wwPDB EM Validation Summary Report (i)

Nov 15, 2022 – 05:35 AM JST

PDB ID	:	6KIF
EMDB ID	:	EMD-9994
Title	:	Structure of cyanobacterial photosystem I-IsiA-flavodoxin supercomplex
Authors	:	Cao, P.; Cao, D.F.; Si, L.; Su, X.D.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on	:	2019-07-18
Resolution	:	3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

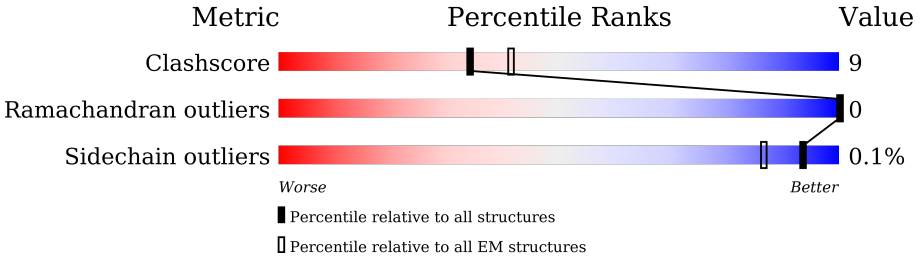
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	763	82% 16%
1	G	763	82% 16%
1	e	763	98%
2	B	734	82% 17%
2	H	734	83% 17%
2	f	734	100%
3	C	81	80% 19%
3	N	81	79% 20%

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Mol	Chain	Length	Quality of chain
3	g	81	99%
4	D	141	81% 19%
4	O	141	81% 19%
4	h	141	100%
5	E	75	11% 81% 13% 5%
5	Q	75	12% 84% 11% 5%
5	i	75	12% 95% 5%
6	F	159	75% 11% 14%
6	R	159	76% 9% 14%
6	j	159	86% 14%
7	I	38	8% 76% 24%
7	S	38	5% 84% 16%
7	k	38	8% 100%
8	J	41	5% 80% 20%
8	T	41	5% 80% 20%
8	l	41	5% 100%
9	K	84	19% 70% 23% 7%
9	U	84	23% 69% 24% 7%
9	m	84	15% 93% 7%
10	L	166	80% 19%
10	V	166	80% 19%
10	n	166	99%
11	M	29	79% 21%
11	W	29	86% 14%
11	o	29	100%

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Mol	Chain	Length	Quality of chain
12	P	172	58% 81% 17%
12	X	172	60% 83% 15%
12	p	172	58% 98%
13	1	342	64% 89% 10%
13	2	342	65% 85% 14%
13	3	342	76% 87% 12%
13	4	342	97% 81% 18%
13	5	342	98% 89% 10%
13	6	342	94% 81% 18%
13	Y	342	65% 88% 11%
13	Z	342	65% 85% 14%
13	a	342	78% 99%
13	b	342	97% 99%
13	c	342	98% 99%
13	d	342	93% 99%
13	q	342	64% 99%
13	r	342	65% 99%
13	s	342	75% 99%
13	t	342	96% 99%
13	u	342	98% 99%
13	v	342	93% 99%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	1	501	X	-	-	-
14	CLA	1	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	1	503	X	-	-	-
14	CLA	1	504	X	-	-	-
14	CLA	1	505	X	-	-	-
14	CLA	1	506	X	-	-	-
14	CLA	1	507	X	-	-	-
14	CLA	1	508	X	-	-	-
14	CLA	1	509	X	-	-	-
14	CLA	1	510	X	-	-	-
14	CLA	1	511	X	-	-	-
14	CLA	1	512	X	-	-	-
14	CLA	1	513	X	-	-	-
14	CLA	1	516	X	-	-	-
14	CLA	1	517	X	-	-	-
14	CLA	1	518	X	-	-	-
14	CLA	1	519	X	-	-	-
14	CLA	2	501	X	-	-	-
14	CLA	2	502	X	-	-	-
14	CLA	2	503	X	-	-	-
14	CLA	2	504	X	-	-	-
14	CLA	2	505	X	-	-	-
14	CLA	2	506	X	-	-	-
14	CLA	2	507	X	-	-	-
14	CLA	2	508	X	-	-	-
14	CLA	2	509	X	-	-	-
14	CLA	2	510	X	-	-	-
14	CLA	2	511	X	-	-	-
14	CLA	2	512	X	-	-	-
14	CLA	2	513	X	-	-	-
14	CLA	2	518	X	-	-	-
14	CLA	2	519	X	-	-	-
14	CLA	3	501	X	-	-	-
14	CLA	3	502	X	-	-	-
14	CLA	3	503	X	-	-	-
14	CLA	3	504	X	-	-	-
14	CLA	3	505	X	-	-	-
14	CLA	3	506	X	-	-	-
14	CLA	3	507	X	-	-	-
14	CLA	3	508	X	-	-	-
14	CLA	3	509	X	-	-	-
14	CLA	3	510	X	-	-	-
14	CLA	3	511	X	-	-	-
14	CLA	3	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	3	513	X	-	-	-
14	CLA	3	516	X	-	-	-
14	CLA	3	517	X	-	-	-
14	CLA	3	518	X	-	-	-
14	CLA	3	519	X	-	-	-
14	CLA	4	501	X	-	-	-
14	CLA	4	502	X	-	-	-
14	CLA	4	503	X	-	-	-
14	CLA	4	504	X	-	-	-
14	CLA	4	505	X	-	-	-
14	CLA	4	506	X	-	-	-
14	CLA	4	507	X	-	-	-
14	CLA	4	508	X	-	-	-
14	CLA	4	509	X	-	-	-
14	CLA	4	510	X	-	-	-
14	CLA	4	511	X	-	-	-
14	CLA	4	512	X	-	-	-
14	CLA	4	513	X	-	-	-
14	CLA	4	516	X	-	-	-
14	CLA	4	517	X	-	-	-
14	CLA	4	518	X	-	-	-
14	CLA	4	519	X	-	-	-
14	CLA	5	501	X	-	-	-
14	CLA	5	502	X	-	-	-
14	CLA	5	503	X	-	-	-
14	CLA	5	504	X	-	-	-
14	CLA	5	505	X	-	-	-
14	CLA	5	506	X	-	-	-
14	CLA	5	507	X	-	-	-
14	CLA	5	508	X	-	-	-
14	CLA	5	509	X	-	-	-
14	CLA	5	510	X	-	-	-
14	CLA	5	511	X	-	-	-
14	CLA	5	512	X	-	-	-
14	CLA	5	513	X	-	-	-
14	CLA	5	516	X	-	-	-
14	CLA	5	517	X	-	-	-
14	CLA	5	518	X	-	-	-
14	CLA	5	519	X	-	-	-
14	CLA	6	501	X	-	-	-
14	CLA	6	502	X	-	-	-
14	CLA	6	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	6	504	X	-	-	-
14	CLA	6	505	X	-	-	-
14	CLA	6	506	X	-	-	-
14	CLA	6	507	X	-	-	-
14	CLA	6	508	X	-	-	-
14	CLA	6	509	X	-	-	-
14	CLA	6	510	X	-	-	-
14	CLA	6	511	X	-	-	-
14	CLA	6	512	X	-	-	-
14	CLA	6	513	X	-	-	-
14	CLA	6	516	X	-	-	-
14	CLA	6	517	X	-	-	-
14	CLA	6	518	X	-	-	-
14	CLA	6	519	X	-	-	-
14	CLA	A	1011	X	-	-	-
14	CLA	A	1013	X	-	-	-
14	CLA	A	1022	X	-	-	-
14	CLA	A	1101	X	-	-	-
14	CLA	A	1102	X	-	-	-
14	CLA	A	1103	X	-	-	-
14	CLA	A	1104	X	-	-	-
14	CLA	A	1105	X	-	-	-
14	CLA	A	1106	X	-	-	-
14	CLA	A	1107	X	-	-	-
14	CLA	A	1108	X	-	-	-
14	CLA	A	1109	X	-	-	-
14	CLA	A	1110	X	-	-	-
14	CLA	A	1111	X	-	-	-
14	CLA	A	1112	X	-	-	-
14	CLA	A	1113	X	-	-	-
14	CLA	A	1114	X	-	-	-
14	CLA	A	1115	X	-	-	-
14	CLA	A	1116	X	-	-	-
14	CLA	A	1117	X	-	-	-
14	CLA	A	1118	X	-	-	-
14	CLA	A	1119	X	-	-	-
14	CLA	A	1120	X	-	-	-
14	CLA	A	1121	X	-	-	-
14	CLA	A	1122	X	-	-	-
14	CLA	A	1123	X	-	-	-
14	CLA	A	1124	X	-	-	-
14	CLA	A	1125	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	1126	X	-	-	-
14	CLA	A	1127	X	-	-	-
14	CLA	A	1128	X	-	-	-
14	CLA	A	1129	X	-	-	-
14	CLA	A	1130	X	-	-	-
14	CLA	A	1131	X	-	-	-
14	CLA	A	1132	X	-	-	-
14	CLA	A	1133	X	-	-	-
14	CLA	A	1134	X	-	-	-
14	CLA	A	1135	X	-	-	-
14	CLA	A	1136	X	-	-	-
14	CLA	A	1137	X	-	-	-
14	CLA	A	1138	X	-	-	-
14	CLA	A	1139	X	-	-	-
14	CLA	A	1140	X	-	-	-
14	CLA	A	1237	X	-	-	-
14	CLA	A	1801	X	-	-	-
14	CLA	B	1012	X	-	-	-
14	CLA	B	1021	X	-	-	-
14	CLA	B	1023	X	-	-	-
14	CLA	B	1201	X	-	-	-
14	CLA	B	1202	X	-	-	-
14	CLA	B	1203	X	-	-	-
14	CLA	B	1204	X	-	-	-
14	CLA	B	1205	X	-	-	-
14	CLA	B	1206	X	-	-	-
14	CLA	B	1207	X	-	-	-
14	CLA	B	1208	X	-	-	-
14	CLA	B	1209	X	-	-	-
14	CLA	B	1210	X	-	-	-
14	CLA	B	1211	X	-	-	-
14	CLA	B	1212	X	-	-	-
14	CLA	B	1213	X	-	-	-
14	CLA	B	1214	X	-	-	-
14	CLA	B	1215	X	-	-	-
14	CLA	B	1216	X	-	-	-
14	CLA	B	1217	X	-	-	-
14	CLA	B	1218	X	-	-	-
14	CLA	B	1219	X	-	-	-
14	CLA	B	1220	X	-	-	-
14	CLA	B	1221	X	-	-	-
14	CLA	B	1222	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	1223	X	-	-	-
14	CLA	B	1224	X	-	-	-
14	CLA	B	1225	X	-	-	-
14	CLA	B	1226	X	-	-	-
14	CLA	B	1227	X	-	-	-
14	CLA	B	1228	X	-	-	-
14	CLA	B	1229	X	-	-	-
14	CLA	B	1230	X	-	-	-
14	CLA	B	1231	X	-	-	-
14	CLA	B	1232	X	-	-	-
14	CLA	B	1234	X	-	-	-
14	CLA	B	1235	X	-	-	-
14	CLA	B	1236	X	-	-	-
14	CLA	B	1238	X	-	-	-
14	CLA	B	1239	X	-	-	-
14	CLA	B	1240	X	-	-	-
14	CLA	F	1301	X	-	-	-
14	CLA	F	1302	X	-	-	-
14	CLA	G	1011	X	-	-	-
14	CLA	G	1013	X	-	-	-
14	CLA	G	1022	X	-	-	-
14	CLA	G	1101	X	-	-	-
14	CLA	G	1102	X	-	-	-
14	CLA	G	1103	X	-	-	-
14	CLA	G	1104	X	-	-	-
14	CLA	G	1105	X	-	-	-
14	CLA	G	1106	X	-	-	-
14	CLA	G	1107	X	-	-	-
14	CLA	G	1108	X	-	-	-
14	CLA	G	1109	X	-	-	-
14	CLA	G	1110	X	-	-	-
14	CLA	G	1111	X	-	-	-
14	CLA	G	1112	X	-	-	-
14	CLA	G	1113	X	-	-	-
14	CLA	G	1114	X	-	-	-
14	CLA	G	1115	X	-	-	-
14	CLA	G	1116	X	-	-	-
14	CLA	G	1117	X	-	-	-
14	CLA	G	1118	X	-	-	-
14	CLA	G	1119	X	-	-	-
14	CLA	G	1120	X	-	-	-
14	CLA	G	1121	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	1122	X	-	-	-
14	CLA	G	1123	X	-	-	-
14	CLA	G	1124	X	-	-	-
14	CLA	G	1125	X	-	-	-
14	CLA	G	1126	X	-	-	-
14	CLA	G	1127	X	-	-	-
14	CLA	G	1128	X	-	-	-
14	CLA	G	1129	X	-	-	-
14	CLA	G	1130	X	-	-	-
14	CLA	G	1131	X	-	-	-
14	CLA	G	1132	X	-	-	-
14	CLA	G	1133	X	-	-	-
14	CLA	G	1134	X	-	-	-
14	CLA	G	1135	X	-	-	-
14	CLA	G	1136	X	-	-	-
14	CLA	G	1137	X	-	-	-
14	CLA	G	1138	X	-	-	-
14	CLA	G	1139	X	-	-	-
14	CLA	G	1140	X	-	-	-
14	CLA	G	1237	X	-	-	-
14	CLA	G	1801	X	-	-	-
14	CLA	H	1012	X	-	-	-
14	CLA	H	1021	X	-	-	-
14	CLA	H	1023	X	-	-	-
14	CLA	H	1201	X	-	-	-
14	CLA	H	1202	X	-	-	-
14	CLA	H	1203	X	-	-	-
14	CLA	H	1204	X	-	-	-
14	CLA	H	1205	X	-	-	-
14	CLA	H	1206	X	-	-	-
14	CLA	H	1207	X	-	-	-
14	CLA	H	1208	X	-	-	-
14	CLA	H	1209	X	-	-	-
14	CLA	H	1210	X	-	-	-
14	CLA	H	1211	X	-	-	-
14	CLA	H	1212	X	-	-	-
14	CLA	H	1213	X	-	-	-
14	CLA	H	1214	X	-	-	-
14	CLA	H	1215	X	-	-	-
14	CLA	H	1216	X	-	-	-
14	CLA	H	1217	X	-	-	-
14	CLA	H	1218	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	1219	X	-	-	-
14	CLA	H	1220	X	-	-	-
14	CLA	H	1221	X	-	-	-
14	CLA	H	1222	X	-	-	-
14	CLA	H	1223	X	-	-	-
14	CLA	H	1224	X	-	-	-
14	CLA	H	1225	X	-	-	-
14	CLA	H	1226	X	-	-	-
14	CLA	H	1227	X	-	-	-
14	CLA	H	1228	X	-	-	-
14	CLA	H	1229	X	-	-	-
14	CLA	H	1230	X	-	-	-
14	CLA	H	1231	X	-	-	-
14	CLA	H	1232	X	-	-	-
14	CLA	H	1234	X	-	-	-
14	CLA	H	1235	X	-	-	-
14	CLA	H	1236	X	-	-	-
14	CLA	H	1238	X	-	-	-
14	CLA	H	1239	X	-	-	-
14	CLA	H	1240	X	-	-	-
14	CLA	J	1302	X	-	-	-
14	CLA	J	1303	X	-	-	-
14	CLA	K	1103	X	-	-	-
14	CLA	K	1105	X	-	-	-
14	CLA	K	1401	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1502	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	R	1301	X	-	-	-
14	CLA	R	1302	X	-	-	-
14	CLA	T	1302	X	-	-	-
14	CLA	T	1303	X	-	-	-
14	CLA	U	1103	X	-	-	-
14	CLA	U	1105	X	-	-	-
14	CLA	U	1401	X	-	-	-
14	CLA	V	1501	X	-	-	-
14	CLA	V	1502	X	-	-	-
14	CLA	V	1503	X	-	-	-
14	CLA	Y	501	X	-	-	-
14	CLA	Y	502	X	-	-	-
14	CLA	Y	503	X	-	-	-
14	CLA	Y	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	Y	505	X	-	-	-
14	CLA	Y	506	X	-	-	-
14	CLA	Y	507	X	-	-	-
14	CLA	Y	508	X	-	-	-
14	CLA	Y	509	X	-	-	-
14	CLA	Y	510	X	-	-	-
14	CLA	Y	511	X	-	-	-
14	CLA	Y	512	X	-	-	-
14	CLA	Y	513	X	-	-	-
14	CLA	Y	516	X	-	-	-
14	CLA	Y	517	X	-	-	-
14	CLA	Y	518	X	-	-	-
14	CLA	Y	519	X	-	-	-
14	CLA	Z	501	X	-	-	-
14	CLA	Z	502	X	-	-	-
14	CLA	Z	503	X	-	-	-
14	CLA	Z	504	X	-	-	-
14	CLA	Z	505	X	-	-	-
14	CLA	Z	506	X	-	-	-
14	CLA	Z	507	X	-	-	-
14	CLA	Z	508	X	-	-	-
14	CLA	Z	509	X	-	-	-
14	CLA	Z	510	X	-	-	-
14	CLA	Z	511	X	-	-	-
14	CLA	Z	512	X	-	-	-
14	CLA	Z	513	X	-	-	-
14	CLA	Z	518	X	-	-	-
14	CLA	Z	519	X	-	-	-
14	CLA	a	501	X	-	-	-
14	CLA	a	502	X	-	-	-
14	CLA	a	503	X	-	-	-
14	CLA	a	504	X	-	-	-
14	CLA	a	505	X	-	-	-
14	CLA	a	506	X	-	-	-
14	CLA	a	507	X	-	-	-
14	CLA	a	508	X	-	-	-
14	CLA	a	509	X	-	-	-
14	CLA	a	510	X	-	-	-
14	CLA	a	511	X	-	-	-
14	CLA	a	512	X	-	-	-
14	CLA	a	513	X	-	-	-
14	CLA	a	516	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	517	X	-	-	-
14	CLA	a	518	X	-	-	-
14	CLA	a	519	X	-	-	-
14	CLA	b	501	X	-	-	-
14	CLA	b	502	X	-	-	-
14	CLA	b	503	X	-	-	-
14	CLA	b	504	X	-	-	-
14	CLA	b	505	X	-	-	-
14	CLA	b	506	X	-	-	-
14	CLA	b	507	X	-	-	-
14	CLA	b	508	X	-	-	-
14	CLA	b	509	X	-	-	-
14	CLA	b	510	X	-	-	-
14	CLA	b	511	X	-	-	-
14	CLA	b	512	X	-	-	-
14	CLA	b	513	X	-	-	-
14	CLA	b	516	X	-	-	-
14	CLA	b	517	X	-	-	-
14	CLA	b	518	X	-	-	-
14	CLA	b	519	X	-	-	-
14	CLA	c	501	X	-	-	-
14	CLA	c	502	X	-	-	-
14	CLA	c	503	X	-	-	-
14	CLA	c	504	X	-	-	-
14	CLA	c	505	X	-	-	-
14	CLA	c	506	X	-	-	-
14	CLA	c	507	X	-	-	-
14	CLA	c	508	X	-	-	-
14	CLA	c	509	X	-	-	-
14	CLA	c	510	X	-	-	-
14	CLA	c	511	X	-	-	-
14	CLA	c	512	X	-	-	-
14	CLA	c	513	X	-	-	-
14	CLA	c	516	X	-	-	-
14	CLA	c	517	X	-	-	-
14	CLA	c	518	X	-	-	-
14	CLA	c	519	X	-	-	-
14	CLA	d	501	X	-	-	-
14	CLA	d	502	X	-	-	-
14	CLA	d	503	X	-	-	-
14	CLA	d	504	X	-	-	-
14	CLA	d	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	d	506	X	-	-	-
14	CLA	d	507	X	-	-	-
14	CLA	d	508	X	-	-	-
14	CLA	d	509	X	-	-	-
14	CLA	d	510	X	-	-	-
14	CLA	d	511	X	-	-	-
14	CLA	d	512	X	-	-	-
14	CLA	d	513	X	-	-	-
14	CLA	d	516	X	-	-	-
14	CLA	d	517	X	-	-	-
14	CLA	d	518	X	-	-	-
14	CLA	d	519	X	-	-	-
14	CLA	e	1011	X	-	-	-
14	CLA	e	1013	X	-	-	-
14	CLA	e	1022	X	-	-	-
14	CLA	e	1101	X	-	-	-
14	CLA	e	1102	X	-	-	-
14	CLA	e	1103	X	-	-	-
14	CLA	e	1104	X	-	-	-
14	CLA	e	1105	X	-	-	-
14	CLA	e	1106	X	-	-	-
14	CLA	e	1107	X	-	-	-
14	CLA	e	1108	X	-	-	-
14	CLA	e	1109	X	-	-	-
14	CLA	e	1110	X	-	-	-
14	CLA	e	1111	X	-	-	-
14	CLA	e	1112	X	-	-	-
14	CLA	e	1113	X	-	-	-
14	CLA	e	1114	X	-	-	-
14	CLA	e	1115	X	-	-	-
14	CLA	e	1116	X	-	-	-
14	CLA	e	1117	X	-	-	-
14	CLA	e	1118	X	-	-	-
14	CLA	e	1119	X	-	-	-
14	CLA	e	1120	X	-	-	-
14	CLA	e	1121	X	-	-	-
14	CLA	e	1122	X	-	-	-
14	CLA	e	1123	X	-	-	-
14	CLA	e	1124	X	-	-	-
14	CLA	e	1125	X	-	-	-
14	CLA	e	1126	X	-	-	-
14	CLA	e	1127	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	e	1128	X	-	-	-
14	CLA	e	1129	X	-	-	-
14	CLA	e	1130	X	-	-	-
14	CLA	e	1131	X	-	-	-
14	CLA	e	1132	X	-	-	-
14	CLA	e	1133	X	-	-	-
14	CLA	e	1134	X	-	-	-
14	CLA	e	1135	X	-	-	-
14	CLA	e	1136	X	-	-	-
14	CLA	e	1137	X	-	-	-
14	CLA	e	1138	X	-	-	-
14	CLA	e	1139	X	-	-	-
14	CLA	e	1140	X	-	-	-
14	CLA	e	1237	X	-	-	-
14	CLA	e	1801	X	-	-	-
14	CLA	f	1012	X	-	-	-
14	CLA	f	1021	X	-	-	-
14	CLA	f	1023	X	-	-	-
14	CLA	f	1201	X	-	-	-
14	CLA	f	1202	X	-	-	-
14	CLA	f	1203	X	-	-	-
14	CLA	f	1204	X	-	-	-
14	CLA	f	1205	X	-	-	-
14	CLA	f	1206	X	-	-	-
14	CLA	f	1207	X	-	-	-
14	CLA	f	1208	X	-	-	-
14	CLA	f	1209	X	-	-	-
14	CLA	f	1210	X	-	-	-
14	CLA	f	1211	X	-	-	-
14	CLA	f	1212	X	-	-	-
14	CLA	f	1213	X	-	-	-
14	CLA	f	1214	X	-	-	-
14	CLA	f	1215	X	-	-	-
14	CLA	f	1216	X	-	-	-
14	CLA	f	1217	X	-	-	-
14	CLA	f	1218	X	-	-	-
14	CLA	f	1219	X	-	-	-
14	CLA	f	1220	X	-	-	-
14	CLA	f	1221	X	-	-	-
14	CLA	f	1222	X	-	-	-
14	CLA	f	1223	X	-	-	-
14	CLA	f	1224	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	f	1225	X	-	-	-
14	CLA	f	1226	X	-	-	-
14	CLA	f	1227	X	-	-	-
14	CLA	f	1228	X	-	-	-
14	CLA	f	1229	X	-	-	-
14	CLA	f	1230	X	-	-	-
14	CLA	f	1231	X	-	-	-
14	CLA	f	1232	X	-	-	-
14	CLA	f	1234	X	-	-	-
14	CLA	f	1235	X	-	-	-
14	CLA	f	1236	X	-	-	-
14	CLA	f	1238	X	-	-	-
14	CLA	f	1239	X	-	-	-
14	CLA	f	1240	X	-	-	-
14	CLA	j	1301	X	-	-	-
14	CLA	j	1302	X	-	-	-
14	CLA	l	1302	X	-	-	-
14	CLA	l	1303	X	-	-	-
14	CLA	m	1103	X	-	-	-
14	CLA	m	1105	X	-	-	-
14	CLA	m	1401	X	-	-	-
14	CLA	n	1501	X	-	-	-
14	CLA	n	1502	X	-	-	-
14	CLA	n	1503	X	-	-	-
14	CLA	q	501	X	-	-	-
14	CLA	q	502	X	-	-	-
14	CLA	q	503	X	-	-	-
14	CLA	q	504	X	-	-	-
14	CLA	q	505	X	-	-	-
14	CLA	q	506	X	-	-	-
14	CLA	q	507	X	-	-	-
14	CLA	q	508	X	-	-	-
14	CLA	q	509	X	-	-	-
14	CLA	q	510	X	-	-	-
14	CLA	q	511	X	-	-	-
14	CLA	q	512	X	-	-	-
14	CLA	q	513	X	-	-	-
14	CLA	q	516	X	-	-	-
14	CLA	q	517	X	-	-	-
14	CLA	q	518	X	-	-	-
14	CLA	q	519	X	-	-	-
14	CLA	r	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	r	502	X	-	-	-
14	CLA	r	503	X	-	-	-
14	CLA	r	504	X	-	-	-
14	CLA	r	505	X	-	-	-
14	CLA	r	506	X	-	-	-
14	CLA	r	507	X	-	-	-
14	CLA	r	508	X	-	-	-
14	CLA	r	509	X	-	-	-
14	CLA	r	510	X	-	-	-
14	CLA	r	511	X	-	-	-
14	CLA	r	512	X	-	-	-
14	CLA	r	513	X	-	-	-
14	CLA	r	518	X	-	-	-
14	CLA	r	519	X	-	-	-
14	CLA	s	501	X	-	-	-
14	CLA	s	502	X	-	-	-
14	CLA	s	503	X	-	-	-
14	CLA	s	504	X	-	-	-
14	CLA	s	505	X	-	-	-
14	CLA	s	506	X	-	-	-
14	CLA	s	507	X	-	-	-
14	CLA	s	508	X	-	-	-
14	CLA	s	509	X	-	-	-
14	CLA	s	510	X	-	-	-
14	CLA	s	511	X	-	-	-
14	CLA	s	512	X	-	-	-
14	CLA	s	513	X	-	-	-
14	CLA	s	516	X	-	-	-
14	CLA	s	517	X	-	-	-
14	CLA	s	518	X	-	-	-
14	CLA	s	519	X	-	-	-
14	CLA	t	501	X	-	-	-
14	CLA	t	502	X	-	-	-
14	CLA	t	503	X	-	-	-
14	CLA	t	504	X	-	-	-
14	CLA	t	505	X	-	-	-
14	CLA	t	506	X	-	-	-
14	CLA	t	507	X	-	-	-
14	CLA	t	508	X	-	-	-
14	CLA	t	509	X	-	-	-
14	CLA	t	510	X	-	-	-
14	CLA	t	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	t	512	X	-	-	-
14	CLA	t	513	X	-	-	-
14	CLA	t	516	X	-	-	-
14	CLA	t	517	X	-	-	-
14	CLA	t	518	X	-	-	-
14	CLA	t	519	X	-	-	-
14	CLA	u	501	X	-	-	-
14	CLA	u	502	X	-	-	-
14	CLA	u	503	X	-	-	-
14	CLA	u	504	X	-	-	-
14	CLA	u	505	X	-	-	-
14	CLA	u	506	X	-	-	-
14	CLA	u	507	X	-	-	-
14	CLA	u	508	X	-	-	-
14	CLA	u	509	X	-	-	-
14	CLA	u	510	X	-	-	-
14	CLA	u	511	X	-	-	-
14	CLA	u	512	X	-	-	-
14	CLA	u	513	X	-	-	-
14	CLA	u	516	X	-	-	-
14	CLA	u	517	X	-	-	-
14	CLA	u	518	X	-	-	-
14	CLA	u	519	X	-	-	-
14	CLA	v	501	X	-	-	-
14	CLA	v	502	X	-	-	-
14	CLA	v	503	X	-	-	-
14	CLA	v	504	X	-	-	-
14	CLA	v	505	X	-	-	-
14	CLA	v	506	X	-	-	-
14	CLA	v	507	X	-	-	-
14	CLA	v	508	X	-	-	-
14	CLA	v	509	X	-	-	-
14	CLA	v	510	X	-	-	-
14	CLA	v	511	X	-	-	-
14	CLA	v	512	X	-	-	-
14	CLA	v	513	X	-	-	-
14	CLA	v	516	X	-	-	-
14	CLA	v	517	X	-	-	-
14	CLA	v	518	X	-	-	-
14	CLA	v	519	X	-	-	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 144312 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	751	5865	3847	1002	999	17	0	0
1	G	751	5865	3847	1002	999	17	0	0
1	e	751	5865	3847	1002	999	17	0	0

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5789	3811	970	994	14	0	0
2	H	733	5789	3811	970	994	14	0	0
2	f	733	5789	3811	970	994	14	0	0

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	598	368	103	116	11	0	0
3	N	80	598	368	103	116	11	0	0
3	g	80	598	368	103	116	11	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	141	1098	702	187	208	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	O	141	1098	702	187	208	1	0	0
4	h	141	1098	702	187	208	1	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	71	543	343	95	105	0	0
5	Q	71	543	343	95	105	0	0
5	i	71	543	343	95	105	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	136	1036	670	174	190	2	0	0
6	R	136	1036	670	174	190	2	0	0
6	j	136	1036	670	174	190	2	0	0

- Molecule 7 is a protein called Photosystem I PsaI protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	38	282	191	38	51	2	0	0
7	S	38	282	191	38	51	2	0	0
7	k	38	282	191	38	51	2	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	41	335	228	52	54	1	0	0
8	T	41	335	228	52	54	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	l	41	335	228	52	54	1	0	0

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	78	549	364	91	93	1	0	0
9	U	78	549	364	91	93	1	0	0
9	m	78	549	364	91	93	1	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	164	1210	782	201	225	2	0	0
10	V	164	1210	782	201	225	2	0	0
10	n	164	1210	782	201	225	2	0	0

- Molecule 11 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	29	228	151	36	40	1	0	0
11	W	29	228	151	36	40	1	0	0
11	o	29	228	151	36	40	1	0	0

- Molecule 12 is a protein called Flavodoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	169	1318	831	210	275	2	0	0
12	X	169	1318	831	210	275	2	0	0
12	p	169	1318	831	210	275	2	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-2	GLY	-	expression tag	UNP P10340
P	-1	SER	-	expression tag	UNP P10340
P	0	HIS	-	expression tag	UNP P10340
X	-2	GLY	-	expression tag	UNP P10340
X	-1	SER	-	expression tag	UNP P10340
X	0	HIS	-	expression tag	UNP P10340
p	-2	GLY	-	expression tag	UNP P10340
p	-1	SER	-	expression tag	UNP P10340
p	0	HIS	-	expression tag	UNP P10340

- Molecule 13 is a protein called Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	1	339	2605	1722	428	448	7	0	0
13	2	339	2605	1722	428	448	7	0	0
13	3	339	2605	1722	428	448	7	0	0
13	4	339	2605	1722	428	448	7	0	0
13	5	339	2605	1722	428	448	7	0	0
13	6	339	2605	1722	428	448	7	0	0
13	Y	339	2605	1722	428	448	7	0	0
13	Z	339	2605	1722	428	448	7	0	0
13	a	339	2605	1722	428	448	7	0	0
13	b	339	2605	1722	428	448	7	0	0
13	c	339	2605	1722	428	448	7	0	0
13	d	339	2605	1722	428	448	7	0	0
13	q	339	2605	1722	428	448	7	0	0
13	r	339	2605	1722	428	448	7	0	0

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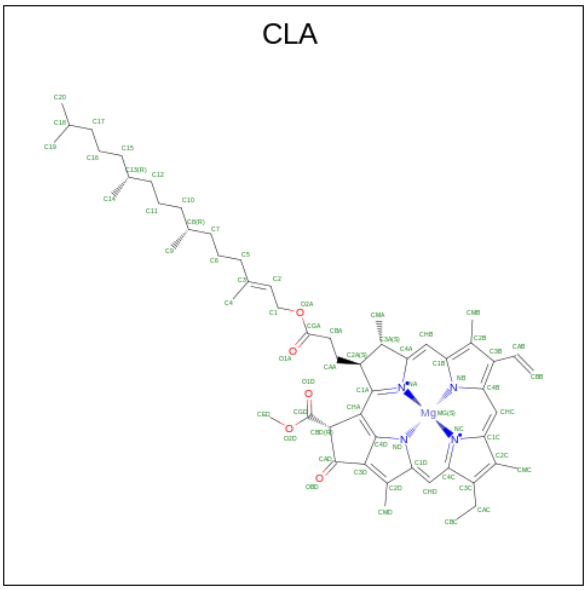
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	s	339	2605	1722	428	448	7	0	0
13	t	339	2605	1722	428	448	7	0	0
13	u	339	2605	1722	428	448	7	0	0
13	v	339	2605	1722	428	448	7	0	0

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
14	A	1	2712	2262	45	180	225	0
14	A	1	2712	2262	45	180	225	0
14	A	1	2712	2262	45	180	225	0
14	A	1	2712	2262	45	180	225	0
14	A	1	2712	2262	45	180	225	0
14	A	1	2712	2262	45	180	225	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	A	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	B	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	F	1	90	70	2	8	10	0
			Total	C	Mg	N	O	
14	F	1	90	70	2	8	10	0
			Total	C	Mg	N	O	
14	J	1	100	80	2	8	10	0
			Total	C	Mg	N	O	
14	J	1	100	80	2	8	10	0
			Total	C	Mg	N	O	
14	K	1	148	118	3	12	15	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	K	1	148	118	3	12	15	0
			Total	C	Mg	N	O	
14	K	1	148	118	3	12	15	0
			Total	C	Mg	N	O	
14	L	1	185	155	3	12	15	0
			Total	C	Mg	N	O	
14	L	1	185	155	3	12	15	0
			Total	C	Mg	N	O	
14	L	1	185	155	3	12	15	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	1	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	2	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	3	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	4	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	5	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	6	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	G	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	H	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	R	1	90	70	2	8	10	0
			Total	C	Mg	N	O	
14	R	1	90	70	2	8	10	0
			Total	C	Mg	N	O	
14	T	1	100	80	2	8	10	0
			Total	C	Mg	N	O	
14	T	1	100	80	2	8	10	0
			Total	C	Mg	N	O	
14	U	1	148	118	3	12	15	0
			Total	C	Mg	N	O	
14	U	1	148	118	3	12	15	0
			Total	C	Mg	N	O	
14	U	1	148	118	3	12	15	0
			Total	C	Mg	N	O	
14	V	1	185	155	3	12	15	0
			Total	C	Mg	N	O	
14	V	1	185	155	3	12	15	0
			Total	C	Mg	N	O	
14	V	1	185	155	3	12	15	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Y	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	Z	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	a	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	b	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	c	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	d	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	e	1	2712	2262	45	180	225	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	f	1	2515	2105	41	164	205	0
			Total	C	Mg	N	O	
14	j	1	90	70	2	8	10	0
			Total	C	Mg	N	O	
14	j	1	90	70	2	8	10	0
			Total	C	Mg	N	O	
14	l	1	100	80	2	8	10	0
			Total	C	Mg	N	O	
14	l	1	100	80	2	8	10	0
			Total	C	Mg	N	O	
14	m	1	148	118	3	12	15	0
			Total	C	Mg	N	O	
14	m	1	148	118	3	12	15	0
			Total	C	Mg	N	O	
14	m	1	148	118	3	12	15	0
			Total	C	Mg	N	O	
14	n	1	185	155	3	12	15	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	n	1	185	155	3	12	15	0
			Total	C	Mg	N	O	
14	n	1	185	155	3	12	15	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	q	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	r	1	850	680	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	s	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	t	1	765	595	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0

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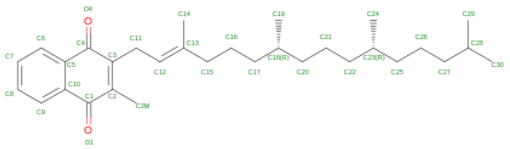
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	u	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0
			Total	C	Mg	N	O	
14	v	1	785	615	17	68	85	0

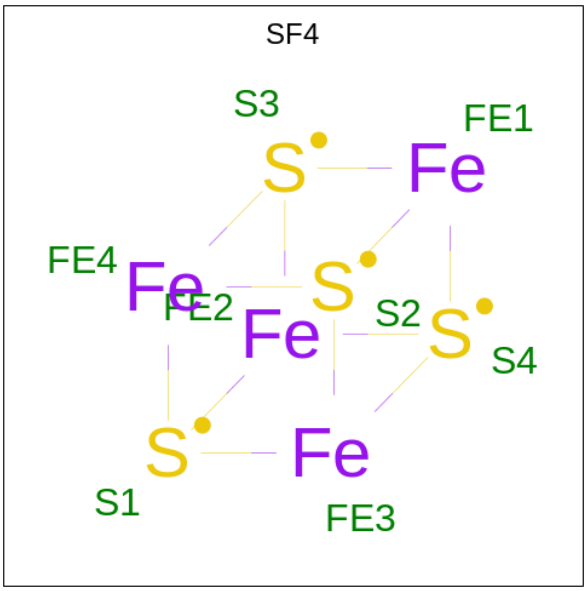
- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).

PQN



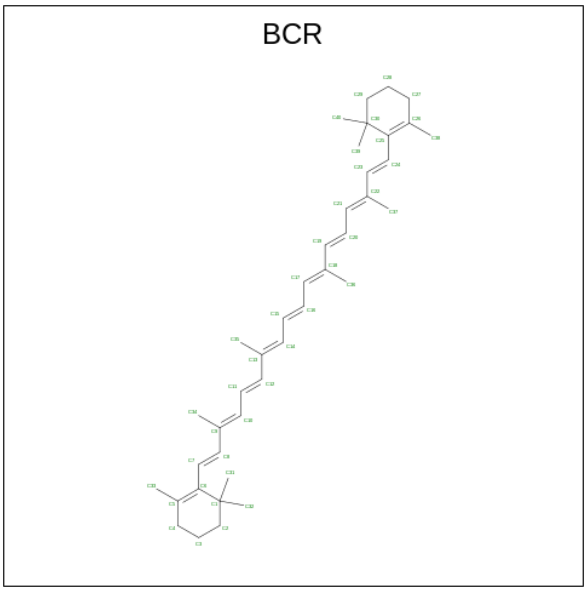
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	A	1	33	31	2	0
15	B	1	33	31	2	0
15	G	1	33	31	2	0
15	H	1	33	31	2	0
15	e	1	33	31	2	0
15	f	1	33	31	2	0

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
16	A	1	8	4	4	0
			Total	Fe	S	
16	C	1	16	8	8	0
			Total	Fe	S	
16	C	1	16	8	8	0
			Total	Fe	S	
16	G	1	8	4	4	0
			Total	Fe	S	
16	N	1	16	8	8	0
			Total	Fe	S	
16	N	1	16	8	8	0
			Total	Fe	S	
16	e	1	8	4	4	0
			Total	Fe	S	
16	g	1	16	8	8	0
			Total	Fe	S	
16	g	1	16	8	8	0

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
17	A	1	240	240	0
			Total	C	
17	A	1	240	240	0
			Total	C	
17	A	1	240	240	0
			Total	C	
17	A	1	240	240	0
			Total	C	
17	A	1	240	240	0
			Total	C	
17	A	1	240	240	0
			Total	C	
17	B	1	280	280	0
			Total	C	
17	B	1	280	280	0
			Total	C	
17	B	1	280	280	0
			Total	C	
17	B	1	280	280	0
			Total	C	
17	B	1	280	280	0
			Total	C	
17	B	1	280	280	0
			Total	C	
17	B	1	280	280	0
			Total	C	
17	F	1	40	40	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
17	I	1	40	40	0
			Total	C	
17	J	1	120	120	0
			Total	C	
17	J	1	120	120	0
			Total	C	
17	J	1	120	120	0
			Total	C	
17	K	1	40	40	0
			Total	C	
17	L	1	160	160	0
			Total	C	
17	L	1	160	160	0
			Total	C	
17	L	1	160	160	0
			Total	C	
17	L	1	160	160	0
			Total	C	
17	M	1	40	40	0
			Total	C	
17	1	1	160	160	0
			Total	C	
17	1	1	160	160	0
			Total	C	
17	1	1	160	160	0
			Total	C	
17	1	1	160	160	0
			Total	C	
17	2	1	160	160	0
			Total	C	
17	2	1	160	160	0
			Total	C	
17	2	1	160	160	0
			Total	C	
17	2	1	160	160	0
			Total	C	
17	3	1	160	160	0
			Total	C	
17	3	1	160	160	0
			Total	C	
17	3	1	160	160	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
17	3	1	160	160	0
			Total	C	
17	4	1	160	160	0
			Total	C	
17	4	1	160	160	0
			Total	C	
17	4	1	160	160	0
			Total	C	
17	4	1	160	160	0
			Total	C	
17	5	1	160	160	0
			Total	C	
17	5	1	160	160	0
			Total	C	
17	5	1	160	160	0
			Total	C	
17	5	1	160	160	0
			Total	C	
17	6	1	160	160	0
			Total	C	
17	6	1	160	160	0
			Total	C	
17	6	1	160	160	0
			Total	C	
17	6	1	160	160	0
			Total	C	
17	G	1	240	240	0
			Total	C	
17	G	1	240	240	0
			Total	C	
17	G	1	240	240	0
			Total	C	
17	G	1	240	240	0
			Total	C	
17	G	1	240	240	0
			Total	C	
17	G	1	240	240	0
			Total	C	
17	H	1	280	280	0
			Total	C	
17	H	1	280	280	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
17	H	1	280	280	0
			Total	C	
17	H	1	280	280	0
			Total	C	
17	H	1	280	280	0
			Total	C	
17	H	1	280	280	0
			Total	C	
17	H	1	280	280	0
			Total	C	
17	R	1	40	40	0
			Total	C	
17	S	1	40	40	0
			Total	C	
17	T	1	120	120	0
			Total	C	
17	T	1	120	120	0
			Total	C	
17	T	1	120	120	0
			Total	C	
17	U	1	40	40	0
			Total	C	
17	V	1	160	160	0
			Total	C	
17	V	1	160	160	0
			Total	C	
17	V	1	160	160	0
			Total	C	
17	V	1	160	160	0
			Total	C	
17	W	1	40	40	0
			Total	C	
17	Y	1	160	160	0
			Total	C	
17	Y	1	160	160	0
			Total	C	
17	Y	1	160	160	0
			Total	C	
17	Y	1	160	160	0
			Total	C	
17	Z	1	160	160	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
17	Z	1	160	160	0
			Total	C	
17	Z	1	160	160	0
			Total	C	
17	Z	1	160	160	0
			Total	C	
17	a	1	160	160	0
			Total	C	
17	a	1	160	160	0
			Total	C	
17	a	1	160	160	0
			Total	C	
17	a	1	160	160	0
			Total	C	
17	b	1	160	160	0
			Total	C	
17	b	1	160	160	0
			Total	C	
17	b	1	160	160	0
			Total	C	
17	b	1	160	160	0
			Total	C	
17	c	1	160	160	0
			Total	C	
17	c	1	160	160	0
			Total	C	
17	c	1	160	160	0
			Total	C	
17	c	1	160	160	0
			Total	C	
17	d	1	160	160	0
			Total	C	
17	d	1	160	160	0
			Total	C	
17	d	1	160	160	0
			Total	C	
17	d	1	160	160	0
			Total	C	
17	e	1	240	240	0
			Total	C	
17	e	1	240	240	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
17	e	1	240	240	0
			Total	C	
17	e	1	240	240	0
			Total	C	
17	e	1	240	240	0
			Total	C	
17	e	1	240	240	0
			Total	C	
17	f	1	280	280	0
			Total	C	
17	f	1	280	280	0
			Total	C	
17	f	1	280	280	0
			Total	C	
17	f	1	280	280	0
			Total	C	
17	f	1	280	280	0
			Total	C	
17	f	1	280	280	0
			Total	C	
17	f	1	280	280	0
			Total	C	
17	j	1	40	40	0
			Total	C	
17	k	1	40	40	0
			Total	C	
17	l	1	120	120	0
			Total	C	
17	l	1	120	120	0
			Total	C	
17	l	1	120	120	0
			Total	C	
17	m	1	40	40	0
			Total	C	
17	n	1	160	160	0
			Total	C	
17	n	1	160	160	0
			Total	C	
17	n	1	160	160	0
			Total	C	
17	n	1	160	160	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
17	o	1	40	40	0
17	q	1	160	160	0
17	q	1	160	160	0
17	q	1	160	160	0
17	q	1	160	160	0
17	r	1	160	160	0
17	r	1	160	160	0
17	r	1	160	160	0
17	r	1	160	160	0
17	s	1	160	160	0
17	s	1	160	160	0
17	s	1	160	160	0
17	s	1	160	160	0
17	t	1	160	160	0
17	t	1	160	160	0
17	t	1	160	160	0
17	t	1	160	160	0
17	u	1	160	160	0
17	u	1	160	160	0
17	u	1	160	160	0
17	u	1	160	160	0

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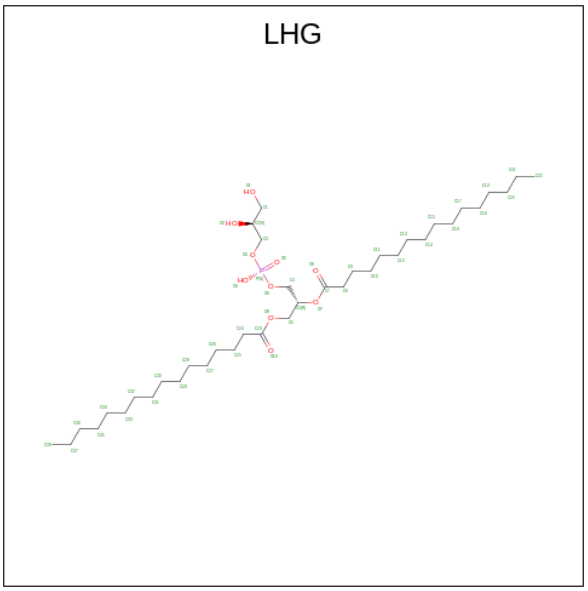
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
17	v	1	160	160	0
			Total	C	
17	v	1	160	160	0
			Total	C	
17	v	1	160	160	0
			Total	C	
17	v	1	160	160	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	A	1	374	275	90	9	0
			Total	C	O	P	
18	A	1	374	275	90	9	0
			Total	C	O	P	
18	A	1	374	275	90	9	0
			Total	C	O	P	
18	A	1	374	275	90	9	0
			Total	C	O	P	
18	A	1	374	275	90	9	0
			Total	C	O	P	
18	A	1	374	275	90	9	0
			Total	C	O	P	
18	A	1	374	275	90	9	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	A	1	374	275	90	9	0
			Total	C	O	P	
18	A	1	374	275	90	9	0
			Total	C	O	P	
18	B	1	78	56	20	2	0
			Total	C	O	P	
18	B	1	78	56	20	2	0
			Total	C	O	P	
18	I	1	48	37	10	1	0
			Total	C	O	P	
18	L	1	127	94	30	3	0
			Total	C	O	P	
18	L	1	127	94	30	3	0
			Total	C	O	P	
18	L	1	127	94	30	3	0
			Total	C	O	P	
18	G	1	374	275	90	9	0
			Total	C	O	P	
18	G	1	374	275	90	9	0
			Total	C	O	P	
18	G	1	374	275	90	9	0
			Total	C	O	P	
18	G	1	374	275	90	9	0
			Total	C	O	P	
18	G	1	374	275	90	9	0
			Total	C	O	P	
18	G	1	374	275	90	9	0
			Total	C	O	P	
18	G	1	374	275	90	9	0
			Total	C	O	P	
18	G	1	374	275	90	9	0
			Total	C	O	P	
18	G	1	374	275	90	9	0
			Total	C	O	P	
18	H	1	78	56	20	2	0
			Total	C	O	P	
18	H	1	78	56	20	2	0
			Total	C	O	P	
18	S	1	48	37	10	1	0
			Total	C	O	P	
18	V	1	127	94	30	3	0

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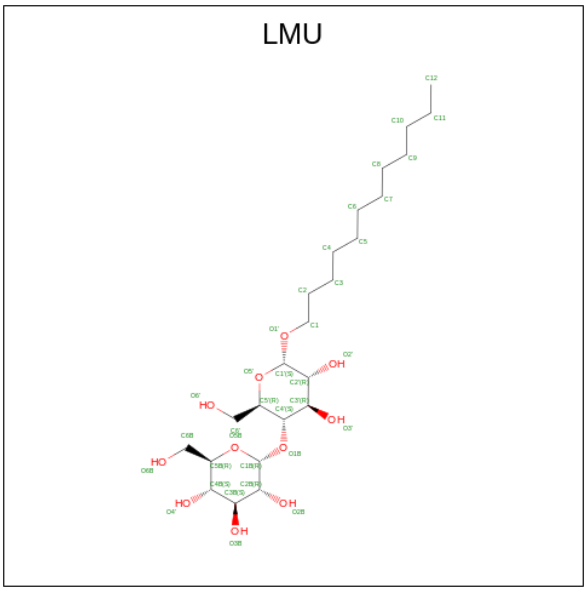
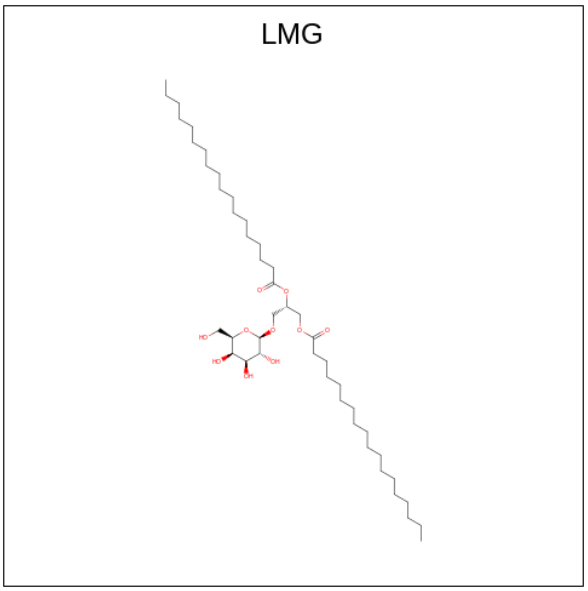
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	V	1	127	94	30	3	0
			Total	C	O	P	
18	V	1	127	94	30	3	0
			Total	C	O	P	
18	e	1	374	275	90	9	0
			Total	C	O	P	
18	e	1	374	275	90	9	0
			Total	C	O	P	
18	e	1	374	275	90	9	0
			Total	C	O	P	
18	e	1	374	275	90	9	0
			Total	C	O	P	
18	e	1	374	275	90	9	0
			Total	C	O	P	
18	e	1	374	275	90	9	0
			Total	C	O	P	
18	e	1	374	275	90	9	0
			Total	C	O	P	
18	e	1	374	275	90	9	0
			Total	C	O	P	
18	e	1	374	275	90	9	0
			Total	C	O	P	
18	f	1	78	56	20	2	0
			Total	C	O	P	
18	f	1	78	56	20	2	0
			Total	C	O	P	
18	k	1	48	37	10	1	0
			Total	C	O	P	
18	n	1	127	94	30	3	0
			Total	C	O	P	
18	n	1	127	94	30	3	0
			Total	C	O	P	
18	n	1	127	94	30	3	0

- Molecule 19 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			58	41	17	
19	A	1	Total	C	O	0
			58	41	17	
19	B	1	Total	C	O	0
			35	24	11	
19	J	1	Total	C	O	0
			22	16	6	
19	G	1	Total	C	O	0
			58	41	17	
19	G	1	Total	C	O	0
			58	41	17	
19	H	1	Total	C	O	0
			35	24	11	
19	T	1	Total	C	O	0
			22	16	6	
19	e	1	Total	C	O	0
			58	41	17	
19	e	1	Total	C	O	0
			58	41	17	
19	f	1	Total	C	O	0
			35	24	11	
19	l	1	Total	C	O	0
			22	16	6	

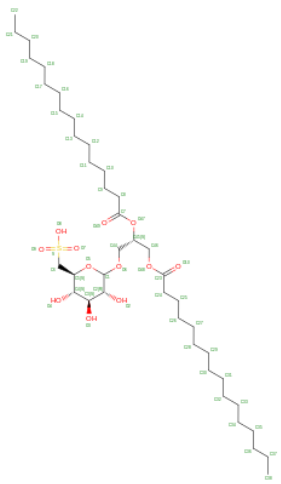
- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	B	1	53	43	10	0
20	J	1	32	22	10	0
20	H	1	53	43	10	0
20	T	1	32	22	10	0
20	f	1	53	43	10	0
20	l	1	32	22	10	0

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

SQD



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
21	B	1	40	27	12	1	0
			Total	C	O	S	
21	L	1	46	33	12	1	0
			Total	C	O	S	
21	1	1	32	19	12	1	0
			Total	C	O	S	
21	2	1	28	15	12	1	0
			Total	C	O	S	
21	3	1	28	15	12	1	0
			Total	C	O	S	
21	4	1	26	13	12	1	0
			Total	C	O	S	
21	5	1	26	13	12	1	0
			Total	C	O	S	
21	6	1	26	13	12	1	0
			Total	C	O	S	
21	H	1	40	27	12	1	0
			Total	C	O	S	
21	V	1	46	33	12	1	0
			Total	C	O	S	
21	Y	1	32	19	12	1	0
			Total	C	O	S	
21	Z	1	28	15	12	1	0
			Total	C	O	S	
21	a	1	28	15	12	1	0
			Total	C	O	S	
21	b	1	26	13	12	1	0

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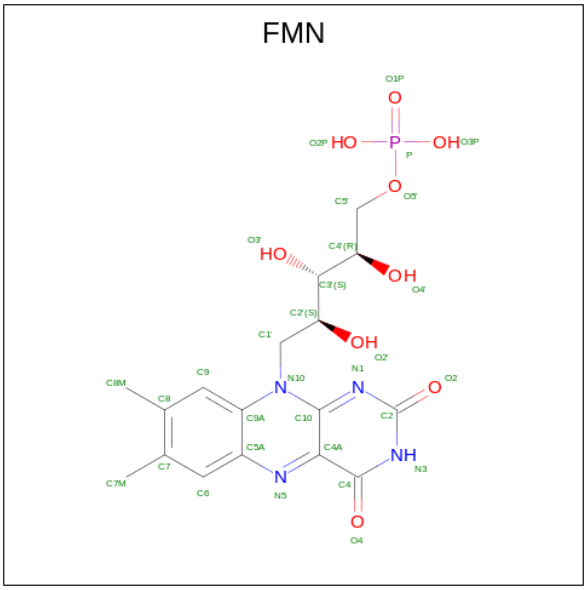
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
21	c	1	26	13	12	1	0
21	d	1	26	13	12	1	0
21	f	1	40	27	12	1	0
21	n	1	46	33	12	1	0
21	q	1	32	19	12	1	0
21	r	1	28	15	12	1	0
21	s	1	28	15	12	1	0
21	t	1	26	13	12	1	0
21	u	1	26	13	12	1	0
21	v	1	26	13	12	1	0

- Molecule 22 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	P	1	31	17	4	9	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	X	1	31	17	4	9	1	0
			Total	C	N	O	P	
22	p	1	31	17	4	9	1	0

- Molecule 23 is water.

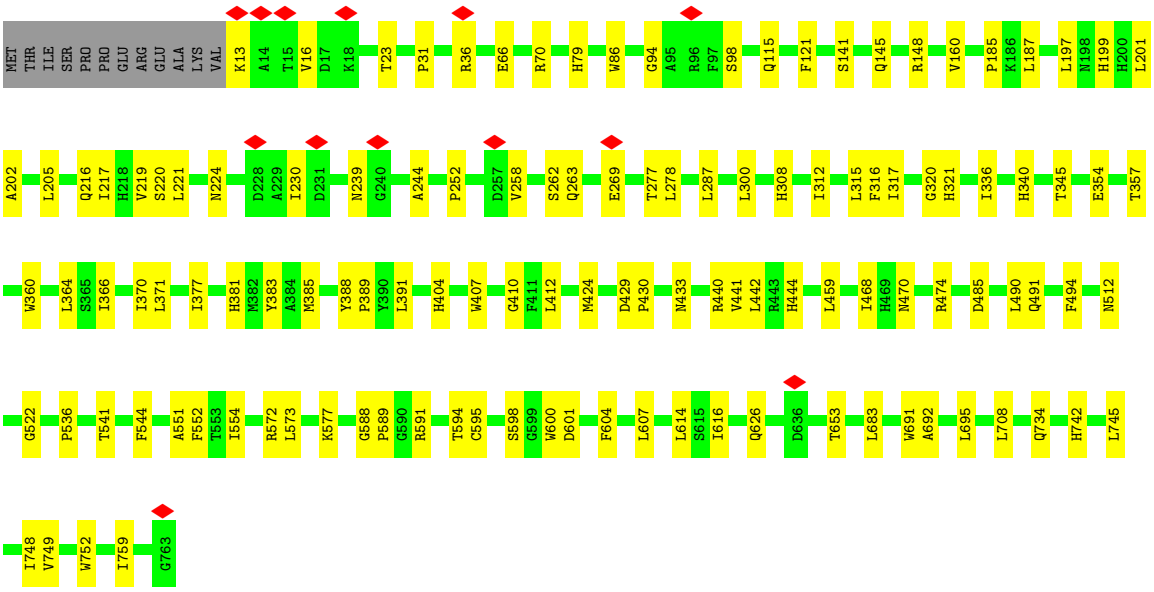
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
23	A	9	9	9	0
			Total	O	
23	B	7	7	7	0
			Total	O	
23	F	1	1	1	0
			Total	O	
23	L	1	1	1	0
			Total	O	
23	G	9	9	9	0
			Total	O	
23	H	7	7	7	0
			Total	O	
23	R	1	1	1	0
			Total	O	
23	V	1	1	1	0
			Total	O	
23	e	9	9	9	0
			Total	O	
23	f	7	7	7	0
			Total	O	
23	j	1	1	1	0
			Total	O	
23	n	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

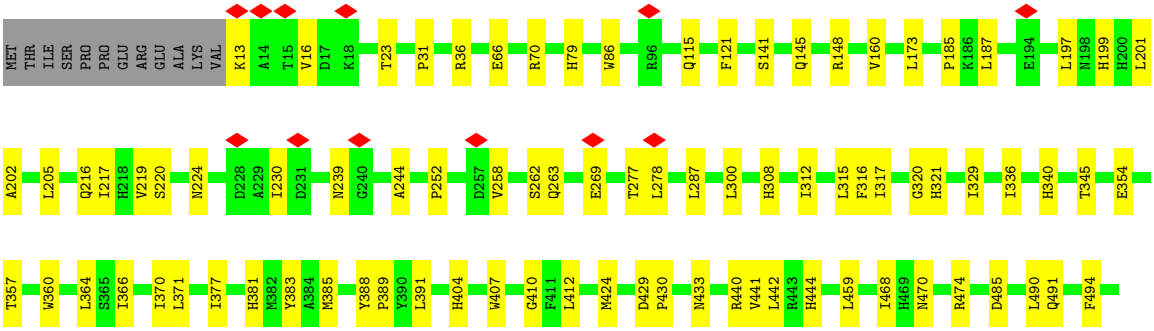
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

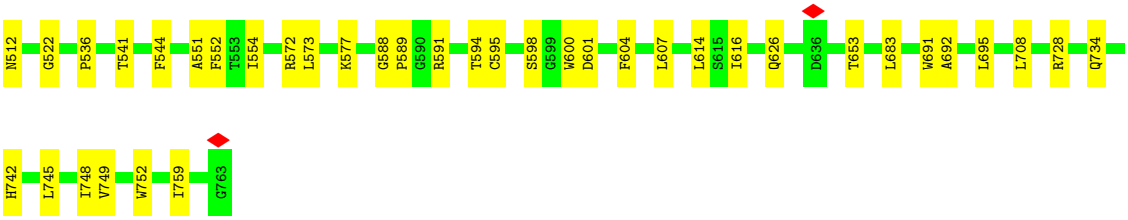
Chain A:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

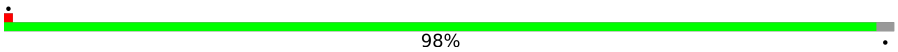
Chain G:

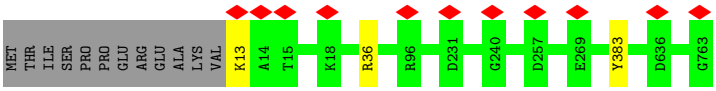




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

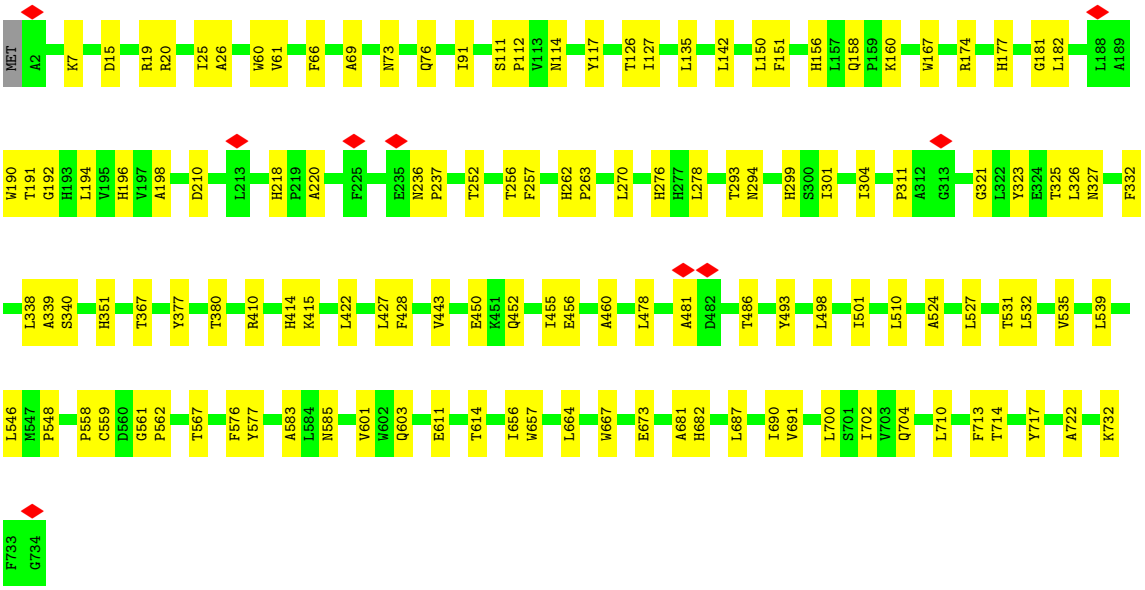
Chain e:





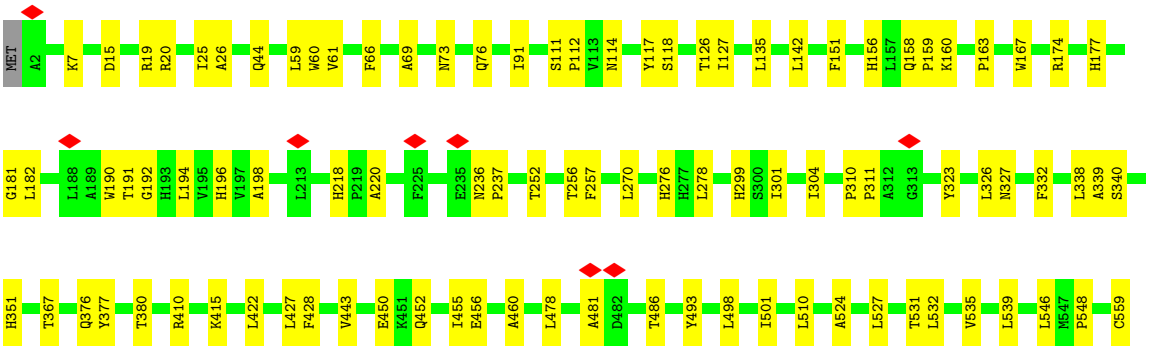
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

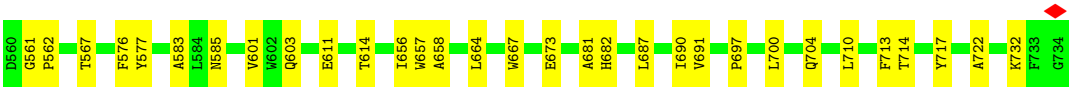
Chain B:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

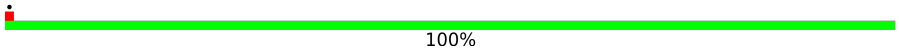
Chain H:

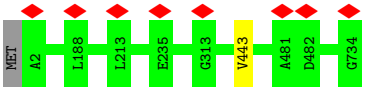




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

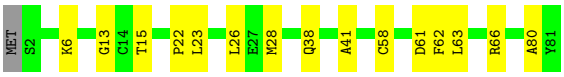
Chain f:





• Molecule 3: Photosystem I iron-sulfur center

Chain C:

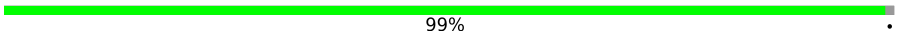


• Molecule 3: Photosystem I iron-sulfur center

Chain N:

• Molecule 3: Photosystem I iron-sulfur center

Chain g:



• Molecule 4: Photosystem I reaction center subunit II

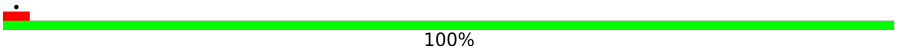
Chain D:

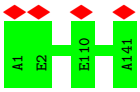
• Molecule 4: Photosystem I reaction center subunit II

Chain O:

• Molecule 4: Photosystem I reaction center subunit II

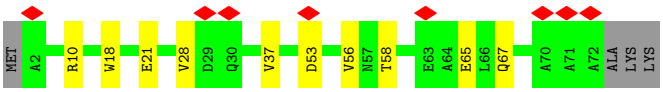
Chain h:





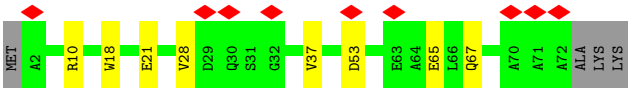
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



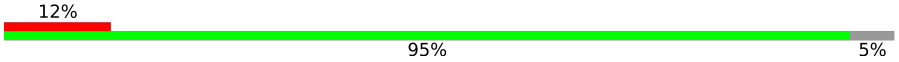
• Molecule 5: Photosystem I reaction center subunit IV

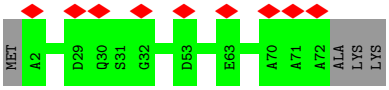
Chain Q:



• Molecule 5: Photosystem I reaction center subunit IV

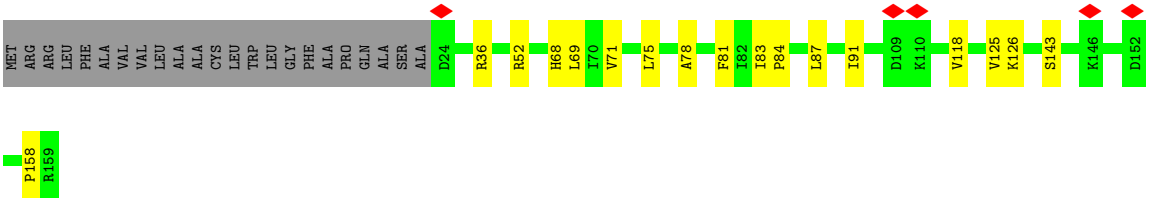
Chain i:





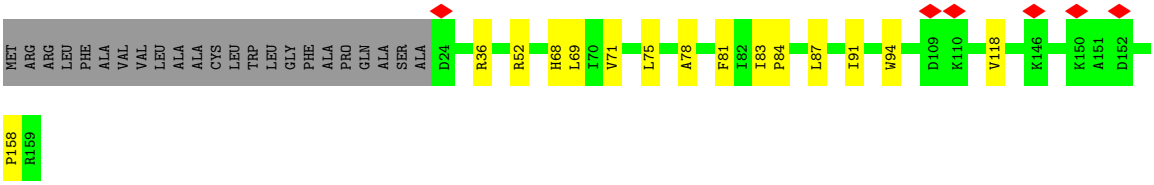
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



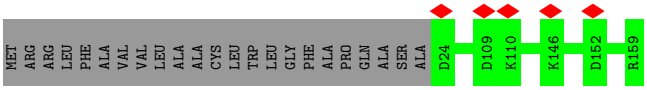
• Molecule 6: Photosystem I reaction center subunit III

Chain R:



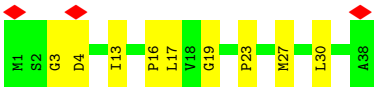
• Molecule 6: Photosystem I reaction center subunit III

Chain j:



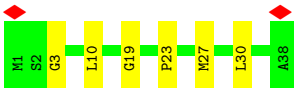
• Molecule 7: Photosystem I PsaI protein

Chain I:



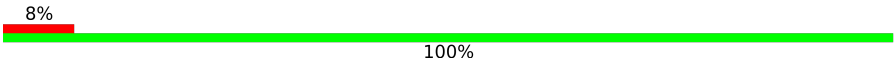
• Molecule 7: Photosystem I PsaI protein

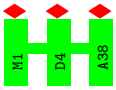
Chain S:



• Molecule 7: Photosystem I PsaI protein

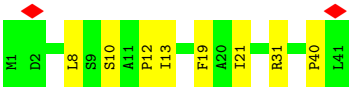
Chain k:





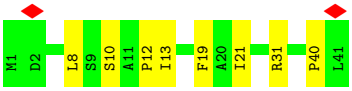
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



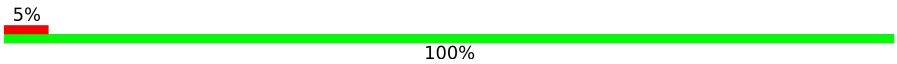
• Molecule 8: Photosystem I reaction center subunit IX

Chain T:



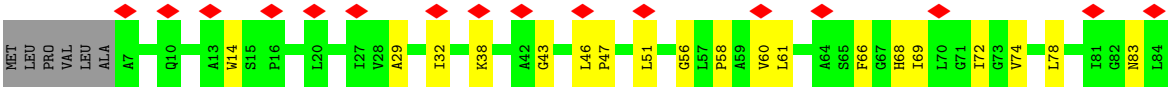
• Molecule 8: Photosystem I reaction center subunit IX

Chain l:



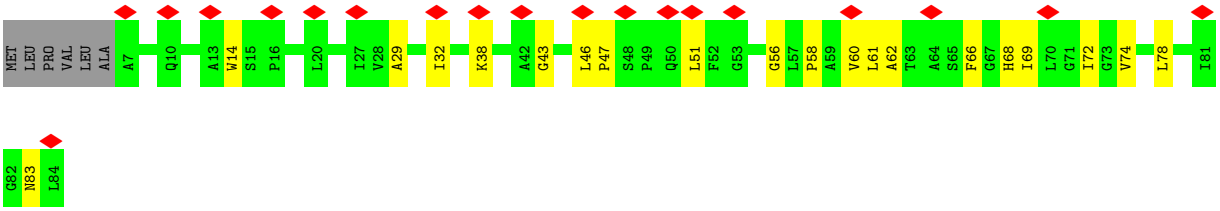
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:



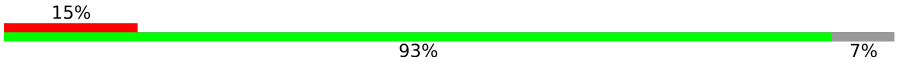
• Molecule 9: Photosystem I reaction center subunit PsaK

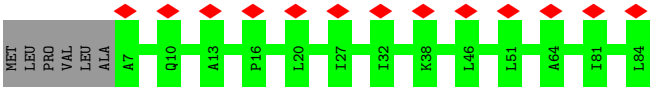
Chain U:



• Molecule 9: Photosystem I reaction center subunit PsaK

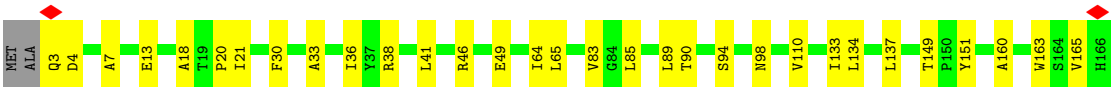
Chain m:





• Molecule 10: Photosystem I reaction center subunit XI

Chain L:

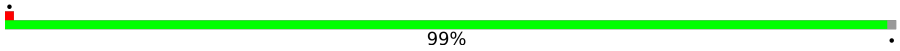


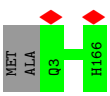
• Molecule 10: Photosystem I reaction center subunit XI

Chain V:

• Molecule 10: Photosystem I reaction center subunit XI

Chain n:





• Molecule 11: PsaM

Chain M: 79% 21%

M1 V6 L11 A20 Y21 Y28 R29

• Molecule 11: PsaM

Chain W: 86% 14%

M1 V6 L11 Y28 R29

• Molecule 11: PsaM

Chain o: 100%

There are no outlier residues recorded for this chain.

• Molecule 12: Flavodoxin

Chain P: 58% 81% 17%

GLY SER HIS A1 K2 I3 G4 L5 F6 T9 T14 Q15 T16 I17 A18 E19 S20 I21 Q22 Q23 E24 F25 G26 G27 E28 S29 I30 V31 D32 L33 N34 D35 I36 A37 N38 A39 D40 A41 S42 D43 L44 N45 A46 Y47 D48 Y49 L50 I51 I52 G53 C54 W57 N58 V59 L62 Q63

S64 D65 W66 E67 G68 I69 Y70 D71 D72 L73 D74 S75 V76 N77 F78 Q79 G80 K81 K82 V83 A84 Y85 F86 V92 D96 A101 I104 L105 E106 E107 K108 I109 S110 S111 L112 G113 S114 Q115 T116 V117 G118 I122 E123 G124 E129 A132 V133 R134 N135 F138 V139 G140

T143 D144 E145 D146 N147 Q148 P149 D150 L151 T152 K153 N154 K157 S161 Q162 L163 K164 S165 E166 F167 G168 L169

• Molecule 12: Flavodoxin

Chain X: 60% 83% 15%

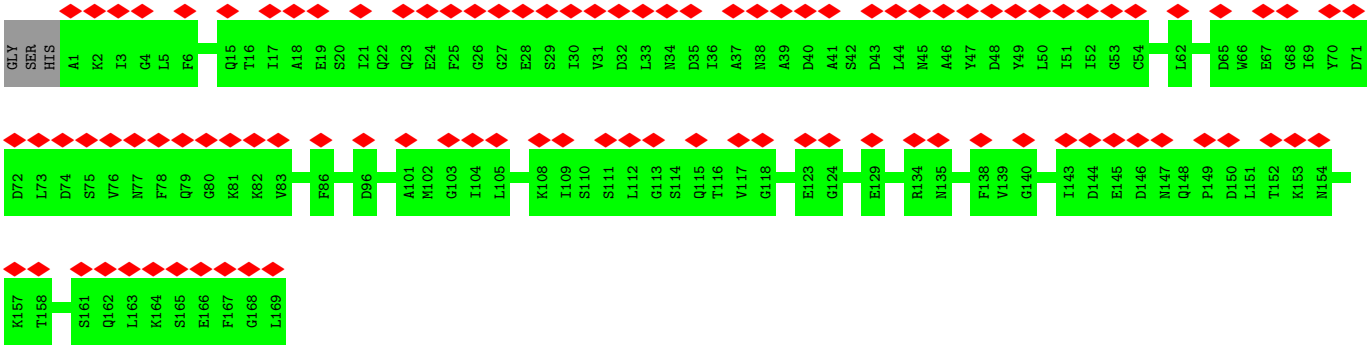
GLY SER HIS A1 K2 I3 G4 L5 F6 T9 Q10 T14 Q15 T16 I17 A18 E19 S20 I21 Q22 Q23 E24 F25 G26 G27 E28 S29 I30 V31 D32 L33 N34 D35 I36 A37 N38 A39 D40 A41 S42 D43 L44 N45 A46 Y47 D48 Y49 L50 I51 I52 G53 C54 W57 N58 V59 L62

Q63 S64 D65 W66 E67 G68 I69 Y70 D71 D72 L73 D74 S75 V76 N77 F78 Q79 G80 K81 K82 V83 F86 V92 D96 A101 M102 G103 I104 L105 K108 I109 S110 S111 L112 G113 S114 Q115 T116 V117 G118 I122 E123 G124 Y125 D126 E129 A132 V133 R134 N135 F138

V139 G140 D144 E145 D146 N147 Q148 P149 D150 L151 T152 K153 N154 K157 T158 S161 Q162 L163 K164 S165 E166 F167 G168 L169

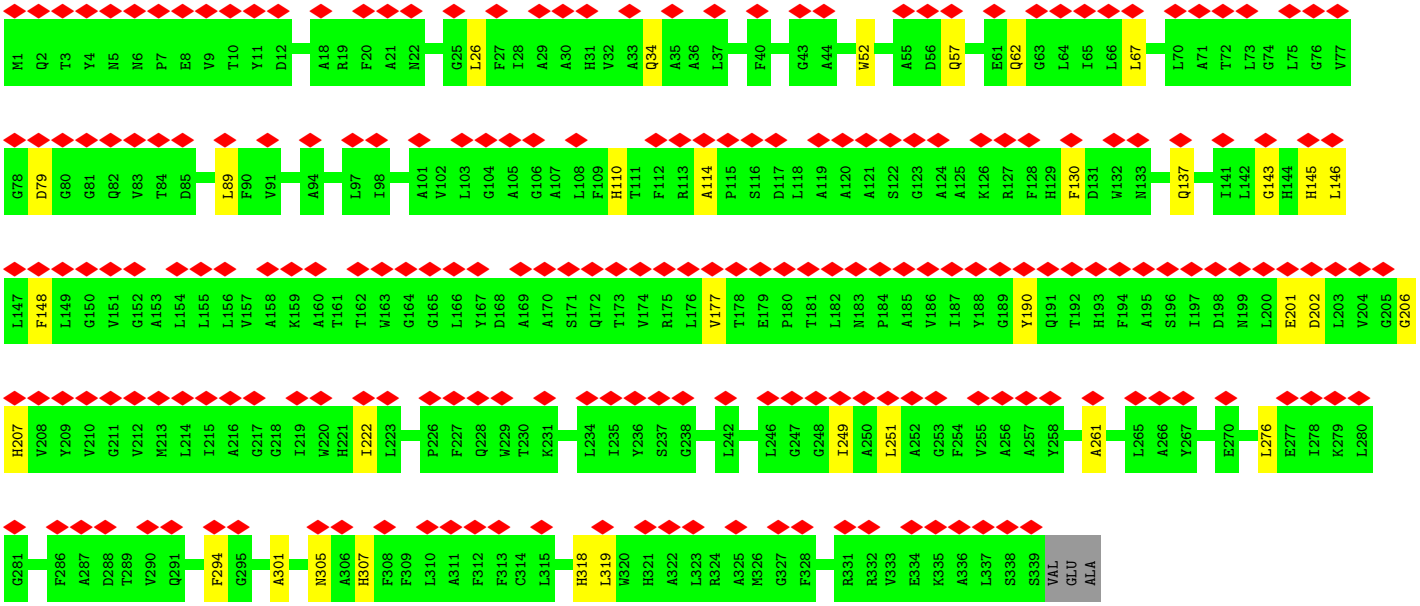
• Molecule 12: Flavodoxin

Chain p: 58% 98%



• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain 1:



• Molecule 13: Iron stress-induced chlorophyll-binding protein

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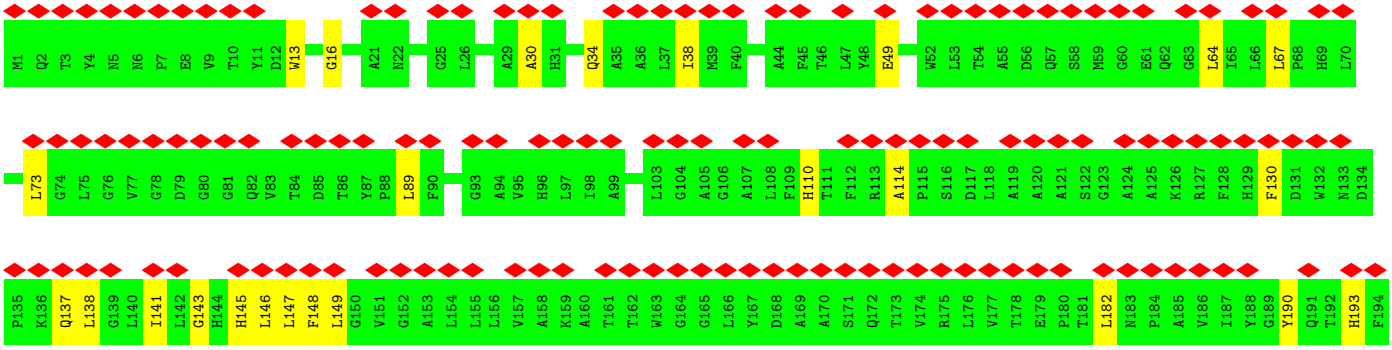
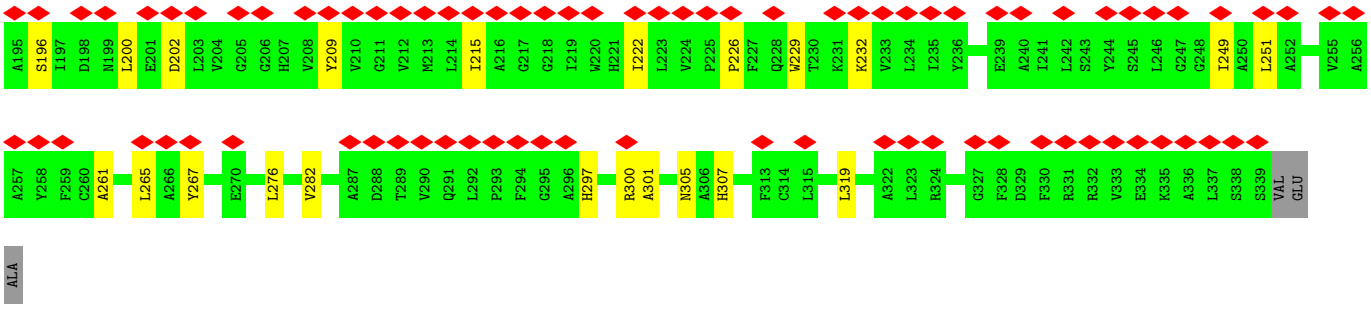
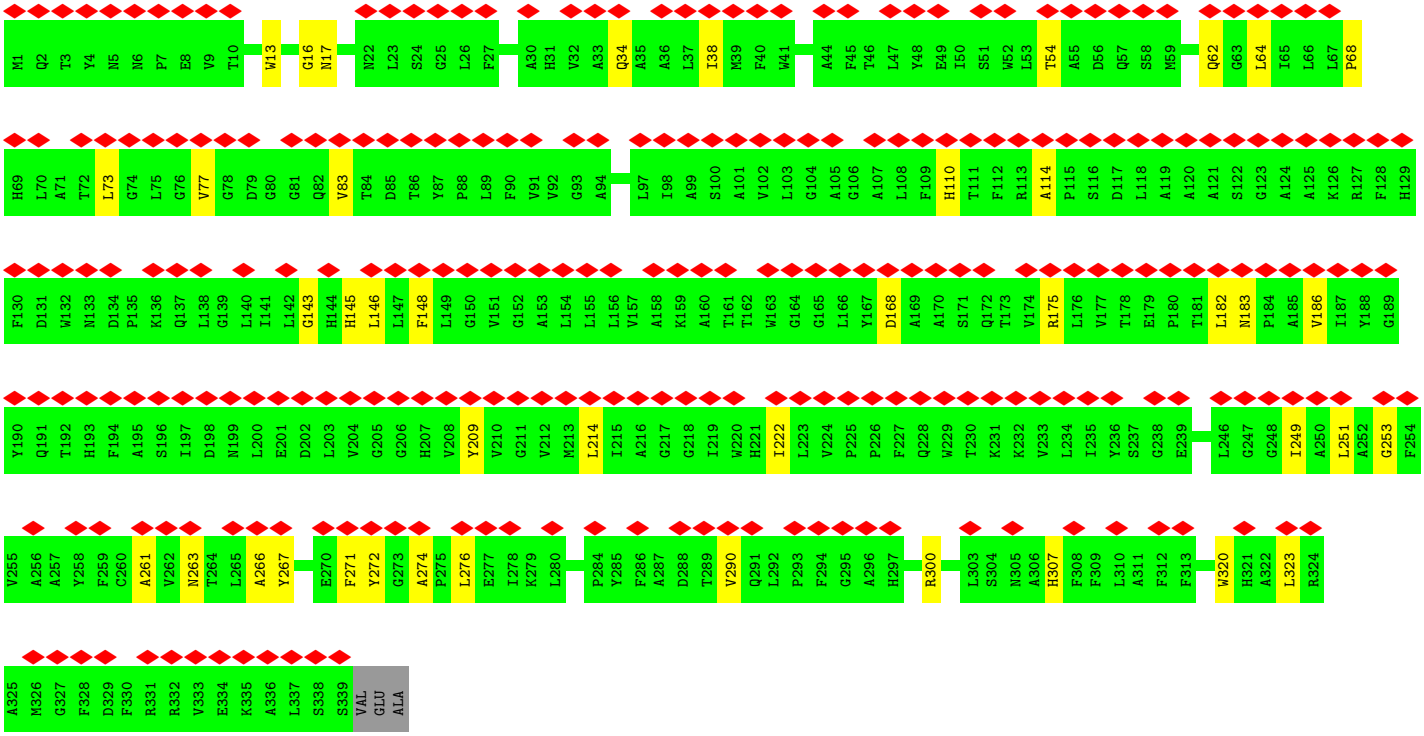




- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain 3:



- Molecule 13: Iron stress-induced chlorophyll-binding protein

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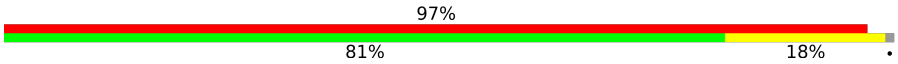

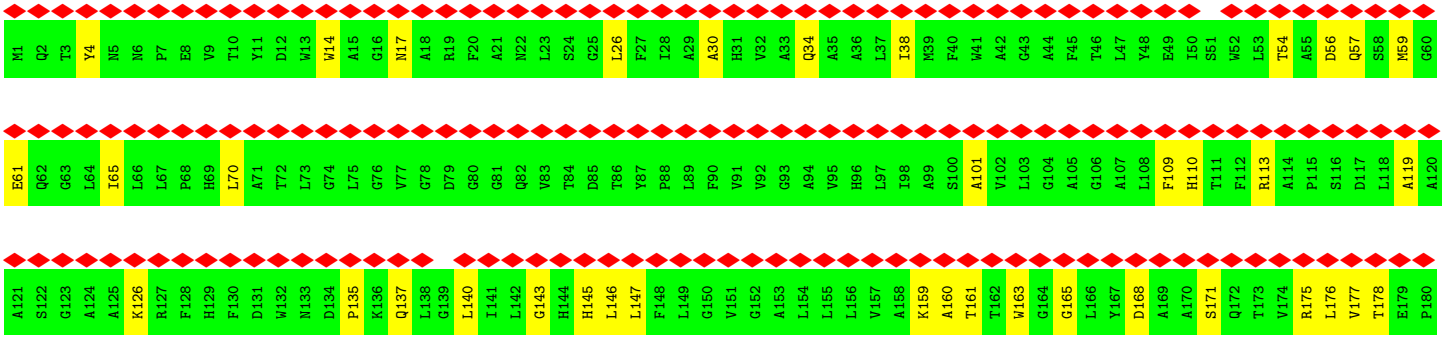

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I241 L242 S243 Y244 S245 L246 G247 G248 I249 A250 L251 A252 G253 F254 V255 A256 A257 Y258 F259 C260 A261 V262 N263 T264 L265 A266 Y267 P268 V269 E270 F271 Y272 G273 A274 P275 L276 E277 I278 K279 L280 G281 V282 T283 P284 Y285 F286 A287 D288 T289 V290 Q291 L292 P293 F294 G295 A296 H297 T298 P299 R300

A301 W302 L303 S304 N305 A306 H307 F308 F309 L310 A311 F312 F313 C314 L315 Q316 G317 H318 L319 W320 H321 A322 L323 R324 A325 M326 G327 F328 D329 F330 R331 R332 V333 E334 K335 A336 L337 S338 S339 VAL GLU ALA

- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain 5: 98% 89% 10%

M1 Q2 T3 Y4 N5 N6 P7 E8 V9 T10 Y11 D12 W13 W14 A15 G16 N17 A18 R19 F20 A21 N22 L23 S24 G25 L26 F27 I28 A29 A30 H31 V32 A33 Q34 A35 A36 L37 I38 M39 F40 W41 A42 G43 A44 F45 T46 L47 Y48 E49 I50 S51 W52 L53 T54 A55 D56 Q57 S58 M59 G60

E61 Q62 G63 L64 I65 L66 L67 P68 H69 L70 A71 T72 L73 G74 L75 G76 V77 G78 D79 G80 G81 Q82 V83 T84 D85 T86 Y87 P88 L89 F90 V91 V92 G93 A94 V95 H96 L97 I98 A99 S100 A101 V102 L103 G104 A105 G106 A107 L108 F109 H110 T111 F112 R113 A114 P115 S116 D117 L118 A119 A120

A121 S122 G123 A124 A125 K126 R127 F128 H129 F130 D131 W132 N133 D134 P135 K136 Q137 L138 G139 L140 I141 L142 G143 H144 H145 L146 L147 F148 L149 G150 V151 G152 A153 L154 L155 L156 V157 A158 K159 A160 T161 T162 W163 G164 G165 L166 Y167 D168 A169 A170 S171 Q172 T173 V174 R175 L176 V177 T178 E179 P180

T181 L182 N183 P184 A185 V186 I187 Y188 G189 Y190 Q191 T192 H193 F194 A195 S196 I197 D198 N199 L200 E201 D202 L203 V204 G205 G206 H207 V208 Y209 V210 G211 V212 M213 L214 I215 A216 G217 G218 I219 W220 H221 I222 L223 V224 P225 P226 F227 Q228 W229 T230 K231 K232 V233 L234 I235 Y236 S237 G238 E239 A240

I241 L242 S243 Y244 S245 L246 G247 G248 I249 A250 L251 A252 G253 F254 V255 A256 A257 Y258 F259 C260 A261 V262 N263 T264 L265 A266 Y267 P268 V269 E270 F271 Y272 G273 A274 P275 L276 E277 I278 K279 L280 G281 V282 T283 P284 Y285 F286 A287 D288 T289 V290 Q291 L292 P293 F294 G295 A296 H297 T298 P299 R300

A301 W302 L303 S304 N305 A306 H307 F308 F309 L310 A311 F312 F313 C314 L315 Q316 G317 H318 L319 W320 H321 A322 L323 R324 A325 M326 G327 F328 D329 F330 R331 R332 V333 E334 K335 A336 L337 S338 S339 VAL GLU ALA

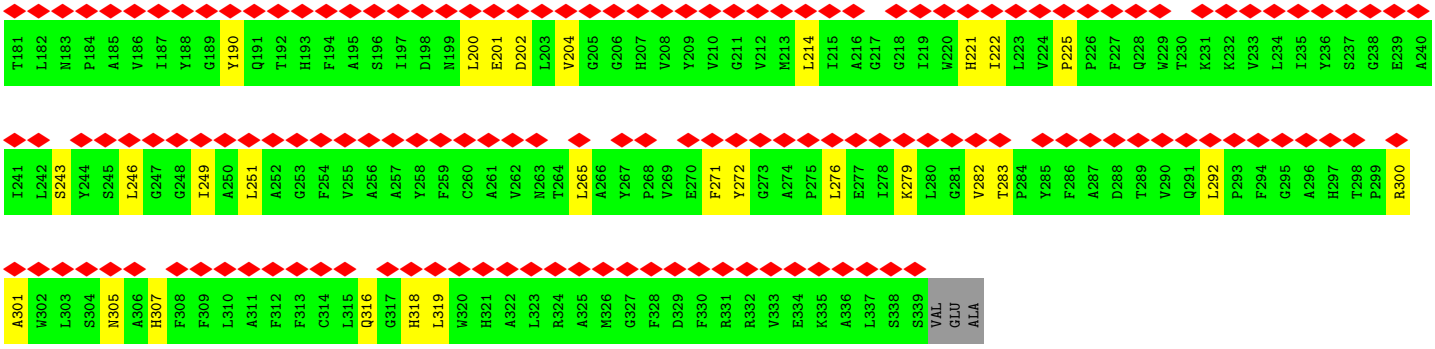
- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain 6: 94% 81% 18%

M1 Q2 T3 Y4 N5 N6 P7 E8 V9 T10 Y11 D12 W13 W14 A15 G16 N17 A18 R19 F20 A21 N22 L23 S24 G25 L26 F27 I28 A29 A30 H31 V32 A33 Q34 A35 A36 L37 I38 M39 F40 W41 A42 G43 A44 F45 T46 L47 Y48 E49 I50 S51 W52 L53 T54 A55 D56 Q57 S58 M59 G60

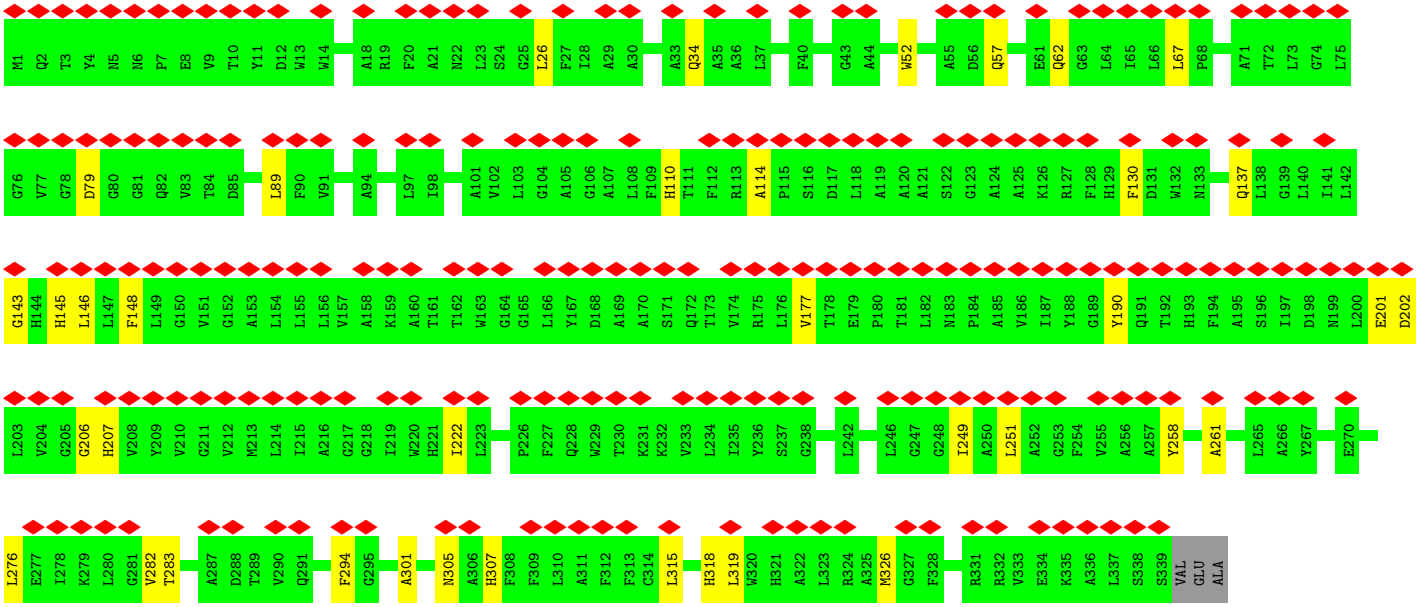
E61 Q62 G63 L64 I65 L66 L67 P68 H69 L70 A71 T72 L73 G74 L75 G76 V77 G78 D79 G80 G81 Q82 V83 T84 D85 T86 Y87 P88 L89 F90 V91 V92 G93 A94 V95 H96 L97 I98 A99 S100 A101 V102 L103 G104 A105 G106 A107 L108 F109 H110 T111 F112 R113 A114 P115 S116 D117 L118 A119 A120

A121 S122 G123 A124 A125 K126 R127 F128 H129 F130 D131 W132 N133 D134 P135 K136 Q137 L138 G139 L140 I141 L142 G143 H144 H145 L146 L147 F148 L149 G150 V151 G152 A153 L154 L155 L156 V157 A158 K159 A160 T161 T162 W163 G164 G165 L166 Y167 D168 A169 A170 S171 Q172 T173 V174 R175 L176 V177 T178 E179 P180



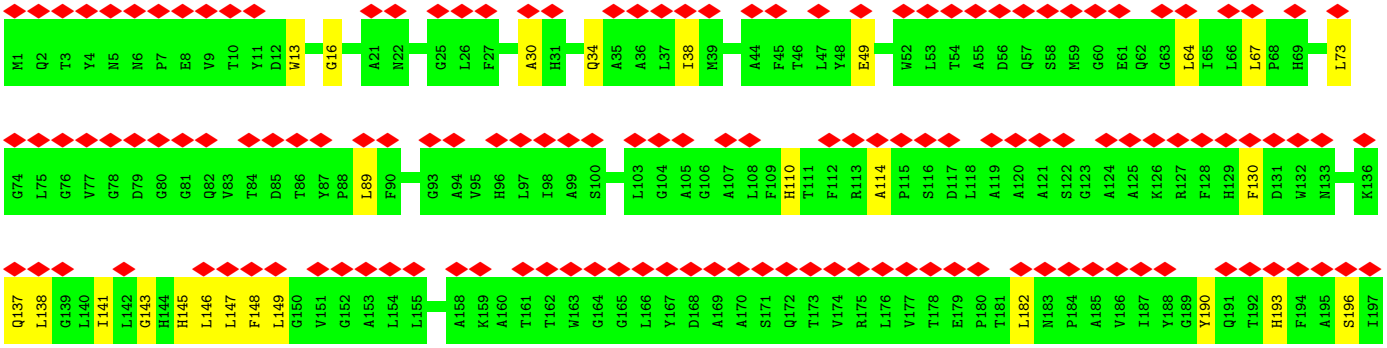
• Molecule 13: Iron stress-induced chlorophyll-binding protein

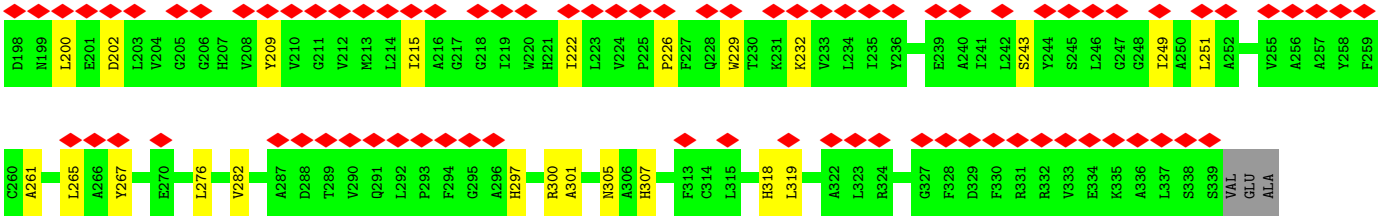
Chain Y:



• Molecule 13: Iron stress-induced chlorophyll-binding protein

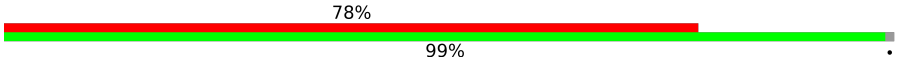
Chain Z:





- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain a:



- Molecule 13: Iron stress-induced chlorophyll-binding protein

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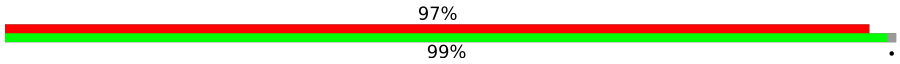
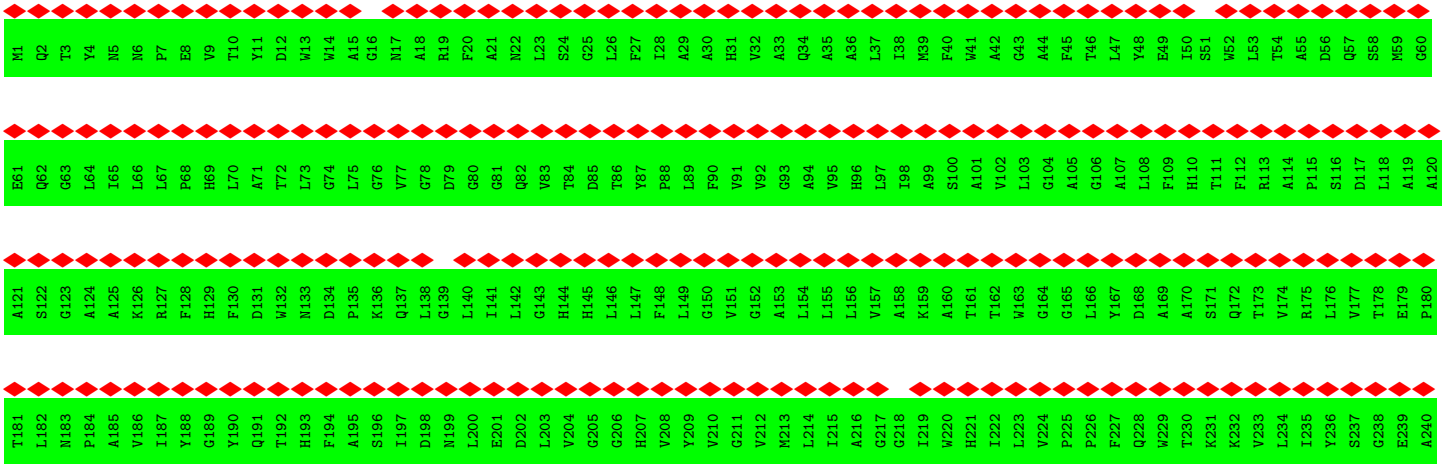




I241 L242 S243 Y244 S245 L246 G247 G248 I249 A250 L251 A252 G253 F254 V255 A256 A257 Y258 F259 C260 A261 V262 N263 T264 L265 A266 Y267 P268 V269 E270 F271 Y272 G273 A274 P275 L276 E277 I278 K279 L280 G281 V282 T283 P284 Y285 F286 A287 D288 T289 V290 Q291 L292 P293 F294 G295 A296 H297 T298 P299 R300

A301 W302 L303 S304 N305 A306 H307 F308 F309 L310 A311 F312 F313 C314 L315 Q316 G317 H318 L319 W320 H321 A322 L323 R324 A325 M326 G327 F328 D329 F330 R331 R332 V333 E334 K335 A336 L337 S338 S339 VAL GLU ALA

- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain c: 98% 99%

M1 Q2 T3 Y4 N5 N6 P7 E8 V9 T10 Y11 D12 W13 W14 A15 G16 N17 A18 R19 F20 A21 N22 L23 S24 G25 L26 F27 I28 A29 A30 H31 V32 A33 Q34 A35 A36 L37 I38 M39 F40 W41 A42 G43 A44 F45 T46 L47 Y48 E49 I50 S51 W52 L53 T54 A55 D56 Q57 S58 M59 G60

E61 Q62 G63 L64 I65 L66 L67 P68 H69 L70 A71 T72 L73 G74 L75 G76 V77 G78 D79 G80 G81 Q82 V83 T84 D85 T86 Y87 P88 L89 F90 V91 V92 G93 A94 V95 H96 L97 I98 A99 S100 A101 V102 L103 G104 A105 G106 A107 L108 F109 H110 T111 F112 R113 A114 P115 S116 D117 L118 A119 A120

A121 S122 G123 A124 A125 K126 R127 F128 H129 F130 D131 W132 N133 D134 P135 K136 Q137 L138 G139 L140 I141 L142 G143 H144 H145 L146 L147 F148 L149 G150 V151 G152 A153 L154 L155 L156 V157 A158 K159 A160 T161 T162 W163 G164 G165 L166 Y167 D168 A169 A170 S171 Q172 T173 V174 R175 L176 V177 T178 E179 P180

T181 L182 N183 P184 A185 V186 I187 Y188 G189 Y190 Q191 T192 H193 F194 A195 S196 I197 D198 N199 L200 E201 D202 L203 V204 G205 G206 H207 V208 Y209 V210 G211 V212 M213 L214 I215 A216 G217 G218 I219 W220 H221 I222 L223 V224 P225 P226 F227 Q228 W229 T230 K231 K232 V233 L234 I235 Y236 S237 G238 E239 A240

I241 L242 S243 Y244 S245 L246 G247 G248 I249 A250 L251 A252 G253 F254 V255 A256 A257 Y258 F259 C260 A261 V262 N263 T264 L265 A266 Y267 P268 V269 E270 F271 Y272 G273 A274 P275 L276 E277 I278 K279 L280 G281 V282 T283 P284 Y285 F286 A287 D288 T289 V290 Q291 L292 P293 F294 G295 A296 H297 T298 P299 R300

A301 W302 L303 S304 N305 A306 H307 F308 F309 L310 A311 F312 F313 C314 L315 Q316 G317 H318 L319 W320 H321 A322 L323 R324 A325 M326 G327 F328 D329 F330 R331 R332 V333 E334 K335 A336 L337 S338 S339 VAL GLU ALA

- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain d: 93% 99%

M1 Q2 T3 Y4 N5 N6 P7 E8 V9 T10 Y11 D12 W13 W14 A15 G16 N17 A18 R19 F20 A21 N22 L23 S24 G25 L26 F27 I28 A29 A30 H31 V32 A33 Q34 A35 A36 L37 I38 M39 F40 W41 A42 G43 A44 F45 T46 L47 Y48 E49 I50 S51 W52 L53 T54 A55 D56 Q57 S58 M59 G60

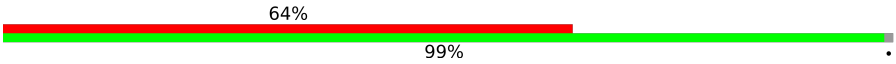
E61 Q62 G63 L64 I65 L66 L67 P68 H69 L70 A71 T72 L73 G74 L75 G76 V77 G78 D79 G80 G81 Q82 V83 T84 D85 T86 Y87 P88 L89 F90 V91 V92 G93 A94 V95 H96 L97 I98 A99 S100 A101 V102 L103 G104 A105 G106 A107 L108 F109 F112 R113 A114 P115 S116 D117 L118 A119 A120 A121

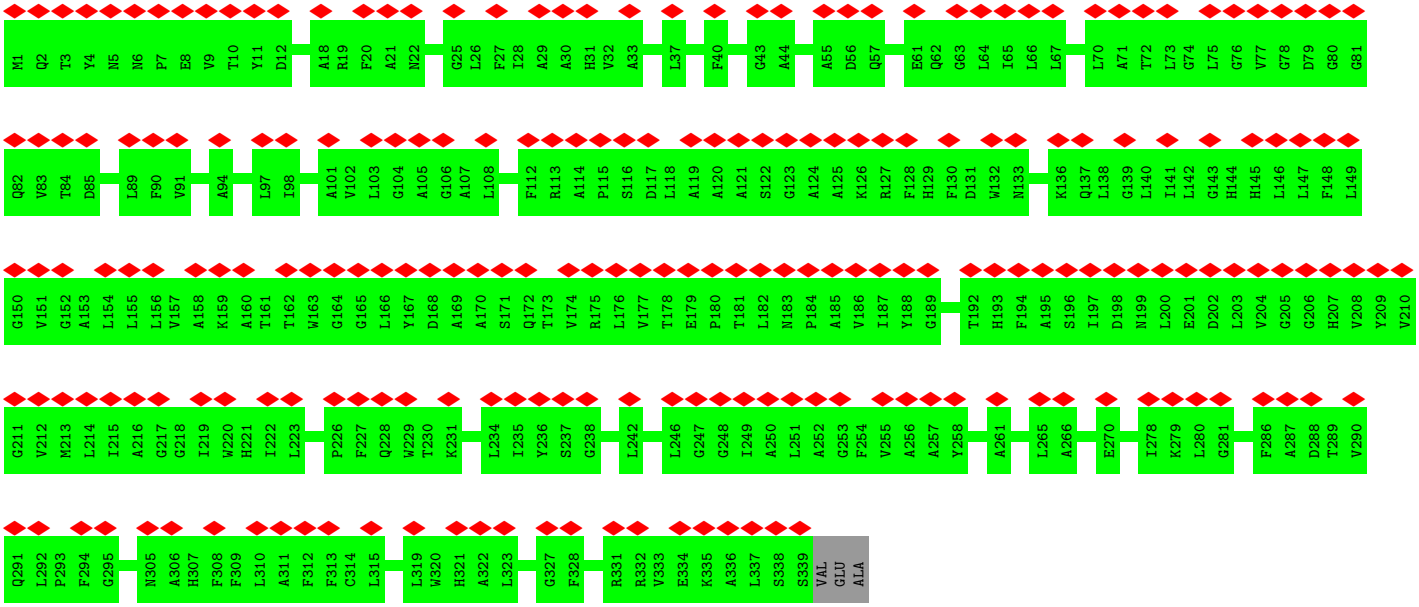
S122 G123 A124 A125 K126 R127 F128 H129 F130 D131 W132 N133 D134 P135 K136 Q137 L138 G139 L140 I141 L142 G143 H144 H145 L146 L147 F148 L149 G150 V151 G152 A153 L154 L155 L156 V157 A158 K159 A160 T161 T162 W163 G164 G165 L166 Y167 D168 A169 A170 S171 Q172 T173 V174 R175 L176 V177 T178 E179 P180 T181

L182 N183 P184 A185 V186 I187 Y188 G189 Y190 Q191 T192 H193 F194 A195 S196 I197 D198 N199 L200 E201 D202 L203 V204 G205 G206 H207 V208 Y209 V210 G211 V212 M213 L214 I215 A216 G217 G218 I219 W220 H221 I222 L223 V224 P225 P226 F227 Q228 W229 T230 K231 K232 V233 L234 I235 Y236 S237 G238 E239 A240 I241

• Molecule 13: Iron stress-induced chlorophyll-binding protein

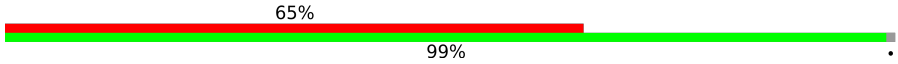
Chain q:

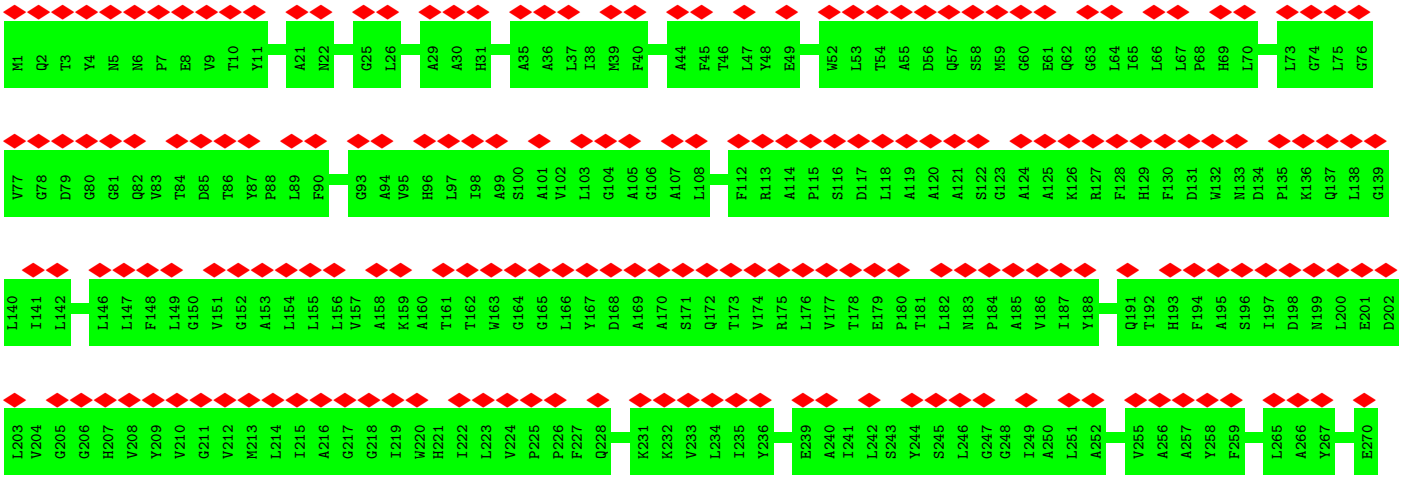


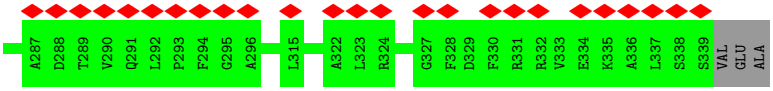


• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain r:

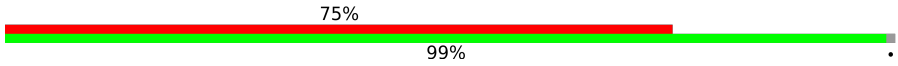


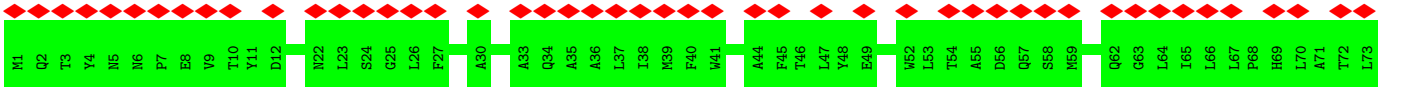


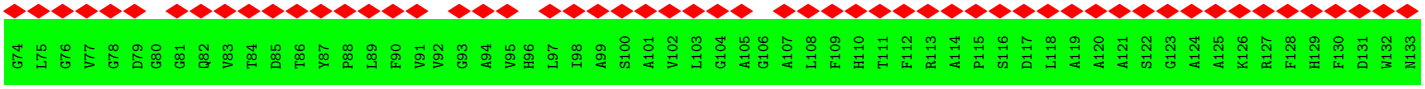


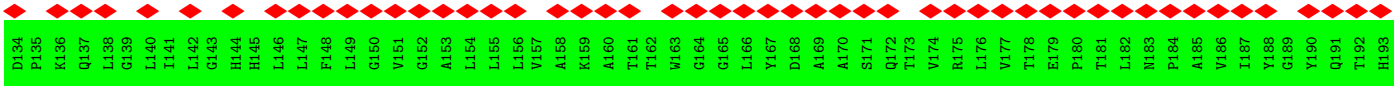
• Molecule 13: Iron stress-induced chlorophyll-binding protein

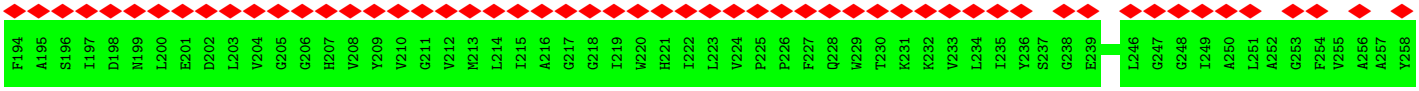
Chain s:

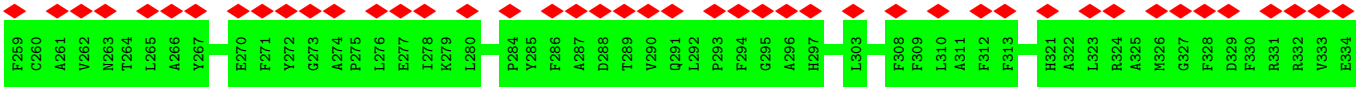


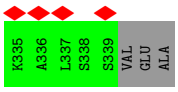






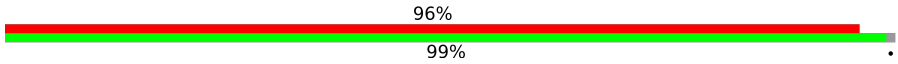


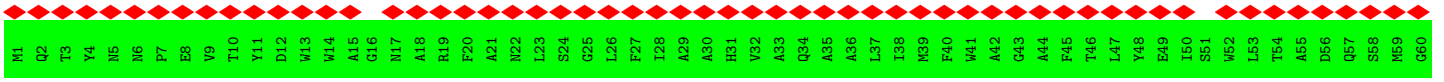


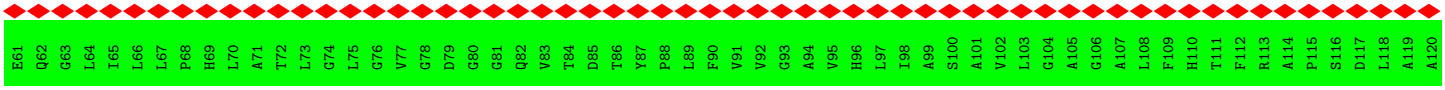


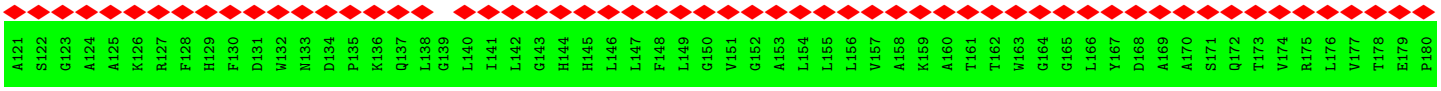
• Molecule 13: Iron stress-induced chlorophyll-binding protein

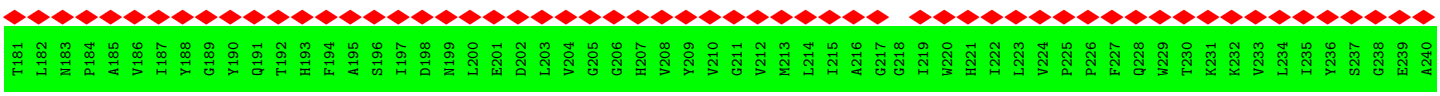
Chain t:











A301 W302 L303 S304 N305 A306 H307 F308 F309 L310 A311 F312 F313 C314 L315 Q316 G317 H318 L319 W320 H321 A322 L323 R324 A325 M326 G327 F328 D329 F330 R331 R332 V333 E334 K335 A336 L337 S338 S339 VAL GLU ALA

- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain u: 98% 99%

M1 Q2 T3 Y4 N5 N6 P7 E8 V9 T10 Y11 D12 W13 W14 A15 G16 N17 A18 R19 F20 A21 N22 L23 S24 G25 L26 F27 I28 A29 A30 H31 V32 A33 Q34 A35 A36 L37 I38 M39 F40 W41 A42 G43 A44 F45 T46 L47 Y48 E49 I50 S51 W52 L53 T54 A55 D56 Q57 S58 M59 G60

E61 Q62 G63 L64 I65 L66 L67 P68 H69 L70 A71 T72 L73 G74 L75 G76 V77 G78 D79 G80 G81 Q82 V83 T84 D85 T86 Y87 P88 L89 F90 V91 V92 G93 A94 V95 H96 L97 I98 A99 S100 A101 V102 L103 G104 A105 G106 A107 L108 F109 H110 T111 F112 R113 A114 P115 S116 D117 L118 A119 A120

A121 S122 G123 A124 A125 K126 R127 F128 H129 F130 D131 W132 N133 D134 P135 K136 Q137 L138 G139 L140 I141 L142 G143 H144 H145 L146 L147 F148 L149 G150 V151 G152 A153 L154 L155 L156 V157 A158 K159 A160 T161 T162 W163 G164 G165 L166 Y167 D168 A169 A170 S171 Q172 T173 V174 R175 L176 V177 T178 E179 P180

T181 L182 N183 P184 A185 V186 I187 Y188 G189 Y190 Q191 T192 H193 F194 A195 S196 I197 D198 N199 L200 E201 D202 L203 V204 G205 G206 H207 V208 Y209 V210 G211 V212 M213 L214 I215 A216 G217 G218 I219 W220 H221 I222 L223 V224 P225 P226 F227 Q228 W229 T230 K231 K232 V233 L234 I235 Y236 S237 G238 E239 A240

I241 L242 S243 Y244 S245 L246 G247 G248 I249 A250 L251 A252 G253 F254 V255 A256 A257 Y258 F259 C260 A261 V262 N263 T264 L265 A266 Y267 P268 V269 E270 F271 Y272 G273 A274 P275 L276 E277 I278 K279 L280 G281 V282 T283 P284 Y285 F286 A287 D288 T289 V290 Q291 L292 P293 F294 G295 A296 H297 T298 P299 R300

A301 W302 L303 S304 N305 A306 H307 F308 F309 L310 A311 F312 F313 C314 L315 Q316 G317 H318 L319 W320 H321 A322 L323 R324 A325 M326 G327 F328 D329 F330 R331 R332 V333 E334 K335 A336 L337 S338 S339 VAL GLU ALA

- Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain v: 93% 99%

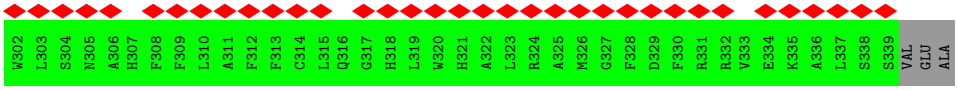
M1 Q2 T3 Y4 N5 N6 P7 E8 V9 T10 Y11 D12 W13 W14 A15 G16 N17 A18 R19 F20 A21 N22 L23 S24 G25 L26 F27 I28 A29 A30 H31 V32 A33 Q34 A35 A36 L37 I38 M39 F40 W41 A42 G43 A44 F45 T46 L47 Y48 E49 I50 S51 W52 L53 T54 A55 D56 Q57 S58 M59 G60

E61 Q62 G63 L64 I65 L66 L67 P68 H69 L70 A71 T72 L73 G74 L75 G76 V77 G78 D79 G80 G81 Q82 V83 T84 D85 T86 Y87 P88 L89 F90 V91 V92 G93 A94 V95 H96 L97 I98 A99 S100 A101 V102 L103 G104 A105 G106 A107 L108 F109 F112 R113 A114 P115 S116 D117 L118 A119 A120 A121

S122 G123 A124 A125 K126 R127 F128 H129 F130 D131 W132 N133 D134 P135 K136 Q137 L138 G139 L140 I141 L142 G143 H144 H145 L146 L147 F148 L149 G150 V151 G152 A153 L154 L155 L156 V157 A158 K159 A160 T161 T162 W163 G164 G165 L166 Y167 D168 A169 A170 S171 Q172 T173 V174 R175 L176 V177 T178 E179 P180 T181

L182 N183 P184 A185 V186 I187 Y188 G189 Y190 Q191 T192 H193 F194 A195 S196 I197 D198 N199 L200 E201 D202 L203 V204 G205 G206 H207 V208 Y209 V210 G211 V212 M213 L214 I215 A216 G217 G218 I219 W220 H221 I222 L223 V224 P225 P226 F227 Q228 W229 T230 K231 K232 V233 L234 I235 Y236 S237 G238 E239 A240 I241

L242 S243 Y244 S245 L246 G247 G248 I249 A250 L251 A252 G253 F254 V255 A256 A257 Y258 F259 C260 A261 V262 N263 T264 L265 A266 Y267 P268 V269 E270 F271 Y272 G273 A274 P275 L276 E277 I278 K279 L280 G281 V282 T283 P284 Y285 F286 A287 D288 T289 V290 Q291 L292 P293 F294 G295 A296 H297 T298 P299 R300 A301


W302
L303
S304
N305
A306
H307
F308
F309
L310
A311
F312
F313
C314
L315
Q316
G317
H318
L319
W320
H321
A322
L323
R324
A325
M326
G327
F328
D329
F330
R331
R332
V333
E334
K335
A336
L337
S338
S339
VAL
GLU
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	29295	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, FMN, LHG, LMG, SQD, CLA, LMU, SF4, PQN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.54	0/6064	0.57	0/8274
1	G	0.54	0/6064	0.57	0/8274
1	e	0.54	0/6064	0.57	0/8274
2	B	0.46	0/5999	0.54	0/8199
2	H	0.46	0/5999	0.54	0/8199
2	f	0.46	0/5999	0.54	0/8199
3	C	0.44	0/608	0.56	0/823
3	N	0.44	0/608	0.56	0/823
3	g	0.44	0/608	0.56	0/823
4	D	0.48	0/1124	0.58	0/1516
4	O	0.48	0/1124	0.58	0/1516
4	h	0.48	0/1124	0.58	0/1516
5	E	0.44	0/553	0.53	0/750
5	Q	0.44	0/553	0.53	0/750
5	i	0.44	0/553	0.53	0/750
6	F	0.43	0/1062	0.54	0/1442
6	R	0.43	0/1062	0.54	0/1442
6	j	0.43	0/1062	0.54	0/1442
7	I	0.49	0/289	0.71	0/393
7	S	0.49	0/289	0.71	0/393
7	k	0.49	0/289	0.71	0/393
8	J	0.37	0/346	0.55	0/469
8	T	0.37	0/346	0.55	0/469
8	l	0.38	0/346	0.55	0/469
9	K	0.33	0/560	0.58	0/765
9	U	0.34	0/560	0.58	0/765
9	m	0.34	0/560	0.58	0/765
10	L	0.42	0/1242	0.55	0/1696
10	V	0.42	0/1242	0.55	0/1696
10	n	0.42	0/1242	0.55	0/1696
11	M	0.42	0/231	0.60	0/314
11	W	0.42	0/231	0.60	0/314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	o	0.42	0/231	0.60	0/314
12	P	0.31	0/1344	0.50	0/1822
12	X	0.31	0/1344	0.50	0/1822
12	p	0.31	0/1344	0.50	0/1822
13	1	0.30	0/2689	0.48	0/3678
13	2	0.30	0/2689	0.48	0/3678
13	3	0.28	0/2689	0.47	0/3678
13	4	0.28	0/2689	0.49	0/3678
13	5	0.29	0/2689	0.48	0/3678
13	6	0.28	0/2689	0.47	0/3678
13	Y	0.30	0/2689	0.48	0/3678
13	Z	0.30	0/2689	0.48	0/3678
13	a	0.28	0/2689	0.47	0/3678
13	b	0.28	0/2689	0.49	0/3678
13	c	0.29	0/2689	0.48	0/3678
13	d	0.28	0/2689	0.48	0/3678
13	q	0.30	0/2689	0.48	0/3678
13	r	0.30	0/2689	0.49	0/3678
13	s	0.28	0/2689	0.47	0/3678
13	t	0.28	0/2689	0.49	0/3678
13	u	0.29	0/2689	0.48	0/3678
13	v	0.29	0/2689	0.48	0/3678
All	All	0.40	0/106668	0.52	0/145593

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5865	0	5744	102	0
1	G	5865	0	5744	103	0
1	e	5865	0	5744	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5789	0	5575	104	0
2	H	5789	0	5575	107	0
2	f	5789	0	5575	0	0
3	C	598	0	579	9	0
3	N	598	0	579	10	0
3	g	598	0	579	0	0
4	D	1098	0	1099	20	0
4	O	1098	0	1099	20	0
4	h	1098	0	1099	0	0
5	E	543	0	525	7	0
5	Q	543	0	525	6	0
5	i	543	0	525	0	0
6	F	1036	0	1031	17	0
6	R	1036	0	1031	13	0
6	j	1036	0	1031	0	0
7	I	282	0	291	8	0
7	S	282	0	291	5	0
7	k	282	0	291	0	0
8	J	335	0	344	8	0
8	T	335	0	344	8	0
8	l	335	0	344	0	0
9	K	549	0	597	15	0
9	U	549	0	597	16	0
9	m	549	0	597	0	0
10	L	1210	0	1206	34	0
10	V	1210	0	1206	31	0
10	n	1210	0	1206	0	0
11	M	228	0	246	6	0
11	W	228	0	246	4	0
11	o	228	0	246	0	0
12	P	1318	0	1233	19	0
12	X	1318	0	1233	17	0
12	p	1318	0	1233	0	0
13	1	2605	0	2564	36	0
13	2	2605	0	2564	42	0
13	3	2605	0	2564	37	0
13	4	2605	0	2564	44	0
13	5	2605	0	2564	31	0
13	6	2605	0	2564	46	0
13	Y	2605	0	2564	40	0
13	Z	2605	0	2564	44	0
13	a	2605	0	2564	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	b	2605	0	2564	0	0
13	c	2605	0	2564	0	0
13	d	2605	0	2564	0	0
13	q	2605	0	2564	0	0
13	r	2605	0	2564	0	0
13	s	2605	0	2564	0	0
13	t	2605	0	2564	0	0
13	u	2605	0	2564	0	0
13	v	2605	0	2564	0	0
14	1	765	0	561	26	0
14	2	850	0	720	31	0
14	3	785	0	593	22	0
14	4	765	0	561	21	0
14	5	785	0	600	20	0
14	6	785	0	600	25	0
14	A	2712	0	2766	133	0
14	B	2515	0	2595	130	0
14	F	90	0	66	4	0
14	G	2712	0	2766	138	0
14	H	2515	0	2595	125	0
14	J	100	0	82	4	0
14	K	148	0	118	3	0
14	L	185	0	190	9	0
14	R	90	0	66	4	0
14	T	100	0	82	4	0
14	U	148	0	118	3	0
14	V	185	0	190	13	0
14	Y	765	0	561	29	0
14	Z	850	0	720	32	0
14	a	785	0	593	0	0
14	b	765	0	561	0	0
14	c	785	0	600	0	0
14	d	785	0	600	0	0
14	e	2712	0	2766	0	0
14	f	2515	0	2595	0	0
14	j	90	0	66	0	0
14	l	100	0	82	0	0
14	m	148	0	118	0	0
14	n	185	0	190	0	0
14	q	765	0	561	0	0
14	r	850	0	720	0	0
14	s	785	0	593	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	t	765	0	561	0	0
14	u	785	0	600	0	0
14	v	785	0	600	0	0
15	A	33	0	46	4	0
15	B	33	0	46	4	0
15	G	33	0	46	3	0
15	H	33	0	46	5	0
15	e	33	0	46	0	0
15	f	33	0	46	0	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
16	G	8	0	0	0	0
16	N	16	0	0	0	0
16	e	8	0	0	0	0
16	g	16	0	0	0	0
17	1	160	0	224	16	0
17	2	160	0	224	16	0
17	3	160	0	224	5	0
17	4	160	0	224	7	0
17	5	160	0	224	7	0
17	6	160	0	224	12	0
17	A	240	0	336	22	0
17	B	280	0	392	31	0
17	F	40	0	56	6	0
17	G	240	0	336	20	0
17	H	280	0	392	29	0
17	I	40	0	56	4	0
17	J	120	0	168	15	0
17	K	40	0	56	3	0
17	L	160	0	224	18	0
17	M	40	0	56	2	0
17	R	40	0	56	6	0
17	S	40	0	56	3	0
17	T	120	0	168	14	0
17	U	40	0	56	3	0
17	V	160	0	224	22	0
17	W	40	0	56	3	0
17	Y	160	0	224	13	0
17	Z	160	0	224	16	0
17	a	160	0	224	0	0
17	b	160	0	224	0	0
17	c	160	0	224	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	d	160	0	224	0	0
17	e	240	0	336	0	0
17	f	280	0	392	0	0
17	j	40	0	56	0	0
17	k	40	0	56	0	0
17	l	120	0	168	0	0
17	m	40	0	56	0	0
17	n	160	0	224	0	0
17	o	40	0	56	0	0
17	q	160	0	224	0	0
17	r	160	0	224	0	0
17	s	160	0	224	0	0
17	t	160	0	224	0	0
17	u	160	0	224	0	0
17	v	160	0	224	0	0
18	A	374	0	493	32	0
18	B	78	0	96	6	0
18	G	374	0	493	32	0
18	H	78	0	96	6	0
18	I	48	0	69	2	0
18	L	127	0	170	7	0
18	S	48	0	69	0	0
18	V	127	0	170	14	0
18	e	374	0	493	0	0
18	f	78	0	96	0	0
18	k	48	0	69	0	0
18	n	127	0	170	0	0
19	A	58	0	76	3	0
19	B	35	0	46	1	0
19	G	58	0	76	3	0
19	H	35	0	46	1	0
19	J	22	0	28	0	0
19	T	22	0	28	0	0
19	e	58	0	76	0	0
19	f	35	0	46	0	0
19	l	22	0	28	0	0
20	B	53	0	76	5	0
20	H	53	0	76	6	0
20	J	32	0	34	0	0
20	T	32	0	34	1	0
20	f	53	0	76	0	0
20	l	32	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	1	32	0	28	1	0
21	2	28	0	20	0	0
21	3	28	0	20	2	0
21	4	26	0	16	0	0
21	5	26	0	16	0	0
21	6	26	0	16	0	0
21	B	40	0	42	8	0
21	H	40	0	42	9	0
21	L	46	0	58	4	0
21	V	46	0	58	6	0
21	Y	32	0	28	1	0
21	Z	28	0	20	0	0
21	a	28	0	20	0	0
21	b	26	0	16	0	0
21	c	26	0	16	0	0
21	d	26	0	16	0	0
21	f	40	0	42	0	0
21	n	46	0	58	0	0
21	q	32	0	28	0	0
21	r	28	0	20	0	0
21	s	28	0	20	0	0
21	t	26	0	16	0	0
21	u	26	0	16	0	0
21	v	26	0	16	0	0
22	P	31	0	19	1	0
22	X	31	0	19	1	0
22	p	31	0	19	0	0
23	A	9	0	0	1	0
23	B	7	0	0	0	0
23	F	1	0	0	0	0
23	G	9	0	0	1	0
23	H	7	0	0	0	0
23	L	1	0	0	0	0
23	R	1	0	0	0	0
23	V	1	0	0	0	0
23	e	9	0	0	0	0
23	f	7	0	0	0	0
23	j	1	0	0	0	0
23	n	1	0	0	0	0
All	All	144312	0	142227	1516	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1516 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:3:GLN:HG2	10:L:4:ASP:H	0.93	1.06
10:V:3:GLN:HG2	10:V:4:ASP:H	0.93	1.05
10:L:3:GLN:HG2	10:L:4:ASP:N	1.75	1.00
10:V:3:GLN:HG2	10:V:4:ASP:N	1.75	0.98
10:L:94:SER:HB2	14:V:1501:CLA:HMD1	1.54	0.87

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	749/763 (98%)	724 (97%)	25 (3%)	0	100	100
1	G	749/763 (98%)	724 (97%)	25 (3%)	0	100	100
1	e	749/763 (98%)	724 (97%)	25 (3%)	0	100	100
2	B	731/734 (100%)	710 (97%)	21 (3%)	0	100	100
2	H	731/734 (100%)	710 (97%)	21 (3%)	0	100	100
2	f	731/734 (100%)	710 (97%)	21 (3%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	N	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	g	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
4	O	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
4	h	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
5	E	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
5	Q	69/75 (92%)	68 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	i	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
6	F	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
6	R	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
6	j	134/159 (84%)	129 (96%)	5 (4%)	0	100	100
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	S	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	k	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
8	T	39/41 (95%)	39 (100%)	0	0	100	100
8	l	39/41 (95%)	39 (100%)	0	0	100	100
9	K	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
9	U	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
9	m	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
10	L	162/166 (98%)	158 (98%)	4 (2%)	0	100	100
10	V	162/166 (98%)	158 (98%)	4 (2%)	0	100	100
10	n	162/166 (98%)	158 (98%)	4 (2%)	0	100	100
11	M	27/29 (93%)	27 (100%)	0	0	100	100
11	W	27/29 (93%)	27 (100%)	0	0	100	100
11	o	27/29 (93%)	27 (100%)	0	0	100	100
12	P	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
12	X	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
12	p	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
13	1	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	2	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	3	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	4	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	5	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	6	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	Y	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	Z	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	a	337/342 (98%)	330 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	b	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	c	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	d	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	q	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
13	r	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	s	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
13	t	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	u	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
13	v	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
All	All	13287/13605 (98%)	12906 (97%)	381 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/611 (98%)	597 (100%)	3 (0%)	88	93
1	G	600/611 (98%)	597 (100%)	3 (0%)	88	93
1	e	600/611 (98%)	597 (100%)	3 (0%)	88	93
2	B	583/584 (100%)	582 (100%)	1 (0%)	93	97
2	H	583/584 (100%)	582 (100%)	1 (0%)	93	97
2	f	583/584 (100%)	582 (100%)	1 (0%)	93	97
3	C	67/68 (98%)	67 (100%)	0	100	100
3	N	67/68 (98%)	67 (100%)	0	100	100
3	g	67/68 (98%)	67 (100%)	0	100	100
4	D	114/114 (100%)	114 (100%)	0	100	100
4	O	114/114 (100%)	114 (100%)	0	100	100
4	h	114/114 (100%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	56/59 (95%)	56 (100%)	0	100	100
5	Q	56/59 (95%)	56 (100%)	0	100	100
5	i	56/59 (95%)	56 (100%)	0	100	100
6	F	105/121 (87%)	105 (100%)	0	100	100
6	R	105/121 (87%)	105 (100%)	0	100	100
6	j	105/121 (87%)	105 (100%)	0	100	100
7	I	30/30 (100%)	30 (100%)	0	100	100
7	S	30/30 (100%)	30 (100%)	0	100	100
7	k	30/30 (100%)	30 (100%)	0	100	100
8	J	35/35 (100%)	35 (100%)	0	100	100
8	T	35/35 (100%)	35 (100%)	0	100	100
8	l	35/35 (100%)	35 (100%)	0	100	100
9	K	56/61 (92%)	56 (100%)	0	100	100
9	U	56/61 (92%)	56 (100%)	0	100	100
9	m	56/61 (92%)	56 (100%)	0	100	100
10	L	127/128 (99%)	127 (100%)	0	100	100
10	V	127/128 (99%)	127 (100%)	0	100	100
10	n	127/128 (99%)	127 (100%)	0	100	100
11	M	24/24 (100%)	24 (100%)	0	100	100
11	W	24/24 (100%)	24 (100%)	0	100	100
11	o	24/24 (100%)	24 (100%)	0	100	100
12	P	140/142 (99%)	140 (100%)	0	100	100
12	X	140/142 (99%)	140 (100%)	0	100	100
12	p	140/142 (99%)	140 (100%)	0	100	100
13	1	257/259 (99%)	257 (100%)	0	100	100
13	2	257/259 (99%)	257 (100%)	0	100	100
13	3	257/259 (99%)	257 (100%)	0	100	100
13	4	257/259 (99%)	257 (100%)	0	100	100
13	5	257/259 (99%)	257 (100%)	0	100	100
13	6	257/259 (99%)	257 (100%)	0	100	100
13	Y	257/259 (99%)	257 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	Z	257/259 (99%)	257 (100%)	0	100	100
13	a	257/259 (99%)	257 (100%)	0	100	100
13	b	257/259 (99%)	257 (100%)	0	100	100
13	c	257/259 (99%)	257 (100%)	0	100	100
13	d	257/259 (99%)	257 (100%)	0	100	100
13	q	257/259 (99%)	257 (100%)	0	100	100
13	r	257/259 (99%)	257 (100%)	0	100	100
13	s	257/259 (99%)	257 (100%)	0	100	100
13	t	257/259 (99%)	257 (100%)	0	100	100
13	u	257/259 (99%)	257 (100%)	0	100	100
13	v	257/259 (99%)	257 (100%)	0	100	100
All	All	10437/10593 (98%)	10425 (100%)	12 (0%)	93	97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	443	VAL
1	e	13	LYS
2	f	443	VAL
1	e	36	ARG
2	B	443	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	34	HIS
4	h	71	GLN
5	Q	67	GLN
2	f	603	GLN
13	t	62	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

843 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	1	512	13	45,53,73	1.74	8 (17%)	52,89,113	1.49	5 (9%)
21	SQD	r	822	-	27,28,54	1.22	4 (14%)	36,39,65	1.86	10 (27%)
14	CLA	d	509	13	45,53,73	1.75	7 (15%)	52,89,113	1.69	7 (13%)
14	CLA	G	1117	1	65,73,73	1.47	10 (15%)	76,113,113	1.57	10 (13%)
14	CLA	t	512	13	45,53,73	1.74	6 (13%)	52,89,113	1.60	6 (11%)
17	BCR	4	521	-	41,41,41	0.67	0	56,56,56	1.79	11 (19%)
14	CLA	2	503	13	65,73,73	1.45	6 (9%)	76,113,113	1.47	8 (10%)
14	CLA	e	1102	1	55,63,73	1.56	9 (16%)	64,101,113	1.62	7 (10%)
17	BCR	H	4014	-	41,41,41	0.83	0	56,56,56	1.89	23 (41%)
14	CLA	u	518	13	45,53,73	1.76	6 (13%)	52,89,113	1.57	8 (15%)
14	CLA	B	1211	2	55,63,73	1.52	8 (14%)	64,101,113	1.68	8 (12%)
18	LHG	H	1842	14	36,36,48	0.81	1 (2%)	39,42,54	1.26	3 (7%)
14	CLA	G	1022	23	65,73,73	1.53	11 (16%)	76,113,113	1.55	11 (14%)
16	SF4	A	3001	2,1	0,12,12	-	-	-		
14	CLA	e	1113	1	45,53,73	1.67	7 (15%)	52,89,113	1.81	7 (13%)
14	CLA	3	512	13	45,53,73	1.77	8 (17%)	52,89,113	1.52	5 (9%)
14	CLA	f	1229	2	65,73,73	1.41	8 (12%)	76,113,113	1.60	8 (10%)
17	BCR	d	522	-	41,41,41	0.71	0	56,56,56	1.89	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	LHG	A	5004	-	34,34,48	0.67	0	37,40,54	1.28	4 (10%)
14	CLA	3	502	13	45,53,73	1.76	7 (15%)	52,89,113	1.72	9 (17%)
14	CLA	H	1218	2	60,68,73	1.51	8 (13%)	70,107,113	1.44	7 (10%)
14	CLA	a	501	13	45,53,73	1.75	7 (15%)	52,89,113	1.67	9 (17%)
14	CLA	A	1128	1	65,73,73	1.58	11 (16%)	76,113,113	1.69	9 (11%)
14	CLA	A	1111	1	65,73,73	1.43	9 (13%)	76,113,113	1.53	8 (10%)
14	CLA	6	502	13	45,53,73	1.77	7 (15%)	52,89,113	1.66	8 (15%)
14	CLA	e	1117	1	65,73,73	1.47	10 (15%)	76,113,113	1.57	10 (13%)
17	BCR	a	522	-	41,41,41	0.70	0	56,56,56	2.03	17 (30%)
14	CLA	f	1204	2	65,73,73	1.40	8 (12%)	76,113,113	1.47	9 (11%)
14	CLA	e	1124	23	60,68,73	1.53	9 (15%)	70,107,113	1.59	10 (14%)
14	CLA	B	1214	2	65,73,73	1.49	9 (13%)	76,113,113	1.51	7 (9%)
18	LHG	A	5003	14	39,39,48	0.86	1 (2%)	42,45,54	1.38	6 (14%)
14	CLA	s	512	13	45,53,73	1.78	8 (17%)	52,89,113	1.52	5 (9%)
14	CLA	4	503	13	45,53,73	1.79	7 (15%)	52,89,113	1.71	8 (15%)
14	CLA	G	1114	23	45,53,73	1.80	8 (17%)	52,89,113	1.69	9 (17%)
14	CLA	H	1235	2	65,73,73	1.47	10 (15%)	76,113,113	1.51	8 (10%)
14	CLA	Z	519	13	45,53,73	1.76	9 (20%)	52,89,113	1.60	8 (15%)
18	LHG	V	5218	-	36,36,48	0.76	2 (5%)	39,42,54	1.20	4 (10%)
21	SQD	c	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.95	11 (32%)
17	BCR	2	524	-	41,41,41	0.73	0	56,56,56	1.76	12 (21%)
14	CLA	c	513	13	45,53,73	1.79	8 (17%)	52,89,113	1.56	6 (11%)
14	CLA	q	508	13	45,53,73	1.77	9 (20%)	52,89,113	1.93	8 (15%)
14	CLA	r	502	13	45,53,73	1.76	7 (15%)	52,89,113	1.70	9 (17%)
14	CLA	c	507	-	45,53,73	1.74	6 (13%)	52,89,113	1.71	9 (17%)
14	CLA	5	519	13	45,53,73	1.78	6 (13%)	52,89,113	1.61	7 (13%)
14	CLA	e	1134	1	56,64,73	1.56	8 (14%)	65,102,113	1.64	11 (16%)
14	CLA	F	1302	6	45,53,73	1.76	9 (20%)	52,89,113	1.58	8 (15%)
14	CLA	B	1204	2	65,73,73	1.40	8 (12%)	76,113,113	1.47	9 (11%)
14	CLA	A	1115	1	60,68,73	1.51	9 (15%)	70,107,113	1.59	7 (10%)
17	BCR	J	4013	-	41,41,41	0.77	0	56,56,56	1.93	16 (28%)
14	CLA	B	1239	2	65,73,73	1.48	8 (12%)	76,113,113	1.72	15 (19%)
14	CLA	3	510	13	45,53,73	1.75	8 (17%)	52,89,113	1.64	7 (13%)
14	CLA	e	1138	1	65,73,73	1.45	9 (13%)	76,113,113	1.54	7 (9%)
14	CLA	H	1201	2	60,68,73	1.49	7 (11%)	70,107,113	1.65	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	H	1224	2	60,68,73	1.50	7 (11%)	70,107,113	1.54	9 (12%)
14	CLA	H	1212	2	51,59,73	1.59	7 (13%)	59,96,113	1.68	6 (10%)
17	BCR	d	524	-	41,41,41	0.79	0	56,56,56	1.84	15 (26%)
14	CLA	f	1201	2	60,68,73	1.49	7 (11%)	70,107,113	1.65	9 (12%)
14	CLA	u	503	13	45,53,73	1.78	7 (15%)	52,89,113	1.68	10 (19%)
18	LHG	e	5005	-	42,42,48	0.65	1 (2%)	45,48,54	1.21	4 (8%)
14	CLA	B	1240	18	65,73,73	1.47	6 (9%)	76,113,113	1.46	8 (10%)
14	CLA	B	1213	2	61,69,73	1.47	7 (11%)	71,108,113	1.60	9 (12%)
14	CLA	B	1205	2	65,73,73	1.46	10 (15%)	76,113,113	1.59	11 (14%)
14	CLA	f	1209	2	53,61,73	1.63	8 (15%)	61,98,113	1.68	8 (13%)
14	CLA	f	1021	2	65,73,73	1.47	9 (13%)	76,113,113	1.45	9 (11%)
14	CLA	t	517	-	45,53,73	1.75	6 (13%)	52,89,113	1.66	8 (15%)
14	CLA	G	1013	-	65,73,73	1.43	8 (12%)	76,113,113	1.88	13 (17%)
14	CLA	a	506	13	45,53,73	1.77	7 (15%)	52,89,113	1.70	6 (11%)
14	CLA	f	1236	2	50,58,73	1.70	9 (18%)	58,95,113	1.55	10 (17%)
16	SF4	G	3001	2,1	0,12,12	-	-	-		
14	CLA	G	1120	1	50,58,73	1.57	8 (16%)	58,95,113	1.73	10 (17%)
21	SQD	4	822	-	25,26,54	1.32	4 (16%)	34,37,65	1.97	9 (26%)
14	CLA	u	504	-	45,53,73	1.77	8 (17%)	52,89,113	1.67	7 (13%)
17	BCR	e	4008	-	41,41,41	0.95	2 (4%)	56,56,56	2.17	16 (28%)
14	CLA	d	501	13	45,53,73	1.75	7 (15%)	52,89,113	1.71	7 (13%)
14	CLA	v	508	13	45,53,73	1.76	7 (15%)	52,89,113	1.78	11 (21%)
14	CLA	Z	516	13	45,53,73	1.77	7 (15%)	52,89,113	1.66	8 (15%)
14	CLA	H	1230	2	60,68,73	1.54	10 (16%)	70,107,113	1.46	7 (10%)
14	CLA	G	1128	1	65,73,73	1.58	11 (16%)	76,113,113	1.69	9 (11%)
14	CLA	d	511	13	45,53,73	1.77	5 (11%)	52,89,113	1.70	7 (13%)
14	CLA	5	517	-	45,53,73	1.79	8 (17%)	52,89,113	1.56	6 (11%)
14	CLA	Y	510	13	45,53,73	1.77	8 (17%)	52,89,113	1.60	6 (11%)
21	SQD	q	822	-	31,32,54	1.20	5 (16%)	40,43,65	2.05	13 (32%)
14	CLA	a	507	-	45,53,73	1.74	6 (13%)	52,89,113	1.68	9 (17%)
18	LHG	n	5221	-	48,48,48	0.62	0	51,54,54	1.28	7 (13%)
14	CLA	B	1202	2	65,73,73	1.41	7 (10%)	76,113,113	1.58	8 (10%)
14	CLA	2	510	13	45,53,73	1.72	7 (15%)	52,89,113	1.62	6 (11%)
19	LMU	l	5105	-	22,22,36	1.21	1 (4%)	27,27,47	1.43	5 (18%)
14	CLA	5	518	13	45,53,73	1.76	6 (13%)	52,89,113	1.56	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	Z	503	13	65,73,73	1.45	6 (9%)	76,113,113	1.47	8 (10%)
14	CLA	u	508	13	45,53,73	1.79	9 (20%)	52,89,113	1.85	7 (13%)
14	CLA	s	516	13	45,53,73	1.75	5 (11%)	52,89,113	1.87	11 (21%)
14	CLA	f	1238	23	65,73,73	1.41	7 (10%)	76,113,113	1.63	10 (13%)
14	CLA	1	510	13	45,53,73	1.76	8 (17%)	52,89,113	1.60	6 (11%)
18	LHG	G	5008	-	34,34,48	0.71	1 (2%)	37,40,54	1.25	3 (8%)
14	CLA	G	1134	1	56,64,73	1.55	8 (14%)	65,102,113	1.64	11 (16%)
14	CLA	b	505	13	45,53,73	1.76	8 (17%)	52,89,113	1.54	6 (11%)
14	CLA	5	503	13	45,53,73	1.78	7 (15%)	52,89,113	1.67	10 (19%)
14	CLA	Y	503	13	45,53,73	1.77	8 (17%)	52,89,113	1.66	7 (13%)
14	CLA	f	1205	2	65,73,73	1.46	10 (15%)	76,113,113	1.59	11 (14%)
19	LMU	G	1849	-	23,23,36	1.18	1 (4%)	28,28,47	1.39	4 (14%)
14	CLA	a	512	13	45,53,73	1.76	8 (17%)	52,89,113	1.53	5 (9%)
14	CLA	L	1501	10	60,68,73	1.56	10 (16%)	70,107,113	1.50	9 (12%)
14	CLA	A	1104	1	65,73,73	1.44	9 (13%)	76,113,113	1.59	13 (17%)
14	CLA	1	503	13	45,53,73	1.76	8 (17%)	52,89,113	1.66	7 (13%)
14	CLA	q	510	13	45,53,73	1.77	7 (15%)	52,89,113	1.59	6 (11%)
17	BCR	H	4006	-	41,41,41	0.78	0	56,56,56	2.09	18 (32%)
14	CLA	e	1103	1	65,73,73	1.45	9 (13%)	76,113,113	1.73	10 (13%)
14	CLA	L	1502	10	65,73,73	1.45	9 (13%)	76,113,113	1.53	8 (10%)
14	CLA	H	1204	2	65,73,73	1.40	8 (12%)	76,113,113	1.47	9 (11%)
14	CLA	A	1122	1	60,68,73	1.50	10 (16%)	70,107,113	1.54	9 (12%)
16	SF4	N	3003	3	0,12,12	-	-	-		
14	CLA	A	1135	1	55,63,73	1.49	10 (18%)	64,101,113	1.76	11 (17%)
14	CLA	f	1230	2	60,68,73	1.54	10 (16%)	70,107,113	1.46	7 (10%)
14	CLA	r	508	13	45,53,73	1.78	9 (20%)	52,89,113	1.76	10 (19%)
17	BCR	Z	524	-	41,41,41	0.74	0	56,56,56	1.75	12 (21%)
16	SF4	g	3003	3	0,12,12	-	-	-		
14	CLA	2	511	13	45,53,73	1.75	7 (15%)	52,89,113	1.70	7 (13%)
17	BCR	n	4022	-	41,41,41	0.79	0	56,56,56	1.82	10 (17%)
14	CLA	c	518	13	45,53,73	1.75	6 (13%)	52,89,113	1.56	8 (15%)
14	CLA	e	1120	1	50,58,73	1.58	8 (16%)	58,95,113	1.73	10 (17%)
14	CLA	t	519	13	45,53,73	1.75	7 (15%)	52,89,113	1.64	7 (13%)
17	BCR	4	522	-	41,41,41	0.73	0	56,56,56	1.91	19 (33%)
14	CLA	m	1103	9	48,56,73	1.66	8 (16%)	55,92,113	1.61	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	j	1301	23	45,53,73	1.73	9 (20%)	52,89,113	1.60	6 (11%)
18	LHG	G	5004	-	34,34,48	0.67	0	37,40,54	1.28	4 (10%)
17	BCR	R	4016	-	41,41,41	0.81	0	56,56,56	1.91	12 (21%)
14	CLA	A	1137	1	60,68,73	1.53	9 (15%)	70,107,113	1.56	10 (14%)
14	CLA	3	503	13	45,53,73	1.77	6 (13%)	52,89,113	1.64	8 (15%)
14	CLA	r	501	13	60,68,73	1.50	8 (13%)	70,107,113	1.57	8 (11%)
17	BCR	l	4015	-	41,41,41	0.80	0	56,56,56	1.73	12 (21%)
18	LHG	e	5007	-	46,46,48	0.61	0	49,52,54	1.20	4 (8%)
14	CLA	f	1215	2	65,73,73	1.46	10 (15%)	76,113,113	1.72	10 (13%)
14	CLA	A	1118	1	60,68,73	1.48	10 (16%)	70,107,113	1.55	8 (11%)
14	CLA	3	509	13	45,53,73	1.75	7 (15%)	52,89,113	1.77	7 (13%)
17	BCR	A	4002	-	41,41,41	0.88	1 (2%)	56,56,56	1.94	16 (28%)
17	BCR	q	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	B	1021	2	65,73,73	1.47	9 (13%)	76,113,113	1.45	9 (11%)
14	CLA	H	1012	23	65,73,73	1.44	9 (13%)	76,113,113	1.58	9 (11%)
14	CLA	u	516	13	45,53,73	1.77	6 (13%)	52,89,113	1.58	6 (11%)
14	CLA	6	508	13	45,53,73	1.78	7 (15%)	52,89,113	1.78	11 (21%)
14	CLA	t	502	13	45,53,73	1.79	8 (17%)	52,89,113	1.67	7 (13%)
14	CLA	U	1401	-	55,63,73	1.58	7 (12%)	64,101,113	1.62	10 (15%)
14	CLA	6	506	13	45,53,73	1.76	7 (15%)	52,89,113	1.67	6 (11%)
14	CLA	A	1133	1	65,73,73	1.41	10 (15%)	76,113,113	1.48	6 (7%)
14	CLA	v	502	13	45,53,73	1.77	7 (15%)	52,89,113	1.66	8 (15%)
17	BCR	J	4015	-	41,41,41	0.80	0	56,56,56	1.73	12 (21%)
14	CLA	B	1216	23	60,68,73	1.60	10 (16%)	70,107,113	1.56	11 (15%)
14	CLA	s	509	13	45,53,73	1.74	7 (15%)	52,89,113	1.77	7 (13%)
14	CLA	e	1135	1	55,63,73	1.50	10 (18%)	64,101,113	1.76	11 (17%)
14	CLA	Z	502	13	45,53,73	1.76	9 (20%)	52,89,113	1.71	9 (17%)
14	CLA	q	517	-	45,53,73	1.74	6 (13%)	52,89,113	1.60	7 (13%)
14	CLA	r	513	13	45,53,73	1.78	9 (20%)	52,89,113	1.55	6 (11%)
17	BCR	1	522	-	41,41,41	0.74	0	56,56,56	1.91	20 (35%)
14	CLA	Z	511	13	45,53,73	1.75	7 (15%)	52,89,113	1.70	7 (13%)
17	BCR	H	4017	-	41,41,41	0.97	4 (9%)	56,56,56	1.82	12 (21%)
14	CLA	r	504	-	45,53,73	1.77	7 (15%)	52,89,113	1.63	8 (15%)
17	BCR	n	4019	-	41,41,41	0.76	0	56,56,56	1.95	15 (26%)
14	CLA	A	1132	1	65,73,73	1.42	10 (15%)	76,113,113	1.55	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	v	509	13	45,53,73	1.75	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	B	1223	2	65,73,73	1.42	8 (12%)	76,113,113	1.63	7 (9%)
14	CLA	Y	512	13	45,53,73	1.74	8 (17%)	52,89,113	1.49	5 (9%)
17	BCR	t	521	-	41,41,41	0.67	0	56,56,56	1.79	10 (17%)
17	BCR	W	4021	-	41,41,41	0.77	0	56,56,56	1.91	15 (26%)
14	CLA	G	1140	1	65,73,73	1.46	9 (13%)	76,113,113	1.56	10 (13%)
14	CLA	e	1116	1	60,68,73	1.52	8 (13%)	70,107,113	1.50	7 (10%)
14	CLA	q	519	13	45,53,73	1.79	9 (20%)	52,89,113	1.56	7 (13%)
14	CLA	Z	504	-	45,53,73	1.77	7 (15%)	52,89,113	1.64	8 (15%)
14	CLA	H	1220	2	55,63,73	1.58	10 (18%)	64,101,113	1.64	10 (15%)
14	CLA	e	1129	1	53,61,73	1.62	10 (18%)	61,98,113	1.59	9 (14%)
17	BCR	L	4020	-	41,41,41	0.98	2 (4%)	56,56,56	1.67	15 (26%)
14	CLA	5	513	13	45,53,73	1.79	8 (17%)	52,89,113	1.55	6 (11%)
14	CLA	T	1303	8	45,53,73	1.77	7 (15%)	52,89,113	1.73	9 (17%)
14	CLA	c	503	13	45,53,73	1.77	7 (15%)	52,89,113	1.68	10 (19%)
14	CLA	s	502	13	45,53,73	1.77	8 (17%)	52,89,113	1.72	9 (17%)
14	CLA	5	504	-	45,53,73	1.76	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	5	508	13	45,53,73	1.79	9 (20%)	52,89,113	1.84	7 (13%)
14	CLA	G	1122	1	60,68,73	1.51	11 (18%)	70,107,113	1.54	9 (12%)
14	CLA	f	1231	23	65,73,73	1.38	7 (10%)	76,113,113	1.52	9 (11%)
16	SF4	g	3002	3	0,12,12	-	-	-		
14	CLA	t	518	13	45,53,73	1.76	6 (13%)	52,89,113	1.61	6 (11%)
14	CLA	H	1202	2	65,73,73	1.41	7 (10%)	76,113,113	1.58	8 (10%)
14	CLA	2	509	13	65,73,73	1.46	7 (10%)	76,113,113	1.52	7 (9%)
17	BCR	G	4007	-	41,41,41	0.87	0	56,56,56	2.11	20 (35%)
21	SQD	H	1852	-	39,40,54	1.18	6 (15%)	48,51,65	1.84	12 (25%)
14	CLA	b	504	-	45,53,73	1.77	5 (11%)	52,89,113	1.64	7 (13%)
14	CLA	t	501	13	45,53,73	1.79	6 (13%)	52,89,113	1.63	7 (13%)
17	BCR	V	4020	-	41,41,41	0.99	2 (4%)	56,56,56	1.67	15 (26%)
14	CLA	B	1201	2	60,68,73	1.49	7 (11%)	70,107,113	1.66	9 (12%)
17	BCR	s	521	-	41,41,41	0.66	0	56,56,56	1.83	11 (19%)
17	BCR	M	4021	-	41,41,41	0.76	0	56,56,56	1.91	15 (26%)
17	BCR	G	4002	-	41,41,41	0.88	1 (2%)	56,56,56	1.94	16 (28%)
14	CLA	v	510	13	45,53,73	1.77	7 (15%)	52,89,113	1.63	6 (11%)
21	SQD	3	822	-	27,28,54	1.29	5 (18%)	36,39,65	1.80	11 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	Z	510	13	45,53,73	1.72	7 (15%)	52,89,113	1.62	6 (11%)
14	CLA	6	505	13	65,73,73	1.45	7 (10%)	76,113,113	1.45	8 (10%)
17	BCR	q	523	-	41,41,41	0.75	0	56,56,56	1.68	13 (23%)
14	CLA	3	516	13	45,53,73	1.75	5 (11%)	52,89,113	1.87	11 (21%)
14	CLA	r	519	13	45,53,73	1.77	9 (20%)	52,89,113	1.59	8 (15%)
17	BCR	H	4010	-	41,41,41	0.91	1 (2%)	56,56,56	2.31	21 (37%)
14	CLA	e	1130	1	56,64,73	1.52	8 (14%)	65,102,113	1.73	9 (13%)
14	CLA	G	1133	1	65,73,73	1.42	10 (15%)	76,113,113	1.49	6 (7%)
14	CLA	B	1236	2	50,58,73	1.70	9 (18%)	58,95,113	1.54	10 (17%)
14	CLA	2	502	13	45,53,73	1.76	8 (17%)	52,89,113	1.70	9 (17%)
14	CLA	e	1127	1	65,73,73	1.42	9 (13%)	76,113,113	1.55	11 (14%)
14	CLA	1	501	13	45,53,73	1.75	6 (13%)	52,89,113	1.67	6 (11%)
14	CLA	s	506	13	45,53,73	1.79	7 (15%)	52,89,113	1.69	6 (11%)
16	SF4	N	3002	3	0,12,12	-	-	-		
21	SQD	n	5216	-	45,46,54	1.02	5 (11%)	54,57,65	1.68	11 (20%)
14	CLA	A	1124	23	60,68,73	1.52	9 (15%)	70,107,113	1.58	9 (12%)
14	CLA	a	510	13	45,53,73	1.75	8 (17%)	52,89,113	1.65	7 (13%)
14	CLA	u	519	13	45,53,73	1.78	6 (13%)	52,89,113	1.60	7 (13%)
14	CLA	B	1234	2	65,73,73	1.44	8 (12%)	76,113,113	1.65	10 (13%)
14	CLA	R	1301	23	45,53,73	1.72	9 (20%)	52,89,113	1.59	6 (11%)
14	CLA	b	517	-	45,53,73	1.76	7 (15%)	52,89,113	1.67	8 (15%)
14	CLA	t	511	13	45,53,73	1.79	6 (13%)	52,89,113	1.67	9 (17%)
17	BCR	G	4001	-	41,41,41	0.79	0	56,56,56	1.68	11 (19%)
14	CLA	B	1227	2	60,68,73	1.54	10 (16%)	70,107,113	1.51	8 (11%)
17	BCR	e	4002	-	41,41,41	0.87	1 (2%)	56,56,56	1.94	16 (28%)
17	BCR	t	523	-	41,41,41	0.73	0	56,56,56	1.77	14 (25%)
21	SQD	d	822	-	25,26,54	1.31	4 (16%)	34,37,65	2.00	10 (29%)
21	SQD	s	822	-	27,28,54	1.29	5 (18%)	36,39,65	1.80	10 (27%)
14	CLA	e	1022	23	65,73,73	1.54	11 (16%)	76,113,113	1.55	11 (14%)
14	CLA	d	513	13	45,53,73	1.77	7 (15%)	52,89,113	1.58	6 (11%)
17	BCR	2	521	-	41,41,41	0.70	0	56,56,56	1.90	13 (23%)
14	CLA	4	511	13	45,53,73	1.78	7 (15%)	52,89,113	1.67	9 (17%)
14	CLA	e	1123	23	65,73,73	1.42	8 (12%)	76,113,113	1.53	8 (10%)
14	CLA	r	512	13	45,53,73	1.75	8 (17%)	52,89,113	1.51	5 (9%)
14	CLA	Y	516	13	45,53,73	1.71	9 (20%)	52,89,113	1.64	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	d	507	-	45,53,73	1.75	7 (15%)	52,89,113	1.69	9 (17%)
14	CLA	A	1107	1	65,73,73	1.52	10 (15%)	76,113,113	1.49	10 (13%)
14	CLA	G	1104	1	65,73,73	1.43	9 (13%)	76,113,113	1.60	13 (17%)
14	CLA	2	505	13	65,73,73	1.42	7 (10%)	76,113,113	1.47	8 (10%)
14	CLA	G	1138	1	65,73,73	1.45	9 (13%)	76,113,113	1.55	7 (9%)
14	CLA	5	506	13	45,53,73	1.73	7 (15%)	52,89,113	1.62	7 (13%)
14	CLA	e	1122	1	60,68,73	1.51	11 (18%)	70,107,113	1.54	9 (12%)
14	CLA	u	502	13	45,53,73	1.79	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	f	1222	23	50,58,73	1.61	9 (18%)	58,95,113	1.73	9 (15%)
14	CLA	A	1237	23	65,73,73	1.46	12 (18%)	76,113,113	1.57	9 (11%)
14	CLA	A	1106	1	65,73,73	1.41	8 (12%)	76,113,113	1.53	9 (11%)
14	CLA	G	1129	1	53,61,73	1.63	10 (18%)	61,98,113	1.60	9 (14%)
14	CLA	4	513	13	45,53,73	1.78	7 (15%)	52,89,113	1.64	6 (11%)
14	CLA	4	507	-	45,53,73	1.72	6 (13%)	52,89,113	1.72	8 (15%)
14	CLA	4	504	-	45,53,73	1.78	6 (13%)	52,89,113	1.65	7 (13%)
14	CLA	b	506	13	45,53,73	1.78	7 (15%)	52,89,113	1.66	6 (11%)
14	CLA	n	1503	23	60,68,73	1.48	8 (13%)	70,107,113	1.57	7 (10%)
14	CLA	f	1213	2	61,69,73	1.47	7 (11%)	71,108,113	1.60	8 (11%)
14	CLA	c	516	13	45,53,73	1.77	6 (13%)	52,89,113	1.58	6 (11%)
14	CLA	q	518	13	45,53,73	1.75	6 (13%)	52,89,113	1.62	7 (13%)
14	CLA	U	1105	9	45,53,73	1.78	8 (17%)	52,89,113	1.85	11 (21%)
16	SF4	C	3002	3	0,12,12	-	-	-		
14	CLA	6	504	-	45,53,73	1.74	7 (15%)	52,89,113	1.69	7 (13%)
18	LHG	A	5008	-	34,34,48	0.70	1 (2%)	37,40,54	1.25	4 (10%)
14	CLA	n	1502	10	65,73,73	1.45	9 (13%)	76,113,113	1.54	8 (10%)
14	CLA	b	513	13	45,53,73	1.78	6 (13%)	52,89,113	1.63	6 (11%)
14	CLA	f	1220	2	55,63,73	1.58	10 (18%)	64,101,113	1.63	10 (15%)
14	CLA	r	517	-	45,53,73	1.76	7 (15%)	52,89,113	1.65	7 (13%)
14	CLA	2	516	13	45,53,73	1.77	7 (15%)	52,89,113	1.66	8 (15%)
17	BCR	e	4007	-	41,41,41	0.87	0	56,56,56	2.10	19 (33%)
14	CLA	G	1137	1	60,68,73	1.52	9 (15%)	70,107,113	1.57	10 (14%)
14	CLA	q	513	13	45,53,73	1.77	7 (15%)	52,89,113	1.63	7 (13%)
14	CLA	A	1101	1	65,73,73	1.50	9 (13%)	76,113,113	1.61	13 (17%)
14	CLA	J	1303	8	45,53,73	1.77	7 (15%)	52,89,113	1.73	9 (17%)
14	CLA	f	1208	2	65,73,73	1.45	7 (10%)	76,113,113	1.39	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	Y	517	-	45,53,73	1.75	7 (15%)	52,89,113	1.61	7 (13%)
14	CLA	1	516	13	45,53,73	1.71	9 (20%)	52,89,113	1.63	8 (15%)
14	CLA	q	504	-	45,53,73	1.79	8 (17%)	52,89,113	1.79	11 (21%)
17	BCR	G	4008	-	41,41,41	0.95	2 (4%)	56,56,56	2.17	16 (28%)
17	BCR	b	524	-	41,41,41	0.69	0	56,56,56	1.85	14 (25%)
14	CLA	v	501	13	45,53,73	1.75	7 (15%)	52,89,113	1.71	7 (13%)
14	CLA	c	504	-	45,53,73	1.76	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	A	1136	1	65,73,73	1.47	10 (15%)	76,113,113	1.54	10 (13%)
21	SQD	b	822	-	25,26,54	1.32	4 (16%)	34,37,65	1.97	9 (26%)
17	BCR	e	4003	-	41,41,41	0.87	1 (2%)	56,56,56	1.78	14 (25%)
14	CLA	d	518	13	45,53,73	1.74	6 (13%)	52,89,113	1.63	6 (11%)
14	CLA	c	508	13	45,53,73	1.79	9 (20%)	52,89,113	1.84	7 (13%)
14	CLA	B	1230	2	60,68,73	1.53	10 (16%)	70,107,113	1.47	7 (10%)
17	BCR	S	4018	-	41,41,41	0.93	2 (4%)	56,56,56	1.93	16 (28%)
14	CLA	T	1302	8	55,63,73	1.55	9 (16%)	64,101,113	1.56	9 (14%)
18	LHG	G	5001	-	48,48,48	0.80	1 (2%)	51,54,54	1.30	7 (13%)
18	LHG	A	5009	-	41,41,48	0.67	0	44,47,54	1.22	5 (11%)
14	CLA	t	509	13	45,53,73	1.77	7 (15%)	52,89,113	1.75	9 (17%)
14	CLA	H	1219	2	63,71,73	1.52	9 (14%)	73,110,113	1.43	10 (13%)
18	LHG	G	5003	14	39,39,48	0.86	1 (2%)	42,45,54	1.38	6 (14%)
14	CLA	u	501	13	45,53,73	1.76	7 (15%)	52,89,113	1.71	8 (15%)
14	CLA	6	510	13	45,53,73	1.77	7 (15%)	52,89,113	1.63	6 (11%)
14	CLA	r	518	13	55,63,73	1.55	7 (12%)	64,101,113	1.53	8 (12%)
14	CLA	e	1126	1	65,73,73	1.39	8 (12%)	76,113,113	1.57	8 (10%)
17	BCR	5	521	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
14	CLA	f	1227	2	60,68,73	1.54	10 (16%)	70,107,113	1.51	8 (11%)
14	CLA	e	1133	1	65,73,73	1.41	10 (15%)	76,113,113	1.48	6 (7%)
17	BCR	H	4004	-	41,41,41	0.73	0	56,56,56	1.85	14 (25%)
14	CLA	A	1129	1	53,61,73	1.62	10 (18%)	61,98,113	1.60	9 (14%)
14	CLA	B	1215	2	65,73,73	1.46	10 (15%)	76,113,113	1.71	10 (13%)
14	CLA	A	1108	1	54,62,73	1.58	9 (16%)	62,99,113	1.58	8 (12%)
14	CLA	Z	509	13	65,73,73	1.46	7 (10%)	76,113,113	1.52	7 (9%)
17	BCR	T	4012	-	41,41,41	0.72	0	56,56,56	1.76	13 (23%)
14	CLA	Y	513	13	45,53,73	1.77	7 (15%)	52,89,113	1.63	7 (13%)
17	BCR	L	4022	-	41,41,41	0.79	0	56,56,56	1.82	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	LMU	B	1843	-	36,36,36	1.16	2 (5%)	47,47,47	1.06	3 (6%)
14	CLA	A	1103	1	65,73,73	1.46	9 (13%)	76,113,113	1.73	11 (14%)
14	CLA	c	511	13	45,53,73	1.75	5 (11%)	52,89,113	1.71	8 (15%)
17	BCR	r	523	-	41,41,41	0.72	0	56,56,56	1.75	17 (30%)
14	CLA	u	509	13	65,73,73	1.43	7 (10%)	76,113,113	1.50	7 (9%)
14	CLA	u	505	13	45,53,73	1.73	7 (15%)	52,89,113	1.60	6 (11%)
17	BCR	G	4011	-	41,41,41	0.81	0	56,56,56	1.78	12 (21%)
17	BCR	3	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
17	BCR	r	522	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	H	1228	2	55,63,73	1.52	7 (12%)	64,101,113	1.71	8 (12%)
14	CLA	q	506	13	45,53,73	1.76	6 (13%)	52,89,113	1.64	6 (11%)
17	BCR	6	521	-	41,41,41	0.67	0	56,56,56	1.79	12 (21%)
14	CLA	A	1120	1	50,58,73	1.58	8 (16%)	58,95,113	1.73	10 (17%)
14	CLA	2	518	13	55,63,73	1.55	6 (10%)	64,101,113	1.53	7 (10%)
14	CLA	5	510	13	45,53,73	1.73	7 (15%)	52,89,113	1.62	7 (13%)
14	CLA	d	519	13	45,53,73	1.77	9 (20%)	52,89,113	1.57	7 (13%)
17	BCR	B	4017	-	41,41,41	0.97	3 (7%)	56,56,56	1.82	12 (21%)
14	CLA	G	1101	1	65,73,73	1.50	9 (13%)	76,113,113	1.62	13 (17%)
17	BCR	T	4013	-	41,41,41	0.78	0	56,56,56	1.93	16 (28%)
14	CLA	H	1208	2	65,73,73	1.44	8 (12%)	76,113,113	1.39	7 (9%)
14	CLA	2	501	13	60,68,73	1.51	7 (11%)	70,107,113	1.57	8 (11%)
21	SQD	6	822	-	25,26,54	1.31	4 (16%)	34,37,65	2.00	10 (29%)
14	CLA	b	510	13	45,53,73	1.72	6 (13%)	52,89,113	1.65	6 (11%)
17	BCR	6	523	-	41,41,41	0.72	0	56,56,56	1.72	14 (25%)
17	BCR	r	521	-	41,41,41	0.70	0	56,56,56	1.90	13 (23%)
14	CLA	6	517	-	45,53,73	1.73	7 (15%)	52,89,113	1.61	7 (13%)
17	BCR	f	4006	-	41,41,41	0.77	0	56,56,56	2.09	18 (32%)
18	LHG	n	5220	-	40,40,48	0.70	1 (2%)	43,46,54	1.30	5 (11%)
14	CLA	G	1108	1	54,62,73	1.57	8 (14%)	62,99,113	1.57	8 (12%)
17	BCR	q	524	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
15	PQN	f	2002	-	34,34,34	2.84	11 (32%)	42,45,45	2.30	6 (14%)
17	BCR	d	521	-	41,41,41	0.67	0	56,56,56	1.79	12 (21%)
14	CLA	H	1023	-	65,73,73	1.41	8 (12%)	76,113,113	1.90	11 (14%)
14	CLA	t	506	13	45,53,73	1.77	7 (15%)	52,89,113	1.65	6 (11%)
14	CLA	G	1119	23	65,73,73	1.49	11 (16%)	76,113,113	1.67	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	BCR	t	524	-	41,41,41	0.70	0	56,56,56	1.85	14 (25%)
14	CLA	f	1012	23	65,73,73	1.45	9 (13%)	76,113,113	1.58	9 (11%)
14	CLA	Y	502	13	45,53,73	1.75	8 (17%)	52,89,113	1.65	8 (15%)
17	BCR	V	4019	-	41,41,41	0.76	0	56,56,56	1.95	15 (26%)
18	LHG	A	5007	-	46,46,48	0.60	0	49,52,54	1.20	4 (8%)
14	CLA	H	1203	2	65,73,73	1.44	9 (13%)	76,113,113	1.53	9 (11%)
14	CLA	3	519	13	45,53,73	1.76	8 (17%)	52,89,113	1.61	7 (13%)
14	CLA	G	1124	23	60,68,73	1.52	9 (15%)	70,107,113	1.59	9 (12%)
17	BCR	V	4022	-	41,41,41	0.78	0	56,56,56	1.81	10 (17%)
14	CLA	B	1226	2	55,63,73	1.71	10 (18%)	64,101,113	1.98	15 (23%)
14	CLA	f	1203	2	65,73,73	1.44	9 (13%)	76,113,113	1.53	9 (11%)
14	CLA	4	518	13	45,53,73	1.76	6 (13%)	52,89,113	1.61	6 (11%)
14	CLA	m	1401	-	55,63,73	1.59	7 (12%)	64,101,113	1.63	10 (15%)
14	CLA	B	1208	2	65,73,73	1.44	7 (10%)	76,113,113	1.38	7 (9%)
17	BCR	B	4009	-	41,41,41	0.77	0	56,56,56	1.90	18 (32%)
14	CLA	Z	505	13	65,73,73	1.42	6 (9%)	76,113,113	1.47	8 (10%)
14	CLA	1	502	13	45,53,73	1.75	8 (17%)	52,89,113	1.66	8 (15%)
14	CLA	G	1112	1	50,58,73	1.62	10 (20%)	58,95,113	1.67	8 (13%)
14	CLA	v	516	13	45,53,73	1.77	6 (13%)	52,89,113	1.60	8 (15%)
14	CLA	H	1209	2	53,61,73	1.62	8 (15%)	61,98,113	1.67	8 (13%)
17	BCR	A	4011	-	41,41,41	0.82	0	56,56,56	1.79	12 (21%)
18	LHG	A	5002	-	42,42,48	0.76	1 (2%)	45,48,54	1.22	4 (8%)
14	CLA	b	519	13	45,53,73	1.77	7 (15%)	52,89,113	1.64	7 (13%)
14	CLA	u	512	13	45,53,73	1.74	7 (15%)	52,89,113	1.57	6 (11%)
17	BCR	b	521	-	41,41,41	0.68	0	56,56,56	1.78	11 (19%)
14	CLA	t	508	13	45,53,73	1.81	10 (22%)	52,89,113	1.79	9 (17%)
17	BCR	5	523	-	41,41,41	0.78	1 (2%)	56,56,56	1.78	15 (26%)
14	CLA	G	1237	23	65,73,73	1.47	12 (18%)	76,113,113	1.57	9 (11%)
14	CLA	G	1106	1	65,73,73	1.41	8 (12%)	76,113,113	1.53	9 (11%)
14	CLA	c	512	13	45,53,73	1.74	7 (15%)	52,89,113	1.56	6 (11%)
21	SQD	V	5216	-	45,46,54	1.01	5 (11%)	54,57,65	1.69	11 (20%)
14	CLA	d	508	13	45,53,73	1.77	7 (15%)	52,89,113	1.78	11 (21%)
14	CLA	2	512	13	45,53,73	1.76	8 (17%)	52,89,113	1.50	5 (9%)
14	CLA	a	516	13	45,53,73	1.74	5 (11%)	52,89,113	1.87	11 (21%)
14	CLA	6	518	13	45,53,73	1.74	6 (13%)	52,89,113	1.63	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	q	511	13	45,53,73	1.76	7 (15%)	52,89,113	1.67	8 (15%)
17	BCR	b	523	-	41,41,41	0.73	0	56,56,56	1.77	14 (25%)
14	CLA	f	1224	2	60,68,73	1.49	7 (11%)	70,107,113	1.54	9 (12%)
14	CLA	1	505	13	45,53,73	1.73	7 (15%)	52,89,113	1.65	6 (11%)
14	CLA	Z	501	13	60,68,73	1.50	8 (13%)	70,107,113	1.57	7 (10%)
17	BCR	A	4008	-	41,41,41	0.95	2 (4%)	56,56,56	2.17	16 (28%)
14	CLA	t	507	-	45,53,73	1.73	6 (13%)	52,89,113	1.73	8 (15%)
20	LMG	l	5104	-	32,32,55	0.96	2 (6%)	40,40,63	1.26	4 (10%)
14	CLA	e	1110	1	53,61,73	1.60	8 (15%)	61,98,113	1.57	8 (13%)
14	CLA	e	1112	1	50,58,73	1.62	10 (20%)	58,95,113	1.67	8 (13%)
18	LHG	G	5007	-	46,46,48	0.60	0	49,52,54	1.20	4 (8%)
14	CLA	A	1011	1	65,73,73	1.46	10 (15%)	76,113,113	1.73	14 (18%)
17	BCR	4	523	-	41,41,41	0.74	0	56,56,56	1.77	14 (25%)
14	CLA	d	503	13	45,53,73	1.76	7 (15%)	52,89,113	1.68	6 (11%)
14	CLA	B	1231	23	65,73,73	1.38	7 (10%)	76,113,113	1.52	9 (11%)
14	CLA	4	517	-	45,53,73	1.76	7 (15%)	52,89,113	1.67	8 (15%)
14	CLA	f	1226	2	55,63,73	1.70	10 (18%)	64,101,113	1.98	15 (23%)
17	BCR	3	523	-	41,41,41	0.69	0	56,56,56	1.82	15 (26%)
14	CLA	a	503	13	45,53,73	1.76	6 (13%)	52,89,113	1.64	8 (15%)
14	CLA	B	1222	23	50,58,73	1.61	9 (18%)	58,95,113	1.72	9 (15%)
14	CLA	2	519	13	45,53,73	1.77	9 (20%)	52,89,113	1.60	8 (15%)
14	CLA	A	1130	1	56,64,73	1.52	8 (14%)	65,102,113	1.73	9 (13%)
14	CLA	A	1138	1	65,73,73	1.44	9 (13%)	76,113,113	1.55	7 (9%)
14	CLA	A	1125	1	65,73,73	1.42	10 (15%)	76,113,113	1.58	9 (11%)
18	LHG	n	5218	-	36,36,48	0.76	2 (5%)	39,42,54	1.20	4 (10%)
14	CLA	H	1232	23	55,63,73	1.54	8 (14%)	64,101,113	1.70	7 (10%)
19	LMU	H	1843	-	36,36,36	1.17	2 (5%)	47,47,47	1.06	3 (6%)
14	CLA	6	519	13	45,53,73	1.78	9 (20%)	52,89,113	1.58	7 (13%)
14	CLA	q	507	-	45,53,73	1.74	7 (15%)	52,89,113	1.70	9 (17%)
14	CLA	H	1223	2	65,73,73	1.42	8 (12%)	76,113,113	1.63	7 (9%)
14	CLA	r	511	13	45,53,73	1.75	7 (15%)	52,89,113	1.71	8 (15%)
18	LHG	G	5009	-	41,41,48	0.67	0	44,47,54	1.22	4 (9%)
14	CLA	c	502	13	45,53,73	1.78	7 (15%)	52,89,113	1.69	7 (13%)
14	CLA	B	1220	2	55,63,73	1.58	10 (18%)	64,101,113	1.64	10 (15%)
17	BCR	e	4001	-	41,41,41	0.79	0	56,56,56	1.69	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	r	506	13	45,53,73	1.75	7 (15%)	52,89,113	1.63	7 (13%)
17	BCR	F	4016	-	41,41,41	0.82	0	56,56,56	1.91	11 (19%)
14	CLA	e	1119	23	65,73,73	1.50	11 (16%)	76,113,113	1.67	13 (17%)
14	CLA	f	1023	-	65,73,73	1.41	8 (12%)	76,113,113	1.89	11 (14%)
14	CLA	Z	518	13	55,63,73	1.55	7 (12%)	64,101,113	1.53	7 (10%)
21	SQD	t	822	-	25,26,54	1.32	4 (16%)	34,37,65	1.97	9 (26%)
14	CLA	d	506	13	45,53,73	1.76	7 (15%)	52,89,113	1.67	6 (11%)
14	CLA	H	1215	2	65,73,73	1.46	10 (15%)	76,113,113	1.71	10 (13%)
14	CLA	e	1237	23	65,73,73	1.46	12 (18%)	76,113,113	1.57	9 (11%)
14	CLA	u	506	13	45,53,73	1.73	7 (15%)	52,89,113	1.63	7 (13%)
14	CLA	G	1103	1	65,73,73	1.46	9 (13%)	76,113,113	1.73	11 (14%)
14	CLA	Y	505	13	45,53,73	1.74	7 (15%)	52,89,113	1.66	6 (11%)
14	CLA	b	503	13	45,53,73	1.78	7 (15%)	52,89,113	1.70	8 (15%)
17	BCR	u	524	-	41,41,41	0.71	0	56,56,56	1.74	11 (19%)
19	LMU	e	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	2 (4%)
17	BCR	r	524	-	41,41,41	0.74	0	56,56,56	1.76	13 (23%)
14	CLA	b	509	13	45,53,73	1.77	7 (15%)	52,89,113	1.75	8 (15%)
14	CLA	B	1203	2	65,73,73	1.44	9 (13%)	76,113,113	1.53	9 (11%)
21	SQD	2	822	-	27,28,54	1.22	4 (14%)	36,39,65	1.86	10 (27%)
14	CLA	r	507	-	45,53,73	1.72	8 (17%)	52,89,113	1.71	10 (19%)
17	BCR	t	522	-	41,41,41	0.74	0	56,56,56	1.91	19 (33%)
17	BCR	2	523	-	41,41,41	0.72	0	56,56,56	1.75	17 (30%)
14	CLA	4	519	13	45,53,73	1.76	7 (15%)	52,89,113	1.64	7 (13%)
14	CLA	c	505	13	45,53,73	1.74	7 (15%)	52,89,113	1.62	6 (11%)
14	CLA	A	1121	1	55,63,73	1.57	10 (18%)	64,101,113	1.66	12 (18%)
14	CLA	Y	501	13	45,53,73	1.75	7 (15%)	52,89,113	1.67	6 (11%)
14	CLA	c	501	13	45,53,73	1.75	7 (15%)	52,89,113	1.70	8 (15%)
14	CLA	c	510	13	45,53,73	1.74	7 (15%)	52,89,113	1.62	7 (13%)
17	BCR	f	4009	-	41,41,41	0.78	0	56,56,56	1.89	18 (32%)
18	LHG	e	5008	-	34,34,48	0.71	1 (2%)	37,40,54	1.25	4 (10%)
17	BCR	c	523	-	41,41,41	0.78	1 (2%)	56,56,56	1.78	15 (26%)
17	BCR	6	524	-	41,41,41	0.78	0	56,56,56	1.85	15 (26%)
17	BCR	A	4003	-	41,41,41	0.88	1 (2%)	56,56,56	1.78	14 (25%)
17	BCR	v	521	-	41,41,41	0.68	0	56,56,56	1.79	12 (21%)
14	CLA	a	502	13	45,53,73	1.77	8 (17%)	52,89,113	1.72	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	LMG	T	5104	-	32,32,55	0.96	2 (6%)	40,40,63	1.26	4 (10%)
14	CLA	B	1218	2	60,68,73	1.51	8 (13%)	70,107,113	1.43	7 (10%)
18	LHG	G	5002	-	42,42,48	0.76	1 (2%)	45,48,54	1.23	4 (8%)
14	CLA	v	512	13	45,53,73	1.76	7 (15%)	52,89,113	1.58	6 (11%)
14	CLA	6	501	13	45,53,73	1.75	7 (15%)	52,89,113	1.71	7 (13%)
15	PQN	A	2001	-	34,34,34	2.81	11 (32%)	42,45,45	2.19	6 (14%)
14	CLA	Z	512	13	45,53,73	1.76	8 (17%)	52,89,113	1.49	5 (9%)
14	CLA	G	1135	1	55,63,73	1.49	10 (18%)	64,101,113	1.76	11 (17%)
14	CLA	j	1302	6	45,53,73	1.76	9 (20%)	52,89,113	1.57	8 (15%)
17	BCR	j	4016	-	41,41,41	0.82	0	56,56,56	1.91	11 (19%)
14	CLA	H	1231	23	65,73,73	1.39	7 (10%)	76,113,113	1.52	9 (11%)
14	CLA	d	504	-	45,53,73	1.74	7 (15%)	52,89,113	1.69	7 (13%)
17	BCR	v	523	-	41,41,41	0.72	0	56,56,56	1.72	15 (26%)
14	CLA	B	1229	2	65,73,73	1.42	7 (10%)	76,113,113	1.59	8 (10%)
14	CLA	H	1222	23	50,58,73	1.61	9 (18%)	58,95,113	1.73	9 (15%)
17	BCR	Z	523	-	41,41,41	0.72	0	56,56,56	1.76	17 (30%)
14	CLA	e	1105	1	55,63,73	1.50	9 (16%)	64,101,113	1.67	8 (12%)
16	SF4	C	3003	3	0,12,12	-	-	-		
17	BCR	a	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	e	1106	1	65,73,73	1.41	8 (12%)	76,113,113	1.53	9 (11%)
14	CLA	1	509	13	45,53,73	1.76	7 (15%)	52,89,113	1.65	9 (17%)
14	CLA	5	516	13	45,53,73	1.77	6 (13%)	52,89,113	1.58	6 (11%)
14	CLA	5	501	13	45,53,73	1.75	7 (15%)	52,89,113	1.71	8 (15%)
14	CLA	f	1207	2	65,73,73	1.44	8 (12%)	76,113,113	1.38	6 (7%)
14	CLA	4	516	13	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)
15	PQN	B	2002	-	34,34,34	2.84	11 (32%)	42,45,45	2.31	6 (14%)
14	CLA	4	508	13	45,53,73	1.80	9 (20%)	52,89,113	1.80	9 (17%)
14	CLA	1	506	13	45,53,73	1.75	7 (15%)	52,89,113	1.64	6 (11%)
14	CLA	B	1012	23	65,73,73	1.44	9 (13%)	76,113,113	1.58	9 (11%)
14	CLA	a	517	-	45,53,73	1.79	8 (17%)	52,89,113	1.58	6 (11%)
14	CLA	G	1123	23	65,73,73	1.42	8 (12%)	76,113,113	1.52	8 (10%)
14	CLA	m	1105	9	45,53,73	1.79	8 (17%)	52,89,113	1.84	11 (21%)
14	CLA	6	511	13	45,53,73	1.78	5 (11%)	52,89,113	1.69	7 (13%)
14	CLA	3	504	-	45,53,73	1.75	7 (15%)	52,89,113	1.73	9 (17%)
14	CLA	b	516	13	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	s	519	13	45,53,73	1.76	8 (17%)	52,89,113	1.61	7 (13%)
17	BCR	2	522	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	c	509	13	65,73,73	1.44	7 (10%)	76,113,113	1.49	7 (9%)
14	CLA	q	505	13	45,53,73	1.74	7 (15%)	52,89,113	1.64	6 (11%)
21	SQD	u	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.95	11 (32%)
17	BCR	n	4219	-	41,41,41	1.09	5 (12%)	56,56,56	2.26	23 (41%)
14	CLA	A	1127	1	65,73,73	1.42	9 (13%)	76,113,113	1.55	11 (14%)
18	LHG	H	1855	-	40,40,48	0.69	1 (2%)	43,46,54	1.24	5 (11%)
14	CLA	G	1011	1	65,73,73	1.46	10 (15%)	76,113,113	1.73	14 (18%)
14	CLA	f	1218	2	60,68,73	1.51	8 (13%)	70,107,113	1.43	7 (10%)
14	CLA	e	1137	1	60,68,73	1.52	9 (15%)	70,107,113	1.56	10 (14%)
17	BCR	B	4014	-	41,41,41	0.83	1 (2%)	56,56,56	1.89	23 (41%)
14	CLA	B	1219	2	63,71,73	1.52	8 (12%)	73,110,113	1.44	10 (13%)
14	CLA	l	1303	8	45,53,73	1.77	8 (17%)	52,89,113	1.74	9 (17%)
14	CLA	v	518	13	45,53,73	1.74	6 (13%)	52,89,113	1.62	6 (11%)
17	BCR	G	4003	-	41,41,41	0.87	1 (2%)	56,56,56	1.78	14 (25%)
18	LHG	B	1842	14	36,36,48	0.81	1 (2%)	39,42,54	1.26	3 (7%)
14	CLA	5	512	13	45,53,73	1.74	7 (15%)	52,89,113	1.56	6 (11%)
18	LHG	e	5009	-	41,41,48	0.67	0	44,47,54	1.22	4 (9%)
14	CLA	3	507	-	45,53,73	1.74	6 (13%)	52,89,113	1.68	9 (17%)
14	CLA	G	1130	1	56,64,73	1.52	8 (14%)	65,102,113	1.74	9 (13%)
14	CLA	6	513	13	45,53,73	1.78	7 (15%)	52,89,113	1.59	6 (11%)
14	CLA	B	1209	2	53,61,73	1.62	8 (15%)	61,98,113	1.68	8 (13%)
17	BCR	u	522	-	41,41,41	0.75	0	56,56,56	1.94	21 (37%)
14	CLA	J	1302	8	55,63,73	1.56	9 (16%)	64,101,113	1.56	9 (14%)
14	CLA	B	1217	2	60,68,73	1.53	6 (10%)	70,107,113	1.42	7 (10%)
14	CLA	3	517	-	45,53,73	1.79	8 (17%)	52,89,113	1.58	6 (11%)
14	CLA	6	507	-	45,53,73	1.76	7 (15%)	52,89,113	1.69	9 (17%)
14	CLA	B	1224	2	60,68,73	1.50	7 (11%)	70,107,113	1.54	9 (12%)
14	CLA	A	1119	23	65,73,73	1.50	11 (16%)	76,113,113	1.67	13 (17%)
18	LHG	A	5005	-	42,42,48	0.65	1 (2%)	45,48,54	1.21	4 (8%)
14	CLA	H	1216	23	60,68,73	1.60	10 (16%)	70,107,113	1.57	11 (15%)
15	PQN	G	2001	-	34,34,34	2.82	11 (32%)	42,45,45	2.20	6 (14%)
17	BCR	Y	524	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	G	1126	1	65,73,73	1.39	8 (12%)	76,113,113	1.57	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	b	508	13	45,53,73	1.81	10 (22%)	52,89,113	1.80	9 (17%)
21	SQD	Y	822	-	31,32,54	1.20	5 (16%)	40,43,65	2.05	13 (32%)
14	CLA	H	1021	2	65,73,73	1.46	9 (13%)	76,113,113	1.45	9 (11%)
14	CLA	B	1232	23	55,63,73	1.54	8 (14%)	64,101,113	1.70	7 (10%)
14	CLA	K	1103	9	48,56,73	1.66	8 (16%)	55,92,113	1.62	8 (14%)
20	LMG	H	5002	-	53,53,55	0.86	3 (5%)	61,61,63	1.51	12 (19%)
21	SQD	a	822	-	27,28,54	1.30	5 (18%)	36,39,65	1.79	10 (27%)
14	CLA	4	512	13	45,53,73	1.74	6 (13%)	52,89,113	1.59	6 (11%)
14	CLA	A	1113	1	45,53,73	1.67	7 (15%)	52,89,113	1.81	7 (13%)
14	CLA	s	507	-	45,53,73	1.75	6 (13%)	52,89,113	1.68	9 (17%)
17	BCR	u	521	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
17	BCR	1	524	-	41,41,41	0.74	0	56,56,56	1.85	17 (30%)
14	CLA	4	506	13	45,53,73	1.77	6 (13%)	52,89,113	1.66	6 (11%)
18	LHG	L	5218	-	36,36,48	0.76	2 (5%)	39,42,54	1.20	4 (10%)
14	CLA	v	505	13	65,73,73	1.45	7 (10%)	76,113,113	1.45	8 (10%)
17	BCR	d	523	-	41,41,41	0.72	0	56,56,56	1.72	14 (25%)
14	CLA	A	1112	1	50,58,73	1.62	10 (20%)	58,95,113	1.68	8 (13%)
14	CLA	3	506	13	45,53,73	1.79	7 (15%)	52,89,113	1.70	6 (11%)
18	LHG	A	5001	-	48,48,48	0.80	1 (2%)	51,54,54	1.30	7 (13%)
14	CLA	d	517	-	45,53,73	1.72	6 (13%)	52,89,113	1.61	7 (13%)
14	CLA	G	1113	1	45,53,73	1.67	7 (15%)	52,89,113	1.80	7 (13%)
14	CLA	H	1238	23	65,73,73	1.40	7 (10%)	76,113,113	1.64	11 (14%)
17	BCR	u	523	-	41,41,41	0.78	0	56,56,56	1.79	15 (26%)
17	BCR	H	4005	-	41,41,41	0.76	0	56,56,56	1.73	12 (21%)
17	BCR	f	4014	-	41,41,41	0.83	1 (2%)	56,56,56	1.90	23 (41%)
17	BCR	T	4015	-	41,41,41	0.80	0	56,56,56	1.73	12 (21%)
14	CLA	G	1111	1	65,73,73	1.43	10 (15%)	76,113,113	1.53	7 (9%)
14	CLA	n	1501	10	60,68,73	1.56	10 (16%)	70,107,113	1.50	9 (12%)
14	CLA	s	518	13	55,63,73	1.59	7 (12%)	64,101,113	1.47	7 (10%)
14	CLA	R	1302	6	45,53,73	1.77	9 (20%)	52,89,113	1.59	8 (15%)
18	LHG	S	5001	-	47,47,48	0.62	0	50,53,54	1.24	5 (10%)
14	CLA	A	1110	1	53,61,73	1.59	8 (15%)	61,98,113	1.57	8 (13%)
17	BCR	c	524	-	41,41,41	0.72	0	56,56,56	1.74	12 (21%)
14	CLA	e	1109	1	65,73,73	1.40	9 (13%)	76,113,113	1.60	8 (10%)
14	CLA	q	509	13	45,53,73	1.76	7 (15%)	52,89,113	1.66	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	BCR	3	524	-	41,41,41	0.78	0	56,56,56	1.93	18 (32%)
14	CLA	f	1217	2	60,68,73	1.52	6 (10%)	70,107,113	1.41	7 (10%)
14	CLA	B	1023	-	65,73,73	1.41	8 (12%)	76,113,113	1.89	11 (14%)
14	CLA	c	517	-	45,53,73	1.79	8 (17%)	52,89,113	1.56	6 (11%)
14	CLA	r	510	13	45,53,73	1.71	7 (15%)	52,89,113	1.62	7 (13%)
14	CLA	f	1212	2	51,59,73	1.60	7 (13%)	59,96,113	1.67	6 (10%)
18	LHG	e	5004	-	34,34,48	0.67	0	37,40,54	1.28	4 (10%)
14	CLA	5	502	13	45,53,73	1.78	7 (15%)	52,89,113	1.70	7 (13%)
14	CLA	t	503	13	45,53,73	1.80	7 (15%)	52,89,113	1.71	8 (15%)
14	CLA	Y	518	13	45,53,73	1.76	6 (13%)	52,89,113	1.64	7 (13%)
14	CLA	1	507	-	45,53,73	1.74	7 (15%)	52,89,113	1.70	9 (17%)
17	BCR	L	4019	-	41,41,41	0.76	0	56,56,56	1.95	15 (26%)
14	CLA	K	1105	9	45,53,73	1.79	8 (17%)	52,89,113	1.85	11 (21%)
14	CLA	e	1011	1	65,73,73	1.45	10 (15%)	76,113,113	1.73	14 (18%)
14	CLA	G	1107	1	65,73,73	1.52	10 (15%)	76,113,113	1.50	10 (13%)
14	CLA	G	1102	1	55,63,73	1.57	9 (16%)	64,101,113	1.61	7 (10%)
14	CLA	H	1236	2	50,58,73	1.70	9 (18%)	58,95,113	1.54	10 (17%)
14	CLA	b	502	13	45,53,73	1.80	8 (17%)	52,89,113	1.67	8 (15%)
17	BCR	b	522	-	41,41,41	0.73	0	56,56,56	1.91	19 (33%)
22	FMN	p	170	-	33,33,33	1.12	2 (6%)	48,50,50	1.24	6 (12%)
17	BCR	o	4021	-	41,41,41	0.77	0	56,56,56	1.91	15 (26%)
14	CLA	1	504	-	45,53,73	1.79	8 (17%)	52,89,113	1.78	9 (17%)
14	CLA	K	1401	-	55,63,73	1.58	7 (12%)	64,101,113	1.63	10 (15%)
14	CLA	5	505	13	45,53,73	1.73	7 (15%)	52,89,113	1.61	6 (11%)
14	CLA	t	504	-	45,53,73	1.79	6 (13%)	52,89,113	1.64	7 (13%)
14	CLA	2	506	13	45,53,73	1.77	8 (17%)	52,89,113	1.62	7 (13%)
19	LMU	G	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	2 (4%)
17	BCR	Z	522	-	41,41,41	0.75	0	56,56,56	1.86	17 (30%)
14	CLA	Y	509	13	45,53,73	1.76	7 (15%)	52,89,113	1.66	9 (17%)
17	BCR	s	522	-	41,41,41	0.70	0	56,56,56	2.04	18 (32%)
14	CLA	a	509	13	45,53,73	1.74	7 (15%)	52,89,113	1.78	7 (13%)
14	CLA	s	503	13	45,53,73	1.77	6 (13%)	52,89,113	1.64	8 (15%)
14	CLA	b	512	13	45,53,73	1.74	6 (13%)	52,89,113	1.60	6 (11%)
14	CLA	e	1111	1	65,73,73	1.42	9 (13%)	76,113,113	1.53	8 (10%)
18	LHG	V	5220	-	40,40,48	0.70	1 (2%)	43,46,54	1.30	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	f	1214	2	65,73,73	1.49	9 (13%)	76,113,113	1.51	7 (9%)
14	CLA	U	1103	9	48,56,73	1.67	8 (16%)	55,92,113	1.62	8 (14%)
14	CLA	G	1121	1	55,63,73	1.57	10 (18%)	64,101,113	1.66	12 (18%)
14	CLA	G	1136	1	65,73,73	1.46	9 (13%)	76,113,113	1.54	10 (13%)
18	LHG	L	5220	-	40,40,48	0.70	1 (2%)	43,46,54	1.30	5 (11%)
20	LMG	f	5002	-	53,53,55	0.85	2 (3%)	61,61,63	1.51	12 (19%)
14	CLA	r	503	13	65,73,73	1.45	6 (9%)	76,113,113	1.47	8 (10%)
14	CLA	G	1139	23	65,73,73	1.47	10 (15%)	76,113,113	1.36	6 (7%)
14	CLA	G	1110	1	53,61,73	1.60	8 (15%)	61,98,113	1.58	8 (13%)
14	CLA	6	509	13	45,53,73	1.75	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	3	505	13	55,63,73	1.56	8 (14%)	64,101,113	1.49	7 (10%)
14	CLA	Y	519	13	45,53,73	1.80	8 (17%)	52,89,113	1.55	7 (13%)
14	CLA	4	510	13	45,53,73	1.73	6 (13%)	52,89,113	1.66	6 (11%)
14	CLA	d	502	13	45,53,73	1.77	7 (15%)	52,89,113	1.67	8 (15%)
17	BCR	Y	522	-	41,41,41	0.74	0	56,56,56	1.91	20 (35%)
14	CLA	1	508	13	45,53,73	1.77	10 (22%)	52,89,113	1.92	7 (13%)
14	CLA	A	1131	1	65,73,73	1.47	10 (15%)	76,113,113	1.42	9 (11%)
14	CLA	G	1109	1	65,73,73	1.40	9 (13%)	76,113,113	1.60	8 (10%)
14	CLA	H	1217	2	60,68,73	1.53	6 (10%)	70,107,113	1.42	7 (10%)
14	CLA	a	519	13	45,53,73	1.76	8 (17%)	52,89,113	1.61	7 (13%)
14	CLA	G	1127	1	65,73,73	1.42	9 (13%)	76,113,113	1.54	11 (14%)
14	CLA	f	1228	2	55,63,73	1.52	7 (12%)	64,101,113	1.70	8 (12%)
14	CLA	s	504	-	45,53,73	1.76	6 (13%)	52,89,113	1.74	9 (17%)
14	CLA	q	501	13	45,53,73	1.75	7 (15%)	52,89,113	1.66	6 (11%)
14	CLA	f	1225	2	65,73,73	1.45	10 (15%)	76,113,113	1.49	9 (11%)
14	CLA	1	519	13	45,53,73	1.79	8 (17%)	52,89,113	1.56	6 (11%)
14	CLA	2	507	-	45,53,73	1.72	8 (17%)	52,89,113	1.71	10 (19%)
17	BCR	k	4018	-	41,41,41	0.93	2 (4%)	56,56,56	1.93	16 (28%)
14	CLA	4	502	13	45,53,73	1.79	8 (17%)	52,89,113	1.67	7 (13%)
17	BCR	n	4020	-	41,41,41	0.98	2 (4%)	56,56,56	1.67	14 (25%)
14	CLA	H	1205	2	65,73,73	1.46	10 (15%)	76,113,113	1.58	11 (14%)
14	CLA	e	1131	1	65,73,73	1.47	10 (15%)	76,113,113	1.42	9 (11%)
17	BCR	f	4010	-	41,41,41	0.91	1 (2%)	56,56,56	2.30	21 (37%)
14	CLA	B	1207	2	65,73,73	1.45	9 (13%)	76,113,113	1.38	6 (7%)
17	BCR	Y	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	BCR	s	524	-	41,41,41	0.77	0	56,56,56	1.93	18 (32%)
15	PQN	e	2001	-	34,34,34	2.81	11 (32%)	42,45,45	2.19	6 (14%)
18	LHG	e	5006	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	5 (11%)
14	CLA	e	1114	23	45,53,73	1.80	8 (17%)	52,89,113	1.68	9 (17%)
14	CLA	t	516	13	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)
17	BCR	3	522	-	41,41,41	0.69	0	56,56,56	2.04	18 (32%)
17	BCR	6	522	-	41,41,41	0.72	0	56,56,56	1.89	19 (33%)
14	CLA	d	505	13	65,73,73	1.45	7 (10%)	76,113,113	1.46	8 (10%)
17	BCR	m	4104	-	41,41,41	0.79	0	56,56,56	1.88	16 (28%)
14	CLA	Z	506	13	45,53,73	1.77	8 (17%)	52,89,113	1.61	7 (13%)
14	CLA	5	511	13	45,53,73	1.76	5 (11%)	52,89,113	1.71	7 (13%)
17	BCR	B	4006	-	41,41,41	0.78	0	56,56,56	2.09	18 (32%)
14	CLA	a	505	13	55,63,73	1.56	8 (14%)	64,101,113	1.49	7 (10%)
14	CLA	d	510	13	45,53,73	1.76	7 (15%)	52,89,113	1.62	6 (11%)
14	CLA	s	508	13	45,53,73	1.79	9 (20%)	52,89,113	1.75	7 (13%)
17	BCR	1	521	-	41,41,41	0.67	0	56,56,56	1.83	11 (19%)
14	CLA	e	1136	1	65,73,73	1.46	9 (13%)	76,113,113	1.54	10 (13%)
14	CLA	f	1234	2	65,73,73	1.44	9 (13%)	76,113,113	1.65	10 (13%)
17	BCR	e	4011	-	41,41,41	0.83	0	56,56,56	1.78	12 (21%)
14	CLA	A	1105	1	55,63,73	1.50	9 (16%)	64,101,113	1.67	8 (12%)
19	LMU	T	5105	-	22,22,36	1.21	1 (4%)	27,27,47	1.43	5 (18%)
21	SQD	B	1852	-	39,40,54	1.18	6 (15%)	48,51,65	1.84	12 (25%)
14	CLA	v	506	13	45,53,73	1.76	7 (15%)	52,89,113	1.67	6 (11%)
18	LHG	B	1855	-	40,40,48	0.69	1 (2%)	43,46,54	1.24	5 (11%)
17	BCR	V	4219	-	41,41,41	1.08	5 (12%)	56,56,56	2.26	23 (41%)
18	LHG	f	1842	14	36,36,48	0.81	1 (2%)	39,42,54	1.25	3 (7%)
17	BCR	a	524	-	41,41,41	0.78	0	56,56,56	1.93	18 (32%)
14	CLA	F	1301	23	45,53,73	1.73	9 (20%)	52,89,113	1.60	6 (11%)
17	BCR	L	4219	-	41,41,41	1.09	5 (12%)	56,56,56	2.26	23 (41%)
14	CLA	Z	513	13	45,53,73	1.78	9 (20%)	52,89,113	1.55	6 (11%)
21	SQD	L	5216	-	45,46,54	1.01	5 (11%)	54,57,65	1.69	11 (20%)
14	CLA	H	1226	2	55,63,73	1.71	10 (18%)	64,101,113	1.99	16 (25%)
14	CLA	v	517	-	45,53,73	1.74	8 (17%)	52,89,113	1.61	7 (13%)
14	CLA	H	1206	2	65,73,73	1.49	11 (16%)	76,113,113	1.61	10 (13%)
14	CLA	H	1211	2	55,63,73	1.53	8 (14%)	64,101,113	1.69	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	Y	508	13	45,53,73	1.77	9 (20%)	52,89,113	1.92	8 (15%)
14	CLA	Z	507	-	45,53,73	1.72	7 (15%)	52,89,113	1.71	10 (19%)
14	CLA	e	1801	18	45,53,73	1.65	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	s	510	13	45,53,73	1.75	8 (17%)	52,89,113	1.64	7 (13%)
14	CLA	f	1206	2	65,73,73	1.49	11 (16%)	76,113,113	1.61	10 (13%)
18	LHG	G	5005	-	42,42,48	0.65	1 (2%)	45,48,54	1.21	4 (8%)
17	BCR	c	521	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
19	LMU	J	5105	-	22,22,36	1.21	1 (4%)	27,27,47	1.43	5 (18%)
14	CLA	a	508	13	45,53,73	1.78	9 (20%)	52,89,113	1.75	7 (13%)
14	CLA	f	1219	2	63,71,73	1.51	9 (14%)	73,110,113	1.44	10 (13%)
14	CLA	q	512	13	45,53,73	1.74	8 (17%)	52,89,113	1.48	5 (9%)
14	CLA	s	511	13	45,53,73	1.75	6 (13%)	52,89,113	1.71	9 (17%)
21	SQD	1	822	-	31,32,54	1.20	5 (16%)	40,43,65	2.05	13 (32%)
14	CLA	e	1139	23	65,73,73	1.47	10 (15%)	76,113,113	1.36	7 (9%)
14	CLA	2	508	13	45,53,73	1.77	9 (20%)	52,89,113	1.76	10 (19%)
14	CLA	A	1801	18	45,53,73	1.65	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	s	513	13	45,53,73	1.79	8 (17%)	52,89,113	1.59	6 (11%)
14	CLA	e	1108	1	54,62,73	1.57	7 (12%)	62,99,113	1.58	8 (12%)
18	LHG	A	5006	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	5 (11%)
14	CLA	e	1132	1	65,73,73	1.42	10 (15%)	76,113,113	1.55	11 (14%)
14	CLA	b	501	13	45,53,73	1.79	6 (13%)	52,89,113	1.63	7 (13%)
14	CLA	v	513	13	45,53,73	1.78	7 (15%)	52,89,113	1.59	6 (11%)
14	CLA	1	517	-	45,53,73	1.75	7 (15%)	52,89,113	1.59	7 (13%)
22	FMN	P	170	-	33,33,33	1.13	2 (6%)	48,50,50	1.24	6 (12%)
14	CLA	Y	511	13	45,53,73	1.76	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	v	504	-	45,53,73	1.75	7 (15%)	52,89,113	1.69	7 (13%)
14	CLA	f	1235	2	65,73,73	1.48	10 (15%)	76,113,113	1.52	8 (10%)
20	LMG	B	5002	-	53,53,55	0.85	3 (5%)	61,61,63	1.51	12 (19%)
14	CLA	a	511	13	45,53,73	1.75	6 (13%)	52,89,113	1.71	9 (17%)
14	CLA	e	1013	-	65,73,73	1.43	8 (12%)	76,113,113	1.88	13 (17%)
14	CLA	c	519	13	45,53,73	1.77	6 (13%)	52,89,113	1.62	7 (13%)
14	CLA	q	516	13	45,53,73	1.72	9 (20%)	52,89,113	1.64	9 (17%)
18	LHG	f	1855	-	40,40,48	0.69	1 (2%)	43,46,54	1.24	5 (11%)
14	CLA	5	509	13	65,73,73	1.44	7 (10%)	76,113,113	1.49	7 (9%)
14	CLA	t	513	13	45,53,73	1.77	6 (13%)	52,89,113	1.63	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	BCR	c	522	-	41,41,41	0.76	0	56,56,56	1.94	20 (35%)
14	CLA	H	1239	2	65,73,73	1.48	8 (12%)	76,113,113	1.73	14 (18%)
17	BCR	B	4005	-	41,41,41	0.76	0	56,56,56	1.72	12 (21%)
14	CLA	H	1207	2	65,73,73	1.45	9 (13%)	76,113,113	1.39	6 (7%)
14	CLA	3	501	13	45,53,73	1.76	7 (15%)	52,89,113	1.66	9 (17%)
18	LHG	I	5001	-	47,47,48	0.62	0	50,53,54	1.24	5 (10%)
17	BCR	v	524	-	41,41,41	0.78	0	56,56,56	1.84	15 (26%)
14	CLA	a	513	13	45,53,73	1.79	8 (17%)	52,89,113	1.60	6 (11%)
14	CLA	r	505	13	65,73,73	1.42	7 (10%)	76,113,113	1.46	8 (10%)
14	CLA	f	1232	23	55,63,73	1.54	8 (14%)	64,101,113	1.70	7 (10%)
14	CLA	a	504	-	45,53,73	1.75	7 (15%)	52,89,113	1.72	9 (17%)
17	BCR	A	4001	-	41,41,41	0.79	0	56,56,56	1.69	11 (19%)
17	BCR	Y	523	-	41,41,41	0.74	0	56,56,56	1.69	14 (25%)
18	LHG	L	5221	-	48,48,48	0.62	0	51,54,54	1.28	7 (13%)
17	BCR	q	522	-	41,41,41	0.74	0	56,56,56	1.91	20 (35%)
14	CLA	H	1210	2	65,73,73	1.44	9 (13%)	76,113,113	1.48	9 (11%)
14	CLA	f	1202	2	65,73,73	1.42	7 (10%)	76,113,113	1.58	8 (10%)
14	CLA	V	1501	10	60,68,73	1.57	10 (16%)	70,107,113	1.51	9 (12%)
21	SQD	f	1852	-	39,40,54	1.18	6 (15%)	48,51,65	1.84	12 (25%)
14	CLA	A	1126	1	65,73,73	1.39	8 (12%)	76,113,113	1.57	8 (10%)
14	CLA	l	1302	8	55,63,73	1.55	9 (16%)	64,101,113	1.56	9 (14%)
14	CLA	2	504	-	45,53,73	1.77	7 (15%)	52,89,113	1.63	8 (15%)
17	BCR	B	4010	-	41,41,41	0.91	1 (2%)	56,56,56	2.30	21 (37%)
14	CLA	B	1221	23	62,70,73	1.50	8 (12%)	72,109,113	1.69	11 (15%)
14	CLA	A	1140	1	65,73,73	1.45	9 (13%)	76,113,113	1.57	10 (13%)
14	CLA	G	1801	18	45,53,73	1.65	7 (15%)	52,89,113	1.74	6 (11%)
14	CLA	e	1128	1	65,73,73	1.58	11 (16%)	76,113,113	1.69	9 (11%)
14	CLA	t	510	13	45,53,73	1.73	6 (13%)	52,89,113	1.67	6 (11%)
14	CLA	e	1121	1	55,63,73	1.57	10 (18%)	64,101,113	1.65	12 (18%)
17	BCR	J	4012	-	41,41,41	0.72	0	56,56,56	1.75	12 (21%)
14	CLA	u	511	13	45,53,73	1.76	5 (11%)	52,89,113	1.72	8 (15%)
17	BCR	K	4104	-	41,41,41	0.78	0	56,56,56	1.88	16 (28%)
14	CLA	A	1123	23	65,73,73	1.42	8 (12%)	76,113,113	1.53	8 (10%)
14	CLA	f	1223	2	65,73,73	1.42	8 (12%)	76,113,113	1.64	7 (9%)
17	BCR	H	4009	-	41,41,41	0.78	0	56,56,56	1.90	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	v	519	13	45,53,73	1.79	9 (20%)	52,89,113	1.58	7 (13%)
18	LHG	k	5001	-	47,47,48	0.62	0	50,53,54	1.24	5 (10%)
20	LMG	J	5104	-	32,32,55	0.96	2 (6%)	40,40,63	1.26	4 (10%)
14	CLA	4	501	13	45,53,73	1.78	5 (11%)	52,89,113	1.63	7 (13%)
14	CLA	G	1125	1	65,73,73	1.42	10 (15%)	76,113,113	1.58	9 (11%)
14	CLA	v	503	13	45,53,73	1.75	6 (13%)	52,89,113	1.69	6 (11%)
14	CLA	u	507	-	45,53,73	1.74	6 (13%)	52,89,113	1.71	9 (17%)
14	CLA	v	507	-	45,53,73	1.76	7 (15%)	52,89,113	1.69	9 (17%)
18	LHG	G	5006	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	5 (11%)
14	CLA	G	1131	1	65,73,73	1.47	10 (15%)	76,113,113	1.42	9 (11%)
17	BCR	U	4104	-	41,41,41	0.78	0	56,56,56	1.88	16 (28%)
14	CLA	2	517	-	45,53,73	1.76	7 (15%)	52,89,113	1.65	7 (13%)
14	CLA	B	1206	2	65,73,73	1.49	11 (16%)	76,113,113	1.61	10 (13%)
14	CLA	d	512	13	45,53,73	1.76	7 (15%)	52,89,113	1.58	6 (11%)
17	BCR	5	524	-	41,41,41	0.71	0	56,56,56	1.74	12 (21%)
14	CLA	H	1214	2	65,73,73	1.49	9 (13%)	76,113,113	1.52	8 (10%)
18	LHG	V	5221	-	48,48,48	0.62	0	51,54,54	1.28	7 (13%)
19	LMU	f	1843	-	36,36,36	1.16	2 (5%)	47,47,47	1.06	3 (6%)
14	CLA	e	1140	1	65,73,73	1.45	9 (13%)	76,113,113	1.56	10 (13%)
14	CLA	3	508	13	45,53,73	1.79	9 (20%)	52,89,113	1.75	7 (13%)
14	CLA	4	509	13	45,53,73	1.77	7 (15%)	52,89,113	1.76	9 (17%)
14	CLA	H	1221	23	62,70,73	1.50	8 (12%)	72,109,113	1.70	11 (15%)
14	CLA	A	1116	1	60,68,73	1.51	8 (13%)	70,107,113	1.50	7 (10%)
14	CLA	r	509	13	65,73,73	1.45	7 (10%)	76,113,113	1.51	7 (9%)
16	SF4	e	3001	2,1	0,12,12	-	-	-		
14	CLA	4	505	13	45,53,73	1.75	9 (20%)	52,89,113	1.54	6 (11%)
14	CLA	f	1221	23	62,70,73	1.50	8 (12%)	72,109,113	1.69	11 (15%)
14	CLA	e	1115	1	60,68,73	1.50	9 (15%)	70,107,113	1.58	7 (10%)
14	CLA	V	1503	23	60,68,73	1.47	8 (13%)	70,107,113	1.56	7 (10%)
14	CLA	H	1213	2	61,69,73	1.46	7 (11%)	71,108,113	1.60	9 (12%)
17	BCR	Z	521	-	41,41,41	0.70	0	56,56,56	1.90	13 (23%)
22	FMN	X	170	-	33,33,33	1.12	2 (6%)	48,50,50	1.24	6 (12%)
14	CLA	Y	504	-	45,53,73	1.79	9 (20%)	52,89,113	1.79	10 (19%)
14	CLA	A	1102	1	55,63,73	1.56	9 (16%)	64,101,113	1.62	7 (10%)
14	CLA	V	1502	10	65,73,73	1.45	9 (13%)	76,113,113	1.53	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	A	1022	23	65,73,73	1.54	11 (16%)	76,113,113	1.55	11 (14%)
14	CLA	e	1107	1	65,73,73	1.53	10 (15%)	76,113,113	1.49	10 (13%)
14	CLA	B	1238	23	65,73,73	1.40	7 (10%)	76,113,113	1.63	10 (13%)
14	CLA	B	1228	2	55,63,73	1.52	7 (12%)	64,101,113	1.70	8 (12%)
14	CLA	G	1105	1	55,63,73	1.49	8 (14%)	64,101,113	1.67	8 (12%)
14	CLA	B	1225	2	65,73,73	1.44	10 (15%)	76,113,113	1.49	8 (10%)
14	CLA	Z	508	13	45,53,73	1.77	9 (20%)	52,89,113	1.77	10 (19%)
17	BCR	4	524	-	41,41,41	0.70	0	56,56,56	1.85	14 (25%)
19	LMU	A	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	2 (4%)
14	CLA	2	513	13	45,53,73	1.78	9 (20%)	52,89,113	1.55	6 (11%)
14	CLA	f	1239	2	65,73,73	1.48	8 (12%)	76,113,113	1.73	14 (18%)
17	BCR	l	4012	-	41,41,41	0.73	0	56,56,56	1.75	12 (21%)
14	CLA	u	513	13	45,53,73	1.79	8 (17%)	52,89,113	1.55	6 (11%)
14	CLA	q	502	13	45,53,73	1.76	8 (17%)	52,89,113	1.66	8 (15%)
21	SQD	5	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.95	11 (32%)
14	CLA	G	1132	1	65,73,73	1.42	10 (15%)	76,113,113	1.55	11 (14%)
14	CLA	G	1118	1	60,68,73	1.47	9 (15%)	70,107,113	1.56	8 (11%)
14	CLA	5	507	-	45,53,73	1.73	6 (13%)	52,89,113	1.71	9 (17%)
17	BCR	f	4005	-	41,41,41	0.77	0	56,56,56	1.72	12 (21%)
14	CLA	f	1240	18	65,73,73	1.47	6 (9%)	76,113,113	1.45	8 (10%)
17	BCR	B	4004	-	41,41,41	0.73	0	56,56,56	1.85	14 (25%)
17	BCR	1	523	-	41,41,41	0.75	0	56,56,56	1.69	13 (23%)
14	CLA	H	1227	2	60,68,73	1.54	10 (16%)	70,107,113	1.50	8 (11%)
17	BCR	v	522	-	41,41,41	0.71	0	56,56,56	1.89	19 (33%)
14	CLA	b	507	-	45,53,73	1.72	6 (13%)	52,89,113	1.72	8 (15%)
14	CLA	B	1210	2	65,73,73	1.43	9 (13%)	76,113,113	1.48	9 (11%)
14	CLA	L	1503	23	60,68,73	1.48	8 (13%)	70,107,113	1.56	7 (10%)
14	CLA	u	510	13	45,53,73	1.73	7 (15%)	52,89,113	1.63	7 (13%)
14	CLA	a	518	13	55,63,73	1.58	8 (14%)	64,101,113	1.48	7 (10%)
14	CLA	s	505	13	55,63,73	1.56	7 (12%)	64,101,113	1.50	7 (10%)
14	CLA	d	516	13	45,53,73	1.77	6 (13%)	52,89,113	1.60	7 (13%)
18	LHG	e	5002	-	42,42,48	0.76	1 (2%)	45,48,54	1.23	4 (8%)
14	CLA	u	517	-	45,53,73	1.80	8 (17%)	52,89,113	1.57	6 (11%)
14	CLA	6	516	13	45,53,73	1.77	6 (13%)	52,89,113	1.60	8 (15%)
19	LMU	e	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.39	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	G	1116	1	60,68,73	1.51	8 (13%)	70,107,113	1.51	7 (10%)
14	CLA	e	1104	1	65,73,73	1.44	9 (13%)	76,113,113	1.60	13 (17%)
14	CLA	A	1117	1	65,73,73	1.47	10 (15%)	76,113,113	1.58	10 (13%)
17	BCR	s	523	-	41,41,41	0.69	0	56,56,56	1.82	15 (26%)
21	SQD	v	822	-	25,26,54	1.31	4 (16%)	34,37,65	2.00	10 (29%)
14	CLA	1	518	13	45,53,73	1.76	6 (13%)	52,89,113	1.63	7 (13%)
17	BCR	l	4013	-	41,41,41	0.77	0	56,56,56	1.93	16 (28%)
21	SQD	Z	822	-	27,28,54	1.22	4 (14%)	36,39,65	1.86	10 (27%)
14	CLA	t	505	13	45,53,73	1.75	9 (20%)	52,89,113	1.54	6 (11%)
14	CLA	A	1013	-	65,73,73	1.43	8 (12%)	76,113,113	1.88	13 (17%)
14	CLA	H	1229	2	65,73,73	1.42	7 (10%)	76,113,113	1.59	9 (11%)
14	CLA	r	516	13	45,53,73	1.77	7 (15%)	52,89,113	1.65	8 (15%)
14	CLA	b	518	13	45,53,73	1.76	6 (13%)	52,89,113	1.61	6 (11%)
15	PQN	H	2002	-	34,34,34	2.84	11 (32%)	42,45,45	2.30	6 (14%)
14	CLA	s	501	13	45,53,73	1.76	7 (15%)	52,89,113	1.67	9 (17%)
17	BCR	f	4017	-	41,41,41	0.97	3 (7%)	56,56,56	1.82	12 (21%)
14	CLA	c	506	13	45,53,73	1.73	7 (15%)	52,89,113	1.62	7 (13%)
14	CLA	6	503	13	45,53,73	1.76	6 (13%)	52,89,113	1.69	6 (11%)
14	CLA	v	511	13	45,53,73	1.78	5 (11%)	52,89,113	1.70	7 (13%)
14	CLA	6	512	13	45,53,73	1.77	6 (13%)	52,89,113	1.59	6 (11%)
17	BCR	f	4004	-	41,41,41	0.74	0	56,56,56	1.85	14 (25%)
14	CLA	1	511	13	45,53,73	1.76	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	Y	507	-	45,53,73	1.74	7 (15%)	52,89,113	1.70	9 (17%)
17	BCR	I	4018	-	41,41,41	0.93	2 (4%)	56,56,56	1.93	17 (30%)
14	CLA	Z	517	-	45,53,73	1.75	7 (15%)	52,89,113	1.65	7 (13%)
14	CLA	B	1235	2	65,73,73	1.47	10 (15%)	76,113,113	1.51	8 (10%)
17	BCR	a	523	-	41,41,41	0.69	0	56,56,56	1.82	15 (26%)
14	CLA	f	1210	2	65,73,73	1.43	8 (12%)	76,113,113	1.48	9 (11%)
14	CLA	q	503	13	45,53,73	1.76	8 (17%)	52,89,113	1.66	7 (13%)
14	CLA	e	1101	1	65,73,73	1.50	9 (13%)	76,113,113	1.61	13 (17%)
14	CLA	3	518	13	55,63,73	1.58	8 (14%)	64,101,113	1.49	7 (10%)
17	BCR	A	4007	-	41,41,41	0.87	0	56,56,56	2.10	20 (35%)
14	CLA	b	511	13	45,53,73	1.79	7 (15%)	52,89,113	1.68	9 (17%)
14	CLA	f	1216	23	60,68,73	1.60	10 (16%)	70,107,113	1.55	11 (15%)
14	CLA	1	513	13	45,53,73	1.77	7 (15%)	52,89,113	1.62	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	BCR	5	522	-	41,41,41	0.76	0	56,56,56	1.94	20 (35%)
14	CLA	s	517	-	45,53,73	1.79	8 (17%)	52,89,113	1.59	6 (11%)
14	CLA	e	1125	1	65,73,73	1.42	10 (15%)	76,113,113	1.59	9 (11%)
14	CLA	A	1114	23	45,53,73	1.80	8 (17%)	52,89,113	1.69	9 (17%)
14	CLA	H	1240	18	65,73,73	1.47	6 (9%)	76,113,113	1.46	8 (10%)
14	CLA	H	1225	2	65,73,73	1.45	10 (15%)	76,113,113	1.49	9 (11%)
14	CLA	3	513	13	45,53,73	1.78	8 (17%)	52,89,113	1.60	6 (11%)
14	CLA	A	1139	23	65,73,73	1.47	10 (15%)	76,113,113	1.36	7 (9%)
14	CLA	A	1109	1	65,73,73	1.41	9 (13%)	76,113,113	1.60	8 (10%)
18	LHG	e	5001	-	48,48,48	0.80	1 (2%)	51,54,54	1.30	7 (13%)
14	CLA	e	1118	1	60,68,73	1.47	10 (16%)	70,107,113	1.56	8 (11%)
14	CLA	3	511	13	45,53,73	1.75	6 (13%)	52,89,113	1.71	9 (17%)
18	LHG	e	5003	14	39,39,48	0.86	1 (2%)	42,45,54	1.38	6 (14%)
14	CLA	A	1134	1	56,64,73	1.56	8 (14%)	65,102,113	1.64	11 (16%)
14	CLA	B	1212	2	51,59,73	1.60	7 (13%)	59,96,113	1.67	6 (10%)
14	CLA	Y	506	13	45,53,73	1.76	7 (15%)	52,89,113	1.64	6 (11%)
14	CLA	G	1115	1	60,68,73	1.50	9 (15%)	70,107,113	1.59	7 (10%)
14	CLA	H	1234	2	65,73,73	1.44	9 (13%)	76,113,113	1.65	10 (13%)
19	LMU	A	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.39	4 (14%)
14	CLA	f	1211	2	55,63,73	1.53	8 (14%)	64,101,113	1.69	8 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	512	13	1/1/11/20	5/13/91/115	-
21	SQD	r	822	-	-	7/22/42/69	0/1/1/1
14	CLA	d	509	13	1/1/11/20	4/13/91/115	-
14	CLA	G	1117	1	1/1/15/20	12/37/115/115	-
14	CLA	t	512	13	1/1/11/20	3/13/91/115	-
17	BCR	4	521	-	-	10/29/63/63	0/2/2/2
14	CLA	2	503	13	1/1/15/20	9/37/115/115	-
14	CLA	e	1102	1	1/1/13/20	7/25/103/115	-
17	BCR	H	4014	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	u	518	13	1/1/11/20	3/13/91/115	-
14	CLA	B	1211	2	1/1/13/20	8/25/103/115	-
18	LHG	H	1842	14	-	19/41/41/53	-
14	CLA	G	1022	23	1/1/15/20	9/37/115/115	-
16	SF4	A	3001	2,1	-	-	0/6/5/5
14	CLA	e	1113	1	1/1/11/20	6/13/91/115	-
14	CLA	3	512	13	1/1/11/20	2/13/91/115	-
14	CLA	f	1229	2	1/1/15/20	12/37/115/115	-
17	BCR	d	522	-	-	5/29/63/63	0/2/2/2
18	LHG	A	5004	-	-	18/39/39/53	-
14	CLA	3	502	13	1/1/11/20	1/13/91/115	-
14	CLA	H	1218	2	1/1/14/20	7/31/109/115	-
14	CLA	a	501	13	1/1/11/20	4/13/91/115	-
14	CLA	A	1128	1	1/1/15/20	10/37/115/115	-
14	CLA	A	1111	1	1/1/15/20	18/37/115/115	-
14	CLA	6	502	13	1/1/11/20	1/13/91/115	-
14	CLA	e	1117	1	1/1/15/20	12/37/115/115	-
17	BCR	a	522	-	-	5/29/63/63	0/2/2/2
14	CLA	f	1204	2	1/1/15/20	12/37/115/115	-
14	CLA	e	1124	23	1/1/14/20	11/31/109/115	-
14	CLA	B	1214	2	1/1/15/20	12/37/115/115	-
18	LHG	A	5003	14	-	17/44/44/53	-
14	CLA	s	512	13	1/1/11/20	2/13/91/115	-
14	CLA	4	503	13	1/1/11/20	2/13/91/115	-
14	CLA	G	1114	23	1/1/11/20	3/13/91/115	-
14	CLA	H	1235	2	1/1/15/20	7/37/115/115	-
14	CLA	Z	519	13	1/1/11/20	5/13/91/115	-
18	LHG	V	5218	-	-	19/41/41/53	-
21	SQD	c	822	-	-	3/19/39/69	0/1/1/1
17	BCR	2	524	-	-	3/29/63/63	0/2/2/2
14	CLA	c	513	13	1/1/11/20	5/13/91/115	-
14	CLA	q	508	13	1/1/11/20	5/13/91/115	-
14	CLA	r	502	13	1/1/11/20	1/13/91/115	-
14	CLA	c	507	-	1/1/11/20	7/13/91/115	-
14	CLA	5	519	13	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	e	1134	1	1/1/13/20	9/27/105/115	-
14	CLA	F	1302	6	1/1/11/20	7/13/91/115	-
14	CLA	B	1204	2	1/1/15/20	12/37/115/115	-
14	CLA	A	1115	1	1/1/14/20	11/31/109/115	-
17	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
14	CLA	B	1239	2	1/1/15/20	14/37/115/115	-
14	CLA	3	510	13	1/1/11/20	6/13/91/115	-
14	CLA	e	1138	1	1/1/15/20	12/37/115/115	-
14	CLA	H	1201	2	1/1/14/20	8/31/109/115	-
14	CLA	H	1224	2	1/1/14/20	7/31/109/115	-
14	CLA	H	1212	2	1/1/12/20	8/21/99/115	-
17	BCR	d	524	-	-	5/29/63/63	0/2/2/2
14	CLA	f	1201	2	1/1/14/20	8/31/109/115	-
14	CLA	u	503	13	1/1/11/20	7/13/91/115	-
18	LHG	e	5005	-	-	28/47/47/53	-
14	CLA	B	1240	18	1/1/15/20	13/37/115/115	-
14	CLA	B	1213	2	1/1/14/20	11/33/111/115	-
14	CLA	B	1205	2	1/1/15/20	8/37/115/115	-
14	CLA	f	1209	2	1/1/12/20	9/23/101/115	-
14	CLA	f	1021	2	1/1/15/20	9/37/115/115	-
14	CLA	t	517	-	1/1/11/20	5/13/91/115	-
14	CLA	G	1013	-	1/1/15/20	14/37/115/115	-
14	CLA	a	506	13	1/1/11/20	8/13/91/115	-
14	CLA	f	1236	2	1/1/12/20	3/19/97/115	-
16	SF4	G	3001	2,1	-	-	0/6/5/5
14	CLA	G	1120	1	1/1/12/20	11/19/97/115	-
21	SQD	4	822	-	-	10/19/39/69	0/1/1/1
14	CLA	u	504	-	1/1/11/20	3/13/91/115	-
17	BCR	e	4008	-	-	7/29/63/63	0/2/2/2
14	CLA	d	501	13	1/1/11/20	7/13/91/115	-
14	CLA	v	508	13	1/1/11/20	4/13/91/115	-
14	CLA	Z	516	13	-	6/13/91/115	-
14	CLA	H	1230	2	1/1/14/20	10/31/109/115	-
14	CLA	G	1128	1	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	d	511	13	1/1/11/20	6/13/91/115	-
14	CLA	5	517	-	1/1/11/20	10/13/91/115	-
14	CLA	Y	510	13	1/1/11/20	4/13/91/115	-
21	SQD	q	822	-	-	10/27/47/69	0/1/1/1
14	CLA	a	507	-	1/1/11/20	5/13/91/115	-
18	LHG	n	5221	-	-	31/53/53/53	-
14	CLA	B	1202	2	1/1/15/20	12/37/115/115	-
14	CLA	2	510	13	1/1/11/20	7/13/91/115	-
19	LMU	l	5105	-	-	9/13/33/61	0/1/1/2
14	CLA	5	518	13	1/1/11/20	3/13/91/115	-
14	CLA	Z	503	13	1/1/15/20	9/37/115/115	-
14	CLA	u	508	13	1/1/11/20	4/13/91/115	-
14	CLA	s	516	13	1/1/11/20	7/13/91/115	-
14	CLA	f	1238	23	1/1/15/20	4/37/115/115	-
14	CLA	1	510	13	1/1/11/20	4/13/91/115	-
18	LHG	G	5008	-	-	18/39/39/53	-
14	CLA	G	1134	1	1/1/13/20	9/27/105/115	-
14	CLA	b	505	13	1/1/11/20	3/13/91/115	-
14	CLA	5	503	13	1/1/11/20	7/13/91/115	-
14	CLA	Y	503	13	1/1/11/20	7/13/91/115	-
14	CLA	f	1205	2	1/1/15/20	8/37/115/115	-
19	LMU	G	1849	-	-	6/14/34/61	0/1/1/2
14	CLA	a	512	13	1/1/11/20	2/13/91/115	-
14	CLA	L	1501	10	1/1/14/20	9/31/109/115	-
14	CLA	A	1104	1	1/1/15/20	10/37/115/115	-
14	CLA	1	503	13	1/1/11/20	7/13/91/115	-
14	CLA	q	510	13	1/1/11/20	4/13/91/115	-
17	BCR	H	4006	-	-	4/29/63/63	0/2/2/2
14	CLA	e	1103	1	1/1/15/20	21/37/115/115	-
14	CLA	L	1502	10	1/1/15/20	8/37/115/115	-
14	CLA	H	1204	2	1/1/15/20	12/37/115/115	-
14	CLA	A	1122	1	1/1/14/20	12/31/109/115	-
16	SF4	N	3003	3	-	-	0/6/5/5
14	CLA	A	1135	1	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	f	1230	2	1/1/14/20	10/31/109/115	-
14	CLA	r	508	13	1/1/11/20	2/13/91/115	-
17	BCR	Z	524	-	-	3/29/63/63	0/2/2/2
16	SF4	g	3003	3	-	-	0/6/5/5
14	CLA	2	511	13	1/1/11/20	4/13/91/115	-
17	BCR	n	4022	-	-	3/29/63/63	0/2/2/2
14	CLA	c	518	13	1/1/11/20	3/13/91/115	-
14	CLA	e	1120	1	1/1/12/20	11/19/97/115	-
14	CLA	t	519	13	1/1/11/20	8/13/91/115	-
17	BCR	4	522	-	-	4/29/63/63	0/2/2/2
14	CLA	m	1103	9	1/1/11/20	8/17/95/115	-
14	CLA	j	1301	23	1/1/11/20	2/13/91/115	-
18	LHG	G	5004	-	-	18/39/39/53	-
17	BCR	R	4016	-	-	2/29/63/63	0/2/2/2
14	CLA	A	1137	1	1/1/14/20	18/31/109/115	-
14	CLA	3	503	13	1/1/11/20	7/13/91/115	-
14	CLA	r	501	13	1/1/14/20	11/31/109/115	-
17	BCR	l	4015	-	-	5/29/63/63	0/2/2/2
18	LHG	e	5007	-	-	23/51/51/53	-
14	CLA	f	1215	2	1/1/15/20	19/37/115/115	-
14	CLA	A	1118	1	1/1/14/20	8/31/109/115	-
14	CLA	3	509	13	1/1/11/20	2/13/91/115	-
17	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
17	BCR	q	521	-	-	7/29/63/63	0/2/2/2
14	CLA	B	1021	2	1/1/15/20	9/37/115/115	-
14	CLA	H	1012	23	1/1/15/20	15/37/115/115	-
14	CLA	u	516	13	1/1/11/20	5/13/91/115	-
14	CLA	6	508	13	1/1/11/20	4/13/91/115	-
14	CLA	t	502	13	1/1/11/20	3/13/91/115	-
14	CLA	U	1401	-	1/1/13/20	8/25/103/115	-
14	CLA	6	506	13	1/1/11/20	6/13/91/115	-
14	CLA	A	1133	1	1/1/15/20	15/37/115/115	-
14	CLA	v	502	13	1/1/11/20	1/13/91/115	-
17	BCR	J	4015	-	-	5/29/63/63	0/2/2/2
14	CLA	B	1216	23	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	s	509	13	1/1/11/20	2/13/91/115	-
14	CLA	e	1135	1	1/1/13/20	10/25/103/115	-
14	CLA	Z	502	13	1/1/11/20	1/13/91/115	-
14	CLA	q	517	-	1/1/11/20	7/13/91/115	-
14	CLA	r	513	13	1/1/11/20	2/13/91/115	-
17	BCR	1	522	-	-	6/29/63/63	0/2/2/2
14	CLA	Z	511	13	1/1/11/20	4/13/91/115	-
17	BCR	H	4017	-	-	2/29/63/63	0/2/2/2
14	CLA	r	504	-	1/1/11/20	7/13/91/115	-
17	BCR	n	4019	-	-	6/29/63/63	0/2/2/2
14	CLA	A	1132	1	1/1/15/20	16/37/115/115	-
14	CLA	v	509	13	1/1/11/20	4/13/91/115	-
14	CLA	B	1223	2	1/1/15/20	9/37/115/115	-
14	CLA	Y	512	13	1/1/11/20	5/13/91/115	-
17	BCR	t	521	-	-	10/29/63/63	0/2/2/2
17	BCR	W	4021	-	-	6/29/63/63	0/2/2/2
14	CLA	G	1140	1	1/1/15/20	12/37/115/115	-
14	CLA	e	1116	1	1/1/14/20	9/31/109/115	-
14	CLA	q	519	13	1/1/11/20	6/13/91/115	-
14	CLA	Z	504	-	1/1/11/20	7/13/91/115	-
14	CLA	H	1220	2	1/1/13/20	9/25/103/115	-
14	CLA	e	1129	1	1/1/12/20	8/23/101/115	-
17	BCR	L	4020	-	-	4/29/63/63	0/2/2/2
14	CLA	5	513	13	1/1/11/20	5/13/91/115	-
14	CLA	T	1303	8	1/1/11/20	4/13/91/115	-
14	CLA	c	503	13	1/1/11/20	7/13/91/115	-
14	CLA	s	502	13	1/1/11/20	1/13/91/115	-
14	CLA	5	504	-	1/1/11/20	3/13/91/115	-
14	CLA	5	508	13	1/1/11/20	4/13/91/115	-
14	CLA	G	1122	1	1/1/14/20	12/31/109/115	-
14	CLA	f	1231	23	1/1/15/20	8/37/115/115	-
16	SF4	g	3002	3	-	-	0/6/5/5
14	CLA	t	518	13	1/1/11/20	4/13/91/115	-
14	CLA	H	1202	2	1/1/15/20	12/37/115/115	-
14	CLA	2	509	13	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	G	4007	-	-	0/29/63/63	0/2/2/2
21	SQD	H	1852	-	-	18/35/55/69	0/1/1/1
14	CLA	b	504	-	1/1/11/20	4/13/91/115	-
14	CLA	t	501	13	1/1/11/20	6/13/91/115	-
17	BCR	V	4020	-	-	4/29/63/63	0/2/2/2
14	CLA	B	1201	2	1/1/14/20	8/31/109/115	-
17	BCR	s	521	-	-	7/29/63/63	0/2/2/2
17	BCR	M	4021	-	-	6/29/63/63	0/2/2/2
17	BCR	G	4002	-	-	0/29/63/63	0/2/2/2
14	CLA	v	510	13	1/1/11/20	8/13/91/115	-
21	SQD	3	822	-	-	9/23/43/69	0/1/1/1
14	CLA	Z	510	13	1/1/11/20	7/13/91/115	-
14	CLA	6	505	13	1/1/15/20	15/37/115/115	-
17	BCR	q	523	-	-	6/29/63/63	0/2/2/2
14	CLA	3	516	13	1/1/11/20	7/13/91/115	-
14	CLA	r	519	13	1/1/11/20	5/13/91/115	-
17	BCR	H	4010	-	-	7/29/63/63	0/2/2/2
14	CLA	e	1130	1	1/1/13/20	7/27/105/115	-
14	CLA	G	1133	1	1/1/15/20	15/37/115/115	-
14	CLA	B	1236	2	1/1/12/20	3/19/97/115	-
14	CLA	2	502	13	1/1/11/20	1/13/91/115	-
14	CLA	e	1127	1	1/1/15/20	12/37/115/115	-
14	CLA	1	501	13	1/1/11/20	9/13/91/115	-
14	CLA	s	506	13	1/1/11/20	8/13/91/115	-
21	SQD	n	5216	-	-	17/41/61/69	0/1/1/1
16	SF4	N	3002	3	-	-	0/6/5/5
14	CLA	A	1124	23	1/1/14/20	11/31/109/115	-
14	CLA	a	510	13	1/1/11/20	6/13/91/115	-
14	CLA	u	519	13	1/1/11/20	6/13/91/115	-
14	CLA	B	1234	2	1/1/15/20	15/37/115/115	-
14	CLA	R	1301	23	1/1/11/20	2/13/91/115	-
14	CLA	b	517	-	1/1/11/20	5/13/91/115	-
14	CLA	t	511	13	1/1/11/20	3/13/91/115	-
17	BCR	G	4001	-	-	8/29/63/63	0/2/2/2
14	CLA	B	1227	2	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	e	4002	-	-	0/29/63/63	0/2/2/2
17	BCR	t	523	-	-	5/29/63/63	0/2/2/2
21	SQD	d	822	-	-	7/19/39/69	0/1/1/1
21	SQD	s	822	-	-	9/23/43/69	0/1/1/1
14	CLA	e	1022	23	1/1/15/20	9/37/115/115	-
14	CLA	d	513	13	1/1/11/20	3/13/91/115	-
17	BCR	2	521	-	-	4/29/63/63	0/2/2/2
14	CLA	4	511	13	1/1/11/20	3/13/91/115	-
14	CLA	e	1123	23	1/1/15/20	11/37/115/115	-
14	CLA	r	512	13	1/1/11/20	4/13/91/115	-
14	CLA	Y	516	13	1/1/11/20	12/13/91/115	-
14	CLA	d	507	-	1/1/11/20	5/13/91/115	-
14	CLA	A	1107	1	1/1/15/20	14/37/115/115	-
14	CLA	G	1104	1	1/1/15/20	10/37/115/115	-
14	CLA	2	505	13	1/1/15/20	14/37/115/115	-
14	CLA	G	1138	1	1/1/15/20	12/37/115/115	-
14	CLA	5	506	13	1/1/11/20	6/13/91/115	-
14	CLA	e	1122	1	1/1/14/20	12/31/109/115	-
14	CLA	u	502	13	1/1/11/20	5/13/91/115	-
14	CLA	f	1222	23	1/1/12/20	2/19/97/115	-
14	CLA	A	1237	23	1/1/15/20	22/37/115/115	-
14	CLA	A	1106	1	1/1/15/20	21/37/115/115	-
14	CLA	G	1129	1	1/1/12/20	8/23/101/115	-
14	CLA	4	513	13	1/1/11/20	5/13/91/115	-
14	CLA	4	507	-	1/1/11/20	6/13/91/115	-
14	CLA	4	504	-	1/1/11/20	4/13/91/115	-
14	CLA	b	506	13	1/1/11/20	4/13/91/115	-
14	CLA	n	1503	23	1/1/14/20	10/31/109/115	-
14	CLA	f	1213	2	1/1/14/20	11/33/111/115	-
14	CLA	c	516	13	1/1/11/20	5/13/91/115	-
14	CLA	q	518	13	1/1/11/20	6/13/91/115	-
14	CLA	U	1105	9	1/1/11/20	8/13/91/115	-
16	SF4	C	3002	3	-	-	0/6/5/5
14	CLA	6	504	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	A	5008	-	-	18/39/39/53	-
14	CLA	n	1502	10	1/1/15/20	8/37/115/115	-
14	CLA	b	513	13	1/1/11/20	5/13/91/115	-
14	CLA	f	1220	2	1/1/13/20	9/25/103/115	-
14	CLA	r	517	-	-	7/13/91/115	-
14	CLA	2	516	13	-	6/13/91/115	-
17	BCR	e	4007	-	-	0/29/63/63	0/2/2/2
14	CLA	G	1137	1	1/1/14/20	18/31/109/115	-
14	CLA	q	513	13	1/1/11/20	4/13/91/115	-
14	CLA	A	1101	1	1/1/15/20	18/37/115/115	-
14	CLA	J	1303	8	1/1/11/20	4/13/91/115	-
14	CLA	f	1208	2	1/1/15/20	15/37/115/115	-
14	CLA	Y	517	-	1/1/11/20	7/13/91/115	-
14	CLA	1	516	13	1/1/11/20	12/13/91/115	-
14	CLA	q	504	-	1/1/11/20	5/13/91/115	-
17	BCR	G	4008	-	-	7/29/63/63	0/2/2/2
17	BCR	b	524	-	-	4/29/63/63	0/2/2/2
14	CLA	v	501	13	1/1/11/20	7/13/91/115	-
14	CLA	c	504	-	1/1/11/20	3/13/91/115	-
14	CLA	A	1136	1	1/1/15/20	10/37/115/115	-
21	SQD	b	822	-	-	10/19/39/69	0/1/1/1
17	BCR	e	4003	-	-	0/29/63/63	0/2/2/2
14	CLA	d	518	13	1/1/11/20	7/13/91/115	-
14	CLA	c	508	13	1/1/11/20	4/13/91/115	-
14	CLA	B	1230	2	1/1/14/20	10/31/109/115	-
17	BCR	S	4018	-	-	0/29/63/63	0/2/2/2
14	CLA	T	1302	8	1/1/13/20	12/25/103/115	-
18	LHG	G	5001	-	-	23/53/53/53	-
18	LHG	A	5009	-	-	28/46/46/53	-
14	CLA	t	509	13	1/1/11/20	6/13/91/115	-
14	CLA	H	1219	2	1/1/14/20	18/35/113/115	-
18	LHG	G	5003	14	-	17/44/44/53	-
14	CLA	u	501	13	1/1/11/20	6/13/91/115	-
14	CLA	6	510	13	1/1/11/20	8/13/91/115	-
14	CLA	r	518	13	1/1/13/20	14/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	e	1126	1	1/1/15/20	18/37/115/115	-
17	BCR	5	521	-	-	7/29/63/63	0/2/2/2
14	CLA	f	1227	2	1/1/14/20	11/31/109/115	-
14	CLA	e	1133	1	1/1/15/20	15/37/115/115	-
17	BCR	H	4004	-	-	8/29/63/63	0/2/2/2
14	CLA	A	1129	1	1/1/12/20	8/23/101/115	-
14	CLA	B	1215	2	1/1/15/20	19/37/115/115	-
14	CLA	A	1108	1	1/1/12/20	14/24/102/115	-
14	CLA	Z	509	13	1/1/15/20	3/37/115/115	-
17	BCR	T	4012	-	-	9/29/63/63	0/2/2/2
14	CLA	Y	513	13	1/1/11/20	4/13/91/115	-
17	BCR	L	4022	-	-	3/29/63/63	0/2/2/2
19	LMU	B	1843	-	-	12/21/61/61	0/2/2/2
14	CLA	A	1103	1	1/1/15/20	21/37/115/115	-
14	CLA	c	511	13	1/1/11/20	3/13/91/115	-
17	BCR	r	523	-	-	6/29/63/63	0/2/2/2
14	CLA	u	509	13	1/1/15/20	13/37/115/115	-
14	CLA	u	505	13	1/1/11/20	3/13/91/115	-
17	BCR	G	4011	-	-	13/29/63/63	0/2/2/2
17	BCR	3	521	-	-	7/29/63/63	0/2/2/2
17	BCR	r	522	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1228	2	1/1/13/20	6/25/103/115	-
14	CLA	q	506	13	1/1/11/20	5/13/91/115	-
17	BCR	6	521	-	-	5/29/63/63	0/2/2/2
14	CLA	A	1120	1	1/1/12/20	11/19/97/115	-
14	CLA	2	518	13	1/1/13/20	14/25/103/115	-
14	CLA	5	510	13	1/1/11/20	7/13/91/115	-
14	CLA	d	519	13	1/1/11/20	6/13/91/115	-
17	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
14	CLA	G	1101	1	1/1/15/20	18/37/115/115	-
17	BCR	T	4013	-	-	4/29/63/63	0/2/2/2
14	CLA	H	1208	2	1/1/15/20	15/37/115/115	-
14	CLA	2	501	13	1/1/14/20	11/31/109/115	-
21	SQD	6	822	-	-	7/19/39/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	510	13	1/1/11/20	5/13/91/115	-
17	BCR	6	523	-	-	4/29/63/63	0/2/2/2
17	BCR	r	521	-	-	4/29/63/63	0/2/2/2
14	CLA	6	517	-	1/1/11/20	10/13/91/115	-
17	BCR	f	4006	-	-	4/29/63/63	0/2/2/2
18	LHG	n	5220	-	-	28/45/45/53	-
14	CLA	G	1108	1	1/1/12/20	14/24/102/115	-
17	BCR	q	524	-	-	2/29/63/63	0/2/2/2
15	PQN	f	2002	-	-	6/23/43/43	0/2/2/2
17	BCR	d	521	-	-	5/29/63/63	0/2/2/2
14	CLA	H	1023	-	1/1/15/20	10/37/115/115	-
14	CLA	t	506	13	1/1/11/20	4/13/91/115	-
14	CLA	G	1119	23	1/1/15/20	13/37/115/115	-
17	BCR	t	524	-	-	4/29/63/63	0/2/2/2
14	CLA	f	1012	23	1/1/15/20	15/37/115/115	-
14	CLA	Y	502	13	1/1/11/20	2/13/91/115	-
17	BCR	V	4019	-	-	6/29/63/63	0/2/2/2
18	LHG	A	5007	-	-	23/51/51/53	-
14	CLA	H	1203	2	1/1/15/20	14/37/115/115	-
14	CLA	3	519	13	1/1/11/20	5/13/91/115	-
14	CLA	G	1124	23	1/1/14/20	11/31/109/115	-
17	BCR	V	4022	-	-	3/29/63/63	0/2/2/2
14	CLA	B	1226	2	1/1/13/20	7/25/103/115	-
14	CLA	f	1203	2	1/1/15/20	14/37/115/115	-
14	CLA	4	518	13	1/1/11/20	4/13/91/115	-
14	CLA	m	1401	-	1/1/13/20	8/25/103/115	-
14	CLA	B	1208	2	1/1/15/20	15/37/115/115	-
17	BCR	B	4009	-	-	1/29/63/63	0/2/2/2
14	CLA	Z	505	13	1/1/15/20	14/37/115/115	-
14	CLA	1	502	13	1/1/11/20	2/13/91/115	-
14	CLA	G	1112	1	1/1/12/20	2/19/97/115	-
14	CLA	v	516	13	1/1/11/20	9/13/91/115	-
14	CLA	H	1209	2	1/1/12/20	9/23/101/115	-
17	BCR	A	4011	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	A	5002	-	-	22/47/47/53	-
14	CLA	b	519	13	1/1/11/20	8/13/91/115	-
14	CLA	u	512	13	1/1/11/20	5/13/91/115	-
17	BCR	b	521	-	-	10/29/63/63	0/2/2/2
14	CLA	t	508	13	1/1/11/20	4/13/91/115	-
17	BCR	5	523	-	-	4/29/63/63	0/2/2/2
14	CLA	G	1237	23	1/1/15/20	23/37/115/115	-
14	CLA	G	1106	1	1/1/15/20	21/37/115/115	-
14	CLA	c	512	13	1/1/11/20	5/13/91/115	-
21	SQD	V	5216	-	-	17/41/61/69	0/1/1/1
14	CLA	d	508	13	1/1/11/20	4/13/91/115	-
14	CLA	2	512	13	1/1/11/20	4/13/91/115	-
14	CLA	a	516	13	1/1/11/20	7/13/91/115	-
14	CLA	6	518	13	1/1/11/20	7/13/91/115	-
14	CLA	q	511	13	1/1/11/20	2/13/91/115	-
17	BCR	b	523	-	-	5/29/63/63	0/2/2/2
14	CLA	f	1224	2	1/1/14/20	7/31/109/115	-
14	CLA	1	505	13	1/1/11/20	6/13/91/115	-
14	CLA	Z	501	13	1/1/14/20	11/31/109/115	-
17	BCR	A	4008	-	-	7/29/63/63	0/2/2/2
14	CLA	t	507	-	1/1/11/20	6/13/91/115	-
20	LMG	l	5104	-	-	13/27/47/70	0/1/1/1
14	CLA	e	1110	1	1/1/12/20	10/23/101/115	-
14	CLA	e	1112	1	1/1/12/20	2/19/97/115	-
18	LHG	G	5007	-	-	23/51/51/53	-
14	CLA	A	1011	1	1/1/15/20	10/37/115/115	-
17	BCR	4	523	-	-	5/29/63/63	0/2/2/2
14	CLA	d	503	13	1/1/11/20	6/13/91/115	-
14	CLA	B	1231	23	1/1/15/20	8/37/115/115	-
14	CLA	4	517	-	1/1/11/20	5/13/91/115	-
14	CLA	f	1226	2	1/1/13/20	7/25/103/115	-
17	BCR	3	523	-	-	4/29/63/63	0/2/2/2
14	CLA	a	503	13	1/1/11/20	7/13/91/115	-
14	CLA	B	1222	23	1/1/12/20	2/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	2	519	13	1/1/11/20	5/13/91/115	-
14	CLA	A	1130	1	1/1/13/20	7/27/105/115	-
14	CLA	A	1138	1	1/1/15/20	12/37/115/115	-
14	CLA	A	1125	1	1/1/15/20	12/37/115/115	-
18	LHG	n	5218	-	-	19/41/41/53	-
14	CLA	H	1232	23	1/1/13/20	6/25/103/115	-
19	LMU	H	1843	-	-	12/21/61/61	0/2/2/2
14	CLA	6	519	13	1/1/11/20	6/13/91/115	-
14	CLA	q	507	-	1/1/11/20	6/13/91/115	-
14	CLA	H	1223	2	1/1/15/20	9/37/115/115	-
14	CLA	r	511	13	1/1/11/20	4/13/91/115	-
18	LHG	G	5009	-	-	28/46/46/53	-
14	CLA	c	502	13	1/1/11/20	5/13/91/115	-
14	CLA	B	1220	2	1/1/13/20	9/25/103/115	-
17	BCR	e	4001	-	-	8/29/63/63	0/2/2/2
14	CLA	r	506	13	1/1/11/20	5/13/91/115	-
17	BCR	F	4016	-	-	2/29/63/63	0/2/2/2
14	CLA	e	1119	23	1/1/15/20	14/37/115/115	-
14	CLA	f	1023	-	1/1/15/20	10/37/115/115	-
14	CLA	Z	518	13	1/1/13/20	14/25/103/115	-
21	SQD	t	822	-	-	10/19/39/69	0/1/1/1
14	CLA	d	506	13	1/1/11/20	6/13/91/115	-
14	CLA	H	1215	2	1/1/15/20	19/37/115/115	-
14	CLA	e	1237	23	1/1/15/20	23/37/115/115	-
14	CLA	u	506	13	1/1/11/20	6/13/91/115	-
14	CLA	G	1103	1	1/1/15/20	21/37/115/115	-
14	CLA	Y	505	13	1/1/11/20	6/13/91/115	-
14	CLA	b	503	13	1/1/11/20	2/13/91/115	-
17	BCR	u	524	-	-	2/29/63/63	0/2/2/2
19	LMU	e	1848	-	-	7/21/61/61	0/2/2/2
17	BCR	r	524	-	-	3/29/63/63	0/2/2/2
14	CLA	b	509	13	1/1/11/20	6/13/91/115	-
14	CLA	B	1203	2	1/1/15/20	14/37/115/115	-
21	SQD	2	822	-	-	7/22/42/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	r	507	-	1/1/11/20	8/13/91/115	-
17	BCR	t	522	-	-	4/29/63/63	0/2/2/2
17	BCR	2	523	-	-	6/29/63/63	0/2/2/2
14	CLA	4	519	13	1/1/11/20	8/13/91/115	-
14	CLA	c	505	13	1/1/11/20	3/13/91/115	-
14	CLA	A	1121	1	1/1/13/20	8/25/103/115	-
14	CLA	Y	501	13	1/1/11/20	9/13/91/115	-
14	CLA	c	501	13	1/1/11/20	6/13/91/115	-
14	CLA	c	510	13	1/1/11/20	7/13/91/115	-
17	BCR	f	4009	-	-	1/29/63/63	0/2/2/2
18	LHG	e	5008	-	-	18/39/39/53	-
17	BCR	c	523	-	-	4/29/63/63	0/2/2/2
17	BCR	6	524	-	-	5/29/63/63	0/2/2/2
17	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
17	BCR	v	521	-	-	5/29/63/63	0/2/2/2
14	CLA	a	502	13	1/1/11/20	1/13/91/115	-
20	LMG	T	5104	-	-	13/27/47/70	0/1/1/1
14	CLA	B	1218	2	1/1/14/20	7/31/109/115	-
18	LHG	G	5002	-	-	22/47/47/53	-
14	CLA	v	512	13	1/1/11/20	7/13/91/115	-
14	CLA	6	501	13	1/1/11/20	7/13/91/115	-
15	PQN	A	2001	-	-	14/23/43/43	0/2/2/2
14	CLA	Z	512	13	1/1/11/20	4/13/91/115	-
14	CLA	G	1135	1	1/1/13/20	10/25/103/115	-
14	CLA	j	1302	6	1/1/11/20	7/13/91/115	-
17	BCR	j	4016	-	-	2/29/63/63	0/2/2/2
14	CLA	H	1231	23	1/1/15/20	8/37/115/115	-
14	CLA	d	504	-	1/1/11/20	4/13/91/115	-
17	BCR	v	523	-	-	4/29/63/63	0/2/2/2
14	CLA	B	1229	2	1/1/15/20	13/37/115/115	-
14	CLA	H	1222	23	1/1/12/20	2/19/97/115	-
17	BCR	Z	523	-	-	6/29/63/63	0/2/2/2
14	CLA	e	1105	1	1/1/13/20	7/25/103/115	-
16	SF4	C	3003	3	-	-	0/6/5/5
17	BCR	a	521	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	e	1106	1	1/1/15/20	21/37/115/115	-
14	CLA	1	509	13	1/1/11/20	3/13/91/115	-
14	CLA	5	516	13	1/1/11/20	5/13/91/115	-
14	CLA	5	501	13	1/1/11/20	6/13/91/115	-
14	CLA	f	1207	2	1/1/15/20	16/37/115/115	-
14	CLA	4	516	13	1/1/11/20	7/13/91/115	-
15	PQN	B	2002	-	-	6/23/43/43	0/2/2/2
14	CLA	4	508	13	1/1/11/20	4/13/91/115	-
14	CLA	1	506	13	1/1/11/20	5/13/91/115	-
14	CLA	B	1012	23	1/1/15/20	15/37/115/115	-
14	CLA	a	517	-	1/1/11/20	7/13/91/115	-
14	CLA	G	1123	23	1/1/15/20	11/37/115/115	-
14	CLA	m	1105	9	1/1/11/20	8/13/91/115	-
14	CLA	6	511	13	1/1/11/20	5/13/91/115	-
14	CLA	3	504	-	1/1/11/20	5/13/91/115	-
14	CLA	b	516	13	1/1/11/20	7/13/91/115	-
14	CLA	s	519	13	1/1/11/20	5/13/91/115	-
17	BCR	2	522	-	-	6/29/63/63	0/2/2/2
14	CLA	c	509	13	1/1/15/20	13/37/115/115	-
14	CLA	q	505	13	1/1/11/20	6/13/91/115	-
21	SQD	u	822	-	-	3/19/39/69	0/1/1/1
17	BCR	n	4219	-	-	2/29/63/63	0/2/2/2
14	CLA	A	1127	1	1/1/15/20	12/37/115/115	-
18	LHG	H	1855	-	-	24/45/45/53	-
14	CLA	G	1011	1	1/1/15/20	10/37/115/115	-
14	CLA	f	1218	2	1/1/14/20	7/31/109/115	-
14	CLA	e	1137	1	1/1/14/20	18/31/109/115	-
17	BCR	B	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	B	1219	2	1/1/14/20	18/35/113/115	-
14	CLA	l	1303	8	1/1/11/20	4/13/91/115	-
14	CLA	v	518	13	1/1/11/20	7/13/91/115	-
17	BCR	G	4003	-	-	0/29/63/63	0/2/2/2
18	LHG	B	1842	14	-	19/41/41/53	-
14	CLA	5	512	13	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	e	5009	-	-	28/46/46/53	-
14	CLA	3	507	-	1/1/11/20	5/13/91/115	-
14	CLA	G	1130	1	1/1/13/20	7/27/105/115	-
14	CLA	6	513	13	1/1/11/20	3/13/91/115	-
14	CLA	B	1209	2	1/1/12/20	9/23/101/115	-
17	BCR	u	522	-	-	5/29/63/63	0/2/2/2
14	CLA	J	1302	8	1/1/13/20	12/25/103/115	-
14	CLA	B	1217	2	1/1/14/20	12/31/109/115	-
14	CLA	3	517	-	1/1/11/20	7/13/91/115	-
14	CLA	6	507	-	1/1/11/20	5/13/91/115	-
14	CLA	B	1224	2	1/1/14/20	7/31/109/115	-
14	CLA	A	1119	23	1/1/15/20	14/37/115/115	-
18	LHG	A	5005	-	-	28/47/47/53	-
14	CLA	H	1216	23	1/1/14/20	11/31/109/115	-
15	PQN	G	2001	-	-	14/23/43/43	0/2/2/2
17	BCR	Y	524	-	-	2/29/63/63	0/2/2/2
14	CLA	G	1126	1	1/1/15/20	18/37/115/115	-
14	CLA	b	508	13	1/1/11/20	4/13/91/115	-
21	SQD	Y	822	-	-	10/27/47/69	0/1/1/1
14	CLA	H	1021	2	1/1/15/20	9/37/115/115	-
14	CLA	B	1232	23	1/1/13/20	6/25/103/115	-
14	CLA	K	1103	9	1/1/11/20	8/17/95/115	-
20	LMG	H	5002	-	-	24/48/68/70	0/1/1/1
21	SQD	a	822	-	-	9/23/43/69	0/1/1/1
14	CLA	4	512	13	1/1/11/20	3/13/91/115	-
14	CLA	A	1113	1	1/1/11/20	6/13/91/115	-
14	CLA	s	507	-	1/1/11/20	5/13/91/115	-
17	BCR	u	521	-	-	7/29/63/63	0/2/2/2
17	BCR	1	524	-	-	2/29/63/63	0/2/2/2
14	CLA	4	506	13	1/1/11/20	4/13/91/115	-
18	LHG	L	5218	-	-	19/41/41/53	-
14	CLA	v	505	13	1/1/15/20	15/37/115/115	-
17	BCR	d	523	-	-	4/29/63/63	0/2/2/2
14	CLA	A	1112	1	1/1/12/20	2/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	3	506	13	1/1/11/20	8/13/91/115	-
18	LHG	A	5001	-	-	23/53/53/53	-
14	CLA	d	517	-	1/1/11/20	10/13/91/115	-
14	CLA	G	1113	1	1/1/11/20	6/13/91/115	-
14	CLA	H	1238	23	1/1/15/20	4/37/115/115	-
17	BCR	u	523	-	-	4/29/63/63	0/2/2/2
17	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
17	BCR	f	4014	-	-	7/29/63/63	0/2/2/2
17	BCR	T	4015	-	-	5/29/63/63	0/2/2/2
14	CLA	G	1111	1	1/1/15/20	18/37/115/115	-
14	CLA	n	1501	10	1/1/14/20	9/31/109/115	-
14	CLA	s	518	13	1/1/13/20	9/25/103/115	-
14	CLA	R	1302	6	1/1/11/20	7/13/91/115	-
18	LHG	S	5001	-	-	25/52/52/53	-
14	CLA	A	1110	1	1/1/12/20	10/23/101/115	-
17	BCR	c	524	-	-	2/29/63/63	0/2/2/2
14	CLA	e	1109	1	1/1/15/20	14/37/115/115	-
14	CLA	q	509	13	1/1/11/20	3/13/91/115	-
17	BCR	3	524	-	-	5/29/63/63	0/2/2/2
14	CLA	f	1217	2	1/1/14/20	12/31/109/115	-
14	CLA	B	1023	-	1/1/15/20	10/37/115/115	-
14	CLA	c	517	-	1/1/11/20	10/13/91/115	-
14	CLA	r	510	13	1/1/11/20	7/13/91/115	-
14	CLA	f	1212	2	1/1/12/20	8/21/99/115	-
18	LHG	e	5004	-	-	18/39/39/53	-
14	CLA	5	502	13	1/1/11/20	5/13/91/115	-
14	CLA	t	503	13	1/1/11/20	2/13/91/115	-
14	CLA	Y	518	13	1/1/11/20	6/13/91/115	-
14	CLA	1	507	-	1/1/11/20	6/13/91/115	-
17	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
14	CLA	K	1105	9	1/1/11/20	8/13/91/115	-
14	CLA	e	1011	1	1/1/15/20	10/37/115/115	-
14	CLA	G	1107	1	1/1/15/20	14/37/115/115	-
14	CLA	G	1102	1	1/1/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1236	2	1/1/12/20	3/19/97/115	-
14	CLA	b	502	13	1/1/11/20	3/13/91/115	-
17	BCR	b	522	-	-	4/29/63/63	0/2/2/2
22	FMN	p	170	-	-	0/18/18/18	0/3/3/3
17	BCR	o	4021	-	-	6/29/63/63	0/2/2/2
14	CLA	1	504	-	1/1/11/20	5/13/91/115	-
14	CLA	K	1401	-	1/1/13/20	8/25/103/115	-
14	CLA	5	505	13	1/1/11/20	3/13/91/115	-
14	CLA	t	504	-	1/1/11/20	4/13/91/115	-
14	CLA	2	506	13	1/1/11/20	5/13/91/115	-
19	LMU	G	1848	-	-	7/21/61/61	0/2/2/2
17	BCR	Z	522	-	-	6/29/63/63	0/2/2/2
14	CLA	Y	509	13	1/1/11/20	3/13/91/115	-
17	BCR	s	522	-	-	5/29/63/63	0/2/2/2
14	CLA	a	509	13	1/1/11/20	2/13/91/115	-
14	CLA	s	503	13	1/1/11/20	7/13/91/115	-
14	CLA	b	512	13	1/1/11/20	3/13/91/115	-
14	CLA	e	1111	1	1/1/15/20	18/37/115/115	-
18	LHG	V	5220	-	-	28/45/45/53	-
14	CLA	f	1214	2	1/1/15/20	12/37/115/115	-
14	CLA	U	1103	9	1/1/11/20	8/17/95/115	-
14	CLA	G	1121	1	1/1/13/20	8/25/103/115	-
14	CLA	G	1136	1	1/1/15/20	10/37/115/115	-
18	LHG	L	5220	-	-	28/45/45/53	-
20	LMG	f	5002	-	-	24/48/68/70	0/1/1/1
14	CLA	r	503	13	1/1/15/20	9/37/115/115	-
14	CLA	G	1139	23	1/1/15/20	18/37/115/115	-
14	CLA	G	1110	1	1/1/12/20	10/23/101/115	-
14	CLA	6	509	13	1/1/11/20	4/13/91/115	-
14	CLA	3	505	13	1/1/13/20	11/25/103/115	-
14	CLA	Y	519	13	1/1/11/20	6/13/91/115	-
14	CLA	4	510	13	1/1/11/20	5/13/91/115	-
14	CLA	d	502	13	1/1/11/20	1/13/91/115	-
17	BCR	Y	522	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	508	13	1/1/11/20	5/13/91/115	-
14	CLA	A	1131	1	1/1/15/20	6/37/115/115	-
14	CLA	G	1109	1	1/1/15/20	14/37/115/115	-
14	CLA	H	1217	2	1/1/14/20	12/31/109/115	-
14	CLA	a	519	13	1/1/11/20	5/13/91/115	-
14	CLA	G	1127	1	1/1/15/20	12/37/115/115	-
14	CLA	f	1228	2	1/1/13/20	6/25/103/115	-
14	CLA	s	504	-	1/1/11/20	5/13/91/115	-
14	CLA	q	501	13	1/1/11/20	9/13/91/115	-
14	CLA	f	1225	2	1/1/15/20	7/37/115/115	-
14	CLA	1	519	13	1/1/11/20	6/13/91/115	-
14	CLA	2	507	-	1/1/11/20	8/13/91/115	-
17	BCR	k	4018	-	-	0/29/63/63	0/2/2/2
14	CLA	4	502	13	1/1/11/20	3/13/91/115	-
17	BCR	n	4020	-	-	4/29/63/63	0/2/2/2
14	CLA	H	1205	2	1/1/15/20	8/37/115/115	-
14	CLA	e	1131	1	1/1/15/20	6/37/115/115	-
17	BCR	f	4010	-	-	7/29/63/63	0/2/2/2
14	CLA	B	1207	2	1/1/15/20	16/37/115/115	-
17	BCR	Y	521	-	-	7/29/63/63	0/2/2/2
17	BCR	s	524	-	-	5/29/63/63	0/2/2/2
15	PQN	e	2001	-	-	14/23/43/43	0/2/2/2
18	LHG	e	5006	-	-	26/44/44/53	-
14	CLA	e	1114	23	1/1/11/20	3/13/91/115	-
14	CLA	t	516	13	1/1/11/20	7/13/91/115	-
17	BCR	3	522	-	-	5/29/63/63	0/2/2/2
17	BCR	6	522	-	-	5/29/63/63	0/2/2/2
14	CLA	d	505	13	1/1/15/20	15/37/115/115	-
17	BCR	m	4104	-	-	2/29/63/63	0/2/2/2
14	CLA	Z	506	13	1/1/11/20	5/13/91/115	-
14	CLA	5	511	13	1/1/11/20	3/13/91/115	-
17	BCR	B	4006	-	-	4/29/63/63	0/2/2/2
14	CLA	a	505	13	1/1/13/20	11/25/103/115	-
14	CLA	d	510	13	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	s	508	13	1/1/11/20	2/13/91/115	-
17	BCR	1	521	-	-	7/29/63/63	0/2/2/2
14	CLA	e	1136	1	1/1/15/20	10/37/115/115	-
14	CLA	f	1234	2	1/1/15/20	15/37/115/115	-
17	BCR	e	4011	-	-	13/29/63/63	0/2/2/2
14	CLA	A	1105	1	1/1/13/20	7/25/103/115	-
19	LMU	T	5105	-	-	9/13/33/61	0/1/1/2
21	SQD	B	1852	-	-	18/35/55/69	0/1/1/1
14	CLA	v	506	13	1/1/11/20	6/13/91/115	-
18	LHG	B	1855	-	-	24/45/45/53	-
17	BCR	V	4219	-	-	2/29/63/63	0/2/2/2
18	LHG	f	1842	14	-	19/41/41/53	-
17	BCR	a	524	-	-	5/29/63/63	0/2/2/2
14	CLA	F	1301	23	1/1/11/20	2/13/91/115	-
17	BCR	L	4219	-	-	2/29/63/63	0/2/2/2
14	CLA	Z	513	13	1/1/11/20	2/13/91/115	-
21	SQD	L	5216	-	-	17/41/61/69	0/1/1/1
14	CLA	H	1226	2	1/1/13/20	7/25/103/115	-
14	CLA	v	517	-	1/1/11/20	10/13/91/115	-
14	CLA	H	1206	2	1/1/15/20	15/37/115/115	-
14	CLA	H	1211	2	1/1/13/20	8/25/103/115	-
14	CLA	Y	508	13	1/1/11/20	5/13/91/115	-
14	CLA	Z	507	-	1/1/11/20	8/13/91/115	-
14	CLA	e	1801	18	1/1/11/20	7/13/91/115	-
14	CLA	s	510	13	1/1/11/20	6/13/91/115	-
14	CLA	f	1206	2	1/1/15/20	15/37/115/115	-
18	LHG	G	5005	-	-	28/47/47/53	-
17	BCR	c	521	-	-	7/29/63/63	0/2/2/2
19	LMU	J	5105	-	-	9/13/33/61	0/1/1/2
14	CLA	a	508	13	1/1/11/20	2/13/91/115	-
14	CLA	f	1219	2	1/1/14/20	18/35/113/115	-
14	CLA	q	512	13	1/1/11/20	5/13/91/115	-
14	CLA	s	511	13	1/1/11/20	2/13/91/115	-
21	SQD	1	822	-	-	10/27/47/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	e	1139	23	1/1/15/20	18/37/115/115	-
14	CLA	2	508	13	1/1/11/20	2/13/91/115	-
14	CLA	A	1801	18	1/1/11/20	7/13/91/115	-
14	CLA	s	513	13	1/1/11/20	3/13/91/115	-
14	CLA	e	1108	1	1/1/12/20	14/24/102/115	-
18	LHG	A	5006	-	-	26/44/44/53	-
14	CLA	e	1132	1	1/1/15/20	16/37/115/115	-
14	CLA	b	501	13	1/1/11/20	6/13/91/115	-
14	CLA	v	513	13	1/1/11/20	3/13/91/115	-
14	CLA	1	517	-	1/1/11/20	7/13/91/115	-
22	FMN	P	170	-	-	0/18/18/18	0/3/3/3
14	CLA	Y	511	13	1/1/11/20	2/13/91/115	-
14	CLA	v	504	-	1/1/11/20	4/13/91/115	-
14	CLA	f	1235	2	1/1/15/20	7/37/115/115	-
20	LMG	B	5002	-	-	24/48/68/70	0/1/1/1
14	CLA	a	511	13	1/1/11/20	2/13/91/115	-
14	CLA	e	1013	-	1/1/15/20	13/37/115/115	-
14	CLA	c	519	13	1/1/11/20	6/13/91/115	-
14	CLA	q	516	13	1/1/11/20	12/13/91/115	-
18	LHG	f	1855	-	-	24/45/45/53	-
14	CLA	5	509	13	1/1/15/20	13/37/115/115	-
14	CLA	t	513	13	1/1/11/20	5/13/91/115	-
17	BCR	c	522	-	-	5/29/63/63	0/2/2/2
14	CLA	H	1239	2	1/1/15/20	14/37/115/115	-
17	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1207	2	1/1/15/20	16/37/115/115	-
14	CLA	3	501	13	1/1/11/20	4/13/91/115	-
18	LHG	I	5001	-	-	25/52/52/53	-
17	BCR	v	524	-	-	5/29/63/63	0/2/2/2
14	CLA	a	513	13	1/1/11/20	3/13/91/115	-
14	CLA	r	505	13	1/1/15/20	14/37/115/115	-
14	CLA	f	1232	23	1/1/13/20	6/25/103/115	-
14	CLA	a	504	-	1/1/11/20	5/13/91/115	-
17	BCR	A	4001	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	Y	523	-	-	6/29/63/63	0/2/2/2
18	LHG	L	5221	-	-	31/53/53/53	-
17	BCR	q	522	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1210	2	1/1/15/20	20/37/115/115	-
14	CLA	f	1202	2	1/1/15/20	12/37/115/115	-
14	CLA	V	1501	10	1/1/14/20	9/31/109/115	-
21	SQD	f	1852	-	-	18/35/55/69	0/1/1/1
14	CLA	A	1126	1	1/1/15/20	18/37/115/115	-
14	CLA	l	1302	8	1/1/13/20	12/25/103/115	-
14	CLA	2	504	-	1/1/11/20	7/13/91/115	-
17	BCR	B	4010	-	-	7/29/63/63	0/2/2/2
14	CLA	B	1221	23	1/1/14/20	14/34/112/115	-
14	CLA	A	1140	1	1/1/15/20	12/37/115/115	-
14	CLA	G	1801	18	1/1/11/20	7/13/91/115	-
14	CLA	e	1128	1	1/1/15/20	10/37/115/115	-
14	CLA	t	510	13	1/1/11/20	5/13/91/115	-
14	CLA	e	1121	1	1/1/13/20	8/25/103/115	-
17	BCR	J	4012	-	-	9/29/63/63	0/2/2/2
14	CLA	u	511	13	1/1/11/20	3/13/91/115	-
17	BCR	K	4104	-	-	2/29/63/63	0/2/2/2
14	CLA	A	1123	23	1/1/15/20	11/37/115/115	-
14	CLA	f	1223	2	1/1/15/20	10/37/115/115	-
17	BCR	H	4009	-	-	1/29/63/63	0/2/2/2
14	CLA	v	519	13	1/1/11/20	6/13/91/115	-
18	LHG	k	5001	-	-	25/52/52/53	-
20	LMG	J	5104	-	-	13/27/47/70	0/1/1/1
14	CLA	4	501	13	1/1/11/20	6/13/91/115	-
14	CLA	G	1125	1	1/1/15/20	12/37/115/115	-
14	CLA	v	503	13	1/1/11/20	6/13/91/115	-
14	CLA	u	507	-	1/1/11/20	7/13/91/115	-
14	CLA	v	507	-	1/1/11/20	5/13/91/115	-
18	LHG	G	5006	-	-	26/44/44/53	-
14	CLA	G	1131	1	1/1/15/20	6/37/115/115	-
17	BCR	U	4104	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	2	517	-	-	7/13/91/115	-
14	CLA	B	1206	2	1/1/15/20	15/37/115/115	-
14	CLA	d	512	13	1/1/11/20	7/13/91/115	-
17	BCR	5	524	-	-	2/29/63/63	0/2/2/2
14	CLA	H	1214	2	1/1/15/20	12/37/115/115	-
18	LHG	V	5221	-	-	31/53/53/53	-
19	LMU	f	1843	-	-	12/21/61/61	0/2/2/2
14	CLA	e	1140	1	1/1/15/20	12/37/115/115	-
14	CLA	3	508	13	1/1/11/20	2/13/91/115	-
14	CLA	4	509	13	1/1/11/20	6/13/91/115	-
14	CLA	H	1221	23	1/1/14/20	14/34/112/115	-
14	CLA	A	1116	1	1/1/14/20	9/31/109/115	-
14	CLA	r	509	13	1/1/15/20	4/37/115/115	-
16	SF4	e	3001	2,1	-	-	0/6/5/5
14	CLA	4	505	13	1/1/11/20	3/13/91/115	-
14	CLA	f	1221	23	1/1/14/20	14/34/112/115	-
14	CLA	e	1115	1	1/1/14/20	10/31/109/115	-
14	CLA	V	1503	23	1/1/14/20	10/31/109/115	-
14	CLA	H	1213	2	1/1/14/20	11/33/111/115	-
17	BCR	Z	521	-	-	4/29/63/63	0/2/2/2
22	FMN	X	170	-	-	0/18/18/18	0/3/3/3
14	CLA	Y	504	-	1/1/11/20	5/13/91/115	-
14	CLA	A	1102	1	1/1/13/20	7/25/103/115	-
14	CLA	V	1502	10	1/1/15/20	8/37/115/115	-
14	CLA	A	1022	23	1/1/15/20	9/37/115/115	-
14	CLA	e	1107	1	1/1/15/20	14/37/115/115	-
14	CLA	B	1238	23	1/1/15/20	4/37/115/115	-
14	CLA	B	1228	2	1/1/13/20	6/25/103/115	-
14	CLA	G	1105	1	1/1/13/20	8/25/103/115	-
14	CLA	B	1225	2	1/1/15/20	7/37/115/115	-
14	CLA	Z	508	13	1/1/11/20	2/13/91/115	-
17	BCR	4	524	-	-	4/29/63/63	0/2/2/2
19	LMU	A	1848	-	-	7/21/61/61	0/2/2/2
14	CLA	2	513	13	1/1/11/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	f	1239	2	1/1/15/20	14/37/115/115	-
17	BCR	l	4012	-	-	9/29/63/63	0/2/2/2
14	CLA	u	513	13	1/1/11/20	5/13/91/115	-
14	CLA	q	502	13	1/1/11/20	2/13/91/115	-
21	SQD	5	822	-	-	3/19/39/69	0/1/1/1
14	CLA	G	1132	1	1/1/15/20	16/37/115/115	-
14	CLA	G	1118	1	1/1/14/20	8/31/109/115	-
14	CLA	5	507	-	1/1/11/20	7/13/91/115	-
17	BCR	f	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	f	1240	18	1/1/15/20	13/37/115/115	-
17	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
17	BCR	1	523	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1227	2	1/1/14/20	11/31/109/115	-
17	BCR	v	522	-	-	5/29/63/63	0/2/2/2
14	CLA	b	507	-	1/1/11/20	6/13/91/115	-
14	CLA	B	1210	2	1/1/15/20	20/37/115/115	-
14	CLA	L	1503	23	1/1/14/20	10/31/109/115	-
14	CLA	u	510	13	1/1/11/20	7/13/91/115	-
14	CLA	a	518	13	1/1/13/20	9/25/103/115	-
14	CLA	s	505	13	1/1/13/20	11/25/103/115	-
14	CLA	d	516	13	1/1/11/20	9/13/91/115	-
18	LHG	e	5002	-	-	22/47/47/53	-
14	CLA	u	517	-	1/1/11/20	10/13/91/115	-
14	CLA	6	516	13	1/1/11/20	9/13/91/115	-
19	LMU	e	1849	-	-	6/14/34/61	0/1/1/2
14	CLA	G	1116	1	1/1/14/20	9/31/109/115	-
14	CLA	e	1104	1	1/1/15/20	10/37/115/115	-
14	CLA	A	1117	1	1/1/15/20	12/37/115/115	-
17	BCR	s	523	-	-	4/29/63/63	0/2/2/2
21	SQD	v	822	-	-	7/19/39/69	0/1/1/1
14	CLA	1	518	13	1/1/11/20	6/13/91/115	-
17	BCR	l	4013	-	-	4/29/63/63	0/2/2/2
21	SQD	Z	822	-	-	7/22/42/69	0/1/1/1
14	CLA	t	505	13	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1013	-	1/1/15/20	13/37/115/115	-
14	CLA	H	1229	2	1/1/15/20	12/37/115/115	-
14	CLA	r	516	13	-	6/13/91/115	-
14	CLA	b	518	13	1/1/11/20	4/13/91/115	-
15	PQN	H	2002	-	-	6/23/43/43	0/2/2/2
14	CLA	s	501	13	1/1/11/20	4/13/91/115	-
17	BCR	f	4017	-	-	2/29/63/63	0/2/2/2
14	CLA	c	506	13	1/1/11/20	6/13/91/115	-
14	CLA	6	503	13	1/1/11/20	6/13/91/115	-
14	CLA	v	511	13	1/1/11/20	5/13/91/115	-
14	CLA	6	512	13	1/1/11/20	7/13/91/115	-
17	BCR	f	4004	-	-	8/29/63/63	0/2/2/2
14	CLA	1	511	13	1/1/11/20	2/13/91/115	-
14	CLA	Y	507	-	1/1/11/20	6/13/91/115	-
17	BCR	I	4018	-	-	0/29/63/63	0/2/2/2
14	CLA	Z	517	-	-	7/13/91/115	-
14	CLA	B	1235	2	1/1/15/20	7/37/115/115	-
17	BCR	a	523	-	-	4/29/63/63	0/2/2/2
14	CLA	f	1210	2	1/1/15/20	20/37/115/115	-
14	CLA	q	503	13	1/1/11/20	7/13/91/115	-
14	CLA	e	1101	1	1/1/15/20	18/37/115/115	-
14	CLA	3	518	13	1/1/13/20	9/25/103/115	-
17	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
14	CLA	b	511	13	1/1/11/20	3/13/91/115	-
14	CLA	f	1216	23	1/1/14/20	11/31/109/115	-
14	CLA	1	513	13	1/1/11/20	4/13/91/115	-
17	BCR	5	522	-	-	5/29/63/63	0/2/2/2
14	CLA	s	517	-	1/1/11/20	7/13/91/115	-
14	CLA	e	1125	1	1/1/15/20	12/37/115/115	-
14	CLA	A	1114	23	1/1/11/20	3/13/91/115	-
14	CLA	H	1240	18	1/1/15/20	13/37/115/115	-
14	CLA	H	1225	2	1/1/15/20	7/37/115/115	-
14	CLA	3	513	13	1/1/11/20	3/13/91/115	-
14	CLA	A	1139	23	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1109	1	1/1/15/20	14/37/115/115	-
18	LHG	e	5001	-	-	23/53/53/53	-
14	CLA	e	1118	1	1/1/14/20	8/31/109/115	-
14	CLA	3	511	13	1/1/11/20	2/13/91/115	-
18	LHG	e	5003	14	-	17/44/44/53	-
14	CLA	A	1134	1	1/1/13/20	9/27/105/115	-
14	CLA	B	1212	2	1/1/12/20	8/21/99/115	-
14	CLA	Y	506	13	1/1/11/20	5/13/91/115	-
14	CLA	G	1115	1	1/1/14/20	11/31/109/115	-
14	CLA	H	1234	2	1/1/15/20	15/37/115/115	-
19	LMU	A	1849	-	-	6/14/34/61	0/1/1/2
14	CLA	f	1211	2	1/1/13/20	8/25/103/115	-

The worst 5 of 5009 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	2001	PQN	C12-C13	8.46	1.53	1.33
15	A	2001	PQN	C12-C13	8.44	1.53	1.33
15	e	2001	PQN	C12-C13	8.44	1.53	1.33
15	B	2002	PQN	C12-C13	8.38	1.53	1.33
15	H	2002	PQN	C12-C13	8.38	1.53	1.33

The worst 5 of 7680 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1023	CLA	C4A-NA-C1A	9.67	111.06	106.71
14	B	1023	CLA	C4A-NA-C1A	9.59	111.02	106.71
14	f	1023	CLA	C4A-NA-C1A	9.53	110.99	106.71
15	G	2001	PQN	C11-C12-C13	-9.51	110.96	126.79
15	A	2001	PQN	C11-C12-C13	-9.50	110.98	126.79

5 of 588 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	1011	CLA	ND
14	A	1013	CLA	ND
14	A	1102	CLA	ND
14	A	1103	CLA	ND
14	A	1104	CLA	ND

5 of 7071 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	1011	CLA	CHA-CBD-CGD-O1D
14	A	1102	CLA	C3A-C2A-CAA-CBA
14	A	1103	CLA	C1A-C2A-CAA-CBA
14	A	1103	CLA	CHA-CBD-CGD-O1D
14	A	1103	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

402 monomers are involved in 1033 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	512	CLA	4	0
14	G	1117	CLA	5	0
17	4	521	BCR	2	0
14	2	503	CLA	3	0
17	H	4014	BCR	5	0
14	B	1211	CLA	1	0
18	H	1842	LHG	3	0
14	G	1022	CLA	2	0
14	3	512	CLA	5	0
18	A	5004	LHG	3	0
14	3	502	CLA	5	0
14	H	1218	CLA	3	0
14	A	1128	CLA	7	0
14	A	1111	CLA	2	0
14	6	502	CLA	2	0
14	B	1214	CLA	3	0
18	A	5003	LHG	2	0
14	4	503	CLA	1	0
14	G	1114	CLA	1	0
14	H	1235	CLA	4	0
14	Z	519	CLA	1	0
18	V	5218	LHG	2	0
17	2	524	BCR	5	0
14	F	1302	CLA	3	0
14	B	1204	CLA	5	0
14	A	1115	CLA	2	0
17	J	4013	BCR	6	0
14	B	1239	CLA	5	0
14	3	510	CLA	3	0
14	H	1201	CLA	3	0
14	H	1224	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1212	CLA	1	0
14	B	1240	CLA	4	0
14	B	1205	CLA	3	0
14	G	1013	CLA	8	0
14	G	1120	CLA	2	0
14	H	1230	CLA	3	0
14	G	1128	CLA	7	0
14	Y	510	CLA	1	0
14	B	1202	CLA	2	0
14	2	510	CLA	2	0
14	Z	503	CLA	3	0
14	1	510	CLA	1	0
18	G	5008	LHG	8	0
14	G	1134	CLA	2	0
19	G	1849	LMU	1	0
14	L	1501	CLA	5	0
14	A	1104	CLA	6	0
17	H	4006	BCR	4	0
14	L	1502	CLA	4	0
14	H	1204	CLA	4	0
14	A	1122	CLA	2	0
14	A	1135	CLA	2	0
17	Z	524	BCR	5	0
14	2	511	CLA	2	0
17	4	522	BCR	1	0
18	G	5004	LHG	2	0
17	R	4016	BCR	6	0
14	A	1137	CLA	5	0
14	3	503	CLA	1	0
14	A	1118	CLA	2	0
14	3	509	CLA	1	0
17	A	4002	BCR	5	0
14	B	1021	CLA	3	0
14	H	1012	CLA	4	0
14	U	1401	CLA	1	0
14	6	506	CLA	2	0
14	A	1133	CLA	2	0
17	J	4015	BCR	6	0
14	B	1216	CLA	5	0
14	Z	502	CLA	3	0
17	1	522	BCR	2	0
14	Z	511	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	4017	BCR	3	0
14	A	1132	CLA	1	0
14	B	1223	CLA	4	0
14	Y	512	CLA	4	0
17	W	4021	BCR	3	0
14	G	1140	CLA	3	0
14	H	1220	CLA	3	0
17	L	4020	BCR	2	0
14	5	513	CLA	2	0
14	T	1303	CLA	3	0
14	G	1122	CLA	3	0
14	H	1202	CLA	3	0
14	2	509	CLA	3	0
17	G	4007	BCR	3	0
21	H	1852	SQD	9	0
17	V	4020	BCR	2	0
14	B	1201	CLA	3	0
17	M	4021	BCR	2	0
17	G	4002	BCR	2	0
21	3	822	SQD	2	0
14	Z	510	CLA	2	0
14	6	505	CLA	5	0
17	H	4010	BCR	7	0
14	G	1133	CLA	2	0
14	B	1236	CLA	4	0
14	2	502	CLA	3	0
14	A	1124	CLA	3	0
14	B	1234	CLA	6	0
14	R	1301	CLA	1	0
17	G	4001	BCR	3	0
14	B	1227	CLA	4	0
17	2	521	BCR	7	0
14	4	511	CLA	3	0
14	Y	516	CLA	6	0
14	A	1107	CLA	2	0
14	G	1104	CLA	6	0
14	2	505	CLA	5	0
14	5	506	CLA	4	0
14	A	1237	CLA	8	0
14	A	1106	CLA	6	0
14	G	1129	CLA	6	0
14	4	513	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	4	507	CLA	1	0
14	U	1105	CLA	2	0
18	A	5008	LHG	7	0
14	G	1137	CLA	5	0
14	A	1101	CLA	5	0
14	J	1303	CLA	3	0
14	1	516	CLA	6	0
17	G	4008	BCR	4	0
14	A	1136	CLA	3	0
14	B	1230	CLA	2	0
17	S	4018	BCR	3	0
14	T	1302	CLA	1	0
18	G	5001	LHG	5	0
18	A	5009	LHG	3	0
14	H	1219	CLA	3	0
18	G	5003	LHG	2	0
14	6	510	CLA	2	0
17	5	521	BCR	3	0
17	H	4004	BCR	5	0
14	A	1129	CLA	6	0
14	B	1215	CLA	3	0
14	A	1108	CLA	2	0
14	Z	509	CLA	3	0
17	T	4012	BCR	4	0
14	Y	513	CLA	2	0
17	L	4022	BCR	6	0
19	B	1843	LMU	1	0
14	A	1103	CLA	5	0
17	G	4011	BCR	5	0
17	3	521	BCR	1	0
14	H	1228	CLA	1	0
14	A	1120	CLA	2	0
14	2	518	CLA	2	0
14	5	510	CLA	2	0
17	B	4017	BCR	4	0
14	G	1101	CLA	5	0
17	T	4013	BCR	6	0
14	H	1208	CLA	5	0
14	2	501	CLA	2	0
17	6	523	BCR	4	0
14	6	517	CLA	2	0
14	G	1108	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1023	CLA	4	0
14	G	1119	CLA	9	0
14	Y	502	CLA	2	0
17	V	4019	BCR	4	0
18	A	5007	LHG	2	0
14	H	1203	CLA	2	0
14	G	1124	CLA	3	0
17	V	4022	BCR	8	0
14	B	1226	CLA	5	0
14	B	1208	CLA	6	0
17	B	4009	BCR	3	0
14	Z	505	CLA	5	0
14	1	502	CLA	2	0
14	G	1112	CLA	1	0
14	H	1209	CLA	2	0
17	A	4011	BCR	4	0
18	A	5002	LHG	1	0
17	5	523	BCR	2	0
14	G	1237	CLA	8	0
14	G	1106	CLA	6	0
21	V	5216	SQD	6	0
14	2	512	CLA	5	0
14	6	518	CLA	1	0
14	1	505	CLA	5	0
14	Z	501	CLA	2	0
17	A	4008	BCR	6	0
18	G	5007	LHG	2	0
14	A	1011	CLA	4	0
17	4	523	BCR	2	0
14	B	1231	CLA	3	0
14	4	517	CLA	1	0
17	3	523	BCR	2	0
14	B	1222	CLA	1	0
14	2	519	CLA	1	0
14	A	1130	CLA	4	0
14	A	1125	CLA	3	0
19	H	1843	LMU	1	0
14	6	519	CLA	1	0
14	H	1223	CLA	4	0
18	G	5009	LHG	3	0
14	B	1220	CLA	3	0
17	F	4016	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	Z	518	CLA	2	0
14	H	1215	CLA	4	0
14	G	1103	CLA	5	0
14	Y	505	CLA	7	0
14	B	1203	CLA	2	0
17	2	523	BCR	2	0
14	A	1121	CLA	4	0
17	6	524	BCR	4	0
17	A	4003	BCR	1	0
20	T	5104	LMG	1	0
14	B	1218	CLA	3	0
18	G	5002	LHG	1	0
15	A	2001	PQN	4	0
14	Z	512	CLA	6	0
14	G	1135	CLA	2	0
14	H	1231	CLA	3	0
14	B	1229	CLA	8	0
14	H	1222	CLA	2	0
17	Z	523	BCR	2	0
14	1	509	CLA	2	0
14	4	516	CLA	2	0
15	B	2002	PQN	4	0
14	4	508	CLA	1	0
14	B	1012	CLA	5	0
14	G	1123	CLA	3	0
14	6	511	CLA	3	0
14	3	504	CLA	1	0
17	2	522	BCR	2	0
14	A	1127	CLA	1	0
18	H	1855	LHG	3	0
14	G	1011	CLA	5	0
17	B	4014	BCR	7	0
14	B	1219	CLA	3	0
17	G	4003	BCR	3	0
18	B	1842	LHG	3	0
14	5	512	CLA	4	0
14	G	1130	CLA	5	0
14	6	513	CLA	3	0
14	B	1209	CLA	2	0
14	J	1302	CLA	1	0
14	B	1217	CLA	2	0
14	3	517	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1224	CLA	4	0
14	A	1119	CLA	7	0
18	A	5005	LHG	7	0
14	H	1216	CLA	6	0
15	G	2001	PQN	3	0
17	Y	524	BCR	6	0
14	G	1126	CLA	10	0
21	Y	822	SQD	1	0
14	H	1021	CLA	4	0
20	H	5002	LMG	6	0
14	4	512	CLA	2	0
14	A	1113	CLA	1	0
17	1	524	BCR	6	0
18	L	5218	LHG	2	0
14	A	1112	CLA	1	0
18	A	5001	LHG	5	0
14	G	1113	CLA	1	0
14	H	1238	CLA	1	0
17	H	4005	BCR	3	0
17	T	4015	BCR	5	0
14	G	1111	CLA	2	0
14	R	1302	CLA	3	0
14	A	1110	CLA	2	0
17	3	524	BCR	1	0
14	B	1023	CLA	2	0
14	5	502	CLA	2	0
14	Y	518	CLA	1	0
14	1	507	CLA	1	0
17	L	4019	BCR	4	0
14	K	1105	CLA	2	0
14	G	1107	CLA	2	0
14	G	1102	CLA	1	0
14	H	1236	CLA	5	0
14	1	504	CLA	1	0
14	K	1401	CLA	1	0
14	5	505	CLA	1	0
14	2	506	CLA	2	0
19	G	1848	LMU	2	0
17	Z	522	BCR	2	0
14	Y	509	CLA	2	0
18	V	5220	LHG	4	0
14	G	1121	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	1136	CLA	4	0
18	L	5220	LHG	4	0
14	G	1139	CLA	1	0
14	G	1110	CLA	1	0
14	6	509	CLA	1	0
14	3	505	CLA	2	0
14	Y	519	CLA	1	0
14	4	510	CLA	3	0
14	A	1131	CLA	3	0
14	G	1109	CLA	2	0
14	H	1217	CLA	1	0
14	G	1127	CLA	1	0
14	4	502	CLA	4	0
14	H	1205	CLA	3	0
14	B	1207	CLA	10	0
17	Y	521	BCR	6	0
17	3	522	BCR	1	0
17	6	522	BCR	4	0
14	Z	506	CLA	2	0
14	5	511	CLA	2	0
17	B	4006	BCR	4	0
17	1	521	BCR	6	0
14	A	1105	CLA	2	0
21	B	1852	SQD	8	0
18	B	1855	LHG	3	0
17	V	4219	BCR	8	0
14	F	1301	CLA	1	0
17	L	4219	BCR	6	0
14	Z	513	CLA	2	0
21	L	5216	SQD	4	0
14	H	1226	CLA	5	0
14	H	1206	CLA	5	0
18	G	5005	LHG	6	0
21	1	822	SQD	1	0
14	A	1801	CLA	3	0
18	A	5006	LHG	4	0
22	P	170	FMN	1	0
14	Y	511	CLA	1	0
20	B	5002	LMG	5	0
14	5	509	CLA	2	0
14	H	1239	CLA	5	0
17	B	4005	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1207	CLA	3	0
18	I	5001	LHG	2	0
17	A	4001	BCR	4	0
17	Y	523	BCR	1	0
18	L	5221	LHG	1	0
14	H	1210	CLA	9	0
14	V	1501	CLA	8	0
14	A	1126	CLA	9	0
17	B	4010	BCR	6	0
14	B	1221	CLA	9	0
14	A	1140	CLA	3	0
14	G	1801	CLA	3	0
17	J	4012	BCR	4	0
17	K	4104	BCR	3	0
14	A	1123	CLA	1	0
17	H	4009	BCR	2	0
14	G	1125	CLA	3	0
18	G	5006	LHG	4	0
14	G	1131	CLA	3	0
17	U	4104	BCR	3	0
14	2	517	CLA	1	0
14	B	1206	CLA	4	0
14	H	1214	CLA	3	0
18	V	5221	LHG	8	0
14	4	509	CLA	4	0
14	H	1221	CLA	9	0
14	A	1116	CLA	5	0
14	V	1503	CLA	2	0
17	Z	521	BCR	7	0
22	X	170	FMN	1	0
14	Y	504	CLA	1	0
14	A	1102	CLA	2	0
14	V	1502	CLA	4	0
14	A	1022	CLA	2	0
14	B	1238	CLA	1	0
14	B	1228	CLA	2	0
14	G	1105	CLA	2	0
14	B	1225	CLA	4	0
17	4	524	BCR	2	0
19	A	1848	LMU	2	0
14	2	513	CLA	2	0
14	G	1132	CLA	1	0

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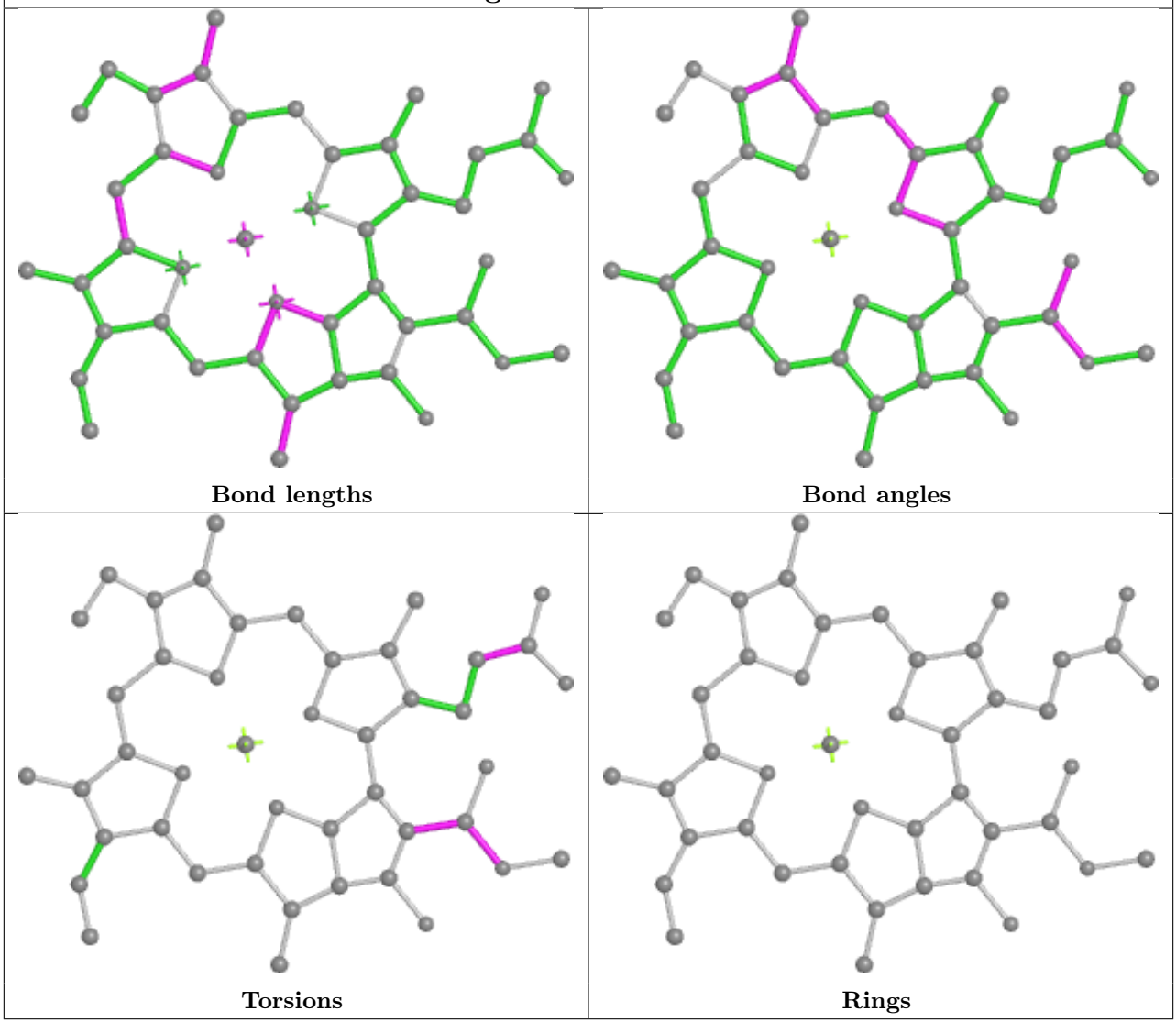
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	1118	CLA	2	0
14	5	507	CLA	1	0
17	B	4004	BCR	3	0
17	1	523	BCR	2	0
14	H	1227	CLA	4	0
14	B	1210	CLA	9	0
14	L	1503	CLA	1	0
14	G	1116	CLA	7	0
14	A	1117	CLA	5	0
14	1	518	CLA	1	0
14	A	1013	CLA	9	0
14	H	1229	CLA	6	0
15	H	2002	PQN	5	0
14	6	512	CLA	4	0
14	1	511	CLA	1	0
14	Y	507	CLA	1	0
17	I	4018	BCR	4	0
14	Z	517	CLA	1	0
14	B	1235	CLA	4	0
14	3	518	CLA	1	0
17	A	4007	BCR	2	0
14	1	513	CLA	2	0
17	5	522	BCR	2	0
14	A	1114	CLA	1	0
14	H	1240	CLA	3	0
14	H	1225	CLA	4	0
14	3	513	CLA	2	0
14	A	1139	CLA	3	0
14	A	1109	CLA	2	0
14	3	511	CLA	1	0
14	A	1134	CLA	3	0
14	B	1212	CLA	1	0
14	G	1115	CLA	3	0
14	H	1234	CLA	7	0
19	A	1849	LMU	1	0

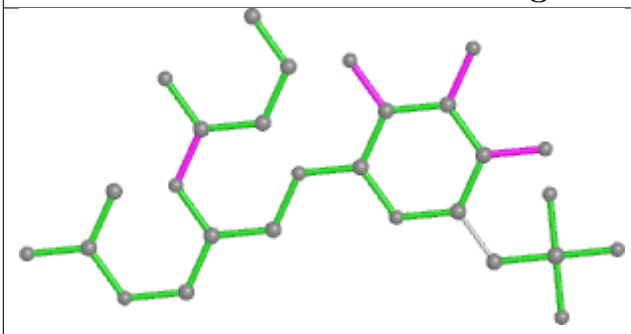
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

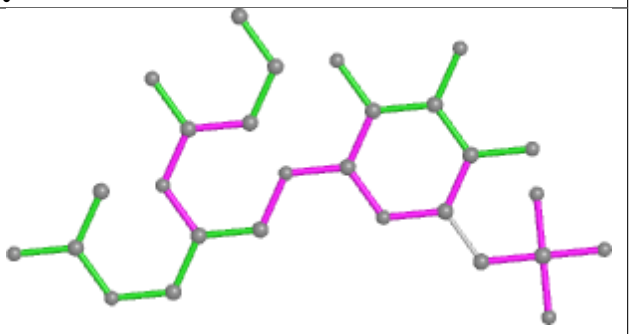
Ligand CLA 1 512



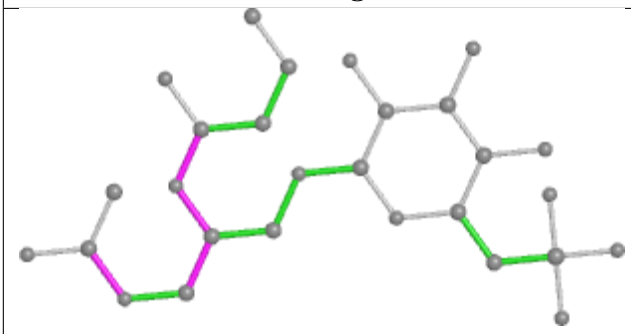
Ligand SQD r 822



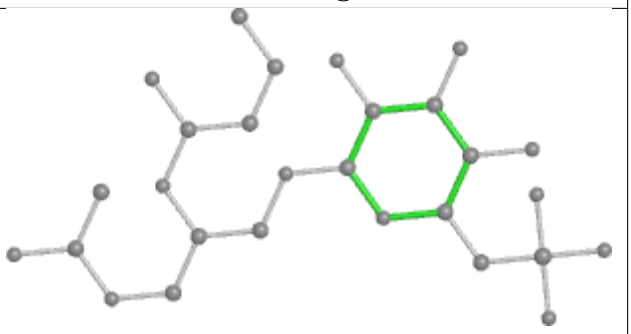
Bond lengths



Bond angles

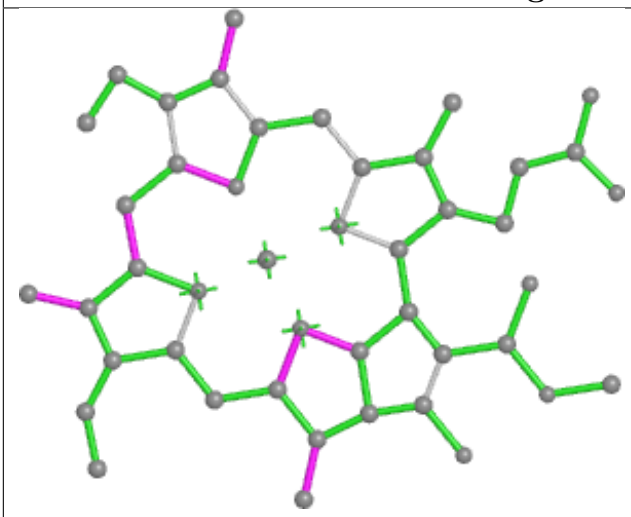


Torsions

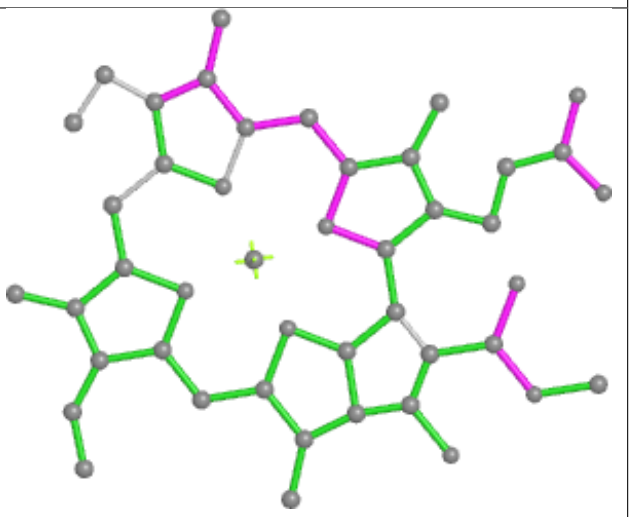


Rings

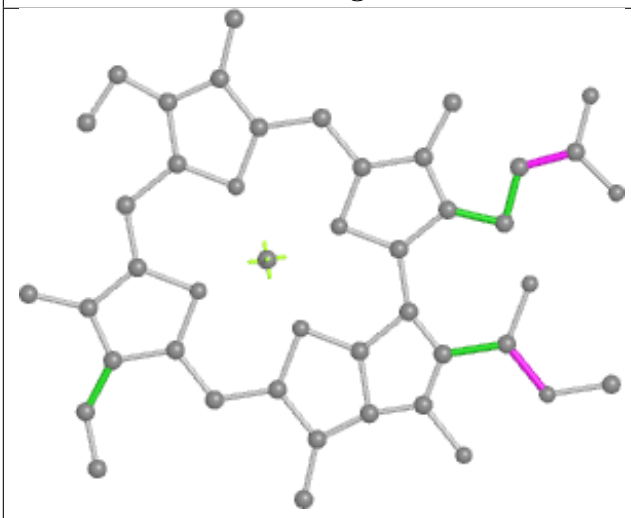
Ligand CLA d 509



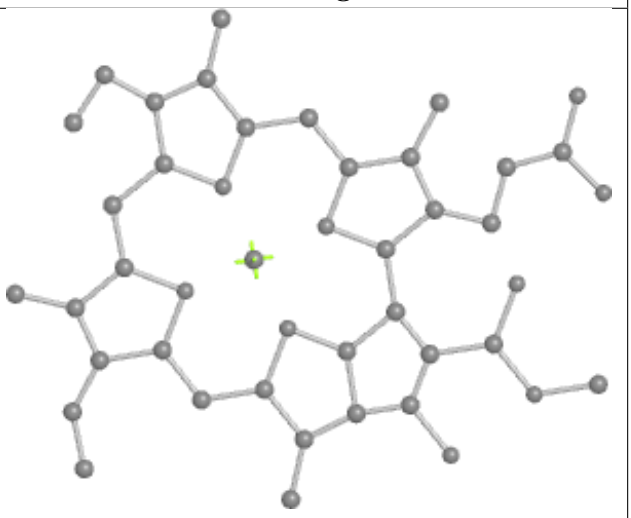
Bond lengths



Bond angles

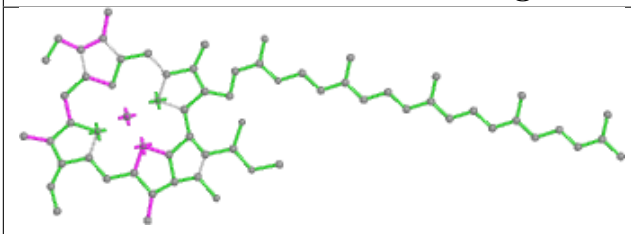


Torsions



Rings

Ligand CLA G 1117



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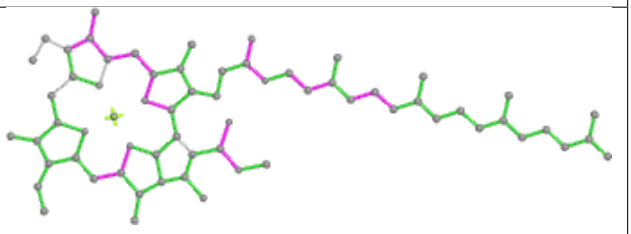

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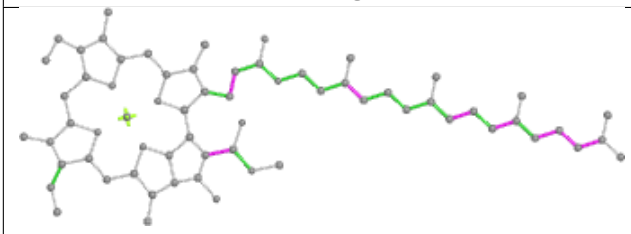

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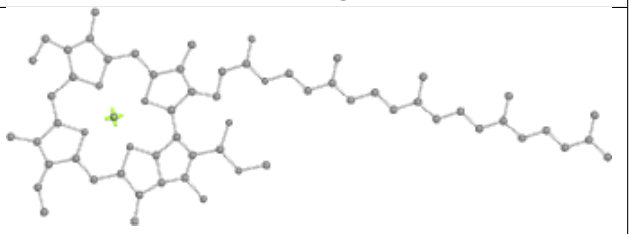
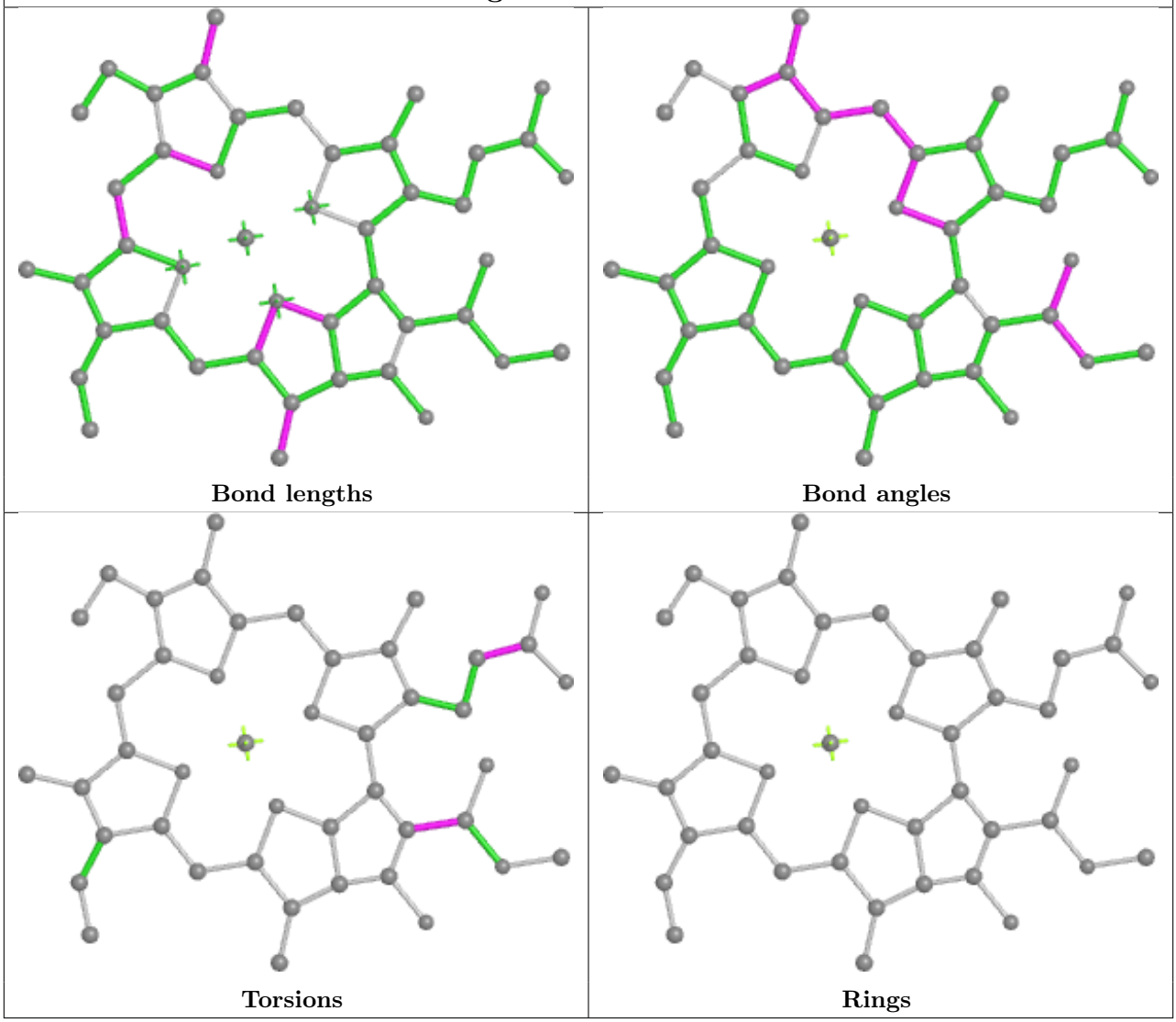
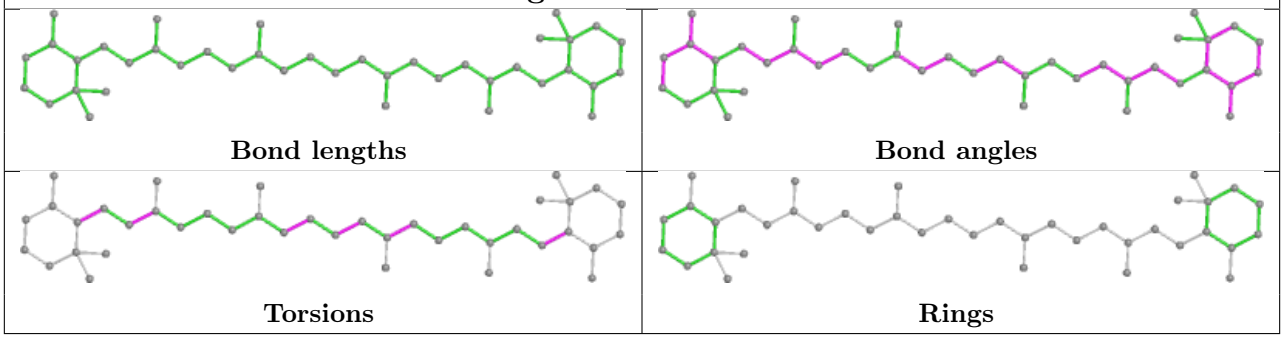


Rings

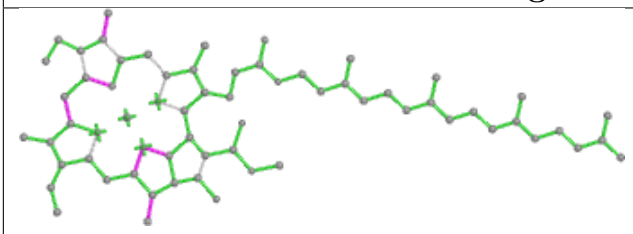
Ligand CLA t 512



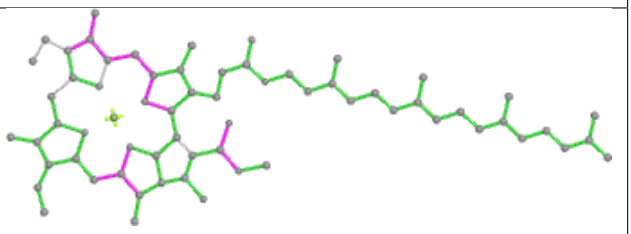
Ligand BCR 4 521



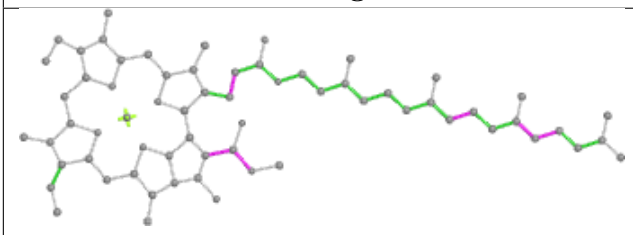
Ligand CLA 2 503



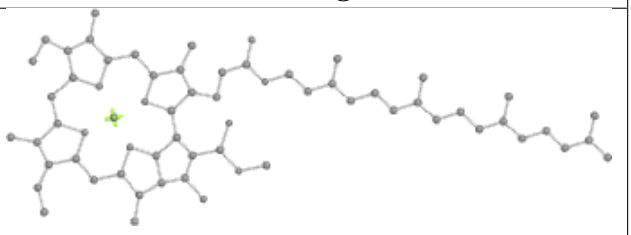
Bond lengths



Bond angles

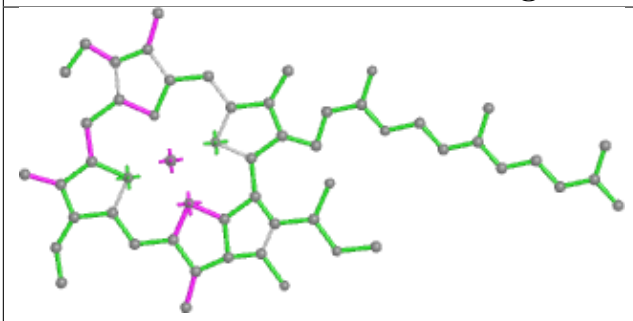


Torsions



Rings

Ligand CLA e 1102



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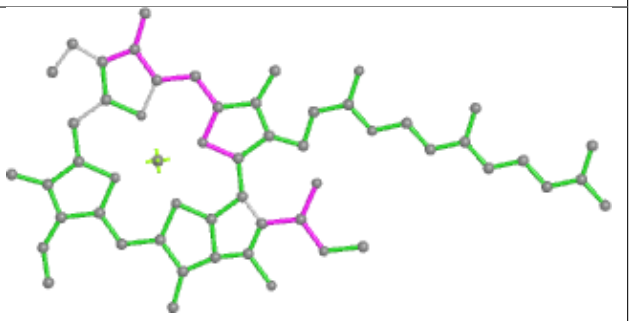

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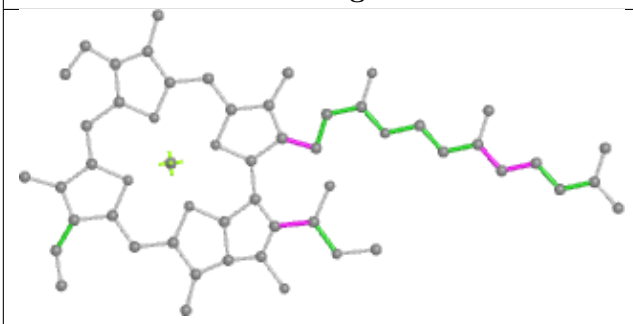

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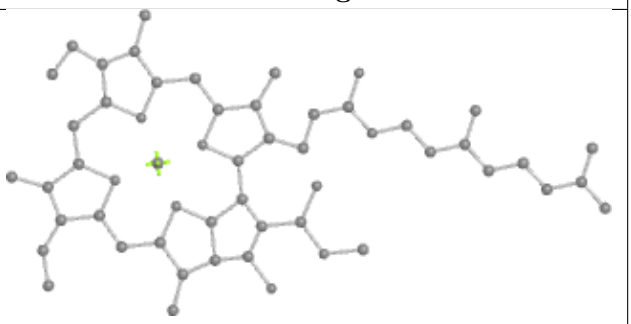
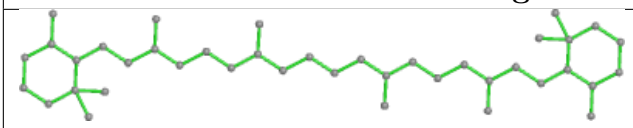


Rings

Ligand BCR H 4014



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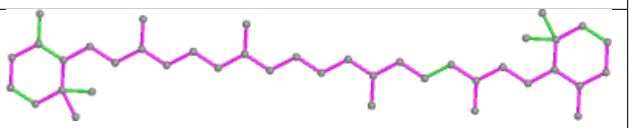

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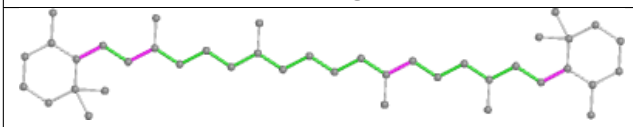

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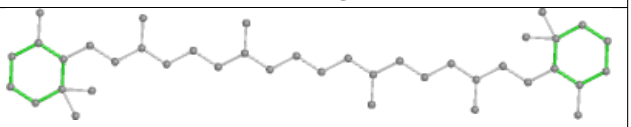
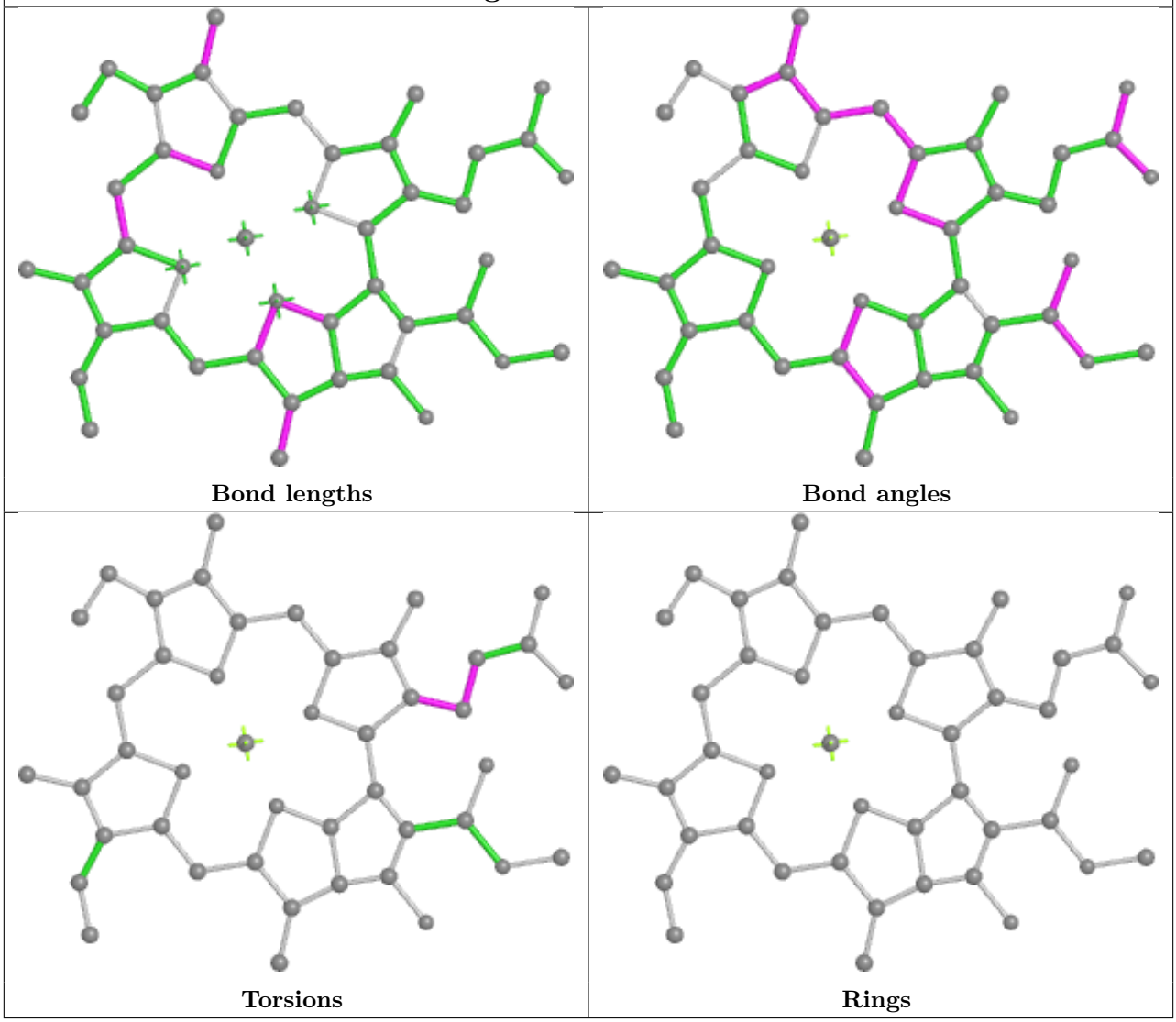
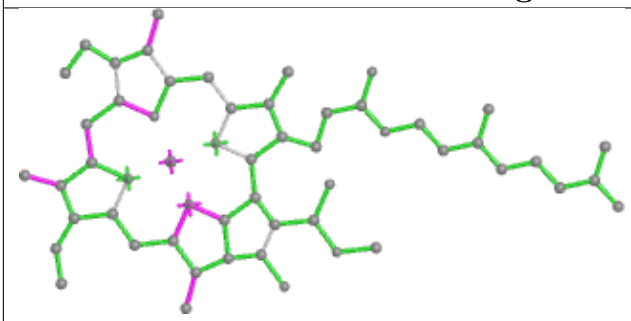


Rings

Ligand CLA u 518



Ligand CLA B 1211



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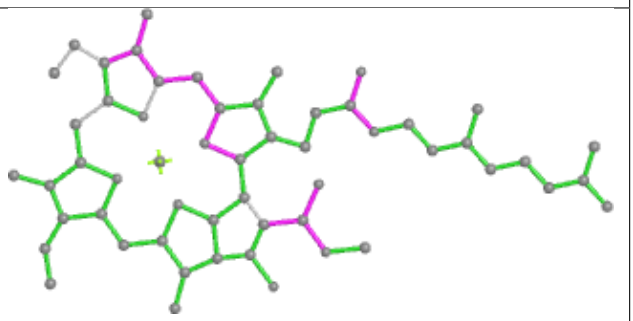
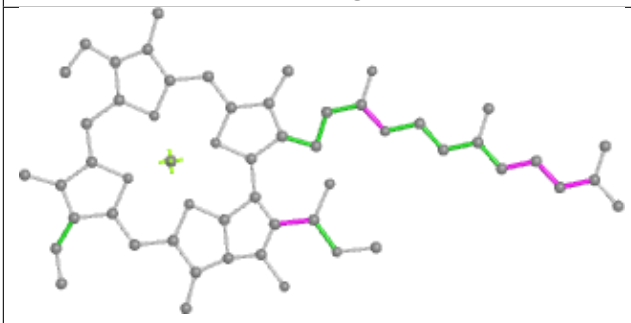


Bond angles



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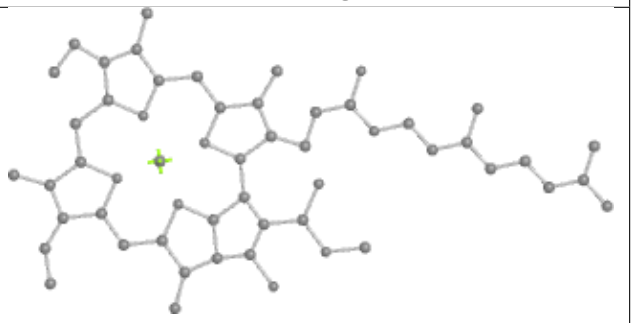
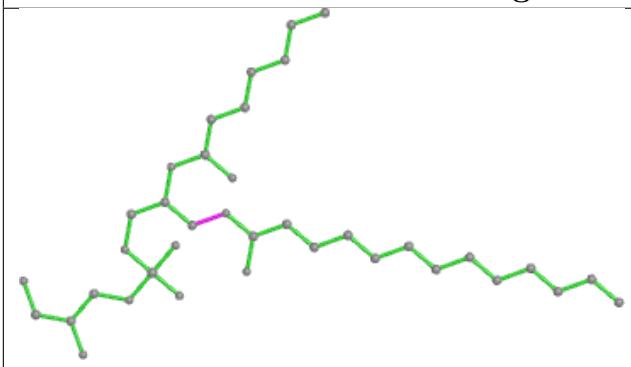


Rings

Ligand LHG H 1842



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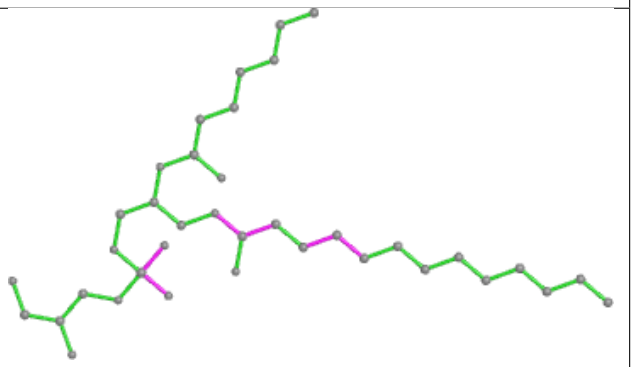
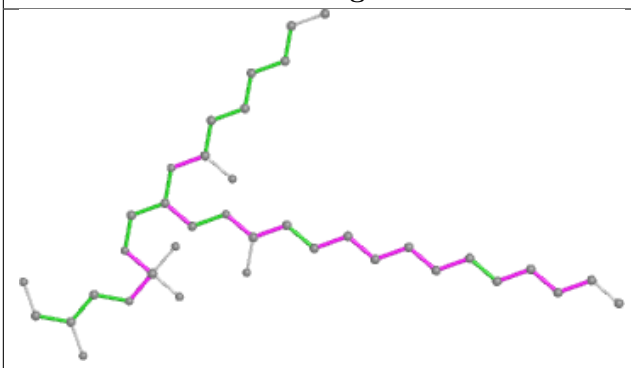


Bond angles



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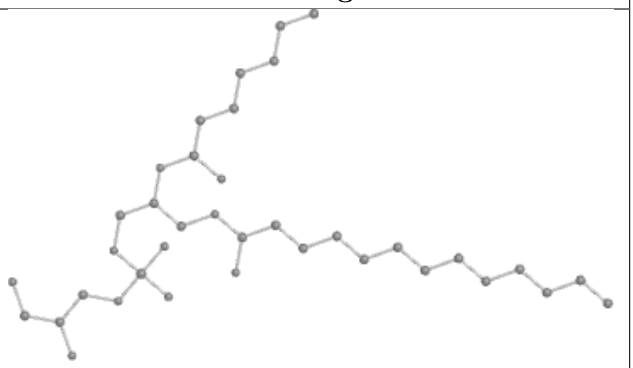
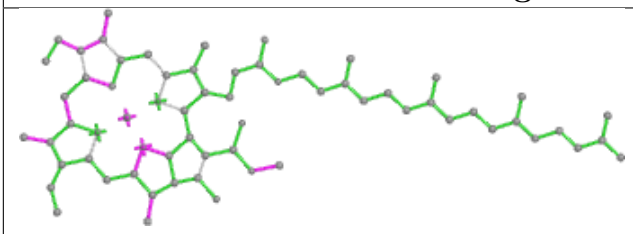


Rings

Ligand CLA G 1022



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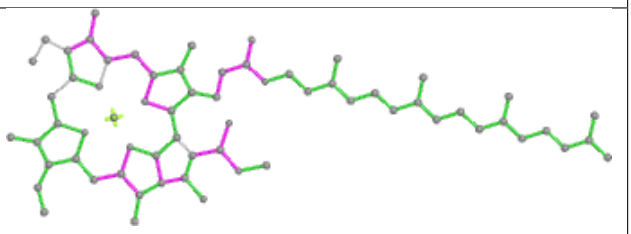

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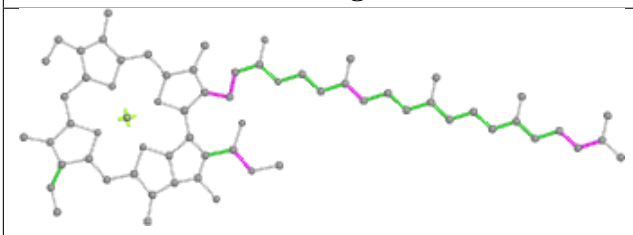

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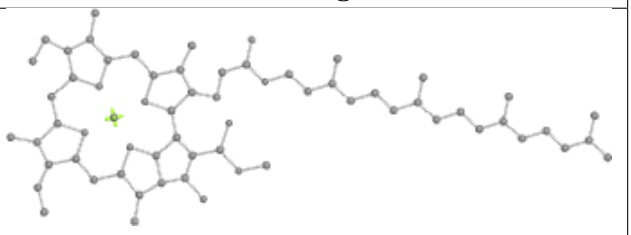

Rings

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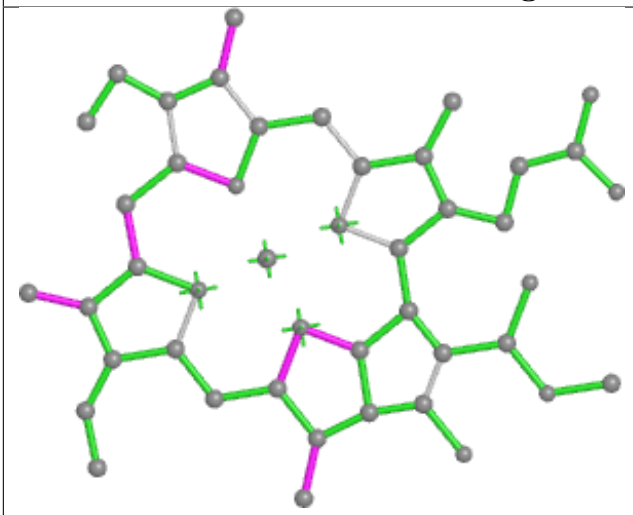

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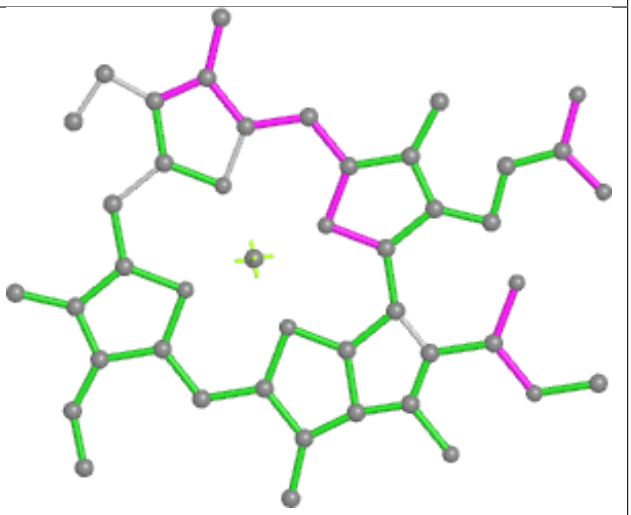

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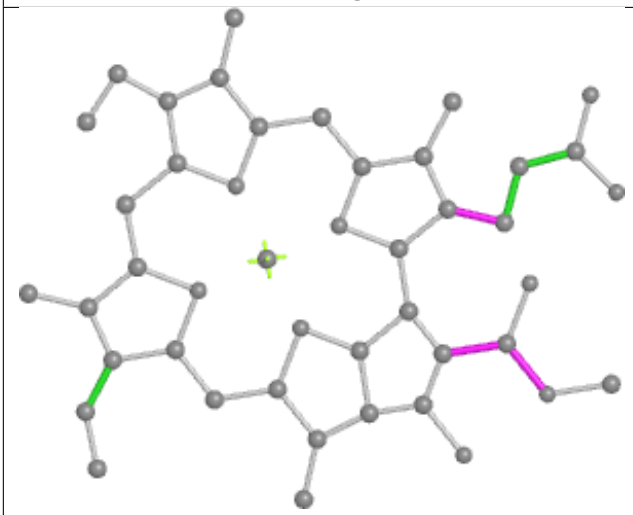

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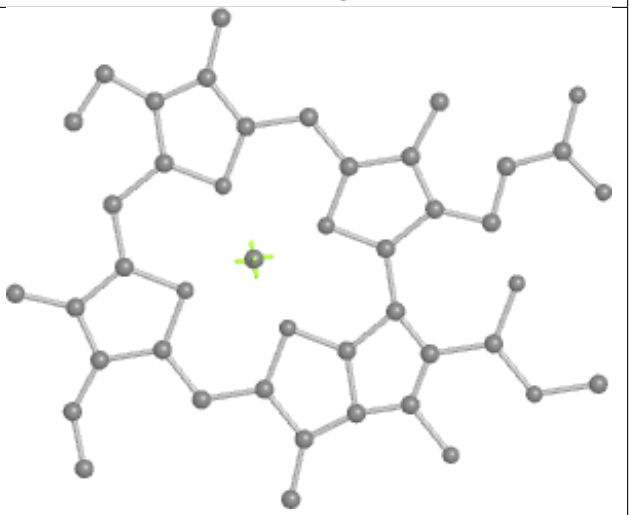
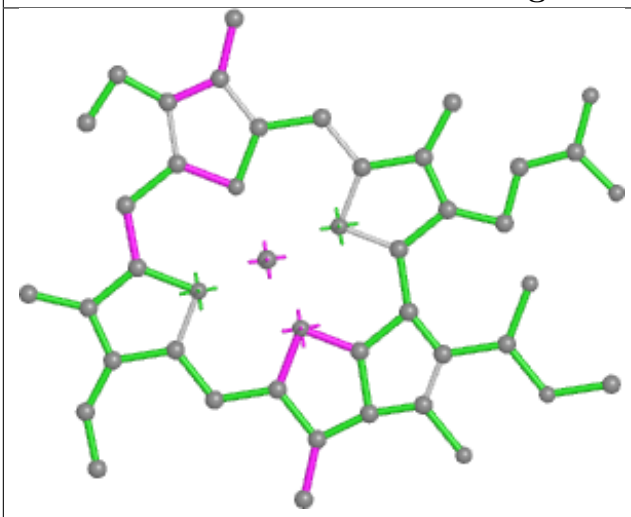


Rings

Ligand CLA 3 512



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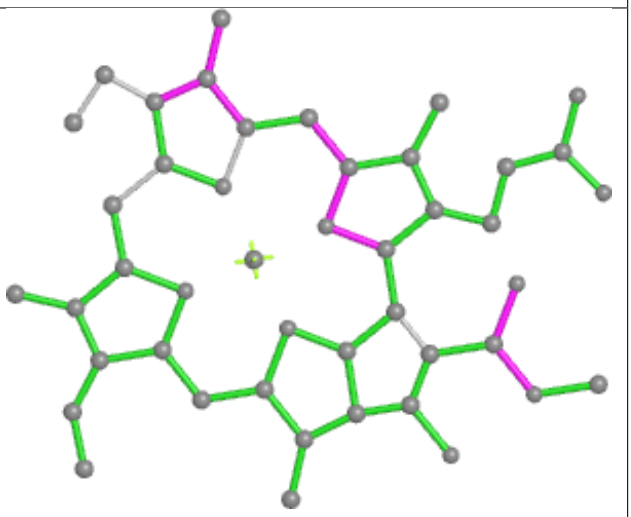

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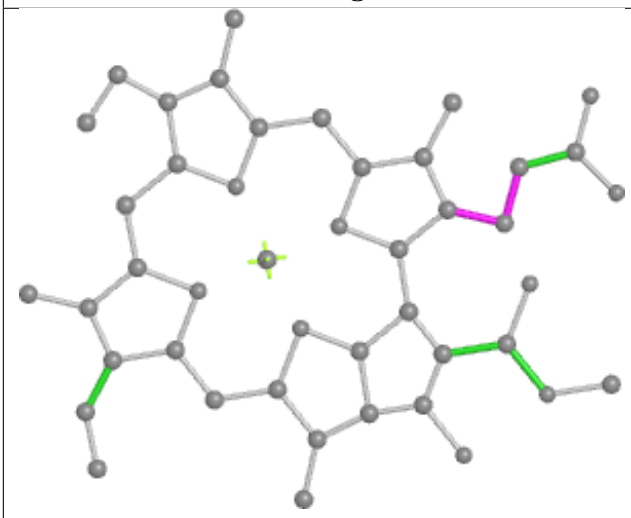

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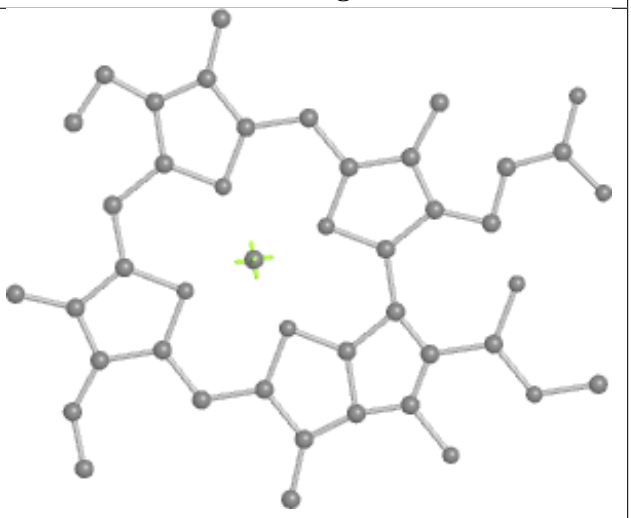
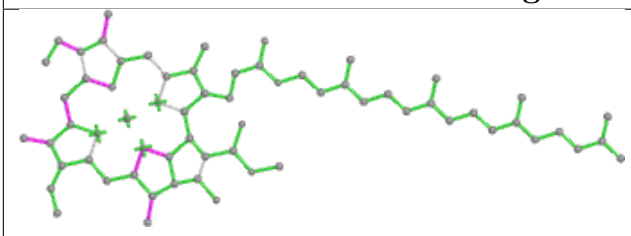


Rings

Ligand CLA f 1229



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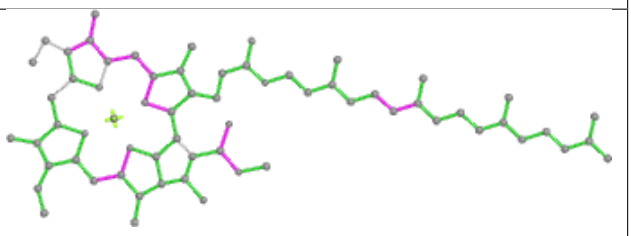
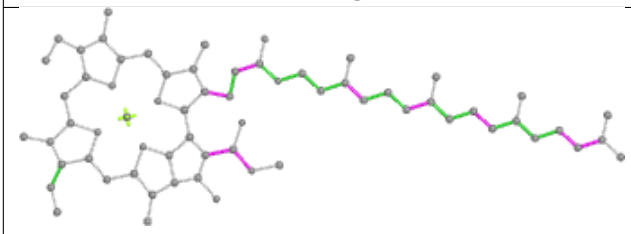
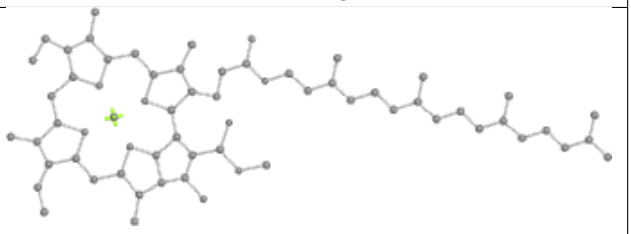


Bond angles

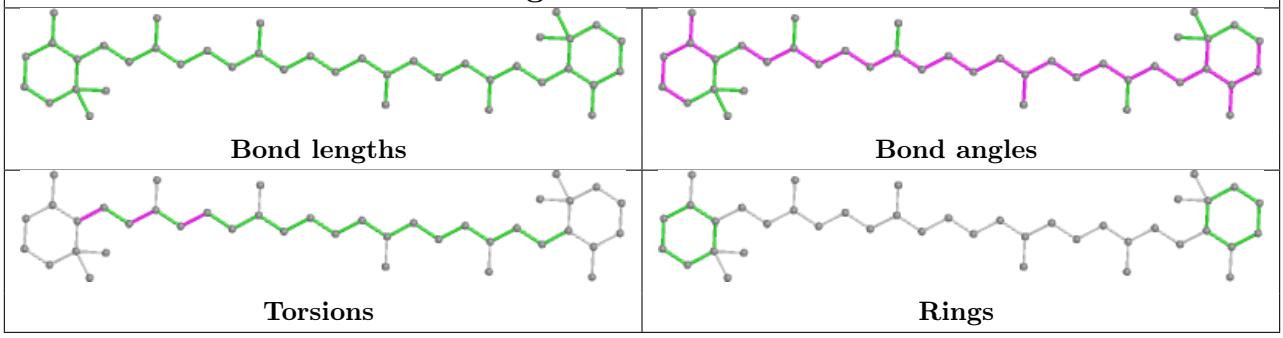


Torsions

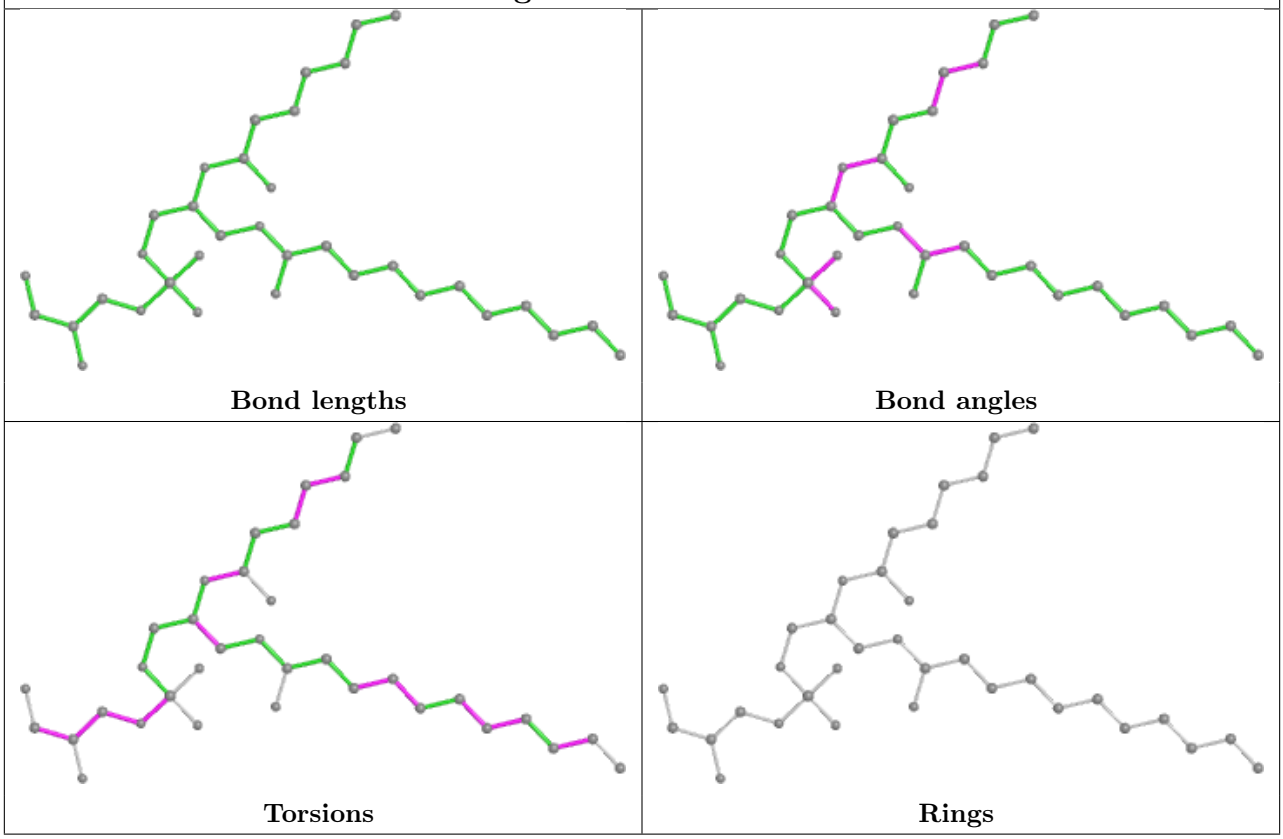


Rings

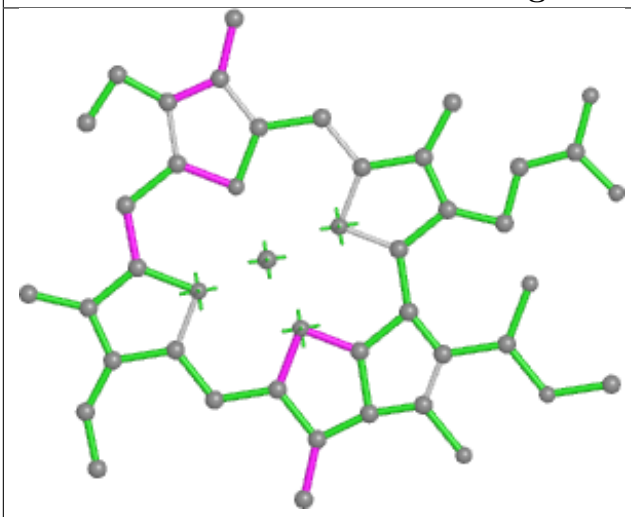
Ligand BCR d 522



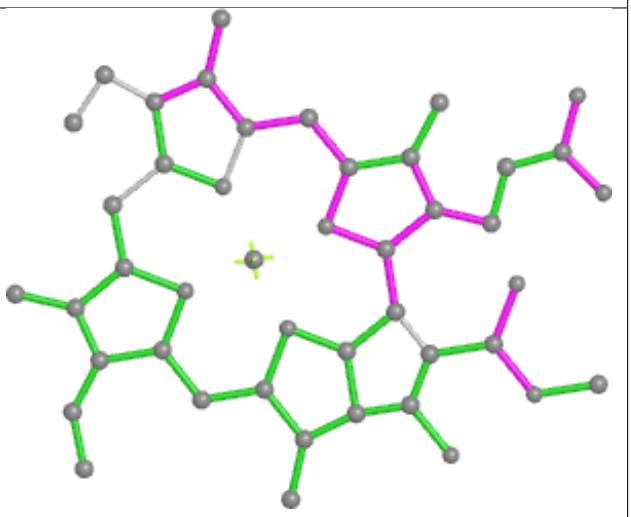
Ligand LHG A 5004



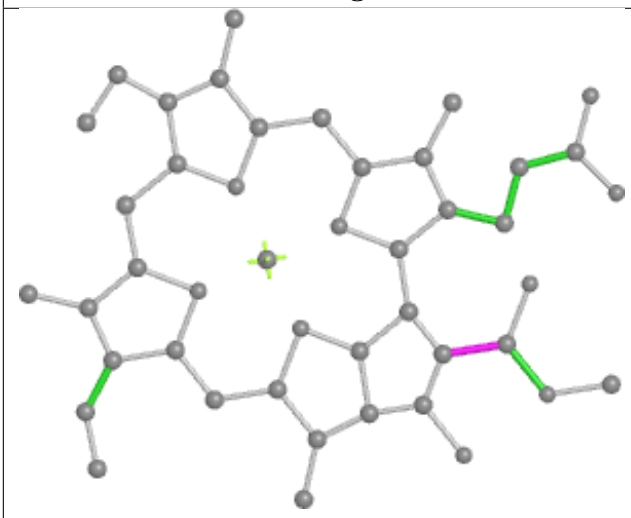
Ligand CLA 3 502



Bond lengths



Bond angles



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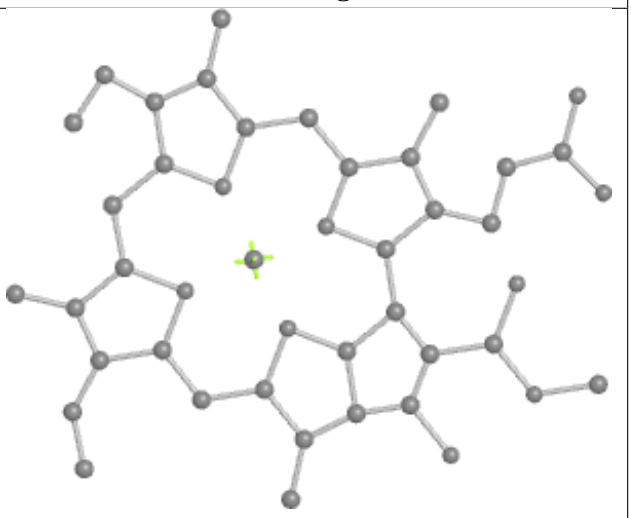
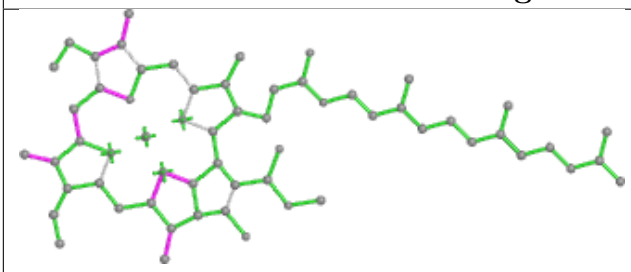
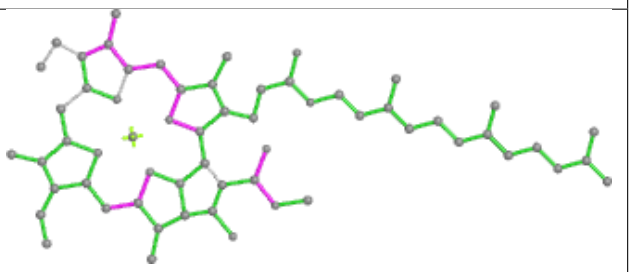


Rings

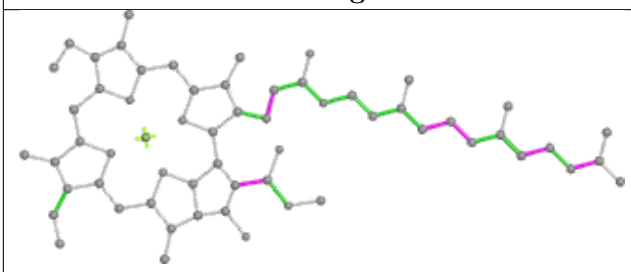
Ligand CLA H 1218



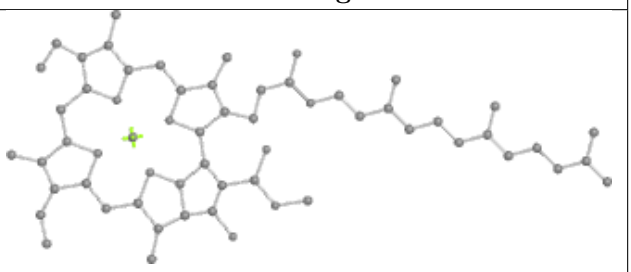
Bond lengths



Bond angles

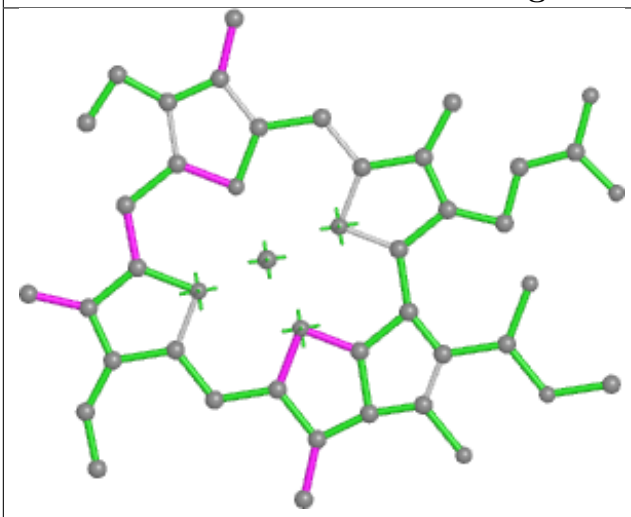


Torsions



Rings

Ligand CLA a 501



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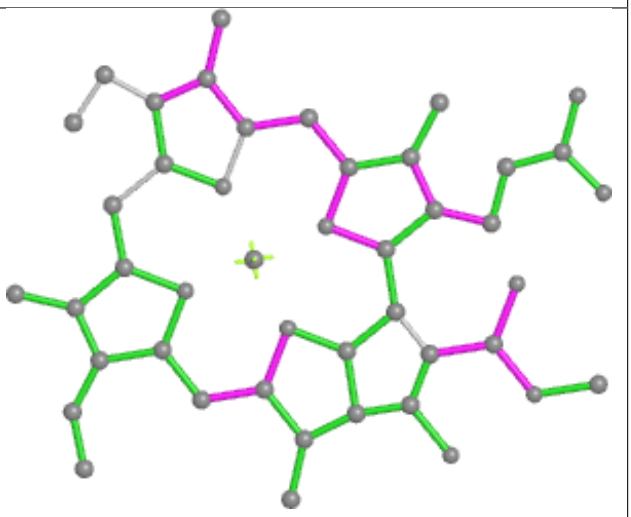
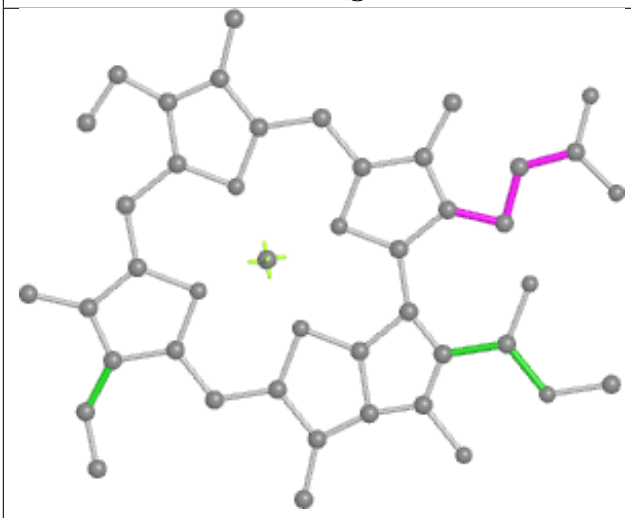


Bond angles



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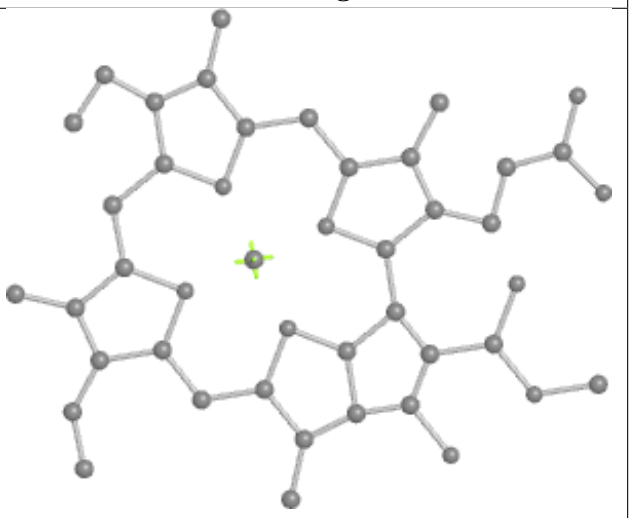
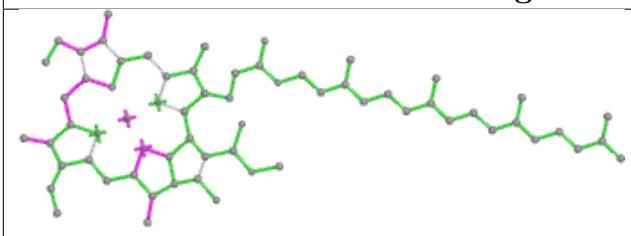


Rings

Ligand CLA A 1128



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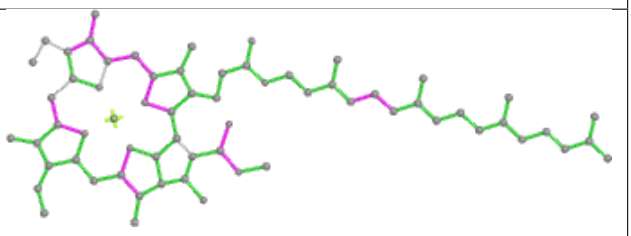
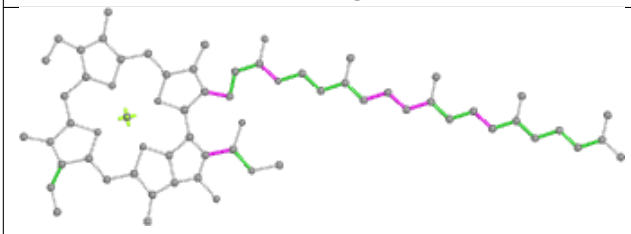


Bond angles



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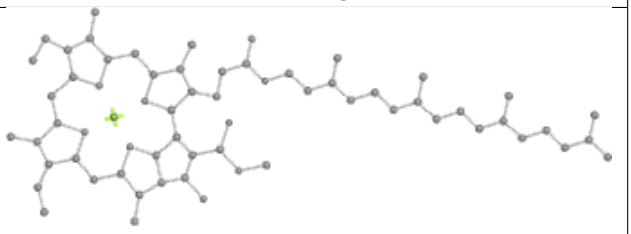
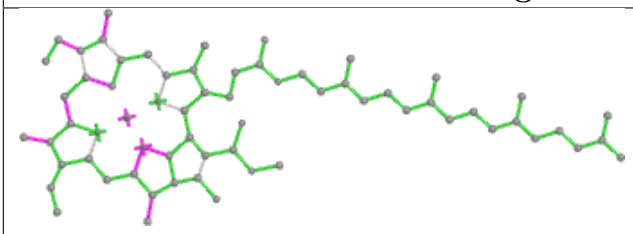


Rings

Ligand CLA A 1111



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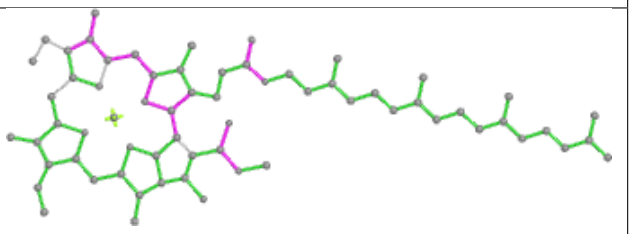
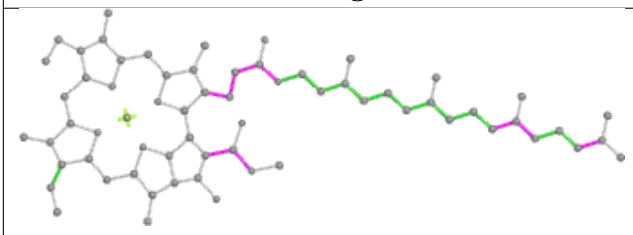


Bond angles



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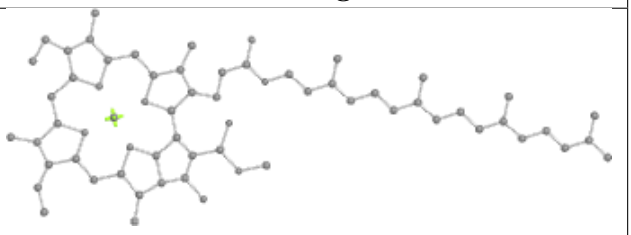
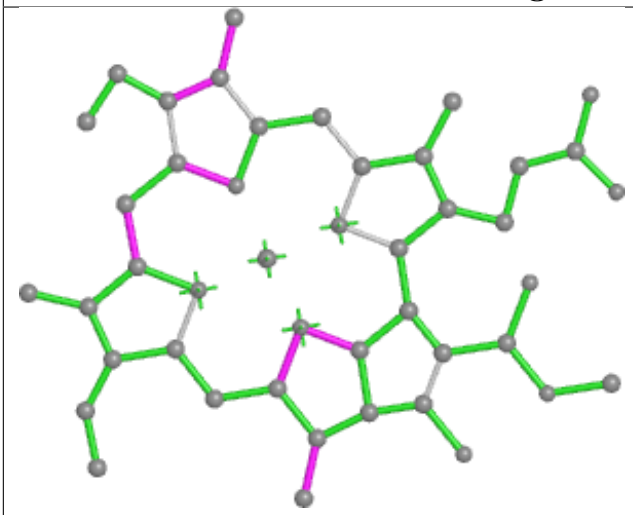


Rings

Ligand CLA 6 502



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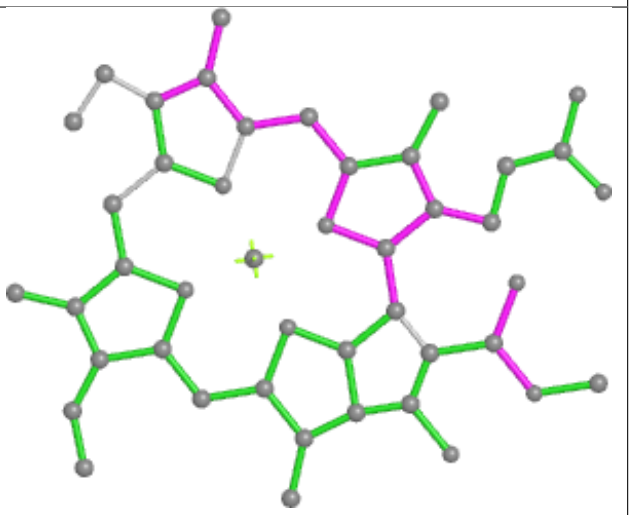

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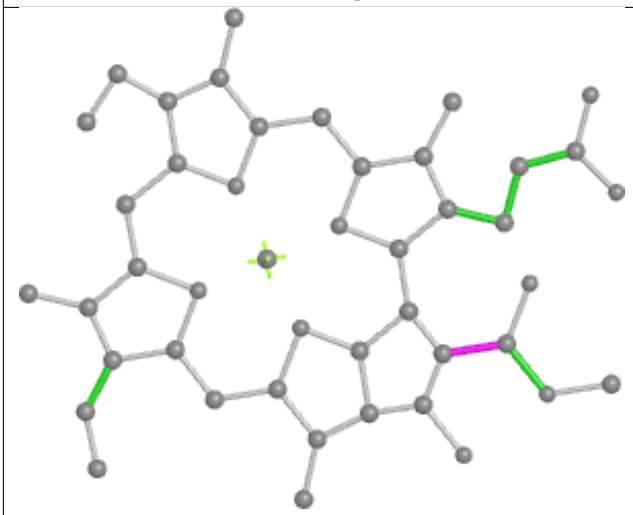

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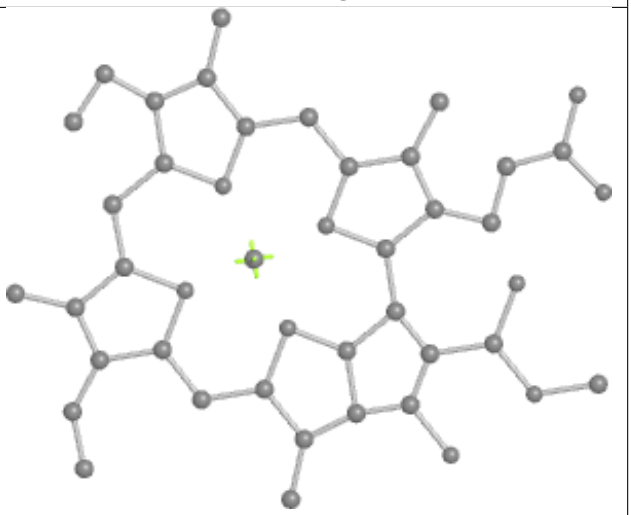
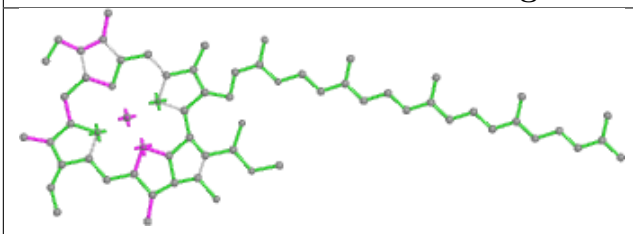


Rings

Ligand CLA e 1117



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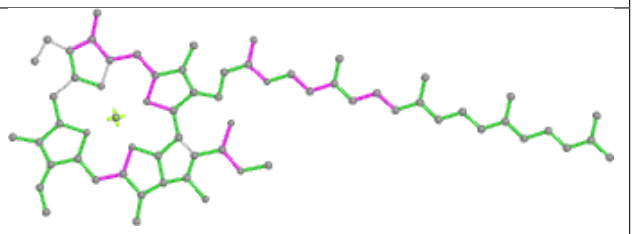
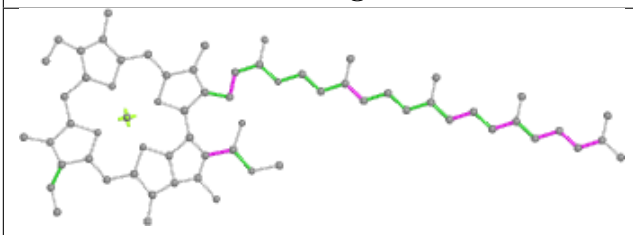


Bond angles



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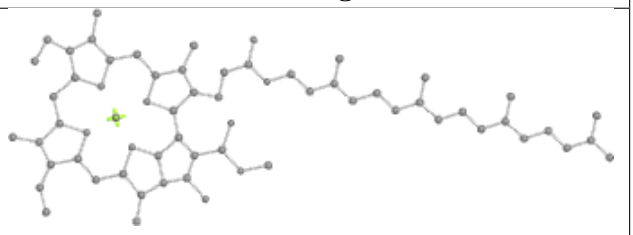
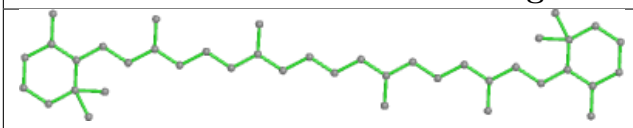


Rings

Ligand BCR a 522



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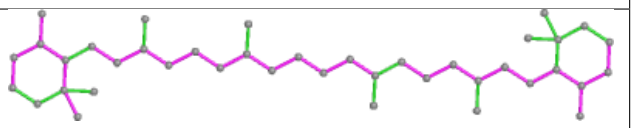
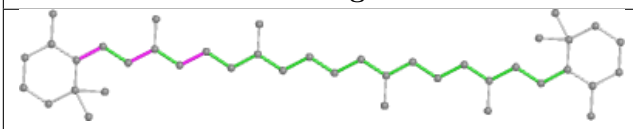


Bond angles



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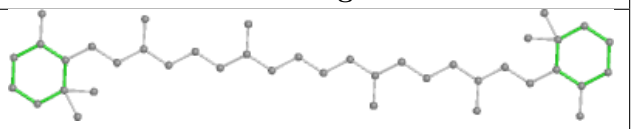
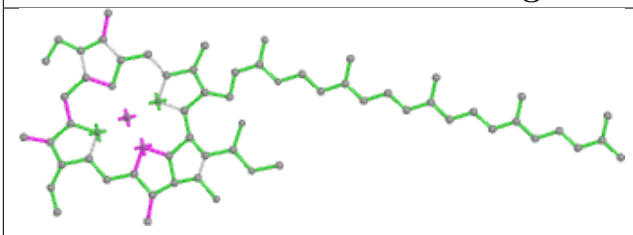


Rings

Ligand CLA f 1204



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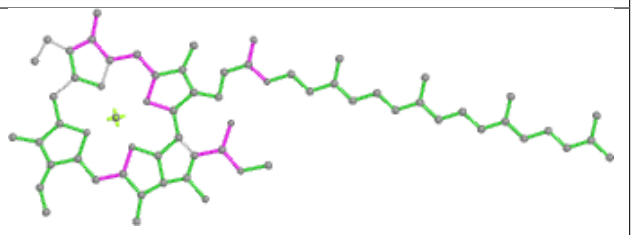
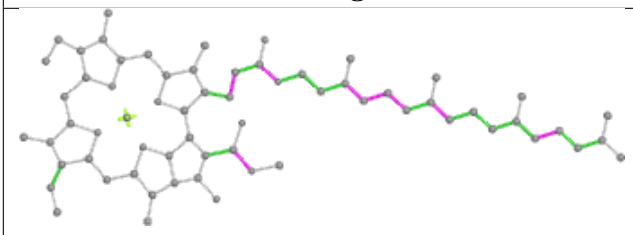
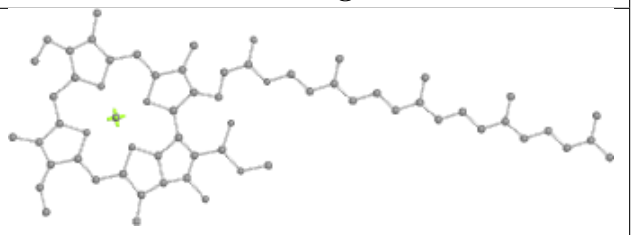


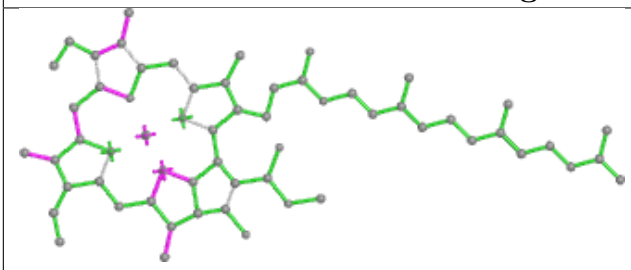
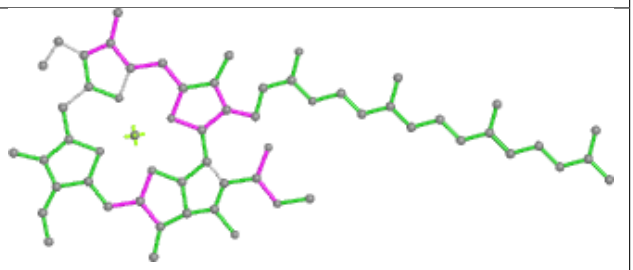
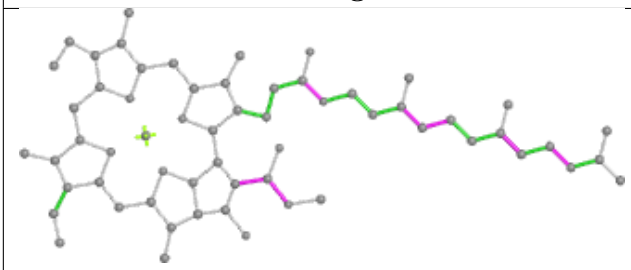
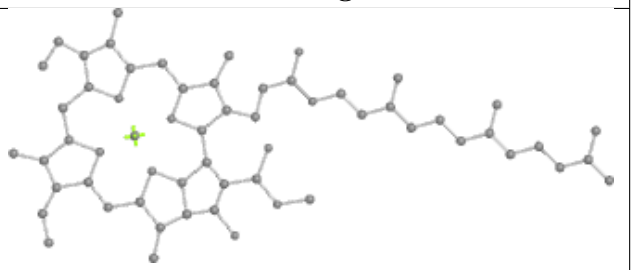
Bond angles



Torsions



Rings

Ligand CLA e 1124	
 Bond lengths	 Bond angles
 Torsions	 Rings

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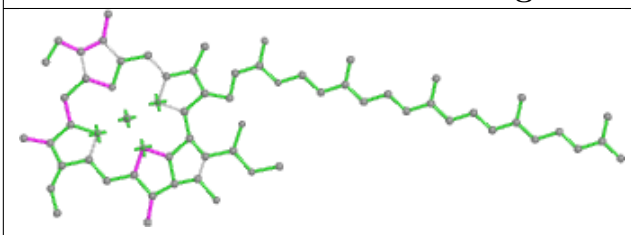
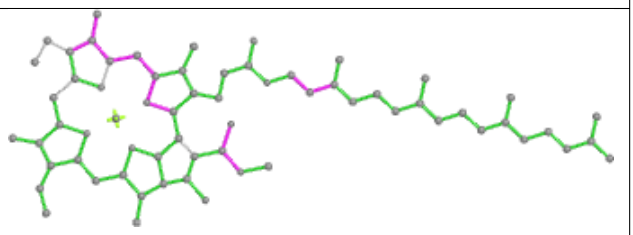
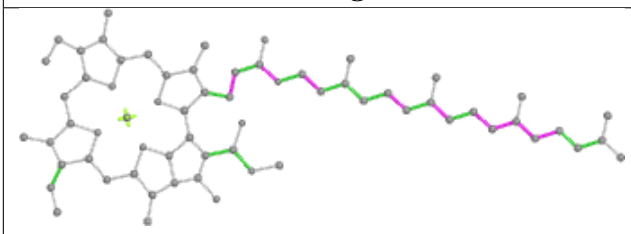
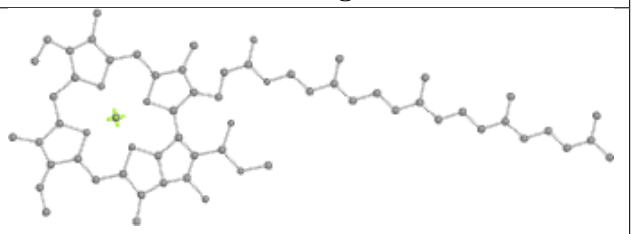
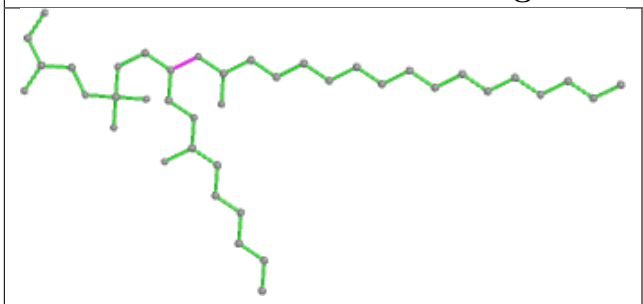
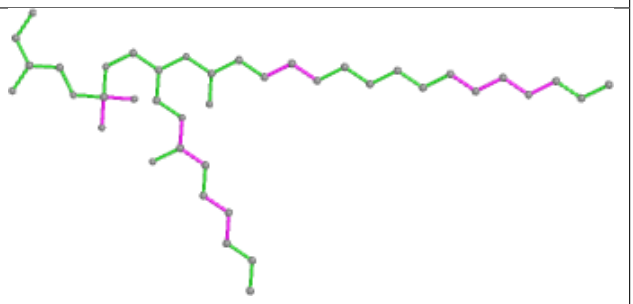
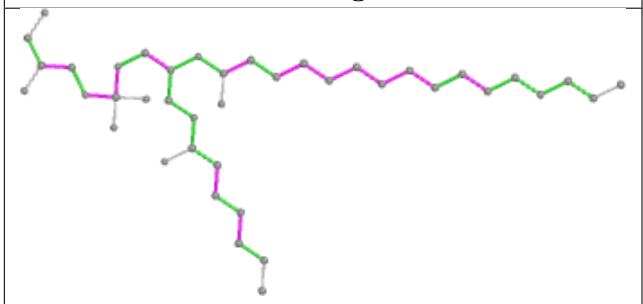
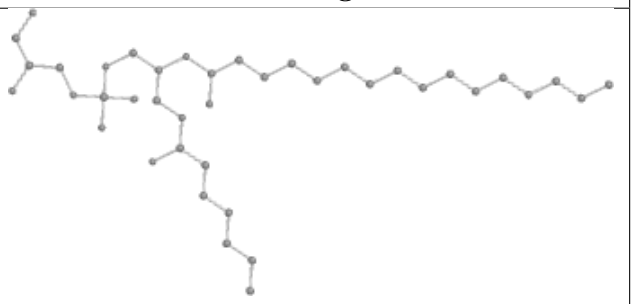
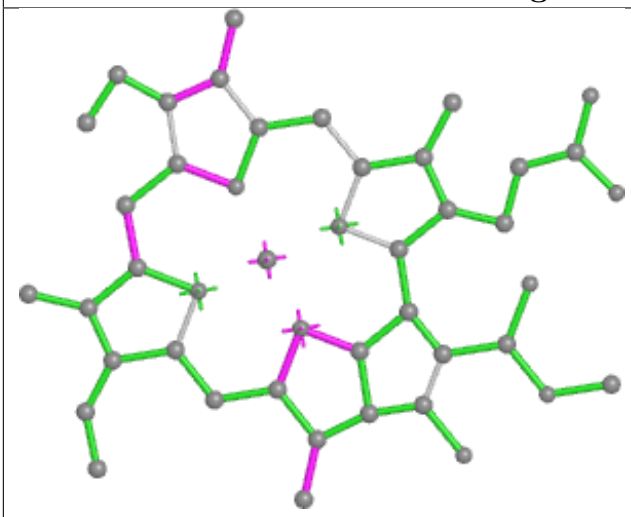
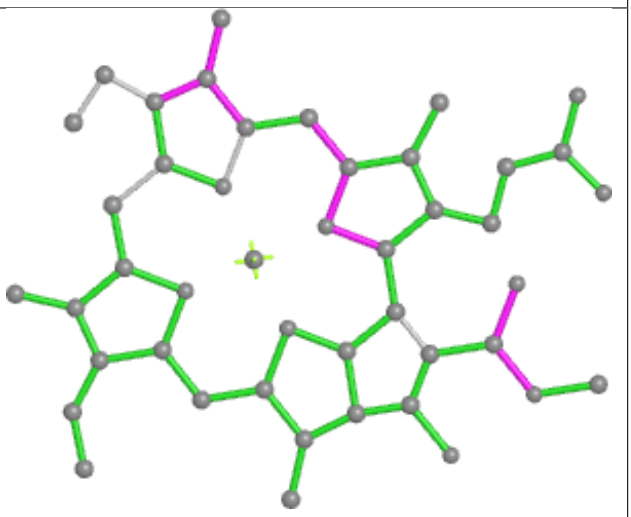
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A 5003	
 Bond lengths	 Bond angles
 Torsions	 Rings

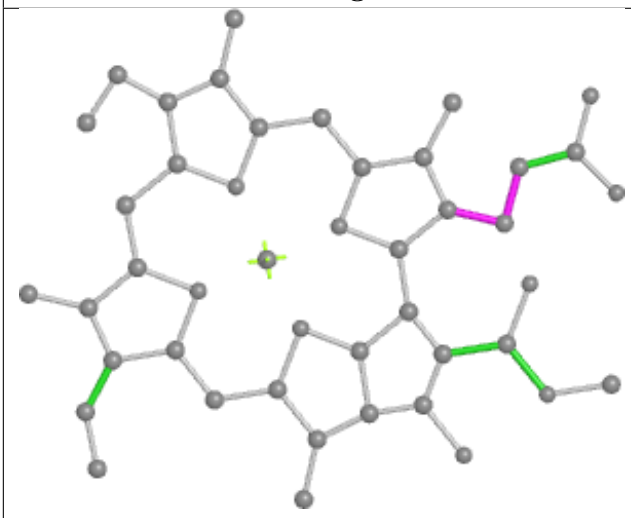
Ligand CLA s 512



Bond lengths



Bond angles



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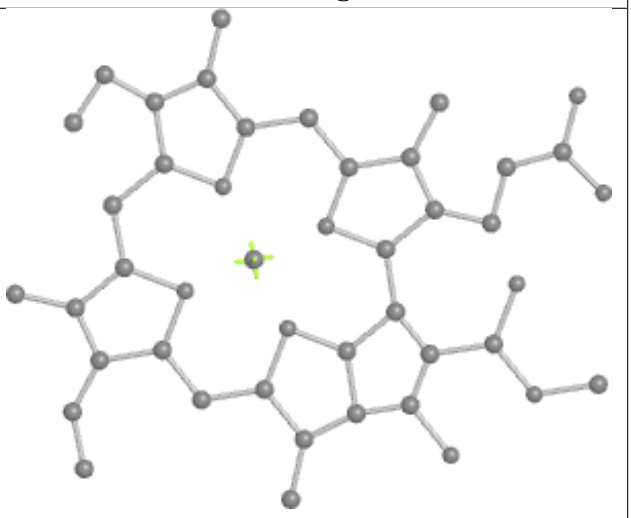
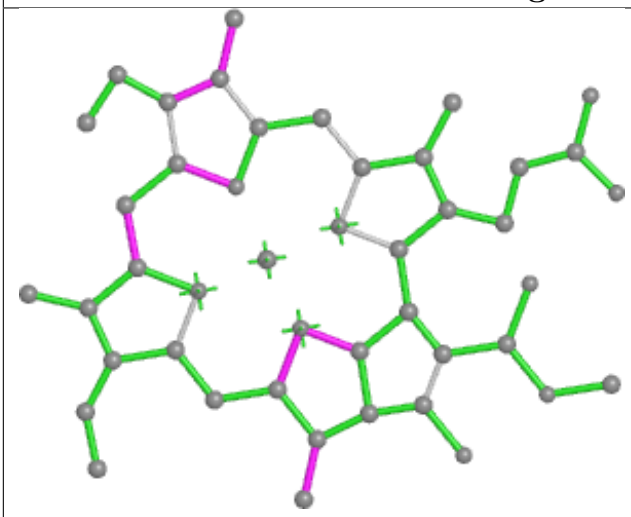


Rings

Ligand CLA 4 503



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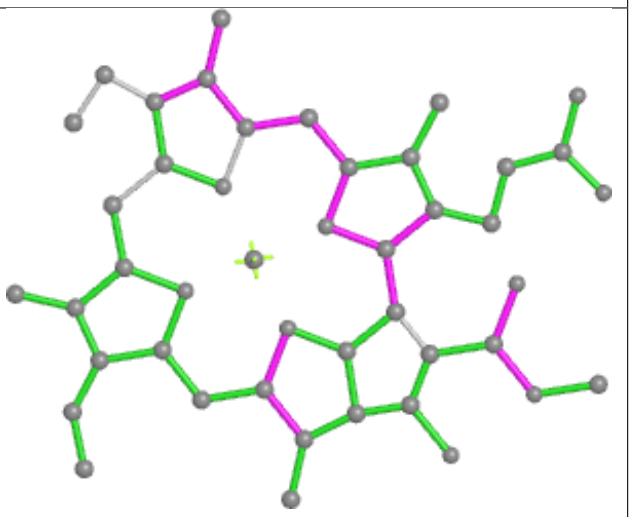
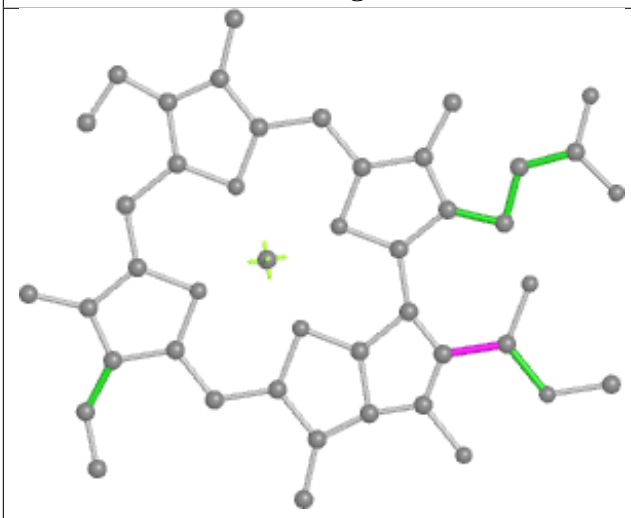
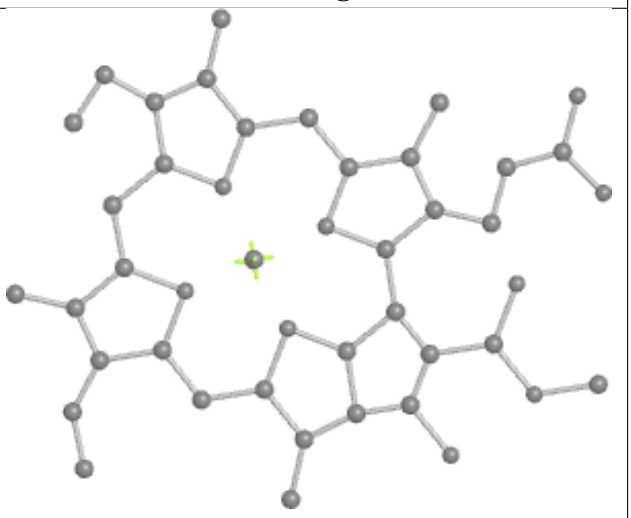


Bond angles

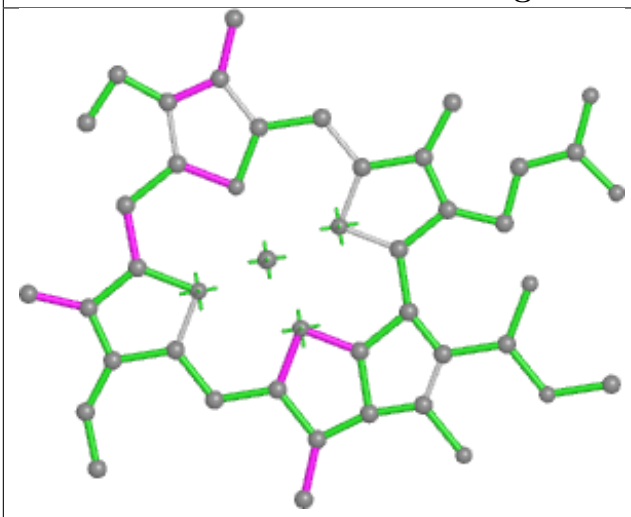


Torsions

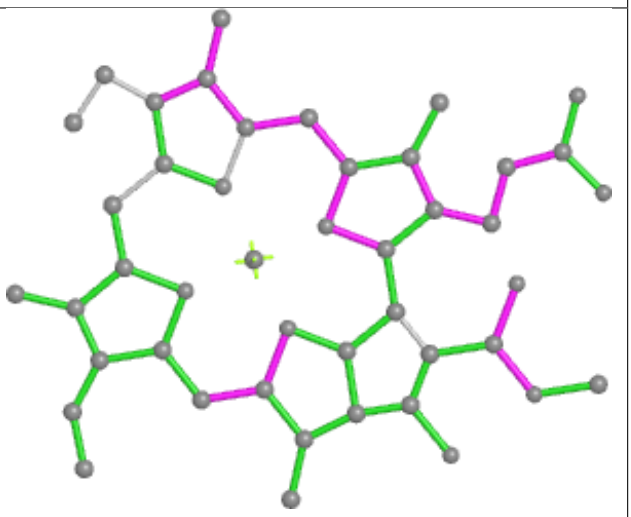


Rings

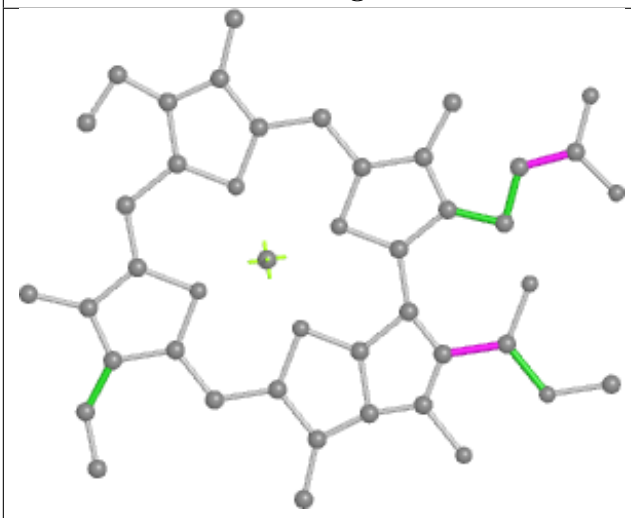
Ligand CLA G 1114



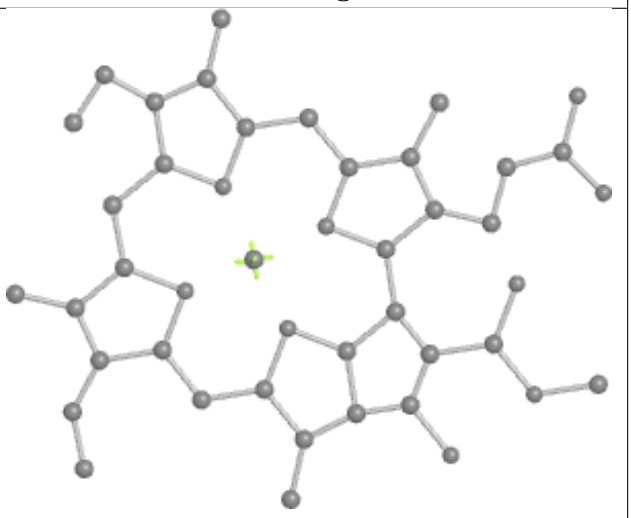
Bond lengths



Bond angles

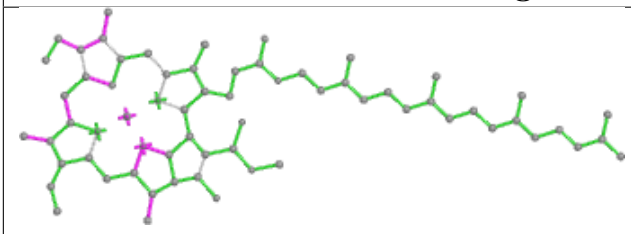


Torsions



Rings

Ligand CLA H 1235



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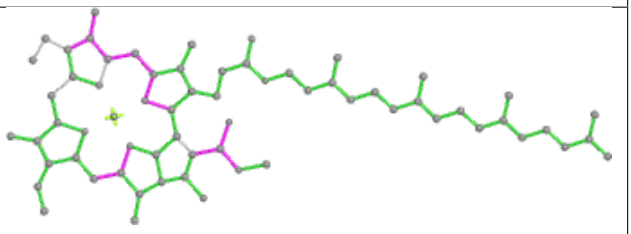

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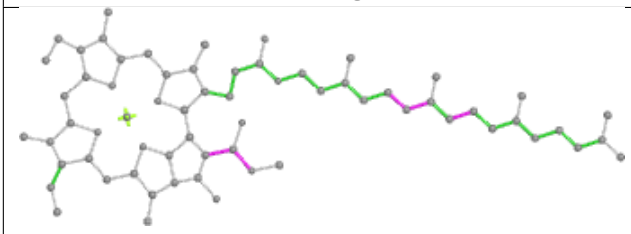

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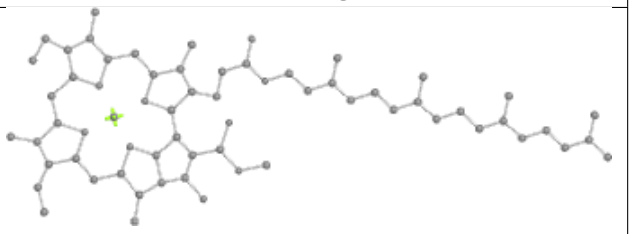
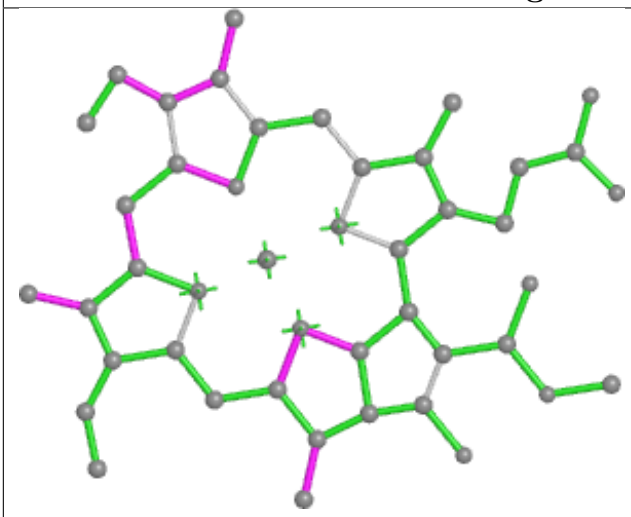


Rings

Ligand CLA Z 519



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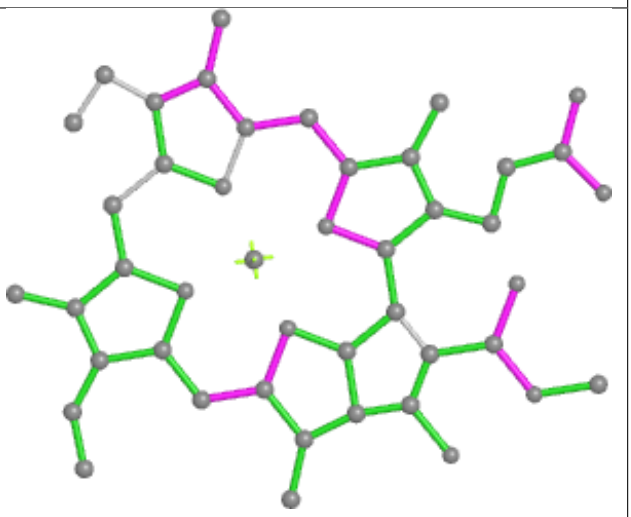

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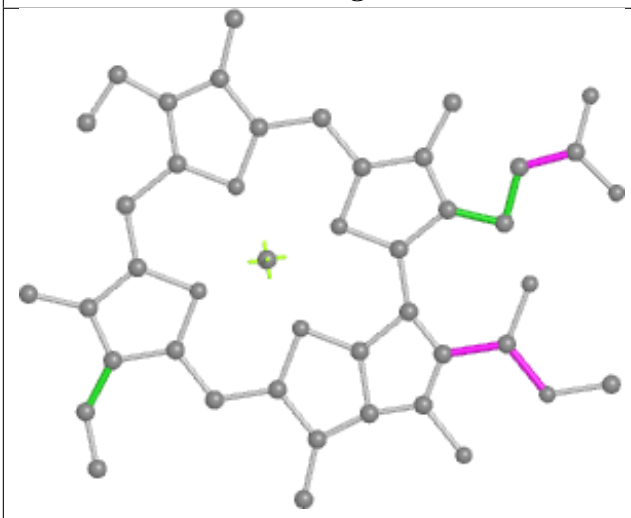

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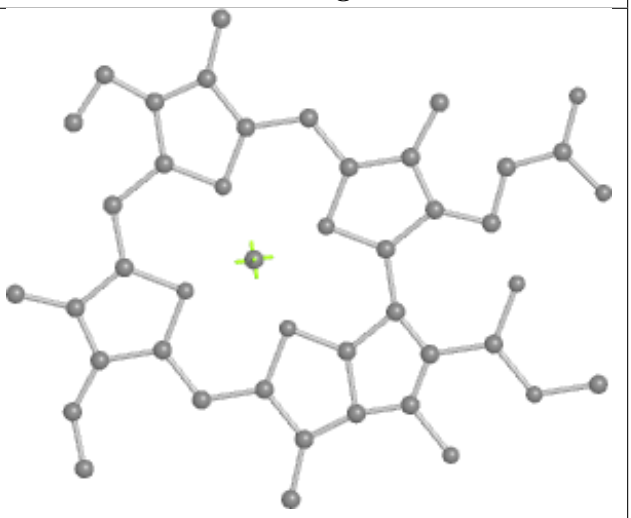
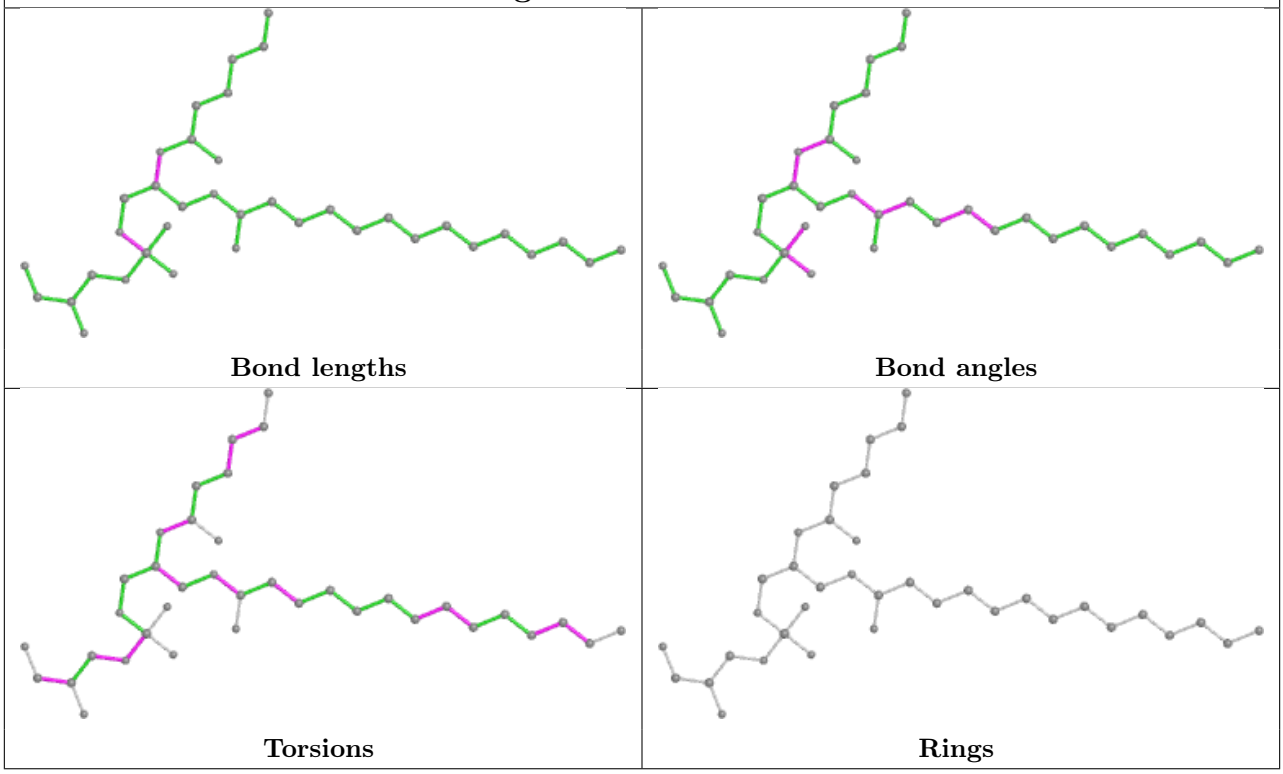


Rings

Ligand LHG V 5218



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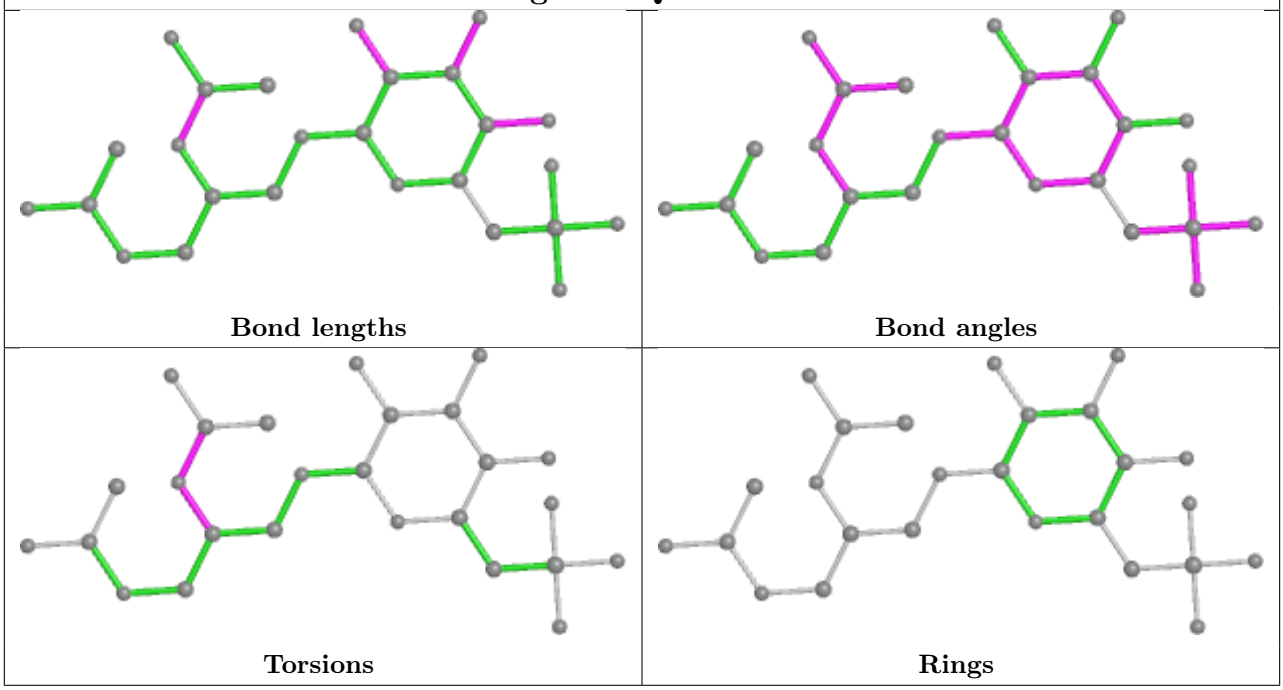
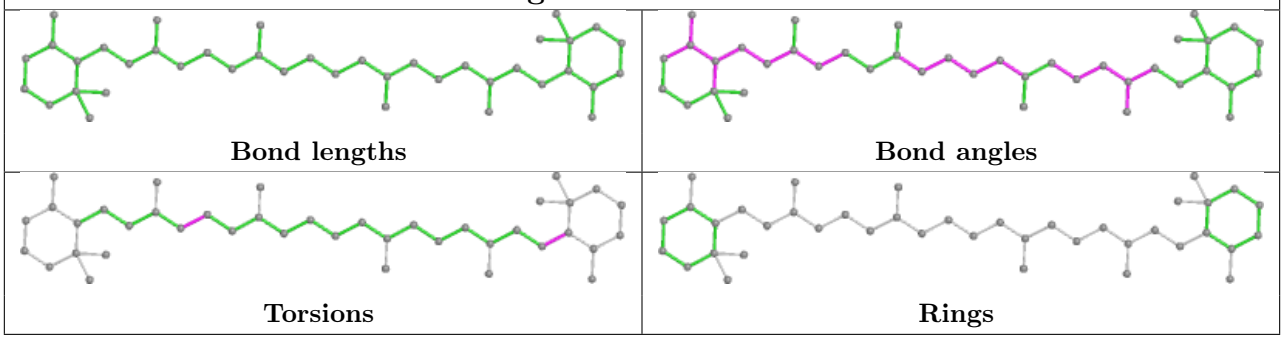


Ligand BCR 2 524



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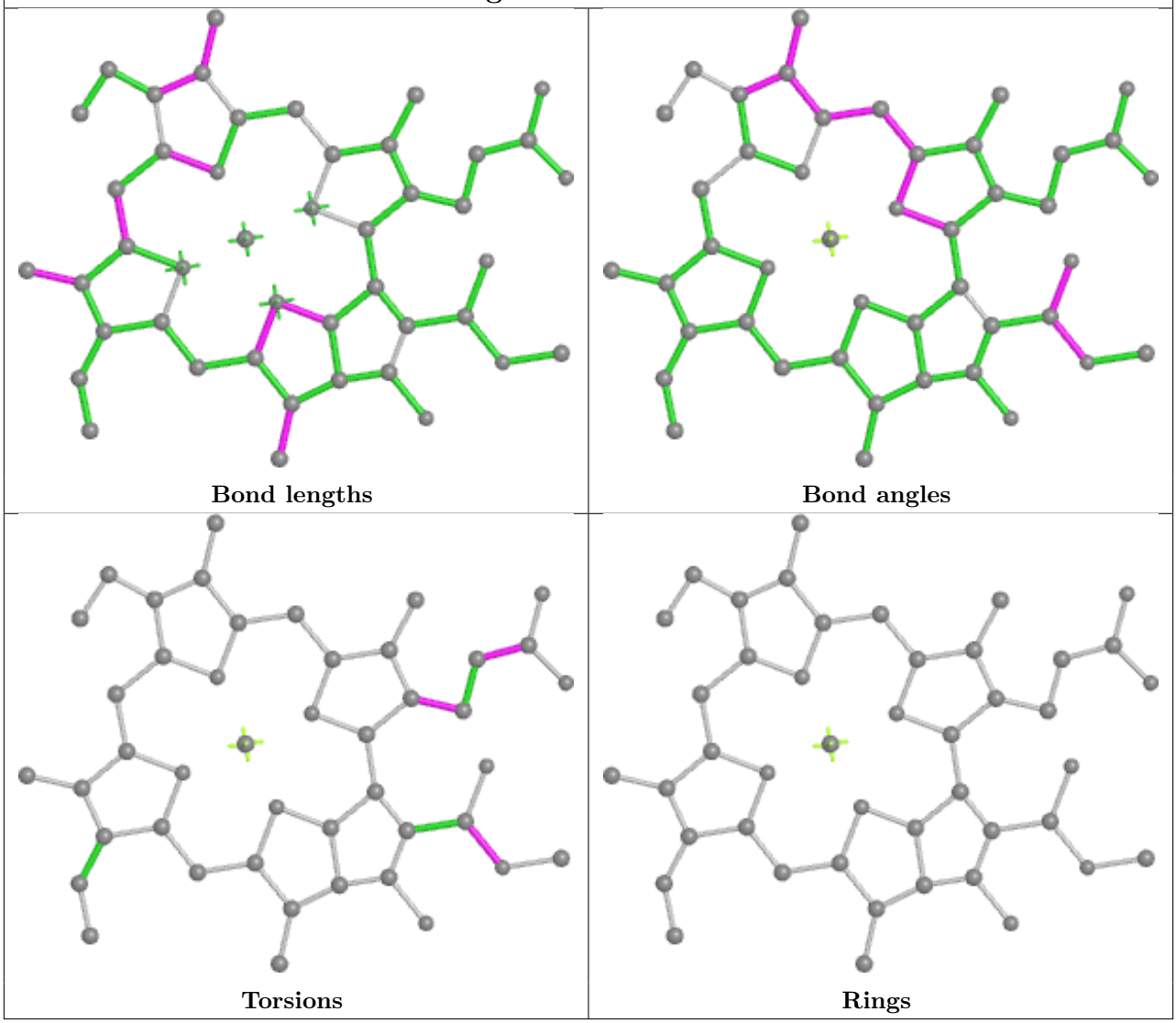

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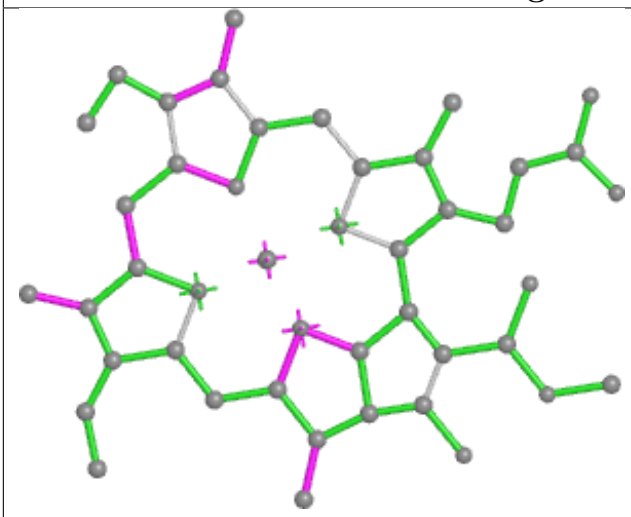
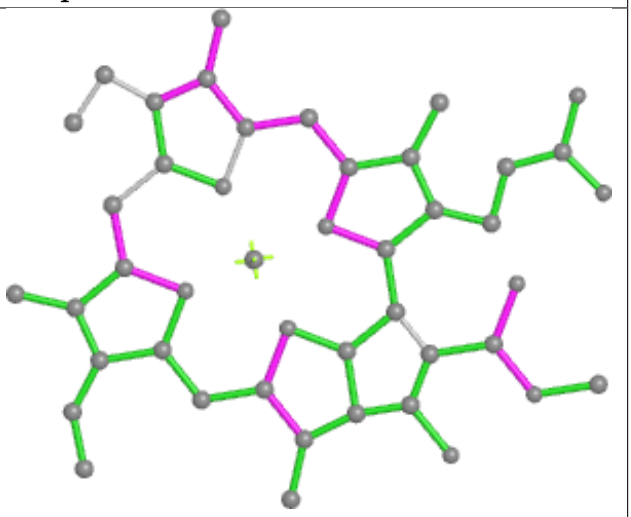
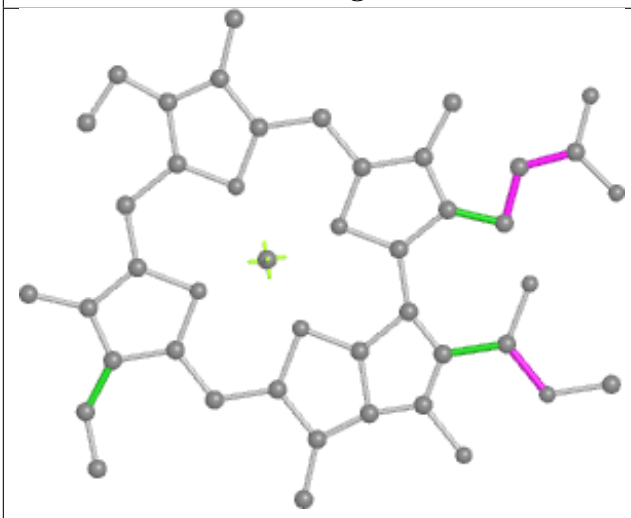


Bond lengths



Bond angles



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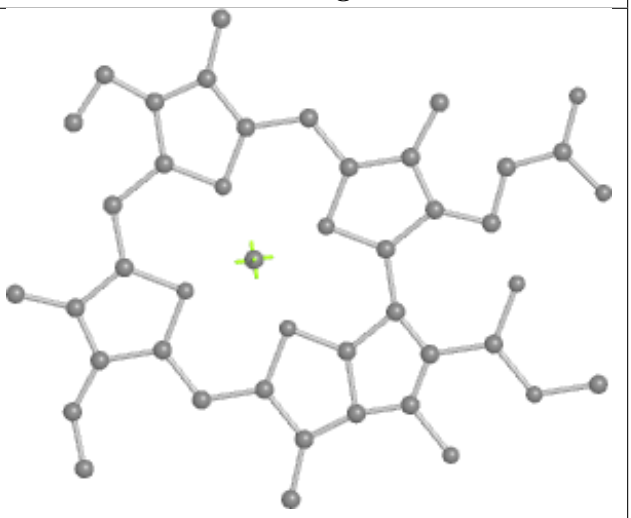

Rings

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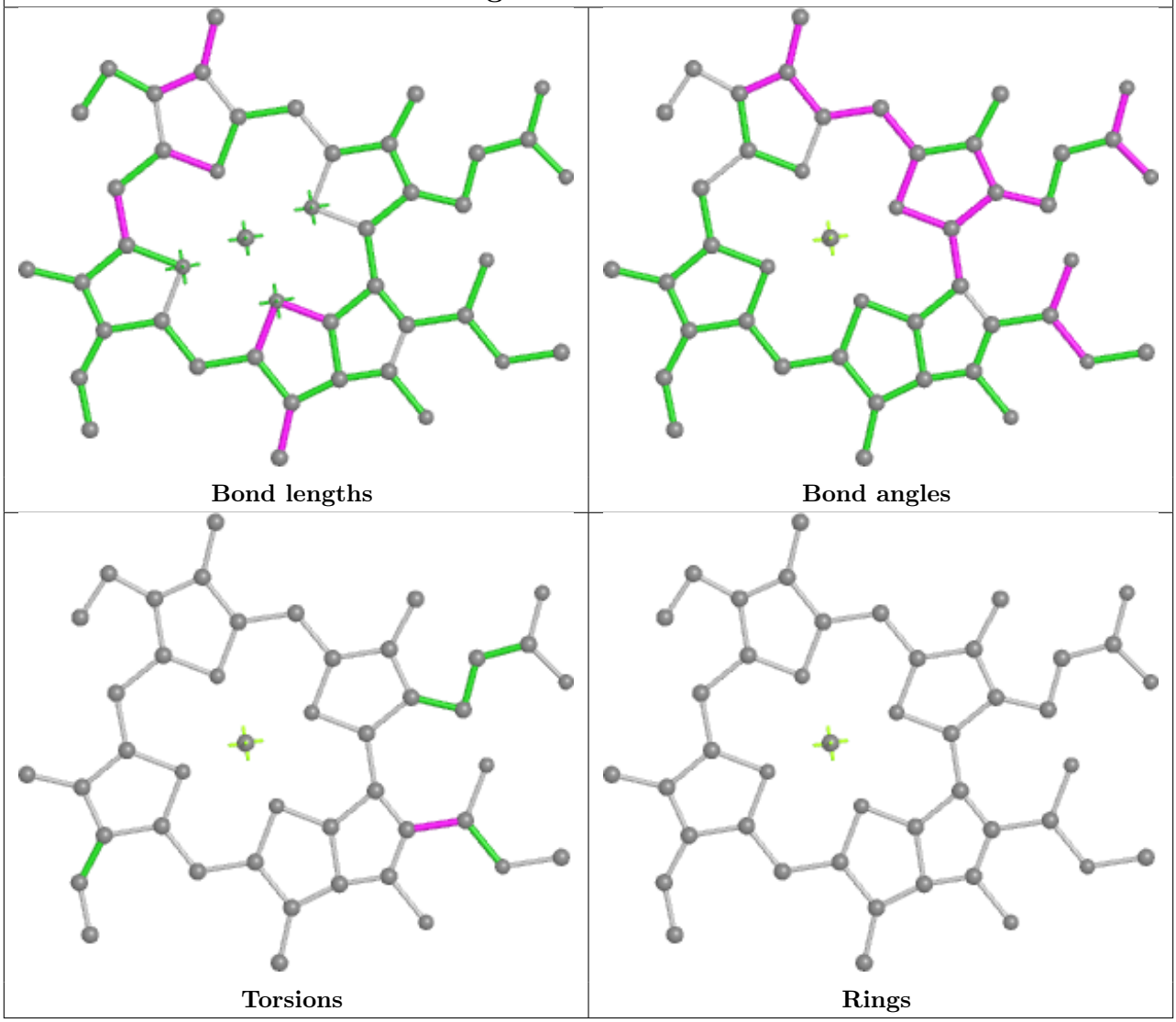

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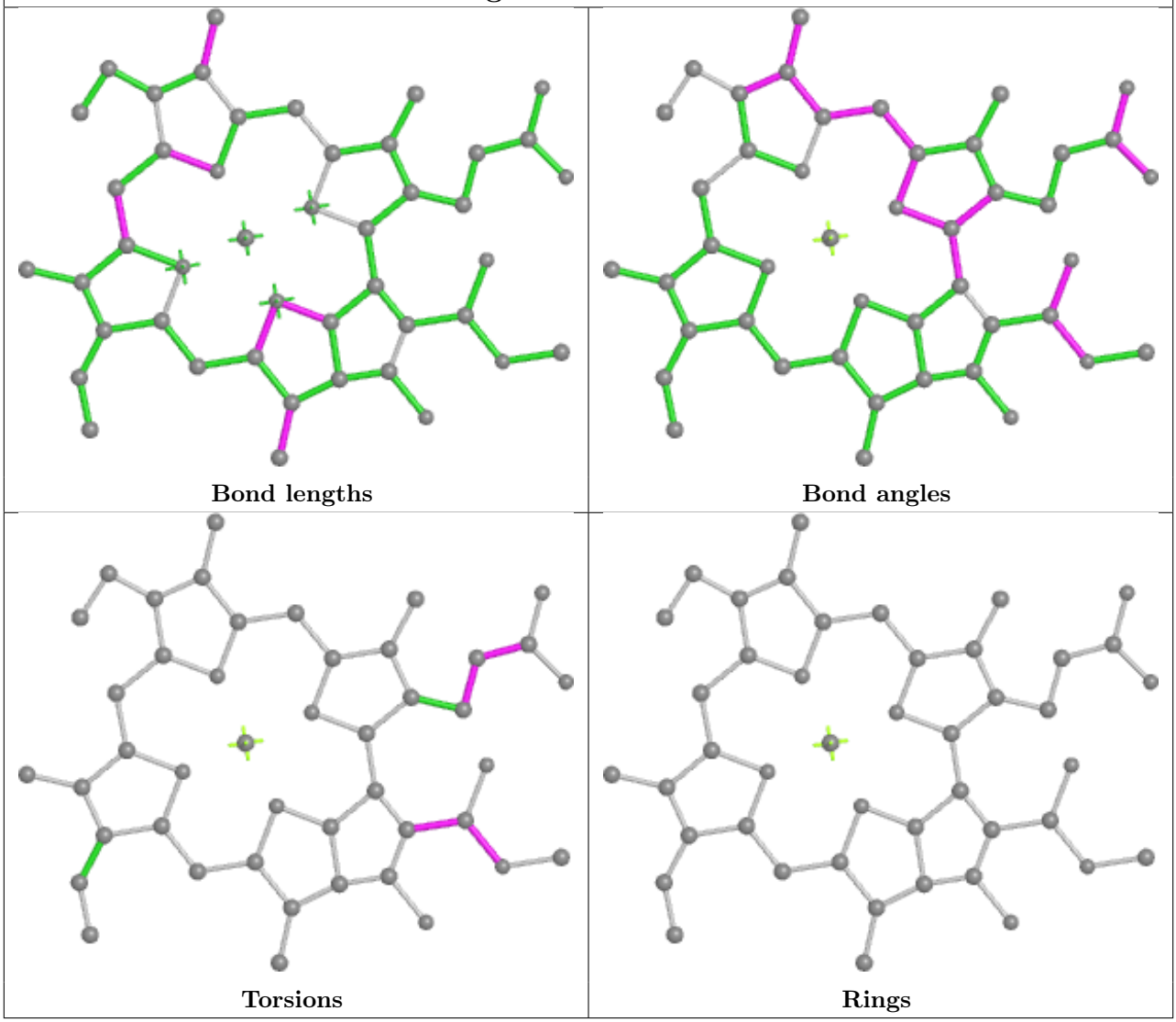

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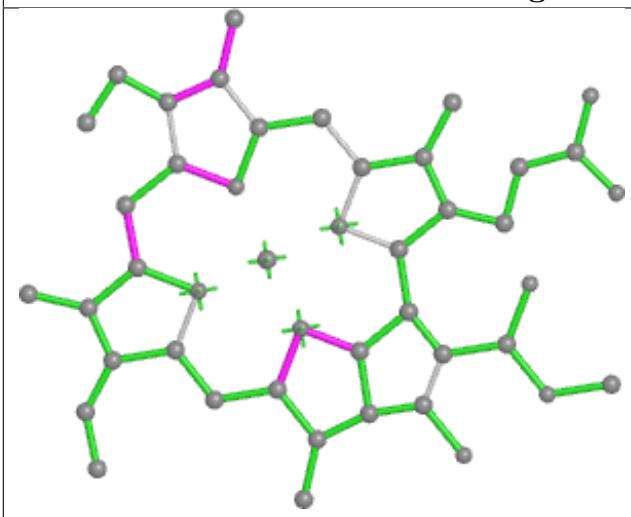

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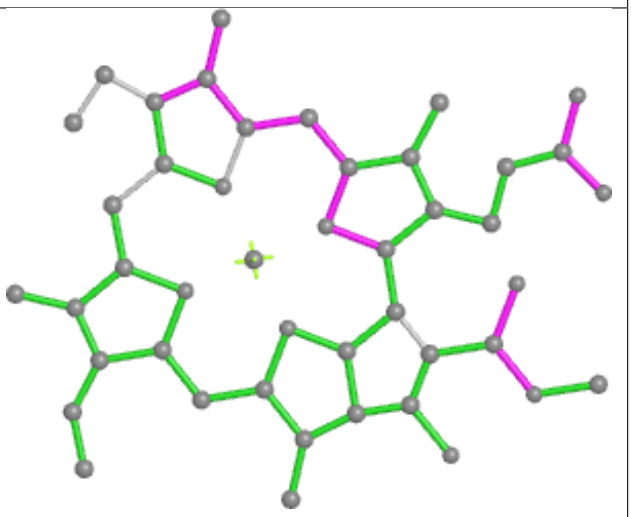

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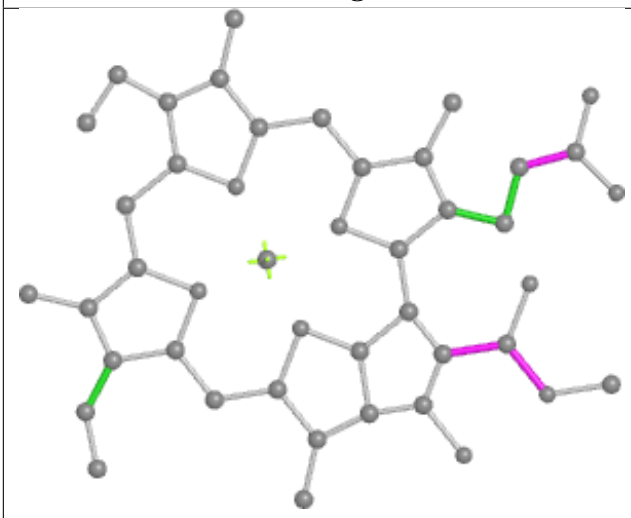

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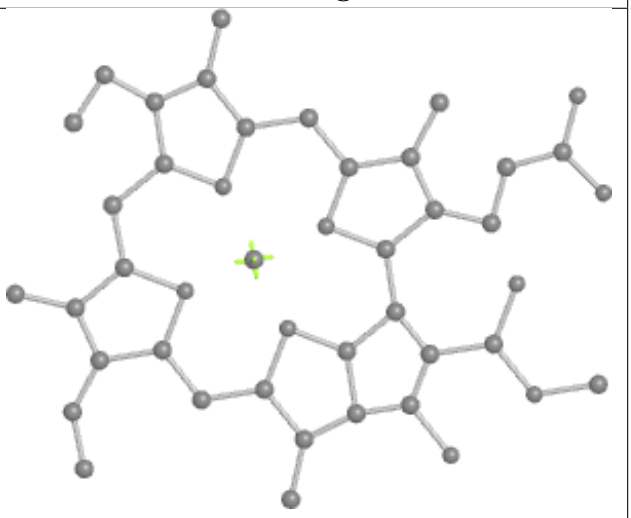
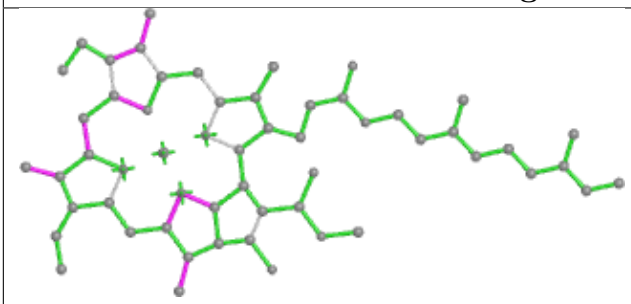
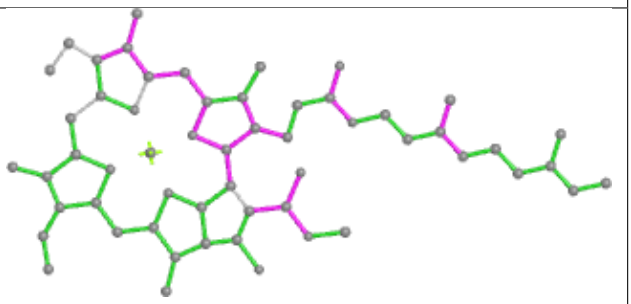
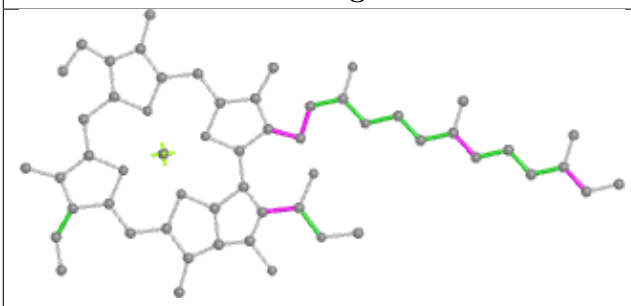
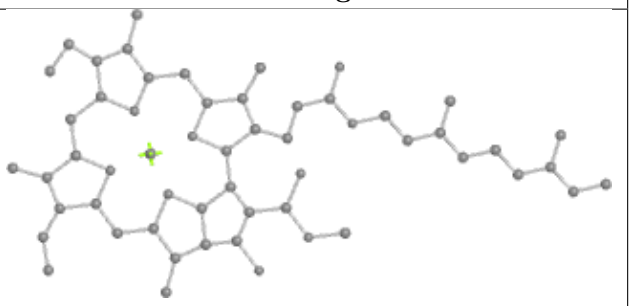
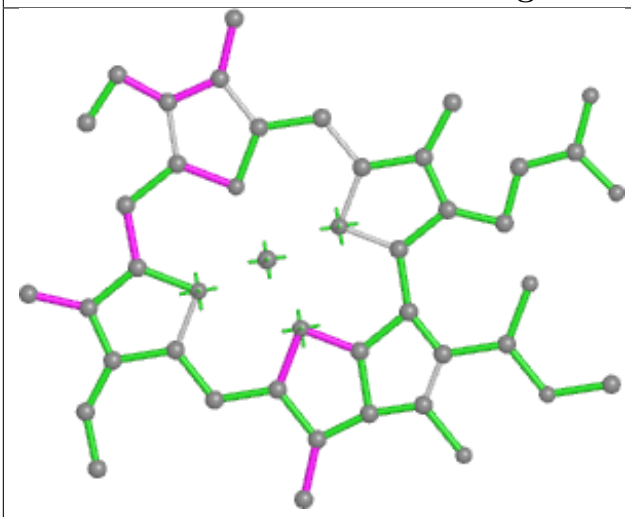


Rings

Ligand CLA e 1134	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 1302



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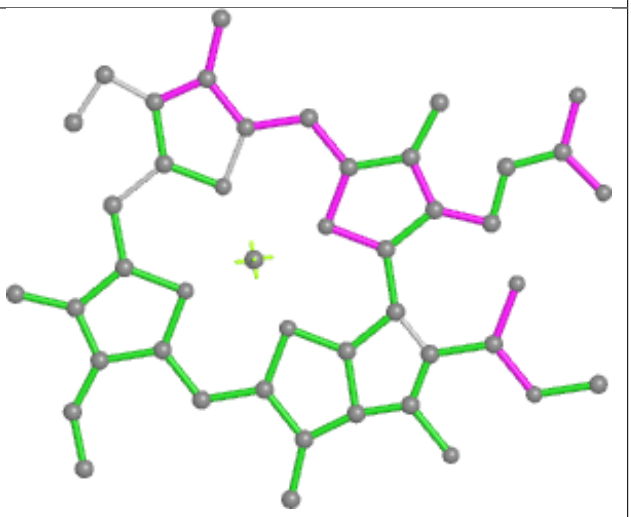
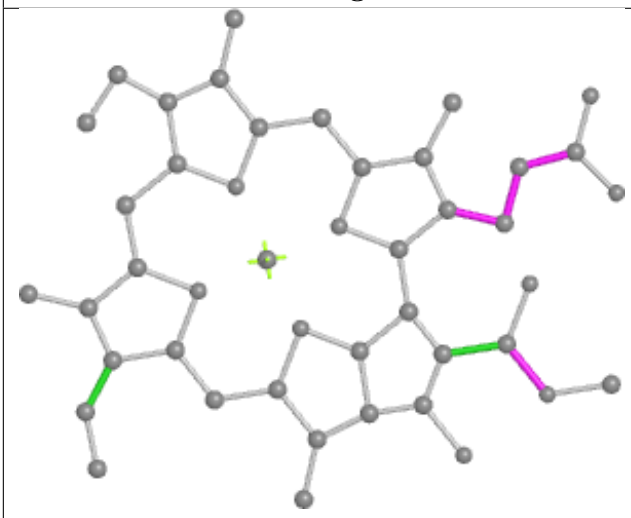


Bond angles



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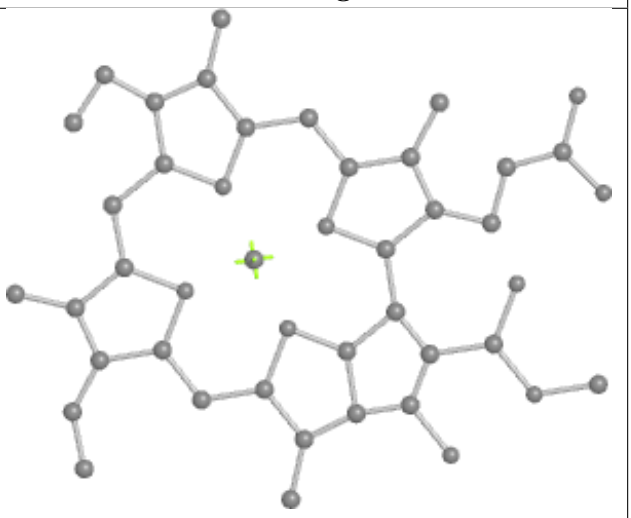
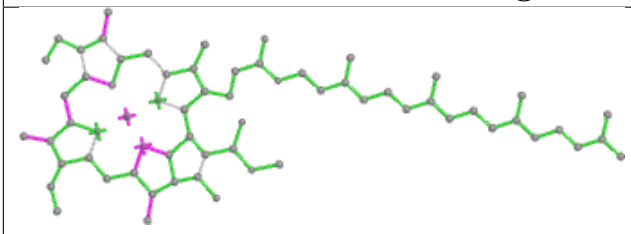


Rings

Ligand CLA B 1204



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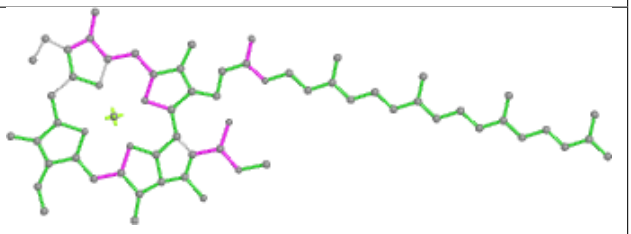

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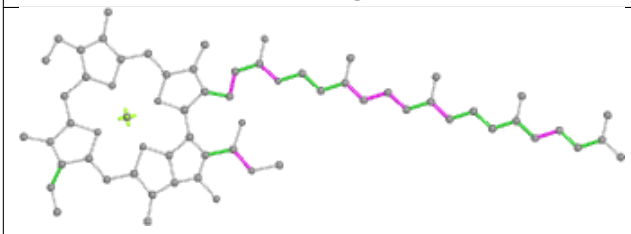

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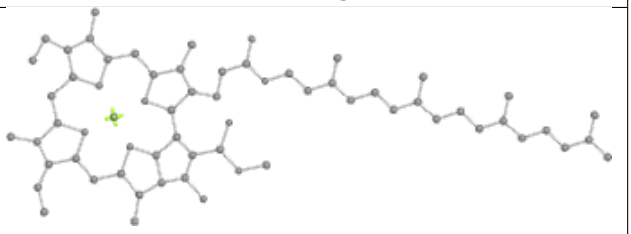
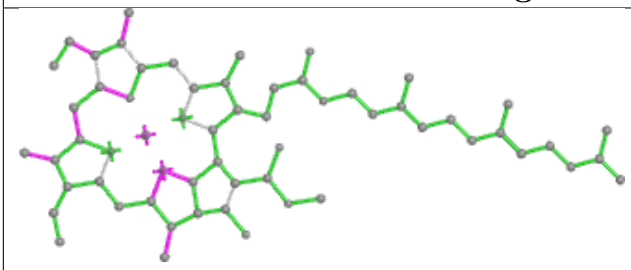


Rings

Ligand CLA A 1115



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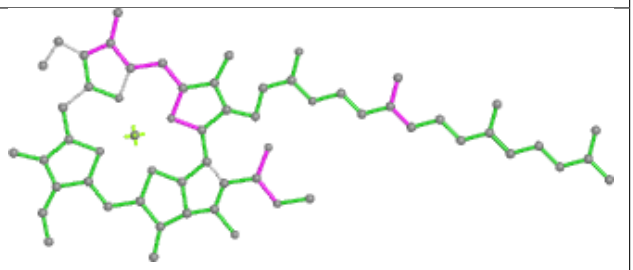

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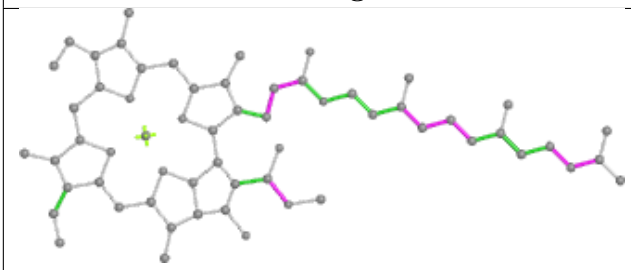

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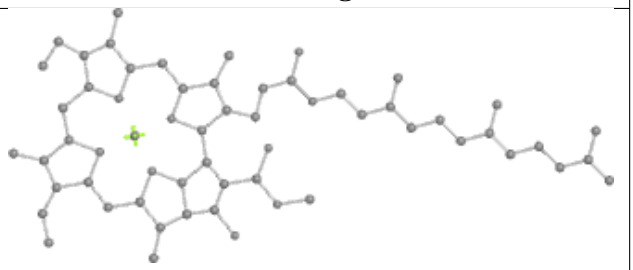
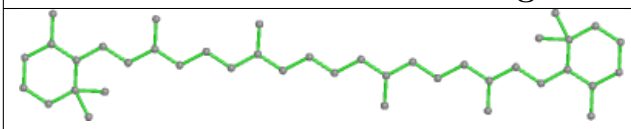


Rings

Ligand BCR J 4013



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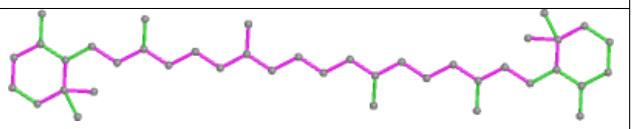
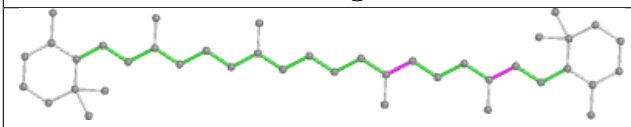


Bond angles



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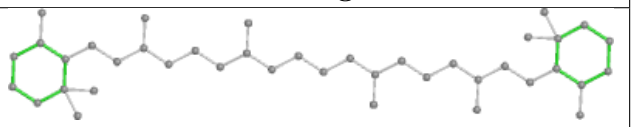
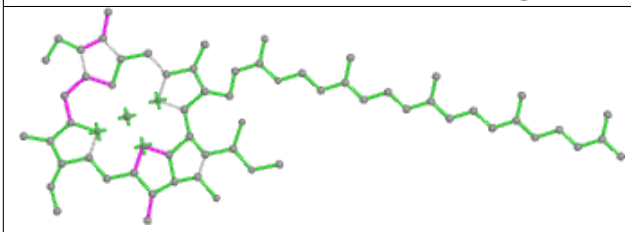


Rings

Ligand CLA B 1239



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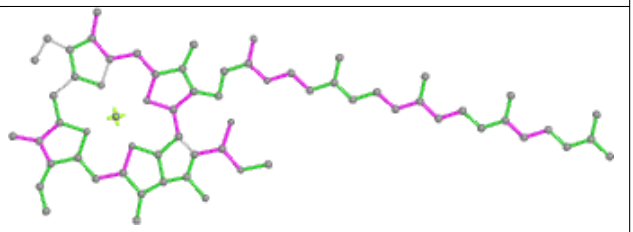

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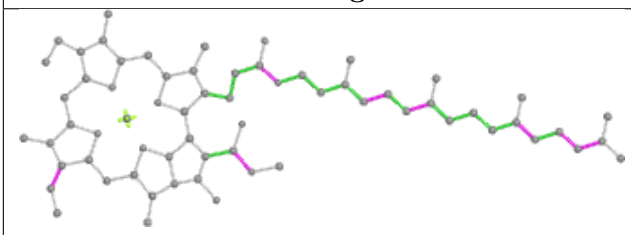

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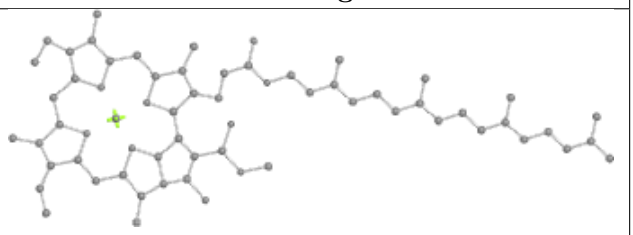
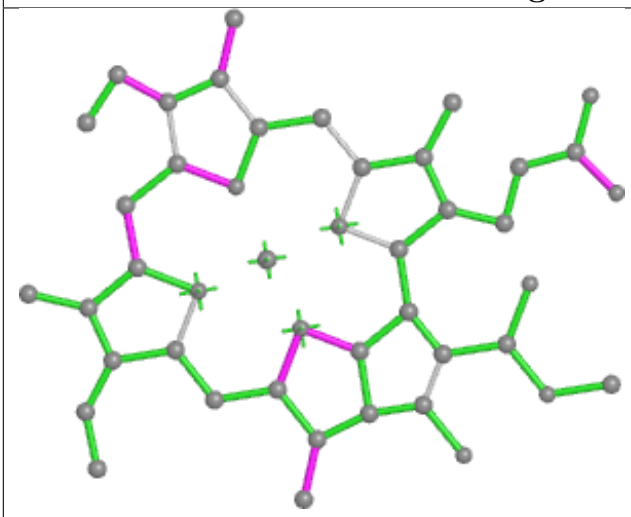


Rings

Ligand CLA 3 510



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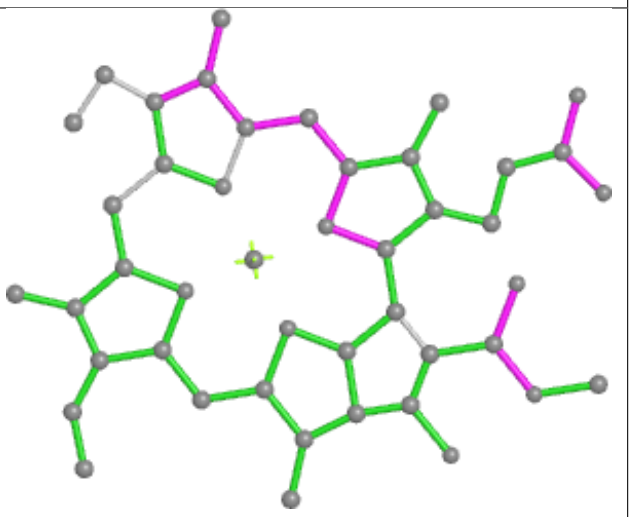
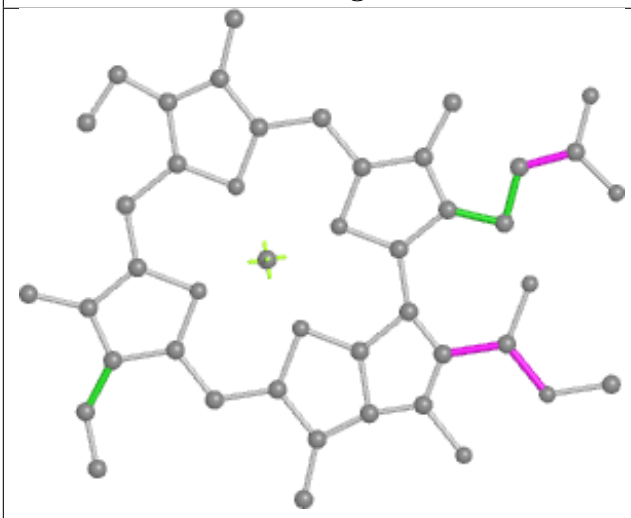
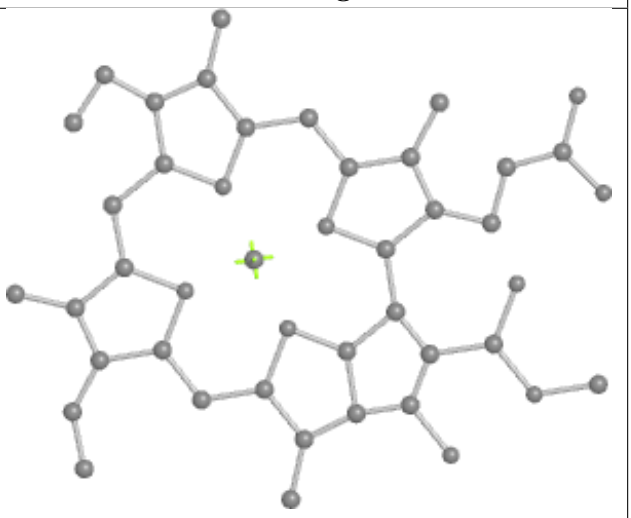


Bond angles

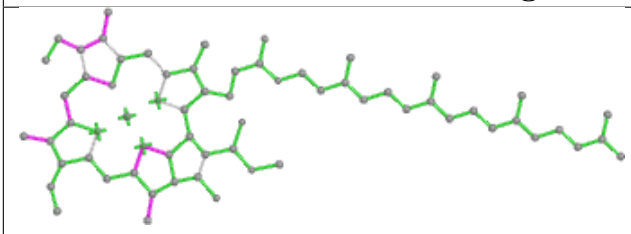


Torsions

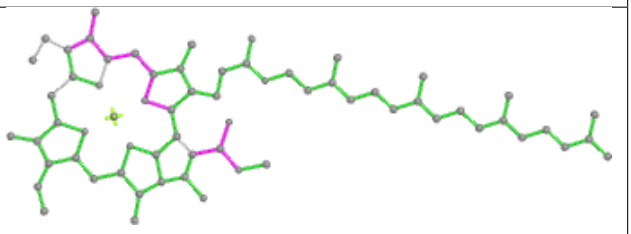


Rings

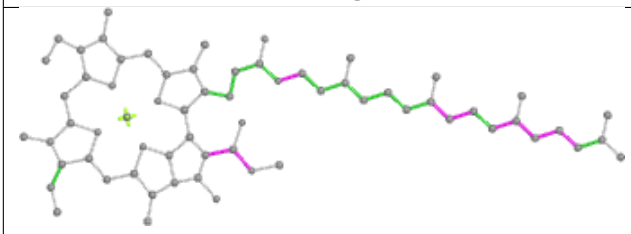
Ligand CLA e 1138



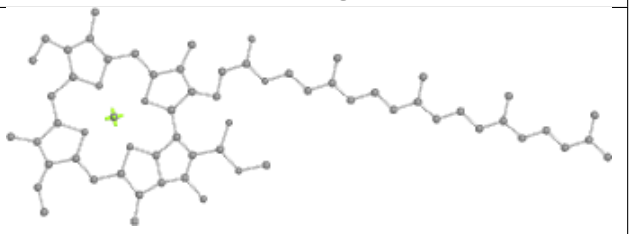
Bond lengths



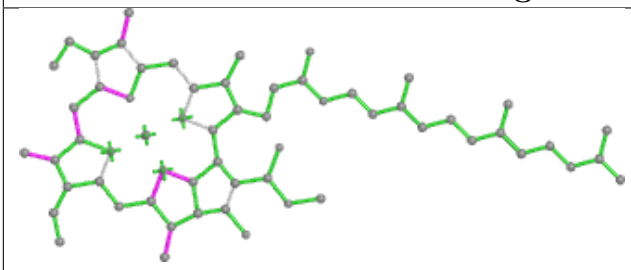
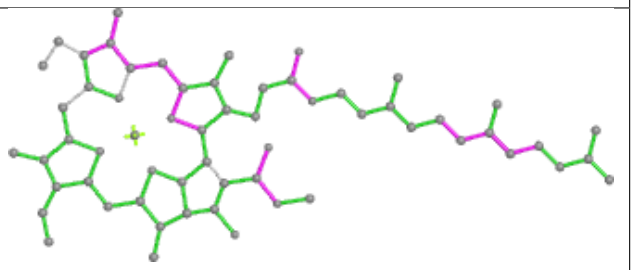
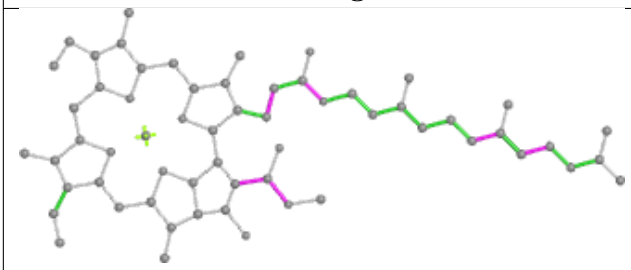
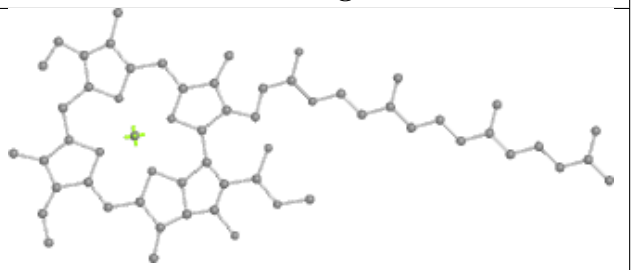
Bond angles



Torsions



Rings

Ligand CLA H 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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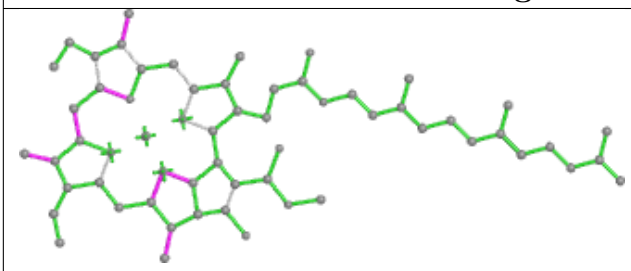
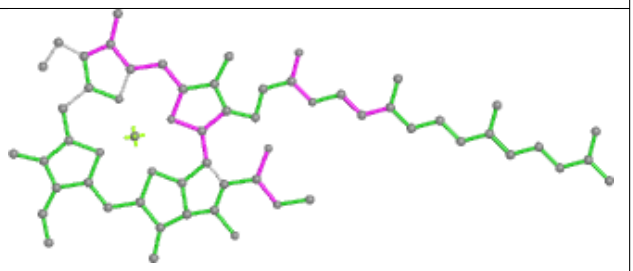
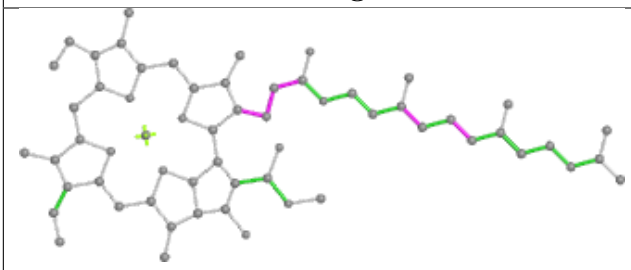
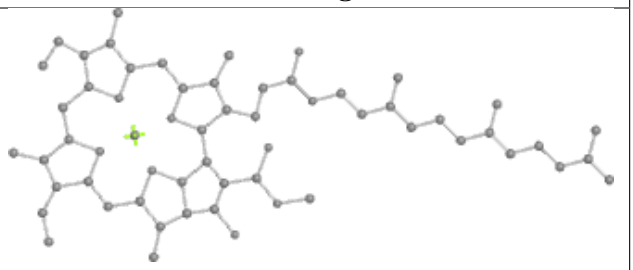
 Bond lengths	 Bond angles
 Torsions	 Rings

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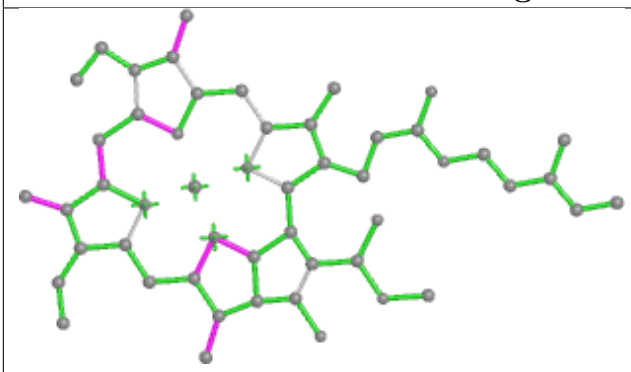

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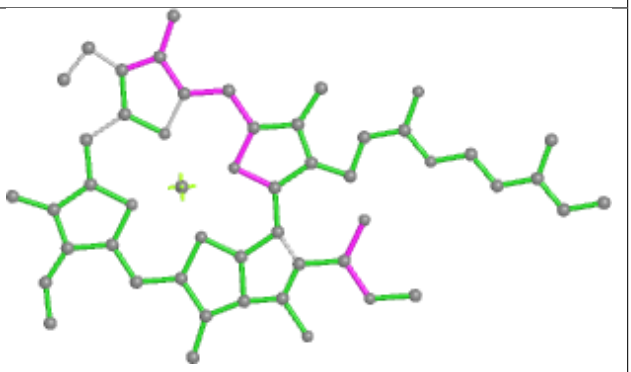
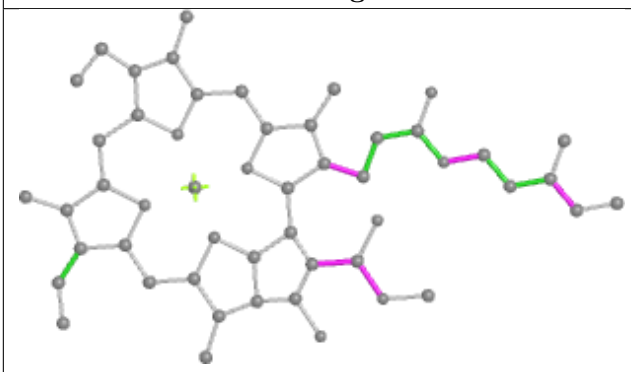


Bond angles



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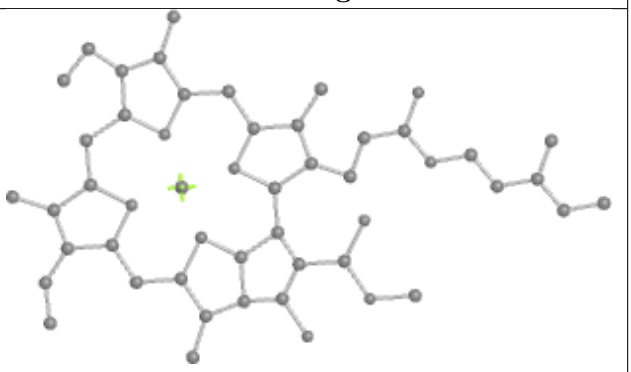
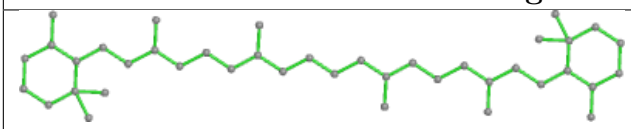


Rings

Ligand BCR d 524



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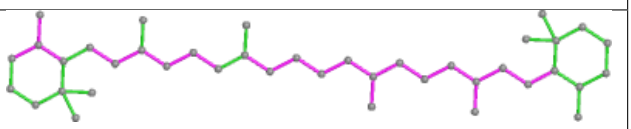
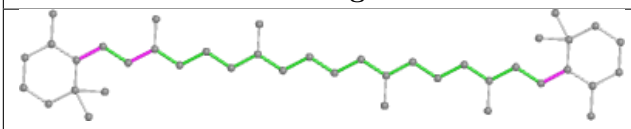


Bond angles



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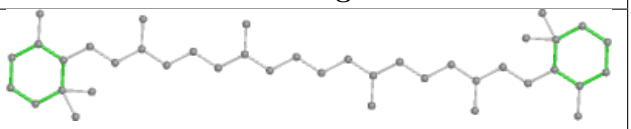
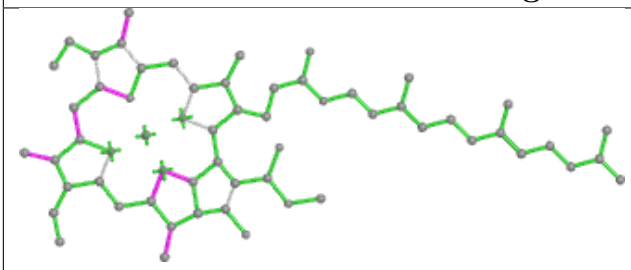


Rings

Ligand CLA f 1201



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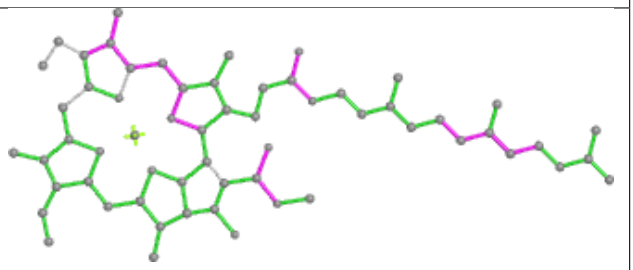
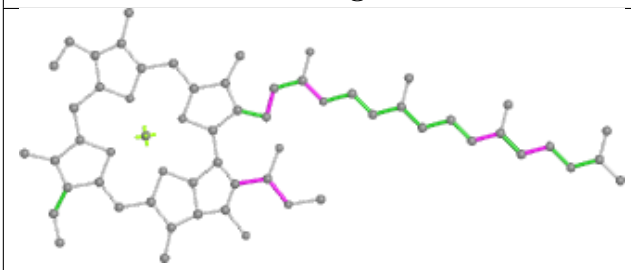


Bond angles



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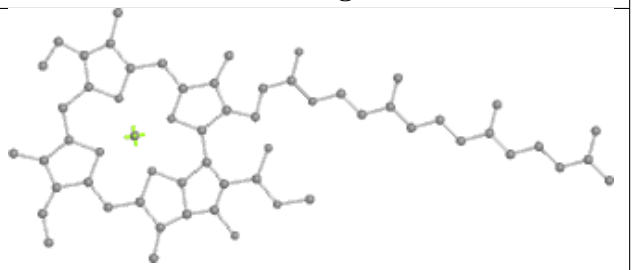
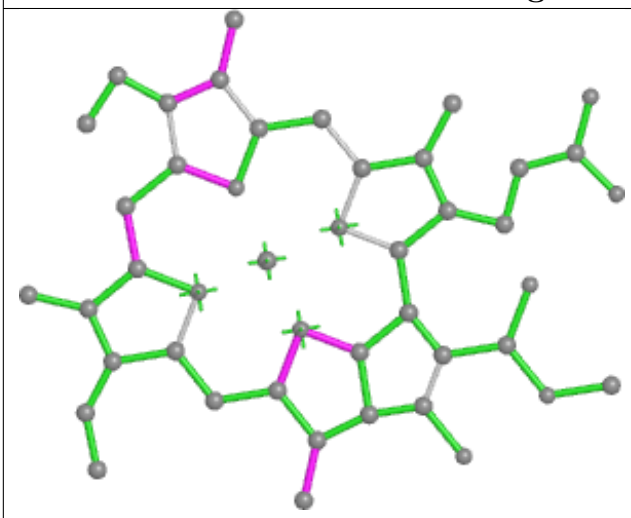


Rings

Ligand CLA u 503



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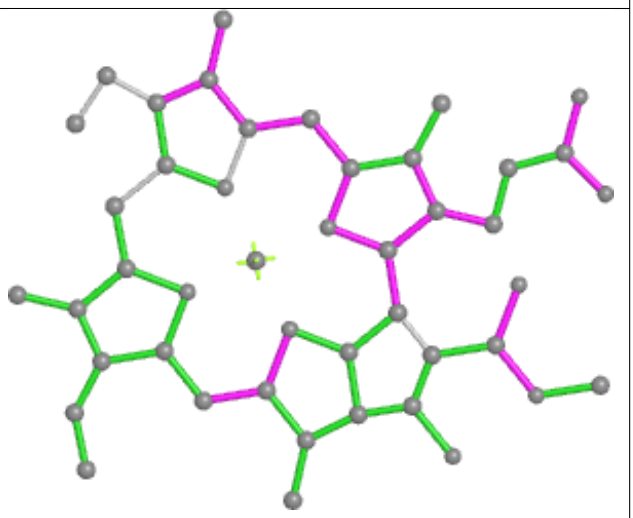
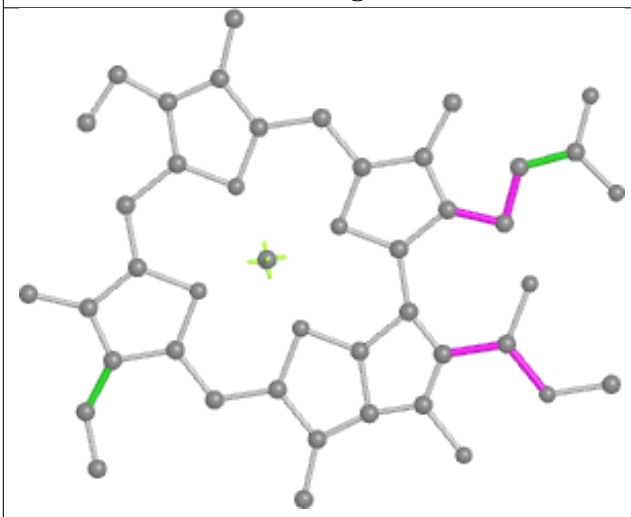


Bond angles



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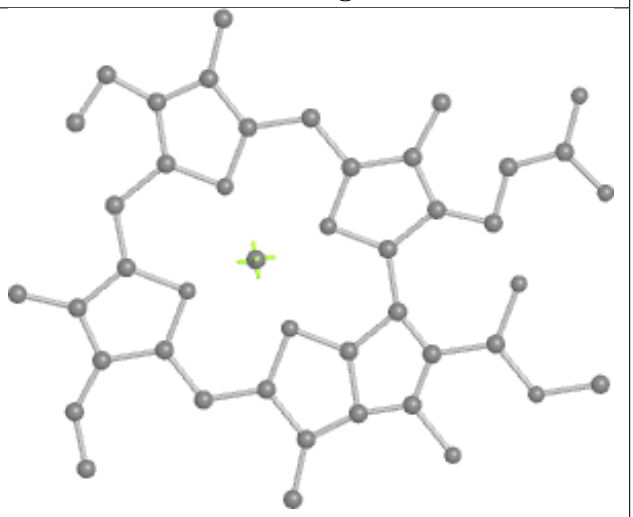
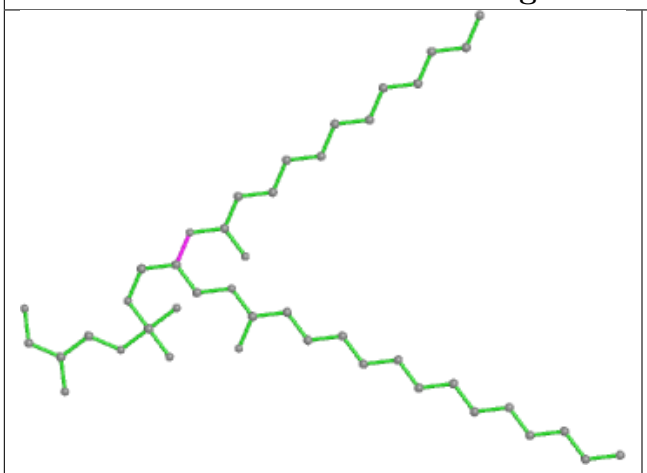


Rings

Ligand LHG e 5005



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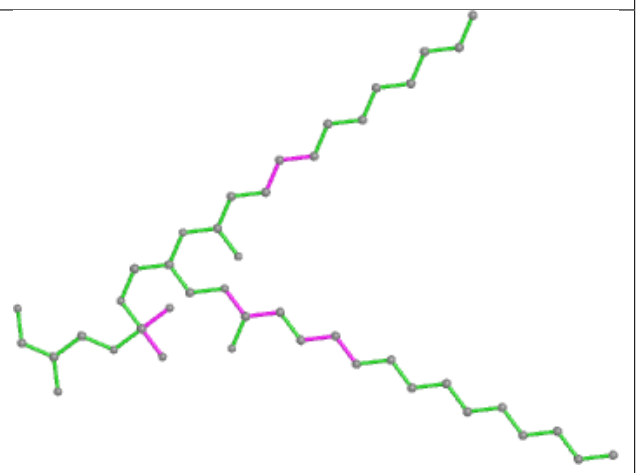

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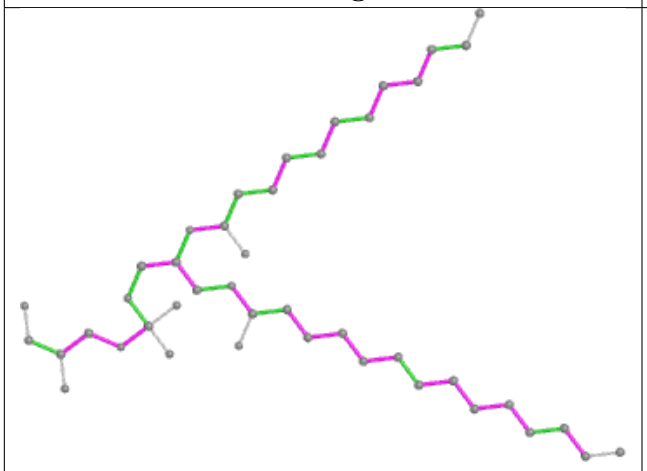

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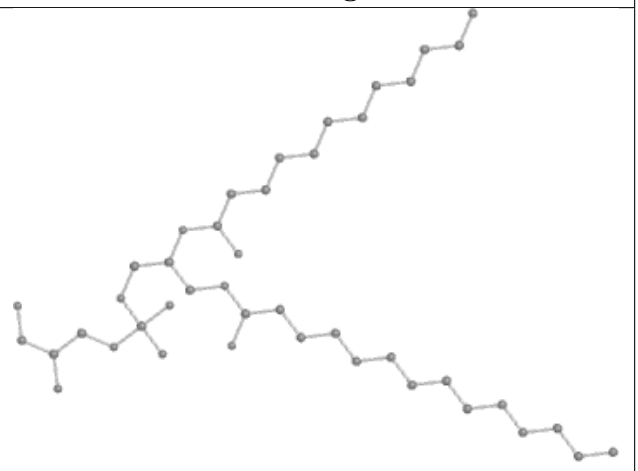
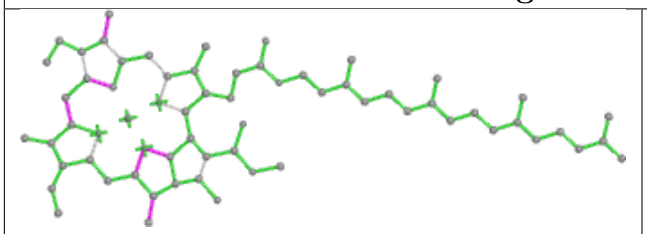
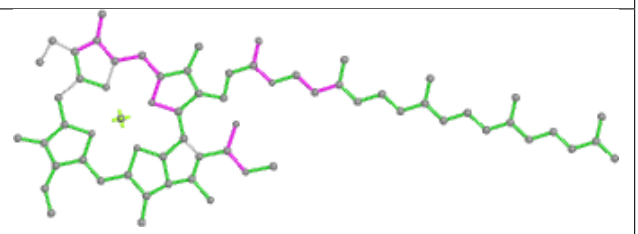


Rings

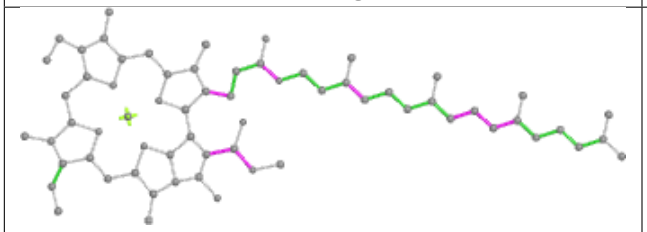
Ligand CLA B 1240



Bond lengths



Bond angles



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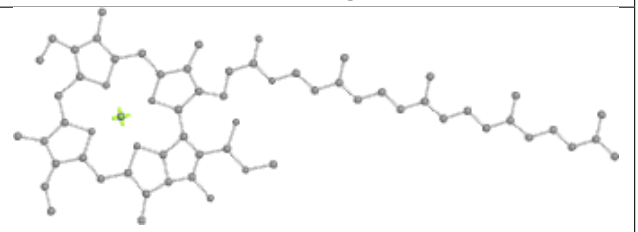

Rings

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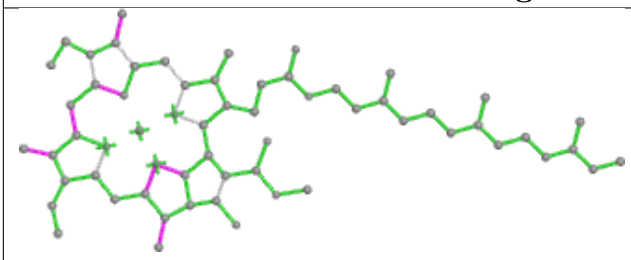
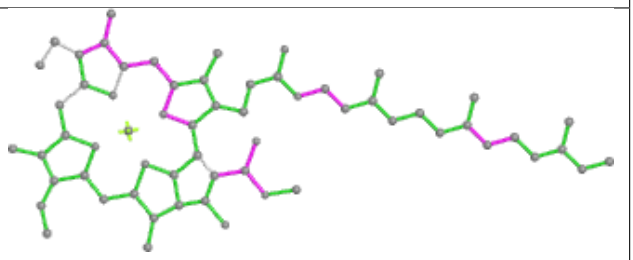
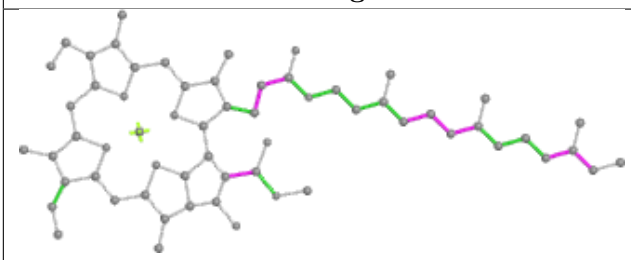
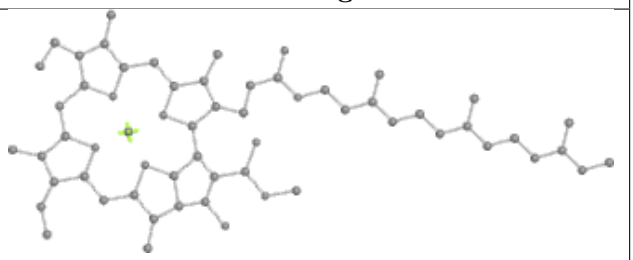
 Bond lengths	 Bond angles
 Torsions	 Rings

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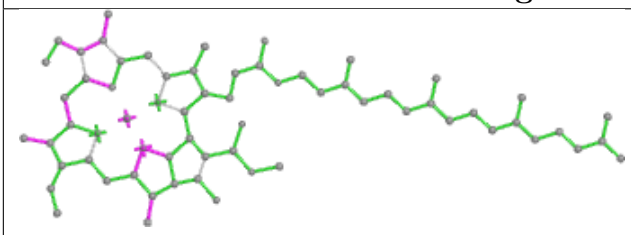
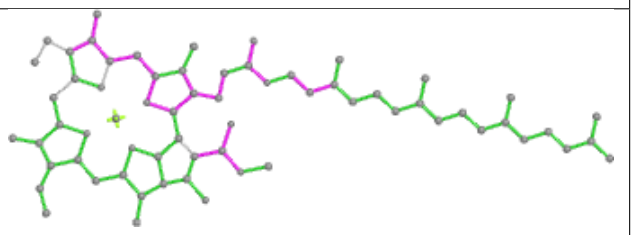
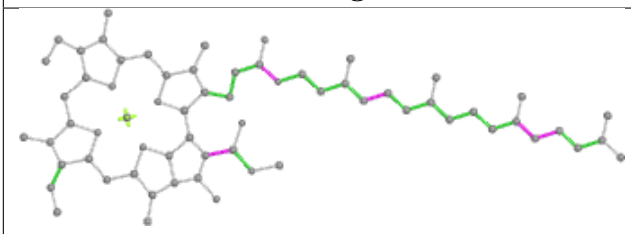
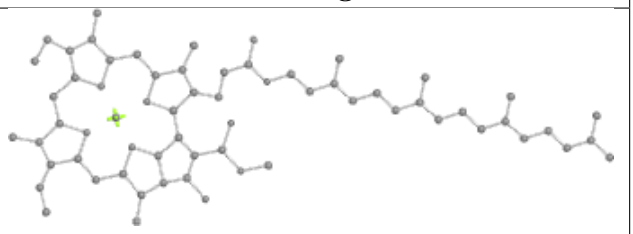
 Bond lengths	 Bond angles
 Torsions	 Rings

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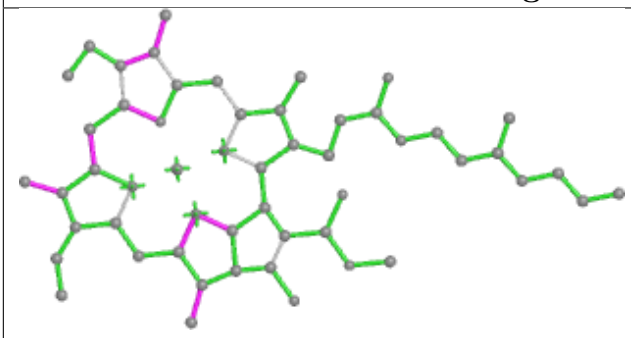
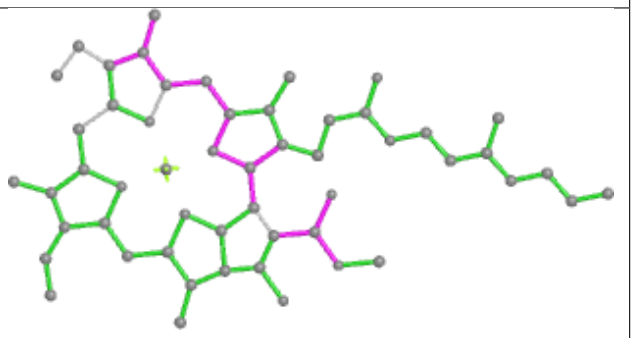
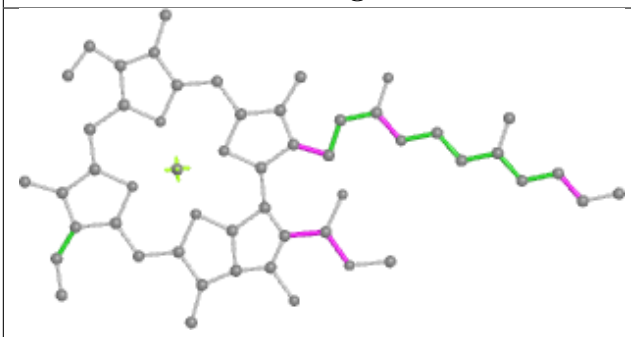
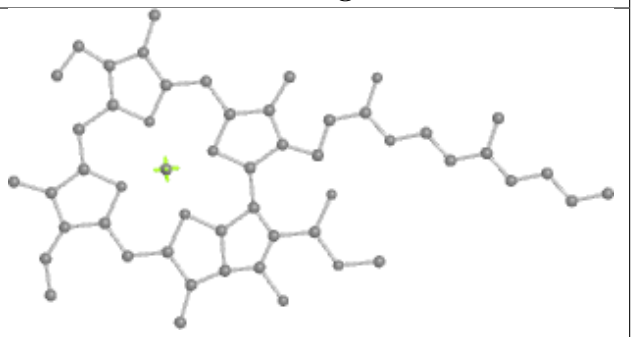
 Bond lengths	 Bond angles
 Torsions	 Rings

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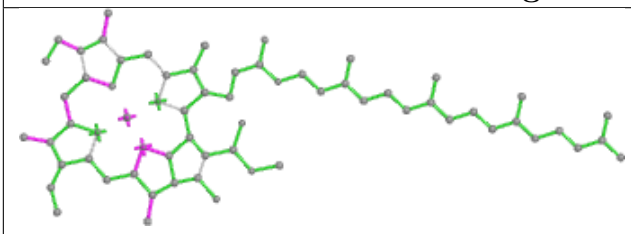
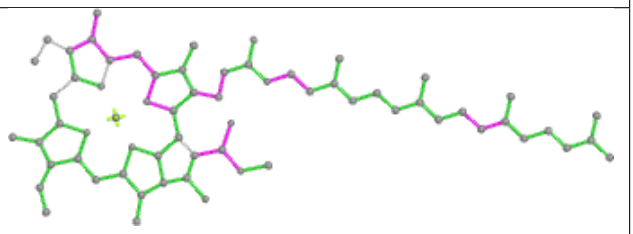
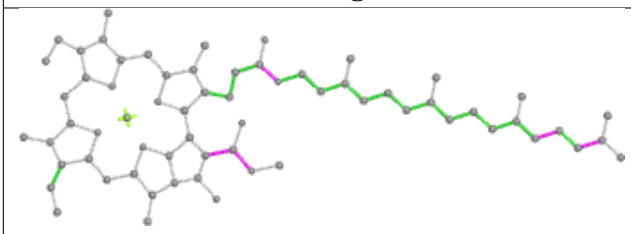
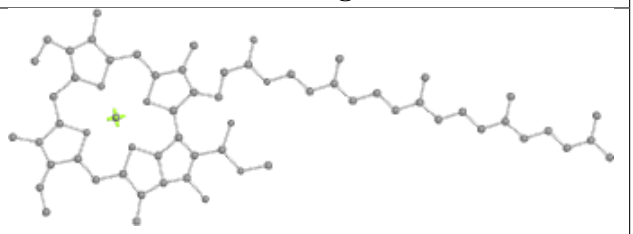
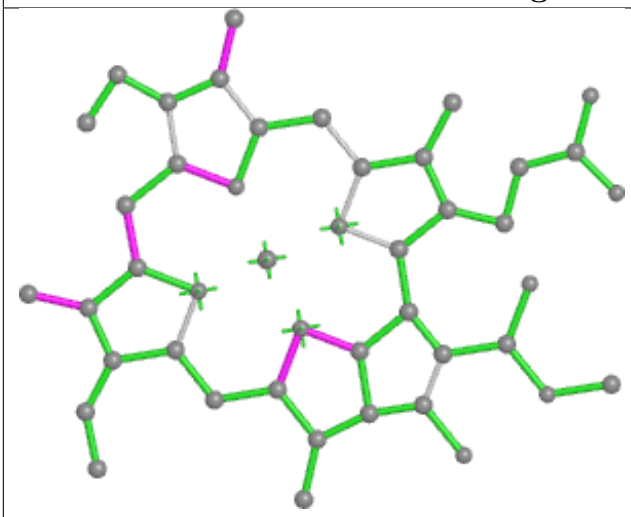
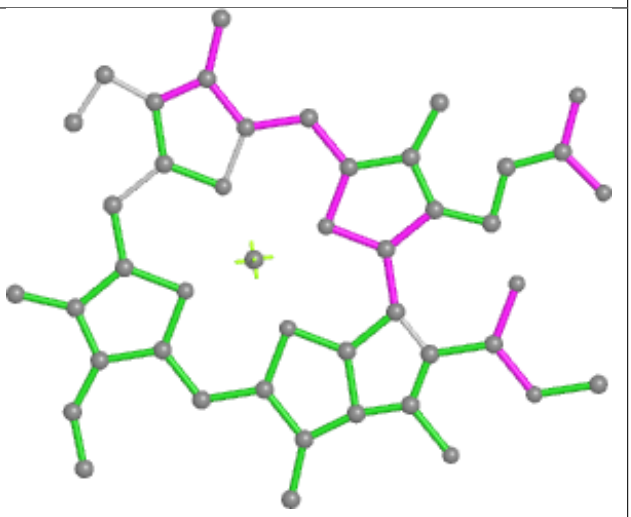
 Bond lengths	 Bond angles
 Torsions	 Rings

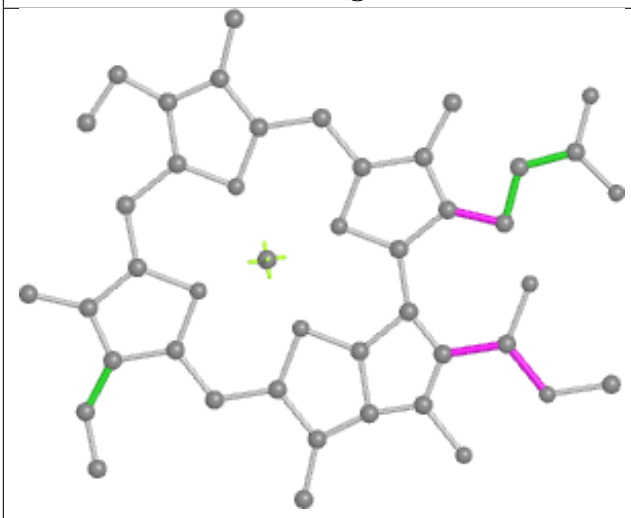
Ligand CLA t 517



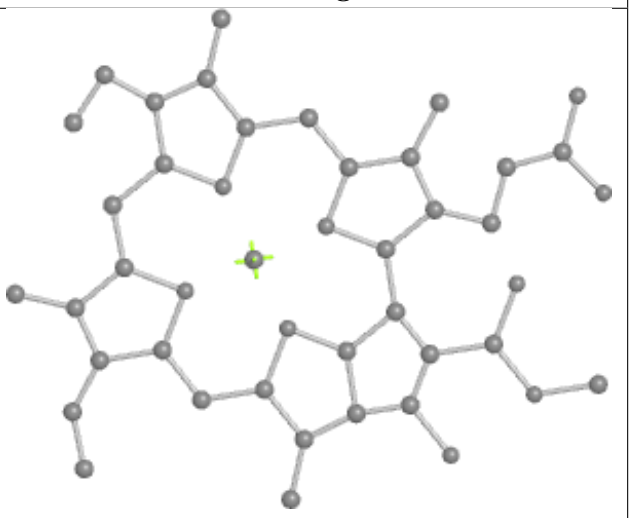
Bond lengths



Bond angles

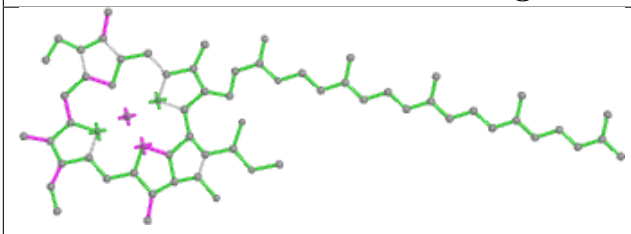


Torsions



Rings

Ligand CLA G 1013



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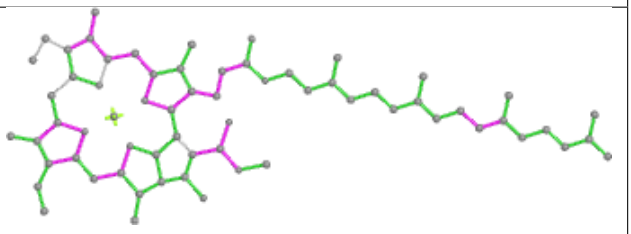
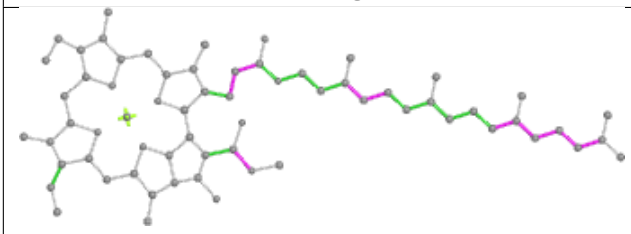


Bond angles



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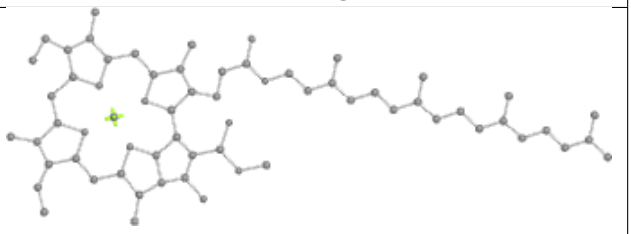
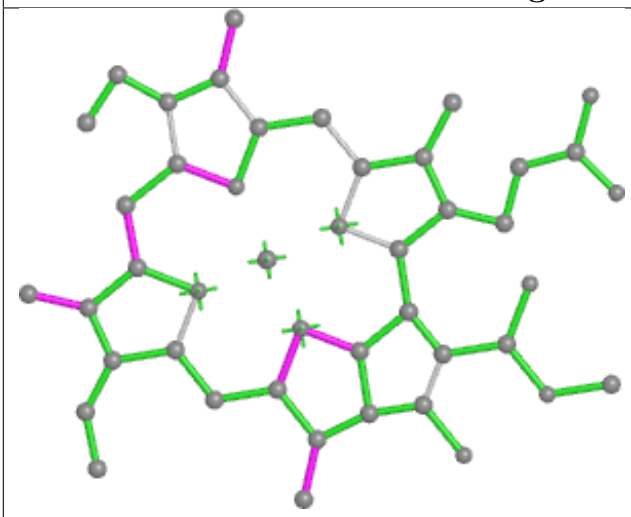


Rings

Ligand CLA a 506



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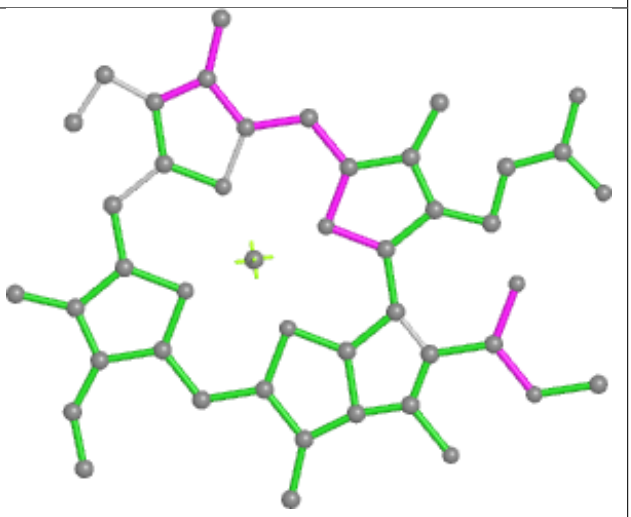
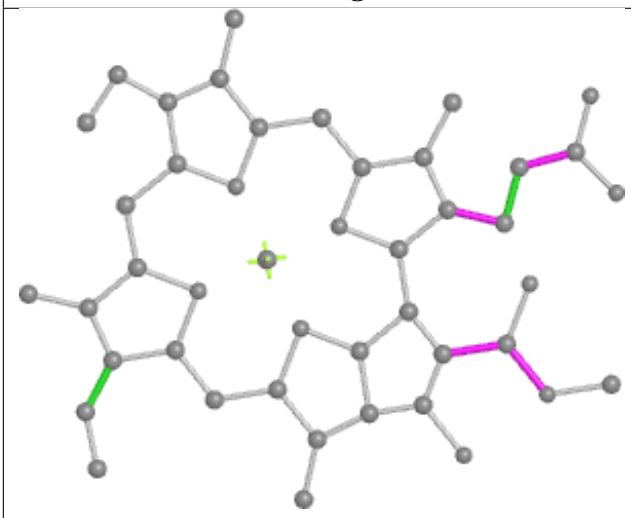


Bond angles



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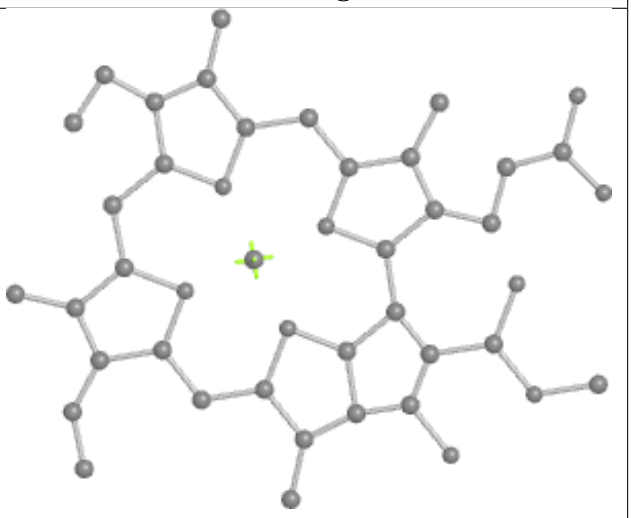
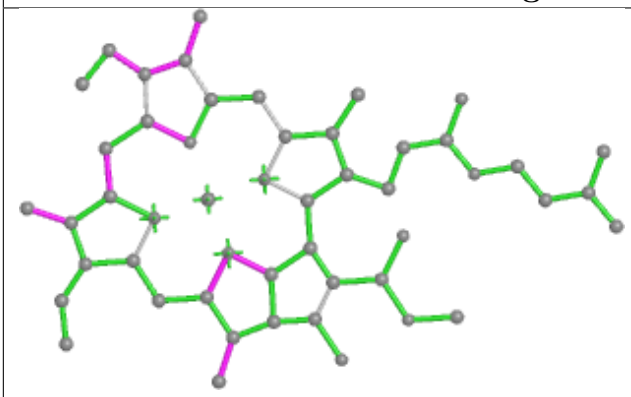
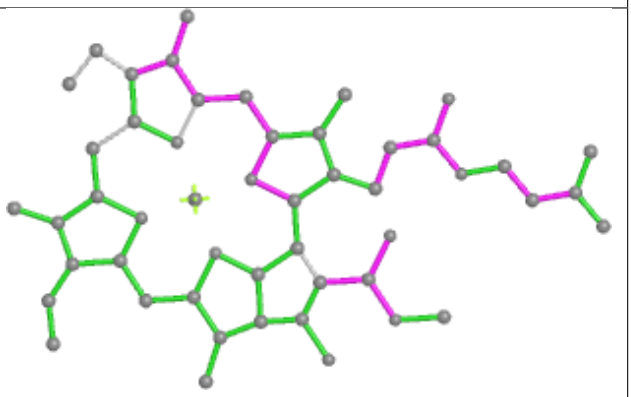
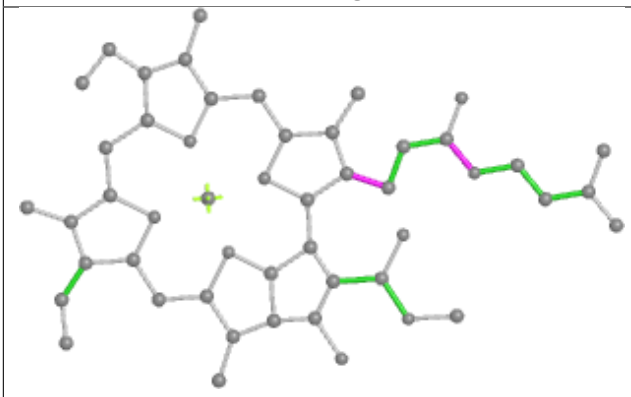
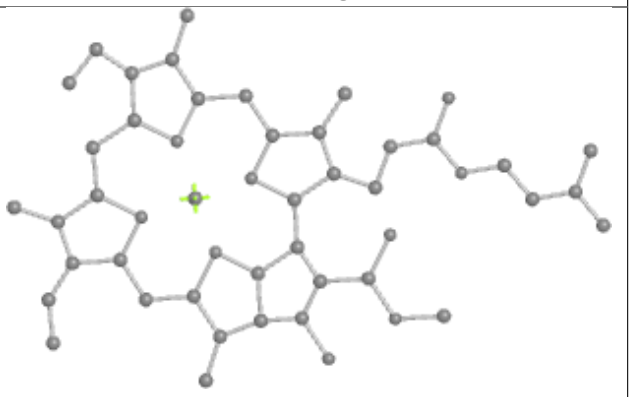
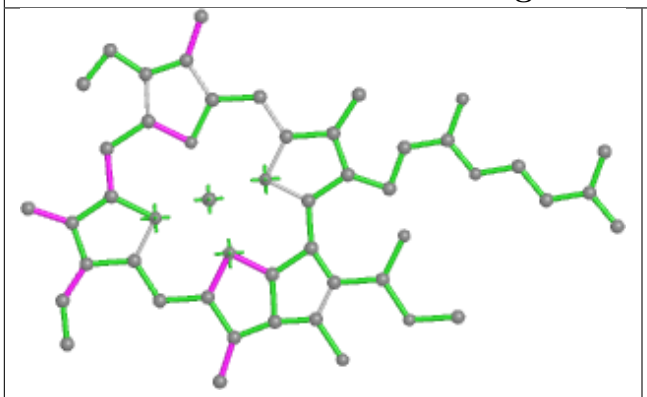


Rings

Ligand CLA f 1236	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1120



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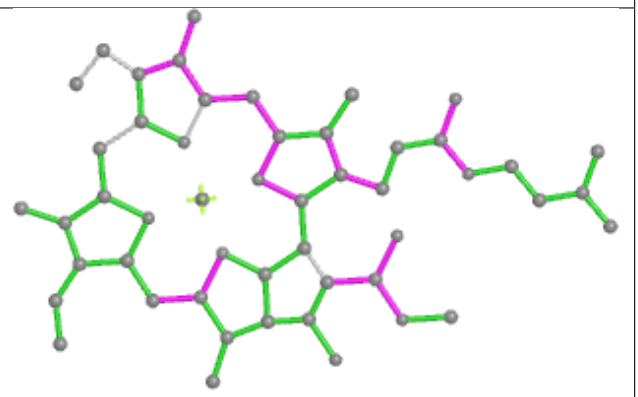

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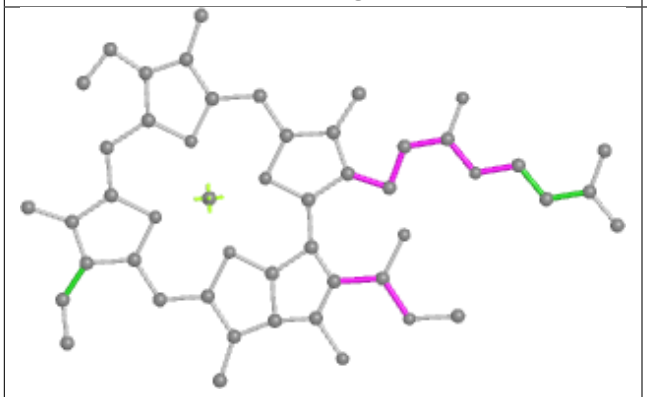

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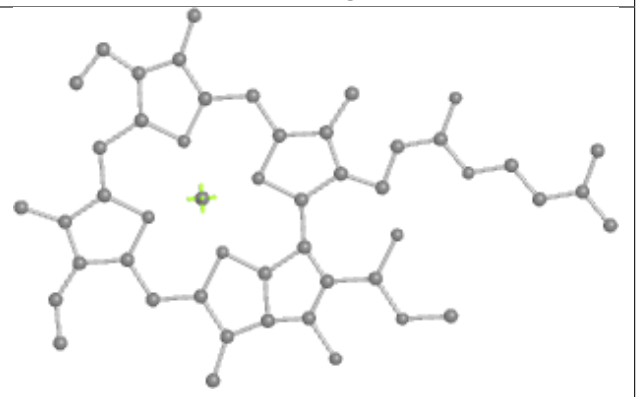
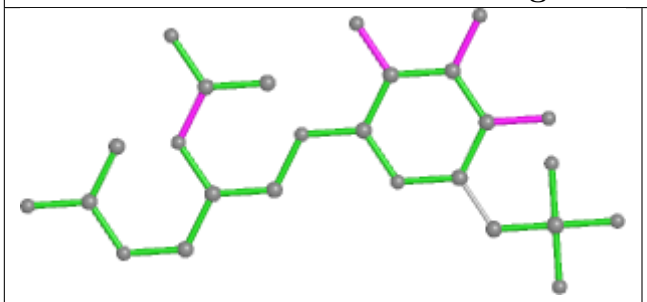


Rings

Ligand SQD 4 822



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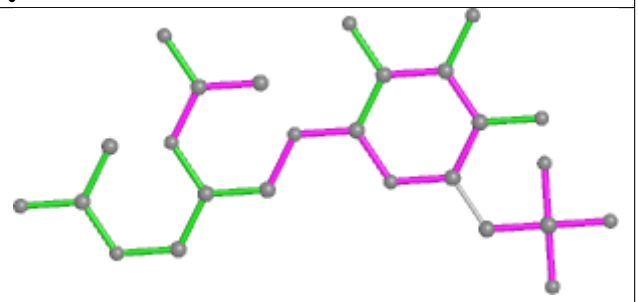

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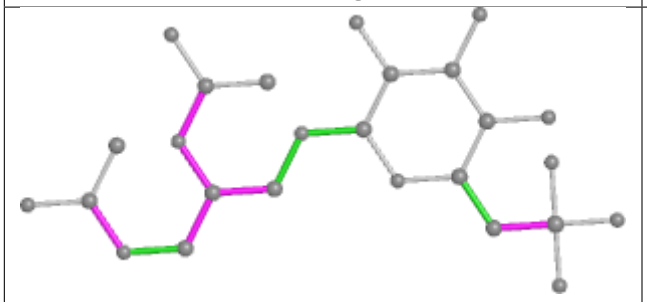

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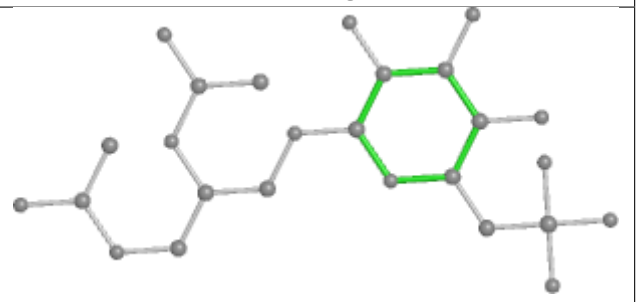
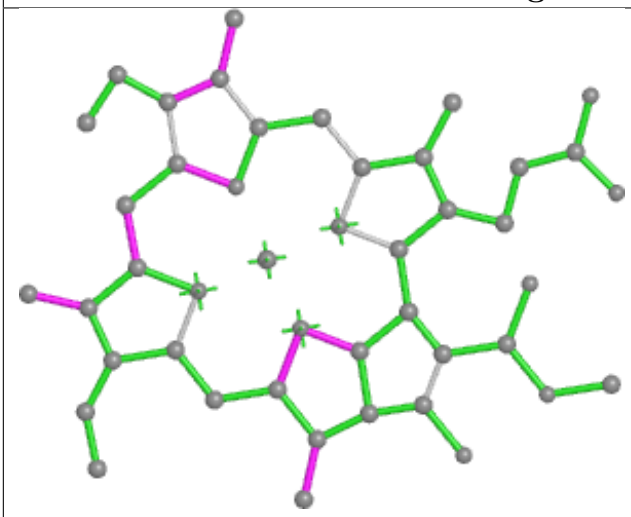


Rings

Ligand CLA u 504



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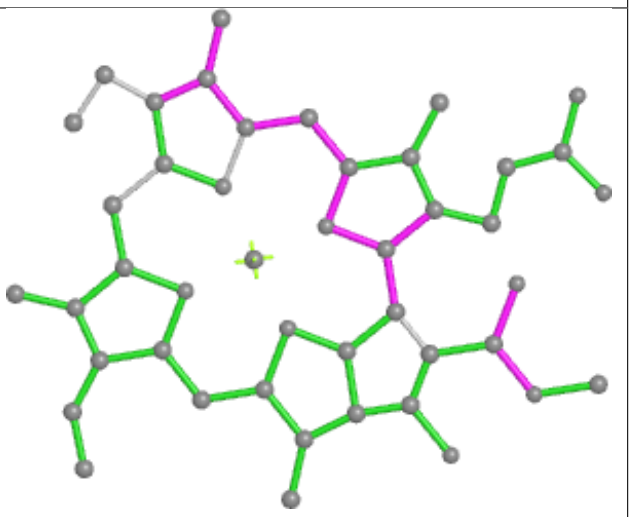

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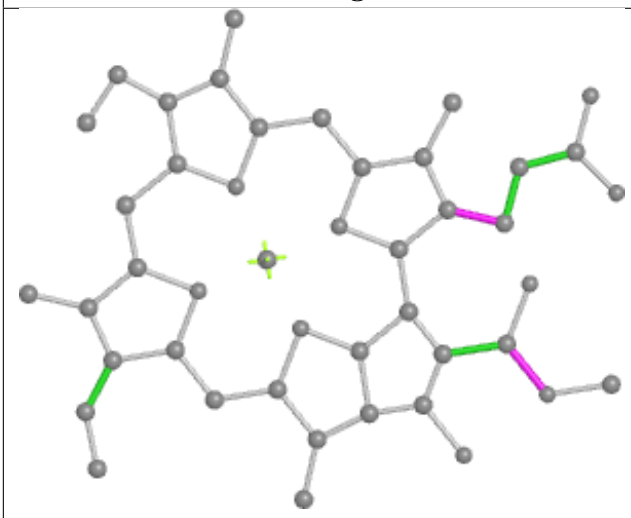

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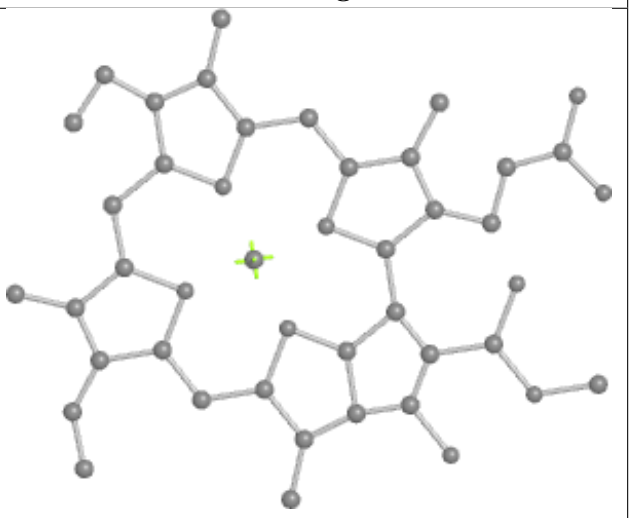

Rings

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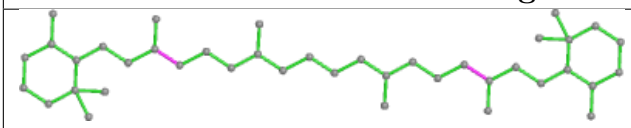

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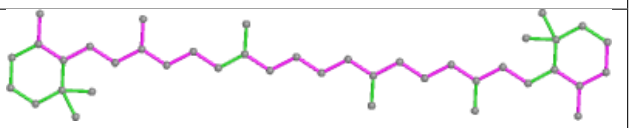

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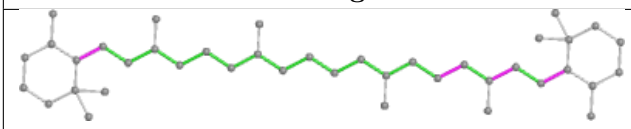
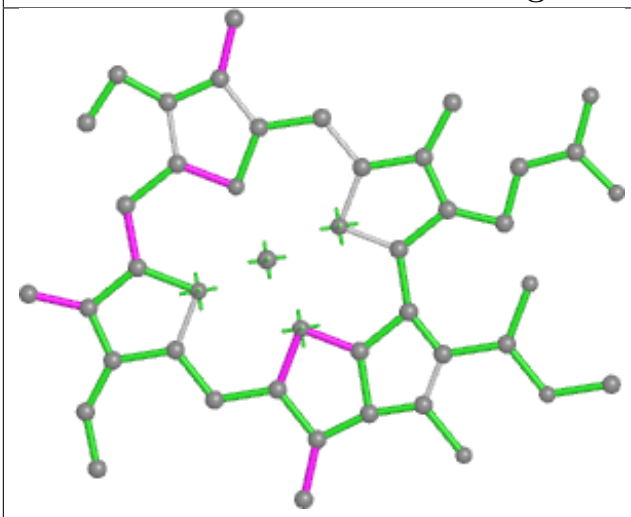


Torsions

Rings

Ligand CLA d 501



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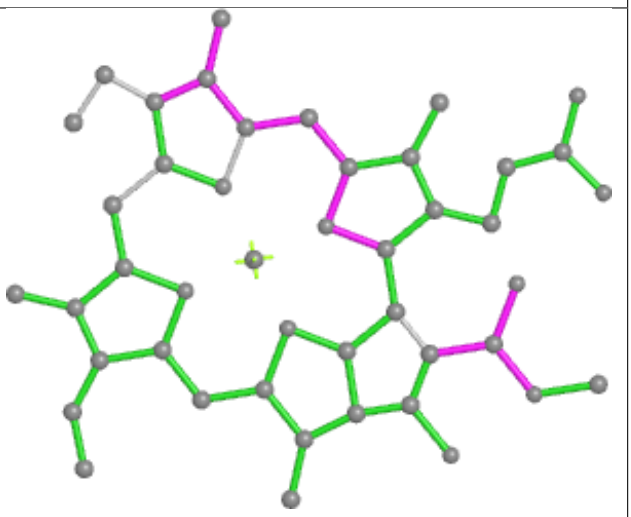

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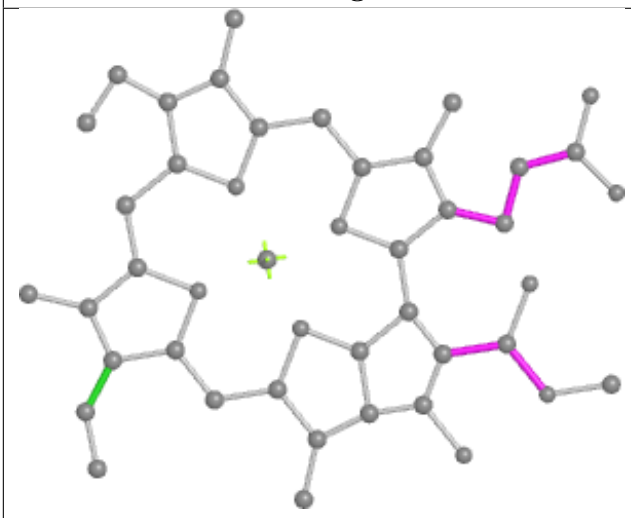

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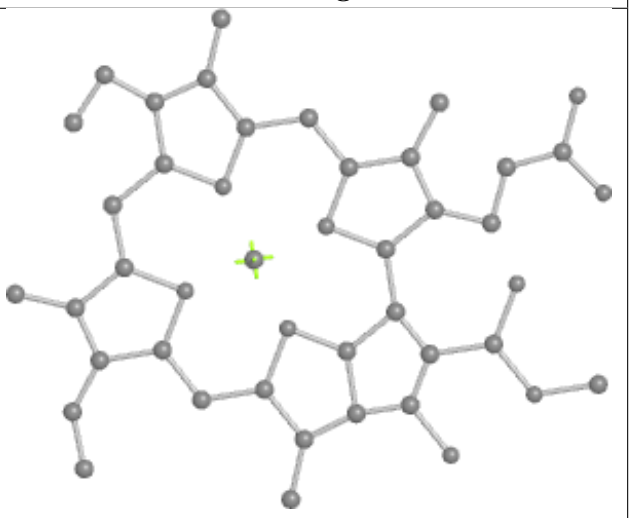
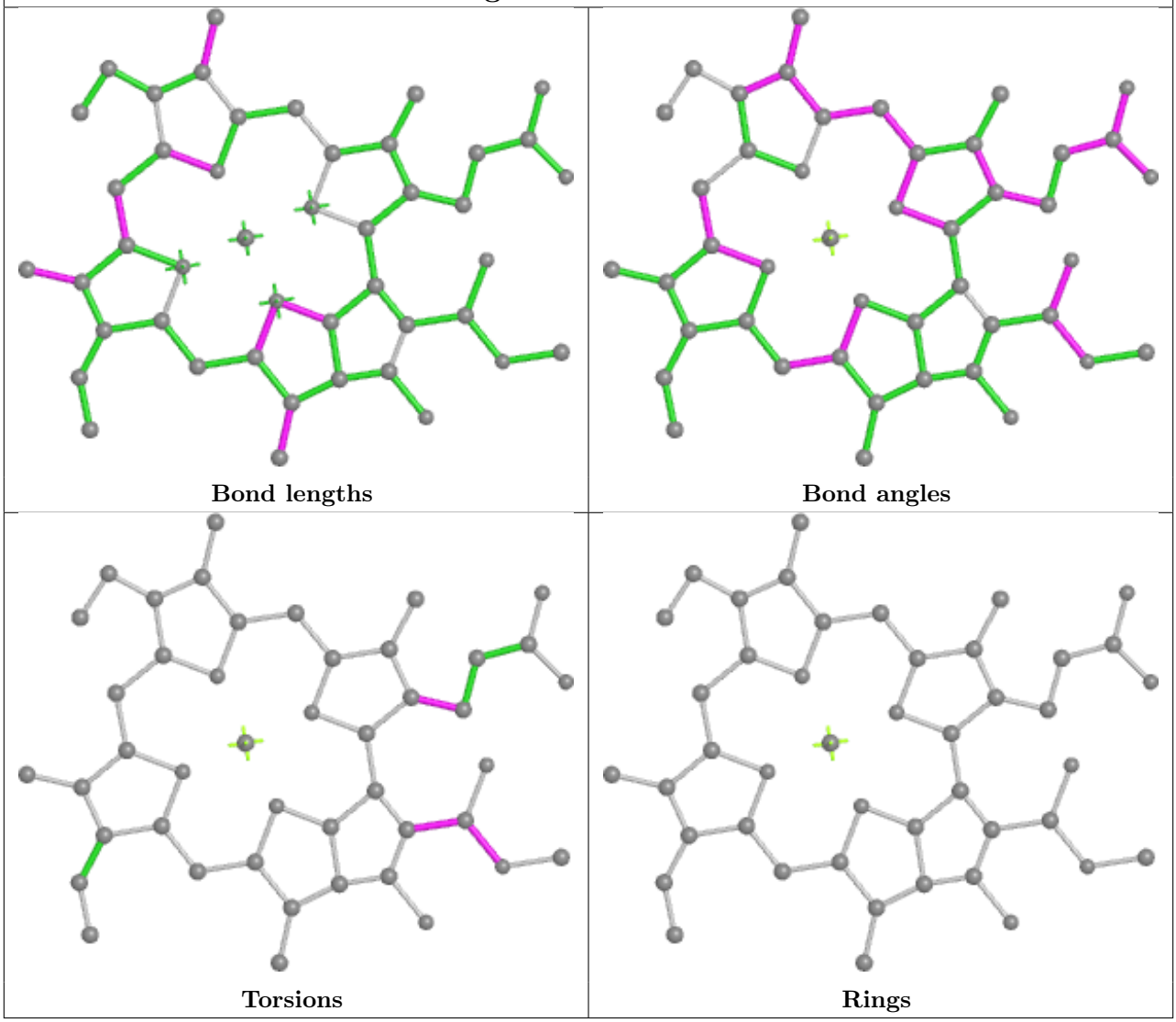


Rings

Ligand CLA v 508



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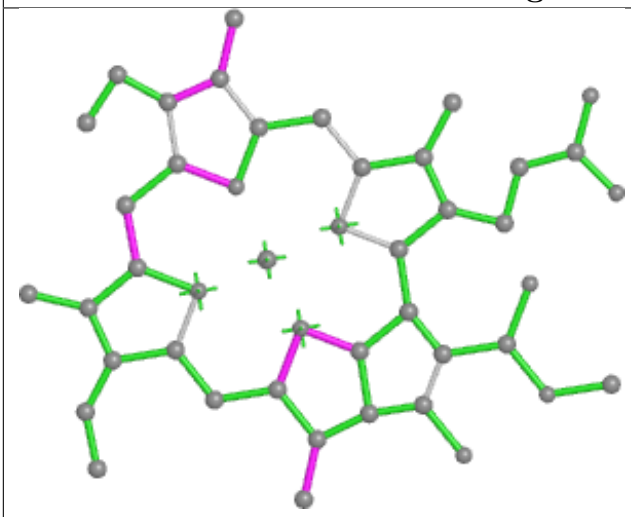

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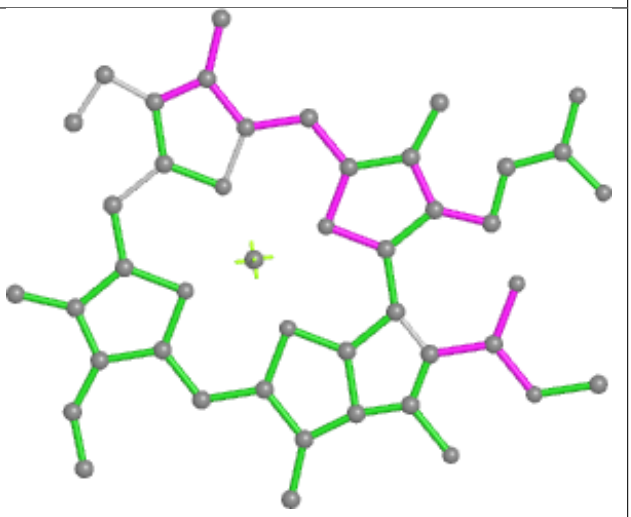

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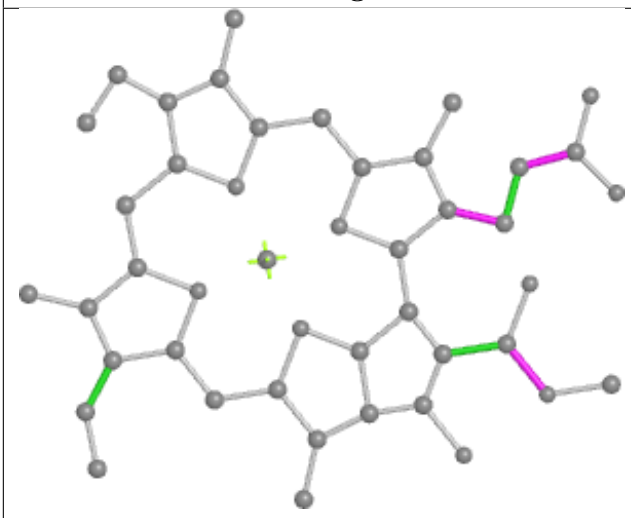

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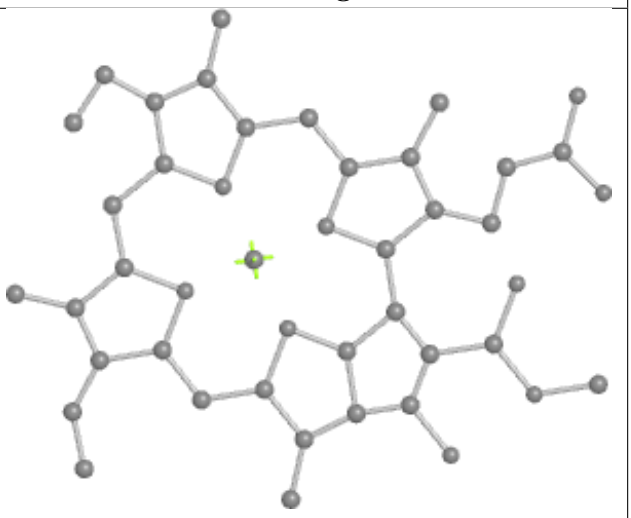
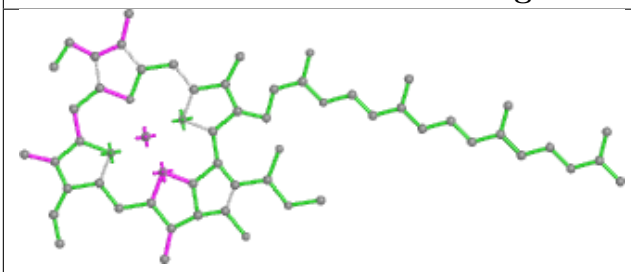


Rings

Ligand CLA H 1230



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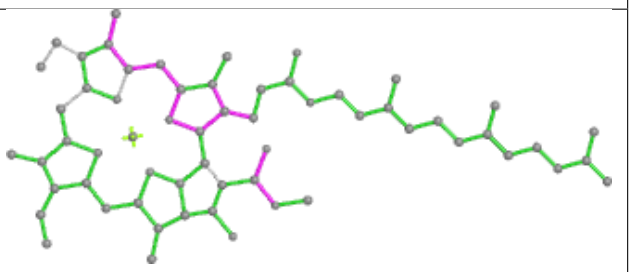

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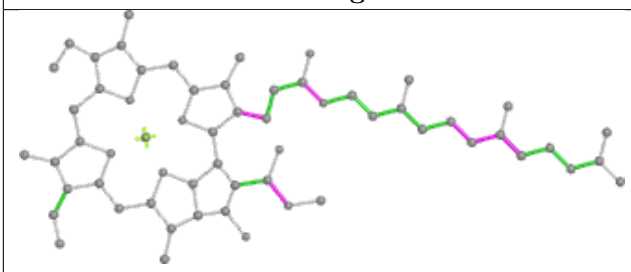

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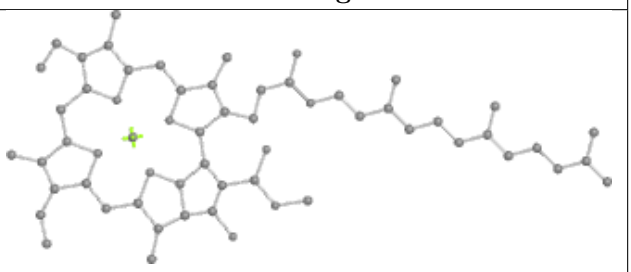
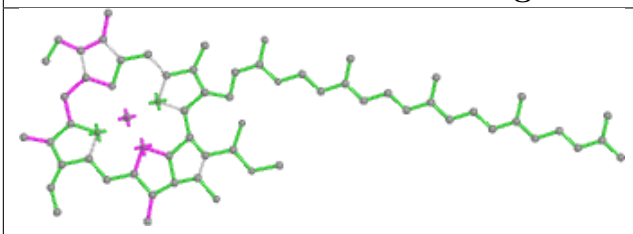


Rings

Ligand CLA G 1128



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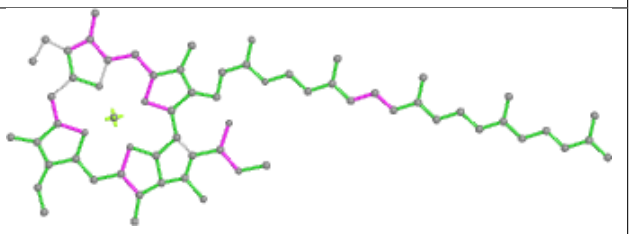

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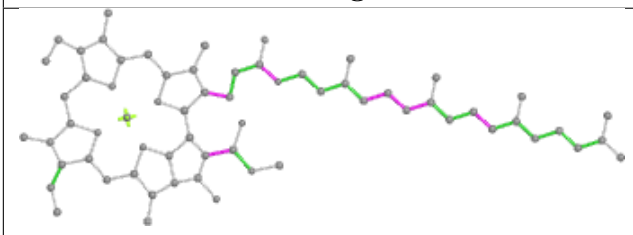

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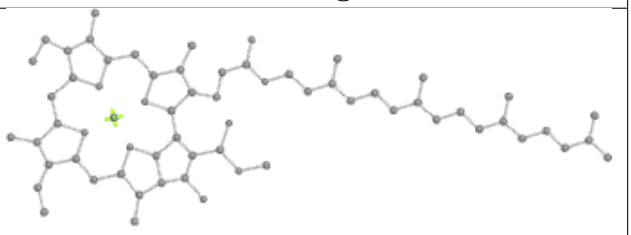
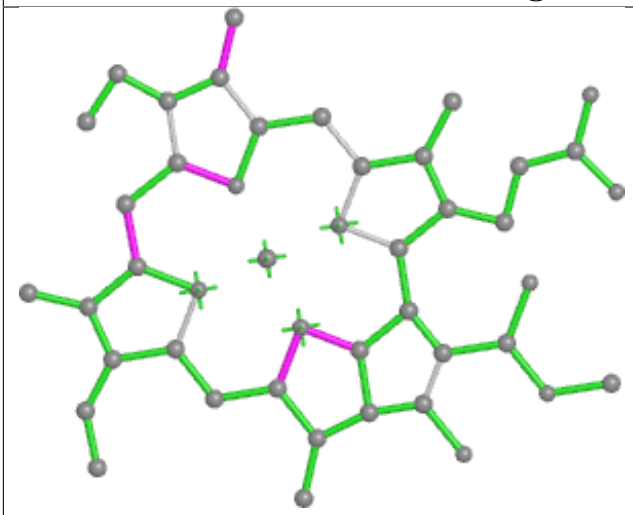


Rings

Ligand CLA d 511



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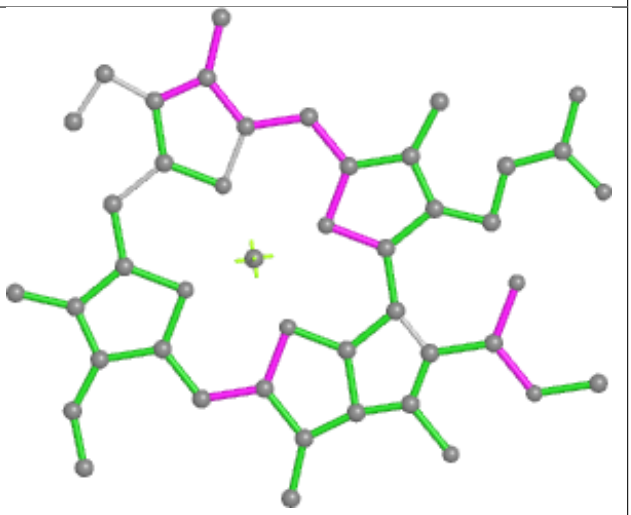
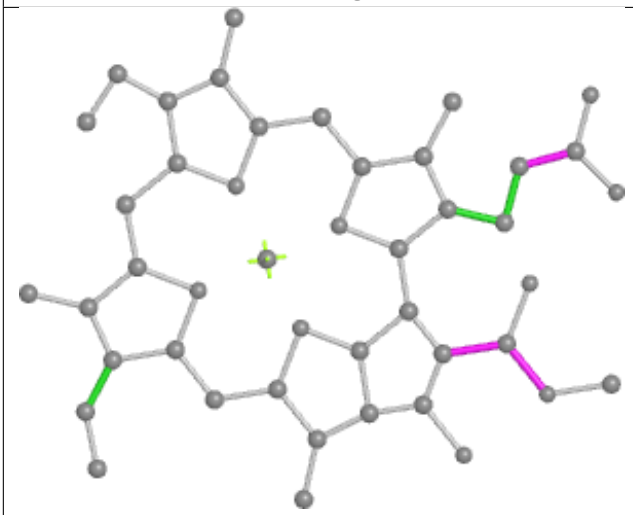


Bond angles



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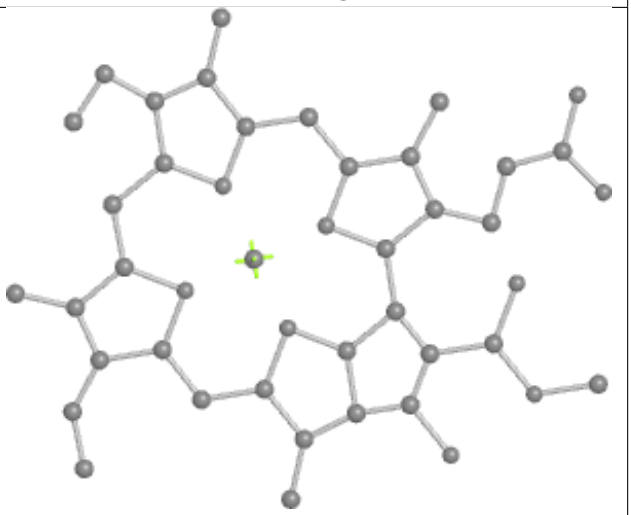
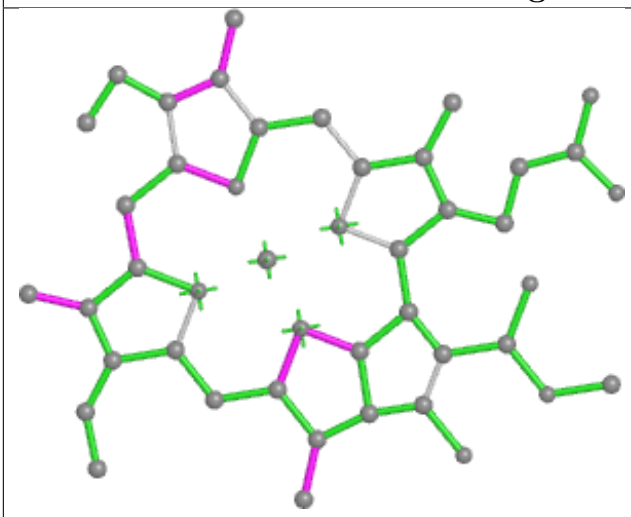


Rings

Ligand CLA 5 517



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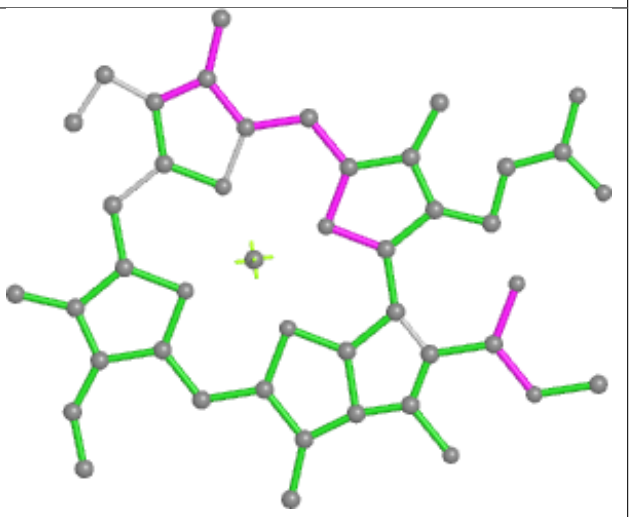
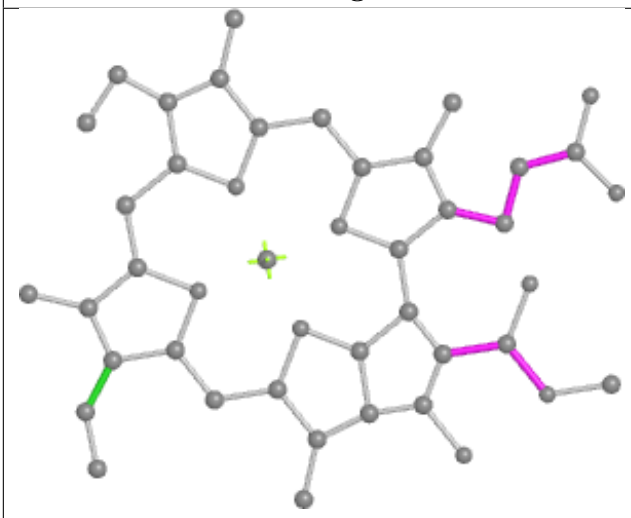
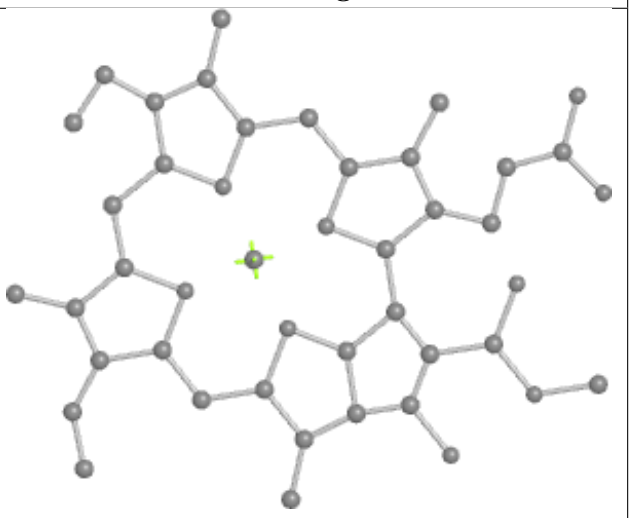


Bond angles

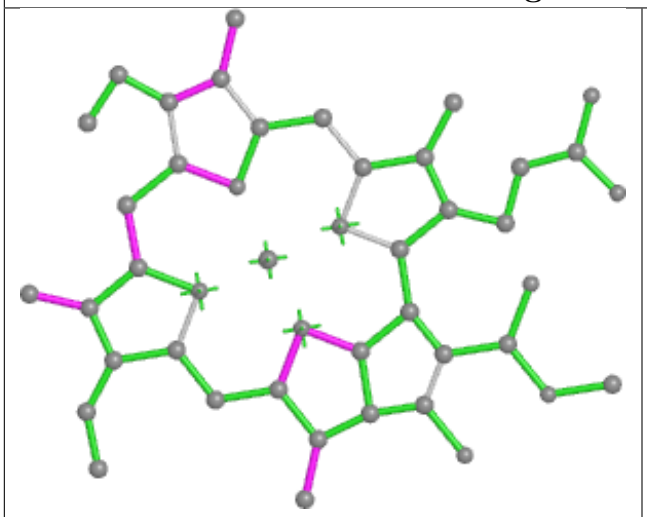


Torsions



Rings

Ligand CLA Y 510



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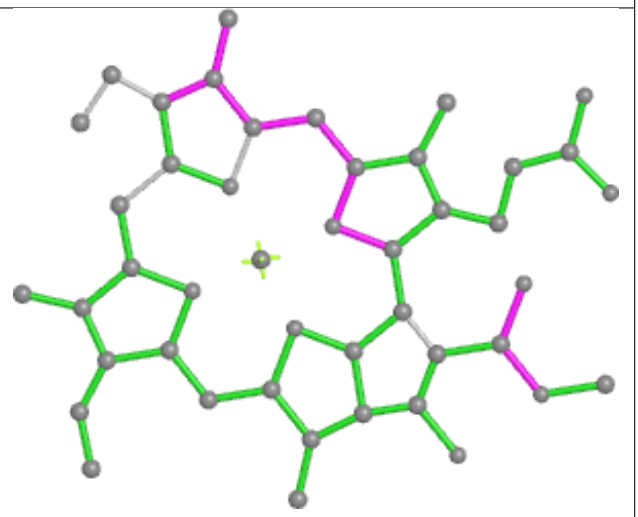
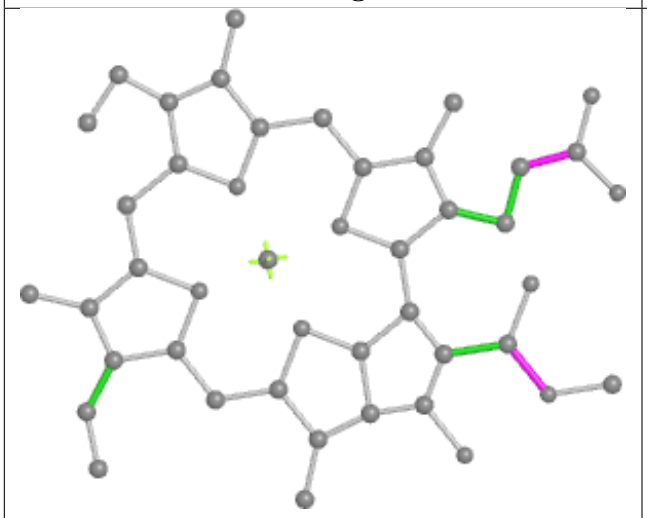
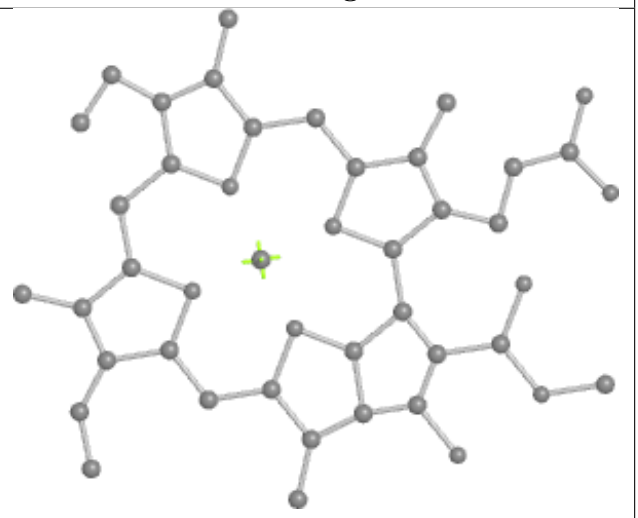


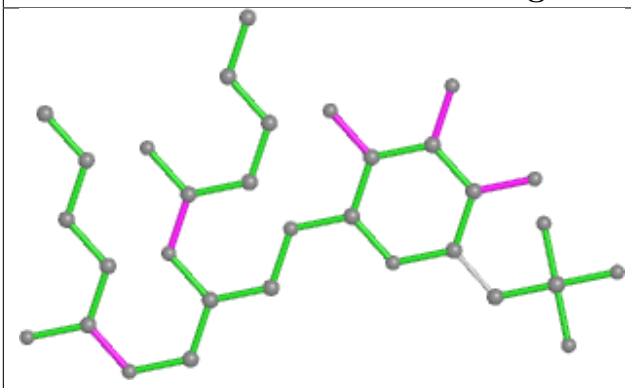
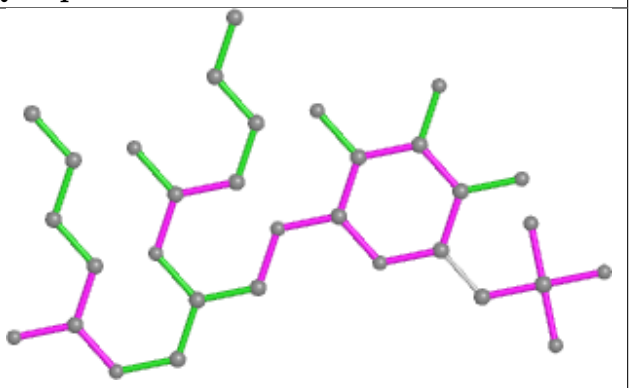
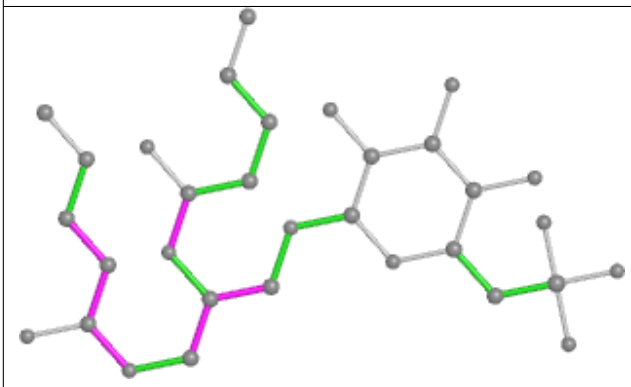
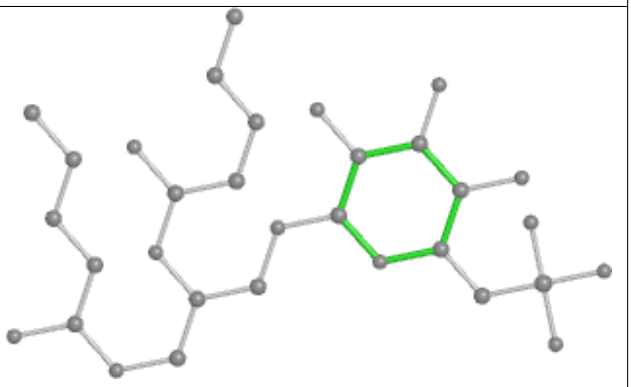
Bond angles



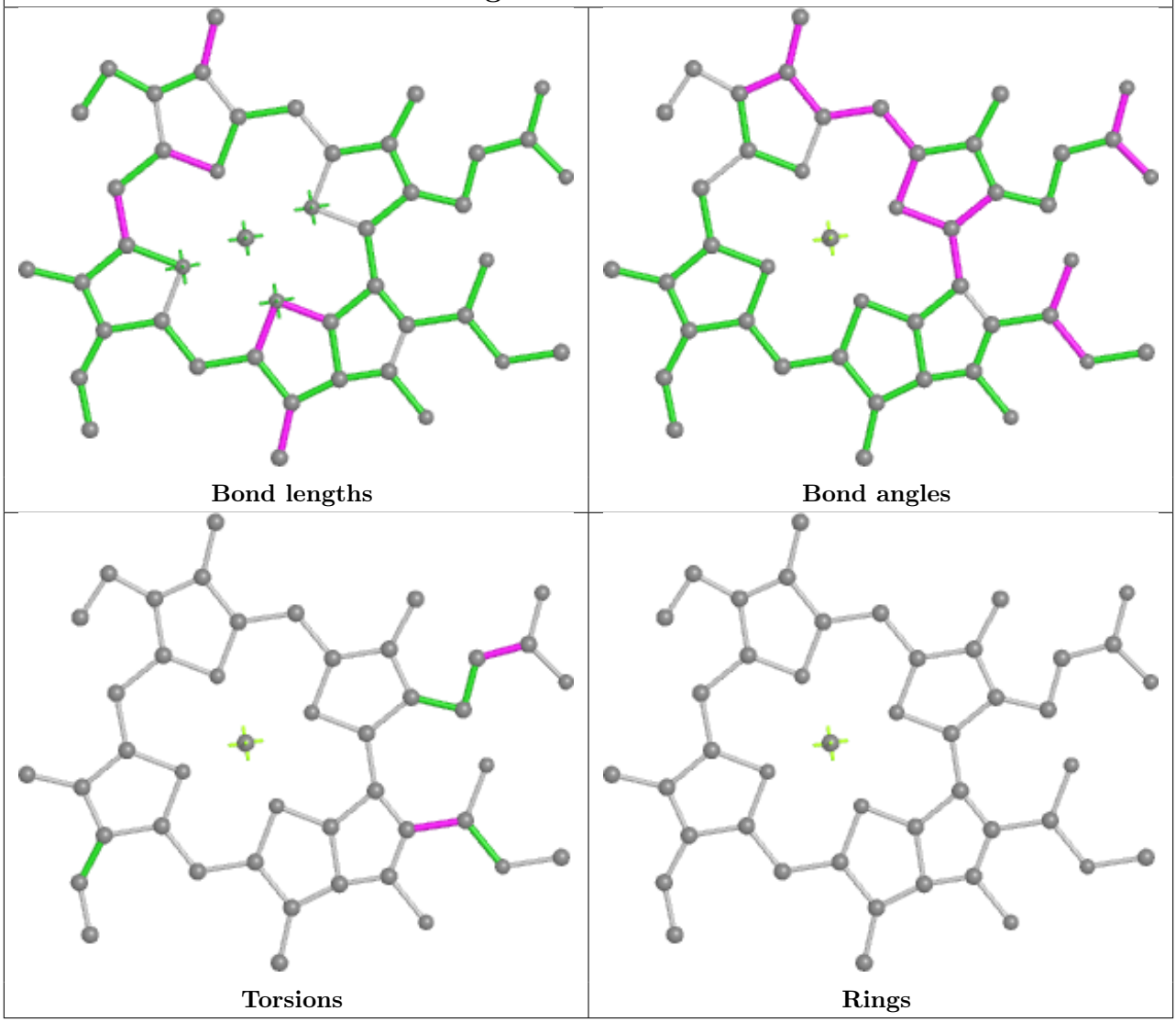
Torsions



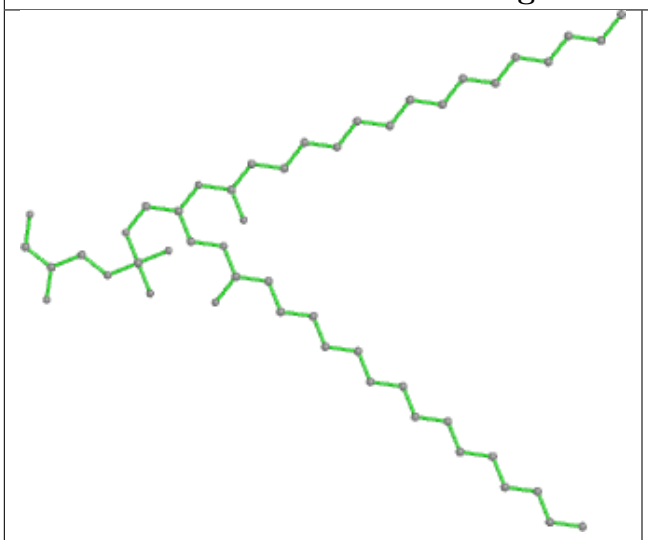
Rings

Ligand SQD q 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 507



Ligand LHG n 5221



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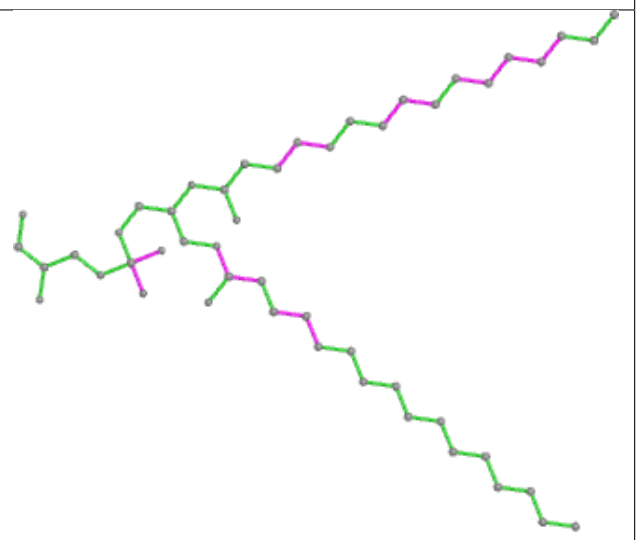
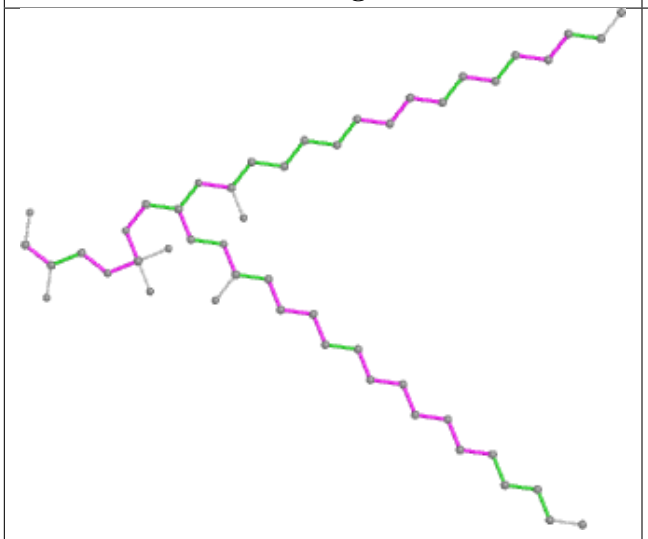


Bond angles



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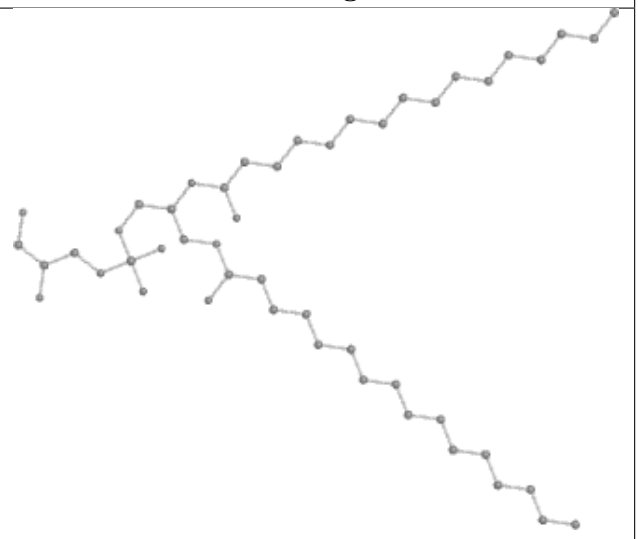

Rings

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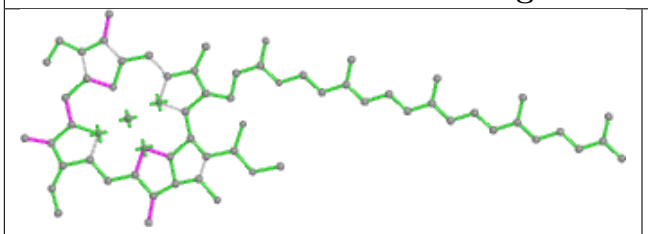

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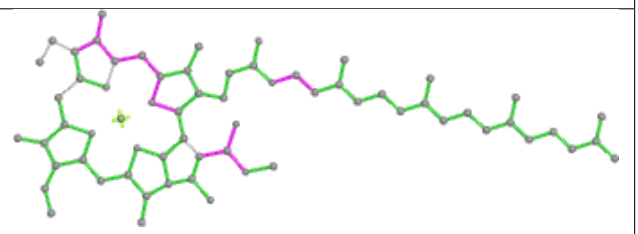
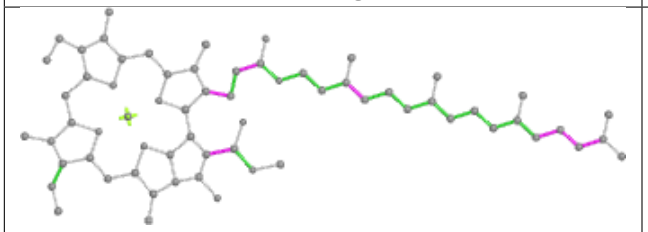


Bond angles



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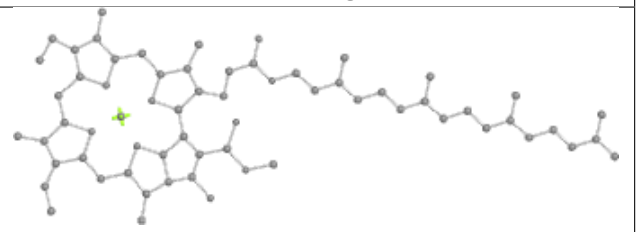
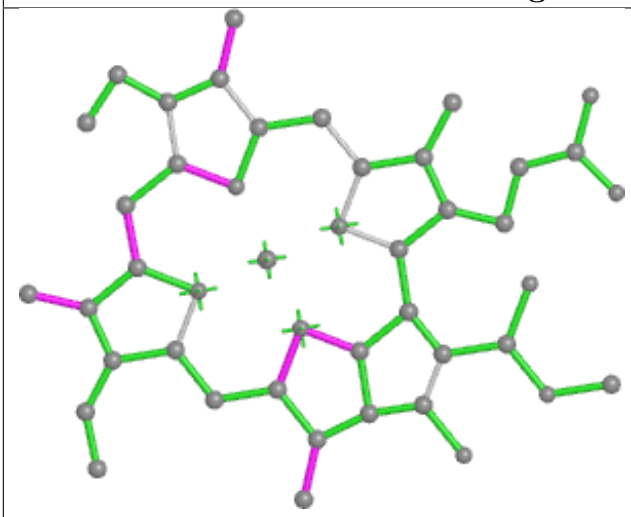


Rings

Ligand CLA 2 510



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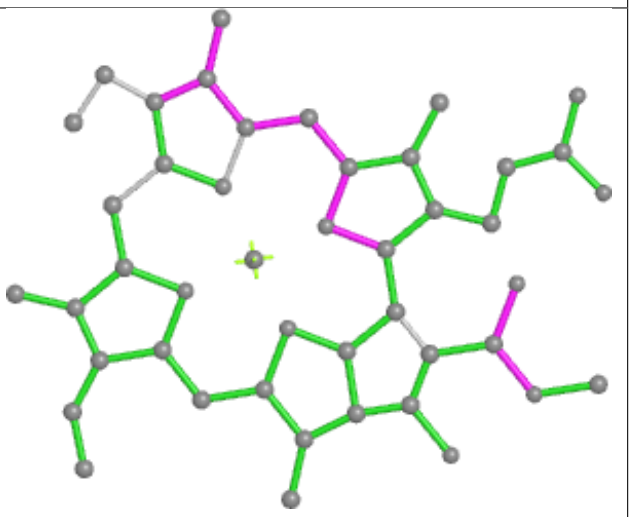

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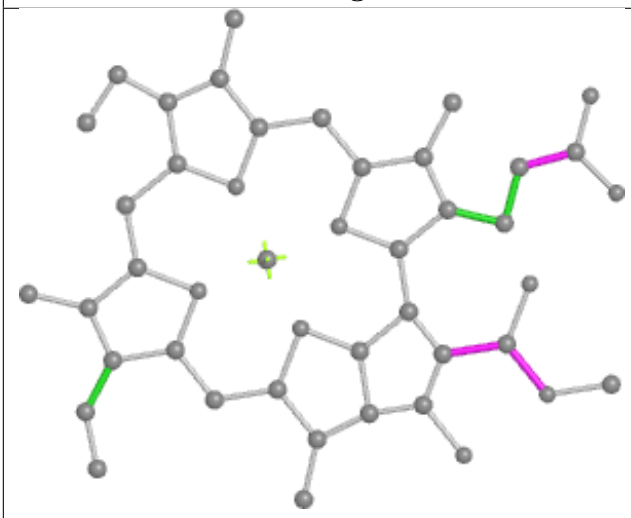

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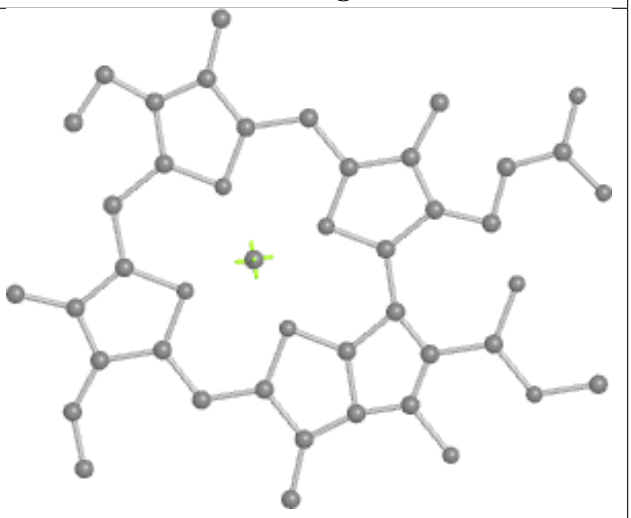

Rings

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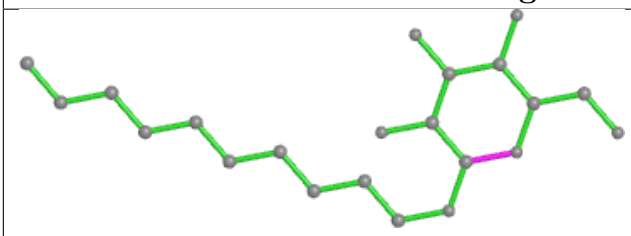

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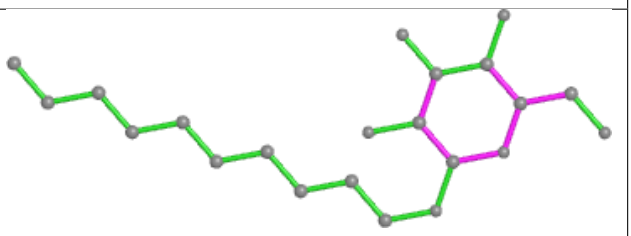

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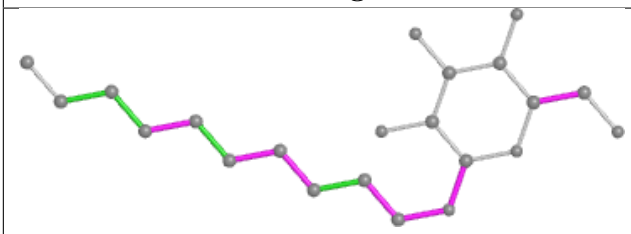

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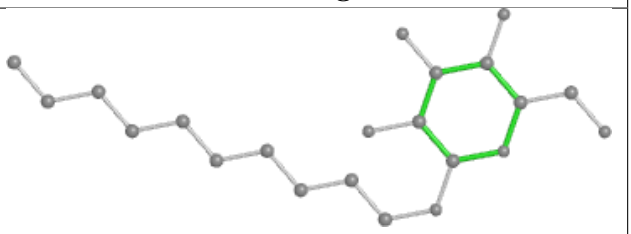

Rings

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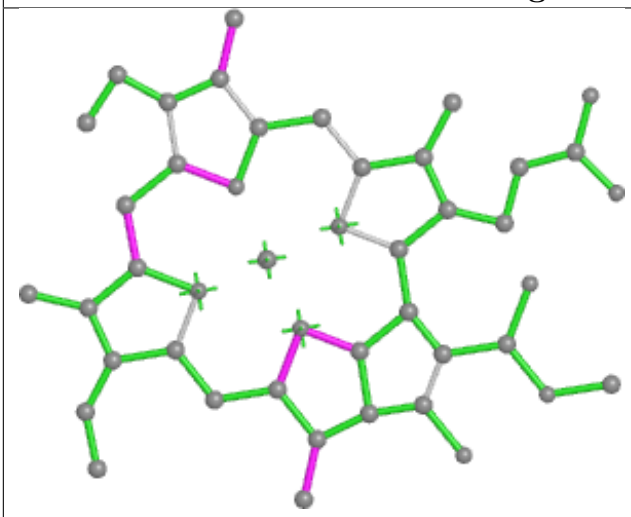

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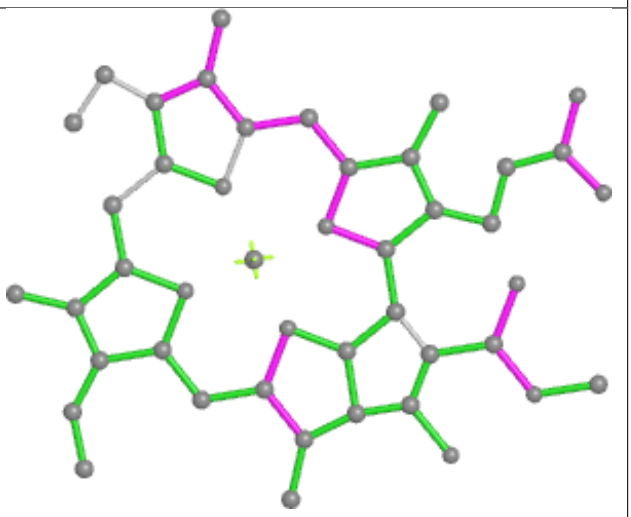

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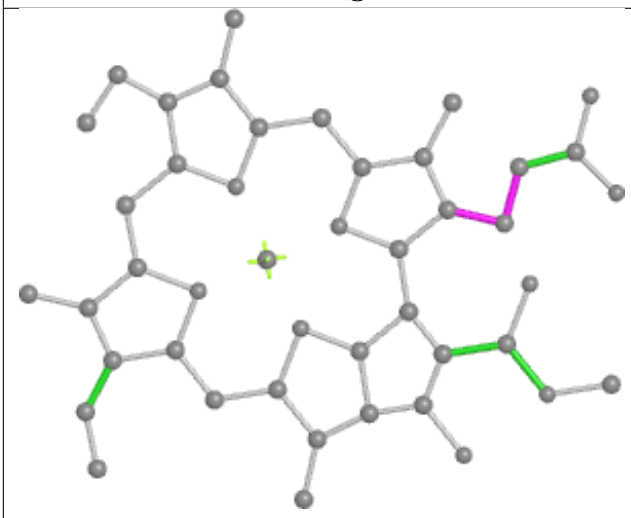

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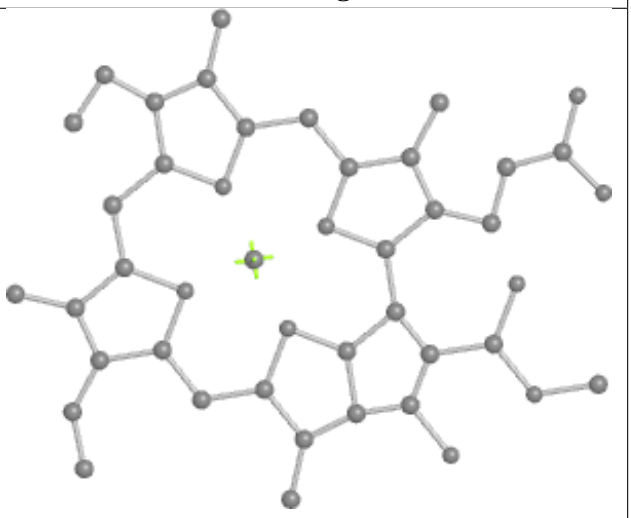
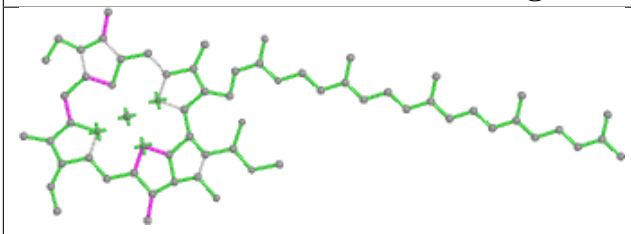


Rings

Ligand CLA Z 503



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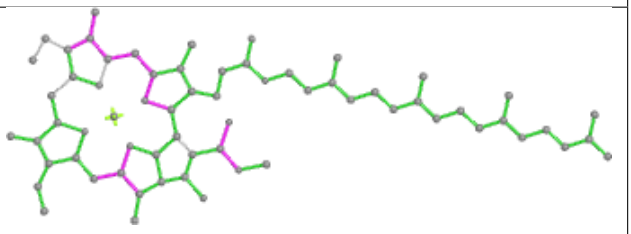

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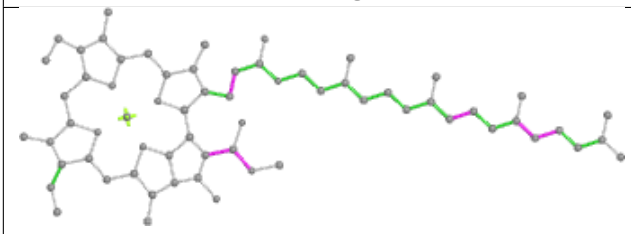

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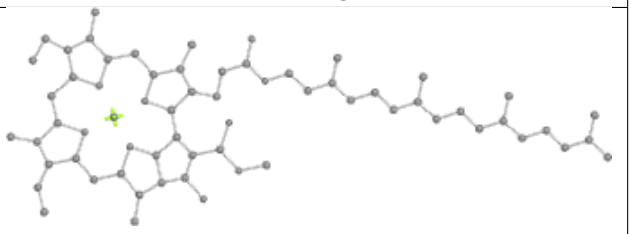
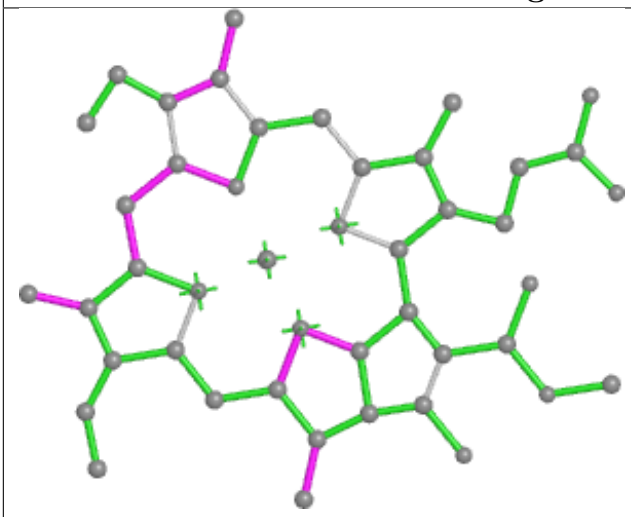


Rings

Ligand CLA u 508



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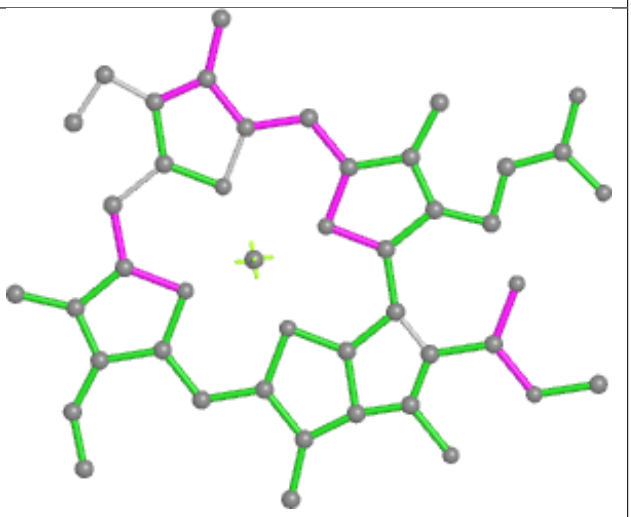

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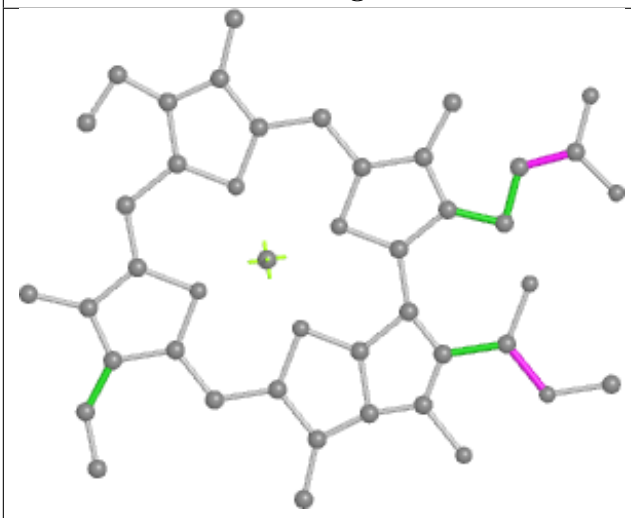

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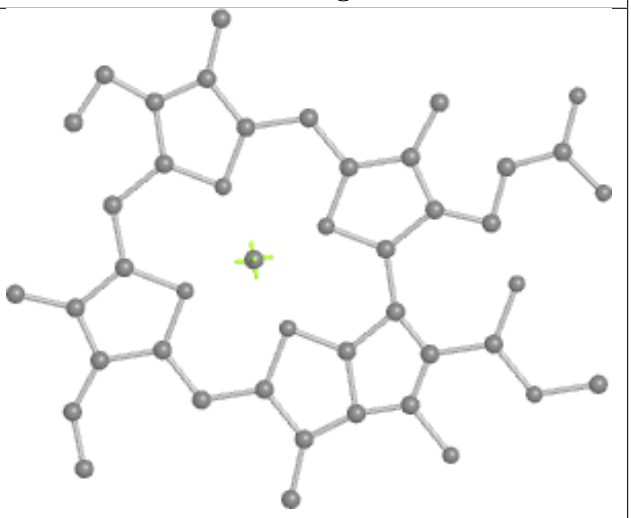

Rings

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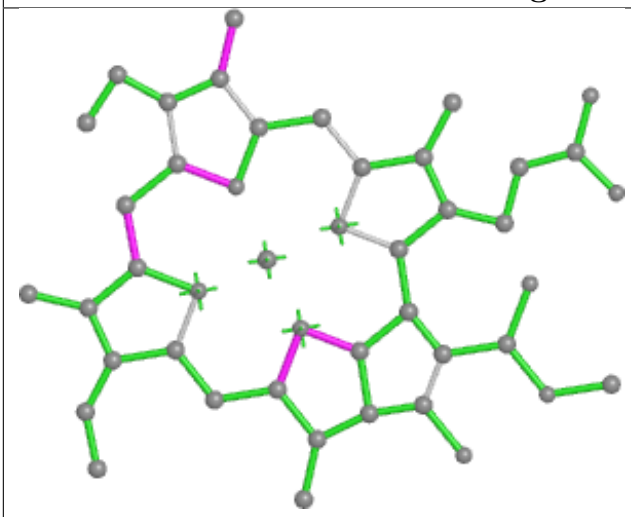

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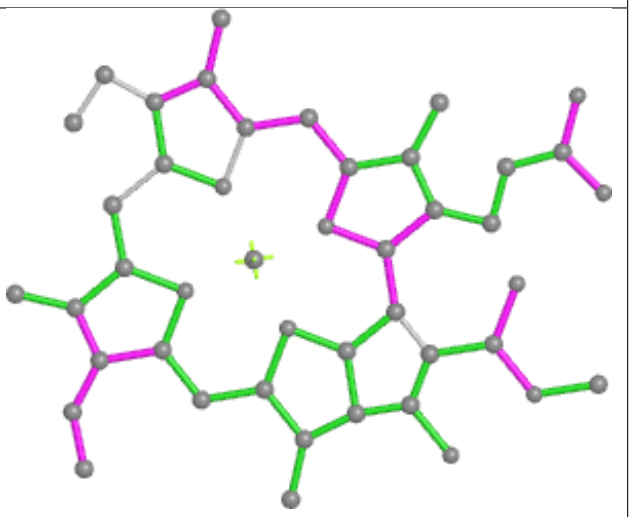

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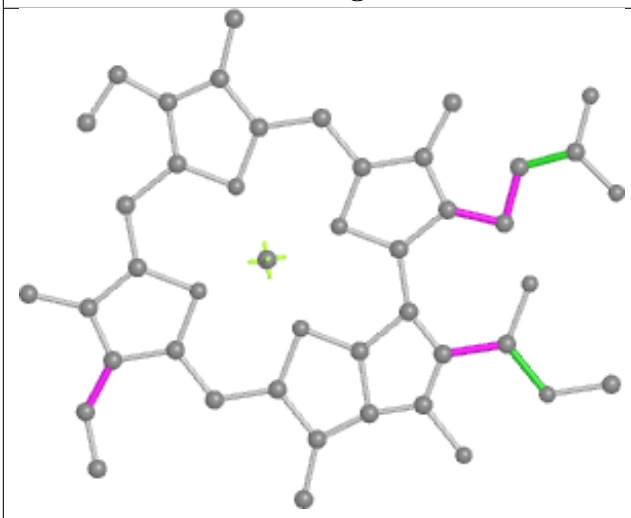

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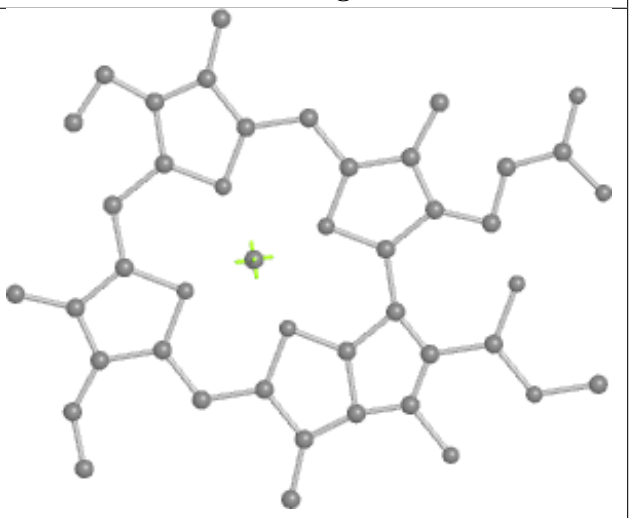
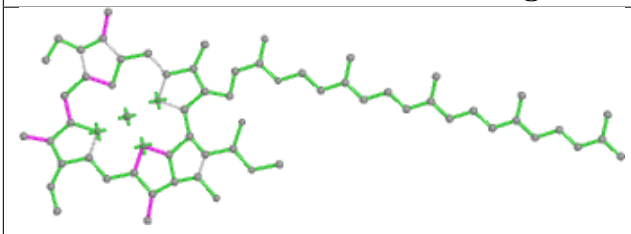


Rings

Ligand CLA f 1238



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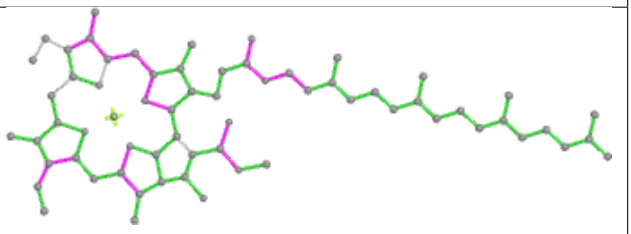

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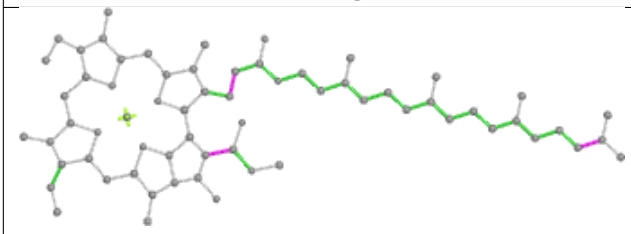

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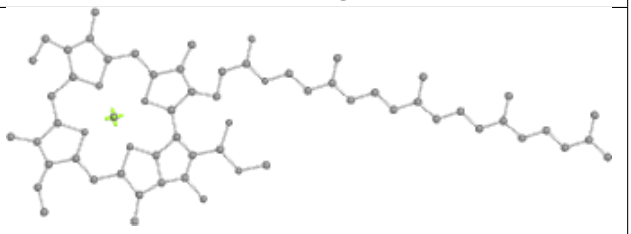
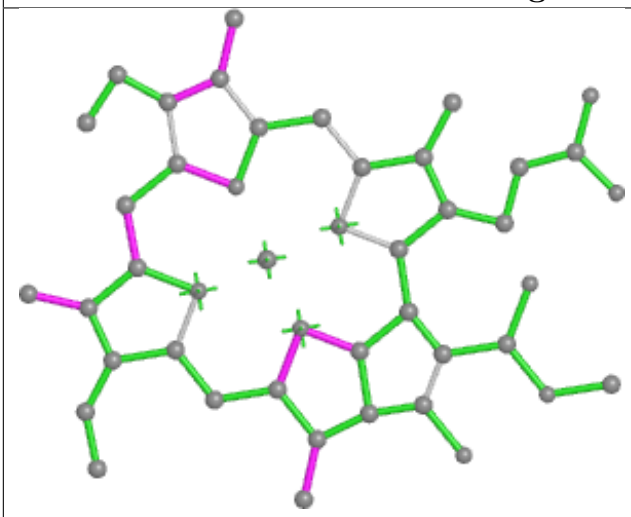


Rings

Ligand CLA 1 510



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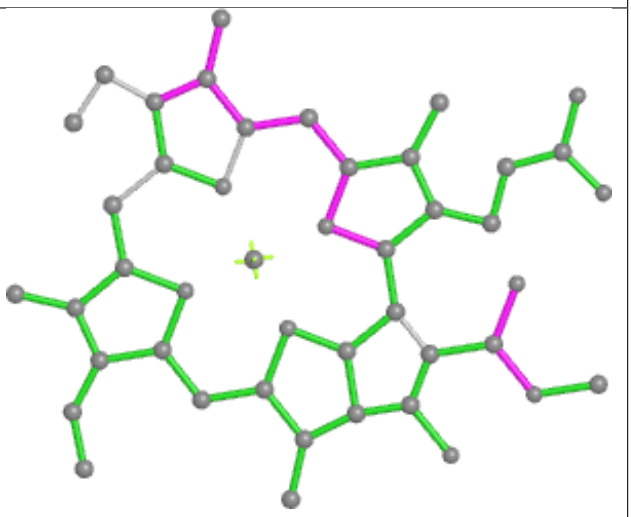

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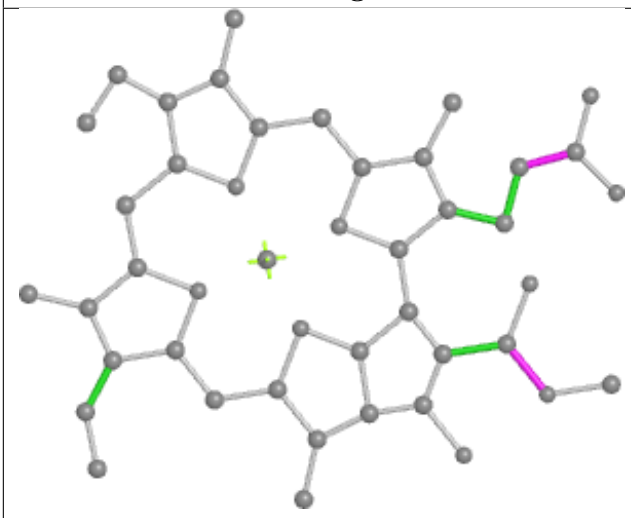

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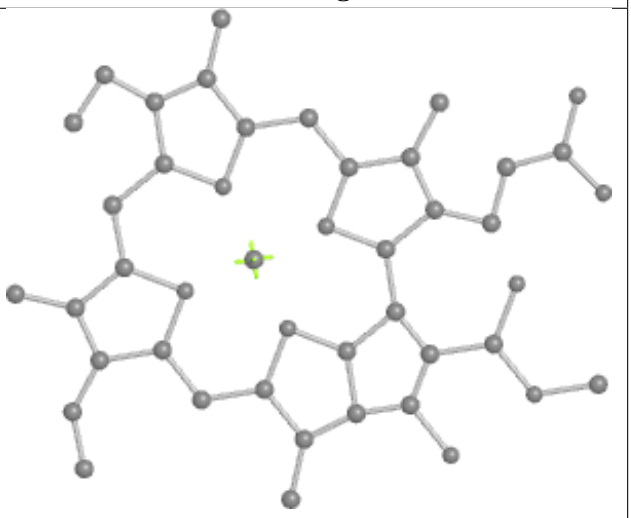

Rings

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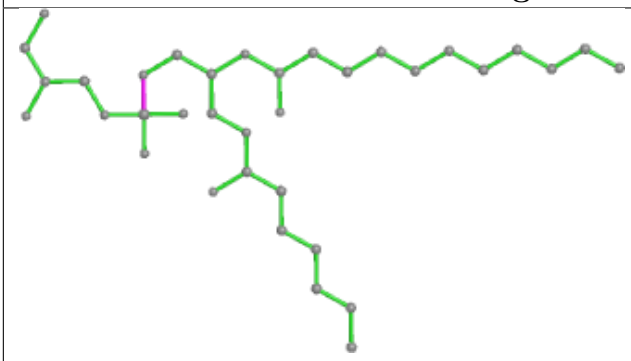

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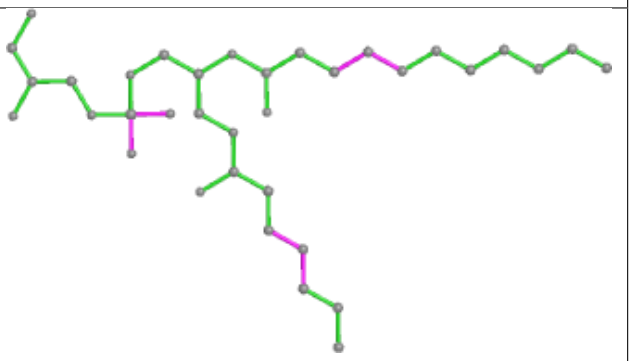

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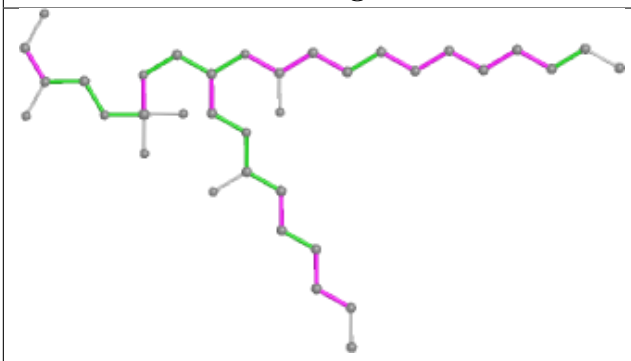
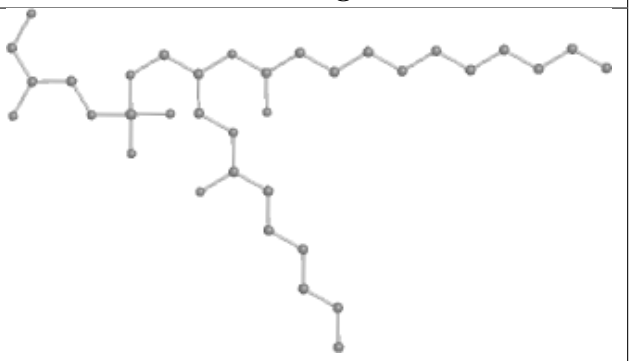
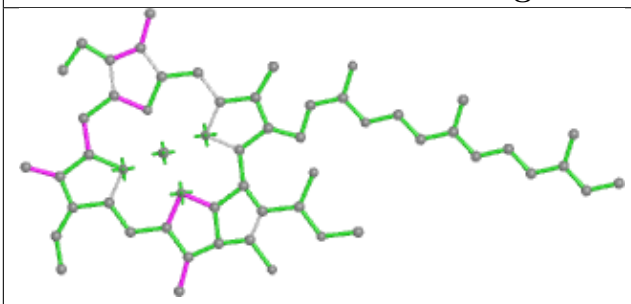


Torsions

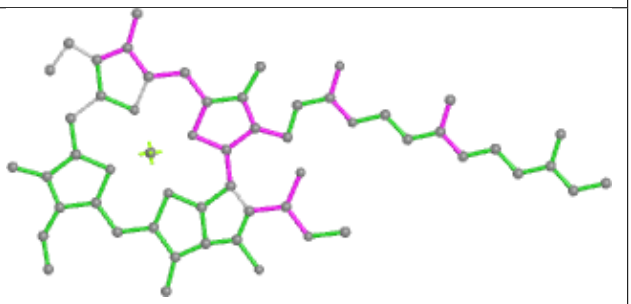


Rings

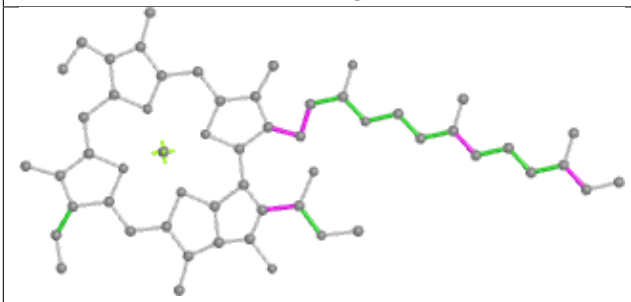
Ligand CLA G 1134



Bond lengths



Bond angles



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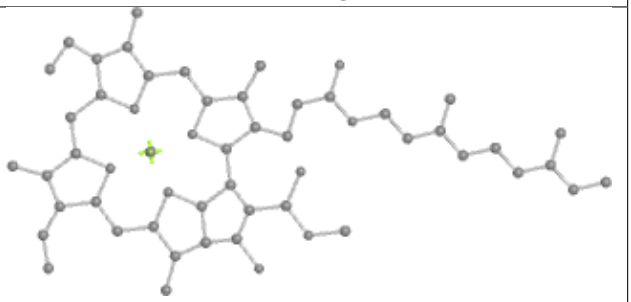
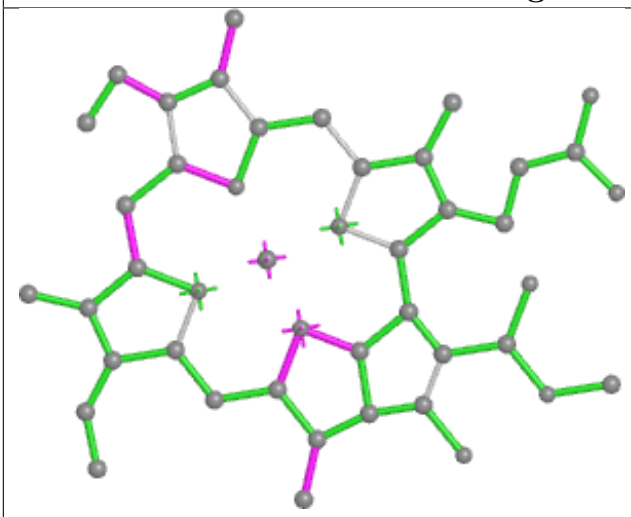


Rings

Ligand CLA b 505



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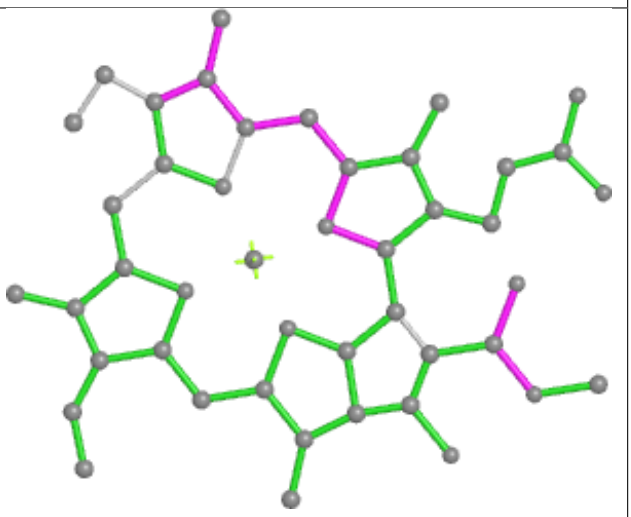

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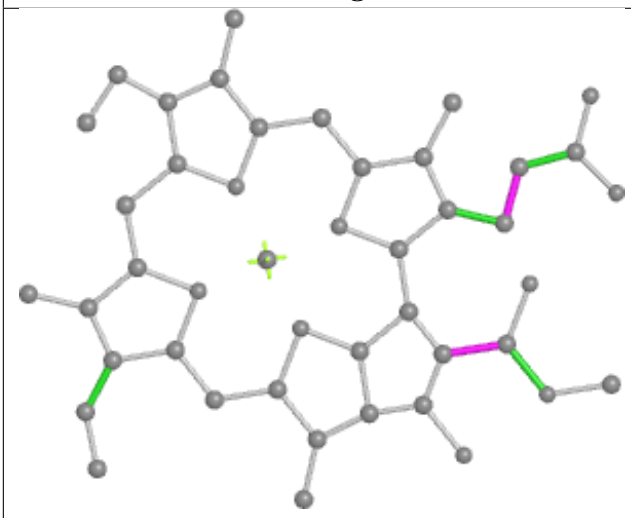

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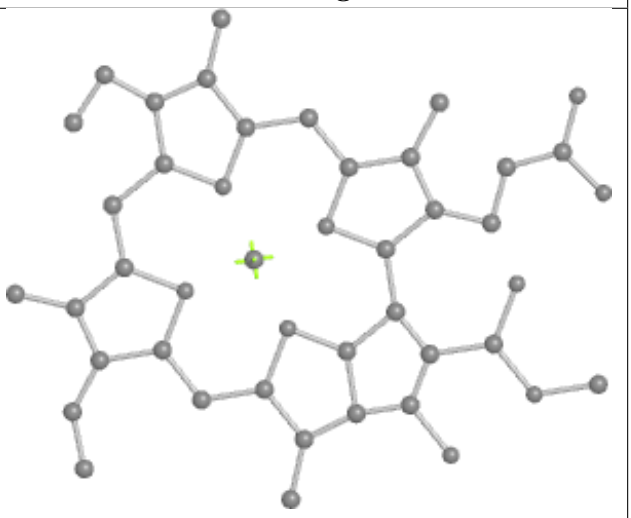
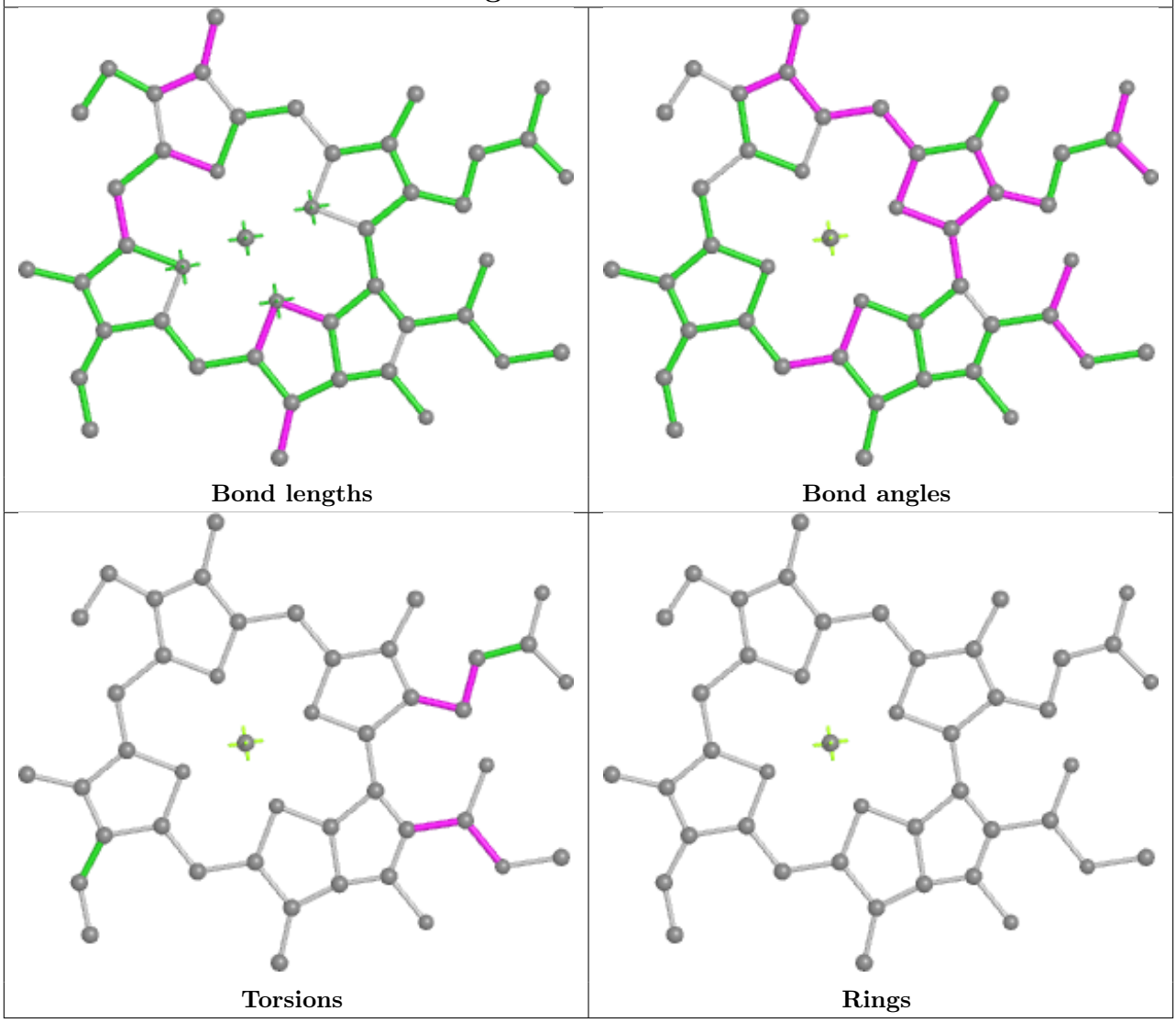
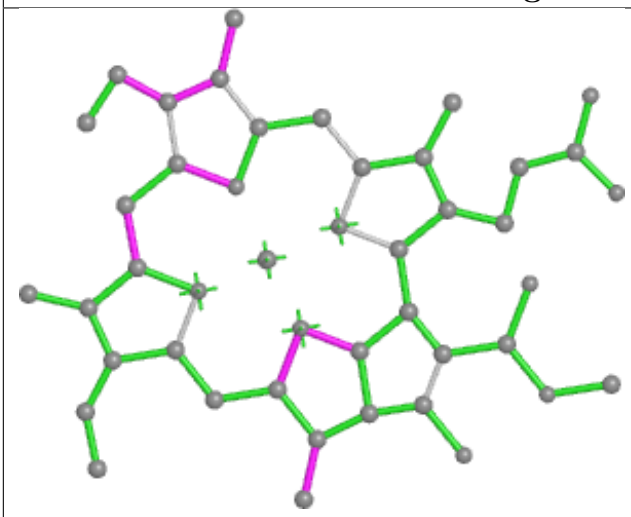


Rings

Ligand CLA 5 503



Ligand CLA Y 503



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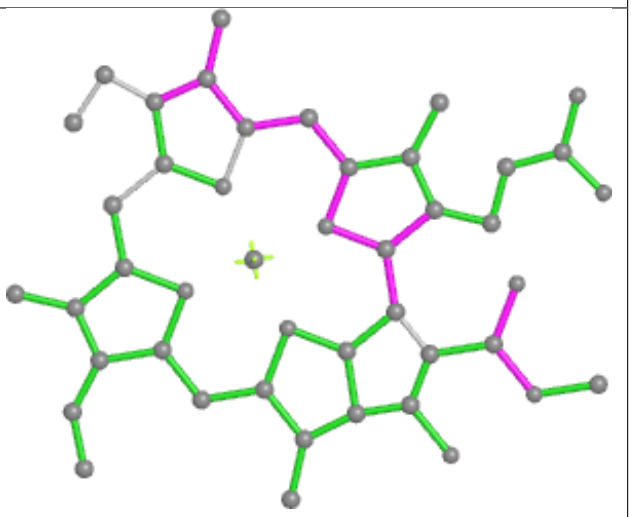
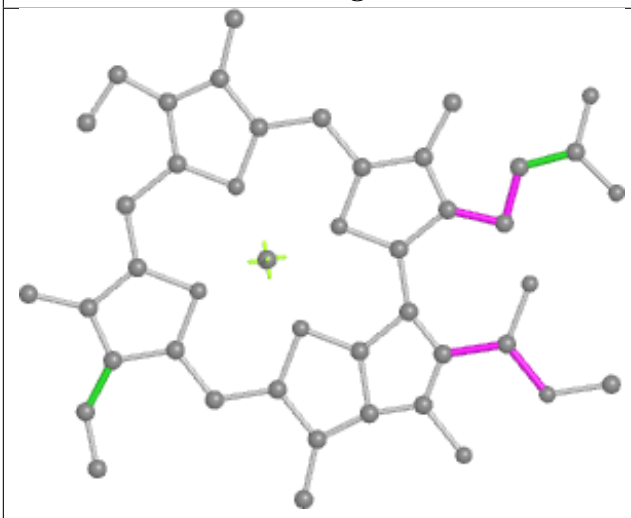


Bond angles



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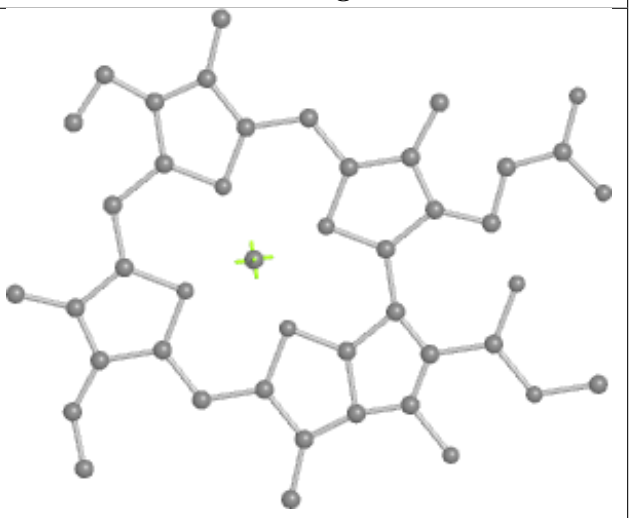
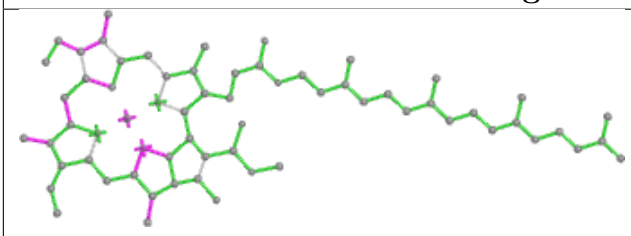


Rings

Ligand CLA f 1205



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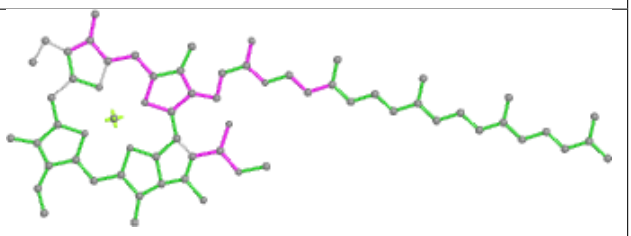

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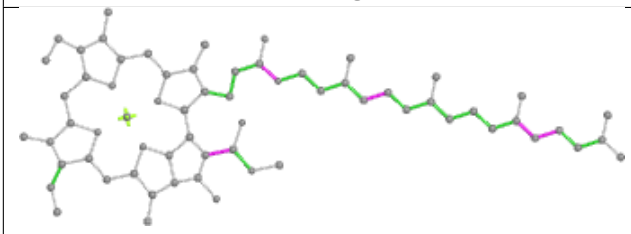

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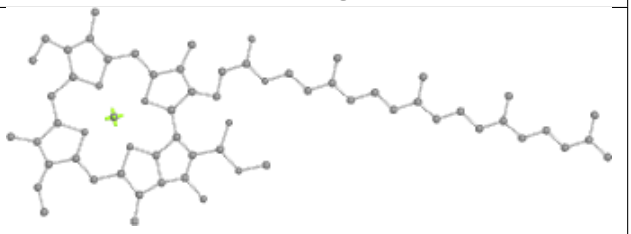

Rings

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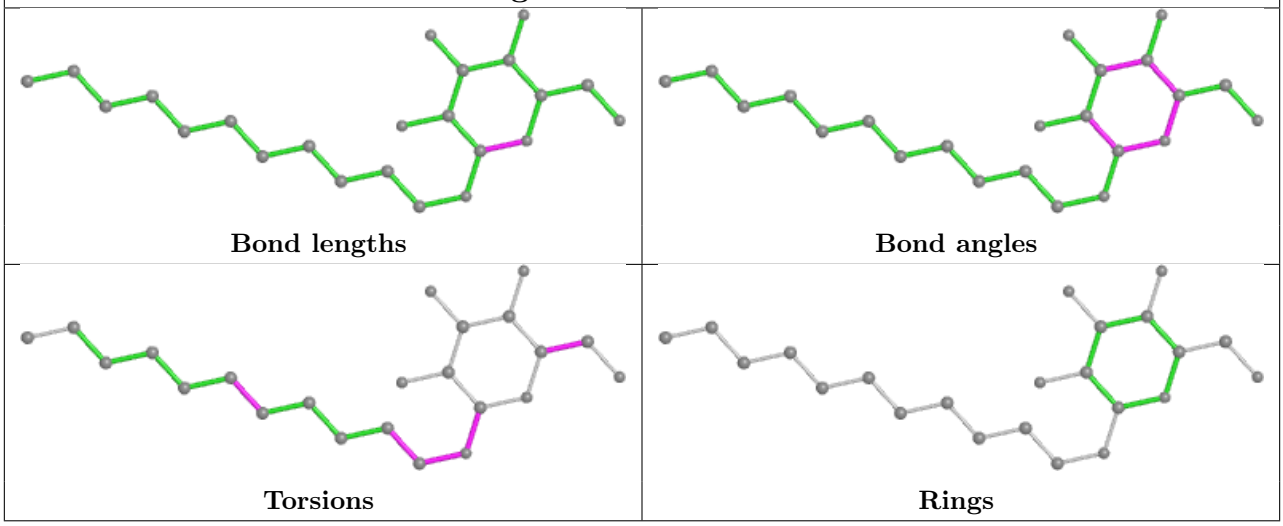
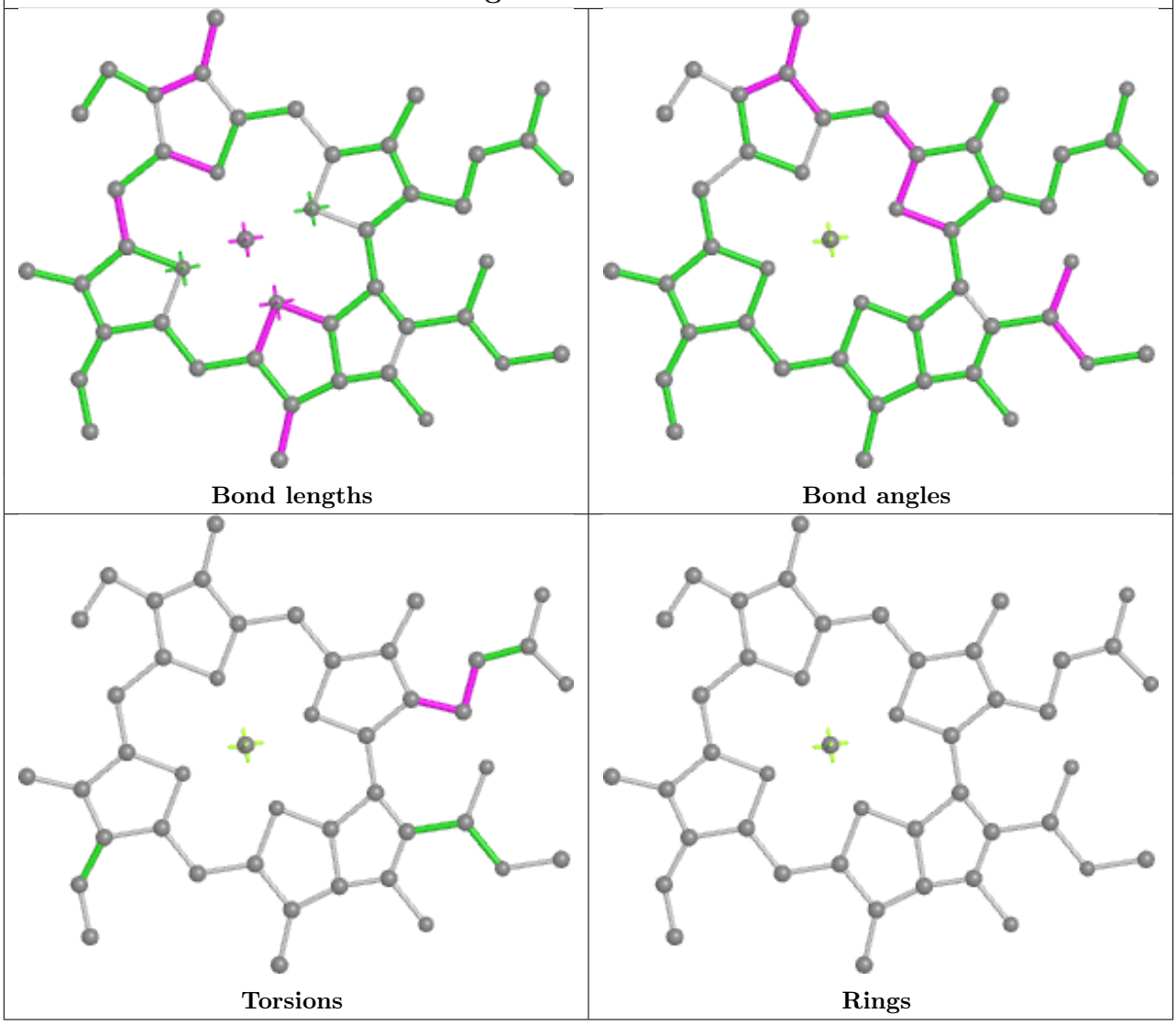


Ligand CLA a 512



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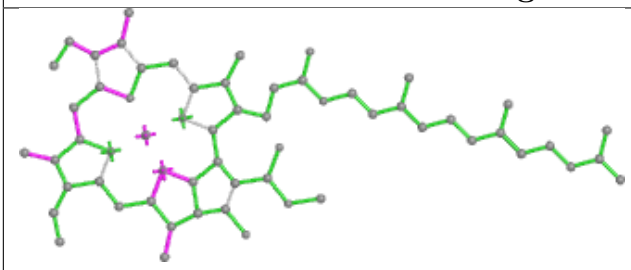
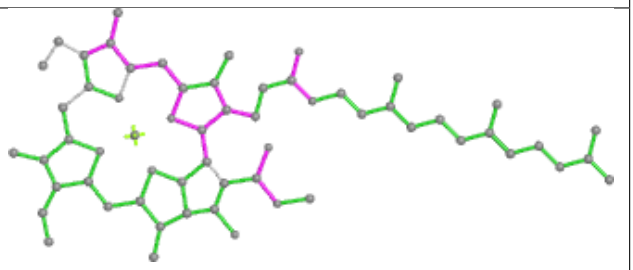
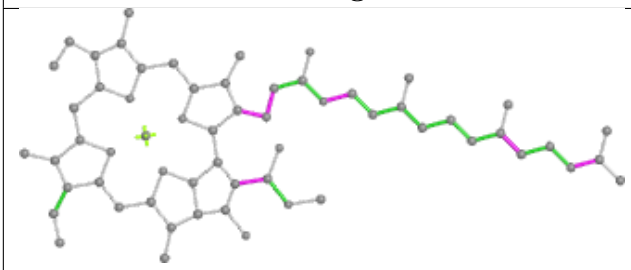
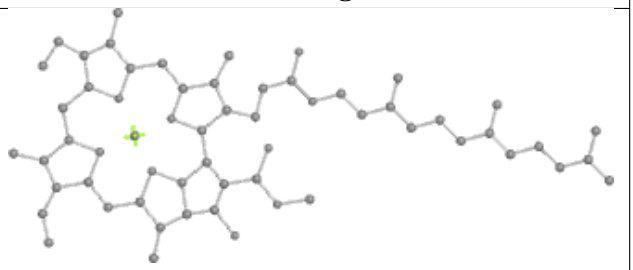
 Bond lengths	 Bond angles
 Torsions	 Rings

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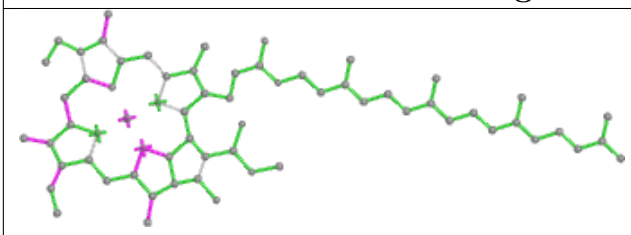
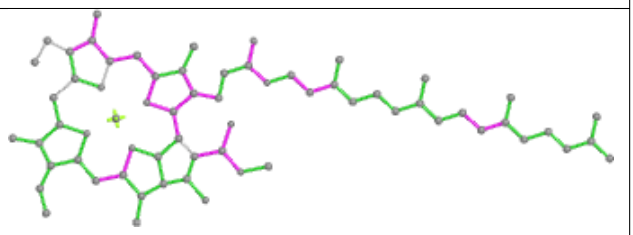
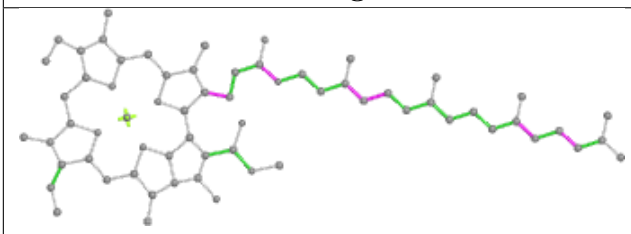
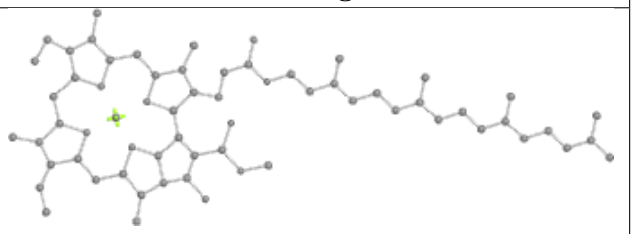
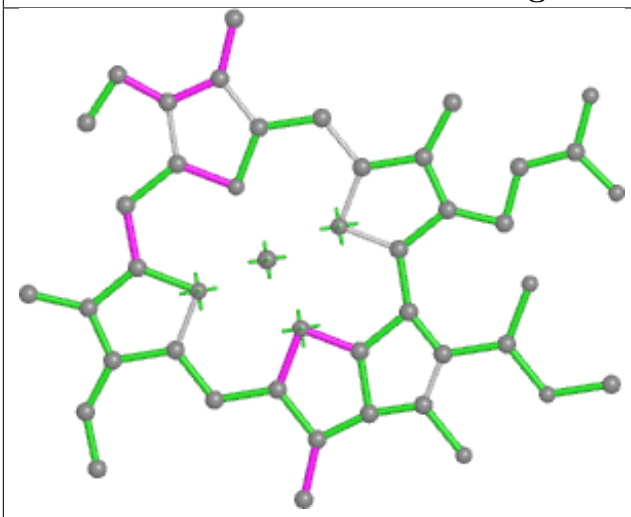
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 503



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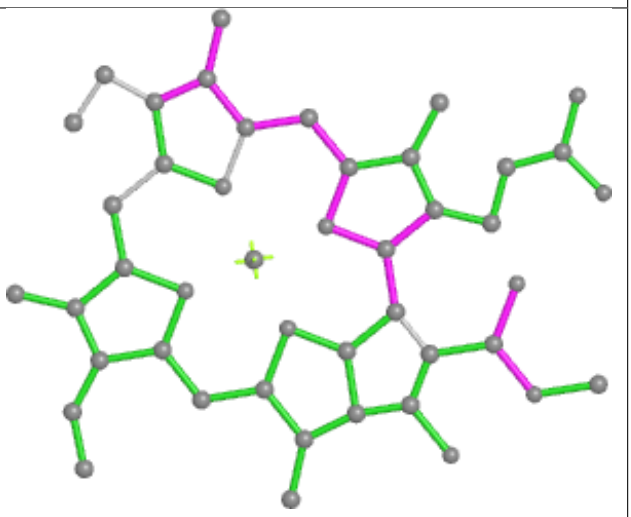
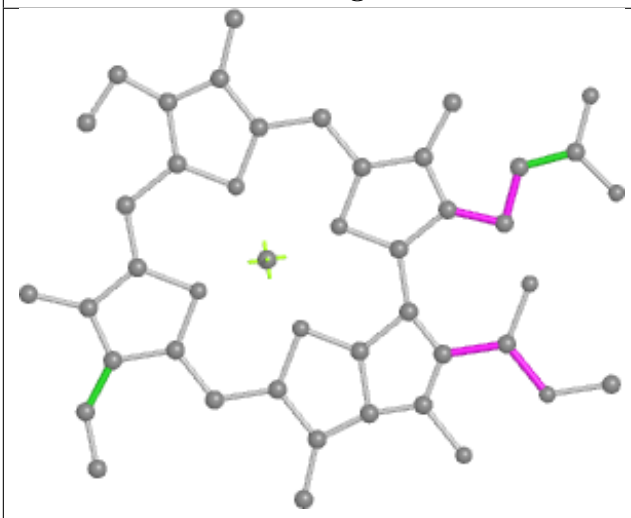


Bond angles



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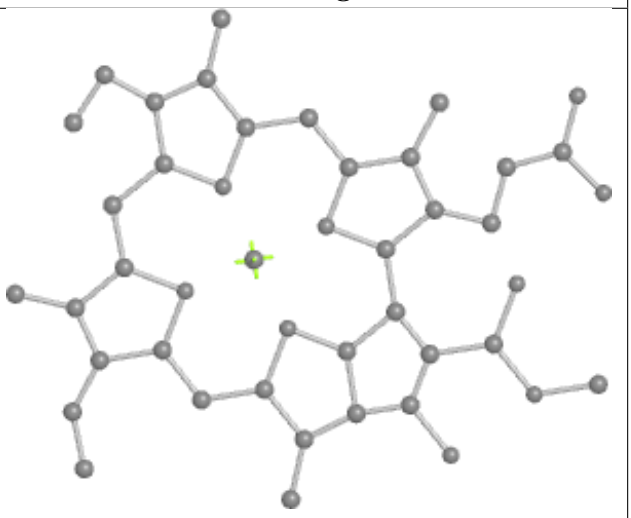
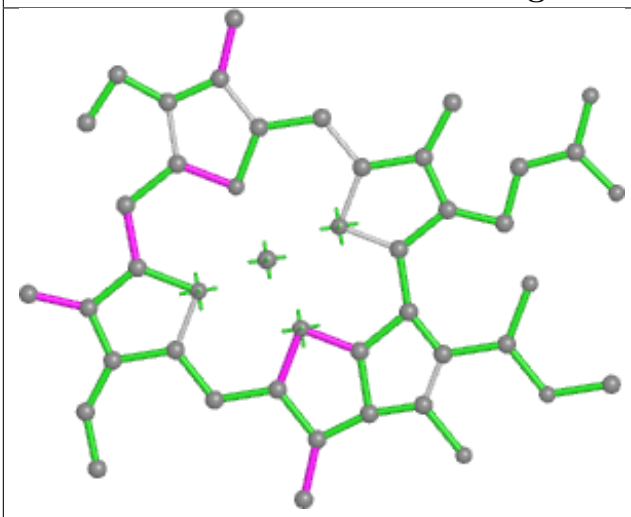


Rings

Ligand CLA q 510



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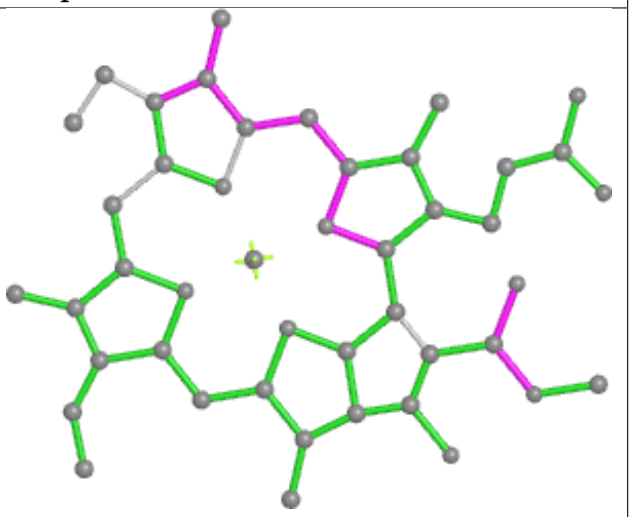

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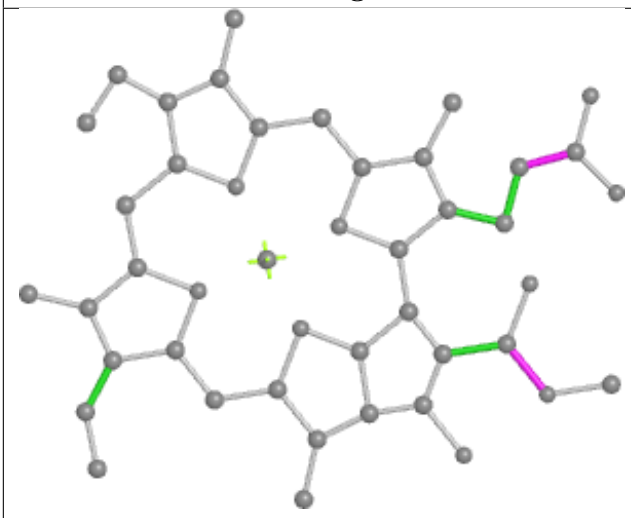

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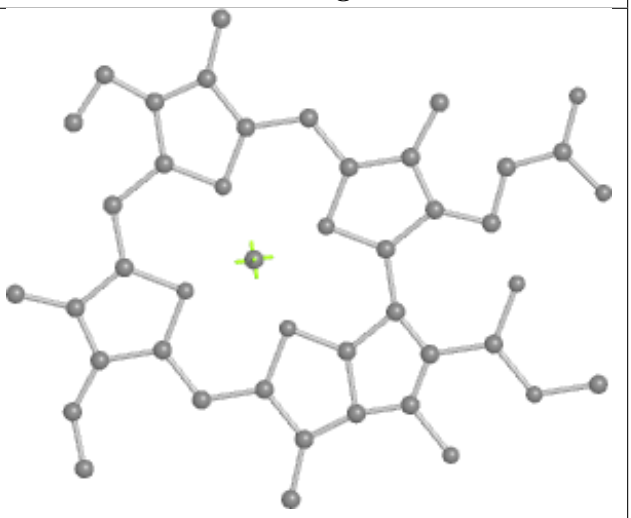
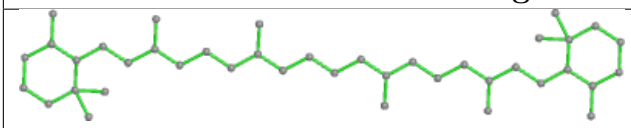


Rings

Ligand BCR H 4006



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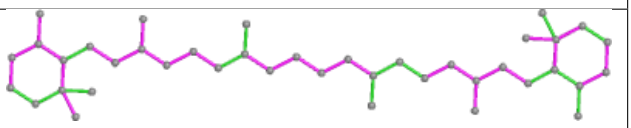

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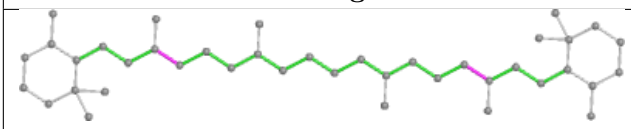
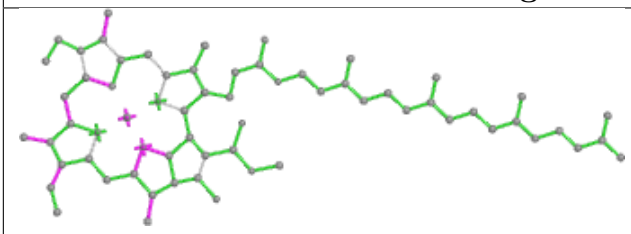


Torsions

Rings

Ligand CLA e 1103



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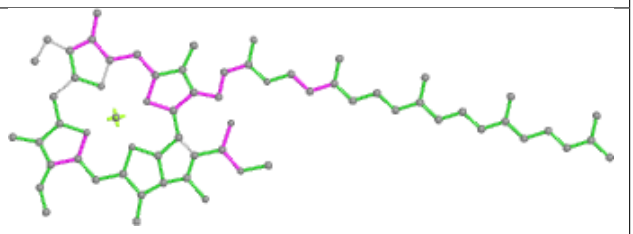

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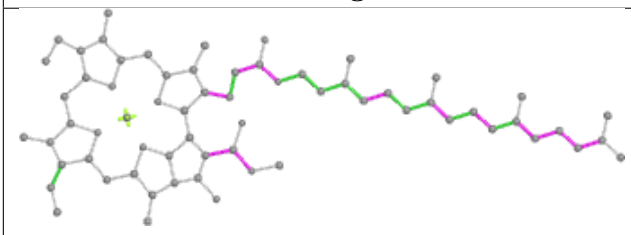

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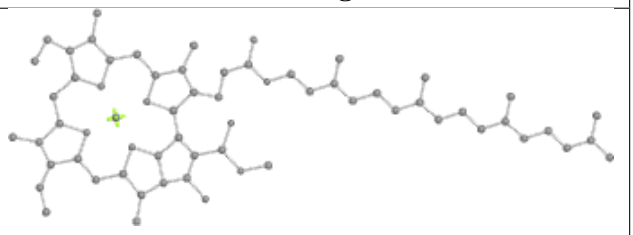

Rings

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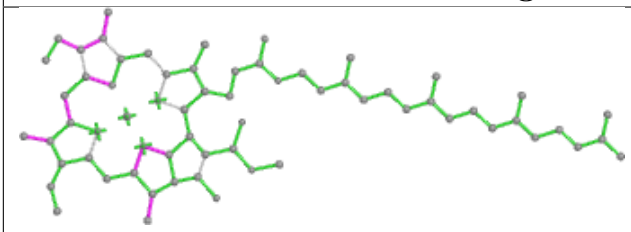

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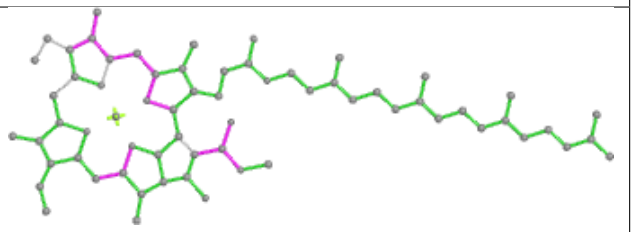

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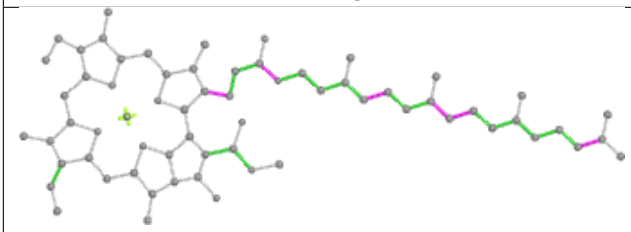

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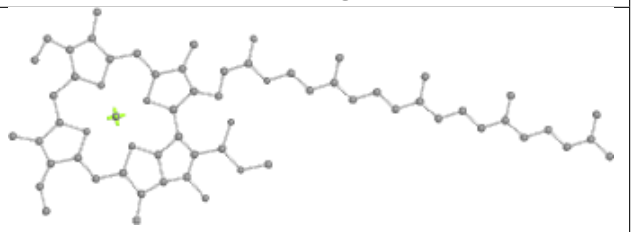

Rings

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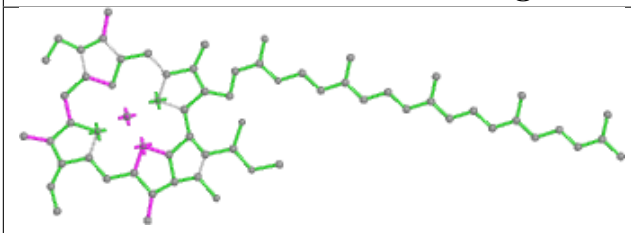

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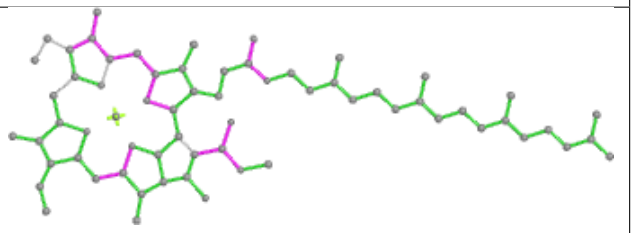
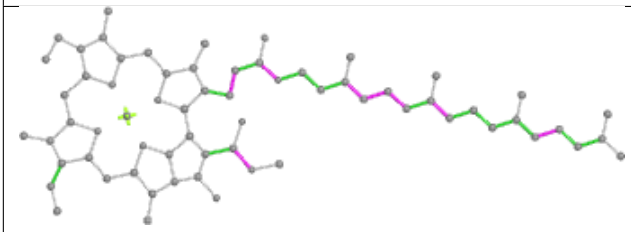


Bond angles



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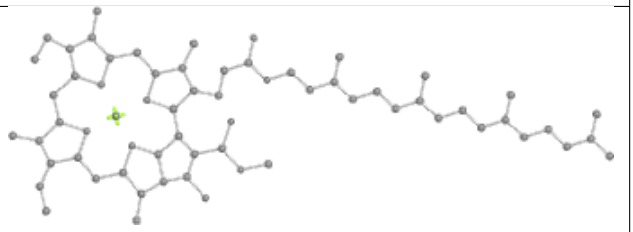

Rings

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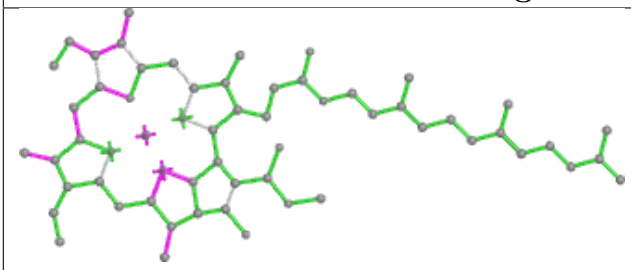
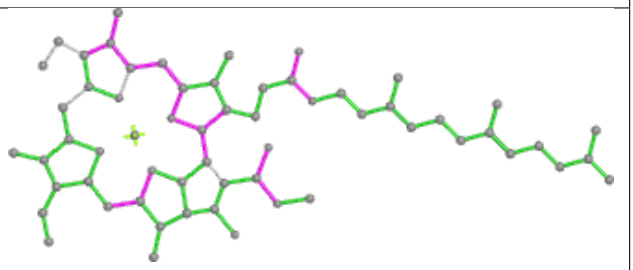
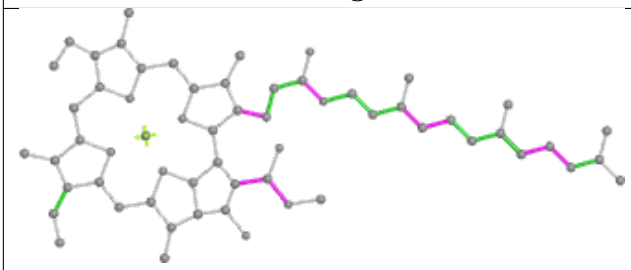
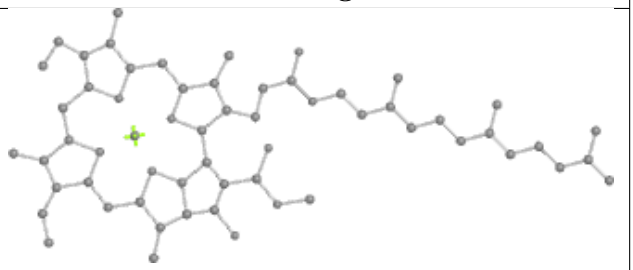
 Bond lengths	 Bond angles
 Torsions	 Rings

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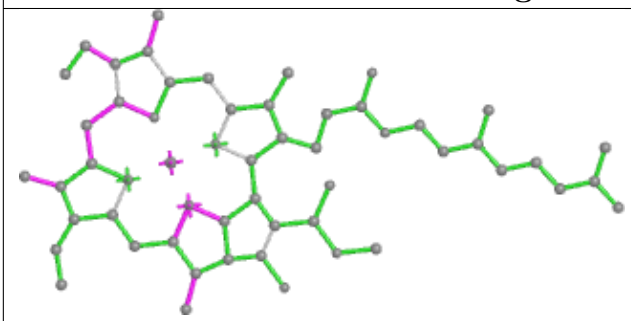
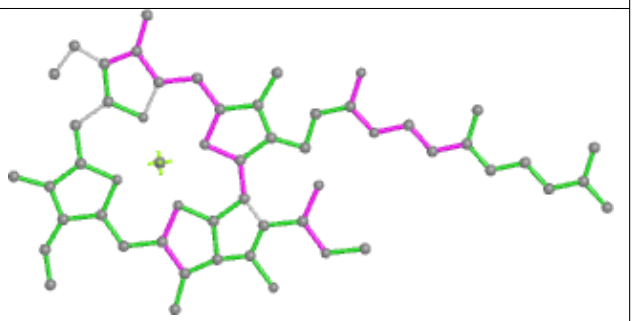
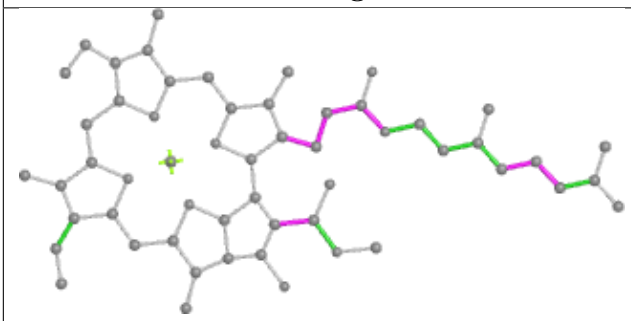
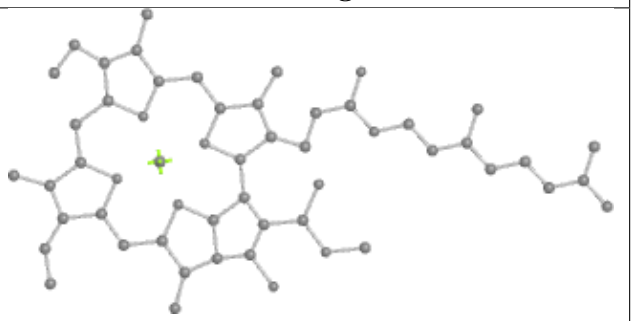
 Bond lengths	 Bond angles
 Torsions	 Rings

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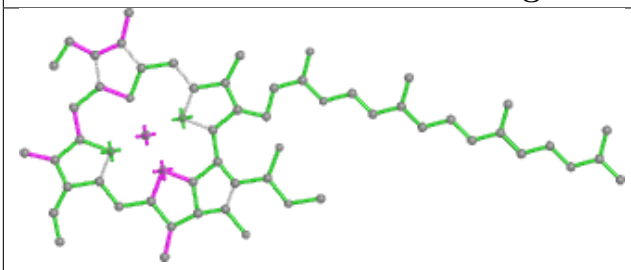

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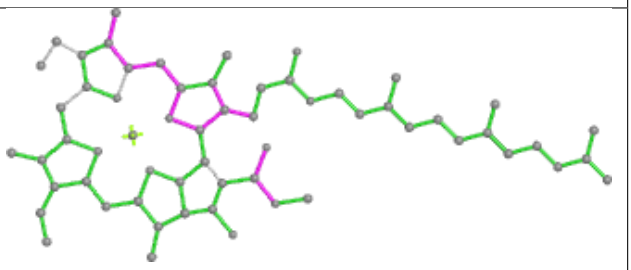

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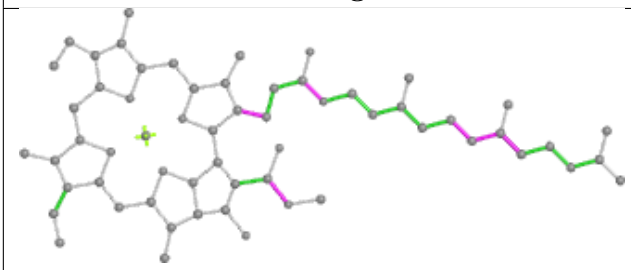

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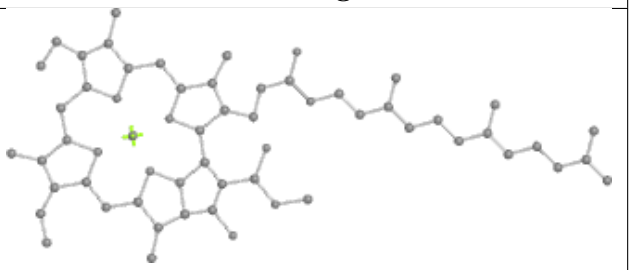
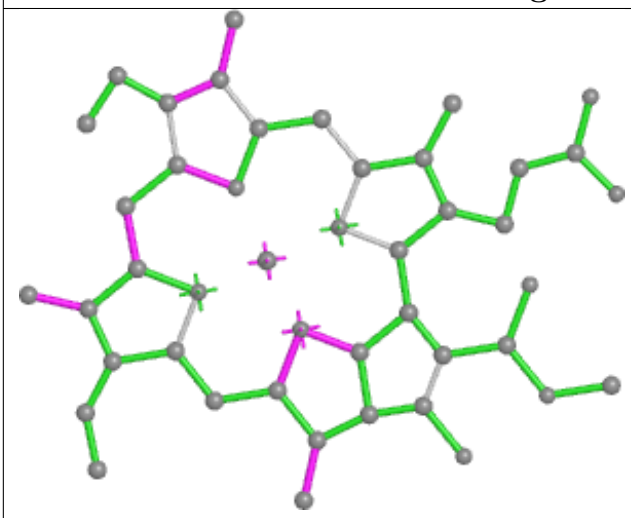


Rings

Ligand CLA r 508



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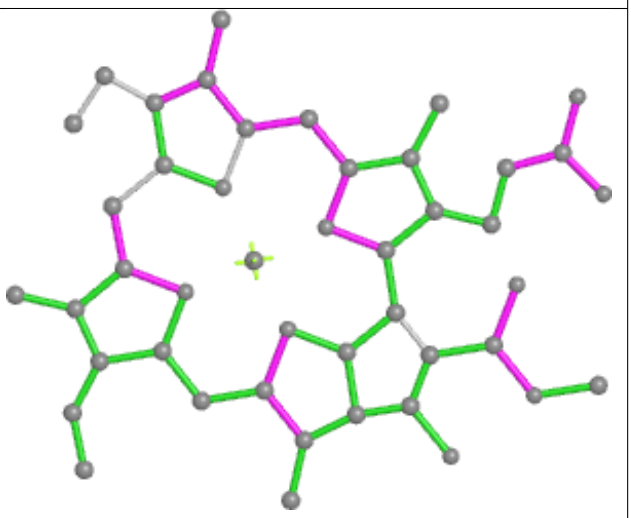

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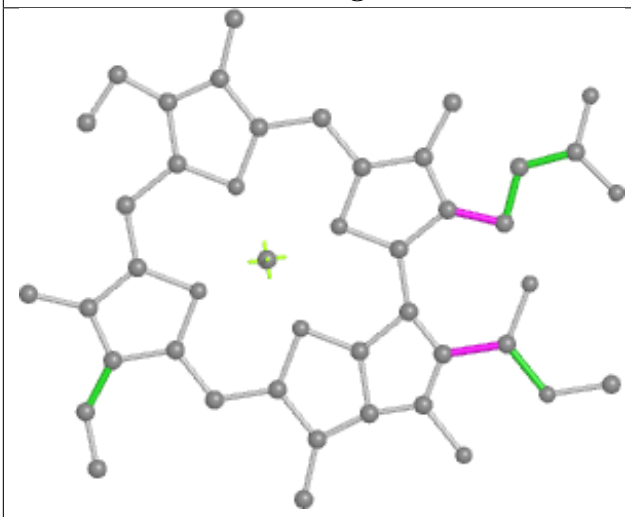

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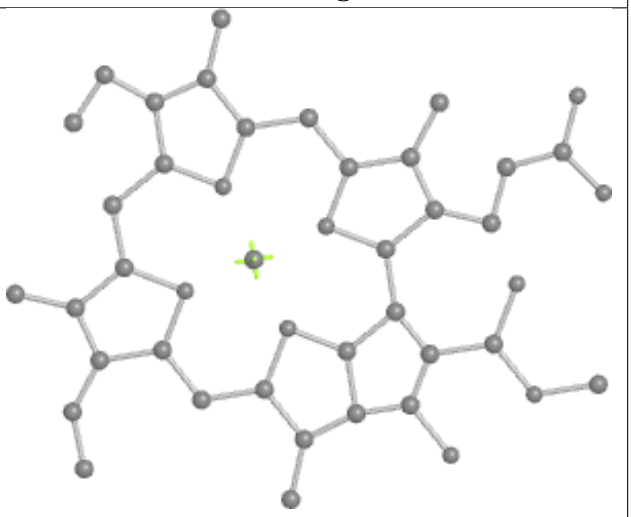
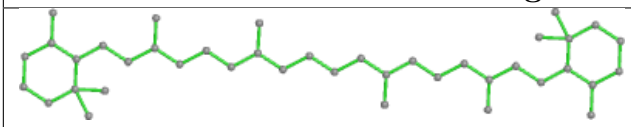


Rings

Ligand BCR Z 524



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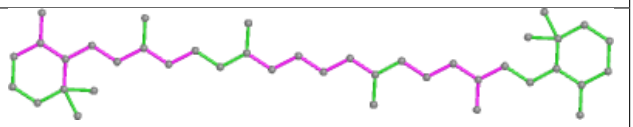

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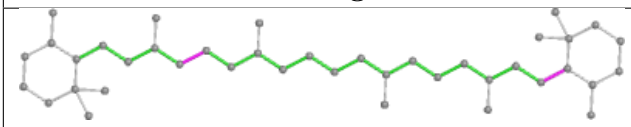

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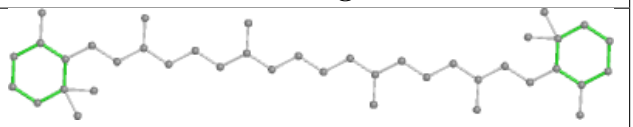

Rings

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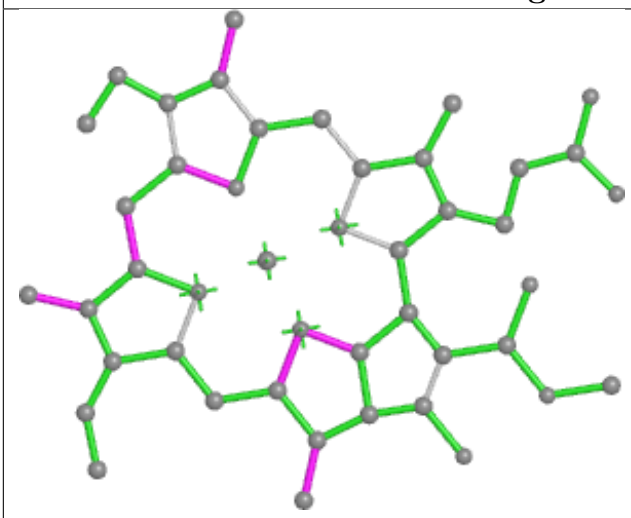

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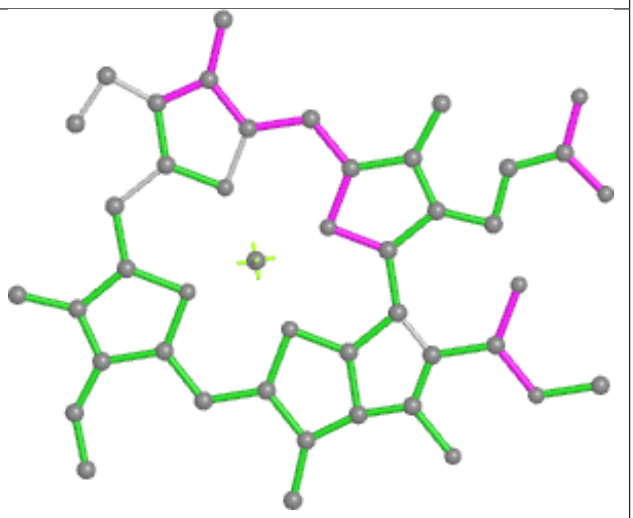

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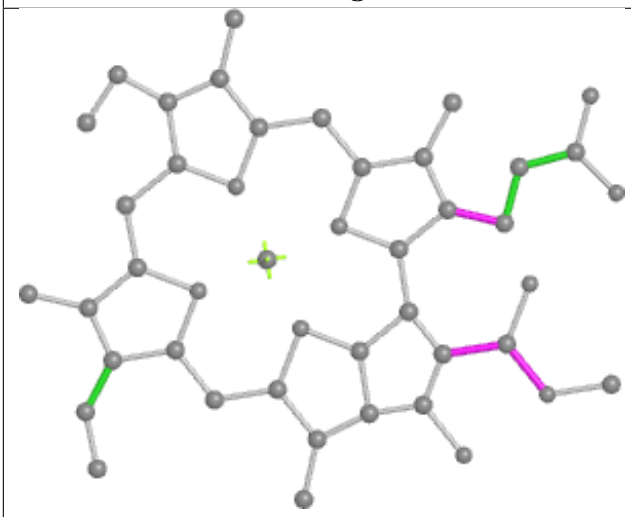

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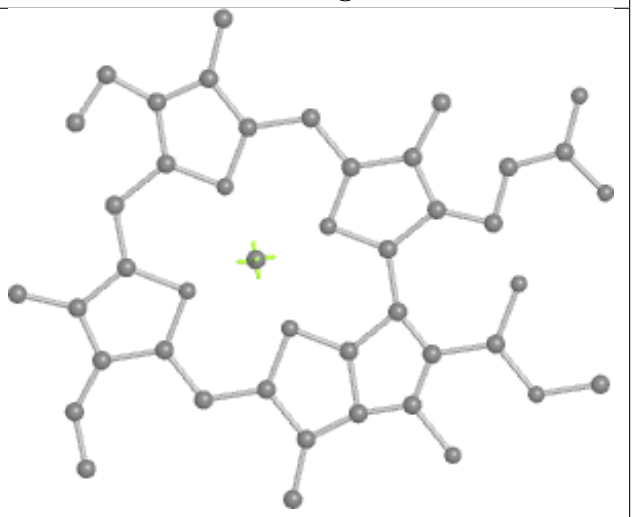

Rings

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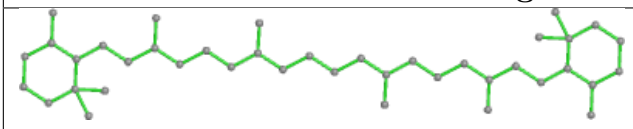

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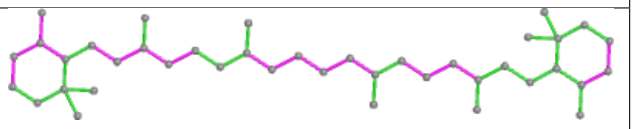
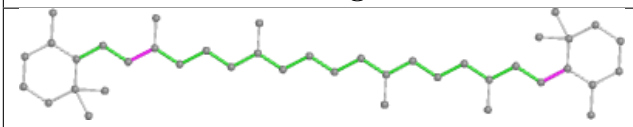


Bond angles



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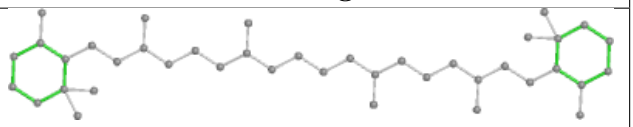

Rings

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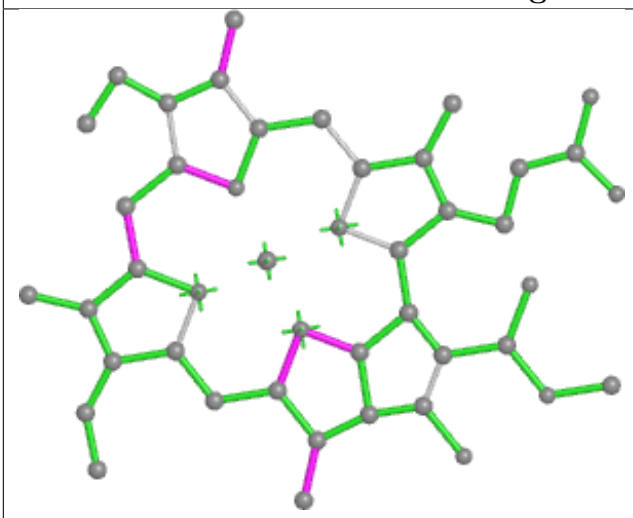

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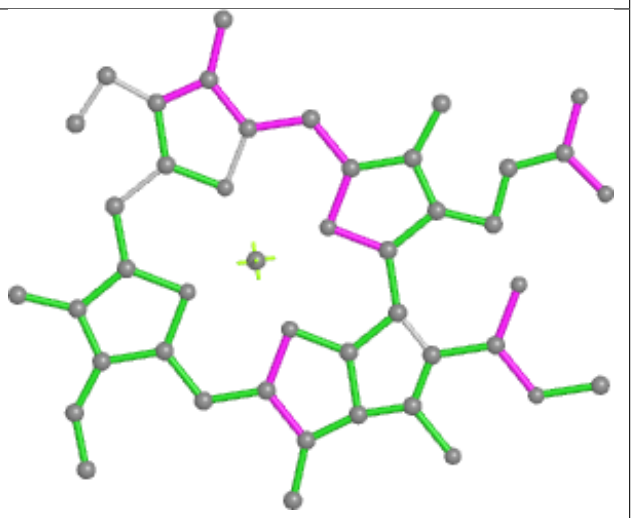

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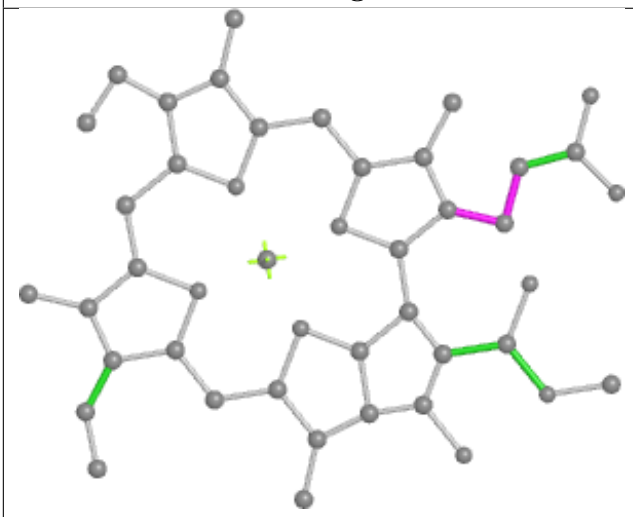

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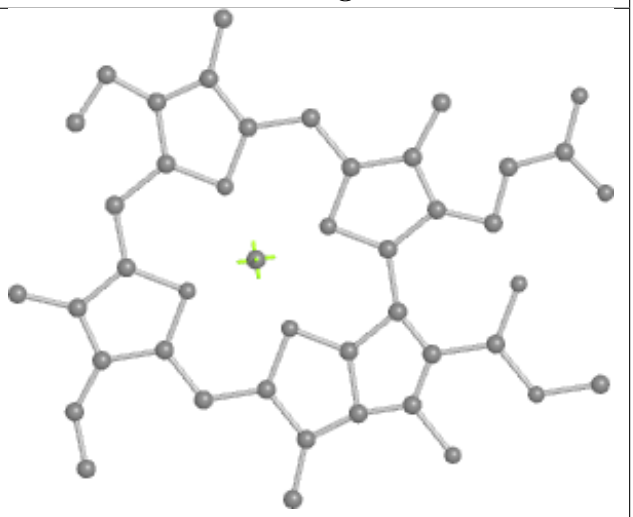

Rings

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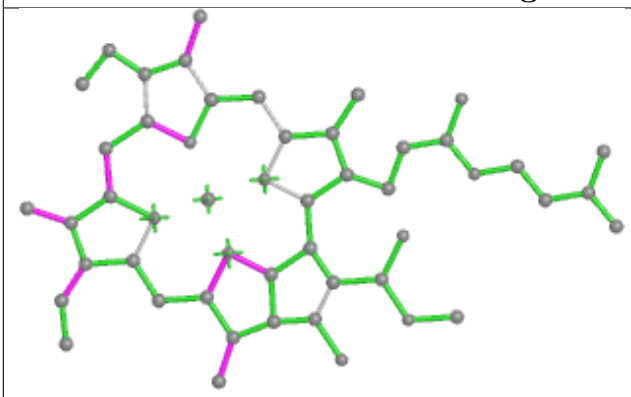
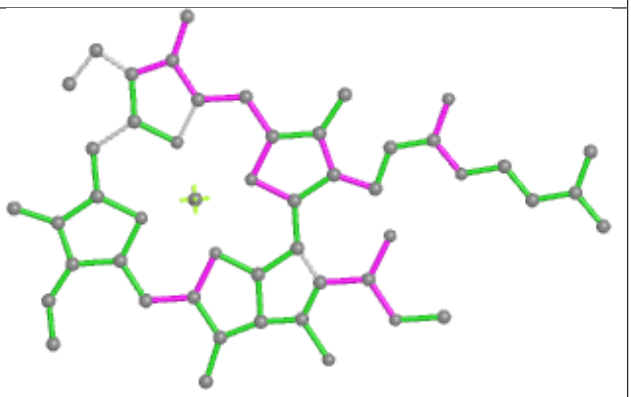
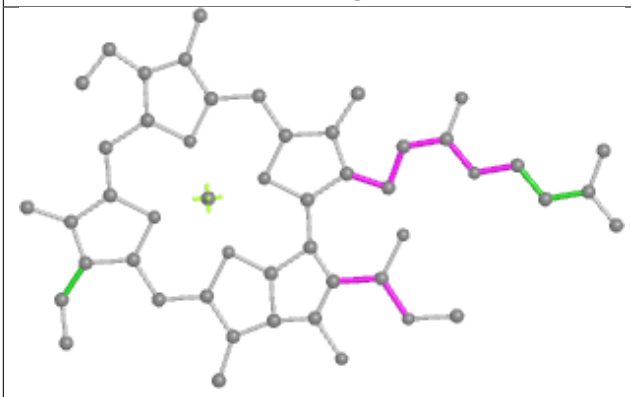
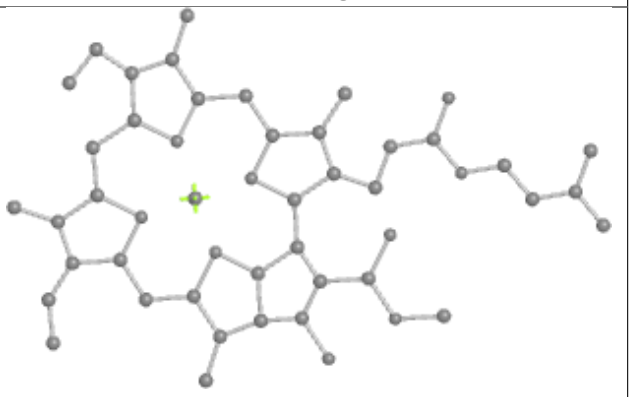
 Bond lengths	 Bond angles
 Torsions	 Rings

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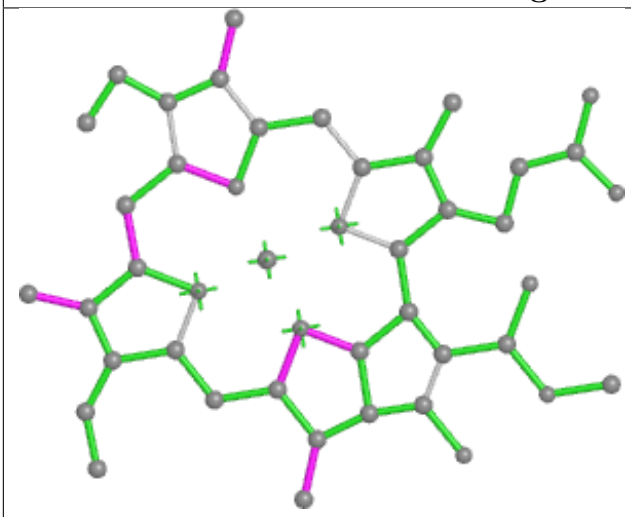

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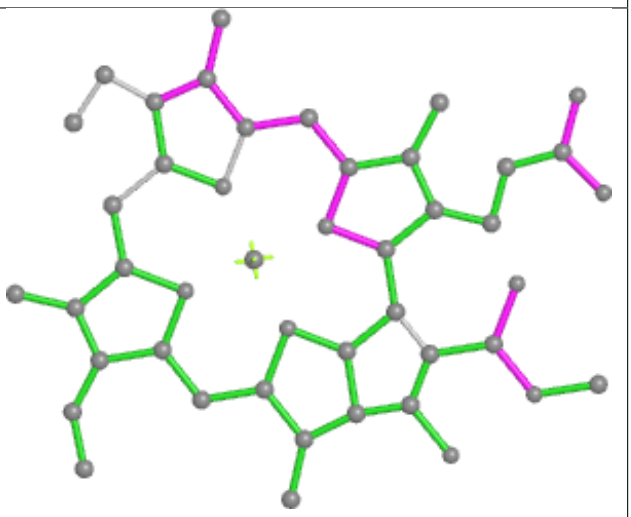
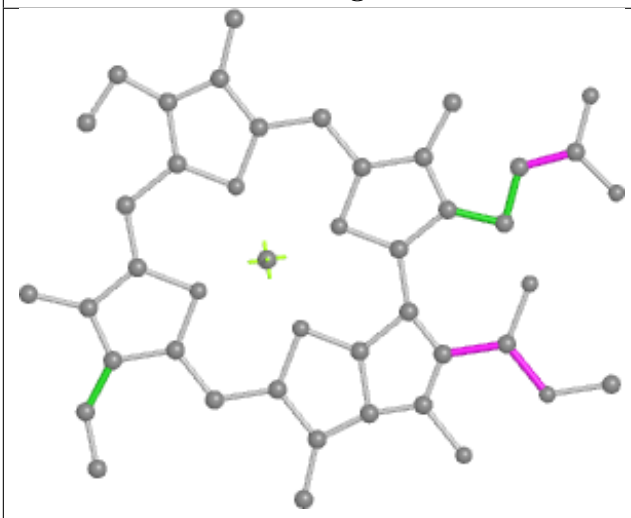


Bond angles



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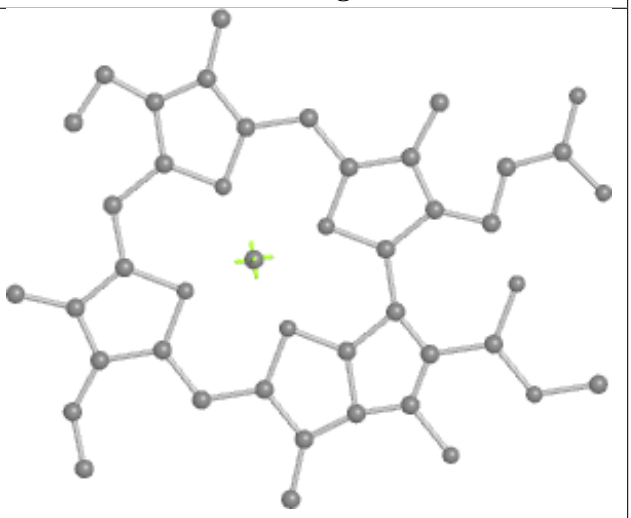
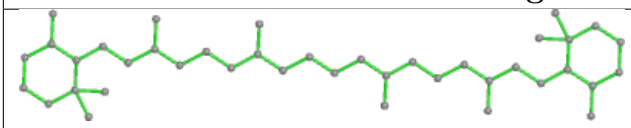


Rings

Ligand BCR 4 522



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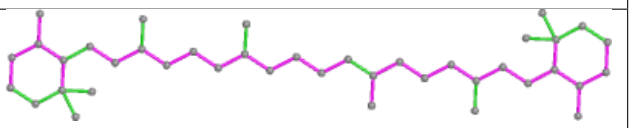

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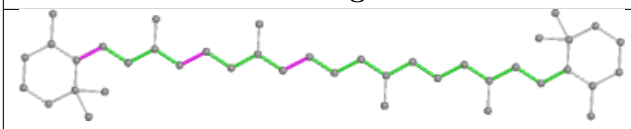

Torsions

Rings

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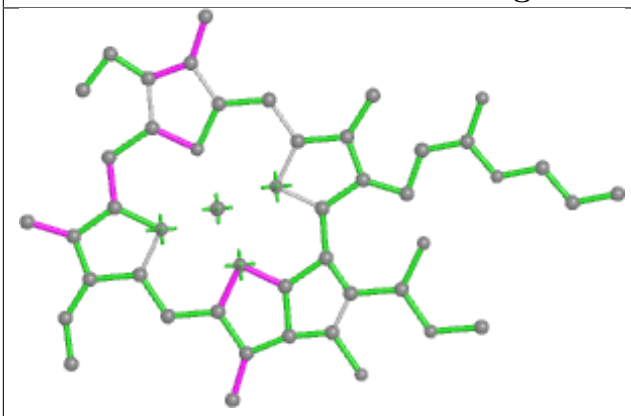
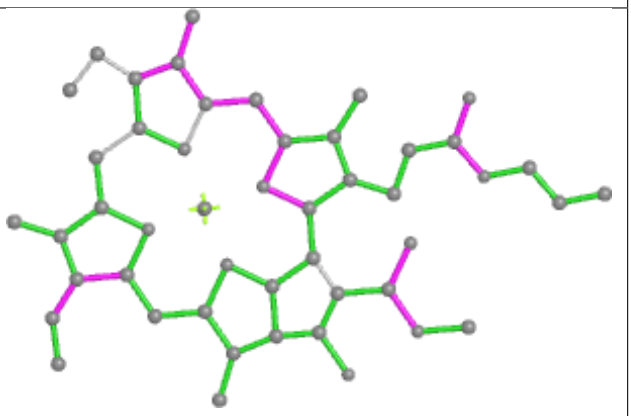
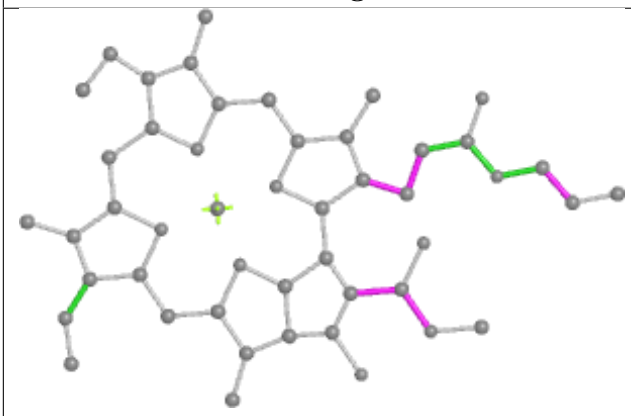
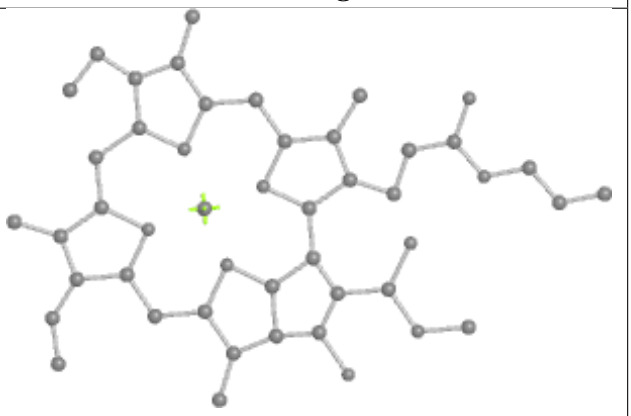
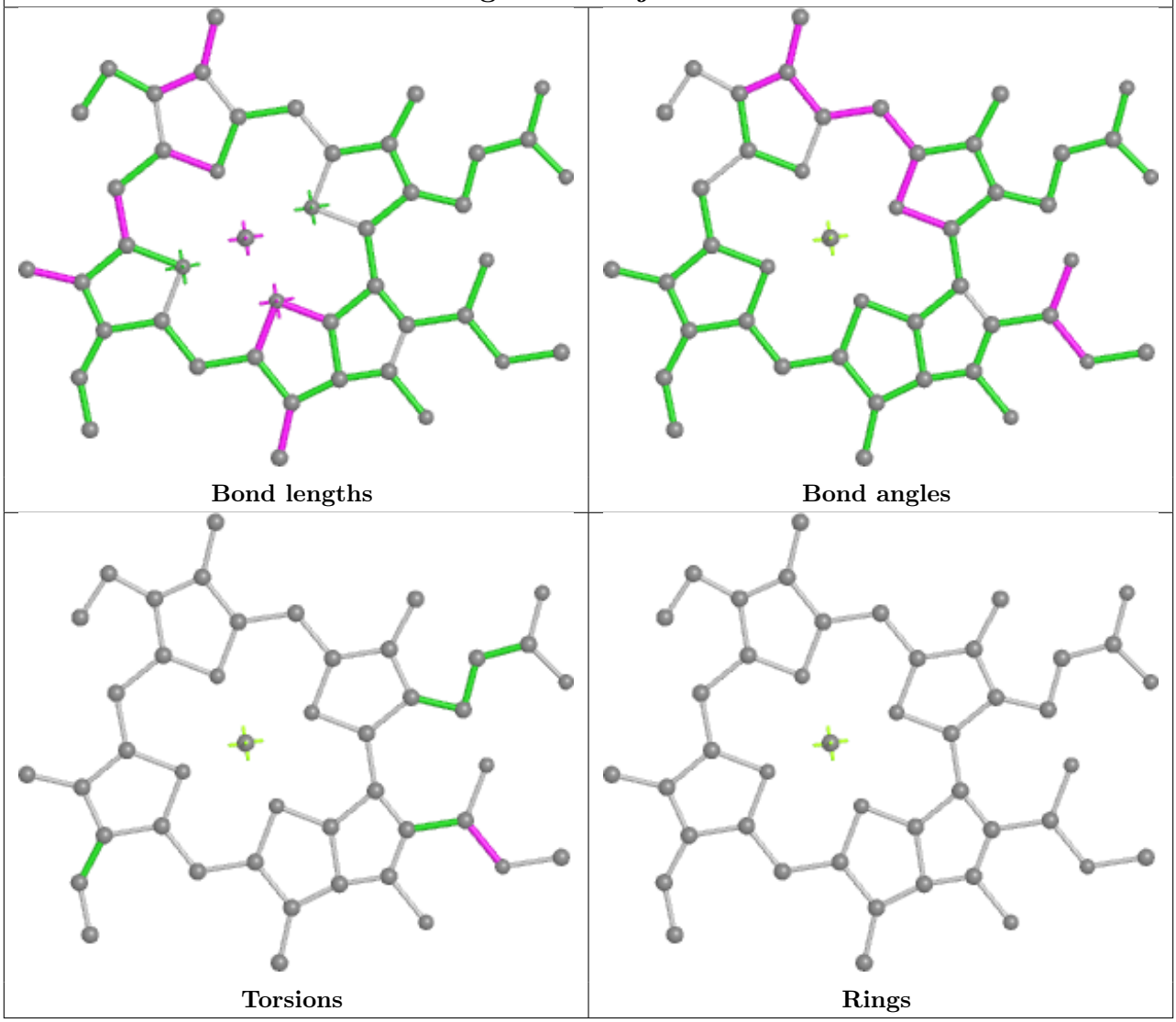
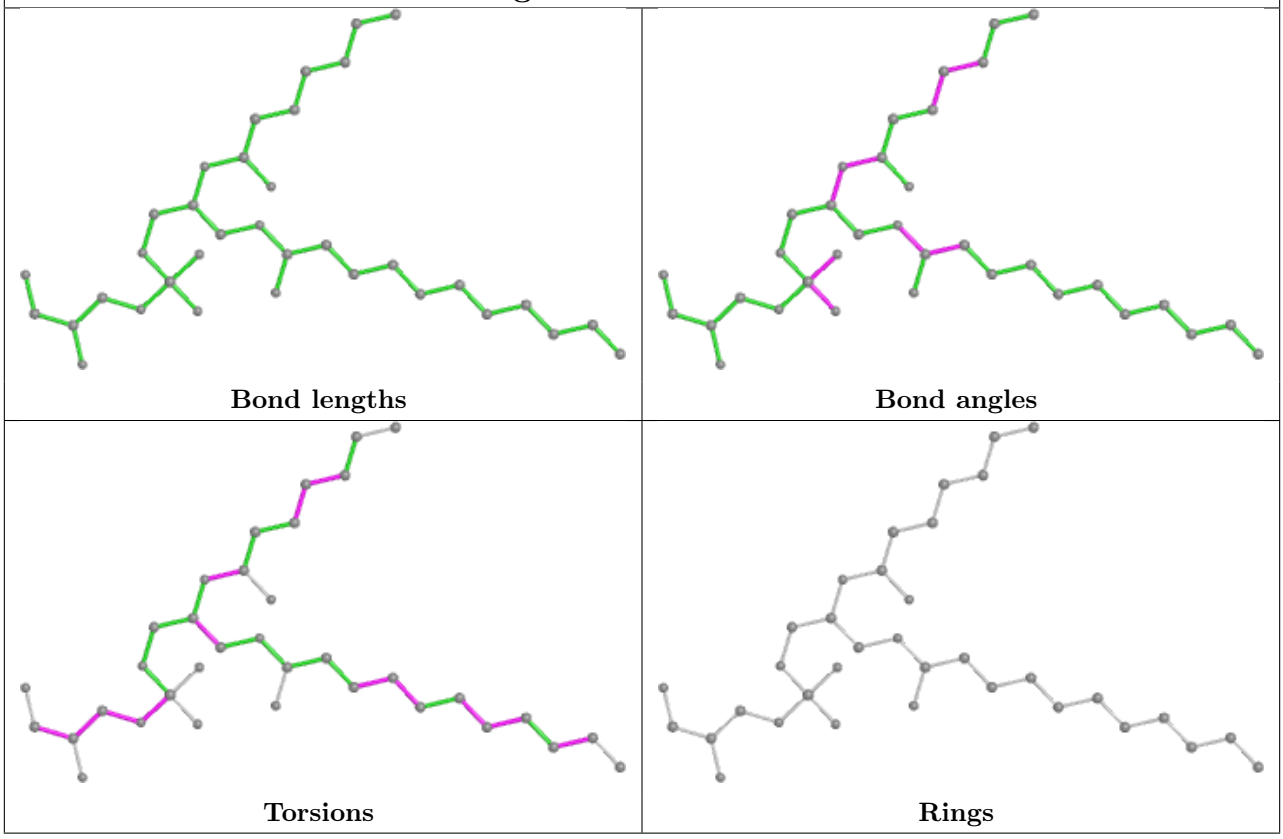
 Bond lengths	 Bond angles
 Torsions	 Rings

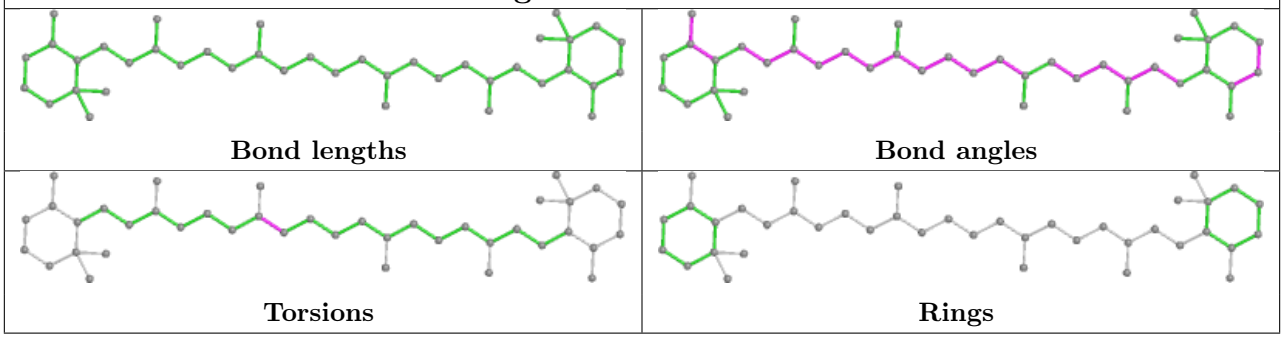
Ligand CLA j 1301



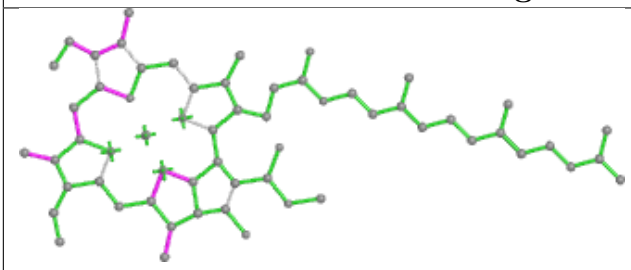
Ligand LHG G 5004



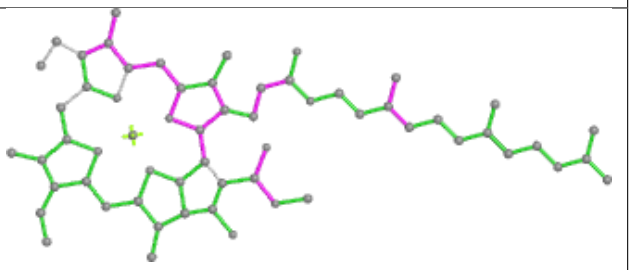
Ligand BCR R 4016



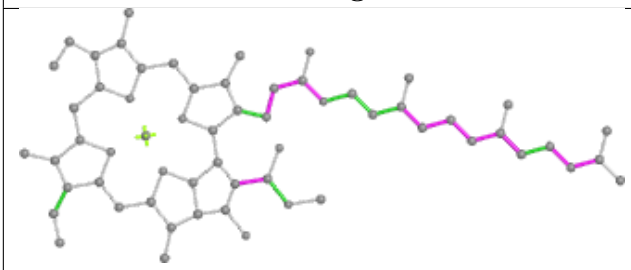
Ligand CLA A 1137



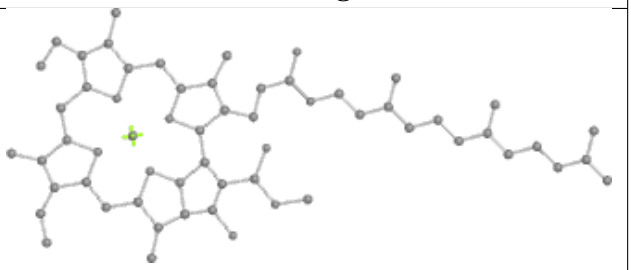
Bond lengths



Bond angles

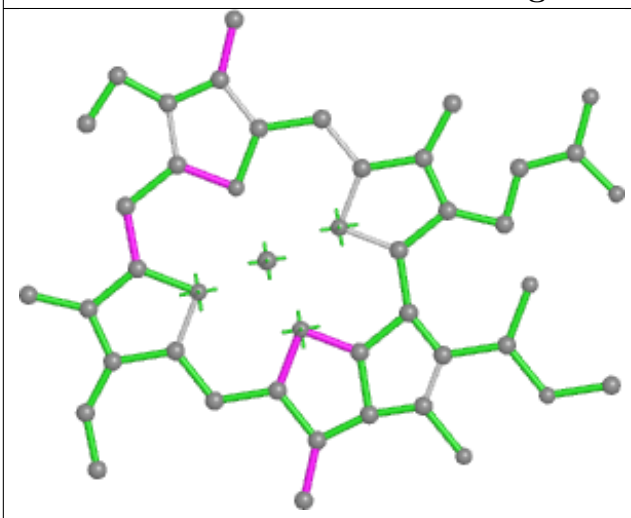


Torsions

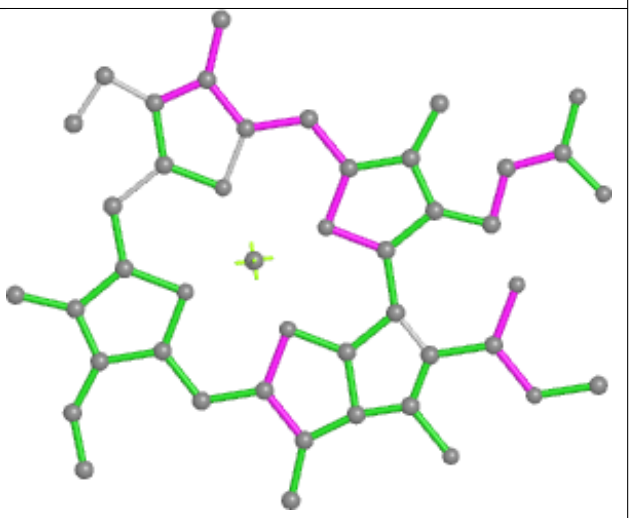


Rings

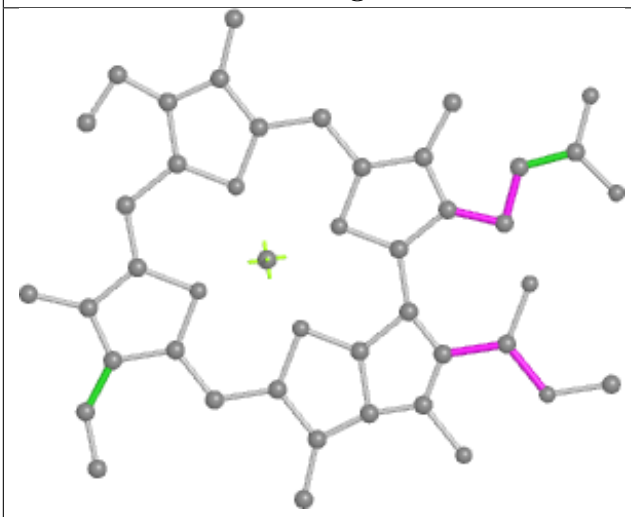
Ligand CLA 3 503



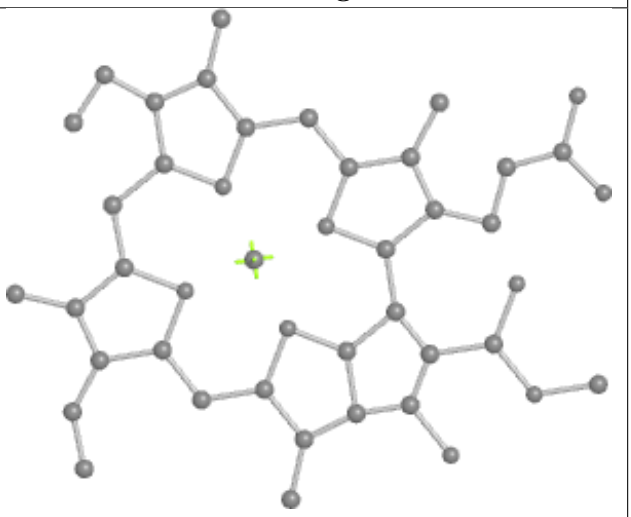
Bond lengths



Bond angles



Torsions



Rings

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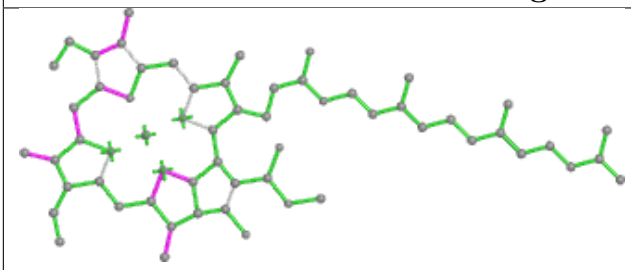
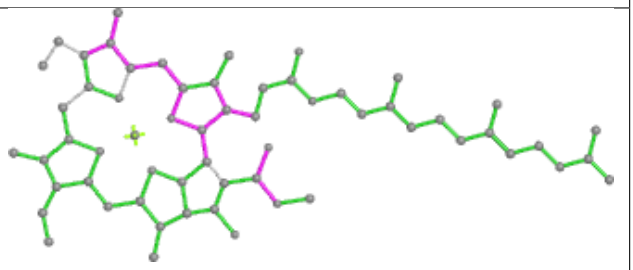
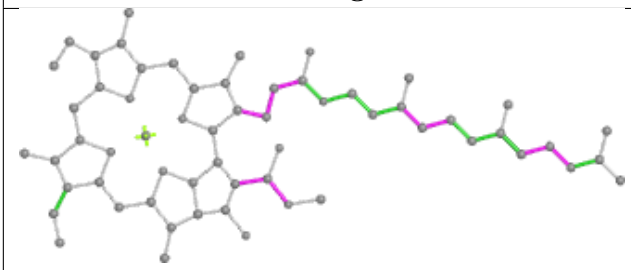
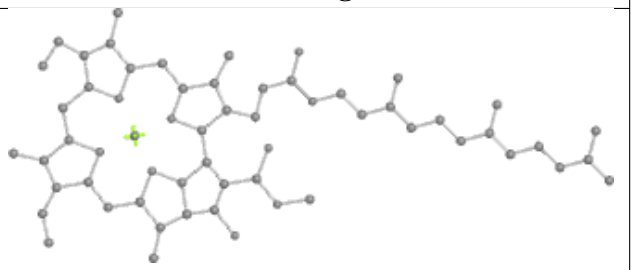
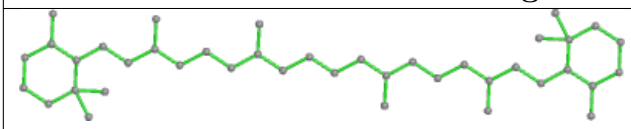
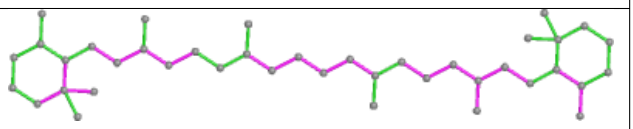
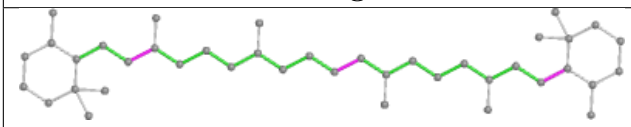
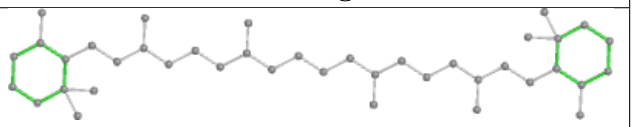
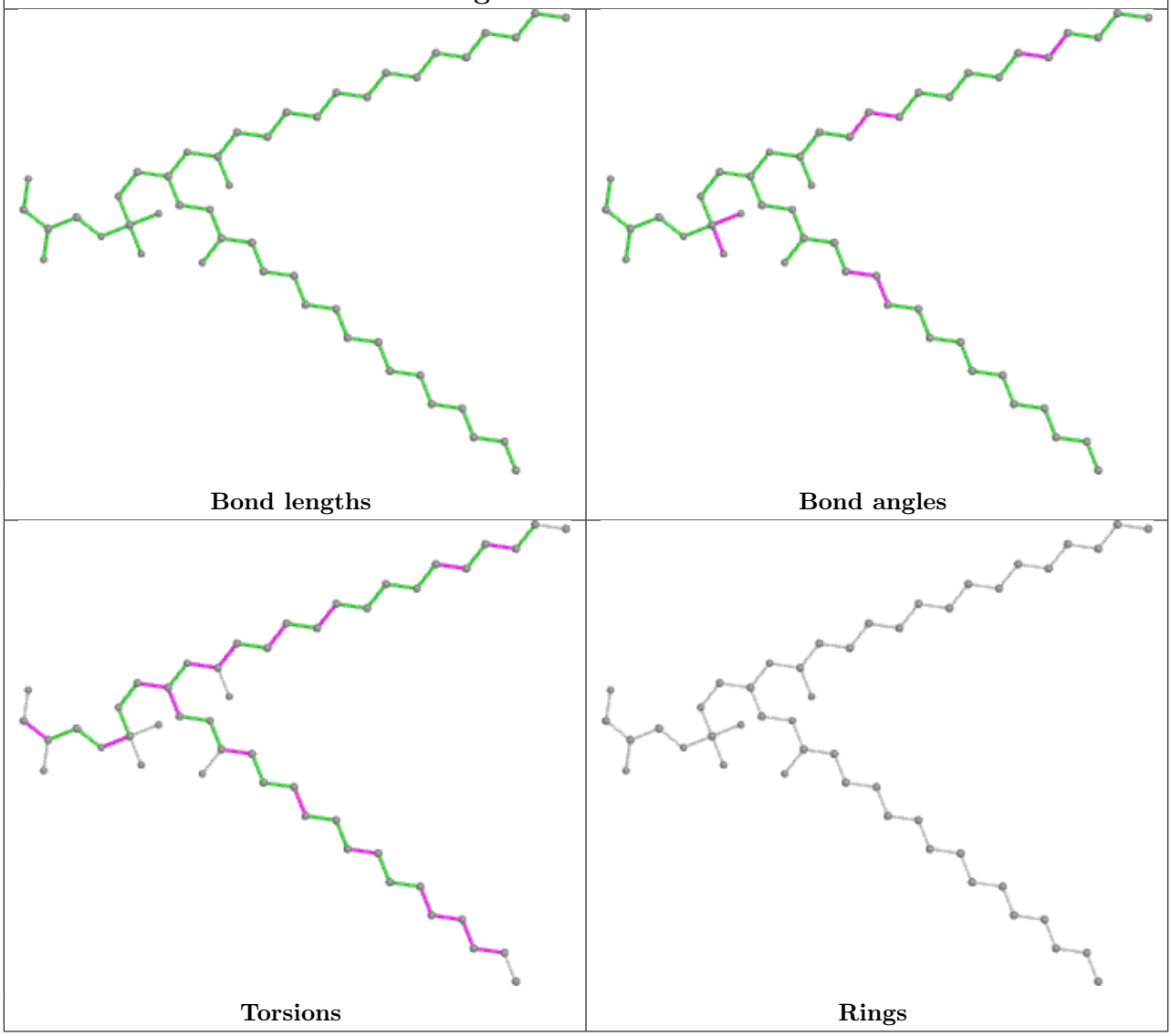
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR l 4015	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG e 5007



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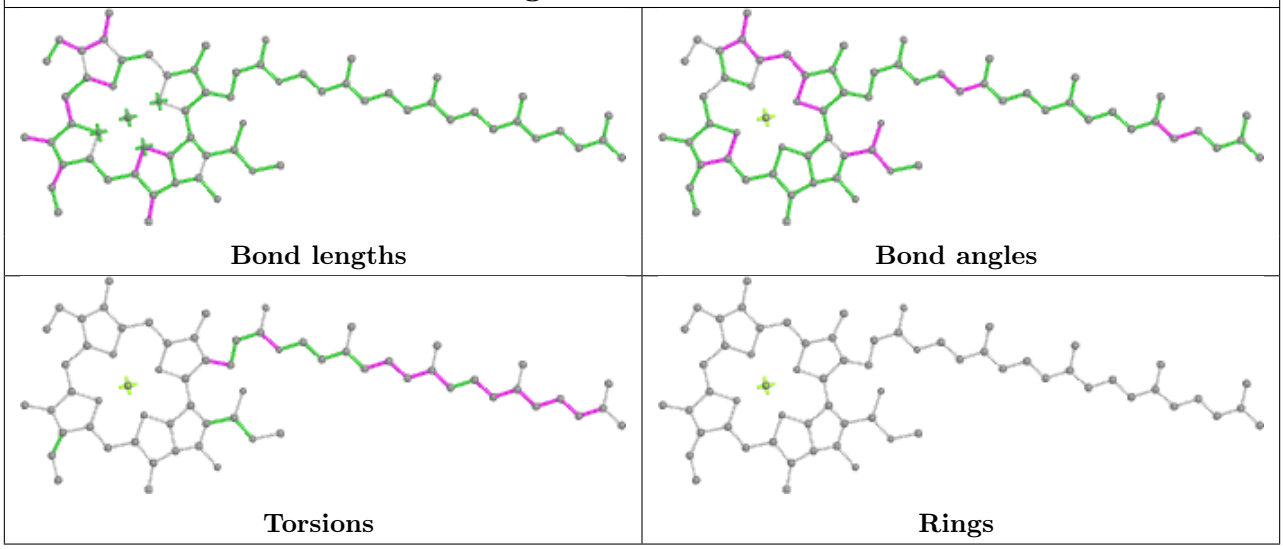
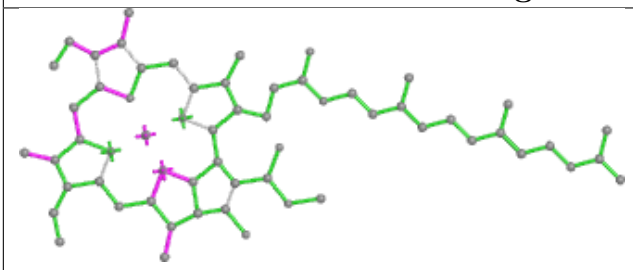
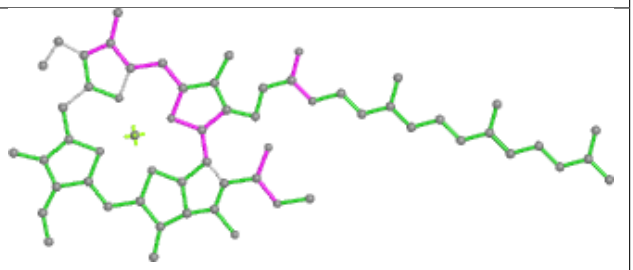


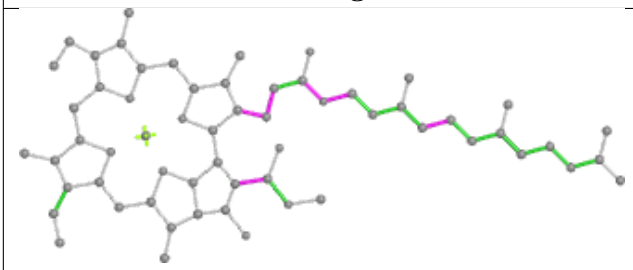
Ligand CLA A 1118



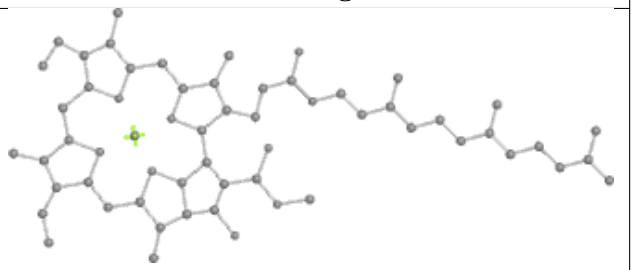
Bond lengths



Bond angles

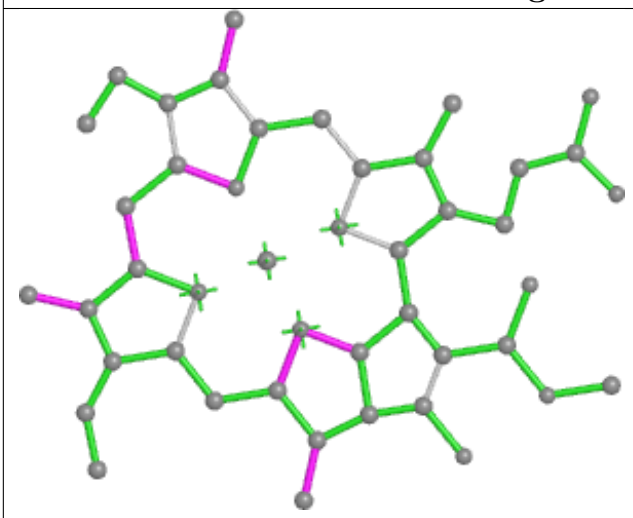


Torsions



Rings

Ligand CLA 3 509



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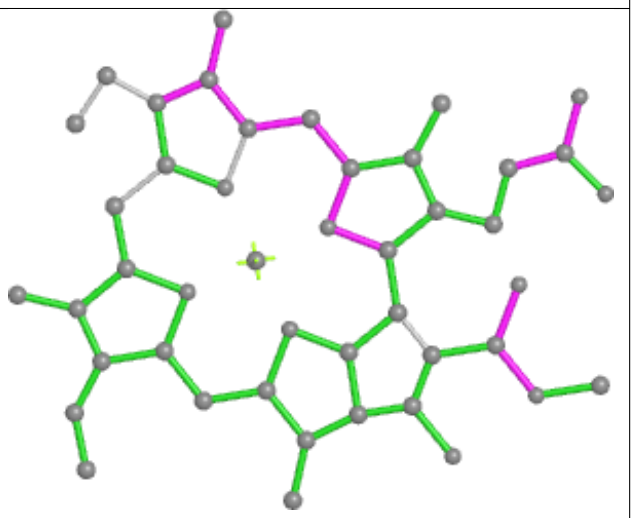

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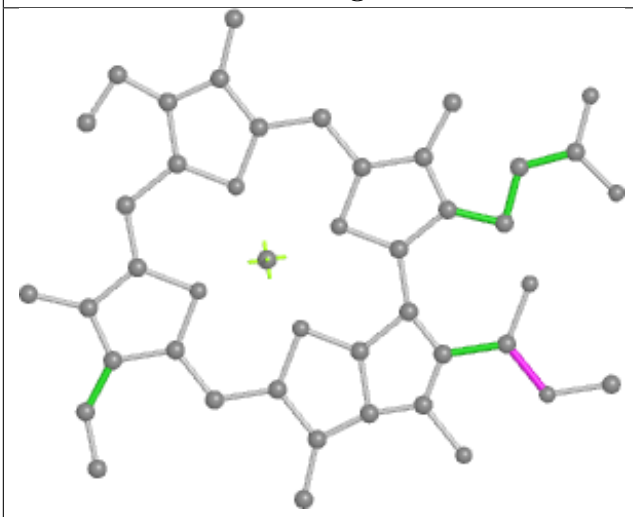

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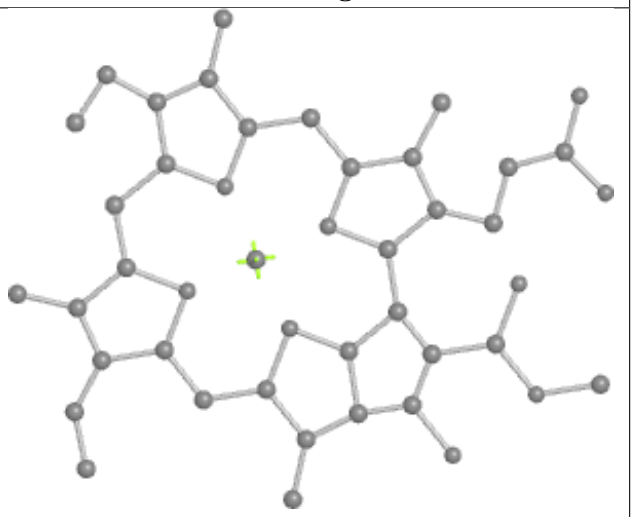
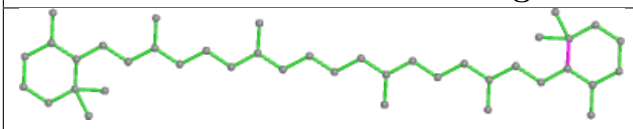


Rings

Ligand BCR A 4002



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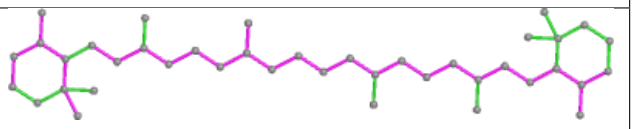
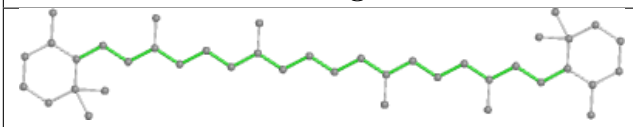


Bond angles



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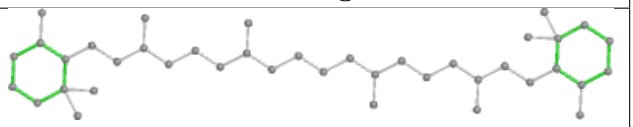
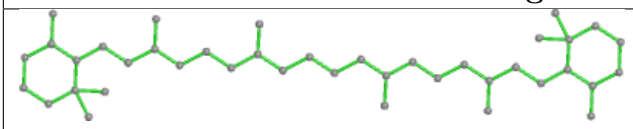


Rings

Ligand BCR q 521



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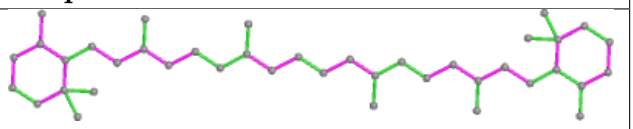

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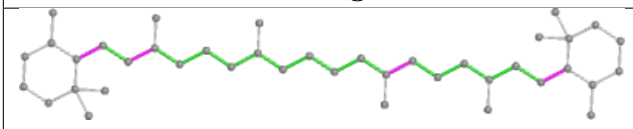

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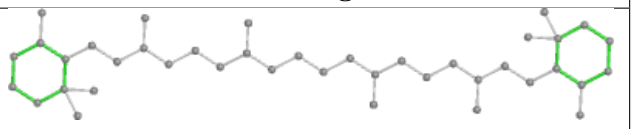
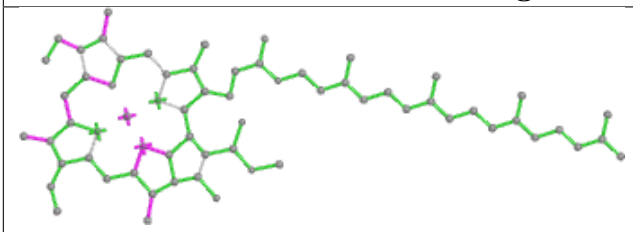


Rings

Ligand CLA B 1021



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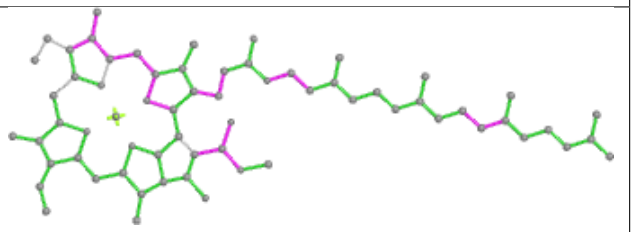
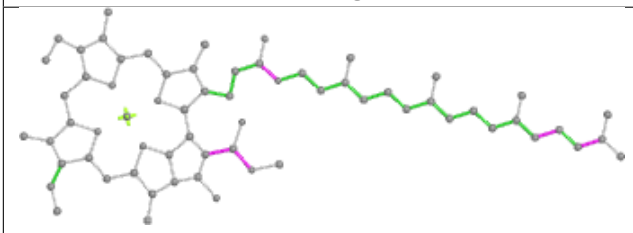


Bond angles



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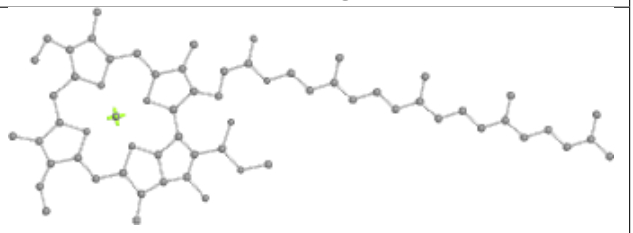

Rings

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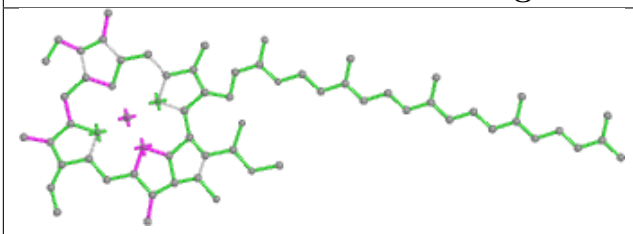

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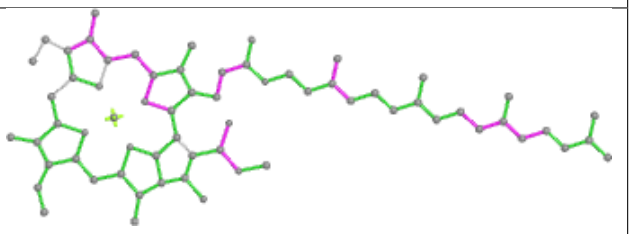

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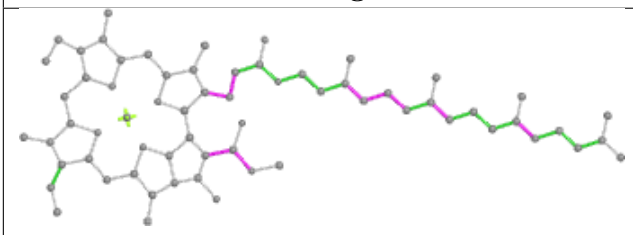

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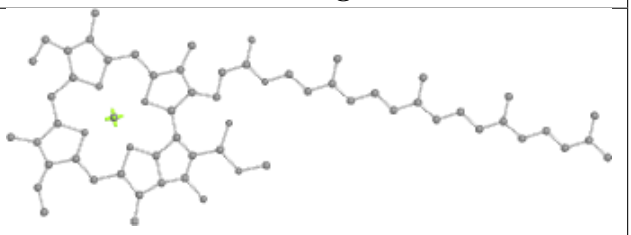
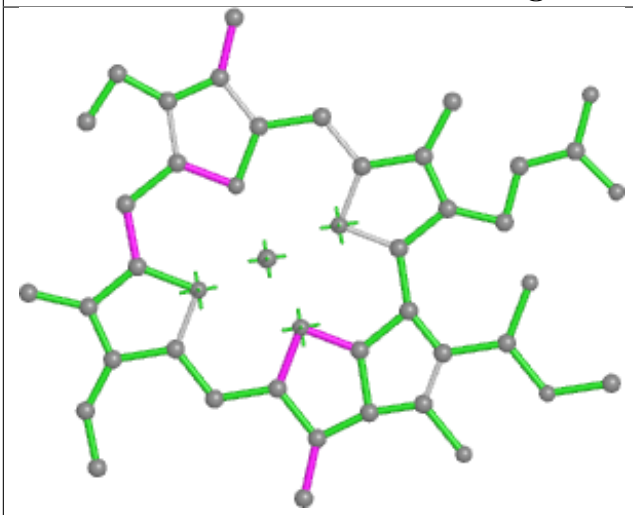


Rings

Ligand CLA u 516



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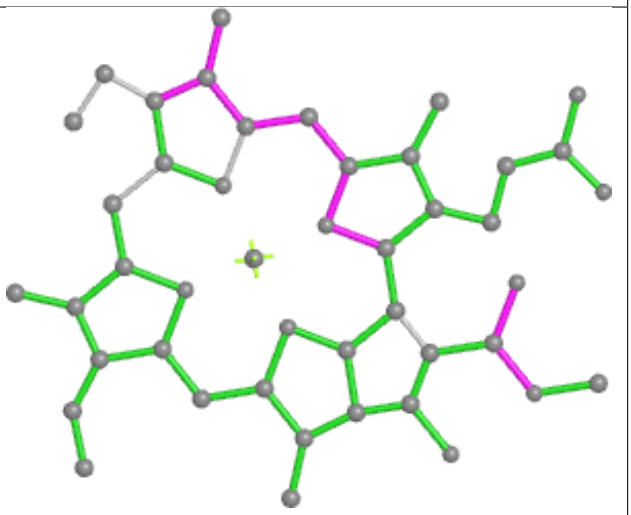

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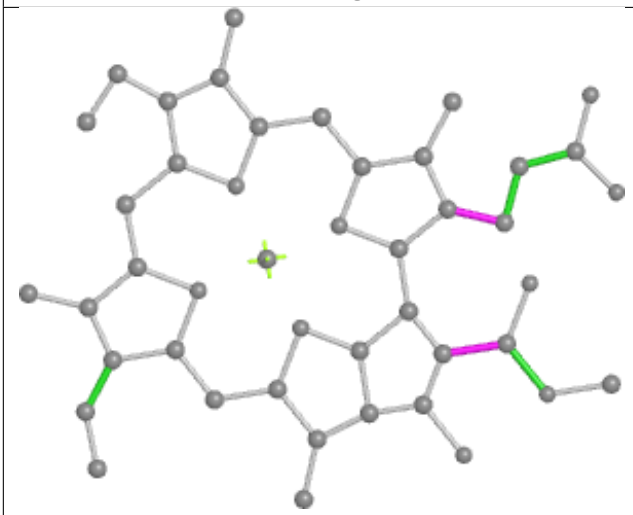

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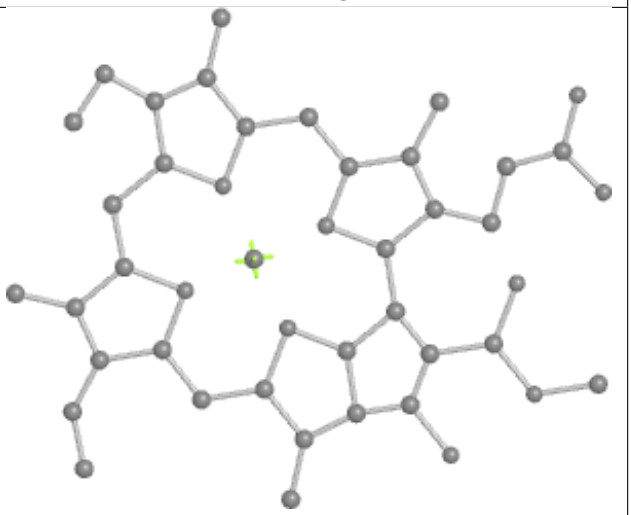

Rings

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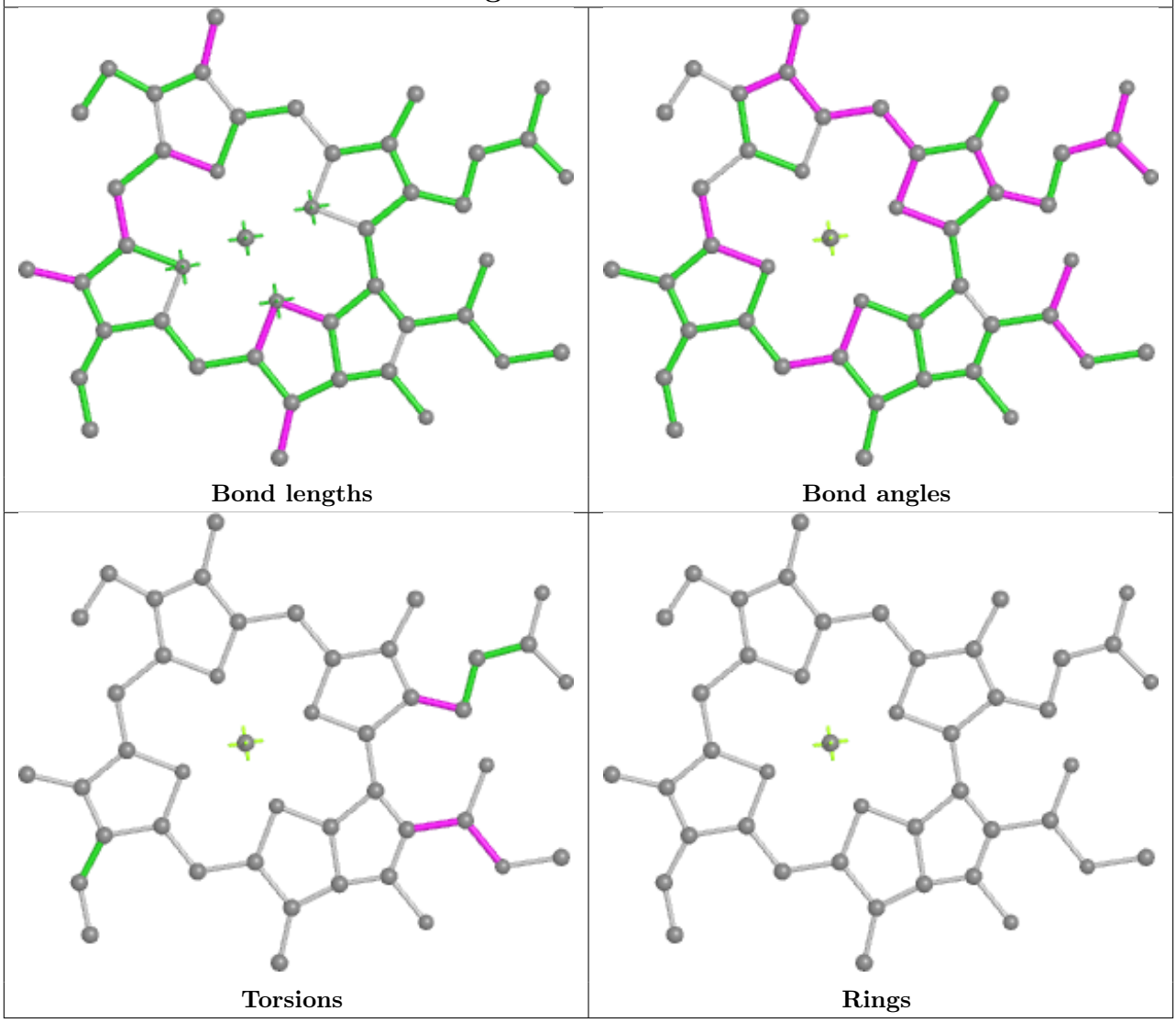

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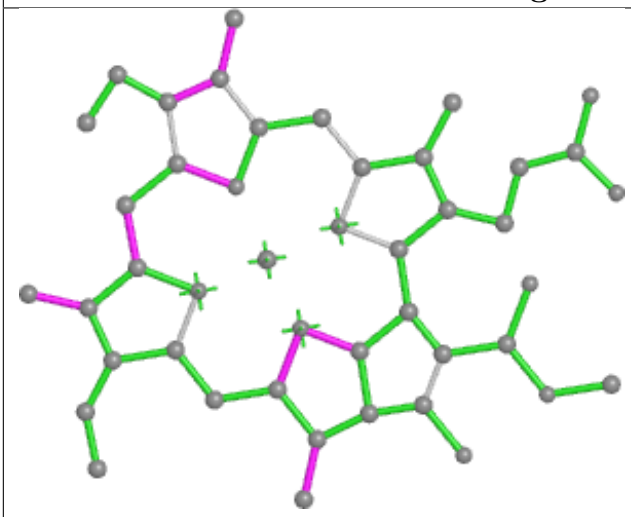

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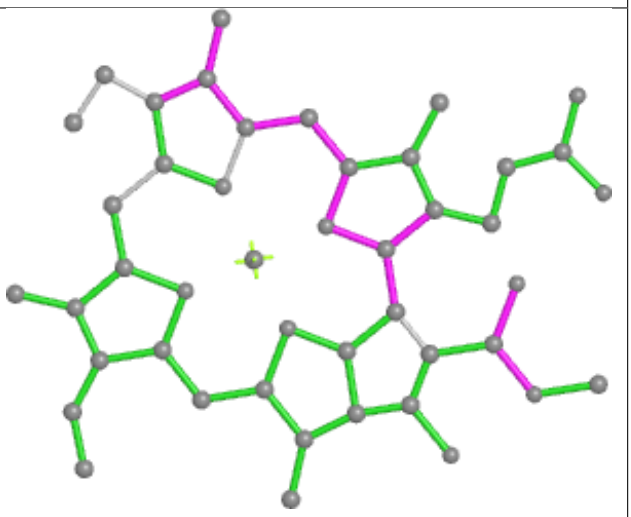
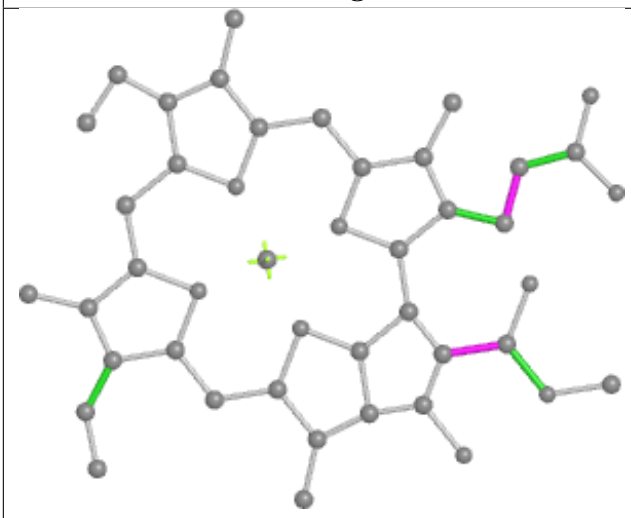
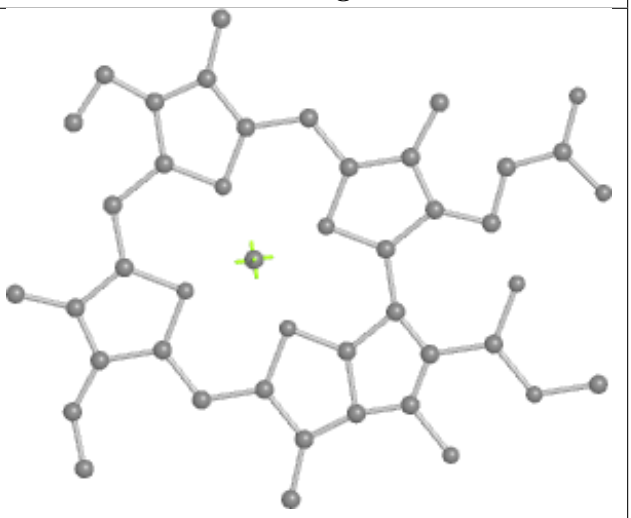


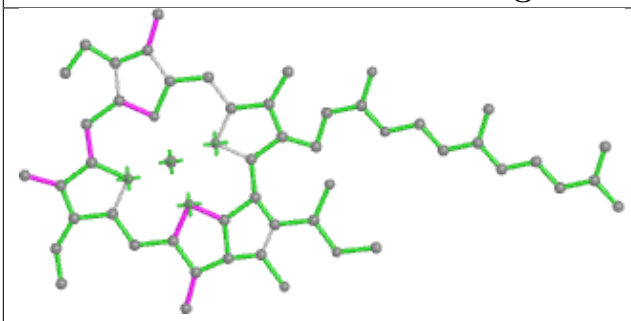
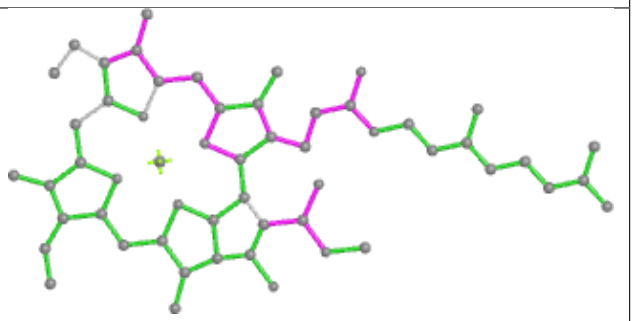
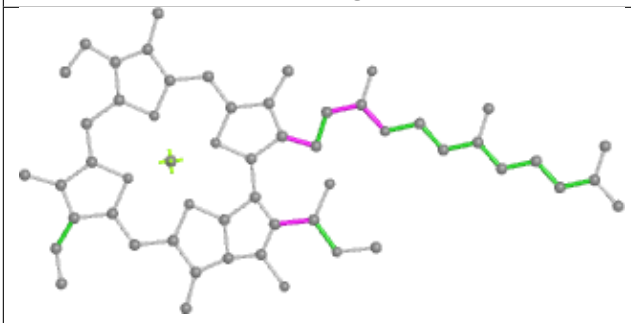
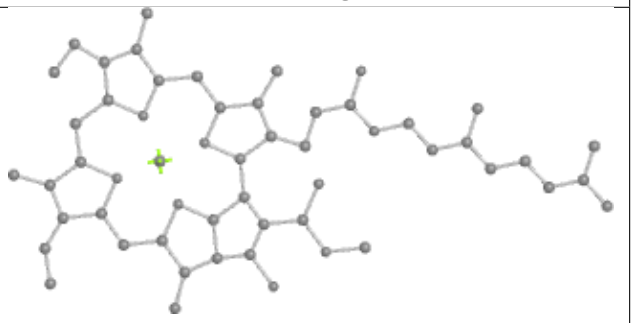
Bond angles



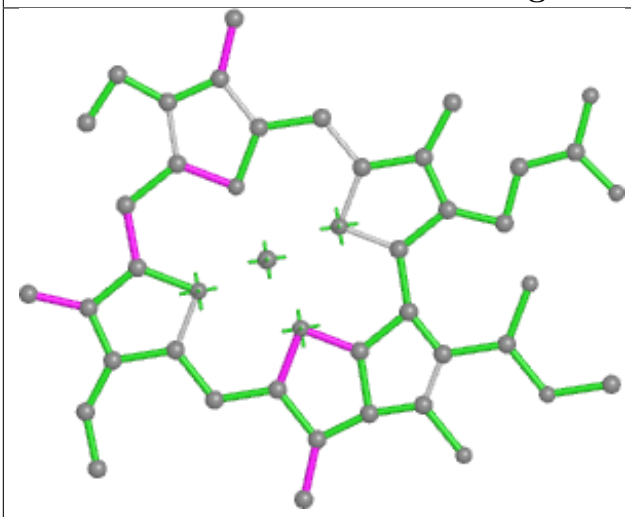
Torsions



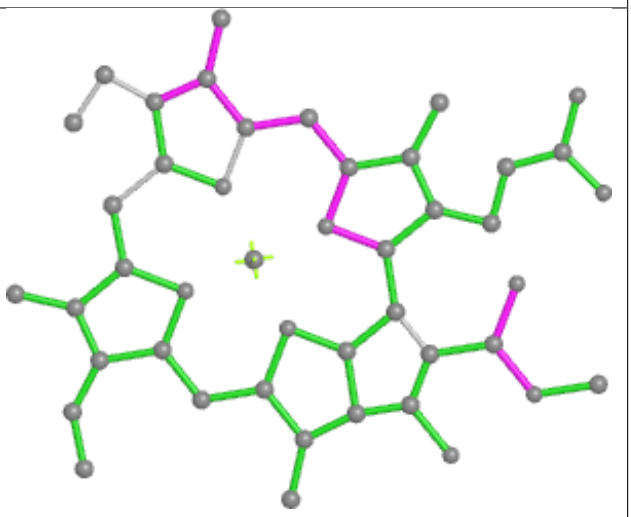
Rings

Ligand CLA U 1401	
 Bond lengths	 Bond angles
 Torsions	 Rings

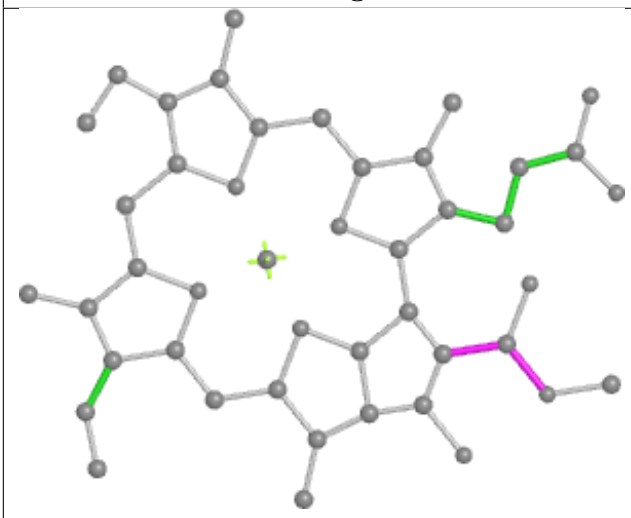
Ligand CLA 6 506



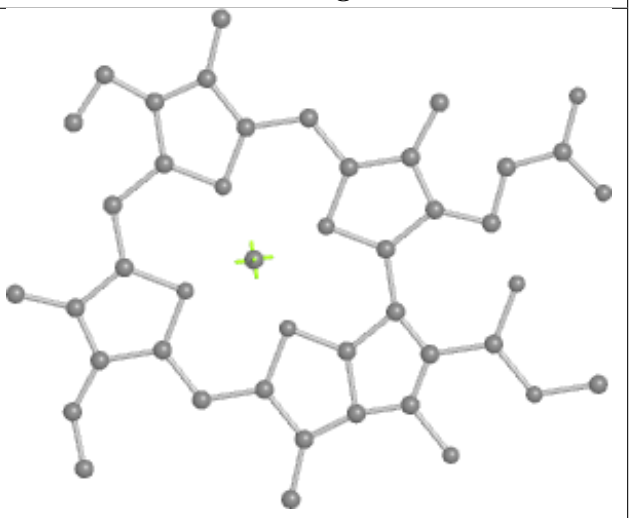
Bond lengths



Bond angles

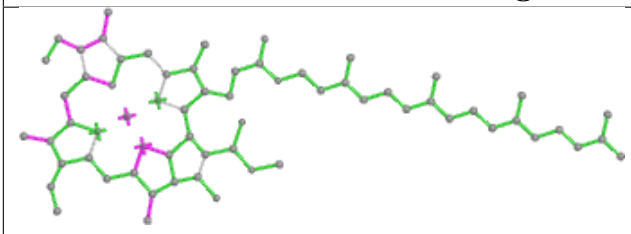


Torsions

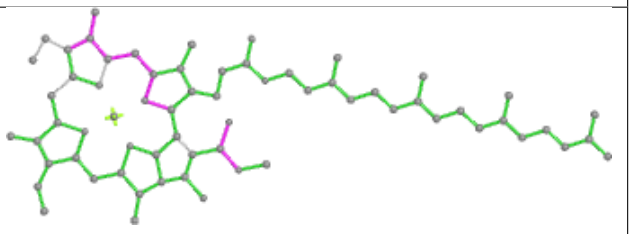


Rings

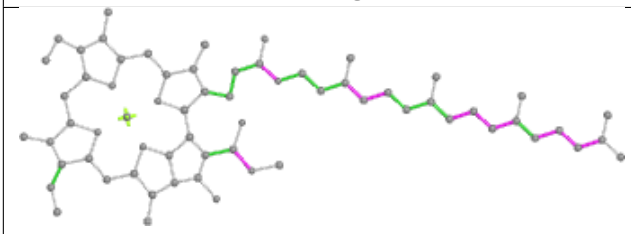
Ligand CLA A 1133



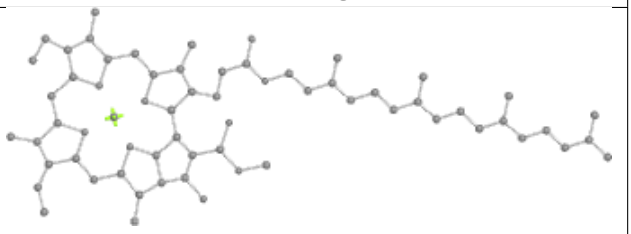
Bond lengths



Bond angles

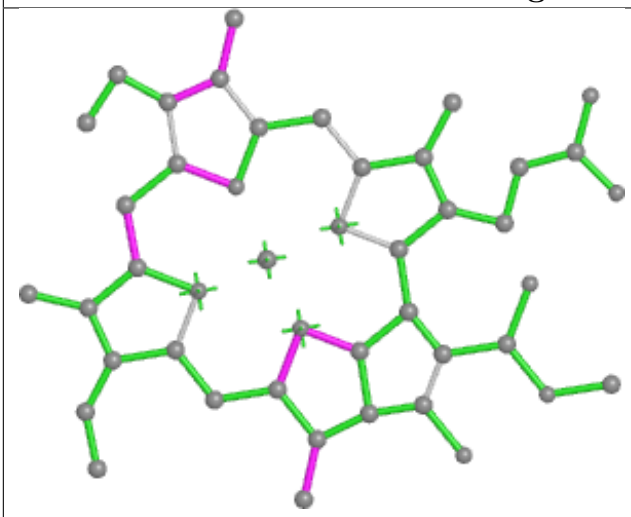


Torsions



Rings

Ligand CLA v 502



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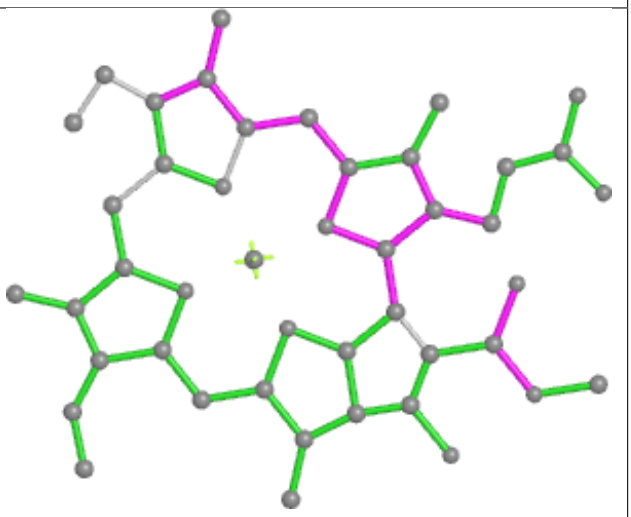

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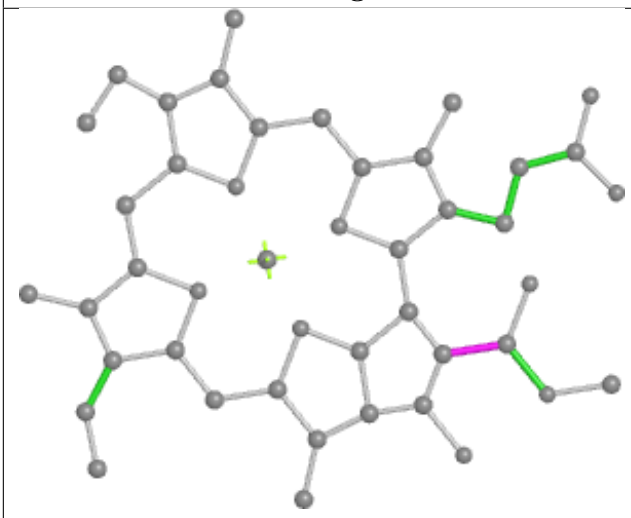

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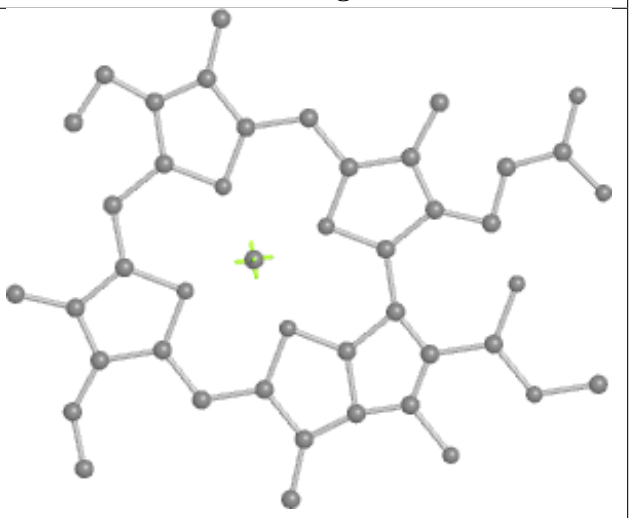
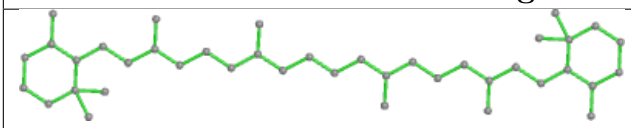


Rings

Ligand BCR J 4015



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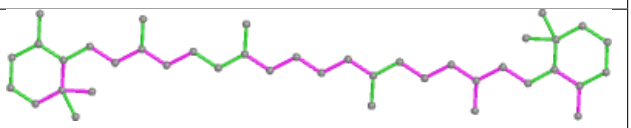
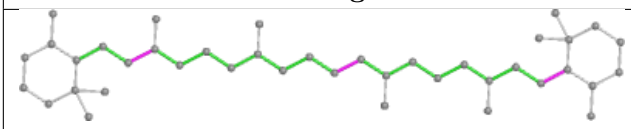


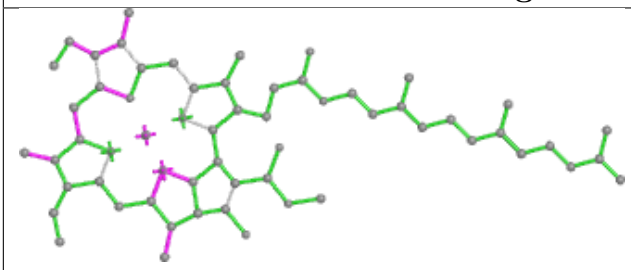
Bond angles



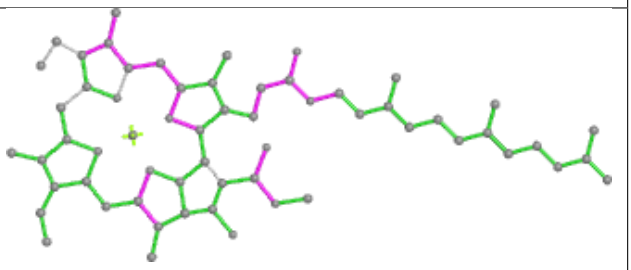
Torsions

Rings

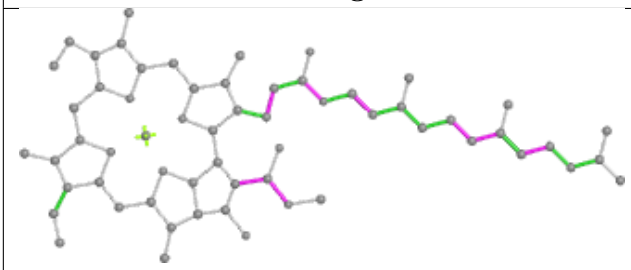
Ligand CLA B 1216



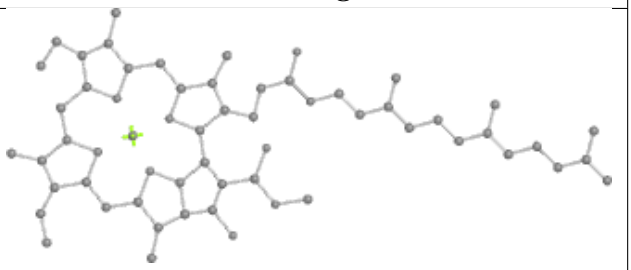
Bond lengths



Bond angles

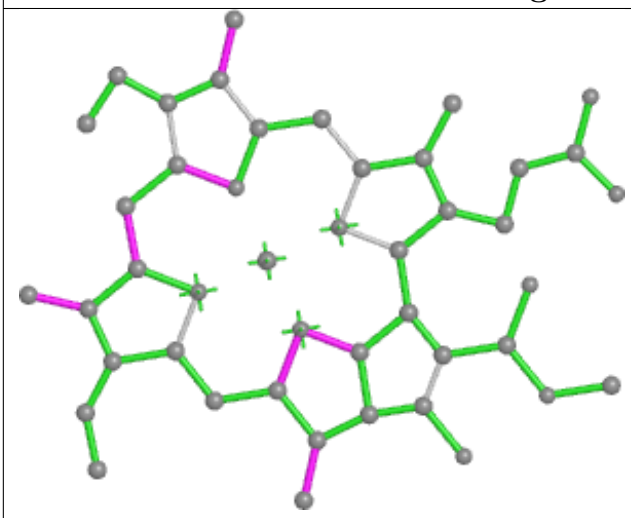


Torsions



Rings

Ligand CLA s 509



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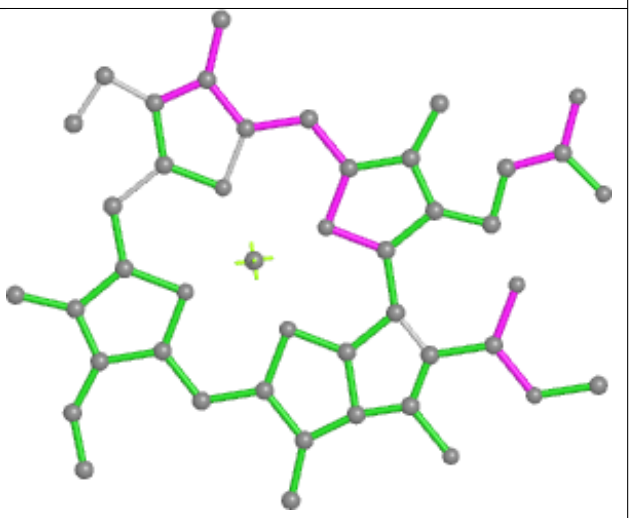
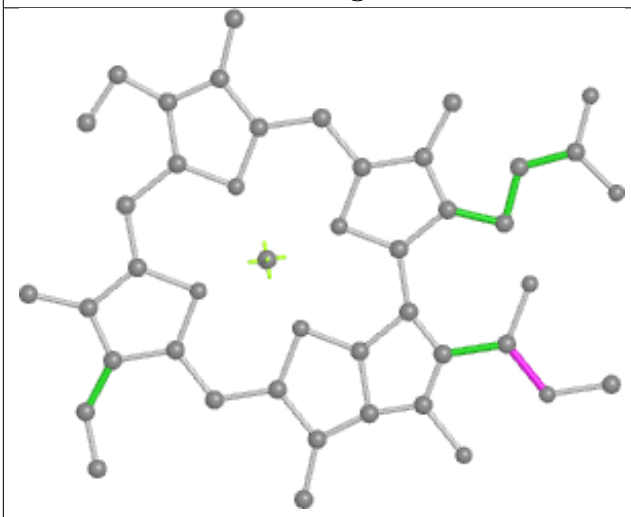


Bond angles



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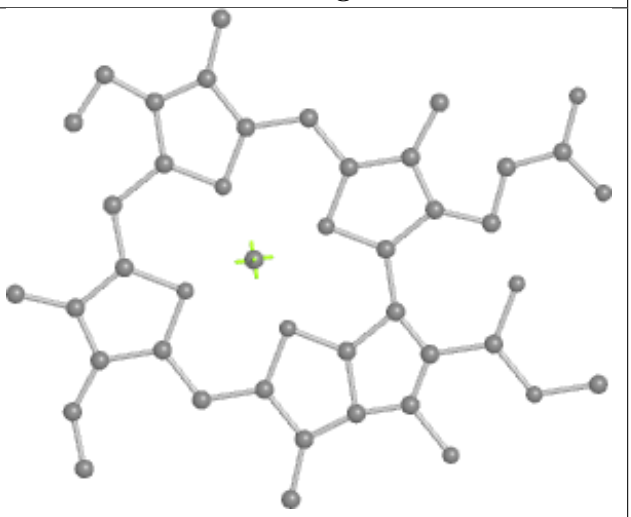
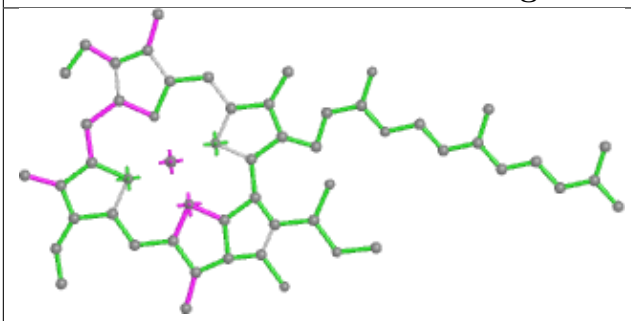
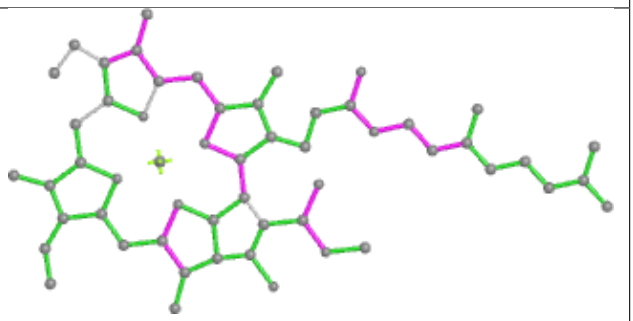
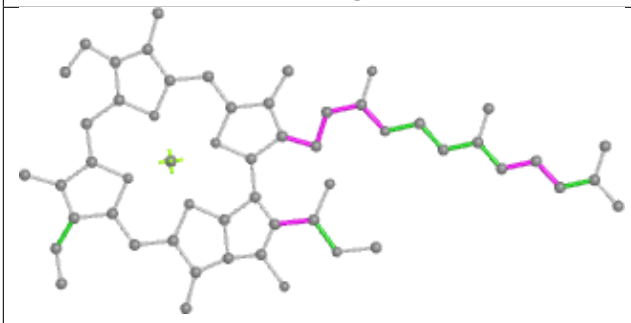
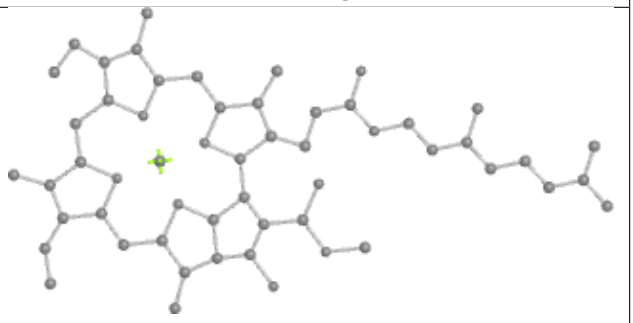
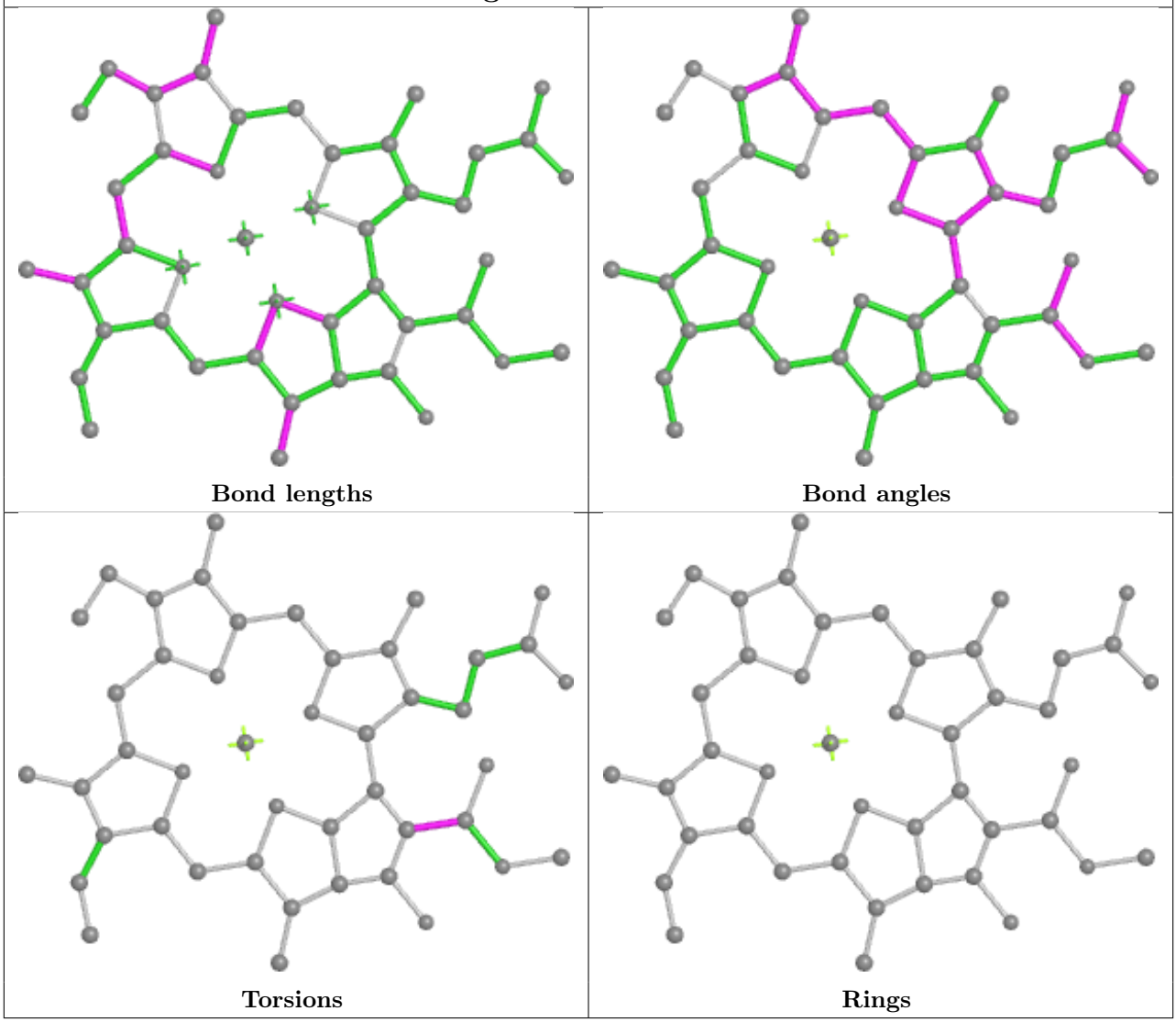


Rings

Ligand CLA e 1135	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 502



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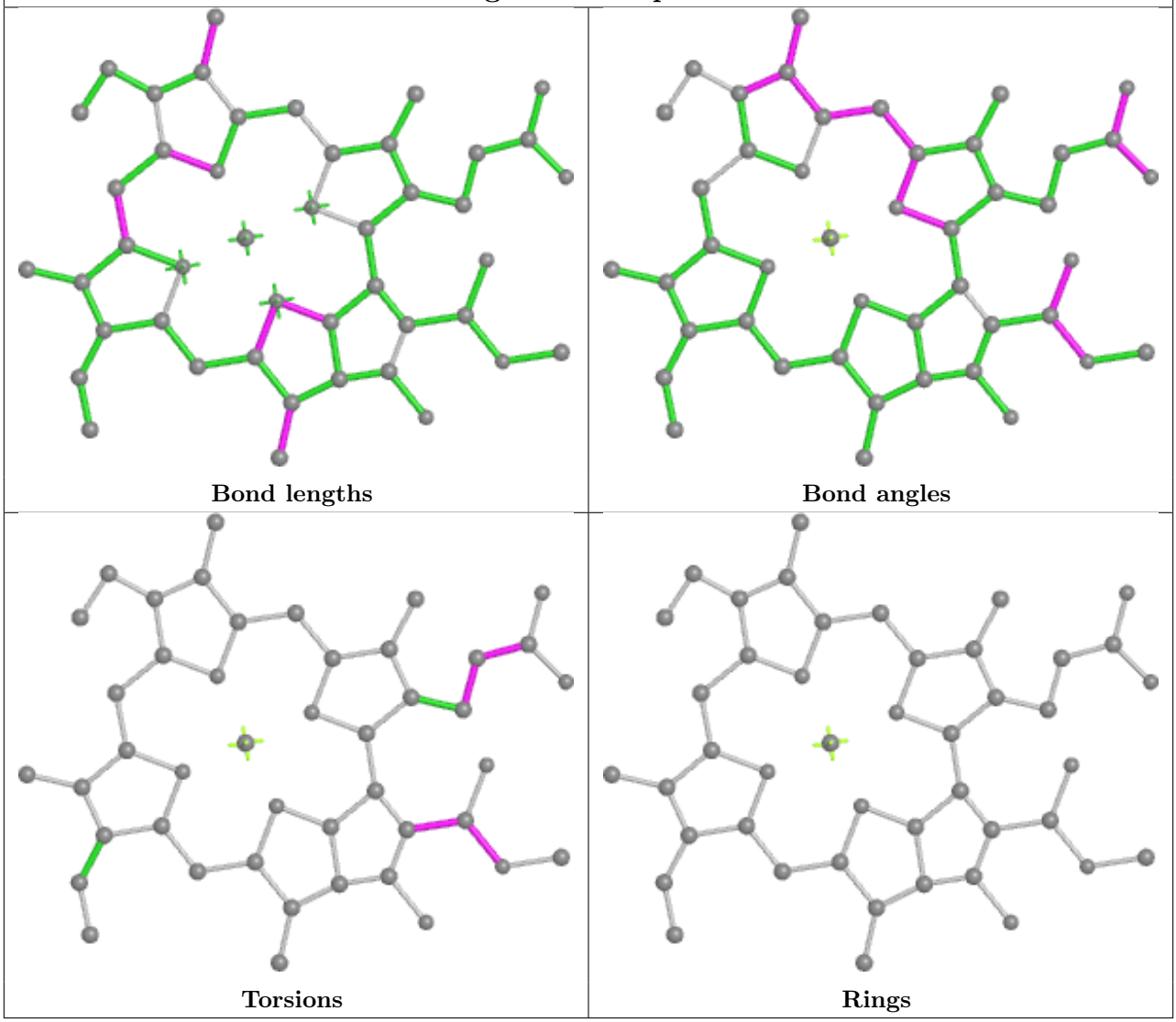
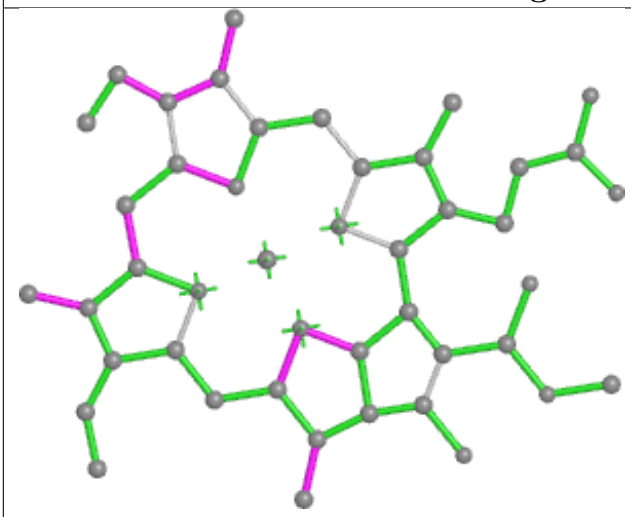
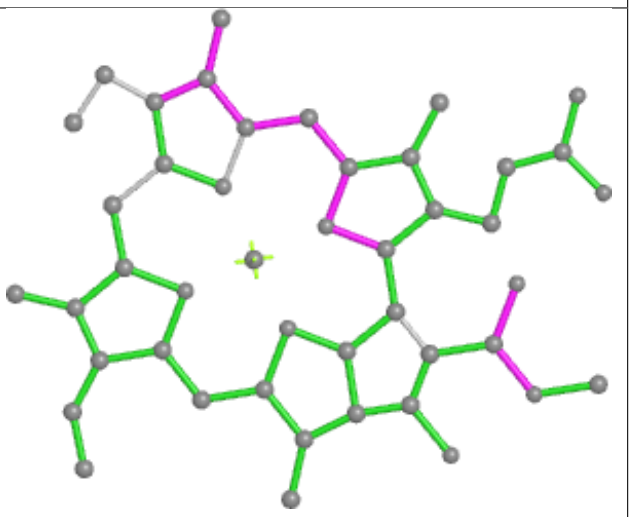


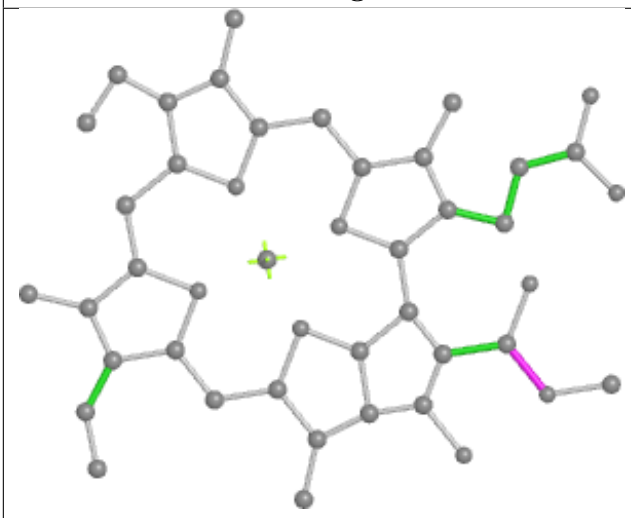
Ligand CLA r 513



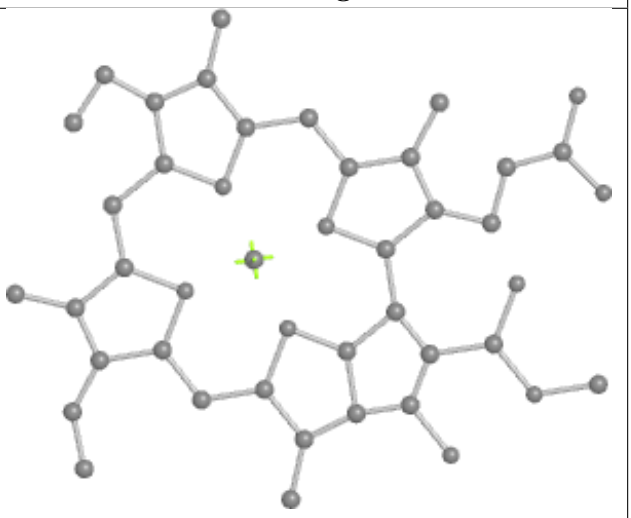
Bond lengths



Bond angles

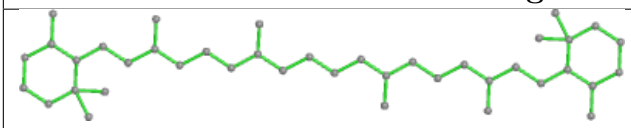


Torsions



Rings

Ligand BCR 1 522



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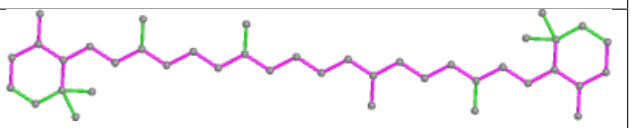
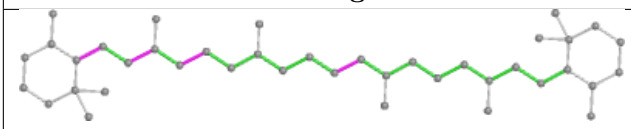


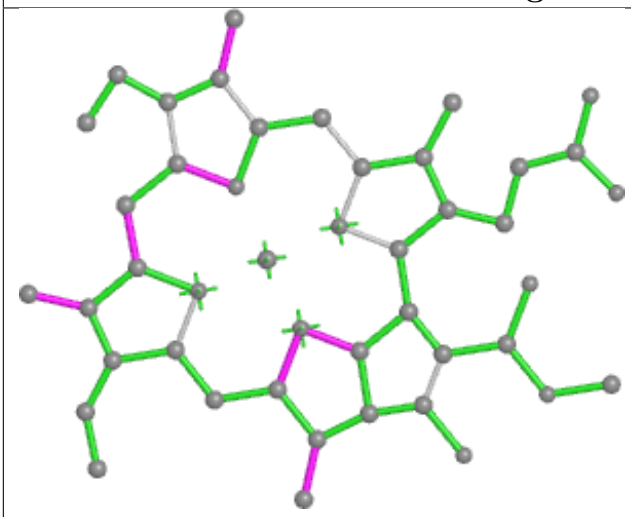
Bond angles



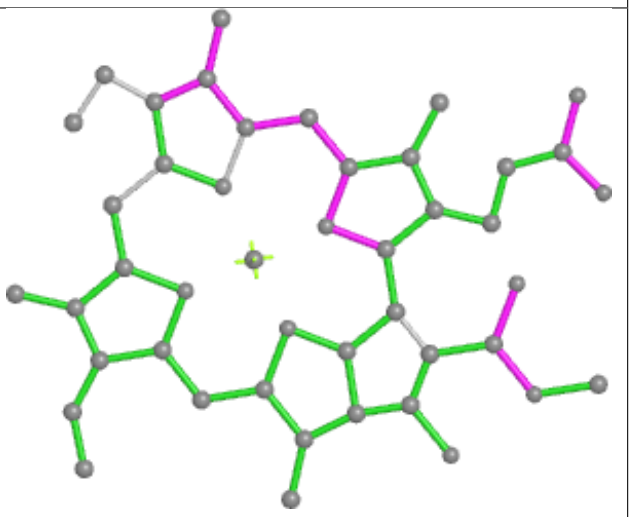
Torsions

Rings

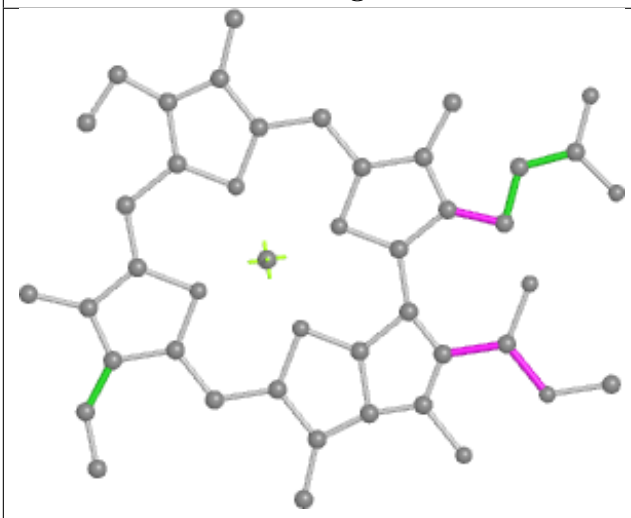
Ligand CLA Z 511



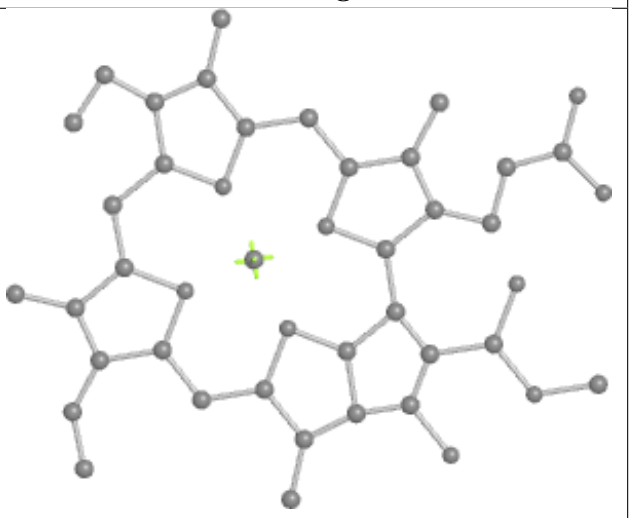
Bond lengths



Bond angles

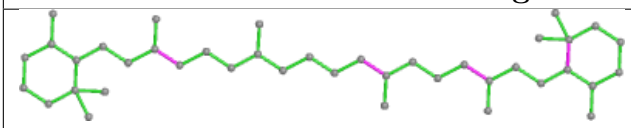


Torsions

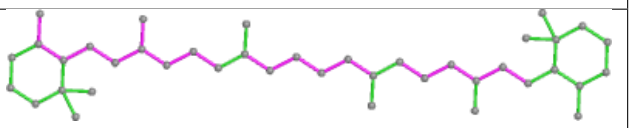


Rings

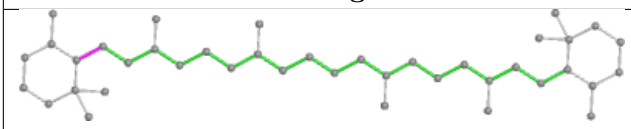
Ligand BCR H 4017



Bond lengths



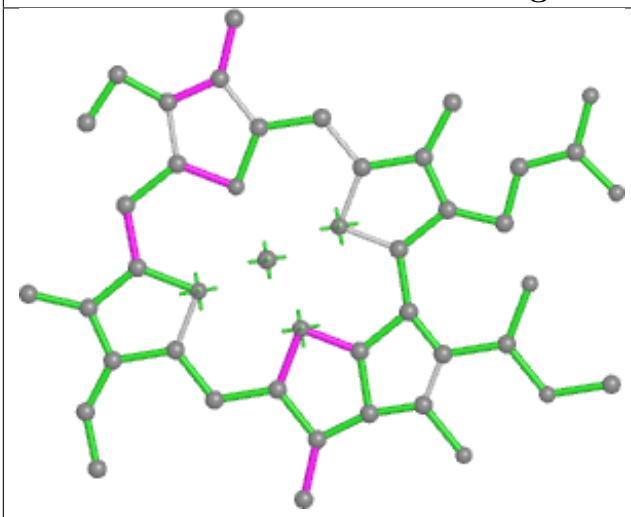
Bond angles



Torsions

Rings

Ligand CLA r 504



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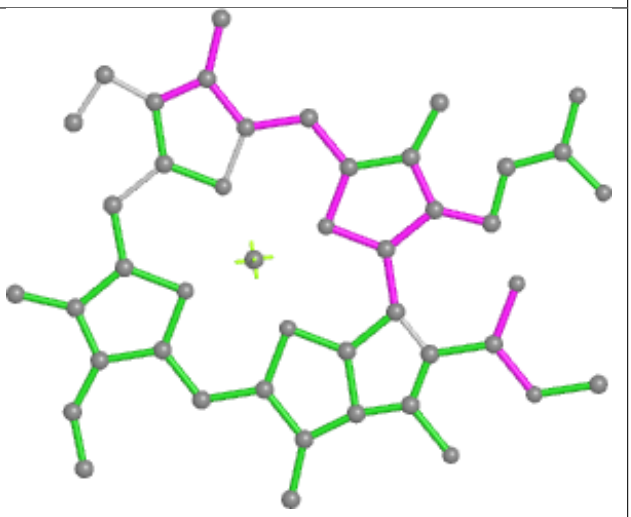
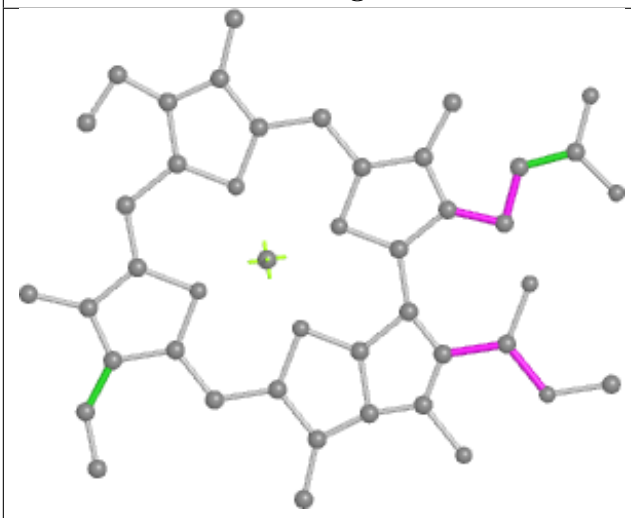
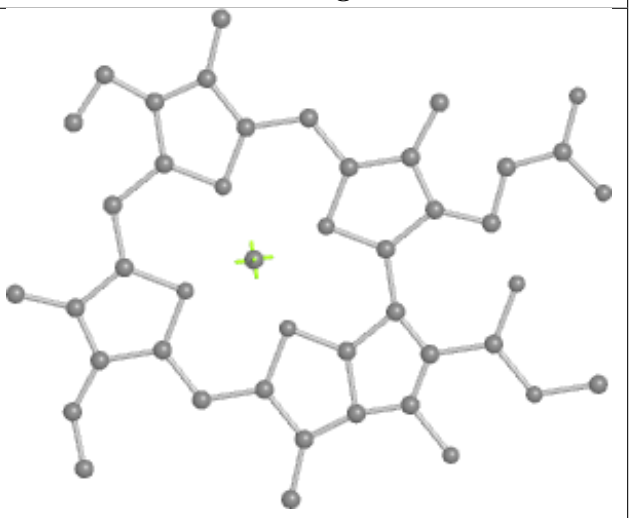


Bond angles

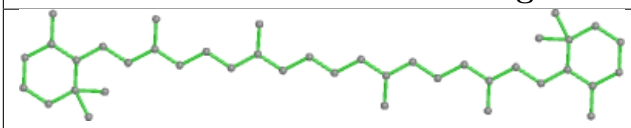


Torsions

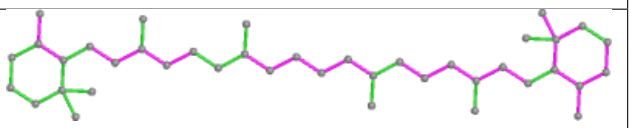


Rings

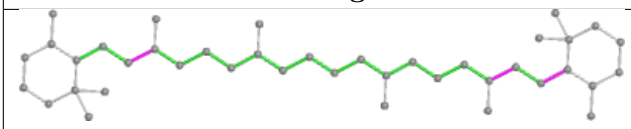
Ligand BCR n 4019



Bond lengths



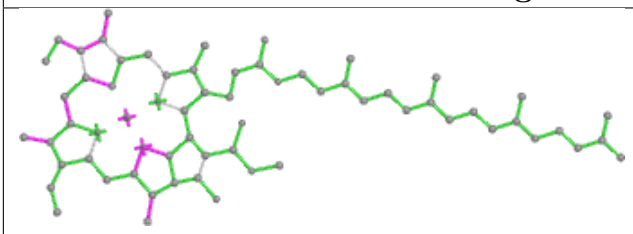
Bond angles



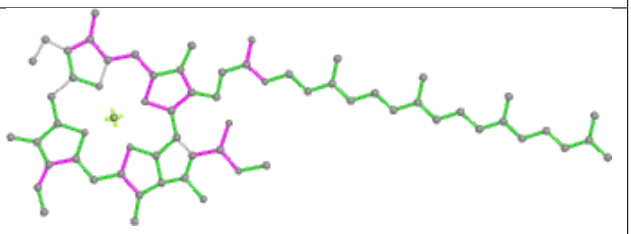
Torsions

Rings

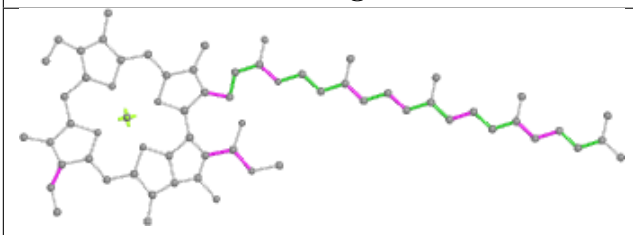
Ligand CLA A 1132



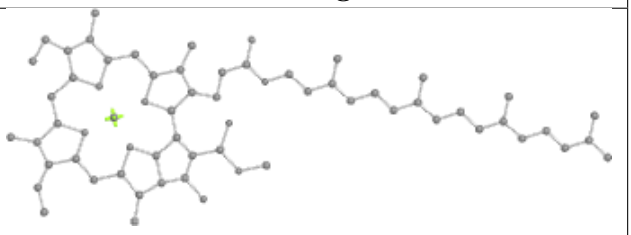
Bond lengths



Bond angles

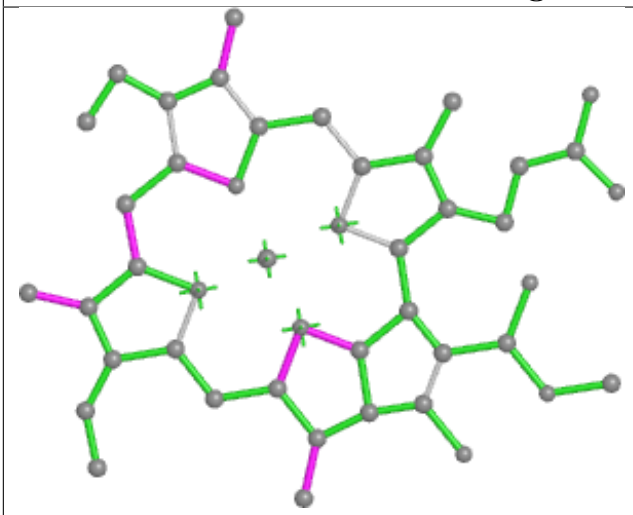


Torsions

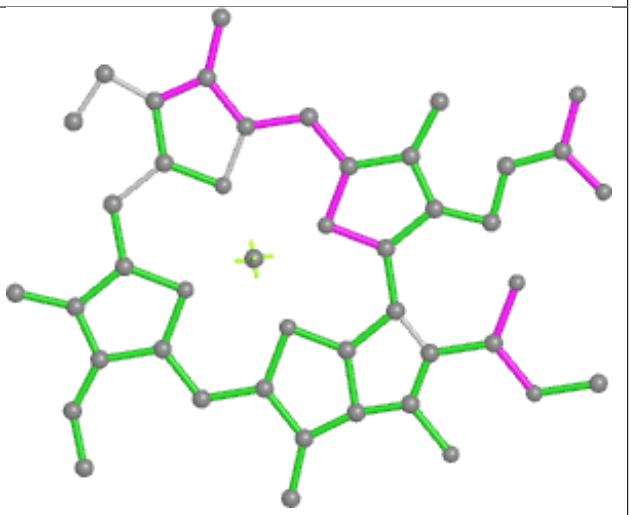


Rings

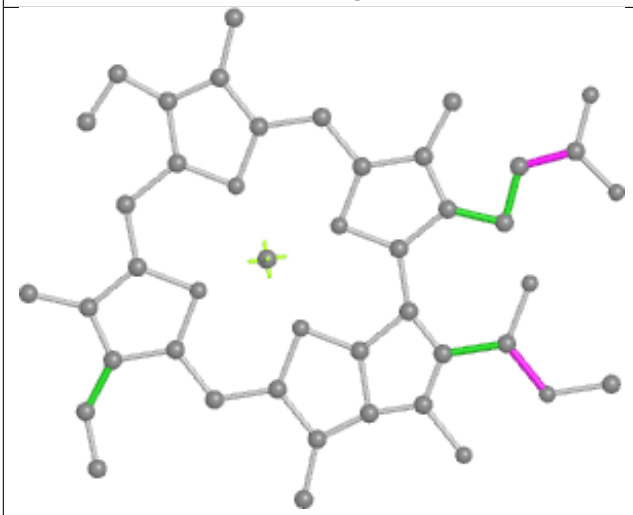
Ligand CLA v 509



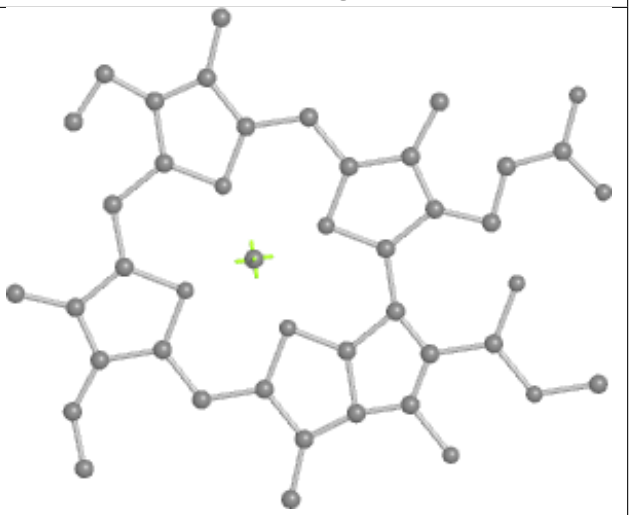
Bond lengths



Bond angles

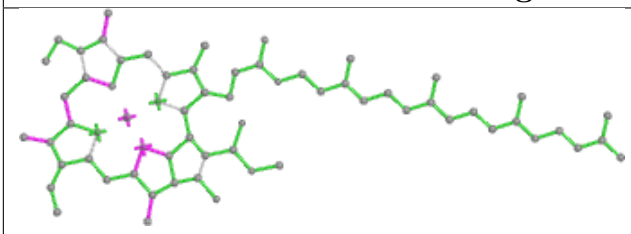


Torsions



Rings

Ligand CLA B 1223



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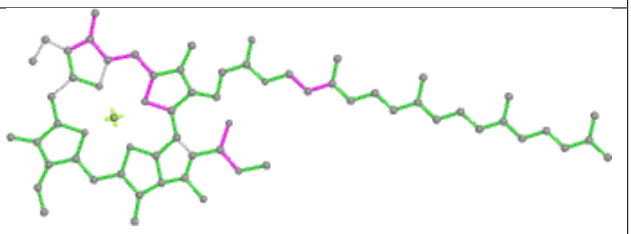

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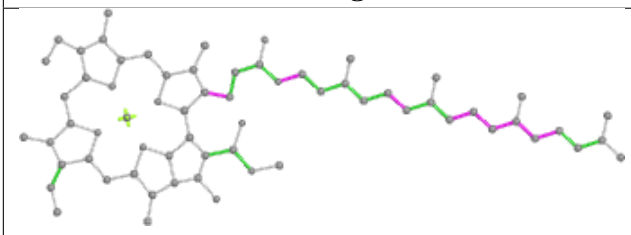

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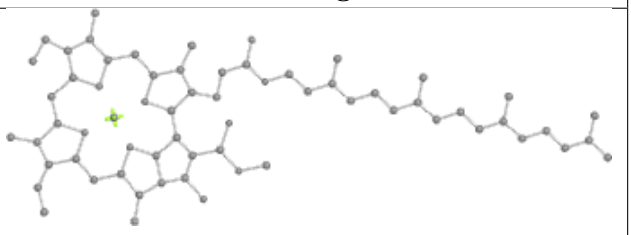
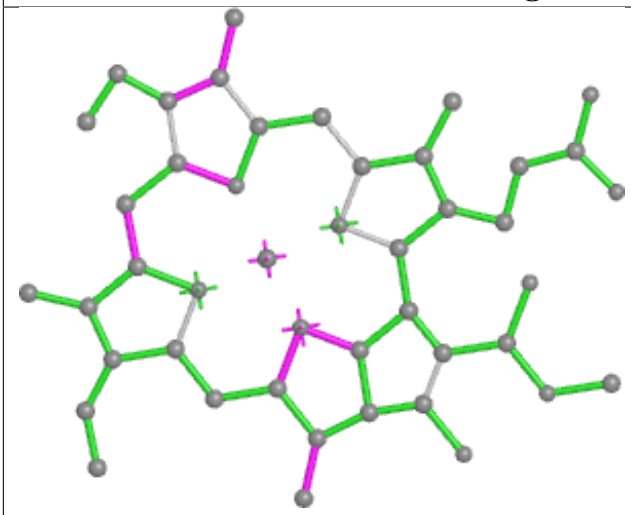


Rings

Ligand CLA Y 512



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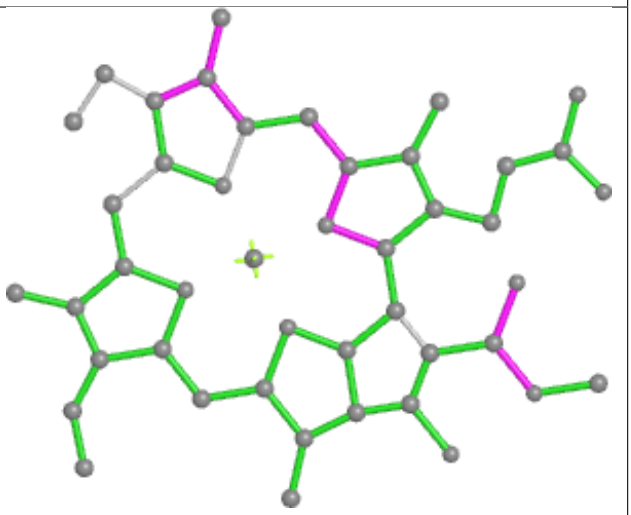

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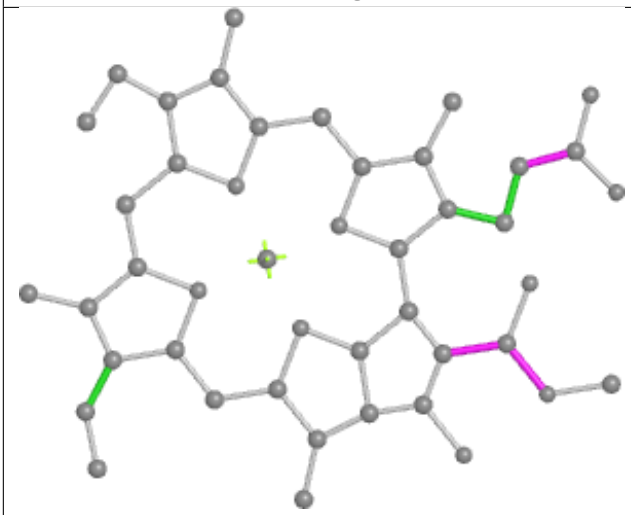

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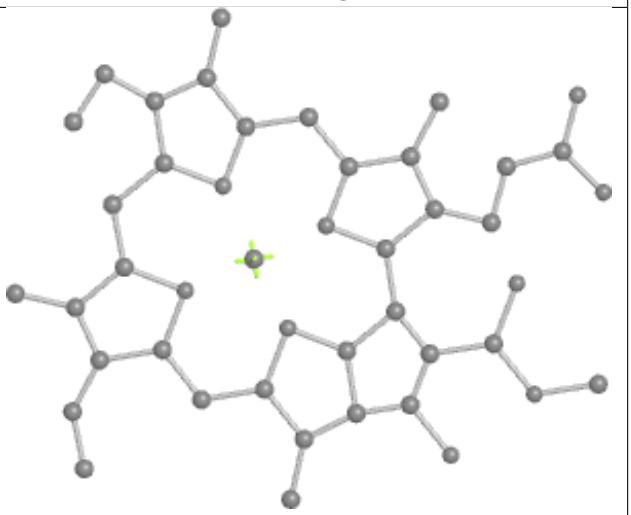
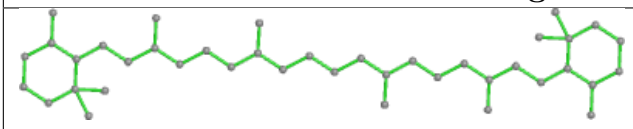


Rings

Ligand BCR t 521



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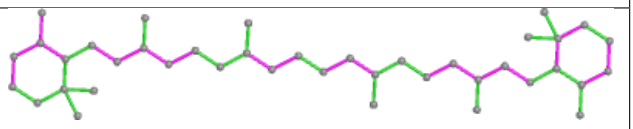

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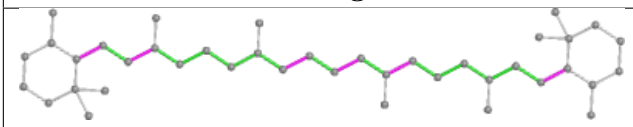

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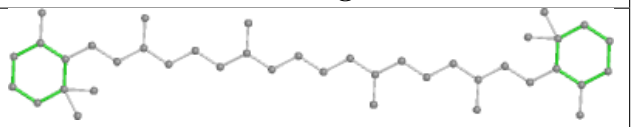
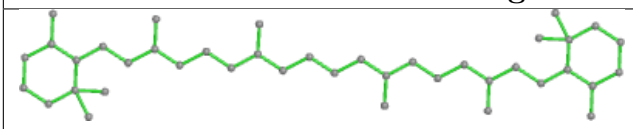


Rings

Ligand BCR W 4021



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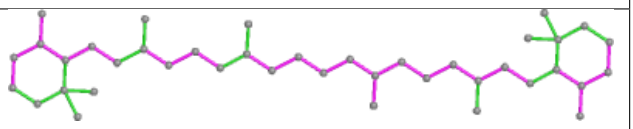
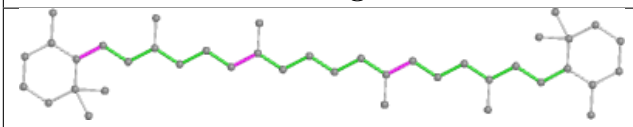


Bond angles



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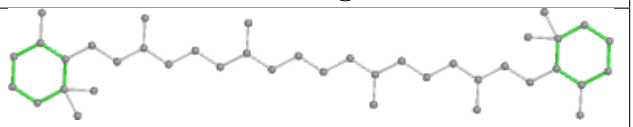
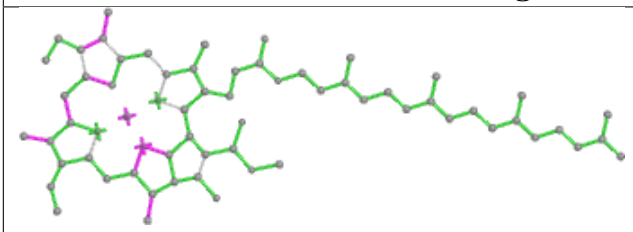


Rings

Ligand CLA G 1140



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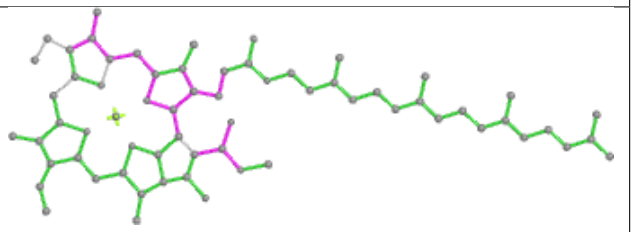

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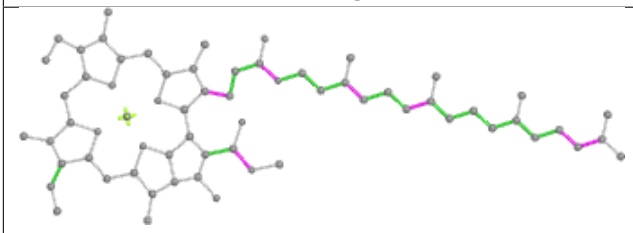

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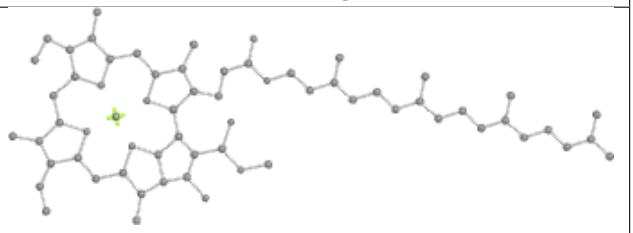
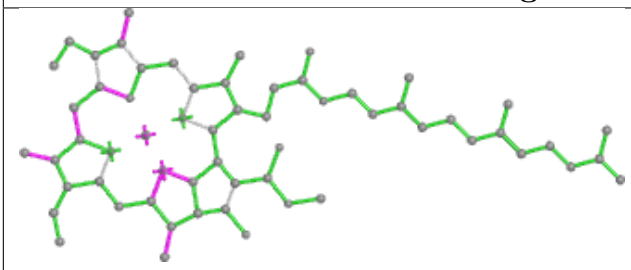


Rings

Ligand CLA e 1116



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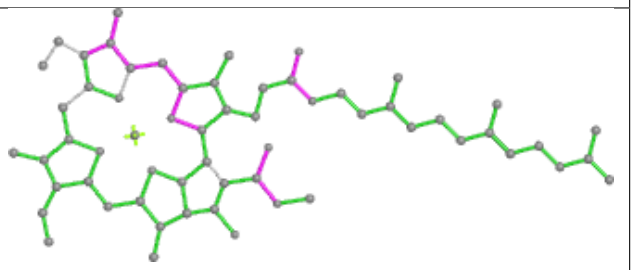
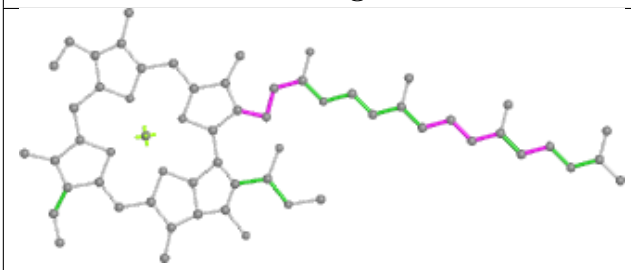


Bond angles



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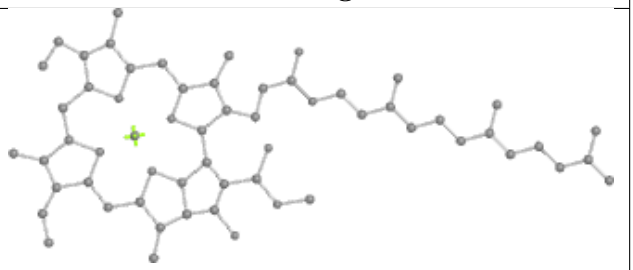
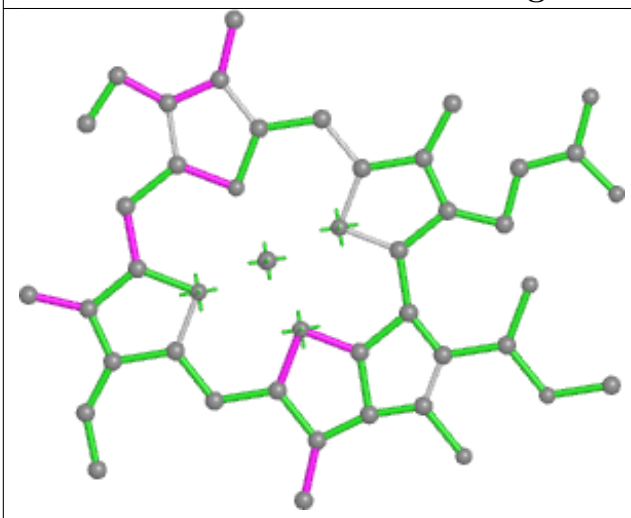


Rings

Ligand CLA q 519



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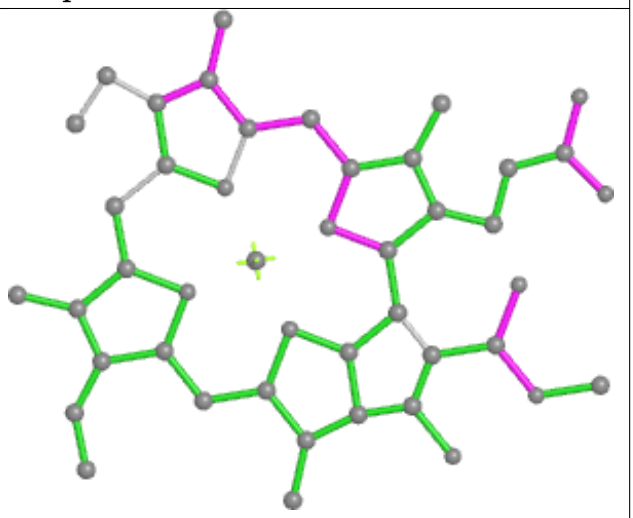

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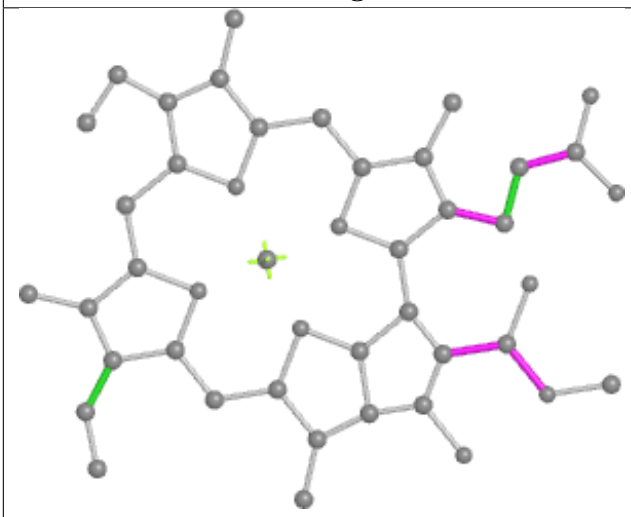

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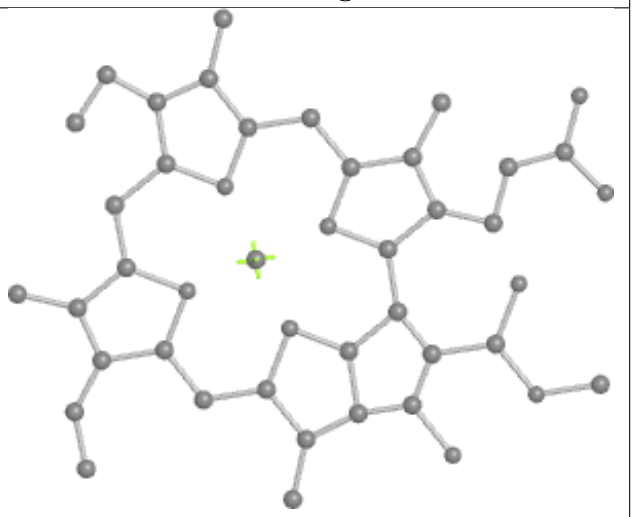
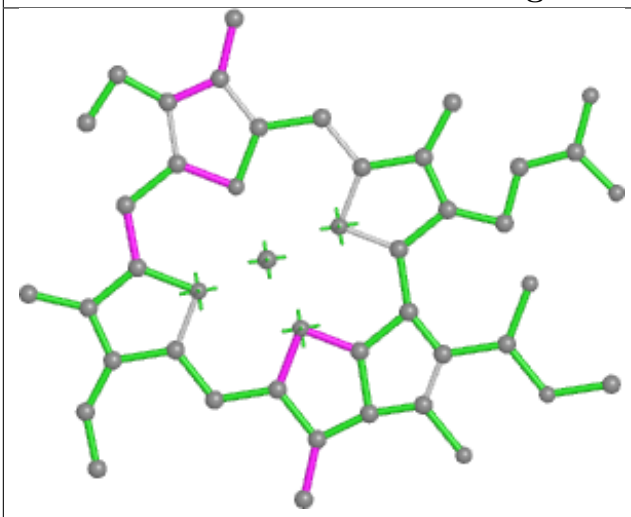


Rings

Ligand CLA Z 504



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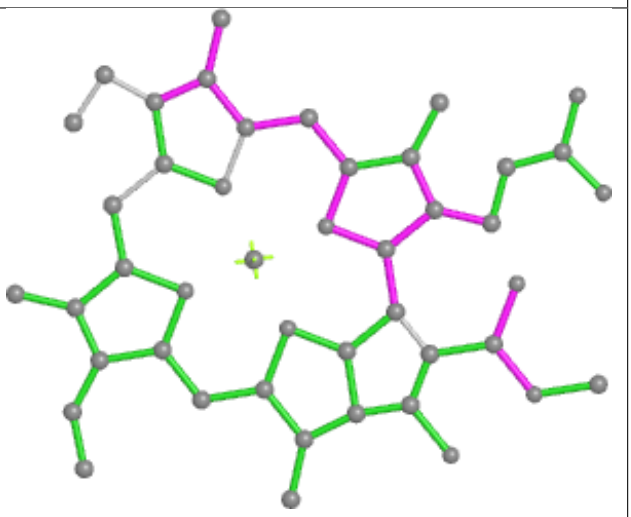
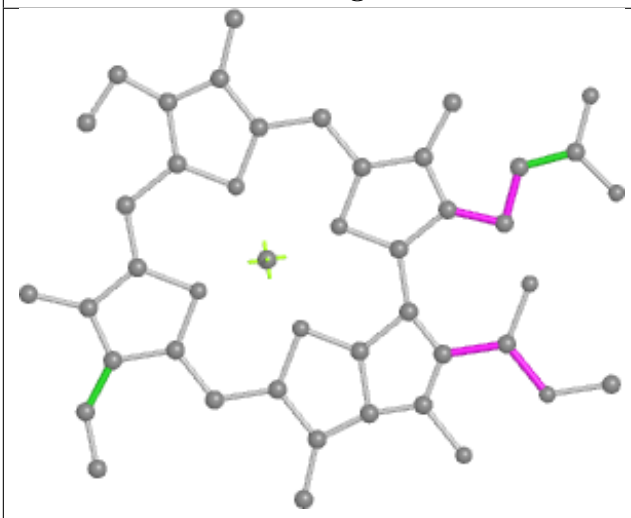


Bond angles



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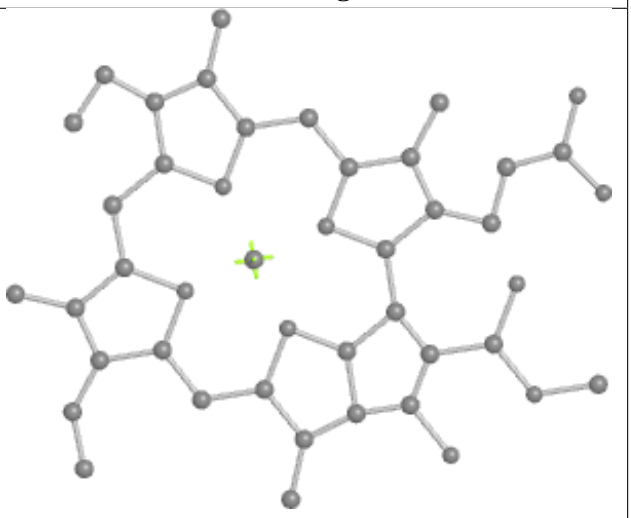
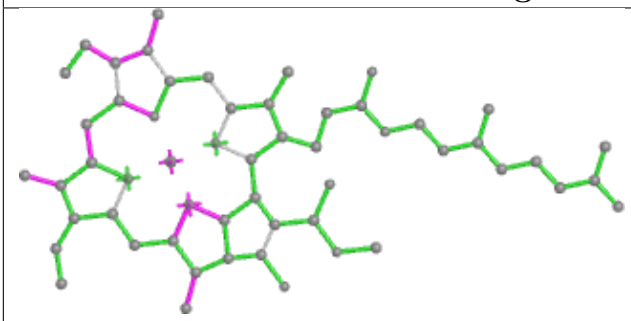


Rings

Ligand CLA H 1220



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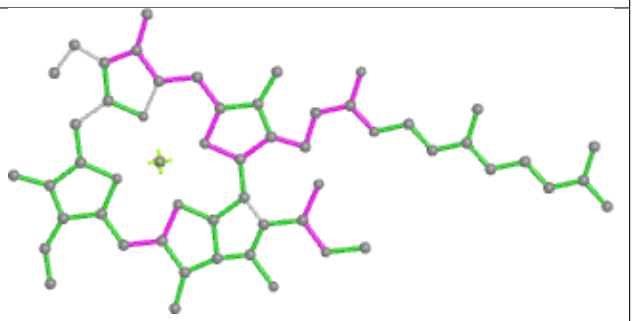
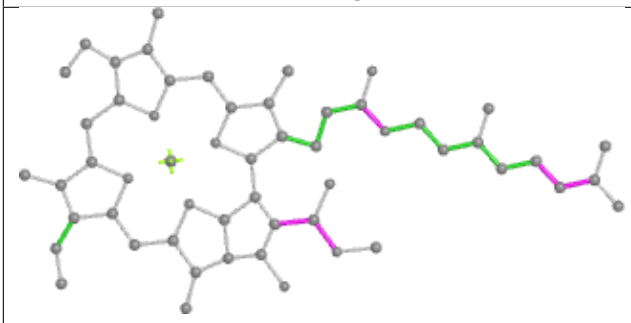
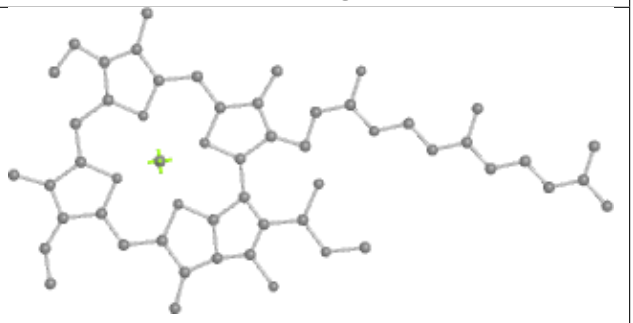


Bond angles

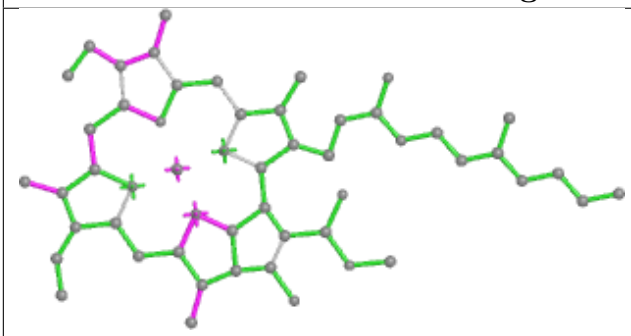


Torsions



Rings

Ligand CLA e 1129



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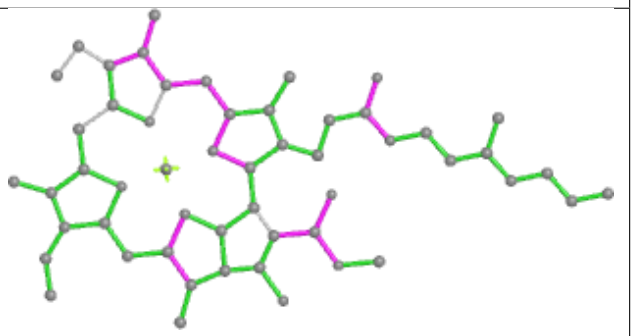
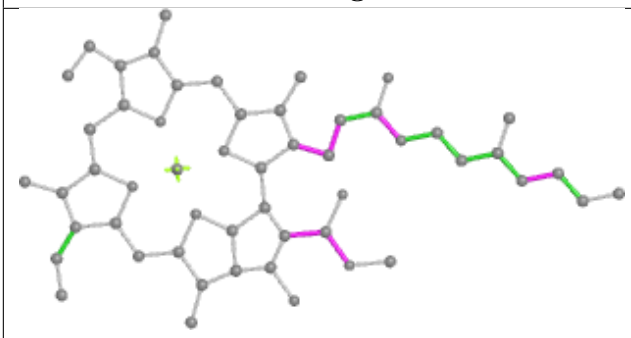


Bond angles



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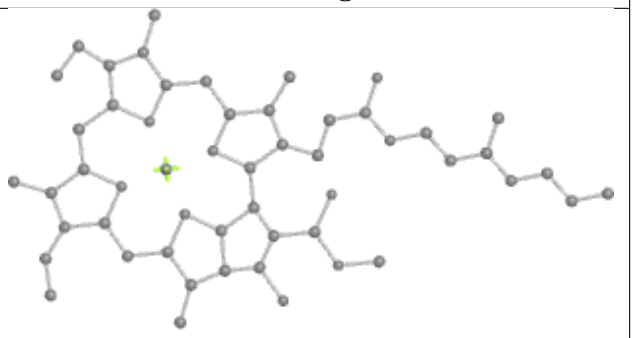
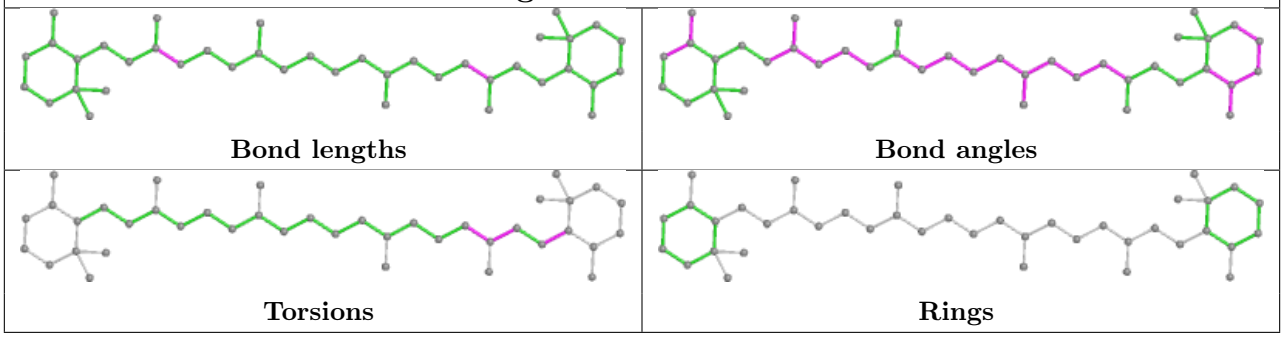
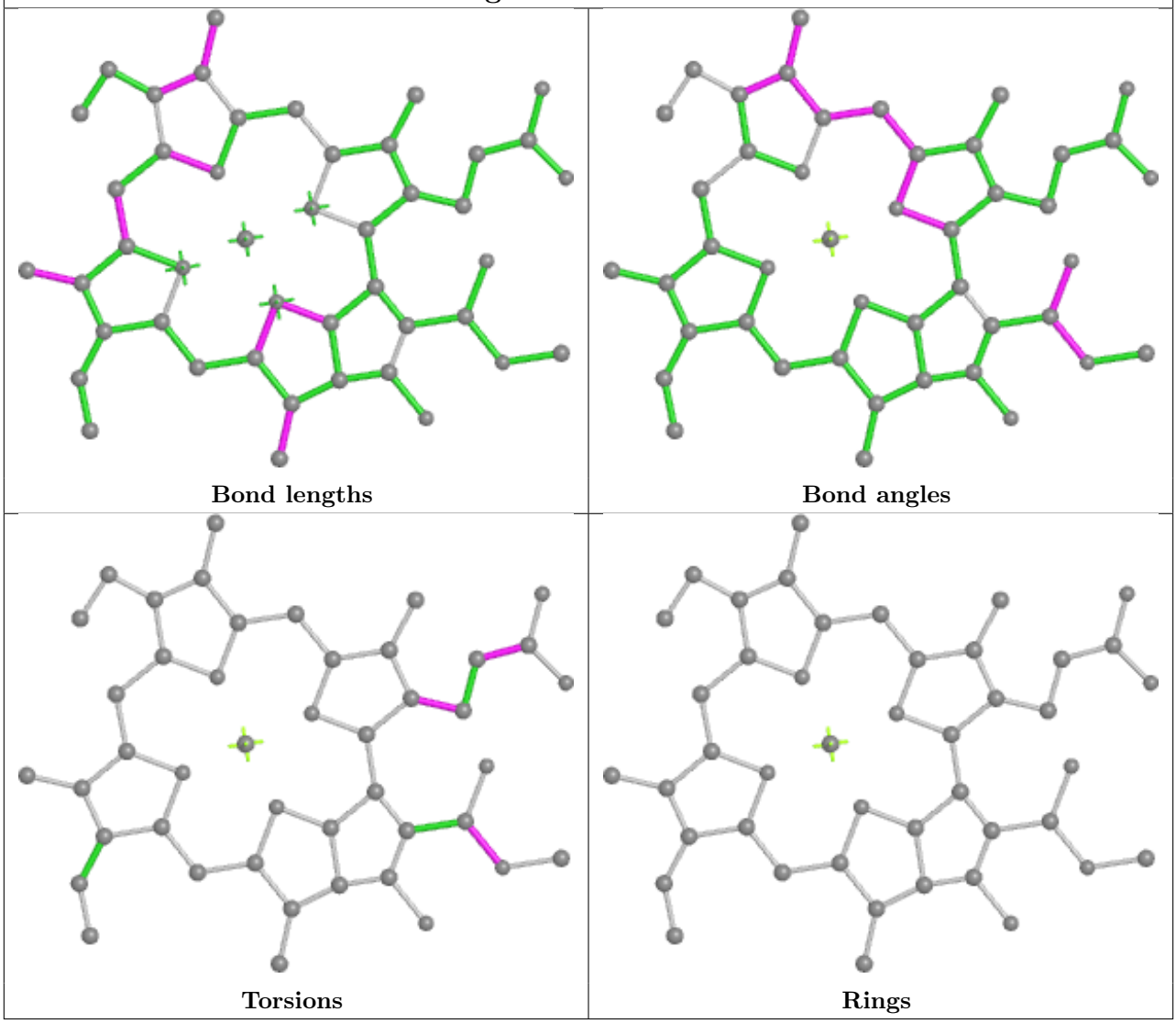


Rings

Ligand BCR L 4020



Ligand CLA 5 513



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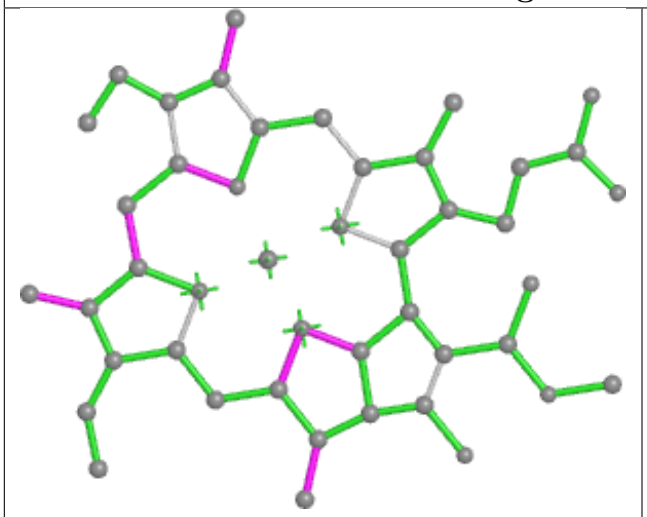
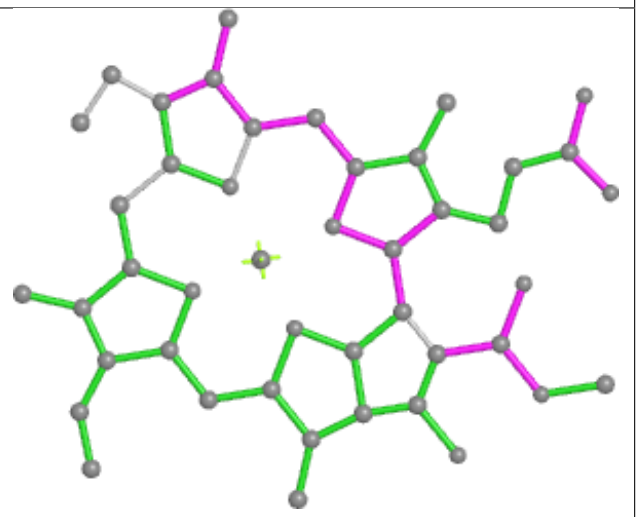
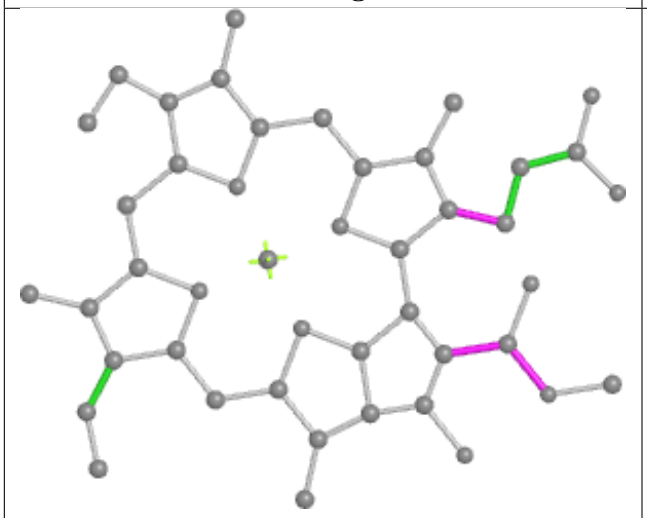


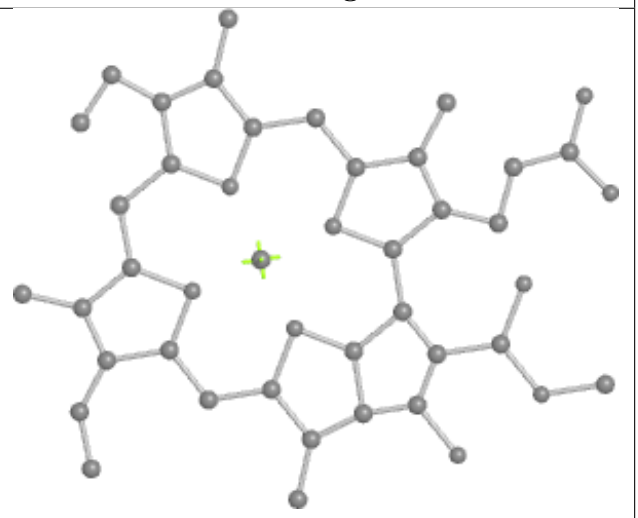
Bond lengths



Bond angles

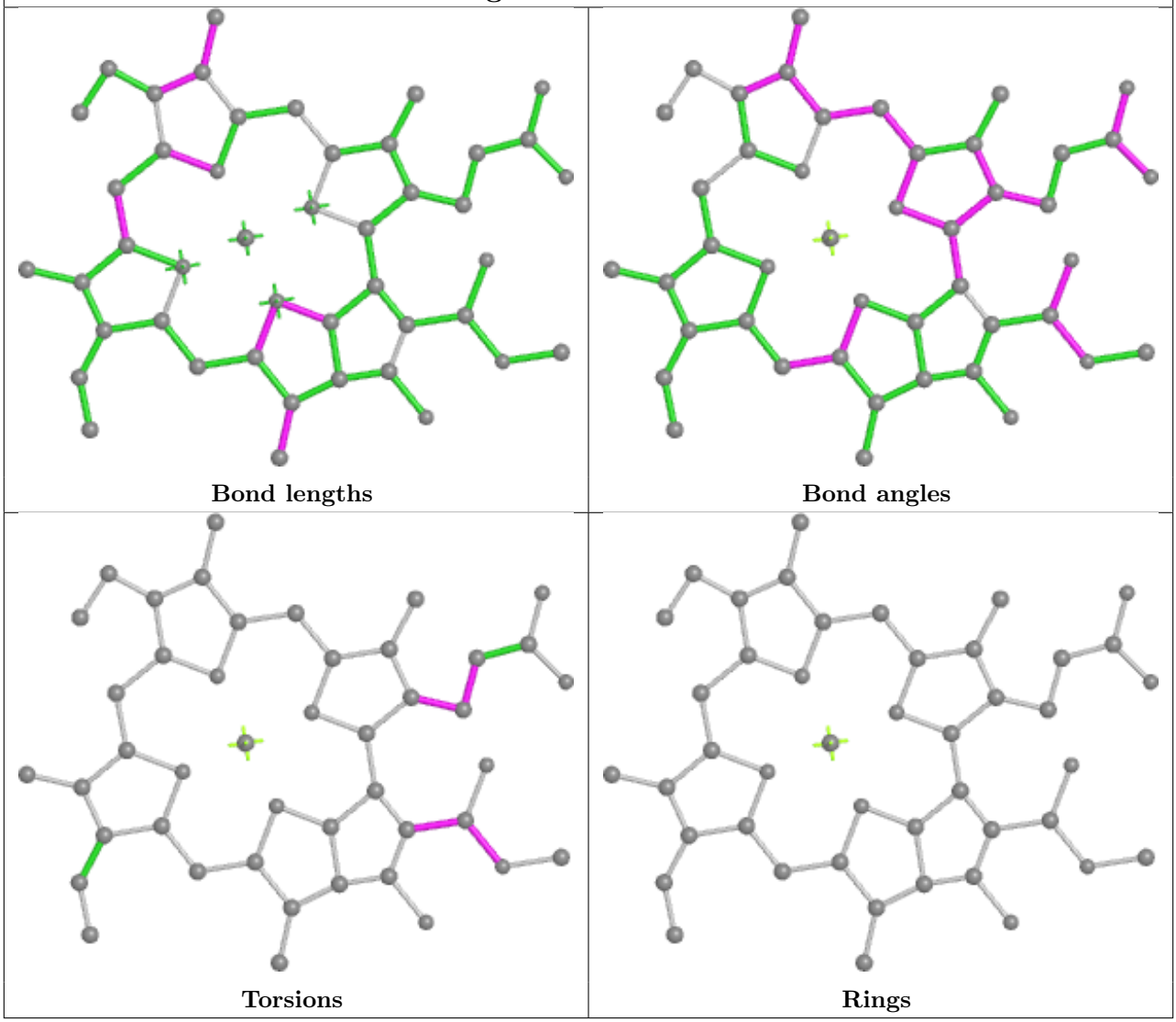


Torsions

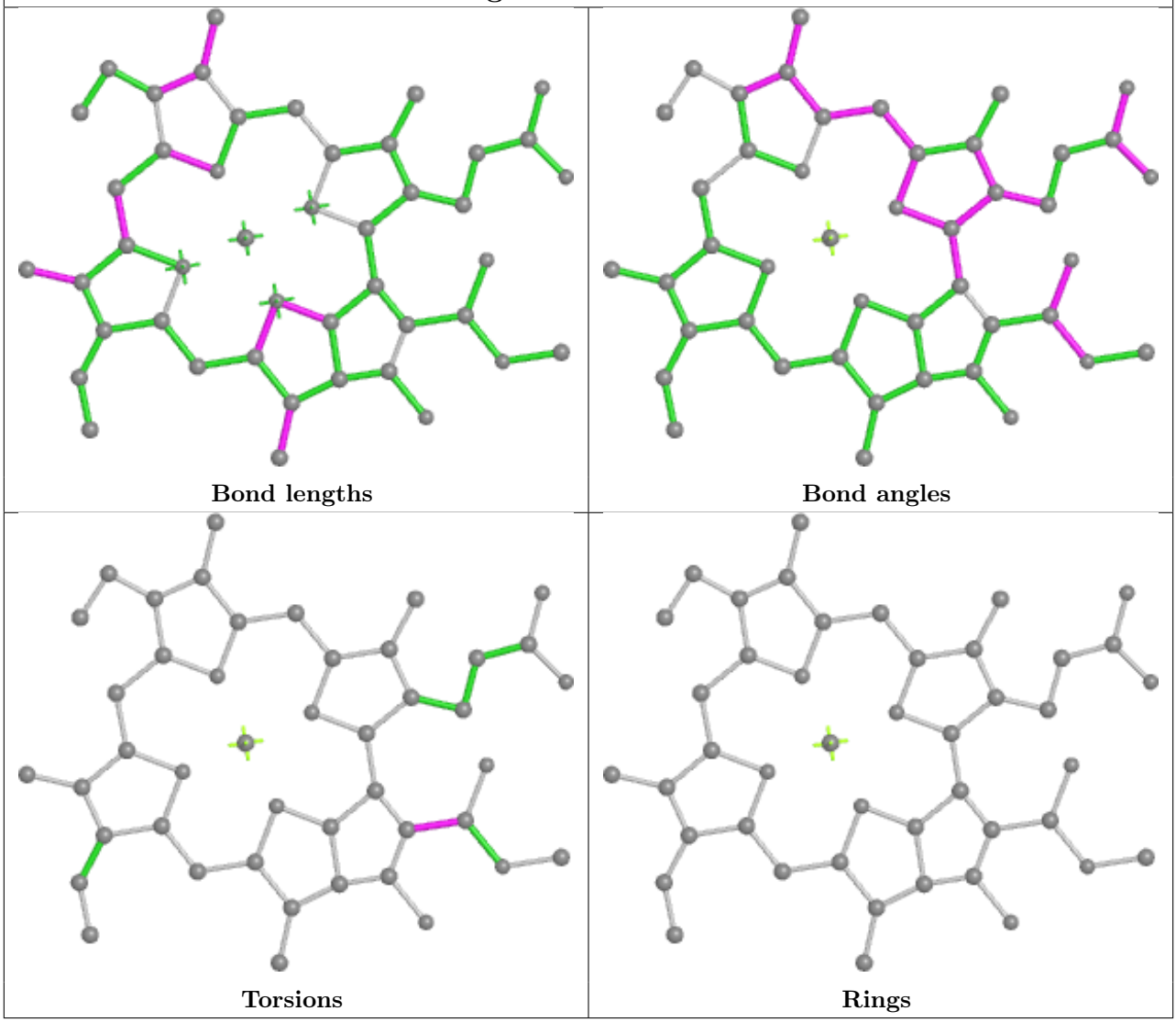


Rings

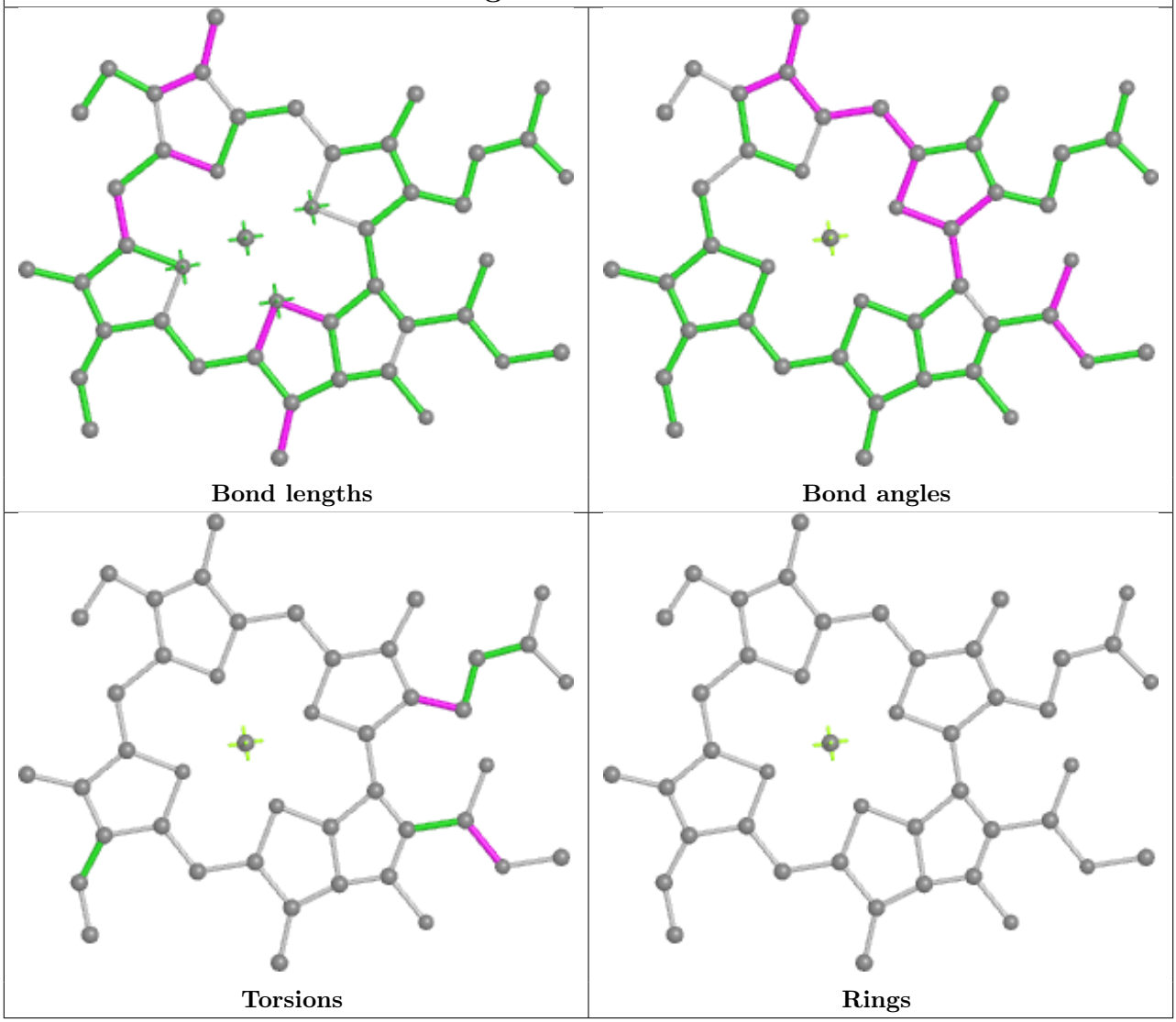
Ligand CLA c 503



Ligand CLA s 502



Ligand CLA 5 504



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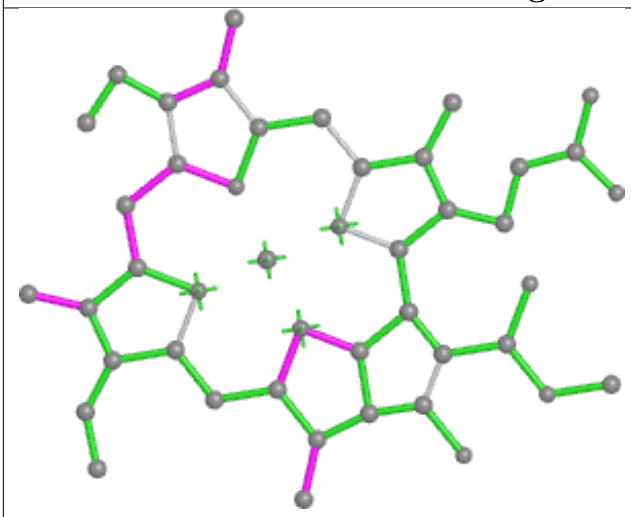
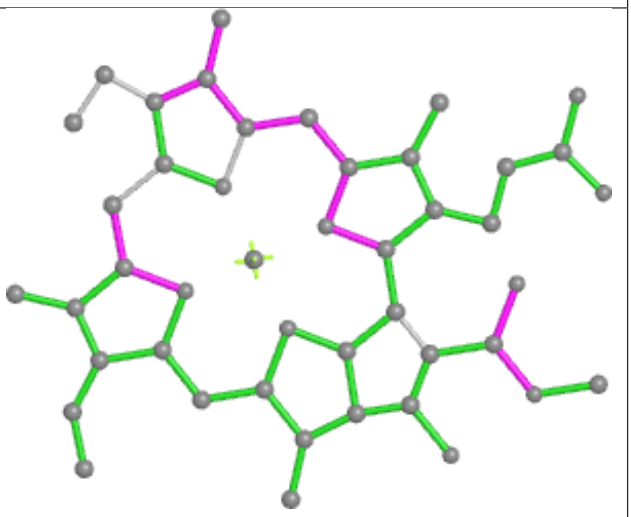
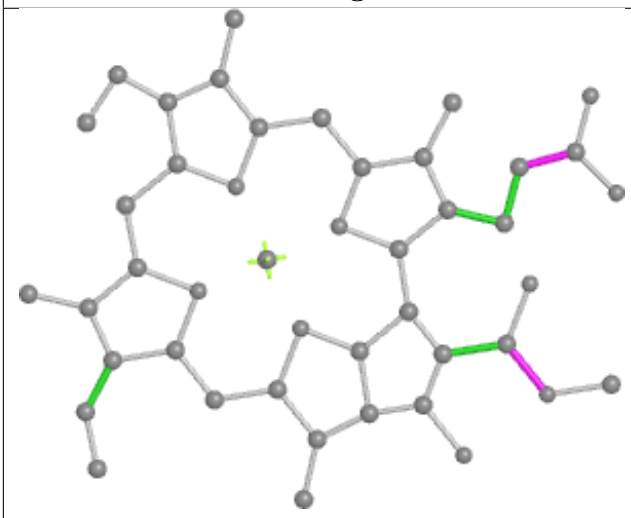


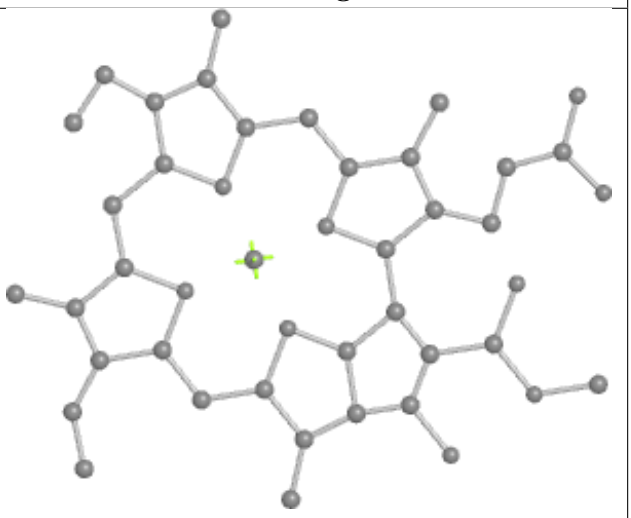
Bond lengths



Bond angles

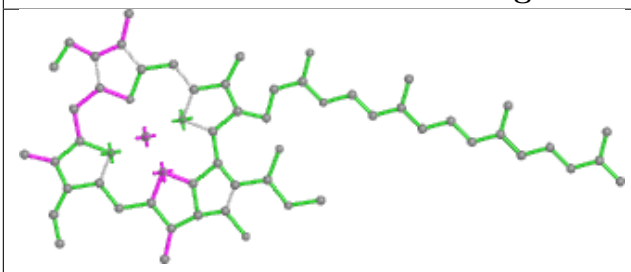


Torsions



Rings

Ligand CLA G 1122



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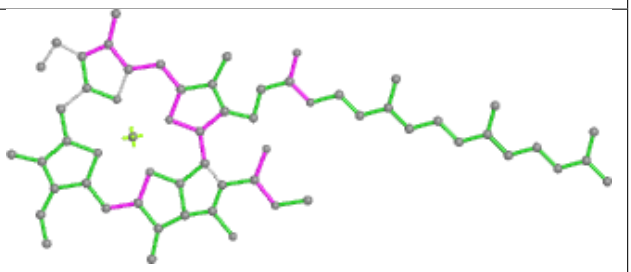

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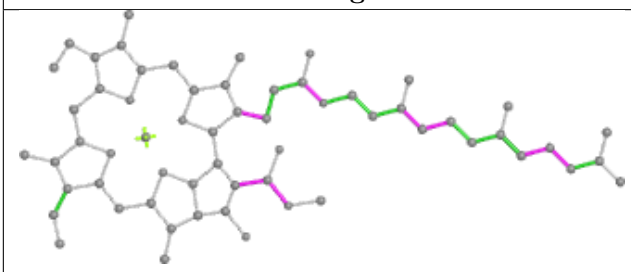

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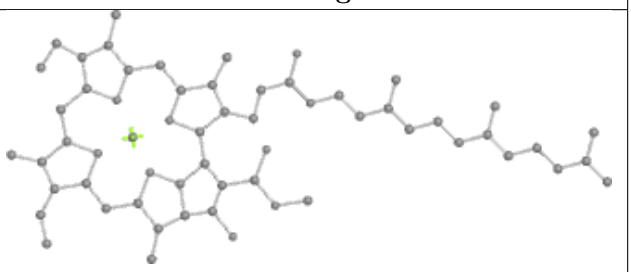
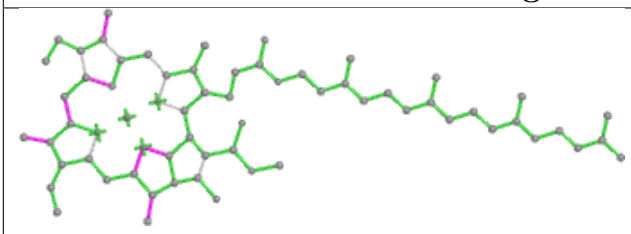


Rings

Ligand CLA f 1231



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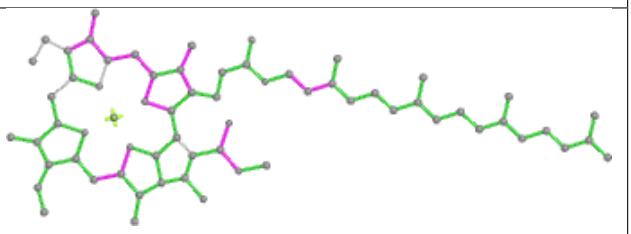
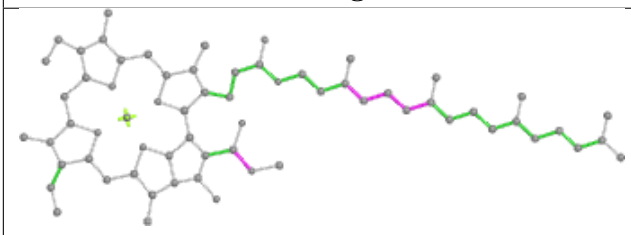


Bond angles



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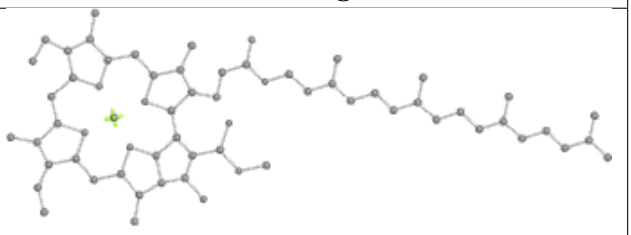
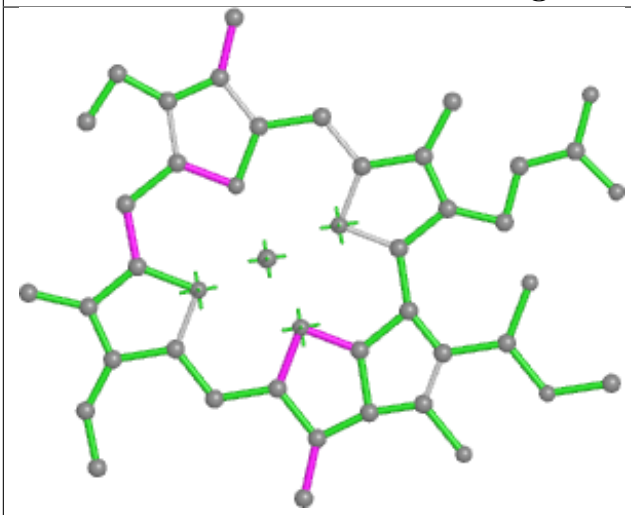


Rings

Ligand CLA t 518



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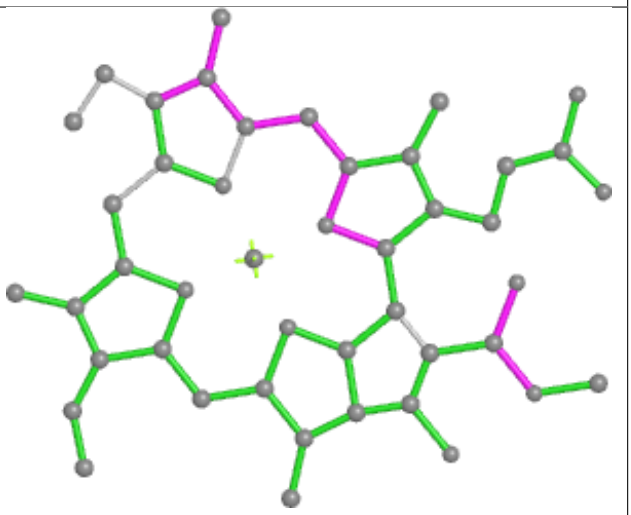
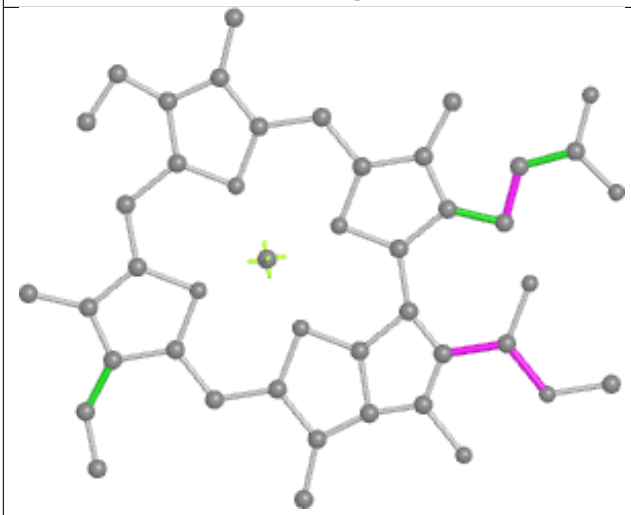


Bond angles



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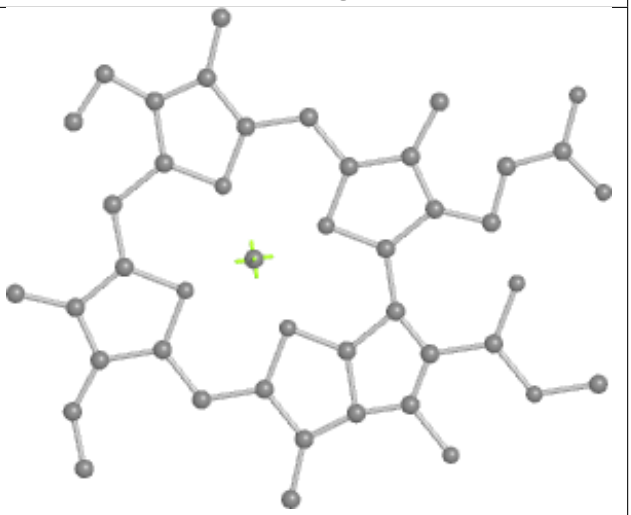
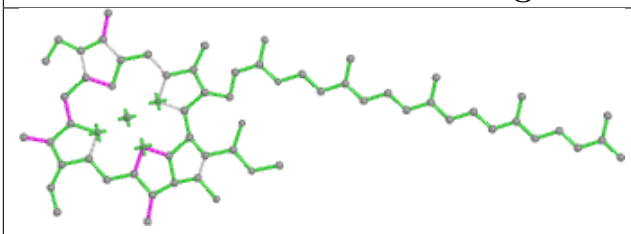


Rings

Ligand CLA H 1202



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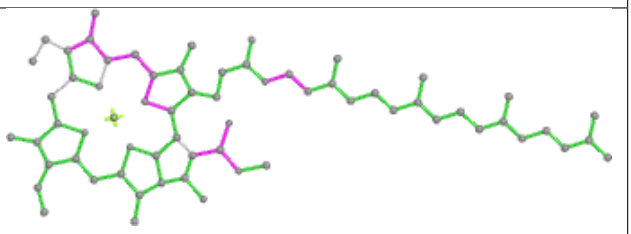
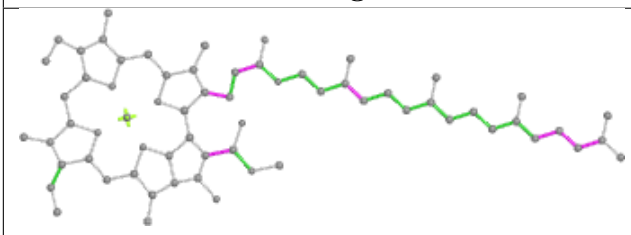


Bond angles



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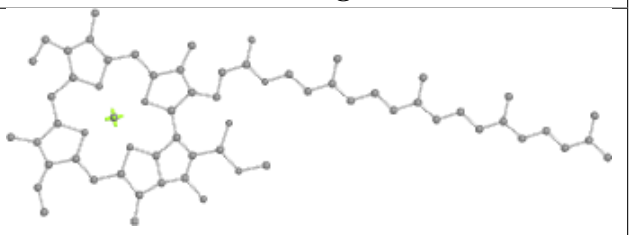
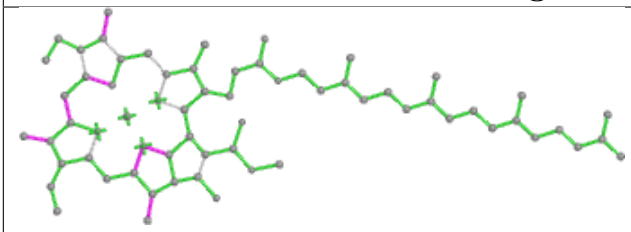


Rings

Ligand CLA 2 509



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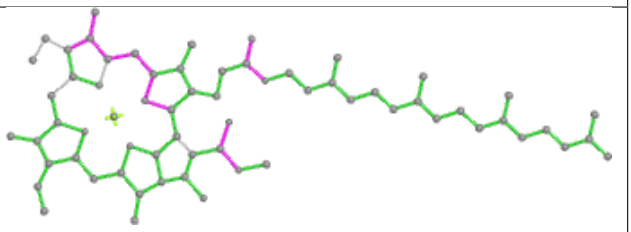
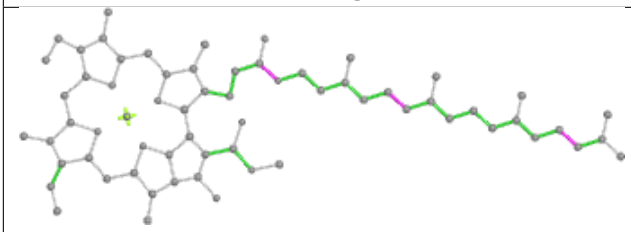


Bond angles



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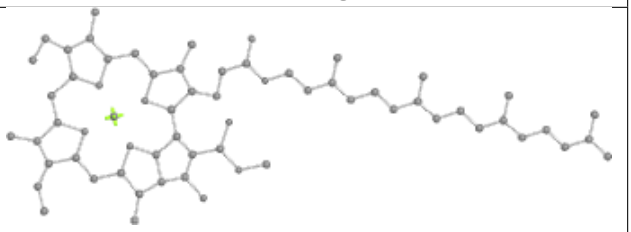
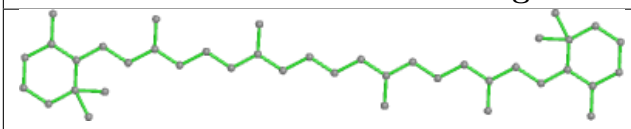


Rings

Ligand BCR G 4007



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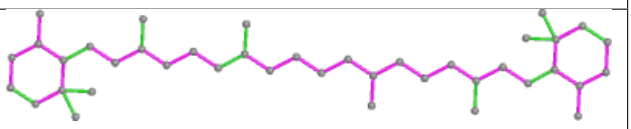
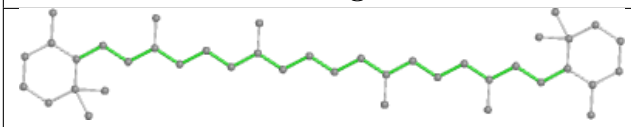


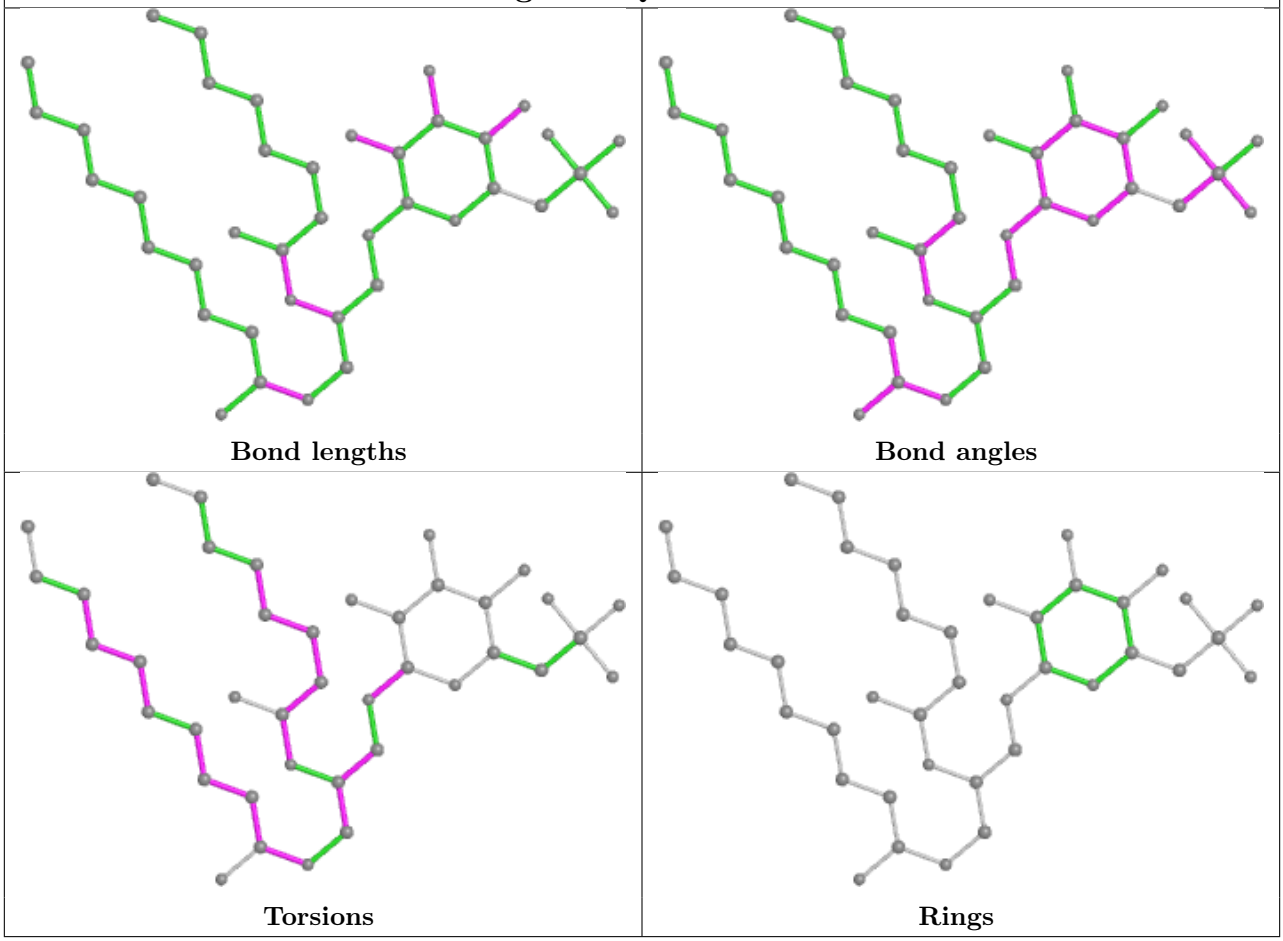
Bond angles



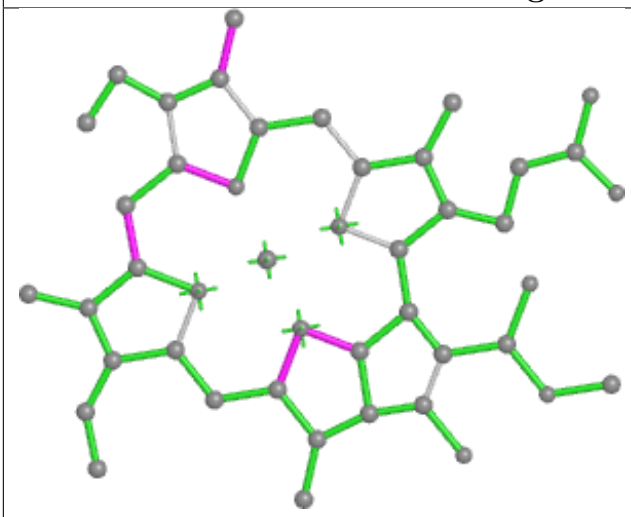
Torsions

Rings

Ligand SQD H 1852



Ligand CLA b 504



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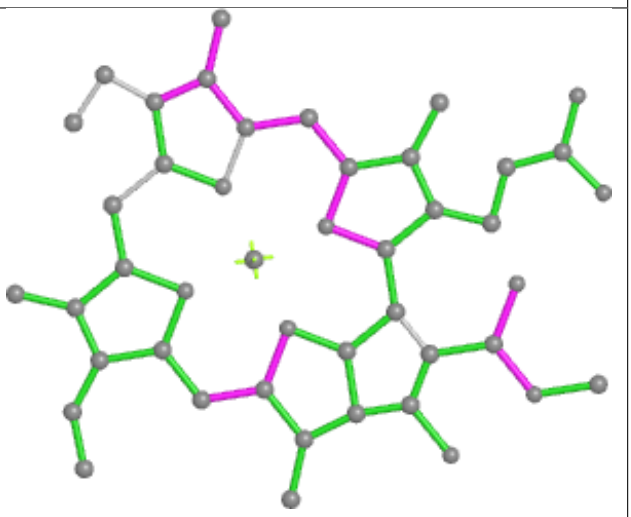

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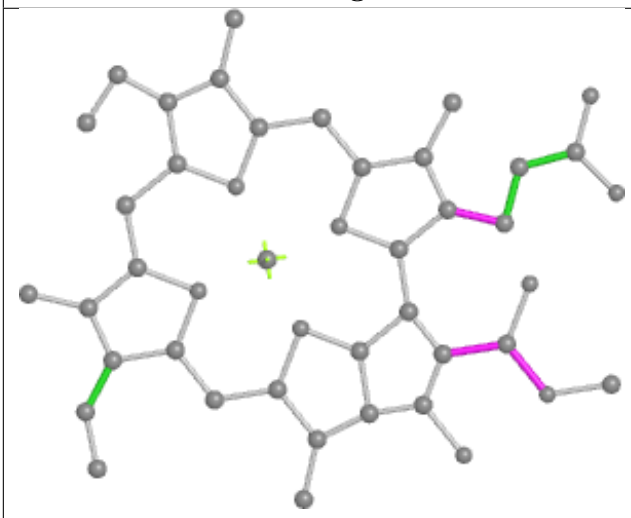

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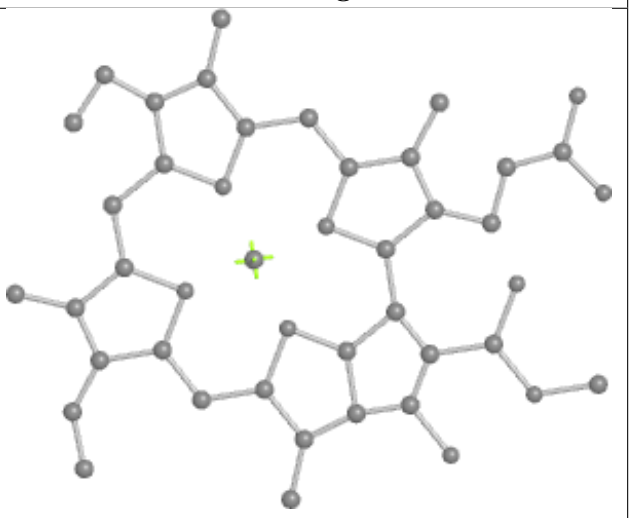
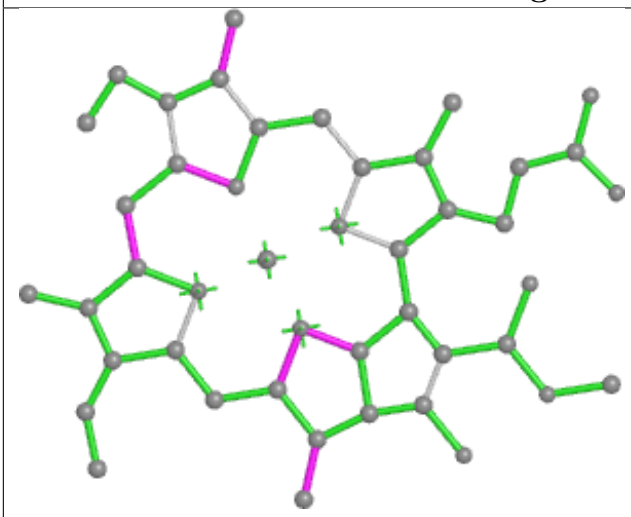


Rings

Ligand CLA t 501



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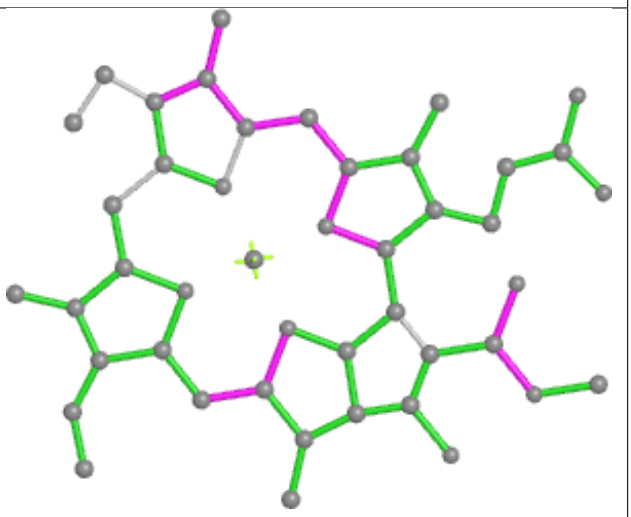
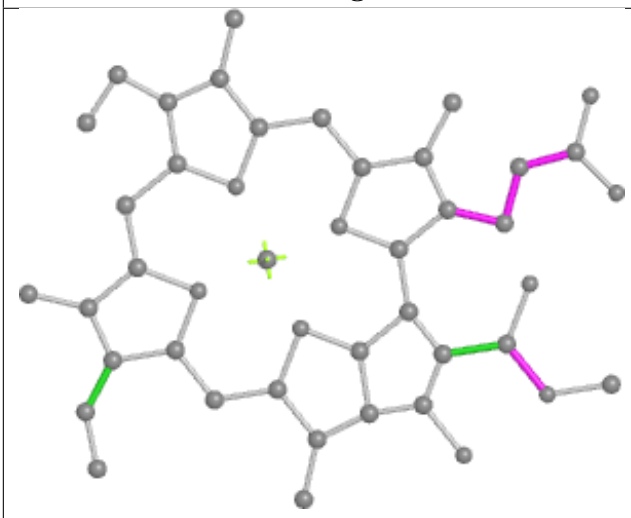


Bond angles



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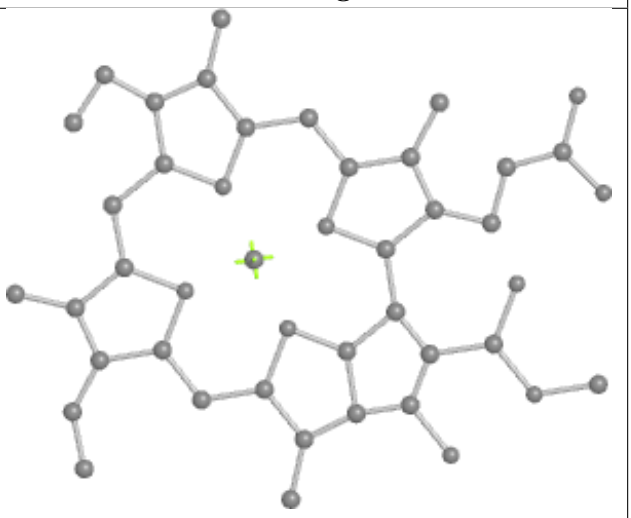
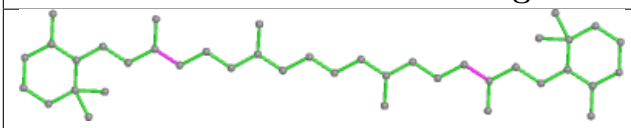


Rings

Ligand BCR V 4020



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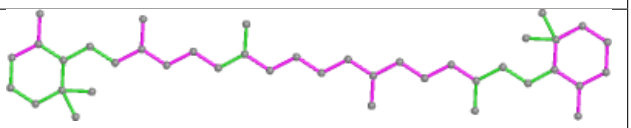

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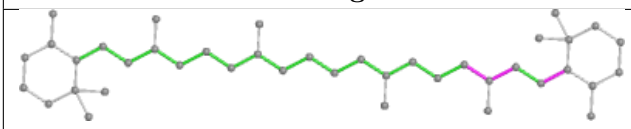
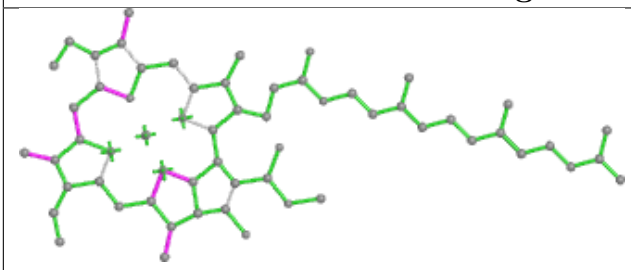


Torsions

Rings

Ligand CLA B 1201



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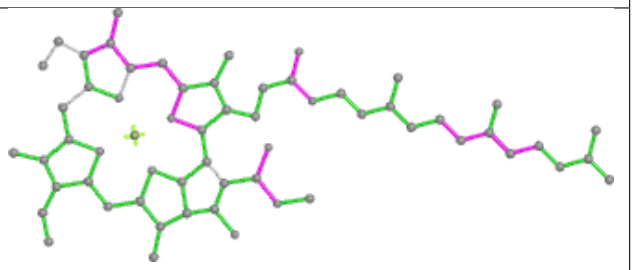
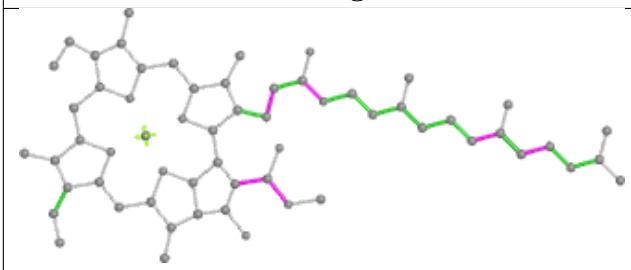
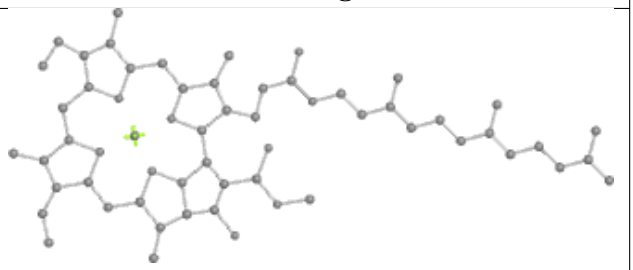


Bond angles

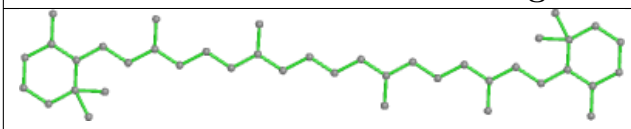


Torsions



Rings

Ligand BCR s 521



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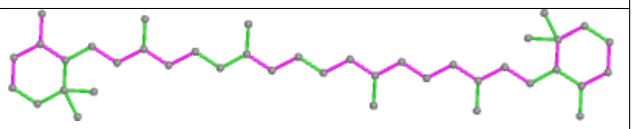
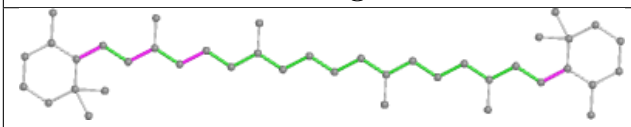


Bond angles



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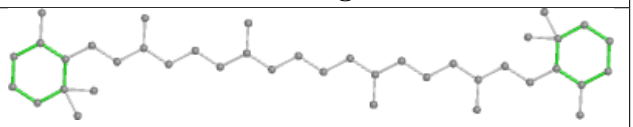
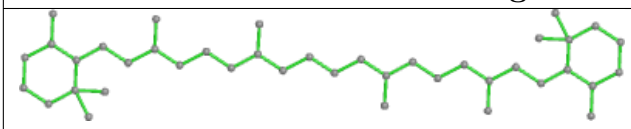


Rings

Ligand BCR M 4021



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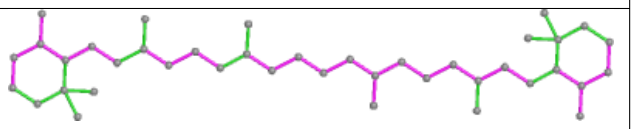
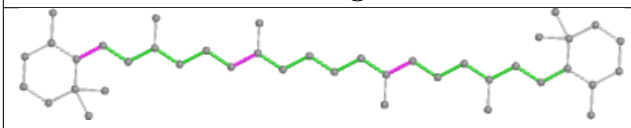


Bond angles



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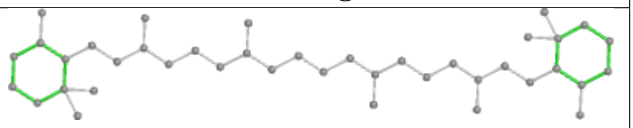
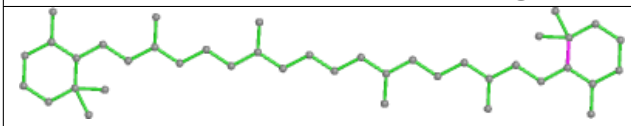


Rings

Ligand BCR G 4002



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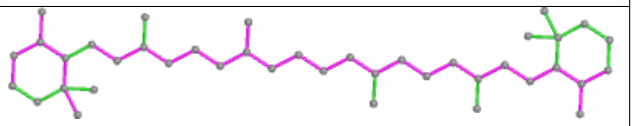
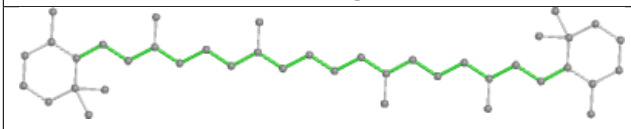


Bond angles



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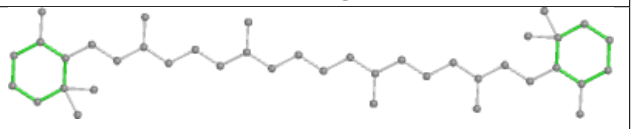
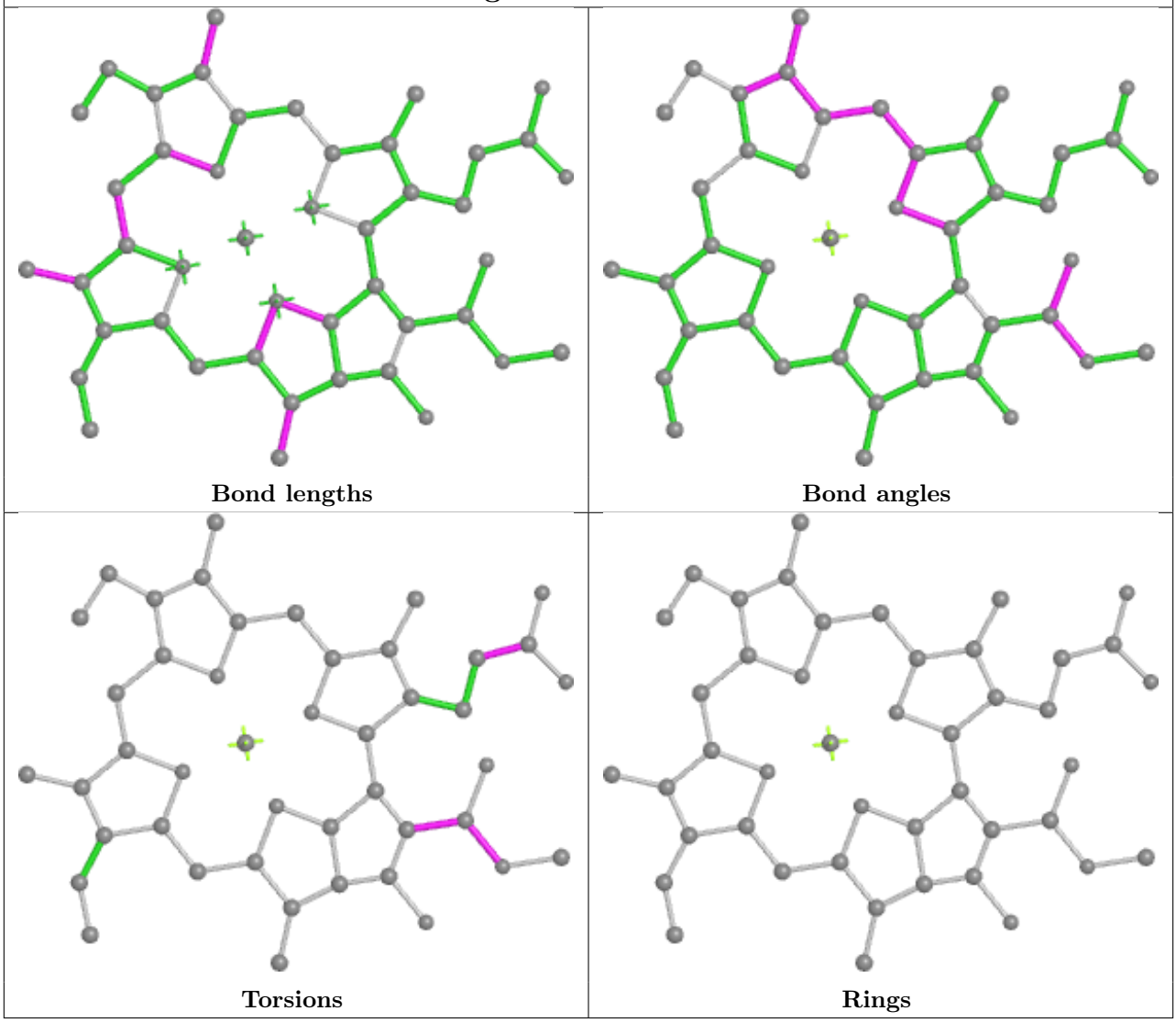


Rings

Ligand CLA v 510



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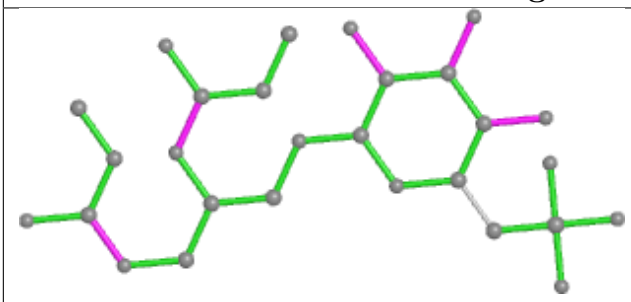
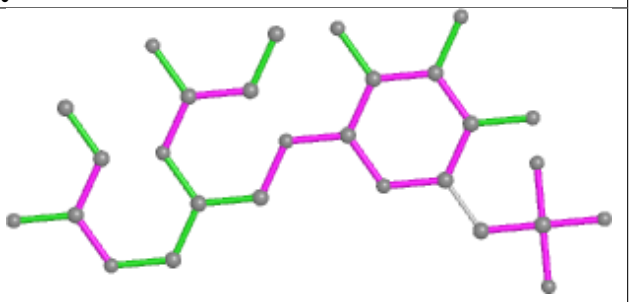
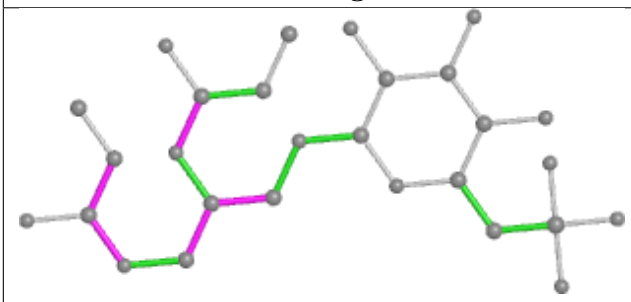
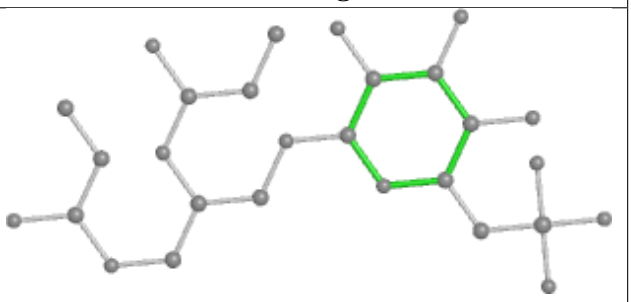
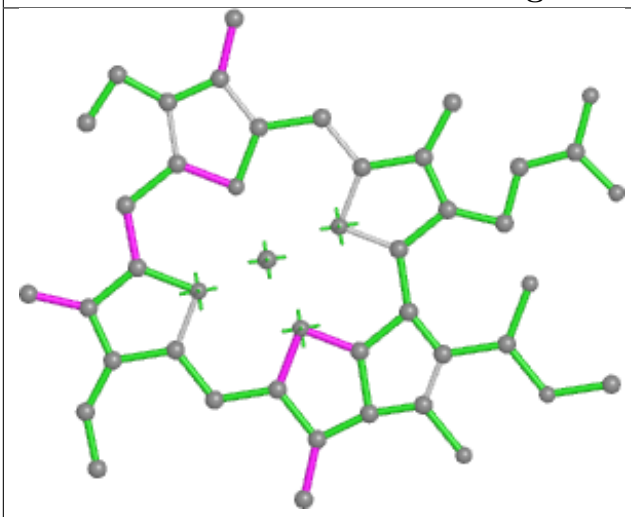
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 510



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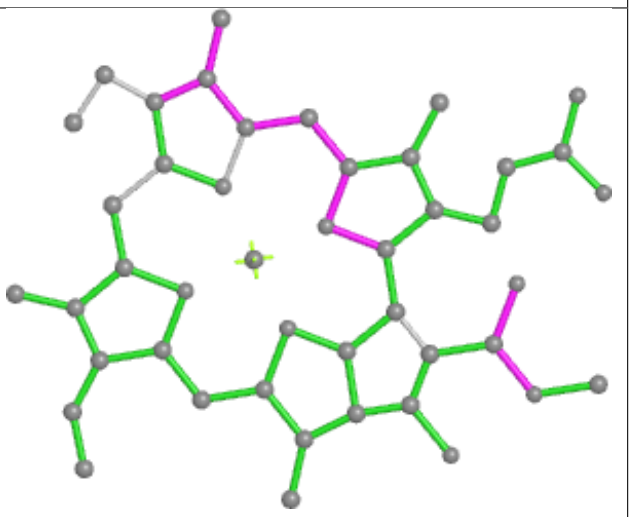

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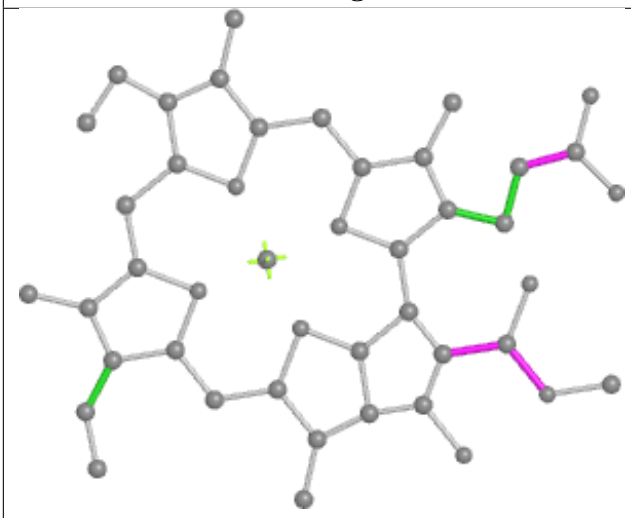

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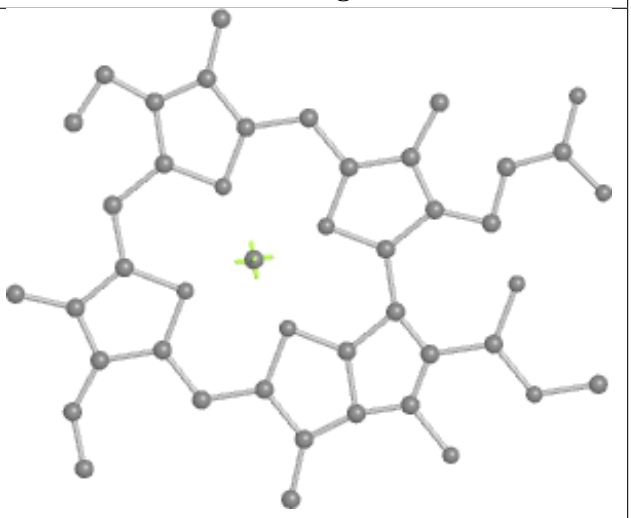

Rings

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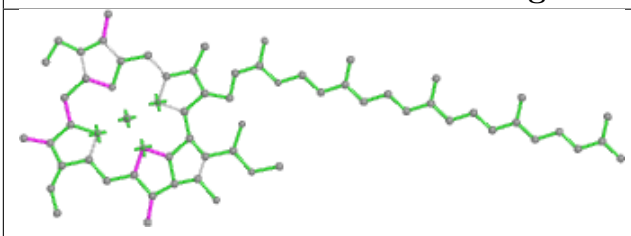

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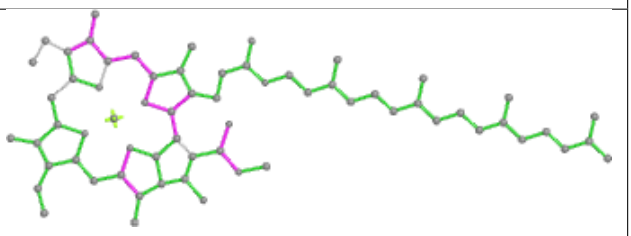

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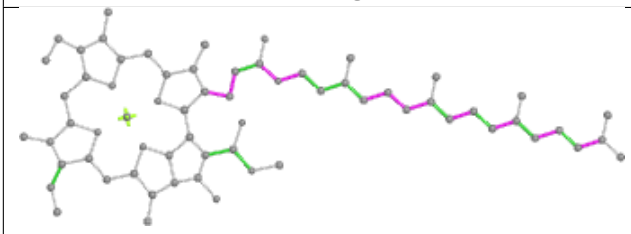

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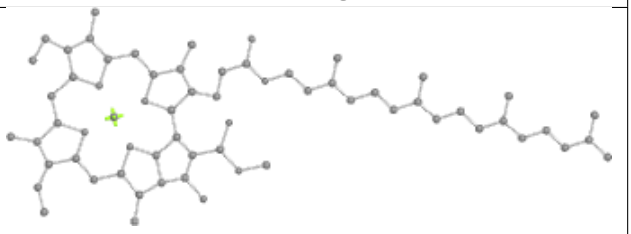
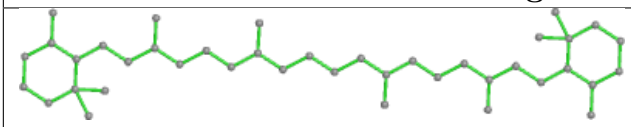


Rings

Ligand BCR q 523



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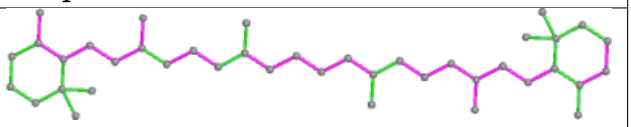

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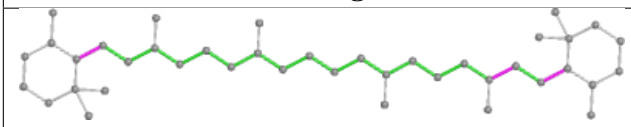
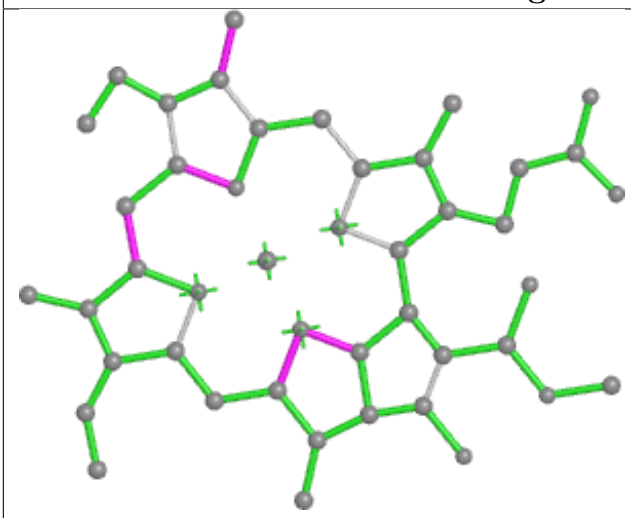


Torsions

Rings

Ligand CLA 3 516



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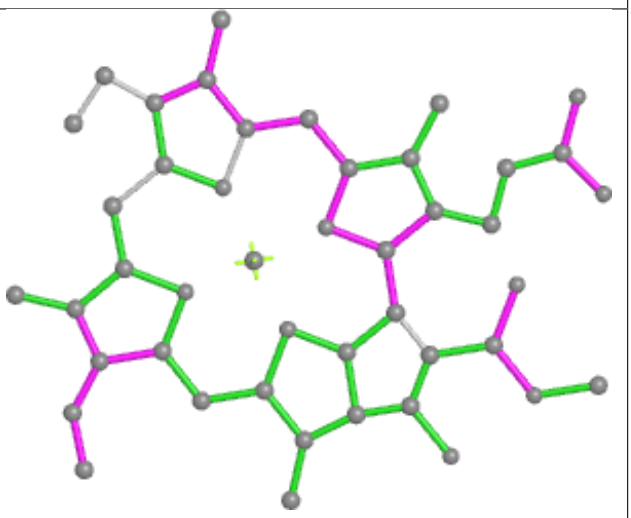

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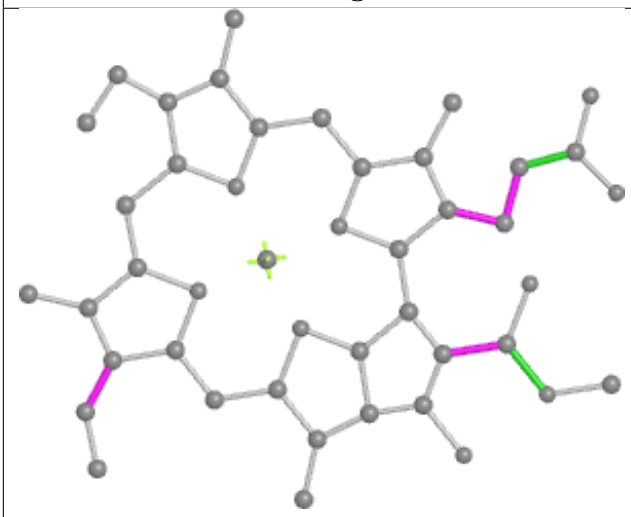

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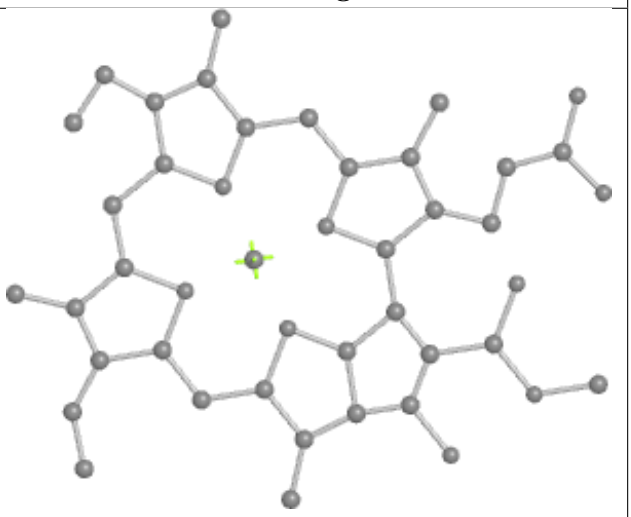

Rings

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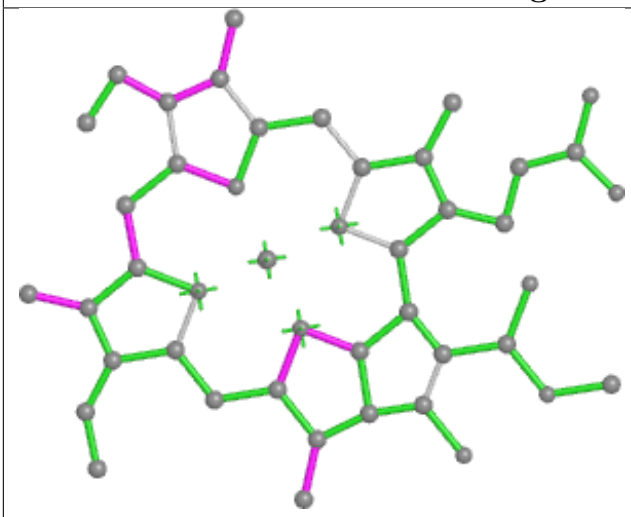

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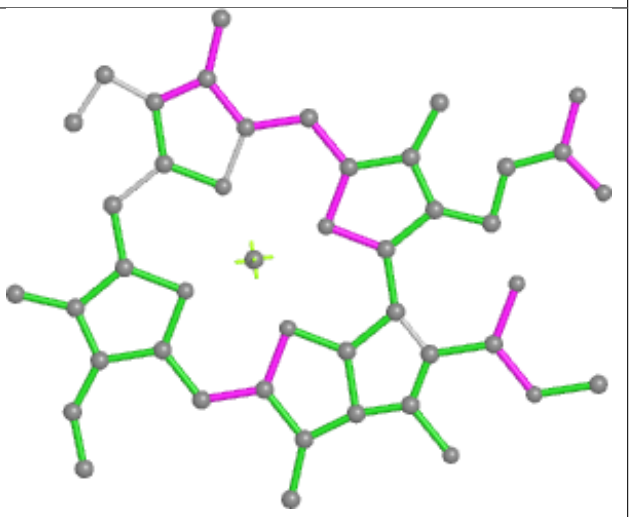

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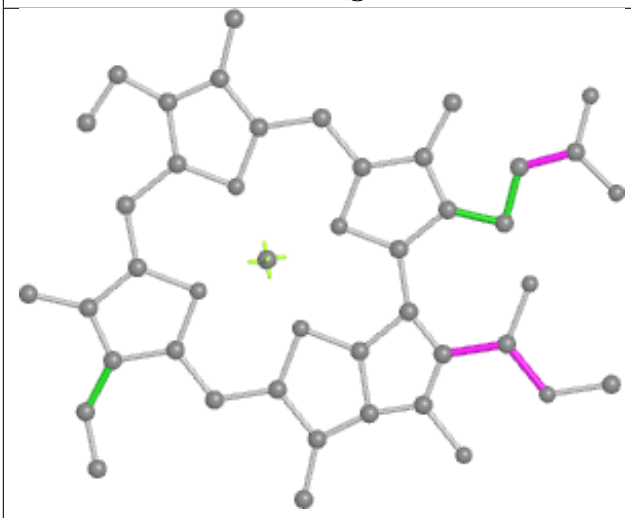

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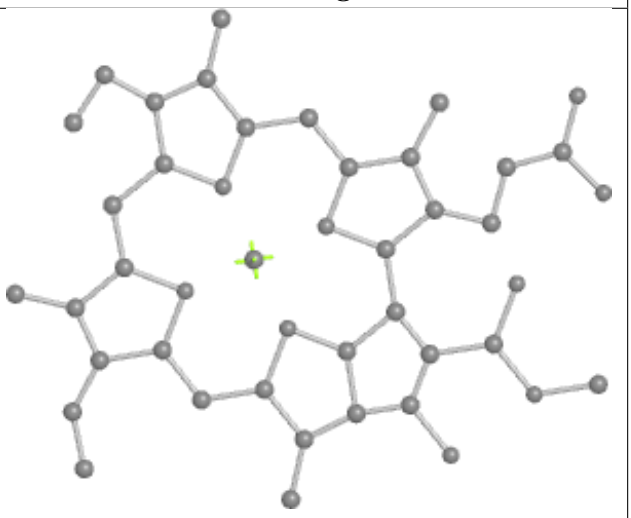
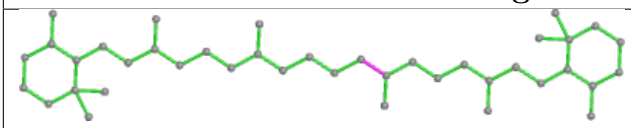


Rings

Ligand BCR H 4010



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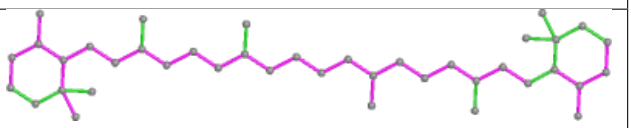

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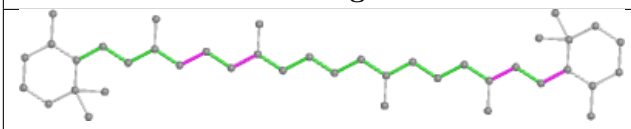
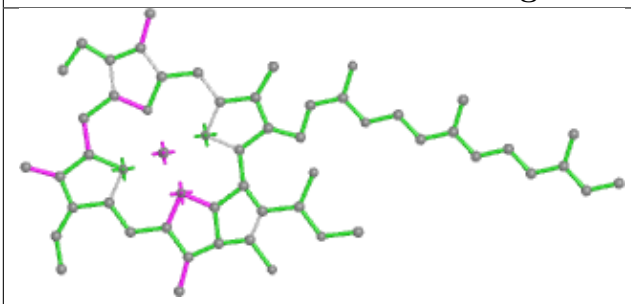
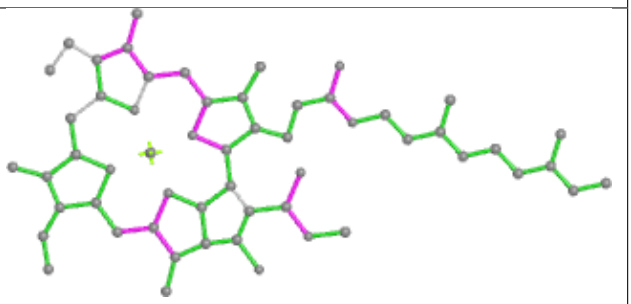
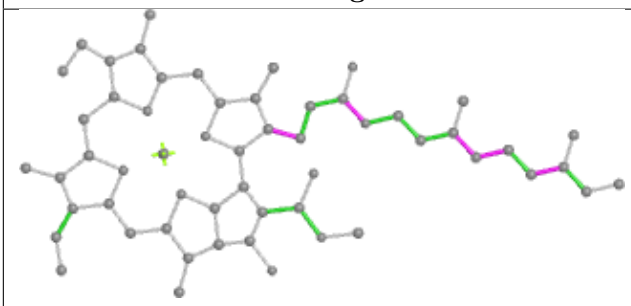
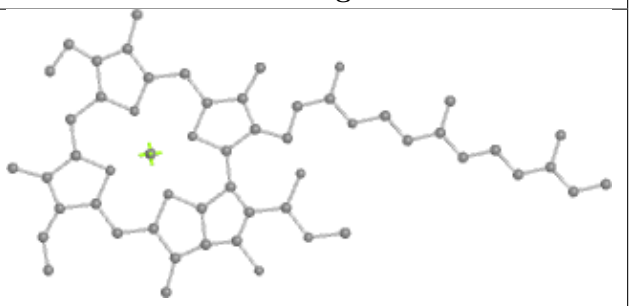


Torsions

Rings

Ligand CLA e 1130	
 Bond lengths	 Bond angles
 Torsions	 Rings

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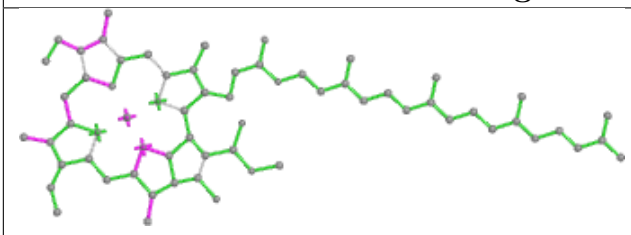
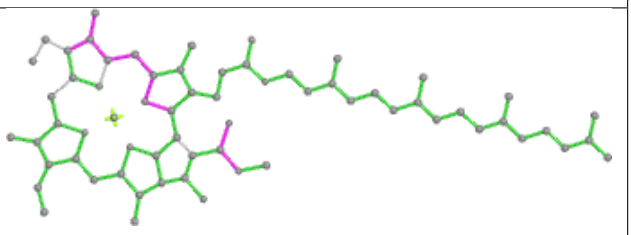
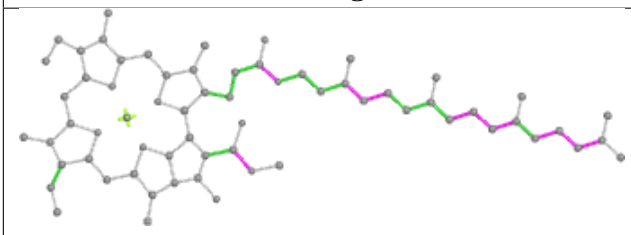
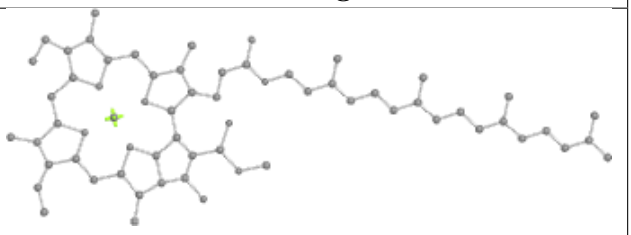
 Bond lengths	 Bond angles
 Torsions	 Rings

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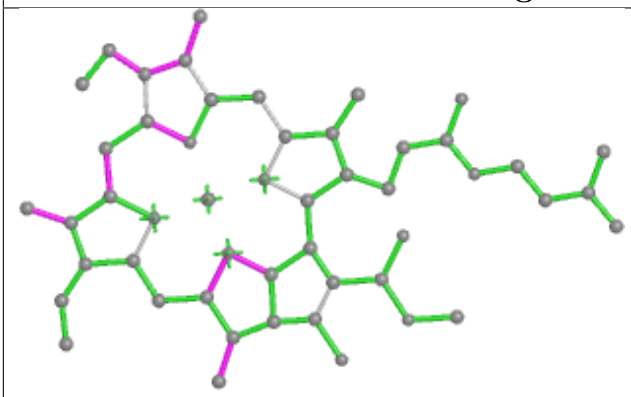
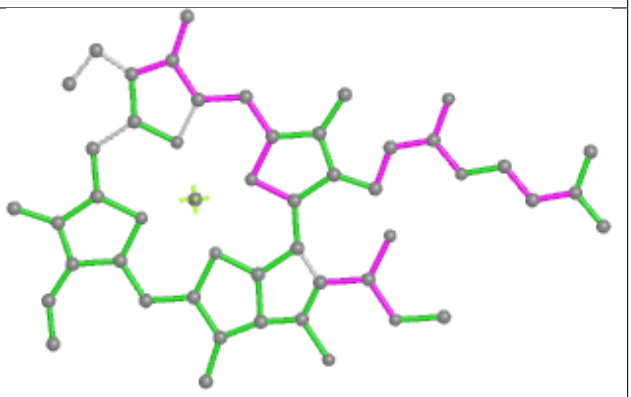
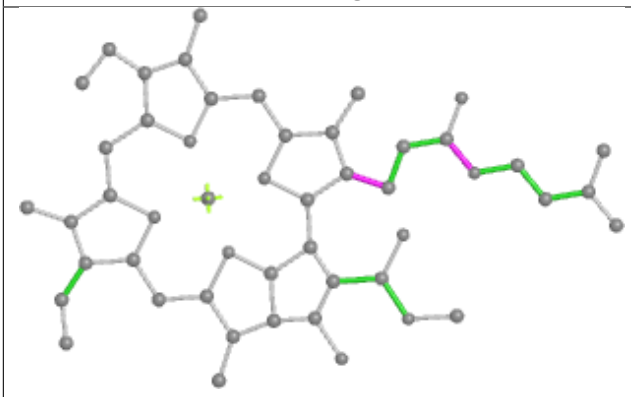
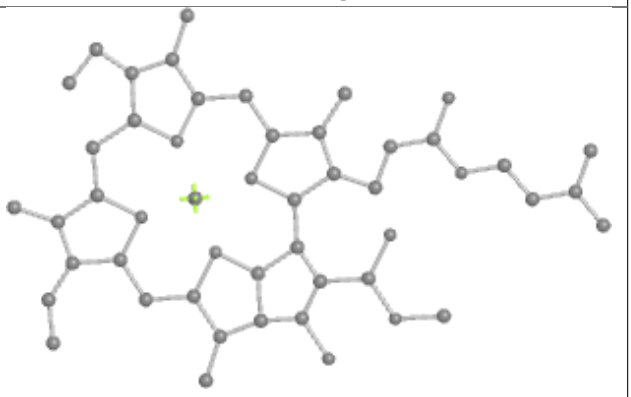
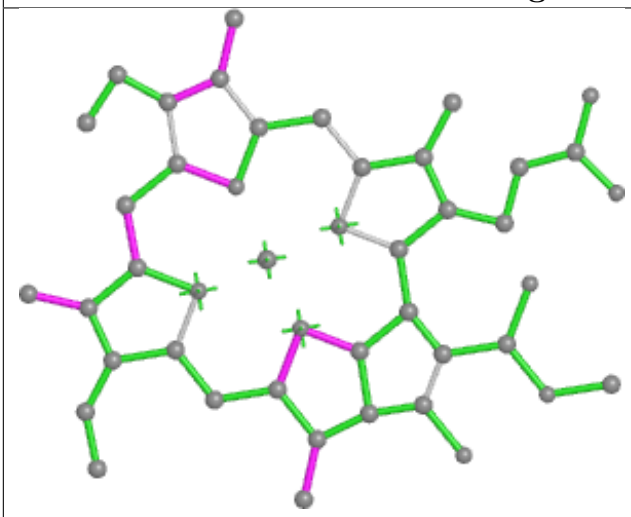
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 502



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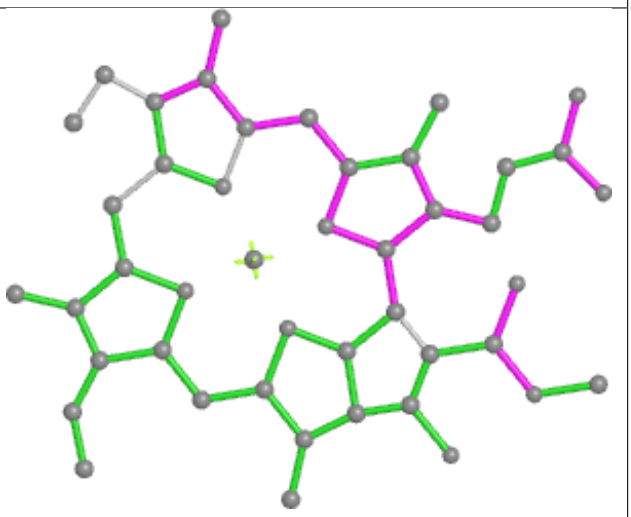

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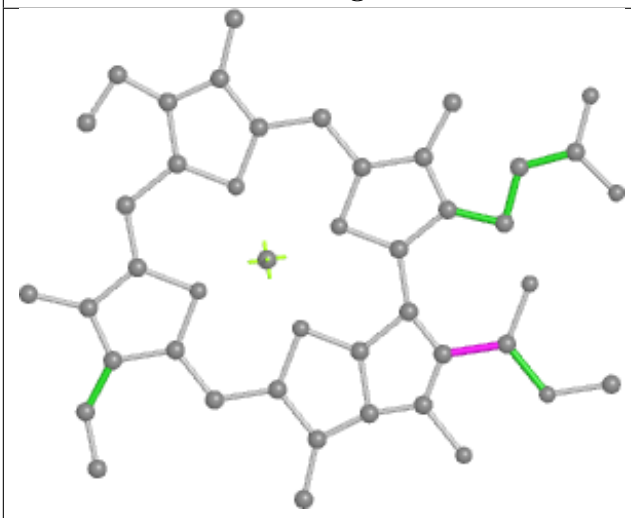

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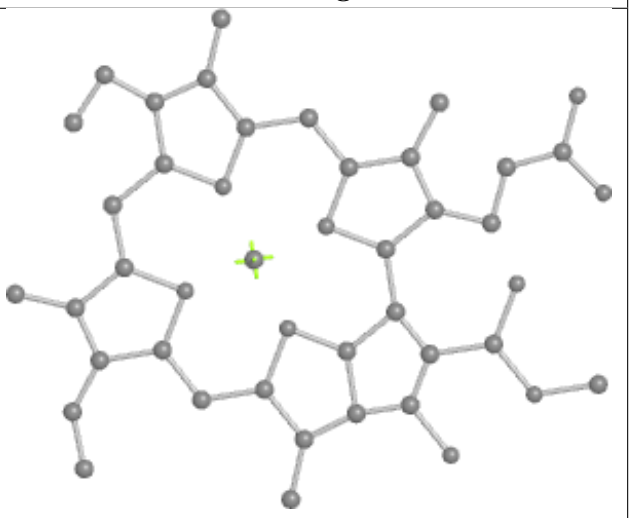
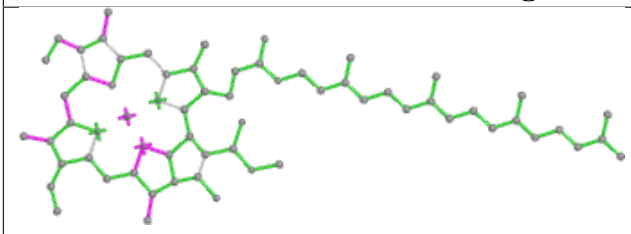


Rings

Ligand CLA e 1127



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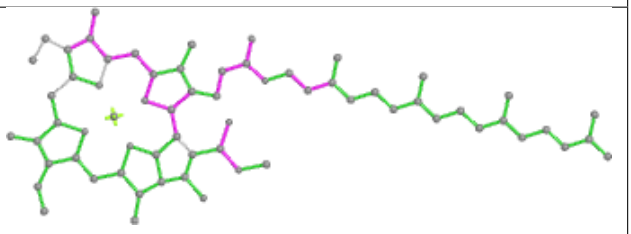

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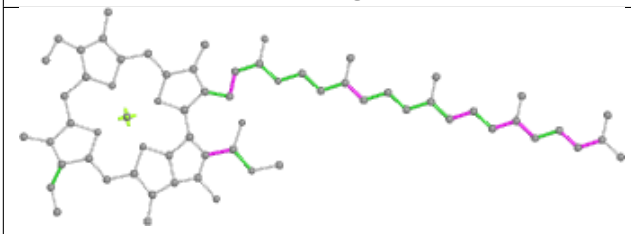

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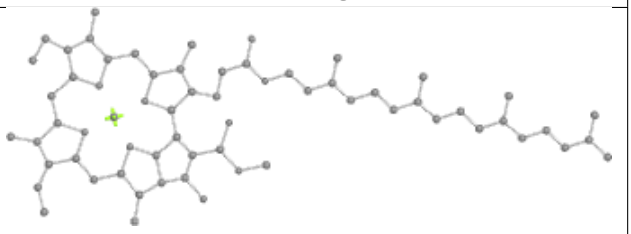
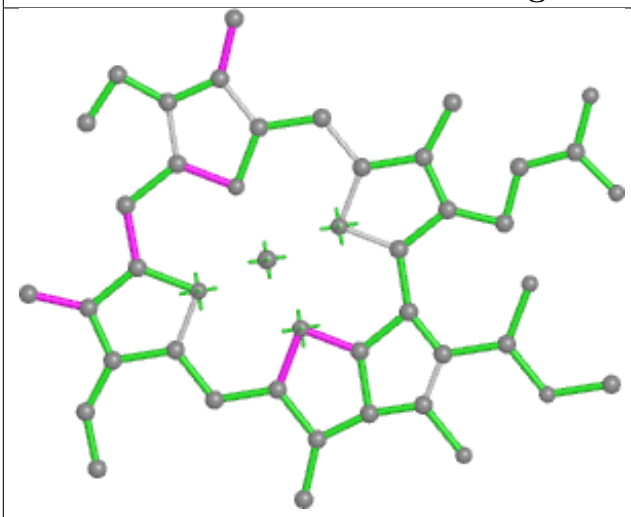


Rings

Ligand CLA 1 501



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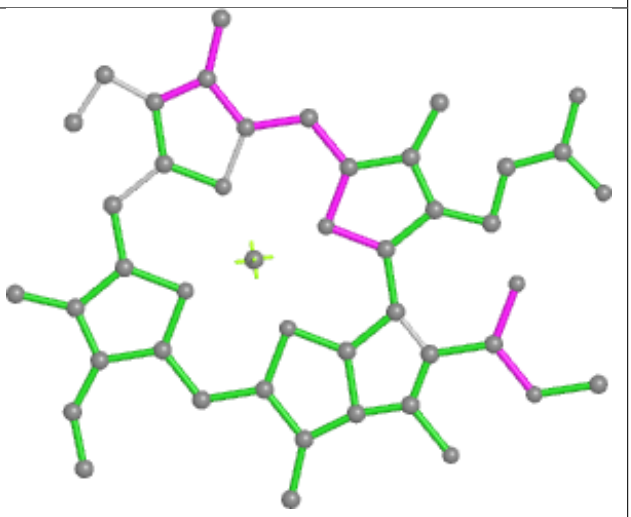
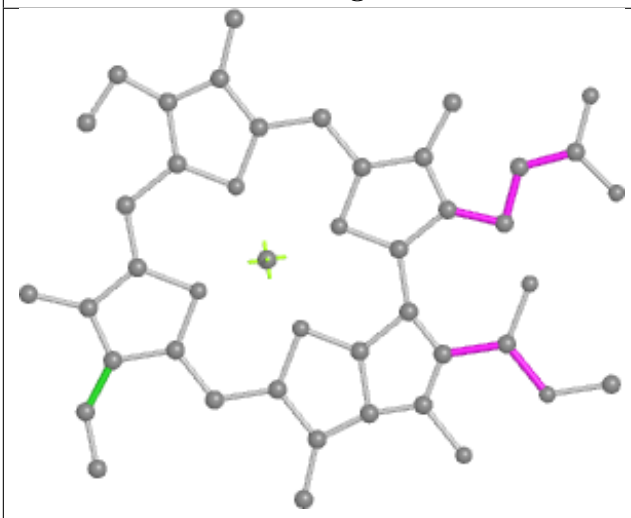


Bond angles



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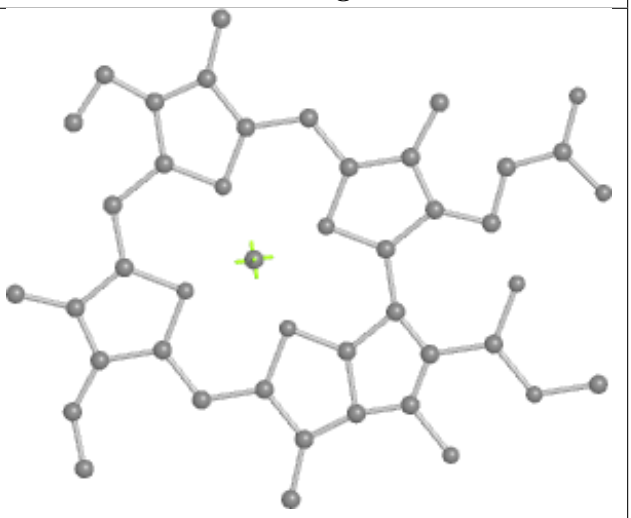
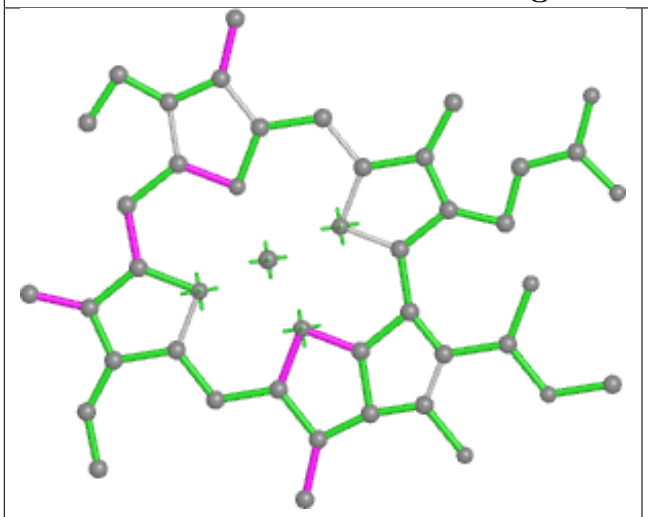


Rings

Ligand CLA s 506



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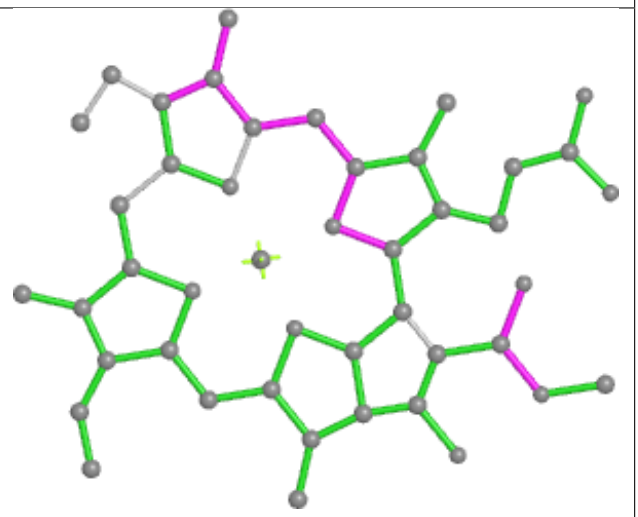
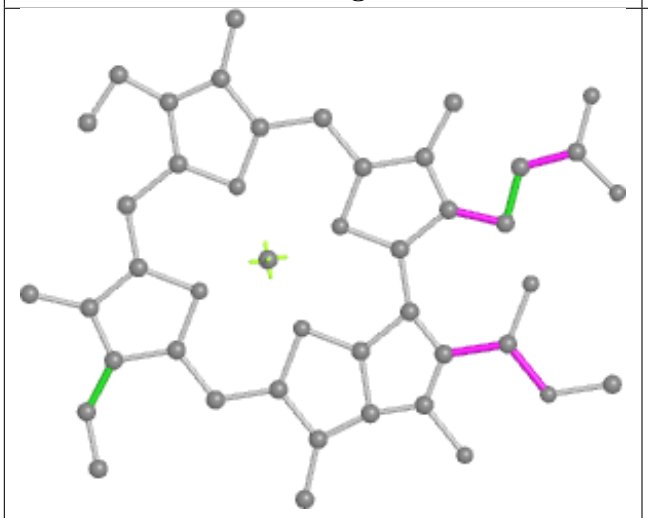
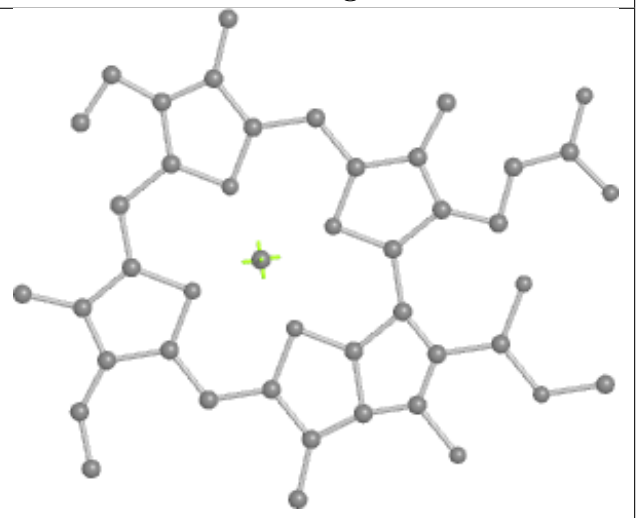


Bond angles

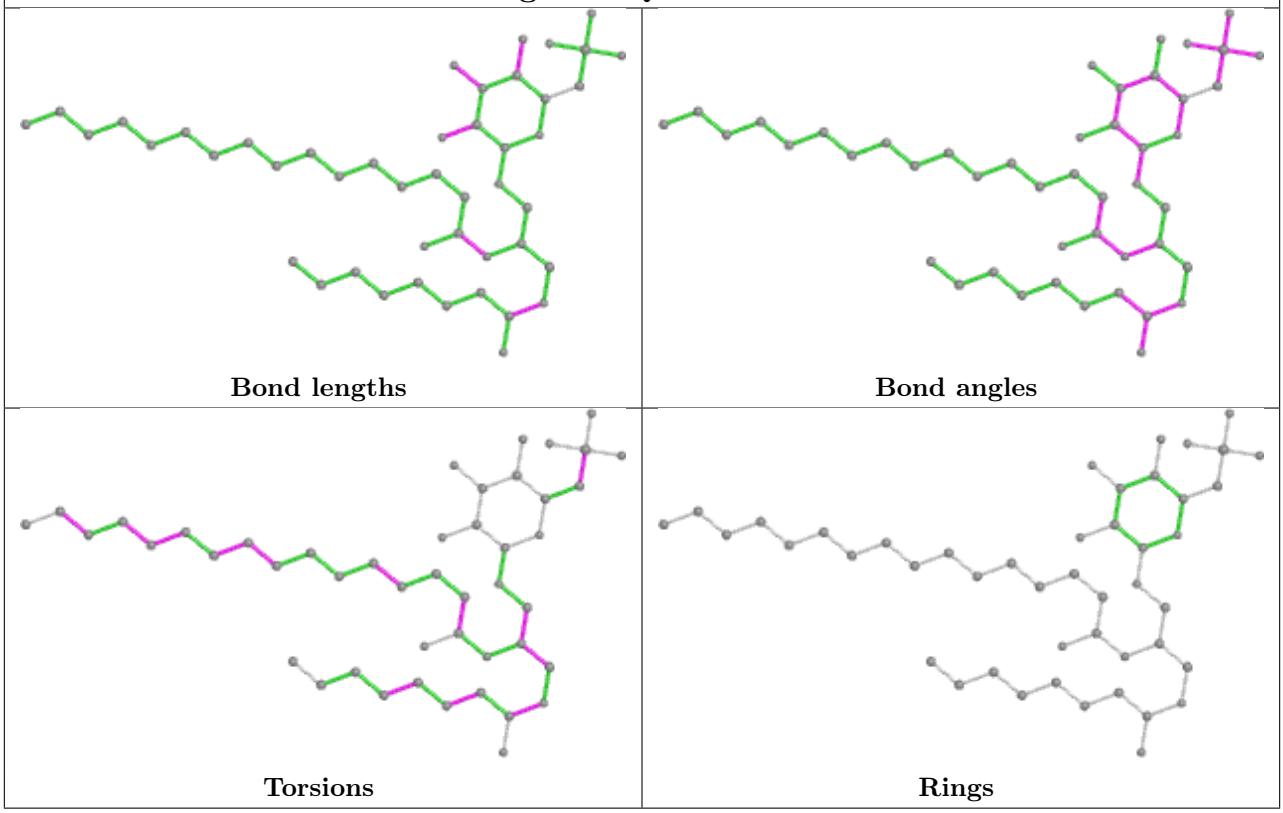


Torsions

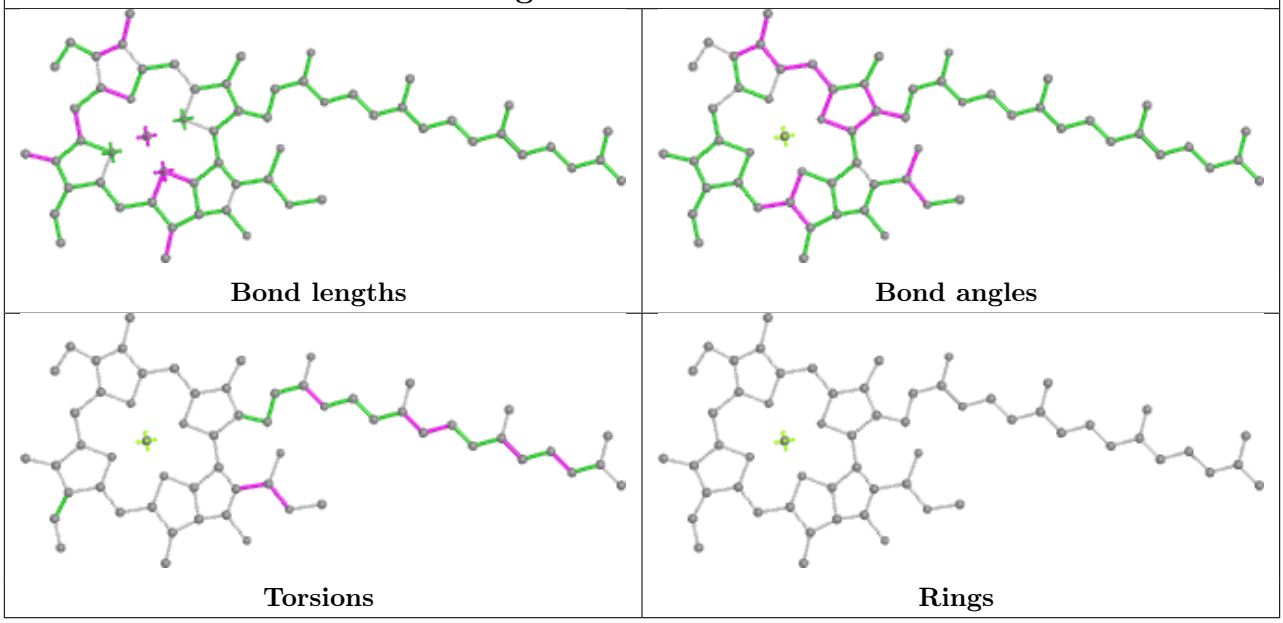


Rings

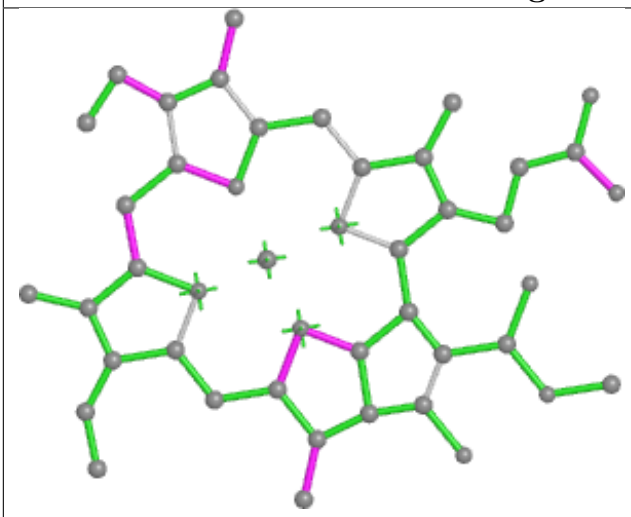
Ligand SQD n 5216



Ligand CLA A 1124



Ligand CLA a 510



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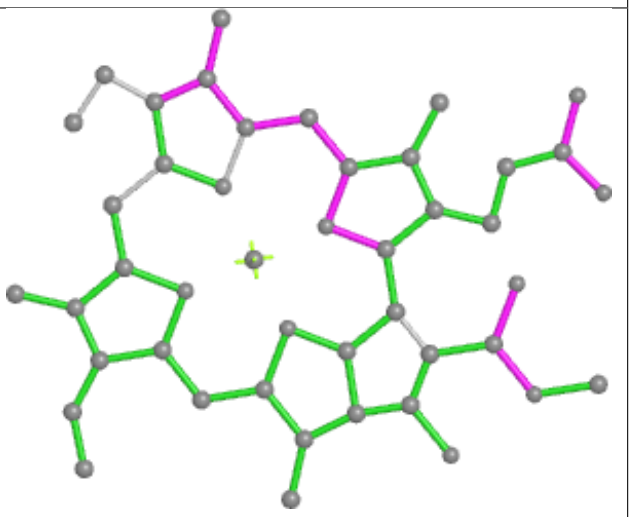
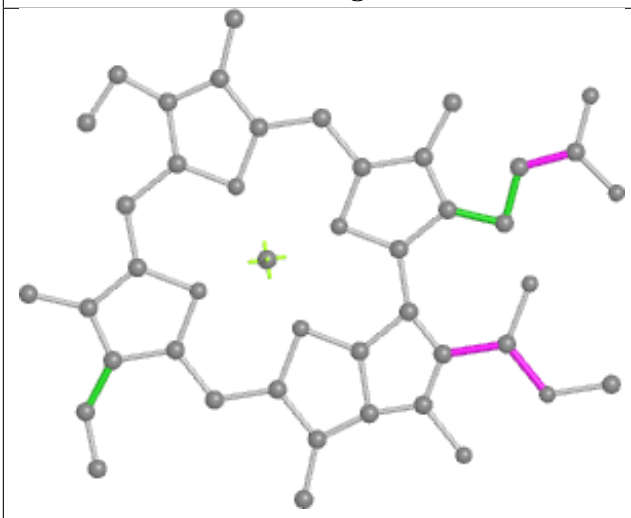
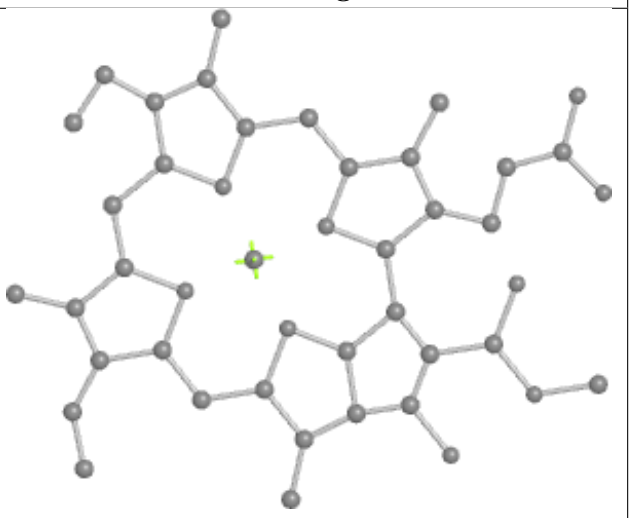


Bond angles

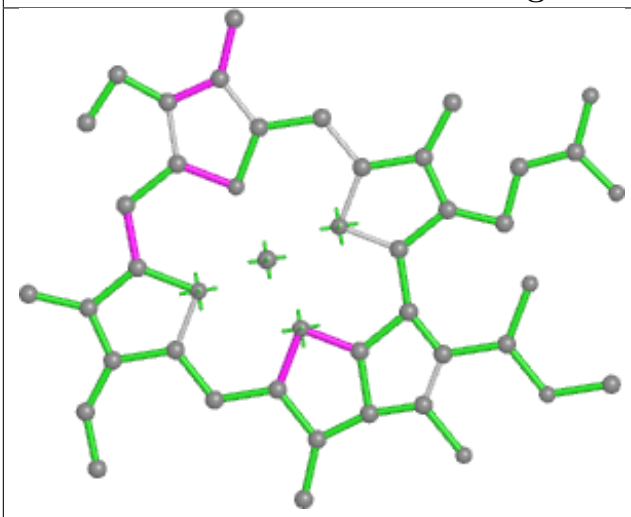


Torsions



Rings

Ligand CLA u 519



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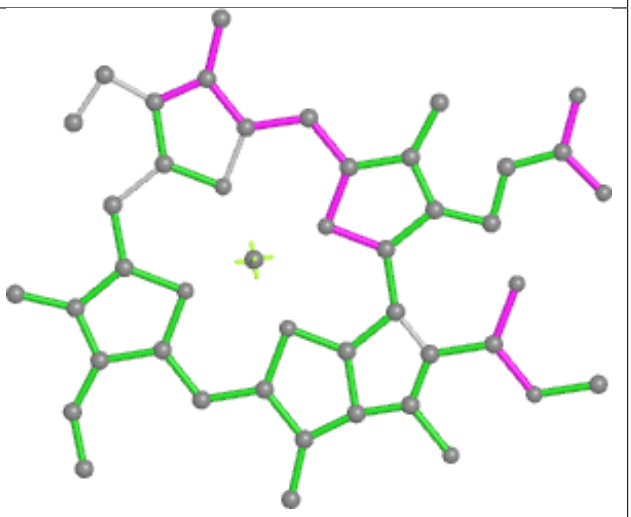

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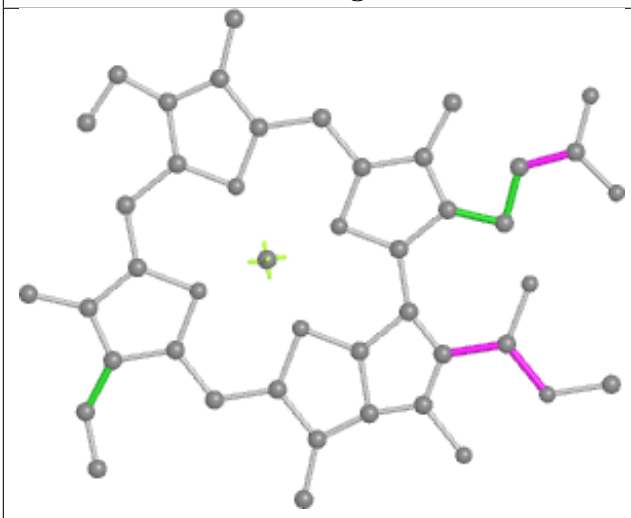

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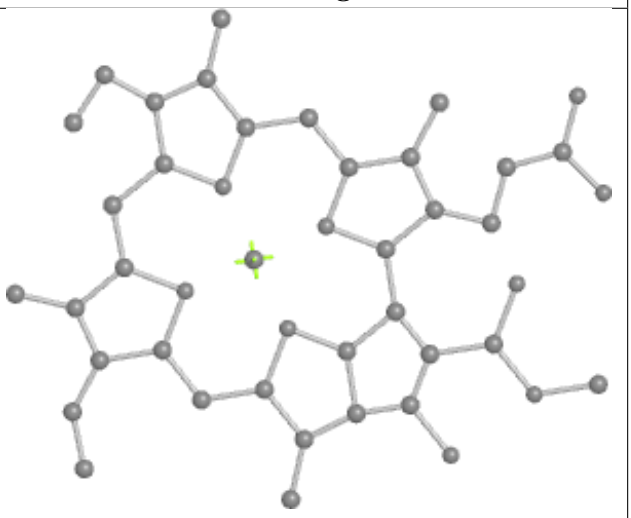
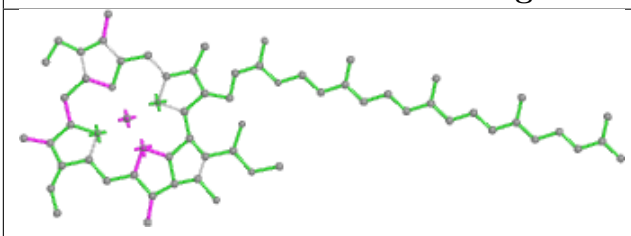


Rings

Ligand CLA B 1234



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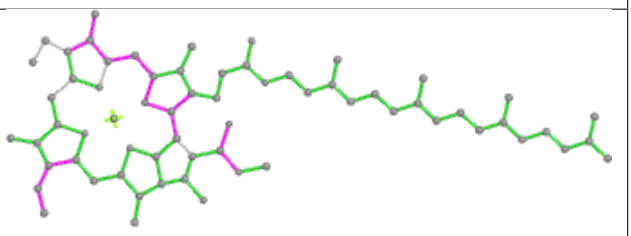
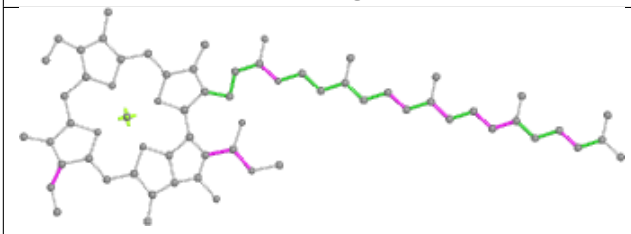


Bond angles



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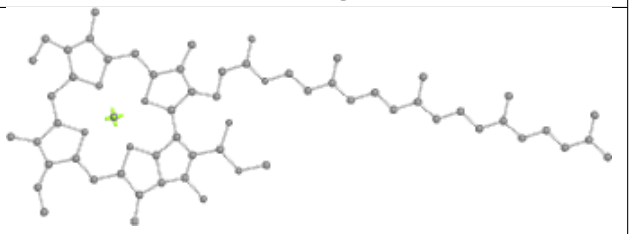
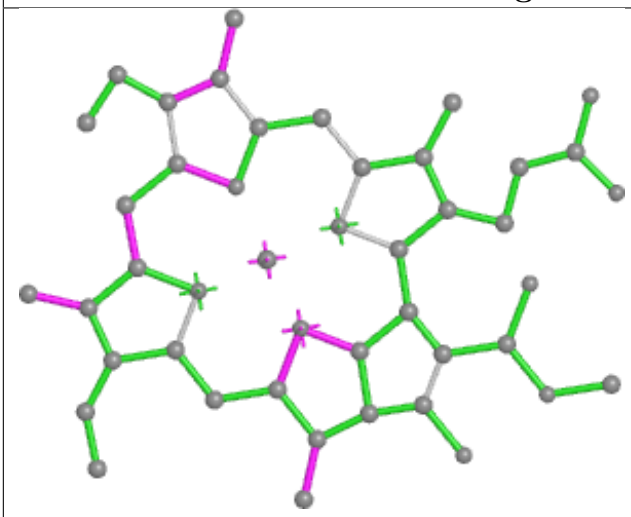


Rings

Ligand CLA R 1301



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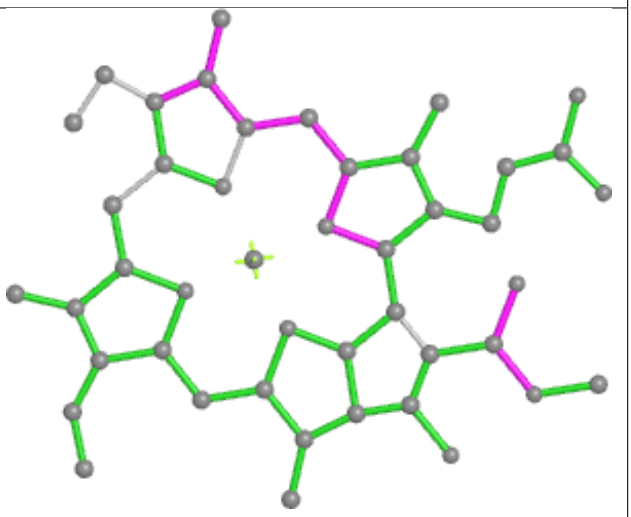

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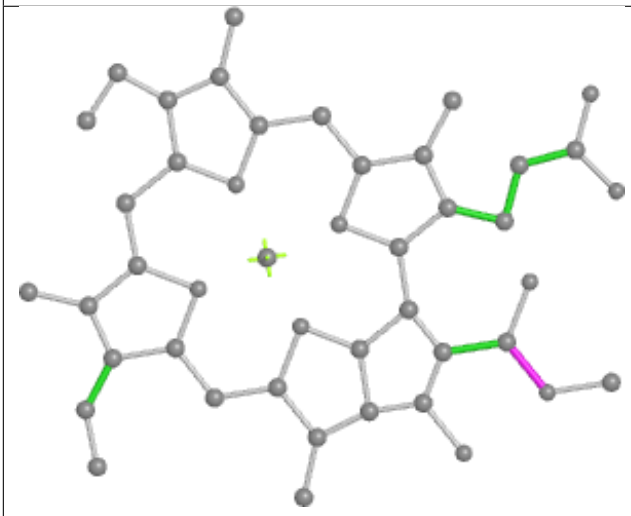

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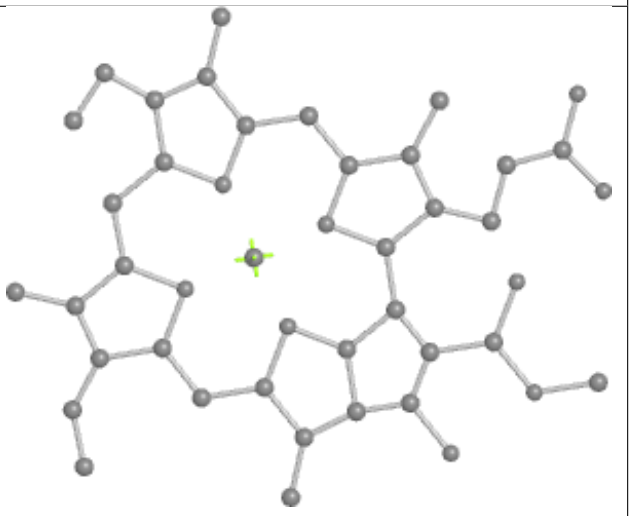
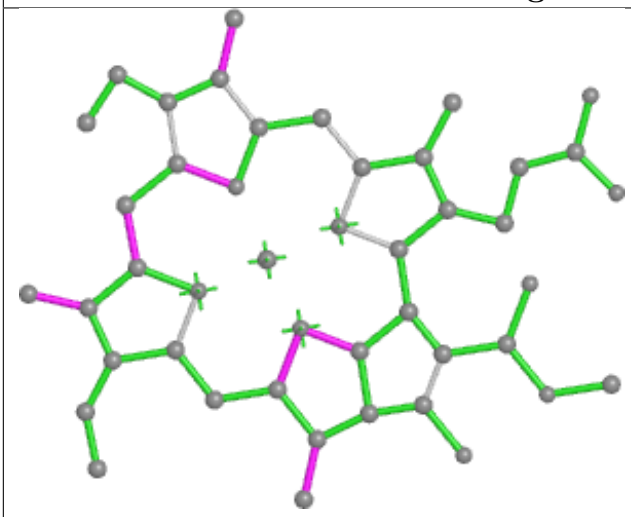


Rings

Ligand CLA b 517



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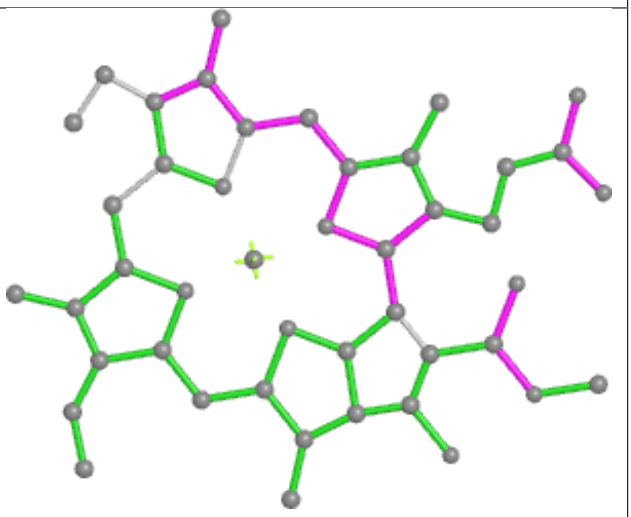

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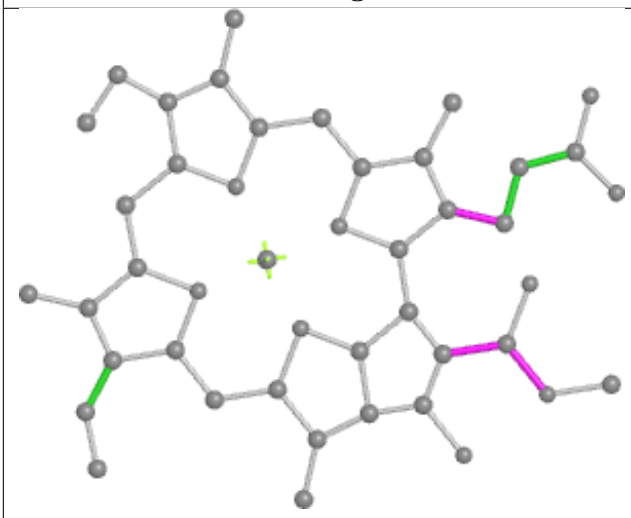

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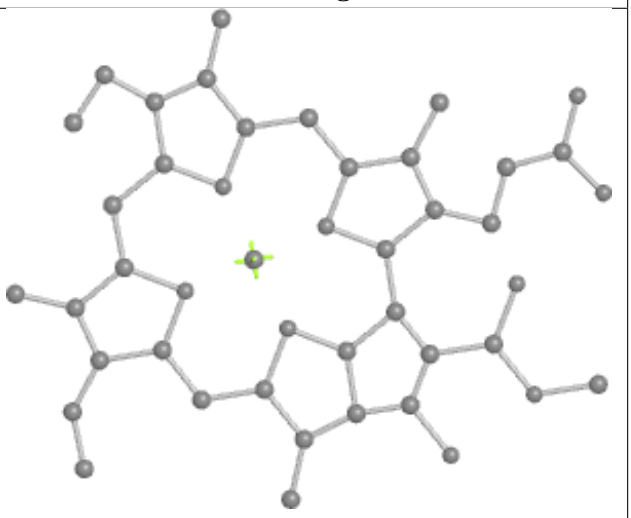
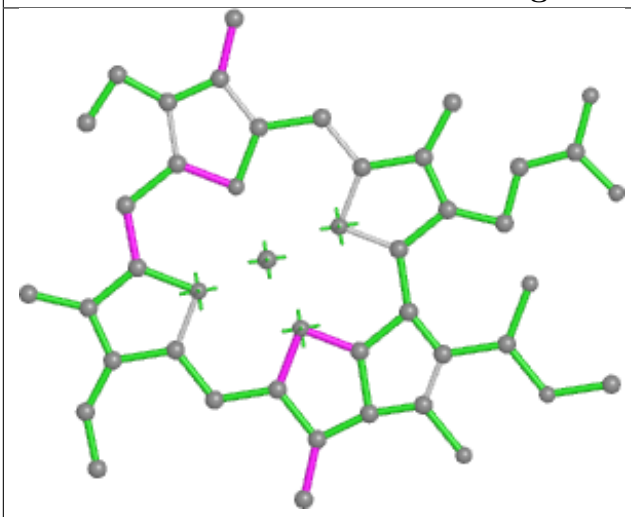


Rings

Ligand CLA t 511



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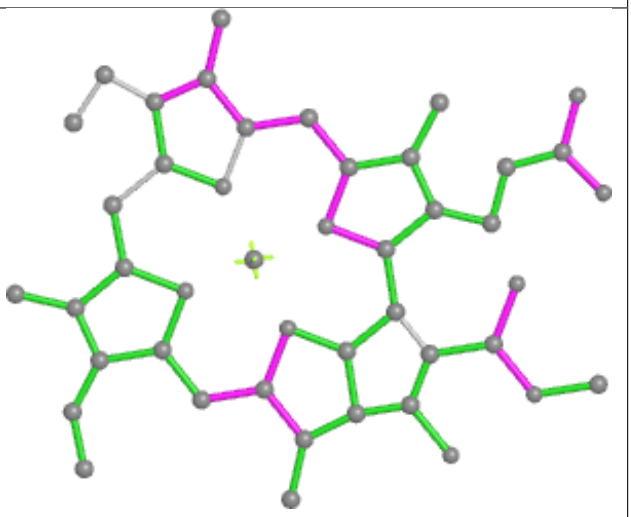
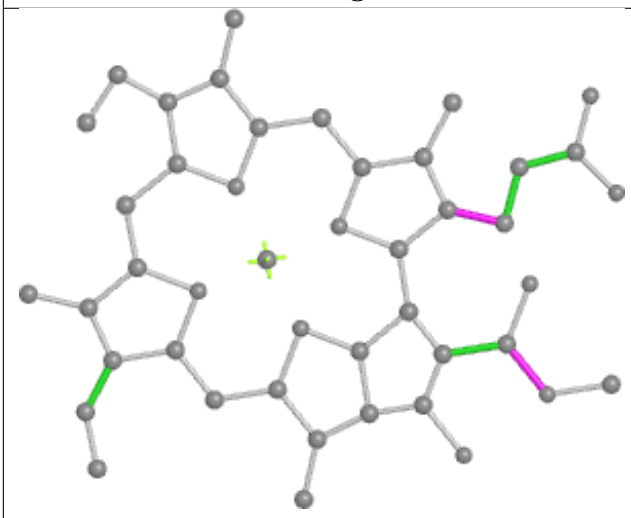


Bond angles



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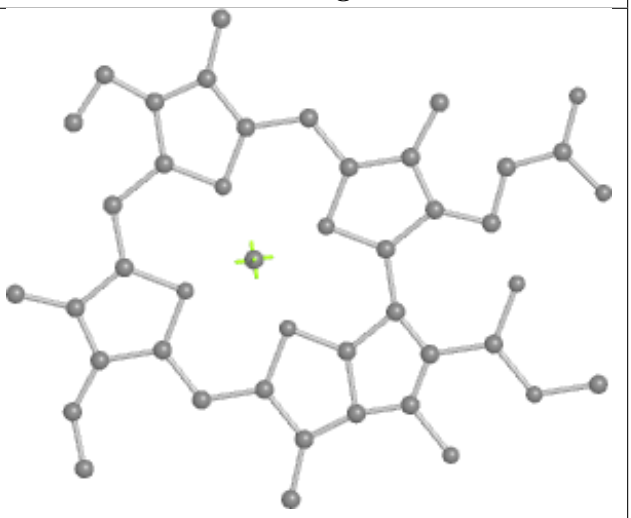
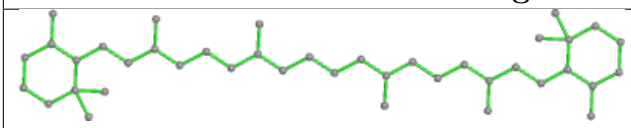


Rings

Ligand BCR G 4001



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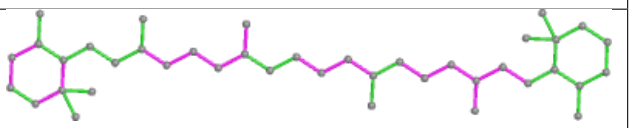
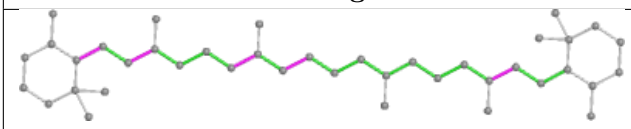
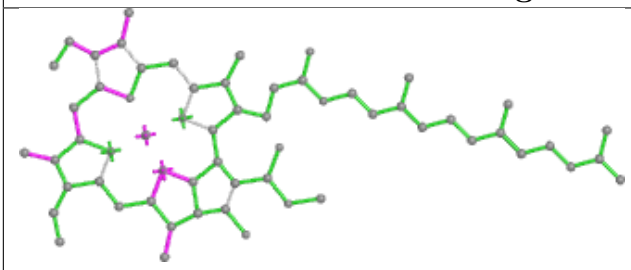
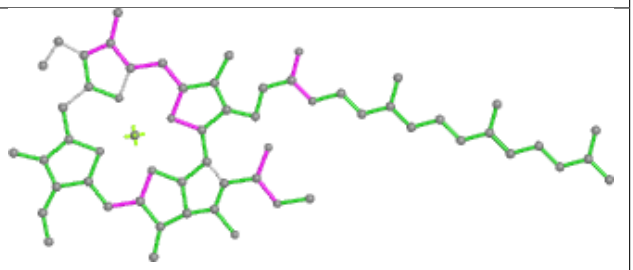
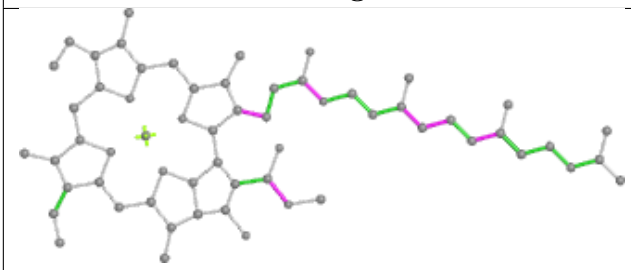
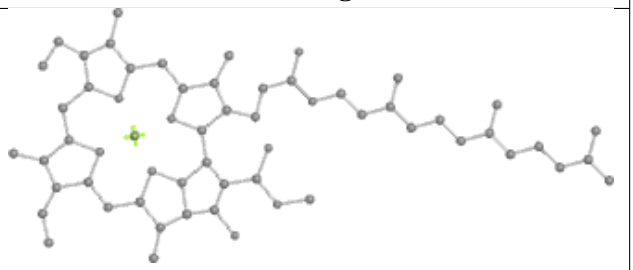


Bond angles



Torsions

Rings

Ligand CLA B 1227	
 Bond lengths	 Bond angles
 Torsions	 Rings

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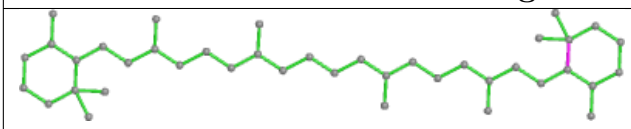
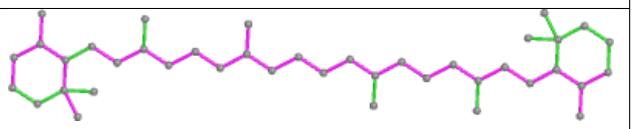
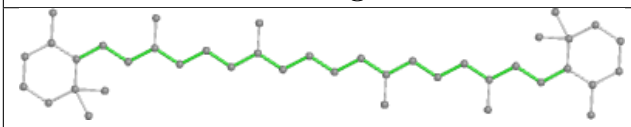
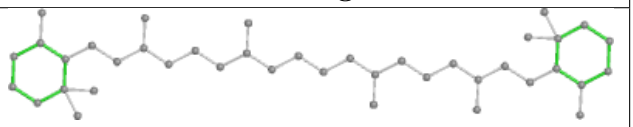
 Bond lengths	 Bond angles
 Torsions	 Rings

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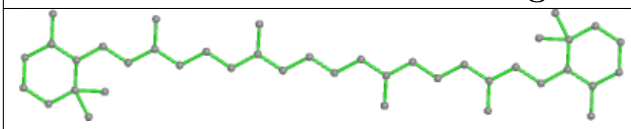
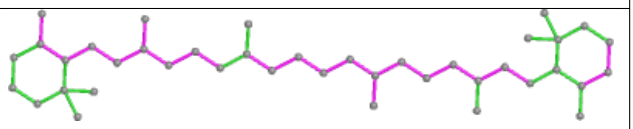
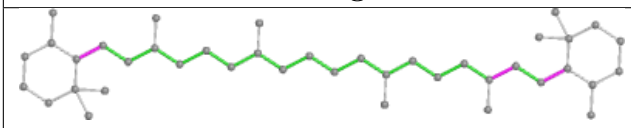
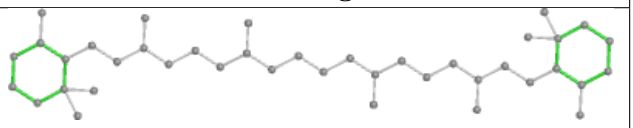
 Bond lengths	 Bond angles
 Torsions	 Rings

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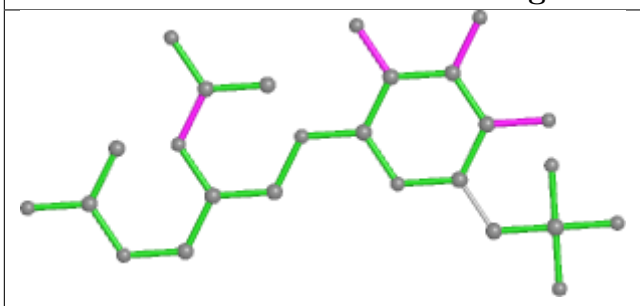
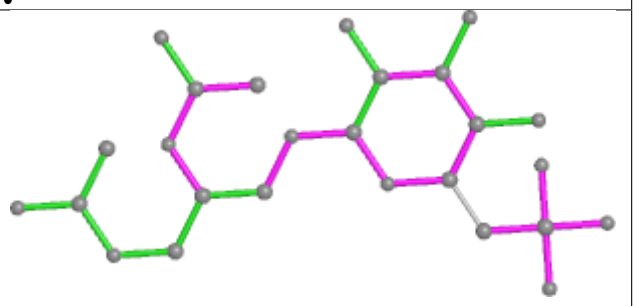
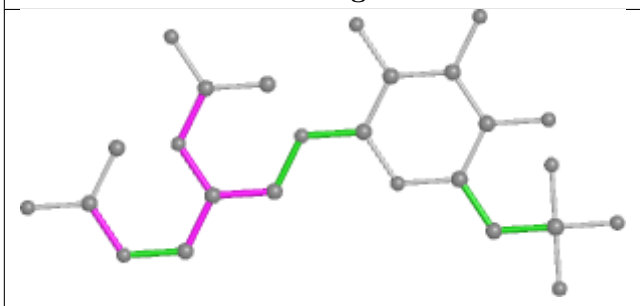
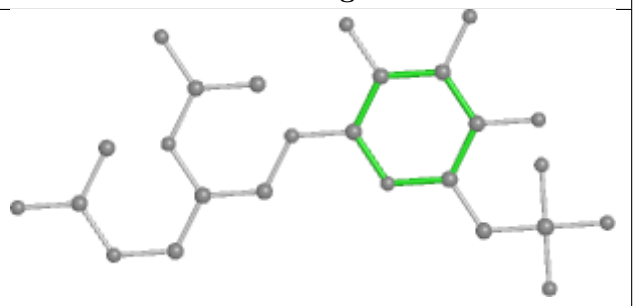
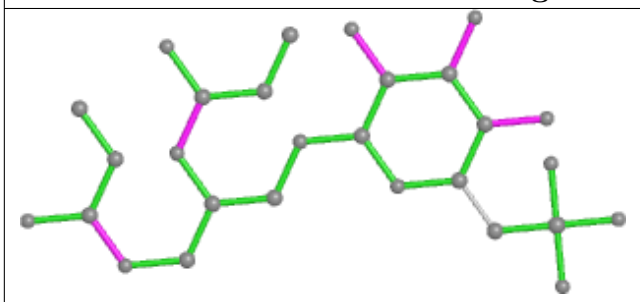
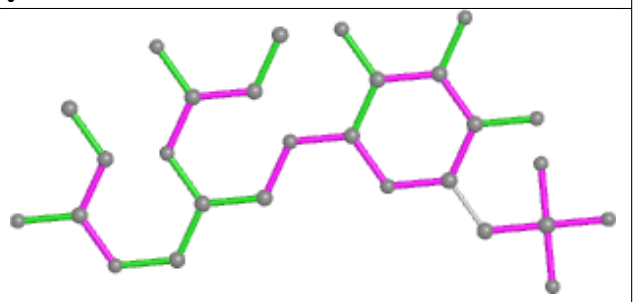
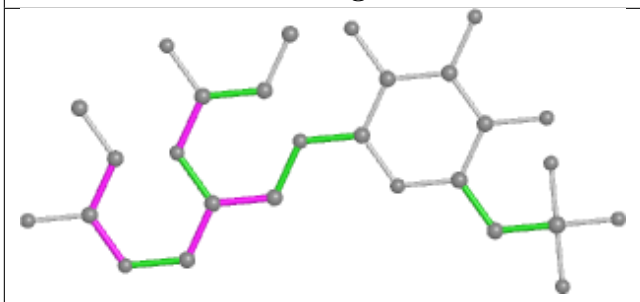
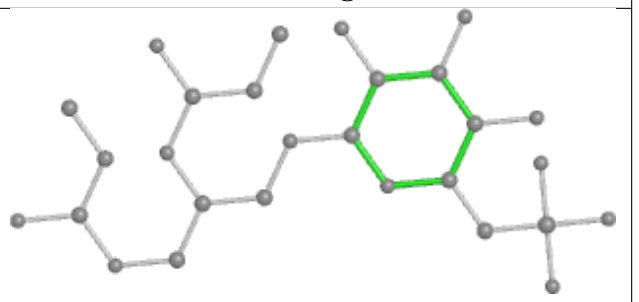
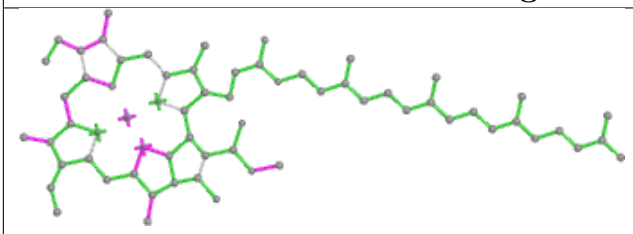
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD s 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA e 1022



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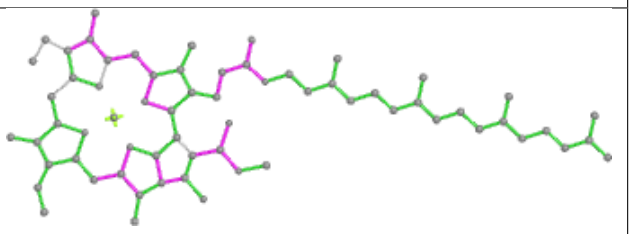
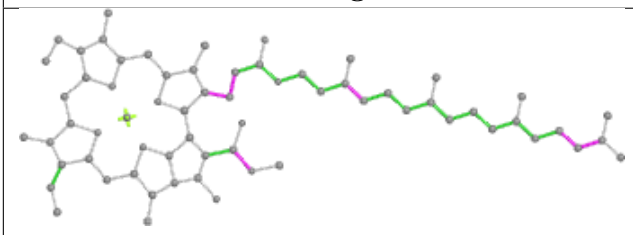
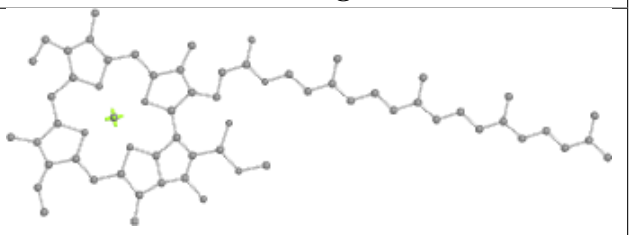


Bond angles

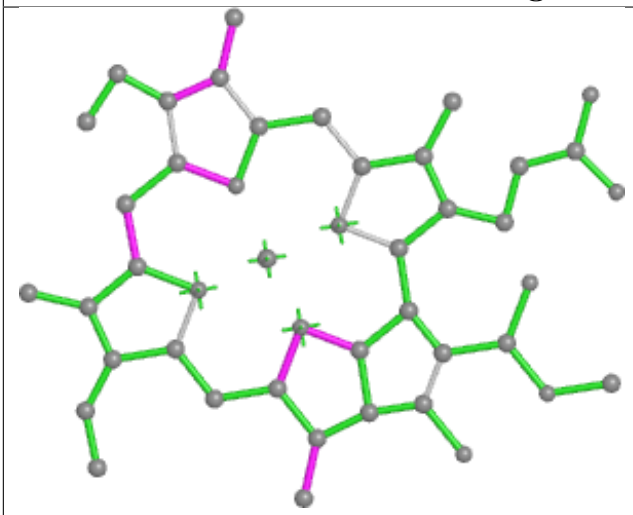


Torsions

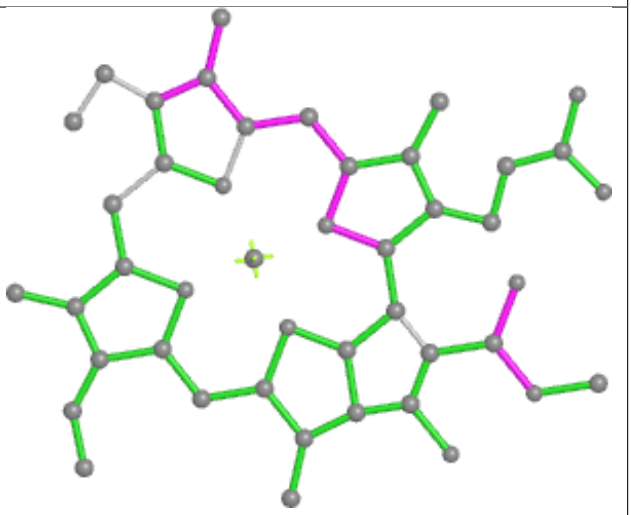


Rings

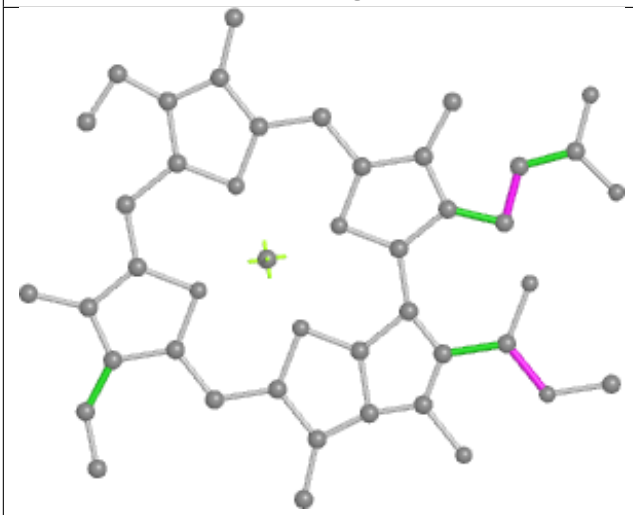
Ligand CLA d 513



Bond lengths



Bond angles



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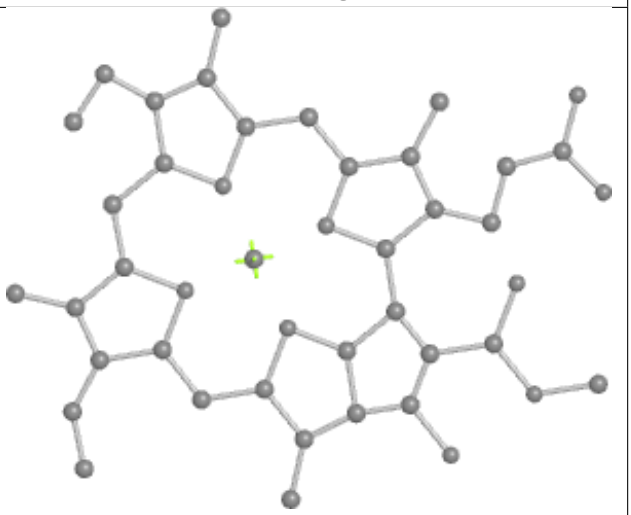
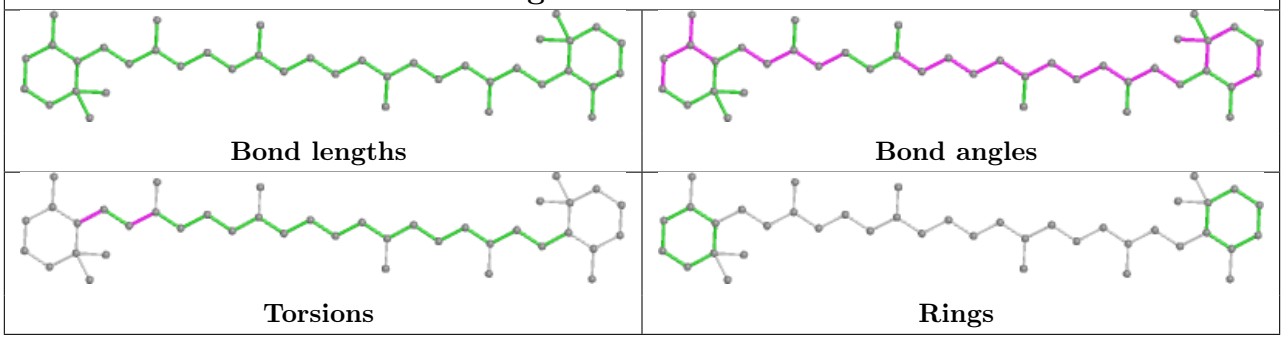
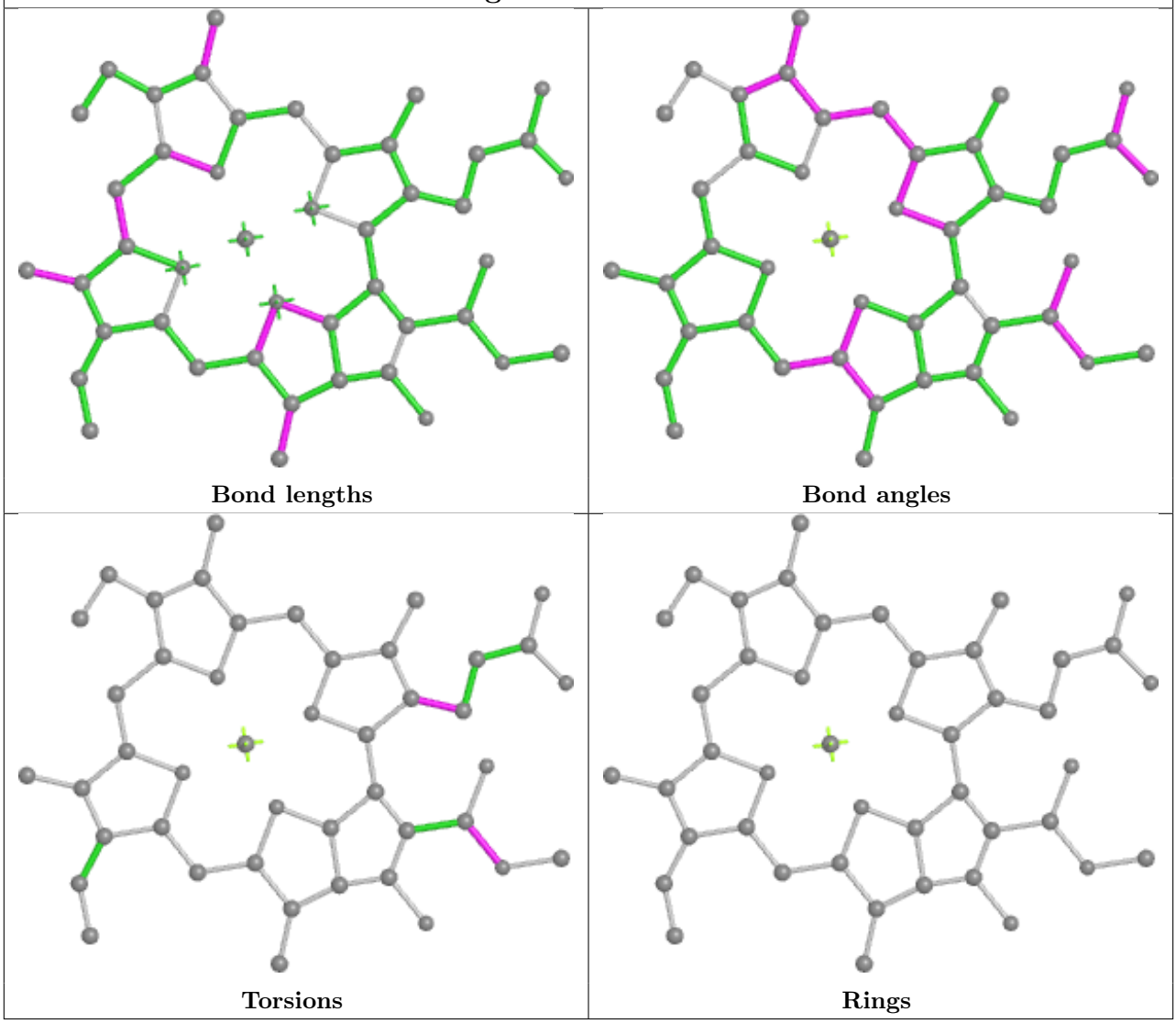


Rings

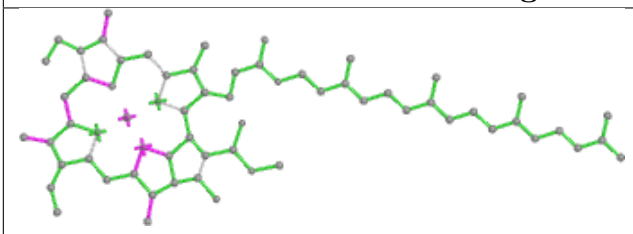
Ligand BCR 2 521



Ligand CLA 4 511



Ligand CLA e 1123



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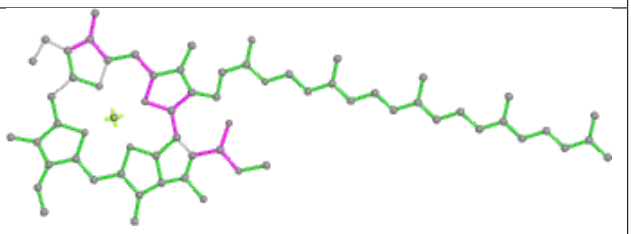
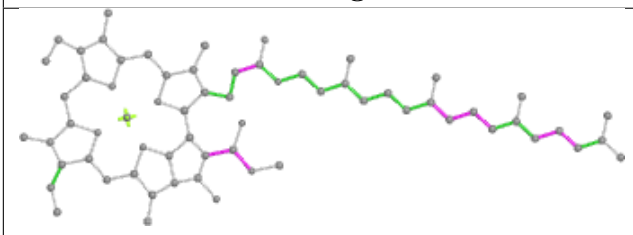


Bond angles



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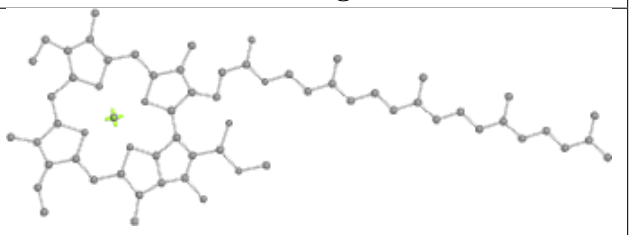
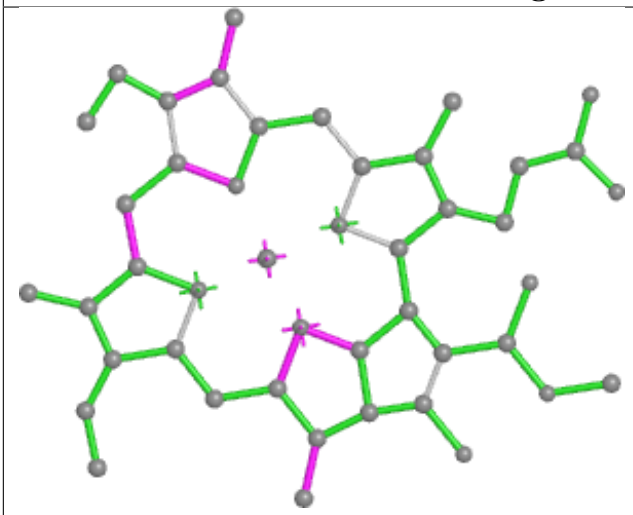


Rings

Ligand CLA r 512



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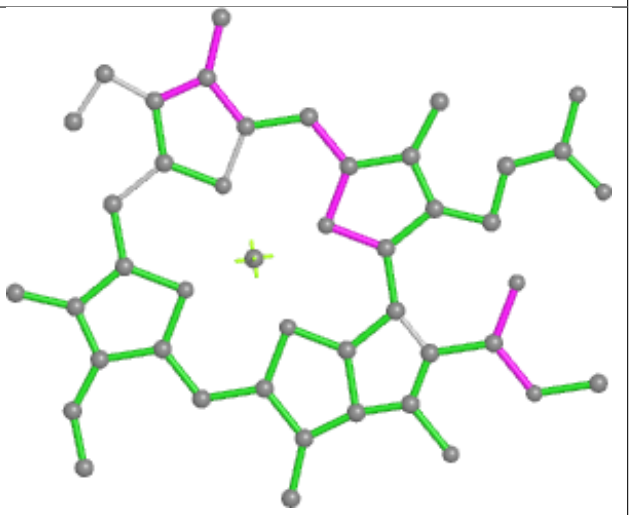
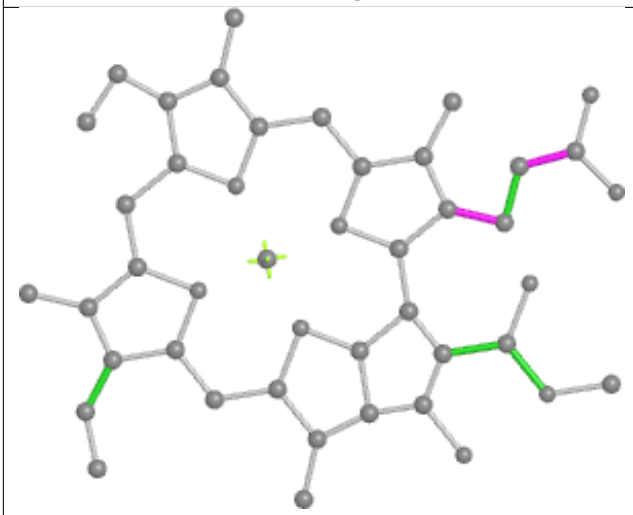


Bond angles



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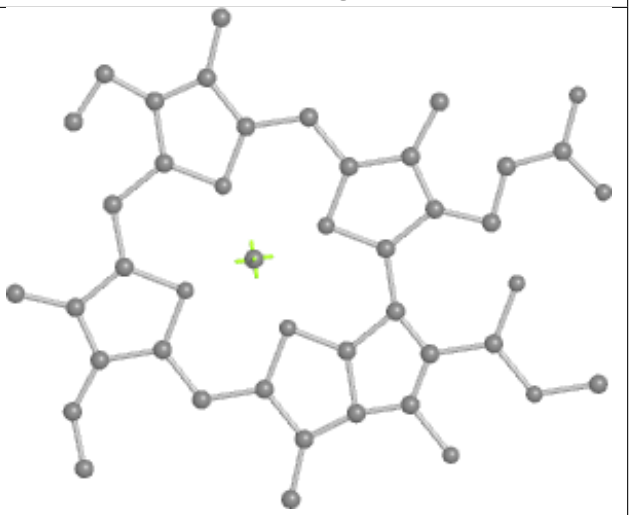
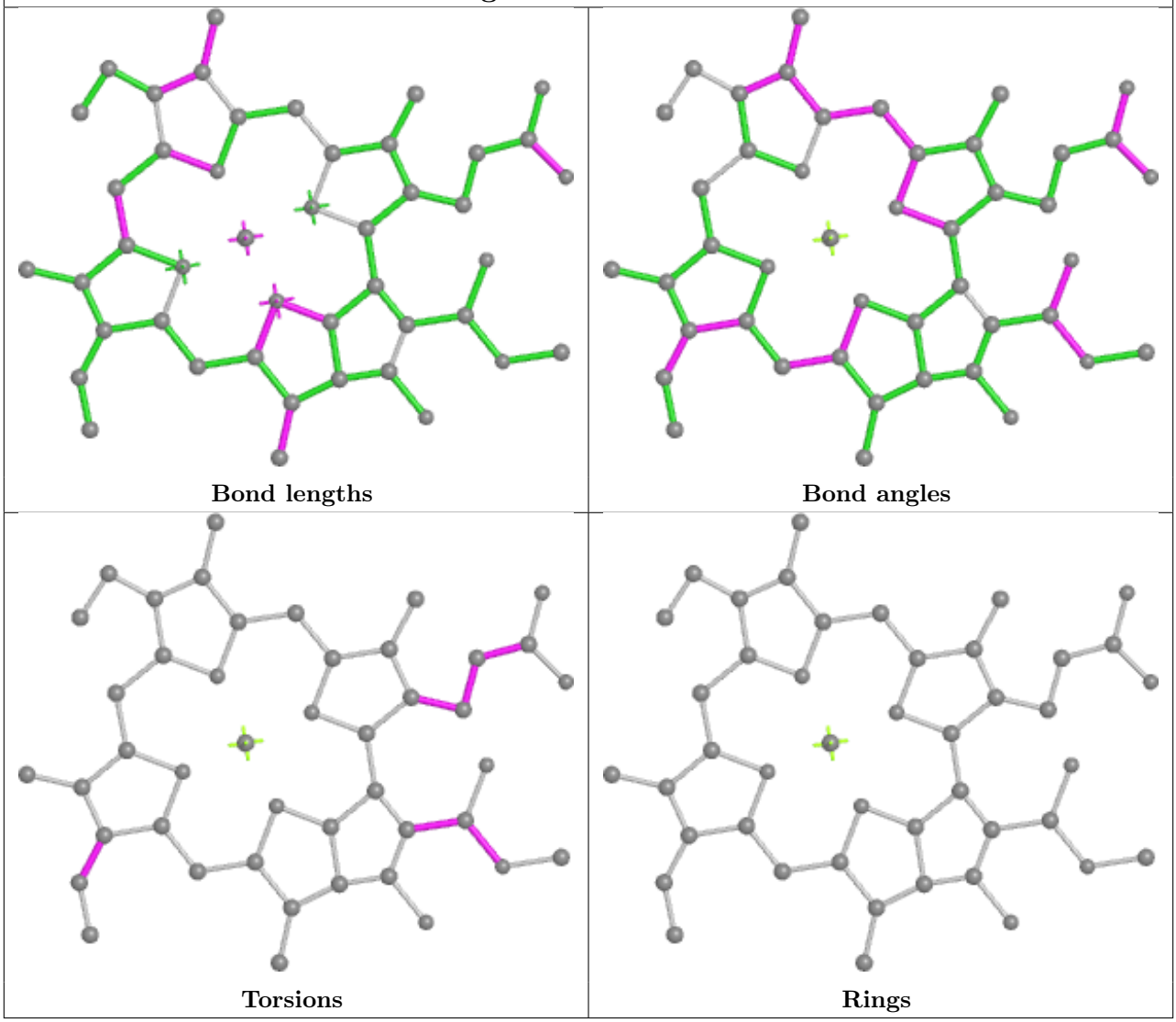
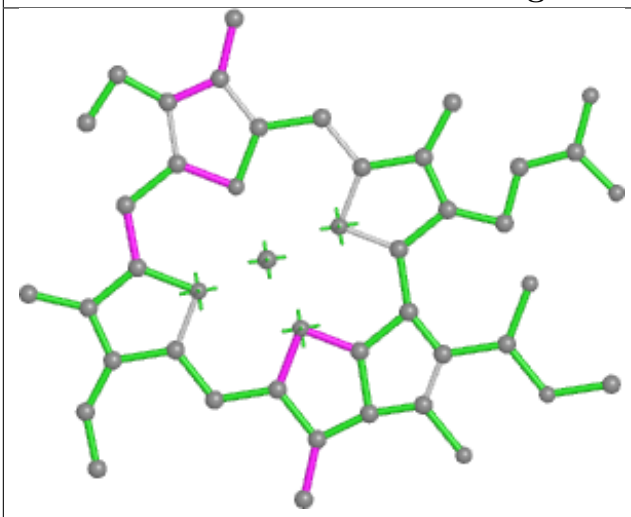


Rings

Ligand CLA Y 516



Ligand CLA d 507



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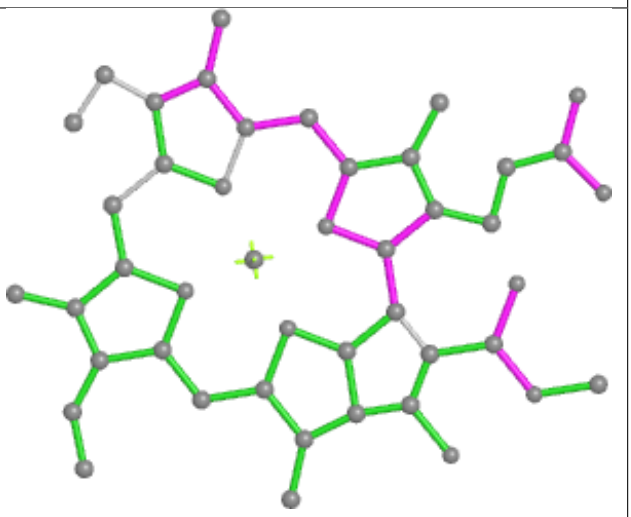
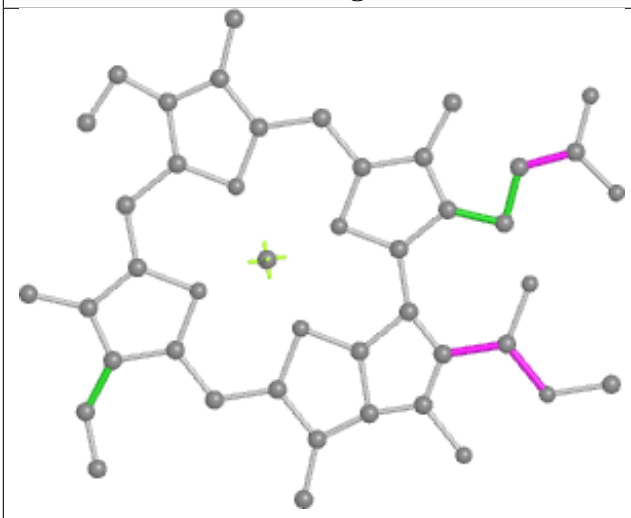


Bond angles



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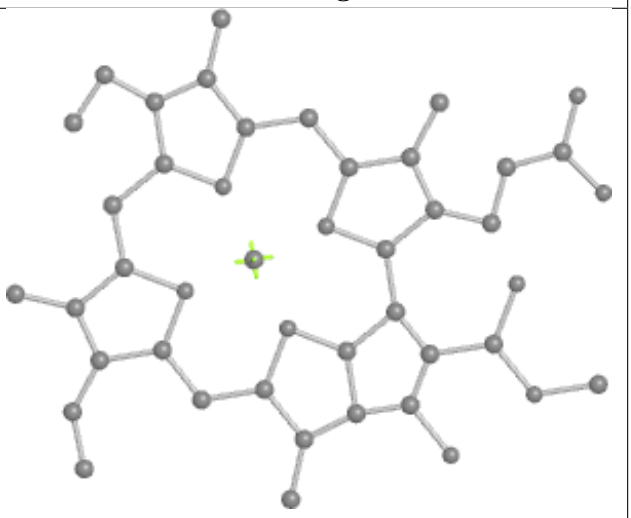
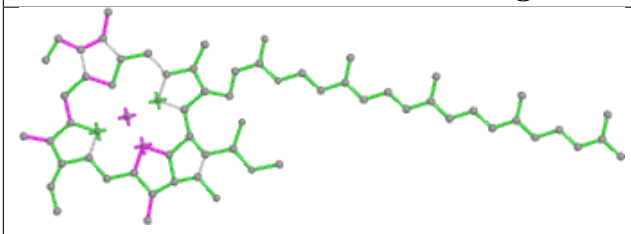


Rings

Ligand CLA A 1107



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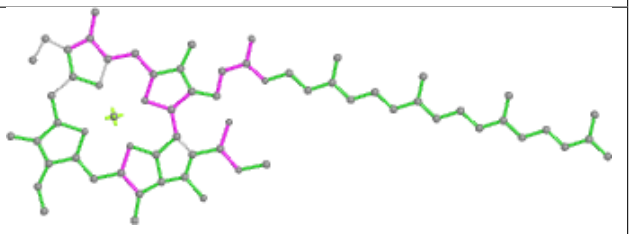

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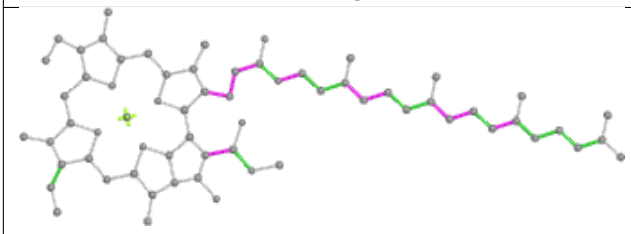

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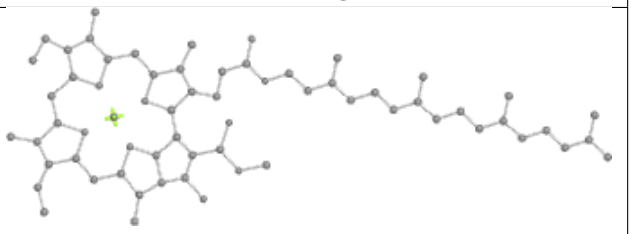
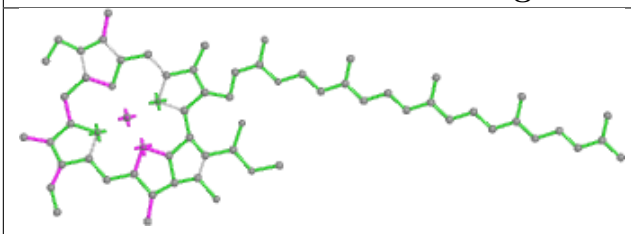


Rings

Ligand CLA G 1104



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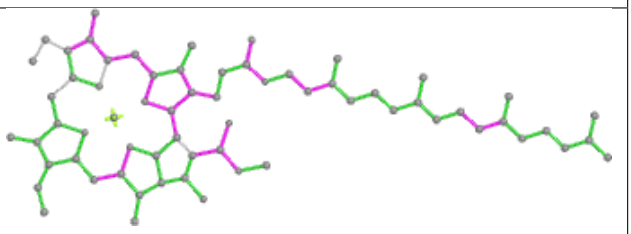

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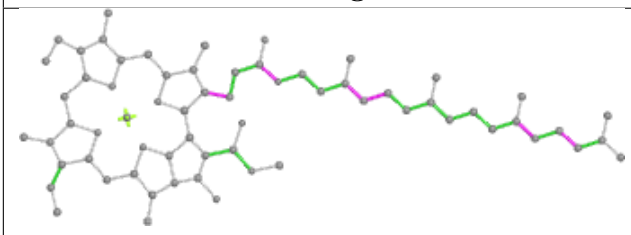

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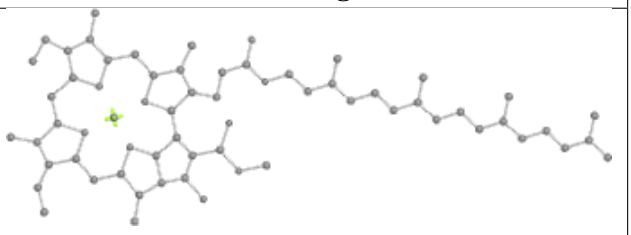
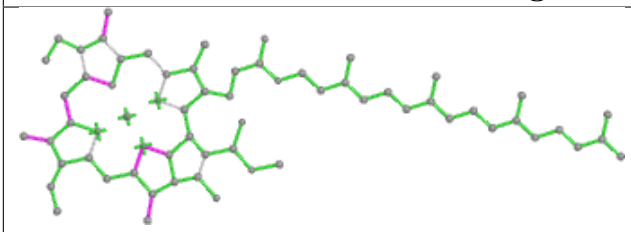


Rings

Ligand CLA 2 505



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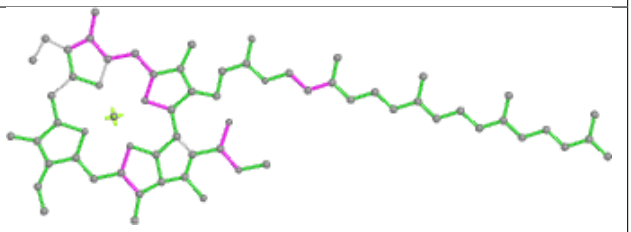
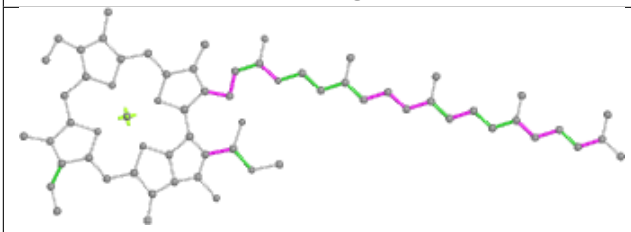


Bond angles



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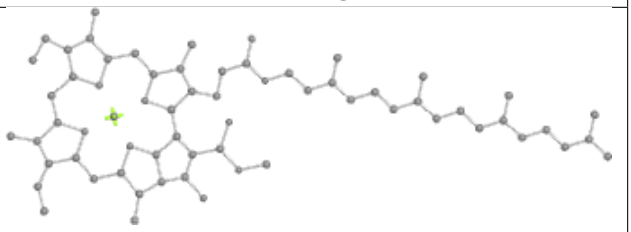

Rings

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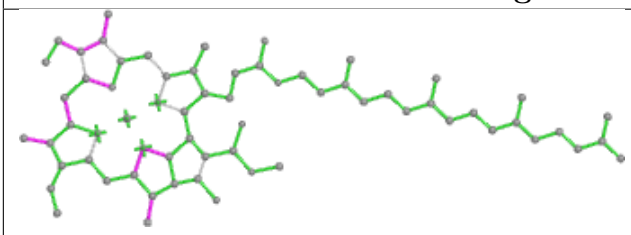

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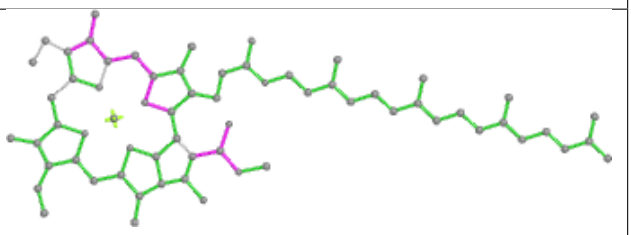

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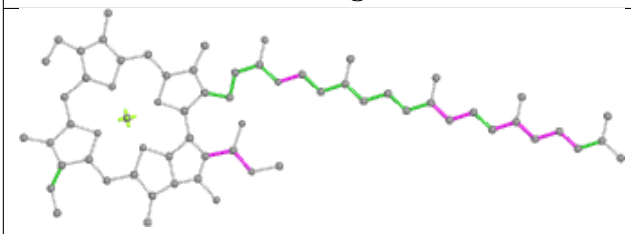

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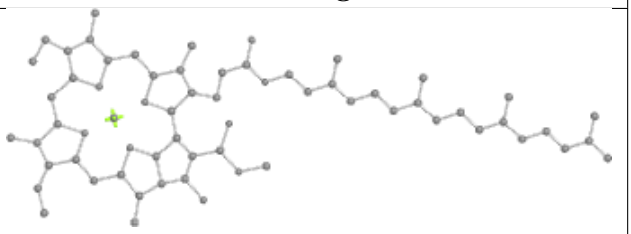
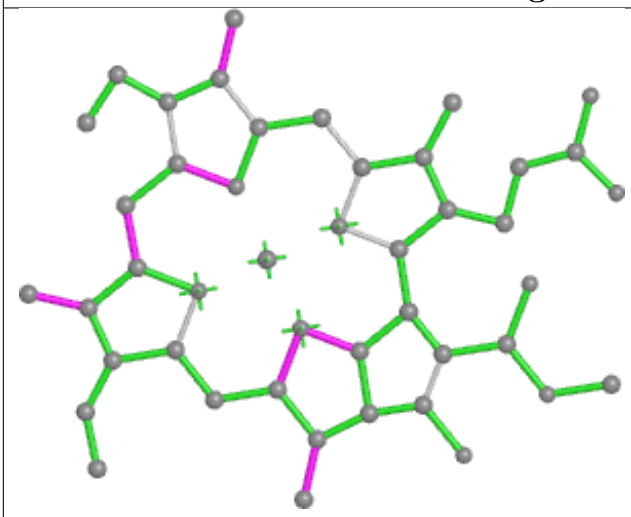


Rings

Ligand CLA 5 506



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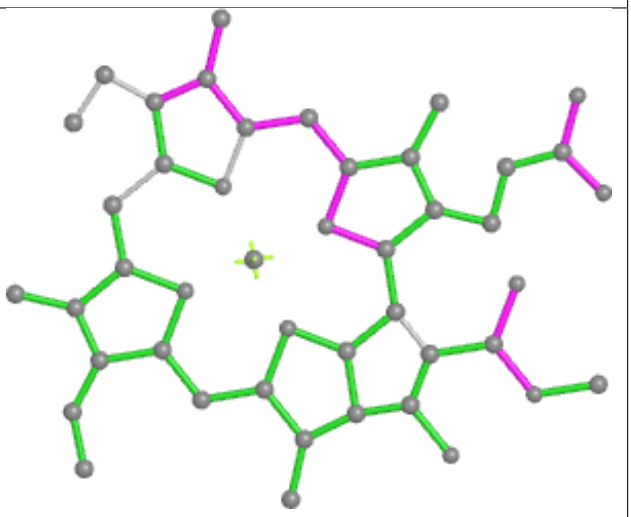

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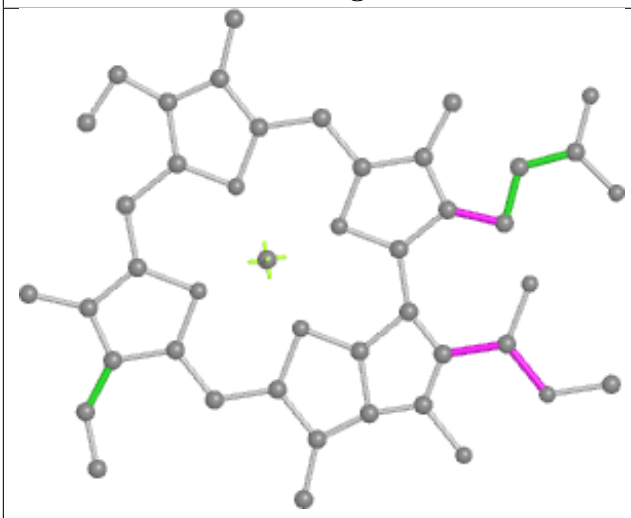

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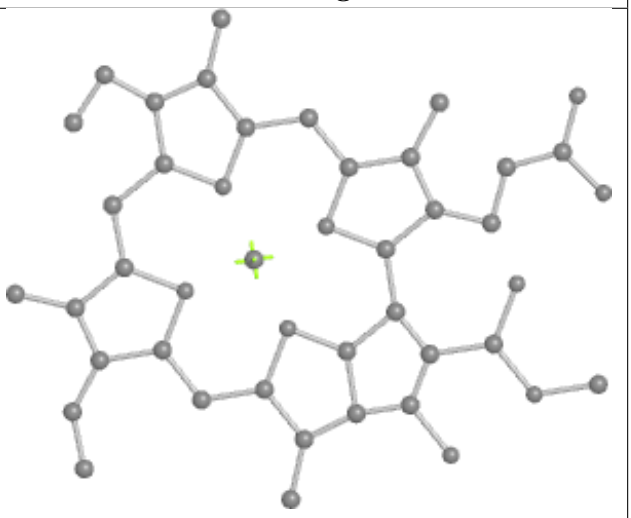

Rings

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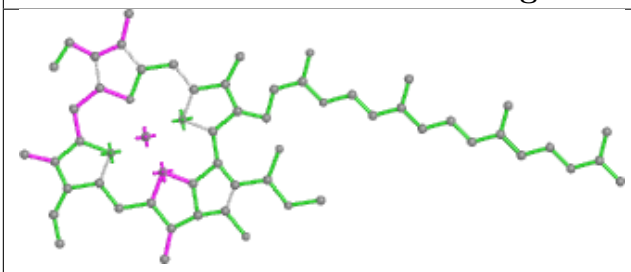

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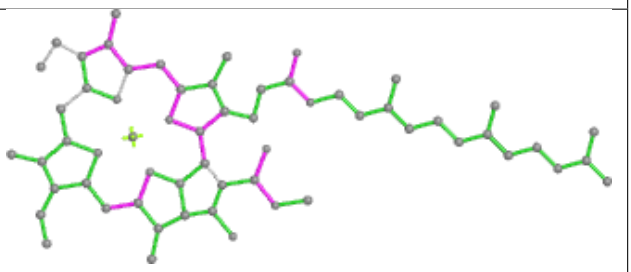

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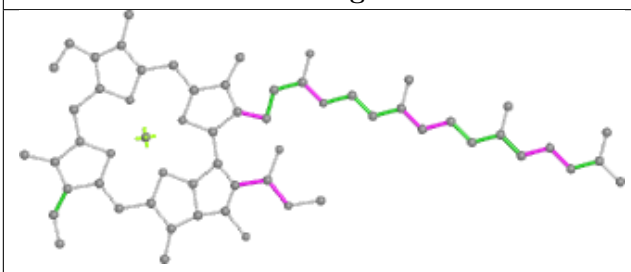

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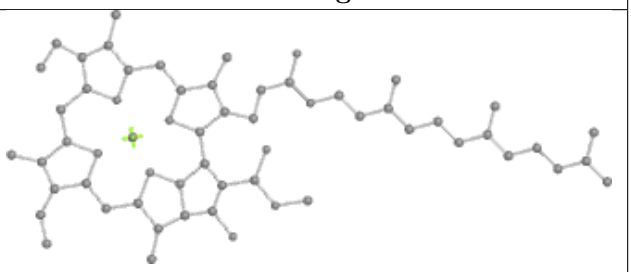
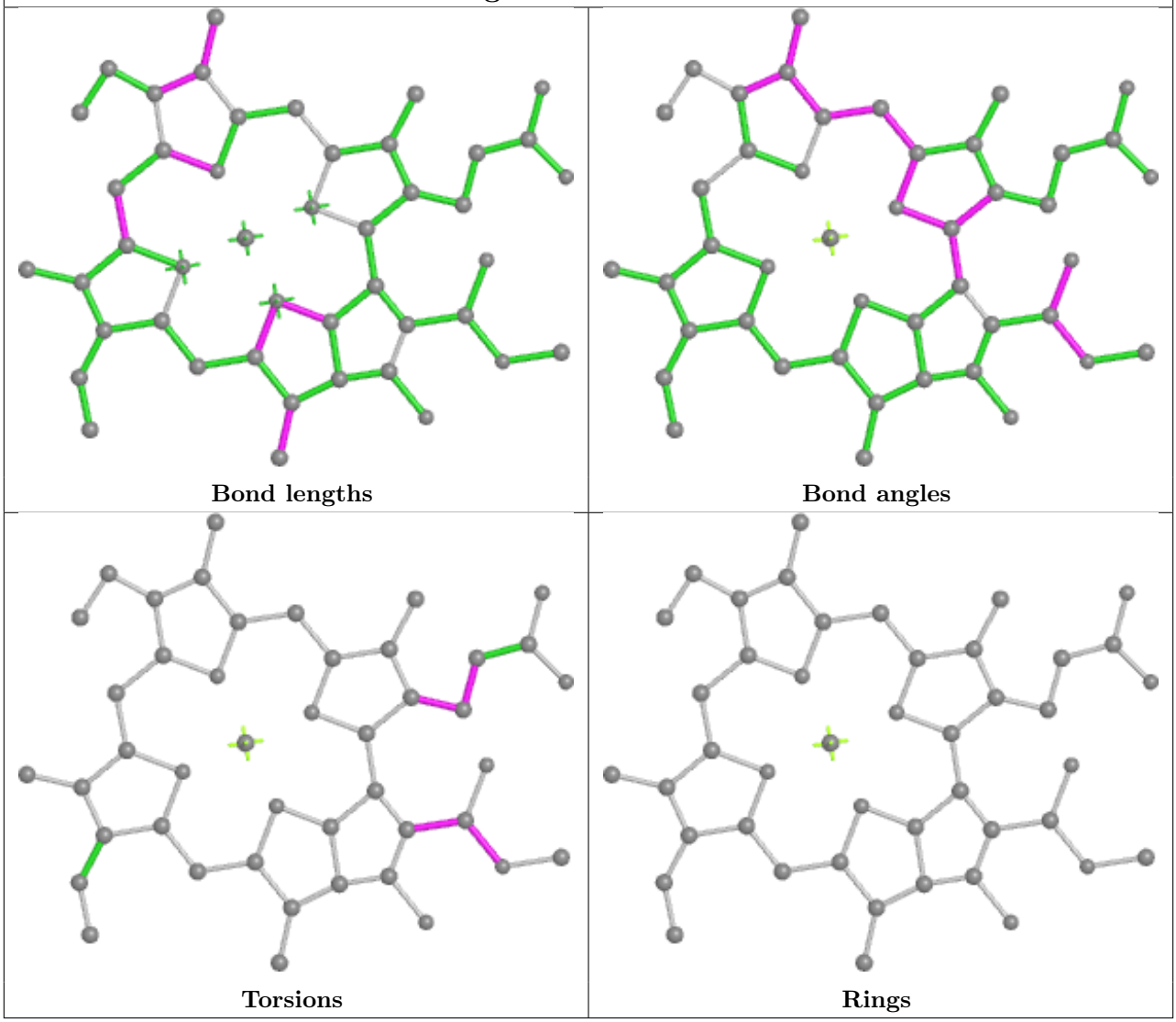
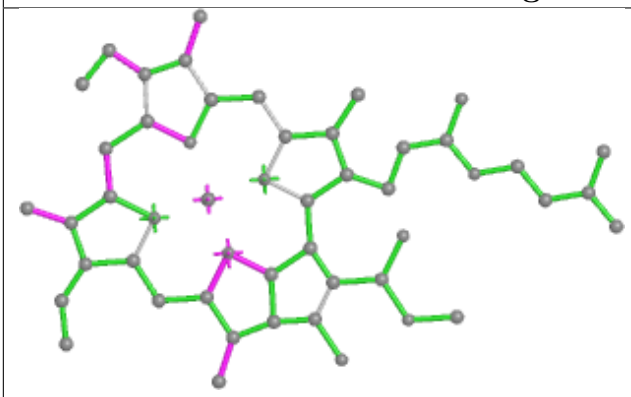
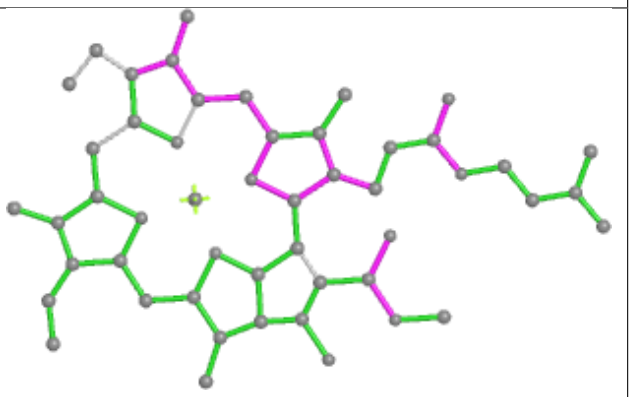
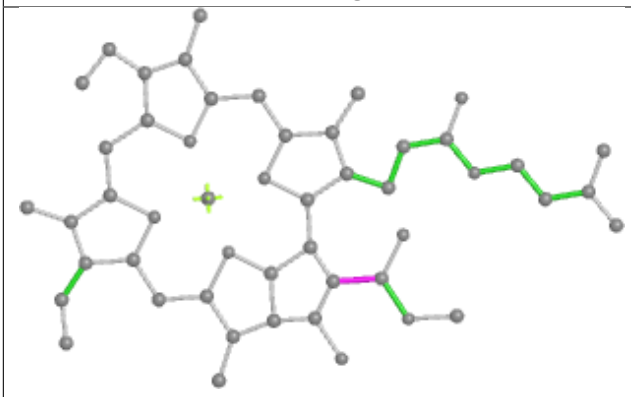
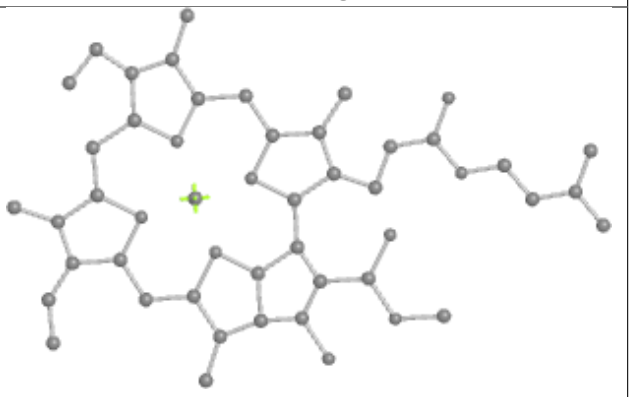


Rings

Ligand CLA u 502



Ligand CLA f 1222	
 Bond lengths	 Bond angles
 Torsions	 Rings

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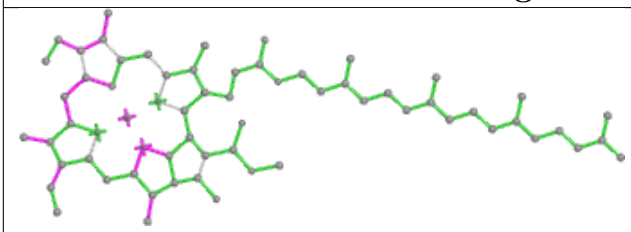
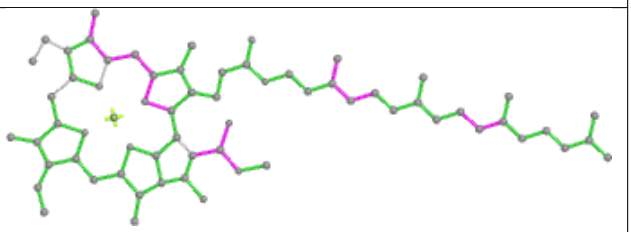
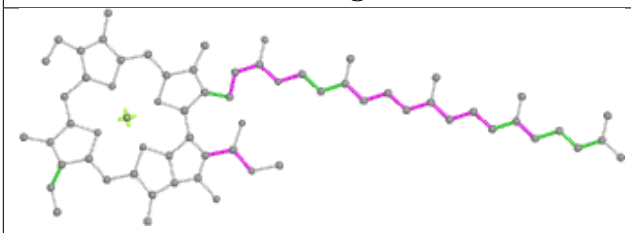
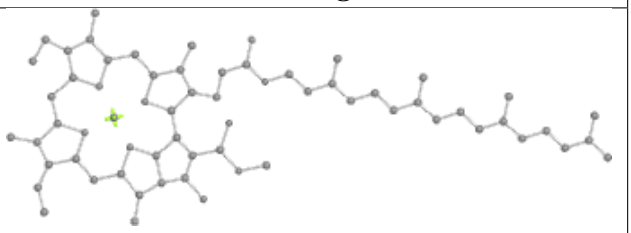
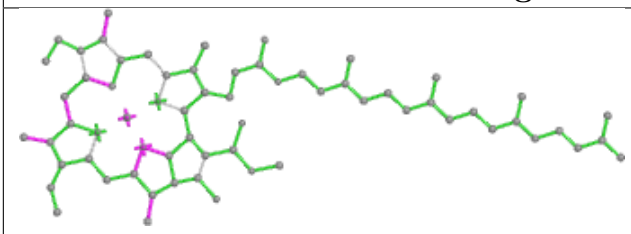
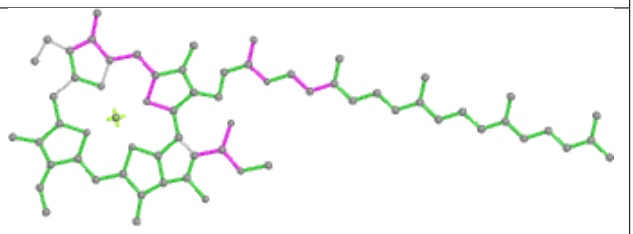
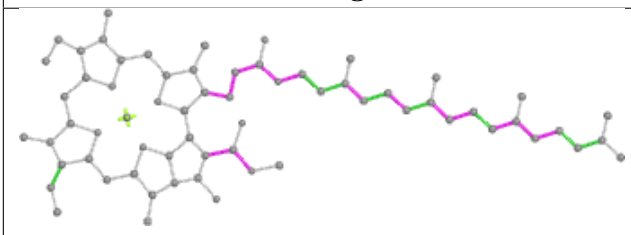
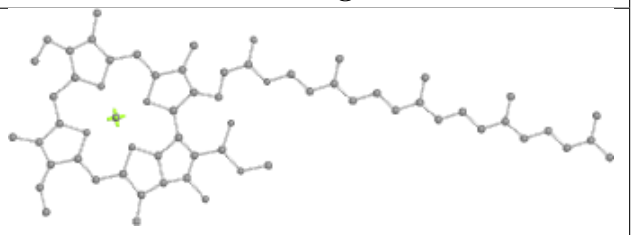
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1106	
 Bond lengths	 Bond angles
 Torsions	 Rings

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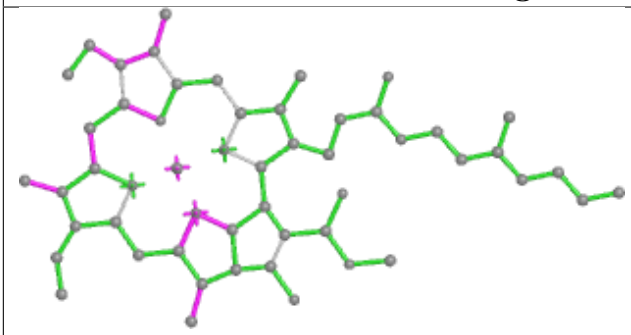
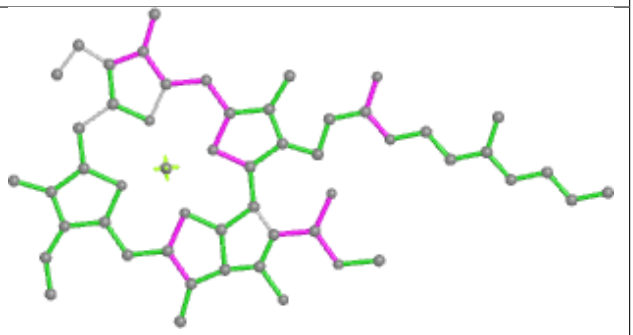
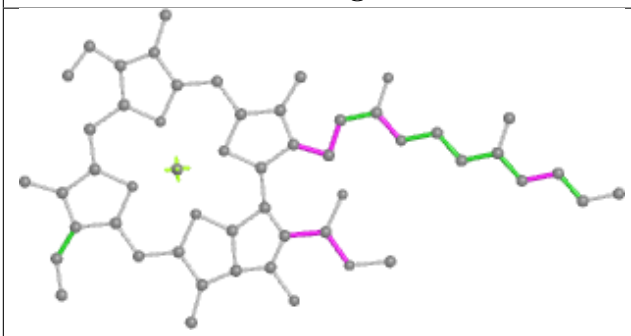
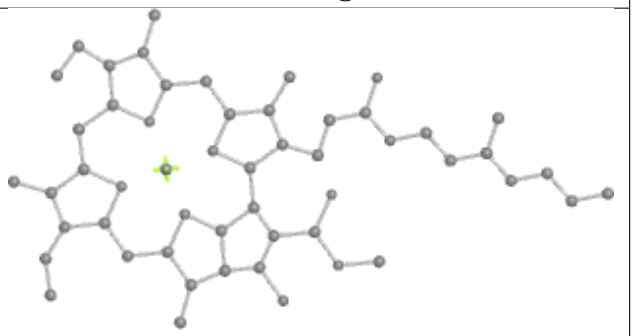
 Bond lengths	 Bond angles
 Torsions	 Rings

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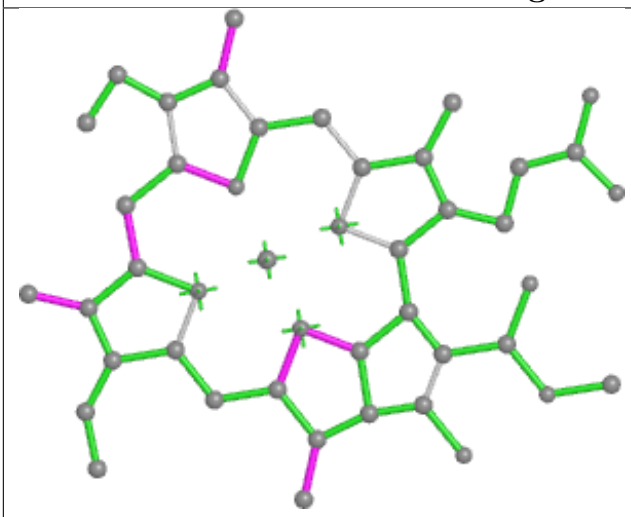

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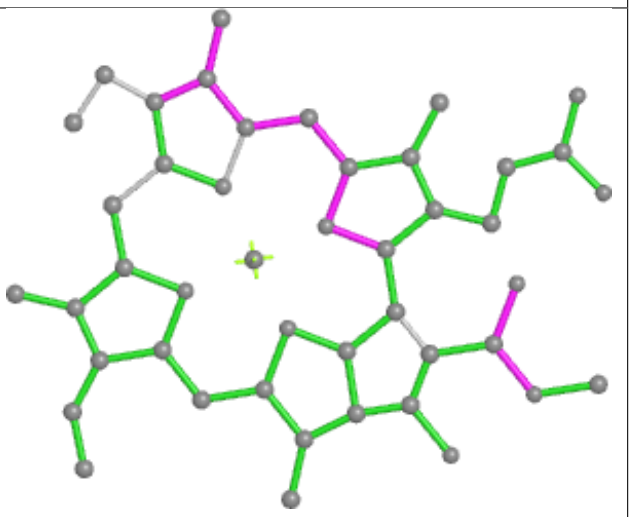

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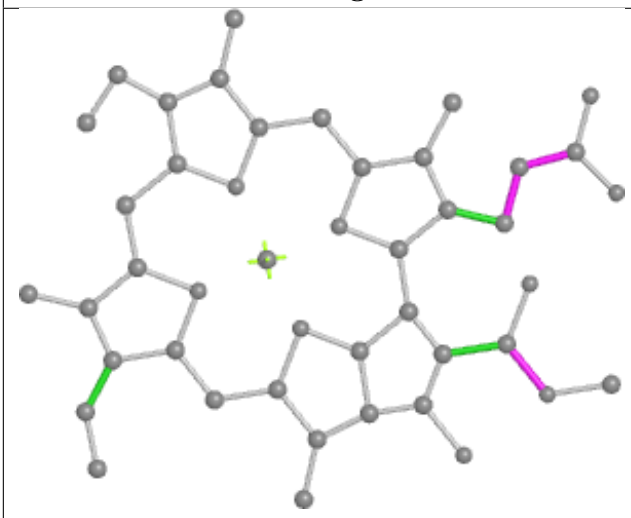

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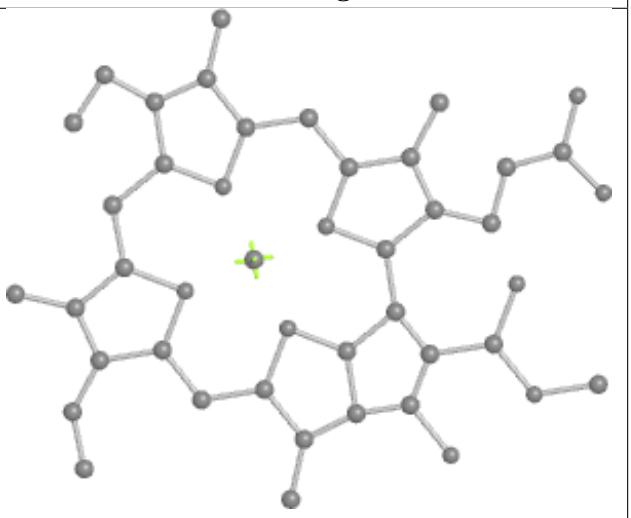

Rings

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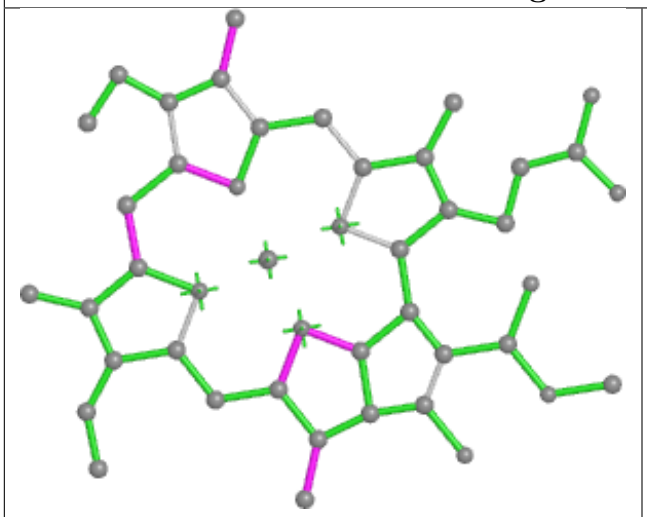

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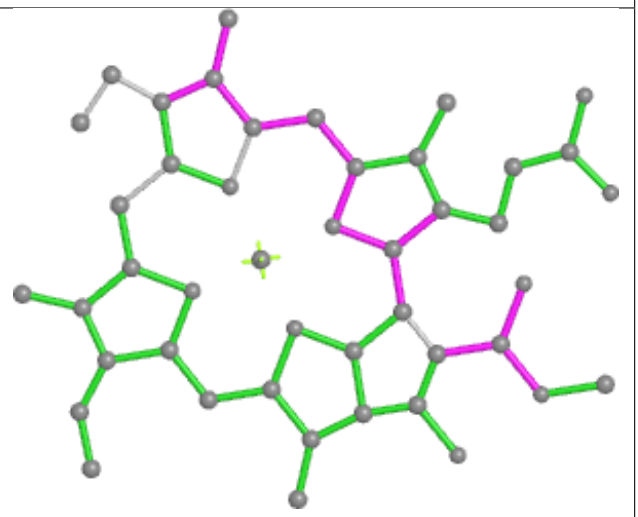

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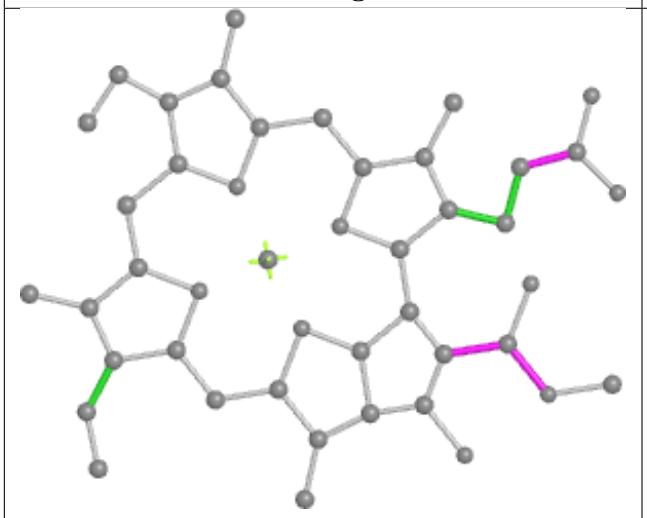

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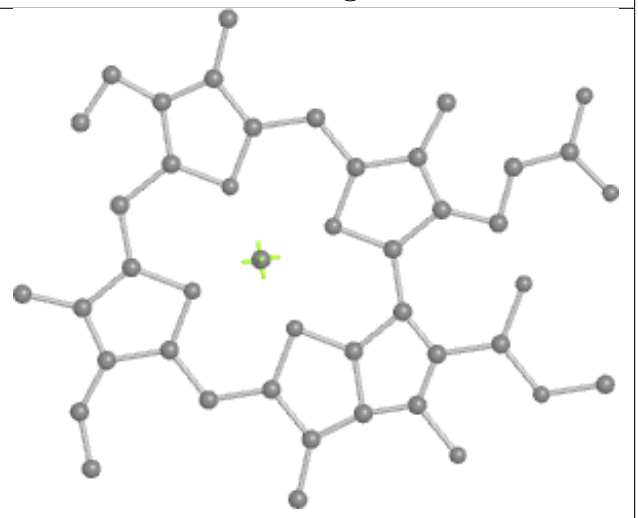

Rings

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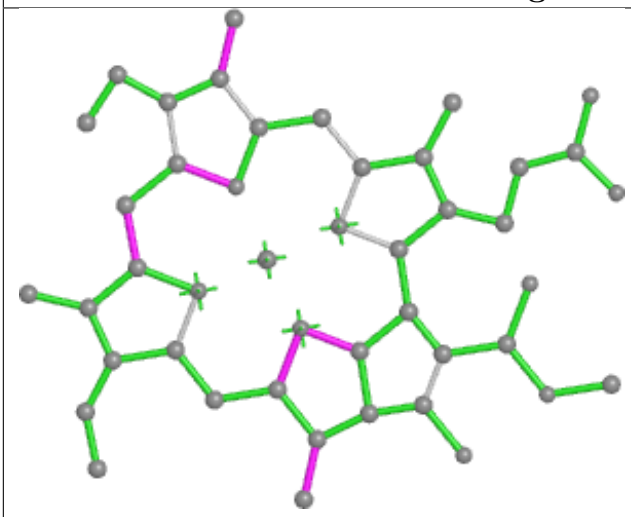

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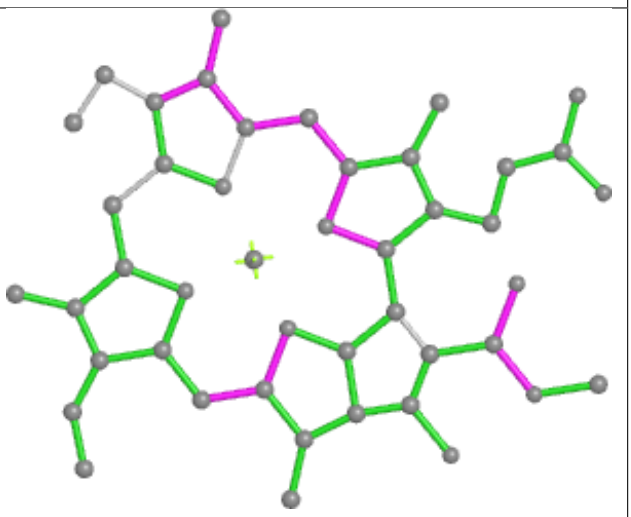

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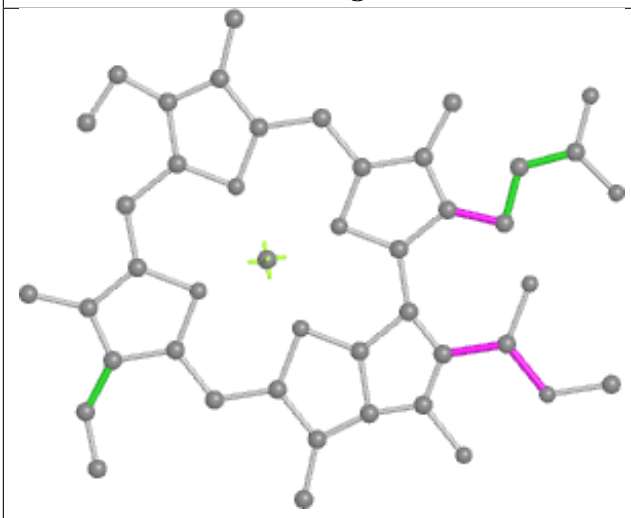

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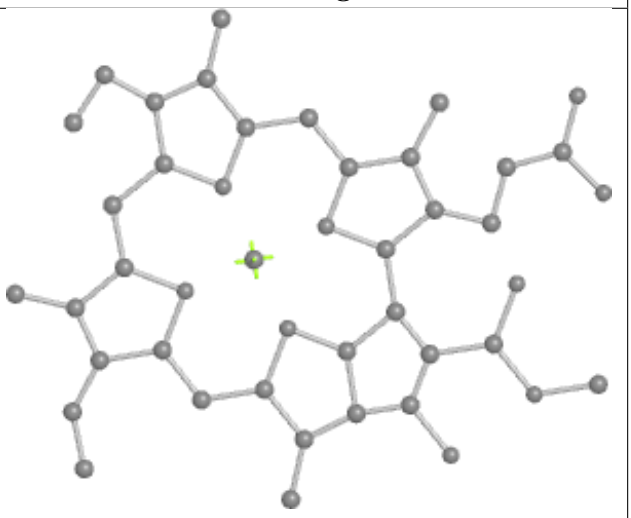
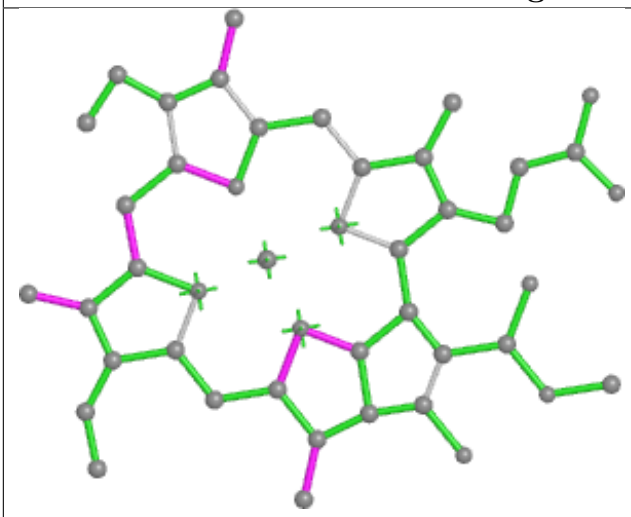


Rings

Ligand CLA b 506



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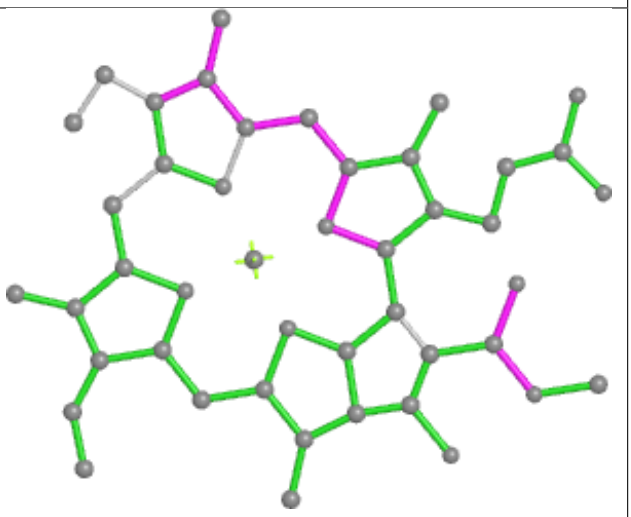

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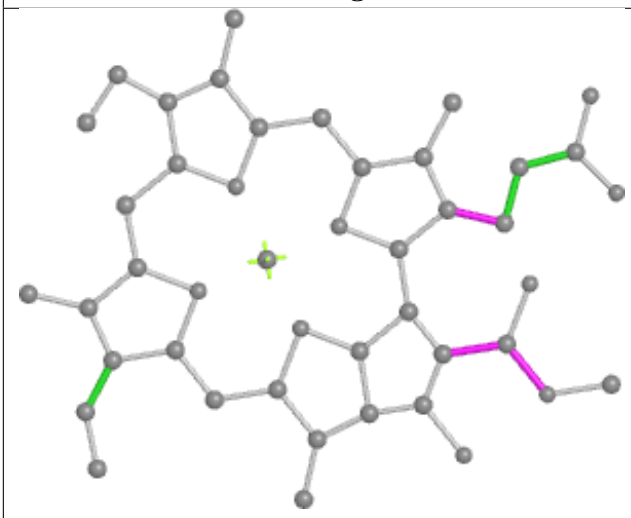

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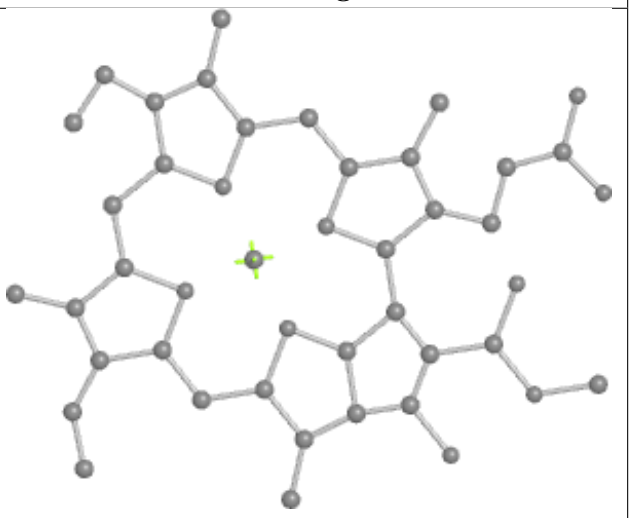
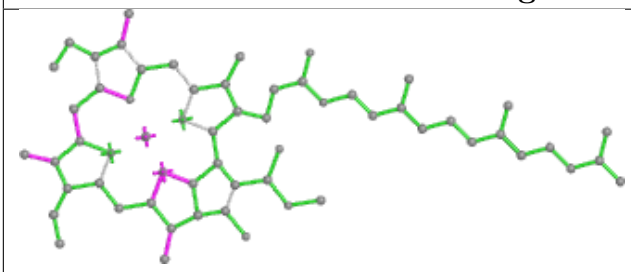


Rings

Ligand CLA n 1503



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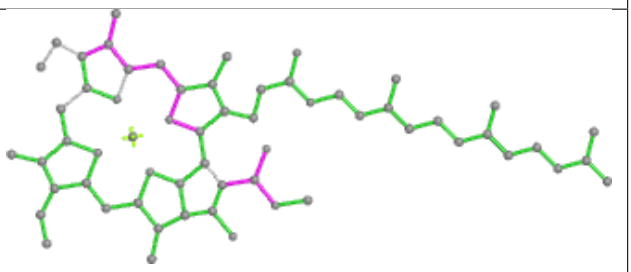

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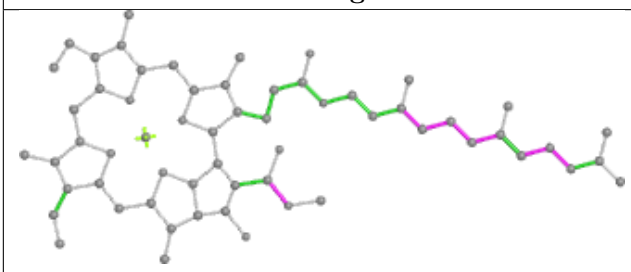

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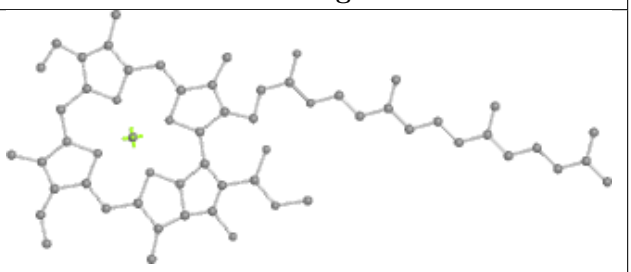
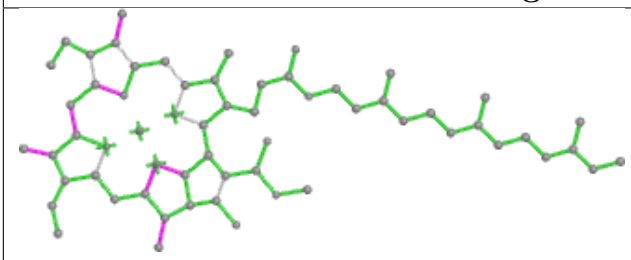


Rings

Ligand CLA f 1213



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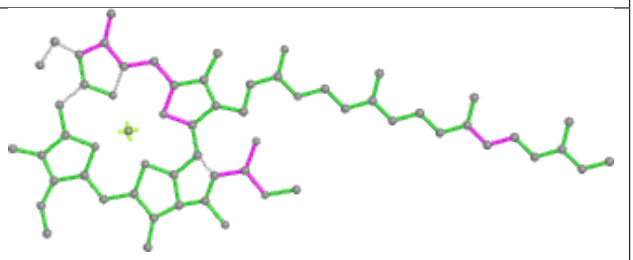

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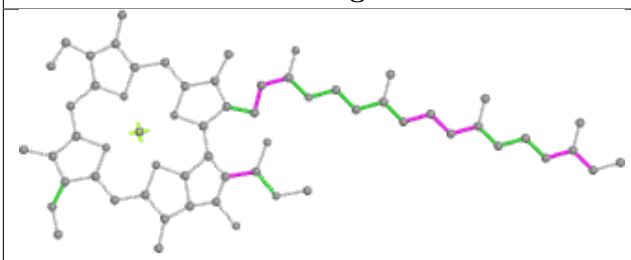

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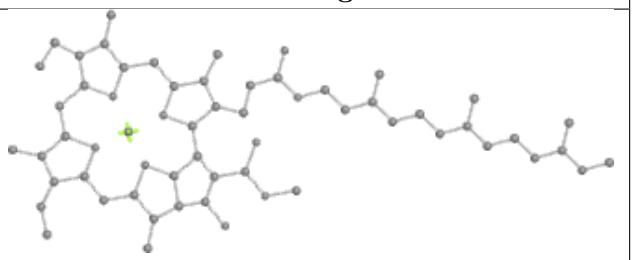
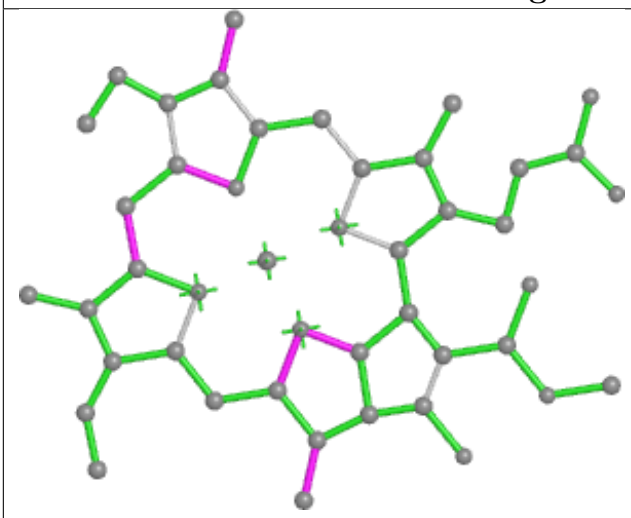


Rings

Ligand CLA c 516



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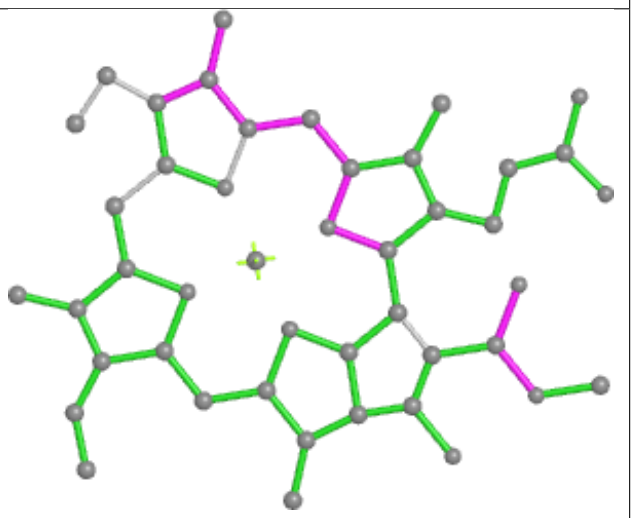

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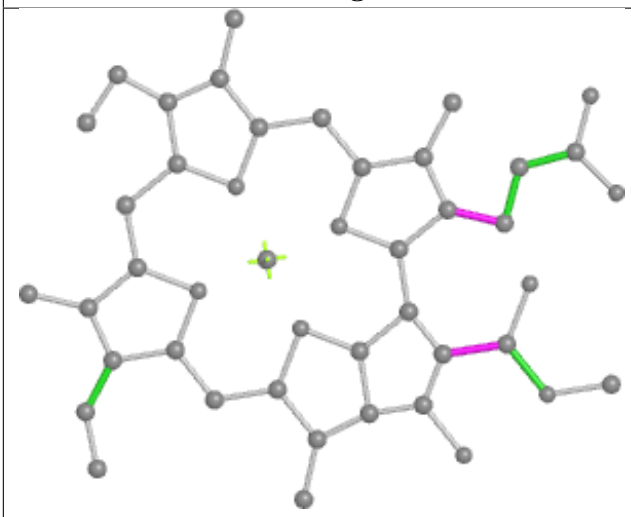

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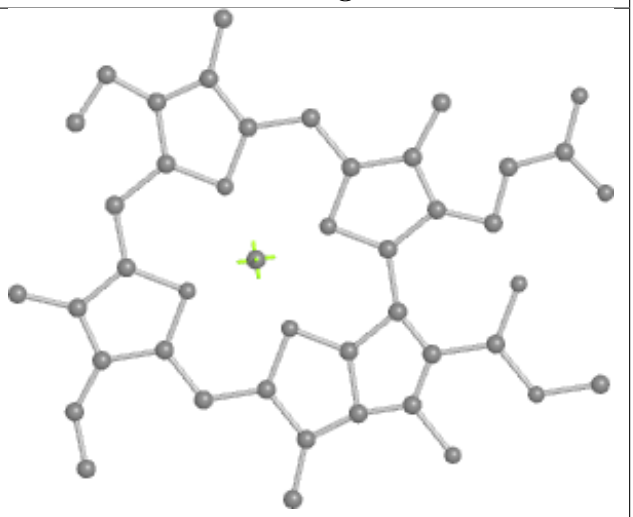

Rings

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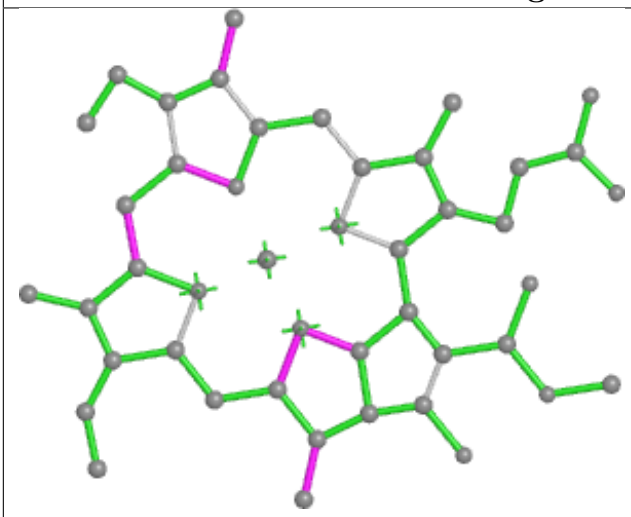

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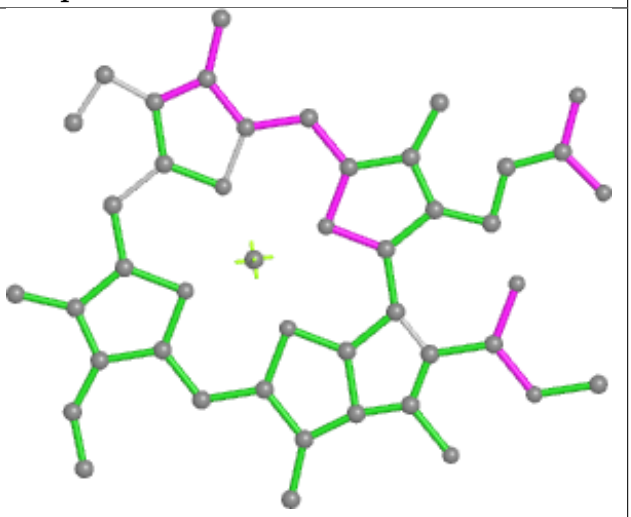

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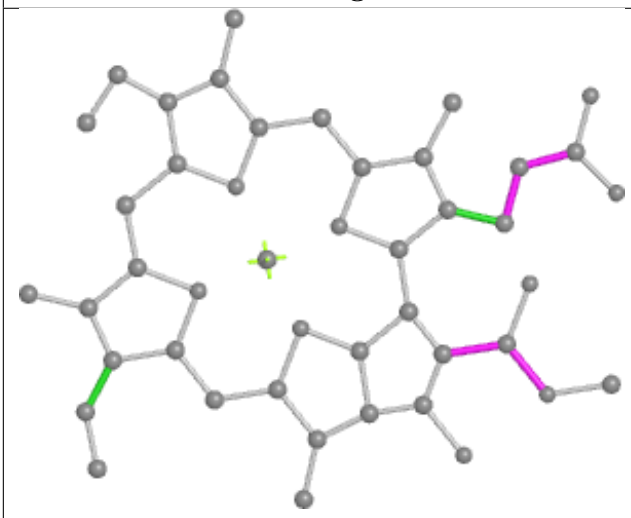

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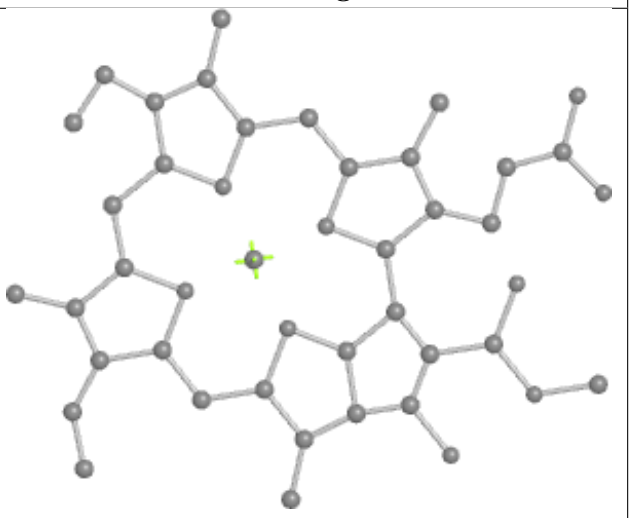

Rings

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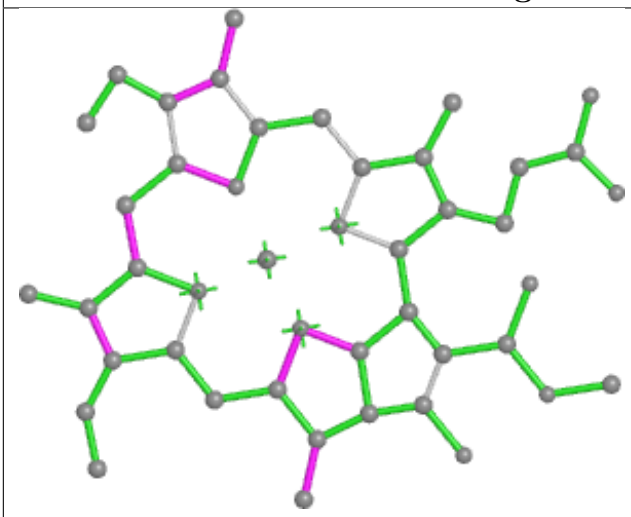

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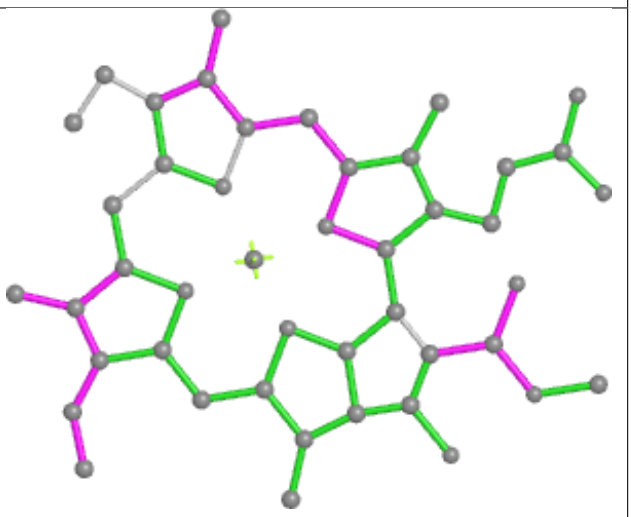

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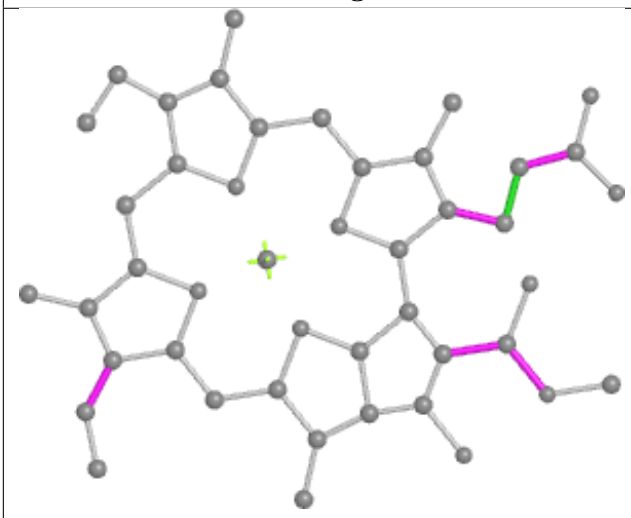

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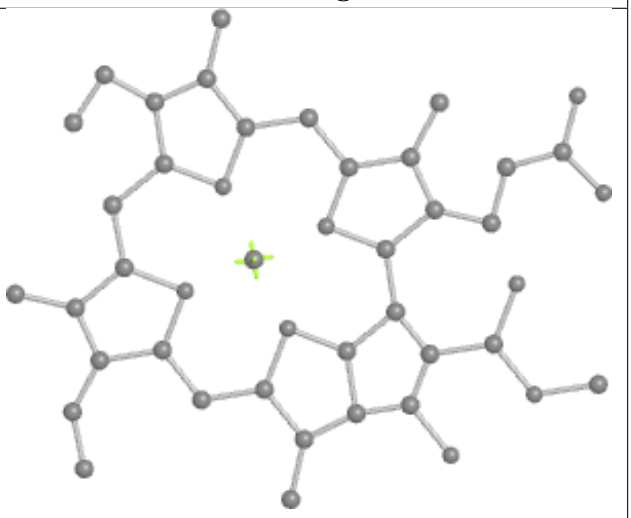

Rings

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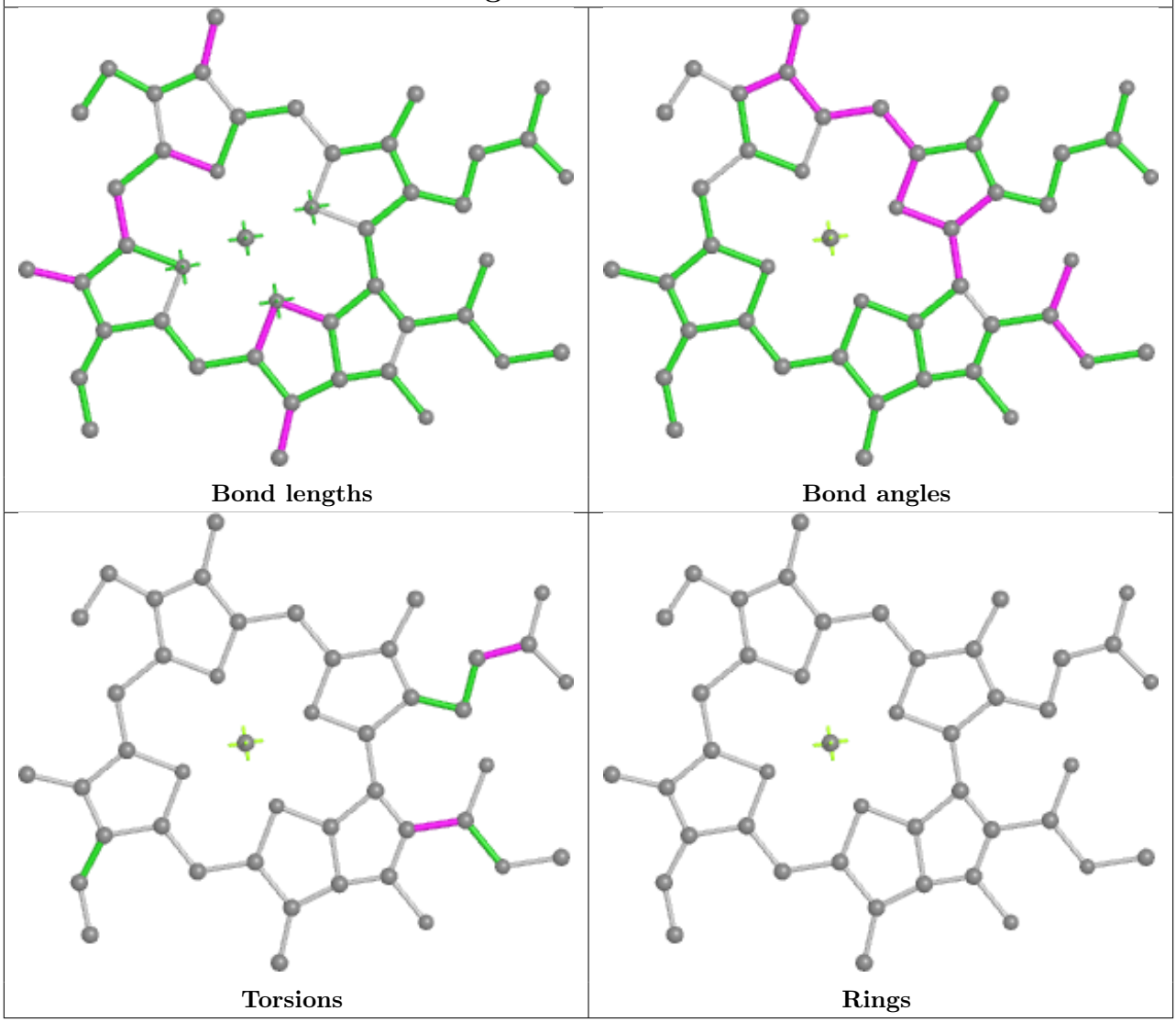
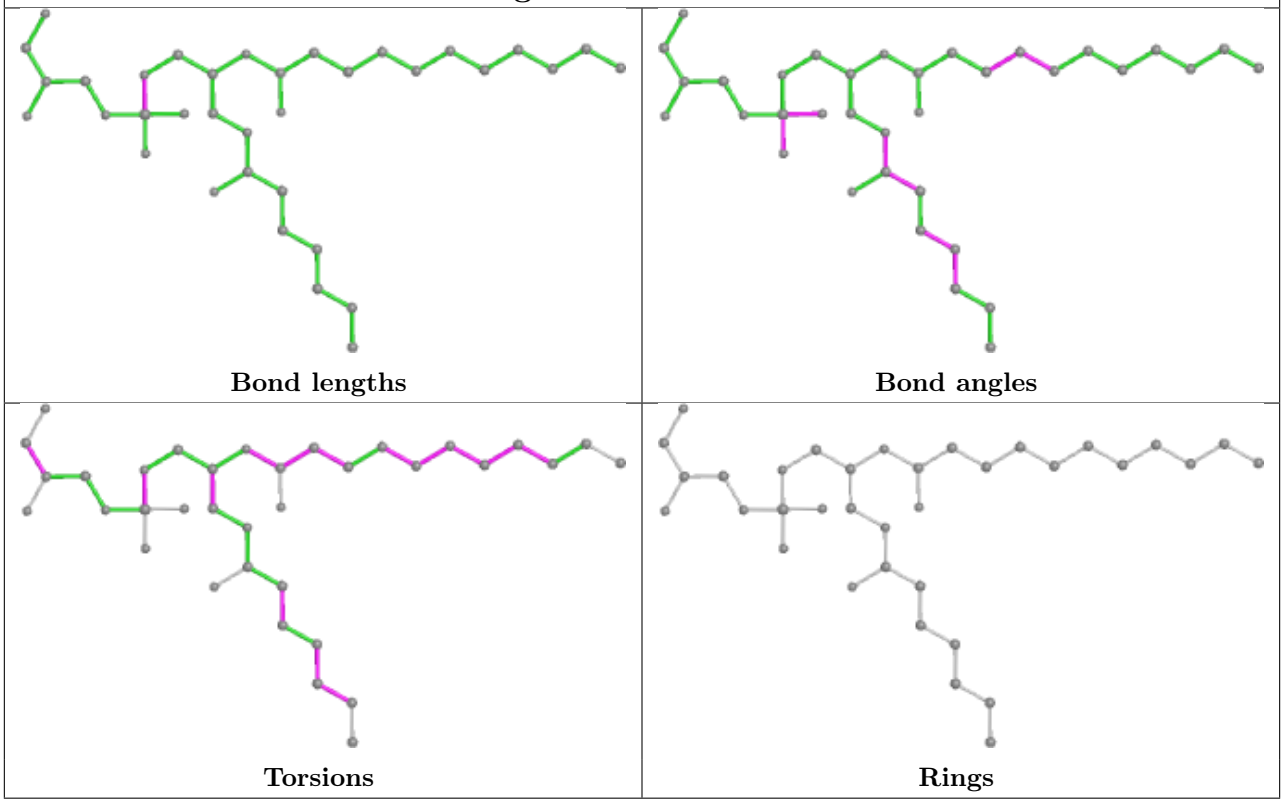


Ligand LHG A 5008



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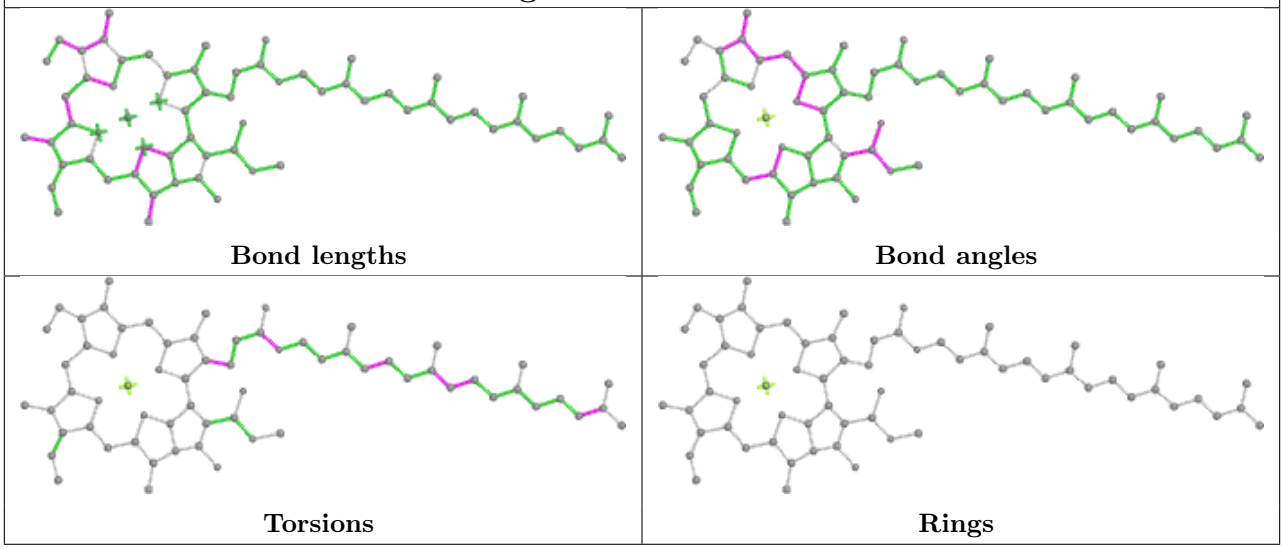
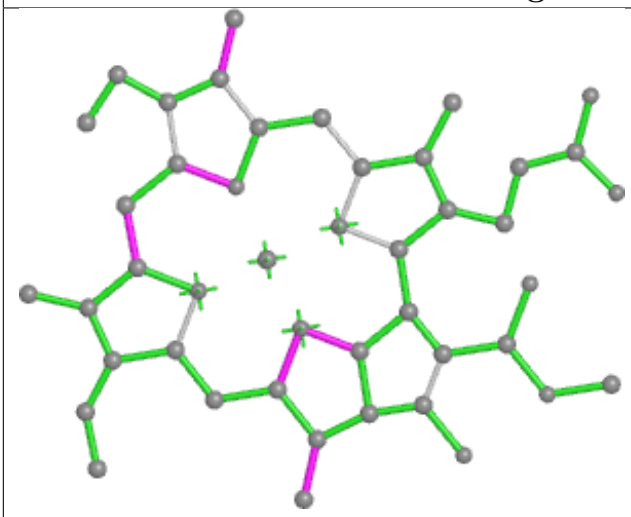


Ligand CLA b 513



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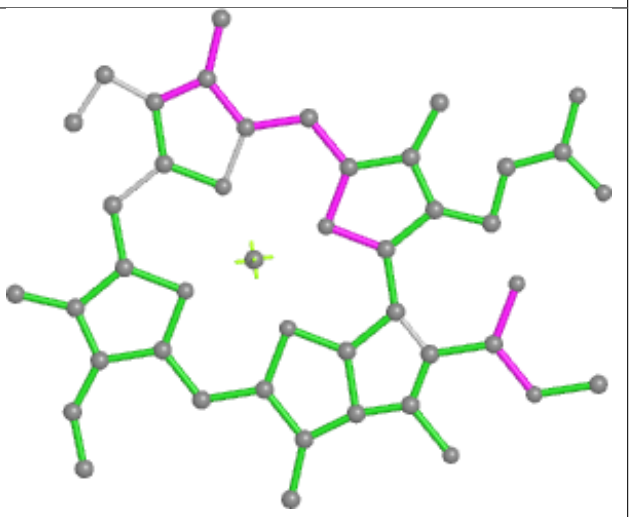
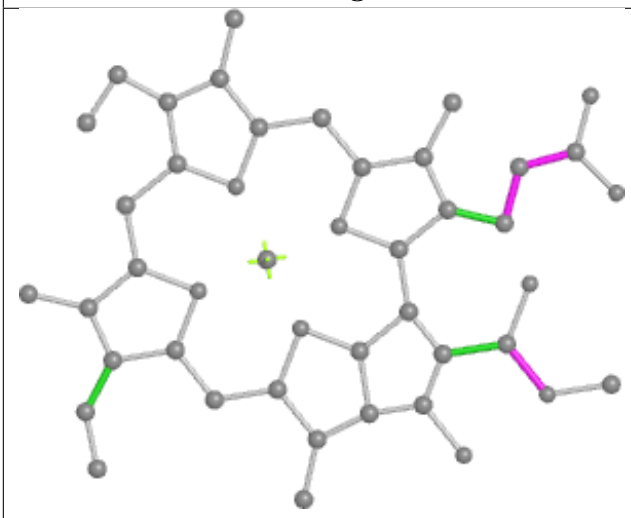


Bond angles



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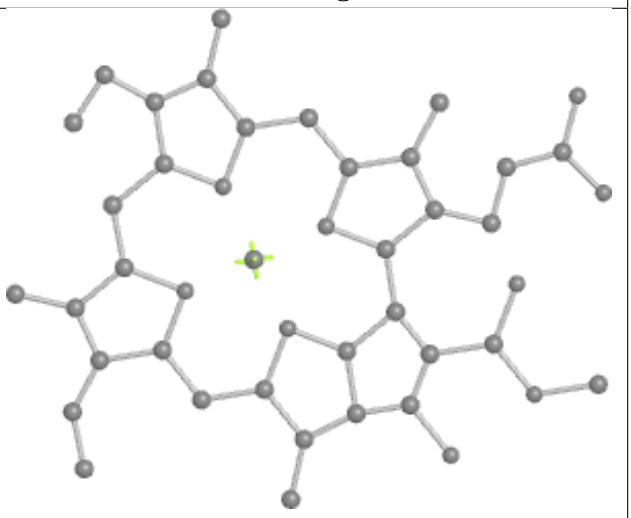
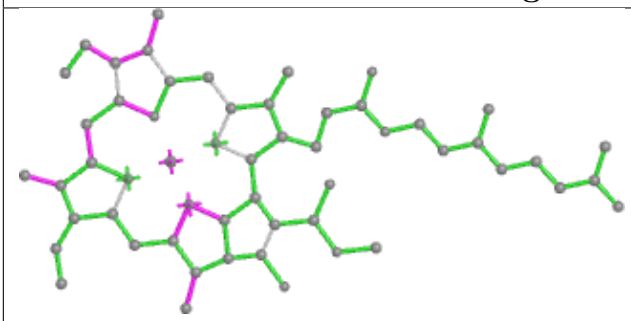
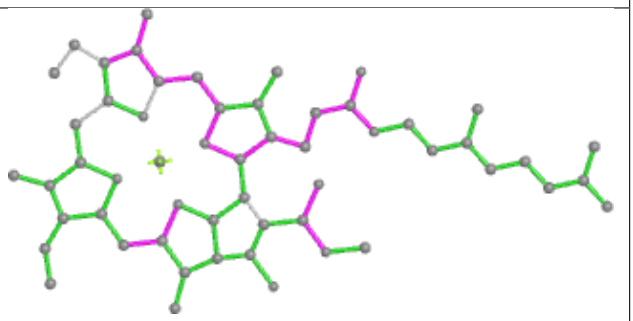
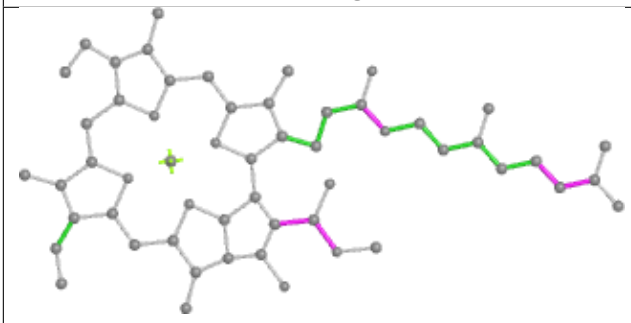
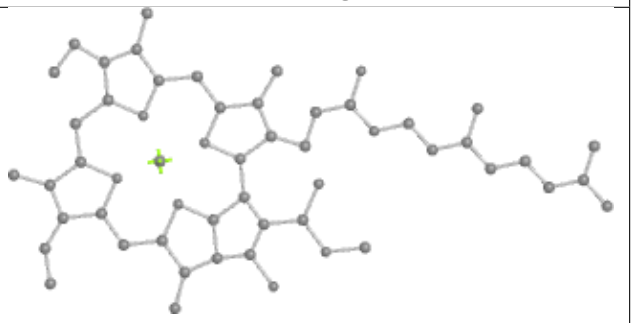
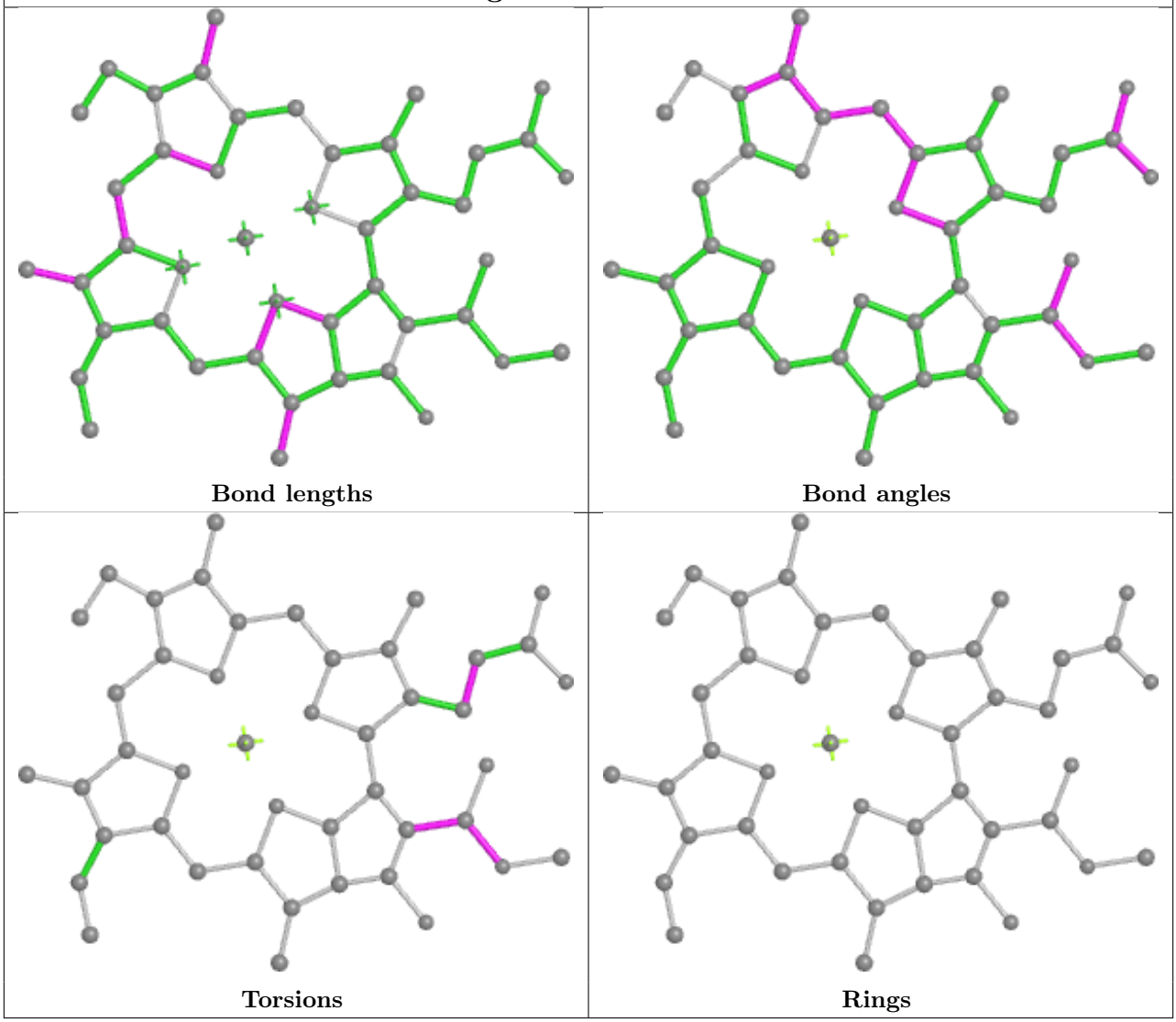


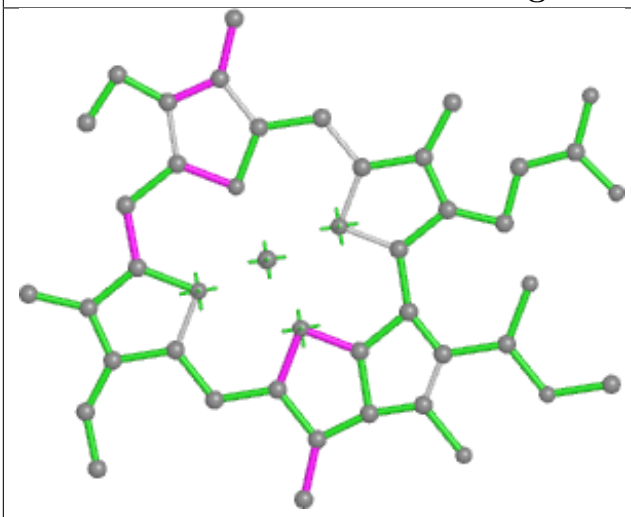
Rings

Ligand CLA f 1220	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 517



Ligand CLA 2 516



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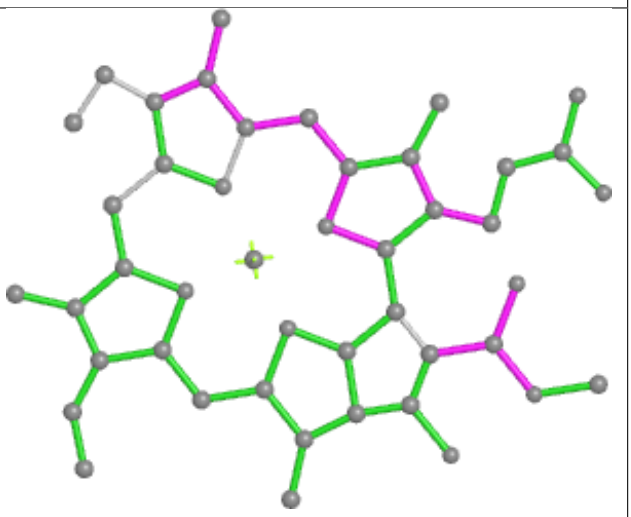

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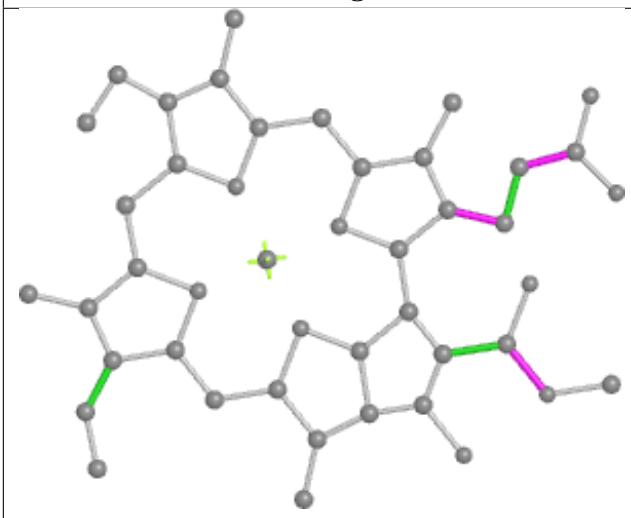

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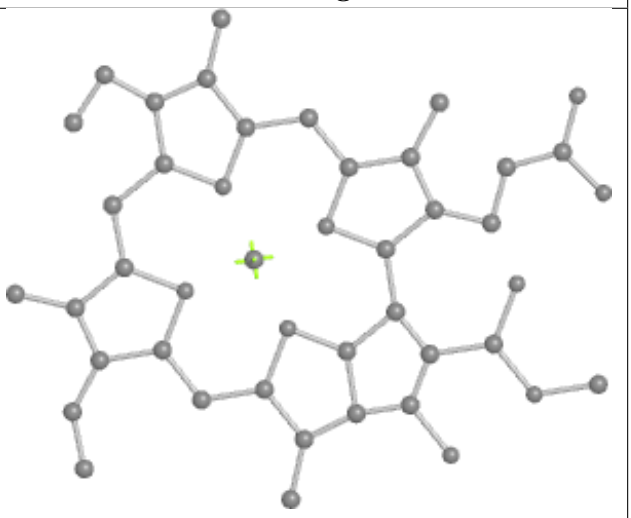
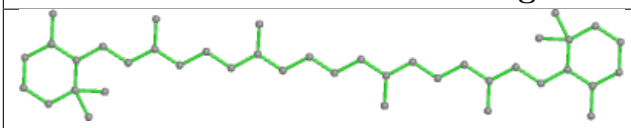


Rings

Ligand BCR e 4007



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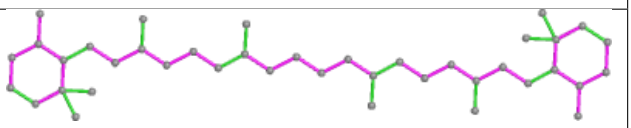

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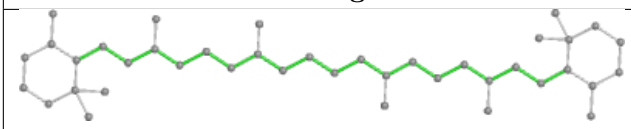
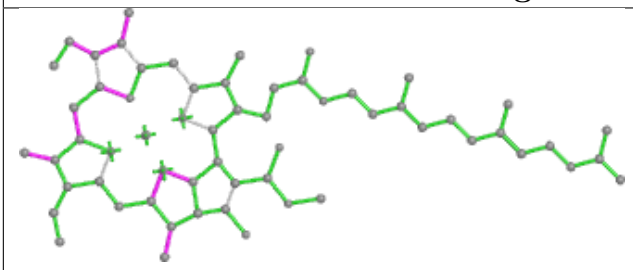


Torsions

Rings

Ligand CLA G 1137



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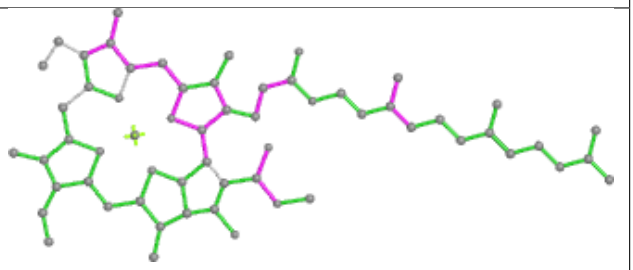

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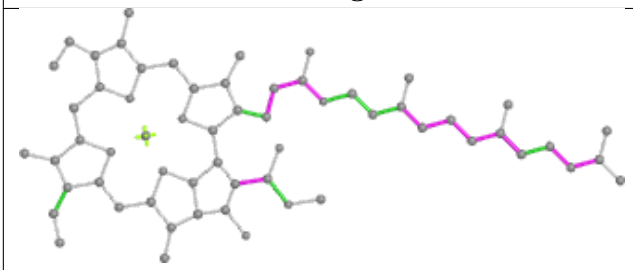

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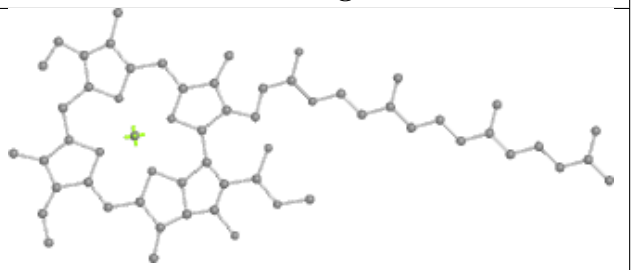
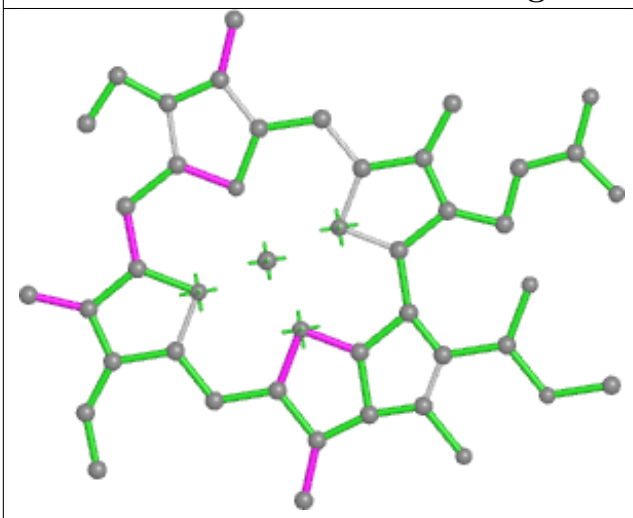


Rings

Ligand CLA q 513



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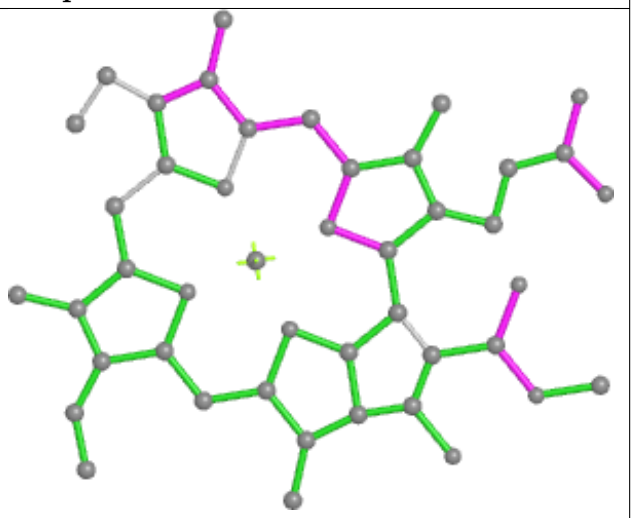

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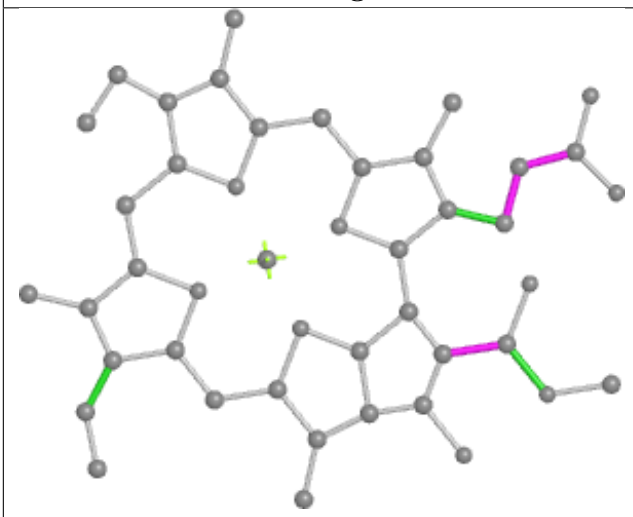

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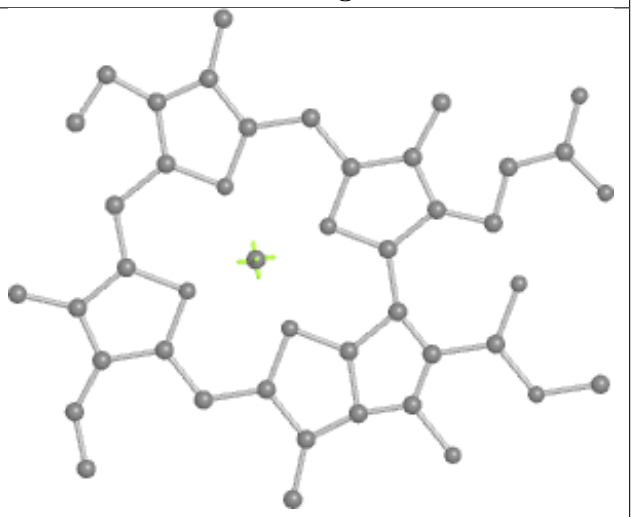

Rings

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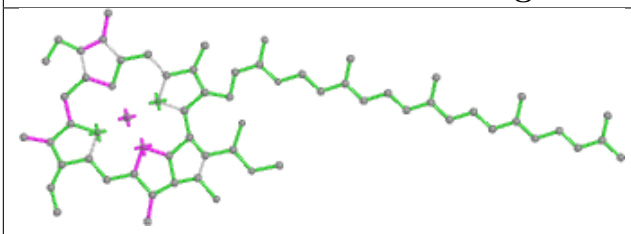

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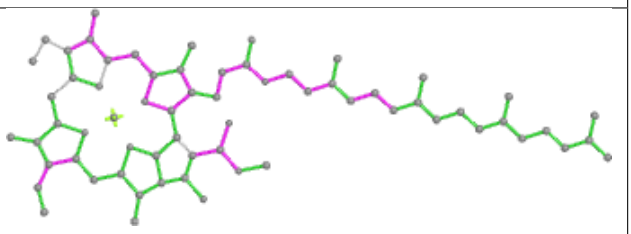

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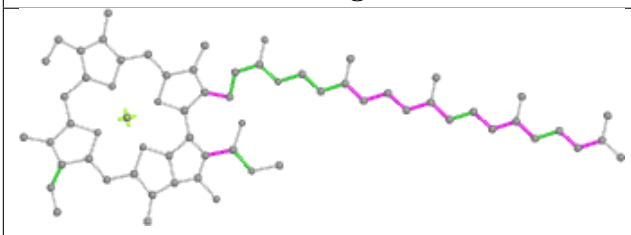

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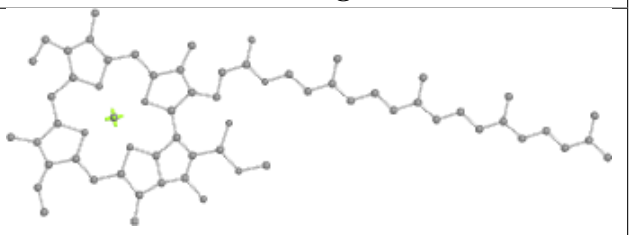
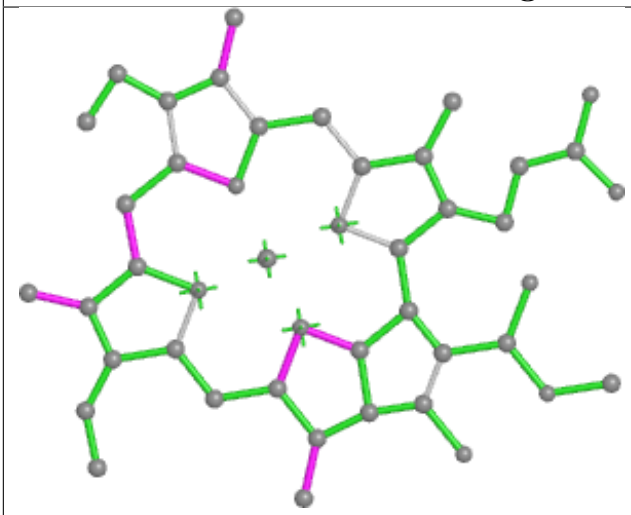


Rings

Ligand CLA J 1303



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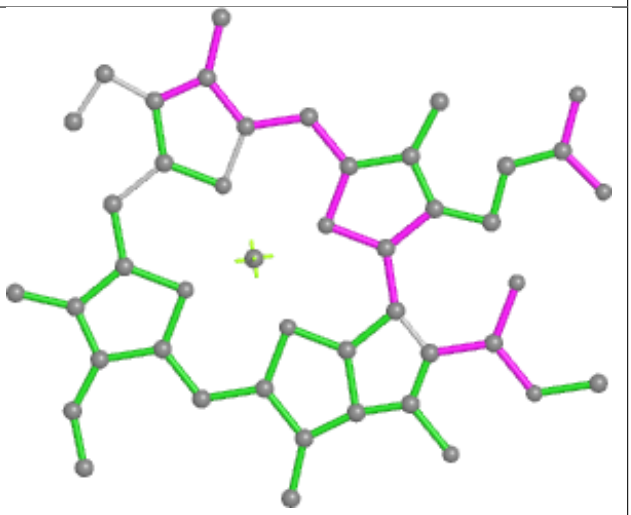

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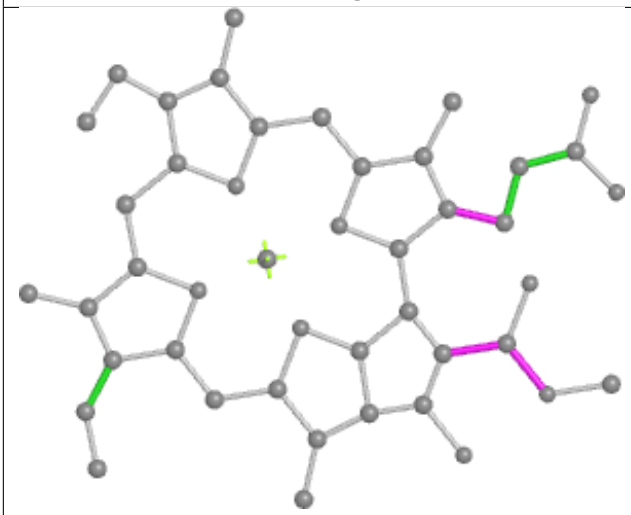

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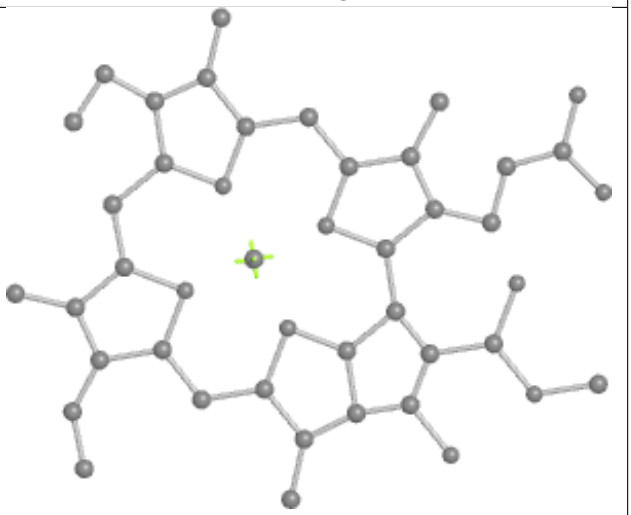

Rings

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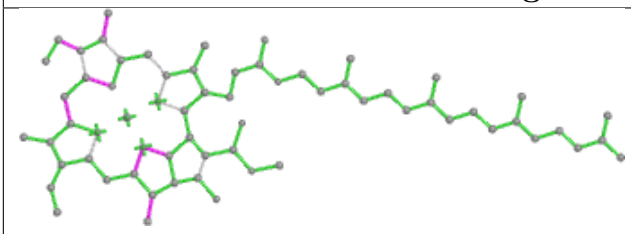

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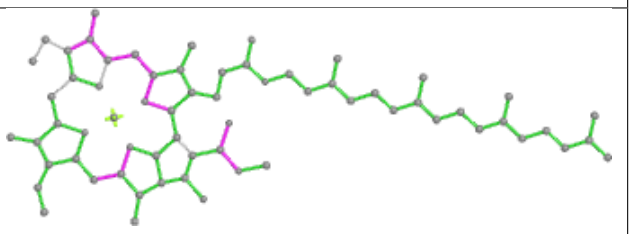

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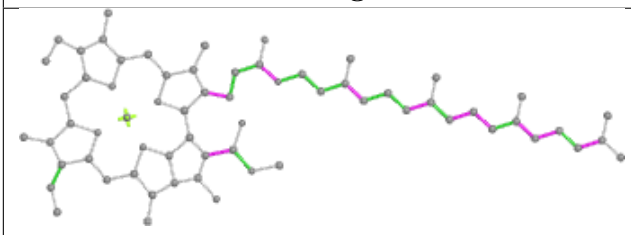

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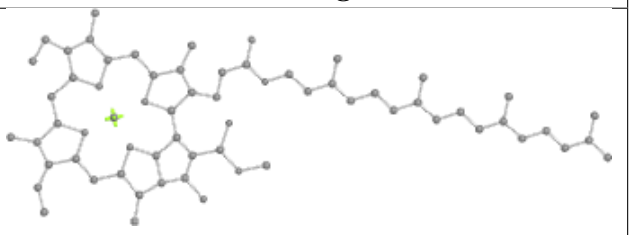
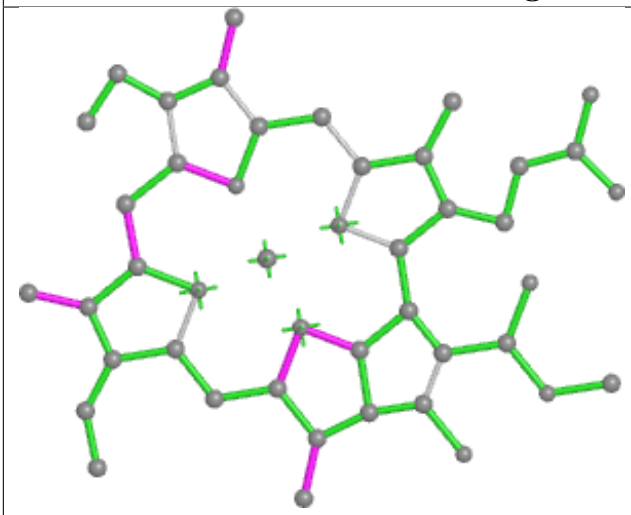


Rings

Ligand CLA Y 517



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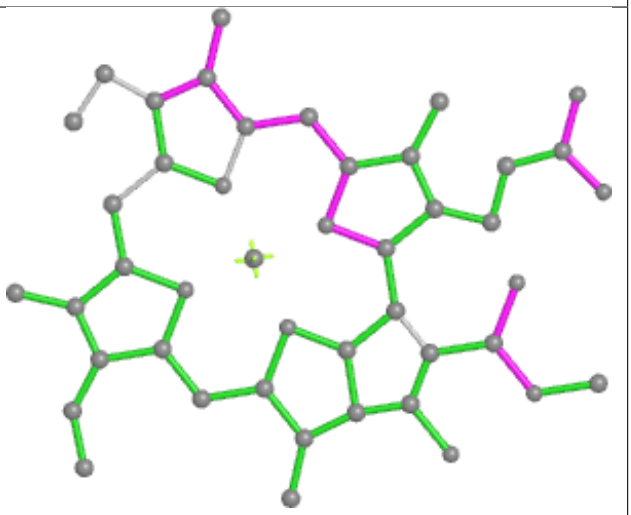

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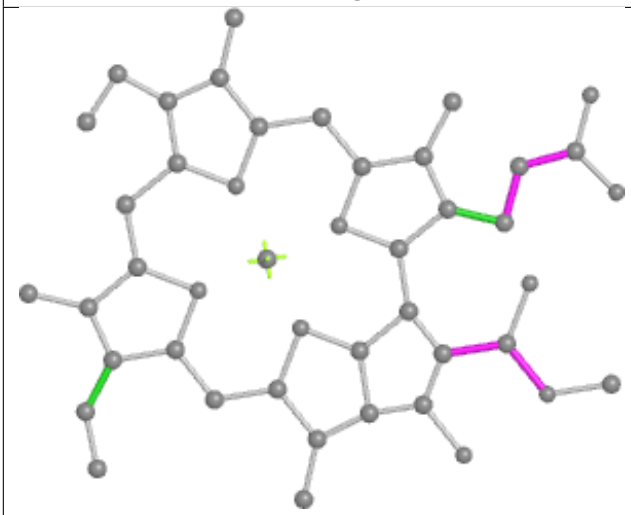

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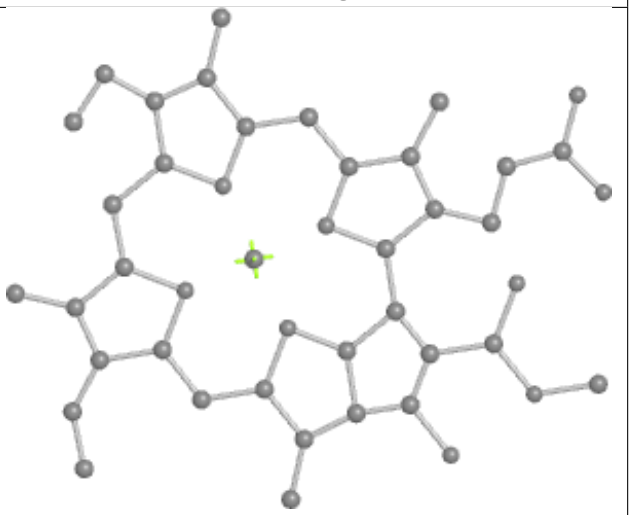

Rings

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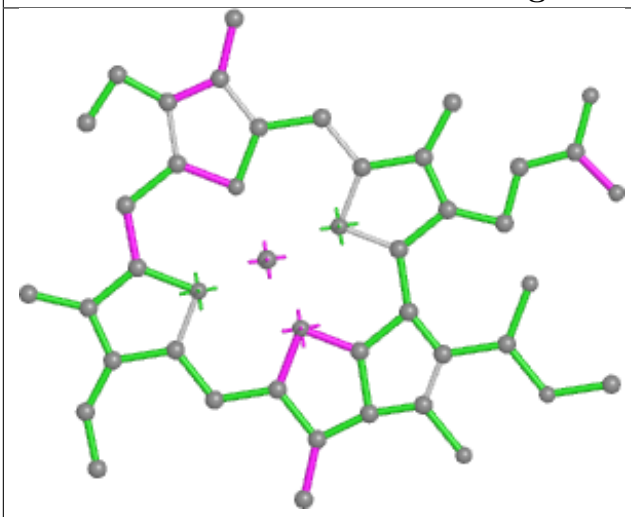

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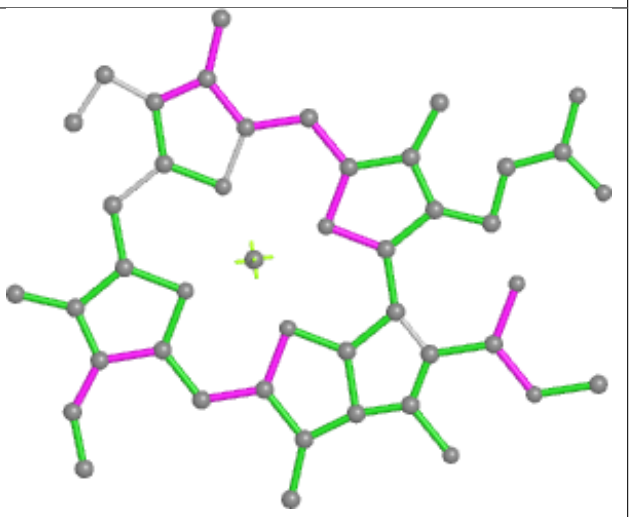

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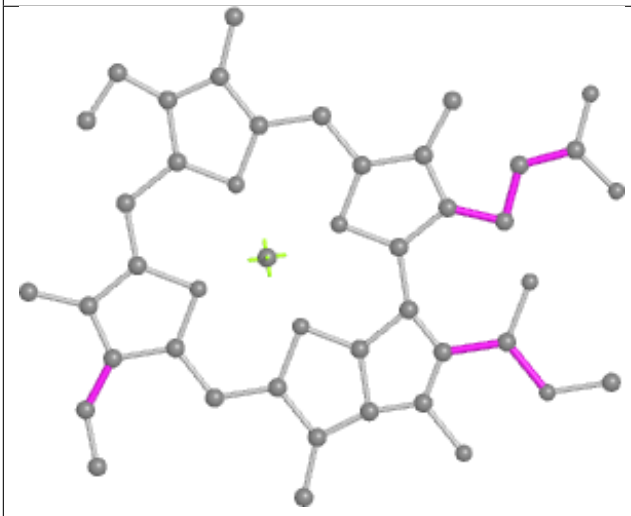

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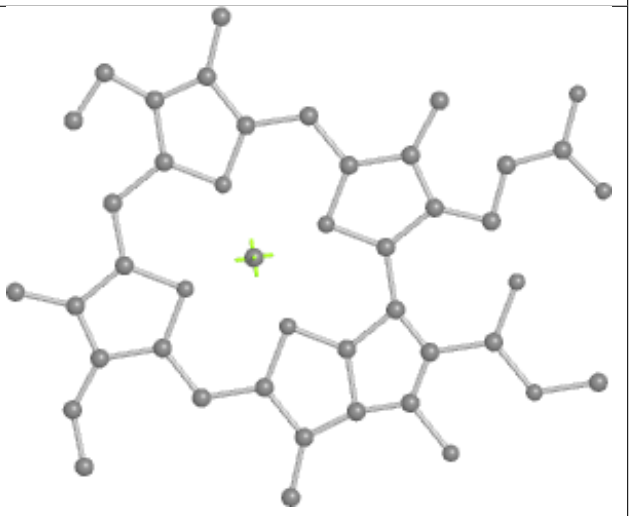

Rings

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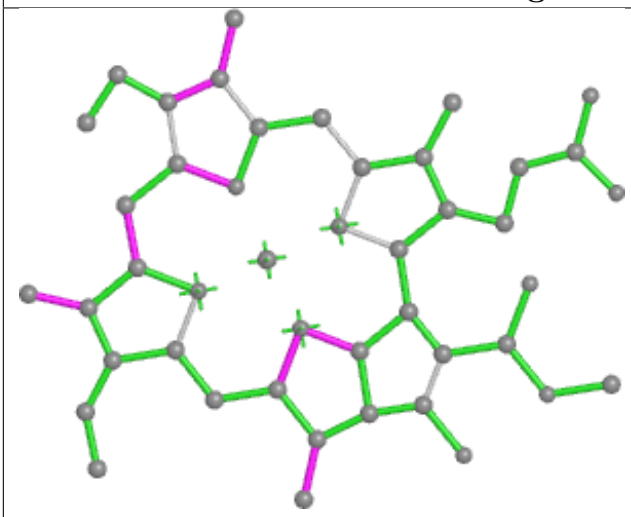

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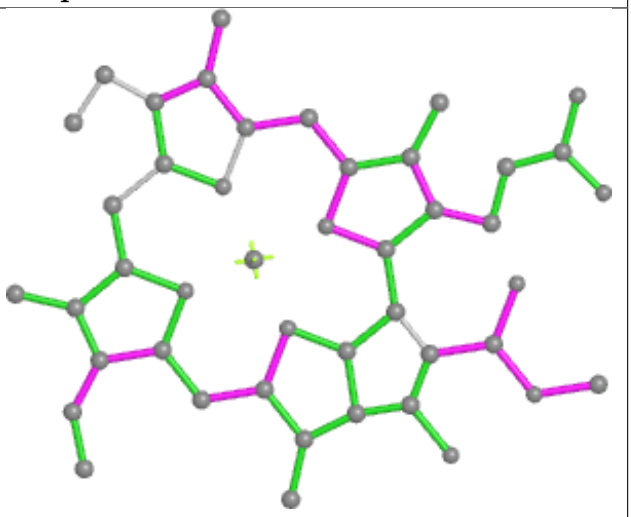

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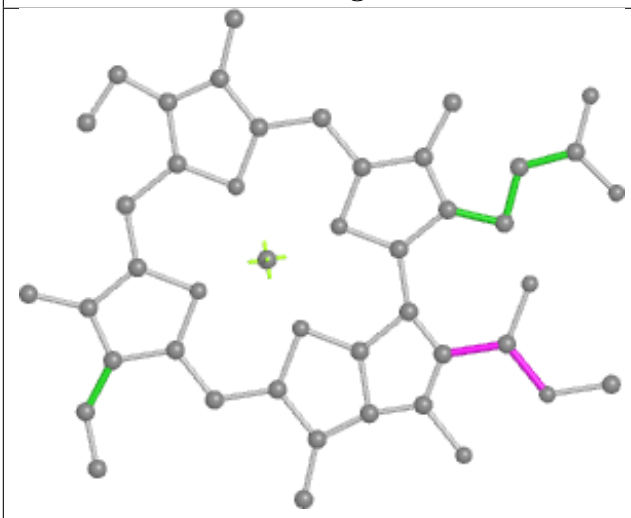

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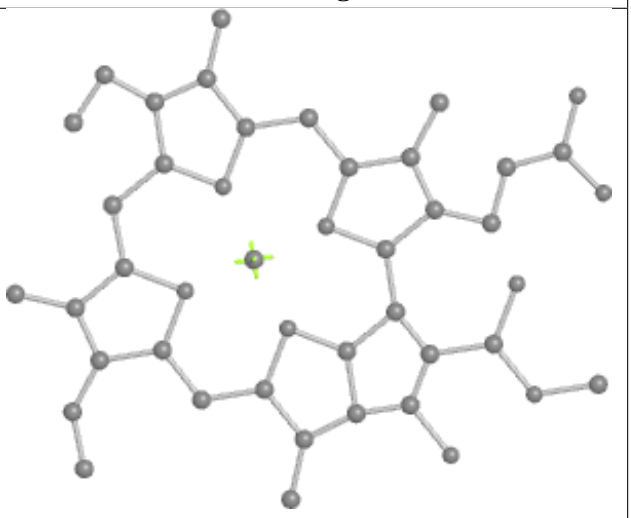
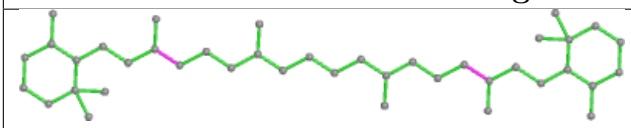


Rings

Ligand BCR G 4008



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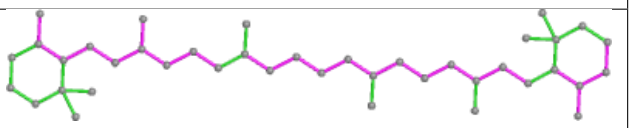

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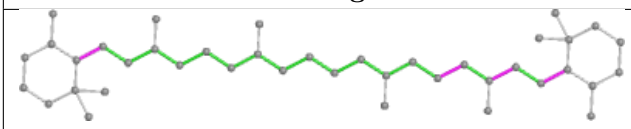
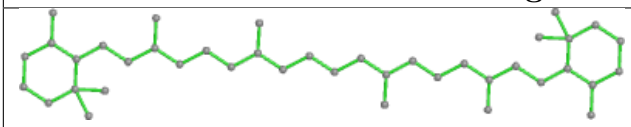


Torsions

Rings

Ligand BCR b 524



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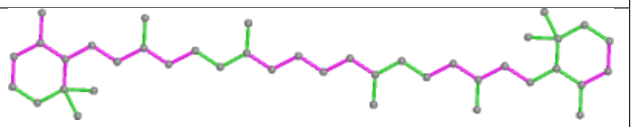
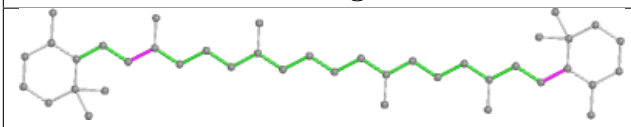
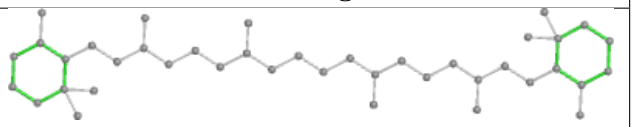


Bond angles

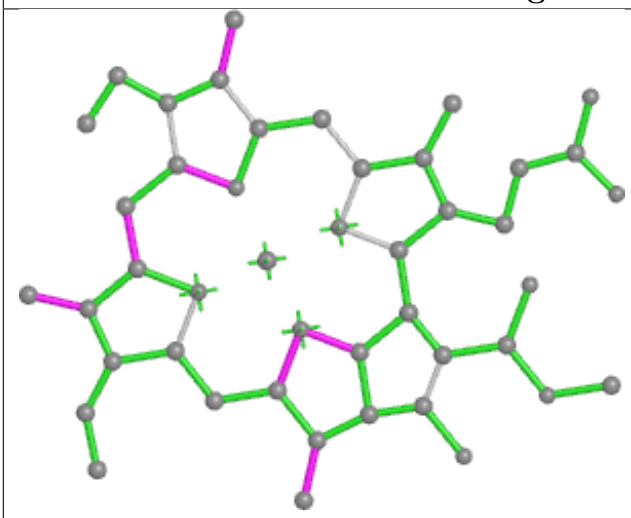


Torsions



Rings

Ligand CLA v 501



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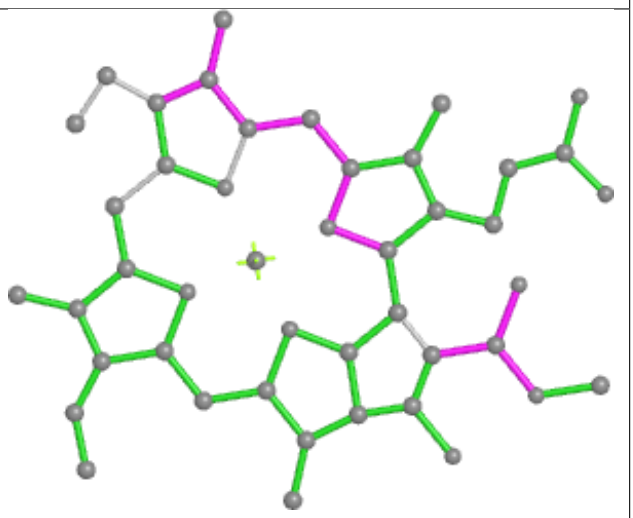
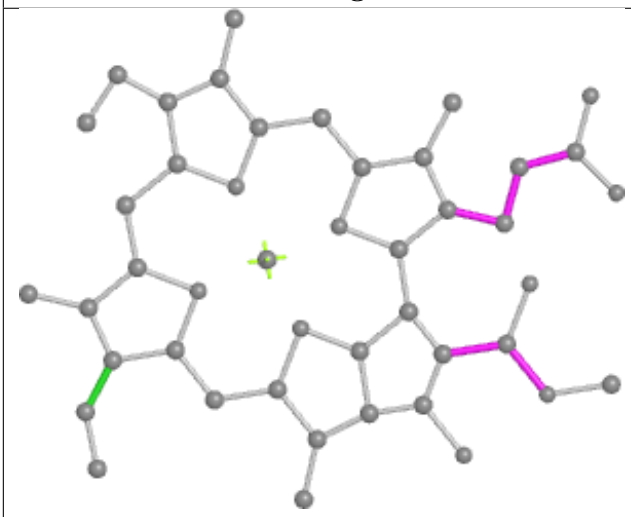
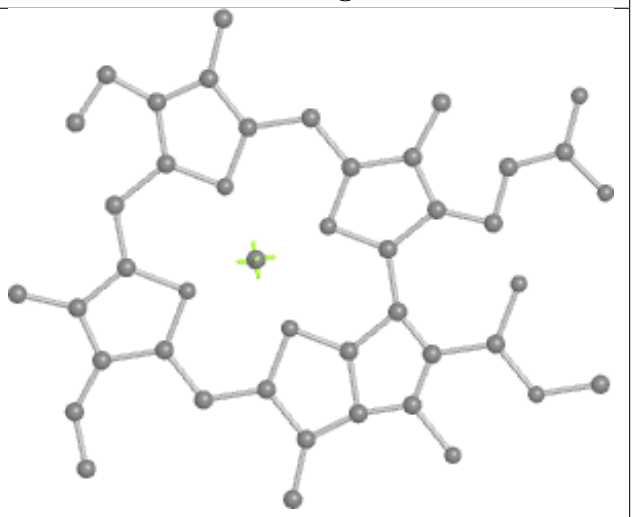


Bond angles

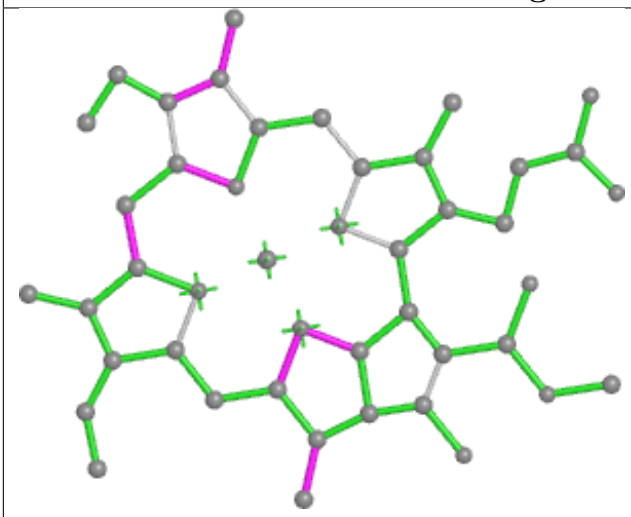


Torsions

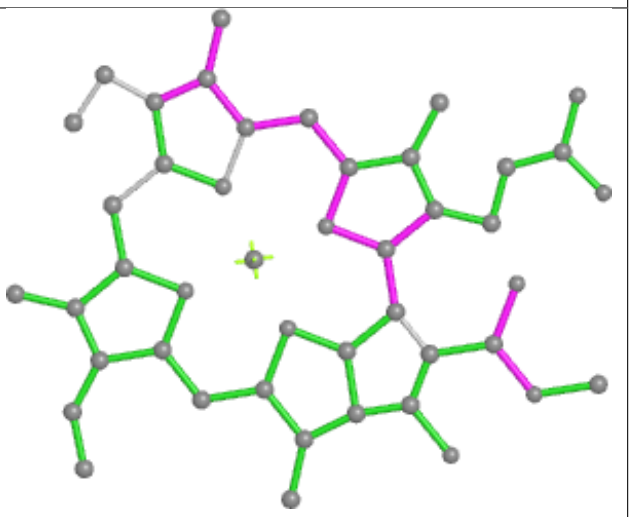


Rings

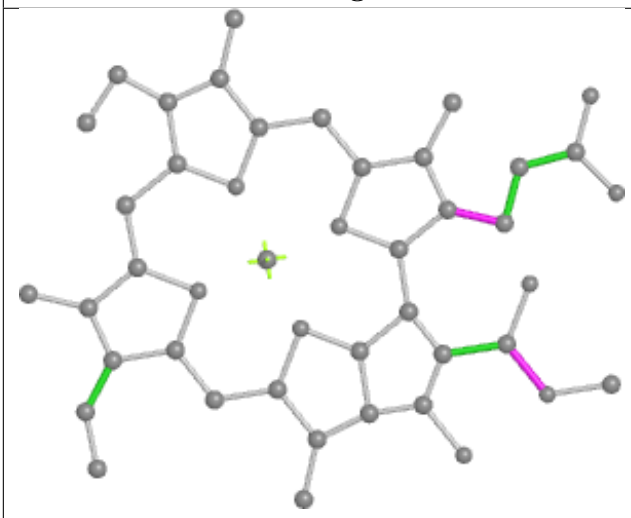
Ligand CLA c 504



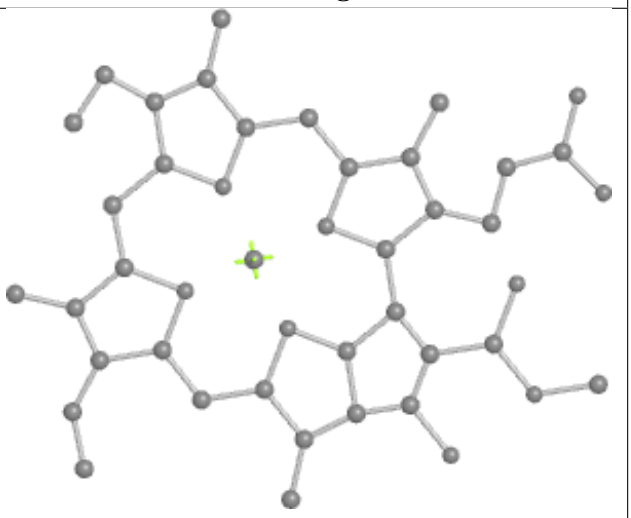
Bond lengths



Bond angles

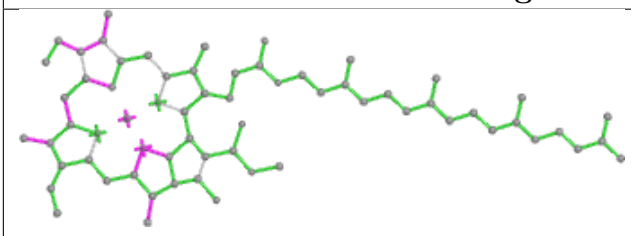


Torsions



Rings

Ligand CLA A 1136



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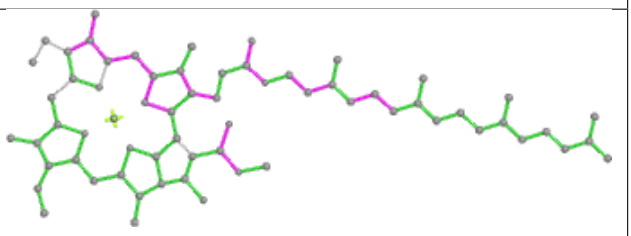

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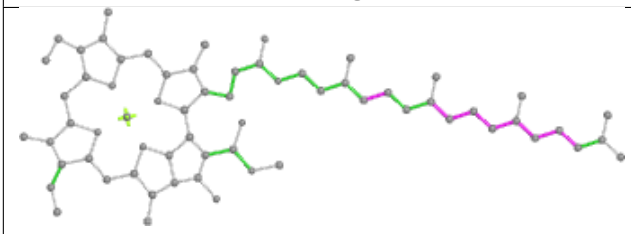
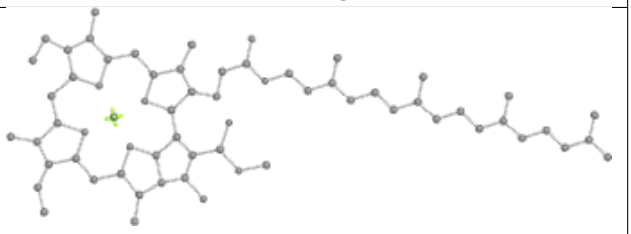
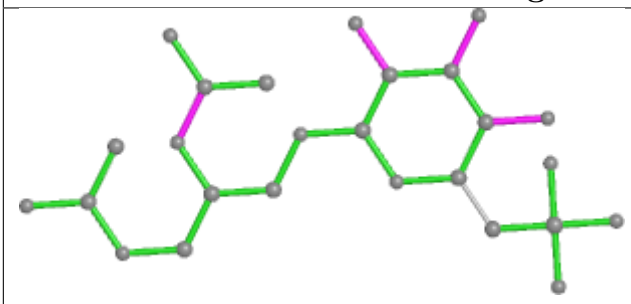
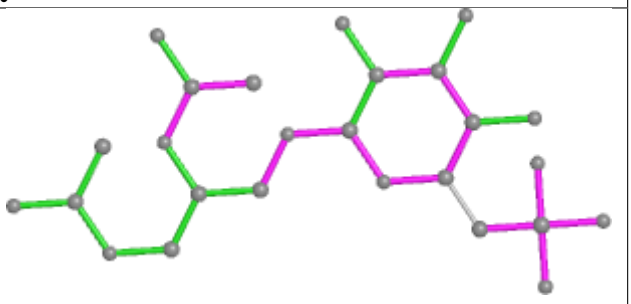
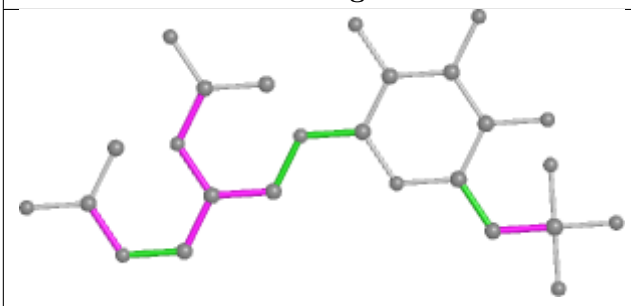
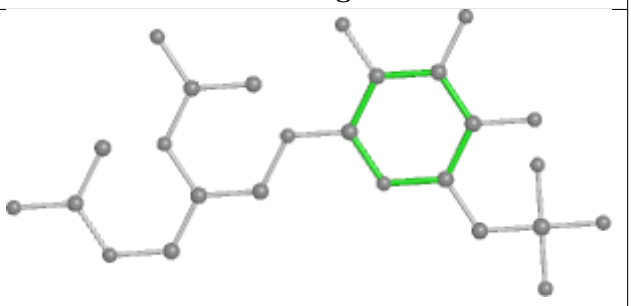
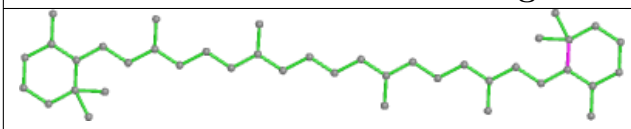
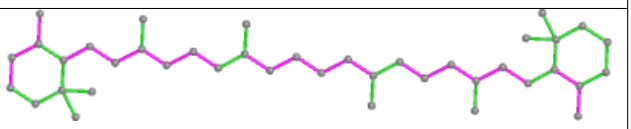
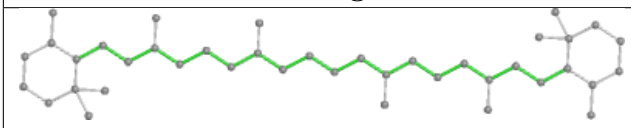
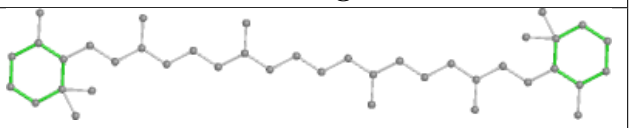


Torsions

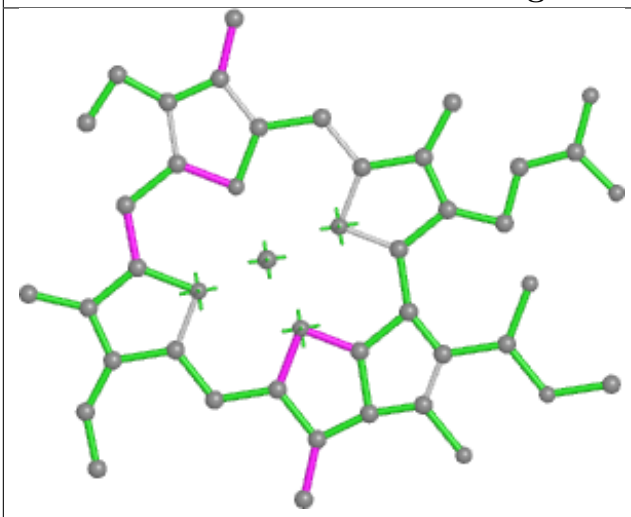


Rings

Ligand SQD b 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR e 4003	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA d 518



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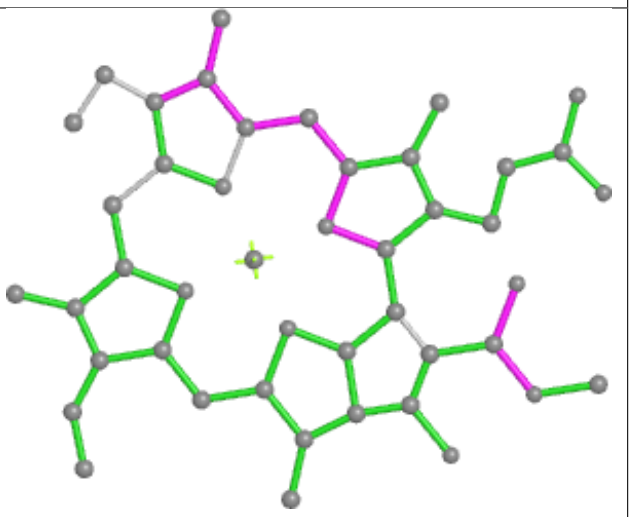

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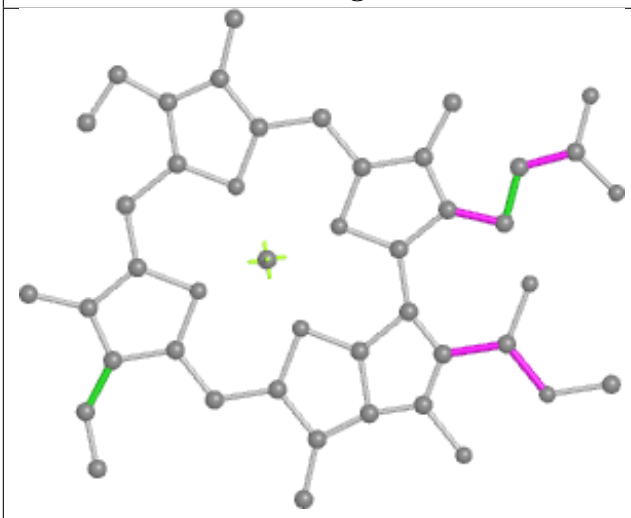

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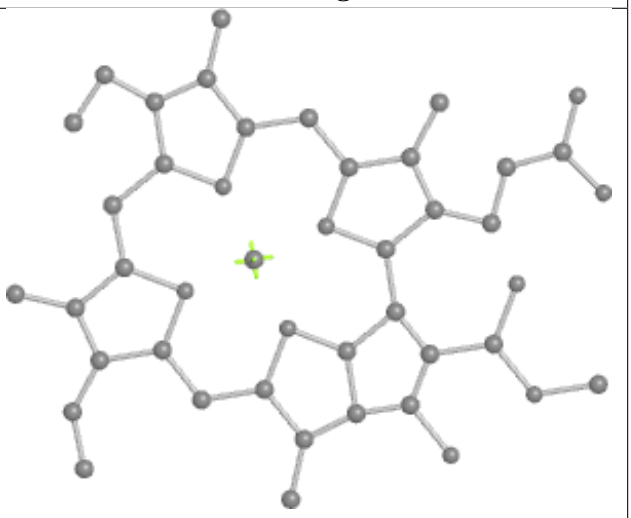
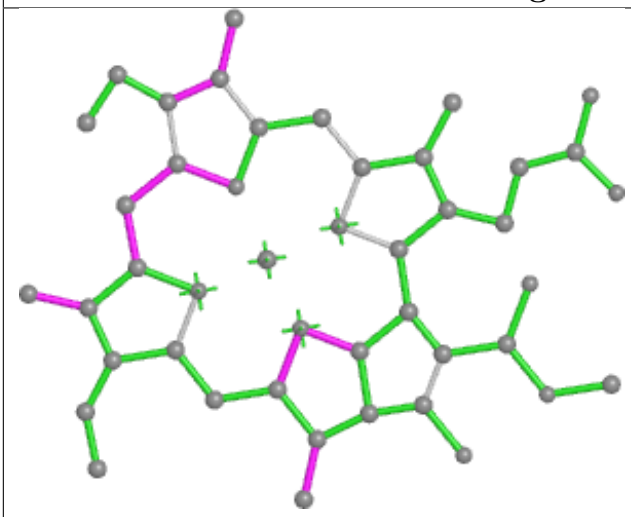


Rings

Ligand CLA c 508



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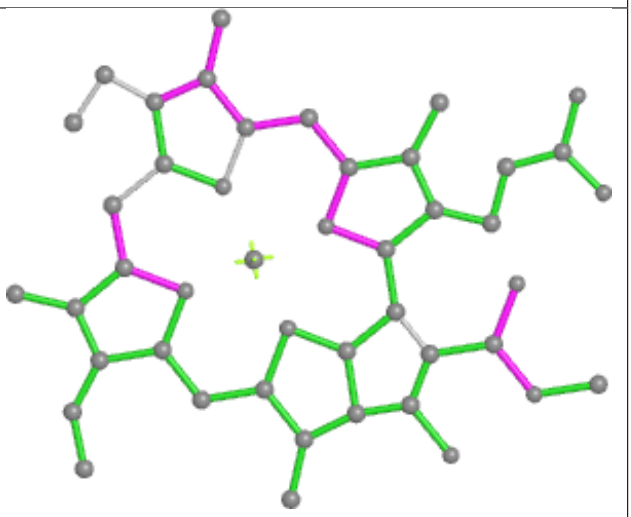

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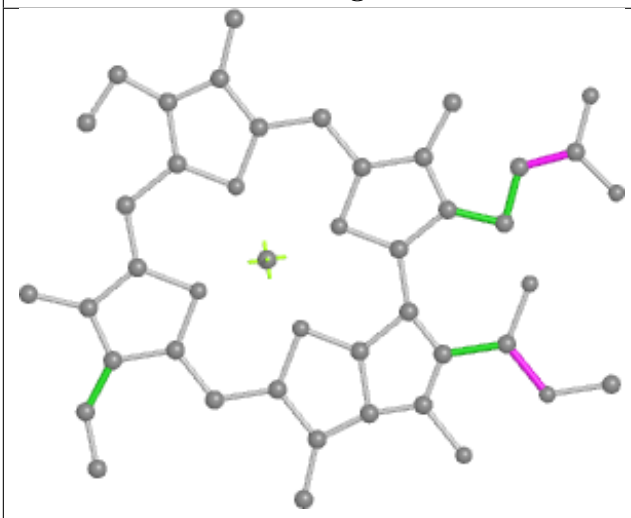

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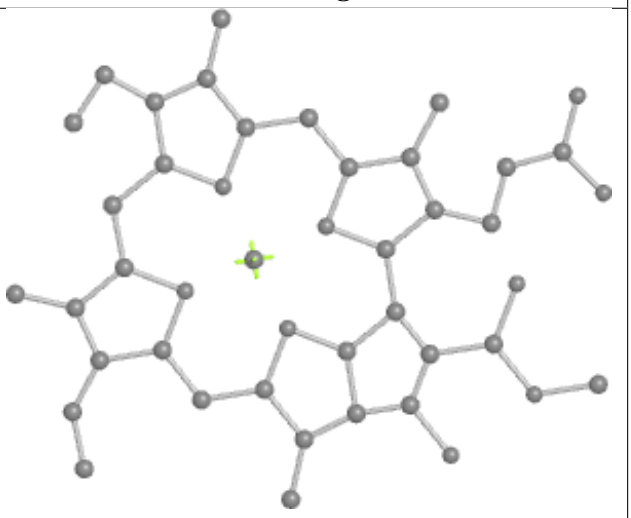
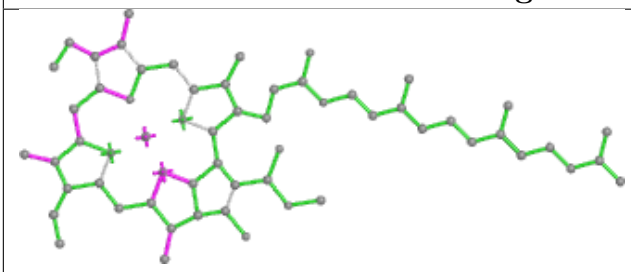


Rings

Ligand CLA B 1230



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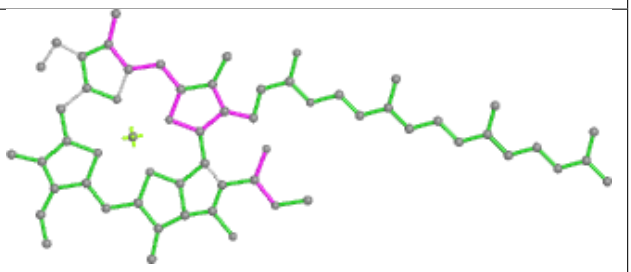
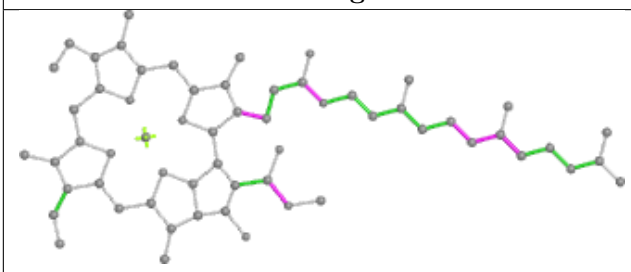


Bond angles



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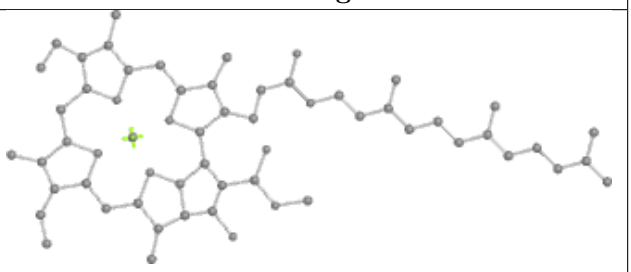
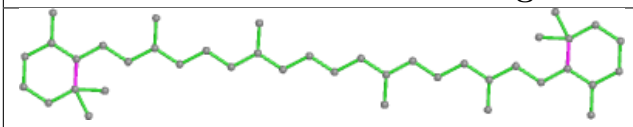


Rings

Ligand BCR S 4018



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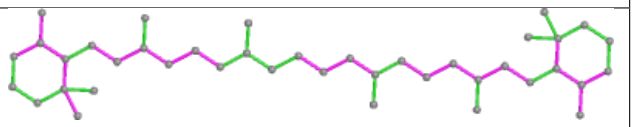
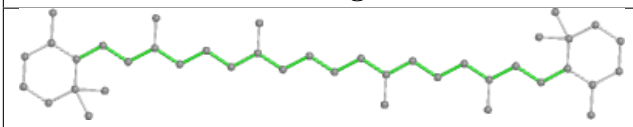


Bond angles



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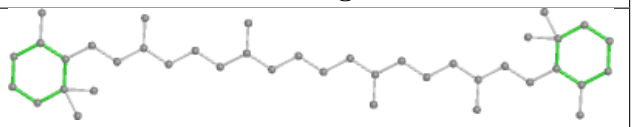
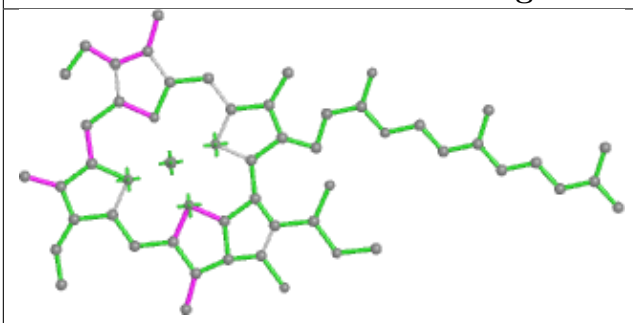


Rings

Ligand CLA T 1302



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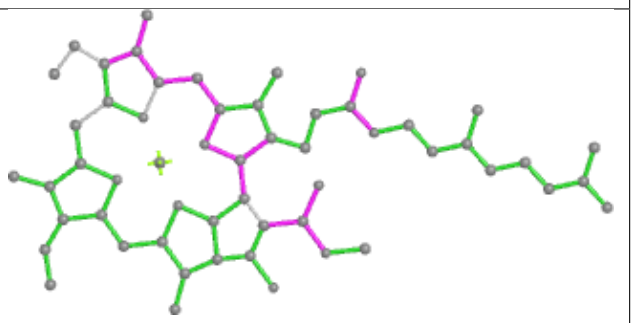
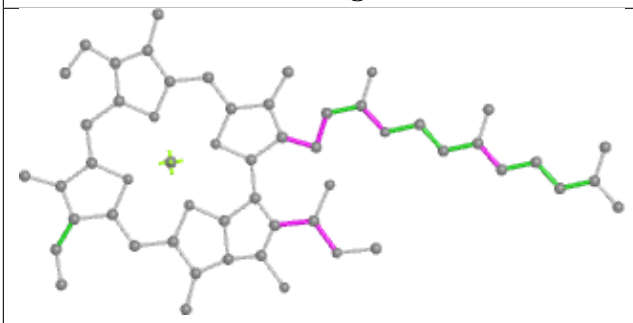


Bond angles



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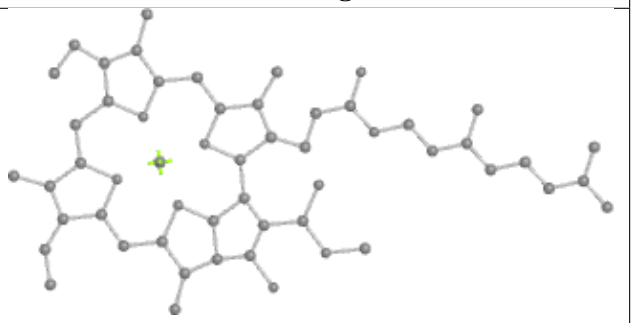
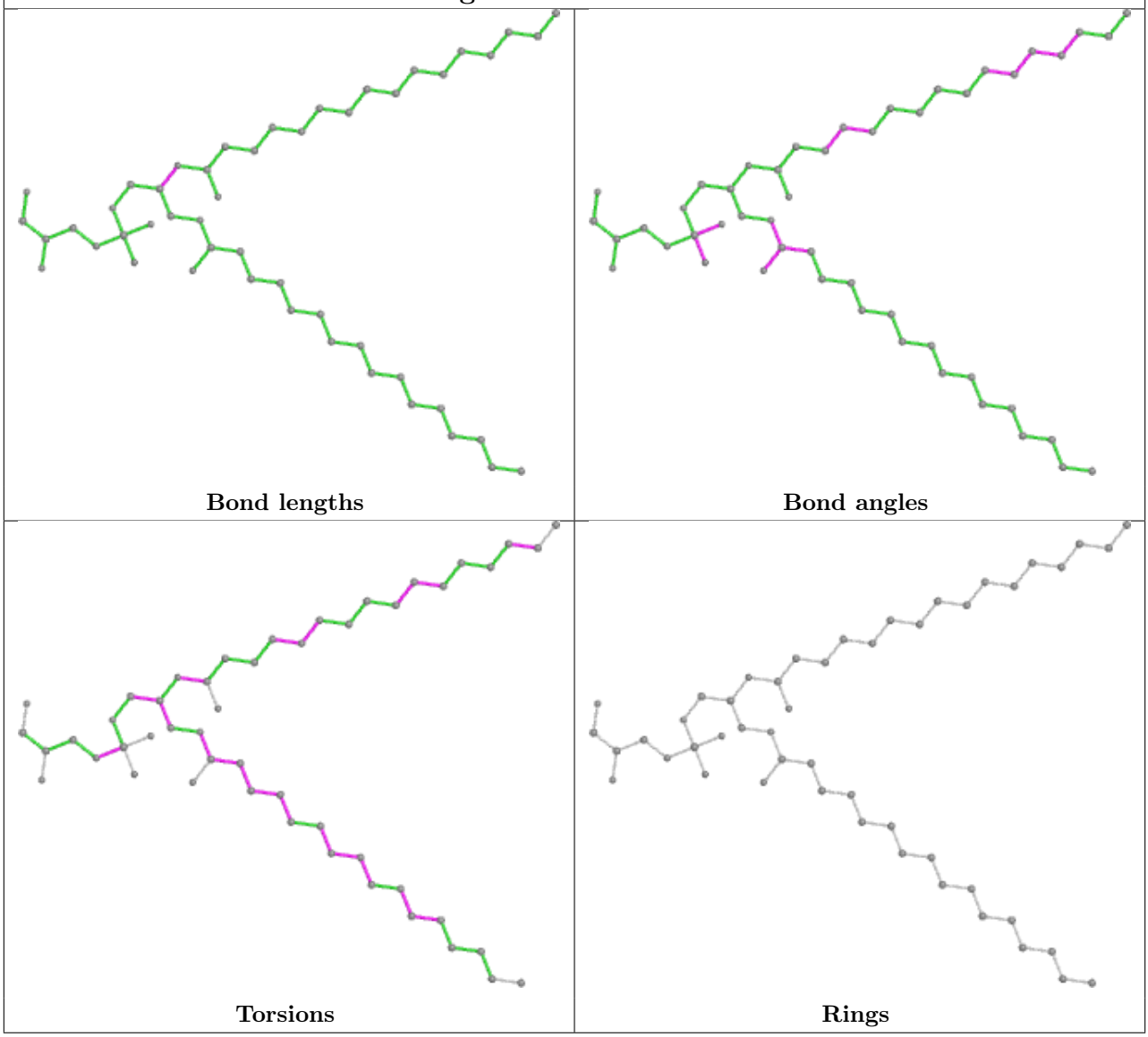
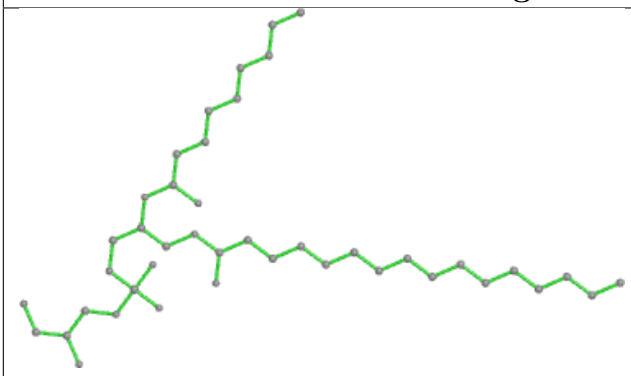
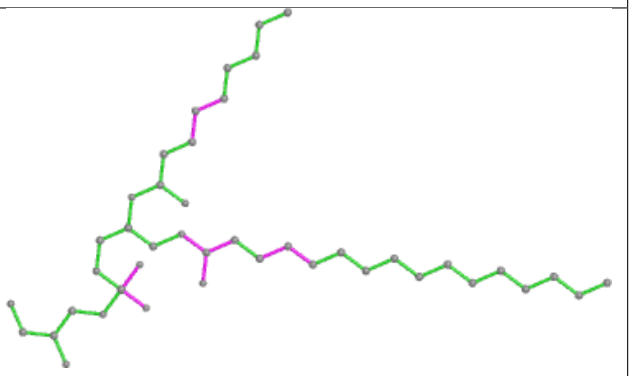
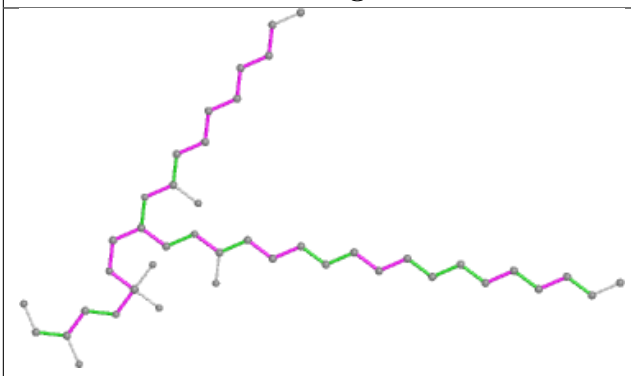
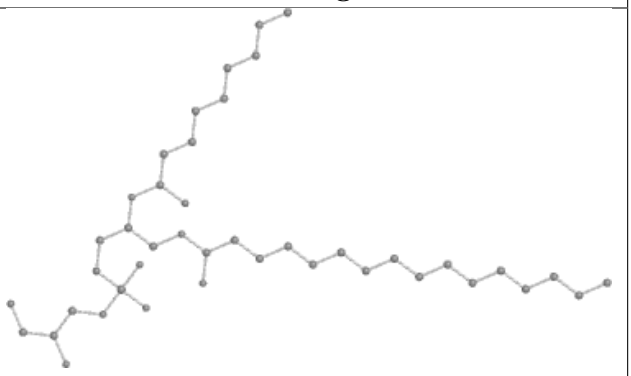


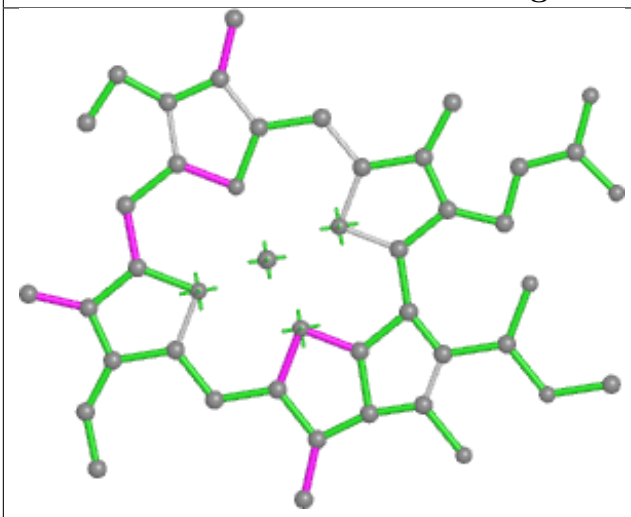
Rings

Ligand LHG G 5001

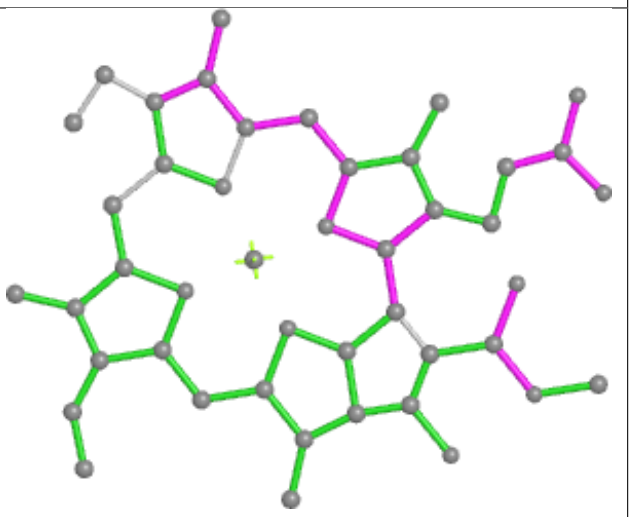


Ligand LHG A 5009	
 Bond lengths	 Bond angles
 Torsions	 Rings

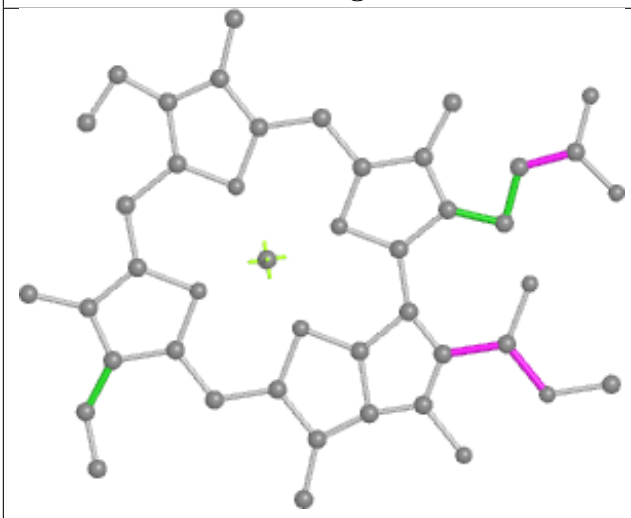
Ligand CLA t 509



Bond lengths



Bond angles



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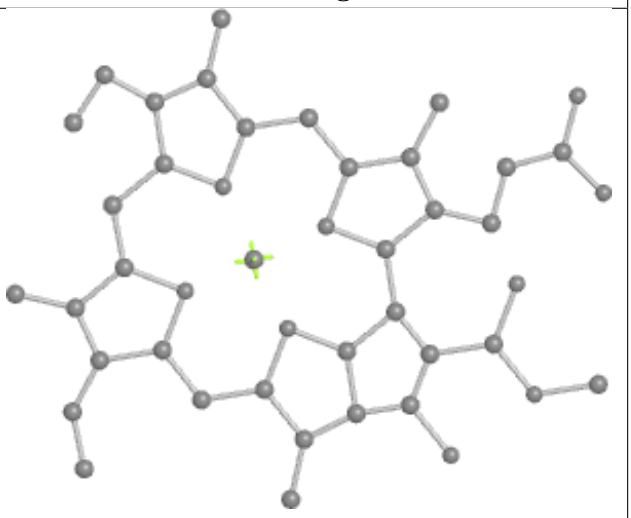
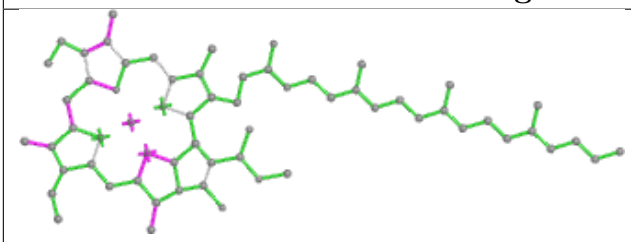


Rings

Ligand CLA H 1219



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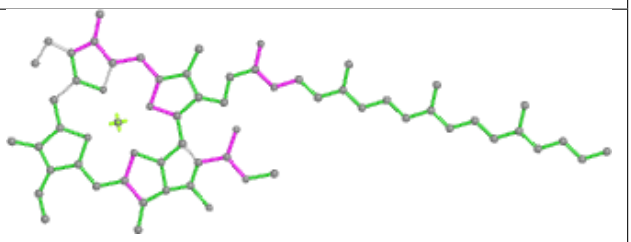

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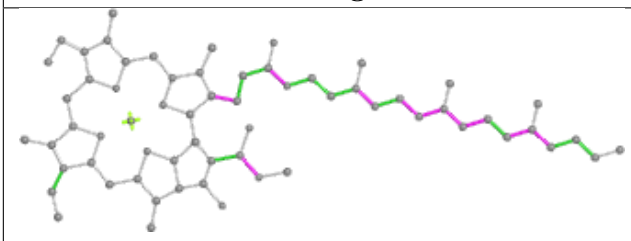

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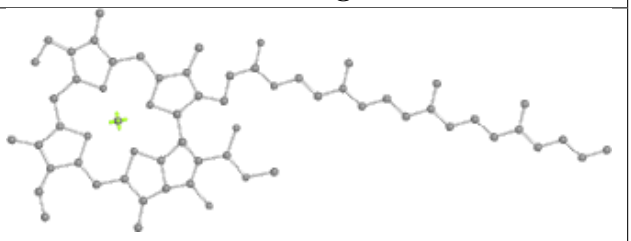
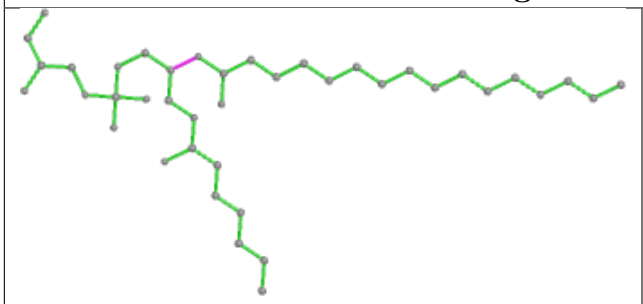
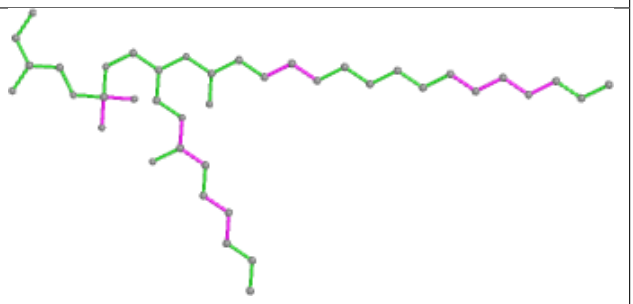
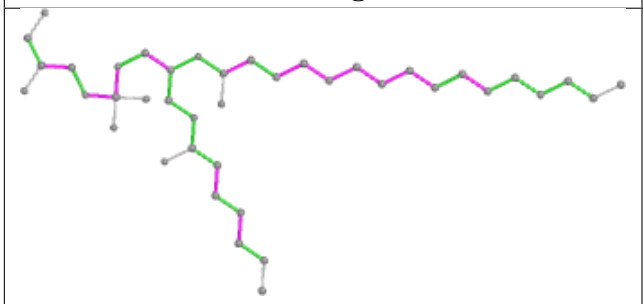
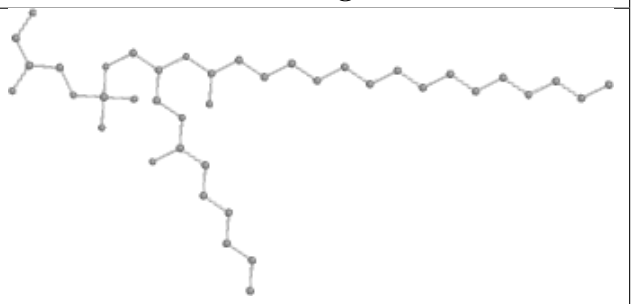
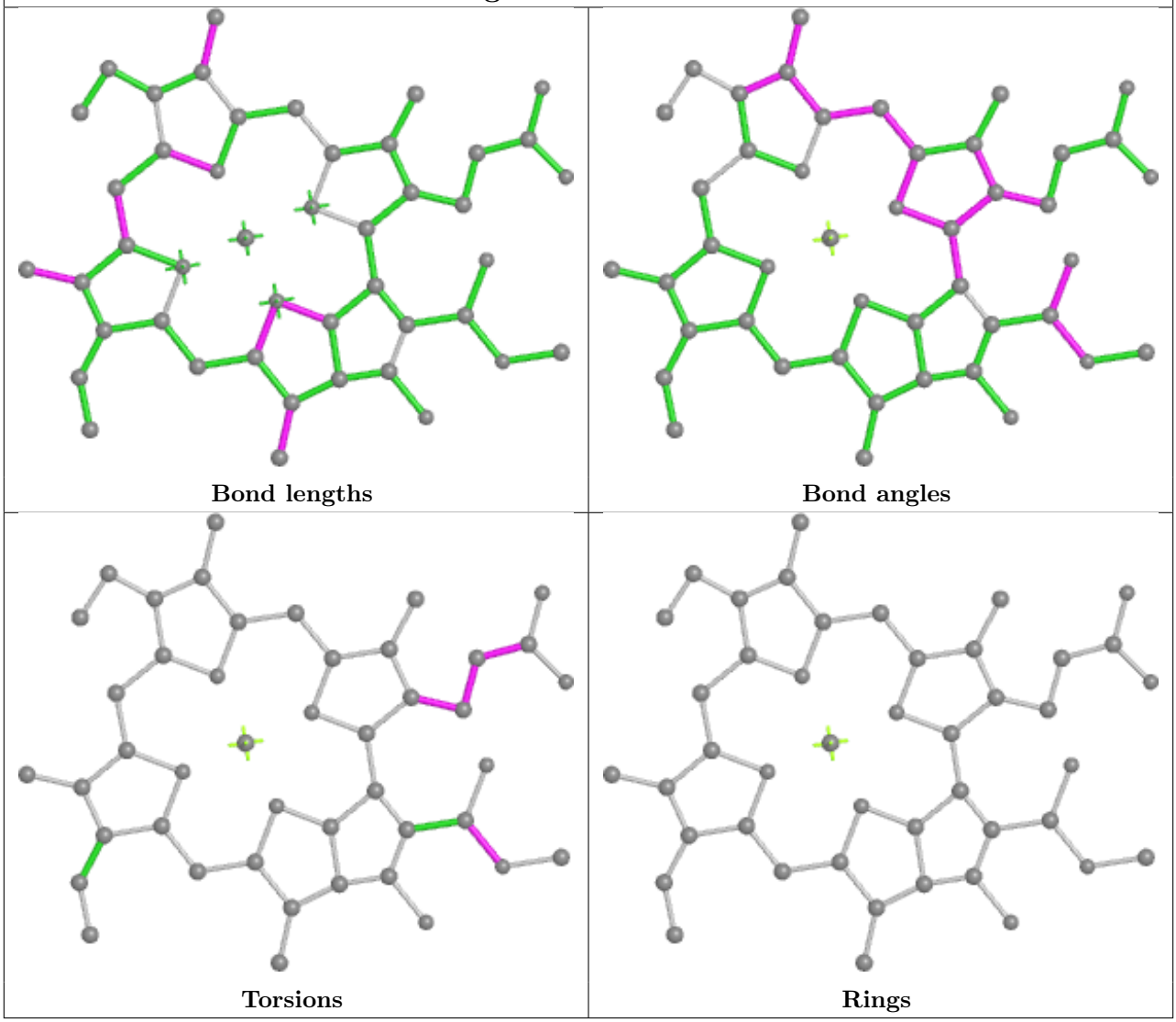


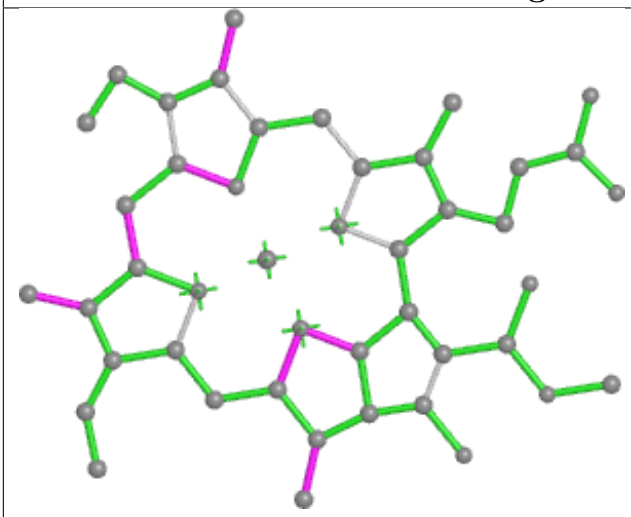
Rings

Ligand LHG G 5003	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA u 501



Ligand CLA 6 510



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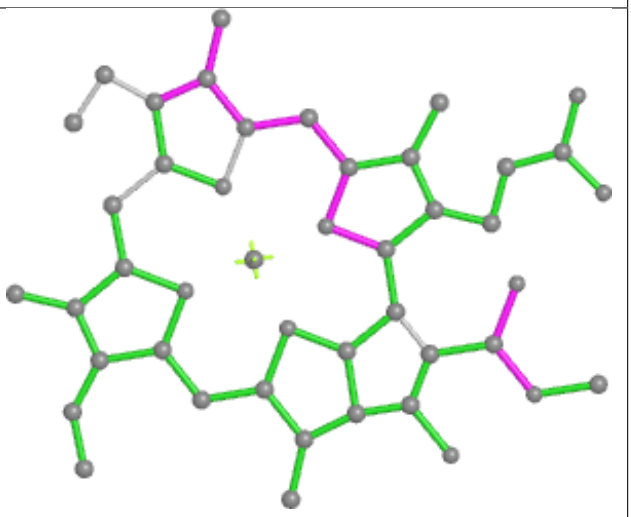

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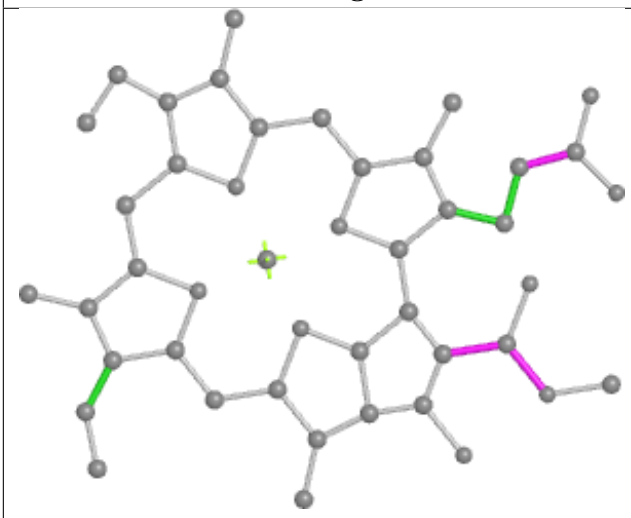

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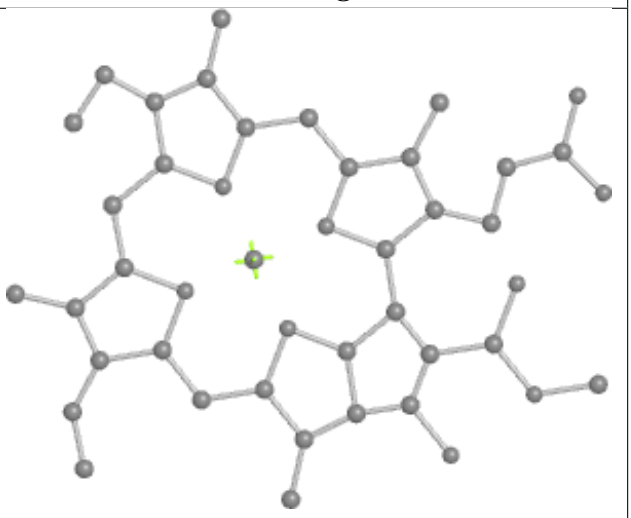
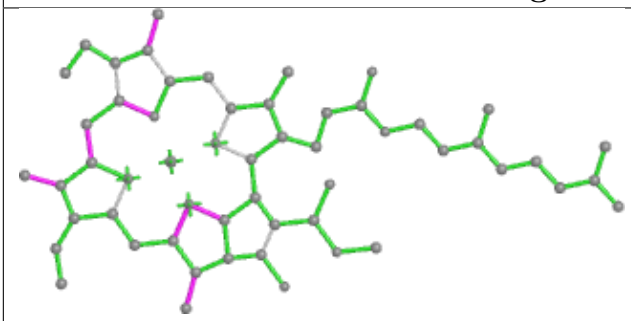


Rings

Ligand CLA r 518



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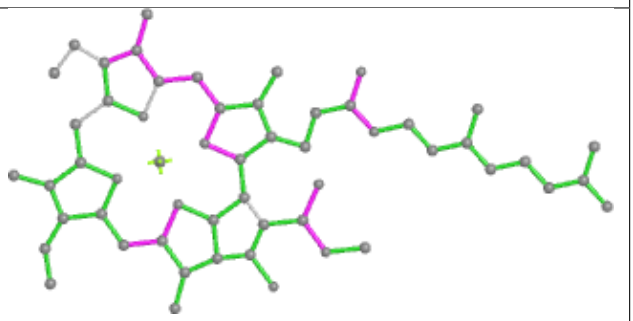

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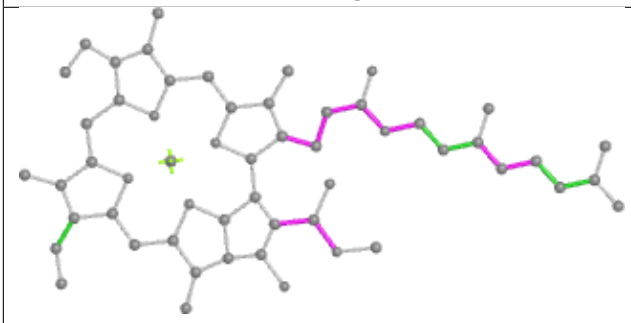

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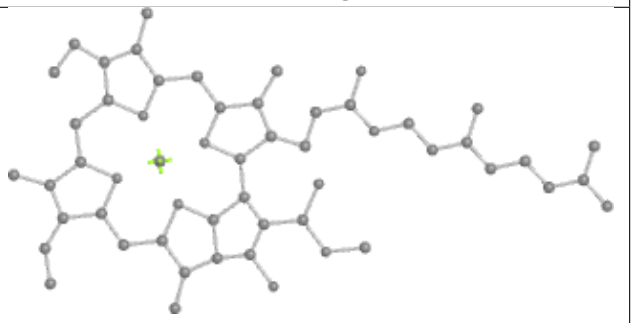
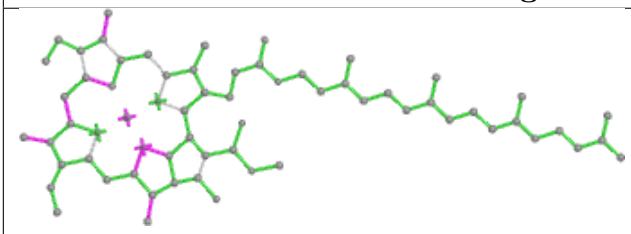


Rings

Ligand CLA e 1126



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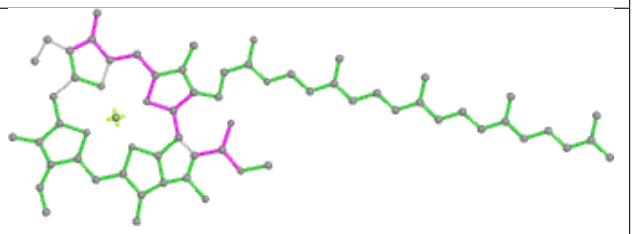

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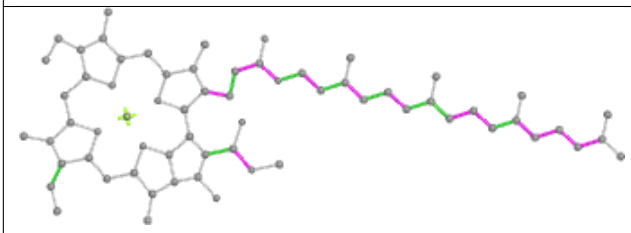

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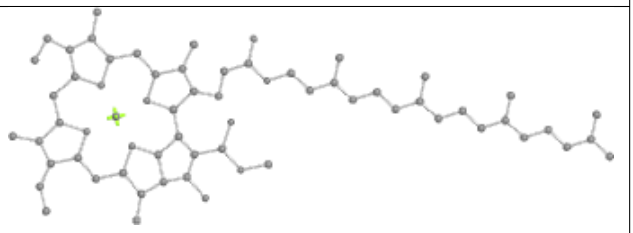

Rings

Ligand BCR 5 521

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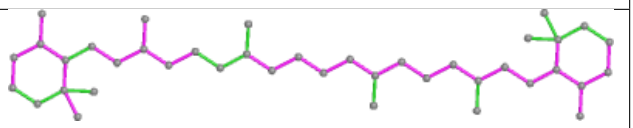

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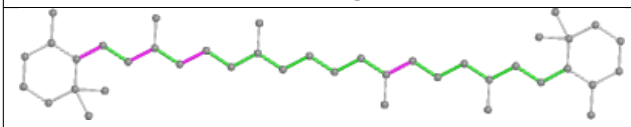

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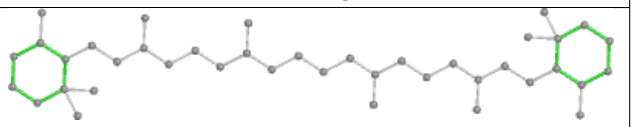
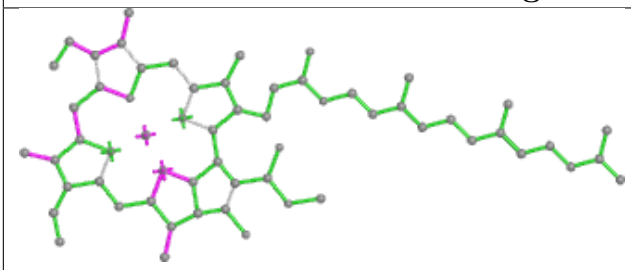


Rings

Ligand CLA f 1227



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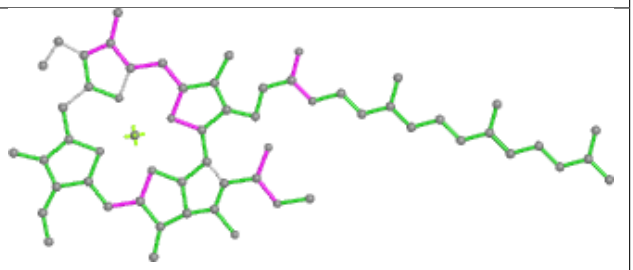

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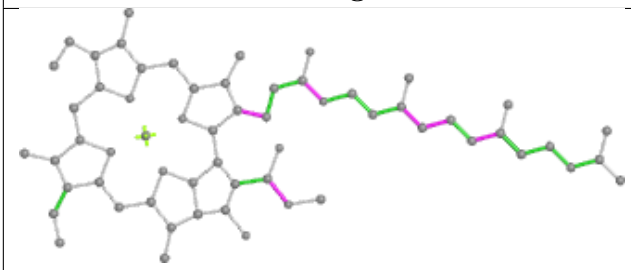

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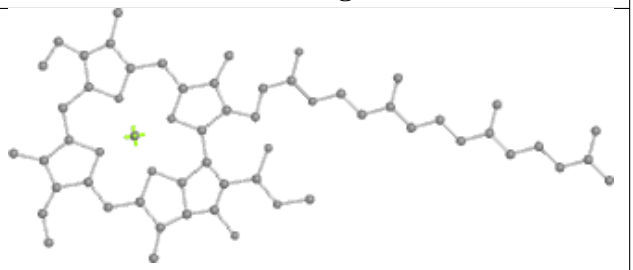
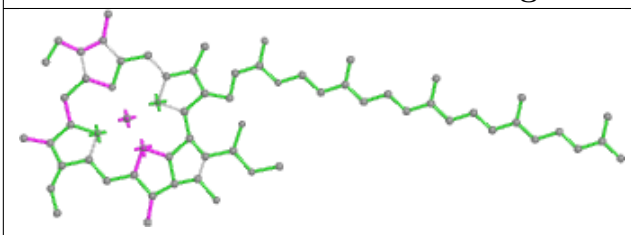


Rings

Ligand CLA e 1133



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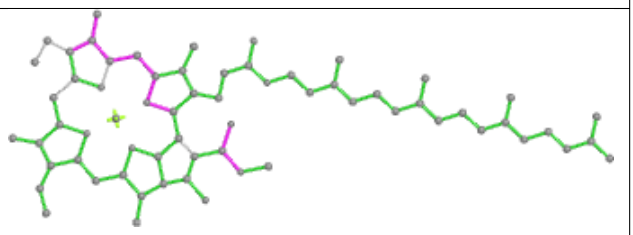

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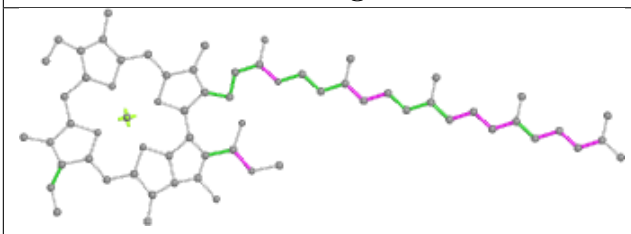

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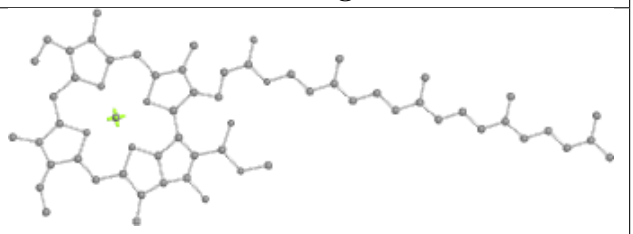
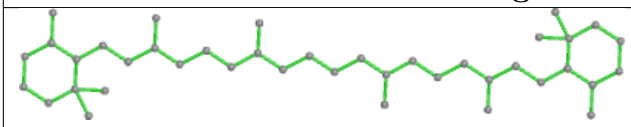


Rings

Ligand BCR H 4004



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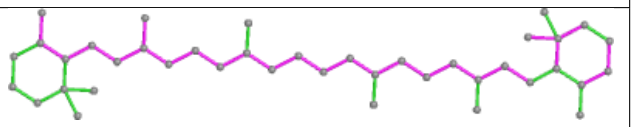

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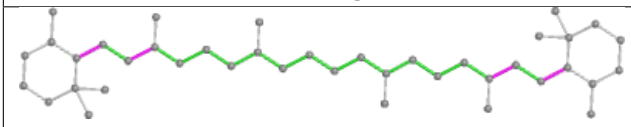

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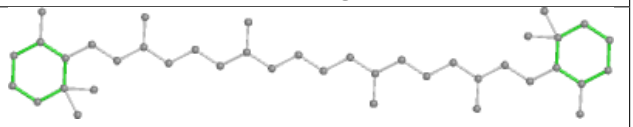
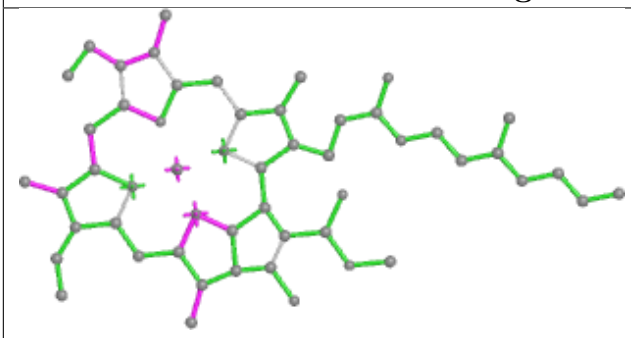
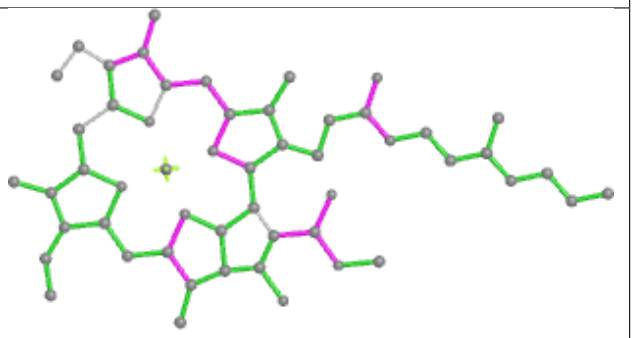
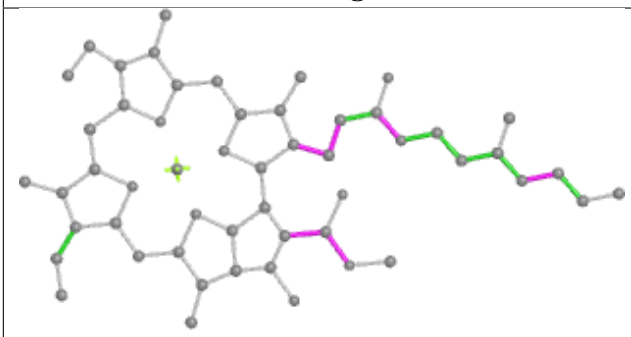
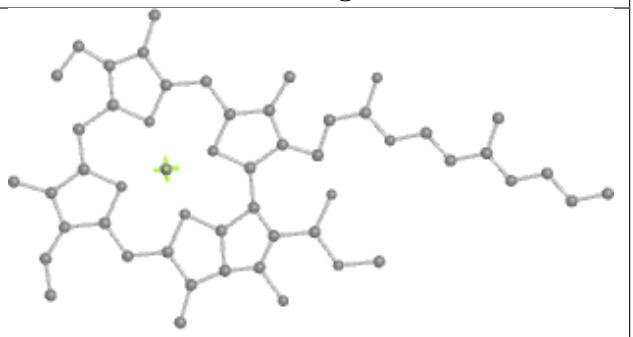


Rings

Ligand CLA A 1129	
 Bond lengths	 Bond angles
 Torsions	 Rings

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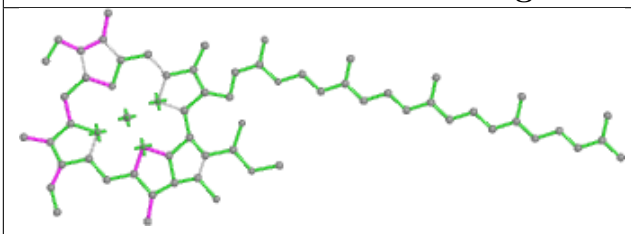
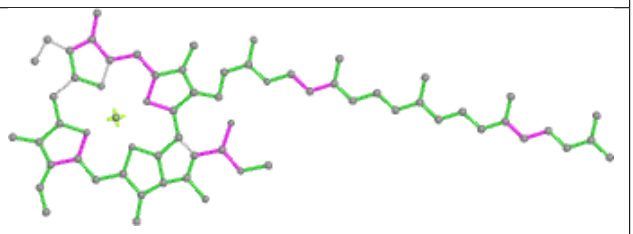
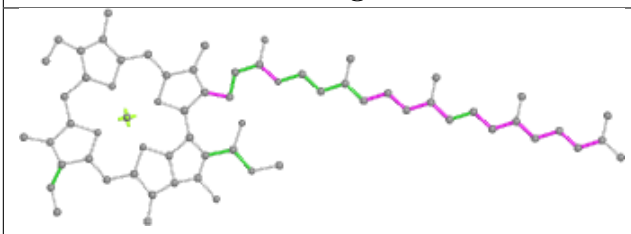
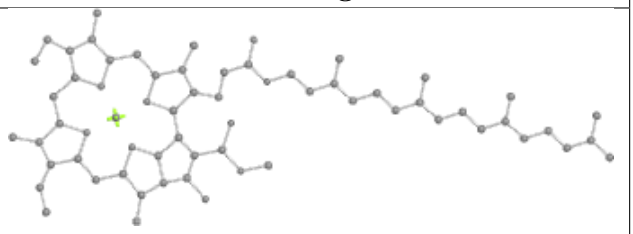
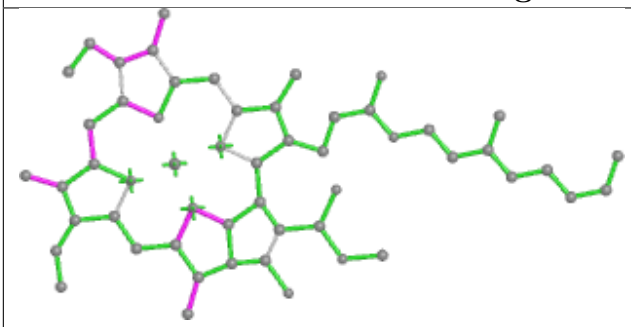
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1108



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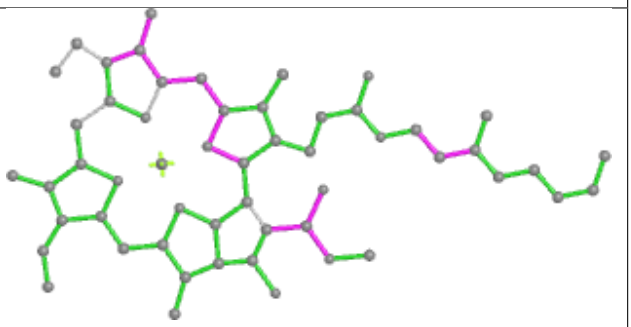
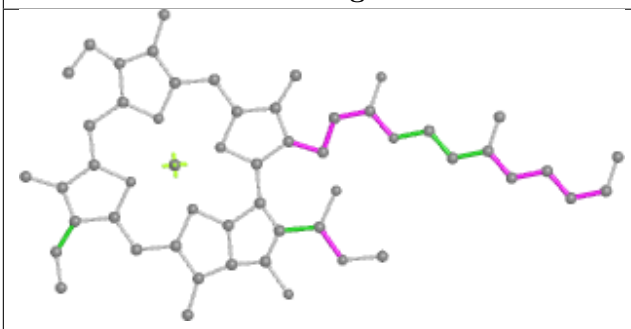


Bond angles



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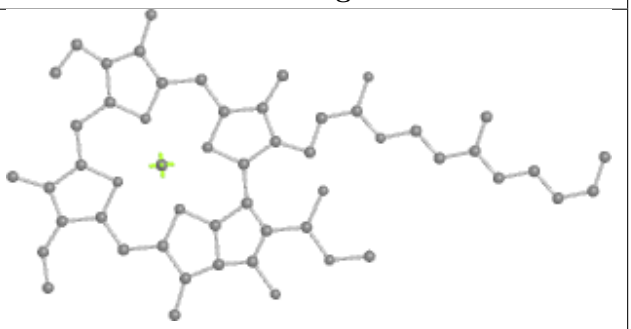
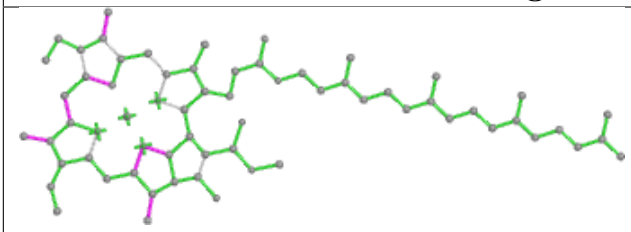


Rings

Ligand CLA Z 509



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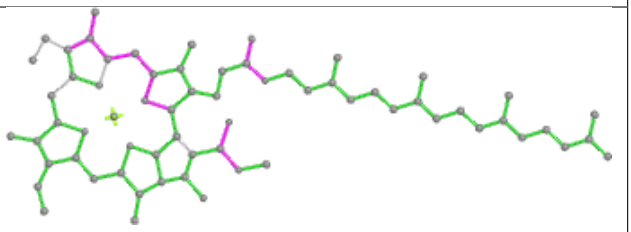

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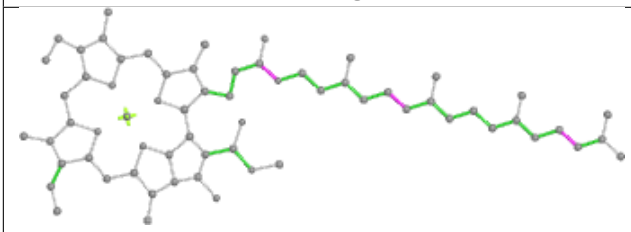

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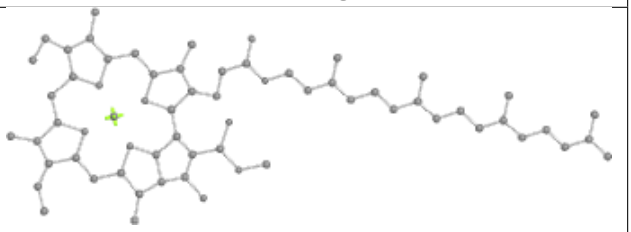
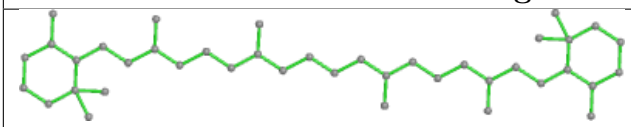


Rings

Ligand BCR T 4012



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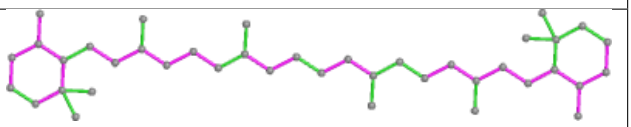
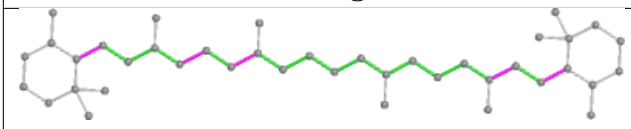


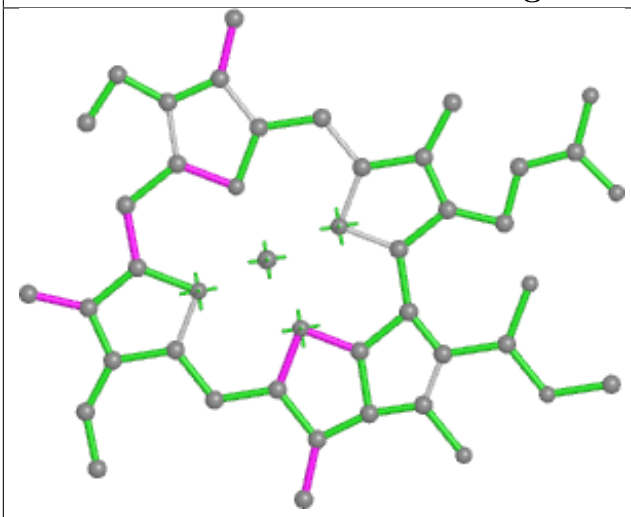
Bond angles



Torsions

Rings

Ligand CLA Y 513



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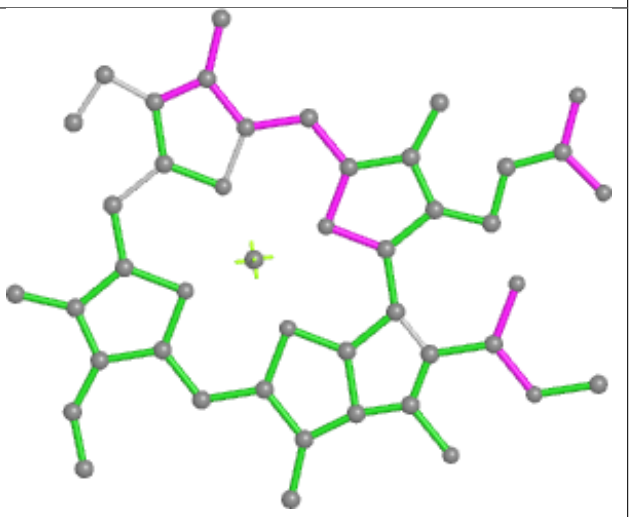
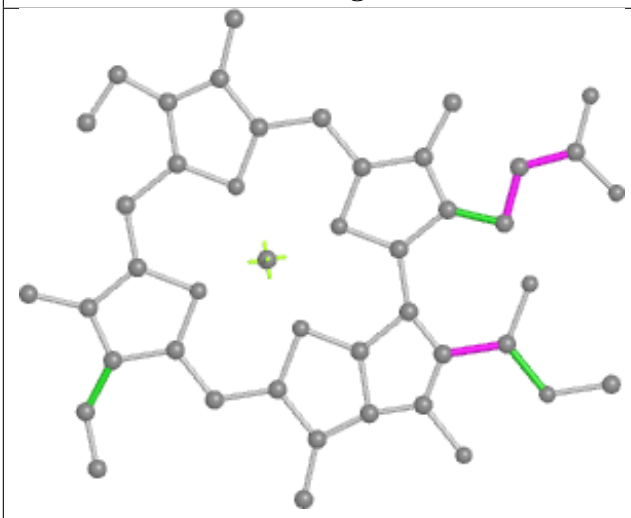
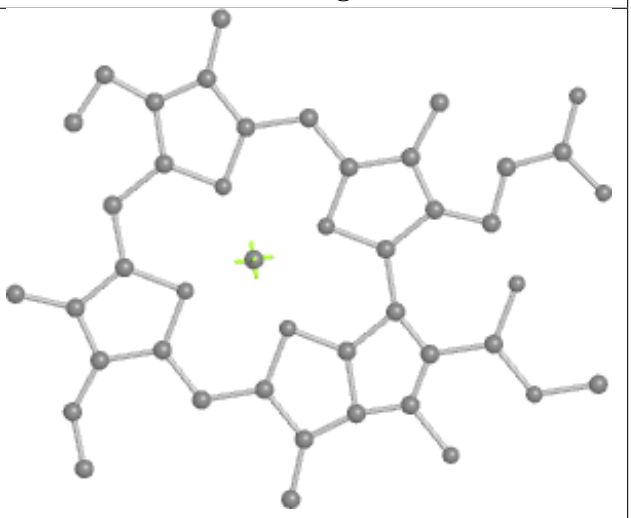


Bond angles

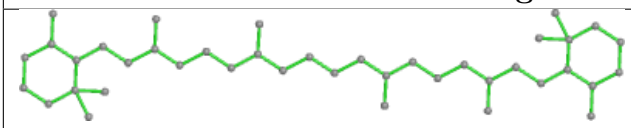


Torsions

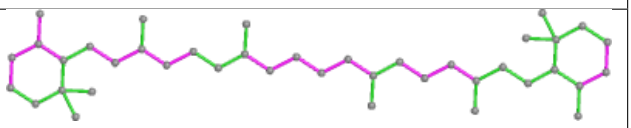


Rings

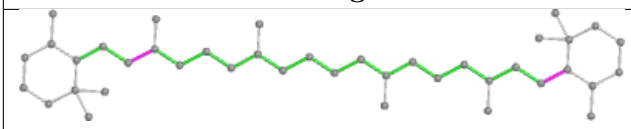
Ligand BCR L 4022



Bond lengths

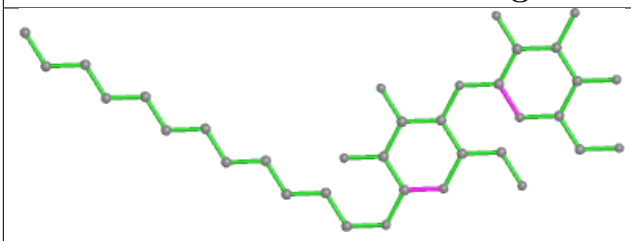
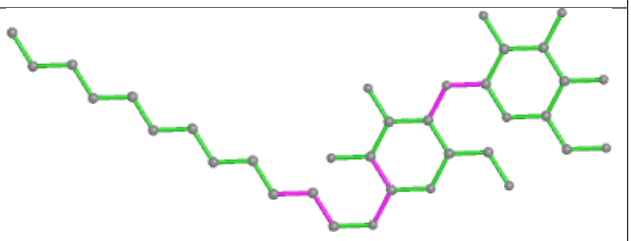
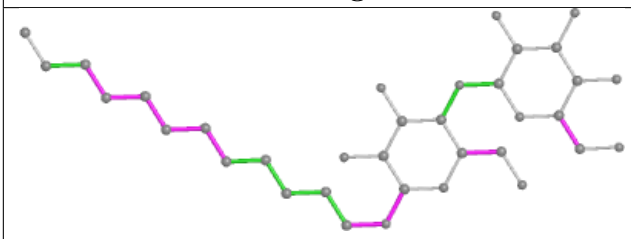
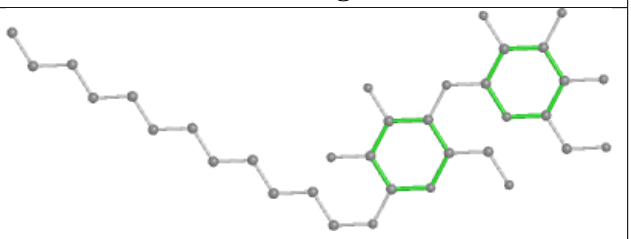


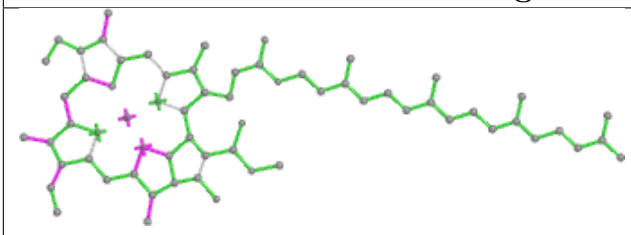
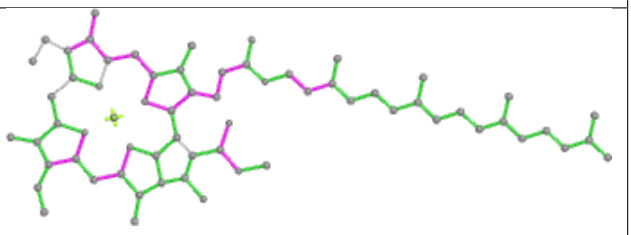
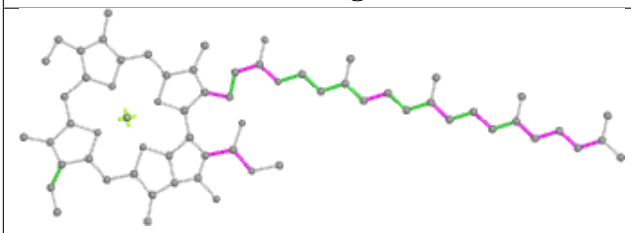
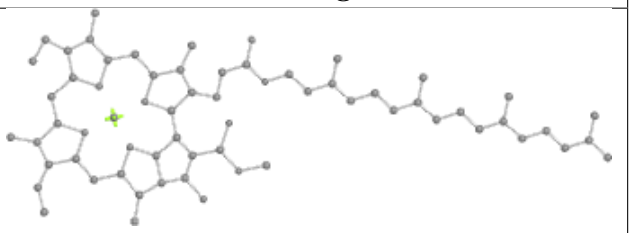
Bond angles



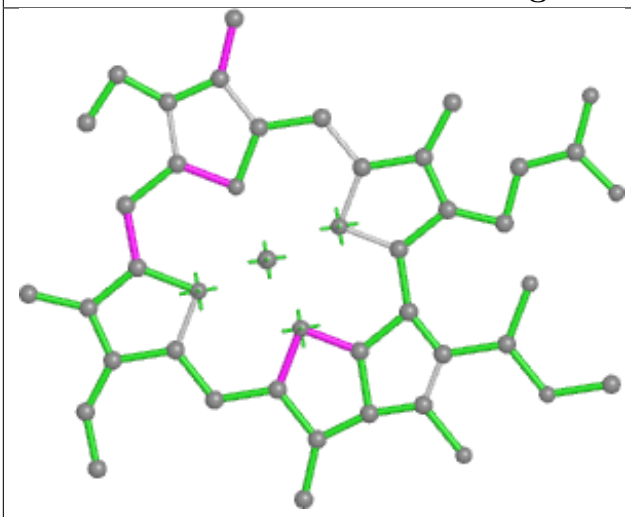
Torsions

Rings

Ligand LMU B 1843	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 511



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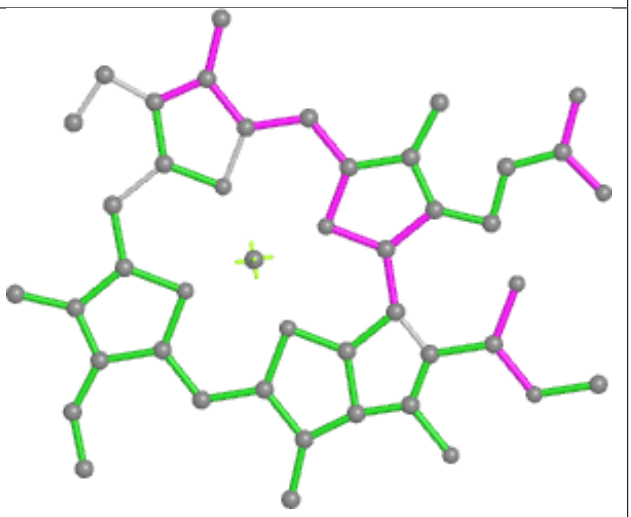
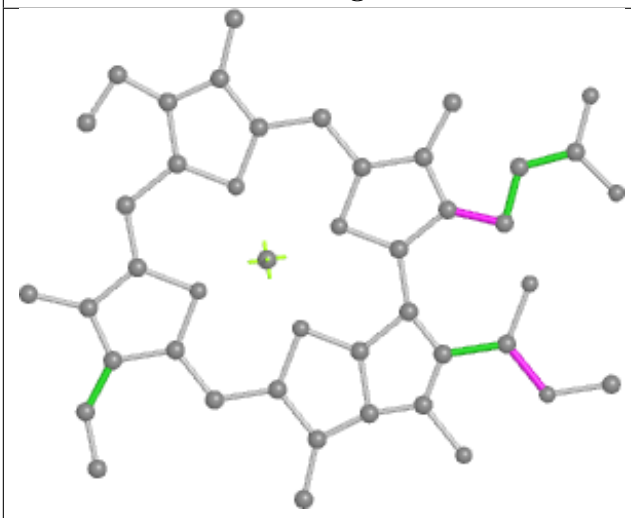


Bond angles



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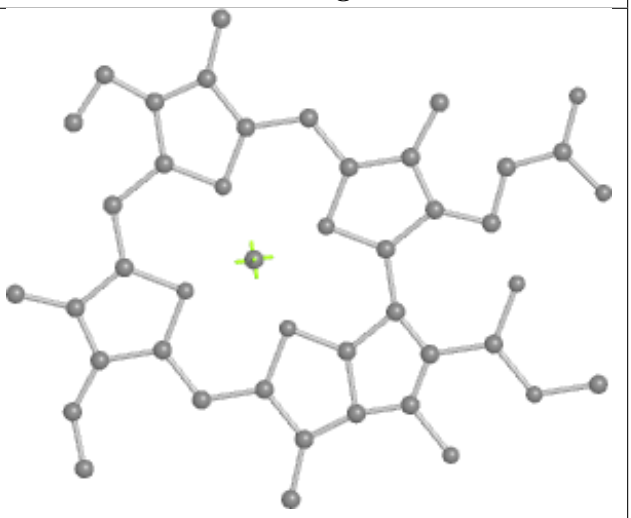
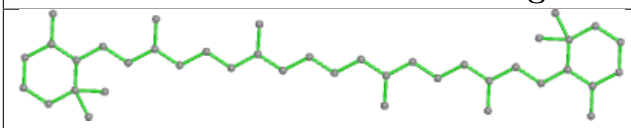


Rings

Ligand BCR r 523



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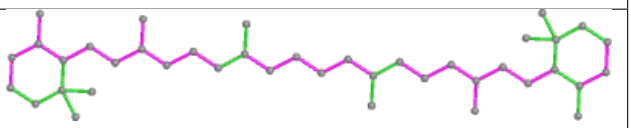
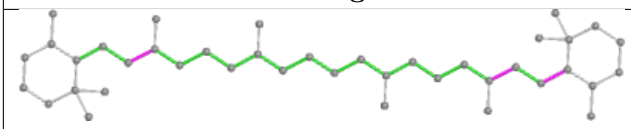


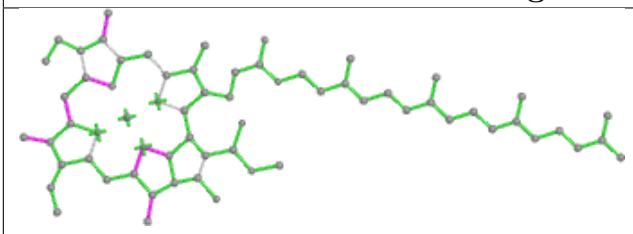
Bond angles



Torsions

Rings

Ligand CLA u 509



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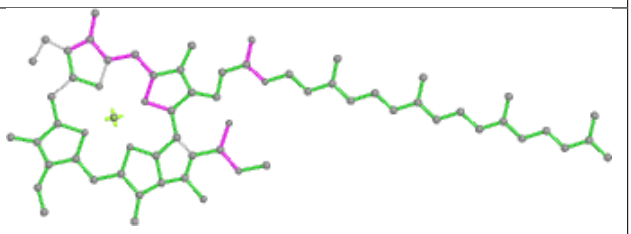
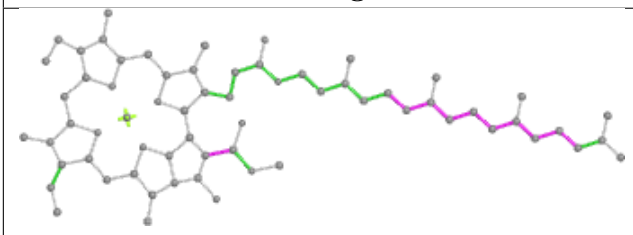


Bond angles



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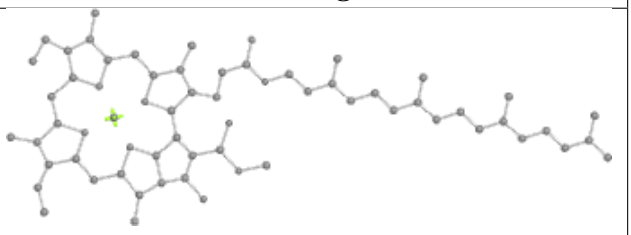
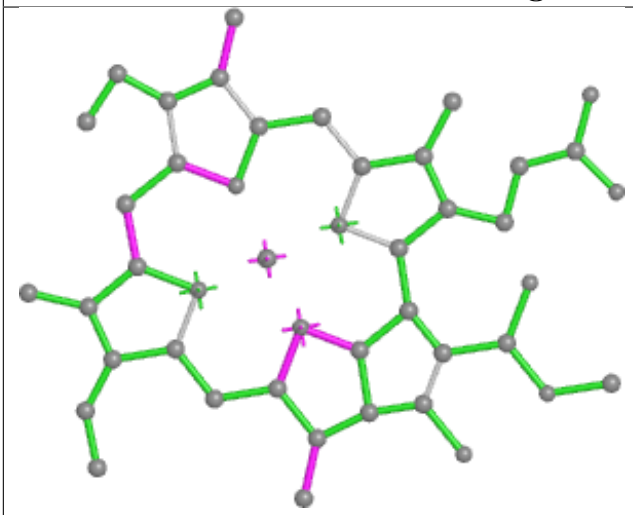


Rings

Ligand CLA u 505



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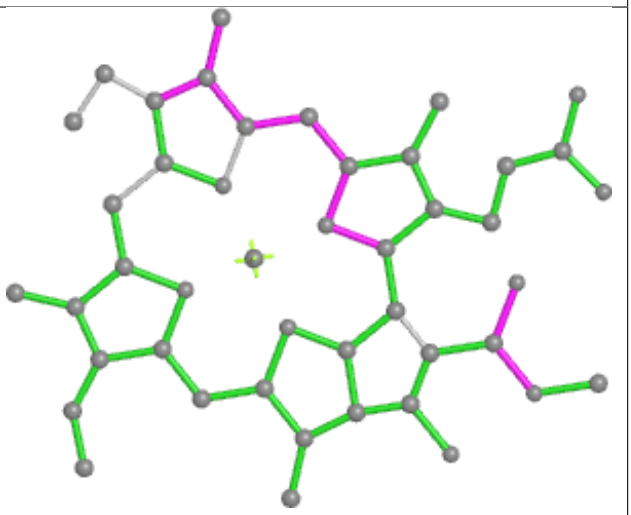
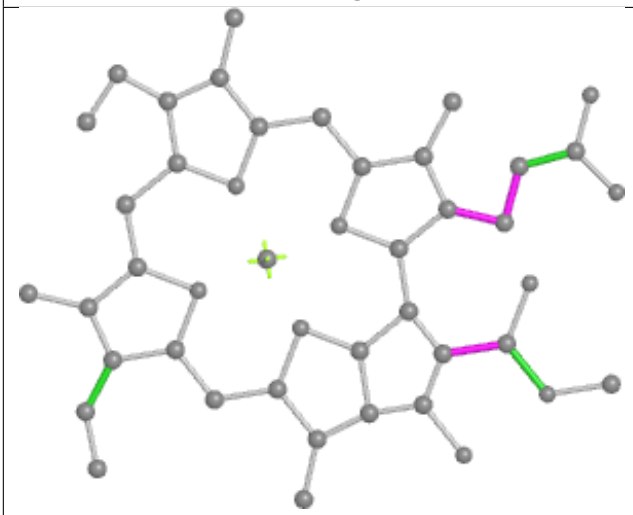


Bond angles



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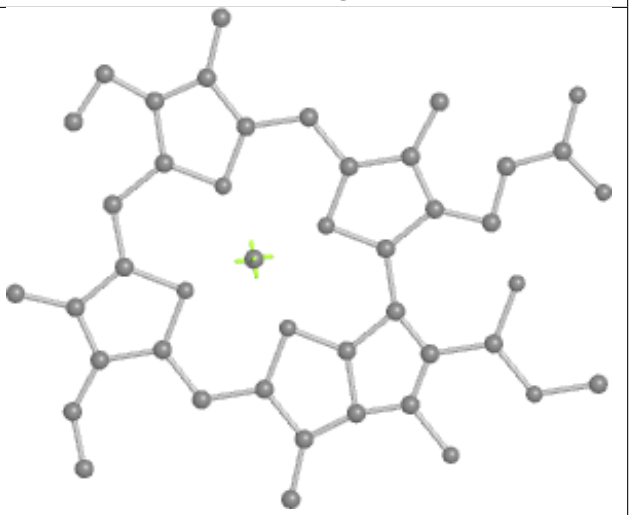
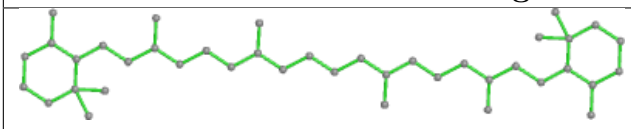


Rings

Ligand BCR G 4011



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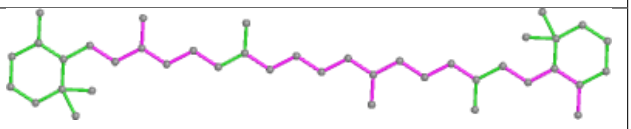
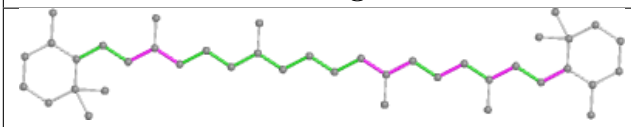


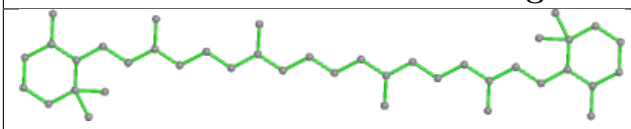
Bond angles



Torsions

Rings

Ligand BCR 3 521



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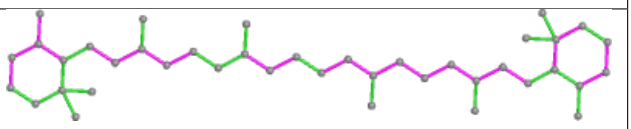
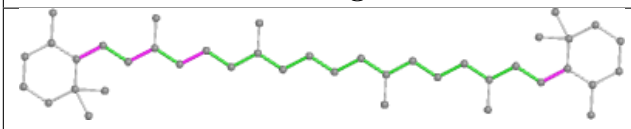


Bond angles



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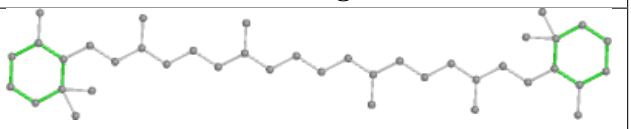
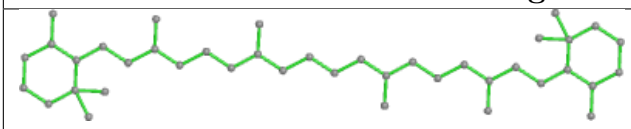


Rings

Ligand BCR r 522



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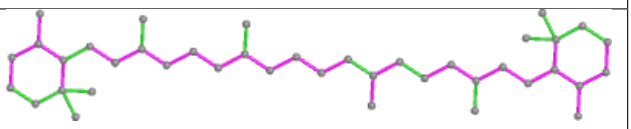

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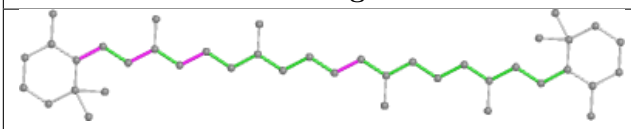

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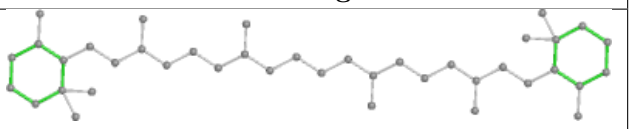
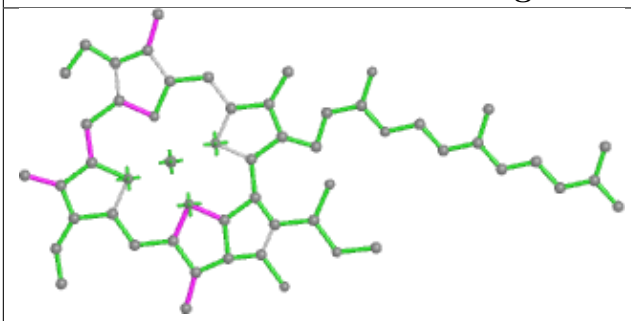
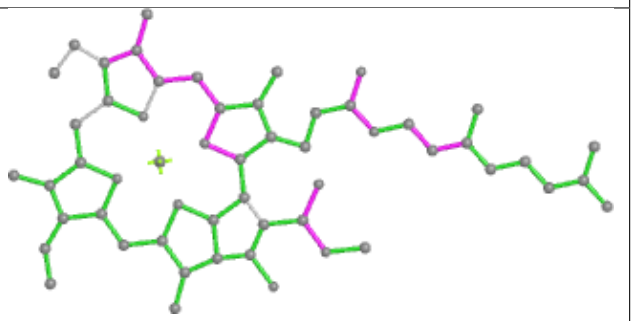
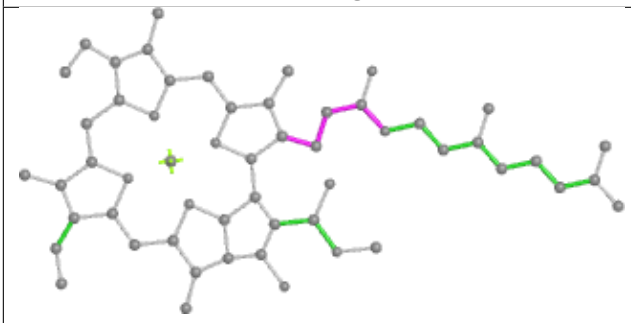
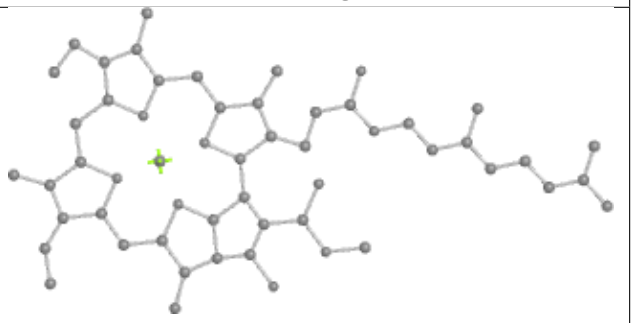
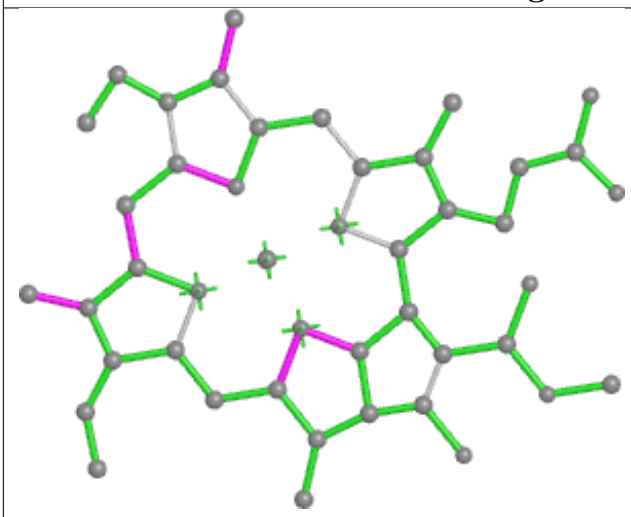


Rings

Ligand CLA H 1228	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 506



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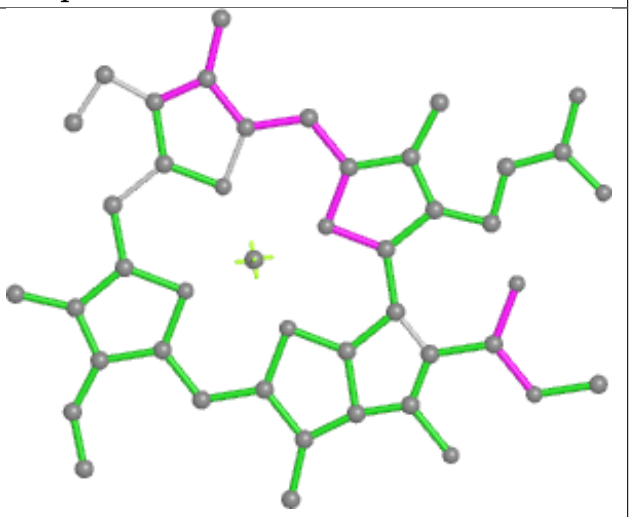
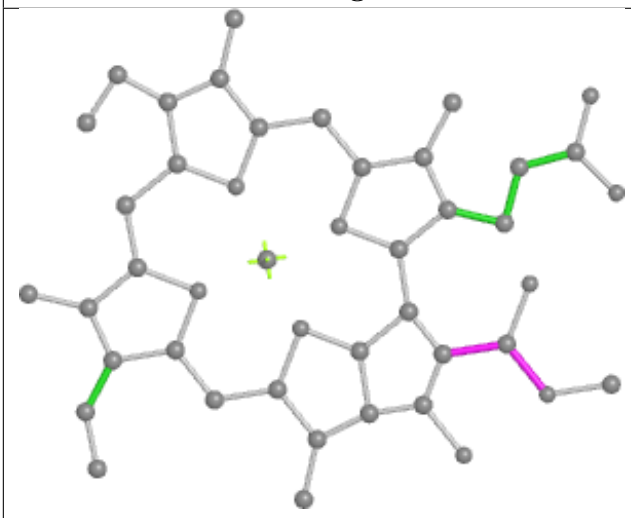


Bond angles



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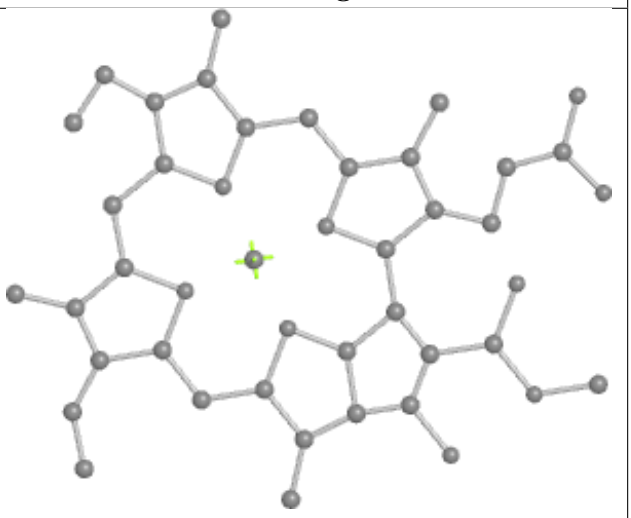
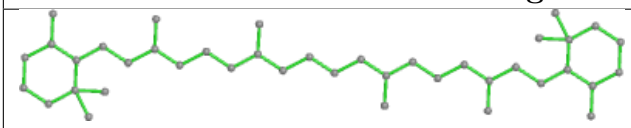


Rings

Ligand BCR 6 521



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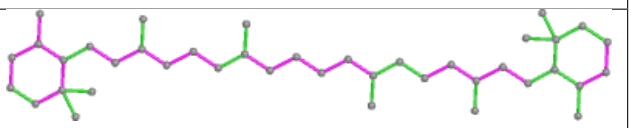
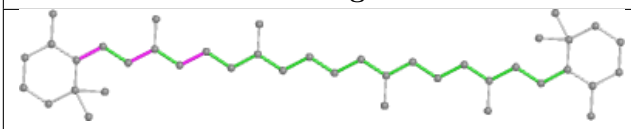


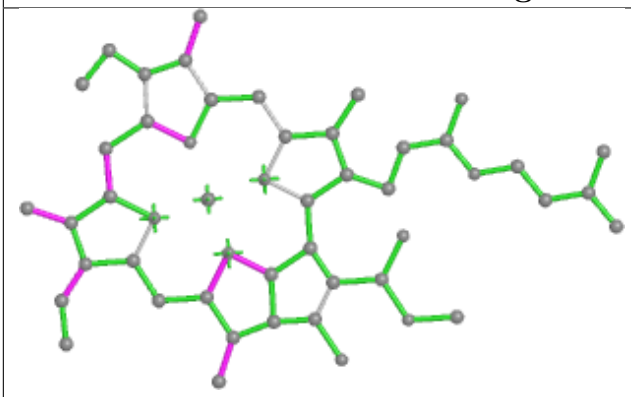
Bond angles



Torsions

Rings

Ligand CLA A 1120



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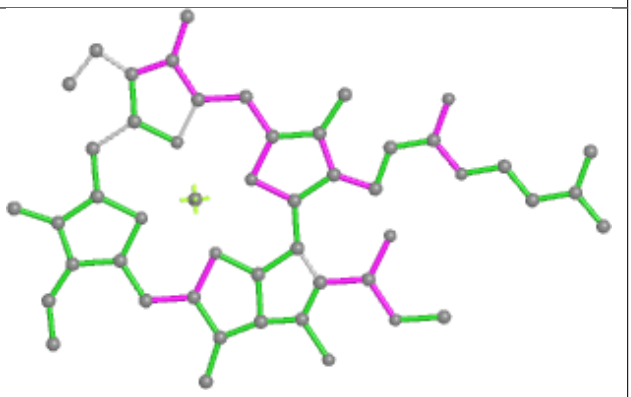
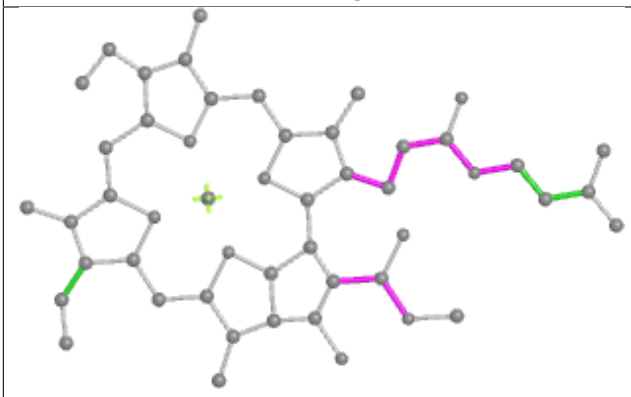
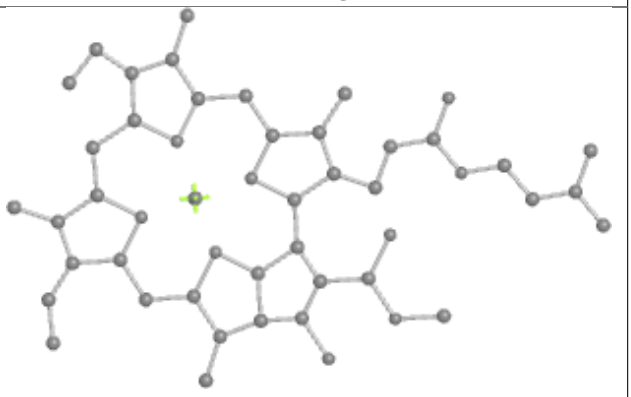


Bond angles

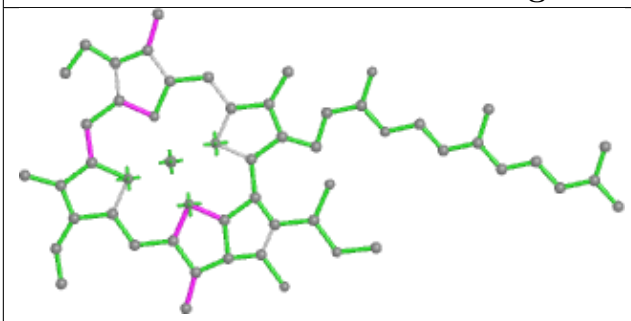


Torsions

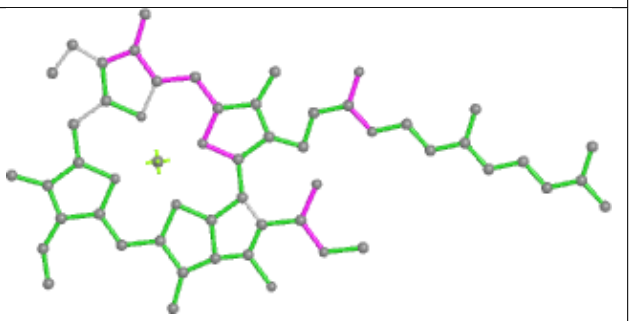


Rings

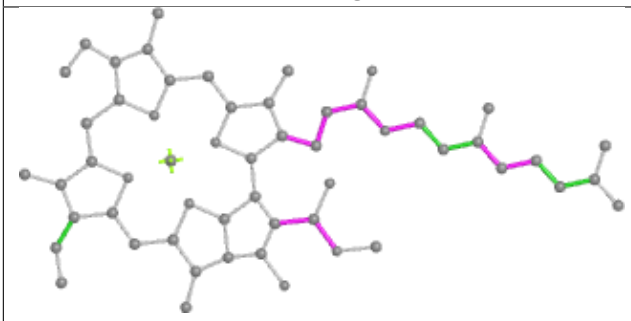
Ligand CLA 2 518



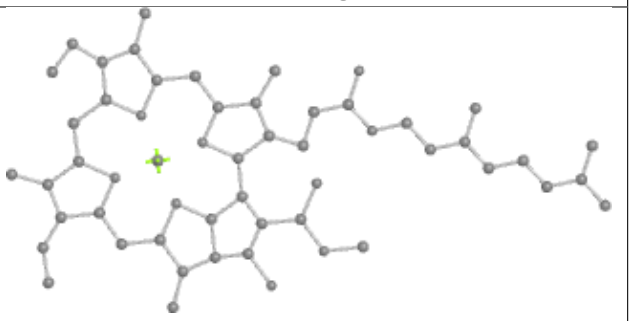
Bond lengths



Bond angles

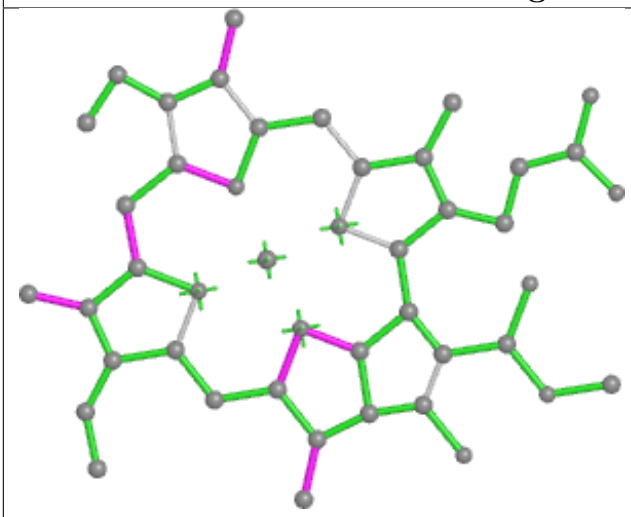


Torsions



Rings

Ligand CLA 5 510



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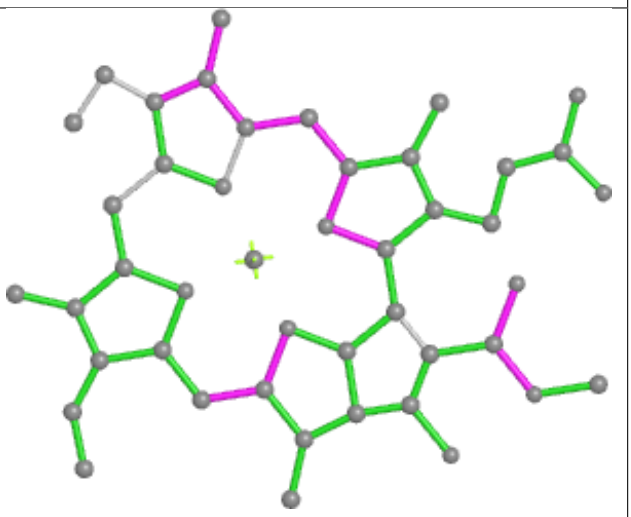

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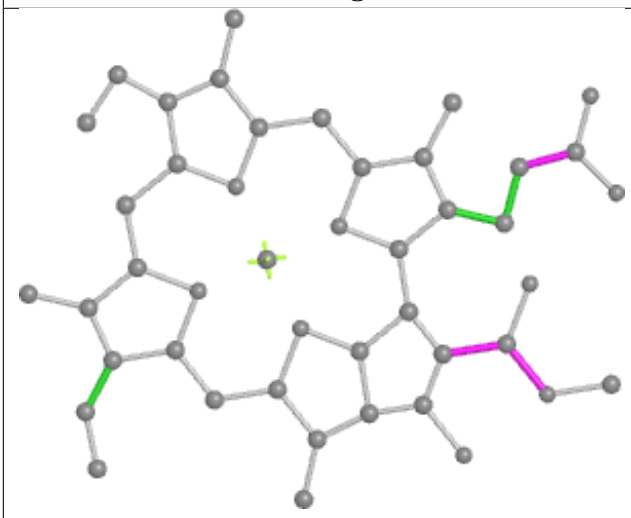

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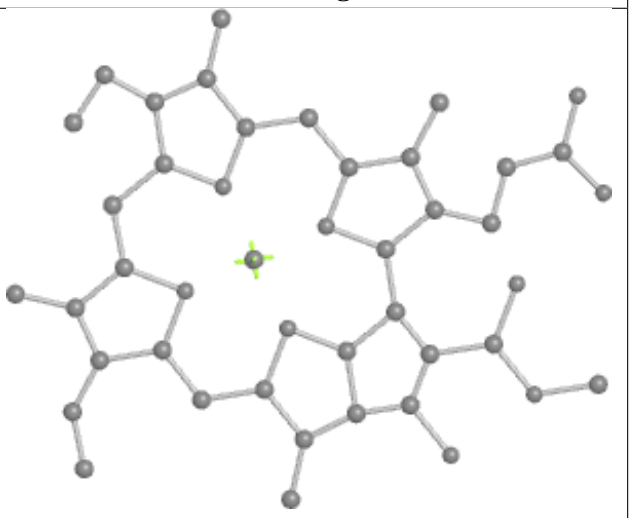
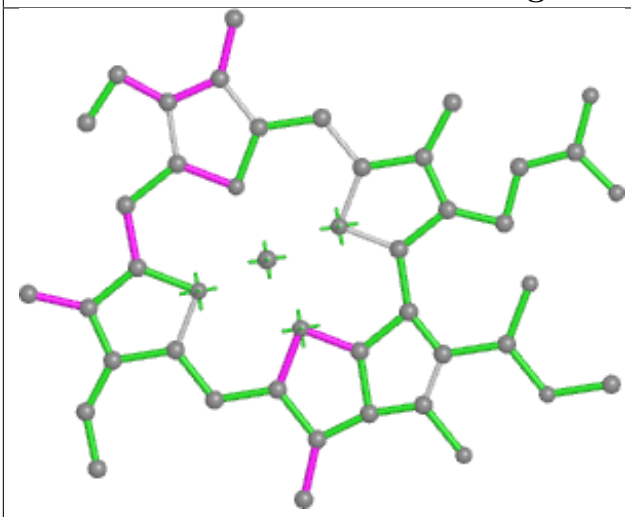


Rings

Ligand CLA d 519



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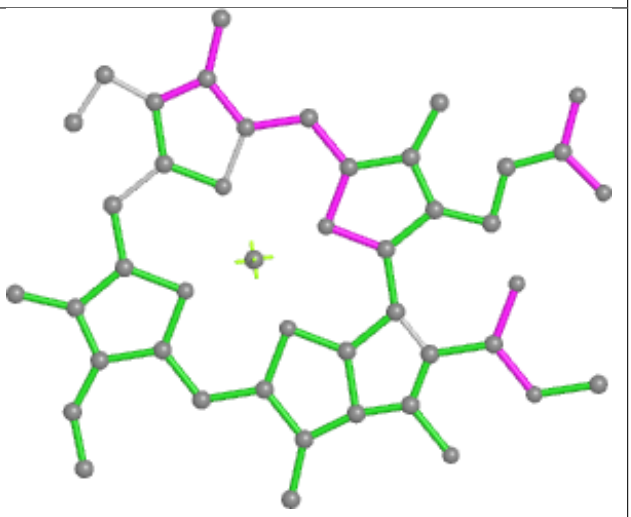
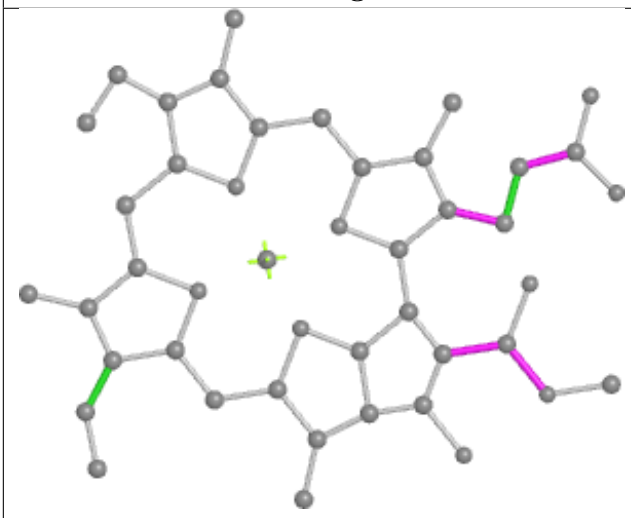


Bond angles



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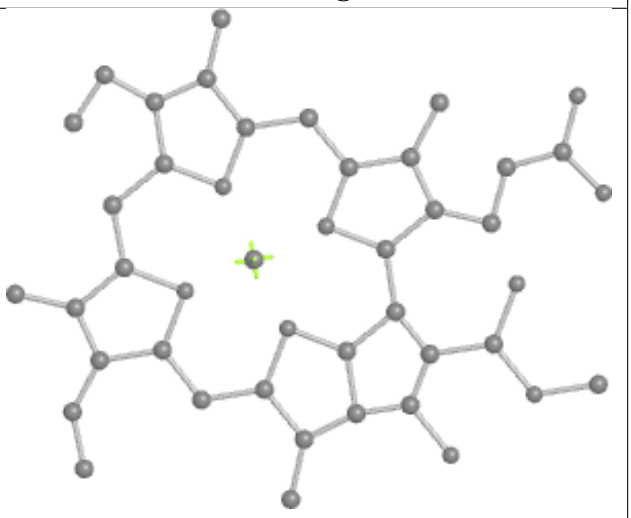
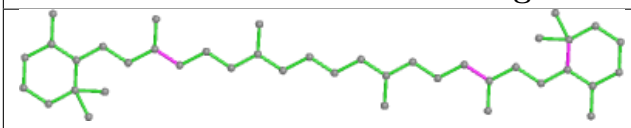


Rings

Ligand BCR B 4017



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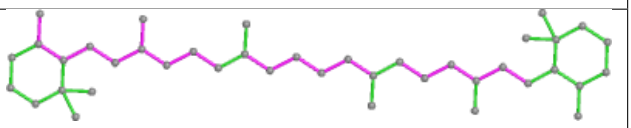

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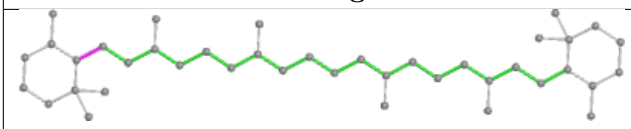
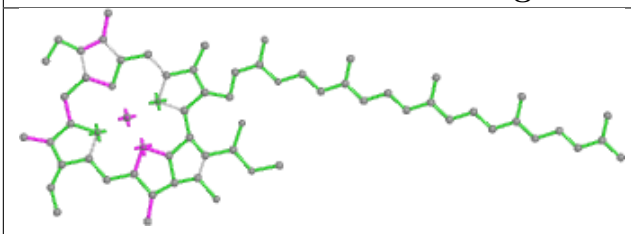


Torsions

Rings

Ligand CLA G 1101



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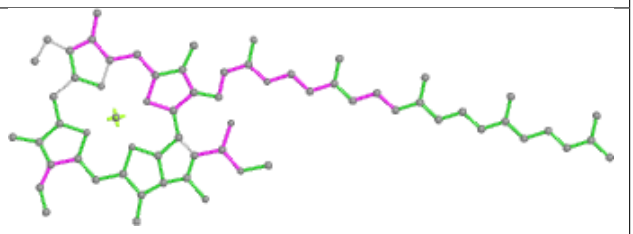
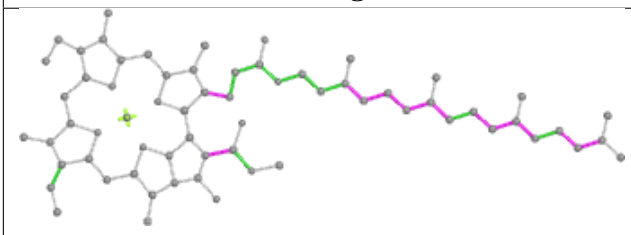


Bond angles



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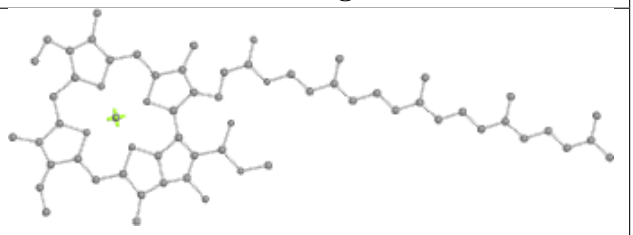
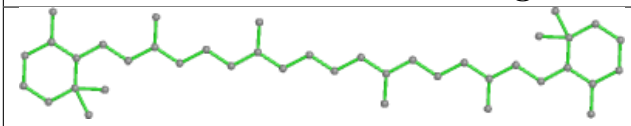


Rings

Ligand BCR T 4013



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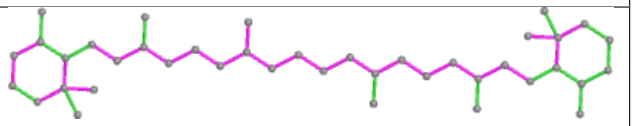

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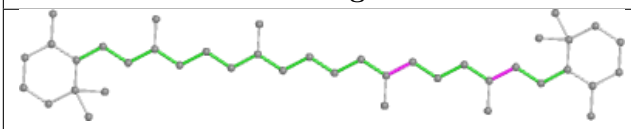

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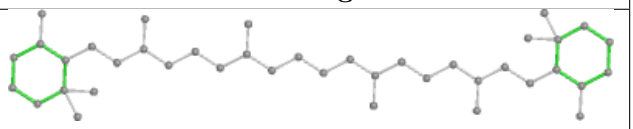
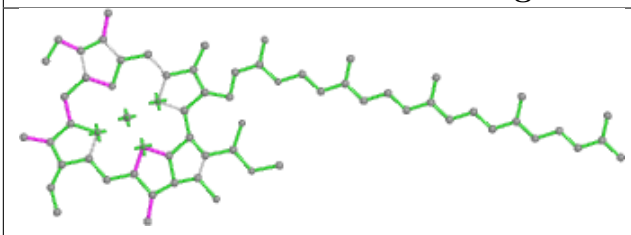


Rings

Ligand CLA H 1208



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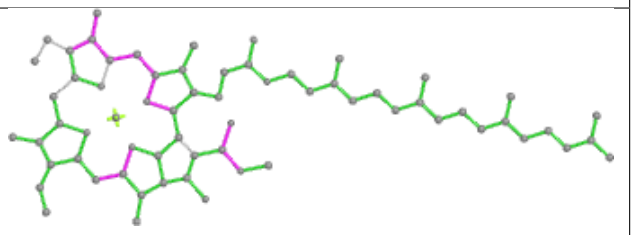
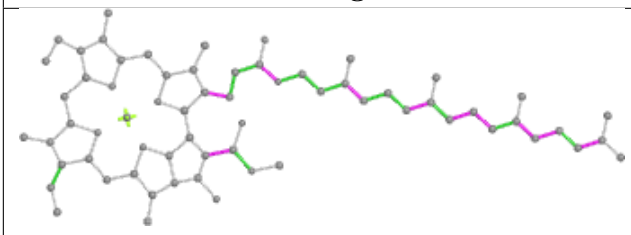


Bond angles



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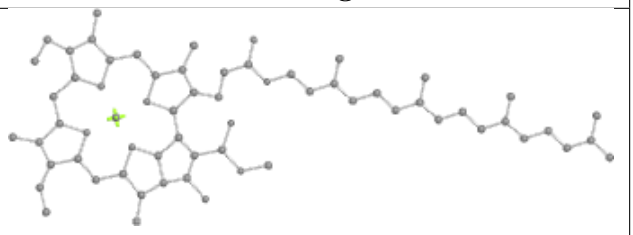
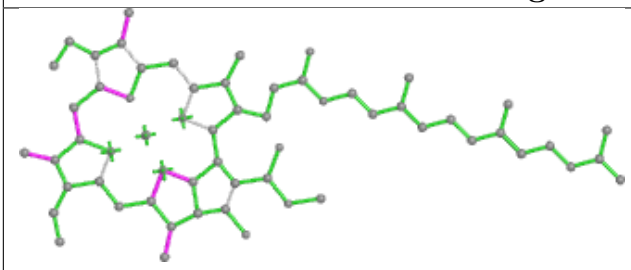
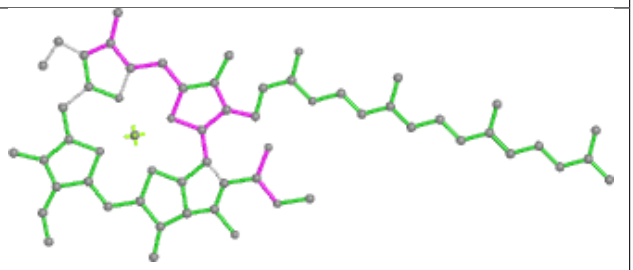
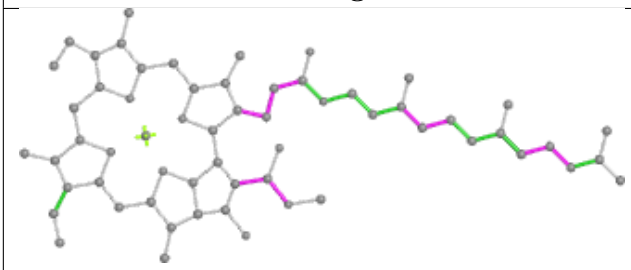
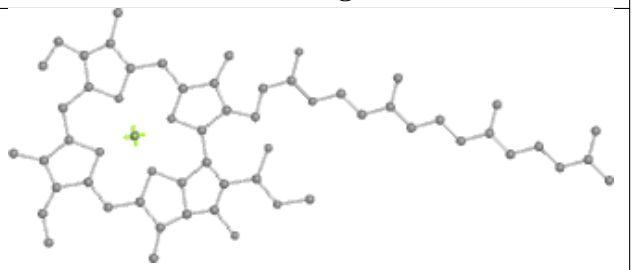


Rings

Ligand CLA 2 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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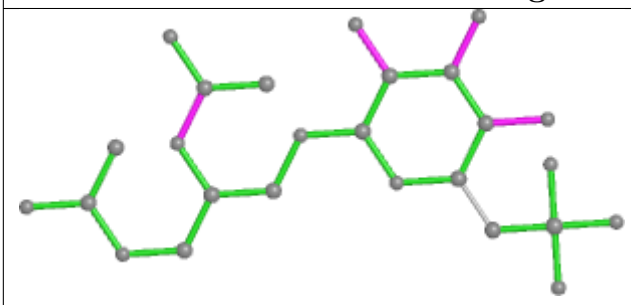
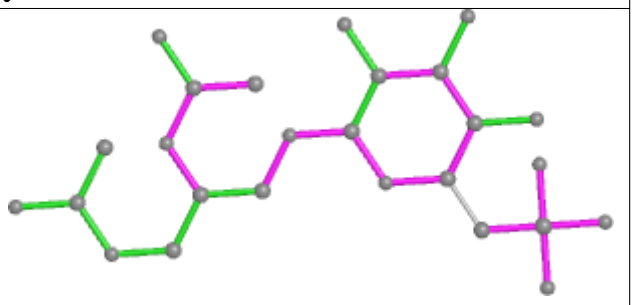
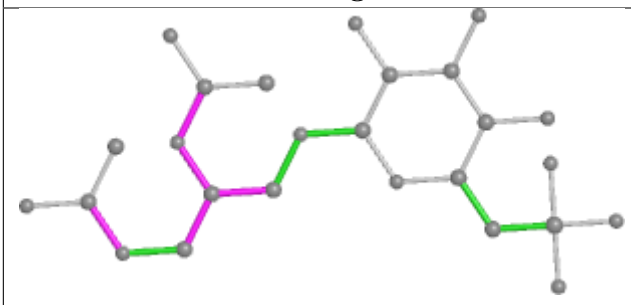
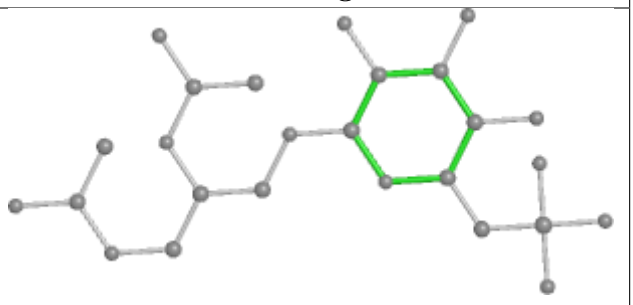
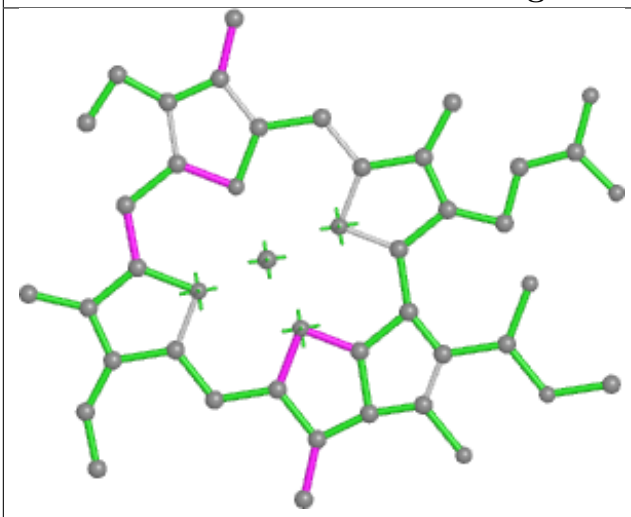
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 510



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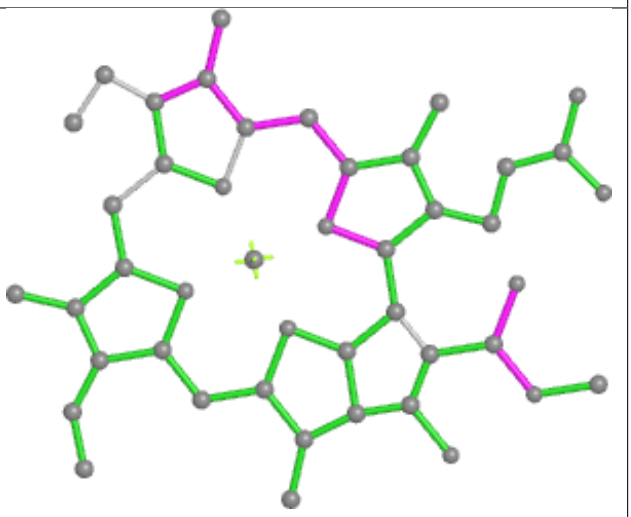

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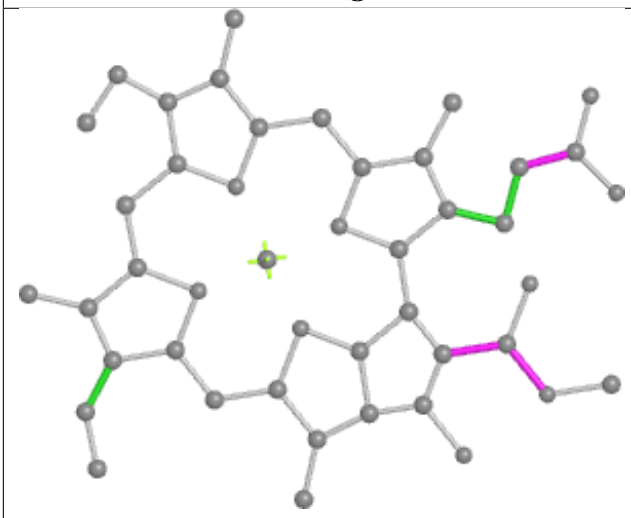
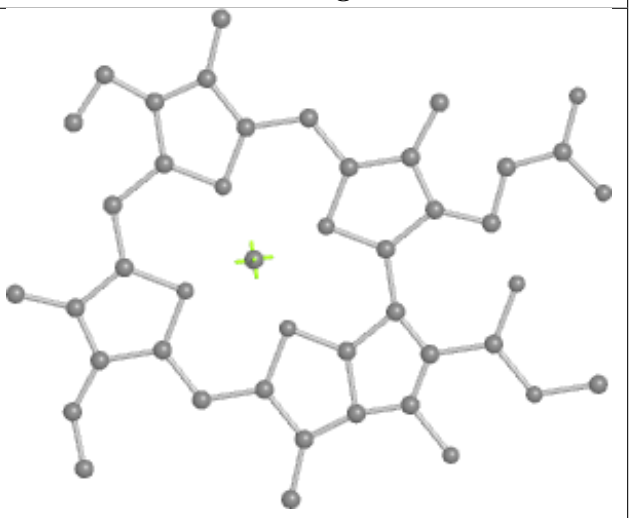
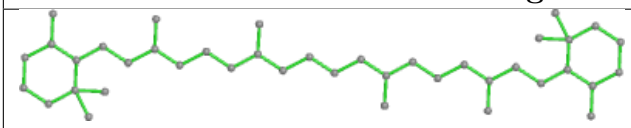


Torsions



Rings

Ligand BCR 6 523



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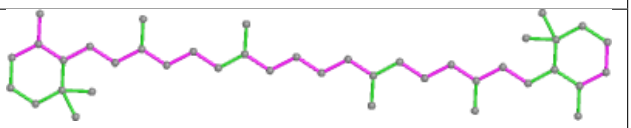
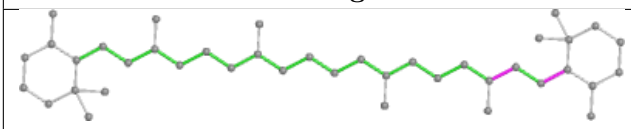


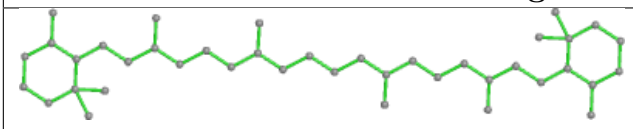
Bond angles



Torsions

Rings

Ligand BCR r 521



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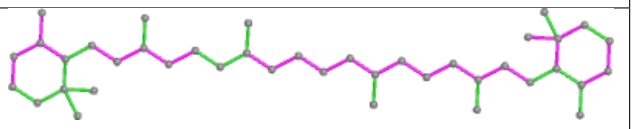
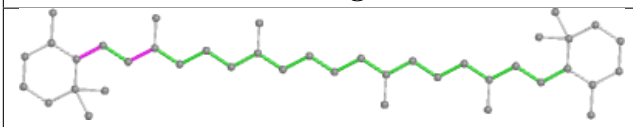
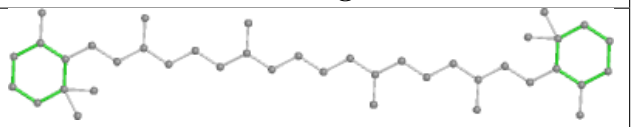


Bond angles

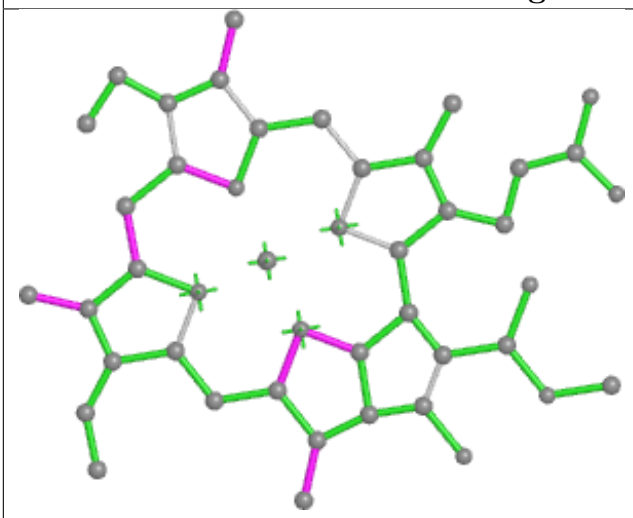


Torsions



Rings

Ligand CLA 6 517



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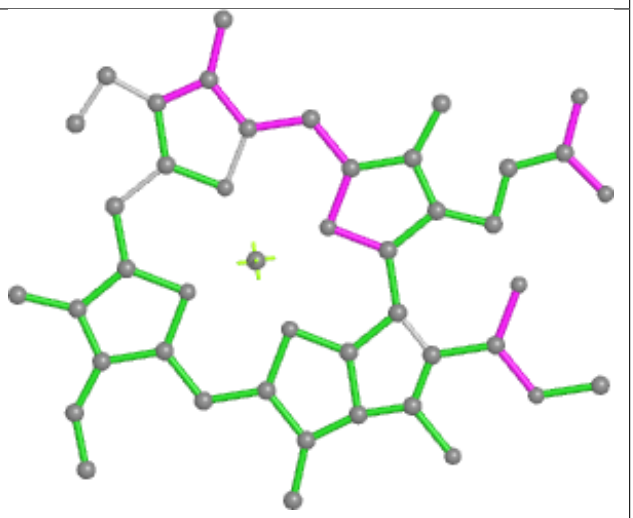
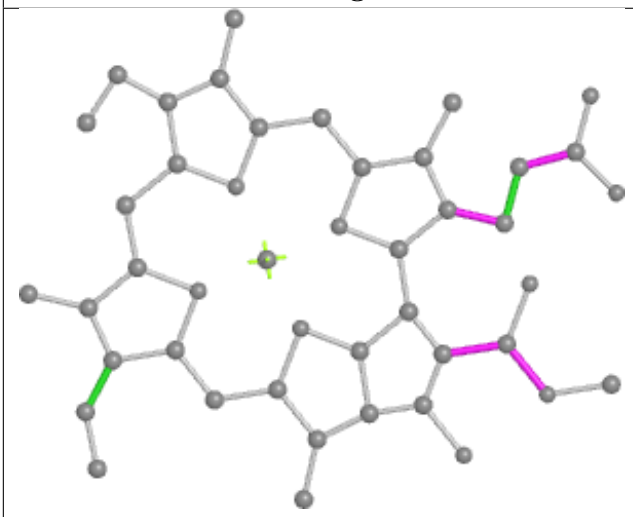
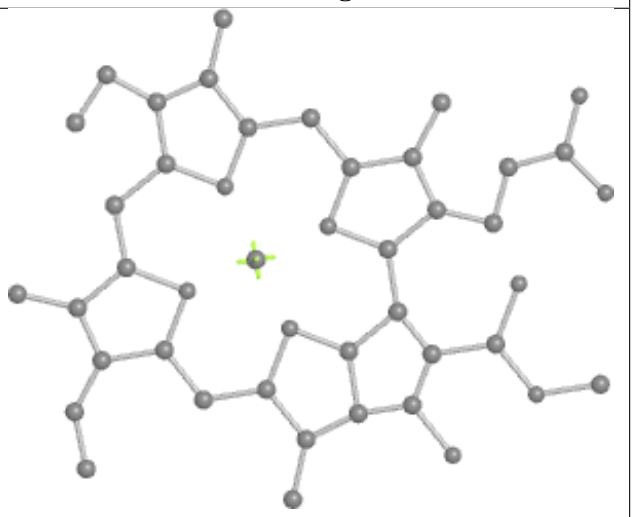


Bond angles

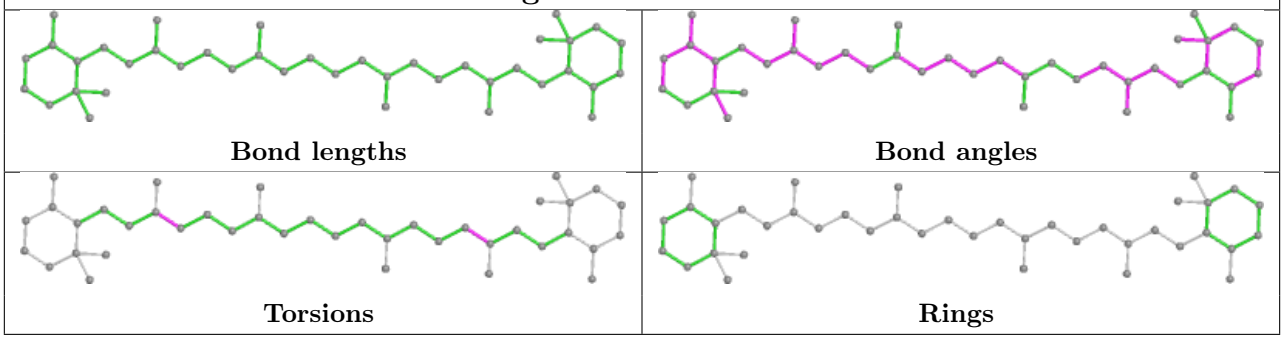


Torsions

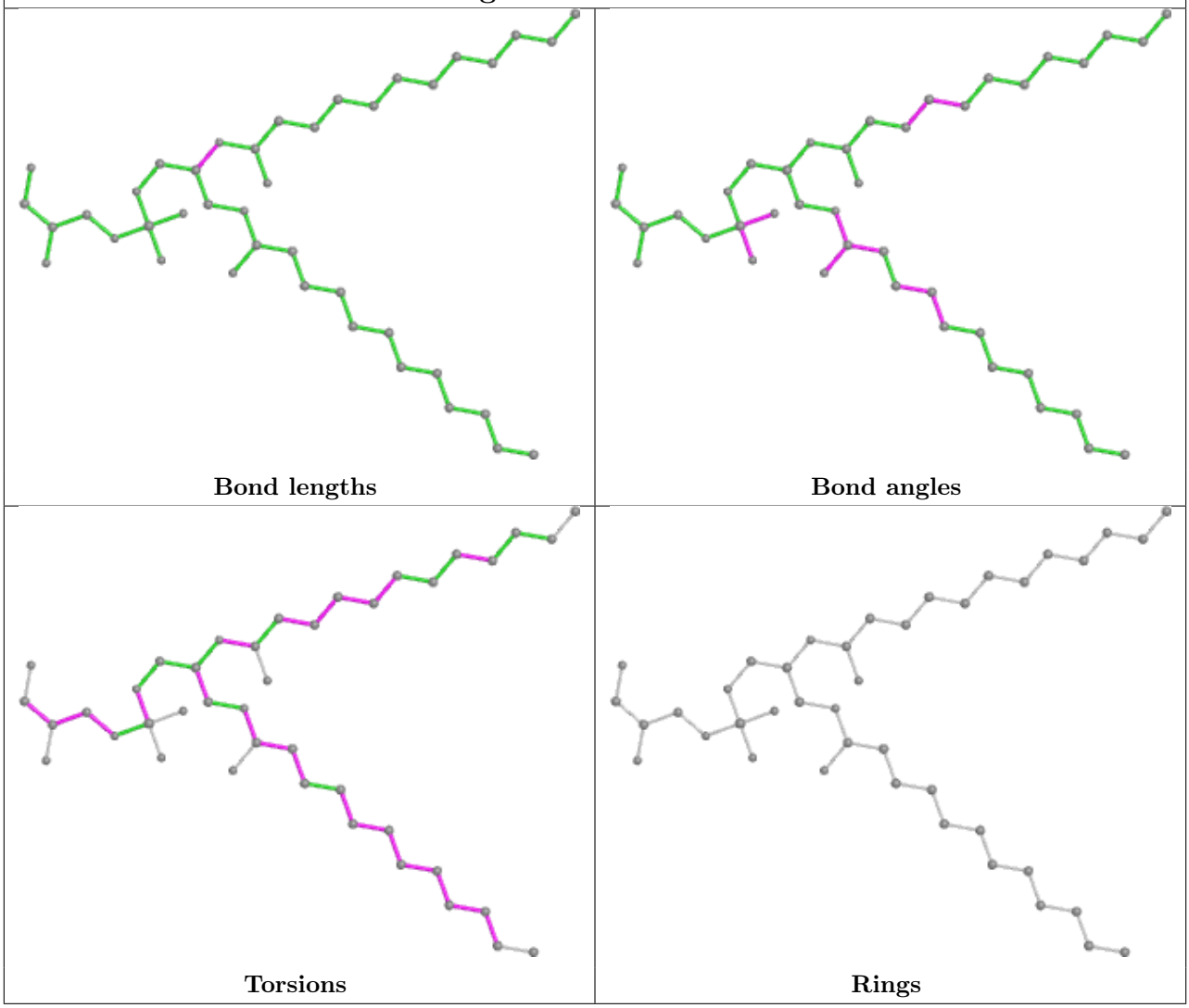


Rings

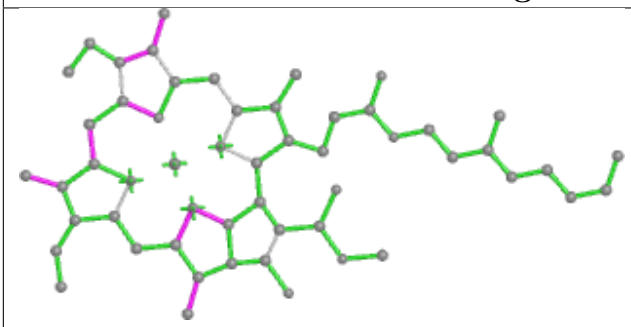
Ligand BCR f 4006



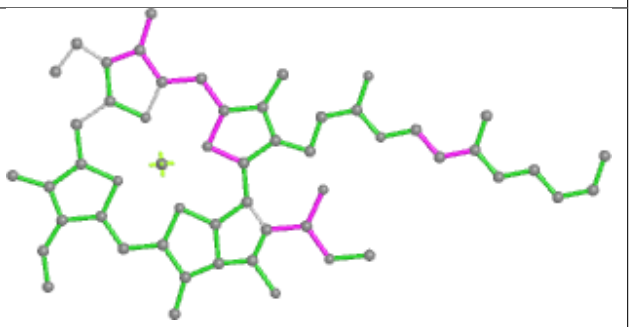
Ligand LHG n 5220



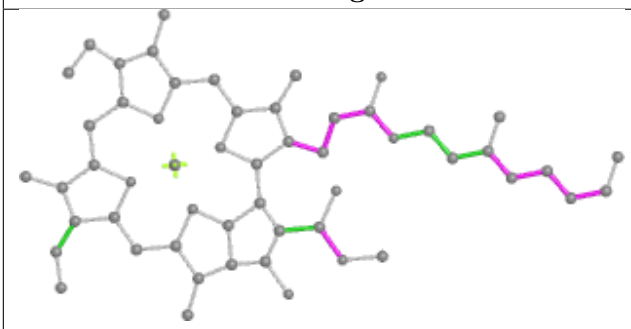
Ligand CLA G 1108



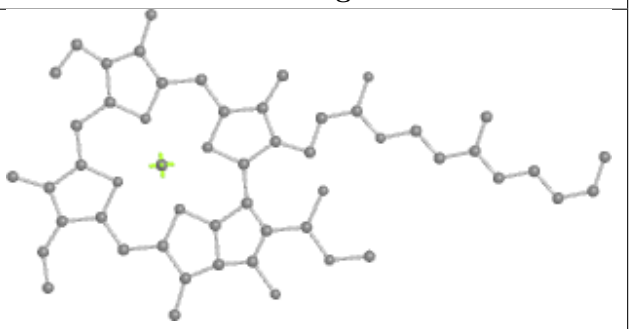
Bond lengths



Bond angles

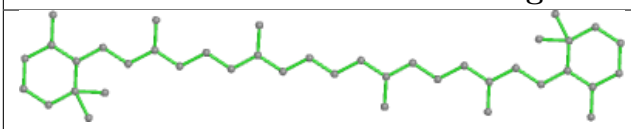


Torsions

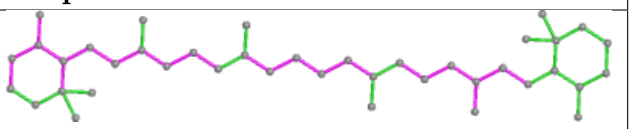


Rings

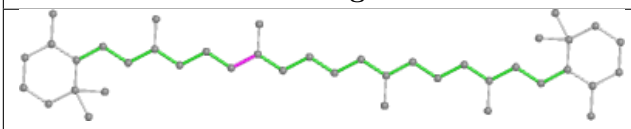
Ligand BCR q 524



Bond lengths



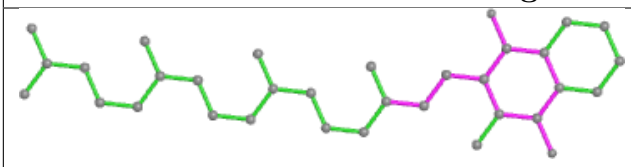
Bond angles



Torsions

Rings

Ligand PQN f 2002



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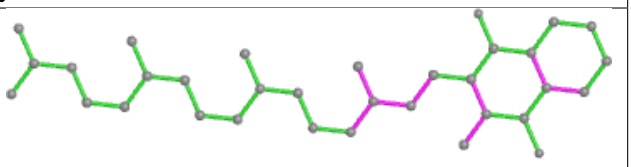
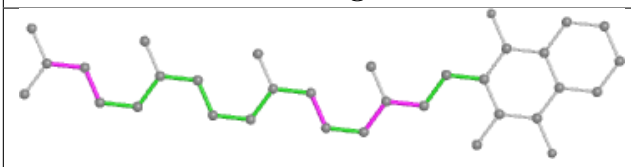
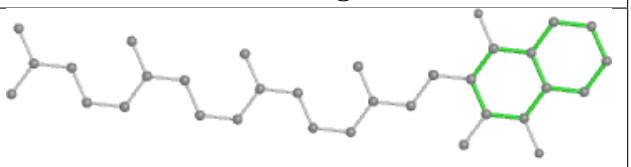


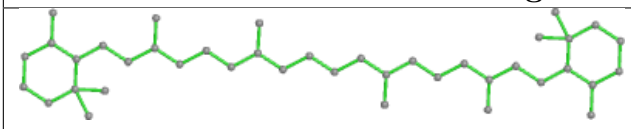
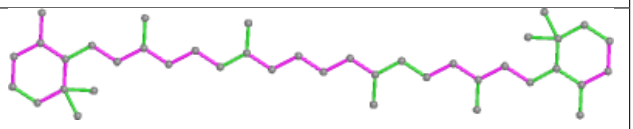
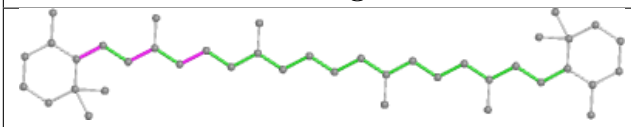
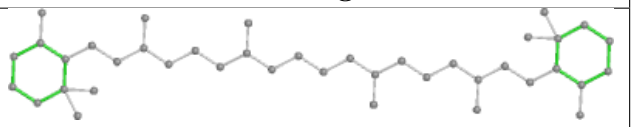
Bond angles

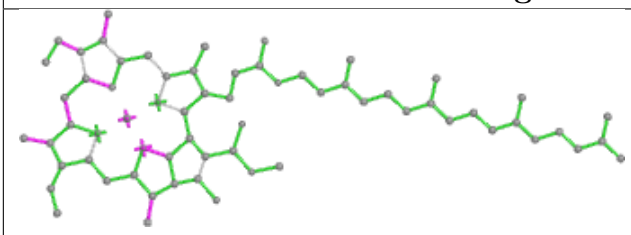
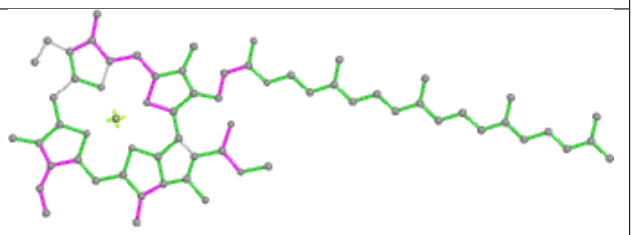
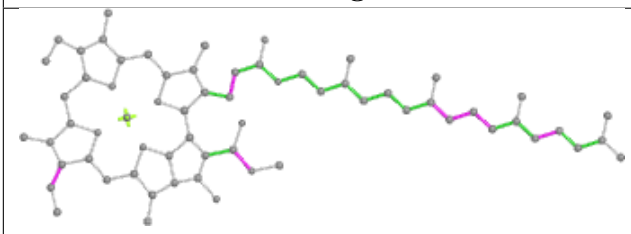
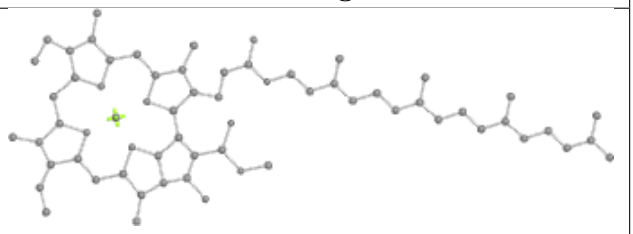


Torsions

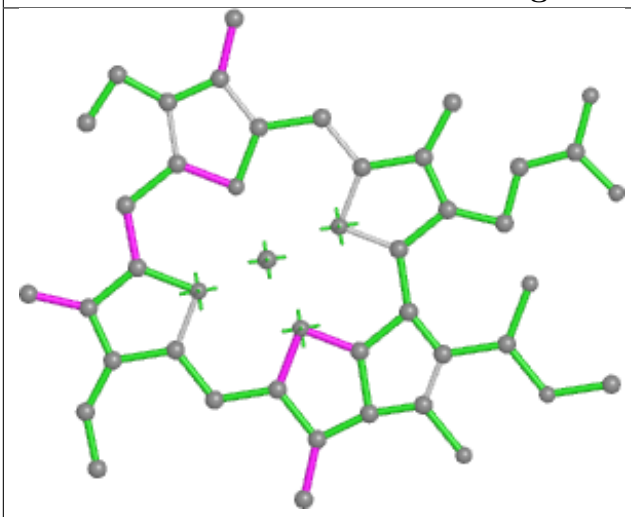


Rings

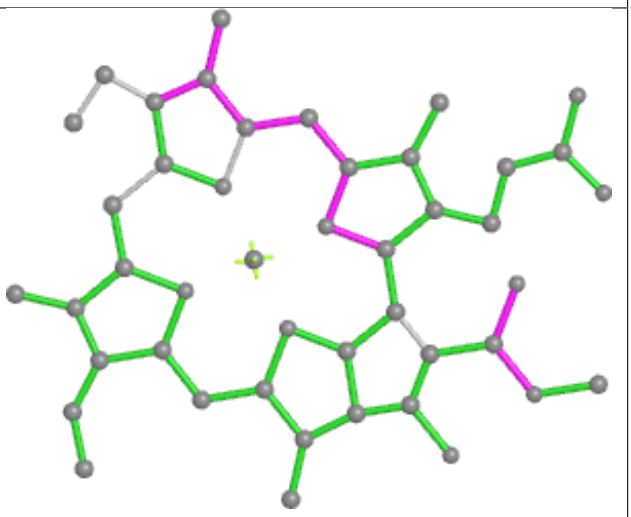
Ligand BCR d 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 1023	
 Bond lengths	 Bond angles
 Torsions	 Rings

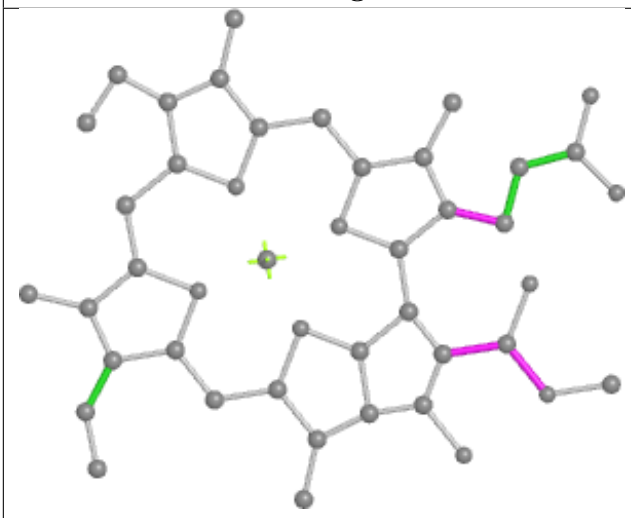
Ligand CLA t 506



Bond lengths



Bond angles



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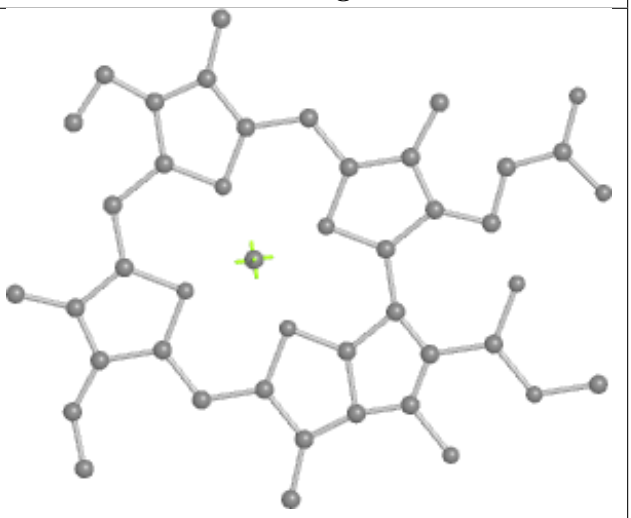
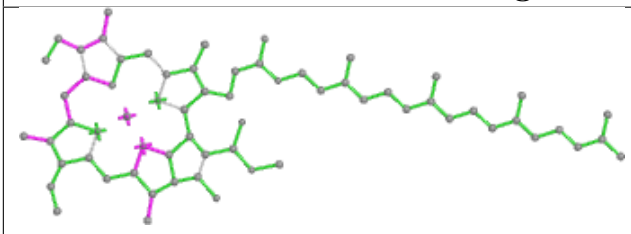


Rings

Ligand CLA G 1119



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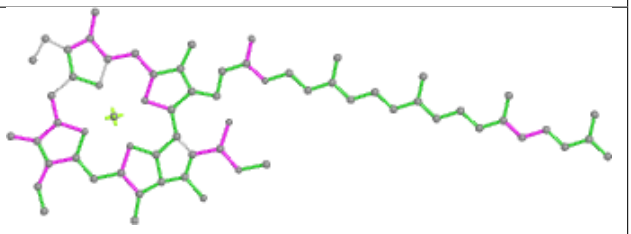
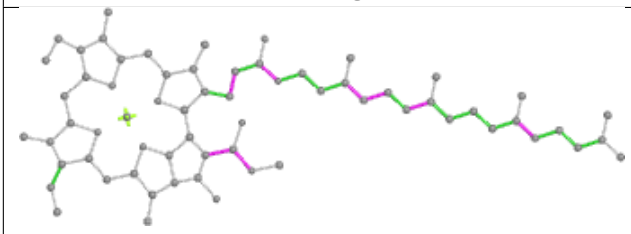


Bond angles



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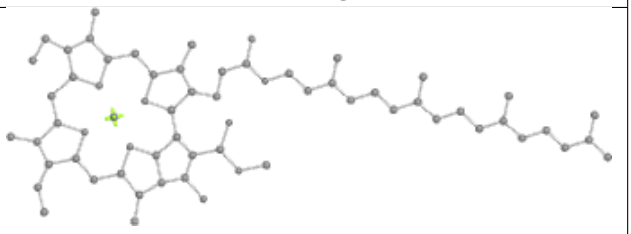
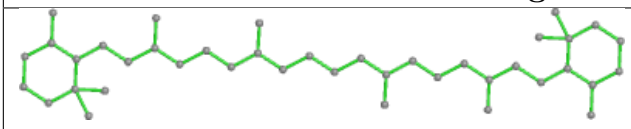
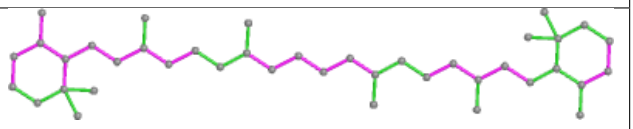
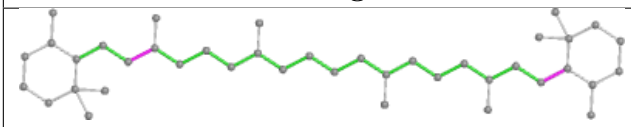
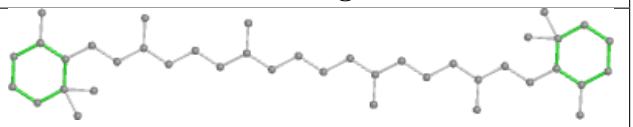


Rings

Ligand BCR t 524	
 Bond lengths	 Bond angles
 Torsions	 Rings

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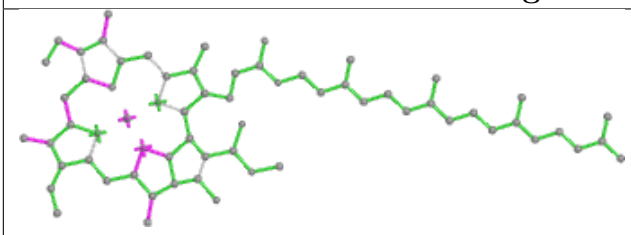
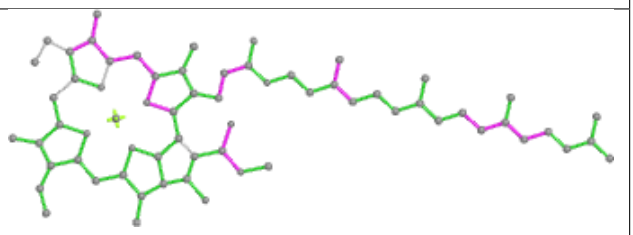
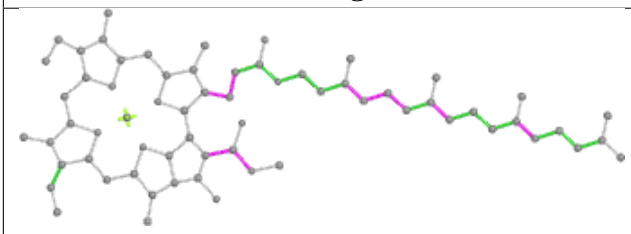
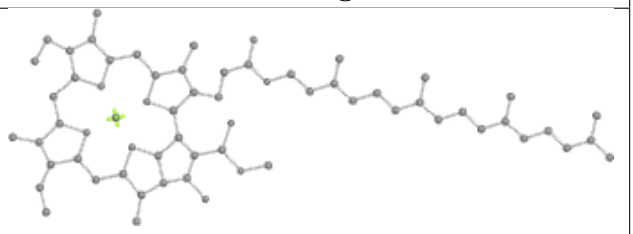
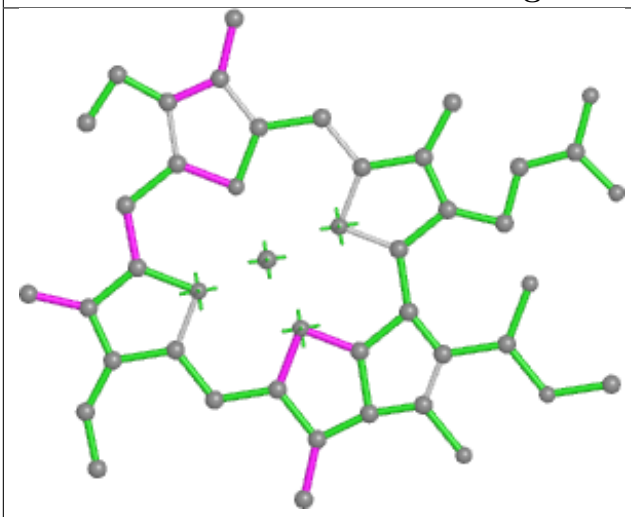
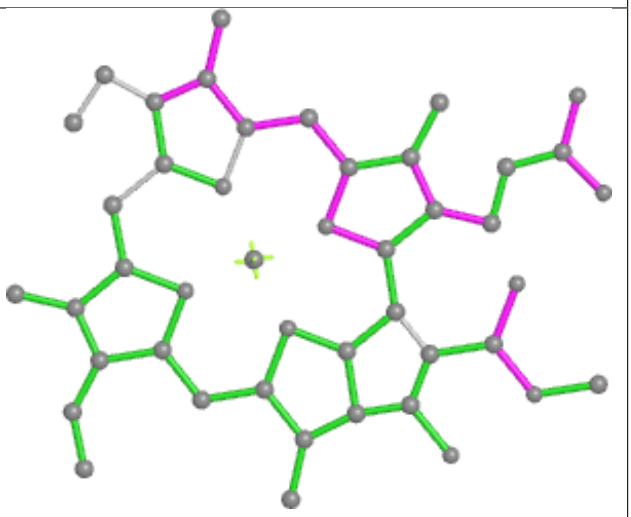
 Bond lengths	 Bond angles
 Torsions	 Rings

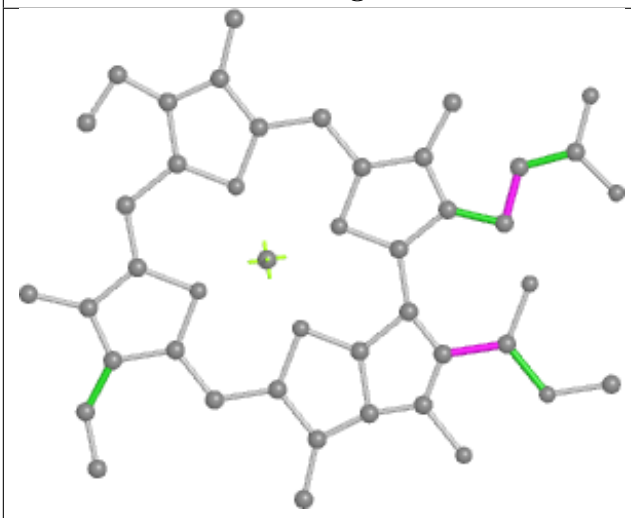
Ligand CLA Y 502



Bond lengths



Bond angles



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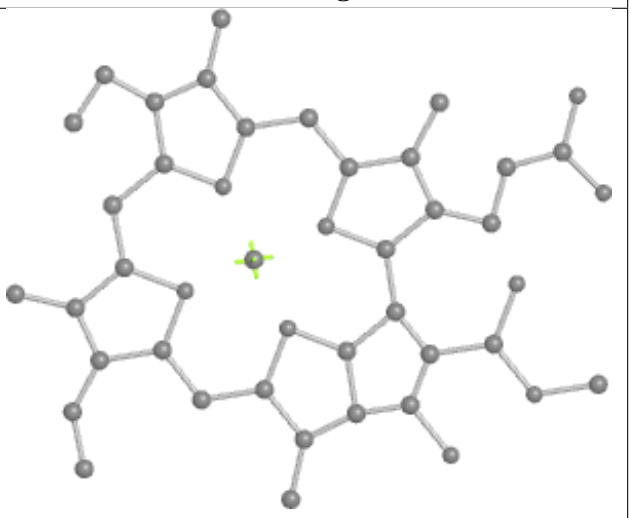
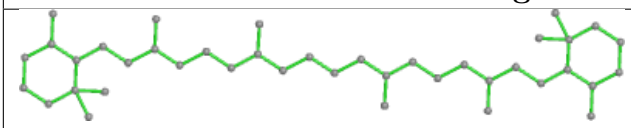


Rings

Ligand BCR V 4019



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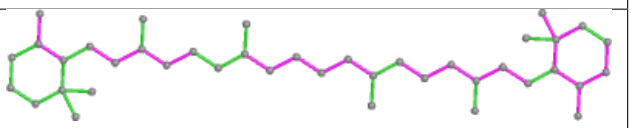
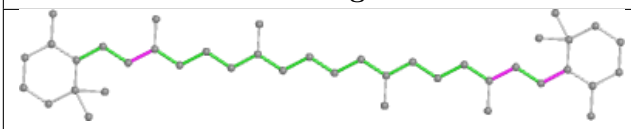


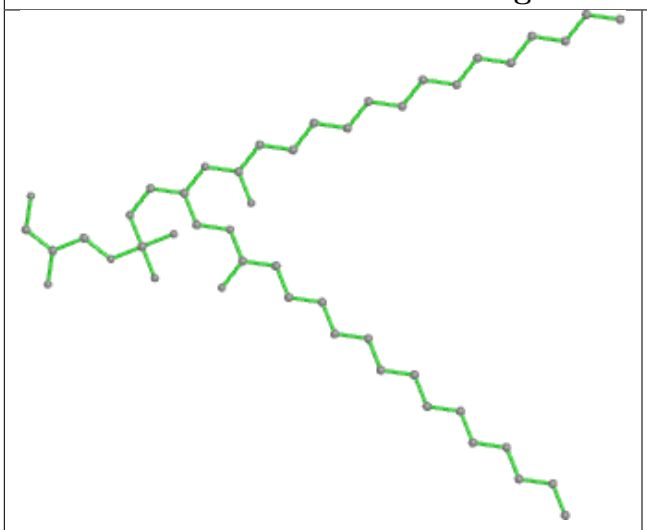
Bond angles



Torsions

Rings

Ligand LHG A 5007



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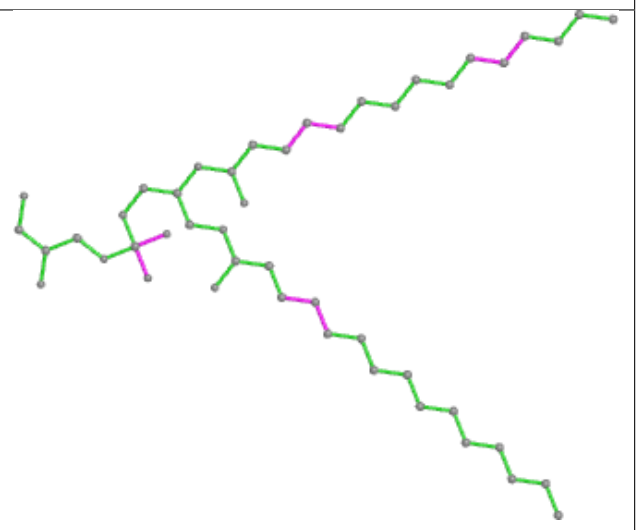
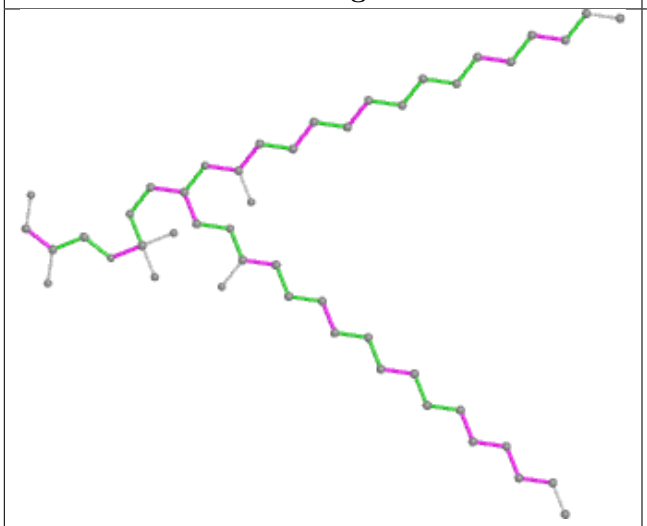
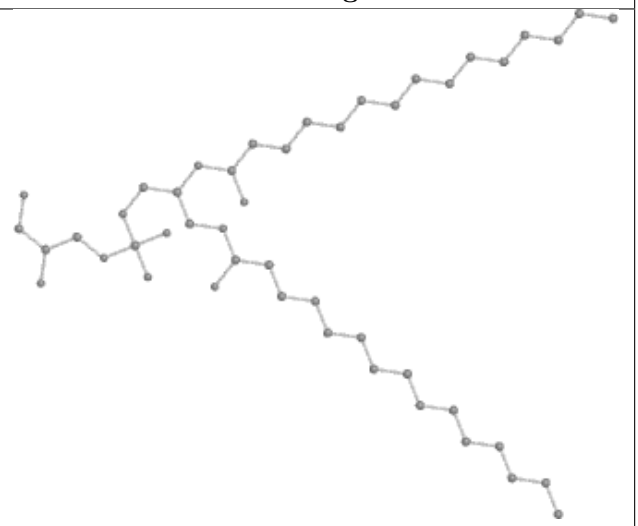


Bond angles

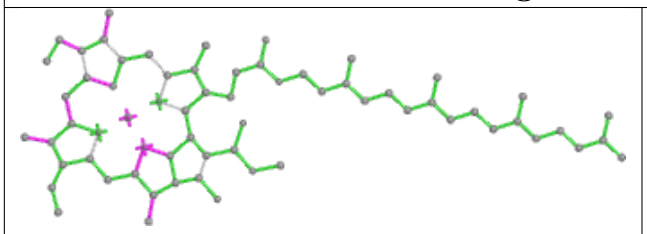


Torsions



Rings

Ligand CLA H 1203



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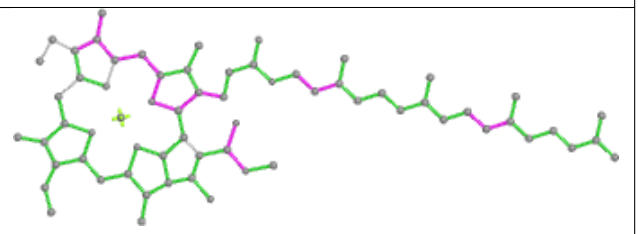
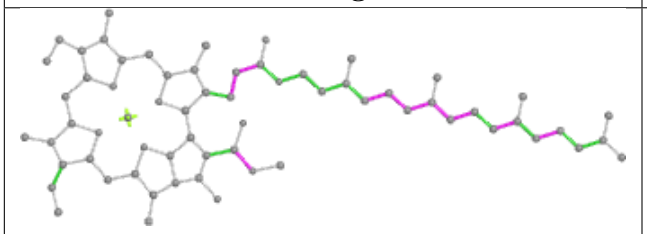


Bond angles



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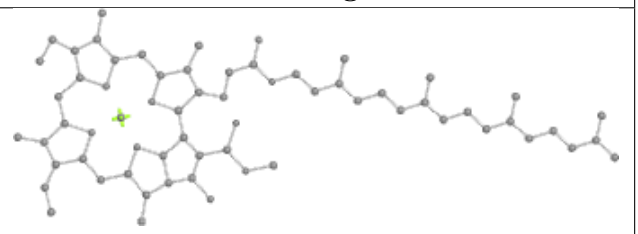
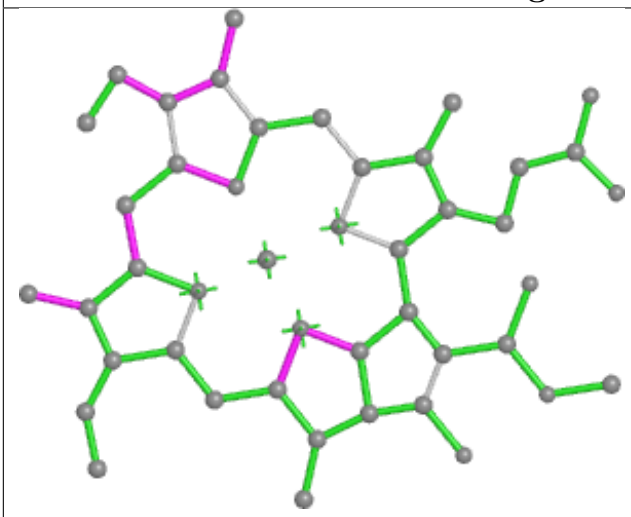


Rings

Ligand CLA 3 519



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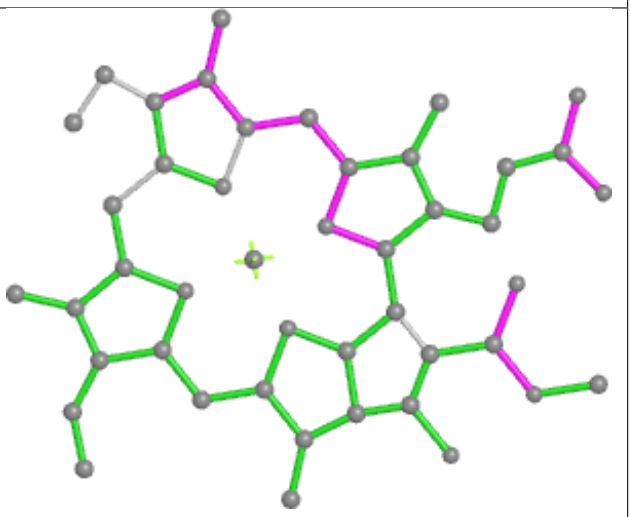
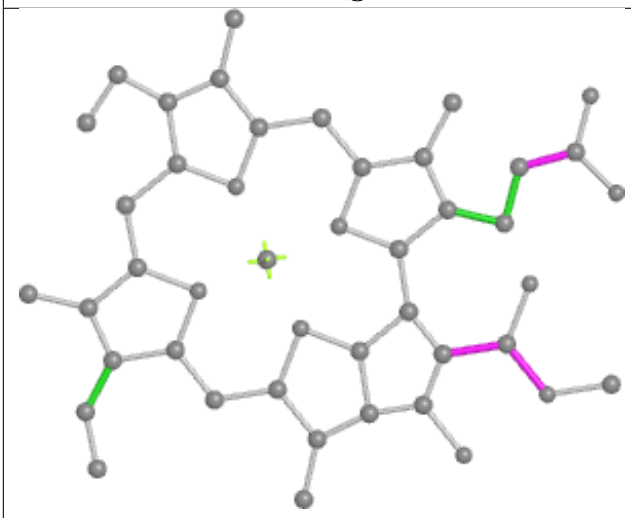
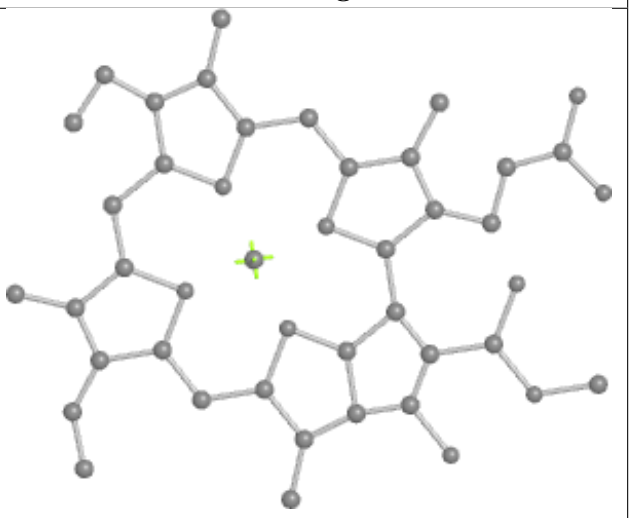


Bond angles

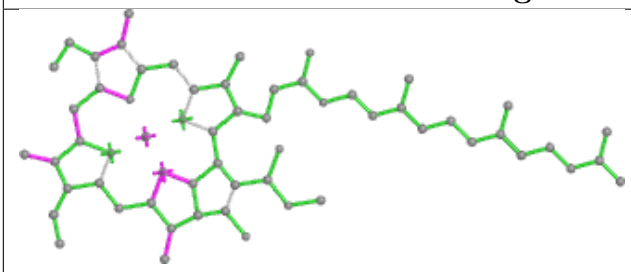


Torsions

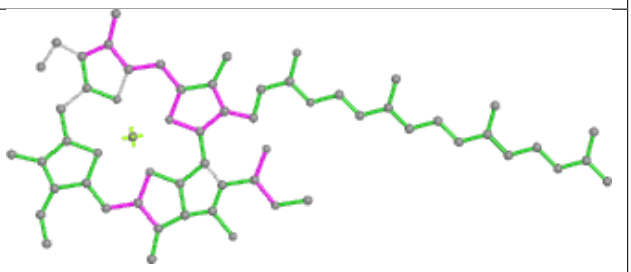


Rings

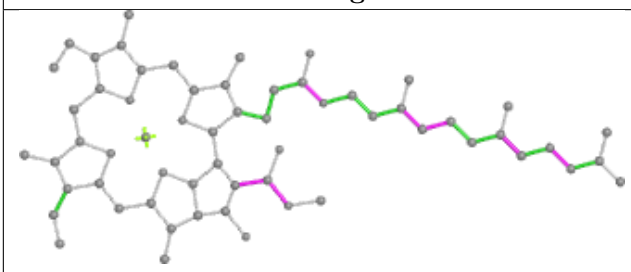
Ligand CLA G 1124



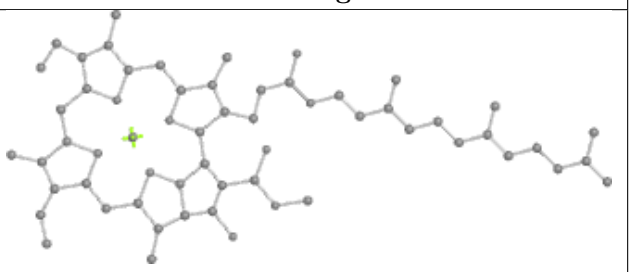
Bond lengths



Bond angles

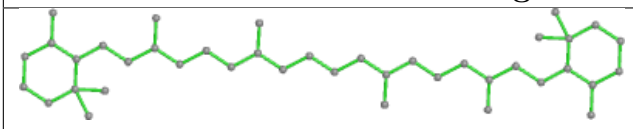


Torsions



Rings

Ligand BCR V 4022



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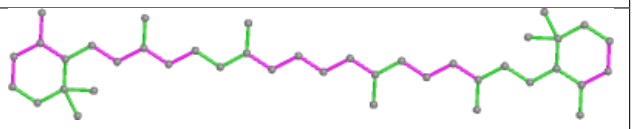

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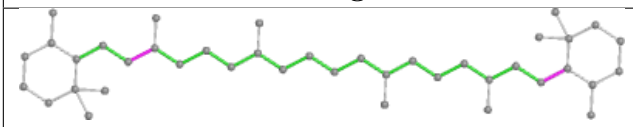

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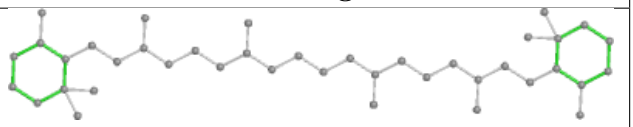
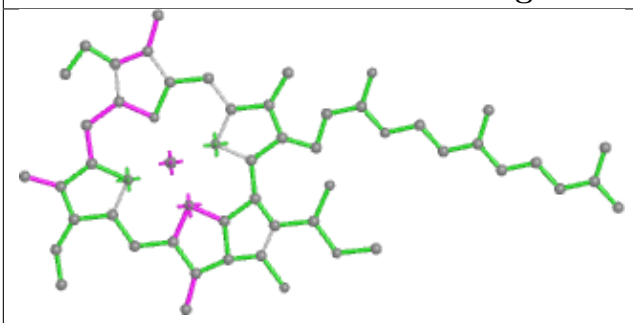


Rings

Ligand CLA B 1226



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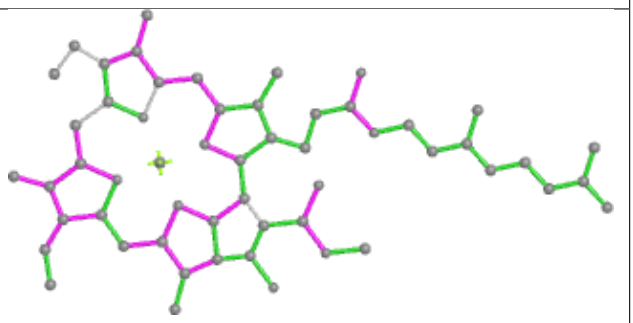
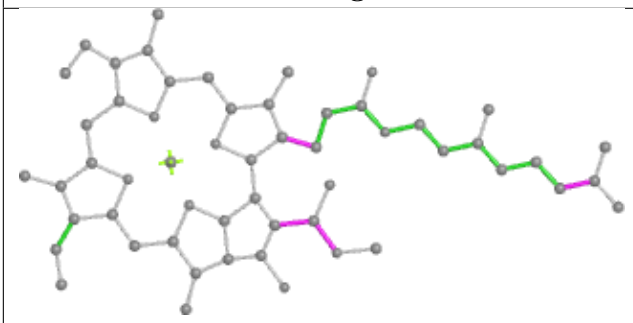
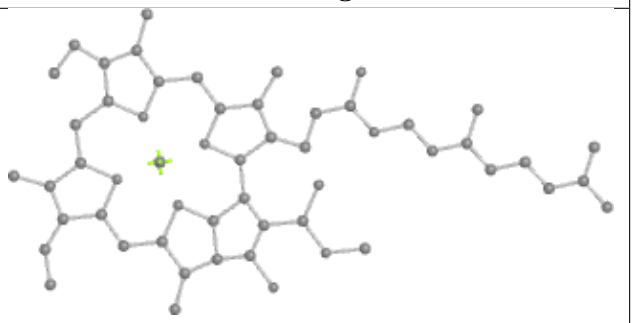


Bond angles

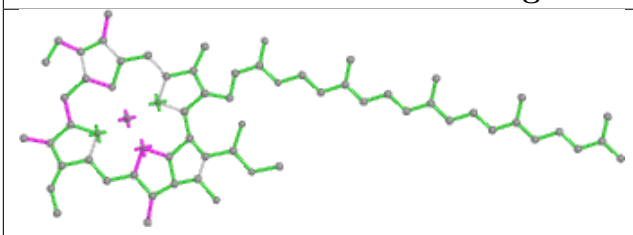


Torsions



Rings

Ligand CLA f 1203



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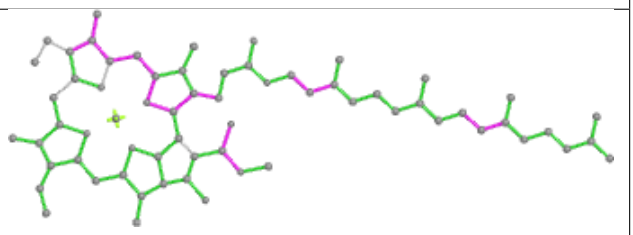
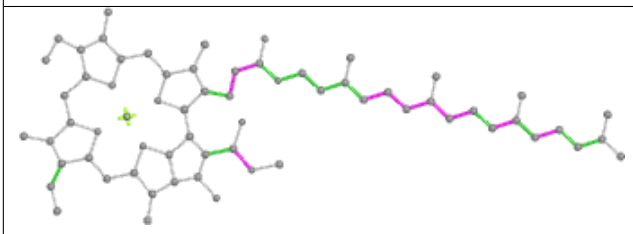


Bond angles



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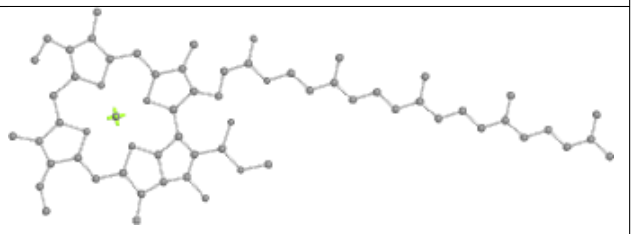
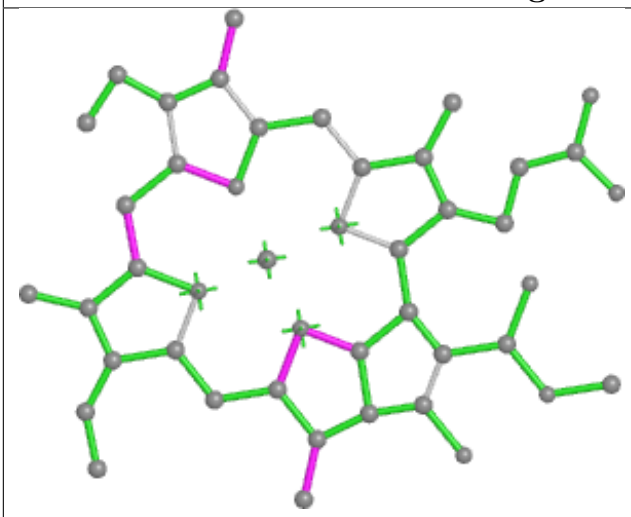


Rings

Ligand CLA 4 518



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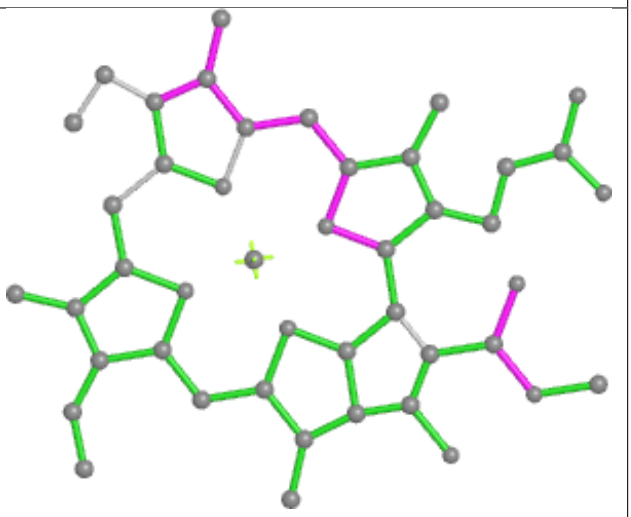
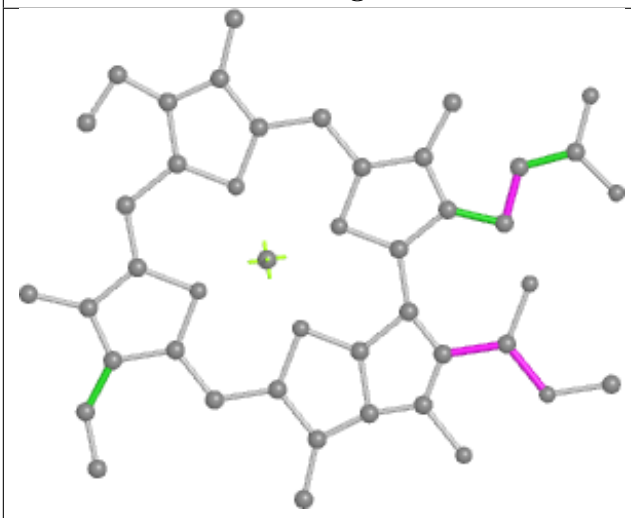


Bond angles



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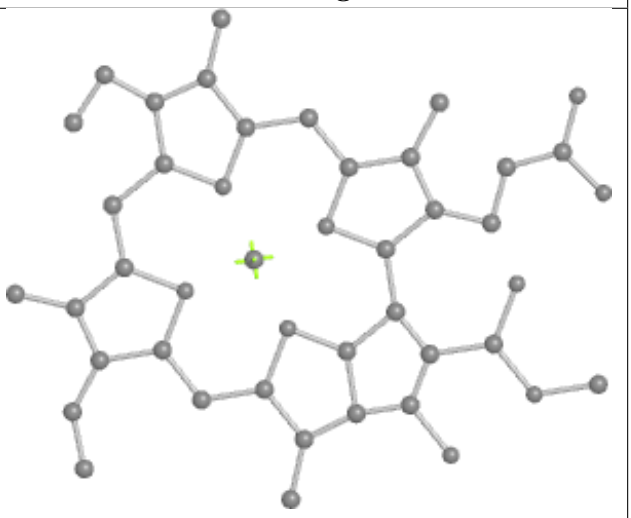
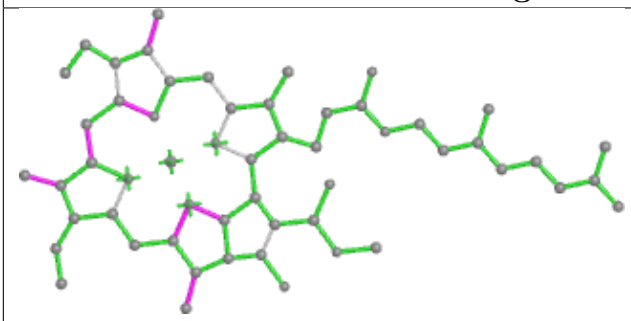


Rings

Ligand CLA m 1401



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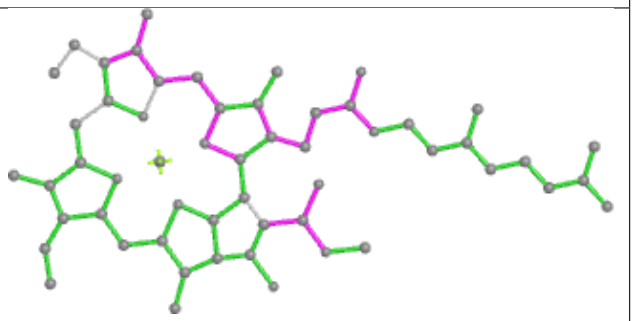
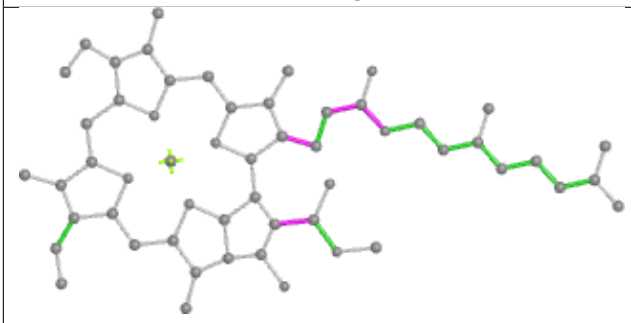


Bond angles



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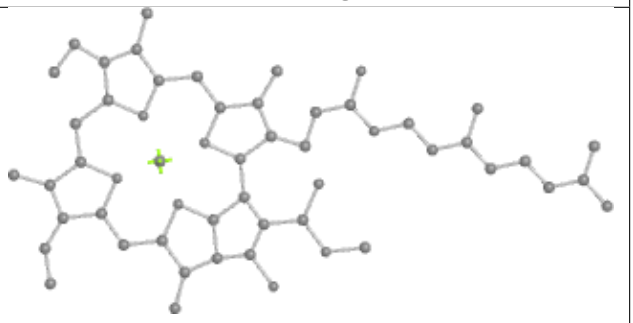
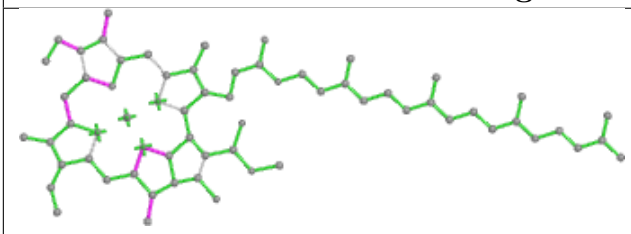


Rings

Ligand CLA B 1208



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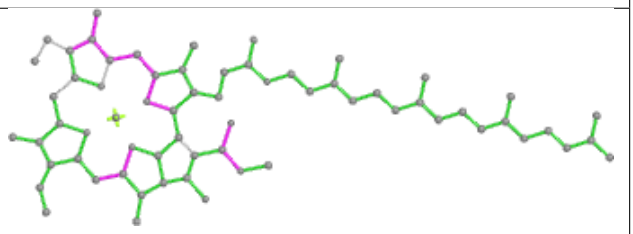
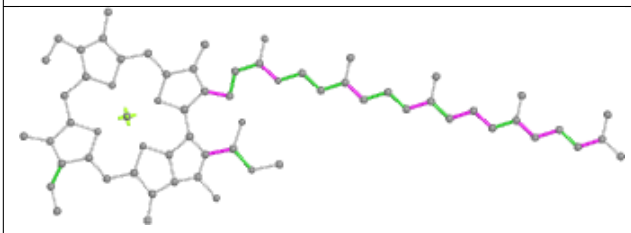


Bond angles



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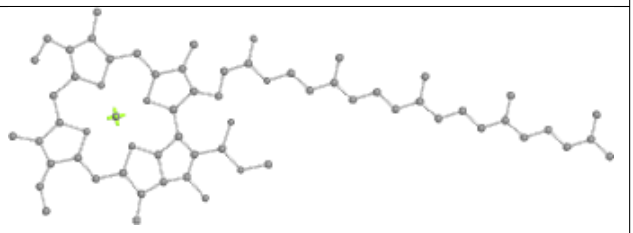
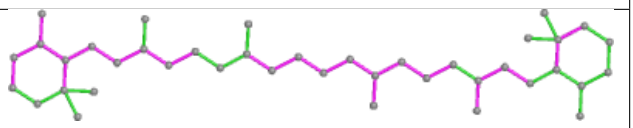


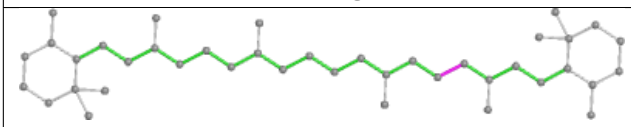
Rings

Ligand BCR B 4009

Bond lengths



Bond angles



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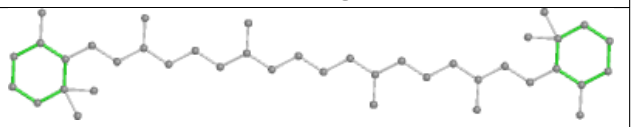
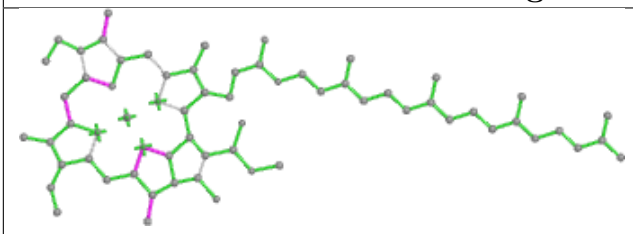
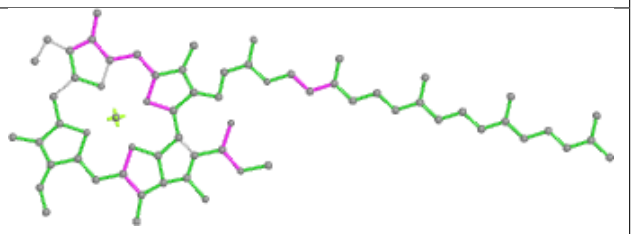


Rings

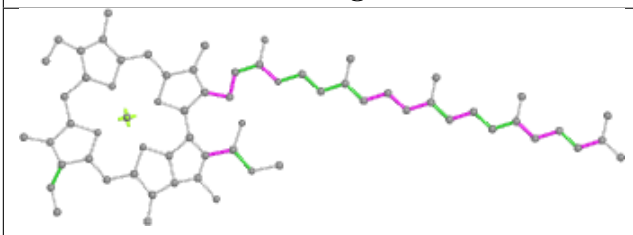
Ligand CLA Z 505



Bond lengths



Bond angles



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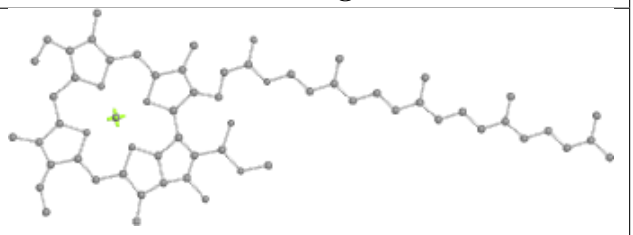
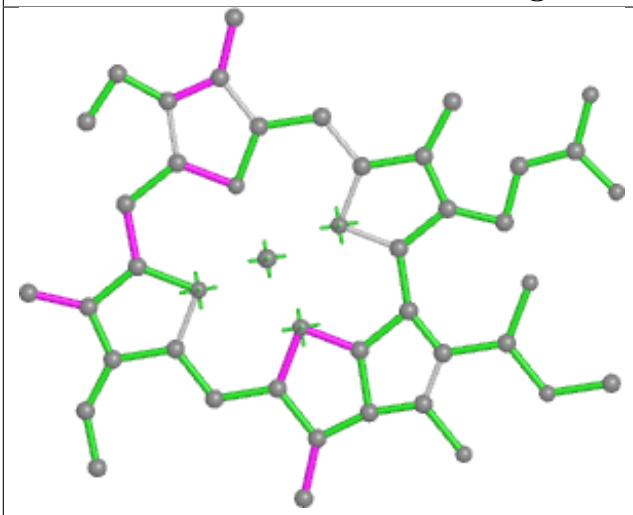


Rings

Ligand CLA 1 502



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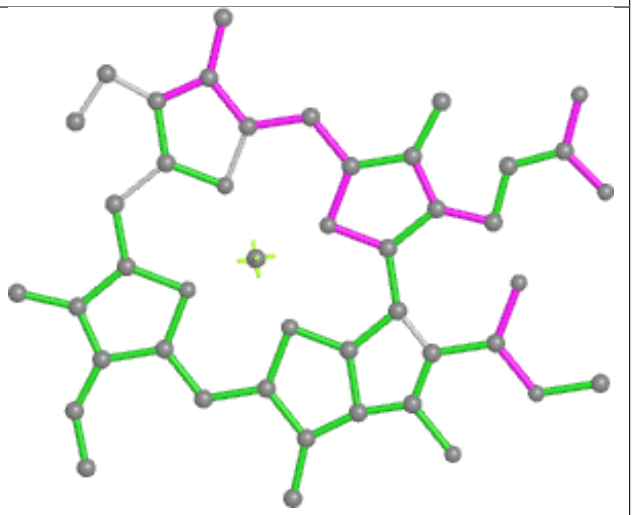
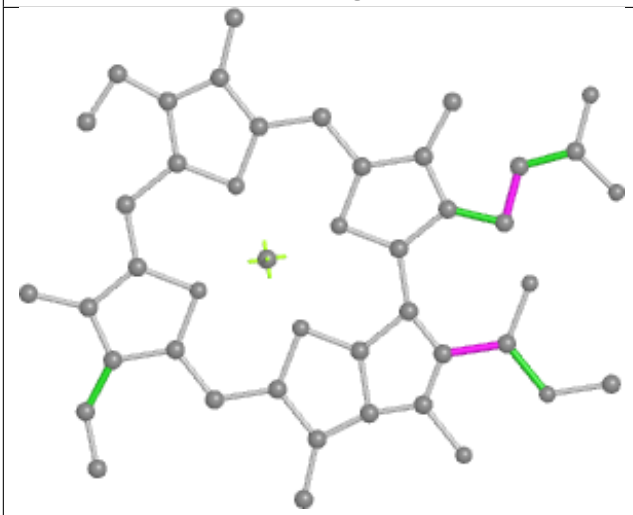


Bond angles



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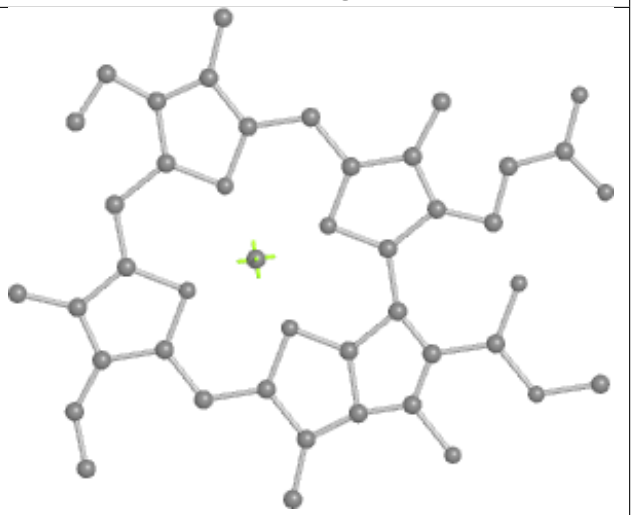
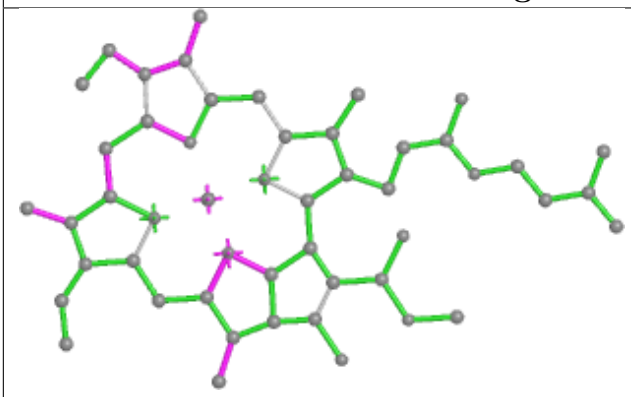
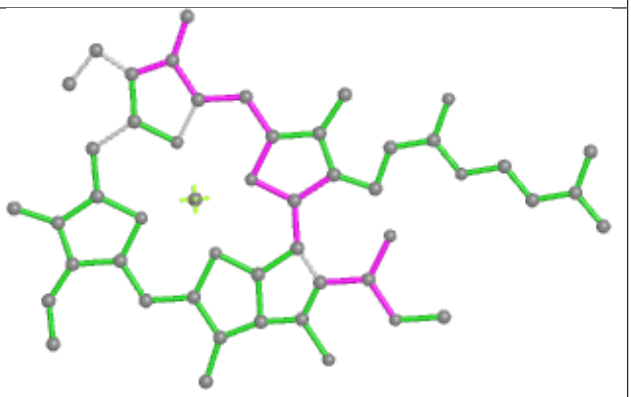
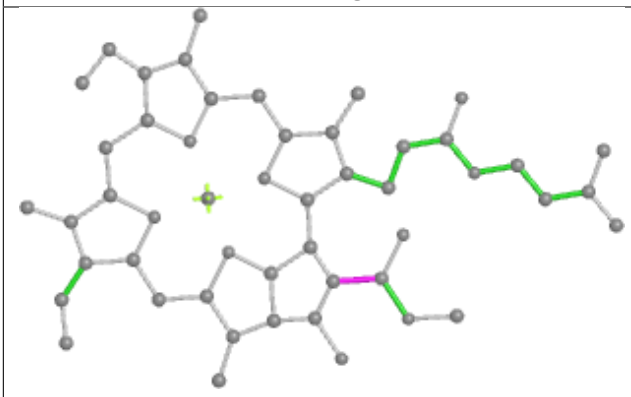
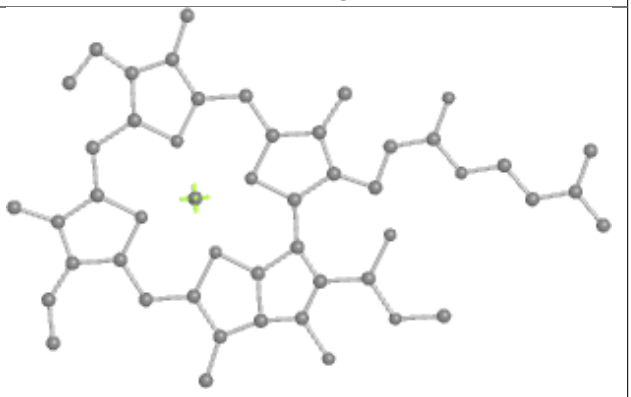
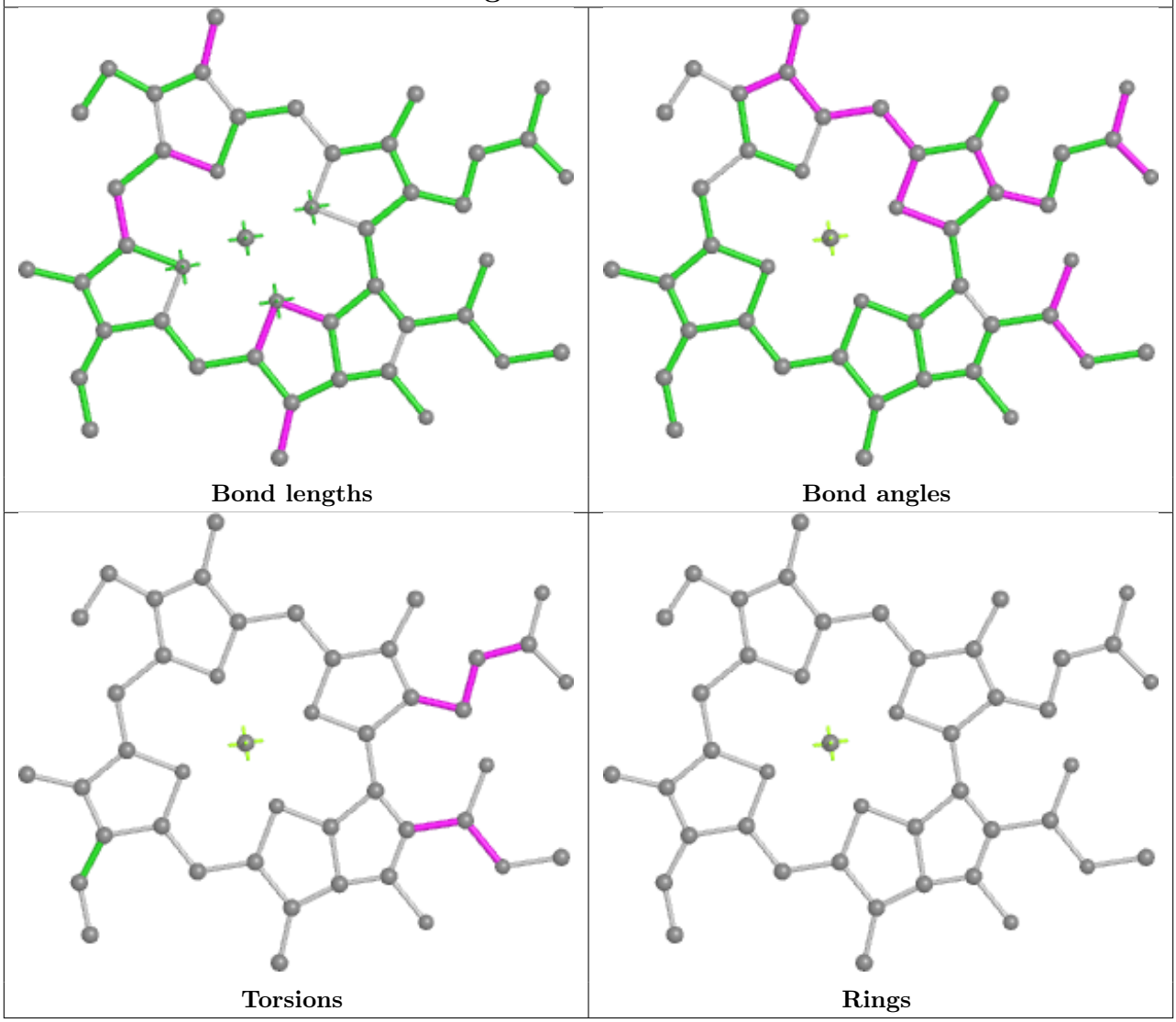


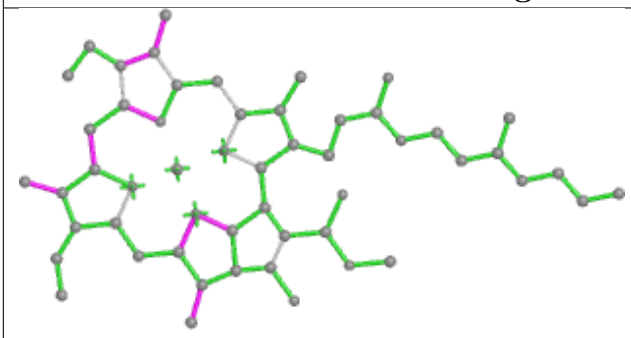
Rings

Ligand CLA G 1112	
 Bond lengths	 Bond angles
 Torsions	 Rings

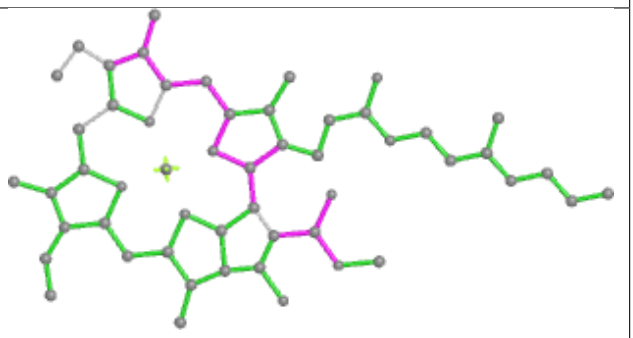
Ligand CLA v 516



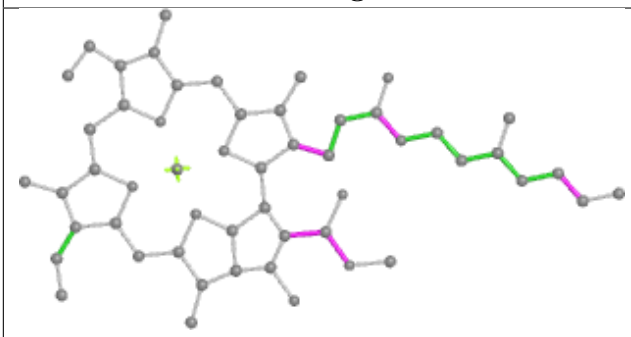
Ligand CLA H 1209



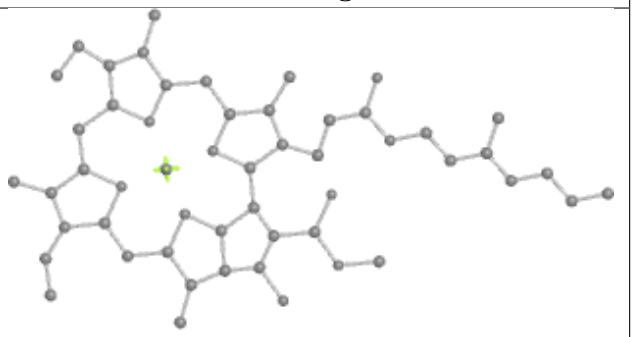
Bond lengths



Bond angles

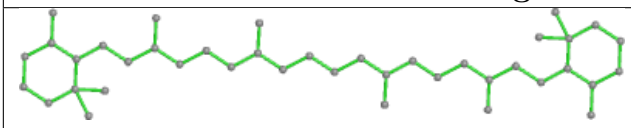


Torsions

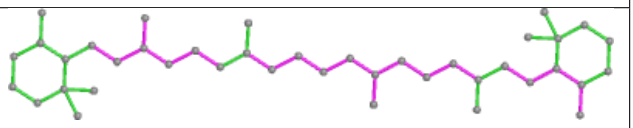


Rings

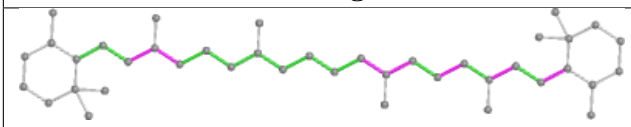
Ligand BCR A 4011



Bond lengths



Bond angles



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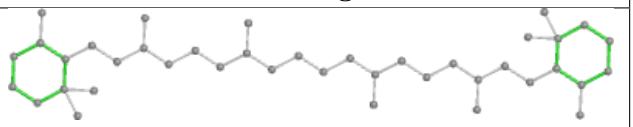
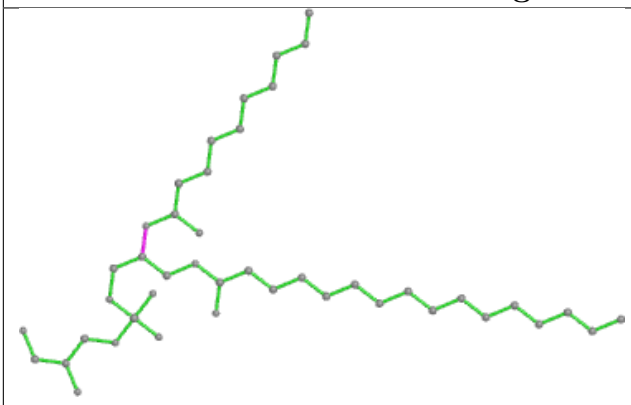
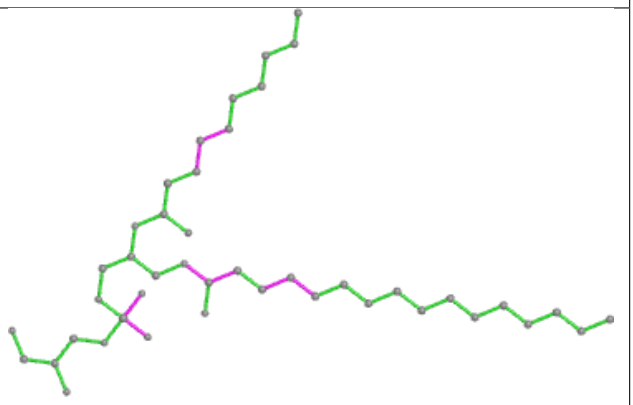
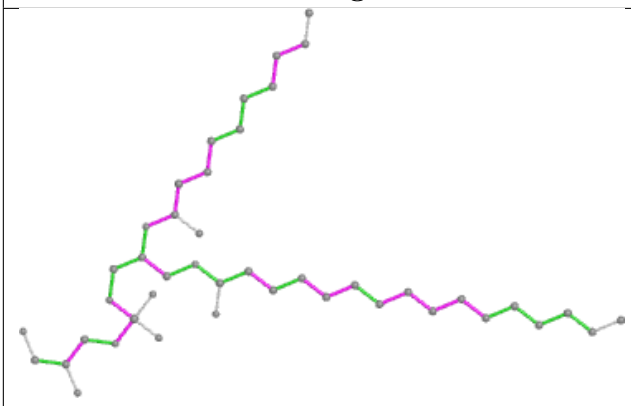
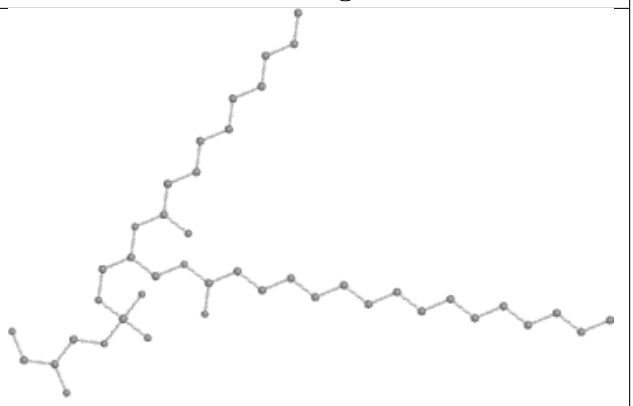
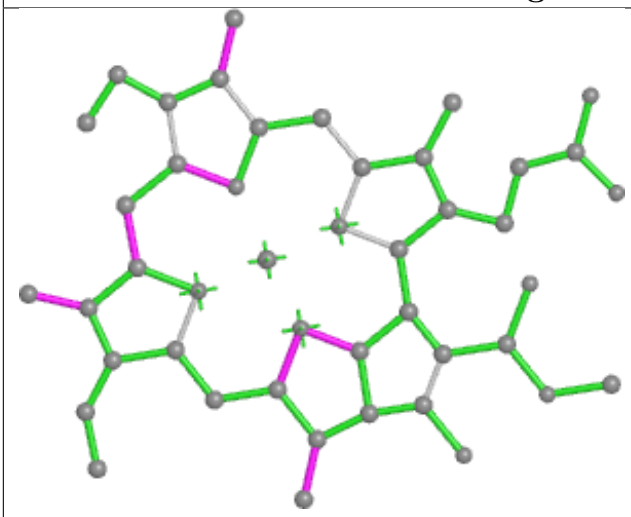


Rings

Ligand LHG A 5002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 519



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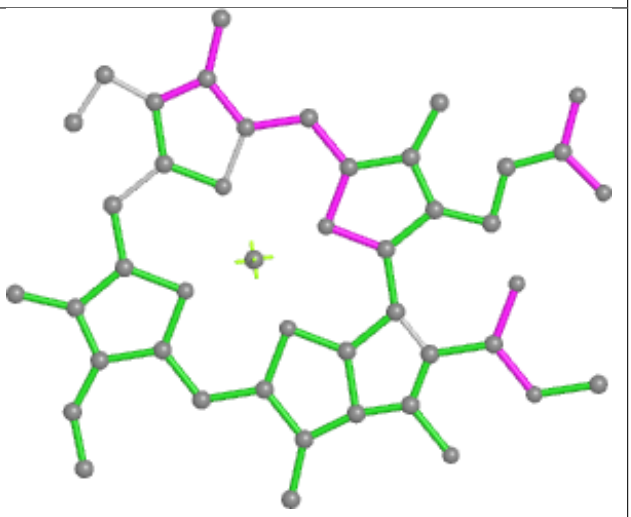

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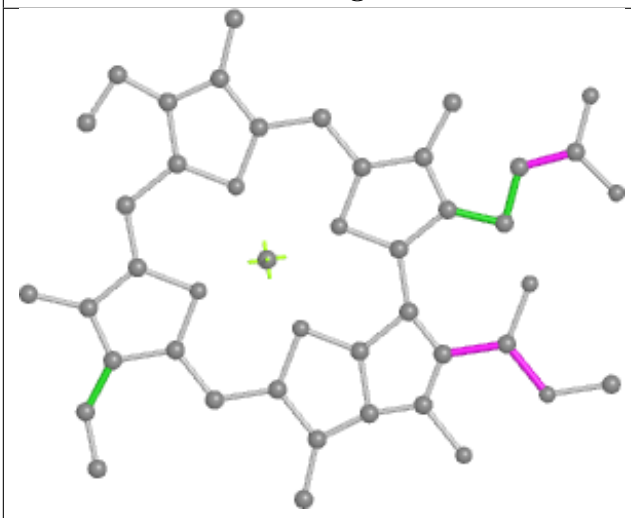

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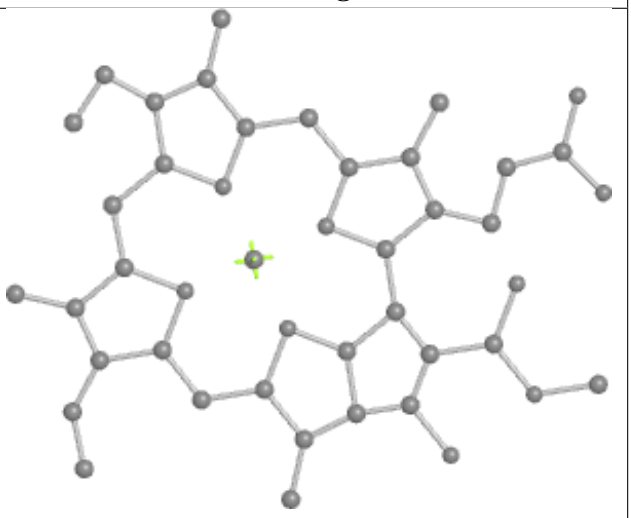
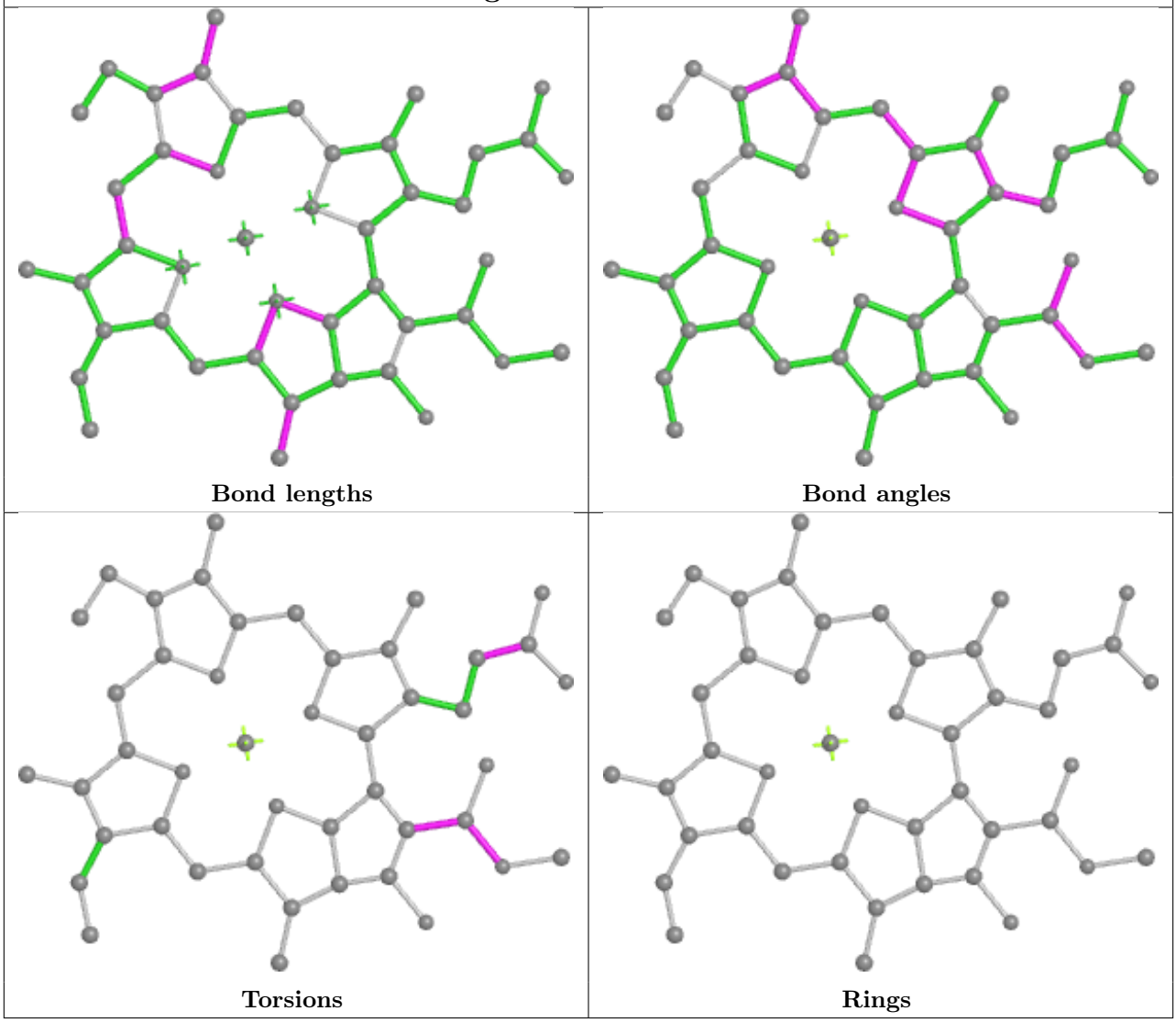


Rings

Ligand CLA u 512



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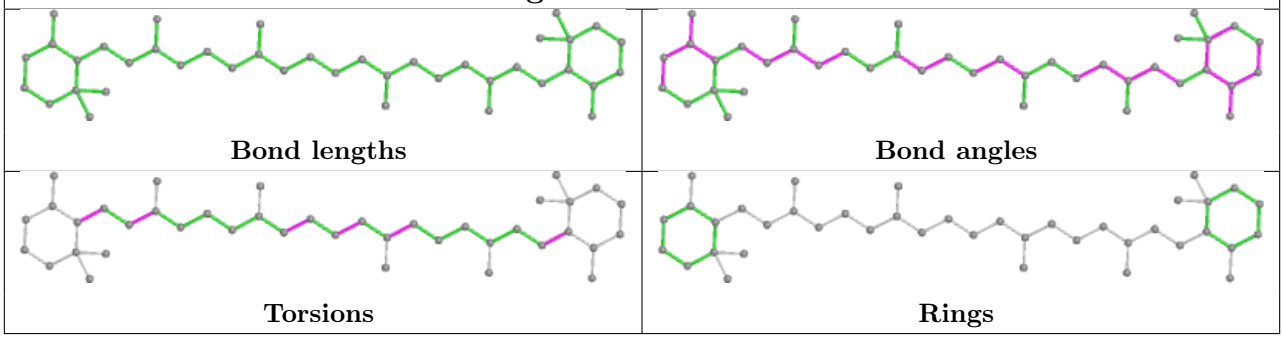

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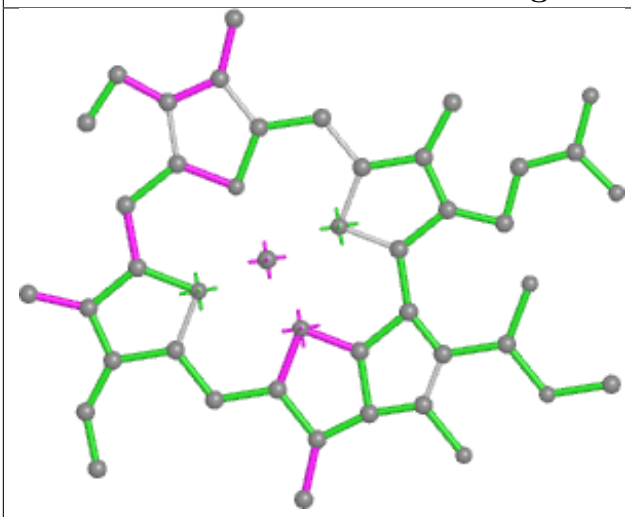

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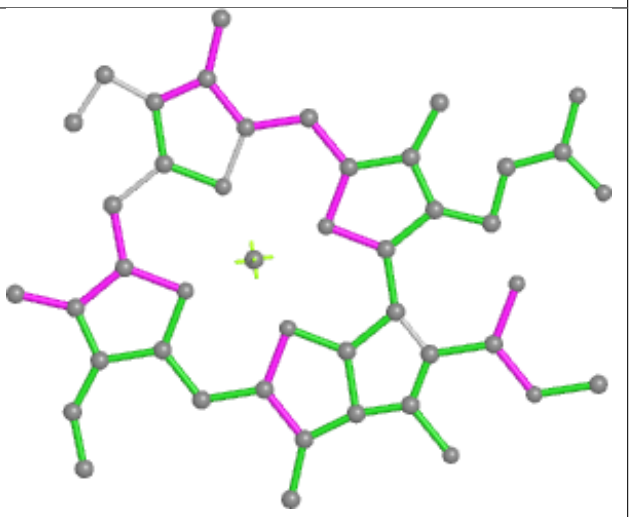

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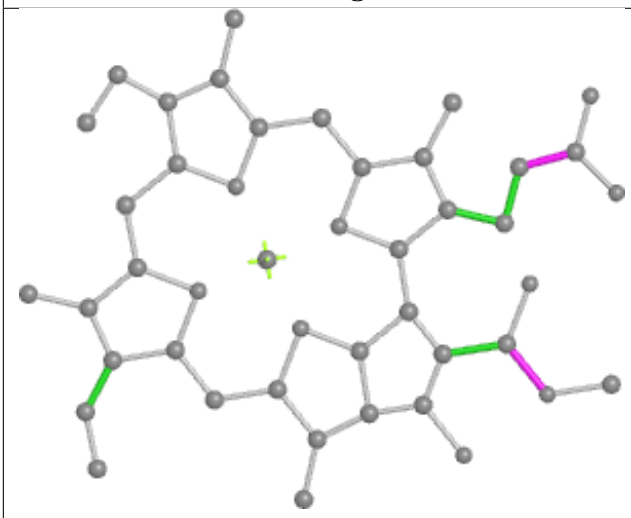

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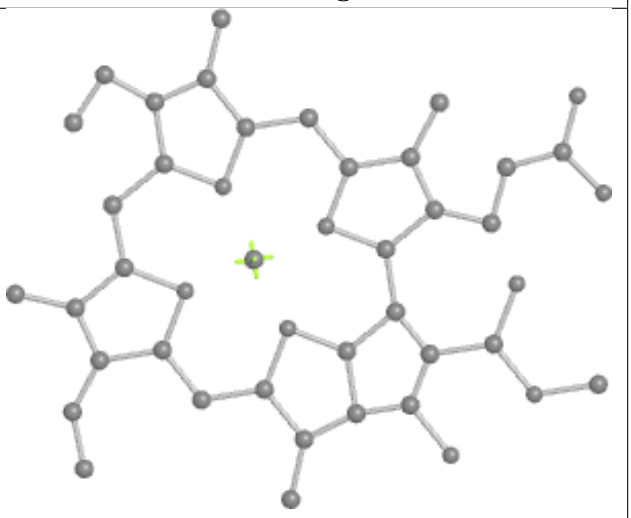

Rings

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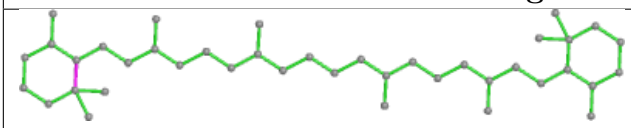

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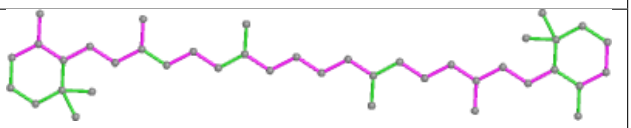
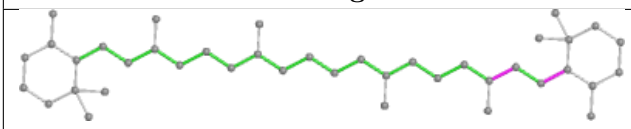


Bond angles



Torsions

Rings

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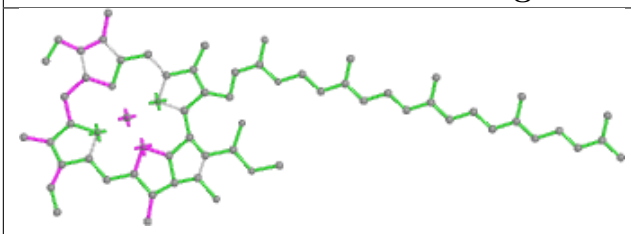
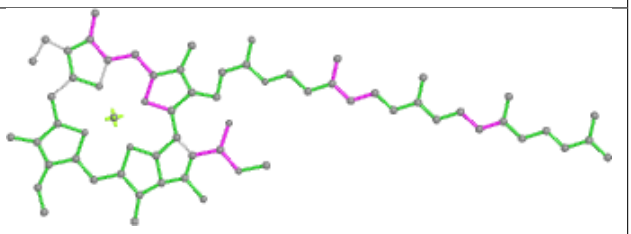
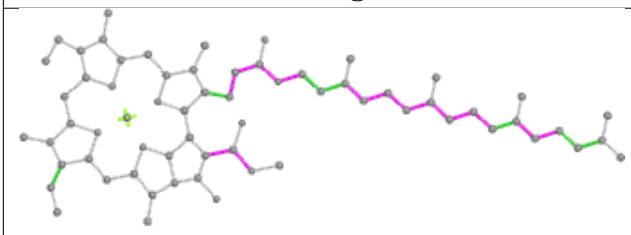
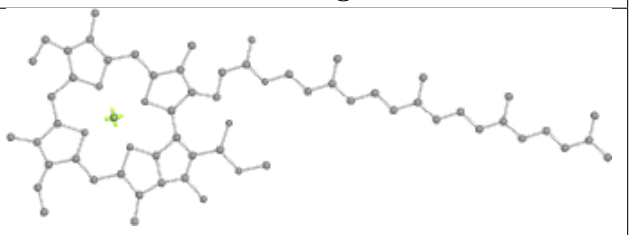
 Bond lengths	 Bond angles
 Torsions	 Rings

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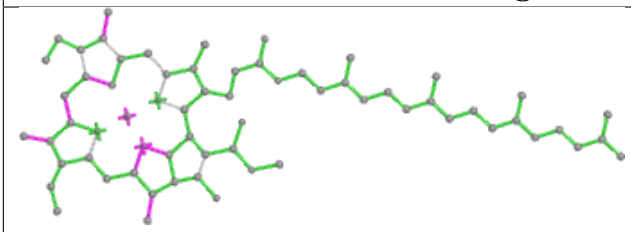
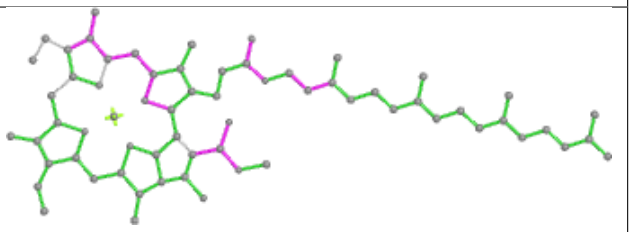
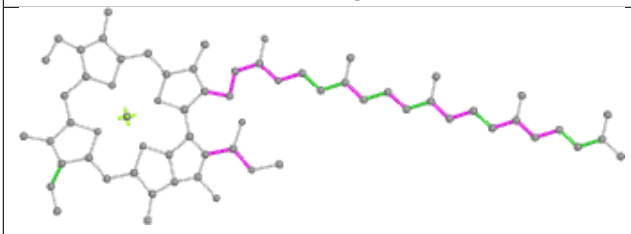
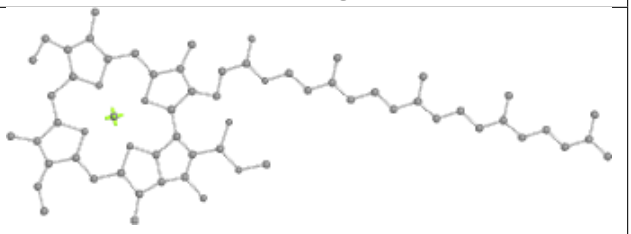
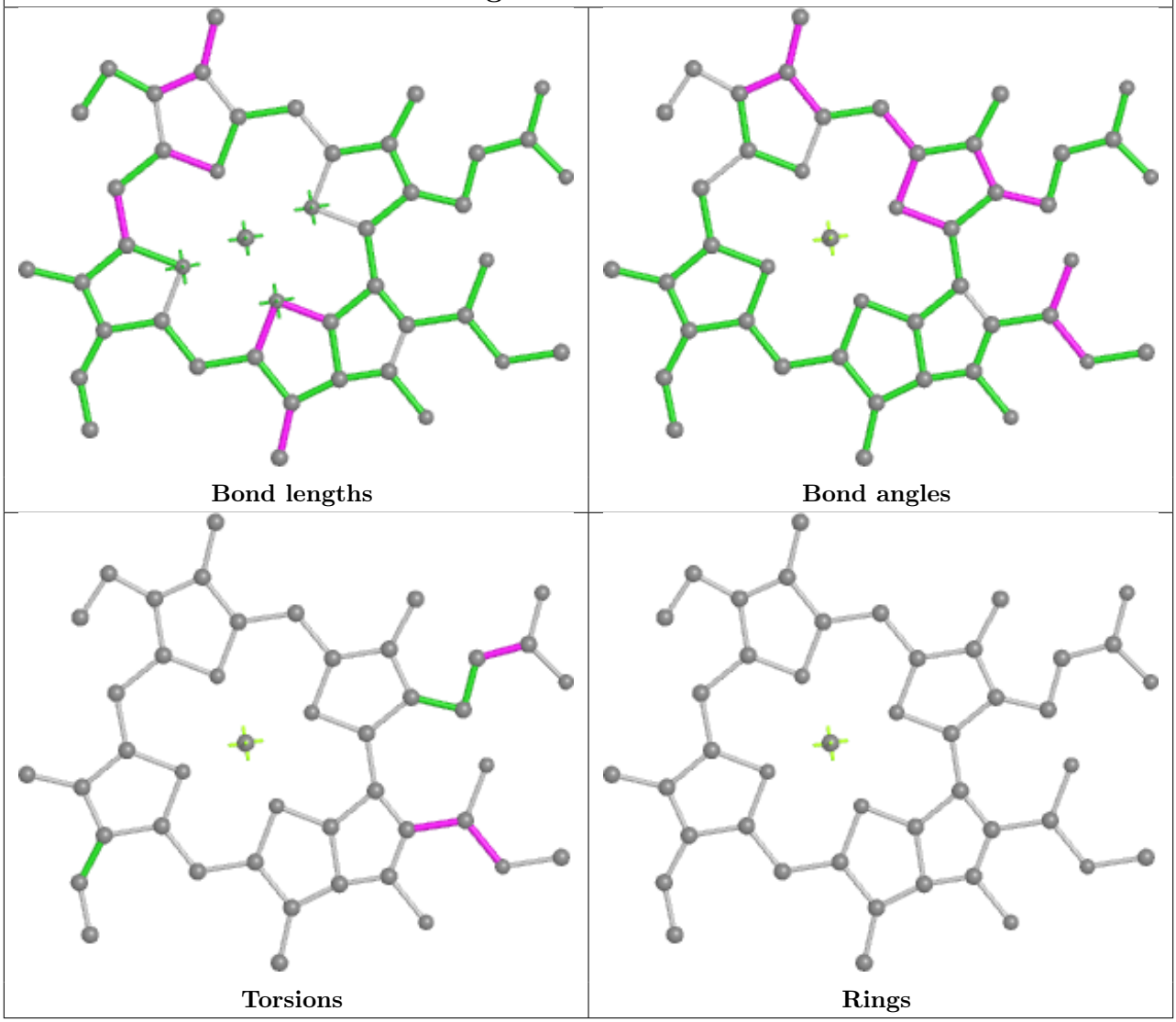
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 512



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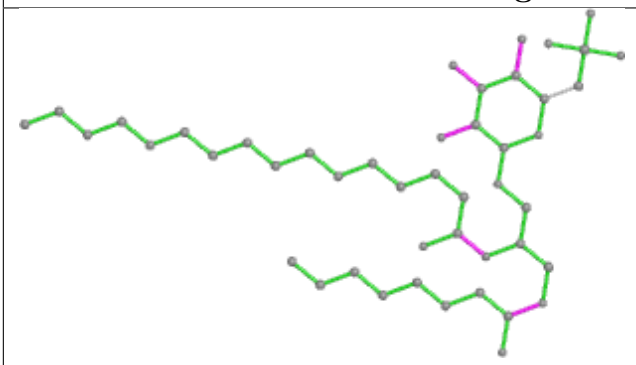
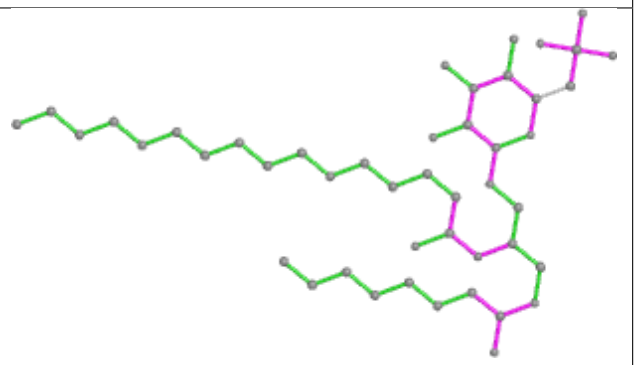
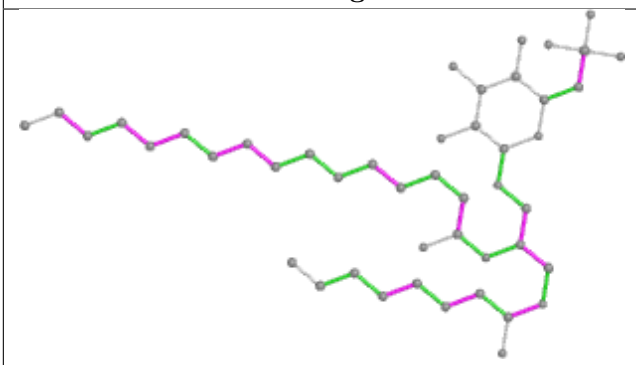
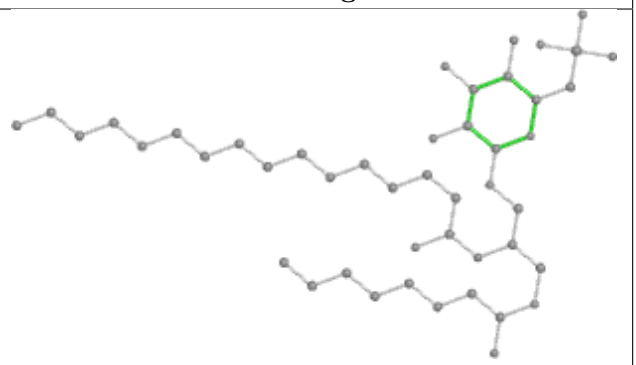
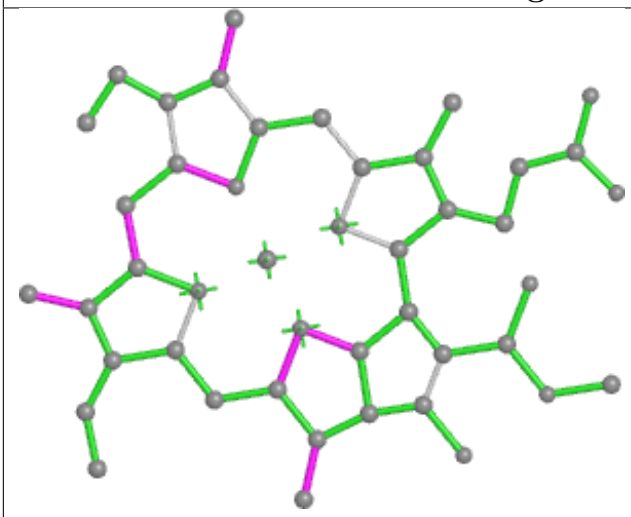
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA d 508



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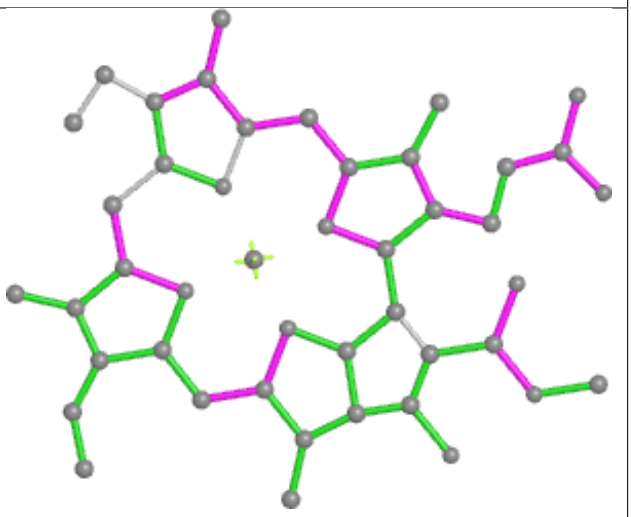

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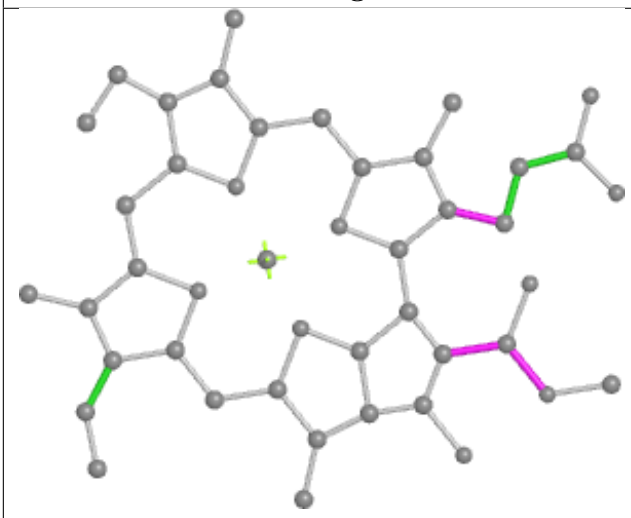

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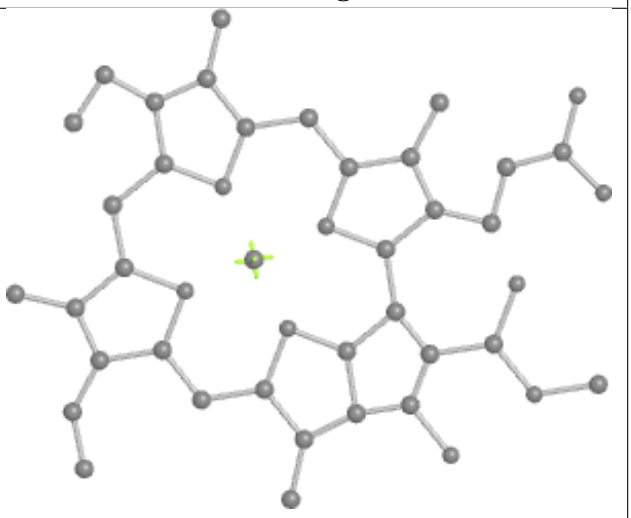
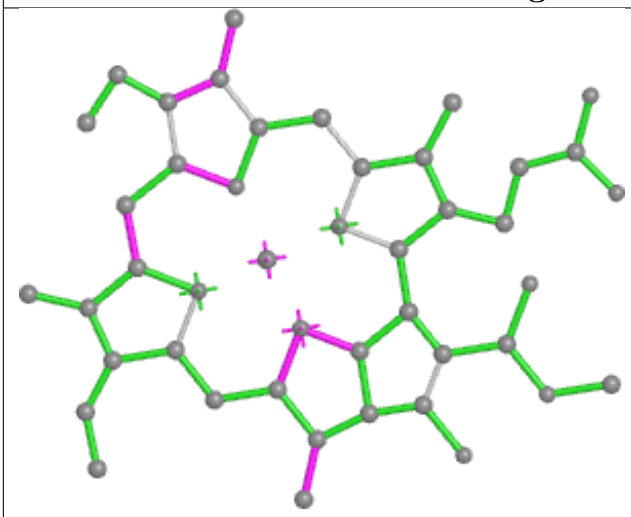


Rings

Ligand CLA 2 512



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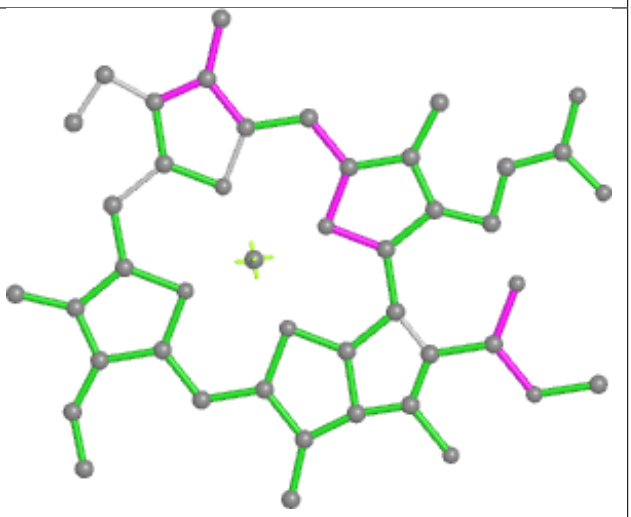

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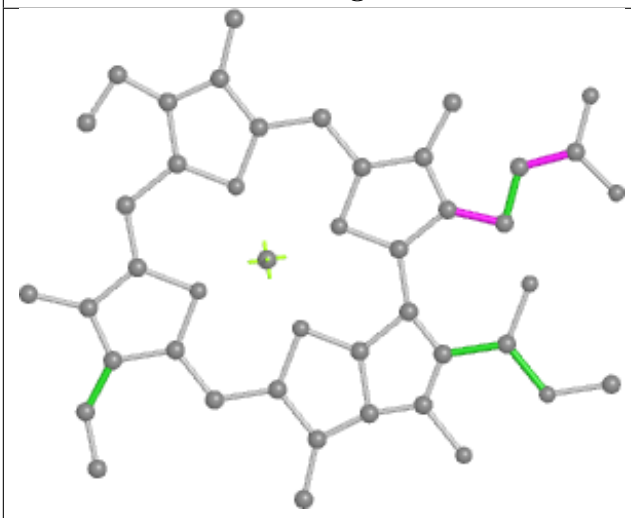

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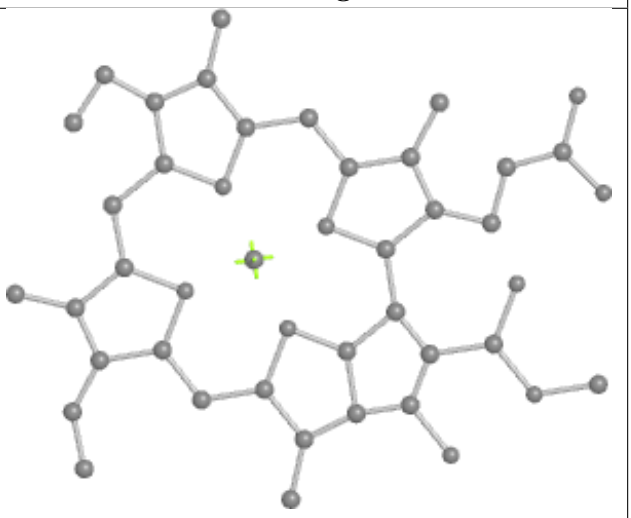
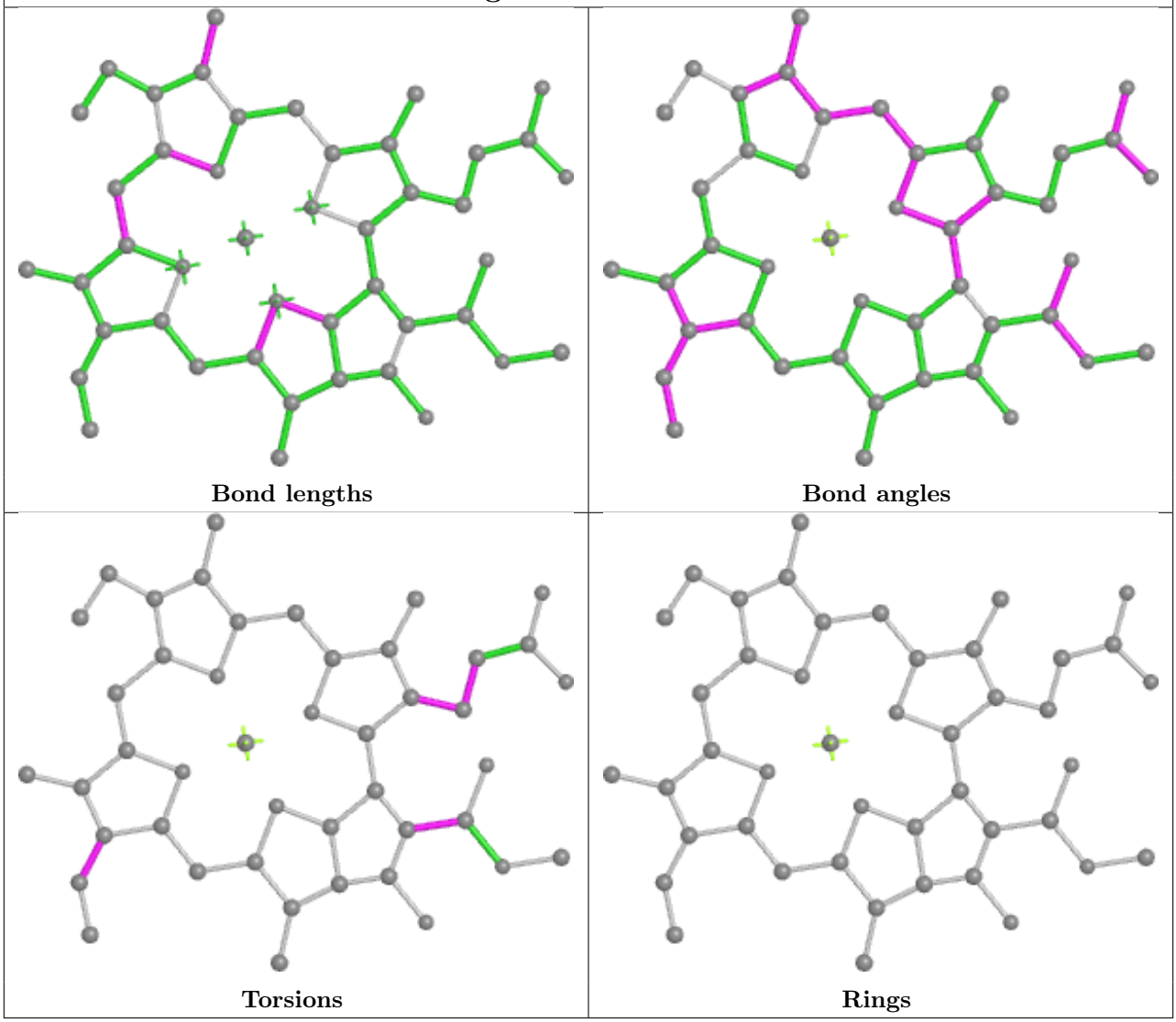


Rings

Ligand CLA a 516



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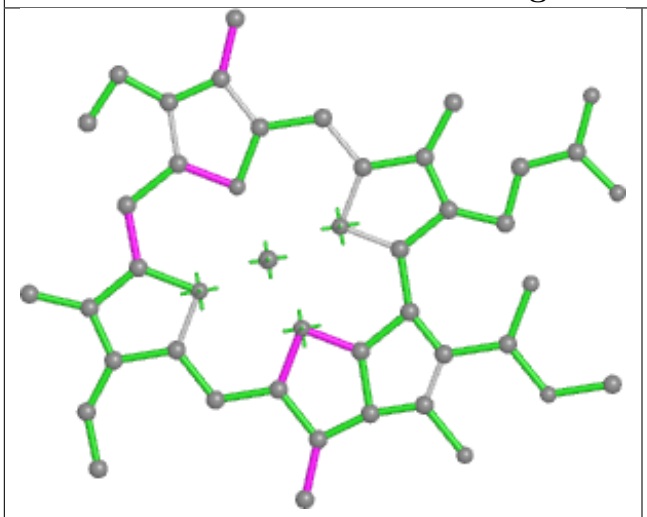

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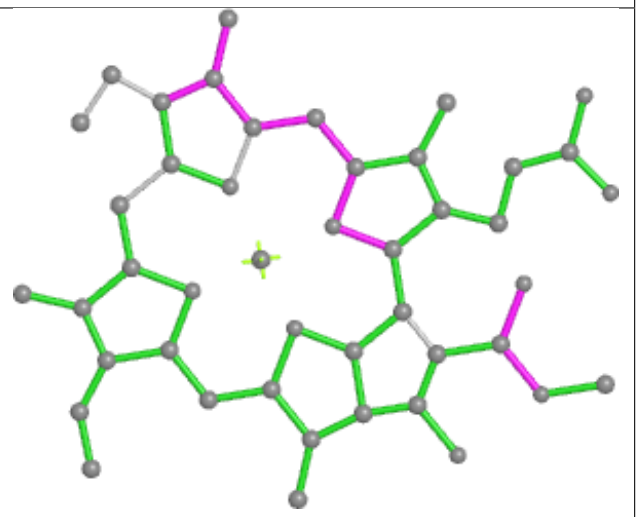

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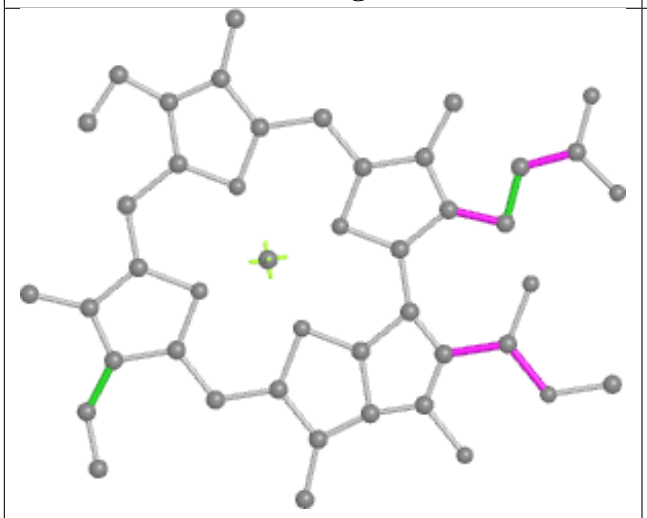

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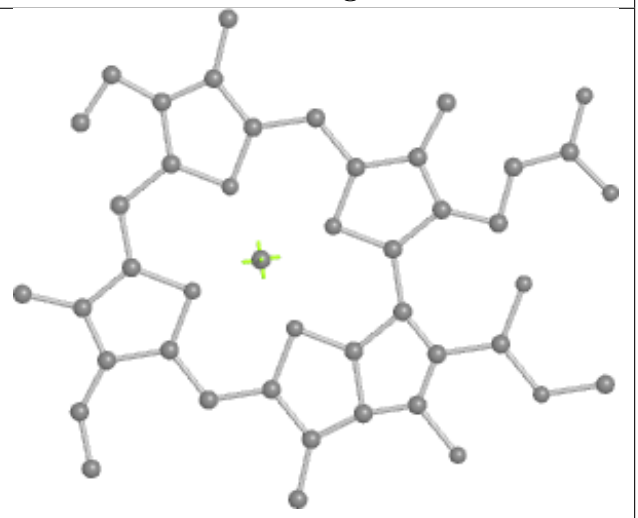
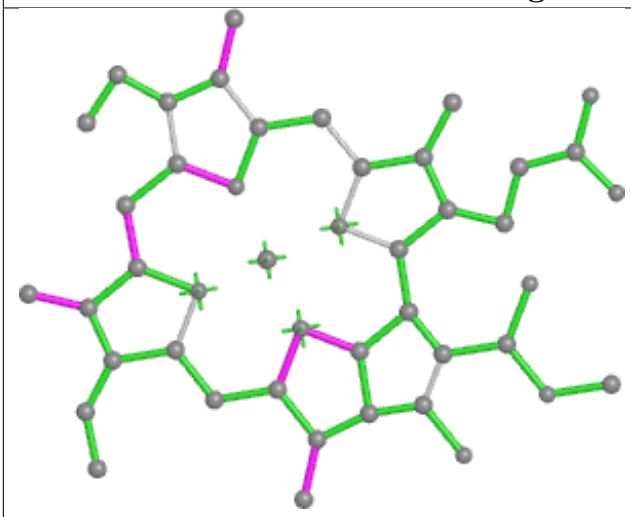


Rings

Ligand CLA q 511



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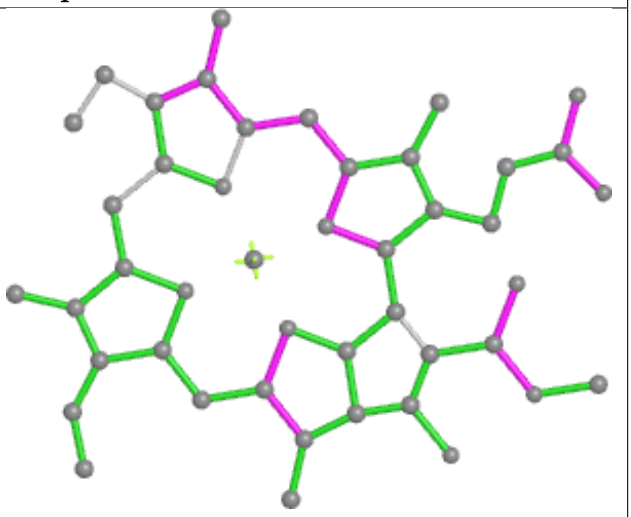

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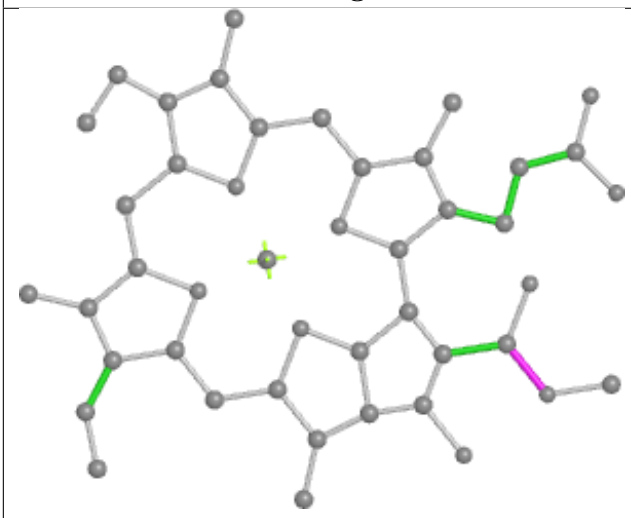

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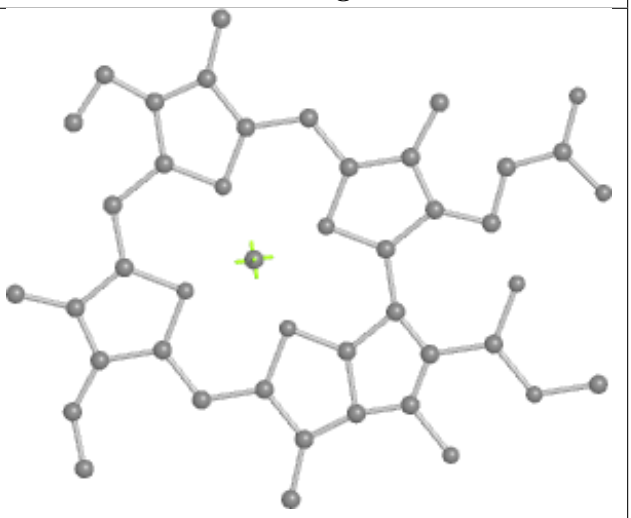
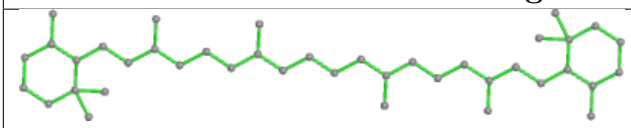


Rings

Ligand BCR b 523



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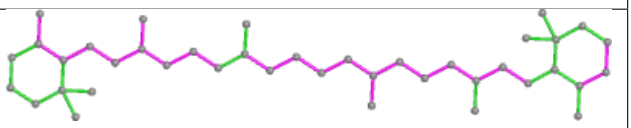
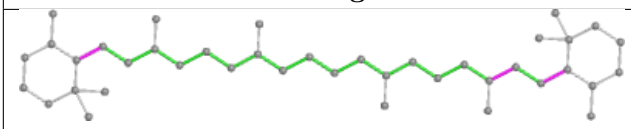


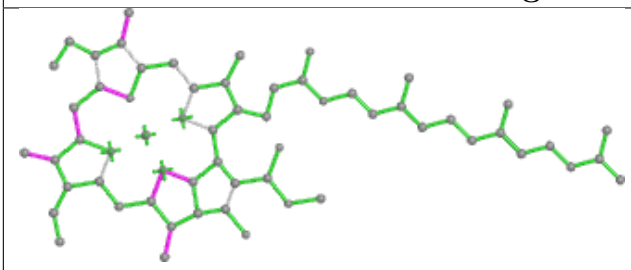
Bond angles



Torsions

Rings

Ligand CLA f 1224



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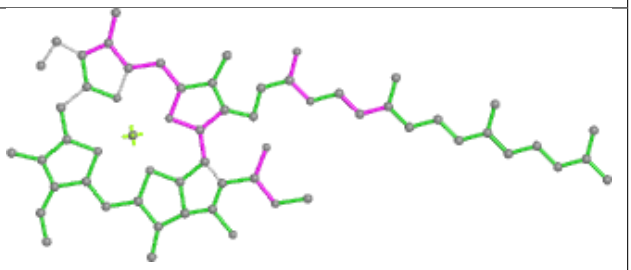

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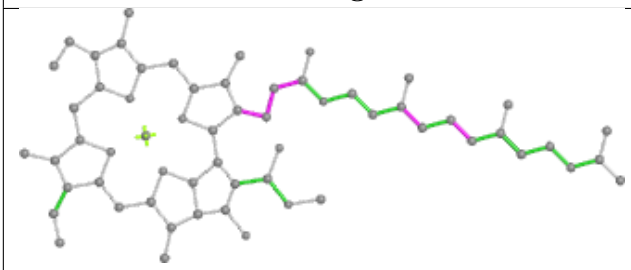
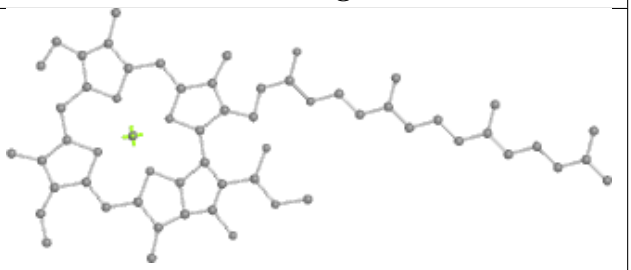
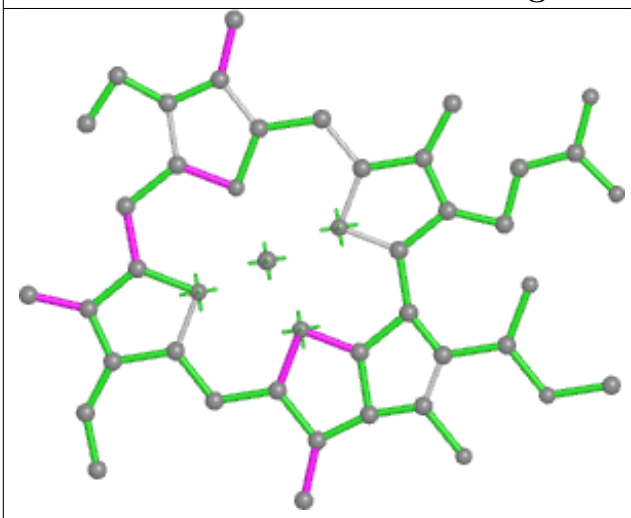


Torsions

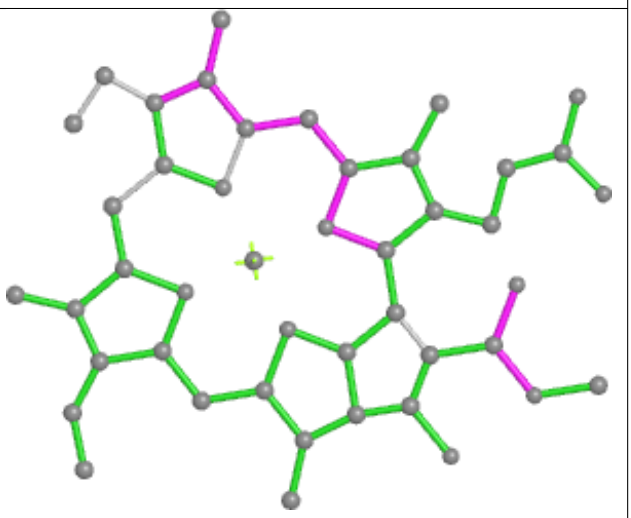


Rings

Ligand CLA 1 505



Bond lengths



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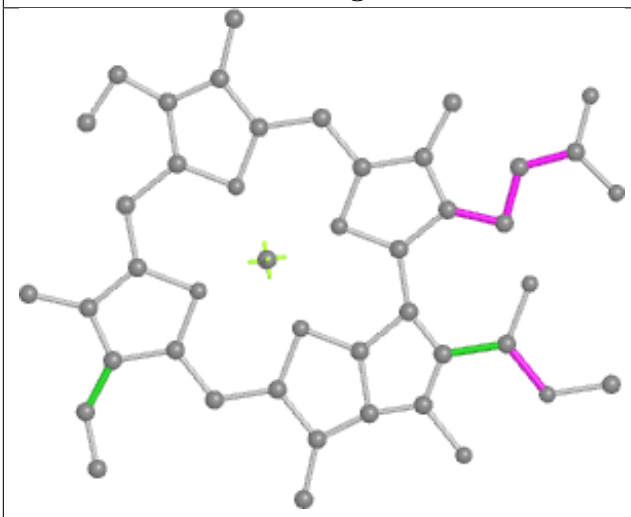
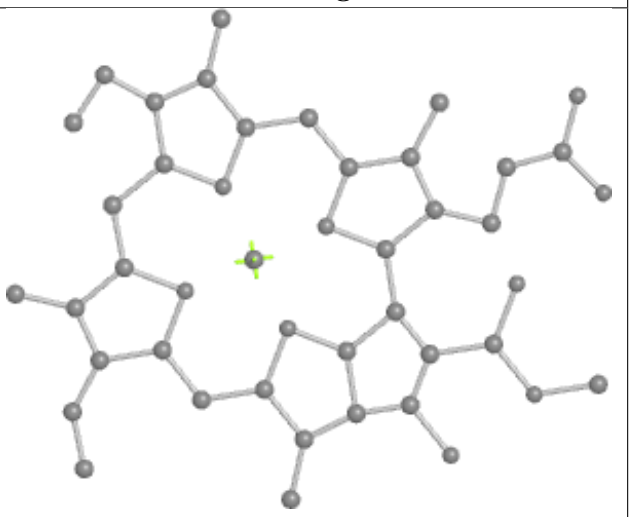
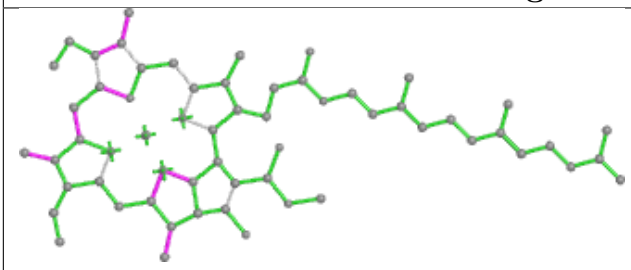
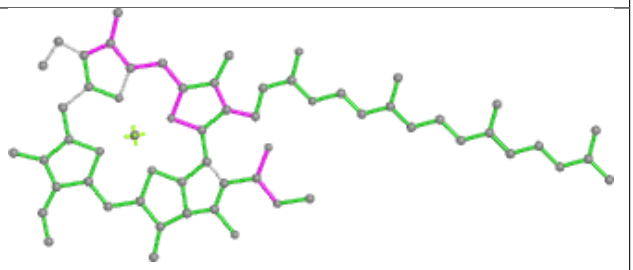
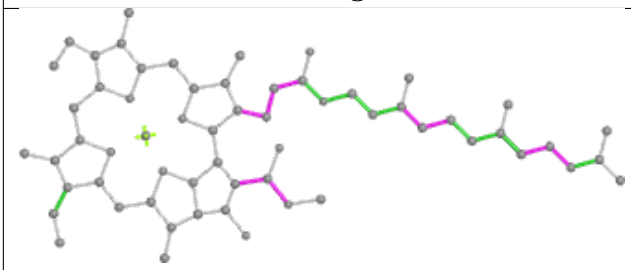
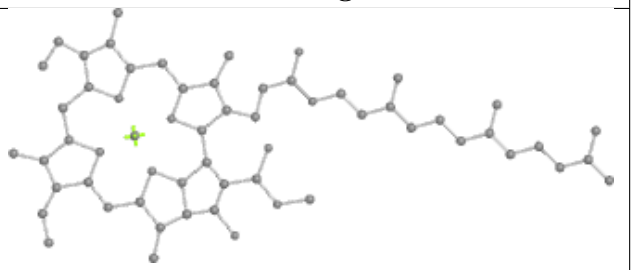
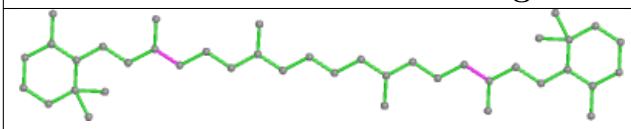
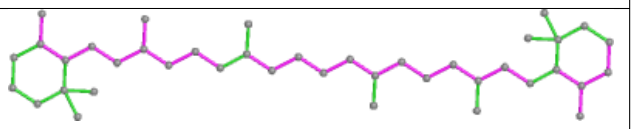
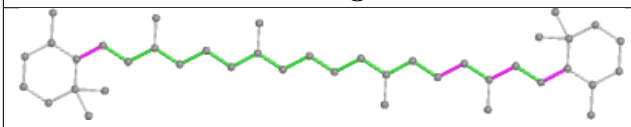
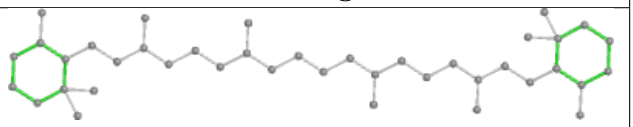


Torsions

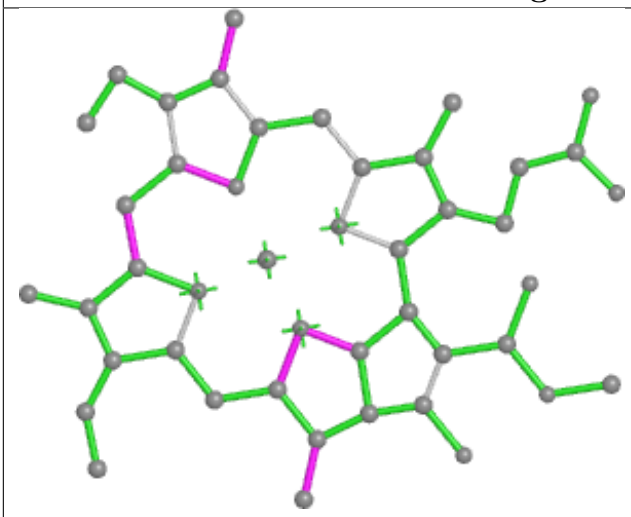


Rings

Ligand CLA Z 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 4008	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA t 507



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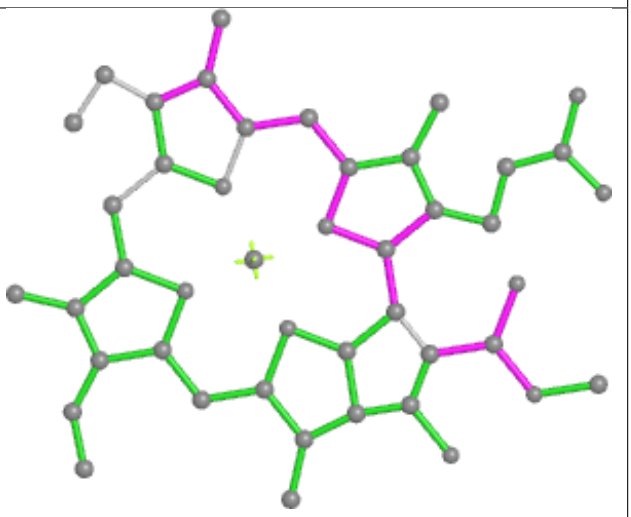

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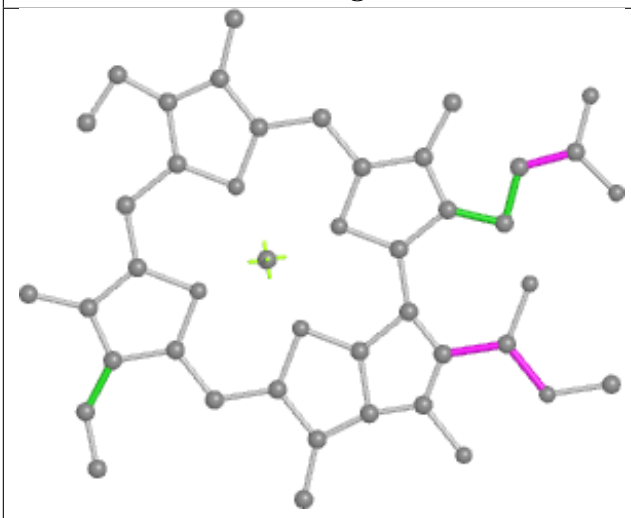

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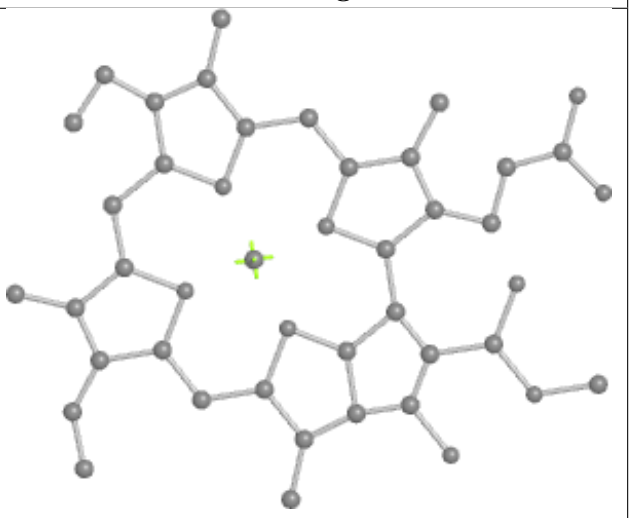
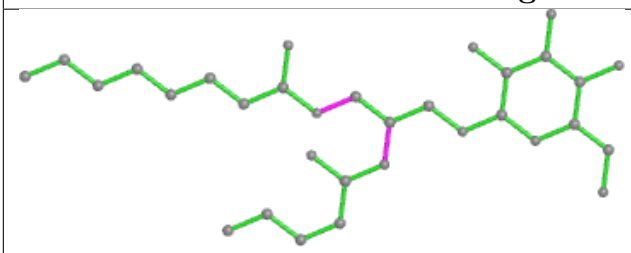


Rings

Ligand LMG l 5104



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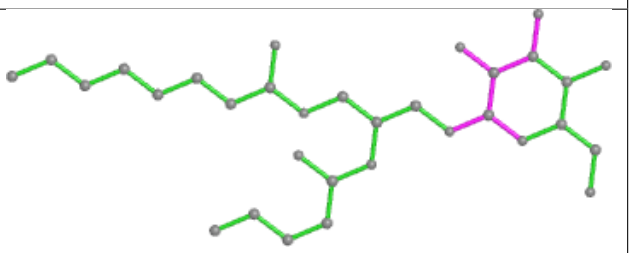

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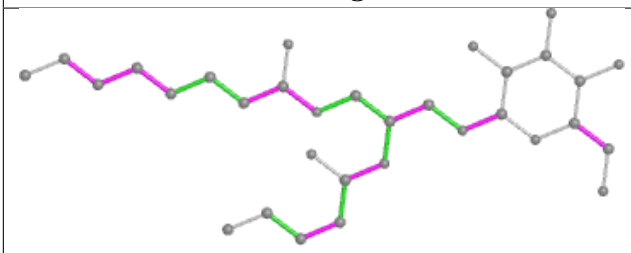

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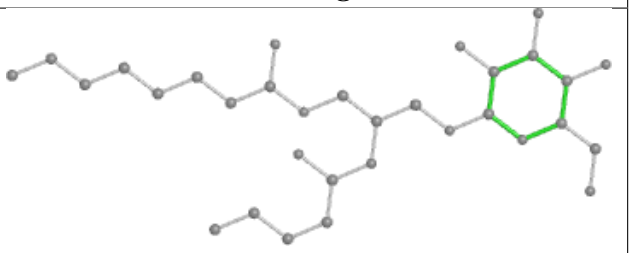

Rings

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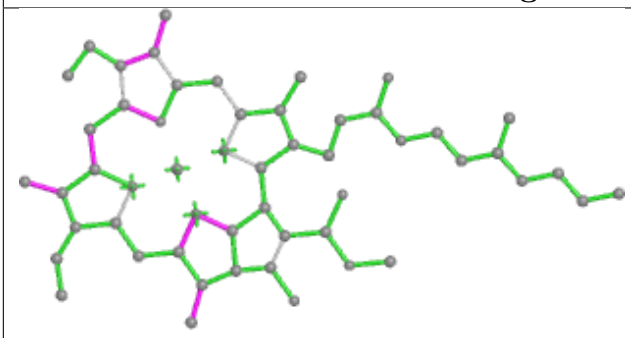
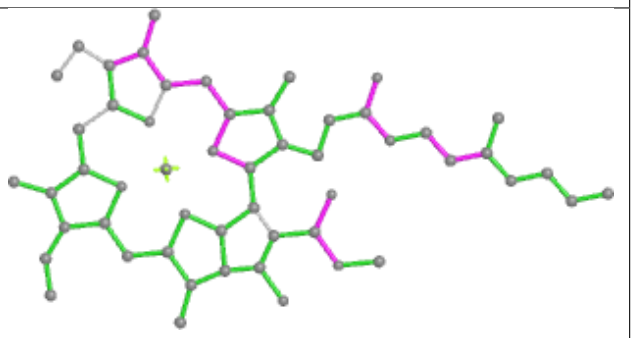
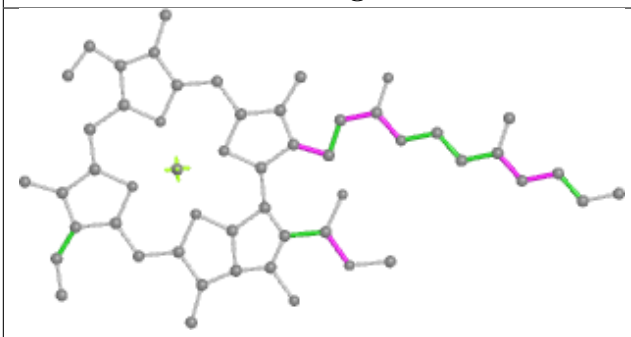
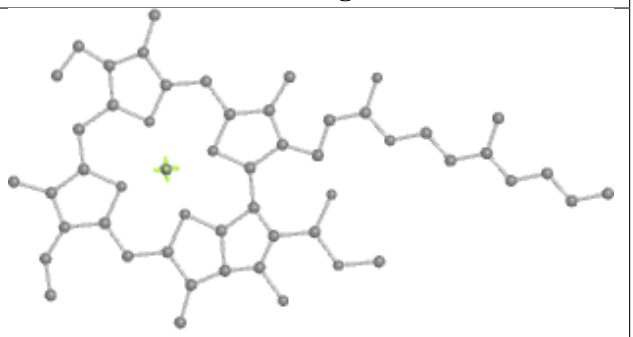
 Bond lengths	 Bond angles
 Torsions	 Rings

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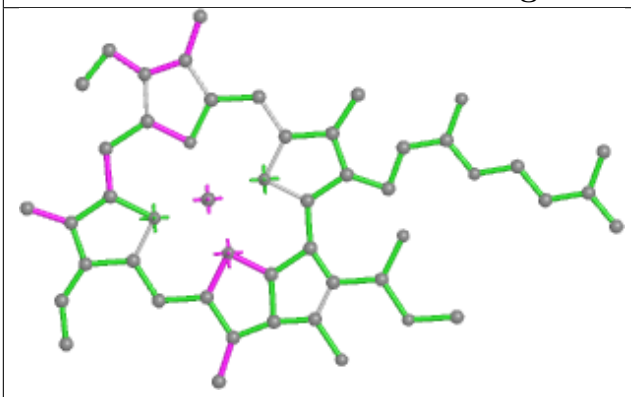
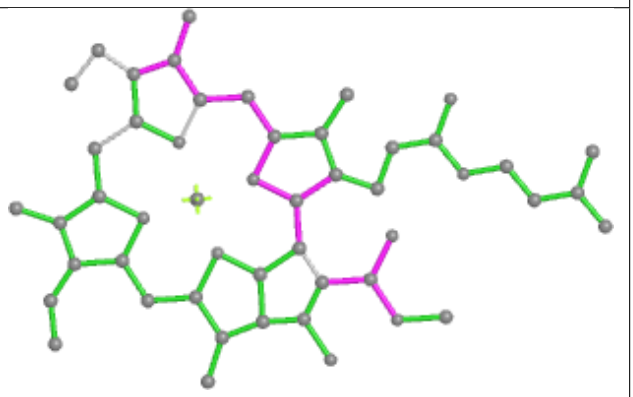
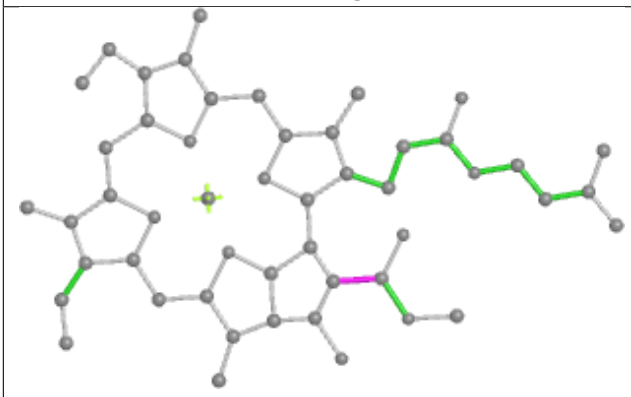
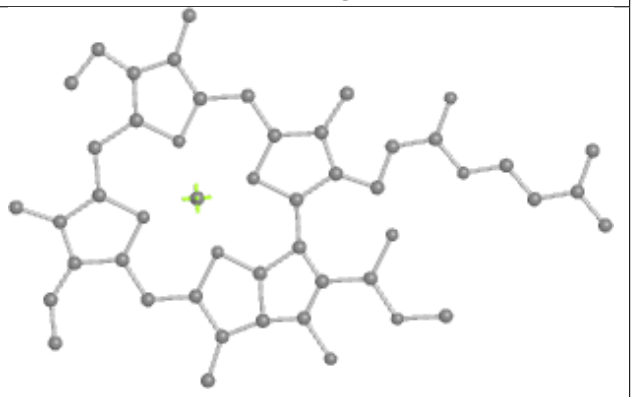
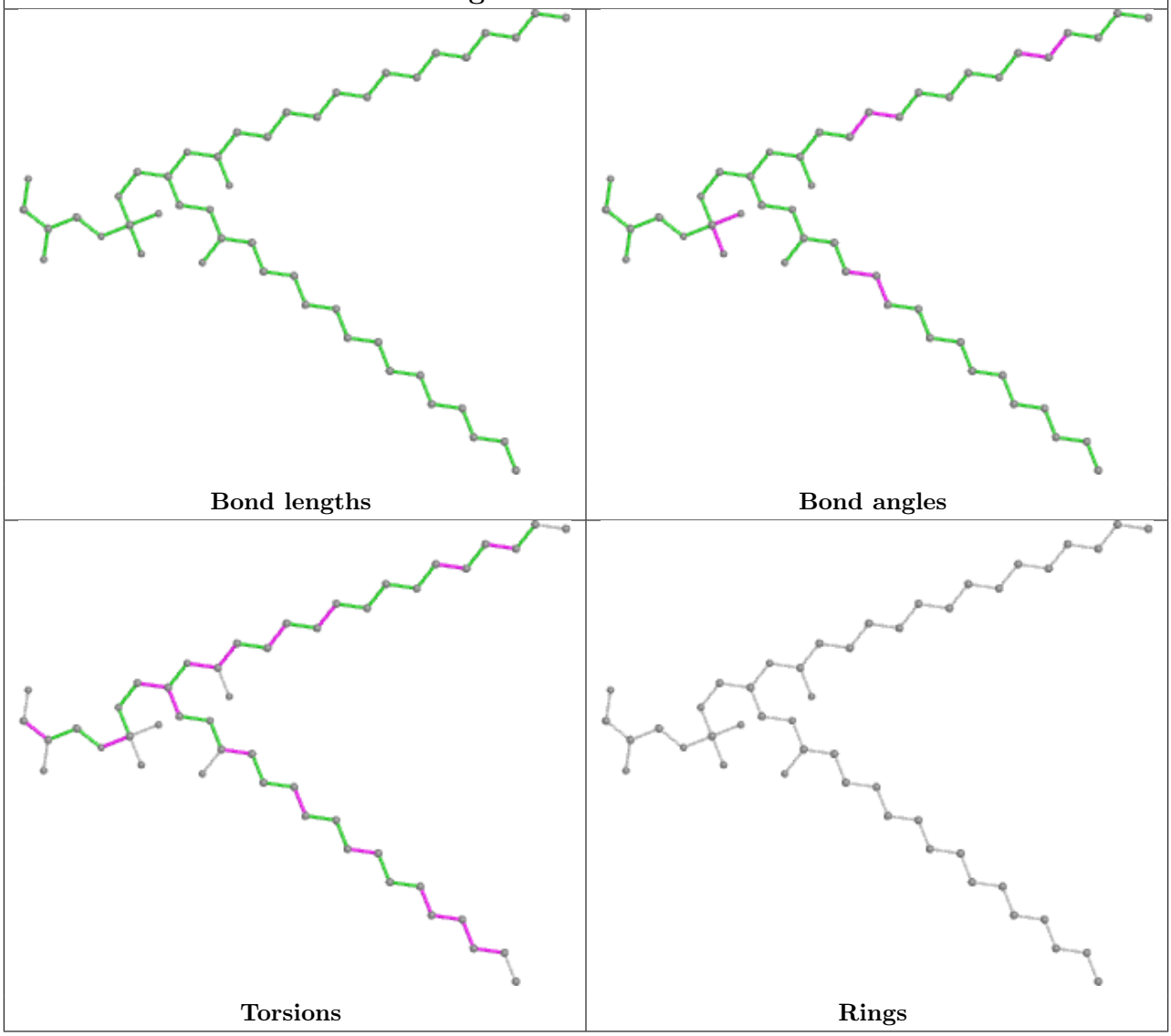
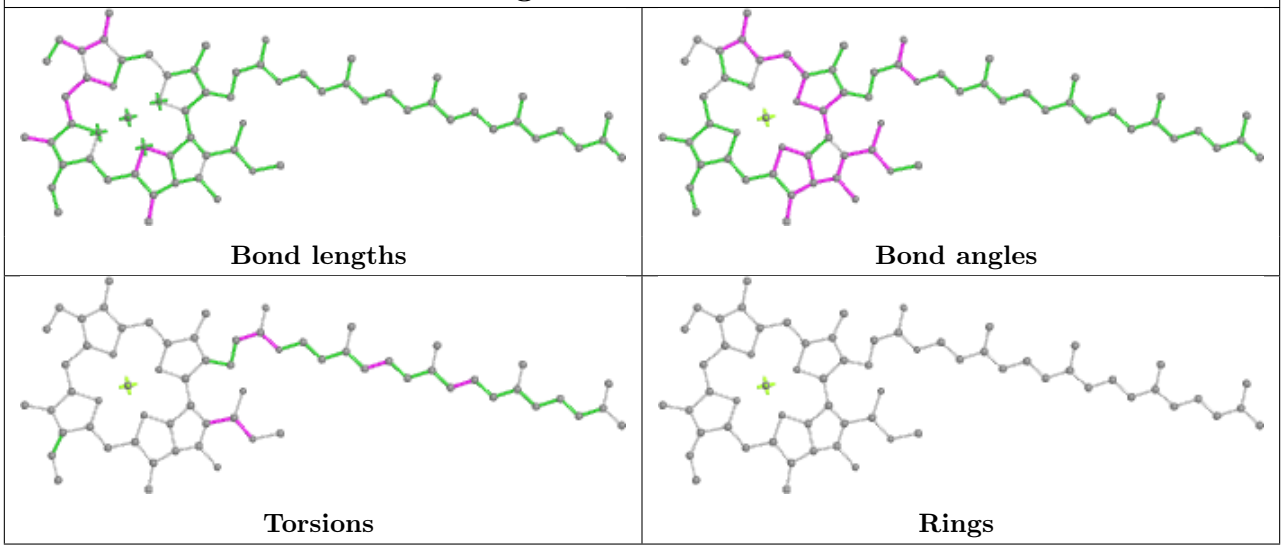
 Bond lengths	 Bond angles
 Torsions	 Rings

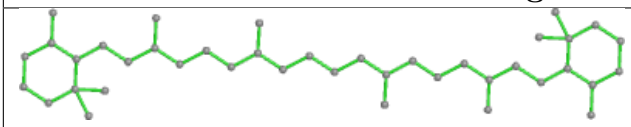
Ligand LHG G 5007



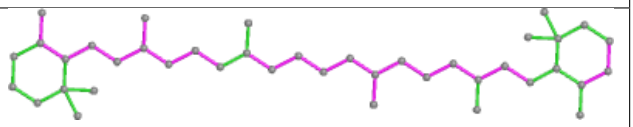
Ligand CLA A 1011



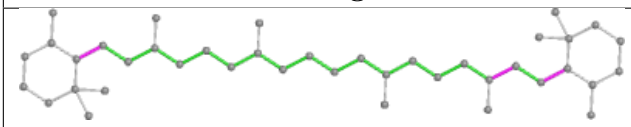
Ligand BCR 4 523



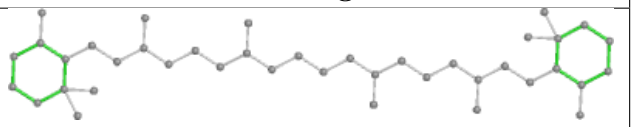
Bond lengths



Bond angles

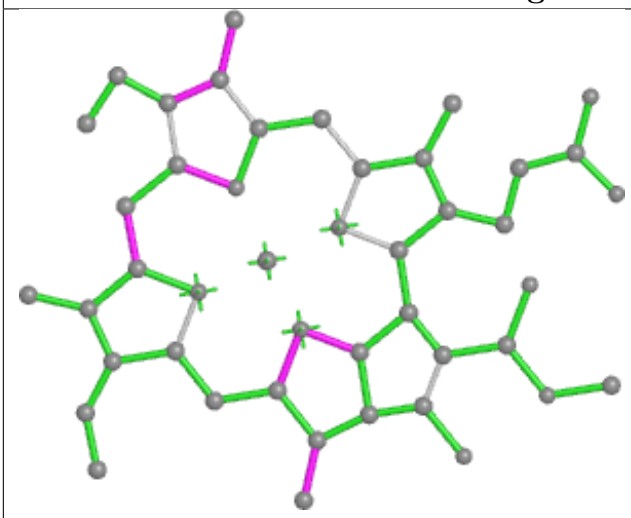


Torsions



Rings

Ligand CLA d 503



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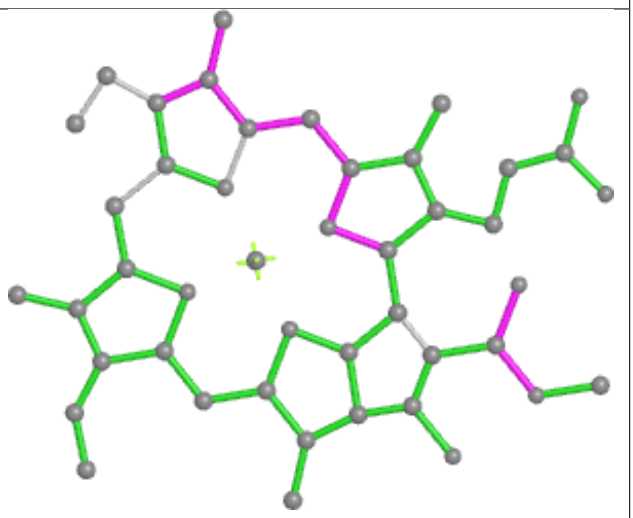

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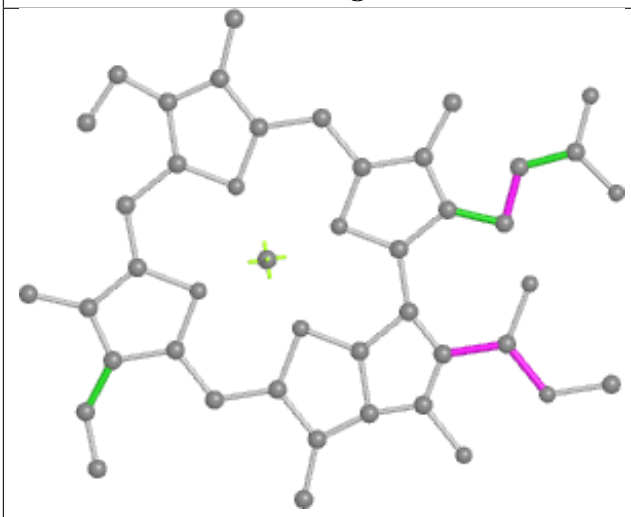

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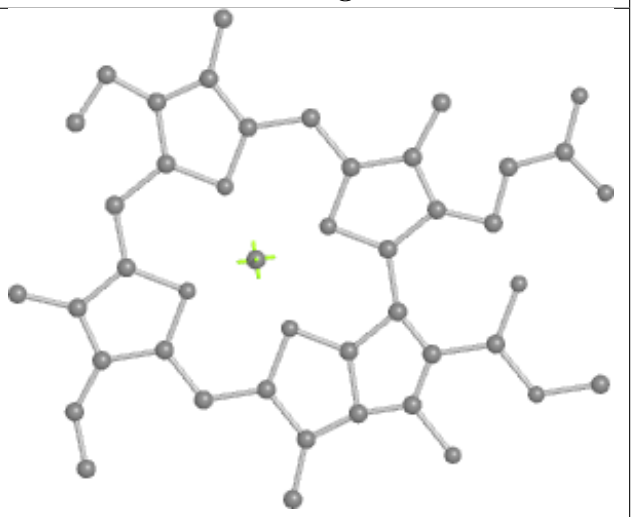
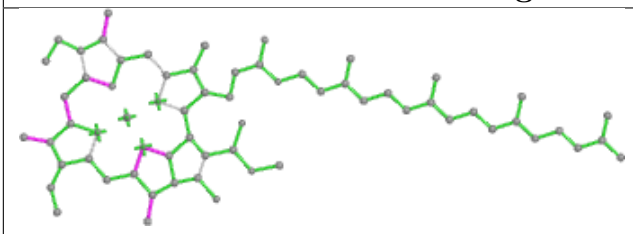


Rings

Ligand CLA B 1231



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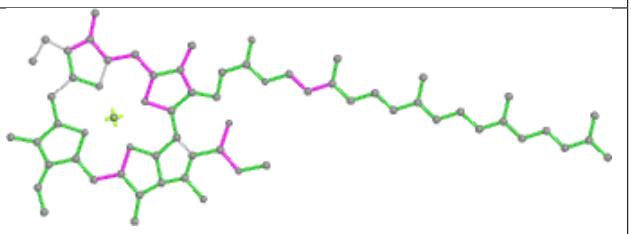

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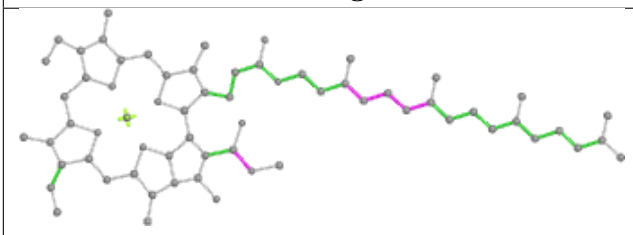

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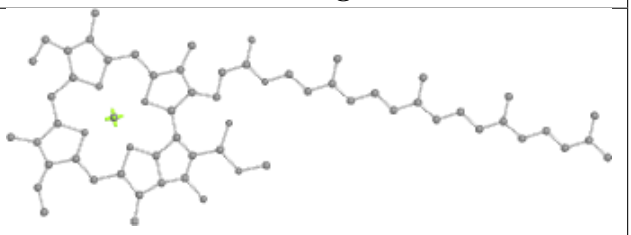
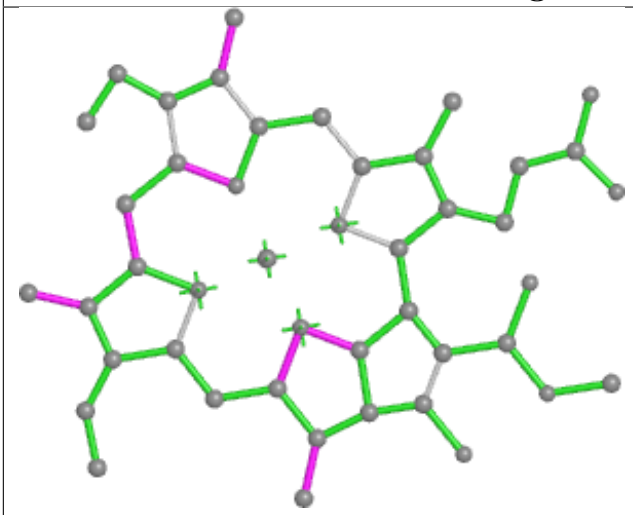


Rings

Ligand CLA 4 517



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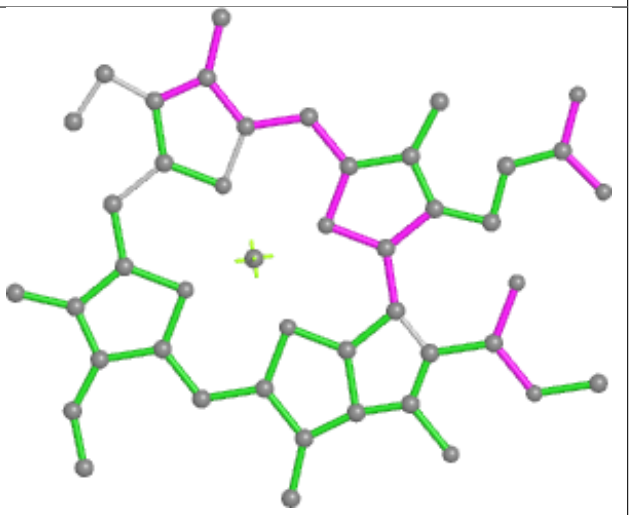

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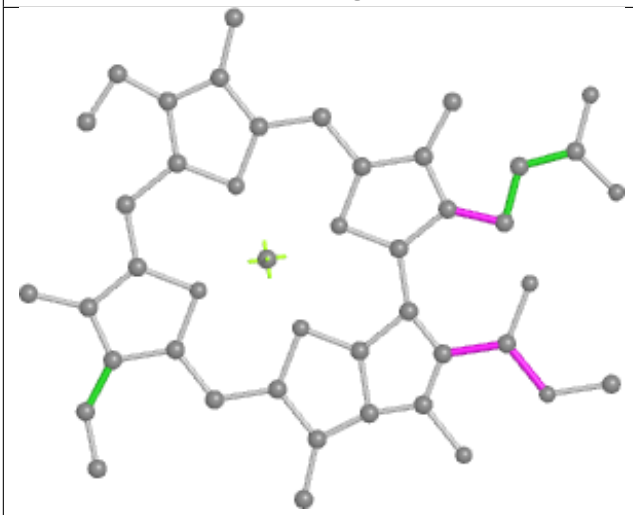

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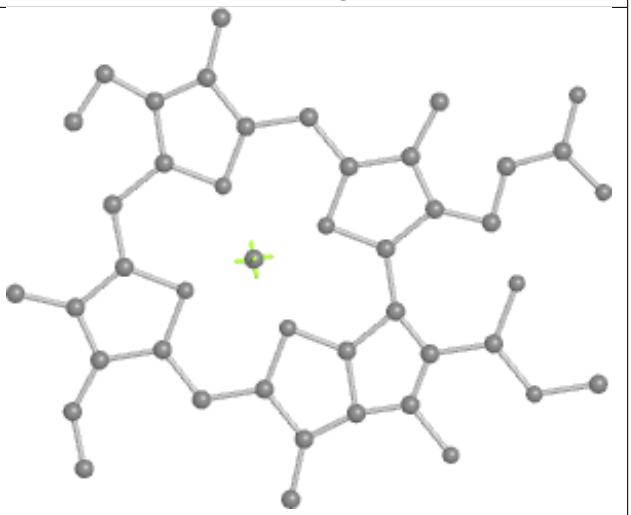
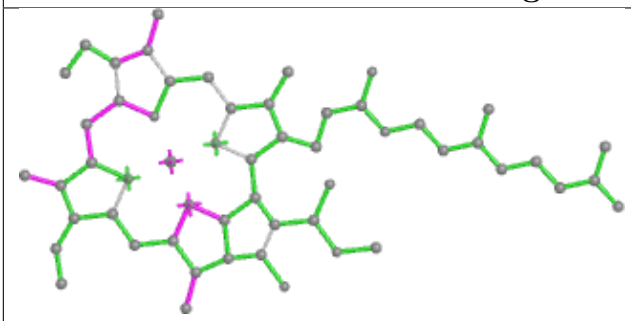


Rings

Ligand CLA f 1226



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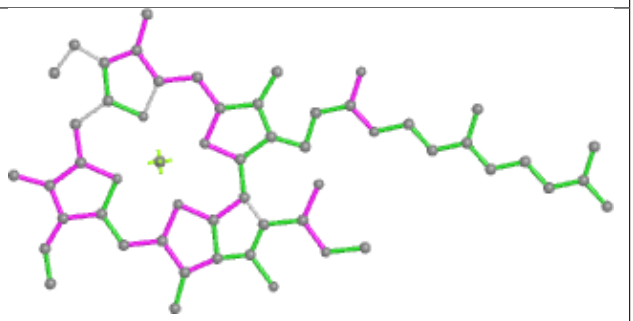
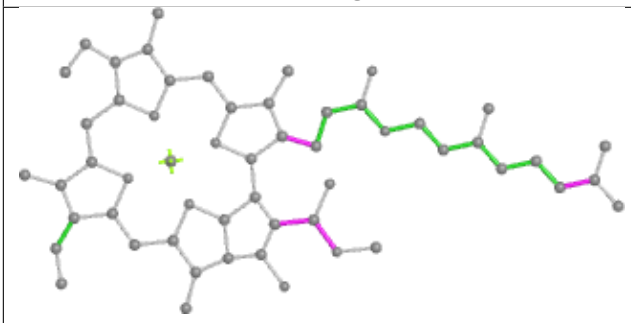


Bond angles



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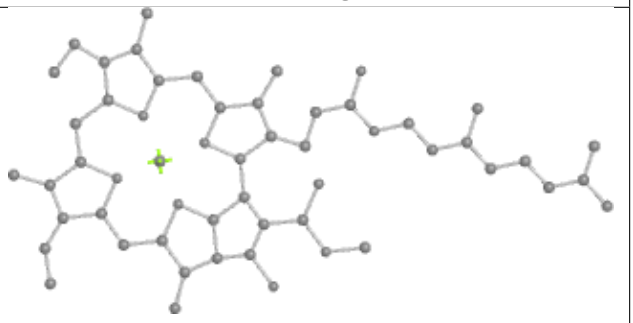
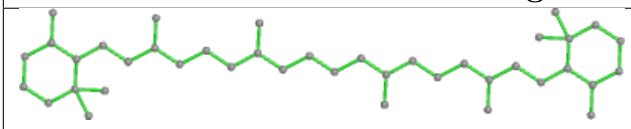


Rings

Ligand BCR 3 523



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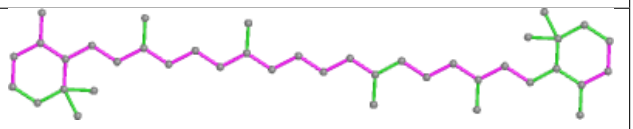
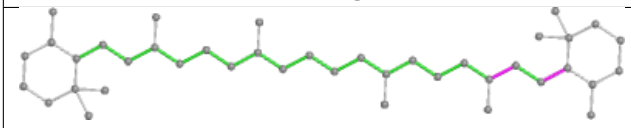


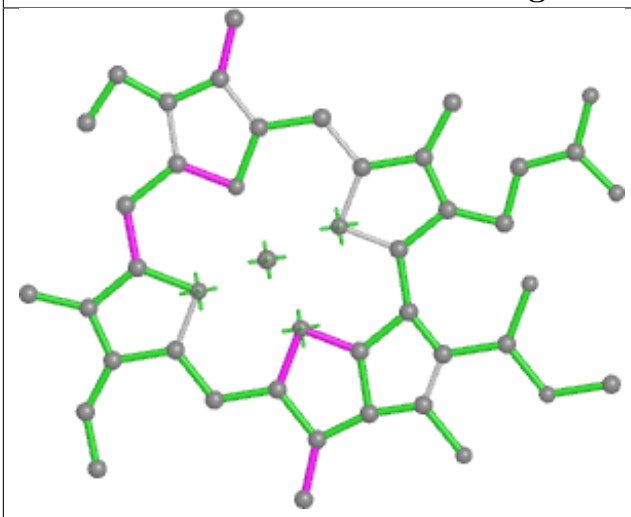
Bond angles



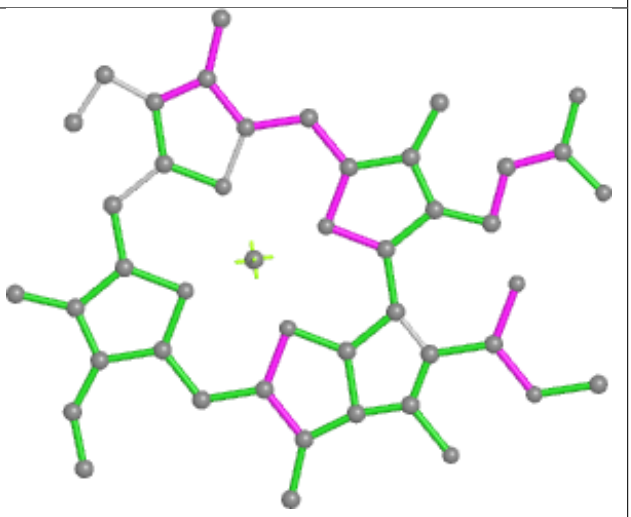
Torsions

Rings

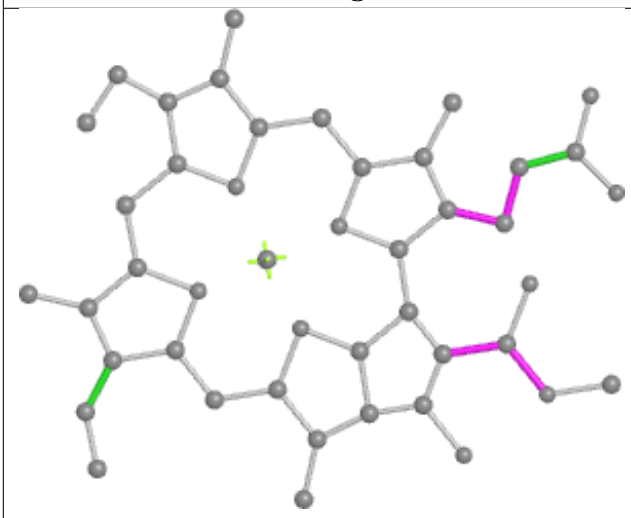
Ligand CLA a 503



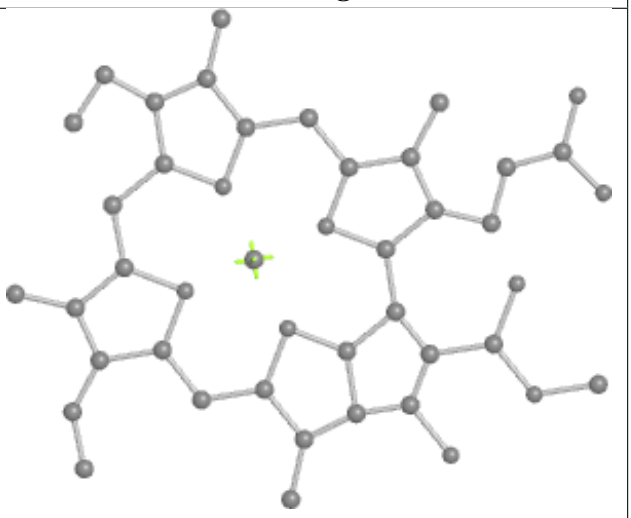
Bond lengths



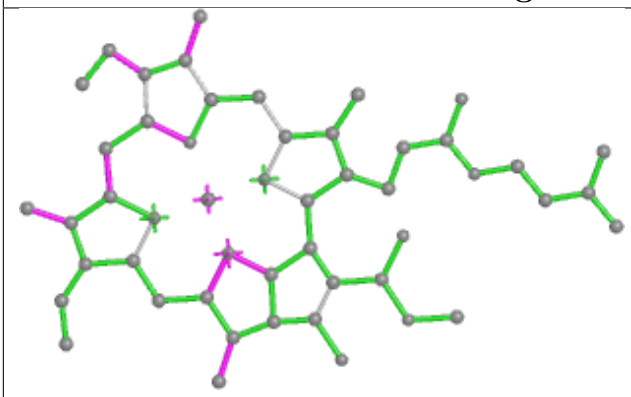
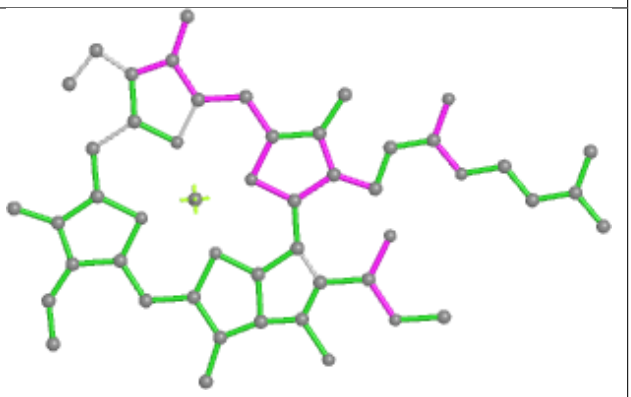
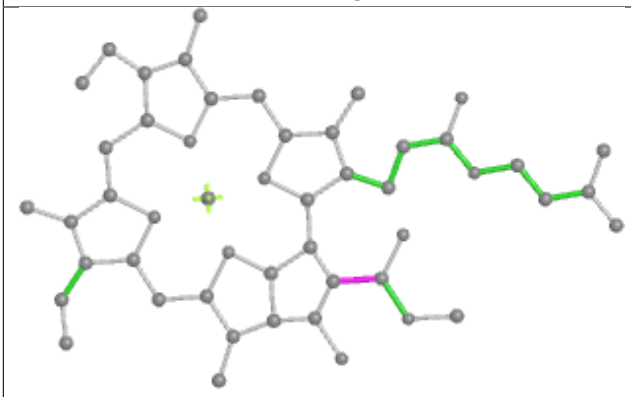
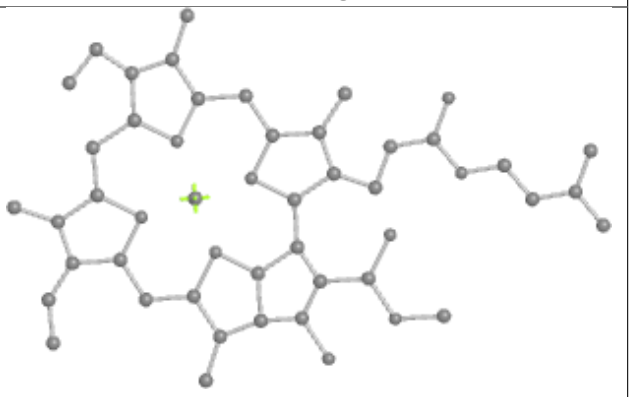
Bond angles



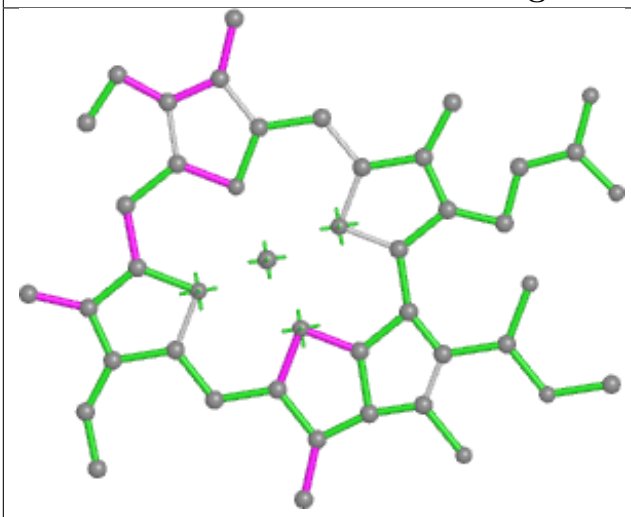
Torsions



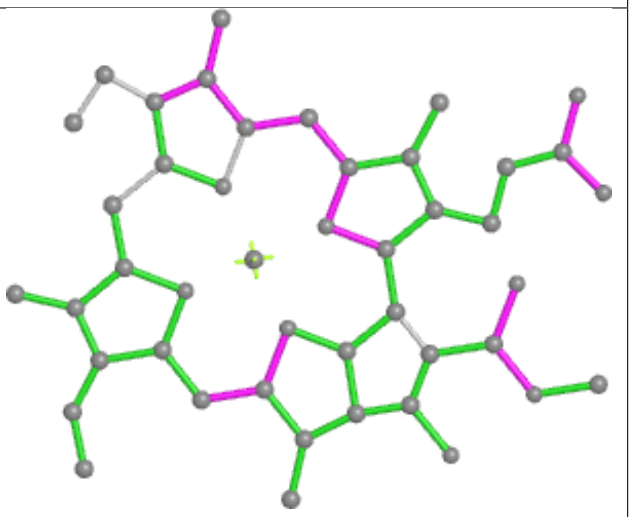
Rings

Ligand CLA B 1222	
 Bond lengths	 Bond angles
 Torsions	 Rings

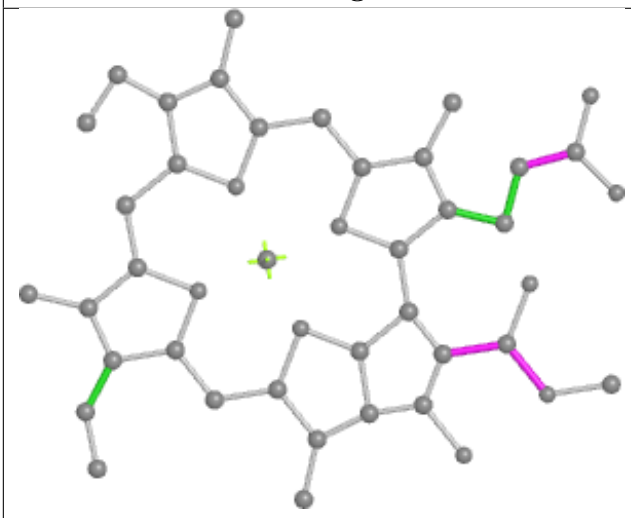
Ligand CLA 2 519



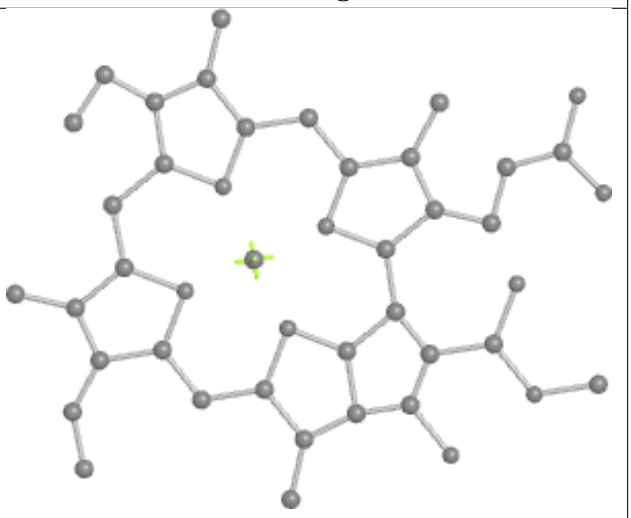
Bond lengths



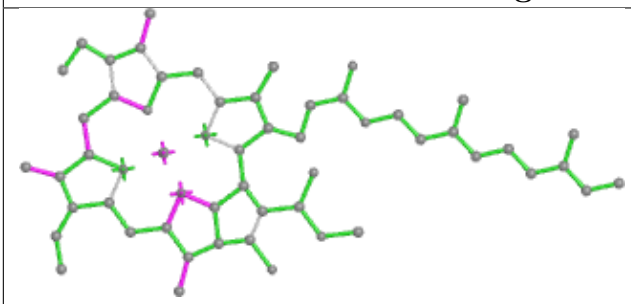
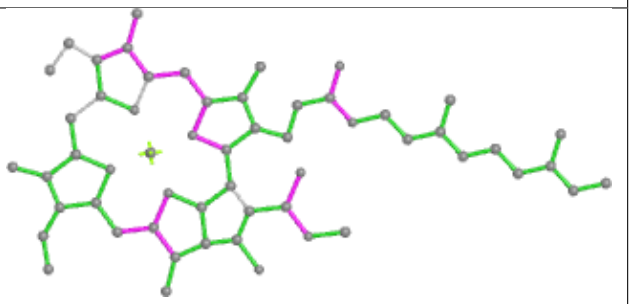
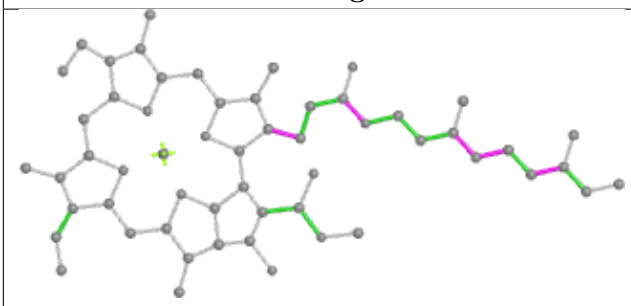
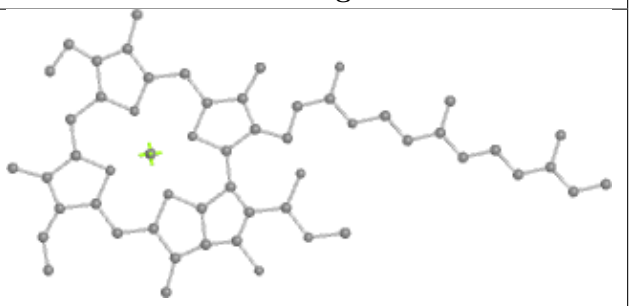
Bond angles

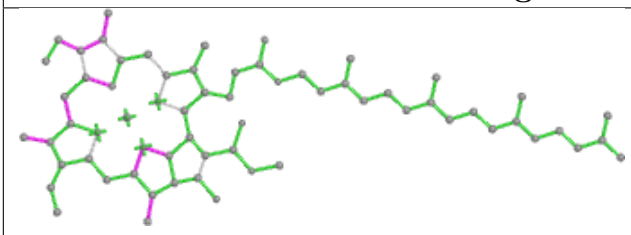
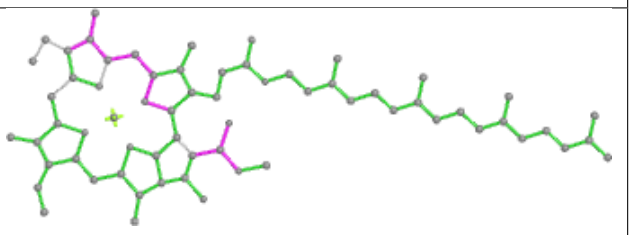
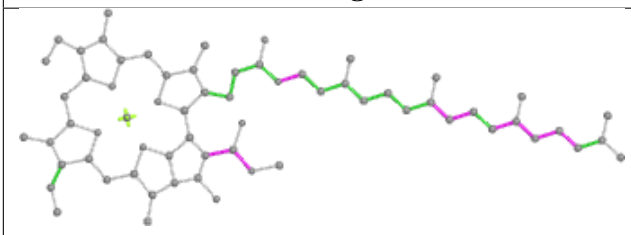
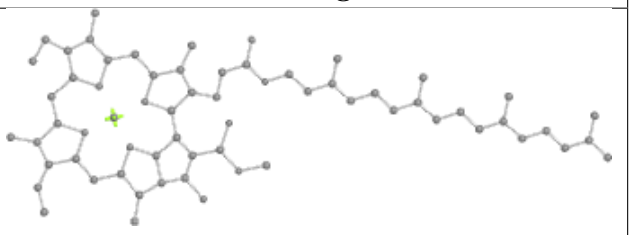


Torsions

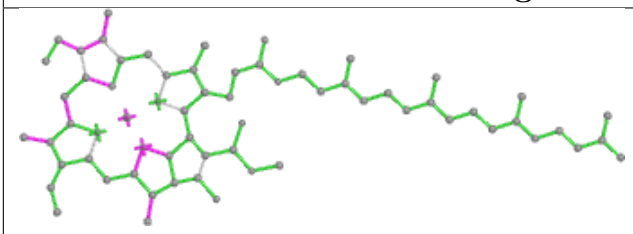


Rings

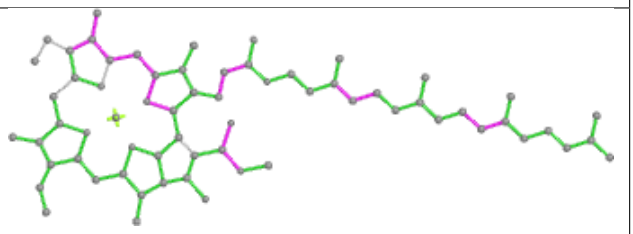
Ligand CLA A 1130	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1138	
 Bond lengths	 Bond angles
 Torsions	 Rings

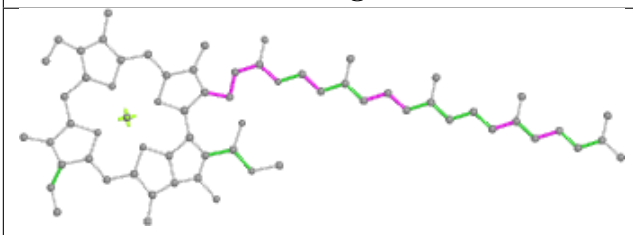
Ligand CLA A 1125



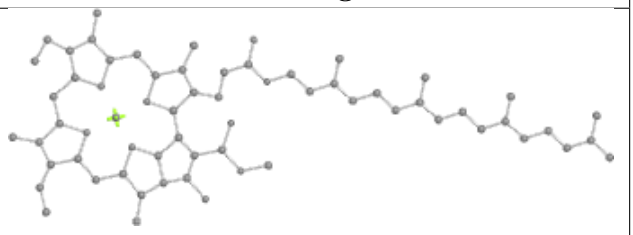
Bond lengths



Bond angles

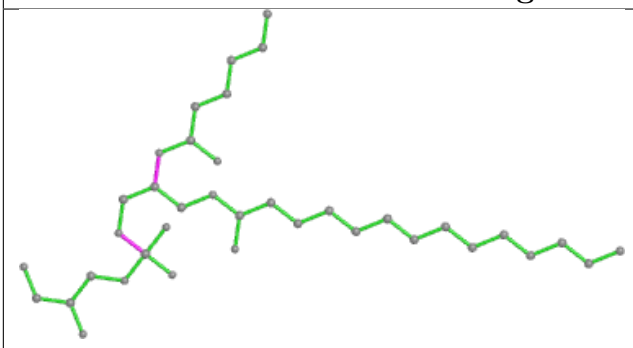


Torsions



Rings

Ligand LHG n 5218



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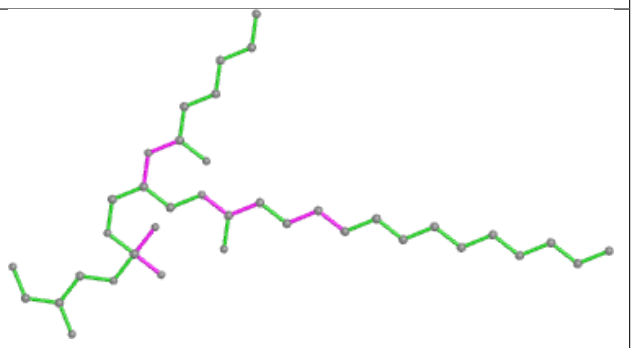
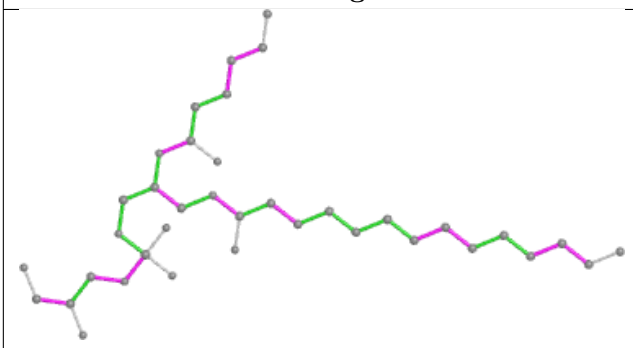


Bond angles



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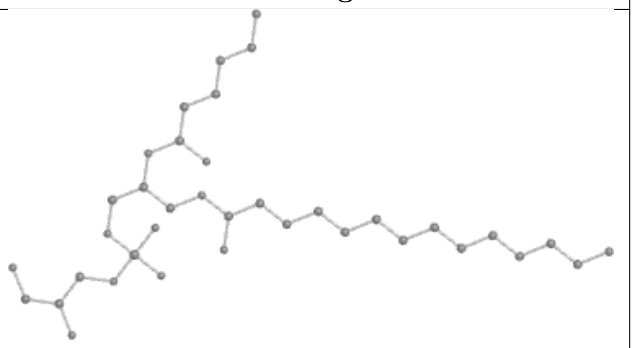
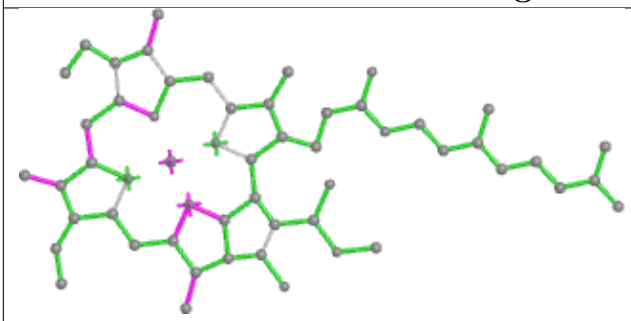


Rings

Ligand CLA H 1232



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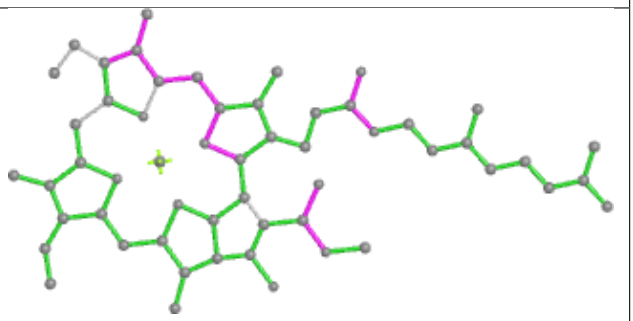
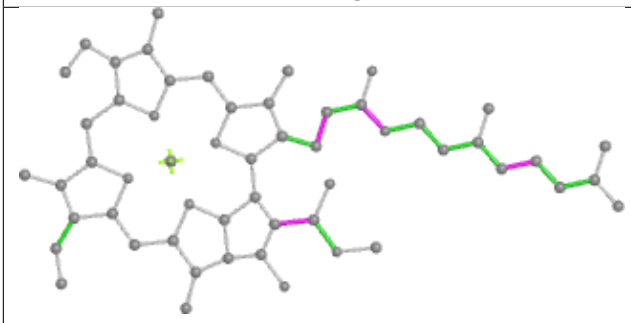


Bond angles



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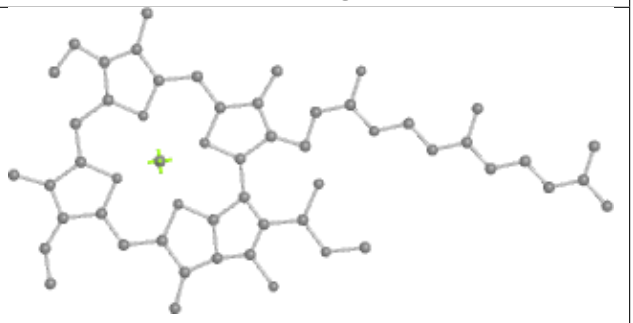
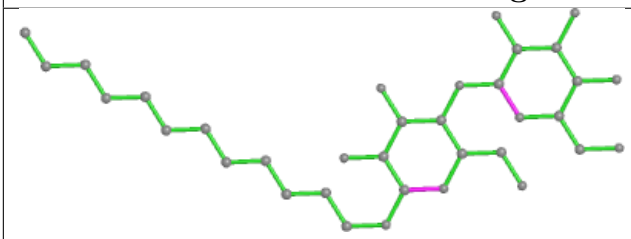
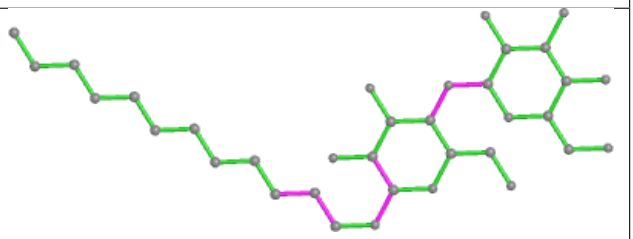


Rings

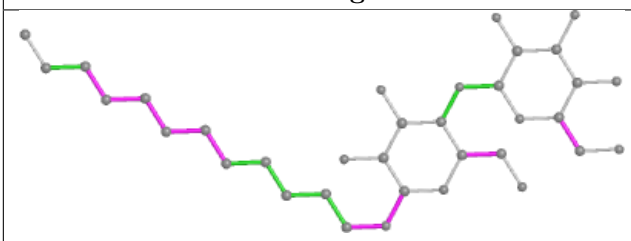
Ligand LMU H 1843



Bond lengths



Bond angles



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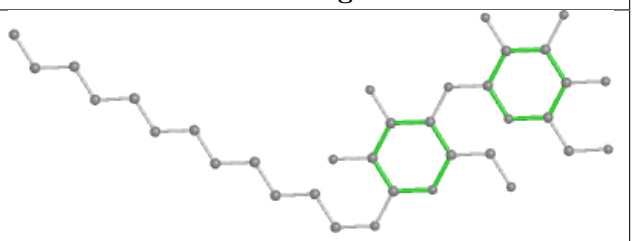
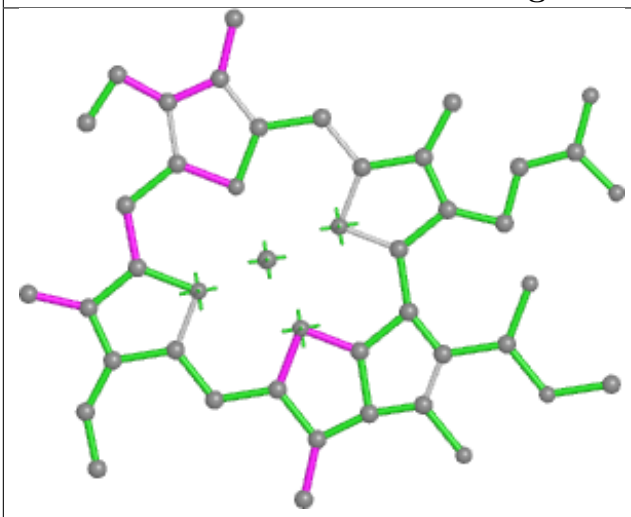


Rings

Ligand CLA 6 519



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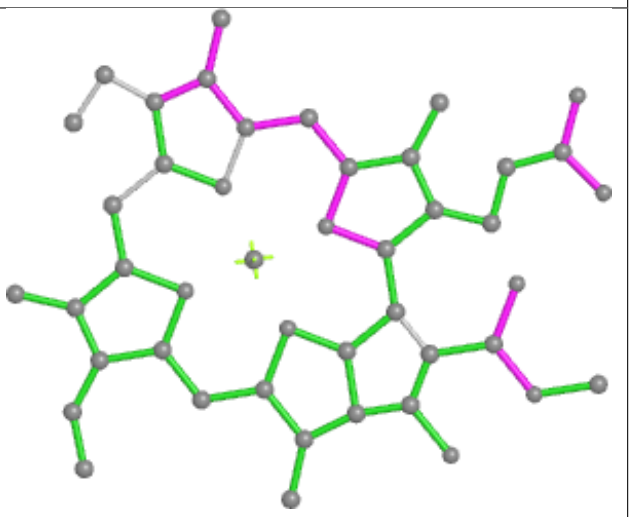
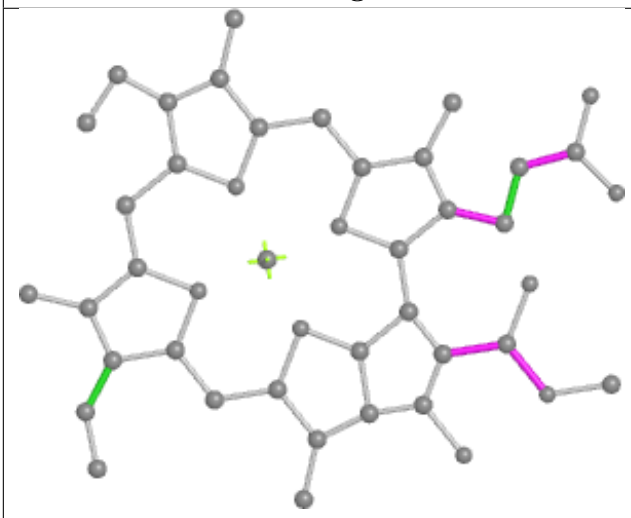


Bond angles



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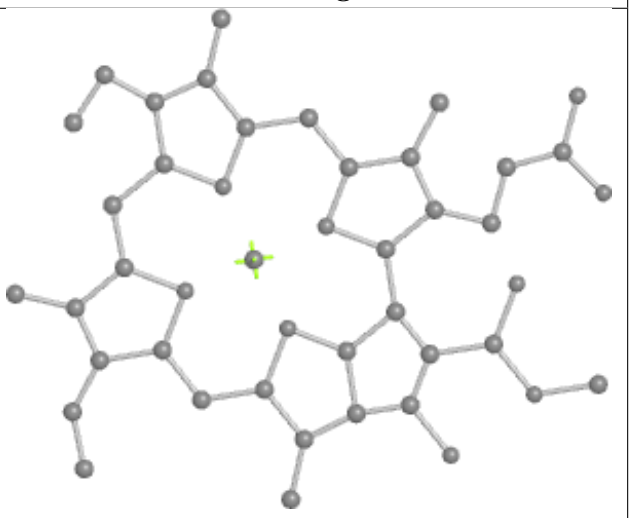
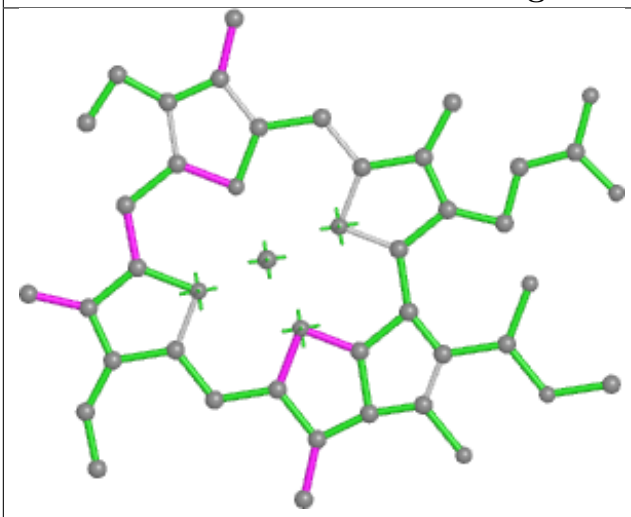


Rings

Ligand CLA q 507



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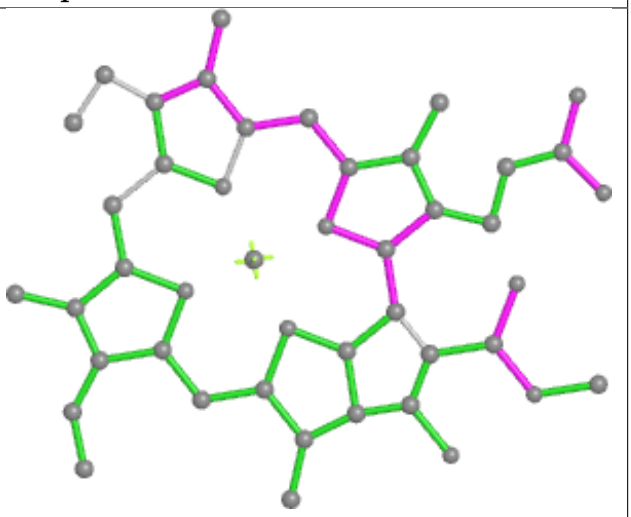
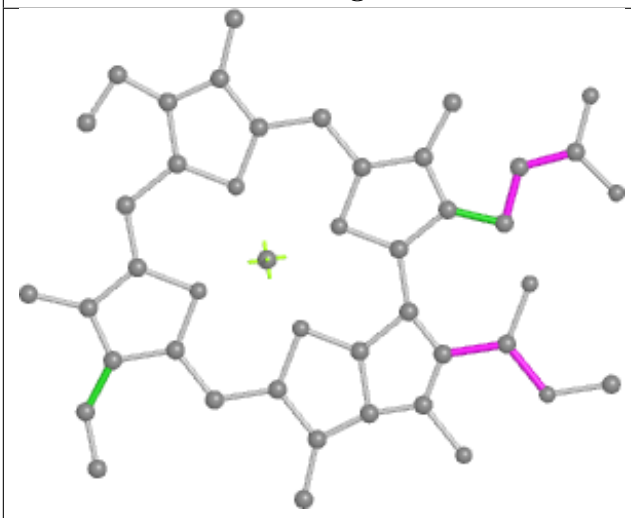


Bond angles



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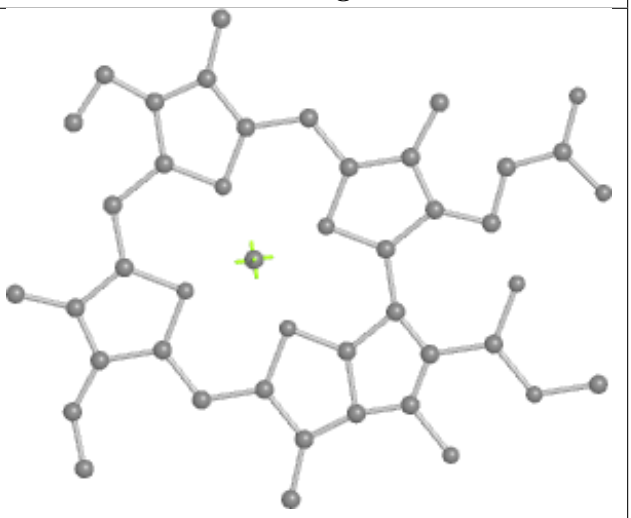
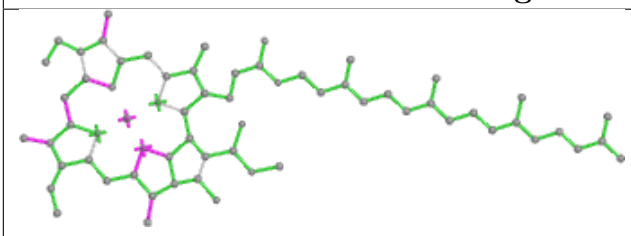


Rings

Ligand CLA H 1223



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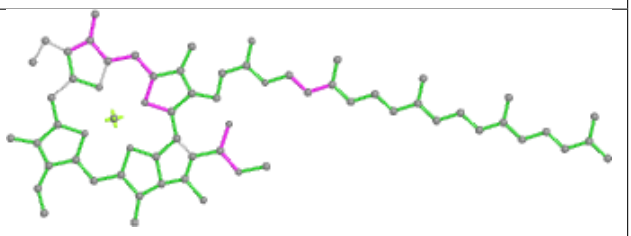
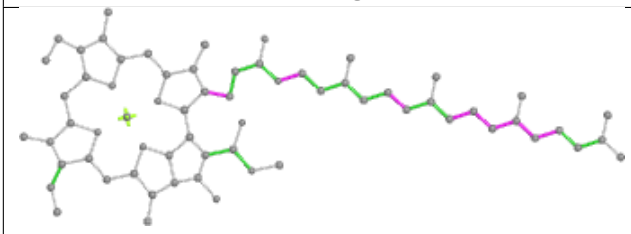


Bond angles



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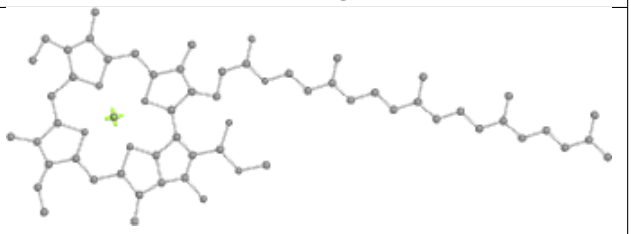
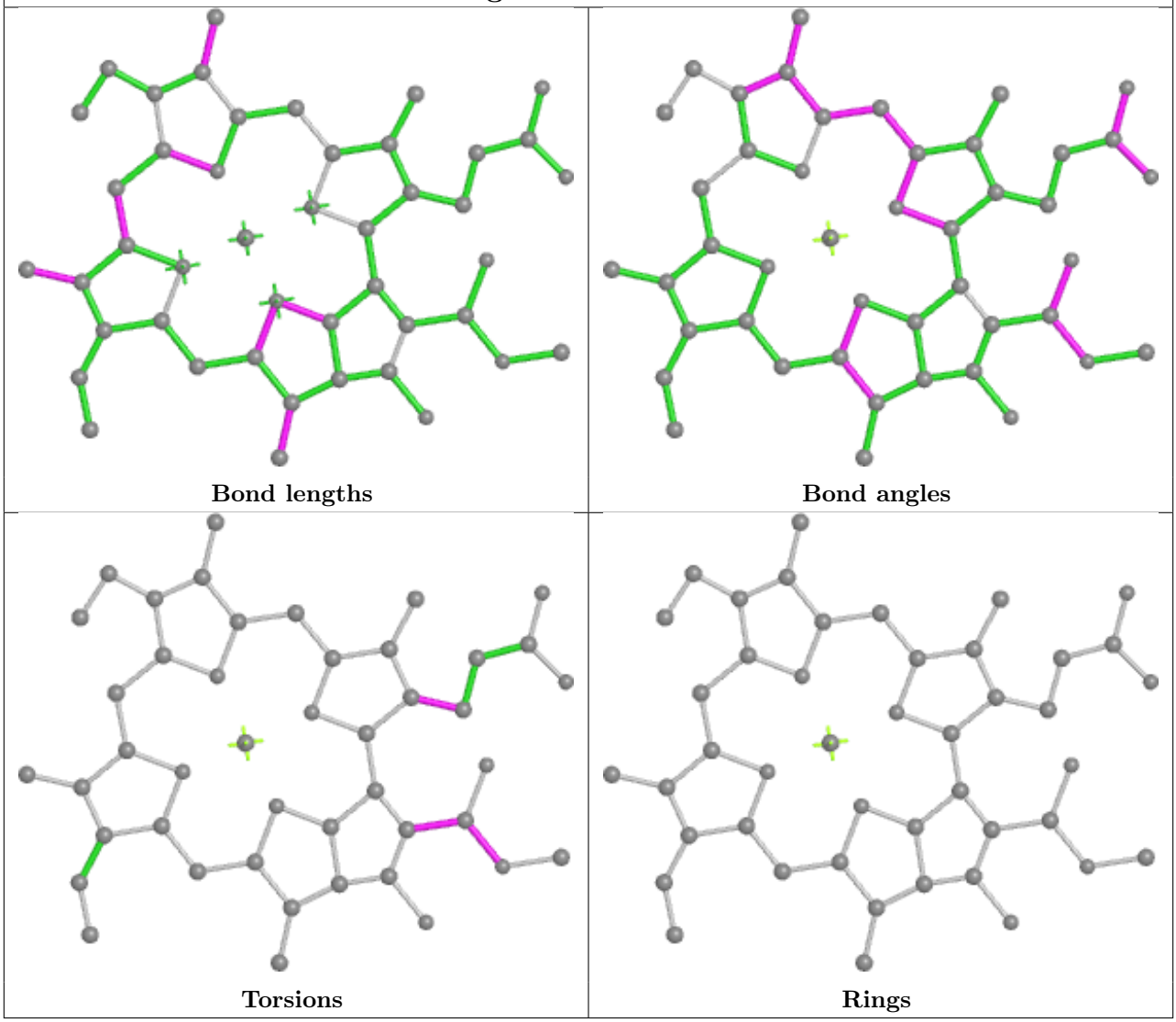
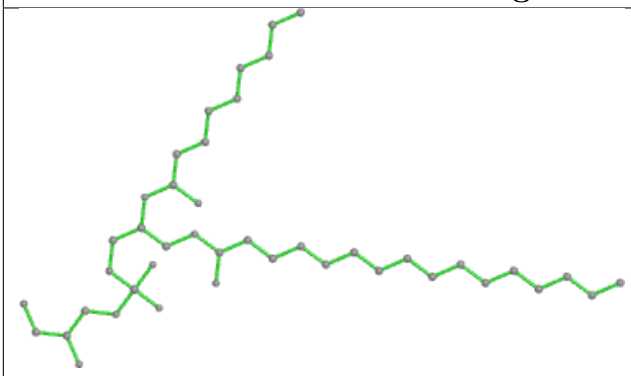
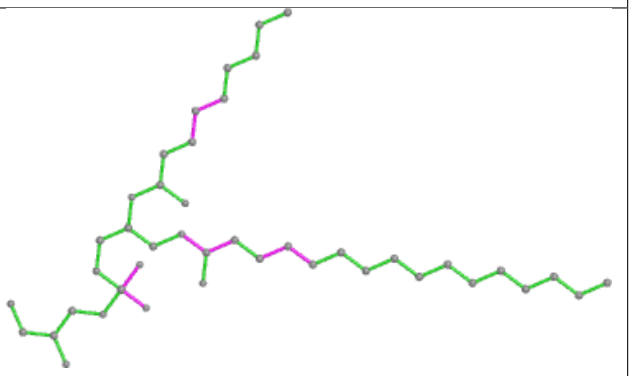
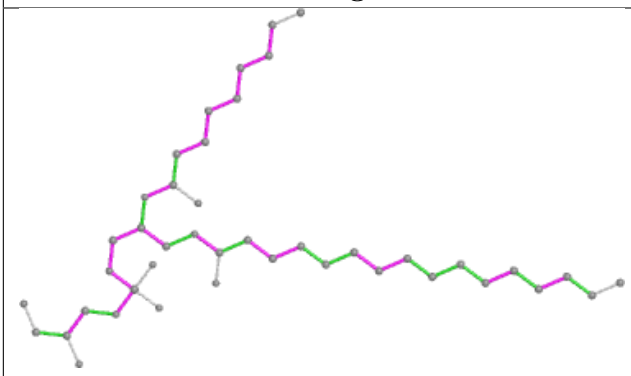
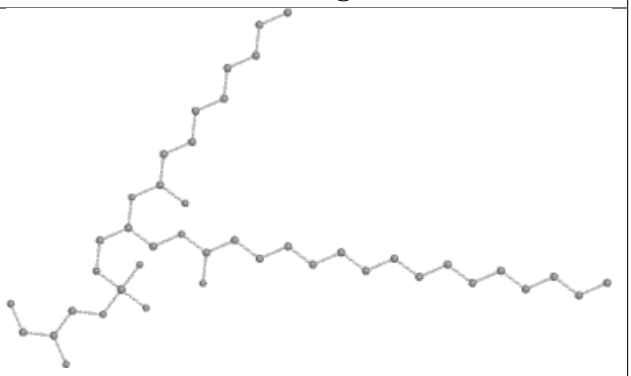


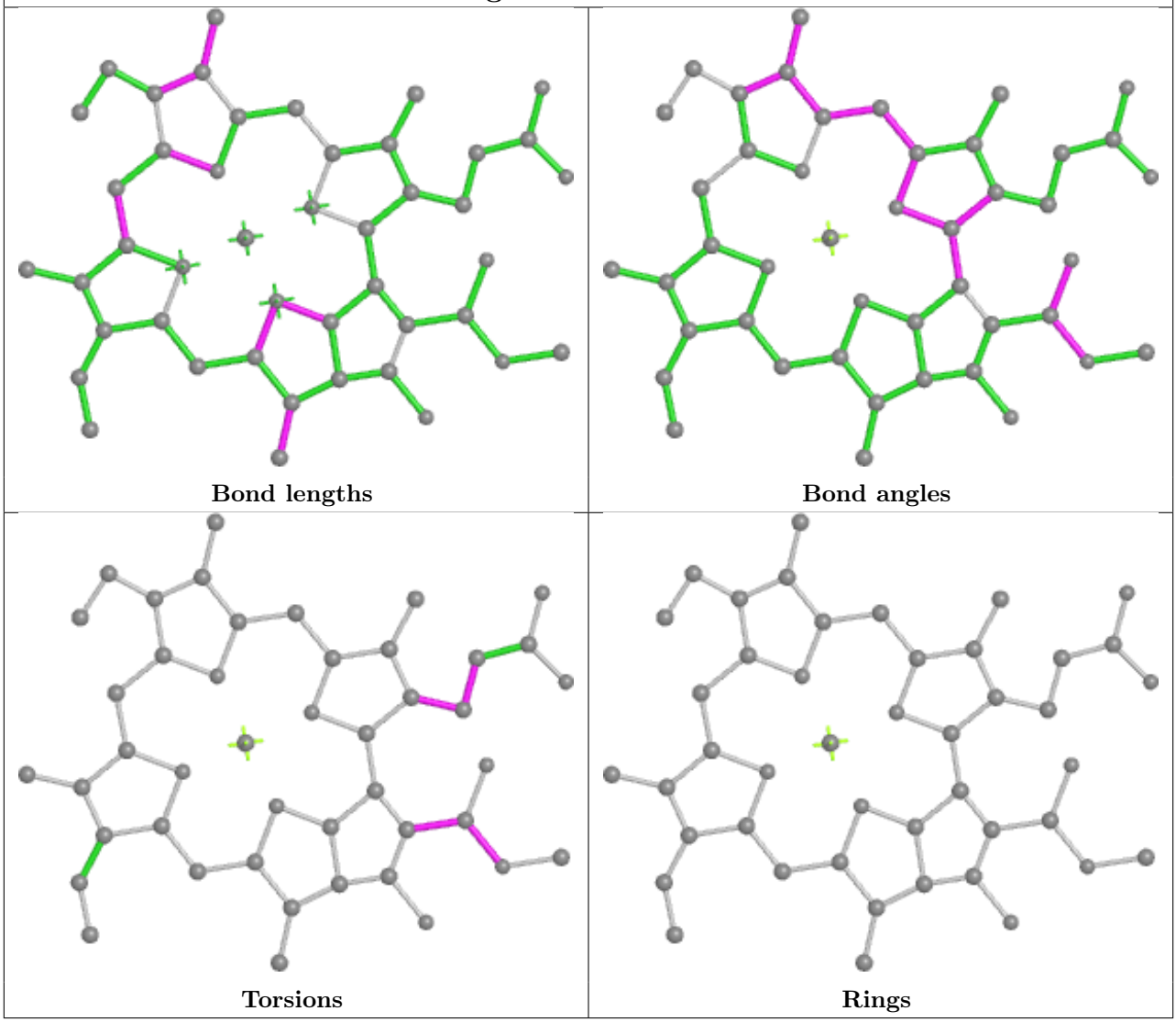
Rings

Ligand CLA r 511

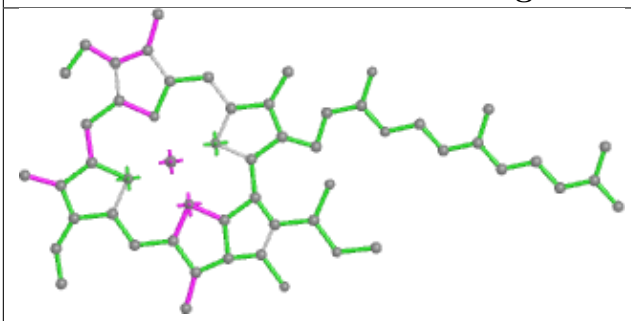


Ligand LHG G 5009	
 Bond lengths	 Bond angles
 Torsions	 Rings

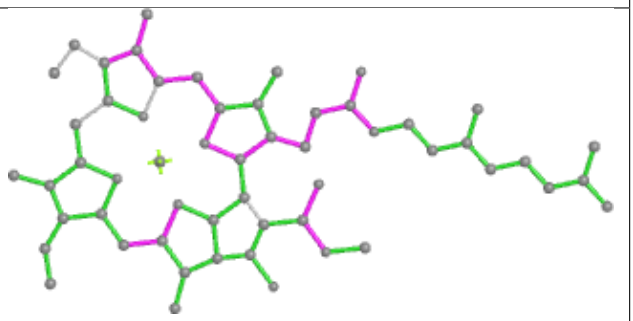
Ligand CLA c 502



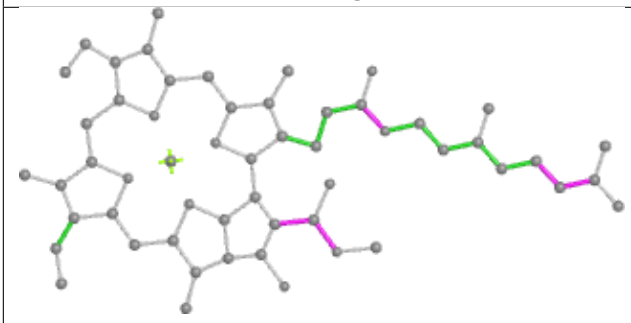
Ligand CLA B 1220



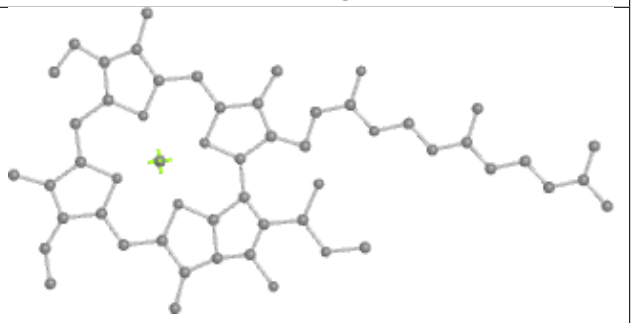
Bond lengths



Bond angles

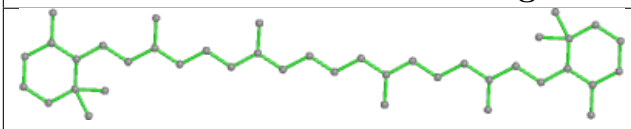


Torsions

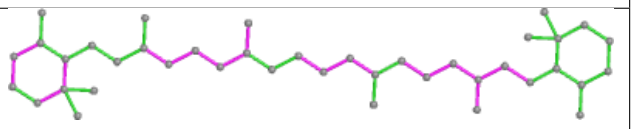


Rings

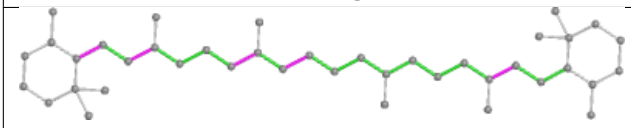
Ligand BCR e 4001



Bond lengths



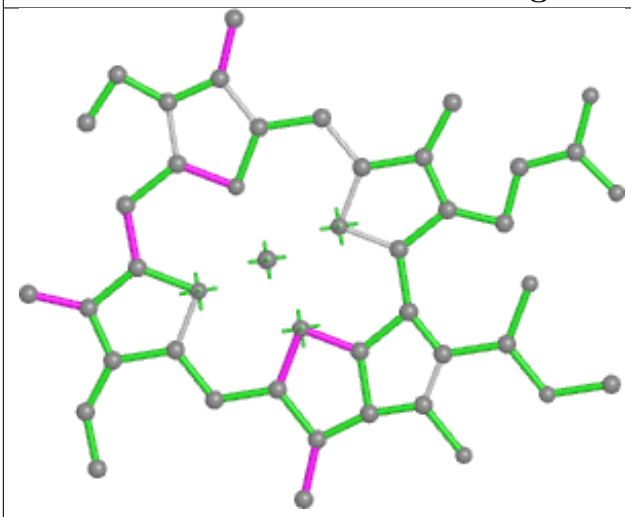
Bond angles



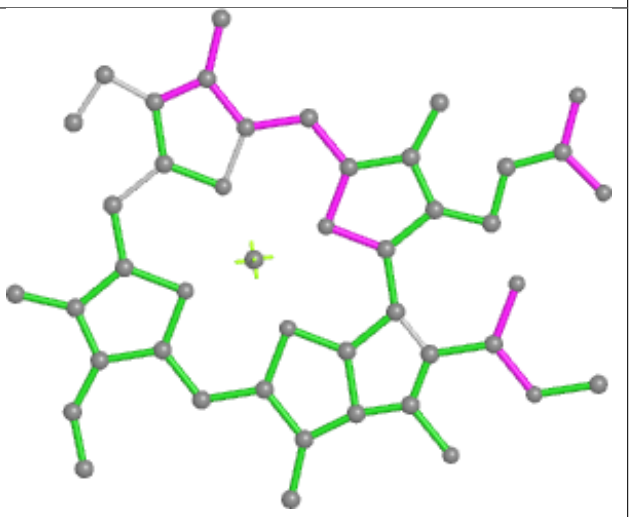
Torsions

Rings

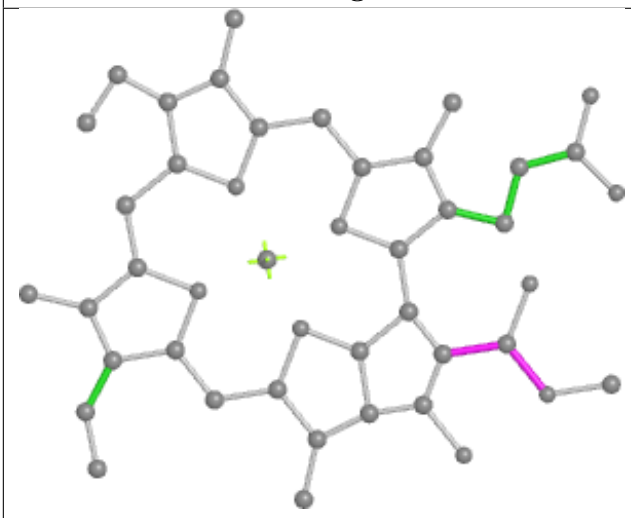
Ligand CLA r 506



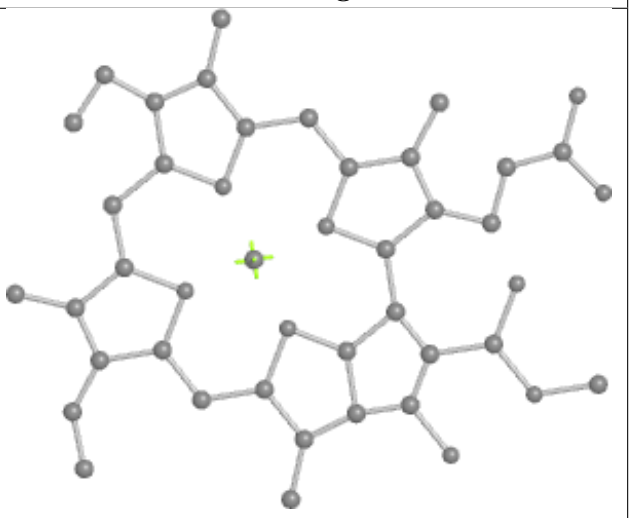
Bond lengths



Bond angles

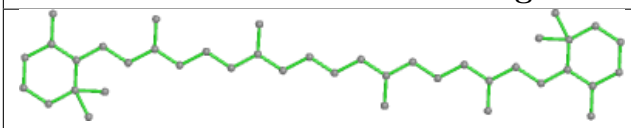


Torsions

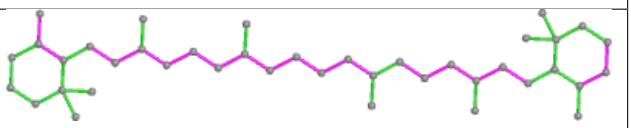


Rings

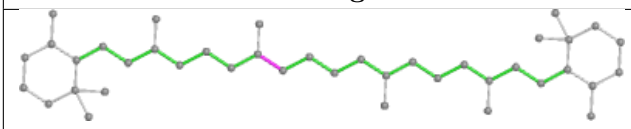
Ligand BCR F 4016



Bond lengths

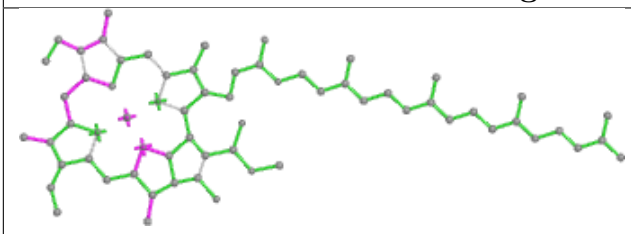
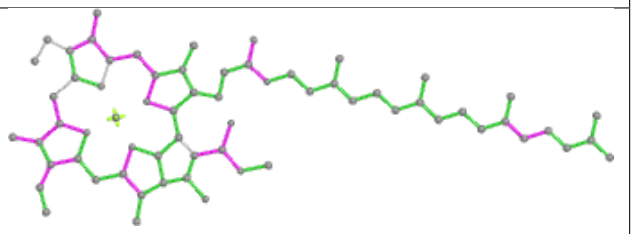
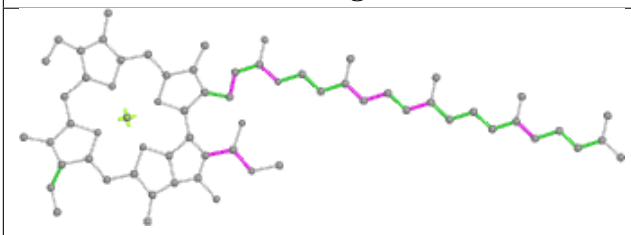
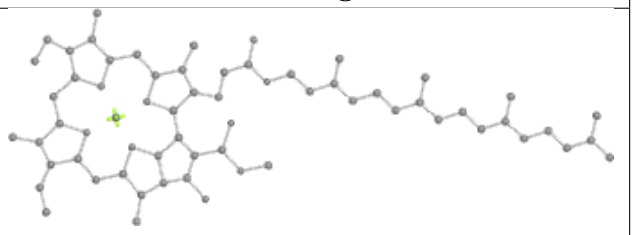


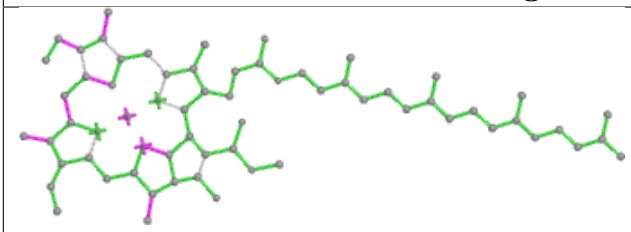
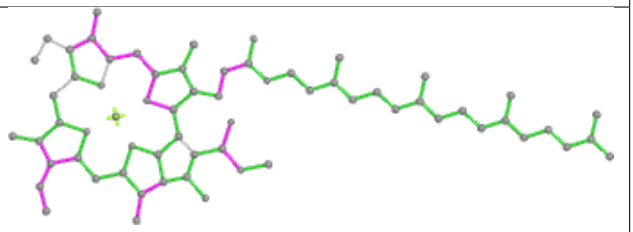
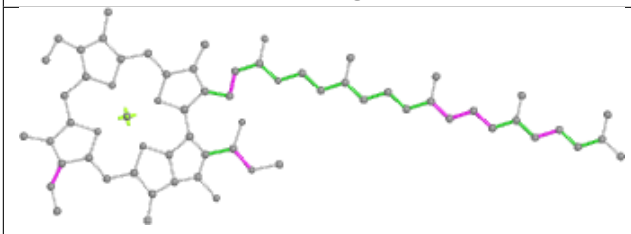
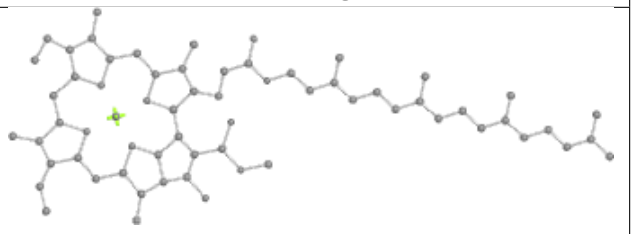
Bond angles



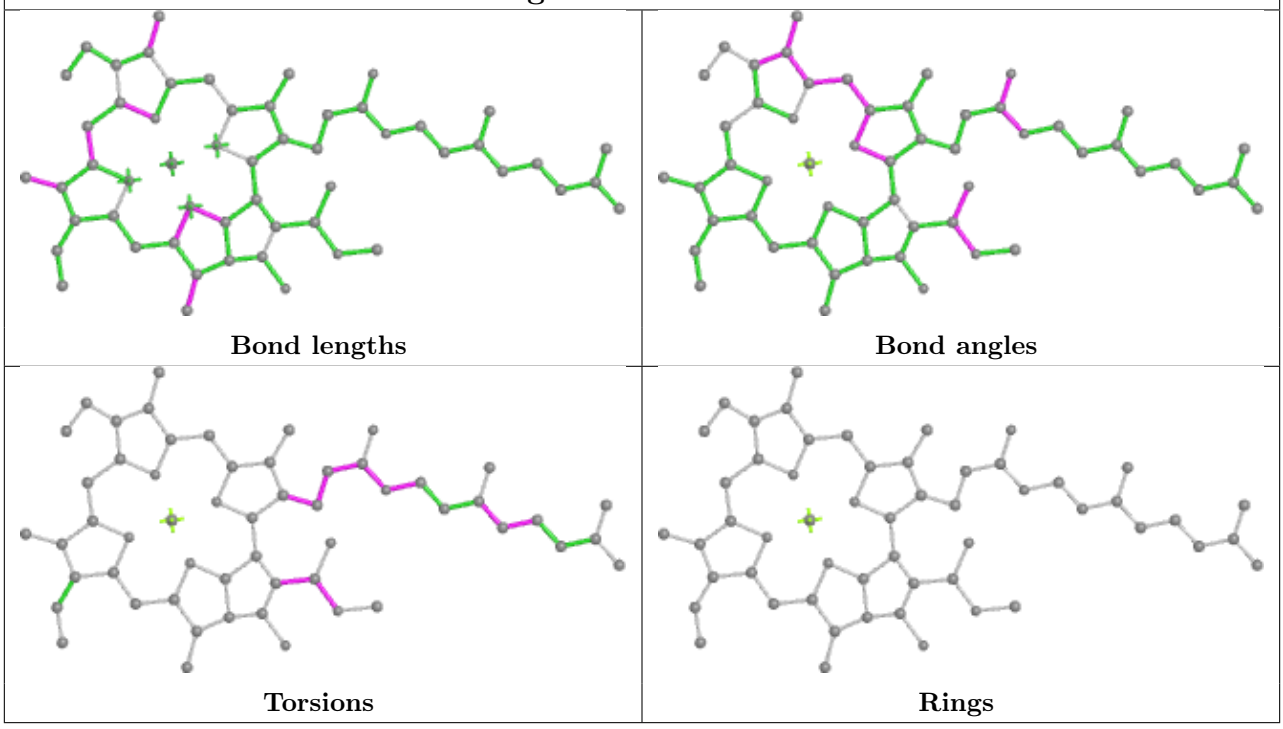
Torsions

Rings

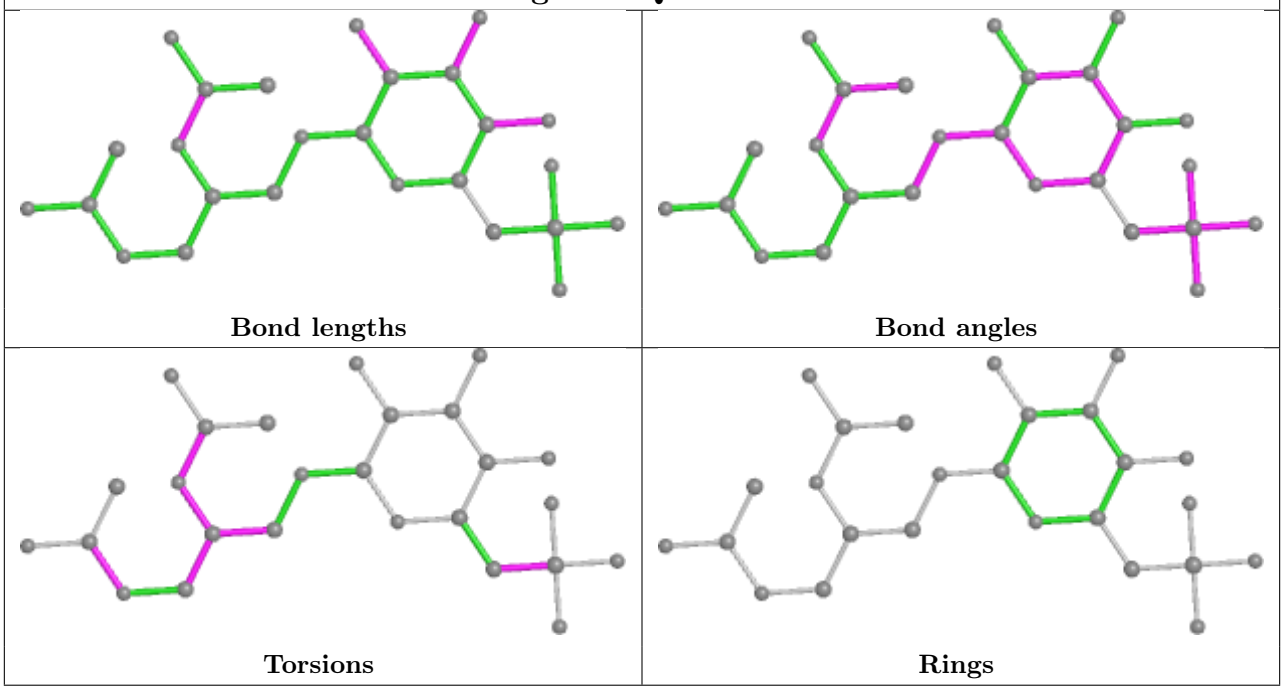
Ligand CLA e 1119	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 1023	
 Bond lengths	 Bond angles
 Torsions	 Rings

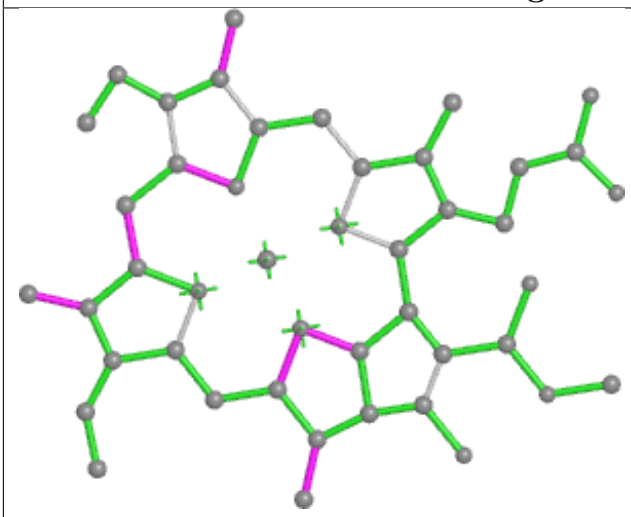
Ligand CLA Z 518



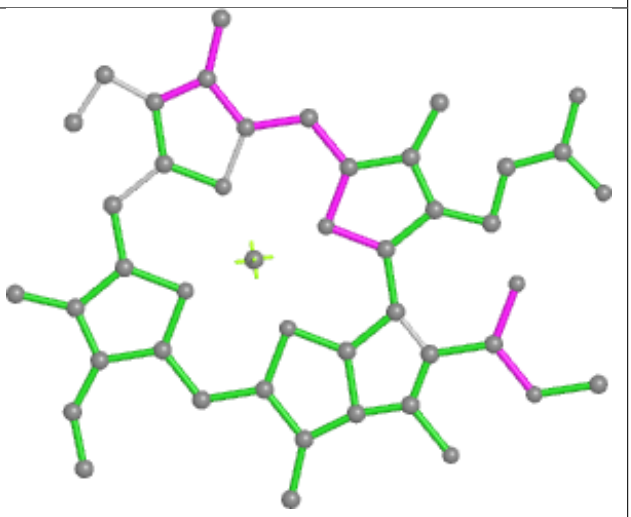
Ligand SQD t 822



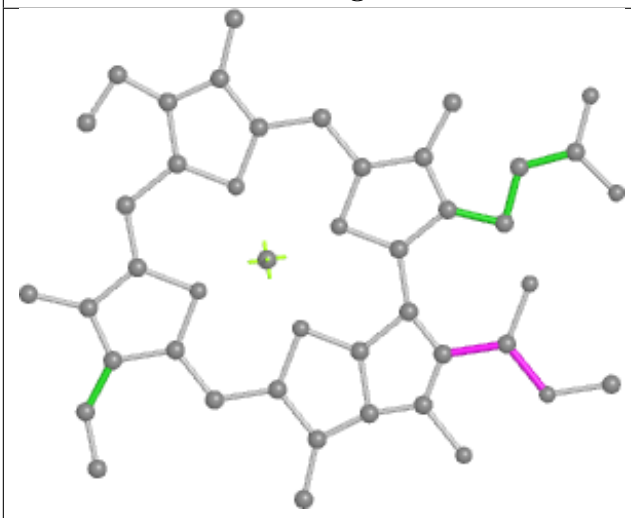
Ligand CLA d 506



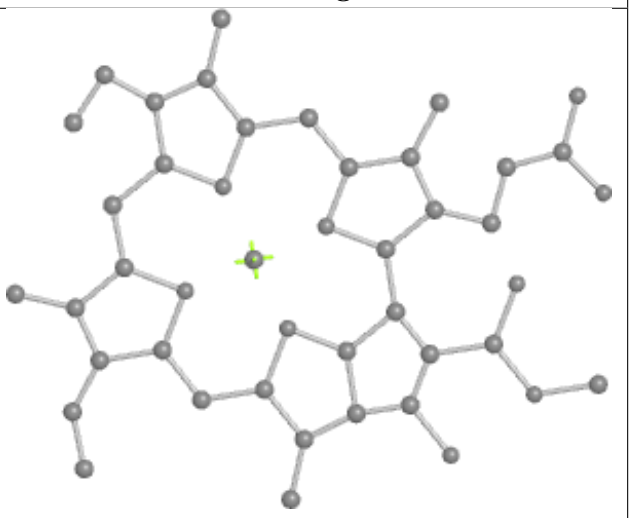
Bond lengths



Bond angles

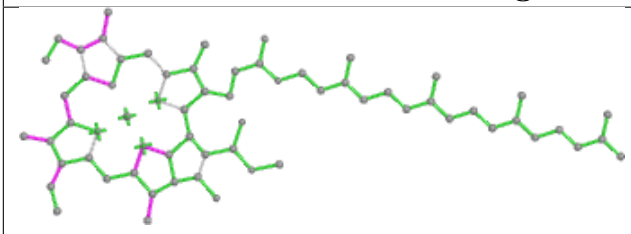


Torsions

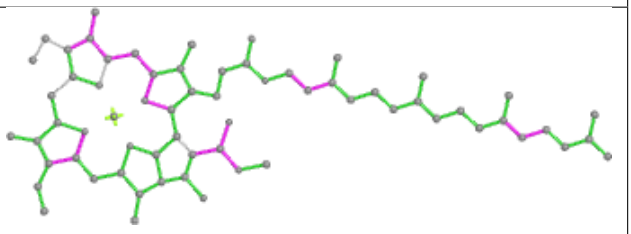


Rings

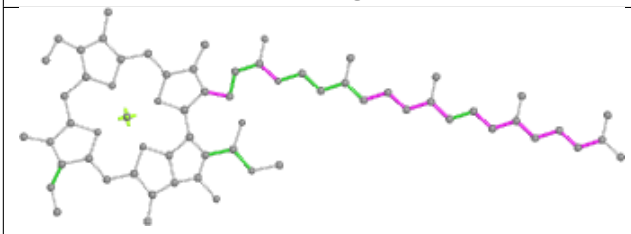
Ligand CLA H 1215



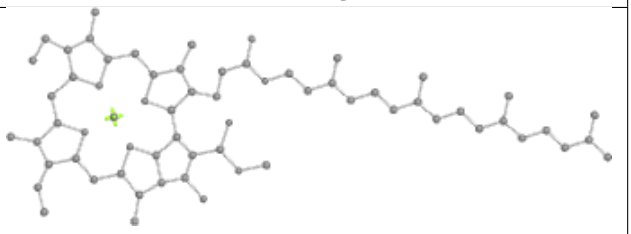
Bond lengths



Bond angles

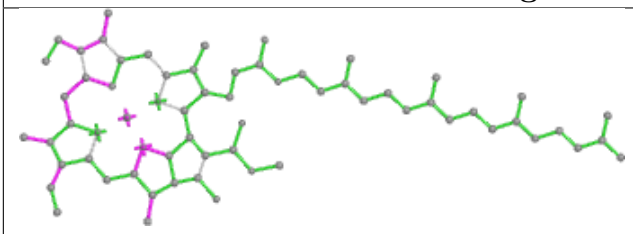


Torsions

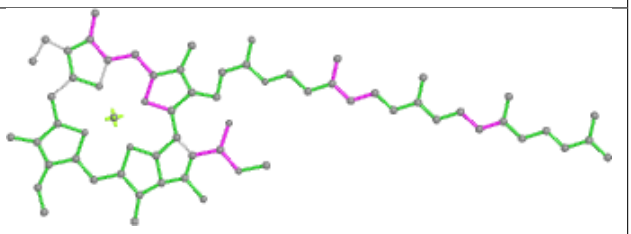


Rings

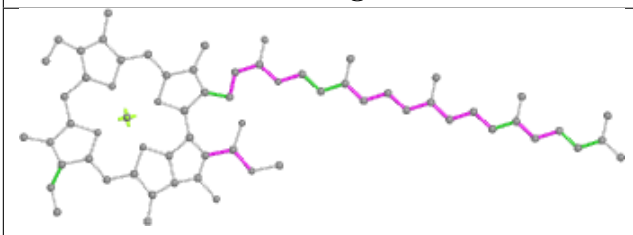
Ligand CLA e 1237



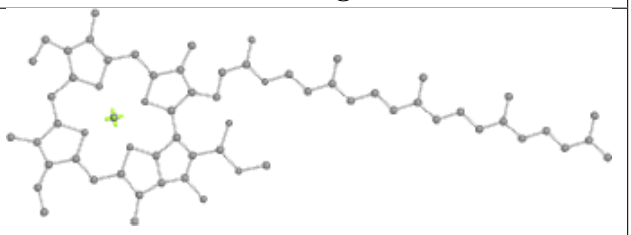
Bond lengths



Bond angles

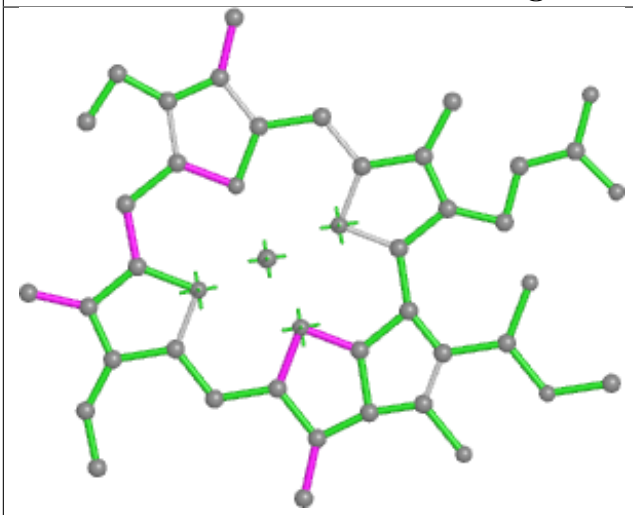


Torsions



Rings

Ligand CLA u 506



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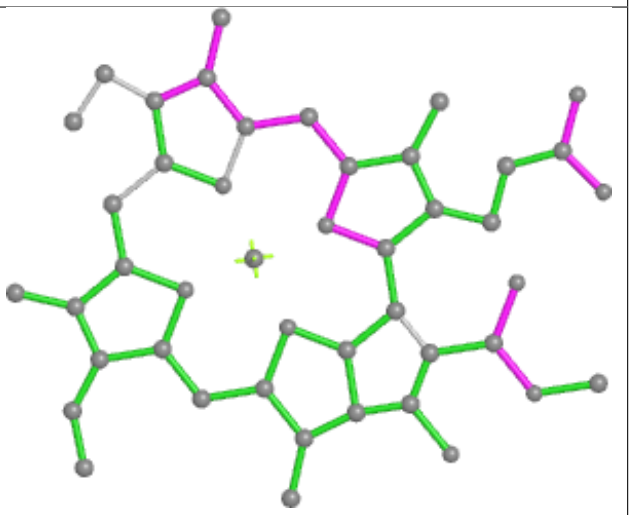
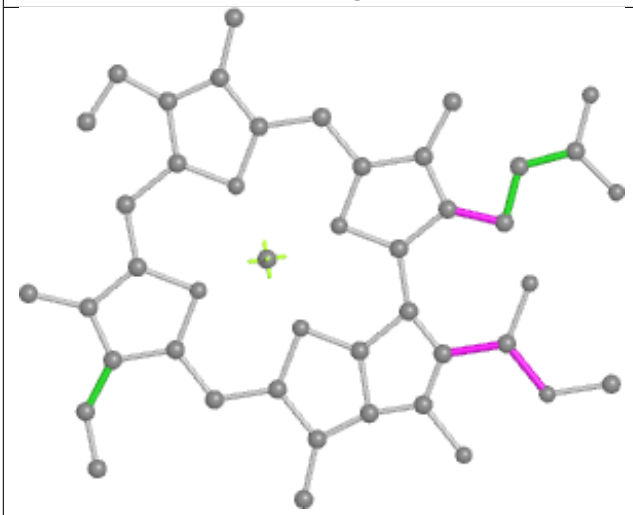
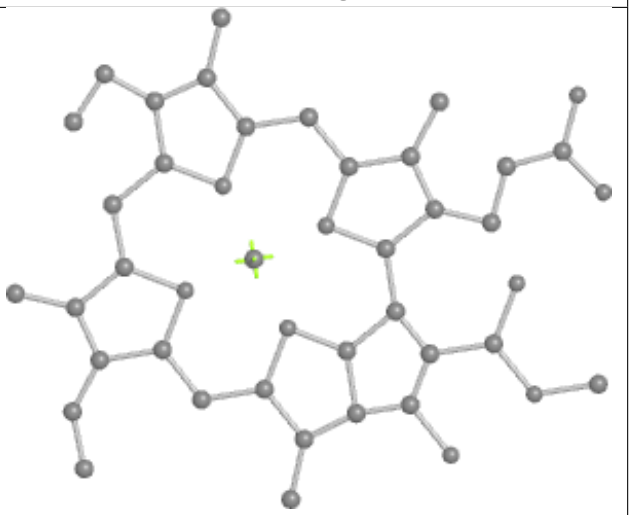


Bond angles

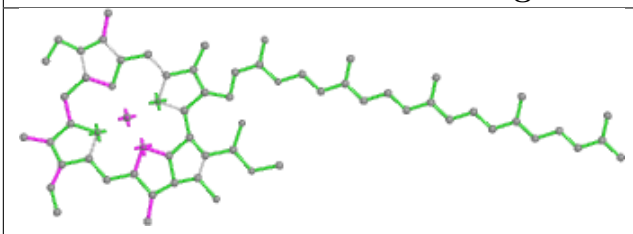


Torsions



Rings

Ligand CLA G 1103



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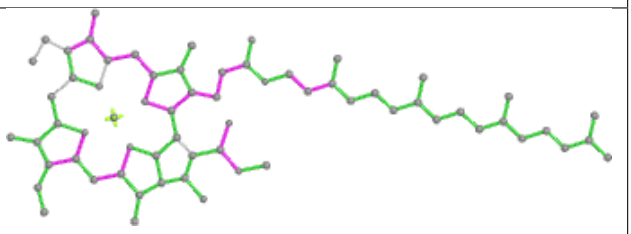
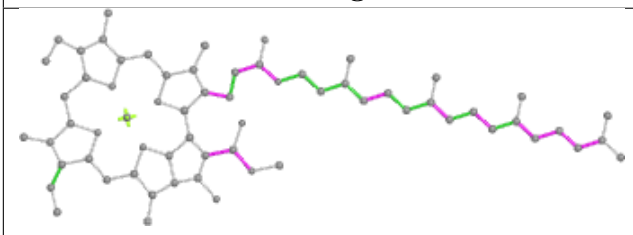
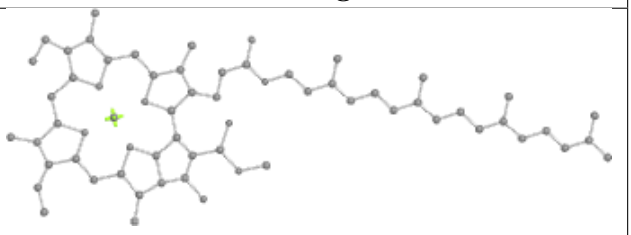


Bond angles

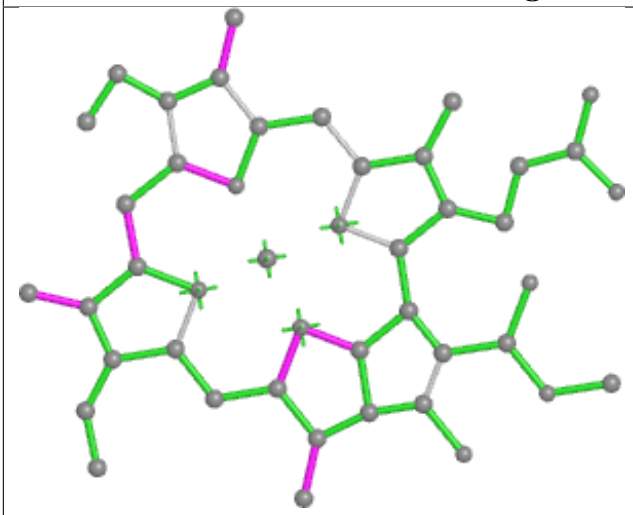


Torsions

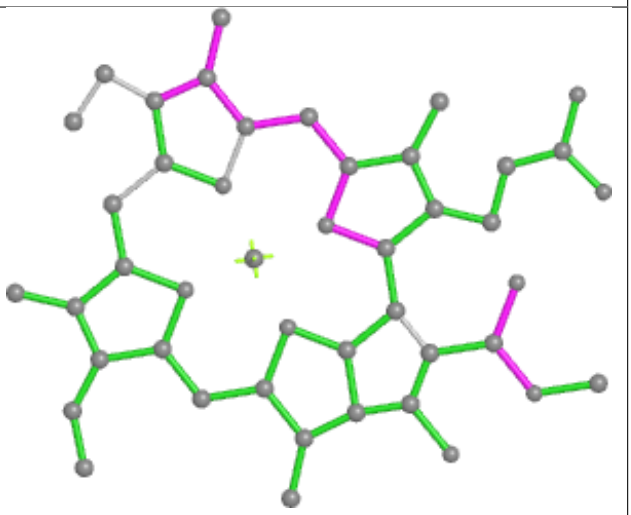


Rings

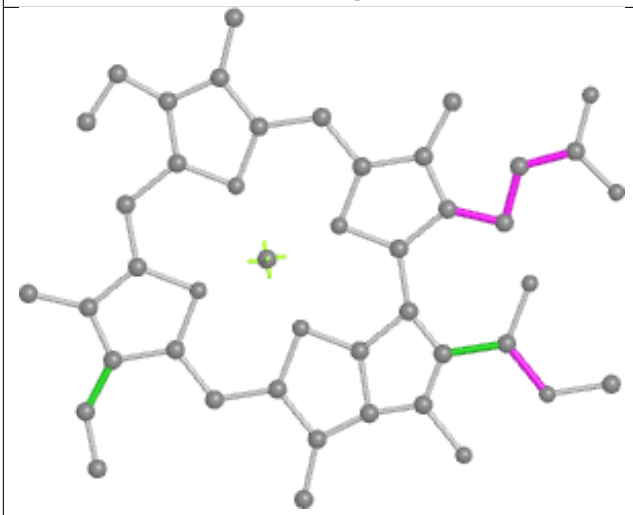
Ligand CLA Y 505



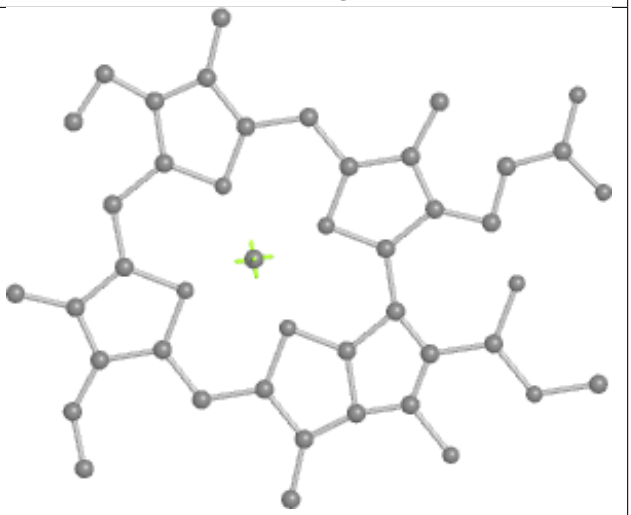
Bond lengths



Bond angles

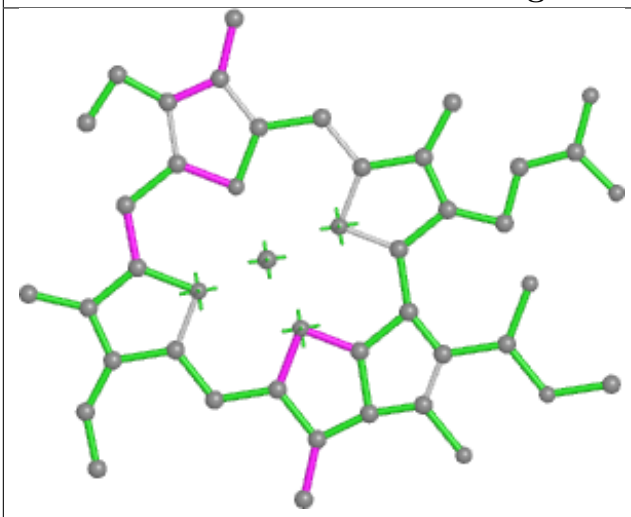


Torsions



Rings

Ligand CLA b 503



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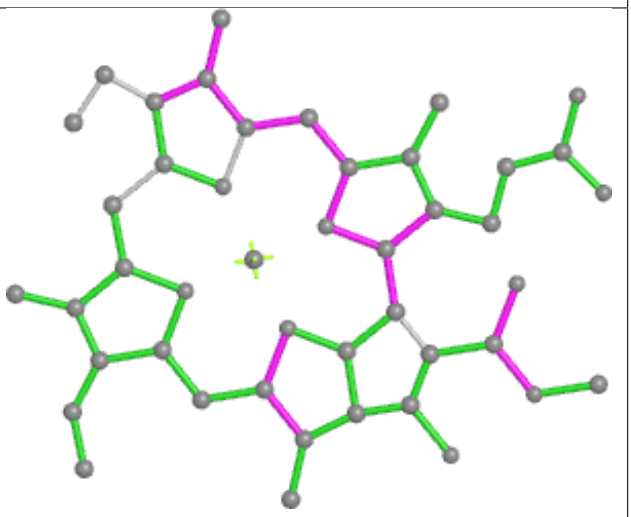
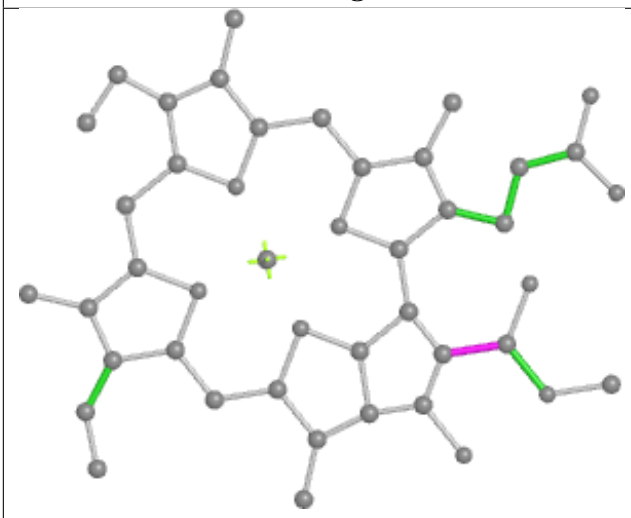
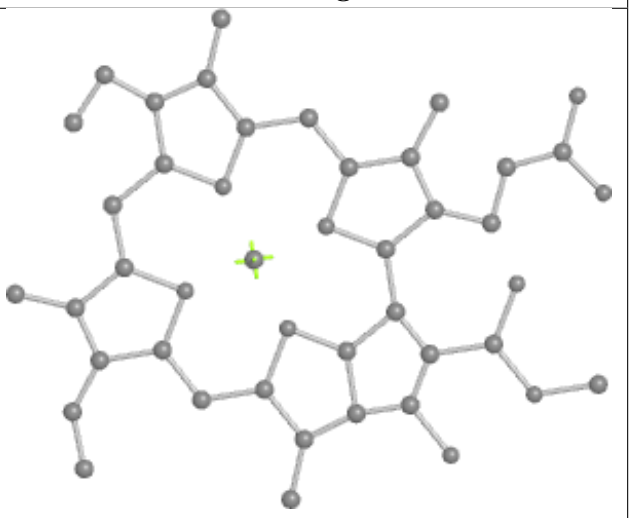


Bond angles

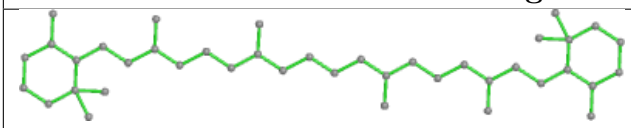


Torsions

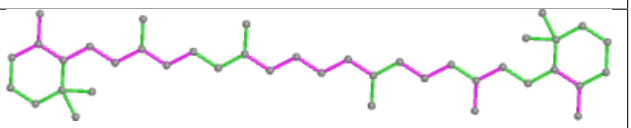


Rings

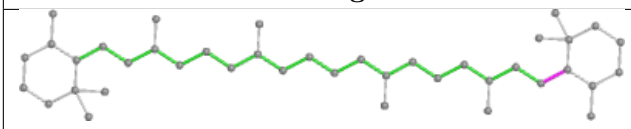
Ligand BCR u 524



Bond lengths

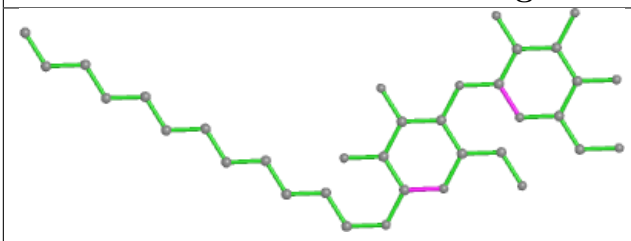
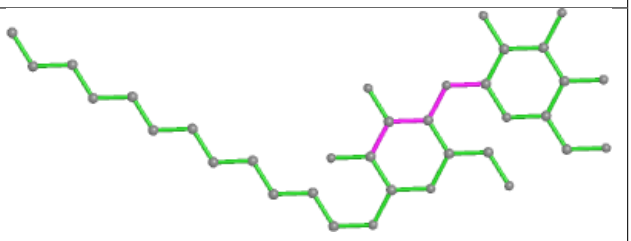
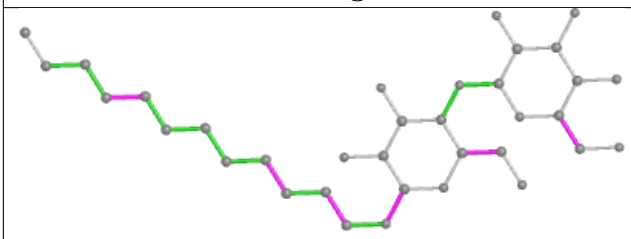
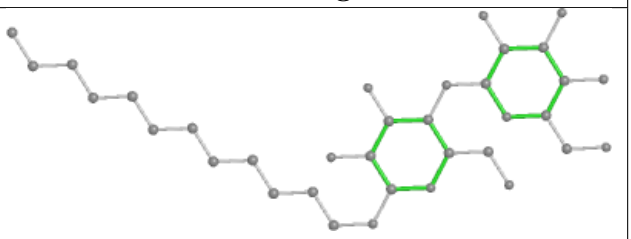


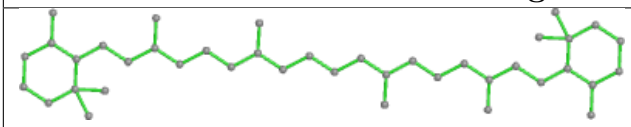
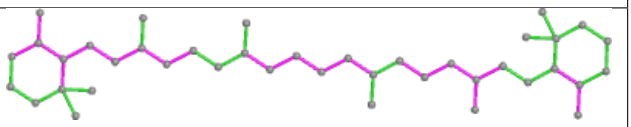
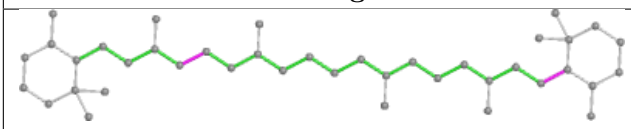
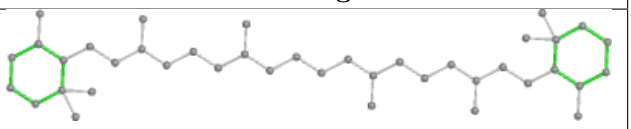
Bond angles



Torsions

Rings

Ligand LMU e 1848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR r 524	
 Bond lengths	 Bond angles
 Torsions	 Rings

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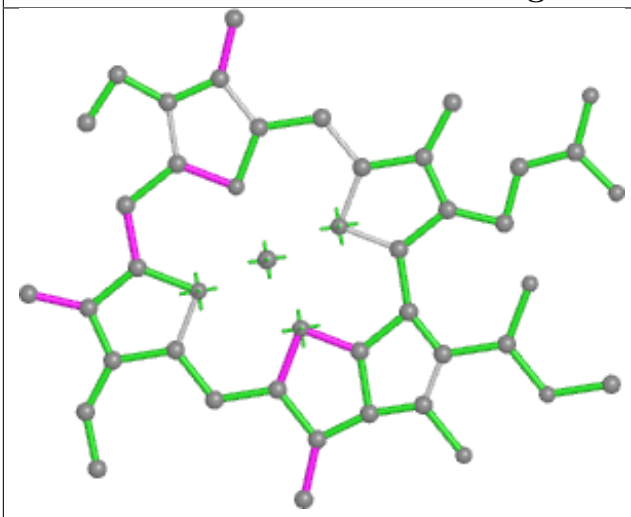

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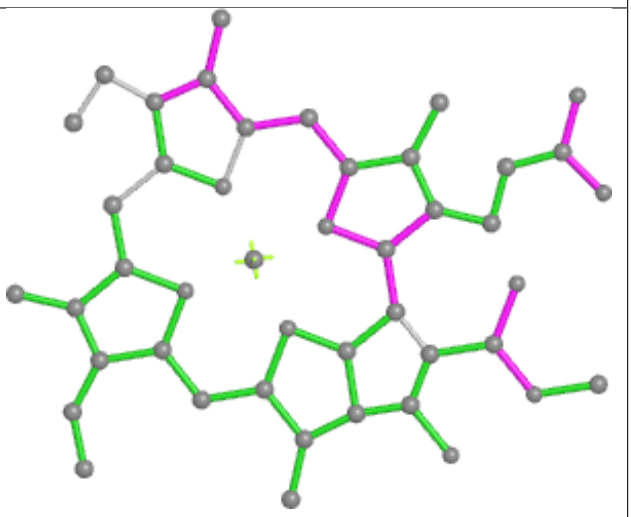

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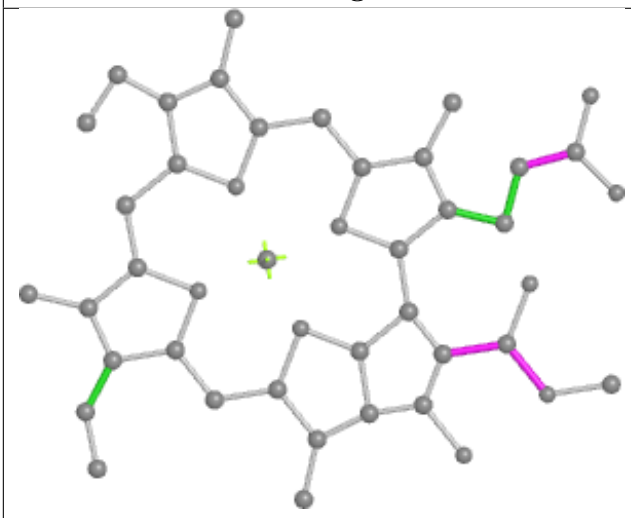
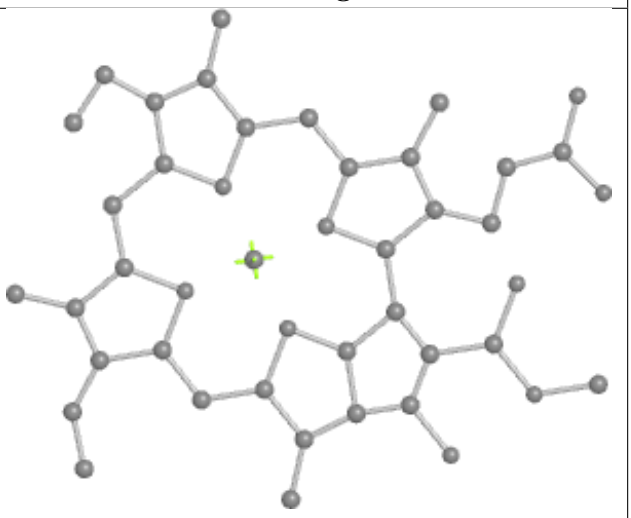
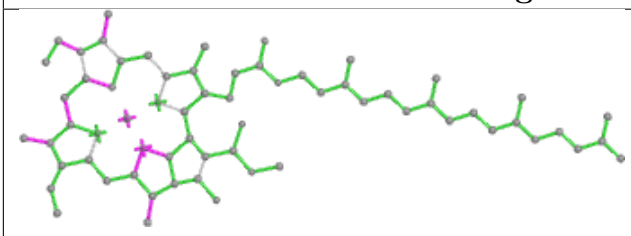


Torsions



Rings

Ligand CLA B 1203



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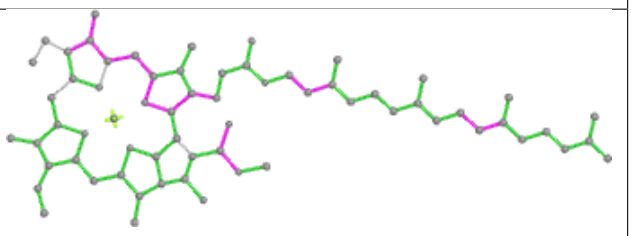

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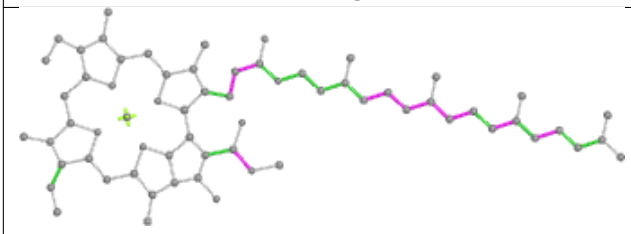

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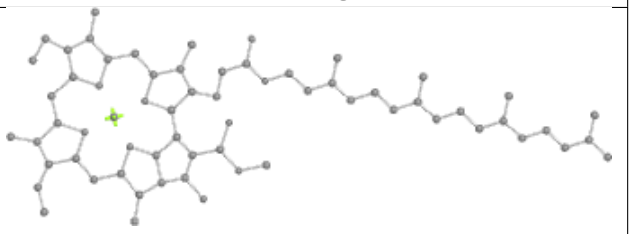
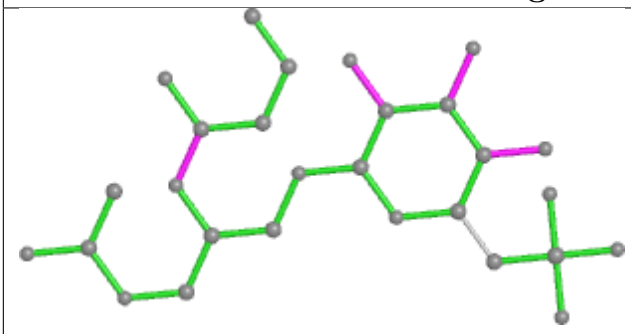


Rings

Ligand SQD 2 822



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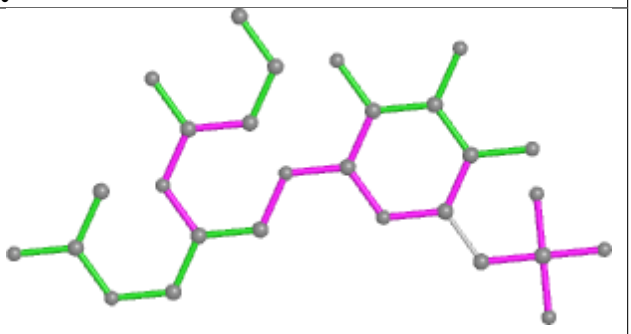

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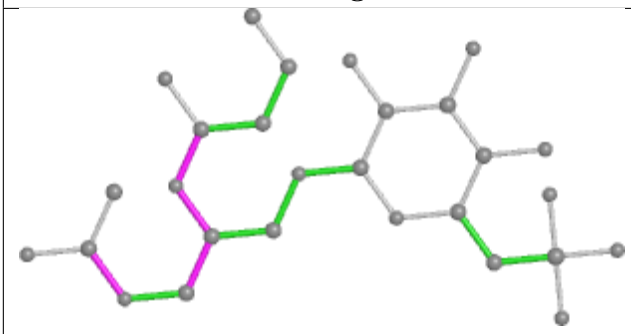

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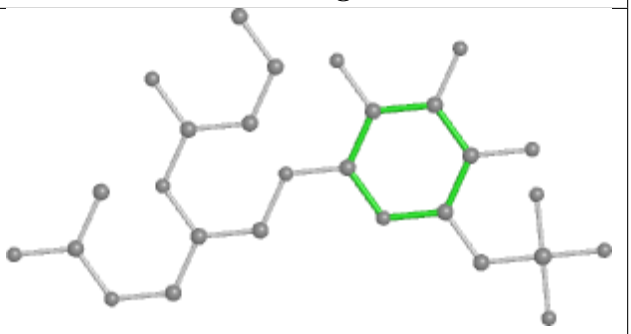
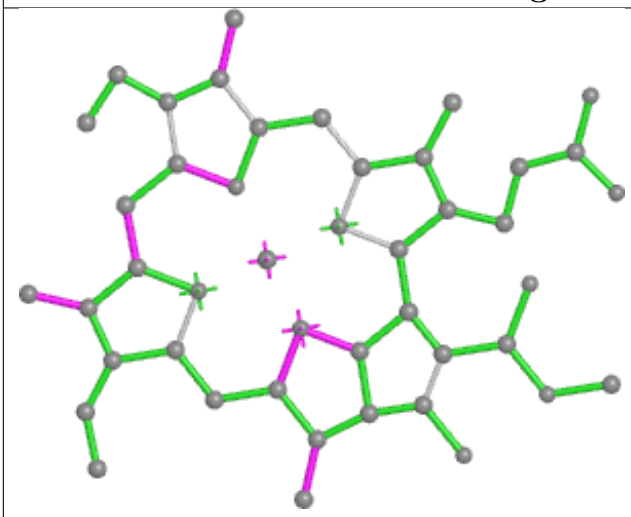


Rings

Ligand CLA r 507



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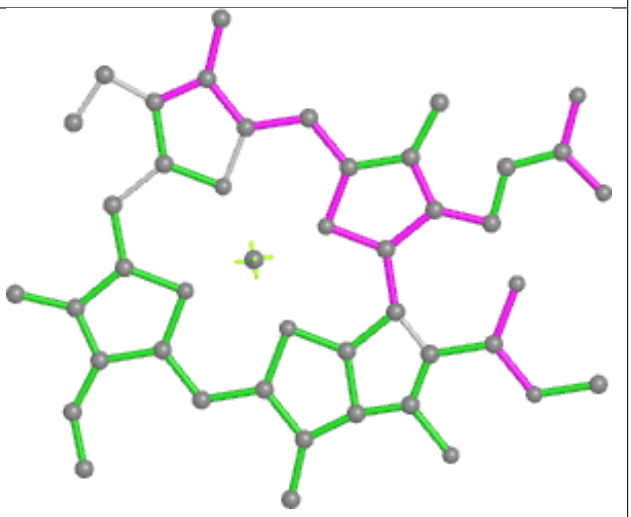

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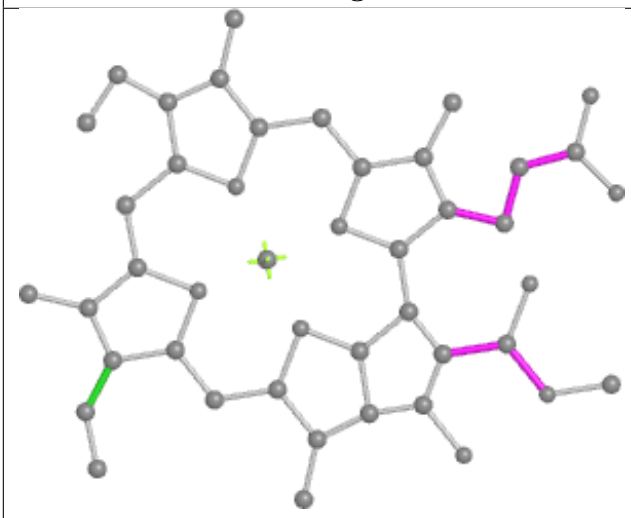

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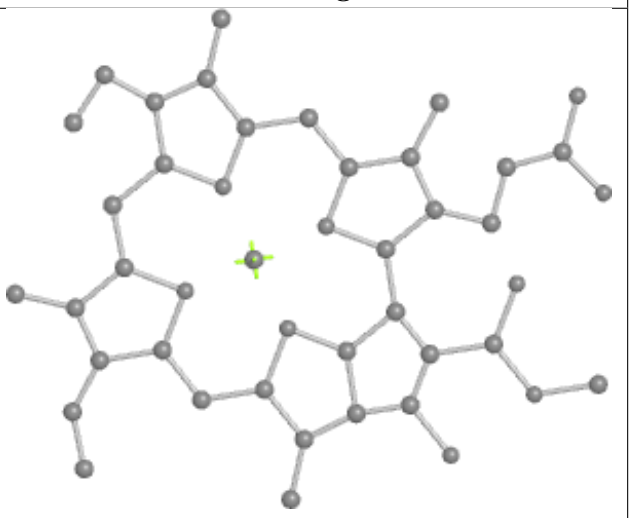
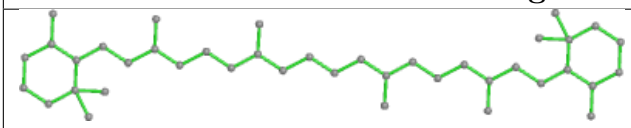


Rings

Ligand BCR t 522



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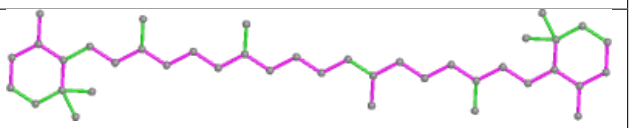
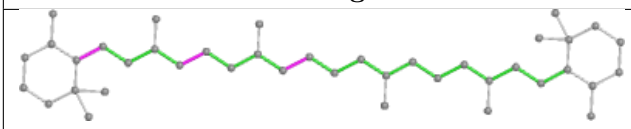


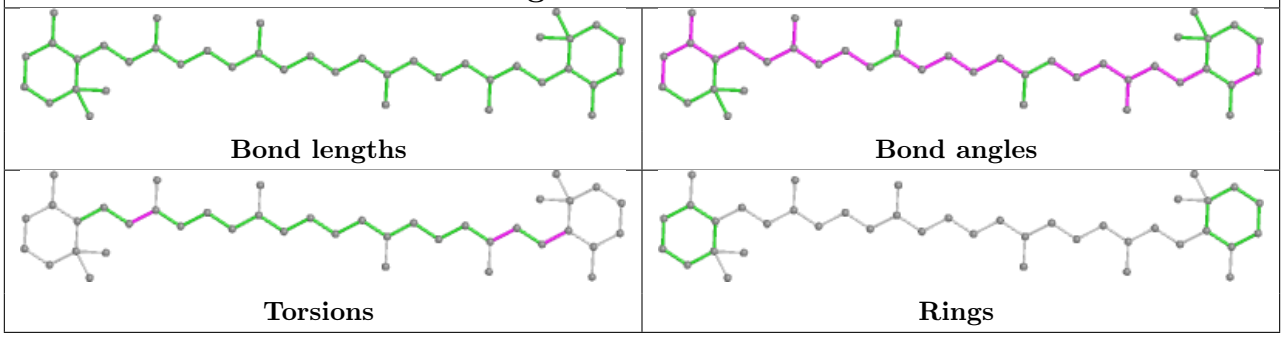
Bond angles



Torsions

Rings

Ligand BCR 2 523



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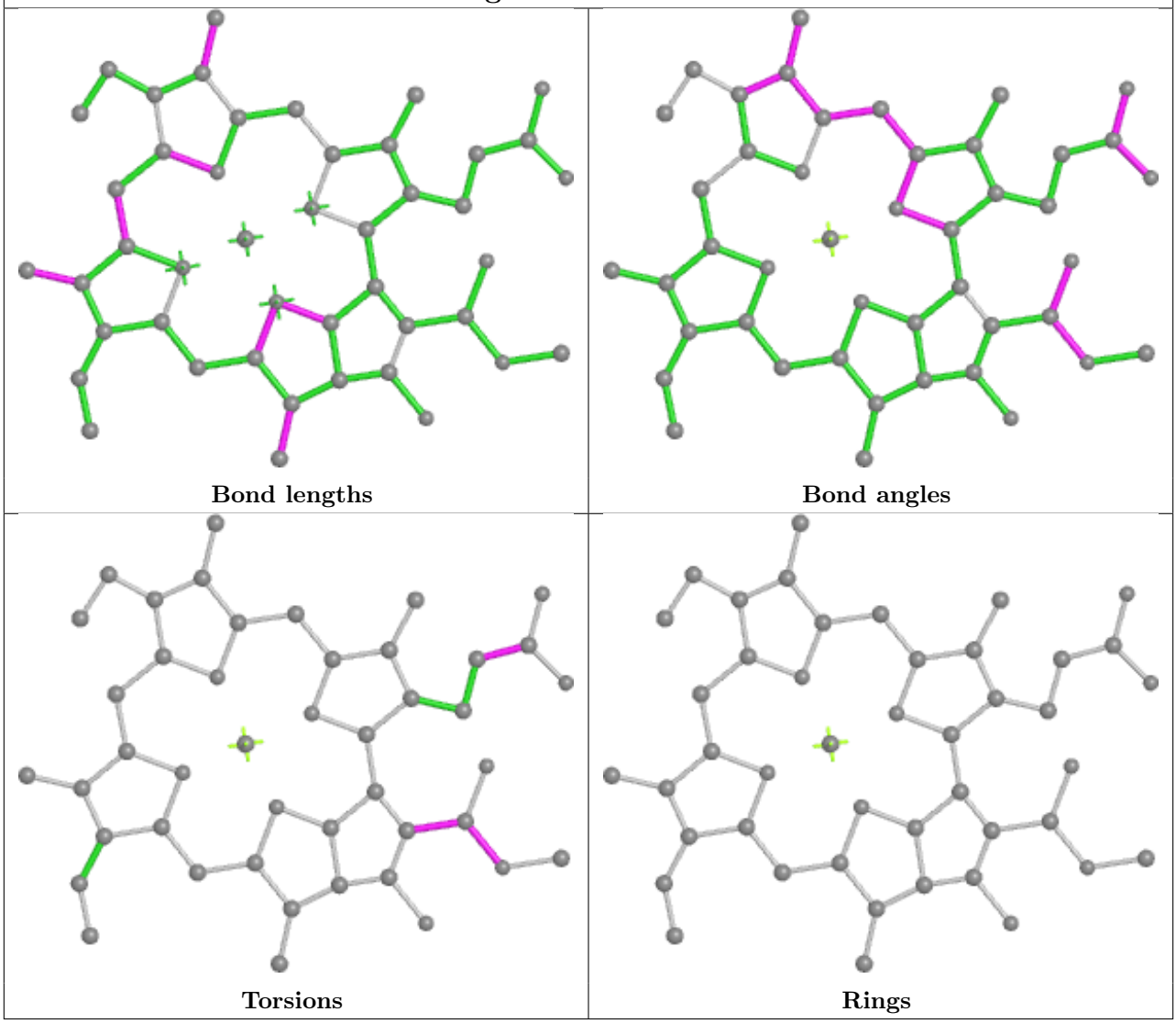
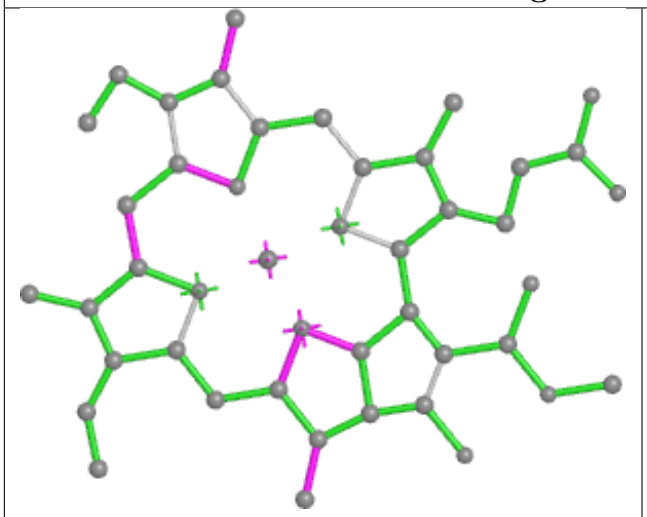
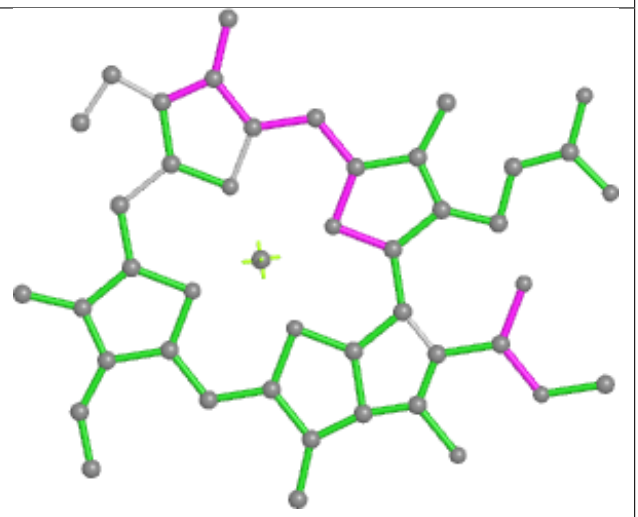


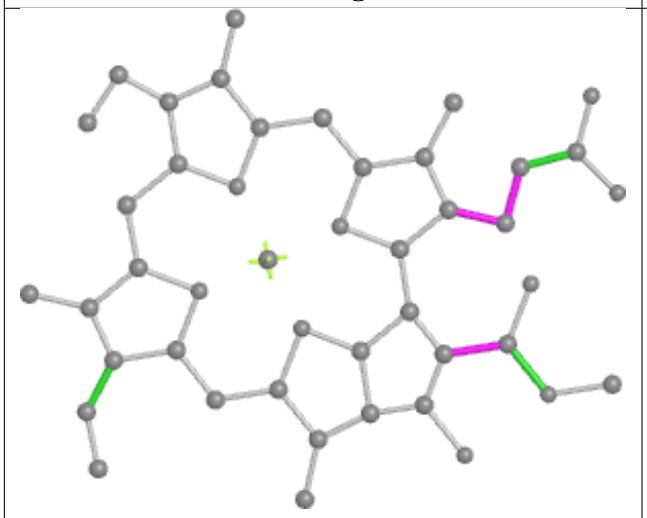
Ligand CLA c 505



Bond lengths



Bond angles



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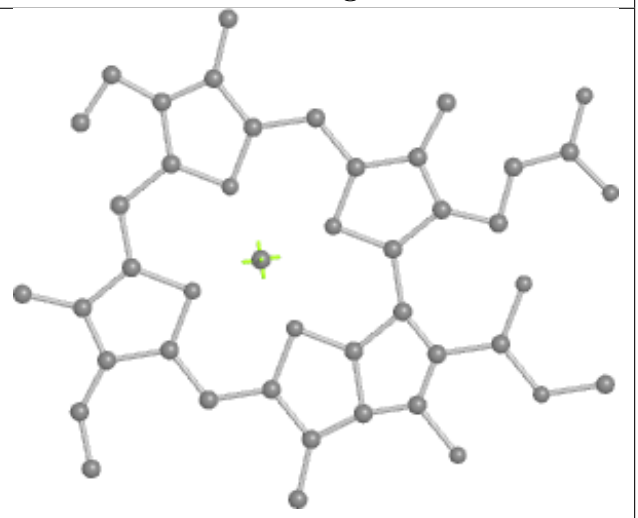
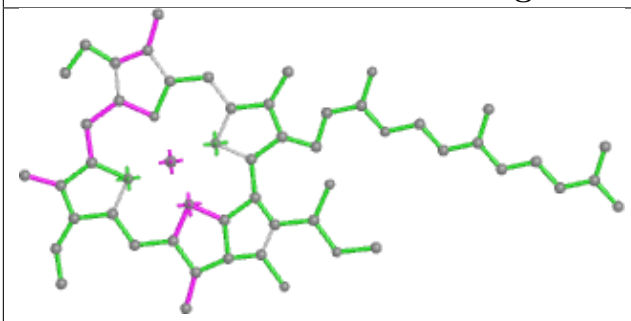
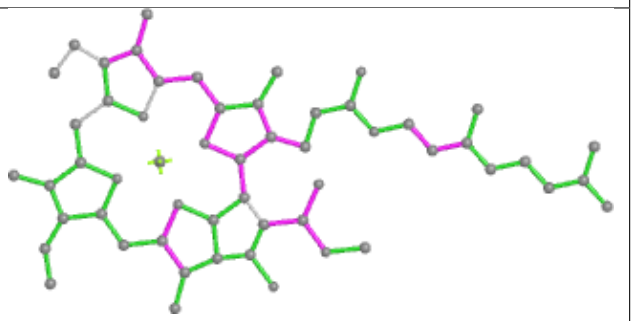
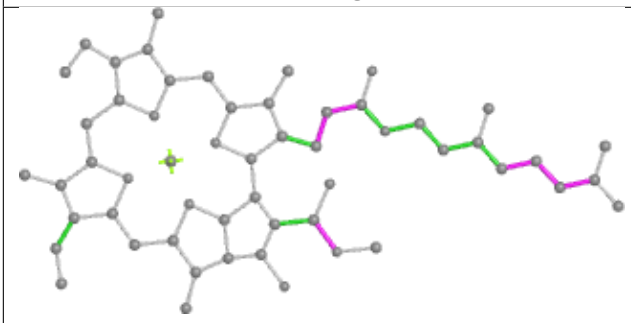
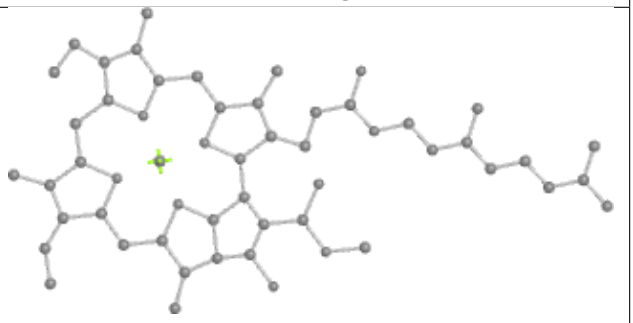
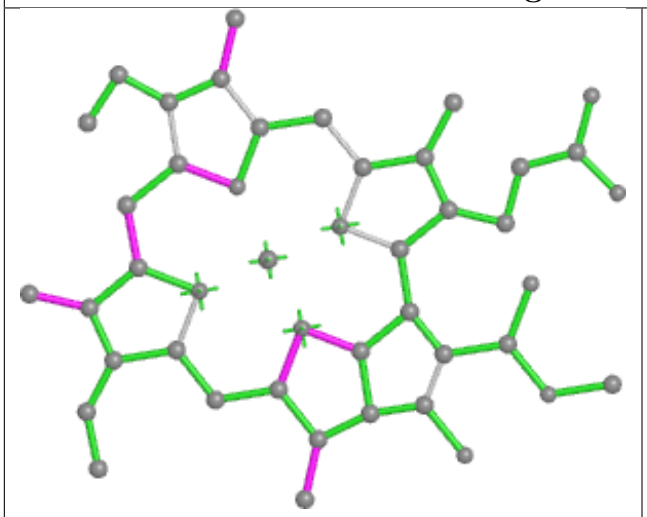


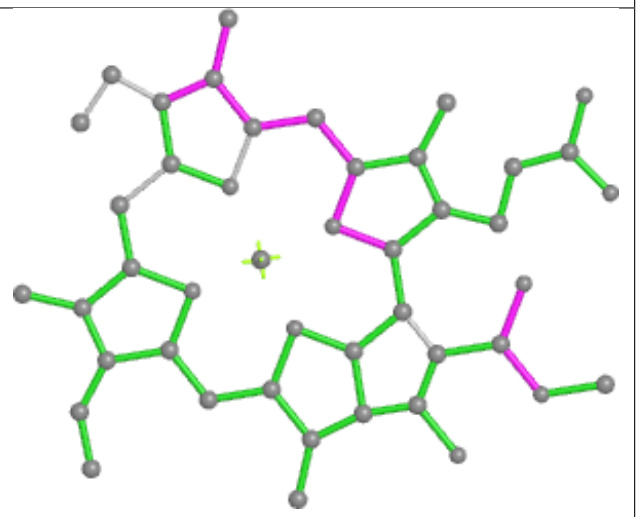
Rings

Ligand CLA A 1121	
 Bond lengths	 Bond angles
 Torsions	 Rings

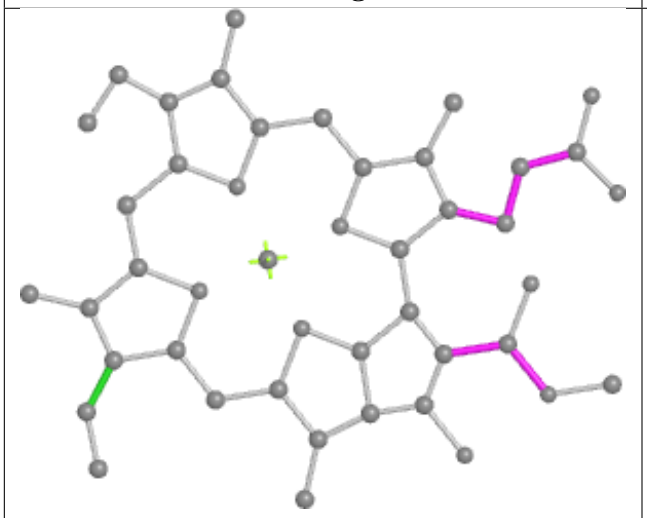
Ligand CLA Y 501



Bond lengths



Bond angles



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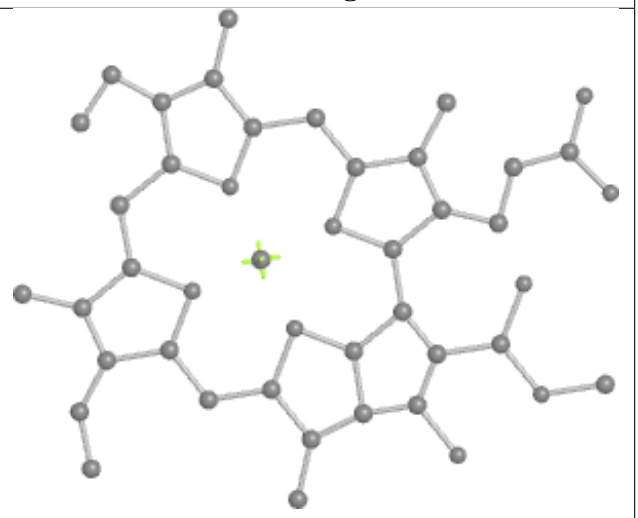
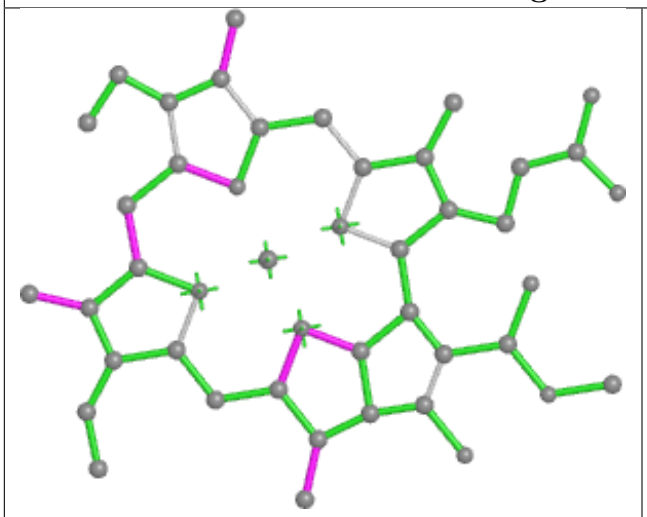


Rings

Ligand CLA c 501



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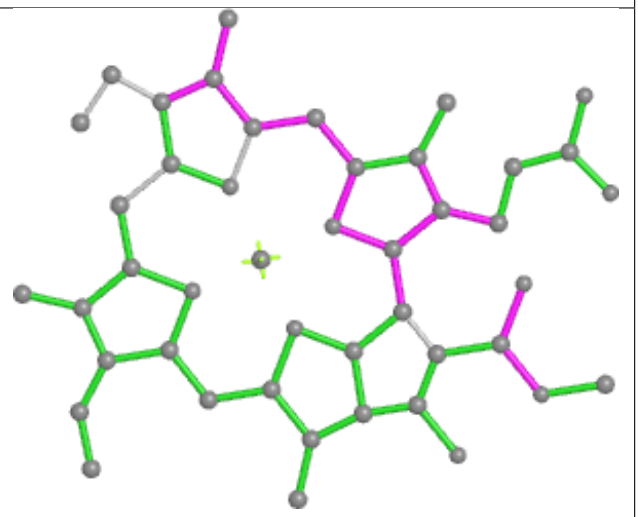
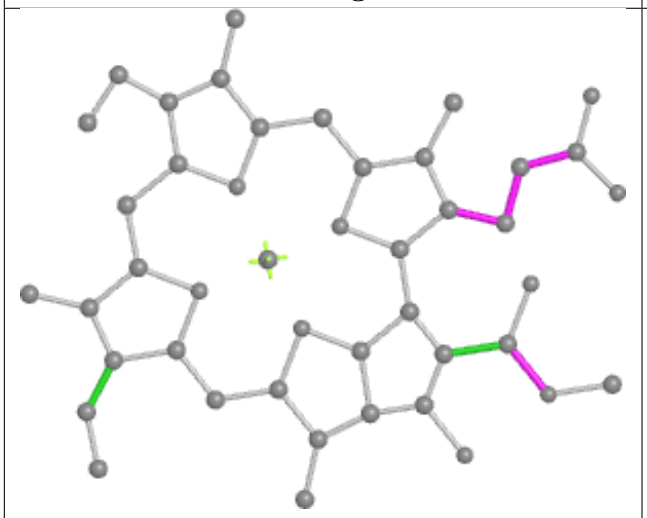


Bond angles



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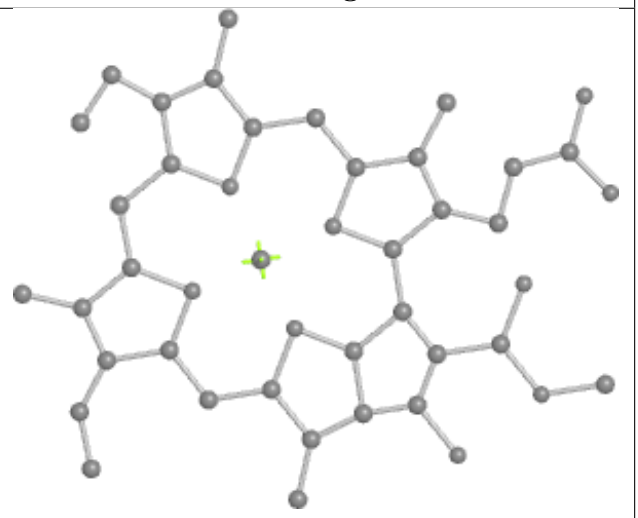
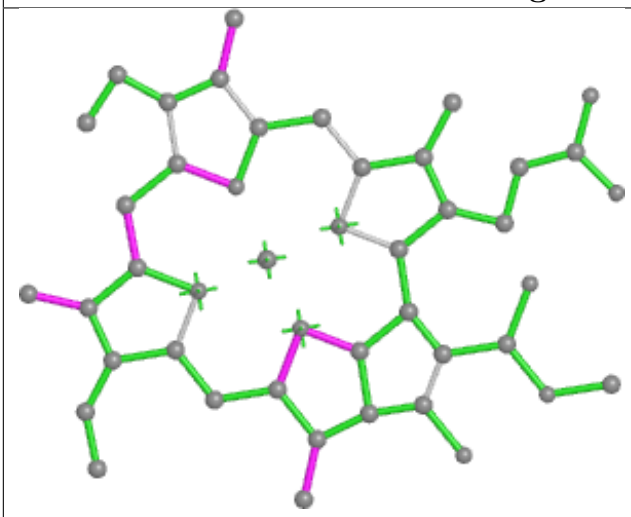


Rings

Ligand CLA c 510



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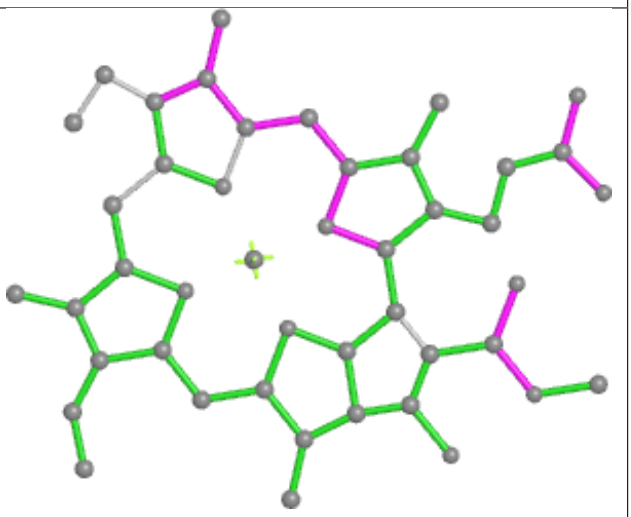
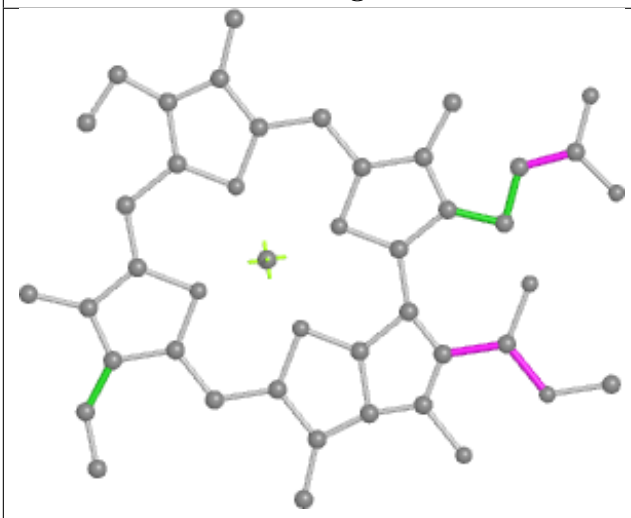
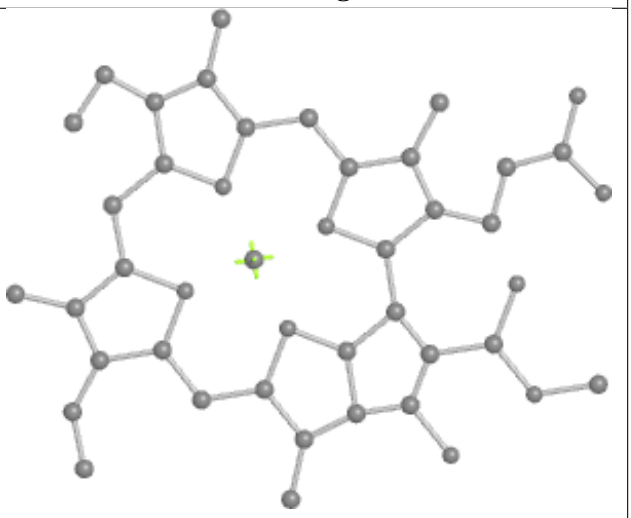


Bond angles

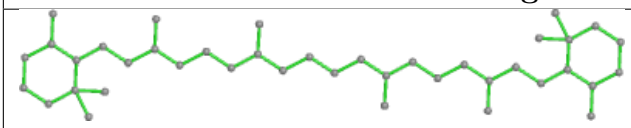


Torsions

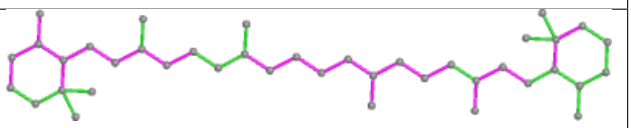


Rings

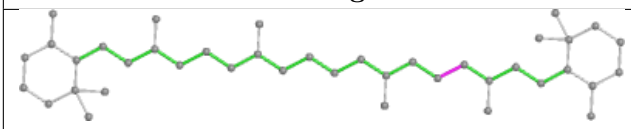
Ligand BCR f 4009



Bond lengths



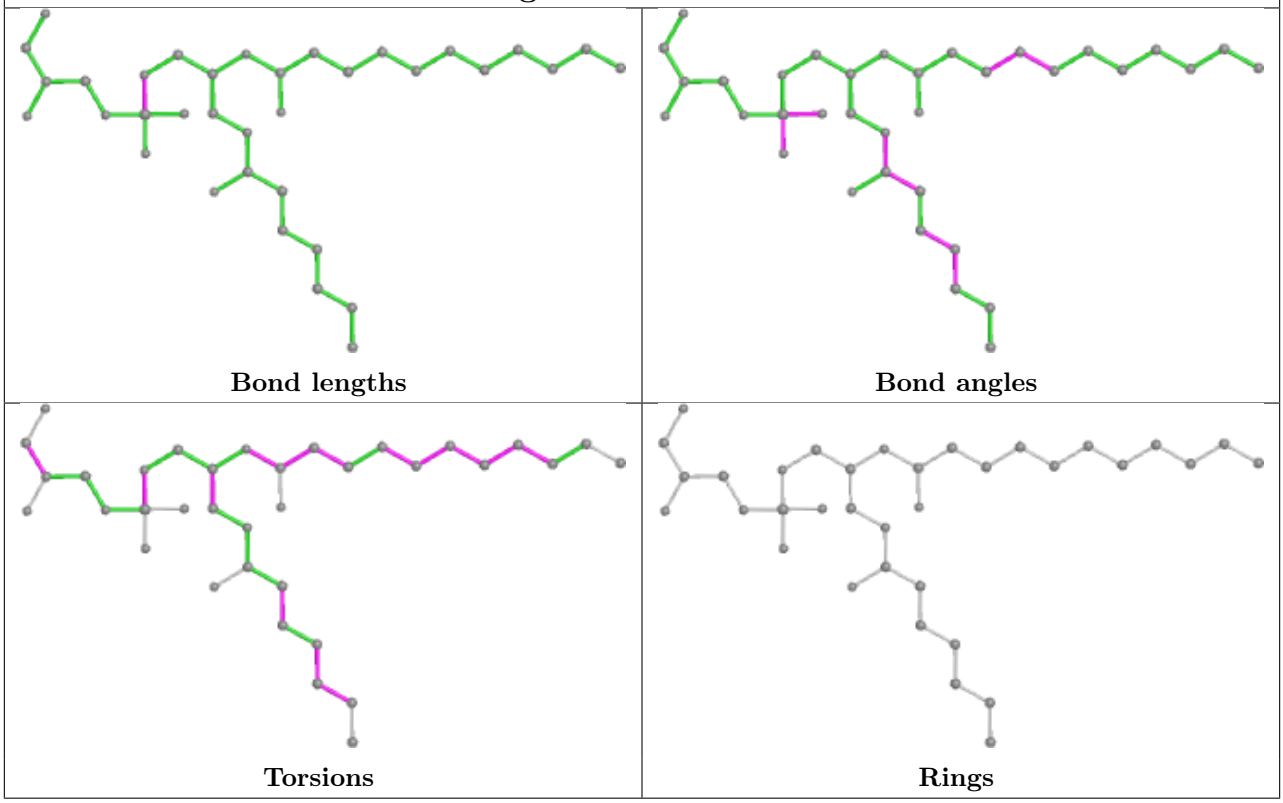
Bond angles



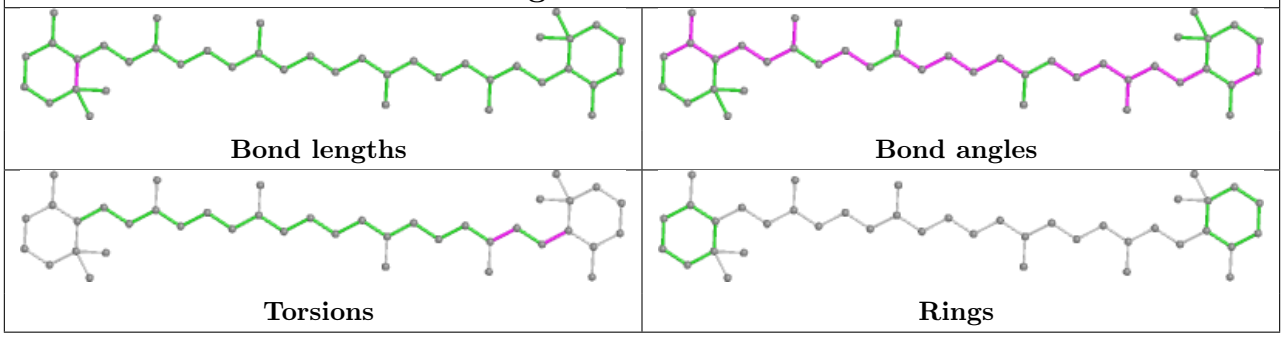
Torsions

Rings

Ligand LHG e 5008



Ligand BCR c 523



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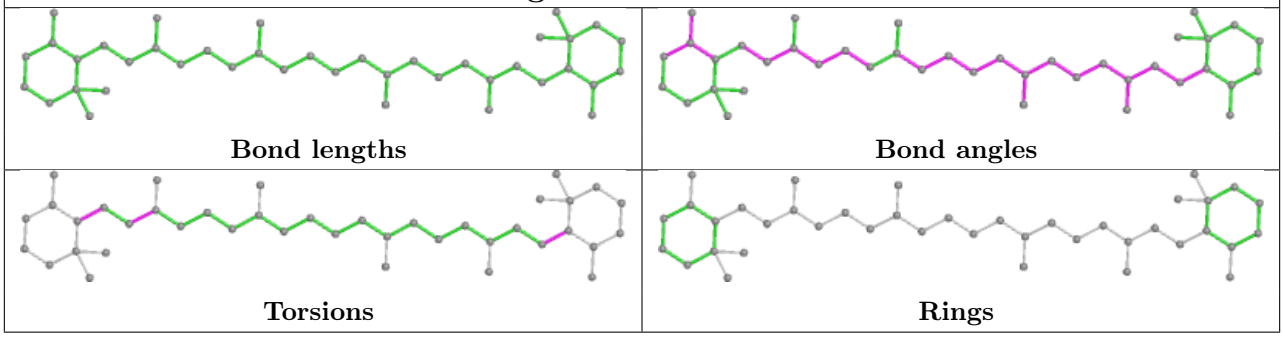

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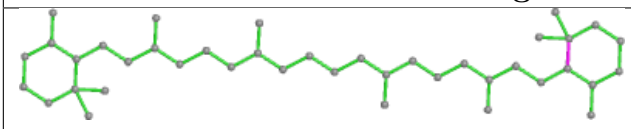
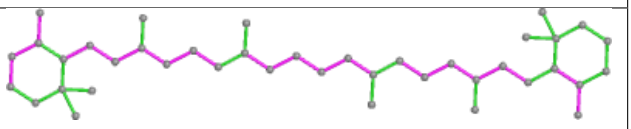
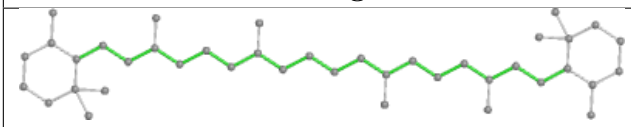
 Bond lengths	 Bond angles
 Torsions	Rings

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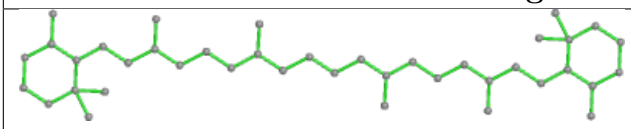
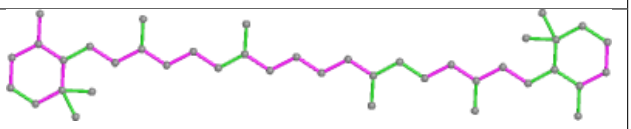
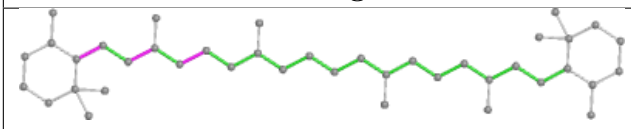
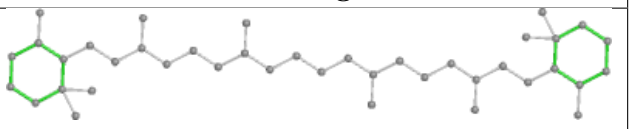
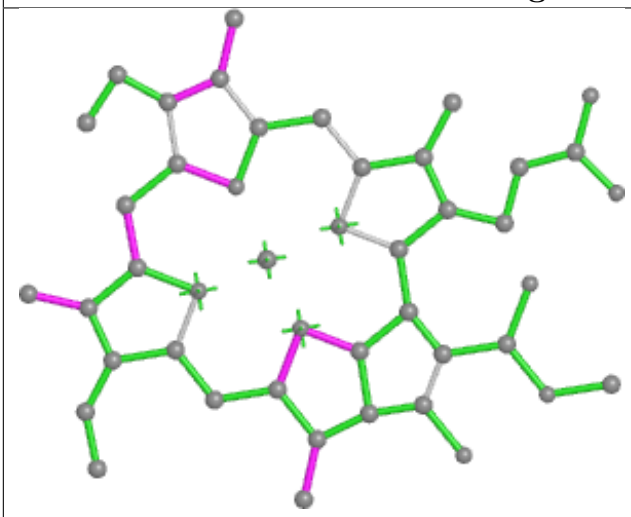
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 502



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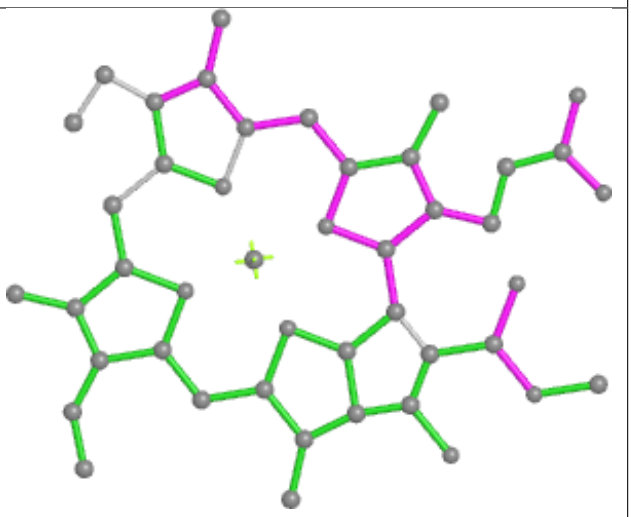
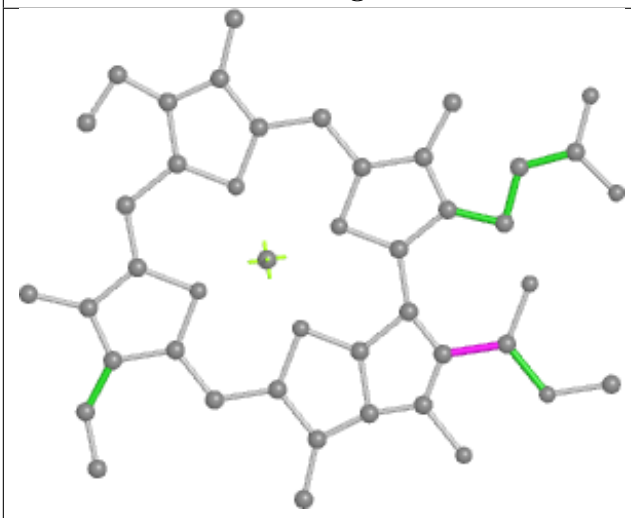


Bond angles



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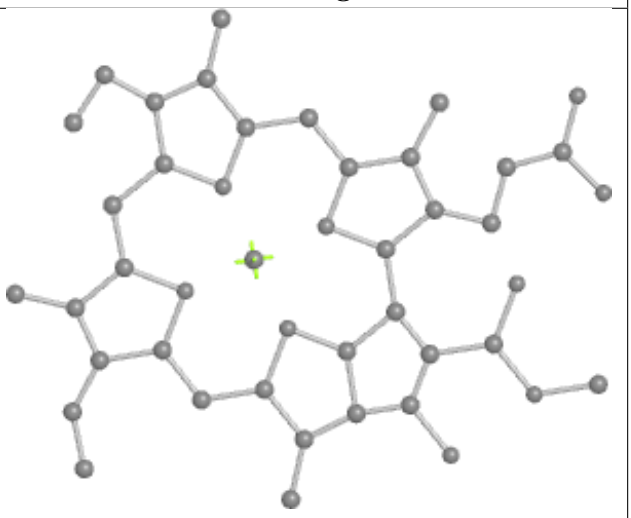
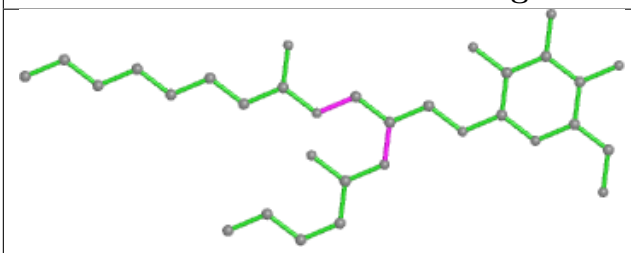


Rings

Ligand LMG T 5104



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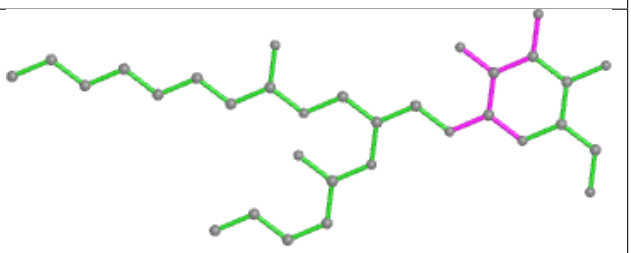

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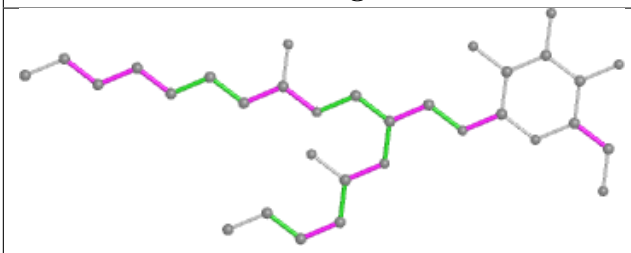

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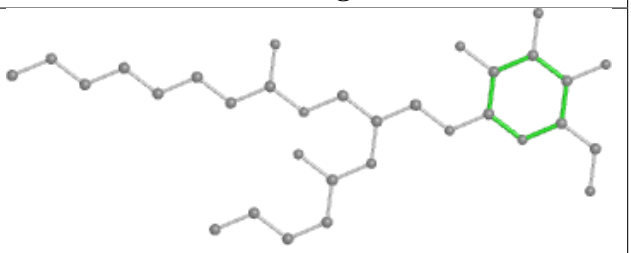
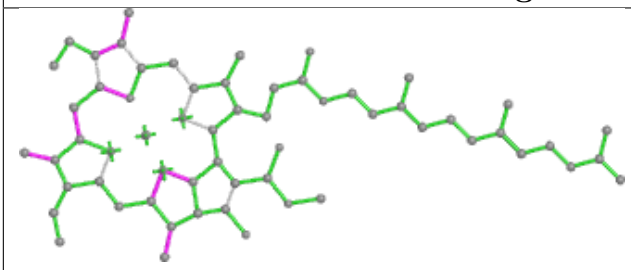


Rings

Ligand CLA B 1218



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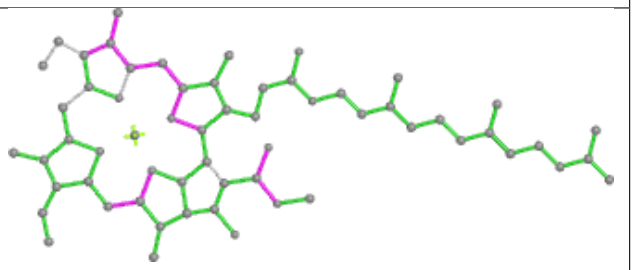

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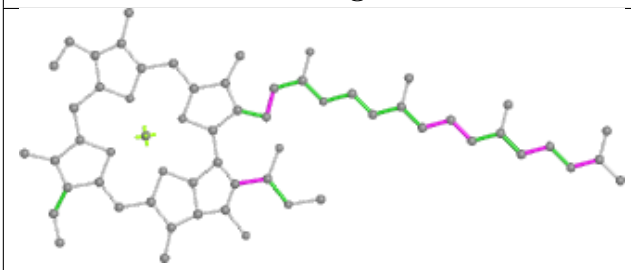

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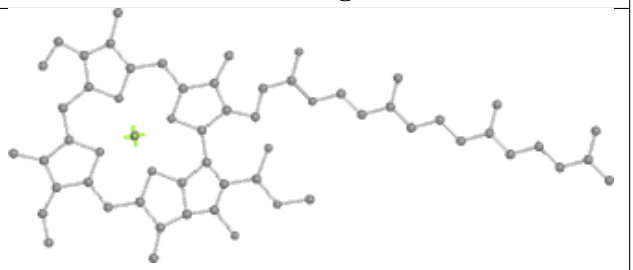
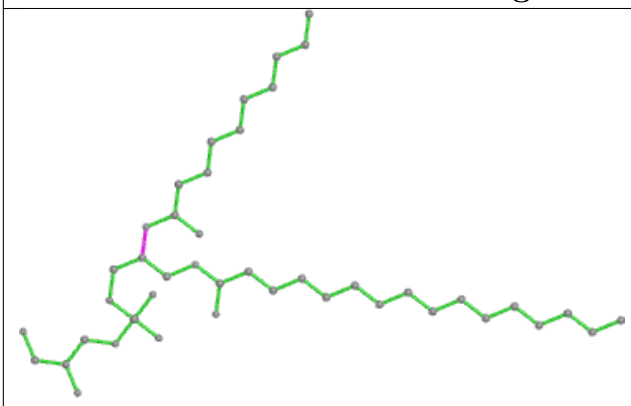


Rings

Ligand LHG G 5002



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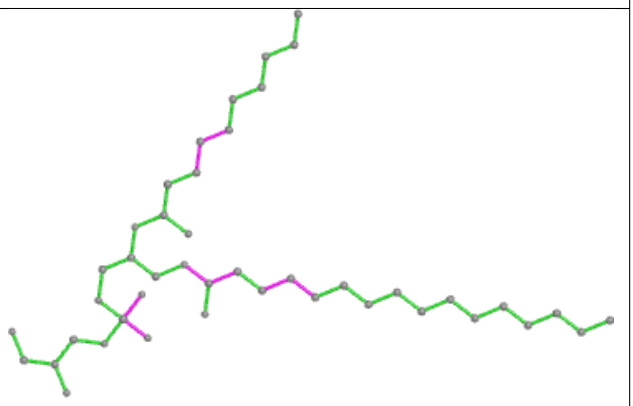

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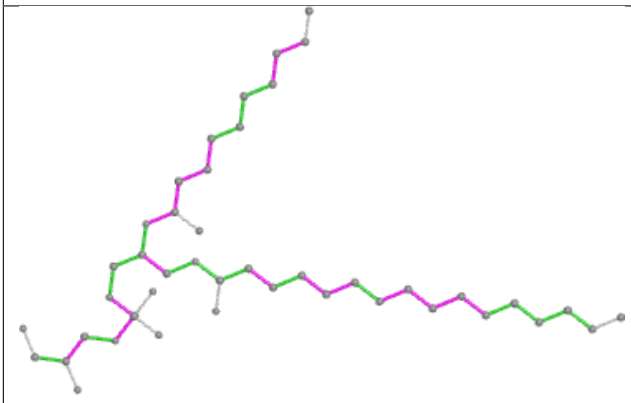

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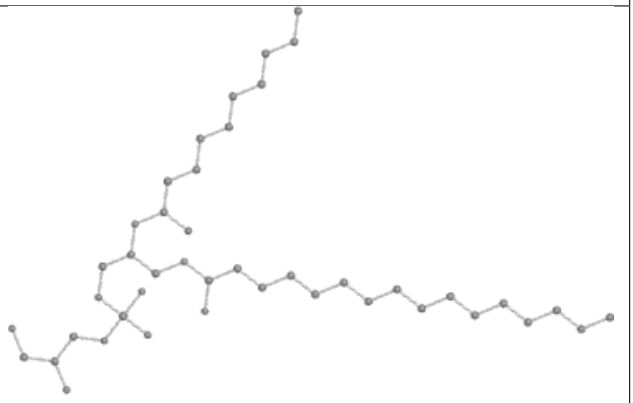
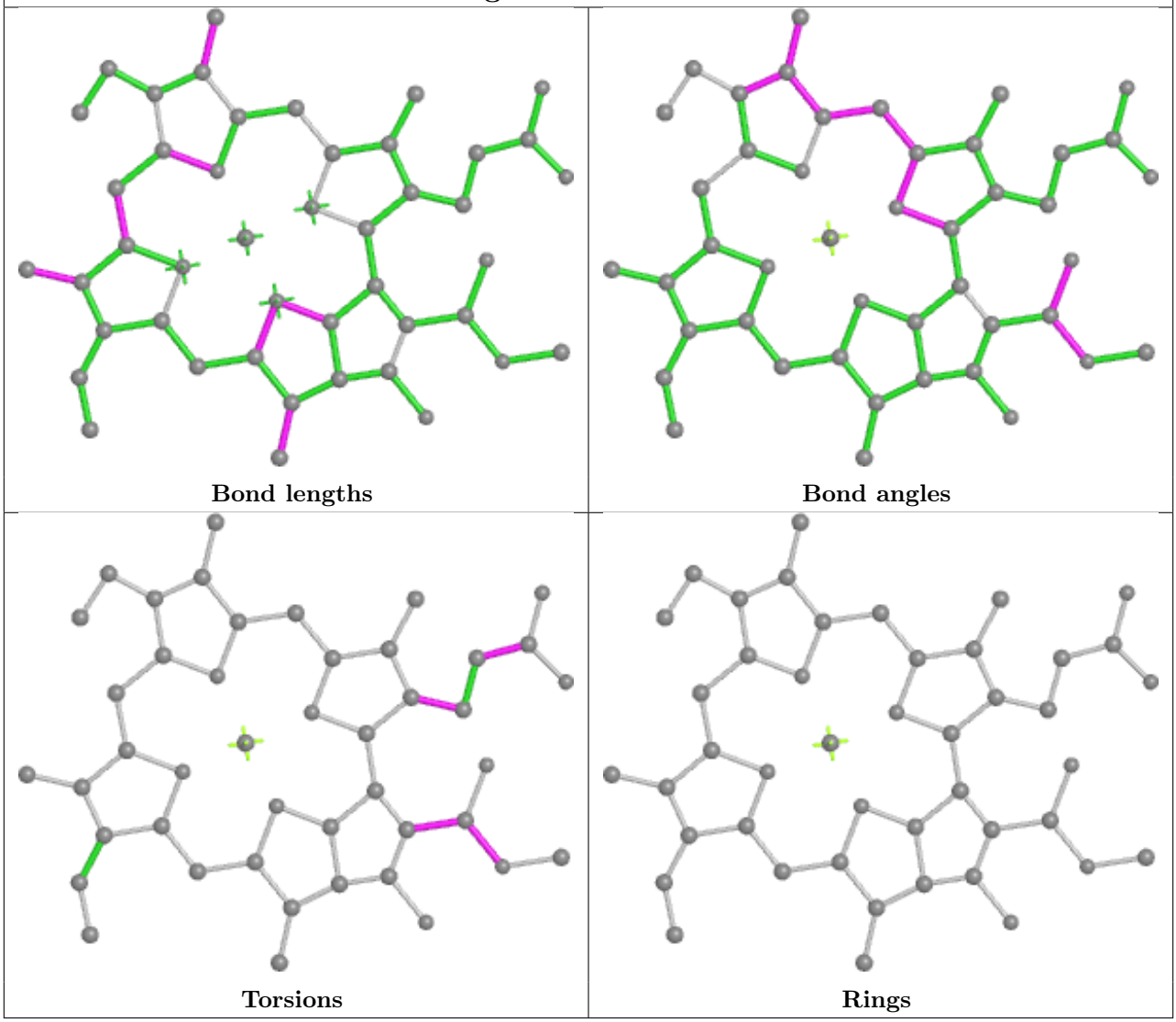


Rings

Ligand CLA v 512



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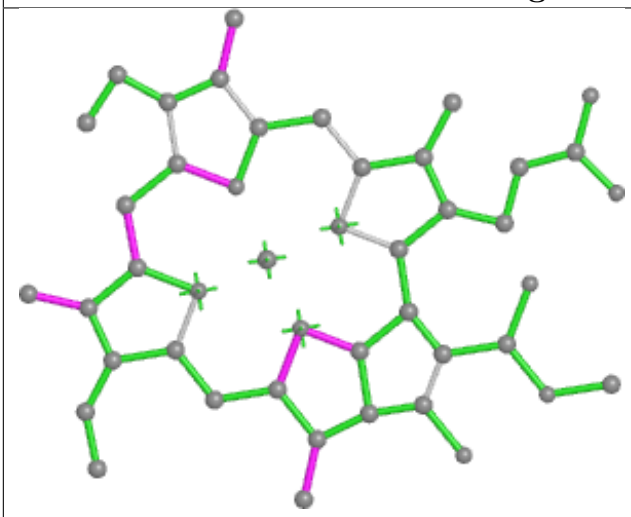

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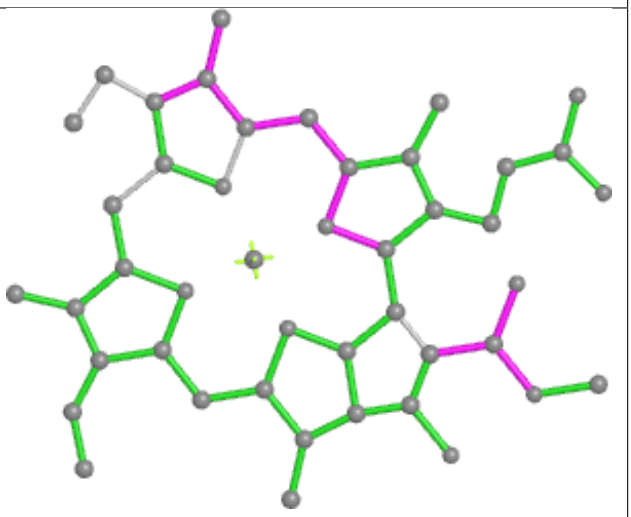
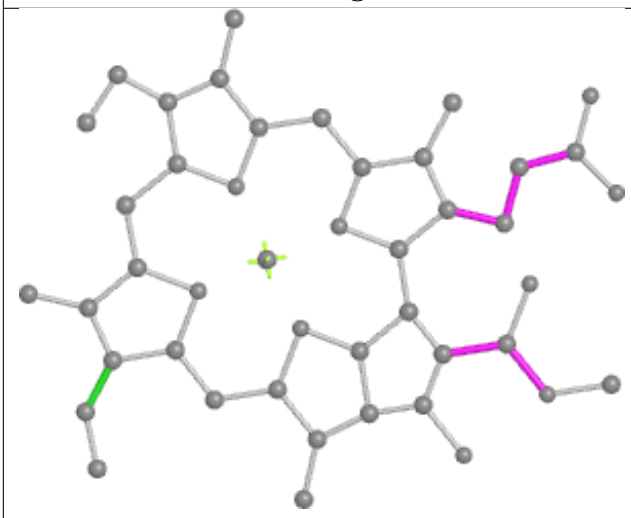


Bond angles



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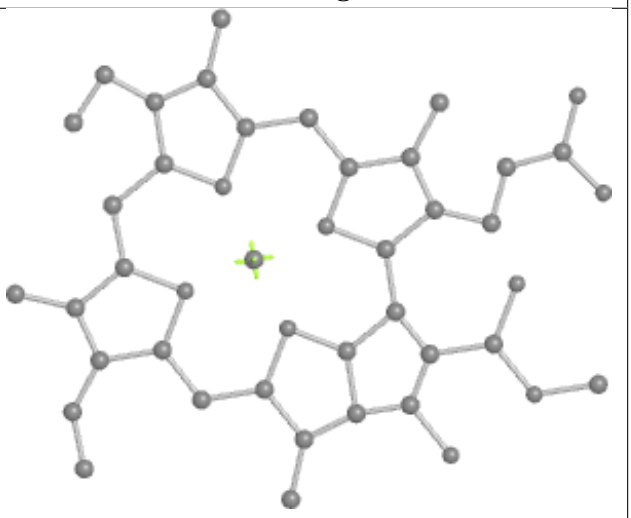
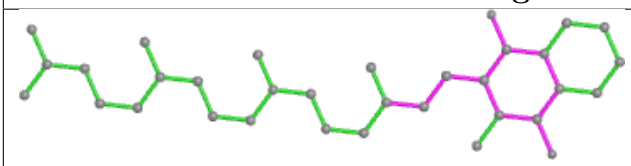


Rings

Ligand PQN A 2001



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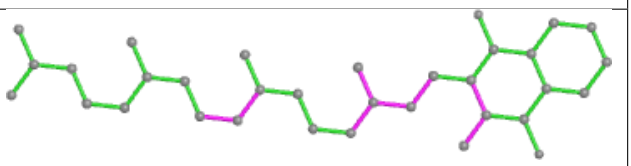

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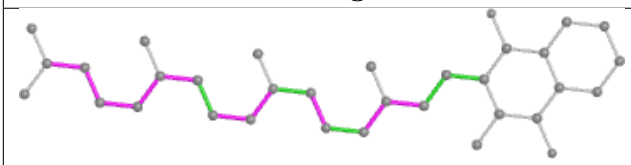

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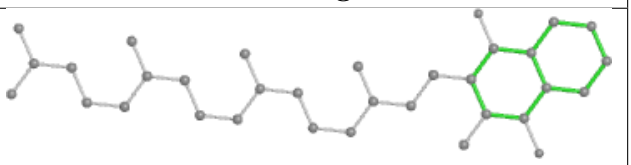
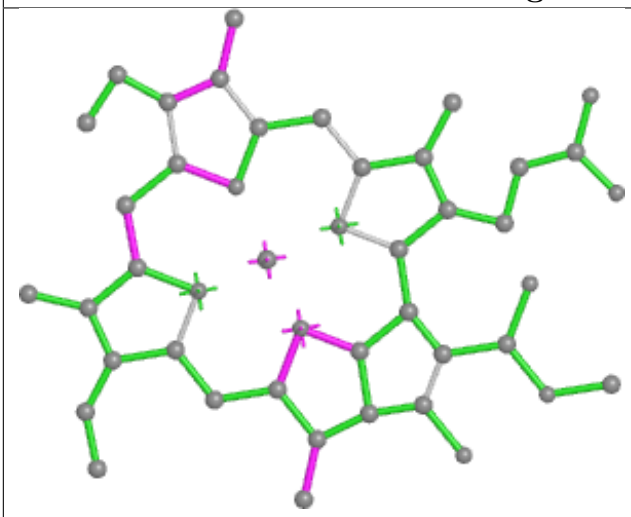


Rings

Ligand CLA Z 512



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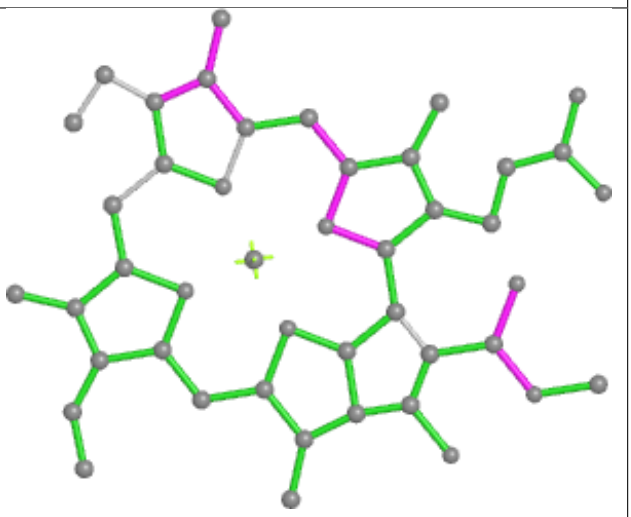

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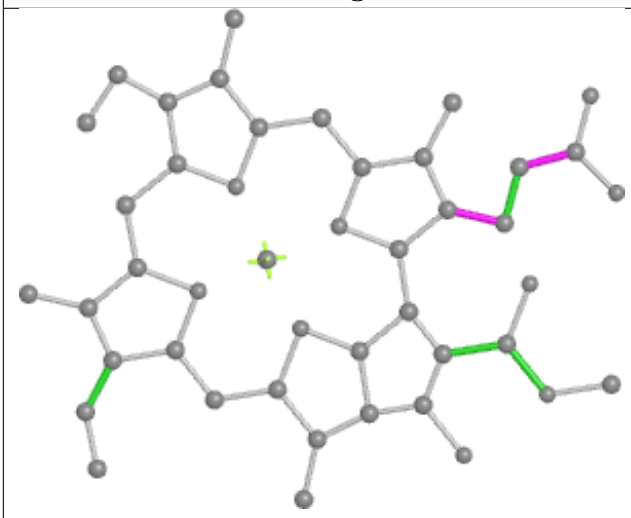

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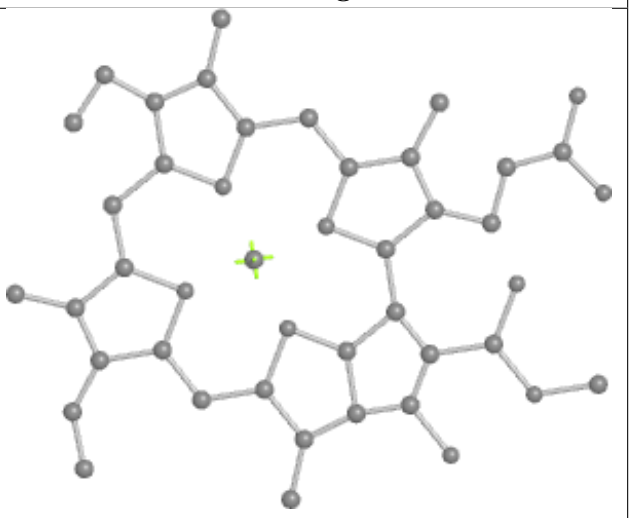
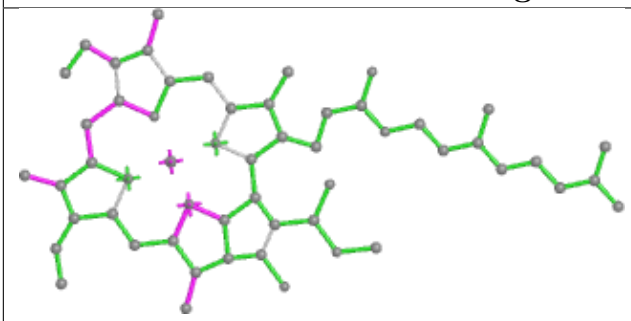
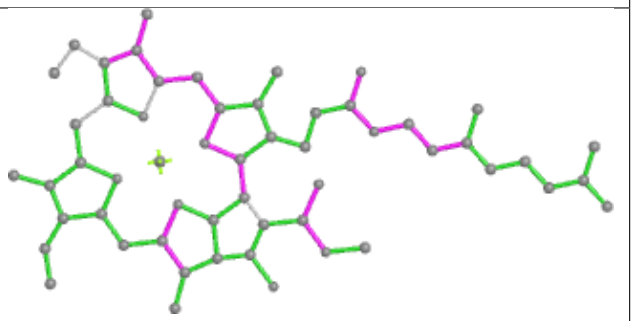
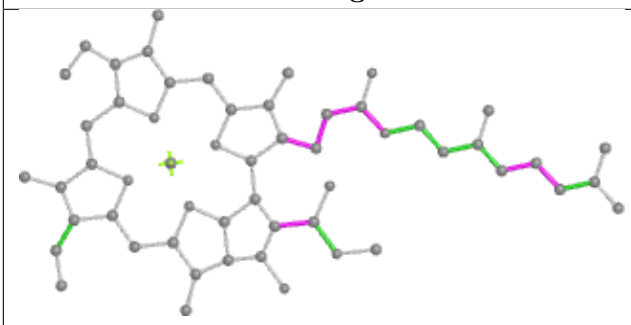
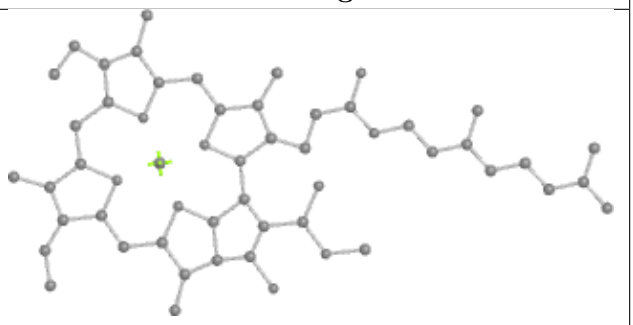
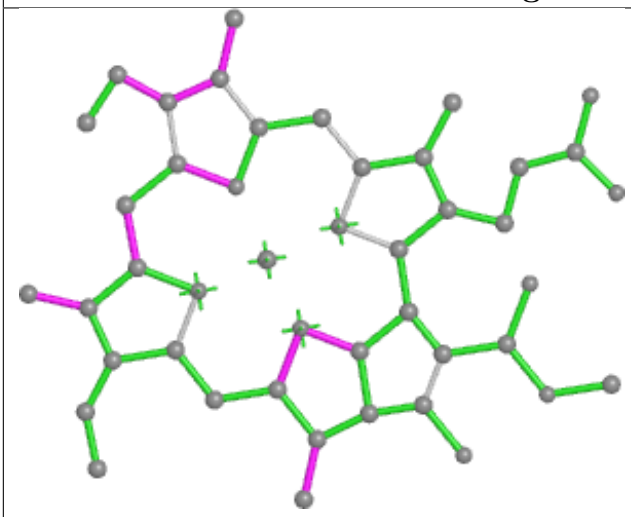


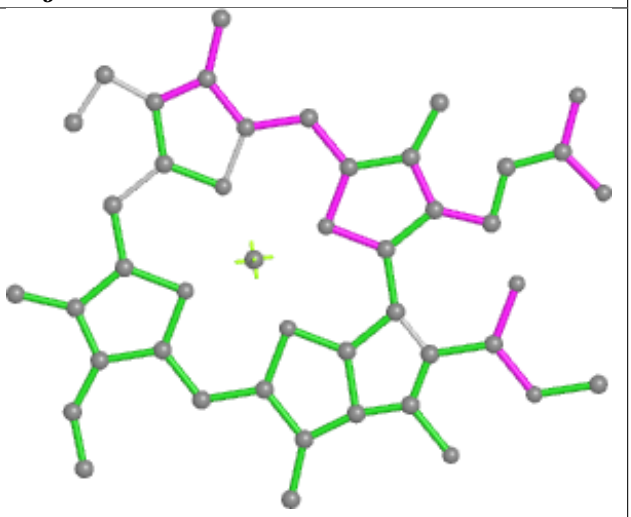
Rings

Ligand CLA G 1135	
 Bond lengths	 Bond angles
 Torsions	 Rings

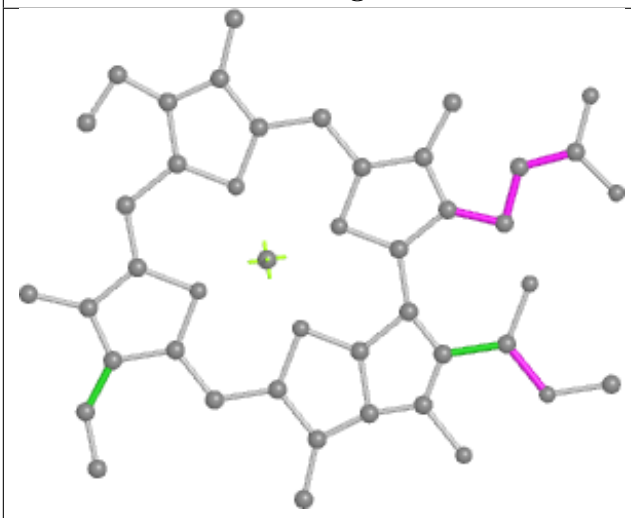
Ligand CLA j 1302



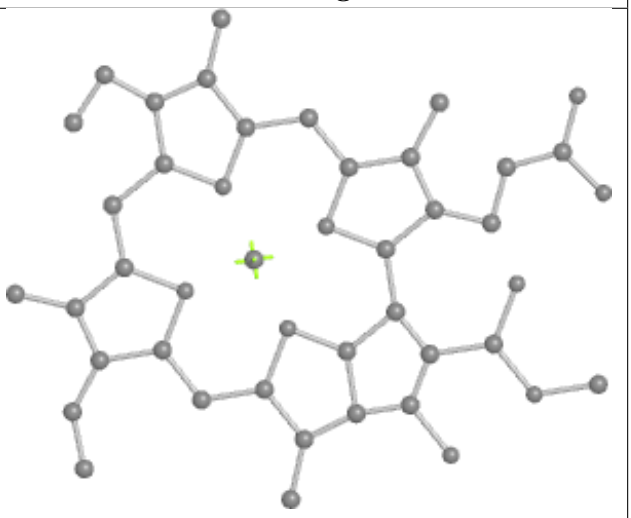
Bond lengths



Bond angles

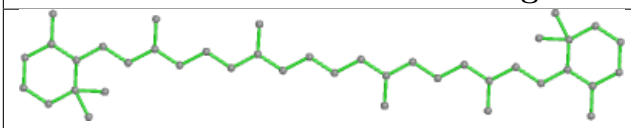


Torsions



Rings

Ligand BCR j 4016



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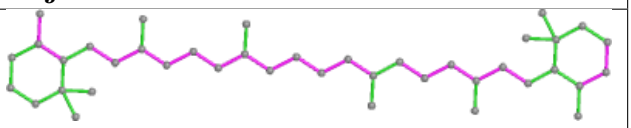
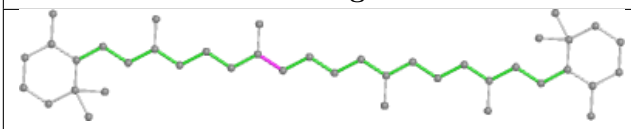


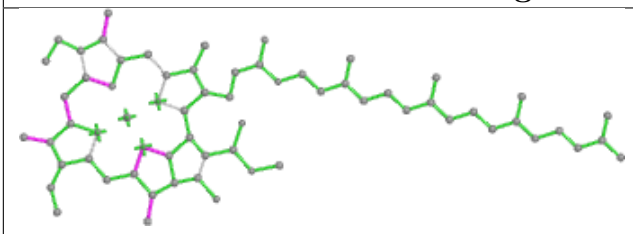
Bond angles



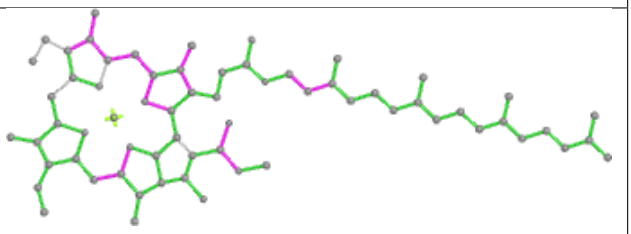
Torsions

Rings

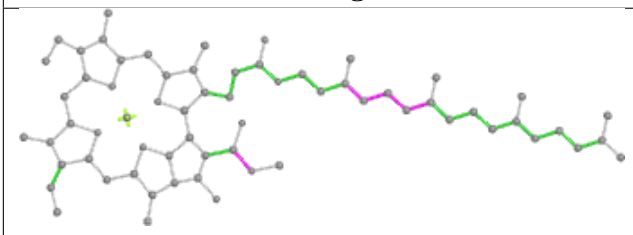
Ligand CLA H 1231



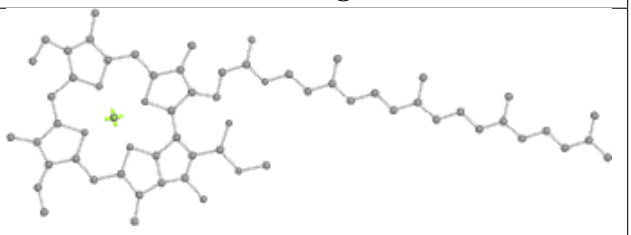
Bond lengths



Bond angles

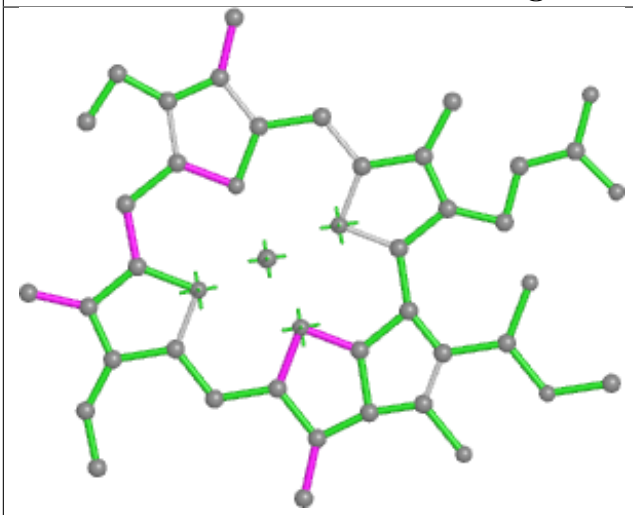


Torsions



Rings

Ligand CLA d 504



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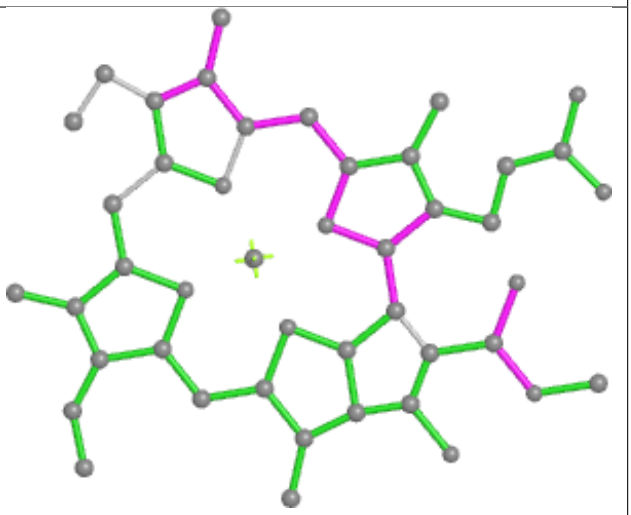

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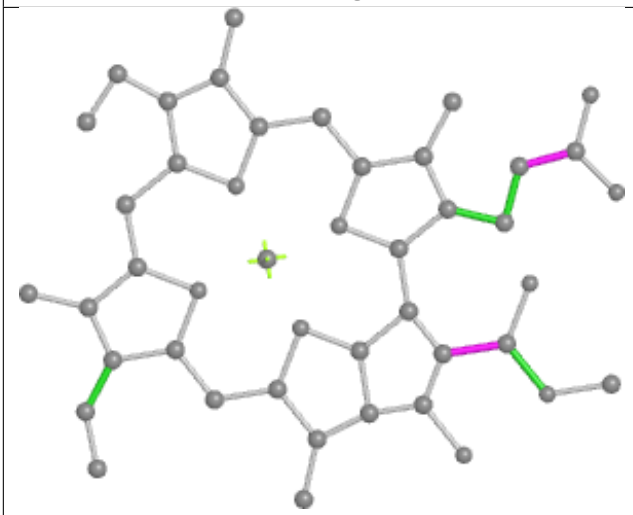

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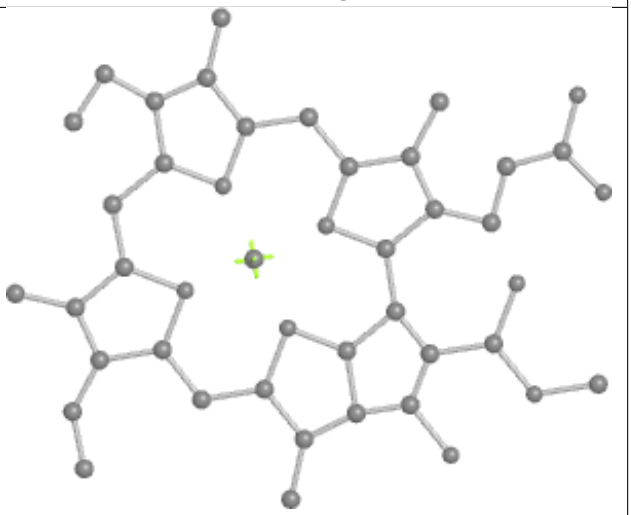
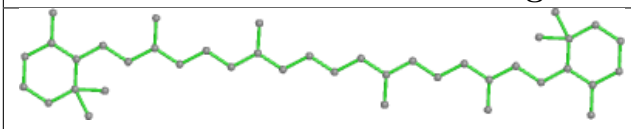
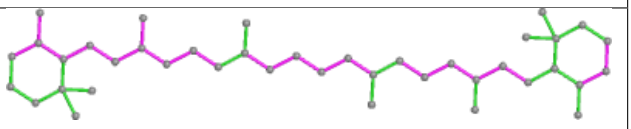
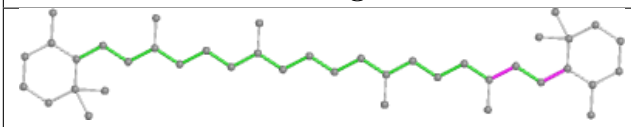


Rings

Ligand BCR v 523	
 Bond lengths	 Bond angles
 Torsions	Rings

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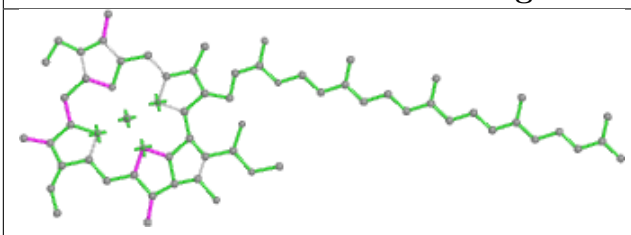
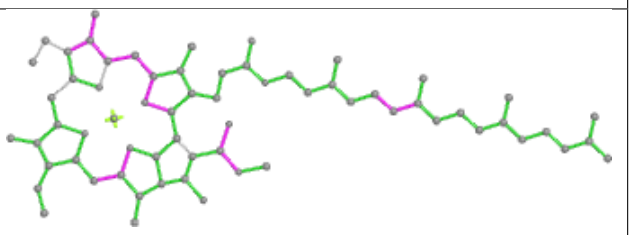
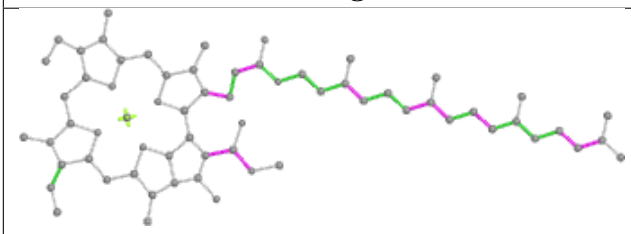
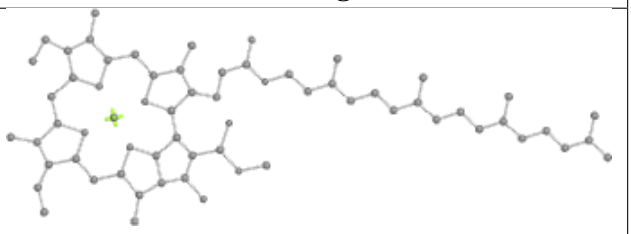
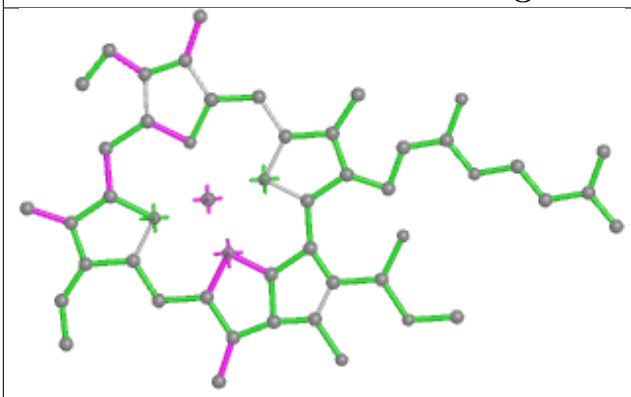
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 1222



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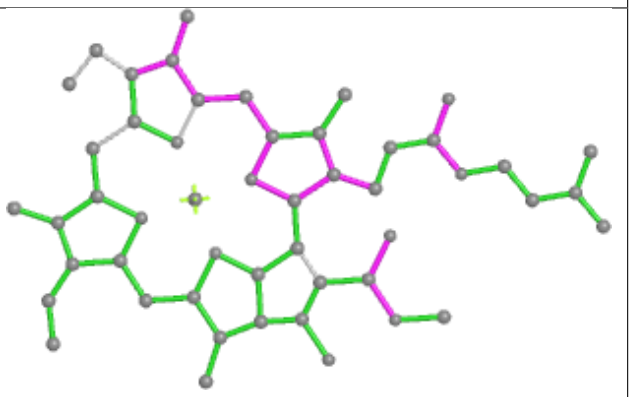
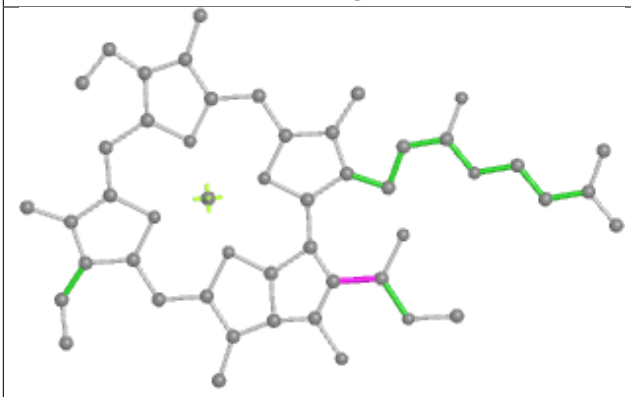


Bond angles



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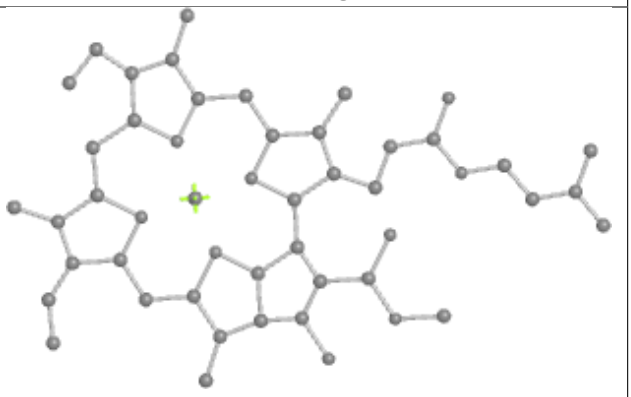
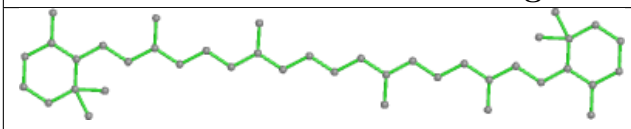


Rings

Ligand BCR Z 523



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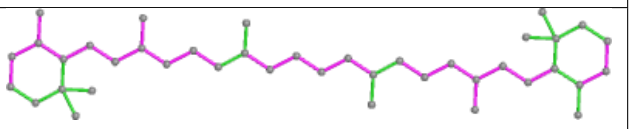

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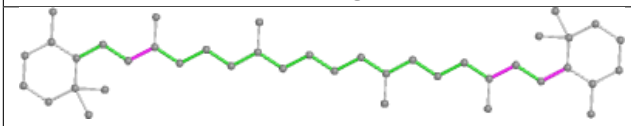

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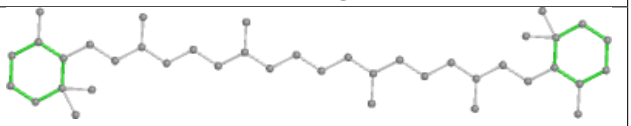
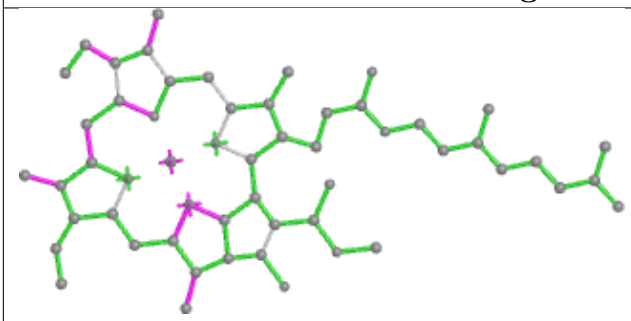


Rings

Ligand CLA e 1105



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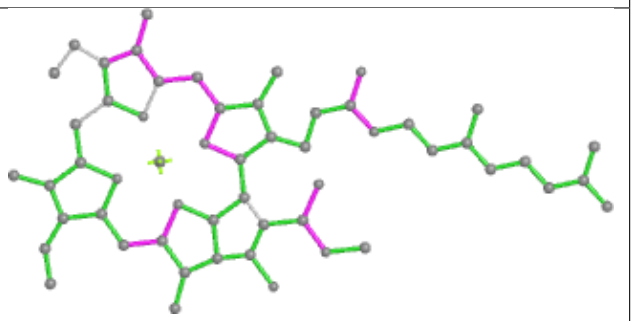

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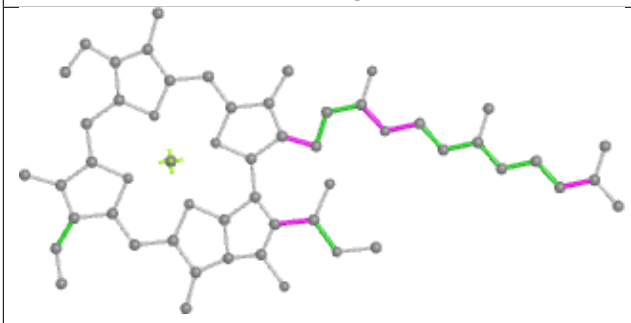

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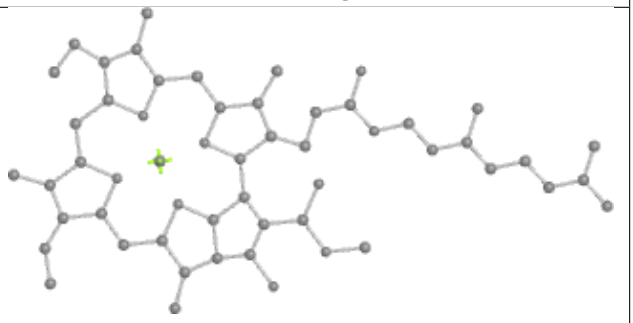
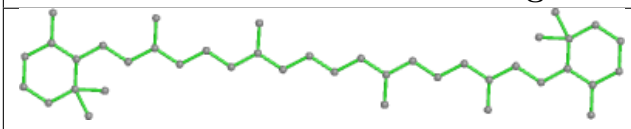


Rings

Ligand BCR a 521



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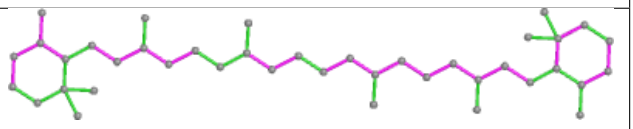

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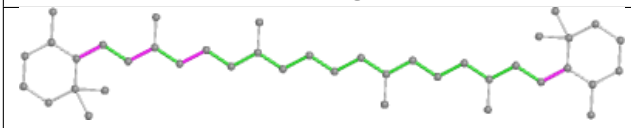
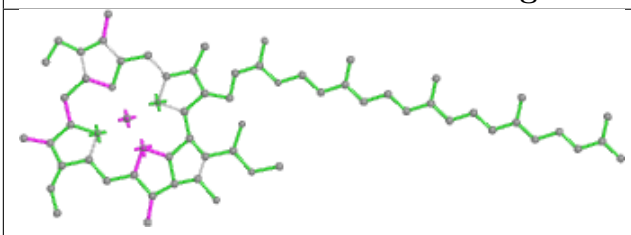


Torsions

Rings

Ligand CLA e 1106



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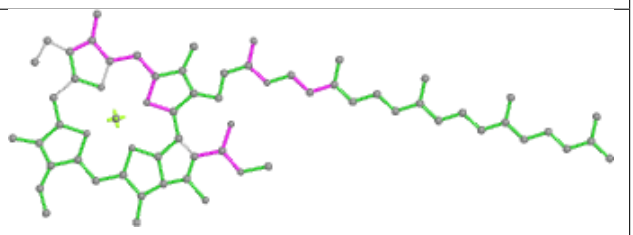

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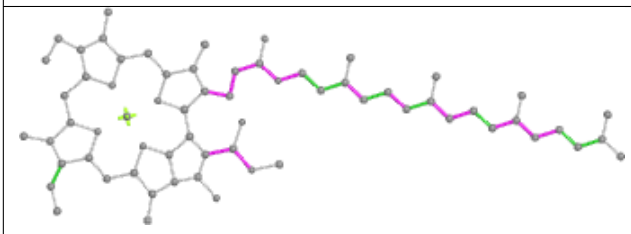

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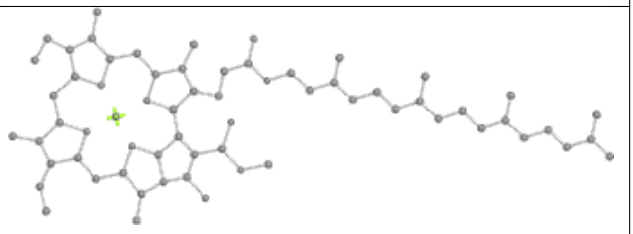
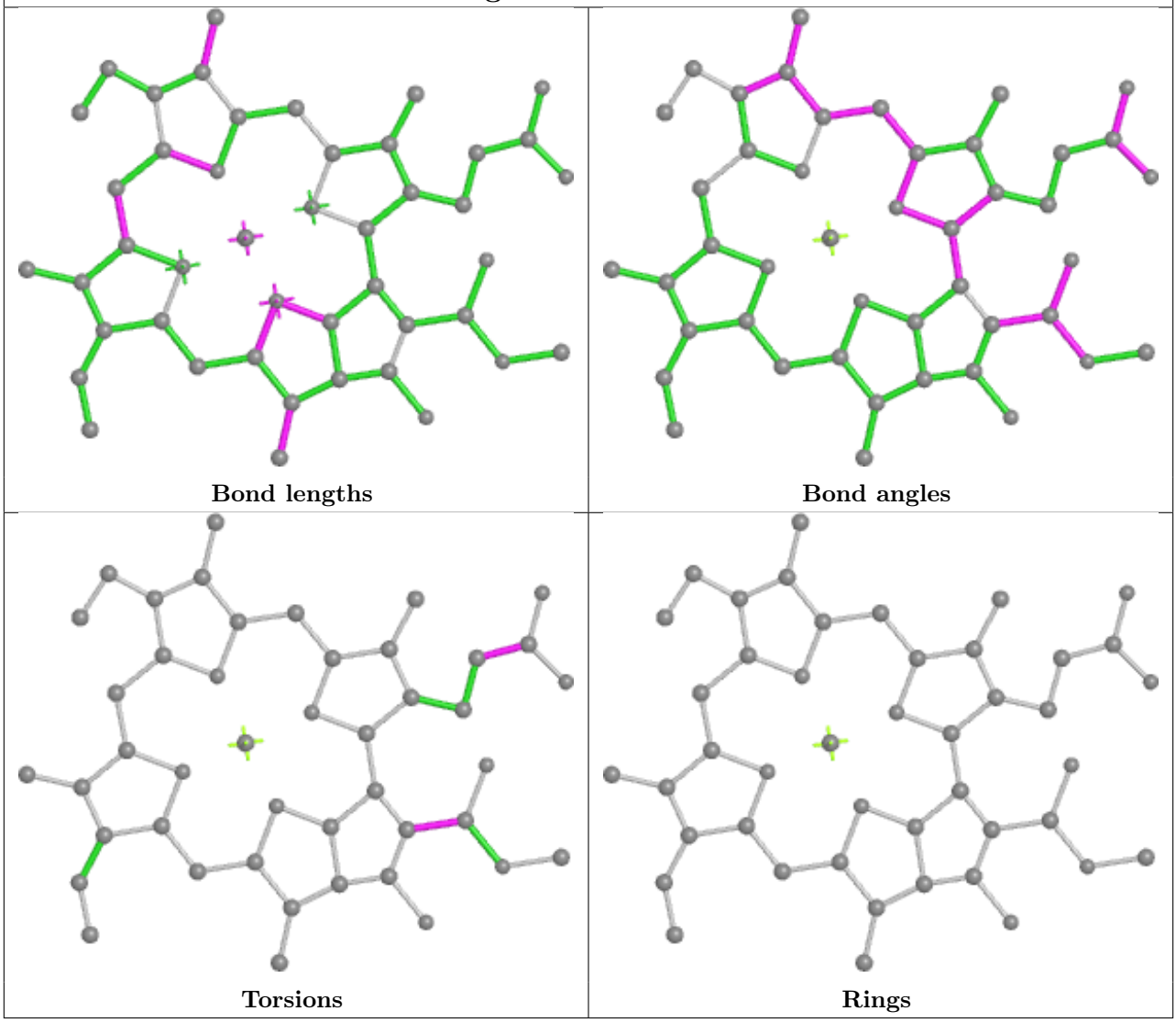


Rings

Ligand CLA 1 509



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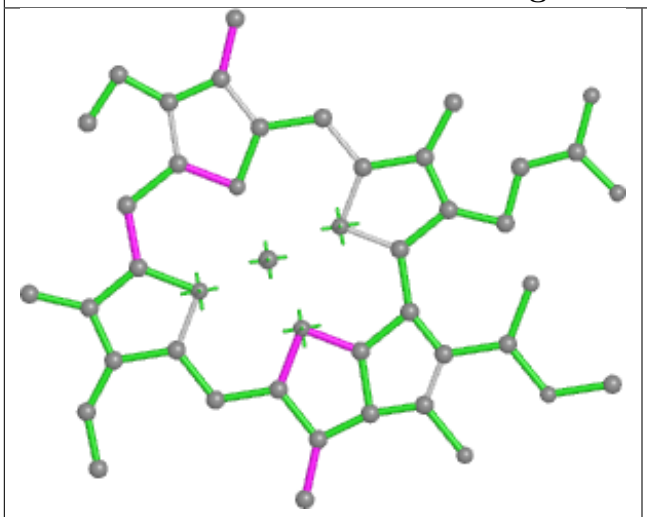

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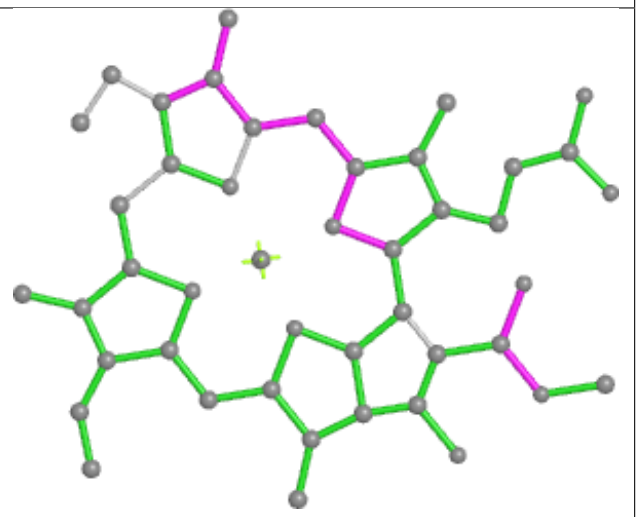

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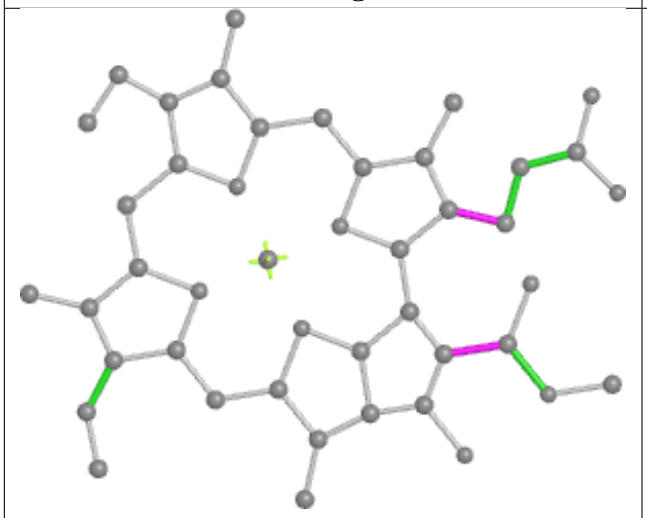

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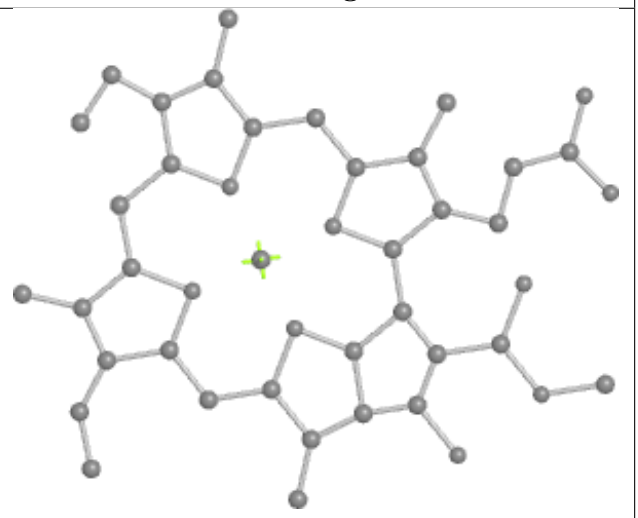

Rings

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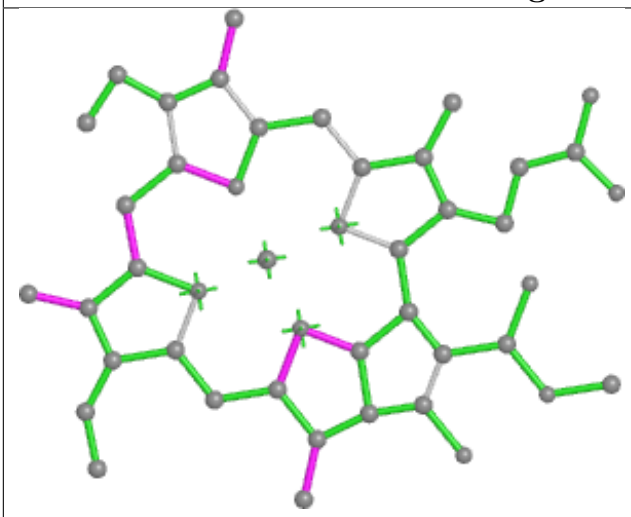

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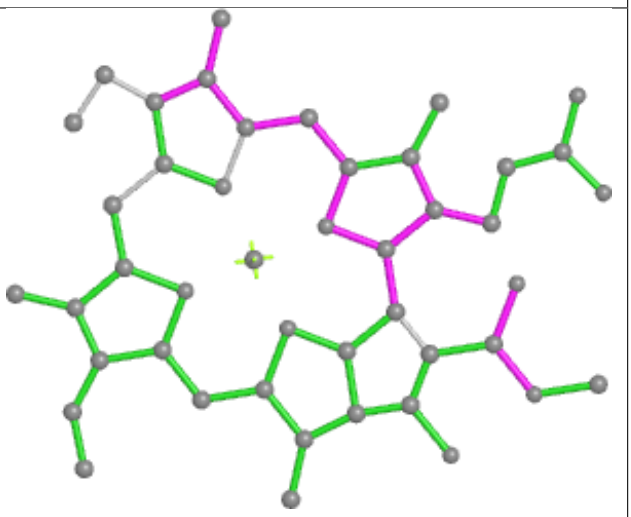

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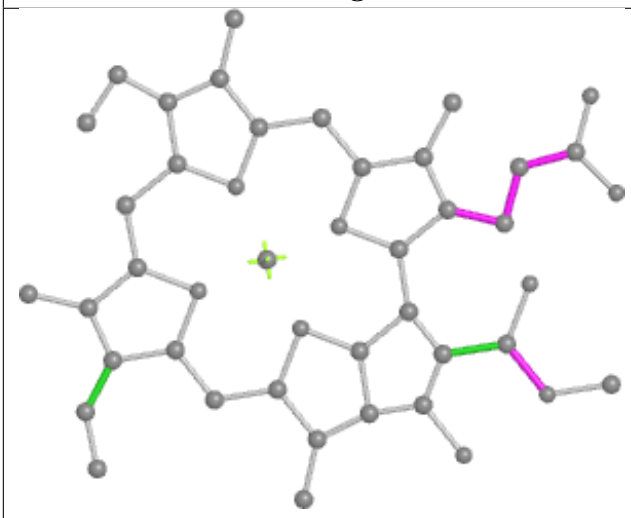

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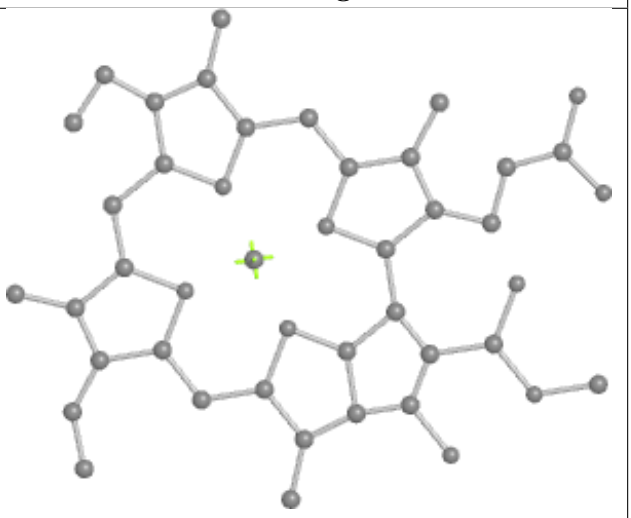
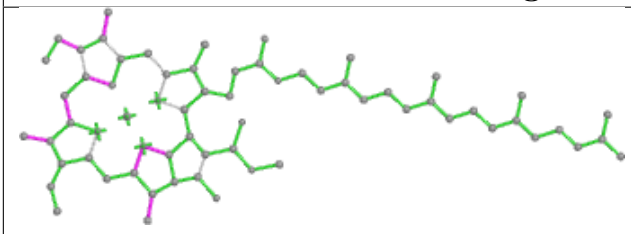


Rings

Ligand CLA f 1207



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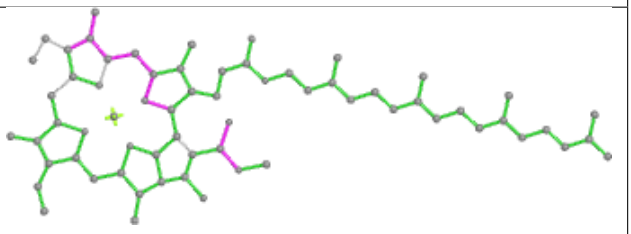

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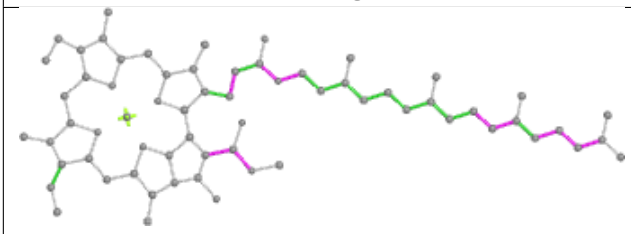

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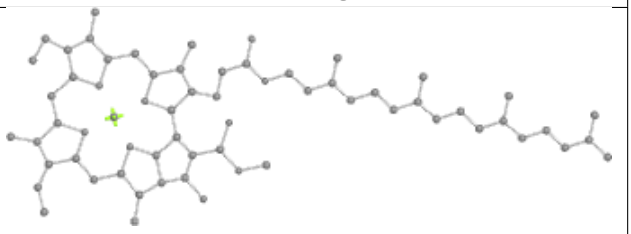
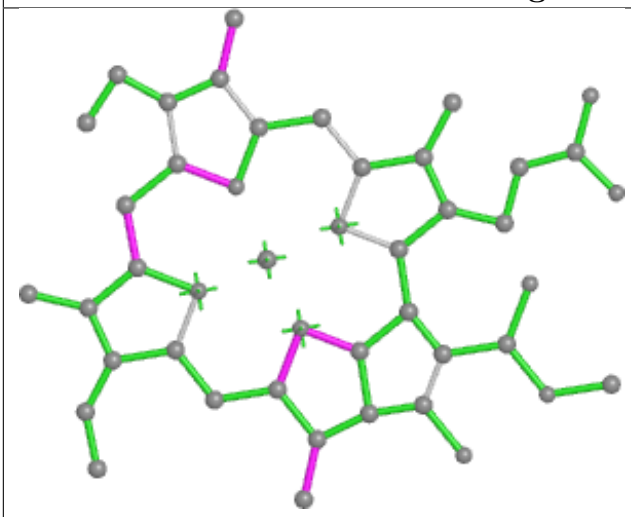


Rings

Ligand CLA 4 516



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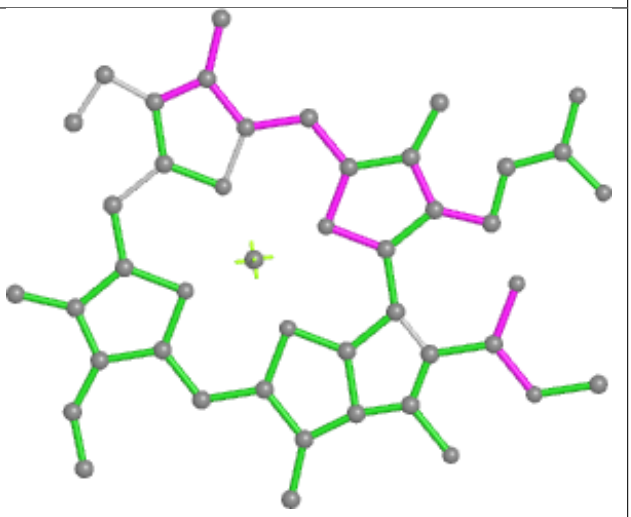
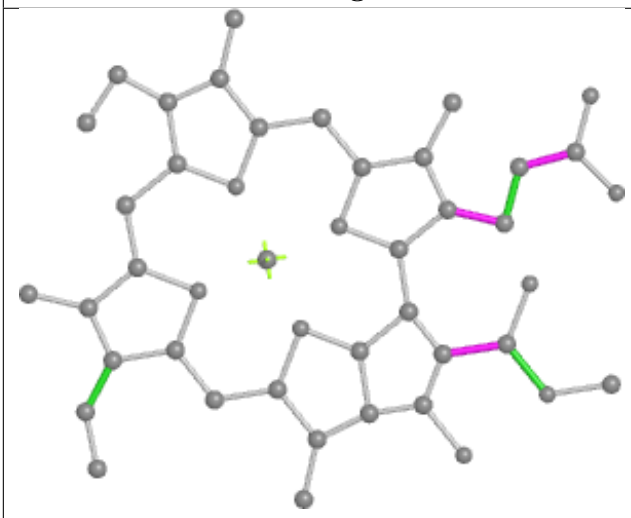


Bond angles



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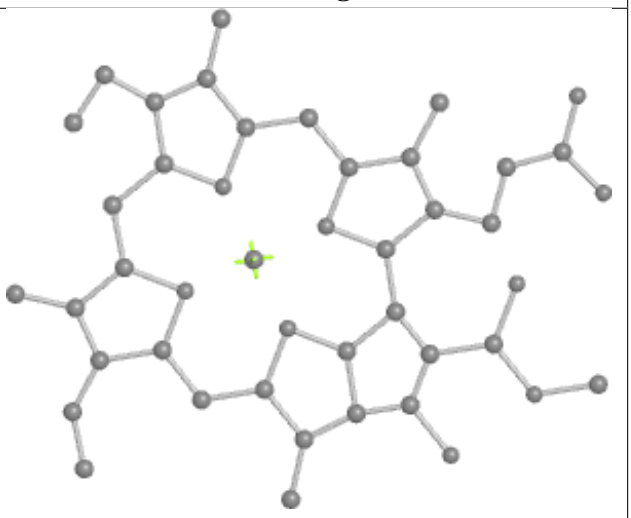
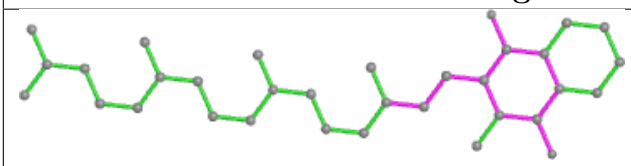


Rings

Ligand PQN B 2002



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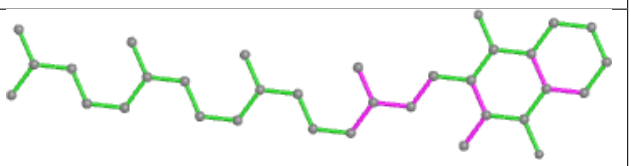
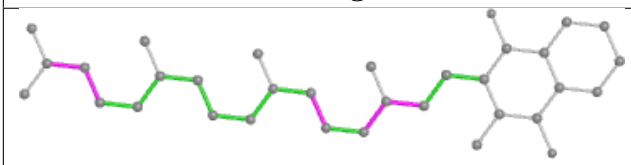


Bond angles



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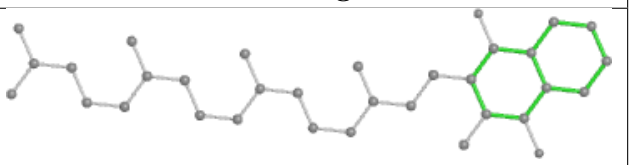
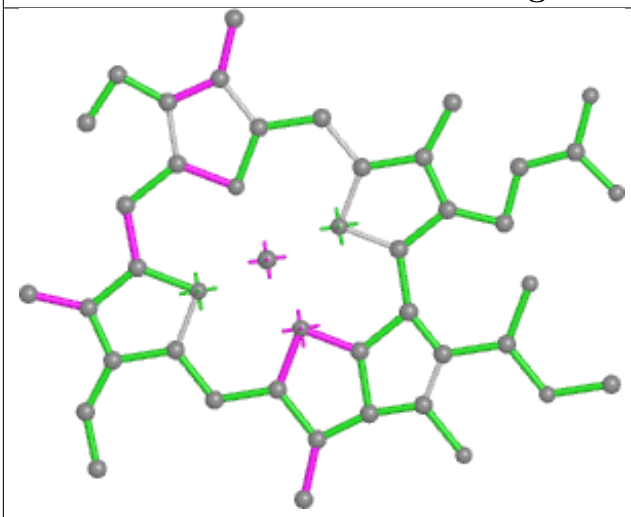
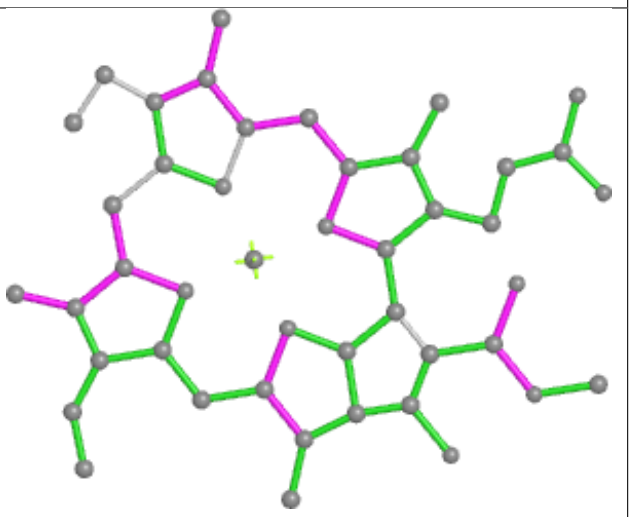


Rings

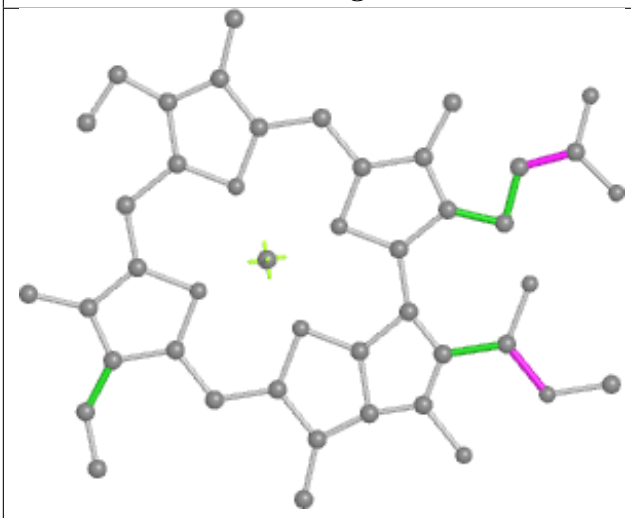
Ligand CLA 4 508



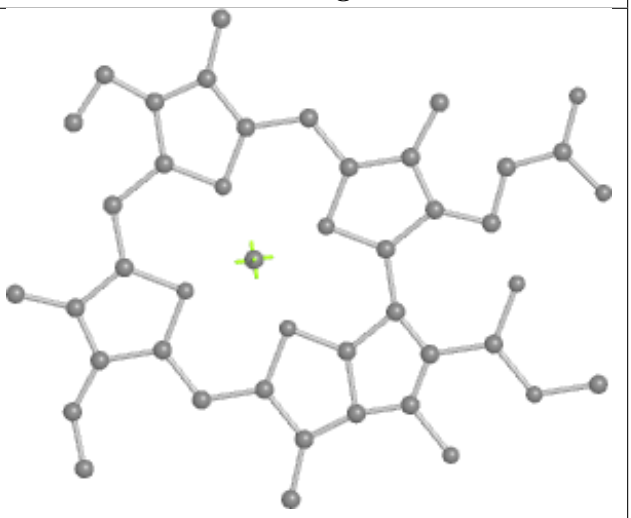
Bond lengths



Bond angles

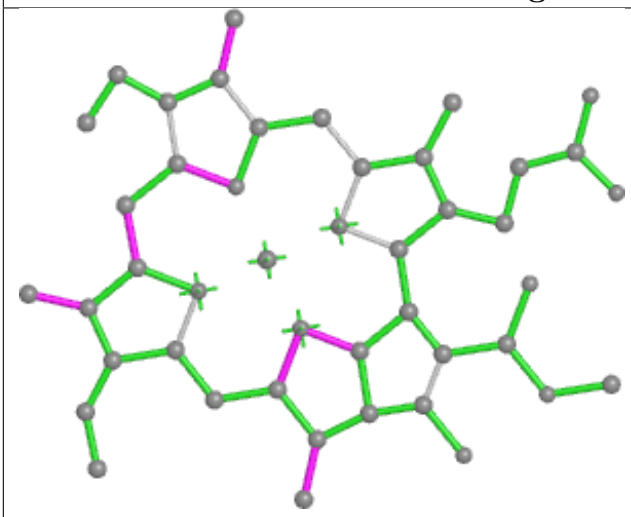


Torsions



Rings

Ligand CLA 1 506



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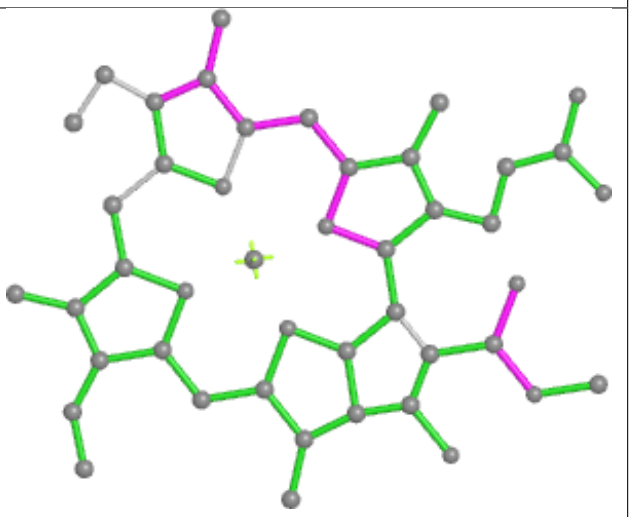

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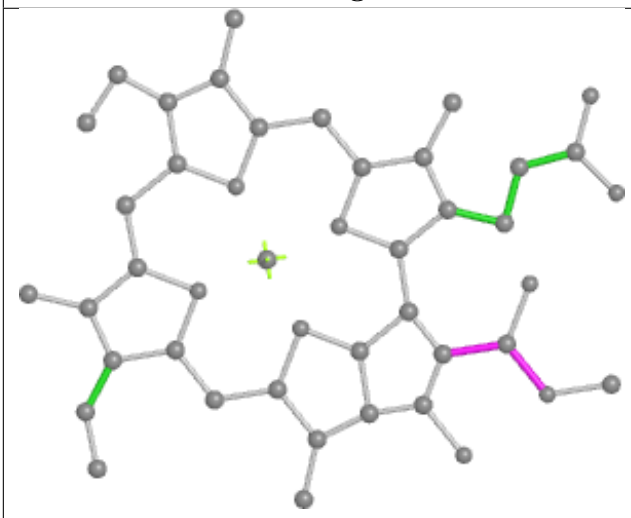

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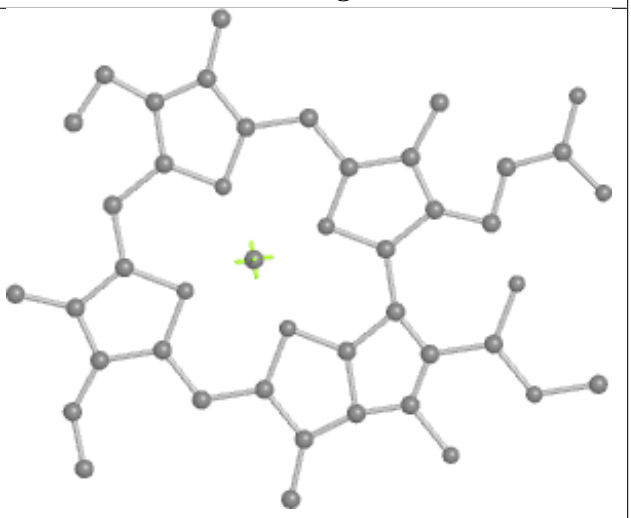
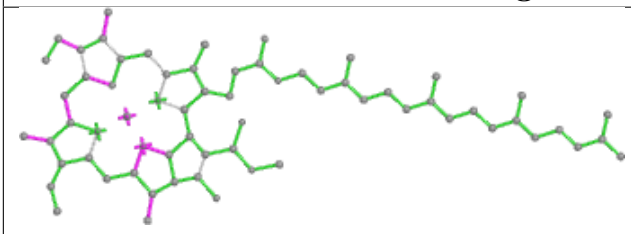


Rings

Ligand CLA B 1012



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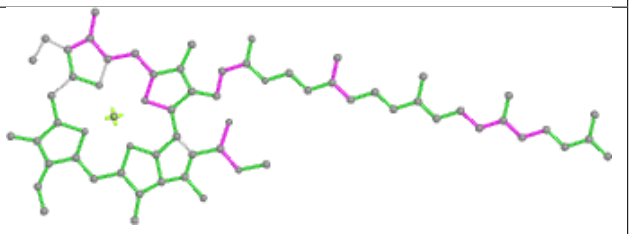
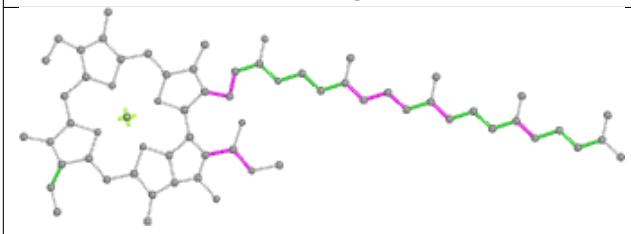


Bond angles



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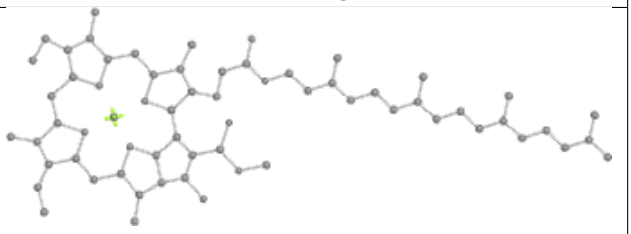
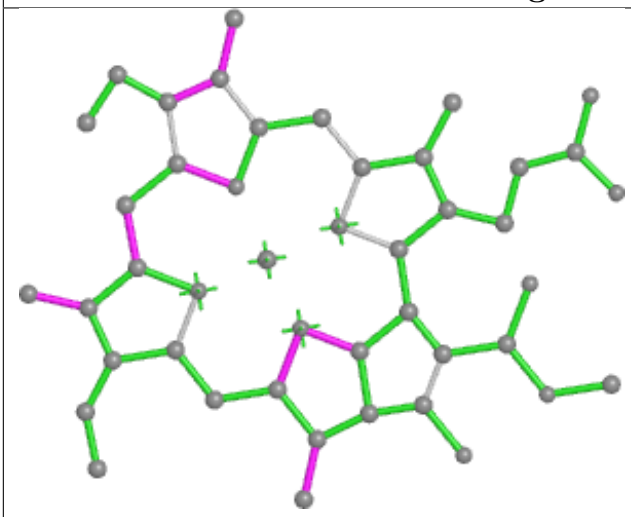


Rings

Ligand CLA a 517



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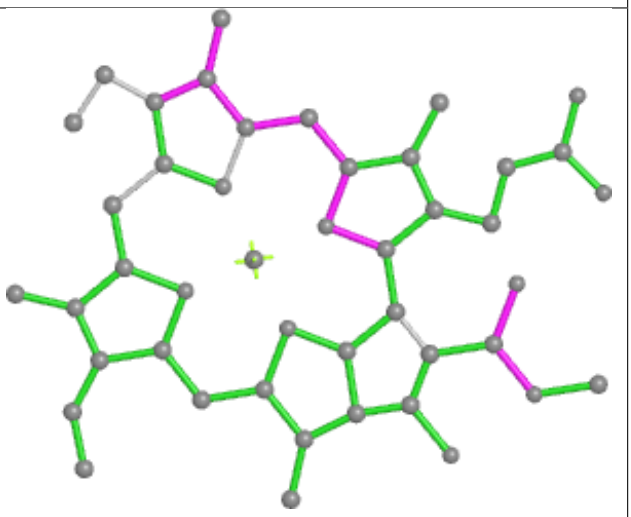

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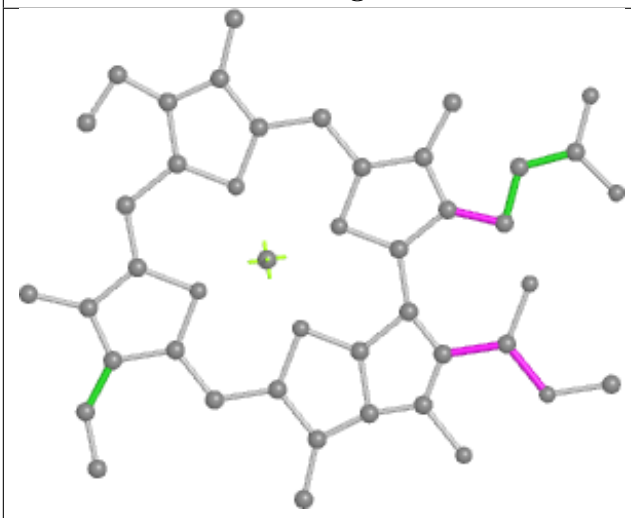

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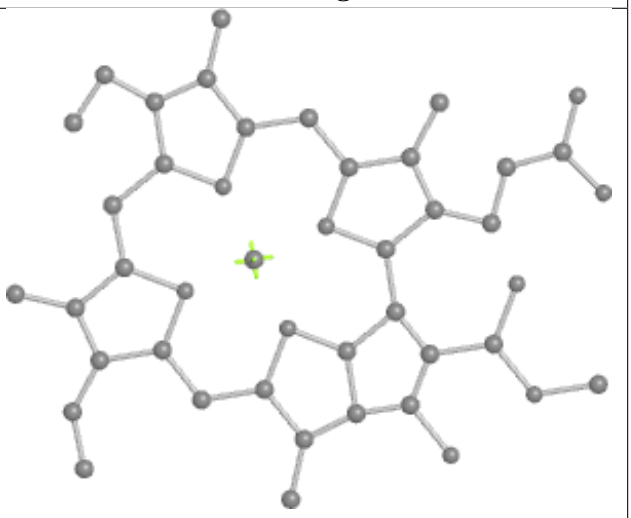
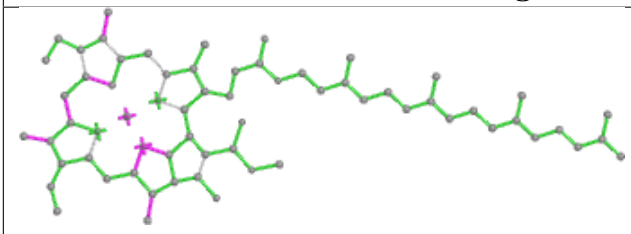


Rings

Ligand CLA G 1123



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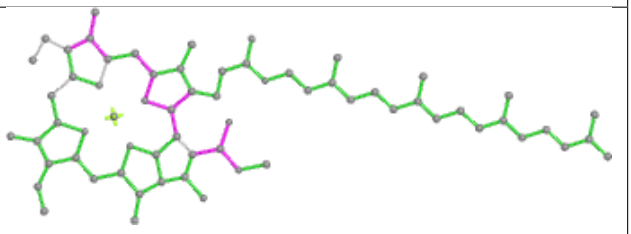

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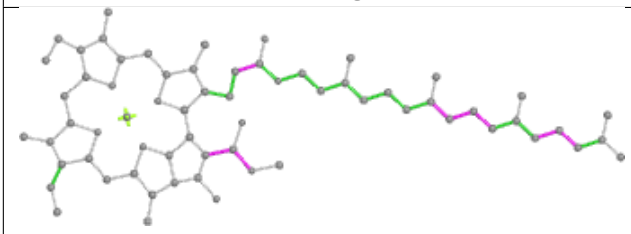

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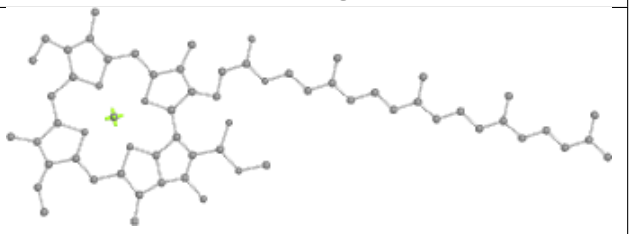

Rings

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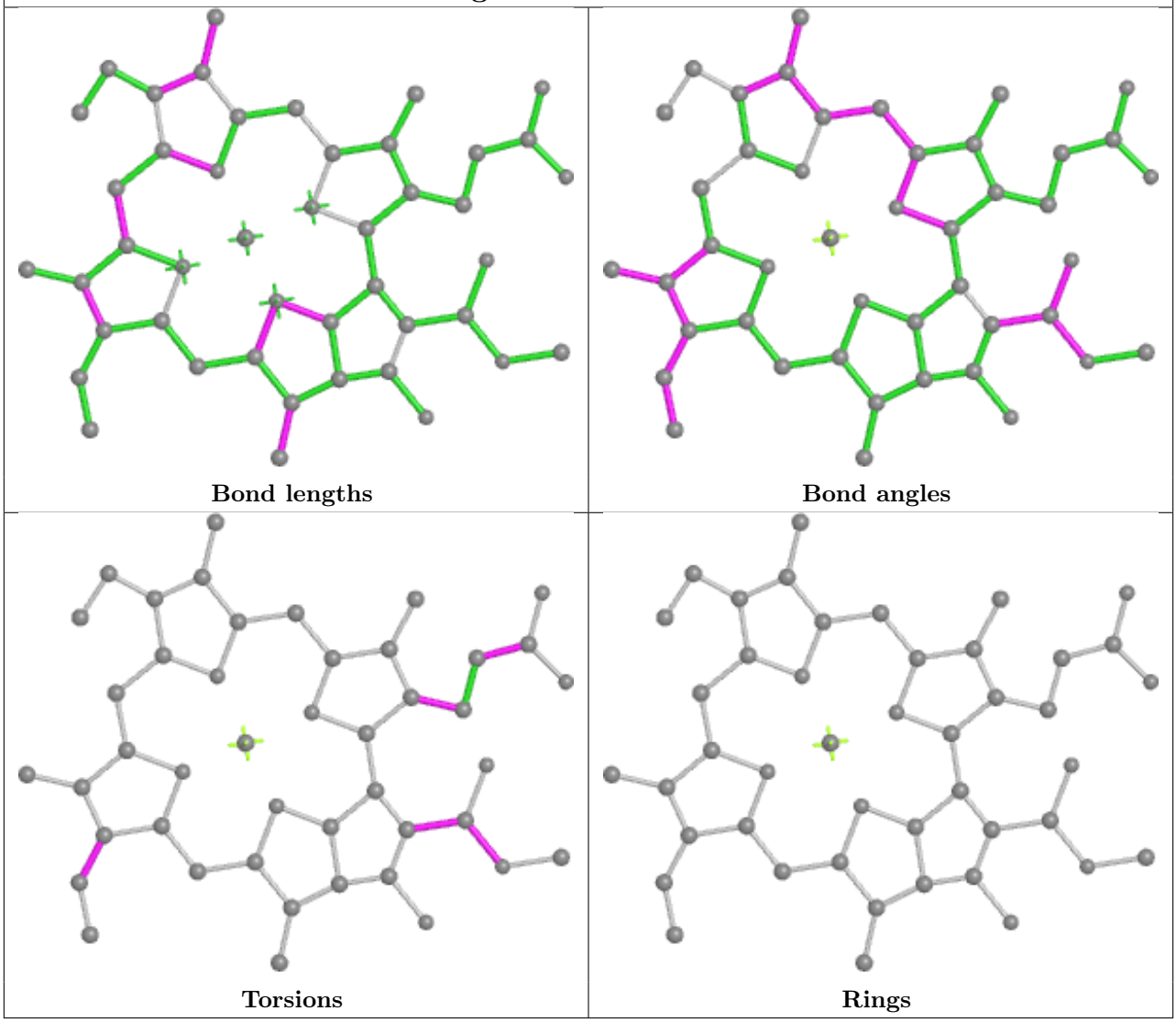

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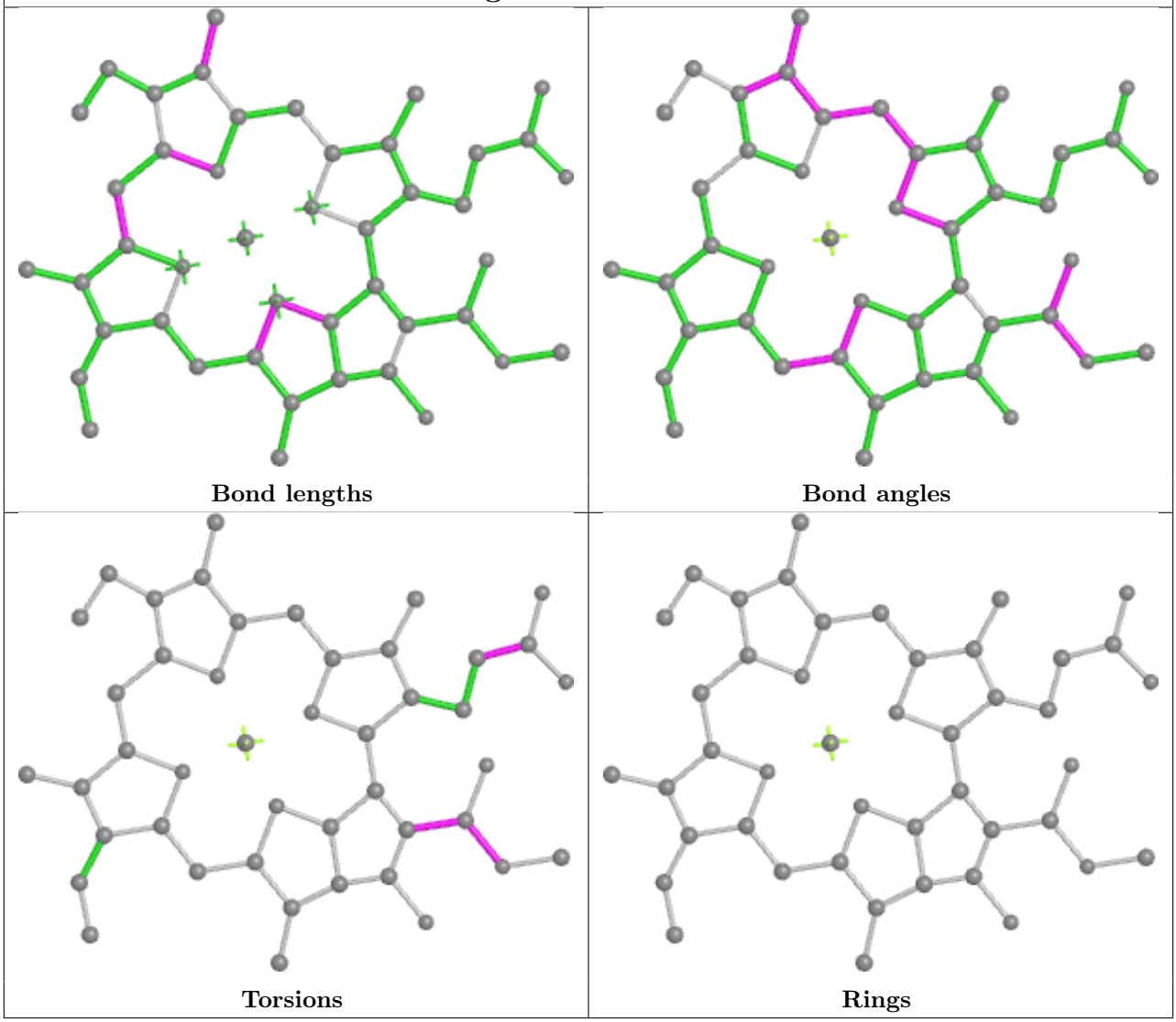

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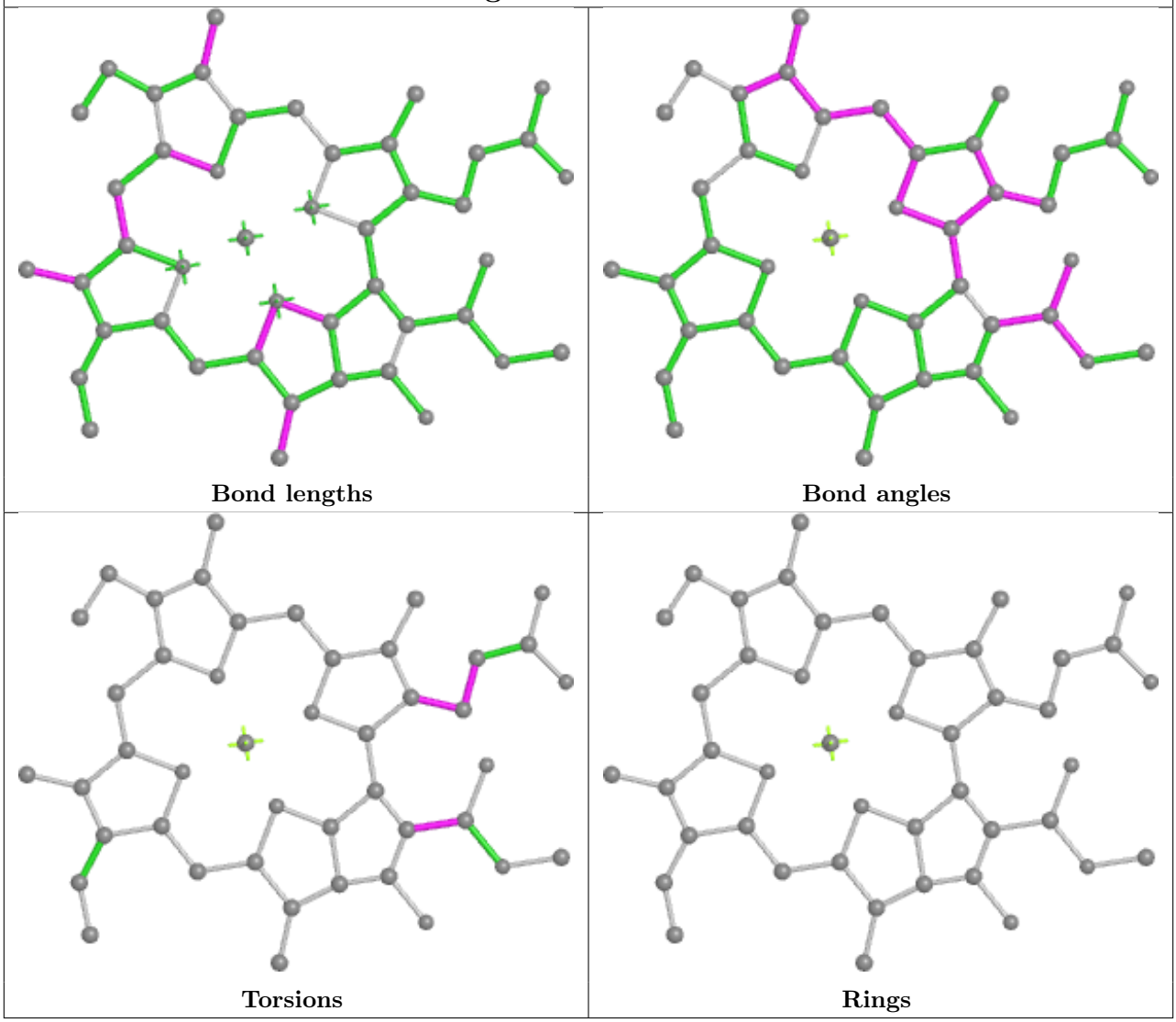

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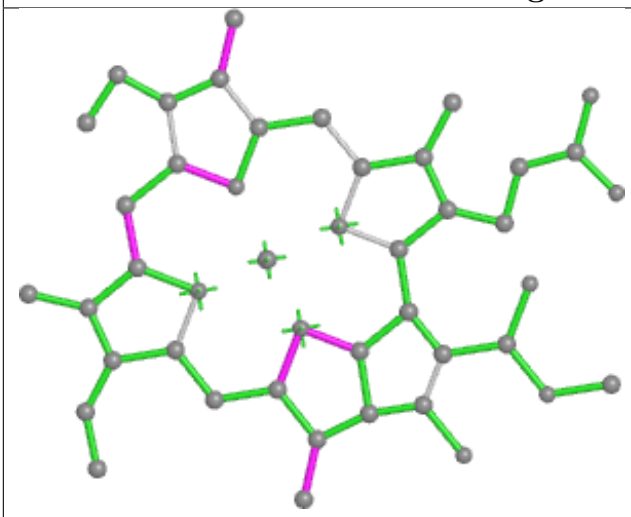
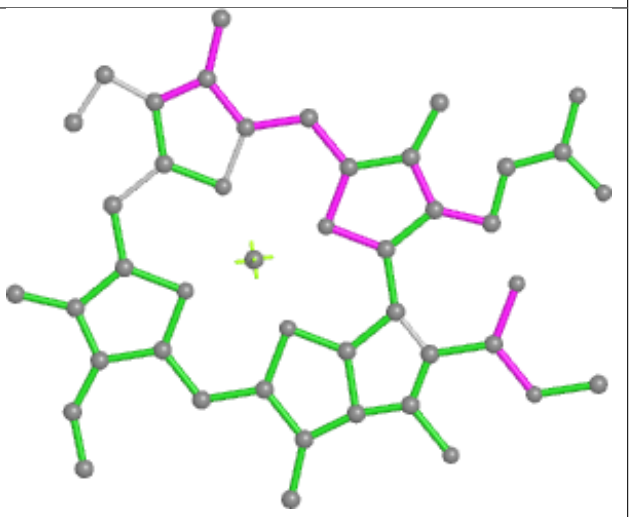
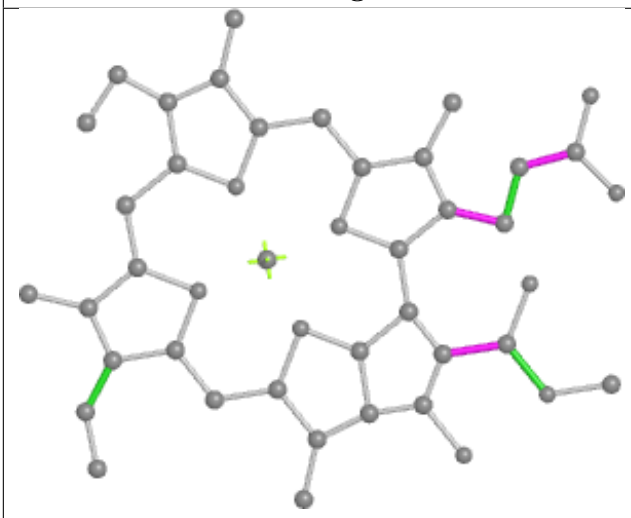


Bond lengths



Bond angles



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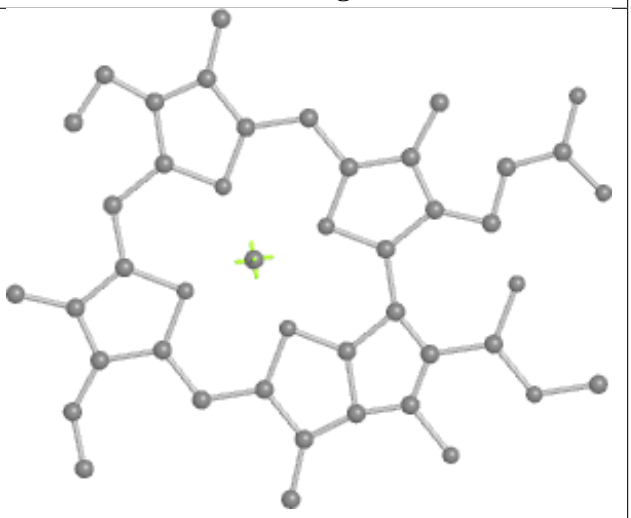

Rings

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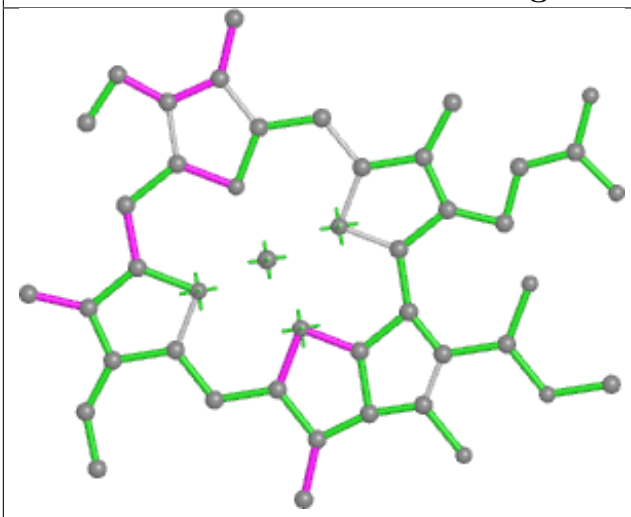

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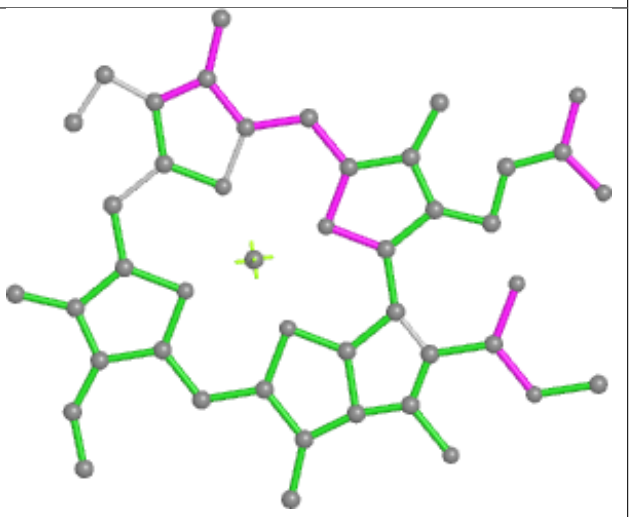

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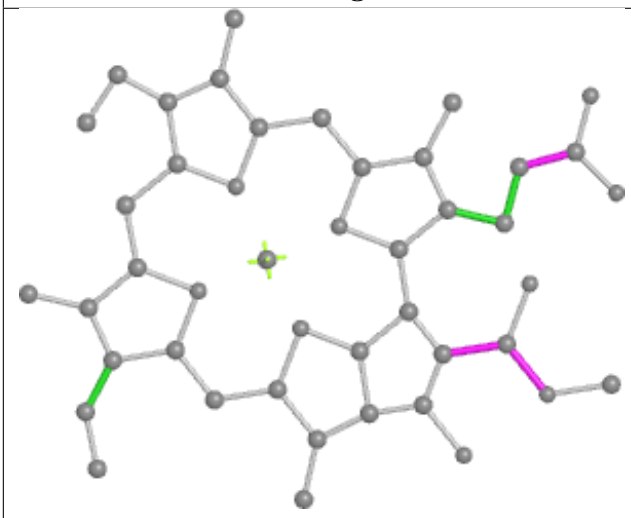

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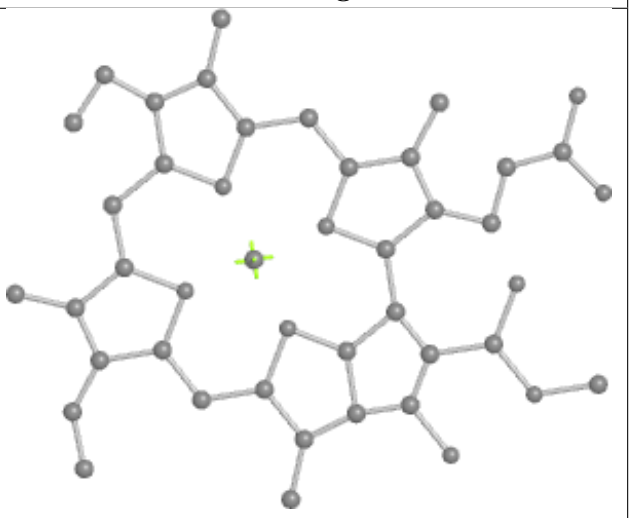
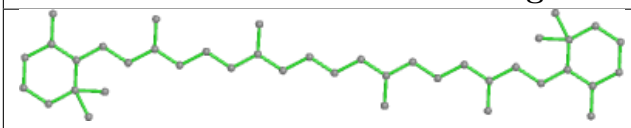


Rings

Ligand BCR 2 522



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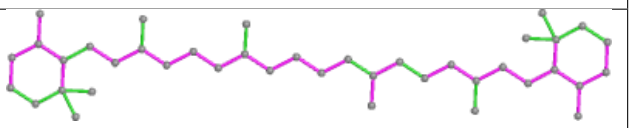

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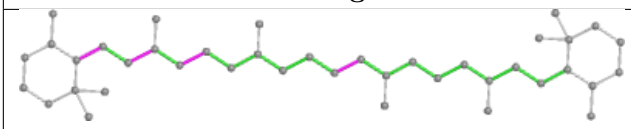
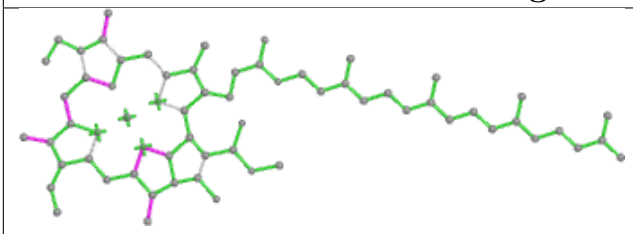


Torsions

Rings

Ligand CLA c 509



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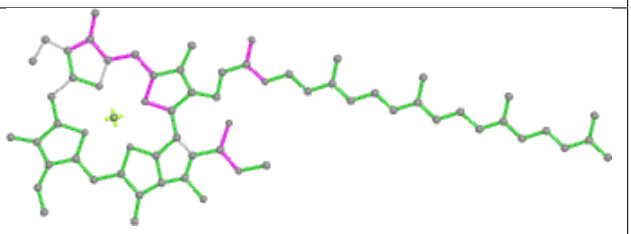

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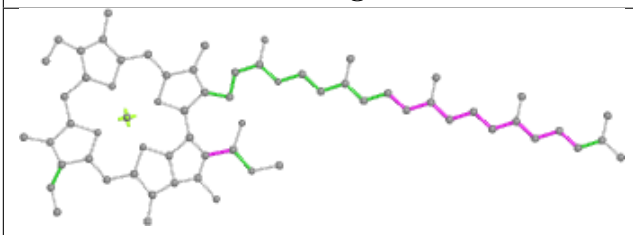

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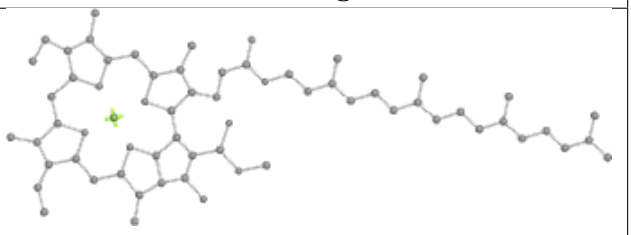
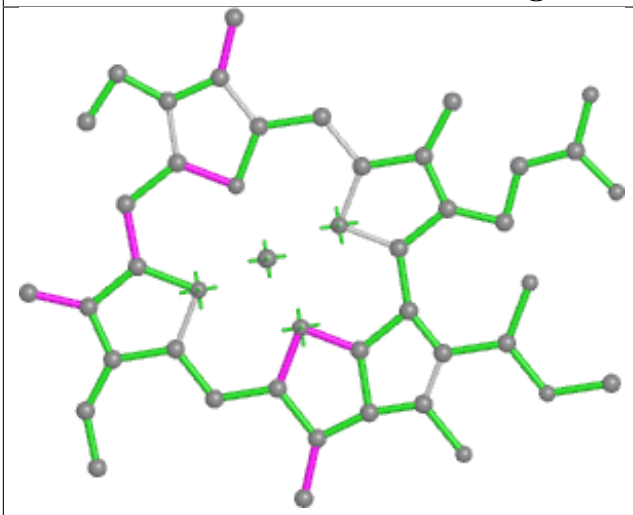


Rings

Ligand CLA q 505



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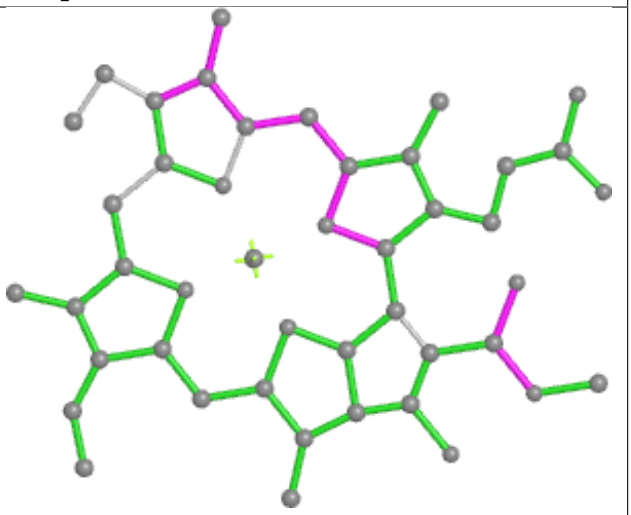

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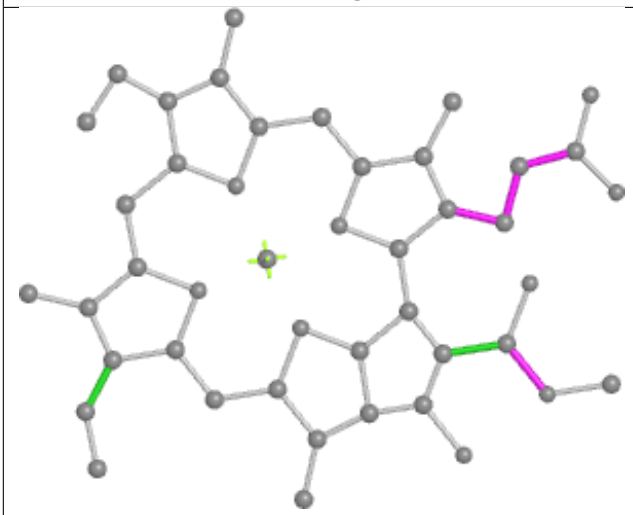

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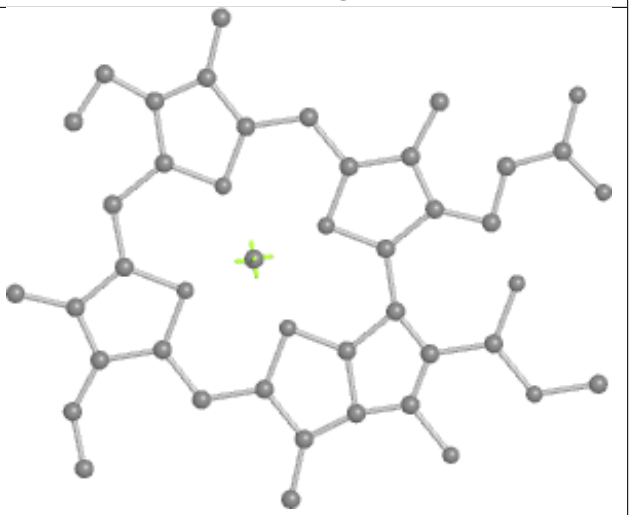
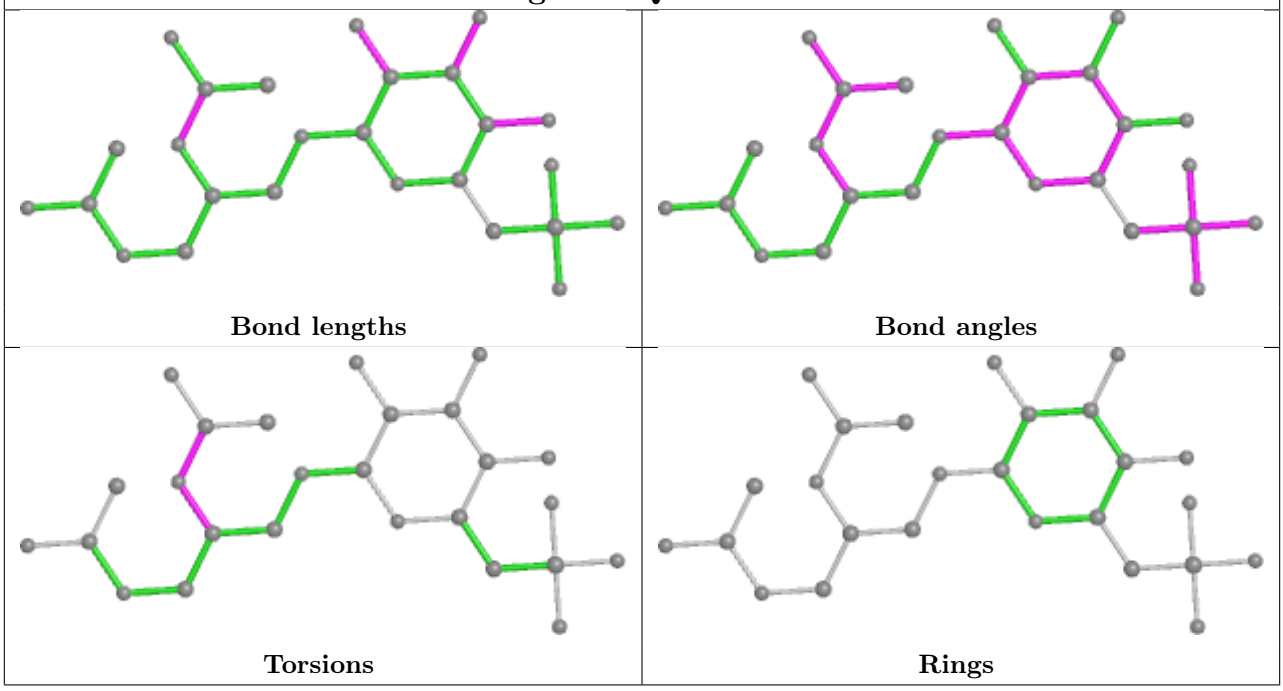


Rings

Ligand SQD u 822



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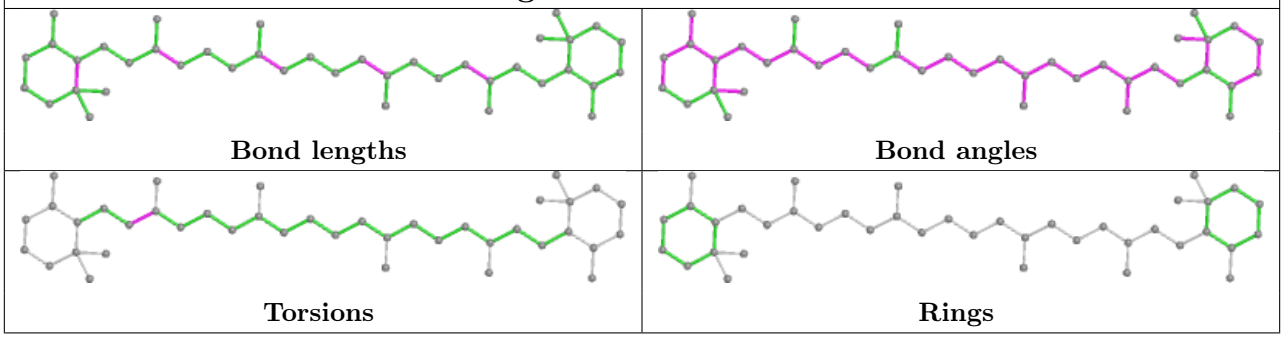
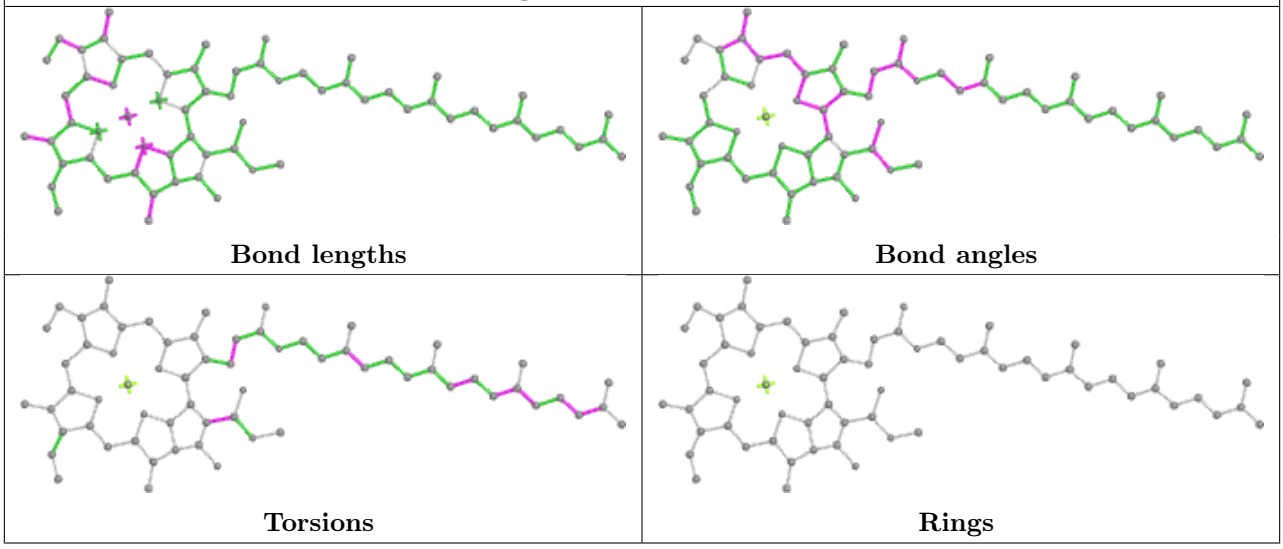
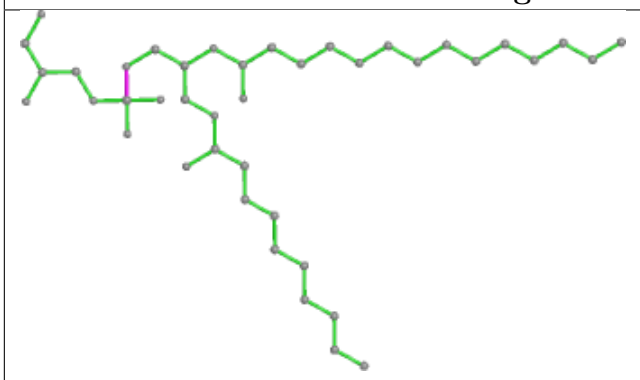
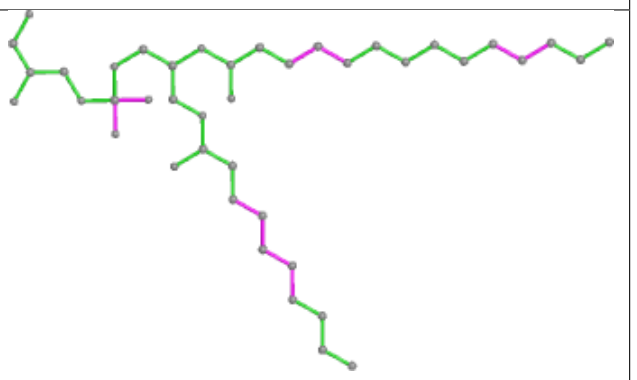
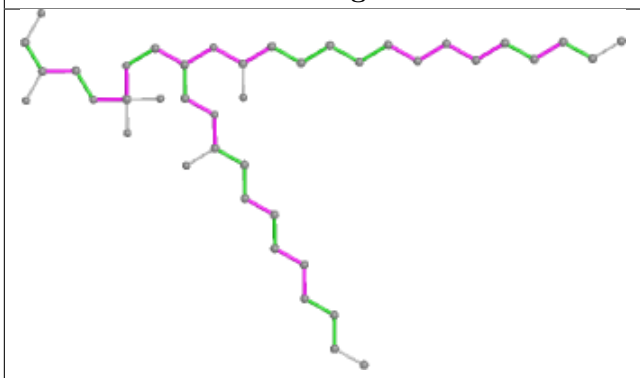
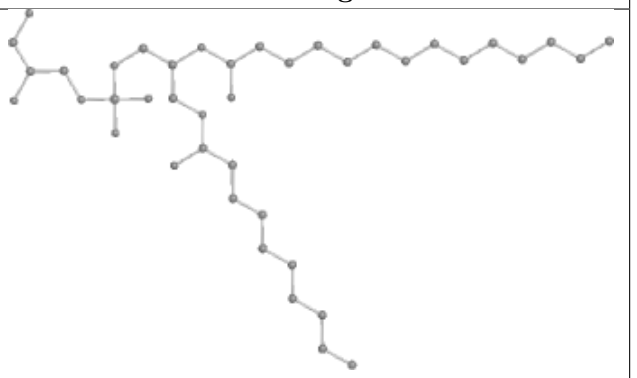


Ligand CLA A 1127



Ligand LHG H 1855	
 Bond lengths	 Bond angles
 Torsions	 Rings

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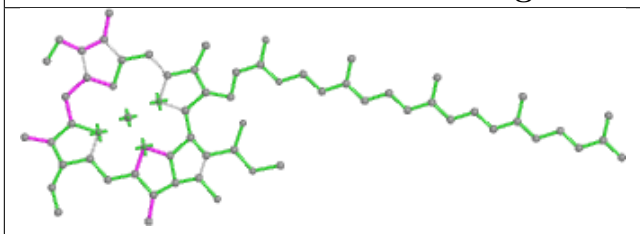
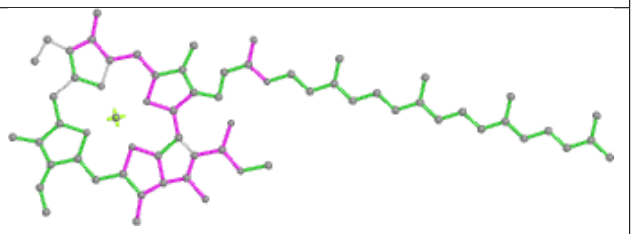
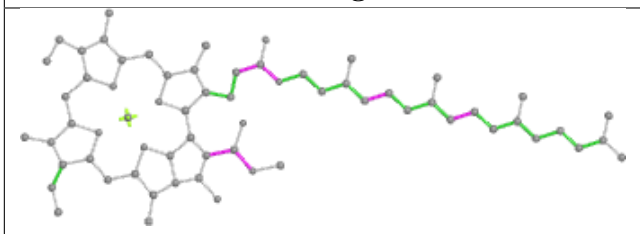
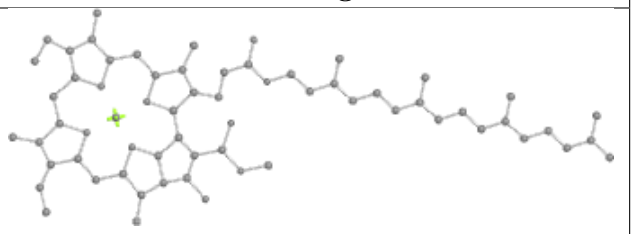
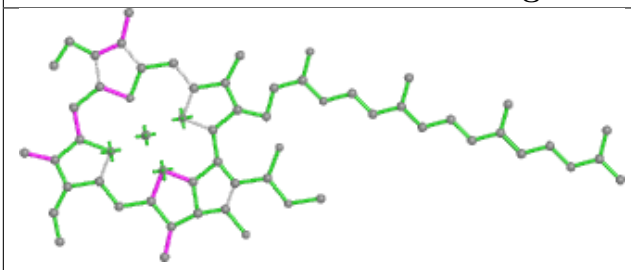
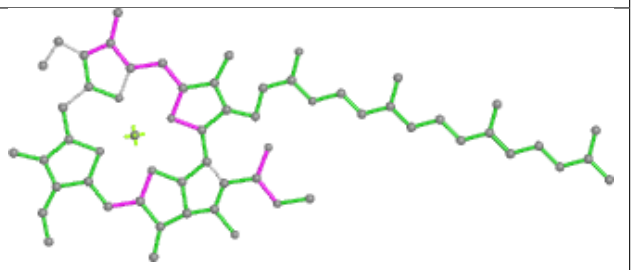
 Bond lengths	 Bond angles
 Torsions	 Rings

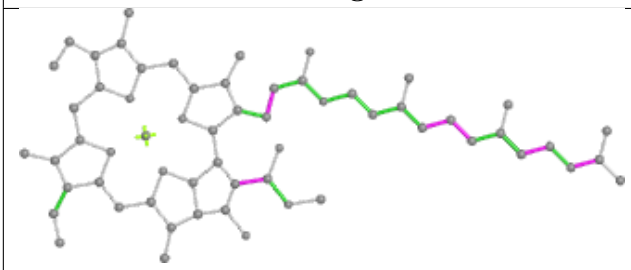
Ligand CLA f 1218



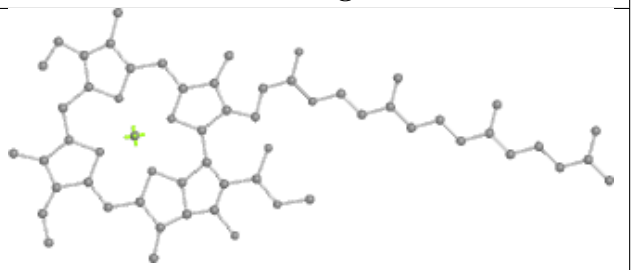
Bond lengths



Bond angles

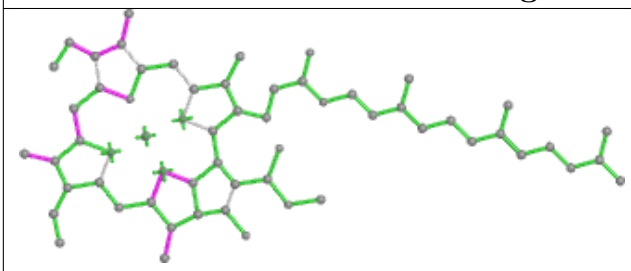


Torsions



Rings

Ligand CLA e 1137



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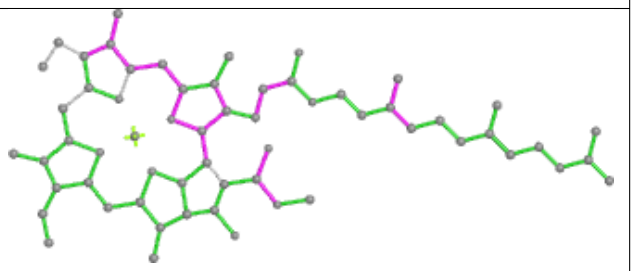

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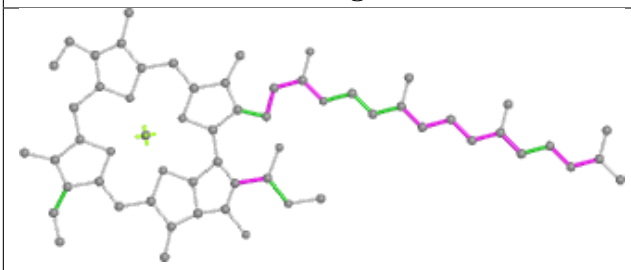

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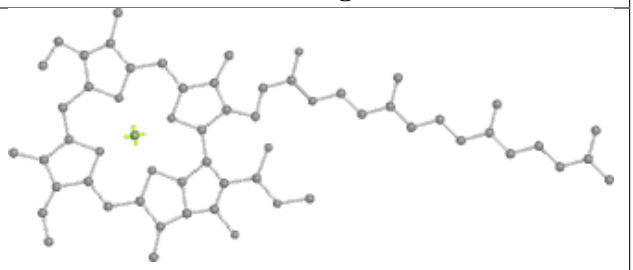
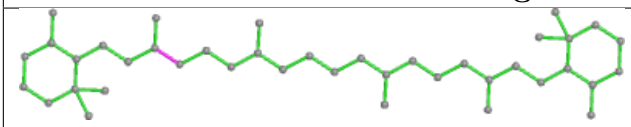


Rings

Ligand BCR B 4014



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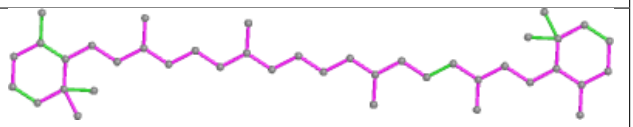
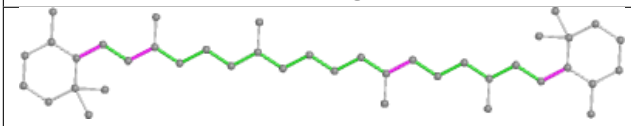


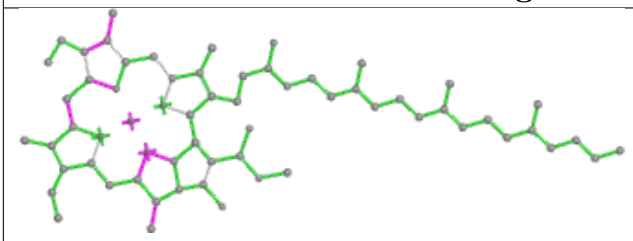
Bond angles



Torsions

Rings

Ligand CLA B 1219



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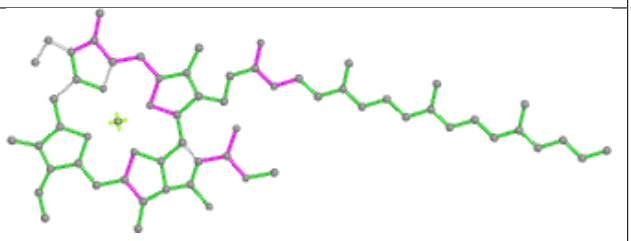

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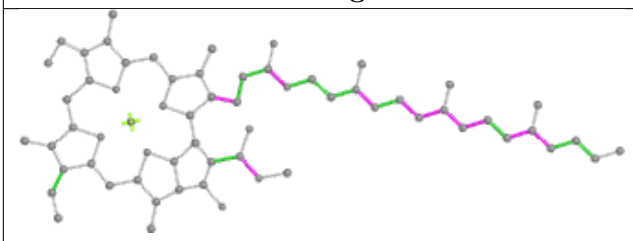

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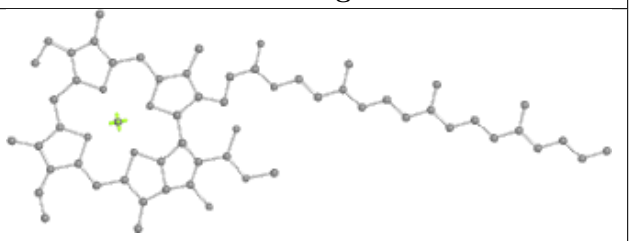
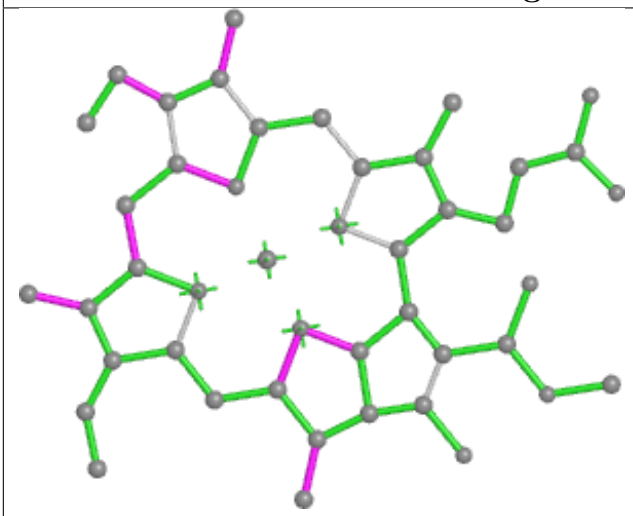


Rings

Ligand CLA l 1303



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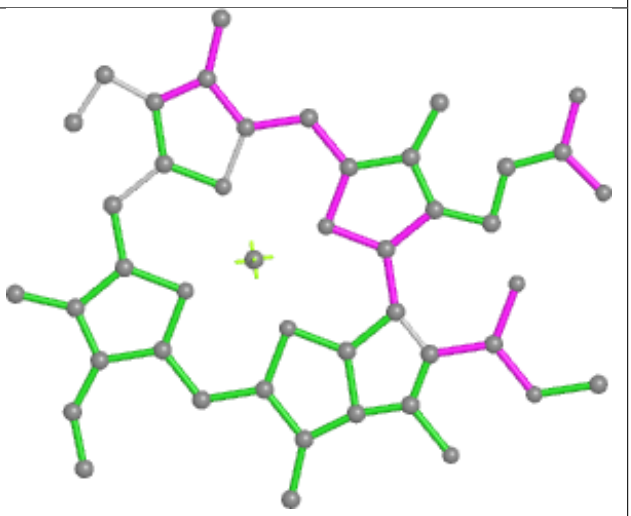
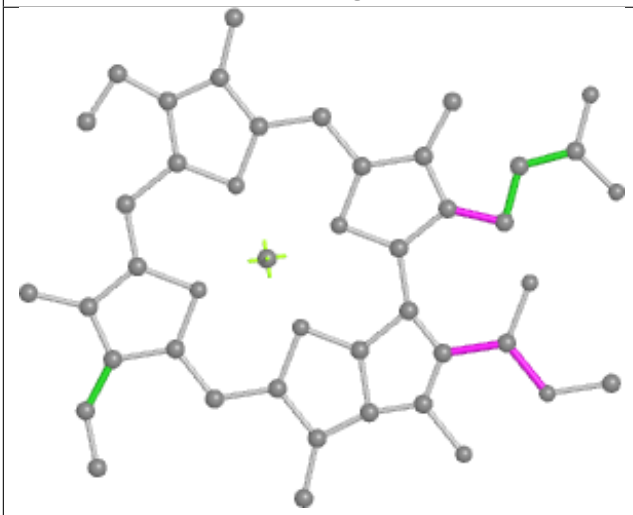


Bond angles



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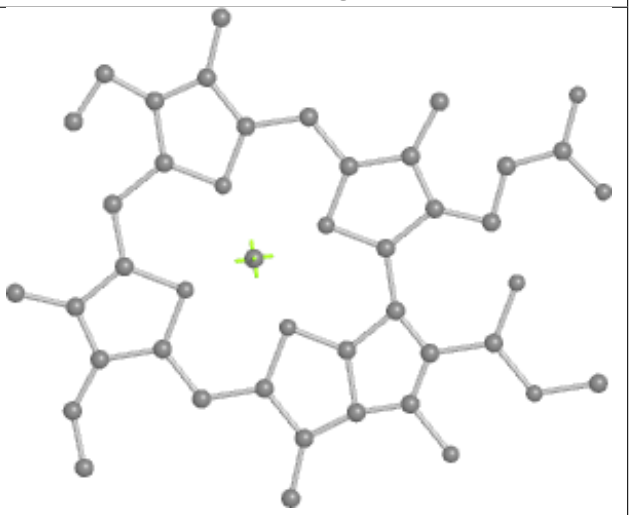
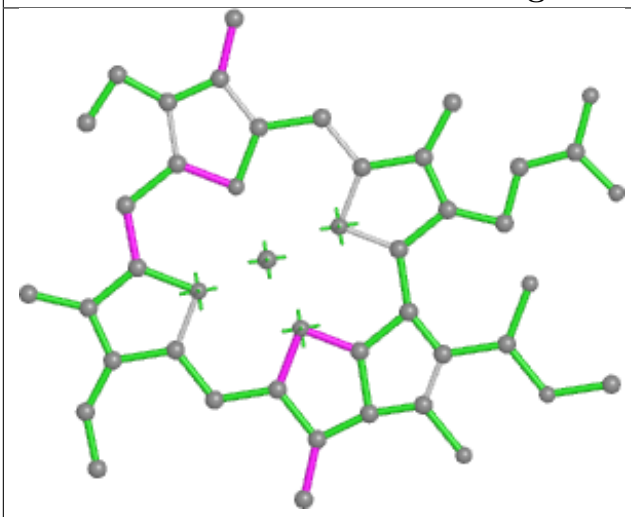


Rings

Ligand CLA v 518



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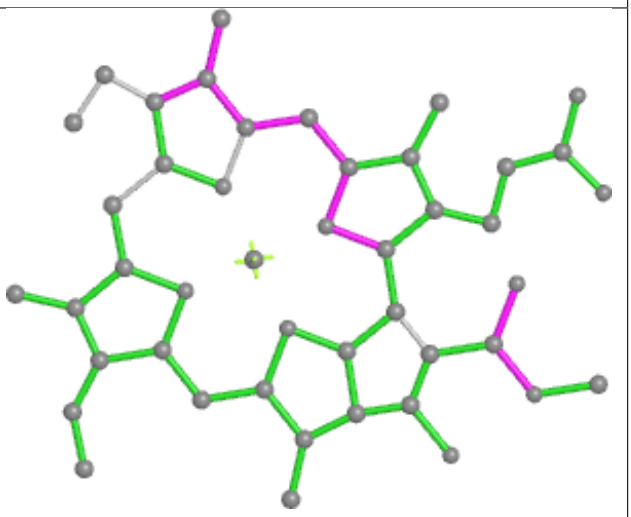
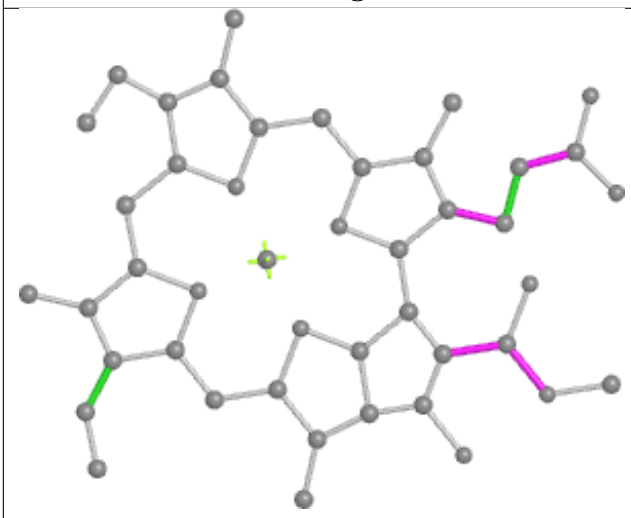


Bond angles



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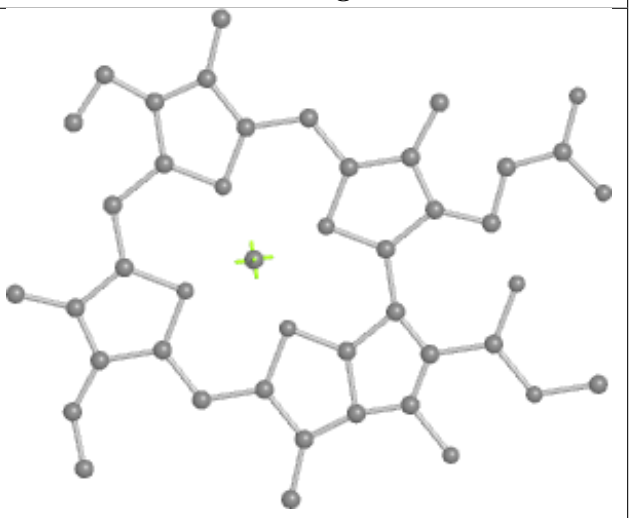
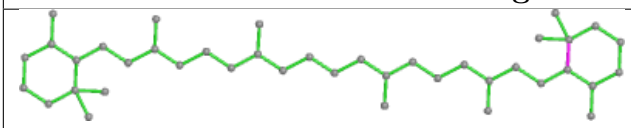


Rings

Ligand BCR G 4003



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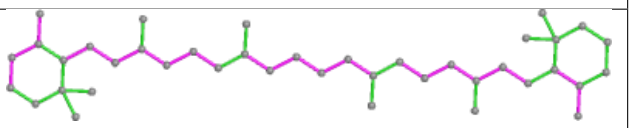
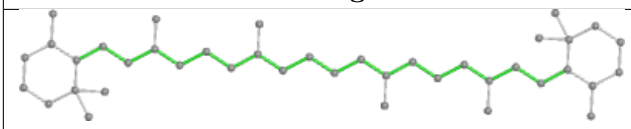
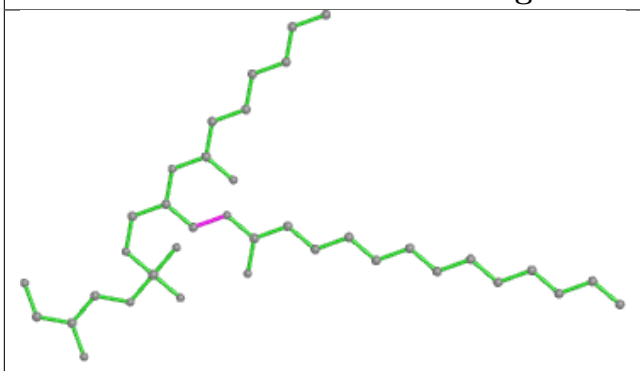
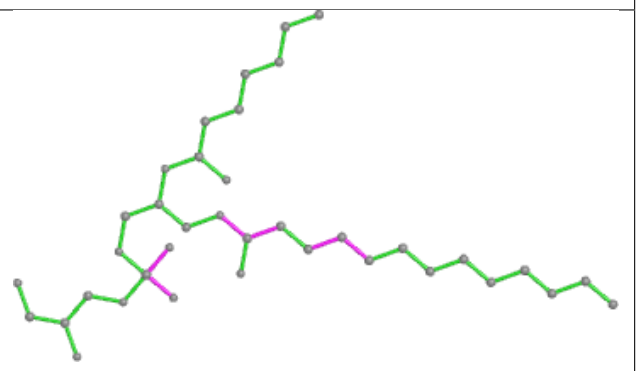
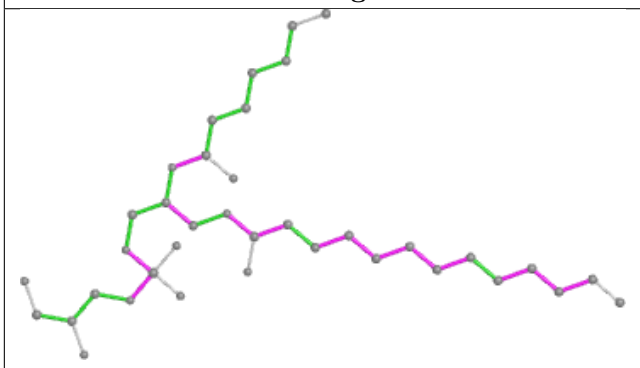
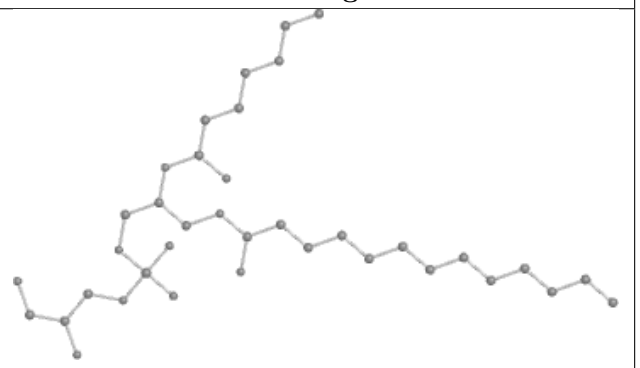


Bond angles

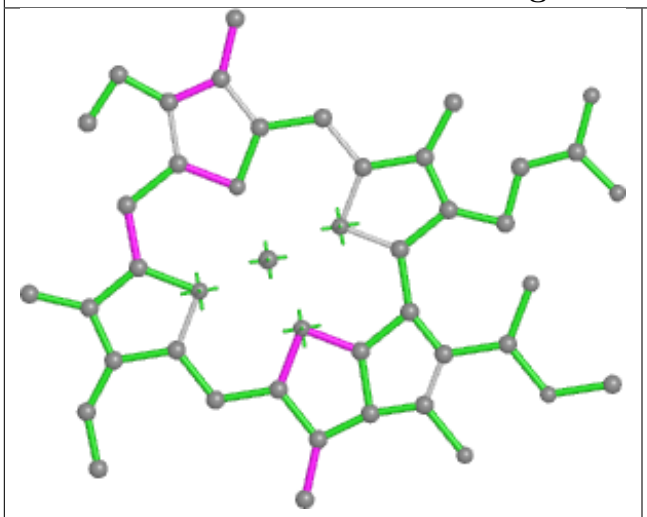


Torsions

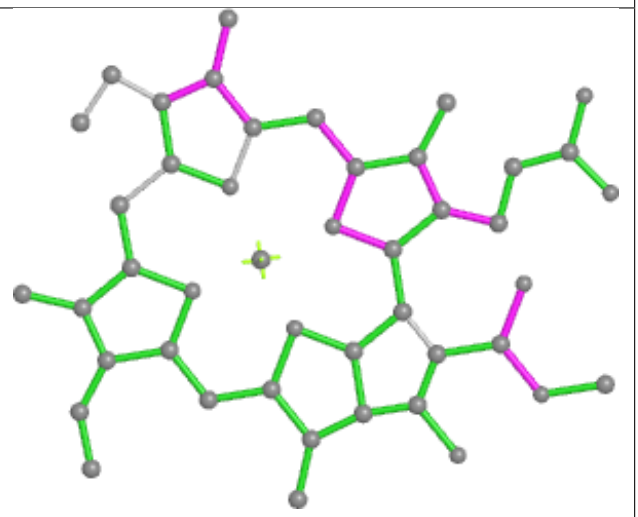
Rings

Ligand LHG B 1842	
 Bond lengths	 Bond angles
 Torsions	 Rings

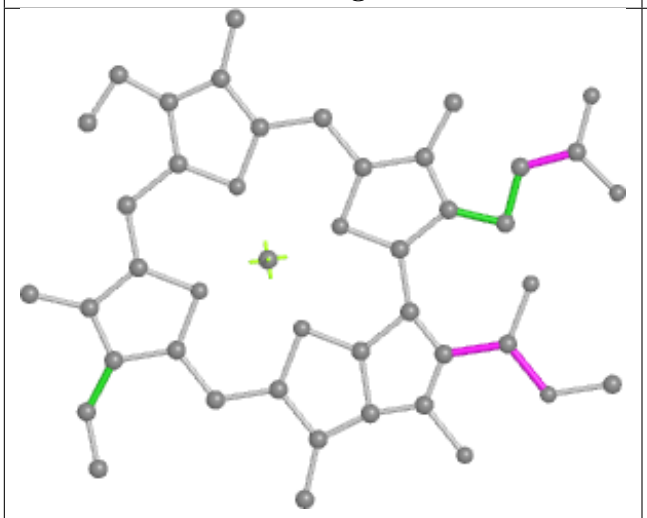
Ligand CLA 5 512



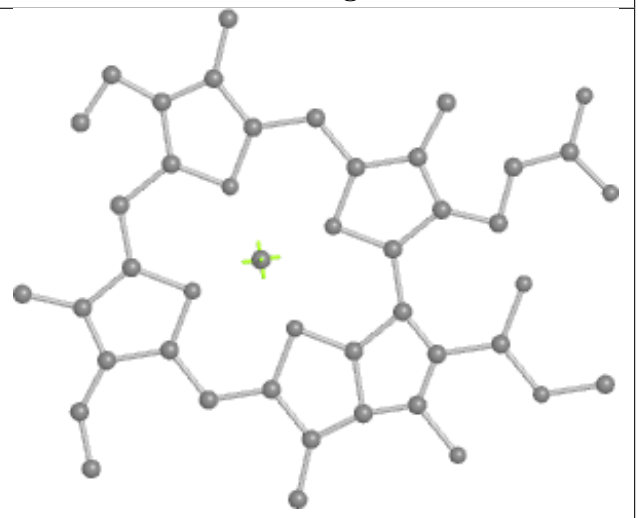
Bond lengths



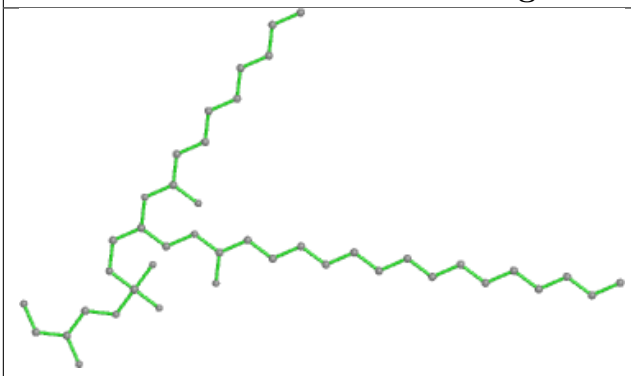
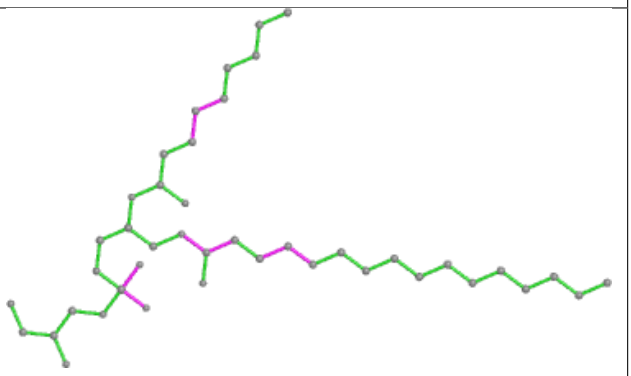
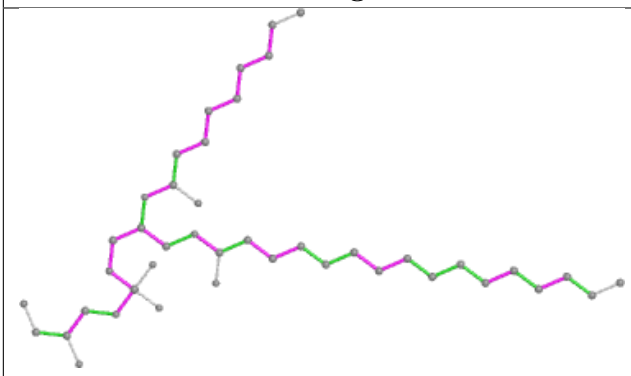
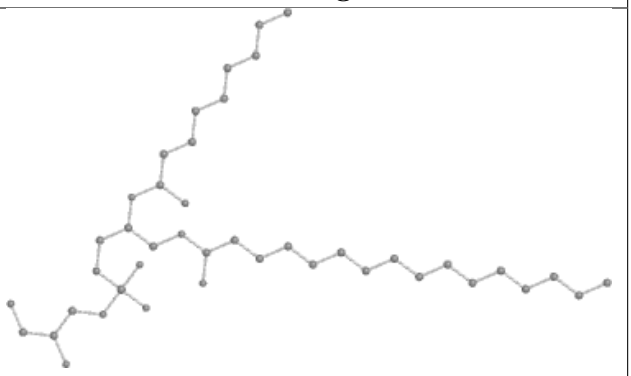
Bond angles



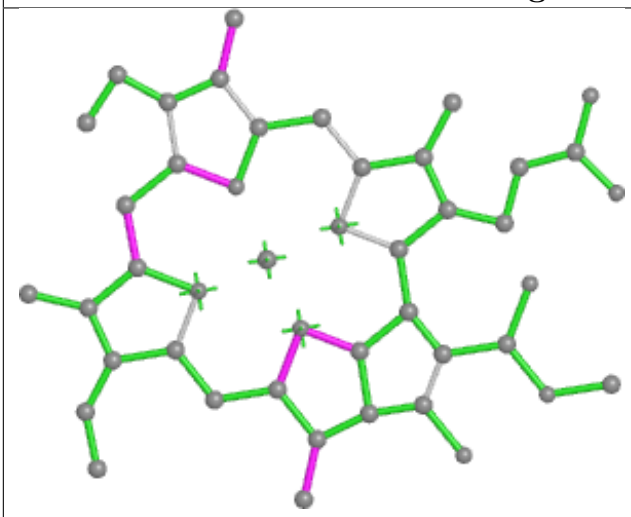
Torsions



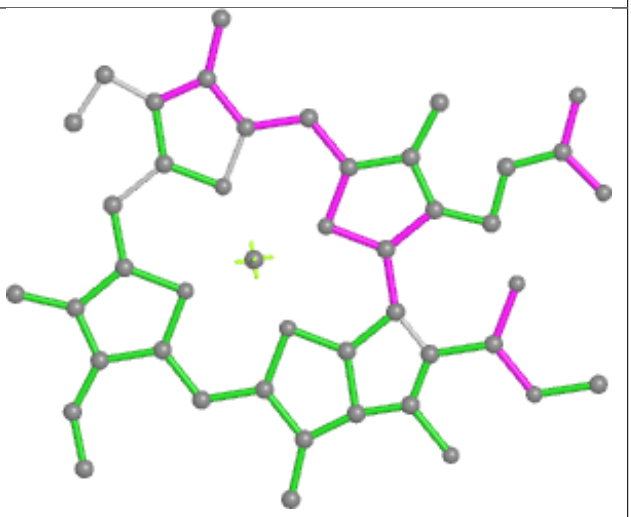
Rings

Ligand LHG e 5009	
 Bond lengths	 Bond angles
 Torsions	 Rings

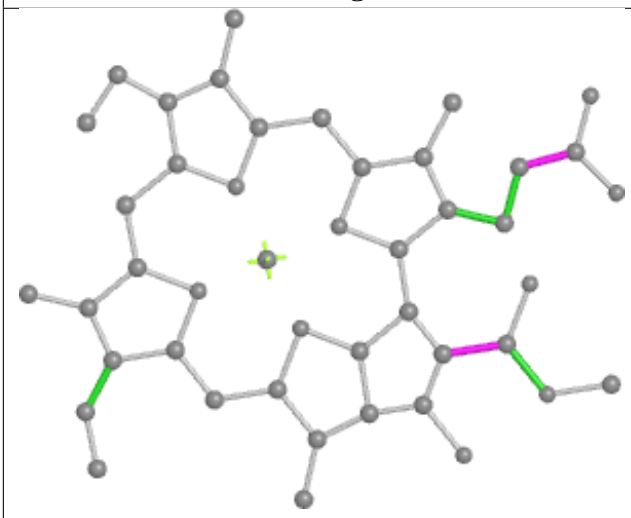
Ligand CLA 3 507



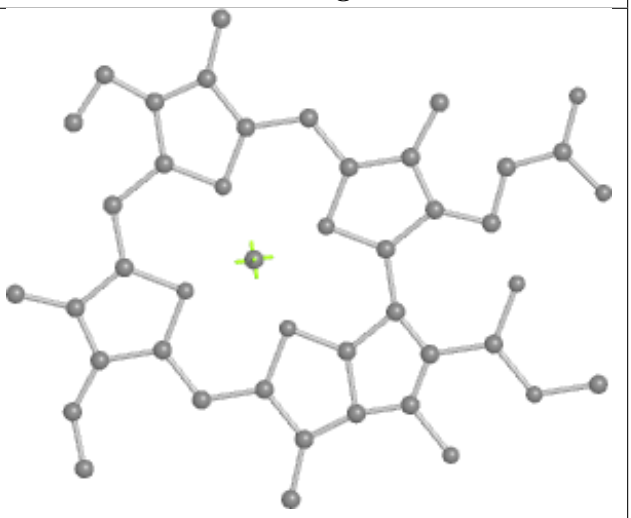
Bond lengths



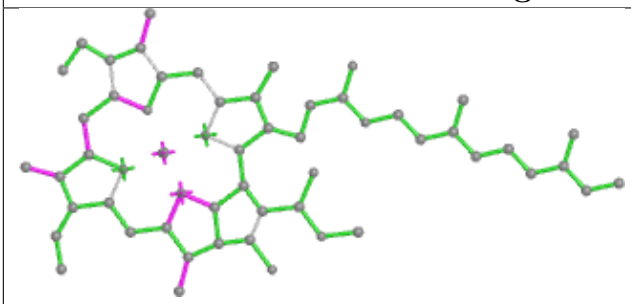
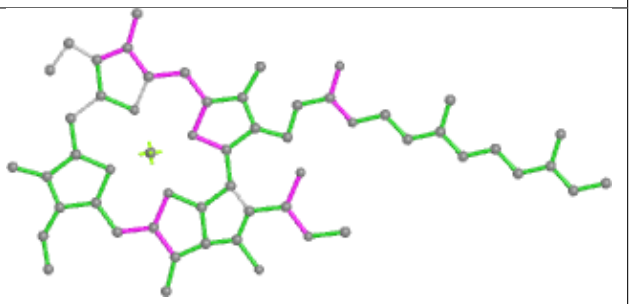
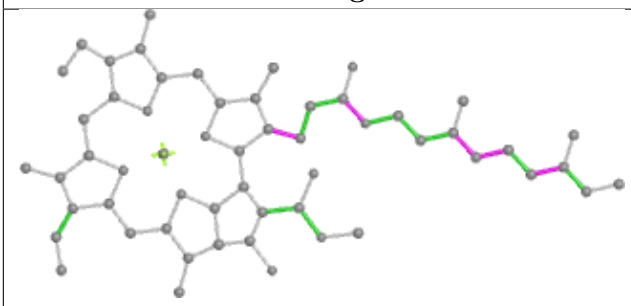
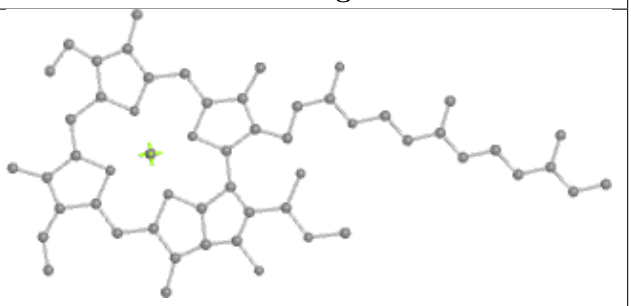
Bond angles



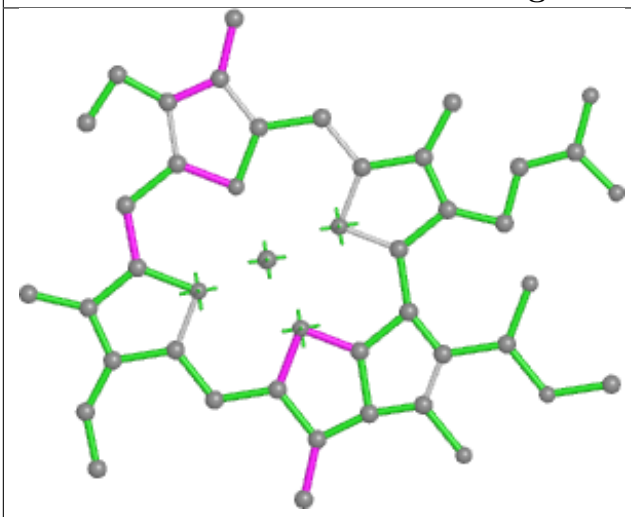
Torsions



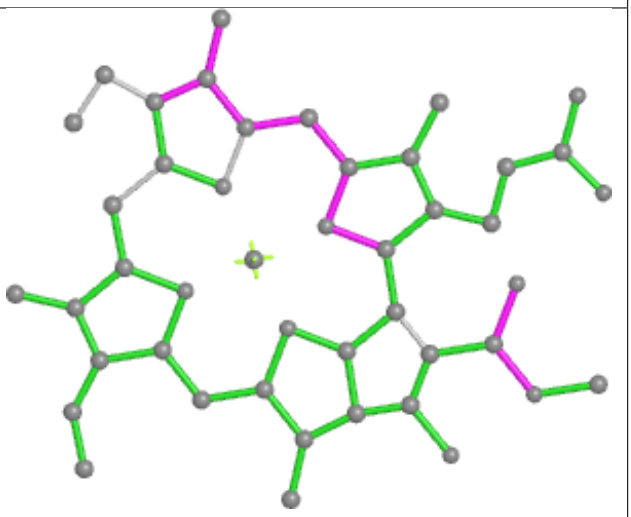
Rings

Ligand CLA G 1130	
 Bond lengths	 Bond angles
 Torsions	 Rings

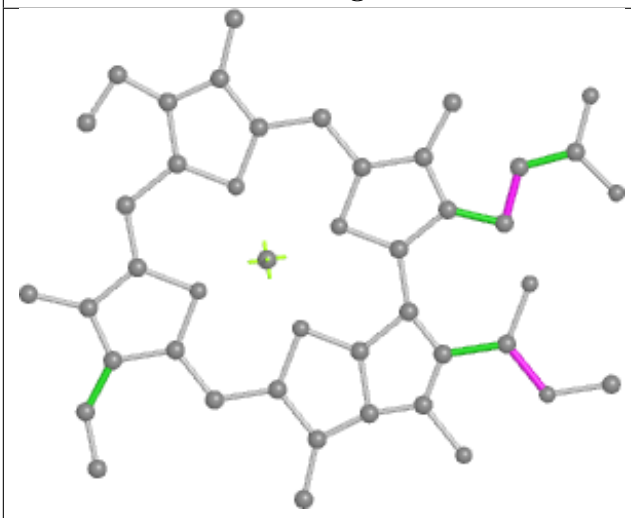
Ligand CLA 6 513



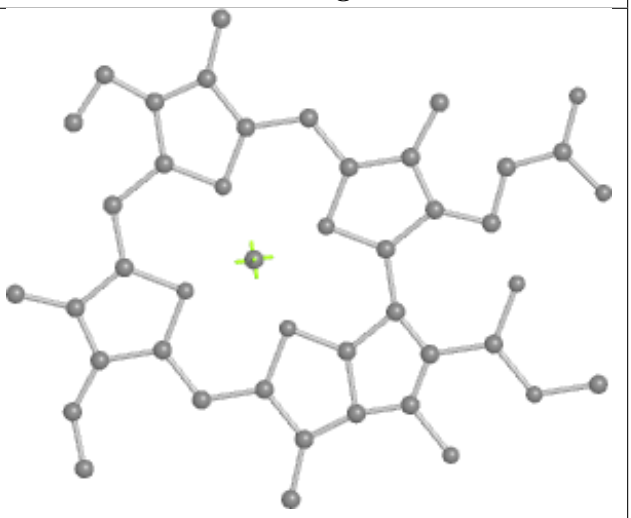
Bond lengths



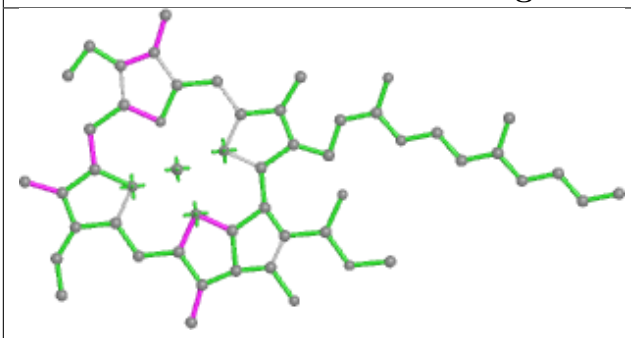
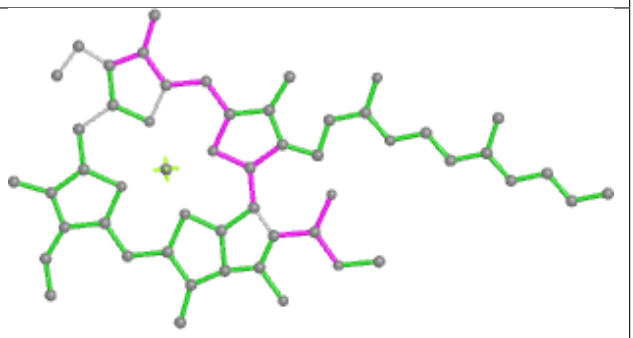
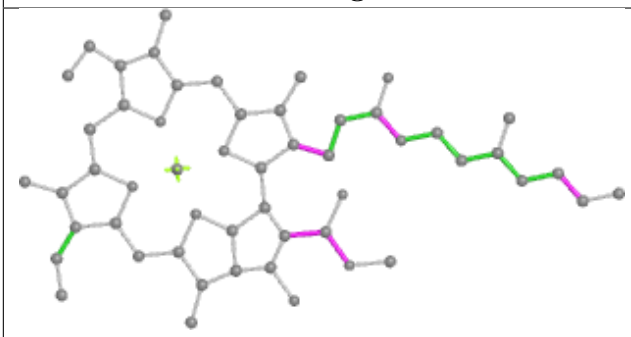
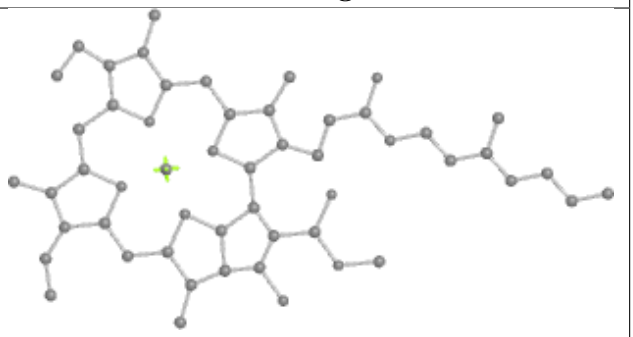
Bond angles

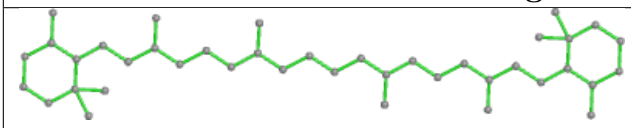
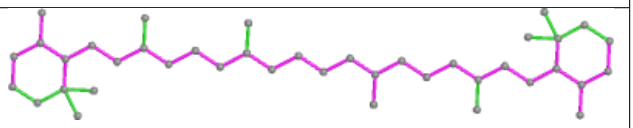
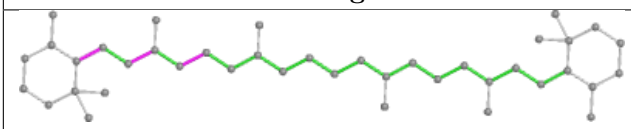
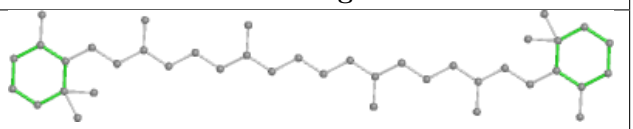


Torsions



Rings

Ligand CLA B 1209	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR u 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

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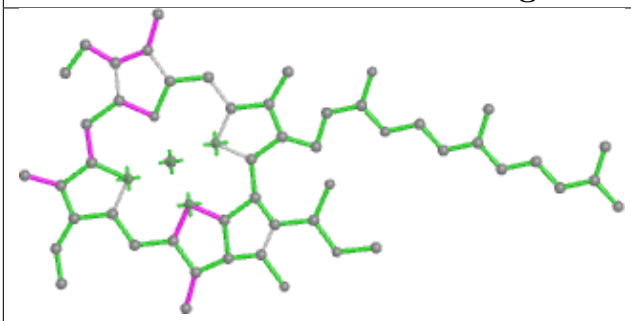
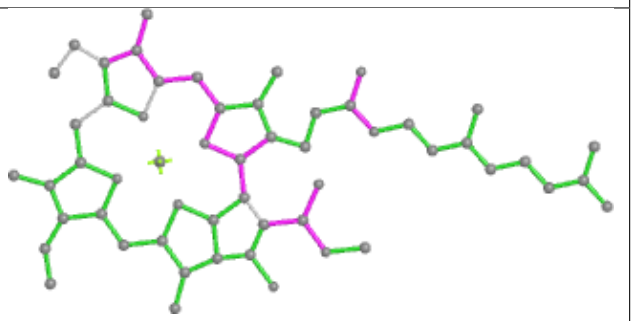
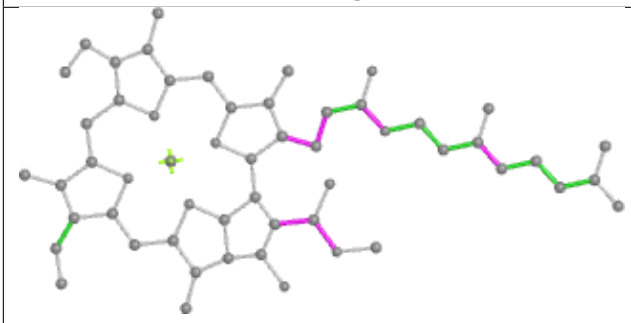
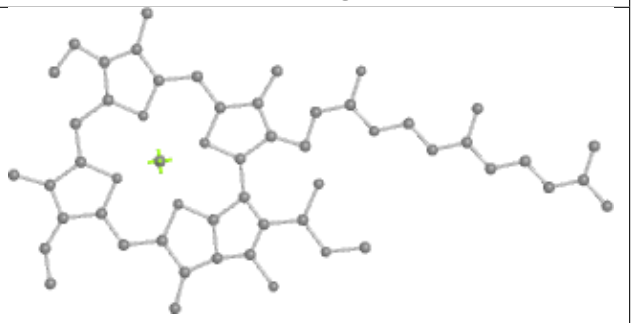
 Bond lengths	 Bond angles
 Torsions	 Rings

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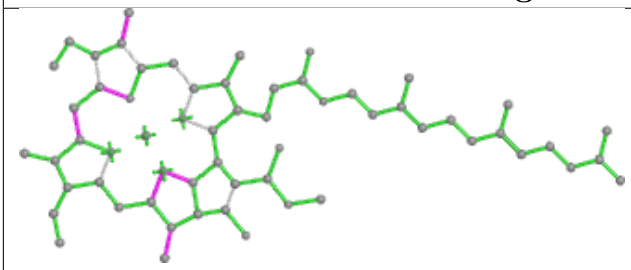
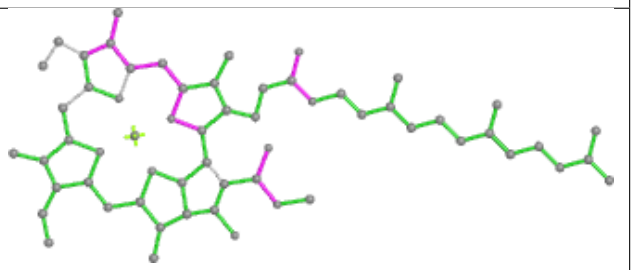
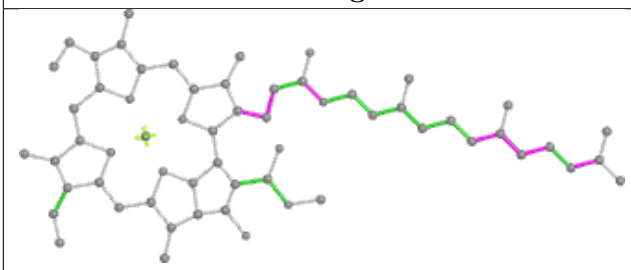
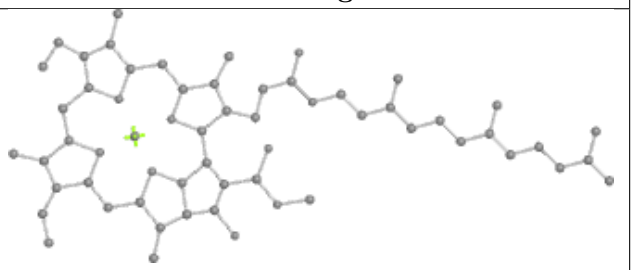
 Bond lengths	 Bond angles
 Torsions	 Rings

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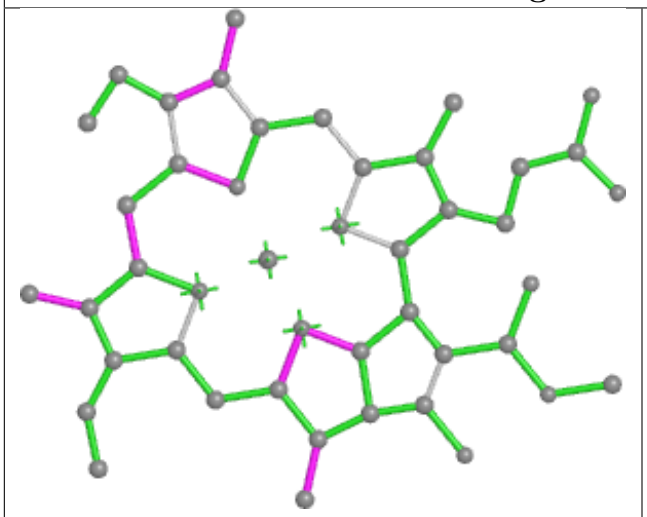

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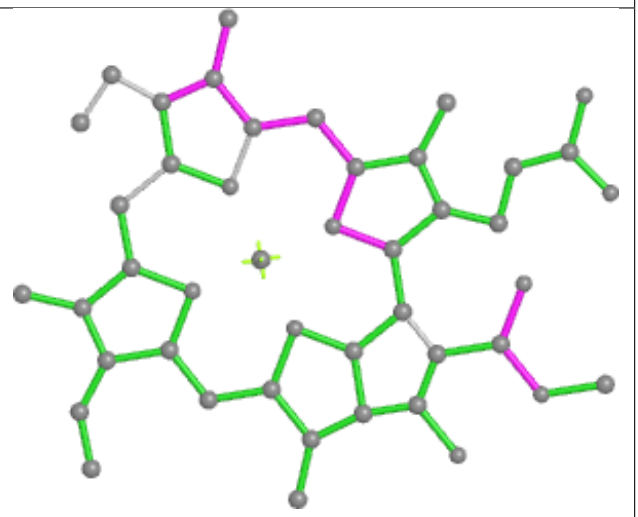
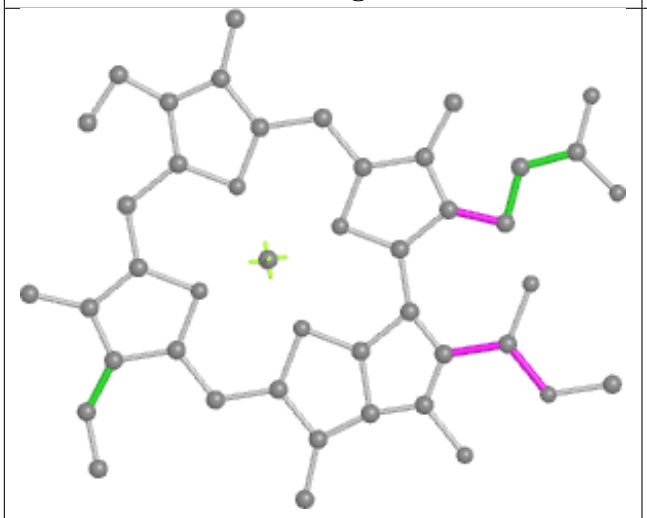


Bond angles



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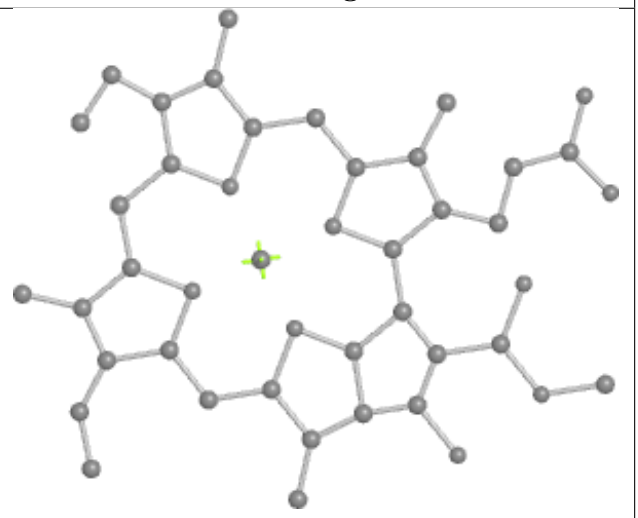

Rings

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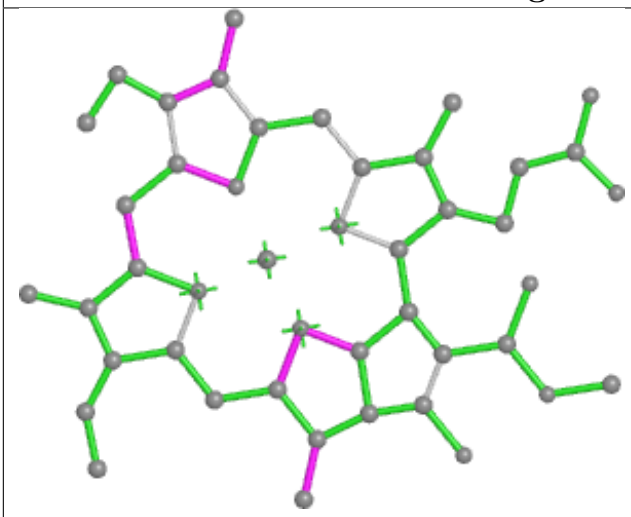

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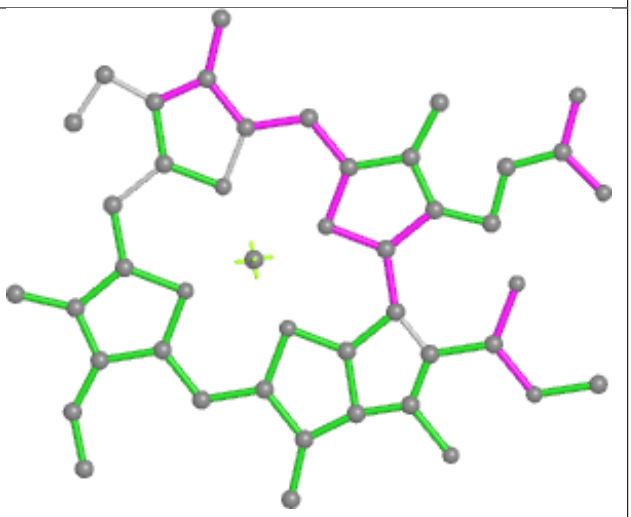

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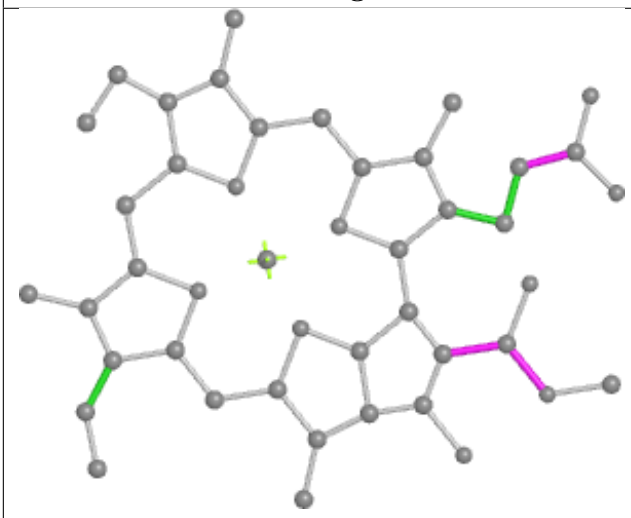

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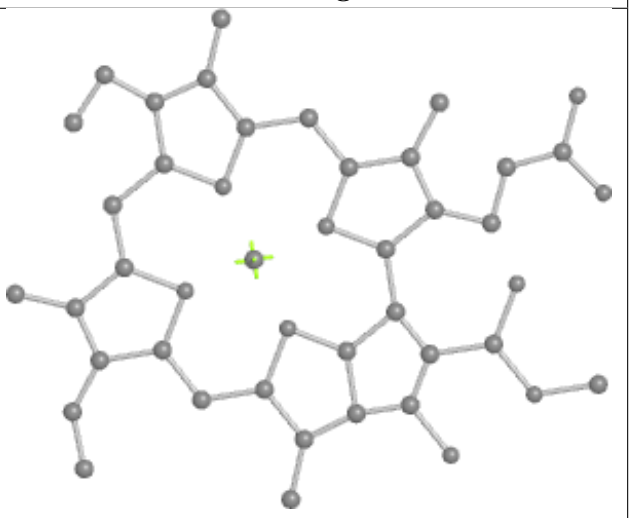
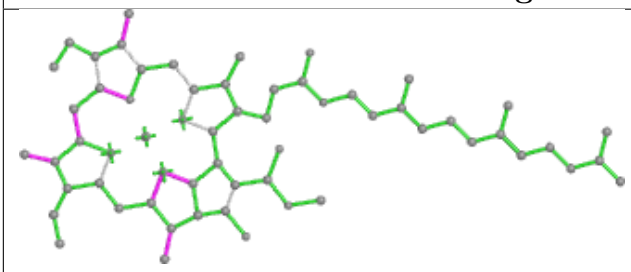


Rings

Ligand CLA B 1224



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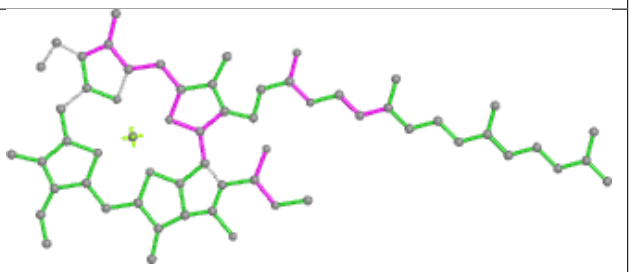

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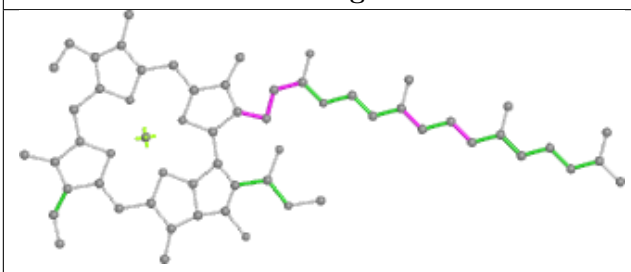

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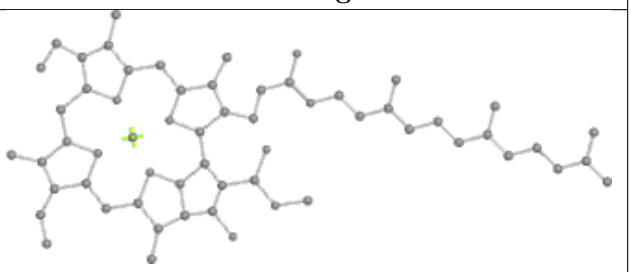
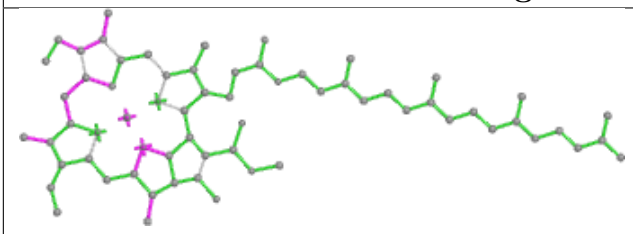


Rings

Ligand CLA A 1119



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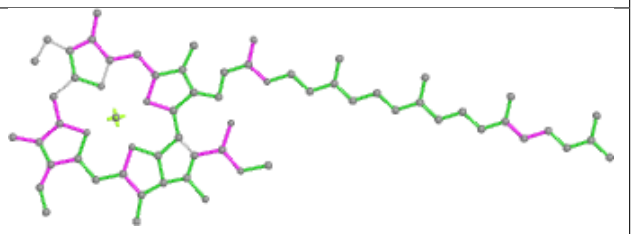

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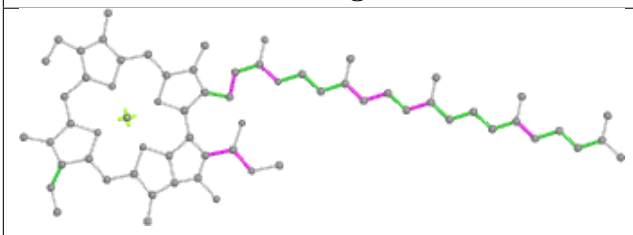

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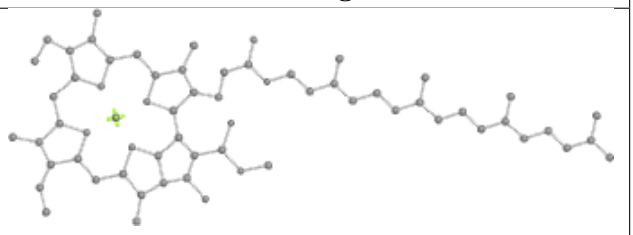

Rings

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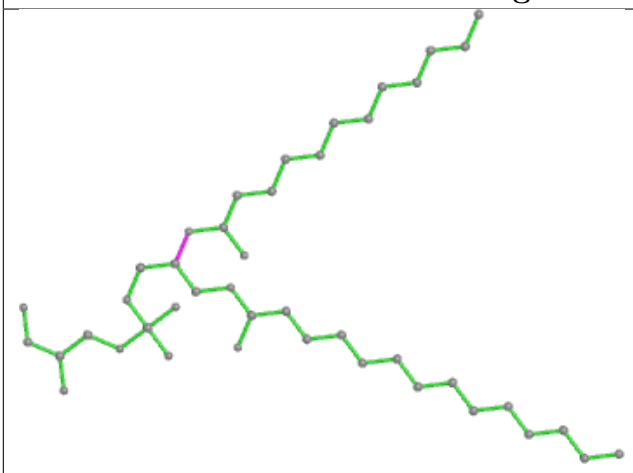

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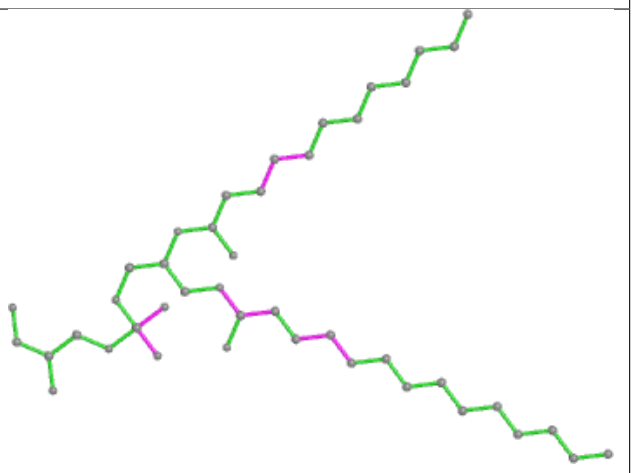

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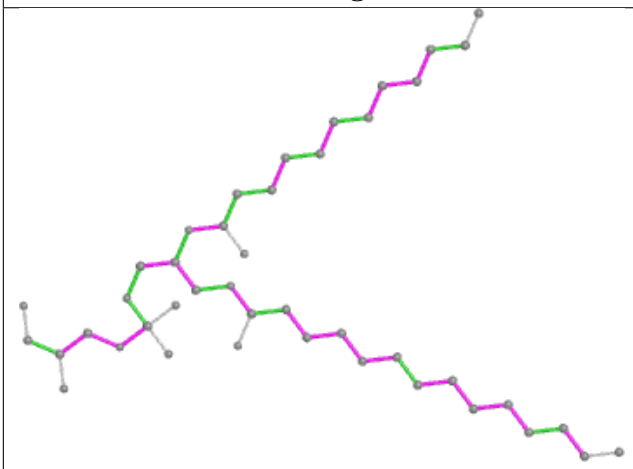

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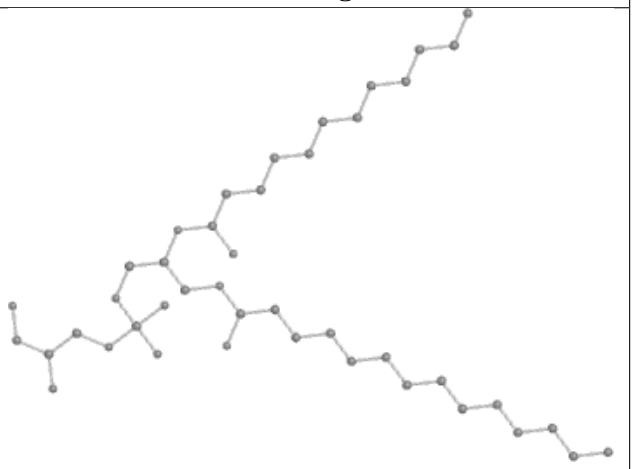
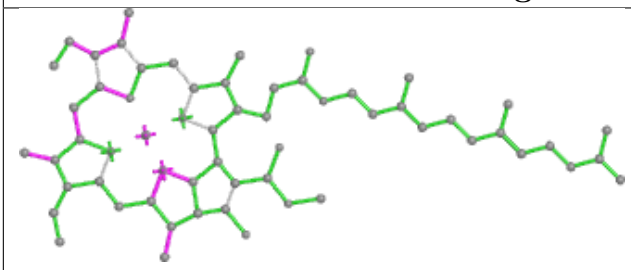


Rings

Ligand CLA H 1216



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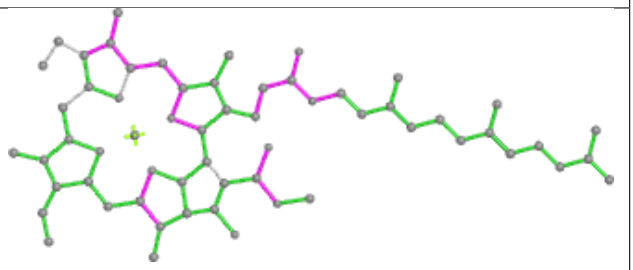

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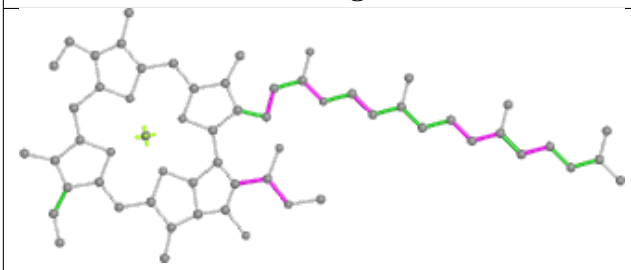

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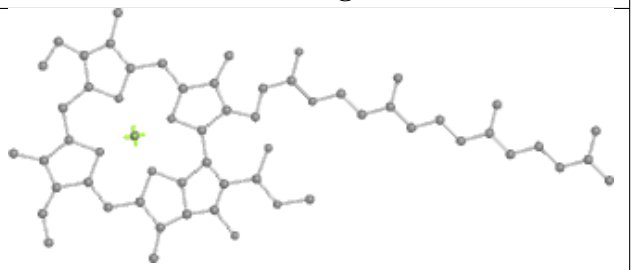
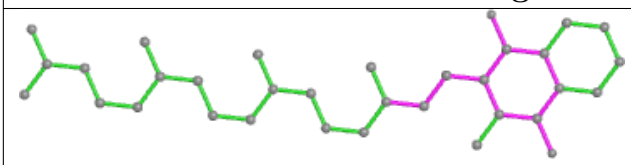


Rings

Ligand PQN G 2001



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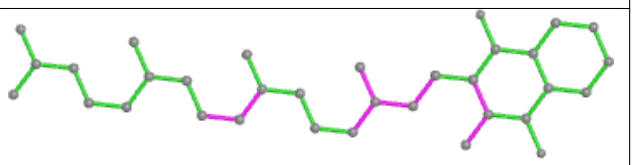

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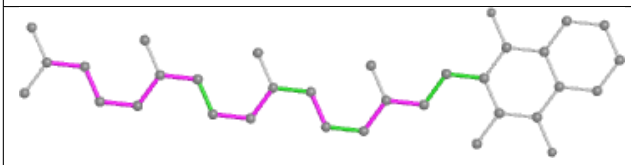

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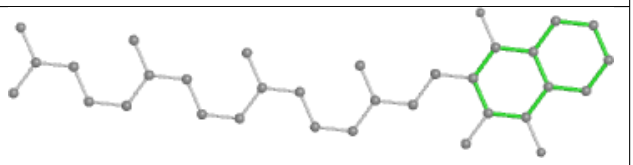
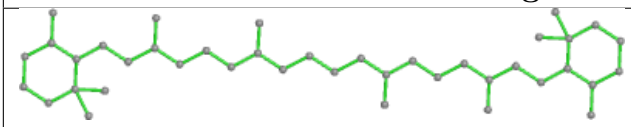


Rings

Ligand BCR Y 524



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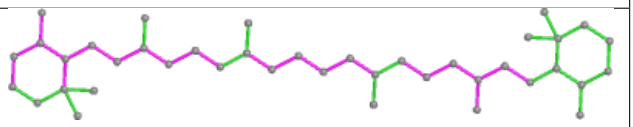

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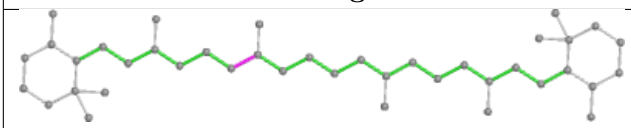
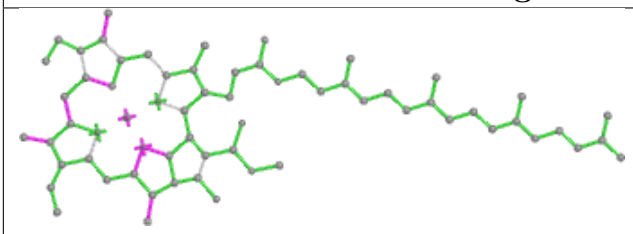


Torsions

Rings

Ligand CLA G 1126



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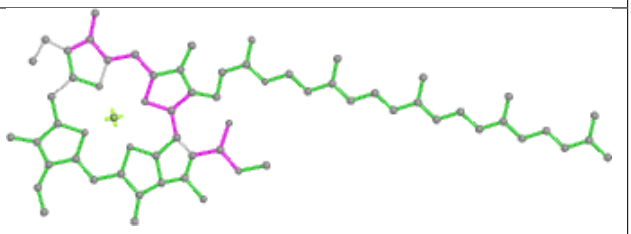

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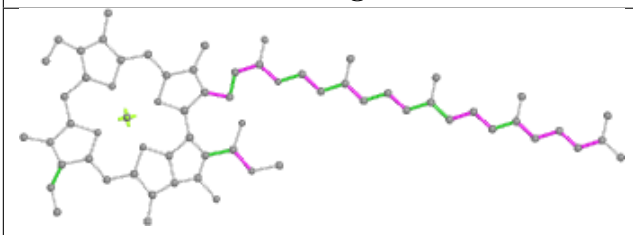

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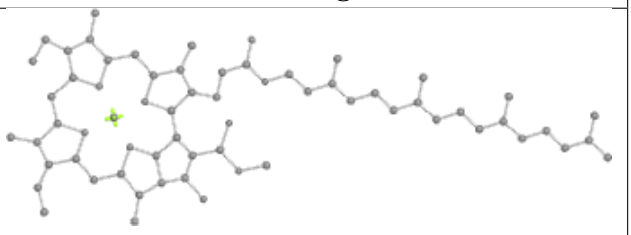
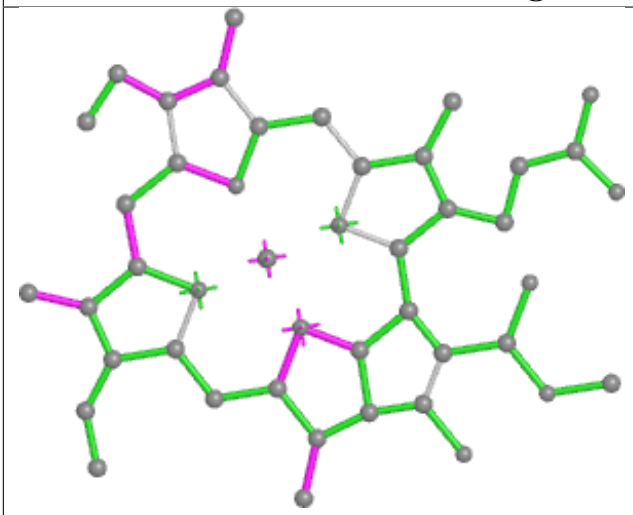


Rings

Ligand CLA b 508



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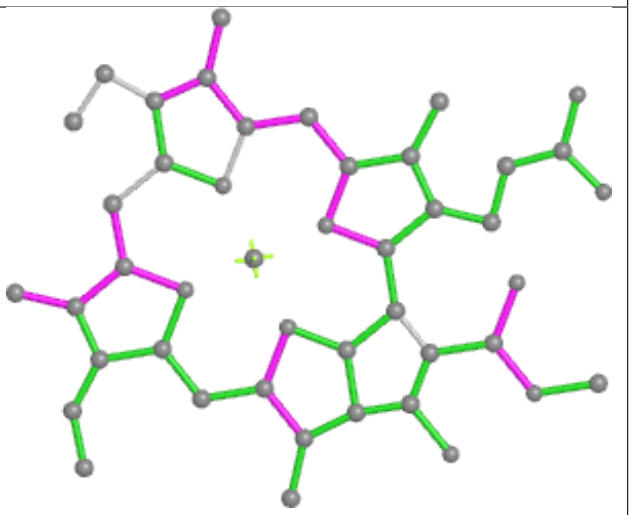
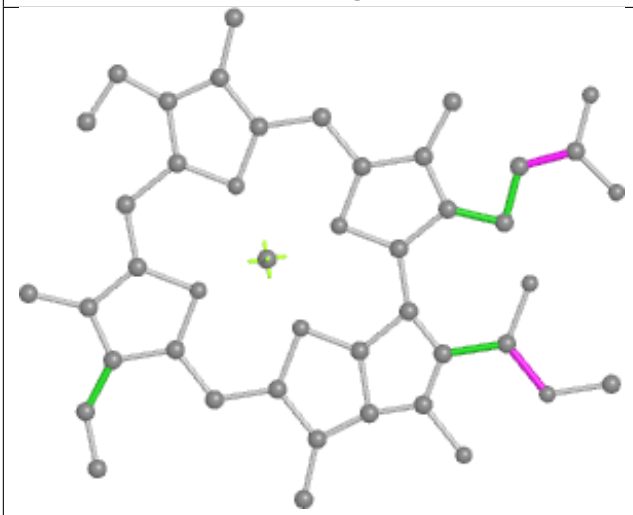


Bond angles



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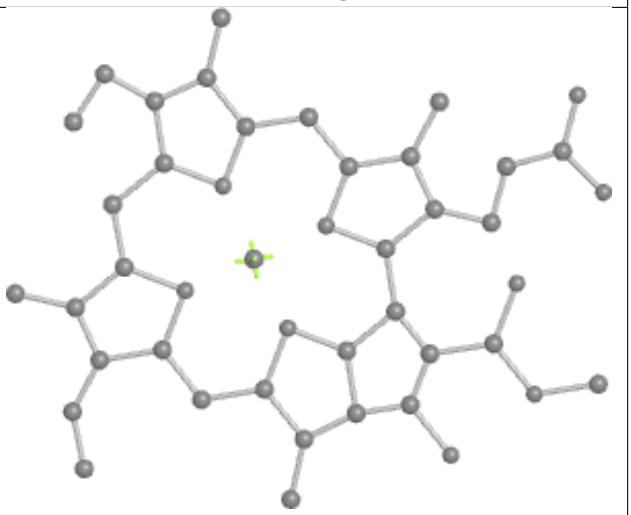
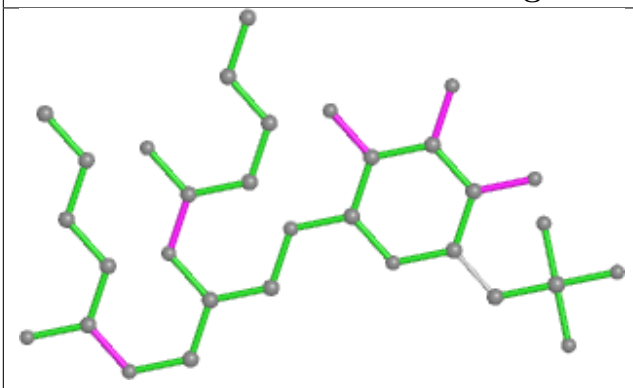
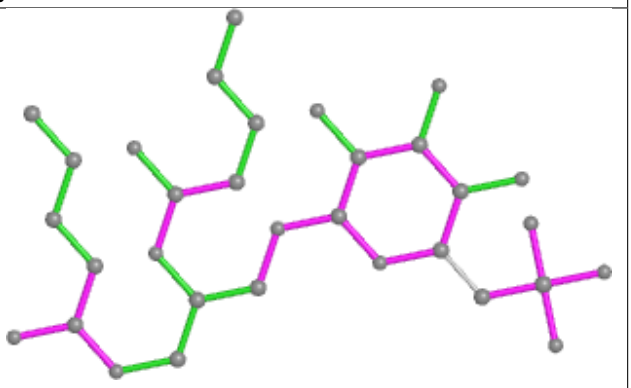


Rings

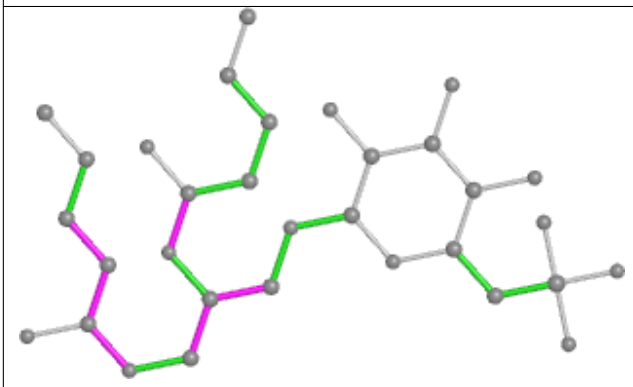
Ligand SQD Y 822



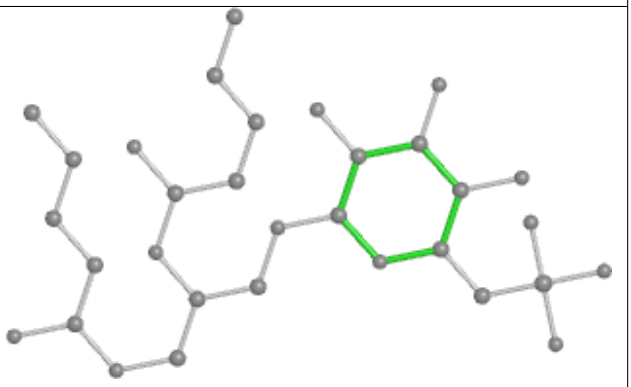
Bond lengths



Bond angles

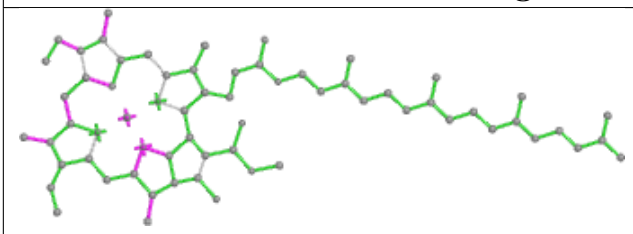


Torsions



Rings

Ligand CLA H 1021



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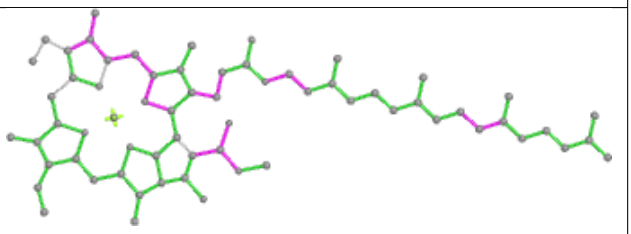

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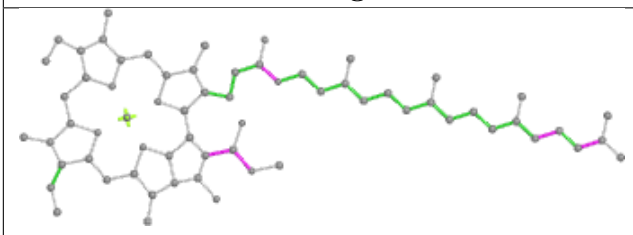
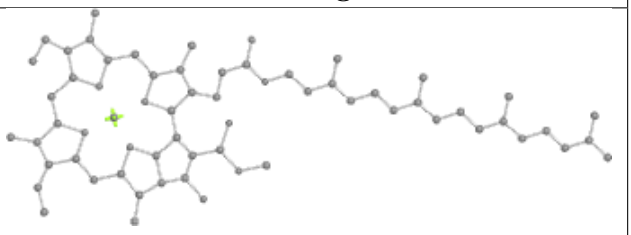
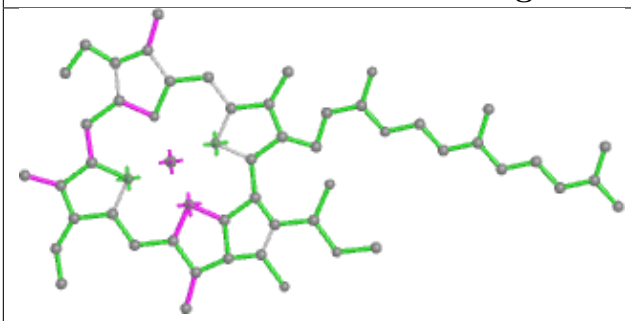


Torsions



Rings

Ligand CLA B 1232



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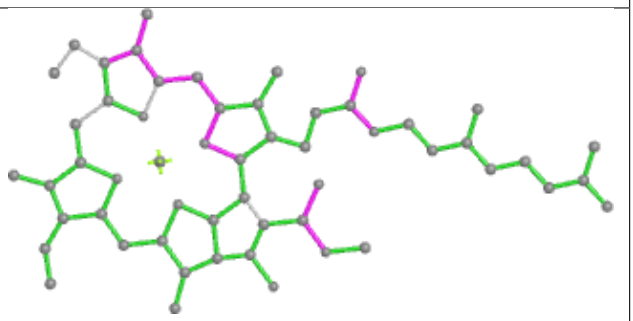
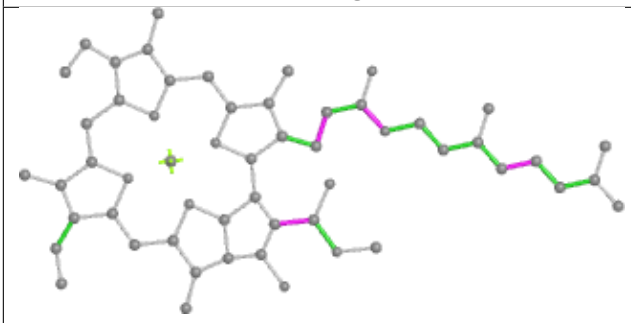
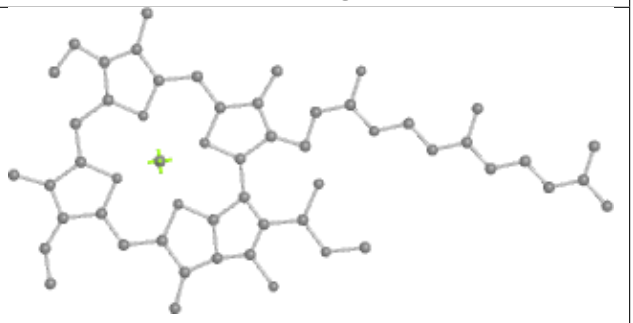


Bond angles

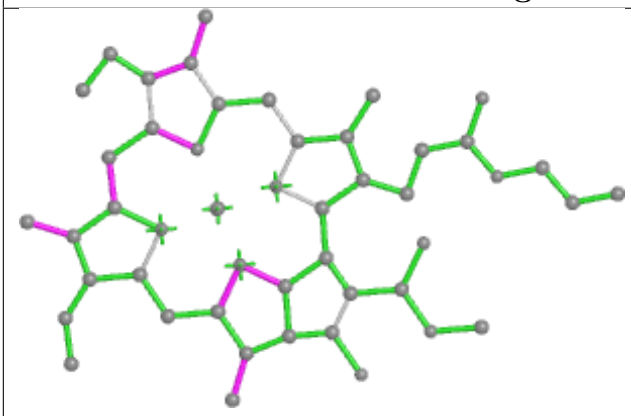


Torsions

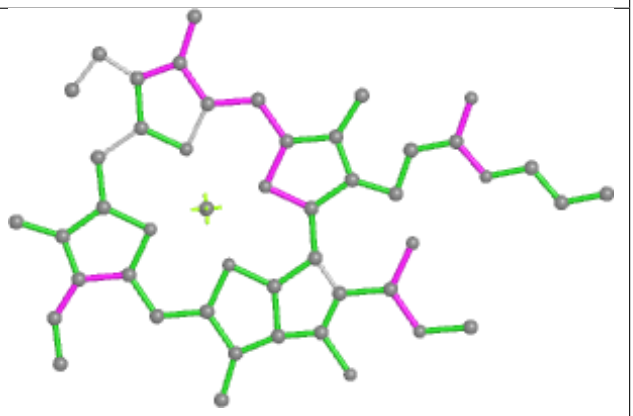


Rings

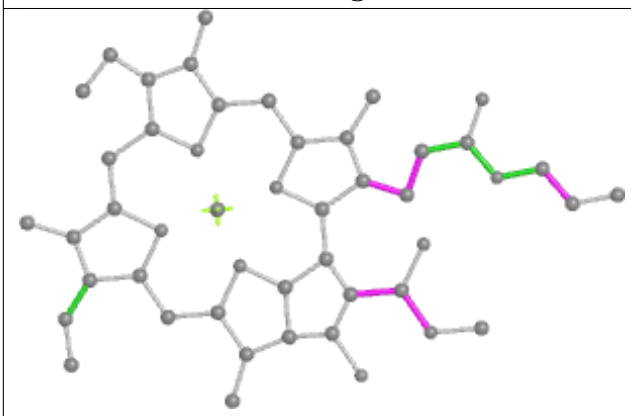
Ligand CLA K 1103



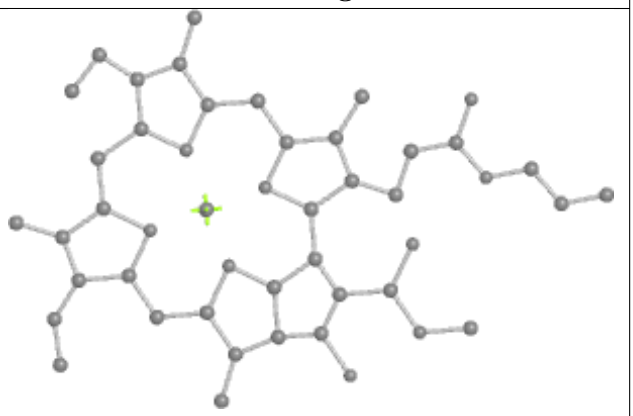
Bond lengths



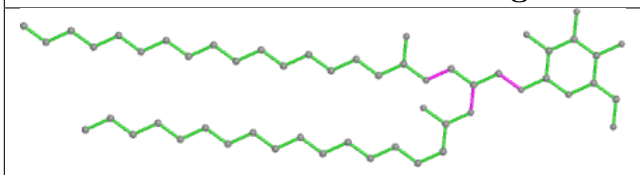
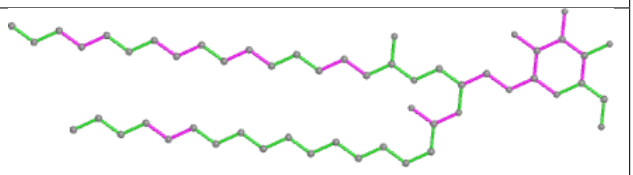
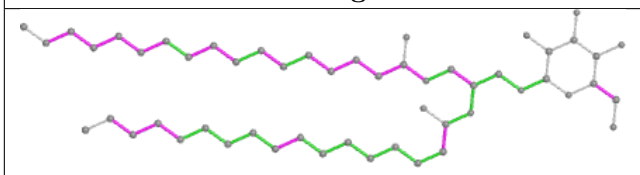
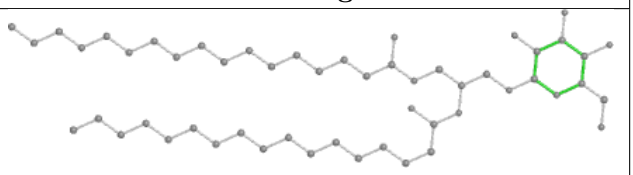
Bond angles



Torsions



Rings

Ligand LMG H 5002	
 Bond lengths	 Bond angles
 Torsions	 Rings

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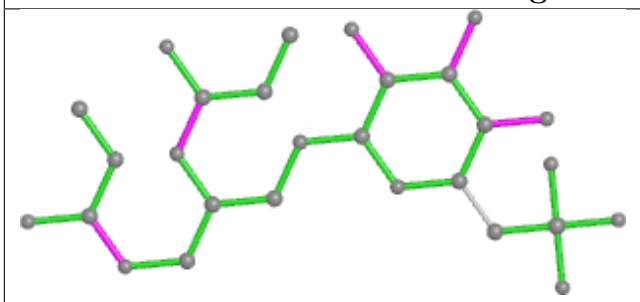
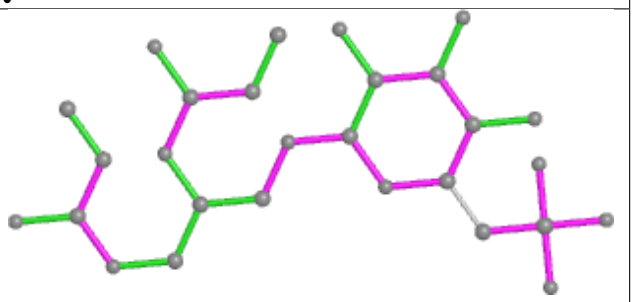
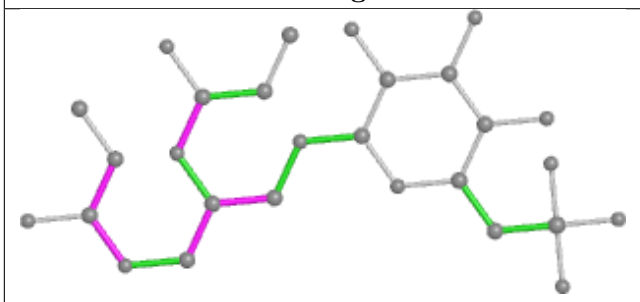
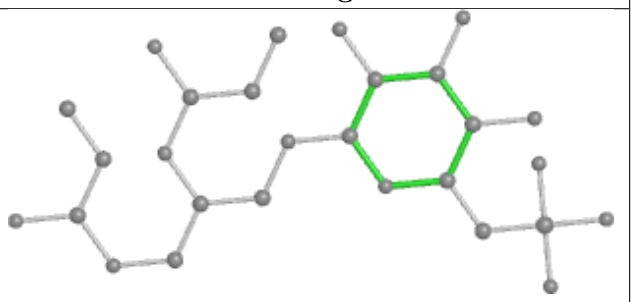
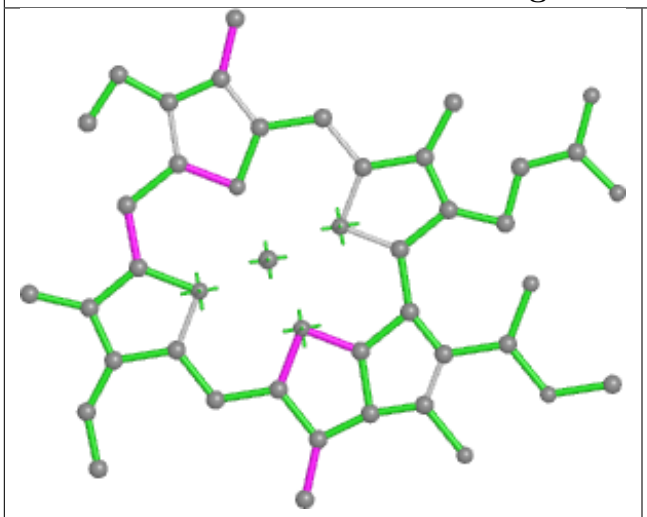
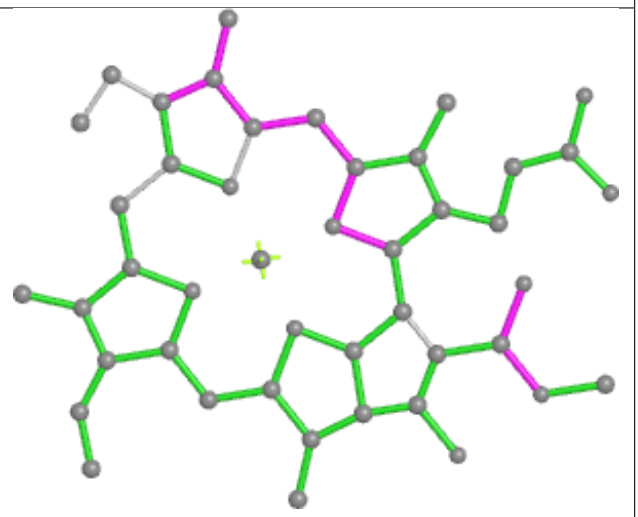
 Bond lengths	 Bond angles
 Torsions	 Rings

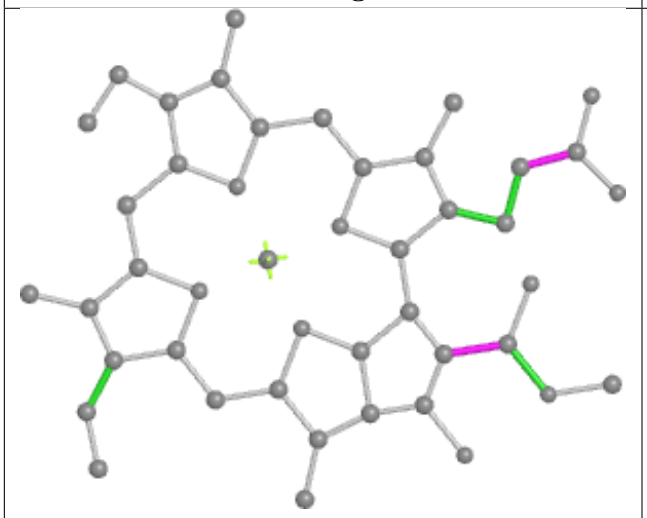
Ligand CLA 4 512



Bond lengths



Bond angles



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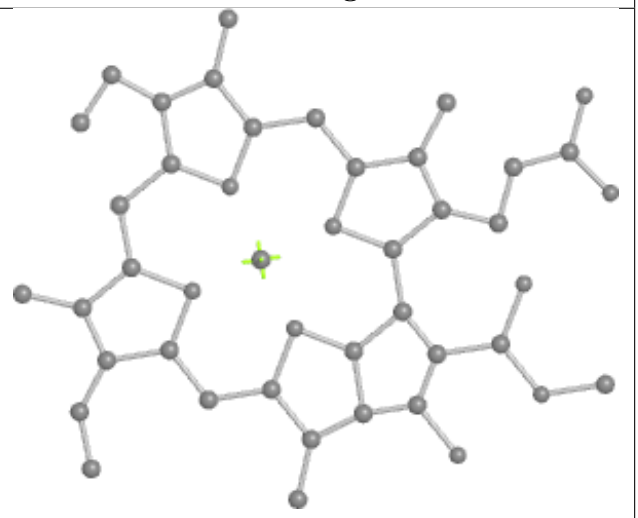
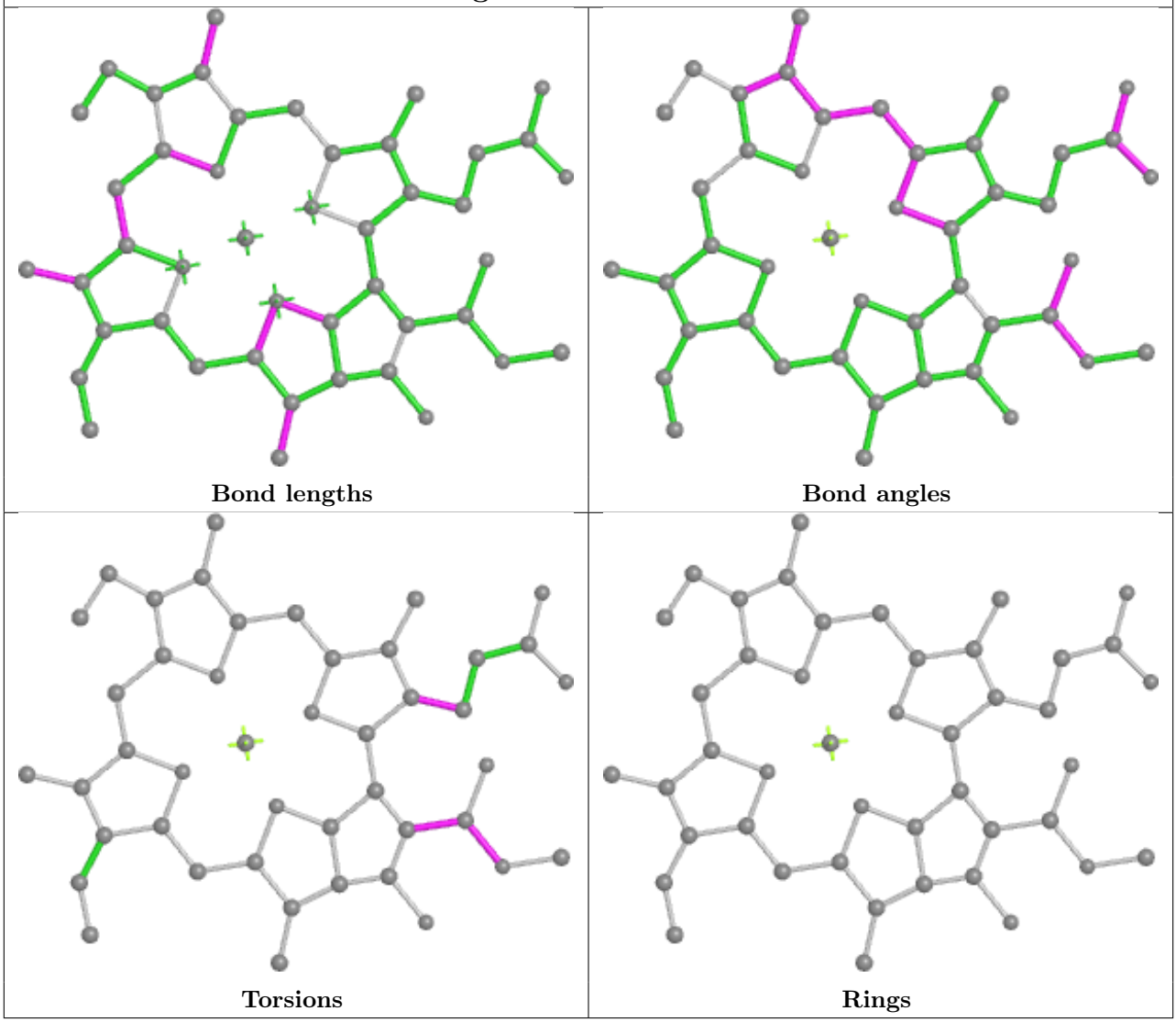
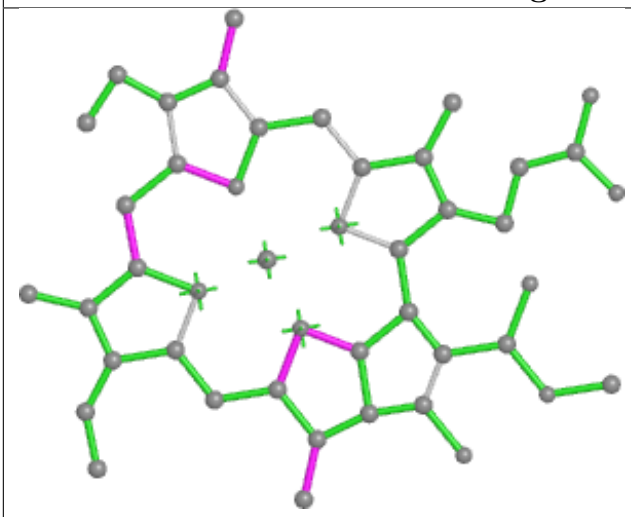


Rings

Ligand CLA A 1113



Ligand CLA s 507



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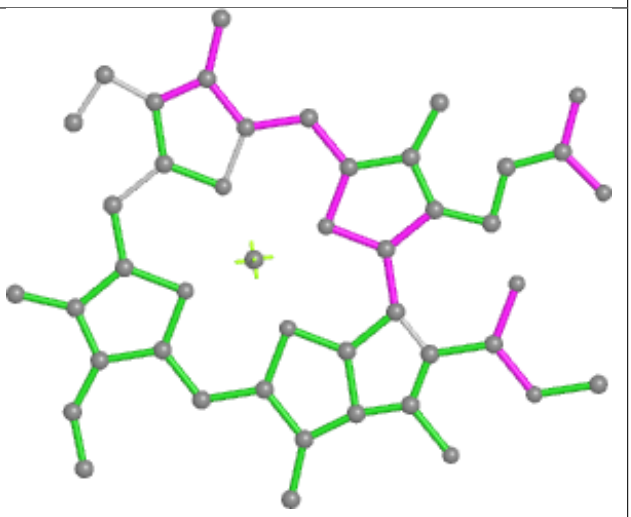
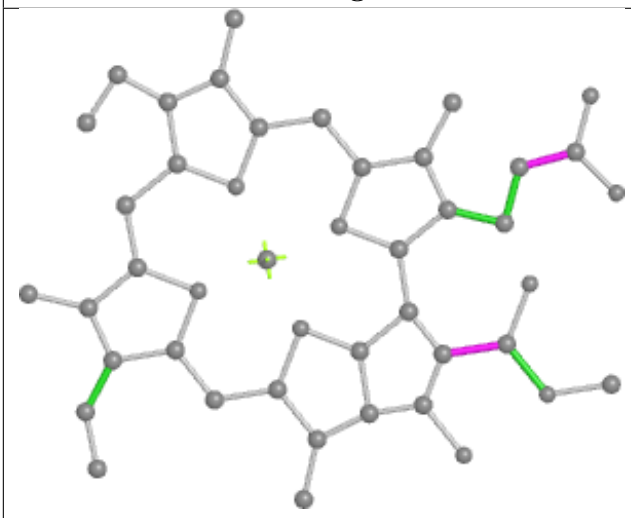
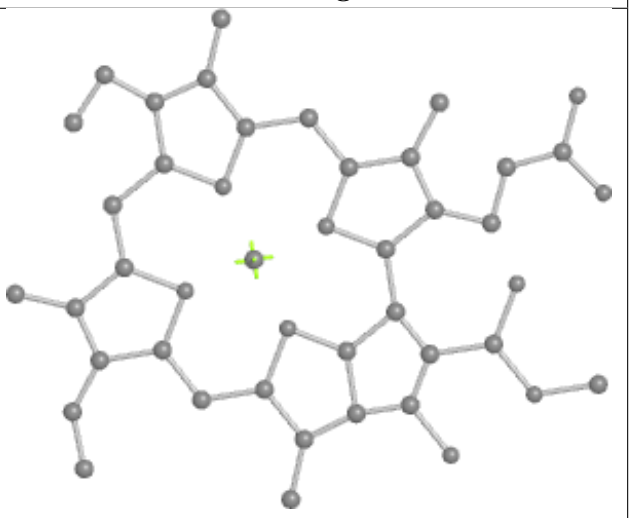


Bond angles

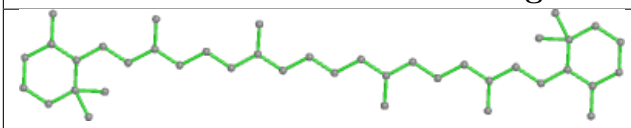


Torsions

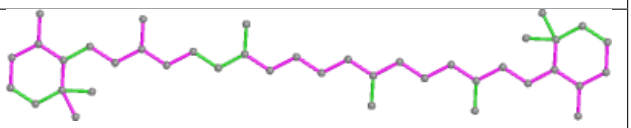


Rings

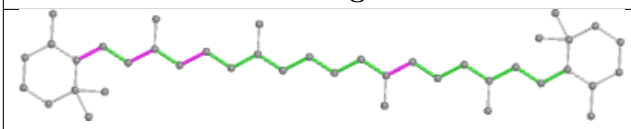
Ligand BCR u 521



Bond lengths



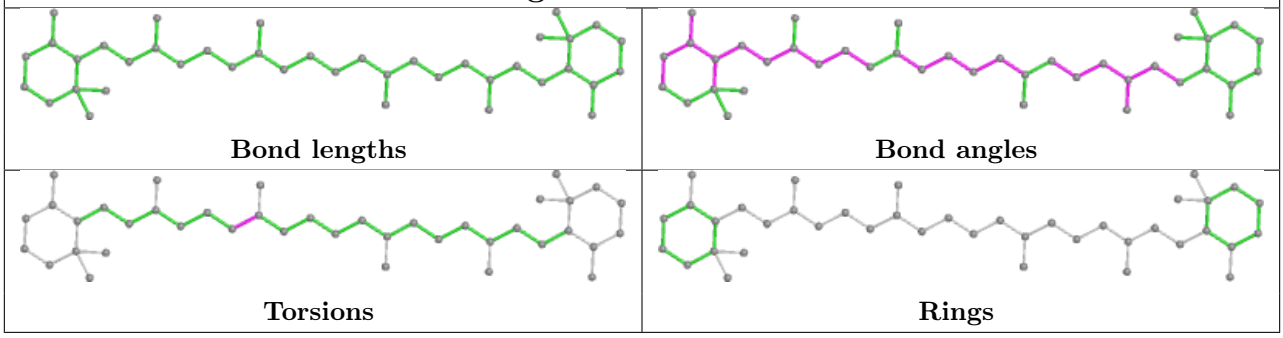
Bond angles



Torsions

Rings

Ligand BCR 1 524



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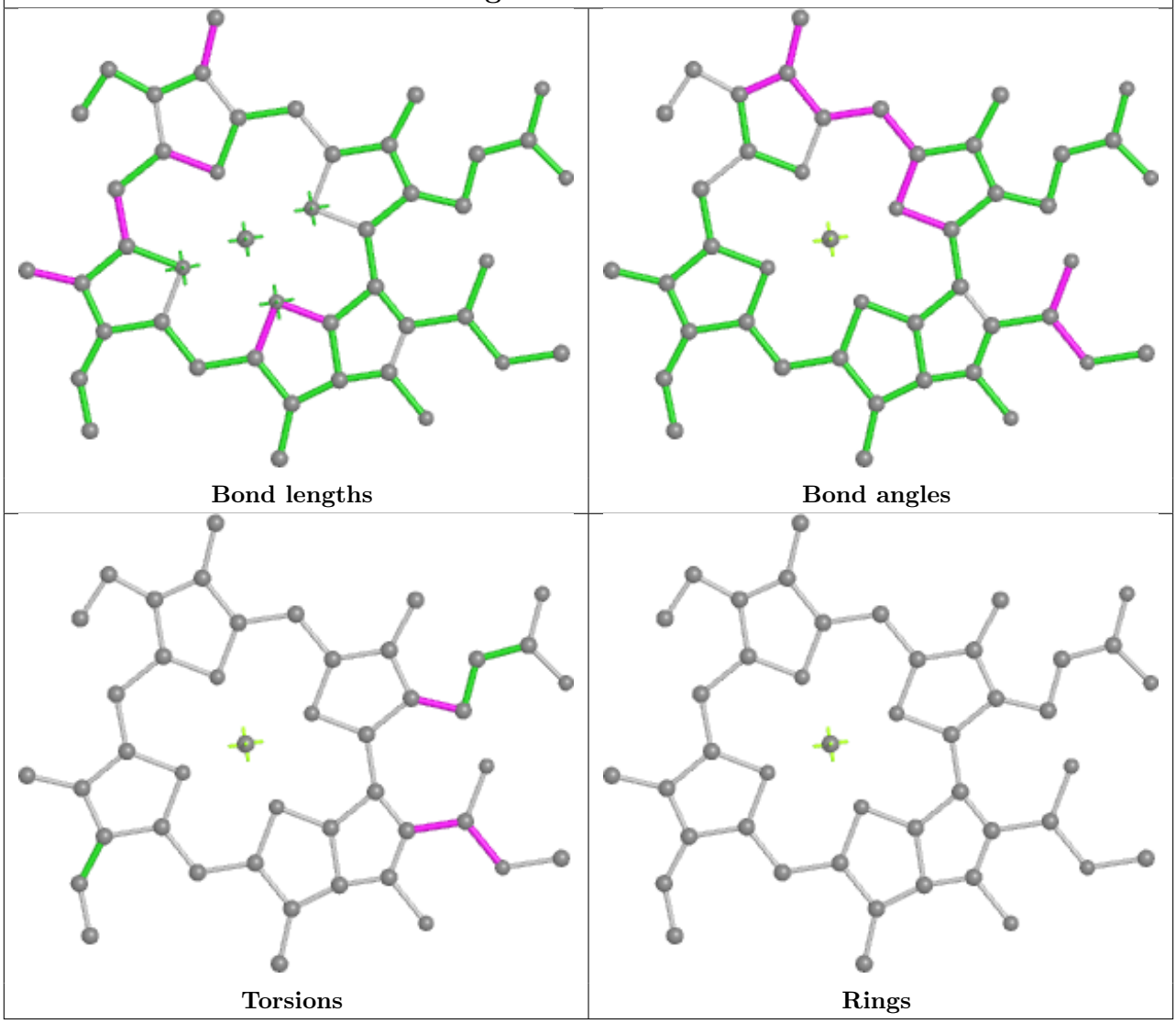
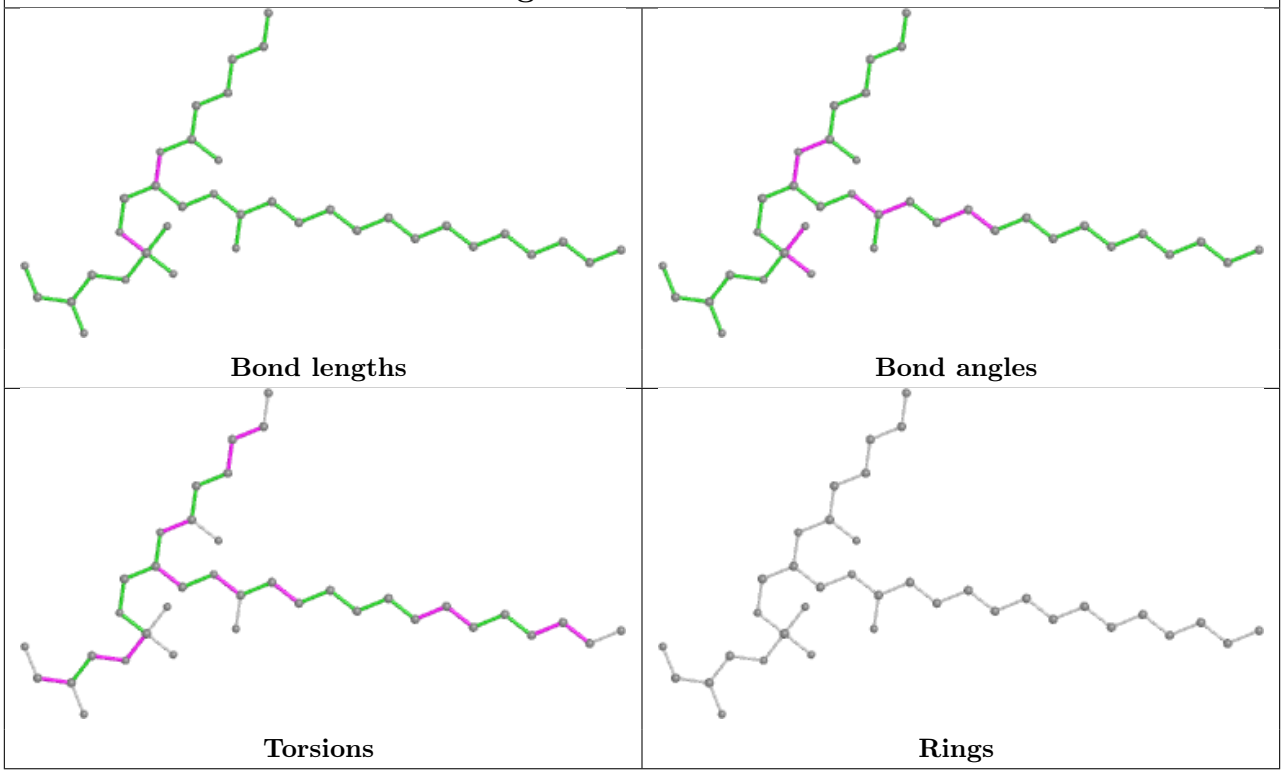


Ligand LHG L 5218



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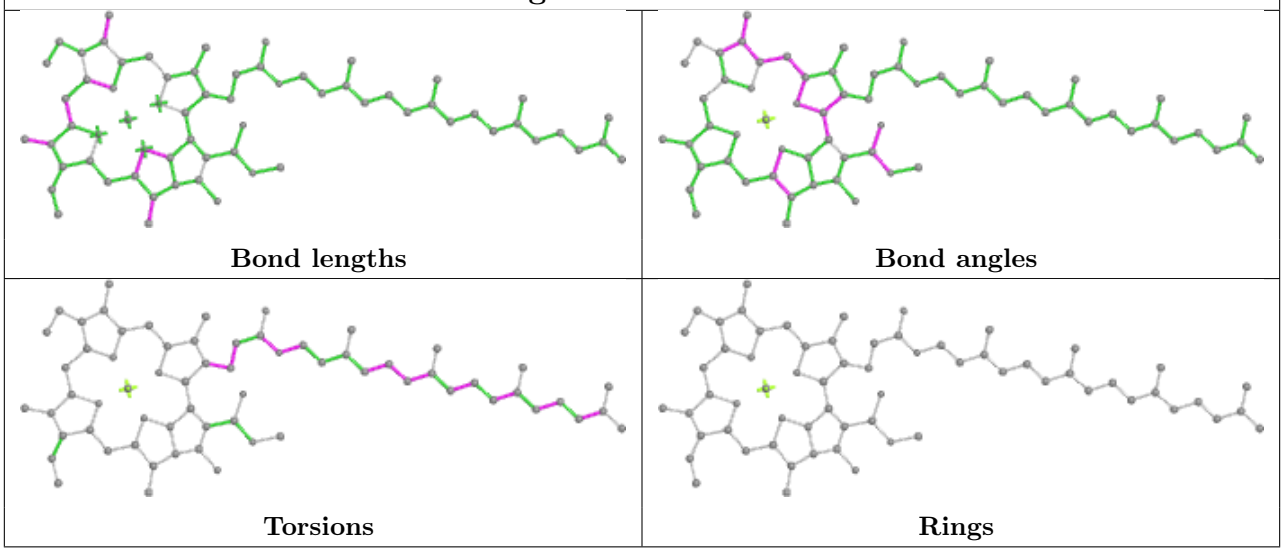

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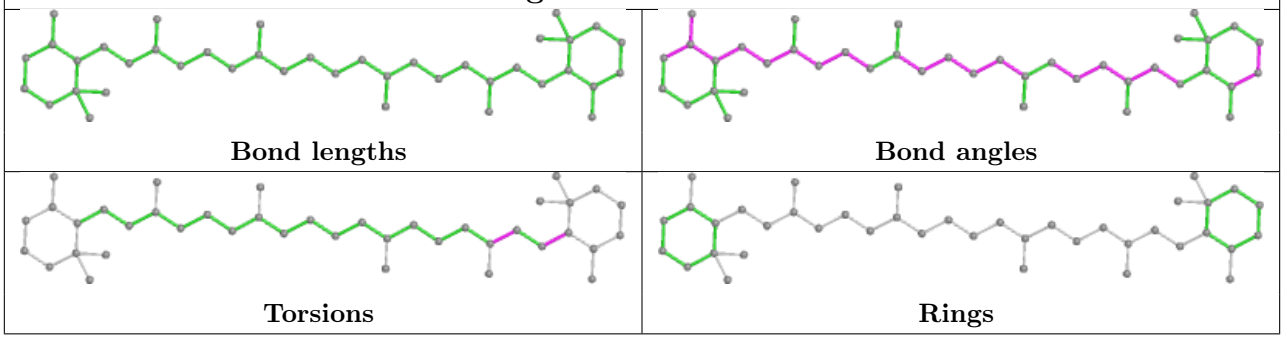

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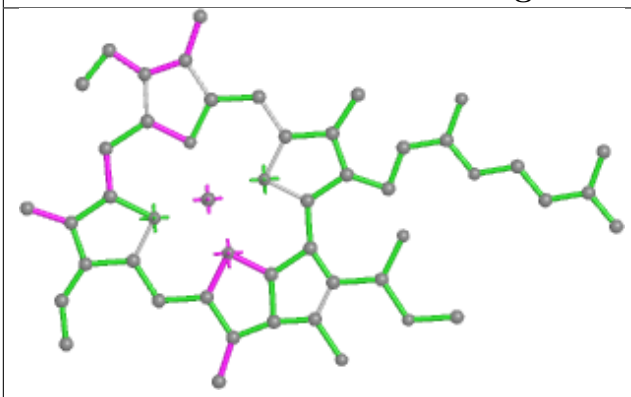
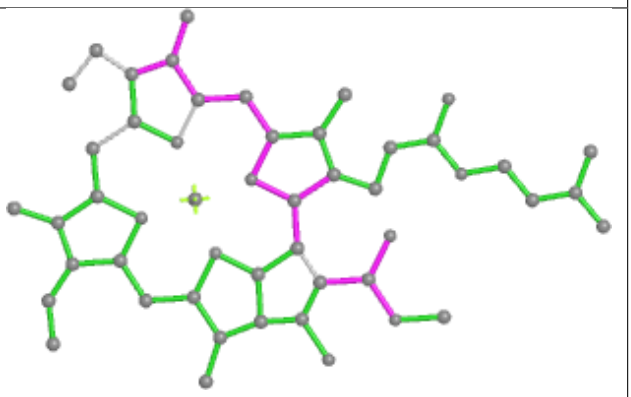
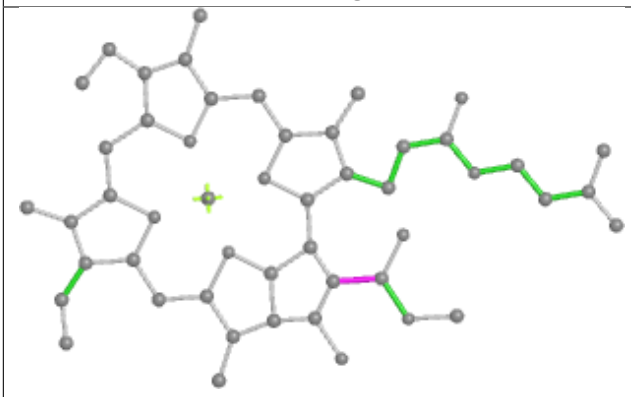
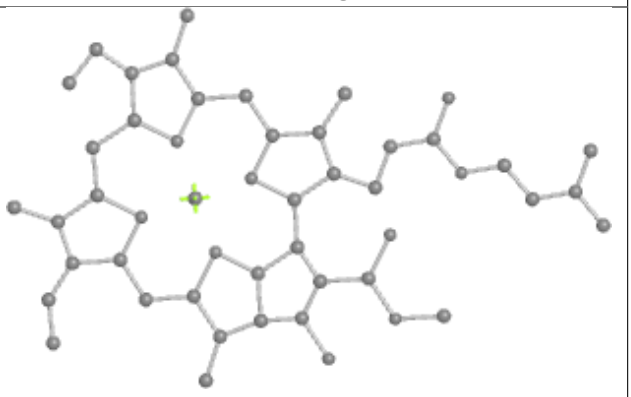
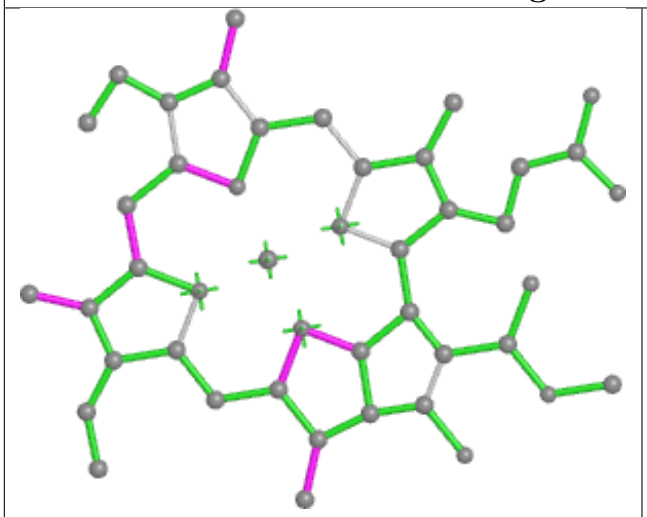
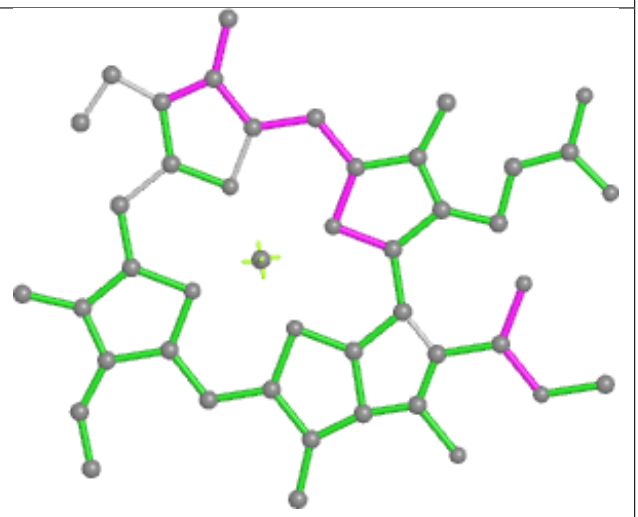
 Bond lengths	 Bond angles
 Torsions	 Rings

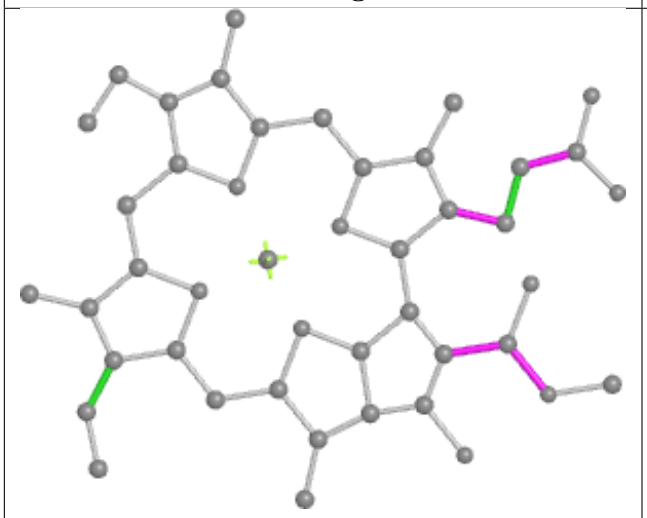
Ligand CLA 3 506



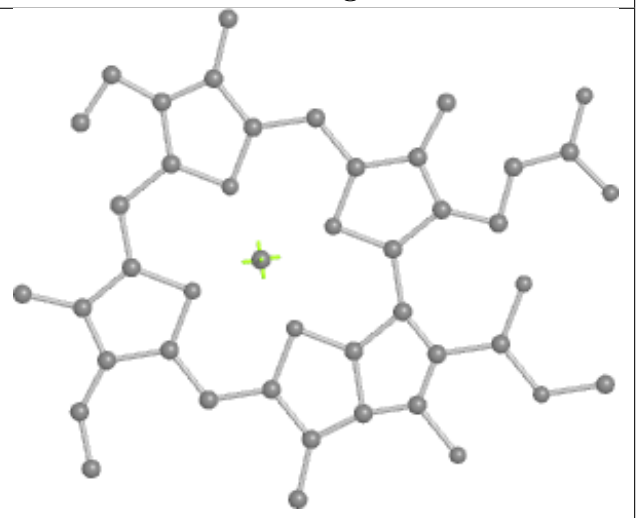
Bond lengths



Bond angles

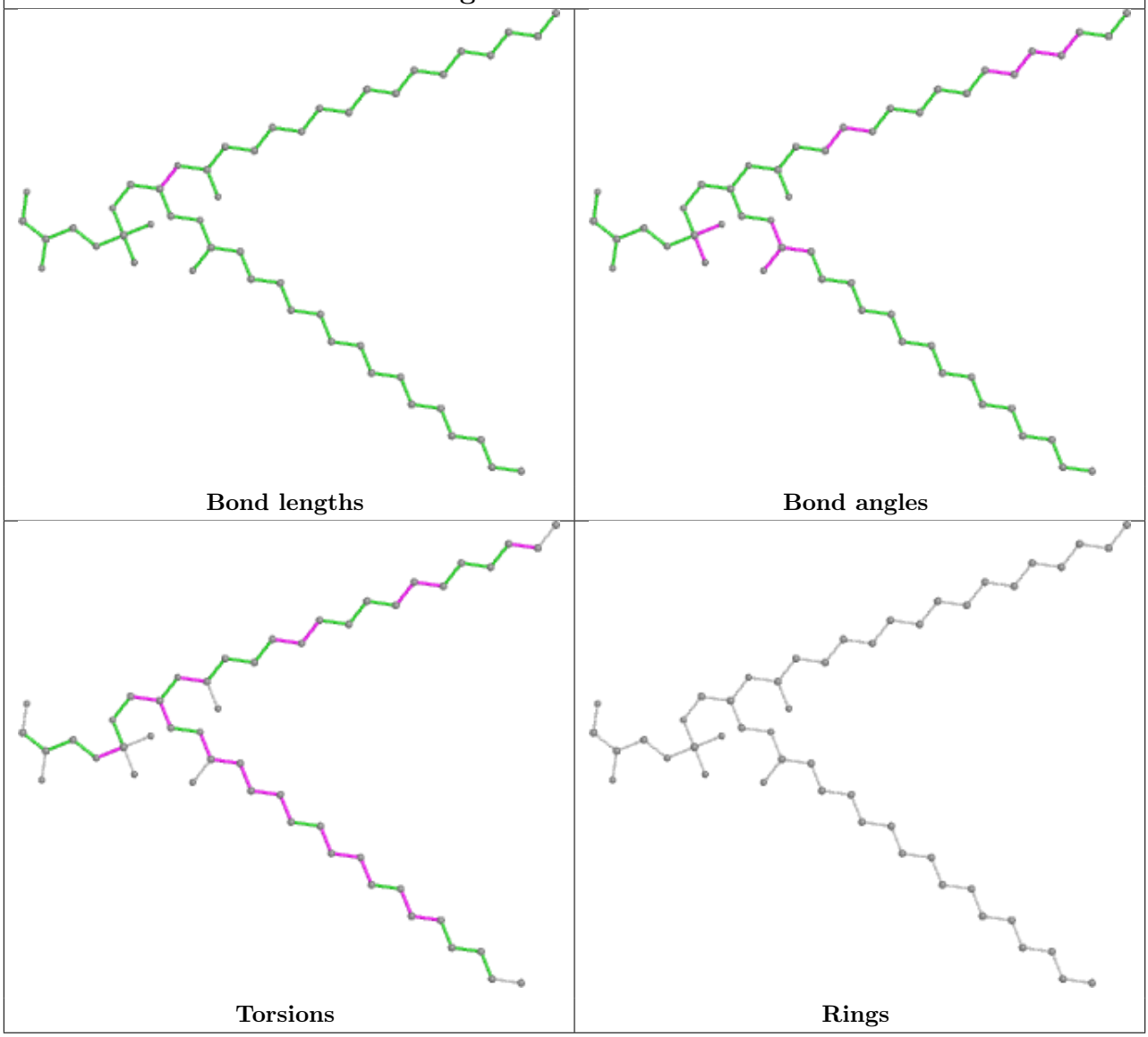


Torsions

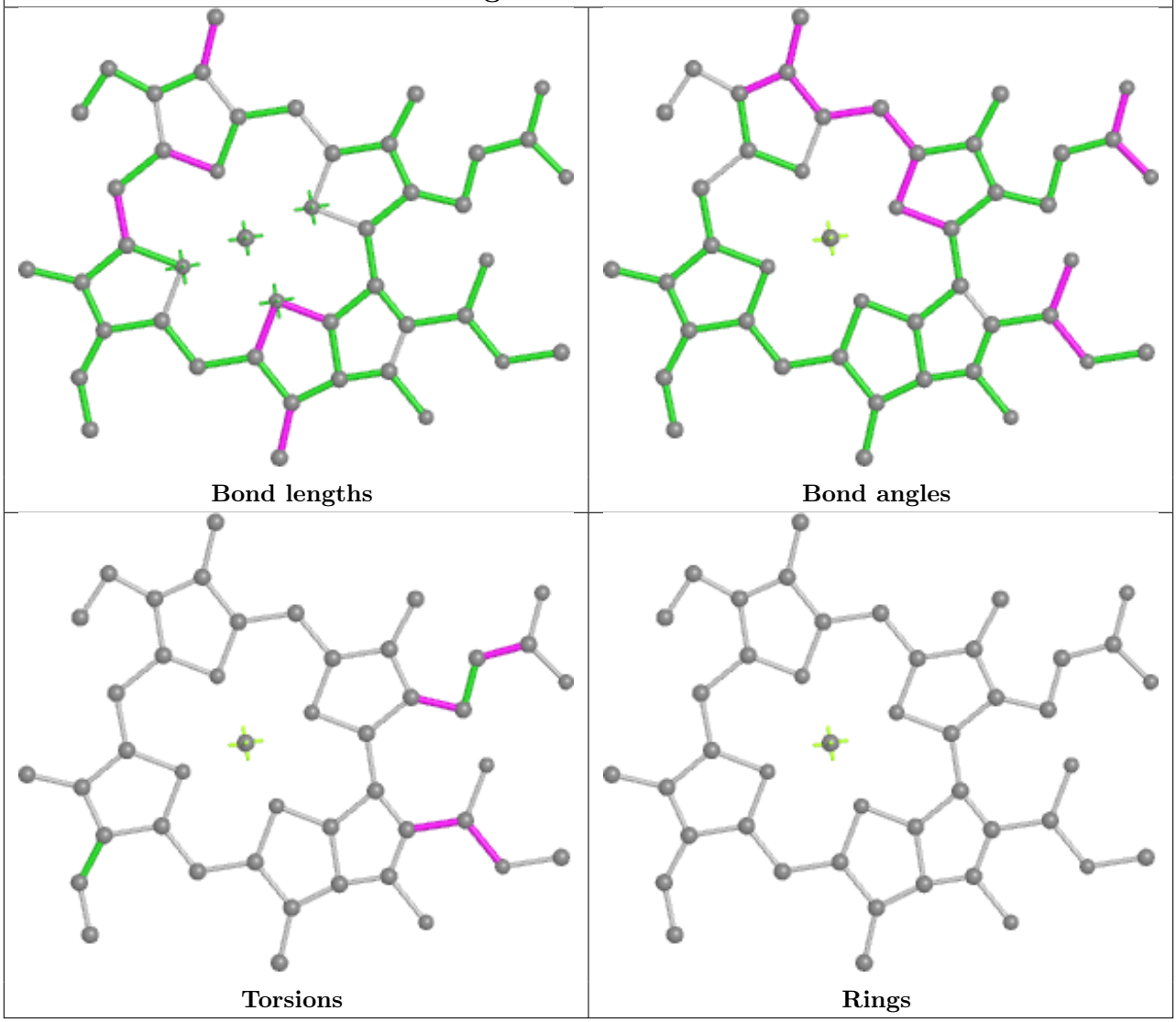


Rings

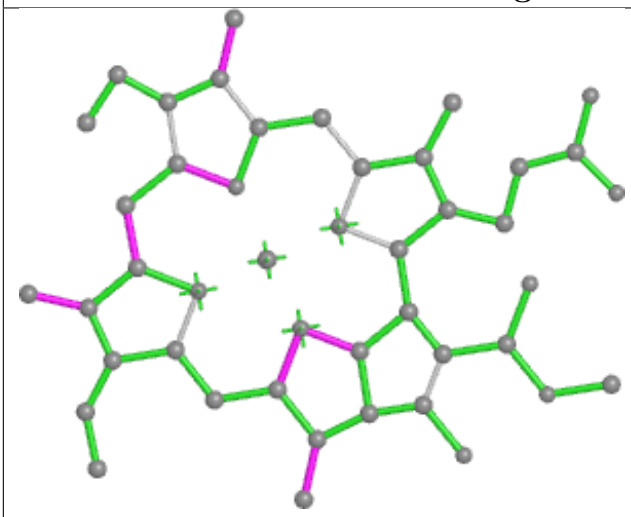
Ligand LHG A 5001



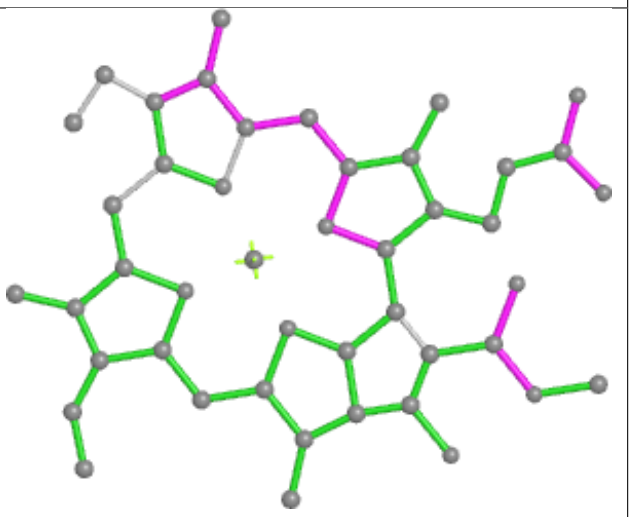
Ligand CLA d 517



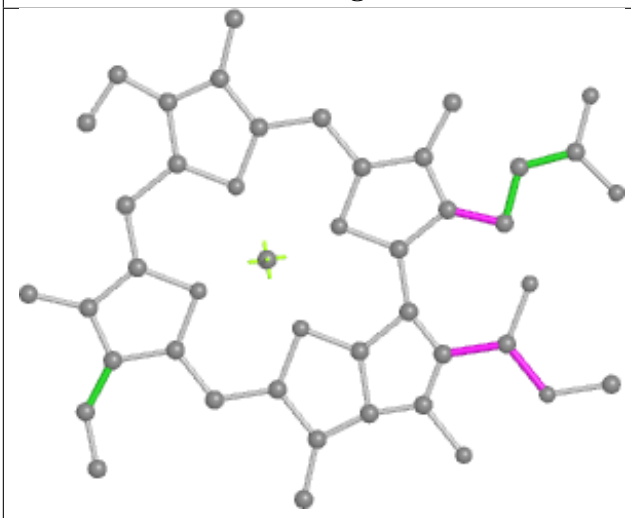
Ligand CLA G 1113



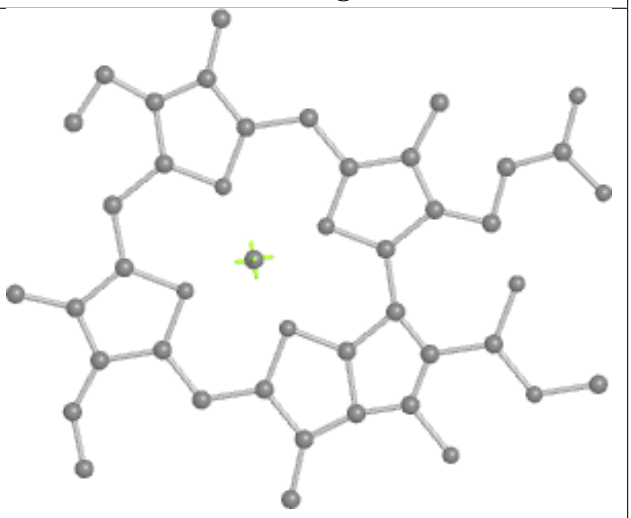
Bond lengths



Bond angles

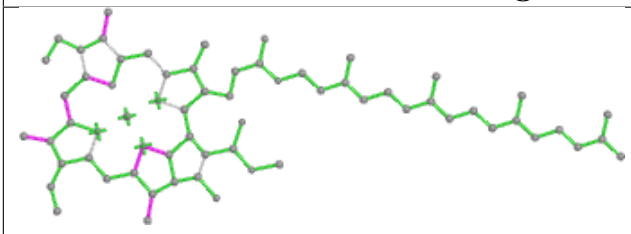


Torsions

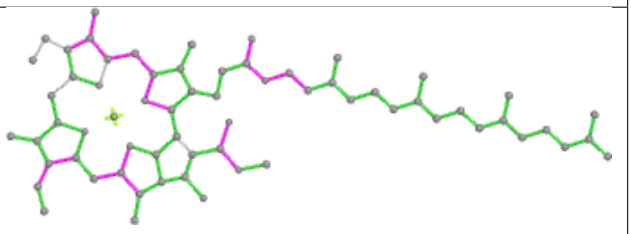


Rings

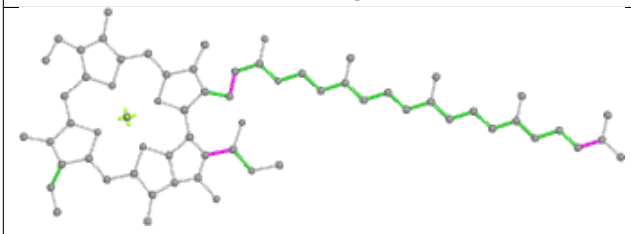
Ligand CLA H 1238



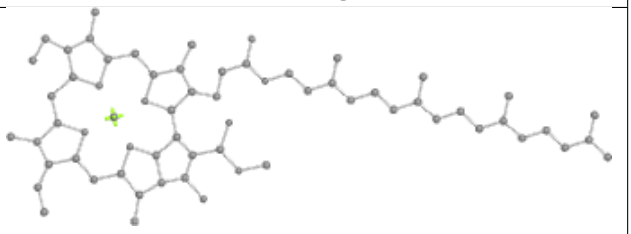
Bond lengths



Bond angles

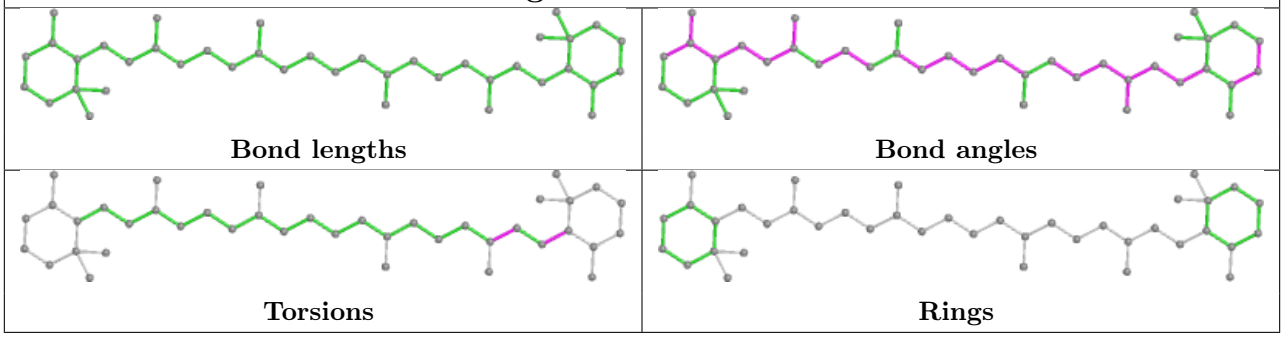


Torsions

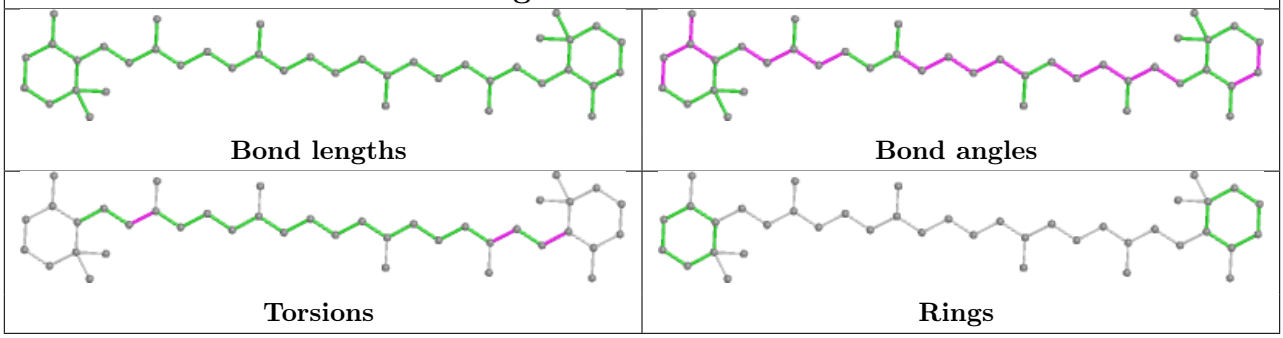


Rings

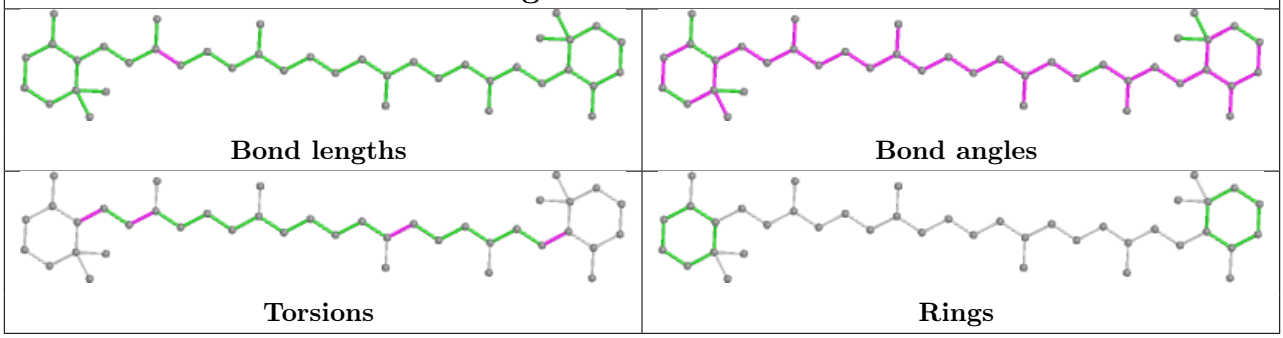
Ligand BCR u 523



Ligand BCR H 4005



Ligand BCR f 4014



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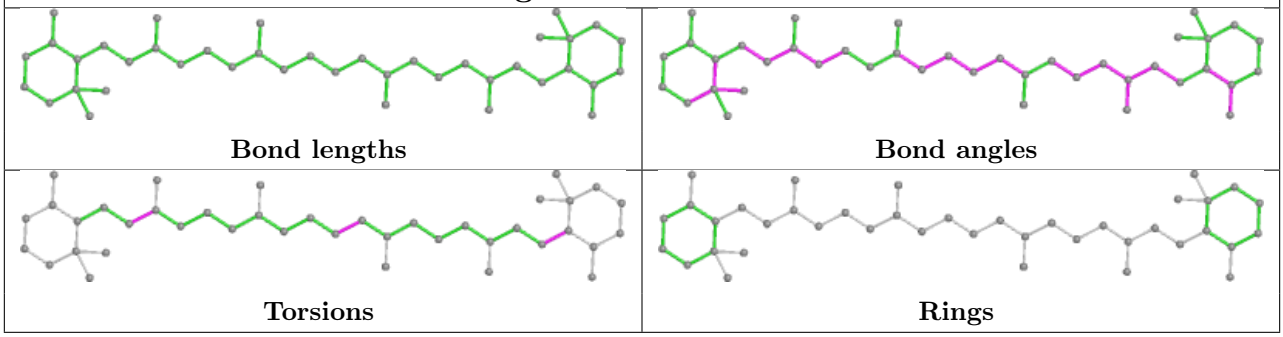
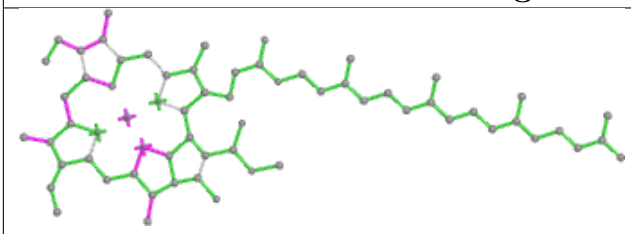
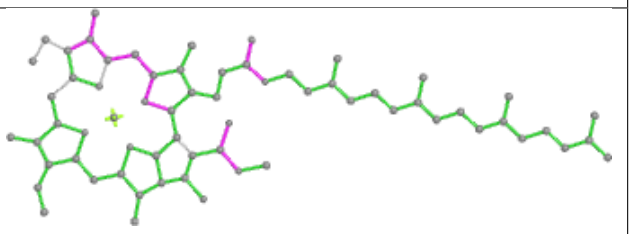
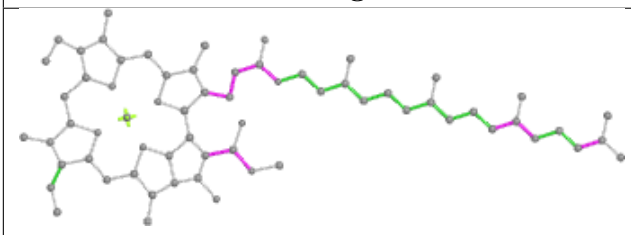
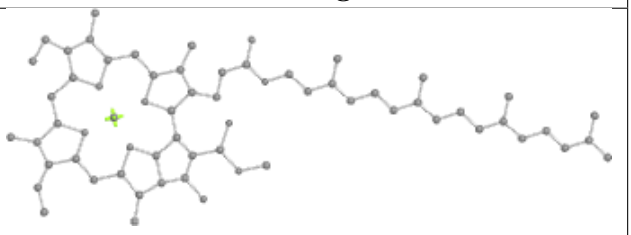
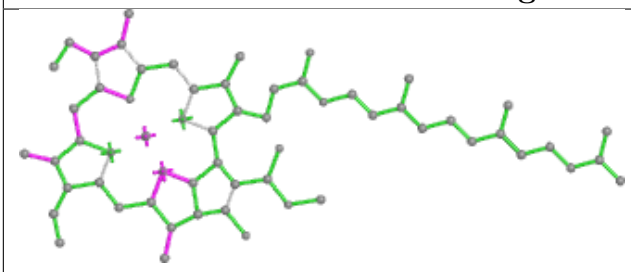
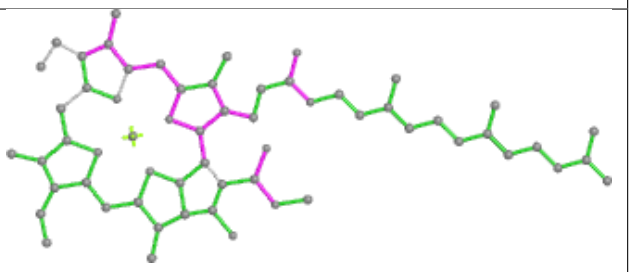
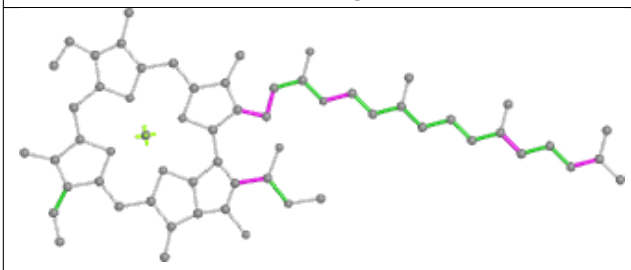
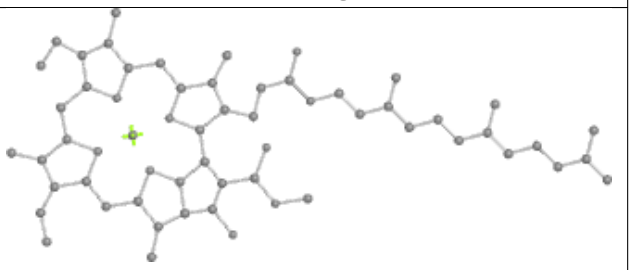
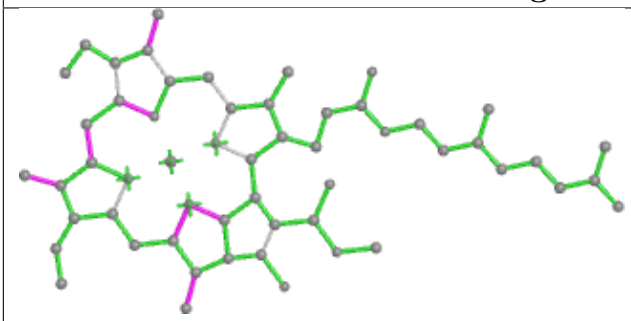
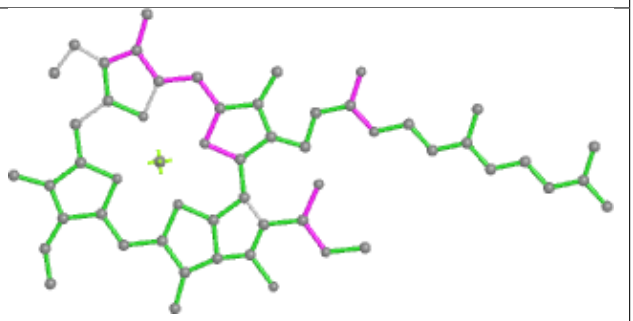
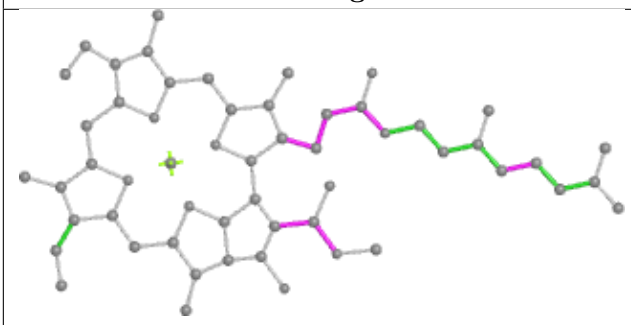
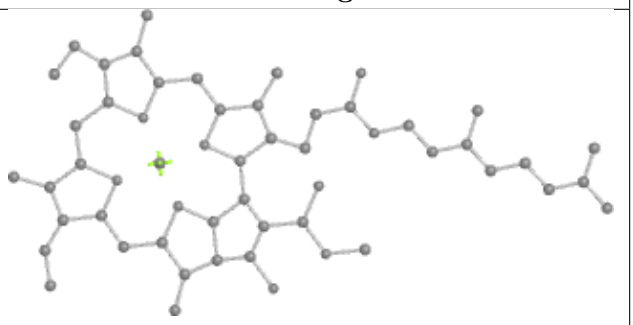
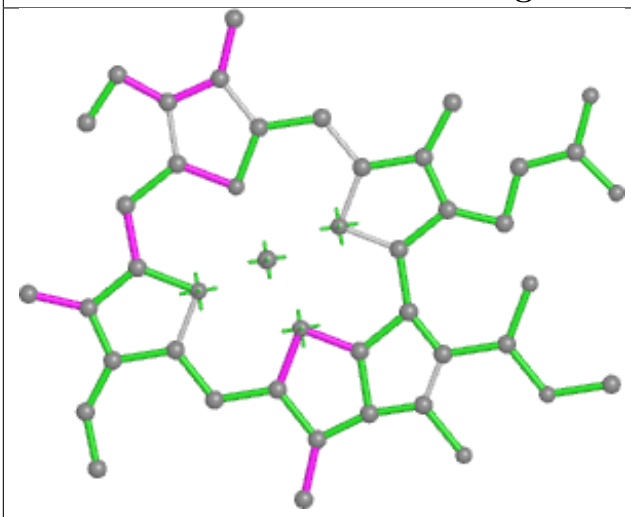


Ligand CLA G 1111	
 Bond lengths	 Bond angles
 Torsions	 Rings

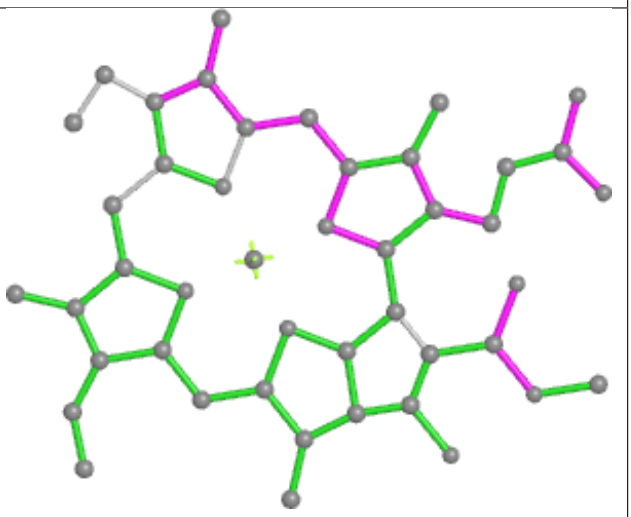
Ligand CLA n 1501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

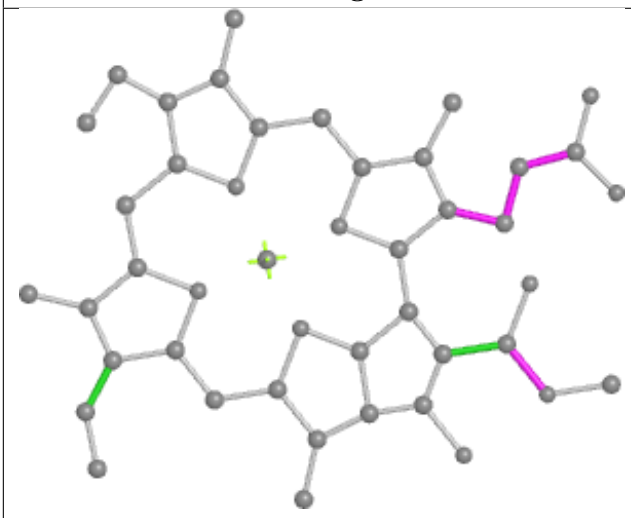
Ligand CLA R 1302



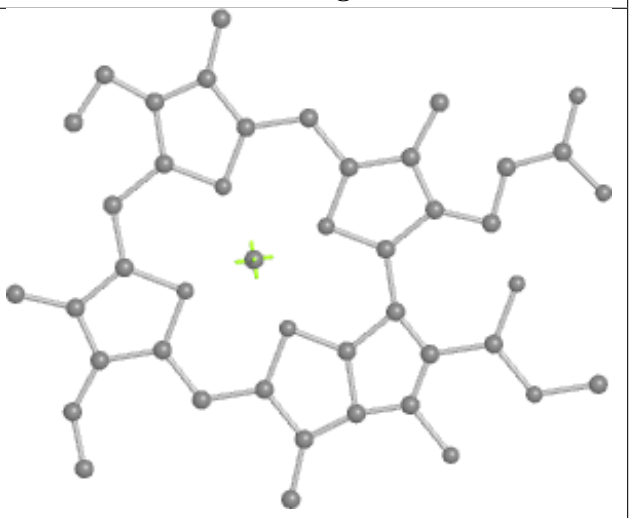
Bond lengths



Bond angles

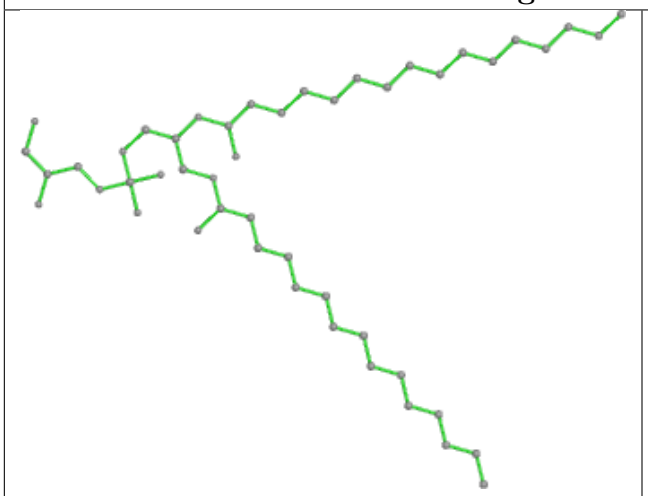


Torsions



Rings

Ligand LHG S 5001



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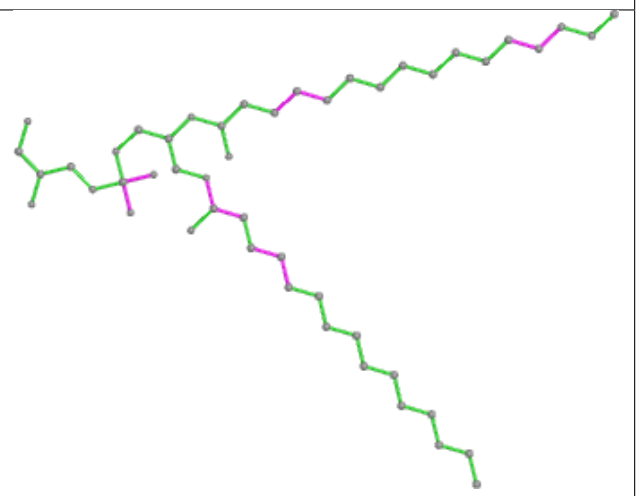
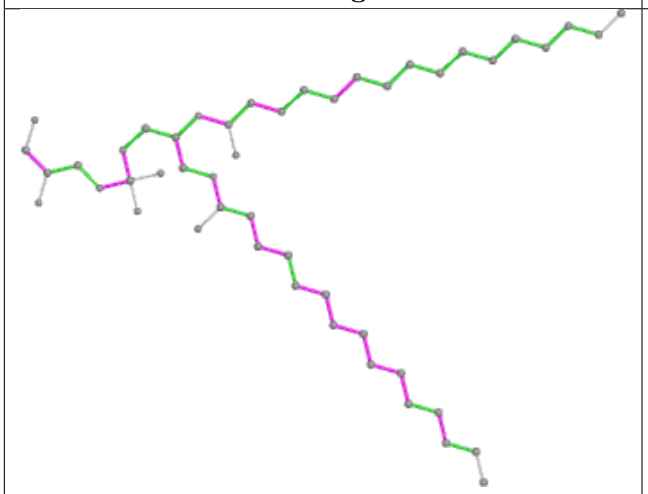


Bond angles



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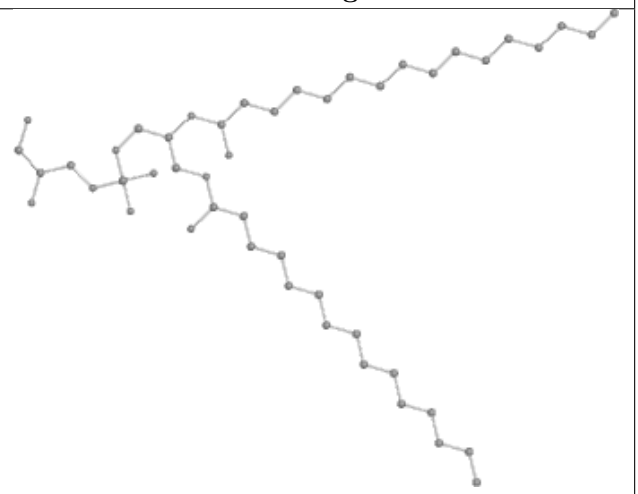
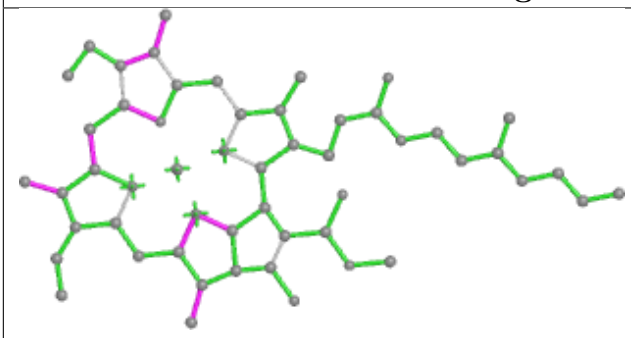


Rings

Ligand CLA A 1110



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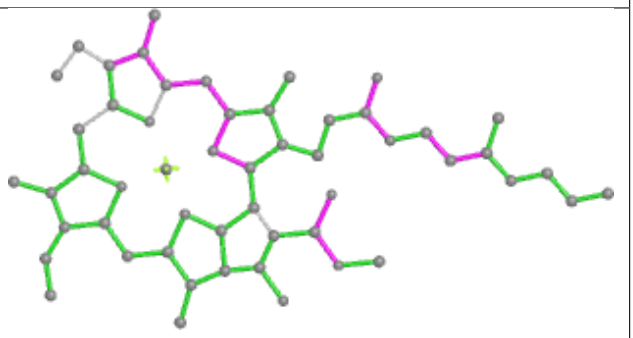
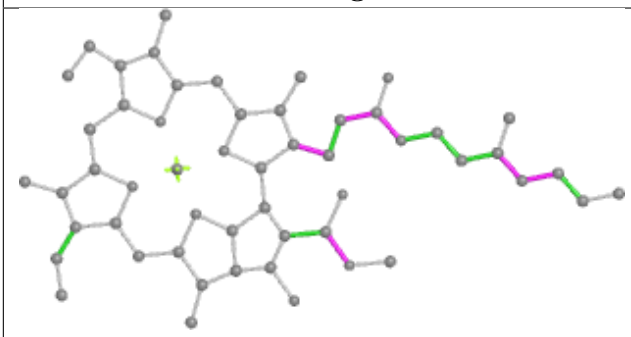


Bond angles



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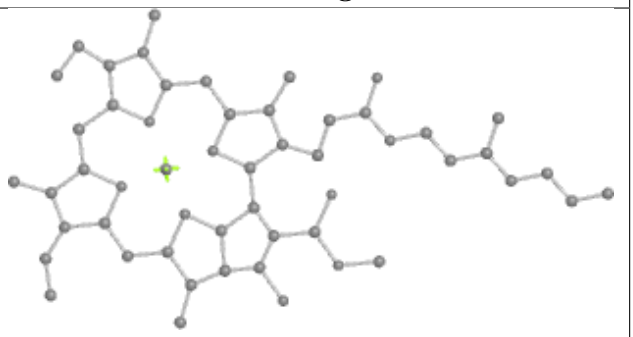
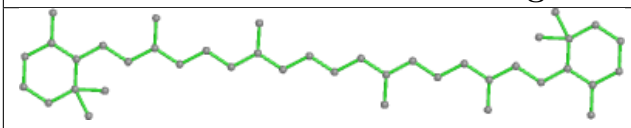


Rings

Ligand BCR c 524



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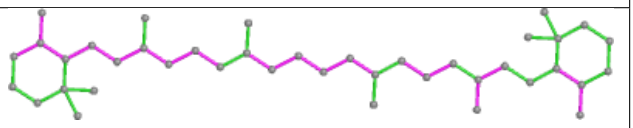
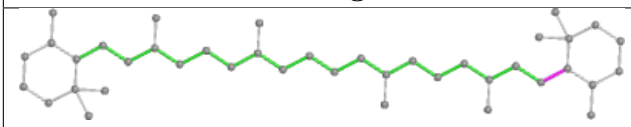


Bond angles



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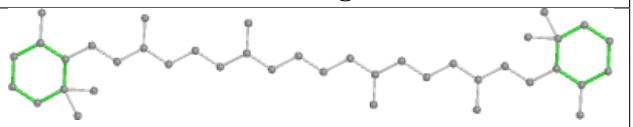
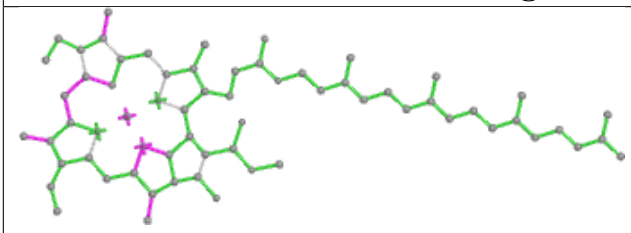


Rings

Ligand CLA e 1109



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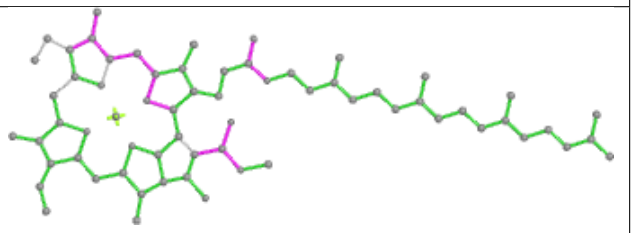
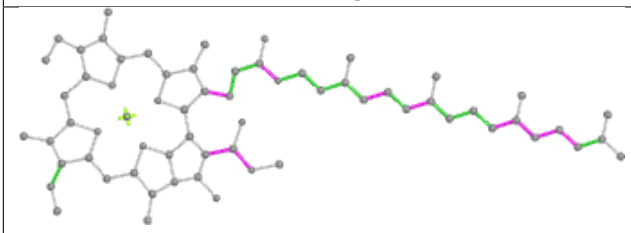


Bond angles



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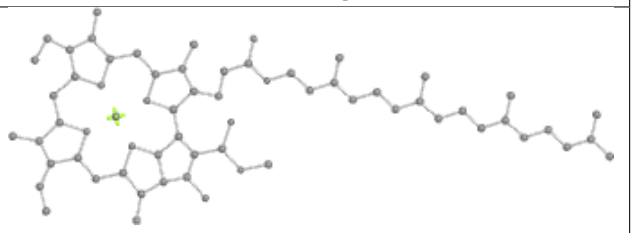
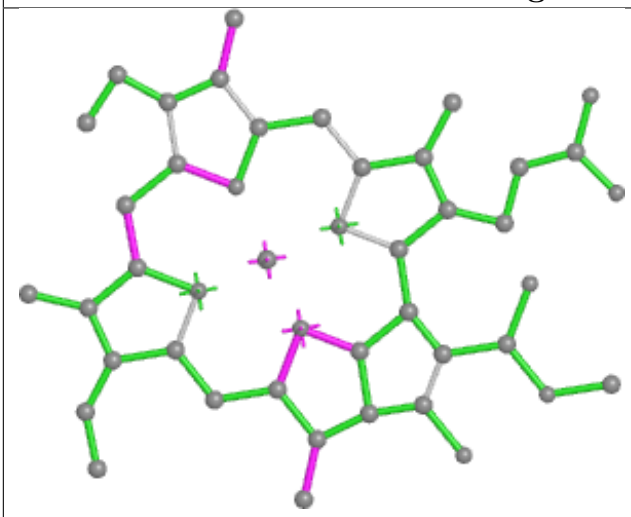


Rings

Ligand CLA q 509



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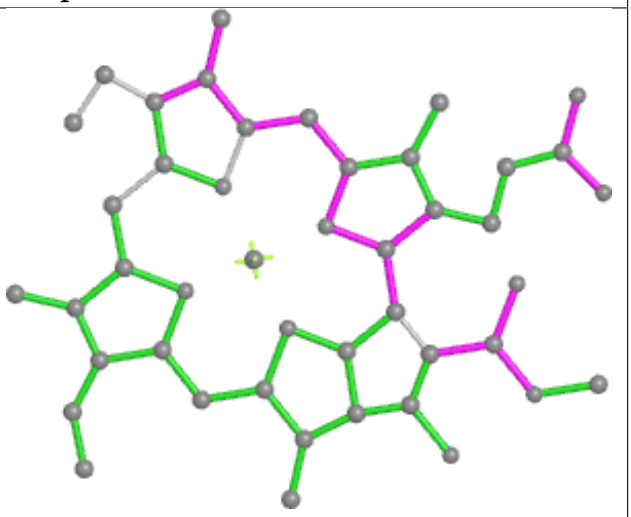
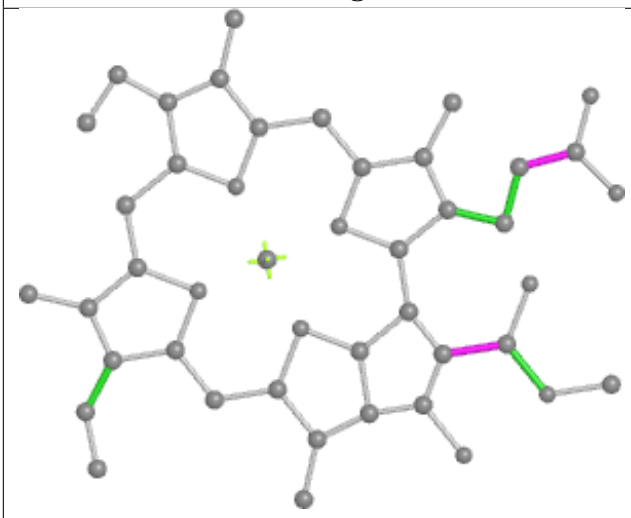


Bond angles



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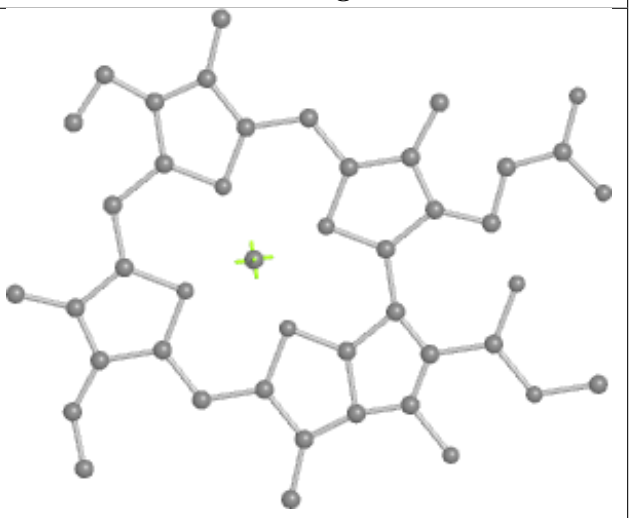
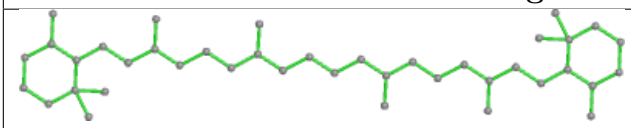


Rings

Ligand BCR 3 524



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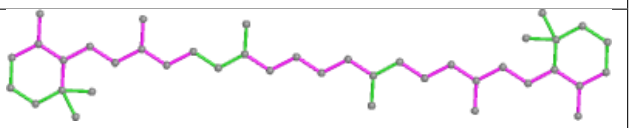
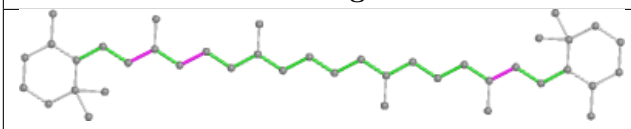
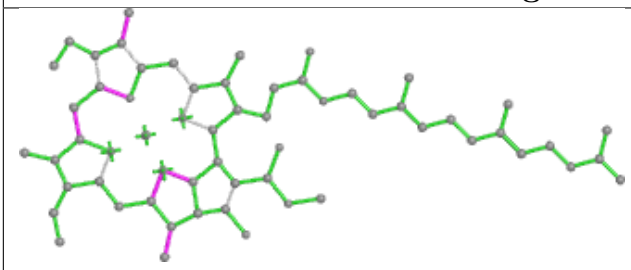
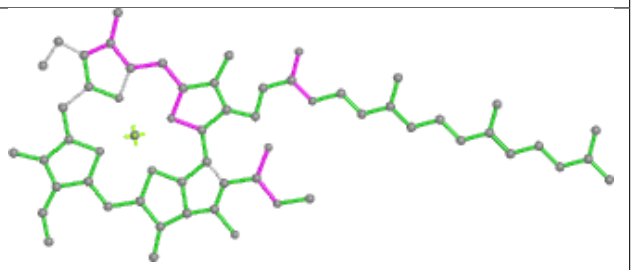
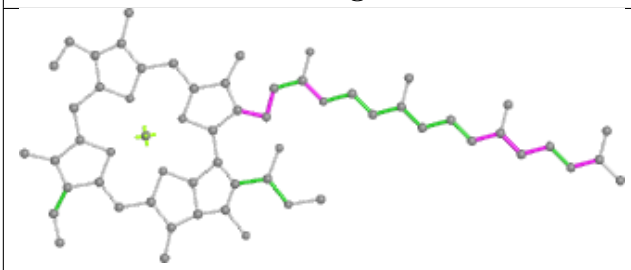
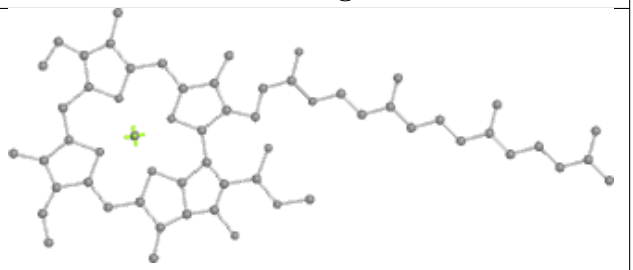


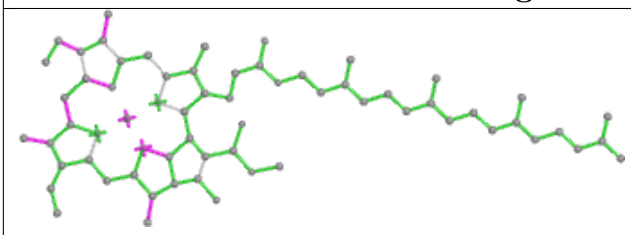
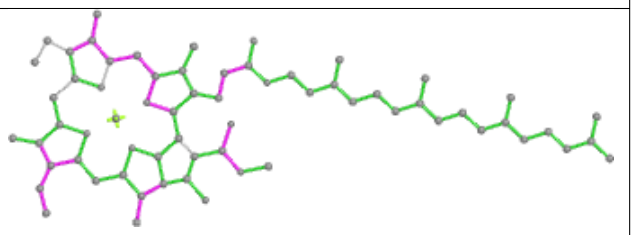
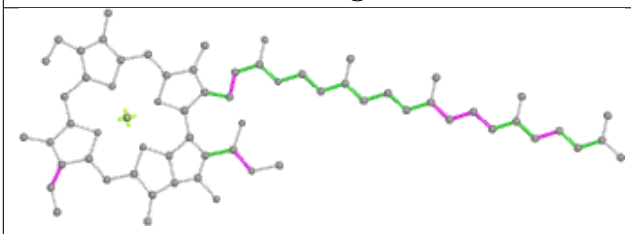
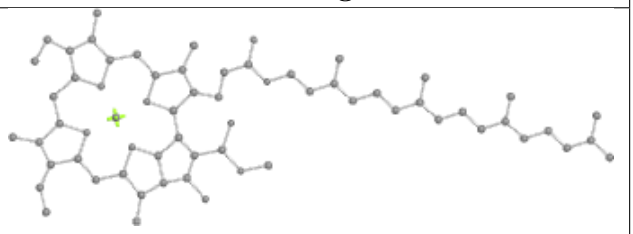
Bond angles



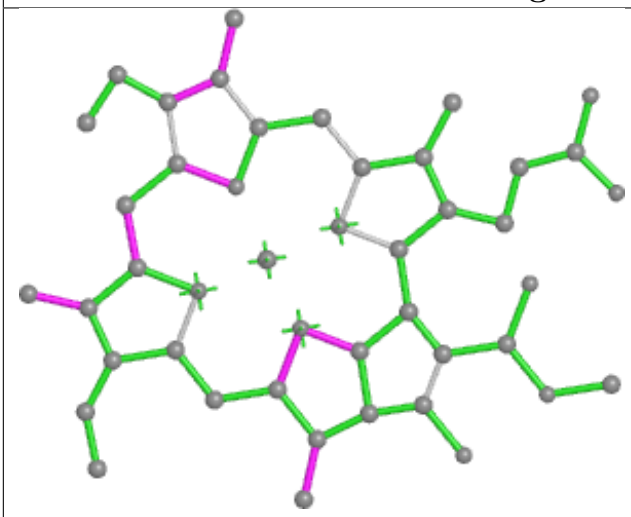
Torsions

Rings

Ligand CLA f 1217	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1023	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 517



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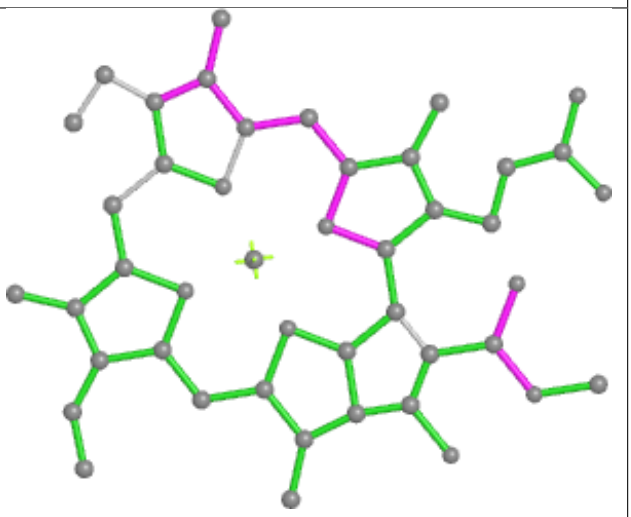

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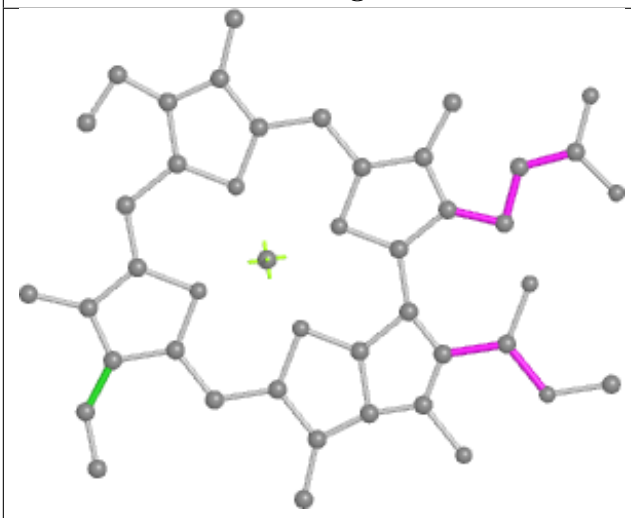

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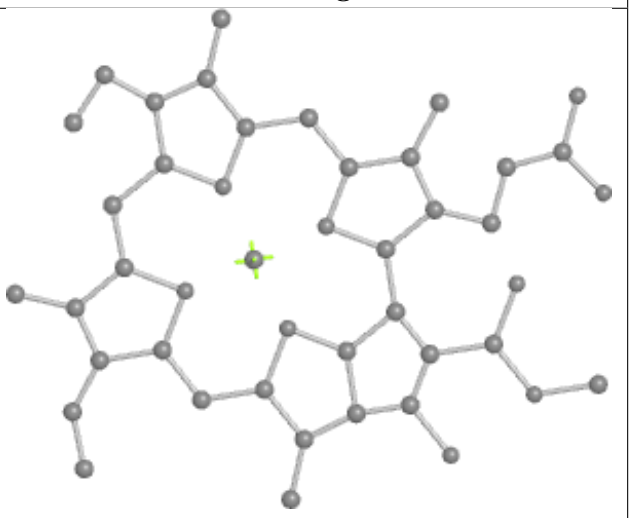
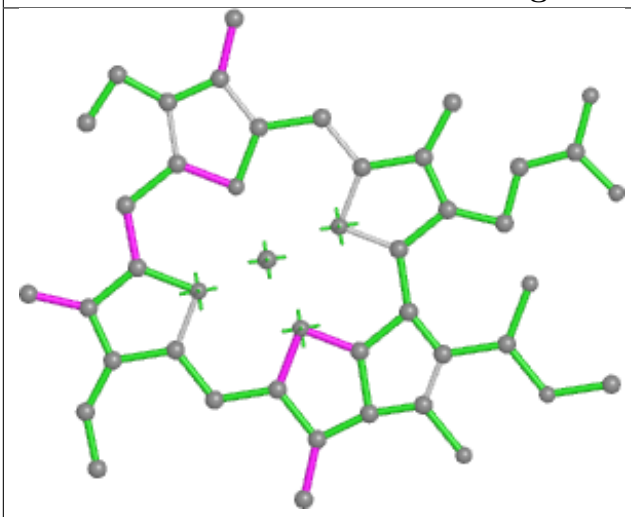


Rings

Ligand CLA r 510



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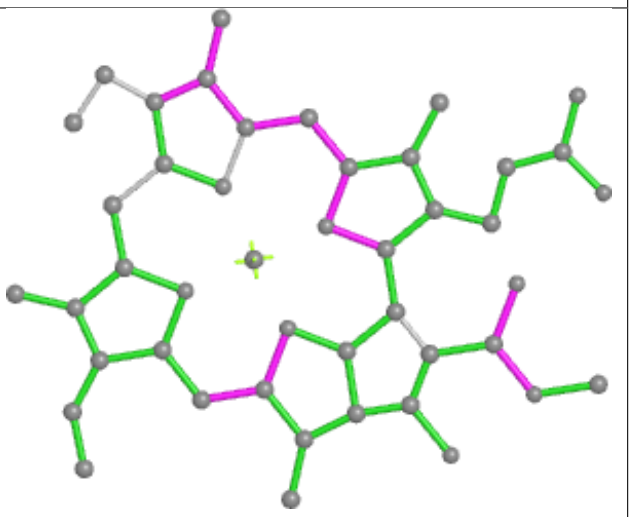

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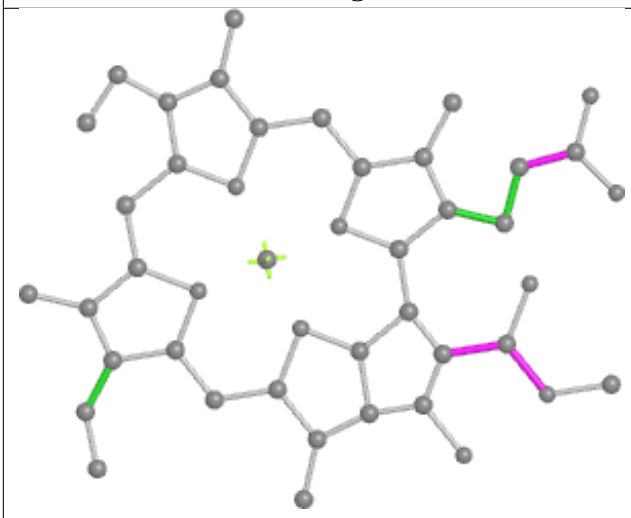

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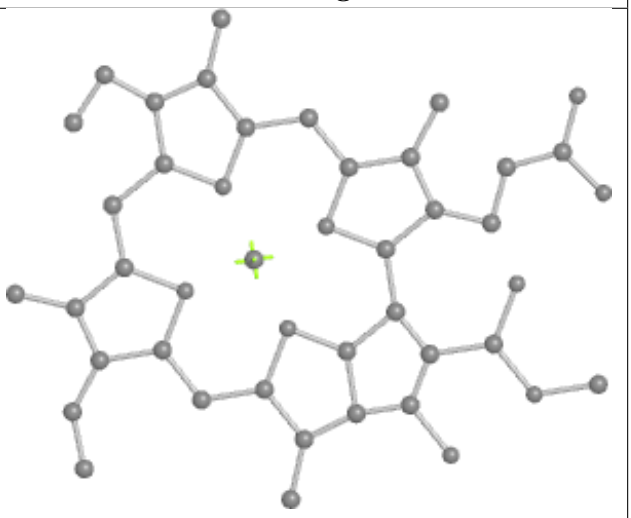
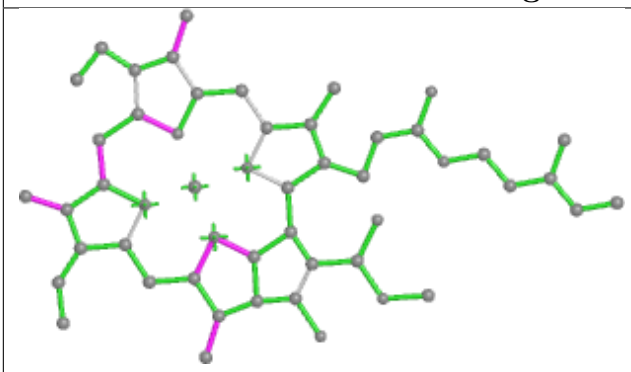


Rings

Ligand CLA f 1212



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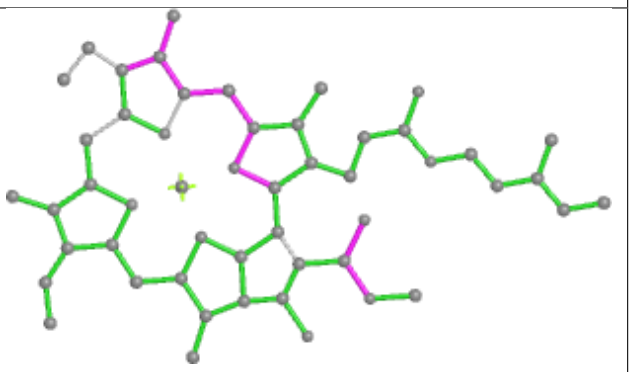

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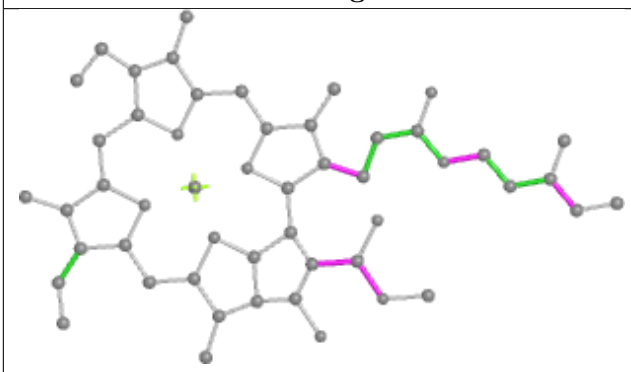

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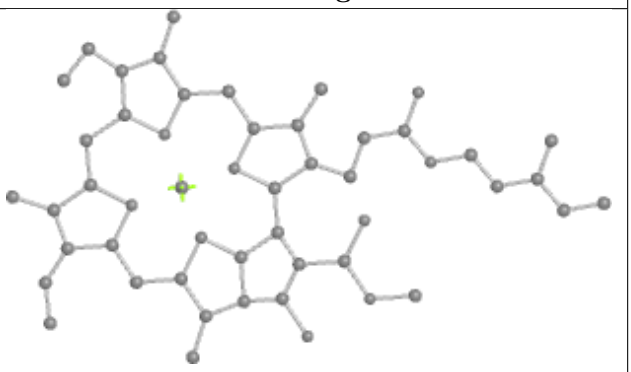
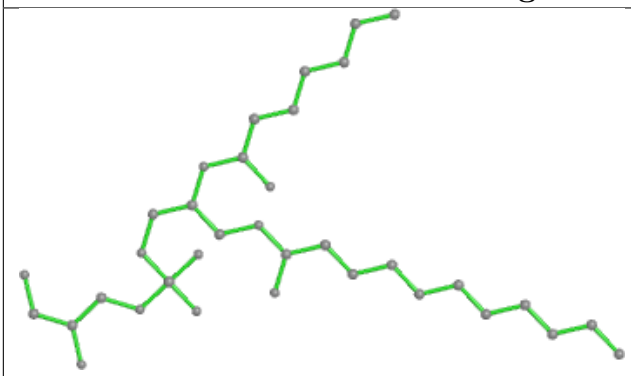


Rings

Ligand LHG e 5004



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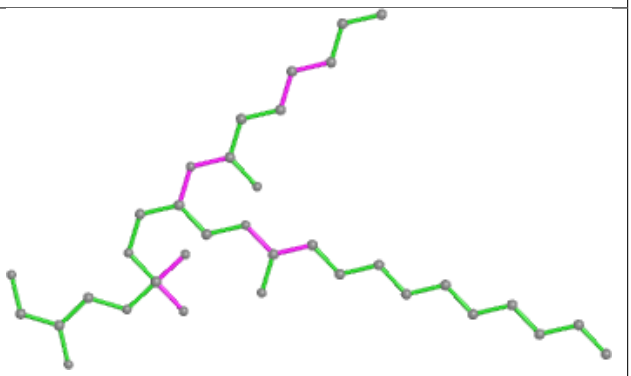

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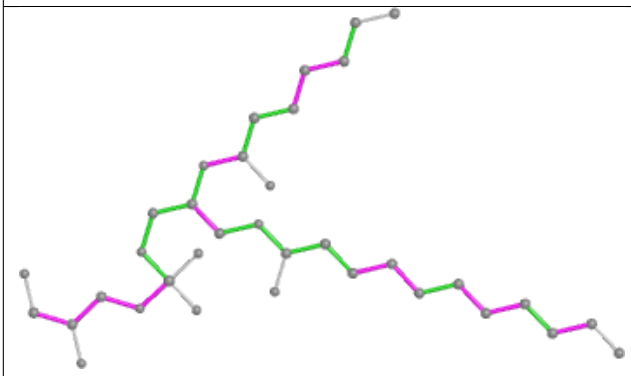

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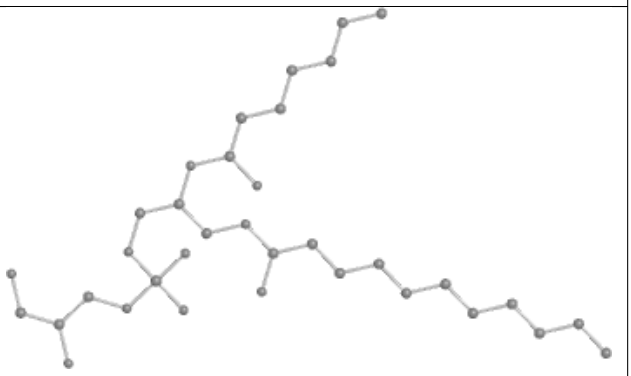

Rings

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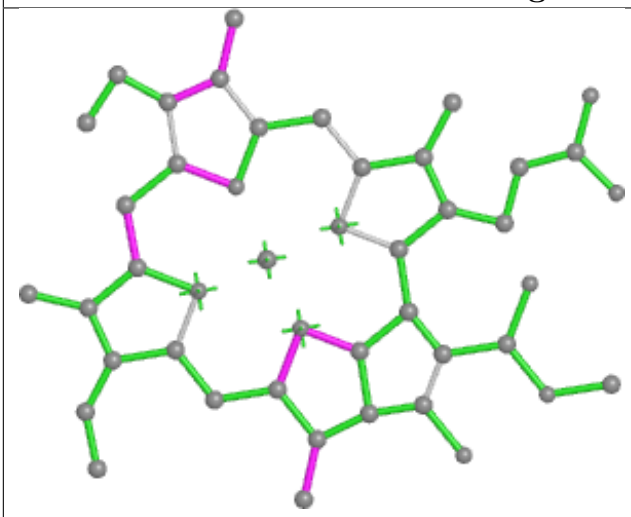

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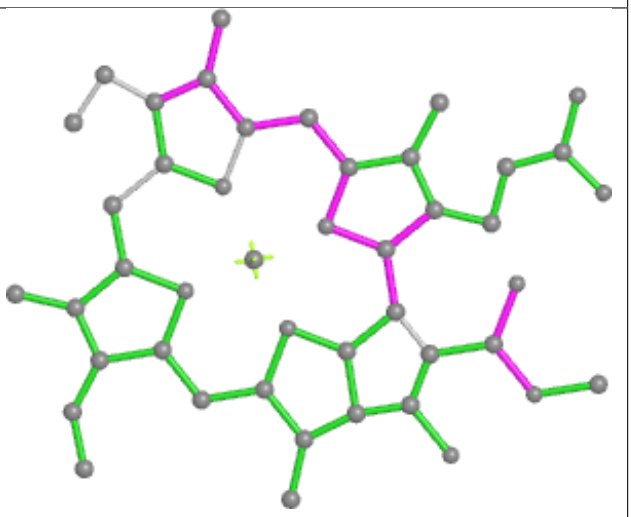

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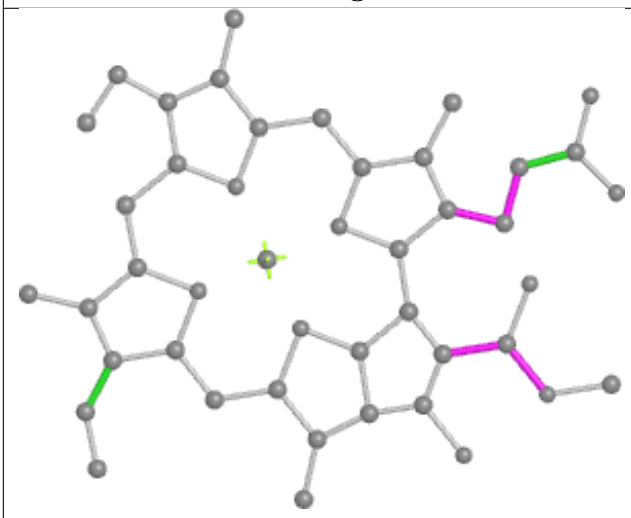

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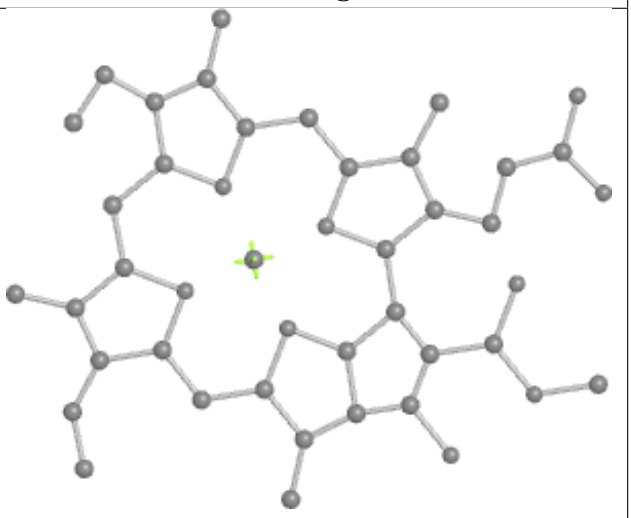
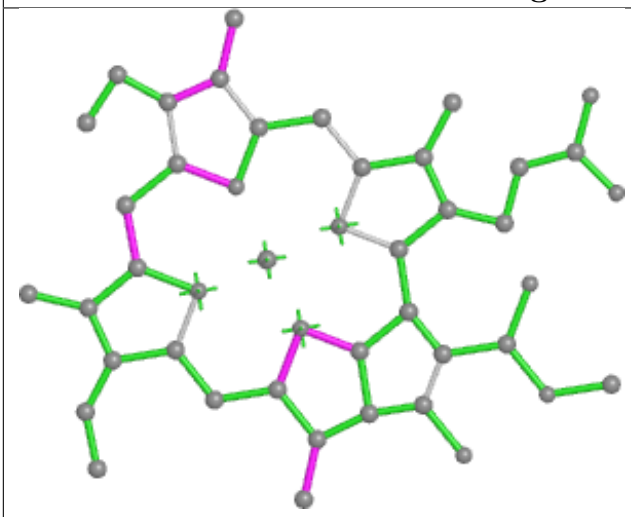


Rings

Ligand CLA t 503



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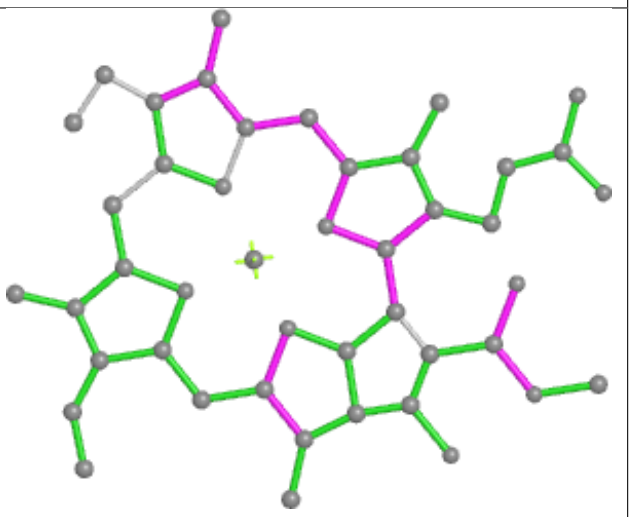

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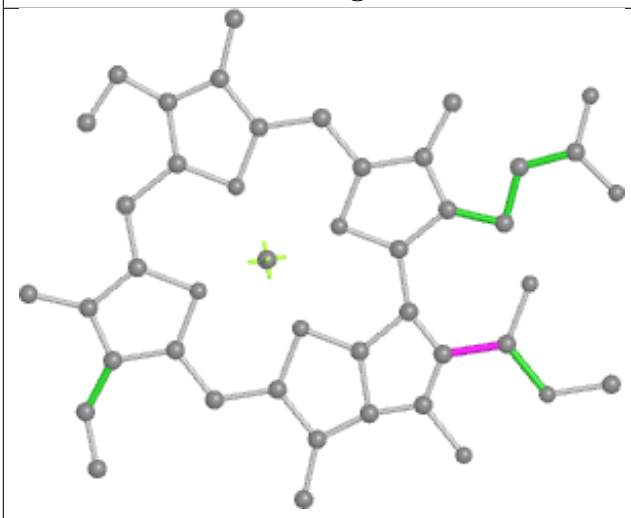

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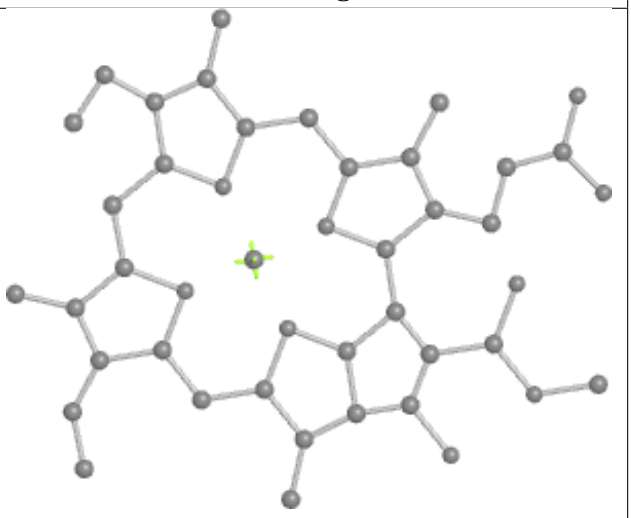

Rings

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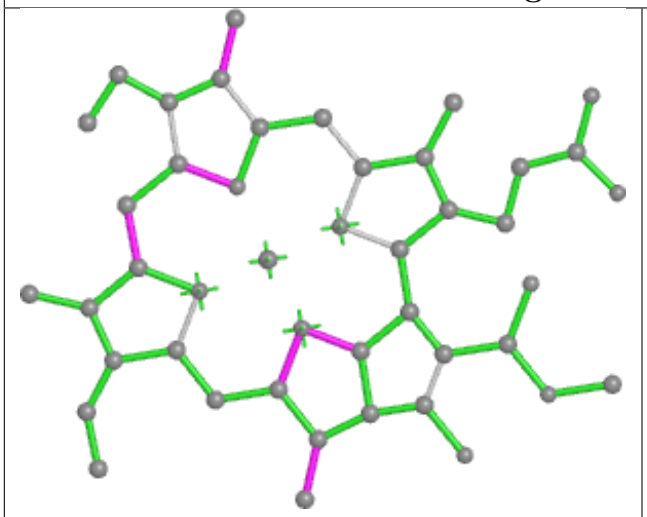

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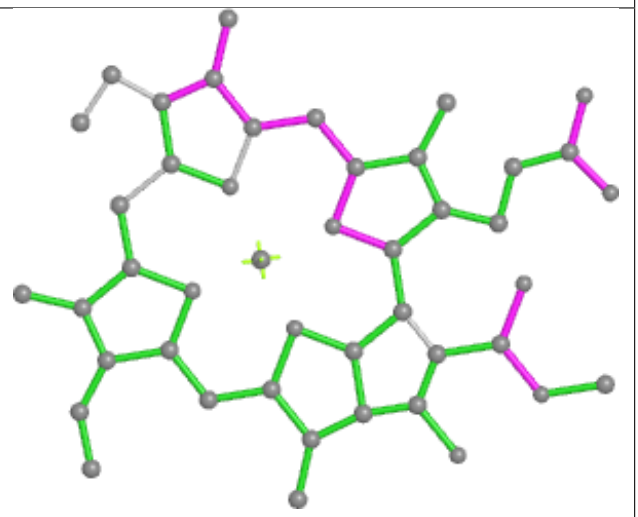

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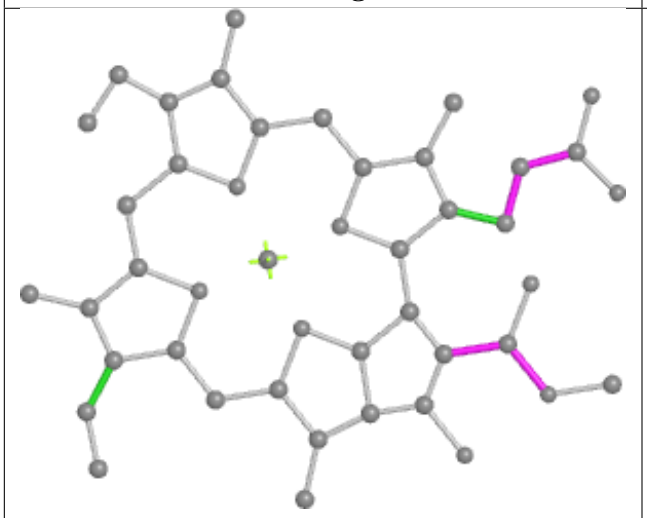

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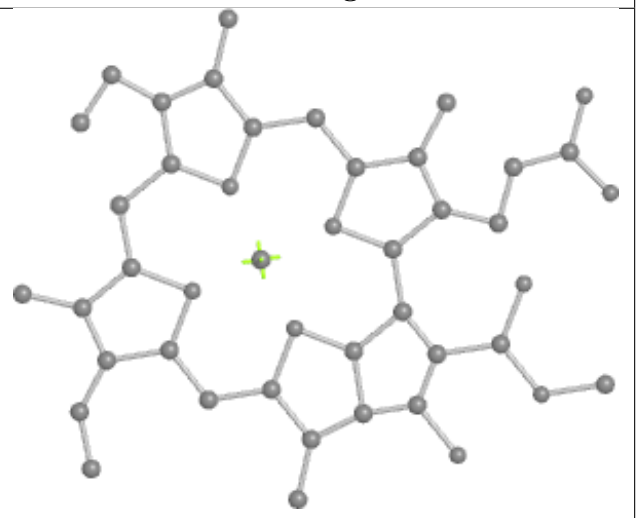

Rings

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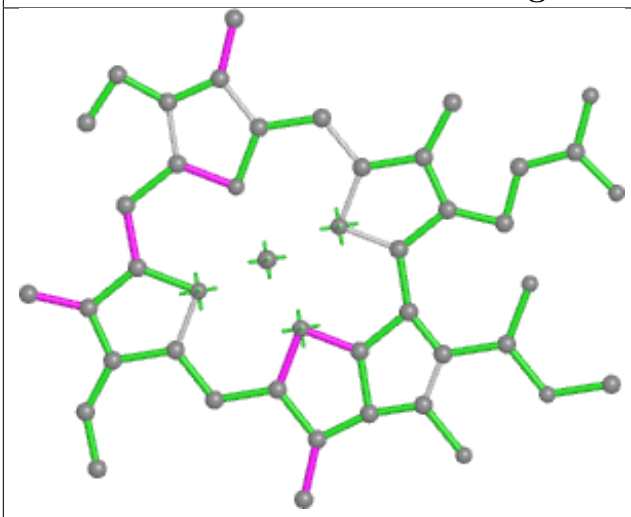

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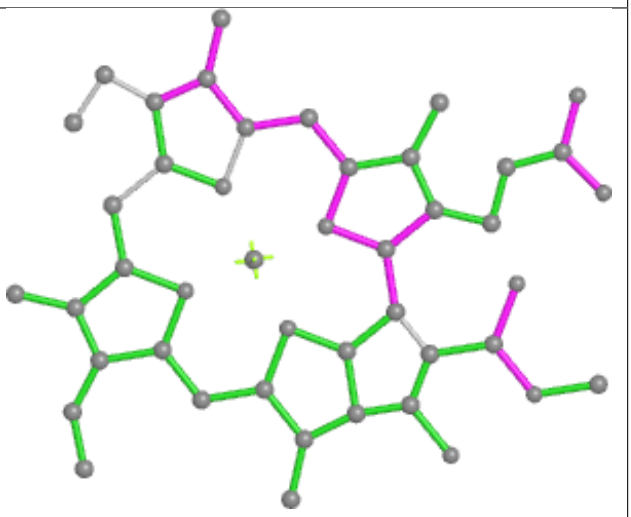

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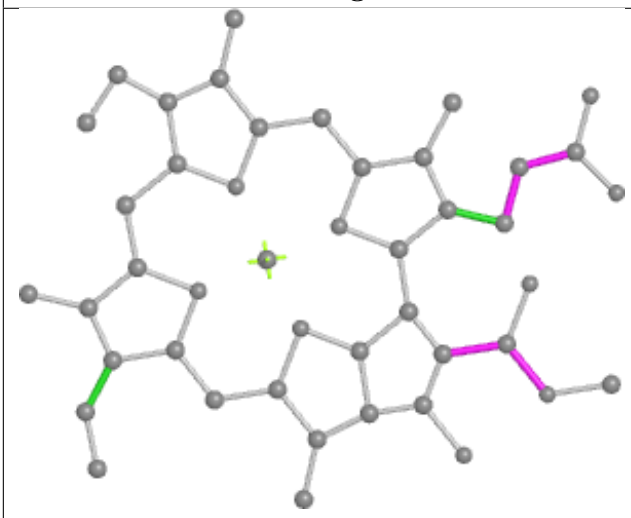

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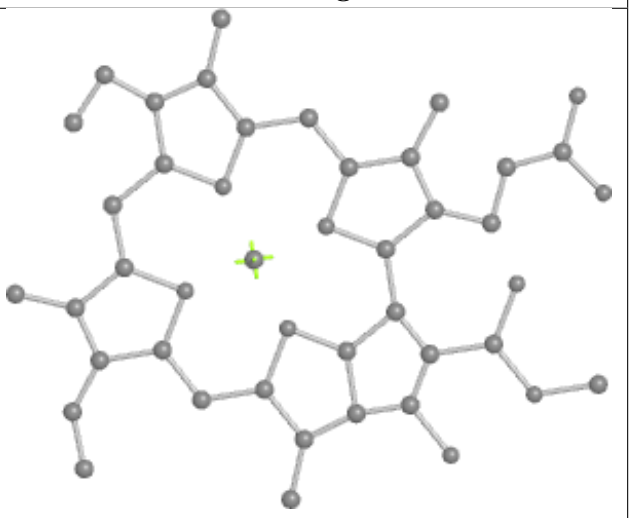
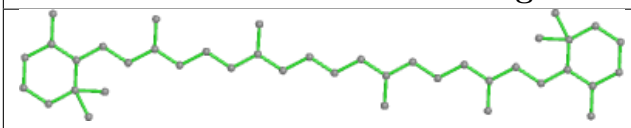


Rings

Ligand BCR L 4019



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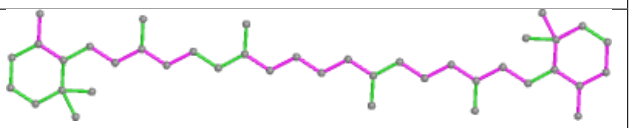

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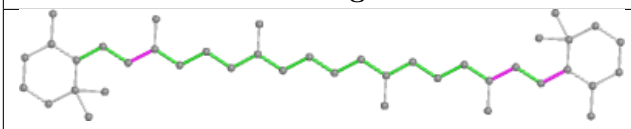
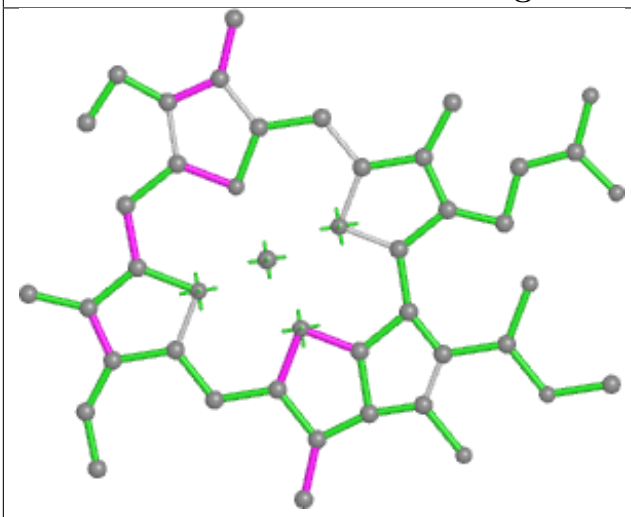


Torsions

Rings

Ligand CLA K 1105



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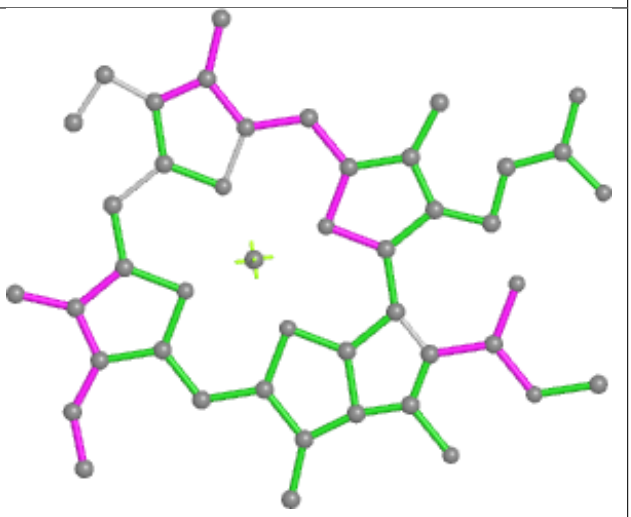

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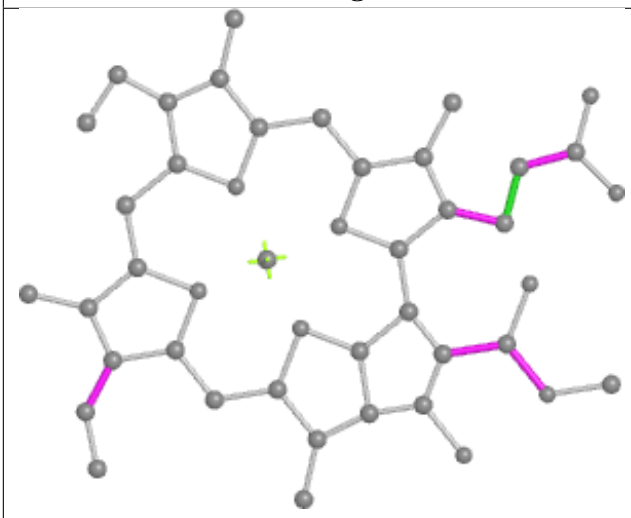

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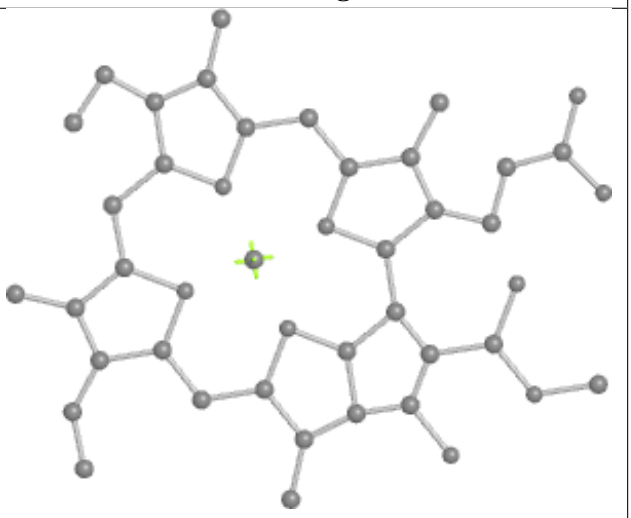
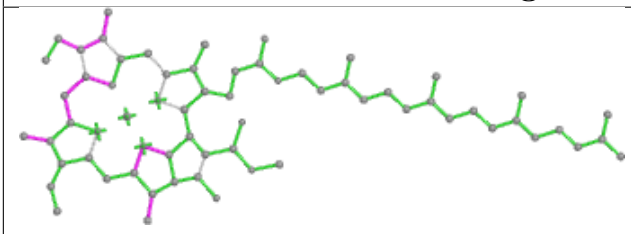


Rings

Ligand CLA e 1011



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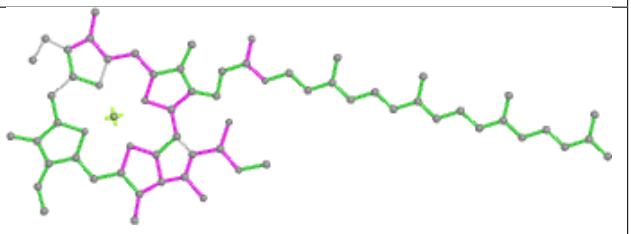

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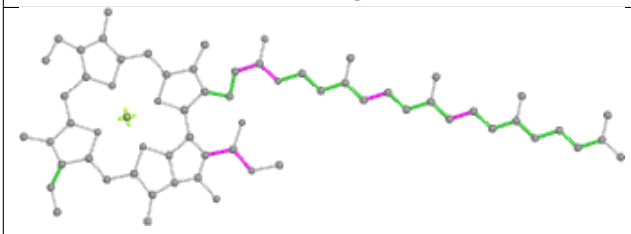

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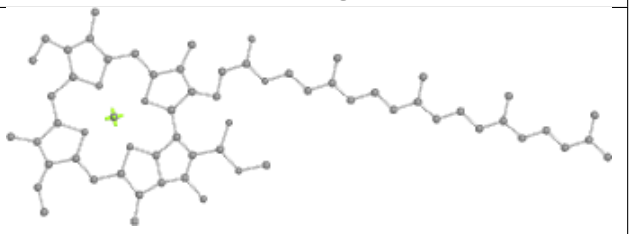
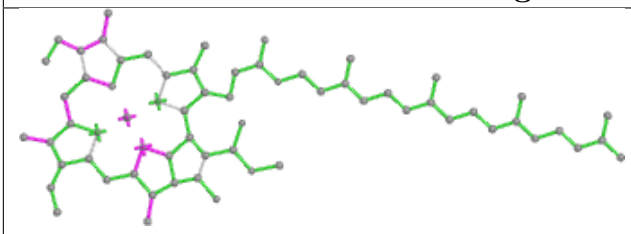
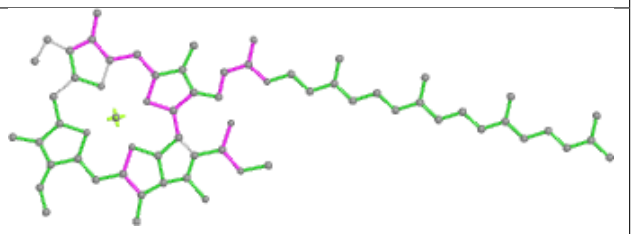
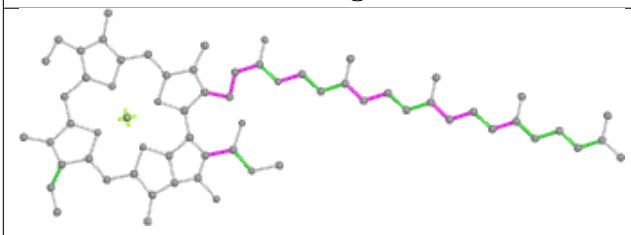
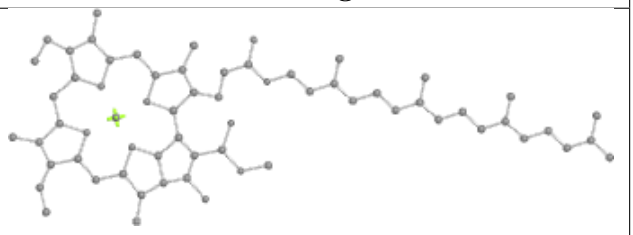
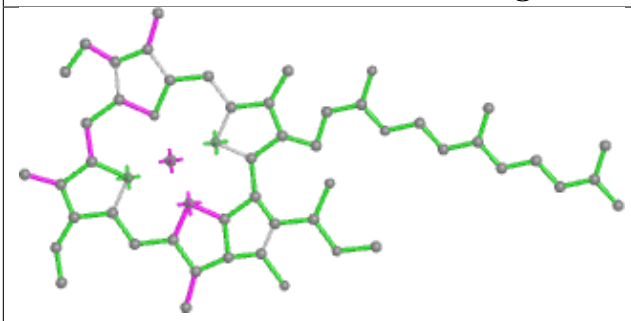
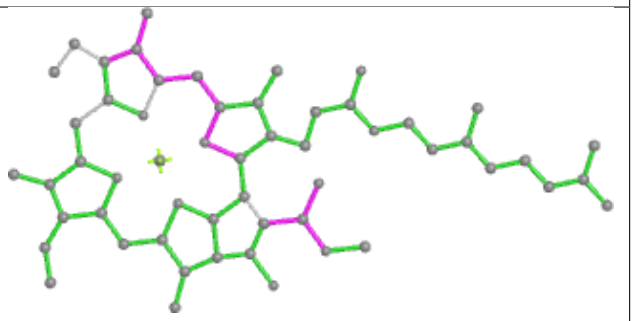
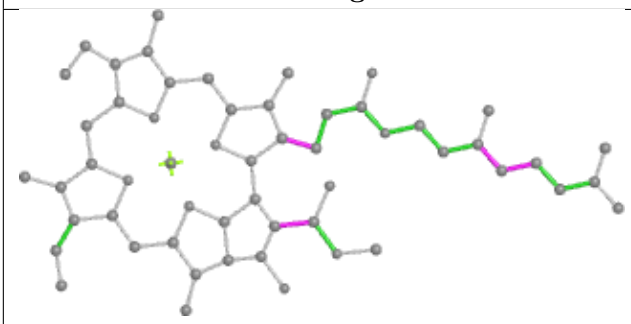
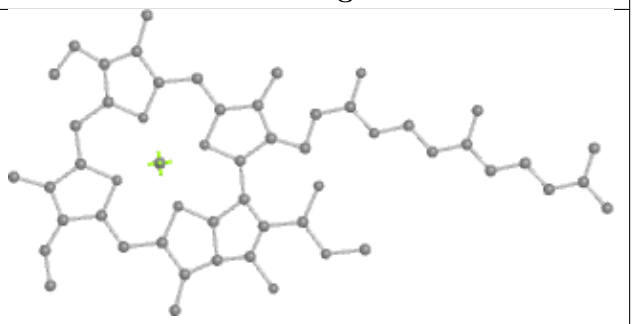


Rings

Ligand CLA G 1107	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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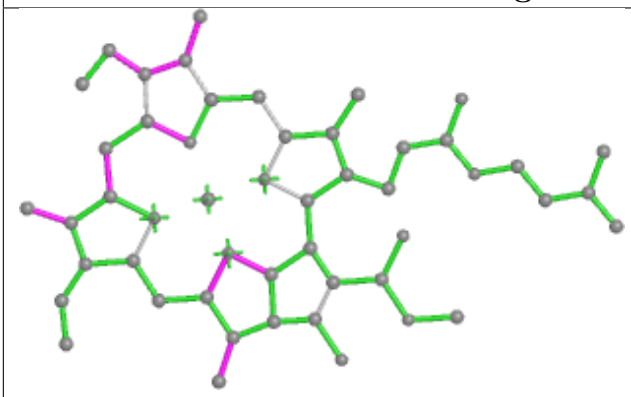
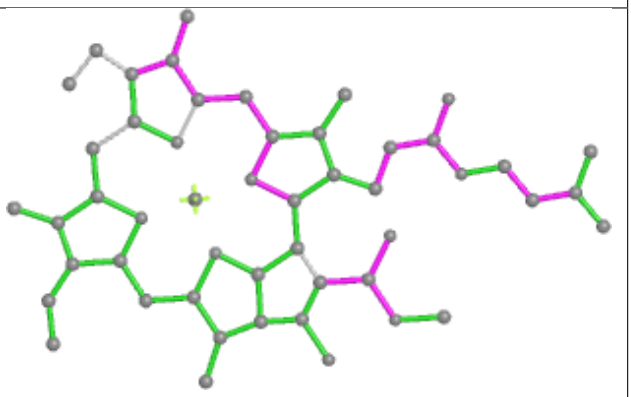
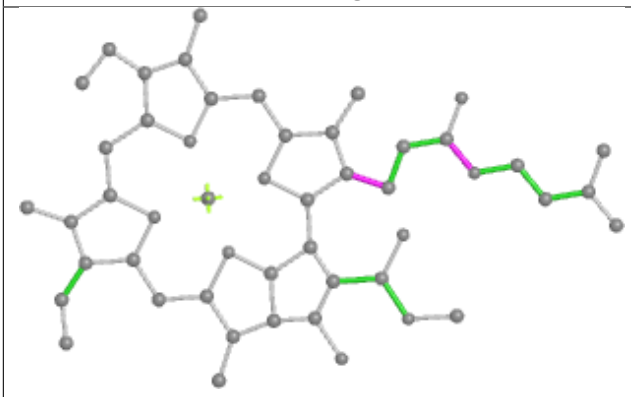
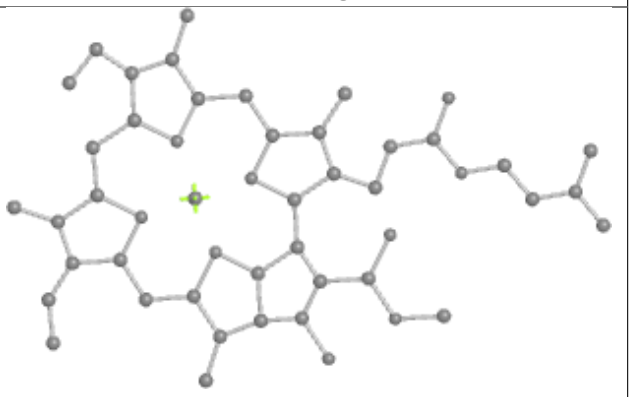
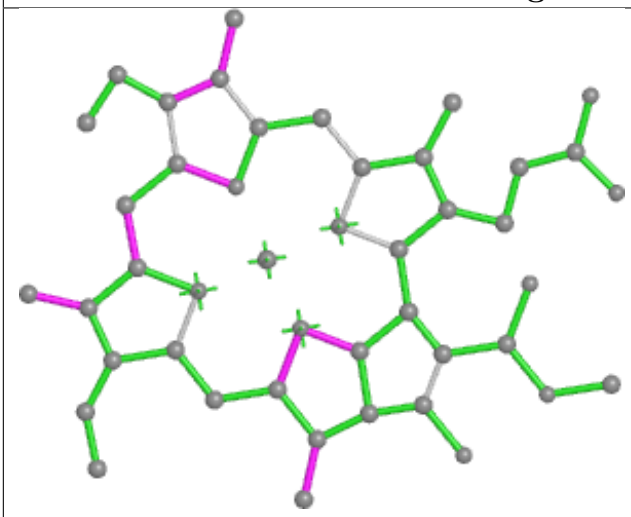
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 502



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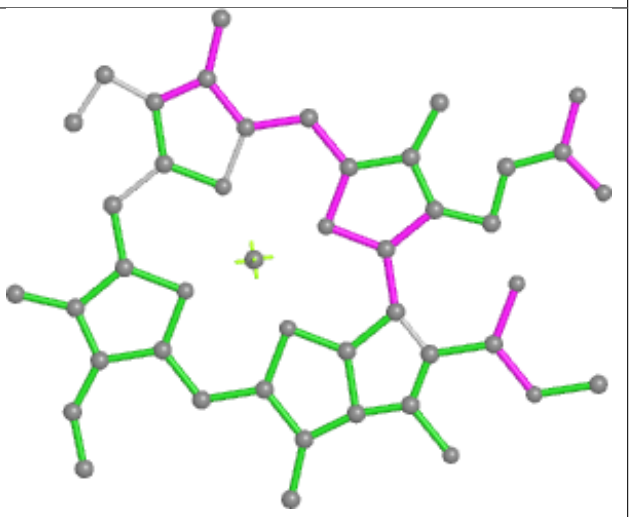

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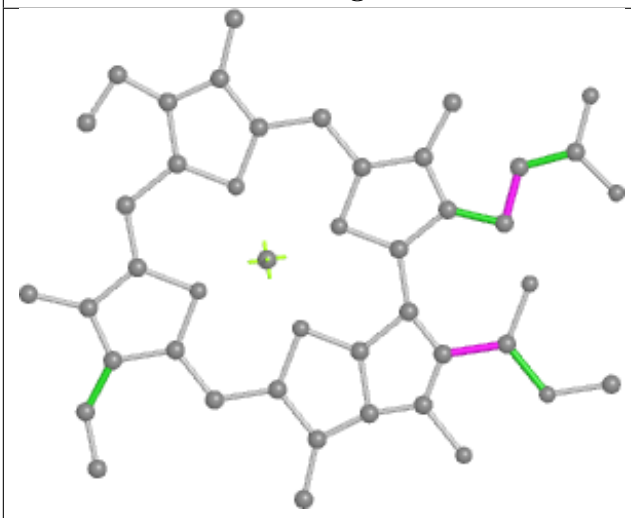

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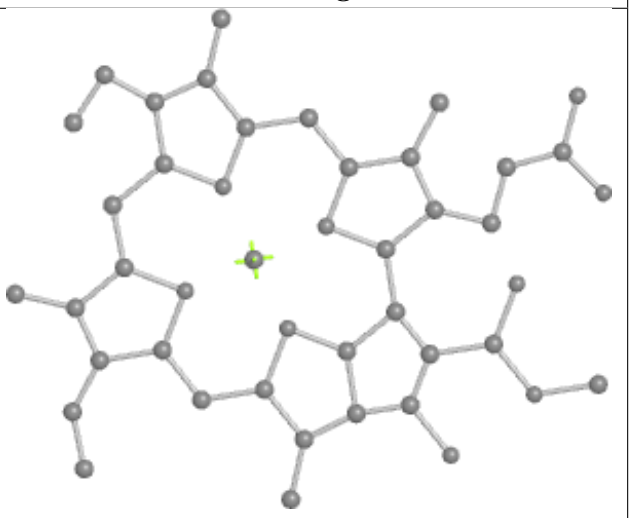
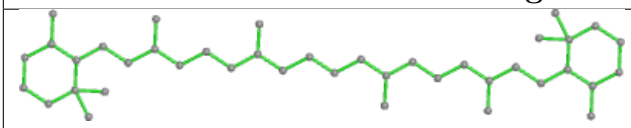


Rings

Ligand BCR b 522



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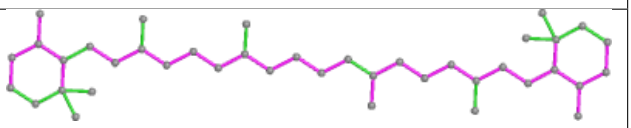

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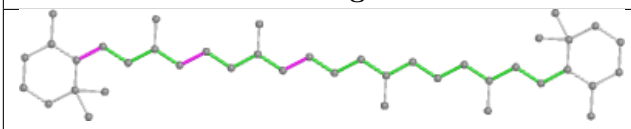
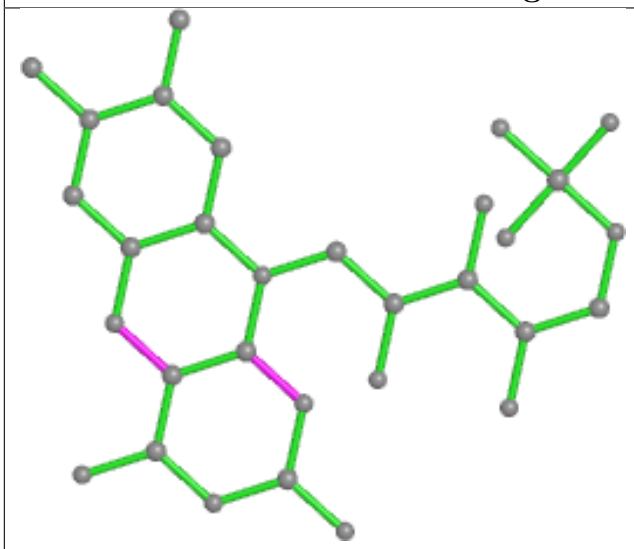


Torsions

Rings

Ligand FMN p 170



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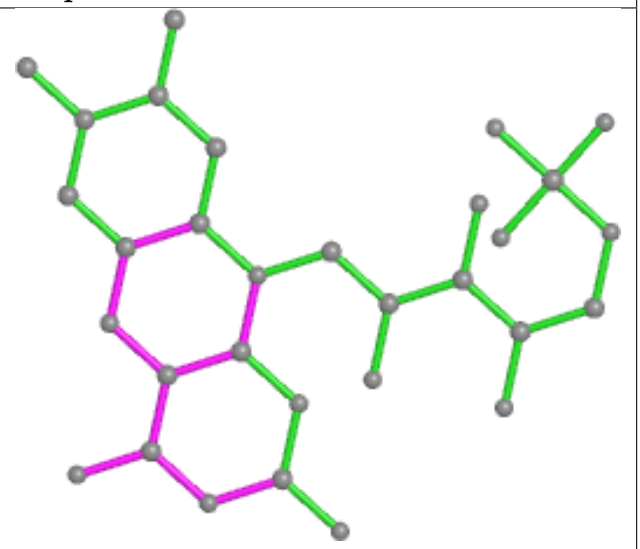

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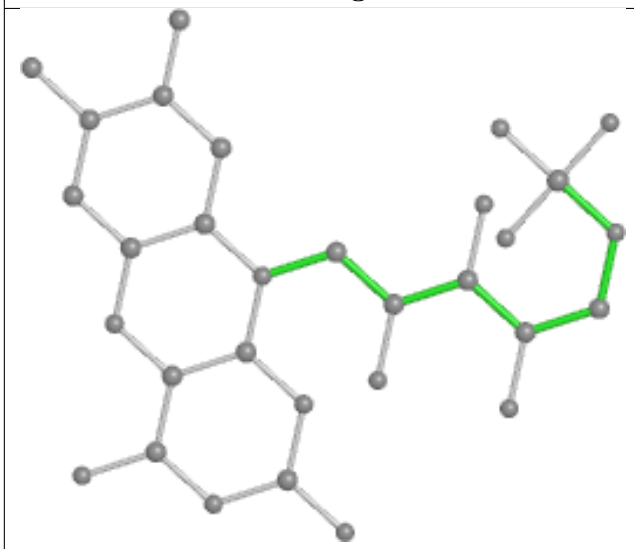

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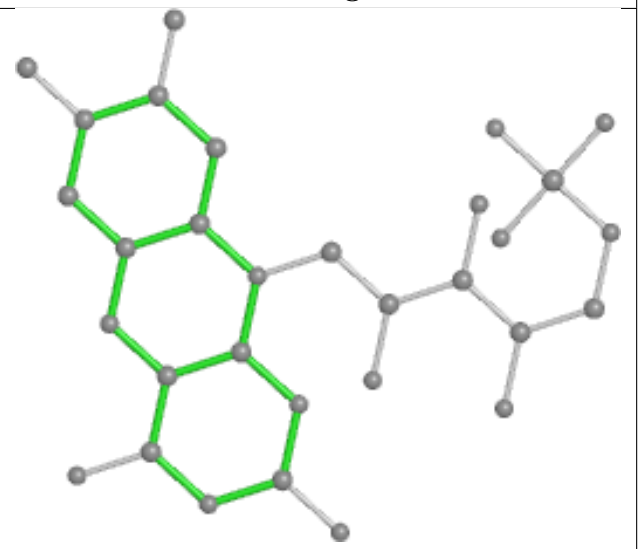
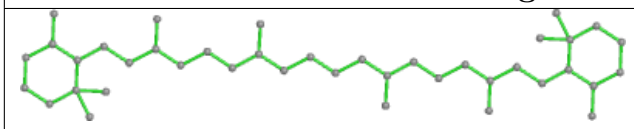


Rings

Ligand BCR o 4021



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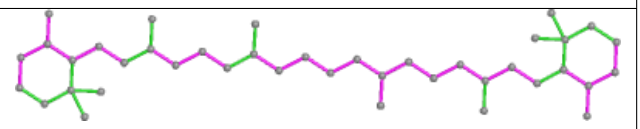

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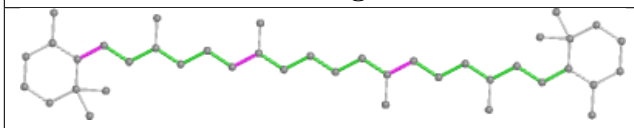

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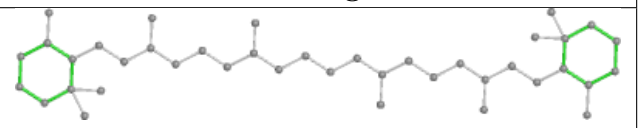
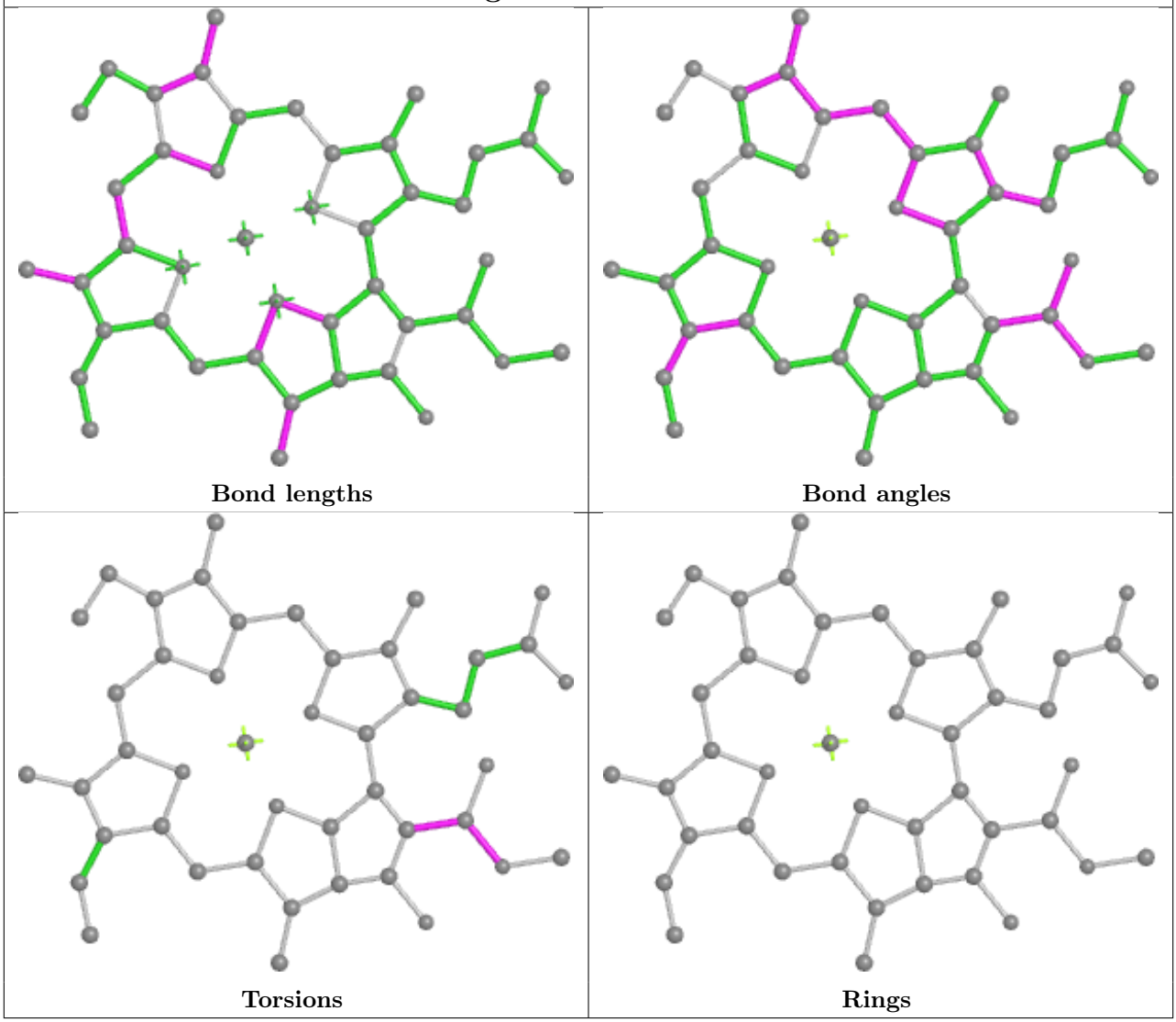


Rings

Ligand CLA 1 504



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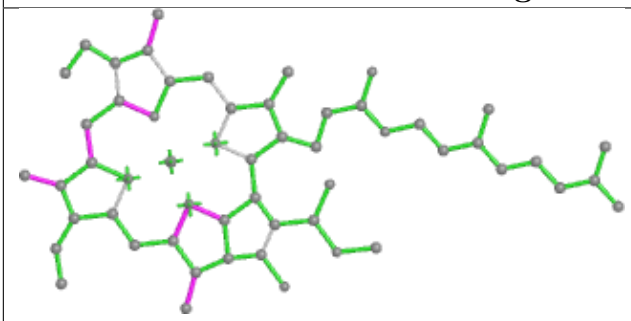
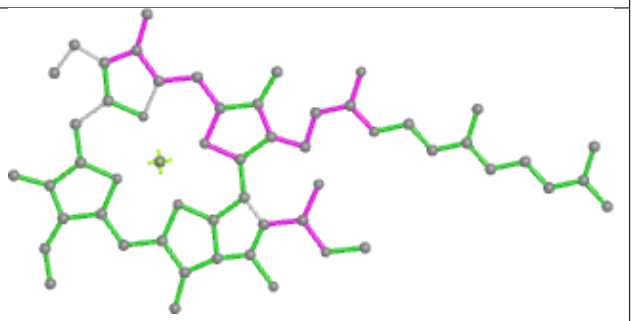
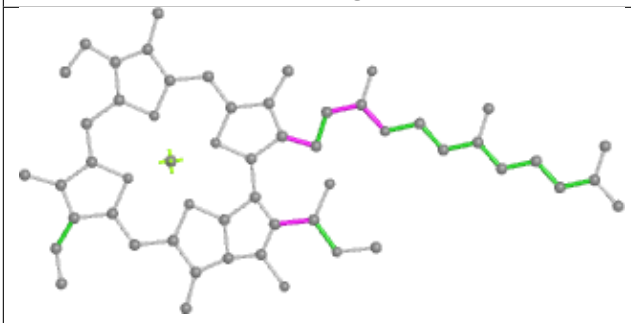
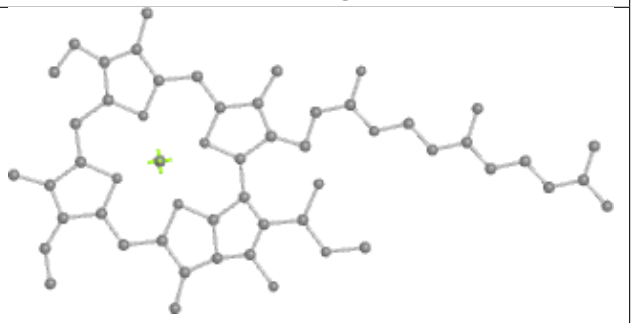
 Bond lengths	 Bond angles
 Torsions	 Rings

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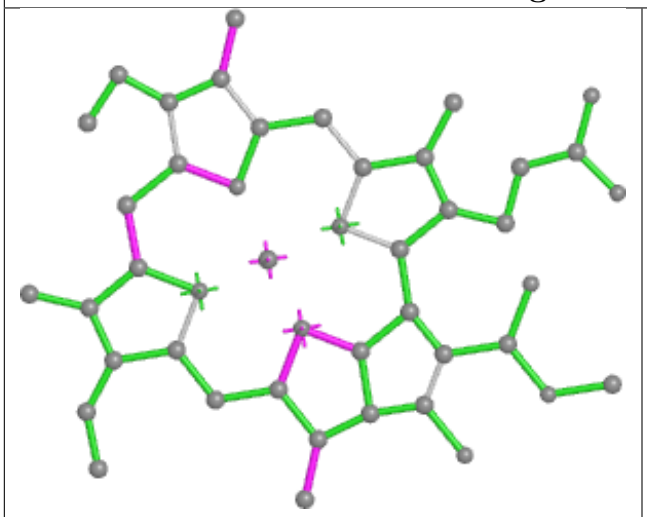

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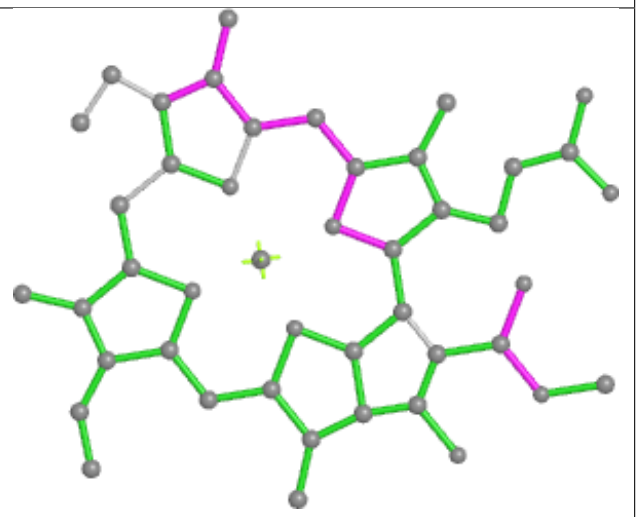

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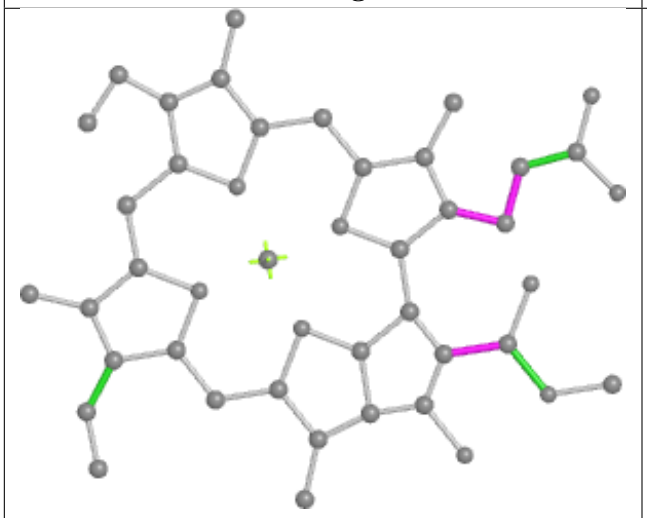

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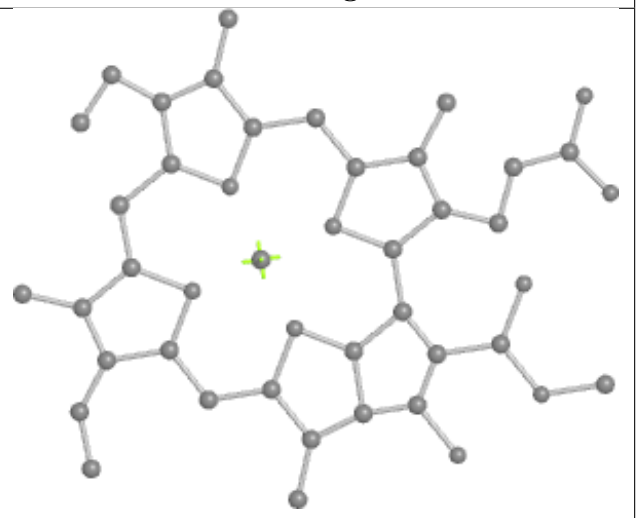
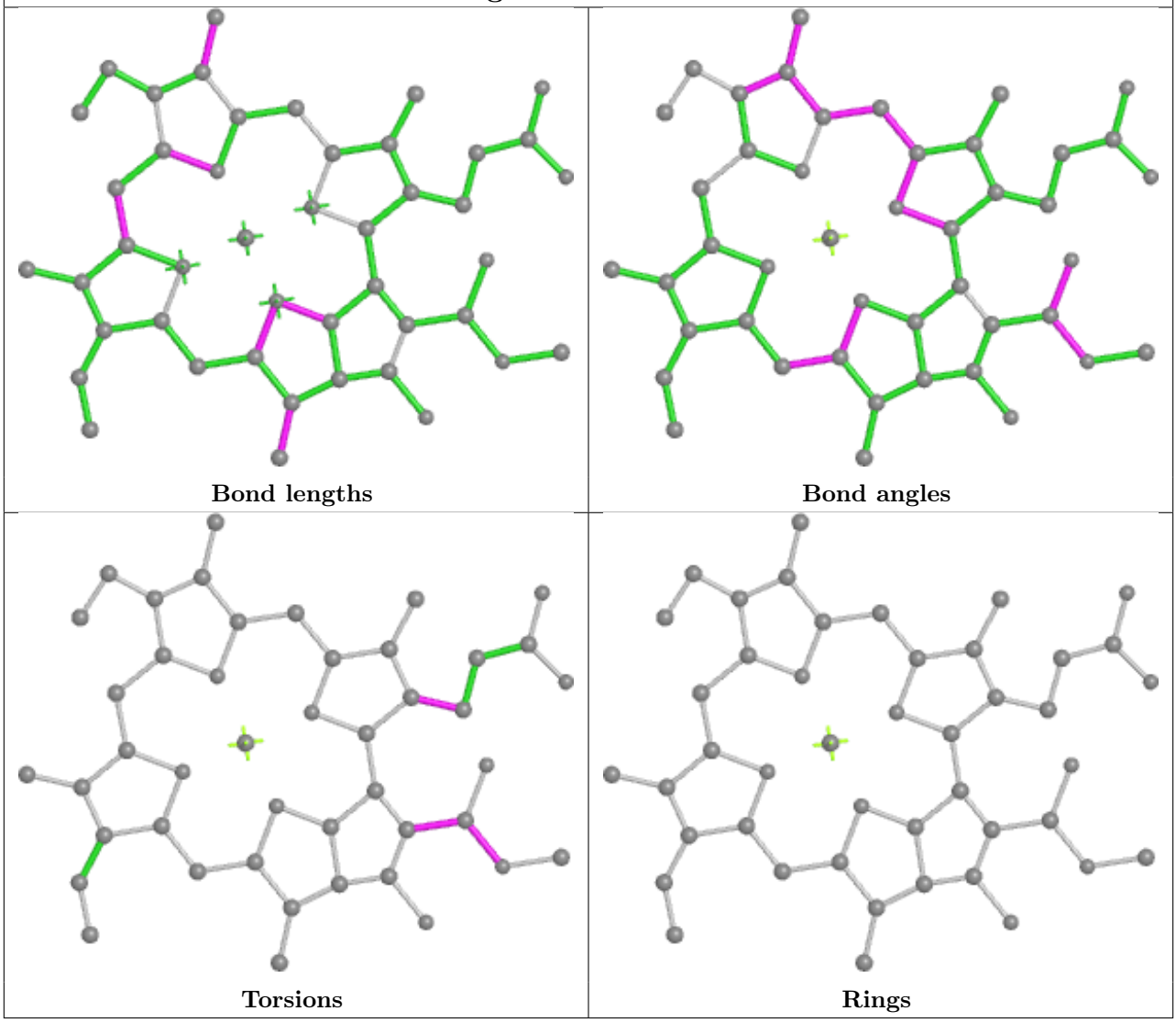


Rings

Ligand CLA t 504



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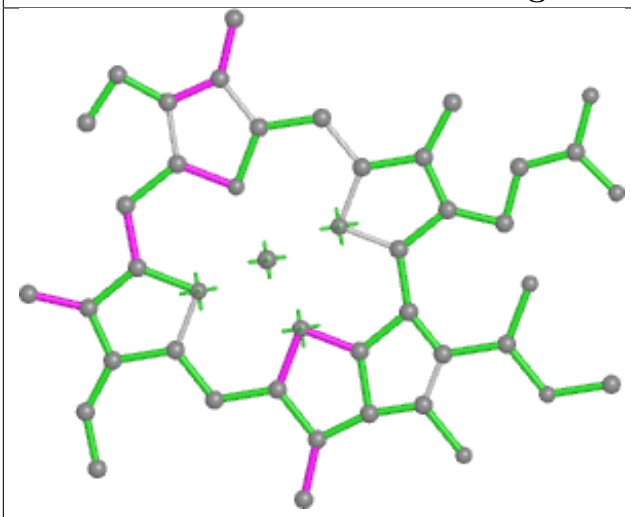

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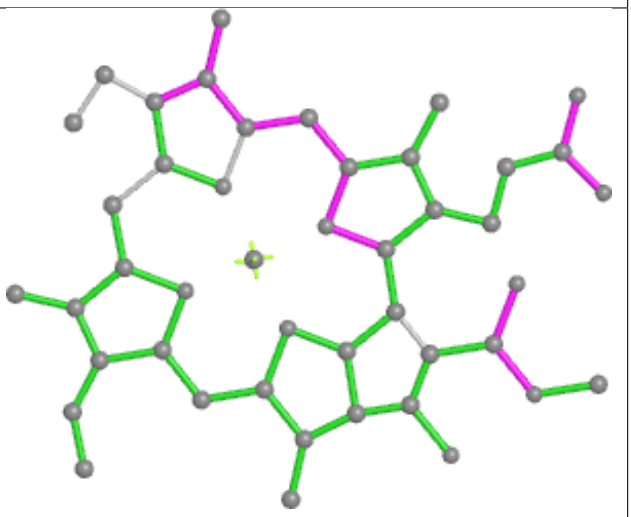

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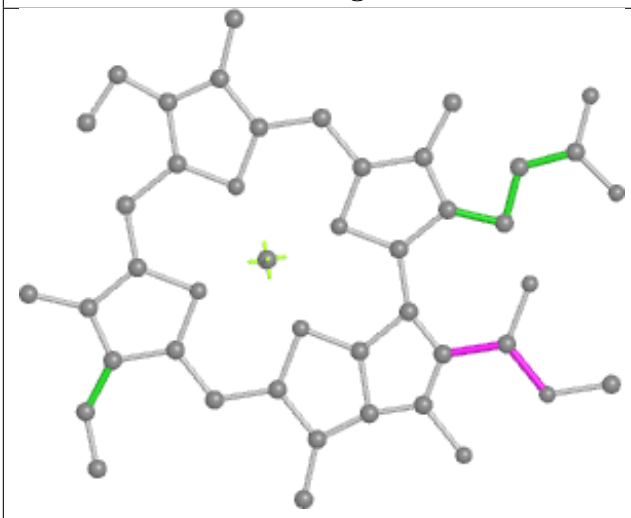

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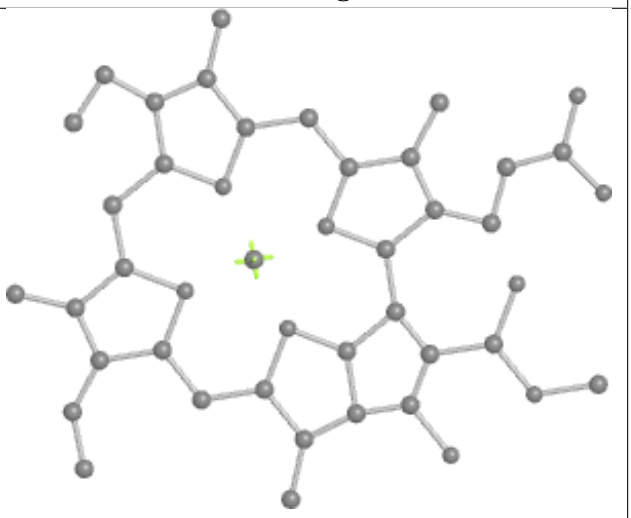

Rings

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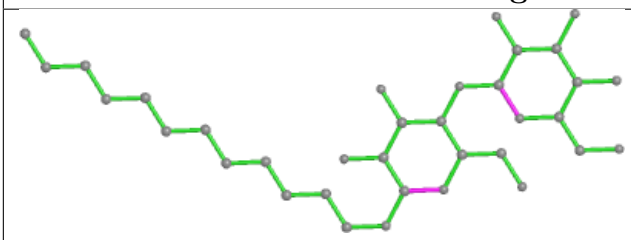

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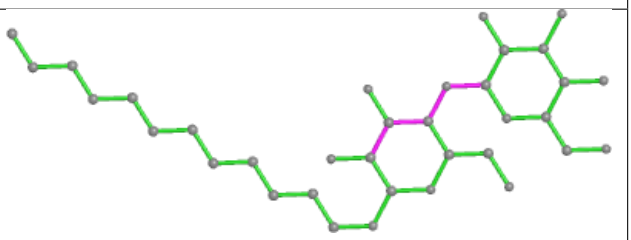

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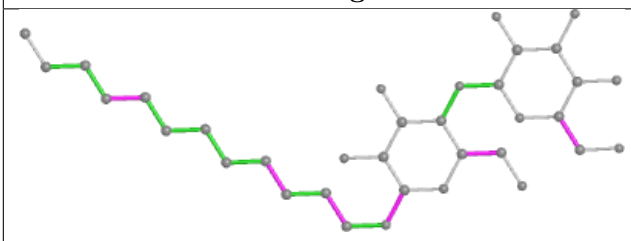

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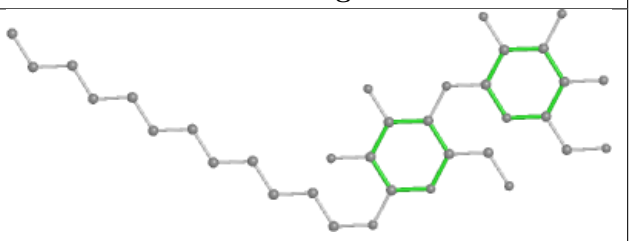
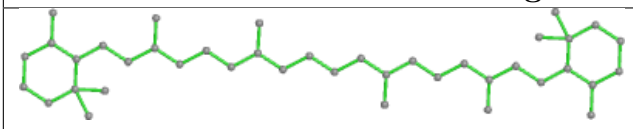


Rings

Ligand BCR Z 522



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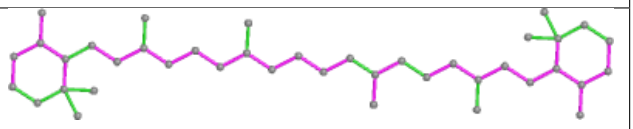

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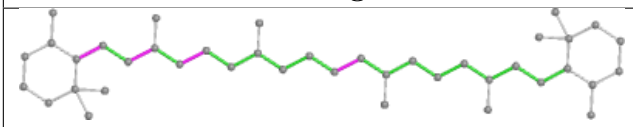

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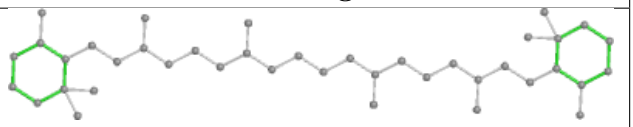
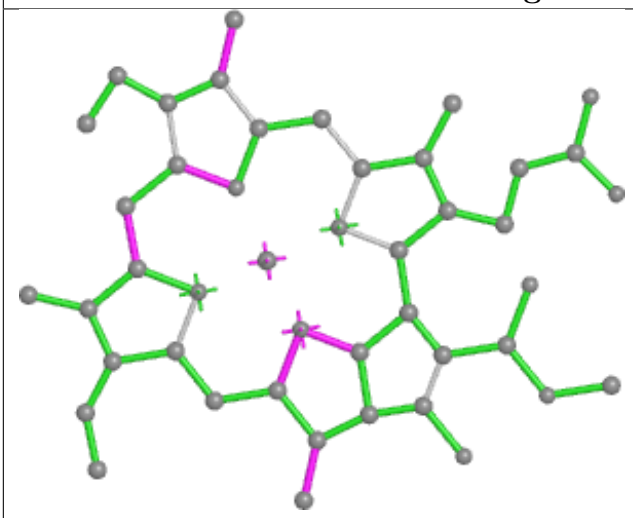


Rings

Ligand CLA Y 509



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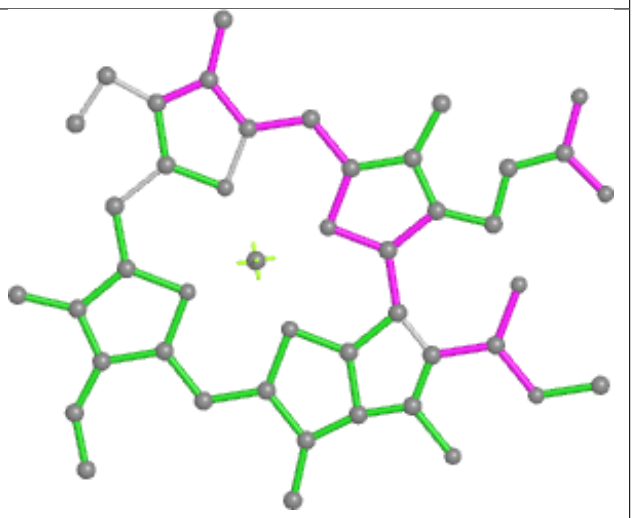

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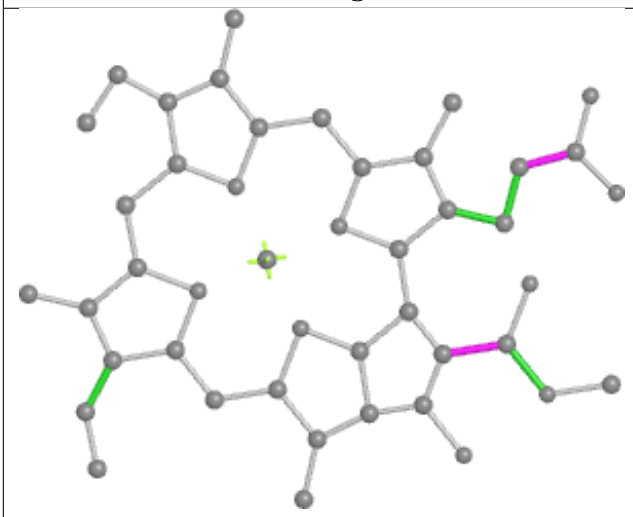

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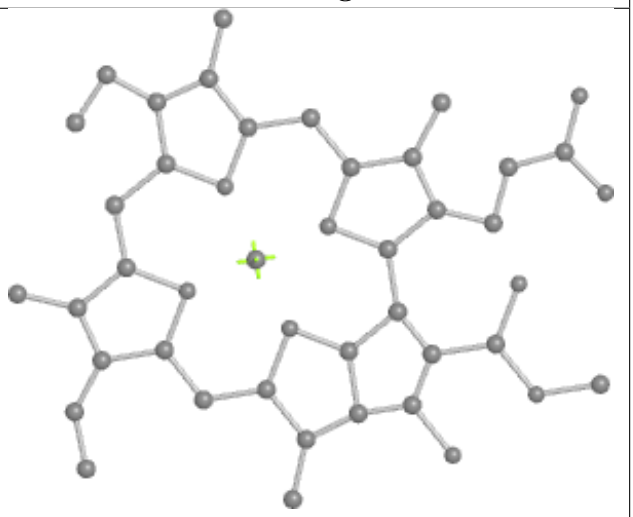
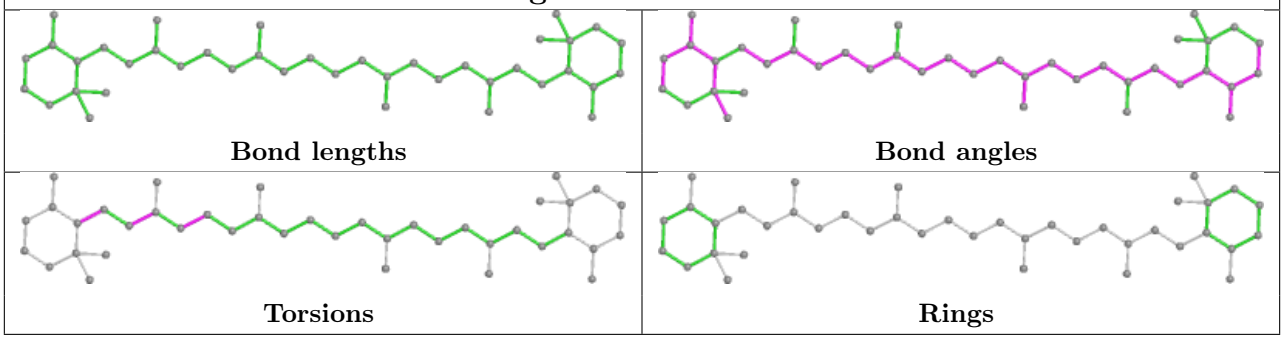
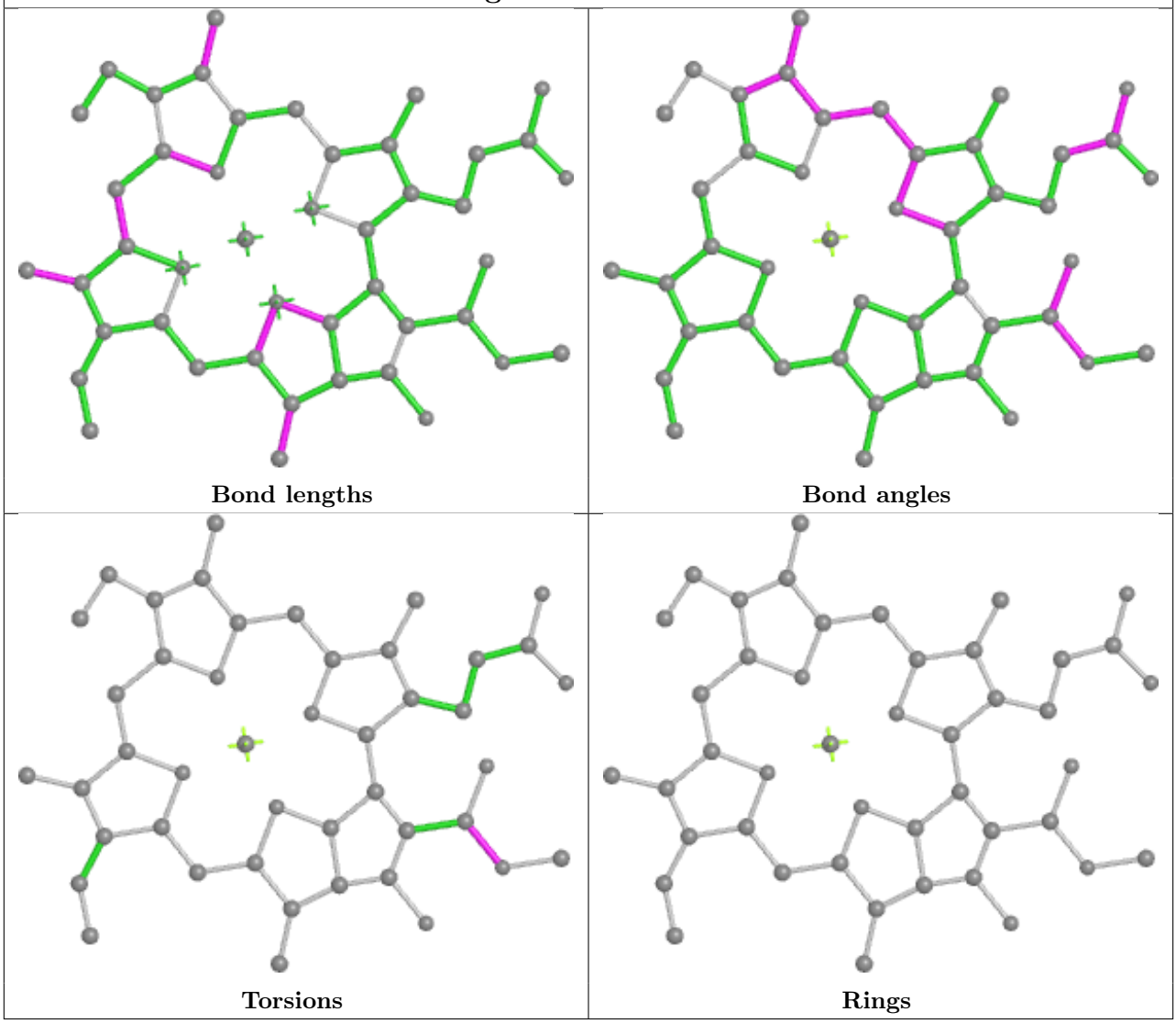


Rings

Ligand BCR s 522



Ligand CLA a 509



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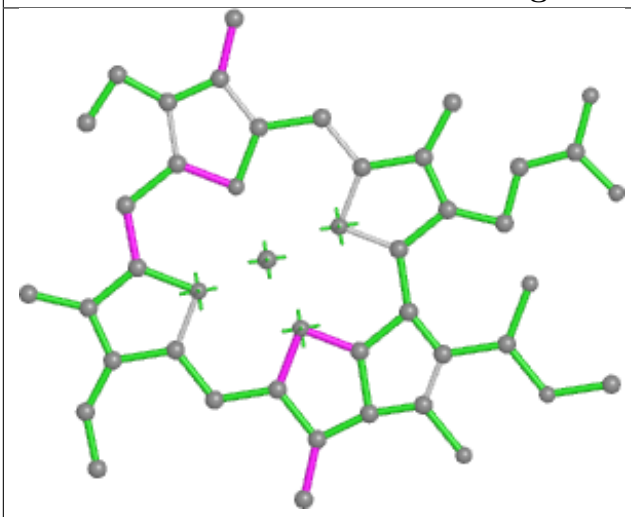
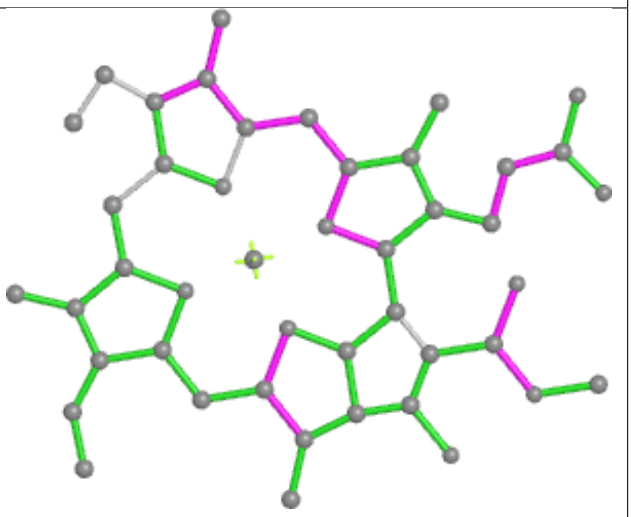
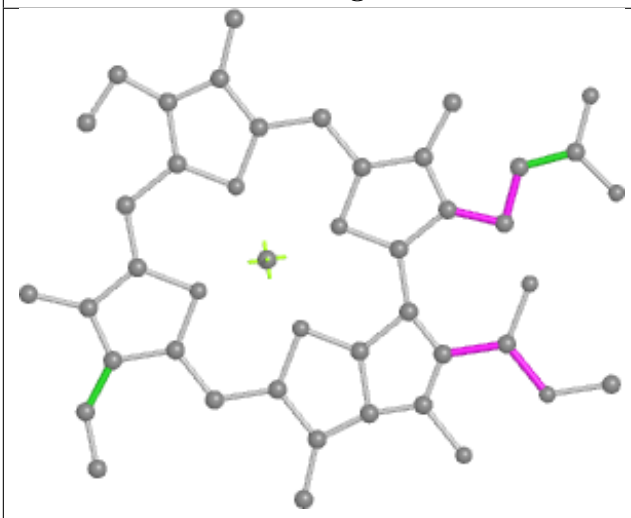


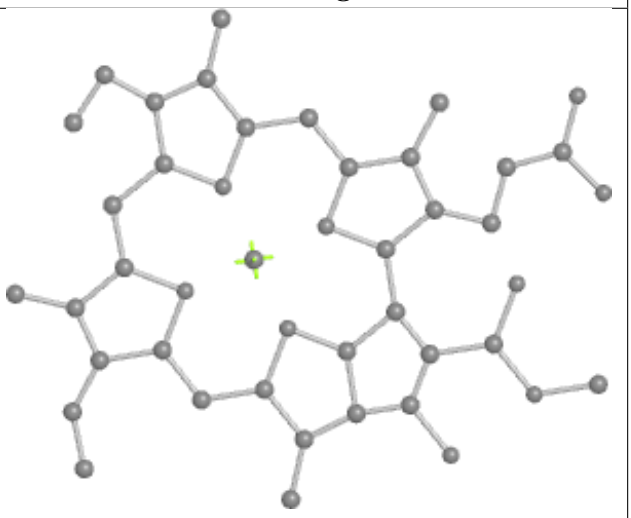
Bond lengths



Bond angles

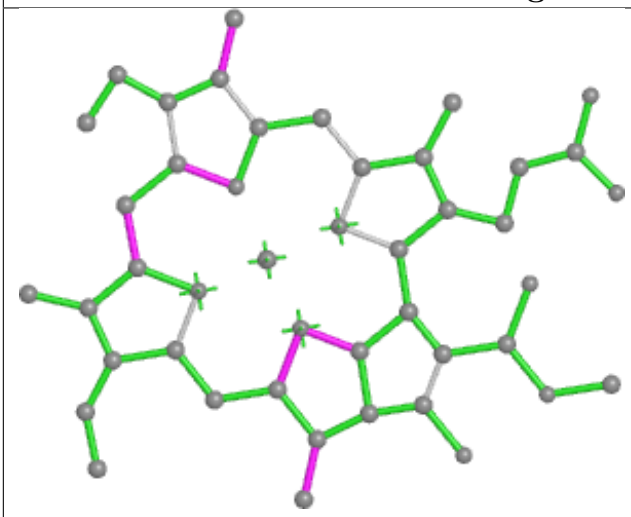


Torsions



Rings

Ligand CLA b 512



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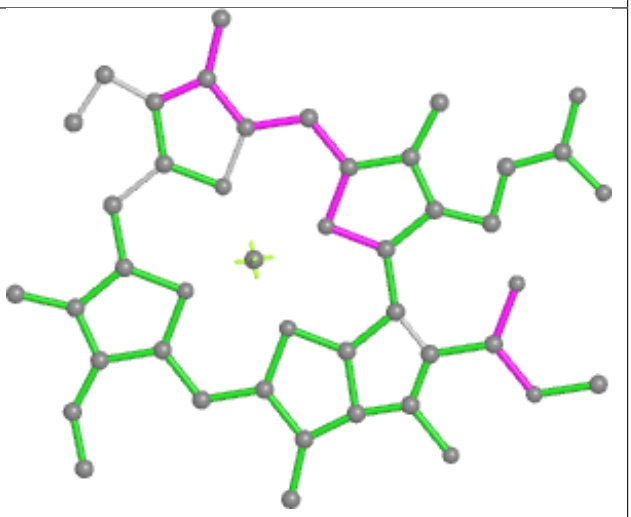

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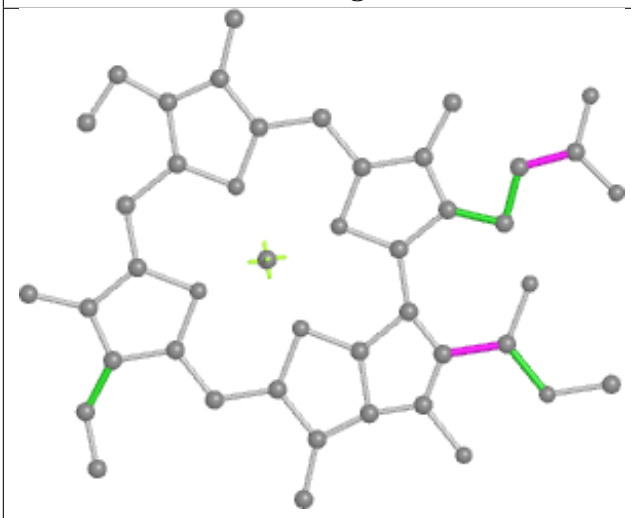

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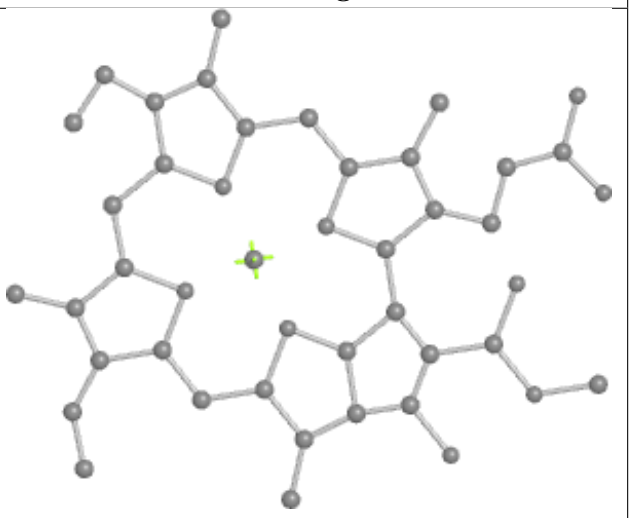
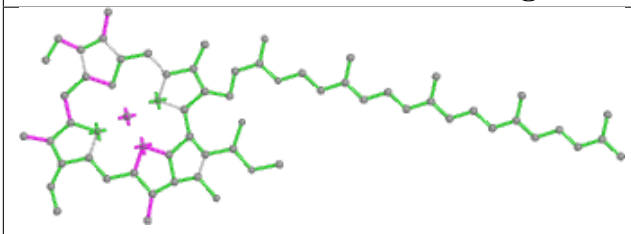


Rings

Ligand CLA e 1111



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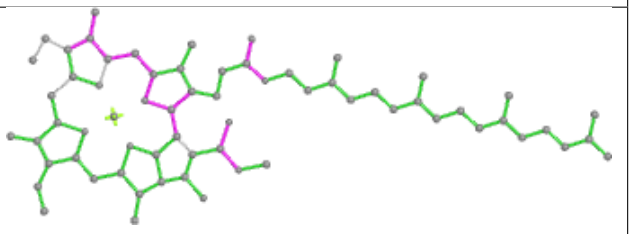

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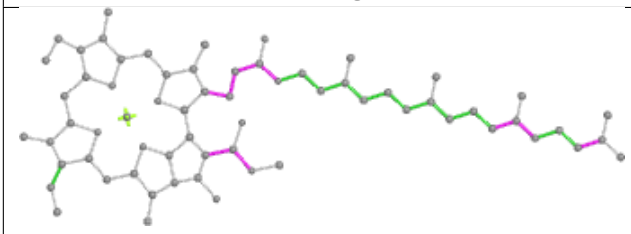

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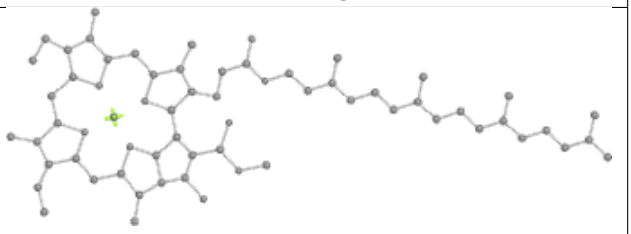
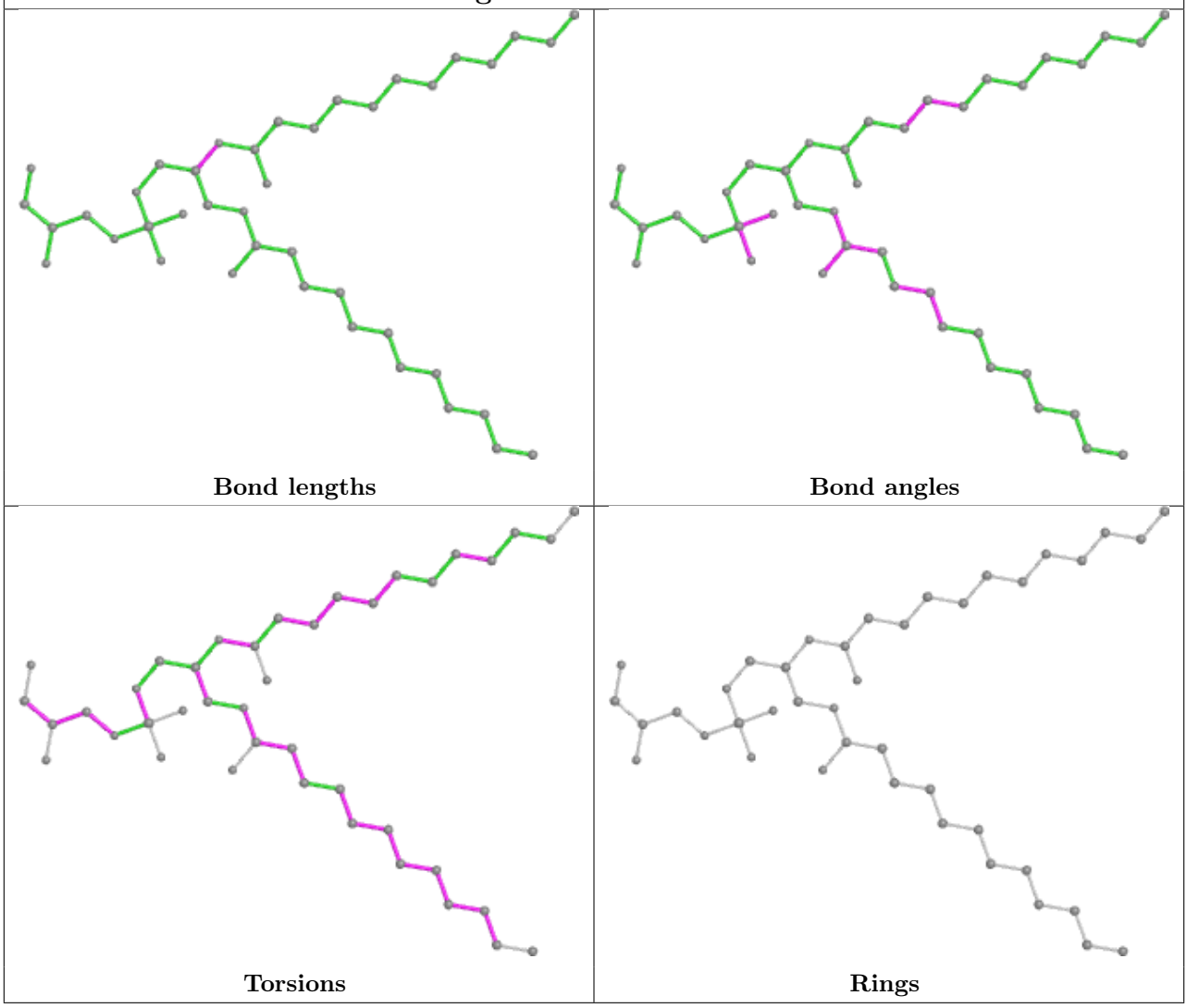
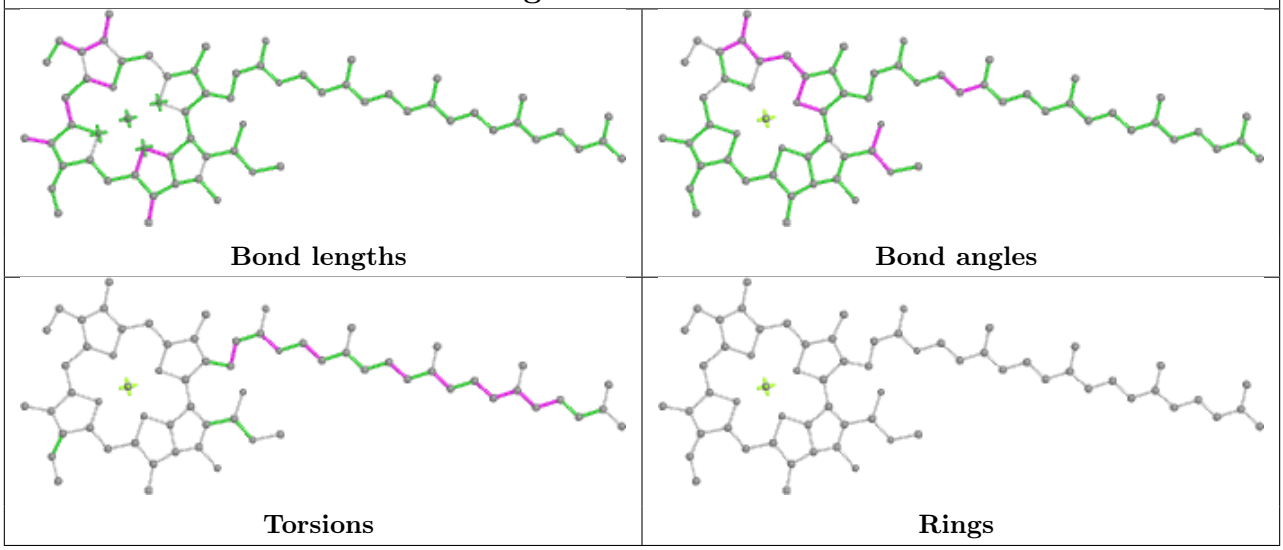


Rings

Ligand LHG V 5220



Ligand CLA f 1214



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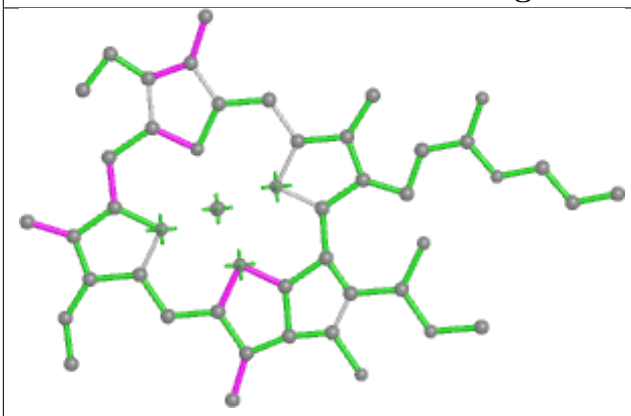
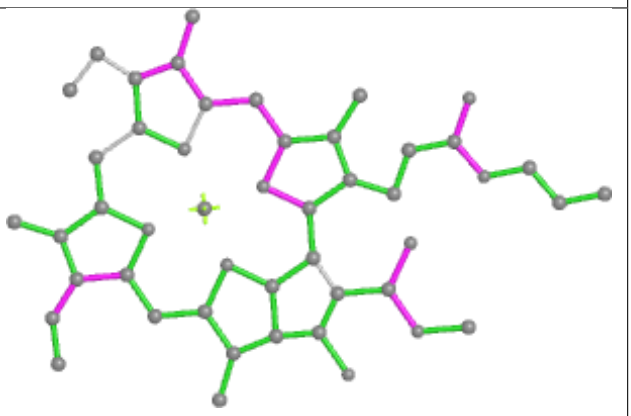
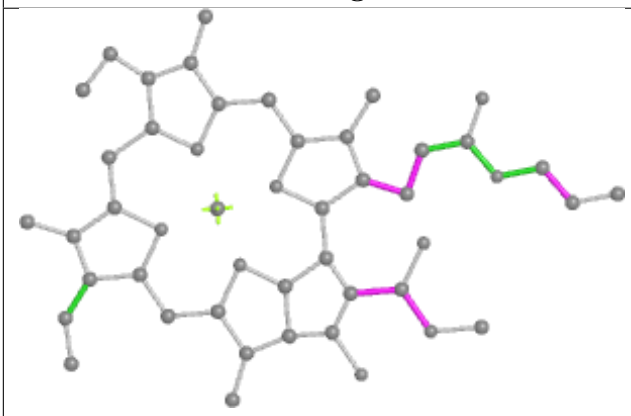


Bond lengths



Bond angles



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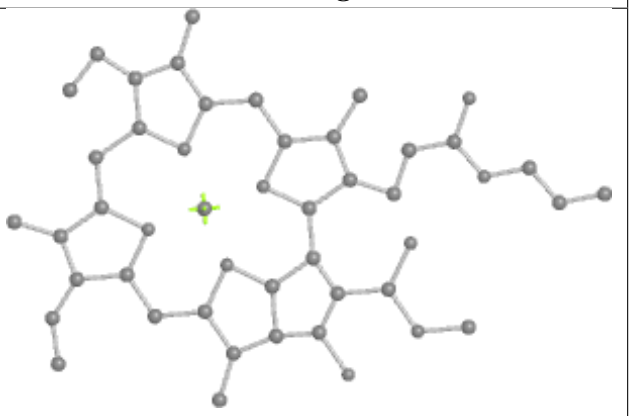
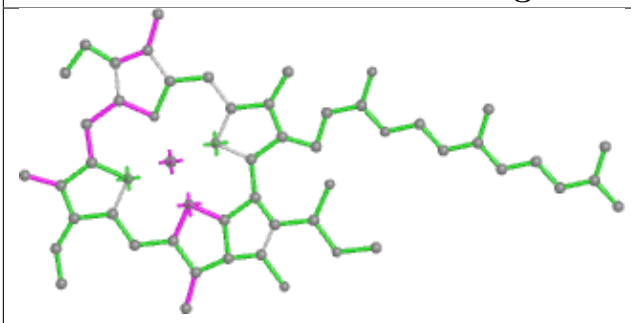


Rings

Ligand CLA G 1121



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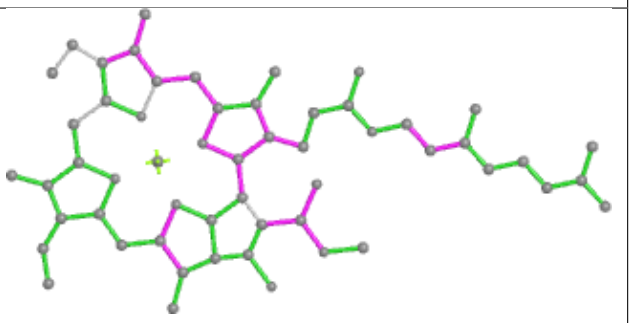

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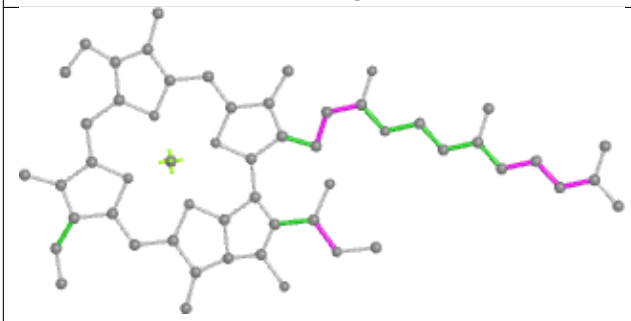

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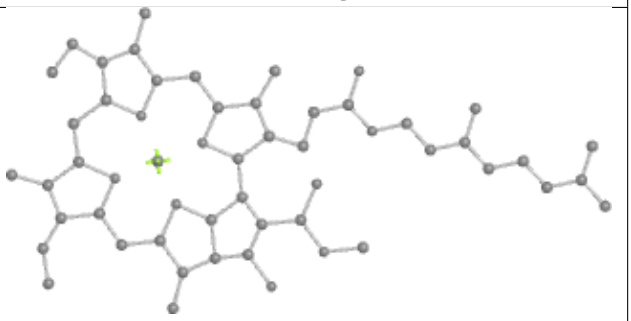
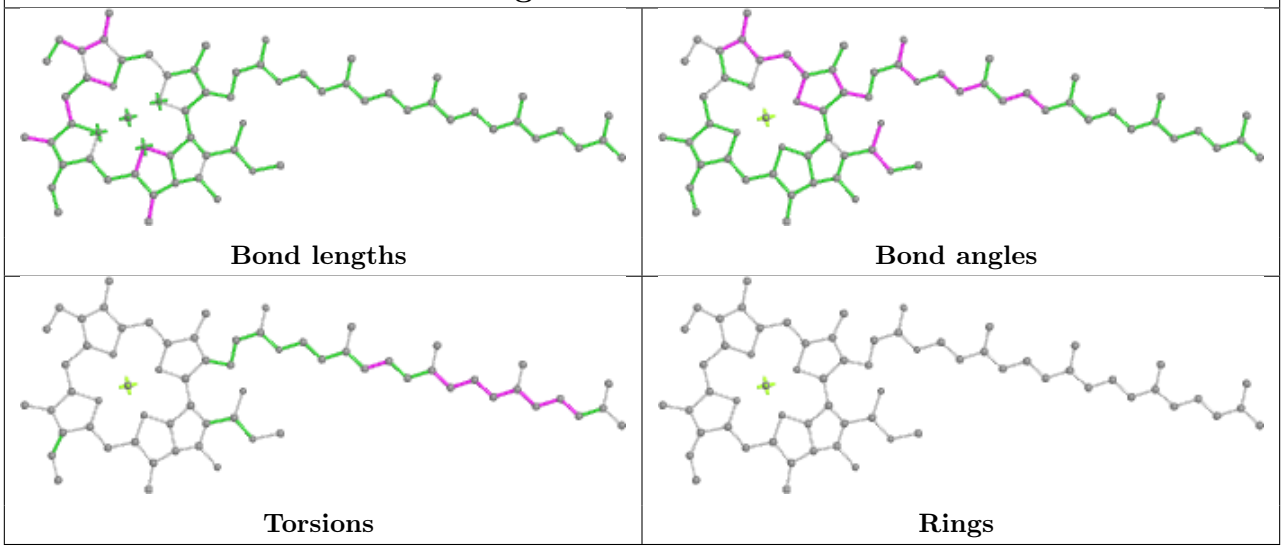
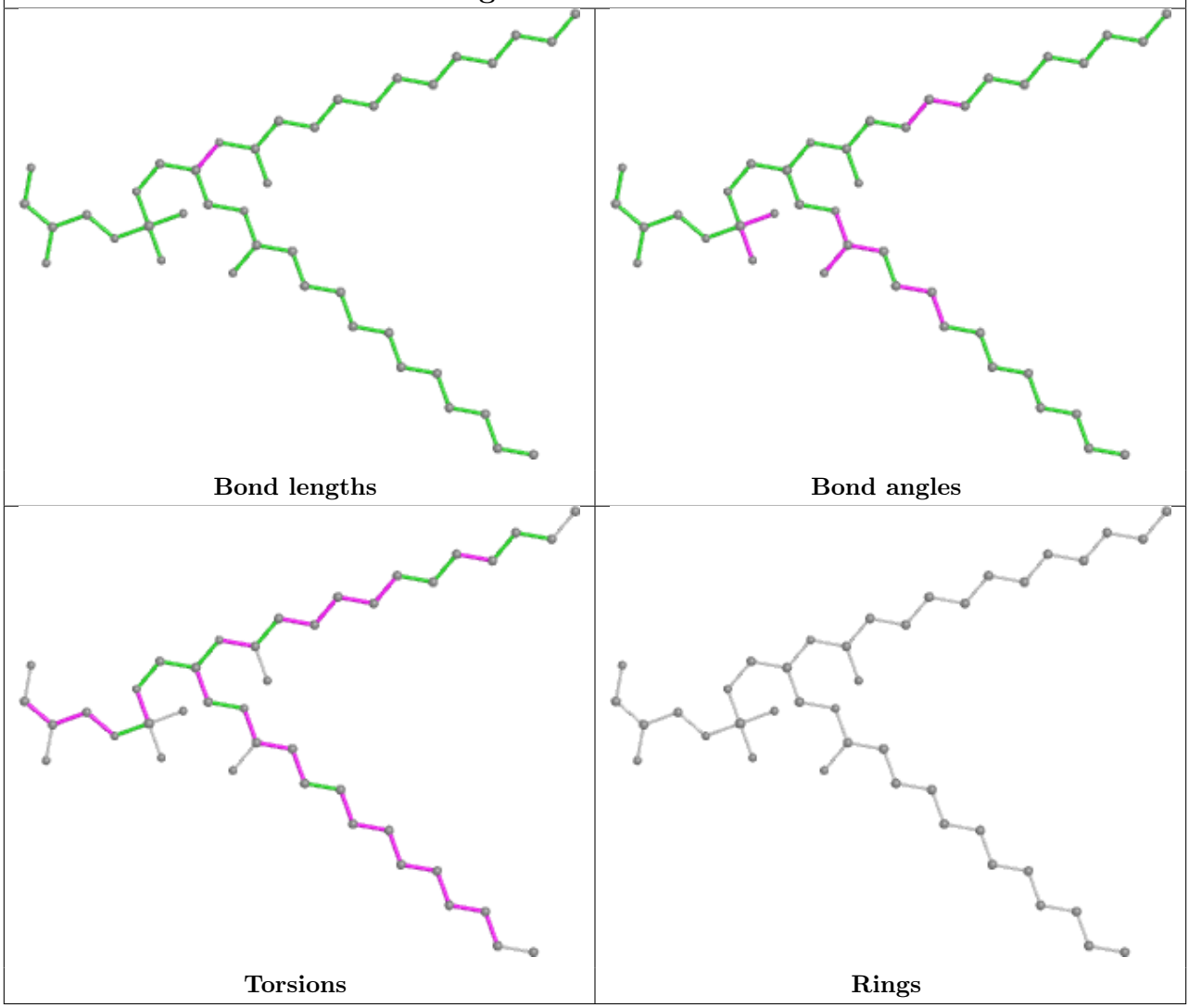


Rings

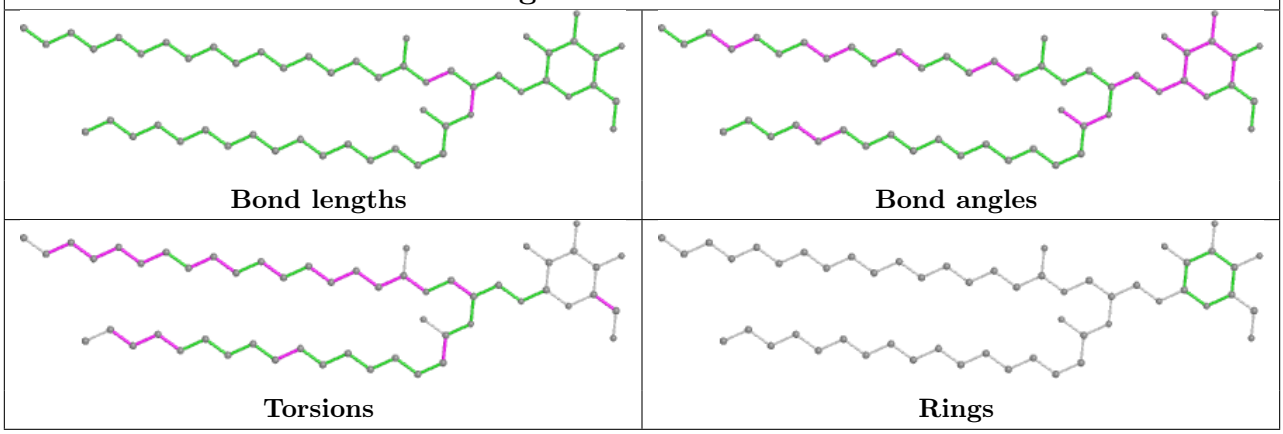
Ligand CLA G 1136



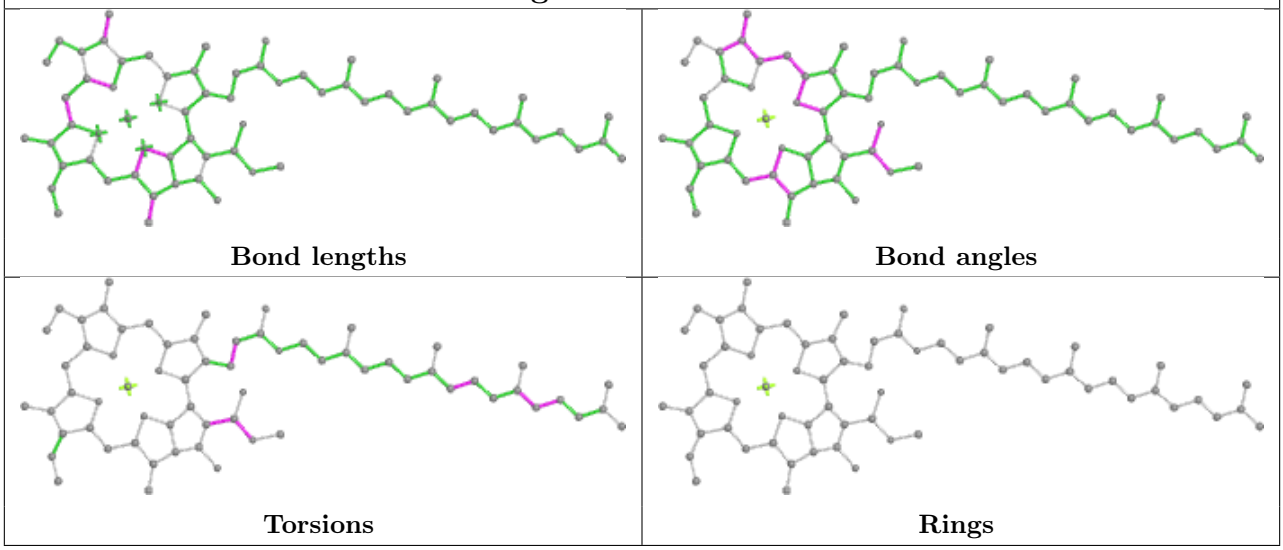
Ligand LHG L 5220



Ligand LMG f 5002



Ligand CLA r 503



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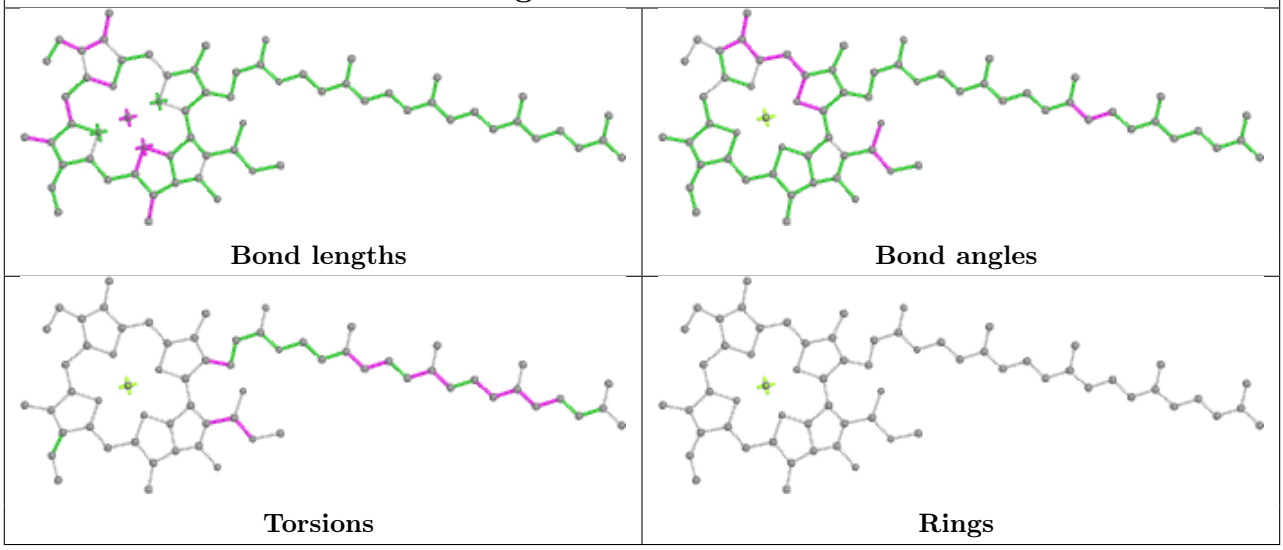

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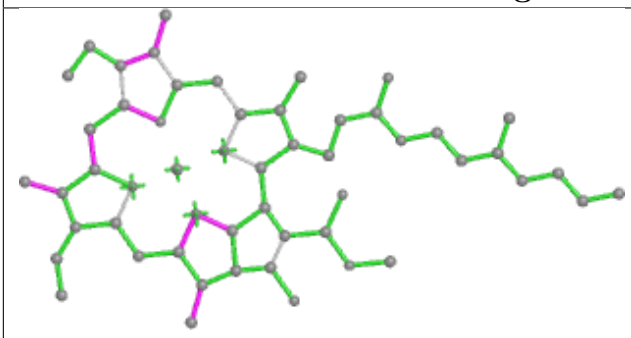
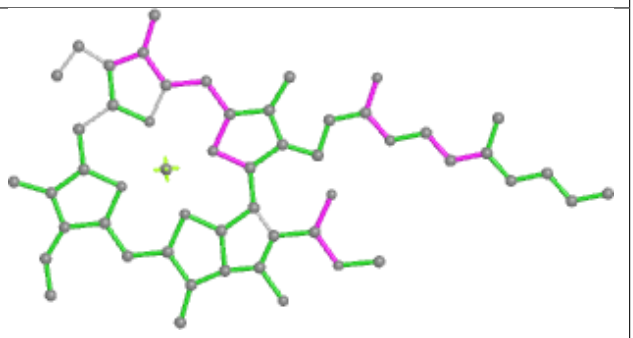
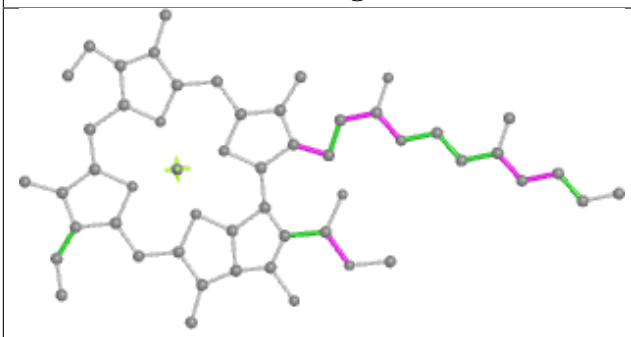
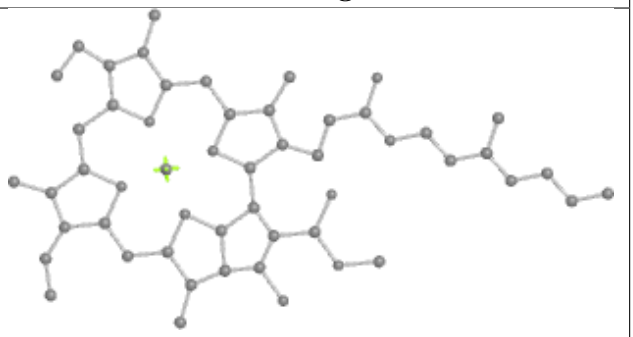
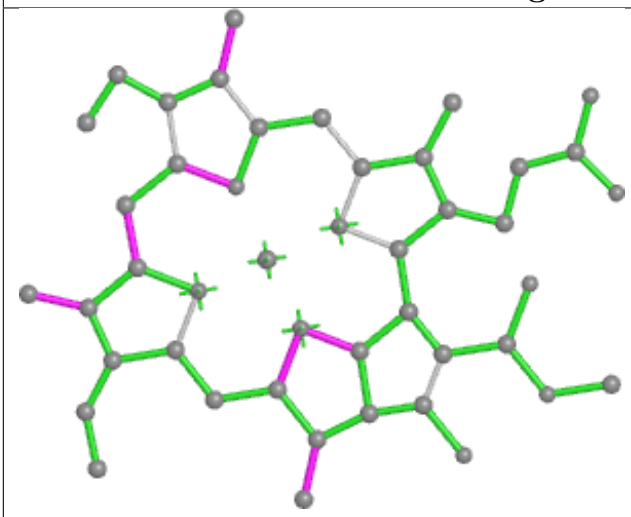
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 509



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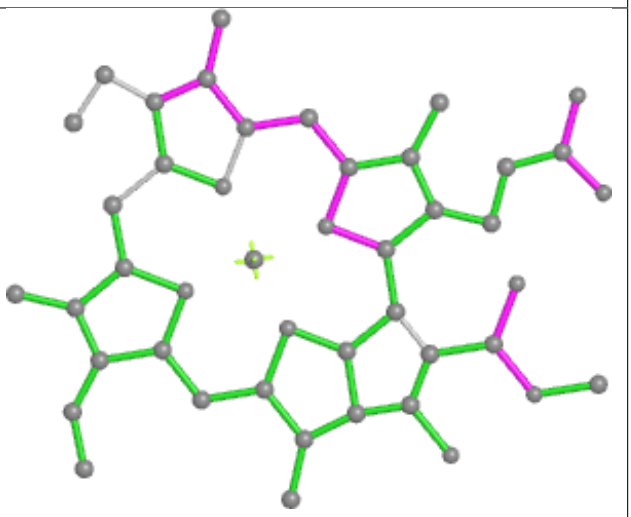
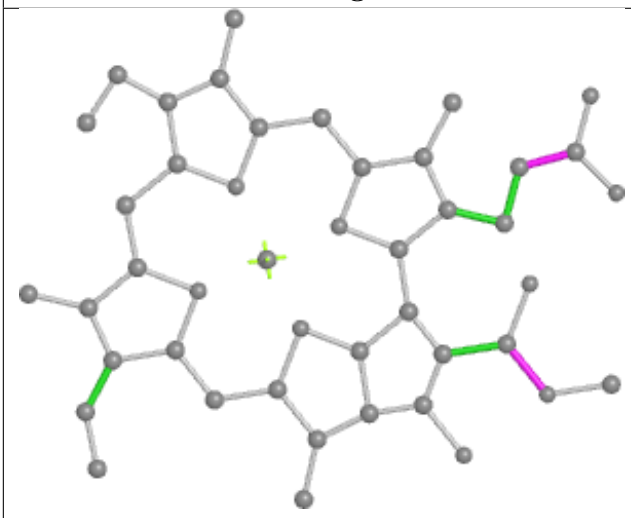


Bond angles



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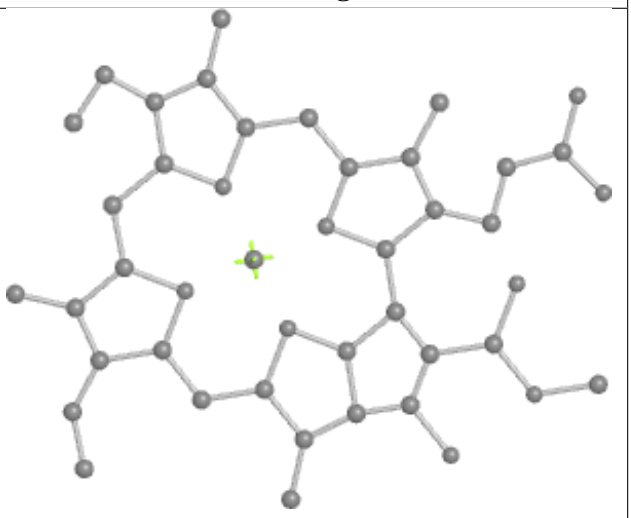

Rings

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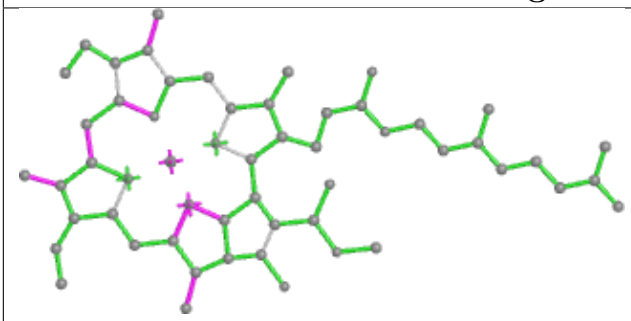
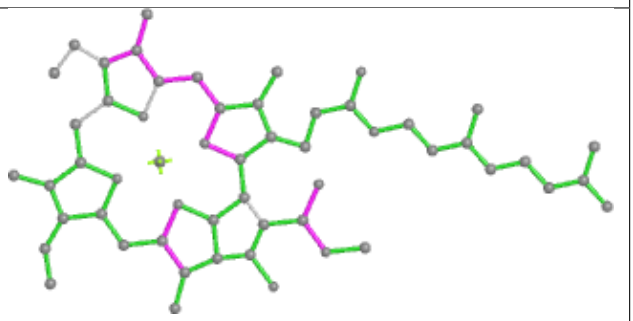
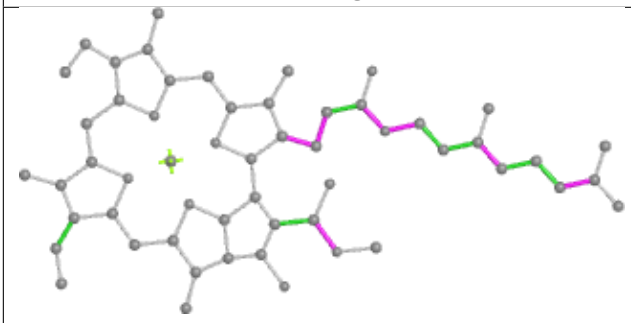
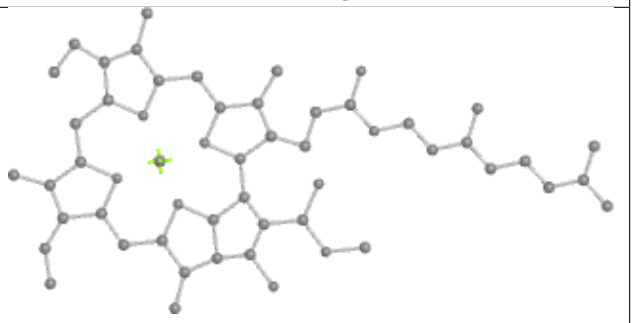
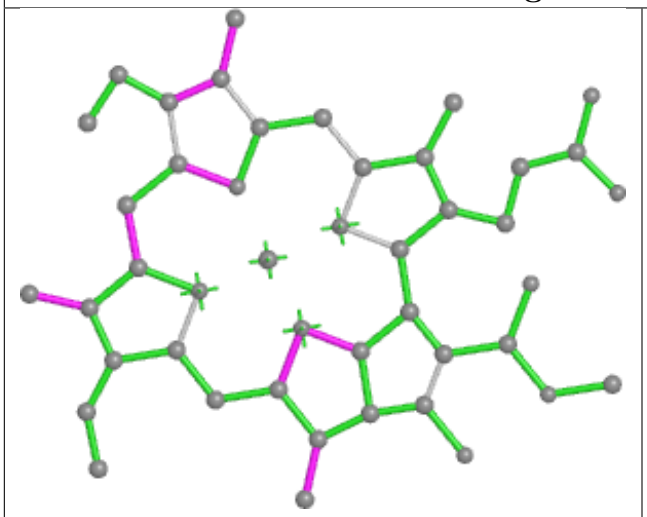
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 519



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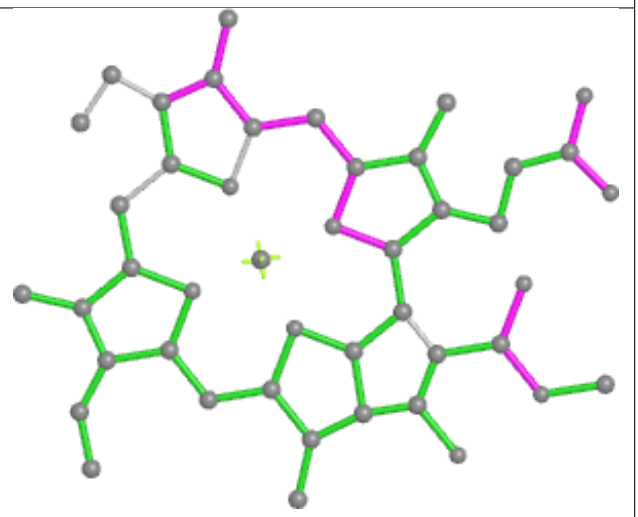

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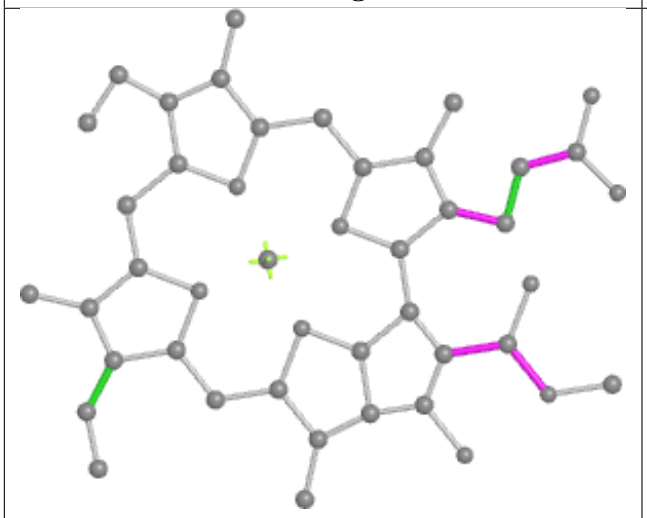

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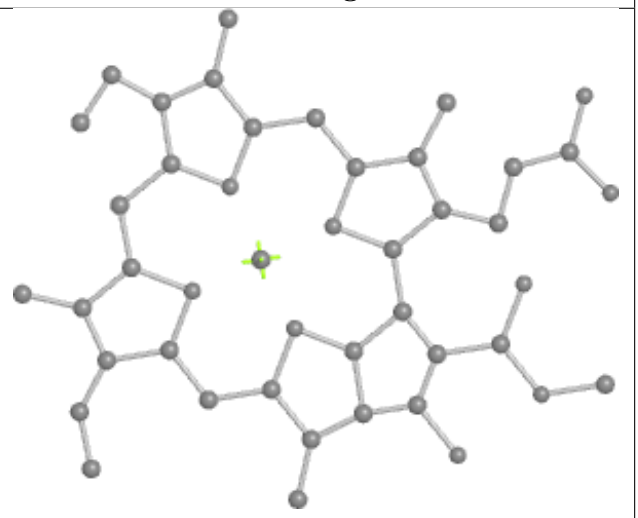

Rings

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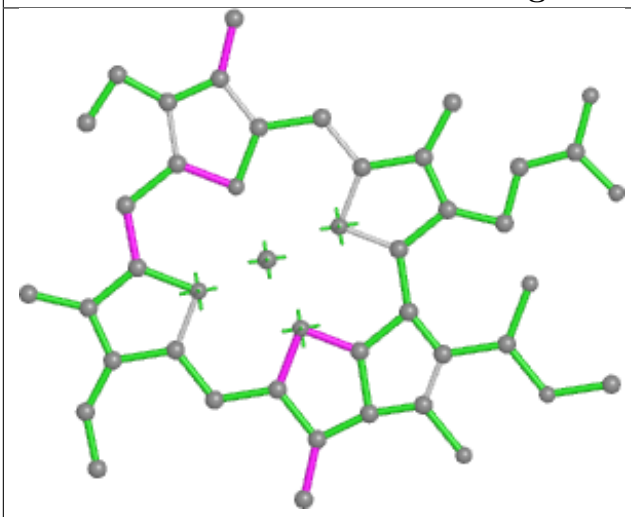

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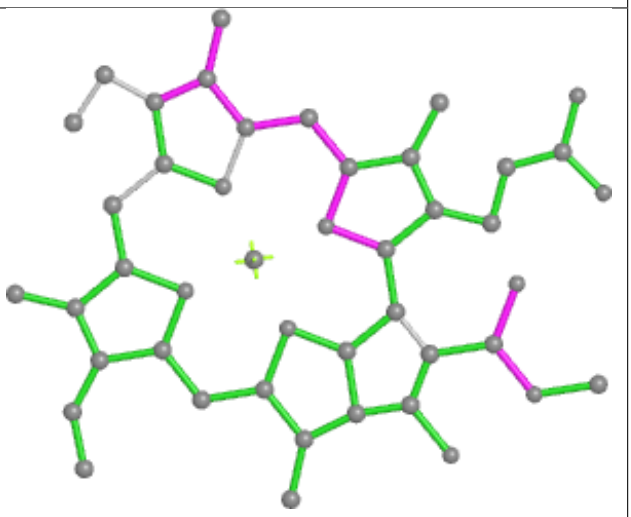

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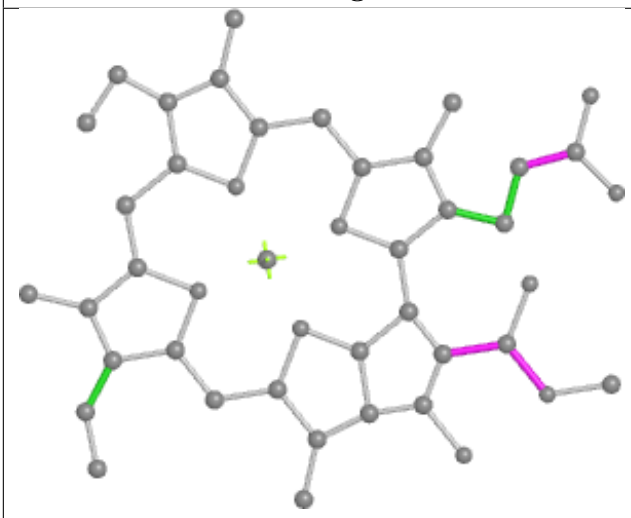

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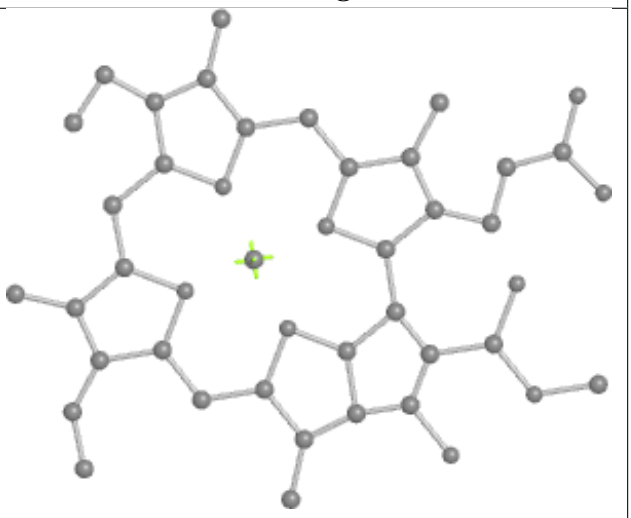
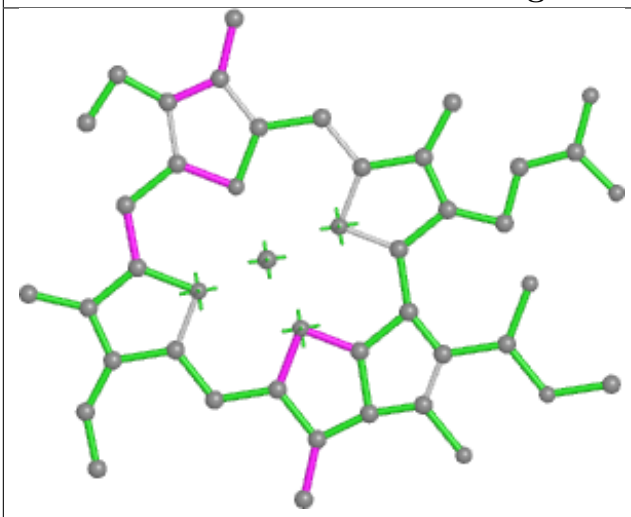


Rings

Ligand CLA d 502



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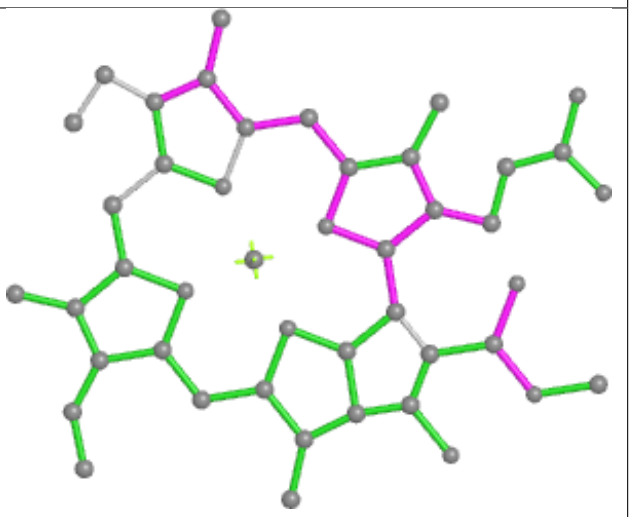

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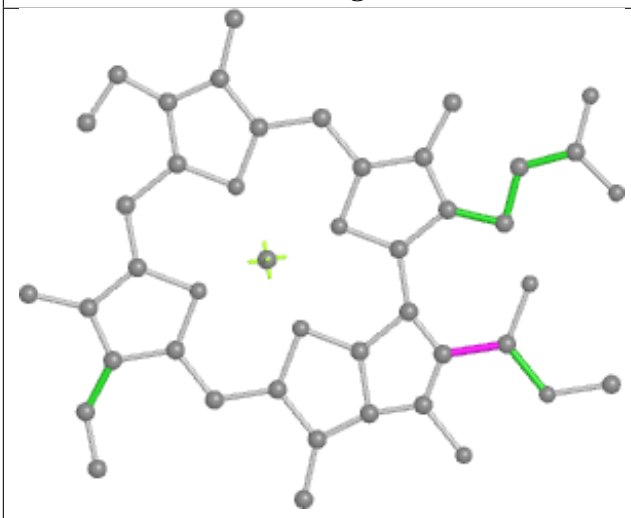

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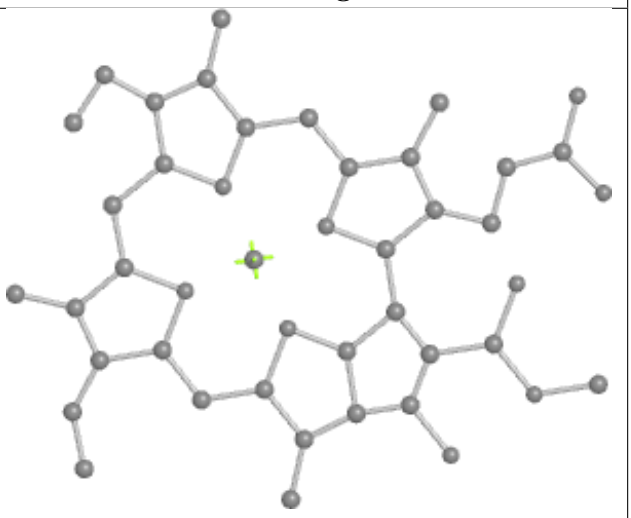
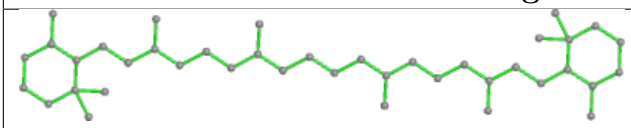


Rings

Ligand BCR Y 522



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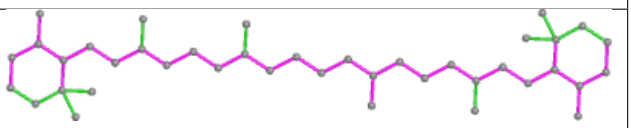
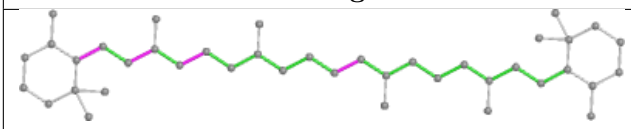


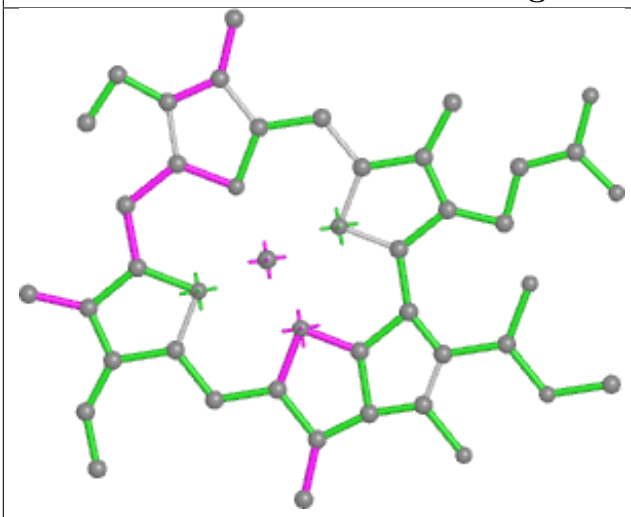
Bond angles



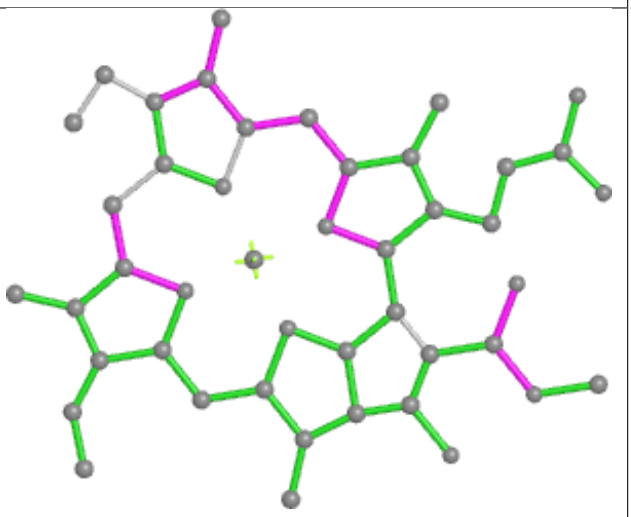
Torsions

Rings

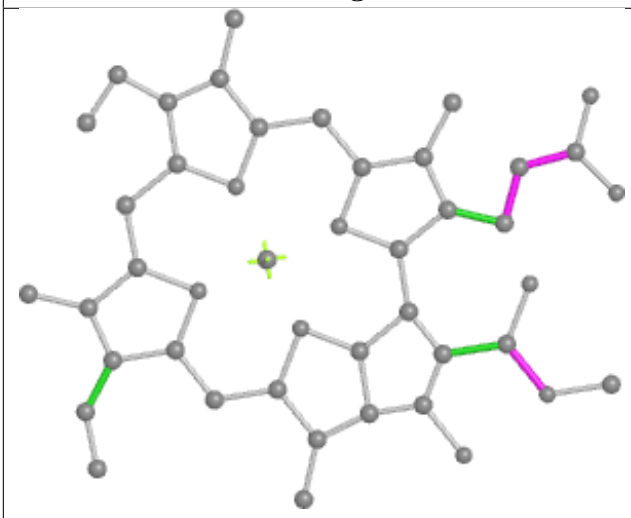
Ligand CLA 1 508



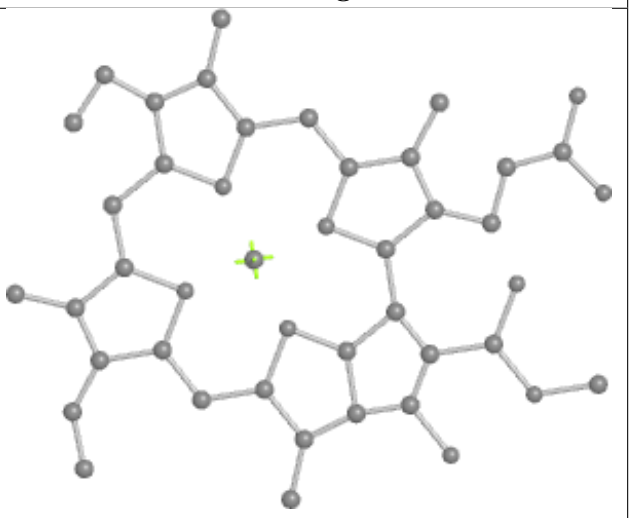
Bond lengths



Bond angles

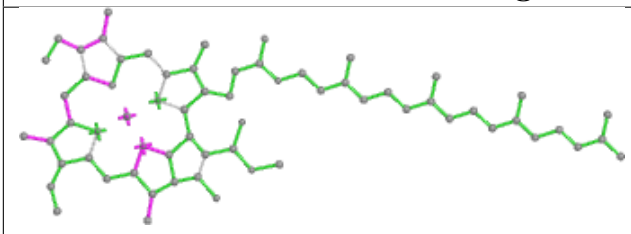


Torsions



Rings

Ligand CLA A 1131



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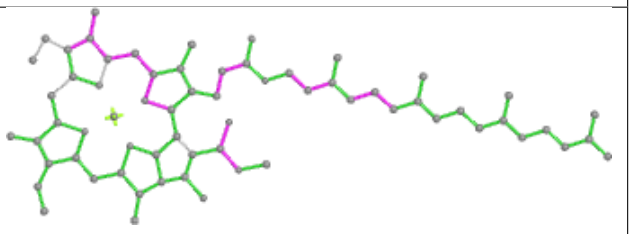

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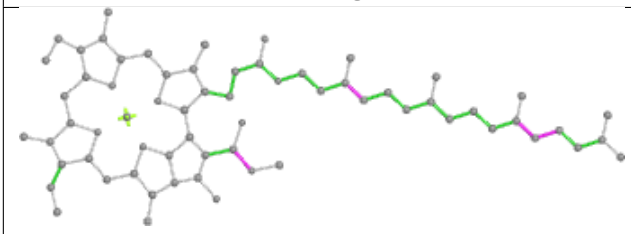
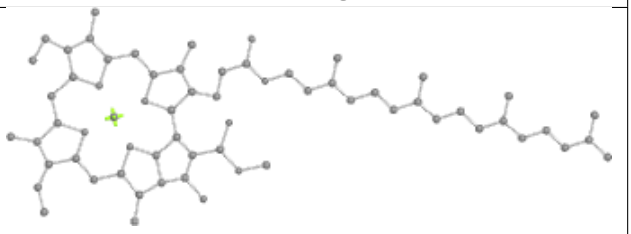
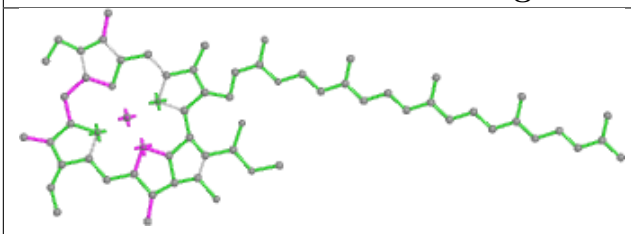
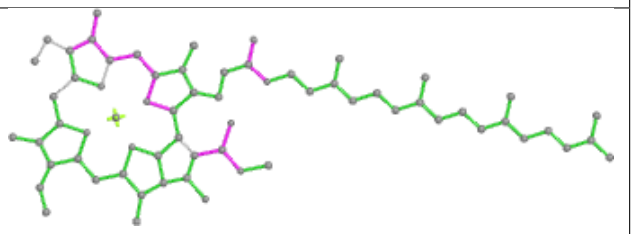
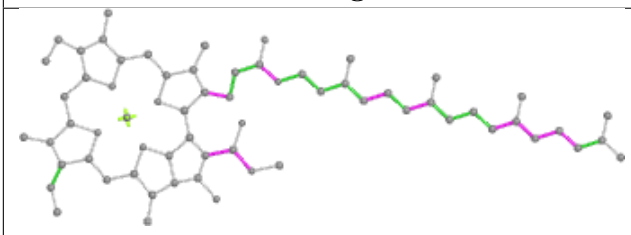
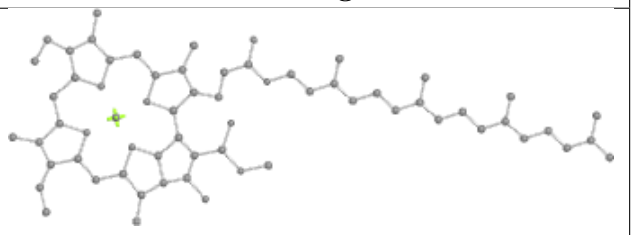


Torsions



Rings

Ligand CLA G 1109	
 Bond lengths	 Bond angles
 Torsions	 Rings

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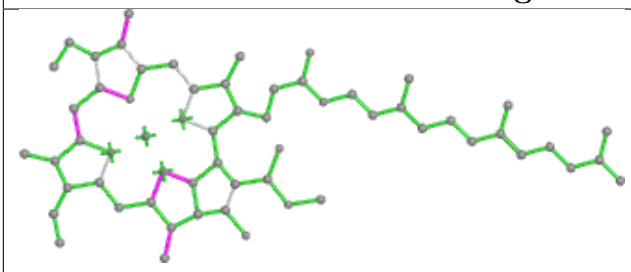
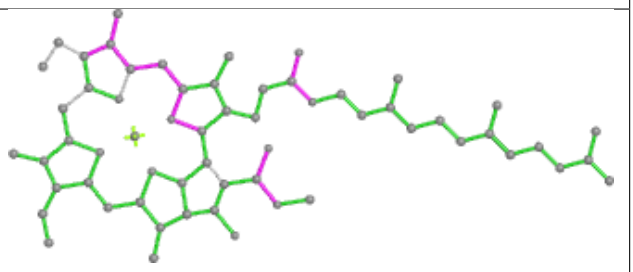
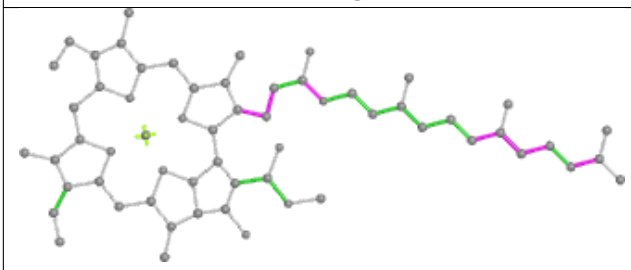
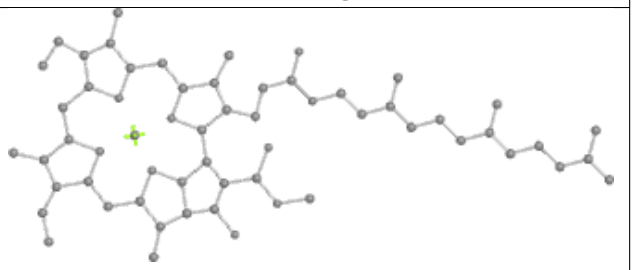
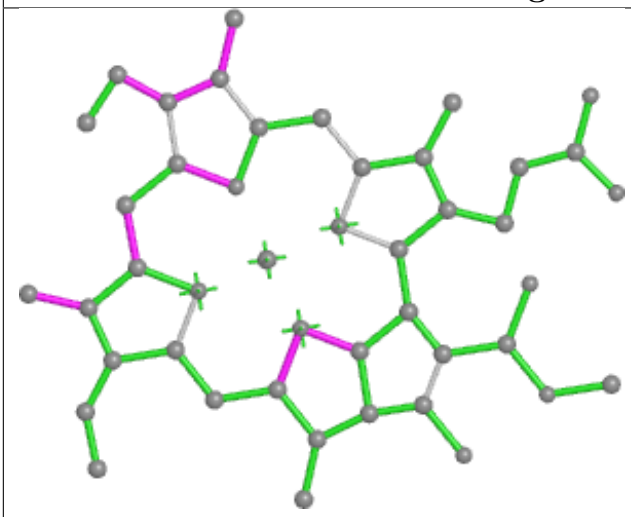
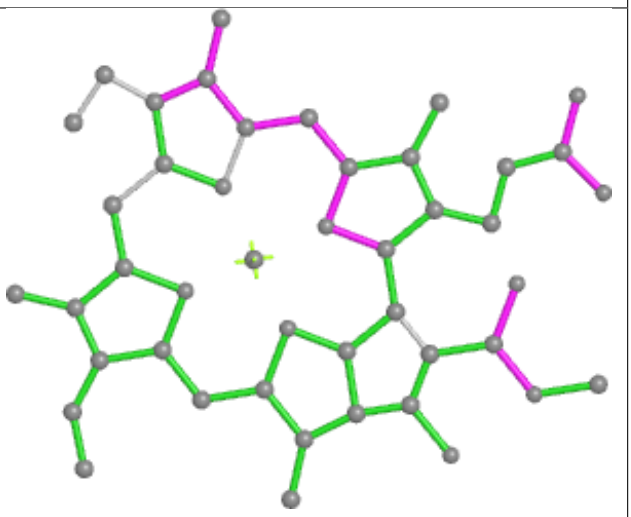
 Bond lengths	 Bond angles
 Torsions	 Rings

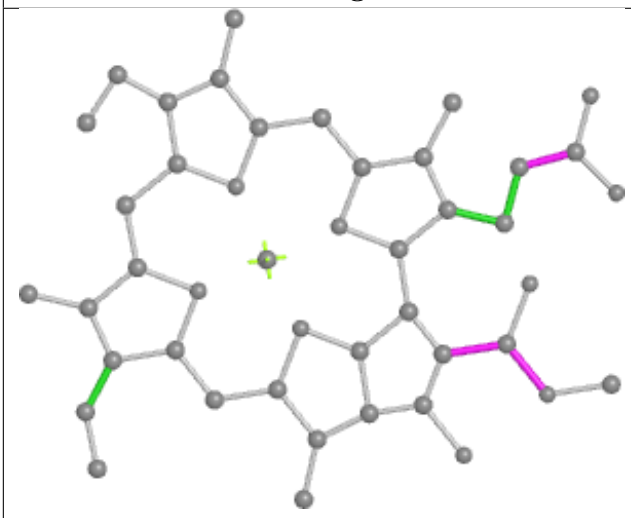
Ligand CLA a 519



Bond lengths



Bond angles



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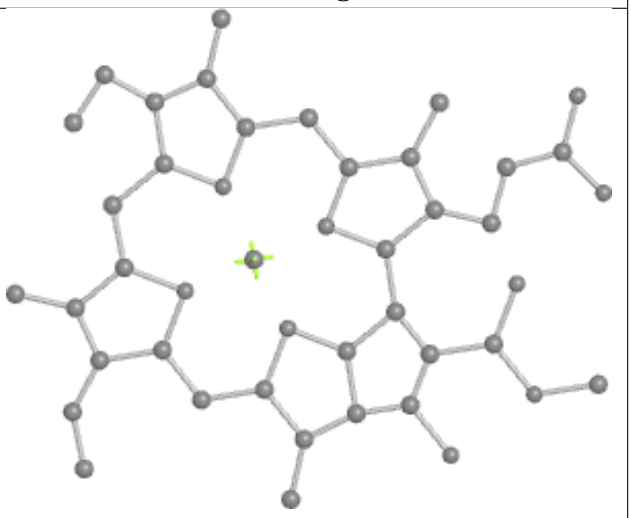
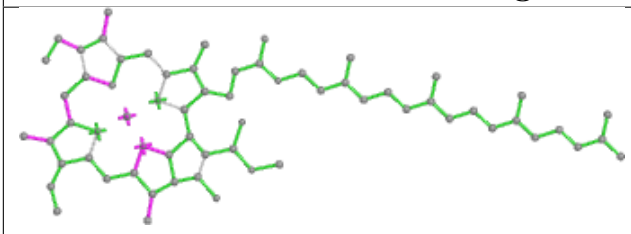


Rings

Ligand CLA G 1127



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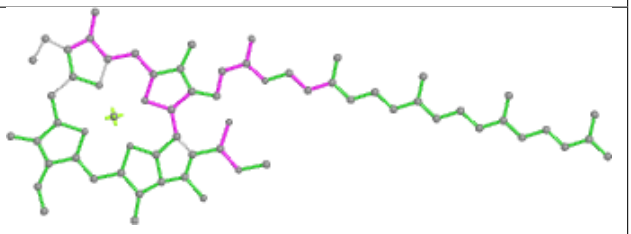
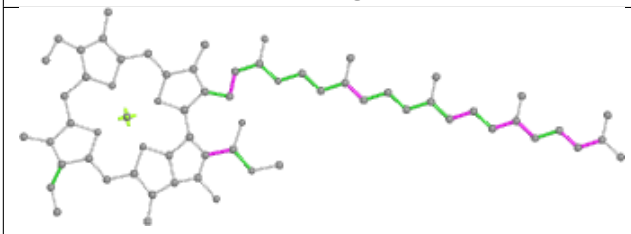


Bond angles



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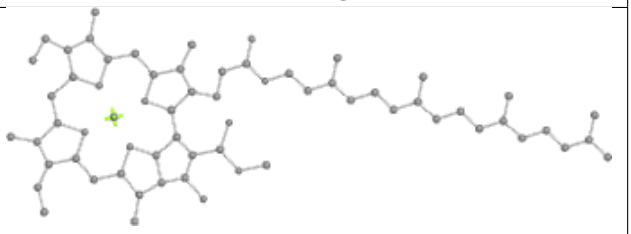
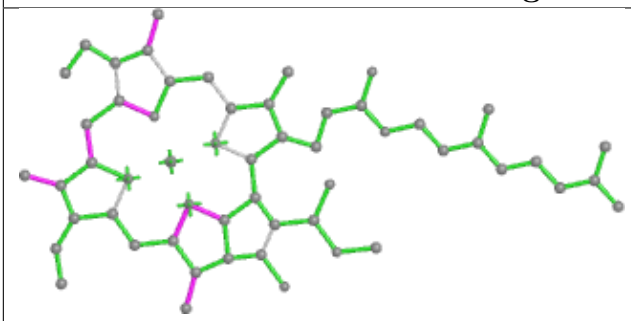
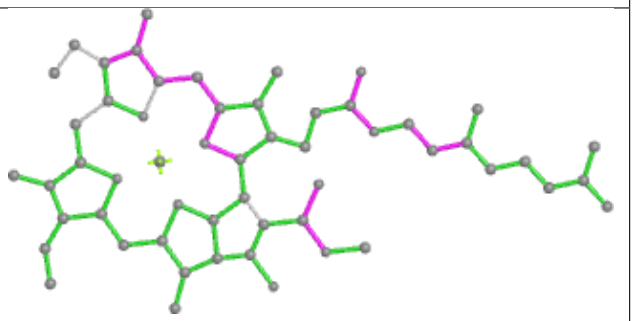
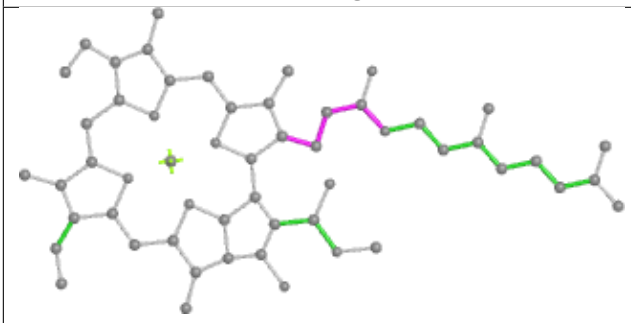
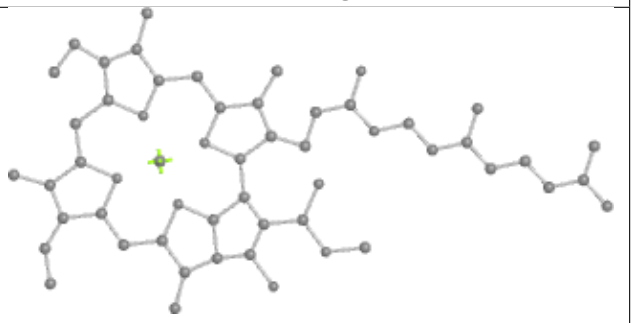
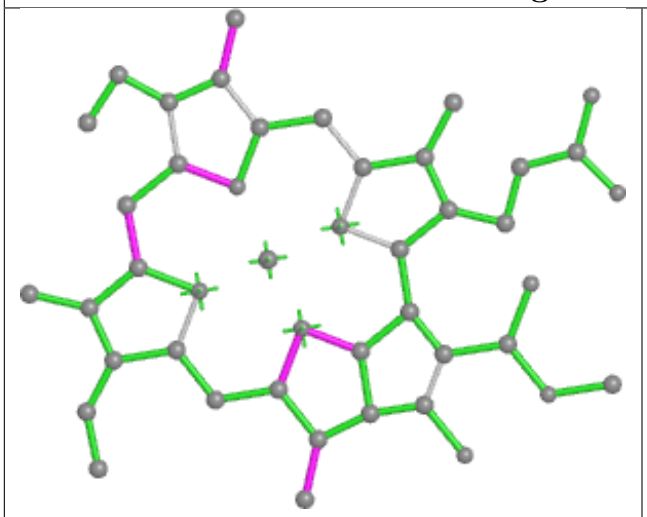


Rings

Ligand CLA f 1228	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 504



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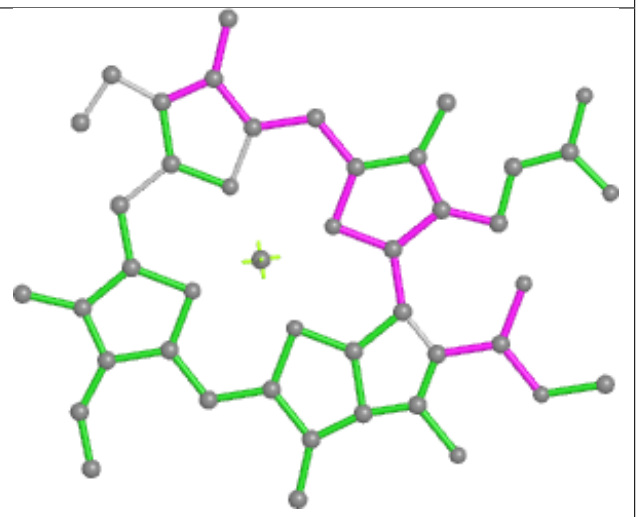
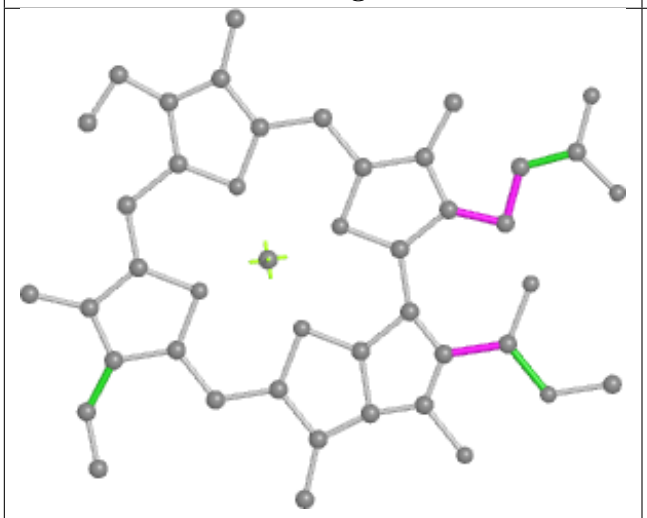
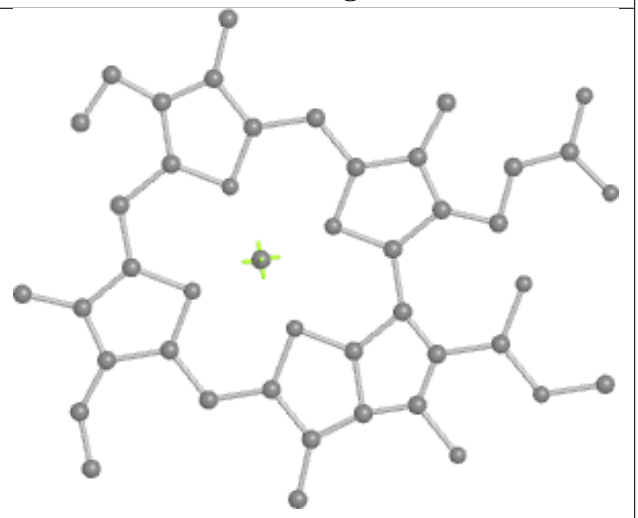


Bond angles

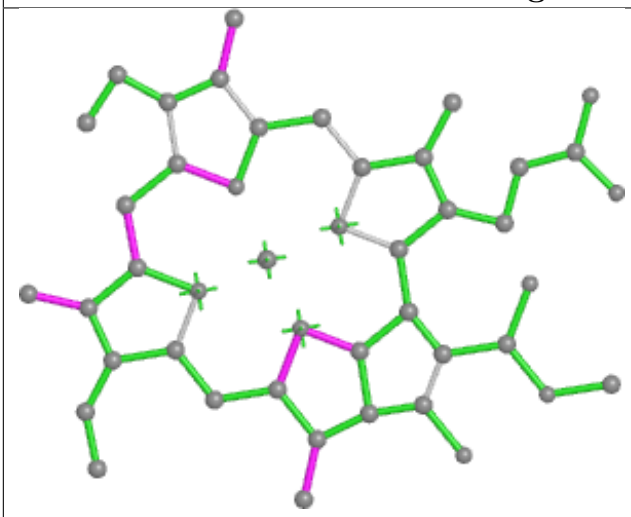


Torsions



Rings

Ligand CLA q 501



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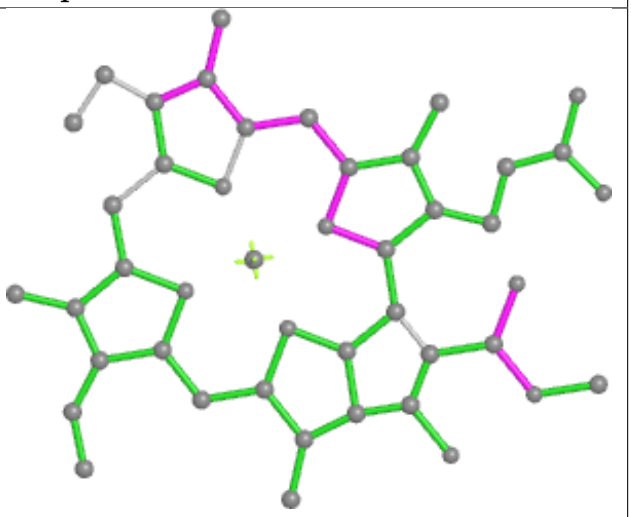

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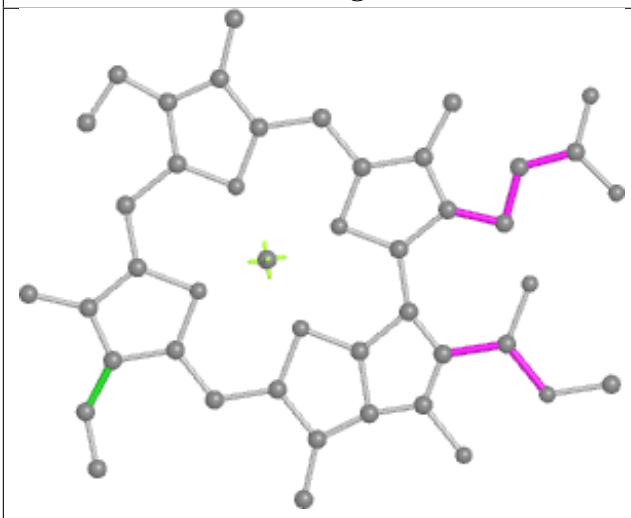

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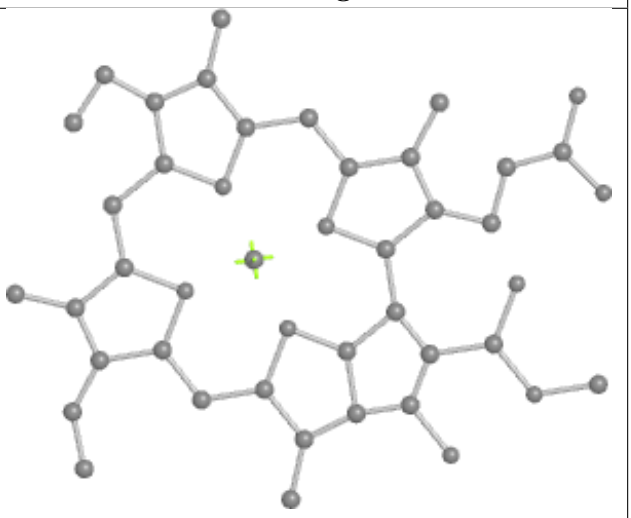
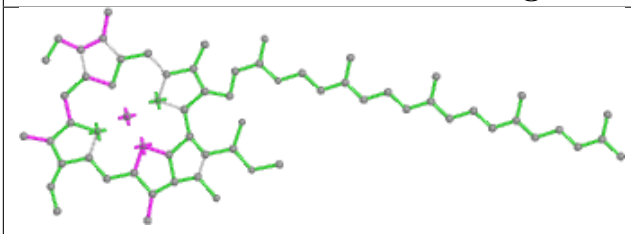


Rings

Ligand CLA f 1225



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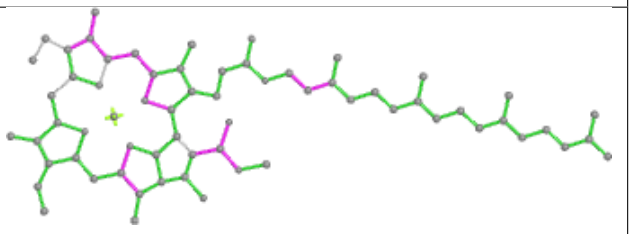

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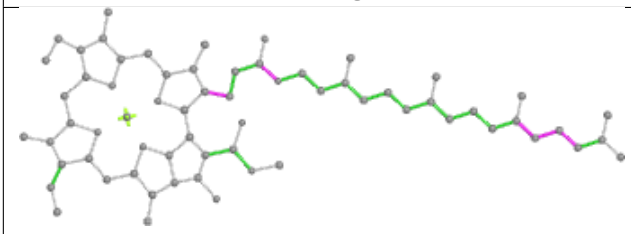

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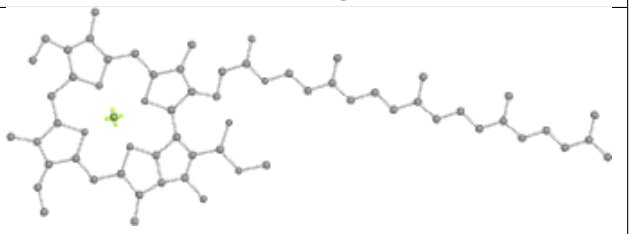
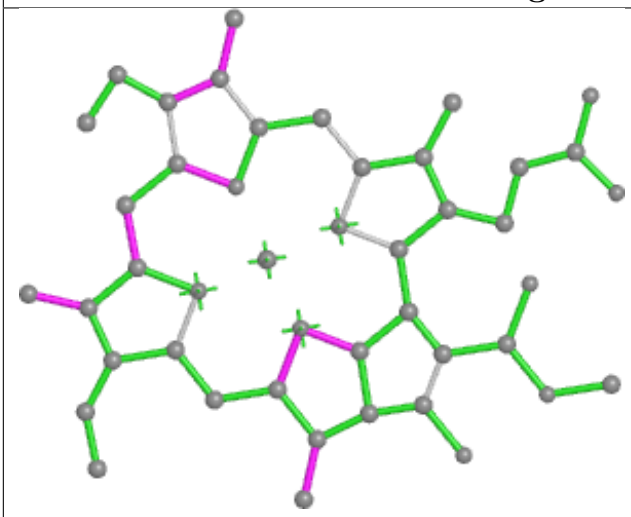


Rings

Ligand CLA 1 519



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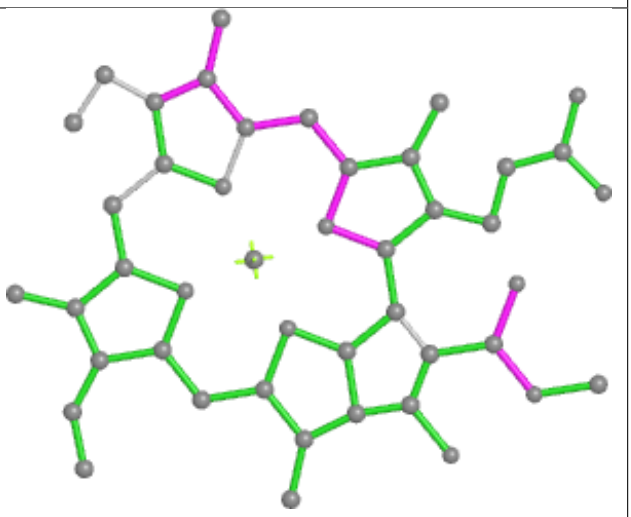

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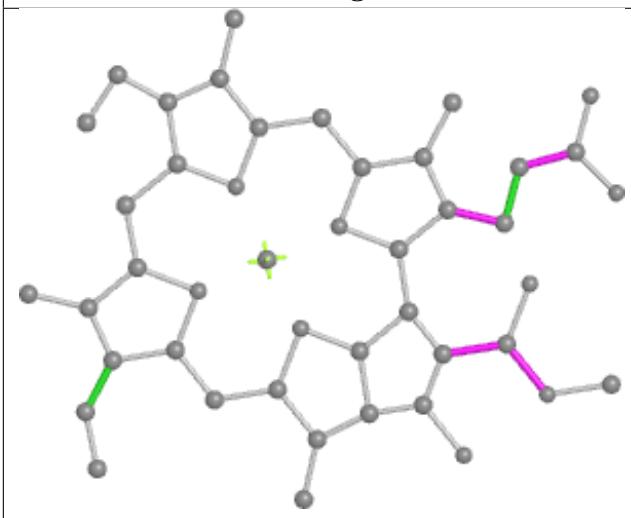

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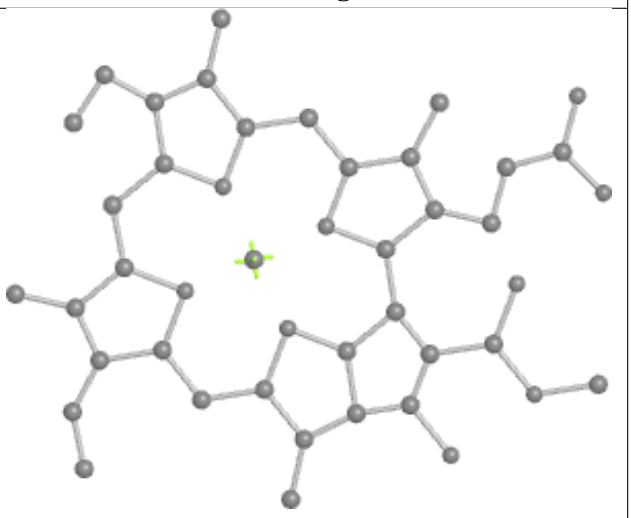
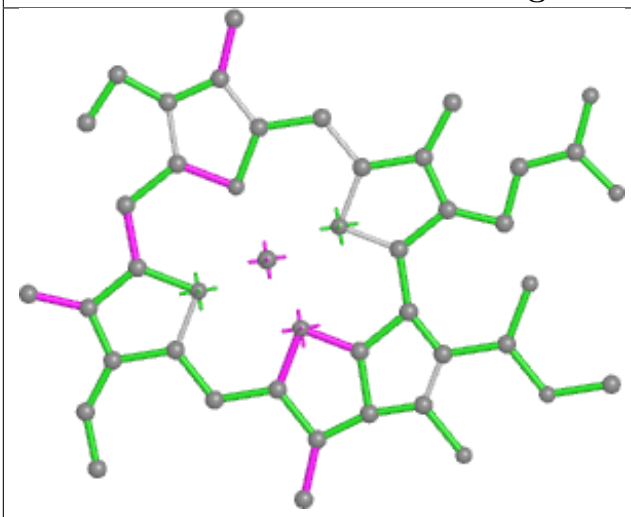


Rings

Ligand CLA 2 507



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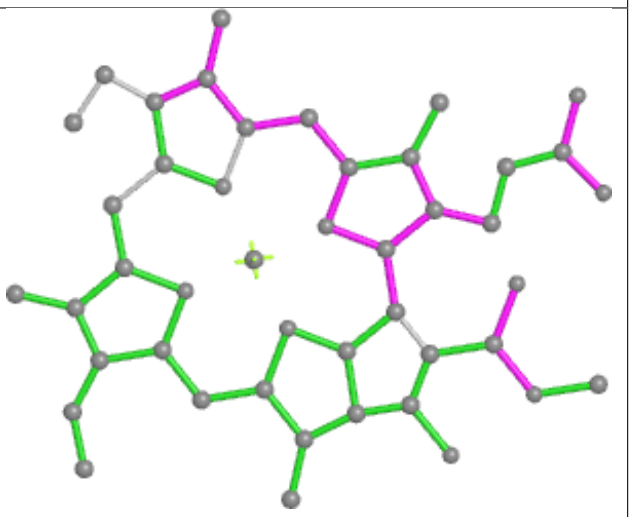
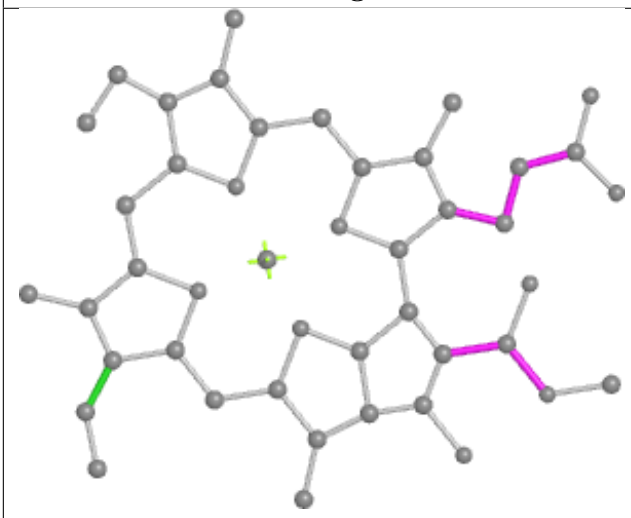


Bond angles



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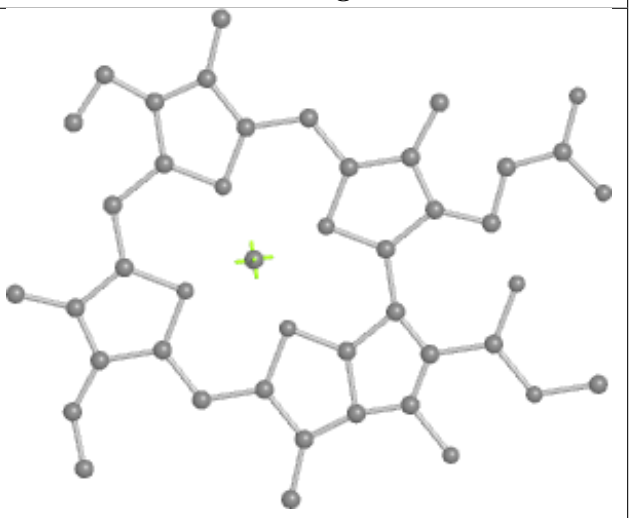
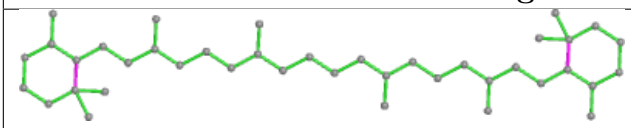


Rings

Ligand BCR k 4018



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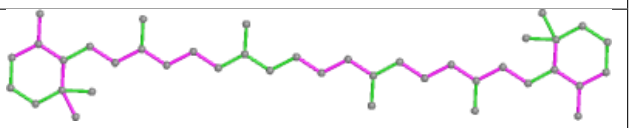
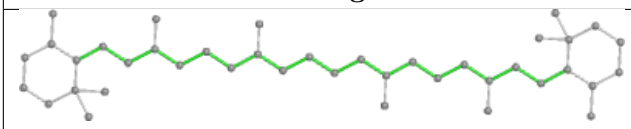


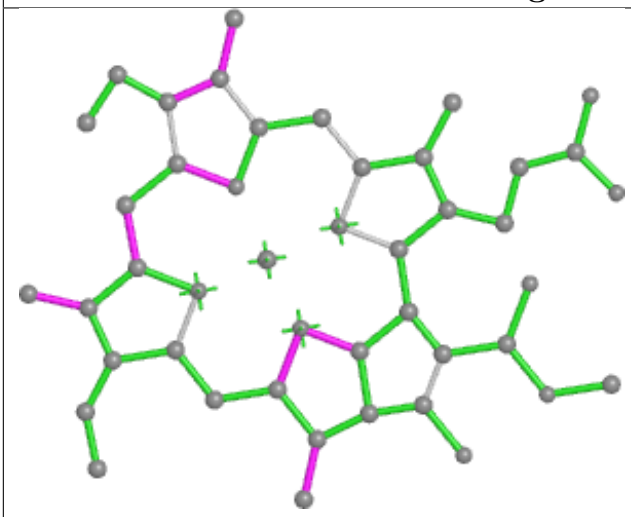
Bond angles



Torsions

Rings

Ligand CLA 4 502



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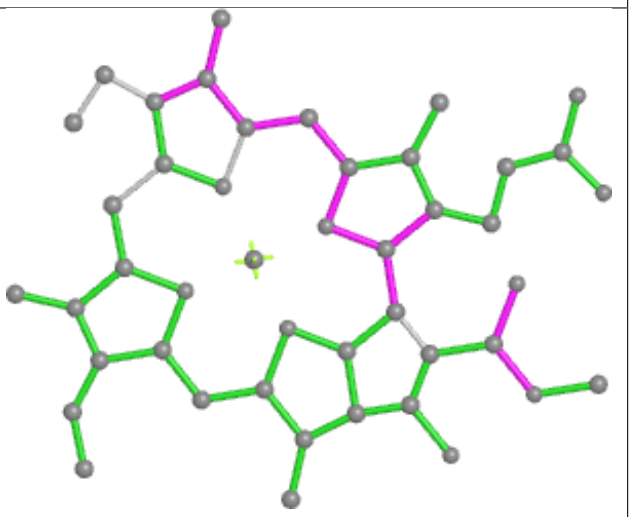
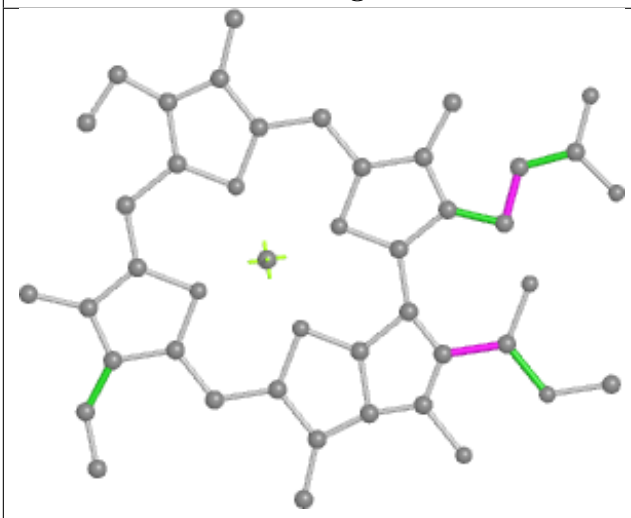
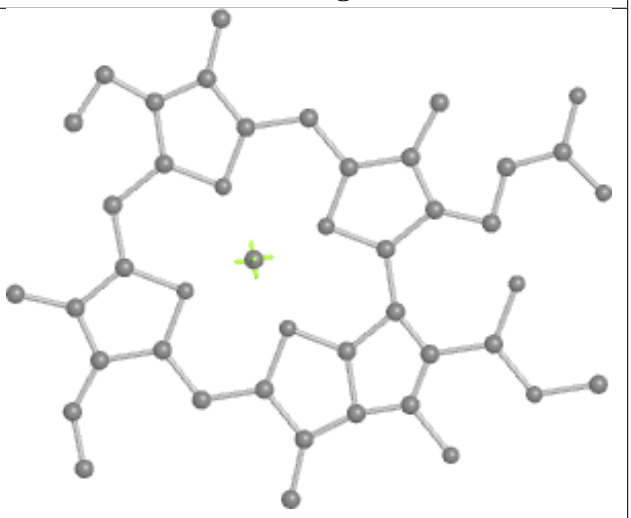


Bond angles

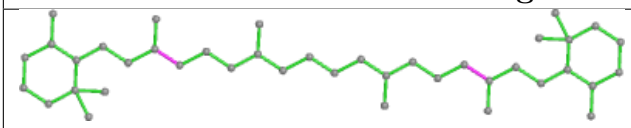


Torsions



Rings

Ligand BCR n 4020



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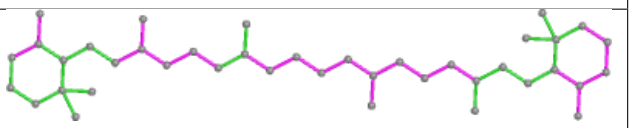
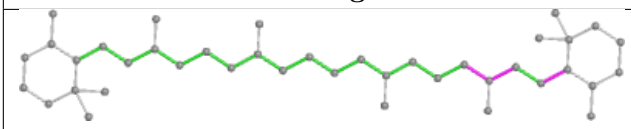


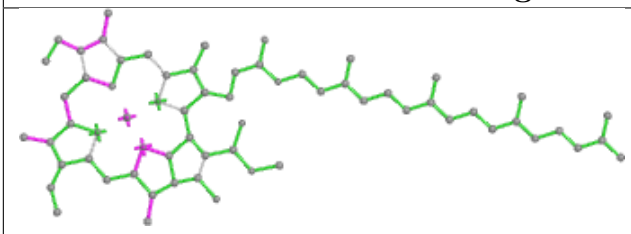
Bond angles



Torsions

Rings

Ligand CLA H 1205



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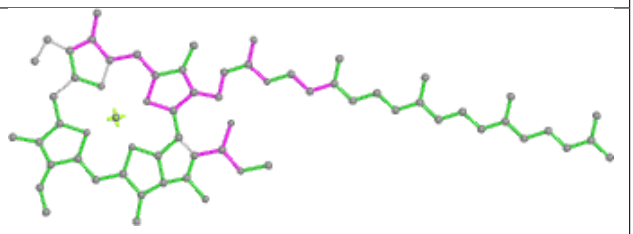

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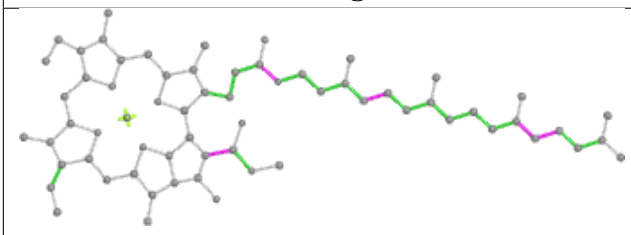

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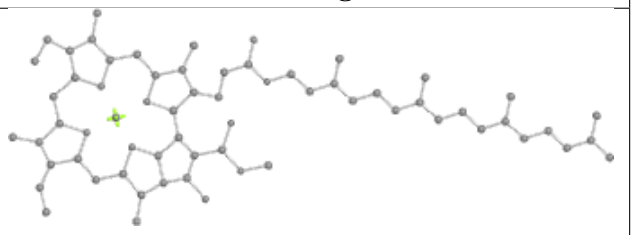
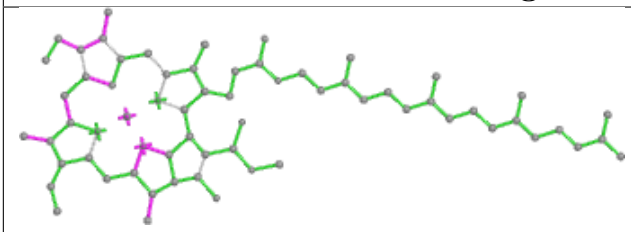


Rings

Ligand CLA e 1131



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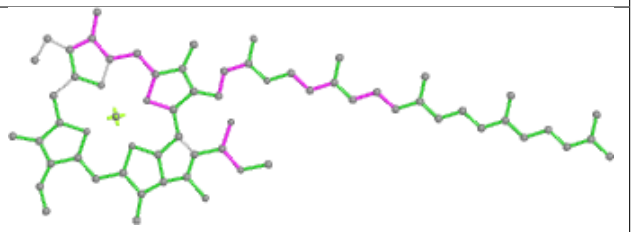

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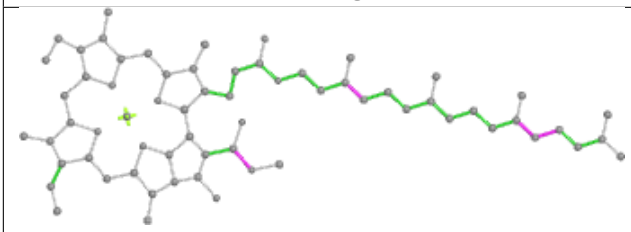

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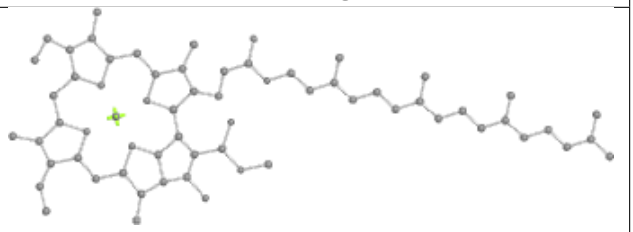
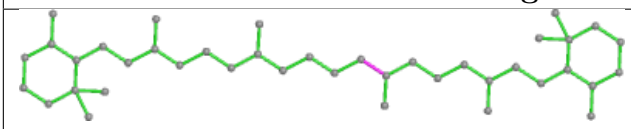


Rings

Ligand BCR f 4010



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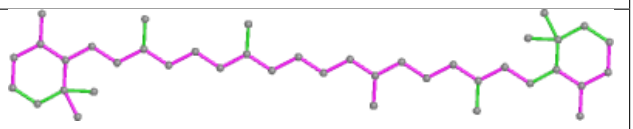

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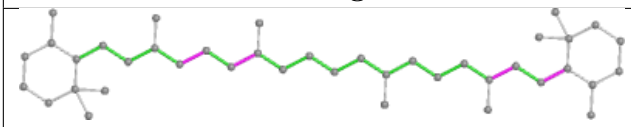
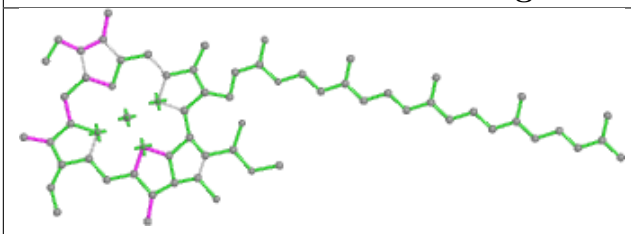


Torsions

Rings

Ligand CLA B 1207



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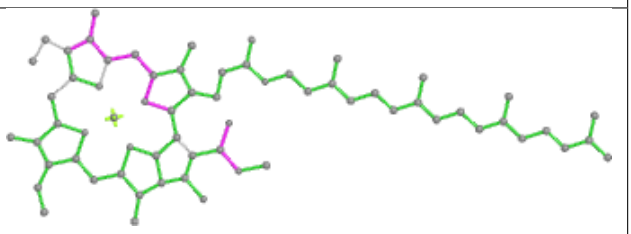

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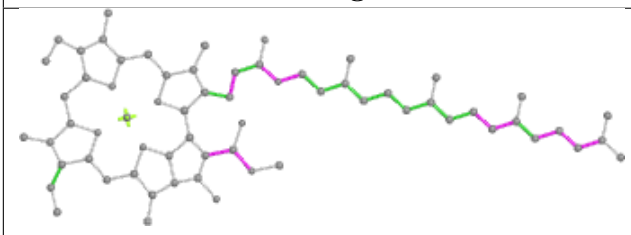

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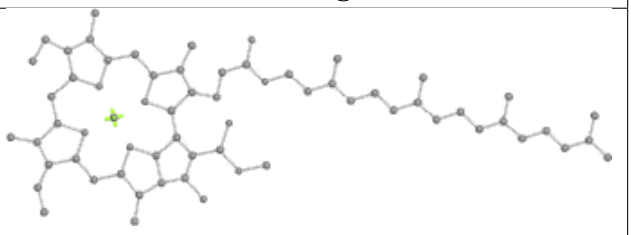
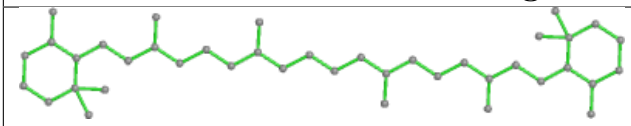


Rings

Ligand BCR Y 521



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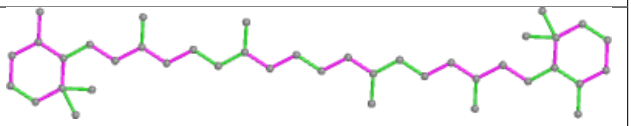

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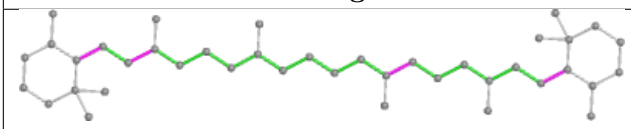

Torsions

Rings

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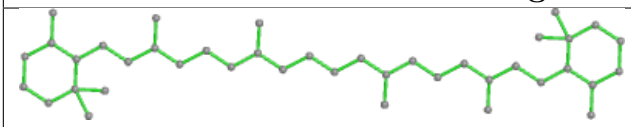

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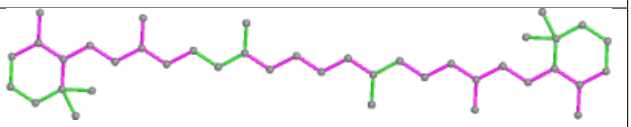

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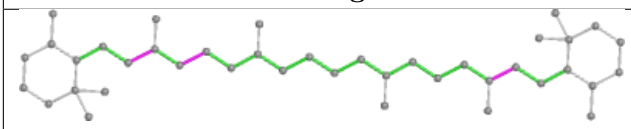

Torsions

Rings

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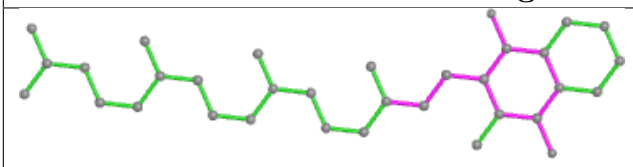

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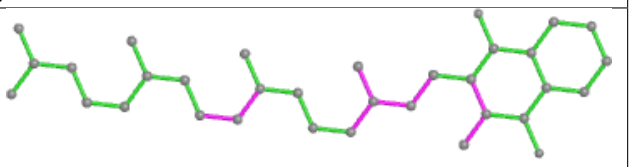

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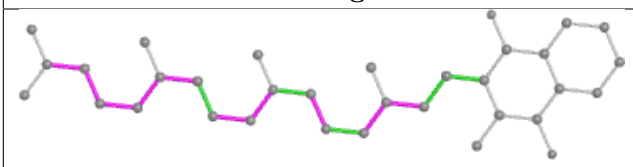

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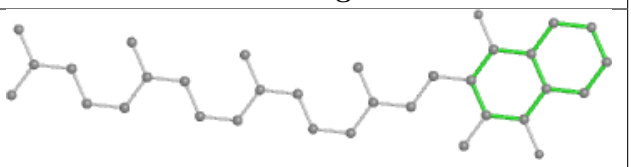

Rings

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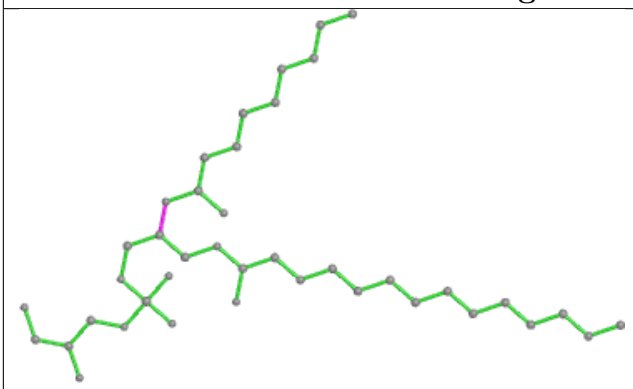

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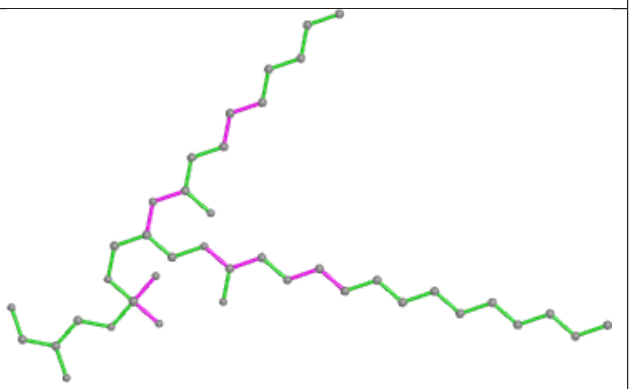

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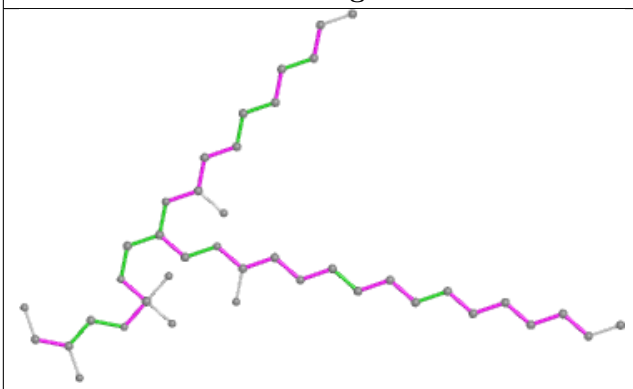

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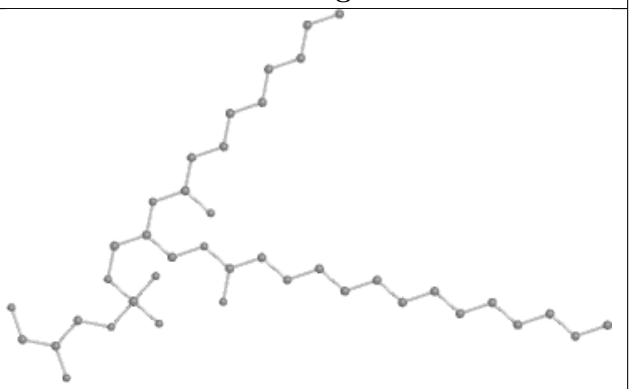

Rings

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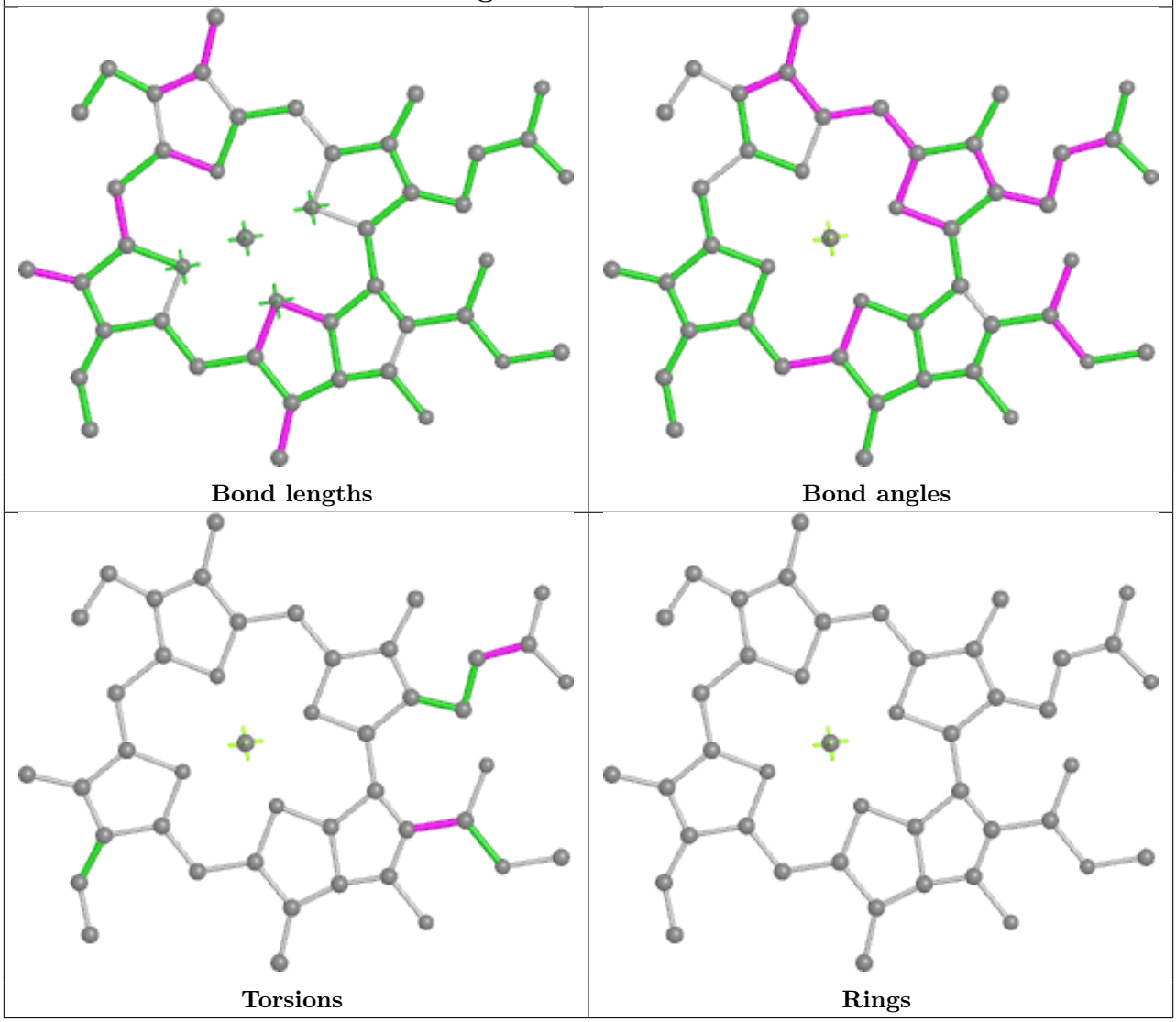
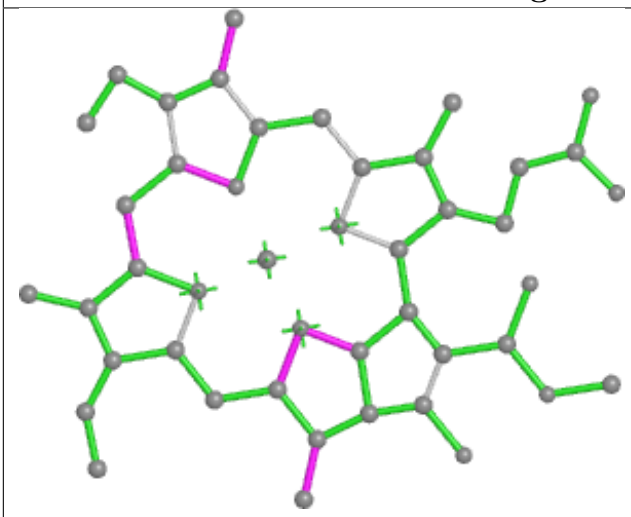


Ligand CLA t 516



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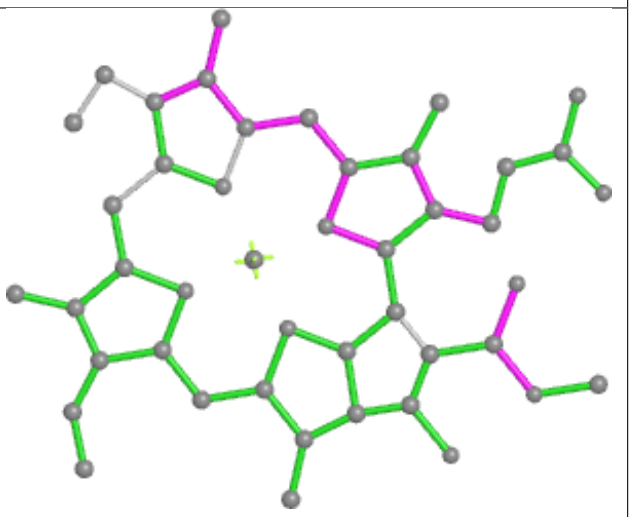

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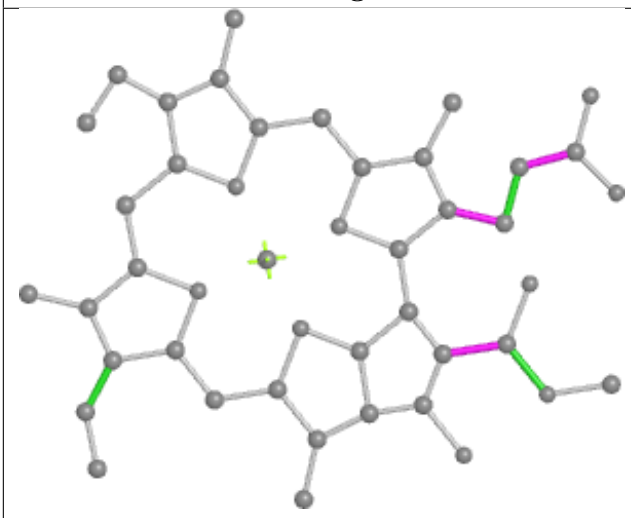

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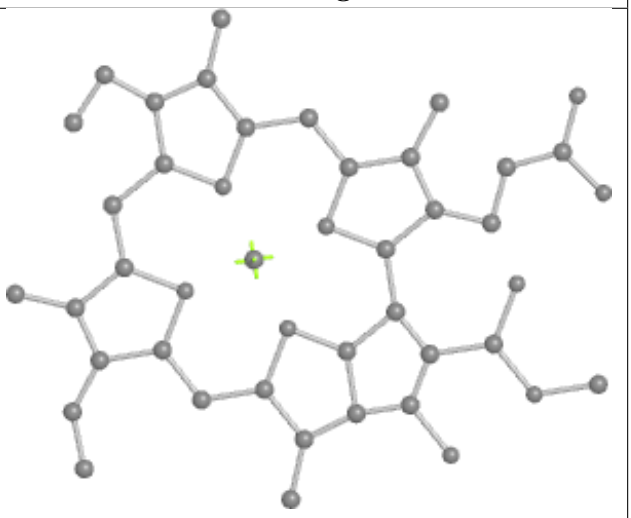
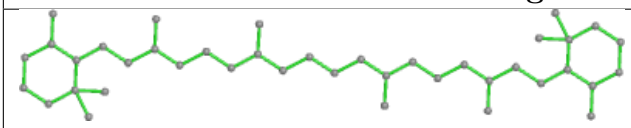


Rings

Ligand BCR 3 522



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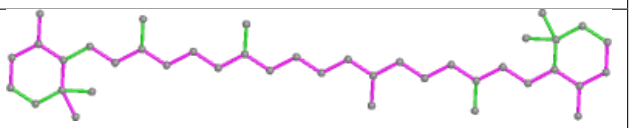

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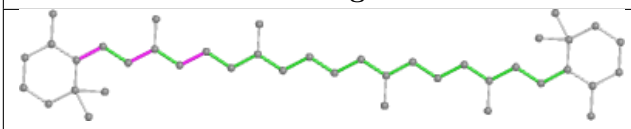

Torsions

Rings

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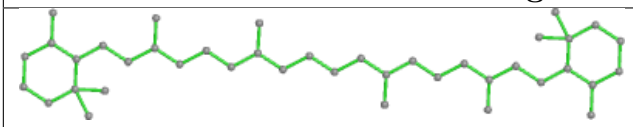

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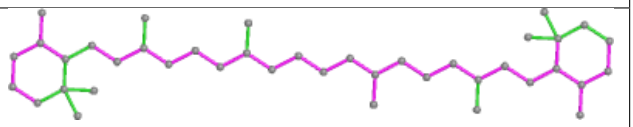

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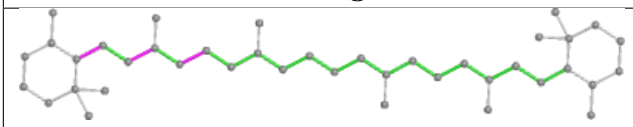

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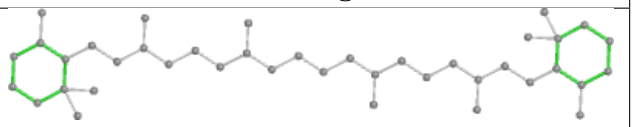
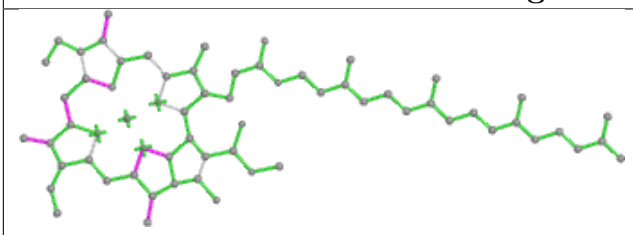


Rings

Ligand CLA d 505



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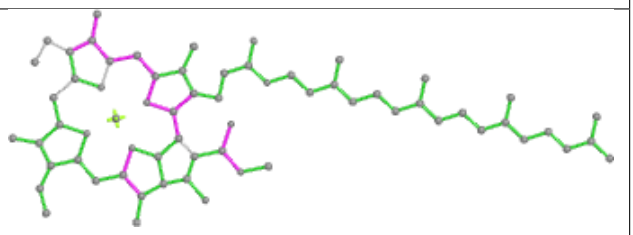

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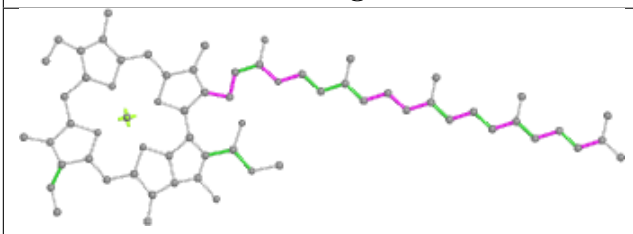

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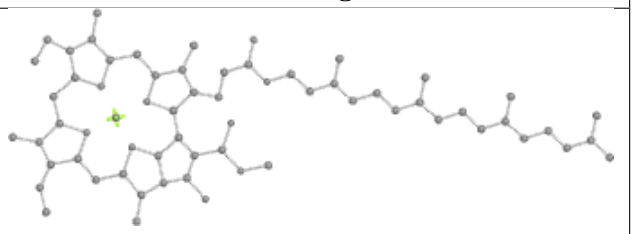
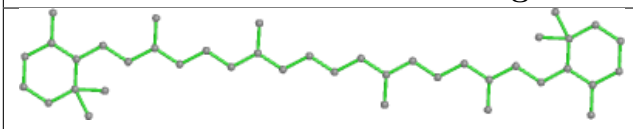


Rings

Ligand BCR m 4104



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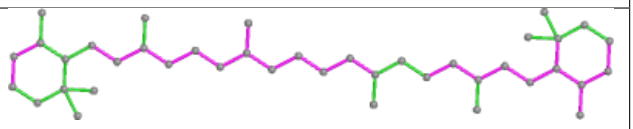
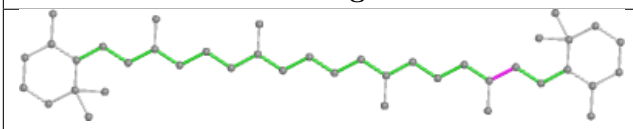
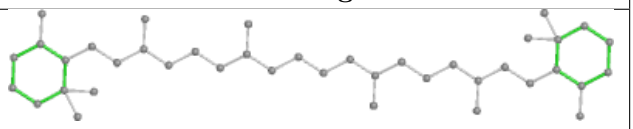


Bond angles

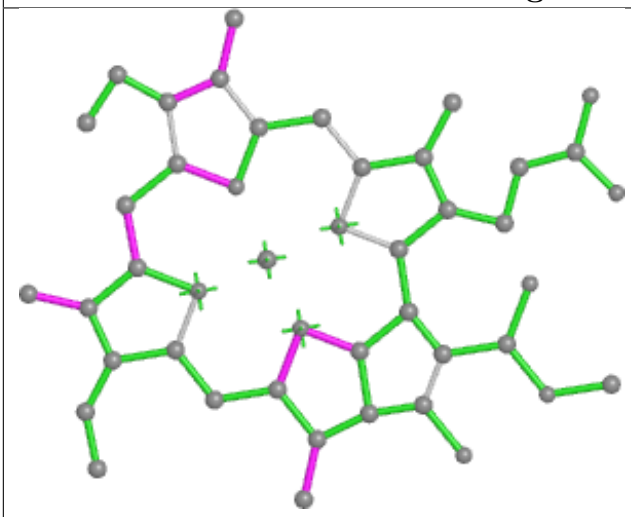


Torsions

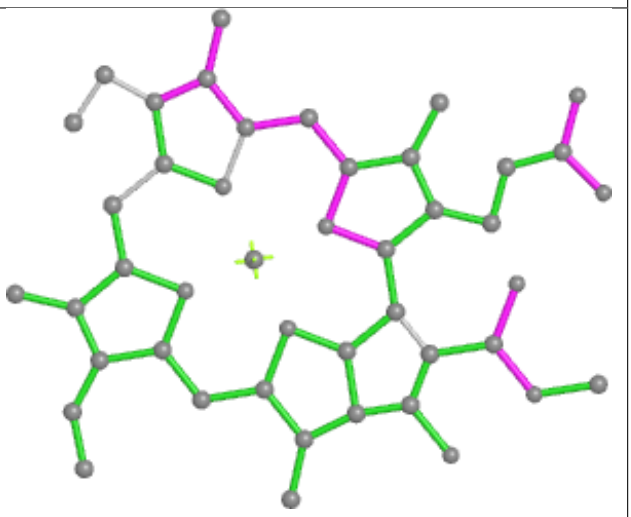


Rings

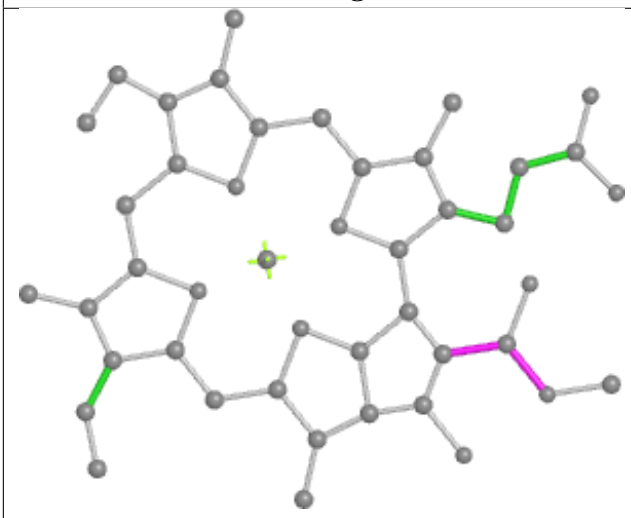
Ligand CLA Z 506



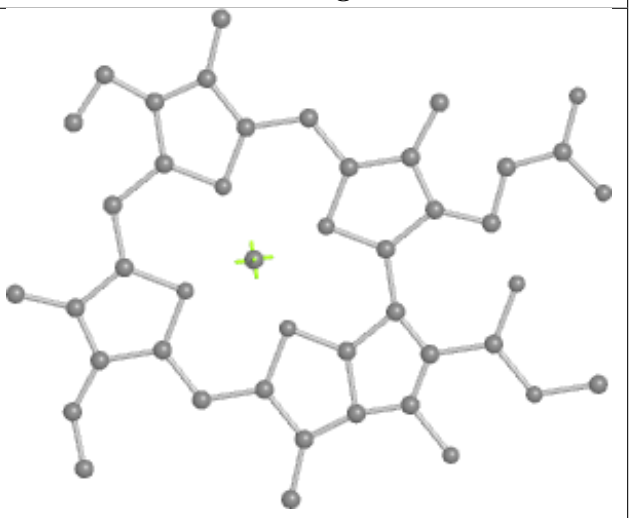
Bond lengths



Bond angles

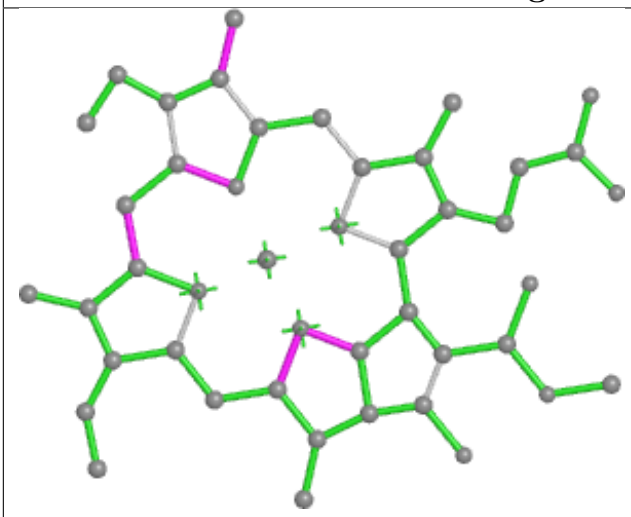


Torsions



Rings

Ligand CLA 5 511



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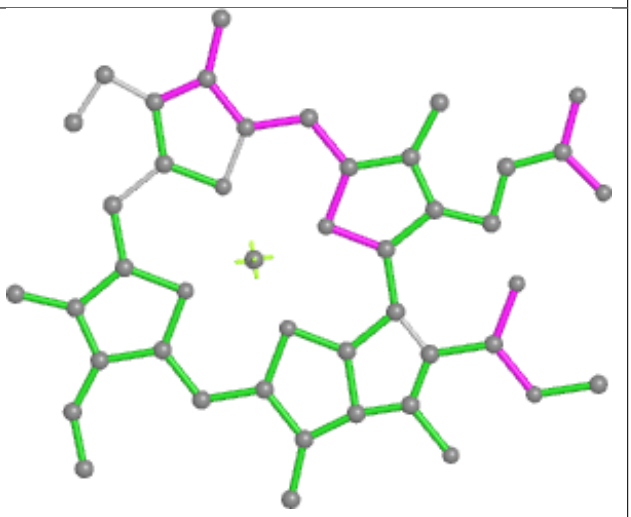

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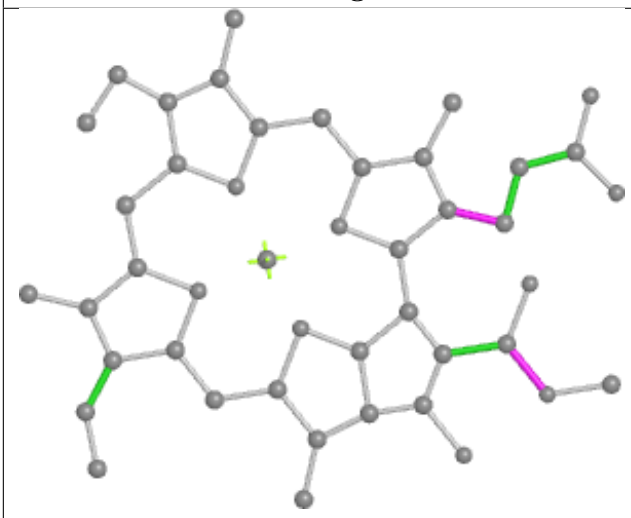

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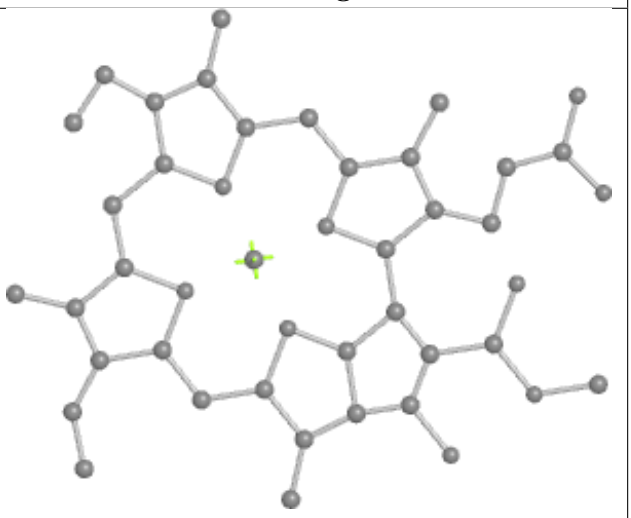
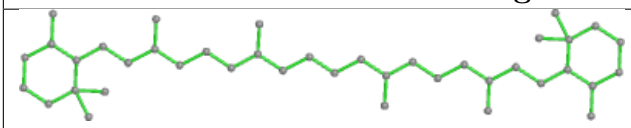


Rings

Ligand BCR B 4006



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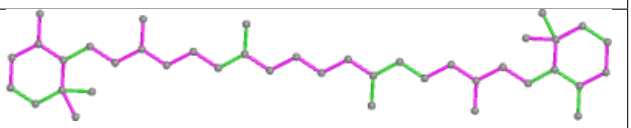

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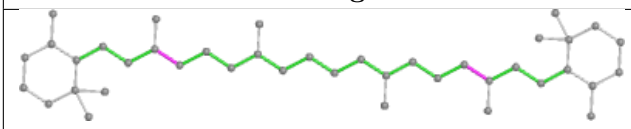
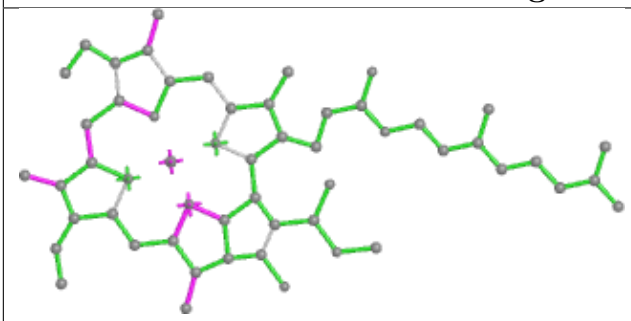
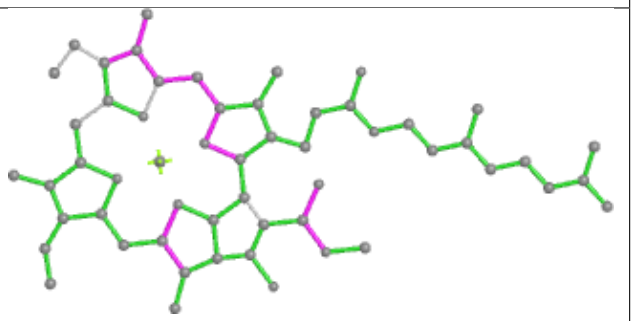
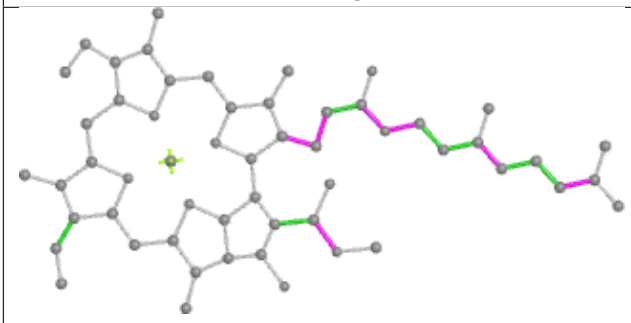
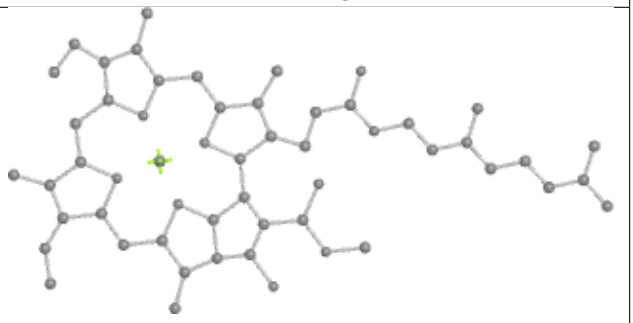
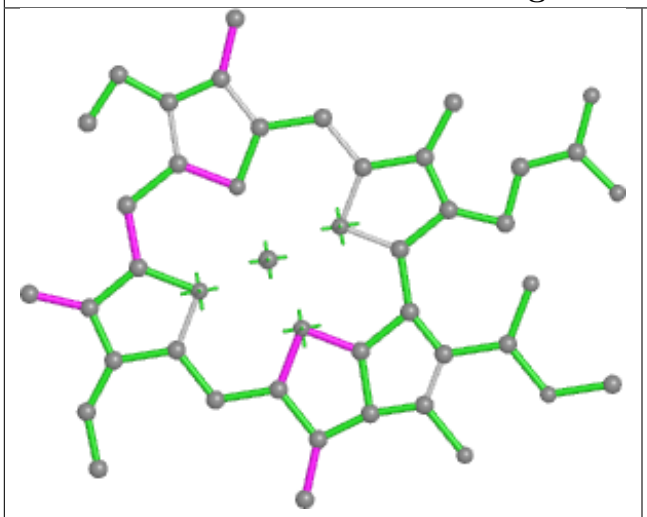


Torsions

Rings

Ligand CLA a 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA d 510



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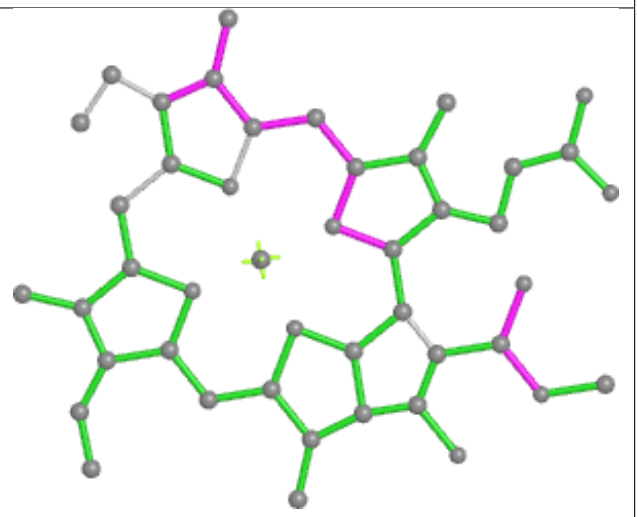

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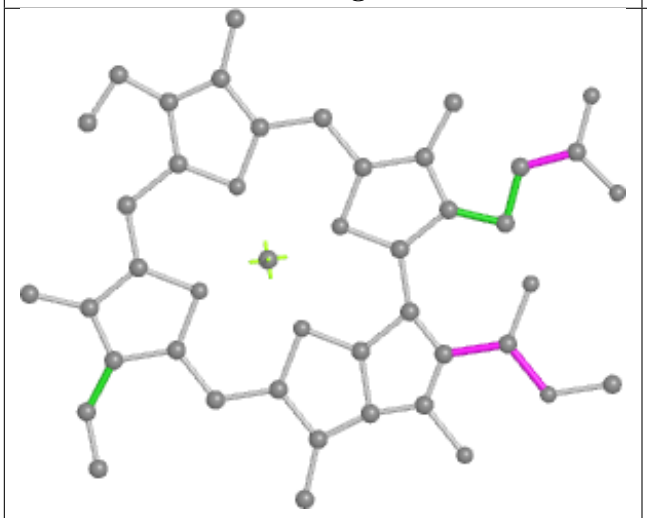

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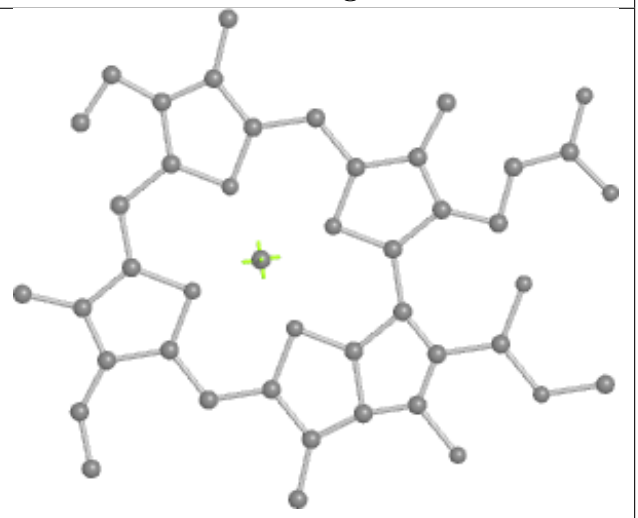

Rings

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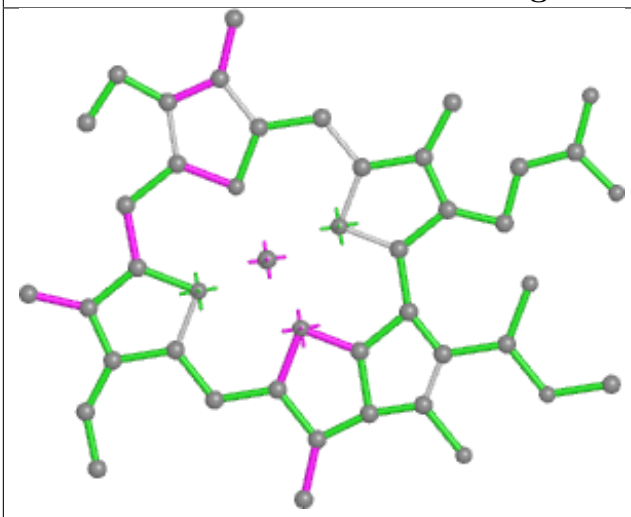

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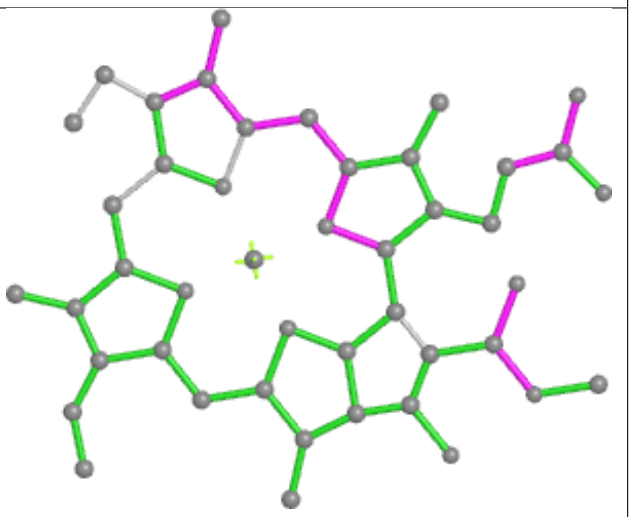

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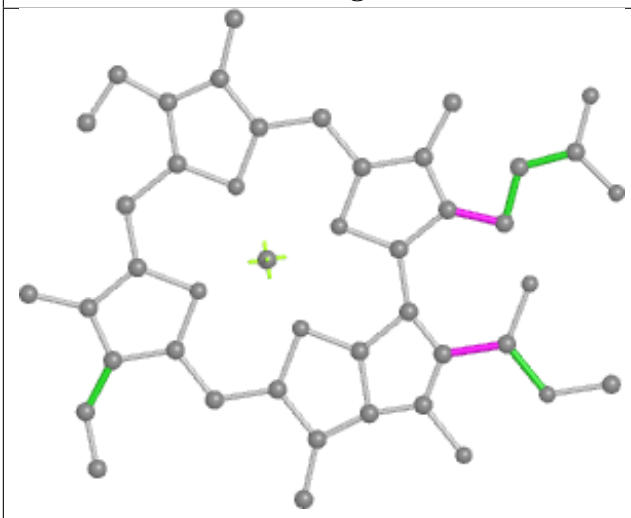

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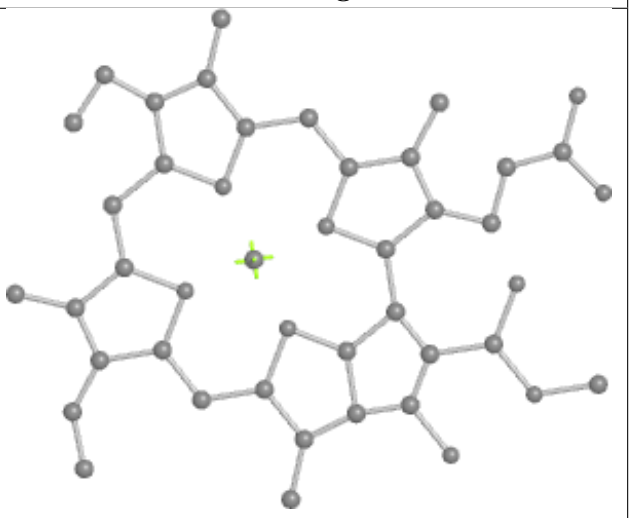
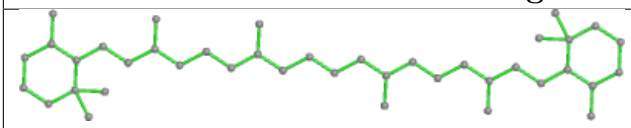


Rings

Ligand BCR 1 521



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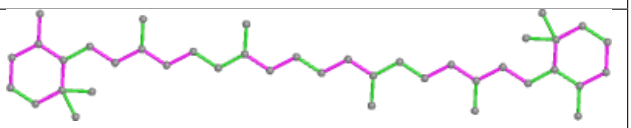

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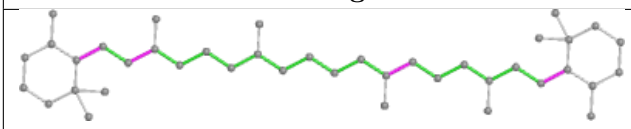
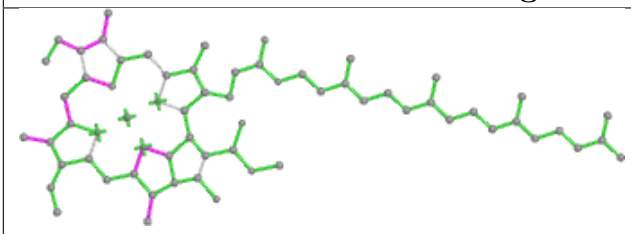


Torsions

Rings

Ligand CLA e 1136



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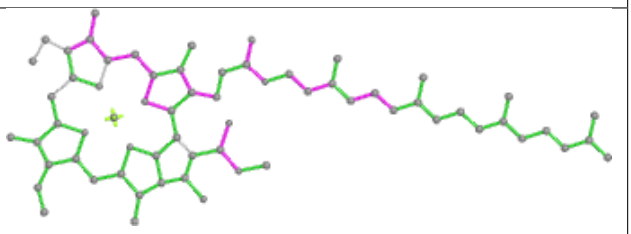

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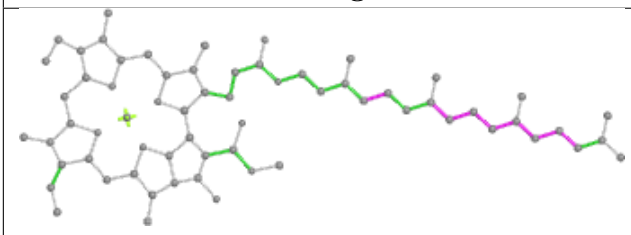

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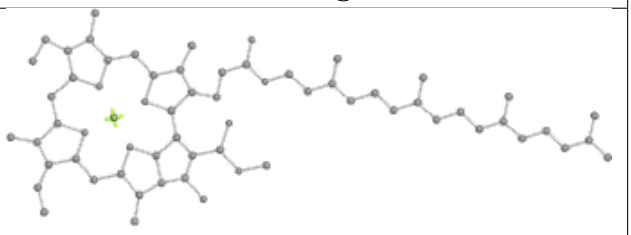
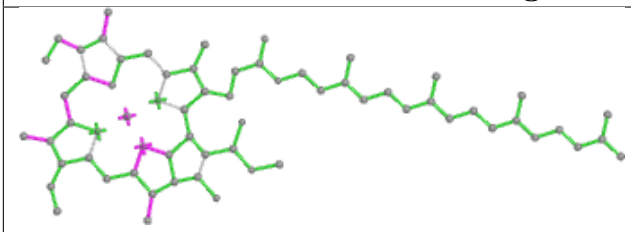


Rings

Ligand CLA f 1234



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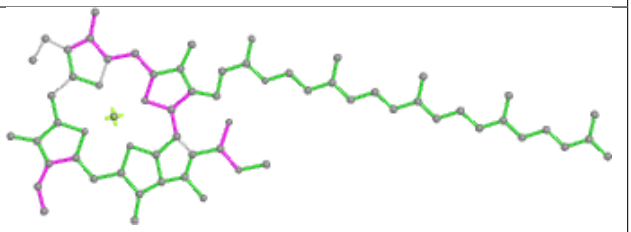

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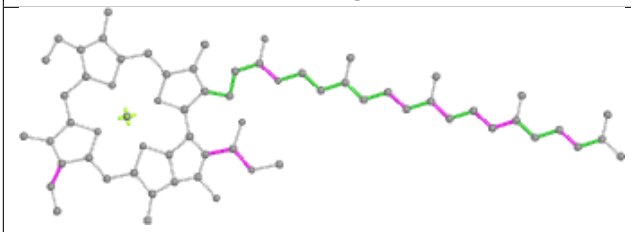

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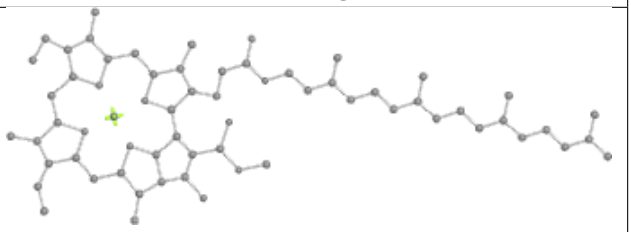
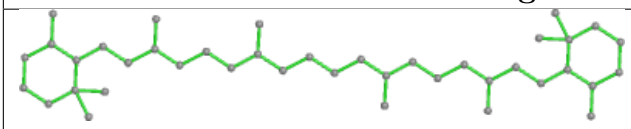


Rings

Ligand BCR e 4011



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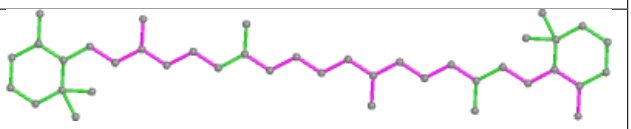

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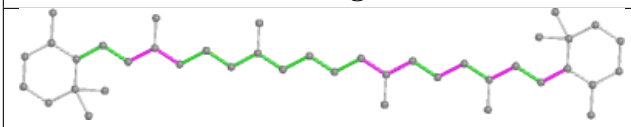
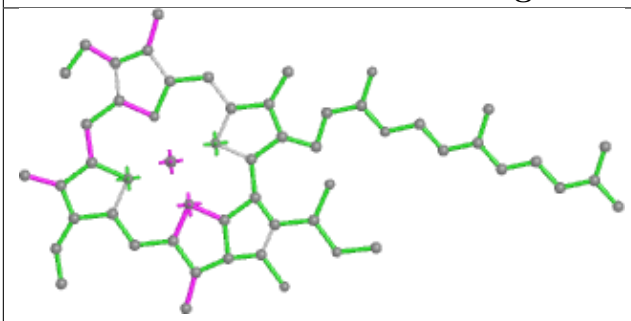


Torsions

Rings

Ligand CLA A 1105



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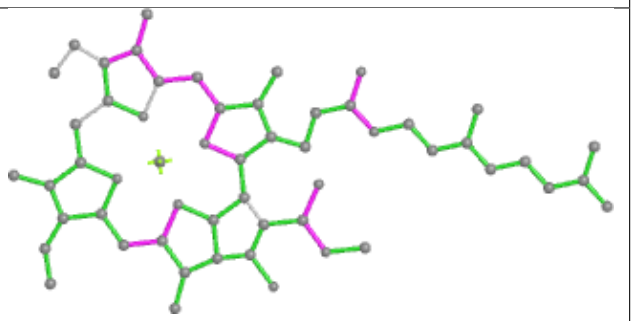

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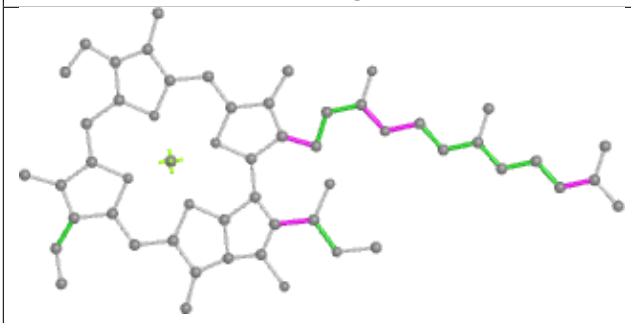

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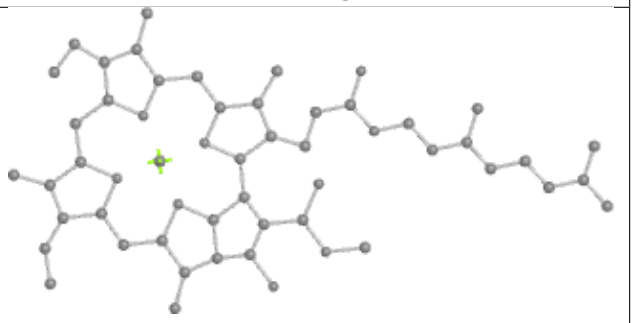
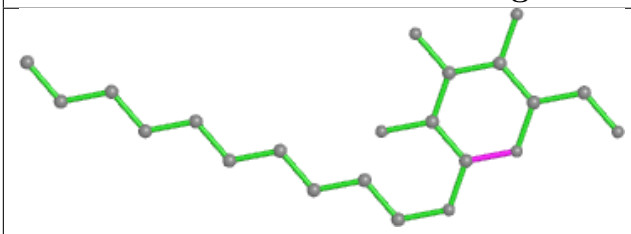


Rings

Ligand LMU T 5105



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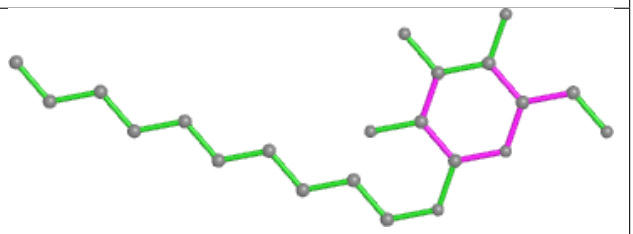

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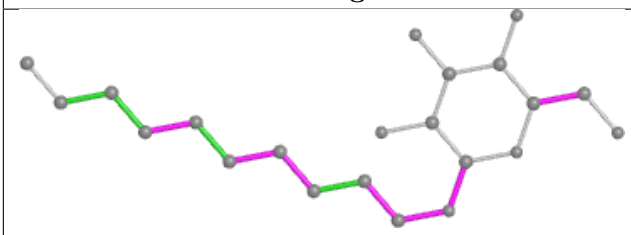

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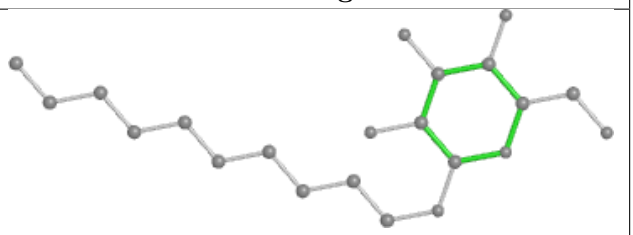
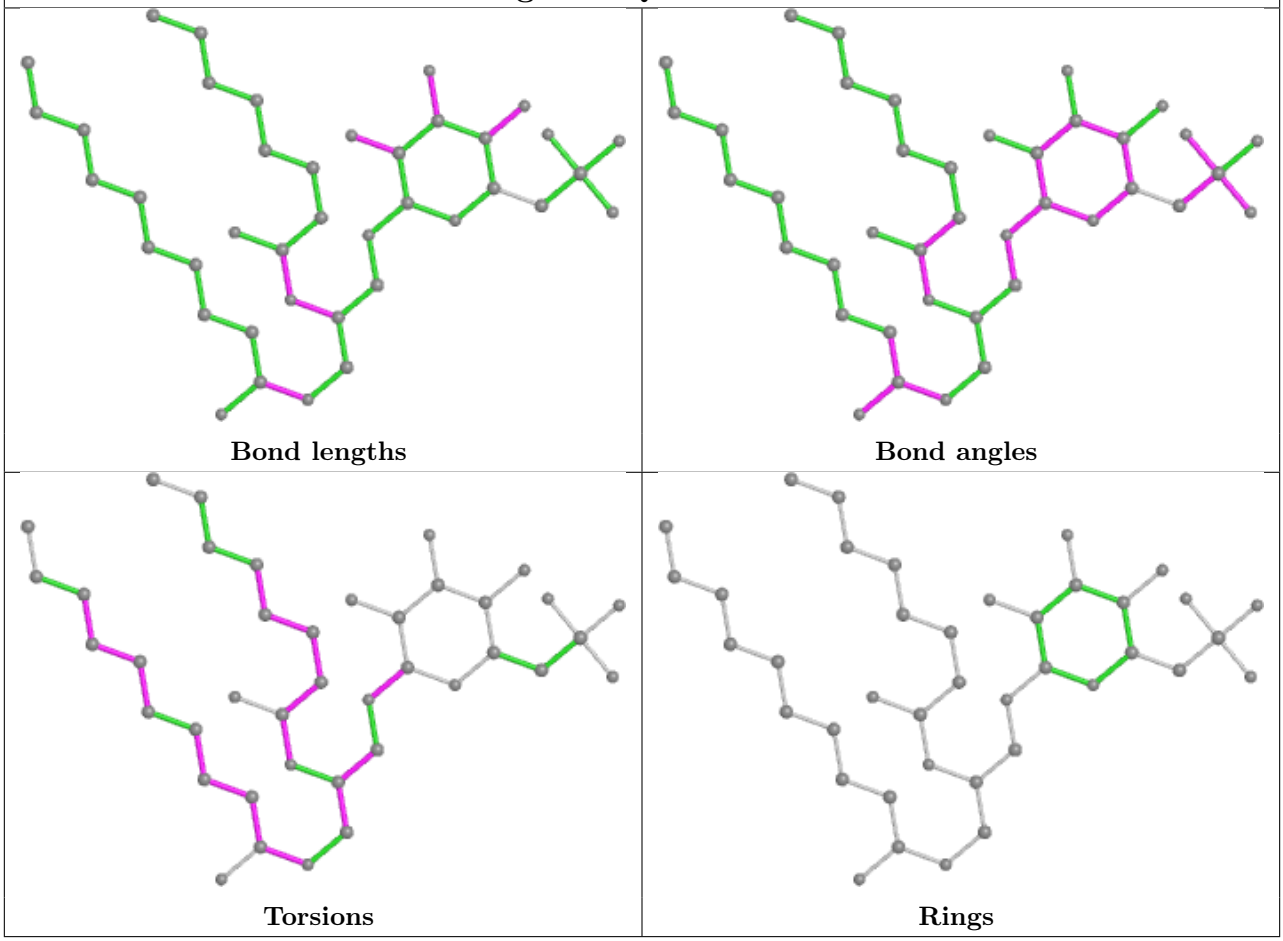
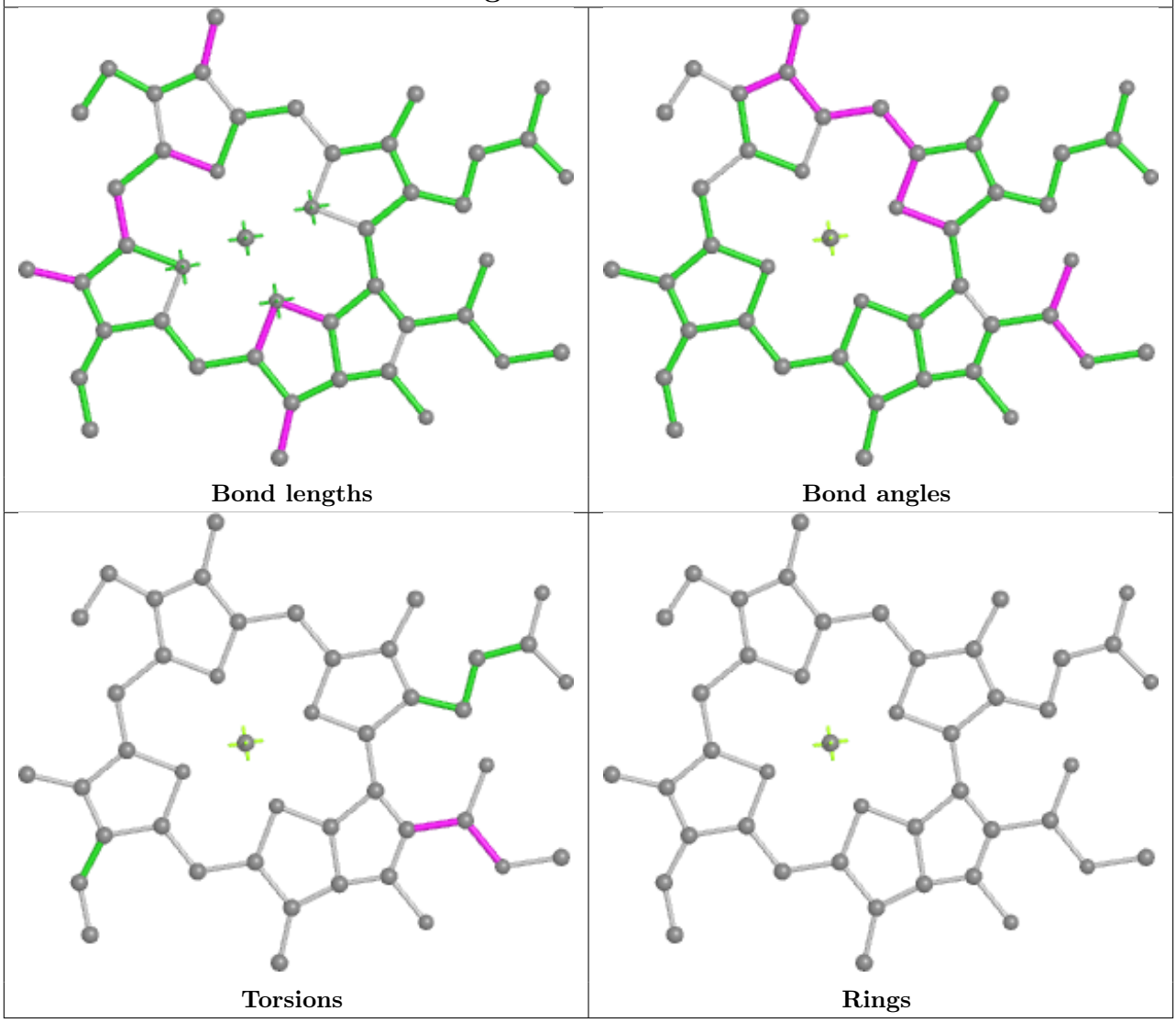


Rings

Ligand SQD B 1852



Ligand CLA v 506



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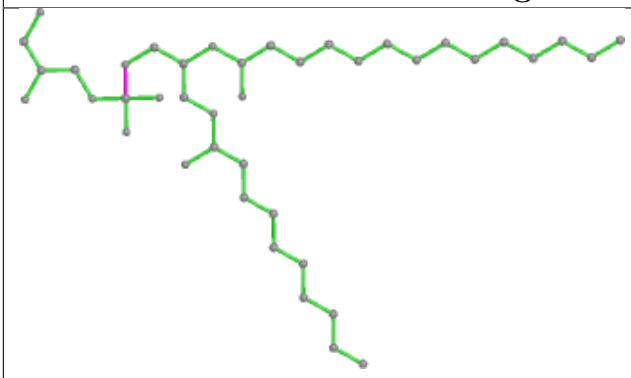
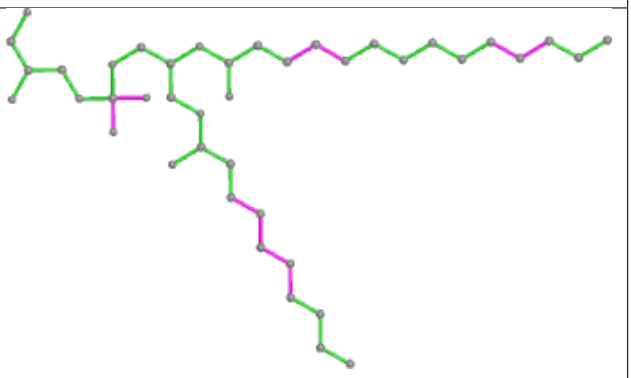
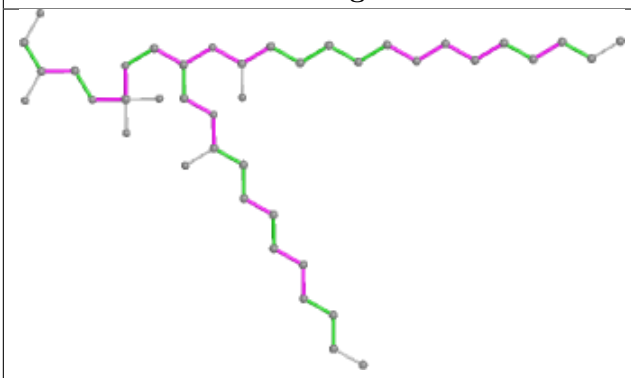
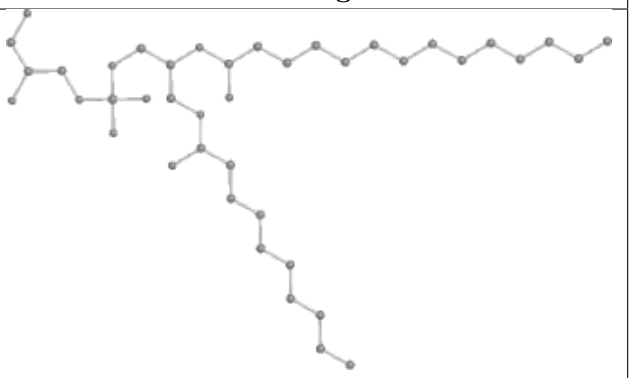
 Bond lengths	 Bond angles
 Torsions	 Rings

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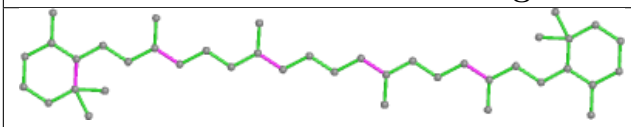
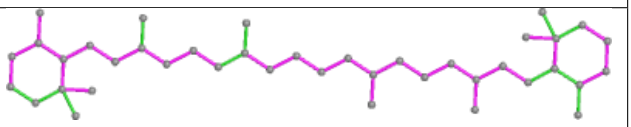
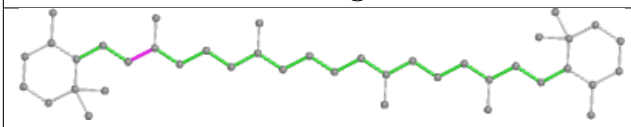
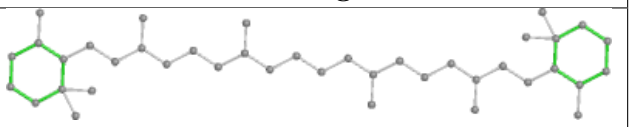
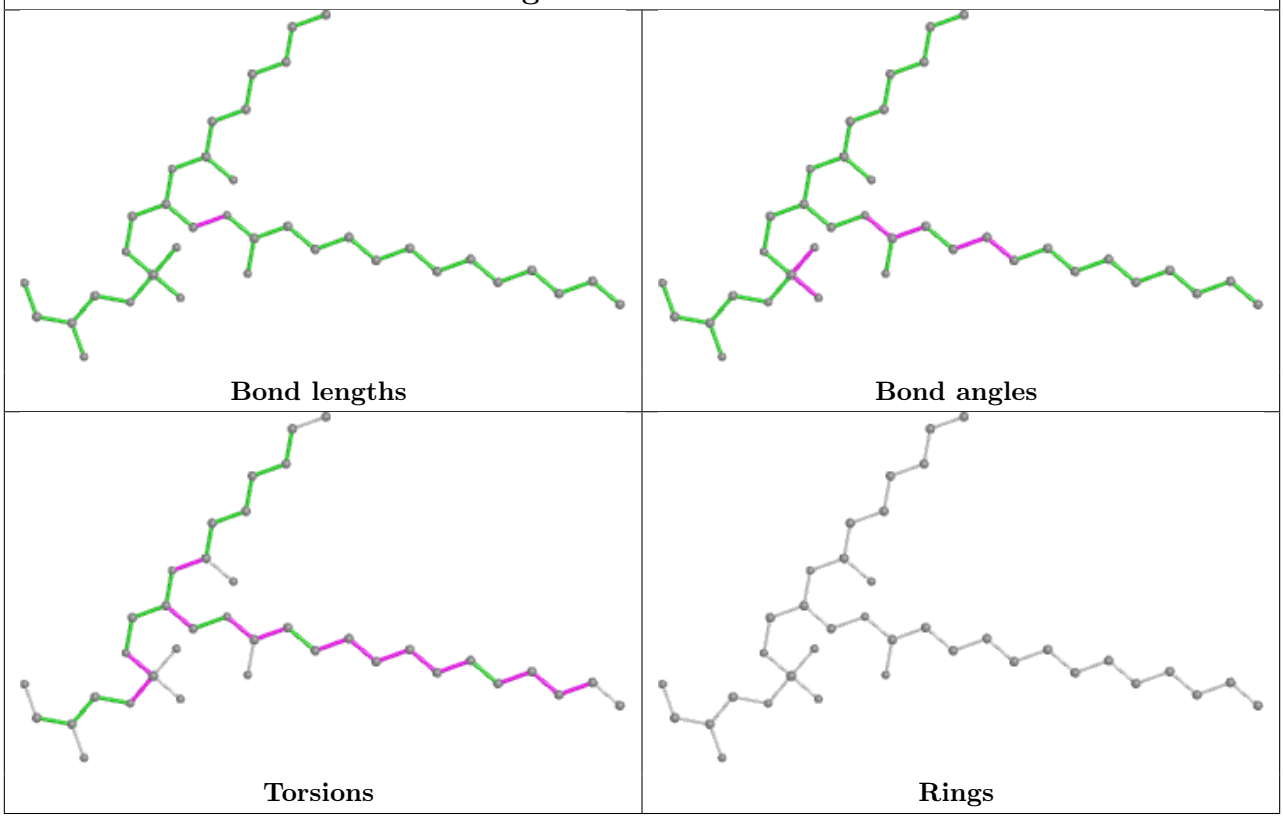
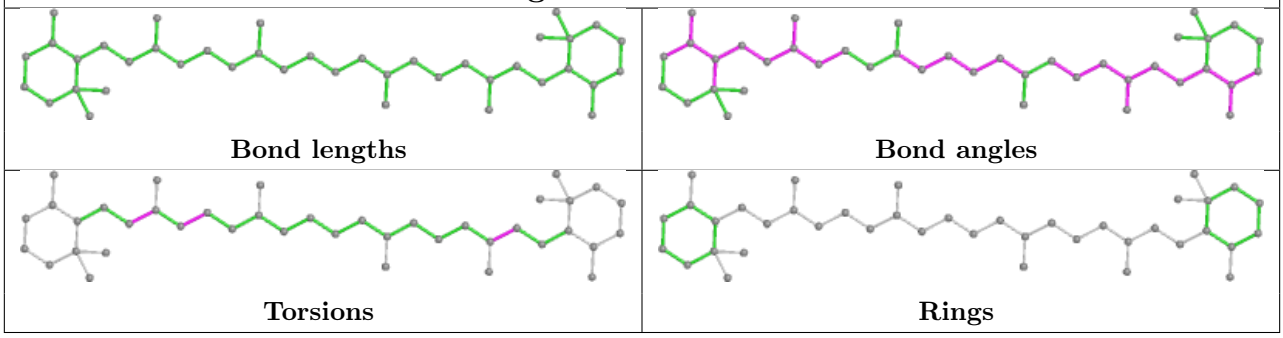
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG f 1842



Ligand BCR a 524



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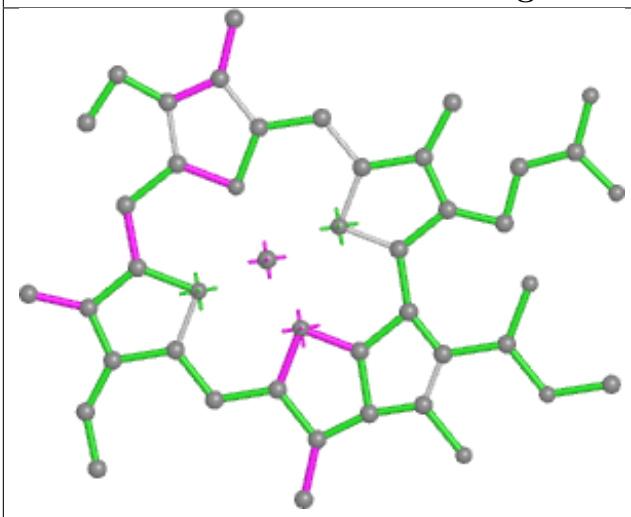

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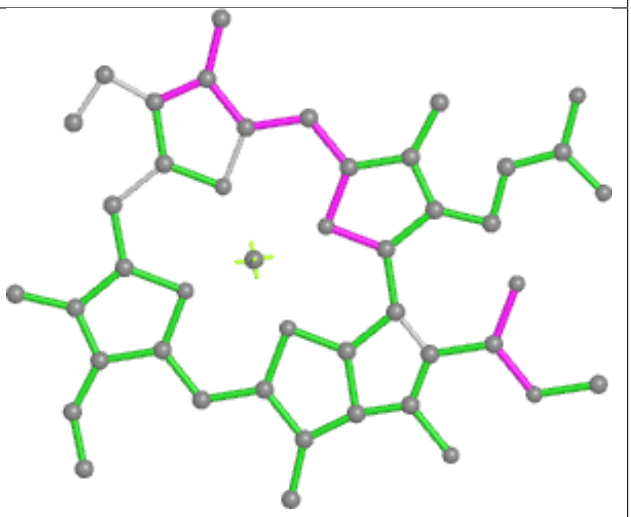
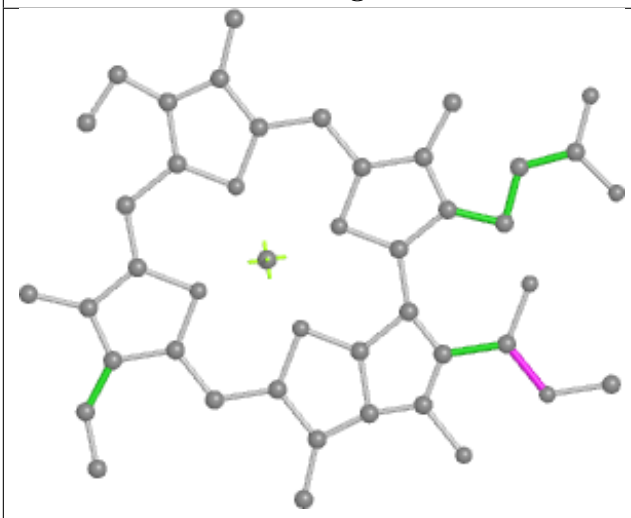
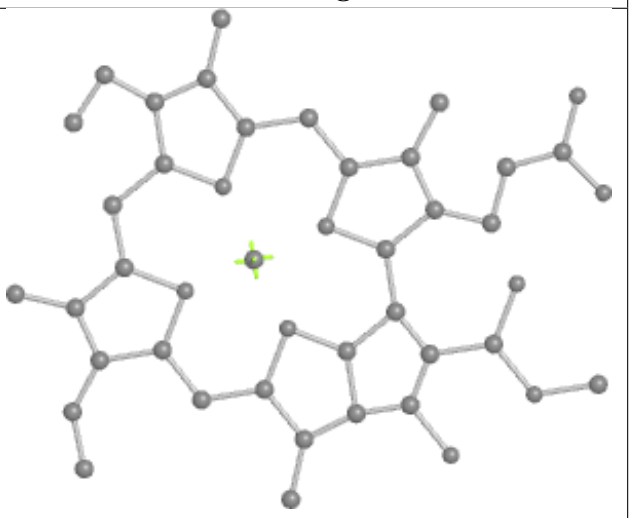


Bond angles

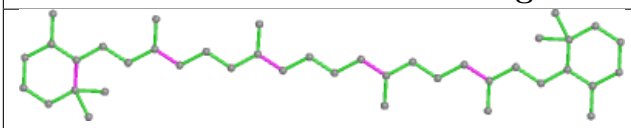


Torsions



Rings

Ligand BCR L 4219



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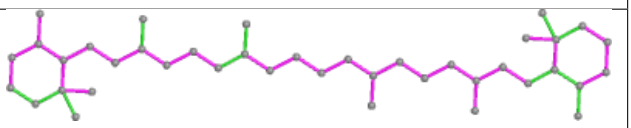

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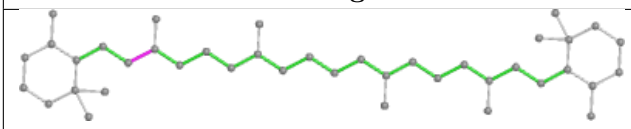
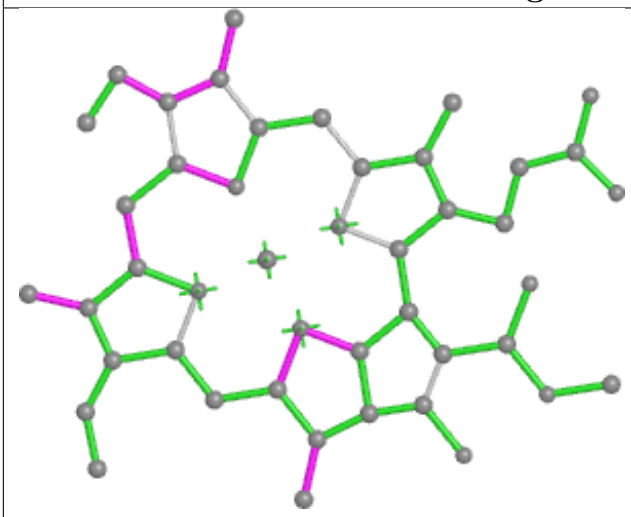


Torsions

Rings

Ligand CLA Z 513



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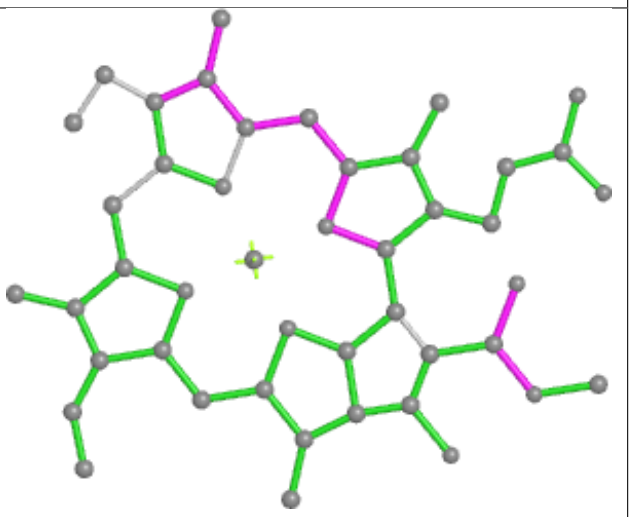

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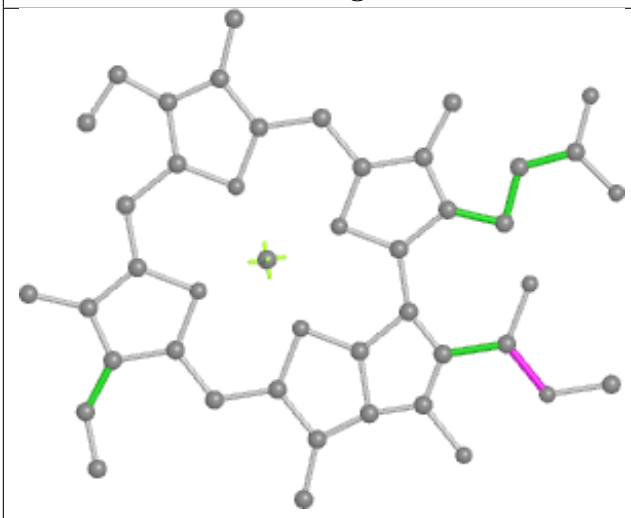

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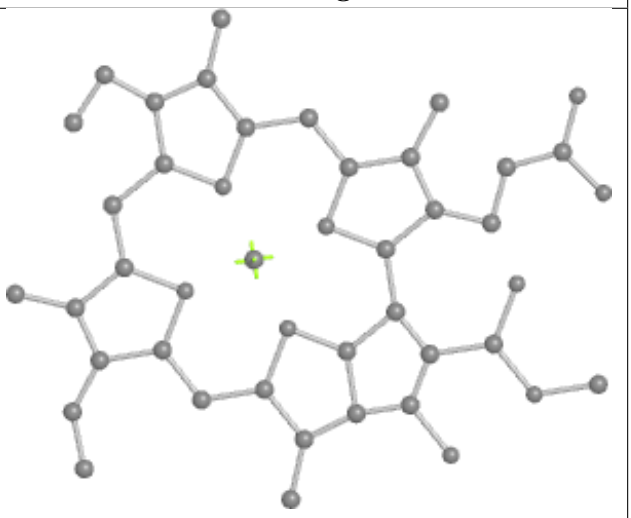

Rings

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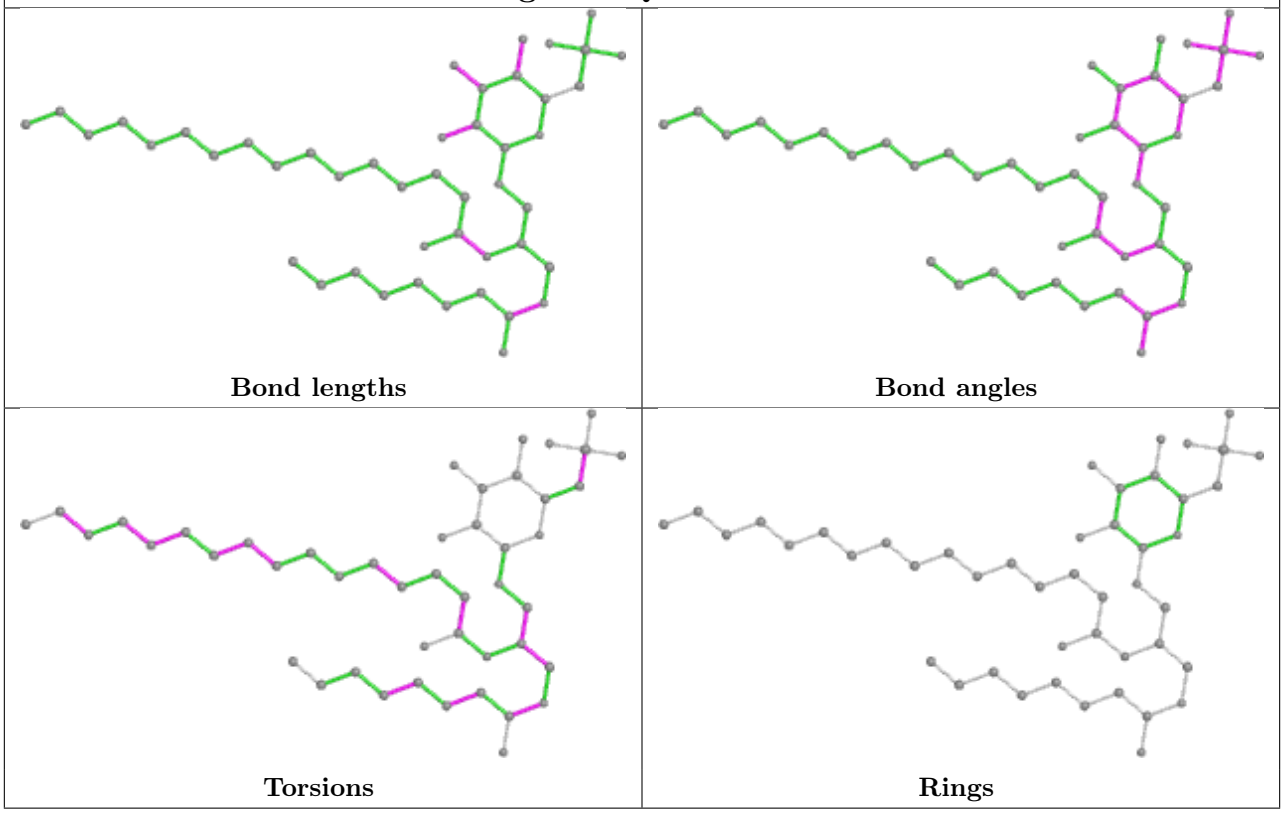

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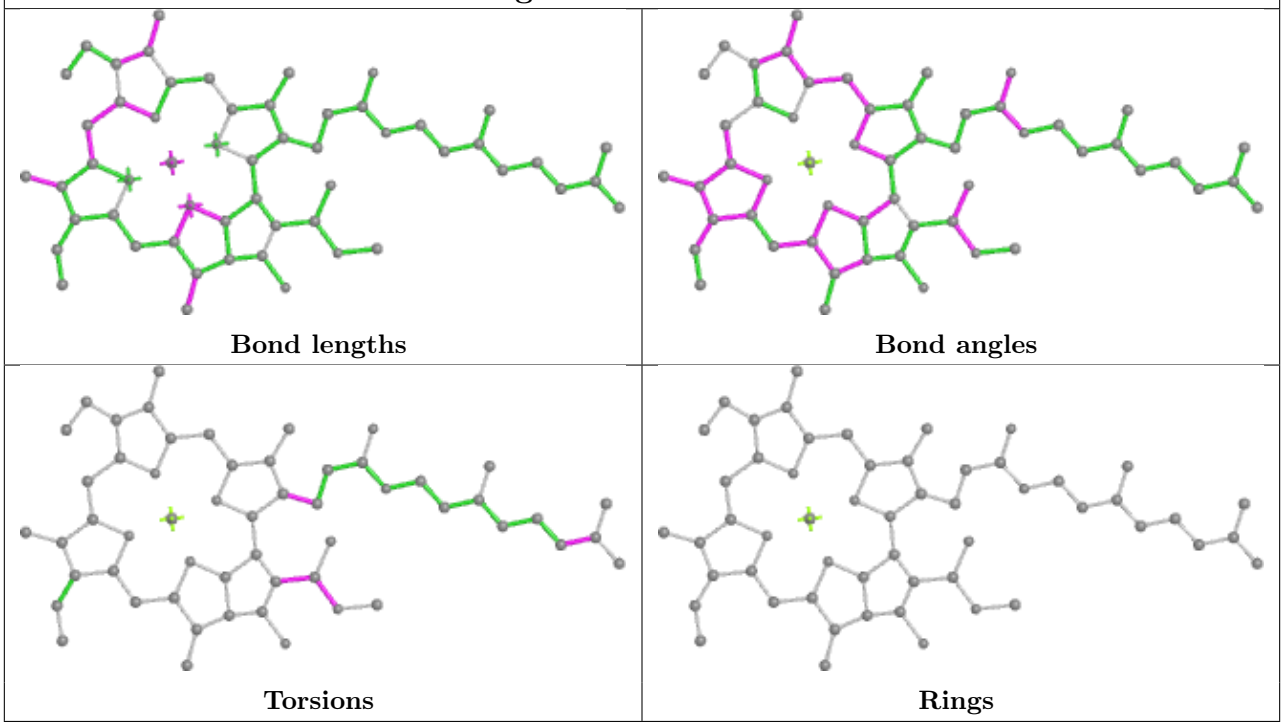

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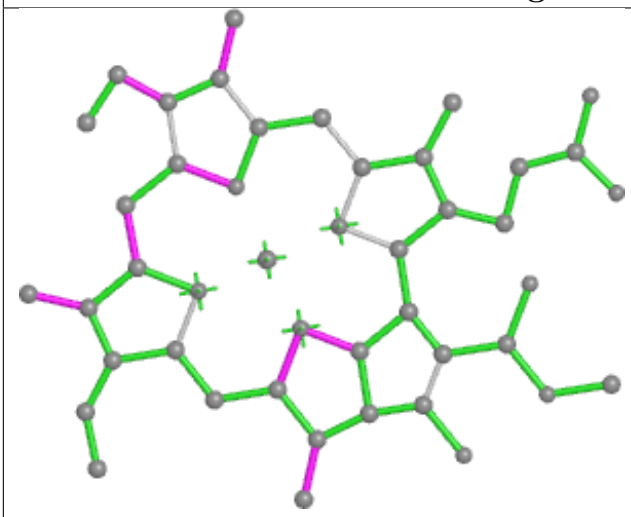

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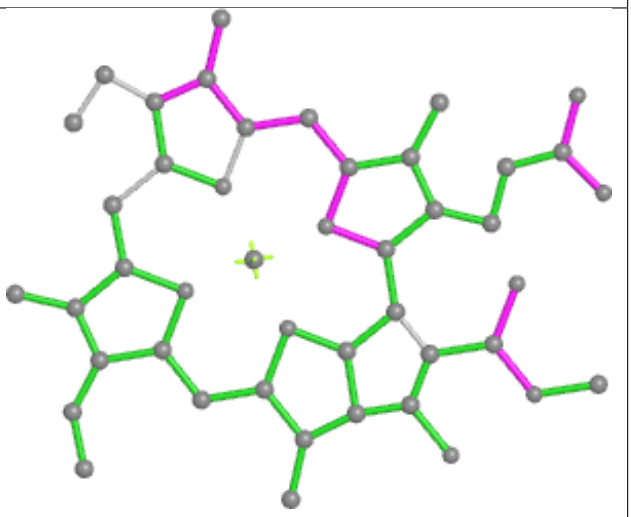

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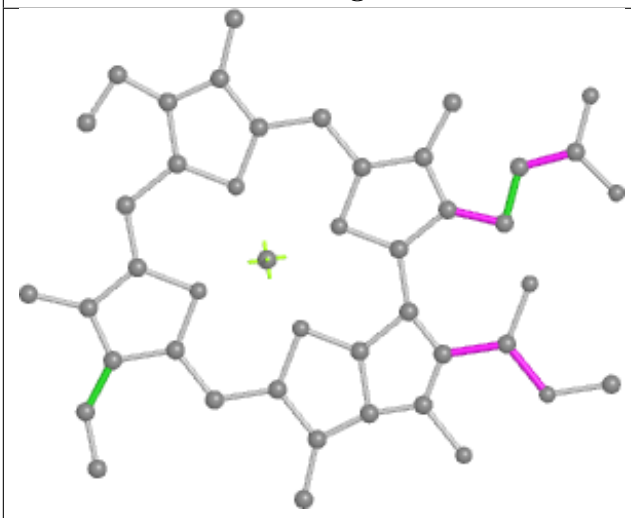

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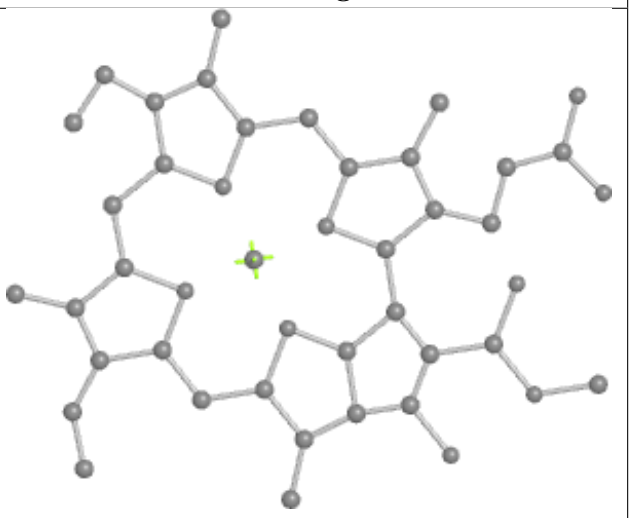

Rings

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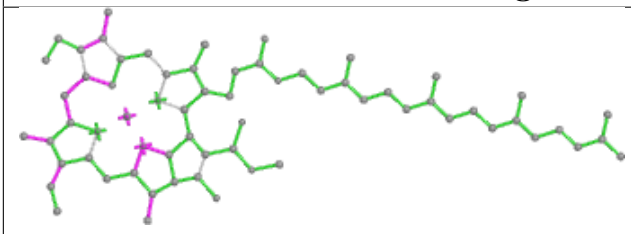

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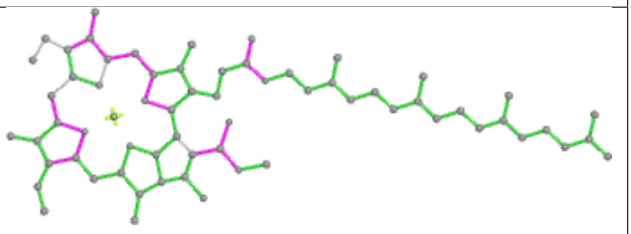

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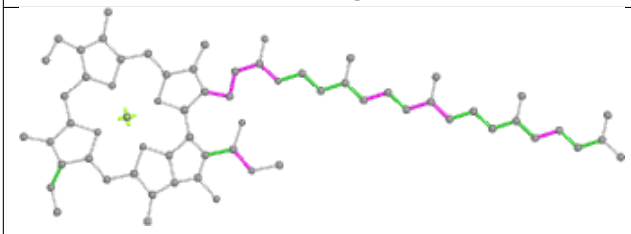

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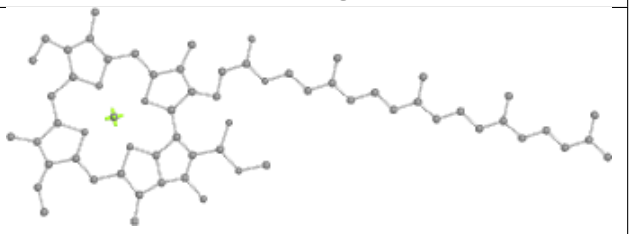

Rings

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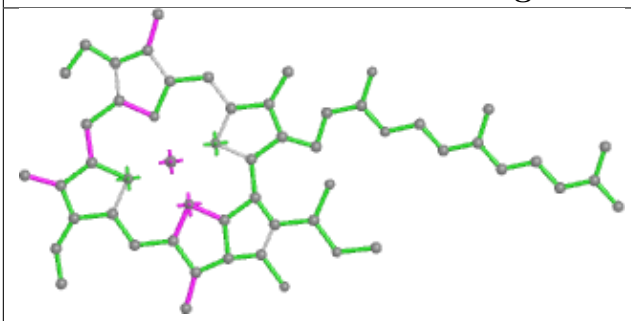
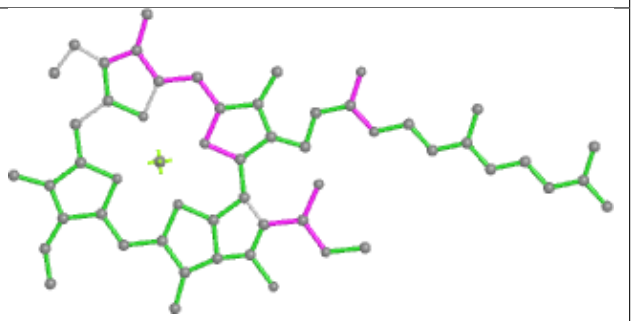
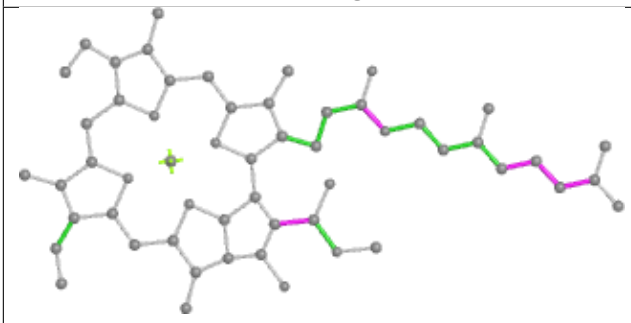
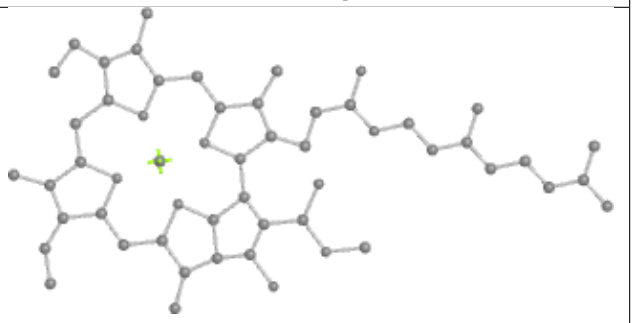
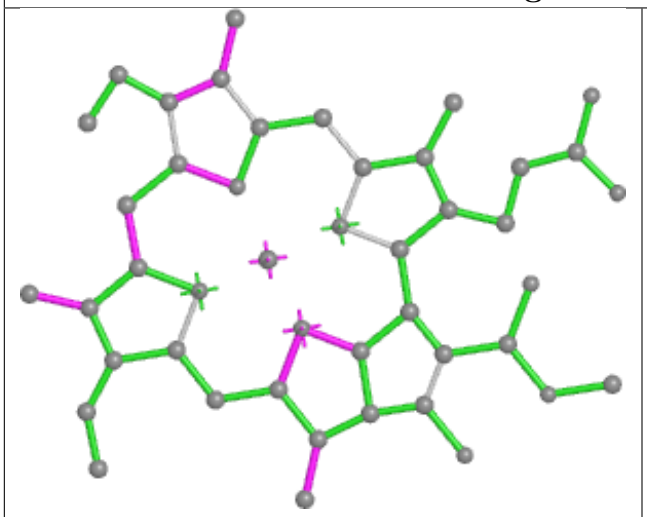
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 508



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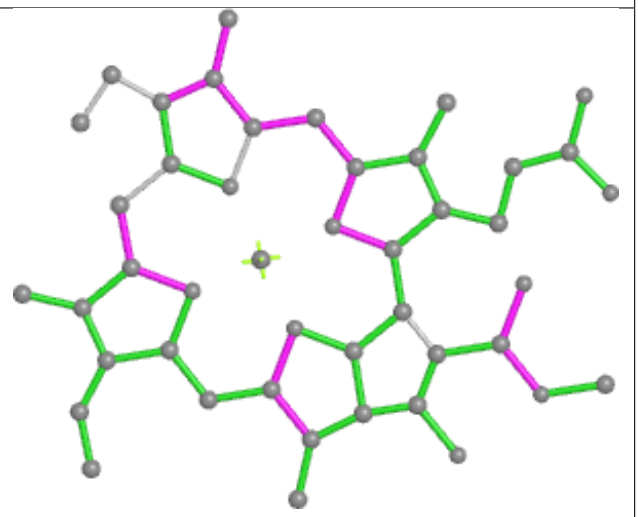

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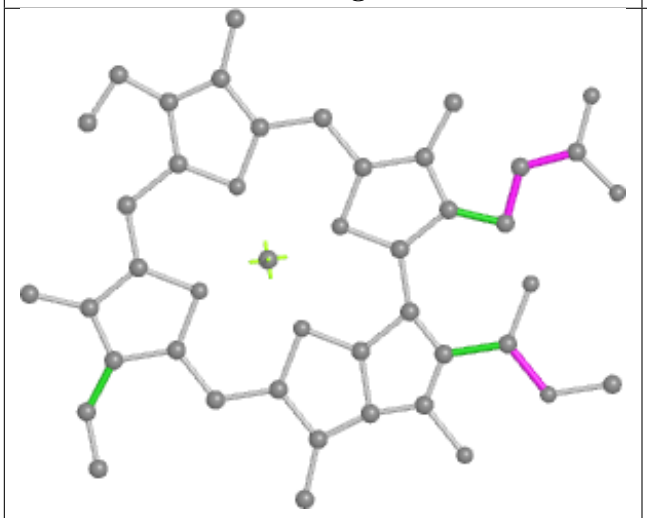

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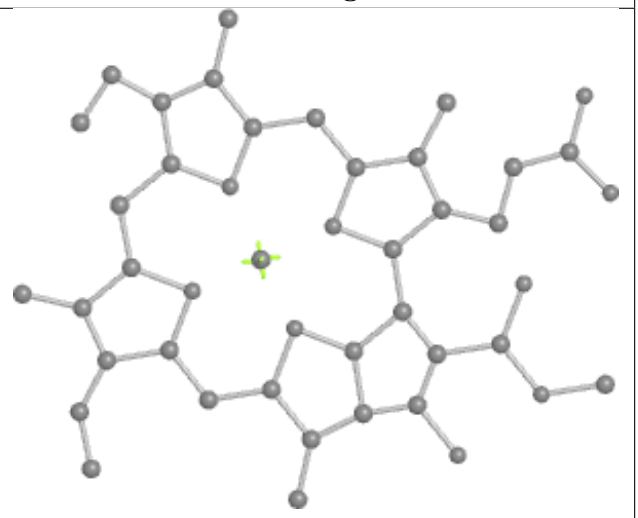

Rings

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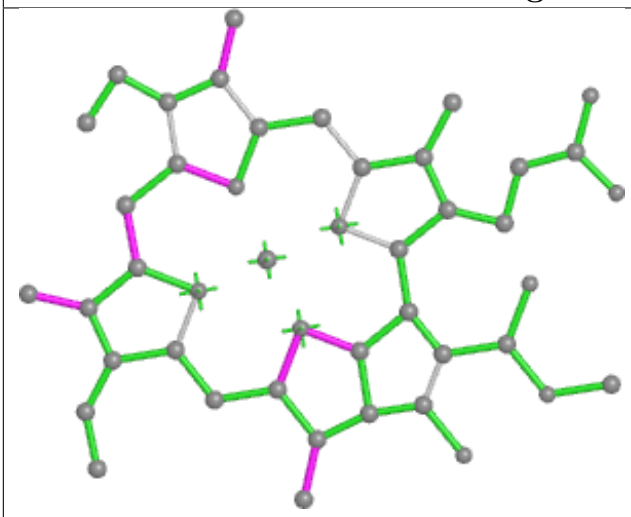

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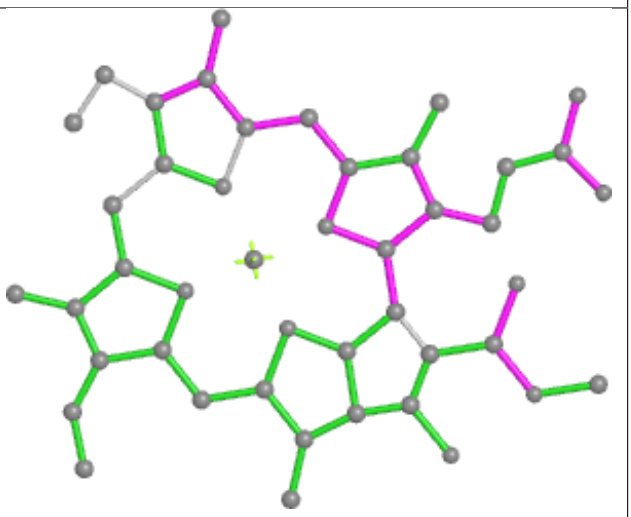

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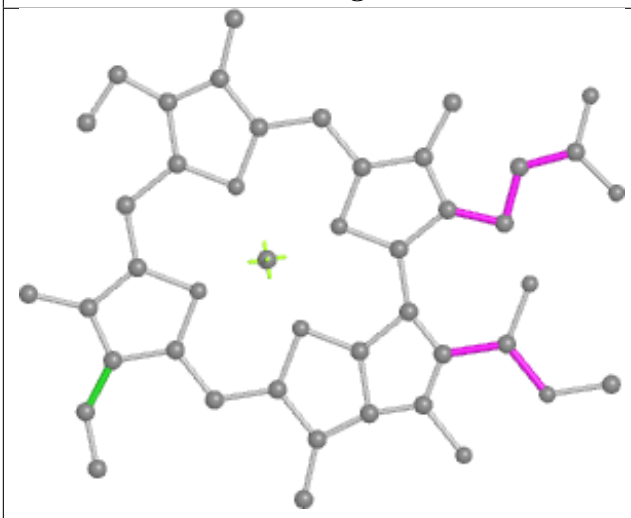

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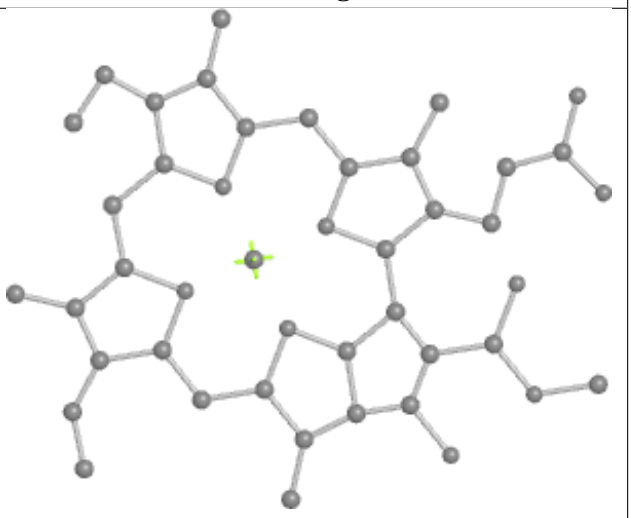

Rings

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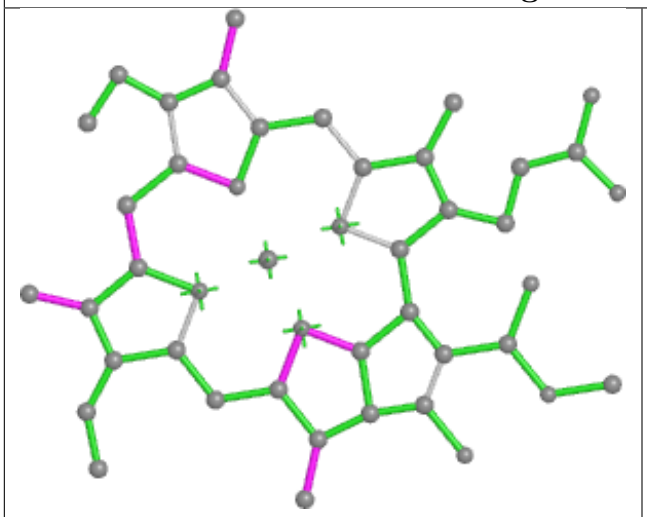

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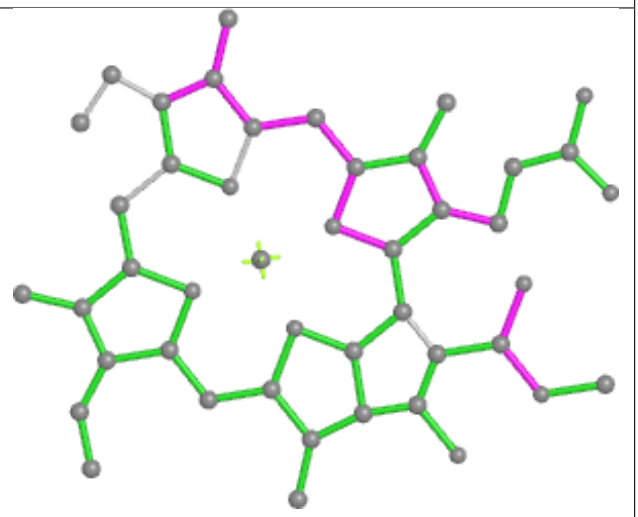

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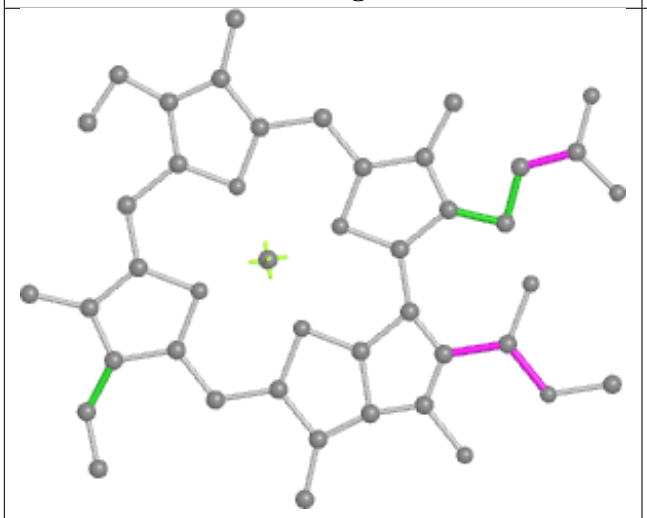

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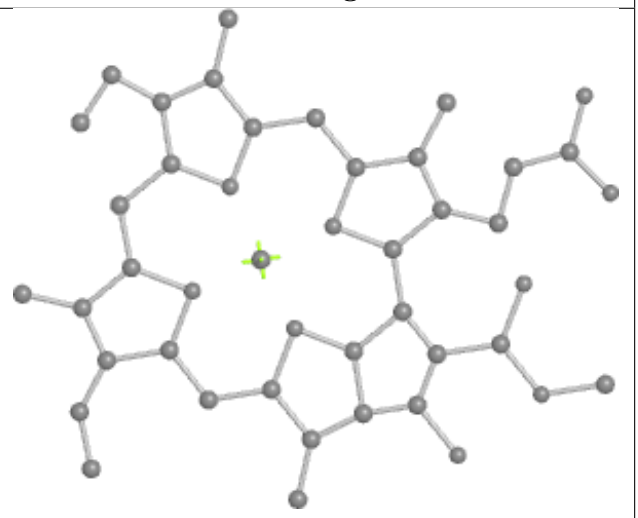
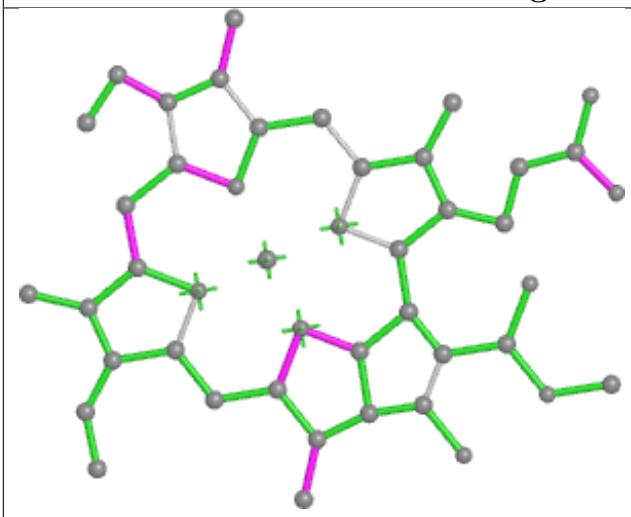


Rings

Ligand CLA s 510



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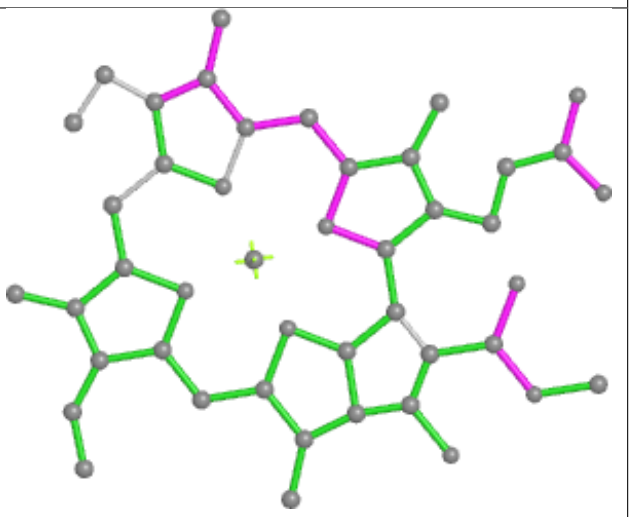

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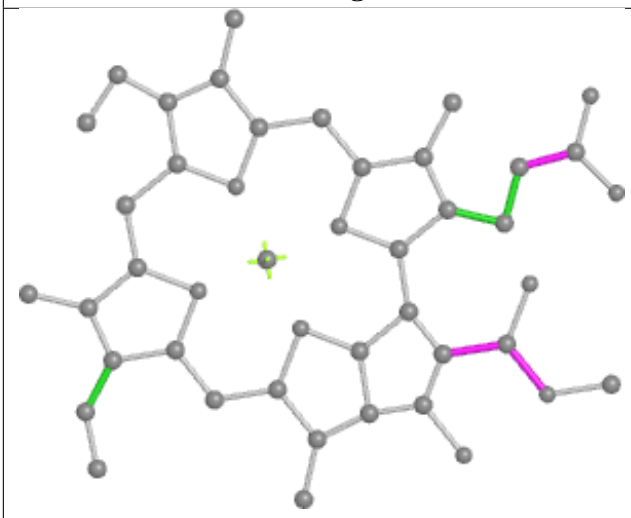

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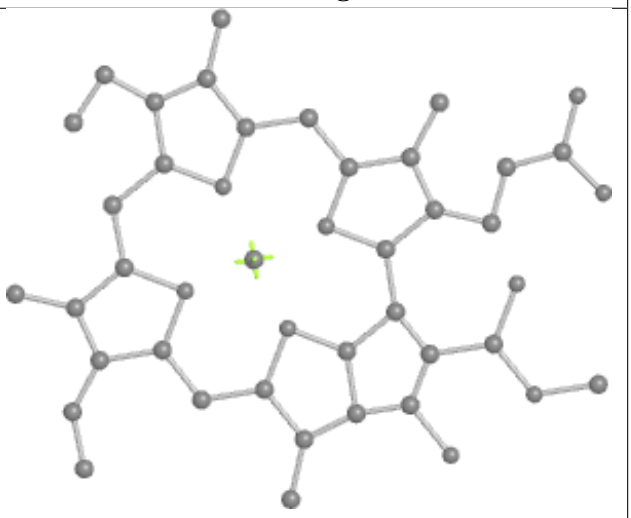
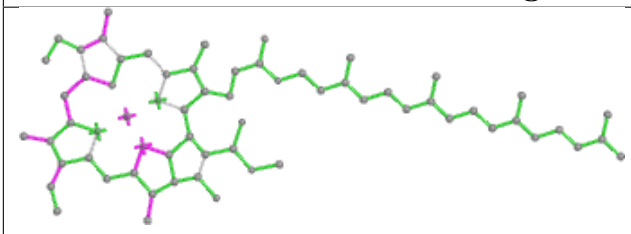


Rings

Ligand CLA f 1206



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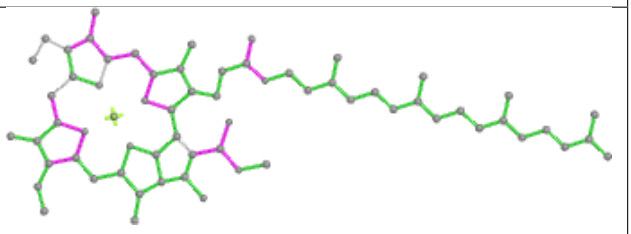

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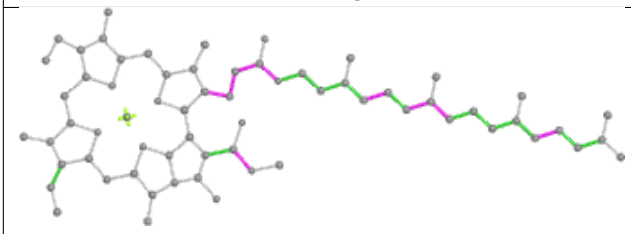

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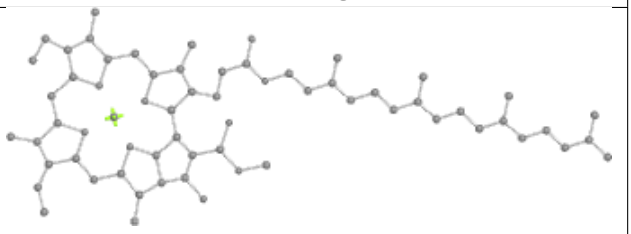
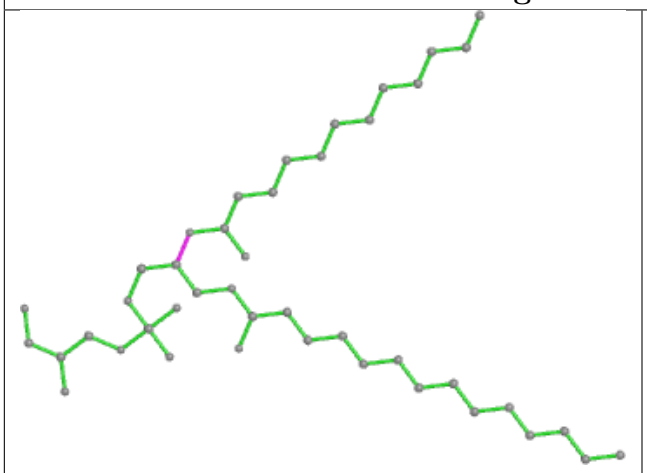


Rings

Ligand LHG G 5005



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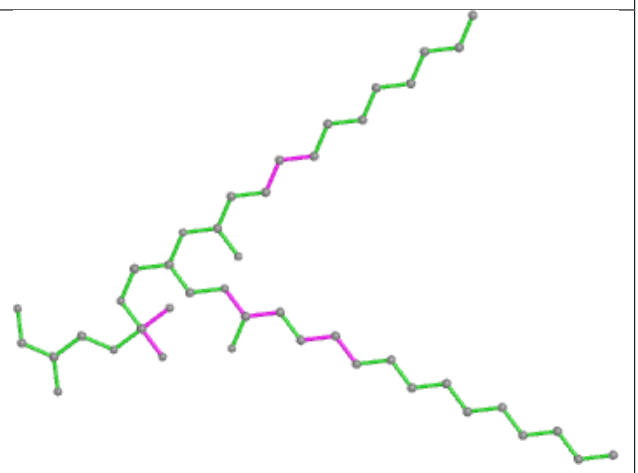
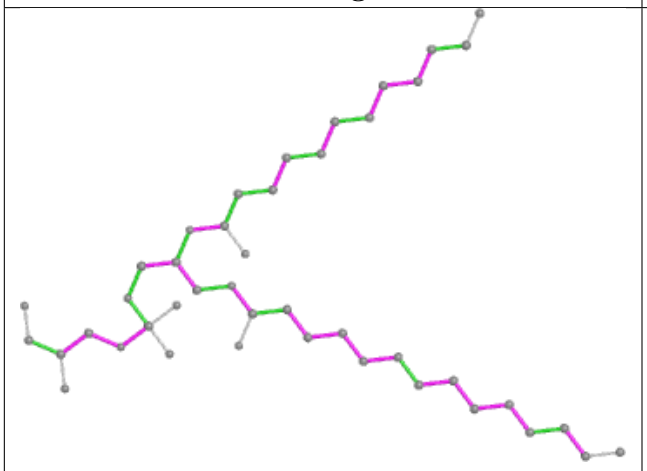
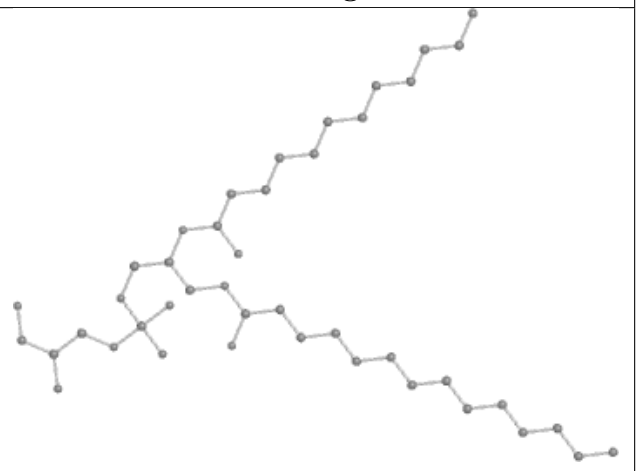


Bond angles

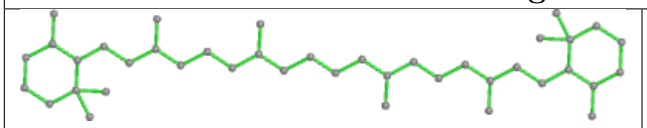


Torsions

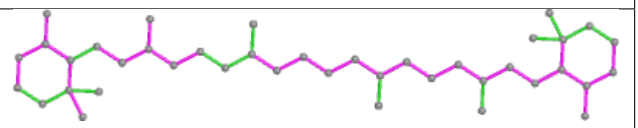


Rings

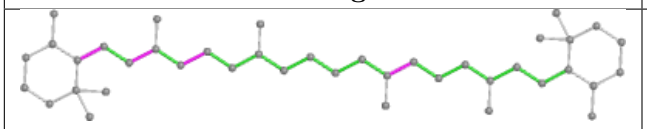
Ligand BCR c 521



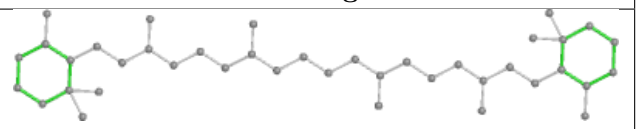
Bond lengths



Bond angles

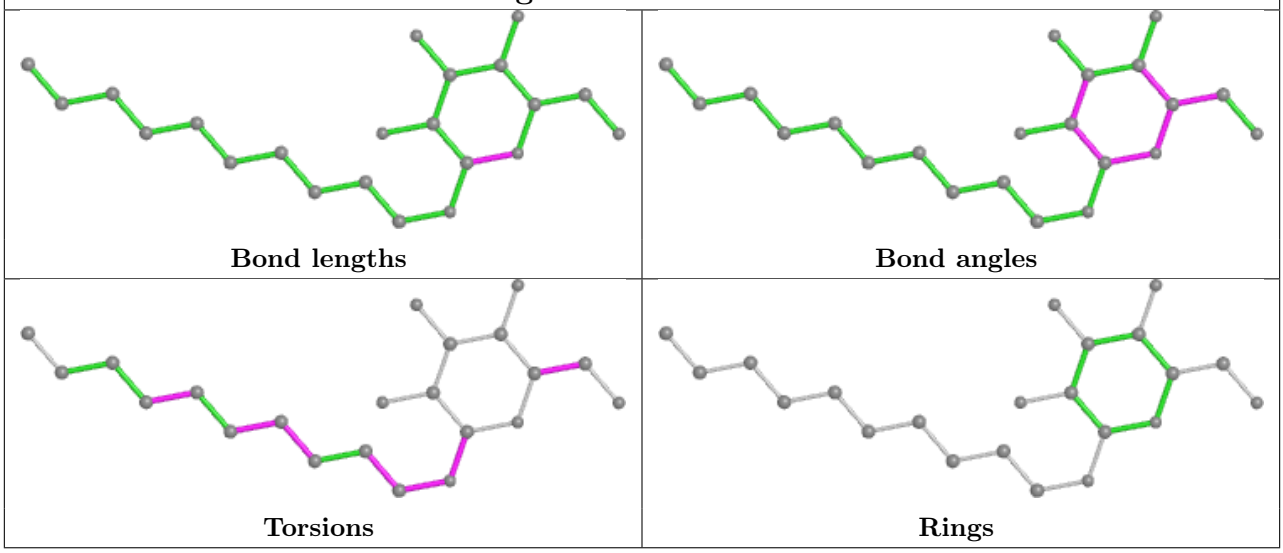


Torsions

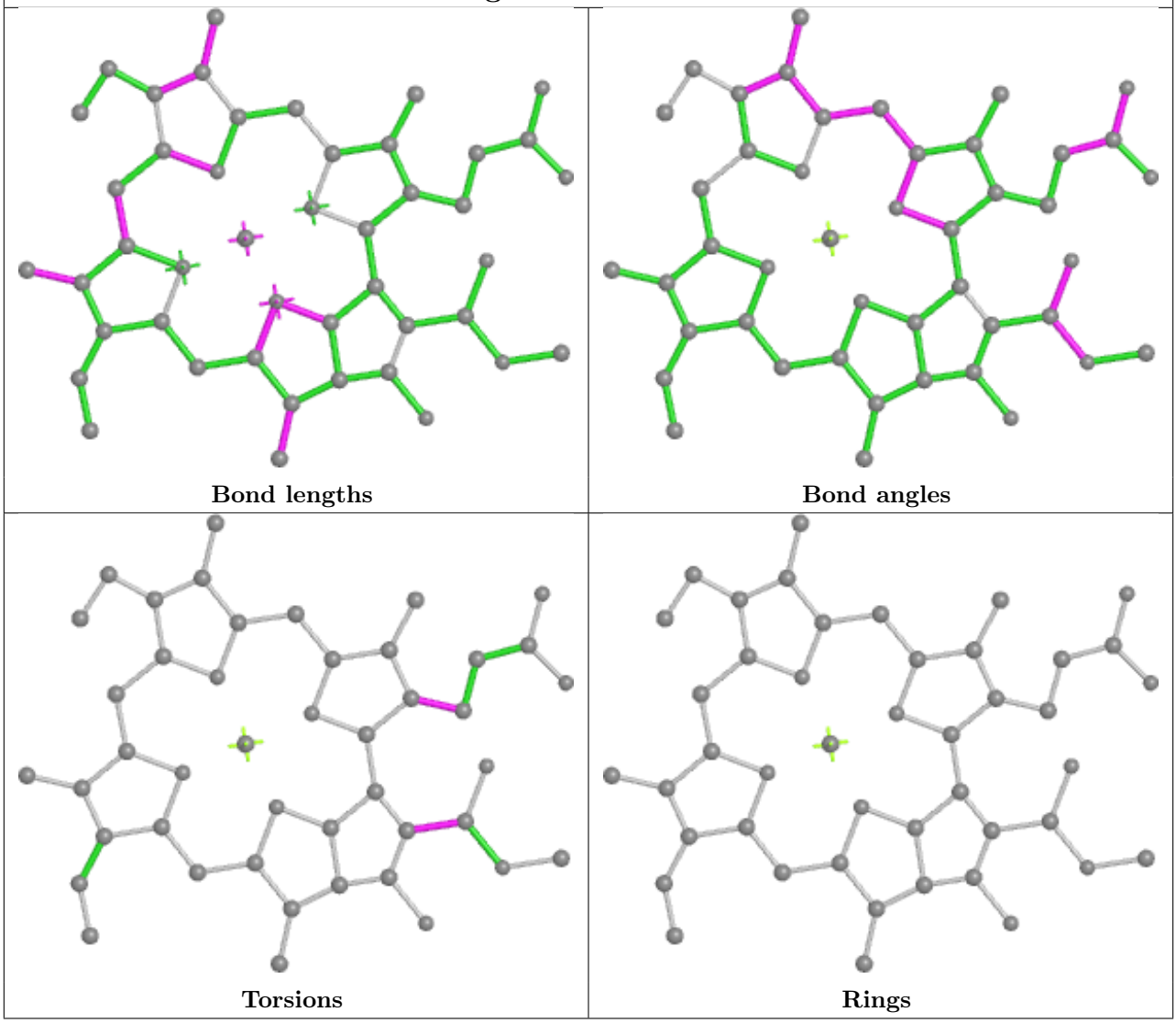


Rings

Ligand LMU J 5105



Ligand CLA a 508



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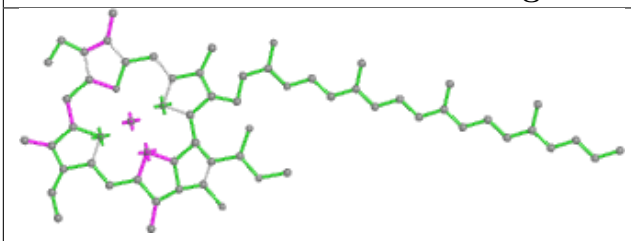
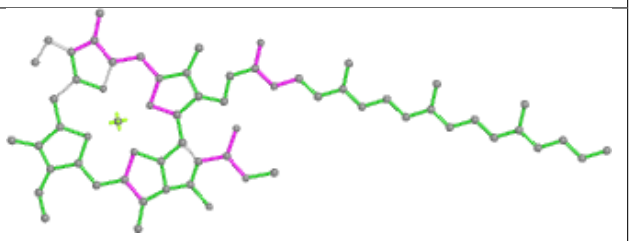
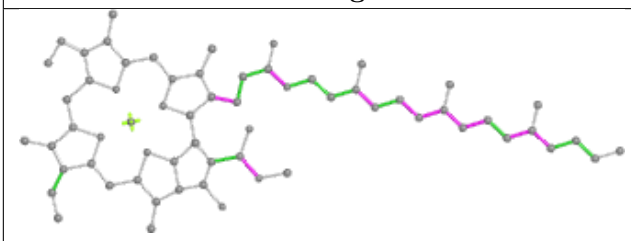


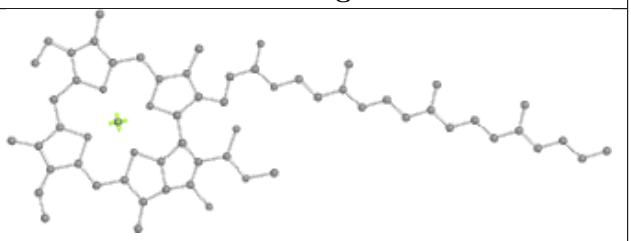
Bond lengths



Bond angles

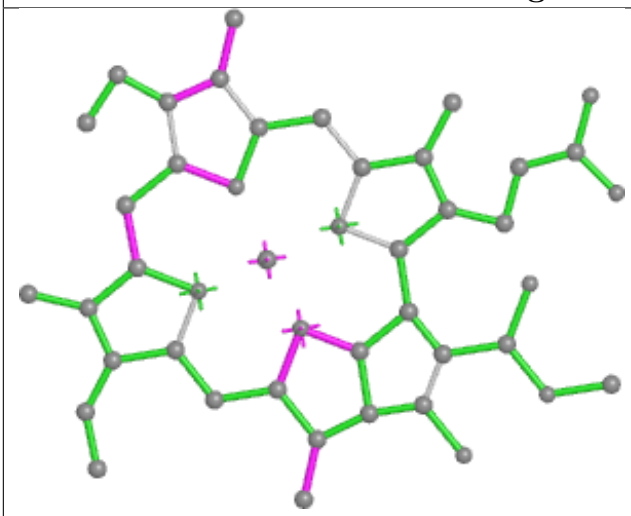


Torsions



Rings

Ligand CLA q 512



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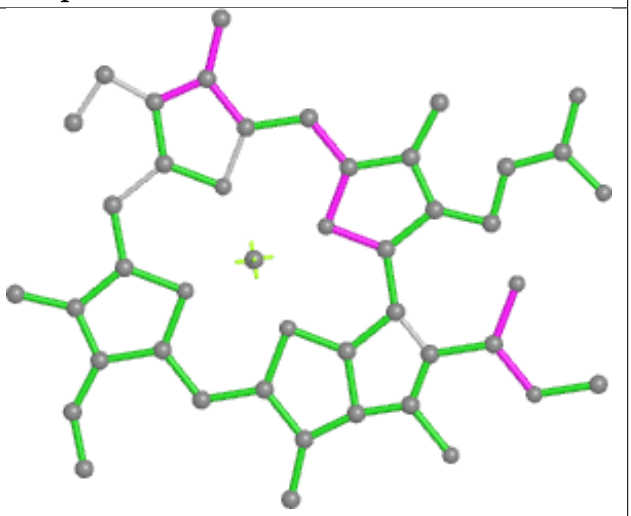
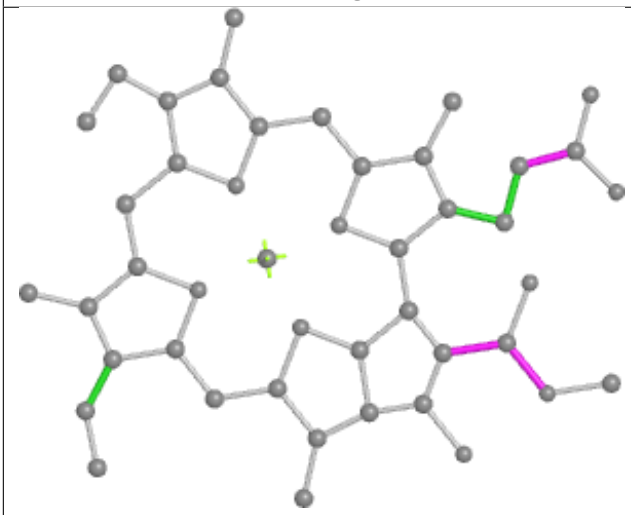
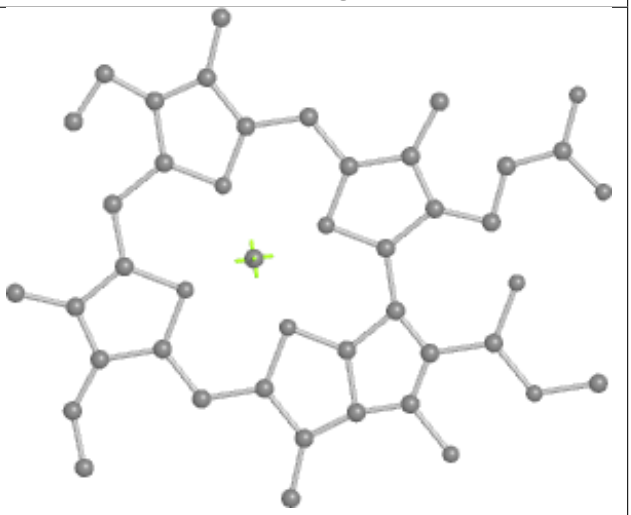


Bond angles

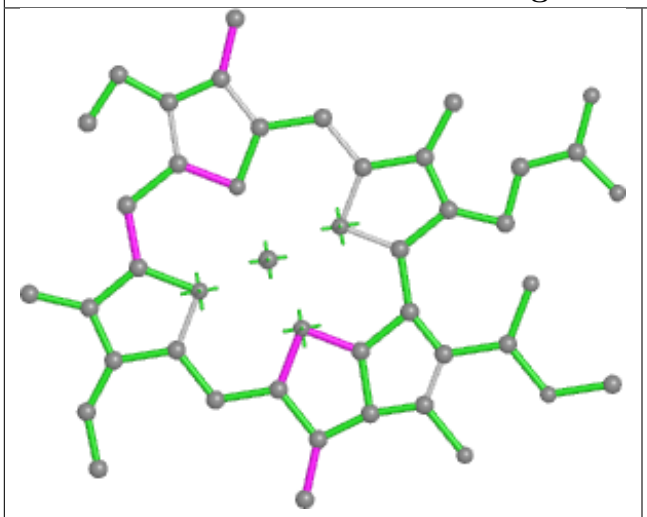


Torsions

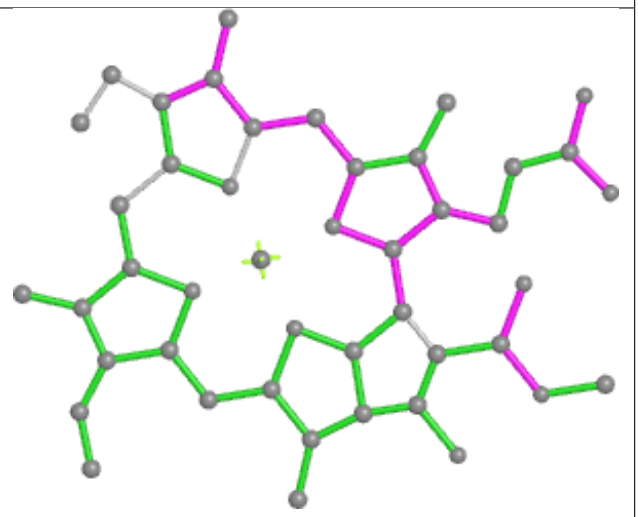


Rings

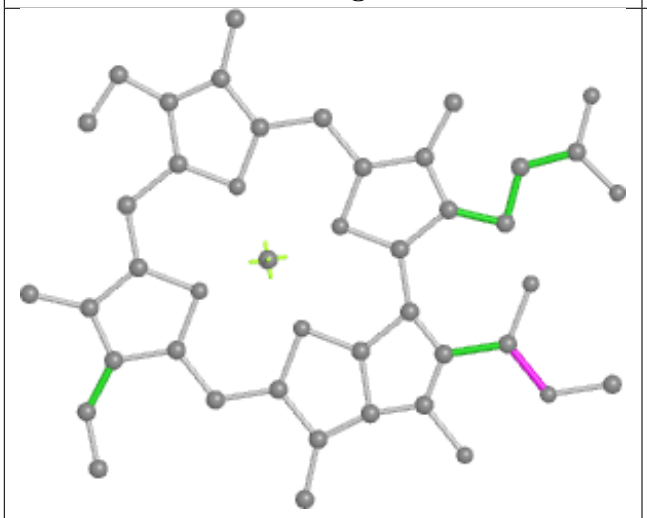
Ligand CLA s 511



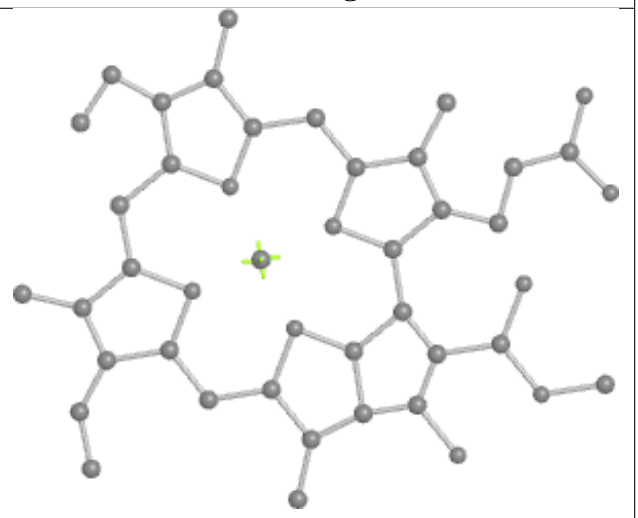
Bond lengths



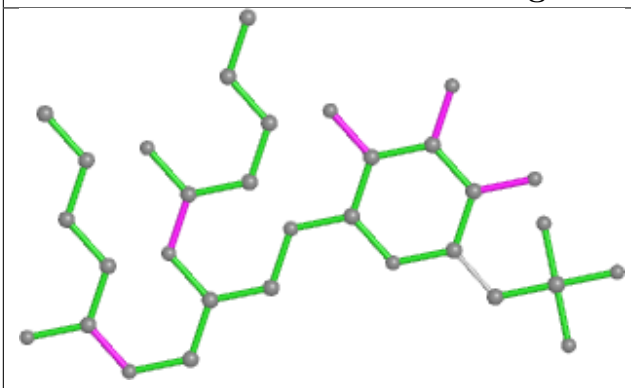
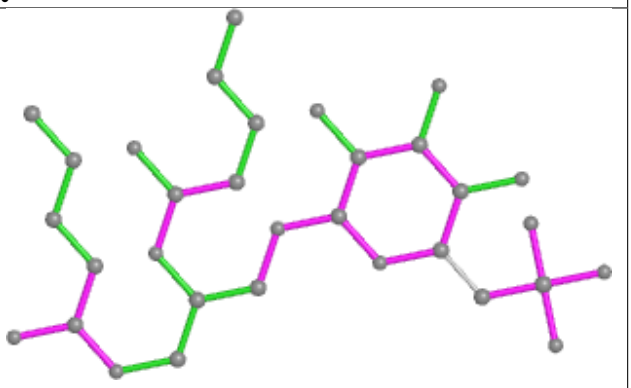
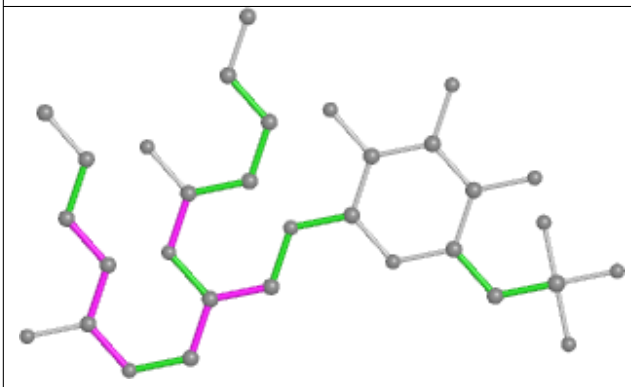
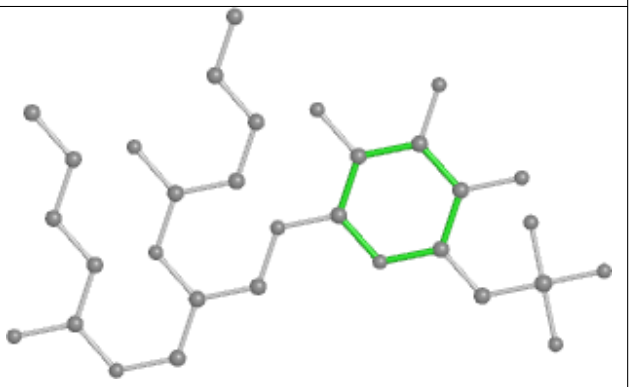
Bond angles

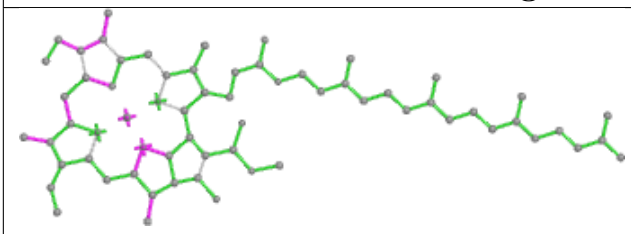
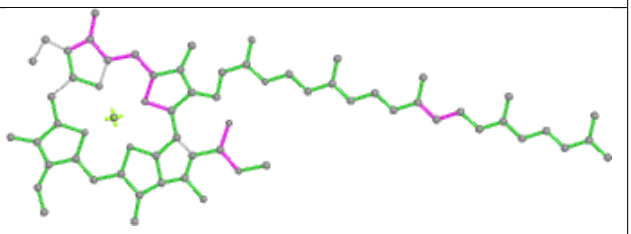
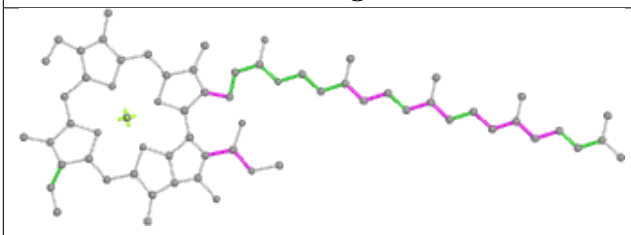
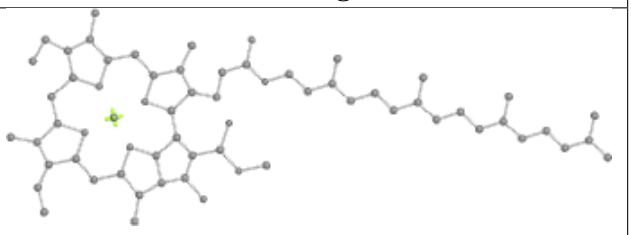


Torsions

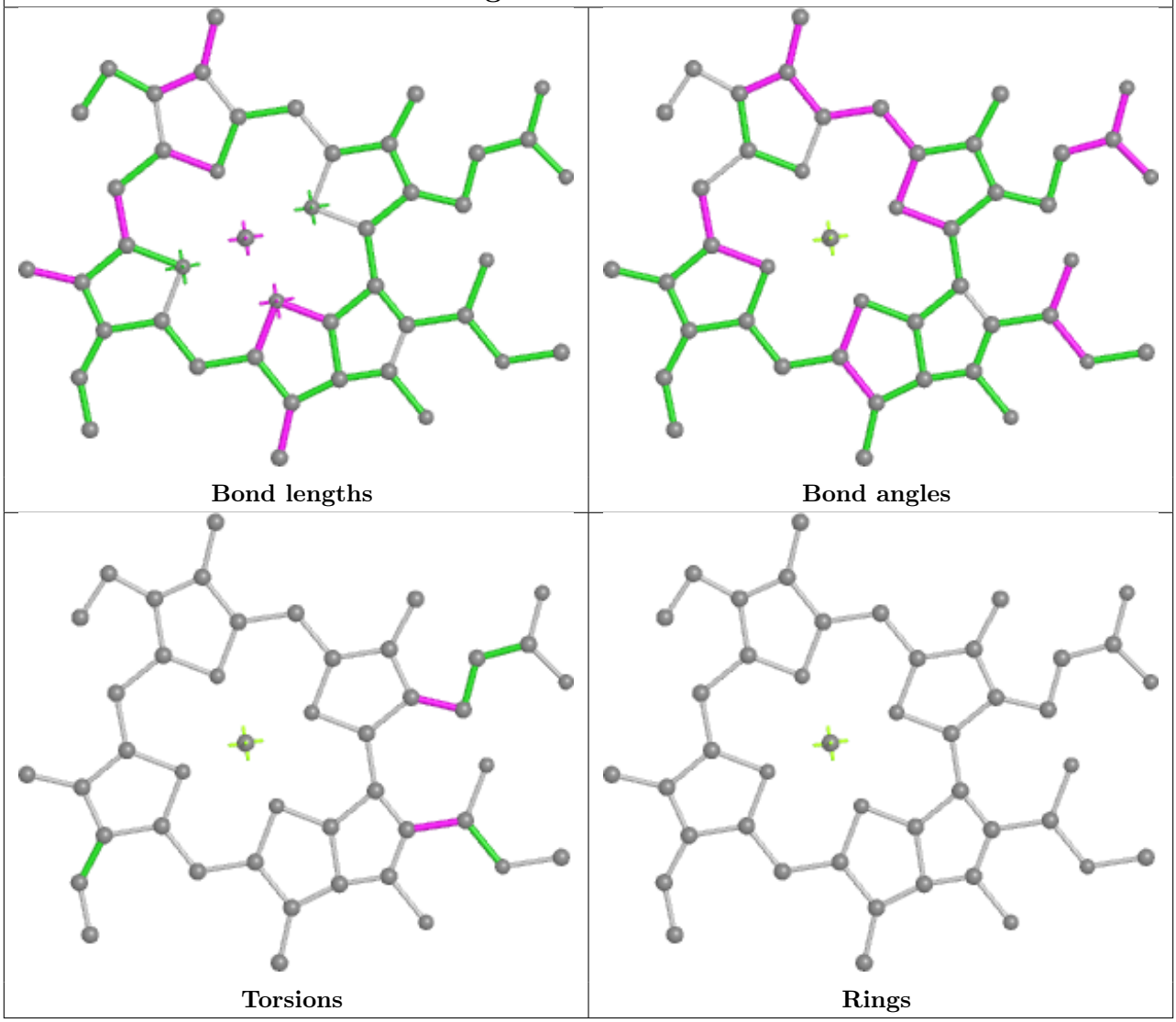


Rings

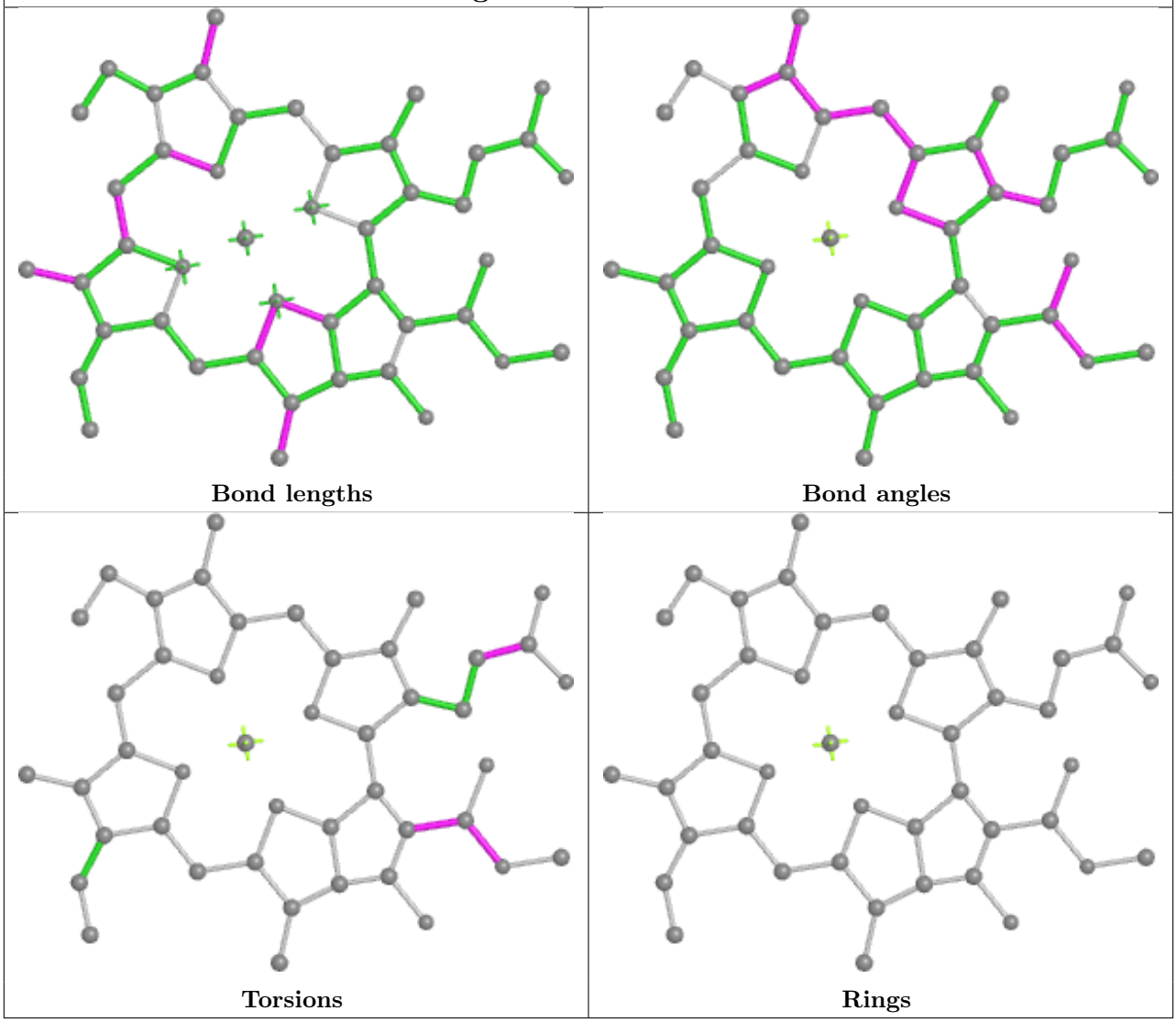
Ligand SQD 1 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA e 1139	
 Bond lengths	 Bond angles
 Torsions	 Rings

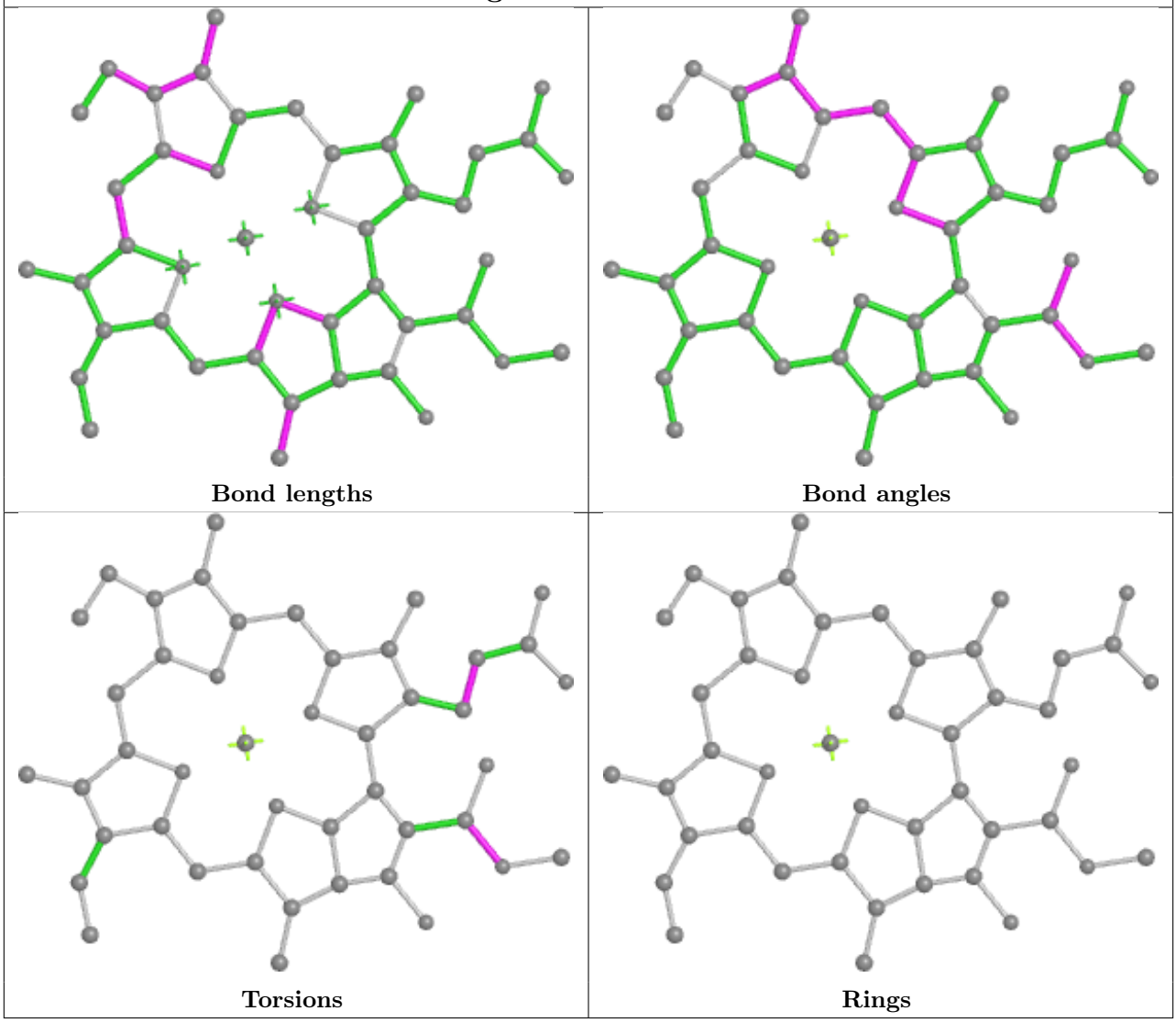
Ligand CLA 2 508



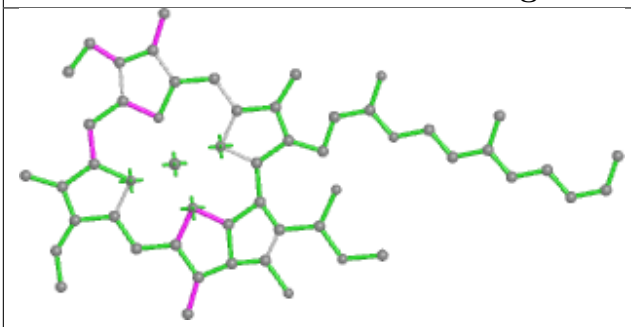
Ligand CLA A 1801



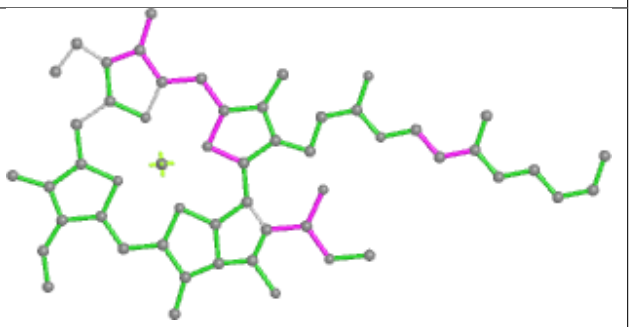
Ligand CLA s 513



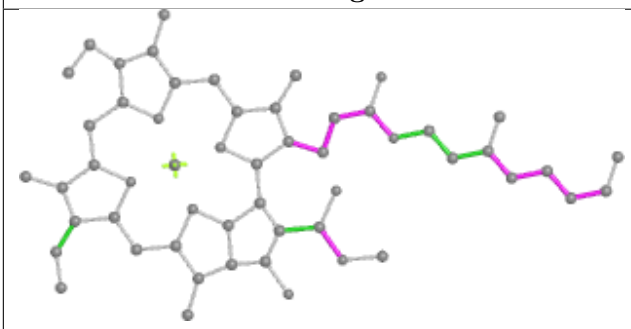
Ligand CLA e 1108



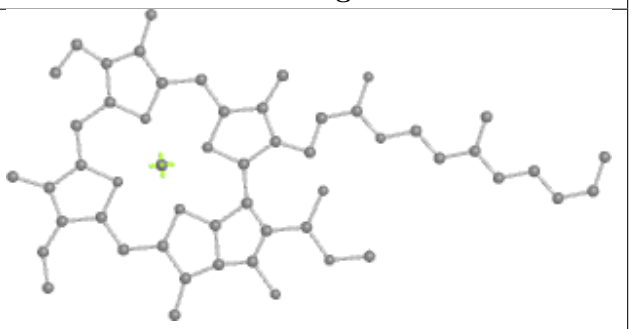
Bond lengths



Bond angles

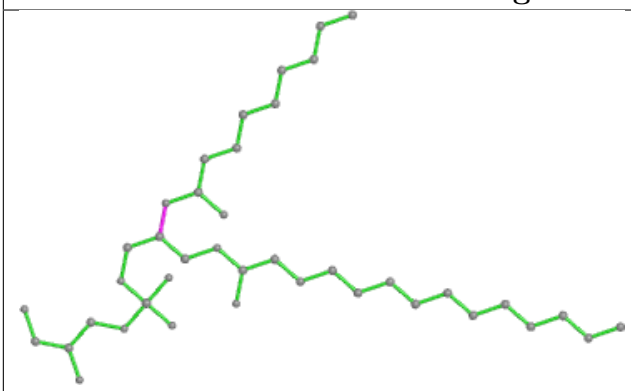


Torsions



Rings

Ligand LHG A 5006



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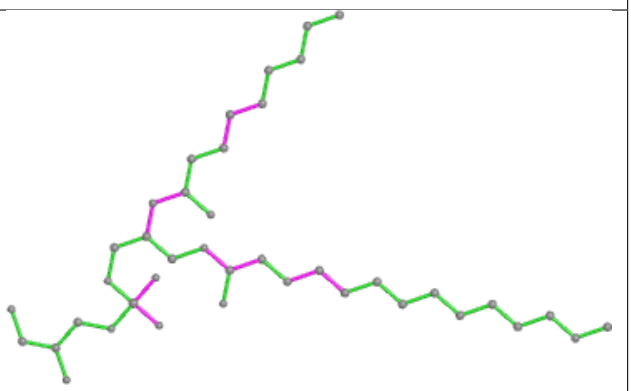
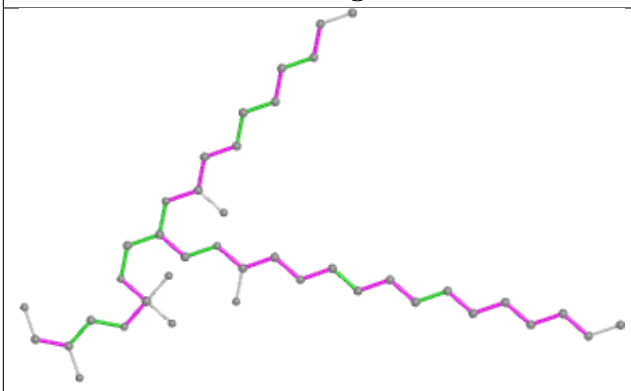
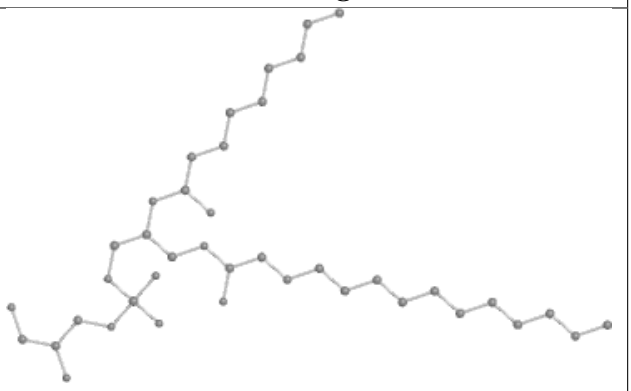


Bond angles

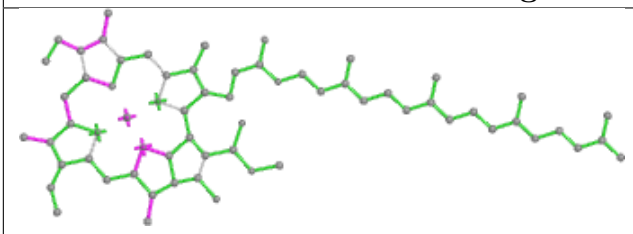


Torsions

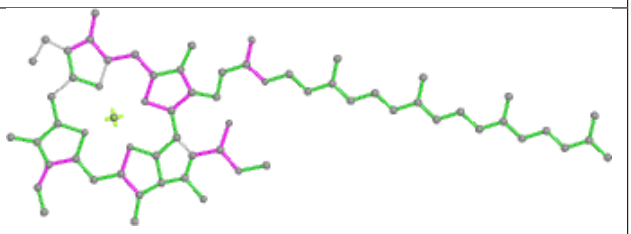


Rings

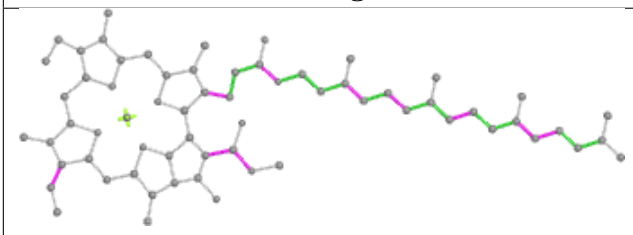
Ligand CLA e 1132



Bond lengths



Bond angles



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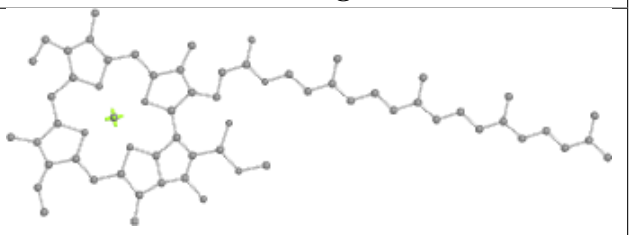
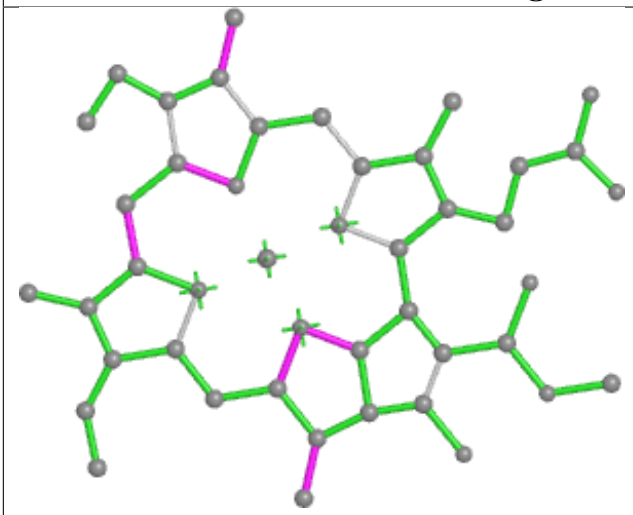
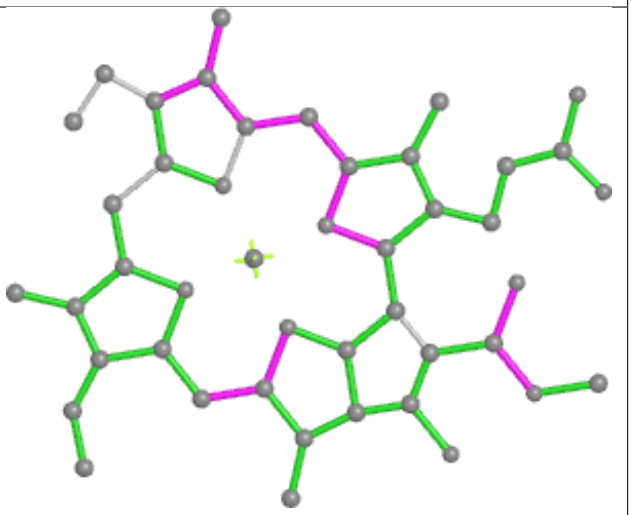


Rings

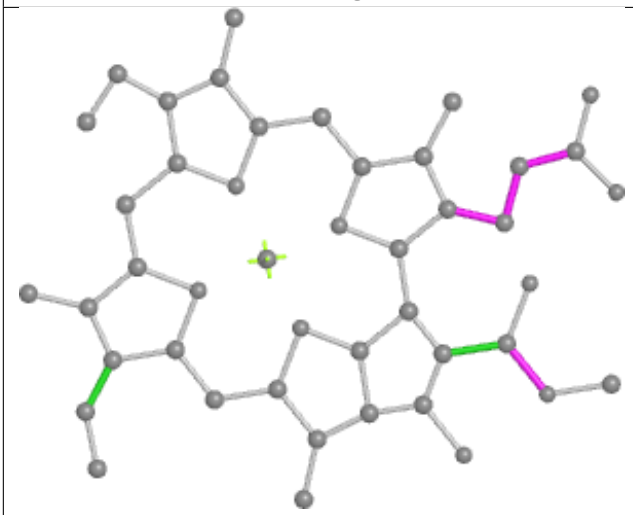
Ligand CLA b 501



Bond lengths



Bond angles



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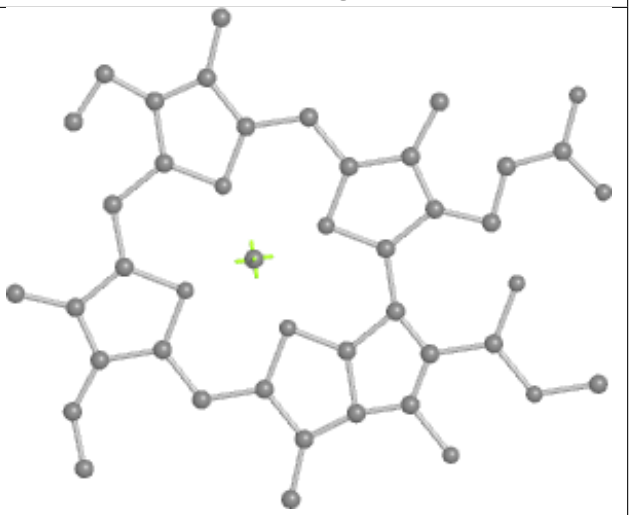
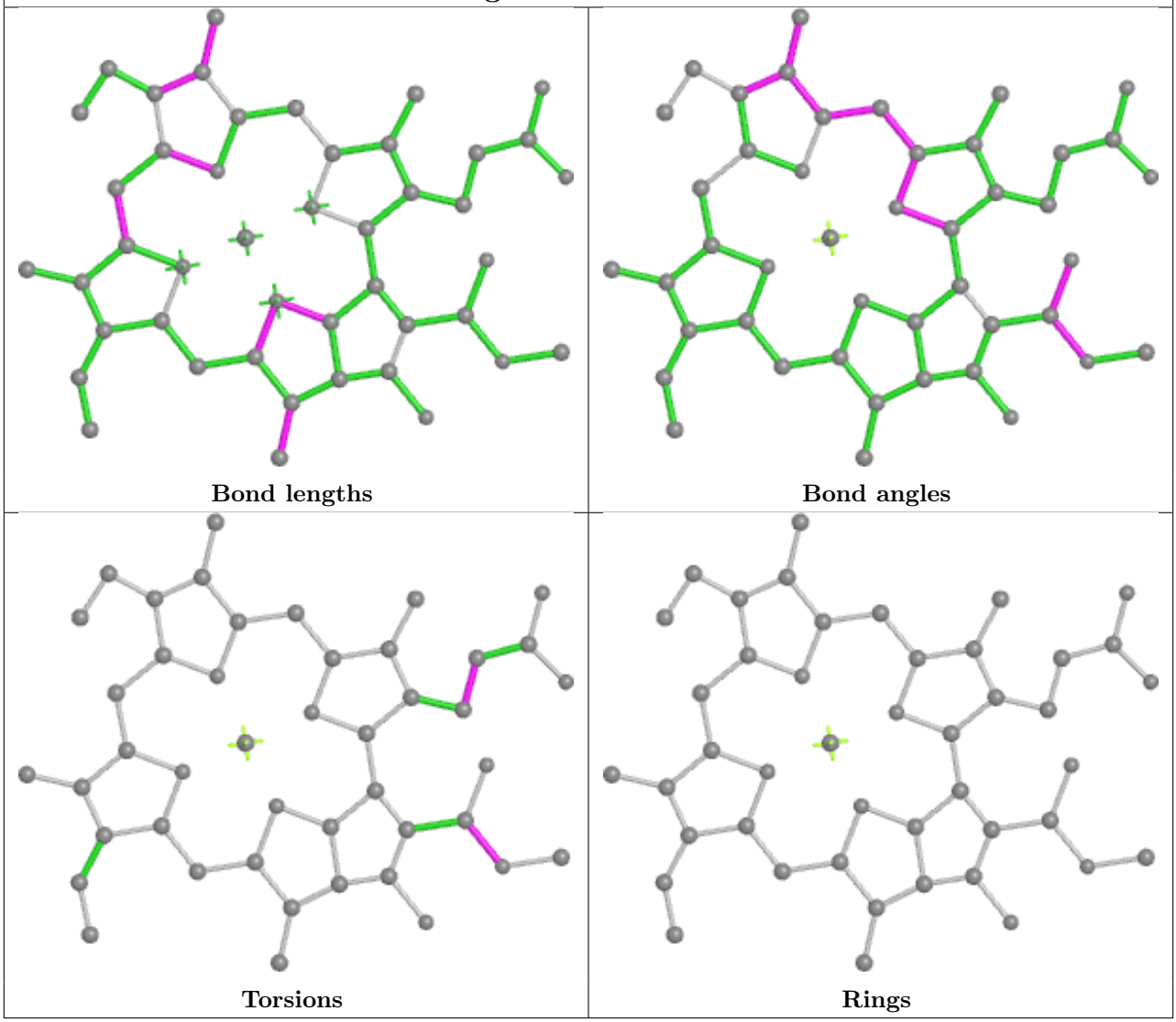
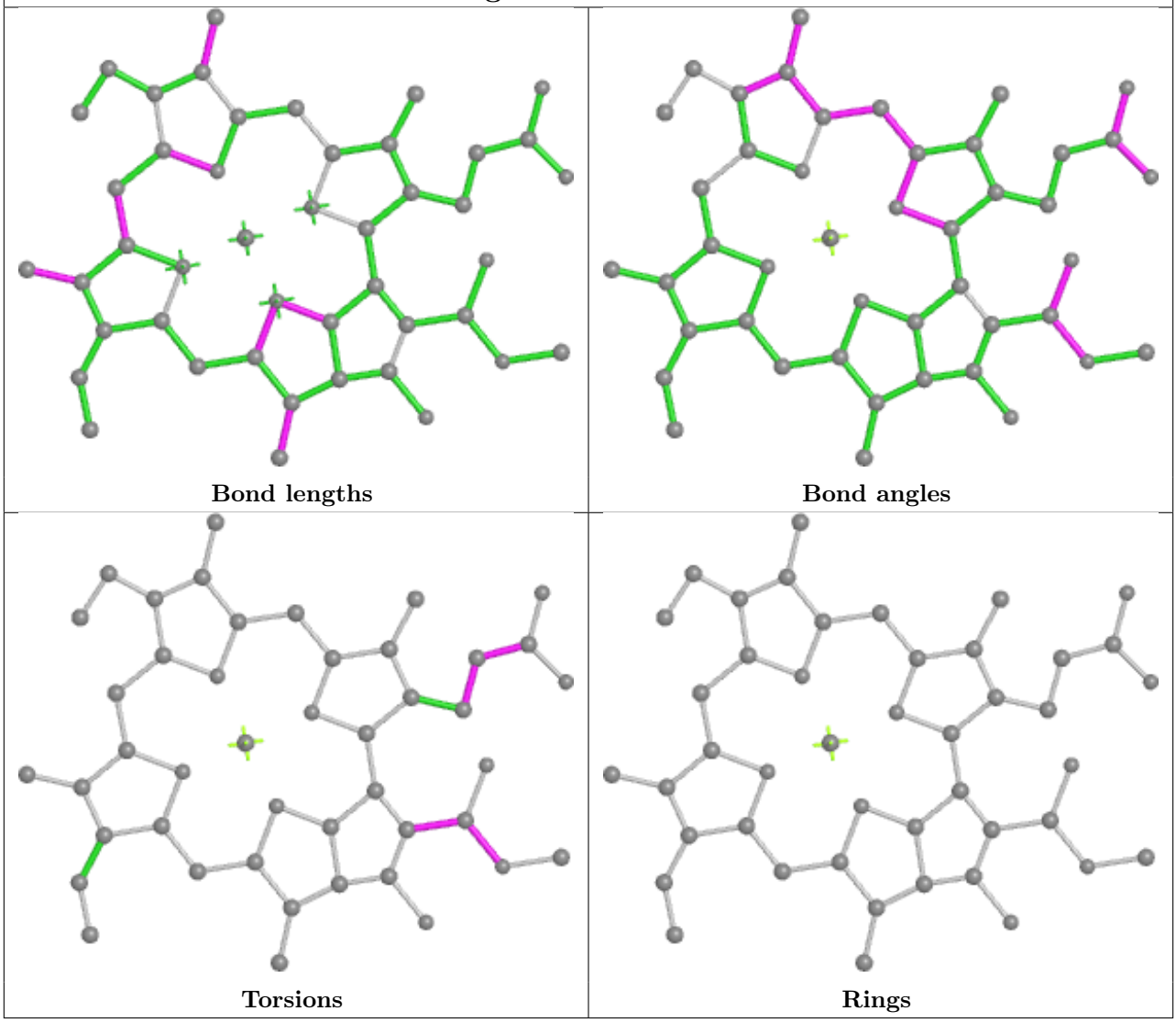


Rings

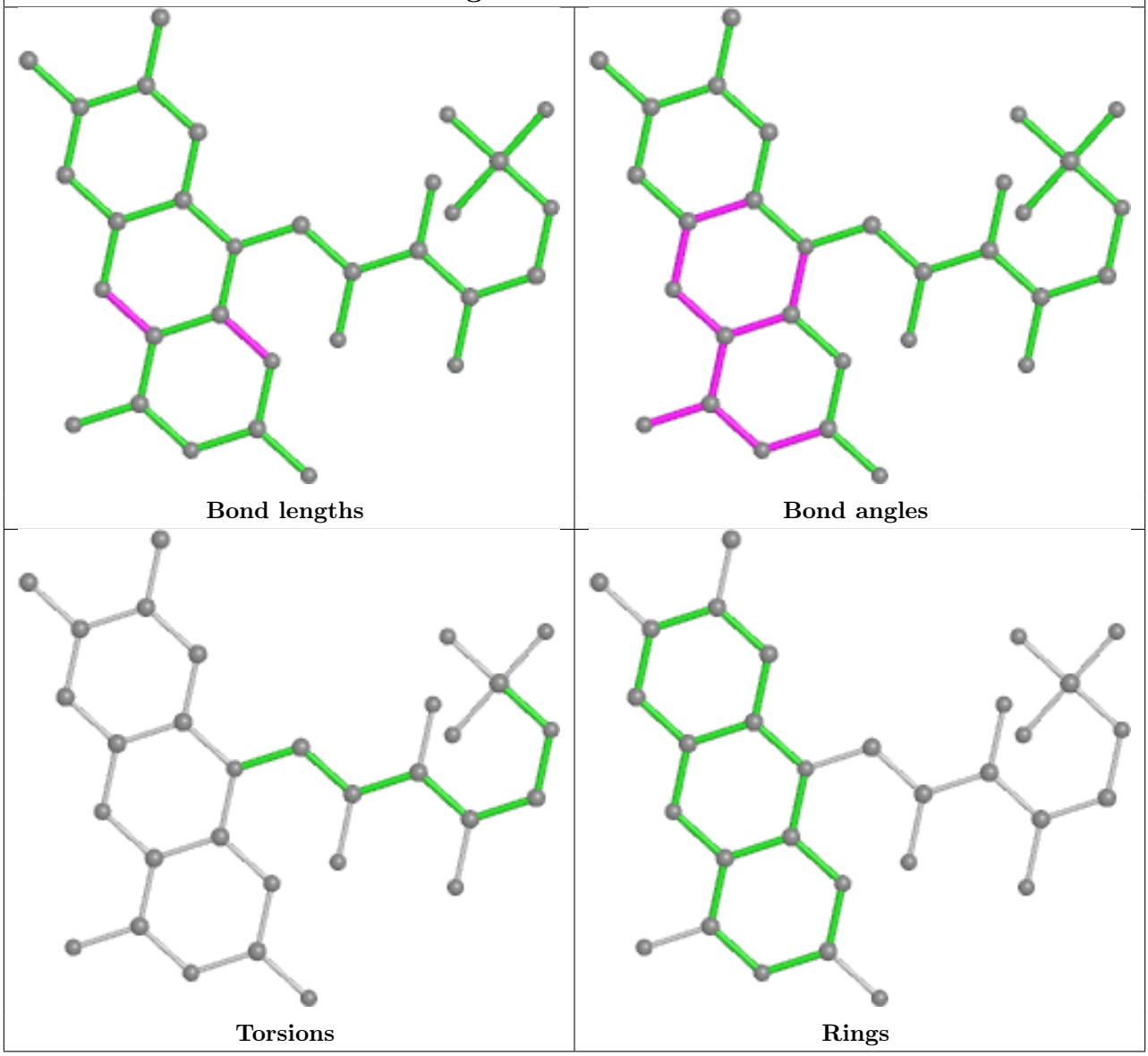
Ligand CLA v 513

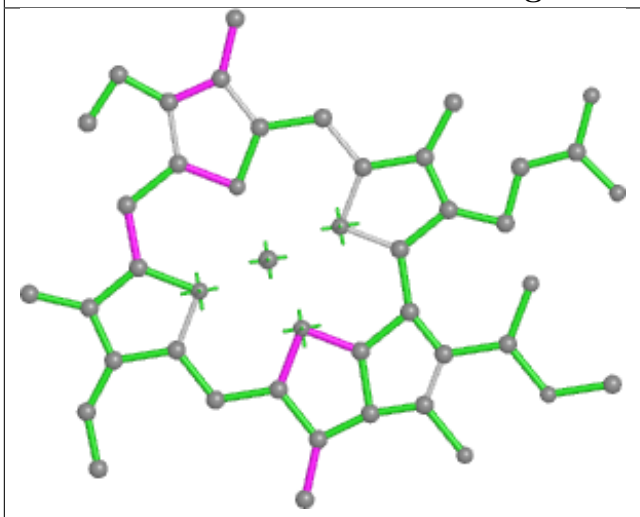
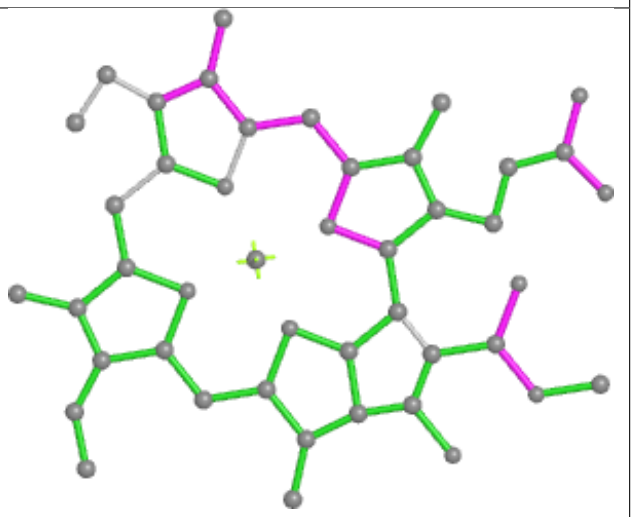
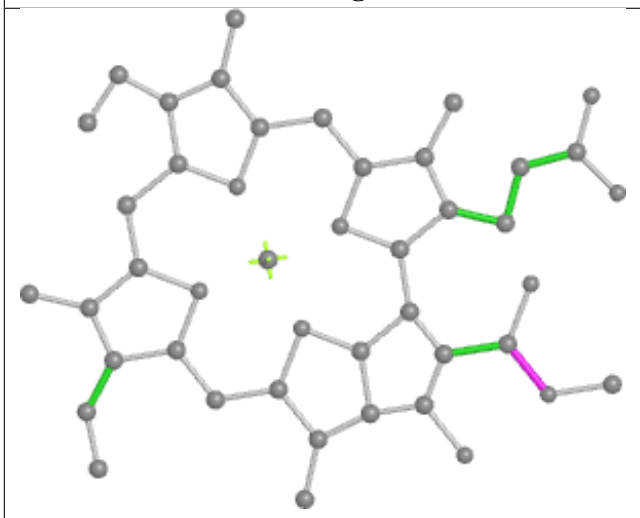
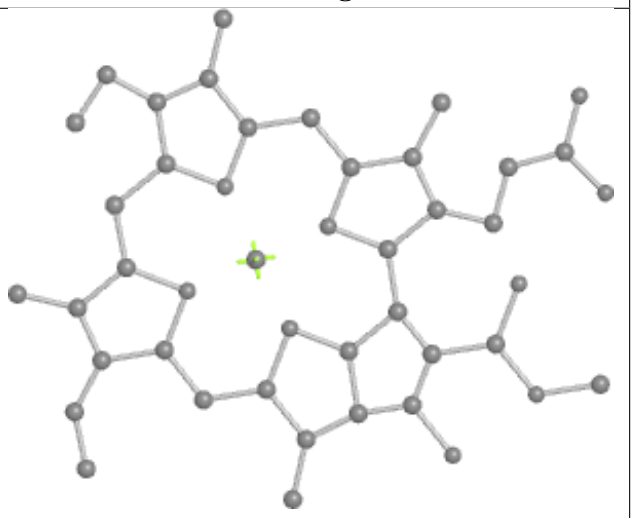


Ligand CLA 1 517

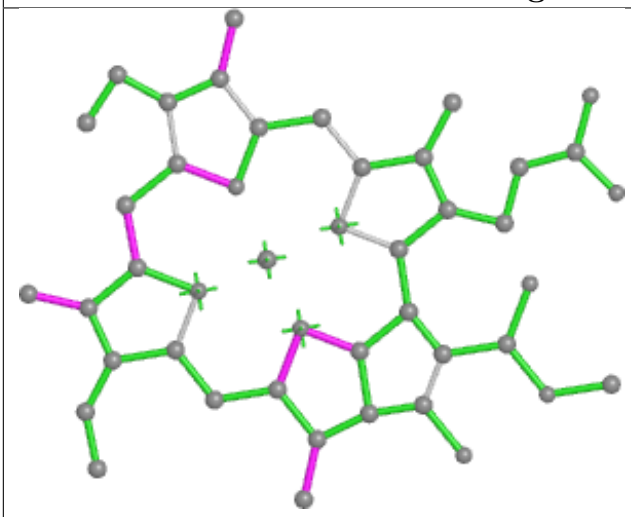


Ligand FMN P 170

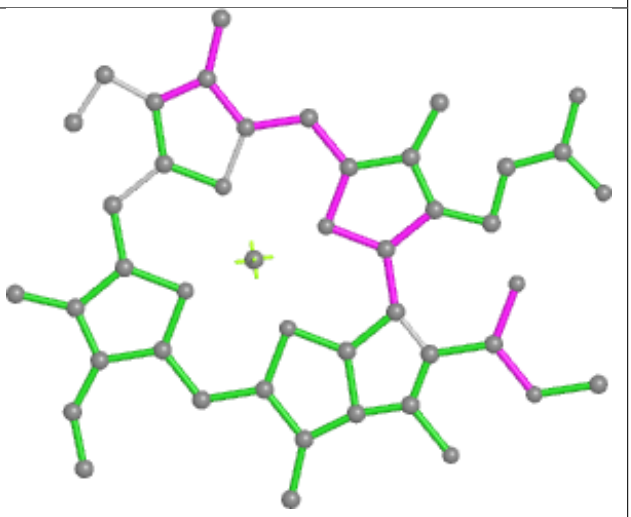


Ligand CLA Y 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

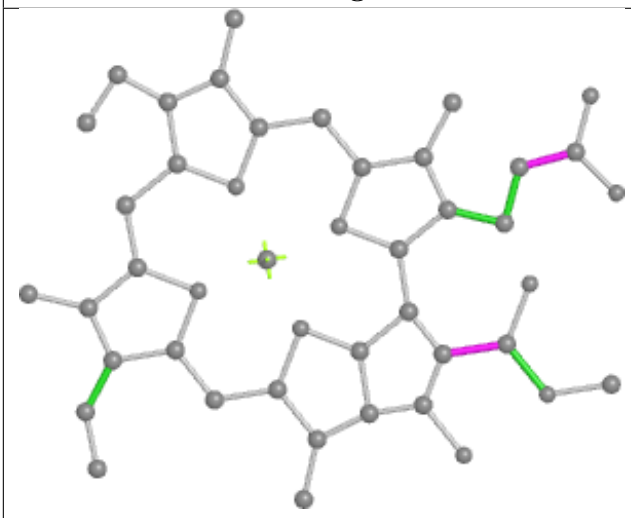
Ligand CLA v 504



Bond lengths



Bond angles



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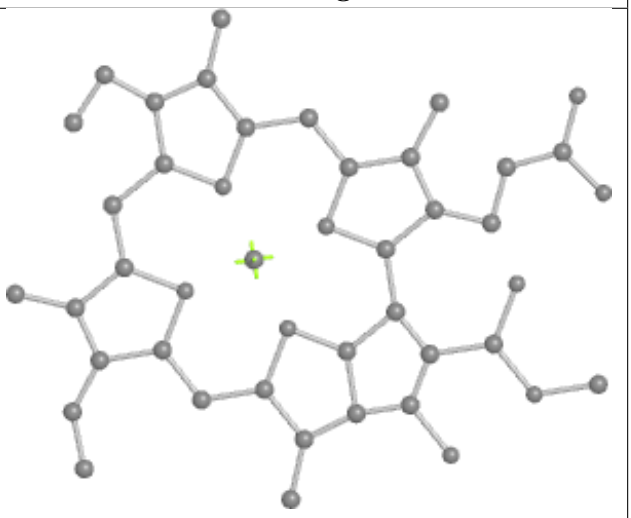
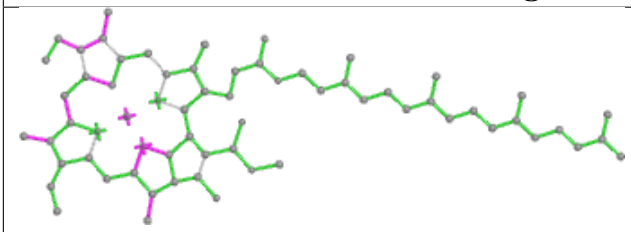


Rings

Ligand CLA f 1235



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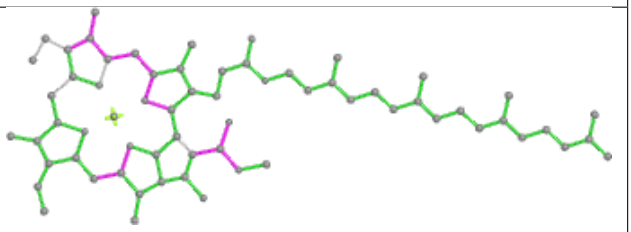

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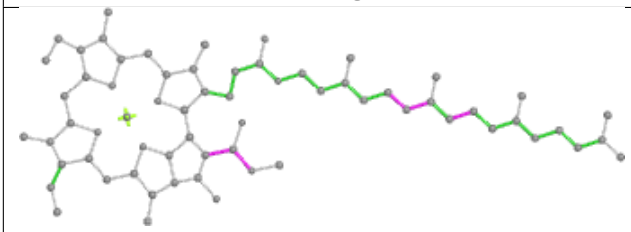

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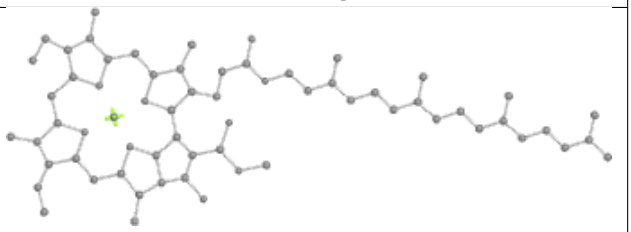
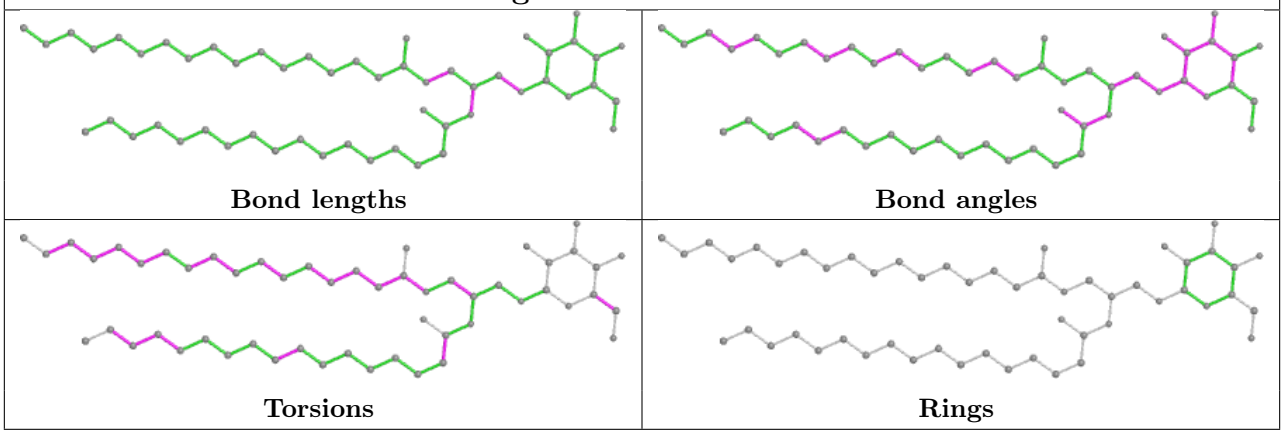
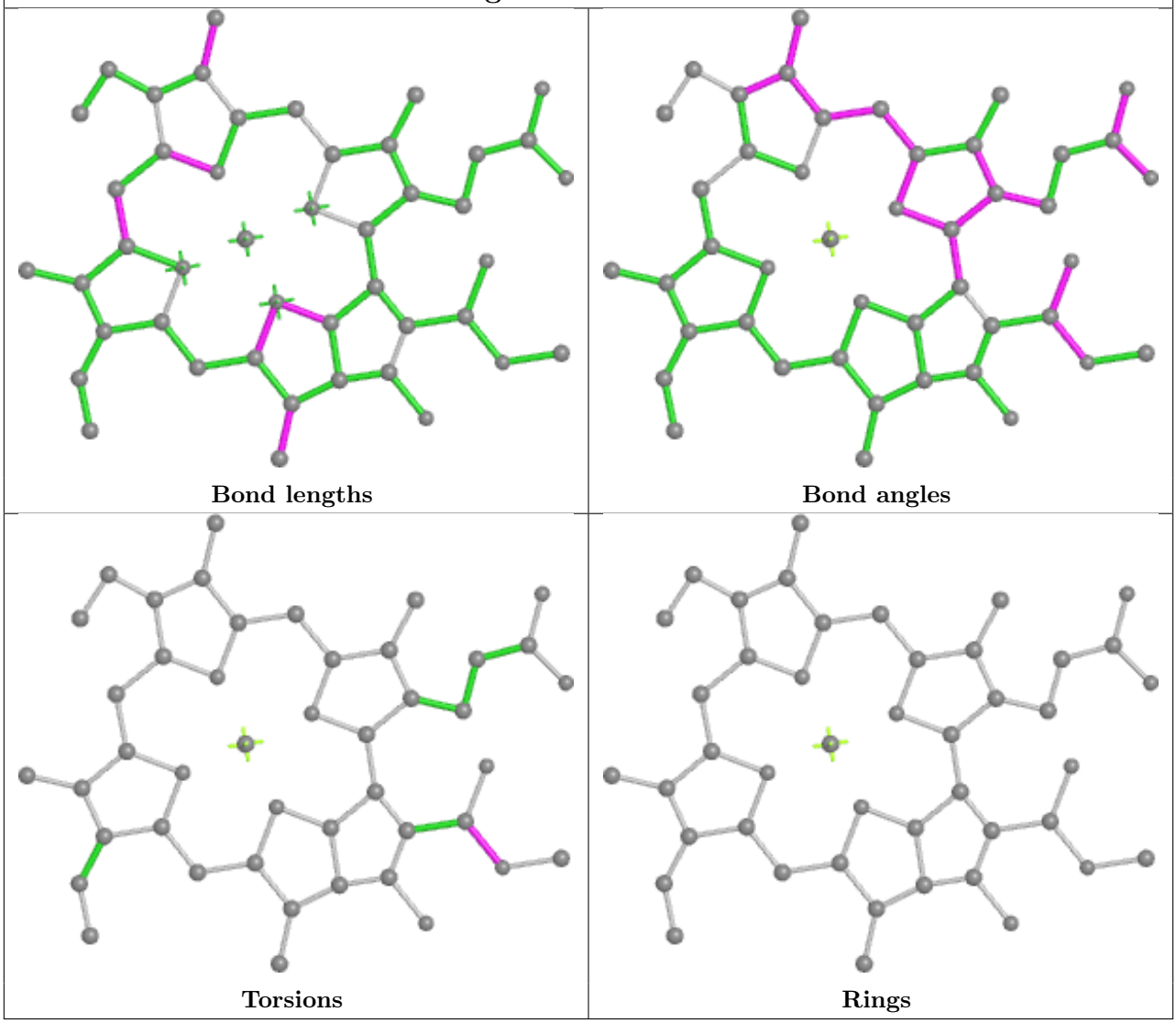


Rings

Ligand LMG B 5002



Ligand CLA a 511



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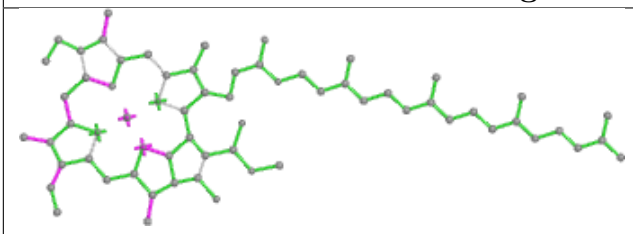

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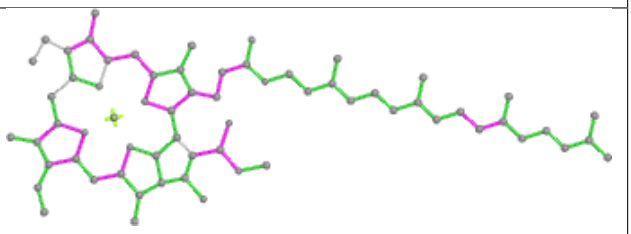
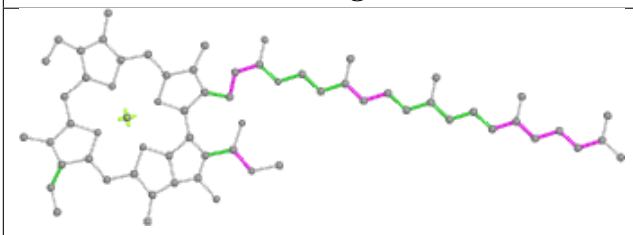


Bond angles



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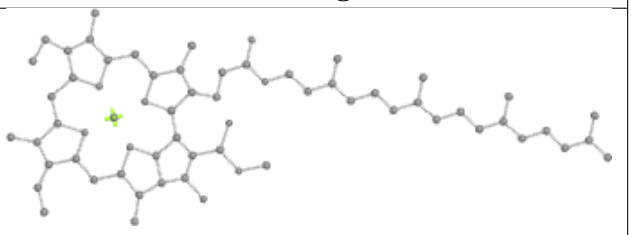
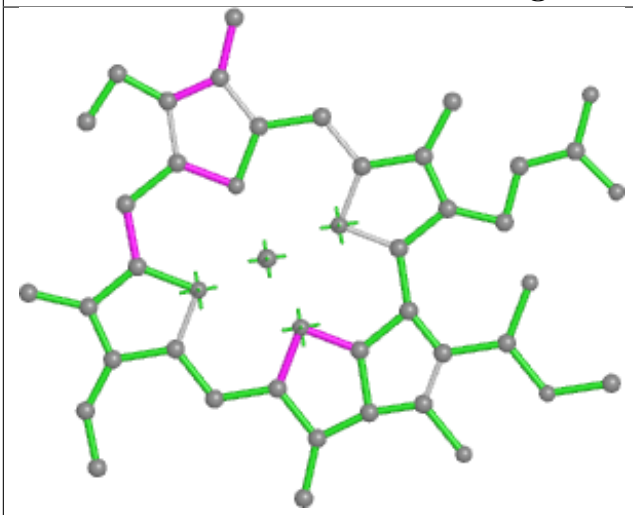


Rings

Ligand CLA c 519



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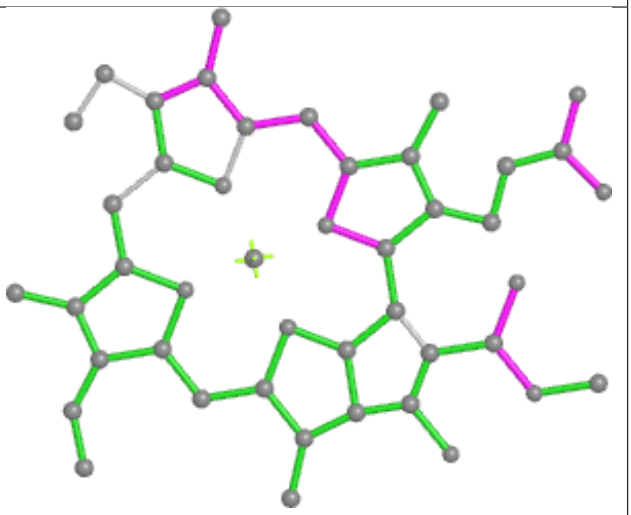

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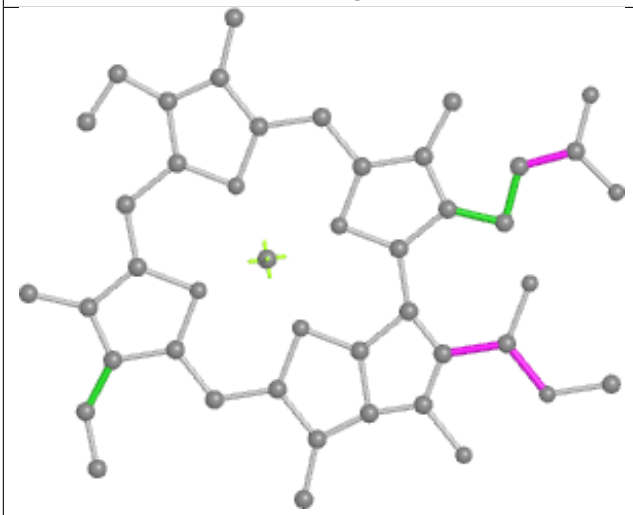

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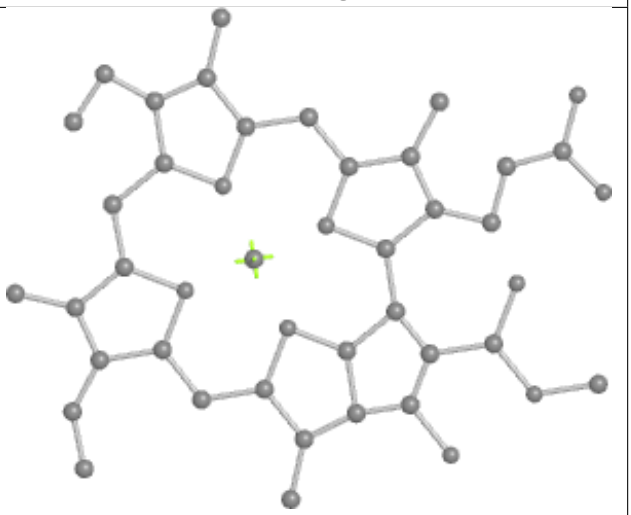

Rings

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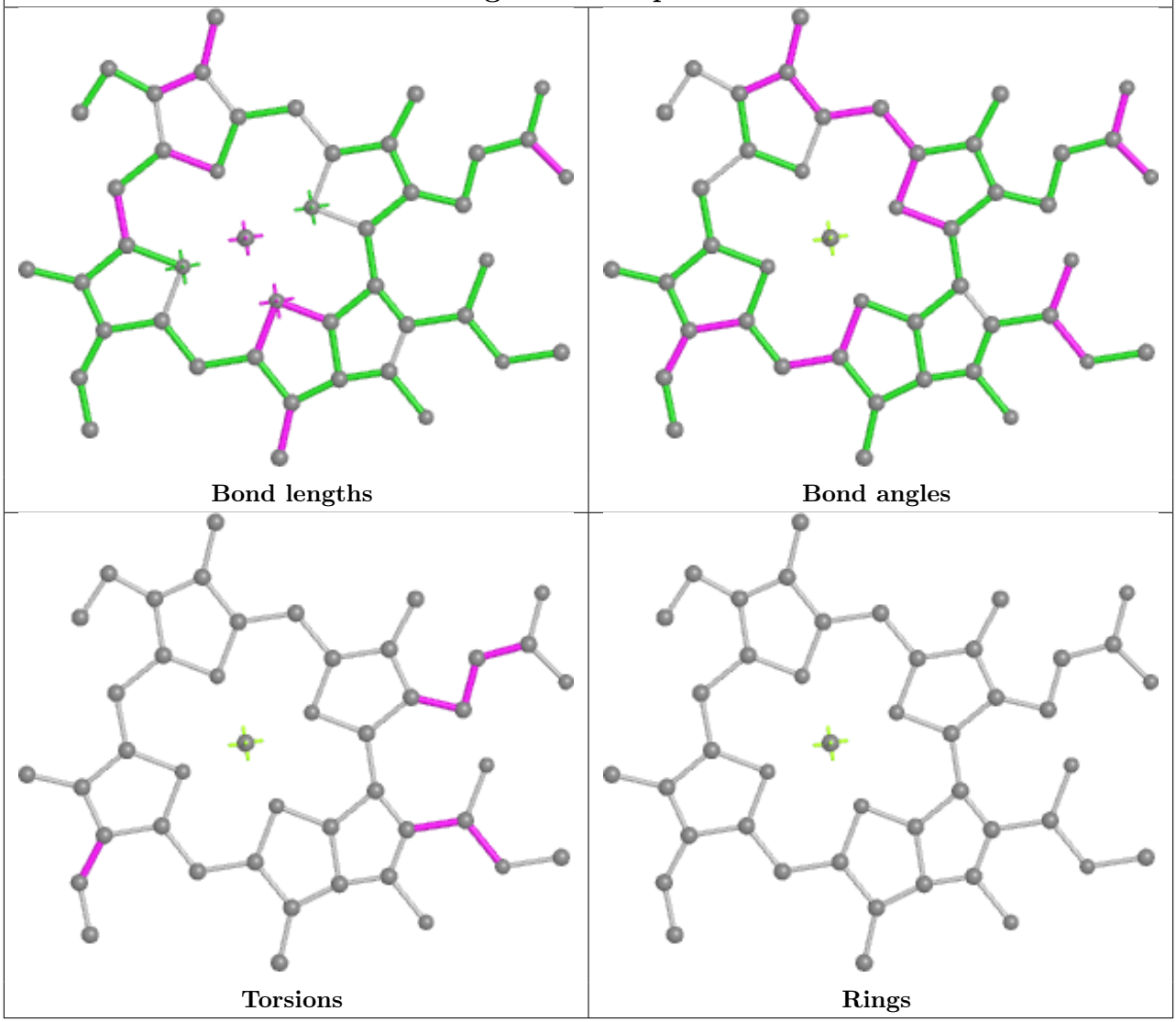
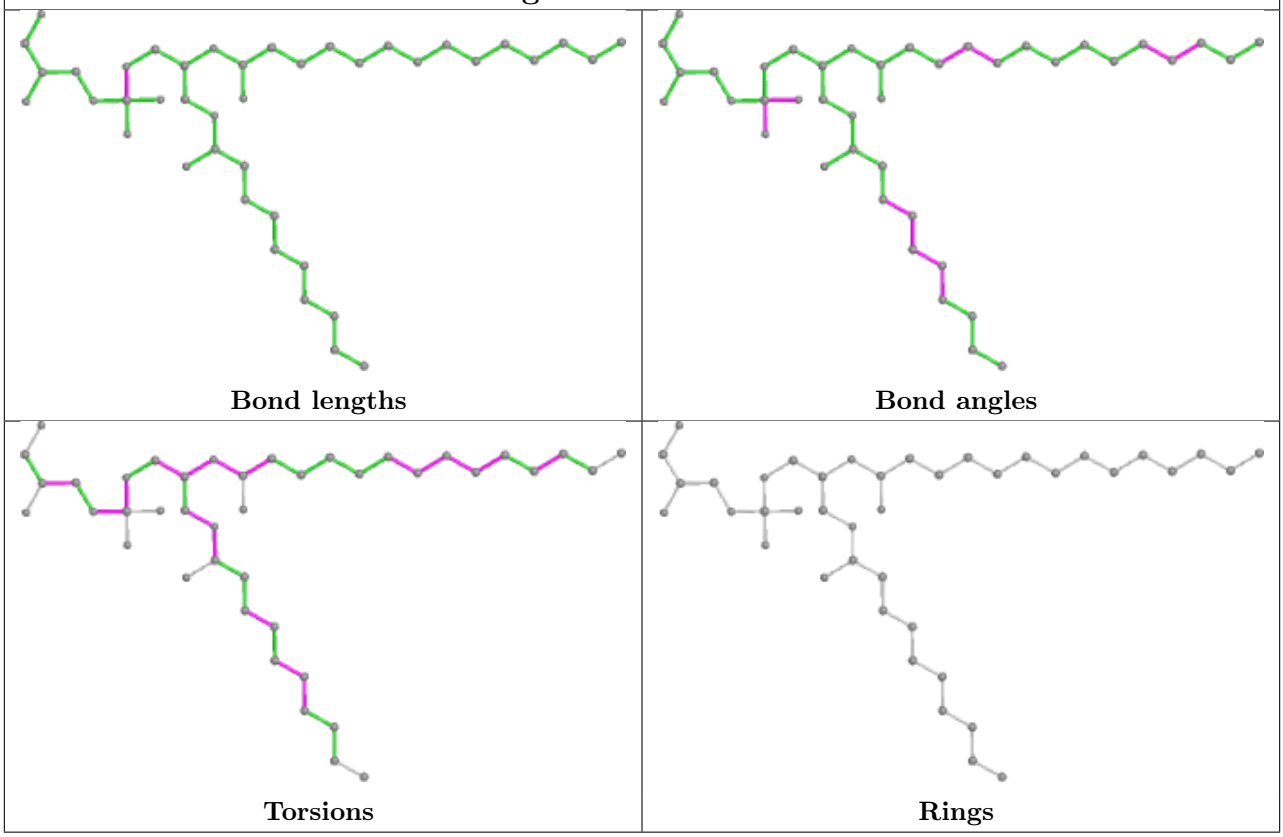


Ligand LHG f 1855



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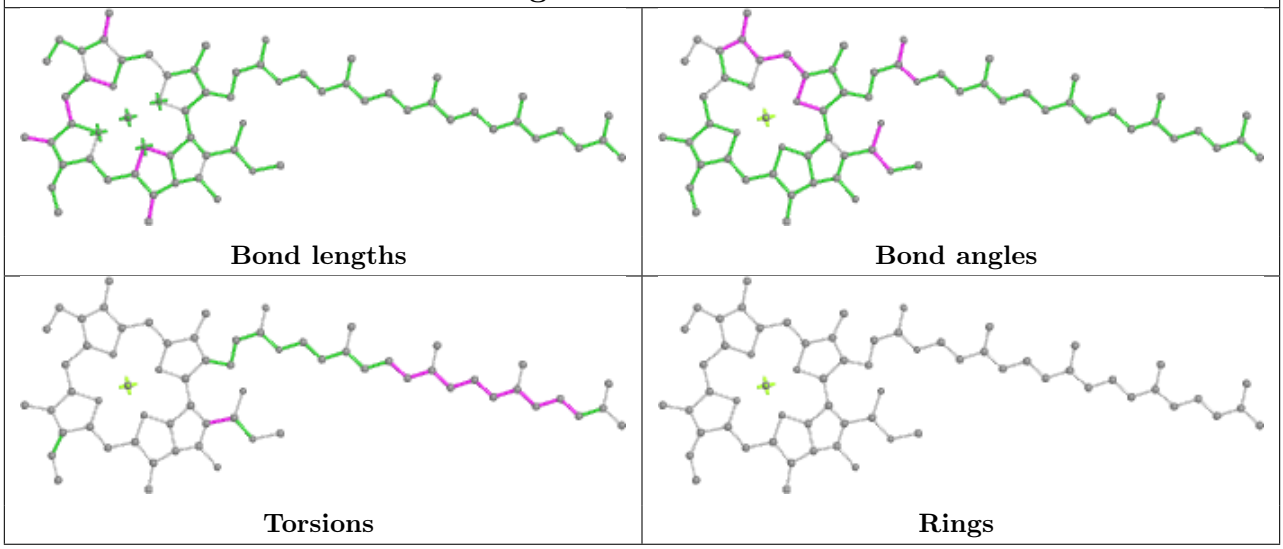

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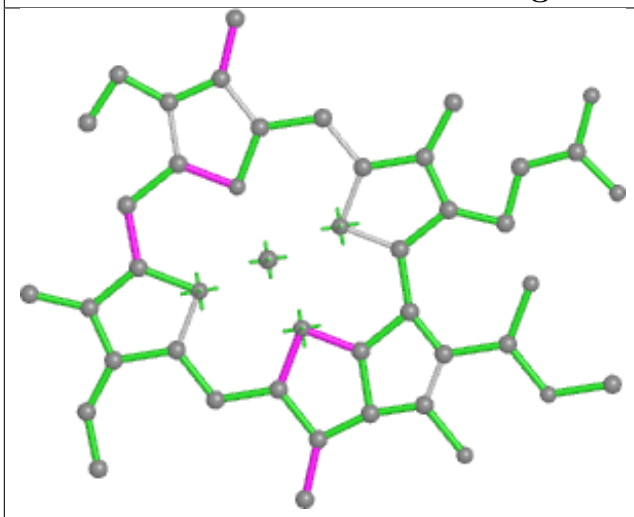
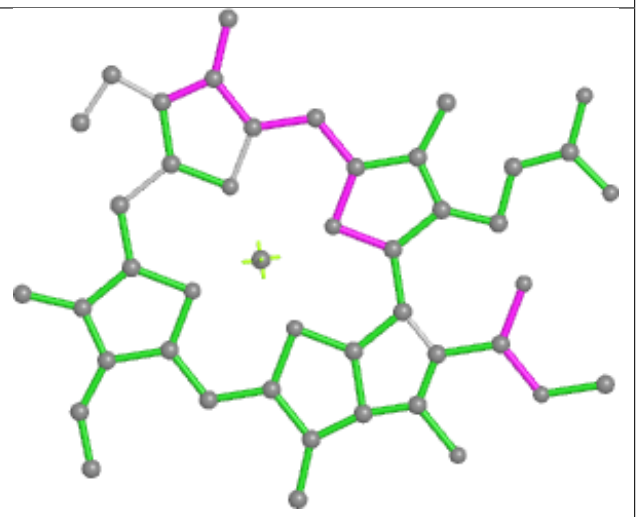
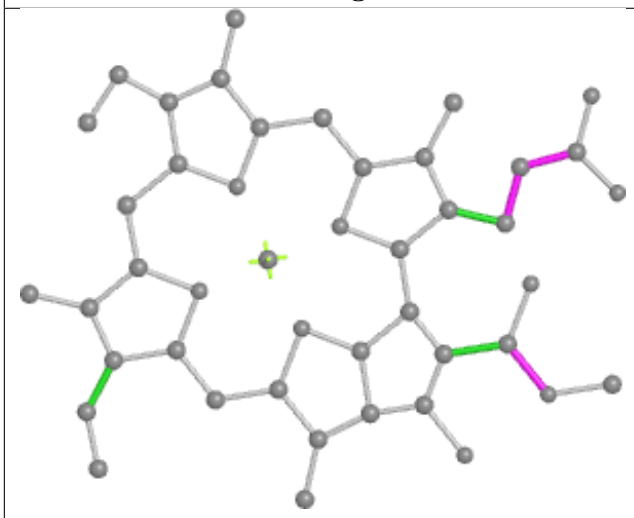


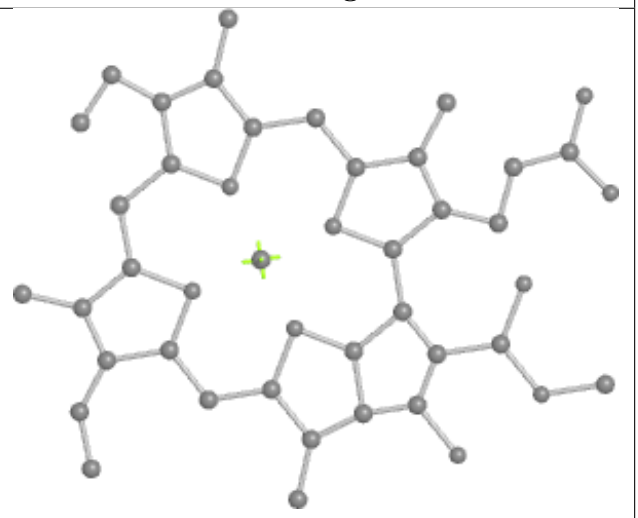
Bond lengths



Bond angles

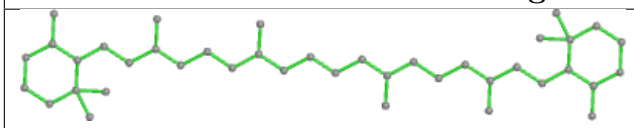


Torsions



Rings

Ligand BCR c 522



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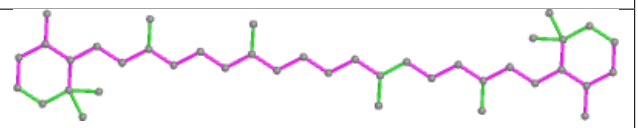
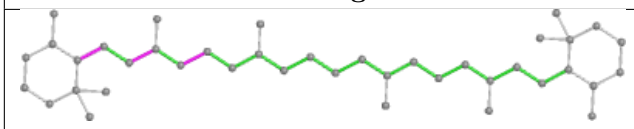


Bond angles



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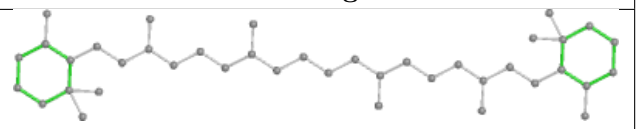
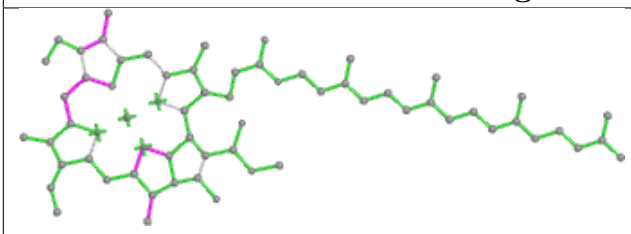


Rings

Ligand CLA H 1239



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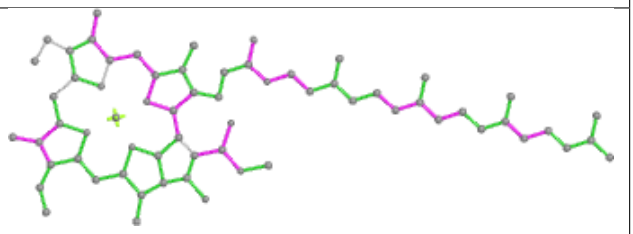
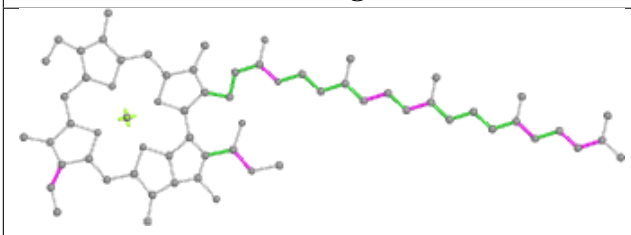


Bond angles



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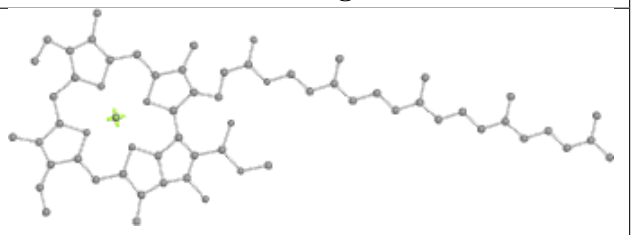
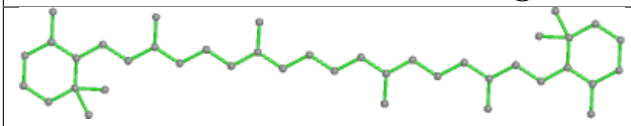


Rings

Ligand BCR B 4005



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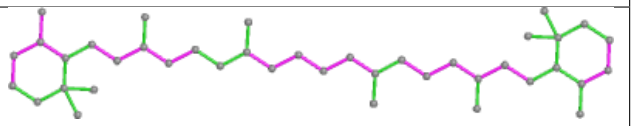
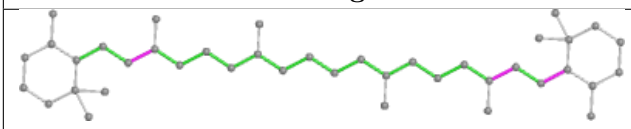
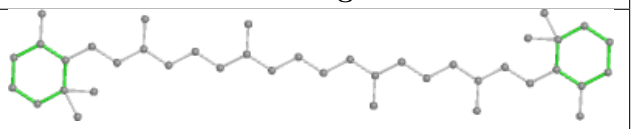


Bond angles

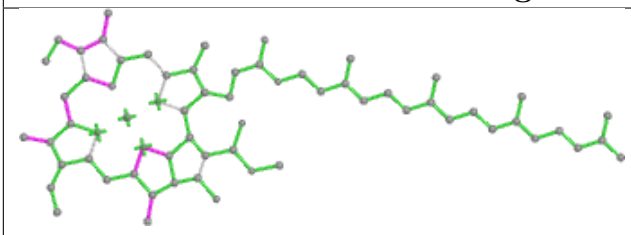


Torsions



Rings

Ligand CLA H 1207



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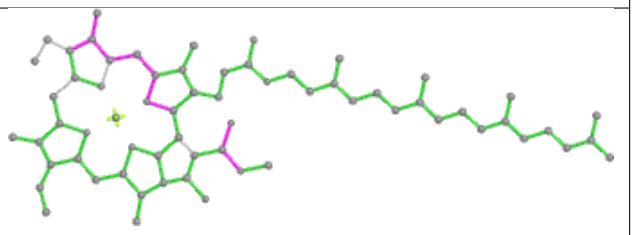

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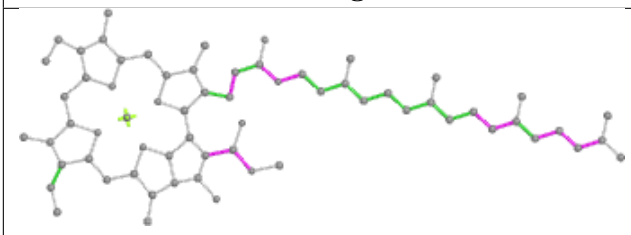

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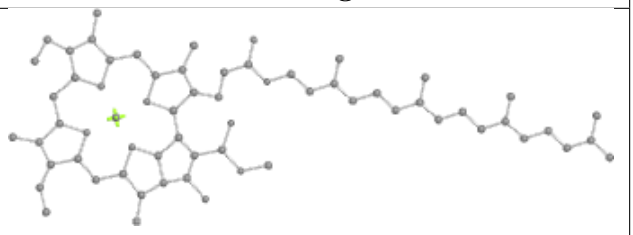
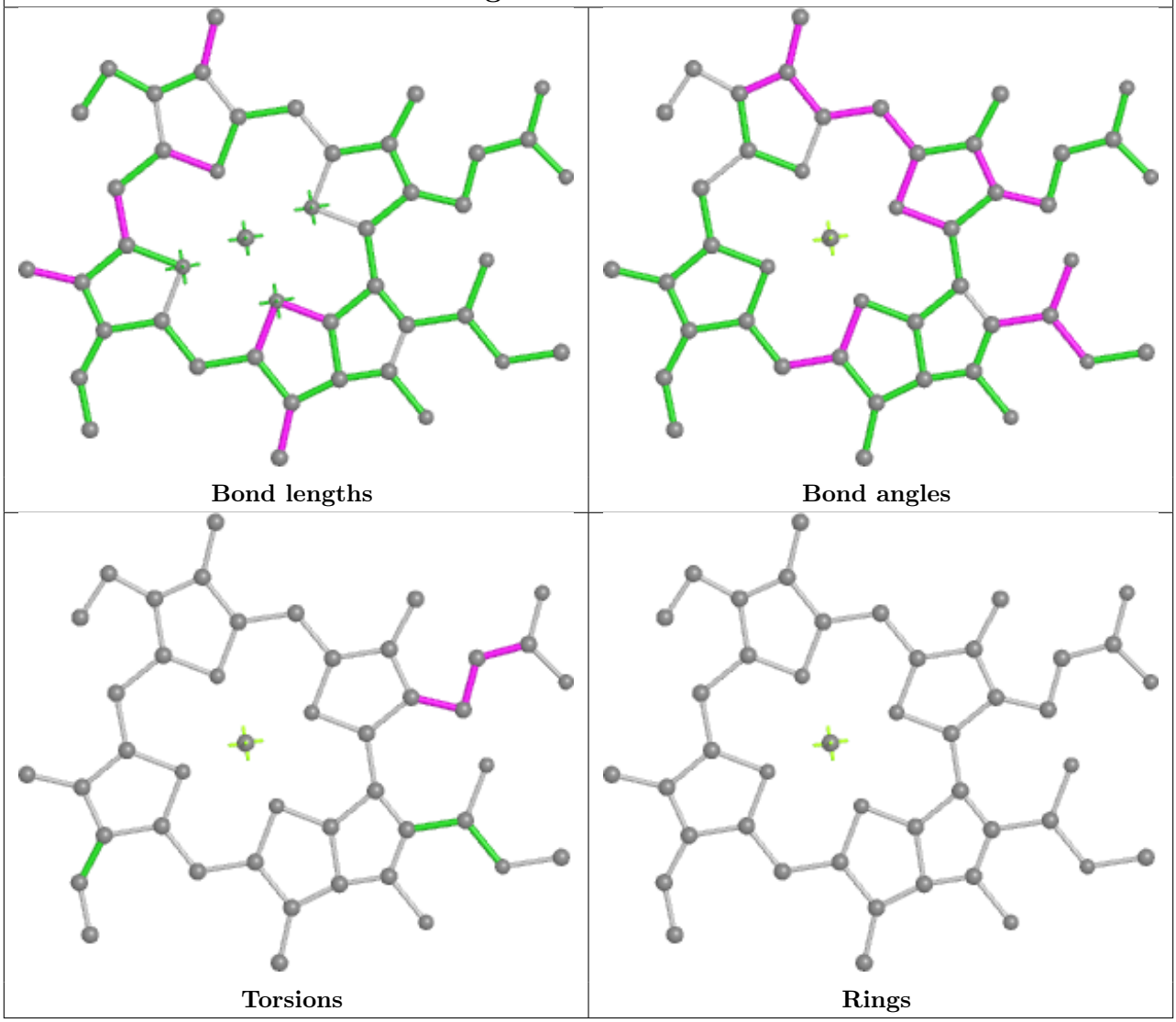
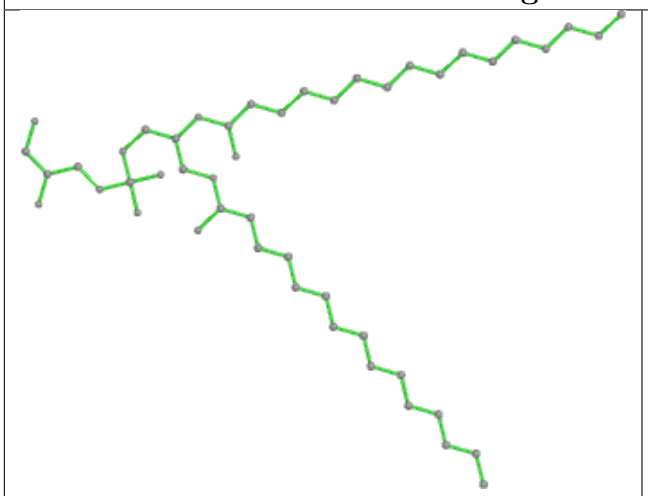


Rings

Ligand CLA 3 501



Ligand LHG I 5001



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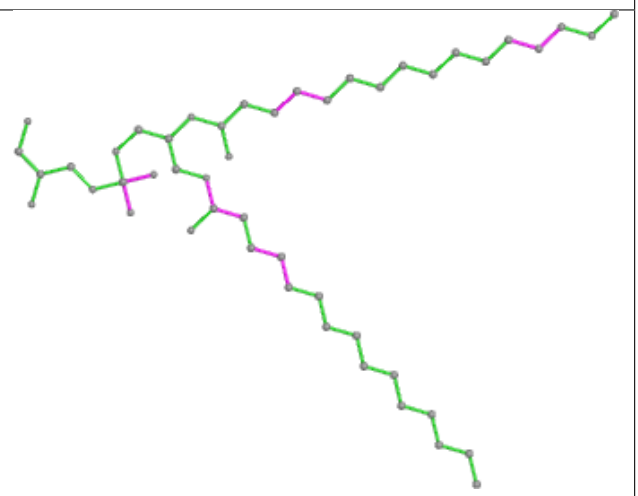
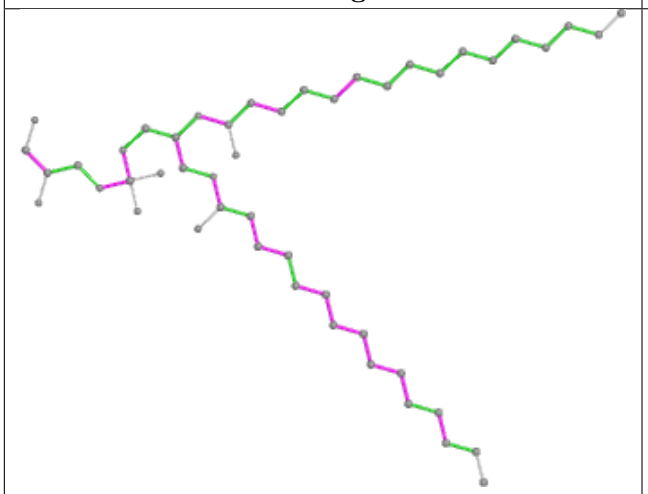


Bond angles



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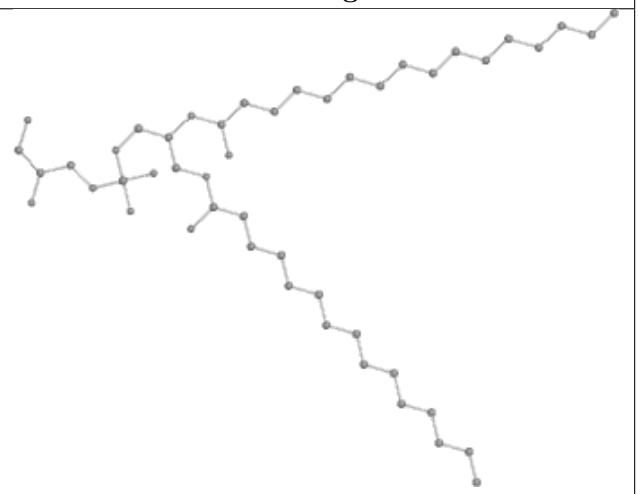
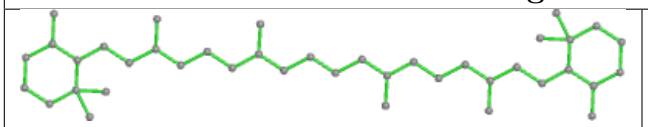


Rings

Ligand BCR v 524



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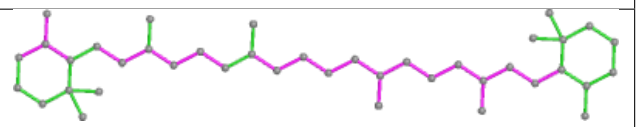

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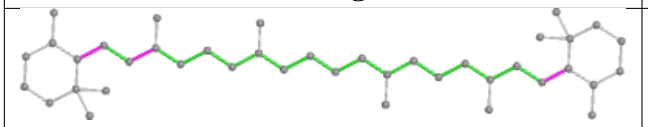

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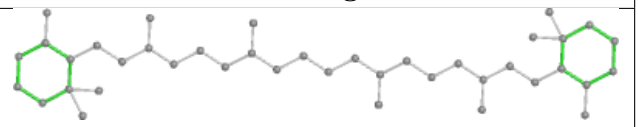
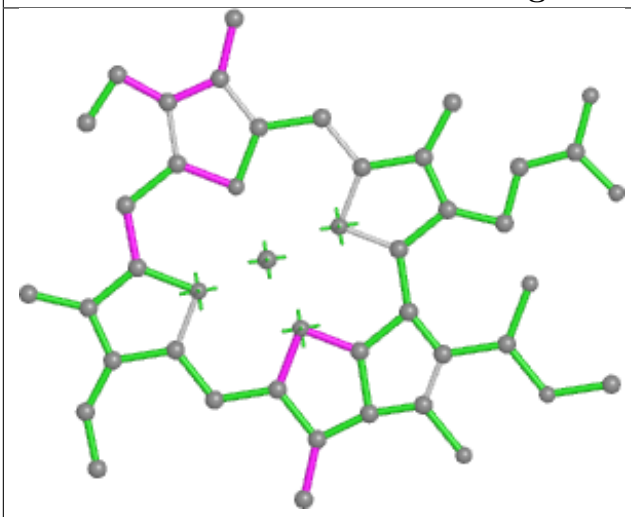


Rings

Ligand CLA a 513



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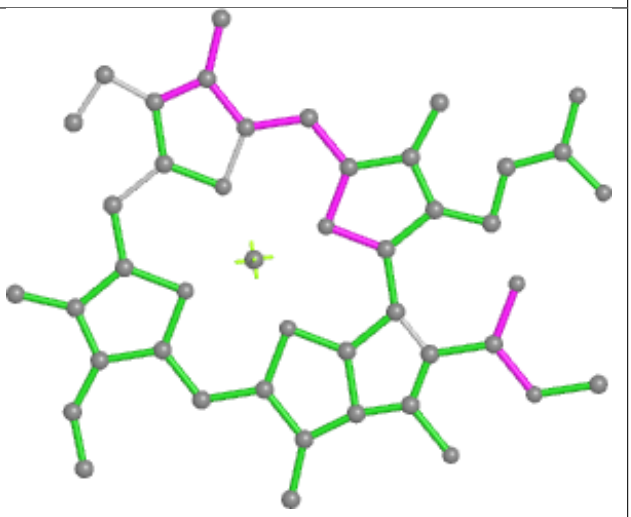
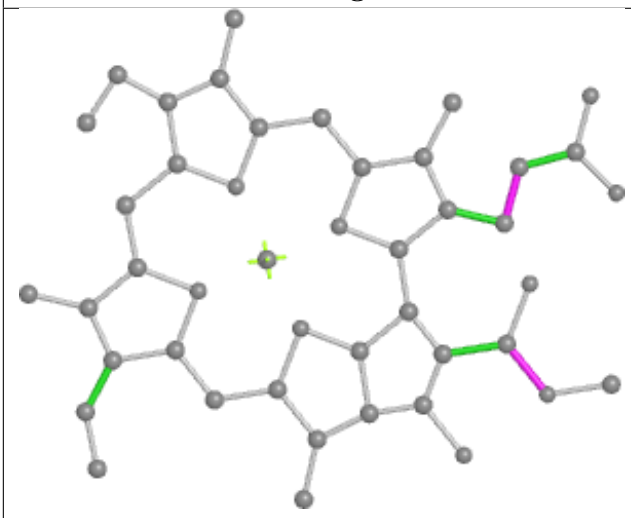
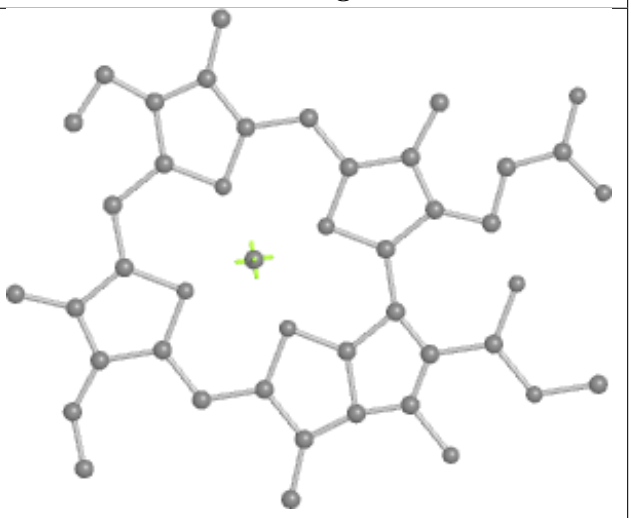


Bond angles

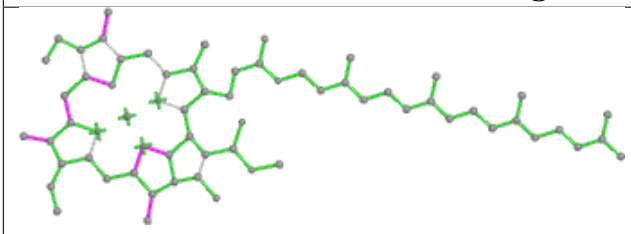


Torsions

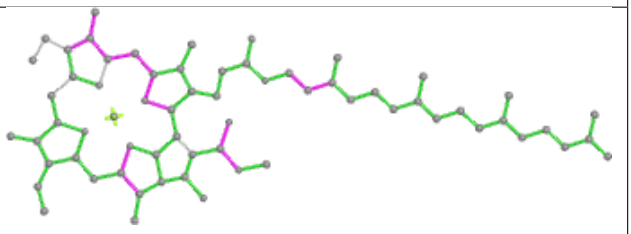


Rings

Ligand CLA r 505



Bond lengths



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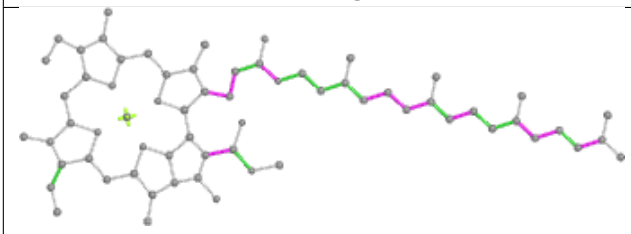

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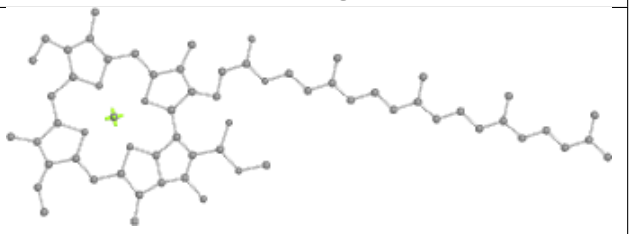
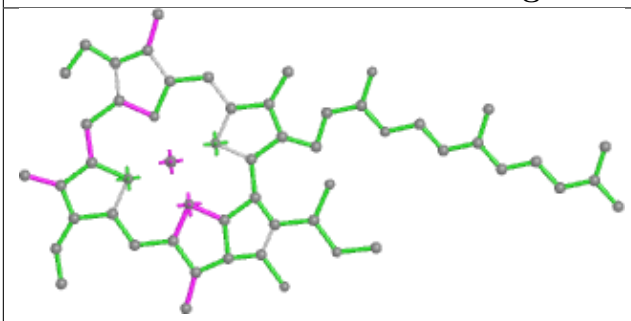
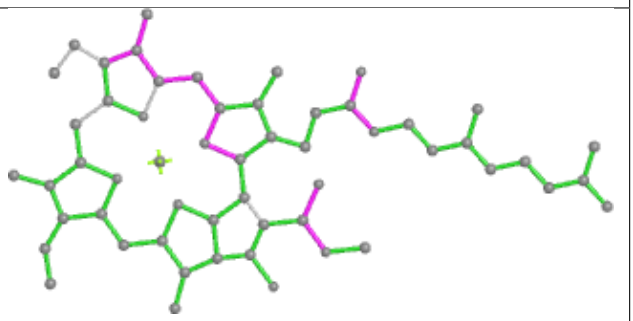
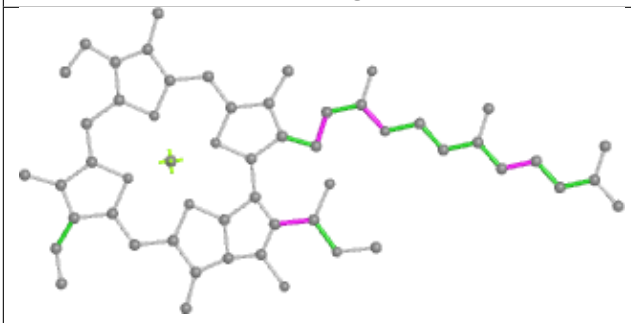
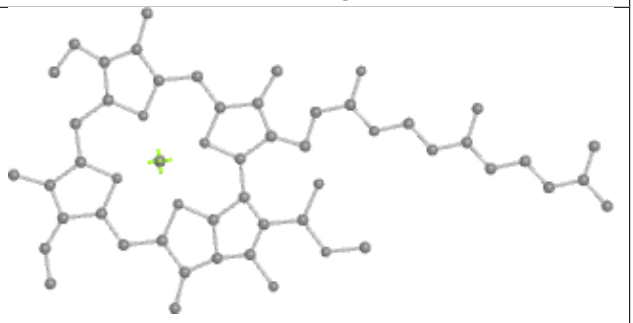
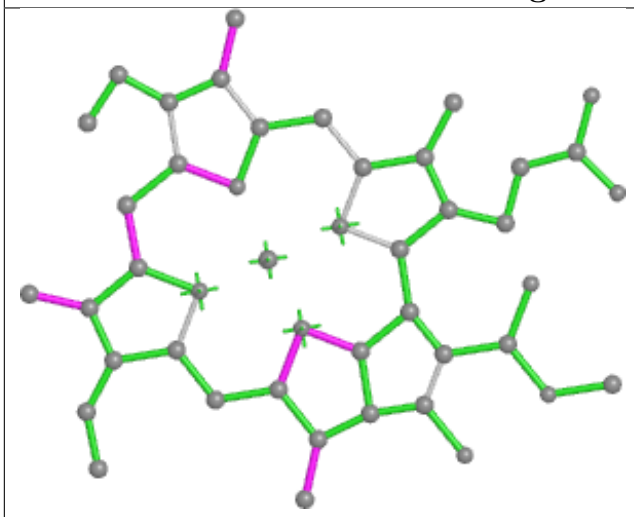


Rings

Ligand CLA f 1232	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 504



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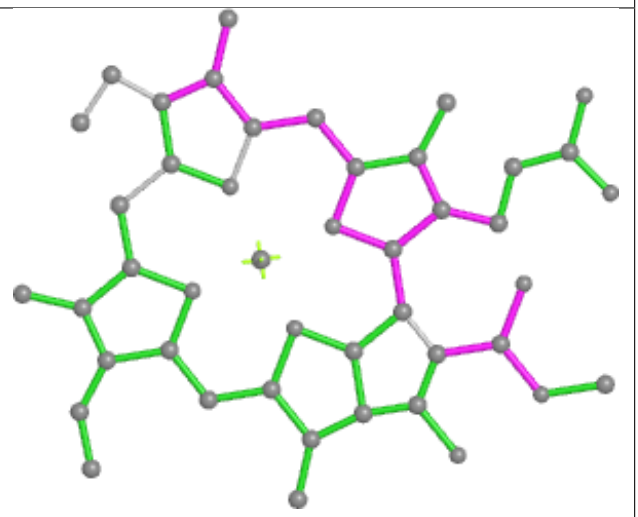
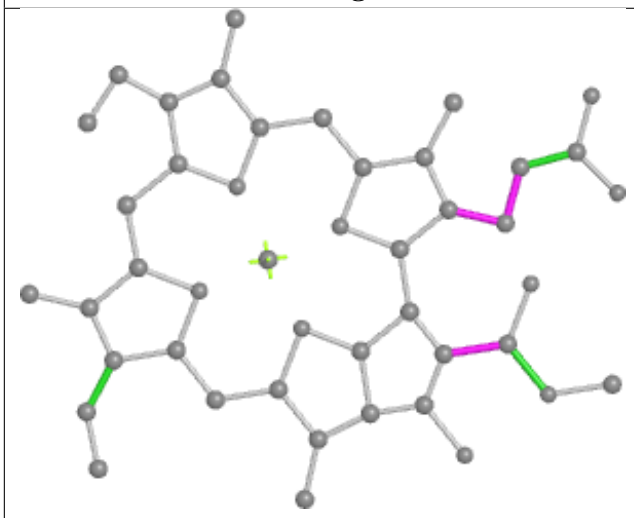


Bond angles



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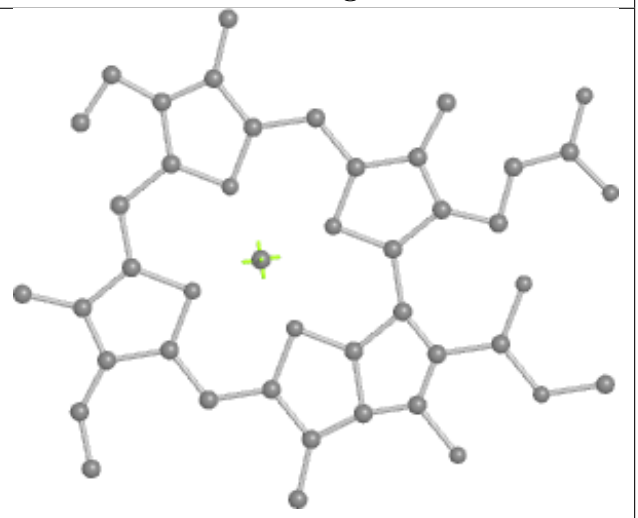
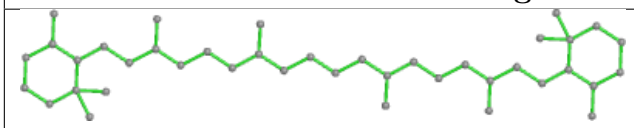


Rings

Ligand BCR A 4001



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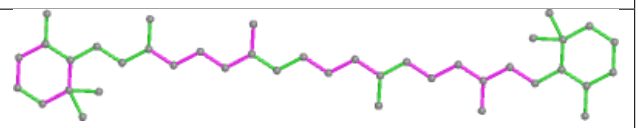
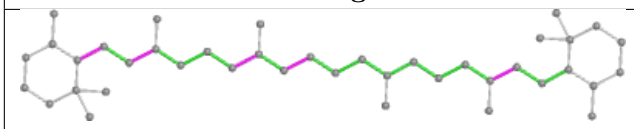


Bond angles



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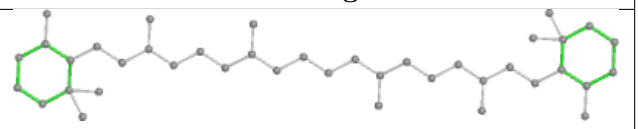
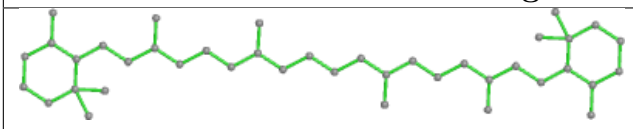


Rings

Ligand BCR Y 523



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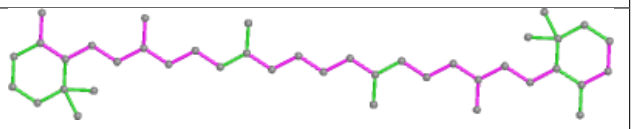

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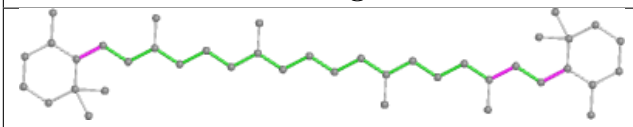

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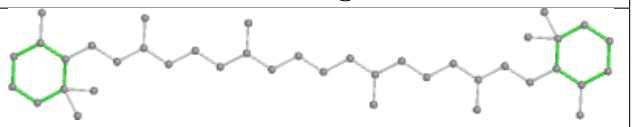
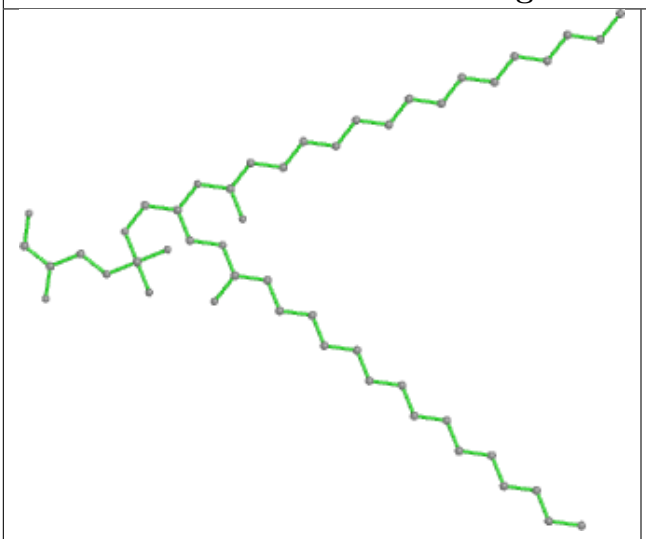


Rings

Ligand LHG L 5221



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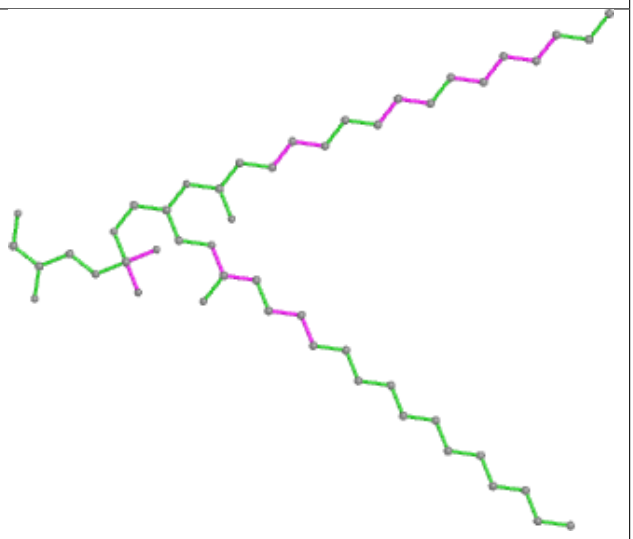

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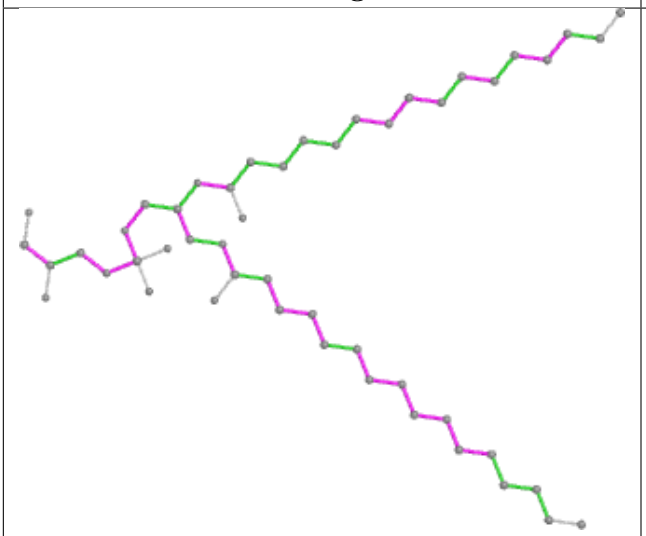

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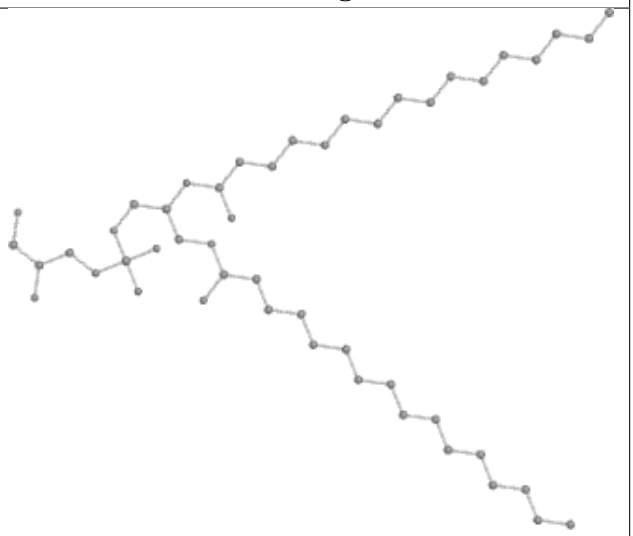

Rings

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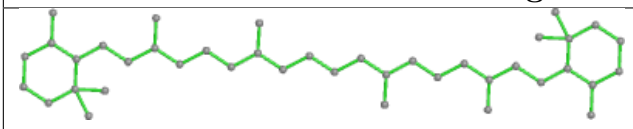

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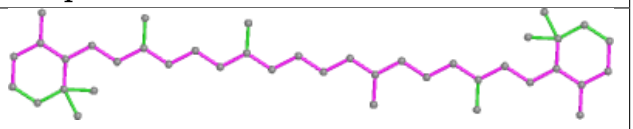

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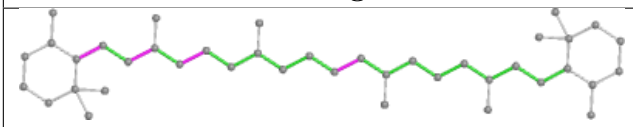

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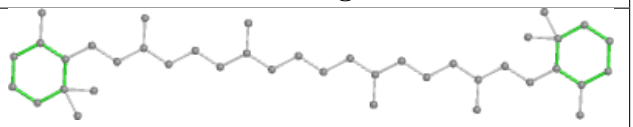
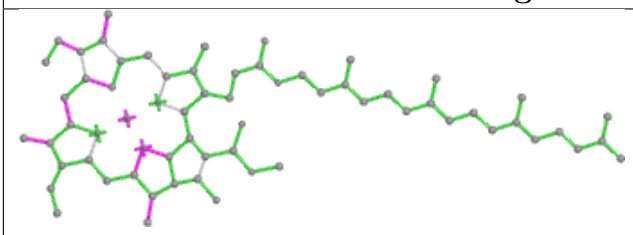


Rings

Ligand CLA H 1210



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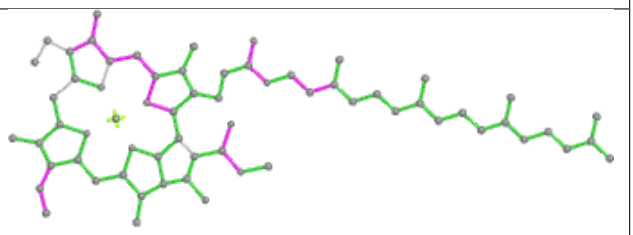
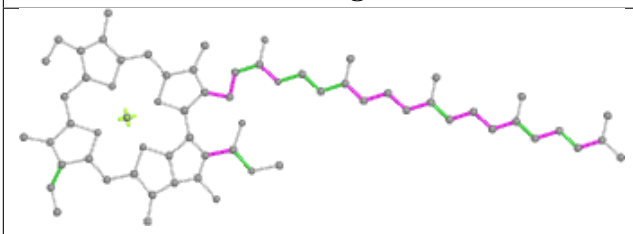


Bond angles



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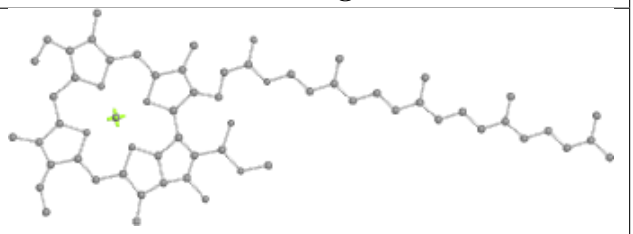
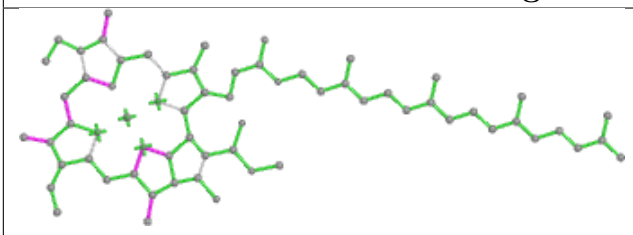


Rings

Ligand CLA f 1202



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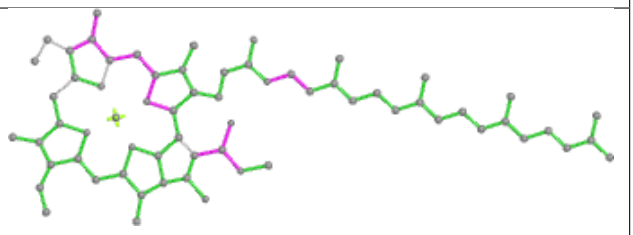

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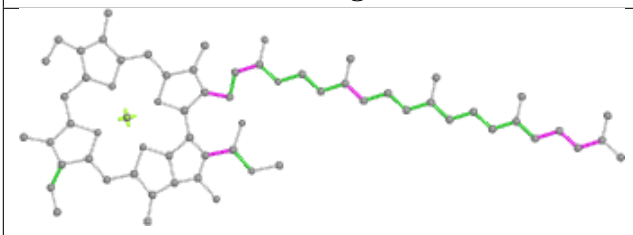

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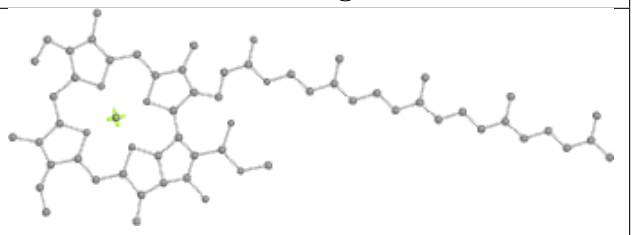
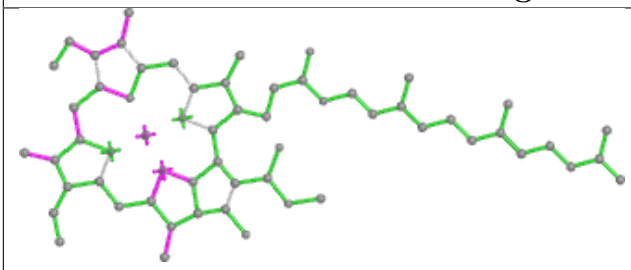


Rings

Ligand CLA V 1501



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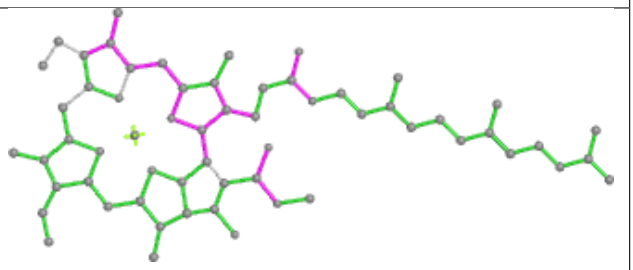

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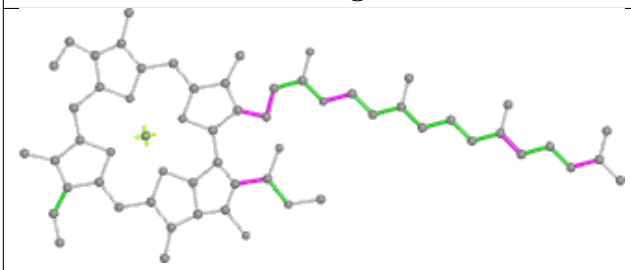

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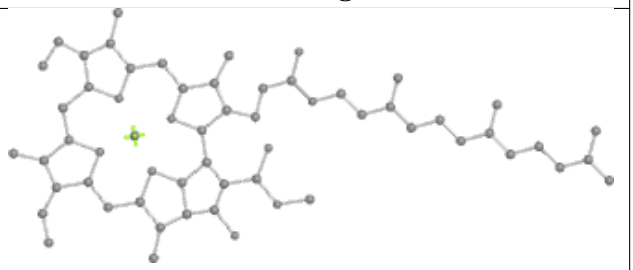
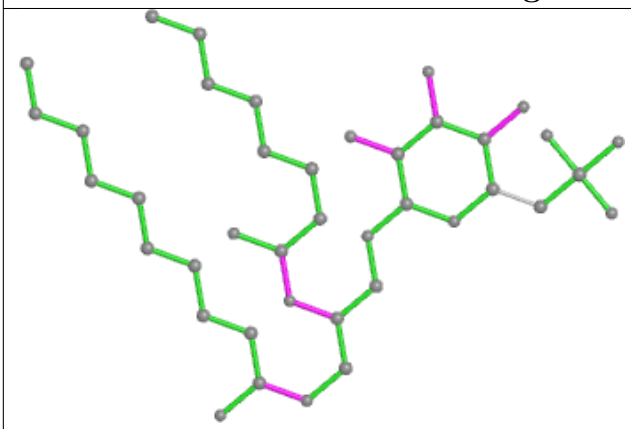


Rings

Ligand SQD f 1852



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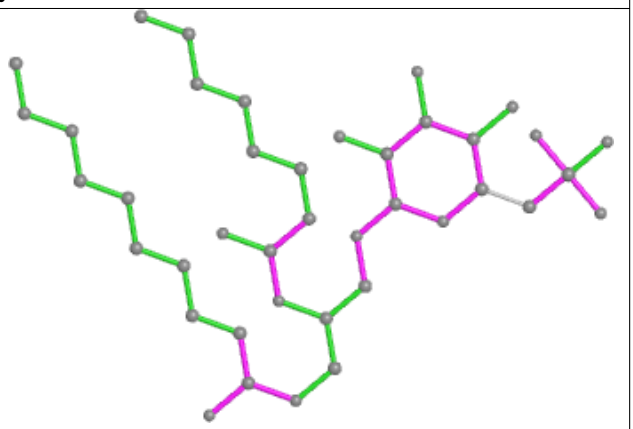
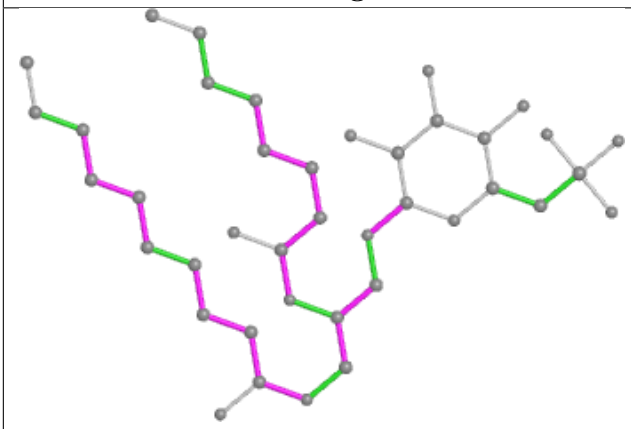


Bond angles



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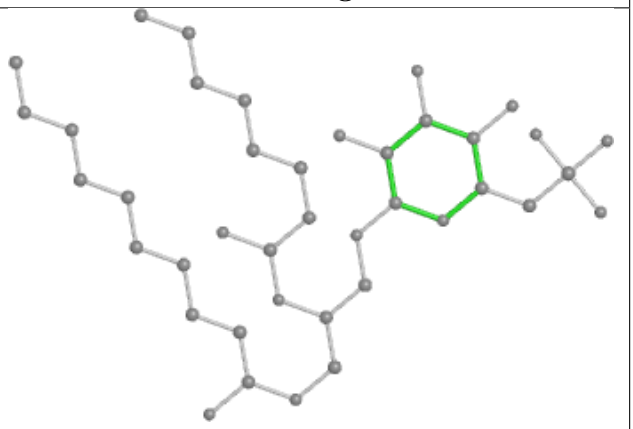

Rings

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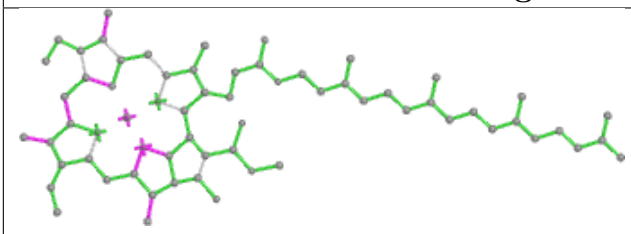
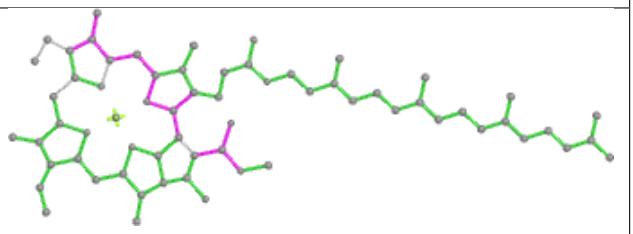
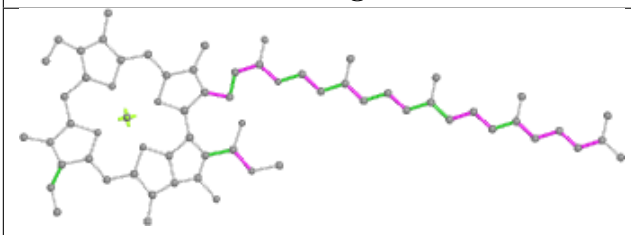
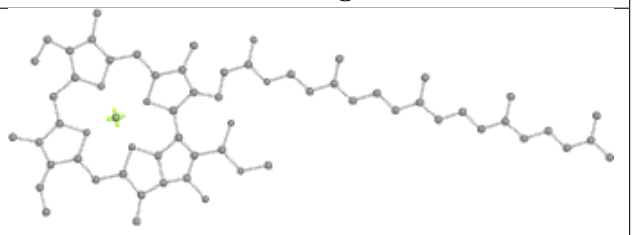
 Bond lengths	 Bond angles
 Torsions	 Rings

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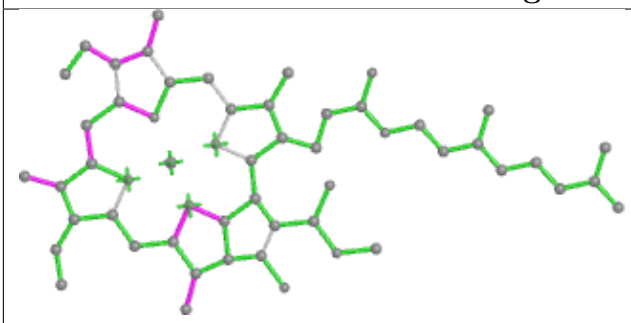
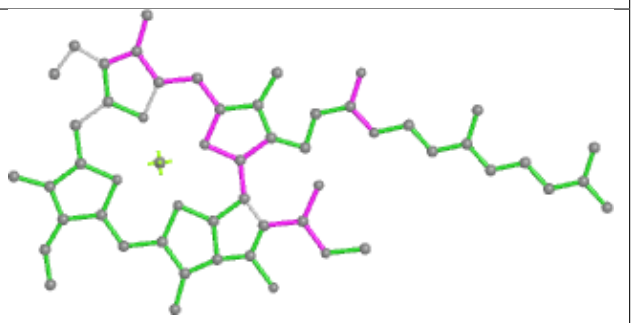
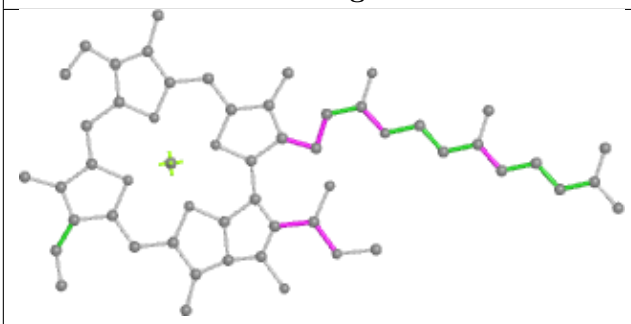
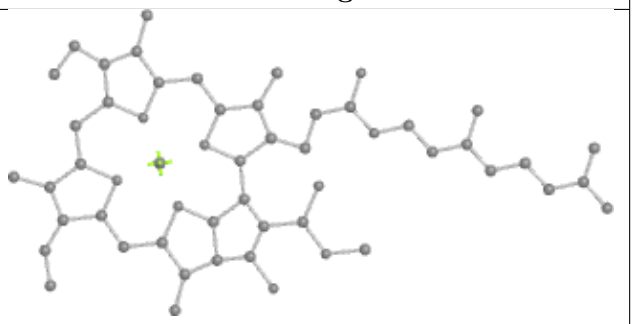
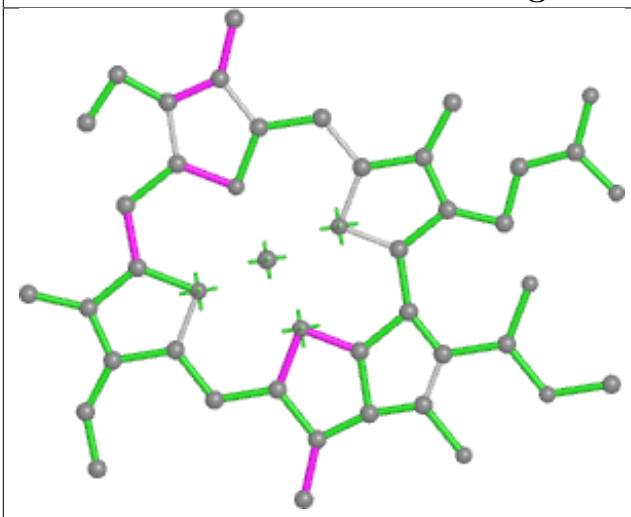
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 504



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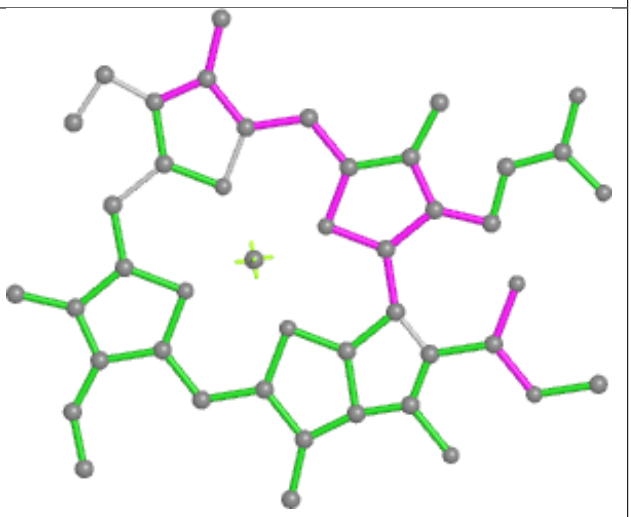

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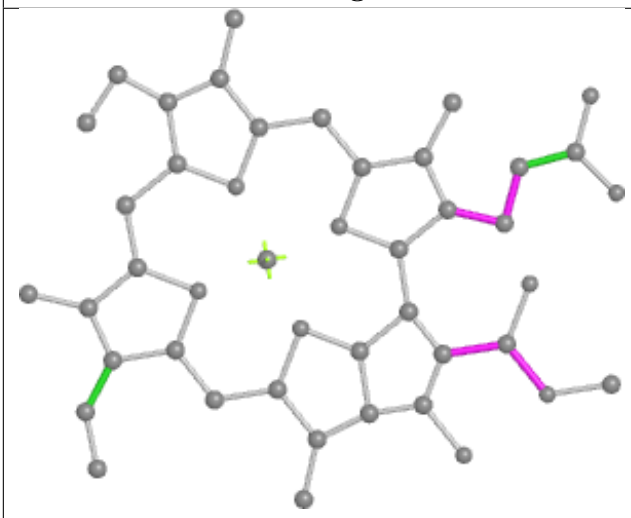

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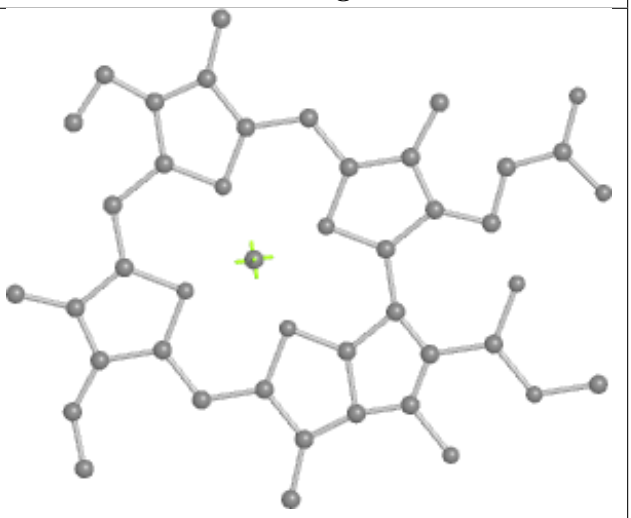
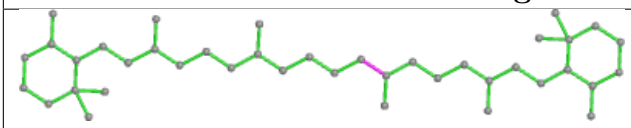


Rings

Ligand BCR B 4010



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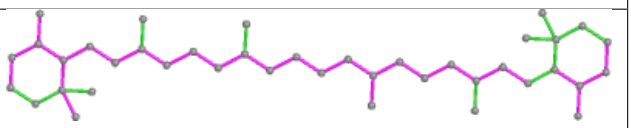

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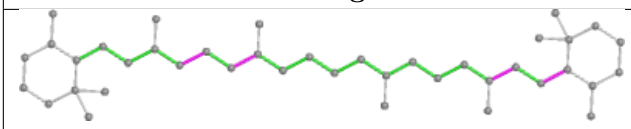

Torsions

Rings

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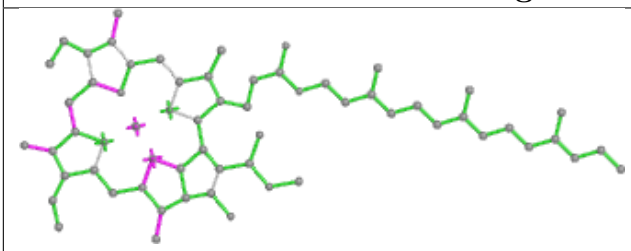
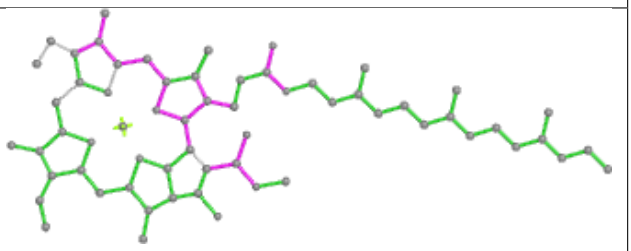
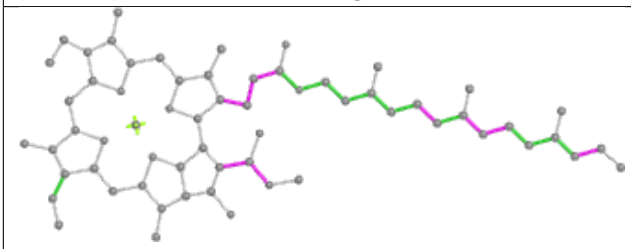
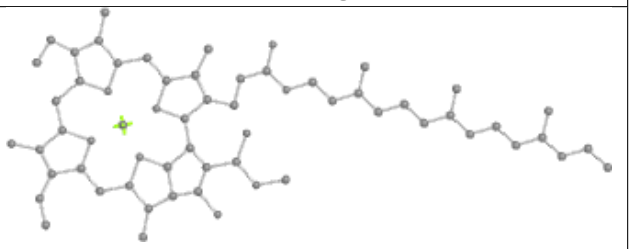
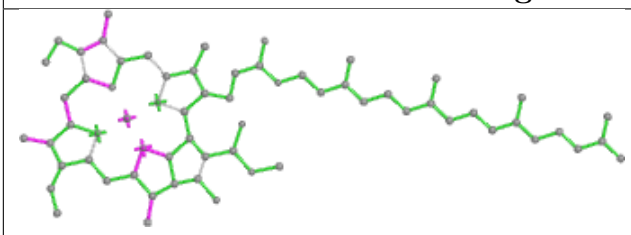
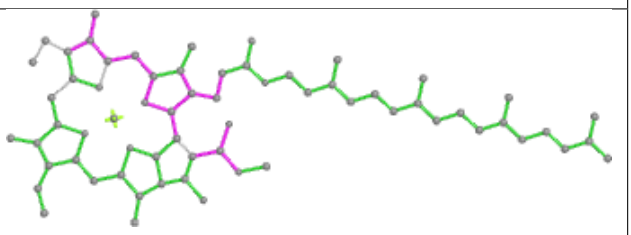
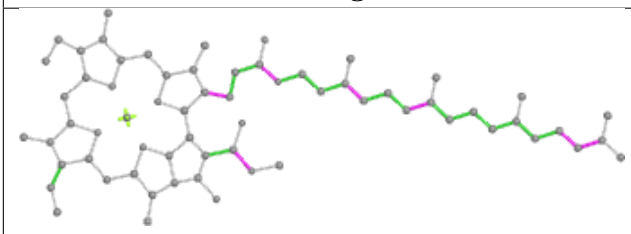
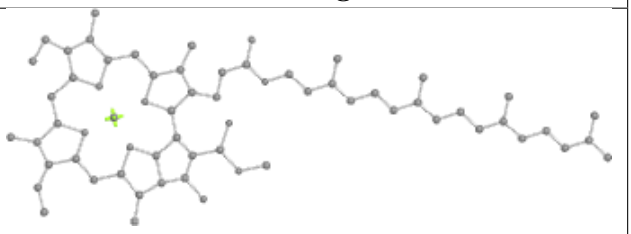
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1140	
 Bond lengths	 Bond angles
 Torsions	 Rings

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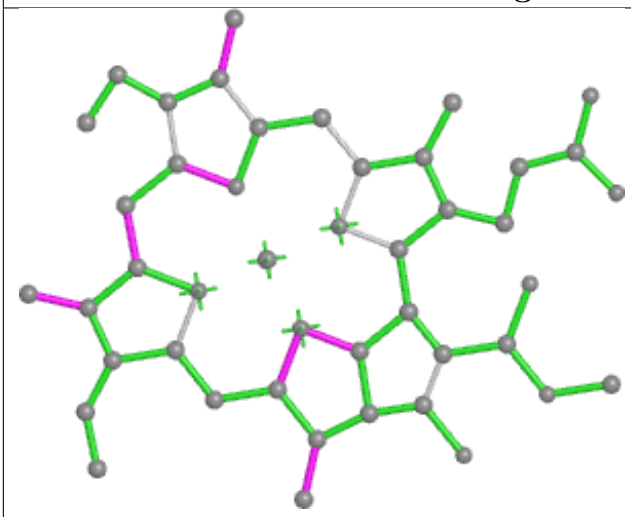

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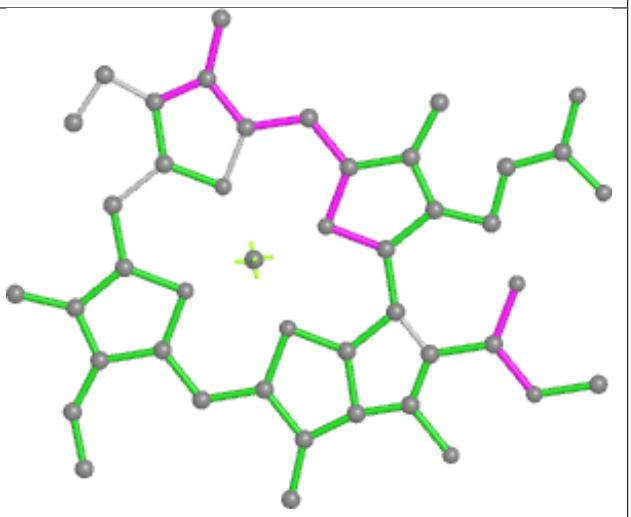

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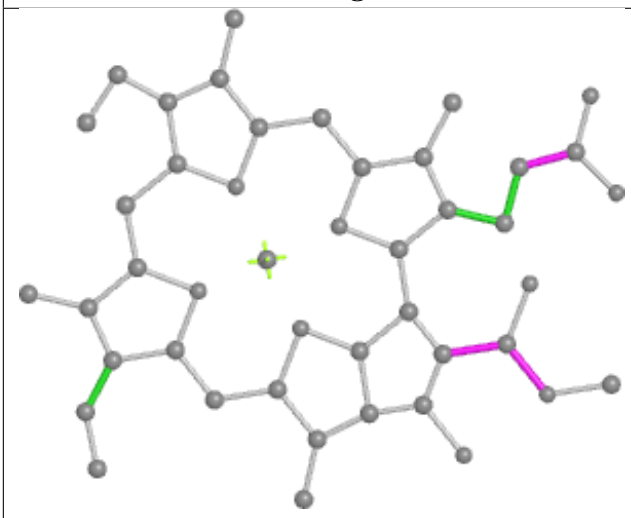

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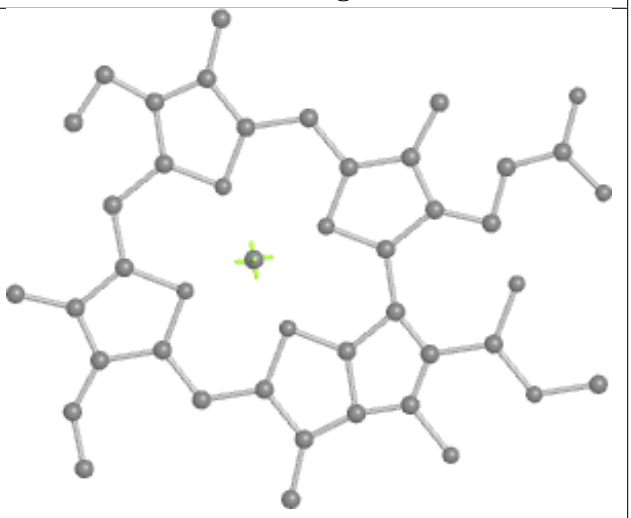
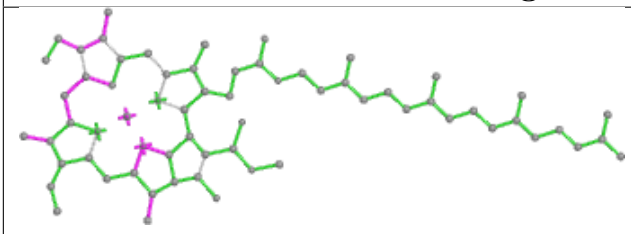


Rings

Ligand CLA e 1128



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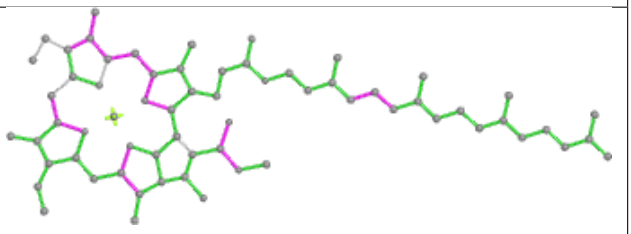
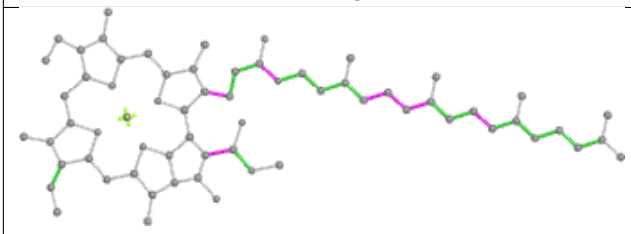


Bond angles



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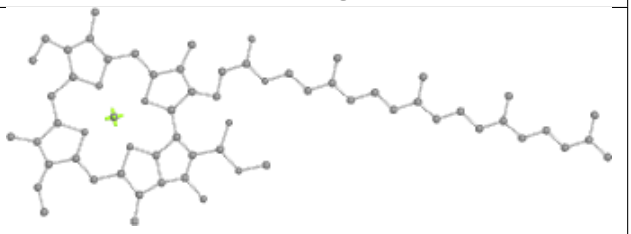
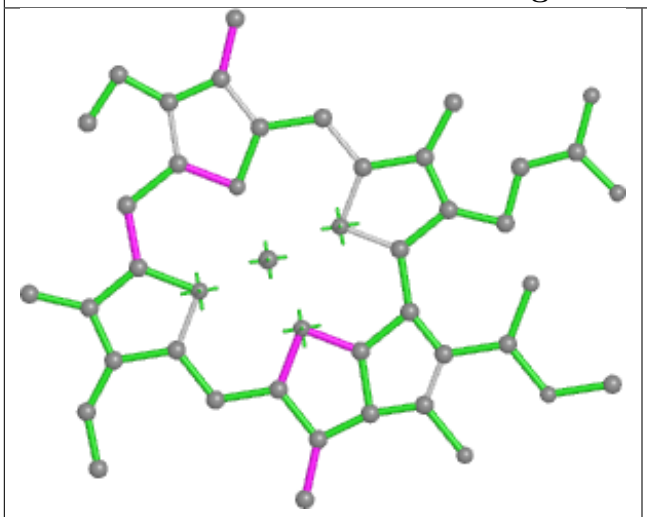


Rings

Ligand CLA t 510



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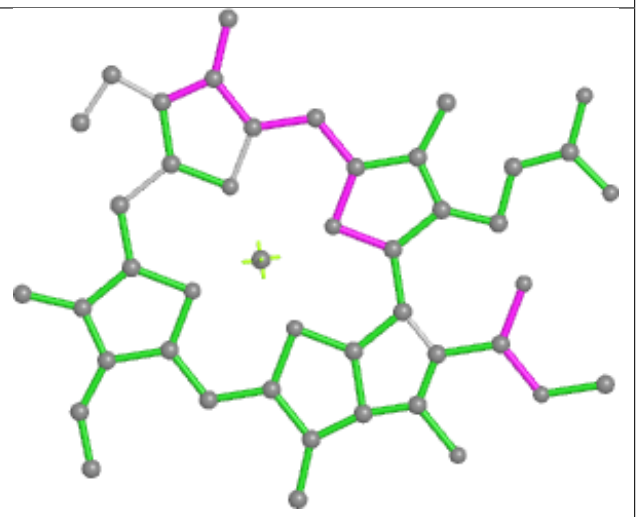

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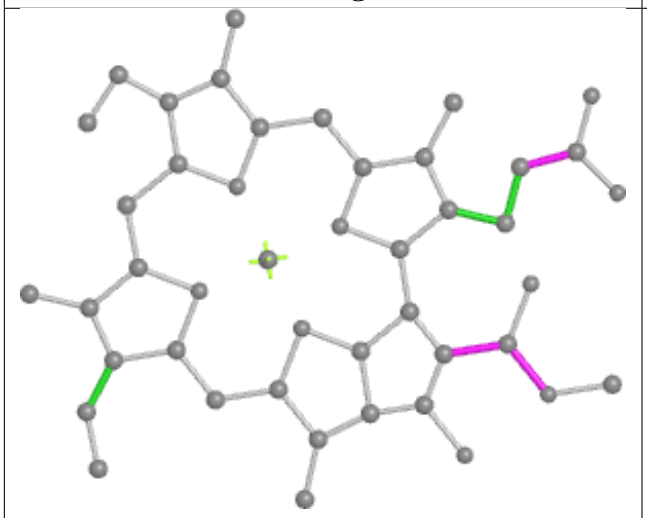

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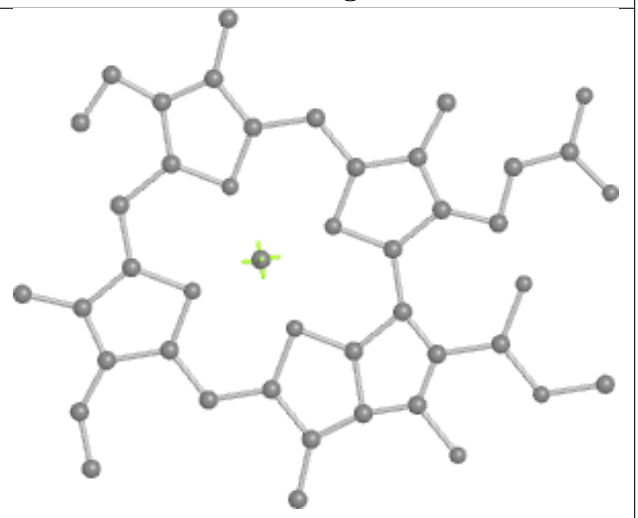
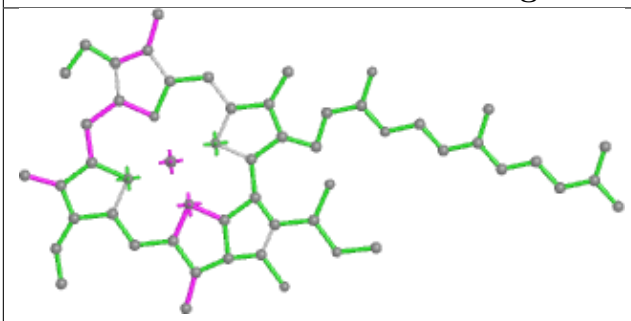


Rings

Ligand CLA e 1121



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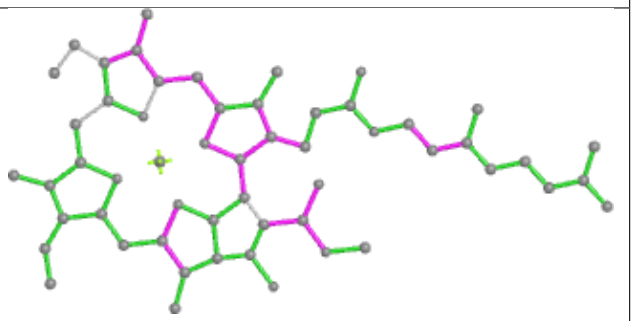

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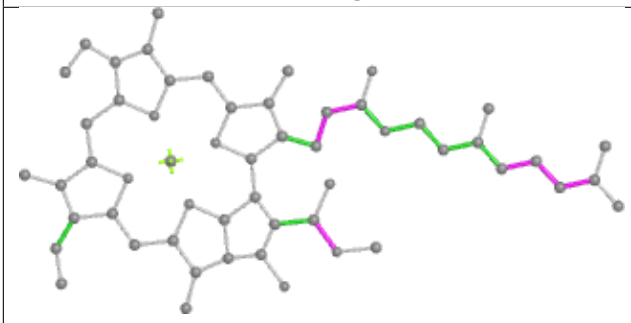

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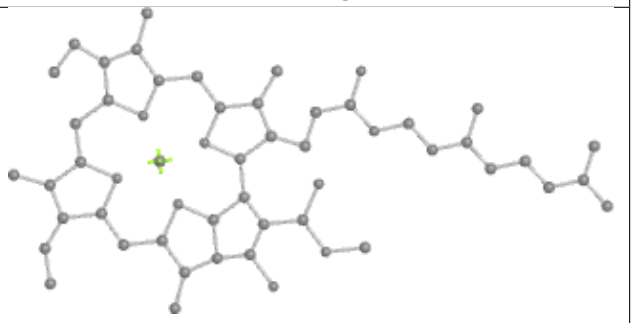
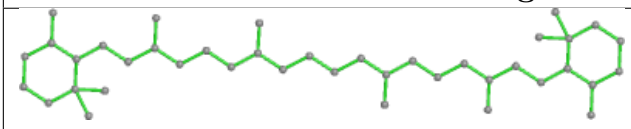


Rings

Ligand BCR J 4012



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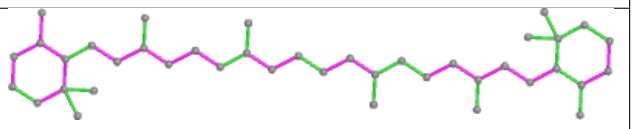

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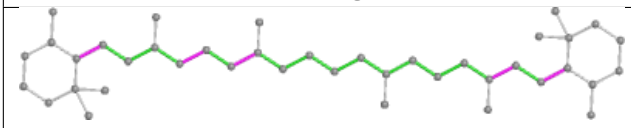
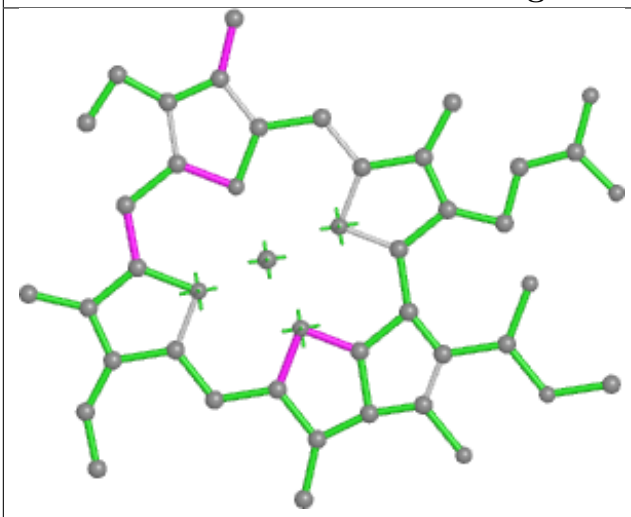


Torsions

Rings

Ligand CLA u 511



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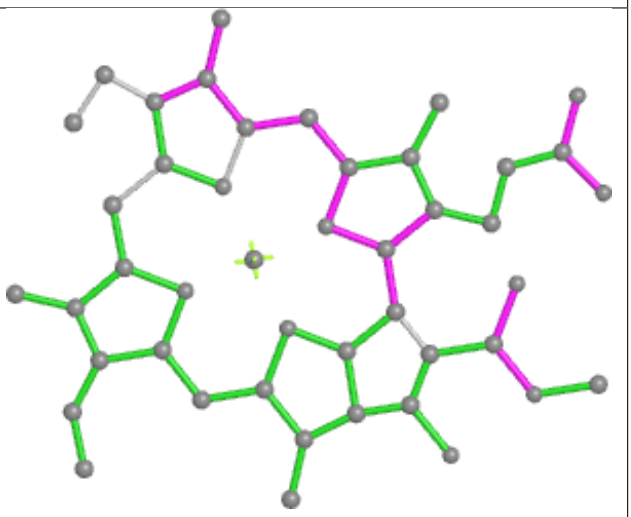

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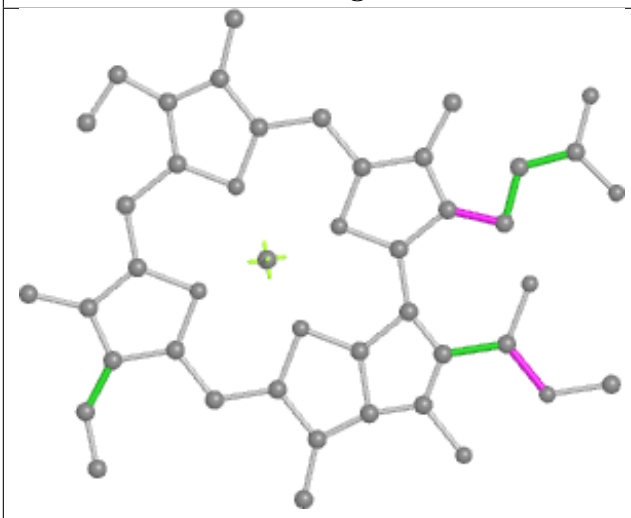

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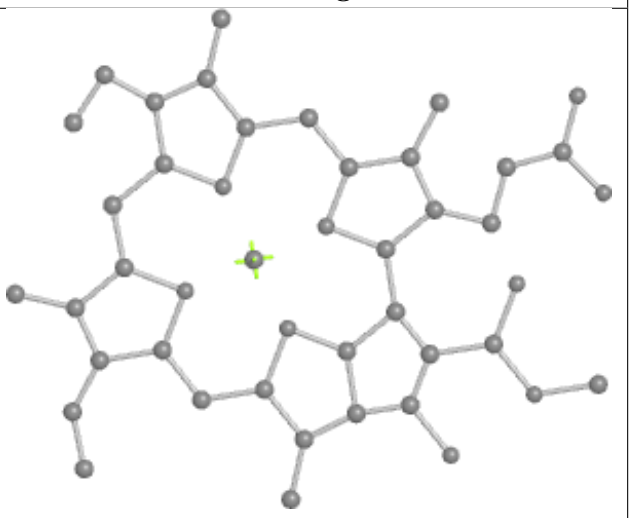
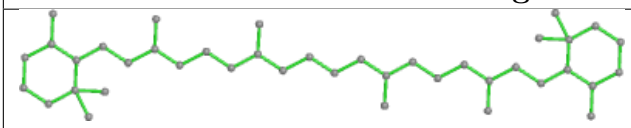


Rings

Ligand BCR K 4104



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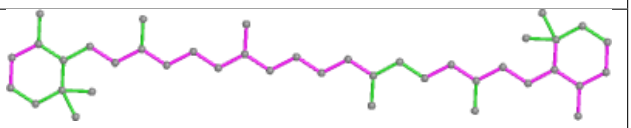

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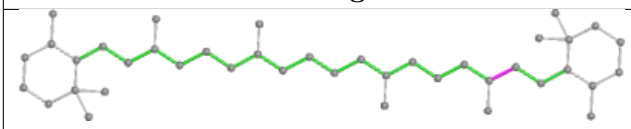
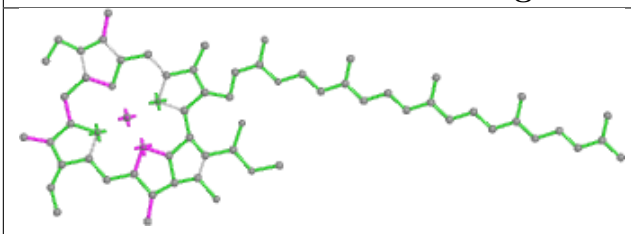


Torsions

Rings

Ligand CLA A 1123



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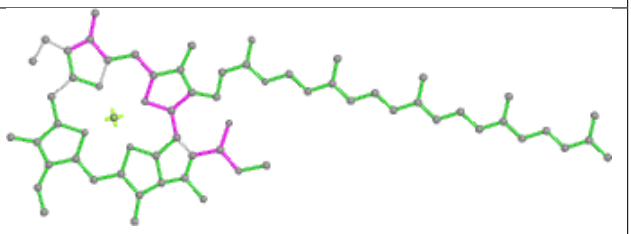

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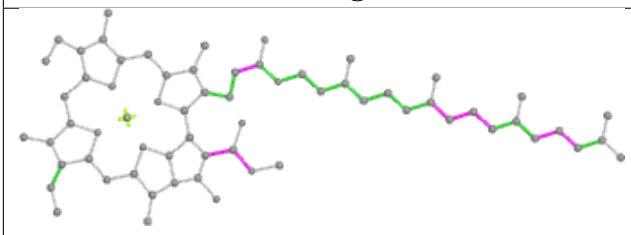

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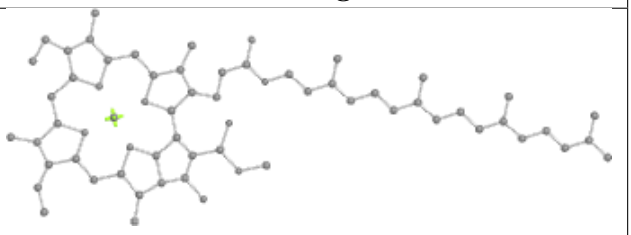
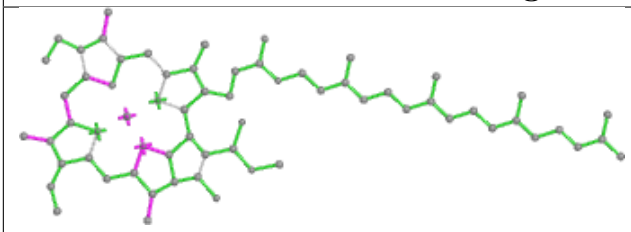


Rings

Ligand CLA f 1223



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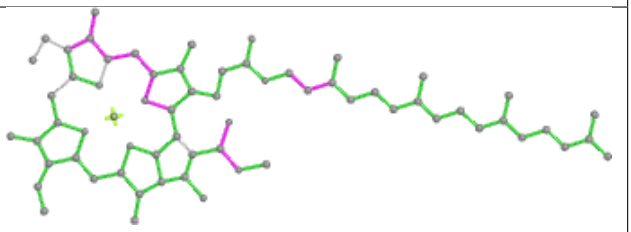
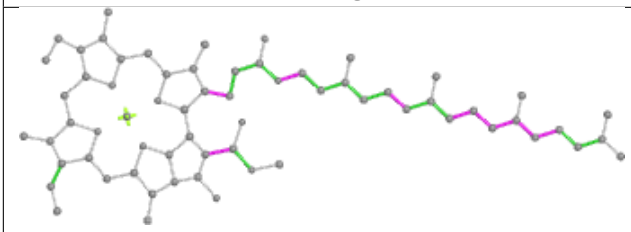


Bond angles



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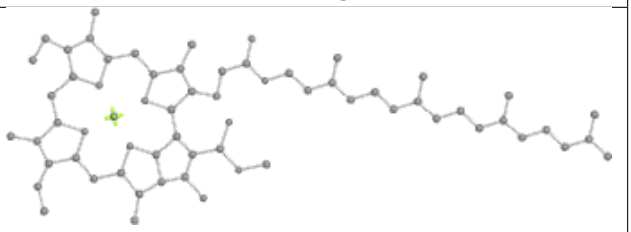
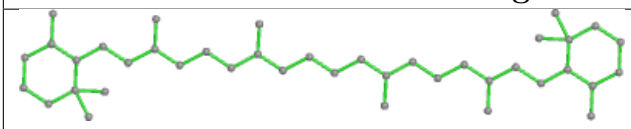
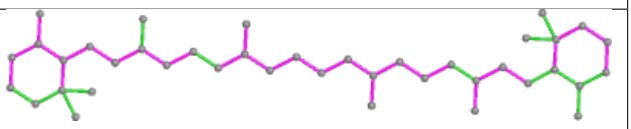


Rings

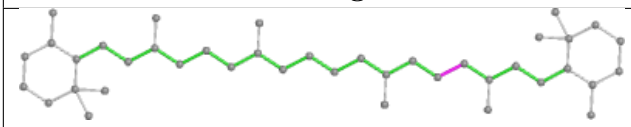
Ligand BCR H 4009



Bond lengths



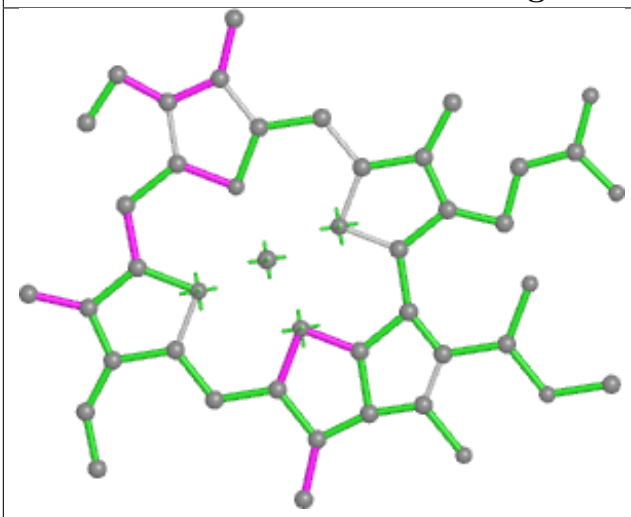
Bond angles



Torsions

Rings

Ligand CLA v 519



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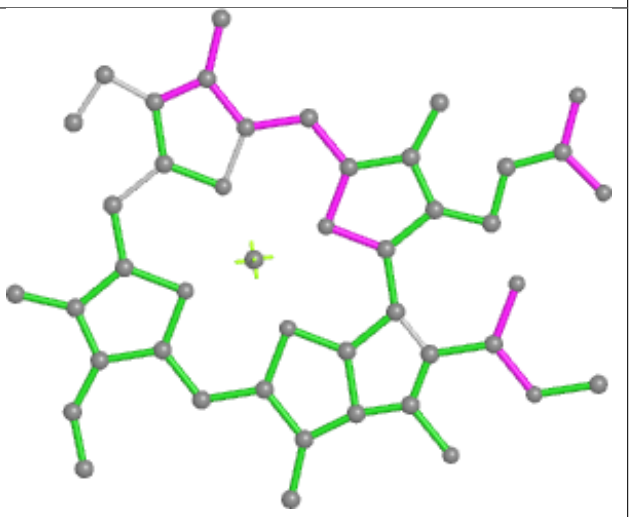

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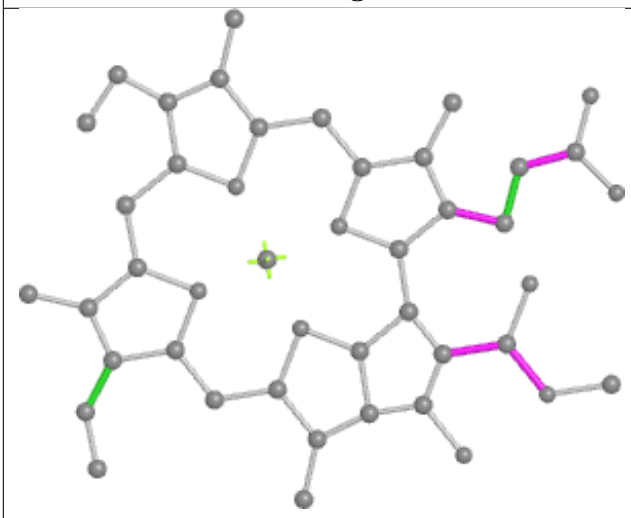

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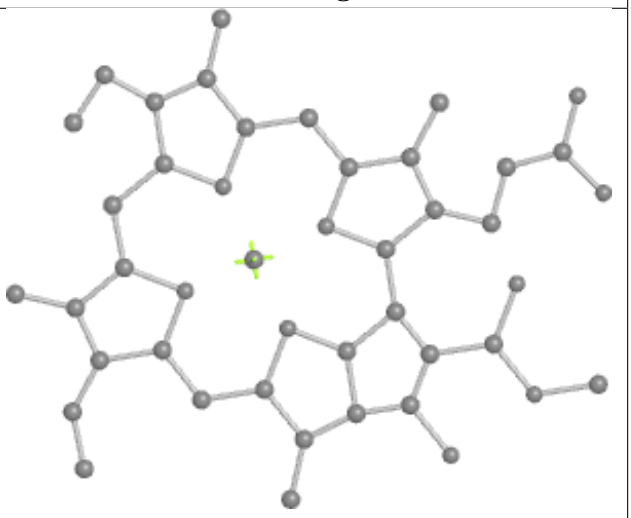
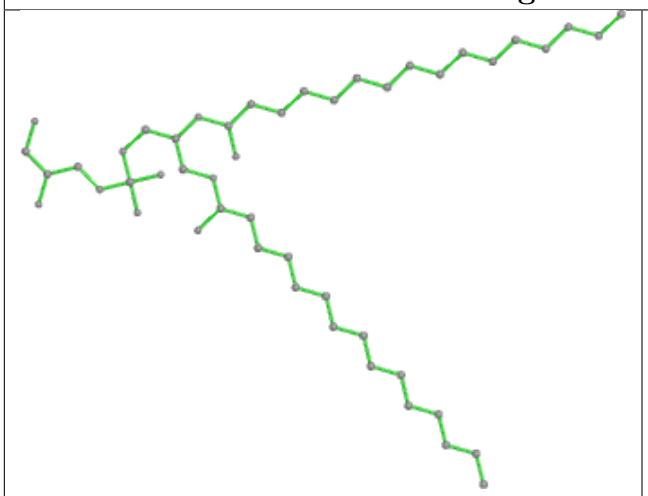


Rings

Ligand LHG k 5001



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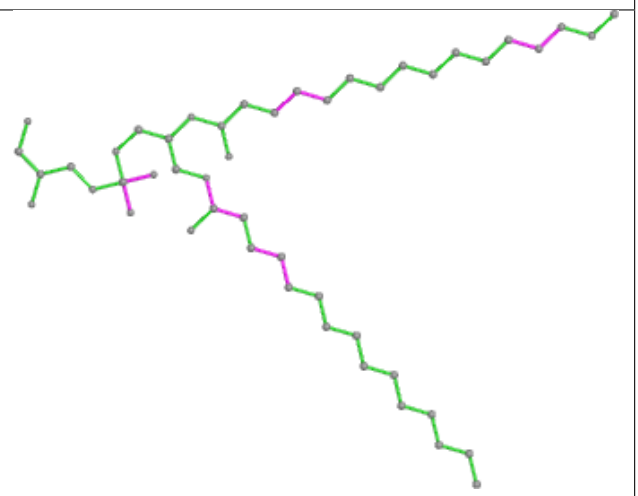
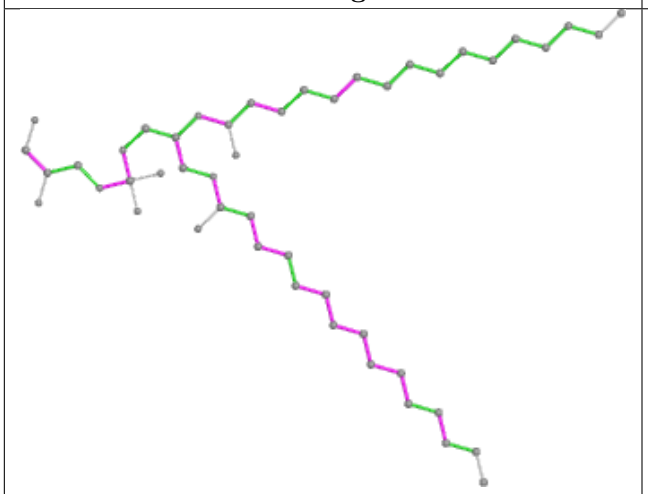


Bond angles



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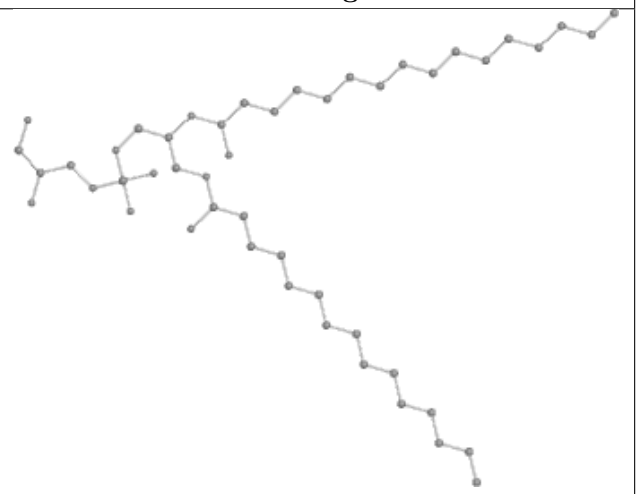
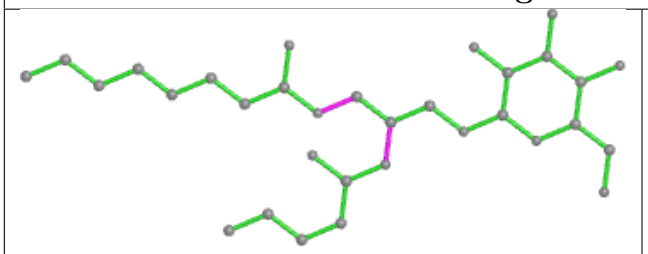


Rings

Ligand LMG J 5104



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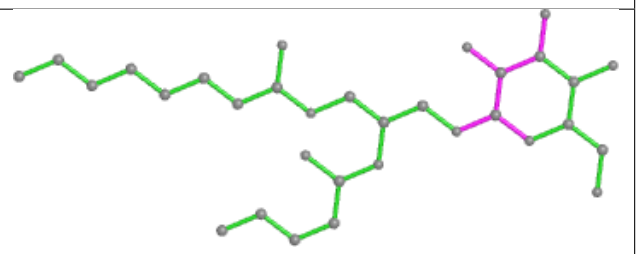
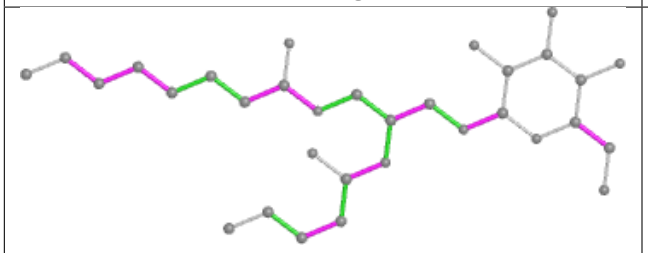


Bond angles



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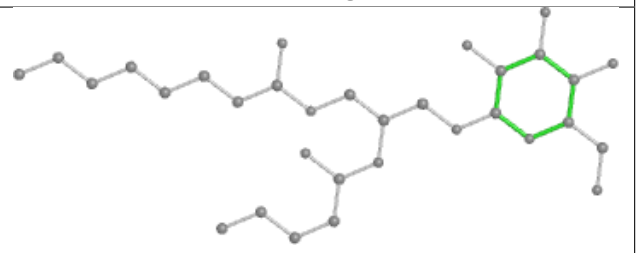
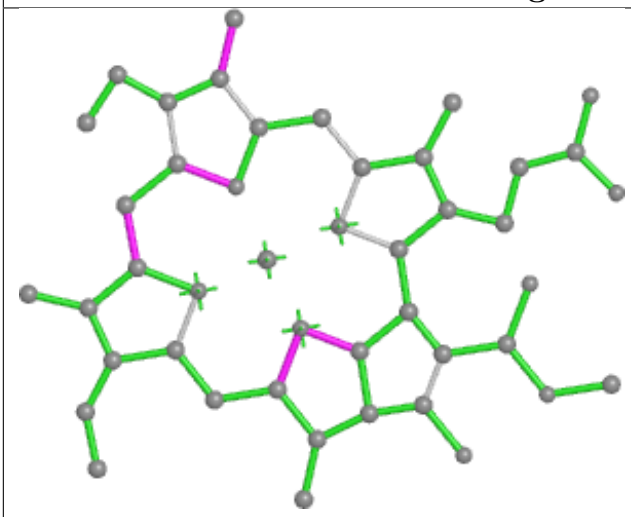


Rings

Ligand CLA 4 501



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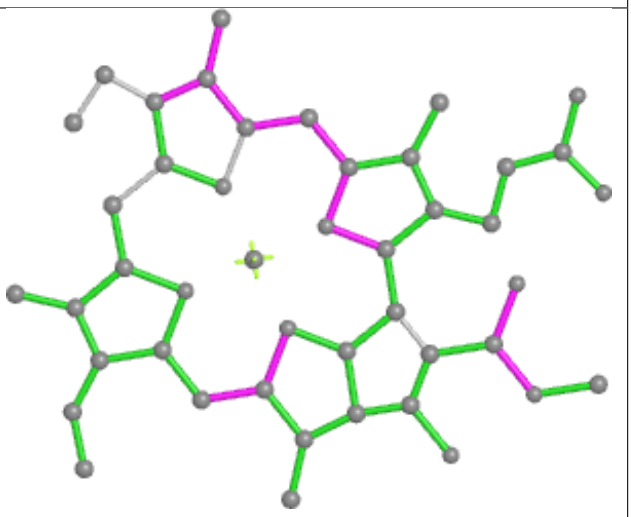
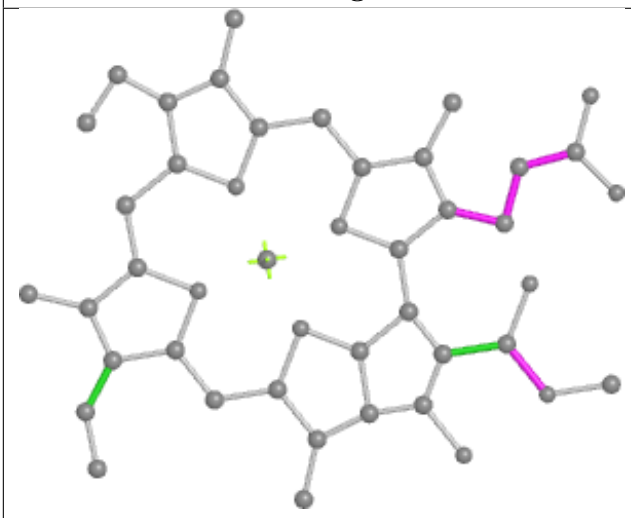


Bond angles



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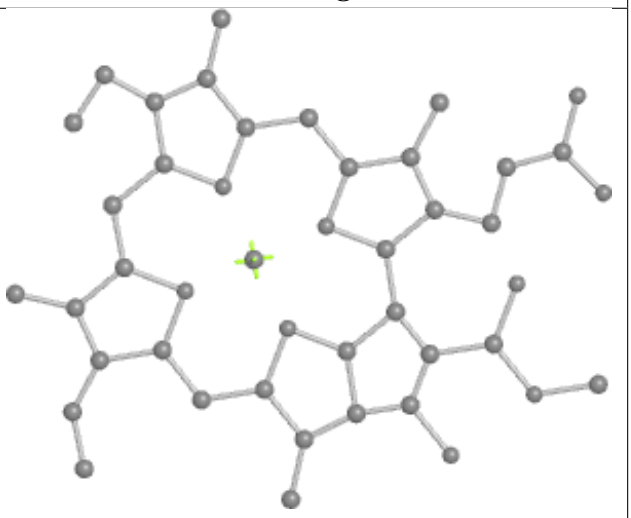
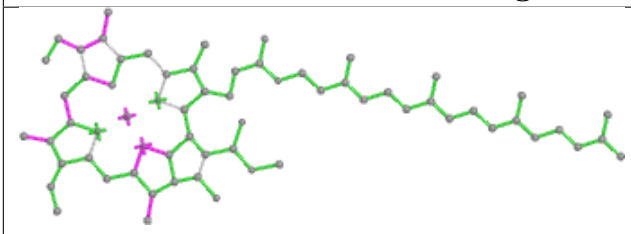


Rings

Ligand CLA G 1125



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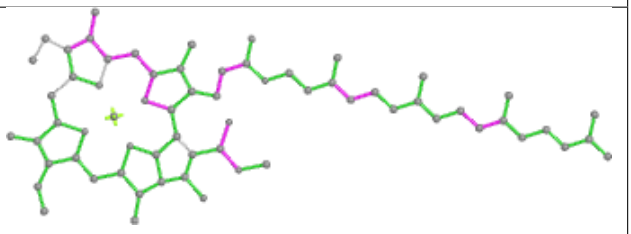
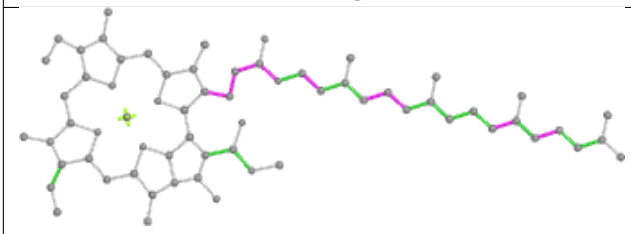


Bond angles



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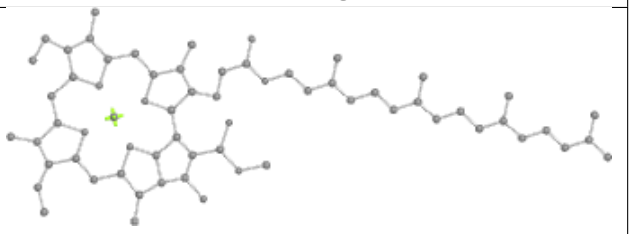
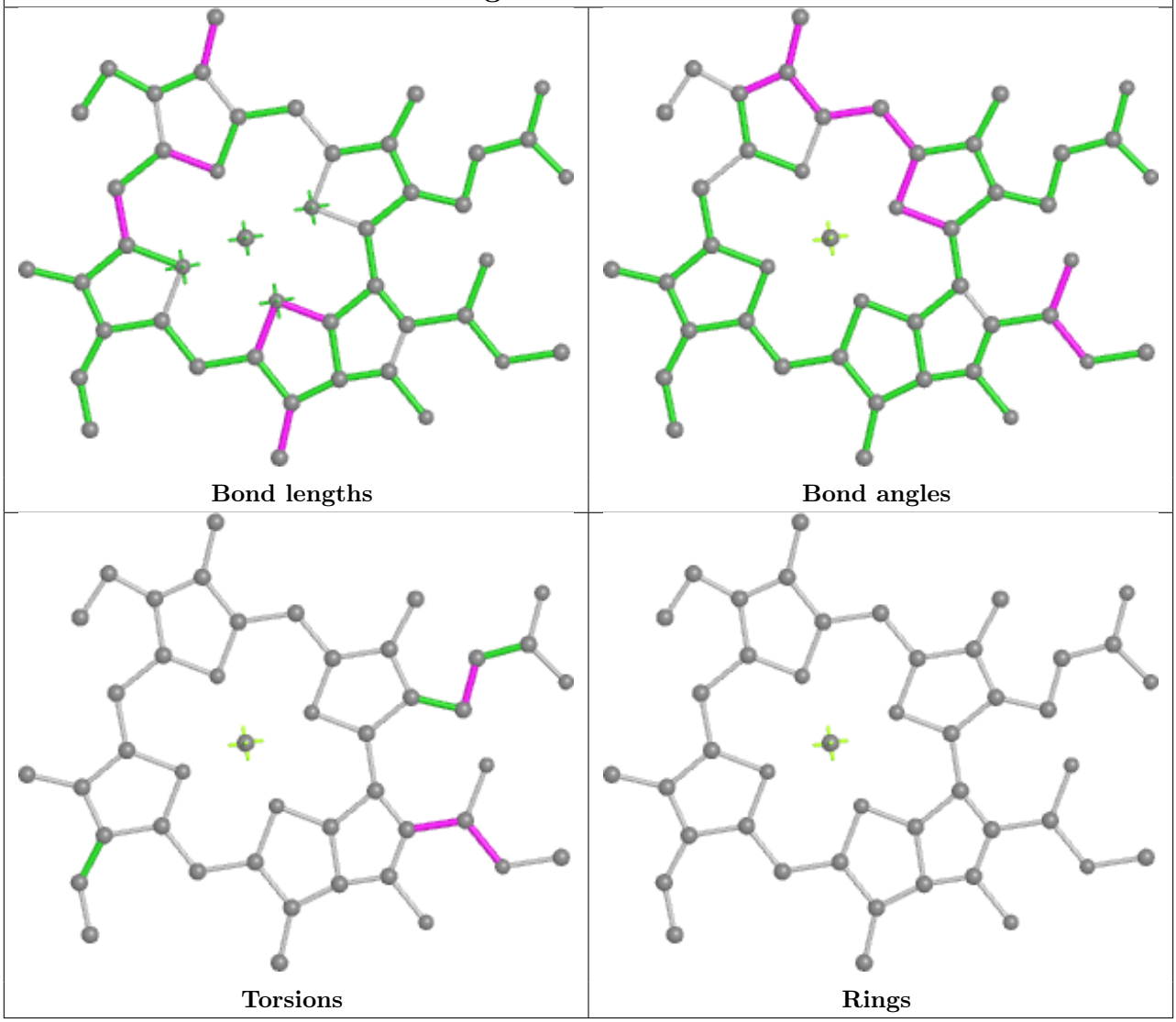
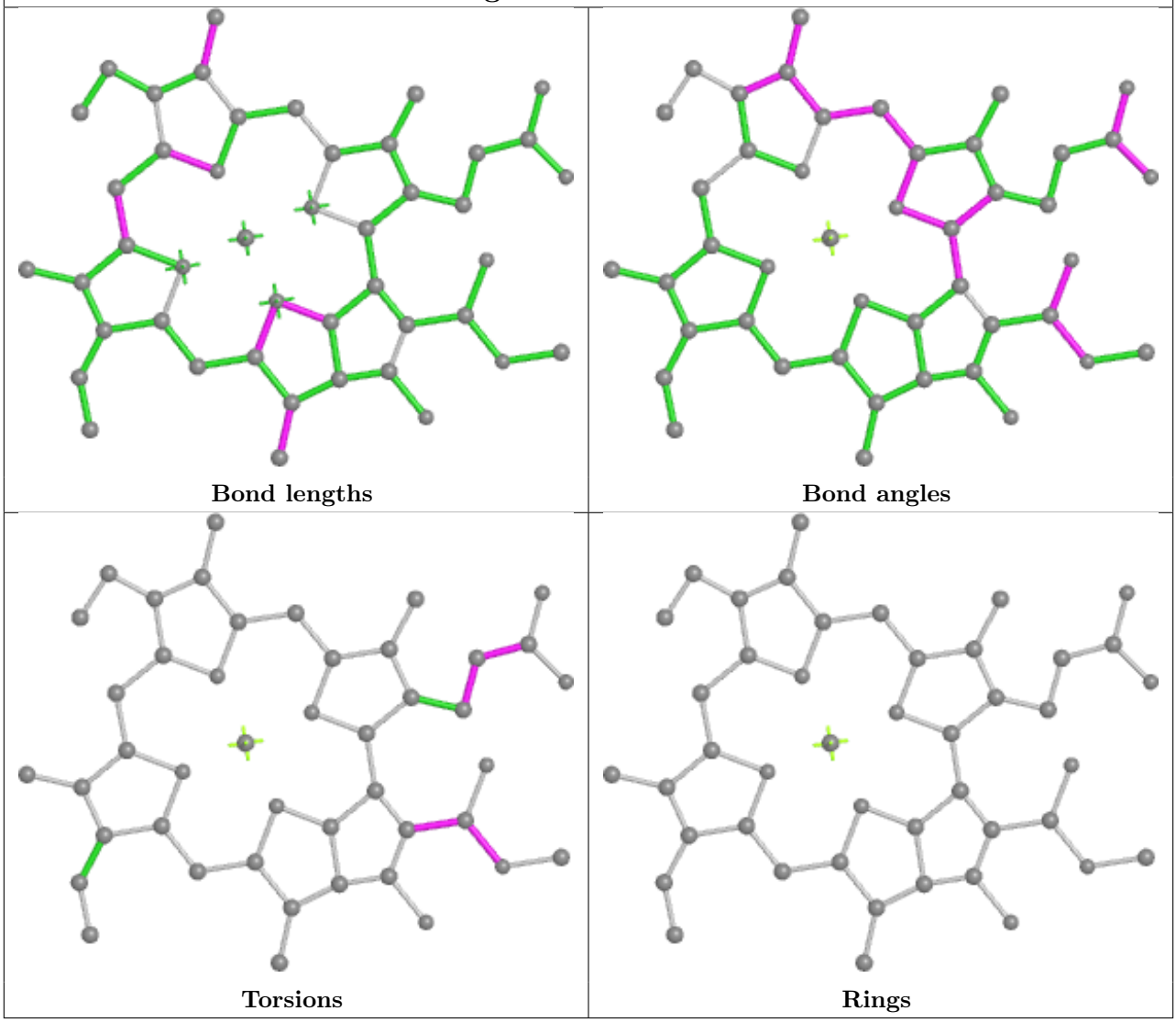


Rings

Ligand CLA v 503



Ligand CLA u 507



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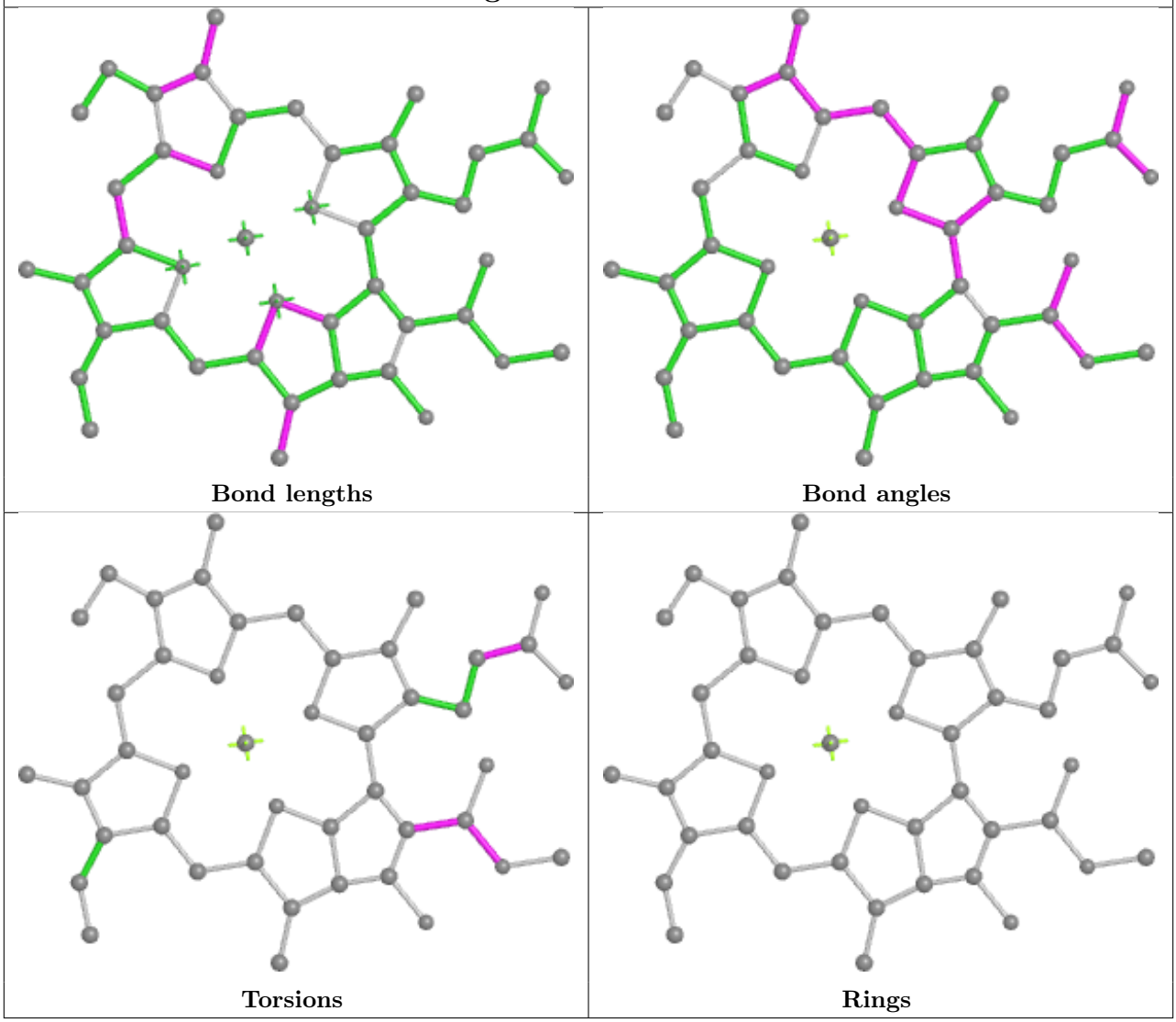
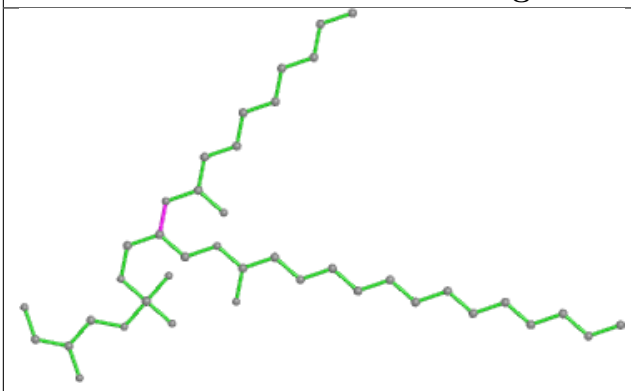
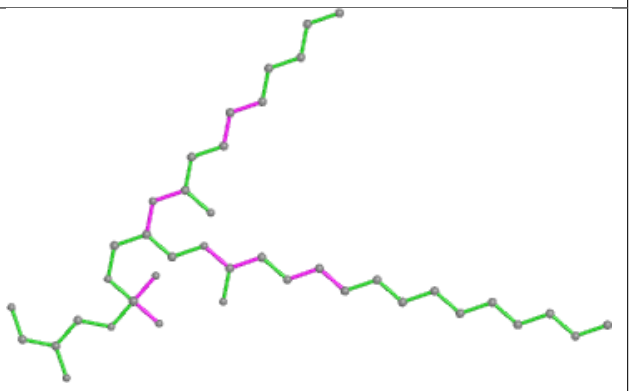


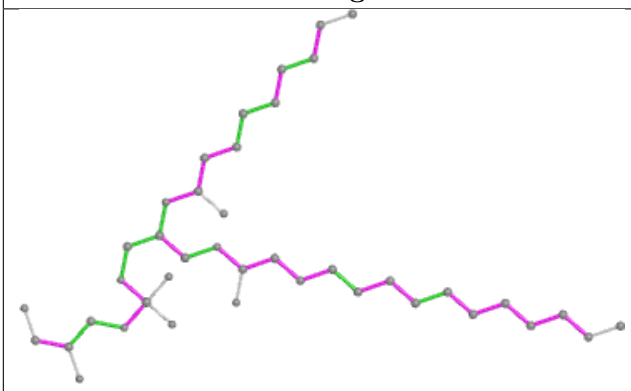
Ligand LHG G 5006



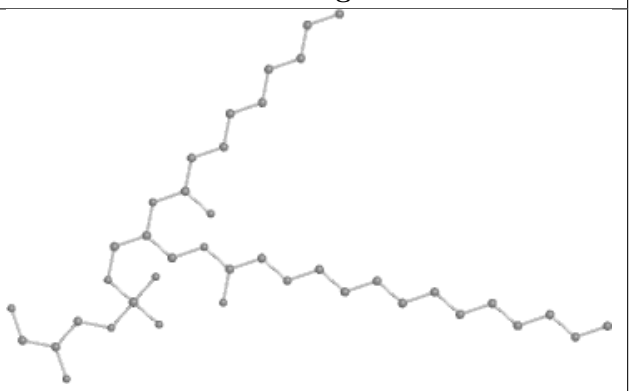
Bond lengths



Bond angles

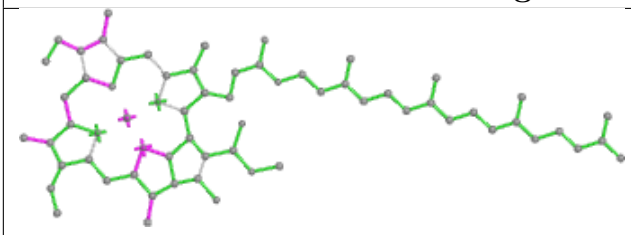


Torsions

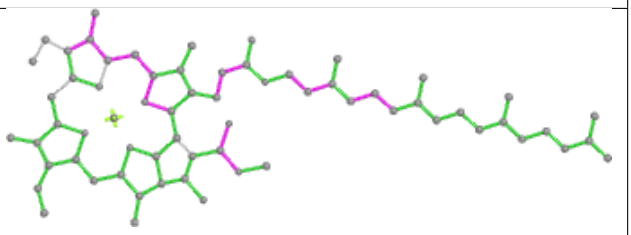


Rings

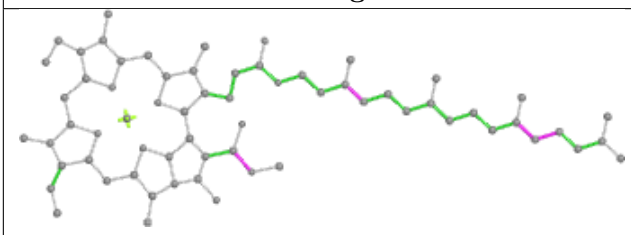
Ligand CLA G 1131



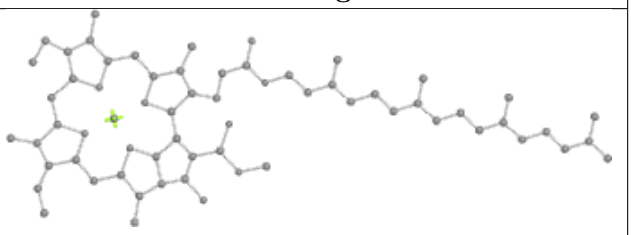
Bond lengths



Bond angles

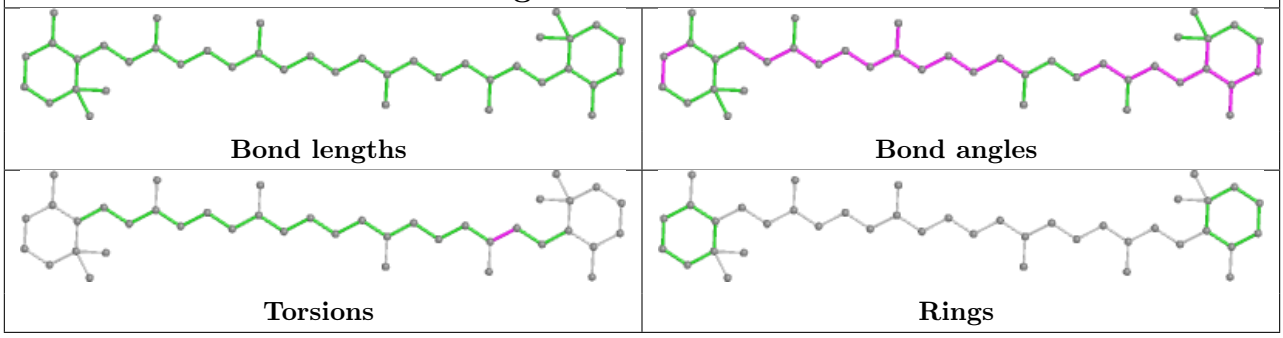


Torsions

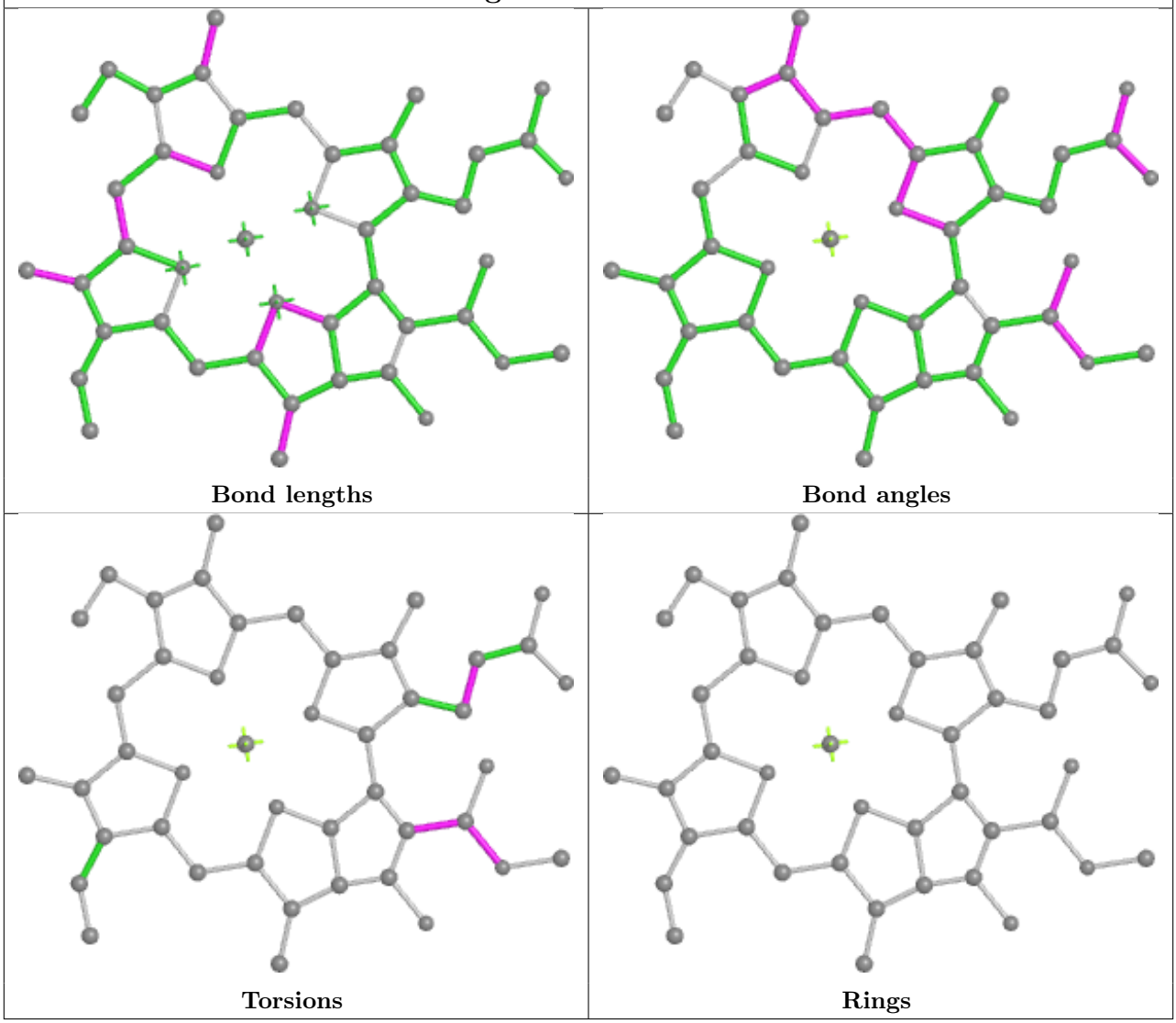


Rings

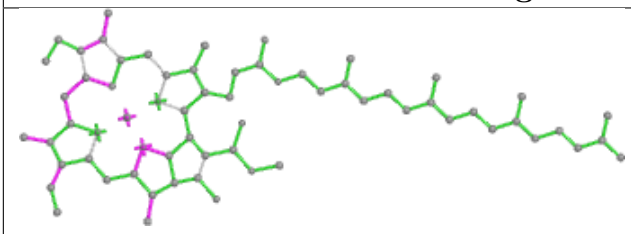
Ligand BCR U 4104



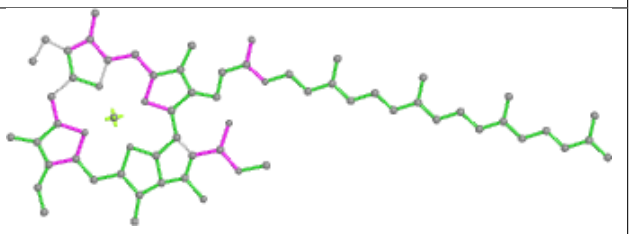
Ligand CLA 2 517



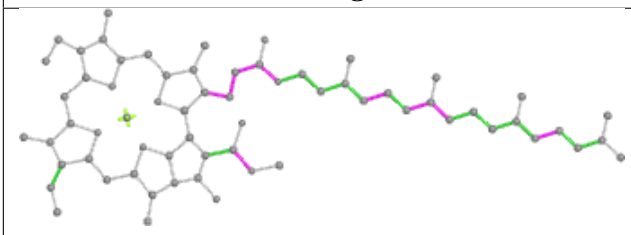
Ligand CLA B 1206



Bond lengths



Bond angles



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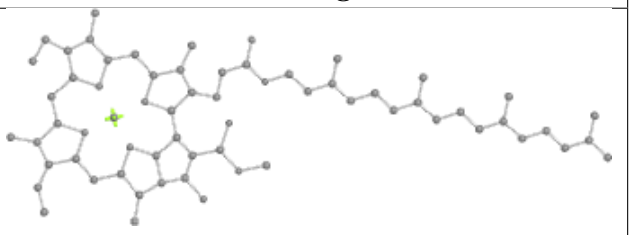
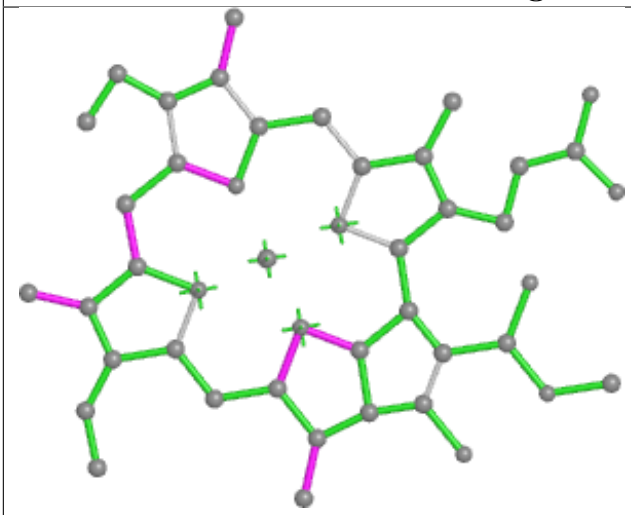


Rings

Ligand CLA d 512



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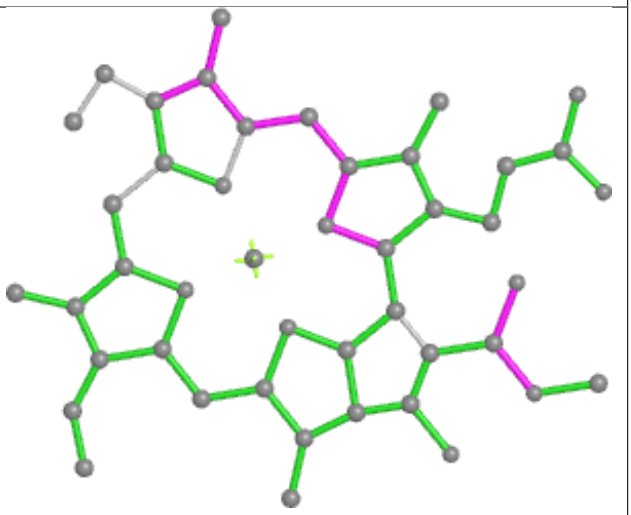
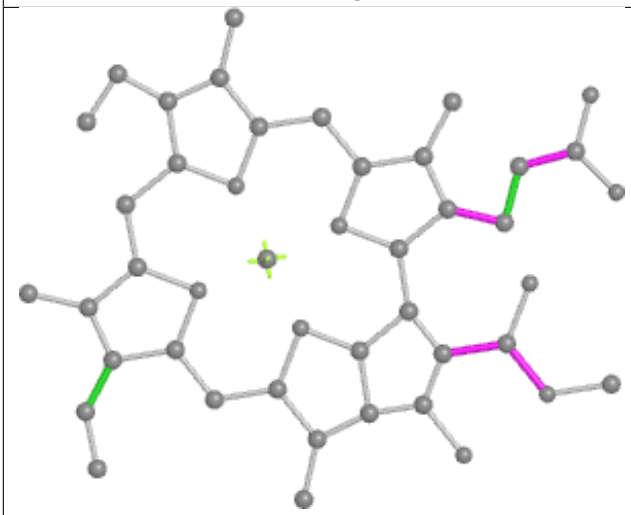


Bond angles



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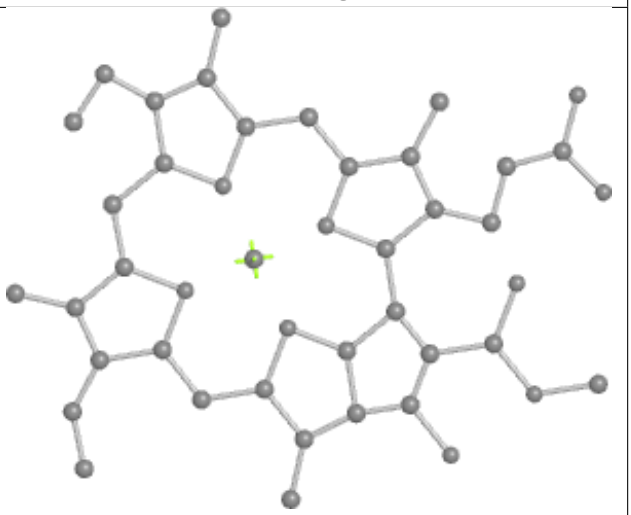
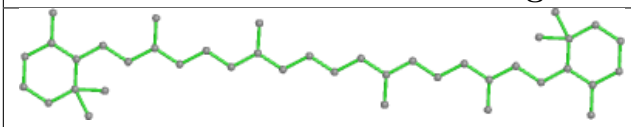
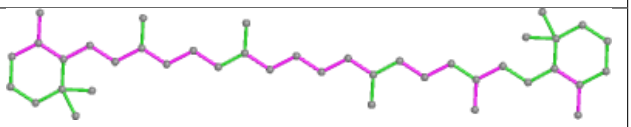
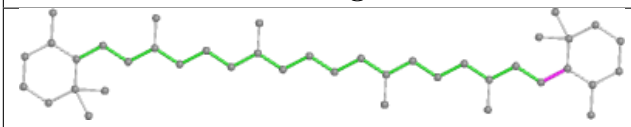
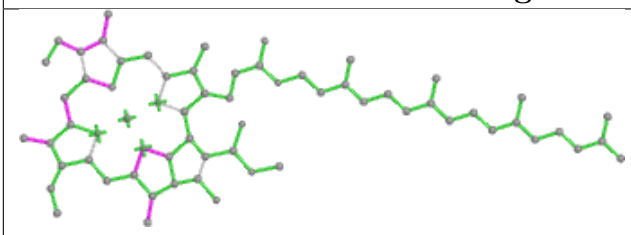
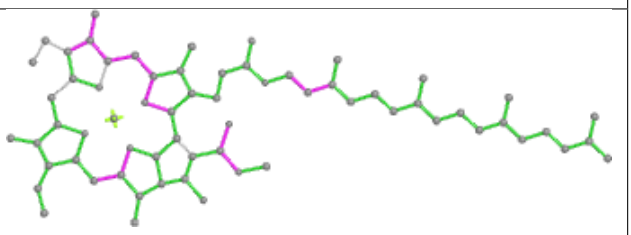
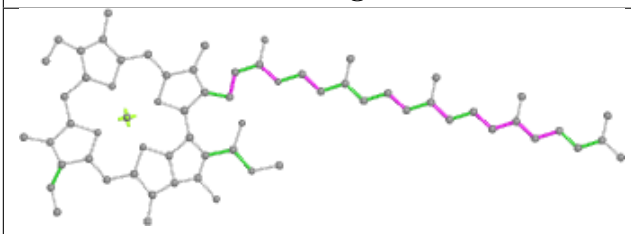
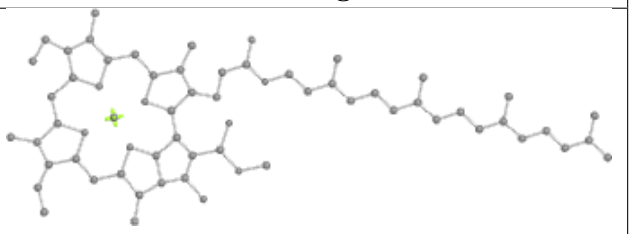
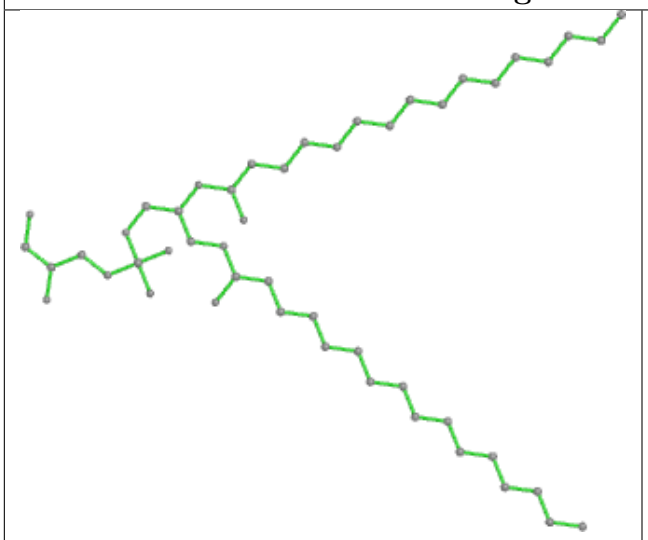


Rings

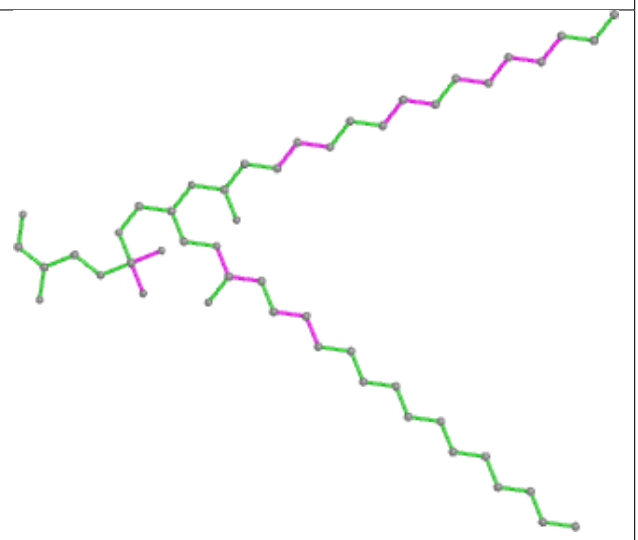
Ligand BCR 5 524	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA H 1214	
 Bond lengths	 Bond angles
 Torsions	 Rings

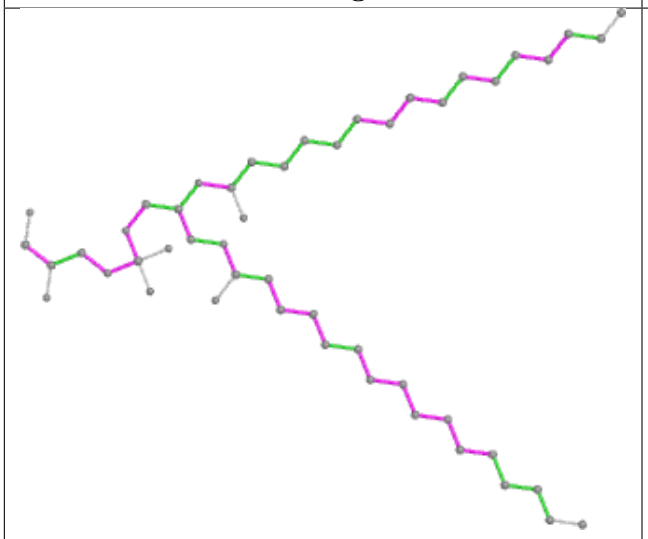
Ligand LHG V 5221



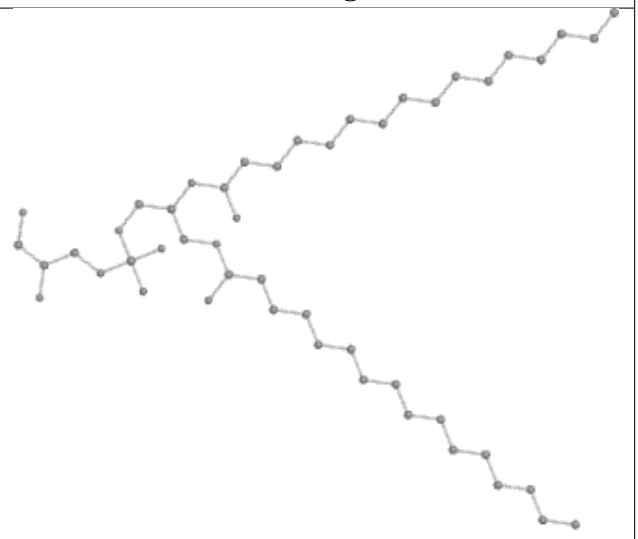
Bond lengths



Bond angles

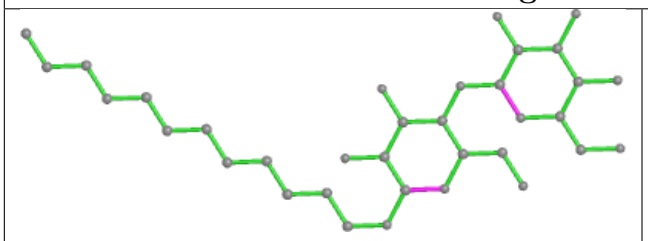


Torsions



Rings

Ligand LMU f 1843



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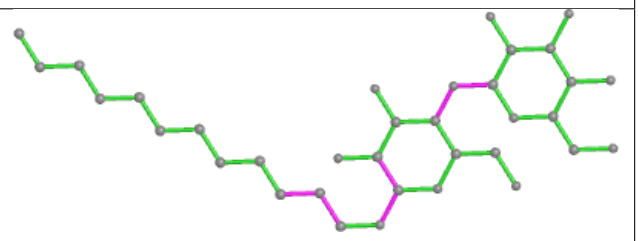
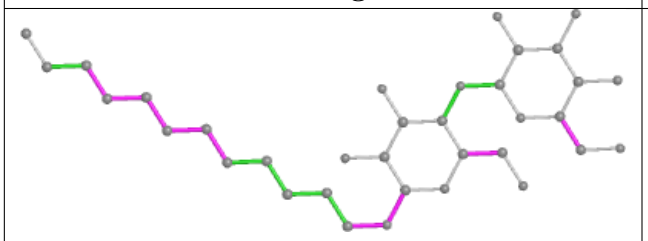


Bond angles



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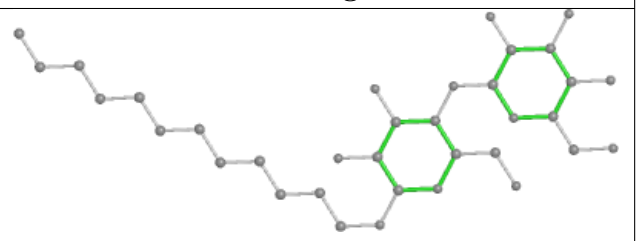
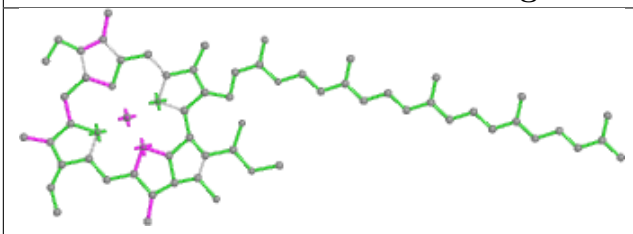


Rings

Ligand CLA e 1140



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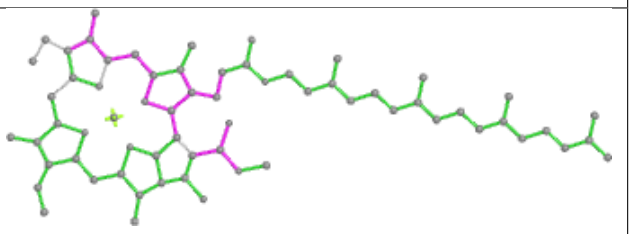
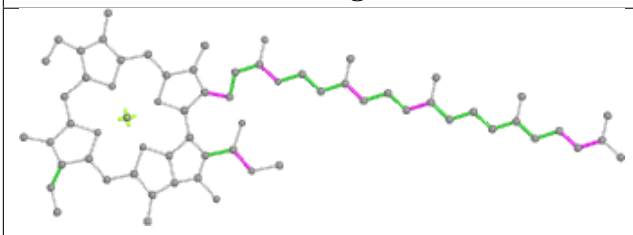


Bond angles



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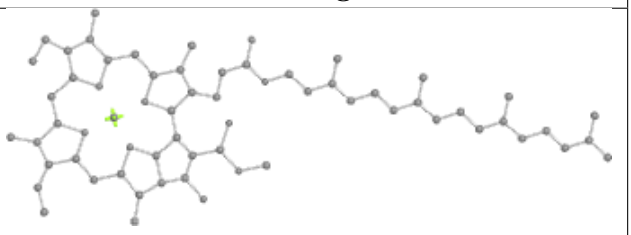
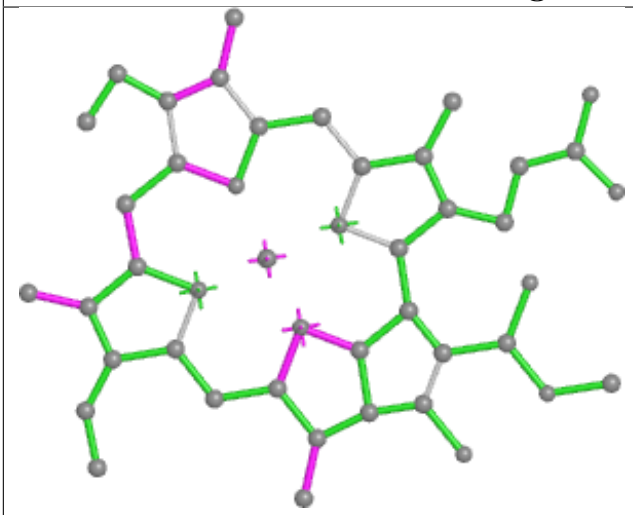


Rings

Ligand CLA 3 508



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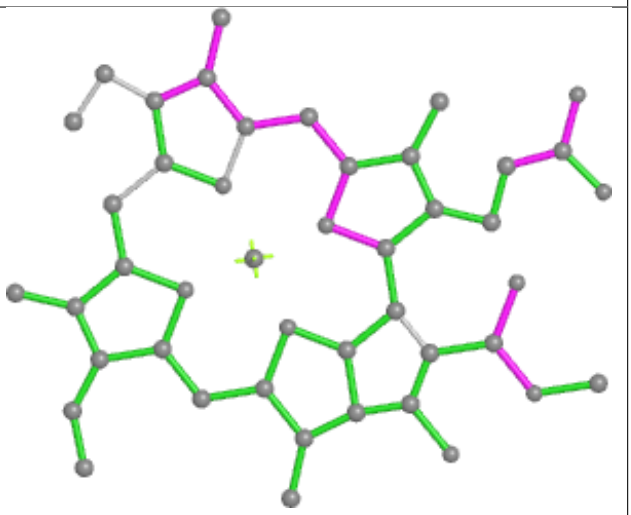

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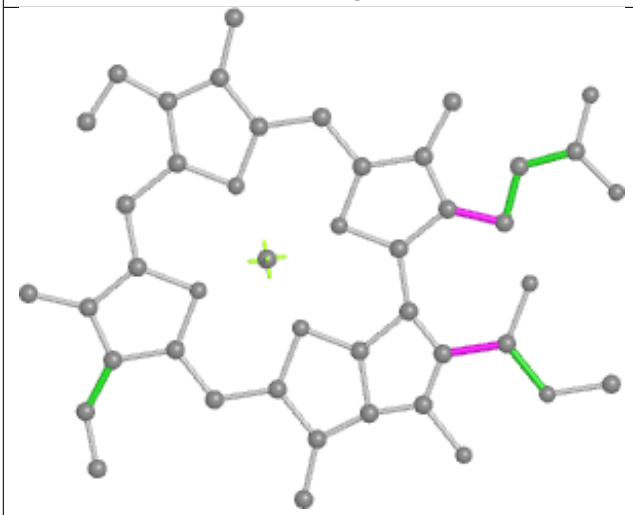

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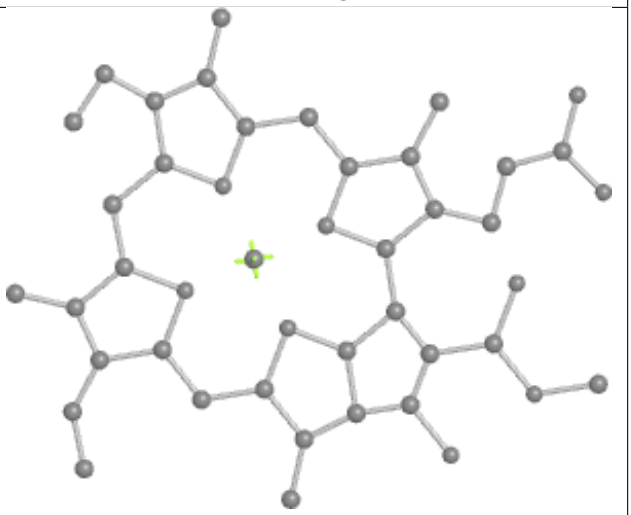
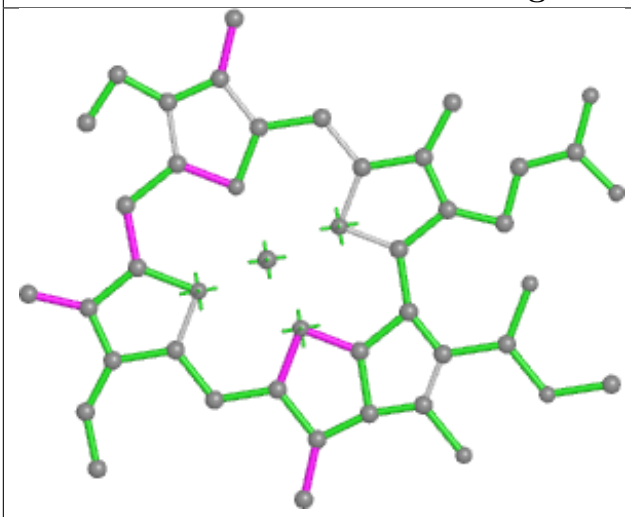


Rings

Ligand CLA 4 509



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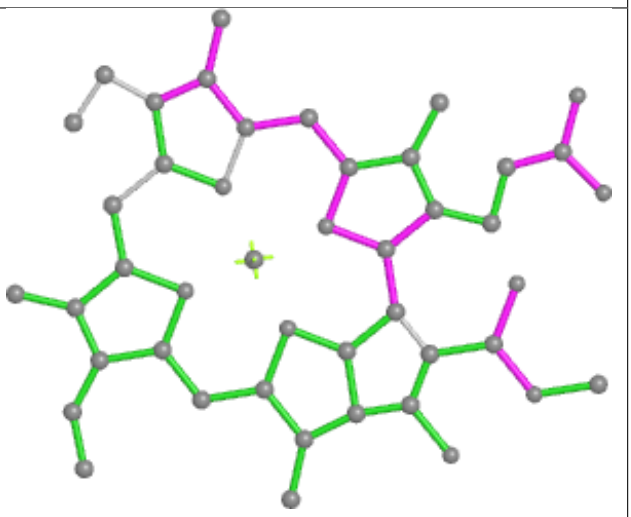
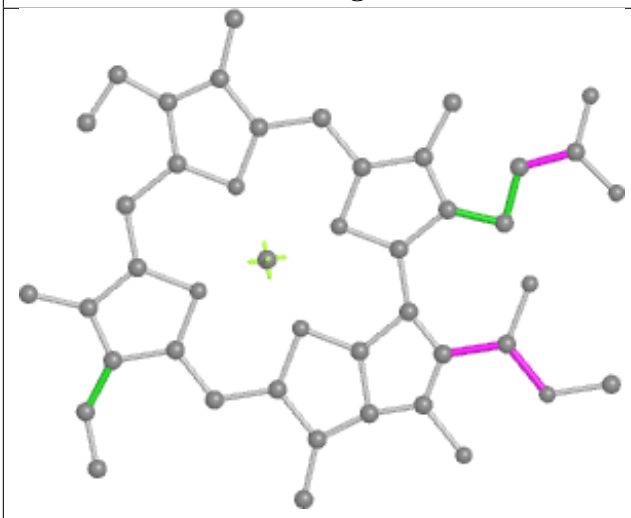


Bond angles



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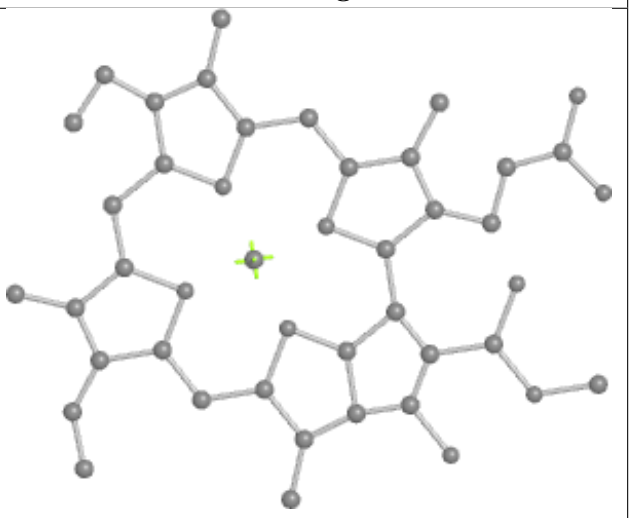
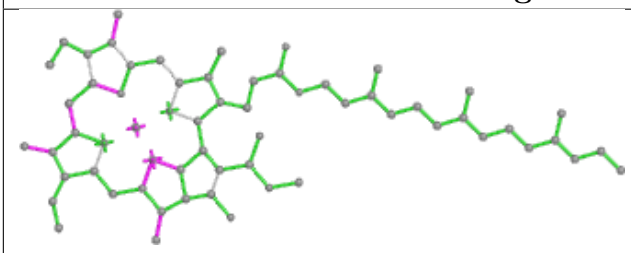


Rings

Ligand CLA H 1221



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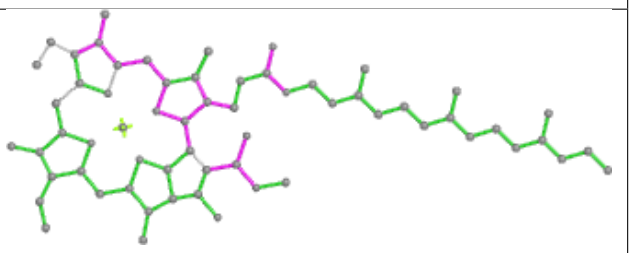

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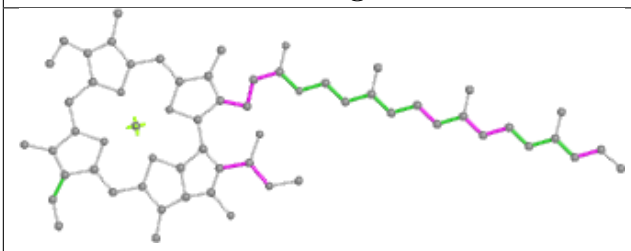

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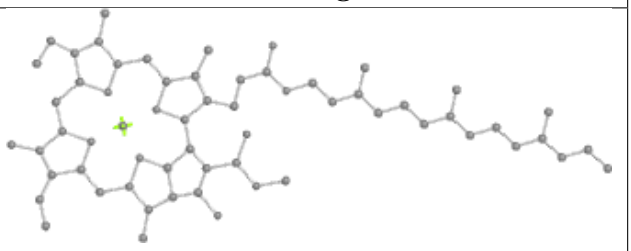
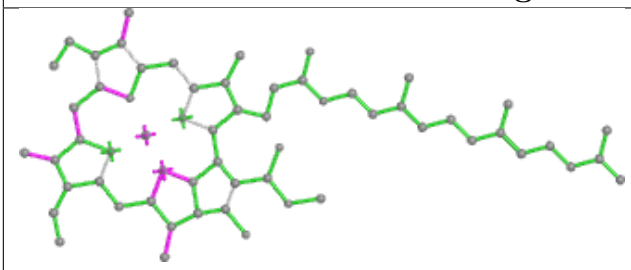
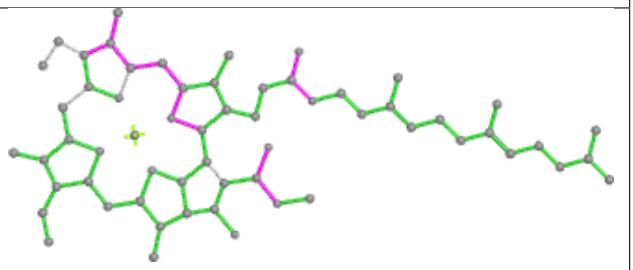
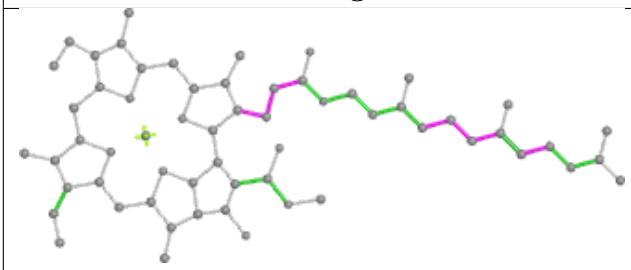
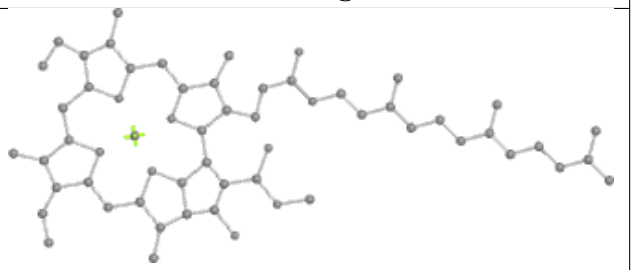


Rings

Ligand CLA A 1116	
 Bond lengths	 Bond angles
 Torsions	 Rings

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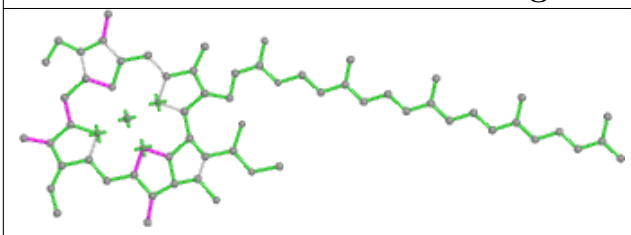
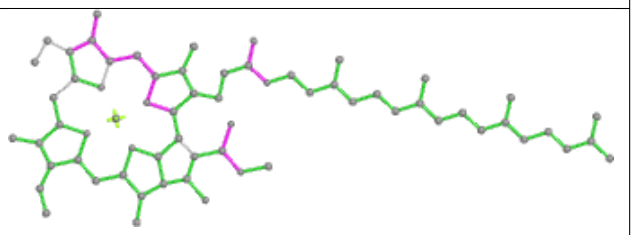
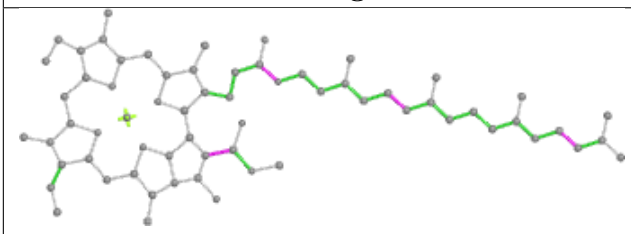
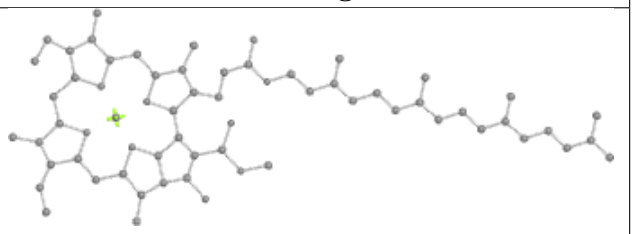
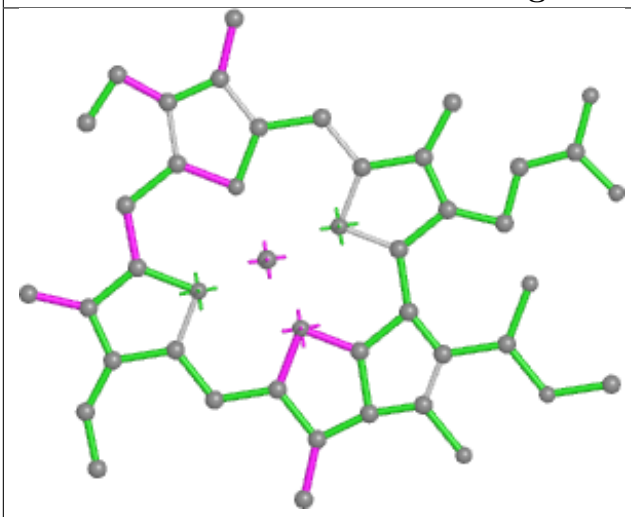
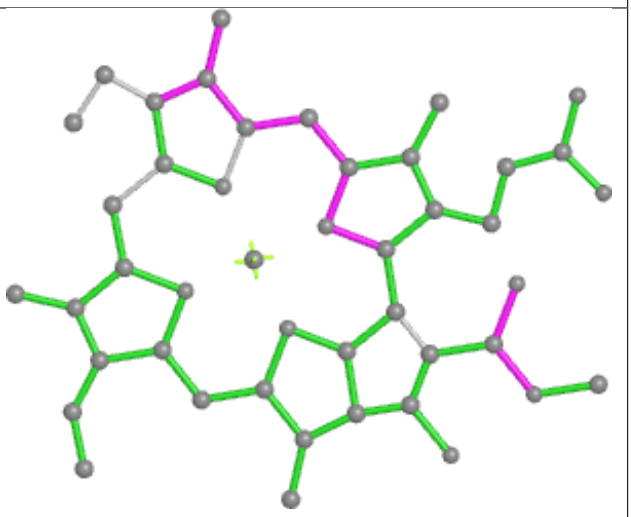
 Bond lengths	 Bond angles
 Torsions	 Rings

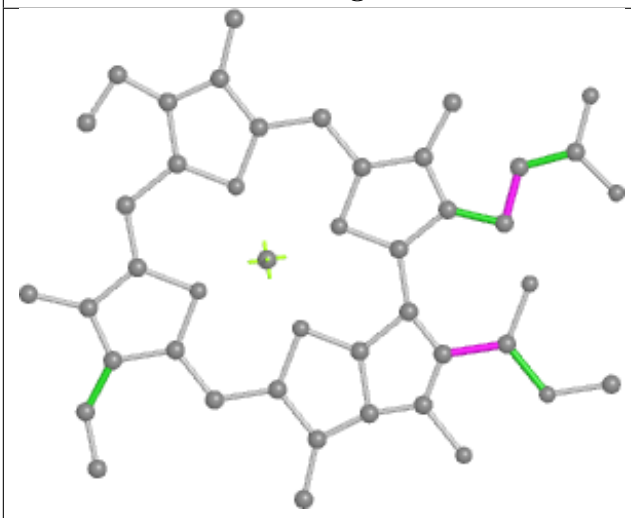
Ligand CLA 4 505



Bond lengths



Bond angles



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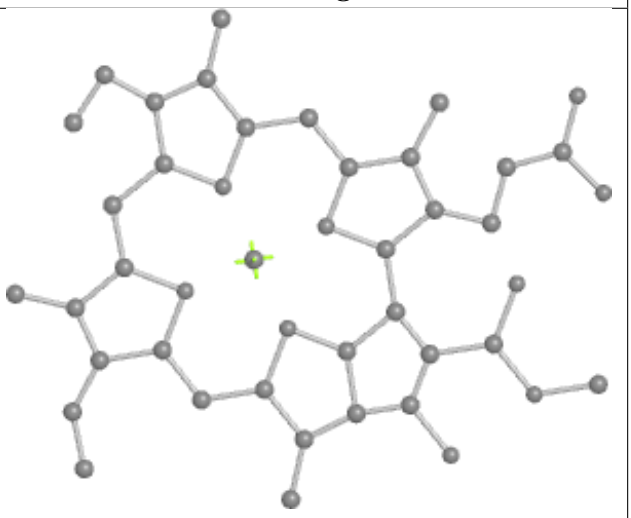
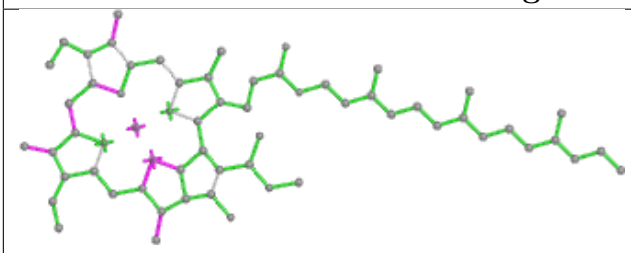


Rings

Ligand CLA f 1221



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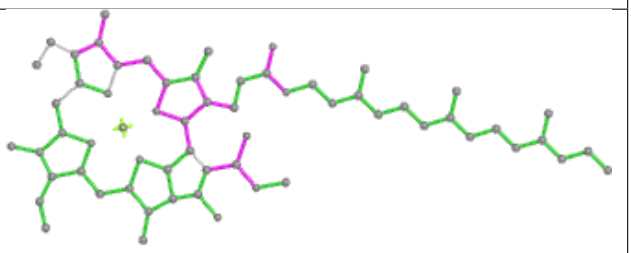
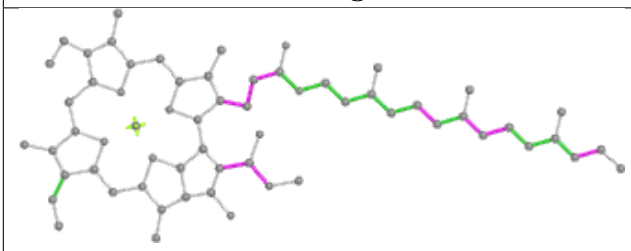


Bond angles



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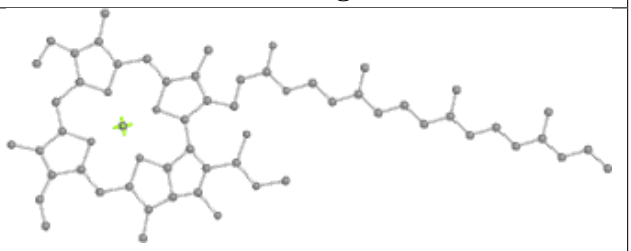
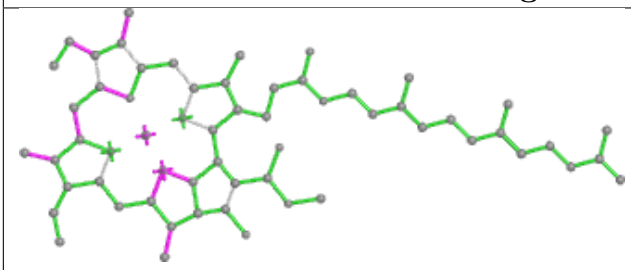
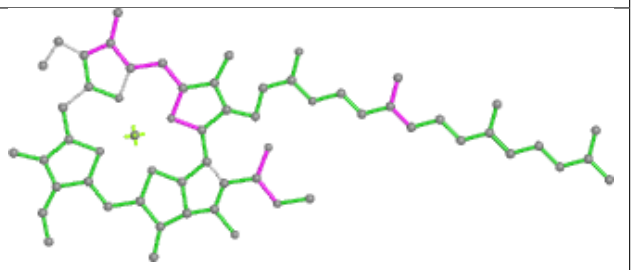
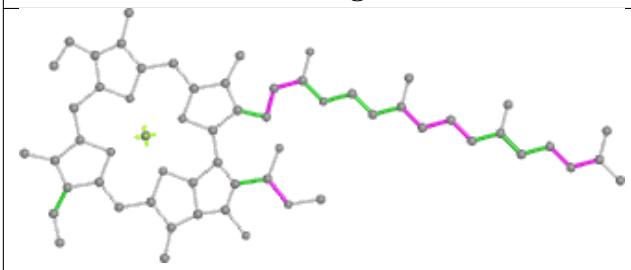
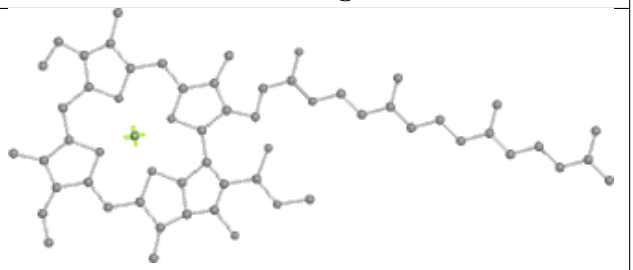


Rings

Ligand CLA e 1115	
 Bond lengths	 Bond angles
 Torsions	 Rings

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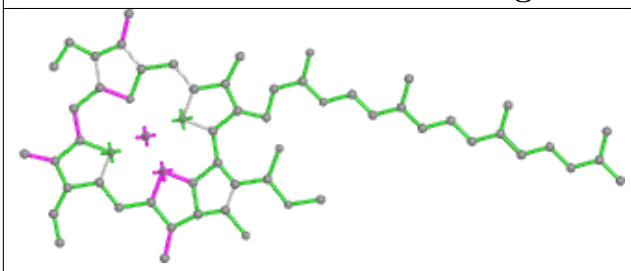
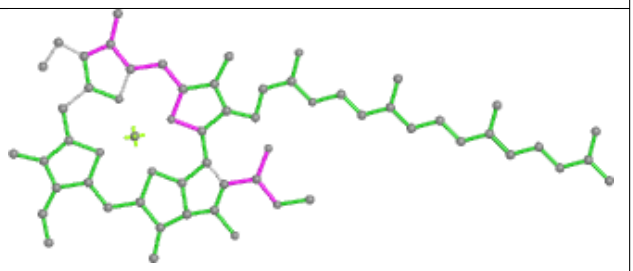
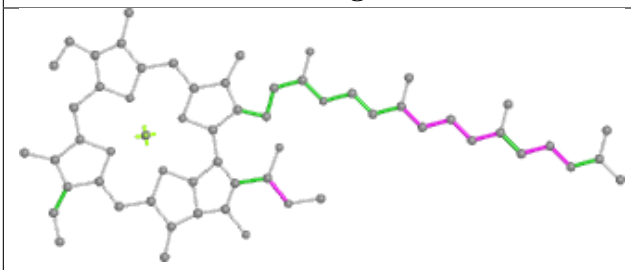
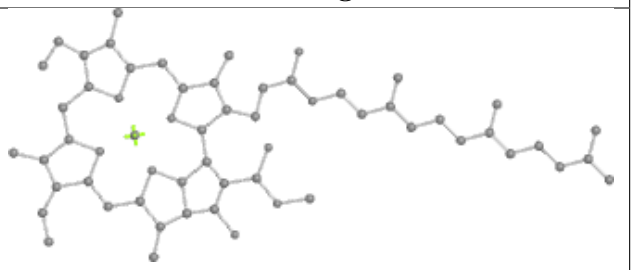
 Bond lengths	 Bond angles
 Torsions	 Rings

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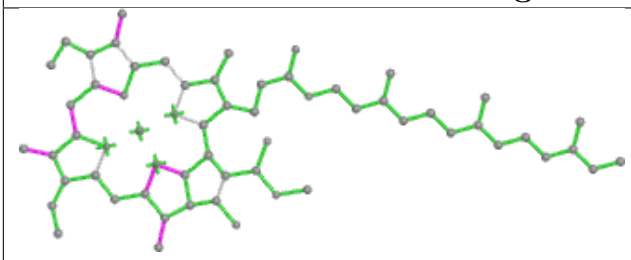
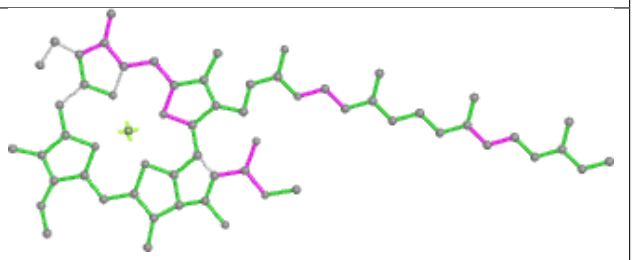
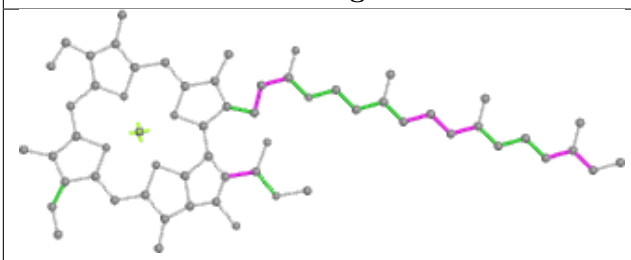
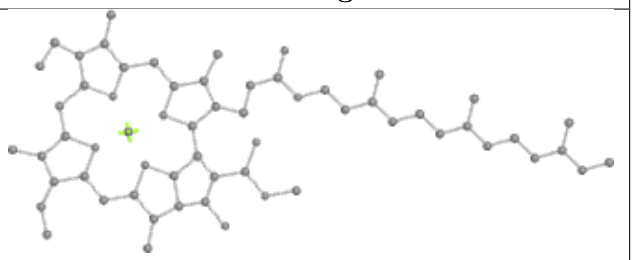
 Bond lengths	 Bond angles
 Torsions	 Rings

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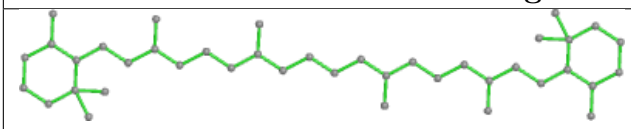
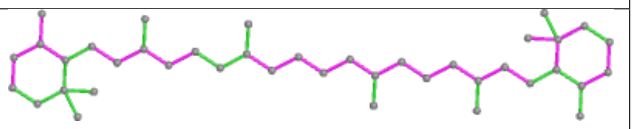
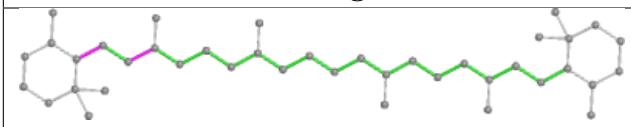
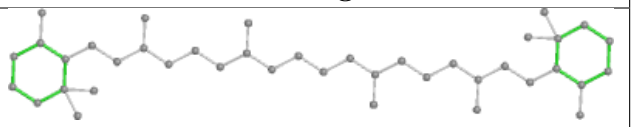
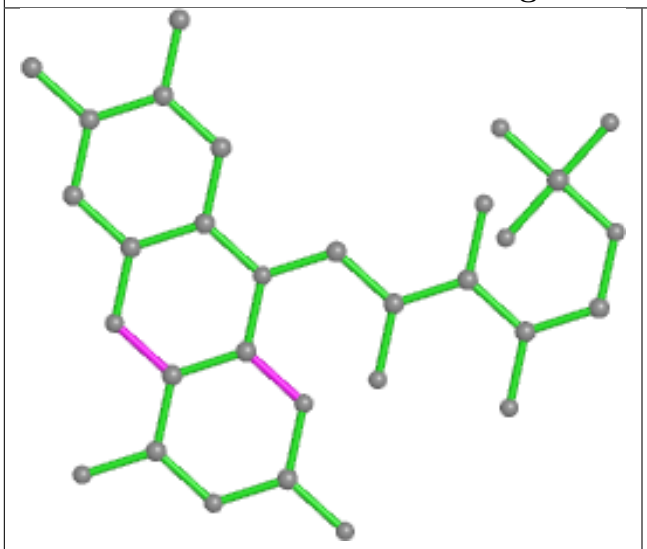
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FMN X 170



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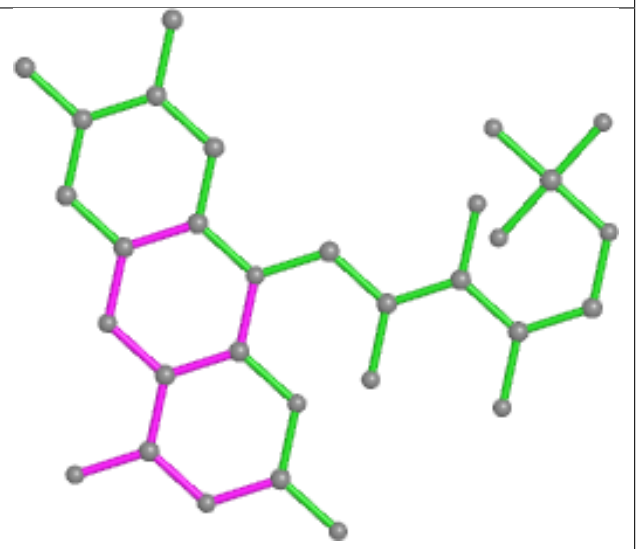
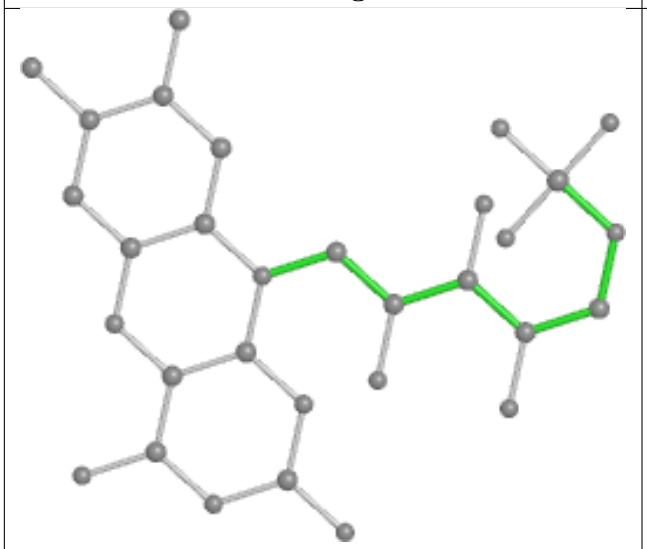


Bond angles



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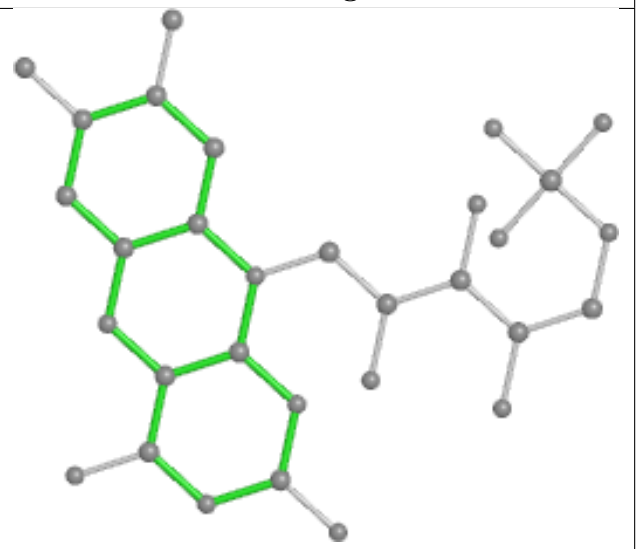
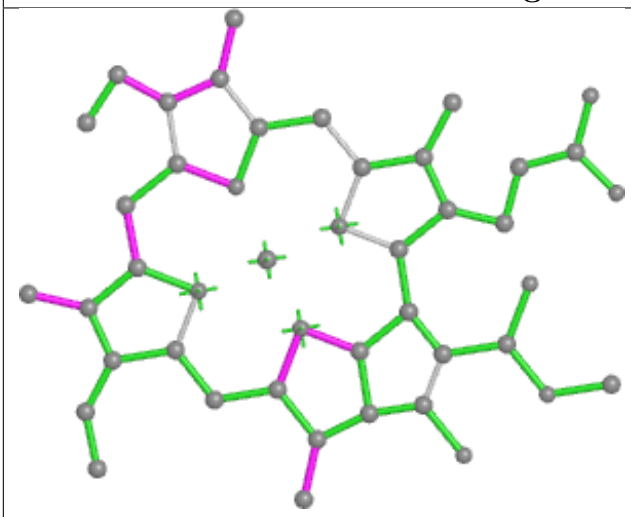


Rings

Ligand CLA Y 504



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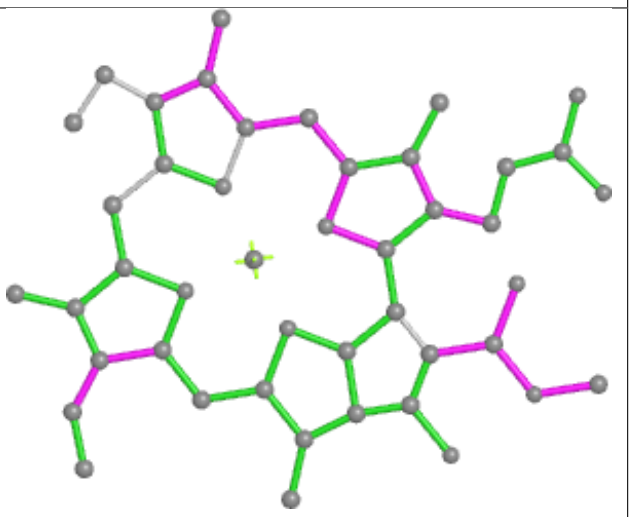

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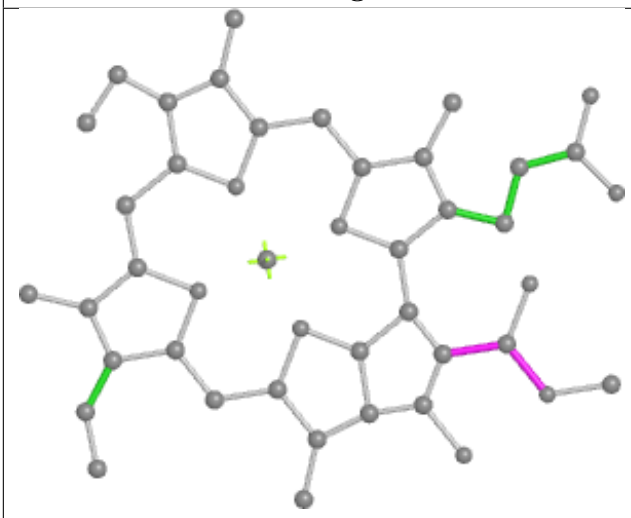

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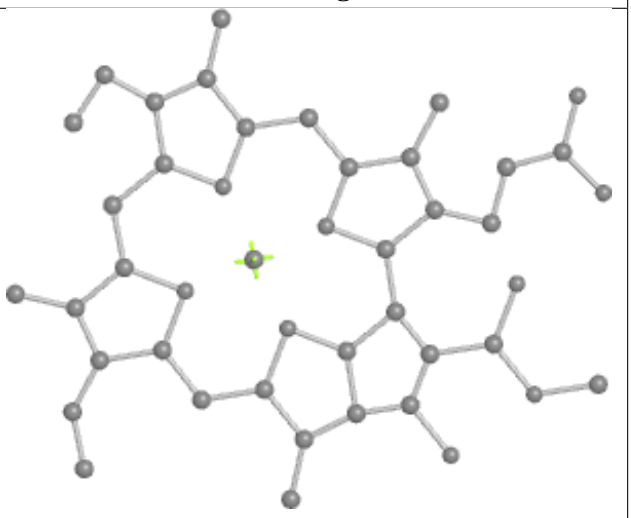
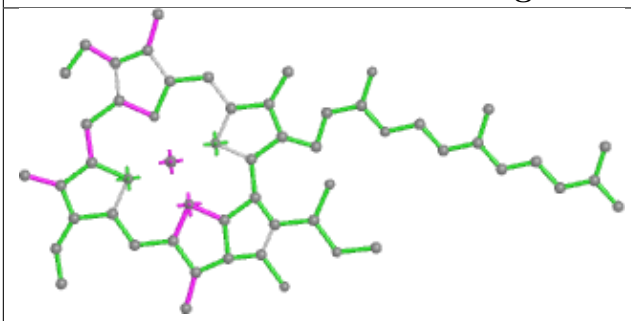


Rings

Ligand CLA A 1102



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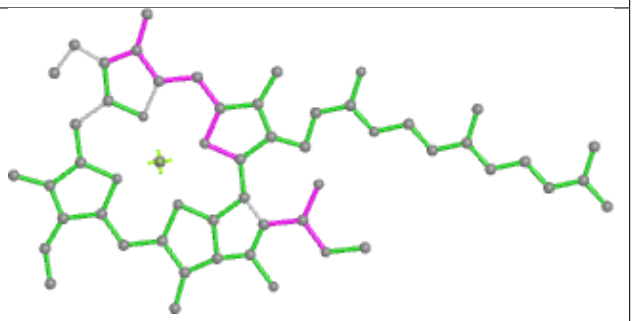

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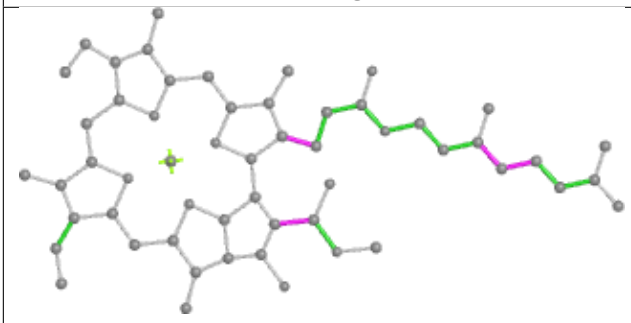

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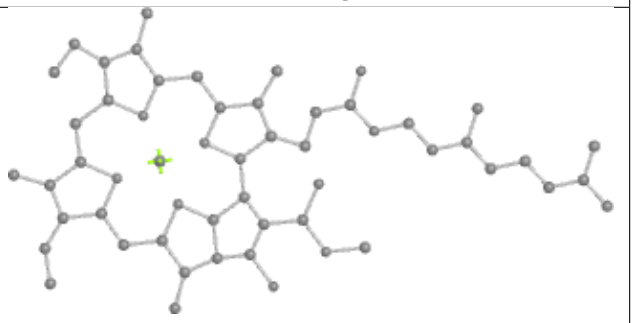

Rings

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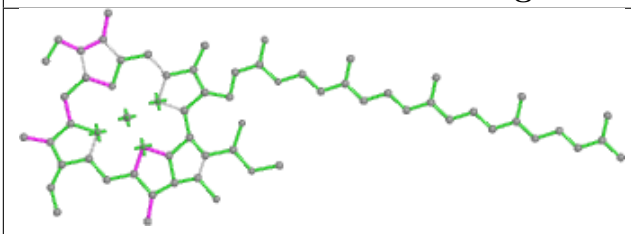

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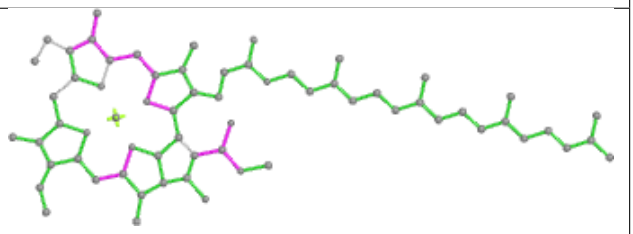

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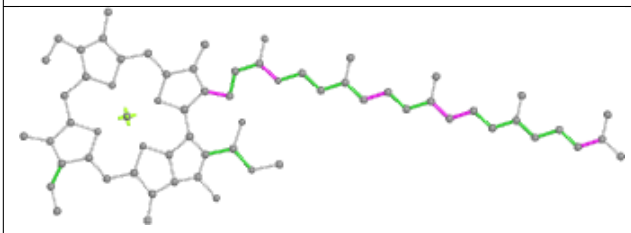

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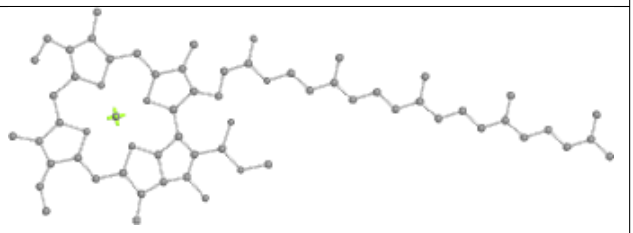

Rings

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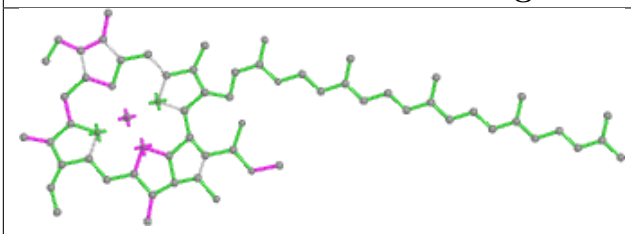

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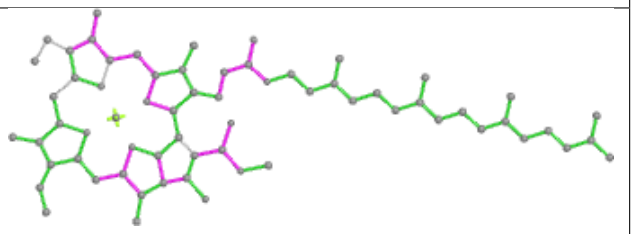

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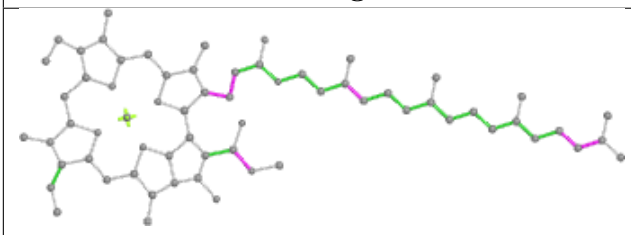

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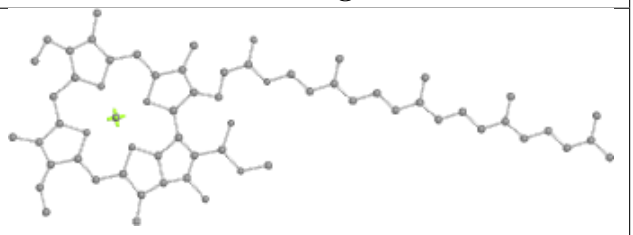

Rings

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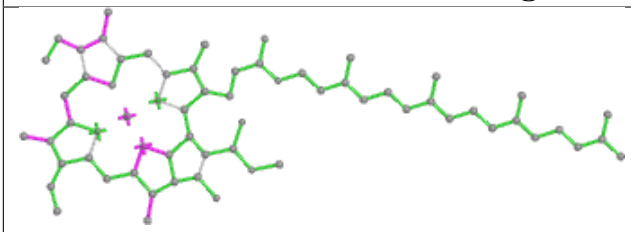

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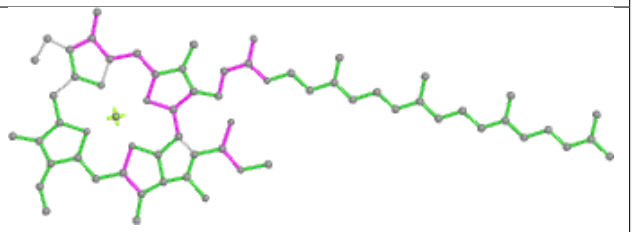

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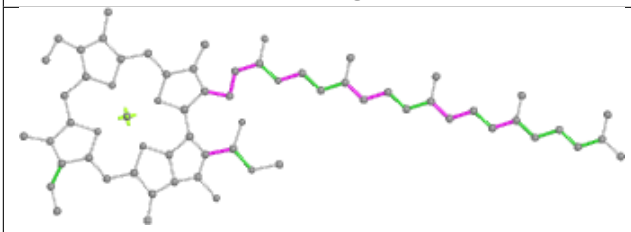

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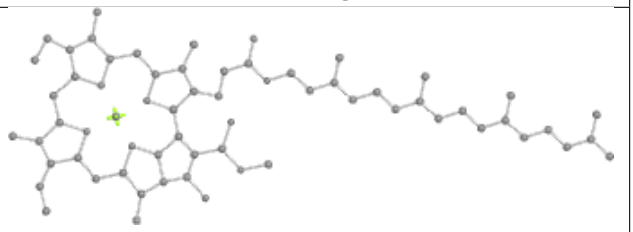
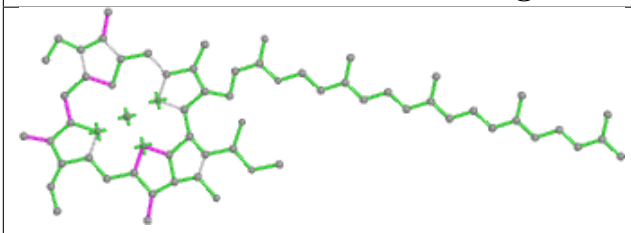


Rings

Ligand CLA B 1238



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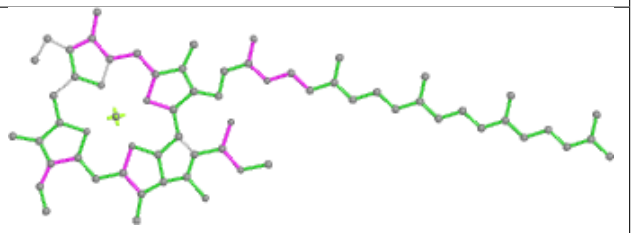

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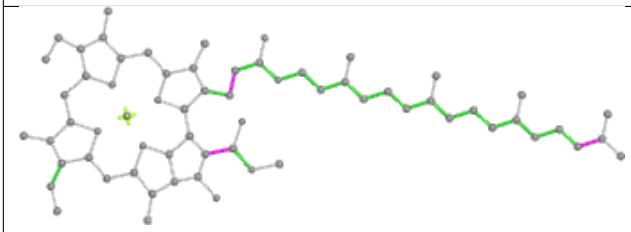

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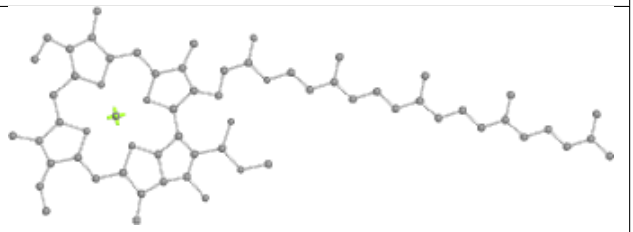

Rings

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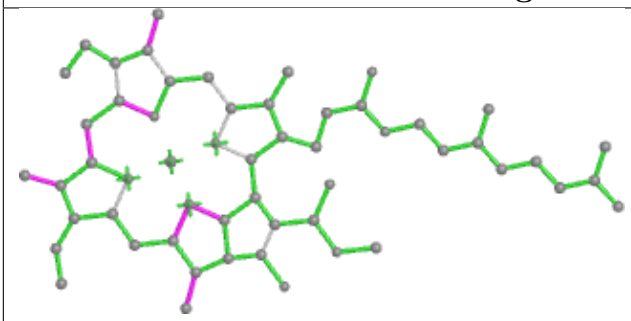

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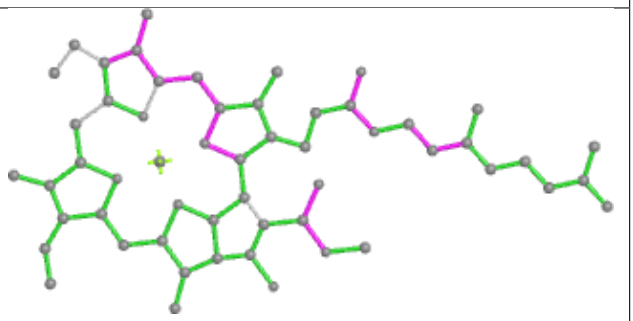

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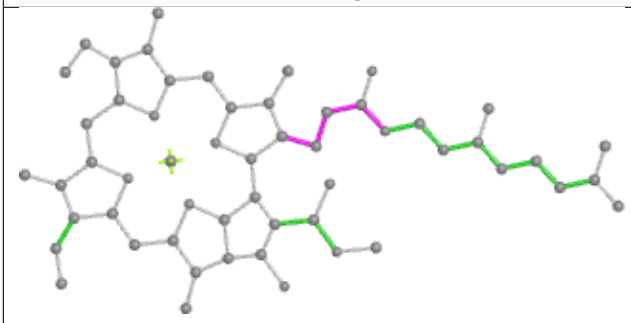

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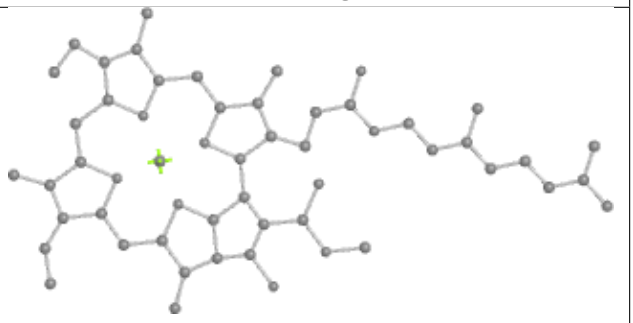

Rings

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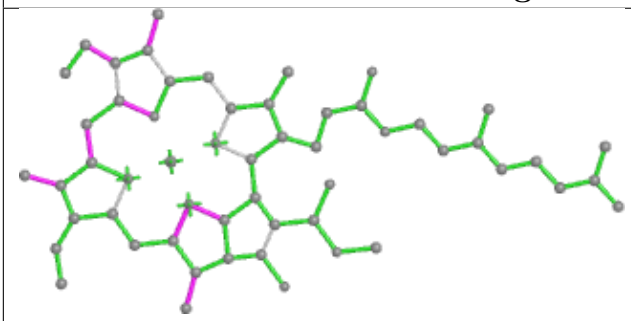

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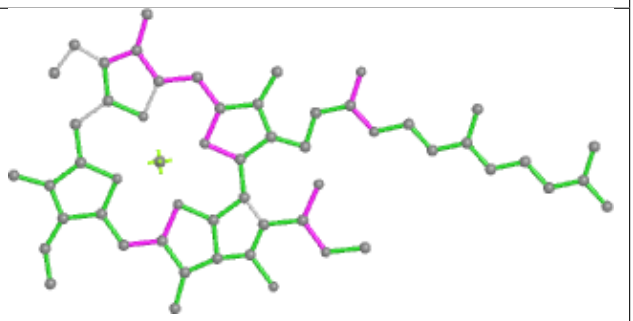

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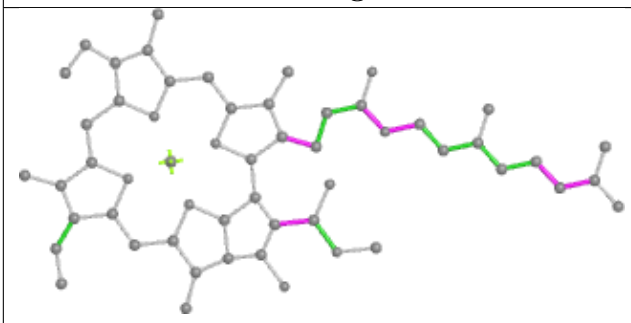

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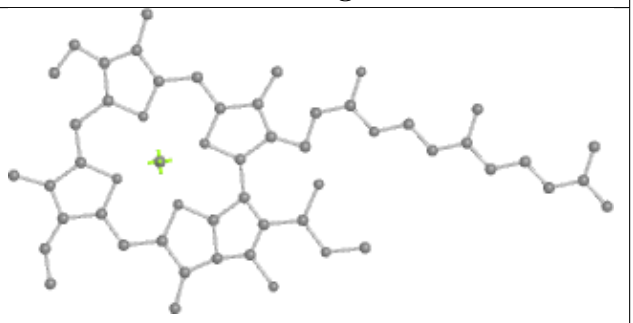

Rings

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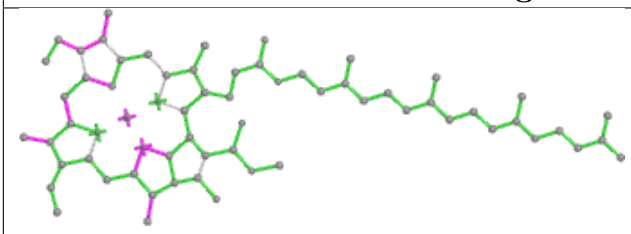

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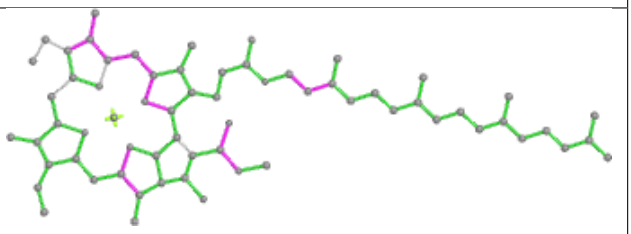

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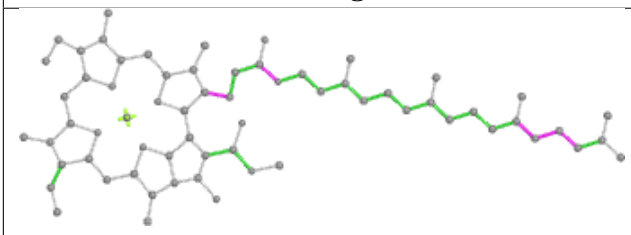

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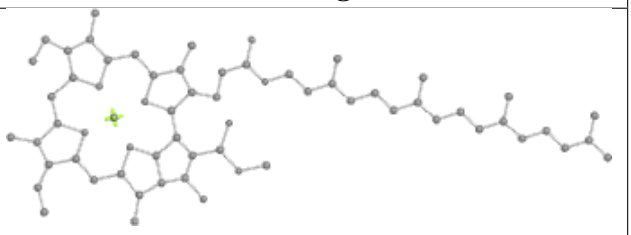
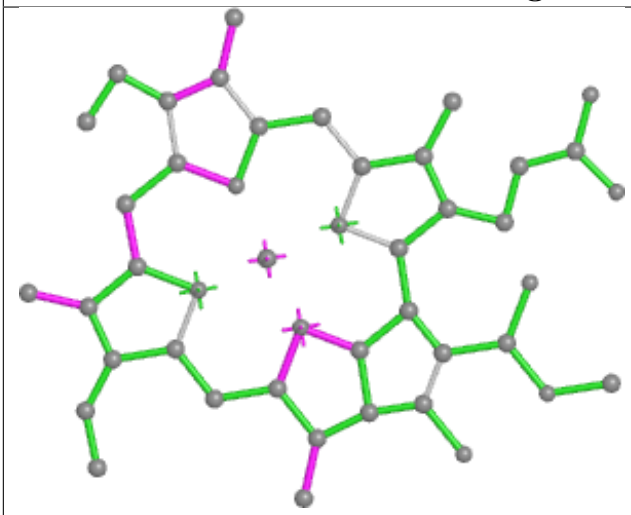


Rings

Ligand CLA Z 508



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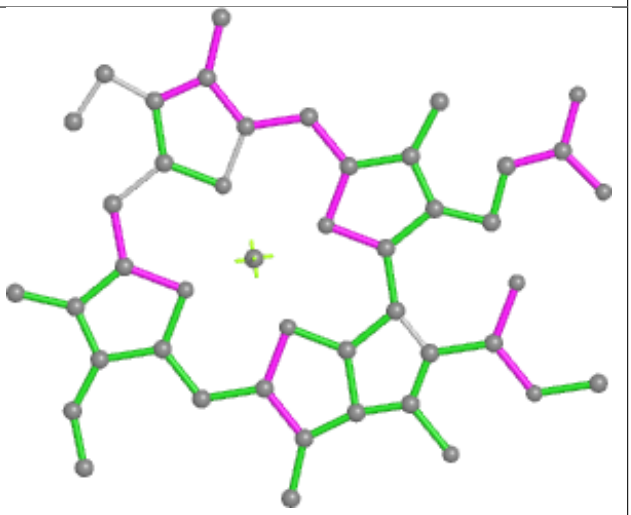

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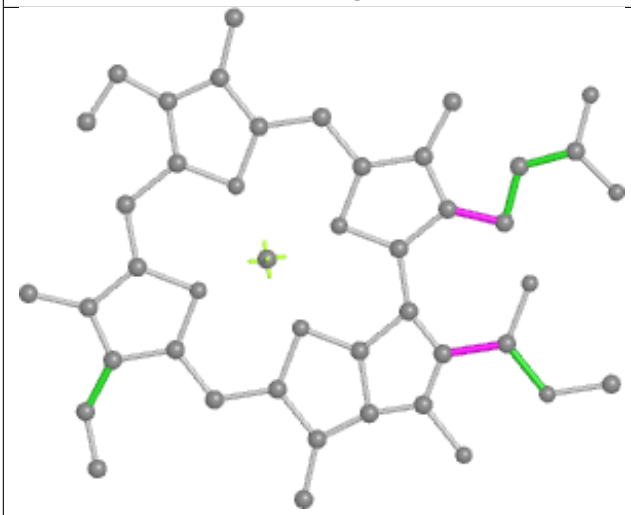

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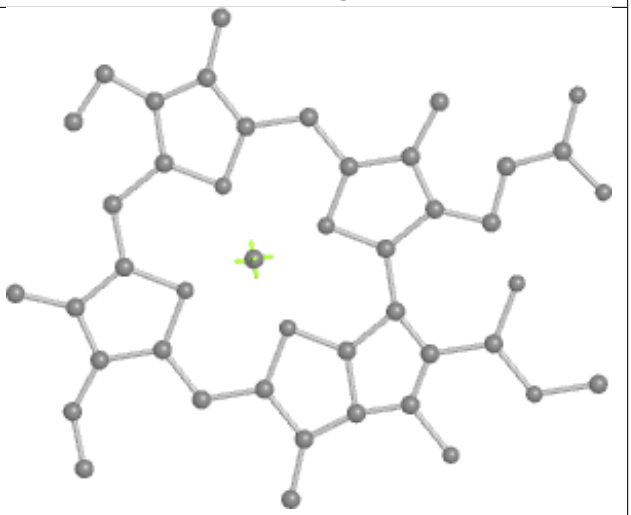

Rings

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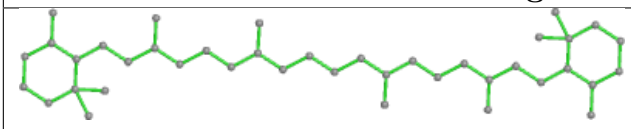
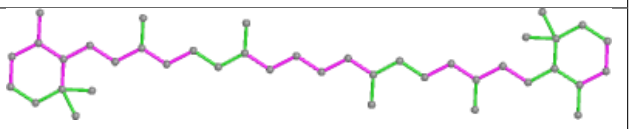
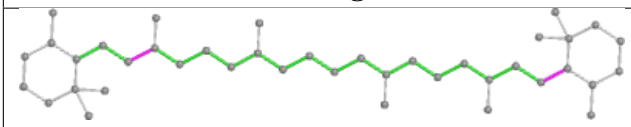
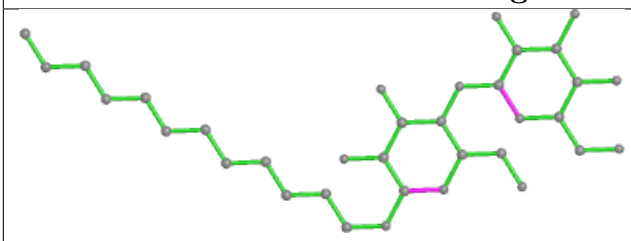
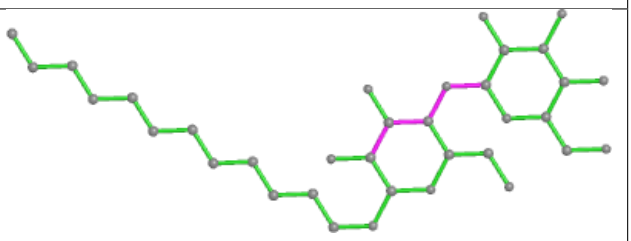
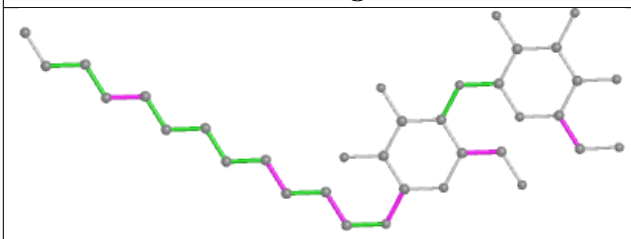
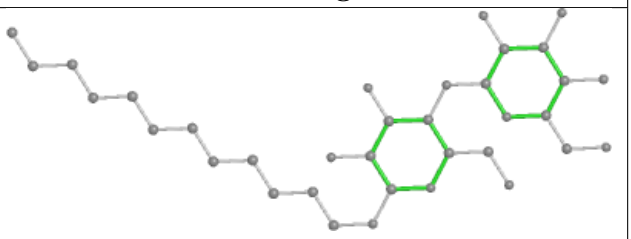
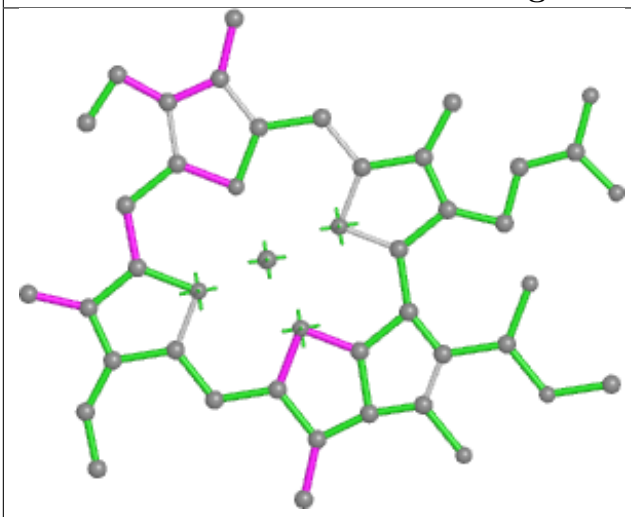
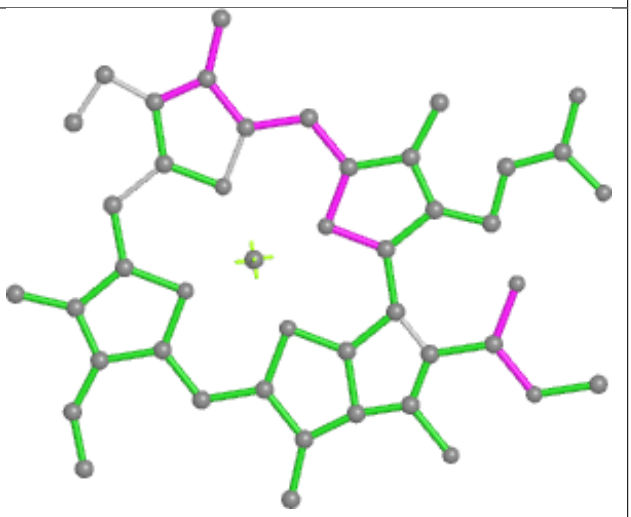
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LMU A 1848	
 Bond lengths	 Bond angles
 Torsions	 Rings

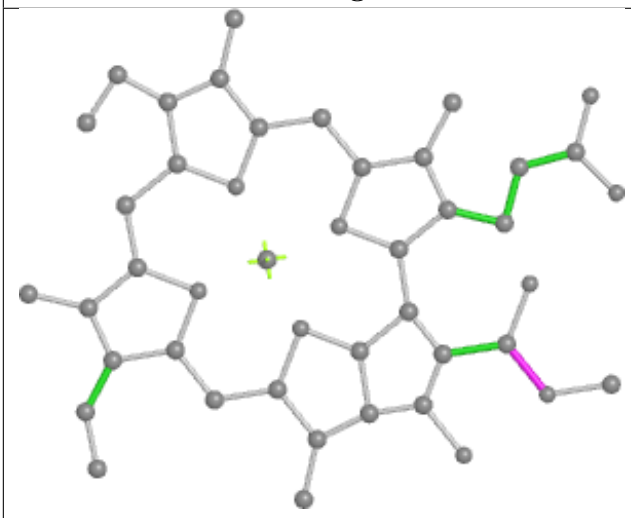
Ligand CLA 2 513



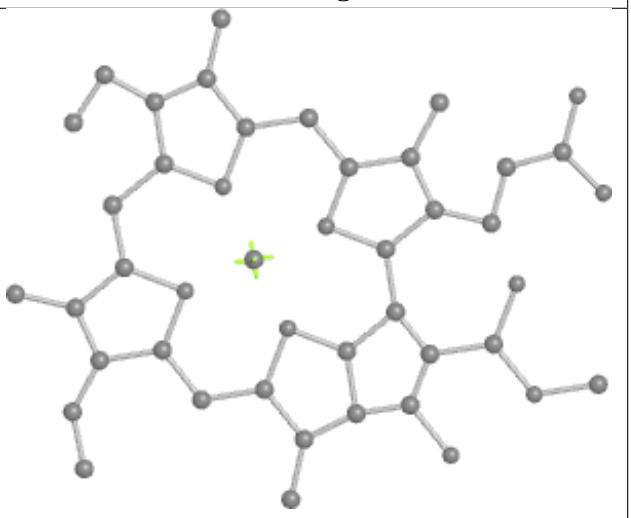
Bond lengths



Bond angles

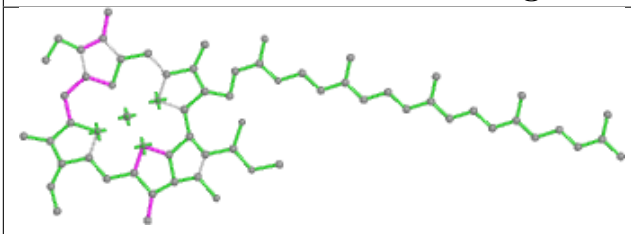


Torsions

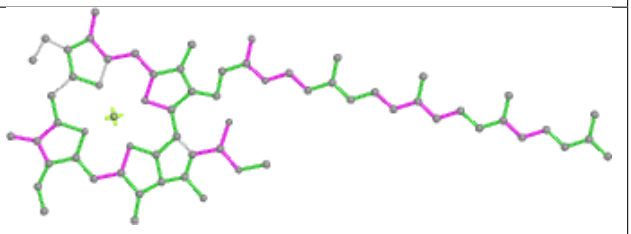


Rings

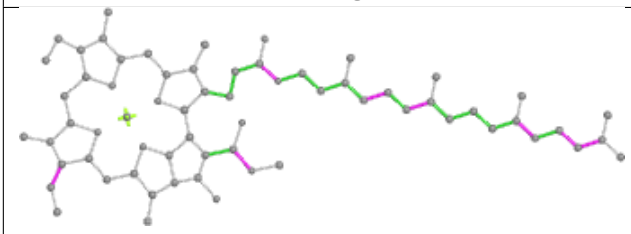
Ligand CLA f 1239



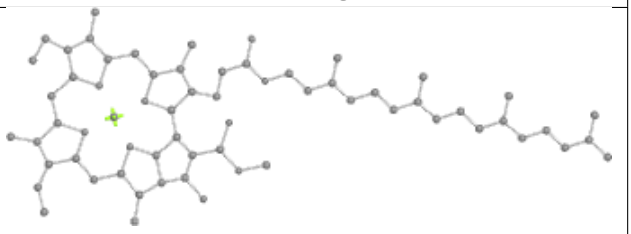
Bond lengths



Bond angles

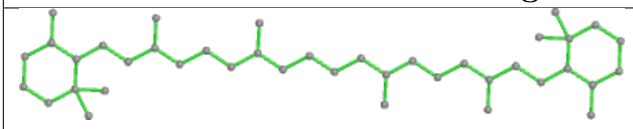


Torsions



Rings

Ligand BCR l 4012



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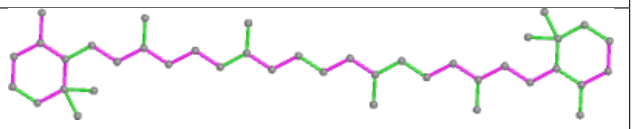
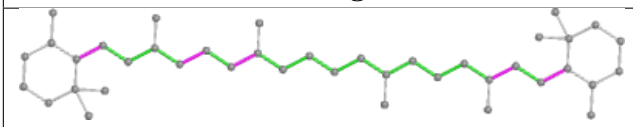
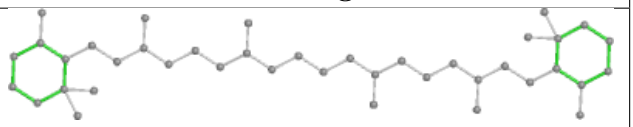


Bond angles

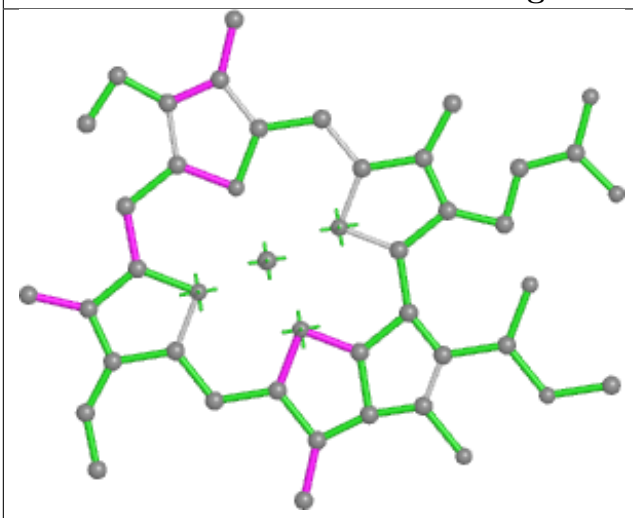


Torsions

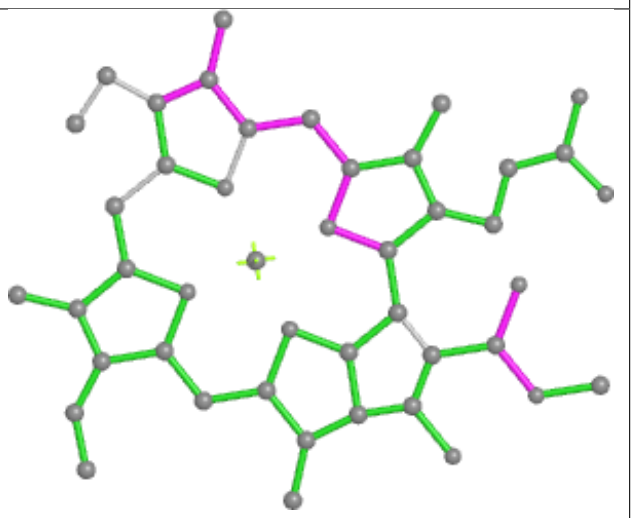


Rings

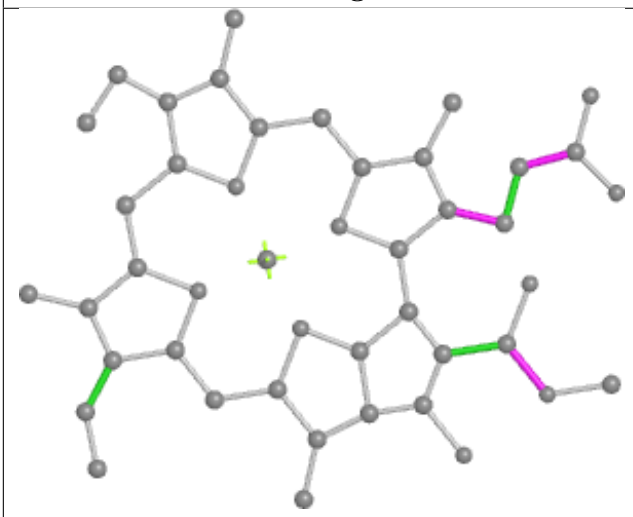
Ligand CLA u 513



Bond lengths



Bond angles



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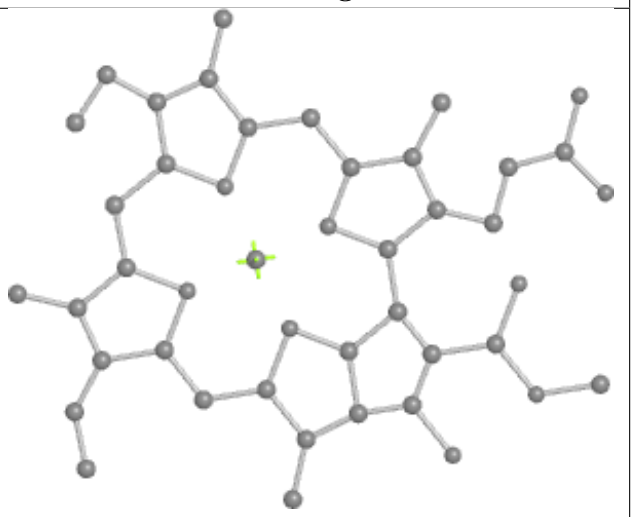
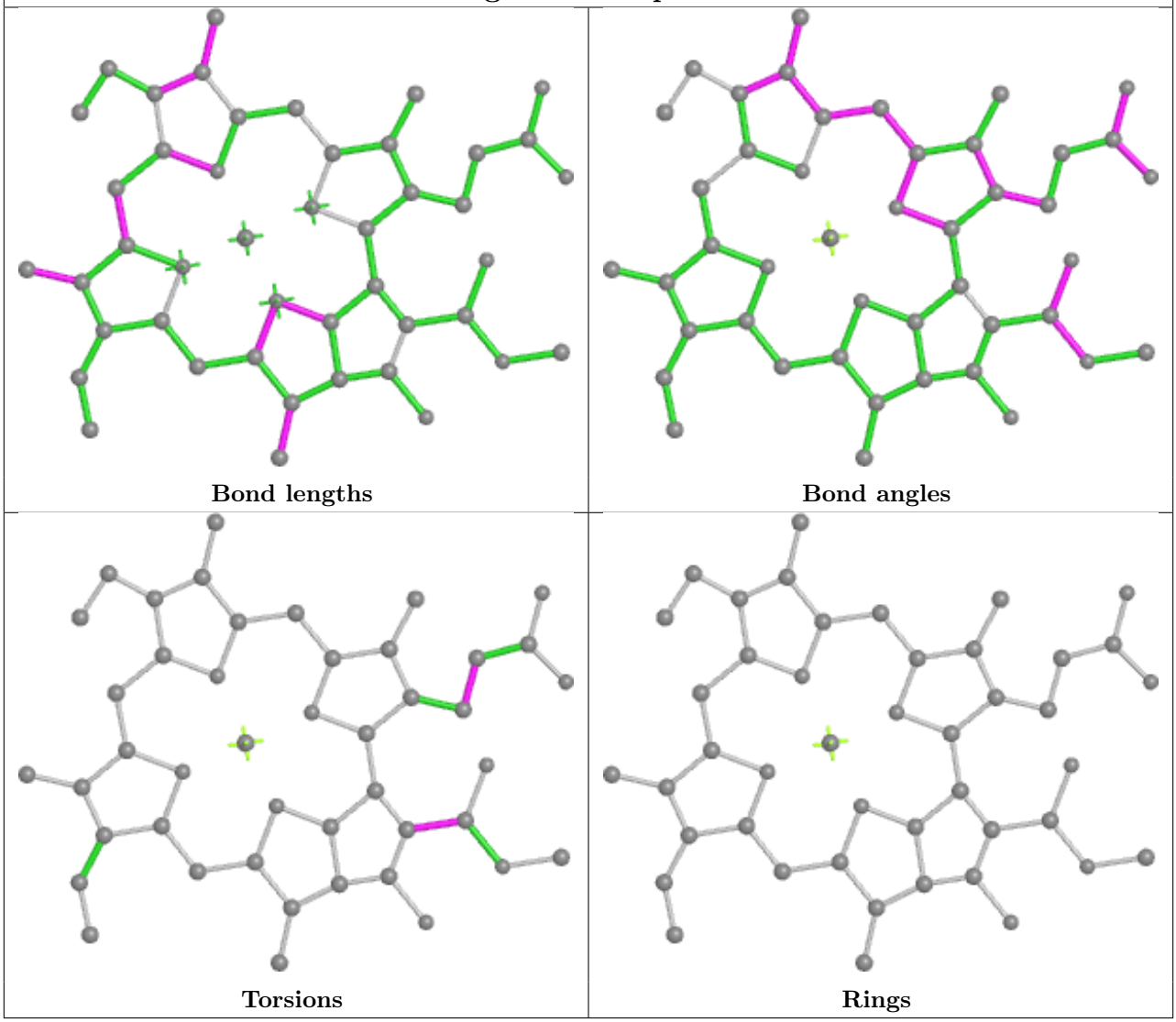
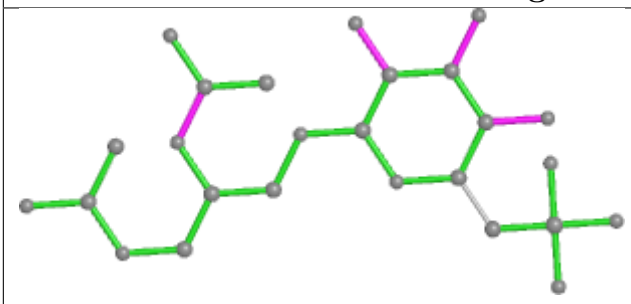
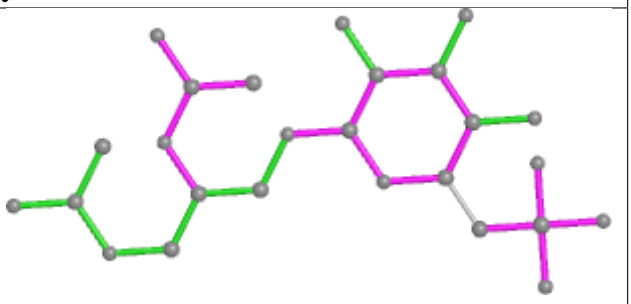
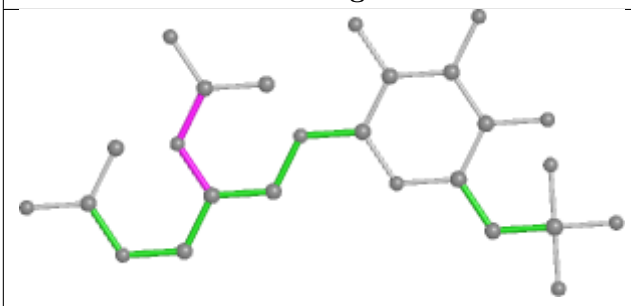
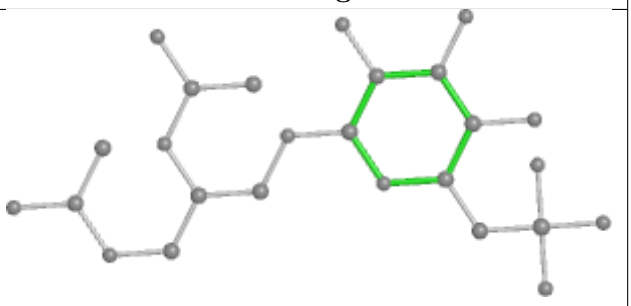
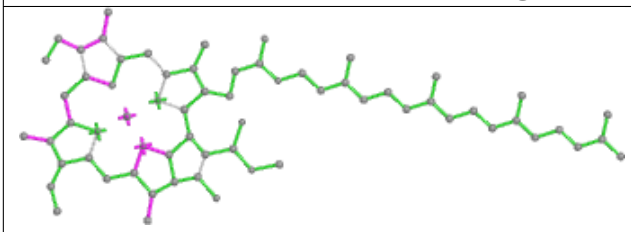
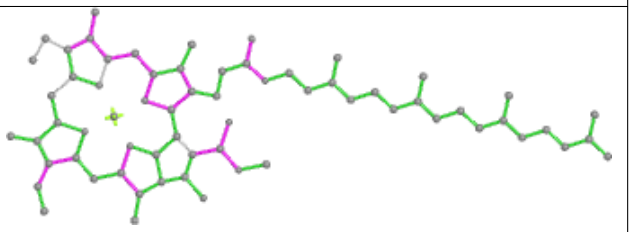
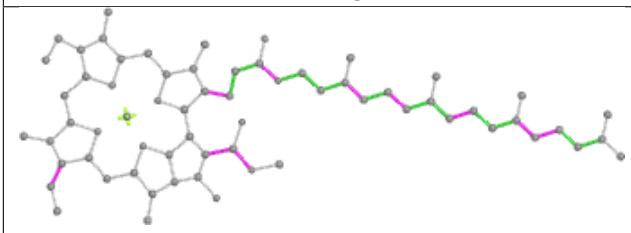
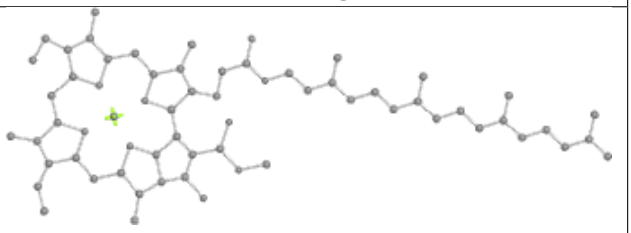


Rings

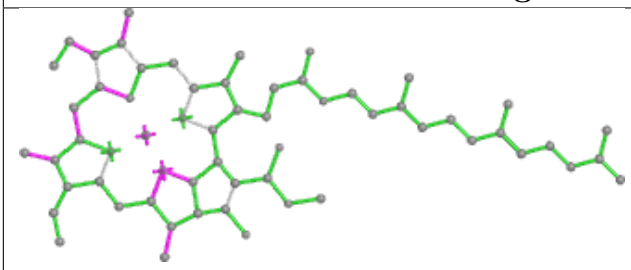
Ligand CLA q 502



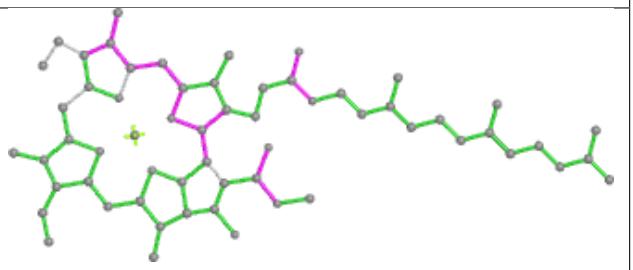
Ligand SQD 5 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1132	
 Bond lengths	 Bond angles
 Torsions	 Rings

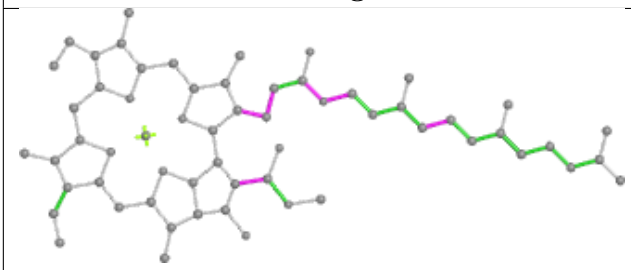
Ligand CLA G 1118



Bond lengths



Bond angles



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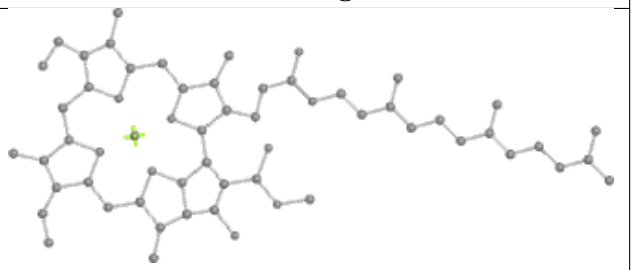
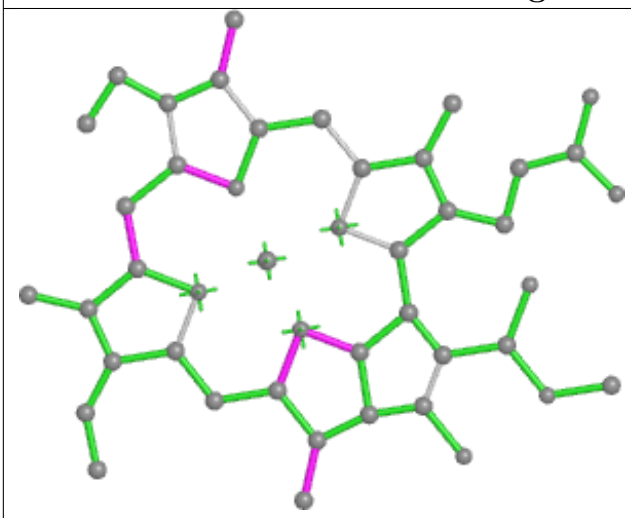


Rings

Ligand CLA 5 507



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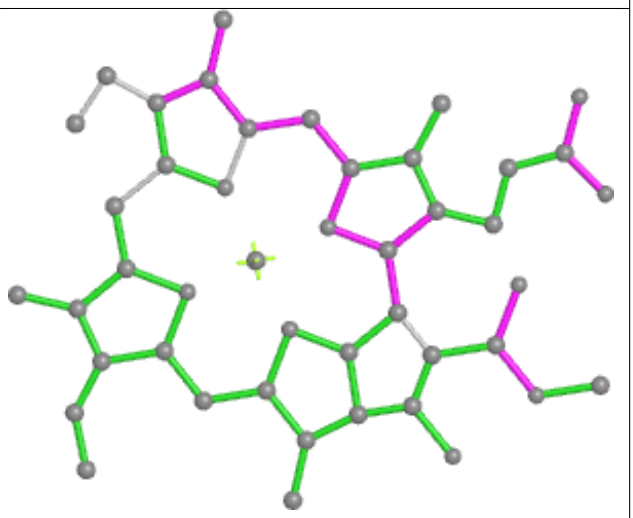
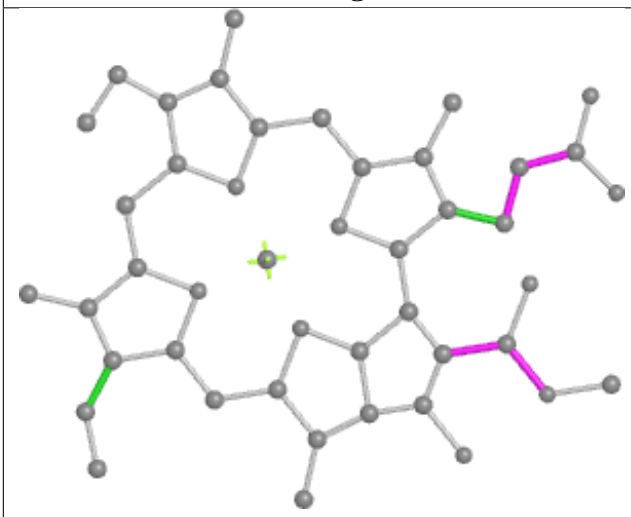
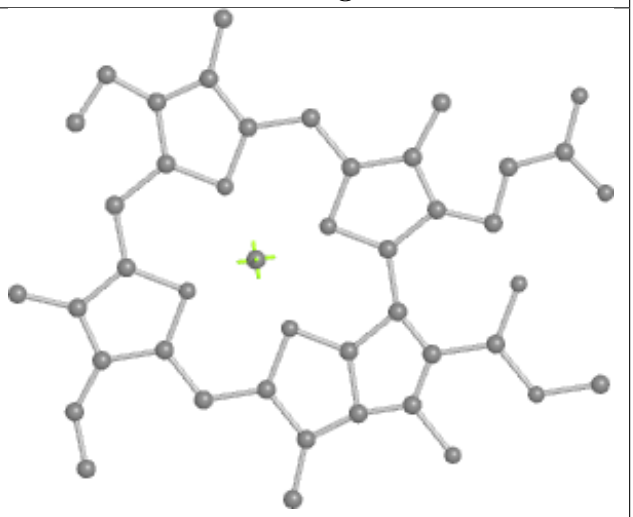


Bond angles

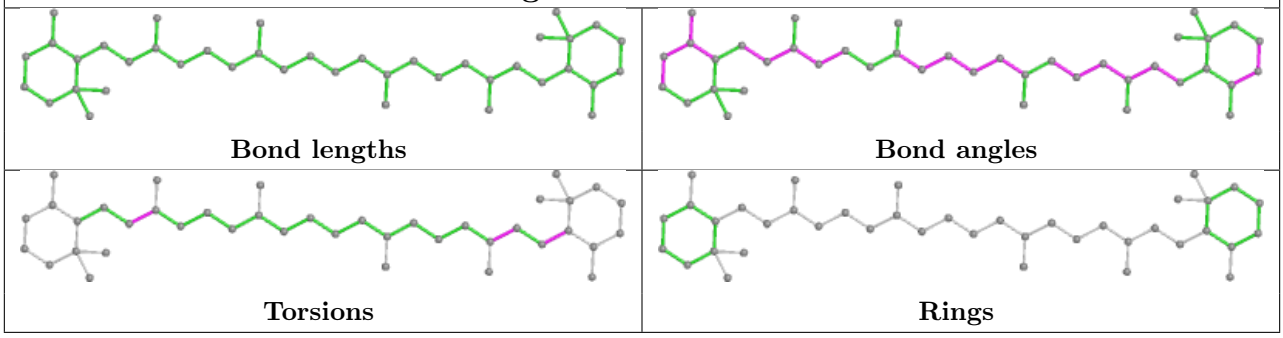


Torsions

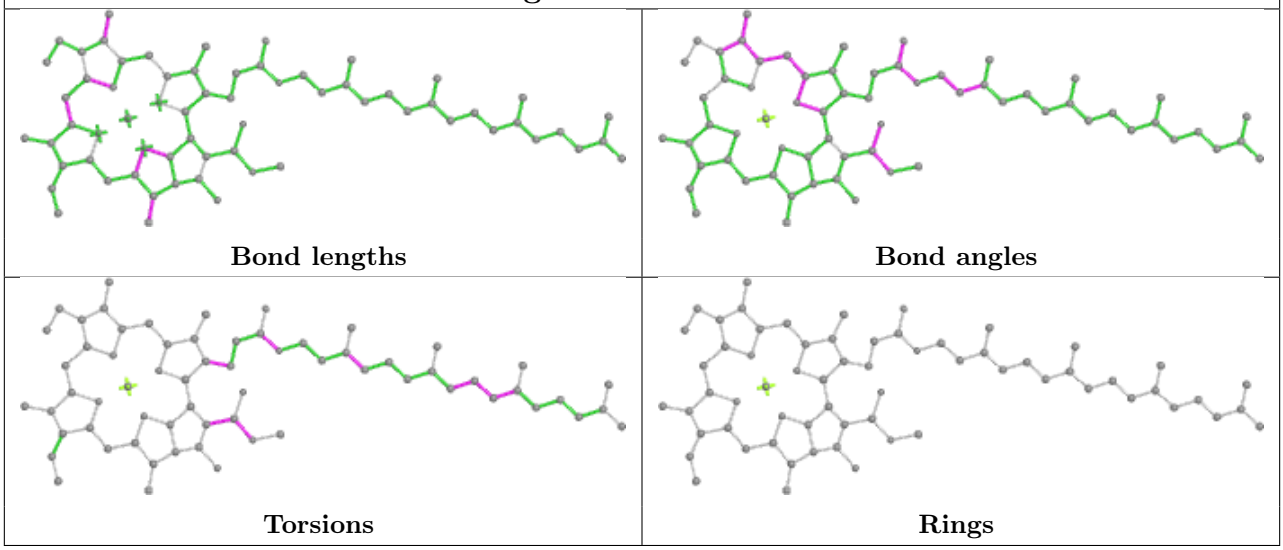


Rings

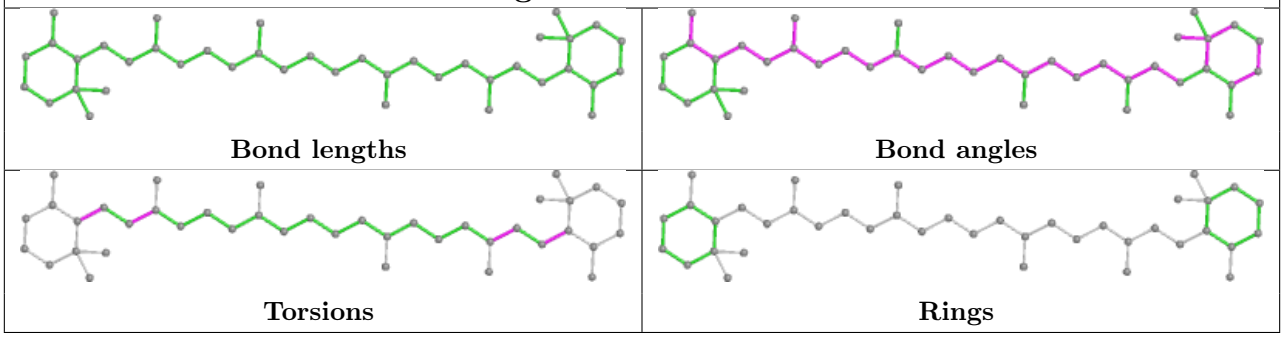
Ligand BCR f 4005



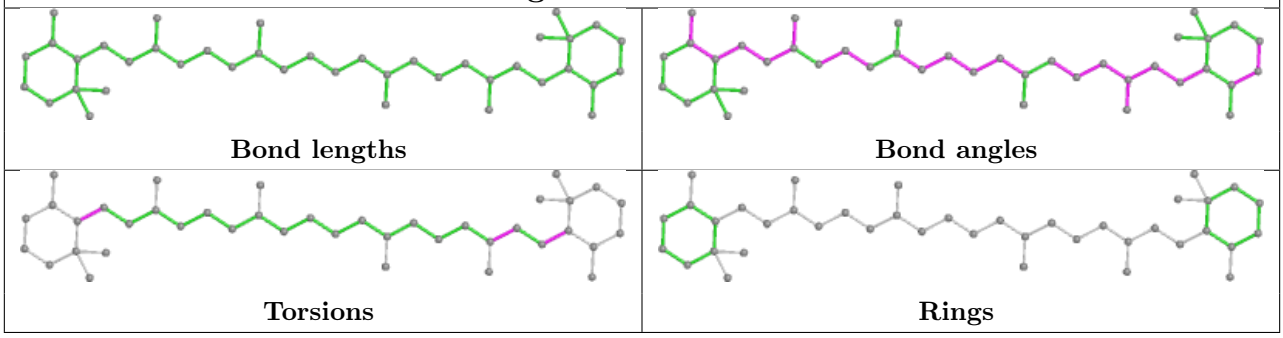
Ligand CLA f 1240

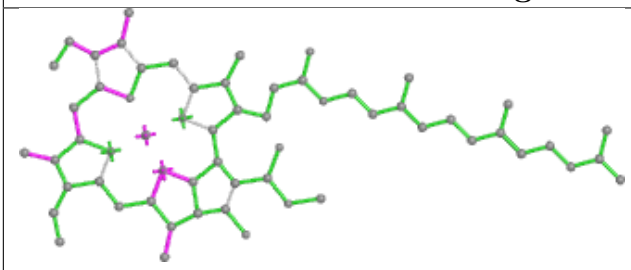
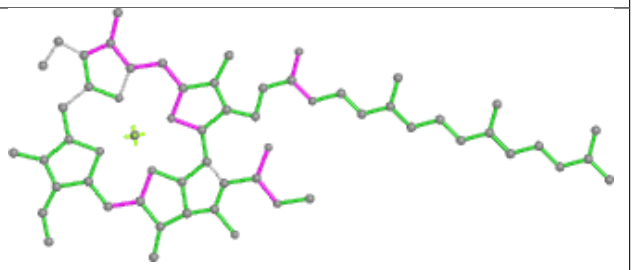
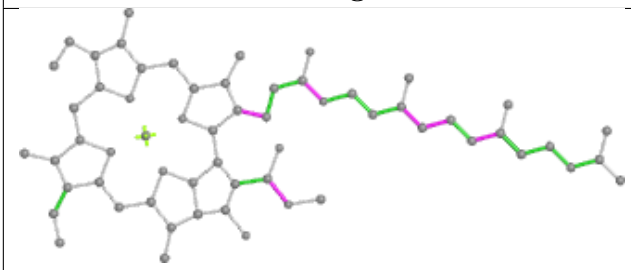
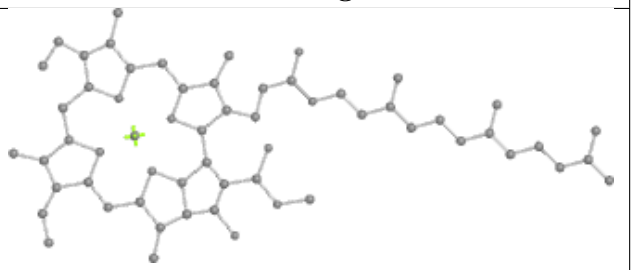


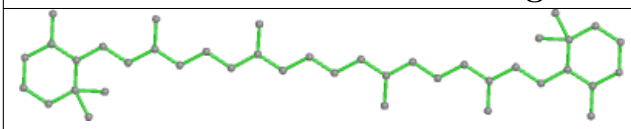
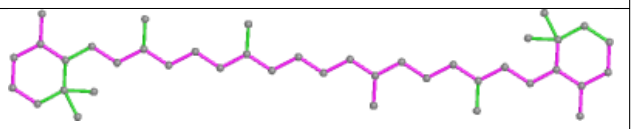
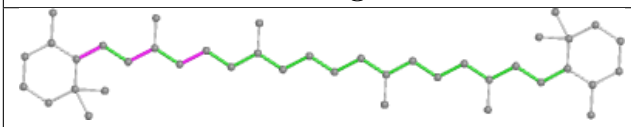
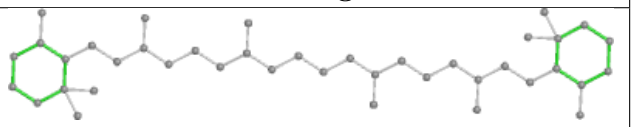
Ligand BCR B 4004



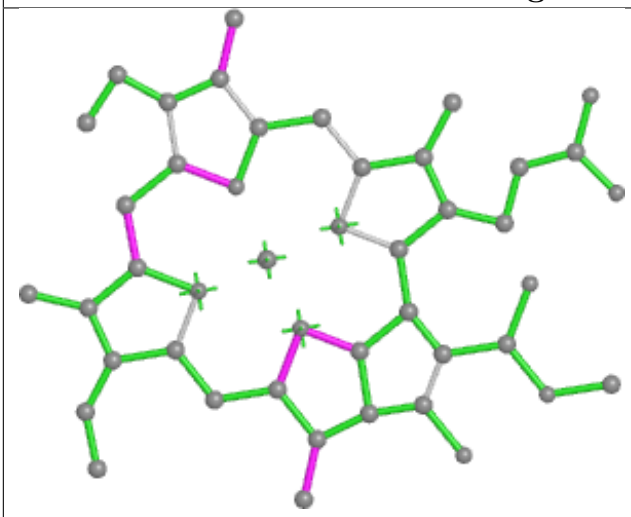
Ligand BCR 1 523



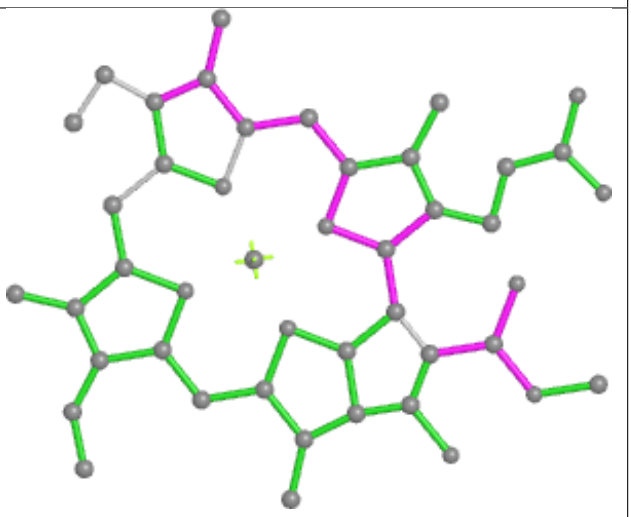
Ligand CLA H 1227	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR v 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

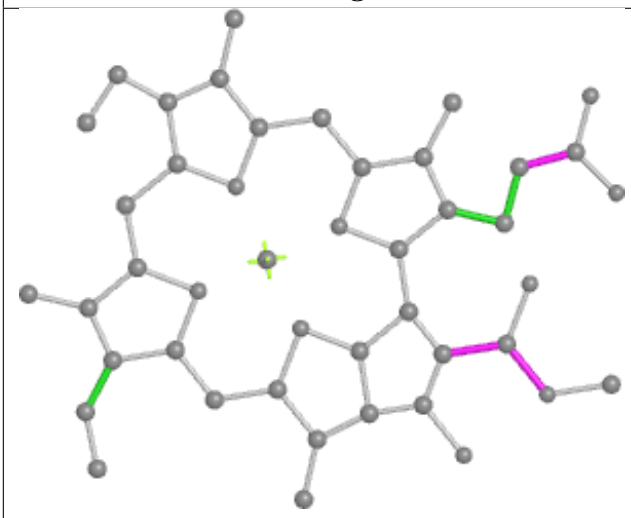
Ligand CLA b 507



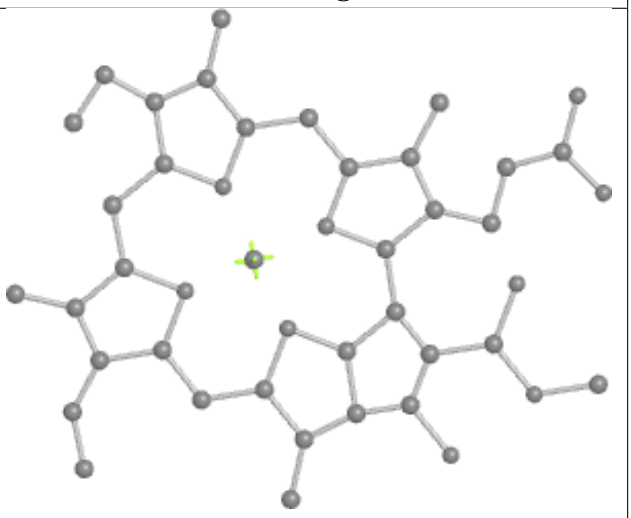
Bond lengths



Bond angles

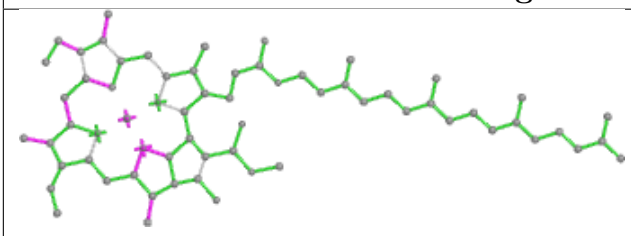


Torsions

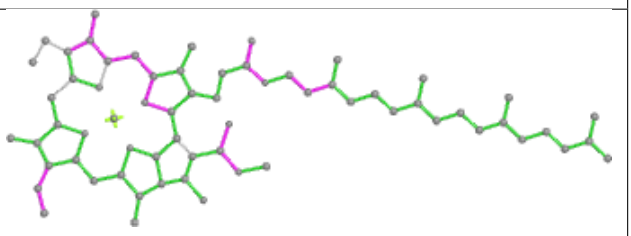


Rings

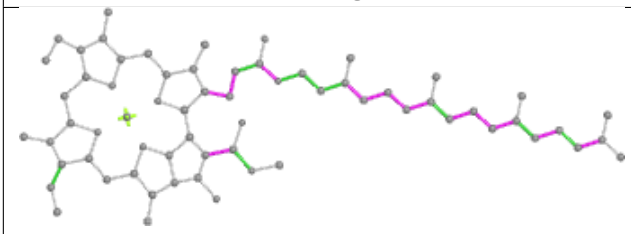
Ligand CLA B 1210



Bond lengths



Bond angles



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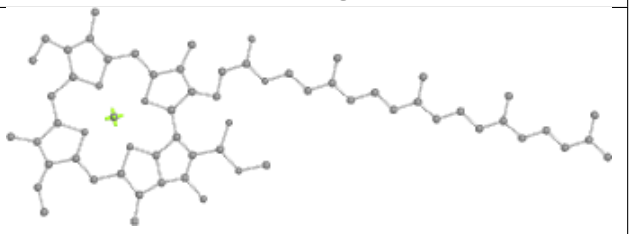
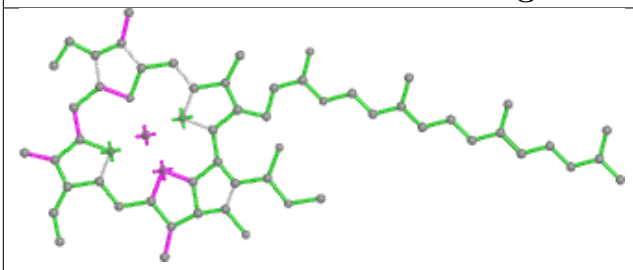
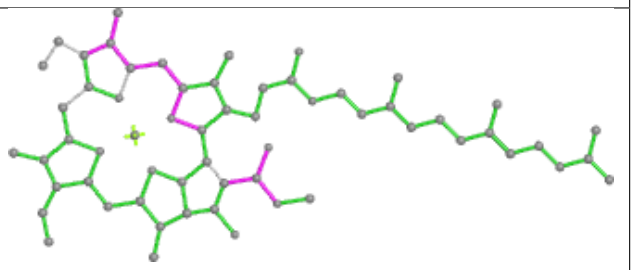


Rings

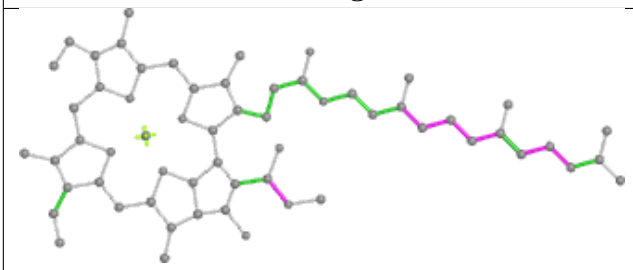
Ligand CLA L 1503



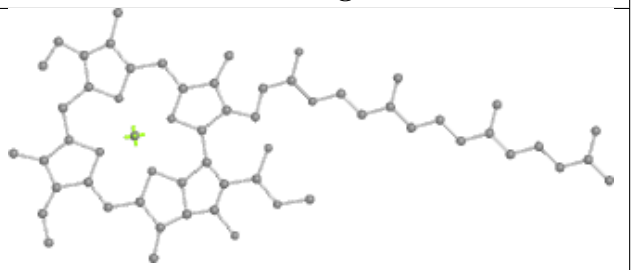
Bond lengths



Bond angles

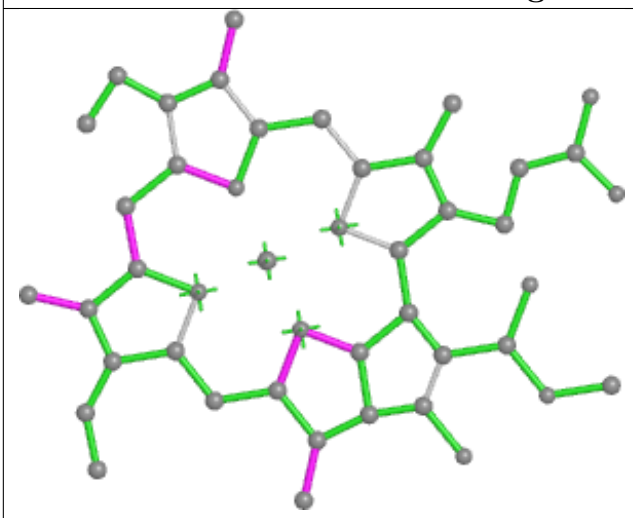


Torsions

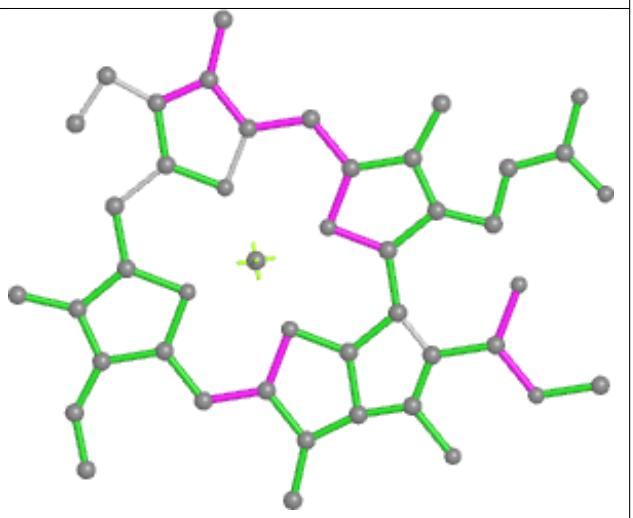


Rings

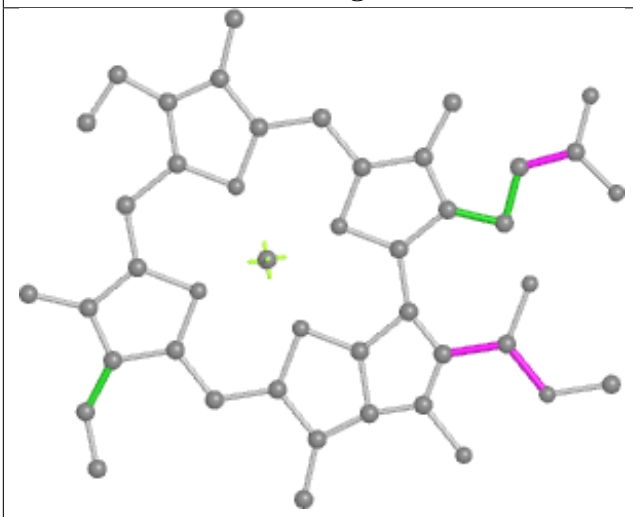
Ligand CLA u 510



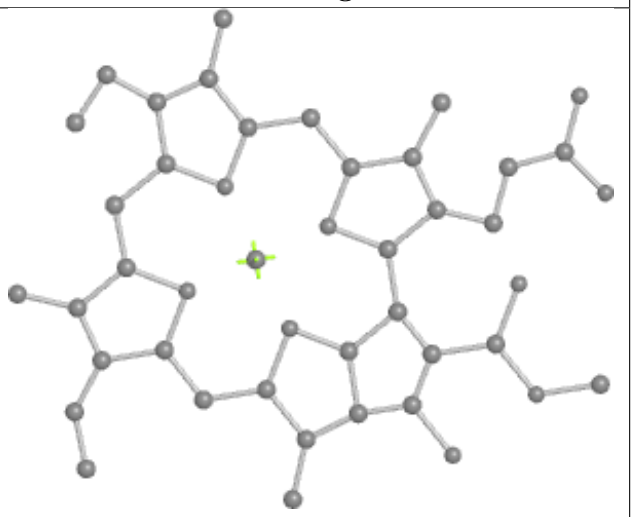
Bond lengths



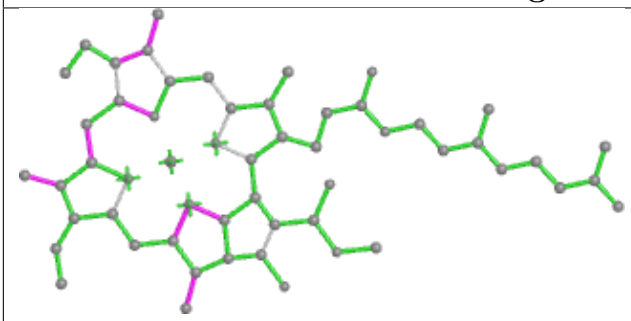
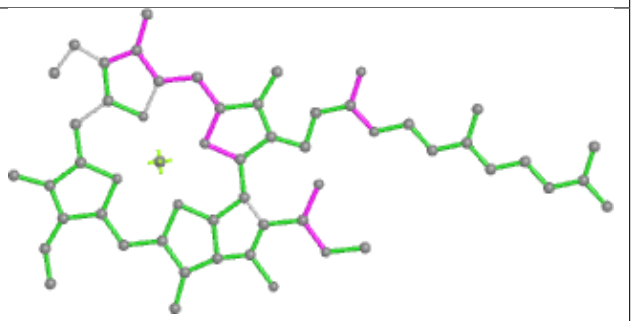
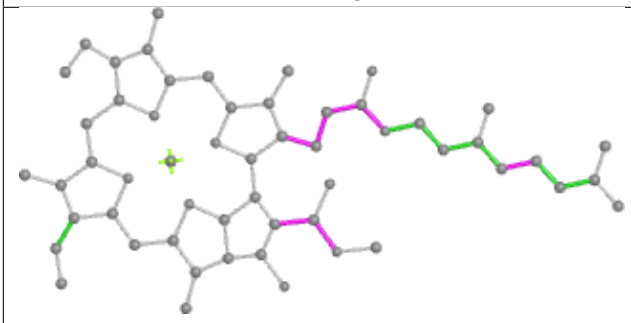
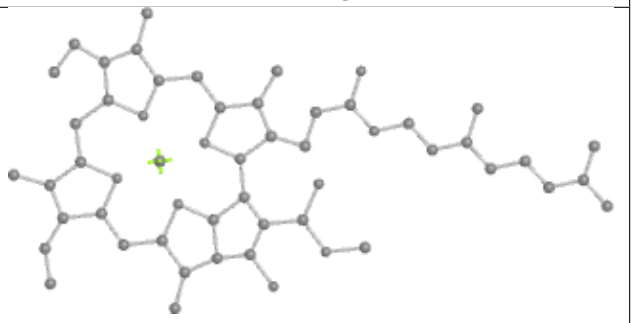
Bond angles

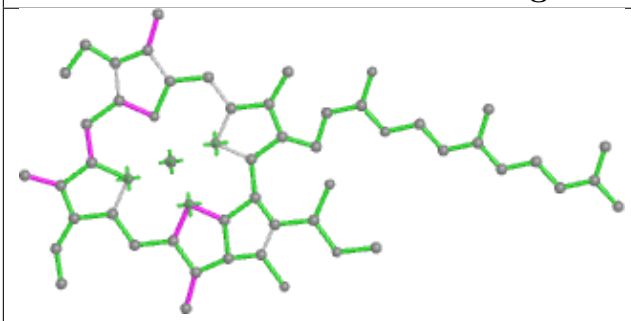
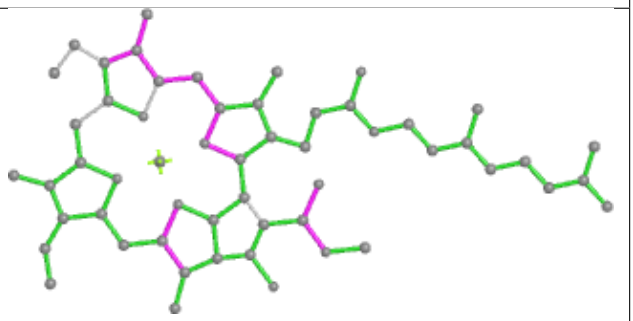
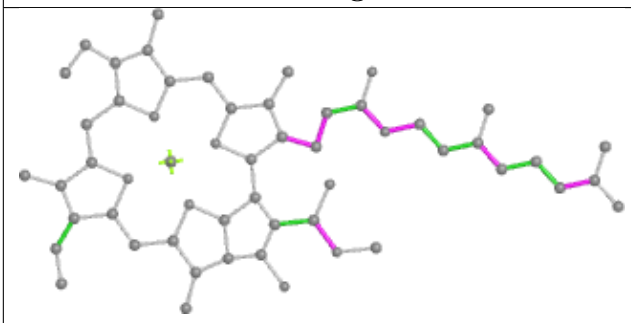
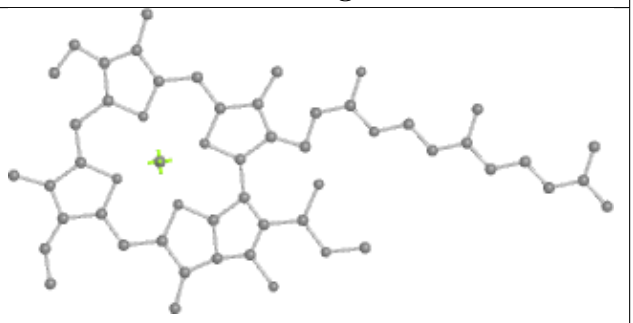


Torsions

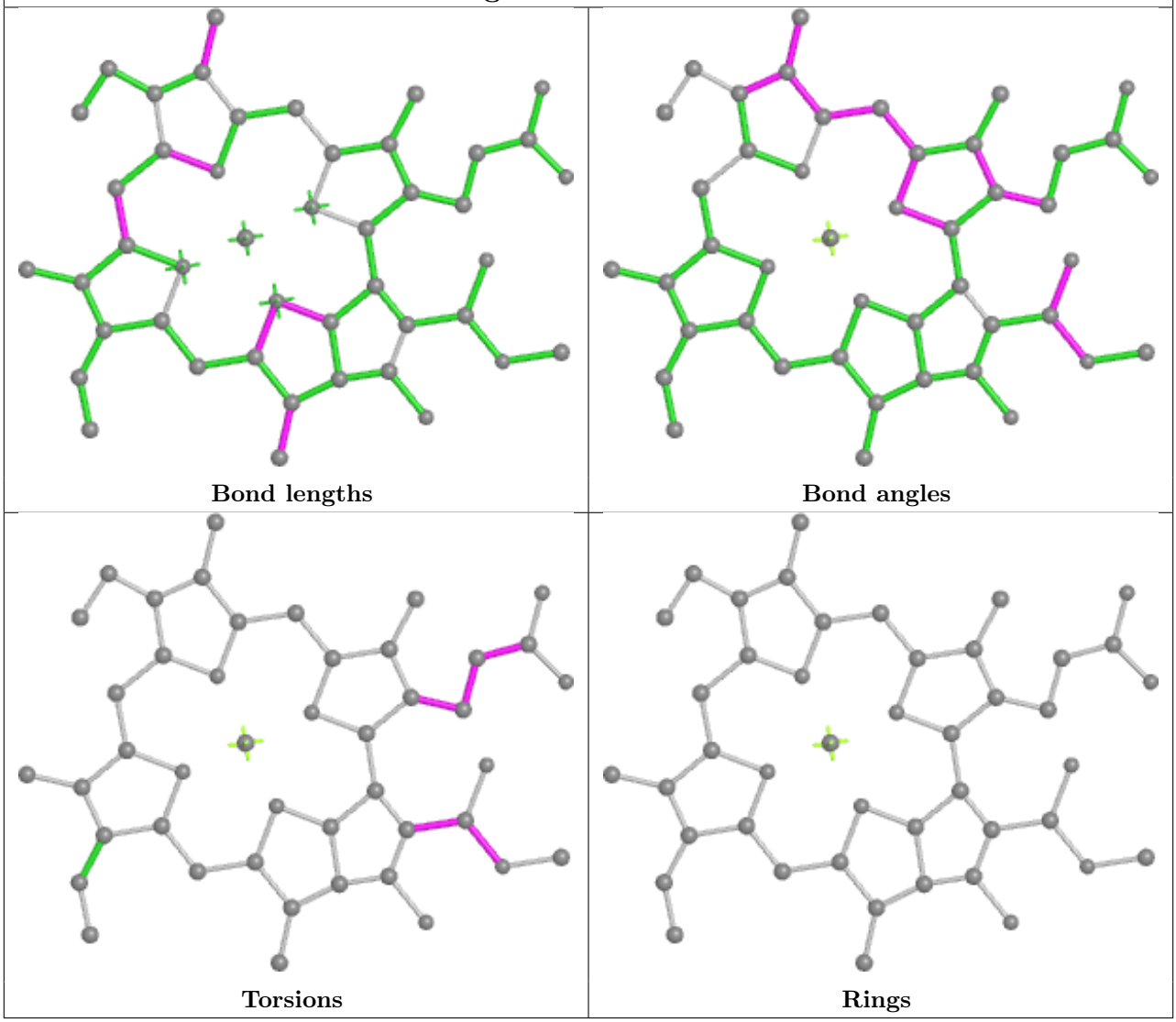


Rings

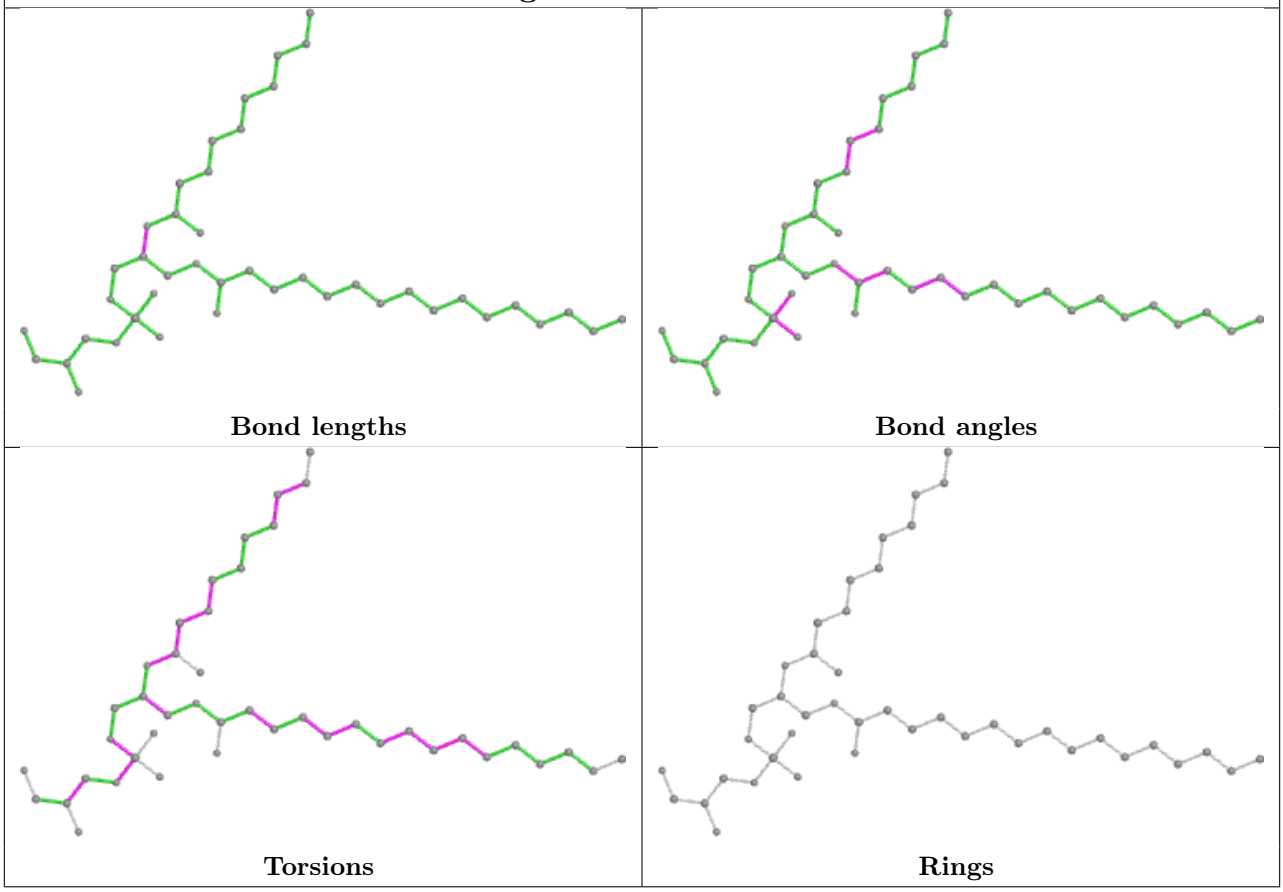
Ligand CLA a 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

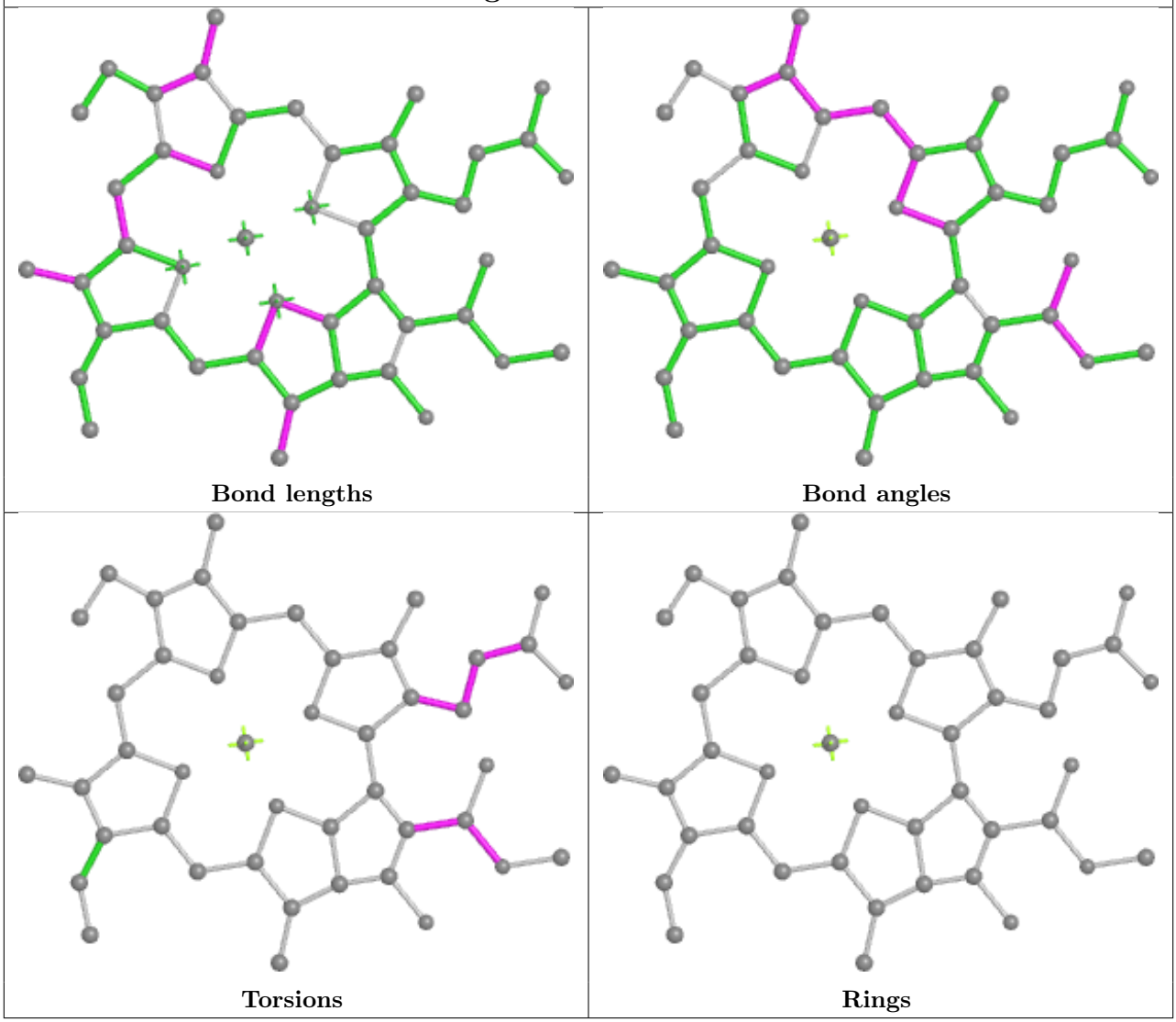
Ligand CLA d 516



Ligand LHG e 5002



Ligand CLA u 517



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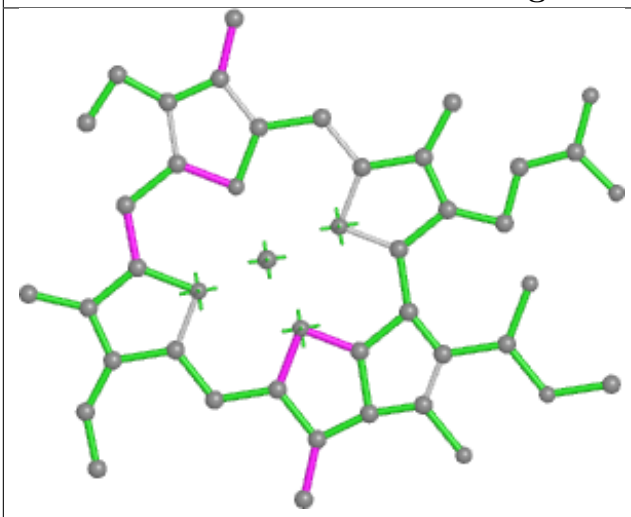
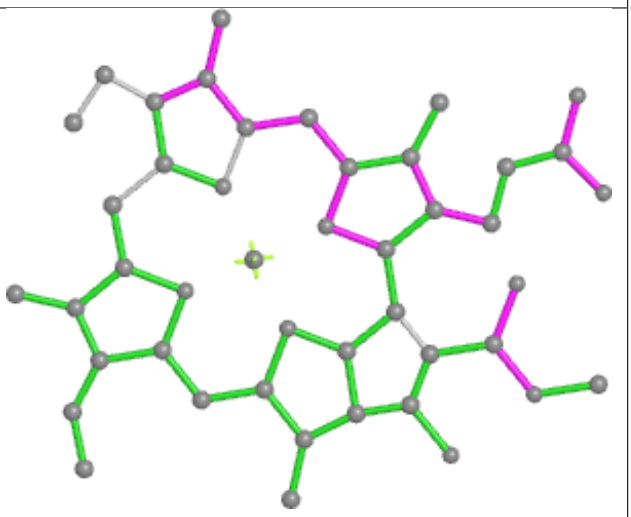
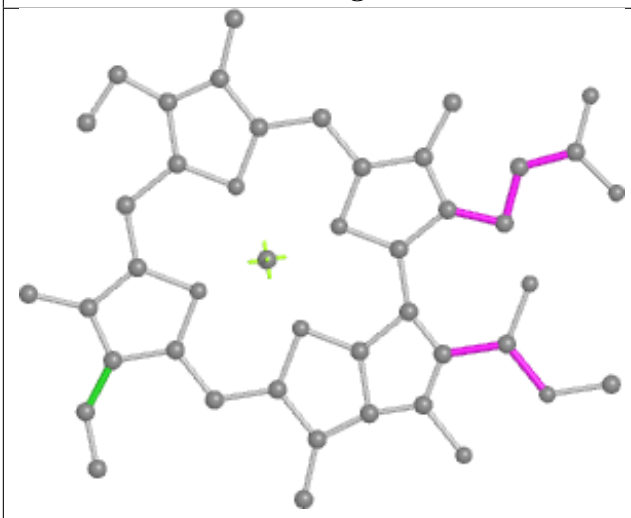


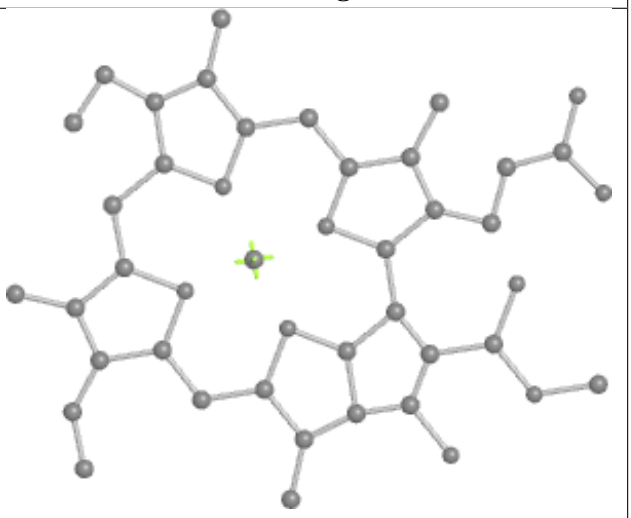
Bond lengths



Bond angles

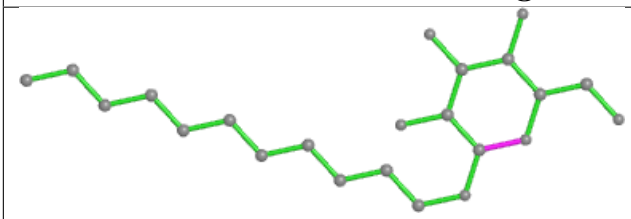


Torsions

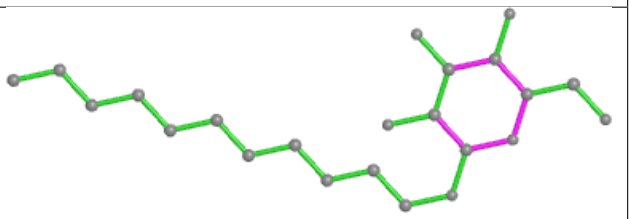


Rings

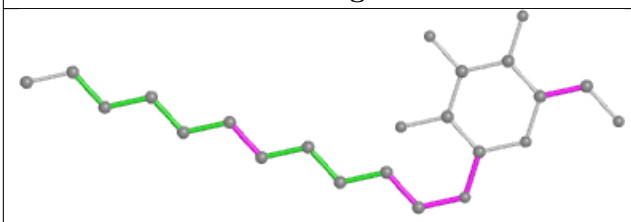
Ligand LMU e 1849



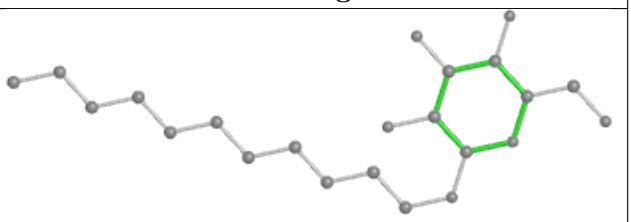
Bond lengths



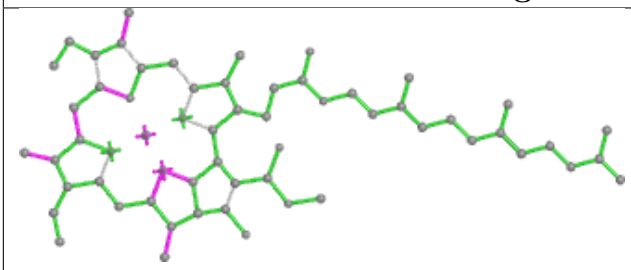
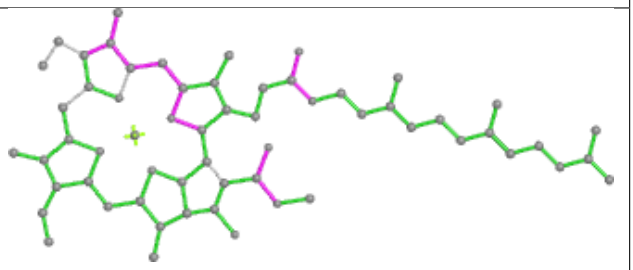
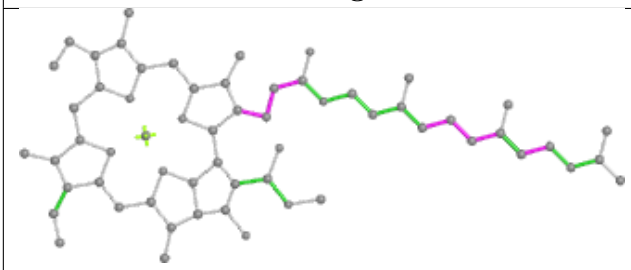
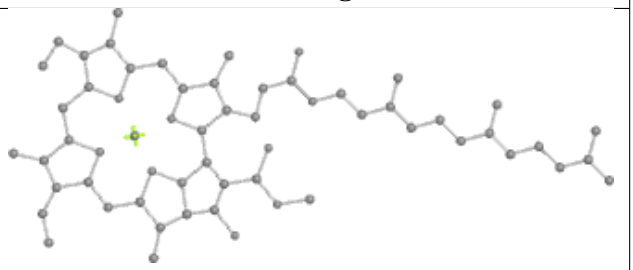
Bond angles



Torsions



Rings

Ligand CLA G 1116	
 Bond lengths	 Bond angles
 Torsions	 Rings

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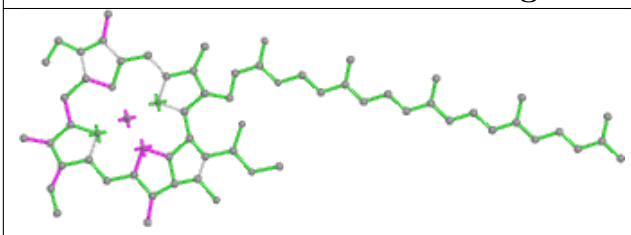
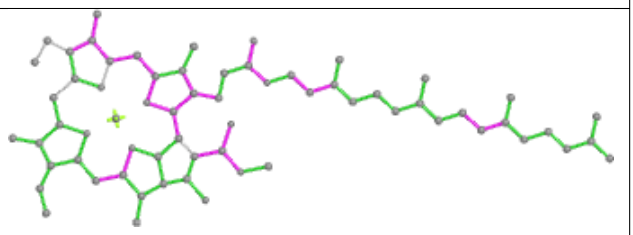
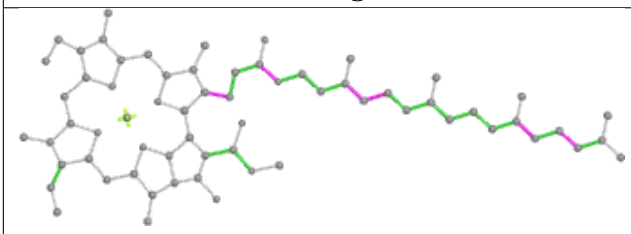
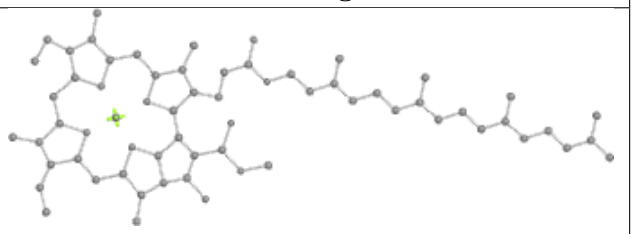
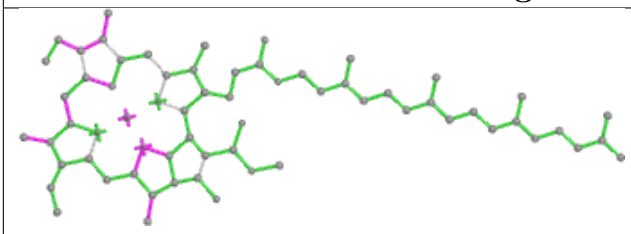
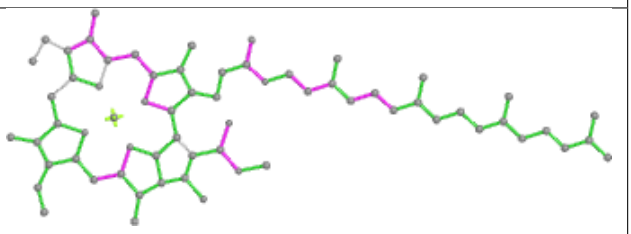
 Bond lengths	 Bond angles
 Torsions	 Rings

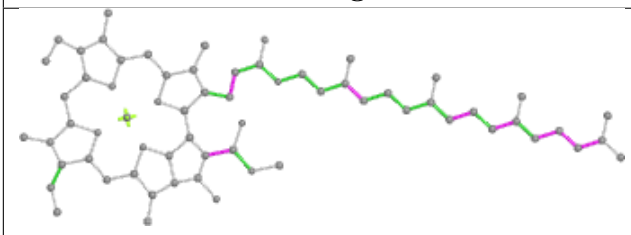
Ligand CLA A 1117



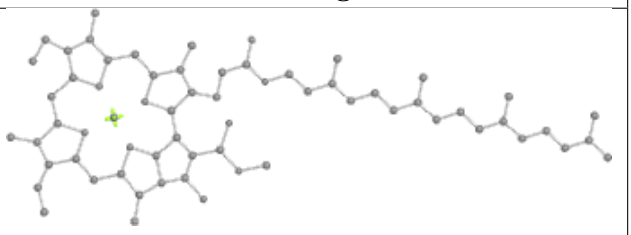
Bond lengths



Bond angles

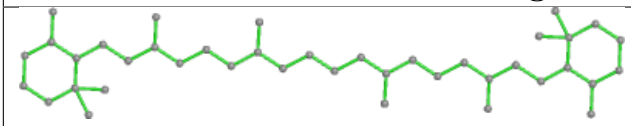


Torsions

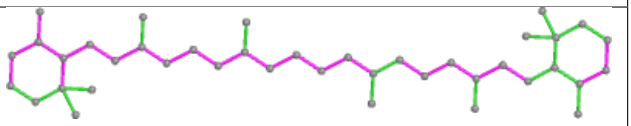


Rings

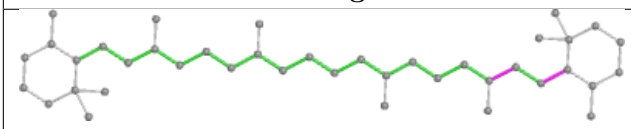
Ligand BCR s 523



Bond lengths



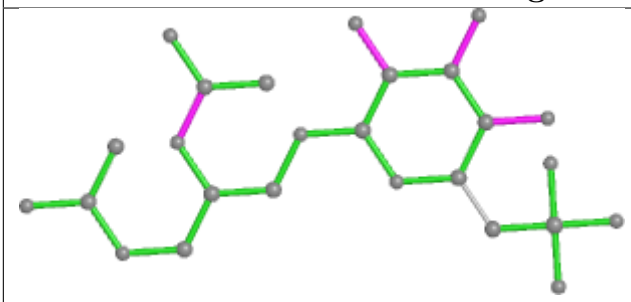
Bond angles



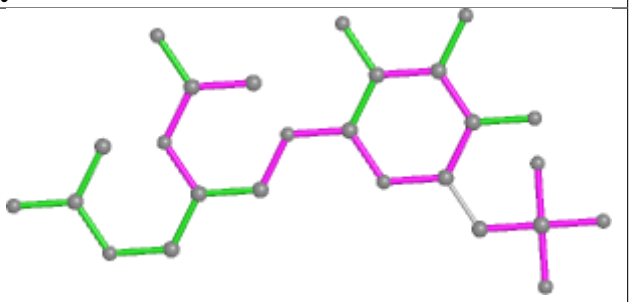
Torsions

Rings

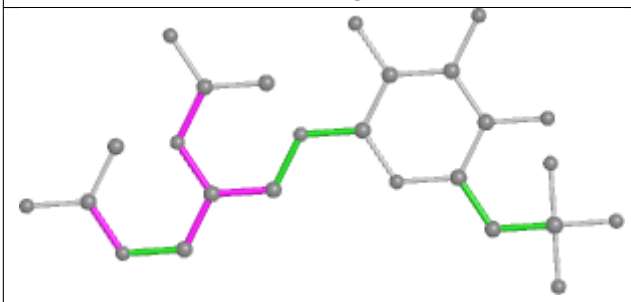
Ligand SQD v 822



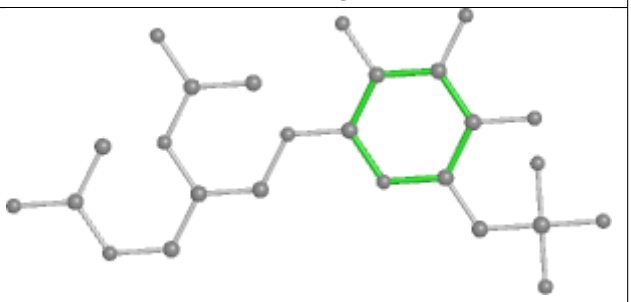
Bond lengths



Bond angles

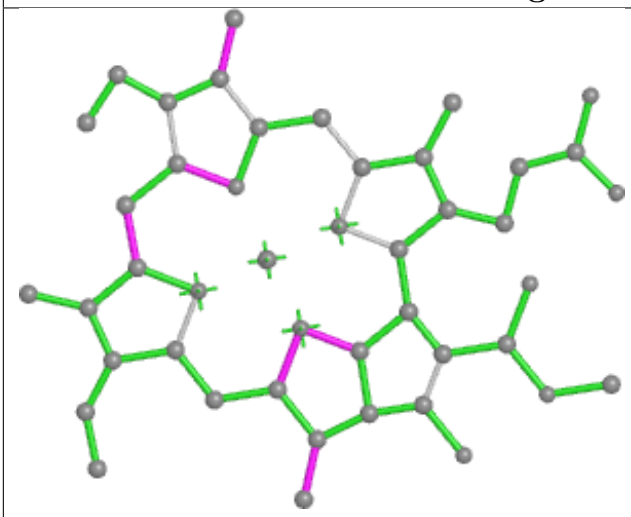


Torsions

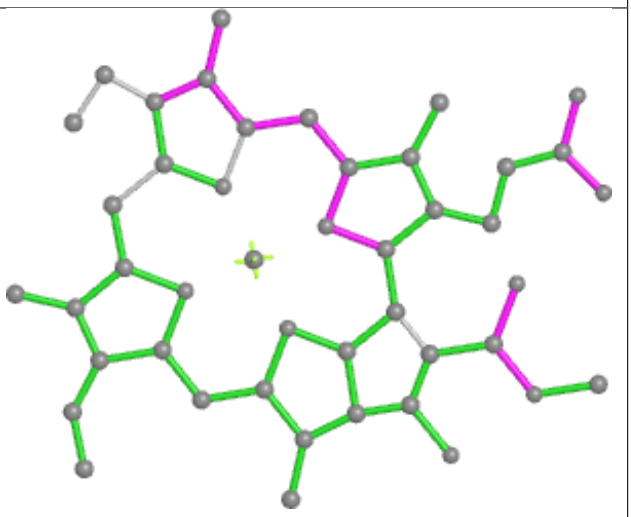


Rings

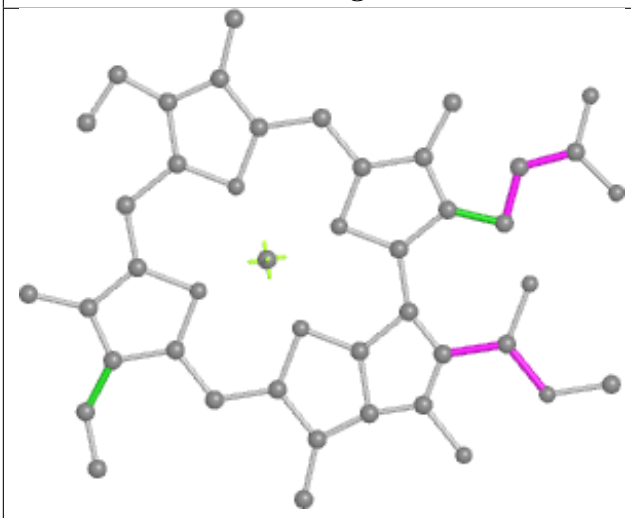
Ligand CLA 1 518



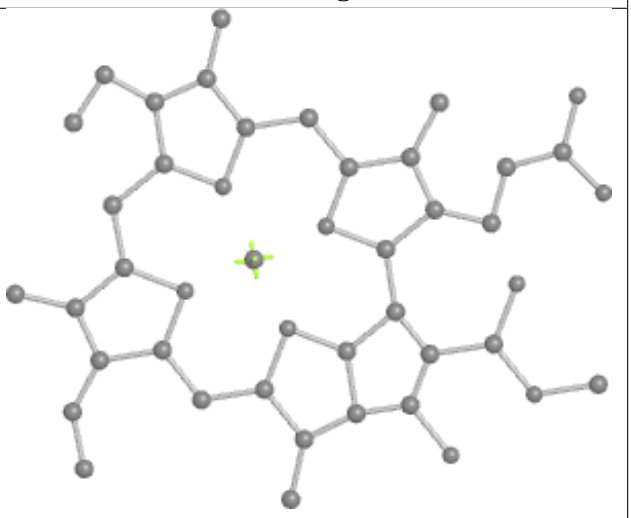
Bond lengths



Bond angles

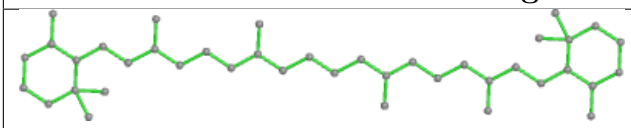


Torsions

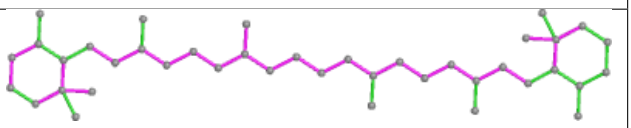


Rings

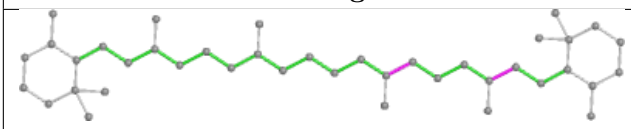
Ligand BCR l 4013



Bond lengths

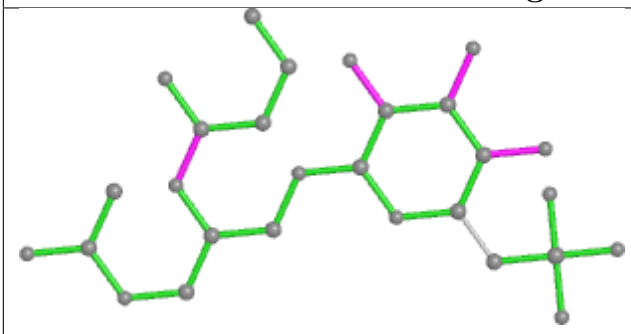
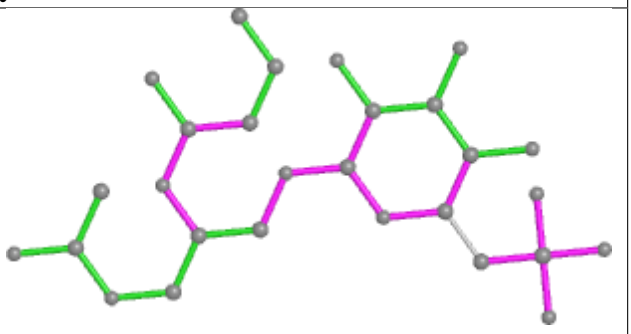
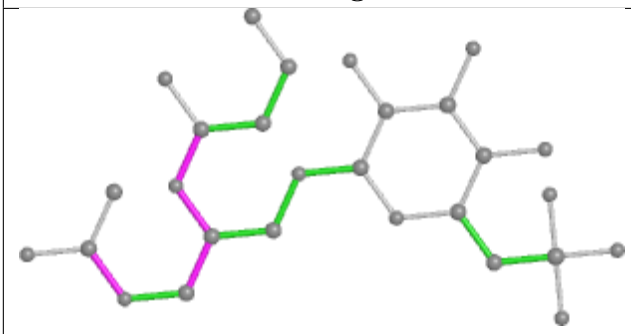
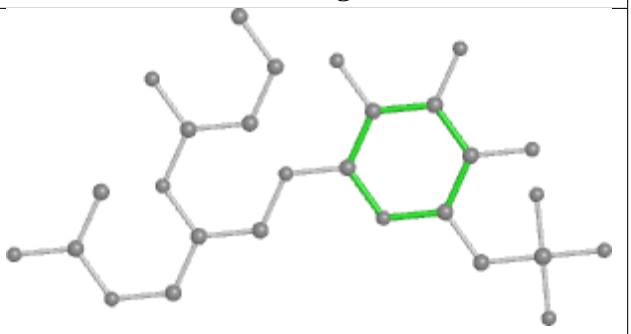


Bond angles

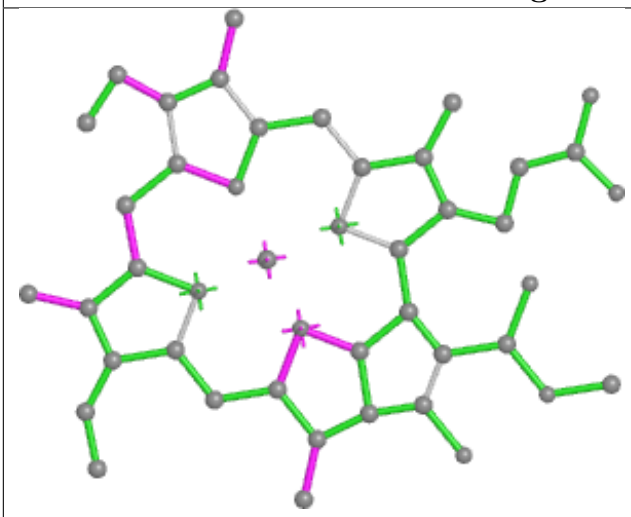


Torsions

Rings

Ligand SQD Z 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA t 505



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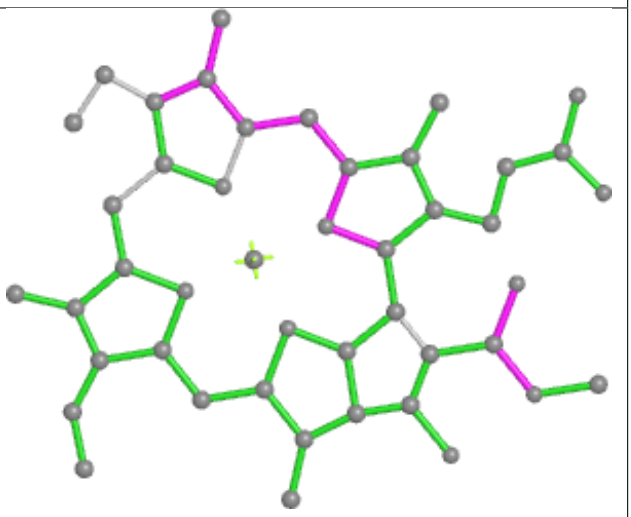

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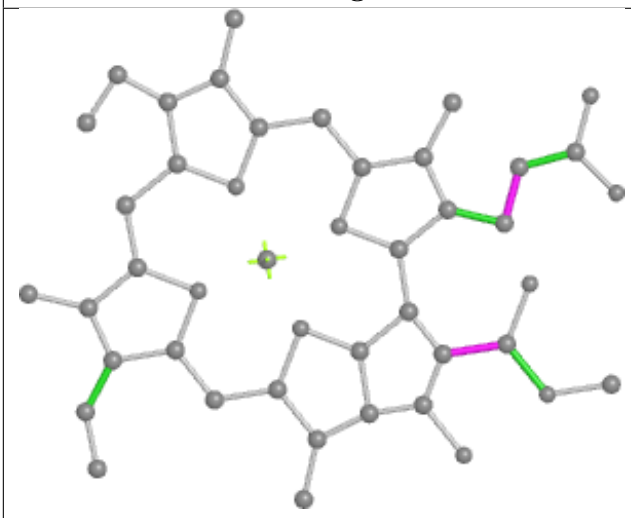

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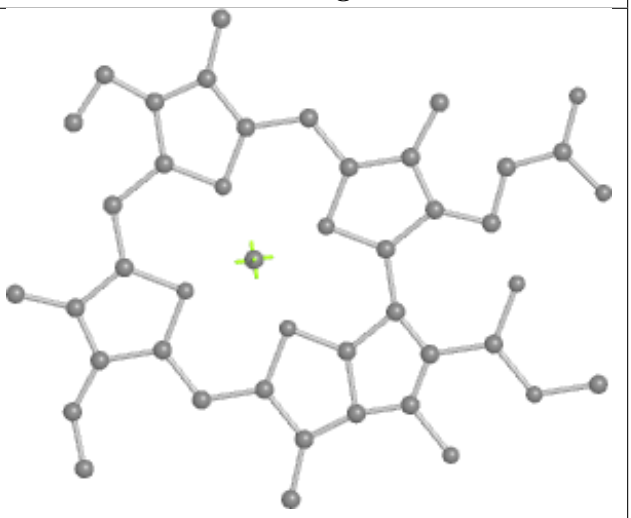
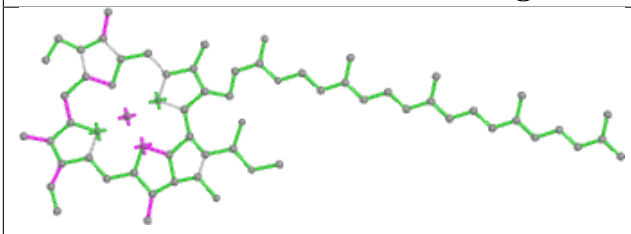


Rings

Ligand CLA A 1013



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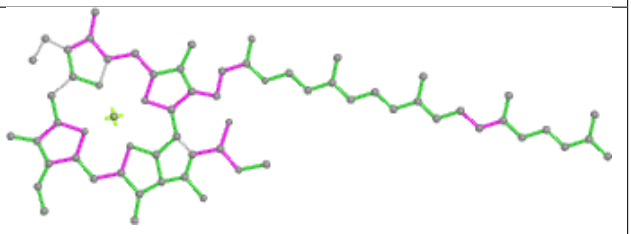

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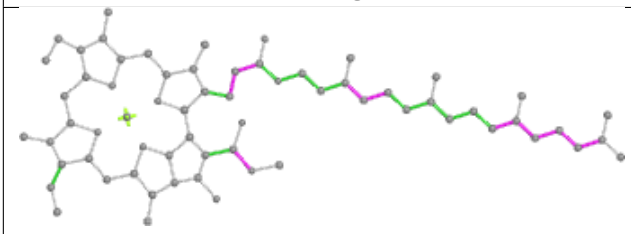

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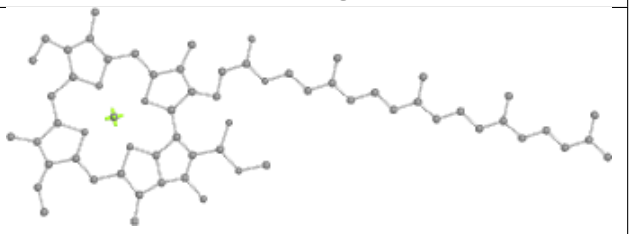
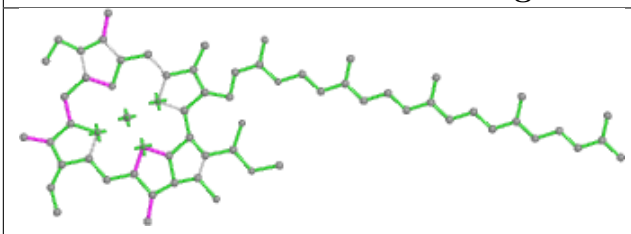


Rings

Ligand CLA H 1229



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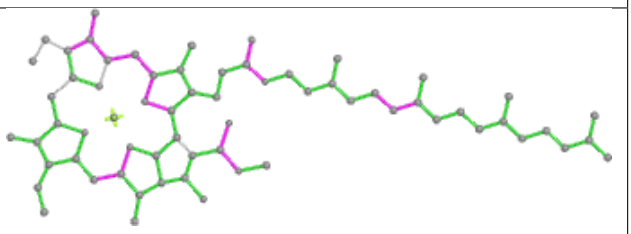

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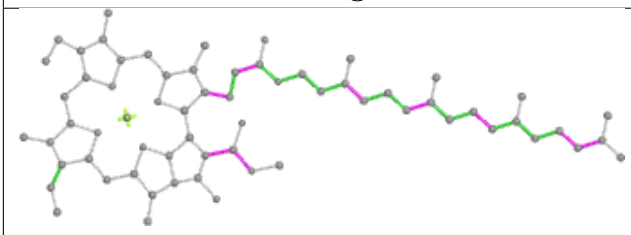

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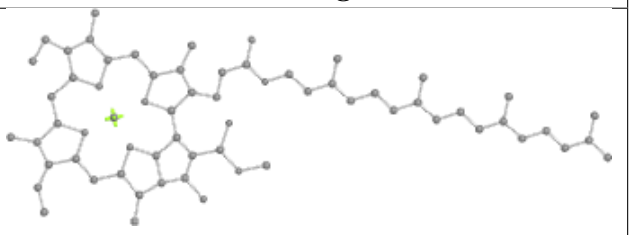
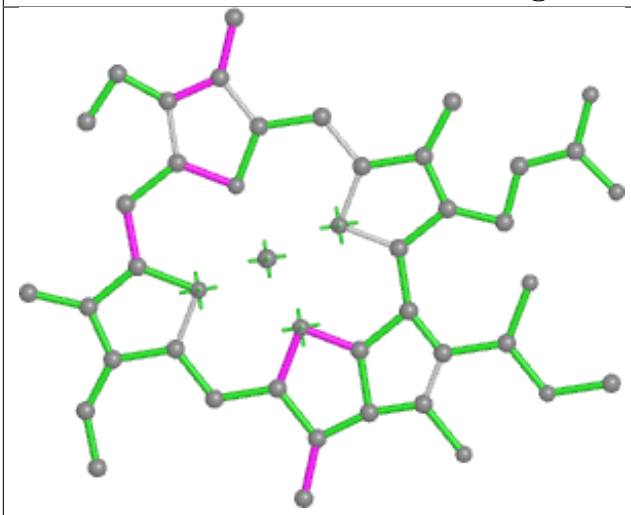


Rings

Ligand CLA r 516



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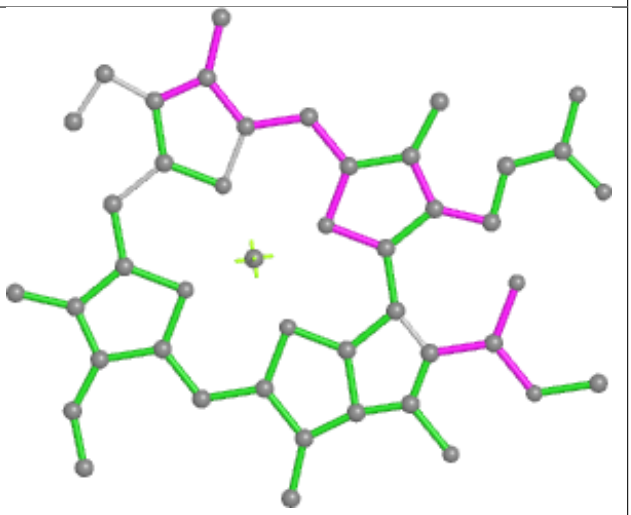

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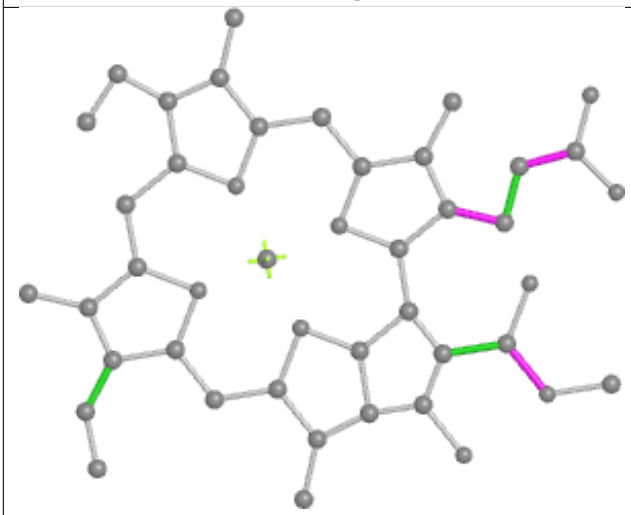

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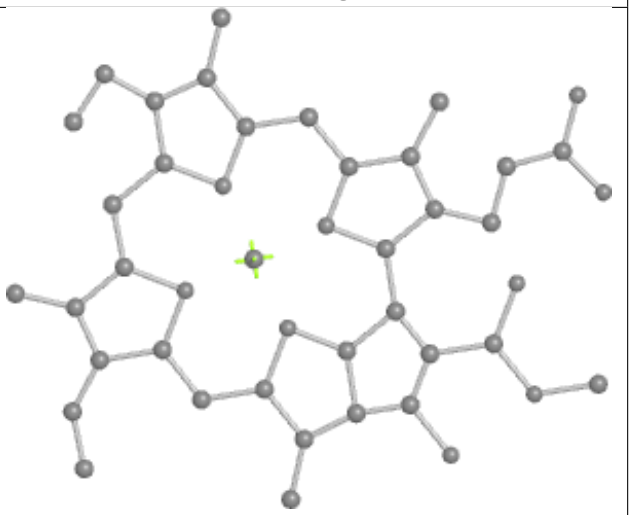

Rings

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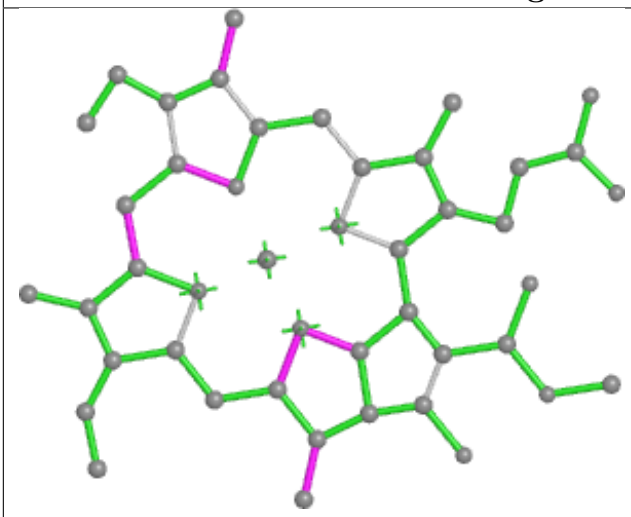

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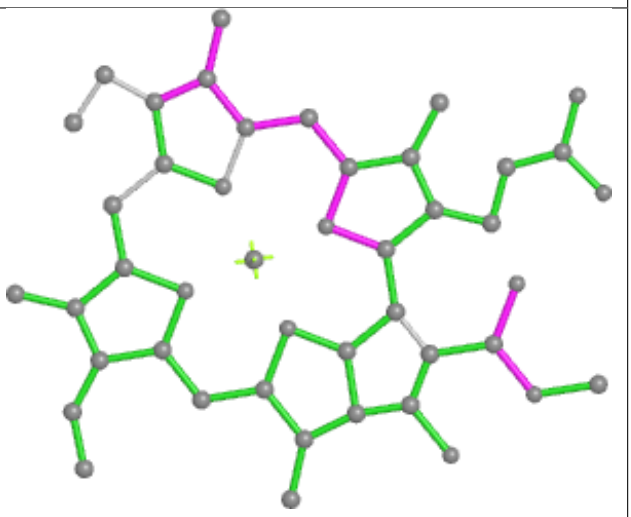

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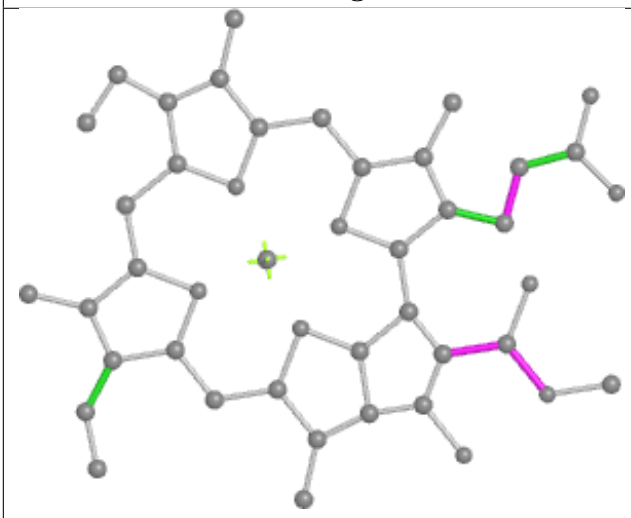

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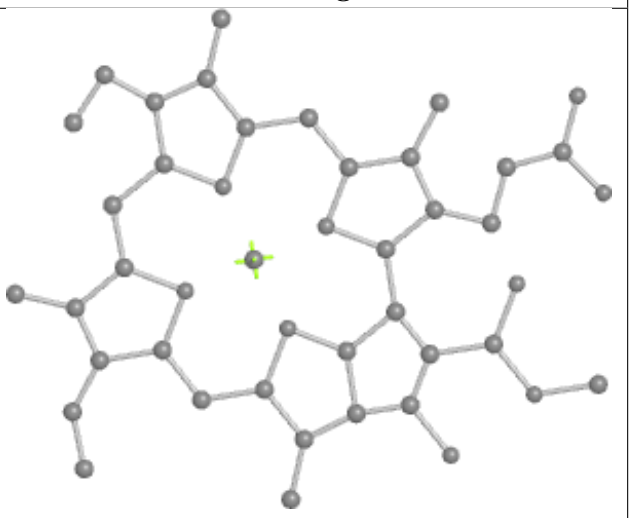
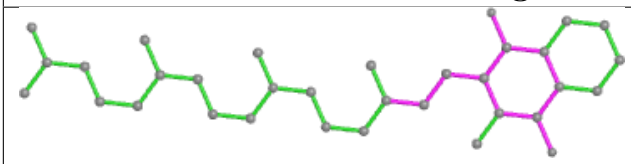


Rings

Ligand PQN H 2002



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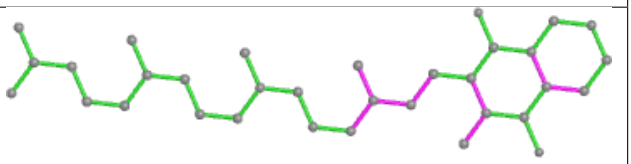

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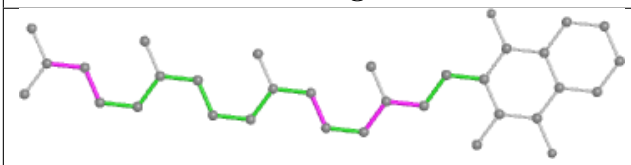

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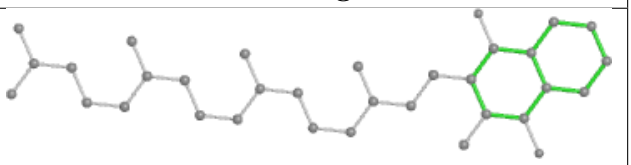
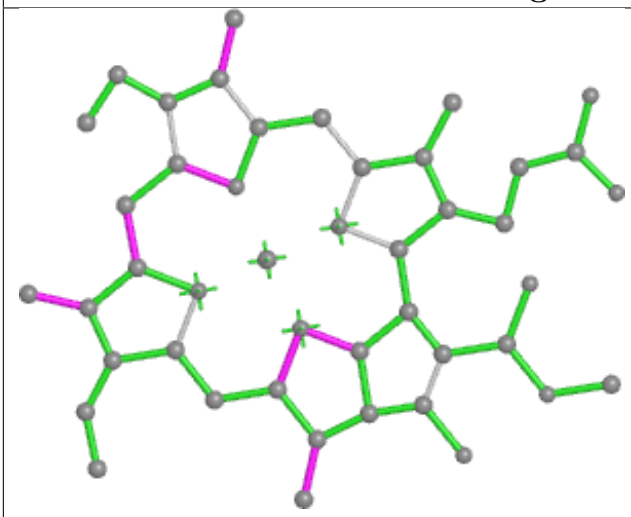


Rings

Ligand CLA s 501



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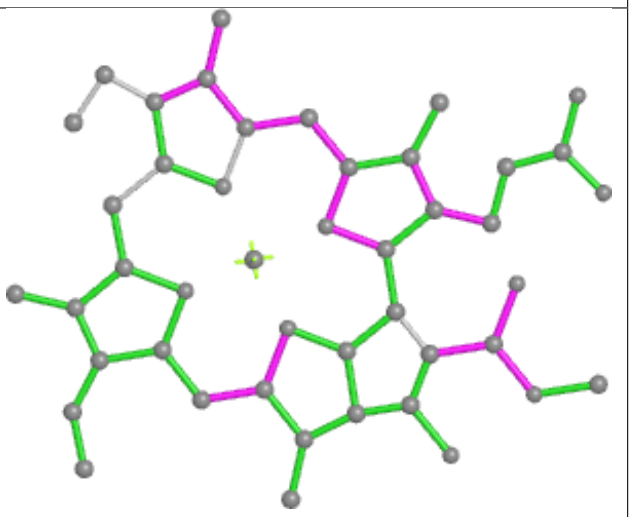

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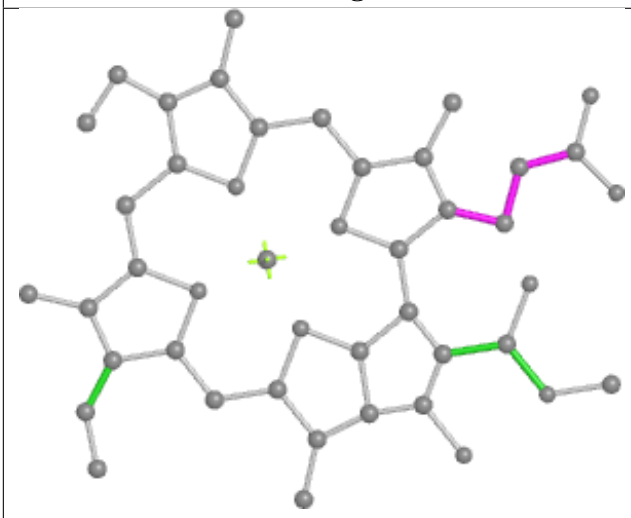

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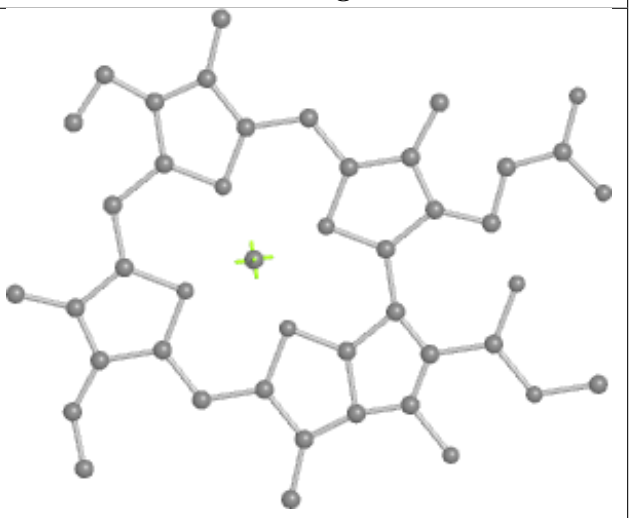
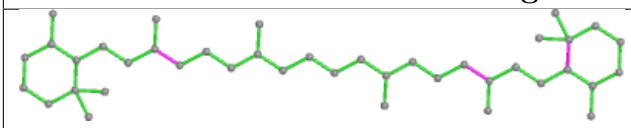


Rings

Ligand BCR f 4017



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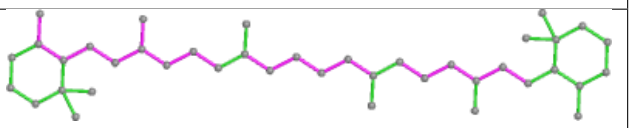

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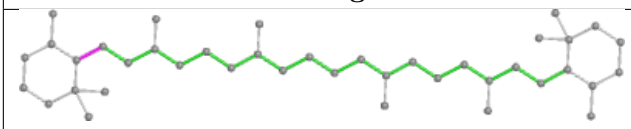
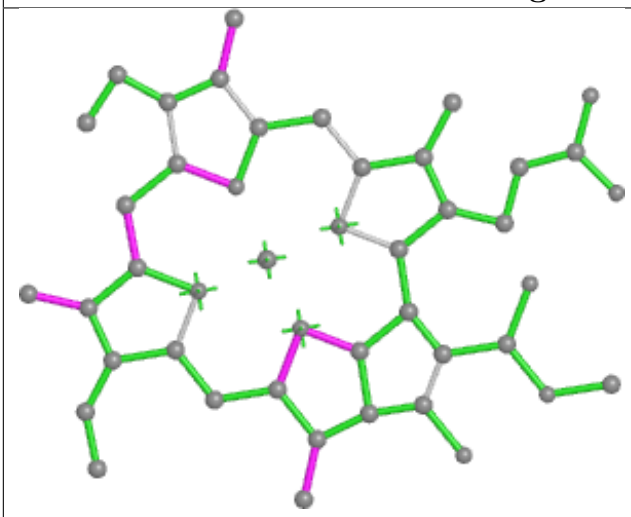


Torsions

Rings

Ligand CLA c 506



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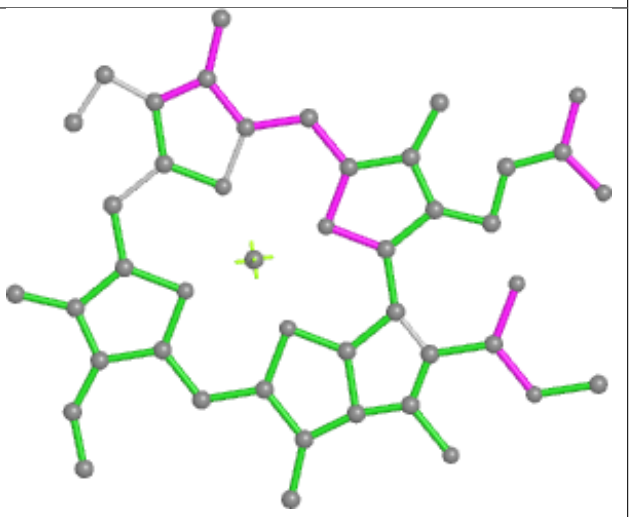

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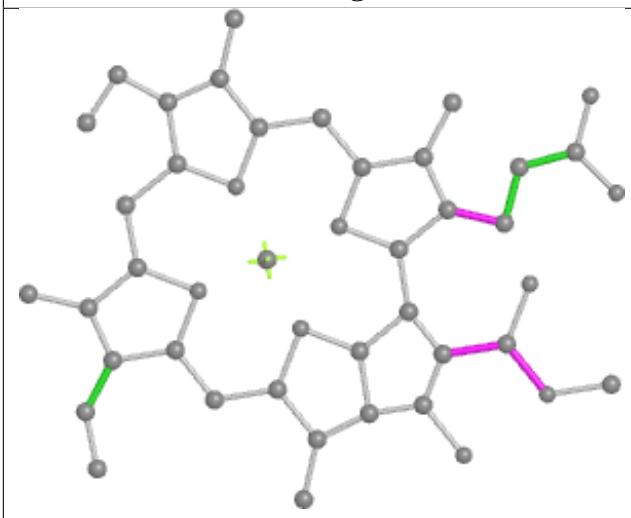

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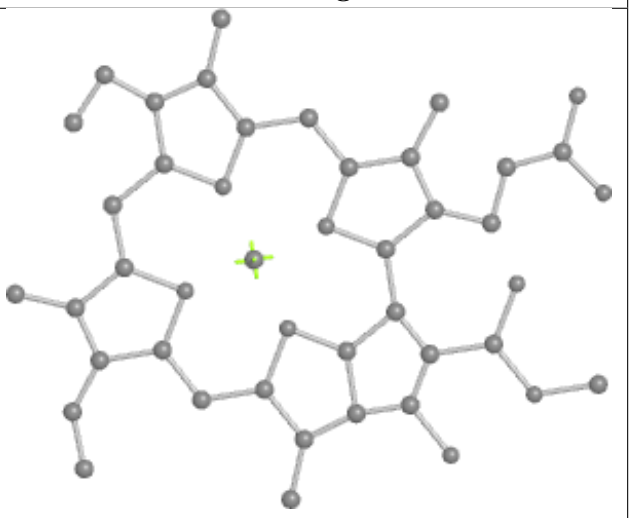
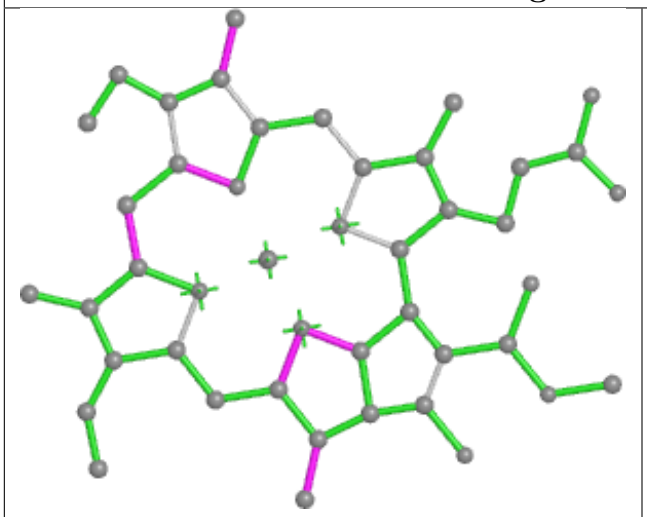


Rings

Ligand CLA 6 503



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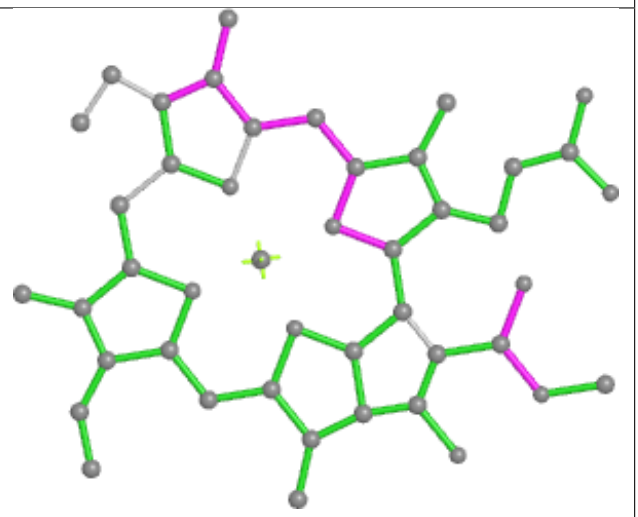

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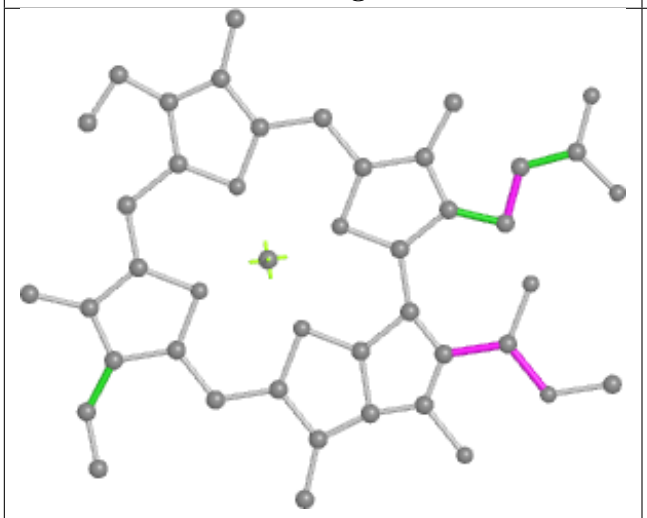

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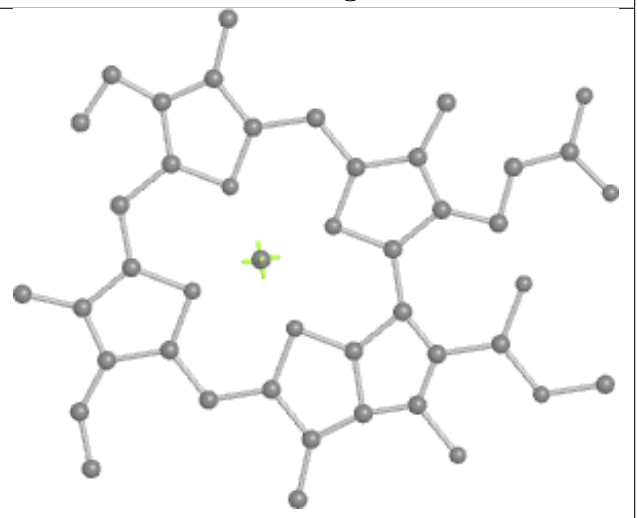

Rings

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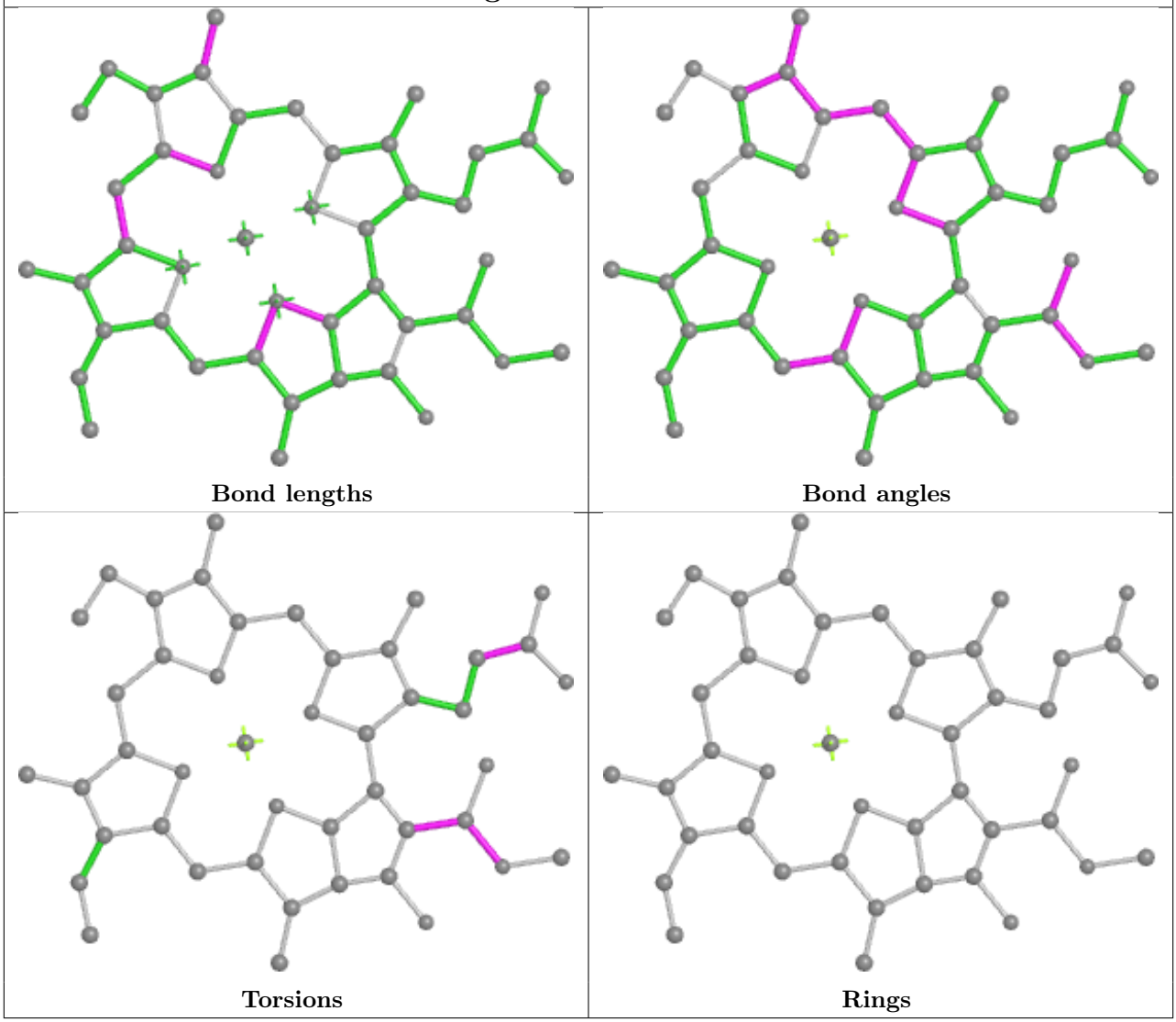

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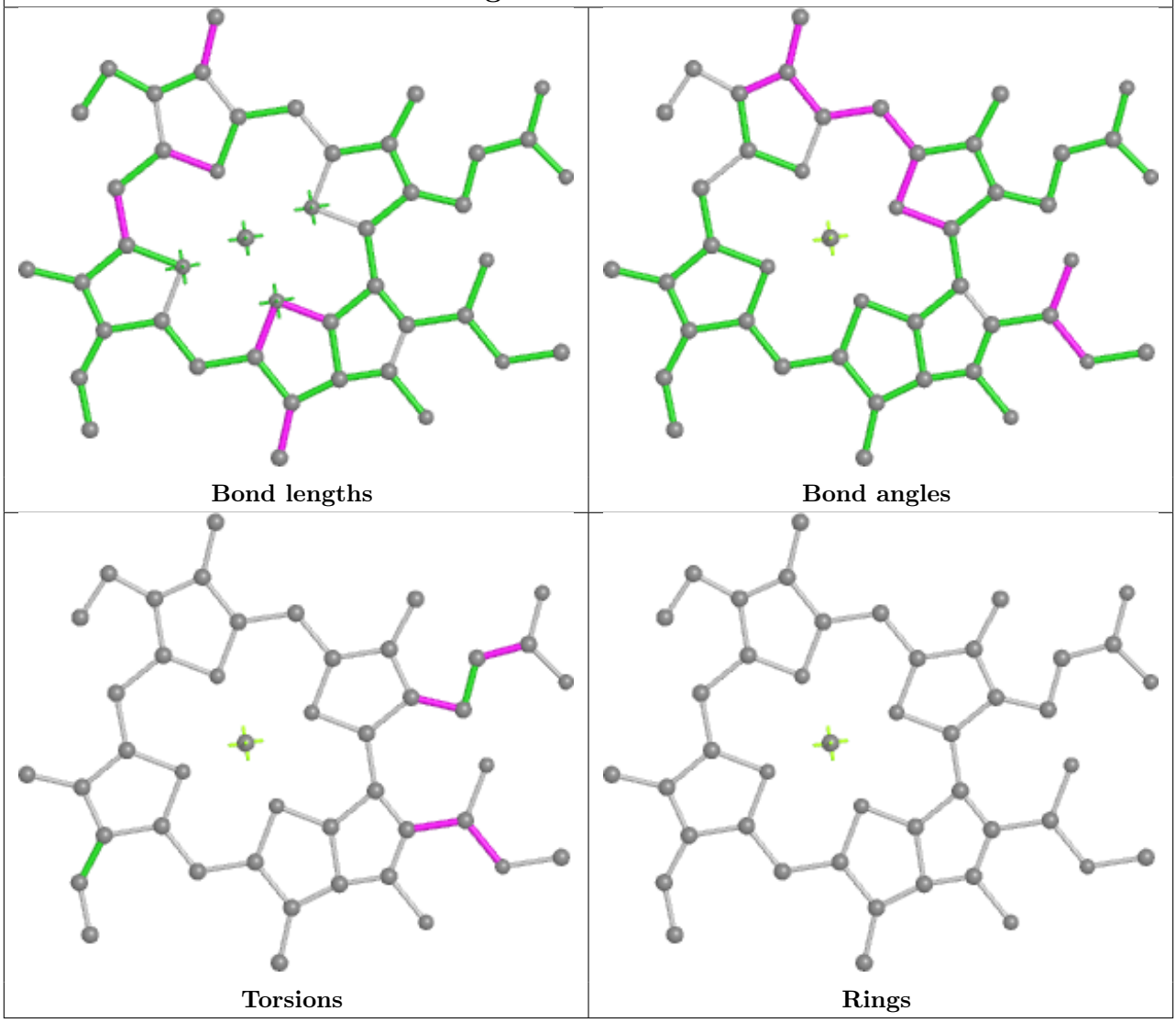
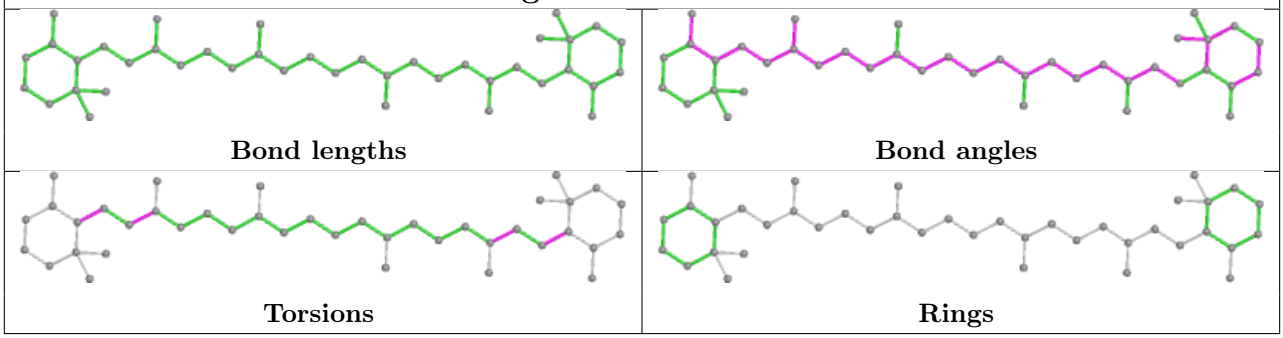
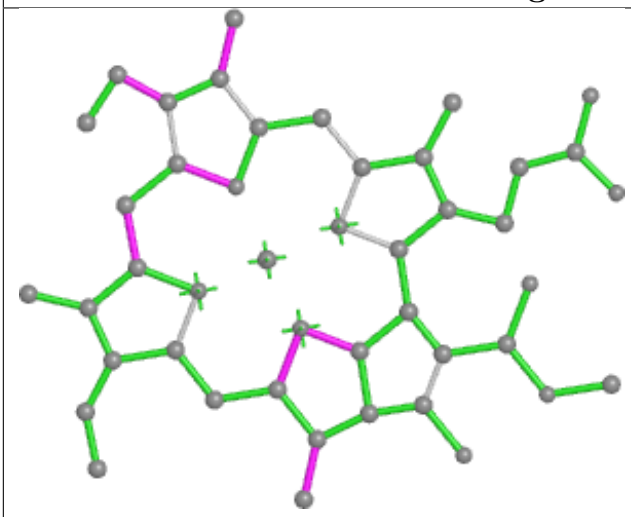


Ligand BCR f 4004



Ligand CLA 1 511



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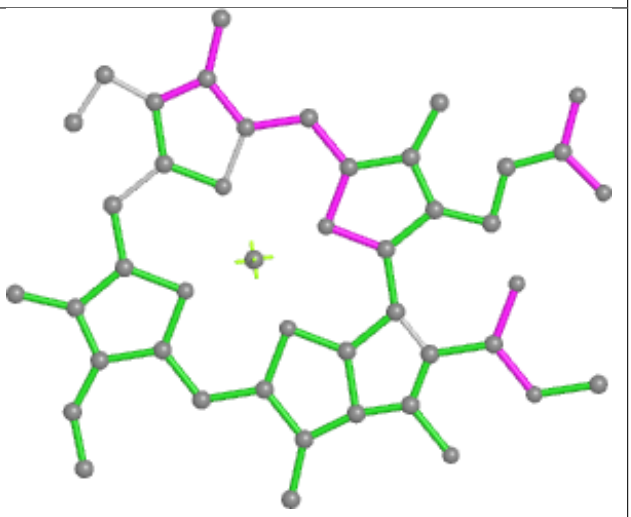

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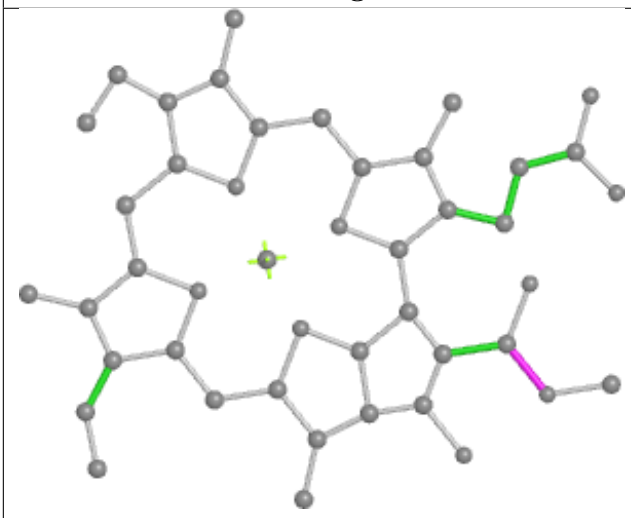
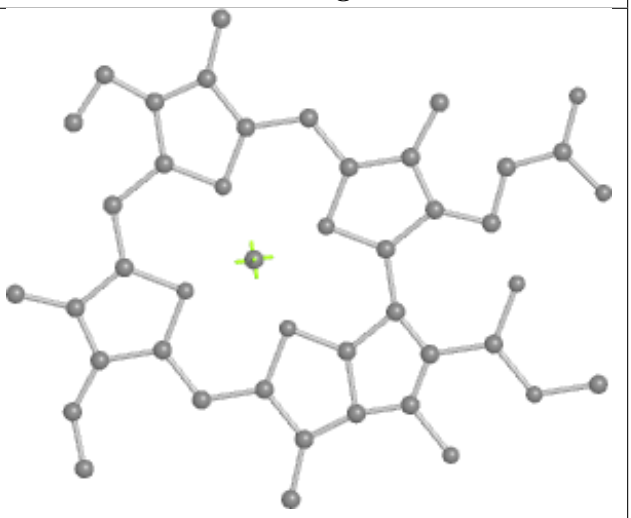
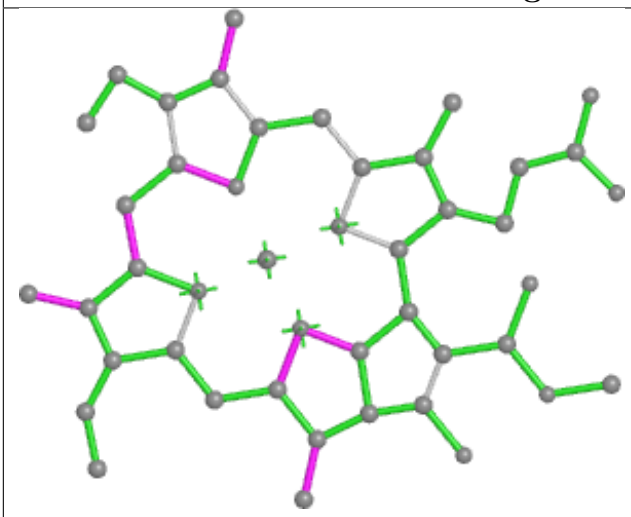


Torsions



Rings

Ligand CLA Y 507



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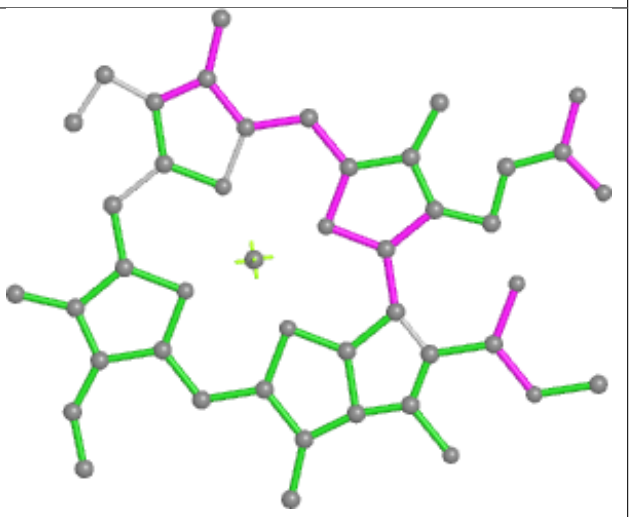

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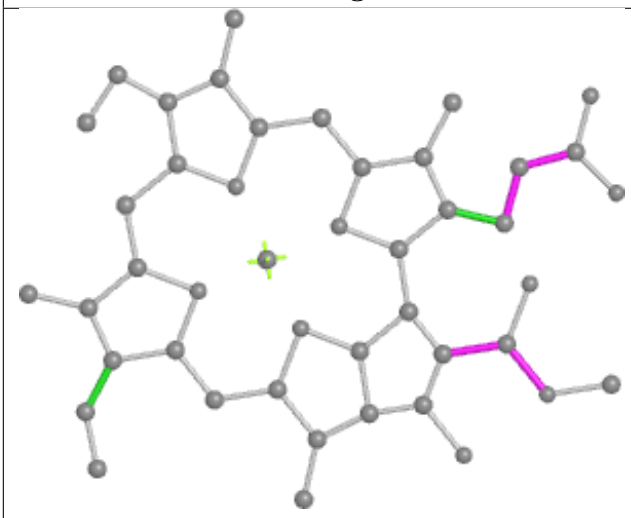

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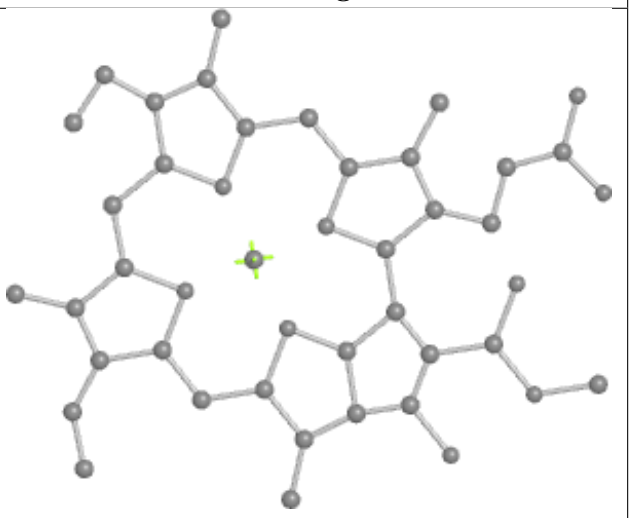
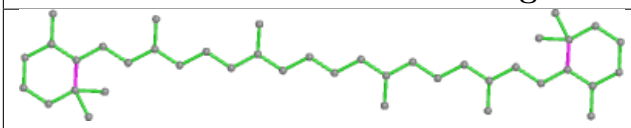
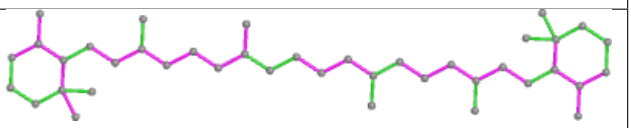


Rings

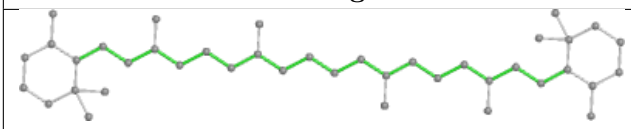
Ligand BCR I 4018



Bond lengths



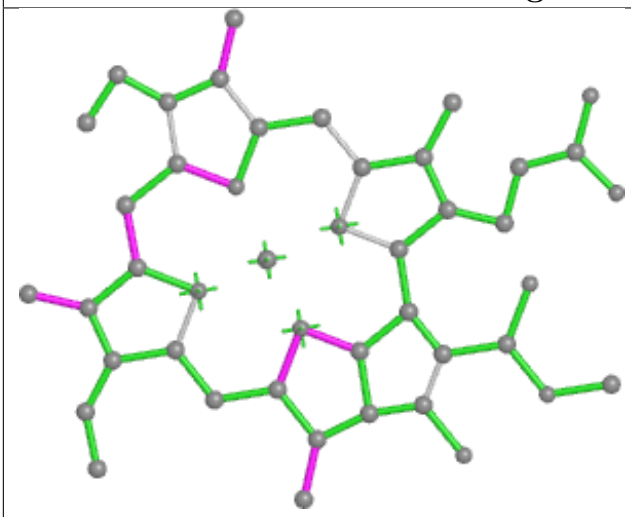
Bond angles



Torsions

Rings

Ligand CLA Z 517



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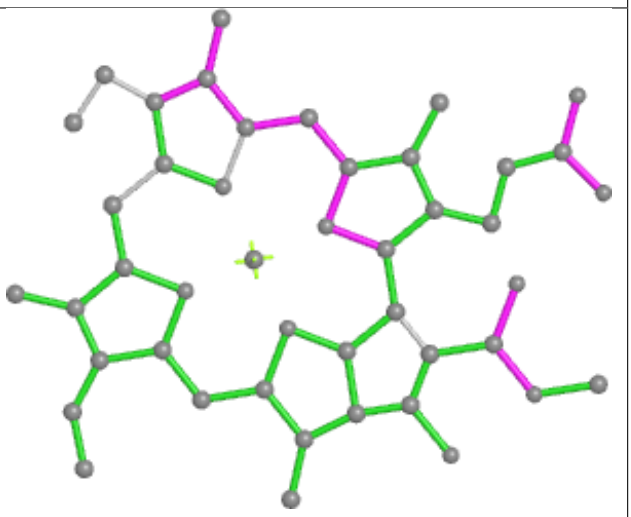
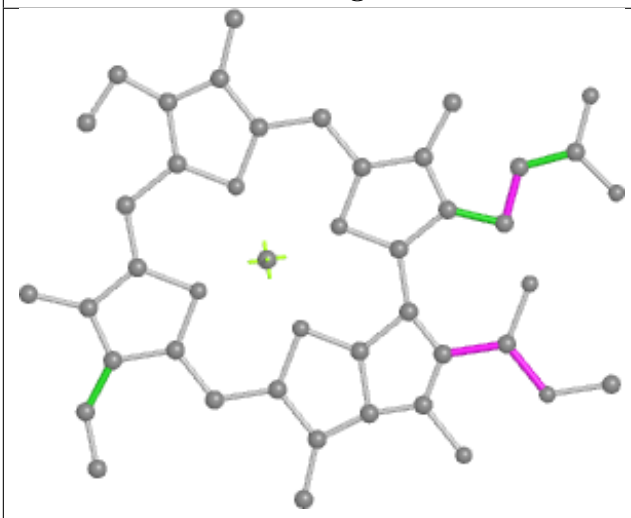
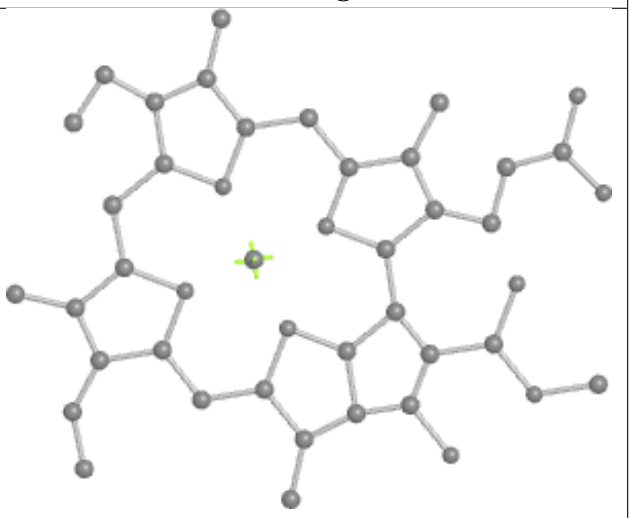


Bond angles

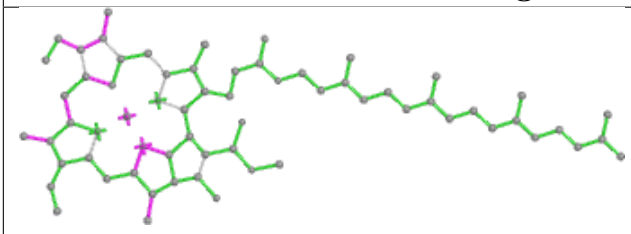


Torsions



Rings

Ligand CLA B 1235



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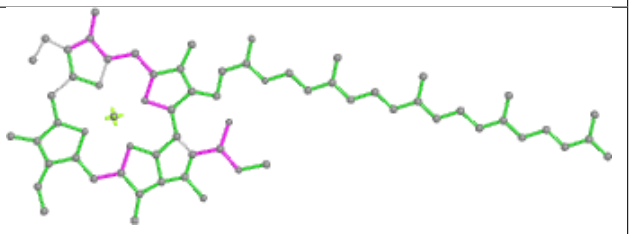

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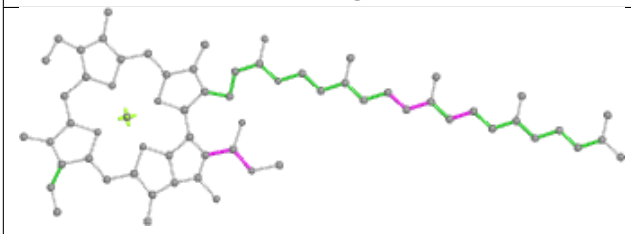
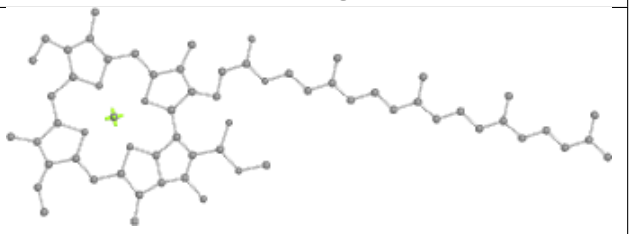
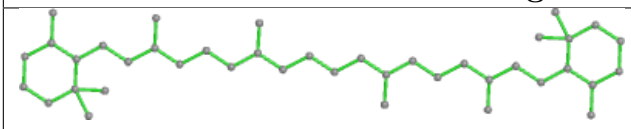
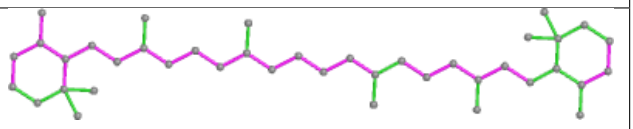
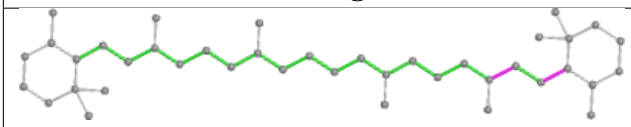
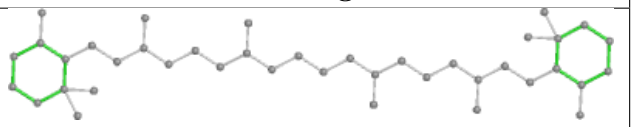
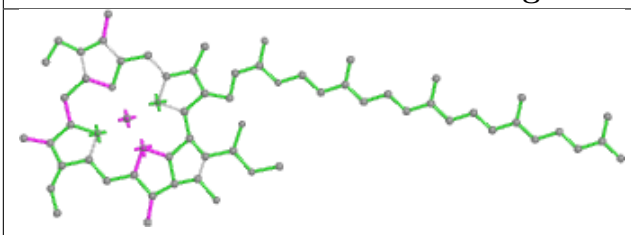
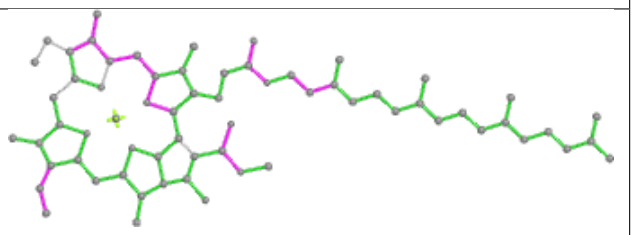
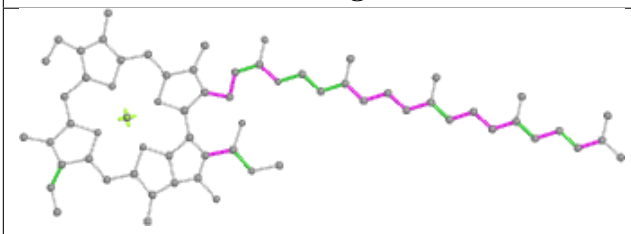
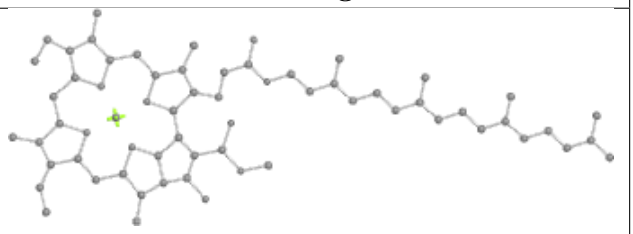


Torsions

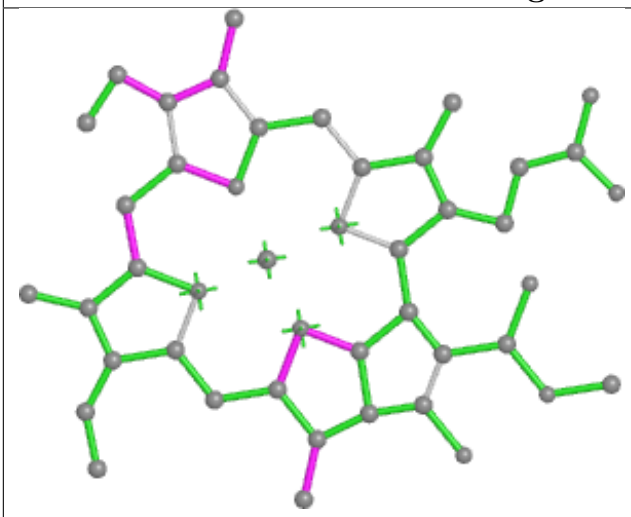


Rings

Ligand BCR a 523	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 1210	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 503



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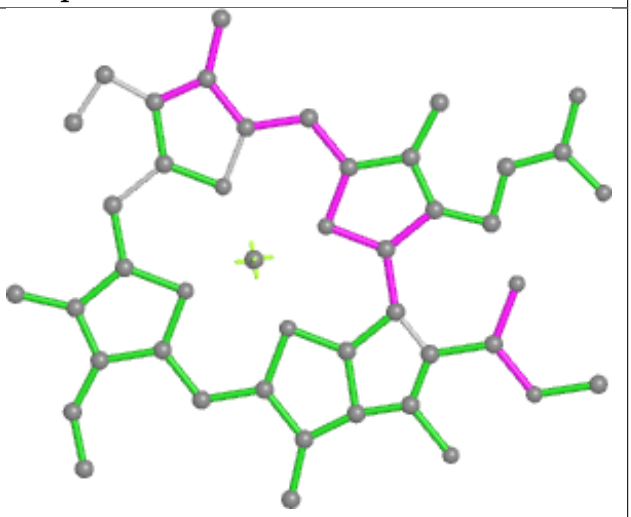
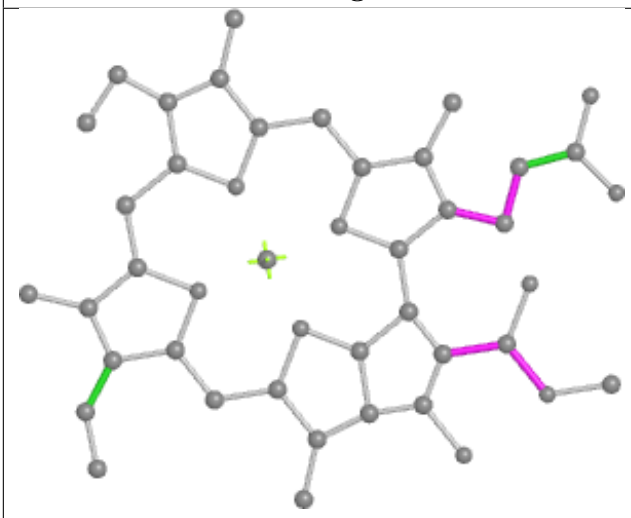


Bond angles



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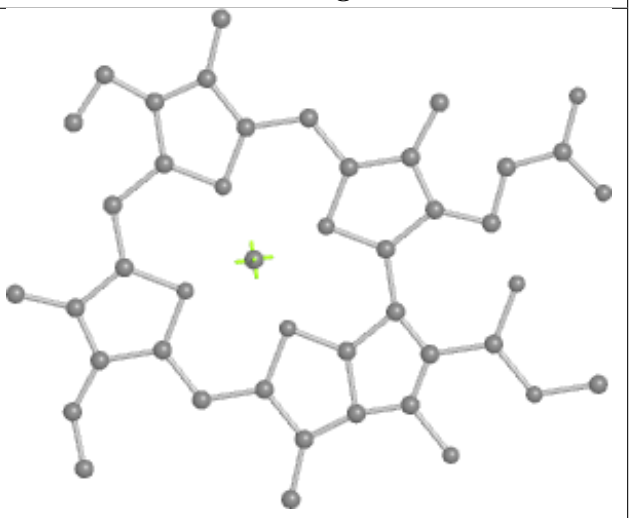
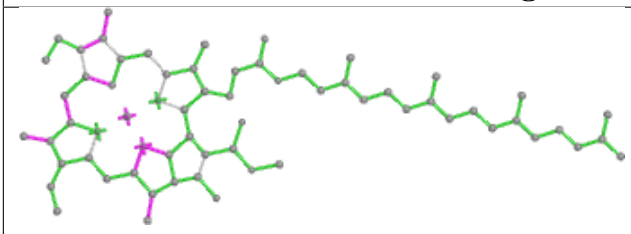


Rings

Ligand CLA e 1101



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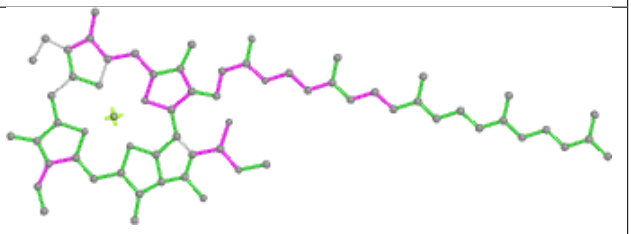

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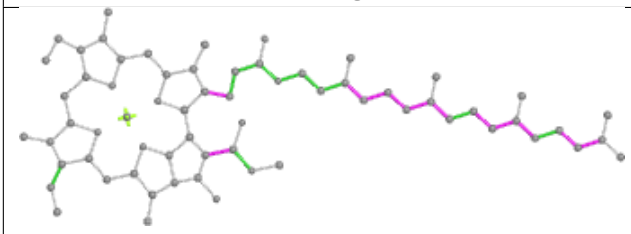

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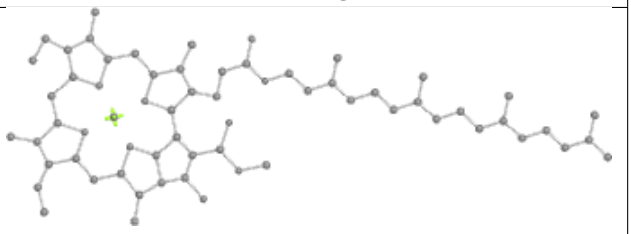
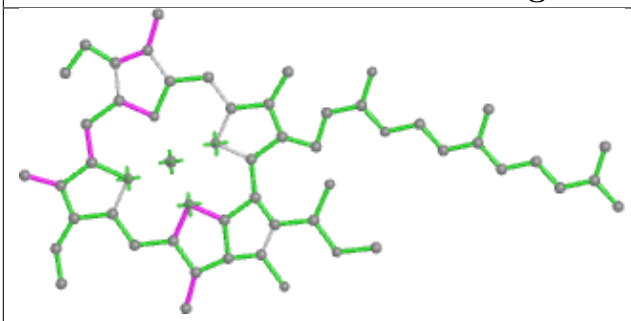


Rings

Ligand CLA 3 518



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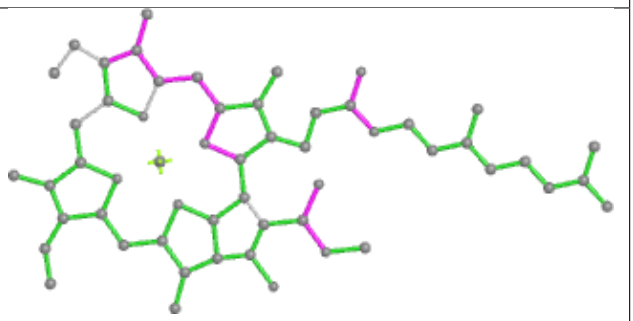

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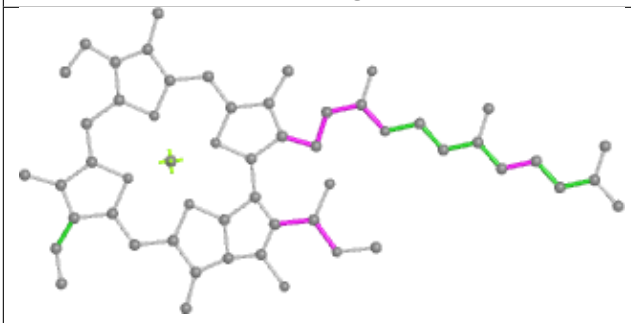

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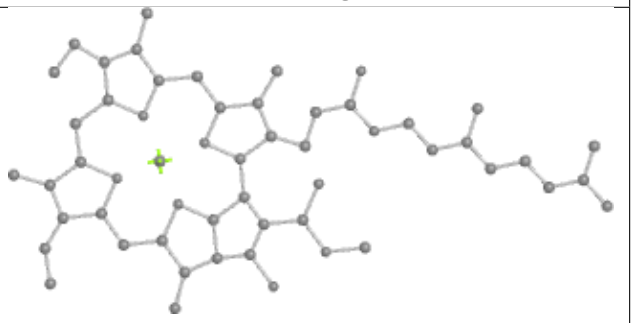
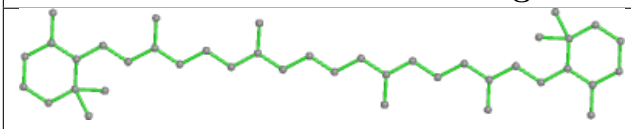


Rings

Ligand BCR A 4007



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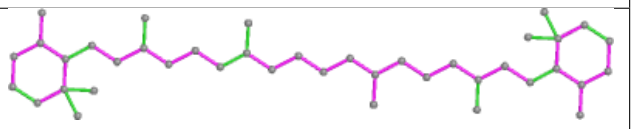

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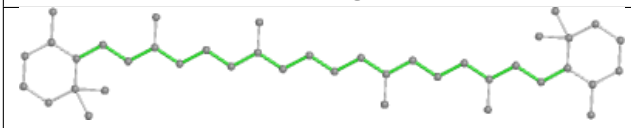
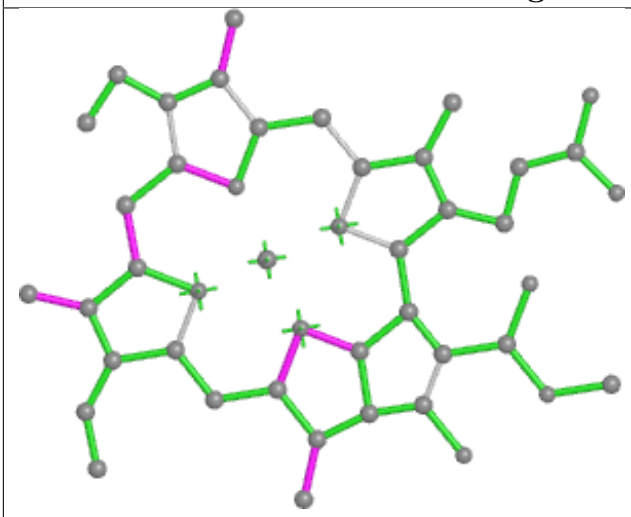


Torsions

Rings

Ligand CLA b 511



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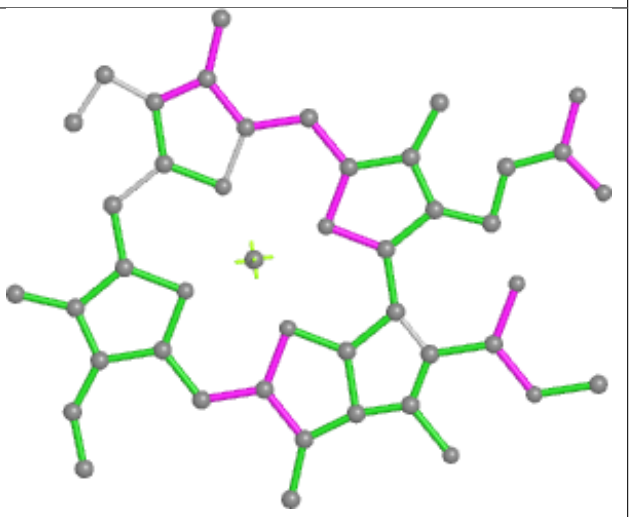

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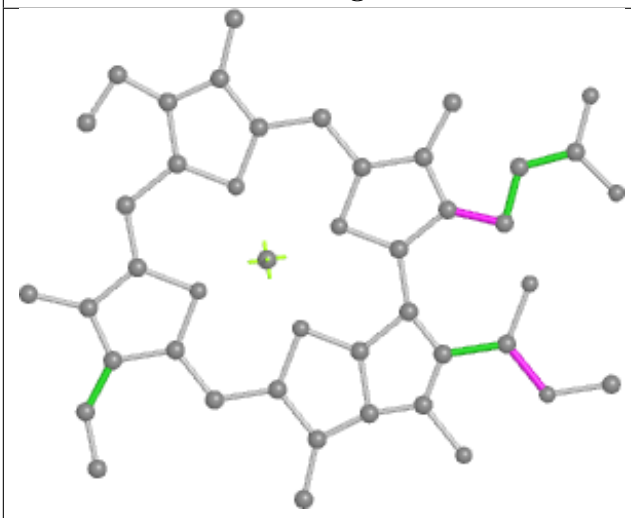

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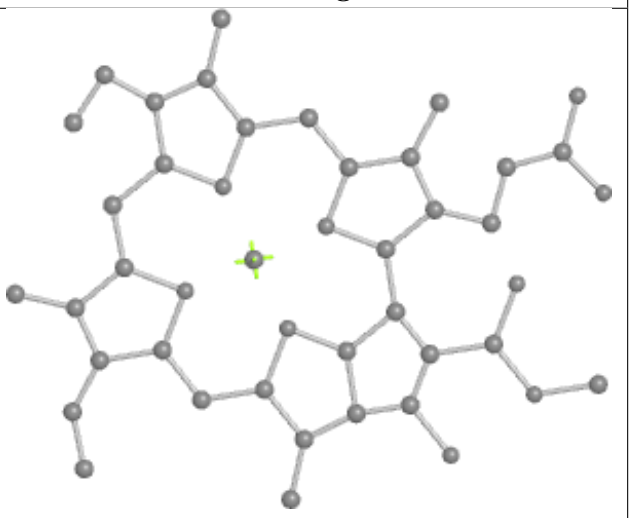
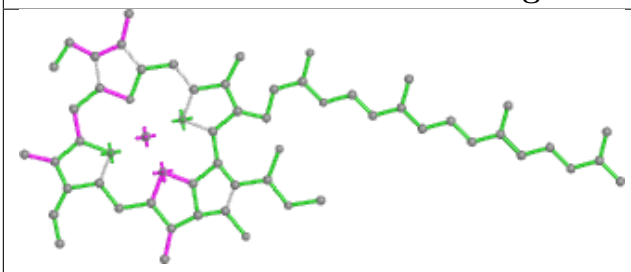


Rings

Ligand CLA f 1216



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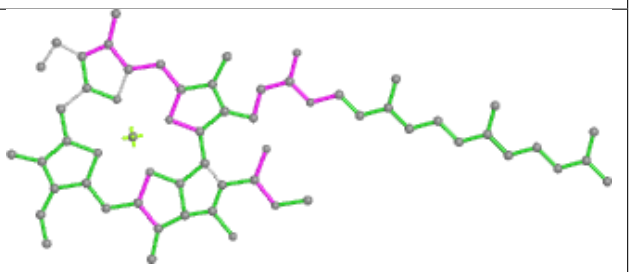
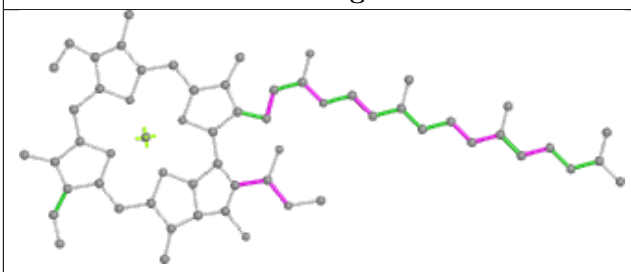
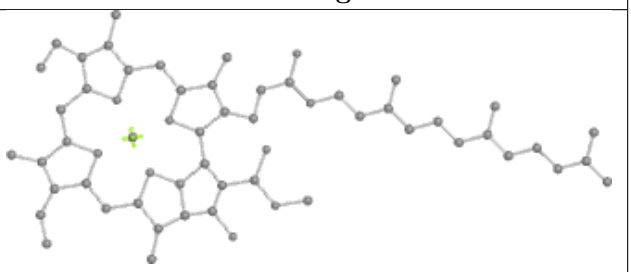


Bond angles

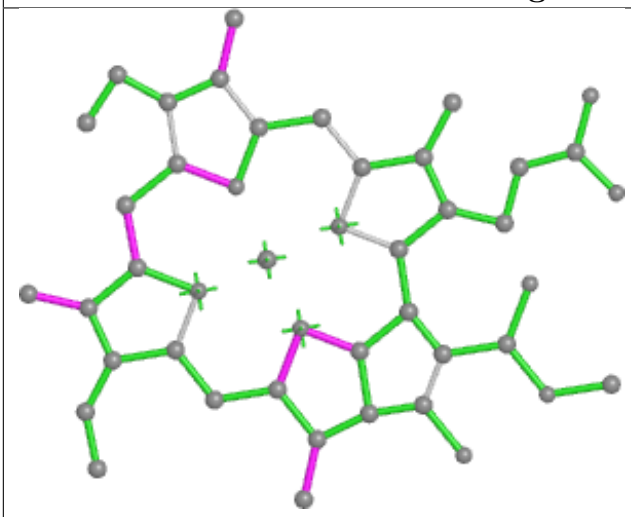


Torsions



Rings

Ligand CLA 1 513



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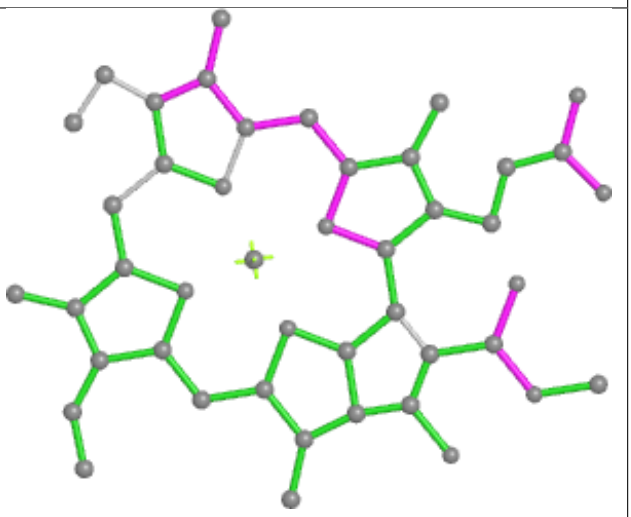
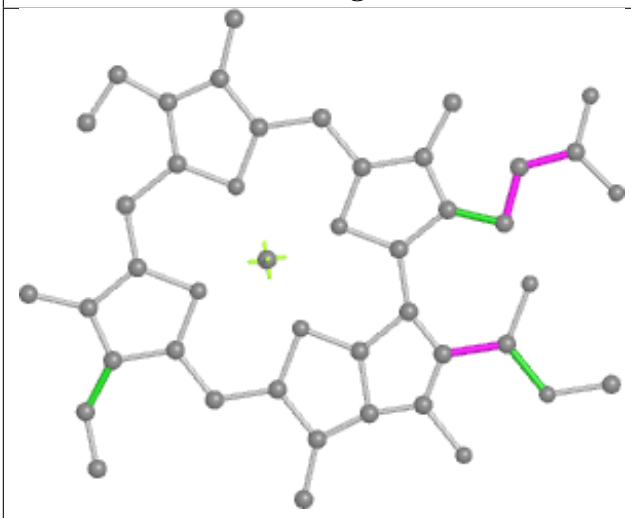
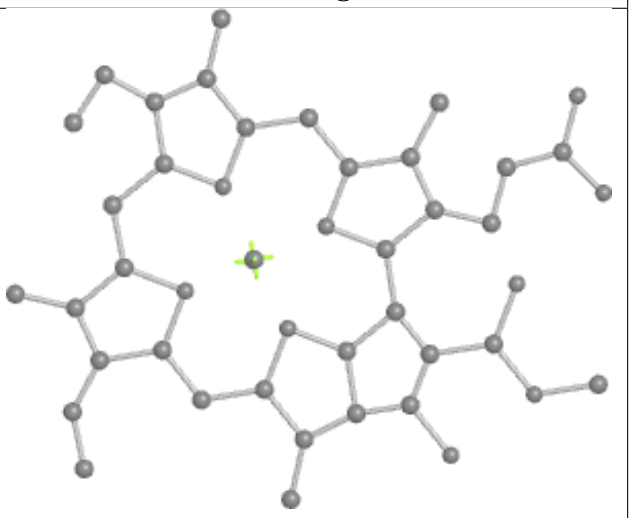


Bond angles

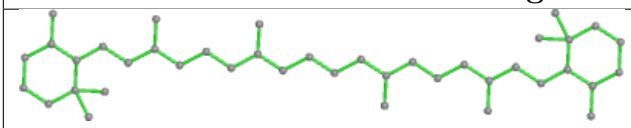


Torsions



Rings

Ligand BCR 5 522



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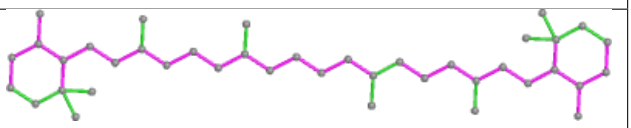
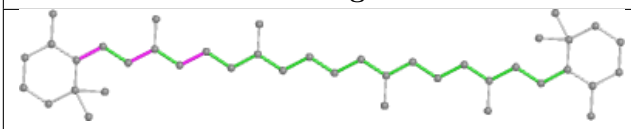


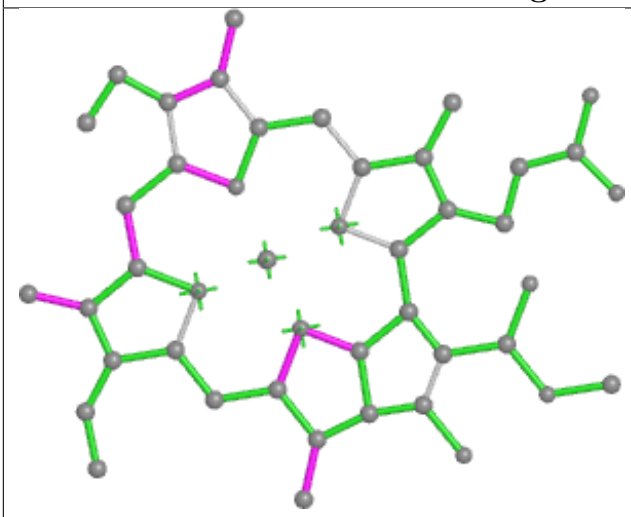
Bond angles



Torsions

Rings

Ligand CLA s 517



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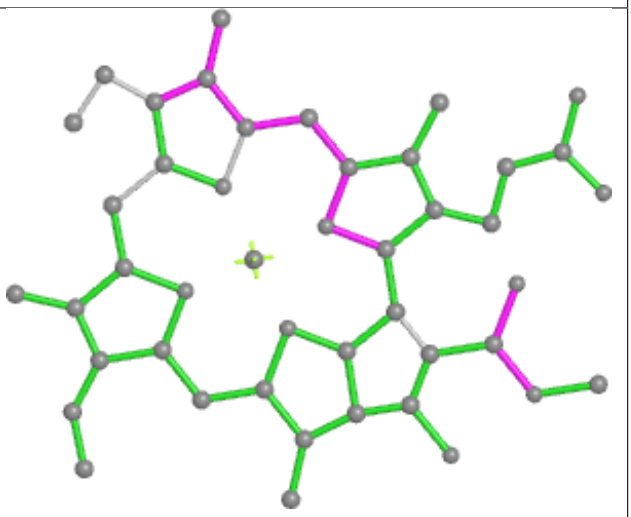
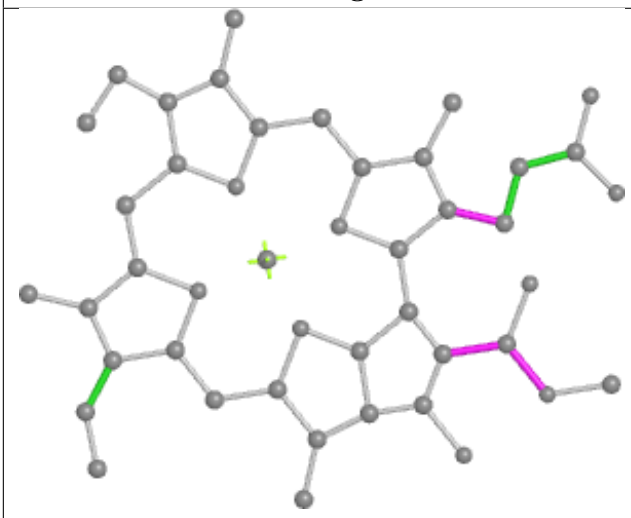
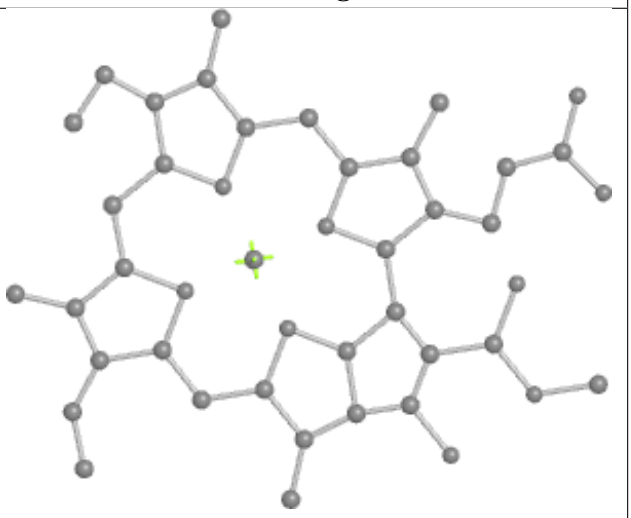


Bond angles

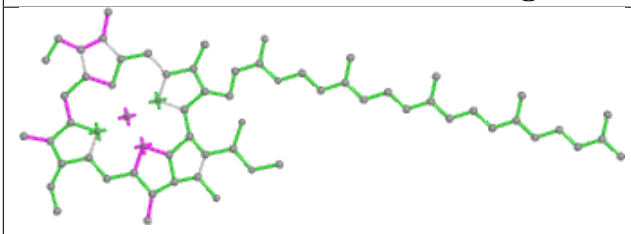


Torsions

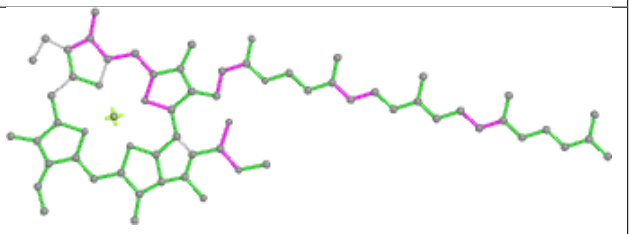


Rings

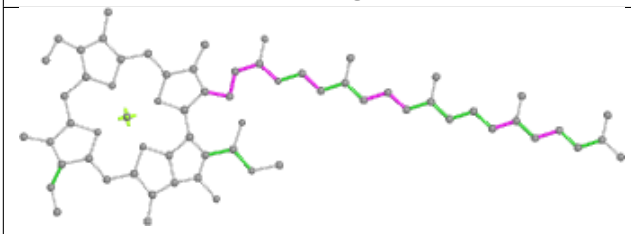
Ligand CLA e 1125



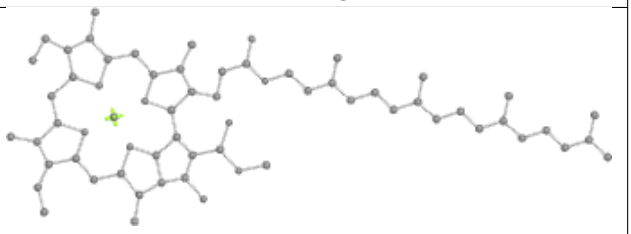
Bond lengths



Bond angles

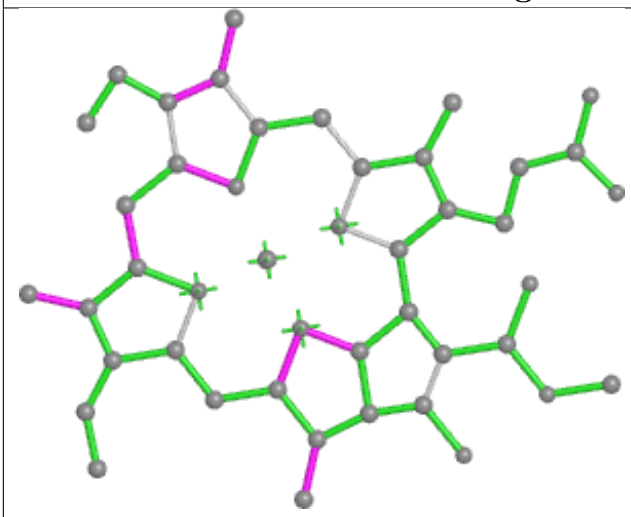


Torsions

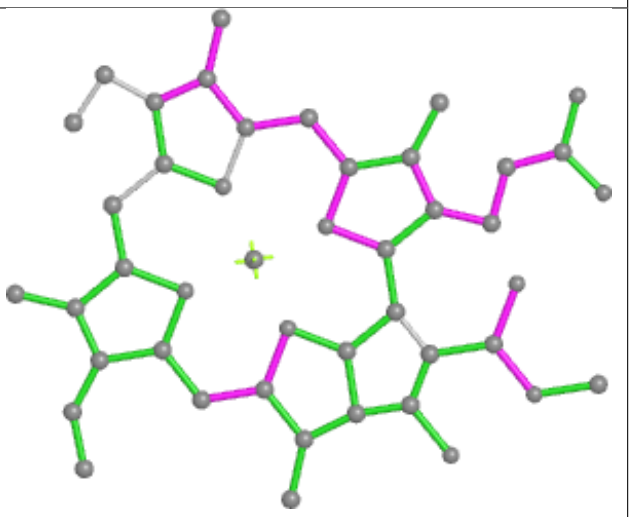


Rings

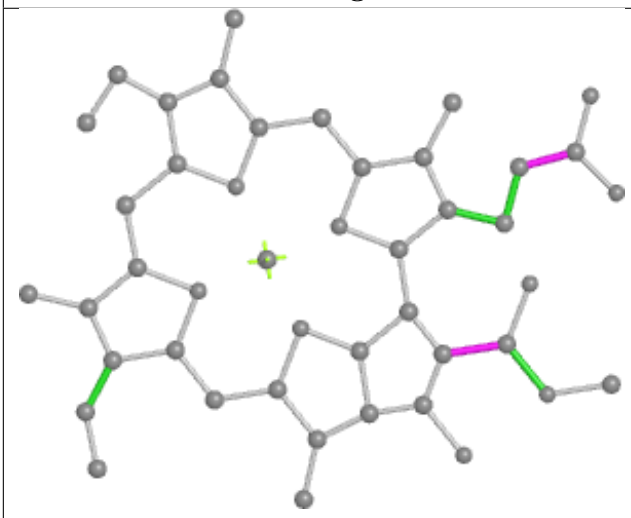
Ligand CLA A 1114



Bond lengths



Bond angles



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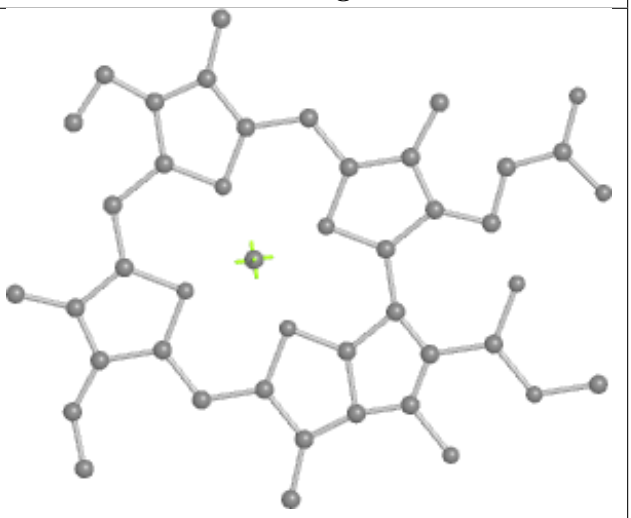
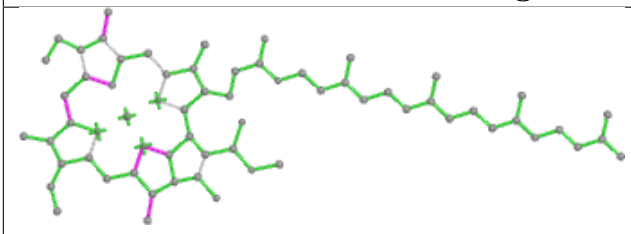


Rings

Ligand CLA H 1240



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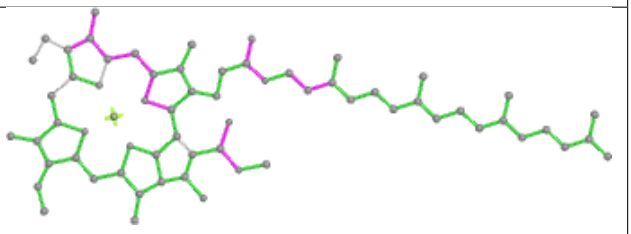
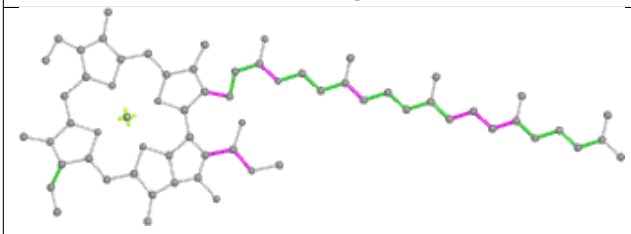
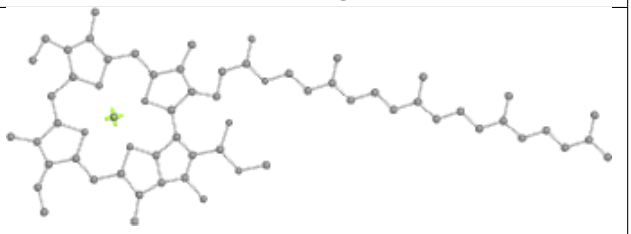


Bond angles

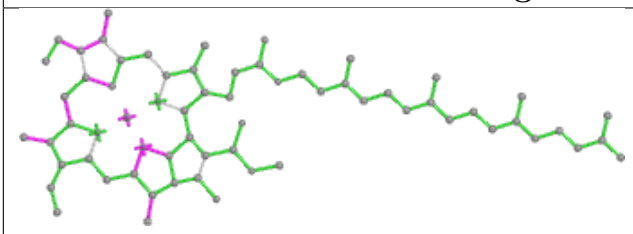


Torsions

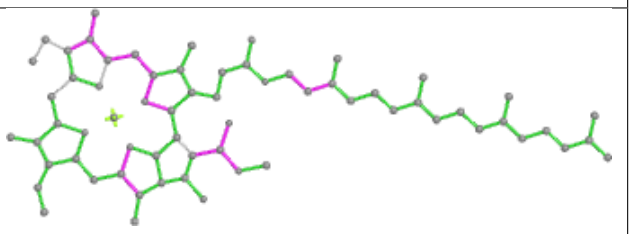


Rings

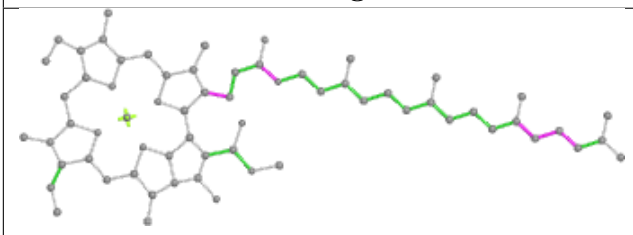
Ligand CLA H 1225



Bond lengths



Bond angles



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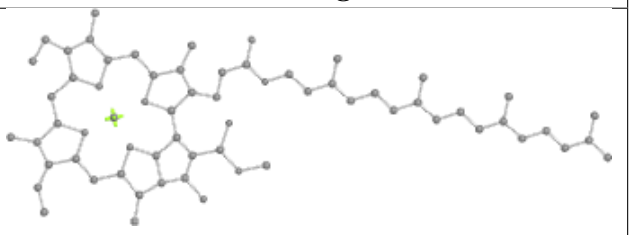
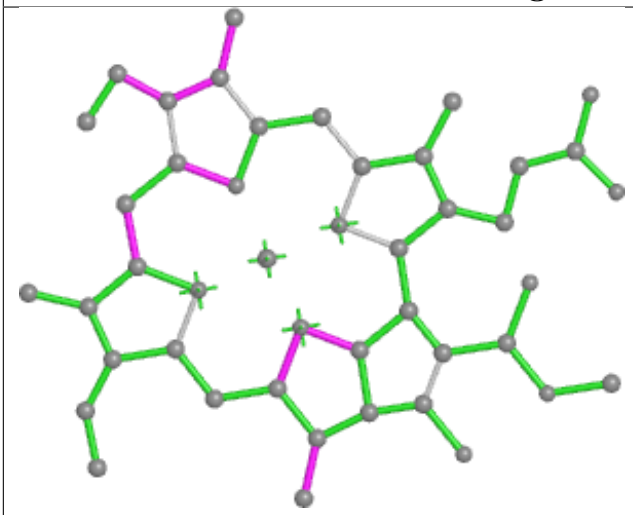


Rings

Ligand CLA 3 513



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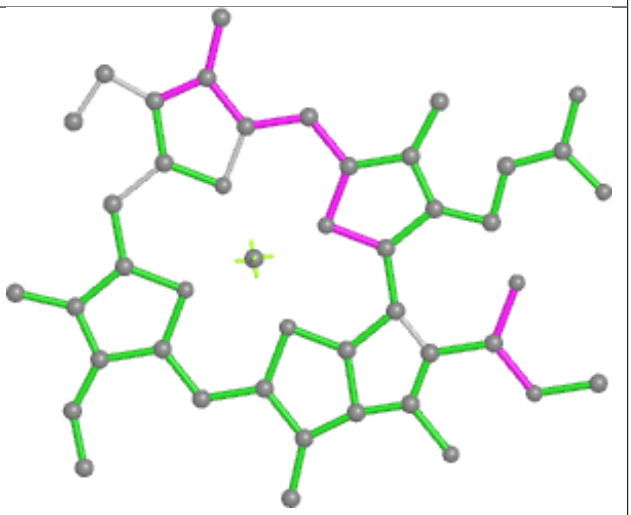
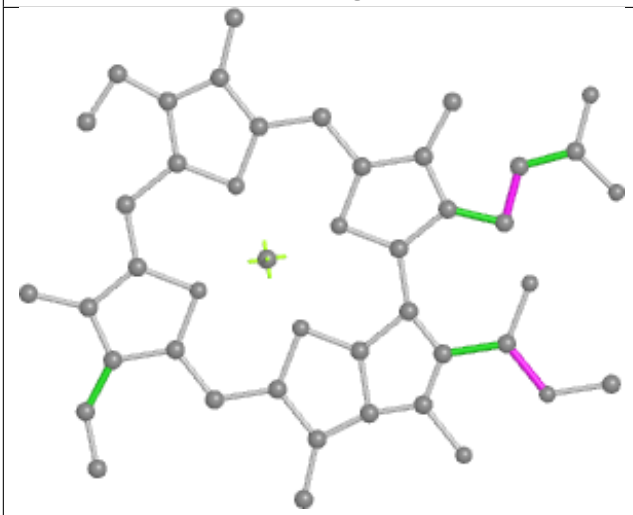


Bond angles



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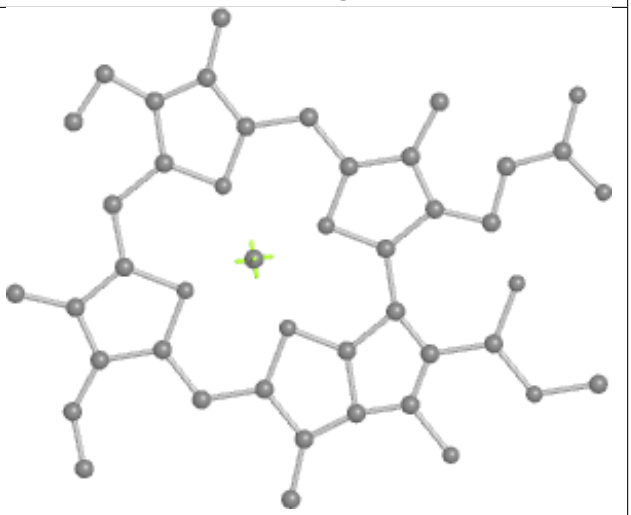
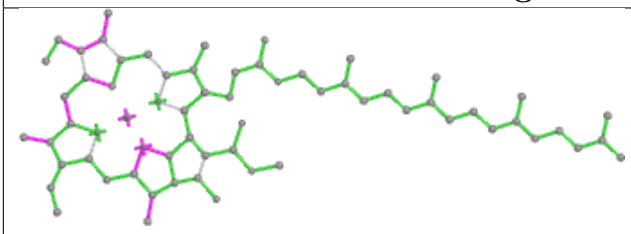
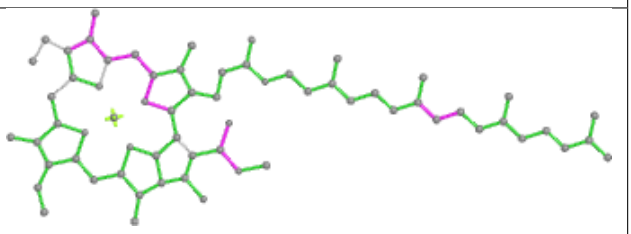
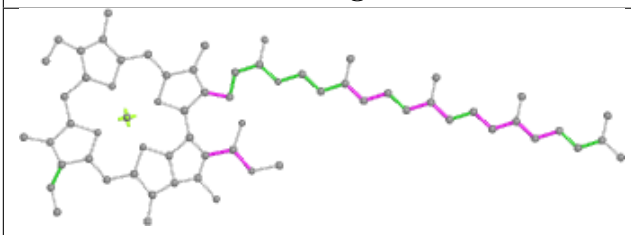
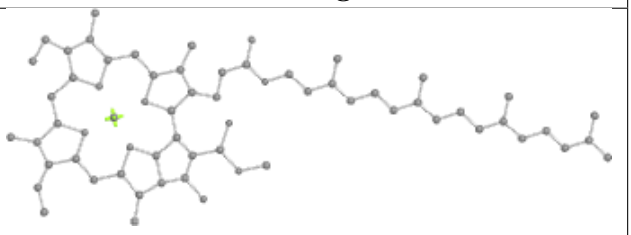
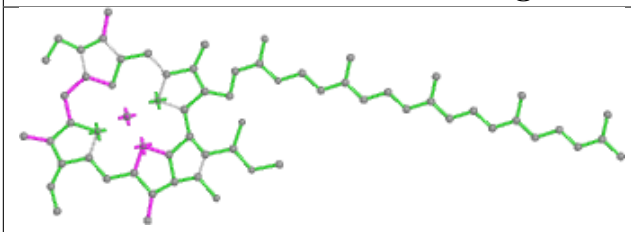
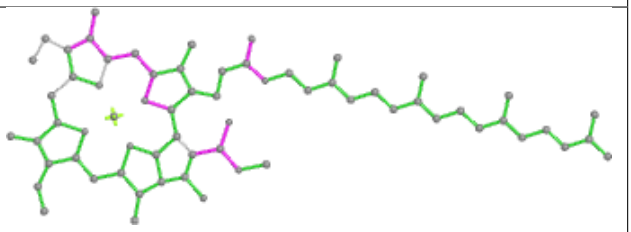
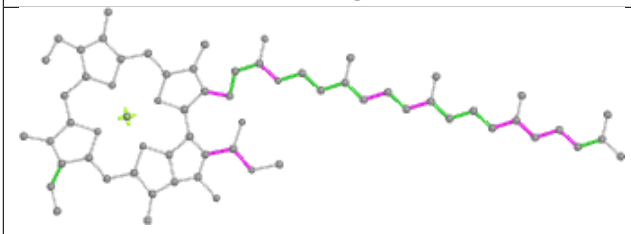
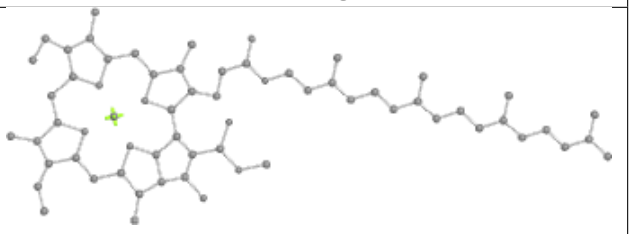
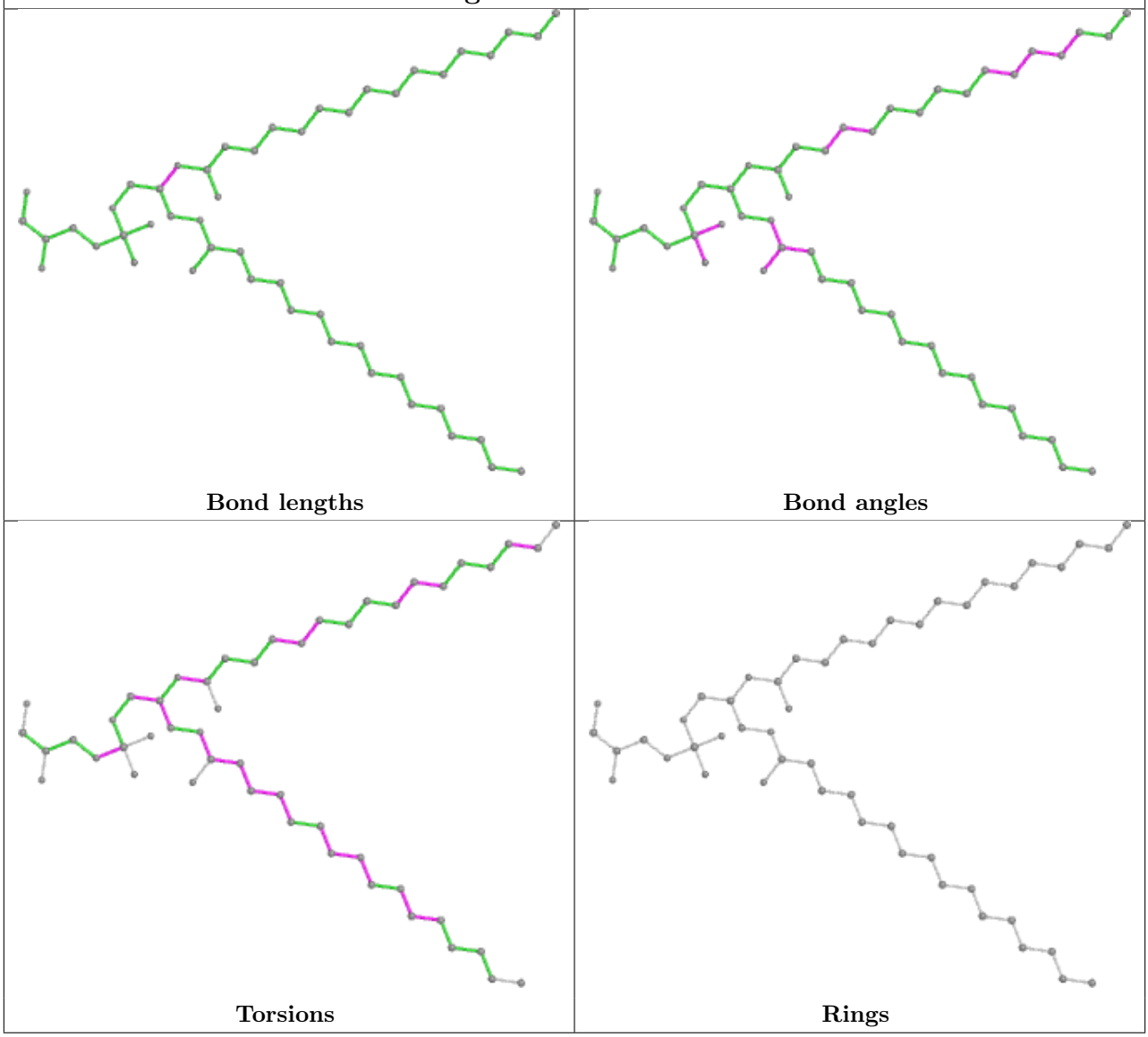


Rings

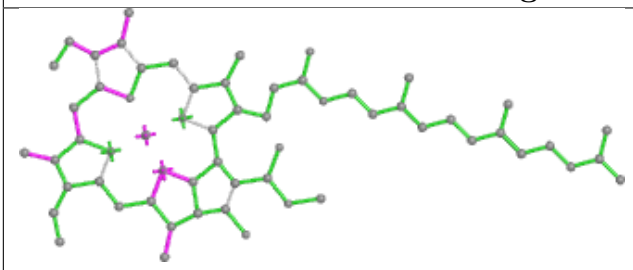
Ligand CLA A 1139	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1109	
 Bond lengths	 Bond angles
 Torsions	 Rings

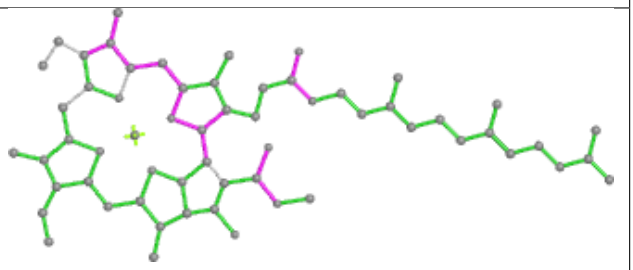
Ligand LHG e 5001



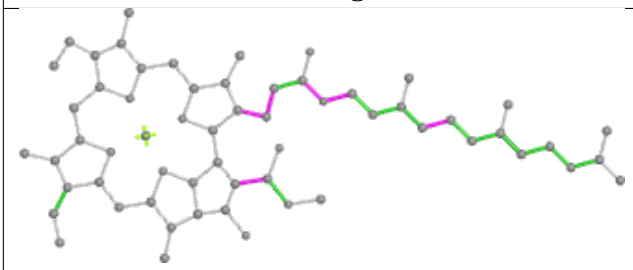
Ligand CLA e 1118



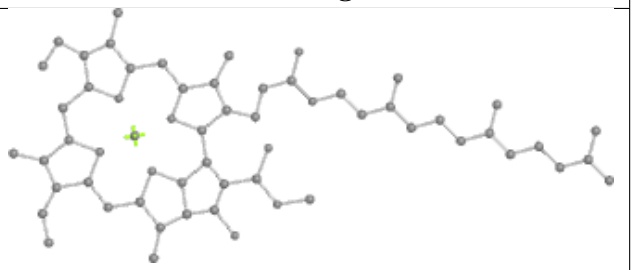
Bond lengths



Bond angles

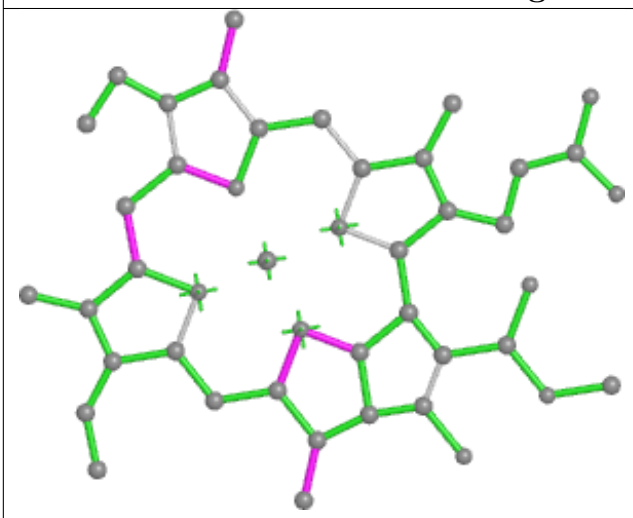


Torsions

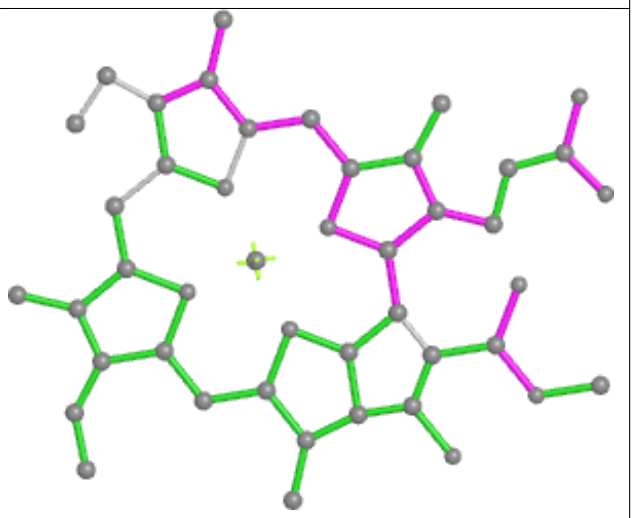


Rings

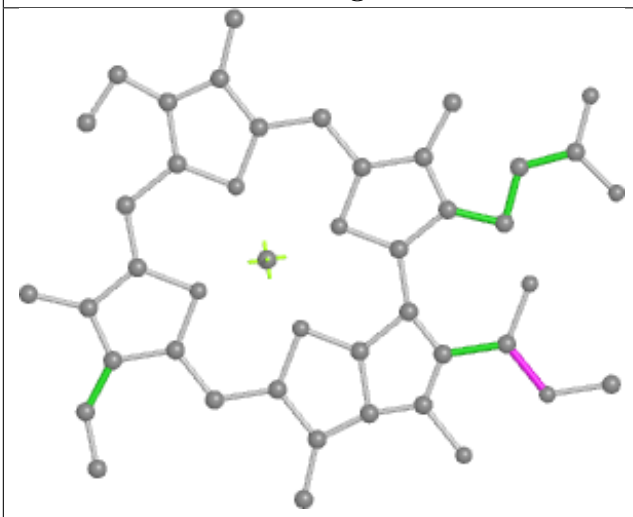
Ligand CLA 3 511



Bond lengths



Bond angles



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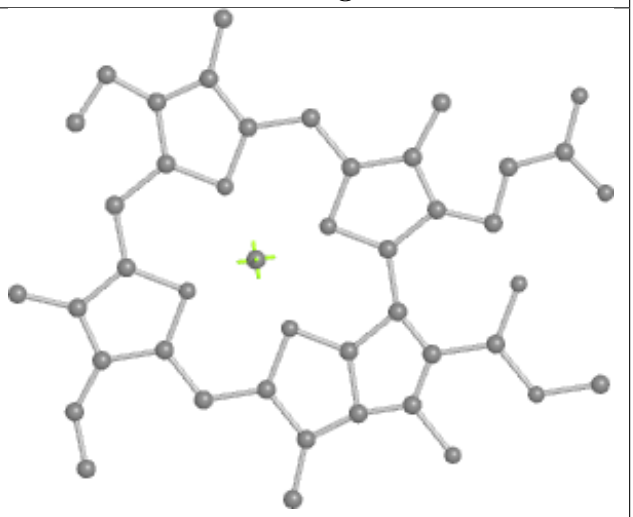
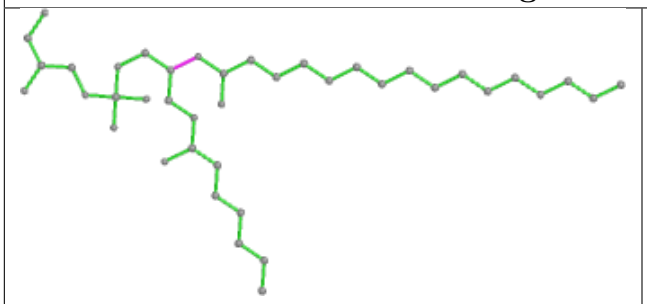
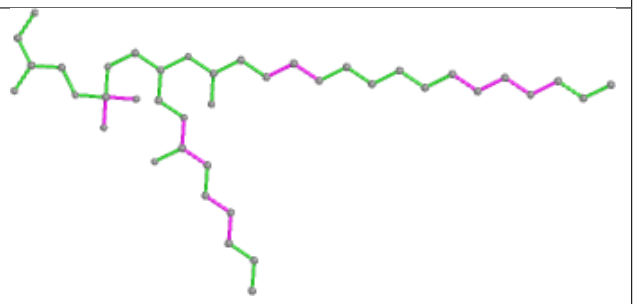


Rings

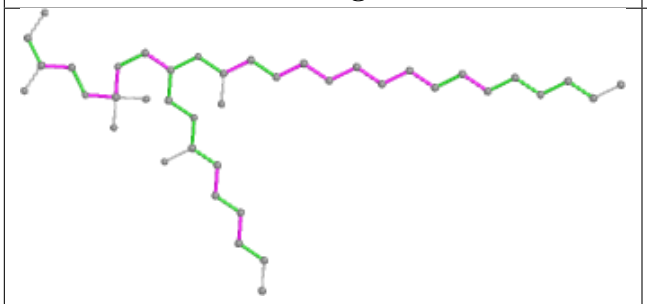
Ligand LHG e 5003



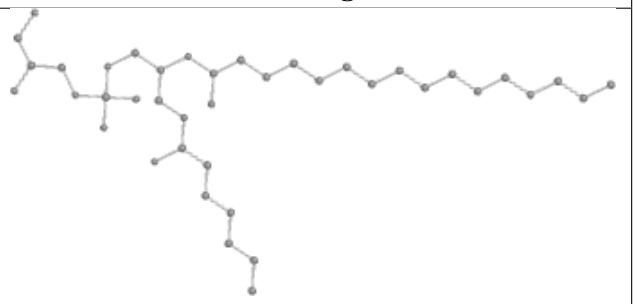
Bond lengths



Bond angles

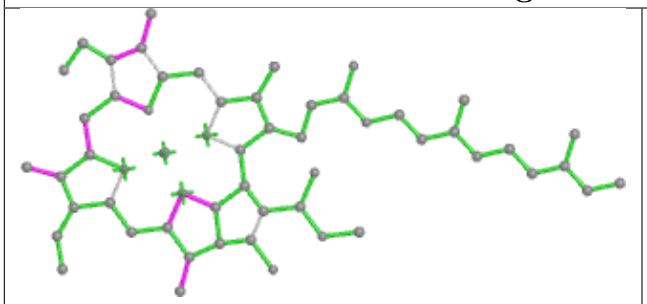


Torsions

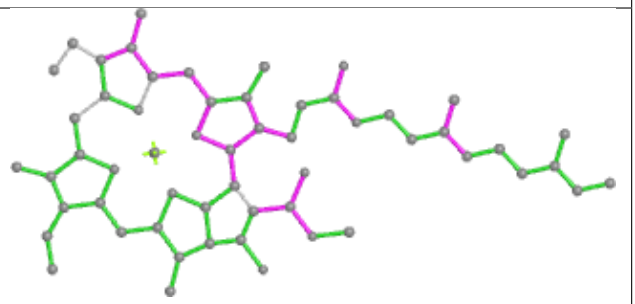


Rings

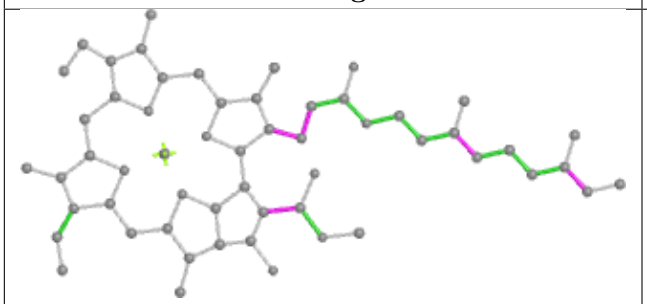
Ligand CLA A 1134



Bond lengths



Bond angles



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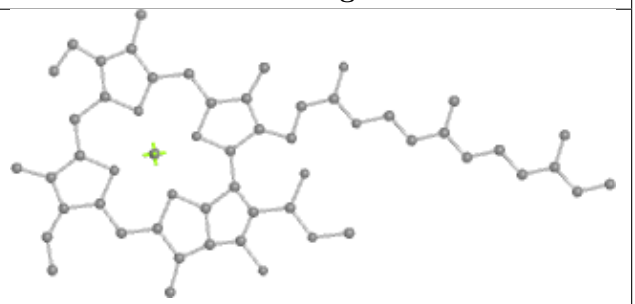
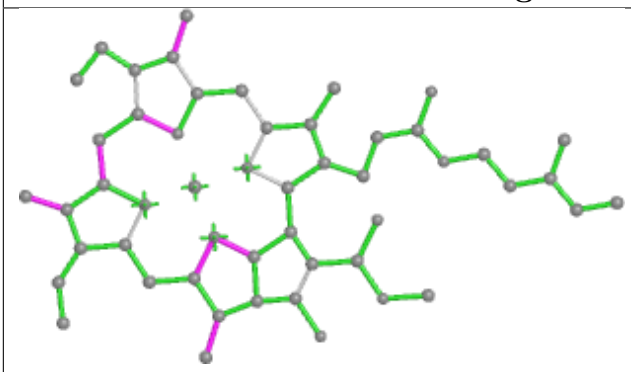
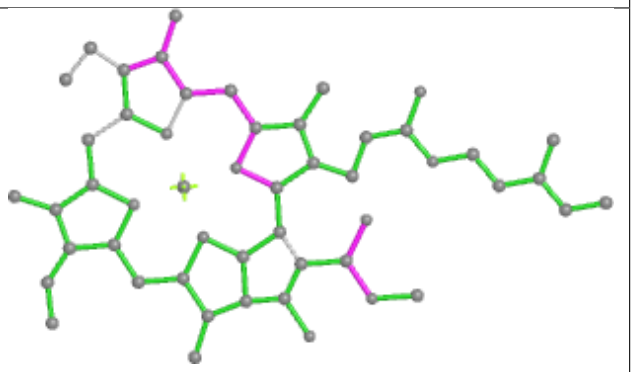
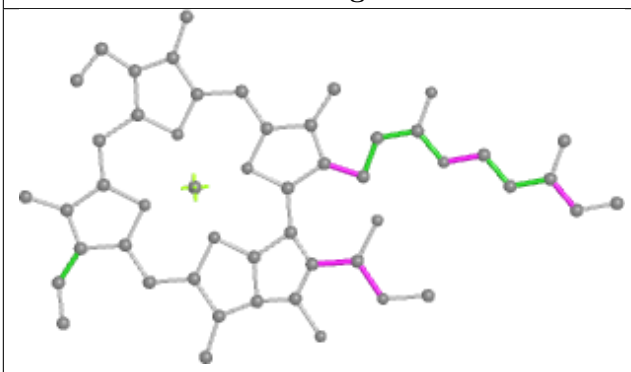
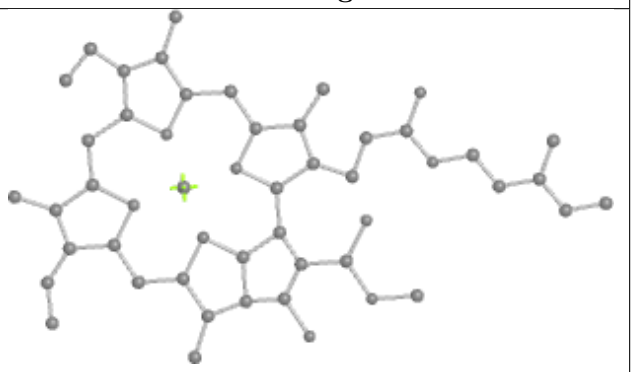
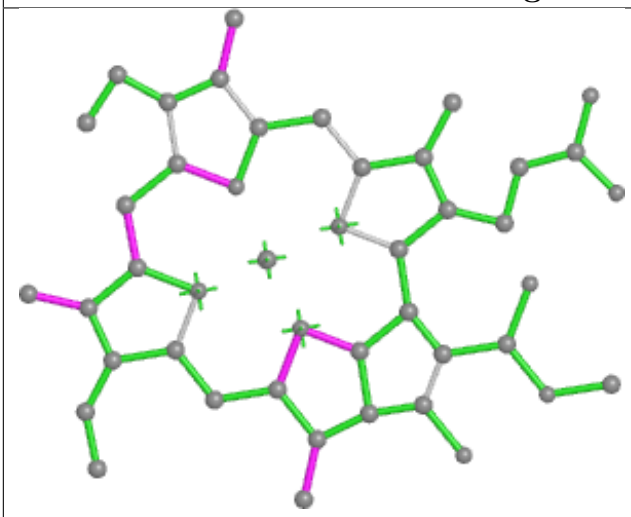


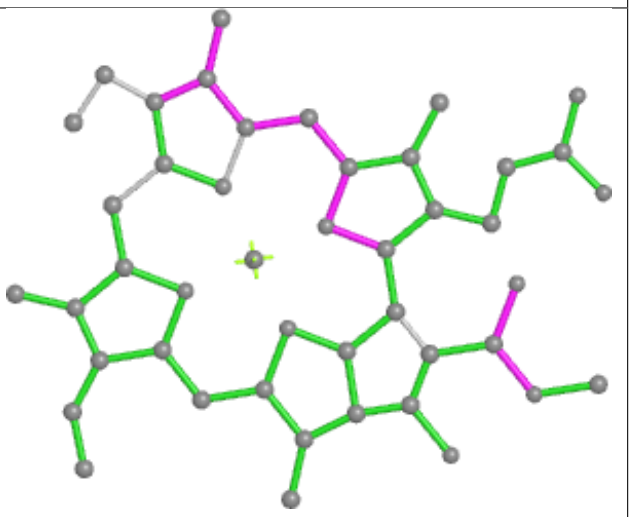
Rings

Ligand CLA B 1212	
 Bond lengths	 Bond angles
 Torsions	 Rings

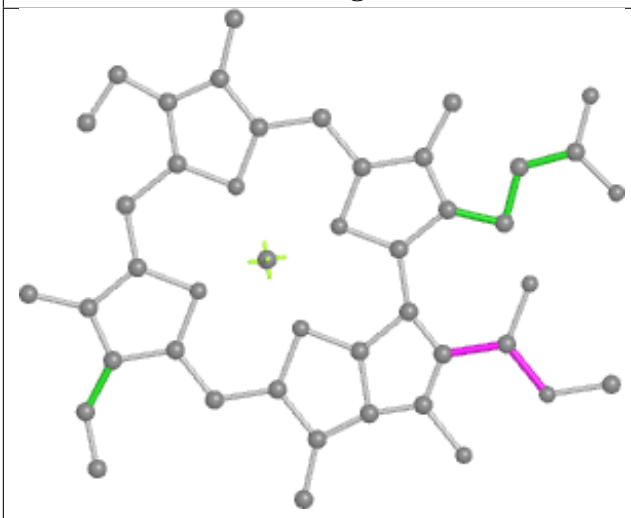
Ligand CLA Y 506



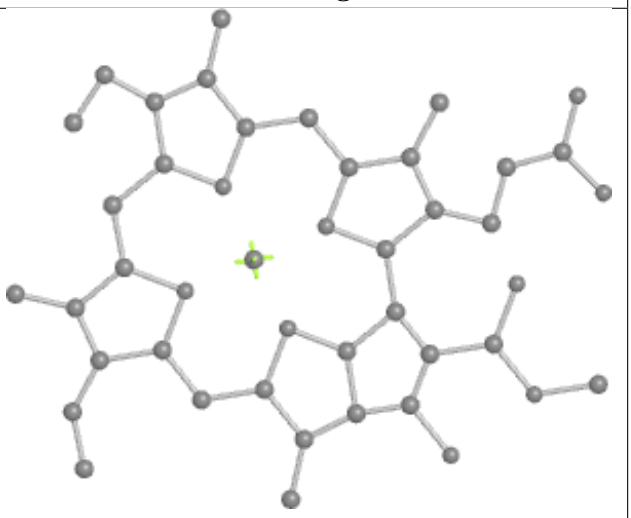
Bond lengths



Bond angles

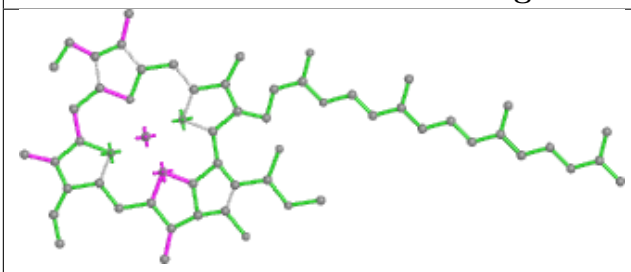


Torsions

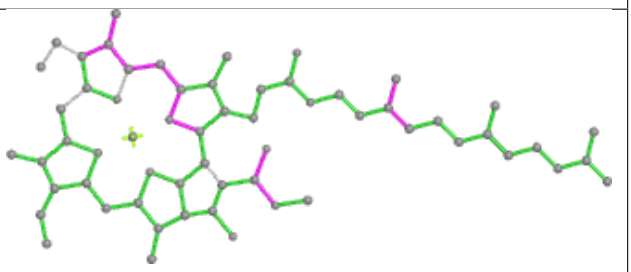


Rings

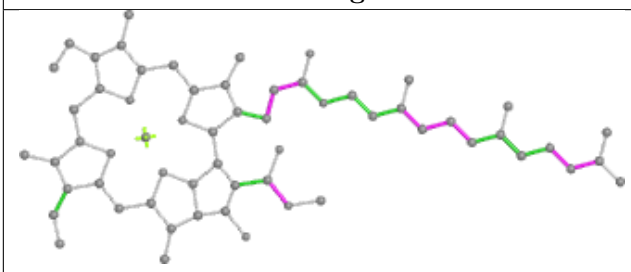
Ligand CLA G 1115



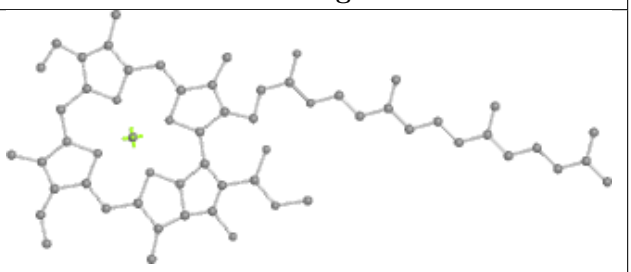
Bond lengths



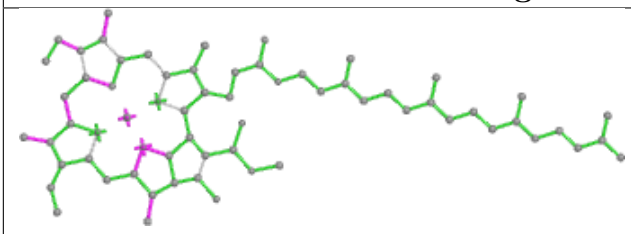
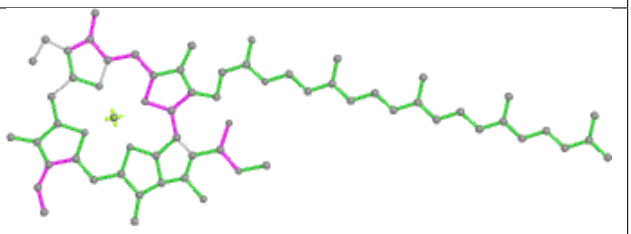
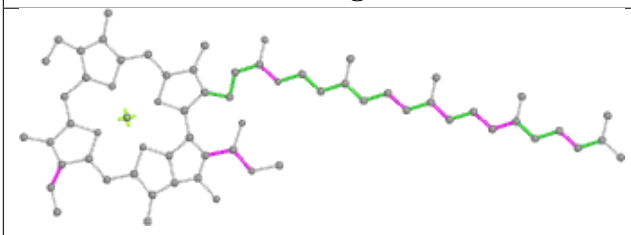
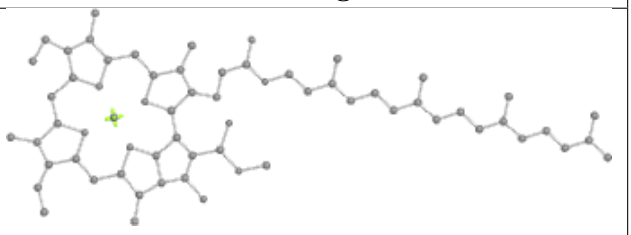
Bond angles

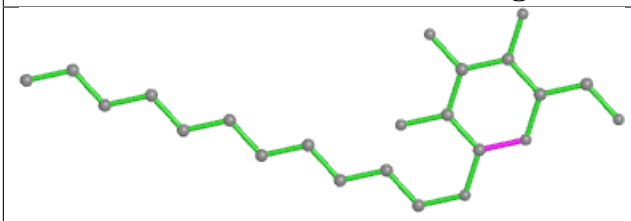
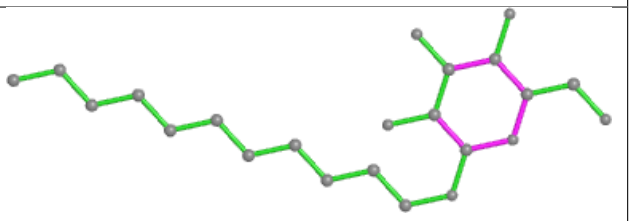
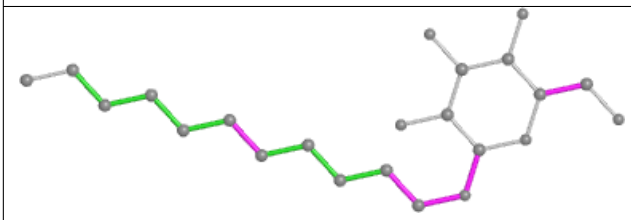
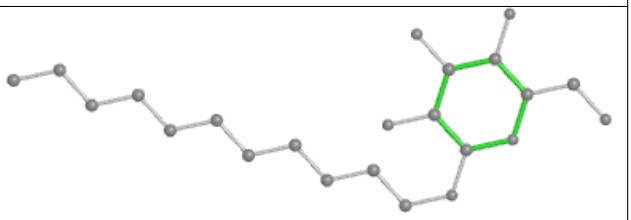


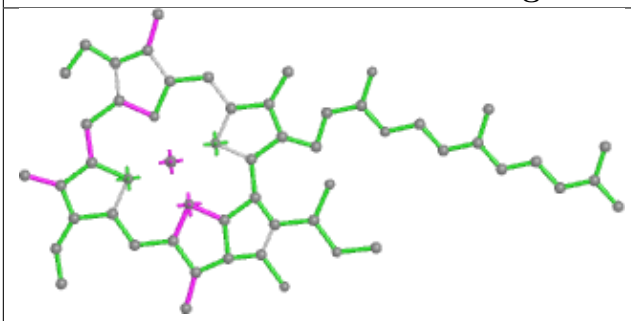
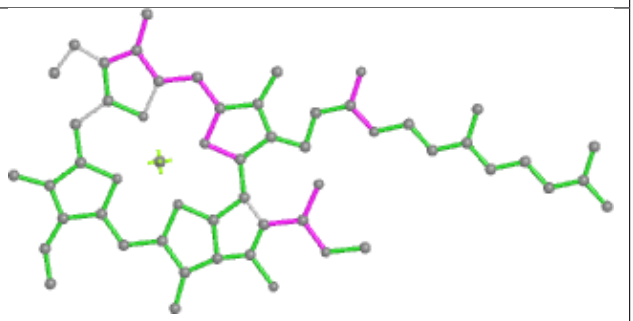
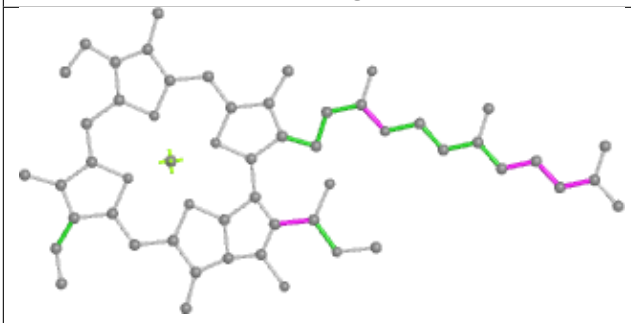
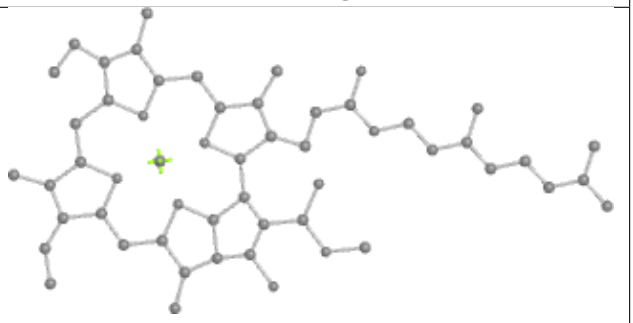
Torsions



Rings

Ligand CLA H 1234	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMU A 1849	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 1211	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

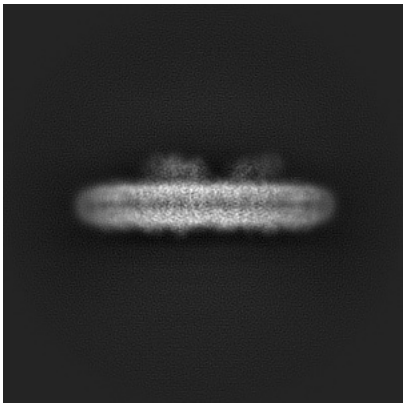
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9994. These allow visual inspection of the internal detail of the map and identification of artifacts.

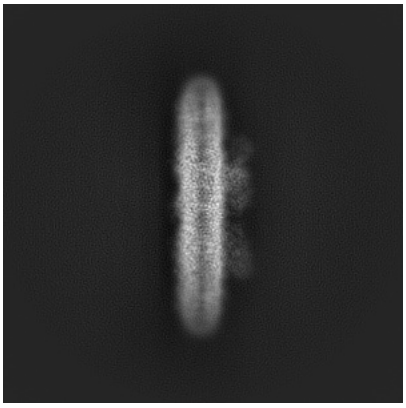
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

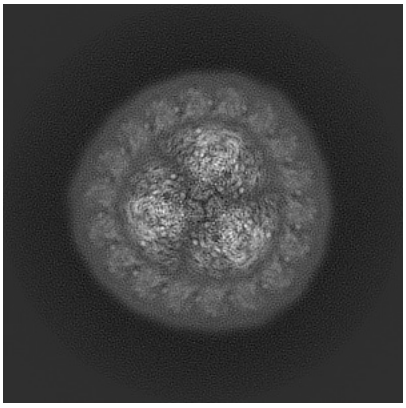
6.1.1 Primary map



X



Y

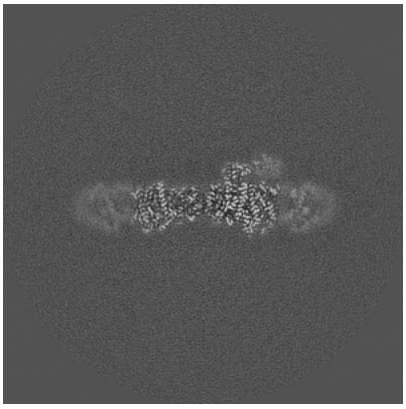


Z

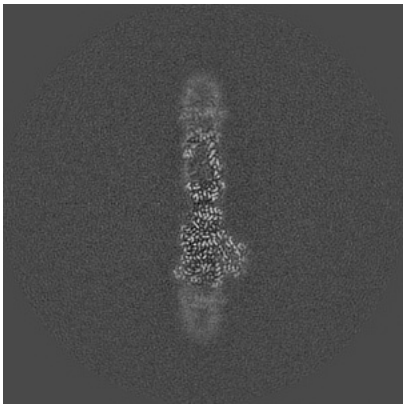
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

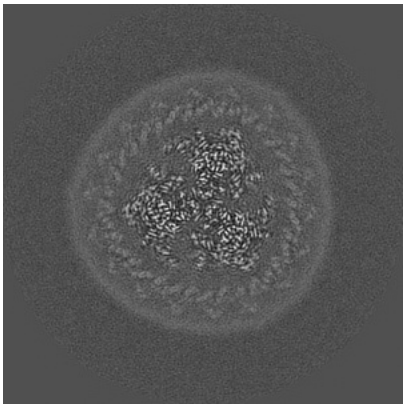
6.2.1 Primary map



X Index: 240



Y Index: 240

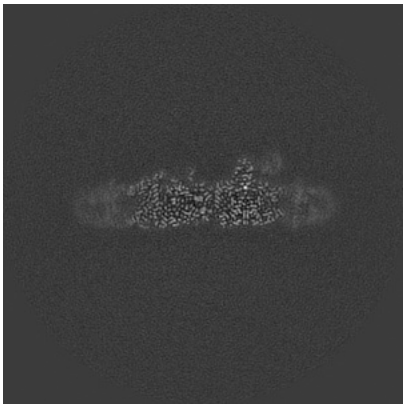


Z Index: 240

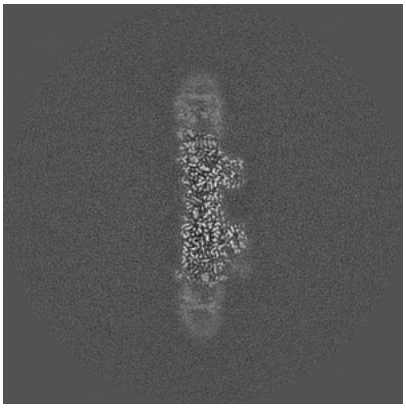
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

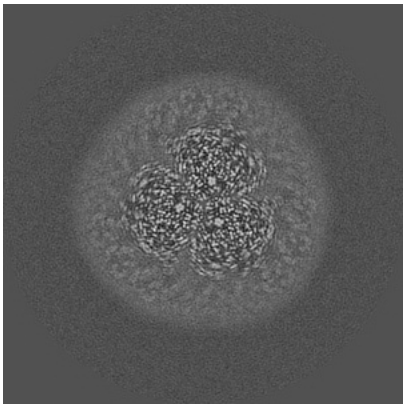
6.3.1 Primary map



X Index: 259



Y Index: 225

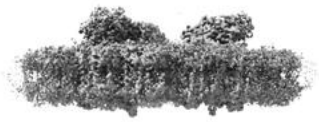


Z Index: 253

The images above show the largest variance slices of the map in three orthogonal directions.

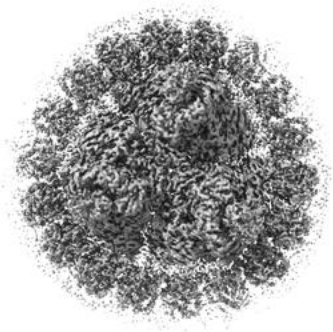
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

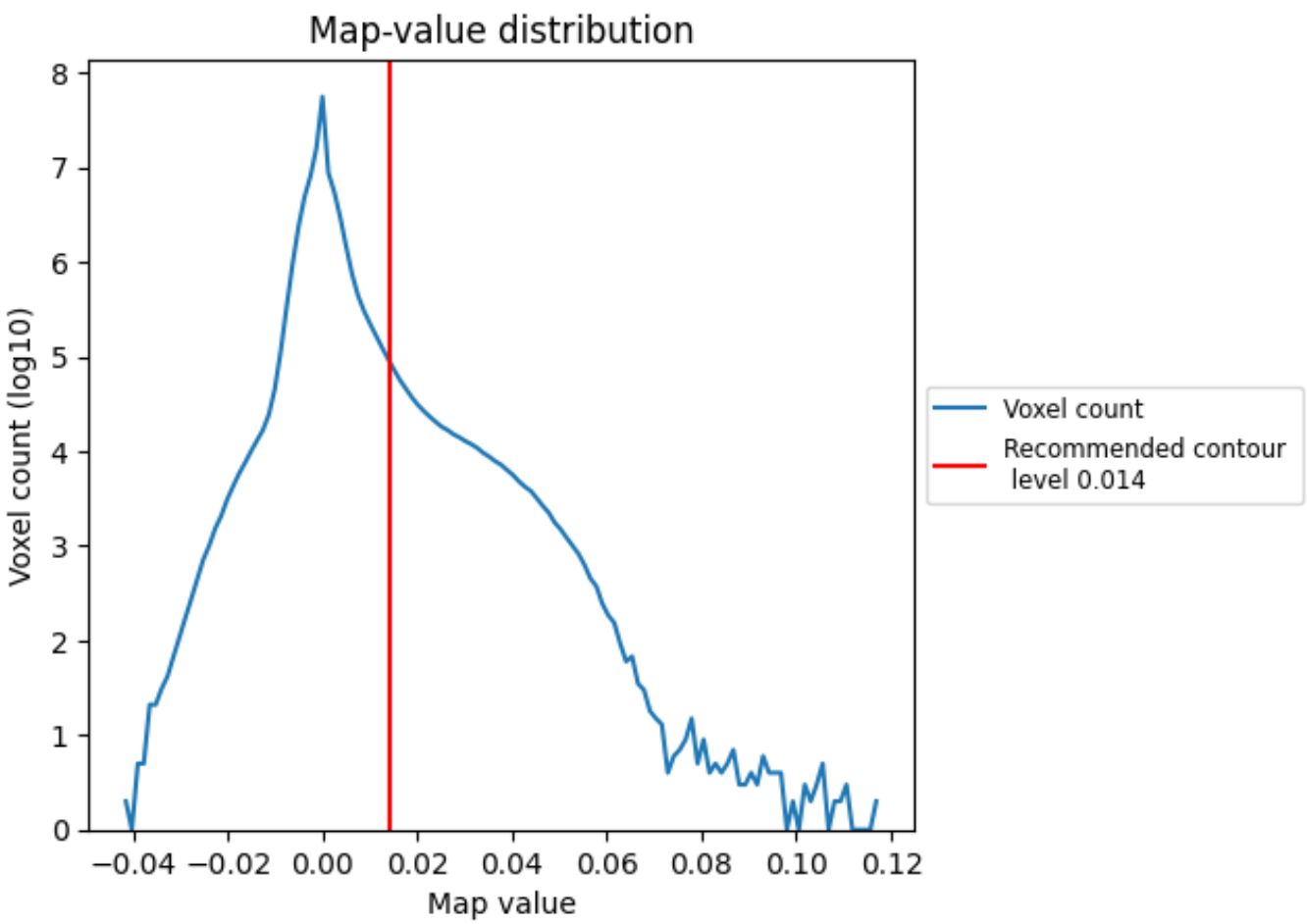
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

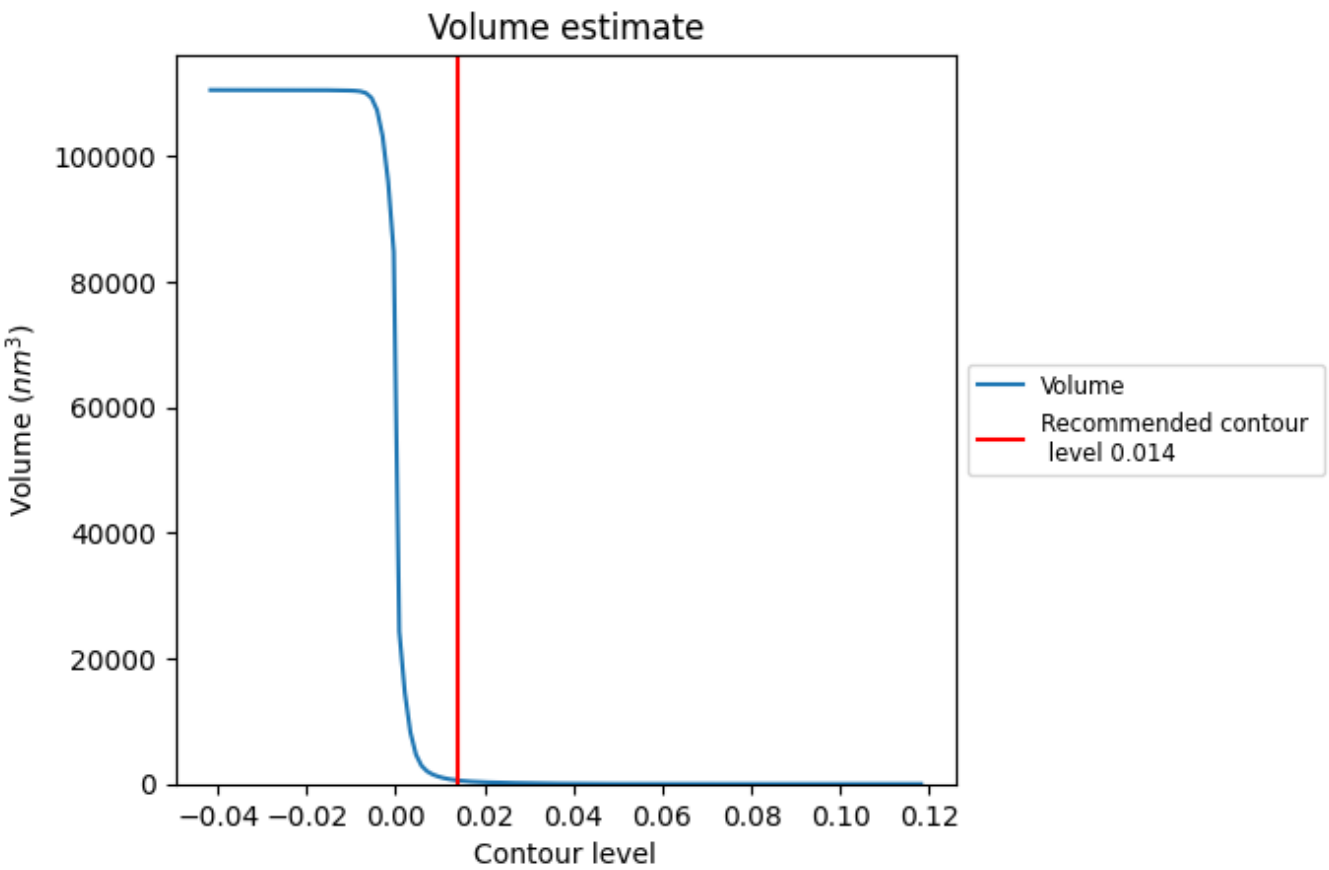
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

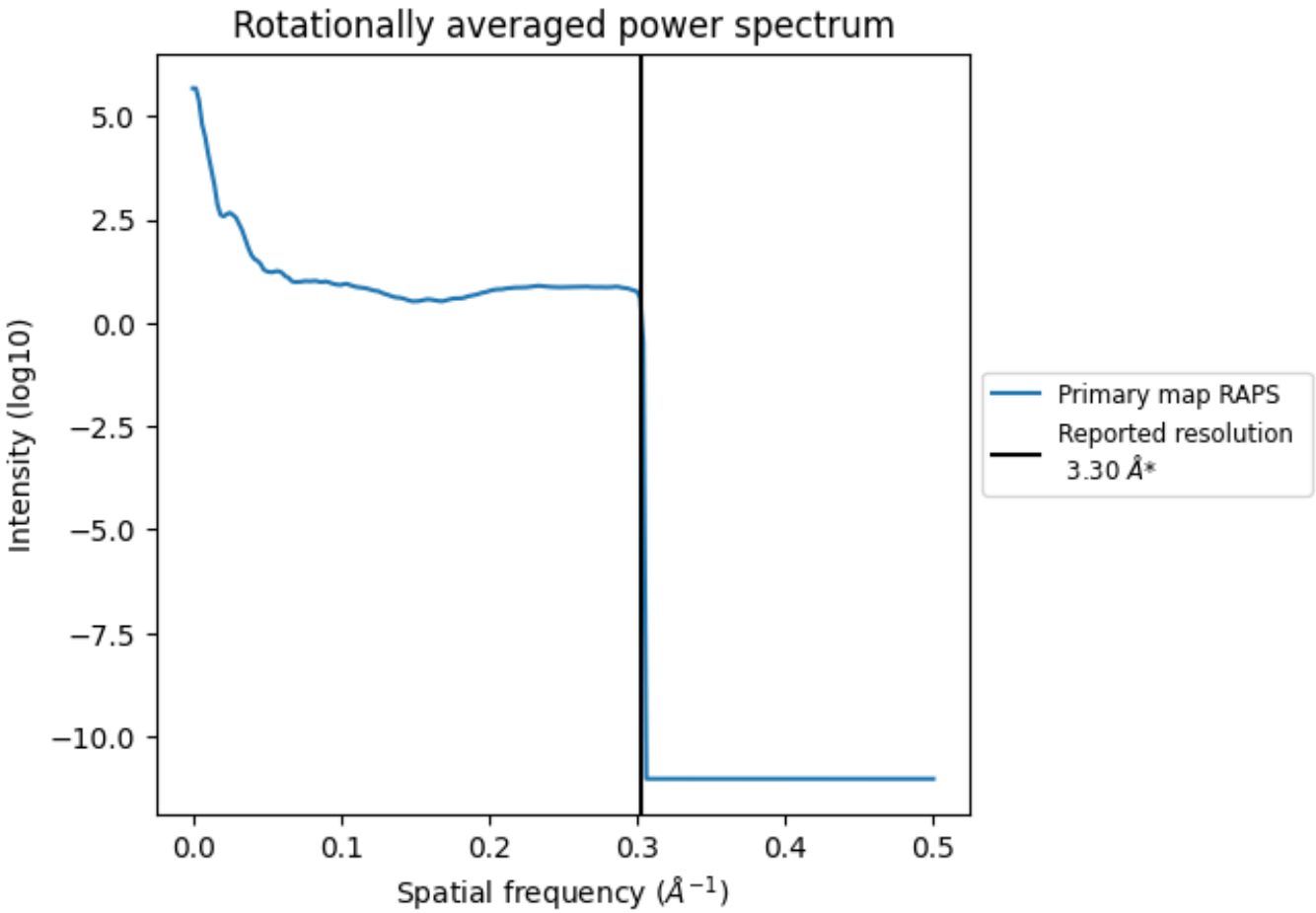
7.2 Volume estimate (i)



The volume at the recommended contour level is 567 nm^3; this corresponds to an approximate mass of 512 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

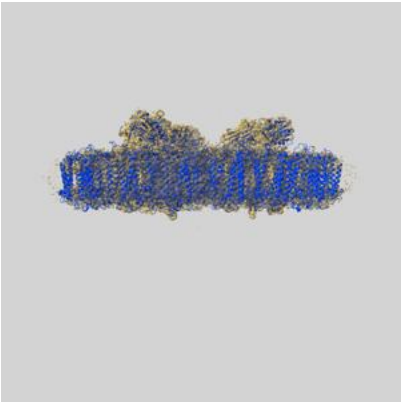
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

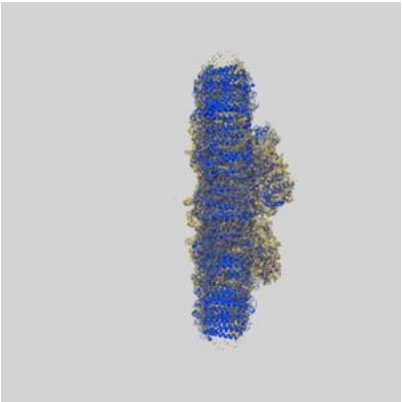
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9994 and PDB model 6KIF. Per-residue inclusion information can be found in section 3 on page 69.

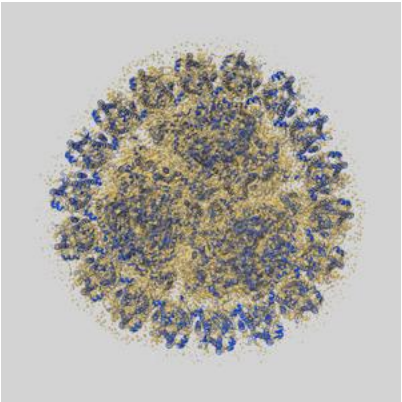
9.1 Map-model overlay (i)



X



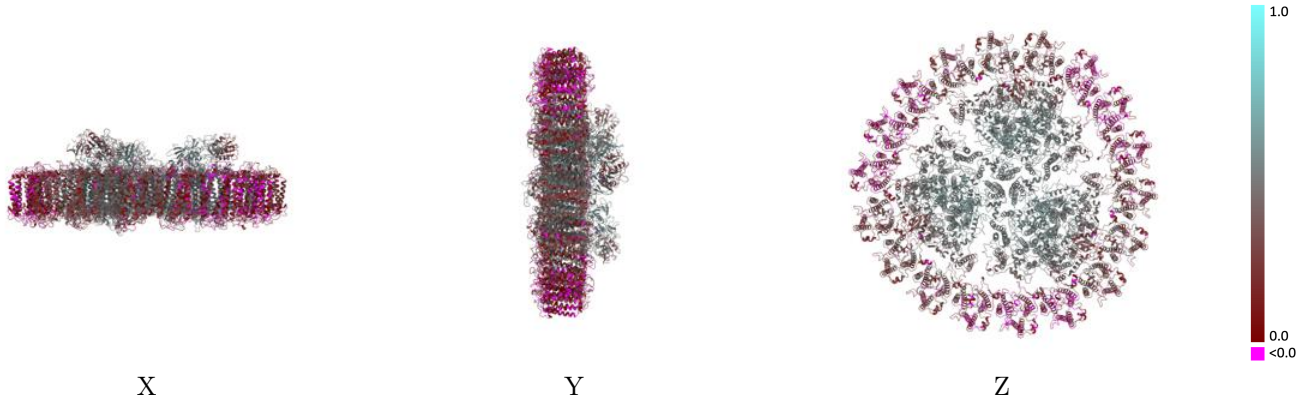
Y



Z

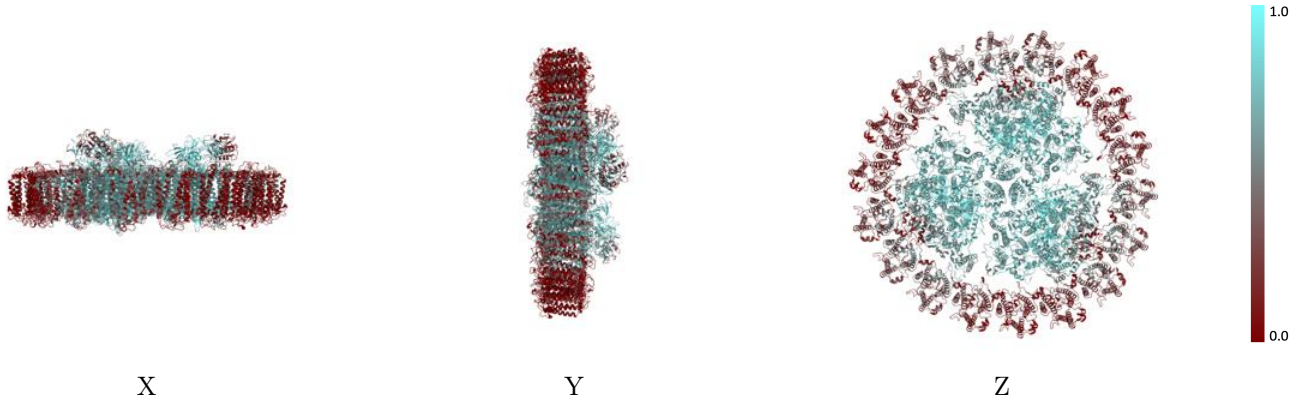
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



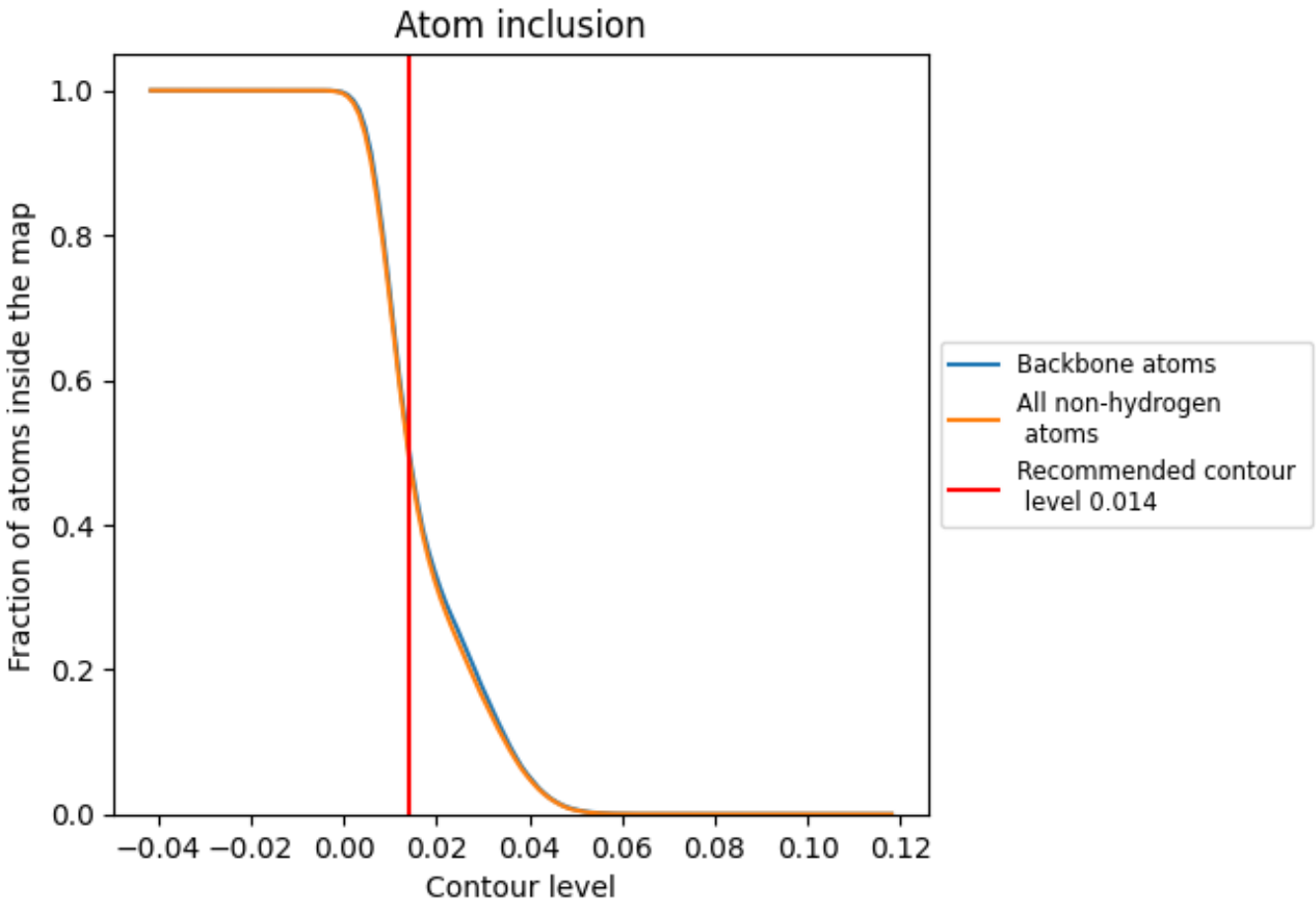
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4953	0.3600
1	0.3257	0.2570
2	0.3296	0.2860
3	0.2646	0.2560
4	0.0824	0.0950
5	0.0787	0.1060
6	0.1419	0.1610
A	0.7563	0.5190
B	0.7499	0.5000
C	0.8750	0.5350
D	0.7924	0.5270
E	0.7269	0.4830
F	0.6904	0.4570
G	0.7554	0.5150
H	0.7495	0.5000
I	0.7507	0.5410
J	0.6790	0.4920
K	0.5304	0.3470
L	0.7814	0.5400
M	0.7061	0.5080
N	0.8717	0.5370
O	0.7933	0.5260
P	0.3706	0.3350
Q	0.7213	0.4810
R	0.6895	0.4570
S	0.7588	0.5440
T	0.6689	0.4930
U	0.5180	0.3330
V	0.7831	0.5400
W	0.6985	0.5040
X	0.3676	0.3320
Y	0.3176	0.2520
Z	0.3279	0.2790
a	0.2614	0.2510
b	0.0832	0.0900

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Chain	Atom inclusion	Q-score
c	0.0758	0.1030
d	0.1459	0.1570
e	0.7556	0.5190
f	0.7495	0.4990
g	0.8683	0.5350
h	0.7924	0.5260
i	0.7175	0.4760
j	0.6886	0.4540
k	0.7534	0.5370
l	0.6689	0.4910
m	0.5359	0.3490
n	0.7855	0.5390
o	0.7023	0.5050
p	0.3781	0.3340
q	0.3243	0.2590
r	0.3347	0.2880
s	0.2640	0.2580
t	0.0809	0.0950
u	0.0767	0.1070
v	0.1482	0.1590