wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 05:56 AM JST

PDB ID	:	6KIG
EMDB ID	:	EMD-9995
Title	:	Structure of cyanobacterial photosystem I-IsiA 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	:	2.90 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 ⓘ 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 ⓘ) were used in the production of this report:

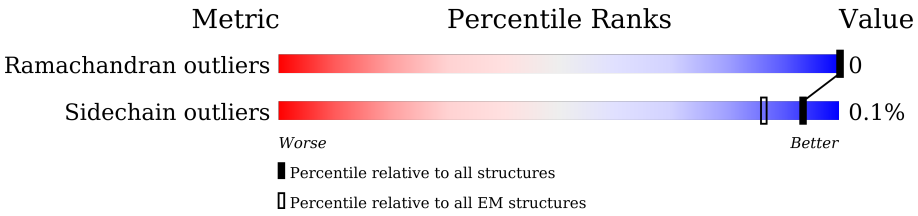
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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)
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	98%
1	G	763	98%
1	e	763	98%
2	B	734	100%
2	H	734	100%
2	f	734	100%
3	C	81	99%
3	N	81	99%
3	g	81	99%

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Mol	Chain	Length	Quality of chain
4	D	141	100%
4	O	141	100%
4	h	141	100%
5	E	75	5% 95% 5%
5	Q	75	5% 95% 5%
5	i	75	5% 95% 5%
6	F	159	86% 14%
6	R	159	86% 14%
6	j	159	86% 14%
7	I	38	5% 100%
7	S	38	5% 100%
7	k	38	5% 100%
8	J	41	100%
8	T	41	100%
8	l	41	100%
9	K	84	15% 93% 7%
9	U	84	13% 93% 7%
9	m	84	14% 93% 7%
10	L	166	99%
10	V	166	99%
10	n	166	99%
11	M	29	100%
11	W	29	100%
11	o	29	100%
12	1	342	49% 99%

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Mol	Chain	Length	Quality of chain
12	2	342	40% 99%
12	3	342	59% 99%
12	4	342	94% 99%
12	5	342	98% 99%
12	6	342	91% 99%
12	Y	342	49% 99%
12	Z	342	38% 99%
12	a	342	60% 99%
12	b	342	95% 99%
12	c	342	98% 99%
12	d	342	90% 99%
12	q	342	51% 99%
12	r	342	41% 99%
12	s	342	59% 99%
12	t	342	93% 99%
12	u	342	99% 99%
12	v	342	90% 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
13	CLA	1	501	X	-	-	-
13	CLA	1	502	X	-	-	-
13	CLA	1	503	X	-	-	-
13	CLA	1	504	X	-	-	-
13	CLA	1	505	X	-	-	-
13	CLA	1	506	X	-	-	-
13	CLA	1	507	X	-	-	-
13	CLA	1	508	X	-	-	-

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	6	508	X	-	-	-
13	CLA	6	509	X	-	-	-
13	CLA	6	510	X	-	-	-
13	CLA	6	511	X	-	-	-
13	CLA	6	512	X	-	-	-
13	CLA	6	513	X	-	-	-
13	CLA	6	516	X	-	-	-
13	CLA	6	517	X	-	-	-
13	CLA	6	518	X	-	-	-
13	CLA	6	519	X	-	-	-
13	CLA	A	1011	X	-	-	-
13	CLA	A	1013	X	-	-	-
13	CLA	A	1022	X	-	-	-
13	CLA	A	1101	X	-	-	-
13	CLA	A	1102	X	-	-	-
13	CLA	A	1103	X	-	-	-
13	CLA	A	1104	X	-	-	-
13	CLA	A	1105	X	-	-	-
13	CLA	A	1106	X	-	-	-
13	CLA	A	1107	X	-	-	-
13	CLA	A	1108	X	-	-	-
13	CLA	A	1109	X	-	-	-
13	CLA	A	1110	X	-	-	-
13	CLA	A	1111	X	-	-	-
13	CLA	A	1112	X	-	-	-
13	CLA	A	1113	X	-	-	-
13	CLA	A	1114	X	-	-	-
13	CLA	A	1115	X	-	-	-
13	CLA	A	1116	X	-	-	-
13	CLA	A	1117	X	-	-	-
13	CLA	A	1118	X	-	-	-
13	CLA	A	1119	X	-	-	-
13	CLA	A	1120	X	-	-	-
13	CLA	A	1121	X	-	-	-
13	CLA	A	1122	X	-	-	-
13	CLA	A	1123	X	-	-	-
13	CLA	A	1124	X	-	-	-
13	CLA	A	1125	X	-	-	-
13	CLA	A	1126	X	-	-	-
13	CLA	A	1127	X	-	-	-
13	CLA	A	1128	X	-	-	-
13	CLA	A	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	1130	X	-	-	-
13	CLA	A	1131	X	-	-	-
13	CLA	A	1132	X	-	-	-
13	CLA	A	1133	X	-	-	-
13	CLA	A	1134	X	-	-	-
13	CLA	A	1135	X	-	-	-
13	CLA	A	1136	X	-	-	-
13	CLA	A	1137	X	-	-	-
13	CLA	A	1138	X	-	-	-
13	CLA	A	1139	X	-	-	-
13	CLA	A	1140	X	-	-	-
13	CLA	A	1237	X	-	-	-
13	CLA	A	1801	X	-	-	-
13	CLA	B	1012	X	-	-	-
13	CLA	B	1021	X	-	-	-
13	CLA	B	1023	X	-	-	-
13	CLA	B	1201	X	-	-	-
13	CLA	B	1202	X	-	-	-
13	CLA	B	1203	X	-	-	-
13	CLA	B	1204	X	-	-	-
13	CLA	B	1205	X	-	-	-
13	CLA	B	1206	X	-	-	-
13	CLA	B	1207	X	-	-	-
13	CLA	B	1208	X	-	-	-
13	CLA	B	1209	X	-	-	-
13	CLA	B	1210	X	-	-	-
13	CLA	B	1211	X	-	-	-
13	CLA	B	1212	X	-	-	-
13	CLA	B	1213	X	-	-	-
13	CLA	B	1214	X	-	-	-
13	CLA	B	1215	X	-	-	-
13	CLA	B	1216	X	-	-	-
13	CLA	B	1217	X	-	-	-
13	CLA	B	1218	X	-	-	-
13	CLA	B	1219	X	-	-	-
13	CLA	B	1220	X	-	-	-
13	CLA	B	1221	X	-	-	-
13	CLA	B	1222	X	-	-	-
13	CLA	B	1223	X	-	-	-
13	CLA	B	1224	X	-	-	-
13	CLA	B	1225	X	-	-	-
13	CLA	B	1226	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	1227	X	-	-	-
13	CLA	B	1228	X	-	-	-
13	CLA	B	1229	X	-	-	-
13	CLA	B	1230	X	-	-	-
13	CLA	B	1231	X	-	-	-
13	CLA	B	1232	X	-	-	-
13	CLA	B	1234	X	-	-	-
13	CLA	B	1235	X	-	-	-
13	CLA	B	1238	X	-	-	-
13	CLA	B	1239	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	F	1302	X	-	-	-
13	CLA	G	1011	X	-	-	-
13	CLA	G	1013	X	-	-	-
13	CLA	G	1022	X	-	-	-
13	CLA	G	1101	X	-	-	-
13	CLA	G	1102	X	-	-	-
13	CLA	G	1103	X	-	-	-
13	CLA	G	1104	X	-	-	-
13	CLA	G	1105	X	-	-	-
13	CLA	G	1106	X	-	-	-
13	CLA	G	1107	X	-	-	-
13	CLA	G	1108	X	-	-	-
13	CLA	G	1109	X	-	-	-
13	CLA	G	1110	X	-	-	-
13	CLA	G	1111	X	-	-	-
13	CLA	G	1112	X	-	-	-
13	CLA	G	1113	X	-	-	-
13	CLA	G	1114	X	-	-	-
13	CLA	G	1115	X	-	-	-
13	CLA	G	1116	X	-	-	-
13	CLA	G	1117	X	-	-	-
13	CLA	G	1118	X	-	-	-
13	CLA	G	1119	X	-	-	-
13	CLA	G	1120	X	-	-	-
13	CLA	G	1121	X	-	-	-
13	CLA	G	1122	X	-	-	-
13	CLA	G	1123	X	-	-	-
13	CLA	G	1124	X	-	-	-
13	CLA	G	1125	X	-	-	-
13	CLA	G	1126	X	-	-	-
13	CLA	G	1127	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	H	1225	X	-	-	-
13	CLA	H	1226	X	-	-	-
13	CLA	H	1227	X	-	-	-
13	CLA	H	1228	X	-	-	-
13	CLA	H	1229	X	-	-	-
13	CLA	H	1230	X	-	-	-
13	CLA	H	1231	X	-	-	-
13	CLA	H	1232	X	-	-	-
13	CLA	H	1234	X	-	-	-
13	CLA	H	1235	X	-	-	-
13	CLA	H	1238	X	-	-	-
13	CLA	H	1239	X	-	-	-
13	CLA	J	1302	X	-	-	-
13	CLA	J	1303	X	-	-	-
13	CLA	K	1103	X	-	-	-
13	CLA	K	1105	X	-	-	-
13	CLA	K	1401	X	-	-	-
13	CLA	L	1501	X	-	-	-
13	CLA	L	1502	X	-	-	-
13	CLA	L	1503	X	-	-	-
13	CLA	R	1301	X	-	-	-
13	CLA	R	1302	X	-	-	-
13	CLA	T	1302	X	-	-	-
13	CLA	T	1303	X	-	-	-
13	CLA	U	1103	X	-	-	-
13	CLA	U	1105	X	-	-	-
13	CLA	U	1401	X	-	-	-
13	CLA	V	1501	X	-	-	-
13	CLA	V	1502	X	-	-	-
13	CLA	V	1503	X	-	-	-
13	CLA	Y	501	X	-	-	-
13	CLA	Y	502	X	-	-	-
13	CLA	Y	503	X	-	-	-
13	CLA	Y	504	X	-	-	-
13	CLA	Y	505	X	-	-	-
13	CLA	Y	506	X	-	-	-
13	CLA	Y	507	X	-	-	-
13	CLA	Y	508	X	-	-	-
13	CLA	Y	509	X	-	-	-
13	CLA	Y	510	X	-	-	-
13	CLA	Y	511	X	-	-	-
13	CLA	Y	512	X	-	-	-

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	d	512	X	-	-	-
13	CLA	d	513	X	-	-	-
13	CLA	d	516	X	-	-	-
13	CLA	d	517	X	-	-	-
13	CLA	d	518	X	-	-	-
13	CLA	d	519	X	-	-	-
13	CLA	e	1011	X	-	-	-
13	CLA	e	1013	X	-	-	-
13	CLA	e	1022	X	-	-	-
13	CLA	e	1101	X	-	-	-
13	CLA	e	1102	X	-	-	-
13	CLA	e	1103	X	-	-	-
13	CLA	e	1104	X	-	-	-
13	CLA	e	1105	X	-	-	-
13	CLA	e	1106	X	-	-	-
13	CLA	e	1107	X	-	-	-
13	CLA	e	1108	X	-	-	-
13	CLA	e	1109	X	-	-	-
13	CLA	e	1110	X	-	-	-
13	CLA	e	1111	X	-	-	-
13	CLA	e	1112	X	-	-	-
13	CLA	e	1113	X	-	-	-
13	CLA	e	1114	X	-	-	-
13	CLA	e	1115	X	-	-	-
13	CLA	e	1116	X	-	-	-
13	CLA	e	1117	X	-	-	-
13	CLA	e	1118	X	-	-	-
13	CLA	e	1119	X	-	-	-
13	CLA	e	1120	X	-	-	-
13	CLA	e	1121	X	-	-	-
13	CLA	e	1122	X	-	-	-
13	CLA	e	1123	X	-	-	-
13	CLA	e	1124	X	-	-	-
13	CLA	e	1125	X	-	-	-
13	CLA	e	1126	X	-	-	-
13	CLA	e	1127	X	-	-	-
13	CLA	e	1128	X	-	-	-
13	CLA	e	1129	X	-	-	-
13	CLA	e	1130	X	-	-	-
13	CLA	e	1131	X	-	-	-
13	CLA	e	1132	X	-	-	-
13	CLA	e	1133	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	e	1134	X	-	-	-
13	CLA	e	1135	X	-	-	-
13	CLA	e	1136	X	-	-	-
13	CLA	e	1137	X	-	-	-
13	CLA	e	1138	X	-	-	-
13	CLA	e	1139	X	-	-	-
13	CLA	e	1140	X	-	-	-
13	CLA	e	1237	X	-	-	-
13	CLA	e	1801	X	-	-	-
13	CLA	f	1012	X	-	-	-
13	CLA	f	1021	X	-	-	-
13	CLA	f	1023	X	-	-	-
13	CLA	f	1201	X	-	-	-
13	CLA	f	1202	X	-	-	-
13	CLA	f	1203	X	-	-	-
13	CLA	f	1204	X	-	-	-
13	CLA	f	1205	X	-	-	-
13	CLA	f	1206	X	-	-	-
13	CLA	f	1207	X	-	-	-
13	CLA	f	1208	X	-	-	-
13	CLA	f	1209	X	-	-	-
13	CLA	f	1210	X	-	-	-
13	CLA	f	1211	X	-	-	-
13	CLA	f	1212	X	-	-	-
13	CLA	f	1213	X	-	-	-
13	CLA	f	1214	X	-	-	-
13	CLA	f	1215	X	-	-	-
13	CLA	f	1216	X	-	-	-
13	CLA	f	1217	X	-	-	-
13	CLA	f	1218	X	-	-	-
13	CLA	f	1219	X	-	-	-
13	CLA	f	1220	X	-	-	-
13	CLA	f	1221	X	-	-	-
13	CLA	f	1222	X	-	-	-
13	CLA	f	1223	X	-	-	-
13	CLA	f	1224	X	-	-	-
13	CLA	f	1225	X	-	-	-
13	CLA	f	1226	X	-	-	-
13	CLA	f	1227	X	-	-	-
13	CLA	f	1228	X	-	-	-
13	CLA	f	1229	X	-	-	-
13	CLA	f	1230	X	-	-	-

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

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

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

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 143022 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
1	A	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		
1	G	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		
1	e	751	Total	C	N	O	S	0	0
			5865	3847	1002	999	17		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called PsaM.

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

- Molecule 12 is a protein called Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	2	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	3	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

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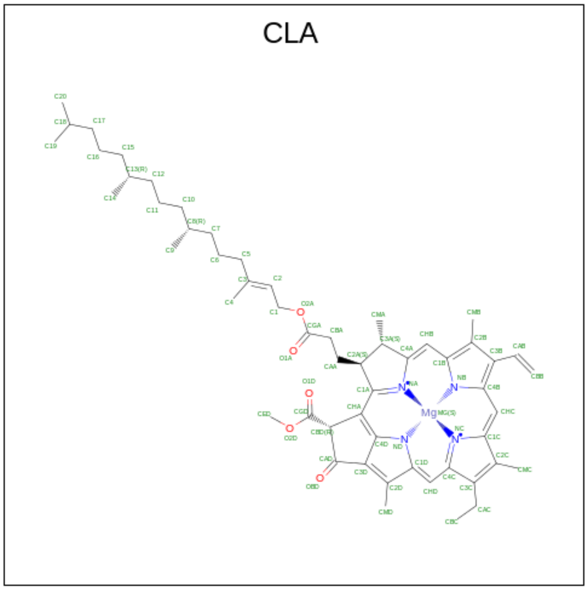
Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	5	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	6	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	Y	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	Z	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	a	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	b	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	c	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	d	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	q	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	r	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	s	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	t	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	u	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		
12	v	339	Total	C	N	O	S	0	0
			2605	1722	428	448	7		

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	A	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	B	1	Total 2550	C 2140	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms	AltConf
13	B	1	Total C Mg N O 2550 2140 41 164 205	0
13	B	1	Total C Mg N O 2550 2140 41 164 205	0
13	B	1	Total C Mg N O 2550 2140 41 164 205	0
13	B	1	Total C Mg N O 2550 2140 41 164 205	0
13	B	1	Total C Mg N O 2550 2140 41 164 205	0
13	B	1	Total C Mg N O 2550 2140 41 164 205	0
13	B	1	Total C Mg N O 2550 2140 41 164 205	0
13	B	1	Total C Mg N O 2550 2140 41 164 205	0
13	B	1	Total C Mg N O 2550 2140 41 164 205	0
13	F	1	Total C Mg N O 110 90 2 8 10	0
13	F	1	Total C Mg N O 110 90 2 8 10	0
13	J	1	Total C Mg N O 123 103 2 8 10	0
13	J	1	Total C Mg N O 123 103 2 8 10	0
13	K	1	Total C Mg N O 150 120 3 12 15	0
13	K	1	Total C Mg N O 150 120 3 12 15	0
13	K	1	Total C Mg N O 150 120 3 12 15	0
13	L	1	Total C Mg N O 190 160 3 12 15	0
13	L	1	Total C Mg N O 190 160 3 12 15	0
13	L	1	Total C Mg N O 190 160 3 12 15	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0

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Mol	Chain	Residues	Atoms	AltConf
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	1	1	Total C Mg N O 951 781 17 68 85	0
13	2	1	Total C Mg N O 993 823 17 68 85	0
13	2	1	Total C Mg N O 993 823 17 68 85	0
13	2	1	Total C Mg N O 993 823 17 68 85	0
13	2	1	Total C Mg N O 993 823 17 68 85	0
13	2	1	Total C Mg N O 993 823 17 68 85	0
13	2	1	Total C Mg N O 993 823 17 68 85	0

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Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	2	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	3	1	Total 950	C 780	Mg 17	N 68	O 85	0
13	3	1	Total 950	C 780	Mg 17	N 68	O 85	0
13	3	1	Total 950	C 780	Mg 17	N 68	O 85	0
13	3	1	Total 950	C 780	Mg 17	N 68	O 85	0
13	3	1	Total 950	C 780	Mg 17	N 68	O 85	0
13	3	1	Total 950	C 780	Mg 17	N 68	O 85	0
13	3	1	Total 950	C 780	Mg 17	N 68	O 85	0
13	3	1	Total 950	C 780	Mg 17	N 68	O 85	0
13	3	1	Total 950	C 780	Mg 17	N 68	O 85	0
13	3	1	Total 950	C 780	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms	AltConf
13	3	1	Total C Mg N O 950 780 17 68 85	0
13	3	1	Total C Mg N O 950 780 17 68 85	0
13	3	1	Total C Mg N O 950 780 17 68 85	0
13	3	1	Total C Mg N O 950 780 17 68 85	0
13	3	1	Total C Mg N O 950 780 17 68 85	0
13	3	1	Total C Mg N O 950 780 17 68 85	0
13	3	1	Total C Mg N O 950 780 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0
13	4	1	Total C Mg N O 860 690 17 68 85	0

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Mol	Chain	Residues	Atoms					AltConf
13	4	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	4	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	4	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	5	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms					AltConf
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	6	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0

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Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0

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Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	G	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	H	1	Total 2550	C 2140	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms	AltConf
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	H	1	Total C Mg N O 2550 2140 41 164 205	0
13	R	1	Total C Mg N O 110 90 2 8 10	0
13	R	1	Total C Mg N O 110 90 2 8 10	0
13	T	1	Total C Mg N O 123 103 2 8 10	0

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Mol	Chain	Residues	Atoms	AltConf
13	T	1	Total C Mg N O 123 103 2 8 10	0
13	U	1	Total C Mg N O 150 120 3 12 15	0
13	U	1	Total C Mg N O 150 120 3 12 15	0
13	U	1	Total C Mg N O 150 120 3 12 15	0
13	V	1	Total C Mg N O 190 160 3 12 15	0
13	V	1	Total C Mg N O 190 160 3 12 15	0
13	V	1	Total C Mg N O 190 160 3 12 15	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0
13	Y	1	Total C Mg N O 951 781 17 68 85	0

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Mol	Chain	Residues	Atoms					AltConf
13	Y	1	Total 951	C 781	Mg 17	N 68	O 85	0
13	Y	1	Total 951	C 781	Mg 17	N 68	O 85	0
13	Y	1	Total 951	C 781	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	Z	1	Total 993	C 823	Mg 17	N 68	O 85	0
13	a	1	Total 950	C 780	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms	AltConf
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	a	1	Total C Mg N O 950 780 17 68 85	0
13	b	1	Total C Mg N O 860 690 17 68 85	0
13	b	1	Total C Mg N O 860 690 17 68 85	0
13	b	1	Total C Mg N O 860 690 17 68 85	0
13	b	1	Total C Mg N O 860 690 17 68 85	0
13	b	1	Total C Mg N O 860 690 17 68 85	0

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	b	1	Total 860	C 690	Mg 17	N 68	O 85	0
13	c	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	c	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	c	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	c	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	c	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	c	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	c	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	c	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	c	1	Total 857	C 687	Mg 17	N 68	O 85	0

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Mol	Chain	Residues	Atoms	AltConf
13	c	1	Total C Mg N O 857 687 17 68 85	0
13	c	1	Total C Mg N O 857 687 17 68 85	0
13	c	1	Total C Mg N O 857 687 17 68 85	0
13	c	1	Total C Mg N O 857 687 17 68 85	0
13	c	1	Total C Mg N O 857 687 17 68 85	0
13	c	1	Total C Mg N O 857 687 17 68 85	0
13	c	1	Total C Mg N O 857 687 17 68 85	0
13	c	1	Total C Mg N O 857 687 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0

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Mol	Chain	Residues	Atoms	AltConf
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	d	1	Total C Mg N O 823 653 17 68 85	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0

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Mol	Chain	Residues	Atoms	AltConf
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0
13	e	1	Total C Mg N O 2728 2278 45 180 225	0

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	e	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	e	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	e	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	e	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	e	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	e	1	Total 2728	C 2278	Mg 45	N 180	O 225	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0
13	f	1	Total 2550	C 2140	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms	AltConf
13	f	1	Total C Mg N O 2550 2140 41 164 205	0
13	f	1	Total C Mg N O 2550 2140 41 164 205	0
13	f	1	Total C Mg N O 2550 2140 41 164 205	0
13	f	1	Total C Mg N O 2550 2140 41 164 205	0
13	f	1	Total C Mg N O 2550 2140 41 164 205	0
13	f	1	Total C Mg N O 2550 2140 41 164 205	0
13	j	1	Total C Mg N O 110 90 2 8 10	0
13	j	1	Total C Mg N O 110 90 2 8 10	0
13	l	1	Total C Mg N O 123 103 2 8 10	0
13	l	1	Total C Mg N O 123 103 2 8 10	0
13	m	1	Total C Mg N O 150 120 3 12 15	0
13	m	1	Total C Mg N O 150 120 3 12 15	0
13	m	1	Total C Mg N O 150 120 3 12 15	0
13	n	1	Total C Mg N O 190 160 3 12 15	0
13	n	1	Total C Mg N O 190 160 3 12 15	0
13	n	1	Total C Mg N O 190 160 3 12 15	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0

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Mol	Chain	Residues	Atoms	AltConf
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	q	1	Total C Mg N O 951 781 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0

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Mol	Chain	Residues	Atoms	AltConf
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	r	1	Total C Mg N O 993 823 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0

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Mol	Chain	Residues	Atoms	AltConf
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	s	1	Total C Mg N O 950 780 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0
13	t	1	Total C Mg N O 860 690 17 68 85	0

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Mol	Chain	Residues	Atoms					AltConf
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	u	1	Total 857	C 687	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0

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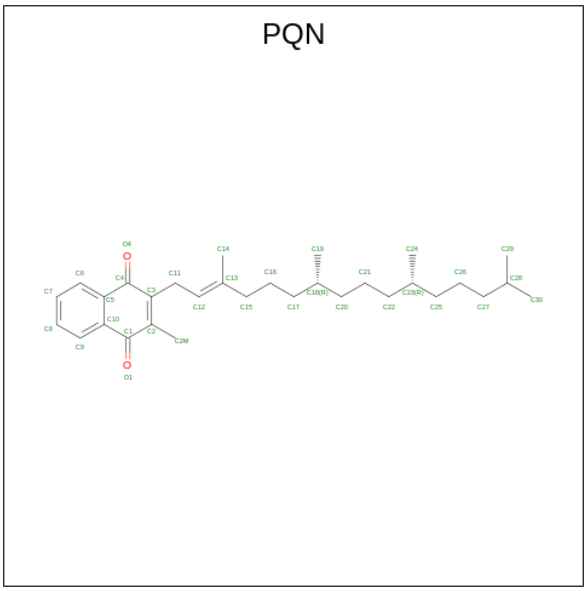
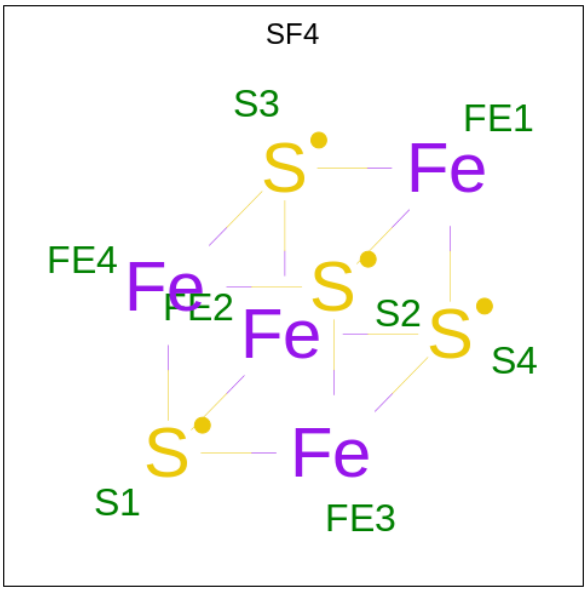
Mol	Chain	Residues	Atoms					AltConf
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0
13	v	1	Total 823	C 653	Mg 17	N 68	O 85	0

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



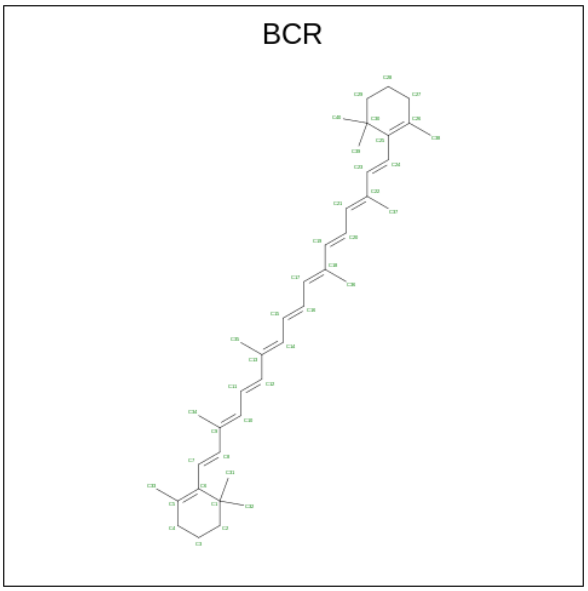
Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C O 33 31 2	0
14	B	1	Total C O 33 31 2	0
14	G	1	Total C O 33 31 2	0
14	H	1	Total C O 33 31 2	0
14	e	1	Total C O 33 31 2	0
14	f	1	Total C O 33 31 2	0

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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Mol	Chain	Residues	Atoms	AltConf
16	I	1	Total C 40 40	0
16	J	1	Total C 120 120	0
16	J	1	Total C 120 120	0
16	J	1	Total C 120 120	0
16	K	1	Total C 40 40	0
16	L	1	Total C 160 160	0
16	L	1	Total C 160 160	0
16	L	1	Total C 160 160	0
16	L	1	Total C 160 160	0
16	M	1	Total C 40 40	0
16	1	1	Total C 160 160	0
16	1	1	Total C 160 160	0
16	1	1	Total C 160 160	0
16	1	1	Total C 160 160	0
16	2	1	Total C 160 160	0
16	2	1	Total C 160 160	0
16	2	1	Total C 160 160	0
16	2	1	Total C 160 160	0
16	3	1	Total C 160 160	0
16	3	1	Total C 160 160	0
16	3	1	Total C 160 160	0

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Mol	Chain	Residues	Atoms	AltConf
16	3	1	Total C 160 160	0
16	4	1	Total C 160 160	0
16	4	1	Total C 160 160	0
16	4	1	Total C 160 160	0
16	4	1	Total C 160 160	0
16	5	1	Total C 160 160	0
16	5	1	Total C 160 160	0
16	5	1	Total C 160 160	0
16	5	1	Total C 160 160	0
16	6	1	Total C 160 160	0
16	6	1	Total C 160 160	0
16	6	1	Total C 160 160	0
16	6	1	Total C 160 160	0
16	G	1	Total C 240 240	0
16	G	1	Total C 240 240	0
16	G	1	Total C 240 240	0
16	G	1	Total C 240 240	0
16	G	1	Total C 240 240	0
16	G	1	Total C 240 240	0
16	H	1	Total C 280 280	0
16	H	1	Total C 280 280	0

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

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

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

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

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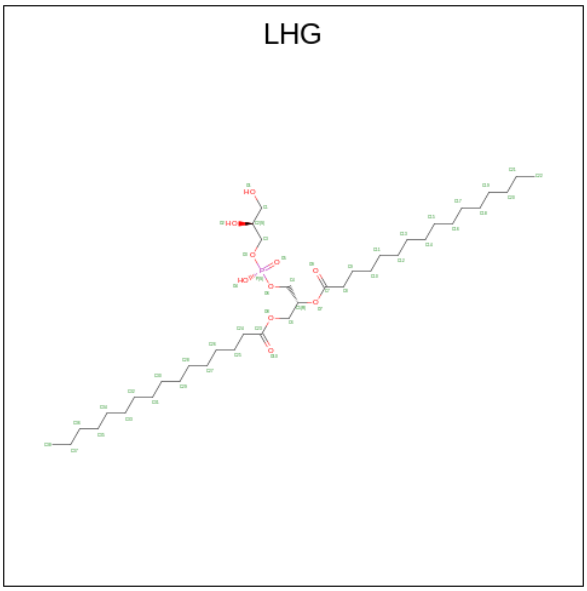
Mol	Chain	Residues	Atoms	AltConf
16	v	1	Total C 160 160	0
16	v	1	Total C 160 160	0
16	v	1	Total C 160 160	0
16	v	1	Total C 160 160	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C O P 386 287 90 9	0
17	A	1	Total C O P 386 287 90 9	0
17	A	1	Total C O P 386 287 90 9	0
17	A	1	Total C O P 386 287 90 9	0
17	A	1	Total C O P 386 287 90 9	0
17	A	1	Total C O P 386 287 90 9	0
17	A	1	Total C O P 386 287 90 9	0

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Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C O P 386 287 90 9	0
17	A	1	Total C O P 386 287 90 9	0
17	B	1	Total C O P 83 61 20 2	0
17	B	1	Total C O P 83 61 20 2	0
17	I	1	Total C O P 44 33 10 1	0
17	L	1	Total C O P 128 95 30 3	0
17	L	1	Total C O P 128 95 30 3	0
17	L	1	Total C O P 128 95 30 3	0
17	G	1	Total C O P 386 287 90 9	0
17	G	1	Total C O P 386 287 90 9	0
17	G	1	Total C O P 386 287 90 9	0
17	G	1	Total C O P 386 287 90 9	0
17	G	1	Total C O P 386 287 90 9	0
17	G	1	Total C O P 386 287 90 9	0
17	G	1	Total C O P 386 287 90 9	0
17	G	1	Total C O P 386 287 90 9	0
17	G	1	Total C O P 386 287 90 9	0
17	H	1	Total C O P 83 61 20 2	0
17	H	1	Total C O P 83 61 20 2	0
17	S	1	Total C O P 44 33 10 1	0
17	V	1	Total C O P 128 95 30 3	0

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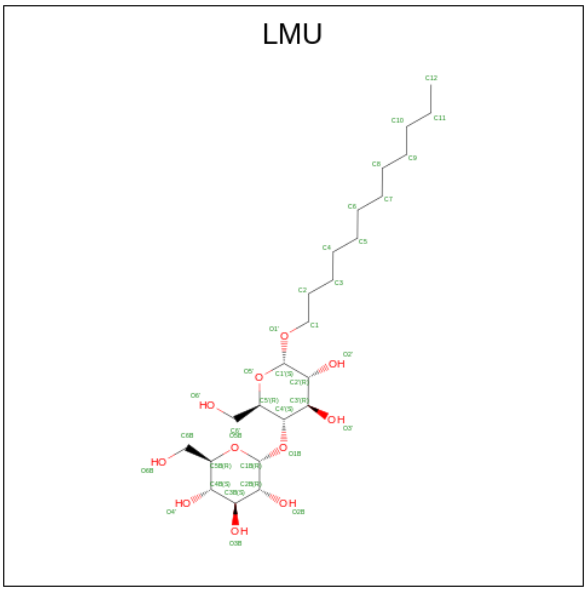
Mol	Chain	Residues	Atoms				AltConf
17	V	1	Total 128	C 95	O 30	P 3	0
17	V	1	Total 128	C 95	O 30	P 3	0
17	e	1	Total 386	C 287	O 90	P 9	0
17	e	1	Total 386	C 287	O 90	P 9	0
17	e	1	Total 386	C 287	O 90	P 9	0
17	e	1	Total 386	C 287	O 90	P 9	0
17	e	1	Total 386	C 287	O 90	P 9	0
17	e	1	Total 386	C 287	O 90	P 9	0
17	e	1	Total 386	C 287	O 90	P 9	0
17	e	1	Total 386	C 287	O 90	P 9	0
17	e	1	Total 386	C 287	O 90	P 9	0
17	f	1	Total 83	C 61	O 20	P 2	0
17	f	1	Total 83	C 61	O 20	P 2	0
17	k	1	Total 44	C 33	O 10	P 1	0
17	n	1	Total 128	C 95	O 30	P 3	0
17	n	1	Total 128	C 95	O 30	P 3	0
17	n	1	Total 128	C 95	O 30	P 3	0

- Molecule 18 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total 58	C 41	O 17	0
18	A	1	Total 58	C 41	O 17	0
18	B	1	Total 35	C 24	O 11	0
18	J	1	Total 22	C 16	O 6	0
18	1	1	Total 19	C 13	O 6	0
18	2	1	Total 23	C 17	O 6	0
18	G	1	Total 58	C 41	O 17	0
18	G	1	Total 58	C 41	O 17	0
18	H	1	Total 35	C 24	O 11	0
18	T	1	Total 22	C 16	O 6	0
18	Y	1	Total 19	C 13	O 6	0
18	Z	1	Total 23	C 17	O 6	0
18	e	1	Total 58	C 41	O 17	0
18	e	1	Total 58	C 41	O 17	0

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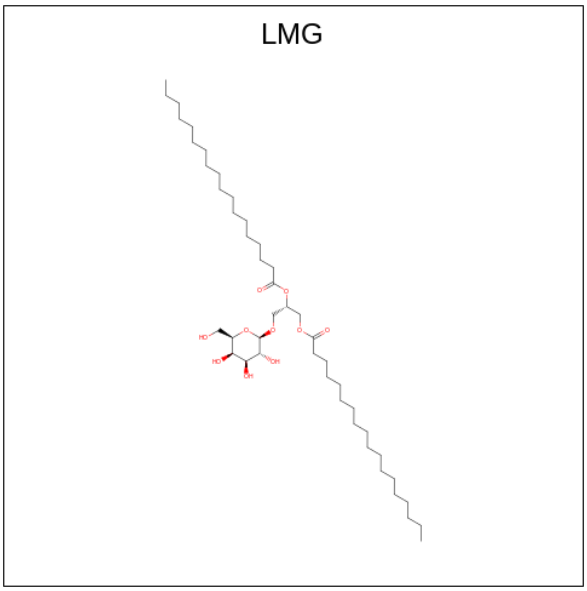
Mol	Chain	Residues	Atoms	AltConf
18	f	1	Total C O 35 24 11	0
18	l	1	Total C O 22 16 6	0
18	q	1	Total C O 19 13 6	0
18	r	1	Total C O 23 17 6	0

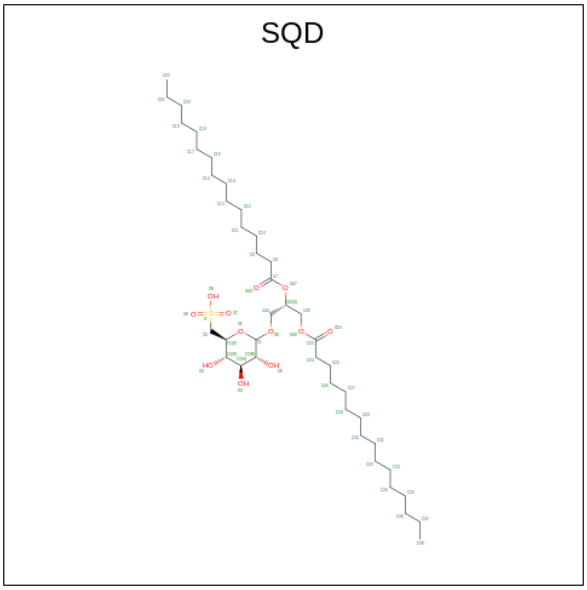
- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C O 54 44 10	0
19	J	1	Total C O 35 25 10	0
19	H	1	Total C O 54 44 10	0
19	T	1	Total C O 35 25 10	0
19	f	1	Total C O 54 44 10	0
19	l	1	Total C O 35 25 10	0

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
20	B	1	Total	C	O	S	0
			45	32	12	1	
20	L	1	Total	C	O	S	0
			51	38	12	1	
20	1	1	Total	C	O	S	0
			48	35	12	1	
20	2	1	Total	C	O	S	0
			43	30	12	1	
20	3	1	Total	C	O	S	0
			43	30	12	1	
20	4	1	Total	C	O	S	0
			26	13	12	1	
20	5	1	Total	C	O	S	0
			29	16	12	1	
20	6	1	Total	C	O	S	0
			26	13	12	1	
20	H	1	Total	C	O	S	0
			45	32	12	1	
20	V	1	Total	C	O	S	0
			51	38	12	1	
20	Y	1	Total	C	O	S	0
			48	35	12	1	
20	Z	1	Total	C	O	S	0
			43	30	12	1	
20	a	1	Total	C	O	S	0
			43	30	12	1	

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Mol	Chain	Residues	Atoms				AltConf
20	b	1	Total	C	O	S	0
			26	13	12	1	
20	c	1	Total	C	O	S	0
			29	16	12	1	
20	d	1	Total	C	O	S	0
			26	13	12	1	
20	f	1	Total	C	O	S	0
			45	32	12	1	
20	n	1	Total	C	O	S	0
			51	38	12	1	
20	q	1	Total	C	O	S	0
			48	35	12	1	
20	r	1	Total	C	O	S	0
			43	30	12	1	
20	s	1	Total	C	O	S	0
			43	30	12	1	
20	t	1	Total	C	O	S	0
			26	13	12	1	
20	u	1	Total	C	O	S	0
			29	16	12	1	
20	v	1	Total	C	O	S	0
			26	13	12	1	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	9	Total	O	0
			9	9	
21	B	7	Total	O	0
			7	7	
21	F	1	Total	O	0
			1	1	
21	L	1	Total	O	0
			1	1	
21	G	9	Total	O	0
			9	9	
21	H	7	Total	O	0
			7	7	
21	R	1	Total	O	0
			1	1	
21	V	1	Total	O	0
			1	1	

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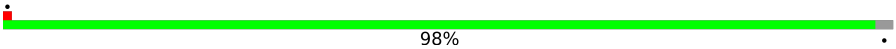
Mol	Chain	Residues	Atoms	AltConf
21	e	9	Total O 9 9	0
21	f	7	Total O 7 7	0
21	j	1	Total O 1 1	0
21	n	1	Total O 1 1	0

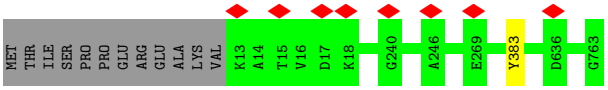
3 Residue-property plots (i)

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

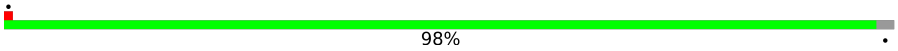
Chain A:

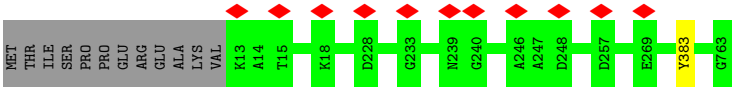




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

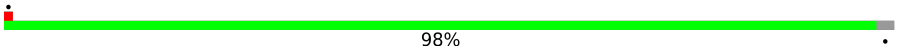
Chain G:

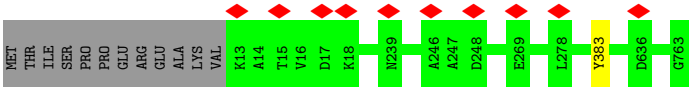




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

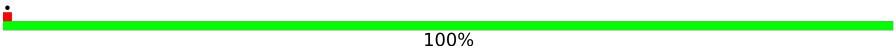
Chain e:

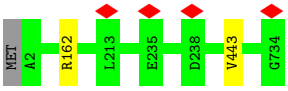




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

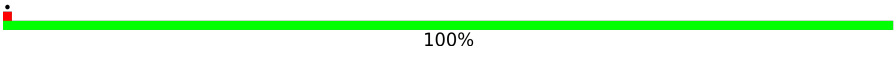
Chain B:

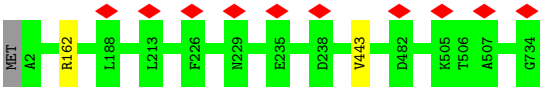




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

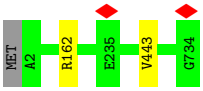
Chain H:





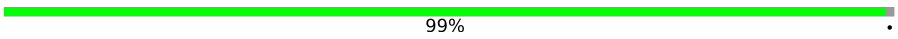
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain f:



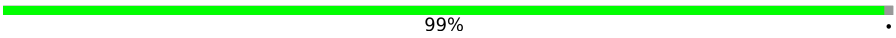
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



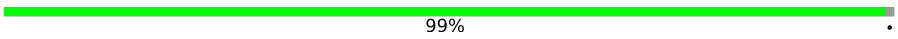
• Molecule 3: Photosystem I iron-sulfur center

Chain N:



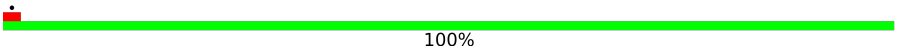
• Molecule 3: Photosystem I iron-sulfur center

Chain g:



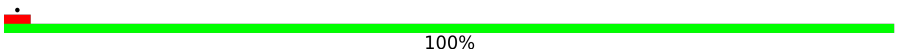
• Molecule 4: Photosystem I reaction center subunit II

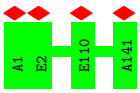
Chain D:



• Molecule 4: Photosystem I reaction center subunit II

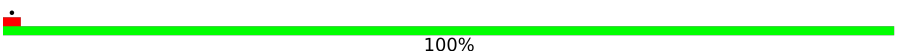
Chain O:





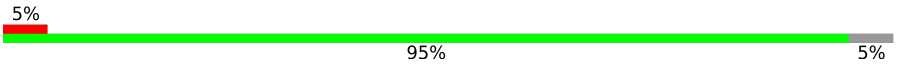
• Molecule 4: Photosystem I reaction center subunit II

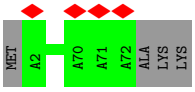
Chain h:



• Molecule 5: Photosystem I reaction center subunit IV

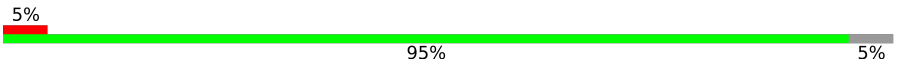
Chain E:

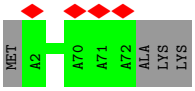




• Molecule 5: Photosystem I reaction center subunit IV

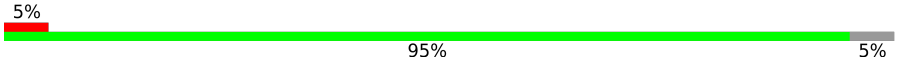
Chain Q:

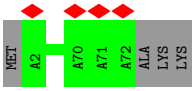




• Molecule 5: Photosystem I reaction center subunit IV

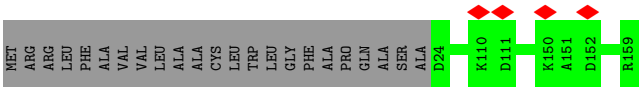
Chain i:





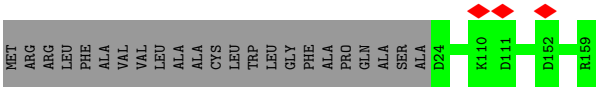
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



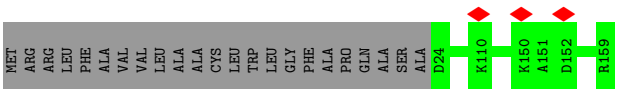
• Molecule 6: Photosystem I reaction center subunit III

Chain R:



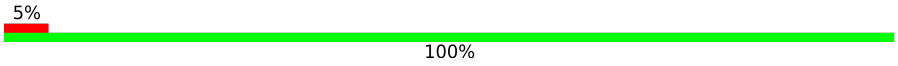
• Molecule 6: Photosystem I reaction center subunit III

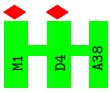
Chain j:



• Molecule 7: Photosystem I PsaI protein

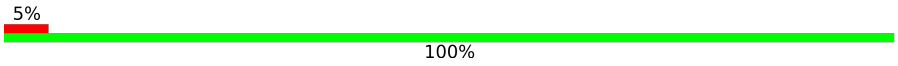
Chain I:

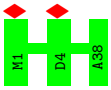




• Molecule 7: Photosystem I PsaI protein

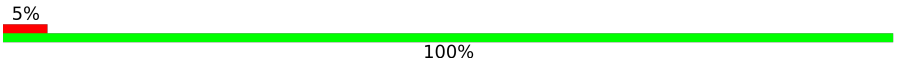
Chain S:

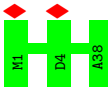




• Molecule 7: Photosystem I PsaI protein

Chain k:





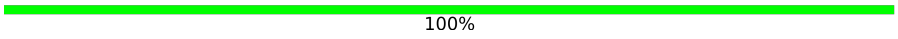
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:

There are no outlier residues recorded for this chain.

• Molecule 8: Photosystem I reaction center subunit IX

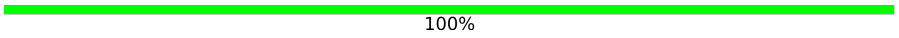
Chain T:



There are no outlier residues recorded for this chain.

• Molecule 8: Photosystem I reaction center subunit IX

Chain l:



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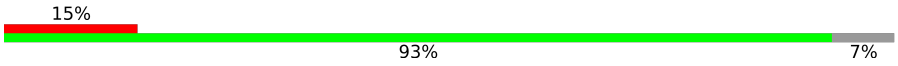
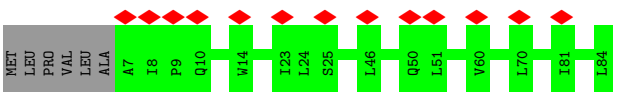
• Molecule 9: Photosystem I reaction center subunit PsaK

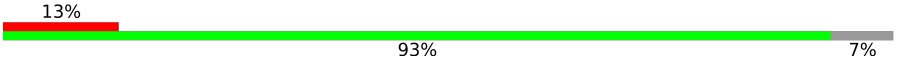
Chain K:

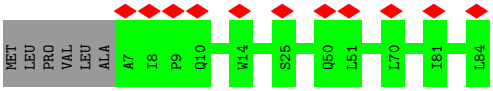




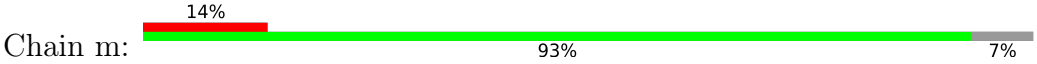
• Molecule 9: Photosystem I reaction center subunit PsaK

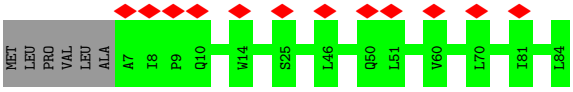
Chain U:



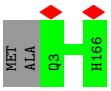


• Molecule 9: Photosystem I reaction center subunit PsaK

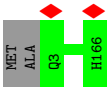




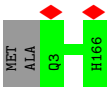
• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 11: PsaM

There are no outlier residues recorded for this chain.

• Molecule 11: PsaM

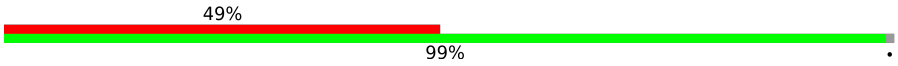
There are no outlier residues recorded for this chain.

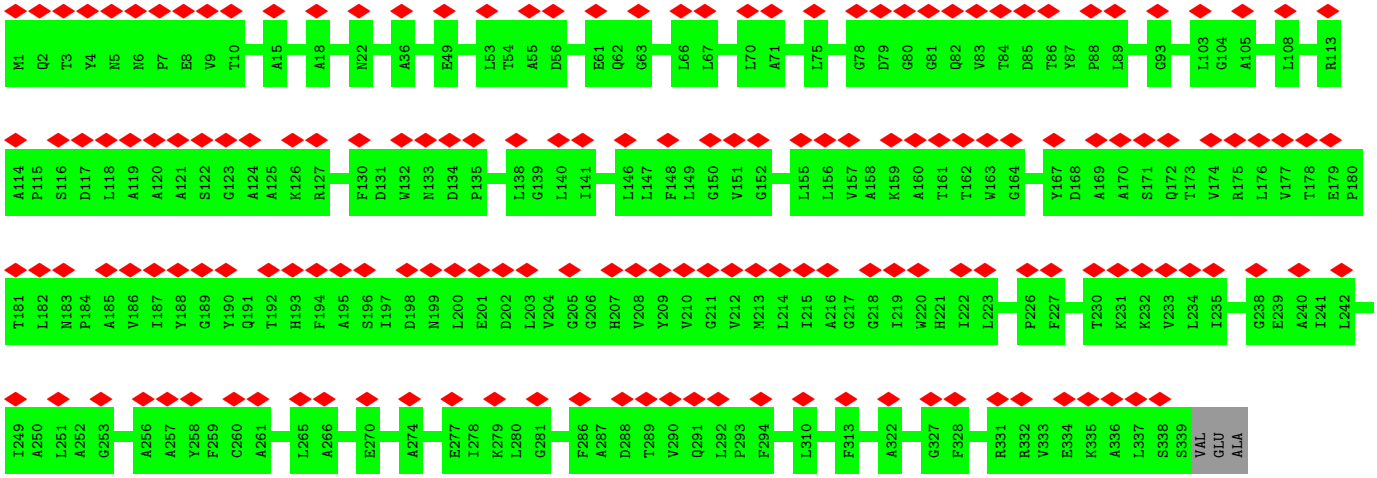
• Molecule 11: PsaM

There are no outlier residues recorded for this chain.

• Molecule 12: Iron stress-induced chlorophyll-binding protein

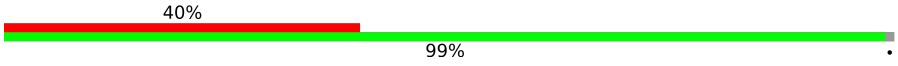
Chain 1:

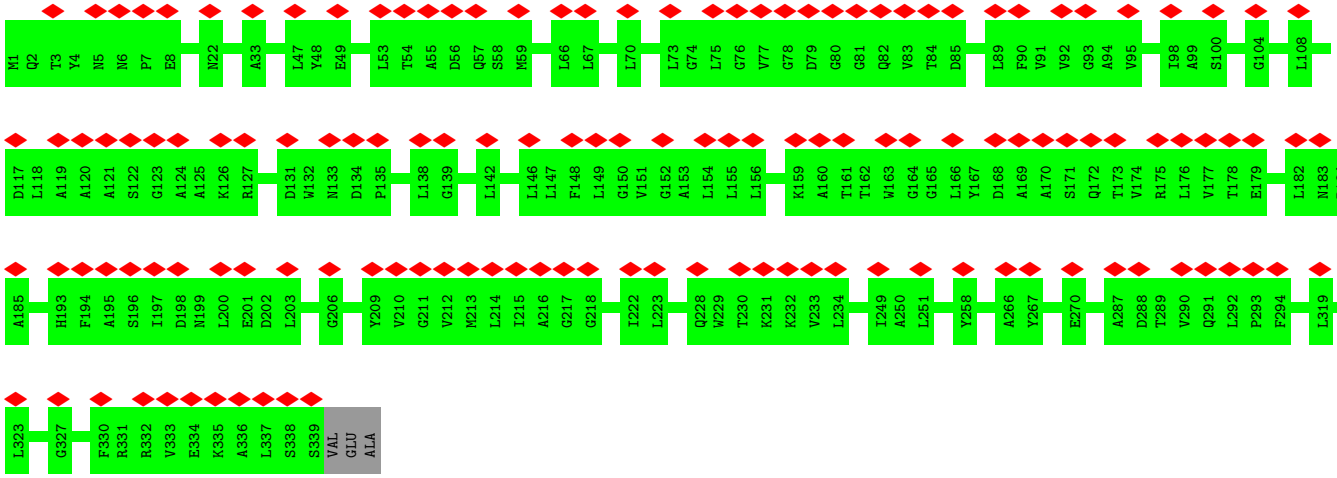




• Molecule 12: Iron stress-induced chlorophyll-binding protein

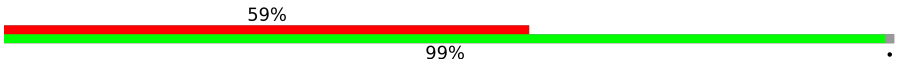
Chain 2:

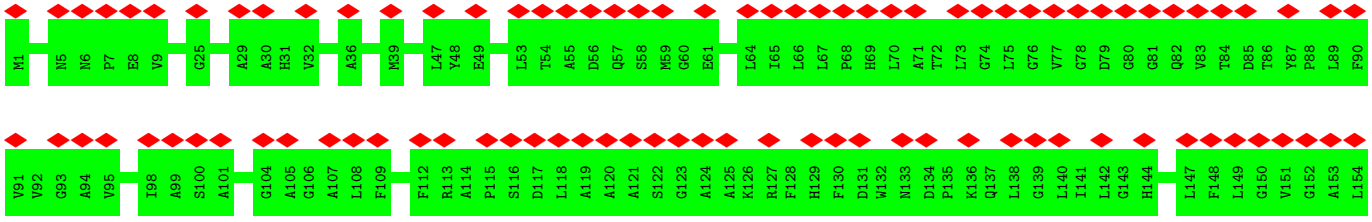


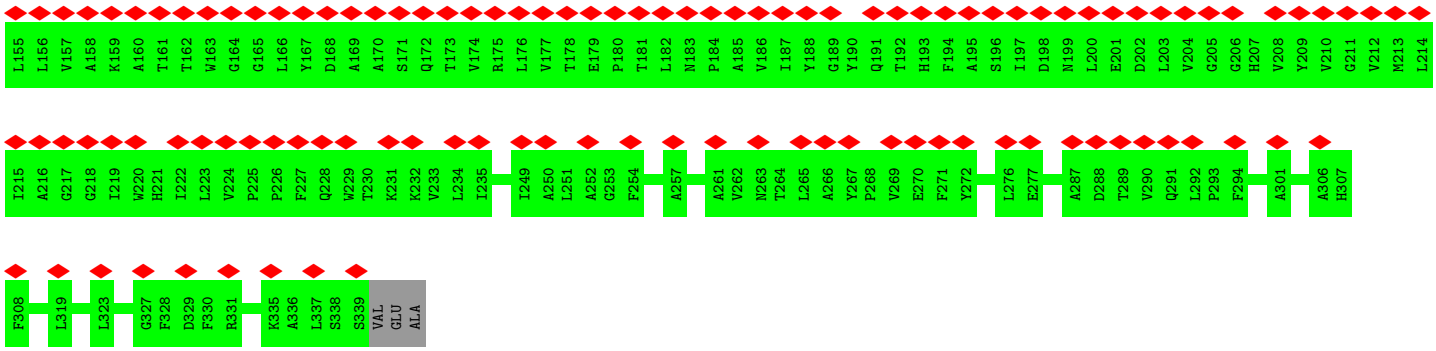


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain 3:

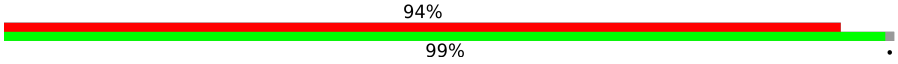


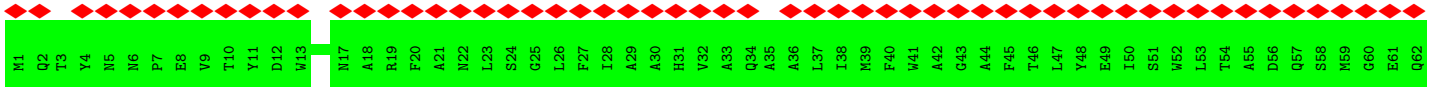


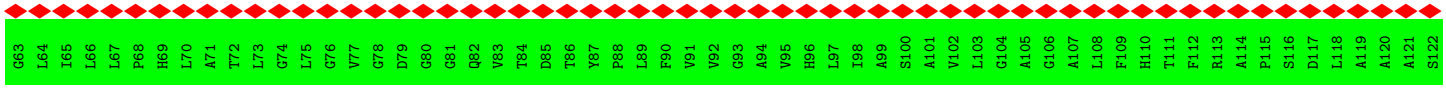


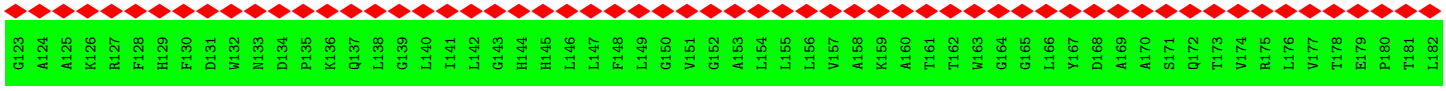
• Molecule 12: Iron stress-induced chlorophyll-binding protein

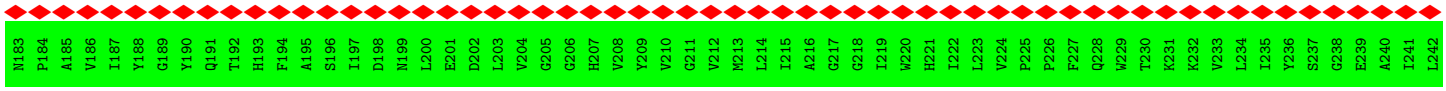
Chain 4:

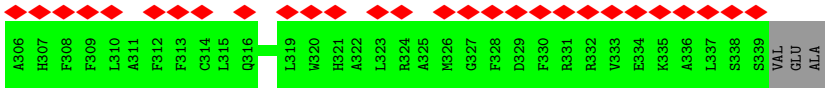






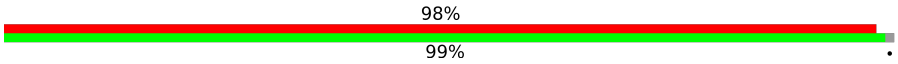


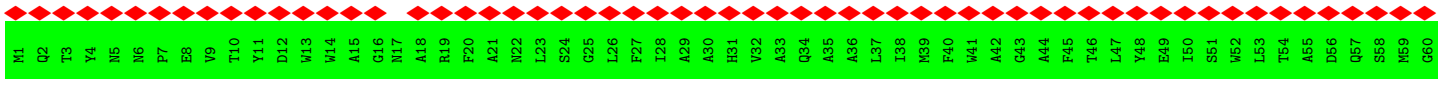


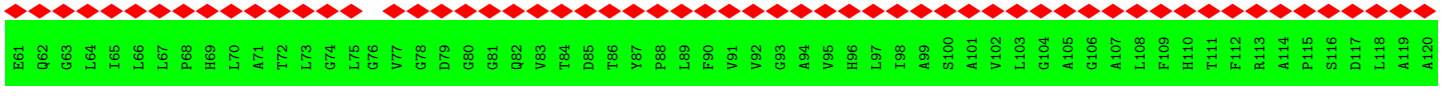


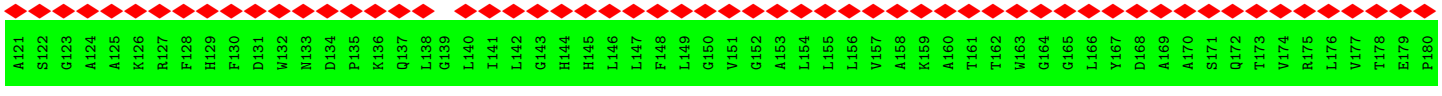
• Molecule 12: Iron stress-induced chlorophyll-binding protein

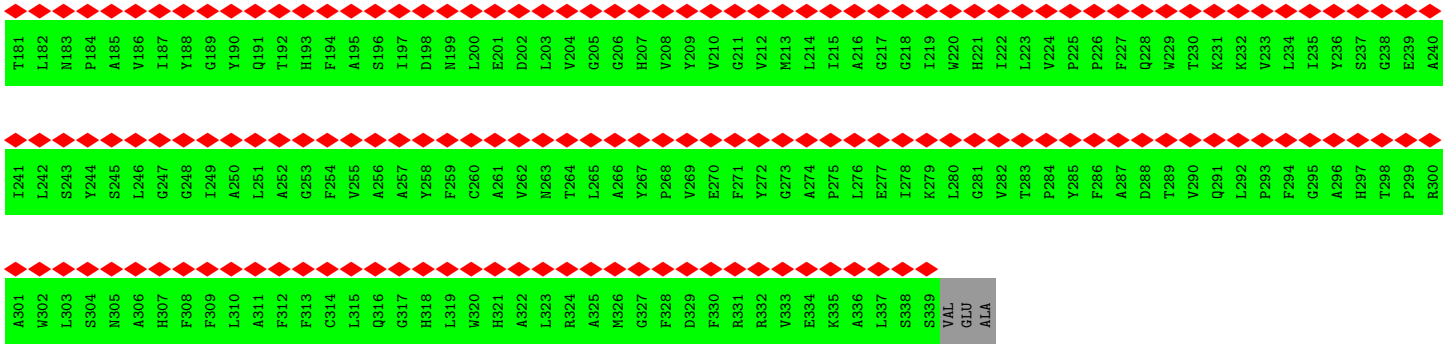
Chain 5:





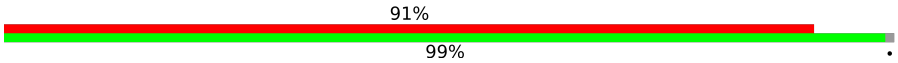






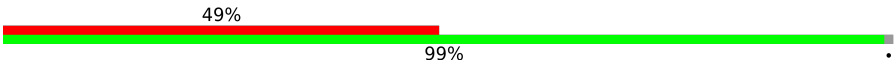
• Molecule 12: Iron stress-induced chlorophyll-binding protein

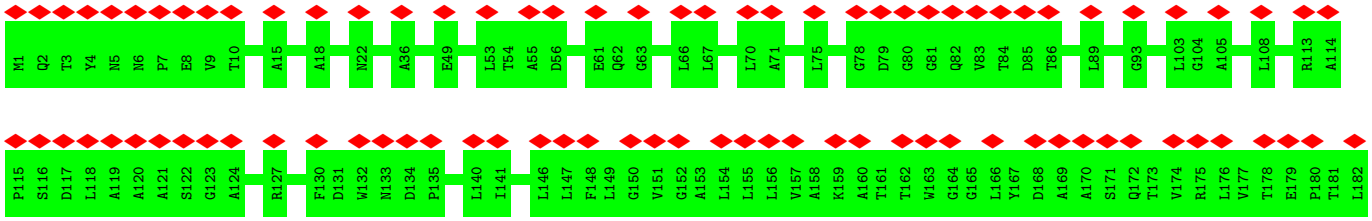
Chain 6:

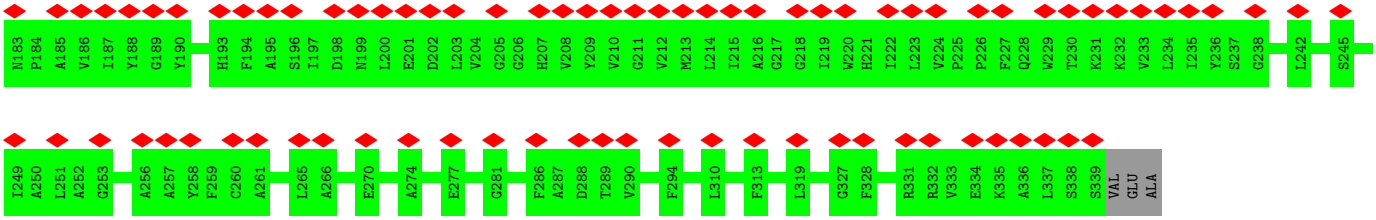


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Y:

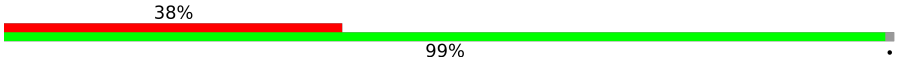


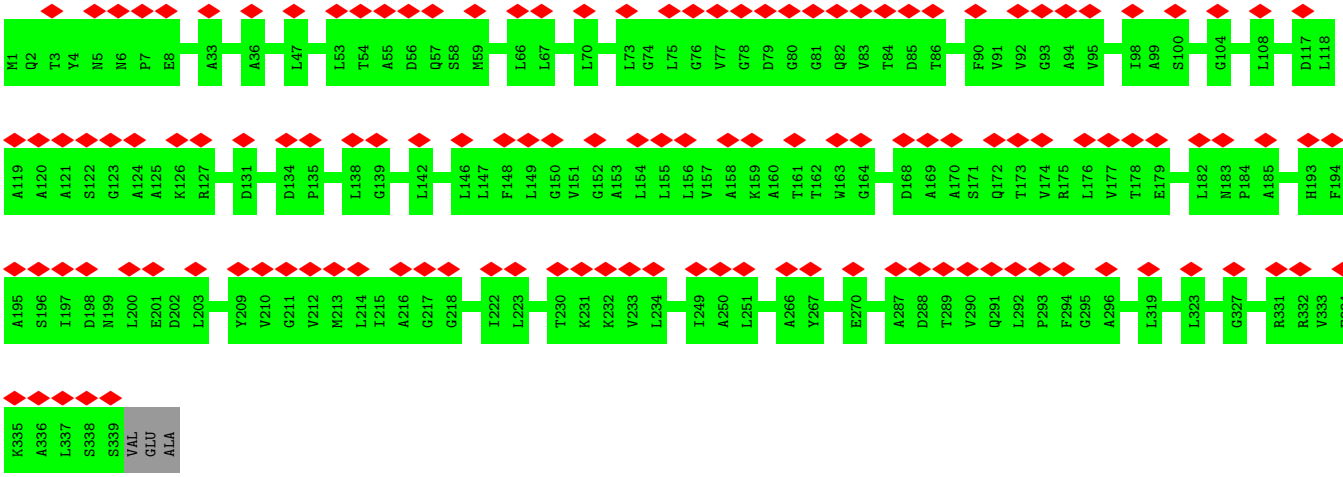




• Molecule 12: Iron stress-induced chlorophyll-binding protein

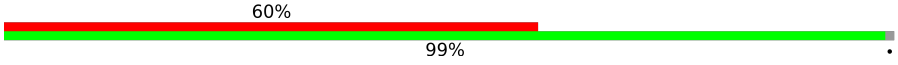
Chain Z:

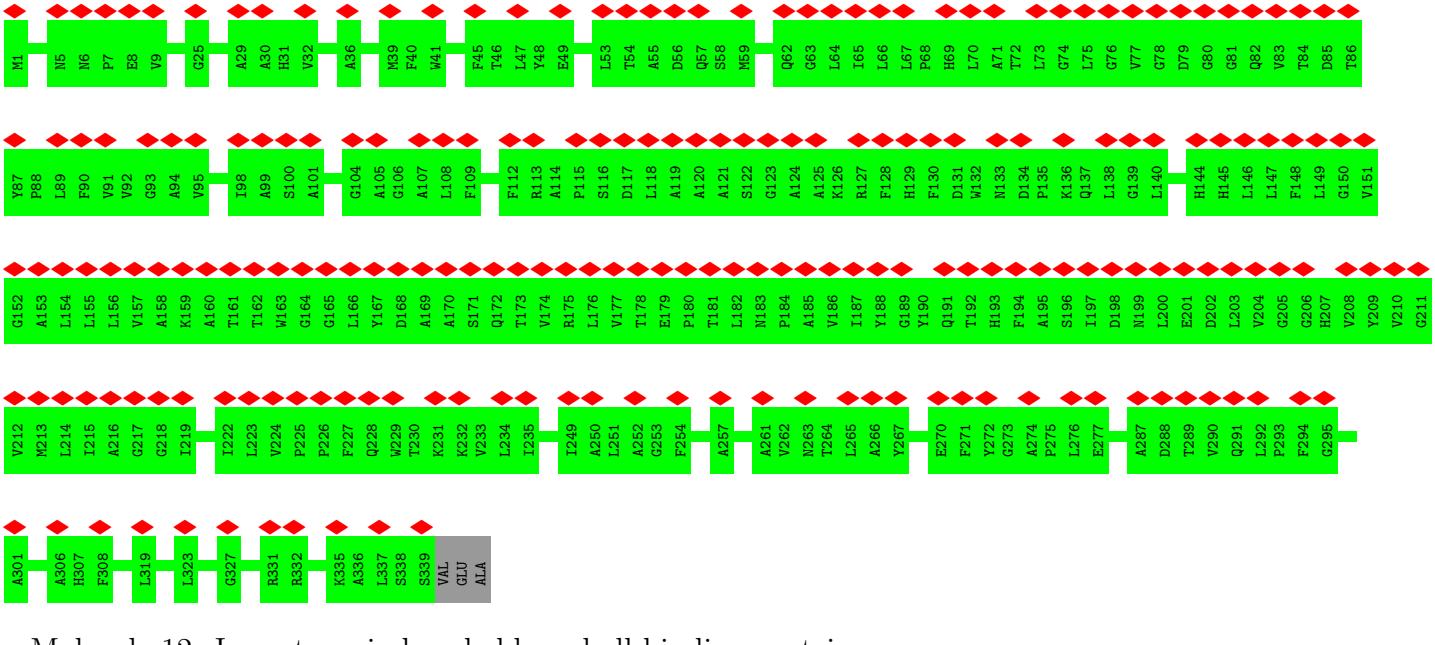




• Molecule 12: Iron stress-induced chlorophyll-binding protein

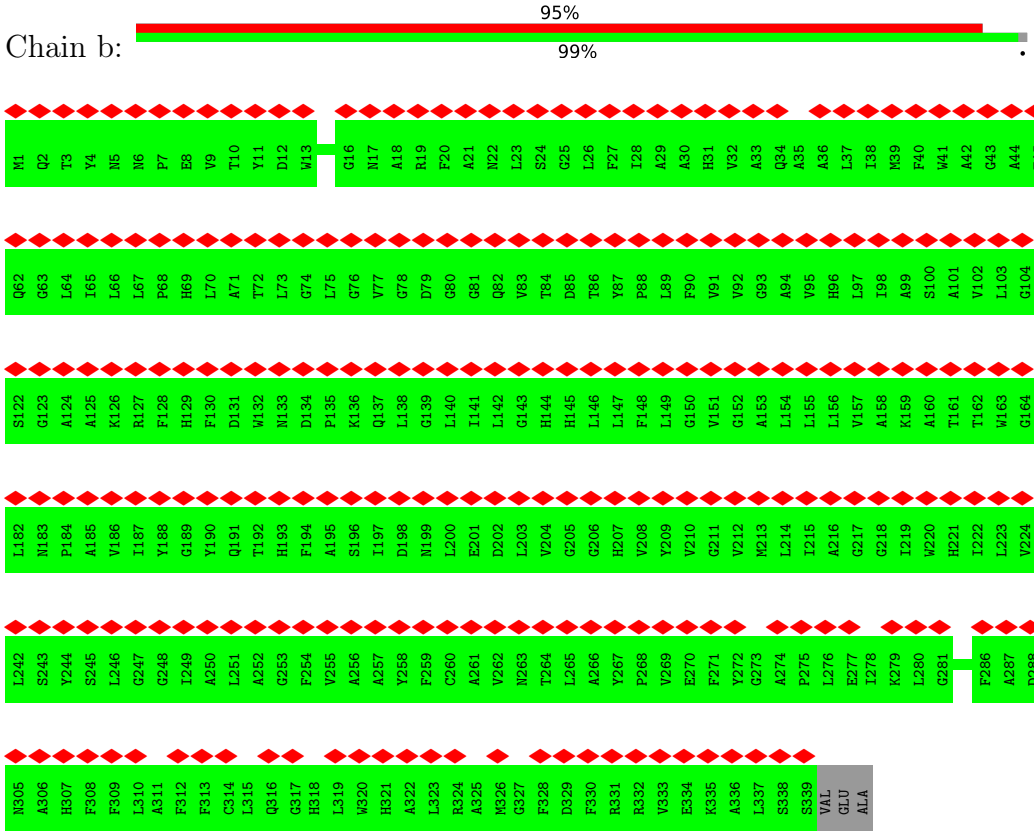
Chain a:





• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain b:

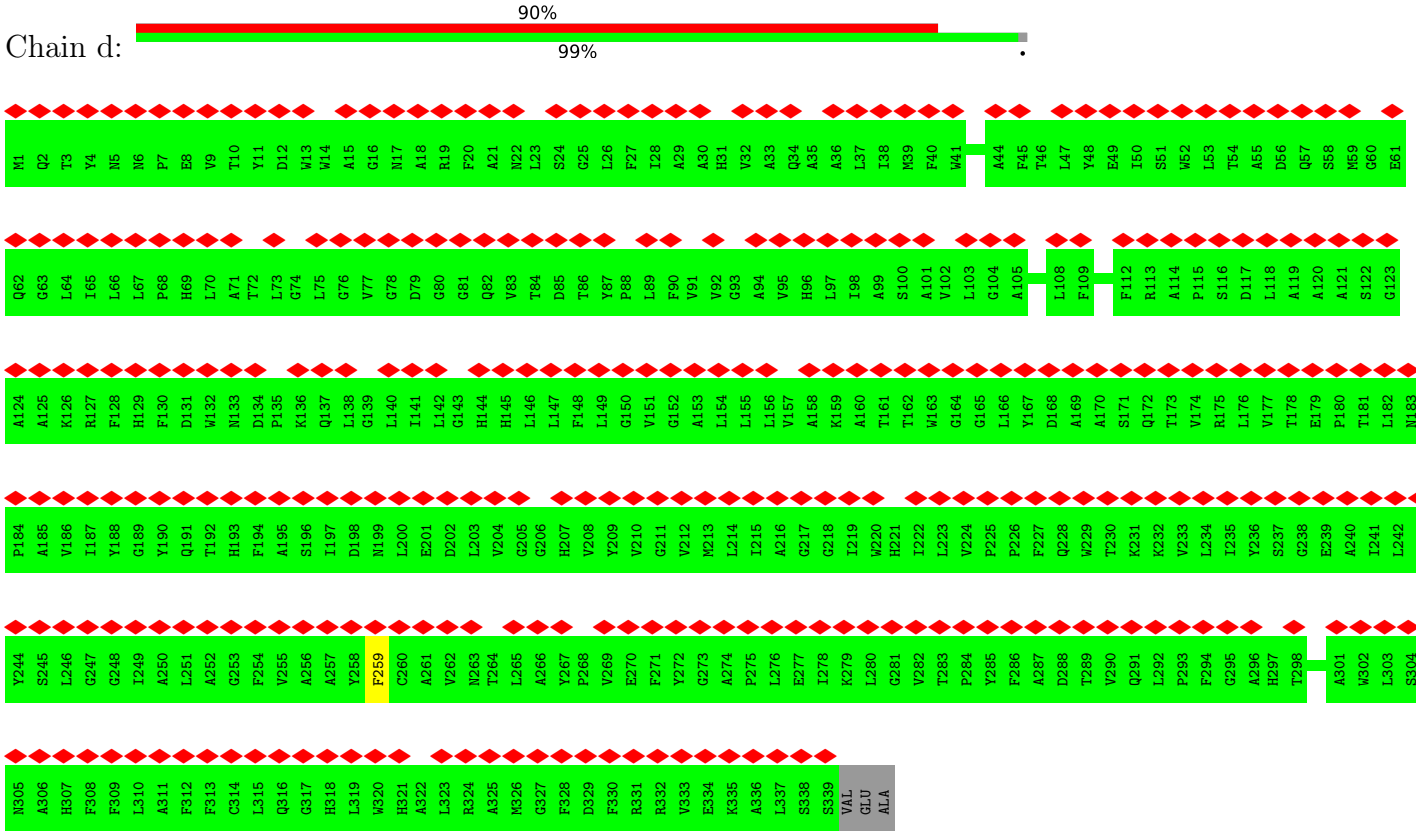


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain c:

• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain d:

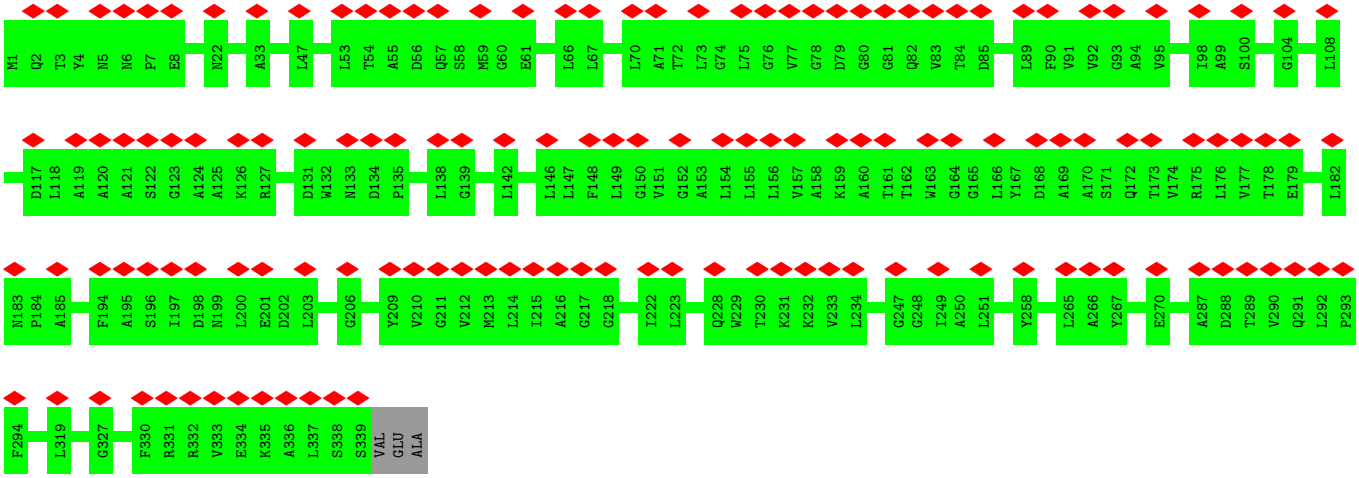


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain q:

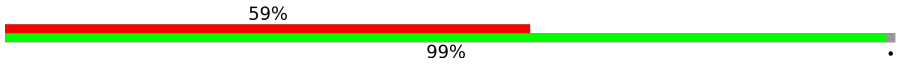
• Molecule 12: Iron stress-induced chlorophyll-binding protein

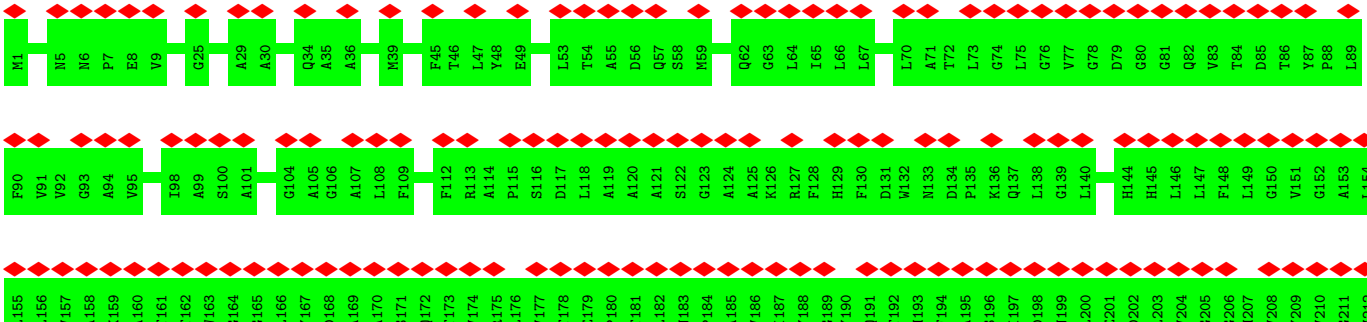
Chain r:



• Molecule 12: Iron stress-induced chlorophyll-binding protein

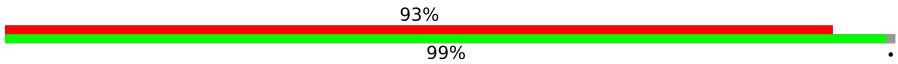
Chain s:

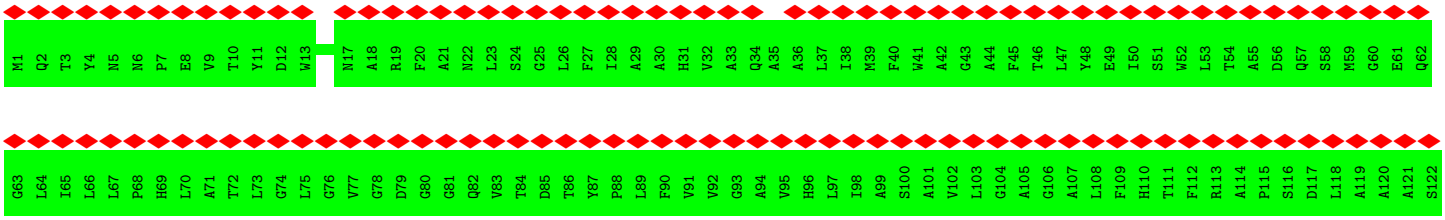


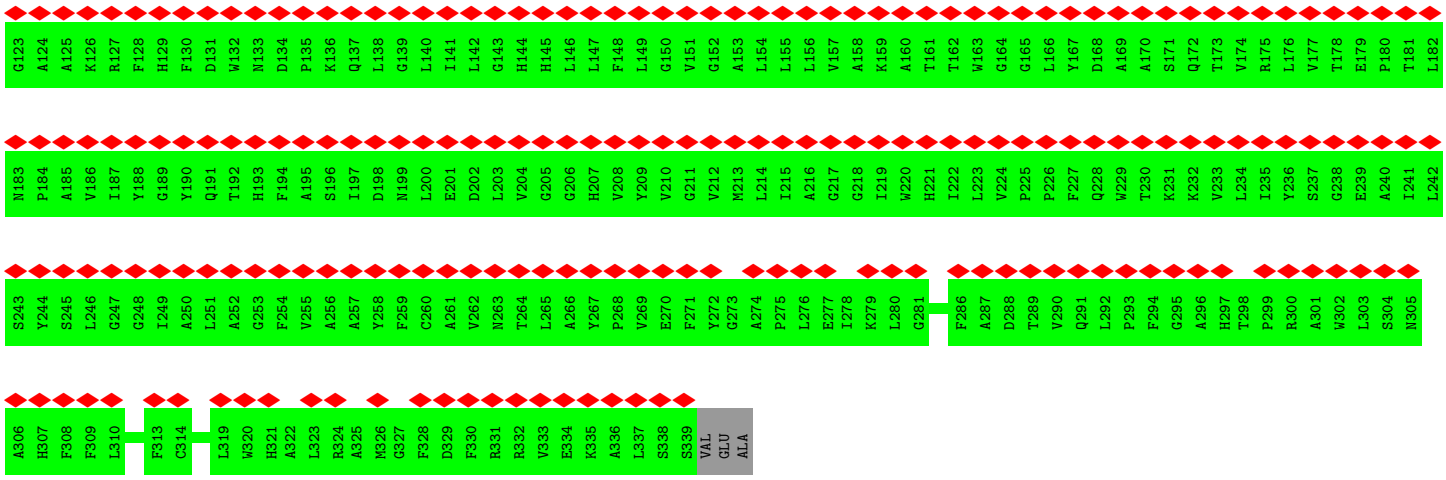


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain t:

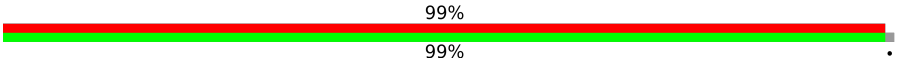


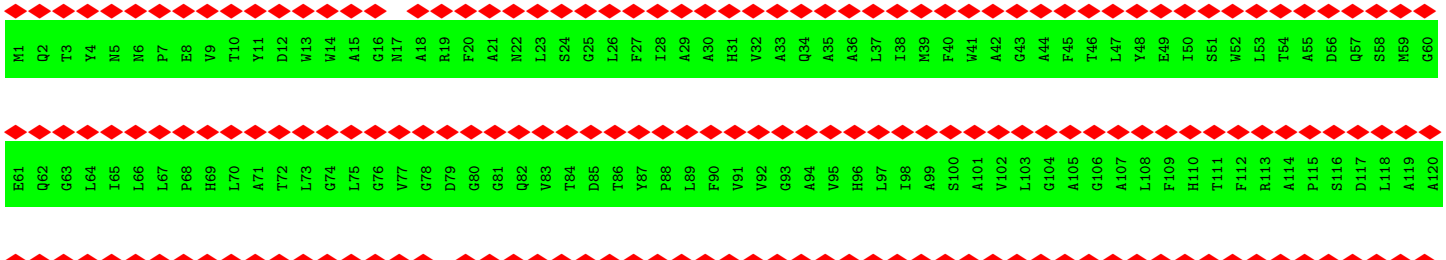




• Molecule 12: Iron stress-induced chlorophyll-binding protein

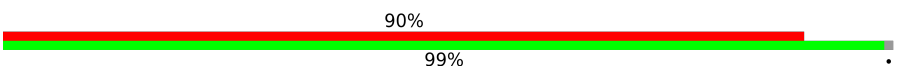
Chain u:

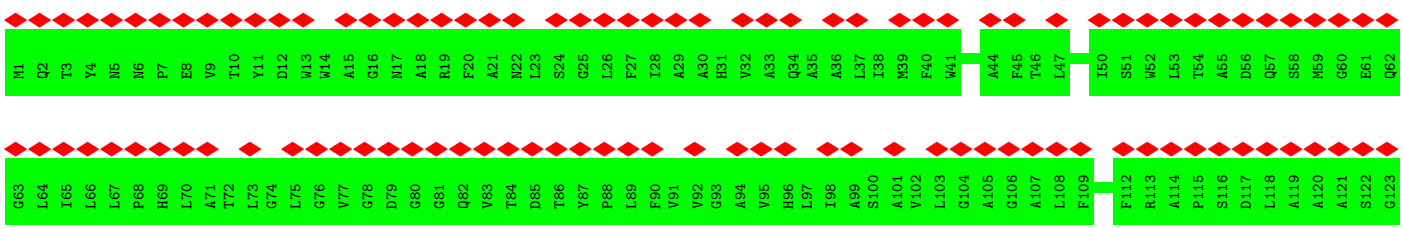


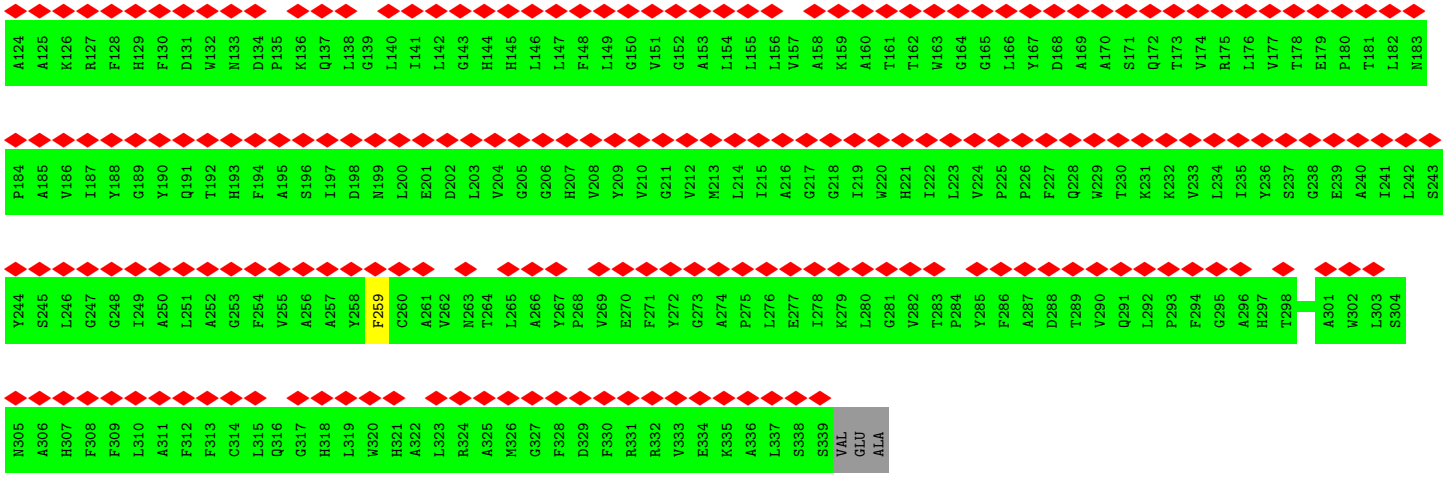


• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain v:






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 A301 W302 L303 S304
N305 A306 H307 F308 P309 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	63332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	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	0.170	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: SQD, SF4, LMU, LHG, CLA, LMG, PQN, BCR

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	0.42	0/6064	0.53	0/8274
1	G	0.42	0/6064	0.53	0/8274
1	e	0.42	0/6064	0.53	0/8274
2	B	0.42	0/5999	0.53	0/8199
2	H	0.42	0/5999	0.53	0/8199
2	f	0.42	0/5999	0.53	0/8199
3	C	0.42	0/608	0.56	0/823
3	N	0.42	0/608	0.56	0/823
3	g	0.43	0/608	0.56	0/823
4	D	0.37	0/1124	0.54	0/1516
4	O	0.37	0/1124	0.54	0/1516
4	h	0.37	0/1124	0.54	0/1516
5	E	0.38	0/553	0.46	0/750
5	Q	0.38	0/553	0.46	0/750
5	i	0.38	0/553	0.46	0/750
6	F	0.36	0/1062	0.50	0/1442
6	R	0.36	0/1062	0.50	0/1442
6	j	0.36	0/1062	0.50	0/1442
7	I	0.38	0/289	0.62	0/393
7	S	0.38	0/289	0.62	0/393
7	k	0.38	0/289	0.62	0/393
8	J	0.41	0/346	0.57	0/469
8	T	0.41	0/346	0.57	0/469
8	l	0.41	0/346	0.57	0/469
9	K	0.31	0/560	0.56	0/765
9	U	0.31	0/560	0.56	0/765
9	m	0.31	0/560	0.56	0/765
10	L	0.36	0/1242	0.51	0/1696
10	V	0.36	0/1242	0.51	0/1696
10	n	0.36	0/1242	0.51	0/1696
11	M	0.37	0/231	0.54	0/314
11	W	0.37	0/231	0.54	0/314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	o	0.37	0/231	0.54	0/314
12	1	0.28	0/2689	0.47	0/3678
12	2	0.28	0/2689	0.48	0/3678
12	3	0.27	0/2689	0.46	0/3678
12	4	0.27	0/2689	0.47	0/3678
12	5	0.27	0/2689	0.46	0/3678
12	6	0.27	0/2689	0.45	0/3678
12	Y	0.29	0/2689	0.47	0/3678
12	Z	0.29	0/2689	0.48	0/3678
12	a	0.27	0/2689	0.46	0/3678
12	b	0.27	0/2689	0.47	0/3678
12	c	0.27	0/2689	0.46	0/3678
12	d	0.27	0/2689	0.45	0/3678
12	q	0.29	0/2689	0.47	0/3678
12	r	0.29	0/2689	0.48	0/3678
12	s	0.27	0/2689	0.46	0/3678
12	t	0.27	0/2689	0.47	0/3678
12	u	0.27	0/2689	0.46	0/3678
12	v	0.27	0/2689	0.45	0/3678
All	All	0.35	0/102636	0.50	0/140127

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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	723 (96%)	26 (4%)	0	100	100
1	G	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
1	e	749/763 (98%)	723 (96%)	26 (4%)	0	100	100
2	B	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
2	H	731/734 (100%)	711 (97%)	20 (3%)	0	100	100
2	f	731/734 (100%)	711 (97%)	20 (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%)	132 (95%)	7 (5%)	0	100	100
4	O	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
4	h	139/141 (99%)	132 (95%)	7 (5%)	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
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%)	34 (94%)	2 (6%)	0	100	100
7	S	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	k	36/38 (95%)	34 (94%)	2 (6%)	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%)	157 (97%)	5 (3%)	0	100	100
10	V	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
10	n	162/166 (98%)	157 (97%)	5 (3%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	o	27/29 (93%)	27 (100%)	0	0	100	100
12	1	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	2	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	3	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	4	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	5	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	6	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	Y	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	Z	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	a	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	b	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	c	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	d	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	q	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
12	r	337/342 (98%)	329 (98%)	8 (2%)	0	100	100
12	s	337/342 (98%)	330 (98%)	7 (2%)	0	100	100
12	t	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
12	u	337/342 (98%)	326 (97%)	11 (3%)	0	100	100
12	v	337/342 (98%)	328 (97%)	9 (3%)	0	100	100
All	All	12786/13089 (98%)	12420 (97%)	366 (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%)	599 (100%)	1 (0%)	93	98
1	G	600/611 (98%)	599 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	600/611 (98%)	599 (100%)	1 (0%)	93	98
2	B	583/584 (100%)	581 (100%)	2 (0%)	92	98
2	H	583/584 (100%)	581 (100%)	2 (0%)	92	98
2	f	583/584 (100%)	581 (100%)	2 (0%)	92	98
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	1	257/259 (99%)	257 (100%)	0	100	100
12	2	257/259 (99%)	257 (100%)	0	100	100
12	3	257/259 (99%)	257 (100%)	0	100	100
12	4	257/259 (99%)	257 (100%)	0	100	100
12	5	257/259 (99%)	257 (100%)	0	100	100
12	6	257/259 (99%)	256 (100%)	1 (0%)	91	97
12	Y	257/259 (99%)	257 (100%)	0	100	100
12	Z	257/259 (99%)	257 (100%)	0	100	100
12	a	257/259 (99%)	257 (100%)	0	100	100
12	b	257/259 (99%)	257 (100%)	0	100	100
12	c	257/259 (99%)	257 (100%)	0	100	100
12	d	257/259 (99%)	256 (100%)	1 (0%)	91	97
12	q	257/259 (99%)	257 (100%)	0	100	100
12	r	257/259 (99%)	257 (100%)	0	100	100
12	s	257/259 (99%)	257 (100%)	0	100	100
12	t	257/259 (99%)	257 (100%)	0	100	100
12	u	257/259 (99%)	257 (100%)	0	100	100
12	v	257/259 (99%)	256 (100%)	1 (0%)	91	97
All	All	10017/10167 (98%)	10005 (100%)	12 (0%)	93	98

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

Mol	Chain	Res	Type
12	d	259	PHE
1	e	383	TYR
12	v	259	PHE
2	f	162	ARG
12	6	259	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	e	179	HIS
2	f	603	GLN
1	e	192	ASN

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Mol	Chain	Res	Type
2	f	34	HIS
10	n	3	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)

846 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	$\#\|Z\| > 2$
13	CLA	3	512	12	45,53,73	1.74	7 (15%)	52,89,113	1.61	5 (9%)
13	CLA	G	1130	1	65,73,73	1.47	7 (10%)	76,113,113	1.52	10 (13%)
13	CLA	A	1134	1	56,64,73	1.57	8 (14%)	65,102,113	1.55	8 (12%)
16	BCR	S	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
18	LMU	T	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
13	CLA	G	1127	1	65,73,73	1.41	7 (10%)	76,113,113	1.50	9 (11%)
17	LHG	A	5007	-	46,46,48	0.67	1 (2%)	49,52,54	1.24	5 (10%)
13	CLA	G	1101	1	65,73,73	1.49	8 (12%)	76,113,113	1.45	9 (11%)
13	CLA	G	1237	21	65,73,73	1.48	9 (13%)	76,113,113	1.50	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	e	1133	1	65,73,73	1.39	7 (10%)	76,113,113	1.48	6 (7%)
13	CLA	G	1117	1	65,73,73	1.43	10 (15%)	76,113,113	1.69	12 (15%)
13	CLA	B	1226	2	65,73,73	1.56	10 (15%)	76,113,113	1.82	14 (18%)
13	CLA	b	502	12	50,58,73	1.69	6 (12%)	58,95,113	1.59	7 (12%)
13	CLA	e	1140	1	65,73,73	1.49	7 (10%)	76,113,113	1.47	12 (15%)
13	CLA	H	1226	2	65,73,73	1.56	10 (15%)	76,113,113	1.82	13 (17%)
13	CLA	f	1238	21	65,73,73	1.41	7 (10%)	76,113,113	1.57	10 (13%)
13	CLA	G	1108	1	54,62,73	1.61	7 (12%)	62,99,113	1.48	6 (9%)
18	LMU	A	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	1 (3%)
15	SF4	N	3003	3	0,12,12	-	-	-		
13	CLA	f	1206	2	65,73,73	1.44	10 (15%)	76,113,113	1.58	7 (9%)
13	CLA	B	1225	2	65,73,73	1.42	9 (13%)	76,113,113	1.45	7 (9%)
13	CLA	e	1121	1	55,63,73	1.59	7 (12%)	64,101,113	1.58	11 (17%)
13	CLA	Z	510	12	65,73,73	1.46	7 (10%)	76,113,113	1.44	6 (7%)
13	CLA	1	503	12	64,72,73	1.50	6 (9%)	74,111,113	1.46	7 (9%)
13	CLA	6	512	12	45,53,73	1.77	6 (13%)	52,89,113	1.58	5 (9%)
13	CLA	H	1229	2	65,73,73	1.43	7 (10%)	76,113,113	1.57	10 (13%)
13	CLA	a	501	12	65,73,73	1.44	7 (10%)	76,113,113	1.53	7 (9%)
16	BCR	q	521	-	41,41,41	0.65	0	56,56,56	1.80	11 (19%)
13	CLA	G	1118	1	60,68,73	1.49	8 (13%)	70,107,113	1.49	8 (11%)
18	LMU	r	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
16	BCR	1	522	-	41,41,41	0.73	0	56,56,56	1.91	19 (33%)
13	CLA	4	501	12	60,68,73	1.54	5 (8%)	70,107,113	1.45	6 (8%)
13	CLA	u	504	-	45,53,73	1.78	6 (13%)	52,89,113	1.64	7 (13%)
13	CLA	t	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.66	8 (15%)
13	CLA	L	1502	10	65,73,73	1.43	7 (10%)	76,113,113	1.49	8 (10%)
13	CLA	d	507	-	45,53,73	1.77	6 (13%)	52,89,113	1.66	8 (15%)
13	CLA	c	507	-	45,53,73	1.74	6 (13%)	52,89,113	1.69	8 (15%)
13	CLA	f	1217	2	57,65,73	1.51	7 (12%)	66,103,113	1.54	8 (12%)
13	CLA	r	512	12	53,61,73	1.61	7 (13%)	61,98,113	1.47	5 (8%)
13	CLA	b	511	12	45,53,73	1.80	6 (13%)	52,89,113	1.69	7 (13%)
20	SQD	Y	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
13	CLA	B	1235	2	65,73,73	1.43	7 (10%)	76,113,113	1.54	10 (13%)
16	BCR	B	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
16	BCR	t	522	-	41,41,41	0.73	0	56,56,56	1.85	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	SQD	u	822	-	28,29,54	1.26	5 (17%)	37,40,65	1.92	13 (35%)
13	CLA	f	1230	2	60,68,73	1.53	9 (15%)	70,107,113	1.53	10 (14%)
13	CLA	Z	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.62	6 (11%)
13	CLA	u	519	12	46,54,73	1.75	9 (19%)	53,90,113	1.55	6 (11%)
13	CLA	A	1131	1	65,73,73	1.45	9 (13%)	76,113,113	1.43	9 (11%)
16	BCR	H	4006	-	41,41,41	0.73	0	56,56,56	1.98	19 (33%)
13	CLA	v	511	12	45,53,73	1.78	6 (13%)	52,89,113	1.67	6 (11%)
16	BCR	G	4002	-	41,41,41	0.81	1 (2%)	56,56,56	1.85	14 (25%)
13	CLA	A	1106	1	65,73,73	1.41	9 (13%)	76,113,113	1.54	9 (11%)
16	BCR	a	521	-	41,41,41	0.68	0	56,56,56	1.75	10 (17%)
13	CLA	5	501	12	65,73,73	1.46	6 (9%)	76,113,113	1.47	7 (9%)
13	CLA	2	507	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	7 (9%)
13	CLA	e	1113	1	45,53,73	1.67	7 (15%)	52,89,113	1.77	6 (11%)
13	CLA	Z	508	12	55,63,73	1.63	8 (14%)	64,101,113	1.58	9 (14%)
13	CLA	B	1023	-	65,73,73	1.41	8 (12%)	76,113,113	1.85	14 (18%)
16	BCR	k	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
13	CLA	6	505	12	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
16	BCR	n	4219	-	41,41,41	0.78	0	56,56,56	1.81	12 (21%)
13	CLA	Z	511	12	55,63,73	1.62	6 (10%)	64,101,113	1.57	7 (10%)
13	CLA	q	508	12	55,63,73	1.60	7 (12%)	64,101,113	1.70	9 (14%)
13	CLA	c	509	12	65,73,73	1.46	7 (10%)	76,113,113	1.49	8 (10%)
16	BCR	s	522	-	41,41,41	0.68	0	56,56,56	1.91	15 (26%)
13	CLA	r	511	12	55,63,73	1.62	6 (10%)	64,101,113	1.56	7 (10%)
13	CLA	t	516	12	45,53,73	1.78	6 (13%)	52,89,113	1.59	7 (13%)
16	BCR	t	521	-	41,41,41	0.65	0	56,56,56	1.78	11 (19%)
18	LMU	f	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.11	3 (6%)
20	SQD	2	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.61	10 (19%)
13	CLA	A	1136	1	60,68,73	1.52	8 (13%)	70,107,113	1.56	11 (15%)
13	CLA	c	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.60	6 (11%)
13	CLA	A	1119	21	65,73,73	1.46	9 (13%)	76,113,113	1.52	9 (11%)
13	CLA	f	1203	2	65,73,73	1.44	8 (12%)	76,113,113	1.46	7 (9%)
20	SQD	r	822	-	42,43,54	1.07	5 (11%)	51,54,65	1.61	10 (19%)
13	CLA	t	501	12	60,68,73	1.55	5 (8%)	70,107,113	1.44	6 (8%)
13	CLA	2	513	12	65,73,73	1.50	8 (12%)	76,113,113	1.38	6 (7%)
13	CLA	u	503	12	55,63,73	1.63	6 (10%)	64,101,113	1.53	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	s	510	12	65,73,73	1.47	6 (9%)	76,113,113	1.46	9 (11%)
13	CLA	T	1302	8	58,66,73	1.53	8 (13%)	67,104,113	1.51	8 (11%)
13	CLA	e	1124	21	56,64,73	1.58	6 (10%)	65,102,113	1.62	12 (18%)
17	LHG	A	5003	13	40,40,48	0.74	1 (2%)	43,46,54	1.34	6 (13%)
13	CLA	Y	506	12	45,53,73	1.77	6 (13%)	52,89,113	1.68	6 (11%)
13	CLA	3	502	12	50,58,73	1.69	7 (14%)	58,95,113	1.62	8 (13%)
13	CLA	s	506	12	50,58,73	1.69	7 (14%)	58,95,113	1.67	6 (10%)
18	LMU	2	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
17	LHG	A	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
18	LMU	Z	901	-	23,23,36	1.10	1 (4%)	28,28,47	0.94	0
13	CLA	H	1234	2	65,73,73	1.43	8 (12%)	76,113,113	1.68	13 (17%)
16	BCR	H	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
16	BCR	v	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
13	CLA	B	1230	2	60,68,73	1.54	9 (15%)	70,107,113	1.53	10 (14%)
13	CLA	s	516	12	45,53,73	1.78	6 (13%)	52,89,113	1.85	12 (23%)
13	CLA	f	1228	2	55,63,73	1.53	7 (12%)	64,101,113	1.67	8 (12%)
13	CLA	1	501	12	65,73,73	1.49	7 (10%)	76,113,113	1.44	8 (10%)
13	CLA	r	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.48	7 (9%)
16	BCR	W	4021	-	41,41,41	0.71	0	56,56,56	1.82	14 (25%)
16	BCR	u	524	-	41,41,41	0.68	0	56,56,56	1.67	14 (25%)
17	LHG	A	5008	-	34,34,48	0.76	1 (2%)	37,40,54	1.28	4 (10%)
13	CLA	G	1105	1	55,63,73	1.51	7 (12%)	64,101,113	1.70	9 (14%)
16	BCR	A	4007	-	41,41,41	0.74	0	56,56,56	2.11	18 (32%)
16	BCR	B	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	f	1202	2	65,73,73	1.44	7 (10%)	76,113,113	1.65	10 (13%)
13	CLA	F	1301	21	65,73,73	1.46	7 (10%)	76,113,113	1.39	8 (10%)
13	CLA	A	1115	1	60,68,73	1.47	7 (11%)	70,107,113	1.59	8 (11%)
13	CLA	2	518	12	65,73,73	1.46	6 (9%)	76,113,113	1.48	7 (9%)
16	BCR	j	4016	-	41,41,41	0.74	0	56,56,56	1.79	13 (23%)
13	CLA	5	513	12	45,53,73	1.81	8 (17%)	52,89,113	1.57	6 (11%)
16	BCR	T	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
16	BCR	r	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
13	CLA	b	509	12	65,73,73	1.47	6 (9%)	76,113,113	1.50	9 (11%)
16	BCR	l	4015	-	41,41,41	0.79	0	56,56,56	1.82	14 (25%)
17	LHG	A	5006	-	44,44,48	0.62	0	47,50,54	1.26	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	4	512	12	45,53,73	1.79	6 (13%)	52,89,113	1.62	6 (11%)
13	CLA	G	1113	1	45,53,73	1.68	7 (15%)	52,89,113	1.76	6 (11%)
13	CLA	1	504	-	45,53,73	1.79	8 (17%)	52,89,113	1.61	8 (15%)
13	CLA	f	1231	21	65,73,73	1.38	7 (10%)	76,113,113	1.57	8 (10%)
13	CLA	4	503	12	55,63,73	1.63	6 (10%)	64,101,113	1.54	11 (17%)
13	CLA	q	507	-	60,68,73	1.53	6 (10%)	70,107,113	1.54	9 (12%)
13	CLA	H	1235	2	65,73,73	1.43	8 (12%)	76,113,113	1.54	10 (13%)
13	CLA	f	1219	2	65,73,73	1.47	7 (10%)	76,113,113	1.33	9 (11%)
13	CLA	G	1107	1	65,73,73	1.47	10 (15%)	76,113,113	1.43	9 (11%)
16	BCR	R	4016	-	41,41,41	0.75	0	56,56,56	1.78	13 (23%)
13	CLA	e	1108	1	54,62,73	1.61	7 (12%)	62,99,113	1.49	6 (9%)
13	CLA	1	508	12	55,63,73	1.60	7 (12%)	64,101,113	1.70	9 (14%)
13	CLA	A	1022	21	65,73,73	1.47	10 (15%)	76,113,113	1.49	9 (11%)
13	CLA	2	505	12	65,73,73	1.44	6 (9%)	76,113,113	1.41	8 (10%)
13	CLA	a	511	12	50,58,73	1.70	6 (12%)	58,95,113	1.61	6 (10%)
13	CLA	e	1104	1	65,73,73	1.40	7 (10%)	76,113,113	1.52	10 (13%)
13	CLA	G	1125	1	65,73,73	1.43	7 (10%)	76,113,113	1.55	9 (11%)
13	CLA	Y	510	12	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
13	CLA	Z	505	12	65,73,73	1.44	6 (9%)	76,113,113	1.41	8 (10%)
13	CLA	u	510	12	45,53,73	1.77	6 (13%)	52,89,113	1.60	7 (13%)
13	CLA	H	1023	-	65,73,73	1.40	8 (12%)	76,113,113	1.85	15 (19%)
13	CLA	d	519	12	46,54,73	1.76	6 (13%)	53,90,113	1.59	6 (11%)
13	CLA	t	510	12	50,58,73	1.68	6 (12%)	58,95,113	1.62	7 (12%)
13	CLA	c	510	12	45,53,73	1.76	6 (13%)	52,89,113	1.60	7 (13%)
16	BCR	Y	521	-	41,41,41	0.65	0	56,56,56	1.80	11 (19%)
13	CLA	f	1220	2	55,63,73	1.54	9 (16%)	64,101,113	1.67	11 (17%)
13	CLA	j	1302	6	45,53,73	1.76	7 (15%)	52,89,113	1.58	6 (11%)
13	CLA	u	506	12	45,53,73	1.78	6 (13%)	52,89,113	1.66	7 (13%)
13	CLA	s	504	-	45,53,73	1.75	6 (13%)	52,89,113	1.69	6 (11%)
13	CLA	H	1236	2	55,63,73	1.63	7 (12%)	64,101,113	1.42	8 (12%)
13	CLA	6	507	-	45,53,73	1.77	6 (13%)	52,89,113	1.66	8 (15%)
20	SQD	s	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
13	CLA	G	1011	1	65,73,73	1.46	6 (9%)	76,113,113	1.63	12 (15%)
17	LHG	G	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
17	LHG	I	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	L	4219	-	41,41,41	0.78	0	56,56,56	1.80	12 (21%)
13	CLA	Z	506	12	55,63,73	1.61	7 (12%)	64,101,113	1.55	6 (9%)
13	CLA	6	518	12	55,63,73	1.61	6 (10%)	64,101,113	1.49	7 (10%)
13	CLA	q	519	12	50,58,73	1.66	10 (20%)	58,95,113	1.50	8 (13%)
13	CLA	2	519	12	55,63,73	1.61	9 (16%)	64,101,113	1.46	9 (14%)
13	CLA	6	511	12	45,53,73	1.78	6 (13%)	52,89,113	1.66	6 (11%)
13	CLA	5	511	12	55,63,73	1.61	6 (10%)	64,101,113	1.52	7 (10%)
15	SF4	A	3001	1,2	0,12,12	-	-	-		
13	CLA	4	509	12	65,73,73	1.47	6 (9%)	76,113,113	1.51	8 (10%)
17	LHG	e	5003	13	40,40,48	0.74	1 (2%)	43,46,54	1.33	6 (13%)
13	CLA	6	504	-	45,53,73	1.78	5 (11%)	52,89,113	1.68	8 (15%)
13	CLA	A	1135	1	52,60,73	1.53	8 (15%)	60,97,113	1.72	10 (16%)
13	CLA	e	1101	1	65,73,73	1.49	8 (12%)	76,113,113	1.45	9 (11%)
16	BCR	B	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
13	CLA	r	507	-	65,73,73	1.44	7 (10%)	76,113,113	1.48	7 (9%)
13	CLA	s	512	12	45,53,73	1.74	7 (15%)	52,89,113	1.62	5 (9%)
20	SQD	1	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
13	CLA	a	502	12	50,58,73	1.68	7 (14%)	58,95,113	1.62	8 (13%)
13	CLA	l	1302	8	58,66,73	1.52	8 (13%)	67,104,113	1.53	8 (11%)
13	CLA	G	1111	1	65,73,73	1.47	7 (10%)	76,113,113	1.49	7 (9%)
13	CLA	A	1126	1	65,73,73	1.39	7 (10%)	76,113,113	1.60	8 (10%)
13	CLA	5	505	12	61,69,73	1.51	6 (9%)	71,108,113	1.39	6 (8%)
13	CLA	f	1216	21	60,68,73	1.57	10 (16%)	70,107,113	1.44	6 (8%)
13	CLA	n	1502	10	65,73,73	1.43	7 (10%)	76,113,113	1.48	8 (10%)
16	BCR	V	4019	-	41,41,41	0.74	0	56,56,56	1.92	14 (25%)
20	SQD	t	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.84	9 (26%)
13	CLA	B	1206	2	65,73,73	1.44	10 (15%)	76,113,113	1.58	7 (9%)
13	CLA	V	1503	21	60,68,73	1.49	7 (11%)	70,107,113	1.56	7 (10%)
16	BCR	e	4007	-	41,41,41	0.74	0	56,56,56	2.11	18 (32%)
13	CLA	1	511	12	55,63,73	1.60	6 (10%)	64,101,113	1.58	8 (12%)
13	CLA	H	1240	17	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
13	CLA	c	502	12	50,58,73	1.71	8 (16%)	58,95,113	1.54	7 (12%)
17	LHG	B	1842	13	38,38,48	0.66	0	41,44,54	1.23	4 (9%)
20	SQD	n	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.63	11 (18%)
13	CLA	5	510	12	45,53,73	1.76	6 (13%)	52,89,113	1.60	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	q	512	12	52,60,73	1.64	6 (11%)	60,97,113	1.53	6 (10%)
17	LHG	H	1842	13	38,38,48	0.66	0	41,44,54	1.23	4 (9%)
13	CLA	r	505	12	65,73,73	1.44	6 (9%)	76,113,113	1.40	8 (10%)
13	CLA	f	1012	21	65,73,73	1.46	9 (13%)	76,113,113	1.54	8 (10%)
13	CLA	B	1215	2	65,73,73	1.44	8 (12%)	76,113,113	1.57	8 (10%)
13	CLA	B	1209	2	52,60,73	1.66	8 (15%)	60,97,113	1.67	8 (13%)
13	CLA	q	503	12	64,72,73	1.50	6 (9%)	74,111,113	1.46	8 (10%)
13	CLA	H	1220	2	55,63,73	1.55	9 (16%)	64,101,113	1.67	11 (17%)
13	CLA	Z	519	12	55,63,73	1.61	9 (16%)	64,101,113	1.46	9 (14%)
13	CLA	b	517	-	45,53,73	1.78	6 (13%)	52,89,113	1.66	8 (15%)
13	CLA	Y	518	12	60,68,73	1.52	9 (15%)	70,107,113	1.52	8 (11%)
13	CLA	f	1232	21	50,58,73	1.62	7 (14%)	58,95,113	1.82	6 (10%)
13	CLA	G	1136	1	60,68,73	1.52	8 (13%)	70,107,113	1.55	11 (15%)
13	CLA	s	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.58	6 (11%)
16	BCR	B	4014	-	41,41,41	0.74	0	56,56,56	1.85	13 (23%)
13	CLA	A	1140	1	65,73,73	1.49	8 (12%)	76,113,113	1.47	12 (15%)
16	BCR	B	4017	-	41,41,41	0.80	0	56,56,56	1.57	11 (19%)
13	CLA	B	1239	2	65,73,73	1.49	7 (10%)	76,113,113	1.63	14 (18%)
18	LMU	q	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
13	CLA	Y	507	-	60,68,73	1.52	6 (10%)	70,107,113	1.53	9 (12%)
13	CLA	r	506	12	55,63,73	1.61	6 (10%)	64,101,113	1.55	6 (9%)
13	CLA	1	502	12	60,68,73	1.55	7 (11%)	70,107,113	1.47	7 (10%)
13	CLA	B	1222	21	60,68,73	1.50	7 (11%)	70,107,113	1.54	10 (14%)
13	CLA	B	1207	2	65,73,73	1.46	9 (13%)	76,113,113	1.38	6 (7%)
13	CLA	G	1126	1	65,73,73	1.38	6 (9%)	76,113,113	1.60	8 (10%)
13	CLA	c	511	12	55,63,73	1.61	6 (10%)	64,101,113	1.53	7 (10%)
13	CLA	f	1239	2	65,73,73	1.49	7 (10%)	76,113,113	1.62	14 (18%)
13	CLA	s	505	12	65,73,73	1.46	6 (9%)	76,113,113	1.37	6 (7%)
17	LHG	G	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
13	CLA	s	502	12	50,58,73	1.68	7 (14%)	58,95,113	1.62	8 (13%)
13	CLA	Y	504	-	45,53,73	1.80	8 (17%)	52,89,113	1.61	8 (15%)
13	CLA	s	513	12	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
13	CLA	B	1238	21	65,73,73	1.41	7 (10%)	76,113,113	1.57	10 (13%)
13	CLA	B	1221	21	65,73,73	1.48	8 (12%)	76,113,113	1.66	12 (15%)
13	CLA	e	1128	1	65,73,73	1.54	10 (15%)	76,113,113	1.61	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	e	1137	1	65,73,73	1.45	7 (10%)	76,113,113	1.50	8 (10%)
13	CLA	H	1213	2	65,73,73	1.40	7 (10%)	76,113,113	1.54	10 (13%)
13	CLA	f	1213	2	65,73,73	1.40	7 (10%)	76,113,113	1.54	10 (13%)
17	LHG	L	5220	-	40,40,48	0.65	0	43,46,54	1.23	4 (9%)
13	CLA	B	1223	2	65,73,73	1.41	7 (10%)	76,113,113	1.56	6 (7%)
13	CLA	G	1139	21	65,73,73	1.45	7 (10%)	76,113,113	1.33	9 (11%)
13	CLA	r	518	12	65,73,73	1.46	7 (10%)	76,113,113	1.48	7 (9%)
13	CLA	e	1117	1	65,73,73	1.43	10 (15%)	76,113,113	1.69	12 (15%)
16	BCR	n	4022	-	41,41,41	0.75	0	56,56,56	1.90	15 (26%)
16	BCR	v	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
13	CLA	f	1229	2	65,73,73	1.44	7 (10%)	76,113,113	1.57	10 (13%)
16	BCR	H	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
13	CLA	e	1125	1	65,73,73	1.42	8 (12%)	76,113,113	1.56	9 (11%)
13	CLA	a	507	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	8 (10%)
13	CLA	1	513	12	55,63,73	1.61	7 (12%)	64,101,113	1.49	6 (9%)
18	LMU	l	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
16	BCR	3	521	-	41,41,41	0.67	0	56,56,56	1.76	10 (17%)
13	CLA	A	1102	1	65,73,73	1.42	6 (9%)	76,113,113	1.49	7 (9%)
13	CLA	H	1223	2	65,73,73	1.40	7 (10%)	76,113,113	1.55	6 (7%)
16	BCR	Y	523	-	41,41,41	0.71	0	56,56,56	1.64	16 (28%)
13	CLA	t	502	12	50,58,73	1.68	7 (14%)	58,95,113	1.59	7 (12%)
13	CLA	H	1206	2	65,73,73	1.44	10 (15%)	76,113,113	1.58	7 (9%)
13	CLA	e	1112	1	50,58,73	1.63	9 (18%)	58,95,113	1.72	8 (13%)
16	BCR	1	521	-	41,41,41	0.66	0	56,56,56	1.81	11 (19%)
13	CLA	3	519	12	55,63,73	1.61	9 (16%)	64,101,113	1.50	7 (10%)
13	CLA	v	517	-	45,53,73	1.79	6 (13%)	52,89,113	1.59	6 (11%)
13	CLA	f	1240	17	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
14	PQN	G	2001	-	34,34,34	2.87	11 (32%)	42,45,45	2.12	7 (16%)
13	CLA	d	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.61	8 (15%)
13	CLA	B	1210	2	65,73,73	1.42	8 (12%)	76,113,113	1.53	12 (15%)
16	BCR	d	524	-	41,41,41	0.75	0	56,56,56	1.87	13 (23%)
13	CLA	H	1232	21	50,58,73	1.62	7 (14%)	58,95,113	1.82	6 (10%)
13	CLA	3	518	12	55,63,73	1.61	7 (12%)	64,101,113	1.48	7 (10%)
16	BCR	q	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
13	CLA	d	508	12	45,53,73	1.77	7 (15%)	52,89,113	1.67	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	J	1302	8	58,66,73	1.52	8 (13%)	67,104,113	1.51	8 (11%)
13	CLA	e	1105	1	55,63,73	1.52	7 (12%)	64,101,113	1.69	9 (14%)
13	CLA	2	506	12	55,63,73	1.61	7 (12%)	64,101,113	1.55	6 (9%)
13	CLA	q	506	12	45,53,73	1.77	7 (15%)	52,89,113	1.69	6 (11%)
16	BCR	G	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
13	CLA	Y	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.58	6 (11%)
16	BCR	u	523	-	41,41,41	0.74	0	56,56,56	1.78	16 (28%)
15	SF4	C	3002	3	0,12,12	-	-	-		
13	CLA	G	1120	1	53,61,73	1.56	7 (13%)	61,98,113	1.68	7 (11%)
13	CLA	Y	502	12	60,68,73	1.55	7 (11%)	70,107,113	1.47	7 (10%)
20	SQD	4	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.84	9 (26%)
13	CLA	A	1124	21	56,64,73	1.58	6 (10%)	65,102,113	1.63	12 (18%)
13	CLA	H	1239	2	65,73,73	1.48	7 (10%)	76,113,113	1.63	14 (18%)
13	CLA	e	1114	21	50,58,73	1.68	8 (16%)	58,95,113	1.64	7 (12%)
16	BCR	H	4017	-	41,41,41	0.79	0	56,56,56	1.58	11 (19%)
16	BCR	f	4006	-	41,41,41	0.72	0	56,56,56	1.98	20 (35%)
13	CLA	a	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.50	8 (10%)
13	CLA	6	513	12	45,53,73	1.83	5 (11%)	52,89,113	1.54	6 (11%)
13	CLA	2	516	12	45,53,73	1.77	6 (13%)	52,89,113	1.64	7 (13%)
13	CLA	a	512	12	45,53,73	1.75	7 (15%)	52,89,113	1.62	5 (9%)
17	LHG	e	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
13	CLA	H	1222	21	60,68,73	1.49	7 (11%)	70,107,113	1.54	10 (14%)
13	CLA	H	1207	2	65,73,73	1.47	9 (13%)	76,113,113	1.39	6 (7%)
13	CLA	G	1102	1	65,73,73	1.42	6 (9%)	76,113,113	1.49	7 (9%)
13	CLA	G	1104	1	65,73,73	1.40	7 (10%)	76,113,113	1.53	10 (13%)
13	CLA	B	1218	2	60,68,73	1.47	7 (11%)	70,107,113	1.52	7 (10%)
13	CLA	H	1221	21	65,73,73	1.48	8 (12%)	76,113,113	1.66	12 (15%)
13	CLA	q	501	12	65,73,73	1.50	7 (10%)	76,113,113	1.43	8 (10%)
13	CLA	q	504	-	45,53,73	1.79	7 (15%)	52,89,113	1.61	8 (15%)
16	BCR	M	4021	-	41,41,41	0.71	0	56,56,56	1.82	14 (25%)
13	CLA	4	519	12	55,63,73	1.58	9 (16%)	64,101,113	1.49	6 (9%)
16	BCR	A	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
13	CLA	5	509	12	65,73,73	1.46	7 (10%)	76,113,113	1.48	8 (10%)
13	CLA	u	512	12	45,53,73	1.77	7 (15%)	52,89,113	1.59	7 (13%)
16	BCR	J	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	G	4007	-	41,41,41	0.75	0	56,56,56	2.10	18 (32%)
13	CLA	s	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.51	8 (10%)
18	LMU	B	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.11	3 (6%)
16	BCR	Z	521	-	41,41,41	0.66	0	56,56,56	1.86	11 (19%)
13	CLA	A	1113	1	45,53,73	1.67	7 (15%)	52,89,113	1.77	6 (11%)
13	CLA	J	1303	8	65,73,73	1.44	7 (10%)	76,113,113	1.51	12 (15%)
13	CLA	4	516	12	45,53,73	1.78	6 (13%)	52,89,113	1.58	7 (13%)
13	CLA	f	1234	2	65,73,73	1.42	8 (12%)	76,113,113	1.69	13 (17%)
16	BCR	b	523	-	41,41,41	0.70	0	56,56,56	1.65	12 (21%)
16	BCR	4	523	-	41,41,41	0.69	0	56,56,56	1.65	12 (21%)
13	CLA	G	1135	1	52,60,73	1.53	8 (15%)	60,97,113	1.71	10 (16%)
19	LMG	J	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
16	BCR	c	524	-	41,41,41	0.69	0	56,56,56	1.67	15 (26%)
13	CLA	d	504	-	45,53,73	1.77	5 (11%)	52,89,113	1.68	7 (13%)
13	CLA	3	507	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	8 (10%)
19	LMG	B	5002	-	54,54,55	0.79	2 (3%)	62,62,63	1.43	10 (16%)
13	CLA	m	1103	9	50,58,73	1.66	9 (18%)	58,95,113	1.68	12 (20%)
13	CLA	v	518	12	55,63,73	1.61	6 (10%)	64,101,113	1.49	7 (10%)
13	CLA	H	1212	2	55,63,73	1.54	8 (14%)	64,101,113	1.64	8 (12%)
13	CLA	A	1103	1	65,73,73	1.43	7 (10%)	76,113,113	1.64	8 (10%)
13	CLA	q	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.79	10 (19%)
16	BCR	e	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
13	CLA	v	507	-	45,53,73	1.77	6 (13%)	52,89,113	1.66	8 (15%)
16	BCR	f	4017	-	41,41,41	0.80	0	56,56,56	1.57	11 (19%)
18	LMU	e	1848	-	36,36,36	1.14	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	t	513	12	45,53,73	1.80	7 (15%)	52,89,113	1.62	6 (11%)
13	CLA	a	510	12	65,73,73	1.47	6 (9%)	76,113,113	1.47	9 (11%)
13	CLA	B	1217	2	57,65,73	1.52	7 (12%)	66,103,113	1.54	8 (12%)
13	CLA	G	1137	1	65,73,73	1.44	7 (10%)	76,113,113	1.51	8 (10%)
17	LHG	e	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
13	CLA	3	511	12	50,58,73	1.70	6 (12%)	58,95,113	1.62	6 (10%)
13	CLA	f	1235	2	65,73,73	1.42	8 (12%)	76,113,113	1.54	10 (13%)
13	CLA	v	504	-	45,53,73	1.76	5 (11%)	52,89,113	1.68	8 (15%)
14	PQN	f	2002	-	34,34,34	2.87	11 (32%)	42,45,45	2.18	4 (9%)
13	CLA	c	505	12	61,69,73	1.51	6 (9%)	71,108,113	1.40	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	e	1011	1	65,73,73	1.45	6 (9%)	76,113,113	1.63	12 (15%)
13	CLA	Z	501	12	65,73,73	1.48	7 (10%)	76,113,113	1.47	7 (9%)
16	BCR	c	521	-	41,41,41	0.69	0	56,56,56	1.94	16 (28%)
13	CLA	3	513	12	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
13	CLA	G	1013	-	65,73,73	1.43	8 (12%)	76,113,113	1.75	9 (11%)
13	CLA	t	509	12	65,73,73	1.48	6 (9%)	76,113,113	1.50	8 (10%)
16	BCR	l	4013	-	41,41,41	0.76	0	56,56,56	1.96	15 (26%)
13	CLA	3	505	12	65,73,73	1.46	6 (9%)	76,113,113	1.36	6 (7%)
13	CLA	f	1023	-	65,73,73	1.41	8 (12%)	76,113,113	1.84	14 (18%)
13	CLA	r	513	12	65,73,73	1.50	8 (12%)	76,113,113	1.38	6 (7%)
16	BCR	e	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.02	17 (30%)
17	LHG	e	5006	-	44,44,48	0.62	0	47,50,54	1.26	5 (10%)
16	BCR	T	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
13	CLA	H	1218	2	60,68,73	1.47	7 (11%)	70,107,113	1.52	6 (8%)
13	CLA	f	1218	2	60,68,73	1.47	7 (11%)	70,107,113	1.53	6 (8%)
16	BCR	q	522	-	41,41,41	0.74	0	56,56,56	1.90	19 (33%)
19	LMG	T	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.25	7 (16%)
16	BCR	J	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
13	CLA	c	519	12	46,54,73	1.76	9 (19%)	53,90,113	1.56	6 (11%)
13	CLA	U	1105	9	45,53,73	1.79	8 (17%)	52,89,113	1.85	11 (21%)
20	SQD	q	822	-	47,48,54	0.99	5 (10%)	56,59,65	1.74	13 (23%)
16	BCR	t	523	-	41,41,41	0.69	0	56,56,56	1.65	13 (23%)
13	CLA	m	1401	-	55,63,73	1.59	8 (14%)	64,101,113	1.56	9 (14%)
13	CLA	c	506	12	45,53,73	1.77	5 (11%)	52,89,113	1.66	7 (13%)
13	CLA	d	503	12	52,60,73	1.66	6 (11%)	60,97,113	1.57	9 (15%)
13	CLA	B	1211	2	56,64,73	1.53	7 (12%)	65,102,113	1.78	6 (9%)
13	CLA	f	1214	2	65,73,73	1.49	9 (13%)	76,113,113	1.51	7 (9%)
13	CLA	K	1103	9	50,58,73	1.64	9 (18%)	58,95,113	1.68	12 (20%)
13	CLA	H	1238	21	65,73,73	1.41	7 (10%)	76,113,113	1.57	10 (13%)
16	BCR	U	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
13	CLA	b	519	12	55,63,73	1.58	9 (16%)	64,101,113	1.49	6 (9%)
18	LMU	H	1843	-	36,36,36	1.19	2 (5%)	47,47,47	1.10	3 (6%)
16	BCR	V	4022	-	41,41,41	0.76	0	56,56,56	1.90	14 (25%)
13	CLA	Y	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.51	7 (9%)
16	BCR	t	524	-	41,41,41	0.68	0	56,56,56	1.84	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	6	509	12	45,53,73	1.77	6 (13%)	52,89,113	1.63	6 (11%)
13	CLA	Z	512	12	53,61,73	1.61	6 (11%)	61,98,113	1.48	5 (8%)
13	CLA	H	1208	2	65,73,73	1.42	7 (10%)	76,113,113	1.43	8 (10%)
13	CLA	A	1117	1	65,73,73	1.43	10 (15%)	76,113,113	1.69	12 (15%)
13	CLA	A	1111	1	65,73,73	1.46	7 (10%)	76,113,113	1.49	7 (9%)
13	CLA	e	1136	1	60,68,73	1.53	8 (13%)	70,107,113	1.56	11 (15%)
13	CLA	c	508	12	45,53,73	1.77	7 (15%)	52,89,113	1.73	6 (11%)
13	CLA	5	507	-	45,53,73	1.75	6 (13%)	52,89,113	1.68	8 (15%)
17	LHG	L	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
13	CLA	H	1205	2	65,73,73	1.46	9 (13%)	76,113,113	1.54	9 (11%)
13	CLA	e	1120	1	53,61,73	1.56	7 (13%)	61,98,113	1.68	7 (11%)
13	CLA	6	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.60	8 (15%)
13	CLA	A	1108	1	54,62,73	1.61	7 (12%)	62,99,113	1.48	6 (9%)
15	SF4	g	3002	3	0,12,12	-	-	-		
16	BCR	6	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
13	CLA	G	1128	1	65,73,73	1.53	10 (15%)	76,113,113	1.61	6 (7%)
13	CLA	e	1131	1	65,73,73	1.44	9 (13%)	76,113,113	1.43	9 (11%)
13	CLA	A	1130	1	65,73,73	1.47	7 (10%)	76,113,113	1.52	10 (13%)
13	CLA	s	508	12	55,63,73	1.63	7 (12%)	64,101,113	1.59	8 (12%)
13	CLA	u	501	12	65,73,73	1.47	6 (9%)	76,113,113	1.47	7 (9%)
13	CLA	u	517	-	45,53,73	1.80	7 (15%)	52,89,113	1.56	6 (11%)
18	LMU	1	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
13	CLA	c	503	12	55,63,73	1.64	6 (10%)	64,101,113	1.53	8 (12%)
13	CLA	q	510	12	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
14	PQN	H	2002	-	34,34,34	2.87	11 (32%)	42,45,45	2.17	4 (9%)
16	BCR	e	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
13	CLA	H	1217	2	57,65,73	1.52	7 (12%)	66,103,113	1.54	9 (13%)
16	BCR	q	523	-	41,41,41	0.71	0	56,56,56	1.64	16 (28%)
13	CLA	d	511	12	45,53,73	1.79	6 (13%)	52,89,113	1.66	6 (11%)
13	CLA	a	518	12	55,63,73	1.61	7 (12%)	64,101,113	1.47	7 (10%)
13	CLA	1	518	12	60,68,73	1.53	10 (16%)	70,107,113	1.53	8 (11%)
13	CLA	V	1502	10	65,73,73	1.43	7 (10%)	76,113,113	1.49	8 (10%)
13	CLA	v	505	12	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
13	CLA	Z	513	12	65,73,73	1.50	8 (12%)	76,113,113	1.38	7 (9%)
16	BCR	e	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	b	503	12	55,63,73	1.64	6 (10%)	64,101,113	1.55	11 (17%)
13	CLA	e	1139	21	65,73,73	1.46	7 (10%)	76,113,113	1.34	9 (11%)
13	CLA	u	509	12	65,73,73	1.45	7 (10%)	76,113,113	1.49	8 (10%)
13	CLA	G	1131	1	65,73,73	1.45	9 (13%)	76,113,113	1.43	9 (11%)
16	BCR	A	4002	-	41,41,41	0.81	1 (2%)	56,56,56	1.85	15 (26%)
16	BCR	d	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
13	CLA	r	508	12	55,63,73	1.63	8 (14%)	64,101,113	1.59	9 (14%)
13	CLA	d	505	12	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
16	BCR	a	524	-	41,41,41	0.74	0	56,56,56	1.81	17 (30%)
13	CLA	q	505	12	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
13	CLA	d	510	12	45,53,73	1.80	5 (11%)	52,89,113	1.57	7 (13%)
13	CLA	e	1115	1	60,68,73	1.46	7 (11%)	70,107,113	1.59	8 (11%)
13	CLA	v	519	12	46,54,73	1.76	6 (13%)	53,90,113	1.59	6 (11%)
16	BCR	b	524	-	41,41,41	0.67	0	56,56,56	1.85	15 (26%)
16	BCR	b	522	-	41,41,41	0.74	0	56,56,56	1.85	18 (32%)
13	CLA	A	1801	17	45,53,73	1.72	7 (15%)	52,89,113	1.83	8 (15%)
13	CLA	e	1126	1	65,73,73	1.39	7 (10%)	76,113,113	1.60	8 (10%)
16	BCR	F	4016	-	41,41,41	0.74	0	56,56,56	1.78	13 (23%)
20	SQD	b	822	-	25,26,54	1.31	4 (16%)	34,37,65	1.85	9 (26%)
13	CLA	t	507	-	45,53,73	1.77	6 (13%)	52,89,113	1.69	8 (15%)
13	CLA	d	506	12	45,53,73	1.79	6 (13%)	52,89,113	1.65	6 (11%)
13	CLA	4	517	-	45,53,73	1.79	6 (13%)	52,89,113	1.66	8 (15%)
18	LMU	G	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	G	1109	1	65,73,73	1.41	7 (10%)	76,113,113	1.52	7 (9%)
13	CLA	5	518	12	55,63,73	1.60	6 (10%)	64,101,113	1.45	7 (10%)
13	CLA	H	1225	2	65,73,73	1.41	9 (13%)	76,113,113	1.44	7 (9%)
13	CLA	d	512	12	45,53,73	1.77	6 (13%)	52,89,113	1.59	5 (9%)
13	CLA	A	1013	-	65,73,73	1.42	8 (12%)	76,113,113	1.75	9 (11%)
13	CLA	e	1129	1	51,59,73	1.60	10 (19%)	59,96,113	1.61	8 (13%)
13	CLA	n	1501	10	65,73,73	1.46	8 (12%)	76,113,113	1.52	9 (11%)
16	BCR	V	4219	-	41,41,41	0.77	0	56,56,56	1.80	12 (21%)
13	CLA	G	1114	21	50,58,73	1.67	8 (16%)	58,95,113	1.64	7 (12%)
13	CLA	a	505	12	65,73,73	1.45	6 (9%)	76,113,113	1.36	6 (7%)
13	CLA	t	511	12	45,53,73	1.80	6 (13%)	52,89,113	1.70	7 (13%)
13	CLA	r	519	12	55,63,73	1.61	8 (14%)	64,101,113	1.46	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	BCR	Z	524	-	41,41,41	0.74	0	56,56,56	1.67	12 (21%)
17	LHG	V	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
13	CLA	A	1110	1	51,59,73	1.66	7 (13%)	59,96,113	1.60	7 (11%)
13	CLA	q	502	12	60,68,73	1.54	7 (11%)	70,107,113	1.47	7 (10%)
13	CLA	2	502	12	60,68,73	1.56	8 (13%)	70,107,113	1.45	7 (10%)
13	CLA	1	507	-	60,68,73	1.52	6 (10%)	70,107,113	1.53	9 (12%)
13	CLA	e	1102	1	65,73,73	1.42	7 (10%)	76,113,113	1.49	7 (9%)
13	CLA	H	1215	2	65,73,73	1.44	8 (12%)	76,113,113	1.57	8 (10%)
16	BCR	f	4005	-	41,41,41	0.70	0	56,56,56	1.78	11 (19%)
13	CLA	s	507	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
13	CLA	A	1127	1	65,73,73	1.41	7 (10%)	76,113,113	1.50	9 (11%)
16	BCR	L	4019	-	41,41,41	0.73	0	56,56,56	1.92	14 (25%)
13	CLA	v	503	12	52,60,73	1.67	6 (11%)	60,97,113	1.58	9 (15%)
13	CLA	2	504	-	50,58,73	1.68	7 (14%)	58,95,113	1.59	8 (13%)
17	LHG	G	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)
13	CLA	a	519	12	55,63,73	1.61	7 (12%)	64,101,113	1.50	7 (10%)
13	CLA	b	510	12	50,58,73	1.69	6 (12%)	58,95,113	1.62	7 (12%)
16	BCR	d	522	-	41,41,41	0.70	0	56,56,56	1.84	14 (25%)
13	CLA	r	504	-	50,58,73	1.68	7 (14%)	58,95,113	1.58	8 (13%)
17	LHG	e	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
16	BCR	L	4020	-	41,41,41	0.83	0	56,56,56	1.95	16 (28%)
16	BCR	v	522	-	41,41,41	0.69	0	56,56,56	1.84	15 (26%)
13	CLA	G	1116	1	60,68,73	1.51	8 (13%)	70,107,113	1.50	7 (10%)
13	CLA	G	1115	1	60,68,73	1.47	7 (11%)	70,107,113	1.59	8 (11%)
13	CLA	s	511	12	50,58,73	1.71	6 (12%)	58,95,113	1.62	6 (10%)
13	CLA	b	506	12	45,53,73	1.79	6 (13%)	52,89,113	1.63	6 (11%)
13	CLA	e	1111	1	65,73,73	1.46	7 (10%)	76,113,113	1.48	7 (9%)
13	CLA	1	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.58	6 (11%)
13	CLA	a	516	12	45,53,73	1.77	6 (13%)	52,89,113	1.85	12 (23%)
13	CLA	4	504	-	45,53,73	1.77	6 (13%)	52,89,113	1.63	7 (13%)
16	BCR	a	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
13	CLA	3	506	12	50,58,73	1.70	7 (14%)	58,95,113	1.67	6 (10%)
13	CLA	3	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.51	8 (10%)
13	CLA	r	503	12	65,73,73	1.48	7 (10%)	76,113,113	1.45	7 (9%)
19	LMG	f	5002	-	54,54,55	0.80	3 (5%)	62,62,63	1.43	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	B	1227	2	65,73,73	1.46	9 (13%)	76,113,113	1.47	9 (11%)
13	CLA	c	501	12	65,73,73	1.46	7 (10%)	76,113,113	1.48	7 (9%)
13	CLA	u	518	12	55,63,73	1.60	6 (10%)	64,101,113	1.45	7 (10%)
13	CLA	e	1135	1	52,60,73	1.54	8 (15%)	60,97,113	1.71	10 (16%)
13	CLA	t	518	12	55,63,73	1.62	7 (12%)	64,101,113	1.49	7 (10%)
13	CLA	v	509	12	45,53,73	1.77	6 (13%)	52,89,113	1.63	6 (11%)
13	CLA	G	1122	1	60,68,73	1.50	9 (15%)	70,107,113	1.53	8 (11%)
13	CLA	u	507	-	45,53,73	1.75	6 (13%)	52,89,113	1.68	8 (15%)
13	CLA	4	508	12	45,53,73	1.82	8 (17%)	52,89,113	1.75	10 (19%)
16	BCR	3	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
16	BCR	o	4021	-	41,41,41	0.71	0	56,56,56	1.81	14 (25%)
13	CLA	f	1222	21	60,68,73	1.50	7 (11%)	70,107,113	1.54	10 (14%)
13	CLA	B	1234	2	65,73,73	1.43	8 (12%)	76,113,113	1.69	13 (17%)
16	BCR	f	4009	-	41,41,41	0.81	0	56,56,56	1.91	21 (37%)
13	CLA	e	1118	1	60,68,73	1.50	7 (11%)	70,107,113	1.49	8 (11%)
13	CLA	G	1134	1	56,64,73	1.57	7 (12%)	65,102,113	1.55	8 (12%)
18	LMU	e	1849	-	23,23,36	1.16	1 (4%)	28,28,47	1.00	2 (7%)
13	CLA	B	1202	2	65,73,73	1.44	7 (10%)	76,113,113	1.65	9 (11%)
13	CLA	5	519	12	46,54,73	1.76	9 (19%)	53,90,113	1.55	6 (11%)
16	BCR	b	521	-	41,41,41	0.64	0	56,56,56	1.78	11 (19%)
13	CLA	1	519	12	50,58,73	1.66	10 (20%)	58,95,113	1.50	8 (13%)
13	CLA	Z	507	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	7 (9%)
17	LHG	G	5007	-	46,46,48	0.67	1 (2%)	49,52,54	1.24	5 (10%)
13	CLA	B	1224	2	60,68,73	1.47	7 (11%)	70,107,113	1.59	8 (11%)
13	CLA	f	1221	21	65,73,73	1.49	8 (12%)	76,113,113	1.65	12 (15%)
16	BCR	e	4002	-	41,41,41	0.81	0	56,56,56	1.85	14 (25%)
17	LHG	A	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)
13	CLA	K	1401	-	55,63,73	1.59	8 (14%)	64,101,113	1.55	9 (14%)
17	LHG	S	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
13	CLA	6	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.59	6 (11%)
13	CLA	H	1209	2	52,60,73	1.66	8 (15%)	60,97,113	1.67	8 (13%)
20	SQD	L	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.63	11 (18%)
13	CLA	t	505	12	65,73,73	1.46	6 (9%)	76,113,113	1.36	6 (7%)
17	LHG	f	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.22	5 (10%)
13	CLA	Y	513	12	55,63,73	1.62	7 (12%)	64,101,113	1.49	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	Z	518	12	65,73,73	1.46	6 (9%)	76,113,113	1.48	7 (9%)
13	CLA	f	1223	2	65,73,73	1.42	7 (10%)	76,113,113	1.56	6 (7%)
13	CLA	u	513	12	45,53,73	1.82	8 (17%)	52,89,113	1.56	7 (13%)
13	CLA	G	1138	1	65,73,73	1.44	7 (10%)	76,113,113	1.45	8 (10%)
13	CLA	2	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.63	6 (11%)
13	CLA	A	1011	1	65,73,73	1.45	6 (9%)	76,113,113	1.63	12 (15%)
13	CLA	f	1201	2	60,68,73	1.48	7 (11%)	70,107,113	1.66	8 (11%)
13	CLA	r	501	12	65,73,73	1.49	7 (10%)	76,113,113	1.47	7 (9%)
13	CLA	4	510	12	50,58,73	1.68	6 (12%)	58,95,113	1.62	7 (12%)
16	BCR	2	522	-	41,41,41	0.71	0	56,56,56	1.75	18 (32%)
13	CLA	e	1103	1	65,73,73	1.43	7 (10%)	76,113,113	1.64	8 (10%)
13	CLA	v	506	12	45,53,73	1.79	7 (15%)	52,89,113	1.65	6 (11%)
13	CLA	s	519	12	55,63,73	1.60	8 (14%)	64,101,113	1.49	7 (10%)
13	CLA	e	1123	21	65,73,73	1.40	7 (10%)	76,113,113	1.51	8 (10%)
16	BCR	T	4015	-	41,41,41	0.78	0	56,56,56	1.82	14 (25%)
13	CLA	3	501	12	65,73,73	1.44	7 (10%)	76,113,113	1.53	7 (9%)
13	CLA	A	1112	1	50,58,73	1.63	9 (18%)	58,95,113	1.72	9 (15%)
20	SQD	B	1852	-	44,45,54	1.02	4 (9%)	53,56,65	1.84	14 (26%)
20	SQD	Z	822	-	42,43,54	1.07	5 (11%)	51,54,65	1.61	10 (19%)
13	CLA	3	510	12	65,73,73	1.46	6 (9%)	76,113,113	1.46	9 (11%)
13	CLA	Y	503	12	64,72,73	1.49	6 (9%)	74,111,113	1.45	8 (10%)
19	LMG	l	5104	-	35,35,55	0.99	1 (2%)	43,43,63	1.24	7 (16%)
13	CLA	G	1112	1	50,58,73	1.63	9 (18%)	58,95,113	1.72	9 (15%)
13	CLA	b	508	12	45,53,73	1.82	8 (17%)	52,89,113	1.75	10 (19%)
17	LHG	A	5005	-	44,44,48	0.67	1 (2%)	47,50,54	1.27	6 (12%)
13	CLA	f	1212	2	55,63,73	1.53	7 (12%)	64,101,113	1.65	8 (12%)
13	CLA	2	503	12	65,73,73	1.47	6 (9%)	76,113,113	1.45	7 (9%)
16	BCR	Y	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
16	BCR	V	4020	-	41,41,41	0.83	0	56,56,56	1.95	16 (28%)
13	CLA	Z	503	12	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
13	CLA	G	1106	1	65,73,73	1.41	9 (13%)	76,113,113	1.55	9 (11%)
13	CLA	f	1225	2	65,73,73	1.41	9 (13%)	76,113,113	1.45	7 (9%)
17	LHG	L	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
13	CLA	Y	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.78	10 (19%)
13	CLA	H	1227	2	65,73,73	1.46	9 (13%)	76,113,113	1.46	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	SQD	c	822	-	28,29,54	1.25	5 (17%)	37,40,65	1.92	13 (35%)
17	LHG	G	5003	13	40,40,48	0.74	0	43,46,54	1.34	6 (13%)
13	CLA	f	1236	2	55,63,73	1.63	7 (12%)	64,101,113	1.43	8 (12%)
16	BCR	5	524	-	41,41,41	0.68	0	56,56,56	1.67	14 (25%)
13	CLA	c	513	12	45,53,73	1.81	8 (17%)	52,89,113	1.57	6 (11%)
13	CLA	e	1022	21	65,73,73	1.48	9 (13%)	76,113,113	1.48	9 (11%)
16	BCR	H	4014	-	41,41,41	0.74	0	56,56,56	1.84	13 (23%)
18	LMU	G	1849	-	23,23,36	1.17	1 (4%)	28,28,47	1.00	2 (7%)
13	CLA	q	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.57	6 (11%)
13	CLA	B	1201	2	60,68,73	1.48	7 (11%)	70,107,113	1.65	8 (11%)
17	LHG	G	5002	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	5 (12%)
15	SF4	C	3003	3	0,12,12	-	-	-		
13	CLA	A	1101	1	65,73,73	1.49	8 (12%)	76,113,113	1.45	9 (11%)
13	CLA	R	1302	6	45,53,73	1.76	7 (15%)	52,89,113	1.59	6 (11%)
20	SQD	v	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.91	10 (29%)
13	CLA	H	1224	2	60,68,73	1.47	7 (11%)	70,107,113	1.58	8 (11%)
13	CLA	f	1224	2	60,68,73	1.47	7 (11%)	70,107,113	1.59	8 (11%)
16	BCR	B	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
13	CLA	Z	504	-	50,58,73	1.68	6 (12%)	58,95,113	1.58	8 (13%)
13	CLA	B	1231	21	65,73,73	1.37	7 (10%)	76,113,113	1.56	8 (10%)
13	CLA	Y	511	12	55,63,73	1.61	6 (10%)	64,101,113	1.58	8 (12%)
13	CLA	4	505	12	65,73,73	1.47	6 (9%)	76,113,113	1.37	7 (9%)
13	CLA	u	511	12	55,63,73	1.62	6 (10%)	64,101,113	1.53	7 (10%)
13	CLA	f	1210	2	65,73,73	1.43	8 (12%)	76,113,113	1.53	12 (15%)
16	BCR	I	4018	-	41,41,41	0.77	0	56,56,56	1.84	15 (26%)
16	BCR	l	4012	-	41,41,41	0.70	0	56,56,56	1.66	13 (23%)
13	CLA	4	502	12	50,58,73	1.69	6 (12%)	58,95,113	1.60	7 (12%)
13	CLA	c	512	12	45,53,73	1.75	6 (13%)	52,89,113	1.59	7 (13%)
17	LHG	n	5221	-	48,48,48	0.65	2 (4%)	51,54,54	1.30	6 (11%)
13	CLA	2	501	12	65,73,73	1.48	7 (10%)	76,113,113	1.47	7 (9%)
16	BCR	6	522	-	41,41,41	0.70	0	56,56,56	1.84	14 (25%)
13	CLA	A	1122	1	60,68,73	1.50	9 (15%)	70,107,113	1.53	8 (11%)
13	CLA	e	1237	21	65,73,73	1.49	9 (13%)	76,113,113	1.50	11 (14%)
13	CLA	a	506	12	50,58,73	1.70	7 (14%)	58,95,113	1.67	6 (10%)
16	BCR	5	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	e	1110	1	51,59,73	1.66	7 (13%)	59,96,113	1.61	7 (11%)
17	LHG	G	5006	-	44,44,48	0.62	0	47,50,54	1.25	5 (10%)
17	LHG	e	5001	-	48,48,48	0.78	1 (2%)	51,54,54	1.26	6 (11%)
13	CLA	G	1110	1	51,59,73	1.65	7 (13%)	59,96,113	1.60	7 (11%)
16	BCR	5	521	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
13	CLA	t	519	12	55,63,73	1.59	9 (16%)	64,101,113	1.50	6 (9%)
16	BCR	H	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
16	BCR	c	523	-	41,41,41	0.74	0	56,56,56	1.78	16 (28%)
18	LMU	J	5105	-	22,22,36	1.14	1 (4%)	27,27,47	0.81	0
13	CLA	e	1116	1	60,68,73	1.51	8 (13%)	70,107,113	1.49	7 (10%)
13	CLA	e	1107	1	65,73,73	1.46	10 (15%)	76,113,113	1.43	10 (13%)
13	CLA	v	512	12	45,53,73	1.77	6 (13%)	52,89,113	1.58	5 (9%)
13	CLA	5	503	12	55,63,73	1.63	6 (10%)	64,101,113	1.53	8 (12%)
13	CLA	F	1302	6	45,53,73	1.76	7 (15%)	52,89,113	1.59	6 (11%)
13	CLA	A	1105	1	55,63,73	1.52	7 (12%)	64,101,113	1.69	9 (14%)
16	BCR	2	521	-	41,41,41	0.66	0	56,56,56	1.87	11 (19%)
13	CLA	A	1139	21	65,73,73	1.45	7 (10%)	76,113,113	1.33	9 (11%)
13	CLA	G	1129	1	51,59,73	1.61	10 (19%)	59,96,113	1.61	8 (13%)
13	CLA	A	1104	1	65,73,73	1.40	7 (10%)	76,113,113	1.53	10 (13%)
13	CLA	5	506	12	45,53,73	1.78	6 (13%)	52,89,113	1.66	7 (13%)
13	CLA	d	518	12	55,63,73	1.61	6 (10%)	64,101,113	1.50	7 (10%)
20	SQD	5	822	-	28,29,54	1.25	5 (17%)	37,40,65	1.92	13 (35%)
16	BCR	n	4019	-	41,41,41	0.73	0	56,56,56	1.92	14 (25%)
16	BCR	A	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.03	17 (30%)
20	SQD	d	822	-	25,26,54	1.30	4 (16%)	34,37,65	1.91	10 (29%)
13	CLA	1	506	12	45,53,73	1.77	6 (13%)	52,89,113	1.68	6 (11%)
13	CLA	1	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.50	7 (9%)
13	CLA	U	1103	9	50,58,73	1.64	9 (18%)	58,95,113	1.69	11 (18%)
13	CLA	e	1122	1	60,68,73	1.49	9 (15%)	70,107,113	1.53	8 (11%)
13	CLA	f	1227	2	65,73,73	1.47	9 (13%)	76,113,113	1.47	9 (11%)
16	BCR	n	4020	-	41,41,41	0.82	0	56,56,56	1.95	15 (26%)
15	SF4	g	3003	3	0,12,12	-	-	-		
13	CLA	b	505	12	65,73,73	1.47	6 (9%)	76,113,113	1.37	6 (7%)
16	BCR	G	4003	-	41,41,41	0.78	0	56,56,56	1.73	11 (19%)
13	CLA	v	513	12	45,53,73	1.82	6 (13%)	52,89,113	1.54	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	s	503	12	65,73,73	1.50	6 (9%)	76,113,113	1.41	9 (11%)
16	BCR	Y	522	-	41,41,41	0.73	0	56,56,56	1.91	20 (35%)
13	CLA	G	1022	21	65,73,73	1.48	9 (13%)	76,113,113	1.48	9 (11%)
13	CLA	Z	502	12	60,68,73	1.56	8 (13%)	70,107,113	1.44	7 (10%)
16	BCR	1	523	-	41,41,41	0.71	0	56,56,56	1.63	16 (28%)
16	BCR	6	524	-	41,41,41	0.75	0	56,56,56	1.86	13 (23%)
17	LHG	e	5007	-	46,46,48	0.66	1 (2%)	49,52,54	1.24	5 (10%)
16	BCR	u	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)
14	PQN	B	2002	-	34,34,34	2.88	11 (32%)	42,45,45	2.18	4 (9%)
13	CLA	H	1201	2	60,68,73	1.48	7 (11%)	70,107,113	1.66	8 (11%)
16	BCR	2	524	-	41,41,41	0.73	0	56,56,56	1.67	12 (21%)
13	CLA	e	1109	1	65,73,73	1.42	7 (10%)	76,113,113	1.52	7 (9%)
16	BCR	H	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
13	CLA	2	508	12	55,63,73	1.62	8 (14%)	64,101,113	1.59	9 (14%)
13	CLA	H	1210	2	65,73,73	1.42	8 (12%)	76,113,113	1.53	12 (15%)
13	CLA	H	1231	21	65,73,73	1.37	7 (10%)	76,113,113	1.56	8 (10%)
17	LHG	B	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.21	5 (10%)
13	CLA	q	513	12	55,63,73	1.61	7 (12%)	64,101,113	1.50	6 (9%)
13	CLA	A	1120	1	53,61,73	1.56	7 (13%)	61,98,113	1.67	7 (11%)
13	CLA	K	1105	9	45,53,73	1.79	8 (17%)	52,89,113	1.86	11 (21%)
13	CLA	m	1105	9	45,53,73	1.79	9 (20%)	52,89,113	1.85	11 (21%)
13	CLA	B	1204	2	65,73,73	1.38	8 (12%)	76,113,113	1.43	9 (11%)
13	CLA	v	510	12	45,53,73	1.80	6 (13%)	52,89,113	1.58	7 (13%)
13	CLA	t	506	12	45,53,73	1.80	6 (13%)	52,89,113	1.65	7 (13%)
13	CLA	H	1204	2	65,73,73	1.38	8 (12%)	76,113,113	1.43	9 (11%)
13	CLA	b	516	12	45,53,73	1.77	6 (13%)	52,89,113	1.58	7 (13%)
16	BCR	A	4011	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
16	BCR	r	522	-	41,41,41	0.70	0	56,56,56	1.75	17 (30%)
14	PQN	A	2001	-	34,34,34	2.88	11 (32%)	42,45,45	2.11	7 (16%)
13	CLA	B	1203	2	65,73,73	1.44	9 (13%)	76,113,113	1.46	7 (9%)
13	CLA	a	508	12	55,63,73	1.65	7 (12%)	64,101,113	1.60	8 (12%)
16	BCR	6	521	-	41,41,41	0.66	0	56,56,56	1.91	12 (21%)
13	CLA	e	1127	1	65,73,73	1.42	7 (10%)	76,113,113	1.50	9 (11%)
17	LHG	n	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
13	CLA	f	1211	2	56,64,73	1.53	7 (12%)	65,102,113	1.77	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	Y	501	12	65,73,73	1.49	7 (10%)	76,113,113	1.43	8 (10%)
13	CLA	B	1021	2	65,73,73	1.42	8 (12%)	76,113,113	1.44	9 (11%)
13	CLA	B	1214	2	65,73,73	1.49	9 (13%)	76,113,113	1.50	7 (9%)
13	CLA	f	1207	2	65,73,73	1.46	9 (13%)	76,113,113	1.38	6 (7%)
13	CLA	a	513	12	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
13	CLA	v	516	12	45,53,73	1.78	5 (11%)	52,89,113	1.60	8 (15%)
16	BCR	A	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
16	BCR	s	521	-	41,41,41	0.66	0	56,56,56	1.76	10 (17%)
17	LHG	V	5218	-	37,37,48	0.75	2 (5%)	40,43,54	1.23	4 (10%)
17	LHG	n	5220	-	40,40,48	0.65	0	43,46,54	1.23	4 (9%)
13	CLA	B	1228	2	55,63,73	1.52	7 (12%)	64,101,113	1.68	8 (12%)
13	CLA	6	510	12	45,53,73	1.80	6 (13%)	52,89,113	1.57	7 (13%)
13	CLA	1	510	12	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
13	CLA	c	504	-	45,53,73	1.77	5 (11%)	52,89,113	1.63	7 (13%)
13	CLA	q	509	12	65,73,73	1.46	7 (10%)	76,113,113	1.50	7 (9%)
13	CLA	s	501	12	65,73,73	1.45	7 (10%)	76,113,113	1.52	7 (9%)
16	BCR	v	524	-	41,41,41	0.76	0	56,56,56	1.87	13 (23%)
16	BCR	4	522	-	41,41,41	0.74	0	56,56,56	1.85	18 (32%)
13	CLA	e	1134	1	56,64,73	1.57	8 (14%)	65,102,113	1.54	8 (12%)
13	CLA	f	1205	2	65,73,73	1.45	9 (13%)	76,113,113	1.53	9 (11%)
16	BCR	f	4014	-	41,41,41	0.74	0	56,56,56	1.84	13 (23%)
13	CLA	6	519	12	46,54,73	1.76	6 (13%)	53,90,113	1.59	6 (11%)
15	SF4	G	3001	1,2	0,12,12	-	-	-		
16	BCR	2	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
13	CLA	b	512	12	45,53,73	1.78	6 (13%)	52,89,113	1.62	6 (11%)
13	CLA	6	506	12	45,53,73	1.79	5 (11%)	52,89,113	1.66	6 (11%)
13	CLA	d	501	12	60,68,73	1.53	6 (10%)	70,107,113	1.51	7 (10%)
13	CLA	d	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.58	6 (11%)
13	CLA	v	508	12	45,53,73	1.77	7 (15%)	52,89,113	1.68	7 (13%)
13	CLA	L	1501	10	65,73,73	1.47	7 (10%)	76,113,113	1.52	9 (11%)
13	CLA	1	516	12	45,53,73	1.79	6 (13%)	52,89,113	1.79	10 (19%)
13	CLA	r	516	12	45,53,73	1.77	6 (13%)	52,89,113	1.66	7 (13%)
13	CLA	Y	505	12	65,73,73	1.45	6 (9%)	76,113,113	1.39	7 (9%)
13	CLA	d	502	12	50,58,73	1.68	6 (12%)	58,95,113	1.60	7 (12%)
13	CLA	G	1103	1	65,73,73	1.43	7 (10%)	76,113,113	1.64	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	H	1230	2	60,68,73	1.53	9 (15%)	70,107,113	1.52	10 (14%)
13	CLA	6	508	12	45,53,73	1.77	7 (15%)	52,89,113	1.67	7 (13%)
16	BCR	G	4001	-	41,41,41	0.76	0	56,56,56	1.72	11 (19%)
13	CLA	A	1118	1	60,68,73	1.49	8 (13%)	70,107,113	1.49	8 (11%)
13	CLA	5	508	12	45,53,73	1.78	7 (15%)	52,89,113	1.73	6 (11%)
17	LHG	G	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
13	CLA	A	1129	1	51,59,73	1.61	10 (19%)	59,96,113	1.61	8 (13%)
16	BCR	4	524	-	41,41,41	0.67	0	56,56,56	1.84	15 (26%)
13	CLA	A	1137	1	65,73,73	1.44	7 (10%)	76,113,113	1.50	8 (10%)
13	CLA	3	503	12	65,73,73	1.50	6 (9%)	76,113,113	1.41	9 (11%)
13	CLA	e	1130	1	65,73,73	1.47	7 (10%)	76,113,113	1.52	10 (13%)
13	CLA	q	511	12	55,63,73	1.60	6 (10%)	64,101,113	1.57	8 (12%)
16	BCR	r	524	-	41,41,41	0.73	0	56,56,56	1.67	12 (21%)
13	CLA	2	511	12	55,63,73	1.62	6 (10%)	64,101,113	1.57	7 (10%)
17	LHG	H	1855	-	43,43,48	0.64	1 (2%)	46,49,54	1.21	5 (10%)
13	CLA	G	1133	1	65,73,73	1.39	7 (10%)	76,113,113	1.49	6 (7%)
16	BCR	u	521	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
17	LHG	e	5008	-	34,34,48	0.77	1 (2%)	37,40,54	1.28	4 (10%)
13	CLA	L	1503	21	60,68,73	1.49	7 (11%)	70,107,113	1.55	7 (10%)
13	CLA	6	503	12	52,60,73	1.67	6 (11%)	60,97,113	1.58	9 (15%)
16	BCR	s	523	-	41,41,41	0.69	0	56,56,56	1.76	15 (26%)
13	CLA	R	1301	21	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
13	CLA	t	504	-	45,53,73	1.77	6 (13%)	52,89,113	1.63	7 (13%)
13	CLA	A	1132	1	65,73,73	1.43	10 (15%)	76,113,113	1.48	10 (13%)
13	CLA	H	1219	2	65,73,73	1.48	7 (10%)	76,113,113	1.33	9 (11%)
13	CLA	4	506	12	45,53,73	1.80	6 (13%)	52,89,113	1.64	6 (11%)
13	CLA	c	518	12	55,63,73	1.60	6 (10%)	64,101,113	1.45	7 (10%)
16	BCR	Z	522	-	41,41,41	0.71	0	56,56,56	1.75	18 (32%)
13	CLA	B	1208	2	65,73,73	1.43	7 (10%)	76,113,113	1.42	8 (10%)
13	CLA	5	512	12	45,53,73	1.76	7 (15%)	52,89,113	1.58	7 (13%)
13	CLA	1	512	12	52,60,73	1.64	6 (11%)	60,97,113	1.53	6 (10%)
13	CLA	B	1219	2	65,73,73	1.48	7 (10%)	76,113,113	1.33	9 (11%)
13	CLA	H	1203	2	65,73,73	1.44	8 (12%)	76,113,113	1.46	7 (9%)
17	LHG	G	5008	-	34,34,48	0.76	1 (2%)	37,40,54	1.28	4 (10%)
13	CLA	f	1209	2	52,60,73	1.66	8 (15%)	60,97,113	1.67	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	u	508	12	45,53,73	1.78	7 (15%)	52,89,113	1.73	6 (11%)
13	CLA	B	1205	2	65,73,73	1.46	9 (13%)	76,113,113	1.53	9 (11%)
13	CLA	Z	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.48	7 (9%)
13	CLA	H	1021	2	65,73,73	1.42	8 (12%)	76,113,113	1.43	9 (11%)
13	CLA	H	1214	2	65,73,73	1.49	9 (13%)	76,113,113	1.51	7 (9%)
13	CLA	f	1021	2	65,73,73	1.42	8 (12%)	76,113,113	1.44	9 (11%)
13	CLA	t	508	12	45,53,73	1.82	8 (17%)	52,89,113	1.75	10 (19%)
13	CLA	H	1228	2	55,63,73	1.52	7 (12%)	64,101,113	1.68	9 (14%)
13	CLA	2	510	12	65,73,73	1.46	6 (9%)	76,113,113	1.44	6 (7%)
13	CLA	t	503	12	55,63,73	1.63	6 (10%)	64,101,113	1.54	12 (18%)
16	BCR	5	523	-	41,41,41	0.75	0	56,56,56	1.78	16 (28%)
13	CLA	e	1106	1	65,73,73	1.41	9 (13%)	76,113,113	1.54	9 (11%)
16	BCR	r	521	-	41,41,41	0.66	0	56,56,56	1.86	11 (19%)
14	PQN	e	2001	-	34,34,34	2.88	11 (32%)	42,45,45	2.11	7 (16%)
20	SQD	6	822	-	25,26,54	1.29	4 (16%)	34,37,65	1.91	10 (29%)
13	CLA	Z	516	12	45,53,73	1.77	7 (15%)	52,89,113	1.64	7 (13%)
13	CLA	j	1301	21	65,73,73	1.46	7 (10%)	76,113,113	1.38	8 (10%)
13	CLA	5	502	12	50,58,73	1.71	8 (16%)	58,95,113	1.54	7 (12%)
19	LMG	H	5002	-	54,54,55	0.79	2 (3%)	62,62,63	1.43	10 (16%)
13	CLA	Y	508	12	55,63,73	1.60	7 (12%)	64,101,113	1.71	10 (15%)
13	CLA	5	516	12	45,53,73	1.78	6 (13%)	52,89,113	1.59	6 (11%)
13	CLA	G	1123	21	65,73,73	1.40	7 (10%)	76,113,113	1.50	8 (10%)
16	BCR	Z	523	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
13	CLA	e	1119	21	65,73,73	1.45	9 (13%)	76,113,113	1.52	9 (11%)
13	CLA	A	1128	1	65,73,73	1.53	10 (15%)	76,113,113	1.61	7 (9%)
16	BCR	4	521	-	41,41,41	0.64	0	56,56,56	1.78	11 (19%)
13	CLA	t	512	12	45,53,73	1.79	6 (13%)	52,89,113	1.62	6 (11%)
13	CLA	e	1132	1	65,73,73	1.43	10 (15%)	76,113,113	1.47	10 (13%)
13	CLA	G	1121	1	55,63,73	1.58	8 (14%)	64,101,113	1.59	11 (17%)
16	BCR	3	522	-	41,41,41	0.67	0	56,56,56	1.91	16 (28%)
13	CLA	G	1124	21	56,64,73	1.58	6 (10%)	65,102,113	1.64	12 (18%)
13	CLA	H	1202	2	65,73,73	1.44	7 (10%)	76,113,113	1.65	9 (11%)
13	CLA	d	513	12	45,53,73	1.84	6 (13%)	52,89,113	1.54	6 (11%)
13	CLA	1	505	12	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
13	CLA	G	1140	1	65,73,73	1.49	8 (12%)	76,113,113	1.48	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	U	1401	-	55,63,73	1.59	7 (12%)	64,101,113	1.55	9 (14%)
13	CLA	A	1138	1	65,73,73	1.44	7 (10%)	76,113,113	1.46	8 (10%)
13	CLA	n	1503	21	60,68,73	1.49	7 (11%)	70,107,113	1.55	7 (10%)
16	BCR	J	4015	-	41,41,41	0.78	0	56,56,56	1.82	14 (25%)
13	CLA	B	1220	2	55,63,73	1.54	9 (16%)	64,101,113	1.67	11 (17%)
13	CLA	T	1303	8	65,73,73	1.44	7 (10%)	76,113,113	1.51	11 (14%)
16	BCR	3	524	-	41,41,41	0.74	0	56,56,56	1.81	17 (30%)
18	LMU	Y	902	-	19,19,36	1.22	1 (5%)	24,24,47	1.10	3 (12%)
13	CLA	Y	519	12	50,58,73	1.65	10 (20%)	58,95,113	1.50	8 (13%)
13	CLA	a	504	-	45,53,73	1.75	6 (13%)	52,89,113	1.69	6 (11%)
13	CLA	d	509	12	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)
13	CLA	B	1216	21	60,68,73	1.56	10 (16%)	70,107,113	1.43	7 (10%)
13	CLA	B	1212	2	55,63,73	1.53	7 (12%)	64,101,113	1.64	8 (12%)
13	CLA	e	1801	17	45,53,73	1.72	7 (15%)	52,89,113	1.83	8 (15%)
13	CLA	6	502	12	50,58,73	1.68	6 (12%)	58,95,113	1.60	7 (12%)
13	CLA	b	501	12	60,68,73	1.54	5 (8%)	70,107,113	1.46	6 (8%)
13	CLA	A	1133	1	65,73,73	1.39	8 (12%)	76,113,113	1.49	6 (7%)
17	LHG	A	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
16	BCR	d	523	-	41,41,41	0.70	0	56,56,56	1.73	14 (25%)
13	CLA	f	1215	2	65,73,73	1.44	8 (12%)	76,113,113	1.57	7 (9%)
13	CLA	B	1012	21	65,73,73	1.46	9 (13%)	76,113,113	1.54	8 (10%)
13	CLA	s	518	12	55,63,73	1.61	7 (12%)	64,101,113	1.48	7 (10%)
13	CLA	c	517	-	45,53,73	1.81	6 (13%)	52,89,113	1.55	6 (11%)
17	LHG	A	5004	-	35,35,48	0.74	1 (2%)	38,41,54	1.25	4 (10%)
13	CLA	A	1116	1	60,68,73	1.51	7 (11%)	70,107,113	1.50	7 (10%)
13	CLA	G	1801	17	45,53,73	1.72	7 (15%)	52,89,113	1.83	8 (15%)
17	LHG	f	1842	13	38,38,48	0.65	0	41,44,54	1.23	4 (9%)
13	CLA	5	504	-	45,53,73	1.77	5 (11%)	52,89,113	1.64	7 (13%)
13	CLA	A	1121	1	55,63,73	1.58	7 (12%)	64,101,113	1.58	11 (17%)
16	BCR	1	524	-	41,41,41	0.73	0	56,56,56	1.82	15 (26%)
13	CLA	4	513	12	45,53,73	1.80	7 (15%)	52,89,113	1.62	6 (11%)
13	CLA	6	501	12	60,68,73	1.53	6 (10%)	70,107,113	1.51	7 (10%)
13	CLA	r	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.64	6 (11%)
13	CLA	B	1213	2	65,73,73	1.40	7 (10%)	76,113,113	1.54	10 (13%)
13	CLA	r	510	12	65,73,73	1.46	7 (10%)	76,113,113	1.43	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	LMU	A	1848	-	36,36,36	1.15	2 (5%)	47,47,47	1.07	2 (4%)
13	CLA	V	1501	10	65,73,73	1.46	7 (10%)	76,113,113	1.52	9 (11%)
13	CLA	Y	512	12	52,60,73	1.65	6 (11%)	60,97,113	1.53	6 (10%)
13	CLA	e	1138	1	65,73,73	1.44	7 (10%)	76,113,113	1.46	8 (10%)
13	CLA	q	518	12	60,68,73	1.52	9 (15%)	70,107,113	1.53	8 (11%)
13	CLA	r	502	12	60,68,73	1.57	8 (13%)	70,107,113	1.44	8 (11%)
13	CLA	u	505	12	61,69,73	1.51	6 (9%)	71,108,113	1.40	6 (8%)
13	CLA	b	518	12	55,63,73	1.62	7 (12%)	64,101,113	1.49	7 (10%)
16	BCR	G	4008	-	41,41,41	0.84	1 (2%)	56,56,56	2.03	16 (28%)
17	LHG	V	5220	-	40,40,48	0.64	0	43,46,54	1.23	4 (9%)
13	CLA	A	1123	21	65,73,73	1.40	7 (10%)	76,113,113	1.51	8 (10%)
13	CLA	4	507	-	45,53,73	1.76	6 (13%)	52,89,113	1.68	8 (15%)
13	CLA	b	507	-	45,53,73	1.75	6 (13%)	52,89,113	1.68	8 (15%)
20	SQD	V	5216	-	50,51,54	0.97	5 (10%)	59,62,65	1.64	10 (16%)
15	SF4	N	3002	3	0,12,12	-	-	-		
13	CLA	A	1125	1	65,73,73	1.43	8 (12%)	76,113,113	1.55	9 (11%)
13	CLA	f	1226	2	65,73,73	1.56	10 (15%)	76,113,113	1.82	14 (18%)
13	CLA	b	504	-	45,53,73	1.76	6 (13%)	52,89,113	1.63	7 (13%)
13	CLA	3	516	12	45,53,73	1.77	6 (13%)	52,89,113	1.85	12 (23%)
13	CLA	B	1232	21	50,58,73	1.62	7 (14%)	58,95,113	1.82	6 (10%)
16	BCR	L	4022	-	41,41,41	0.76	0	56,56,56	1.90	14 (25%)
13	CLA	B	1236	2	55,63,73	1.63	7 (12%)	64,101,113	1.43	8 (12%)
13	CLA	B	1229	2	65,73,73	1.43	7 (10%)	76,113,113	1.57	10 (13%)
13	CLA	4	518	12	55,63,73	1.61	6 (10%)	64,101,113	1.48	7 (10%)
13	CLA	l	1303	8	65,73,73	1.43	7 (10%)	76,113,113	1.51	12 (15%)
20	SQD	H	1852	-	44,45,54	1.02	4 (9%)	53,56,65	1.84	14 (26%)
20	SQD	f	1852	-	44,45,54	1.01	4 (9%)	53,56,65	1.84	14 (26%)
16	BCR	K	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
13	CLA	f	1204	2	65,73,73	1.38	8 (12%)	76,113,113	1.43	9 (11%)
13	CLA	A	1109	1	65,73,73	1.41	7 (10%)	76,113,113	1.52	7 (9%)
13	CLA	4	511	12	45,53,73	1.79	6 (13%)	52,89,113	1.70	7 (13%)
13	CLA	B	1240	17	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
13	CLA	a	517	-	45,53,73	1.77	7 (15%)	52,89,113	1.58	6 (11%)
13	CLA	2	509	12	65,73,73	1.47	7 (10%)	76,113,113	1.48	7 (9%)
13	CLA	e	1013	-	65,73,73	1.42	8 (12%)	76,113,113	1.75	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	A	1114	21	50,58,73	1.68	8 (16%)	58,95,113	1.64	7 (12%)
13	CLA	2	512	12	53,61,73	1.61	7 (13%)	61,98,113	1.48	5 (8%)
16	BCR	a	522	-	41,41,41	0.67	0	56,56,56	1.91	16 (28%)
13	CLA	f	1208	2	65,73,73	1.42	7 (10%)	76,113,113	1.42	8 (10%)
20	SQD	3	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
13	CLA	v	501	12	60,68,73	1.53	7 (11%)	70,107,113	1.51	7 (10%)
13	CLA	H	1216	21	60,68,73	1.56	10 (16%)	70,107,113	1.43	6 (8%)
20	SQD	a	822	-	42,43,54	1.06	5 (11%)	51,54,65	1.59	12 (23%)
13	CLA	A	1237	21	65,73,73	1.49	9 (13%)	76,113,113	1.50	11 (14%)
16	BCR	m	4104	-	41,41,41	0.74	0	56,56,56	1.86	15 (26%)
13	CLA	b	513	12	45,53,73	1.80	7 (15%)	52,89,113	1.62	6 (11%)
15	SF4	e	3001	1,2	0,12,12	-	-	-		
13	CLA	u	502	12	50,58,73	1.71	8 (16%)	58,95,113	1.55	7 (12%)
13	CLA	G	1119	21	65,73,73	1.46	9 (13%)	76,113,113	1.51	9 (11%)
16	BCR	s	524	-	41,41,41	0.73	0	56,56,56	1.82	17 (30%)
16	BCR	B	4006	-	41,41,41	0.72	0	56,56,56	1.99	19 (33%)
13	CLA	u	516	12	45,53,73	1.78	6 (13%)	52,89,113	1.59	6 (11%)
13	CLA	3	504	-	45,53,73	1.75	6 (13%)	52,89,113	1.69	6 (11%)
13	CLA	v	502	12	50,58,73	1.68	6 (12%)	58,95,113	1.60	6 (10%)
13	CLA	H	1211	2	56,64,73	1.53	7 (12%)	65,102,113	1.79	6 (9%)
13	CLA	3	517	-	45,53,73	1.78	7 (15%)	52,89,113	1.58	6 (11%)
16	BCR	f	4004	-	41,41,41	0.72	0	56,56,56	1.85	13 (23%)
17	LHG	k	5001	-	43,43,48	0.64	0	46,49,54	1.22	4 (8%)
13	CLA	a	503	12	65,73,73	1.50	6 (9%)	76,113,113	1.41	9 (11%)
13	CLA	H	1012	21	65,73,73	1.46	9 (13%)	76,113,113	1.54	8 (10%)
13	CLA	A	1107	1	65,73,73	1.47	10 (15%)	76,113,113	1.43	9 (11%)
13	CLA	5	517	-	45,53,73	1.80	7 (15%)	52,89,113	1.55	6 (11%)
13	CLA	G	1132	1	65,73,73	1.42	9 (13%)	76,113,113	1.47	10 (13%)
16	BCR	f	4010	-	41,41,41	0.94	3 (7%)	56,56,56	2.28	23 (41%)
17	LHG	e	5009	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
13	CLA	3	508	12	55,63,73	1.65	7 (12%)	64,101,113	1.60	8 (12%)
16	BCR	c	522	-	41,41,41	0.74	0	56,56,56	1.93	20 (35%)

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
13	CLA	3	512	12	1/1/11/20	3/13/91/115	-
13	CLA	G	1130	1	1/1/15/20	7/37/115/115	-
13	CLA	A	1134	1	1/1/13/20	11/27/105/115	-
16	BCR	S	4018	-	-	1/29/63/63	0/2/2/2
18	LMU	T	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	G	1127	1	1/1/15/20	12/37/115/115	-
17	LHG	A	5007	-	-	24/51/51/53	-
13	CLA	G	1101	1	1/1/15/20	13/37/115/115	-
13	CLA	G	1237	21	1/1/15/20	18/37/115/115	-
13	CLA	e	1133	1	1/1/15/20	15/37/115/115	-
13	CLA	G	1117	1	1/1/15/20	12/37/115/115	-
13	CLA	B	1226	2	1/1/15/20	12/37/115/115	-
13	CLA	b	502	12	1/1/12/20	5/19/97/115	-
13	CLA	e	1140	1	1/1/15/20	11/37/115/115	-
13	CLA	H	1226	2	1/1/15/20	12/37/115/115	-
13	CLA	f	1238	21	1/1/15/20	4/37/115/115	-
13	CLA	G	1108	1	1/1/12/20	16/24/102/115	-
18	LMU	A	1849	-	-	6/14/34/61	0/1/1/2
15	SF4	N	3003	3	-	-	0/6/5/5
13	CLA	f	1206	2	1/1/15/20	15/37/115/115	-
13	CLA	B	1225	2	1/1/15/20	8/37/115/115	-
13	CLA	e	1121	1	1/1/13/20	6/25/103/115	-
13	CLA	Z	510	12	1/1/15/20	9/37/115/115	-
13	CLA	1	503	12	1/1/14/20	9/36/114/115	-
13	CLA	6	512	12	1/1/11/20	6/13/91/115	-
13	CLA	H	1229	2	1/1/15/20	13/37/115/115	-
13	CLA	a	501	12	1/1/15/20	6/37/115/115	-
16	BCR	q	521	-	-	7/29/63/63	0/2/2/2
13	CLA	G	1118	1	1/1/14/20	12/31/109/115	-
18	LMU	r	901	-	-	8/14/34/61	0/1/1/2
16	BCR	1	522	-	-	6/29/63/63	0/2/2/2
13	CLA	4	501	12	1/1/14/20	12/31/109/115	-
13	CLA	u	504	-	1/1/11/20	3/13/91/115	-
13	CLA	t	517	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	L	1502	10	1/1/15/20	8/37/115/115	-
13	CLA	d	507	-	1/1/11/20	4/13/91/115	-
13	CLA	c	507	-	1/1/11/20	5/13/91/115	-
13	CLA	f	1217	2	1/1/13/20	12/28/106/115	-
13	CLA	r	512	12	1/1/12/20	5/23/101/115	-
13	CLA	b	511	12	1/1/11/20	3/13/91/115	-
20	SQD	Y	822	-	-	20/43/63/69	0/1/1/1
13	CLA	B	1235	2	1/1/15/20	6/37/115/115	-
16	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
16	BCR	t	522	-	-	4/29/63/63	0/2/2/2
20	SQD	u	822	-	-	7/24/44/69	0/1/1/1
13	CLA	f	1230	2	1/1/14/20	10/31/109/115	-
13	CLA	Z	517	-	1/1/11/20	4/13/91/115	-
13	CLA	u	519	12	1/1/11/20	8/15/93/115	-
13	CLA	A	1131	1	1/1/15/20	6/37/115/115	-
16	BCR	H	4006	-	-	4/29/63/63	0/2/2/2
13	CLA	v	511	12	1/1/11/20	4/13/91/115	-
16	BCR	G	4002	-	-	0/29/63/63	0/2/2/2
13	CLA	A	1106	1	1/1/15/20	21/37/115/115	-
16	BCR	a	521	-	-	7/29/63/63	0/2/2/2
13	CLA	5	501	12	1/1/15/20	19/37/115/115	-
13	CLA	2	507	-	1/1/15/20	14/37/115/115	-
13	CLA	e	1113	1	1/1/11/20	5/13/91/115	-
13	CLA	Z	508	12	1/1/13/20	6/25/103/115	-
13	CLA	B	1023	-	1/1/15/20	10/37/115/115	-
16	BCR	k	4018	-	-	1/29/63/63	0/2/2/2
13	CLA	6	505	12	1/1/15/20	15/37/115/115	-
16	BCR	n	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	Z	511	12	1/1/13/20	4/25/103/115	-
13	CLA	q	508	12	1/1/13/20	9/25/103/115	-
13	CLA	c	509	12	1/1/15/20	12/37/115/115	-
16	BCR	s	522	-	-	5/29/63/63	0/2/2/2
13	CLA	r	511	12	1/1/13/20	4/25/103/115	-
13	CLA	t	516	12	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	t	521	-	-	10/29/63/63	0/2/2/2
18	LMU	f	1843	-	-	12/21/61/61	0/2/2/2
20	SQD	2	822	-	-	13/38/58/69	0/1/1/1
13	CLA	A	1136	1	1/1/14/20	5/31/109/115	-
13	CLA	c	516	12	1/1/11/20	2/13/91/115	-
13	CLA	A	1119	21	1/1/15/20	15/37/115/115	-
13	CLA	f	1203	2	1/1/15/20	16/37/115/115	-
20	SQD	r	822	-	-	13/38/58/69	0/1/1/1
13	CLA	t	501	12	1/1/14/20	12/31/109/115	-
13	CLA	2	513	12	1/1/15/20	15/37/115/115	-
13	CLA	u	503	12	1/1/13/20	10/25/103/115	-
13	CLA	s	510	12	1/1/15/20	17/37/115/115	-
13	CLA	T	1302	8	1/1/13/20	13/29/107/115	-
13	CLA	e	1124	21	1/1/13/20	11/27/105/115	-
17	LHG	A	5003	13	-	17/45/45/53	-
13	CLA	Y	506	12	1/1/11/20	6/13/91/115	-
13	CLA	3	502	12	1/1/12/20	4/19/97/115	-
13	CLA	s	506	12	1/1/12/20	5/19/97/115	-
18	LMU	2	901	-	-	8/14/34/61	0/1/1/2
17	LHG	A	5002	-	-	26/43/43/53	-
18	LMU	Z	901	-	-	8/14/34/61	0/1/1/2
13	CLA	H	1234	2	1/1/15/20	13/37/115/115	-
16	BCR	H	4009	-	-	1/29/63/63	0/2/2/2
16	BCR	v	523	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1230	2	1/1/14/20	10/31/109/115	-
13	CLA	s	516	12	1/1/11/20	9/13/91/115	-
13	CLA	f	1228	2	1/1/13/20	8/25/103/115	-
13	CLA	1	501	12	1/1/15/20	18/37/115/115	-
13	CLA	r	509	12	1/1/15/20	6/37/115/115	-
16	BCR	W	4021	-	-	7/29/63/63	0/2/2/2
16	BCR	u	524	-	-	2/29/63/63	0/2/2/2
17	LHG	A	5008	-	-	19/39/39/53	-
13	CLA	G	1105	1	1/1/13/20	6/25/103/115	-
16	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
16	BCR	B	4009	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1202	2	1/1/15/20	13/37/115/115	-
13	CLA	F	1301	21	1/1/15/20	11/37/115/115	-
13	CLA	A	1115	1	1/1/14/20	10/31/109/115	-
13	CLA	2	518	12	1/1/15/20	16/37/115/115	-
16	BCR	j	4016	-	-	2/29/63/63	0/2/2/2
13	CLA	5	513	12	1/1/11/20	4/13/91/115	-
16	BCR	T	4013	-	-	4/29/63/63	0/2/2/2
16	BCR	r	523	-	-	6/29/63/63	0/2/2/2
13	CLA	b	509	12	1/1/15/20	7/37/115/115	-
16	BCR	l	4015	-	-	5/29/63/63	0/2/2/2
17	LHG	A	5006	-	-	24/49/49/53	-
13	CLA	4	512	12	1/1/11/20	3/13/91/115	-
13	CLA	G	1113	1	1/1/11/20	5/13/91/115	-
13	CLA	1	504	-	1/1/11/20	5/13/91/115	-
13	CLA	f	1231	21	1/1/15/20	8/37/115/115	-
13	CLA	4	503	12	1/1/13/20	1/25/103/115	-
13	CLA	q	507	-	1/1/14/20	15/31/109/115	-
13	CLA	H	1235	2	1/1/15/20	6/37/115/115	-
13	CLA	f	1219	2	1/1/15/20	17/37/115/115	-
13	CLA	G	1107	1	1/1/15/20	14/37/115/115	-
16	BCR	R	4016	-	-	2/29/63/63	0/2/2/2
13	CLA	e	1108	1	1/1/12/20	16/24/102/115	-
13	CLA	1	508	12	1/1/13/20	9/25/103/115	-
13	CLA	A	1022	21	1/1/15/20	8/37/115/115	-
13	CLA	2	505	12	1/1/15/20	14/37/115/115	-
13	CLA	a	511	12	1/1/12/20	5/19/97/115	-
13	CLA	e	1104	1	1/1/15/20	12/37/115/115	-
13	CLA	G	1125	1	1/1/15/20	14/37/115/115	-
13	CLA	Y	510	12	1/1/15/20	11/37/115/115	-
13	CLA	Z	505	12	1/1/15/20	14/37/115/115	-
13	CLA	u	510	12	1/1/11/20	7/13/91/115	-
13	CLA	H	1023	-	1/1/15/20	10/37/115/115	-
13	CLA	d	519	12	1/1/11/20	6/15/93/115	-
13	CLA	t	510	12	1/1/12/20	5/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	c	510	12	1/1/11/20	7/13/91/115	-
16	BCR	Y	521	-	-	6/29/63/63	0/2/2/2
13	CLA	f	1220	2	1/1/13/20	9/25/103/115	-
13	CLA	j	1302	6	1/1/11/20	8/13/91/115	-
13	CLA	u	506	12	1/1/11/20	5/13/91/115	-
13	CLA	s	504	-	1/1/11/20	6/13/91/115	-
13	CLA	H	1236	2	-	3/25/103/115	-
13	CLA	6	507	-	1/1/11/20	4/13/91/115	-
20	SQD	s	822	-	-	21/38/58/69	0/1/1/1
13	CLA	G	1011	1	1/1/15/20	10/37/115/115	-
17	LHG	G	5009	-	-	28/53/53/53	-
17	LHG	I	5001	-	-	22/48/48/53	-
16	BCR	L	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	Z	506	12	1/1/13/20	8/25/103/115	-
13	CLA	6	518	12	1/1/13/20	10/25/103/115	-
13	CLA	q	519	12	1/1/12/20	6/19/97/115	-
13	CLA	2	519	12	1/1/13/20	9/25/103/115	-
13	CLA	6	511	12	1/1/11/20	4/13/91/115	-
13	CLA	5	511	12	1/1/13/20	5/25/103/115	-
15	SF4	A	3001	1,2	-	-	0/6/5/5
13	CLA	4	509	12	1/1/15/20	7/37/115/115	-
17	LHG	e	5003	13	-	17/45/45/53	-
13	CLA	6	504	-	1/1/11/20	6/13/91/115	-
13	CLA	A	1135	1	1/1/12/20	10/22/100/115	-
13	CLA	e	1101	1	1/1/15/20	13/37/115/115	-
16	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
13	CLA	r	507	-	1/1/15/20	14/37/115/115	-
13	CLA	s	512	12	1/1/11/20	3/13/91/115	-
20	SQD	1	822	-	-	20/43/63/69	0/1/1/1
13	CLA	a	502	12	1/1/12/20	4/19/97/115	-
13	CLA	l	1302	8	1/1/13/20	13/29/107/115	-
13	CLA	G	1111	1	1/1/15/20	14/37/115/115	-
13	CLA	A	1126	1	1/1/15/20	18/37/115/115	-
13	CLA	5	505	12	1/1/14/20	16/33/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1216	21	1/1/14/20	5/31/109/115	-
13	CLA	n	1502	10	1/1/15/20	8/37/115/115	-
16	BCR	V	4019	-	-	6/29/63/63	0/2/2/2
20	SQD	t	822	-	-	8/19/39/69	0/1/1/1
13	CLA	B	1206	2	1/1/15/20	15/37/115/115	-
13	CLA	V	1503	21	1/1/14/20	10/31/109/115	-
16	BCR	e	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	1	511	12	1/1/13/20	4/25/103/115	-
13	CLA	H	1240	17	-	13/37/115/115	-
13	CLA	c	502	12	1/1/12/20	5/19/97/115	-
17	LHG	B	1842	13	-	22/43/43/53	-
20	SQD	n	5216	-	-	17/46/66/69	0/1/1/1
13	CLA	5	510	12	1/1/11/20	7/13/91/115	-
13	CLA	q	512	12	1/1/12/20	10/22/100/115	-
17	LHG	H	1842	13	-	22/43/43/53	-
13	CLA	r	505	12	1/1/15/20	14/37/115/115	-
13	CLA	f	1012	21	1/1/15/20	16/37/115/115	-
13	CLA	B	1215	2	1/1/15/20	19/37/115/115	-
13	CLA	B	1209	2	1/1/12/20	8/22/100/115	-
13	CLA	q	503	12	1/1/14/20	9/36/114/115	-
13	CLA	H	1220	2	1/1/13/20	9/25/103/115	-
13	CLA	Z	519	12	1/1/13/20	9/25/103/115	-
13	CLA	b	517	-	1/1/11/20	5/13/91/115	-
13	CLA	Y	518	12	1/1/14/20	15/31/109/115	-
13	CLA	f	1232	21	1/1/12/20	6/19/97/115	-
13	CLA	G	1136	1	1/1/14/20	5/31/109/115	-
13	CLA	s	517	-	1/1/11/20	7/13/91/115	-
16	BCR	B	4014	-	-	9/29/63/63	0/2/2/2
13	CLA	A	1140	1	1/1/15/20	11/37/115/115	-
16	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1239	2	1/1/15/20	15/37/115/115	-
18	LMU	q	902	-	-	6/10/30/61	0/1/1/2
13	CLA	Y	507	-	1/1/14/20	15/31/109/115	-
13	CLA	r	506	12	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	1	502	12	1/1/14/20	14/31/109/115	-
13	CLA	B	1222	21	1/1/14/20	7/31/109/115	-
13	CLA	B	1207	2	1/1/15/20	14/37/115/115	-
13	CLA	G	1126	1	1/1/15/20	18/37/115/115	-
13	CLA	c	511	12	1/1/13/20	5/25/103/115	-
13	CLA	f	1239	2	1/1/15/20	15/37/115/115	-
13	CLA	s	505	12	1/1/15/20	18/37/115/115	-
17	LHG	G	5005	-	-	29/49/49/53	-
13	CLA	s	502	12	1/1/12/20	4/19/97/115	-
13	CLA	Y	504	-	1/1/11/20	5/13/91/115	-
13	CLA	s	513	12	1/1/15/20	13/37/115/115	-
13	CLA	B	1238	21	1/1/15/20	4/37/115/115	-
13	CLA	B	1221	21	1/1/15/20	14/37/115/115	-
13	CLA	e	1128	1	1/1/15/20	12/37/115/115	-
13	CLA	e	1137	1	1/1/15/20	19/37/115/115	-
13	CLA	H	1213	2	1/1/15/20	14/37/115/115	-
13	CLA	f	1213	2	1/1/15/20	14/37/115/115	-
17	LHG	L	5220	-	-	24/45/45/53	-
13	CLA	B	1223	2	1/1/15/20	14/37/115/115	-
13	CLA	G	1139	21	1/1/15/20	12/37/115/115	-
13	CLA	r	518	12	1/1/15/20	16/37/115/115	-
13	CLA	e	1117	1	1/1/15/20	12/37/115/115	-
16	BCR	n	4022	-	-	2/29/63/63	0/2/2/2
16	BCR	v	521	-	-	5/29/63/63	0/2/2/2
13	CLA	f	1229	2	1/1/15/20	13/37/115/115	-
16	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
13	CLA	e	1125	1	1/1/15/20	14/37/115/115	-
13	CLA	a	507	-	1/1/15/20	13/37/115/115	-
13	CLA	1	513	12	1/1/13/20	2/25/103/115	-
18	LMU	l	5105	-	-	8/13/33/61	0/1/1/2
16	BCR	3	521	-	-	7/29/63/63	0/2/2/2
13	CLA	A	1102	1	1/1/15/20	11/37/115/115	-
13	CLA	H	1223	2	1/1/15/20	14/37/115/115	-
16	BCR	Y	523	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	t	502	12	1/1/12/20	5/19/97/115	-
13	CLA	H	1206	2	1/1/15/20	15/37/115/115	-
13	CLA	e	1112	1	1/1/12/20	3/19/97/115	-
16	BCR	1	521	-	-	7/29/63/63	0/2/2/2
13	CLA	3	519	12	1/1/13/20	8/25/103/115	-
13	CLA	v	517	-	1/1/11/20	9/13/91/115	-
13	CLA	f	1240	17	-	13/37/115/115	-
14	PQN	G	2001	-	-	14/23/43/43	0/2/2/2
13	CLA	d	516	12	1/1/11/20	8/13/91/115	-
13	CLA	B	1210	2	1/1/15/20	19/37/115/115	-
16	BCR	d	524	-	-	5/29/63/63	0/2/2/2
13	CLA	H	1232	21	1/1/12/20	6/19/97/115	-
13	CLA	3	518	12	1/1/13/20	10/25/103/115	-
16	BCR	q	524	-	-	2/29/63/63	0/2/2/2
13	CLA	d	508	12	1/1/11/20	3/13/91/115	-
13	CLA	J	1302	8	1/1/13/20	13/29/107/115	-
13	CLA	e	1105	1	1/1/13/20	6/25/103/115	-
13	CLA	2	506	12	1/1/13/20	8/25/103/115	-
13	CLA	q	506	12	1/1/11/20	6/13/91/115	-
16	BCR	G	4011	-	-	12/29/63/63	0/2/2/2
13	CLA	Y	517	-	1/1/11/20	4/13/91/115	-
16	BCR	u	523	-	-	4/29/63/63	0/2/2/2
15	SF4	C	3002	3	-	-	0/6/5/5
13	CLA	G	1120	1	1/1/12/20	4/23/101/115	-
13	CLA	Y	502	12	1/1/14/20	14/31/109/115	-
20	SQD	4	822	-	-	8/19/39/69	0/1/1/1
13	CLA	A	1124	21	1/1/13/20	11/27/105/115	-
13	CLA	H	1239	2	1/1/15/20	15/37/115/115	-
13	CLA	e	1114	21	1/1/12/20	2/19/97/115	-
16	BCR	H	4017	-	-	2/29/63/63	0/2/2/2
16	BCR	f	4006	-	-	4/29/63/63	0/2/2/2
13	CLA	a	509	12	1/1/15/20	4/37/115/115	-
13	CLA	6	513	12	1/1/11/20	3/13/91/115	-
13	CLA	2	516	12	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	512	12	1/1/11/20	3/13/91/115	-
17	LHG	e	5005	-	-	29/49/49/53	-
13	CLA	H	1222	21	1/1/14/20	7/31/109/115	-
13	CLA	H	1207	2	1/1/15/20	14/37/115/115	-
13	CLA	G	1102	1	1/1/15/20	11/37/115/115	-
13	CLA	G	1104	1	1/1/15/20	12/37/115/115	-
13	CLA	B	1218	2	1/1/14/20	7/31/109/115	-
13	CLA	H	1221	21	1/1/15/20	14/37/115/115	-
13	CLA	q	501	12	1/1/15/20	18/37/115/115	-
13	CLA	q	504	-	1/1/11/20	5/13/91/115	-
16	BCR	M	4021	-	-	7/29/63/63	0/2/2/2
13	CLA	4	519	12	1/1/13/20	12/25/103/115	-
16	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	5	509	12	1/1/15/20	12/37/115/115	-
13	CLA	u	512	12	1/1/11/20	5/13/91/115	-
16	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
16	BCR	G	4007	-	-	0/29/63/63	0/2/2/2
13	CLA	s	509	12	1/1/15/20	4/37/115/115	-
18	LMU	B	1843	-	-	12/21/61/61	0/2/2/2
16	BCR	Z	521	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1113	1	1/1/11/20	5/13/91/115	-
13	CLA	J	1303	8	1/1/15/20	18/37/115/115	-
13	CLA	4	516	12	1/1/11/20	7/13/91/115	-
13	CLA	f	1234	2	1/1/15/20	13/37/115/115	-
16	BCR	b	523	-	-	5/29/63/63	0/2/2/2
16	BCR	4	523	-	-	5/29/63/63	0/2/2/2
13	CLA	G	1135	1	1/1/12/20	10/22/100/115	-
19	LMG	J	5104	-	-	17/30/50/70	0/1/1/1
16	BCR	c	524	-	-	2/29/63/63	0/2/2/2
13	CLA	d	504	-	1/1/11/20	6/13/91/115	-
13	CLA	3	507	-	1/1/15/20	13/37/115/115	-
19	LMG	B	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	m	1103	9	1/1/12/20	7/19/97/115	-
13	CLA	v	518	12	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	H	1212	2	1/1/13/20	11/25/103/115	-
13	CLA	A	1103	1	1/1/15/20	20/37/115/115	-
13	CLA	q	516	12	1/1/11/20	13/13/91/115	-
16	BCR	e	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	v	507	-	1/1/11/20	4/13/91/115	-
16	BCR	f	4017	-	-	2/29/63/63	0/2/2/2
18	LMU	e	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	t	513	12	1/1/11/20	7/13/91/115	-
13	CLA	a	510	12	1/1/15/20	17/37/115/115	-
13	CLA	B	1217	2	1/1/13/20	12/28/106/115	-
13	CLA	G	1137	1	1/1/15/20	19/37/115/115	-
17	LHG	e	5002	-	-	26/43/43/53	-
13	CLA	3	511	12	1/1/12/20	5/19/97/115	-
13	CLA	f	1235	2	1/1/15/20	6/37/115/115	-
13	CLA	v	504	-	1/1/11/20	6/13/91/115	-
14	PQN	f	2002	-	-	9/23/43/43	0/2/2/2
13	CLA	c	505	12	1/1/14/20	16/33/111/115	-
13	CLA	e	1011	1	1/1/15/20	10/37/115/115	-
13	CLA	Z	501	12	1/1/15/20	12/37/115/115	-
16	BCR	c	521	-	-	7/29/63/63	0/2/2/2
13	CLA	3	513	12	1/1/15/20	13/37/115/115	-
13	CLA	G	1013	-	1/1/15/20	11/37/115/115	-
13	CLA	t	509	12	1/1/15/20	7/37/115/115	-
16	BCR	l	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	3	505	12	1/1/15/20	17/37/115/115	-
13	CLA	f	1023	-	1/1/15/20	10/37/115/115	-
13	CLA	r	513	12	1/1/15/20	15/37/115/115	-
16	BCR	e	4008	-	-	7/29/63/63	0/2/2/2
17	LHG	e	5006	-	-	24/49/49/53	-
16	BCR	T	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	H	1218	2	1/1/14/20	7/31/109/115	-
13	CLA	f	1218	2	1/1/14/20	7/31/109/115	-
16	BCR	q	522	-	-	6/29/63/63	0/2/2/2
19	LMG	T	5104	-	-	17/30/50/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	J	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	c	519	12	1/1/11/20	8/15/93/115	-
13	CLA	U	1105	9	1/1/11/20	9/13/91/115	-
20	SQD	q	822	-	-	20/43/63/69	0/1/1/1
16	BCR	t	523	-	-	5/29/63/63	0/2/2/2
13	CLA	m	1401	-	1/1/13/20	8/25/103/115	-
13	CLA	c	506	12	1/1/11/20	5/13/91/115	-
13	CLA	d	503	12	1/1/12/20	8/22/100/115	-
13	CLA	B	1211	2	1/1/13/20	4/27/105/115	-
13	CLA	f	1214	2	1/1/15/20	13/37/115/115	-
13	CLA	K	1103	9	1/1/12/20	7/19/97/115	-
13	CLA	H	1238	21	1/1/15/20	4/37/115/115	-
16	BCR	U	4104	-	-	2/29/63/63	0/2/2/2
13	CLA	b	519	12	1/1/13/20	12/25/103/115	-
18	LMU	H	1843	-	-	12/21/61/61	0/2/2/2
16	BCR	V	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	Y	509	12	1/1/15/20	6/37/115/115	-
16	BCR	t	524	-	-	4/29/63/63	0/2/2/2
13	CLA	6	509	12	1/1/11/20	5/13/91/115	-
13	CLA	Z	512	12	1/1/12/20	5/23/101/115	-
13	CLA	H	1208	2	1/1/15/20	15/37/115/115	-
13	CLA	A	1117	1	1/1/15/20	12/37/115/115	-
13	CLA	A	1111	1	1/1/15/20	14/37/115/115	-
13	CLA	e	1136	1	1/1/14/20	5/31/109/115	-
13	CLA	c	508	12	1/1/11/20	4/13/91/115	-
13	CLA	5	507	-	1/1/11/20	5/13/91/115	-
17	LHG	L	5218	-	-	23/42/42/53	-
13	CLA	H	1205	2	1/1/15/20	10/37/115/115	-
13	CLA	e	1120	1	1/1/12/20	4/23/101/115	-
13	CLA	6	516	12	1/1/11/20	8/13/91/115	-
13	CLA	A	1108	1	1/1/12/20	16/24/102/115	-
15	SF4	g	3002	3	-	-	0/6/5/5
16	BCR	6	523	-	-	4/29/63/63	0/2/2/2
13	CLA	G	1128	1	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	1131	1	1/1/15/20	6/37/115/115	-
13	CLA	A	1130	1	1/1/15/20	7/37/115/115	-
13	CLA	s	508	12	1/1/13/20	7/25/103/115	-
13	CLA	u	501	12	1/1/15/20	19/37/115/115	-
13	CLA	u	517	-	1/1/11/20	9/13/91/115	-
18	LMU	1	902	-	-	6/10/30/61	0/1/1/2
13	CLA	c	503	12	1/1/13/20	10/25/103/115	-
13	CLA	q	510	12	1/1/15/20	11/37/115/115	-
14	PQN	H	2002	-	-	9/23/43/43	0/2/2/2
16	BCR	e	4011	-	-	13/29/63/63	0/2/2/2
13	CLA	H	1217	2	1/1/13/20	12/28/106/115	-
16	BCR	q	523	-	-	6/29/63/63	0/2/2/2
13	CLA	d	511	12	1/1/11/20	4/13/91/115	-
13	CLA	a	518	12	1/1/13/20	10/25/103/115	-
13	CLA	1	518	12	1/1/14/20	15/31/109/115	-
13	CLA	V	1502	10	1/1/15/20	8/37/115/115	-
13	CLA	v	505	12	1/1/15/20	15/37/115/115	-
13	CLA	Z	513	12	1/1/15/20	15/37/115/115	-
16	BCR	e	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	b	503	12	1/1/13/20	1/25/103/115	-
13	CLA	e	1139	21	1/1/15/20	12/37/115/115	-
13	CLA	u	509	12	1/1/15/20	12/37/115/115	-
13	CLA	G	1131	1	1/1/15/20	6/37/115/115	-
16	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
16	BCR	d	521	-	-	5/29/63/63	0/2/2/2
13	CLA	r	508	12	1/1/13/20	6/25/103/115	-
13	CLA	d	505	12	1/1/15/20	15/37/115/115	-
16	BCR	a	524	-	-	5/29/63/63	0/2/2/2
13	CLA	q	505	12	1/1/15/20	11/37/115/115	-
13	CLA	d	510	12	1/1/11/20	7/13/91/115	-
13	CLA	e	1115	1	1/1/14/20	10/31/109/115	-
13	CLA	v	519	12	1/1/11/20	6/15/93/115	-
16	BCR	b	524	-	-	4/29/63/63	0/2/2/2
16	BCR	b	522	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1801	17	1/1/11/20	5/13/91/115	-
13	CLA	e	1126	1	1/1/15/20	18/37/115/115	-
16	BCR	F	4016	-	-	2/29/63/63	0/2/2/2
20	SQD	b	822	-	-	8/19/39/69	0/1/1/1
13	CLA	t	507	-	1/1/11/20	6/13/91/115	-
13	CLA	d	506	12	1/1/11/20	5/13/91/115	-
13	CLA	4	517	-	1/1/11/20	5/13/91/115	-
18	LMU	G	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	G	1109	1	1/1/15/20	9/37/115/115	-
13	CLA	5	518	12	1/1/13/20	11/25/103/115	-
13	CLA	H	1225	2	1/1/15/20	7/37/115/115	-
13	CLA	d	512	12	1/1/11/20	6/13/91/115	-
13	CLA	A	1013	-	1/1/15/20	11/37/115/115	-
13	CLA	e	1129	1	1/1/12/20	5/21/99/115	-
13	CLA	n	1501	10	1/1/15/20	18/37/115/115	-
16	BCR	V	4219	-	-	2/29/63/63	0/2/2/2
13	CLA	G	1114	21	1/1/12/20	2/19/97/115	-
13	CLA	a	505	12	1/1/15/20	17/37/115/115	-
13	CLA	t	511	12	1/1/11/20	3/13/91/115	-
13	CLA	r	519	12	1/1/13/20	9/25/103/115	-
16	BCR	Z	524	-	-	2/29/63/63	0/2/2/2
17	LHG	V	5221	-	-	30/53/53/53	-
13	CLA	A	1110	1	1/1/12/20	9/21/99/115	-
13	CLA	q	502	12	1/1/14/20	14/31/109/115	-
13	CLA	2	502	12	1/1/14/20	11/31/109/115	-
13	CLA	1	507	-	1/1/14/20	15/31/109/115	-
13	CLA	e	1102	1	1/1/15/20	11/37/115/115	-
13	CLA	H	1215	2	1/1/15/20	19/37/115/115	-
16	BCR	f	4005	-	-	6/29/63/63	0/2/2/2
13	CLA	s	507	-	1/1/15/20	13/37/115/115	-
13	CLA	A	1127	1	1/1/15/20	12/37/115/115	-
16	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
13	CLA	v	503	12	1/1/12/20	8/22/100/115	-
13	CLA	2	504	-	1/1/12/20	5/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	G	5001	-	-	25/53/53/53	-
13	CLA	a	519	12	1/1/13/20	8/25/103/115	-
13	CLA	b	510	12	1/1/12/20	5/19/97/115	-
16	BCR	d	522	-	-	5/29/63/63	0/2/2/2
13	CLA	r	504	-	1/1/12/20	5/19/97/115	-
17	LHG	e	5004	-	-	21/40/40/53	-
16	BCR	L	4020	-	-	4/29/63/63	0/2/2/2
16	BCR	v	522	-	-	5/29/63/63	0/2/2/2
13	CLA	G	1116	1	1/1/14/20	15/31/109/115	-
13	CLA	G	1115	1	1/1/14/20	10/31/109/115	-
13	CLA	s	511	12	1/1/12/20	5/19/97/115	-
13	CLA	b	506	12	1/1/11/20	2/13/91/115	-
13	CLA	e	1111	1	1/1/15/20	14/37/115/115	-
13	CLA	1	517	-	1/1/11/20	4/13/91/115	-
13	CLA	a	516	12	1/1/11/20	9/13/91/115	-
13	CLA	4	504	-	1/1/11/20	5/13/91/115	-
16	BCR	a	523	-	-	4/29/63/63	0/2/2/2
13	CLA	3	506	12	1/1/12/20	5/19/97/115	-
13	CLA	3	509	12	1/1/15/20	4/37/115/115	-
13	CLA	r	503	12	1/1/15/20	9/37/115/115	-
19	LMG	f	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	B	1227	2	1/1/15/20	12/37/115/115	-
13	CLA	c	501	12	1/1/15/20	19/37/115/115	-
13	CLA	u	518	12	1/1/13/20	11/25/103/115	-
13	CLA	e	1135	1	1/1/12/20	10/22/100/115	-
13	CLA	t	518	12	1/1/13/20	8/25/103/115	-
13	CLA	v	509	12	1/1/11/20	6/13/91/115	-
13	CLA	G	1122	1	1/1/14/20	14/31/109/115	-
13	CLA	u	507	-	1/1/11/20	5/13/91/115	-
13	CLA	4	508	12	1/1/11/20	4/13/91/115	-
16	BCR	3	523	-	-	4/29/63/63	0/2/2/2
16	BCR	o	4021	-	-	7/29/63/63	0/2/2/2
13	CLA	f	1222	21	1/1/14/20	7/31/109/115	-
13	CLA	B	1234	2	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	f	4009	-	-	1/29/63/63	0/2/2/2
13	CLA	e	1118	1	1/1/14/20	12/31/109/115	-
13	CLA	G	1134	1	1/1/13/20	11/27/105/115	-
18	LMU	e	1849	-	-	6/14/34/61	0/1/1/2
13	CLA	B	1202	2	1/1/15/20	13/37/115/115	-
13	CLA	5	519	12	1/1/11/20	8/15/93/115	-
16	BCR	b	521	-	-	10/29/63/63	0/2/2/2
13	CLA	1	519	12	1/1/12/20	6/19/97/115	-
13	CLA	Z	507	-	1/1/15/20	14/37/115/115	-
17	LHG	G	5007	-	-	24/51/51/53	-
13	CLA	B	1224	2	1/1/14/20	13/31/109/115	-
13	CLA	f	1221	21	1/1/15/20	14/37/115/115	-
16	BCR	e	4002	-	-	0/29/63/63	0/2/2/2
17	LHG	A	5001	-	-	25/53/53/53	-
13	CLA	K	1401	-	1/1/13/20	8/25/103/115	-
17	LHG	S	5001	-	-	22/48/48/53	-
13	CLA	6	517	-	1/1/11/20	9/13/91/115	-
13	CLA	H	1209	2	1/1/12/20	8/22/100/115	-
20	SQD	L	5216	-	-	17/46/66/69	0/1/1/1
13	CLA	t	505	12	1/1/15/20	11/37/115/115	-
17	LHG	f	1855	-	-	28/48/48/53	-
13	CLA	Y	513	12	1/1/13/20	2/25/103/115	-
13	CLA	Z	518	12	1/1/15/20	16/37/115/115	-
13	CLA	f	1223	2	1/1/15/20	14/37/115/115	-
13	CLA	u	513	12	1/1/11/20	4/13/91/115	-
13	CLA	G	1138	1	1/1/15/20	12/37/115/115	-
13	CLA	2	517	-	1/1/11/20	4/13/91/115	-
13	CLA	A	1011	1	1/1/15/20	10/37/115/115	-
13	CLA	f	1201	2	1/1/14/20	11/31/109/115	-
13	CLA	r	501	12	1/1/15/20	12/37/115/115	-
13	CLA	4	510	12	1/1/12/20	5/19/97/115	-
16	BCR	2	522	-	-	6/29/63/63	0/2/2/2
13	CLA	e	1103	1	1/1/15/20	20/37/115/115	-
13	CLA	v	506	12	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	s	519	12	1/1/13/20	8/25/103/115	-
13	CLA	e	1123	21	1/1/15/20	11/37/115/115	-
16	BCR	T	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	3	501	12	1/1/15/20	6/37/115/115	-
13	CLA	A	1112	1	1/1/12/20	3/19/97/115	-
20	SQD	B	1852	-	-	19/40/60/69	0/1/1/1
20	SQD	Z	822	-	-	13/38/58/69	0/1/1/1
13	CLA	3	510	12	1/1/15/20	17/37/115/115	-
13	CLA	Y	503	12	1/1/14/20	9/36/114/115	-
19	LMG	l	5104	-	-	17/30/50/70	0/1/1/1
13	CLA	G	1112	1	1/1/12/20	3/19/97/115	-
13	CLA	b	508	12	1/1/11/20	4/13/91/115	-
17	LHG	A	5005	-	-	29/49/49/53	-
13	CLA	f	1212	2	1/1/13/20	11/25/103/115	-
13	CLA	2	503	12	1/1/15/20	9/37/115/115	-
16	BCR	Y	524	-	-	2/29/63/63	0/2/2/2
16	BCR	V	4020	-	-	4/29/63/63	0/2/2/2
13	CLA	Z	503	12	1/1/15/20	9/37/115/115	-
13	CLA	G	1106	1	1/1/15/20	21/37/115/115	-
13	CLA	f	1225	2	1/1/15/20	7/37/115/115	-
17	LHG	L	5221	-	-	30/53/53/53	-
13	CLA	Y	516	12	1/1/11/20	13/13/91/115	-
13	CLA	H	1227	2	1/1/15/20	12/37/115/115	-
20	SQD	c	822	-	-	7/24/44/69	0/1/1/1
17	LHG	G	5003	13	-	16/45/45/53	-
13	CLA	f	1236	2	-	3/25/103/115	-
16	BCR	5	524	-	-	2/29/63/63	0/2/2/2
13	CLA	c	513	12	1/1/11/20	4/13/91/115	-
13	CLA	e	1022	21	1/1/15/20	8/37/115/115	-
16	BCR	H	4014	-	-	9/29/63/63	0/2/2/2
18	LMU	G	1849	-	-	6/14/34/61	0/1/1/2
13	CLA	q	517	-	1/1/11/20	4/13/91/115	-
13	CLA	B	1201	2	1/1/14/20	11/31/109/115	-
17	LHG	G	5002	-	-	26/43/43/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SF4	C	3003	3	-	-	0/6/5/5
13	CLA	A	1101	1	1/1/15/20	13/37/115/115	-
13	CLA	R	1302	6	1/1/11/20	8/13/91/115	-
20	SQD	v	822	-	-	9/19/39/69	0/1/1/1
13	CLA	H	1224	2	1/1/14/20	13/31/109/115	-
13	CLA	f	1224	2	1/1/14/20	13/31/109/115	-
16	BCR	B	4010	-	-	5/29/63/63	0/2/2/2
13	CLA	Z	504	-	1/1/12/20	5/19/97/115	-
13	CLA	B	1231	21	1/1/15/20	8/37/115/115	-
13	CLA	Y	511	12	1/1/13/20	4/25/103/115	-
13	CLA	4	505	12	1/1/15/20	11/37/115/115	-
13	CLA	u	511	12	1/1/13/20	5/25/103/115	-
13	CLA	f	1210	2	1/1/15/20	19/37/115/115	-
16	BCR	I	4018	-	-	1/29/63/63	0/2/2/2
16	BCR	l	4012	-	-	9/29/63/63	0/2/2/2
13	CLA	4	502	12	1/1/12/20	5/19/97/115	-
13	CLA	c	512	12	1/1/11/20	5/13/91/115	-
17	LHG	n	5221	-	-	30/53/53/53	-
13	CLA	2	501	12	1/1/15/20	12/37/115/115	-
16	BCR	6	522	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1122	1	1/1/14/20	14/31/109/115	-
13	CLA	e	1237	21	1/1/15/20	19/37/115/115	-
13	CLA	a	506	12	1/1/12/20	5/19/97/115	-
16	BCR	5	522	-	-	5/29/63/63	0/2/2/2
13	CLA	e	1110	1	1/1/12/20	9/21/99/115	-
17	LHG	G	5006	-	-	24/49/49/53	-
17	LHG	e	5001	-	-	25/53/53/53	-
13	CLA	G	1110	1	1/1/12/20	9/21/99/115	-
16	BCR	5	521	-	-	7/29/63/63	0/2/2/2
13	CLA	t	519	12	1/1/13/20	12/25/103/115	-
16	BCR	H	4010	-	-	5/29/63/63	0/2/2/2
16	BCR	c	523	-	-	4/29/63/63	0/2/2/2
18	LMU	J	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	e	1116	1	1/1/14/20	15/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	1107	1	1/1/15/20	14/37/115/115	-
13	CLA	v	512	12	1/1/11/20	6/13/91/115	-
13	CLA	5	503	12	1/1/13/20	10/25/103/115	-
13	CLA	F	1302	6	1/1/11/20	8/13/91/115	-
13	CLA	A	1105	1	1/1/13/20	6/25/103/115	-
16	BCR	2	521	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1139	21	1/1/15/20	12/37/115/115	-
13	CLA	G	1129	1	1/1/12/20	5/21/99/115	-
13	CLA	A	1104	1	1/1/15/20	12/37/115/115	-
13	CLA	5	506	12	1/1/11/20	5/13/91/115	-
13	CLA	d	518	12	1/1/13/20	10/25/103/115	-
20	SQD	5	822	-	-	7/24/44/69	0/1/1/1
16	BCR	n	4019	-	-	6/29/63/63	0/2/2/2
16	BCR	A	4008	-	-	7/29/63/63	0/2/2/2
20	SQD	d	822	-	-	9/19/39/69	0/1/1/1
13	CLA	1	506	12	1/1/11/20	6/13/91/115	-
13	CLA	1	509	12	1/1/15/20	6/37/115/115	-
13	CLA	U	1103	9	1/1/12/20	7/19/97/115	-
13	CLA	e	1122	1	1/1/14/20	14/31/109/115	-
13	CLA	f	1227	2	1/1/15/20	12/37/115/115	-
16	BCR	n	4020	-	-	4/29/63/63	0/2/2/2
15	SF4	g	3003	3	-	-	0/6/5/5
13	CLA	b	505	12	1/1/15/20	11/37/115/115	-
16	BCR	G	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	v	513	12	1/1/11/20	3/13/91/115	-
13	CLA	s	503	12	1/1/15/20	7/37/115/115	-
16	BCR	Y	522	-	-	6/29/63/63	0/2/2/2
13	CLA	G	1022	21	1/1/15/20	8/37/115/115	-
13	CLA	Z	502	12	1/1/14/20	11/31/109/115	-
16	BCR	1	523	-	-	6/29/63/63	0/2/2/2
16	BCR	6	524	-	-	5/29/63/63	0/2/2/2
17	LHG	e	5007	-	-	24/51/51/53	-
16	BCR	u	522	-	-	5/29/63/63	0/2/2/2
14	PQN	B	2002	-	-	9/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	H	1201	2	1/1/14/20	11/31/109/115	-
16	BCR	2	524	-	-	2/29/63/63	0/2/2/2
13	CLA	e	1109	1	1/1/15/20	9/37/115/115	-
16	BCR	H	4004	-	-	8/29/63/63	0/2/2/2
13	CLA	2	508	12	1/1/13/20	6/25/103/115	-
13	CLA	H	1210	2	1/1/15/20	19/37/115/115	-
13	CLA	H	1231	21	1/1/15/20	8/37/115/115	-
17	LHG	B	1855	-	-	28/48/48/53	-
13	CLA	q	513	12	1/1/13/20	2/25/103/115	-
13	CLA	A	1120	1	1/1/12/20	4/23/101/115	-
13	CLA	K	1105	9	1/1/11/20	9/13/91/115	-
13	CLA	m	1105	9	1/1/11/20	9/13/91/115	-
13	CLA	B	1204	2	1/1/15/20	12/37/115/115	-
13	CLA	v	510	12	1/1/11/20	7/13/91/115	-
13	CLA	t	506	12	1/1/11/20	2/13/91/115	-
13	CLA	H	1204	2	1/1/15/20	12/37/115/115	-
13	CLA	b	516	12	1/1/11/20	7/13/91/115	-
16	BCR	A	4011	-	-	12/29/63/63	0/2/2/2
16	BCR	r	522	-	-	6/29/63/63	0/2/2/2
14	PQN	A	2001	-	-	14/23/43/43	0/2/2/2
13	CLA	B	1203	2	1/1/15/20	16/37/115/115	-
13	CLA	a	508	12	1/1/13/20	7/25/103/115	-
16	BCR	6	521	-	-	5/29/63/63	0/2/2/2
13	CLA	e	1127	1	1/1/15/20	12/37/115/115	-
17	LHG	n	5218	-	-	23/42/42/53	-
13	CLA	f	1211	2	1/1/13/20	4/27/105/115	-
13	CLA	Y	501	12	1/1/15/20	18/37/115/115	-
13	CLA	B	1021	2	1/1/15/20	10/37/115/115	-
13	CLA	B	1214	2	1/1/15/20	13/37/115/115	-
13	CLA	f	1207	2	1/1/15/20	14/37/115/115	-
13	CLA	a	513	12	1/1/15/20	13/37/115/115	-
13	CLA	v	516	12	1/1/11/20	8/13/91/115	-
16	BCR	A	4001	-	-	8/29/63/63	0/2/2/2
16	BCR	s	521	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	V	5218	-	-	23/42/42/53	-
17	LHG	n	5220	-	-	24/45/45/53	-
13	CLA	B	1228	2	1/1/13/20	8/25/103/115	-
13	CLA	6	510	12	1/1/11/20	7/13/91/115	-
13	CLA	1	510	12	1/1/15/20	11/37/115/115	-
13	CLA	c	504	-	1/1/11/20	3/13/91/115	-
13	CLA	q	509	12	1/1/15/20	6/37/115/115	-
13	CLA	s	501	12	1/1/15/20	6/37/115/115	-
16	BCR	v	524	-	-	5/29/63/63	0/2/2/2
16	BCR	4	522	-	-	4/29/63/63	0/2/2/2
13	CLA	e	1134	1	1/1/13/20	11/27/105/115	-
13	CLA	f	1205	2	1/1/15/20	10/37/115/115	-
16	BCR	f	4014	-	-	9/29/63/63	0/2/2/2
13	CLA	6	519	12	1/1/11/20	6/15/93/115	-
15	SF4	G	3001	1,2	-	-	0/6/5/5
16	BCR	2	523	-	-	6/29/63/63	0/2/2/2
13	CLA	b	512	12	1/1/11/20	3/13/91/115	-
13	CLA	6	506	12	1/1/11/20	5/13/91/115	-
13	CLA	d	501	12	1/1/14/20	16/31/109/115	-
13	CLA	d	517	-	1/1/11/20	9/13/91/115	-
13	CLA	v	508	12	1/1/11/20	3/13/91/115	-
13	CLA	L	1501	10	1/1/15/20	18/37/115/115	-
13	CLA	1	516	12	1/1/11/20	13/13/91/115	-
13	CLA	r	516	12	1/1/11/20	8/13/91/115	-
13	CLA	Y	505	12	1/1/15/20	11/37/115/115	-
13	CLA	d	502	12	1/1/12/20	5/19/97/115	-
13	CLA	G	1103	1	1/1/15/20	20/37/115/115	-
13	CLA	H	1230	2	1/1/14/20	10/31/109/115	-
13	CLA	6	508	12	1/1/11/20	3/13/91/115	-
16	BCR	G	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	A	1118	1	1/1/14/20	12/31/109/115	-
13	CLA	5	508	12	1/1/11/20	4/13/91/115	-
17	LHG	G	5004	-	-	21/40/40/53	-
13	CLA	A	1129	1	1/1/12/20	5/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	4	524	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1137	1	1/1/15/20	19/37/115/115	-
13	CLA	3	503	12	1/1/15/20	7/37/115/115	-
13	CLA	e	1130	1	1/1/15/20	7/37/115/115	-
13	CLA	q	511	12	1/1/13/20	4/25/103/115	-
16	BCR	r	524	-	-	2/29/63/63	0/2/2/2
13	CLA	2	511	12	1/1/13/20	4/25/103/115	-
17	LHG	H	1855	-	-	28/48/48/53	-
13	CLA	G	1133	1	1/1/15/20	15/37/115/115	-
16	BCR	u	521	-	-	7/29/63/63	0/2/2/2
17	LHG	e	5008	-	-	19/39/39/53	-
13	CLA	L	1503	21	1/1/14/20	10/31/109/115	-
13	CLA	6	503	12	1/1/12/20	8/22/100/115	-
16	BCR	s	523	-	-	4/29/63/63	0/2/2/2
13	CLA	R	1301	21	1/1/15/20	11/37/115/115	-
13	CLA	t	504	-	1/1/11/20	5/13/91/115	-
13	CLA	A	1132	1	1/1/15/20	15/37/115/115	-
13	CLA	H	1219	2	1/1/15/20	17/37/115/115	-
13	CLA	4	506	12	1/1/11/20	2/13/91/115	-
13	CLA	c	518	12	1/1/13/20	11/25/103/115	-
16	BCR	Z	522	-	-	6/29/63/63	0/2/2/2
13	CLA	B	1208	2	1/1/15/20	15/37/115/115	-
13	CLA	5	512	12	1/1/11/20	5/13/91/115	-
13	CLA	1	512	12	1/1/12/20	10/22/100/115	-
13	CLA	B	1219	2	1/1/15/20	17/37/115/115	-
13	CLA	H	1203	2	1/1/15/20	16/37/115/115	-
17	LHG	G	5008	-	-	19/39/39/53	-
13	CLA	f	1209	2	1/1/12/20	8/22/100/115	-
13	CLA	u	508	12	1/1/11/20	4/13/91/115	-
13	CLA	B	1205	2	1/1/15/20	10/37/115/115	-
13	CLA	Z	509	12	1/1/15/20	6/37/115/115	-
13	CLA	H	1021	2	1/1/15/20	11/37/115/115	-
13	CLA	H	1214	2	1/1/15/20	13/37/115/115	-
13	CLA	f	1021	2	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	t	508	12	1/1/11/20	4/13/91/115	-
13	CLA	H	1228	2	1/1/13/20	8/25/103/115	-
13	CLA	2	510	12	1/1/15/20	9/37/115/115	-
13	CLA	t	503	12	1/1/13/20	1/25/103/115	-
16	BCR	5	523	-	-	4/29/63/63	0/2/2/2
13	CLA	e	1106	1	1/1/15/20	21/37/115/115	-
16	BCR	r	521	-	-	4/29/63/63	0/2/2/2
14	PQN	e	2001	-	-	14/23/43/43	0/2/2/2
20	SQD	6	822	-	-	9/19/39/69	0/1/1/1
13	CLA	Z	516	12	1/1/11/20	8/13/91/115	-
13	CLA	j	1301	21	1/1/15/20	11/37/115/115	-
13	CLA	5	502	12	1/1/12/20	5/19/97/115	-
19	LMG	H	5002	-	-	24/49/69/70	0/1/1/1
13	CLA	Y	508	12	1/1/13/20	9/25/103/115	-
13	CLA	5	516	12	1/1/11/20	2/13/91/115	-
13	CLA	G	1123	21	1/1/15/20	11/37/115/115	-
16	BCR	Z	523	-	-	6/29/63/63	0/2/2/2
13	CLA	e	1119	21	1/1/15/20	15/37/115/115	-
13	CLA	A	1128	1	1/1/15/20	12/37/115/115	-
16	BCR	4	521	-	-	10/29/63/63	0/2/2/2
13	CLA	t	512	12	1/1/11/20	3/13/91/115	-
13	CLA	e	1132	1	1/1/15/20	15/37/115/115	-
13	CLA	G	1121	1	1/1/13/20	6/25/103/115	-
16	BCR	3	522	-	-	5/29/63/63	0/2/2/2
13	CLA	G	1124	21	1/1/13/20	11/27/105/115	-
13	CLA	H	1202	2	1/1/15/20	13/37/115/115	-
13	CLA	d	513	12	1/1/11/20	3/13/91/115	-
13	CLA	1	505	12	1/1/15/20	11/37/115/115	-
13	CLA	G	1140	1	1/1/15/20	11/37/115/115	-
13	CLA	U	1401	-	1/1/13/20	8/25/103/115	-
13	CLA	A	1138	1	1/1/15/20	12/37/115/115	-
13	CLA	n	1503	21	1/1/14/20	10/31/109/115	-
16	BCR	J	4015	-	-	5/29/63/63	0/2/2/2
13	CLA	B	1220	2	1/1/13/20	9/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	T	1303	8	1/1/15/20	18/37/115/115	-
16	BCR	3	524	-	-	5/29/63/63	0/2/2/2
18	LMU	Y	902	-	-	6/10/30/61	0/1/1/2
13	CLA	Y	519	12	1/1/12/20	6/19/97/115	-
13	CLA	a	504	-	1/1/11/20	6/13/91/115	-
13	CLA	d	509	12	1/1/11/20	6/13/91/115	-
13	CLA	B	1216	21	1/1/14/20	5/31/109/115	-
13	CLA	B	1212	2	1/1/13/20	11/25/103/115	-
13	CLA	e	1801	17	1/1/11/20	5/13/91/115	-
13	CLA	6	502	12	1/1/12/20	5/19/97/115	-
13	CLA	b	501	12	1/1/14/20	12/31/109/115	-
13	CLA	A	1133	1	1/1/15/20	15/37/115/115	-
17	LHG	A	5009	-	-	28/53/53/53	-
16	BCR	d	523	-	-	4/29/63/63	0/2/2/2
13	CLA	f	1215	2	1/1/15/20	19/37/115/115	-
13	CLA	B	1012	21	1/1/15/20	16/37/115/115	-
13	CLA	s	518	12	1/1/13/20	10/25/103/115	-
13	CLA	c	517	-	1/1/11/20	9/13/91/115	-
17	LHG	A	5004	-	-	21/40/40/53	-
13	CLA	A	1116	1	1/1/14/20	15/31/109/115	-
13	CLA	G	1801	17	1/1/11/20	5/13/91/115	-
17	LHG	f	1842	13	-	22/43/43/53	-
13	CLA	5	504	-	1/1/11/20	3/13/91/115	-
13	CLA	A	1121	1	1/1/13/20	6/25/103/115	-
16	BCR	1	524	-	-	2/29/63/63	0/2/2/2
13	CLA	4	513	12	1/1/11/20	7/13/91/115	-
13	CLA	6	501	12	1/1/14/20	16/31/109/115	-
13	CLA	r	517	-	1/1/11/20	4/13/91/115	-
13	CLA	B	1213	2	1/1/15/20	14/37/115/115	-
13	CLA	r	510	12	1/1/15/20	9/37/115/115	-
18	LMU	A	1848	-	-	7/21/61/61	0/2/2/2
13	CLA	V	1501	10	1/1/15/20	18/37/115/115	-
13	CLA	Y	512	12	1/1/12/20	9/22/100/115	-
13	CLA	e	1138	1	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	q	518	12	1/1/14/20	15/31/109/115	-
13	CLA	r	502	12	1/1/14/20	11/31/109/115	-
13	CLA	u	505	12	1/1/14/20	16/33/111/115	-
13	CLA	b	518	12	1/1/13/20	8/25/103/115	-
16	BCR	G	4008	-	-	7/29/63/63	0/2/2/2
17	LHG	V	5220	-	-	24/45/45/53	-
13	CLA	A	1123	21	1/1/15/20	11/37/115/115	-
13	CLA	4	507	-	1/1/11/20	6/13/91/115	-
13	CLA	b	507	-	1/1/11/20	6/13/91/115	-
20	SQD	V	5216	-	-	17/46/66/69	0/1/1/1
15	SF4	N	3002	3	-	-	0/6/5/5
13	CLA	A	1125	1	1/1/15/20	14/37/115/115	-
13	CLA	f	1226	2	1/1/15/20	12/37/115/115	-
13	CLA	b	504	-	1/1/11/20	5/13/91/115	-
13	CLA	3	516	12	1/1/11/20	9/13/91/115	-
13	CLA	B	1232	21	1/1/12/20	6/19/97/115	-
16	BCR	L	4022	-	-	2/29/63/63	0/2/2/2
13	CLA	4	518	12	1/1/13/20	8/25/103/115	-
13	CLA	B	1229	2	1/1/15/20	13/37/115/115	-
13	CLA	l	1303	8	1/1/15/20	18/37/115/115	-
13	CLA	B	1236	2	-	3/25/103/115	-
20	SQD	H	1852	-	-	19/40/60/69	0/1/1/1
20	SQD	f	1852	-	-	19/40/60/69	0/1/1/1
16	BCR	K	4104	-	-	2/29/63/63	0/2/2/2
13	CLA	f	1204	2	1/1/15/20	12/37/115/115	-
13	CLA	A	1109	1	1/1/15/20	9/37/115/115	-
13	CLA	4	511	12	1/1/11/20	3/13/91/115	-
13	CLA	a	517	-	1/1/11/20	7/13/91/115	-
13	CLA	B	1240	17	-	13/37/115/115	-
13	CLA	2	509	12	1/1/15/20	6/37/115/115	-
13	CLA	e	1013	-	1/1/15/20	11/37/115/115	-
13	CLA	A	1114	21	1/1/12/20	2/19/97/115	-
13	CLA	2	512	12	1/1/12/20	5/23/101/115	-
16	BCR	a	522	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	1208	2	1/1/15/20	15/37/115/115	-
20	SQD	3	822	-	-	21/38/58/69	0/1/1/1
13	CLA	v	501	12	1/1/14/20	16/31/109/115	-
13	CLA	H	1216	21	1/1/14/20	5/31/109/115	-
20	SQD	a	822	-	-	21/38/58/69	0/1/1/1
13	CLA	A	1237	21	1/1/15/20	19/37/115/115	-
16	BCR	m	4104	-	-	2/29/63/63	0/2/2/2
13	CLA	b	513	12	1/1/11/20	7/13/91/115	-
15	SF4	e	3001	1,2	-	-	0/6/5/5
13	CLA	u	502	12	1/1/12/20	5/19/97/115	-
13	CLA	G	1119	21	1/1/15/20	15/37/115/115	-
16	BCR	s	524	-	-	5/29/63/63	0/2/2/2
16	BCR	B	4006	-	-	4/29/63/63	0/2/2/2
13	CLA	u	516	12	1/1/11/20	2/13/91/115	-
13	CLA	3	504	-	1/1/11/20	6/13/91/115	-
13	CLA	v	502	12	1/1/12/20	5/19/97/115	-
13	CLA	H	1211	2	1/1/13/20	4/27/105/115	-
13	CLA	3	517	-	1/1/11/20	7/13/91/115	-
16	BCR	f	4004	-	-	8/29/63/63	0/2/2/2
17	LHG	k	5001	-	-	22/48/48/53	-
13	CLA	a	503	12	1/1/15/20	7/37/115/115	-
13	CLA	H	1012	21	1/1/15/20	16/37/115/115	-
13	CLA	A	1107	1	1/1/15/20	14/37/115/115	-
13	CLA	5	517	-	1/1/11/20	9/13/91/115	-
13	CLA	G	1132	1	1/1/15/20	15/37/115/115	-
16	BCR	f	4010	-	-	5/29/63/63	0/2/2/2
17	LHG	e	5009	-	-	28/53/53/53	-
13	CLA	3	508	12	1/1/13/20	7/25/103/115	-
16	BCR	c	522	-	-	5/29/63/63	0/2/2/2

The worst 5 of 4509 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	2002	PQN	C12-C13	8.71	1.53	1.33
14	f	2002	PQN	C12-C13	8.70	1.53	1.33
14	H	2002	PQN	C12-C13	8.70	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	2001	PQN	C12-C13	8.66	1.53	1.33
14	e	2001	PQN	C12-C13	8.66	1.53	1.33

The worst 5 of 7438 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	2002	PQN	C11-C12-C13	-9.00	111.81	126.79
14	B	2002	PQN	C11-C12-C13	-9.00	111.81	126.79
13	H	1211	CLA	C4A-NA-C1A	8.99	110.75	106.71
14	H	2002	PQN	C11-C12-C13	-8.98	111.85	126.79
13	B	1211	CLA	C4A-NA-C1A	8.88	110.70	106.71

5 of 588 chirality outliers are listed below:

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

5 of 8073 torsion outliers are listed below:

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

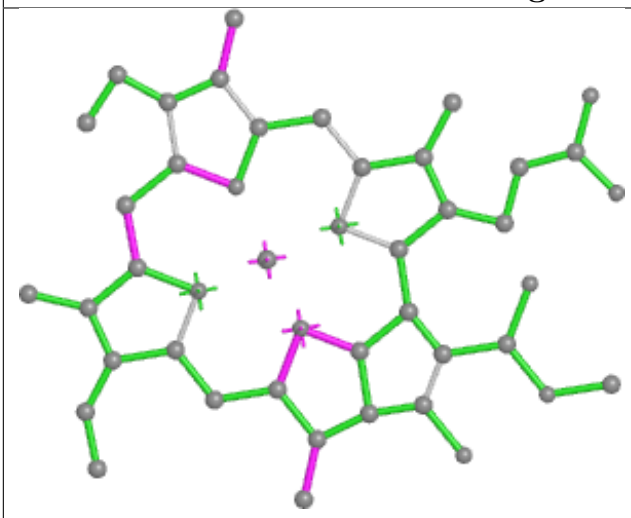
There are no ring outliers.

No monomer is involved in short contacts.

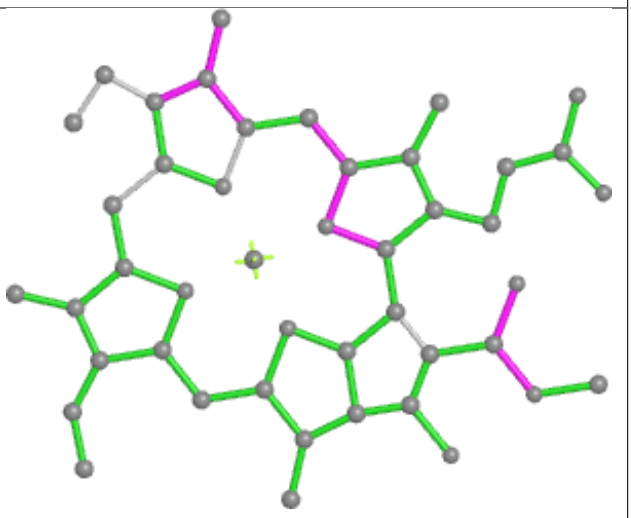
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

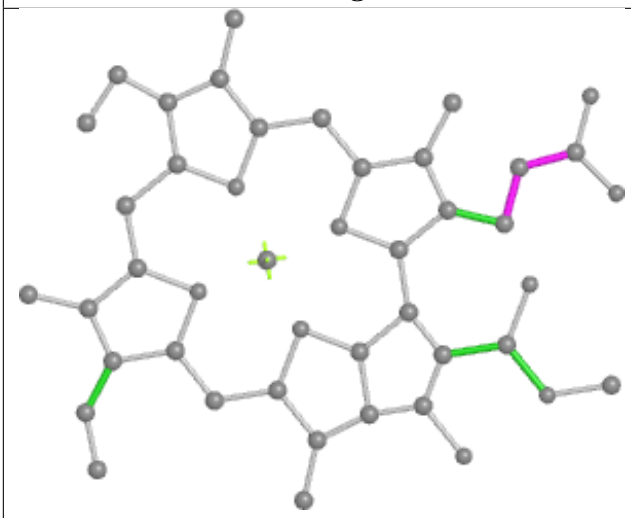
Ligand CLA 3 512



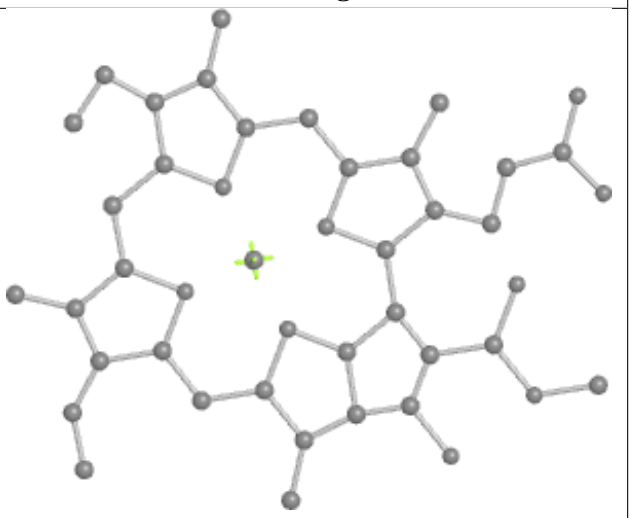
Bond lengths



Bond angles

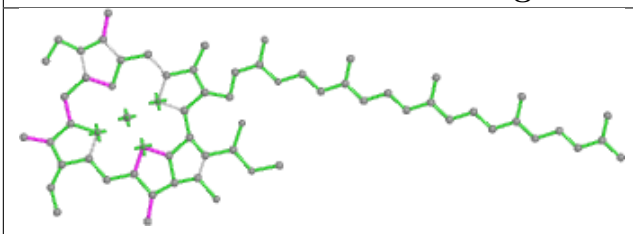


Torsions

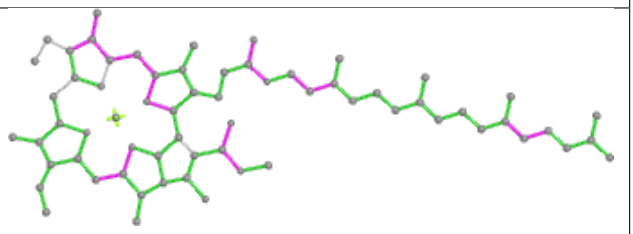


Rings

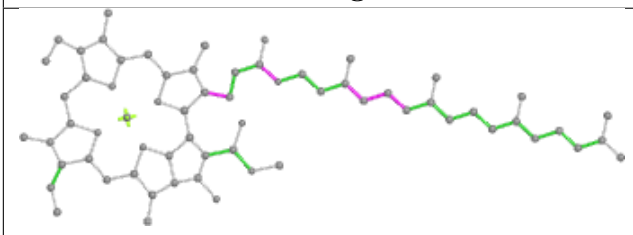
Ligand CLA G 1130



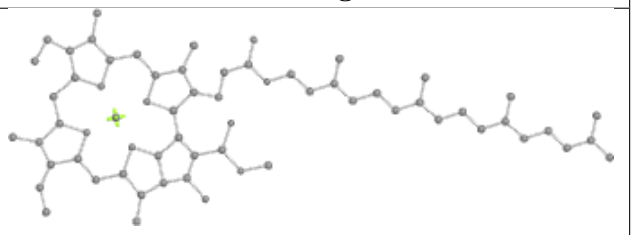
Bond lengths



Bond angles

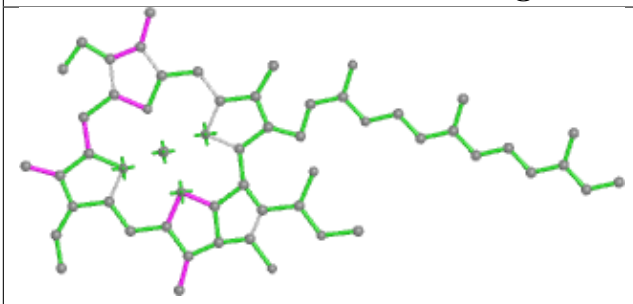


Torsions

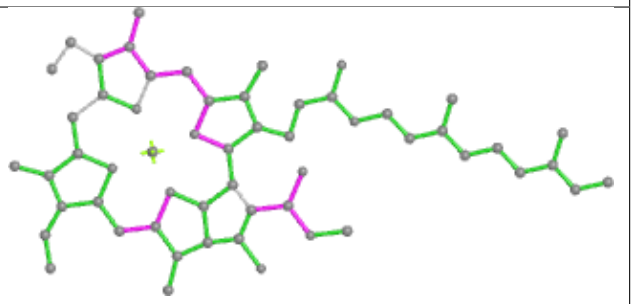


Rings

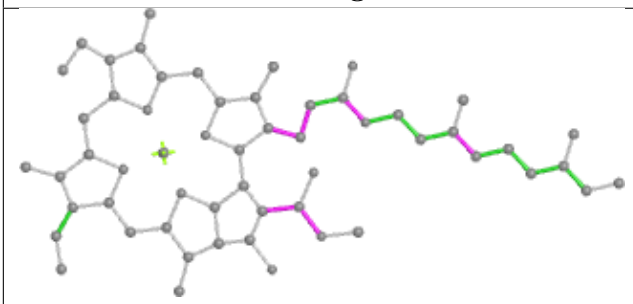
Ligand CLA A 1134



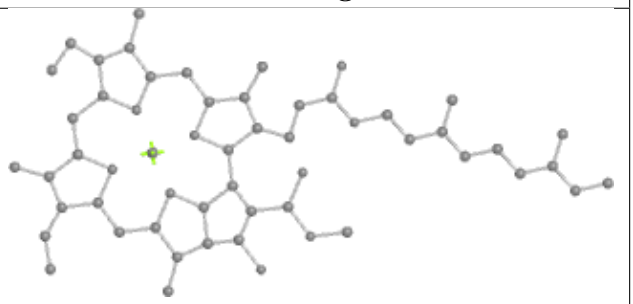
Bond lengths



Bond angles

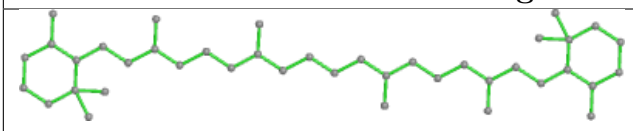


Torsions

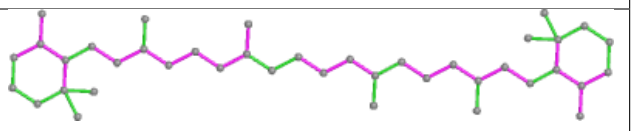


Rings

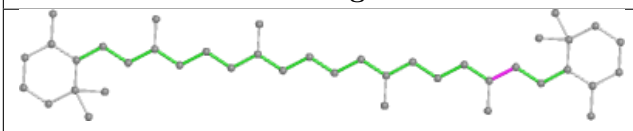
Ligand BCR S 4018



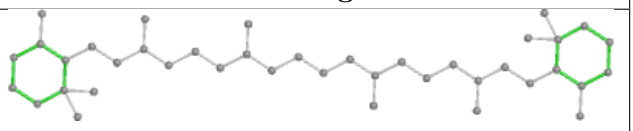
Bond lengths



Bond angles

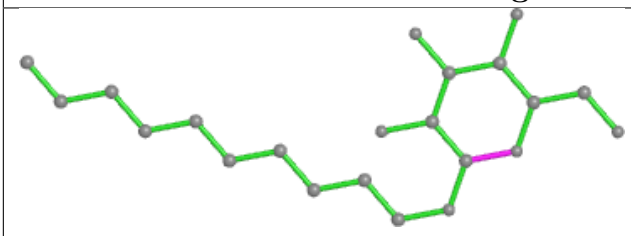


Torsions

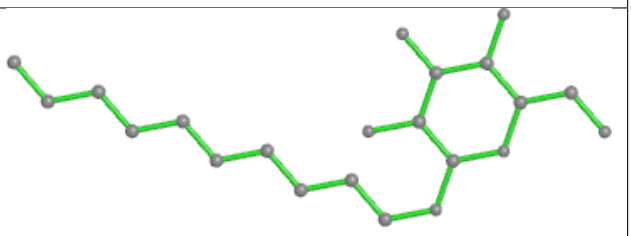


Rings

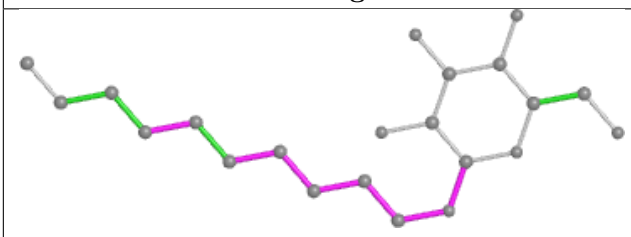
Ligand LMU T 5105



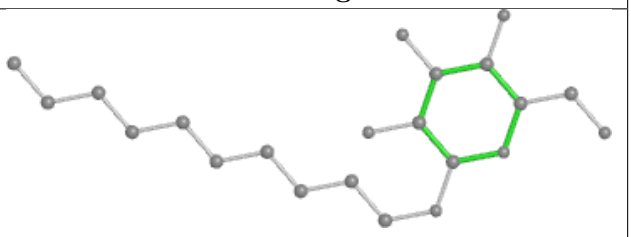
Bond lengths



Bond angles

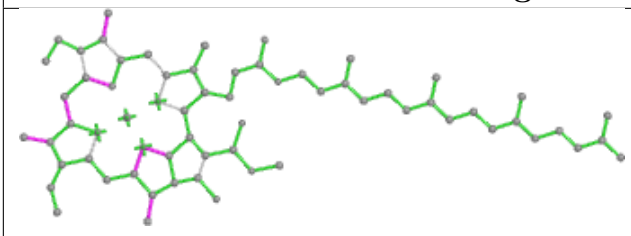


Torsions

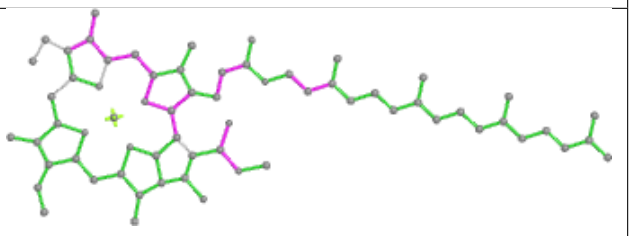


Rings

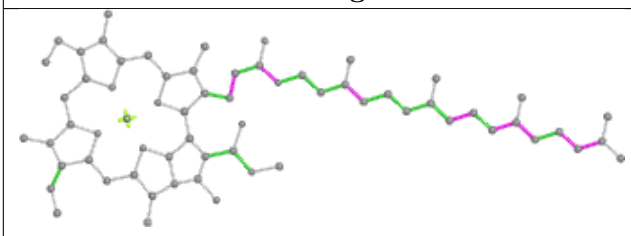
Ligand CLA G 1127



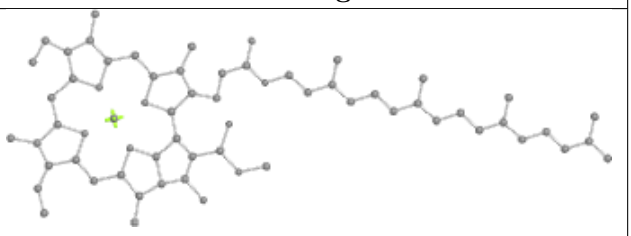
Bond lengths



Bond angles

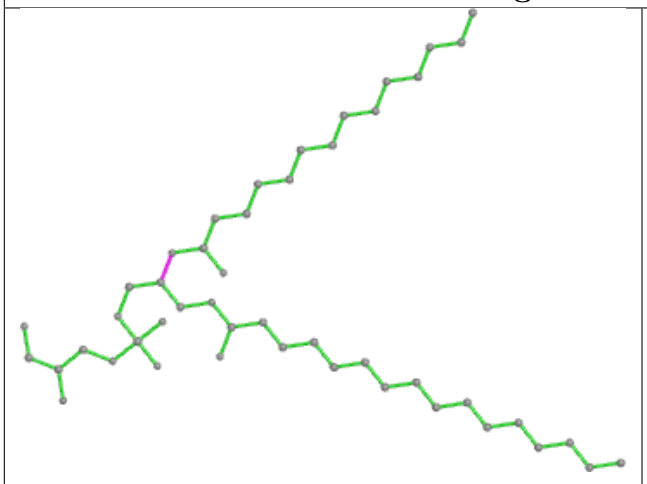


Torsions

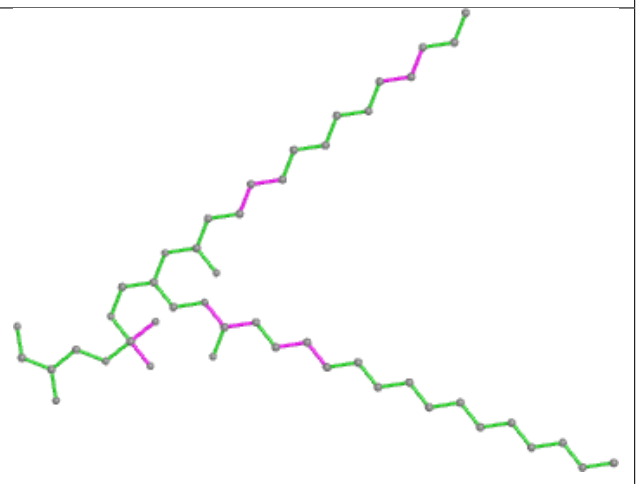


Rings

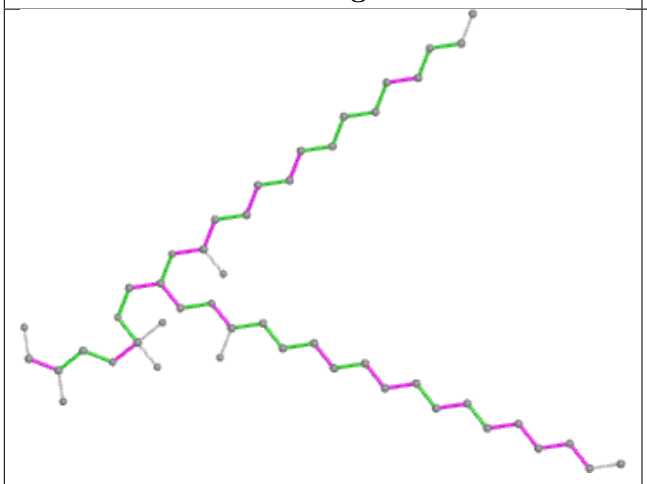
Ligand LHG A 5007



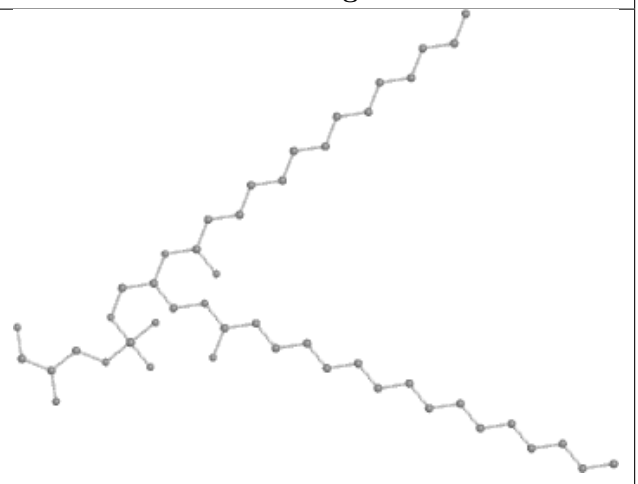
Bond lengths



Bond angles

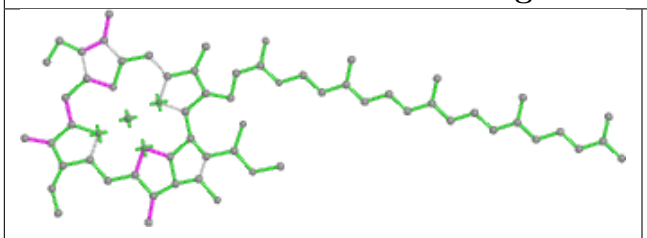


Torsions

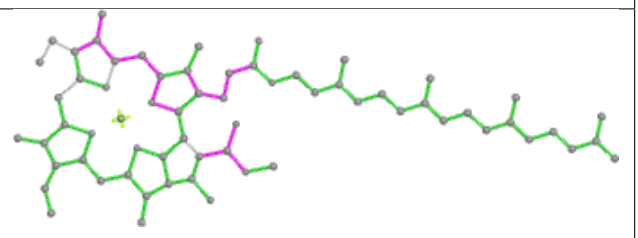


Rings

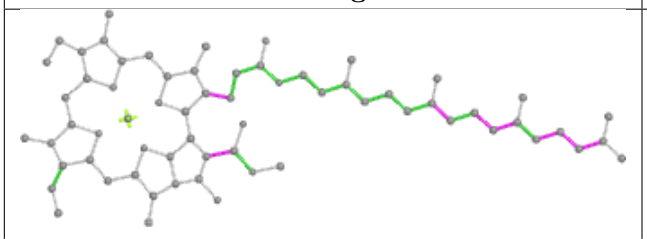
Ligand CLA G 1101



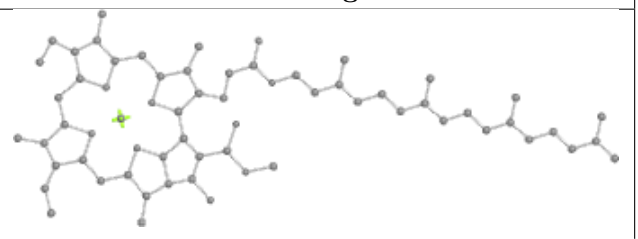
Bond lengths



Bond angles

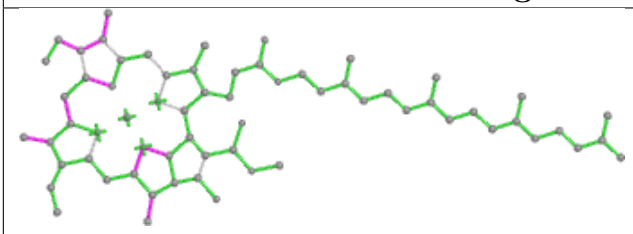


Torsions



Rings

Ligand CLA G 1237



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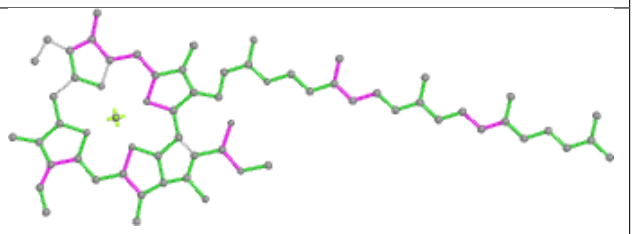

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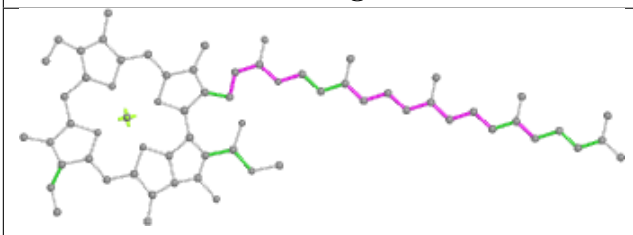
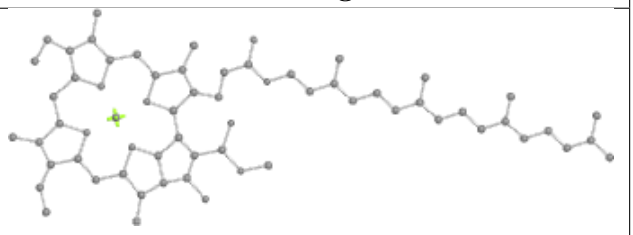
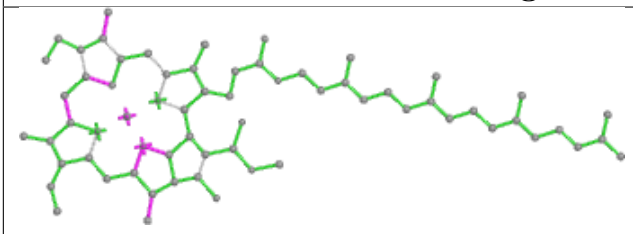


Torsions



Rings

Ligand CLA e 1133



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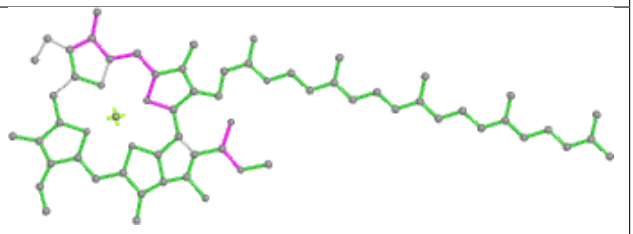
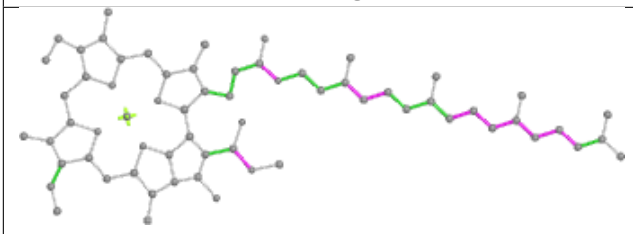
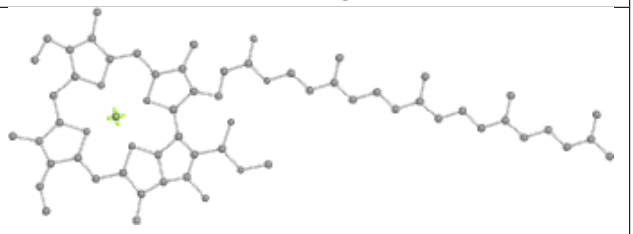


Bond angles

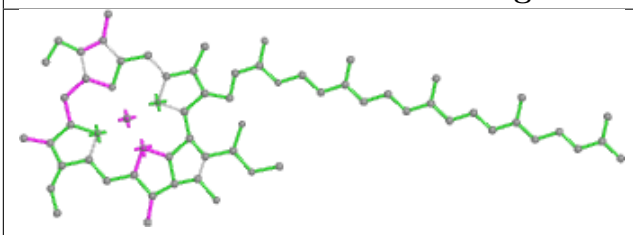


Torsions



Rings

Ligand CLA G 1117



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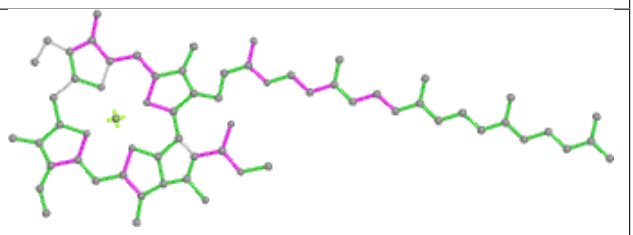
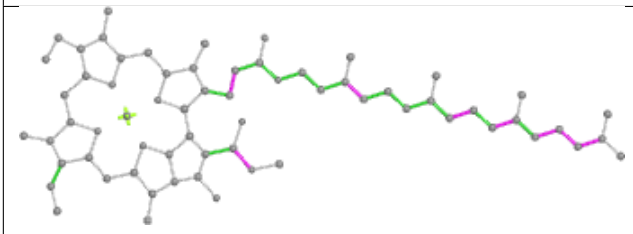


Bond angles



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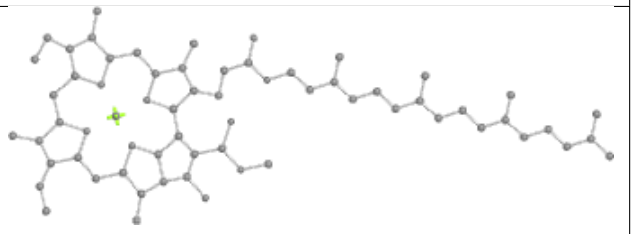
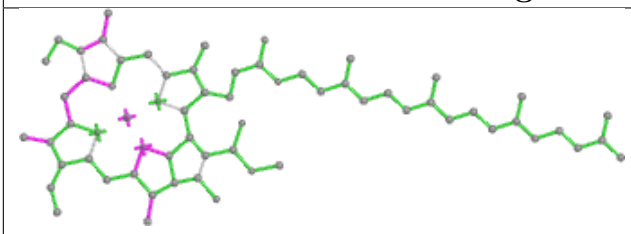


Rings

Ligand CLA B 1226



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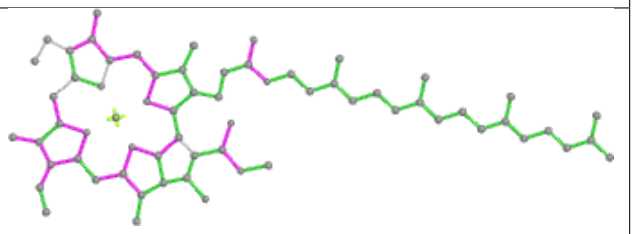
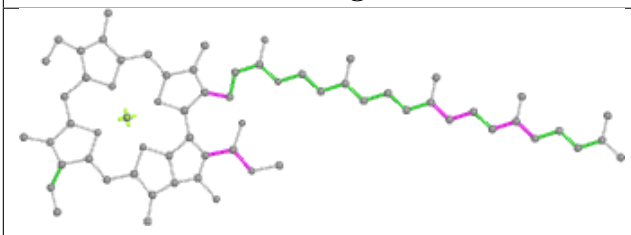


Bond angles



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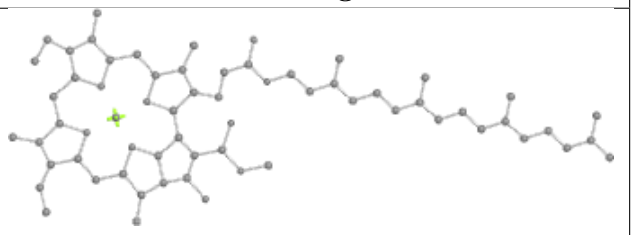
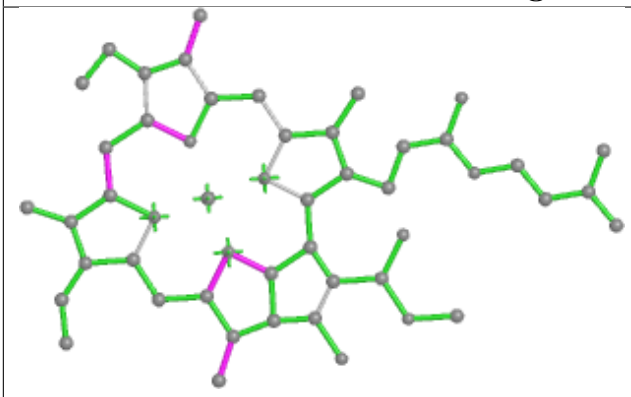


Rings

Ligand CLA b 502



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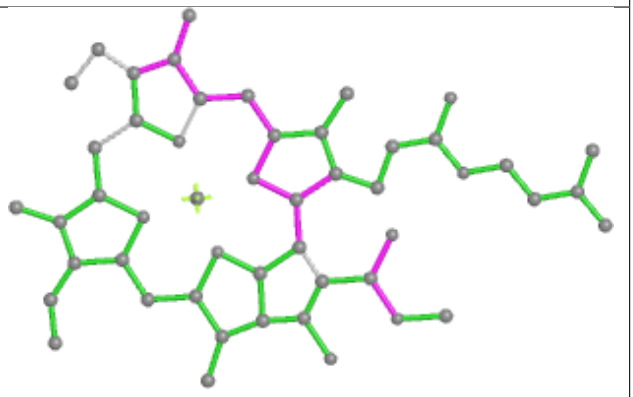
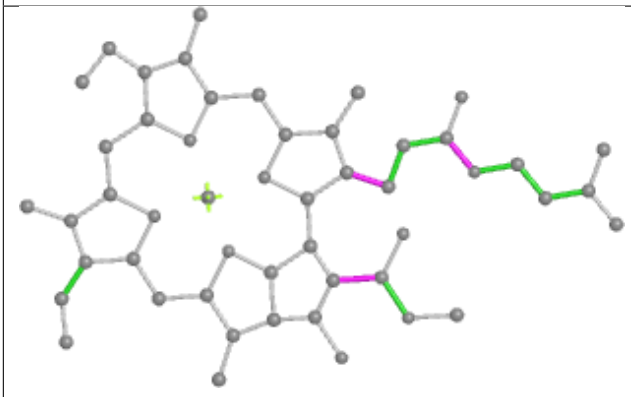


Bond angles



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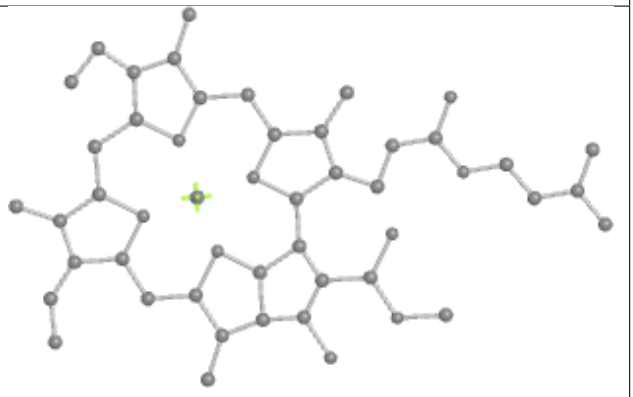
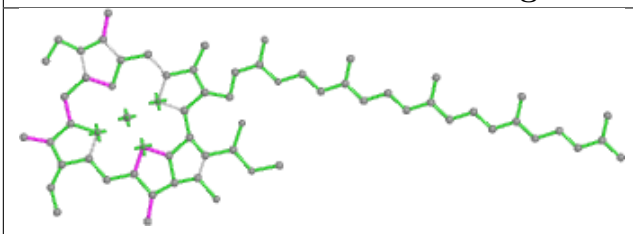


Rings

Ligand CLA e 1140



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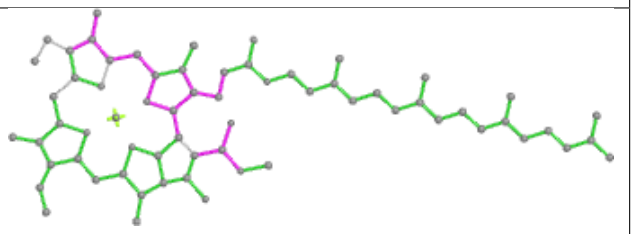
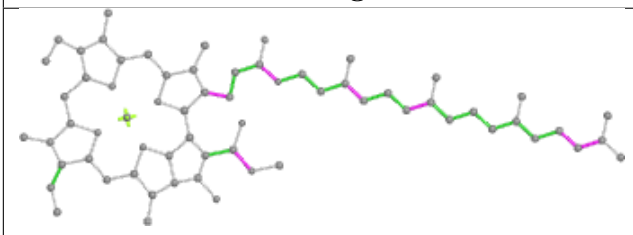


Bond angles



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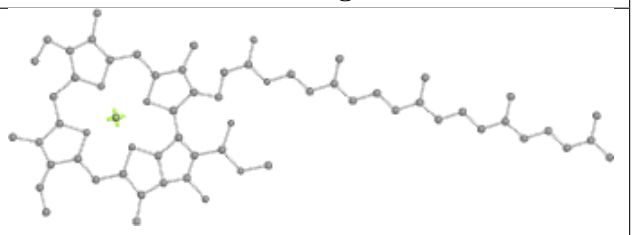
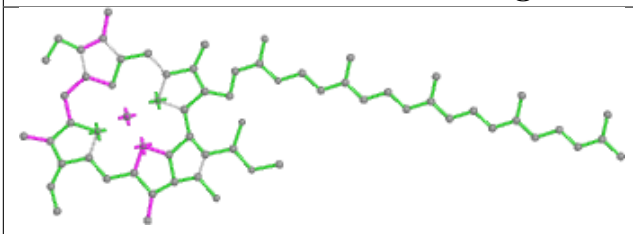


Rings

Ligand CLA H 1226



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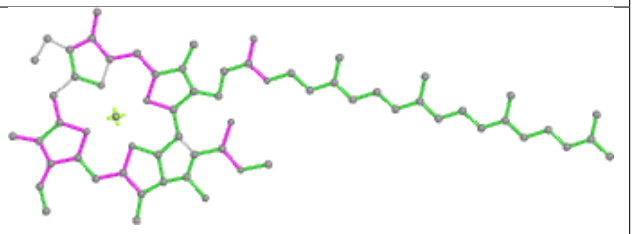
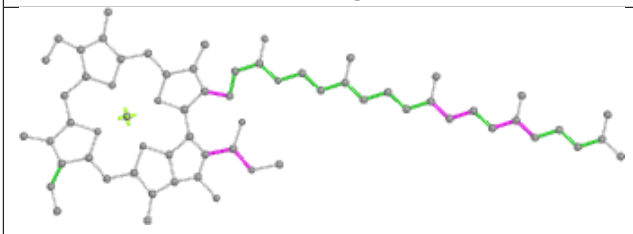


Bond angles



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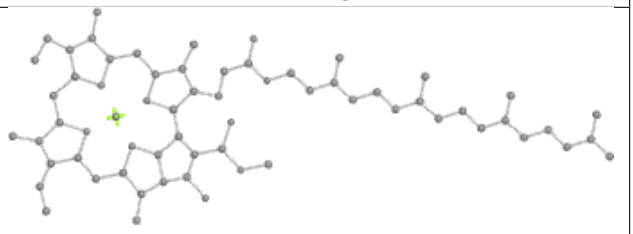
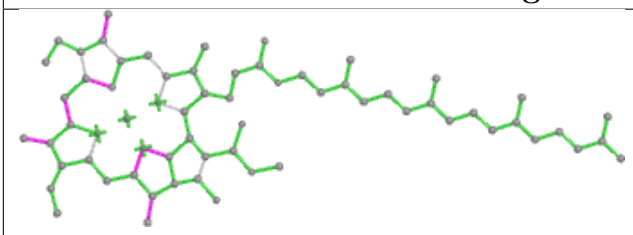


Rings

Ligand CLA f 1238



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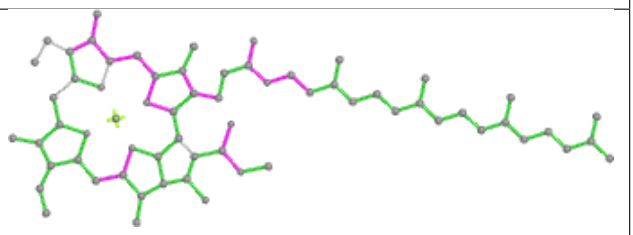
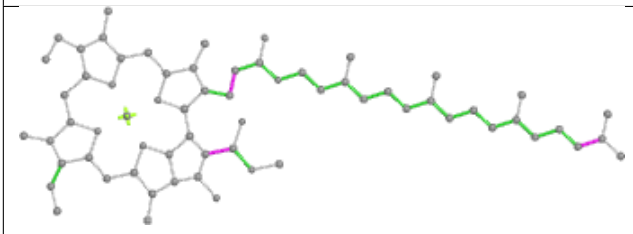


Bond angles



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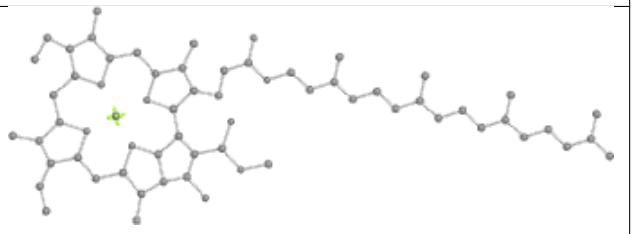
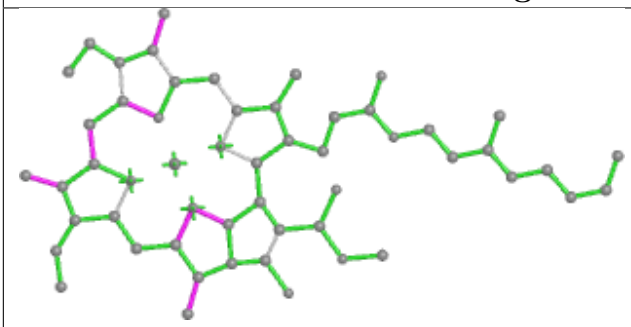


Rings

Ligand CLA G 1108



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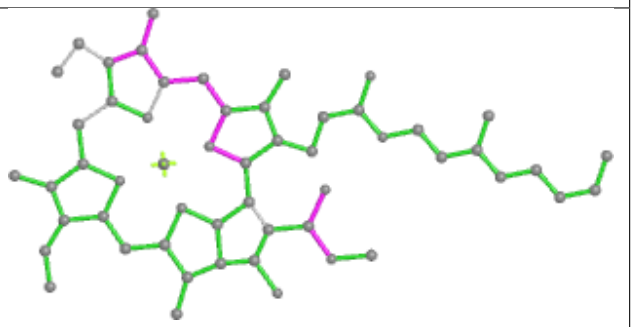

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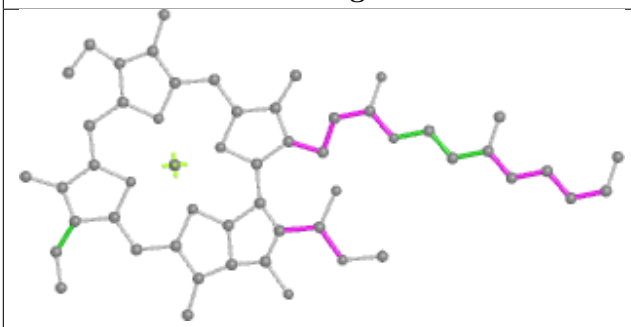

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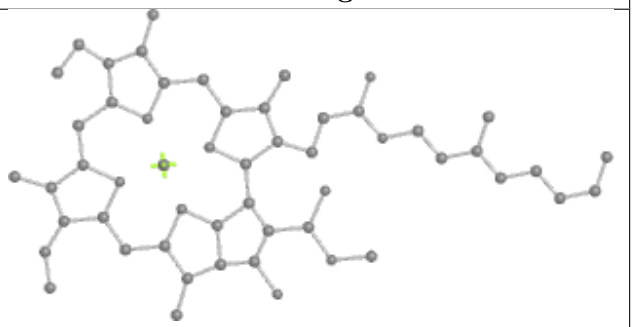
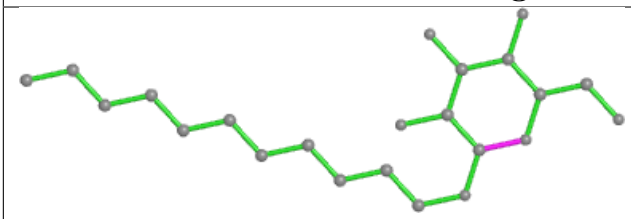


Rings

Ligand LMU A 1849



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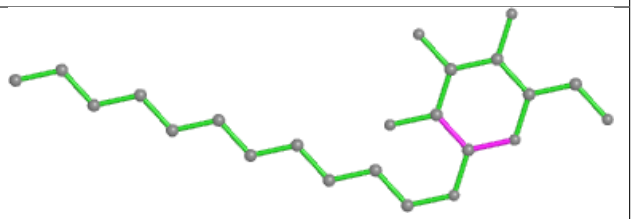
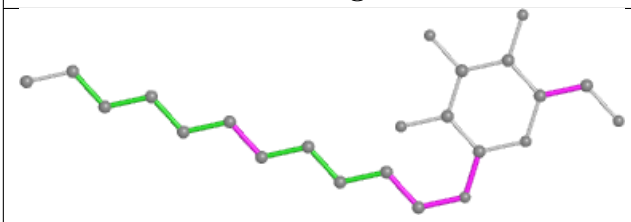


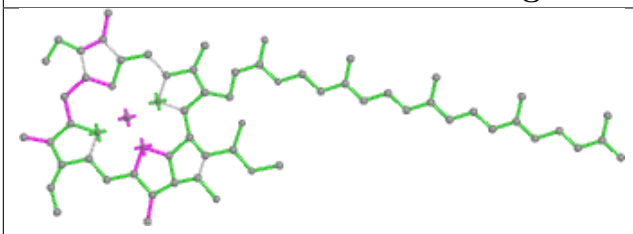
Bond angles



Torsions

Rings

Ligand CLA f 1206



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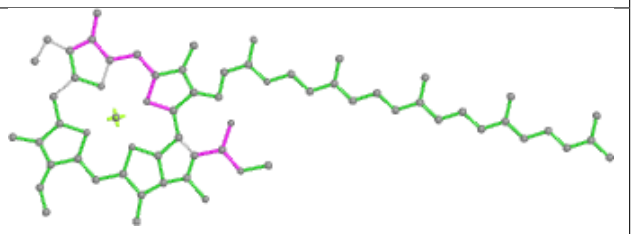

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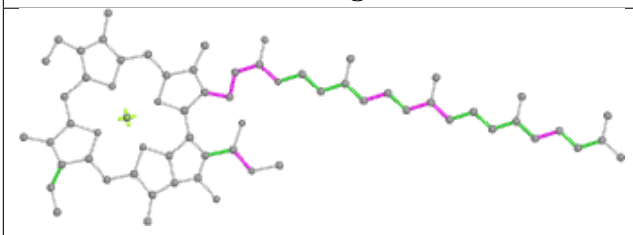

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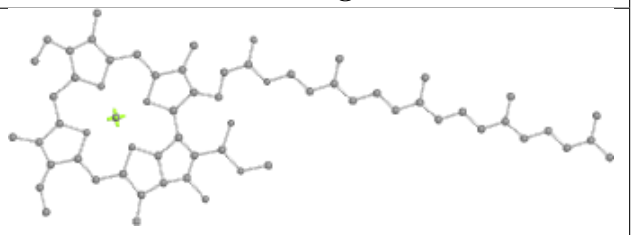
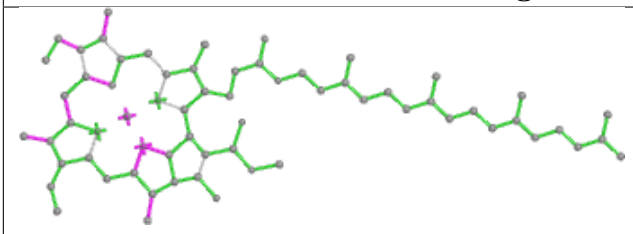


Rings

Ligand CLA B 1225



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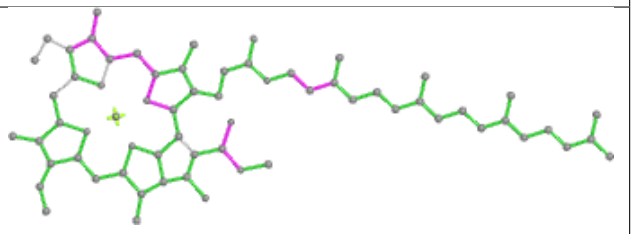
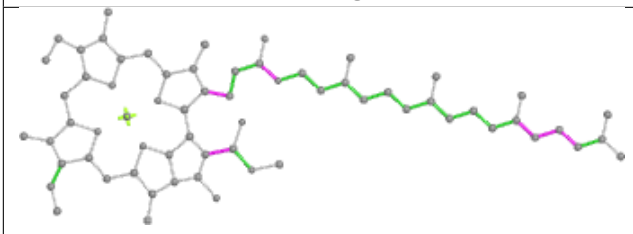
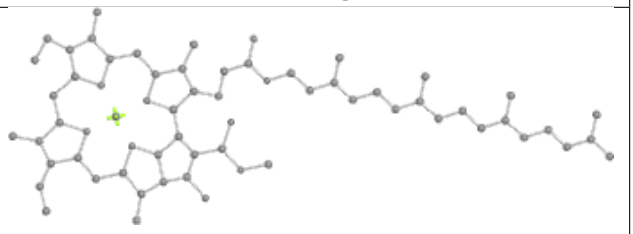


Bond angles

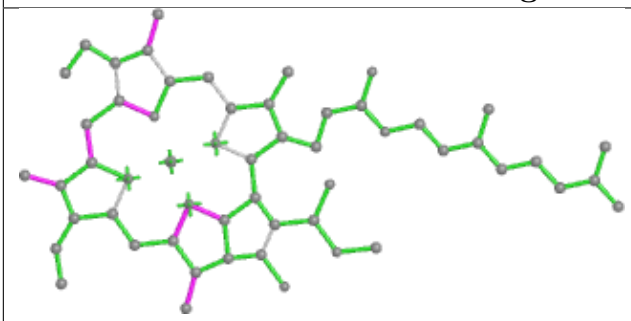


Torsions



Rings

Ligand CLA e 1121



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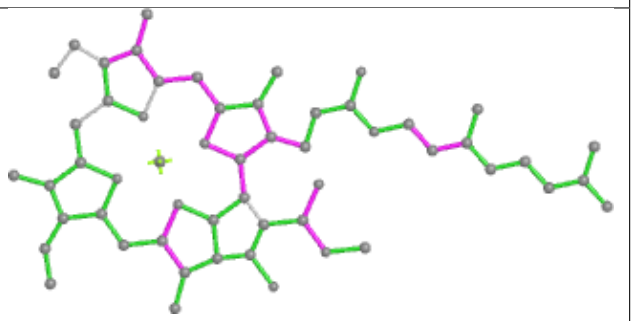
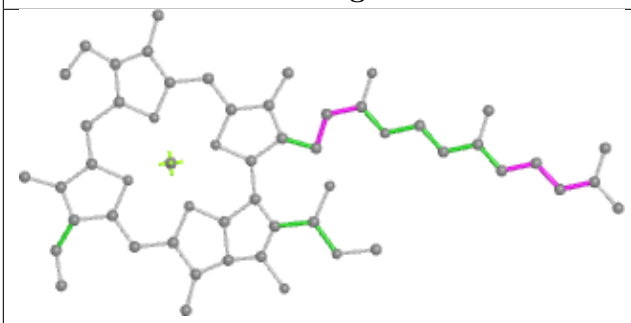


Bond angles



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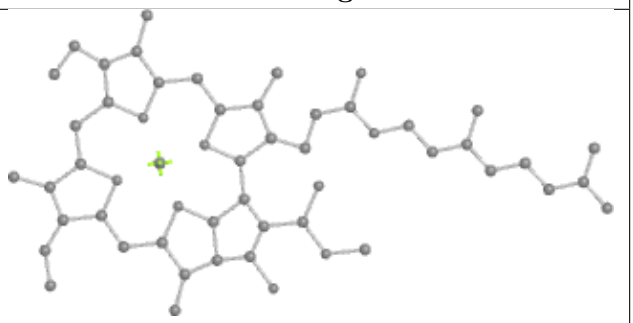
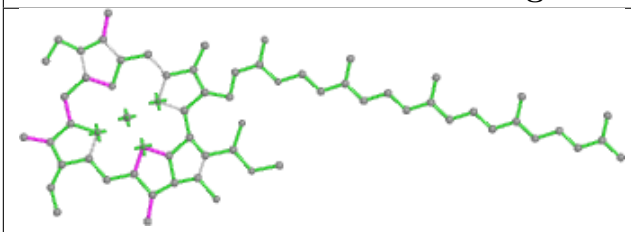


Rings

Ligand CLA Z 510



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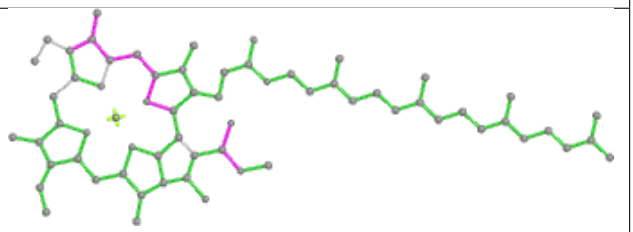
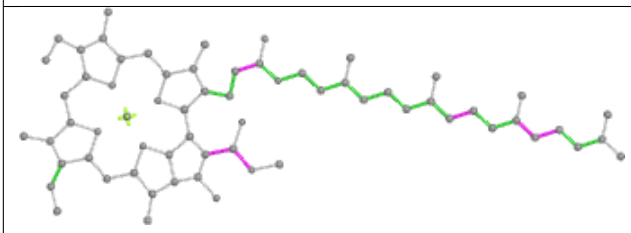
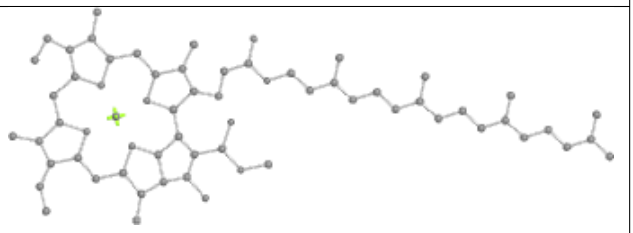


Bond angles

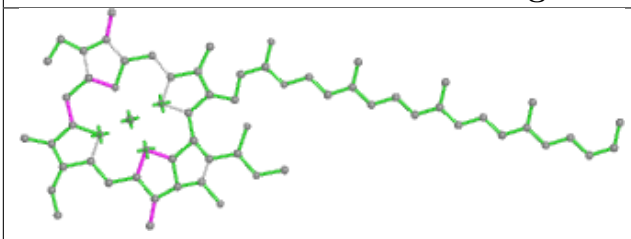


Torsions

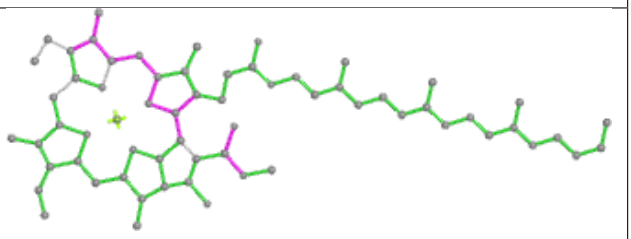


Rings

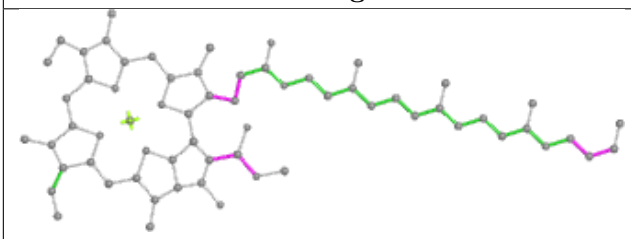
Ligand CLA 1 503



Bond lengths



Bond angles



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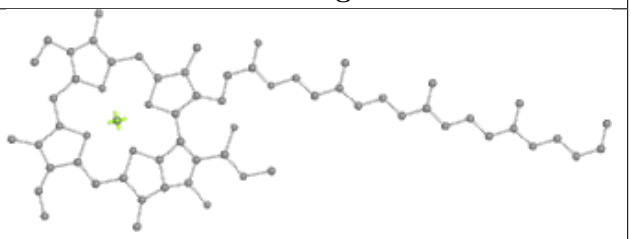
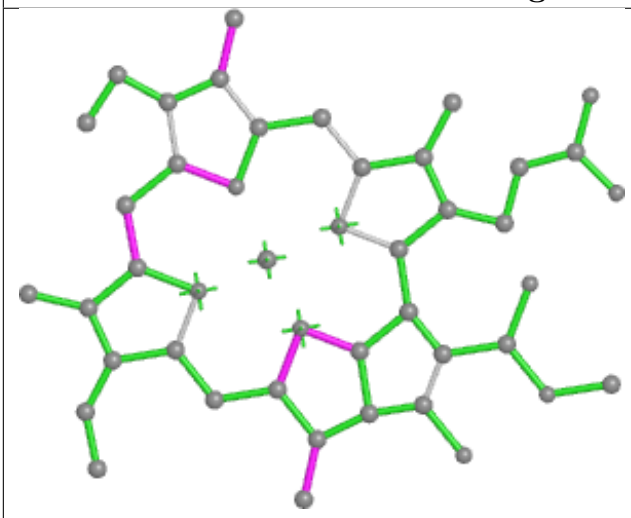


Rings

Ligand CLA 6 512



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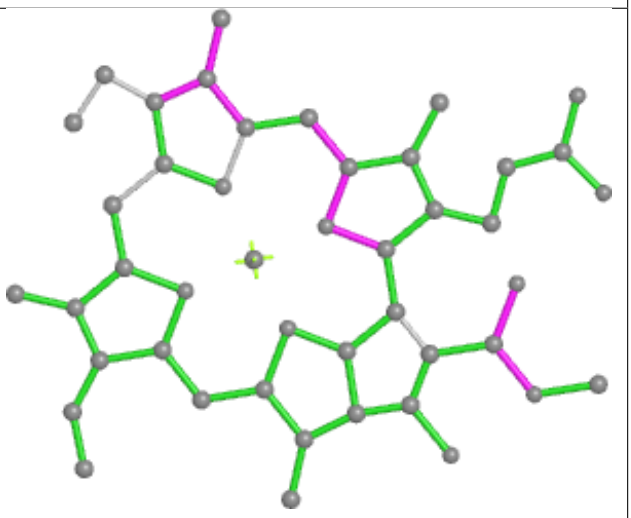

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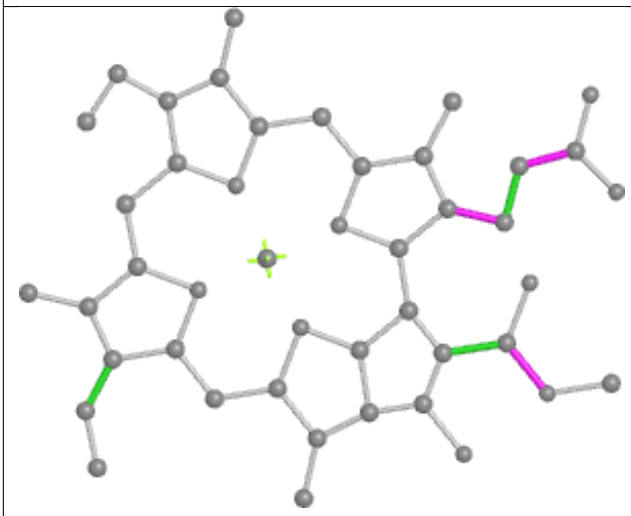
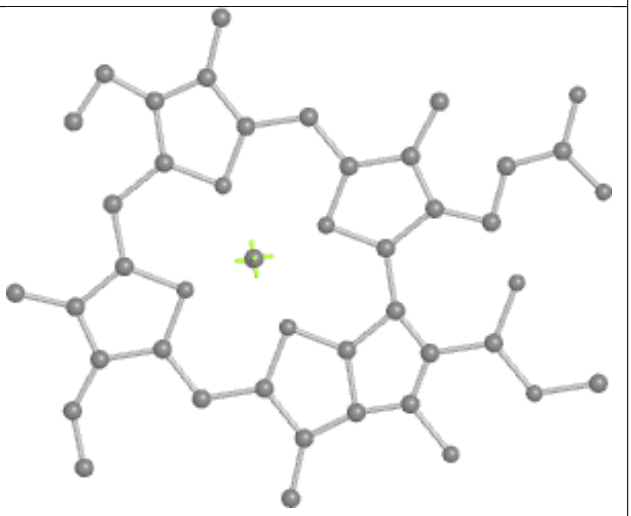
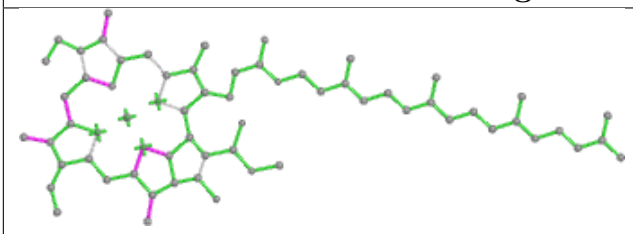


Torsions



Rings

Ligand CLA H 1229



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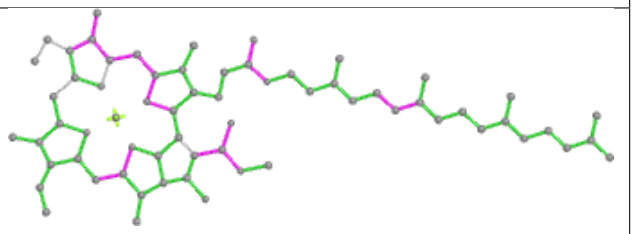

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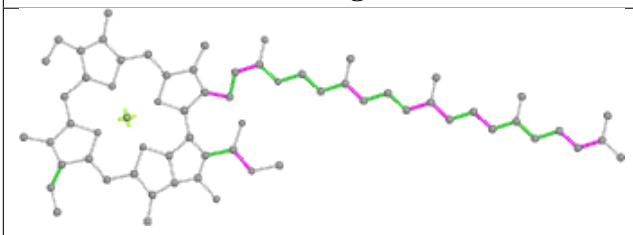

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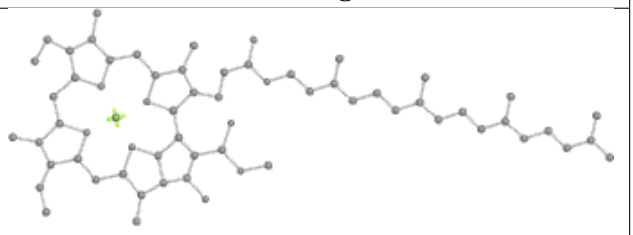
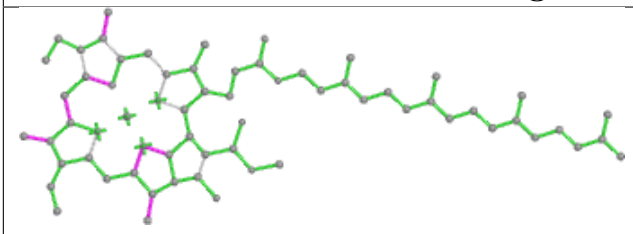


Rings

Ligand CLA a 501



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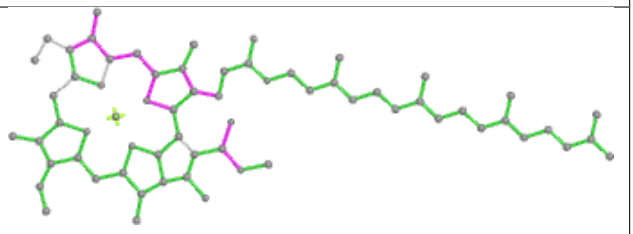

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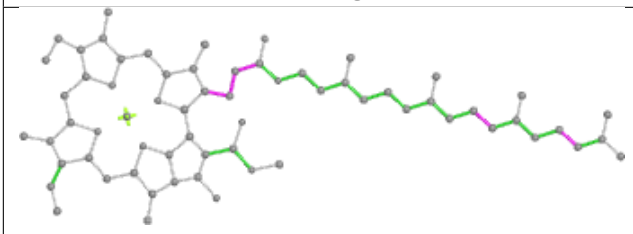

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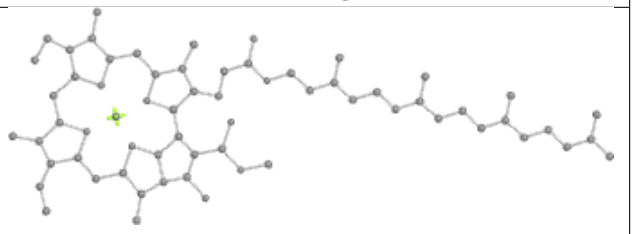
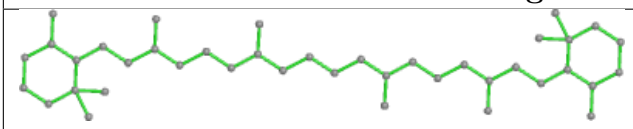


Rings

Ligand BCR q 521



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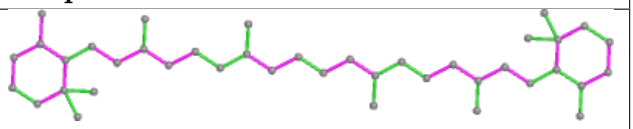

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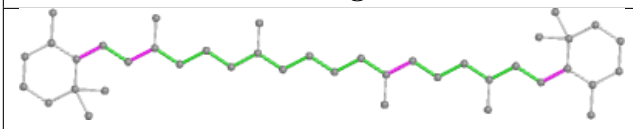
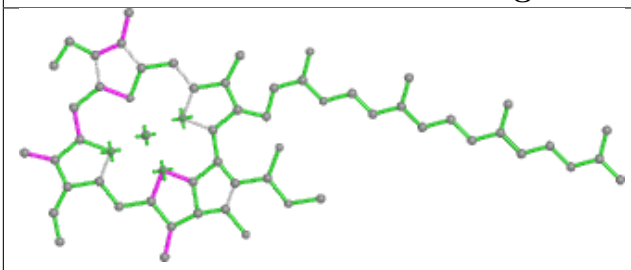


Torsions

Rings

Ligand CLA G 1118



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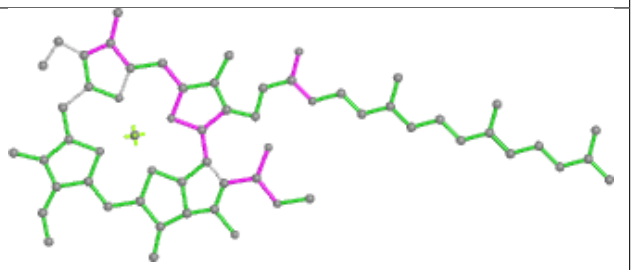

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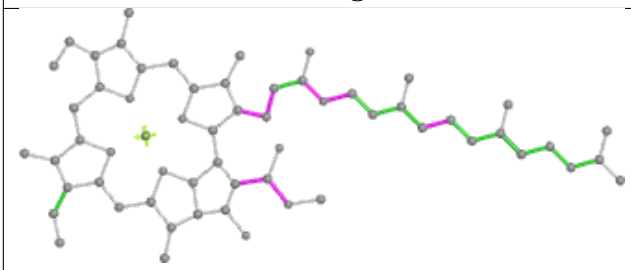

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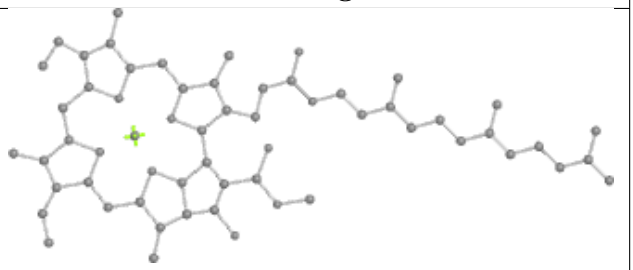
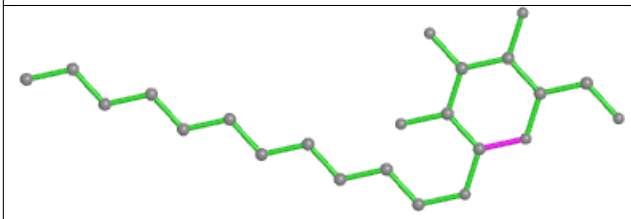


Rings

Ligand LMU r 901



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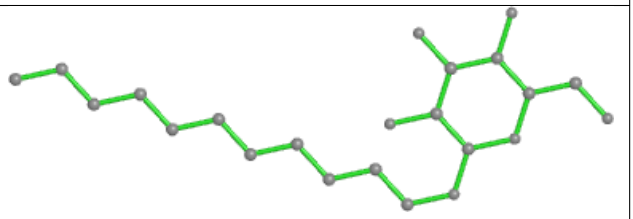

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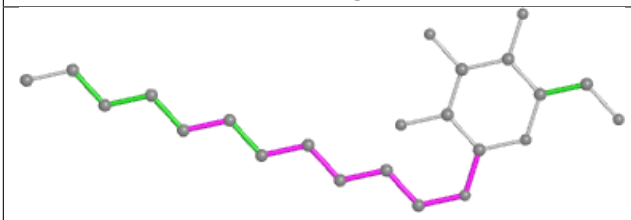

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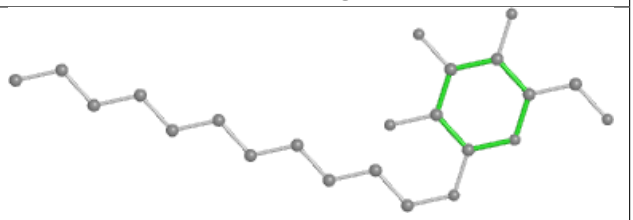
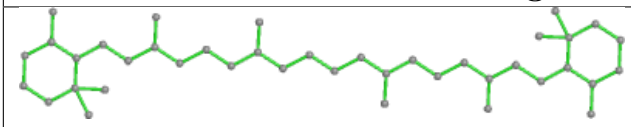


Rings

Ligand BCR 1 522



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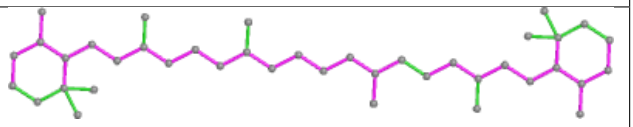

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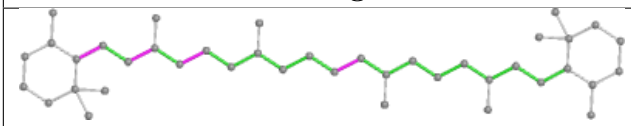
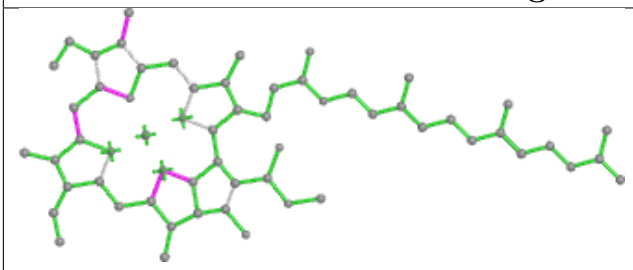


Torsions

Rings

Ligand CLA 4 501



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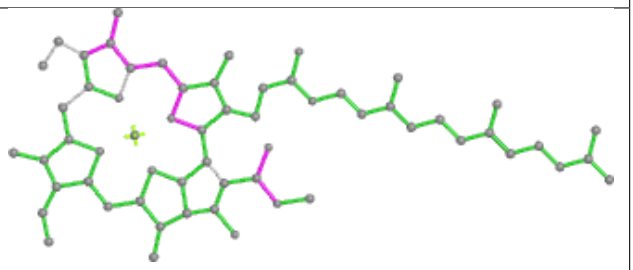
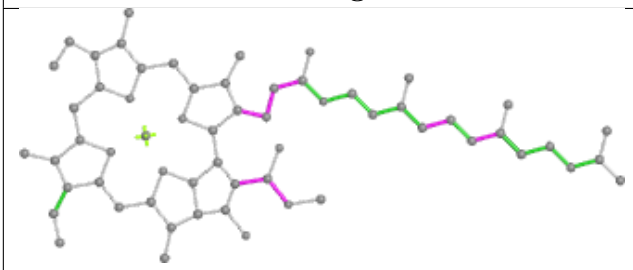


Bond angles



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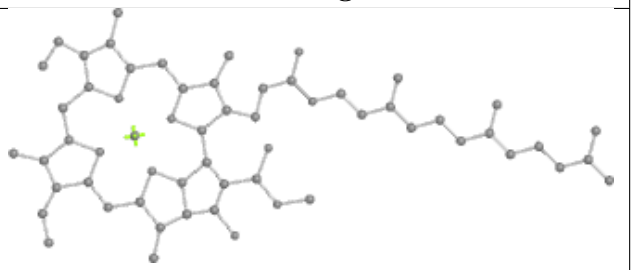
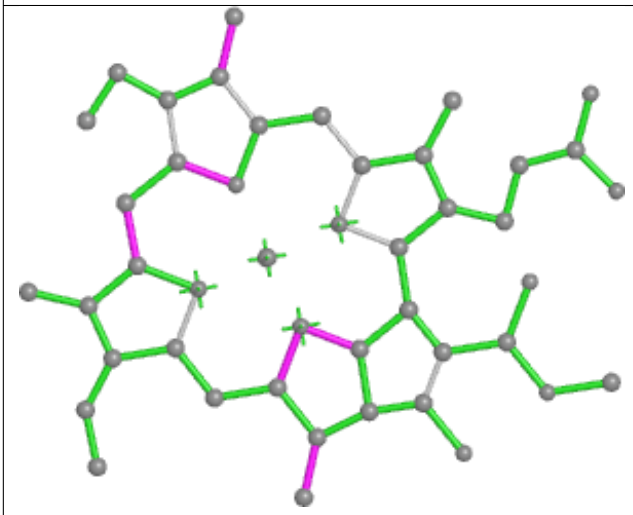


Rings

Ligand CLA u 504



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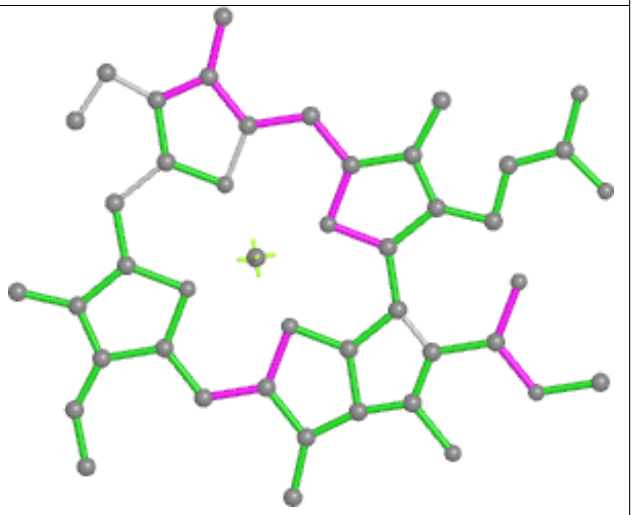

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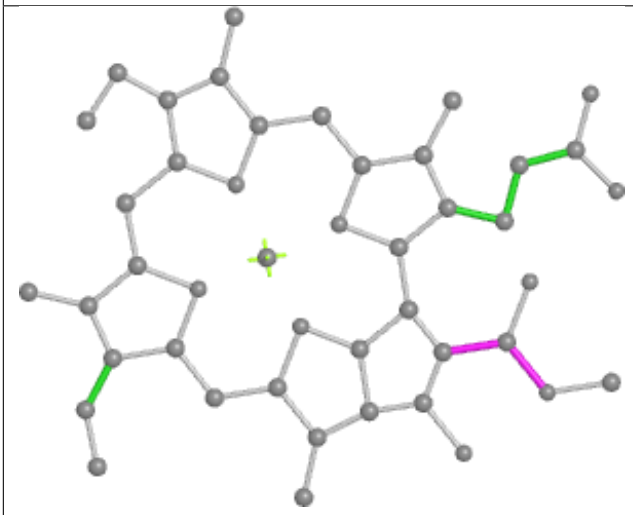

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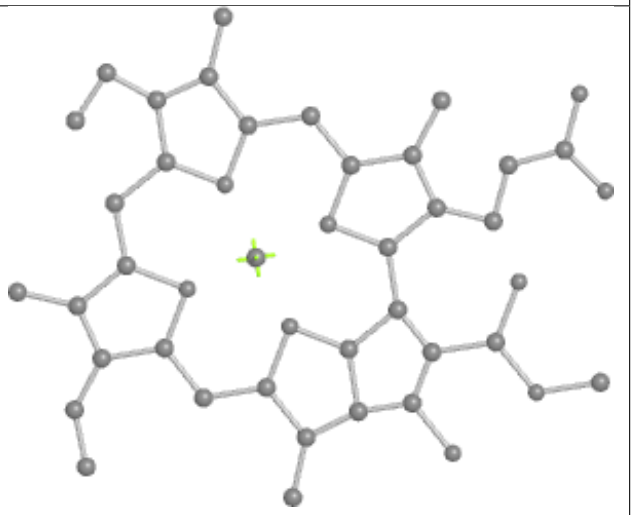
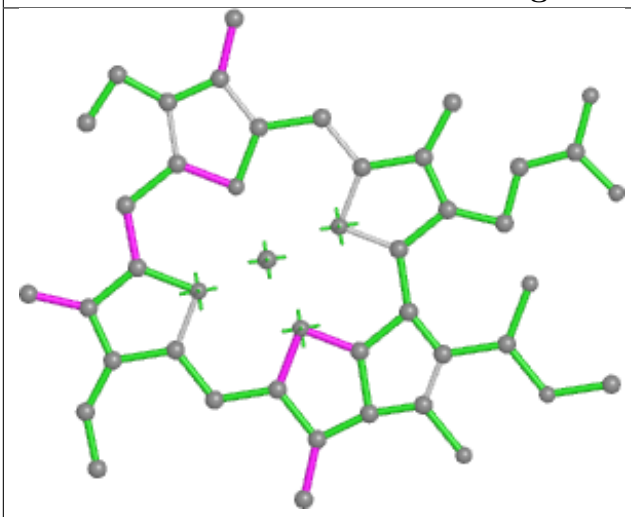


Rings

Ligand CLA t 517



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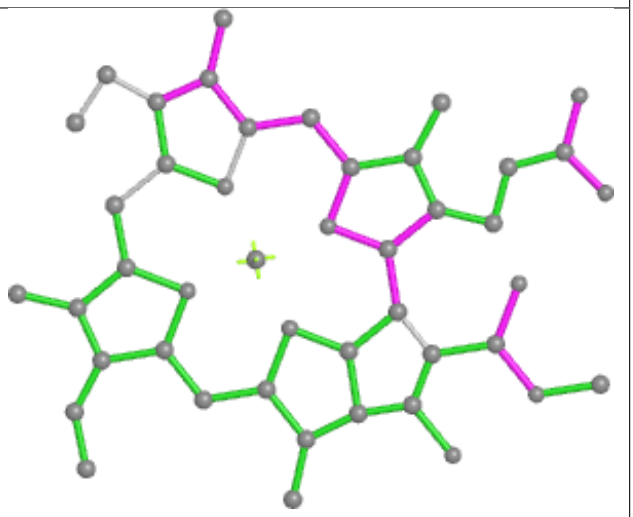

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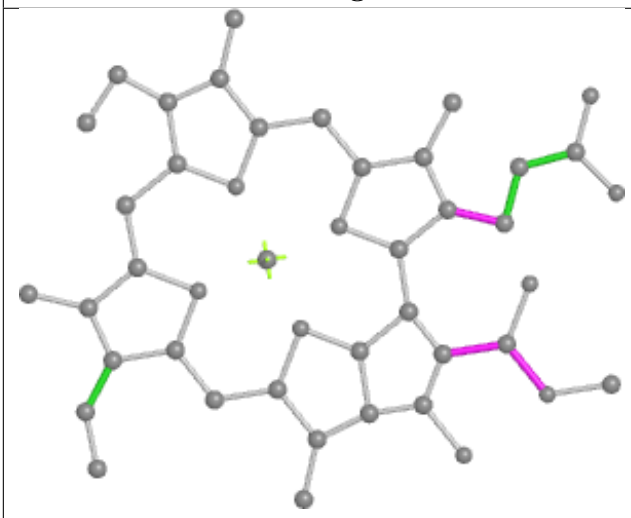

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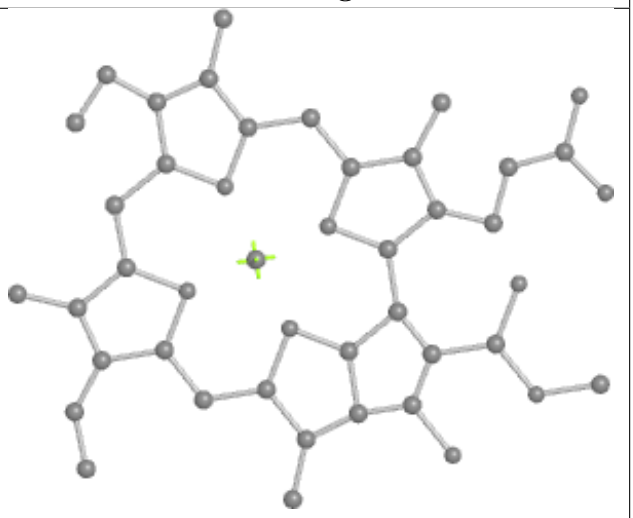
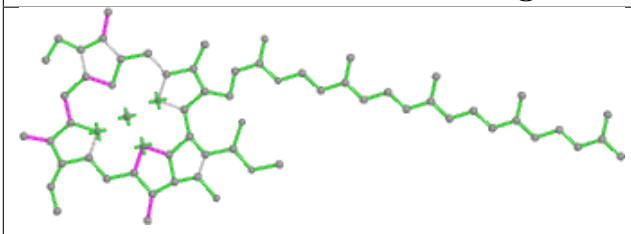


Rings

Ligand CLA L 1502



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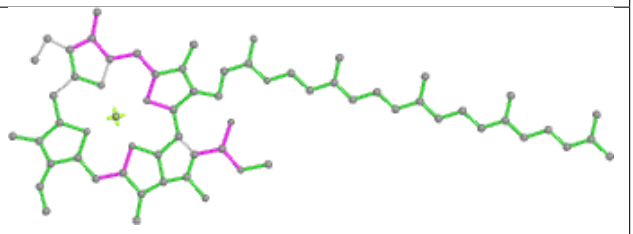
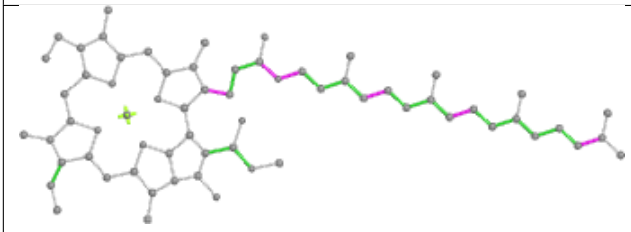


Bond angles



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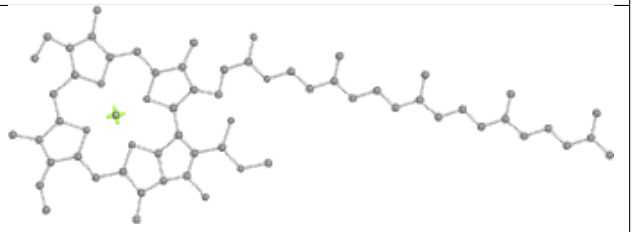
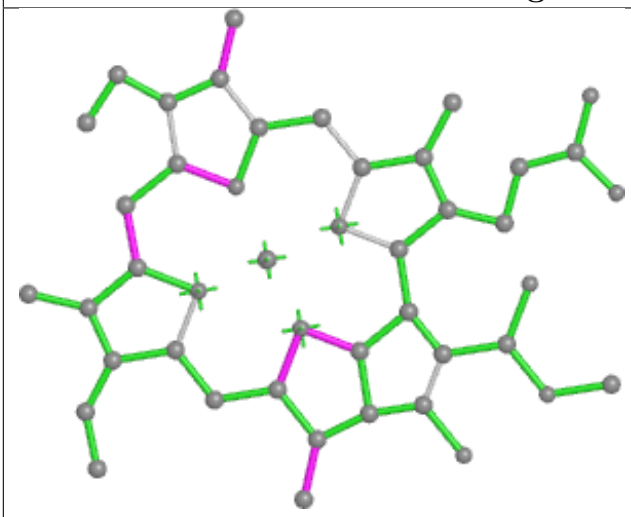


Rings

Ligand CLA d 507



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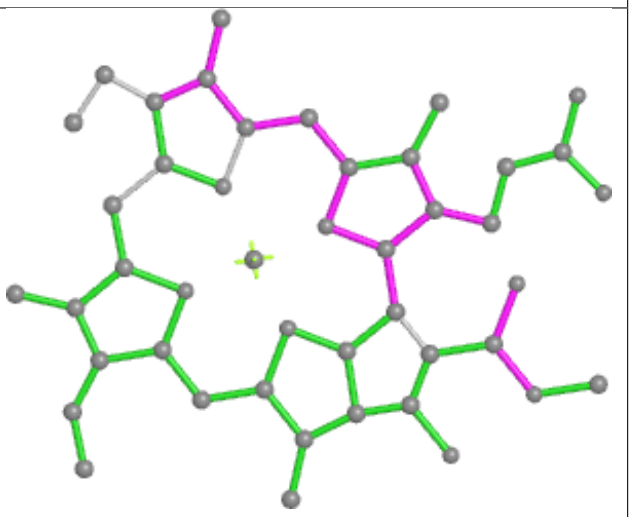
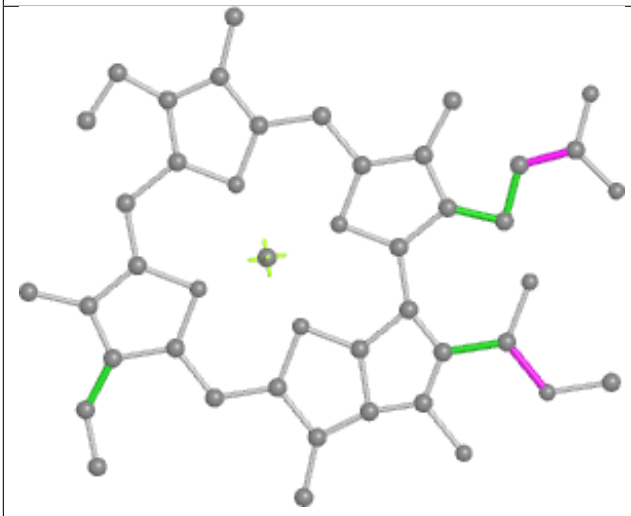


Bond angles



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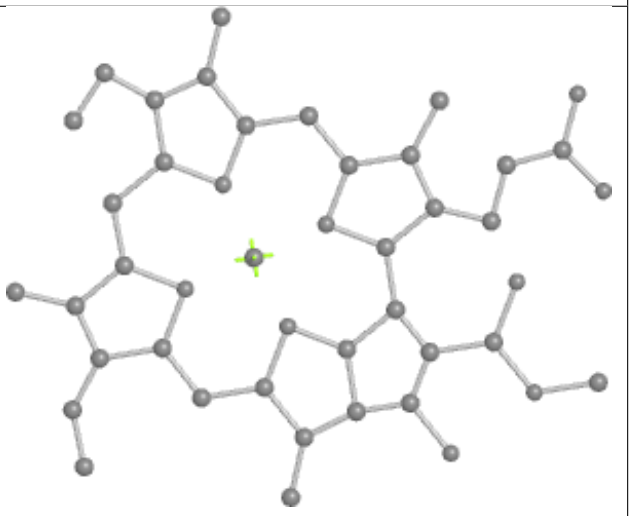
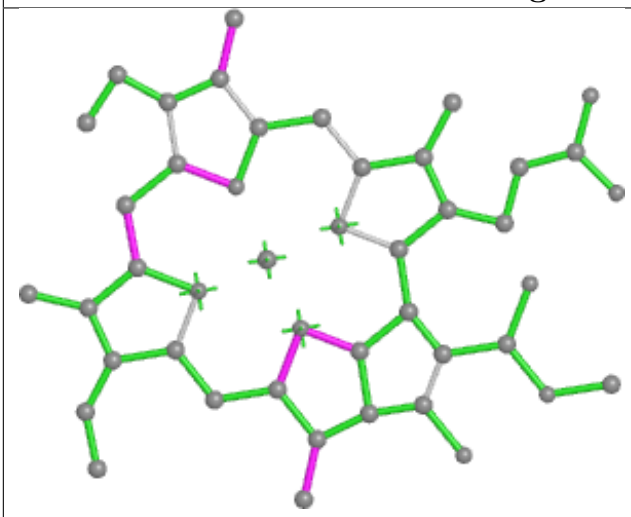


Rings

Ligand CLA c 507



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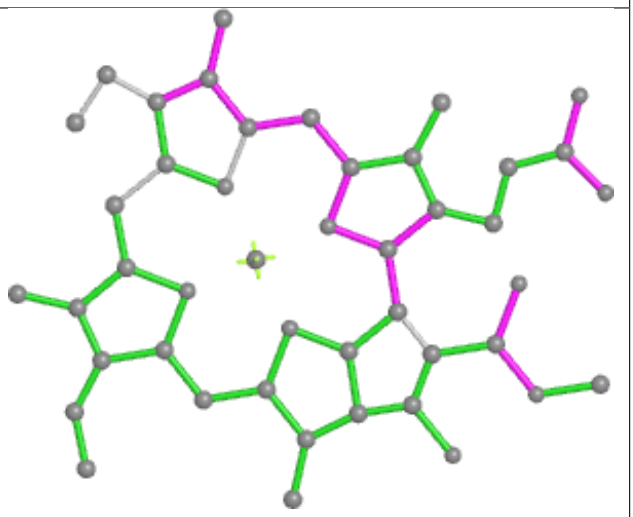
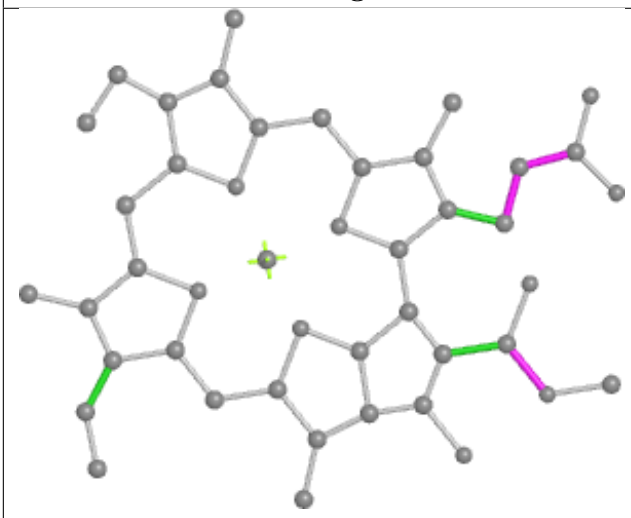


Bond angles



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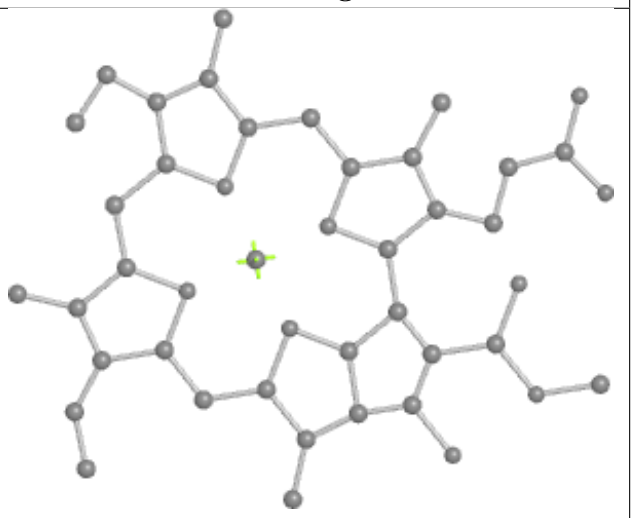
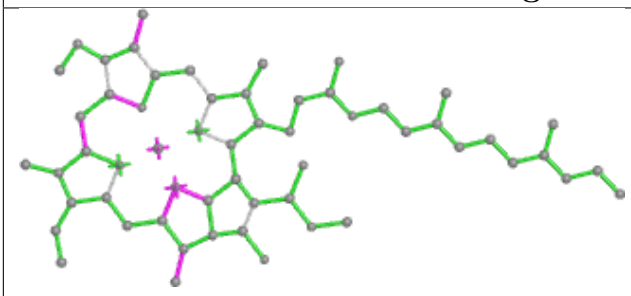
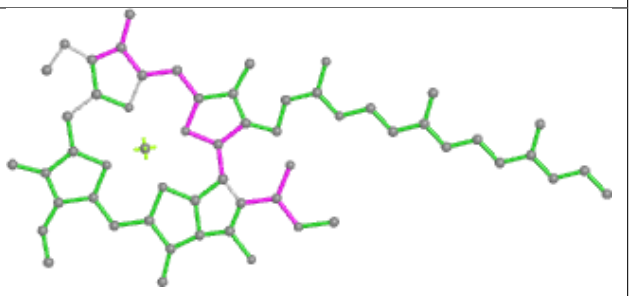


Rings

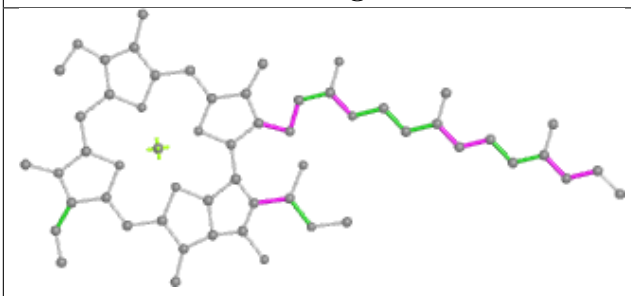
Ligand CLA f 1217



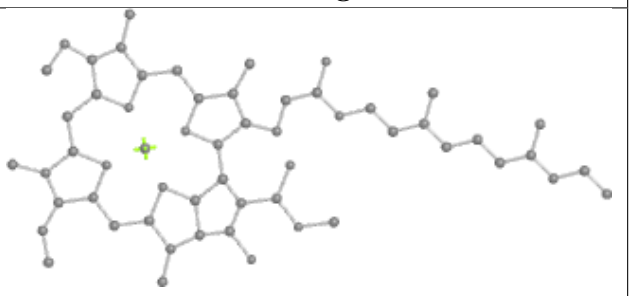
Bond lengths



Bond angles

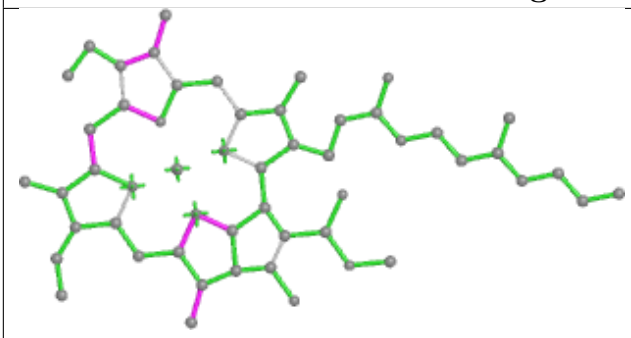


Torsions

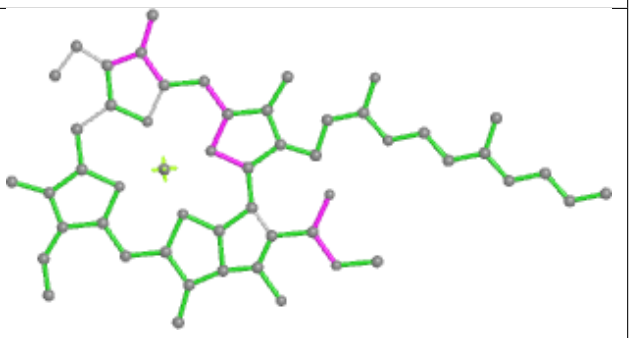


Rings

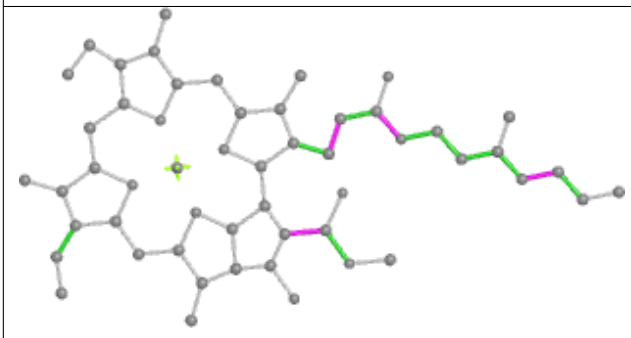
Ligand CLA r 512



Bond lengths



Bond angles



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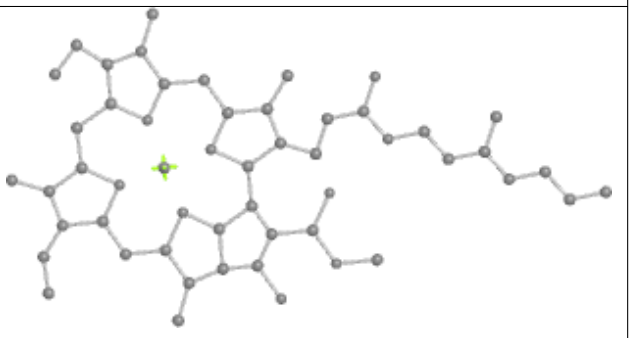
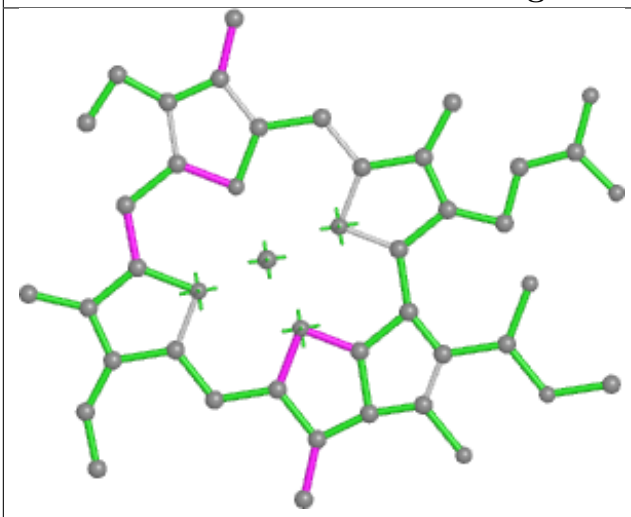


Rings

Ligand CLA b 511



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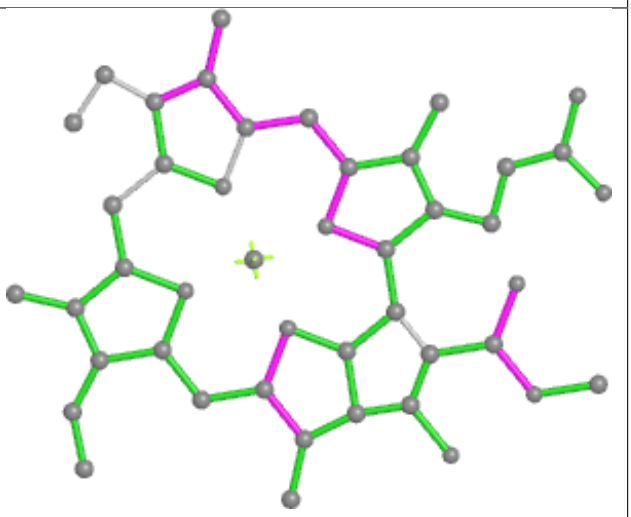
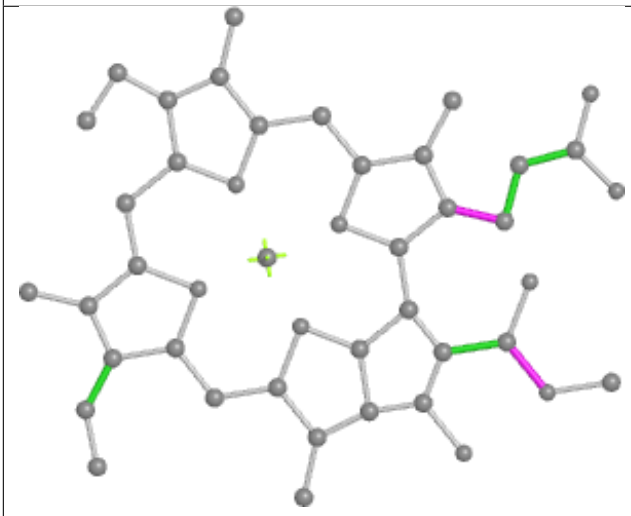


Bond angles



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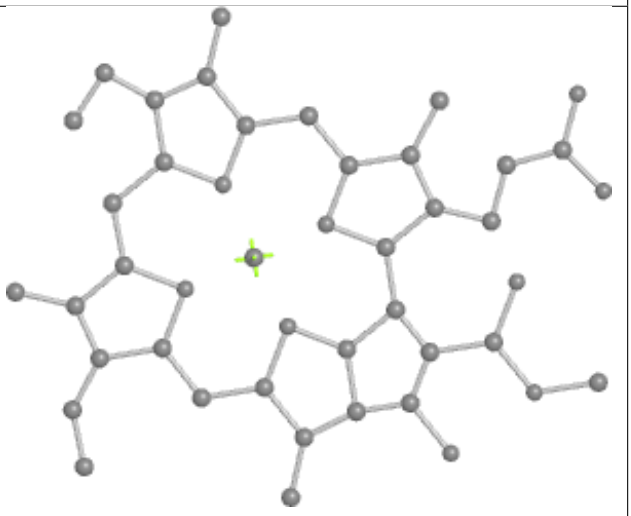
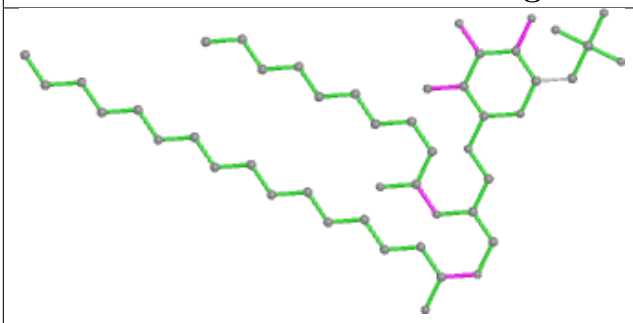


Rings

Ligand SQD Y 822



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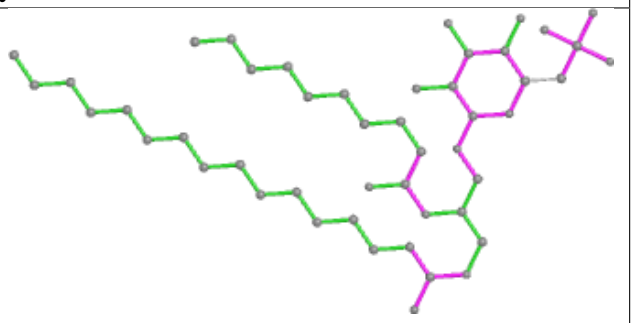
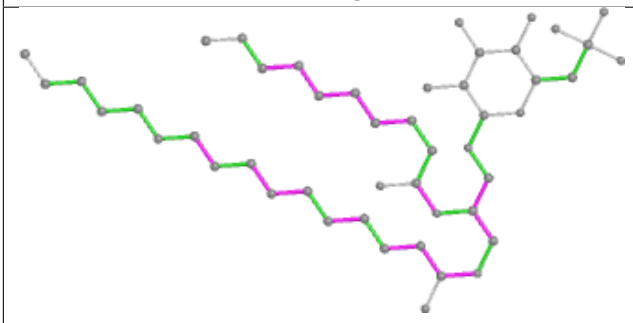
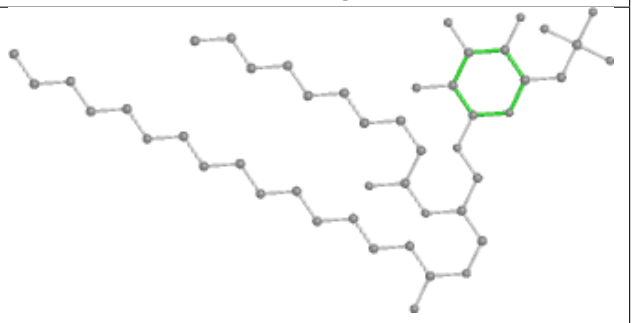


Bond angles

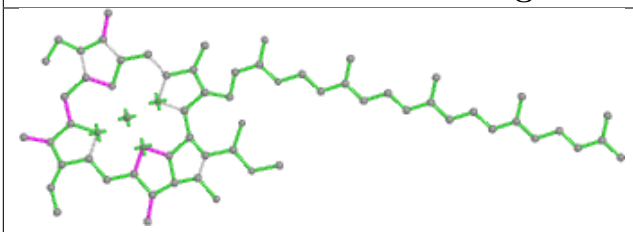


Torsions



Rings

Ligand CLA B 1235



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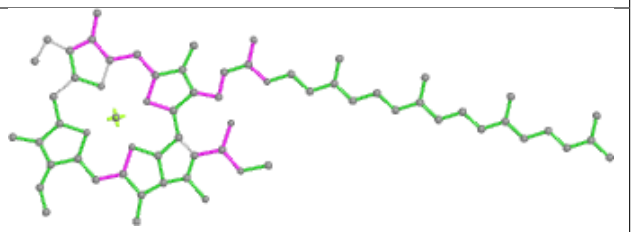
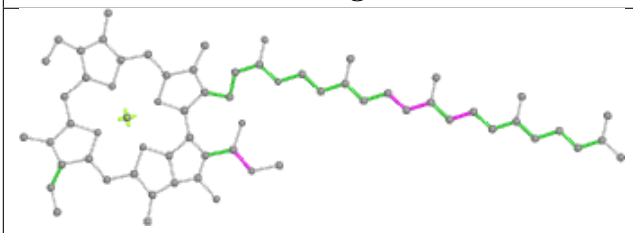


Bond angles



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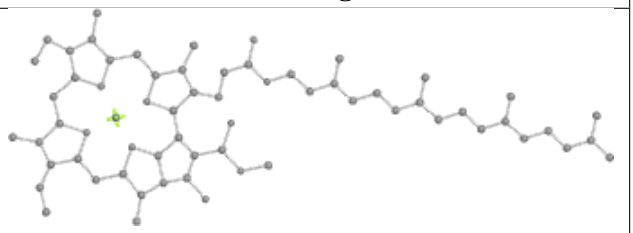
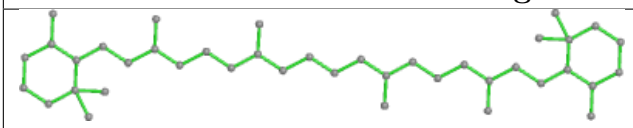


Rings

Ligand BCR B 4004



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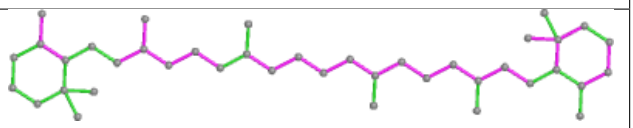
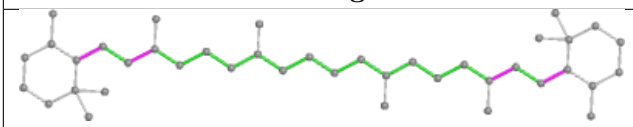


Bond angles



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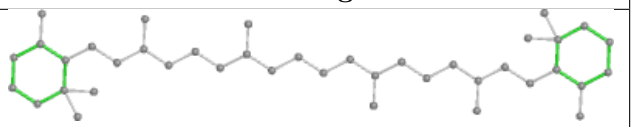
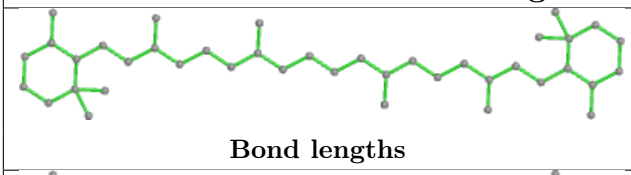


Rings

Ligand BCR t 522



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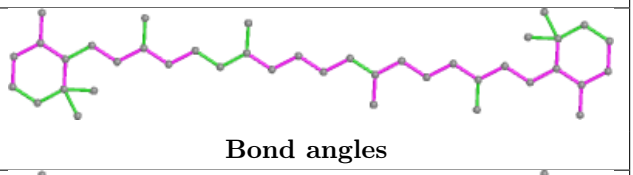
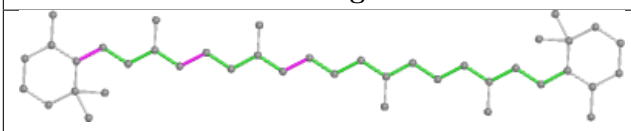


Bond angles



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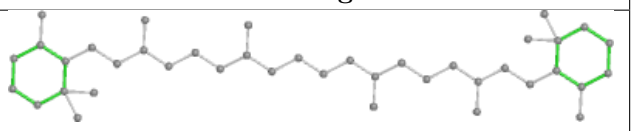
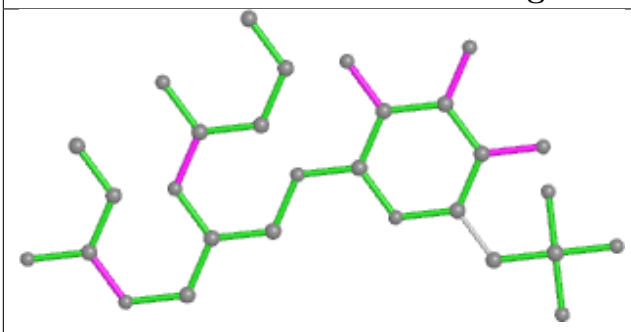


Rings

Ligand SQD u 822



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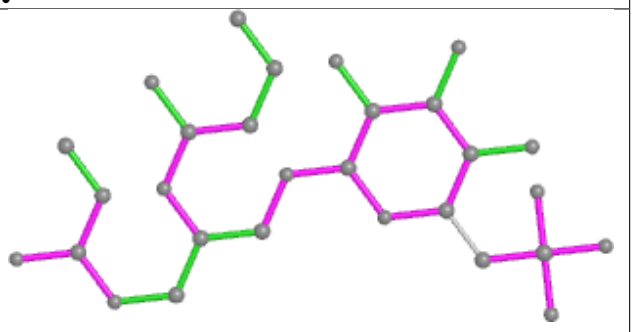
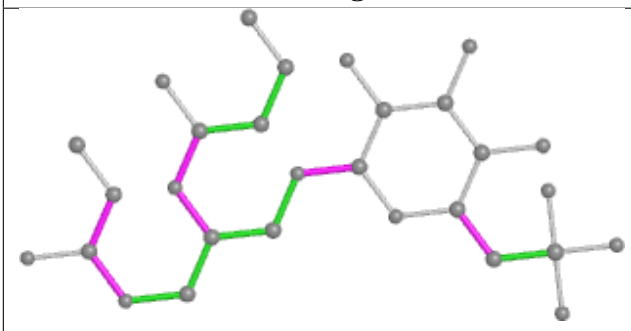


Bond angles



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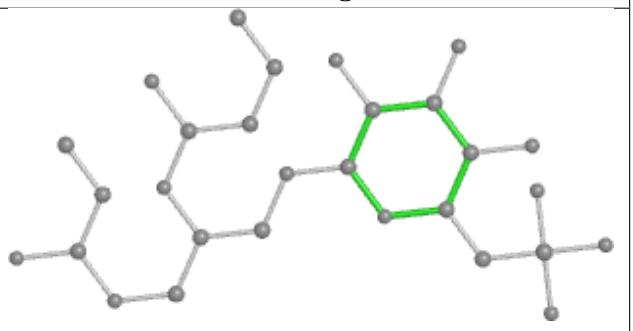
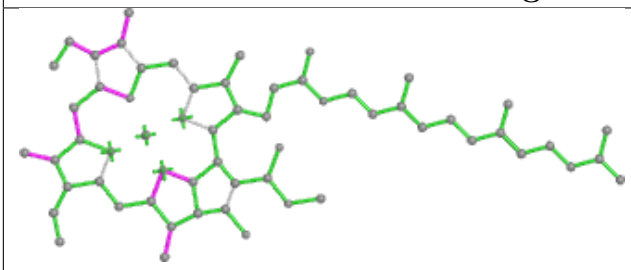


Rings

Ligand CLA f 1230



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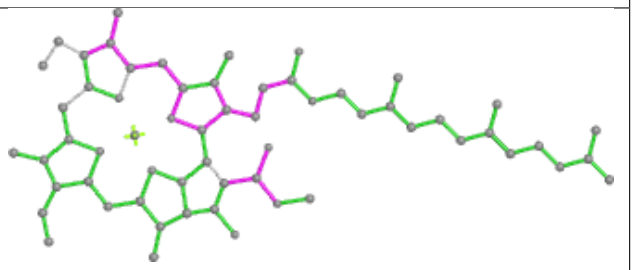
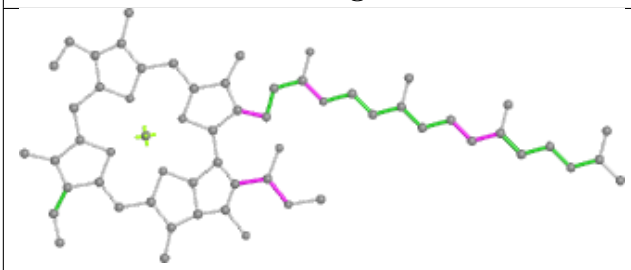


Bond angles



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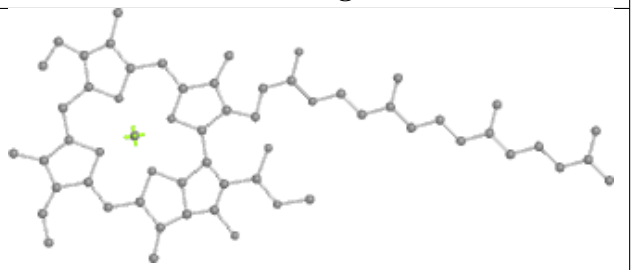
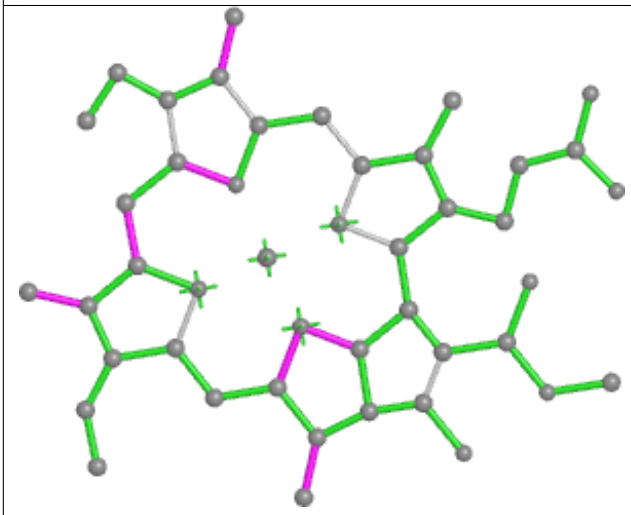


Rings

Ligand CLA Z 517



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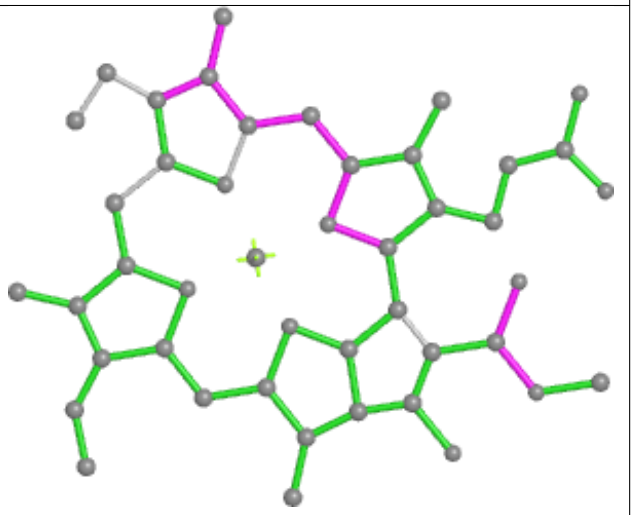
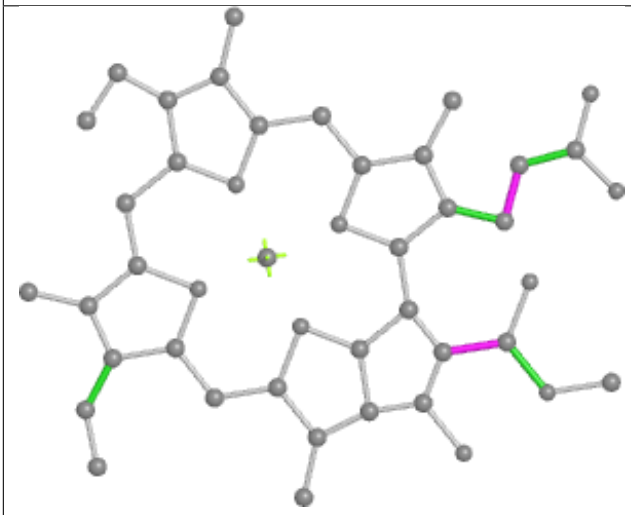


Bond angles



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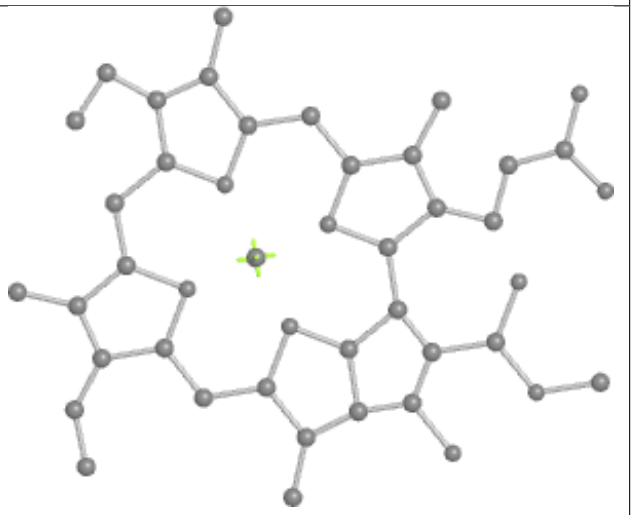
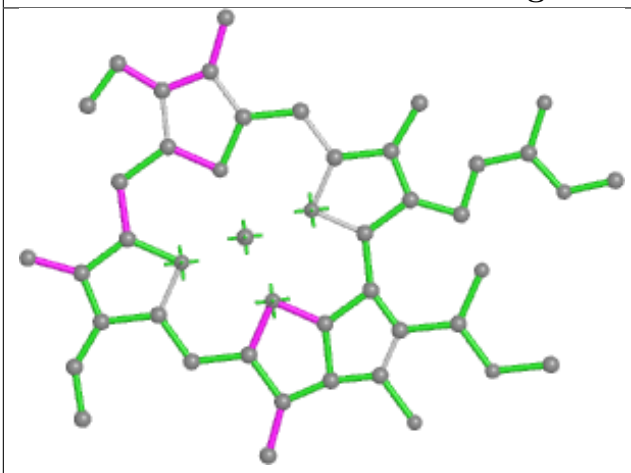


Rings

Ligand CLA u 519



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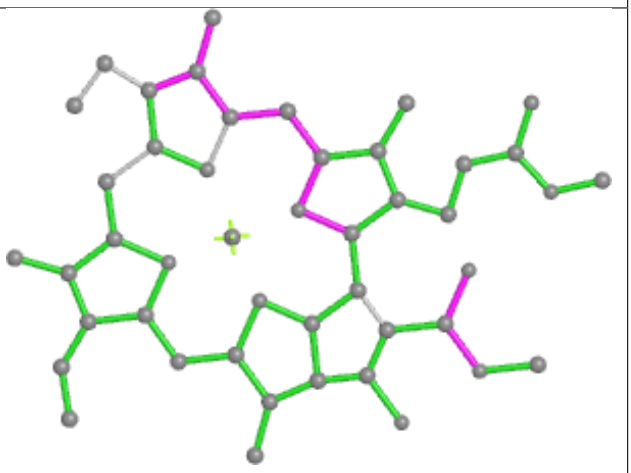

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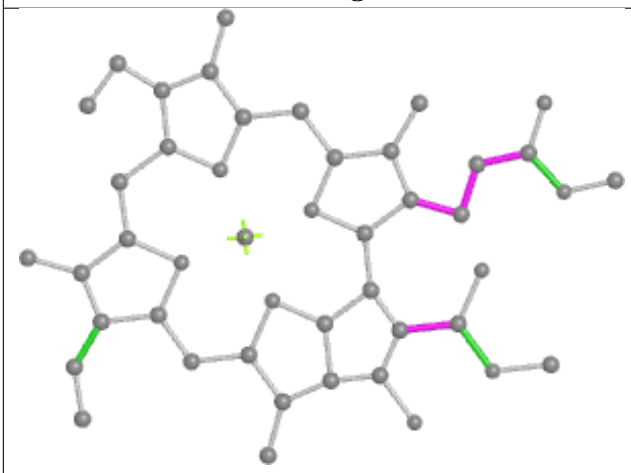

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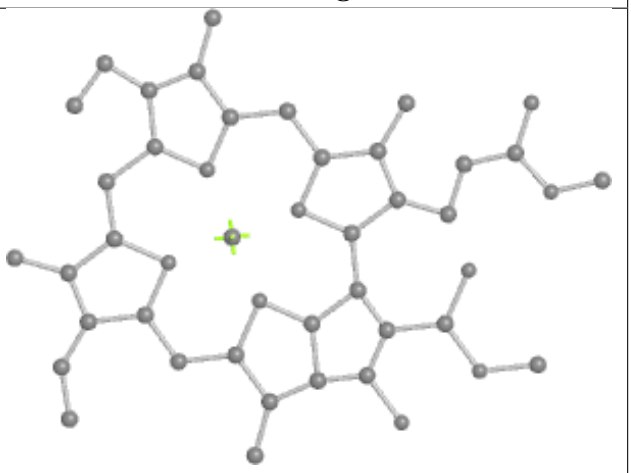
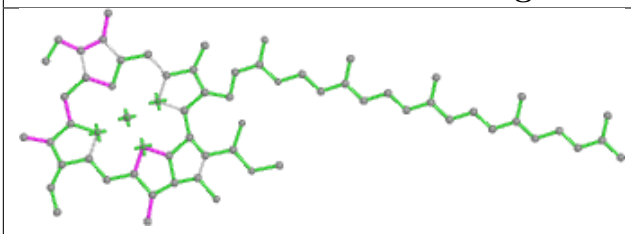


Rings

Ligand CLA A 1131



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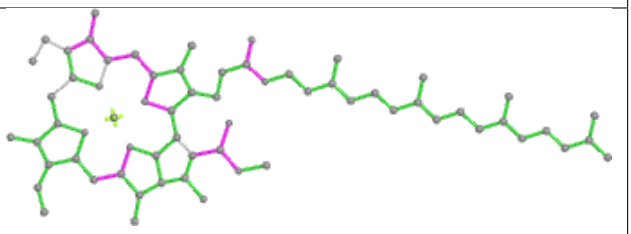
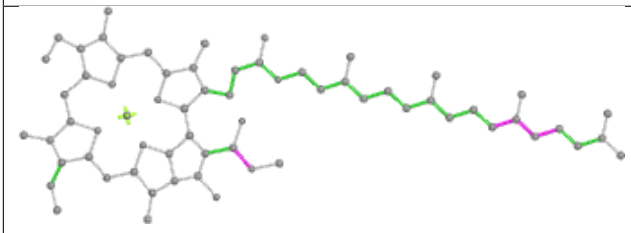


Bond angles



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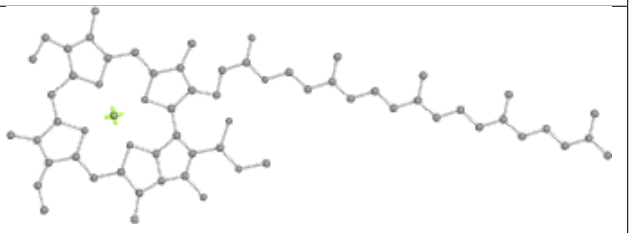
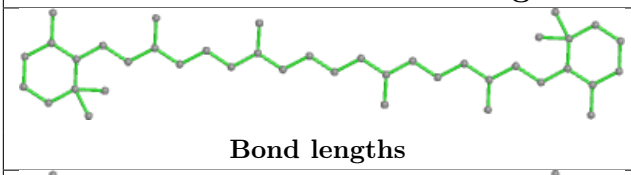


Rings

Ligand BCR H 4006



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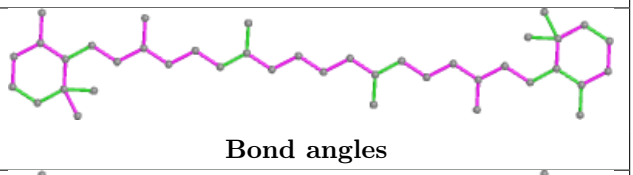
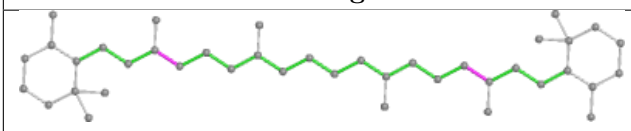


Bond angles



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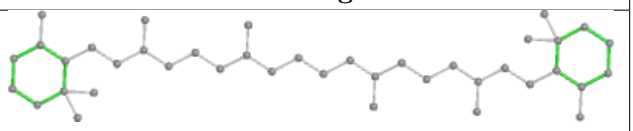
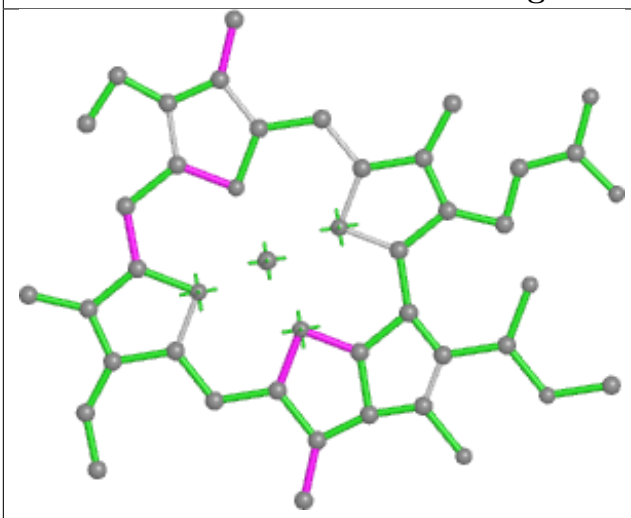


Rings

Ligand CLA v 511



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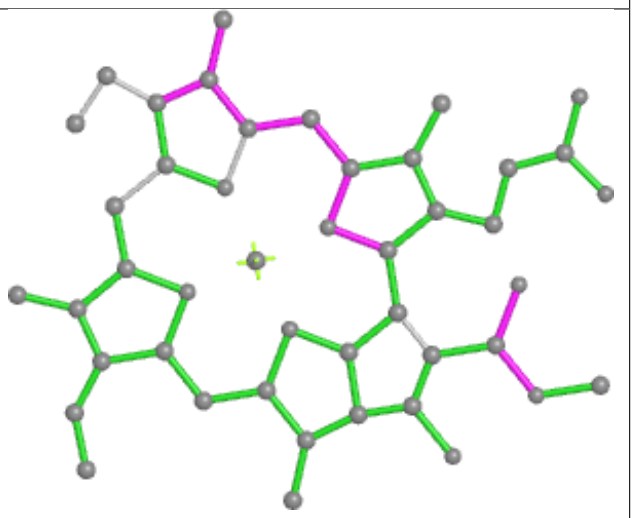
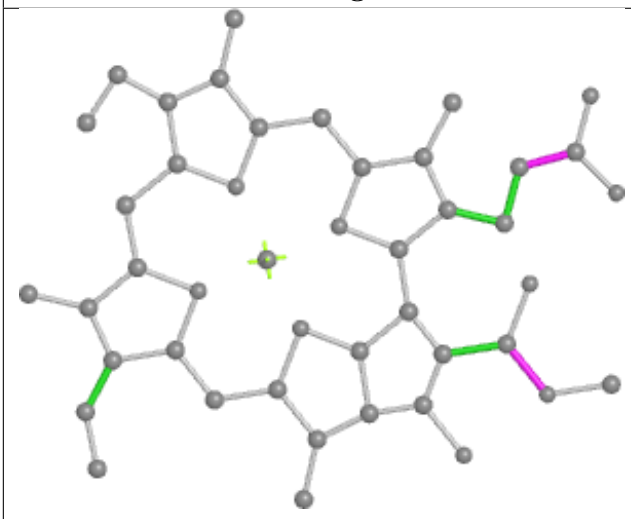
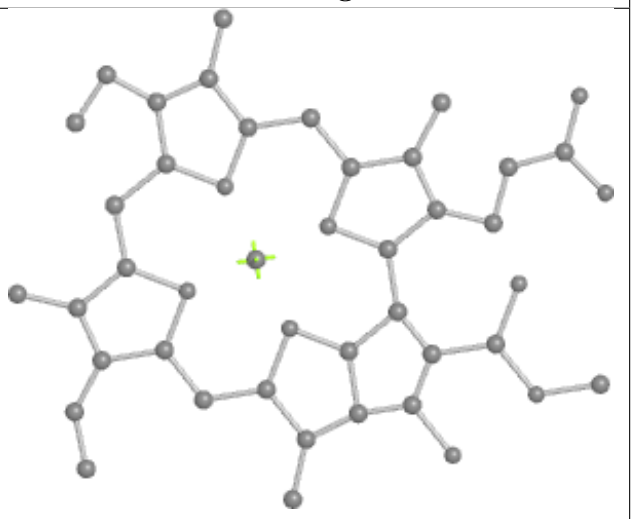


Bond angles

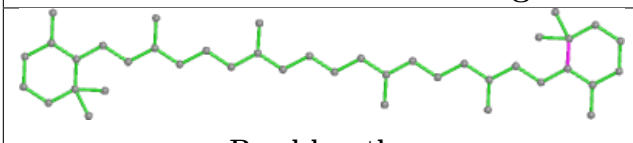


Torsions

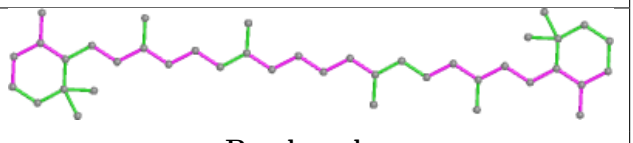


Rings

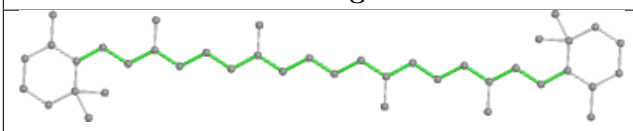
Ligand BCR G 4002



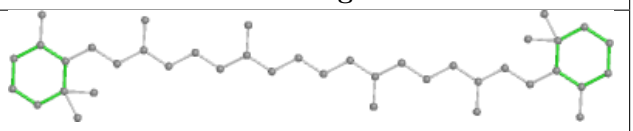
Bond lengths



Bond angles

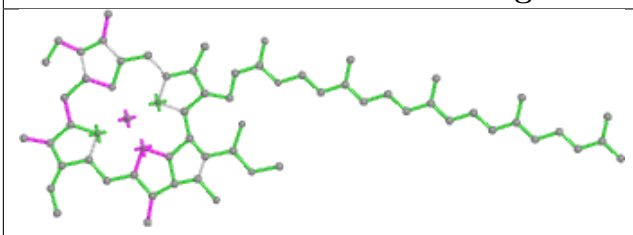


Torsions

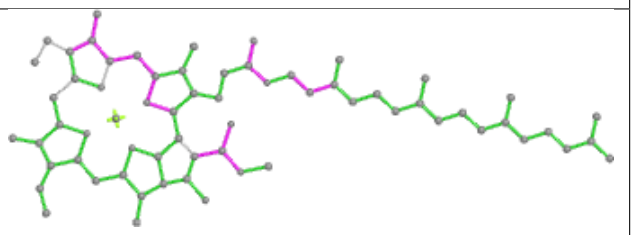


Rings

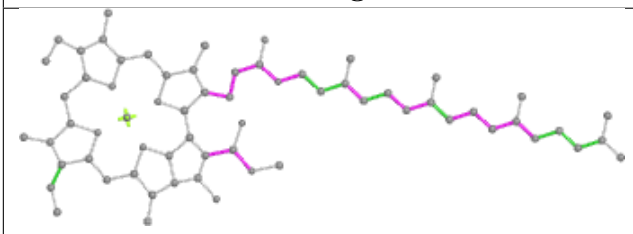
Ligand CLA A 1106



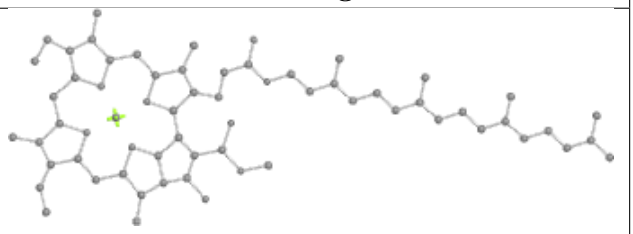
Bond lengths



Bond angles

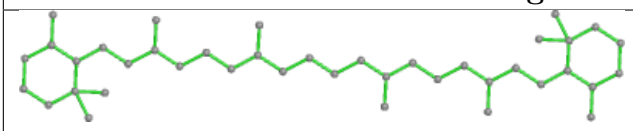


Torsions



Rings

Ligand BCR a 521



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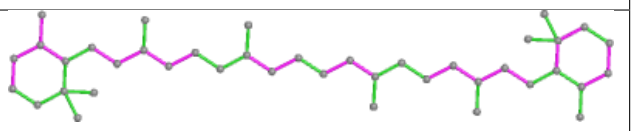

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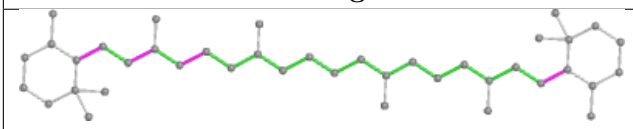

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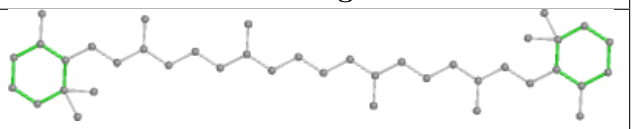
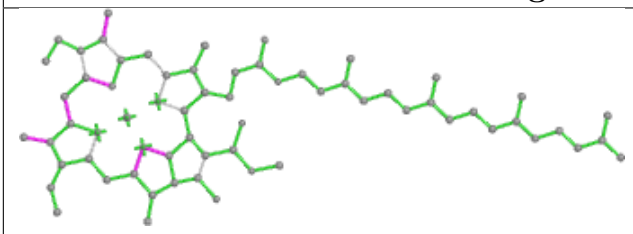


Rings

Ligand CLA 5 501



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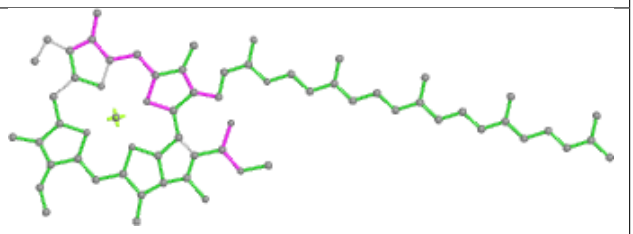
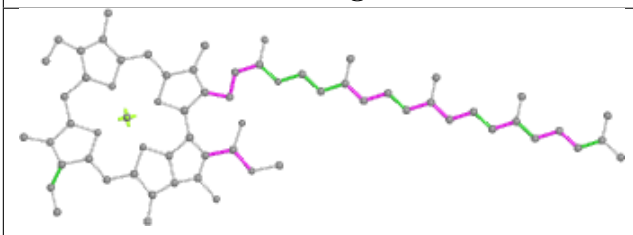


Bond angles



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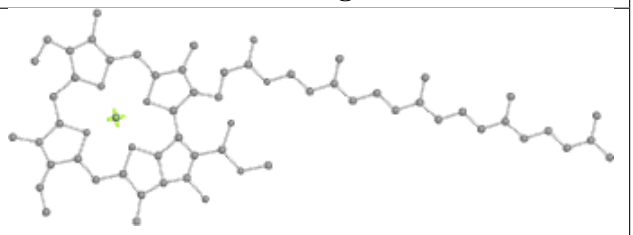
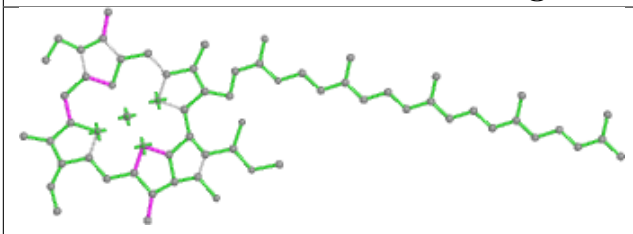


Rings

Ligand CLA 2 507



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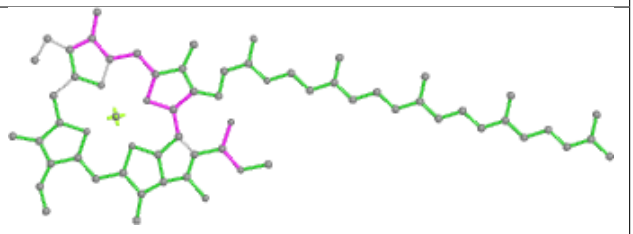

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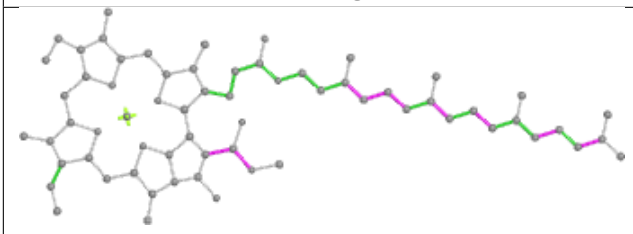

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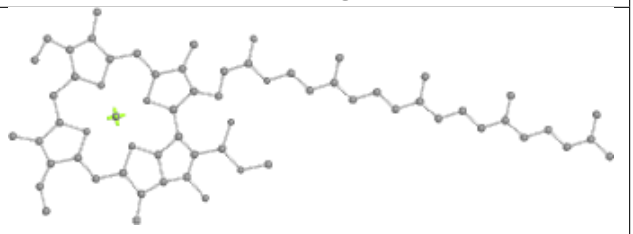
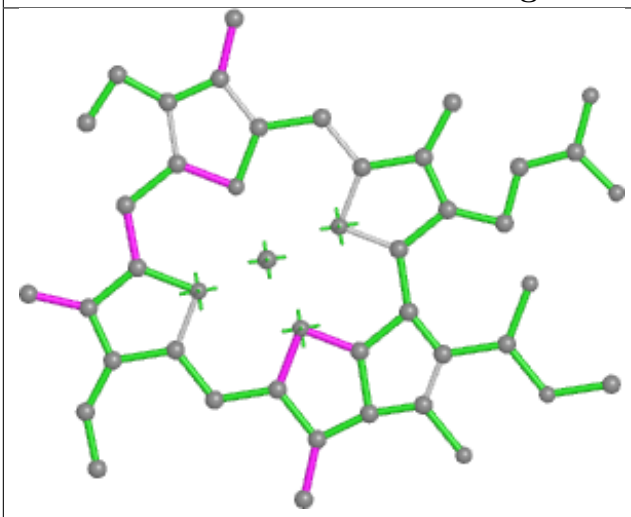


Rings

Ligand CLA e 1113



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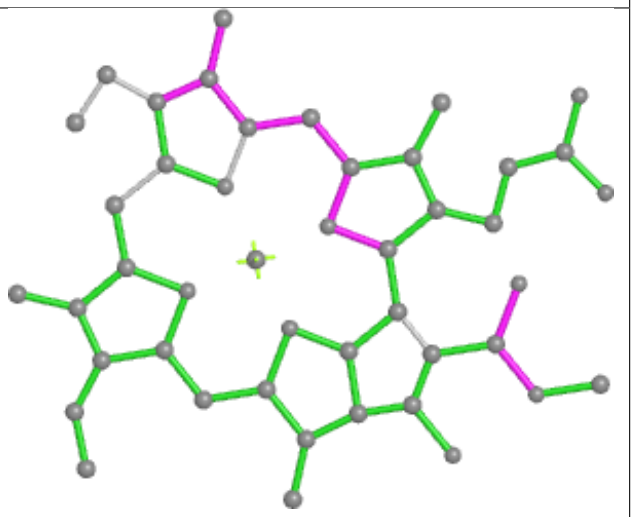

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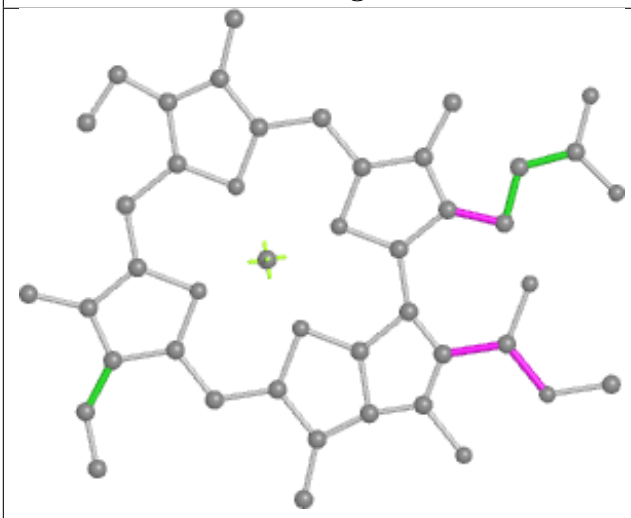

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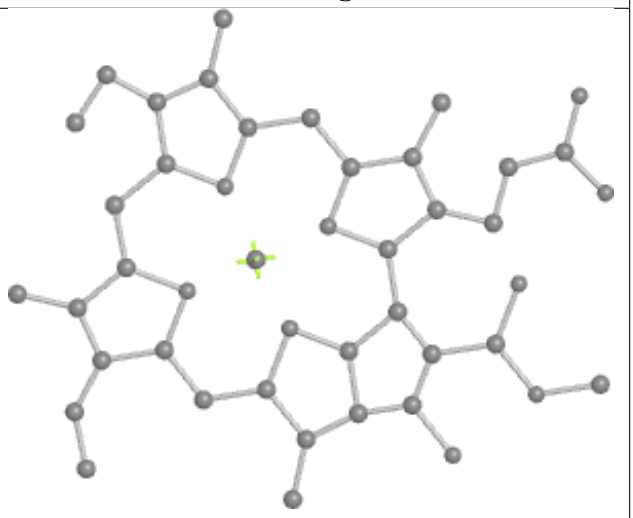
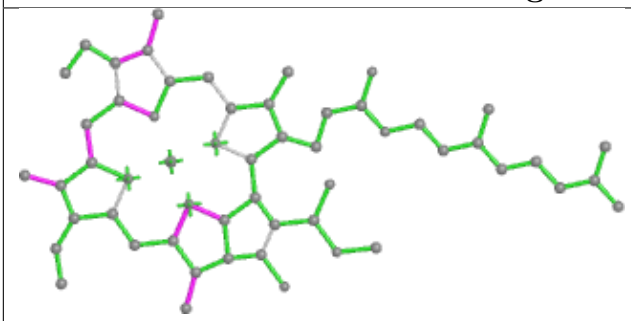


Rings

Ligand CLA Z 508



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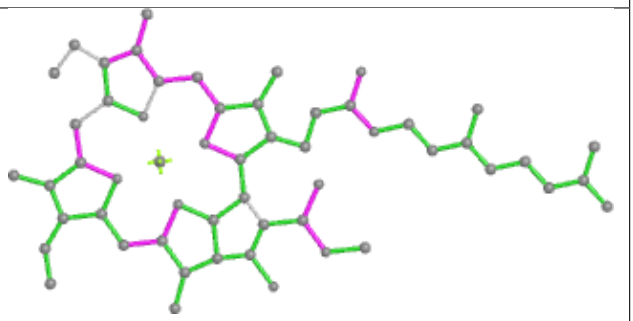
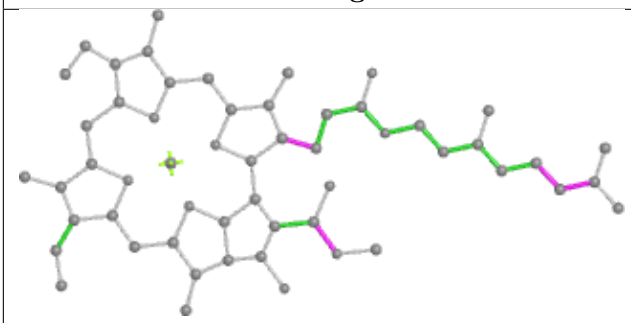


Bond angles



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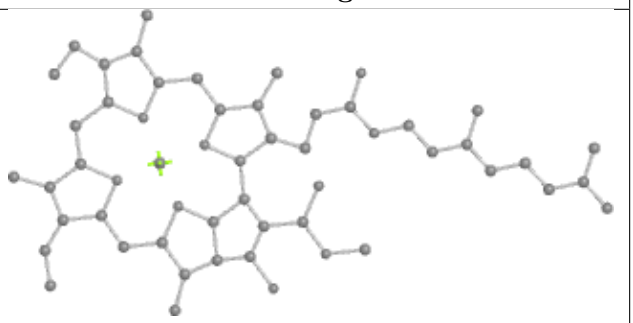
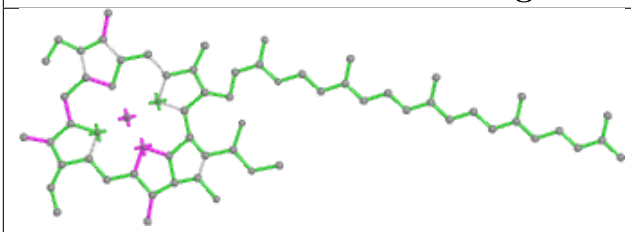


Rings

Ligand CLA B 1023



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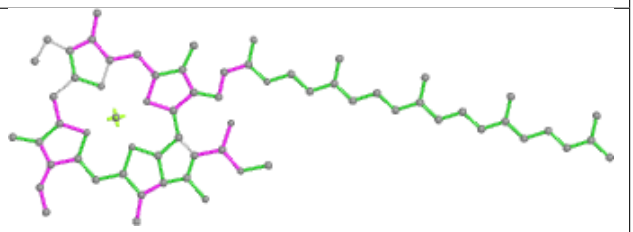

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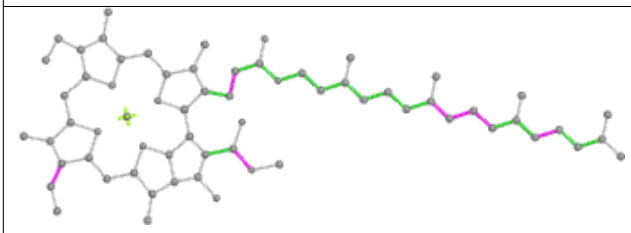

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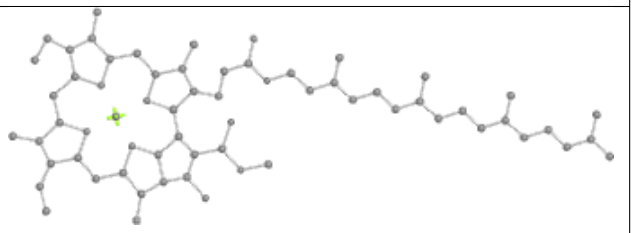
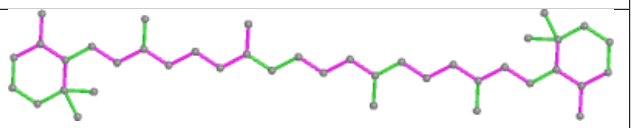


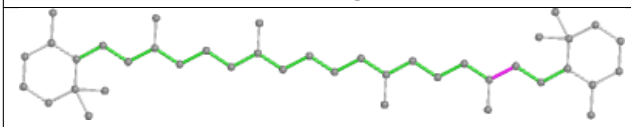
Rings

Ligand BCR k 4018

Bond lengths



Bond angles



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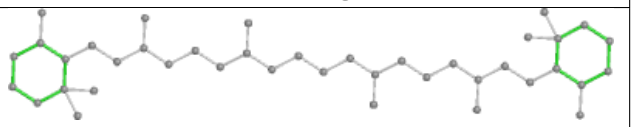
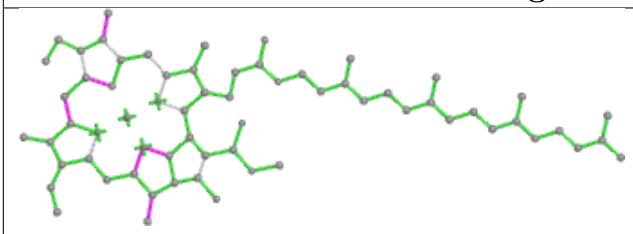


Rings

Ligand CLA 6 505



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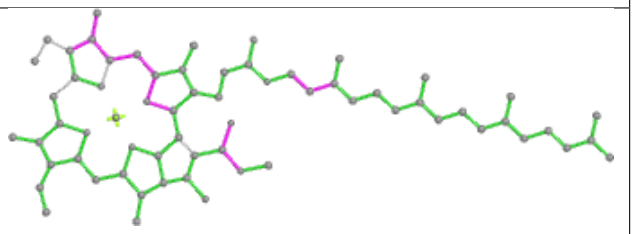

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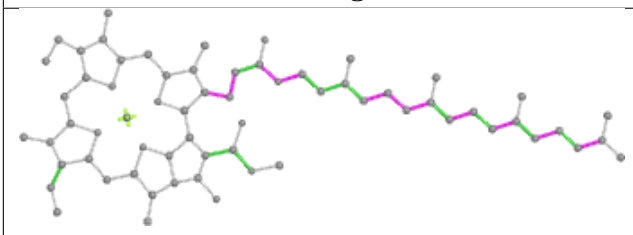

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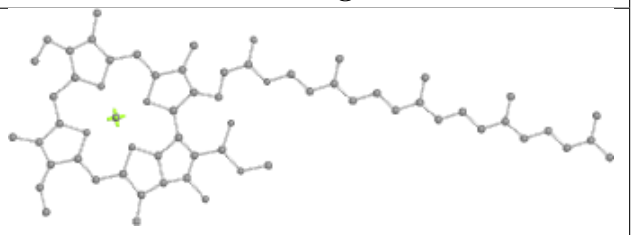
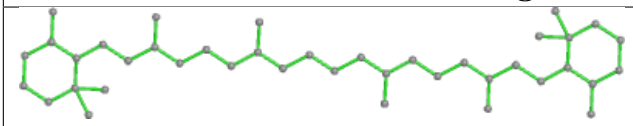


Rings

Ligand BCR n 4219



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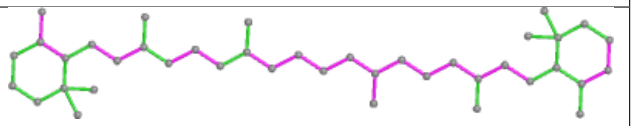

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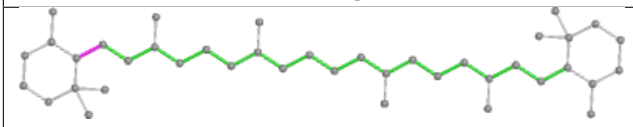
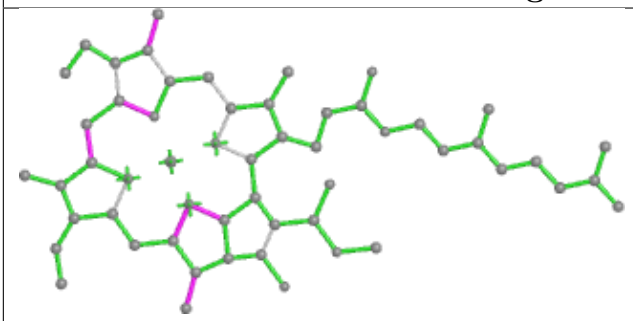


Torsions

Rings

Ligand CLA Z 511



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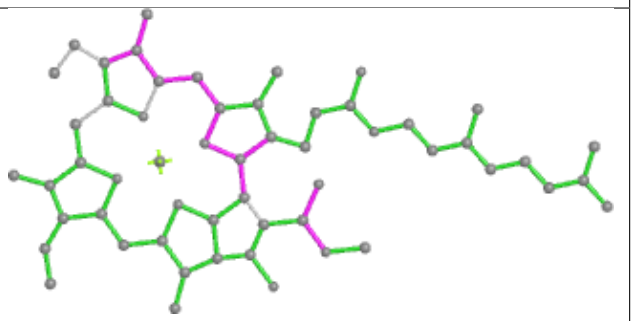
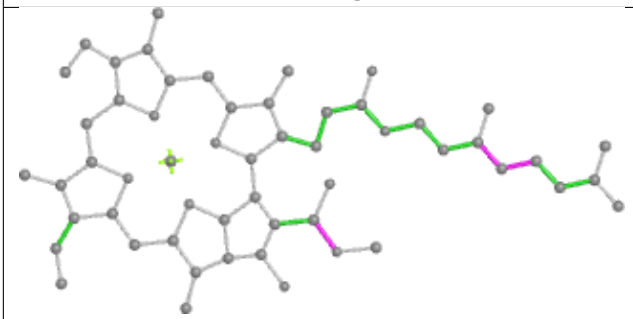


Bond angles



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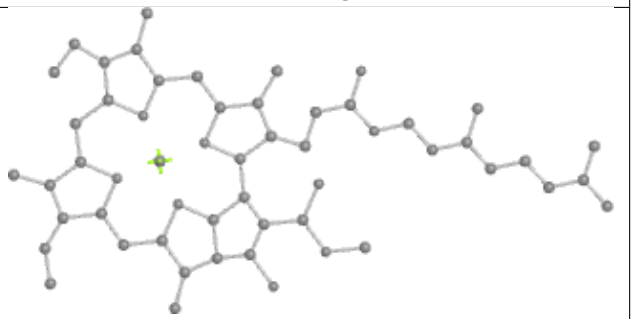
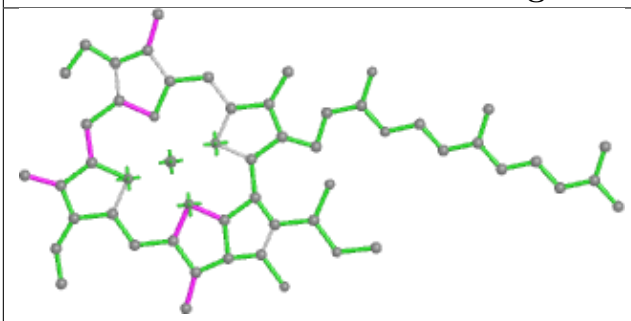


Rings

Ligand CLA q 508



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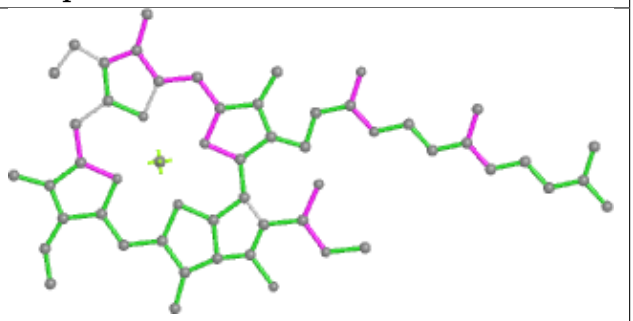

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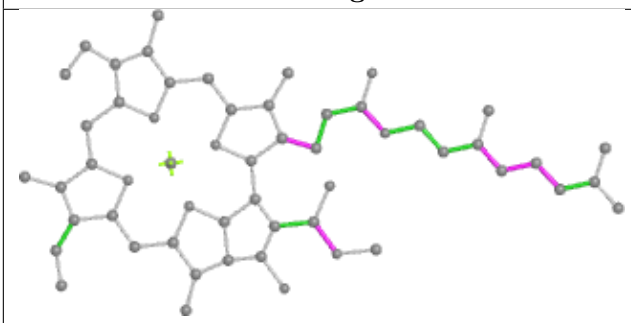

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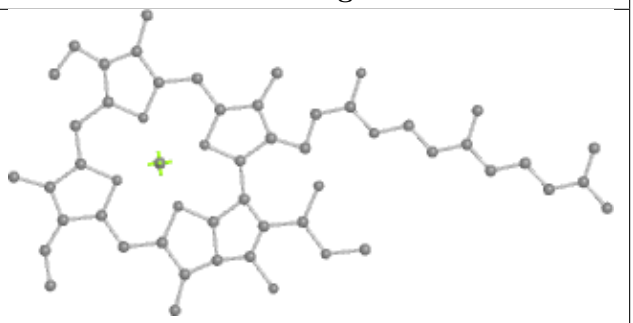
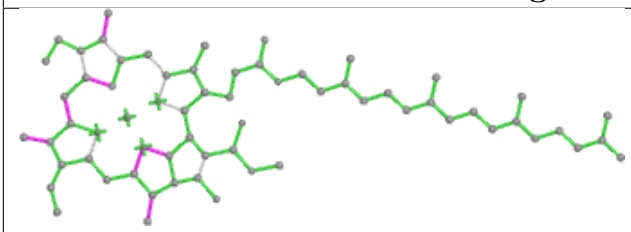


Rings

Ligand CLA c 509



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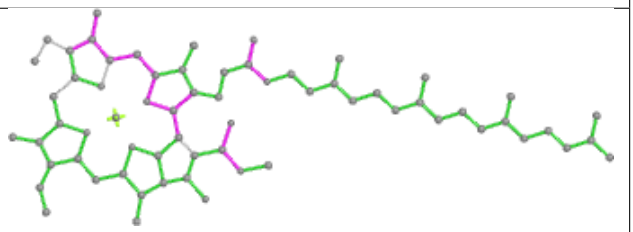
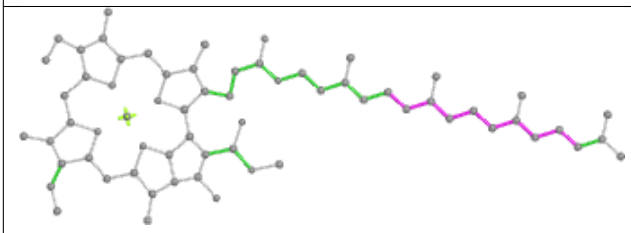


Bond angles



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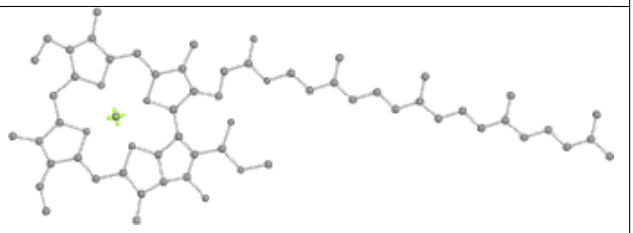
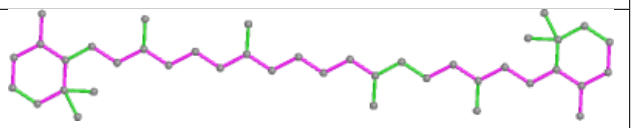


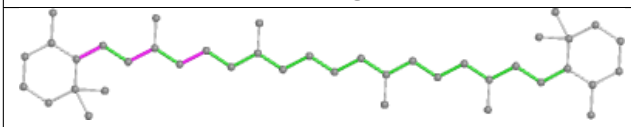
Rings

Ligand BCR s 522

Bond lengths



Bond angles



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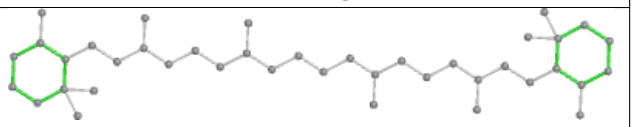
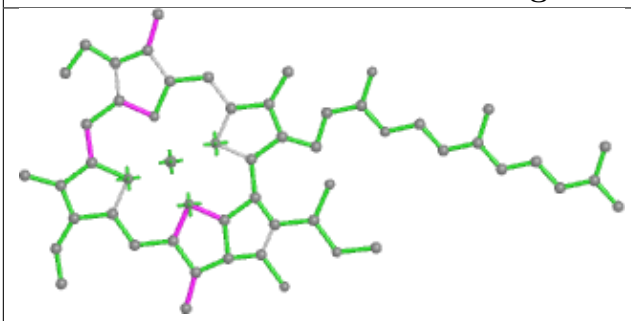


Rings

Ligand CLA r 511



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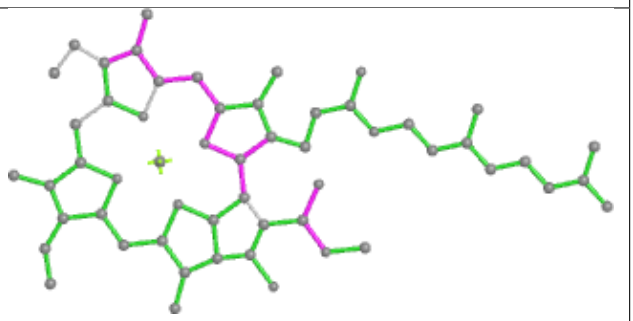
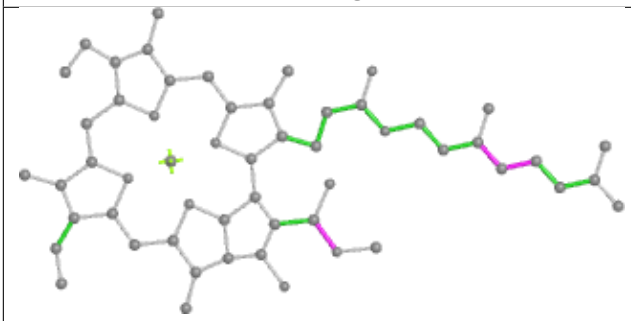


Bond angles



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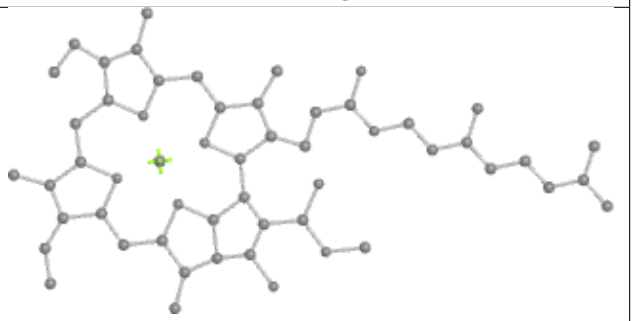
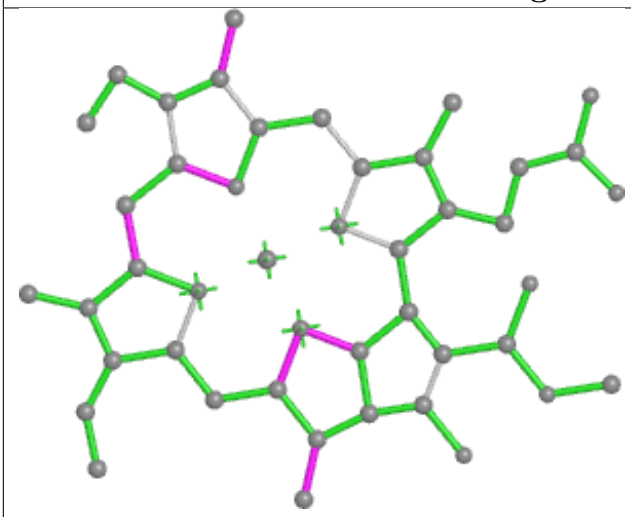
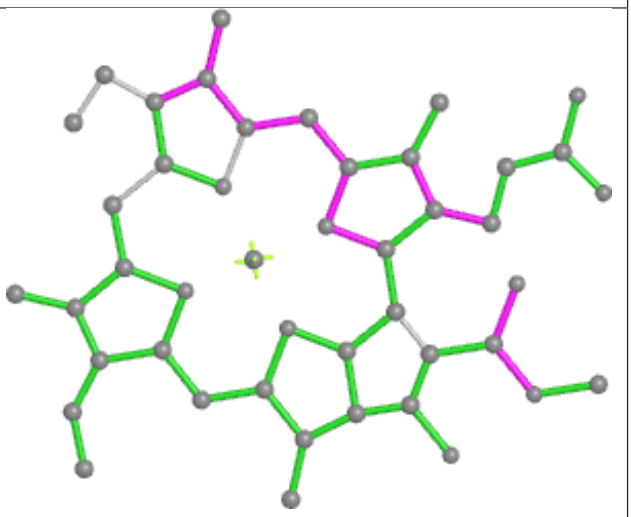


Rings

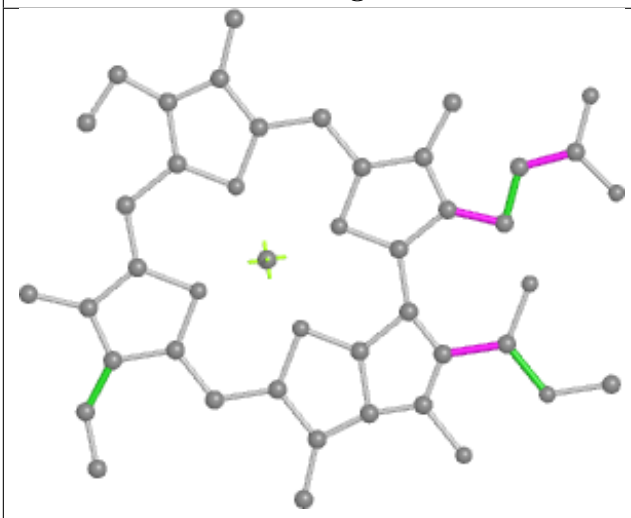
Ligand CLA t 516



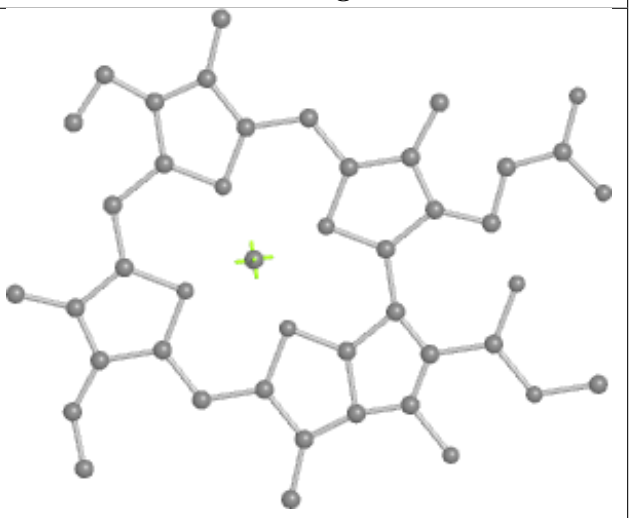
Bond lengths



Bond angles

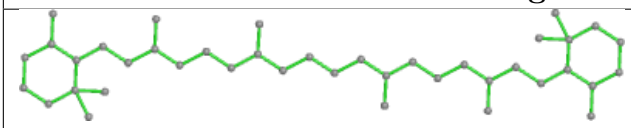


Torsions



Rings

Ligand BCR t 521



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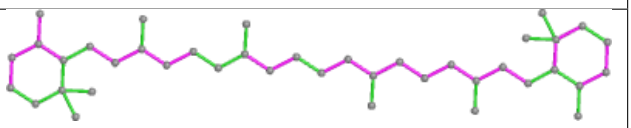

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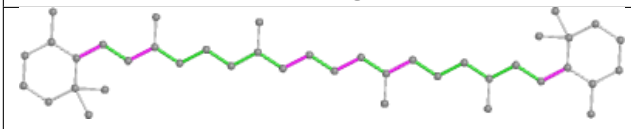
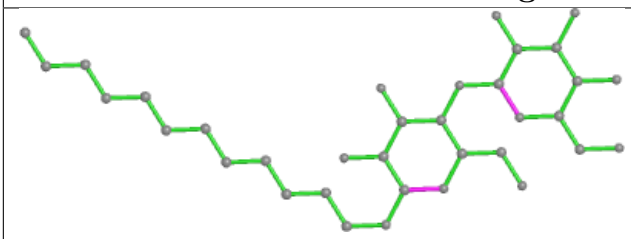


Torsions

Rings

Ligand LMU f 1843



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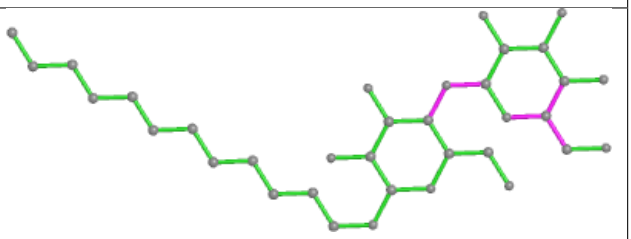

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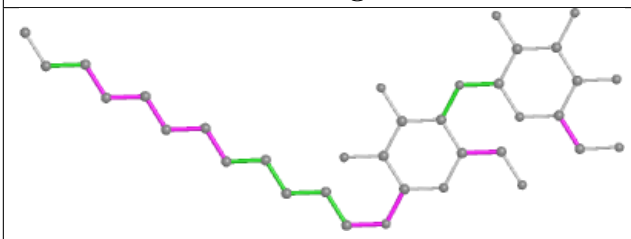

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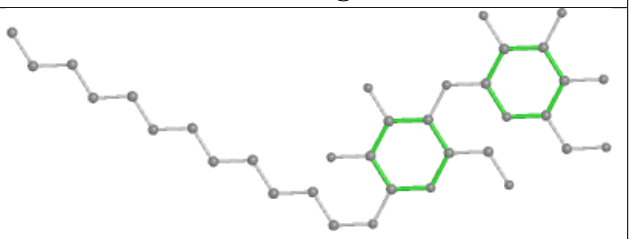
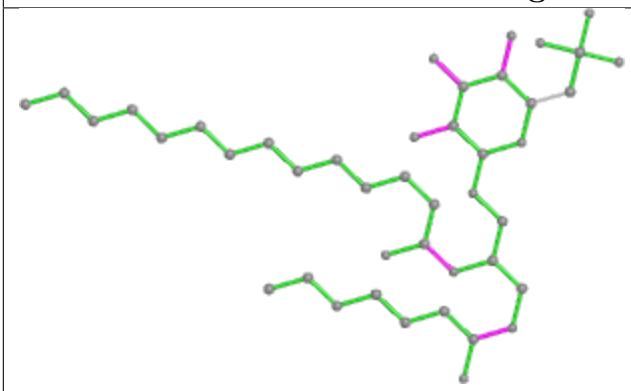


Rings

Ligand SQD 2 822



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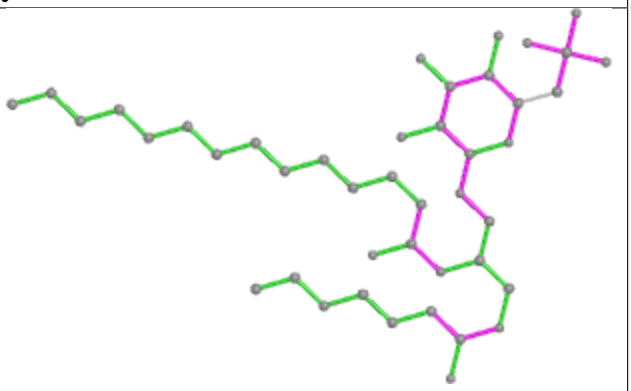
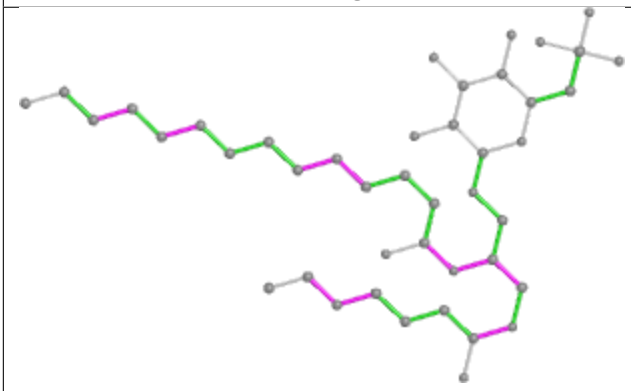
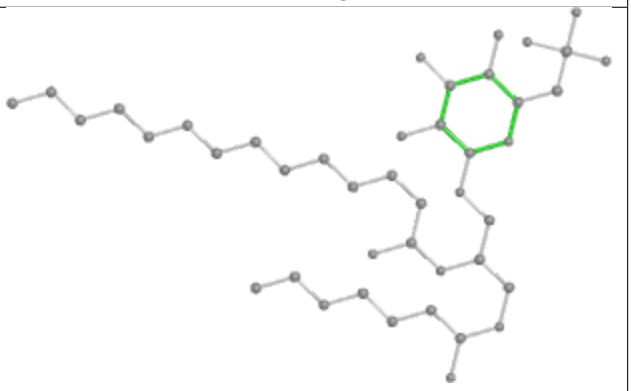


Bond angles

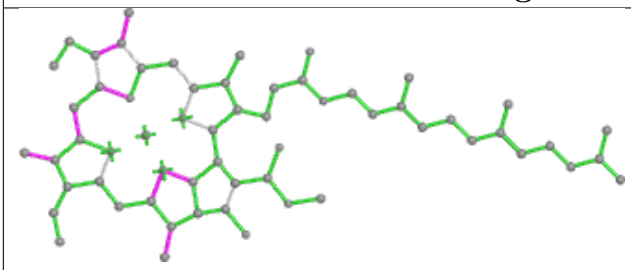


Torsions



Rings

Ligand CLA A 1136



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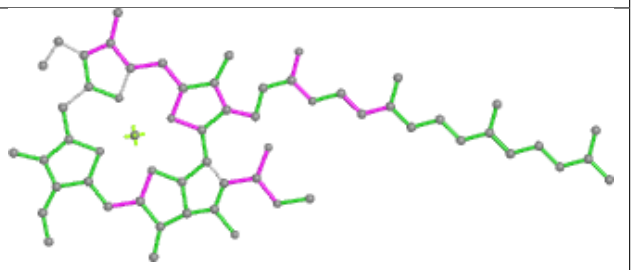
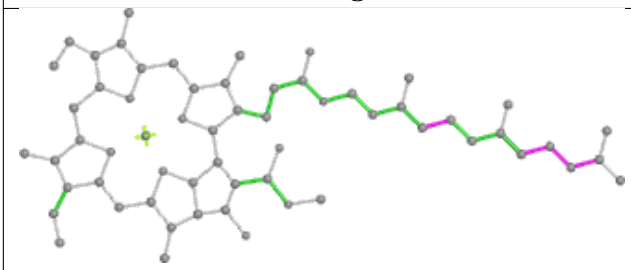


Bond angles



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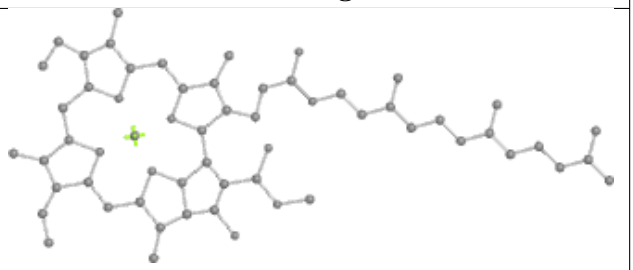
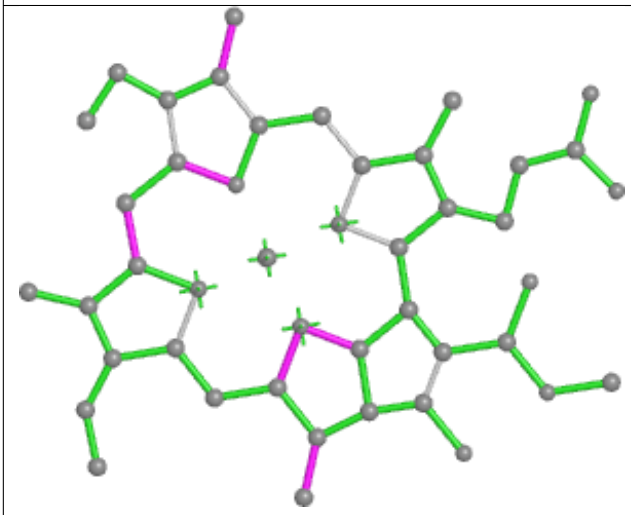


Rings

Ligand CLA c 516



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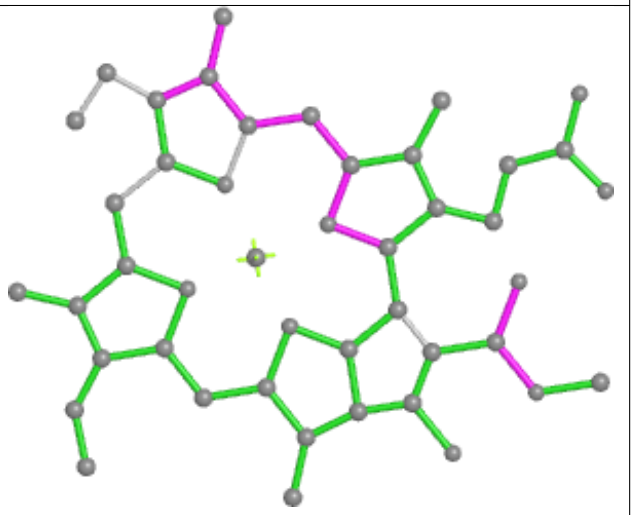
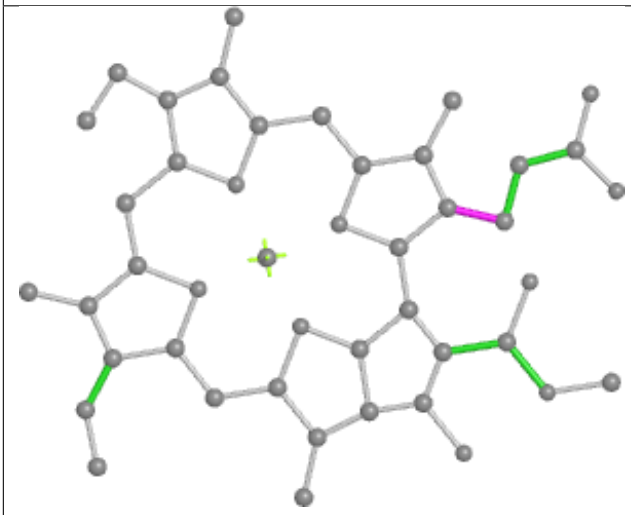


Bond angles



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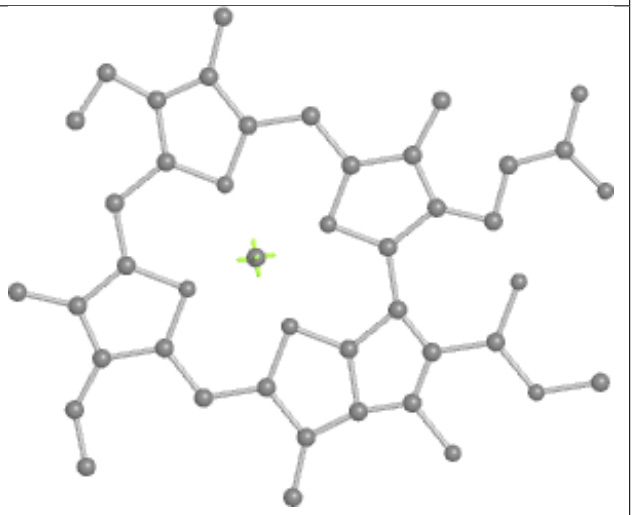
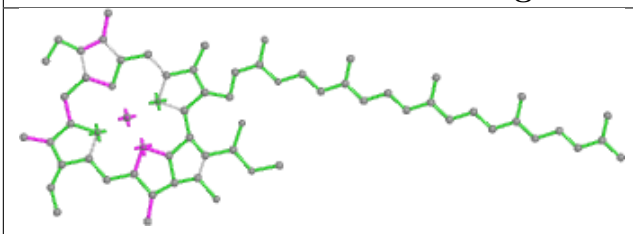


Rings

Ligand CLA A 1119



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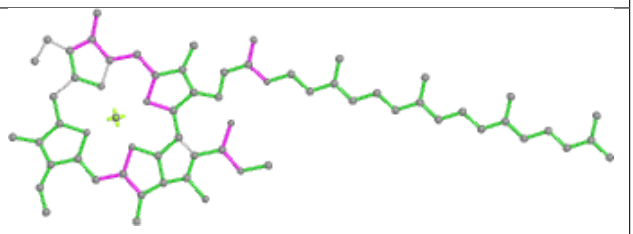

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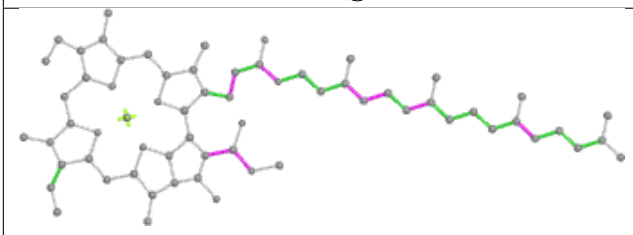

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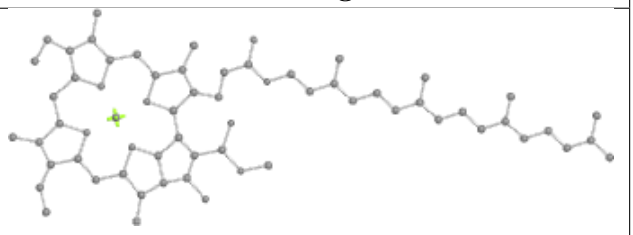
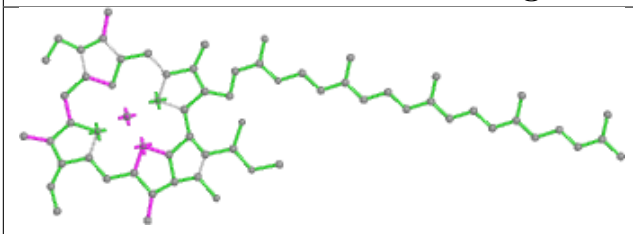


Rings

Ligand CLA f 1203



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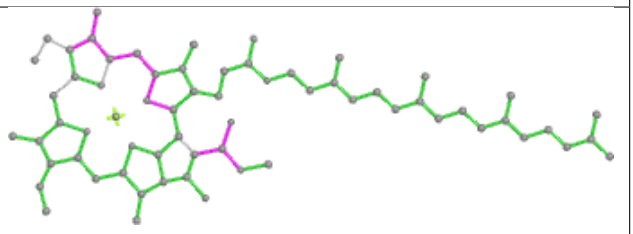
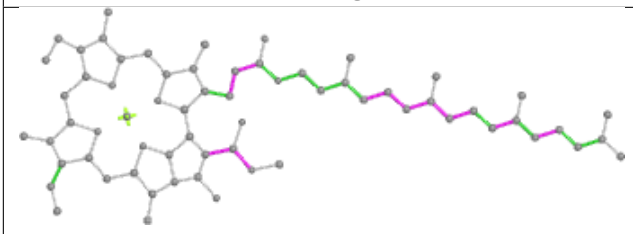


Bond angles



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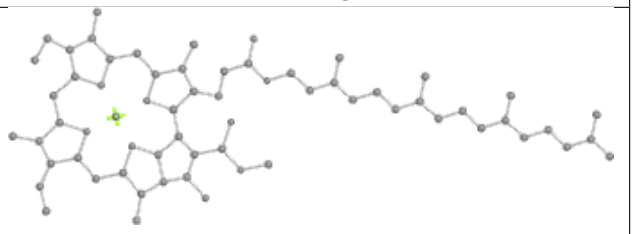
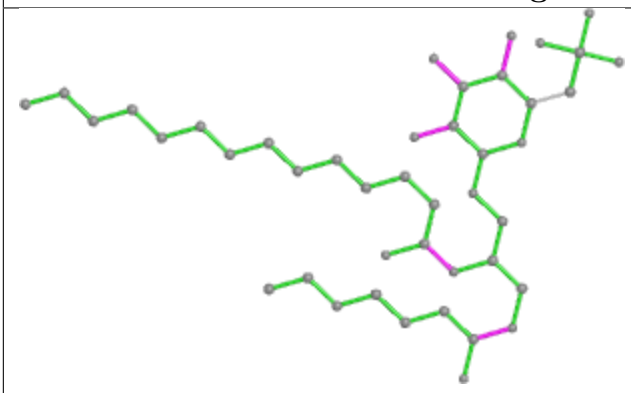


Rings

Ligand SQD r 822



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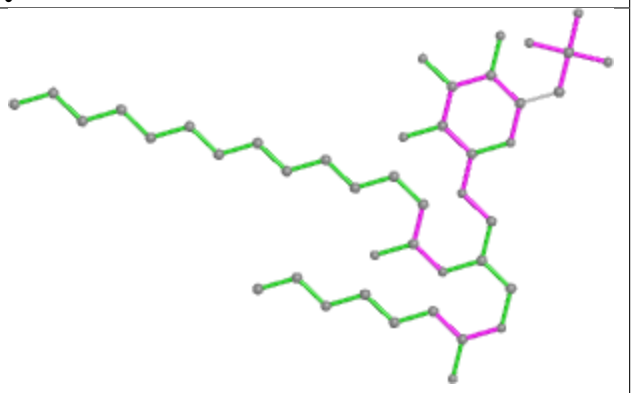
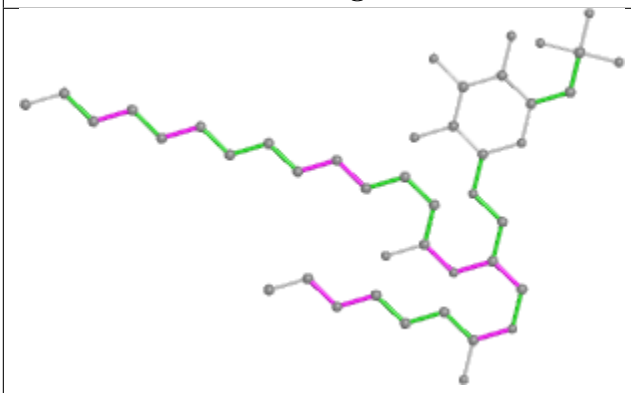


Bond angles



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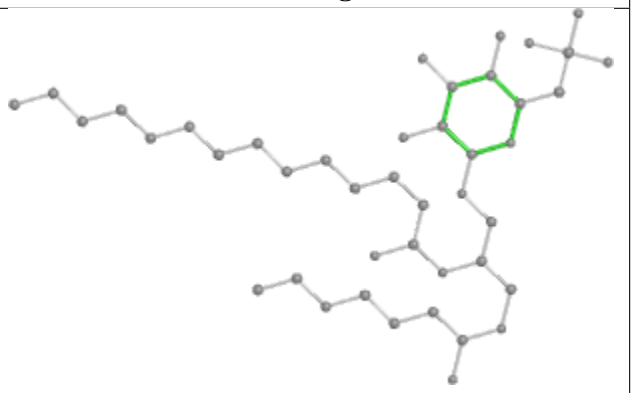
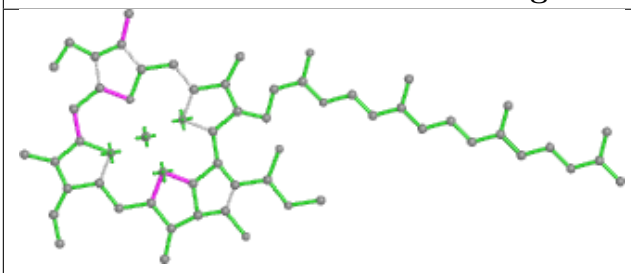


Rings

Ligand CLA t 501



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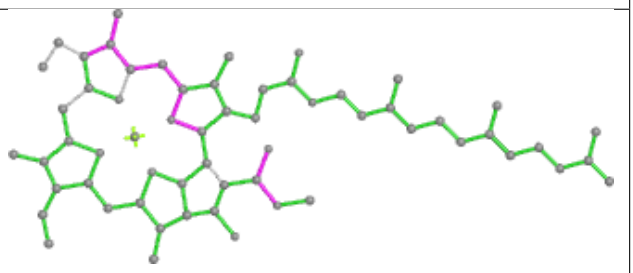
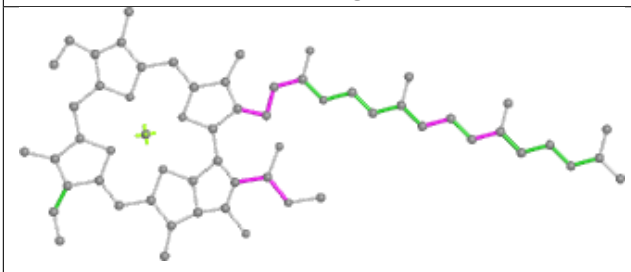


Bond angles



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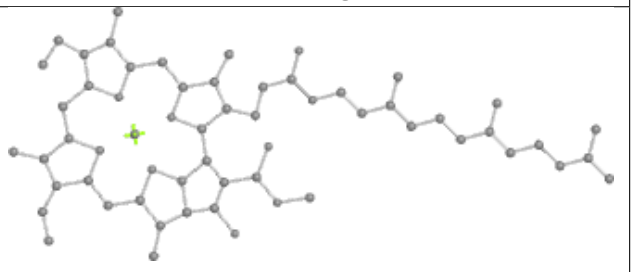
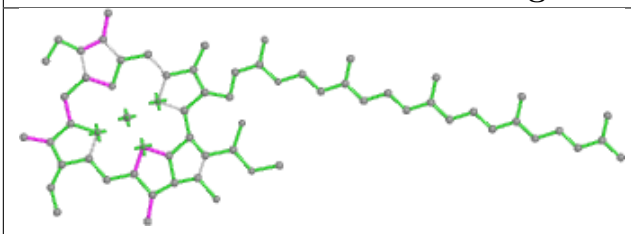


Rings

Ligand CLA 2 513



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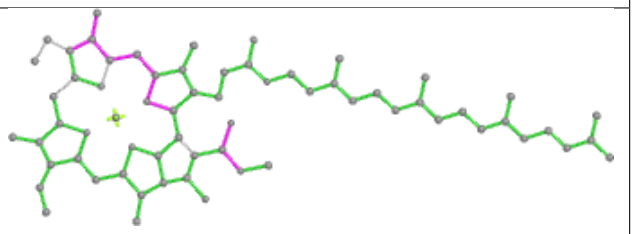
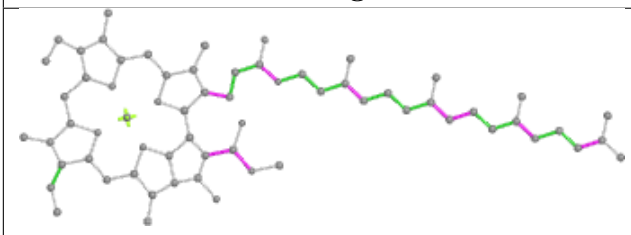


Bond angles



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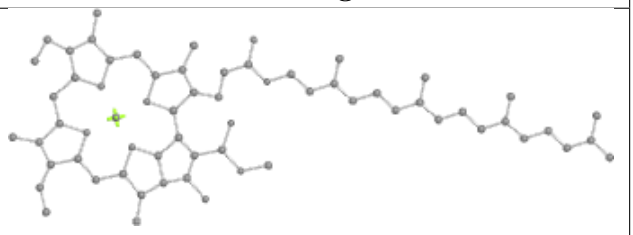
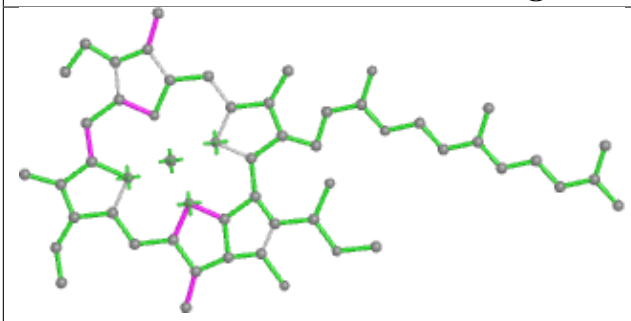


Rings

Ligand CLA u 503



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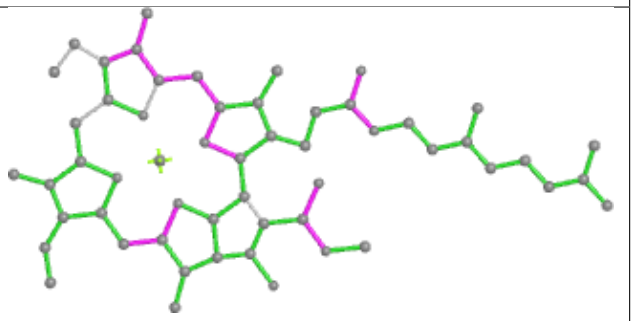
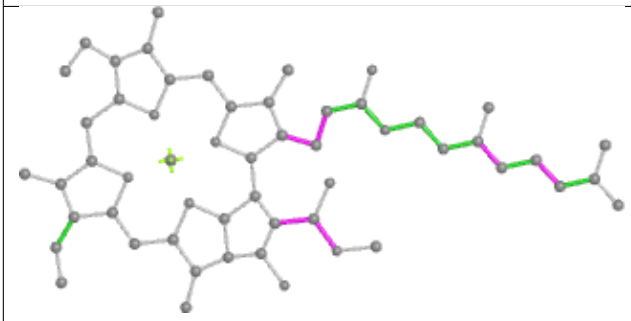


Bond angles



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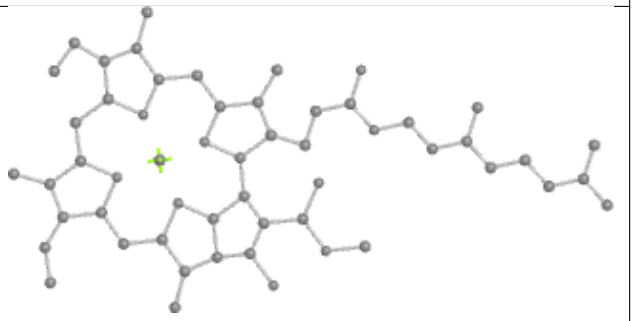
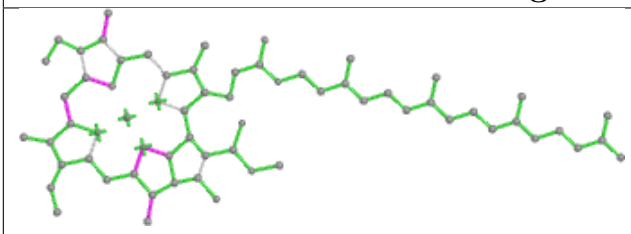


Rings

Ligand CLA s 510



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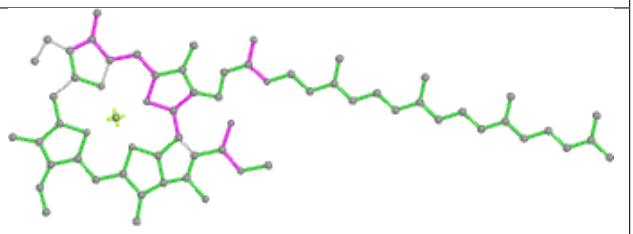
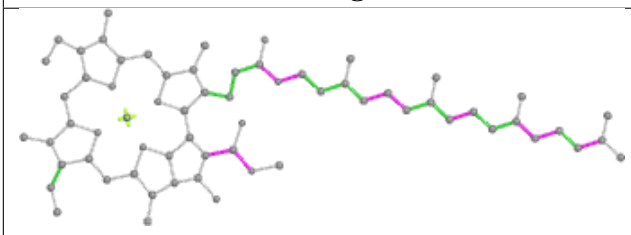
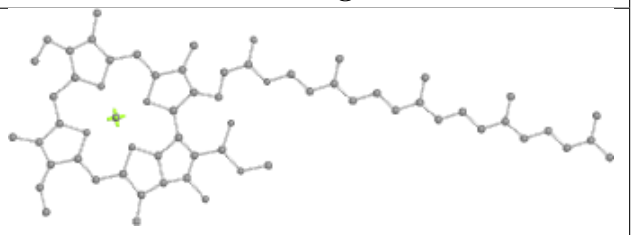


Bond angles

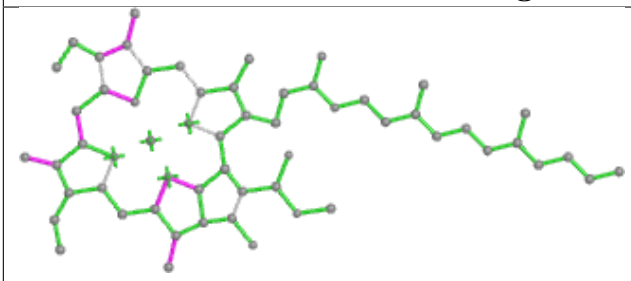


Torsions



Rings

Ligand CLA T 1302



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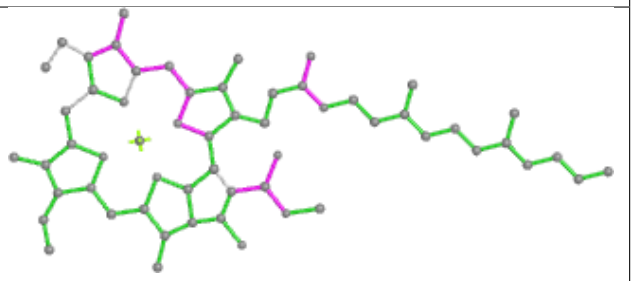
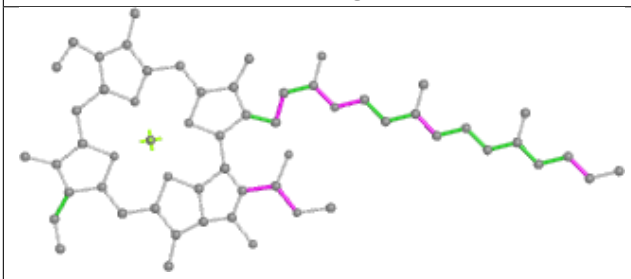


Bond angles



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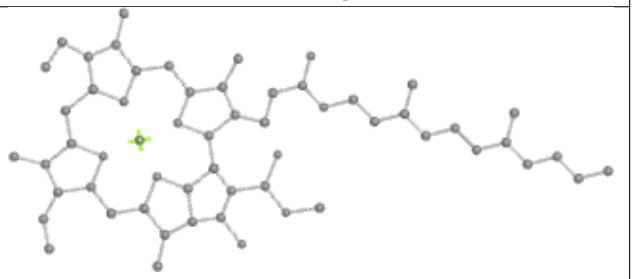
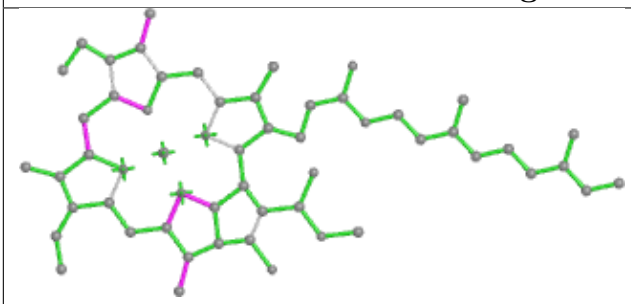
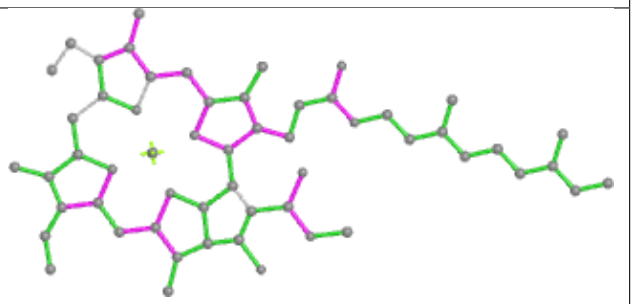


Rings

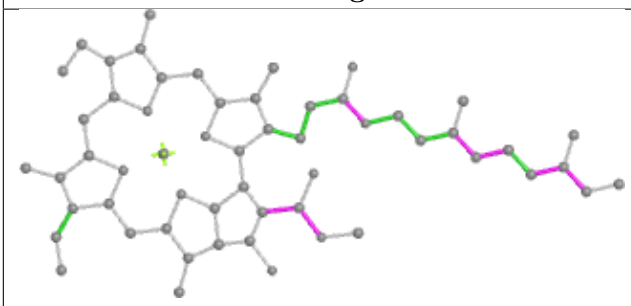
Ligand CLA e 1124



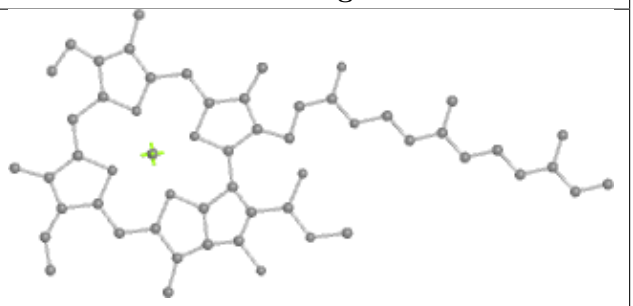
Bond lengths



Bond angles

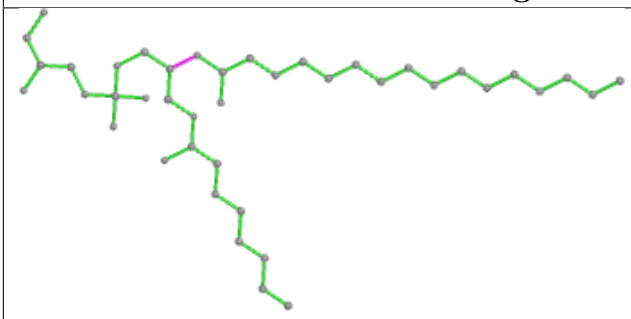


Torsions

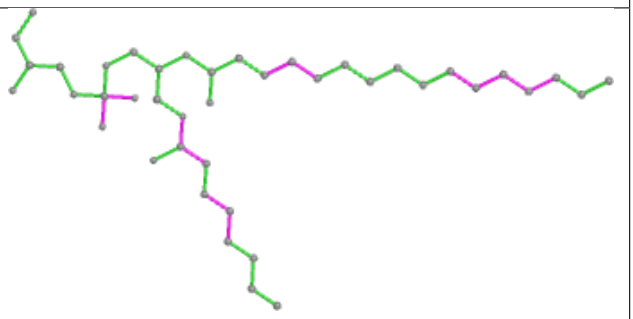


Rings

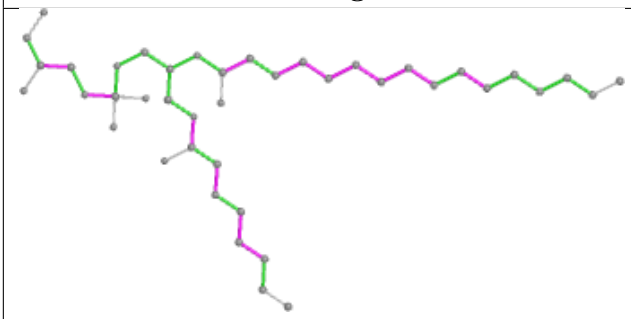
Ligand LHG A 5003



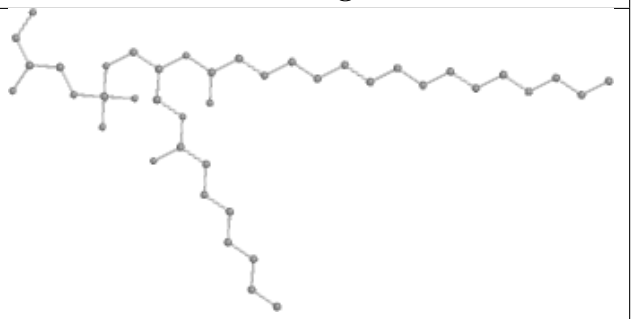
Bond lengths



Bond angles

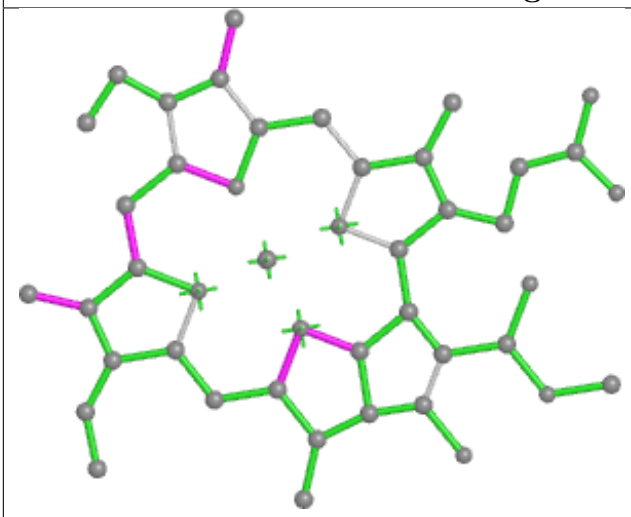


Torsions



Rings

Ligand CLA Y 506



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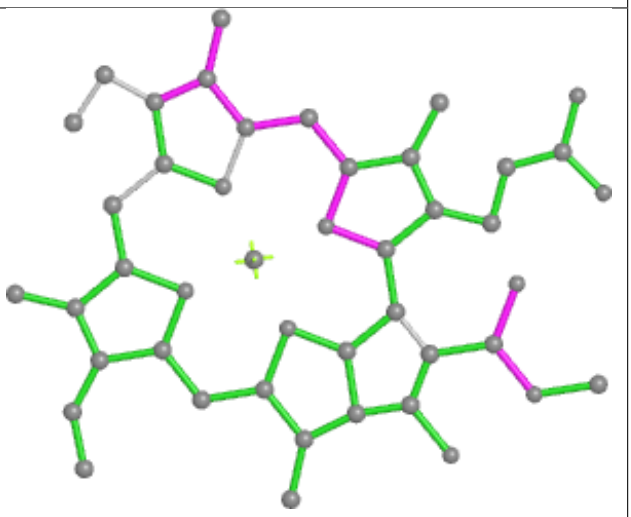
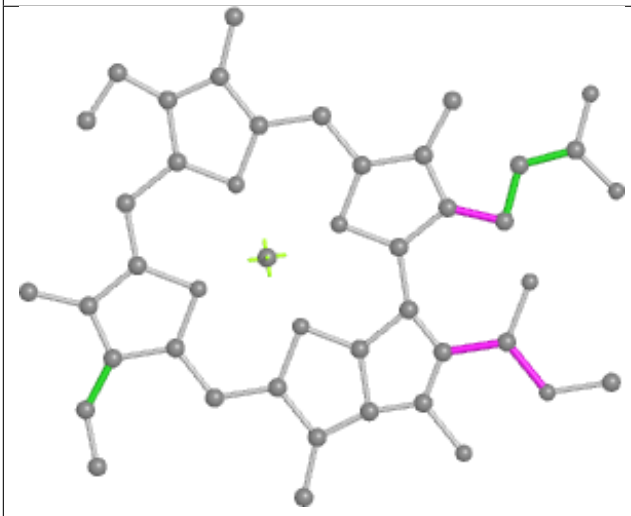
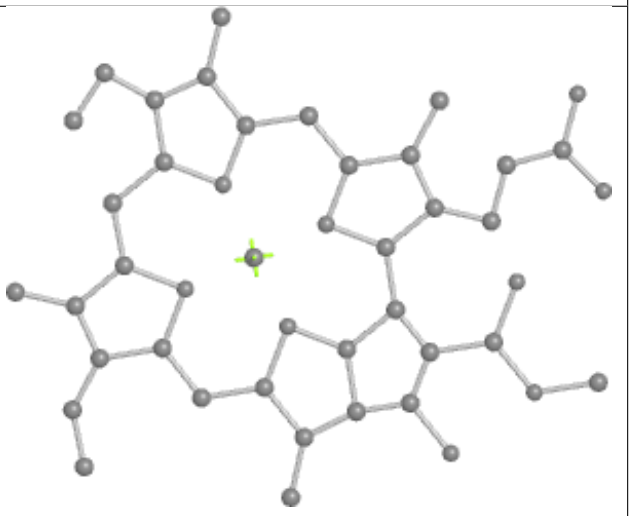


Bond angles

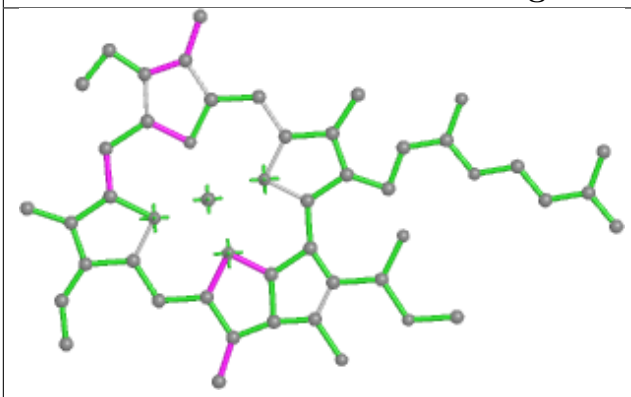


Torsions

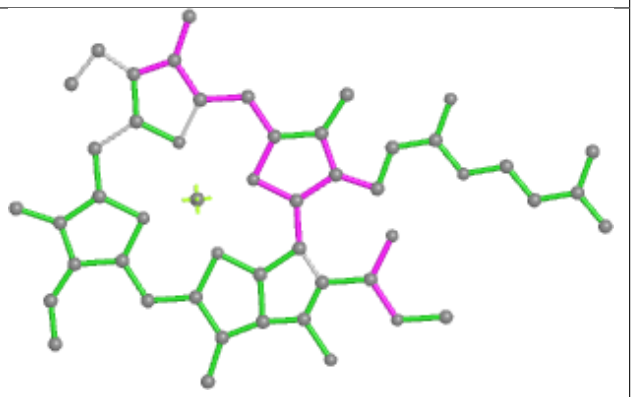


Rings

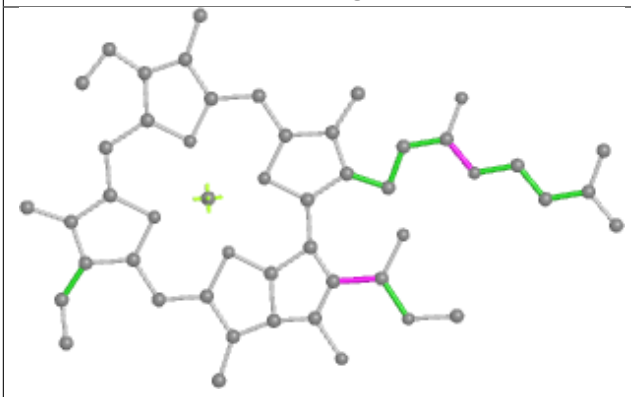
Ligand CLA 3 502



Bond lengths



Bond angles



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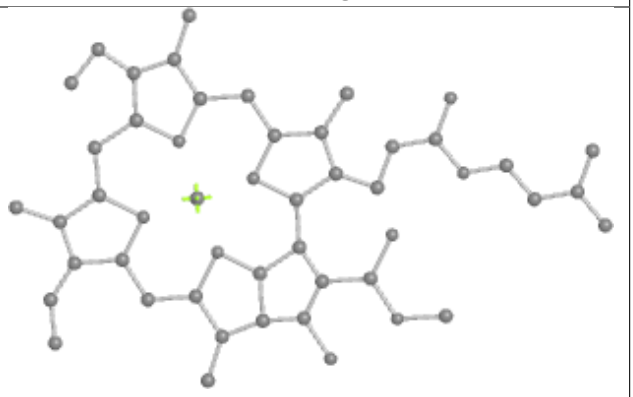
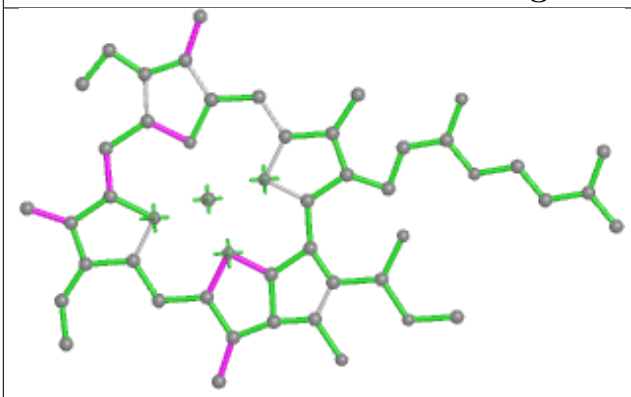


Rings

Ligand CLA s 506



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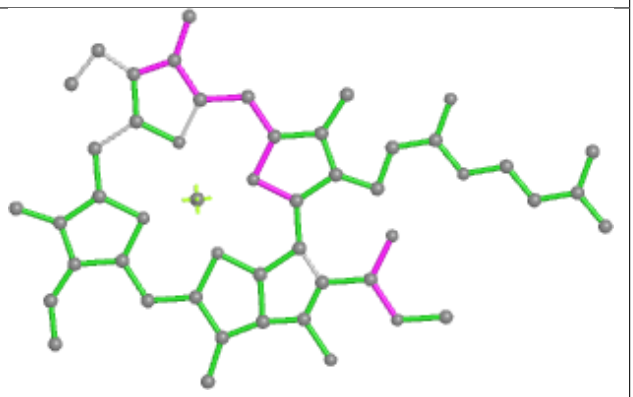
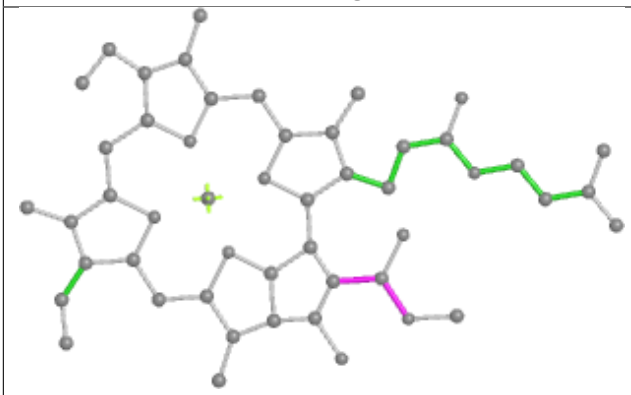


Bond angles



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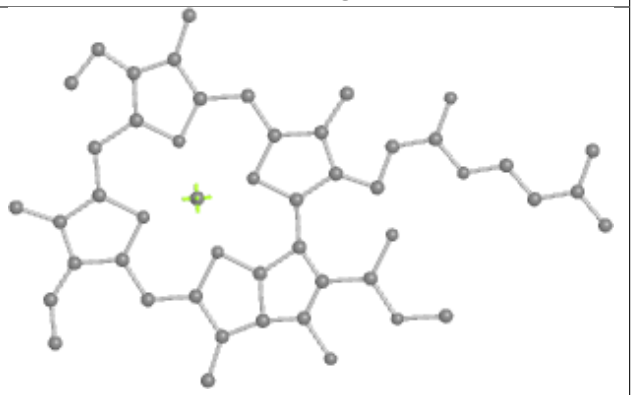
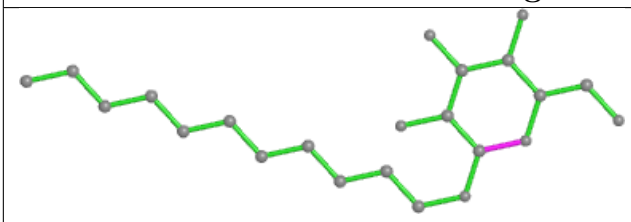


Rings

Ligand LMU 2 901



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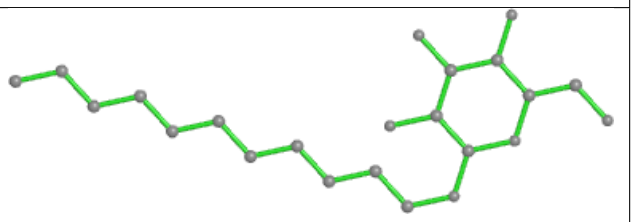
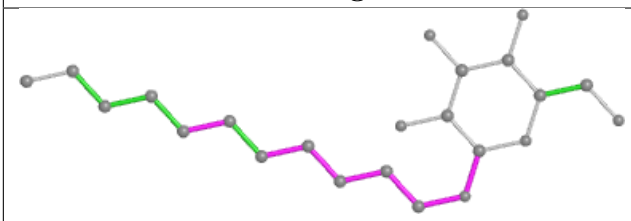


Bond angles



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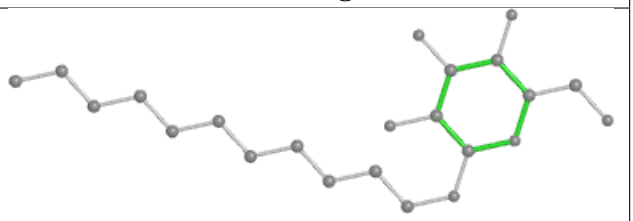
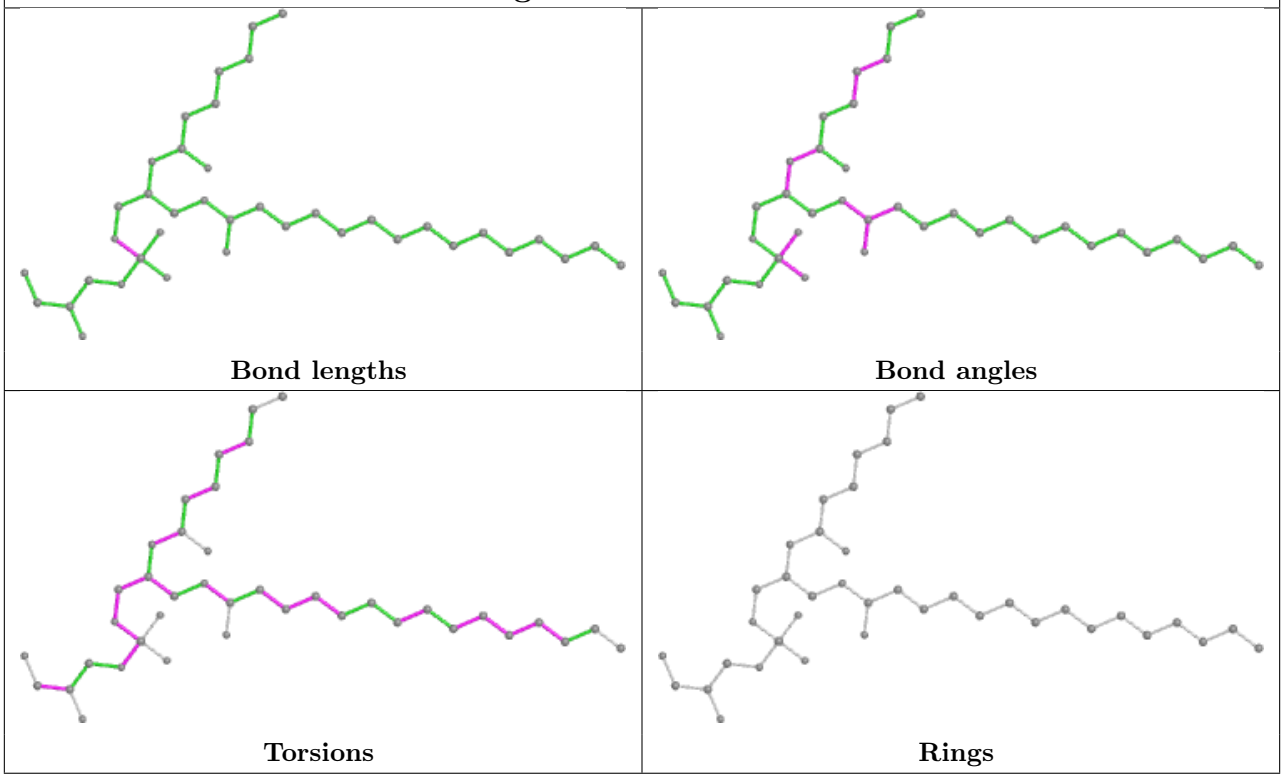
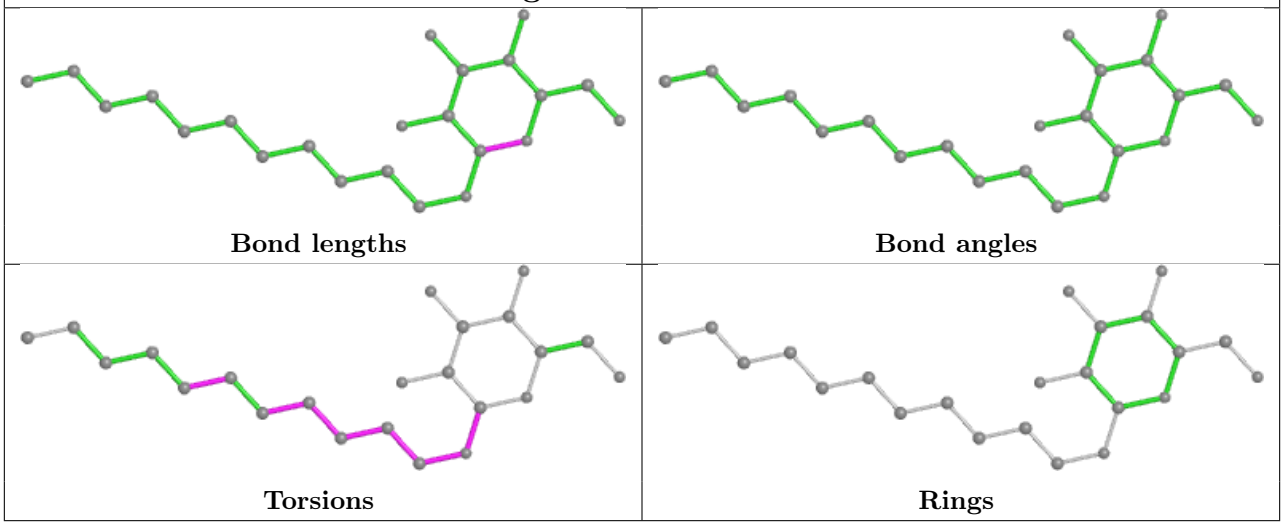


Rings

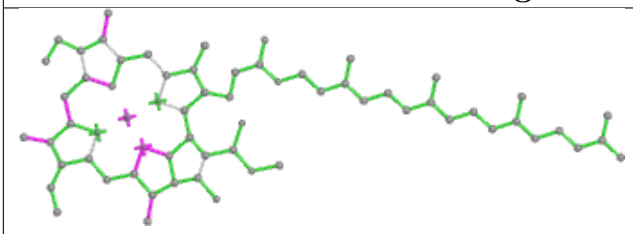
Ligand LHG A 5002



Ligand LMU Z 901



Ligand CLA H 1234



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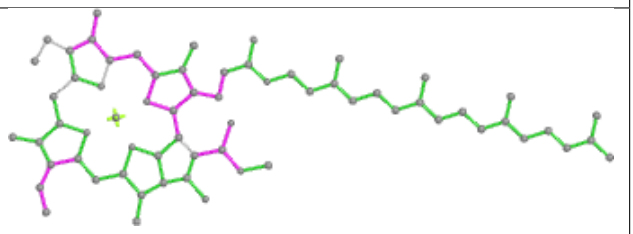
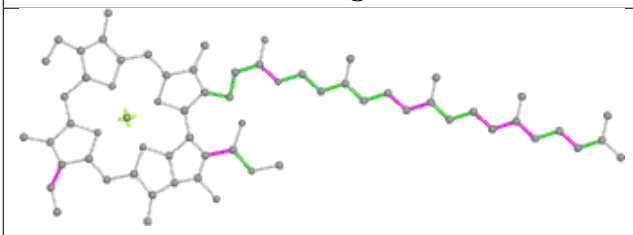


Bond angles



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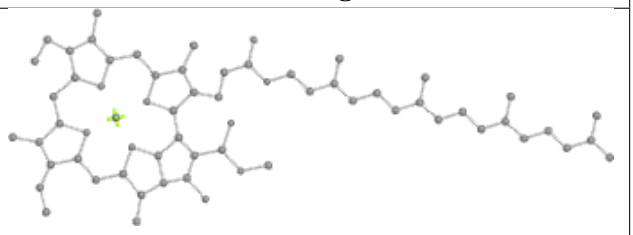
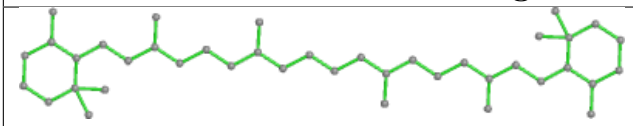


Rings

Ligand BCR H 4009



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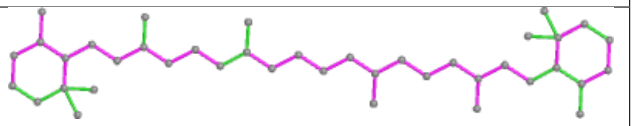
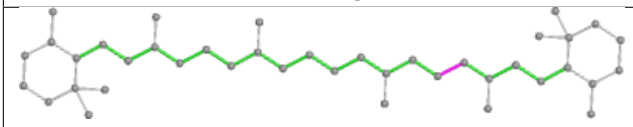


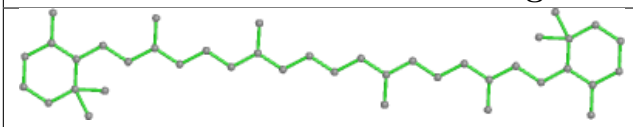
Bond angles



Torsions

Rings

Ligand BCR v 523



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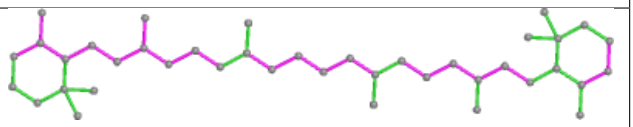
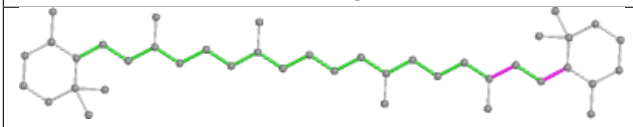


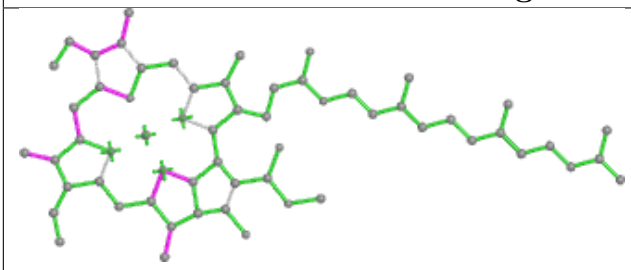
Bond angles



Torsions

Rings

Ligand CLA B 1230



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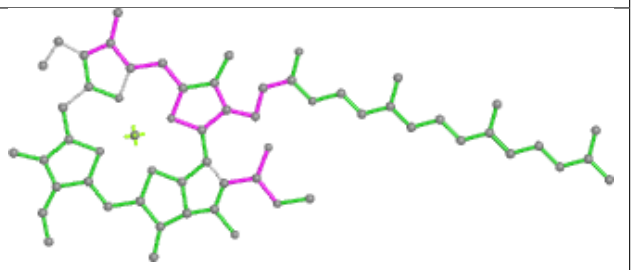
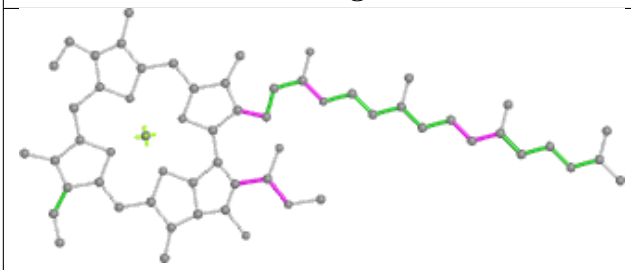
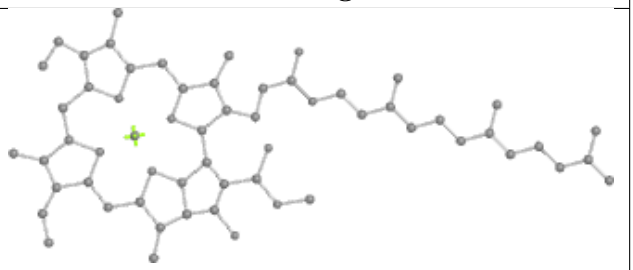


Bond angles

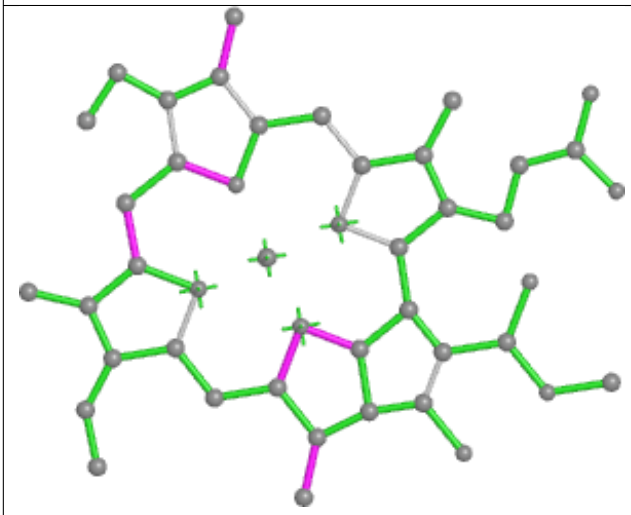


Torsions



Rings

Ligand CLA s 516



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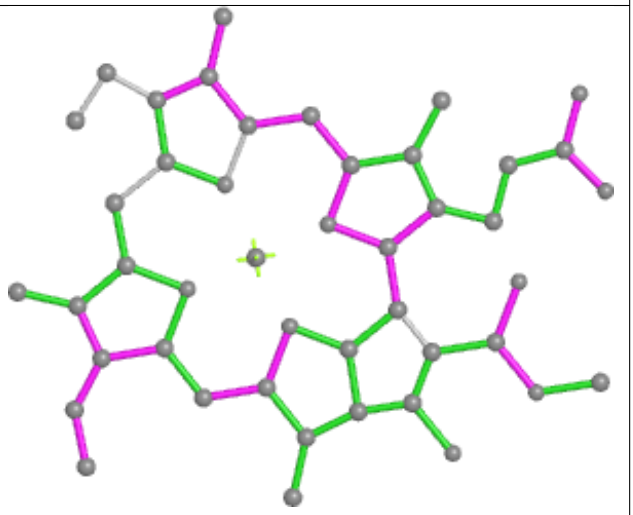
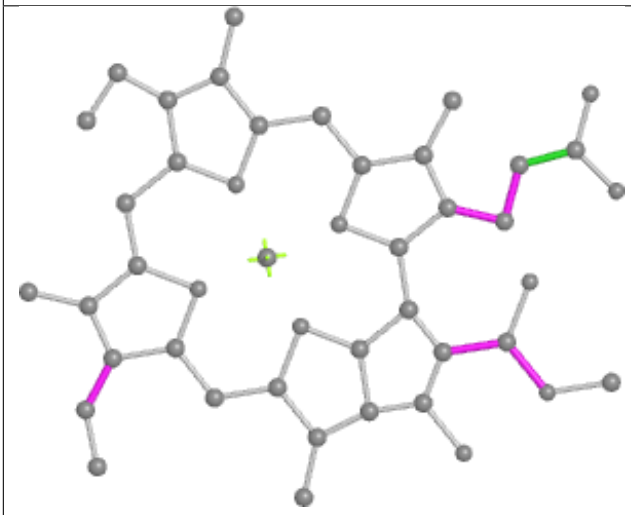


Bond angles



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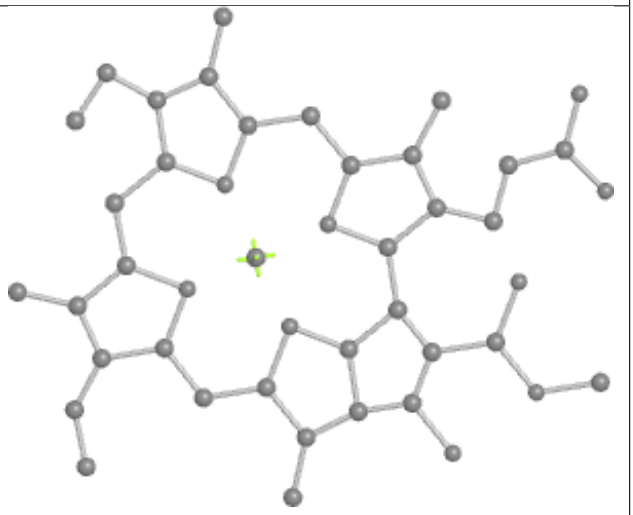
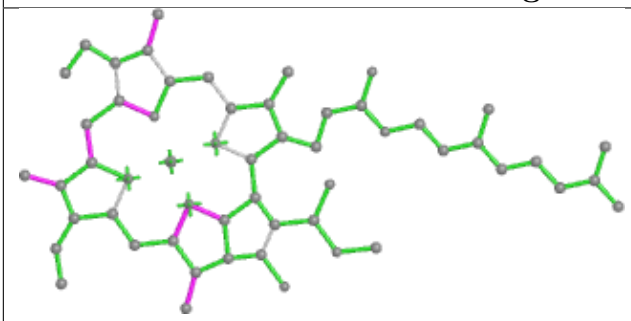


Rings

Ligand CLA f 1228



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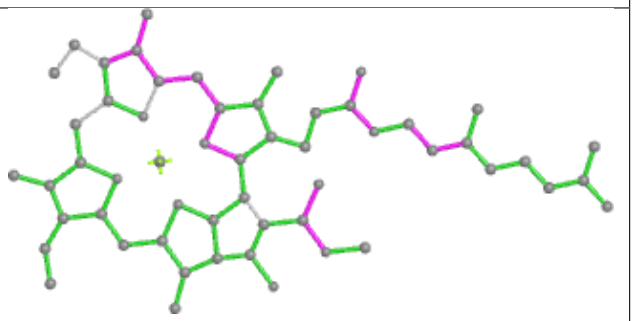
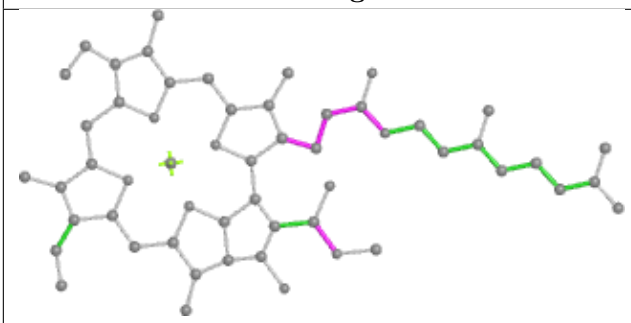


Bond angles



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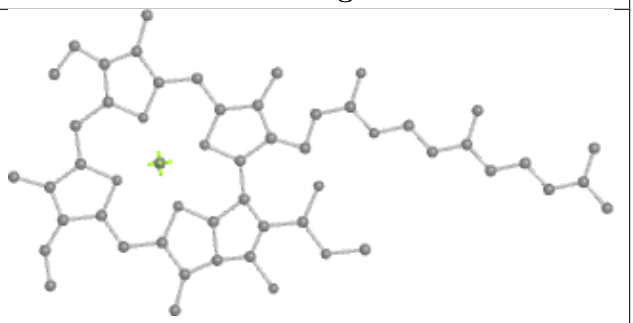
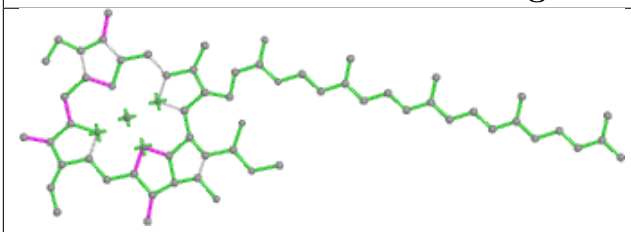


Rings

Ligand CLA 1 501



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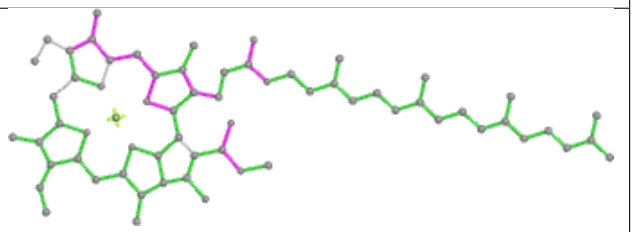
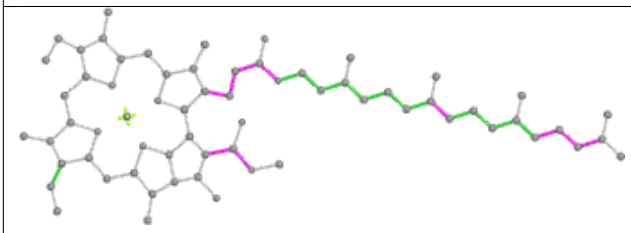


Bond angles



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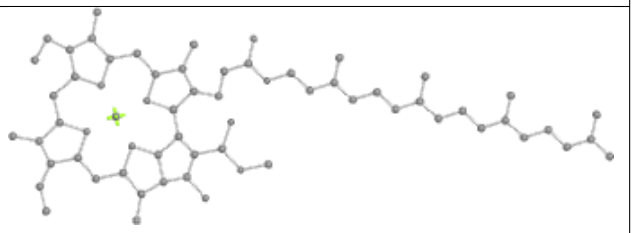
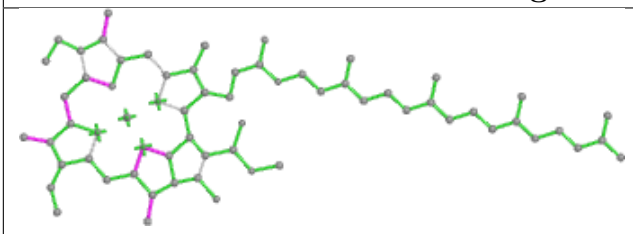


Rings

Ligand CLA r 509



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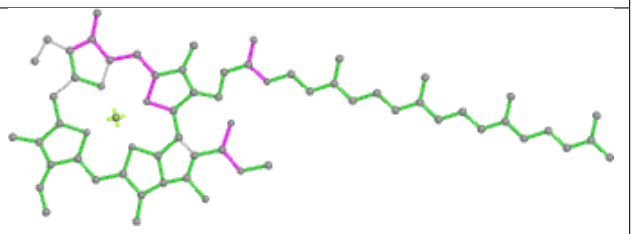
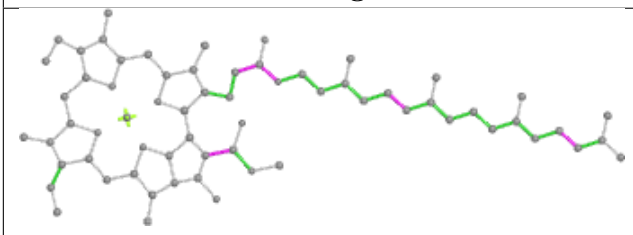


Bond angles



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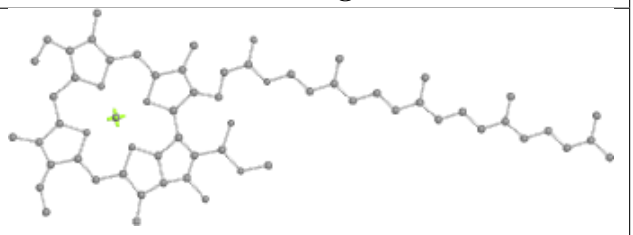
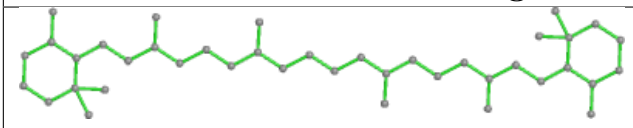


Rings

Ligand BCR W 4021



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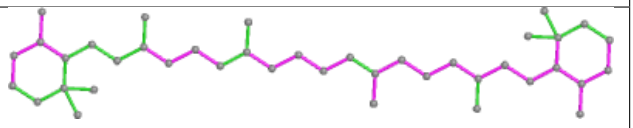
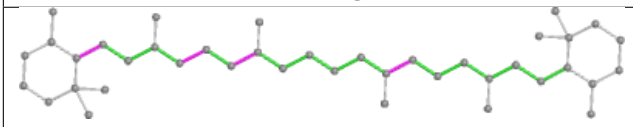


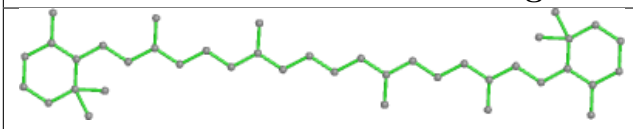
Bond angles



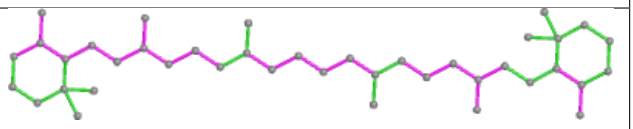
Torsions

Rings

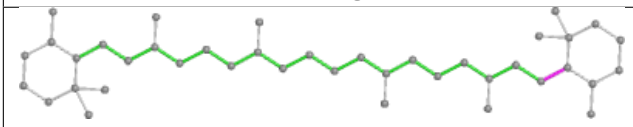
Ligand BCR u 524



Bond lengths



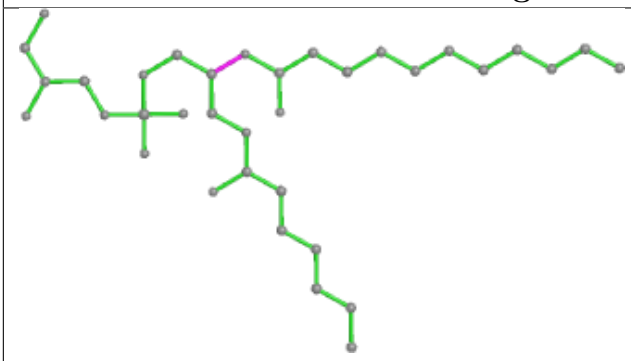
Bond angles



Torsions

Rings

Ligand LHG A 5008



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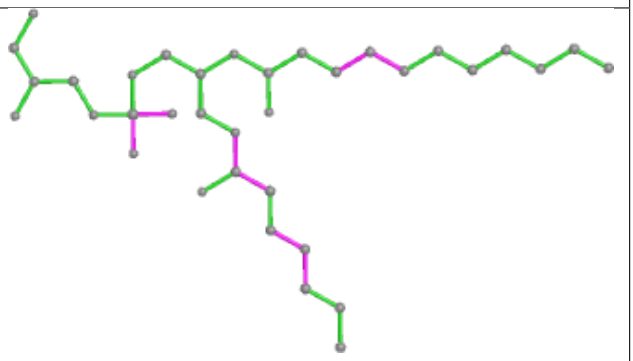
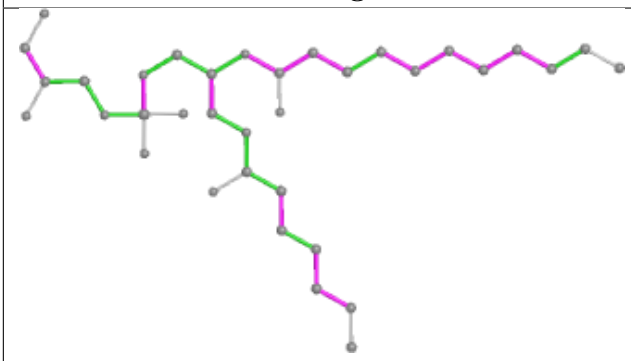
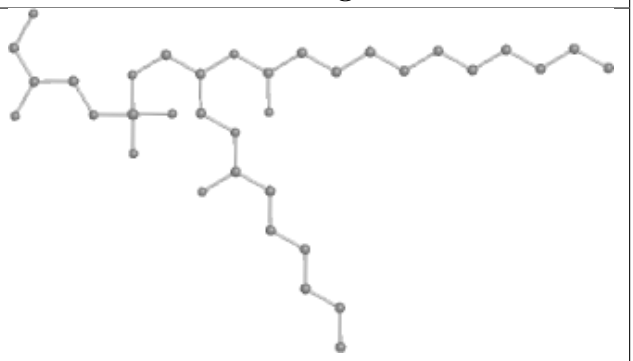


Bond angles

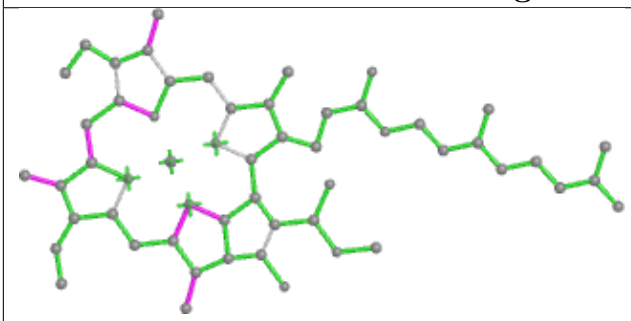


Torsions



Rings

Ligand CLA G 1105



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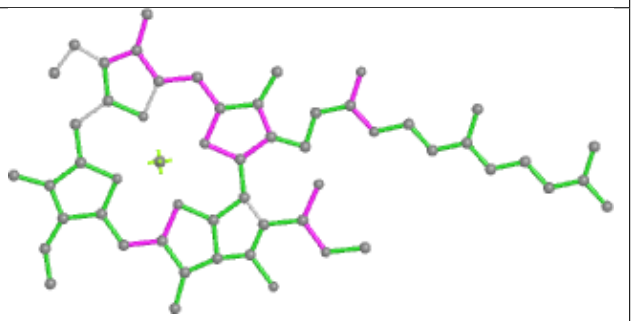
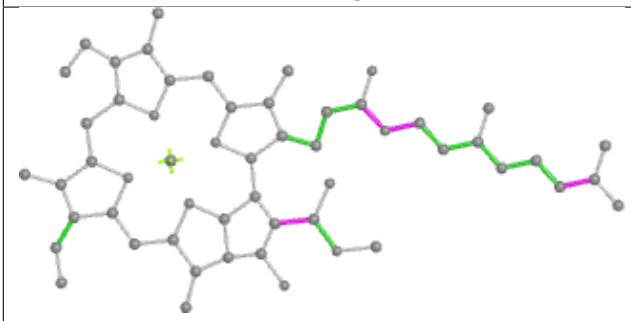
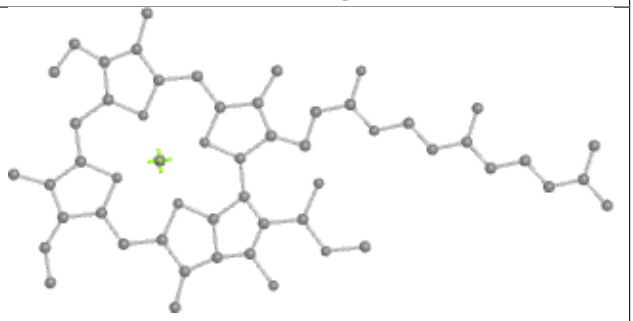


Bond angles

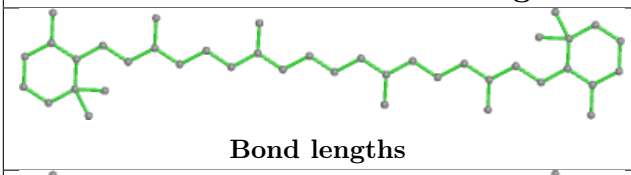


Torsions



Rings

Ligand BCR A 4007



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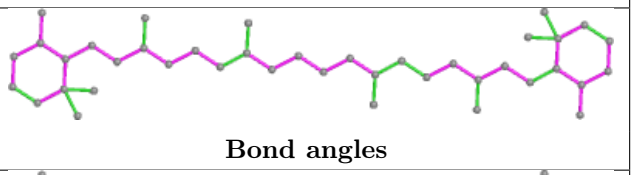
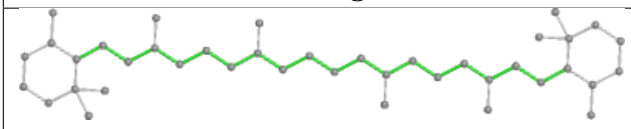


Bond angles



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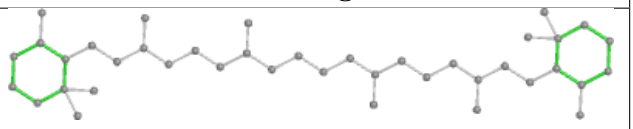
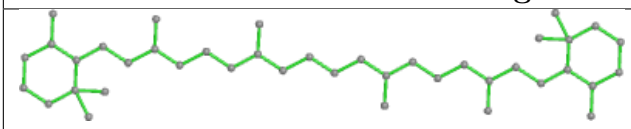


Rings

Ligand BCR B 4009



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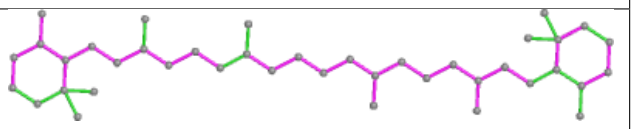
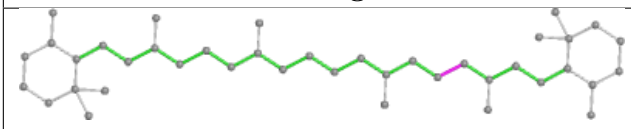


Bond angles



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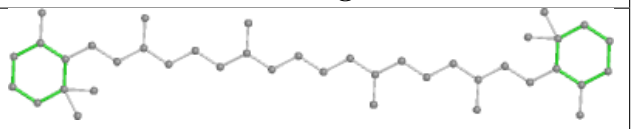
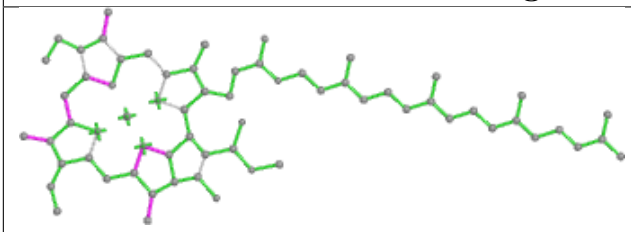
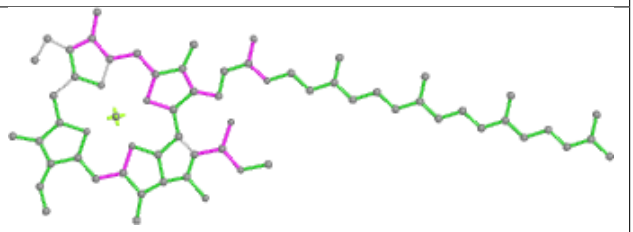


Rings

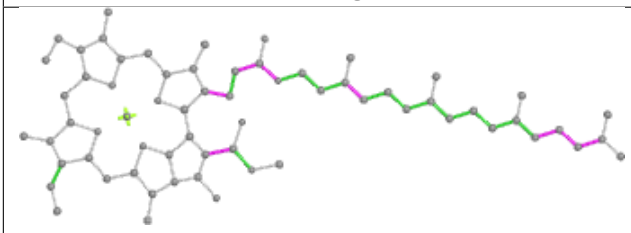
Ligand CLA f 1202



Bond lengths



Bond angles



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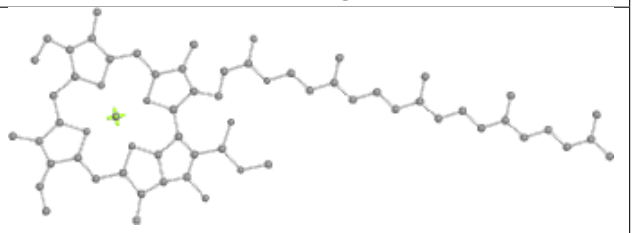
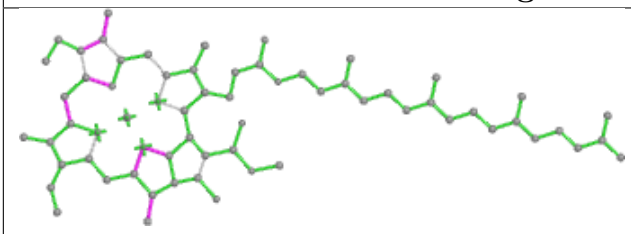
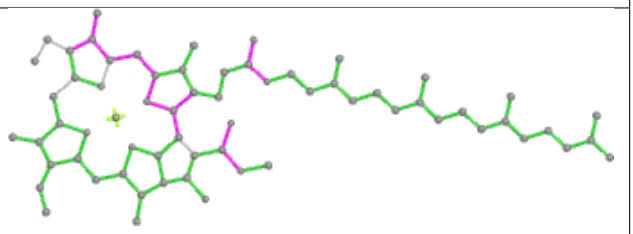
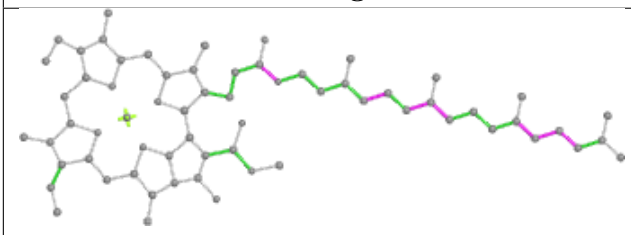
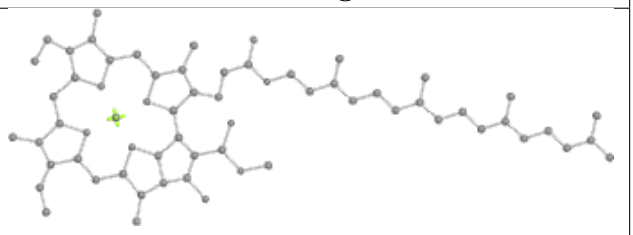
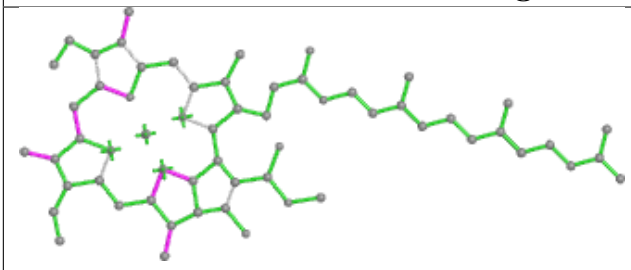
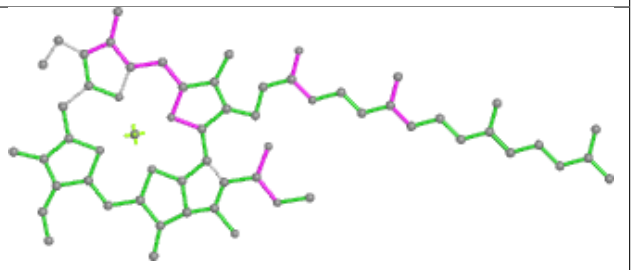
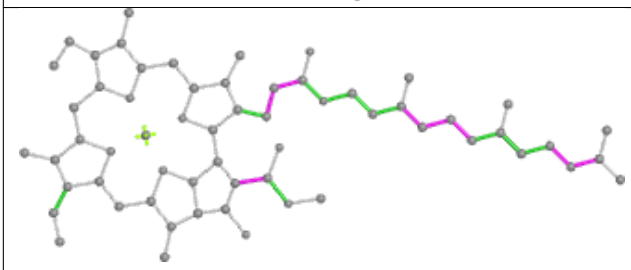
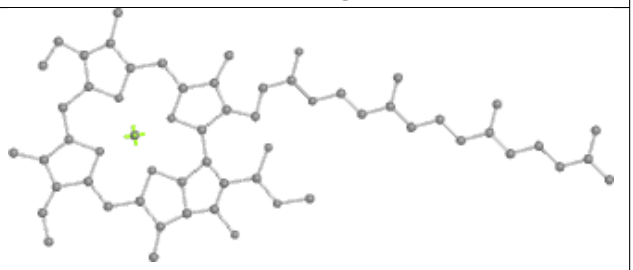
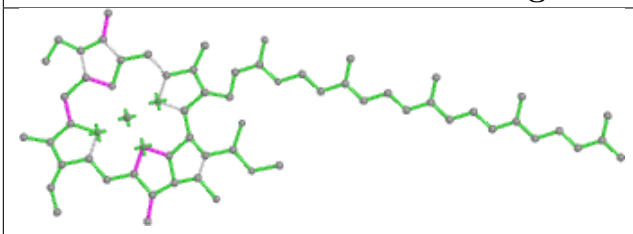


Rings

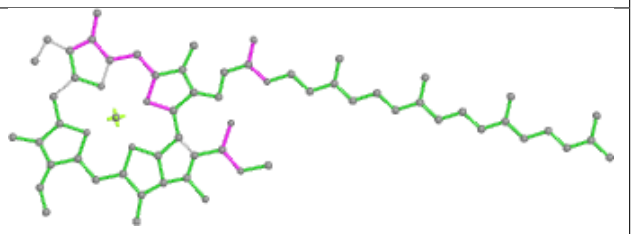
Ligand CLA F 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1115	
 Bond lengths	 Bond angles
 Torsions	 Rings

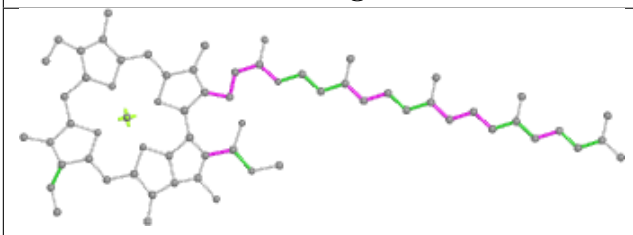
Ligand CLA 2 518



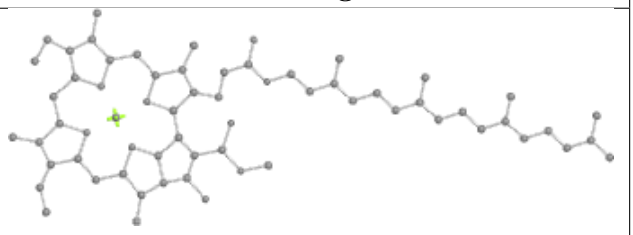
Bond lengths



Bond angles

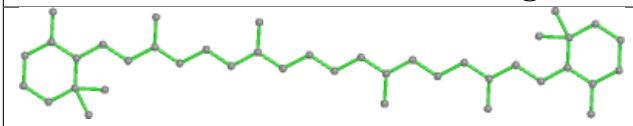


Torsions

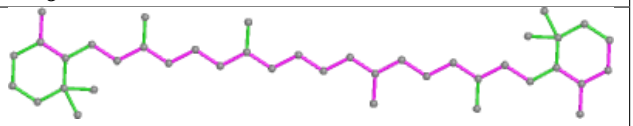


Rings

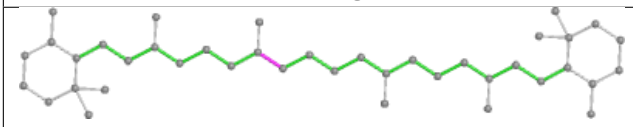
Ligand BCR j 4016



Bond lengths



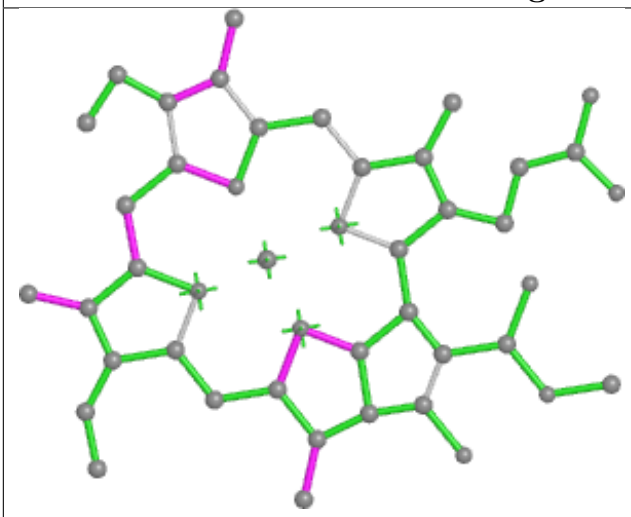
Bond angles



Torsions

Rings

Ligand CLA 5 513



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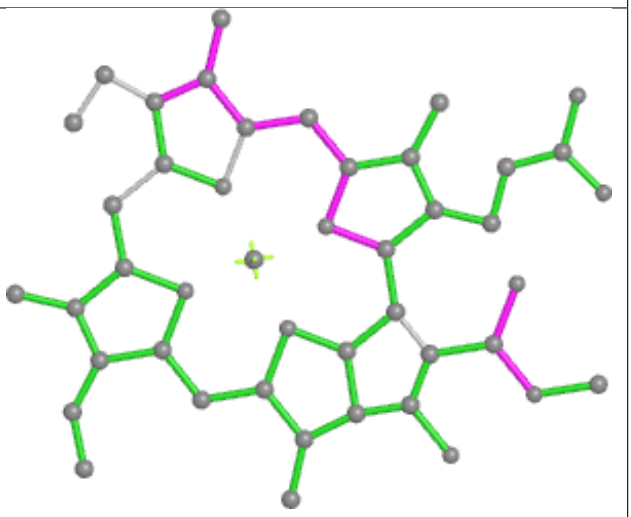

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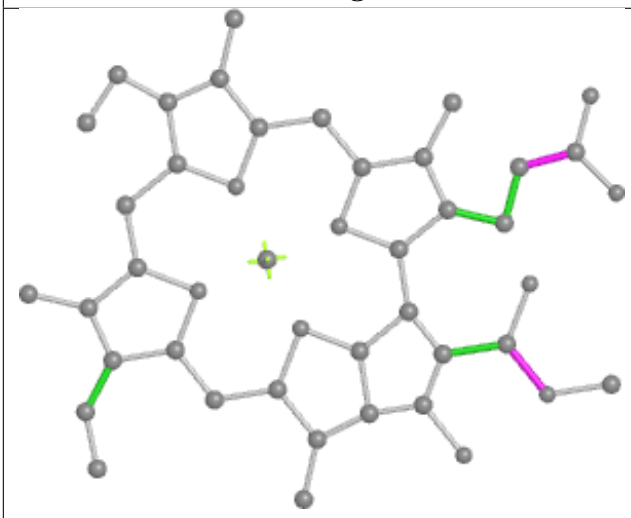
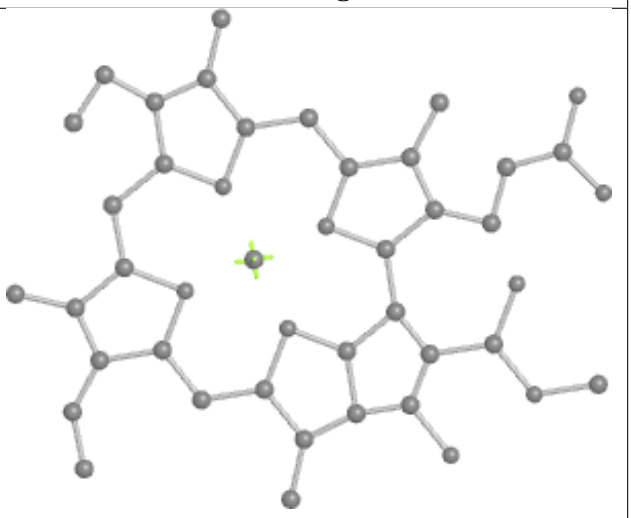
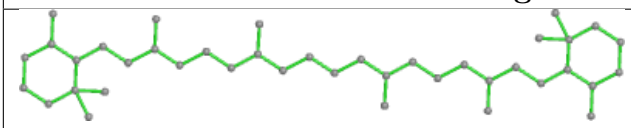


Torsions



Rings

Ligand BCR T 4013



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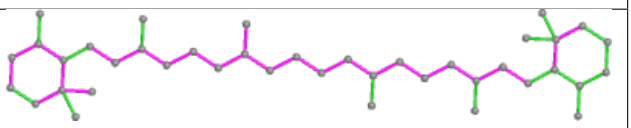
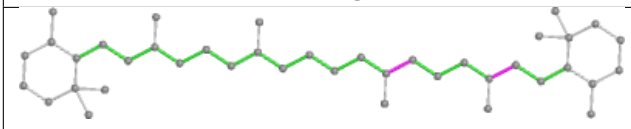


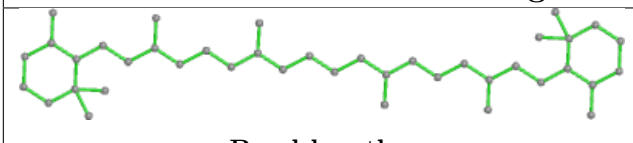
Bond angles



Torsions

Rings

Ligand BCR r 523



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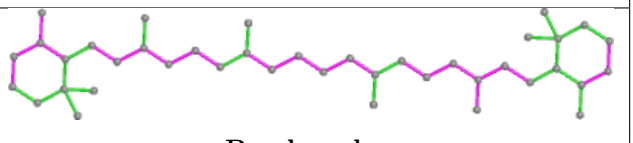
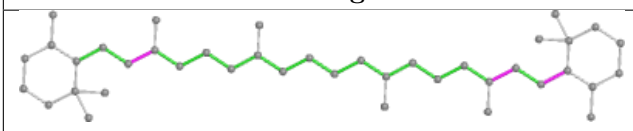
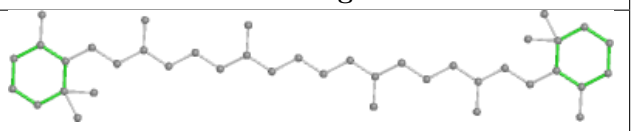


Bond angles

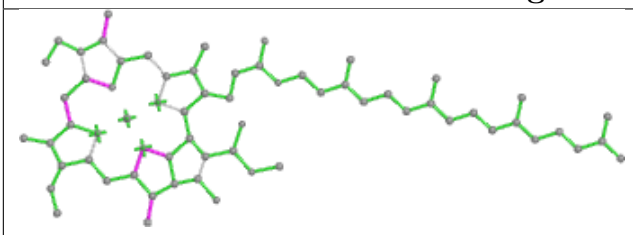


Torsions



Rings

Ligand CLA b 509



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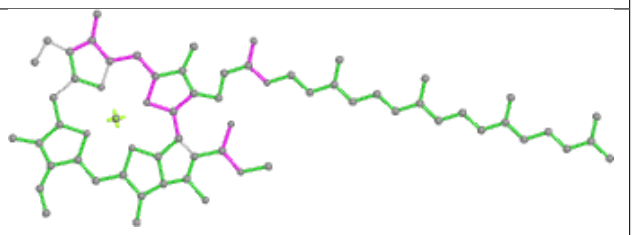
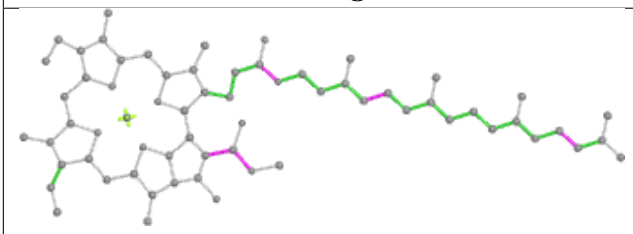
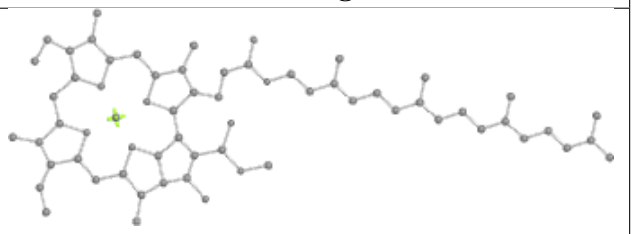


Bond angles

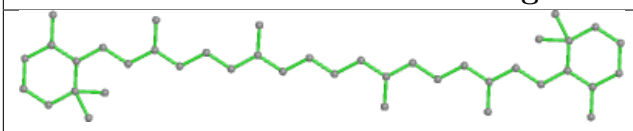


Torsions

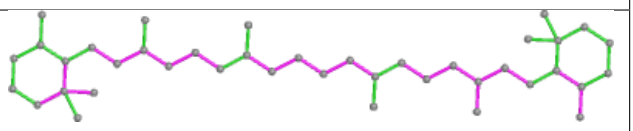


Rings

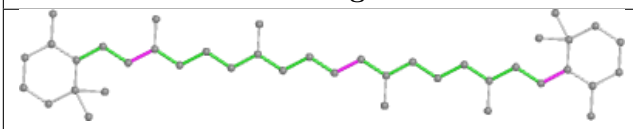
Ligand BCR l 4015



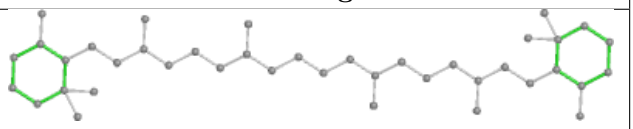
Bond lengths



Bond angles

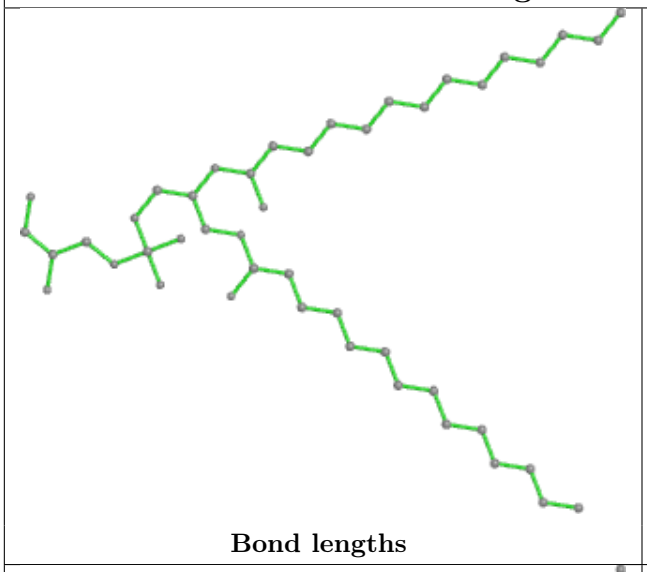


Torsions

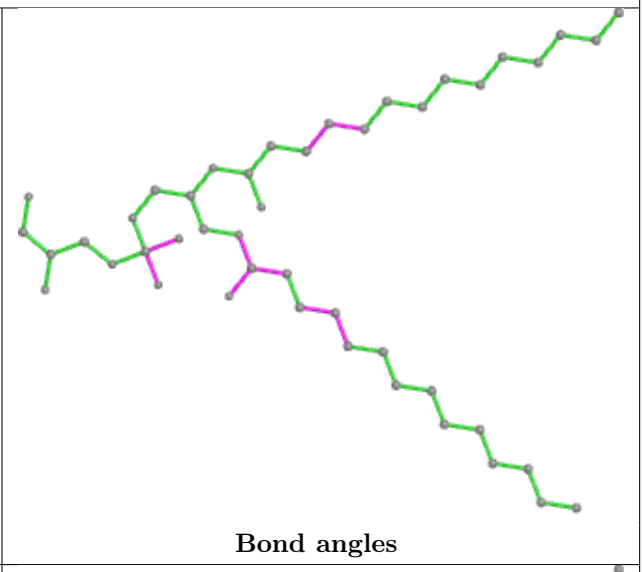


Rings

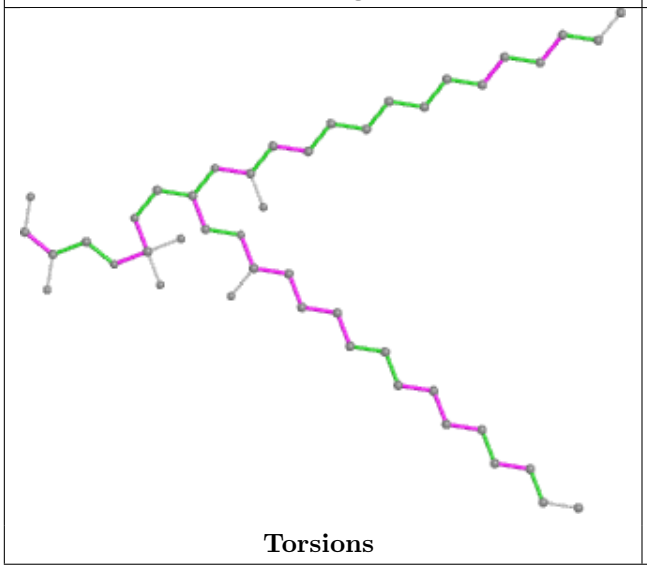
Ligand LHG A 5006



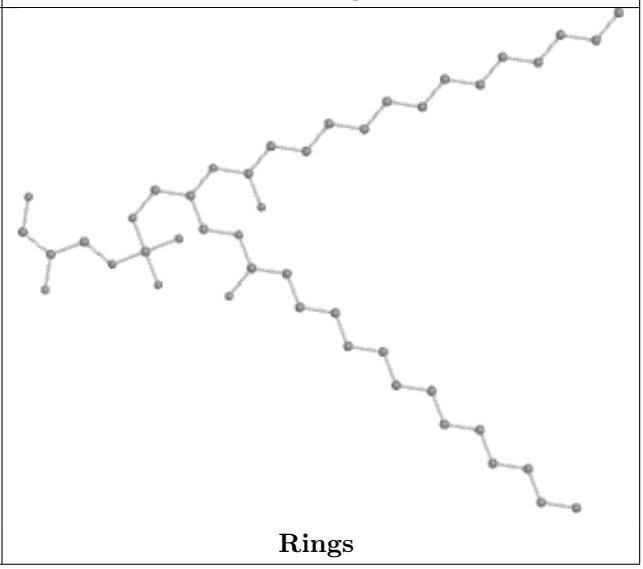
Bond lengths



Bond angles

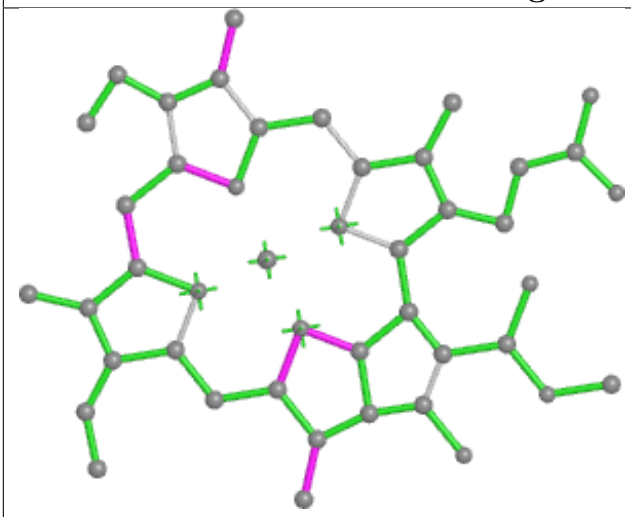


Torsions



Rings

Ligand CLA 4 512



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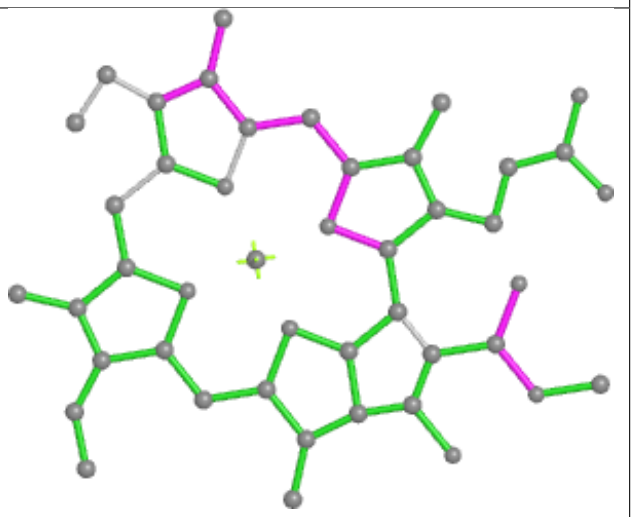
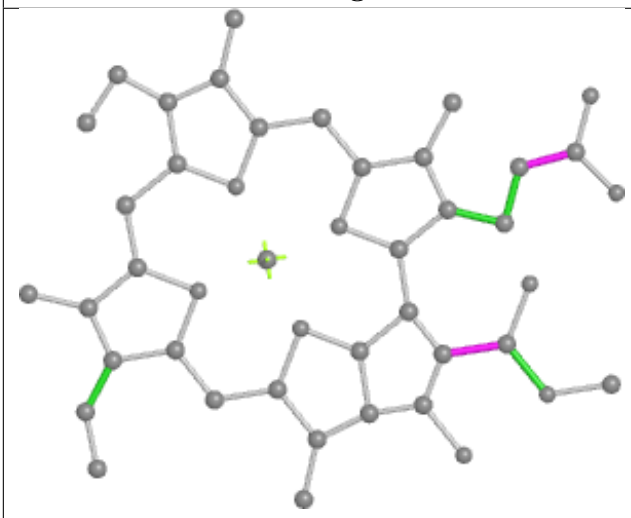


Bond angles



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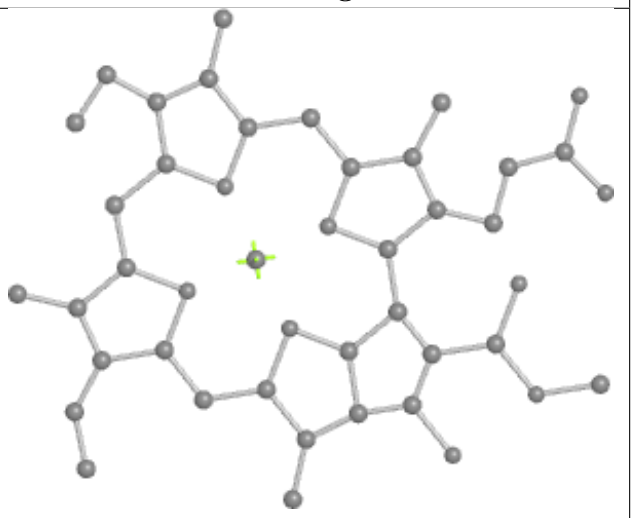
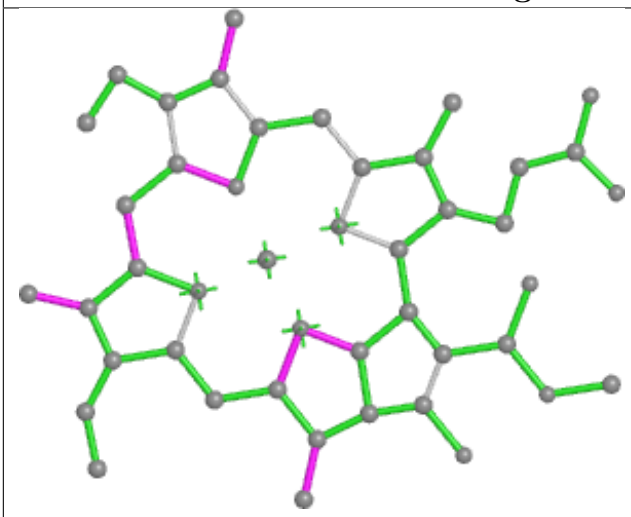


Rings

Ligand CLA G 1113



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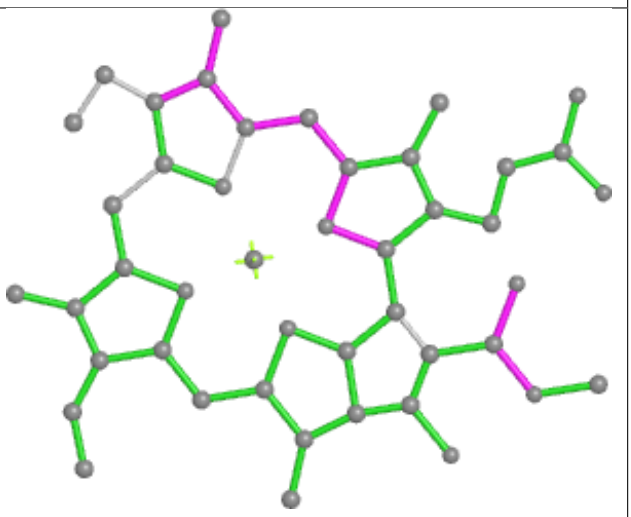

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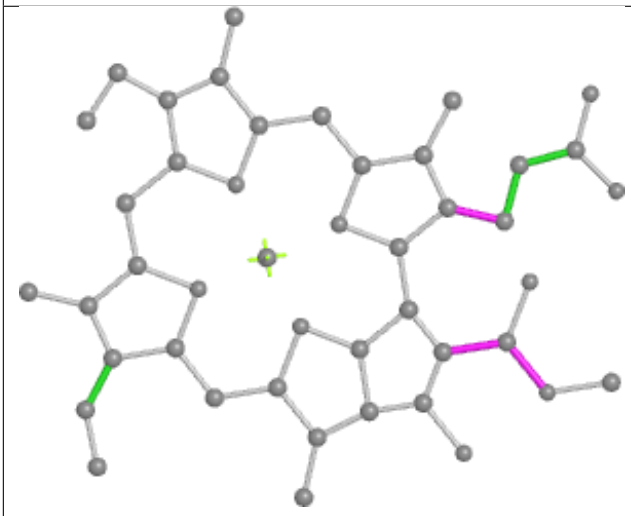

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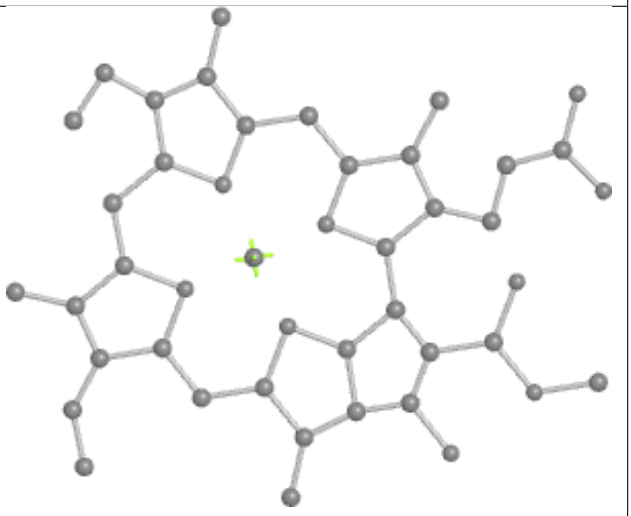
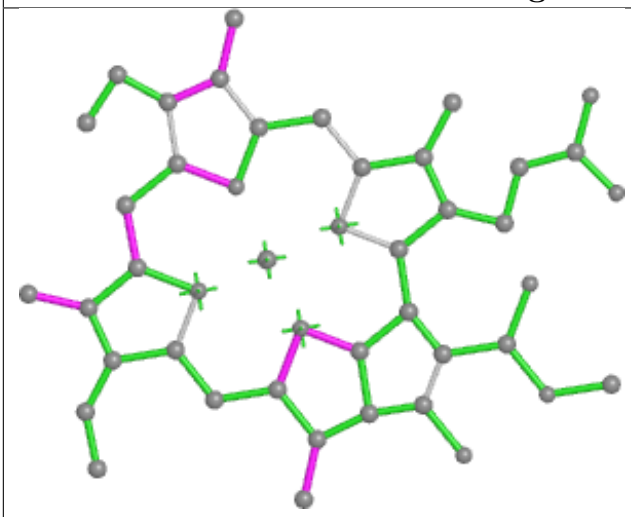


Rings

Ligand CLA 1 504



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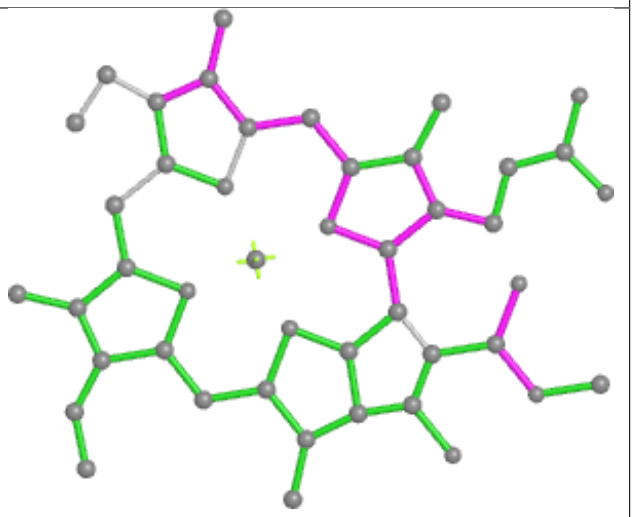
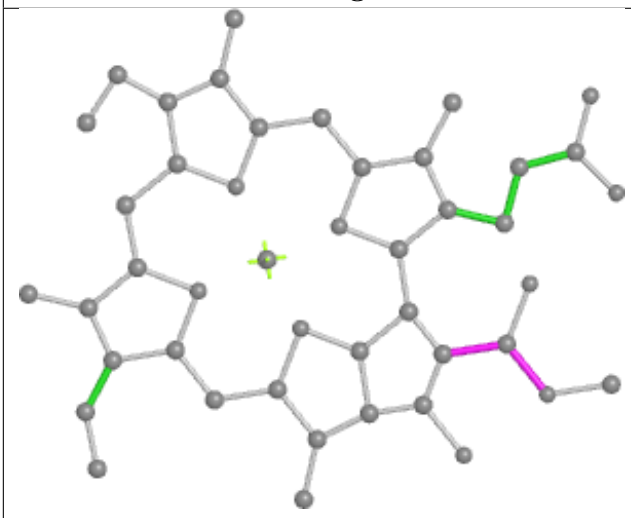
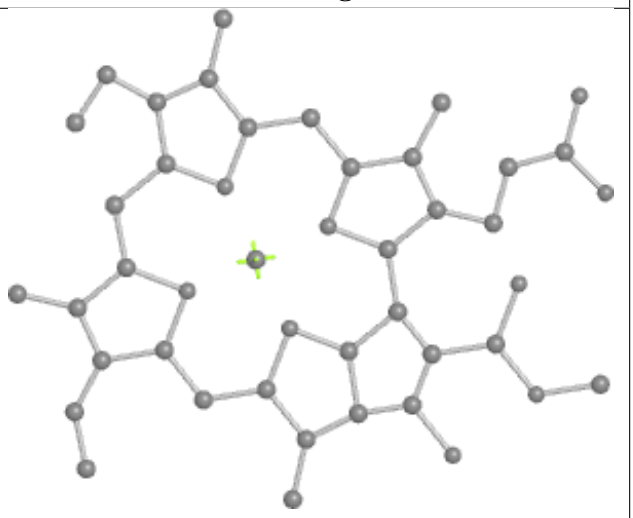


Bond angles

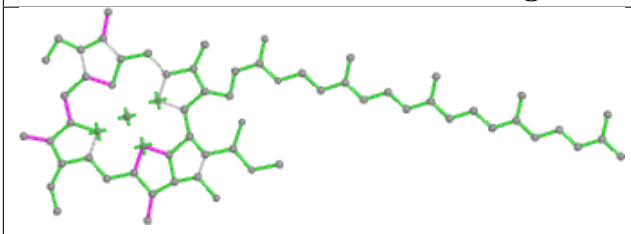


Torsions



Rings

Ligand CLA f 1231



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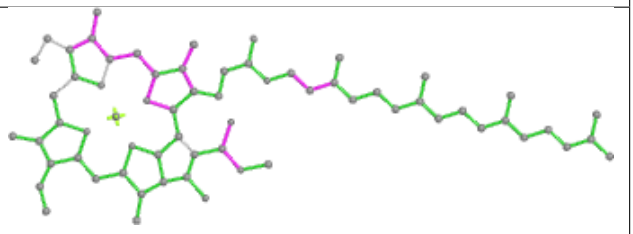
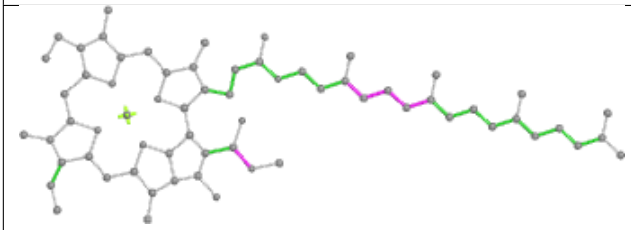


Bond angles



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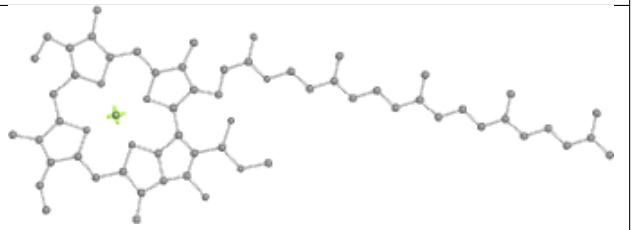
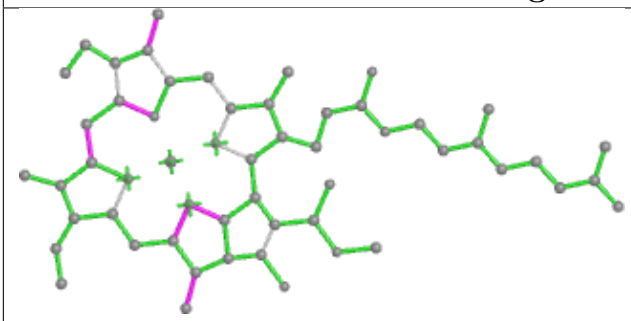


Rings

Ligand CLA 4 503



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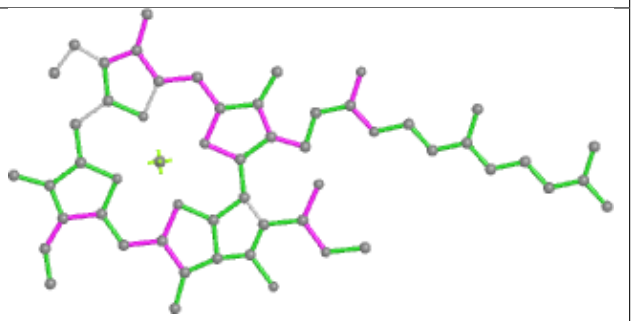

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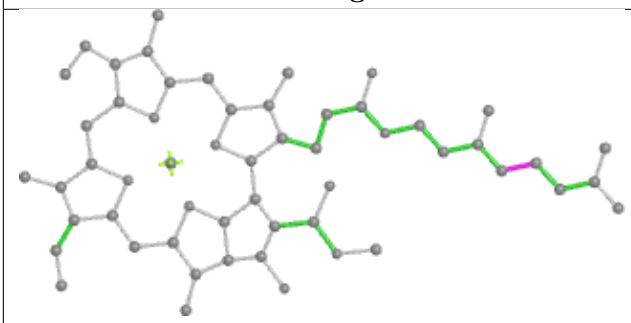

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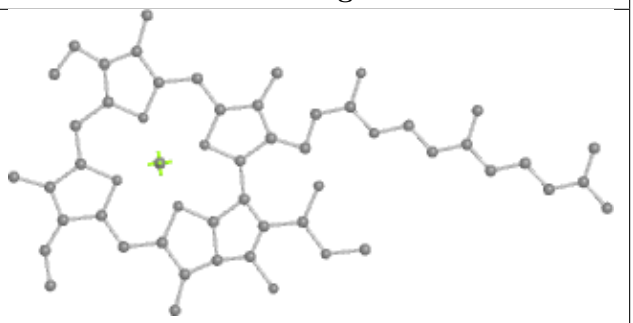
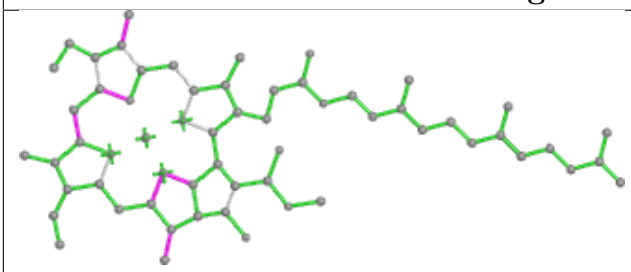


Rings

Ligand CLA q 507



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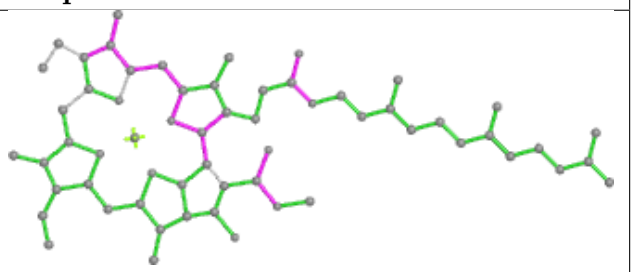
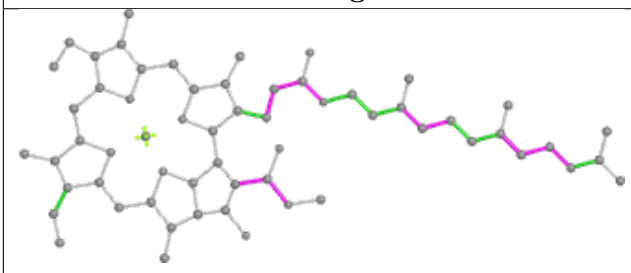


Bond angles



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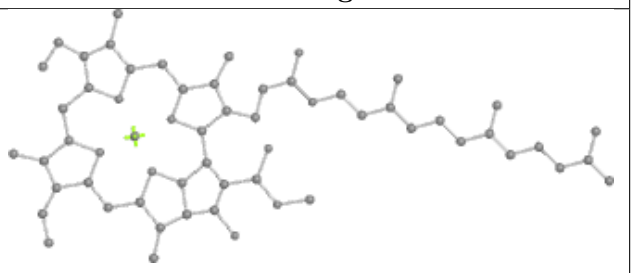
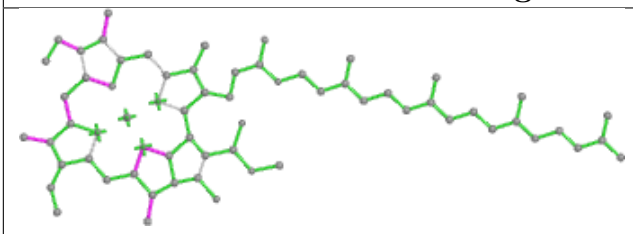


Rings

Ligand CLA H 1235



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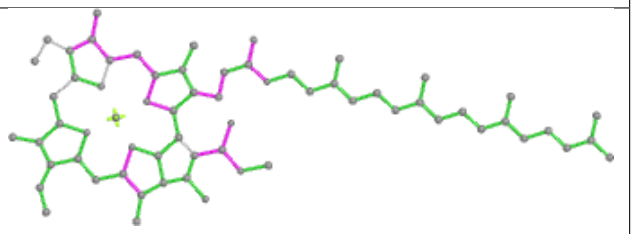
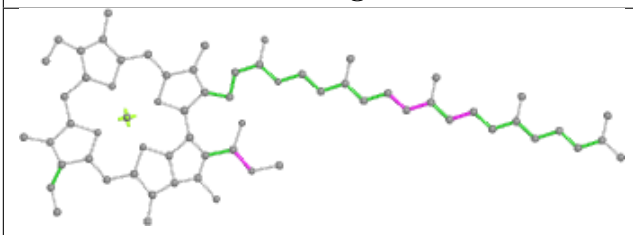


Bond angles



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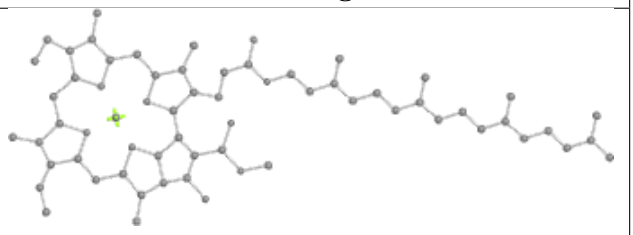
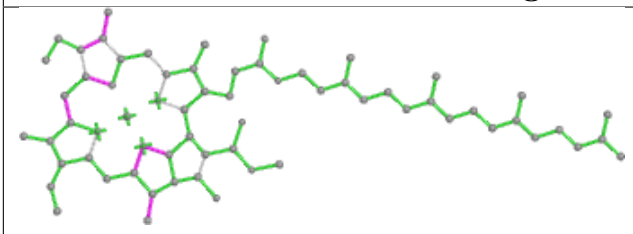


Rings

Ligand CLA f 1219



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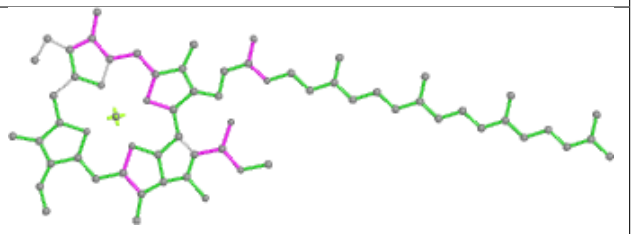
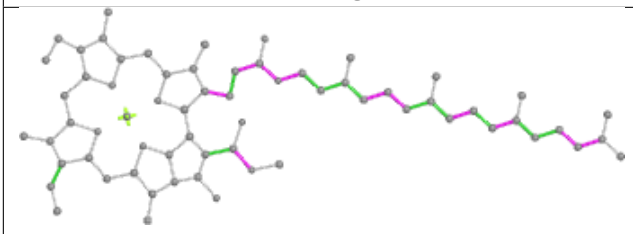


Bond angles



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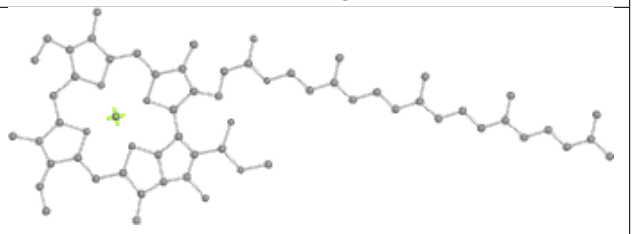
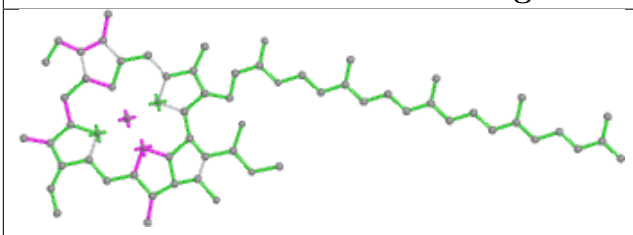


Rings

Ligand CLA G 1107



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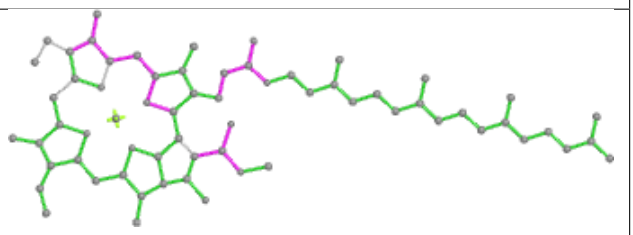
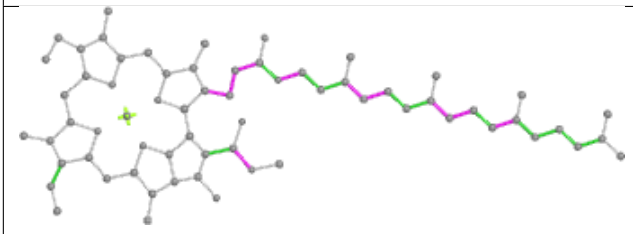


Bond angles



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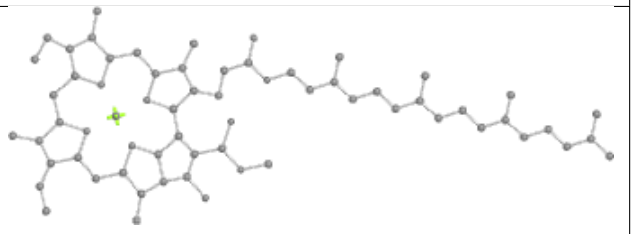
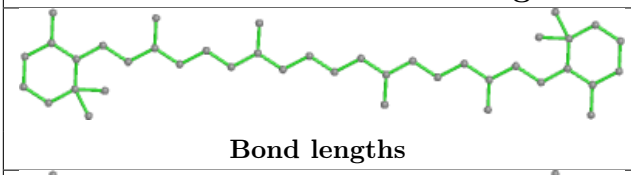


Rings

Ligand BCR R 4016



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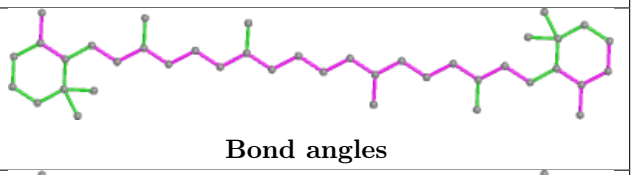
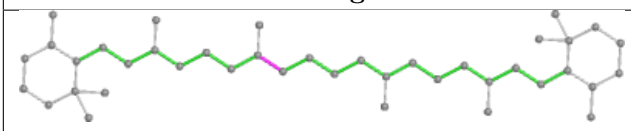


Bond angles



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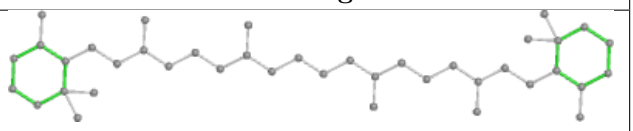
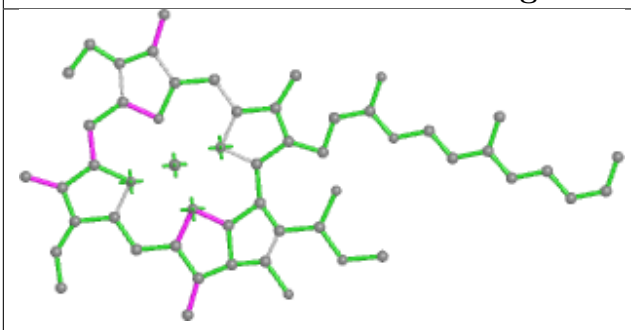


Rings

Ligand CLA e 1108



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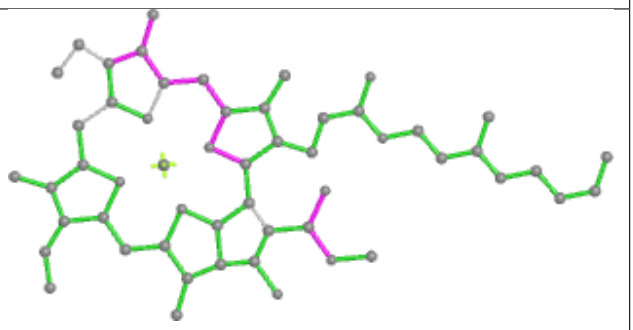
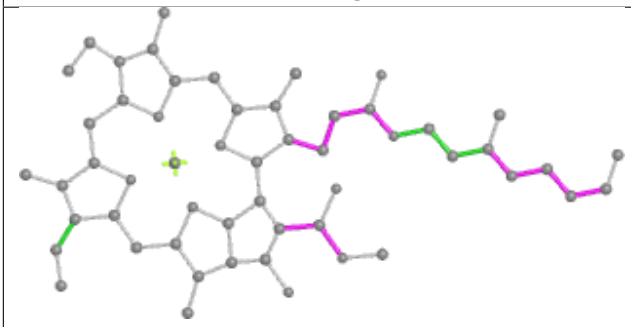


Bond angles



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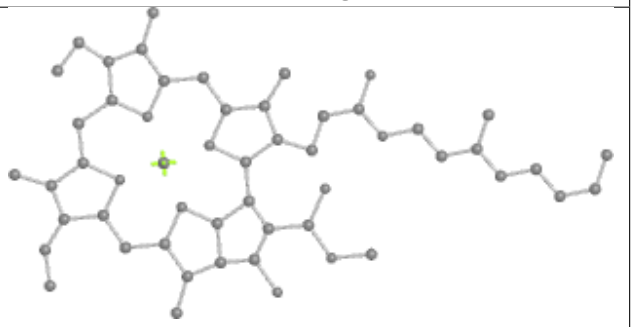
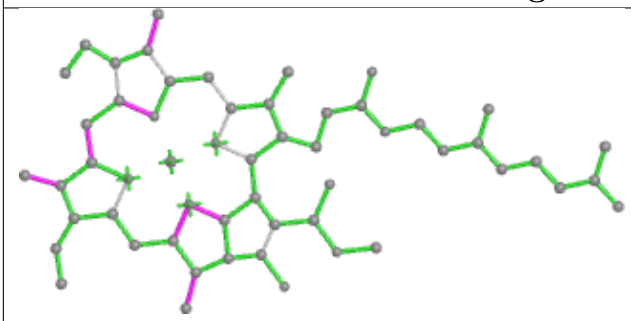


Rings

Ligand CLA 1 508



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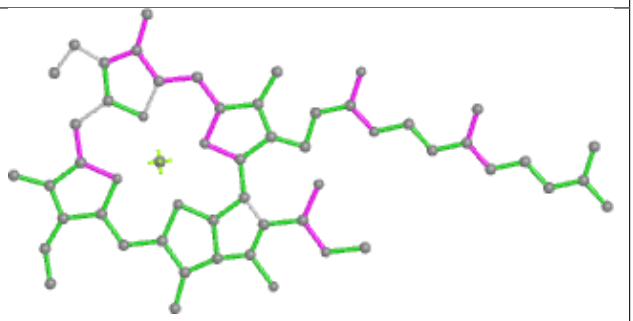
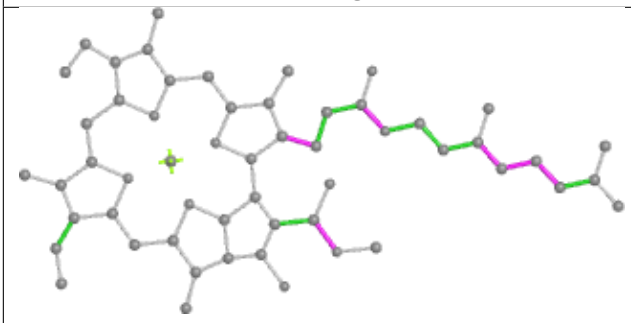


Bond angles



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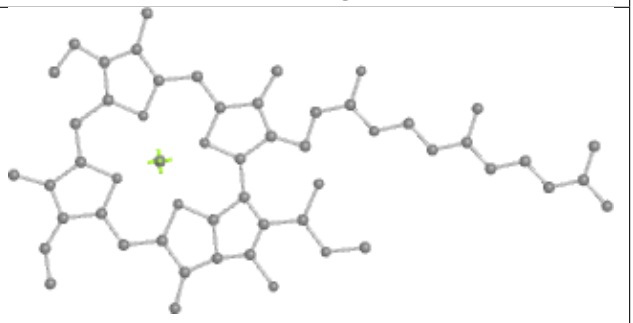
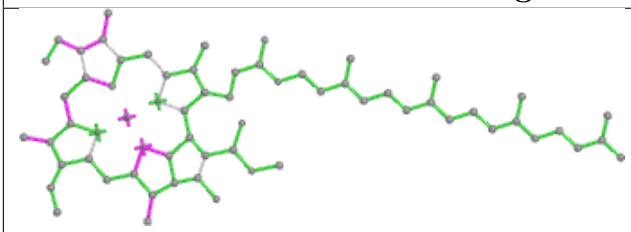


Rings

Ligand CLA A 1022



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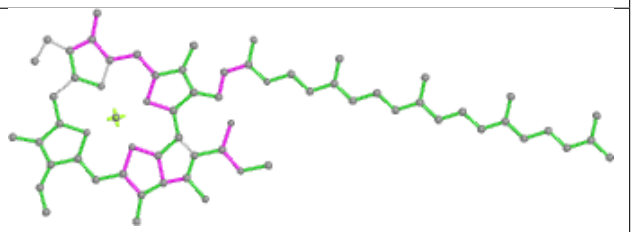
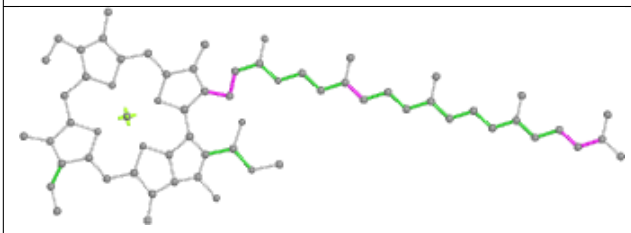
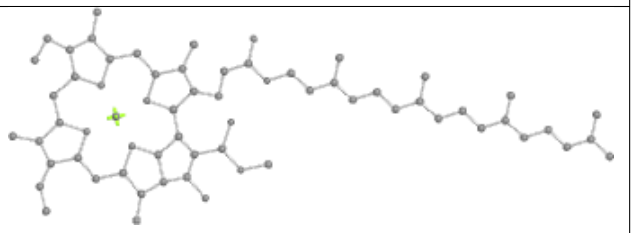


Bond angles

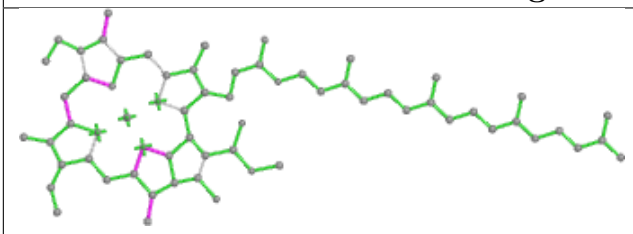


Torsions



Rings

Ligand CLA 2 505



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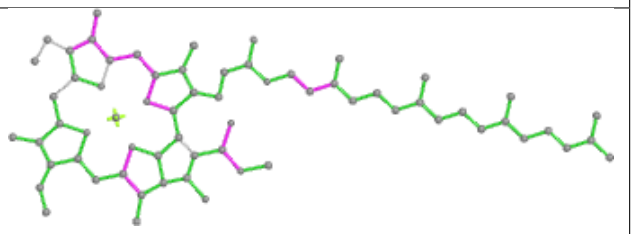
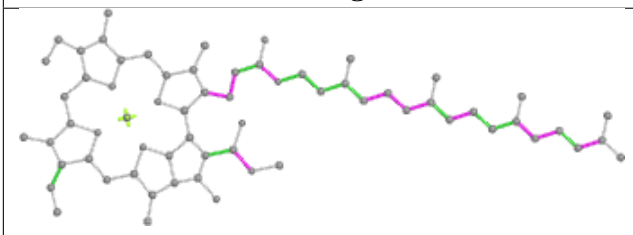
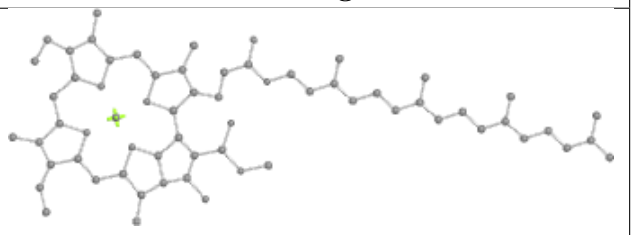


Bond angles

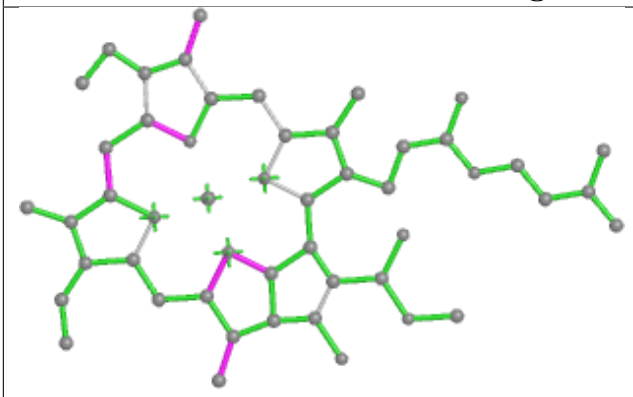


Torsions



Rings

Ligand CLA a 511



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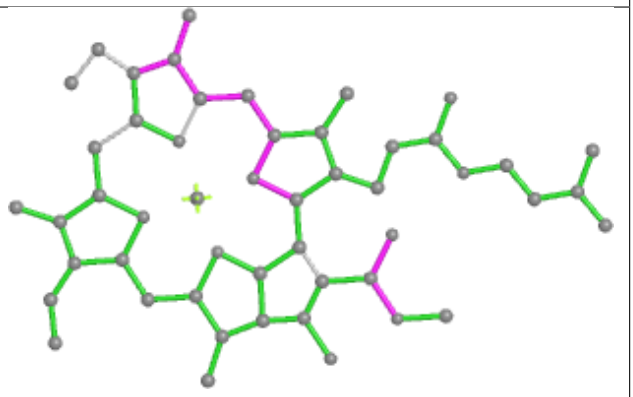

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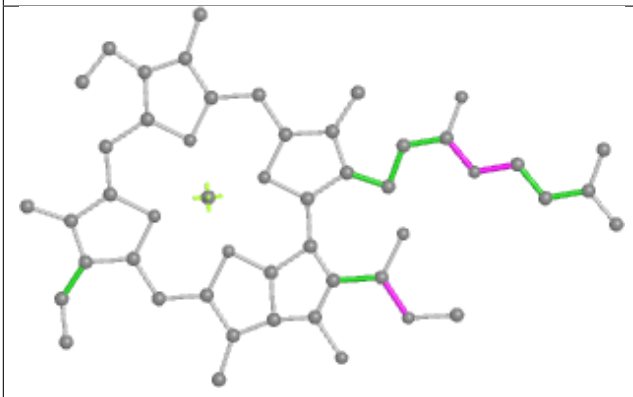

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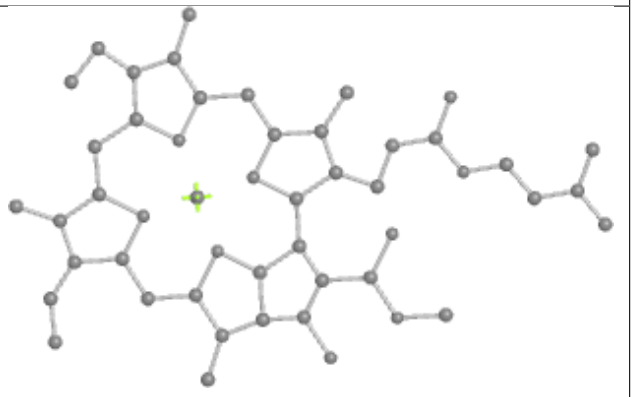
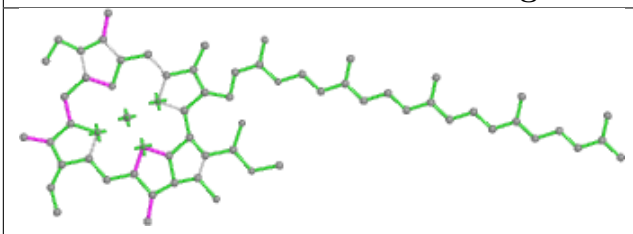


Rings

Ligand CLA e 1104



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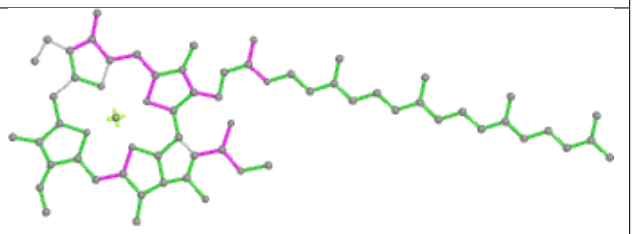

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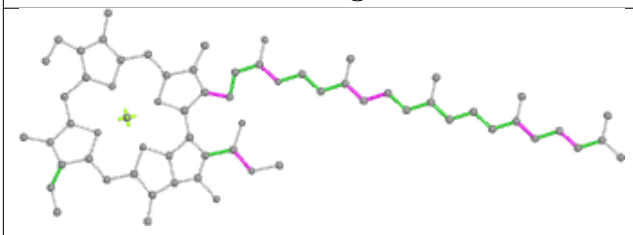

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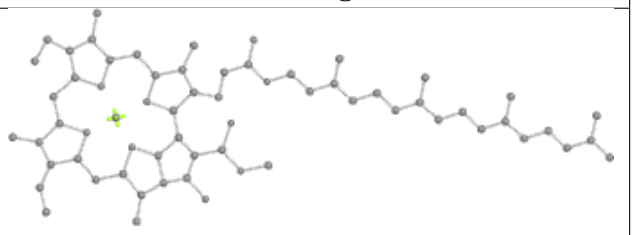
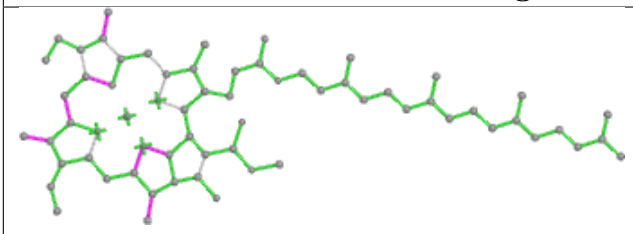


Rings

Ligand CLA G 1125



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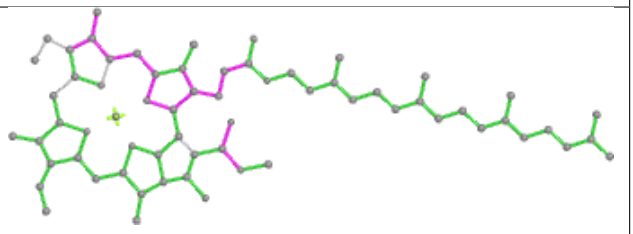

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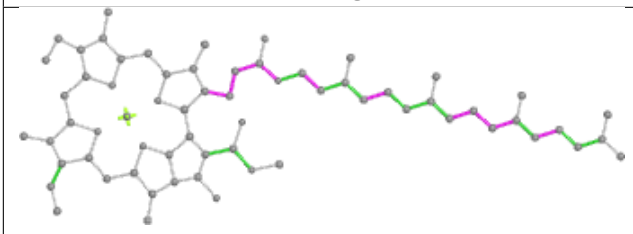

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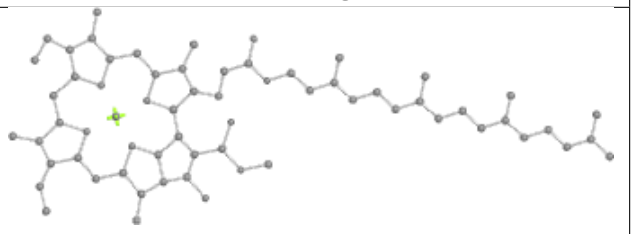
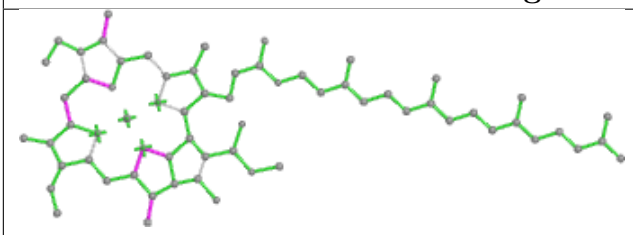


Rings

Ligand CLA Y 510



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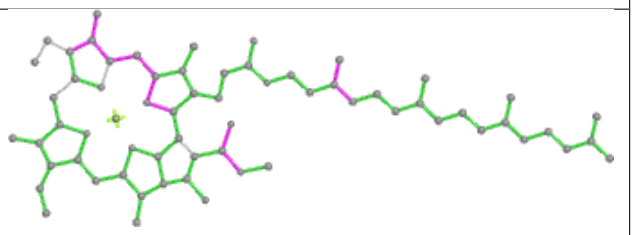

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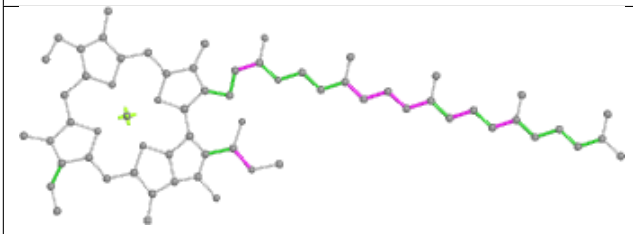

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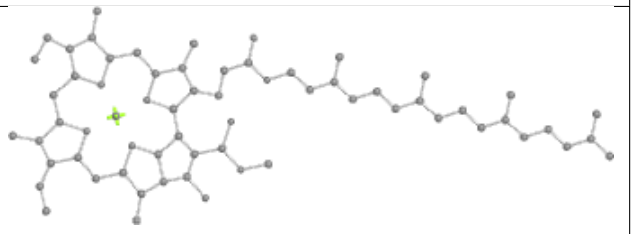
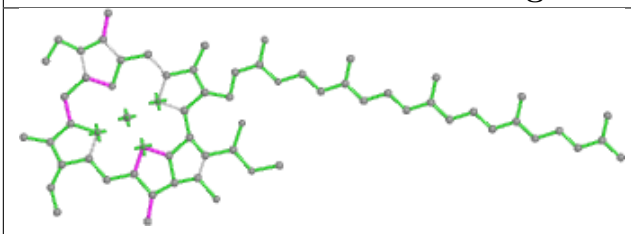


Rings

Ligand CLA Z 505



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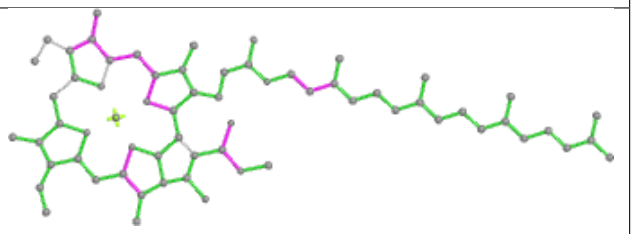

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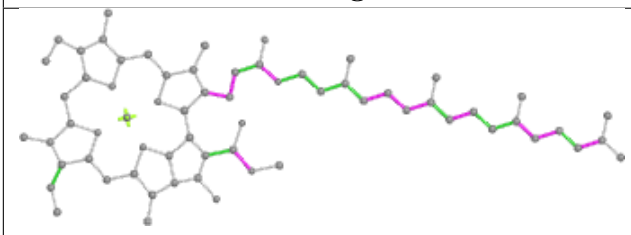

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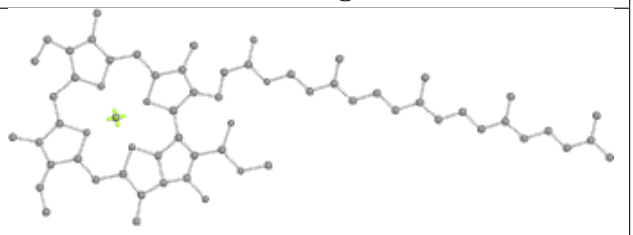
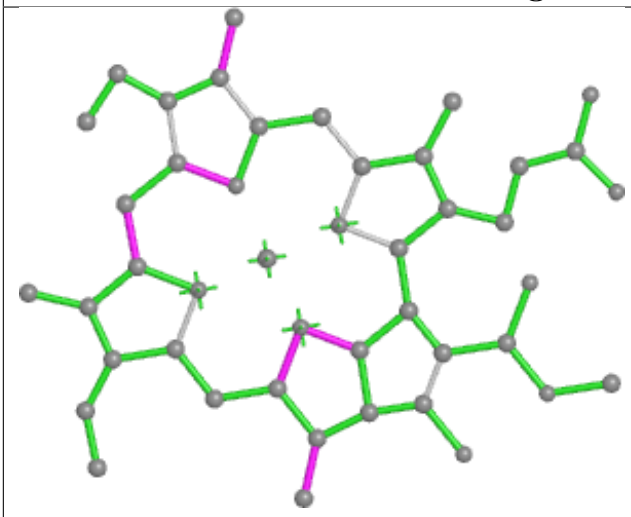


Rings

Ligand CLA u 510



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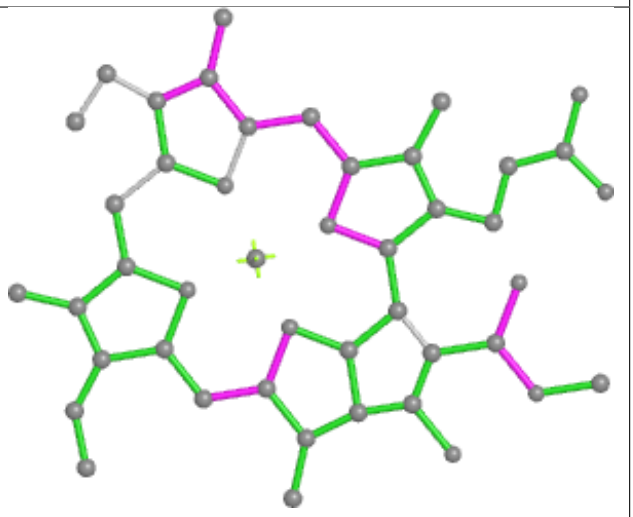

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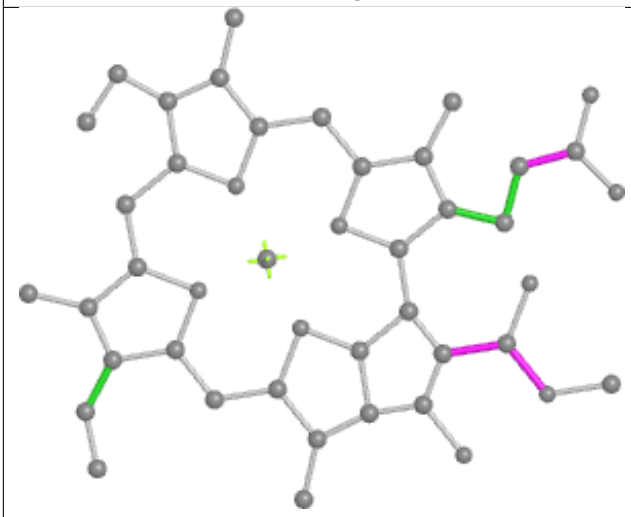

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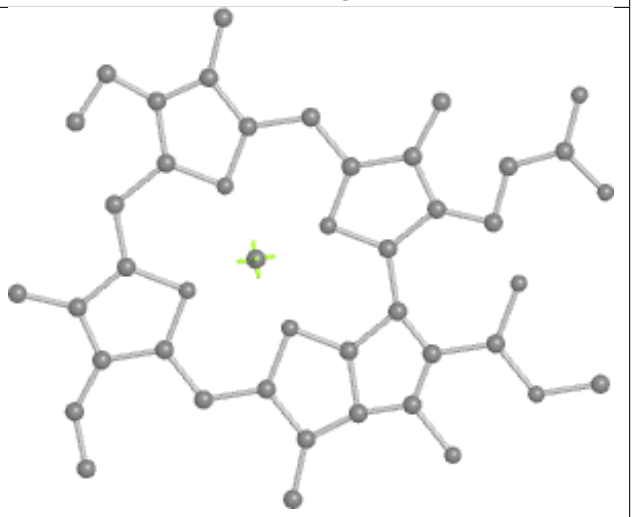
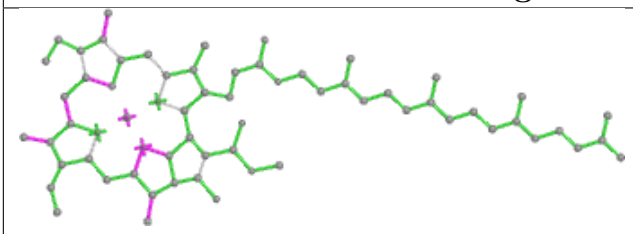


Rings

Ligand CLA H 1023



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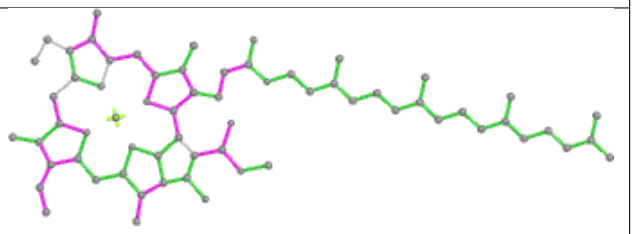

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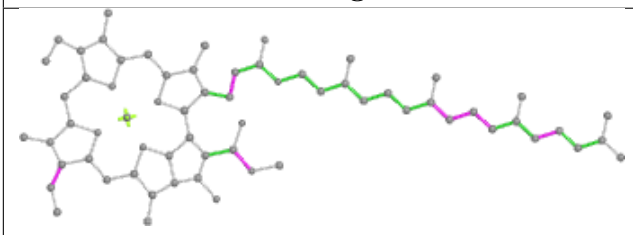

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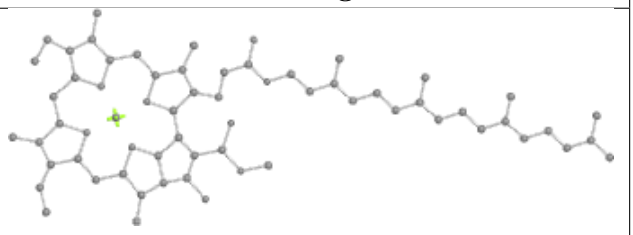
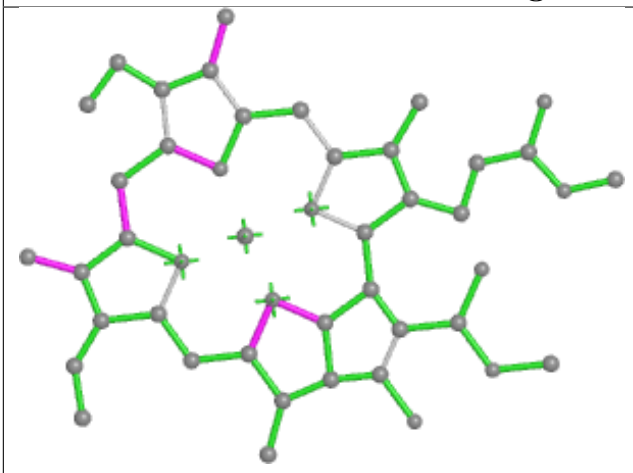


Rings

Ligand CLA d 519



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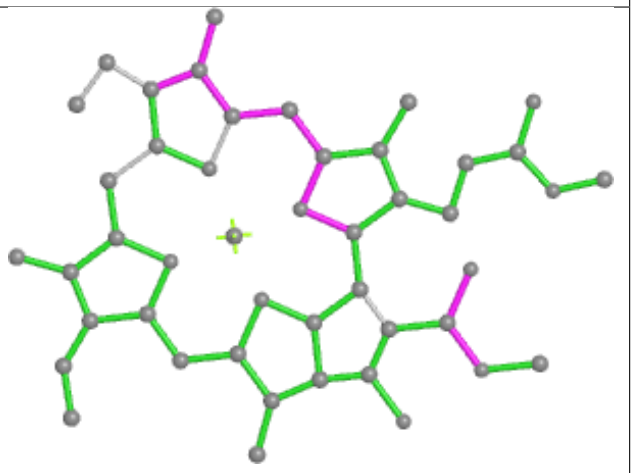

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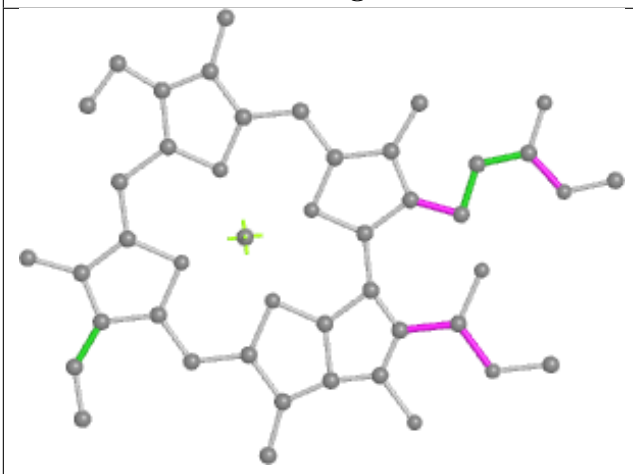

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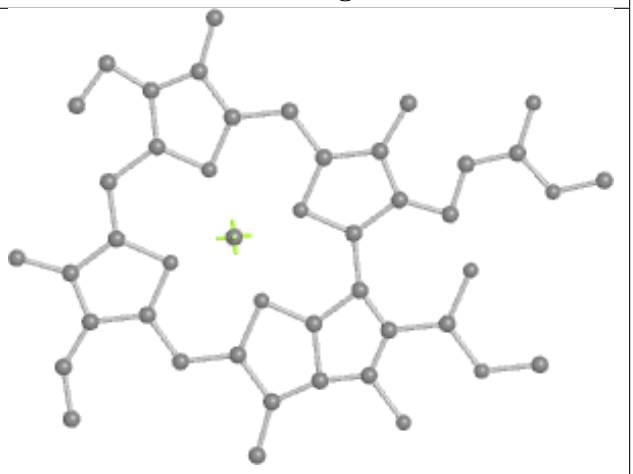
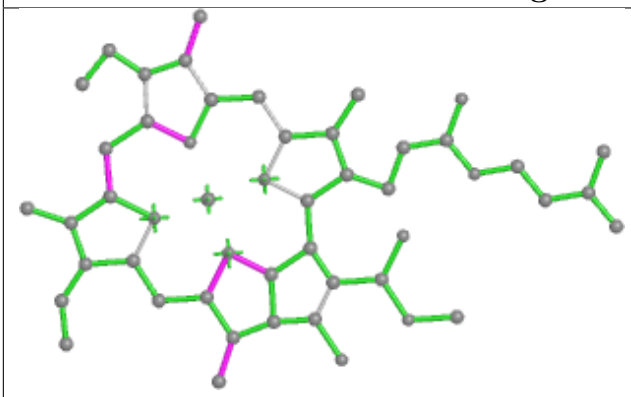


Rings

Ligand CLA t 510



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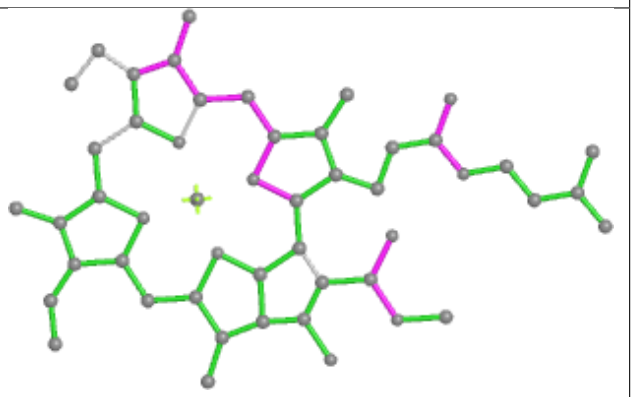

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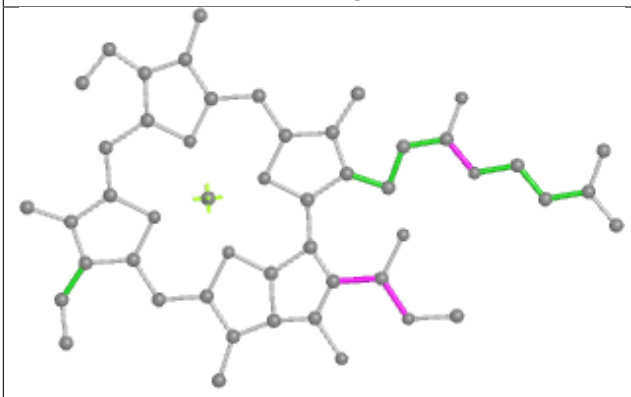

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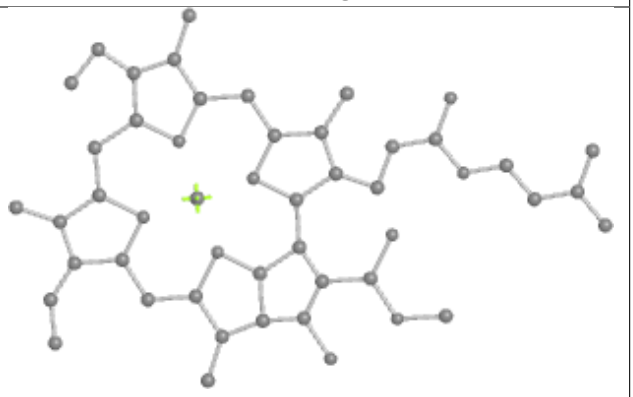
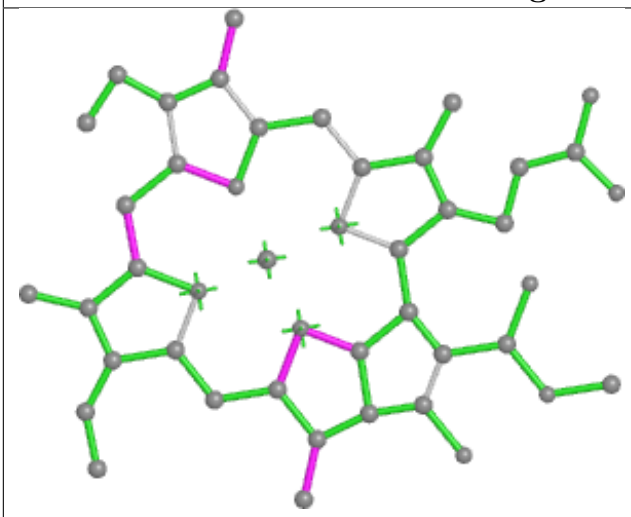


Rings

Ligand CLA c 510



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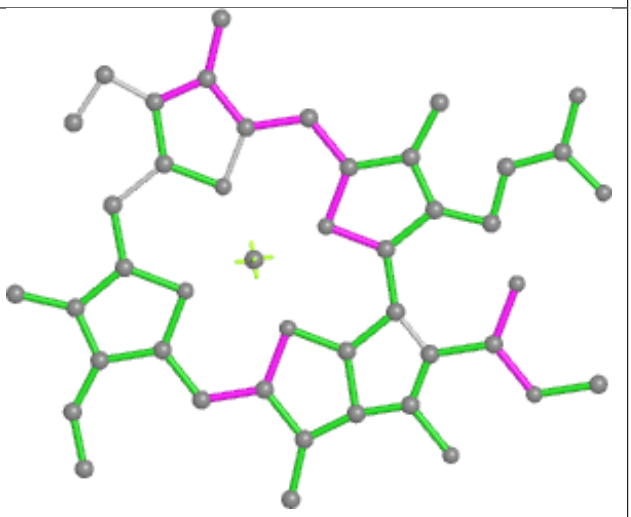

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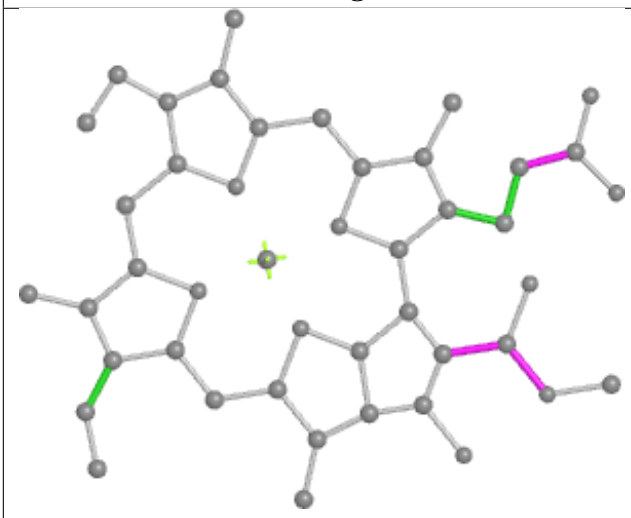

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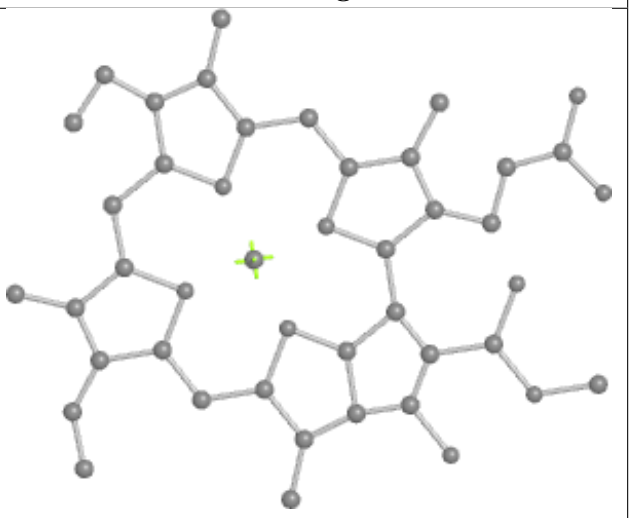
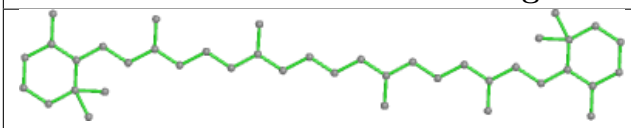


Rings

Ligand BCR Y 521



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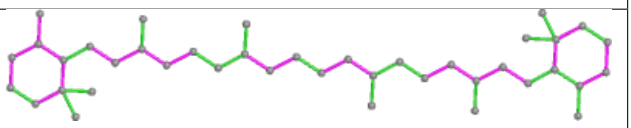

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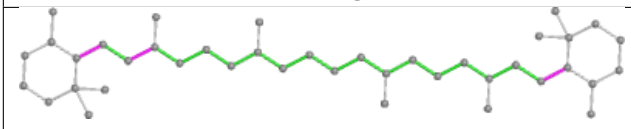
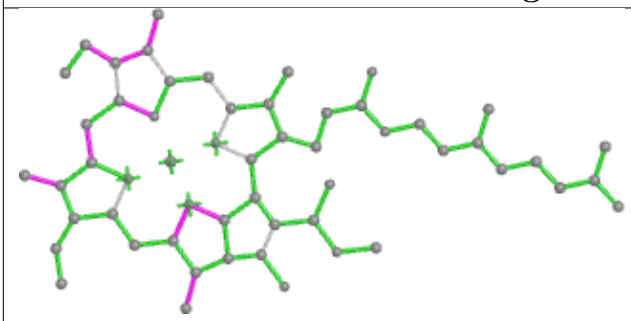


Torsions

Rings

Ligand CLA f 1220



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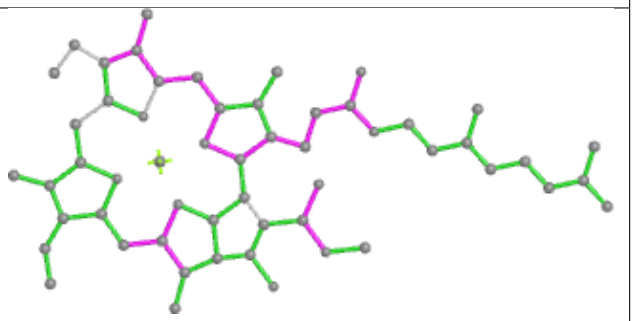

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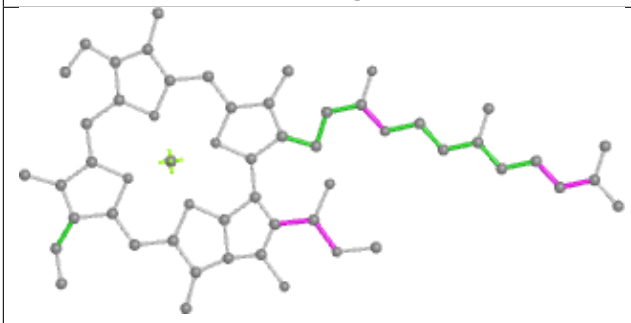

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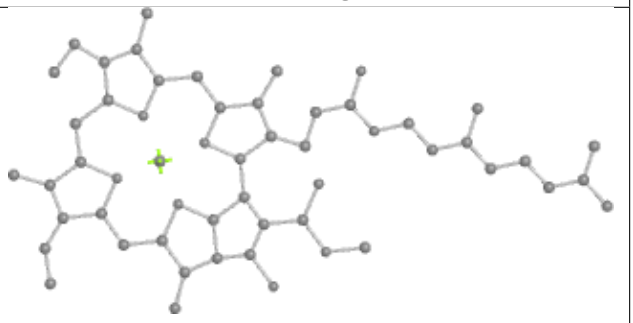
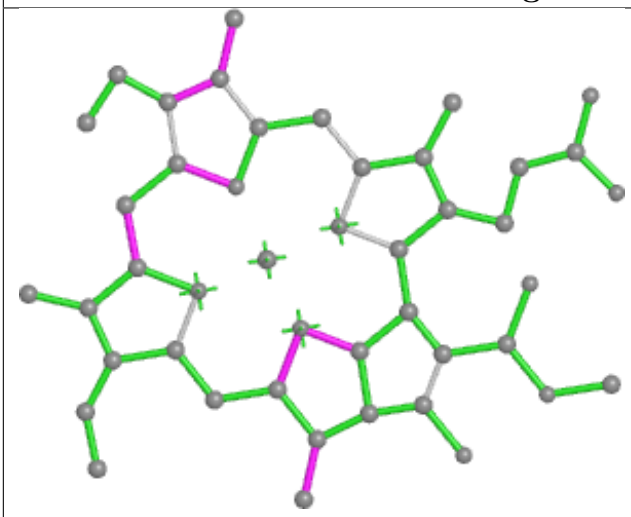


Rings

Ligand CLA j 1302



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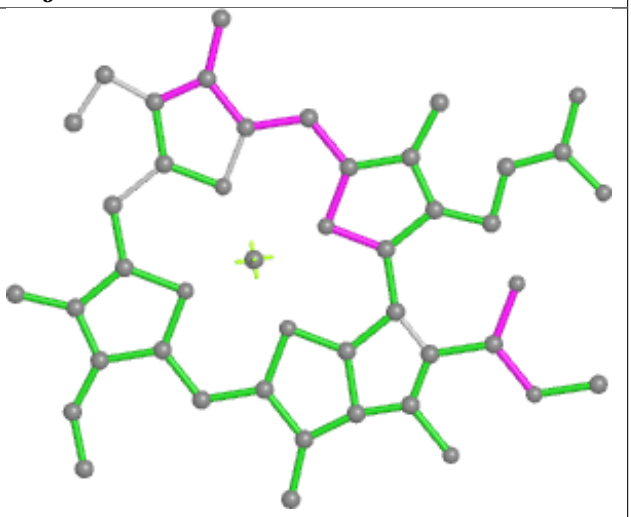
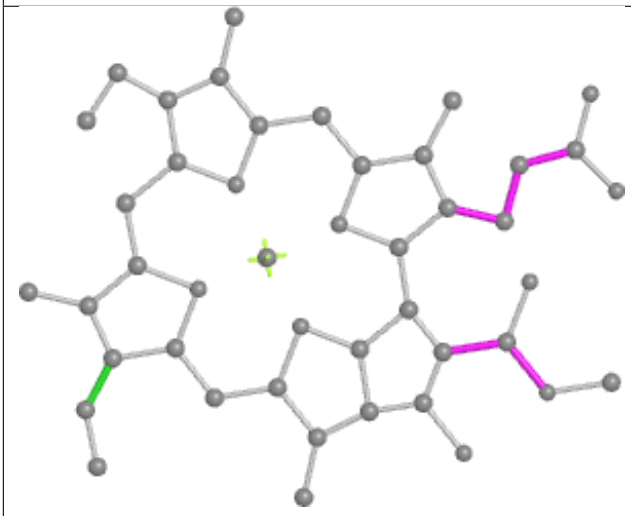


Bond angles



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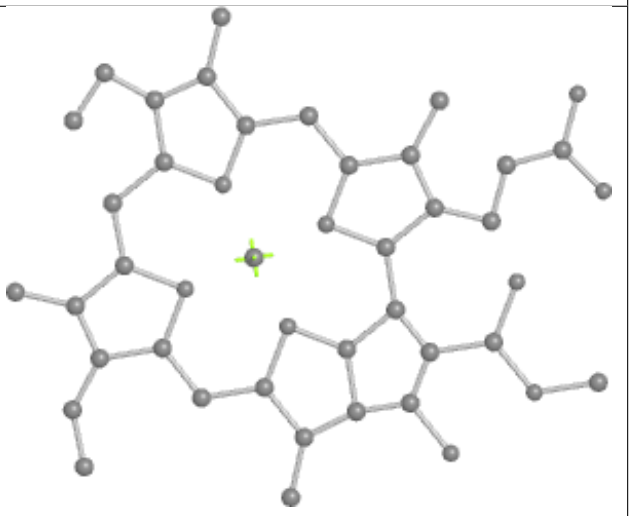
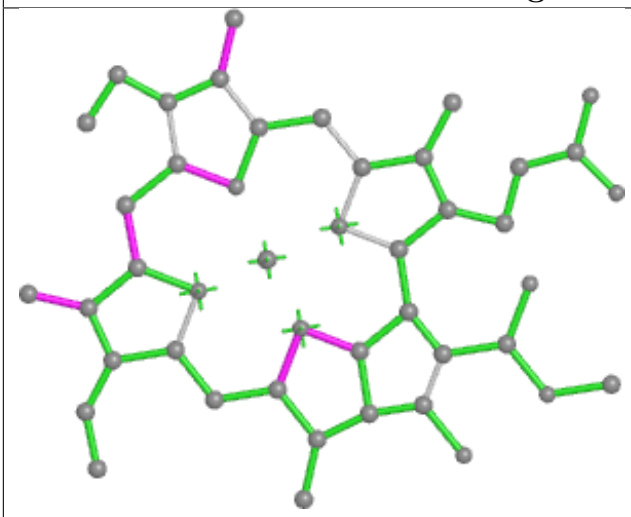


Rings

Ligand CLA u 506



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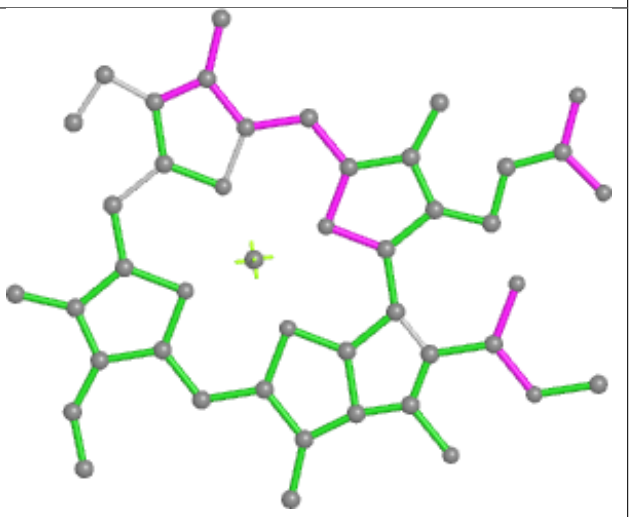
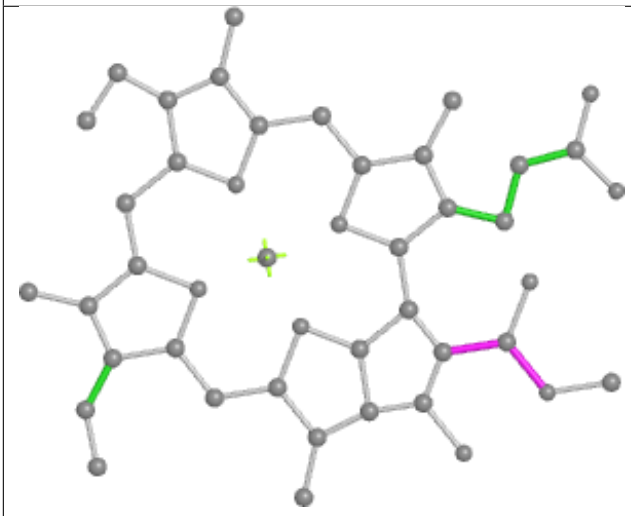


Bond angles



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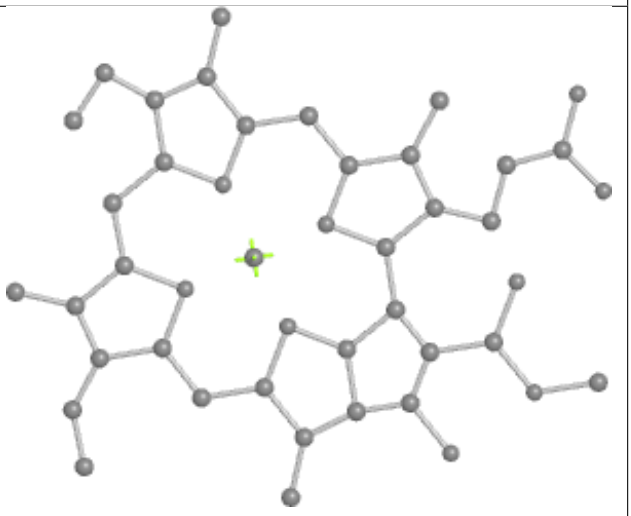
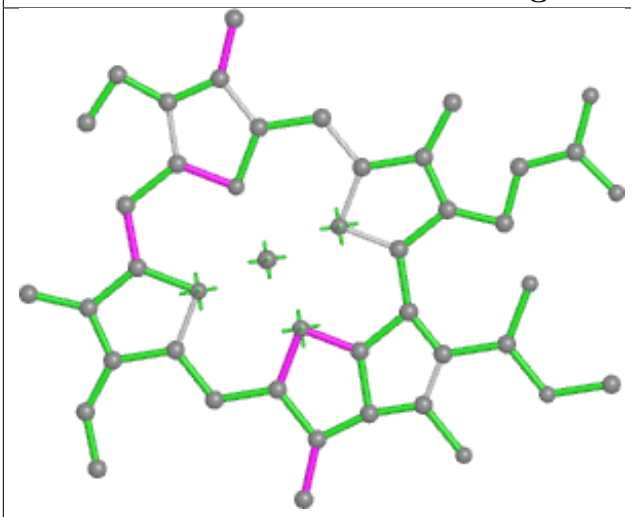
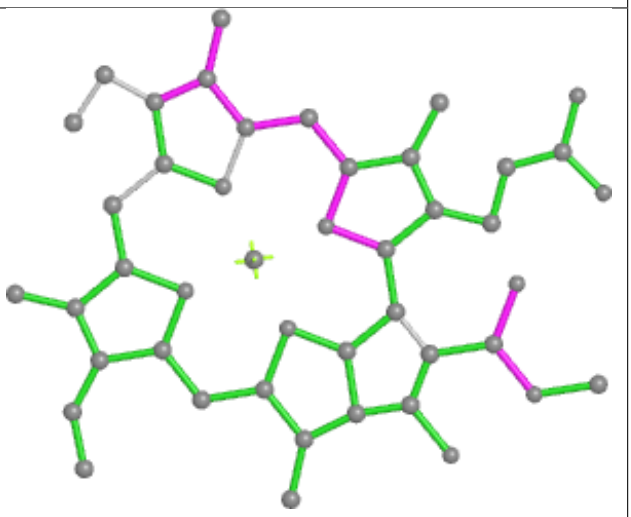


Rings

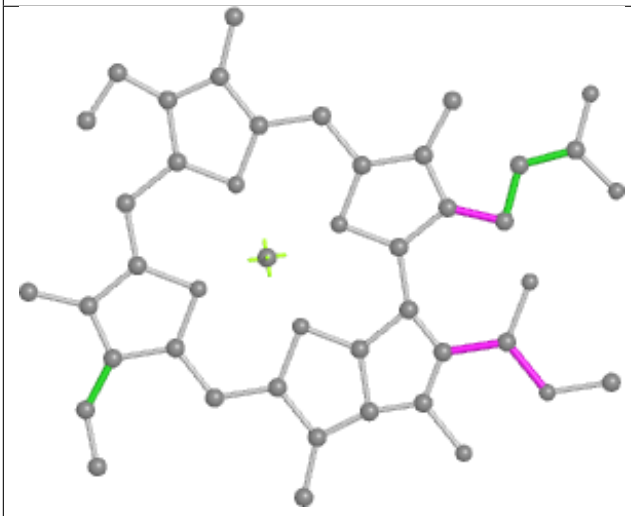
Ligand CLA s 504



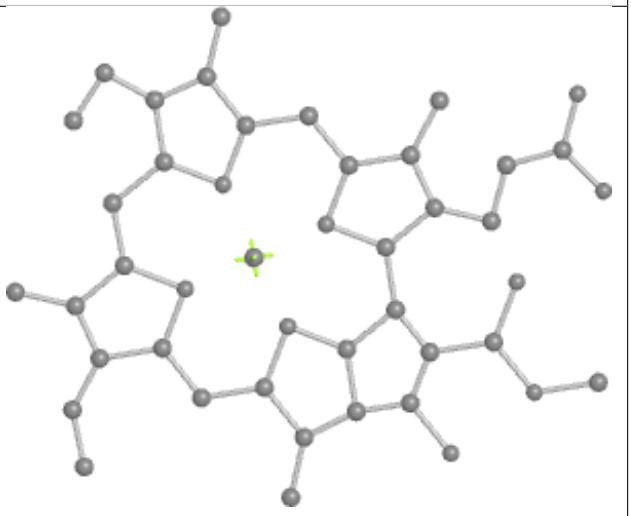
Bond lengths



Bond angles

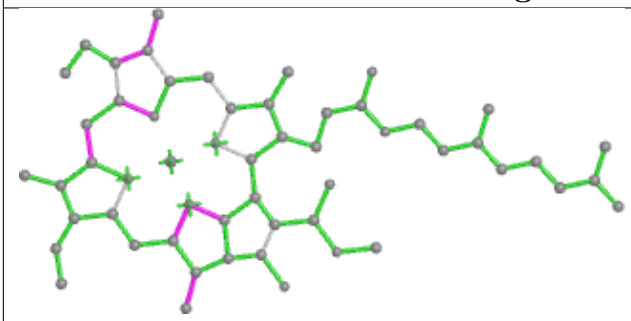


Torsions



Rings

Ligand CLA H 1236



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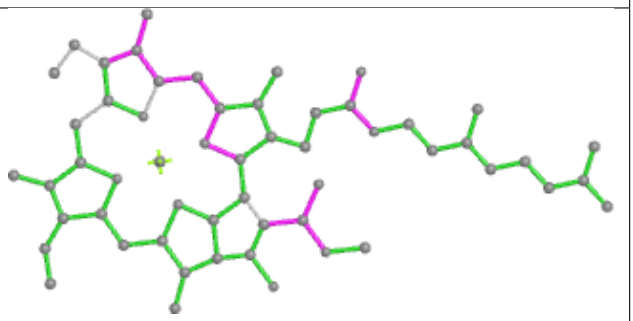
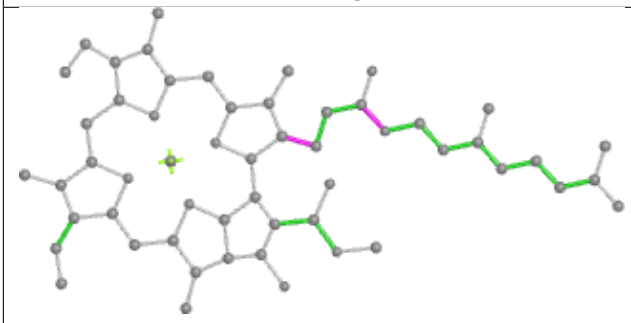


Bond angles



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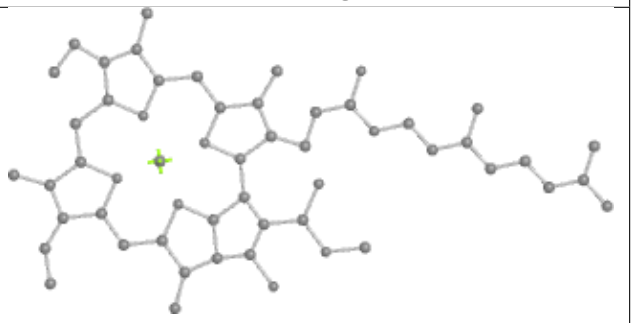
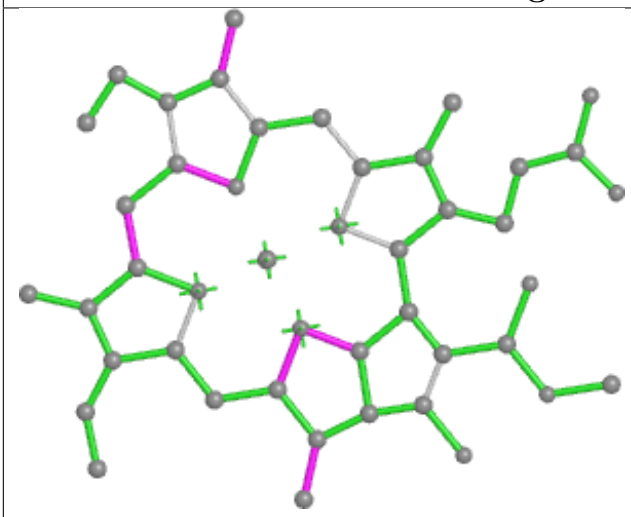


Rings

Ligand CLA 6 507



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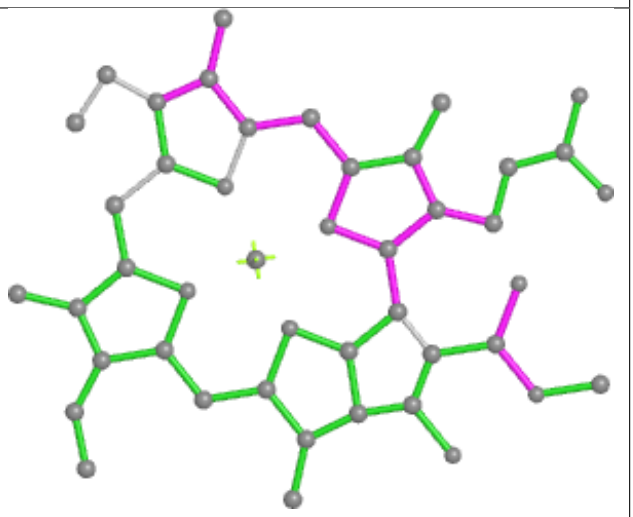
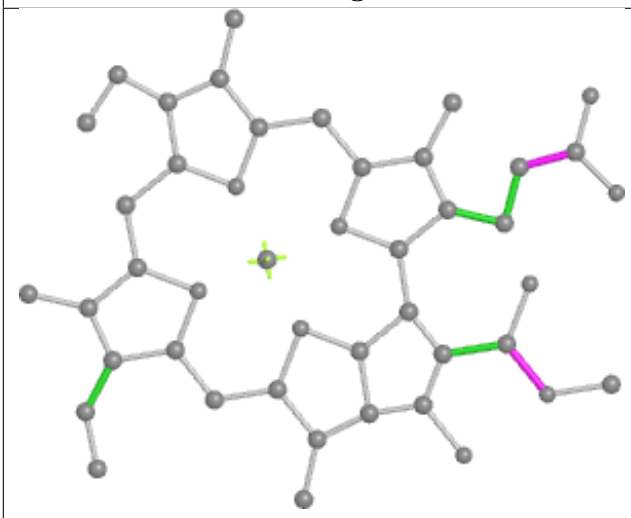


Bond angles



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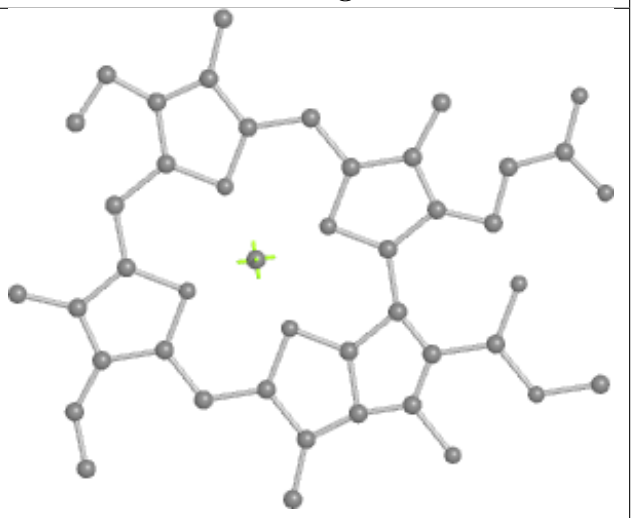
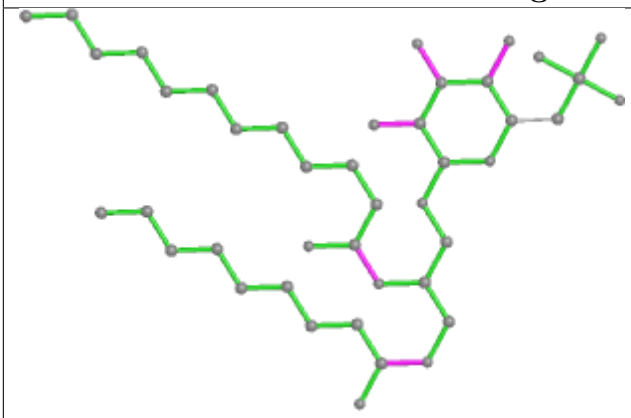


Rings

Ligand SQD s 822



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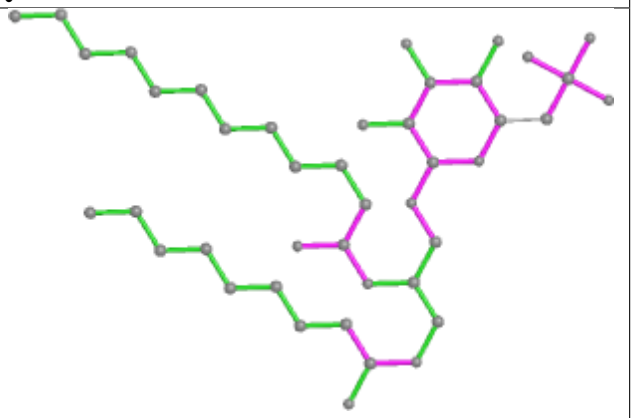
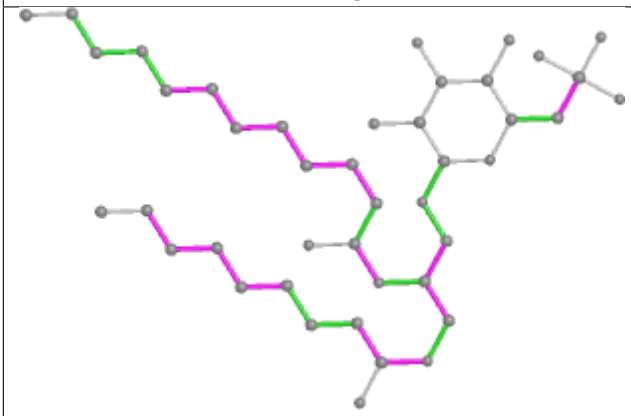
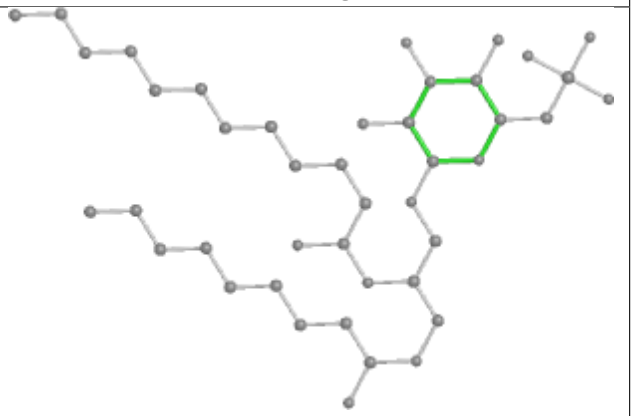


Bond angles

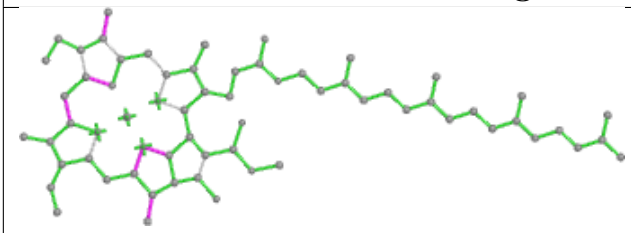


Torsions



Rings

Ligand CLA G 1011



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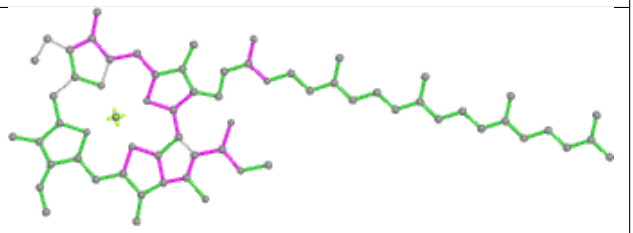
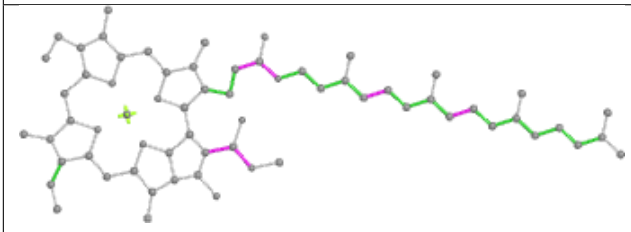


Bond angles



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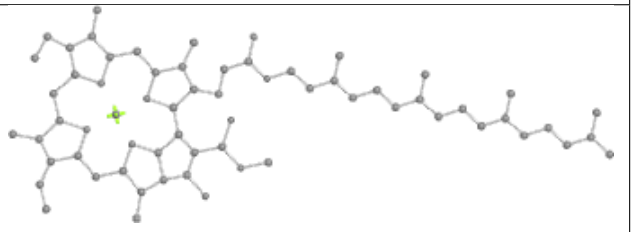
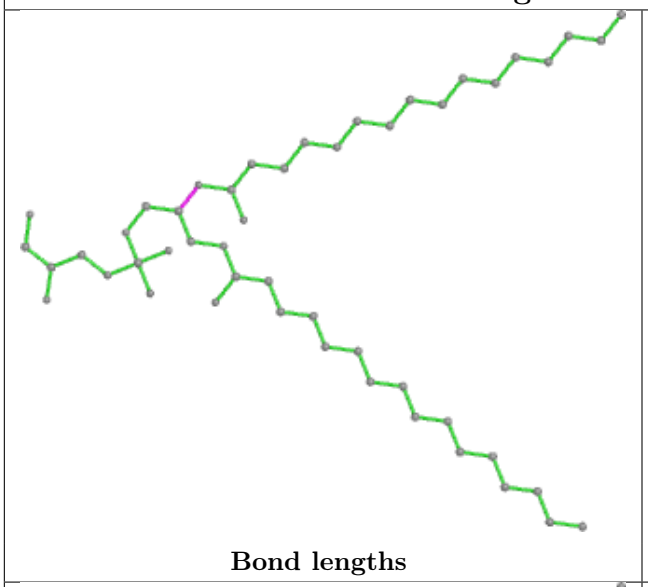


Rings

Ligand LHG G 5009



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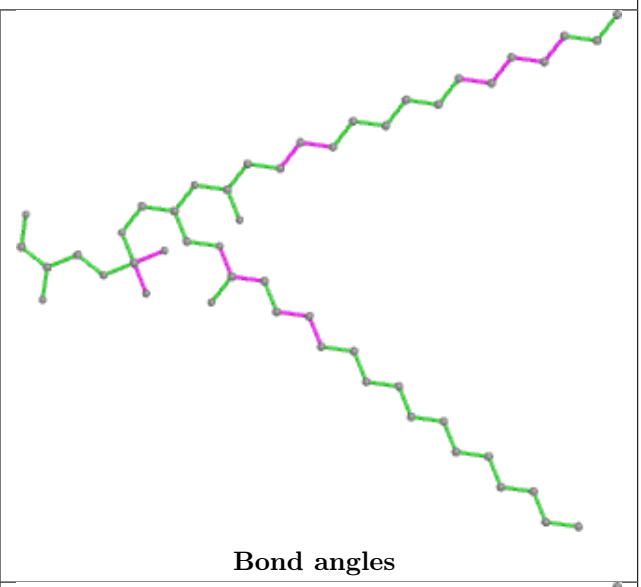

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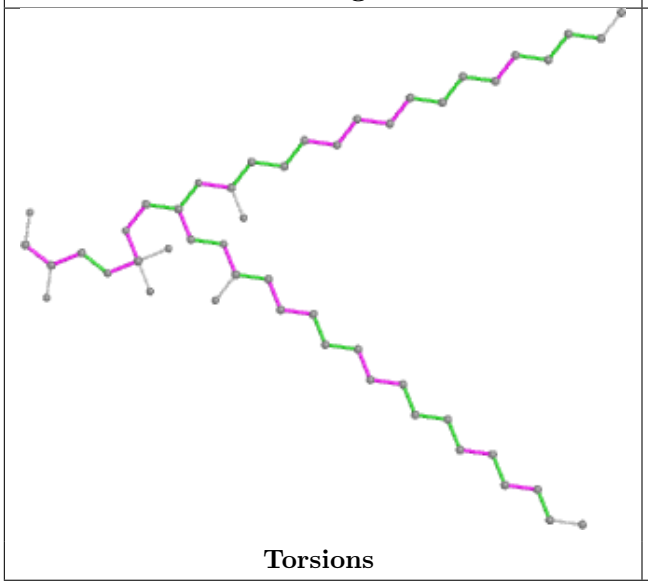

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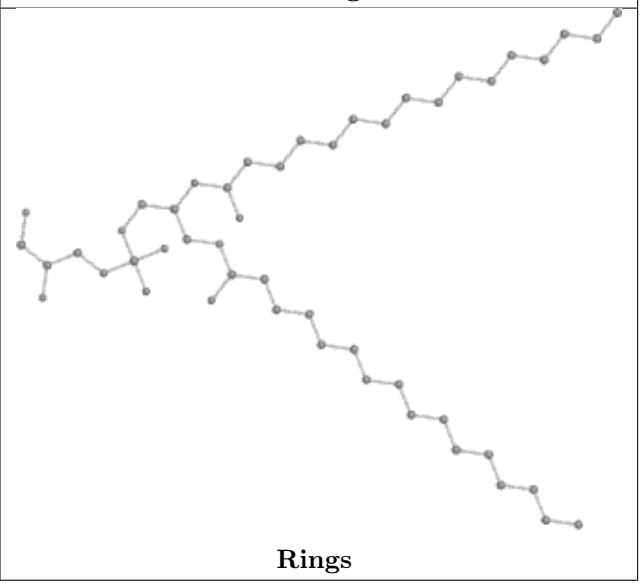
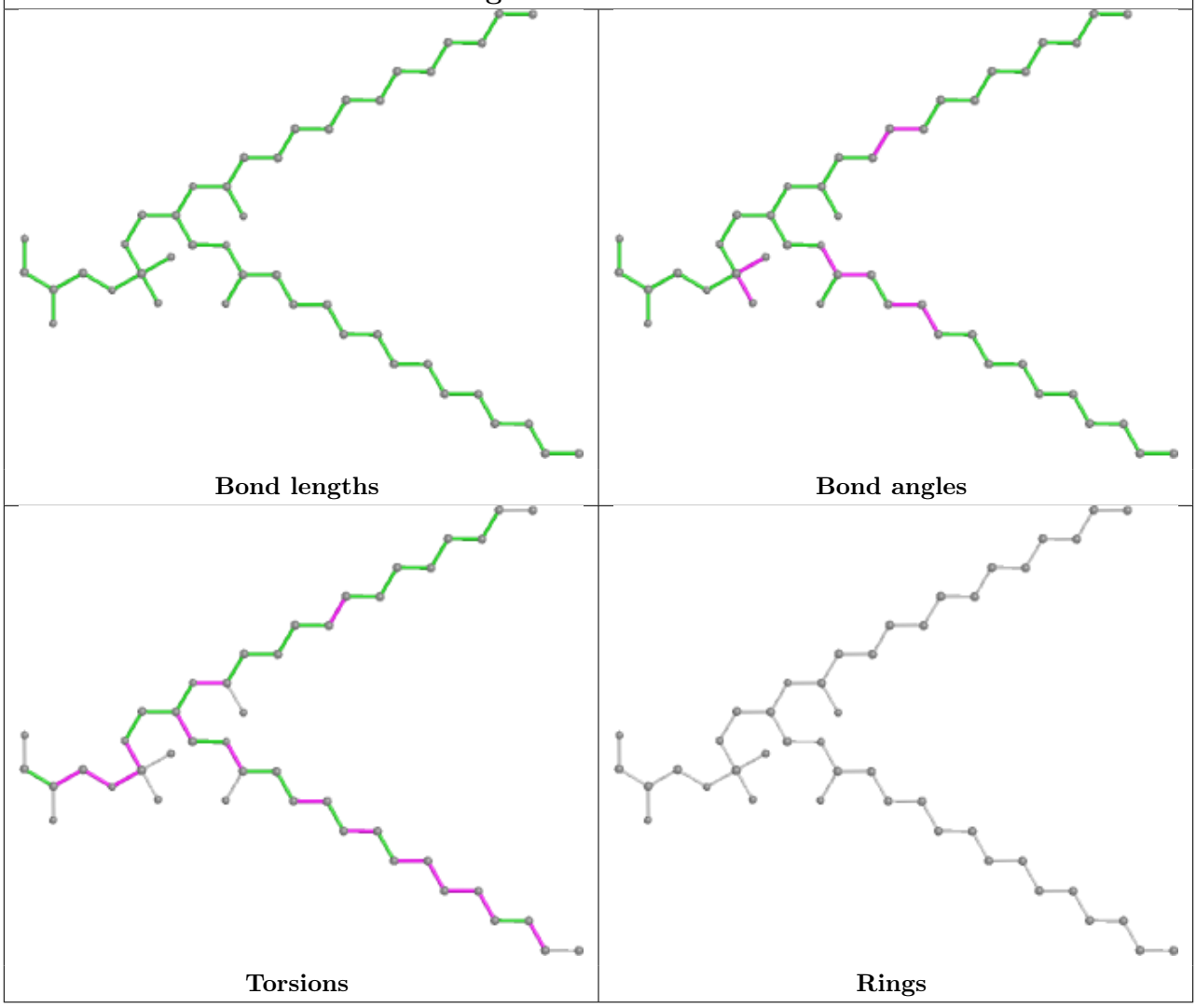
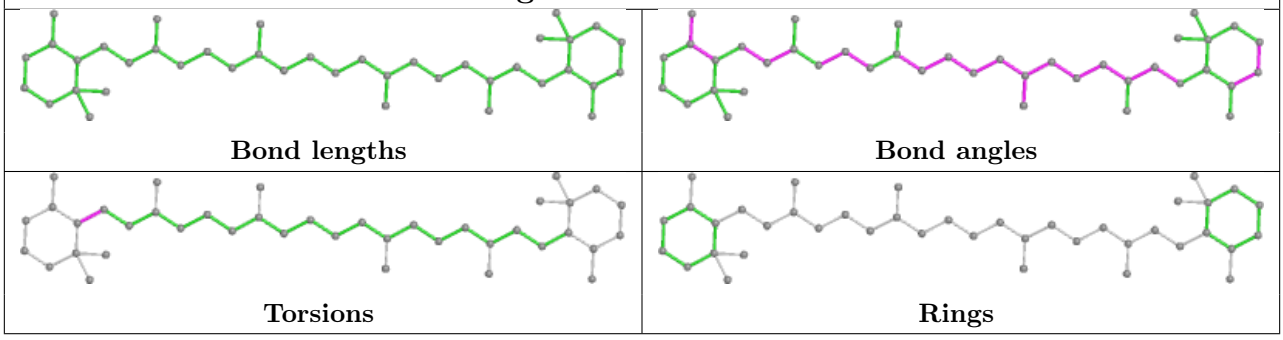


Rings

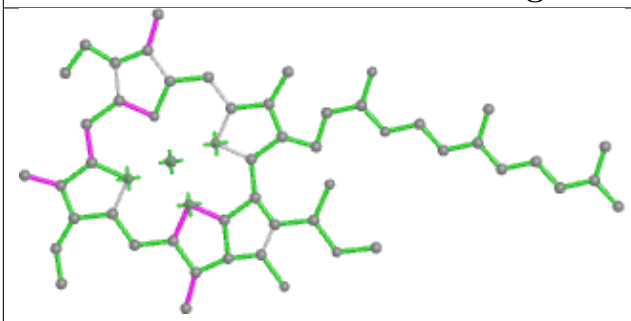
Ligand LHG I 5001



Ligand BCR L 4219



Ligand CLA Z 506



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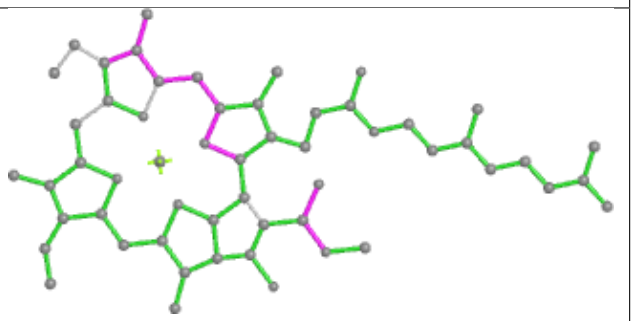
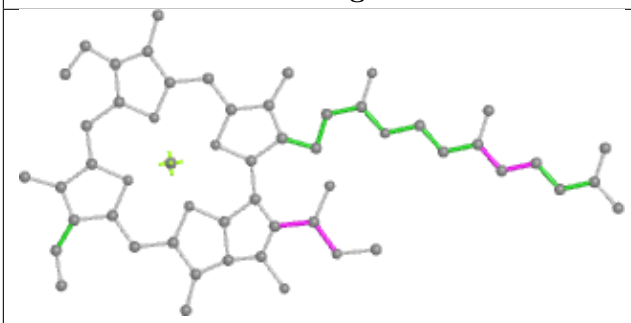


Bond angles



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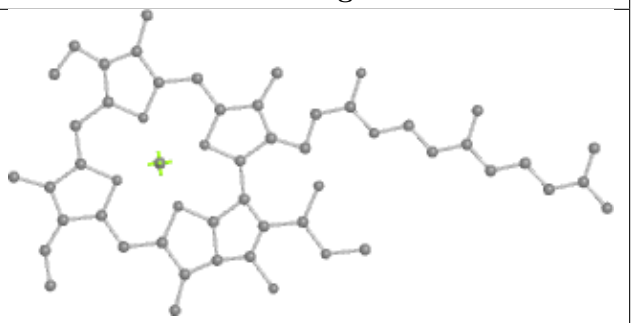
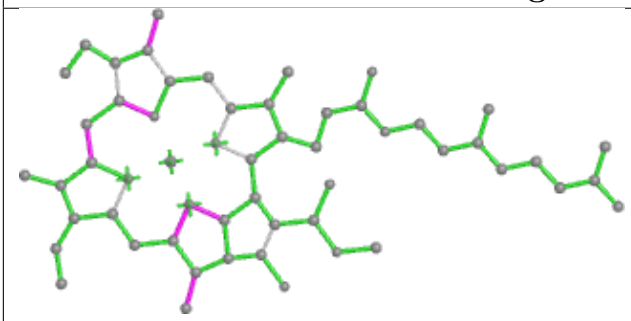


Rings

Ligand CLA 6 518



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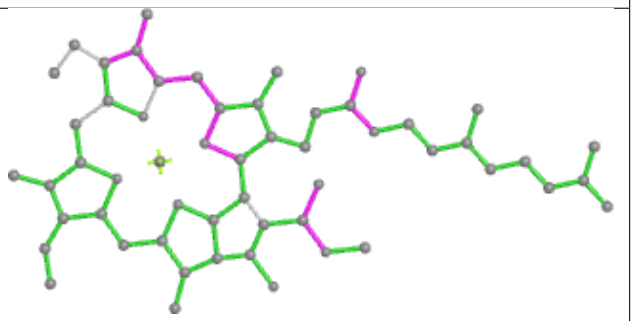

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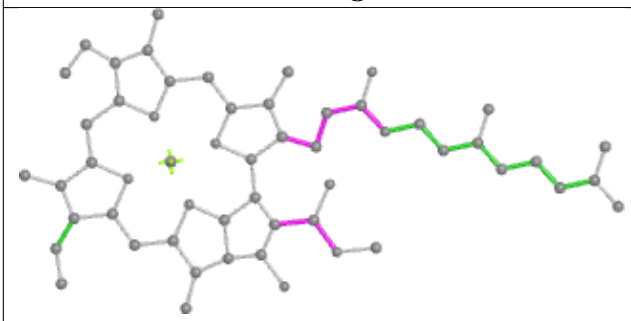

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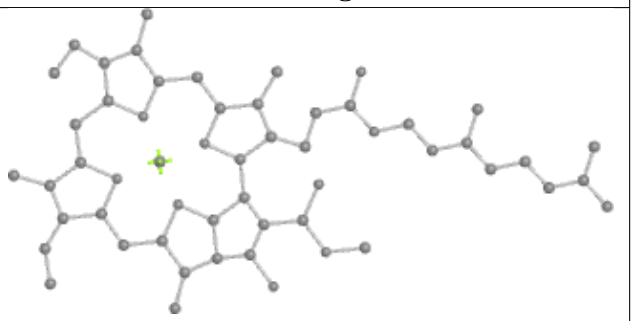
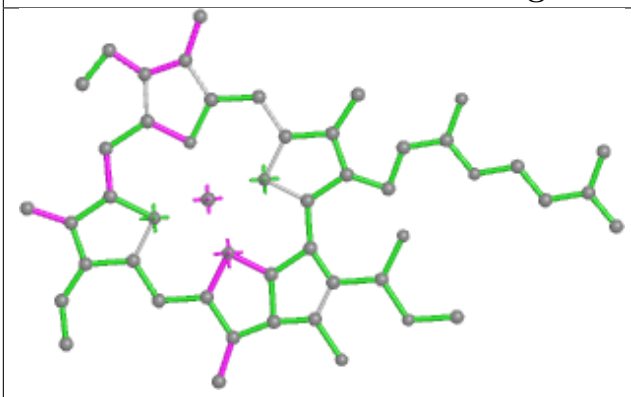


Rings

Ligand CLA q 519



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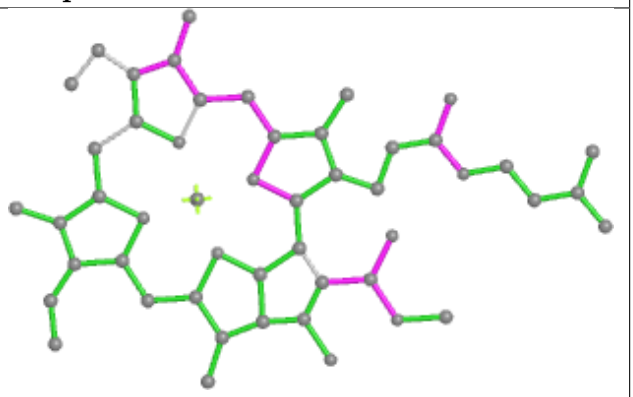
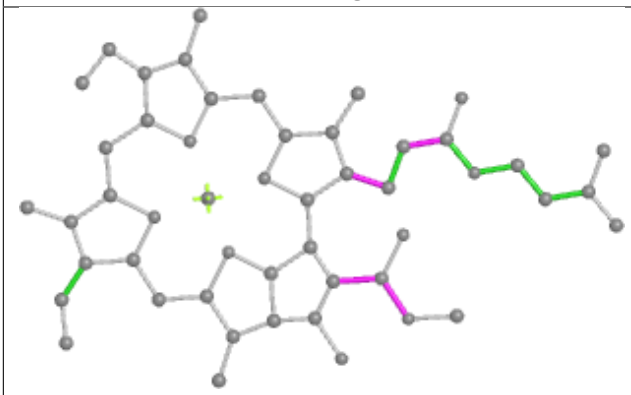
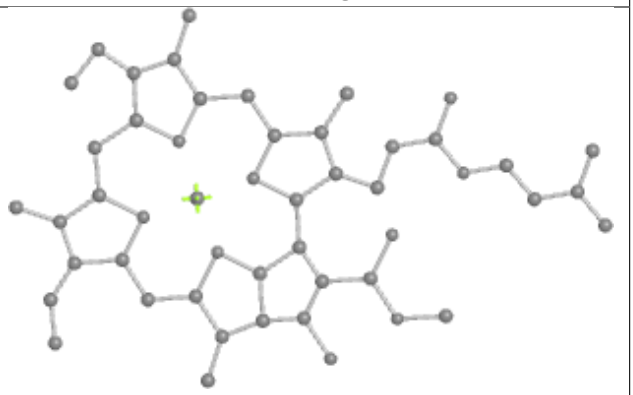


Bond angles

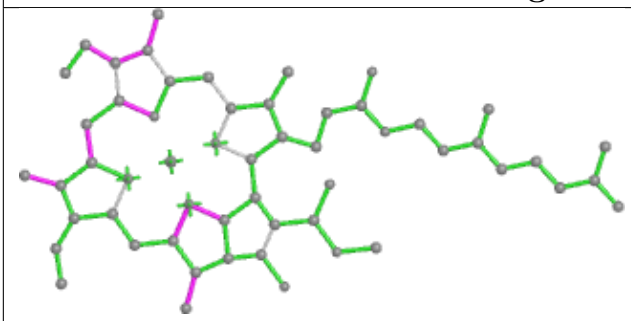


Torsions



Rings

Ligand CLA 2 519



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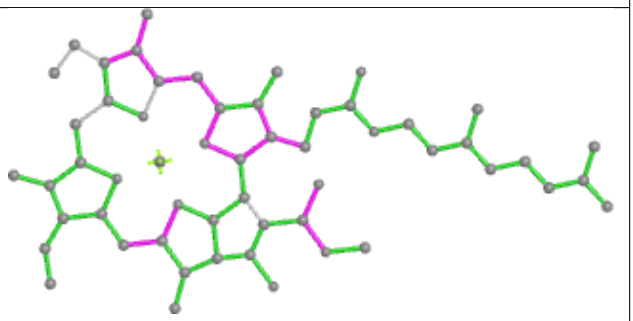

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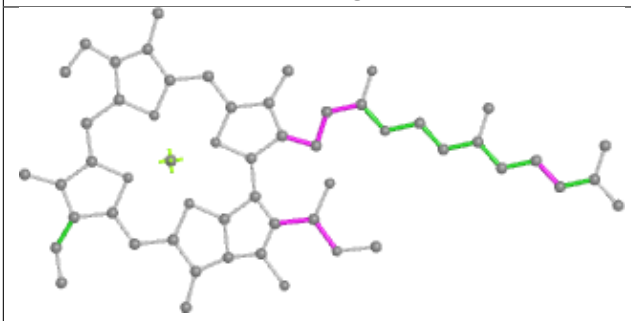

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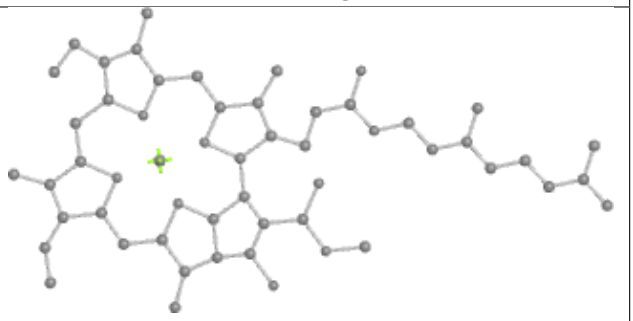
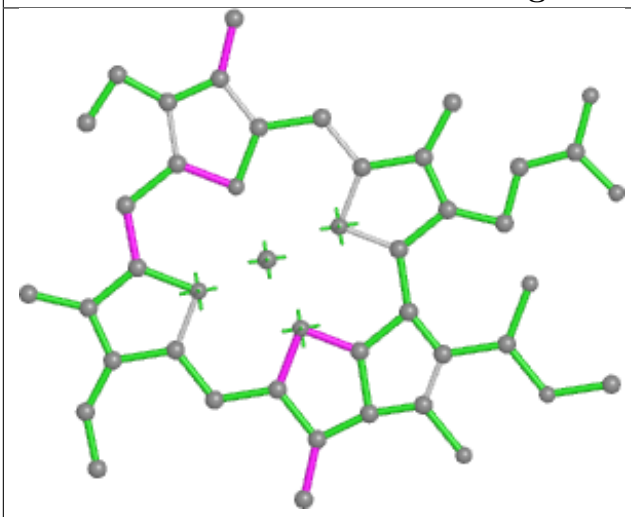


Rings

Ligand CLA 6 511



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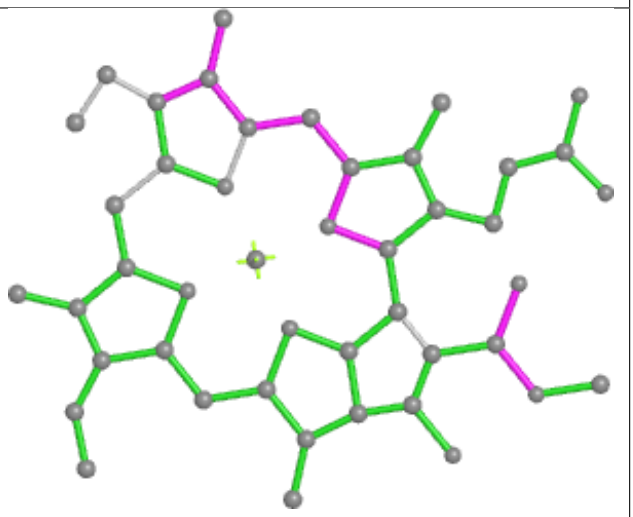
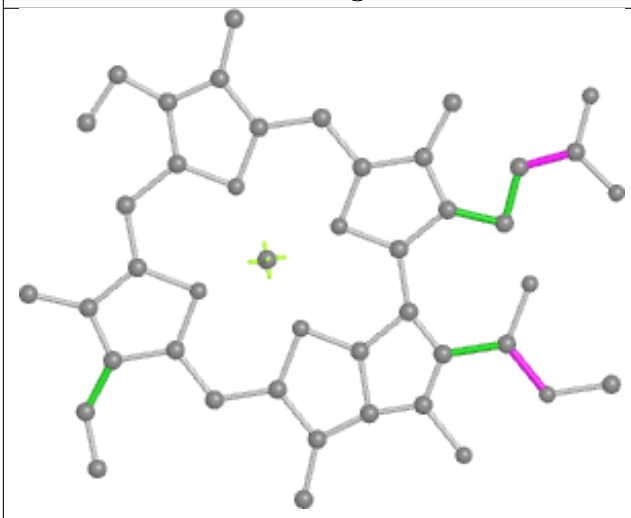


Bond angles



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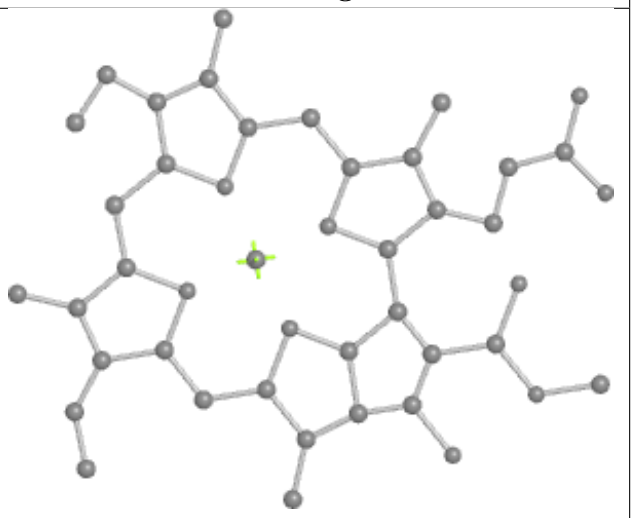

Rings

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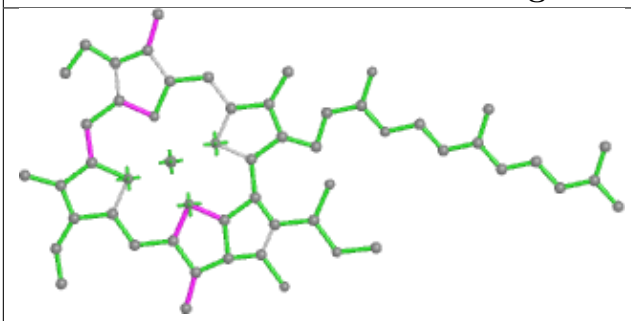

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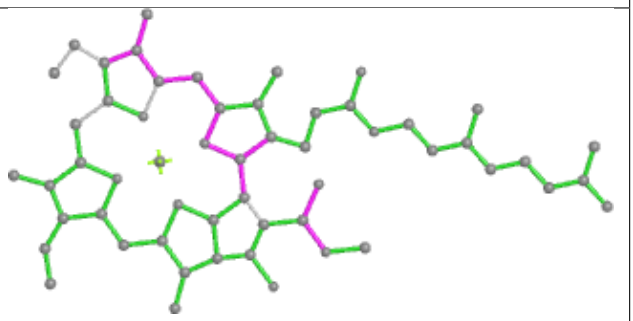
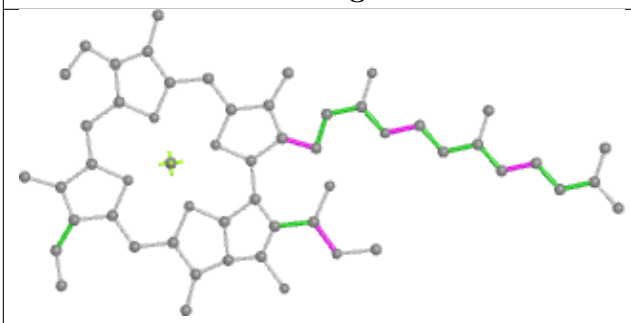


Bond angles



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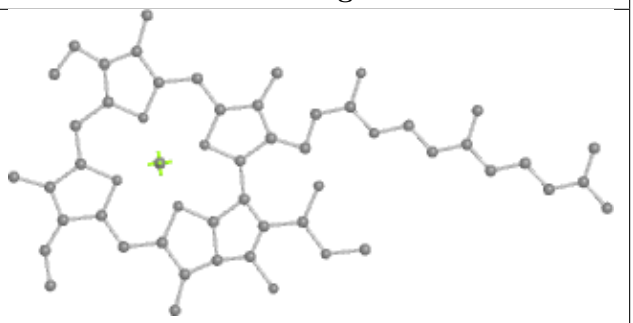
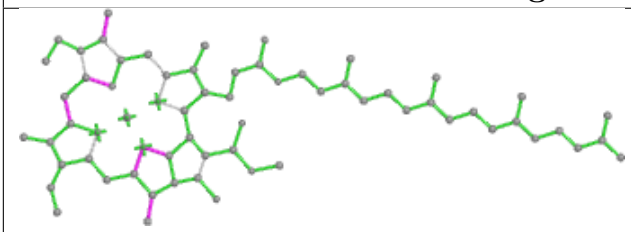


Rings

Ligand CLA 4 509



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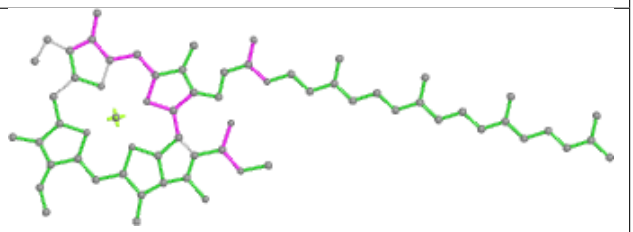
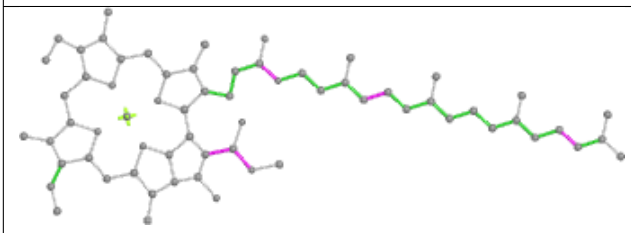


Bond angles



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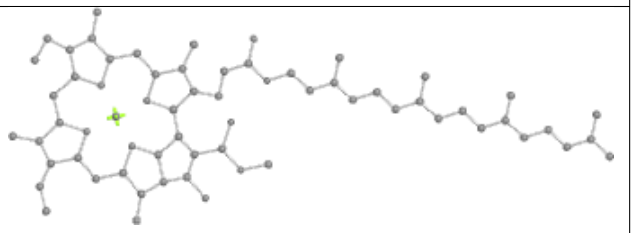
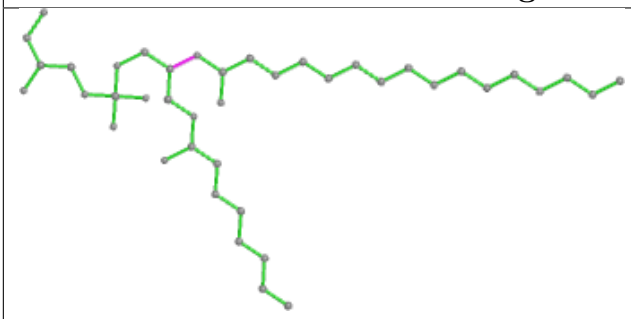
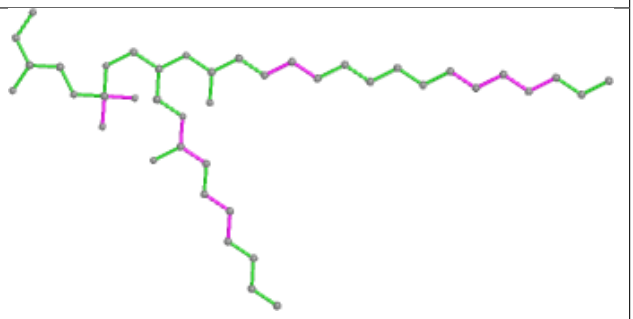


Rings

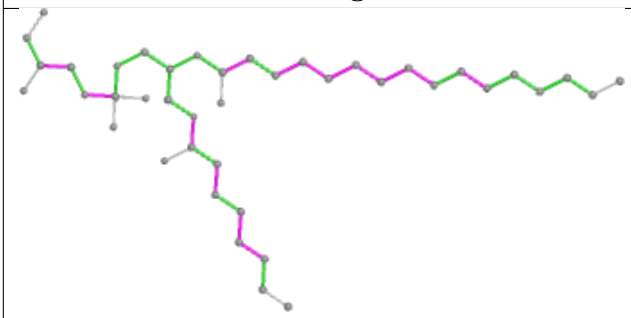
Ligand LHG e 5003



Bond lengths



Bond angles



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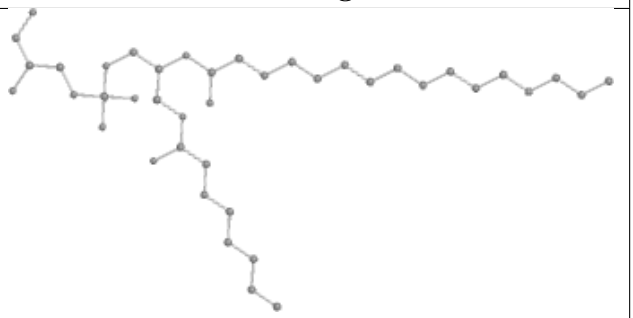
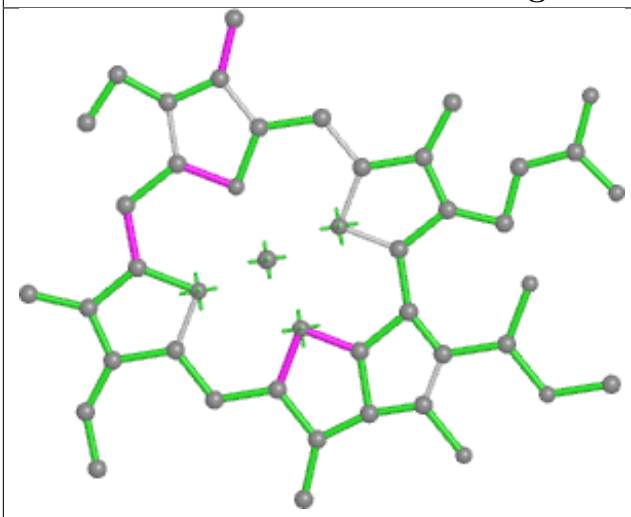
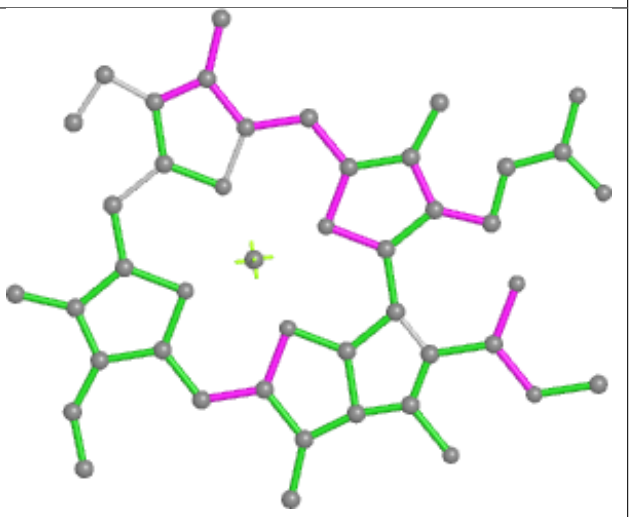


Rings

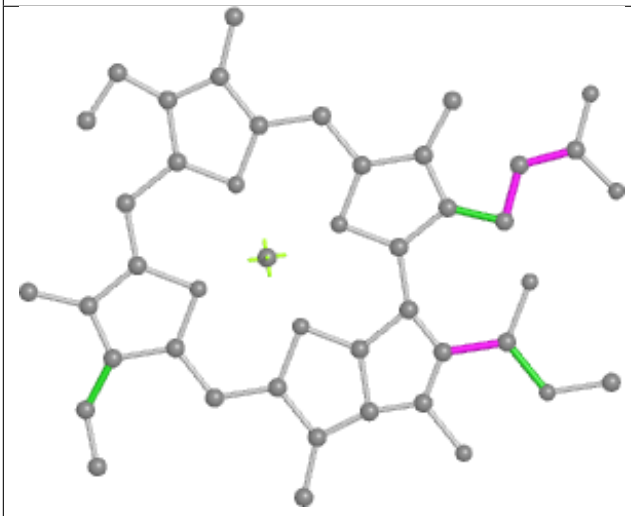
Ligand CLA 6 504



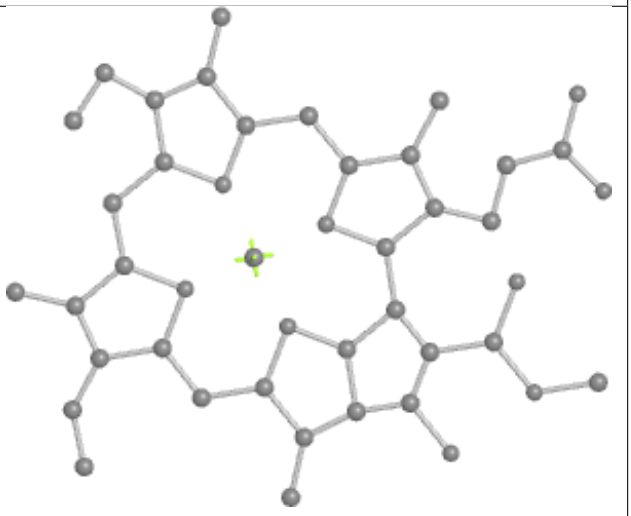
Bond lengths



Bond angles

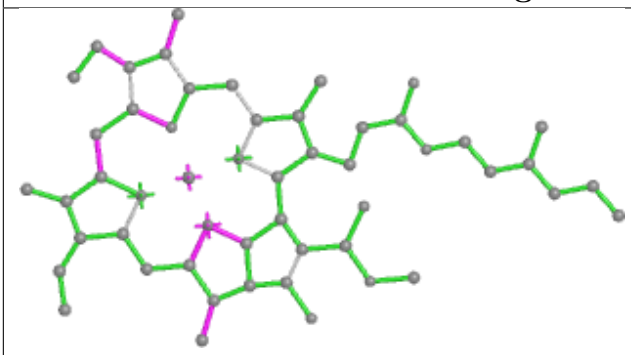


Torsions



Rings

Ligand CLA A 1135



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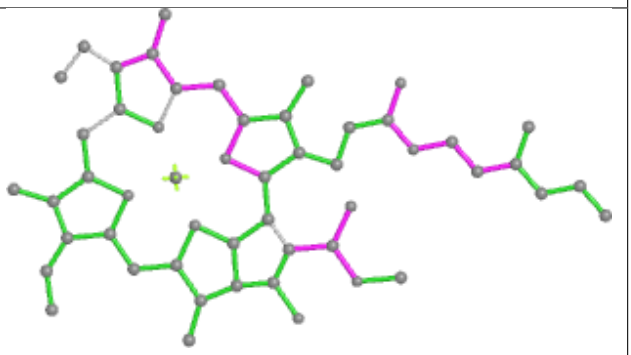

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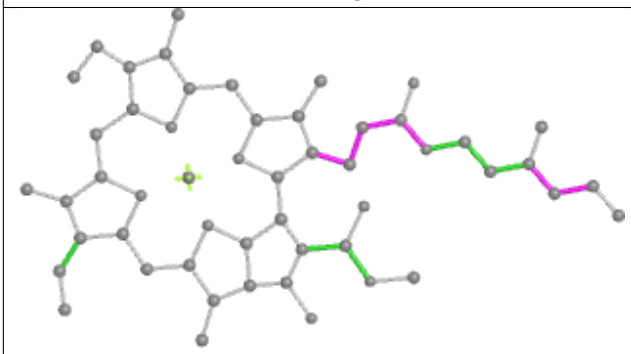

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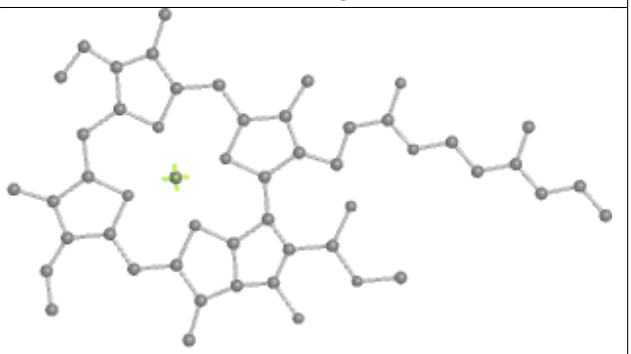
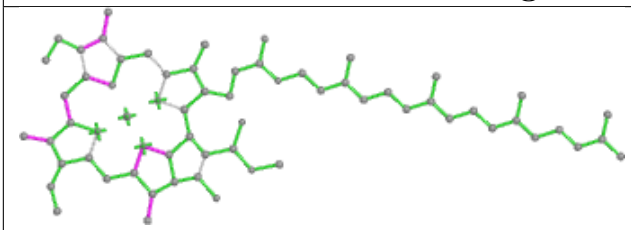
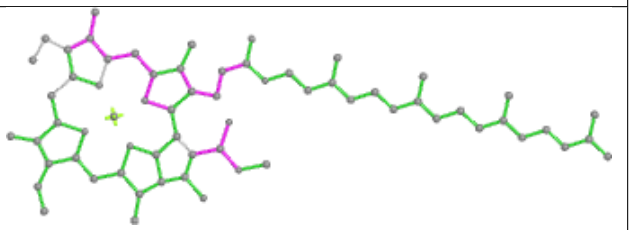


Rings

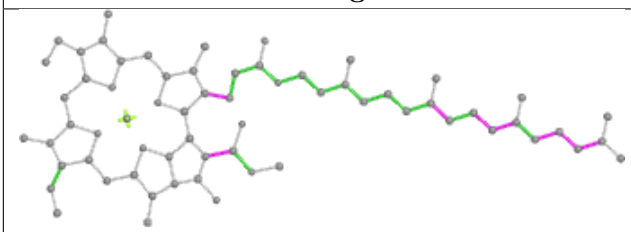
Ligand CLA e 1101



Bond lengths



Bond angles



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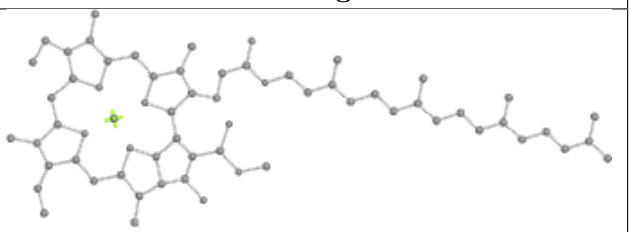
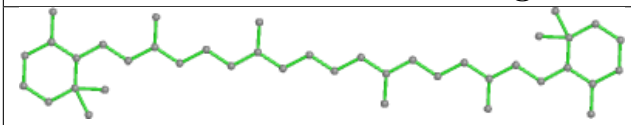


Rings

Ligand BCR B 4005



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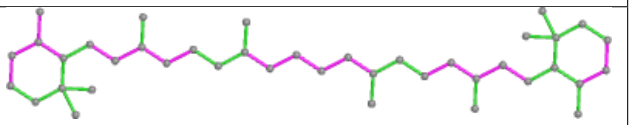
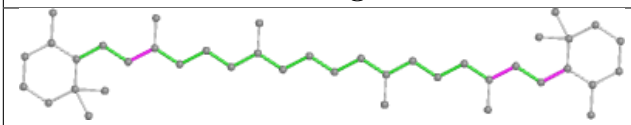


Bond angles



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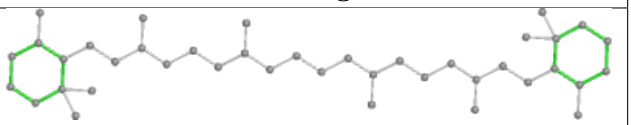
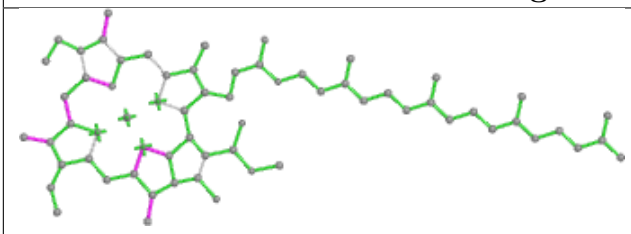


Rings

Ligand CLA r 507



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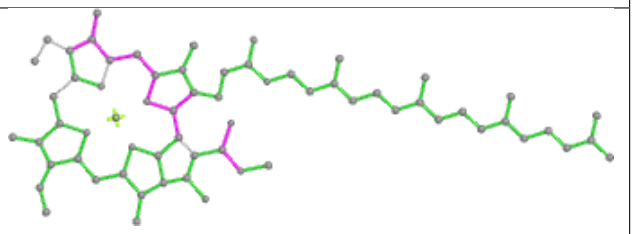

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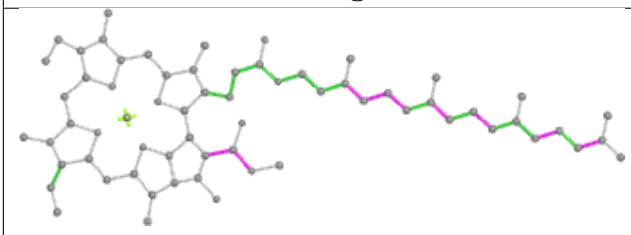

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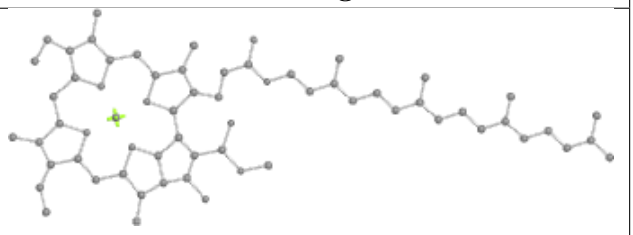
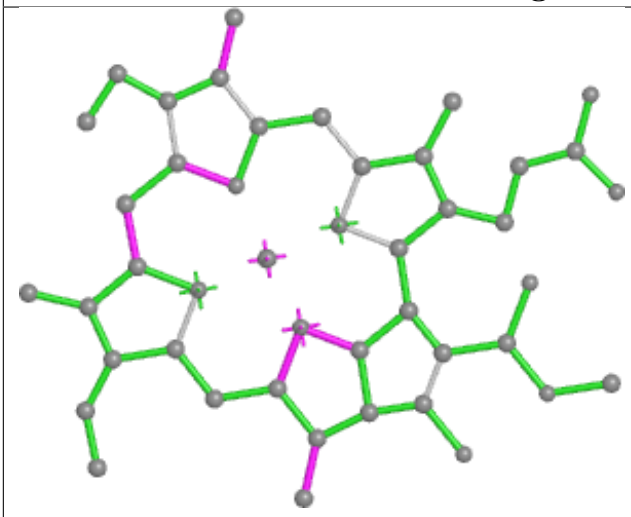


Rings

Ligand CLA s 512



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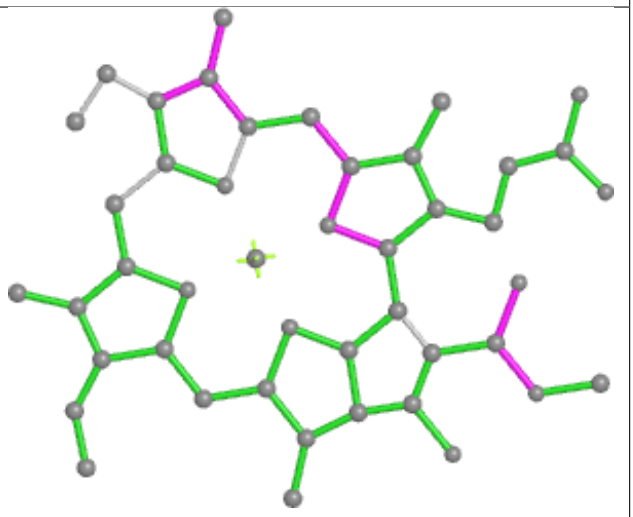
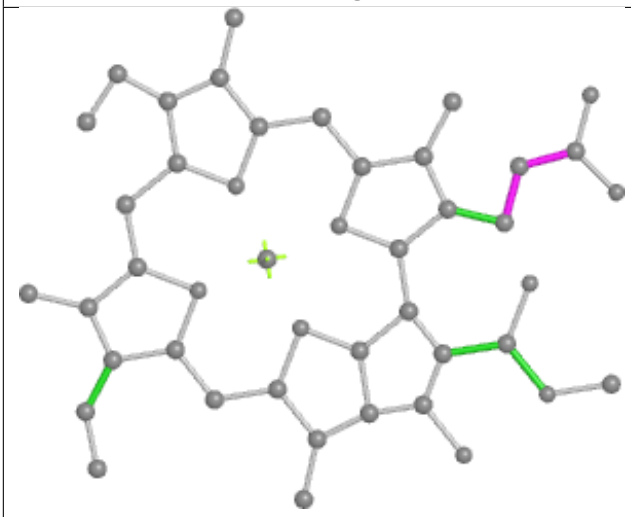


Bond angles



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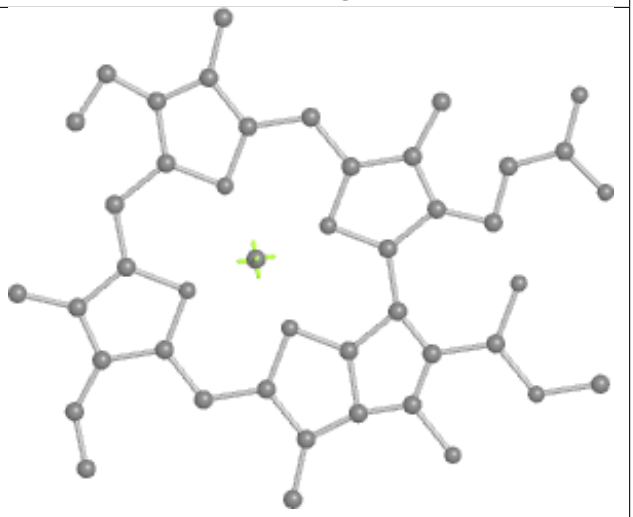
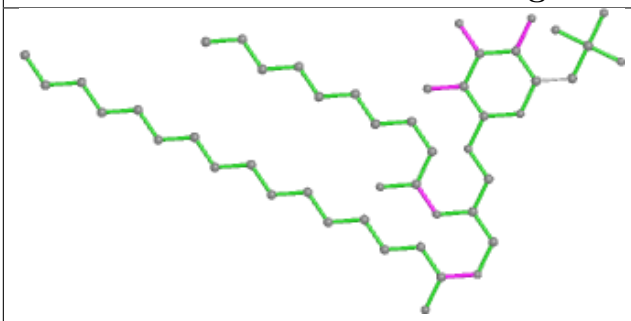


Rings

Ligand SQD 1 822



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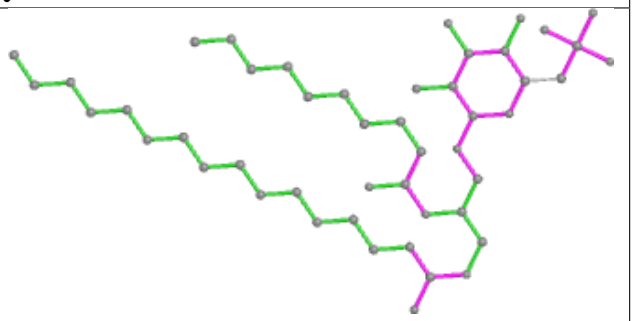
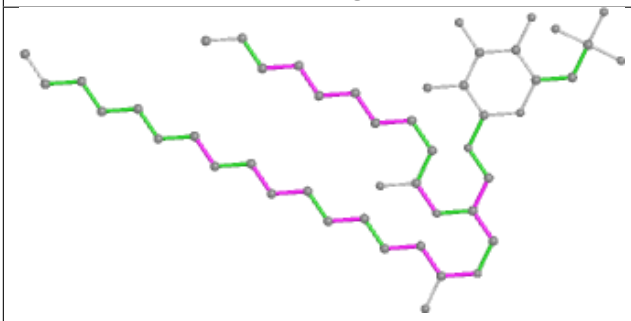


Bond angles



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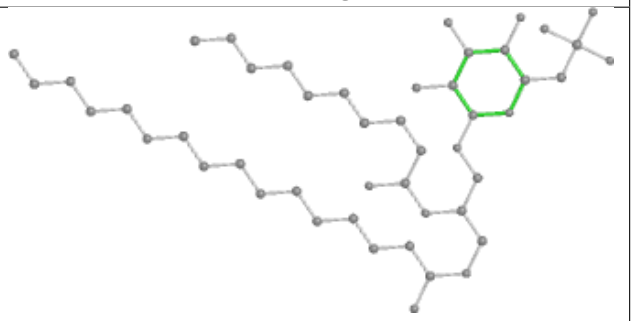
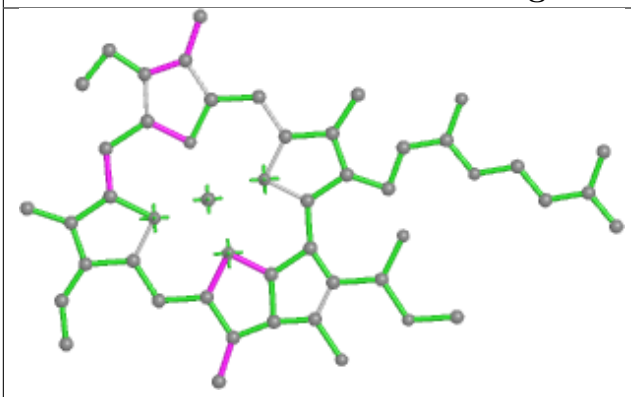


Rings

Ligand CLA a 502



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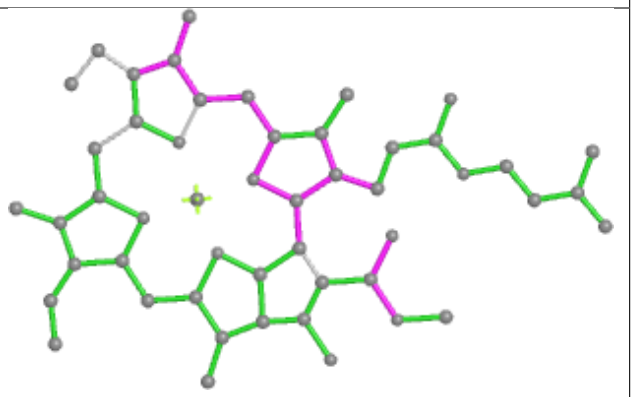
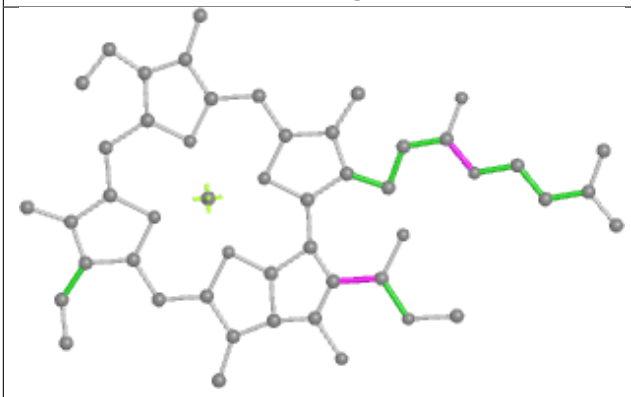
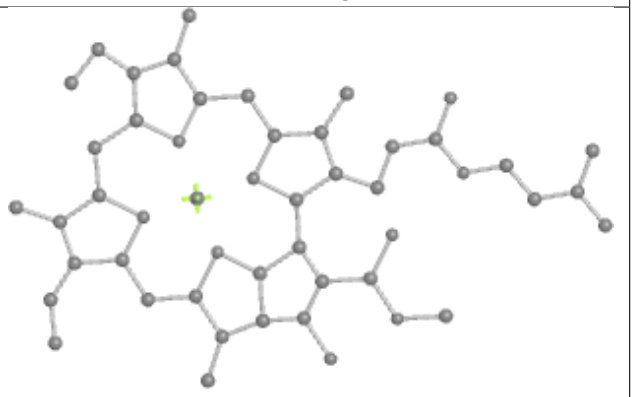


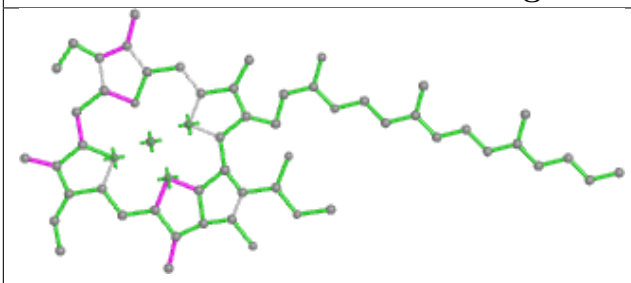
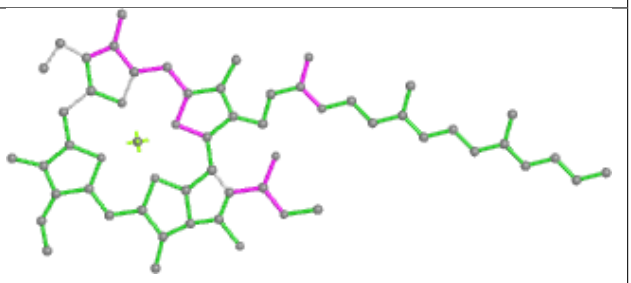
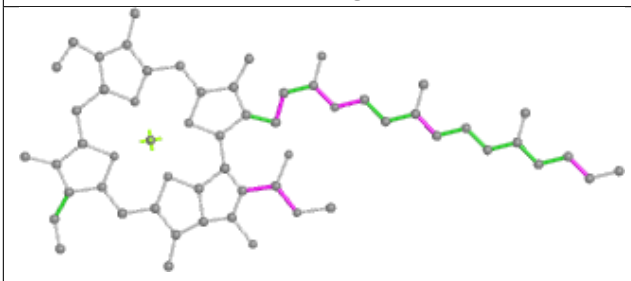
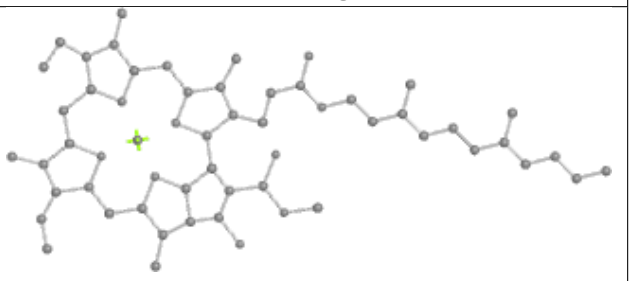
Bond angles

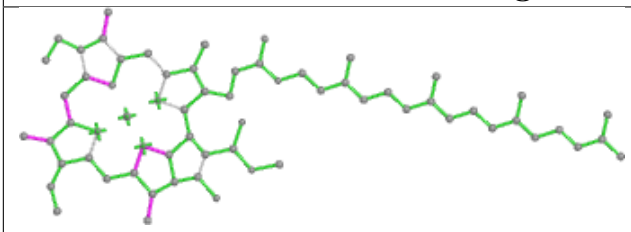
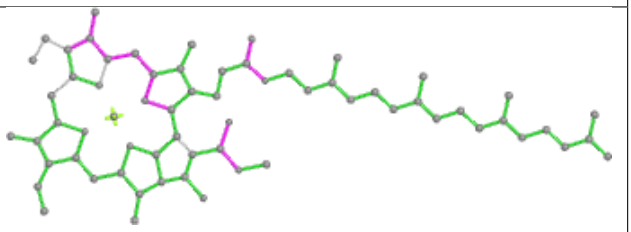


Torsions



Rings

Ligand CLA l 1302	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA G 1111	
	
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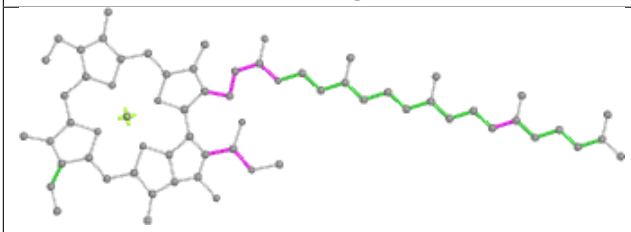
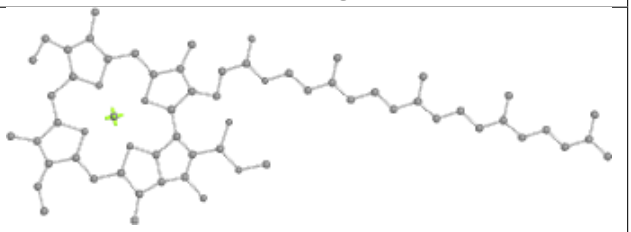
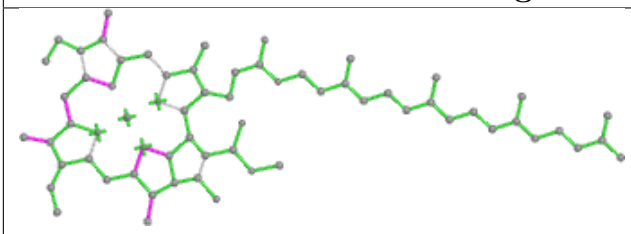
	
Torsions	**Rings**

Ligand CLA A 1126



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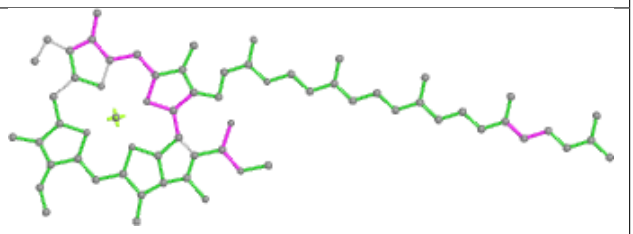
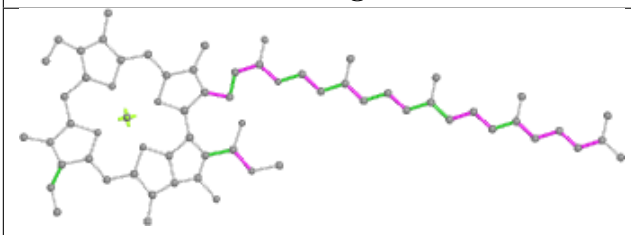


Bond angles



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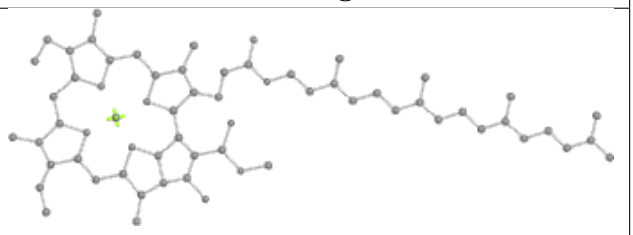
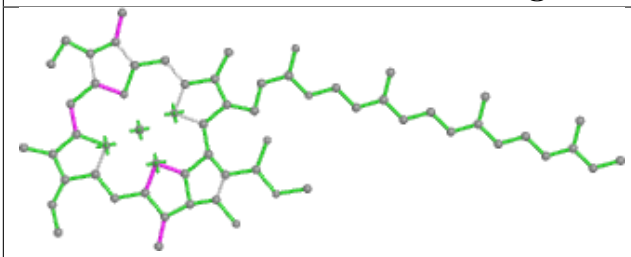


Rings

Ligand CLA 5 505



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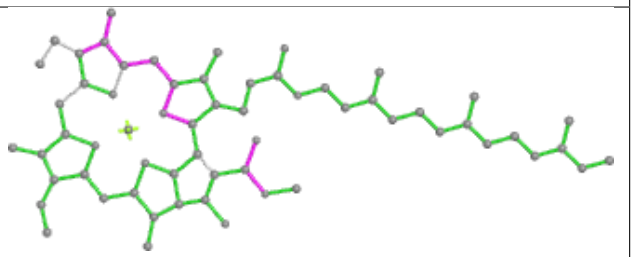
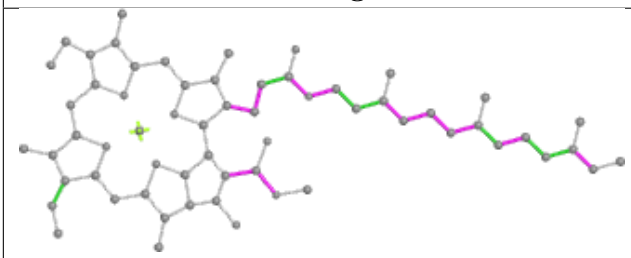
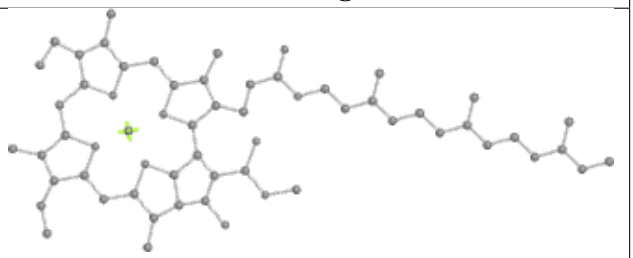


Bond angles

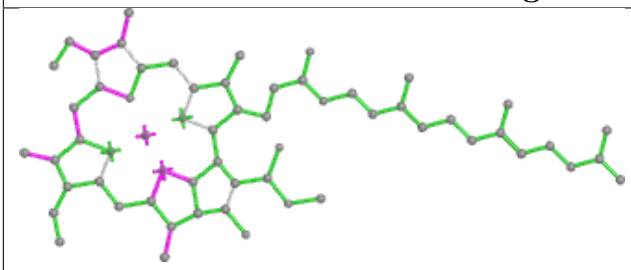


Torsions

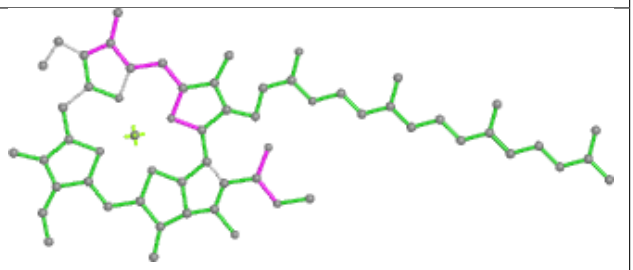


Rings

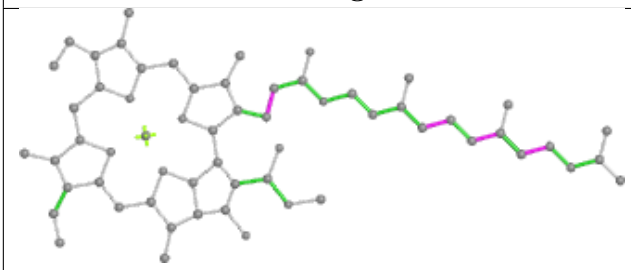
Ligand CLA f 1216



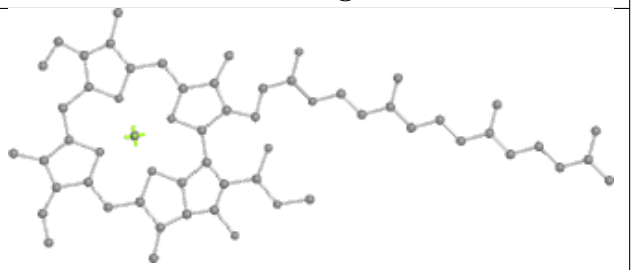
Bond lengths



Bond angles

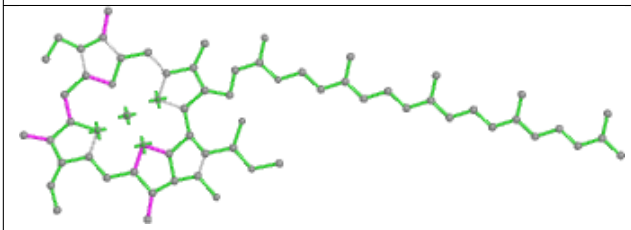


Torsions

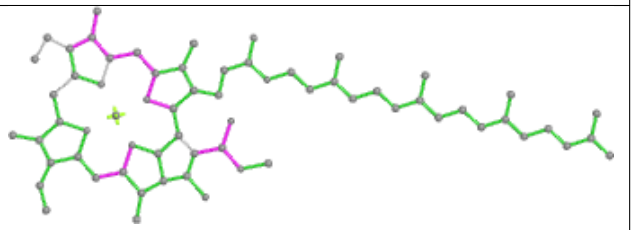


Rings

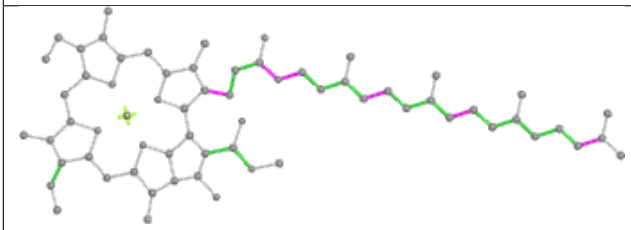
Ligand CLA n 1502



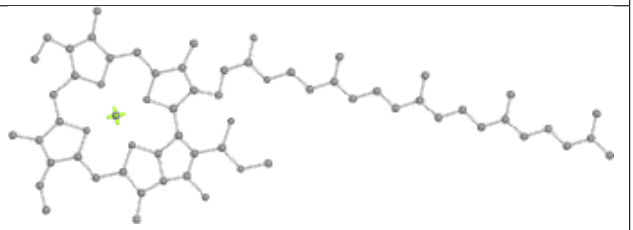
Bond lengths



Bond angles

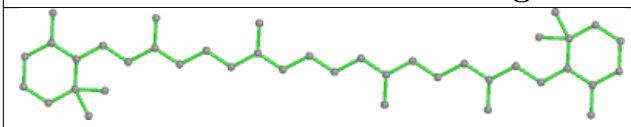


Torsions

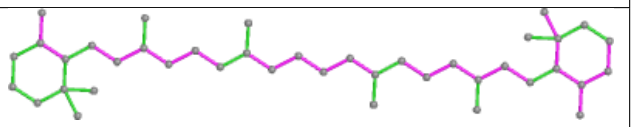


Rings

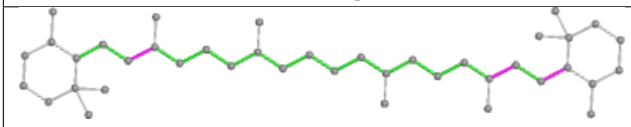
Ligand BCR V 4019



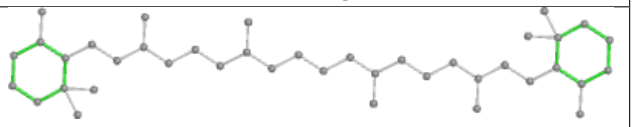
Bond lengths



Bond angles

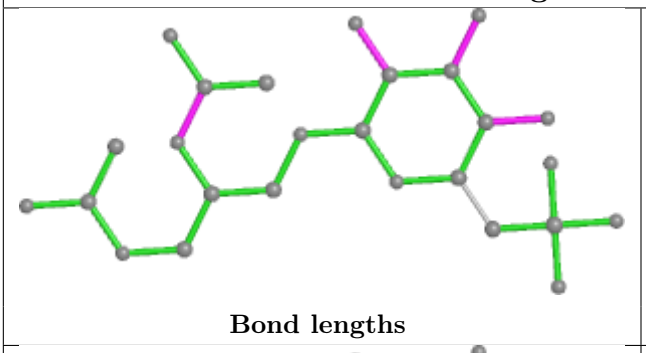


Torsions



Rings

Ligand SQD t 822



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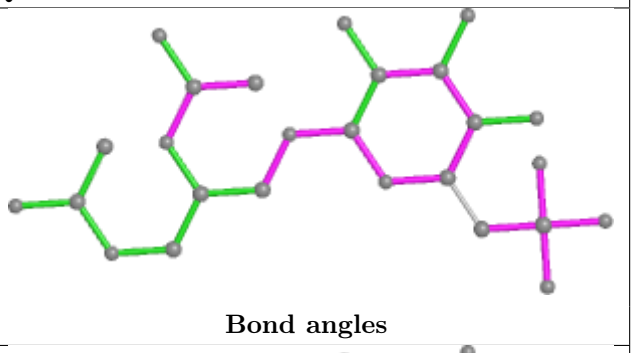

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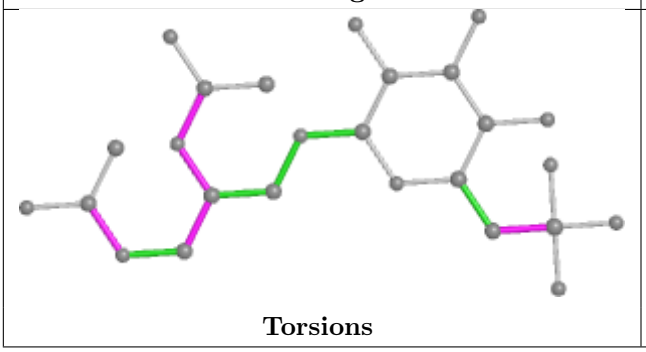

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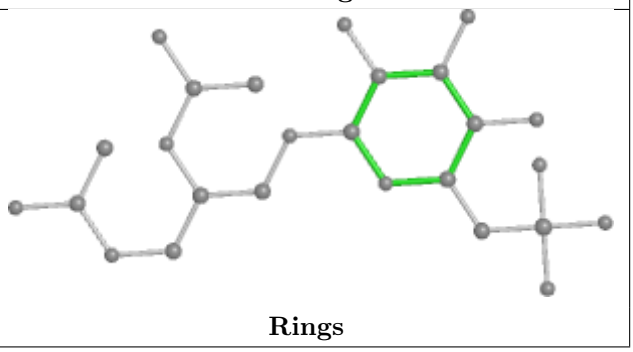
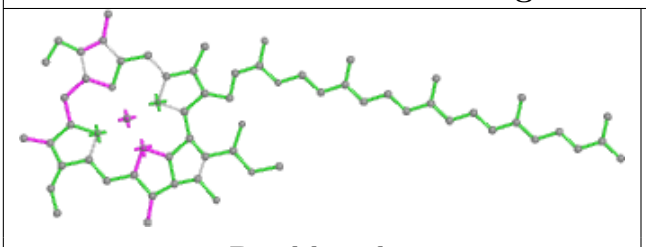


Rings

Ligand CLA B 1206



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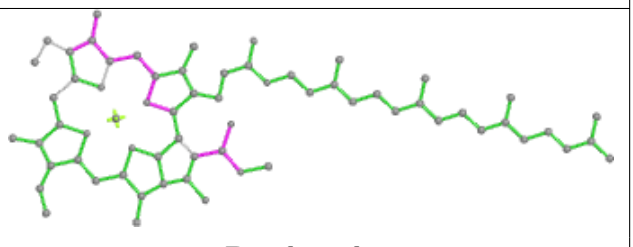
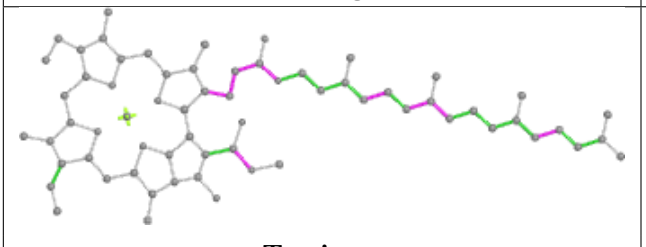


Bond angles



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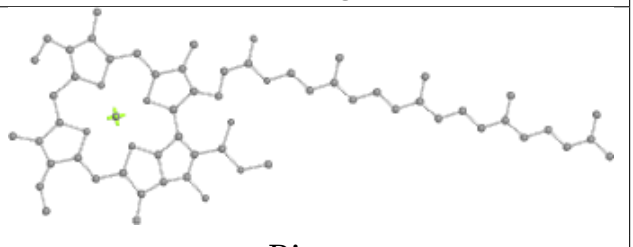
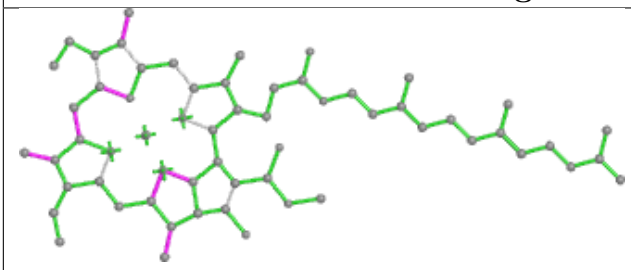


Rings

Ligand CLA V 1503



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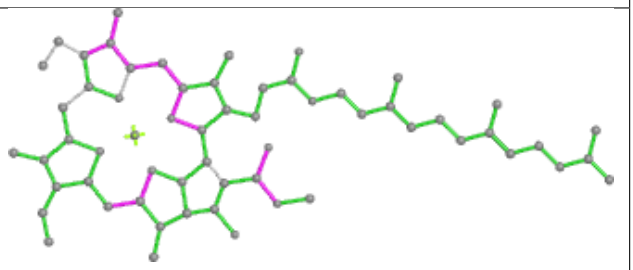

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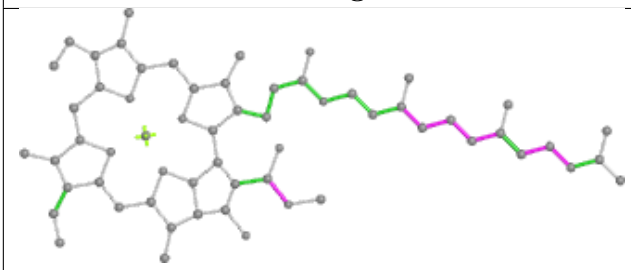
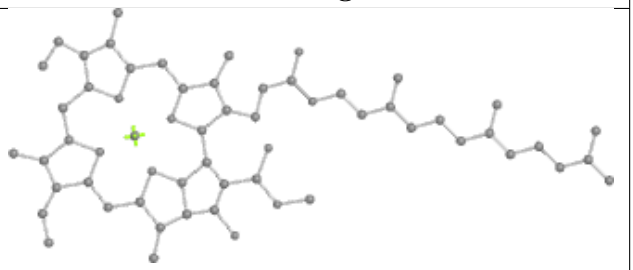
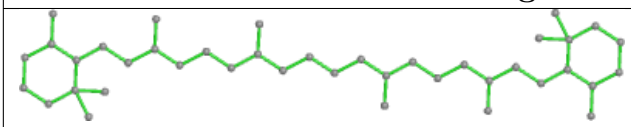


Torsions



Rings

Ligand BCR e 4007



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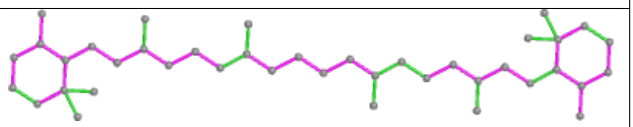

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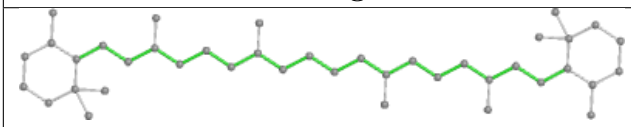

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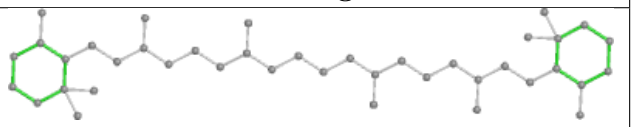
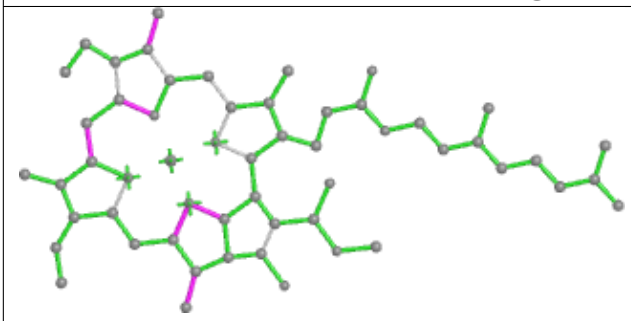


Rings

Ligand CLA 1 511



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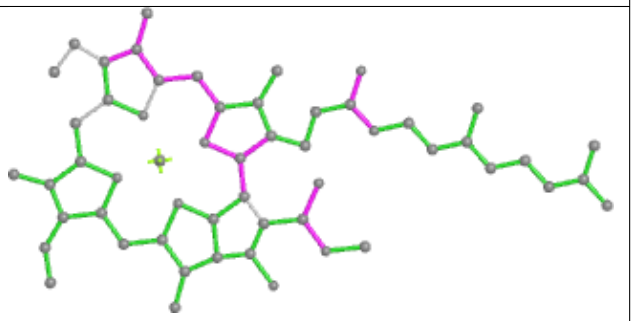

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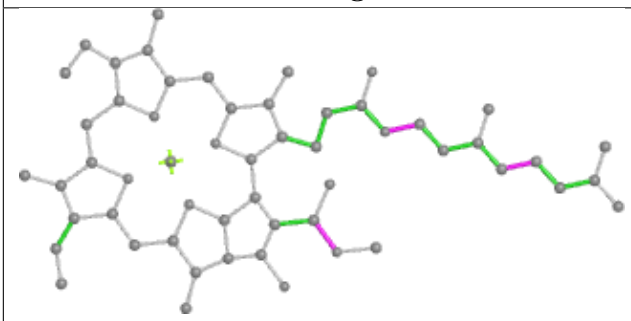

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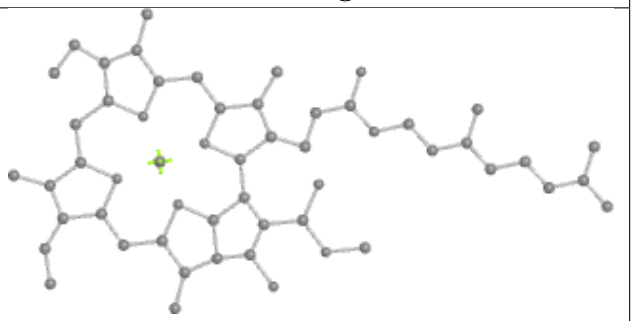
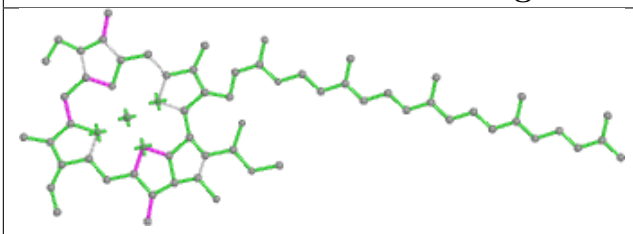


Rings

Ligand CLA H 1240



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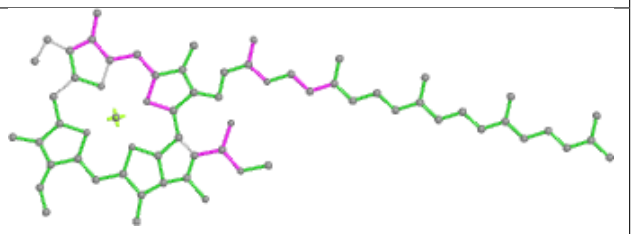
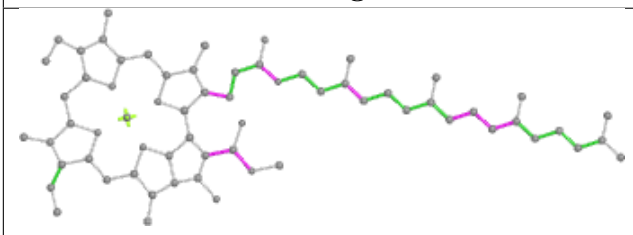


Bond angles



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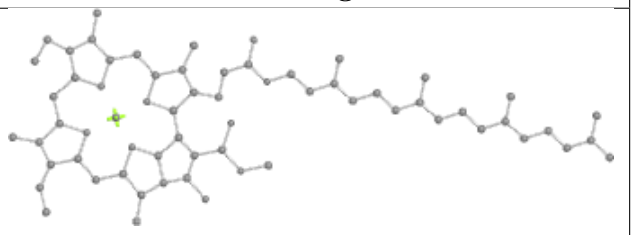
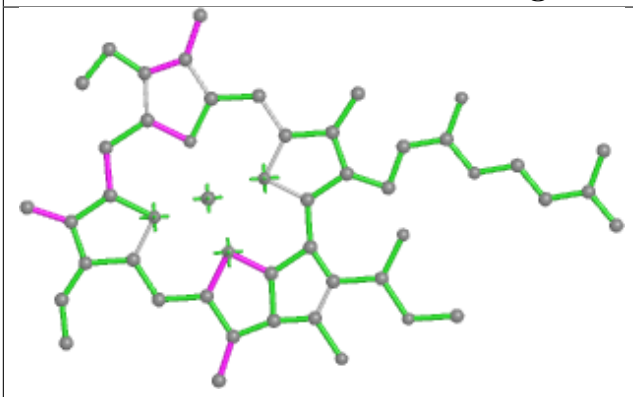


Rings

Ligand CLA c 502



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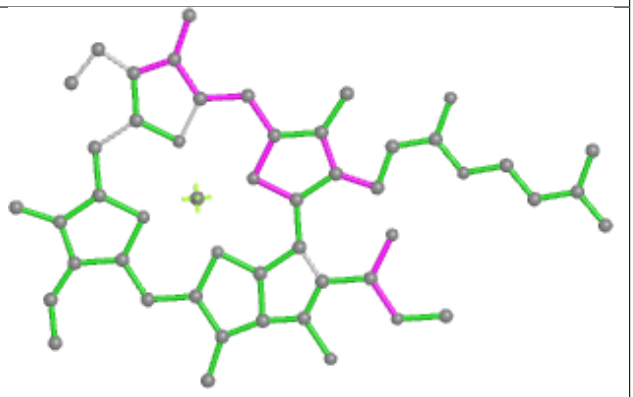
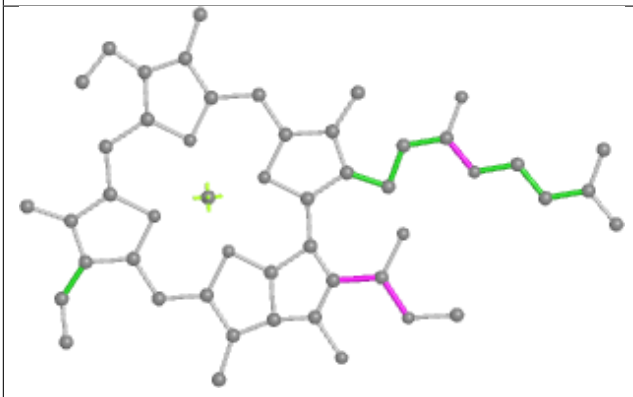


Bond angles



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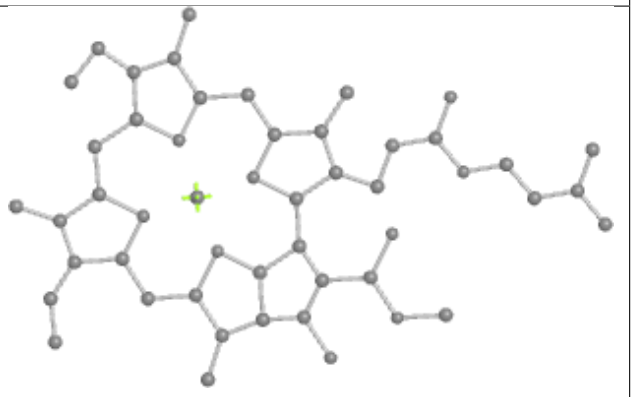
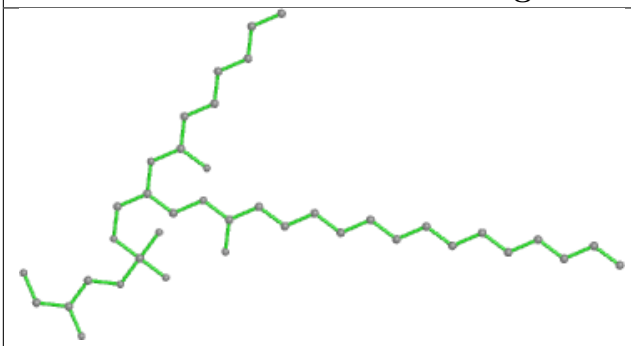


Rings

Ligand LHG B 1842



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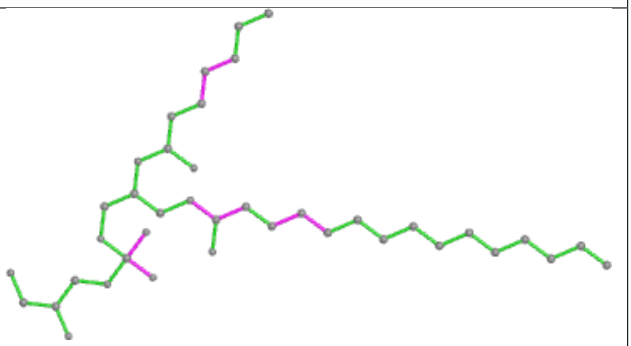
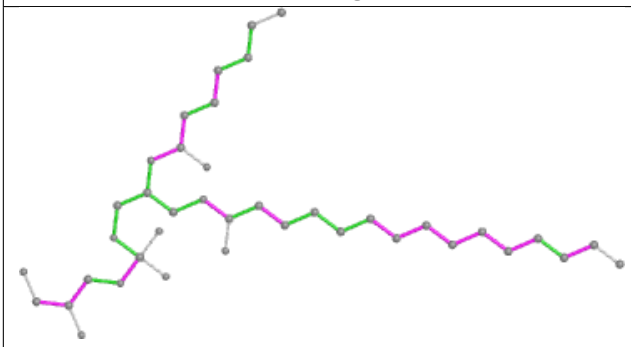


Bond angles



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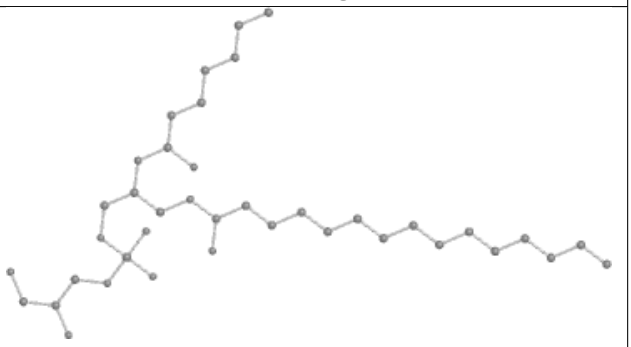
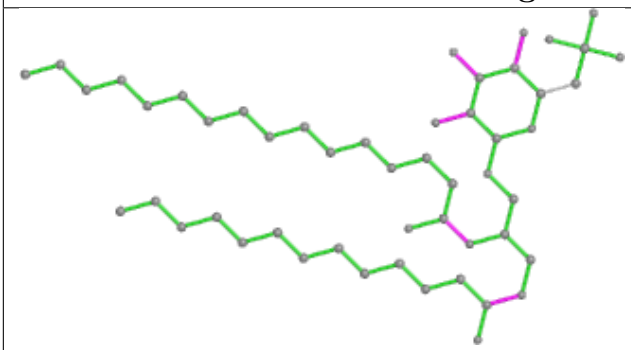


Rings

Ligand SQD n 5216



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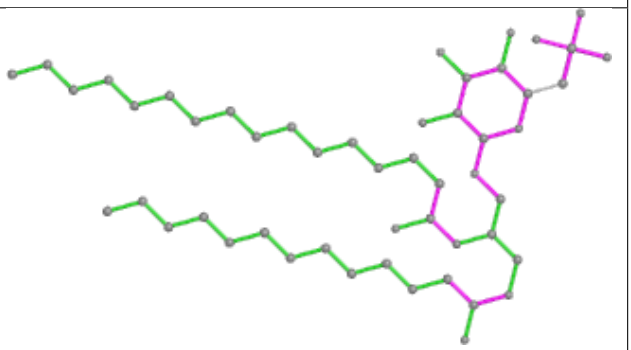
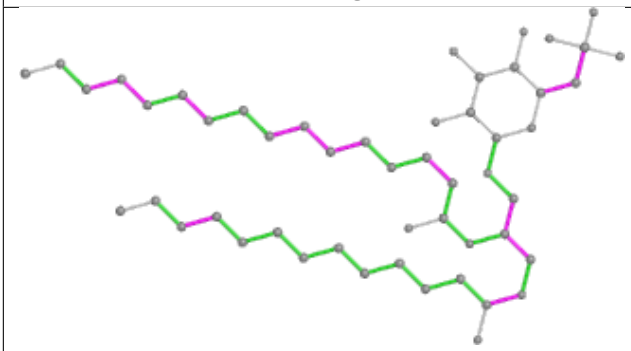


Bond angles



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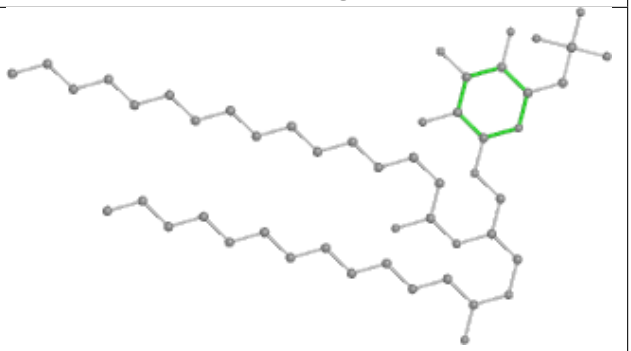
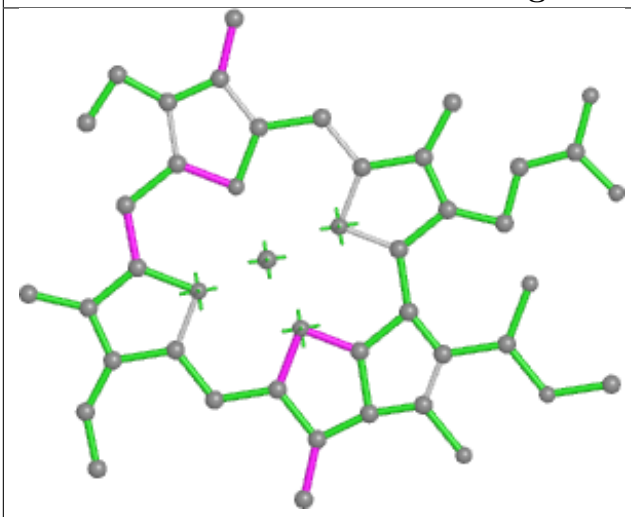


Rings

Ligand CLA 5 510



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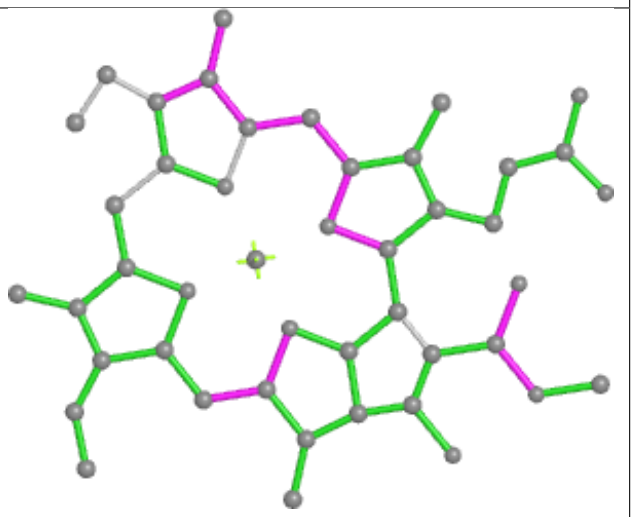
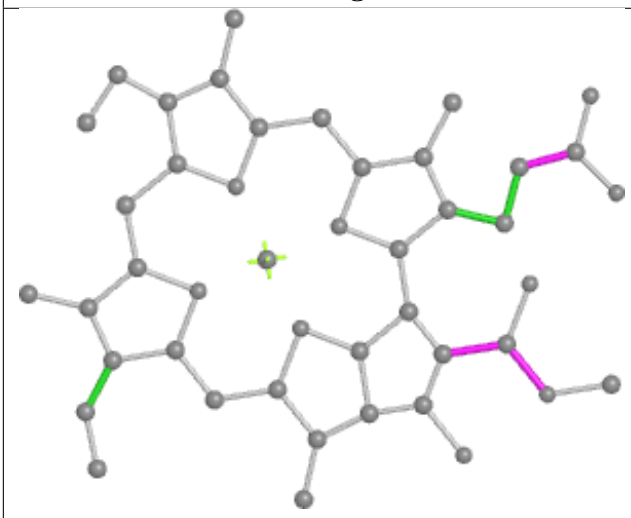


Bond angles



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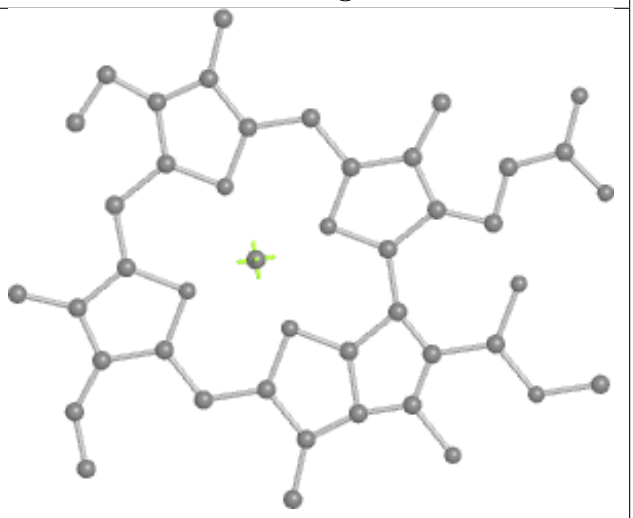
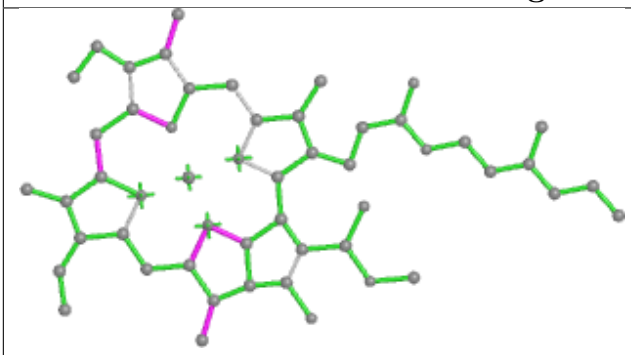


Rings

Ligand CLA q 512



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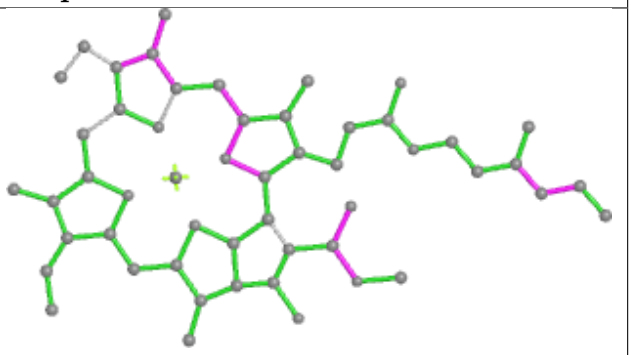
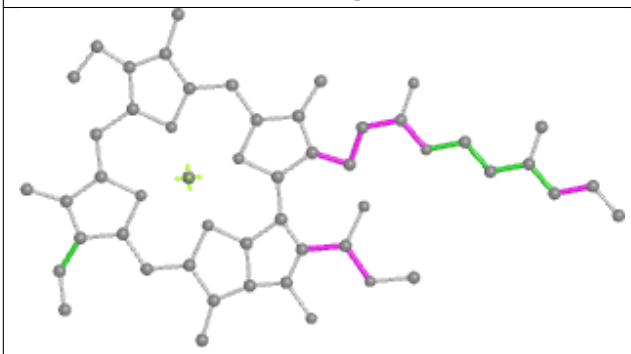


Bond angles



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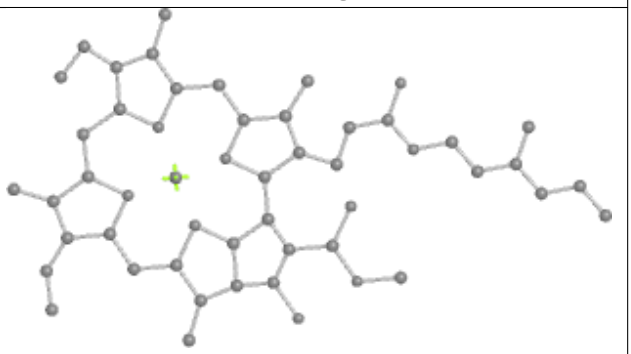
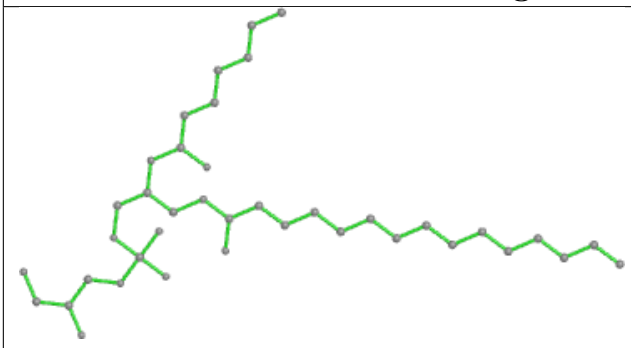


Rings

Ligand LHG H 1842



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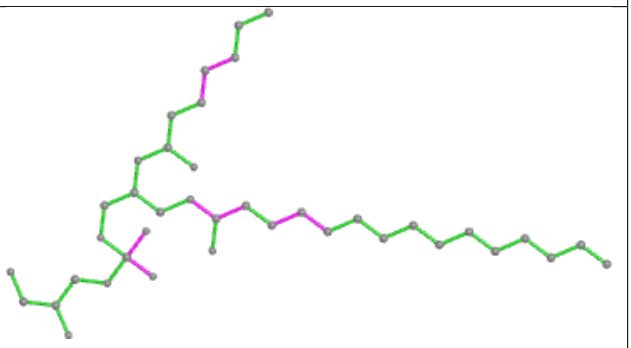
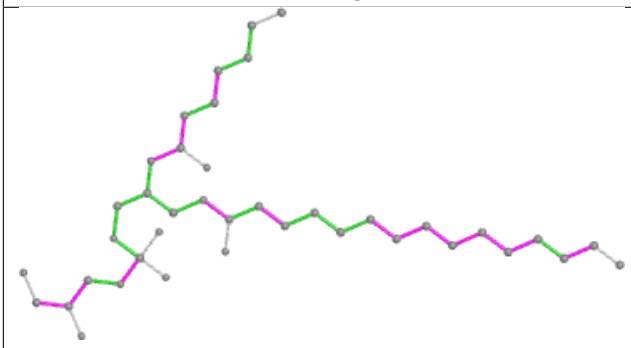


Bond angles



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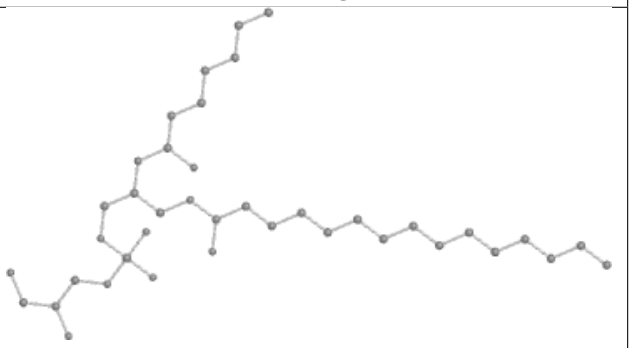
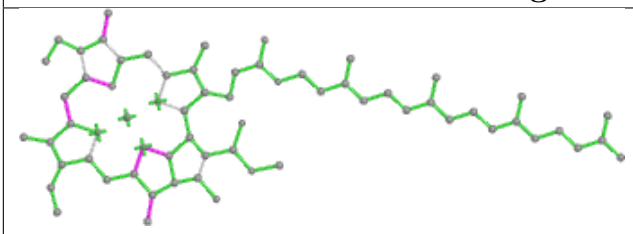


Rings

Ligand CLA r 505



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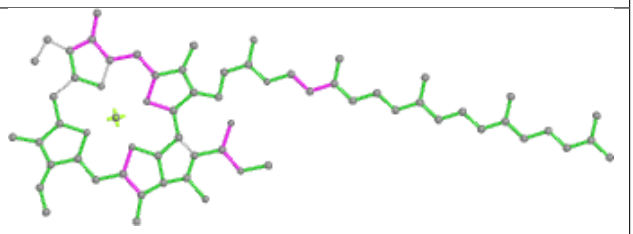
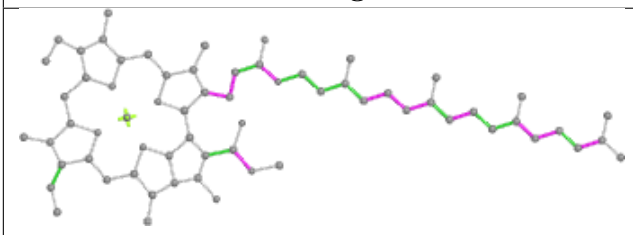


Bond angles



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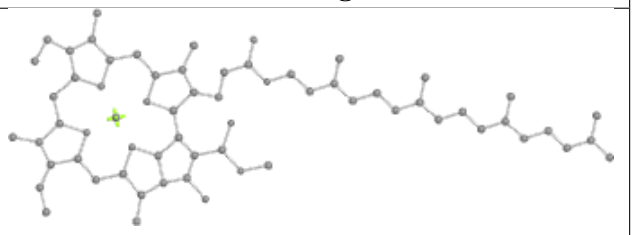
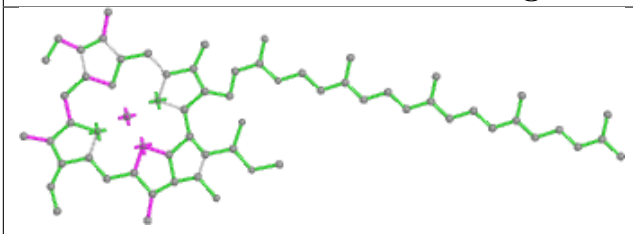
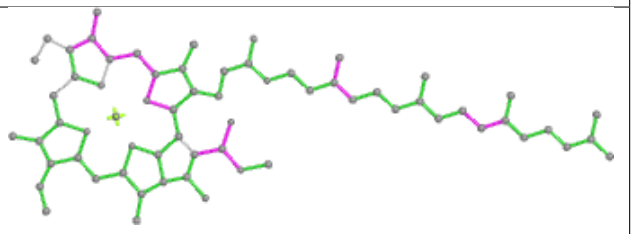


Rings

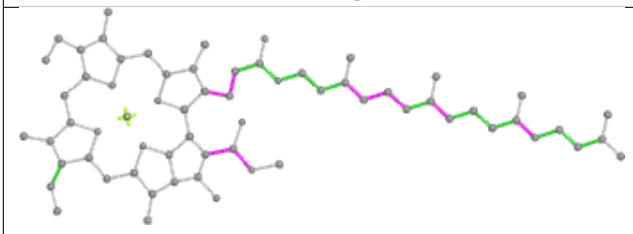
Ligand CLA f 1012



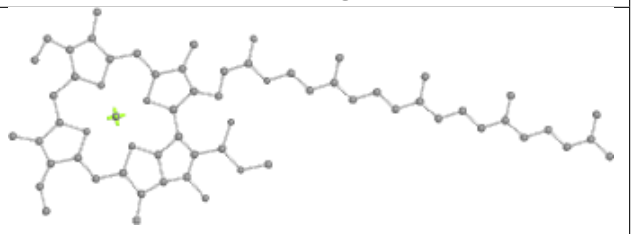
Bond lengths



Bond angles

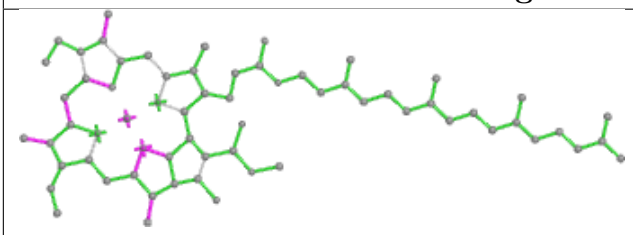


Torsions

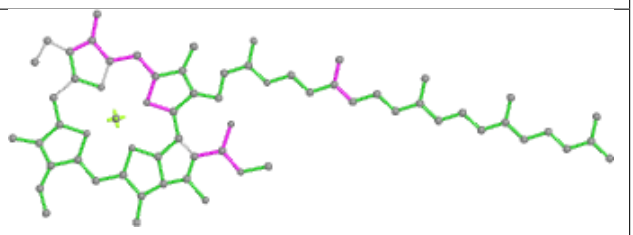


Rings

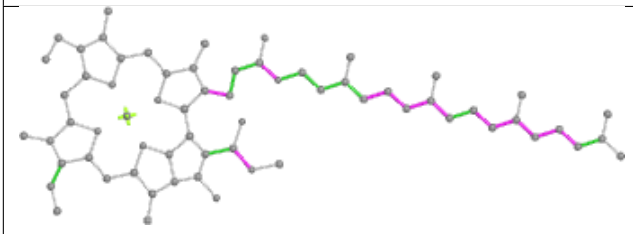
Ligand CLA B 1215



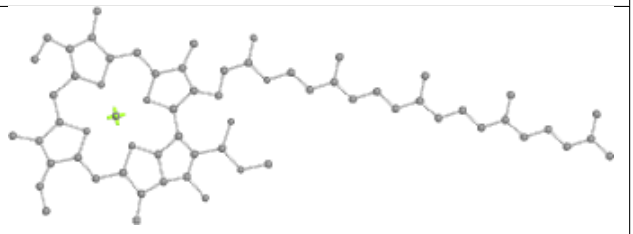
Bond lengths



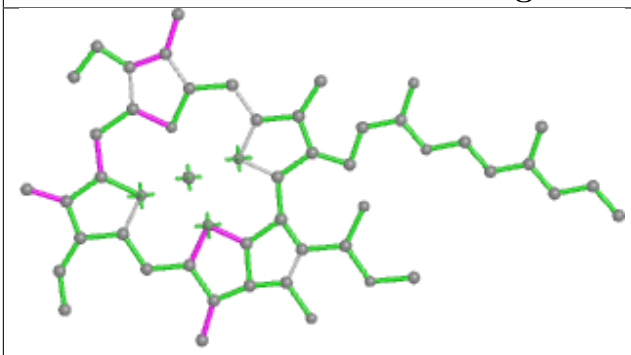
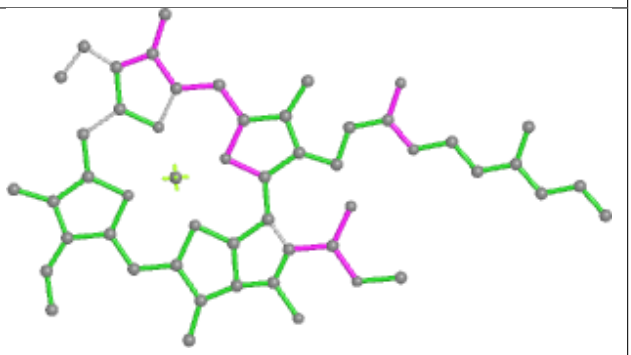
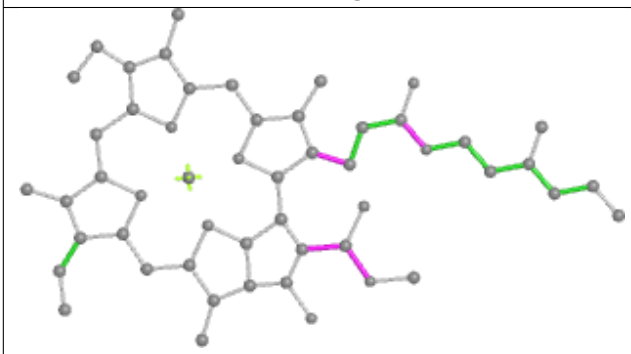
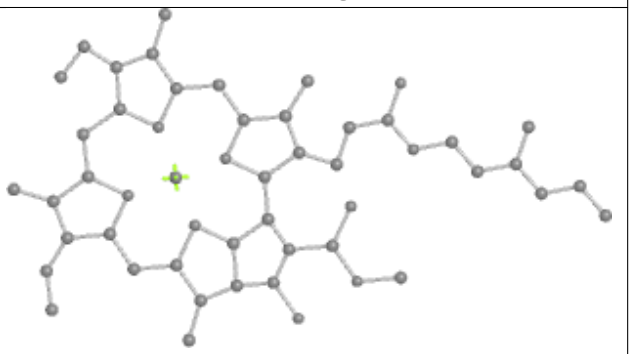
Bond angles

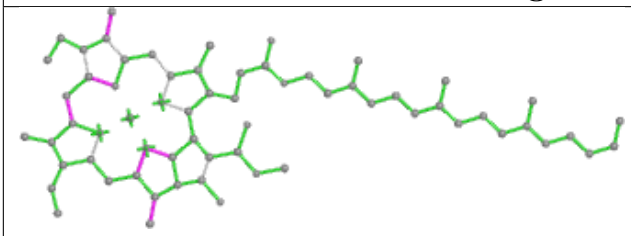
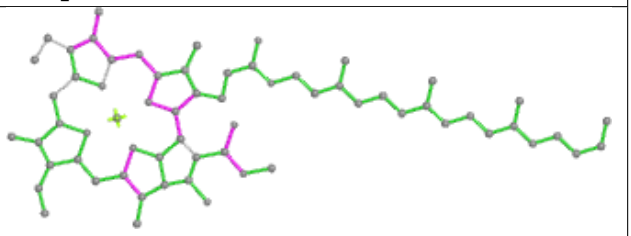
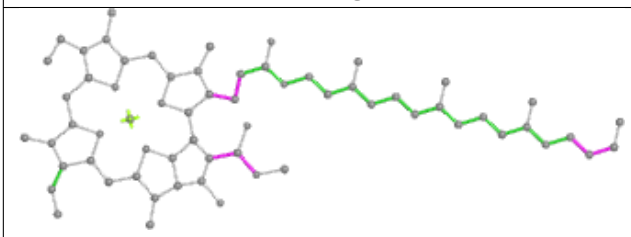
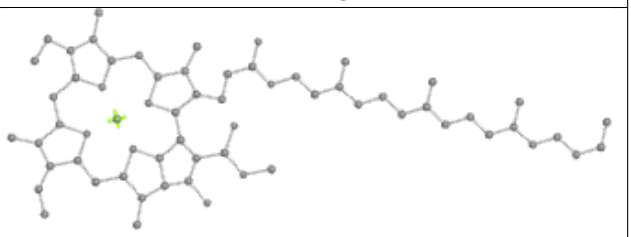


Torsions

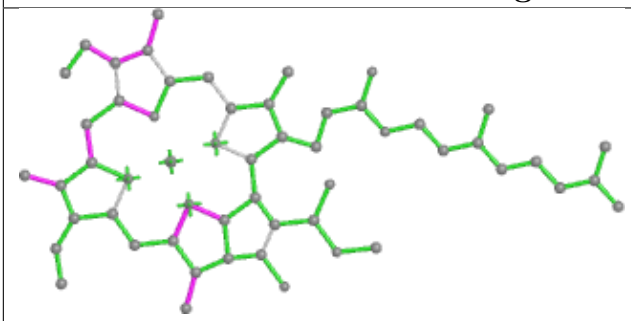


Rings

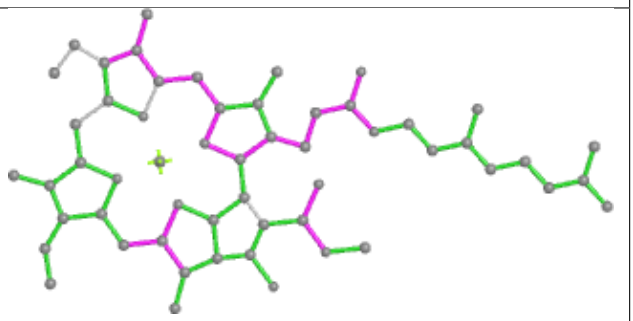
Ligand CLA B 1209	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA q 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

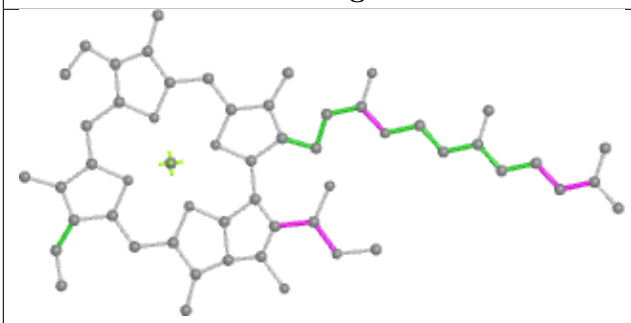
Ligand CLA H 1220



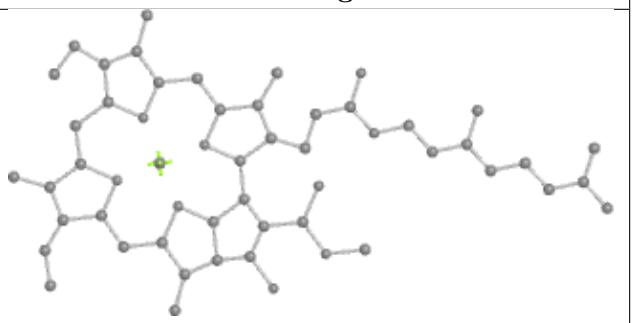
Bond lengths



Bond angles

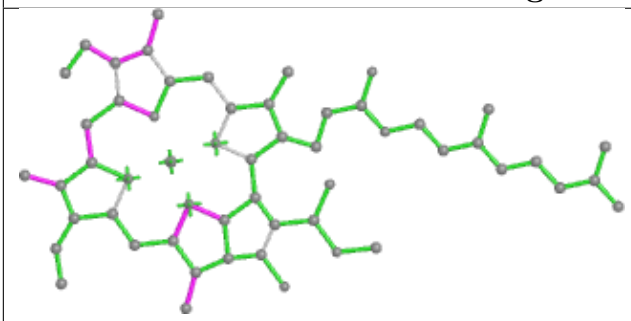


Torsions



Rings

Ligand CLA Z 519



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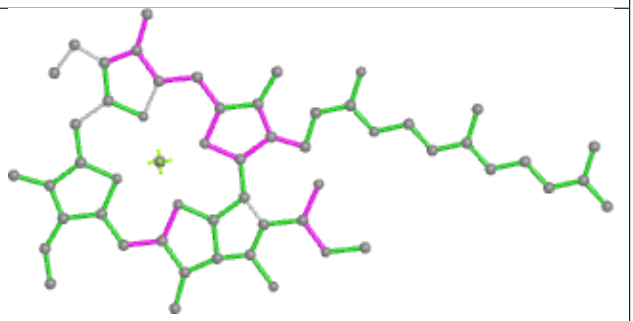
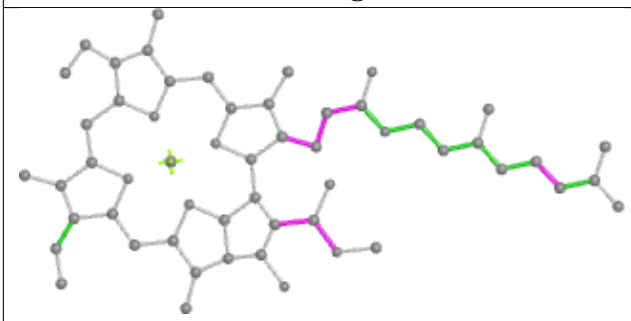


Bond angles



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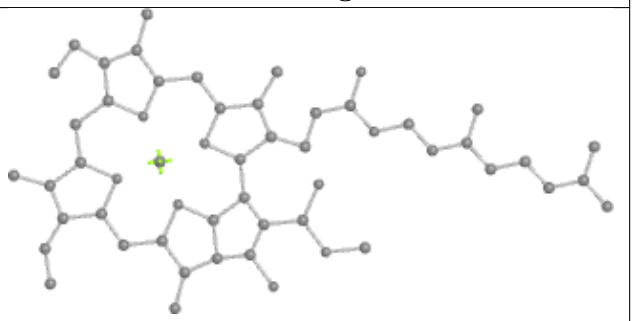
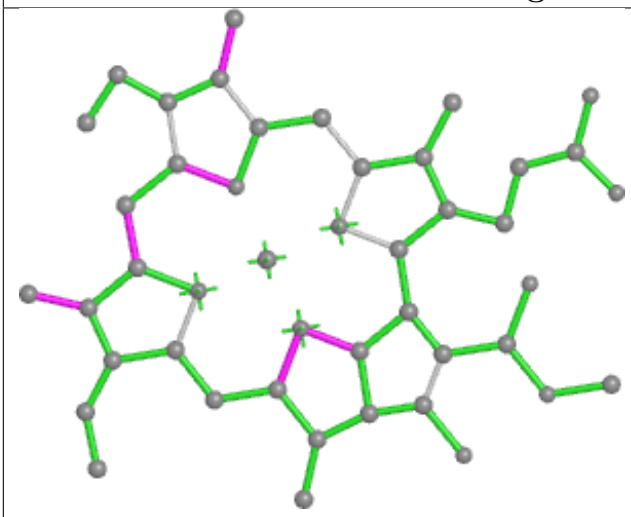


Rings

Ligand CLA b 517



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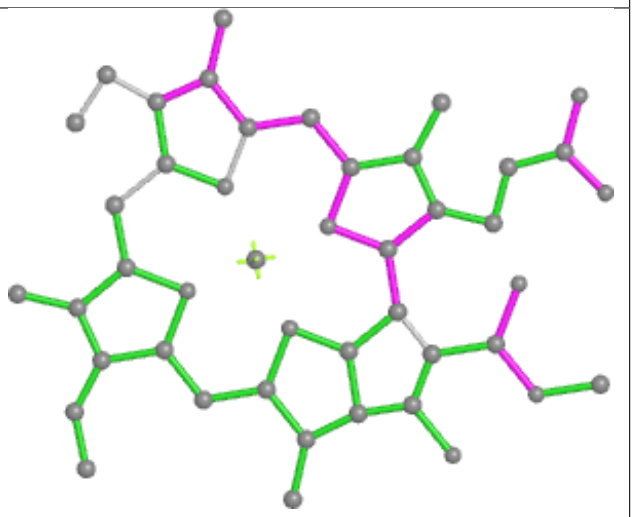
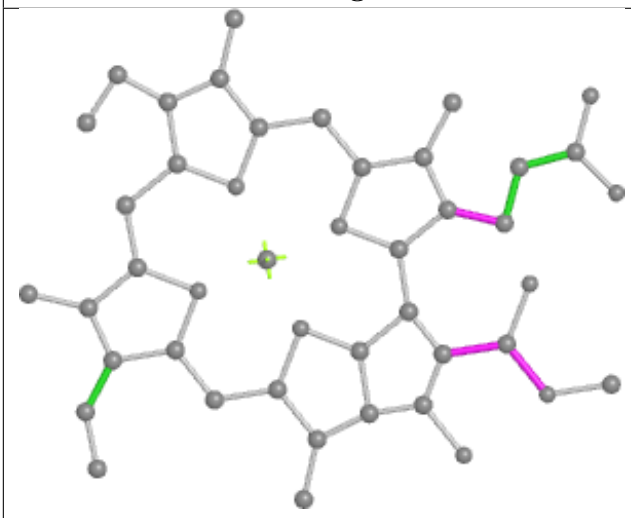


Bond angles



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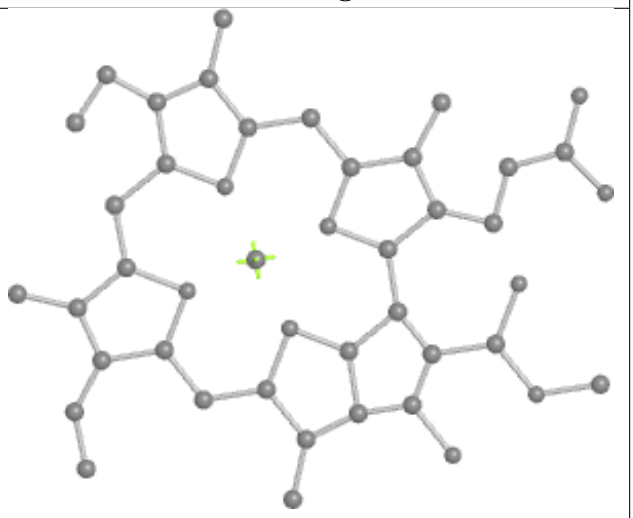
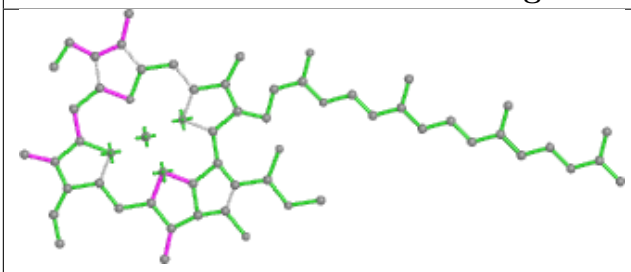


Rings

Ligand CLA Y 518



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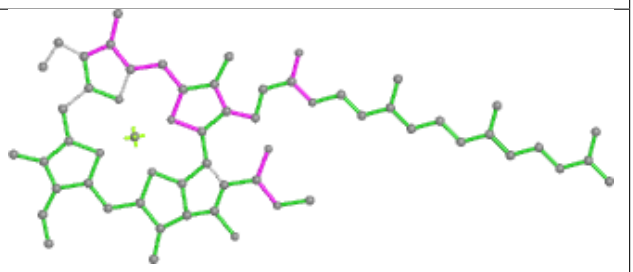
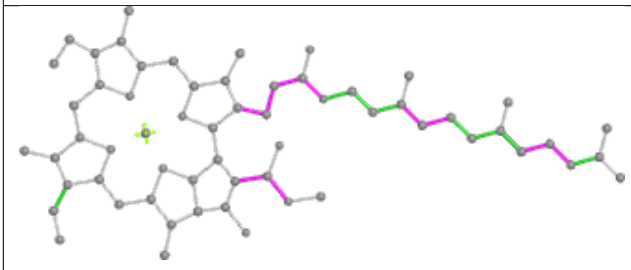


Bond angles



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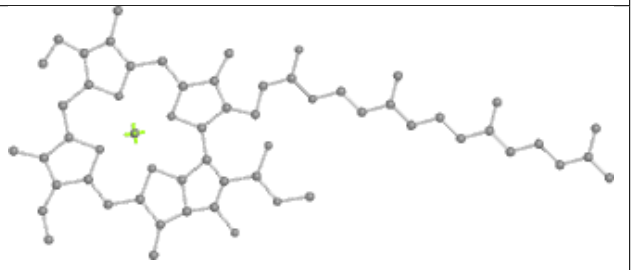
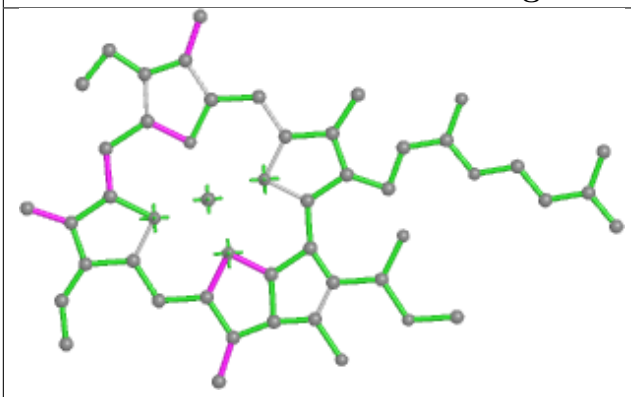


Rings

Ligand CLA f 1232



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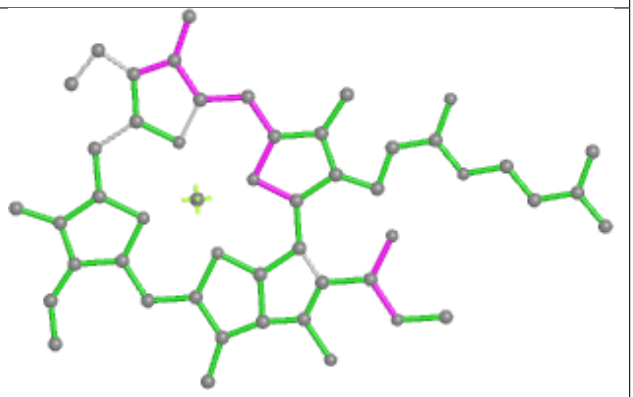
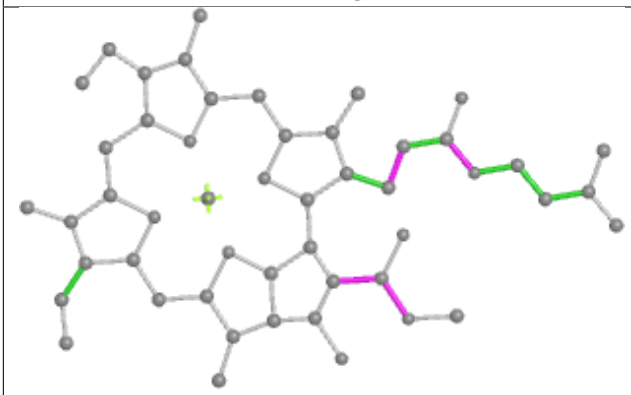


Bond angles



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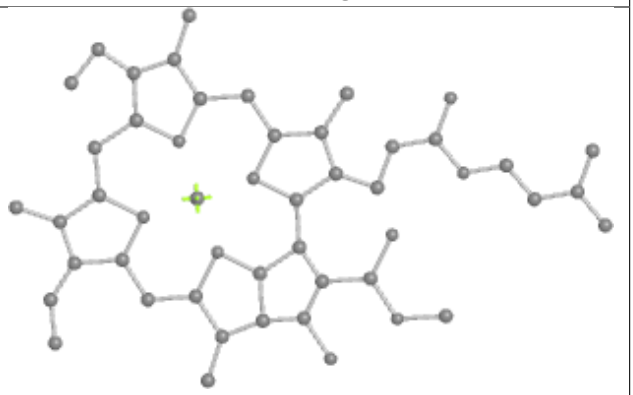
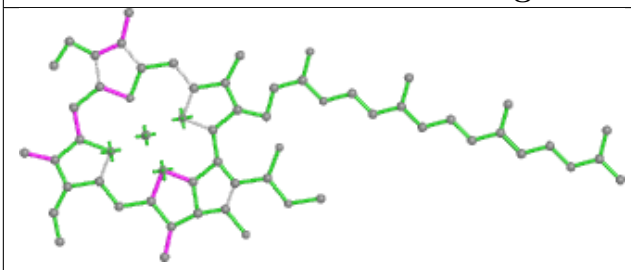


Rings

Ligand CLA G 1136



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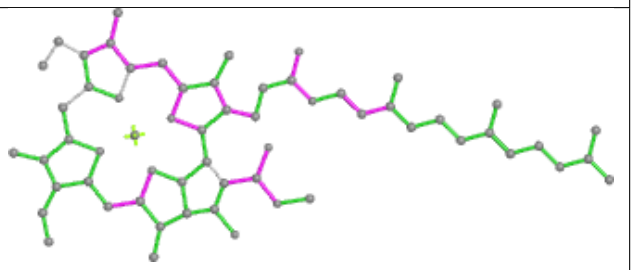
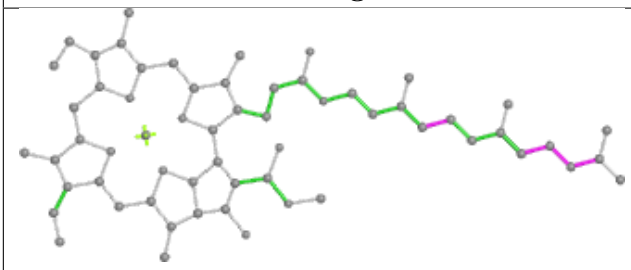
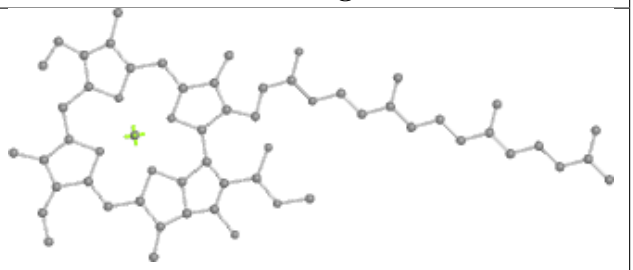


Bond angles

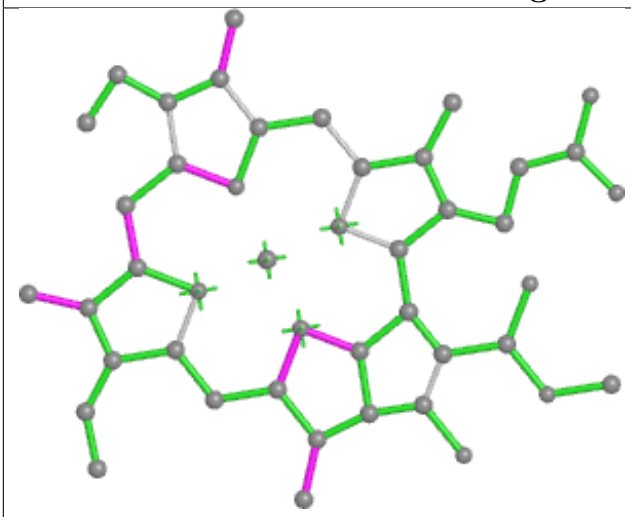


Torsions



Rings

Ligand CLA s 517



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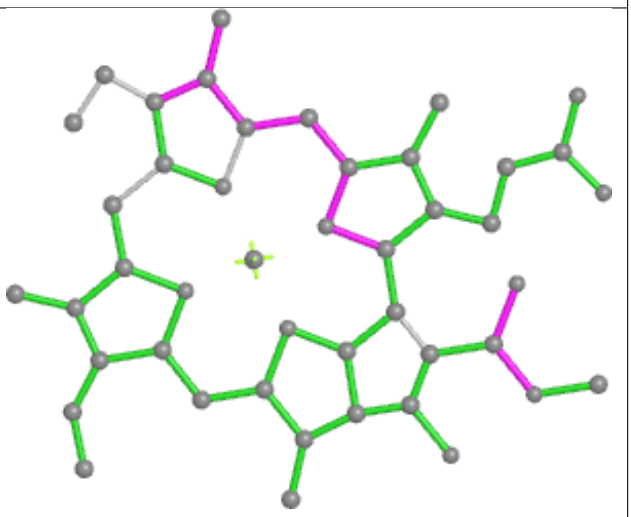

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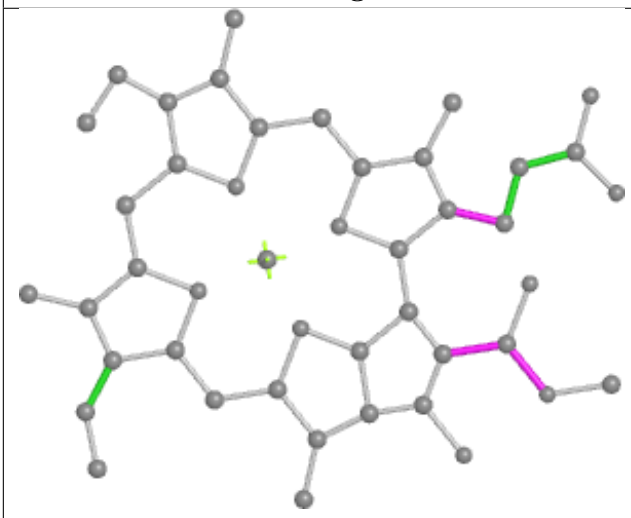

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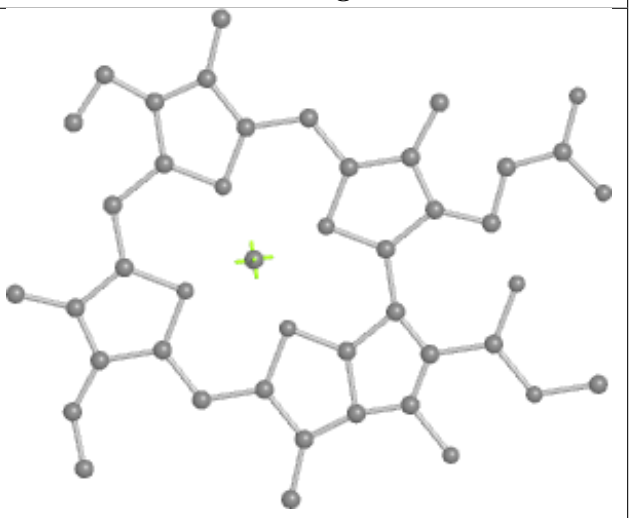
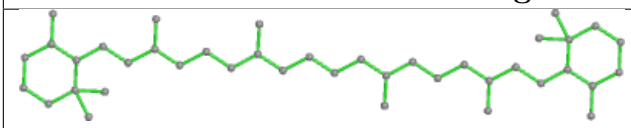


Rings

Ligand BCR B 4014



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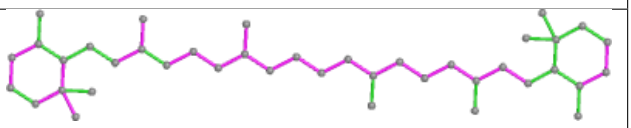
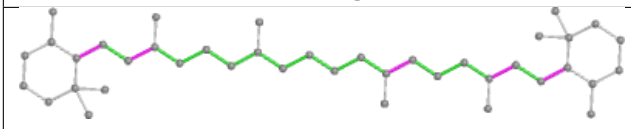


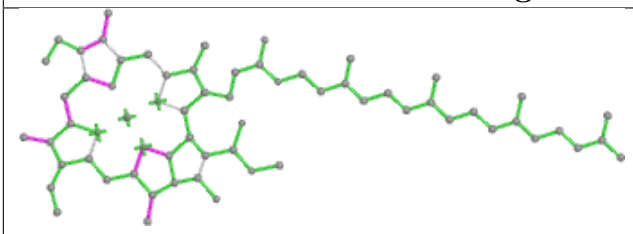
Bond angles



Torsions

Rings

Ligand CLA A 1140



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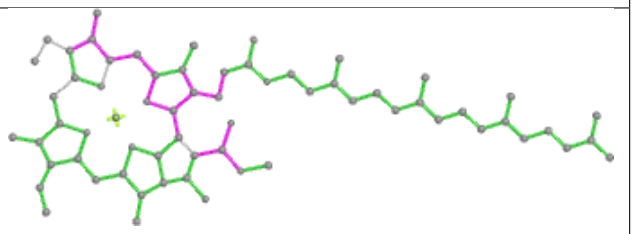
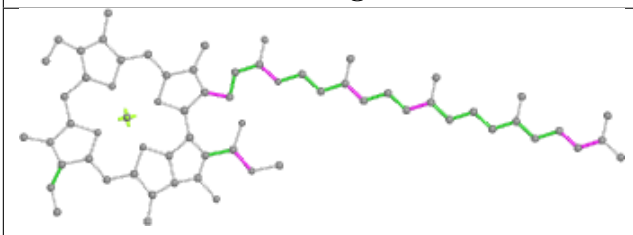
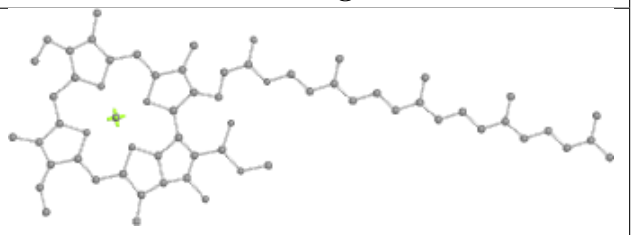


Bond angles

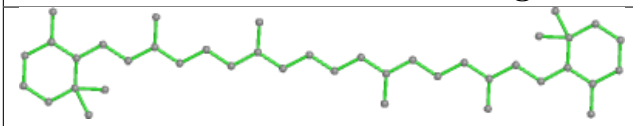


Torsions

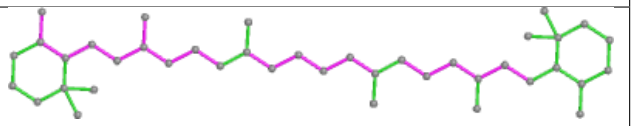


Rings

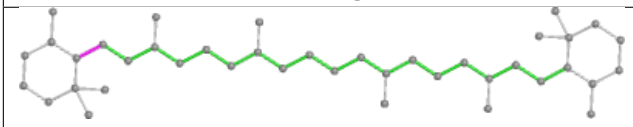
Ligand BCR B 4017



Bond lengths



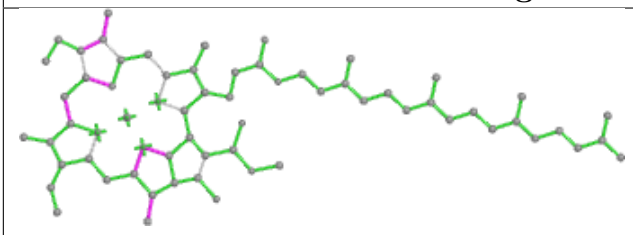
Bond angles



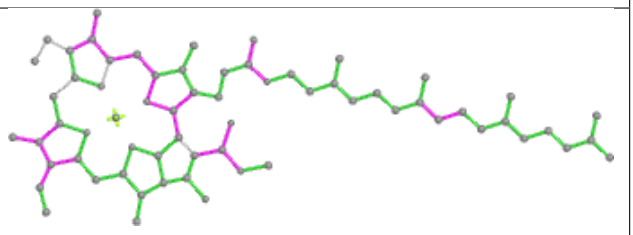
Torsions

Rings

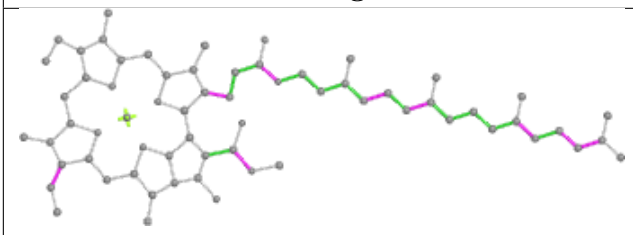
Ligand CLA B 1239



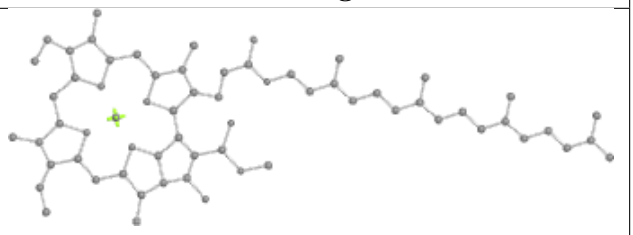
Bond lengths



Bond angles

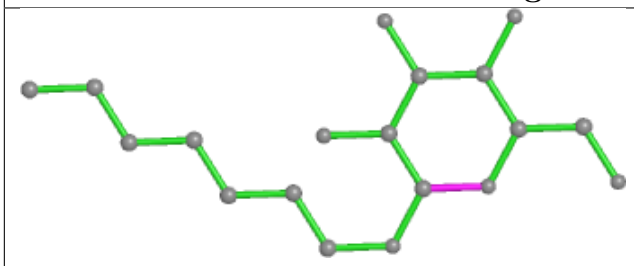


Torsions



Rings

Ligand LMU q 902



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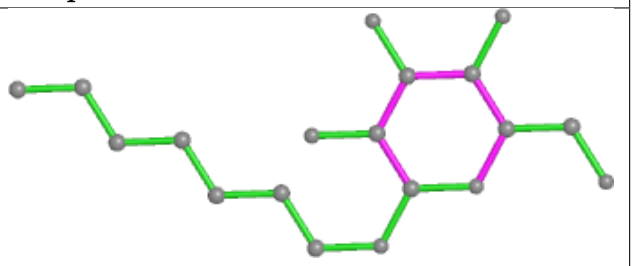
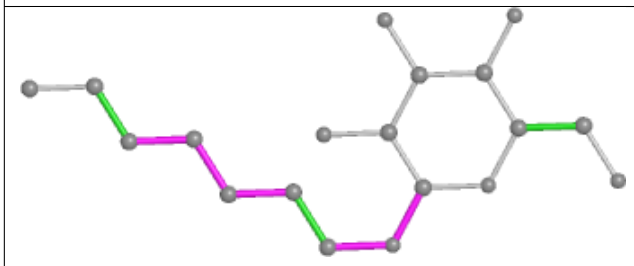
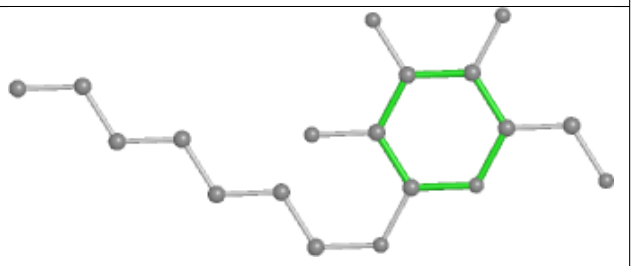


Bond angles

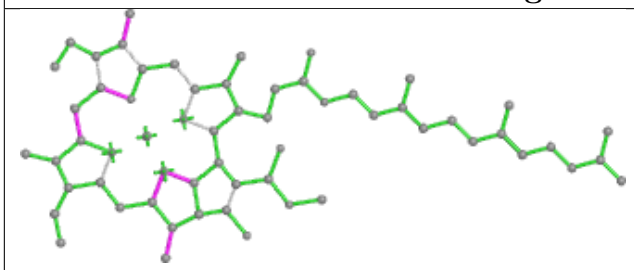


Torsions

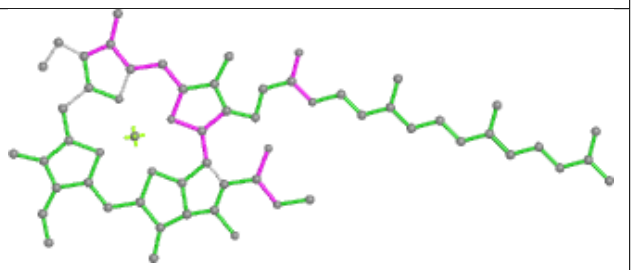


Rings

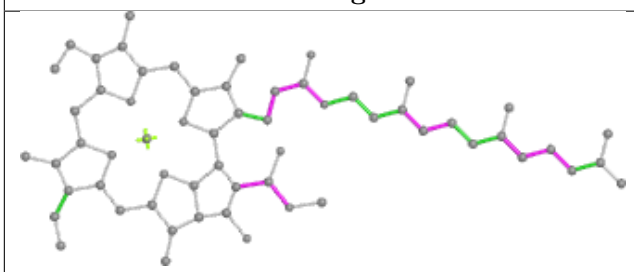
Ligand CLA Y 507



Bond lengths



Bond angles



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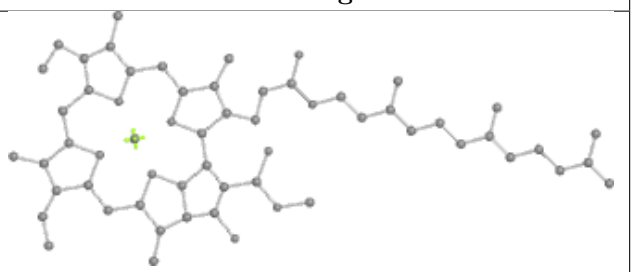
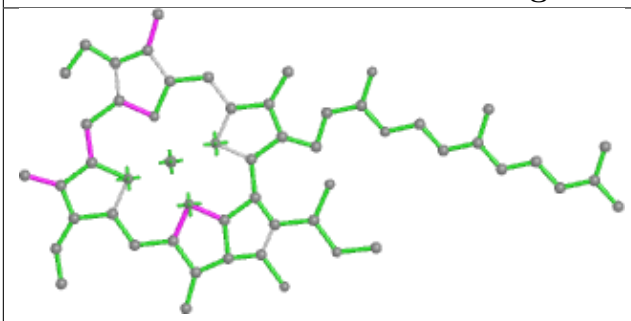


Rings

Ligand CLA r 506



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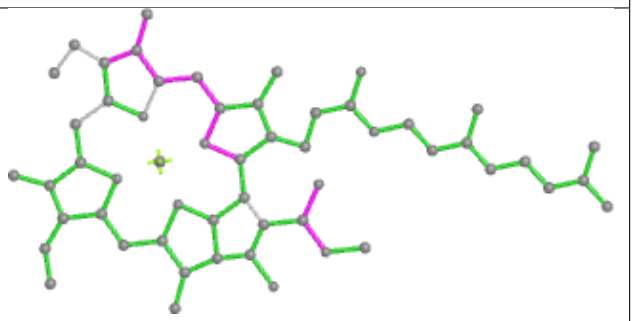
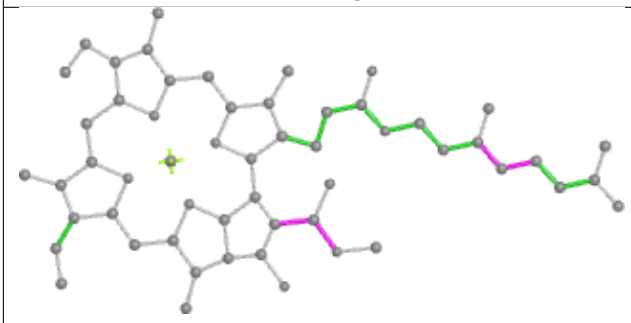


Bond angles



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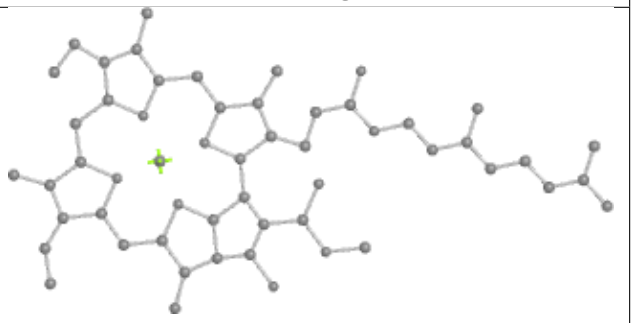
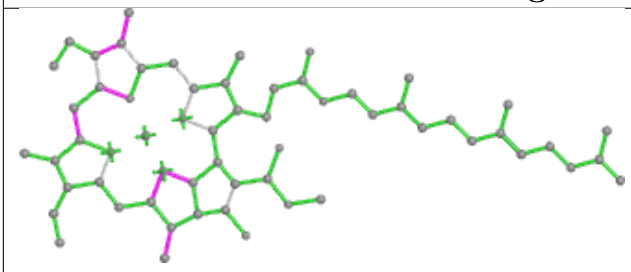


Rings

Ligand CLA 1 502



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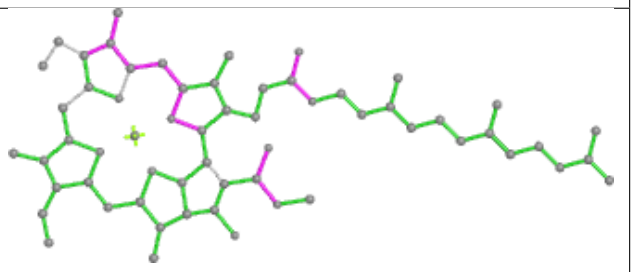
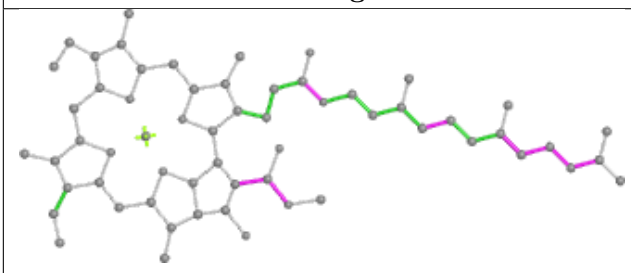


Bond angles



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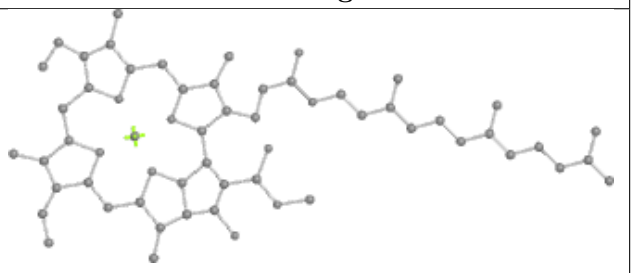
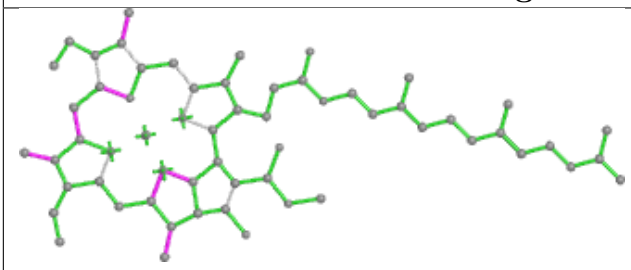
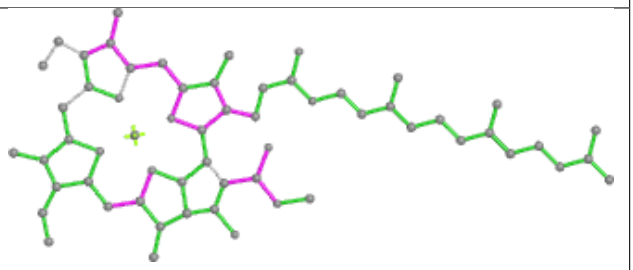
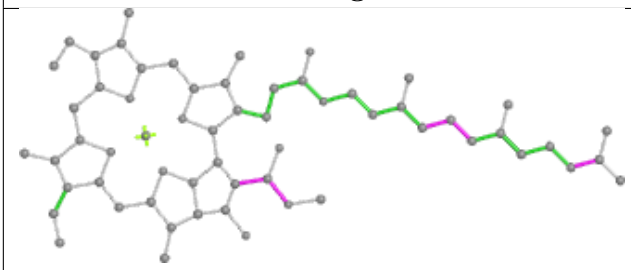
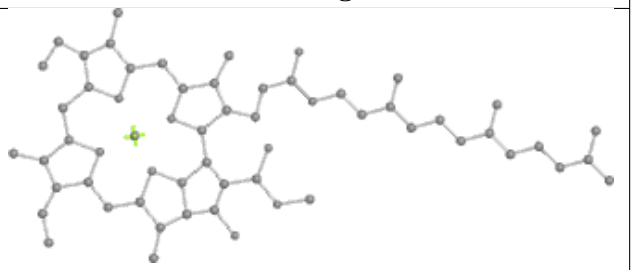


Rings

Ligand CLA B 1222	
 Bond lengths	 Bond angles
 Torsions	 Rings

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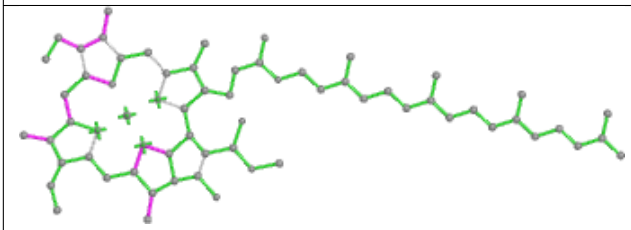
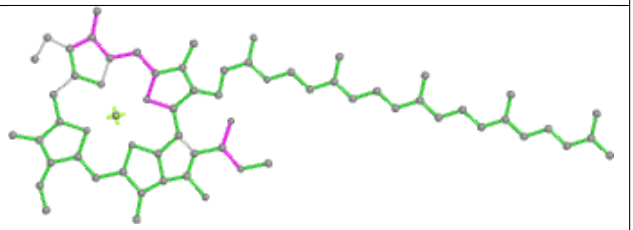
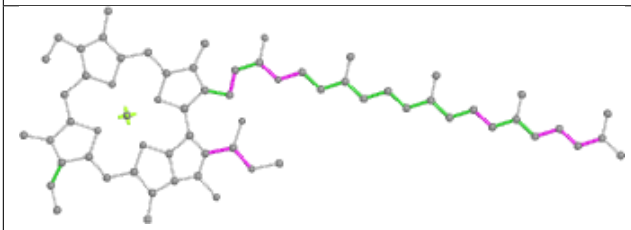
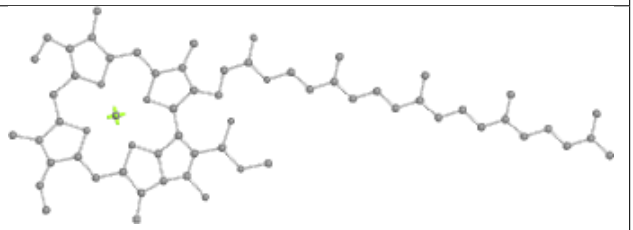
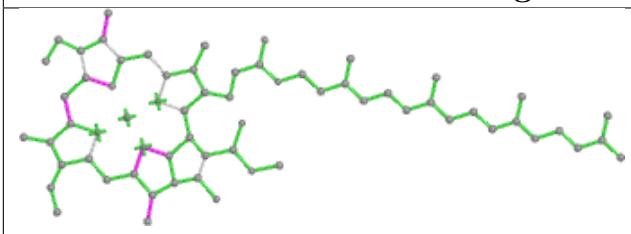
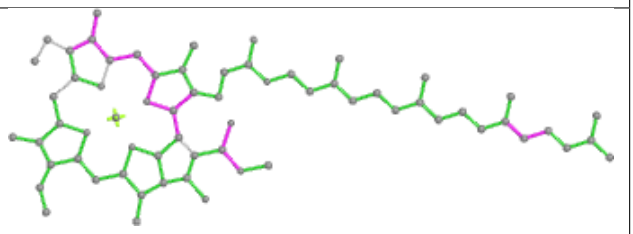
 Bond lengths	 Bond angles
 Torsions	 Rings

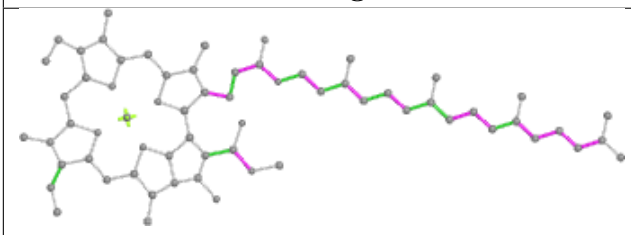
Ligand CLA G 1126



Bond lengths



Bond angles



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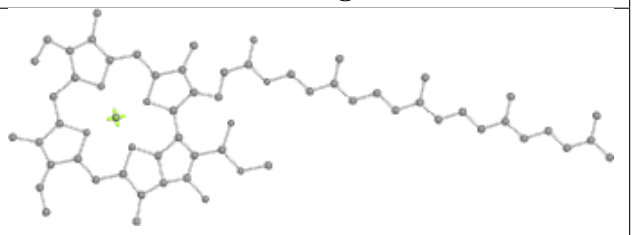
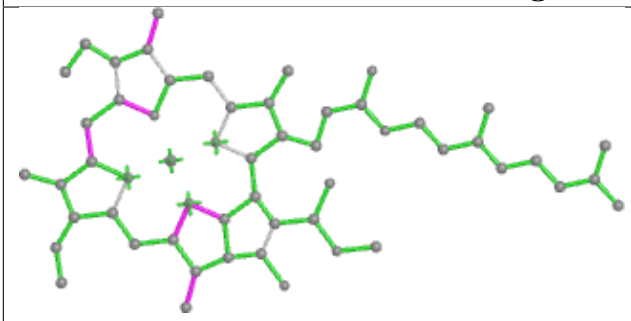


Rings

Ligand CLA c 511



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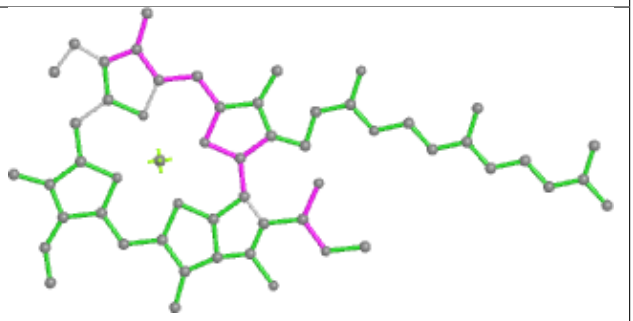
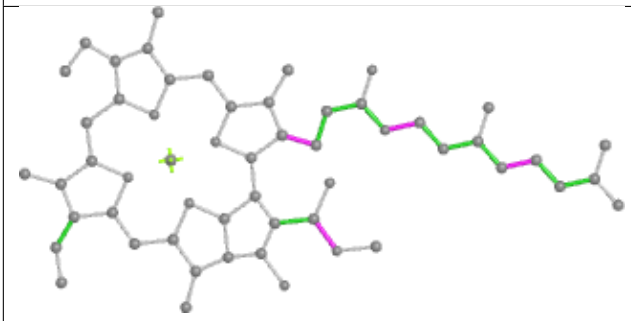


Bond angles



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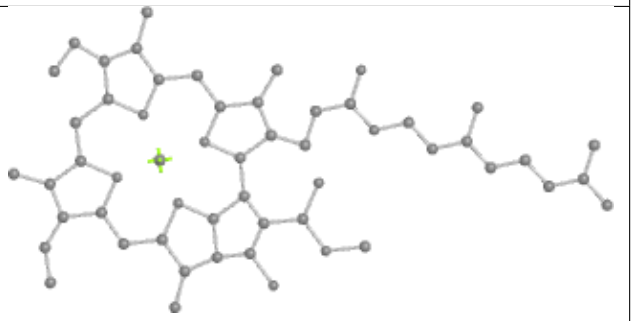
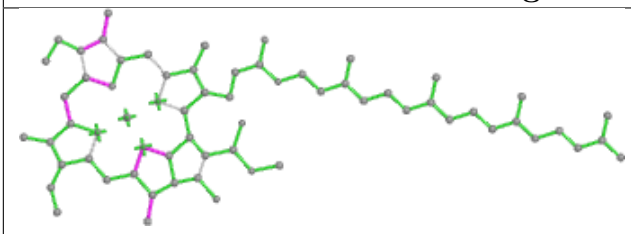


Rings

Ligand CLA f 1239



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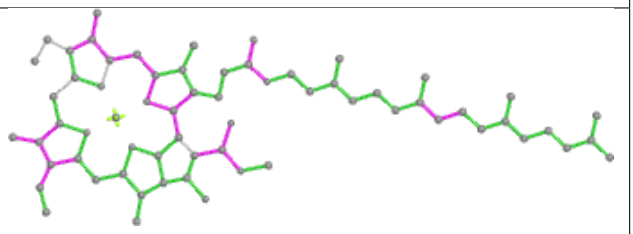
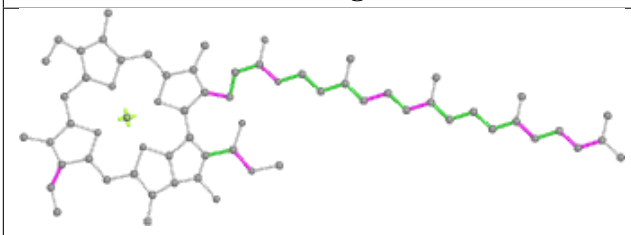


Bond angles



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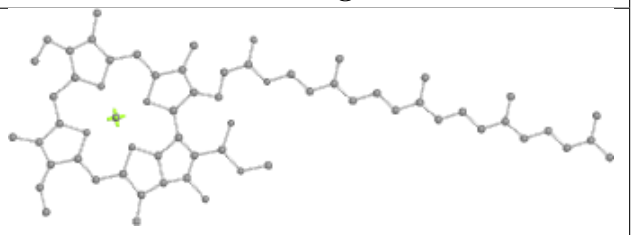
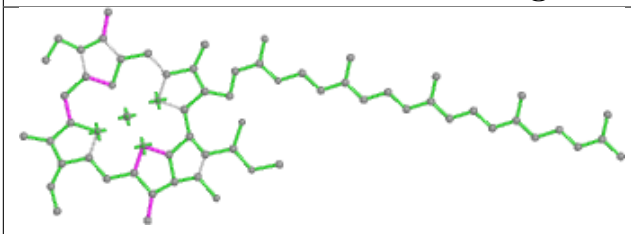
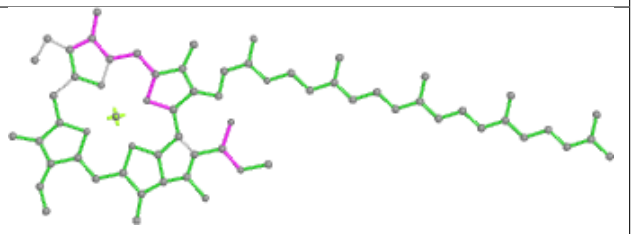


Rings

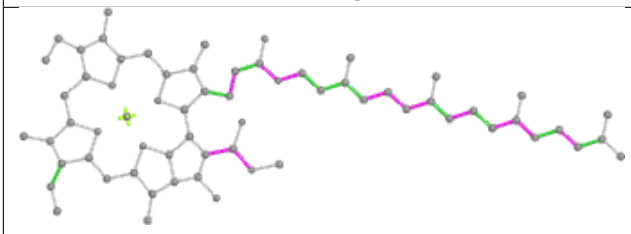
Ligand CLA s 505



Bond lengths



Bond angles



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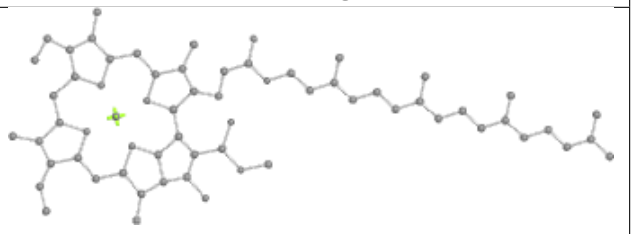
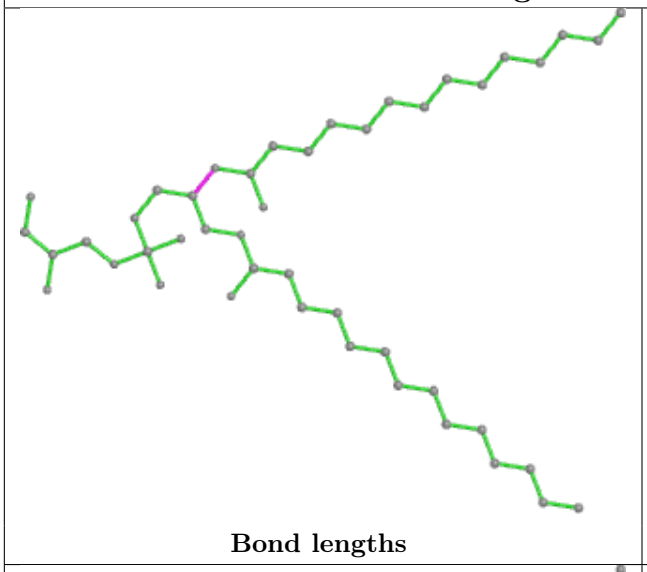


Rings

Ligand LHG G 5005



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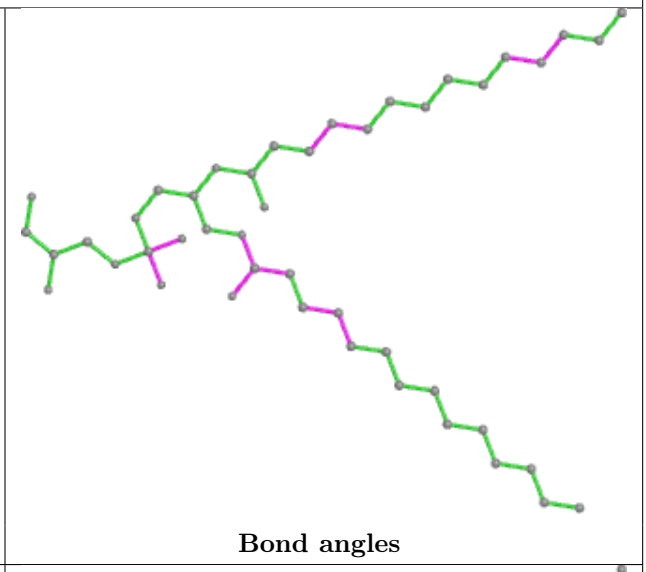
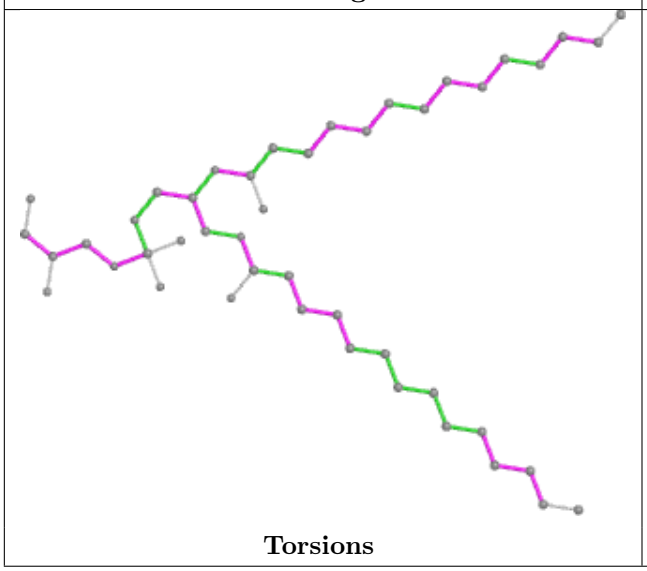


Bond angles



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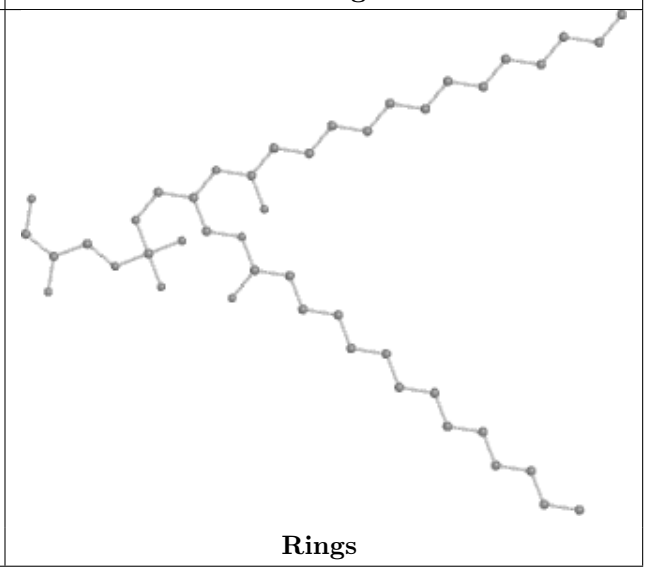
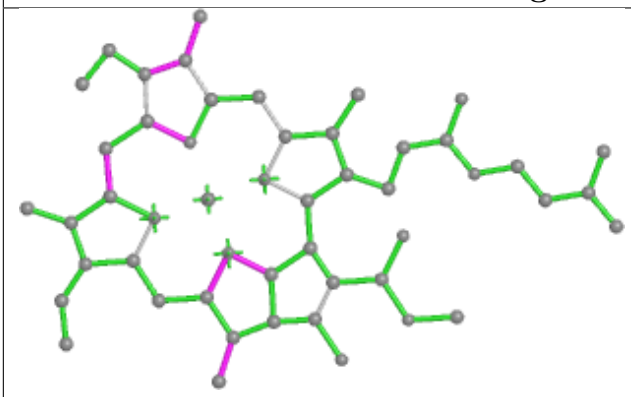


Rings

Ligand CLA s 502



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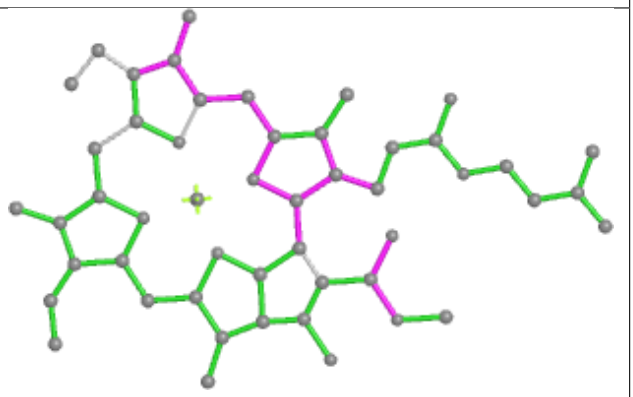
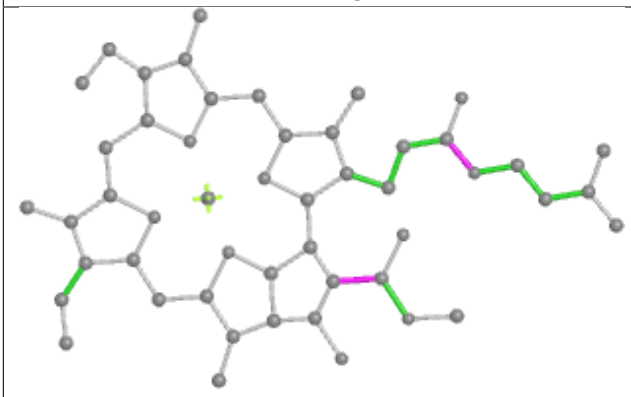


Bond angles



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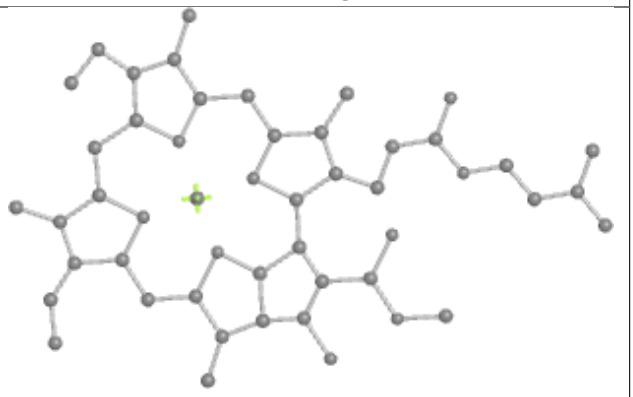
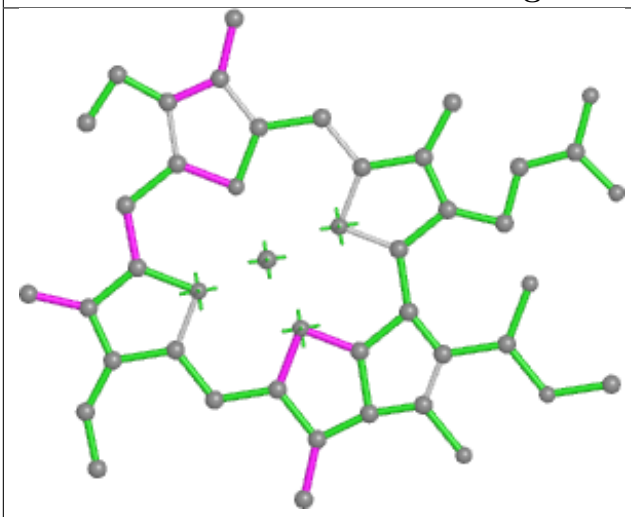


Rings

Ligand CLA Y 504



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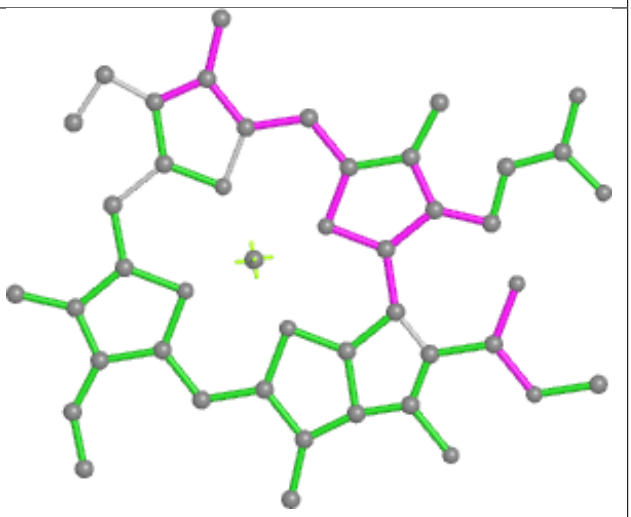
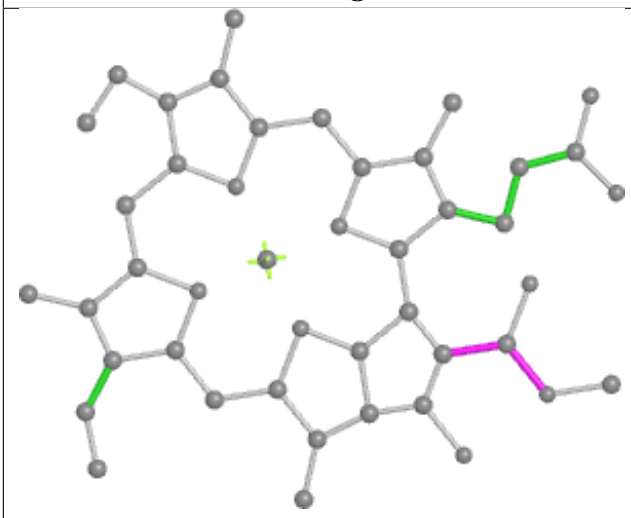
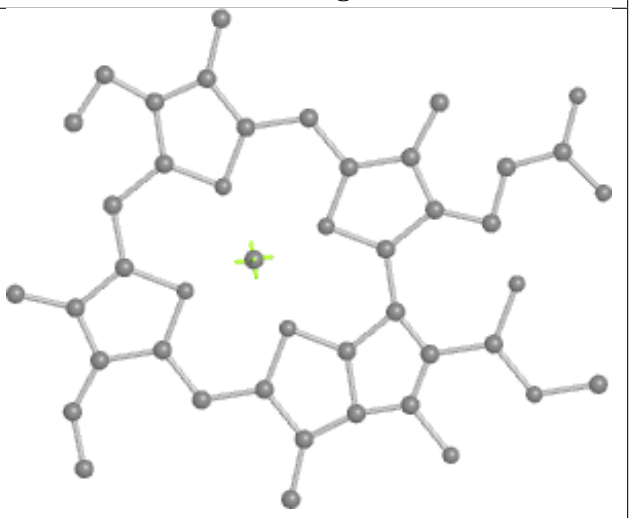


Bond angles

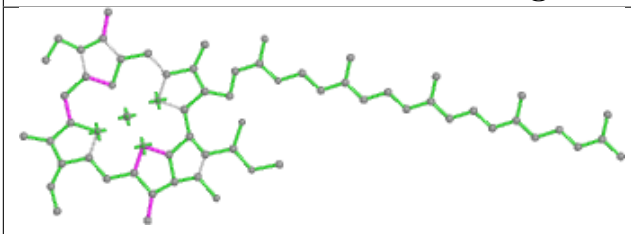


Torsions



Rings

Ligand CLA s 513



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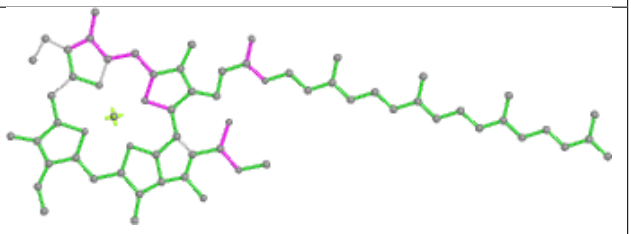
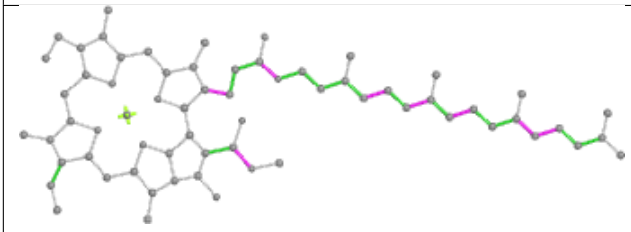


Bond angles



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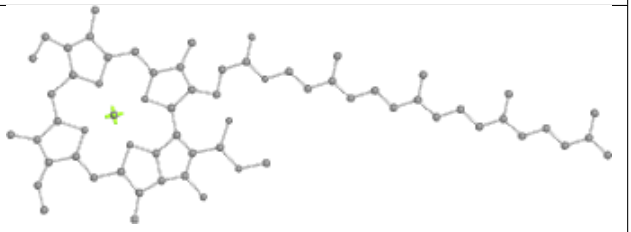
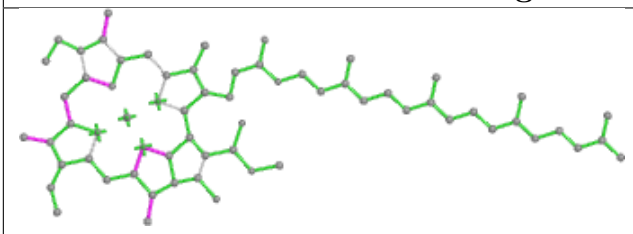
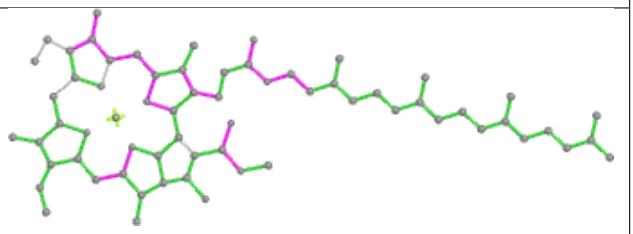


Rings

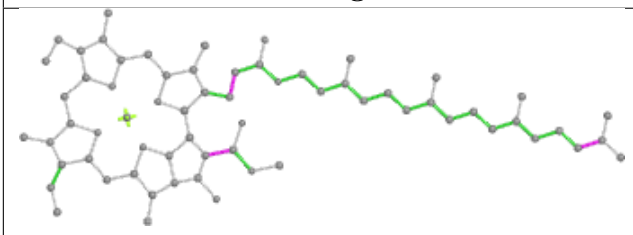
Ligand CLA B 1238



Bond lengths



Bond angles



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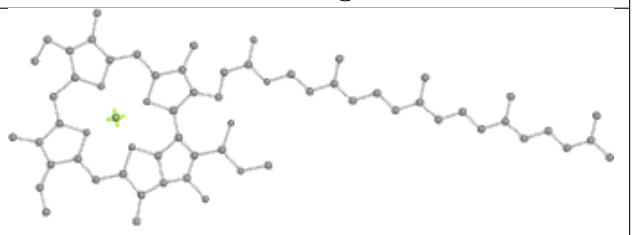
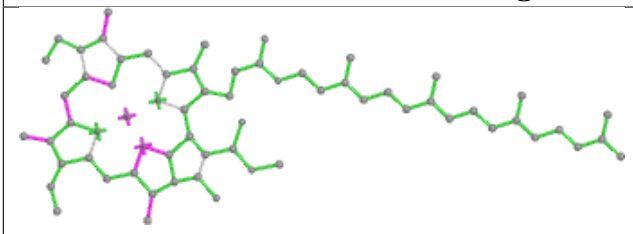
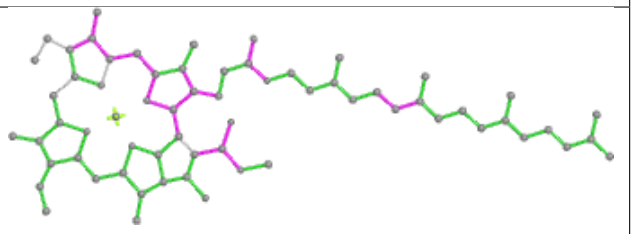


Rings

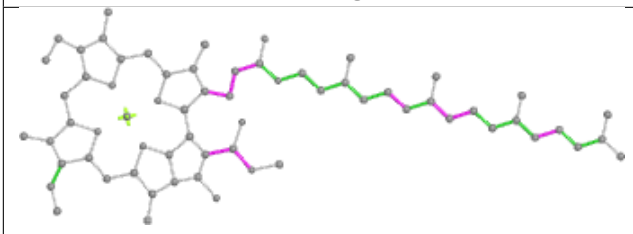
Ligand CLA B 1221



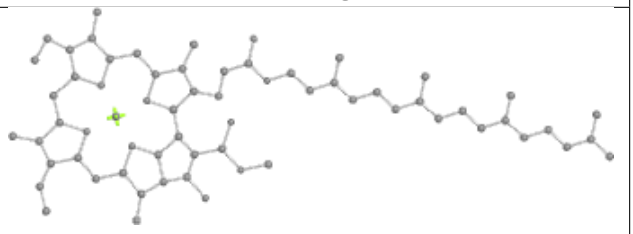
Bond lengths



Bond angles

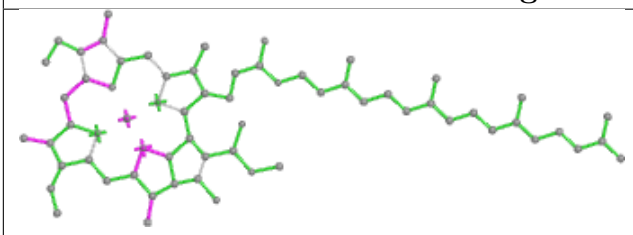


Torsions

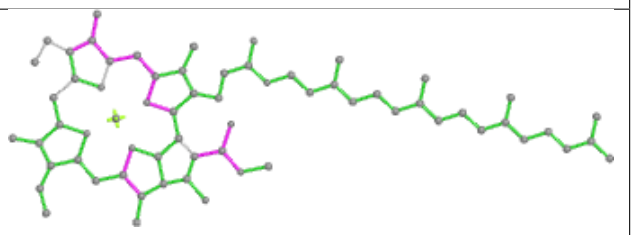


Rings

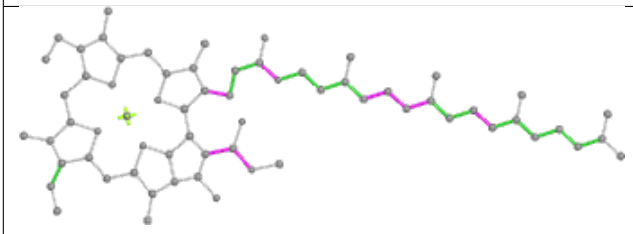
Ligand CLA e 1128



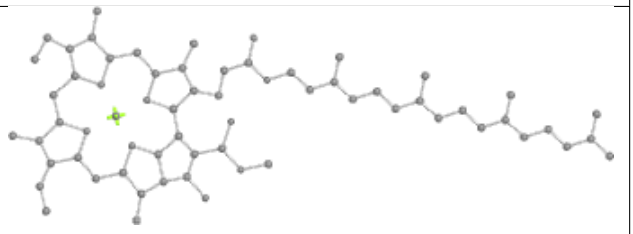
Bond lengths



Bond angles

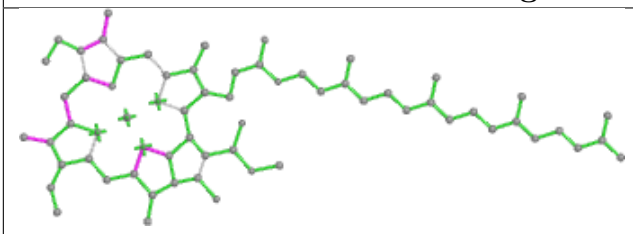


Torsions



Rings

Ligand CLA e 1137



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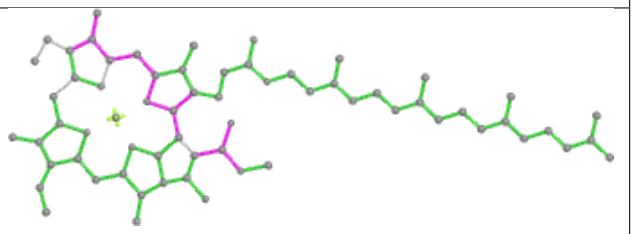
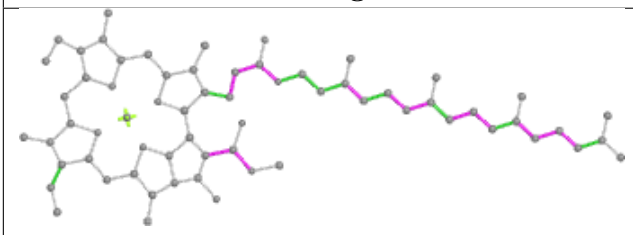


Bond angles



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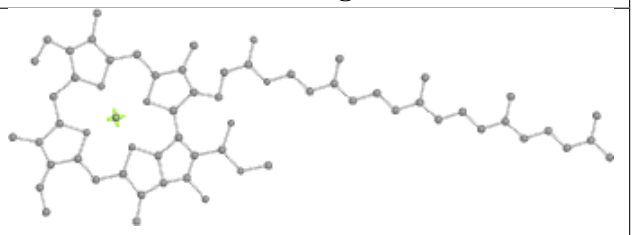
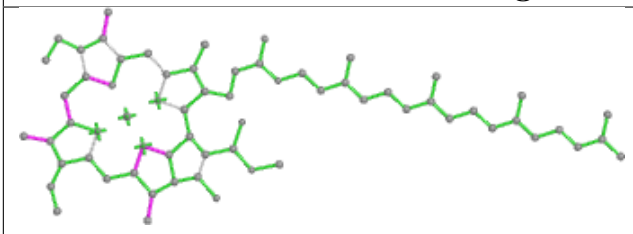
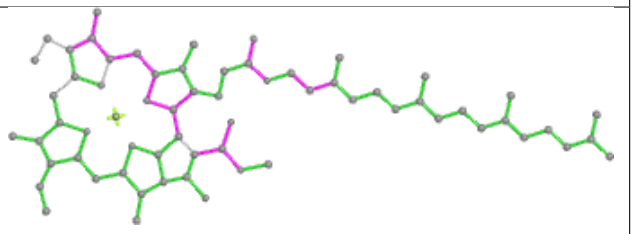


Rings

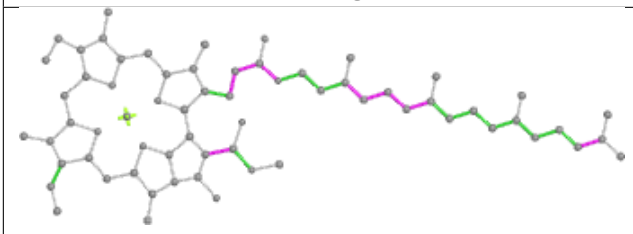
Ligand CLA H 1213



Bond lengths



Bond angles



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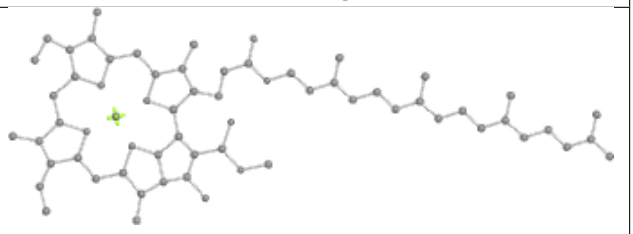
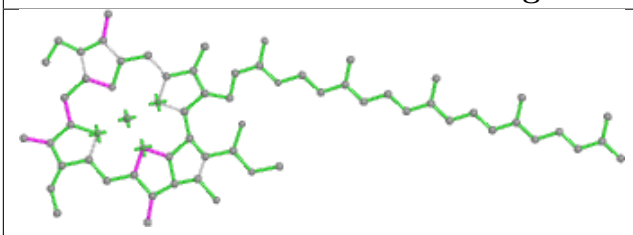


Rings

Ligand CLA f 1213



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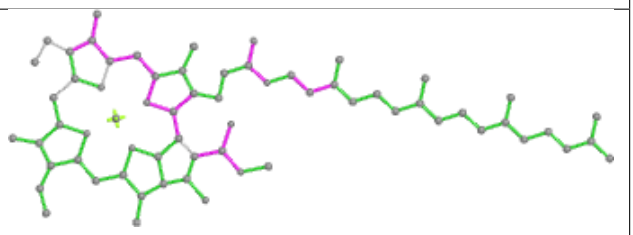
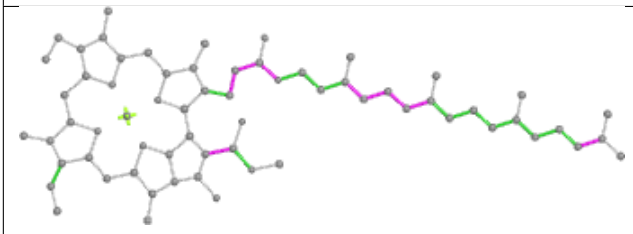


Bond angles



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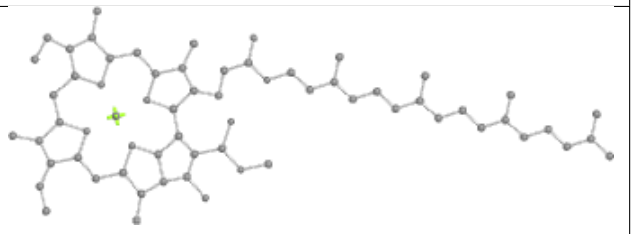
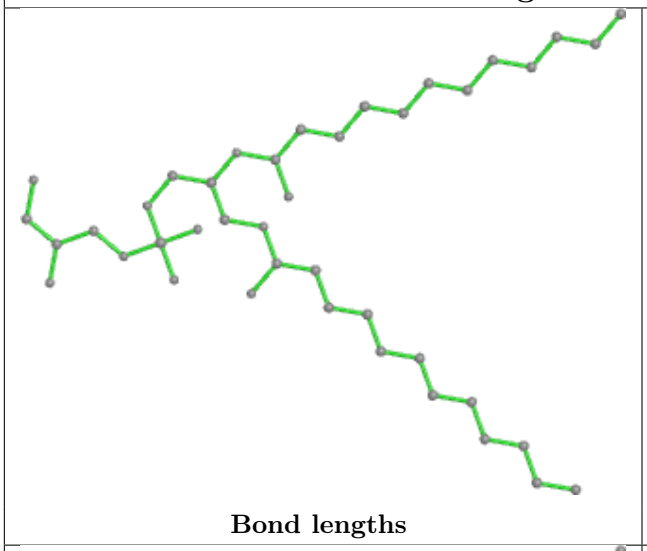


Rings

Ligand LHG L 5220



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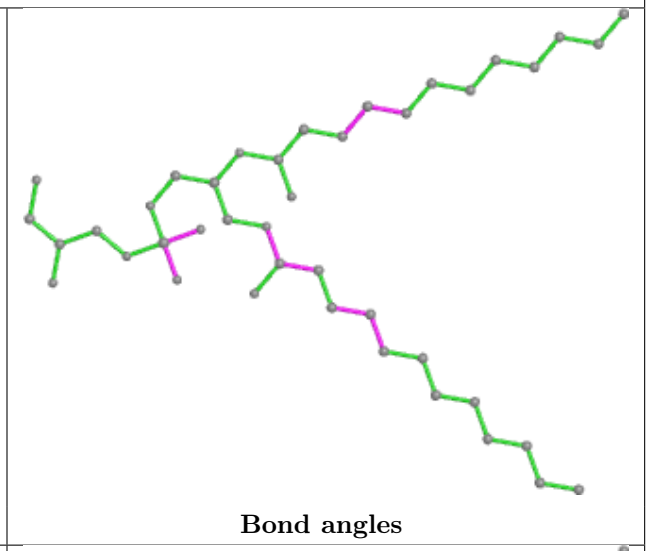
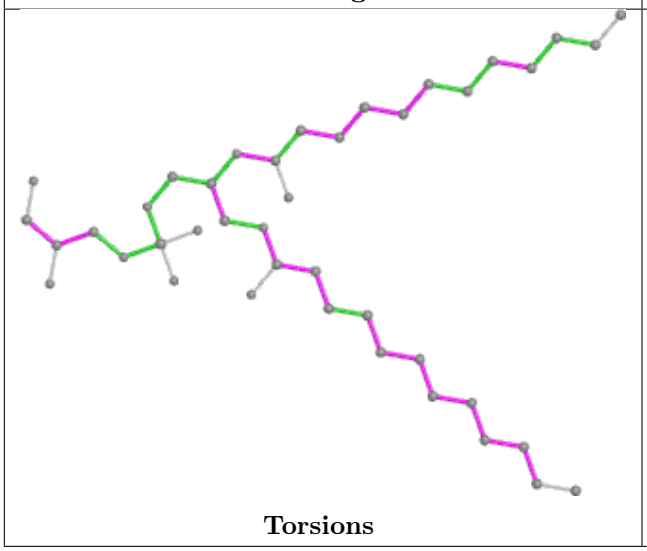


Bond angles



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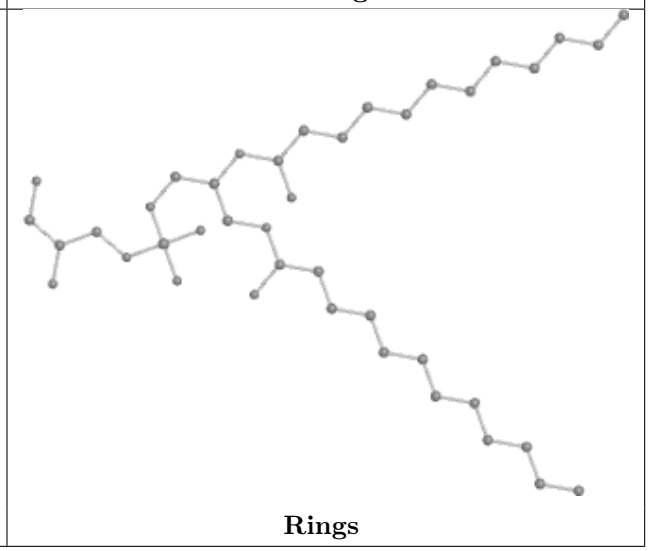
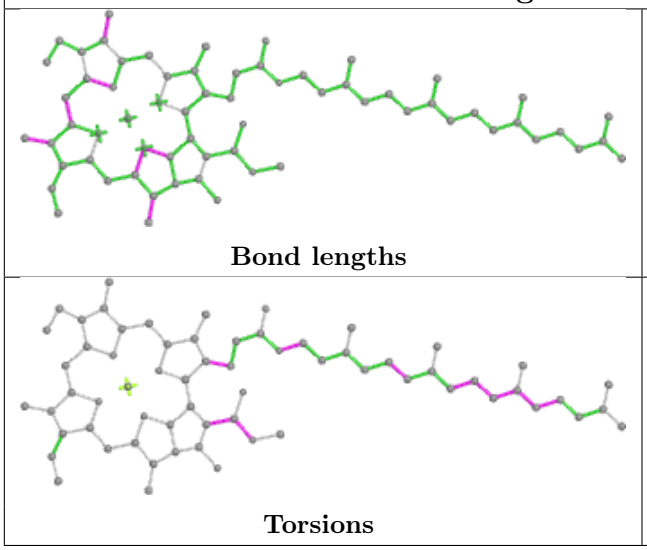
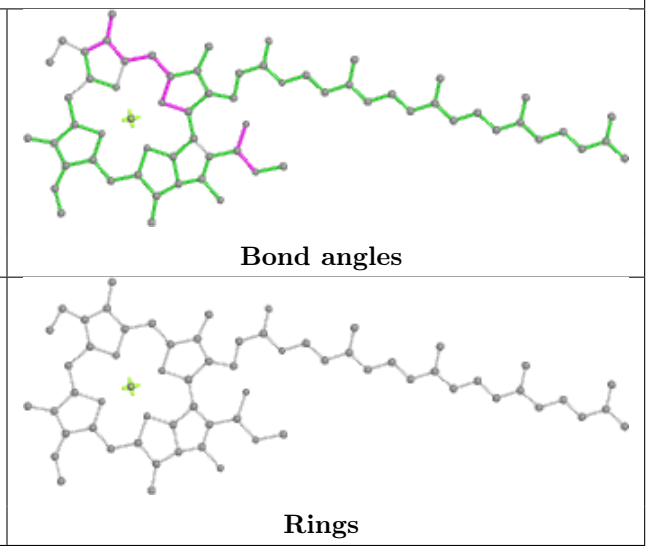


Rings

Ligand CLA B 1223



Bond lengths

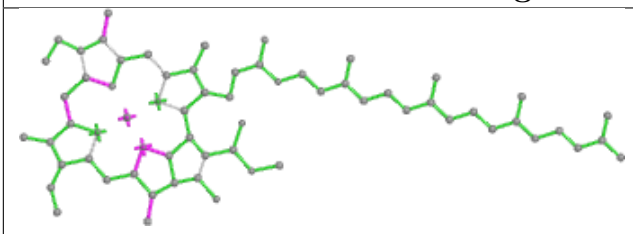


Bond angles

Torsions

Rings

Ligand CLA G 1139



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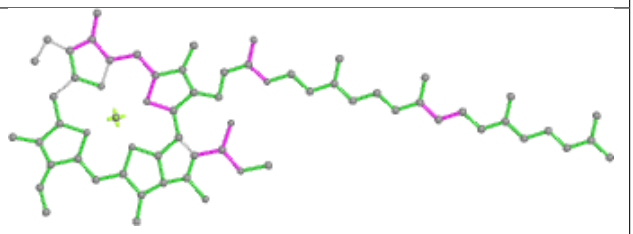
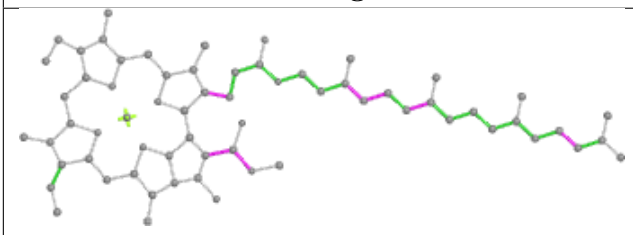


Bond angles



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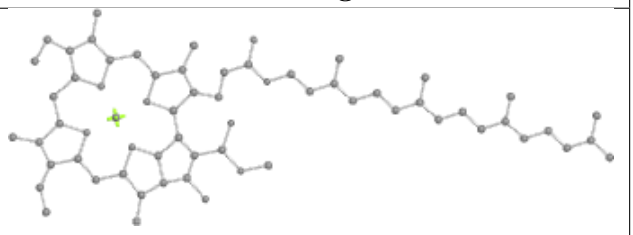
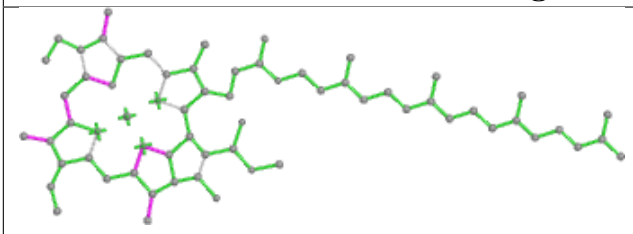


Rings

Ligand CLA r 518



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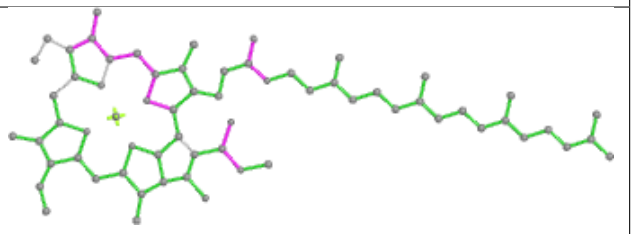
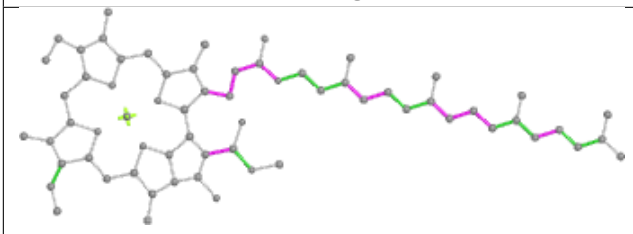
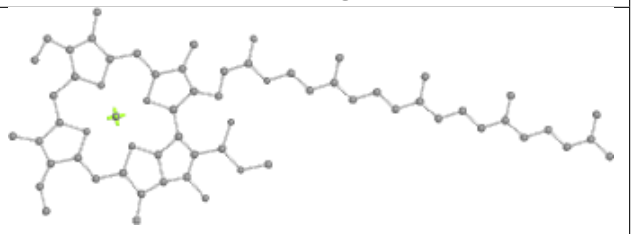


Bond angles

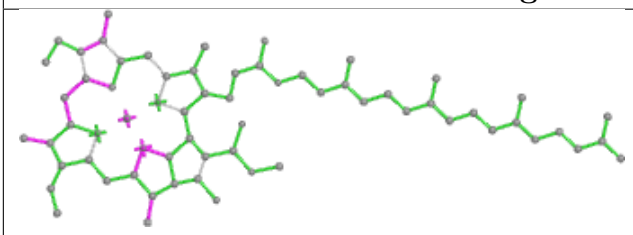


Torsions



Rings

Ligand CLA e 1117



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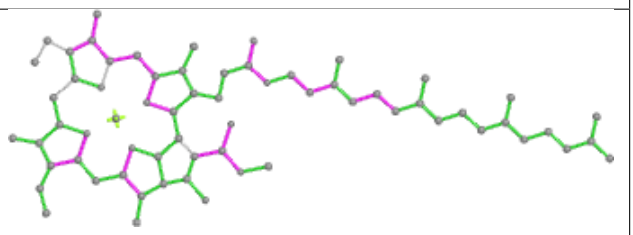
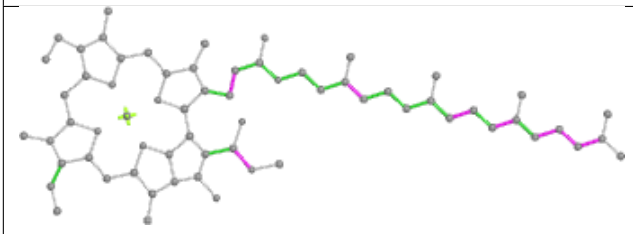
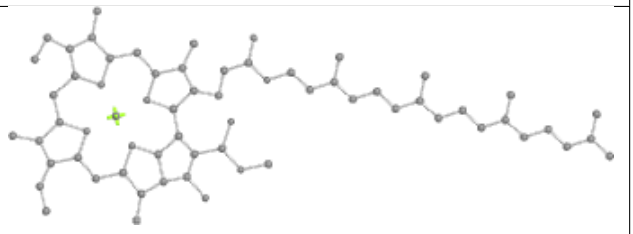


Bond angles

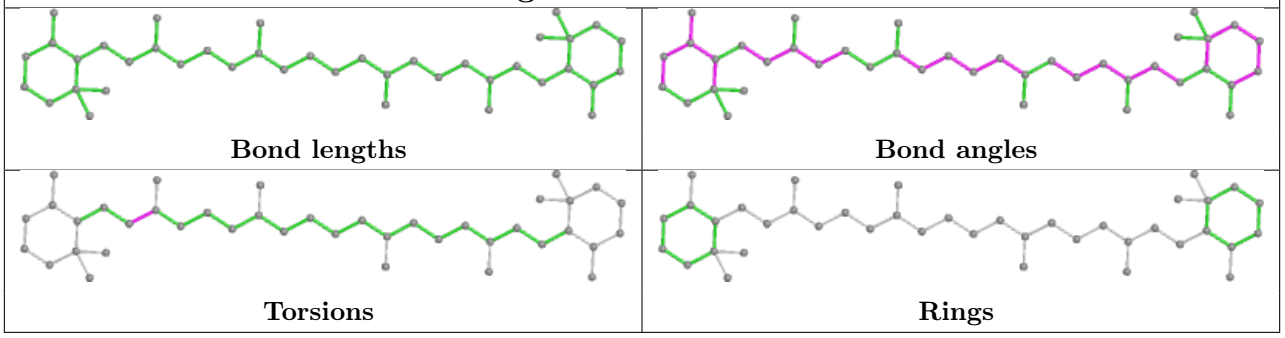


Torsions

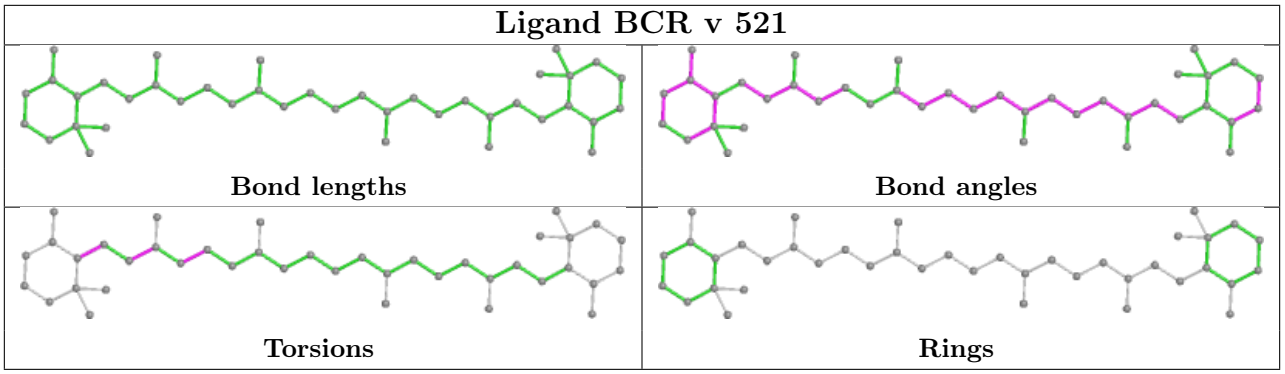


Rings

Ligand BCR n 4022



Ligand BCR v 521



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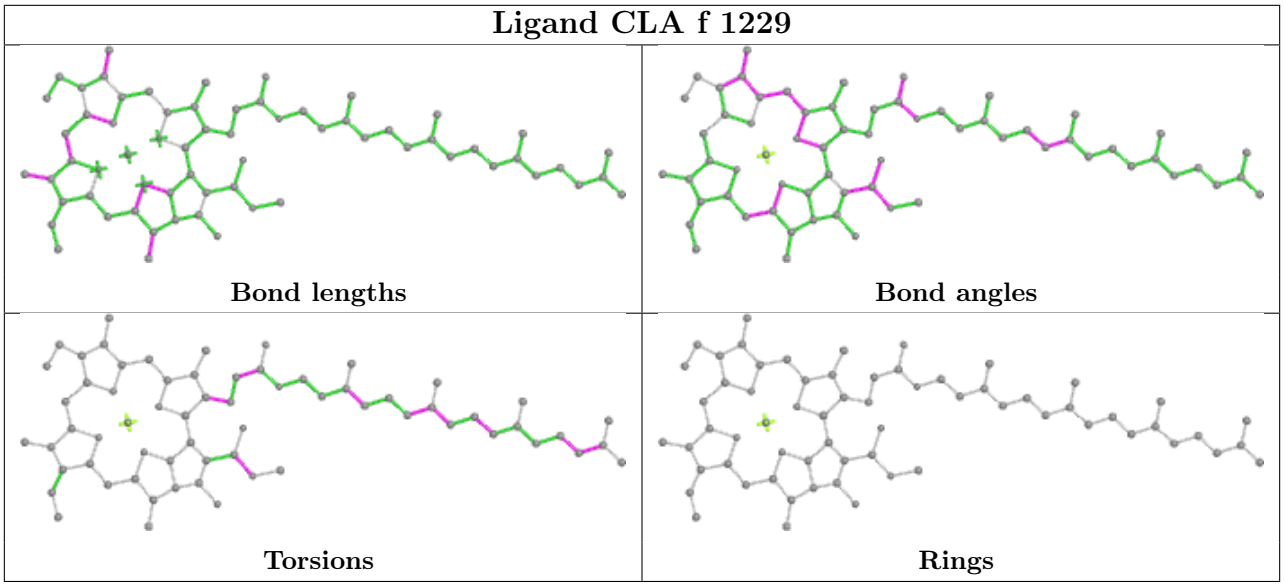

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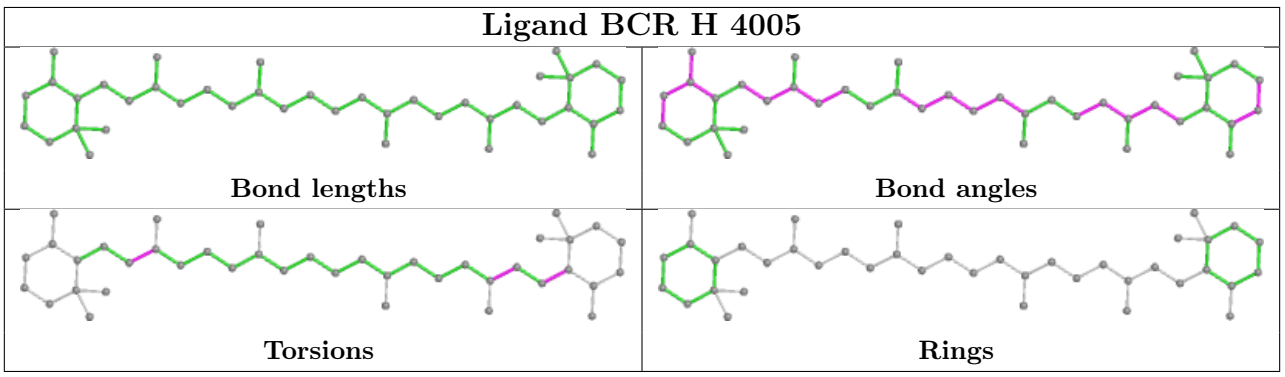
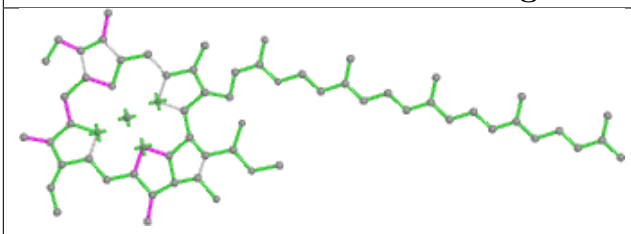
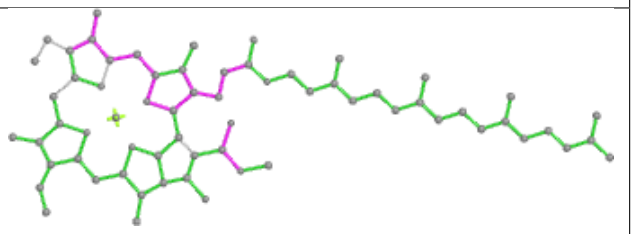


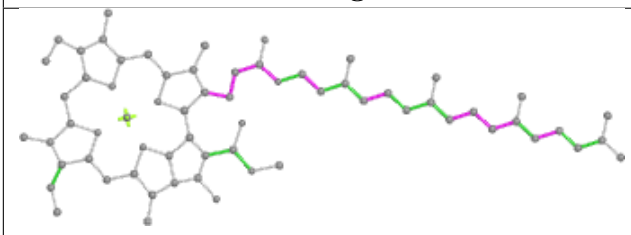
Ligand CLA e 1125



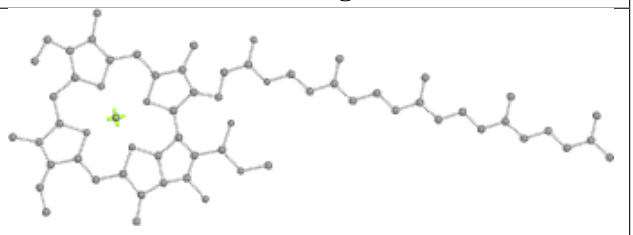
Bond lengths



Bond angles

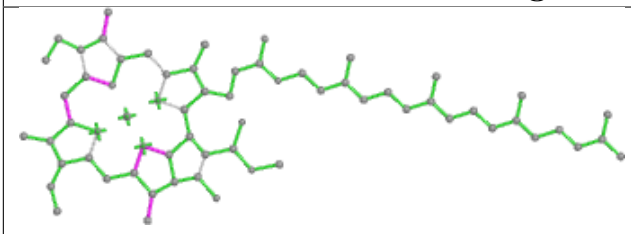


Torsions



Rings

Ligand CLA a 507



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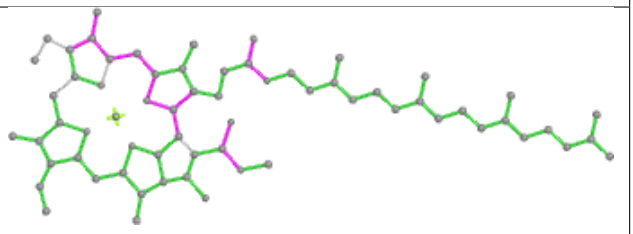
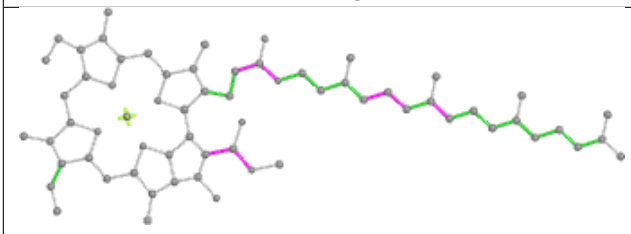
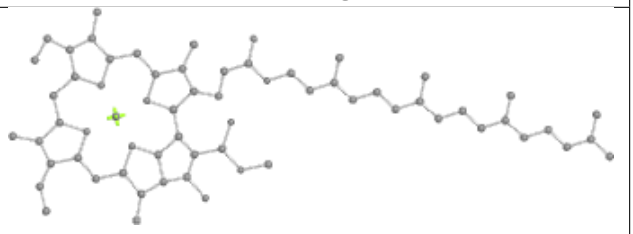


Bond angles

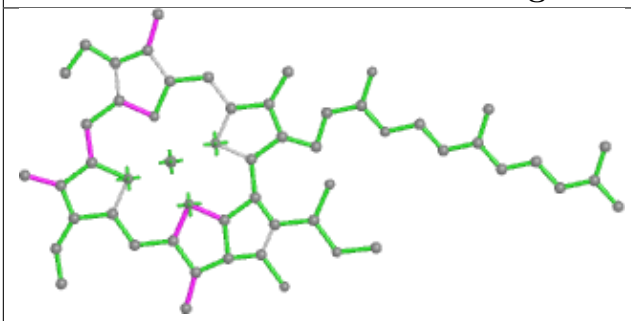


Torsions



Rings

Ligand CLA 1 513



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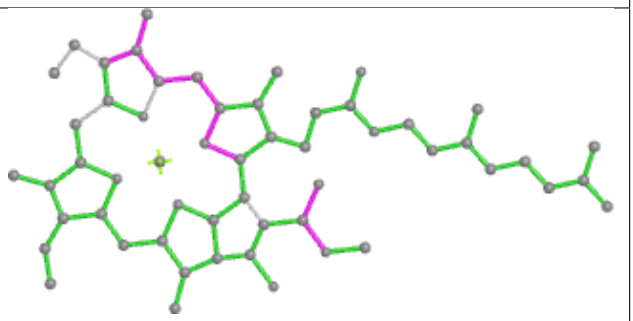
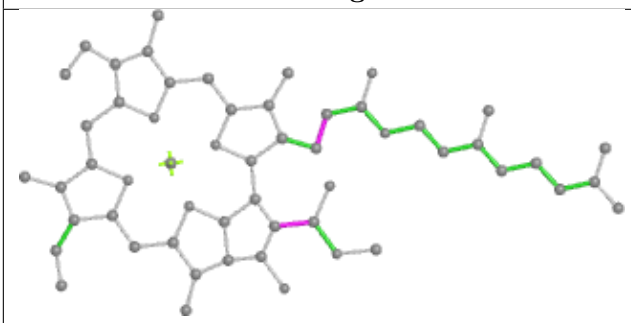
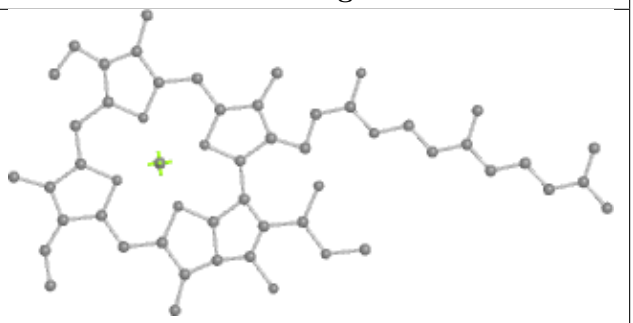


Bond angles

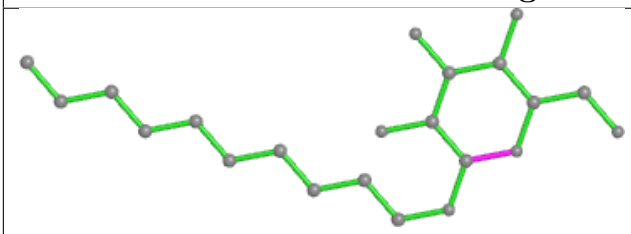


Torsions

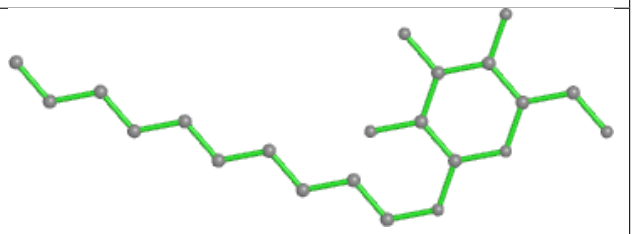


Rings

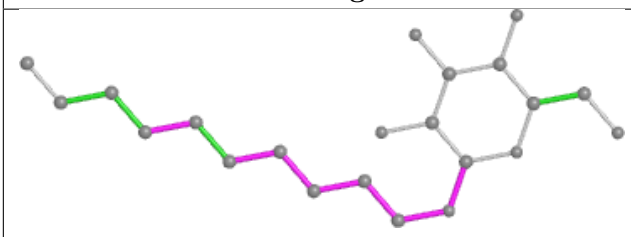
Ligand LMU l 5105



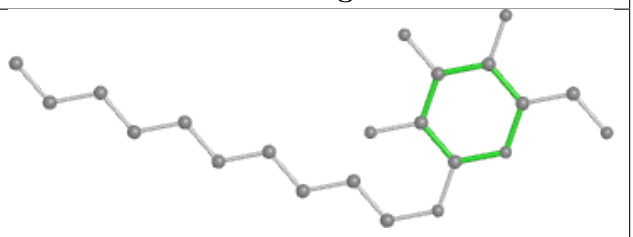
Bond lengths



Bond angles

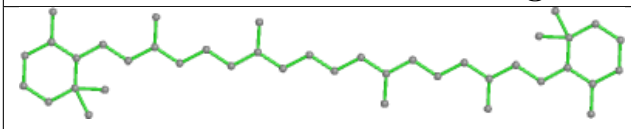


Torsions

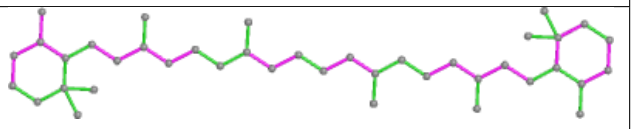


Rings

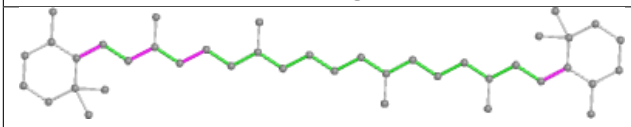
Ligand BCR 3 521



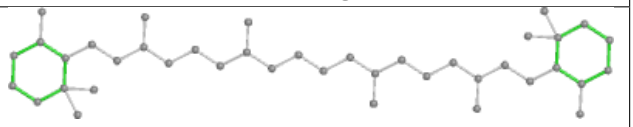
Bond lengths



Bond angles

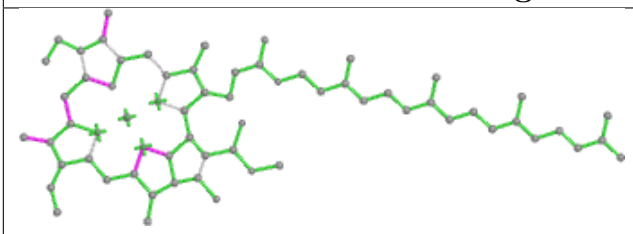


Torsions



Rings

Ligand CLA A 1102



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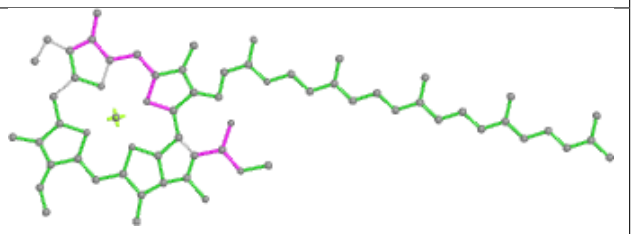

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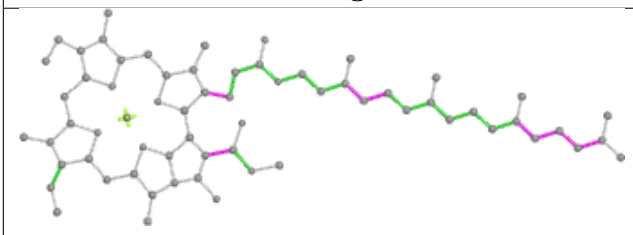
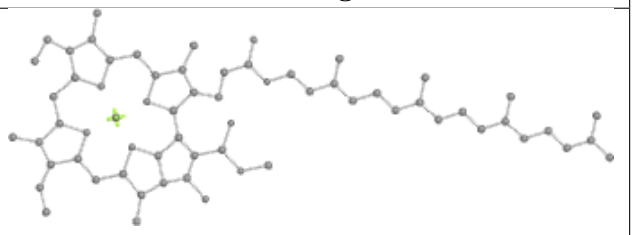
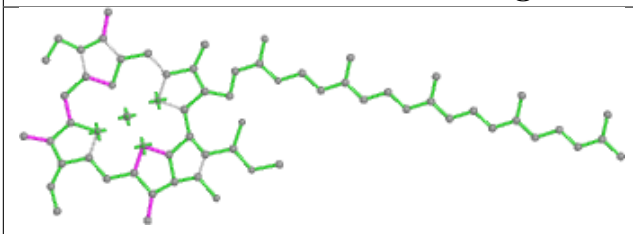


Torsions

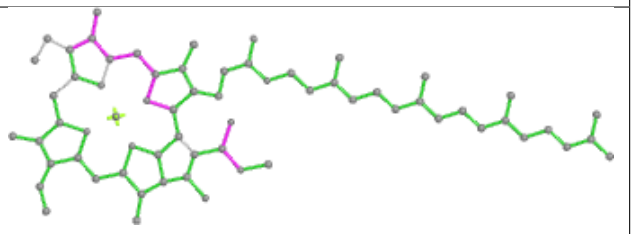


Rings

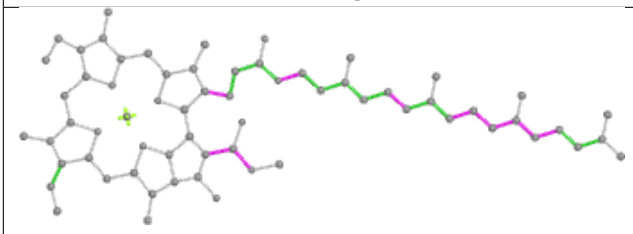
Ligand CLA H 1223



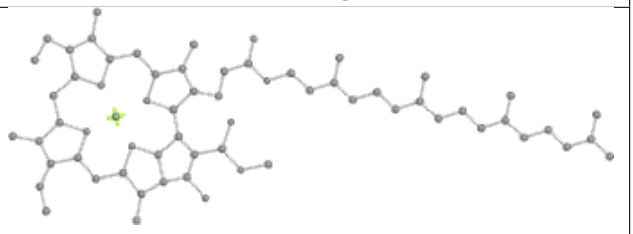
Bond lengths



Bond angles

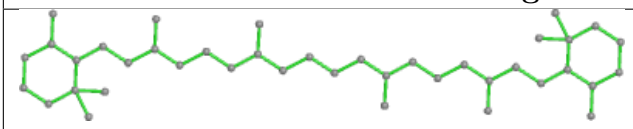


Torsions

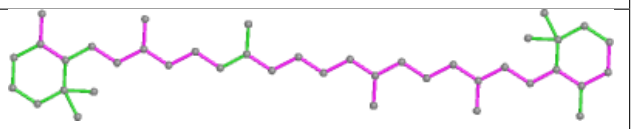


Rings

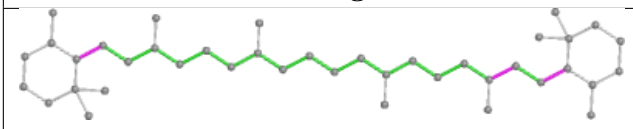
Ligand BCR Y 523



Bond lengths

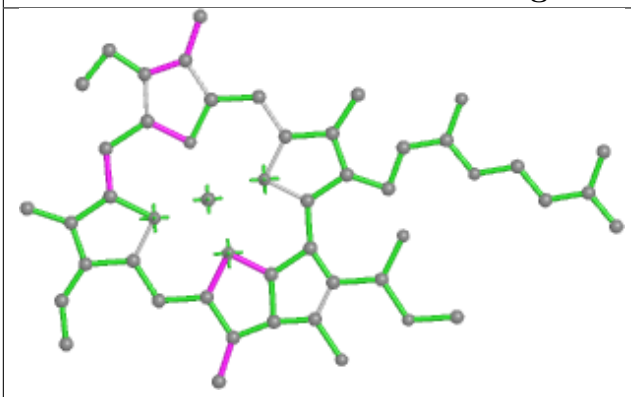
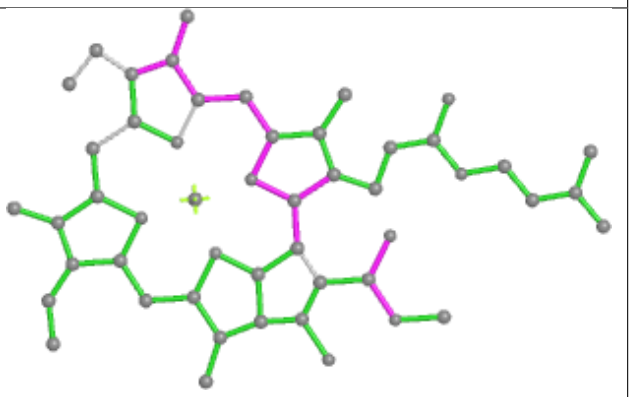
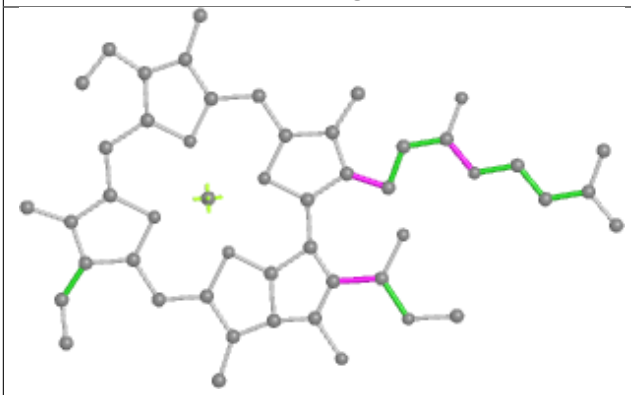
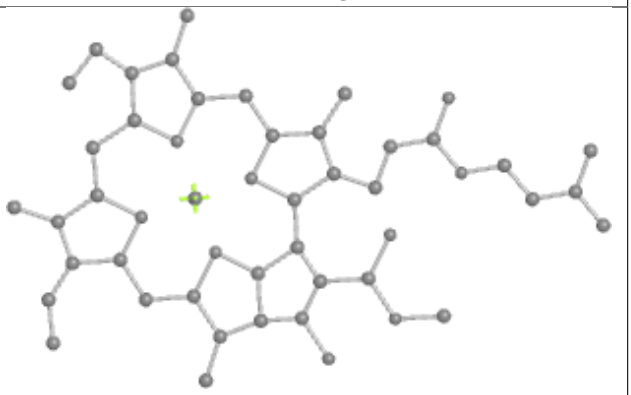


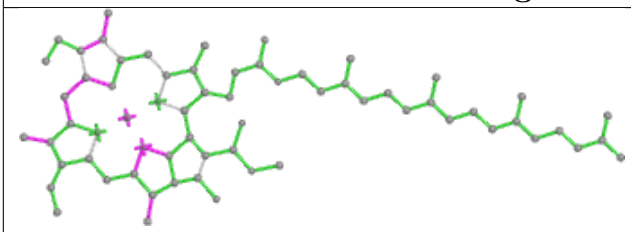
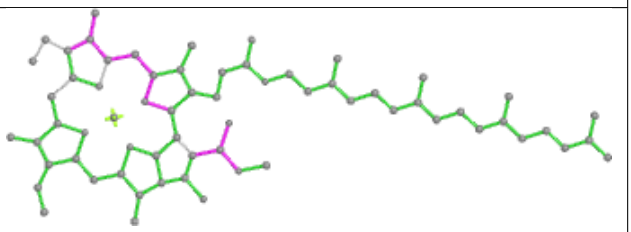
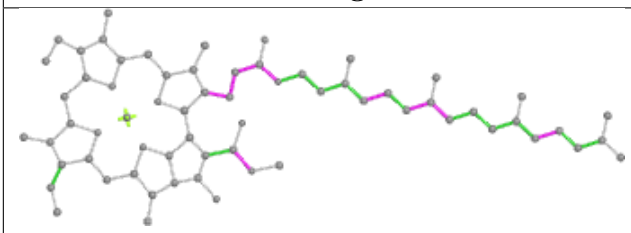
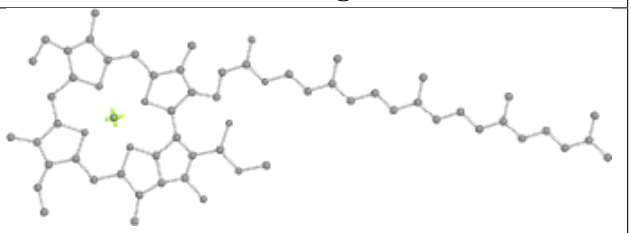
Bond angles



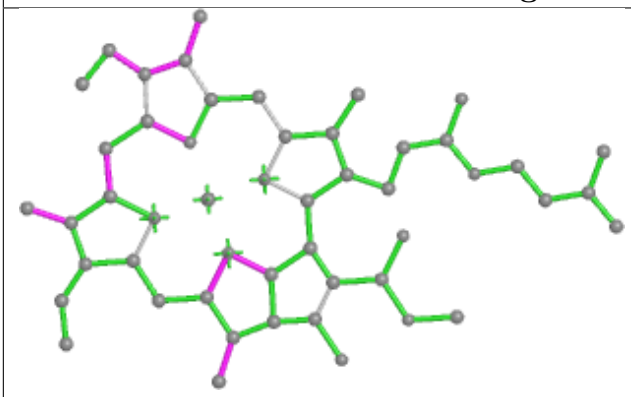
Torsions

Rings

Ligand CLA t 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1206	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA e 1112



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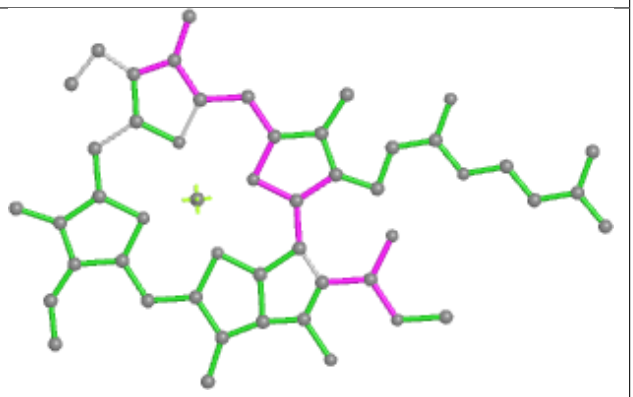
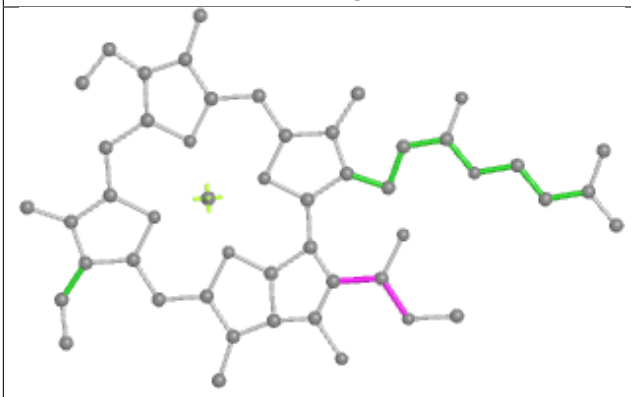
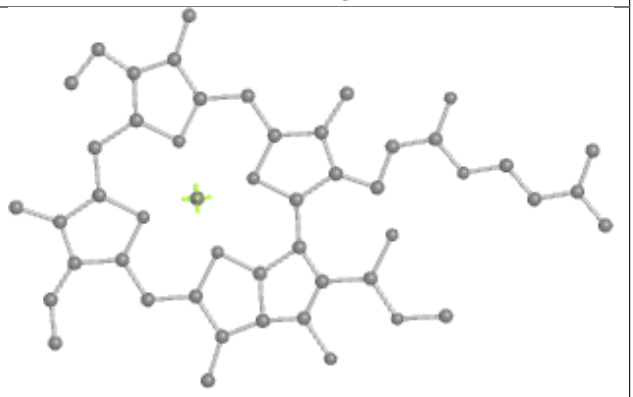


Bond angles

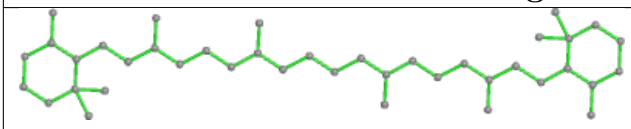


Torsions



Rings

Ligand BCR 1 521



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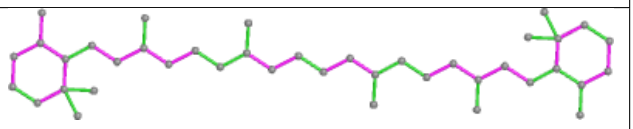
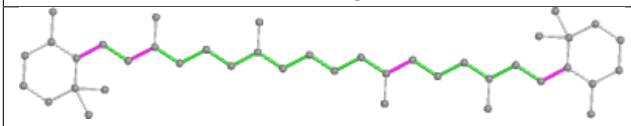


Bond angles



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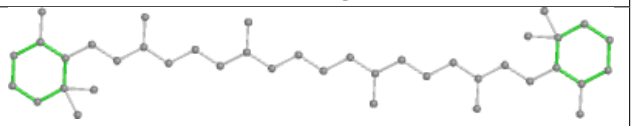
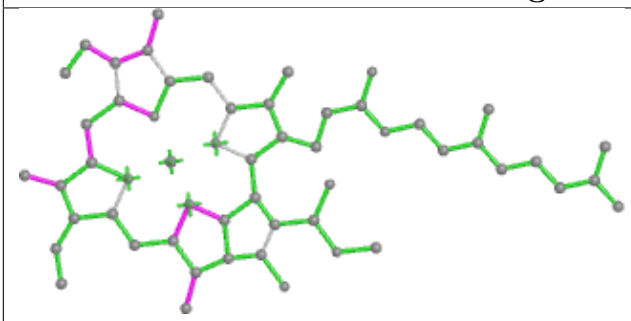
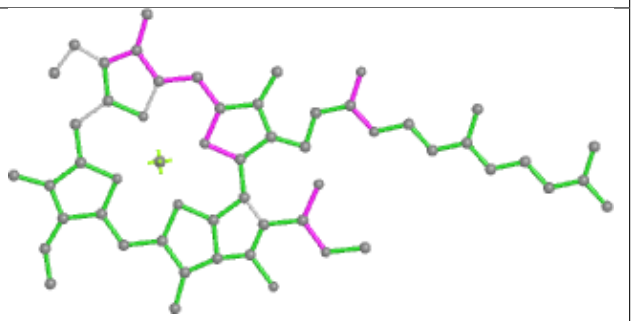


Rings

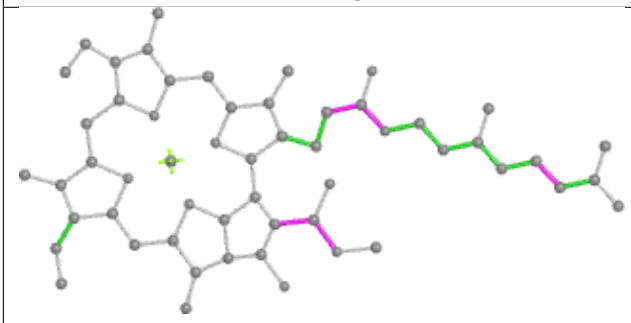
Ligand CLA 3 519



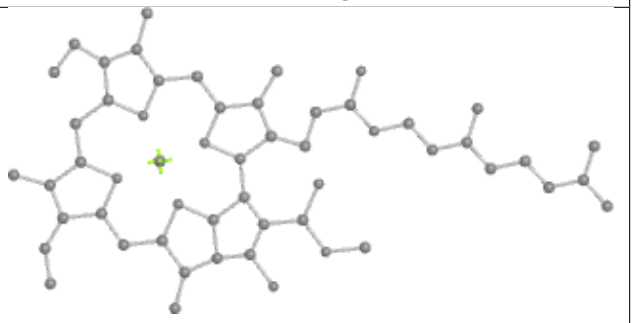
Bond lengths



Bond angles

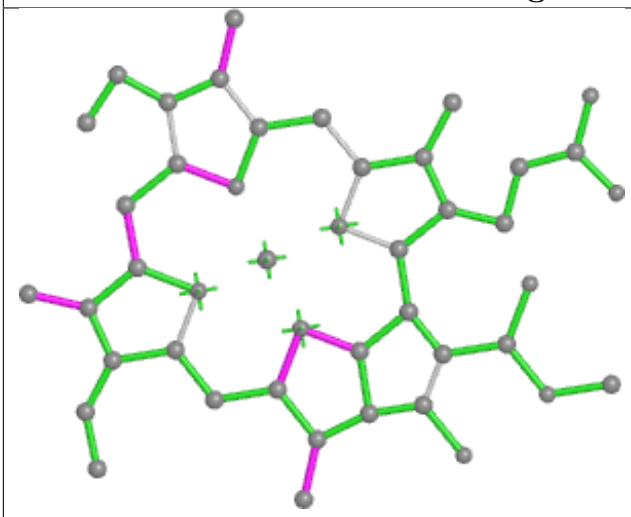


Torsions



Rings

Ligand CLA v 517



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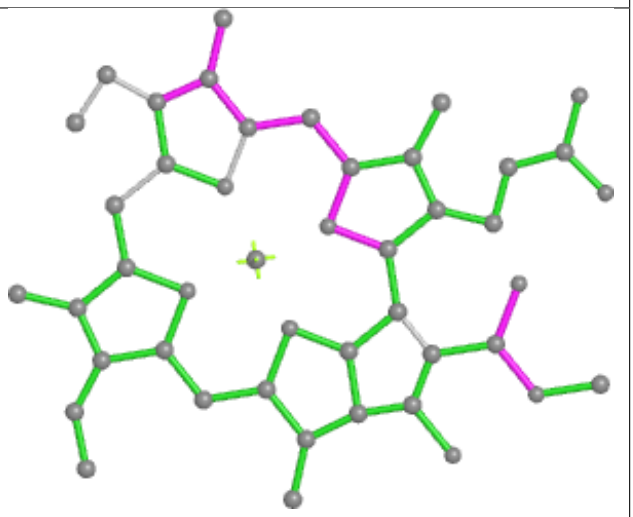
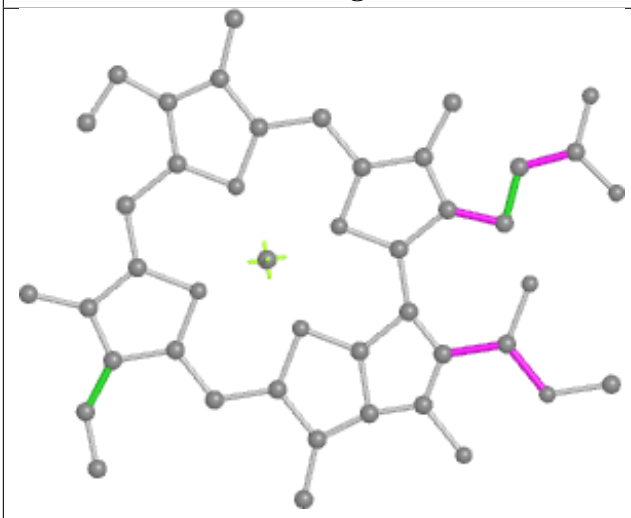
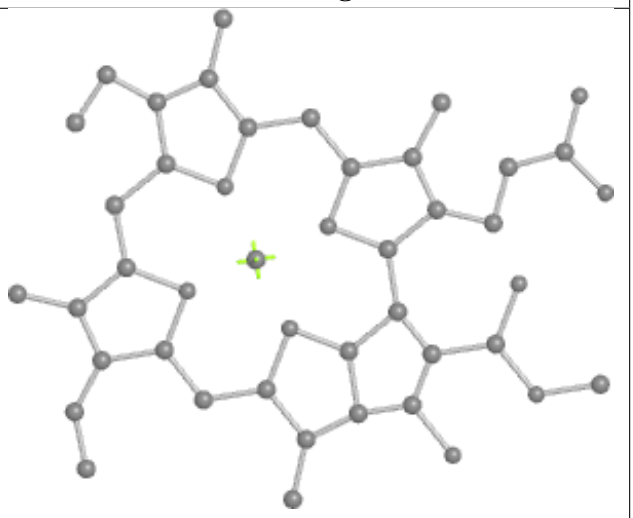


Bond angles

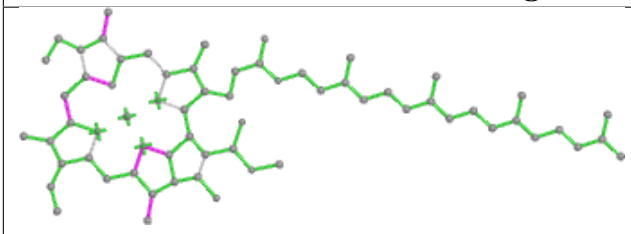


Torsions



Rings

Ligand CLA f 1240



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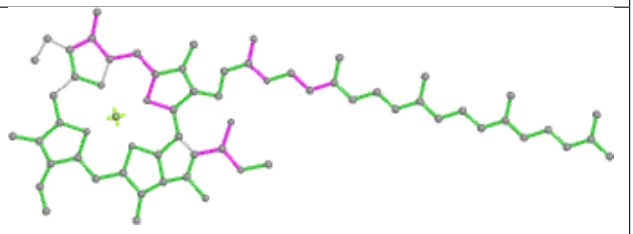
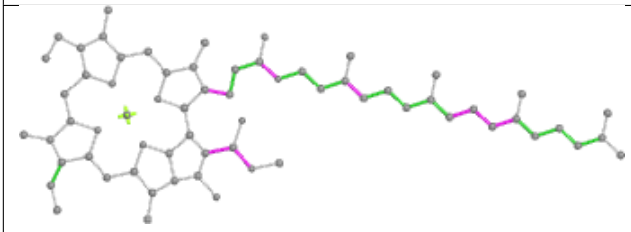


Bond angles



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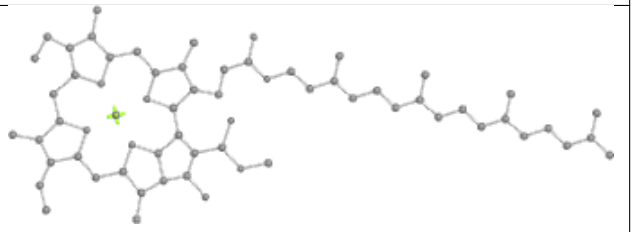
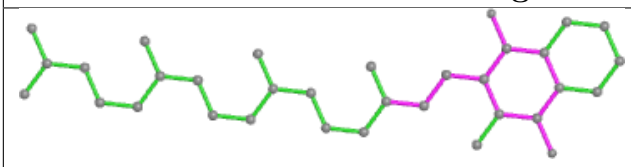


Rings

Ligand PQN G 2001



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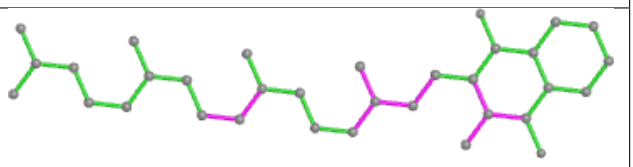
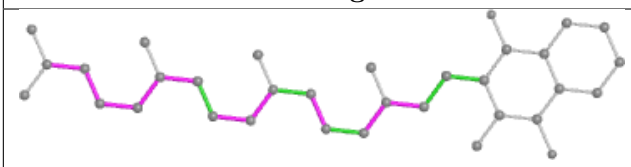
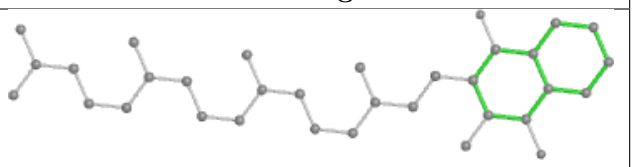


Bond angles

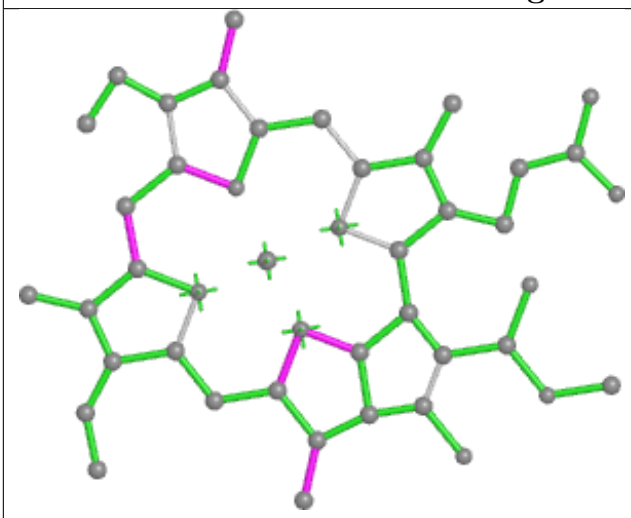


Torsions

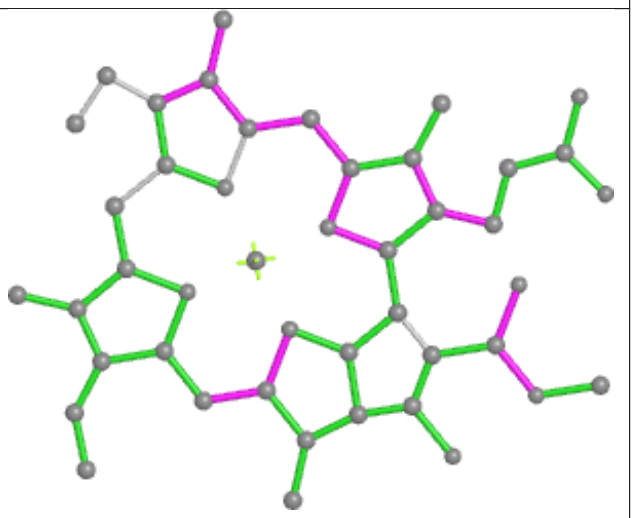


Rings

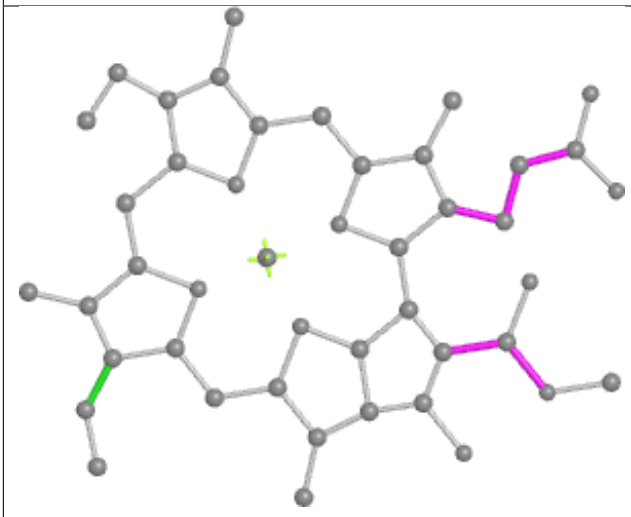
Ligand CLA d 516



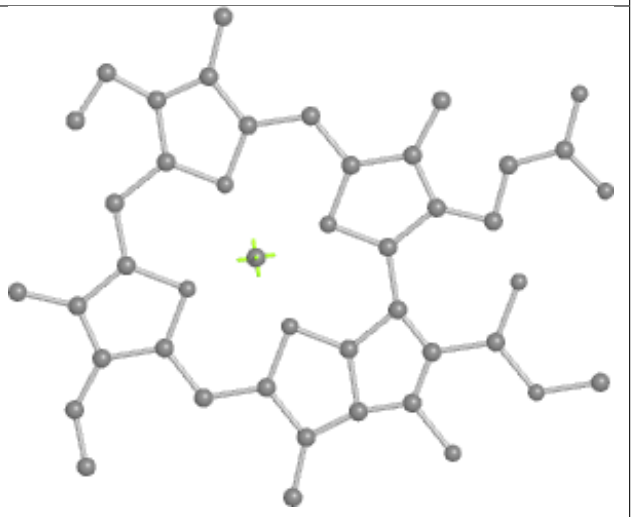
Bond lengths



Bond angles

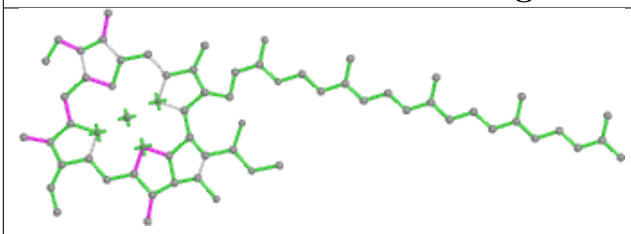


Torsions

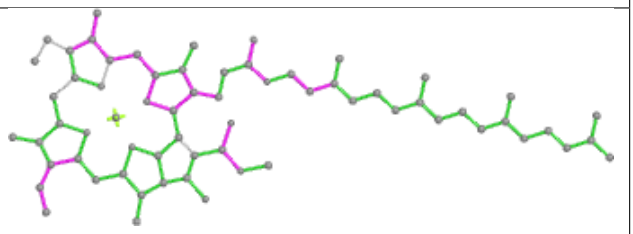


Rings

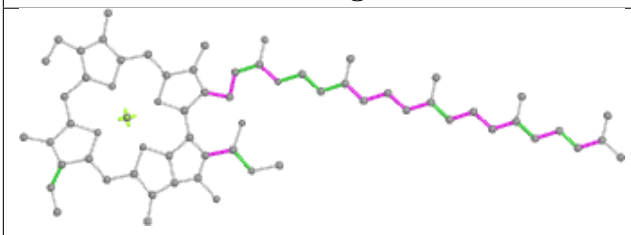
Ligand CLA B 1210



Bond lengths



Bond angles



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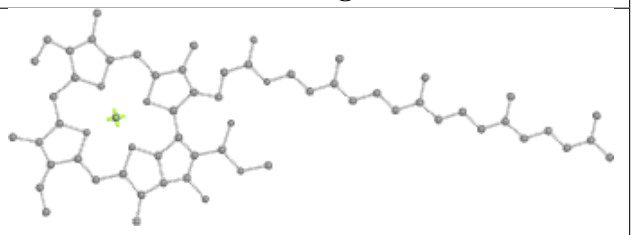
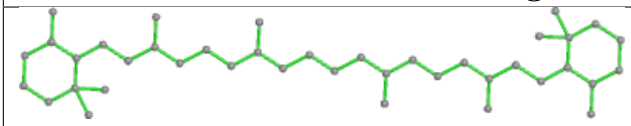
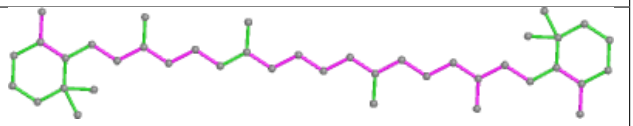


Rings

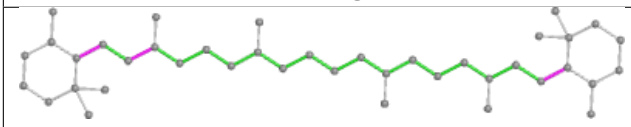
Ligand BCR d 524



Bond lengths



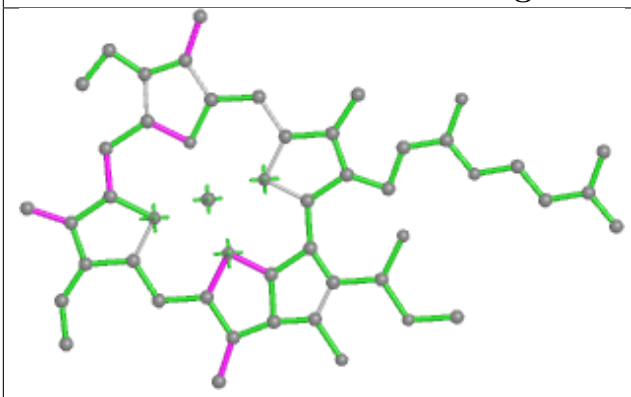
Bond angles



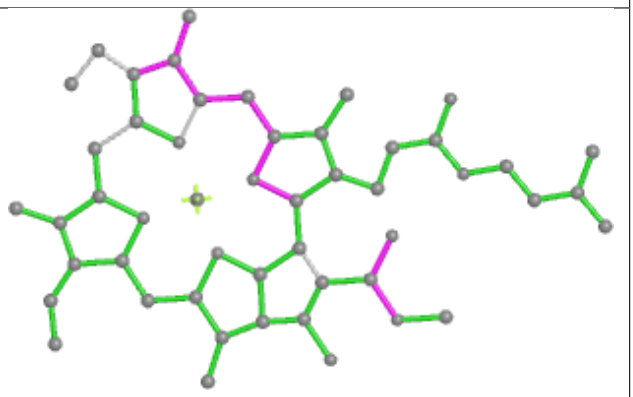
Torsions

Rings

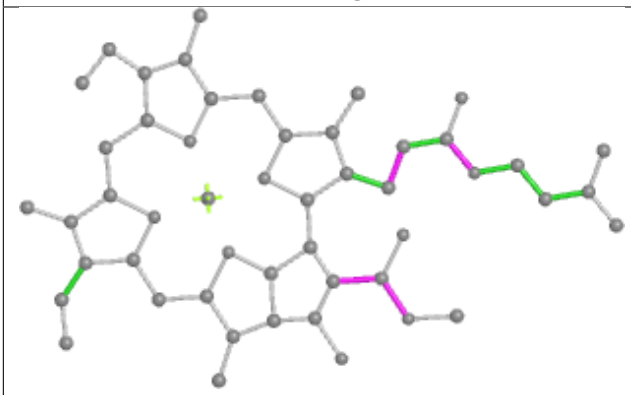
Ligand CLA H 1232



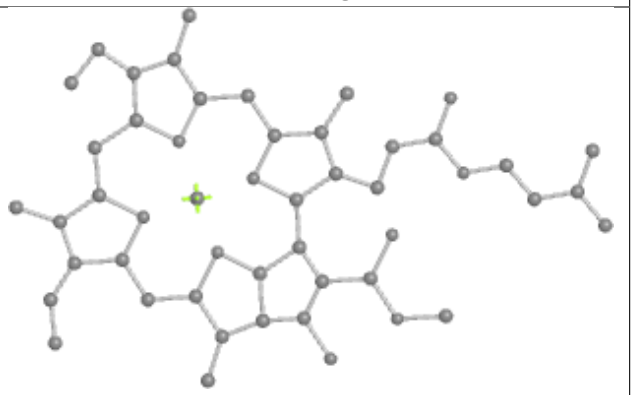
Bond lengths



Bond angles

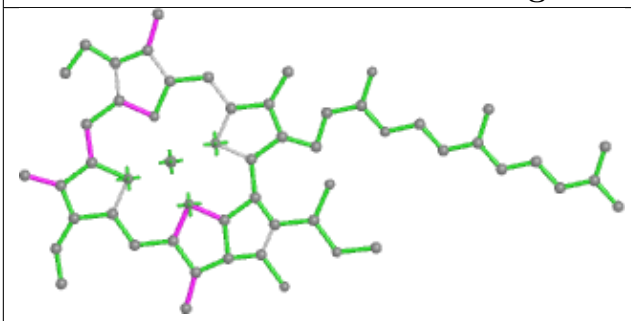


Torsions



Rings

Ligand CLA 3 518



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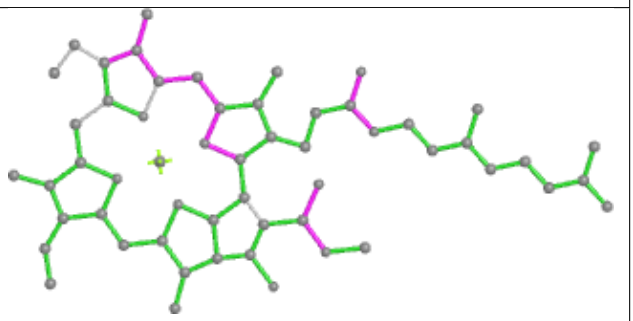

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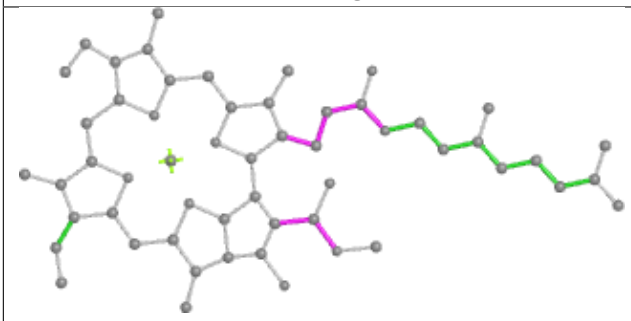
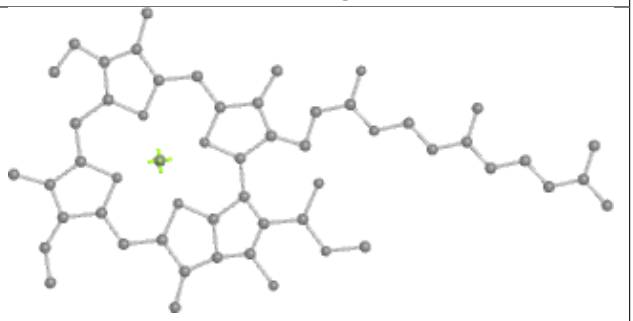
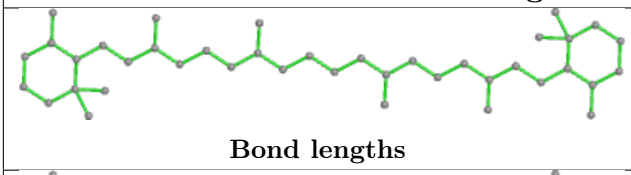


Torsions



Rings

Ligand BCR q 524



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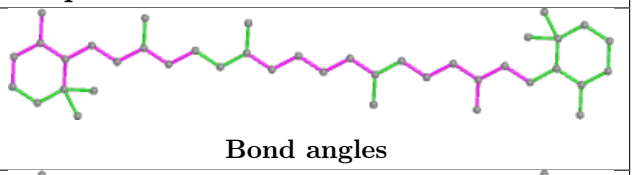
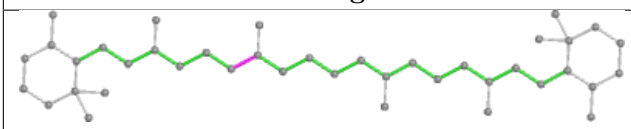


Bond angles



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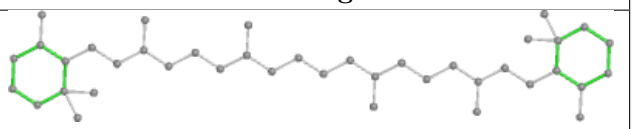
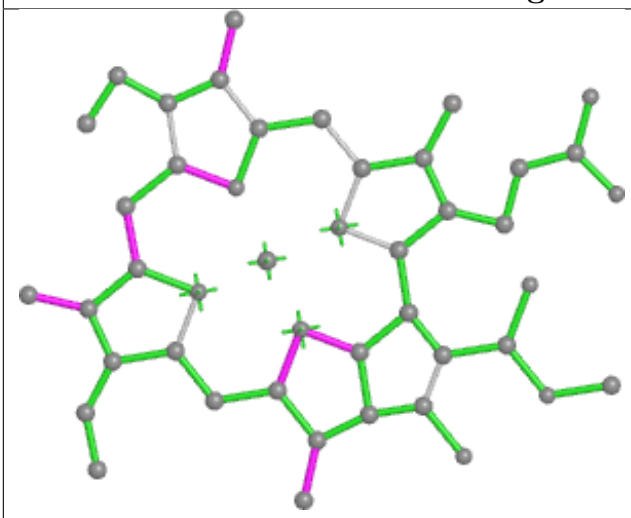


Rings

Ligand CLA d 508



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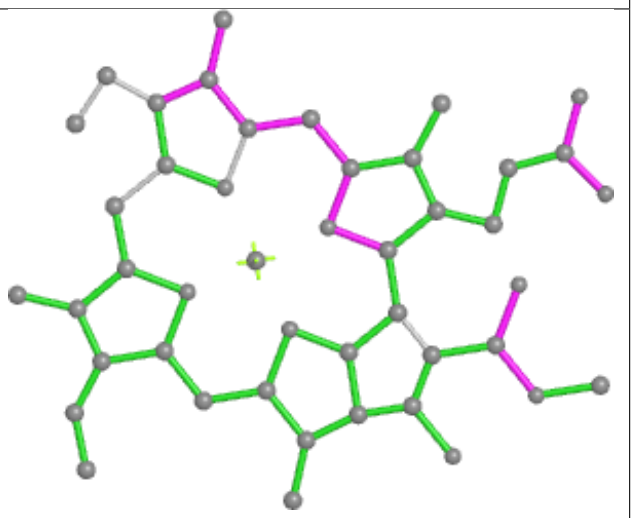
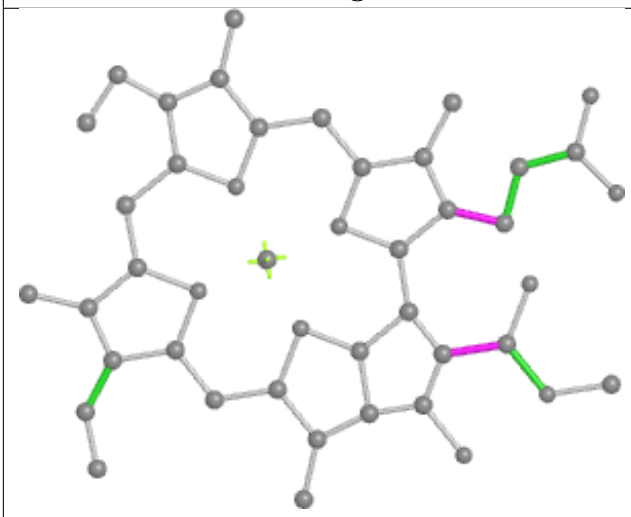


Bond angles



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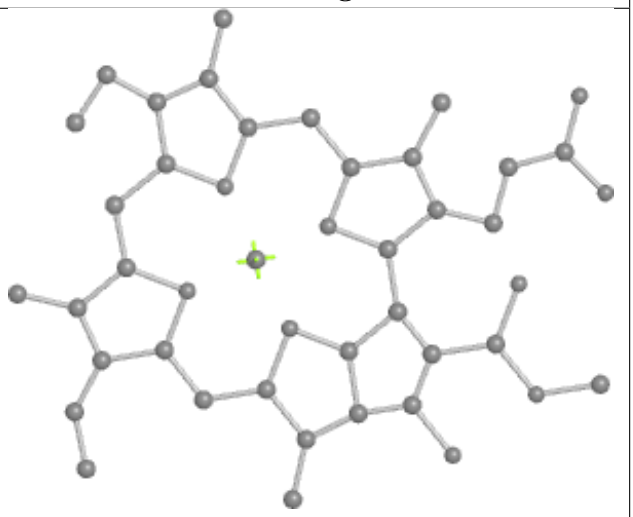
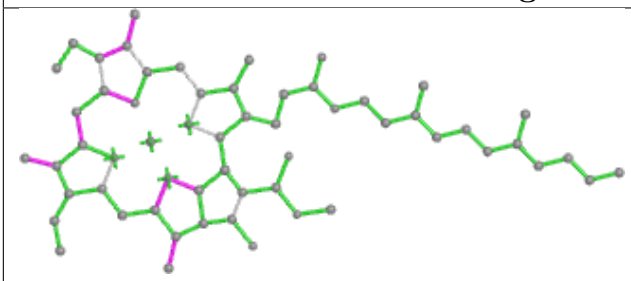


Rings

Ligand CLA J 1302



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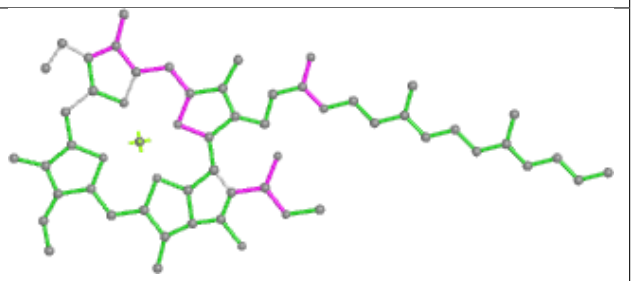
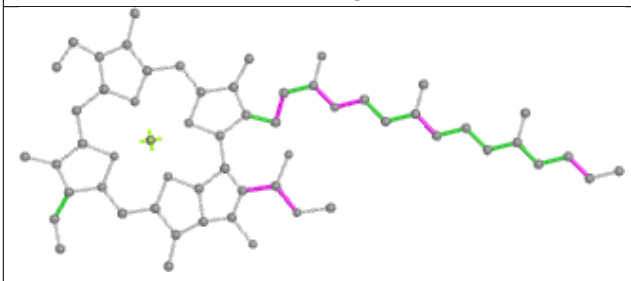


Bond angles



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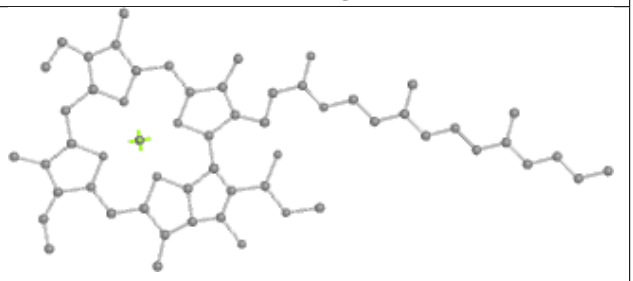
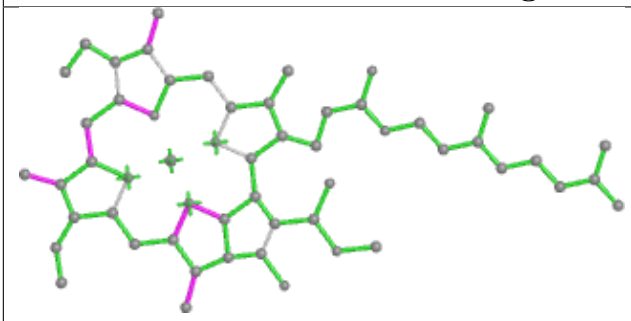


Rings

Ligand CLA e 1105



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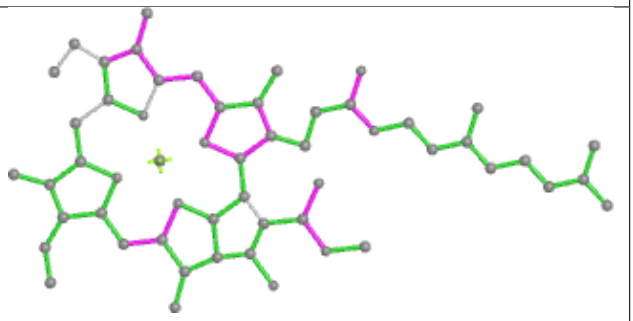
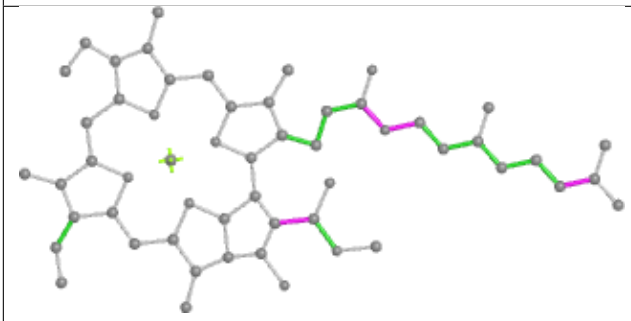


Bond angles



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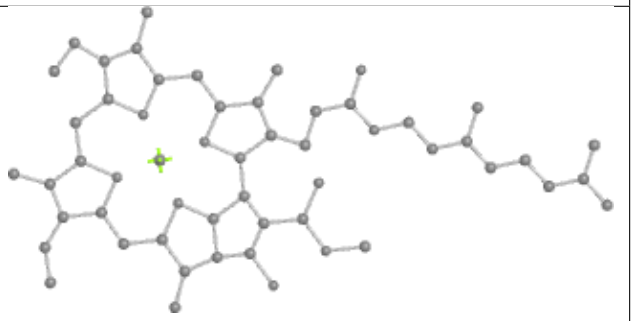
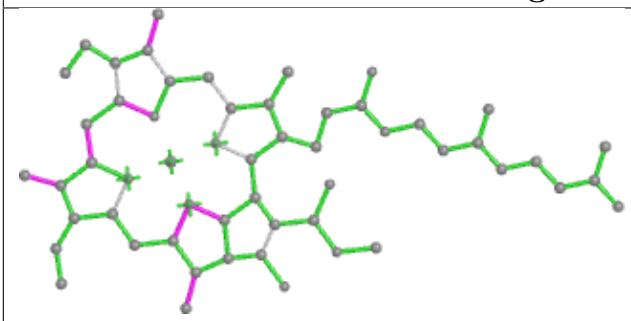


Rings

Ligand CLA 2 506



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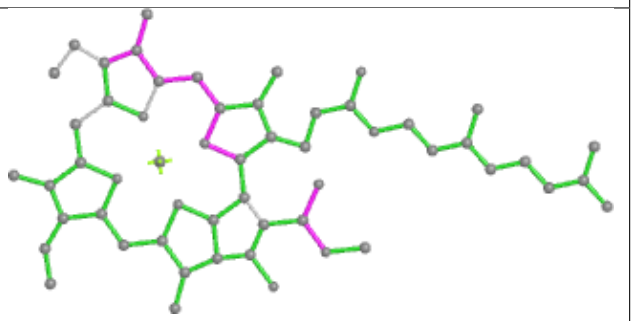
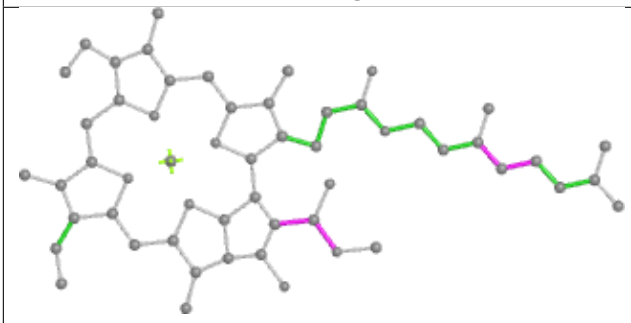


Bond angles



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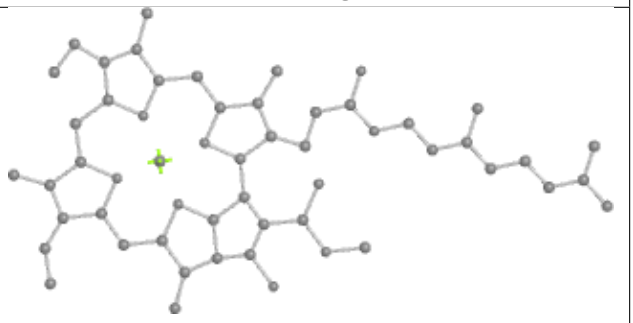
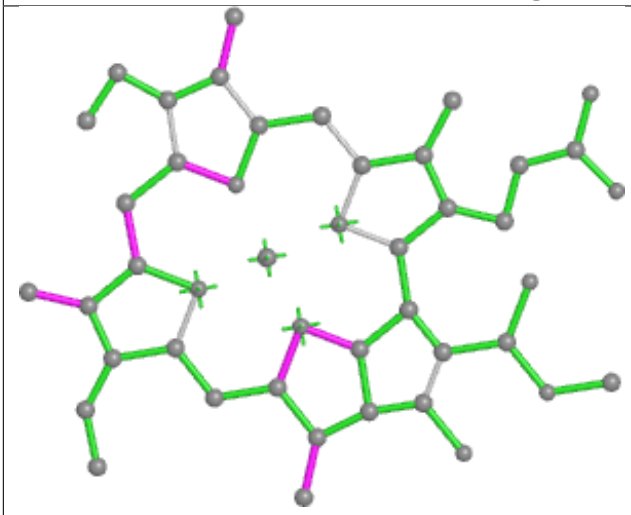


Rings

Ligand CLA q 506



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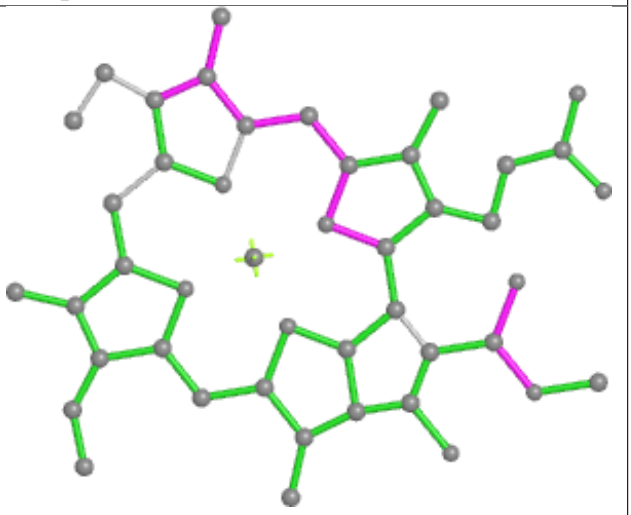
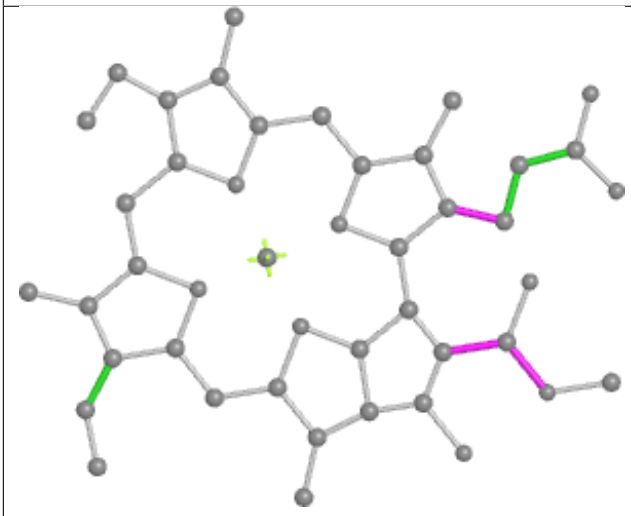


Bond angles



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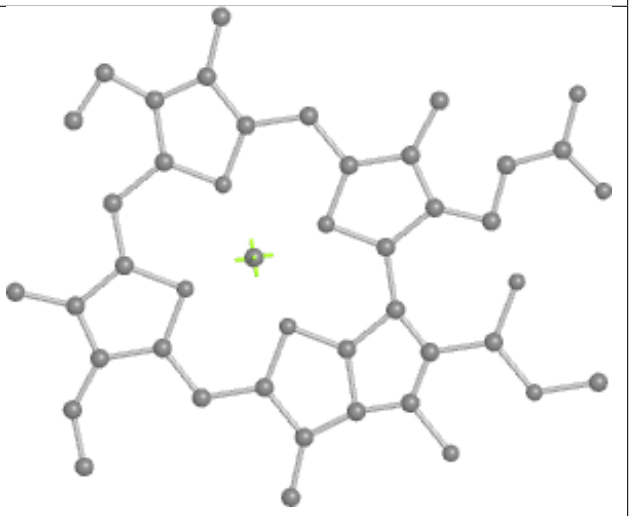
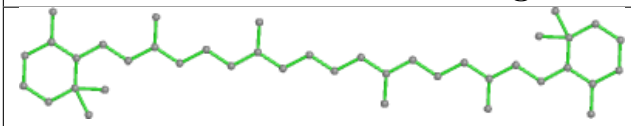
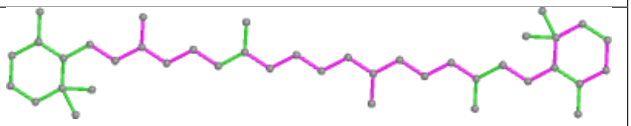


Rings

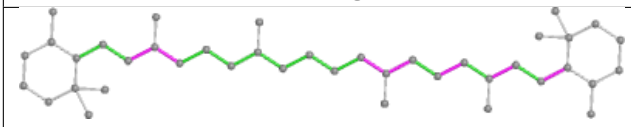
Ligand BCR G 4011



Bond lengths



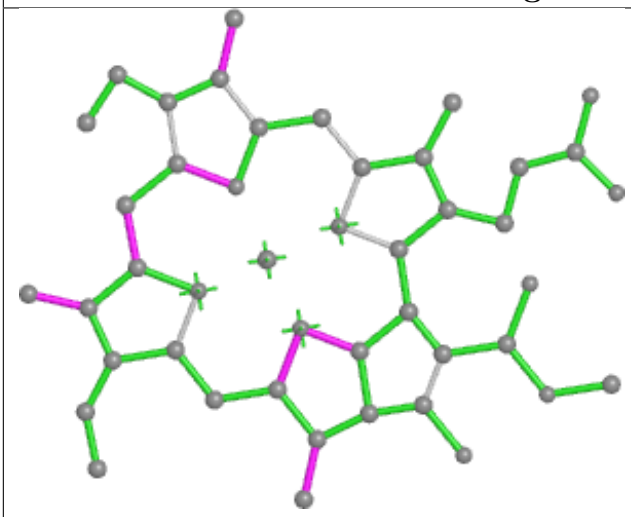
Bond angles



Torsions

Rings

Ligand CLA Y 517



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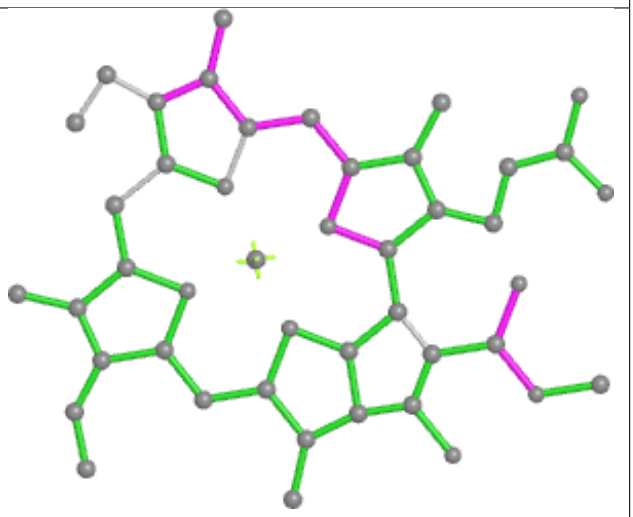
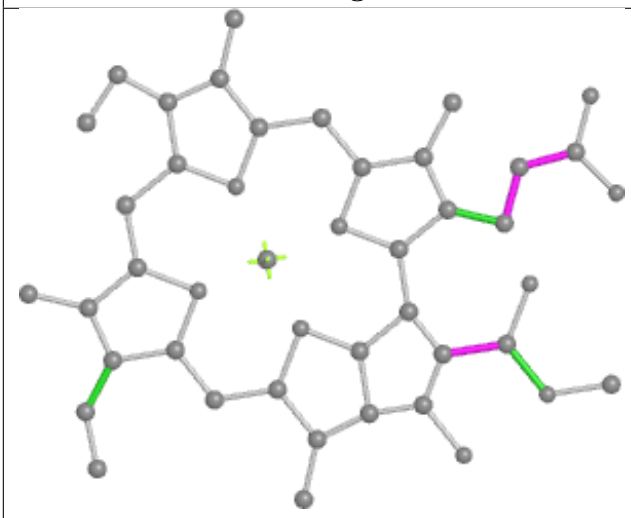
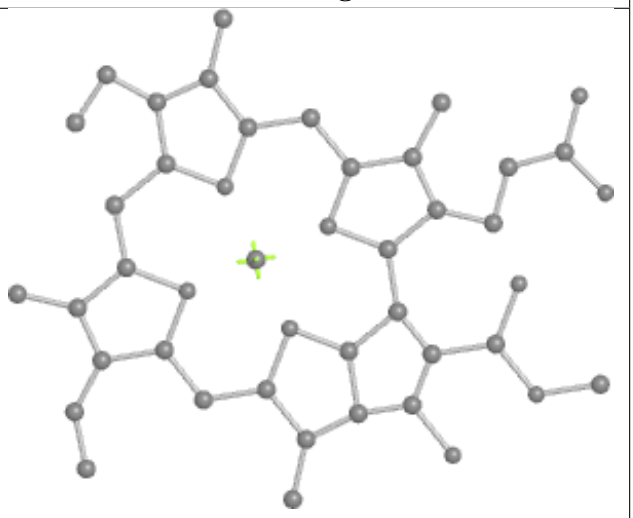


Bond angles

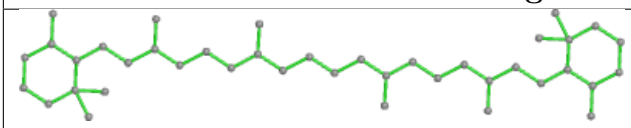


Torsions



Rings

Ligand BCR u 523



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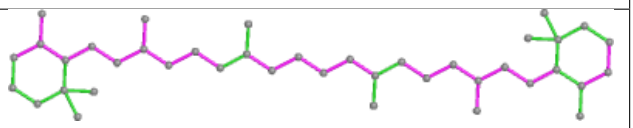

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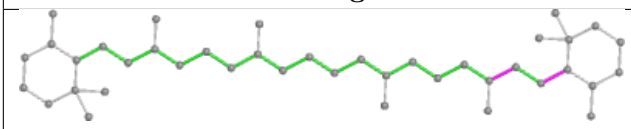

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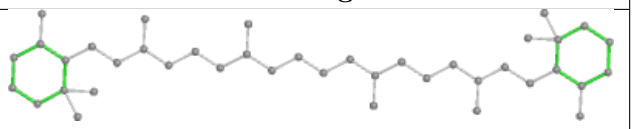
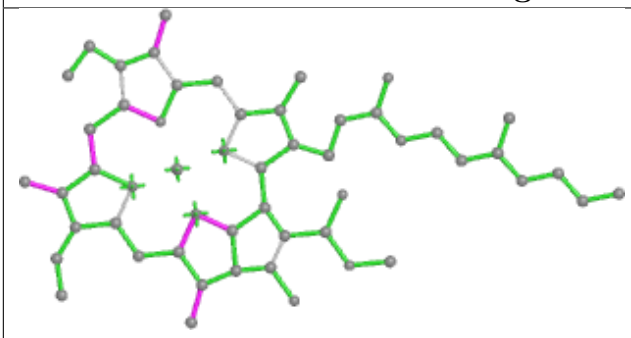


Rings

Ligand CLA G 1120



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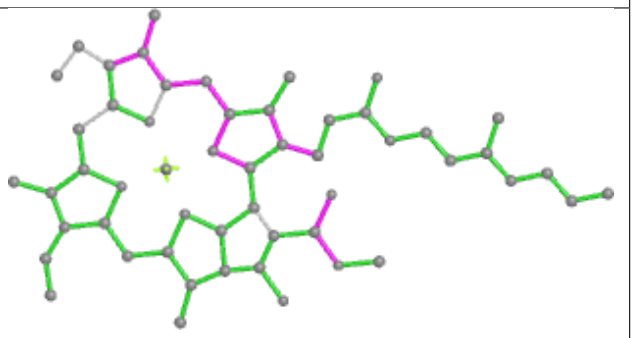
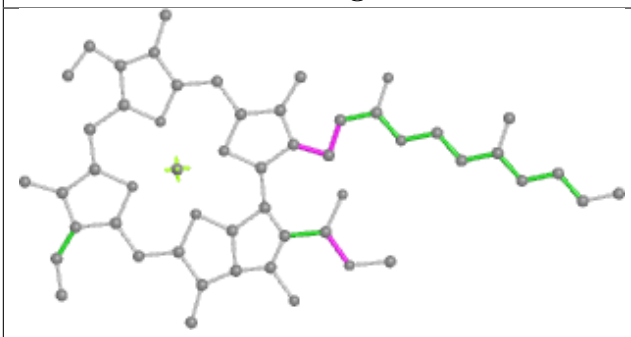


Bond angles



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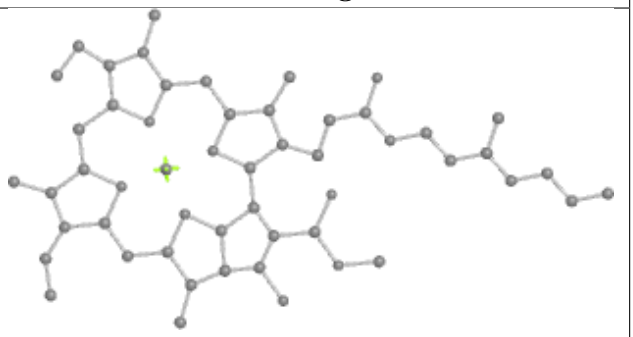
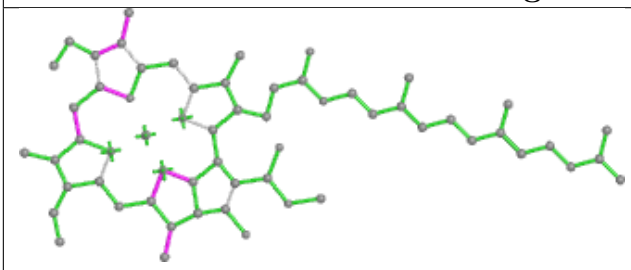
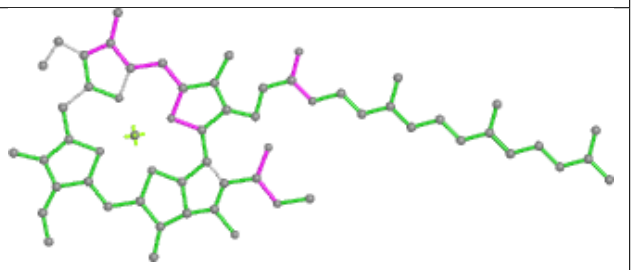


Rings

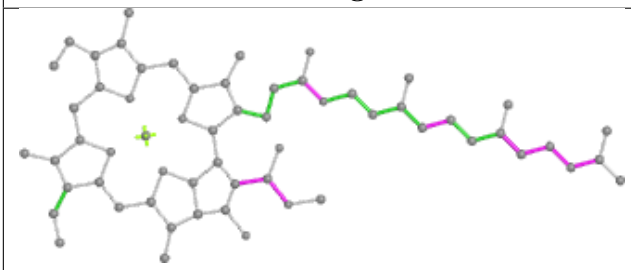
Ligand CLA Y 502



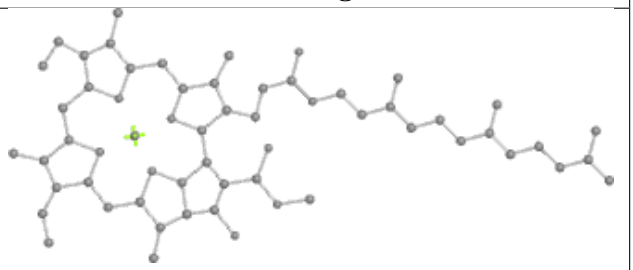
Bond lengths



Bond angles

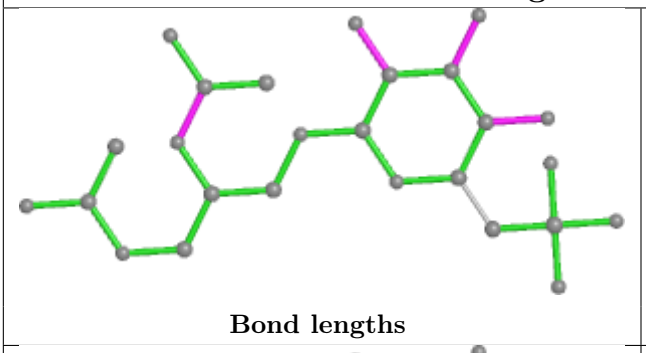


Torsions

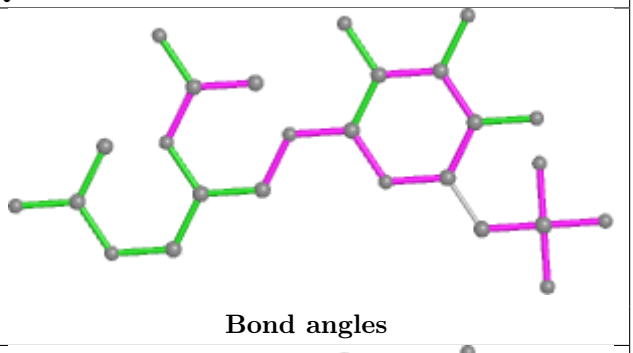


Rings

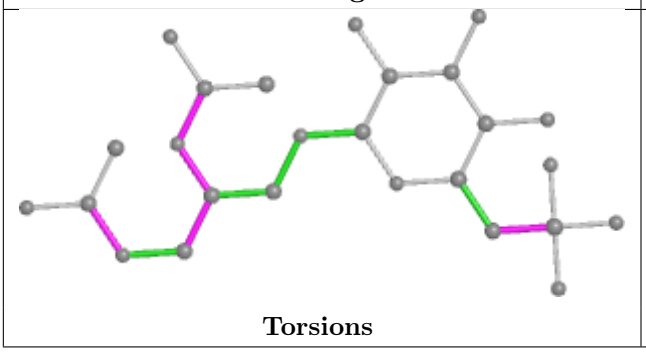
Ligand SQD 4 822



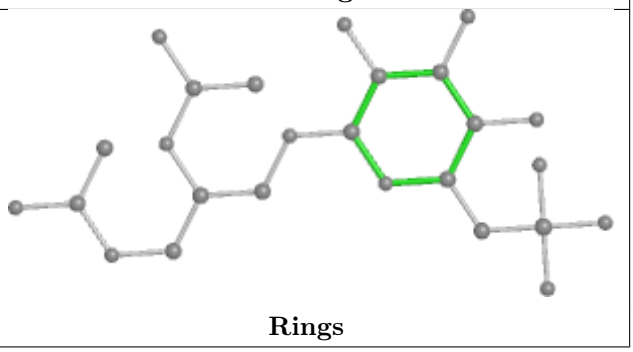
Bond lengths



Bond angles

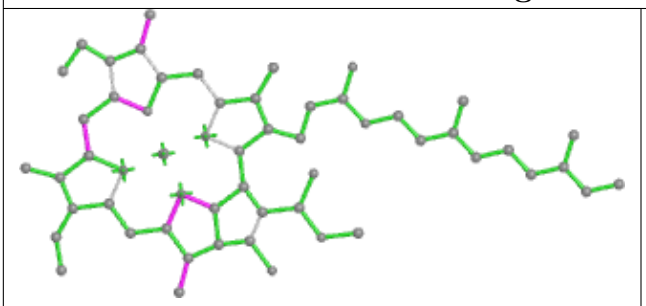


Torsions

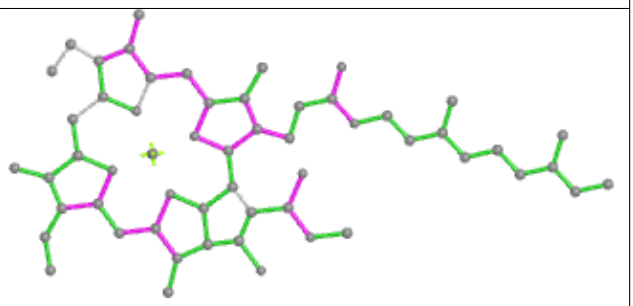


Rings

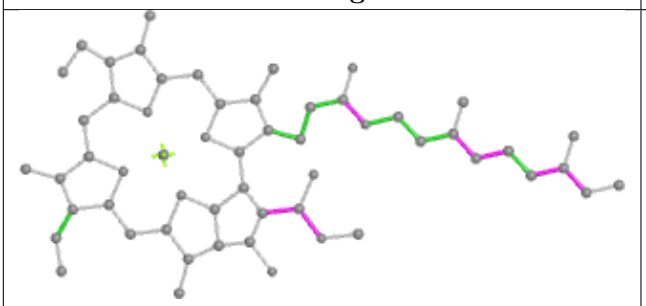
Ligand CLA A 1124



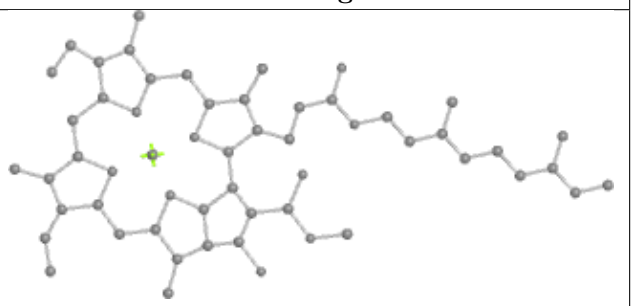
Bond lengths



Bond angles

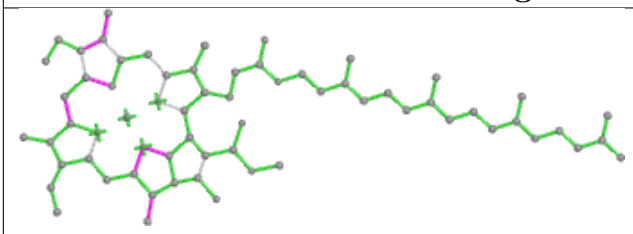


Torsions

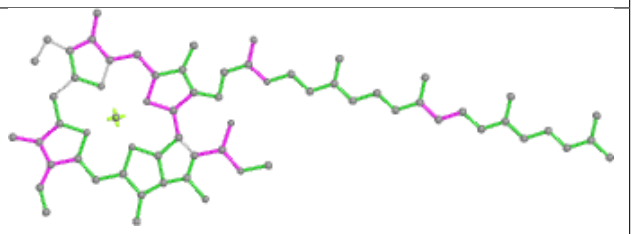


Rings

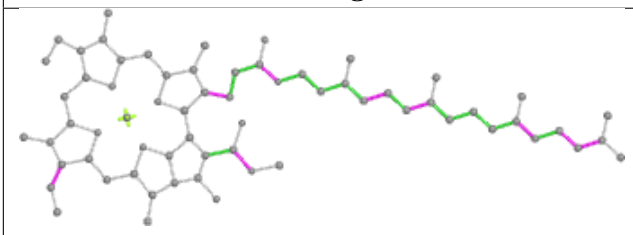
Ligand CLA H 1239



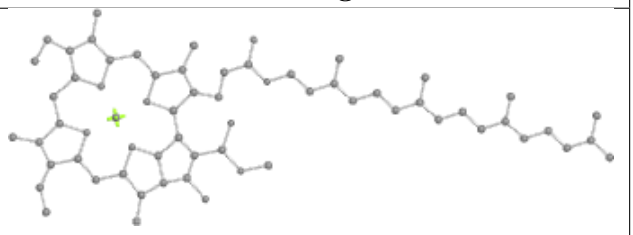
Bond lengths



Bond angles

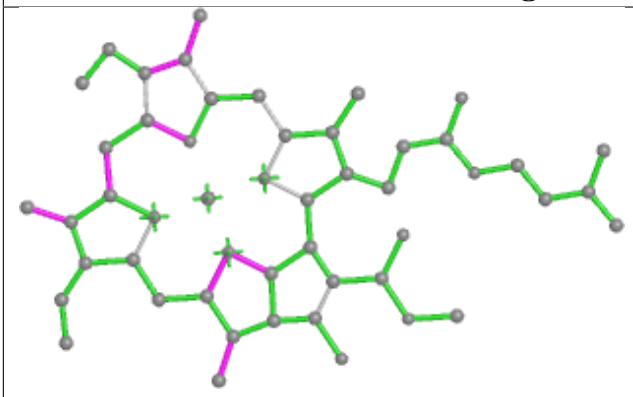


Torsions



Rings

Ligand CLA e 1114



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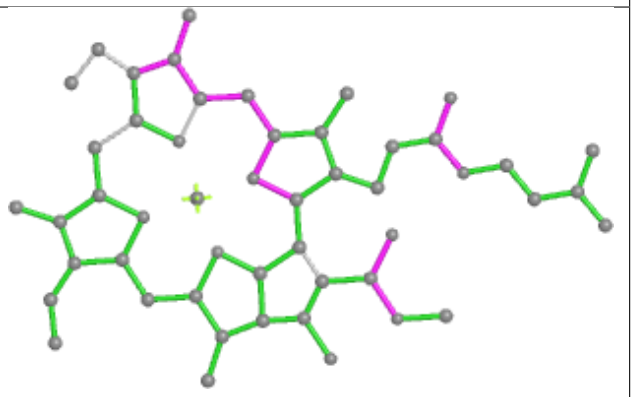
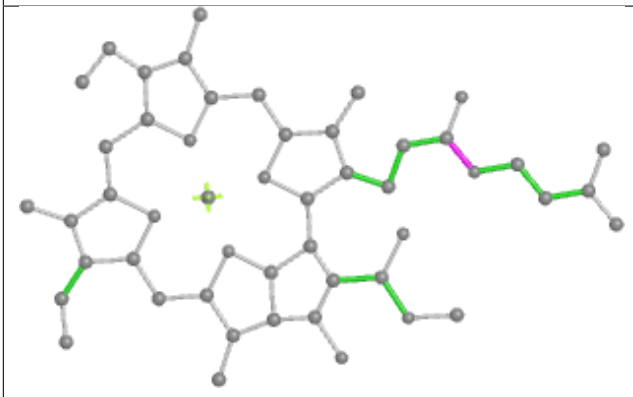
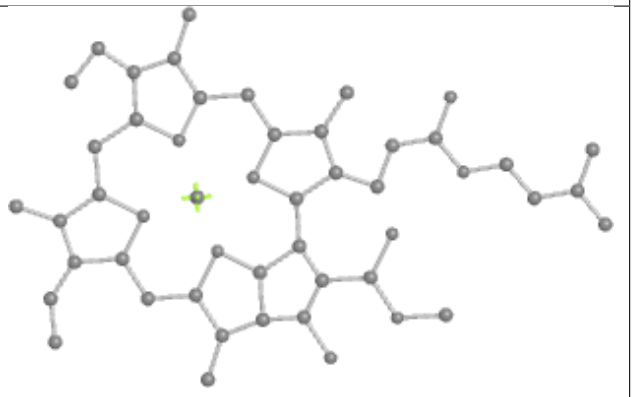


Bond angles

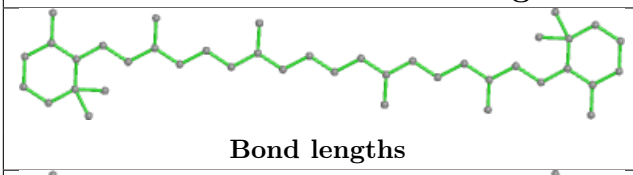


Torsions



Rings

Ligand BCR H 4017



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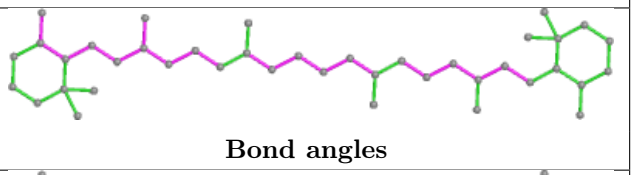
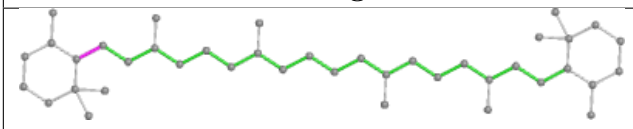
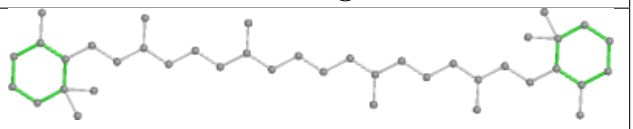


Bond angles

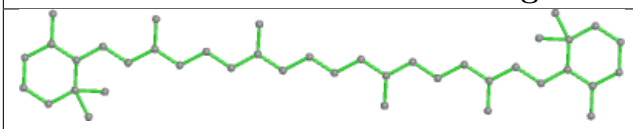


Torsions



Rings

Ligand BCR f 4006



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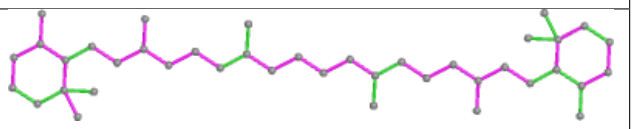
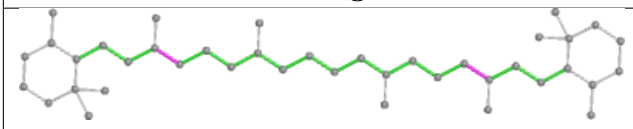
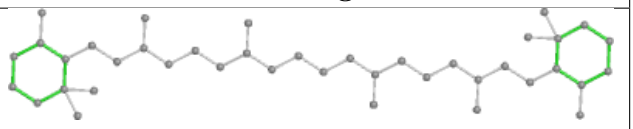


Bond angles

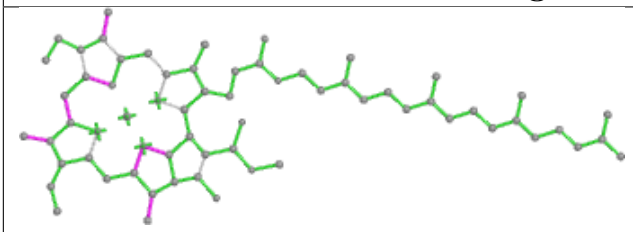


Torsions



Rings

Ligand CLA a 509



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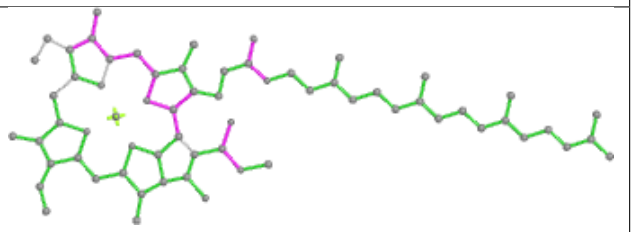
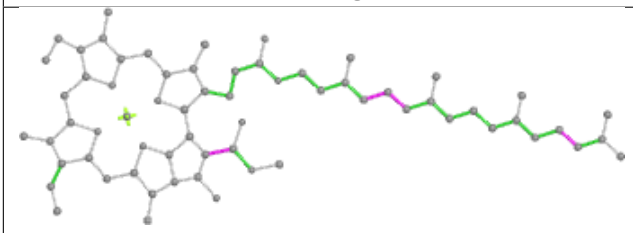


Bond angles



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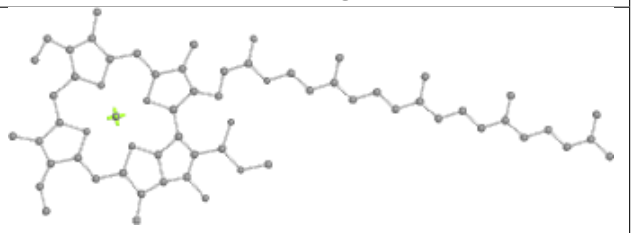
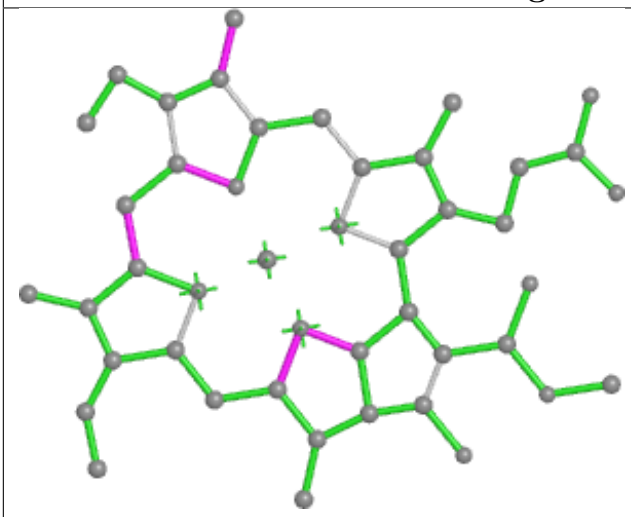


Rings

Ligand CLA 6 513



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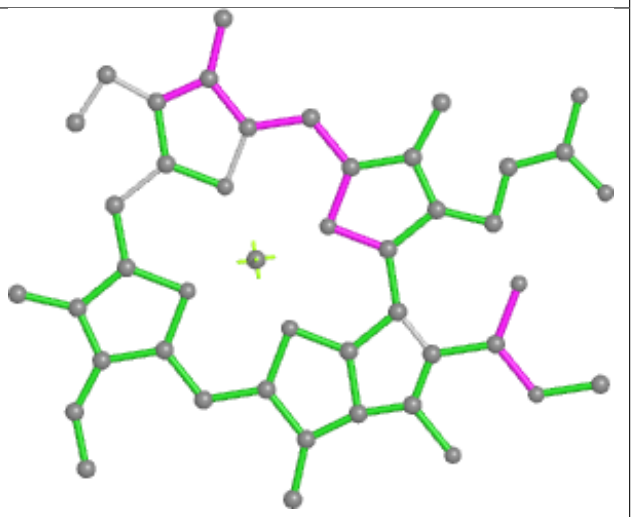
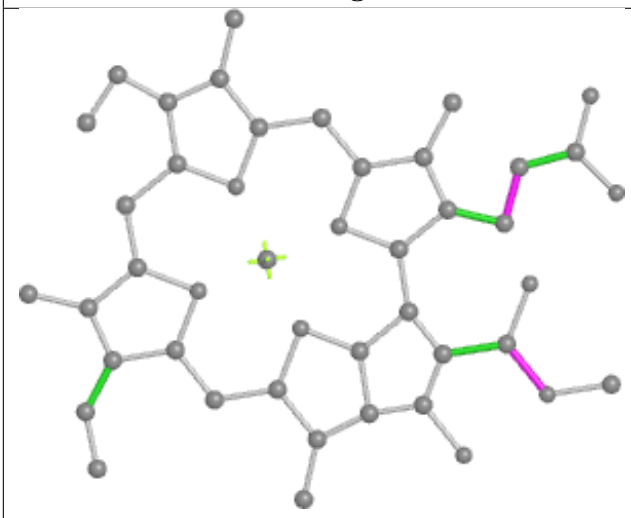


Bond angles



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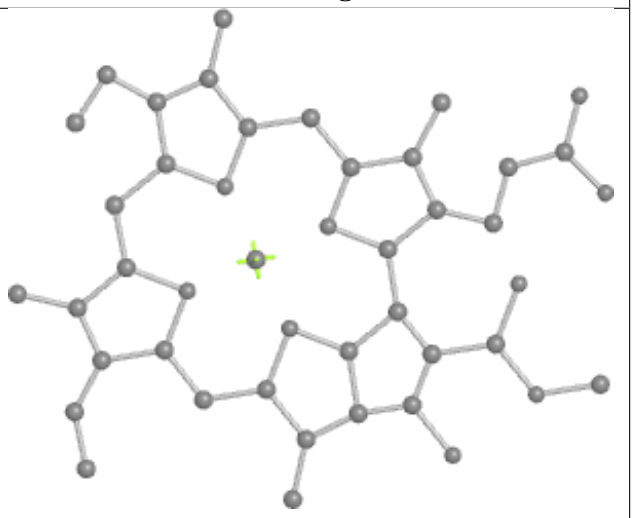
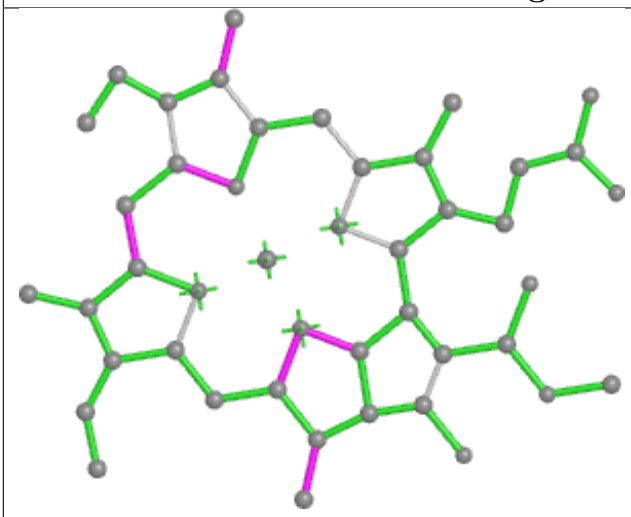


Rings

Ligand CLA 2 516



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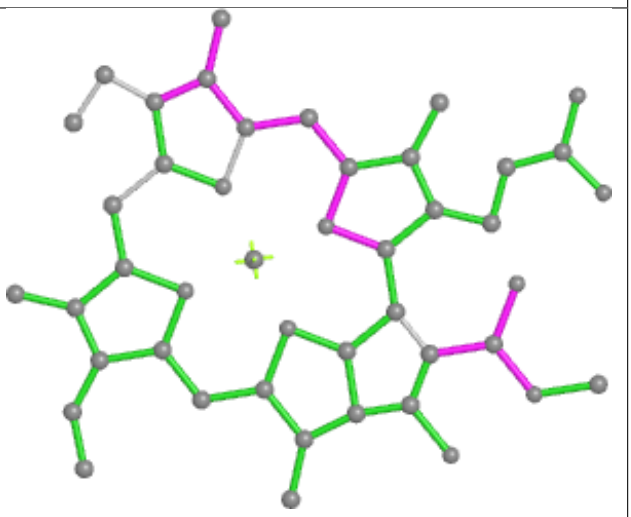
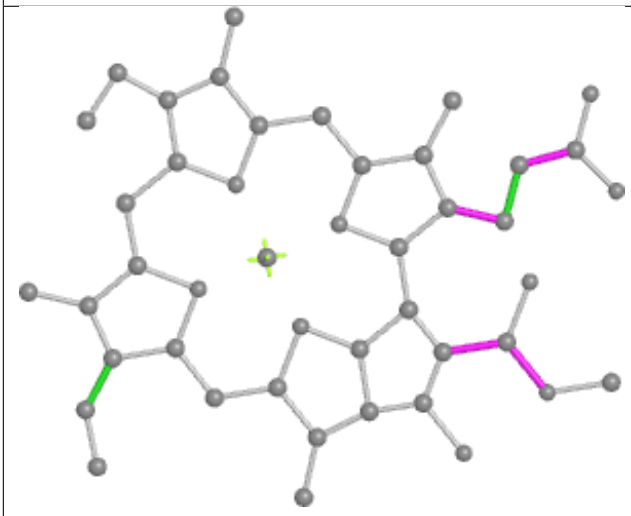


Bond angles



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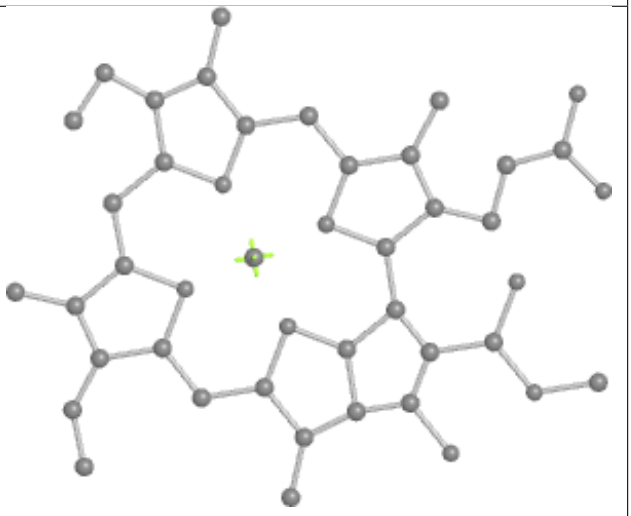
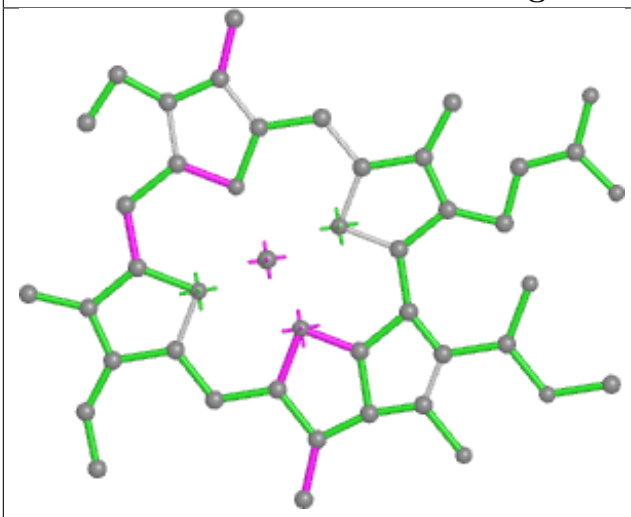


Rings

Ligand CLA a 512



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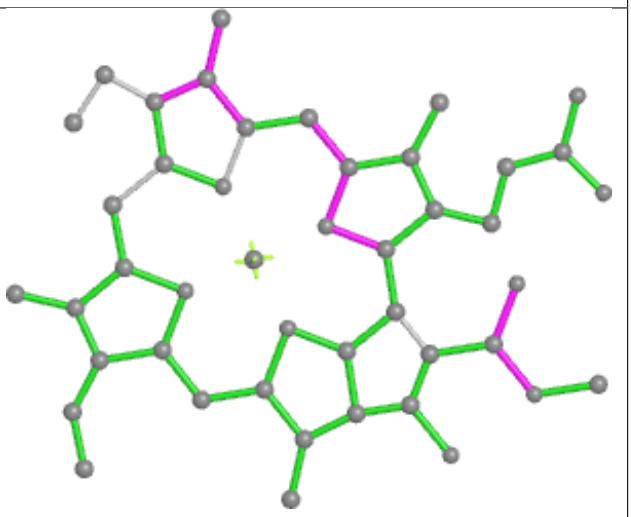
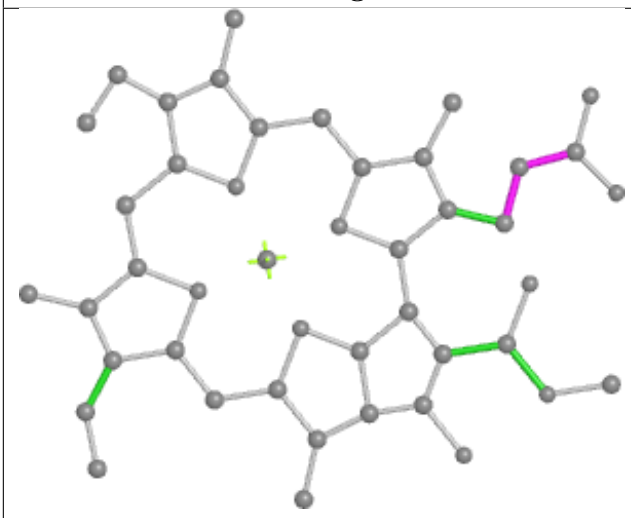


Bond angles



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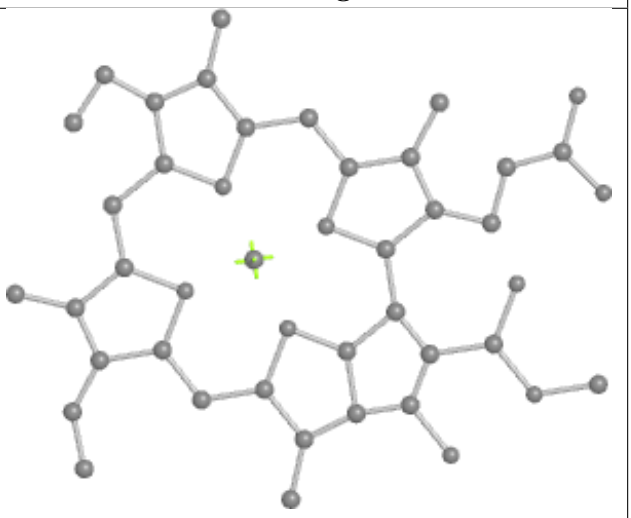
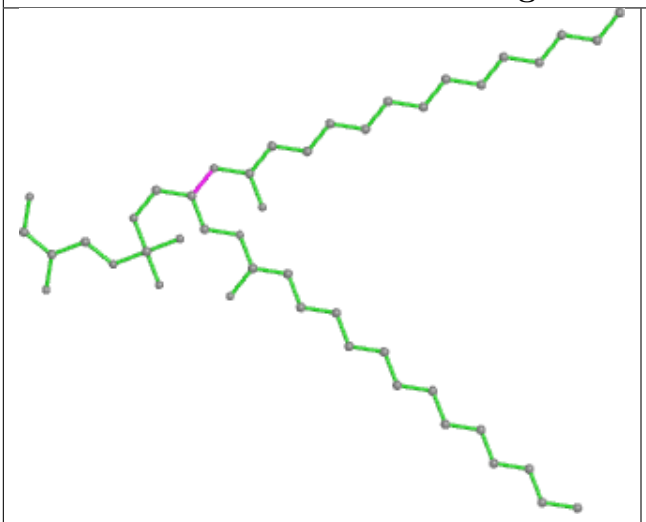
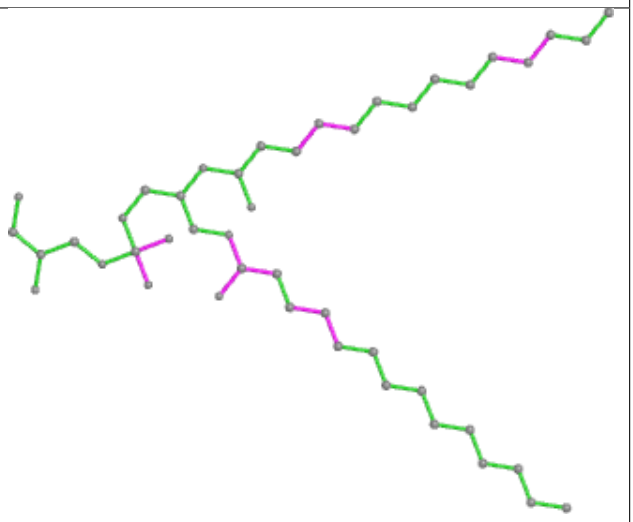


Rings

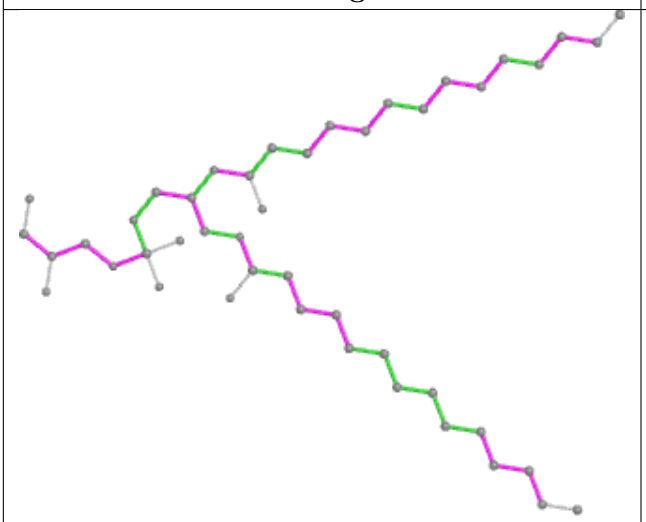
Ligand LHG e 5005



Bond lengths



Bond angles



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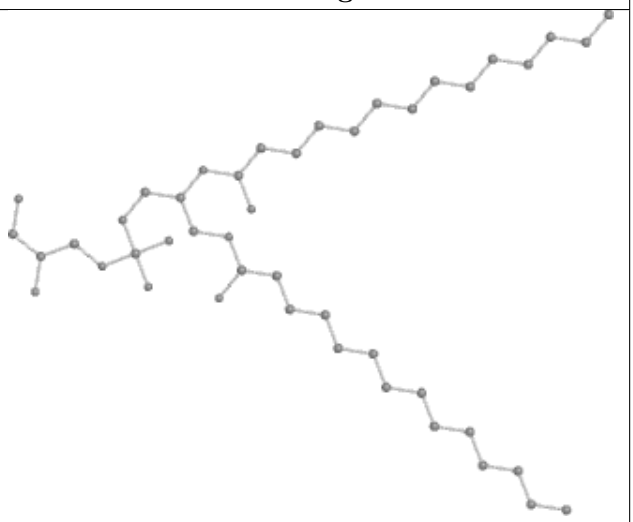
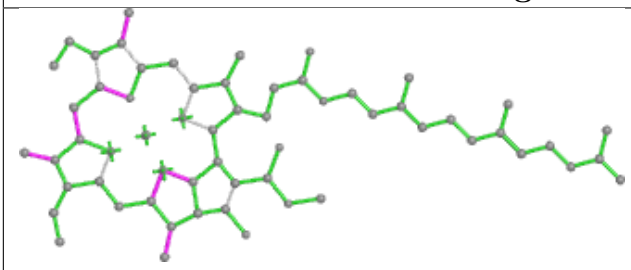
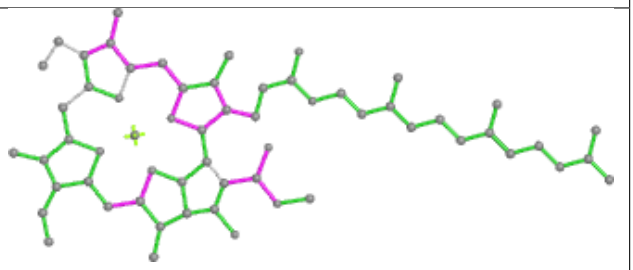
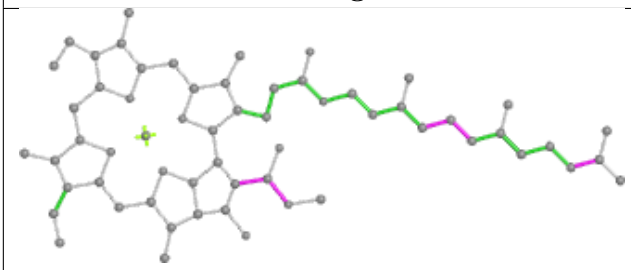
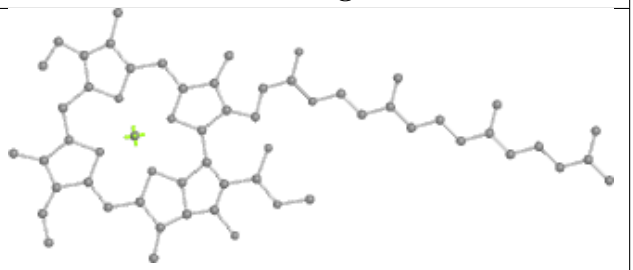
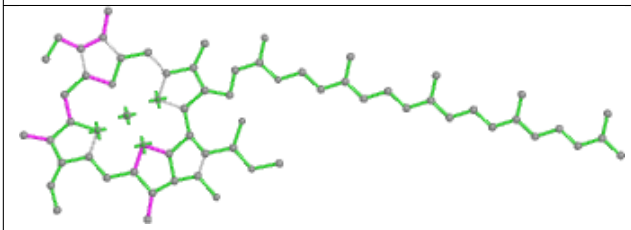
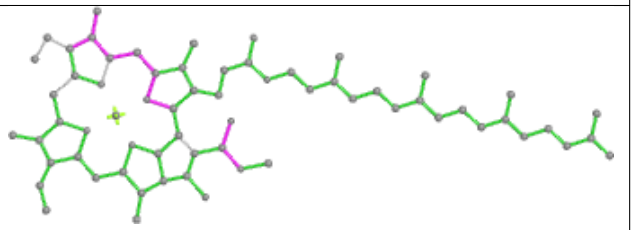
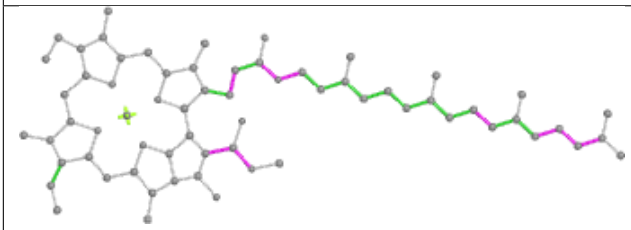
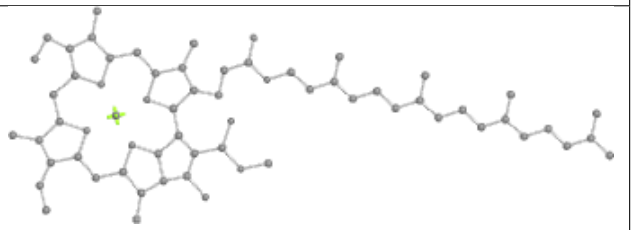
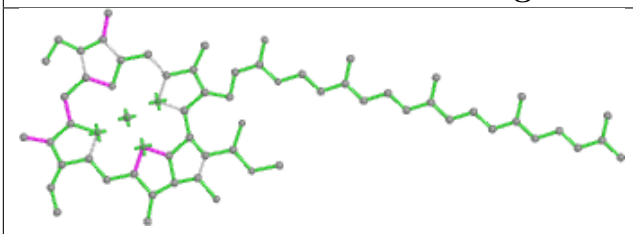


Rings

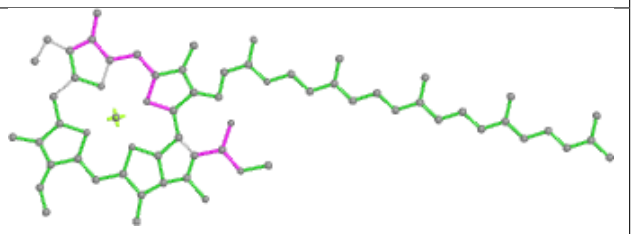
Ligand CLA H 1222	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1207	
	
Bond lengths	Bond angles
	
Torsions	Rings

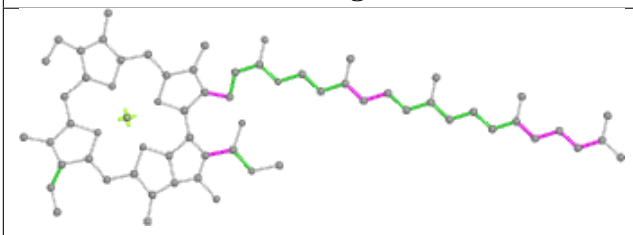
Ligand CLA G 1102



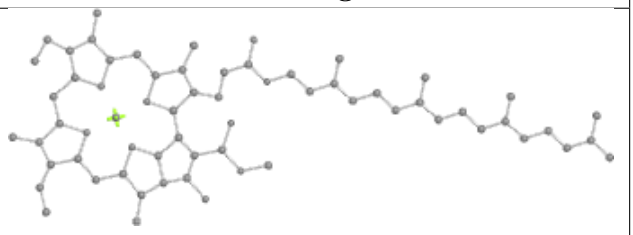
Bond lengths



Bond angles

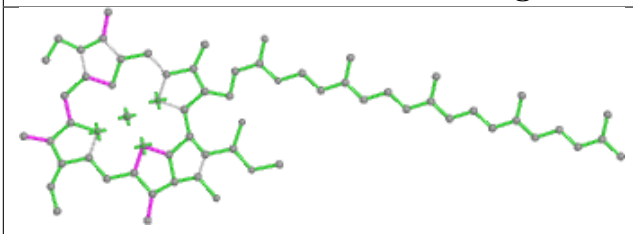


Torsions

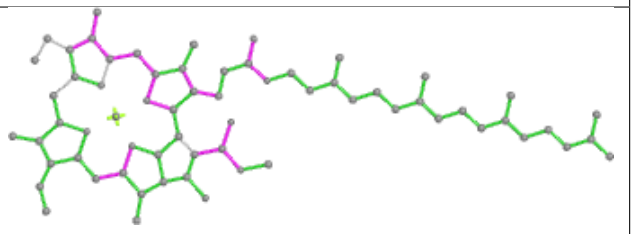


Rings

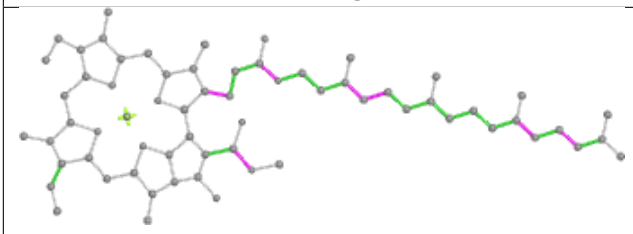
Ligand CLA G 1104



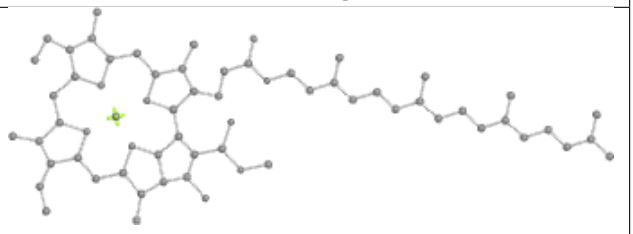
Bond lengths



Bond angles

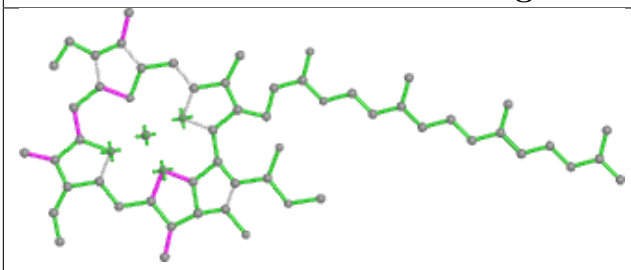


Torsions

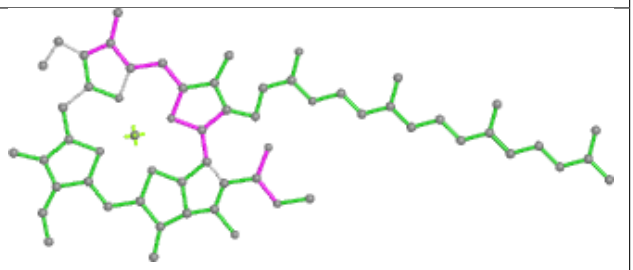


Rings

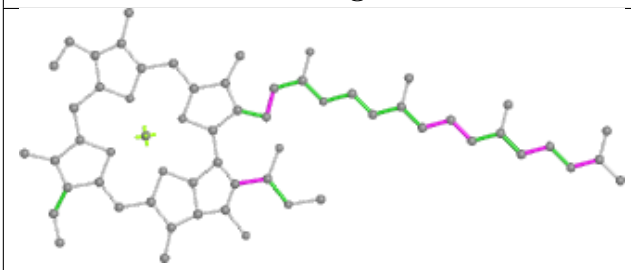
Ligand CLA B 1218



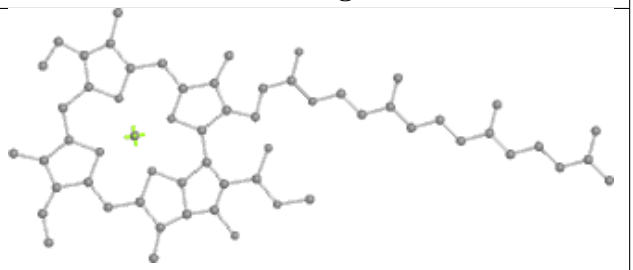
Bond lengths



Bond angles

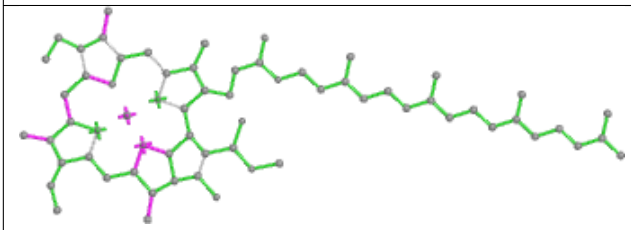


Torsions

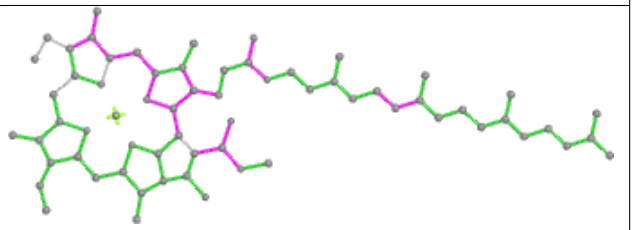


Rings

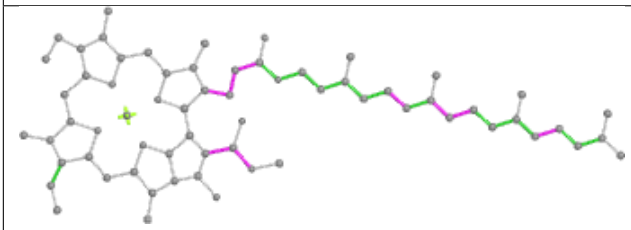
Ligand CLA H 1221



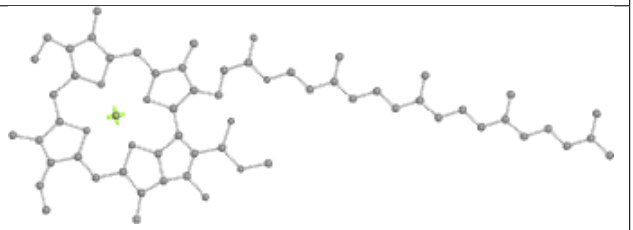
Bond lengths



Bond angles

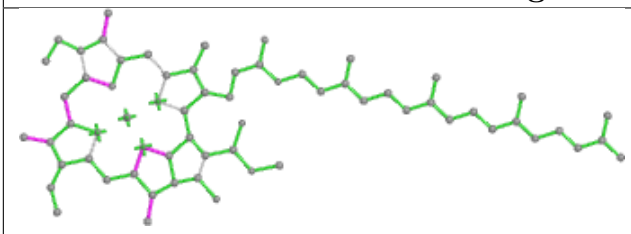


Torsions

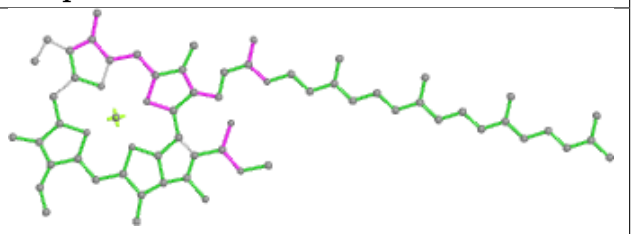


Rings

Ligand CLA q 501



Bond lengths



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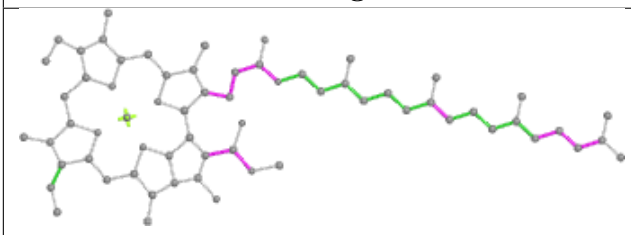
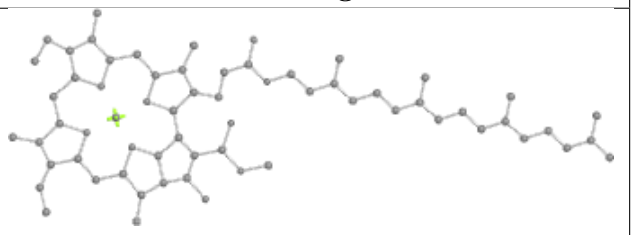


Torsions



Rings

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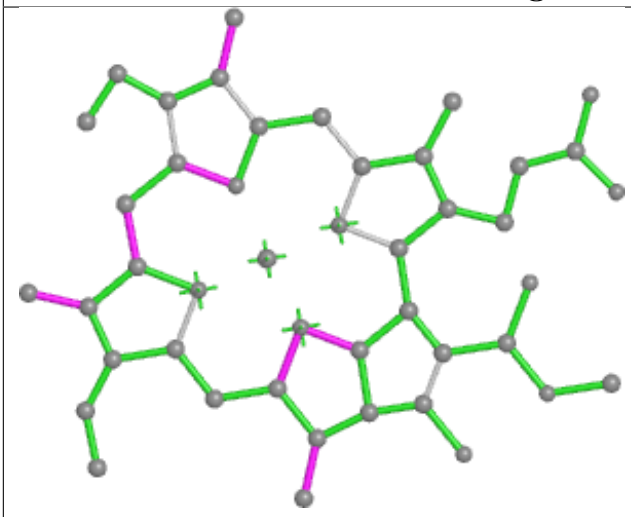

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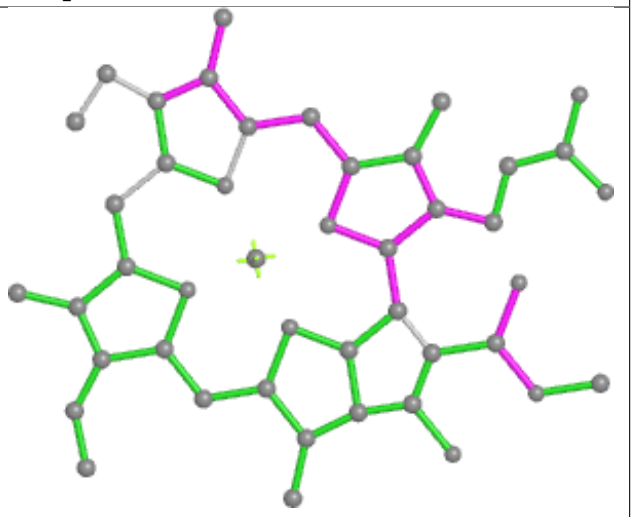
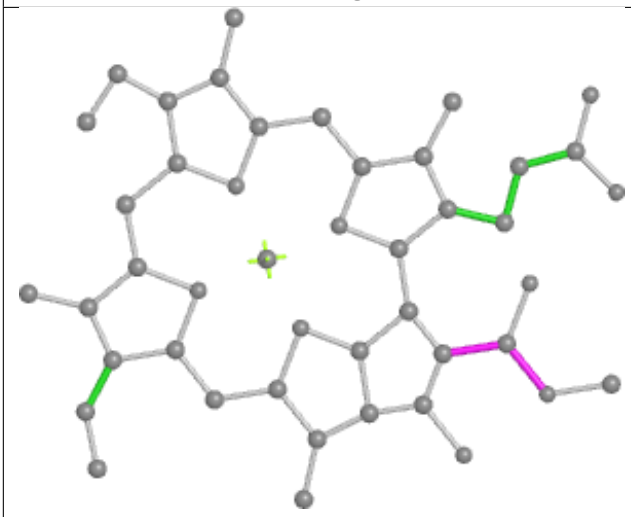
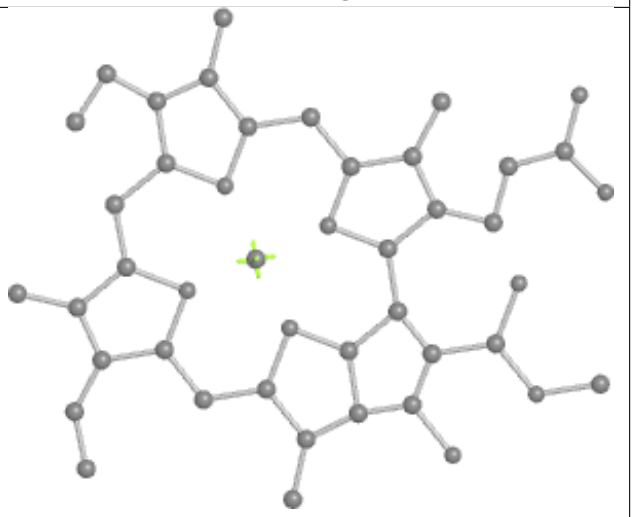


Bond angles

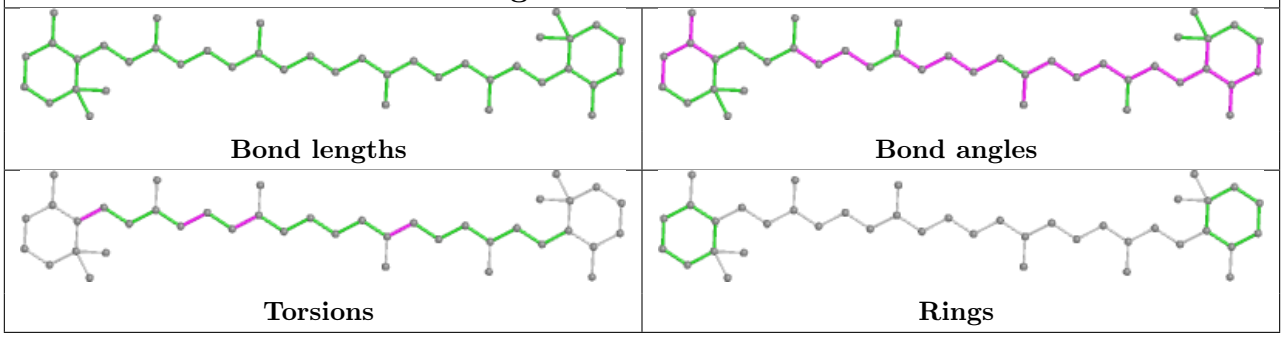


Torsions

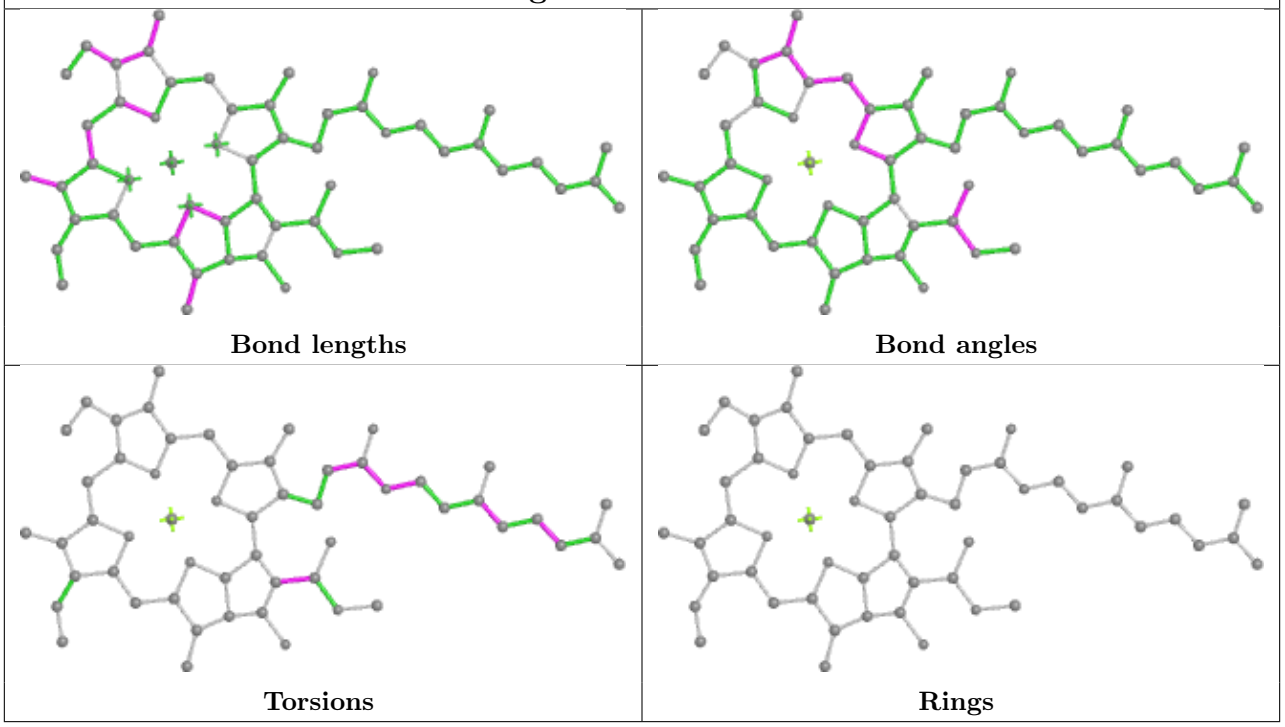


Rings

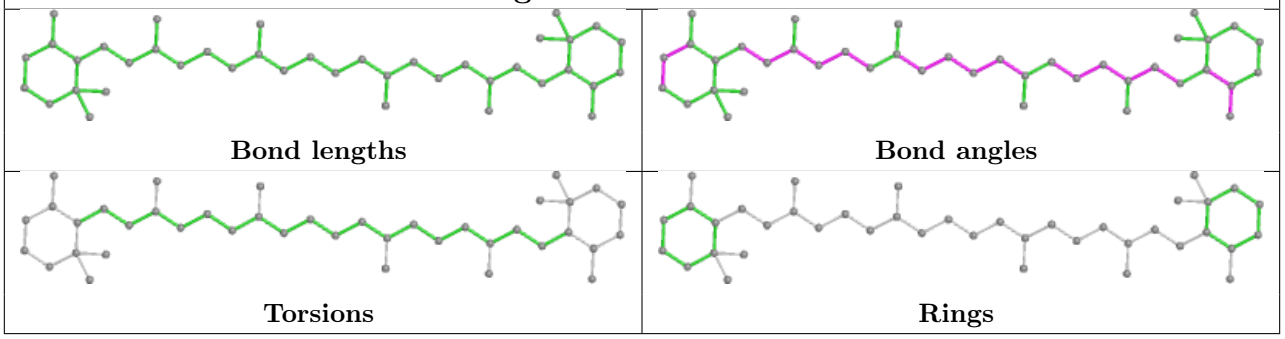
Ligand BCR M 4021



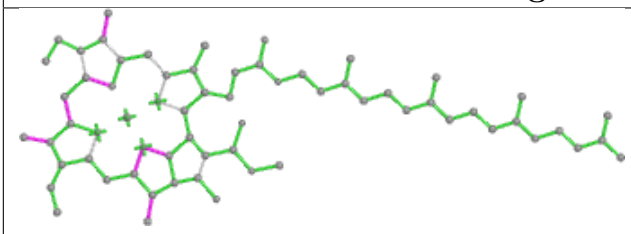
Ligand CLA 4 519



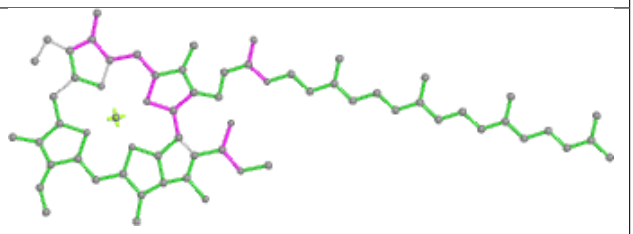
Ligand BCR A 4003



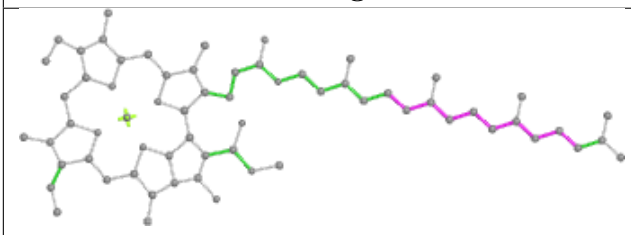
Ligand CLA 5 509



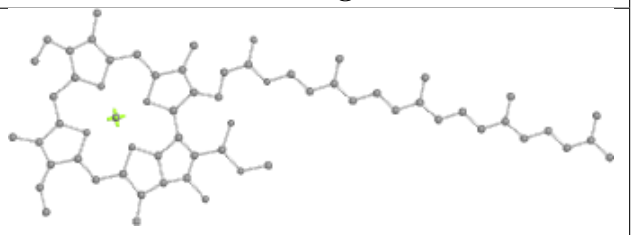
Bond lengths



Bond angles

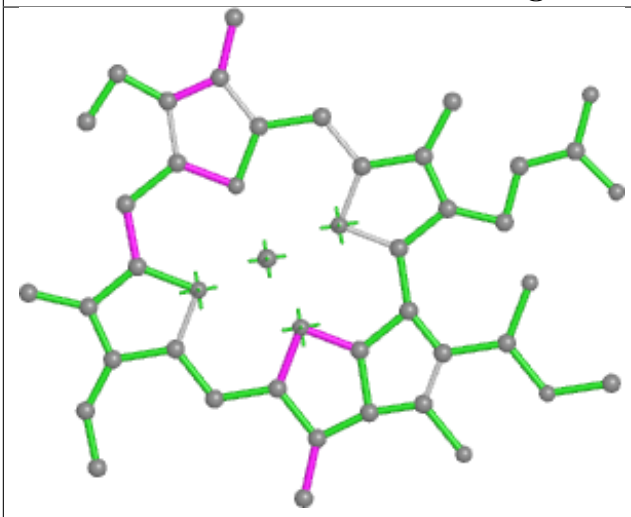


Torsions



Rings

Ligand CLA u 512



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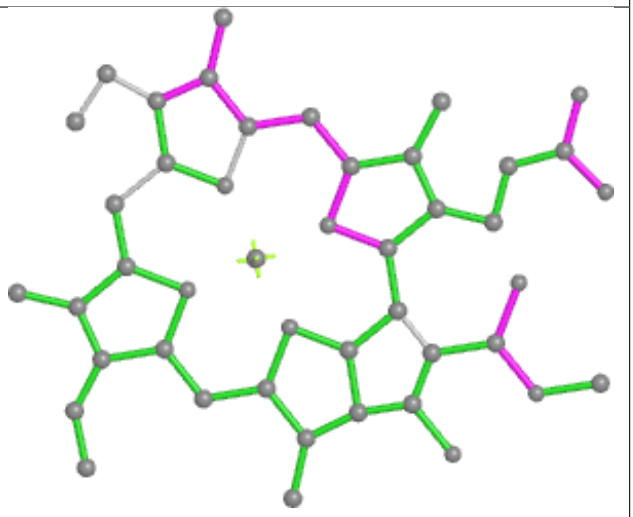
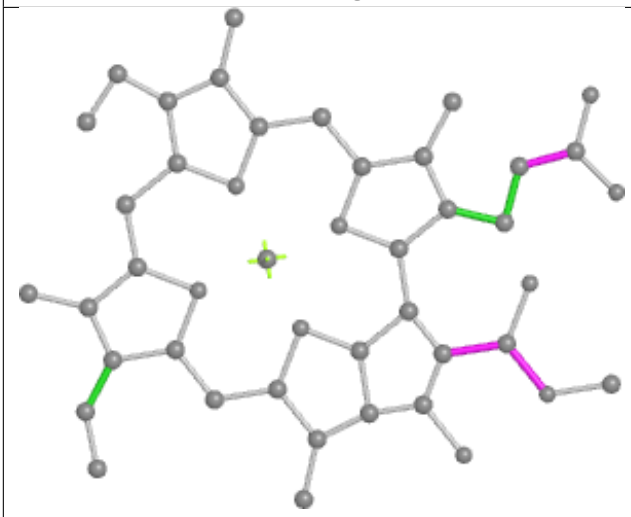


Bond angles



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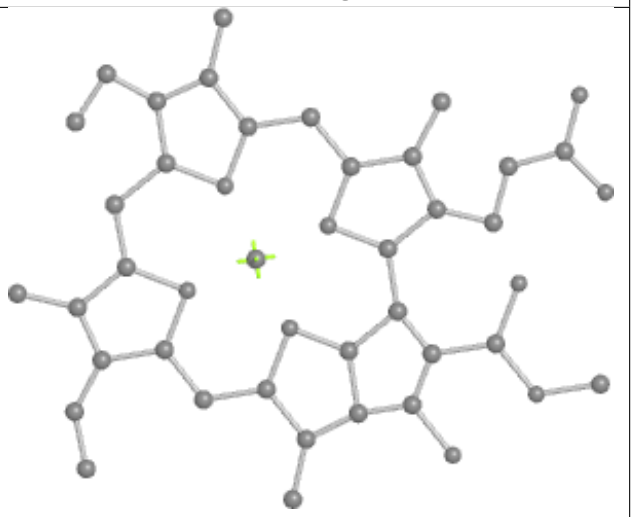
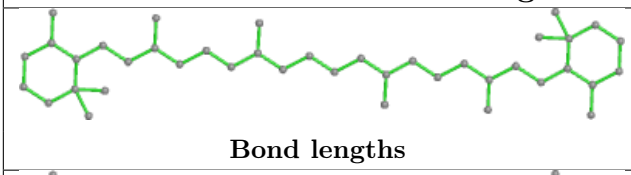


Rings

Ligand BCR J 4013



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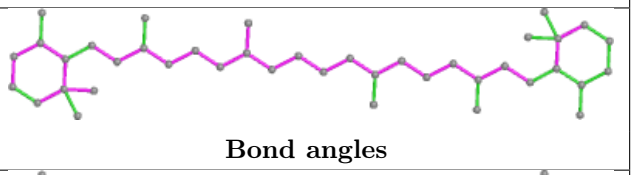
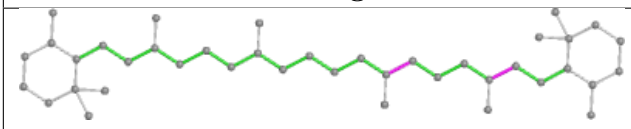
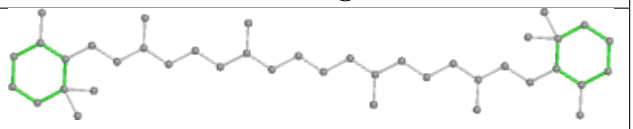


Bond angles

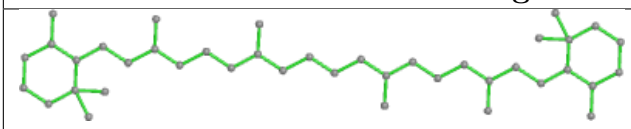


Torsions



Rings

Ligand BCR G 4007



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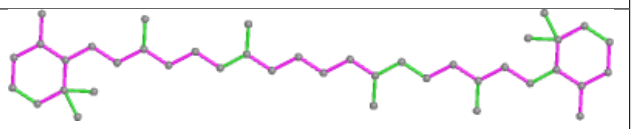
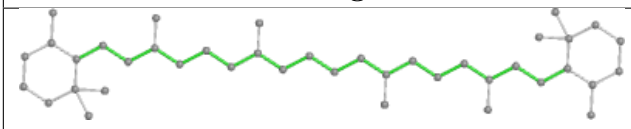
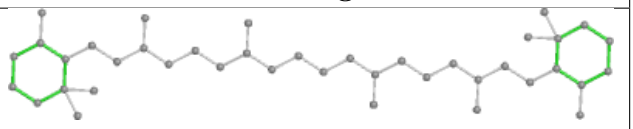


Bond angles

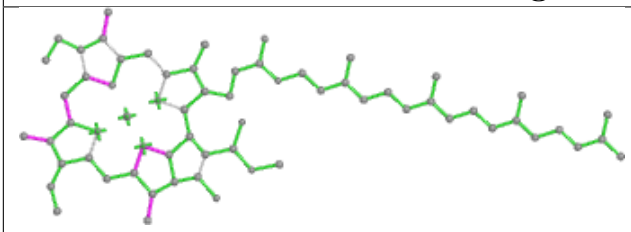


Torsions



Rings

Ligand CLA s 509



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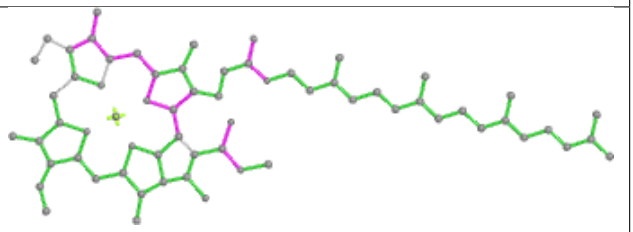
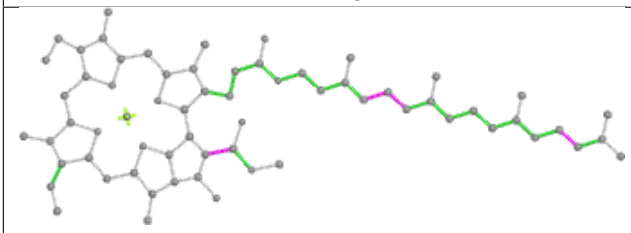
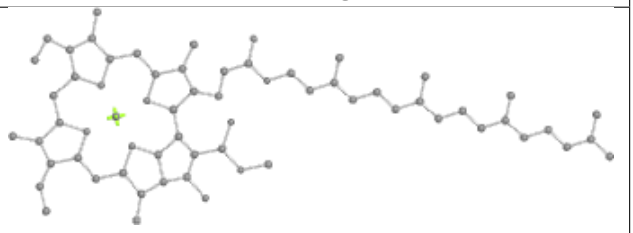


Bond angles

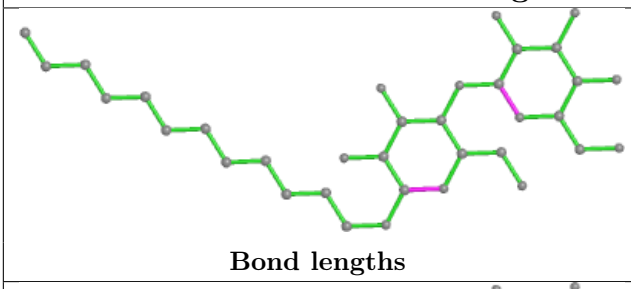


Torsions



Rings

Ligand LMU B 1843



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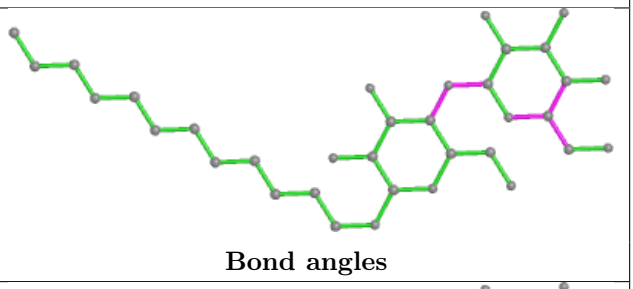
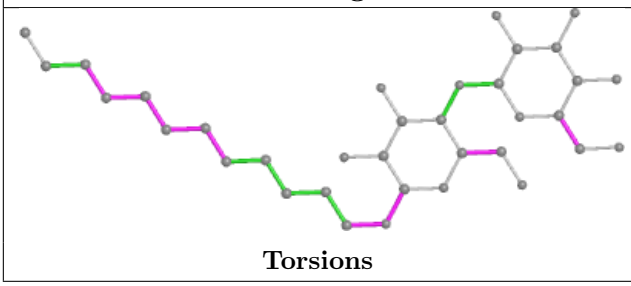


Bond angles



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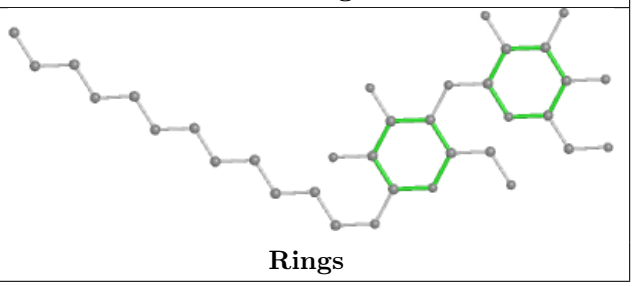
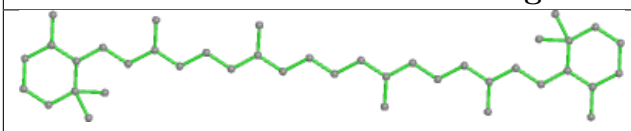


Rings

Ligand BCR Z 521



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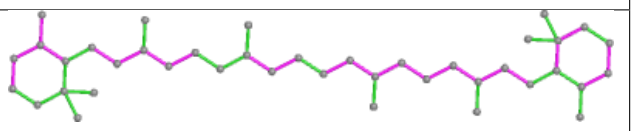
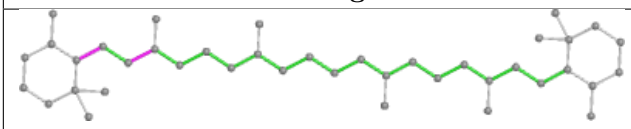


Bond angles



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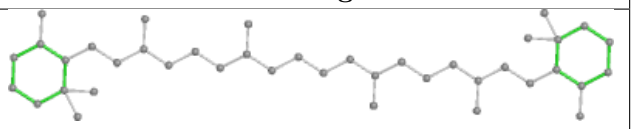
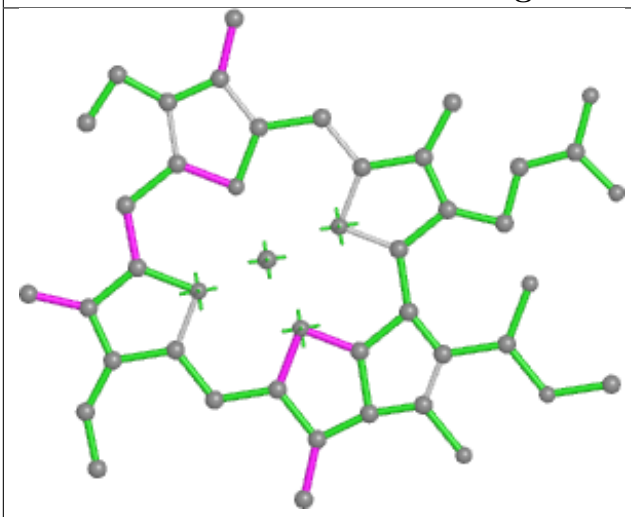


Rings

Ligand CLA A 1113



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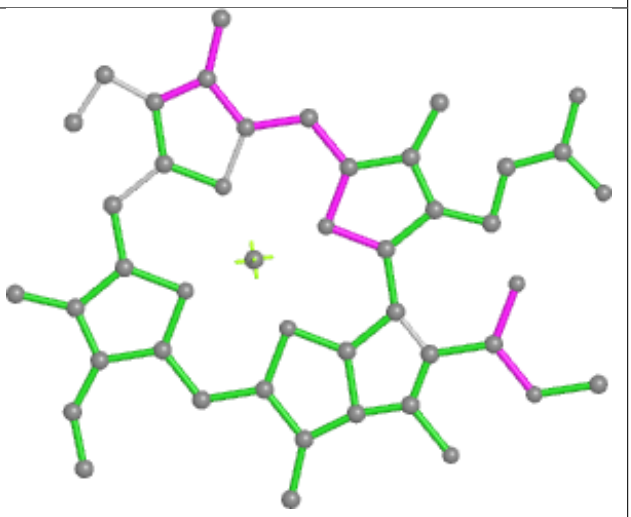
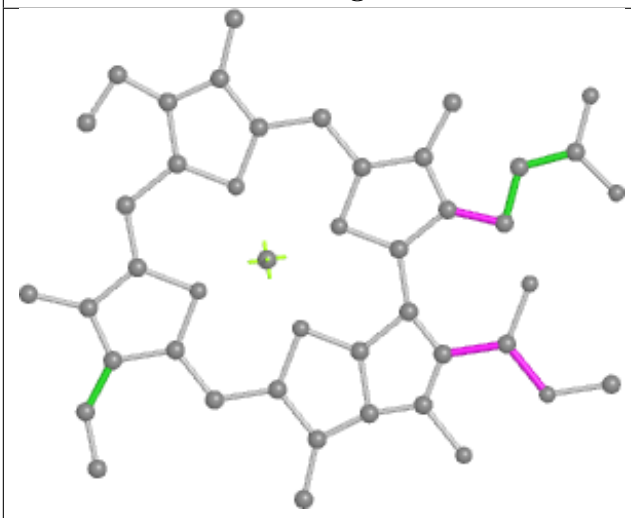
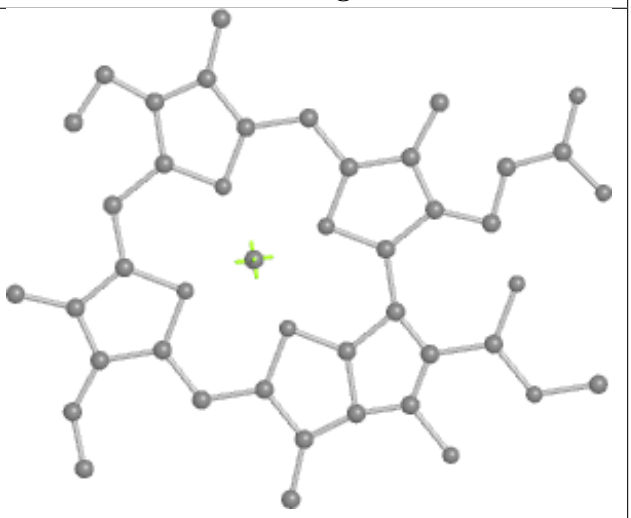


Bond angles

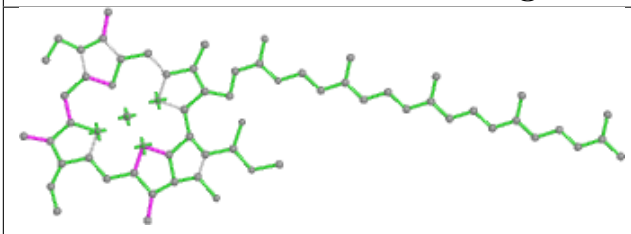


Torsions



Rings

Ligand CLA J 1303



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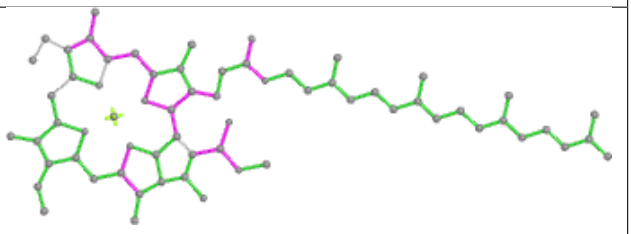
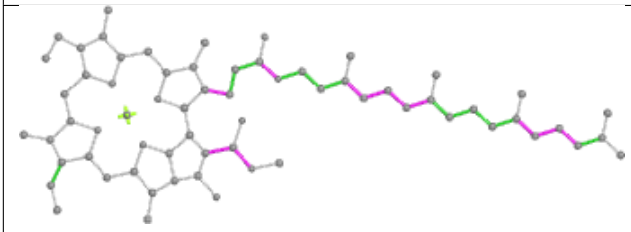
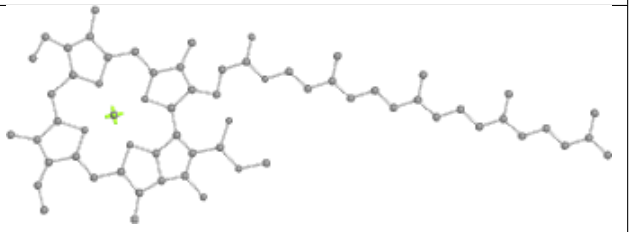


Bond angles

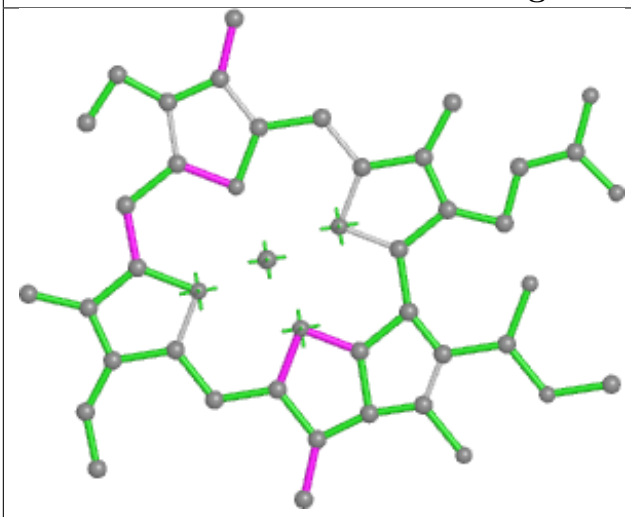


Torsions



Rings

Ligand CLA 4 516



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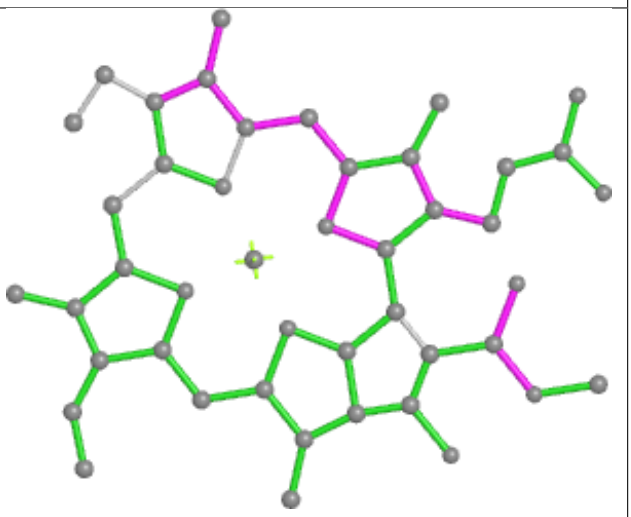
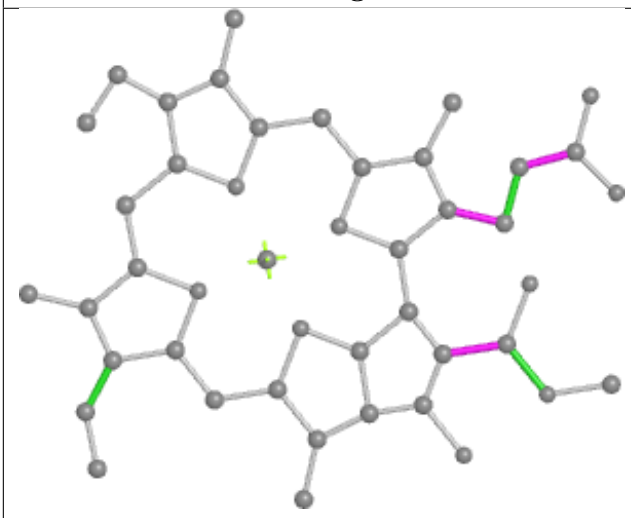
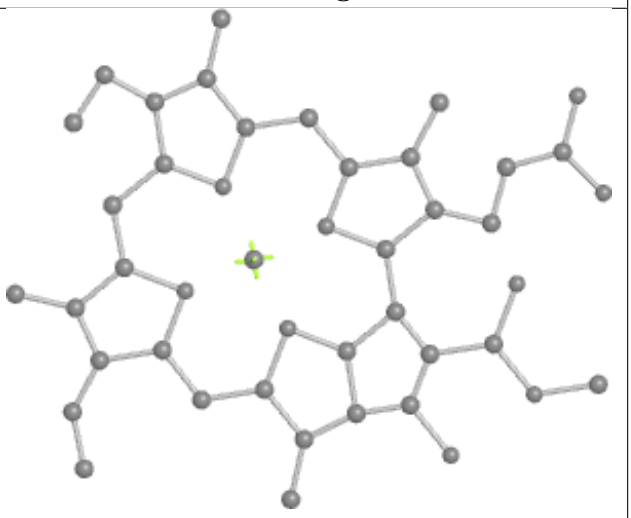


Bond angles

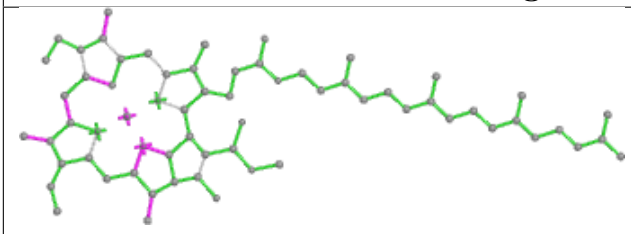


Torsions

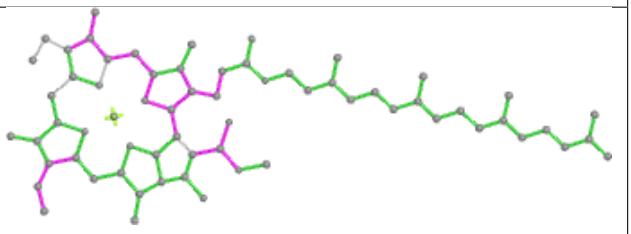


Rings

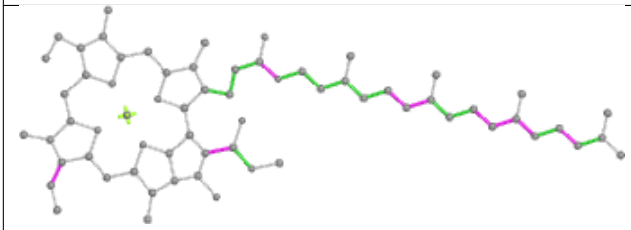
Ligand CLA f 1234



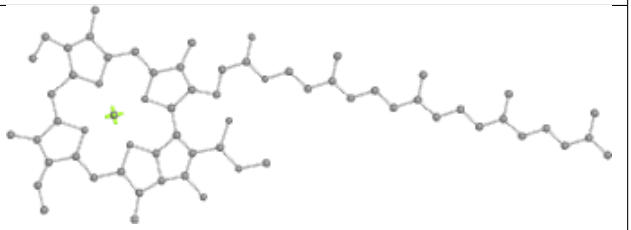
Bond lengths



Bond angles

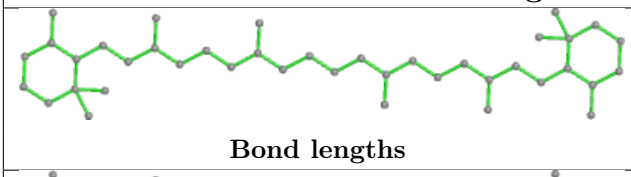


Torsions

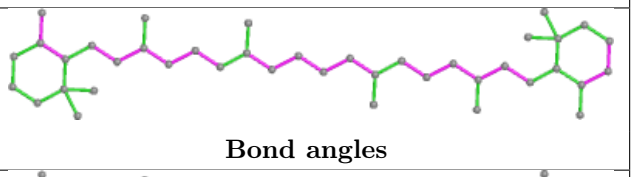


Rings

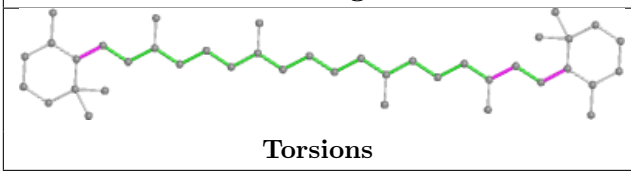
Ligand BCR b 523



Bond lengths



Bond angles



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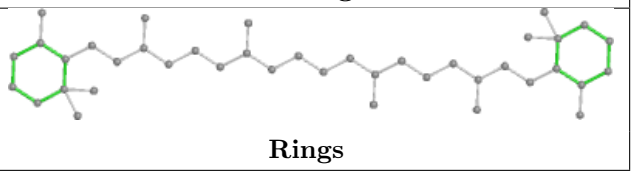
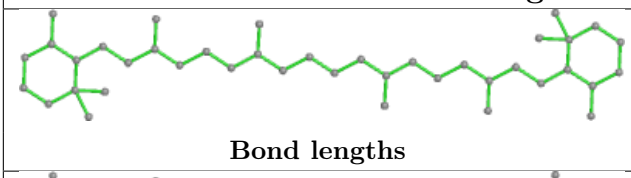


Rings

Ligand BCR 4 523



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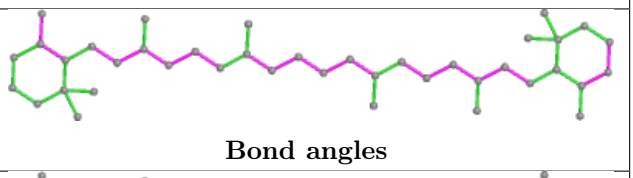
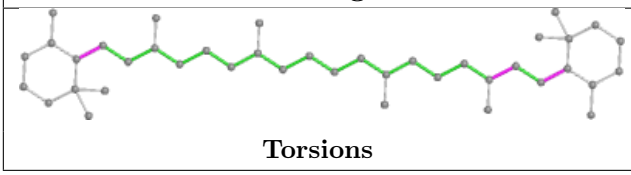
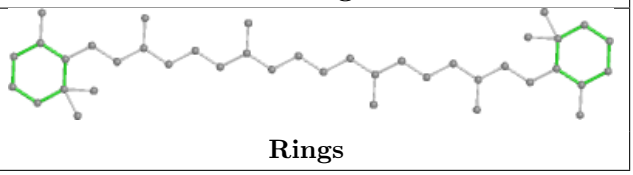


Bond angles

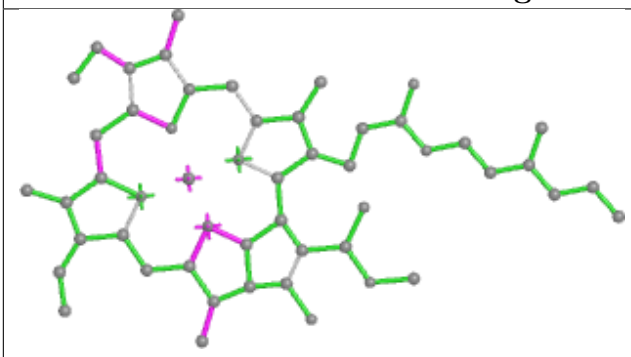


Torsions



Rings

Ligand CLA G 1135



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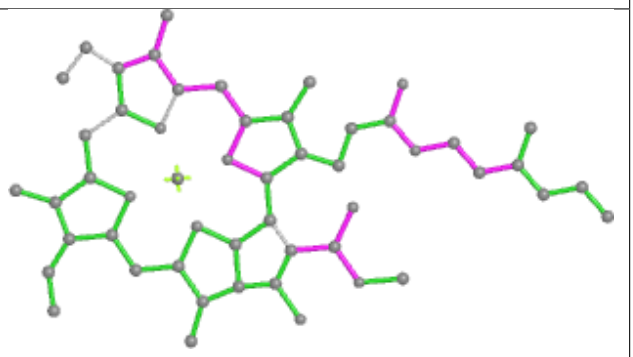
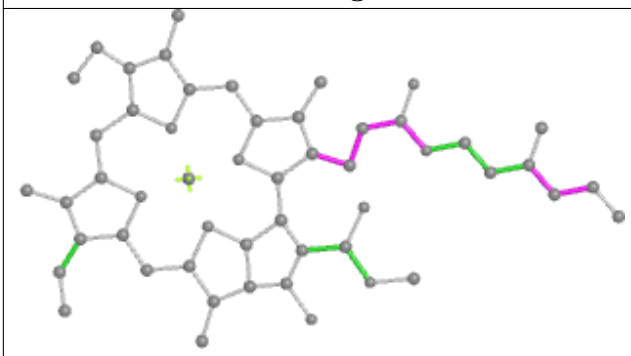
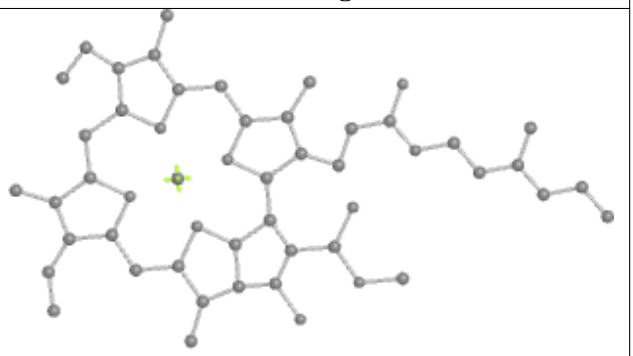


Bond angles

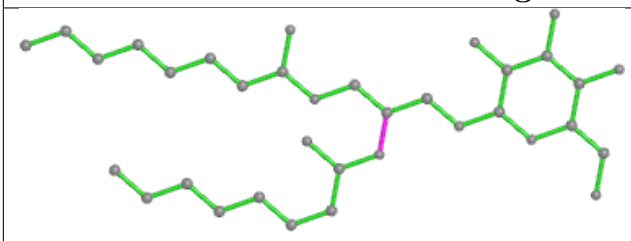


Torsions

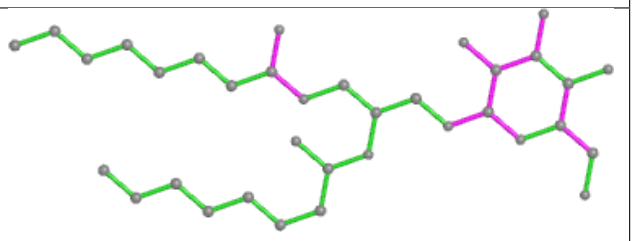


Rings

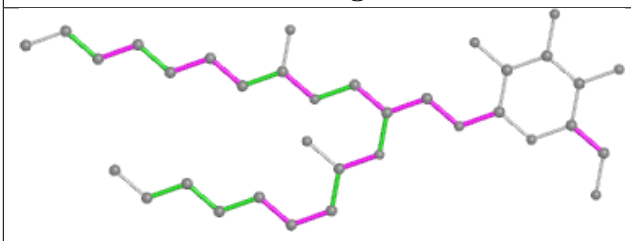
Ligand LMG J 5104



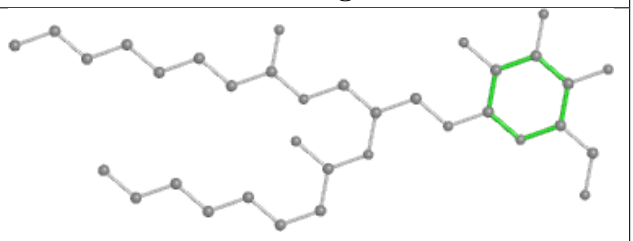
Bond lengths



Bond angles

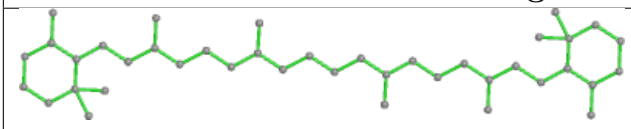


Torsions



Rings

Ligand BCR c 524



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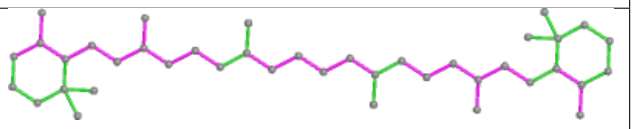
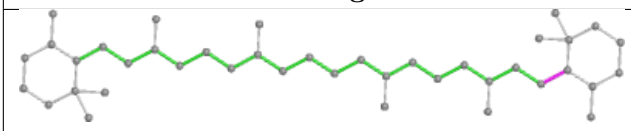


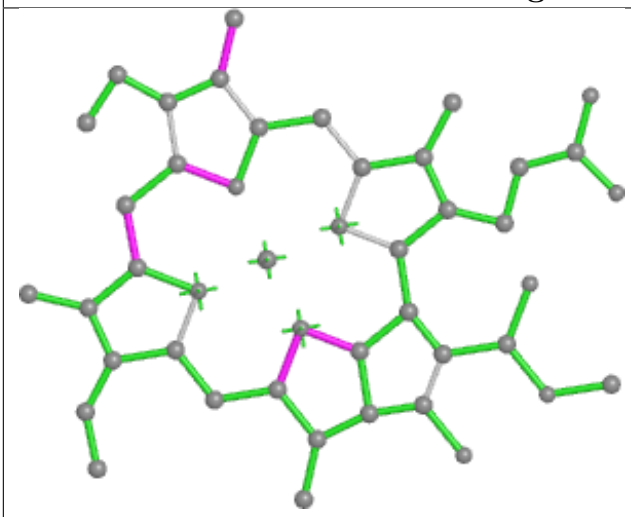
Bond angles



Torsions

Rings

Ligand CLA d 504



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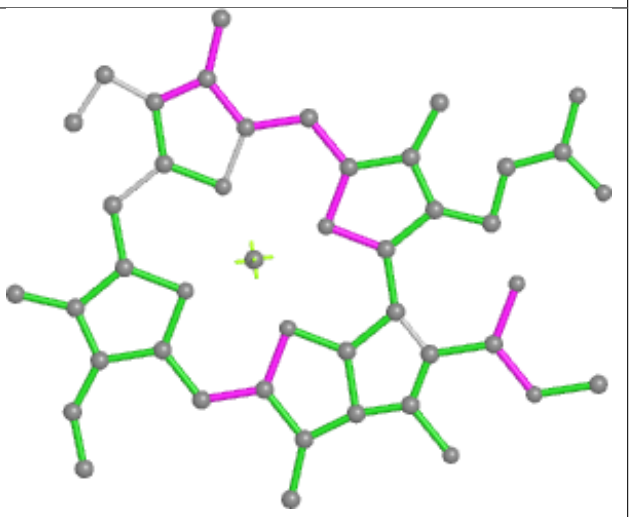
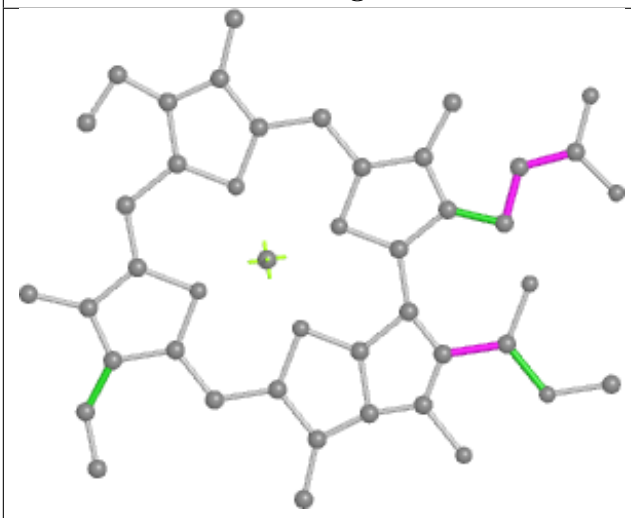


Bond angles



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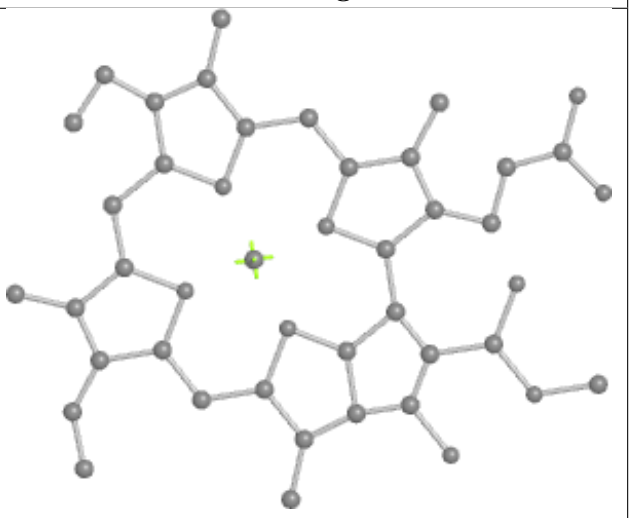
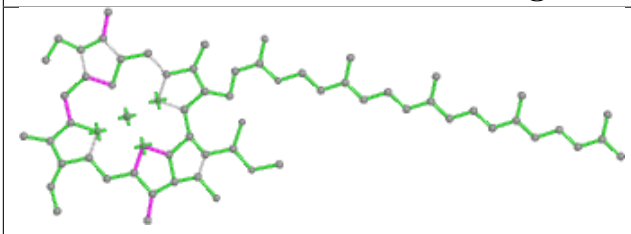
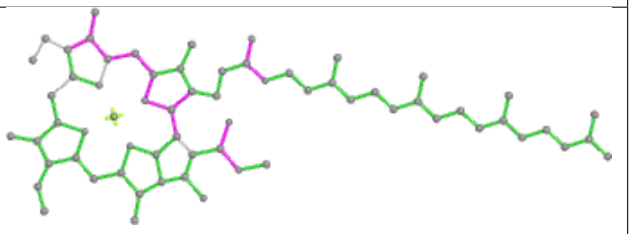


Rings

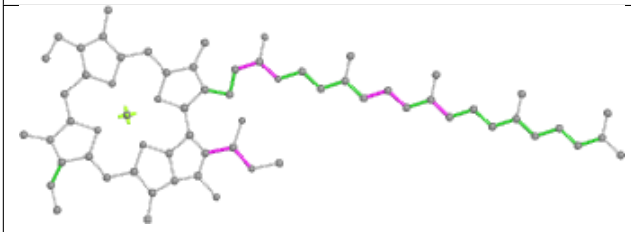
Ligand CLA 3 507



Bond lengths



Bond angles



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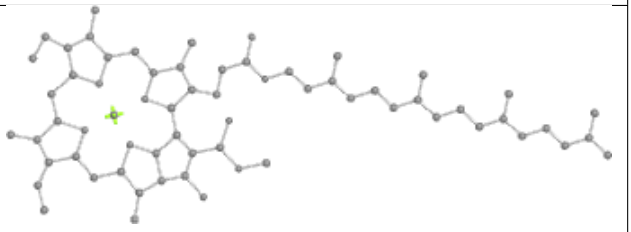
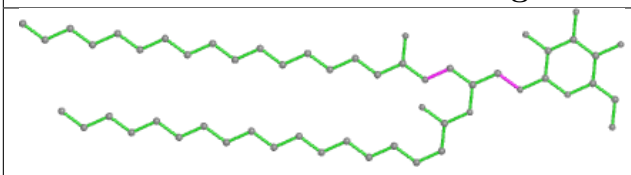
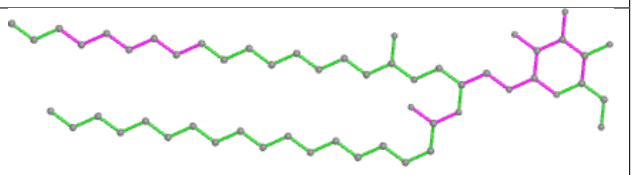


Rings

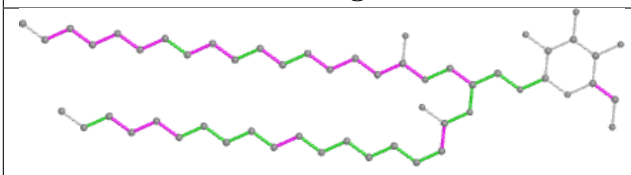
Ligand LMG B 5002



Bond lengths



Bond angles



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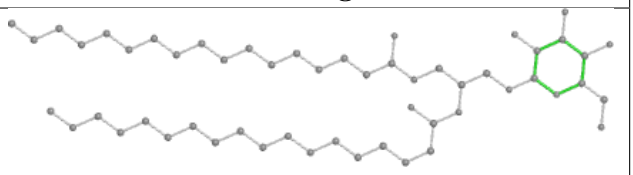
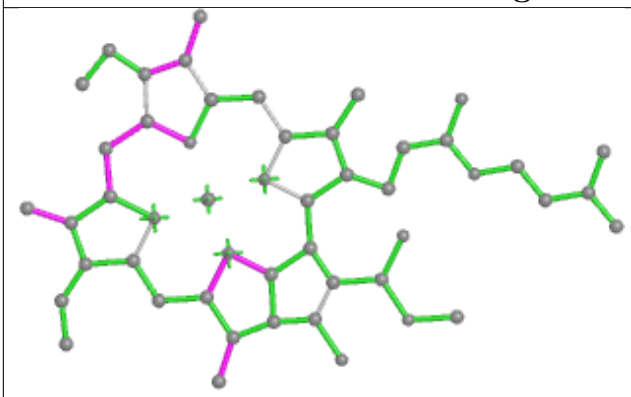
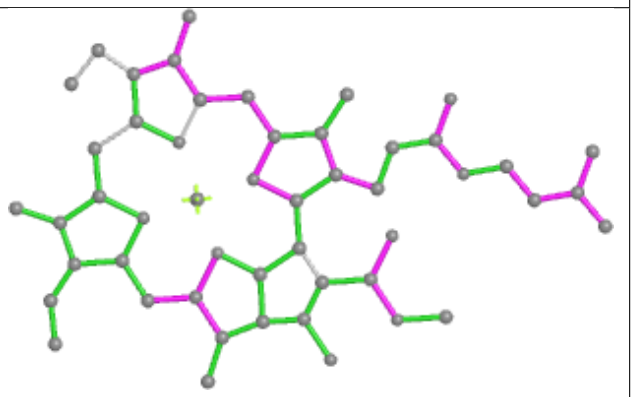


Rings

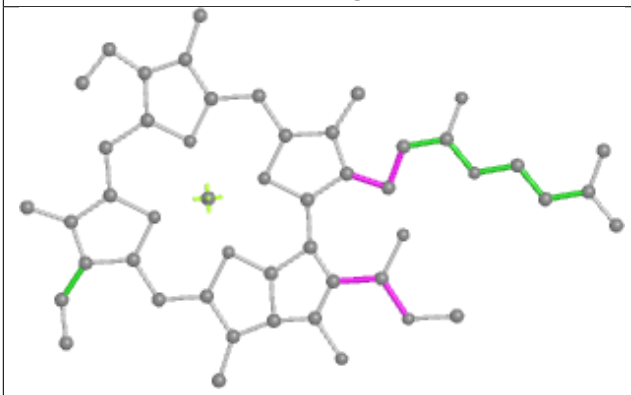
Ligand CLA m 1103



Bond lengths



Bond angles



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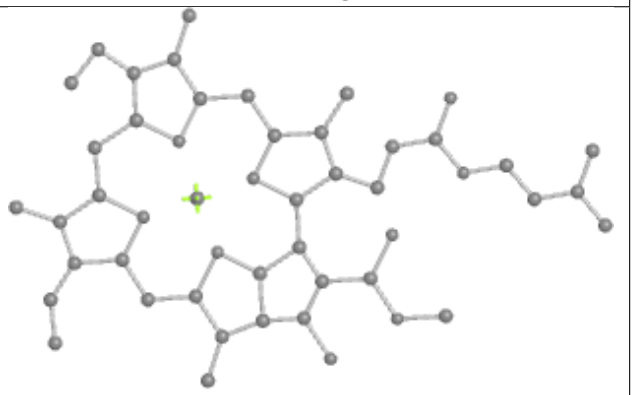
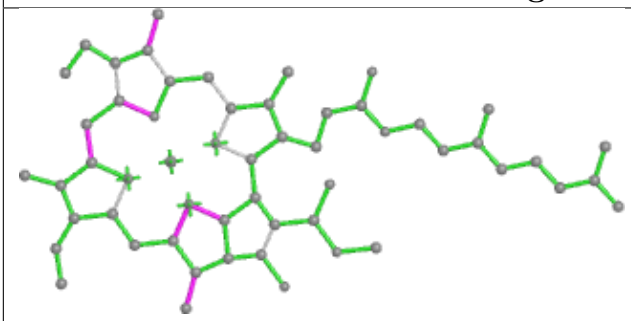


Rings

Ligand CLA v 518



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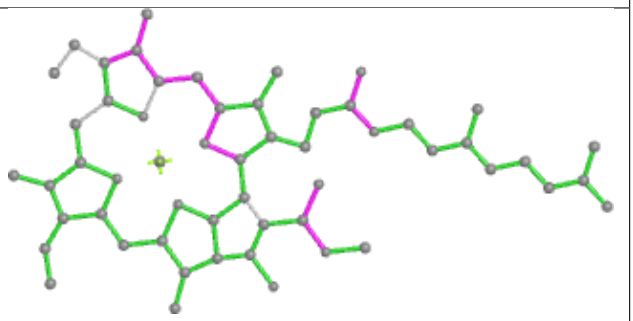
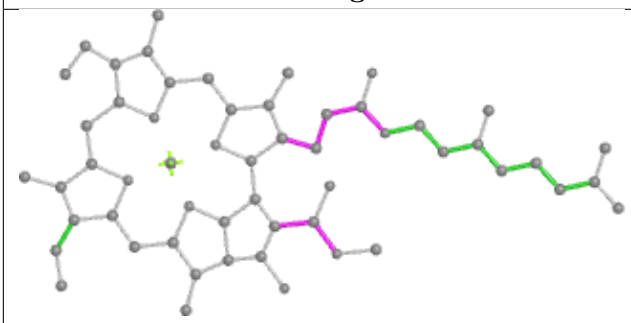


Bond angles



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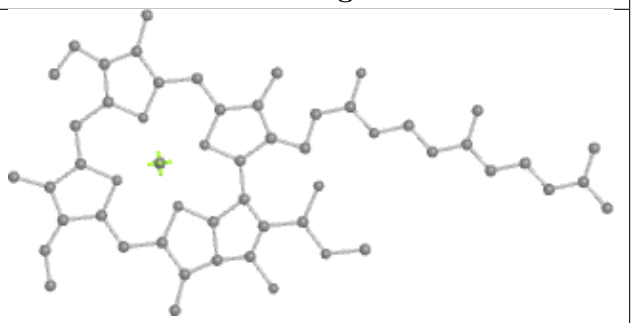
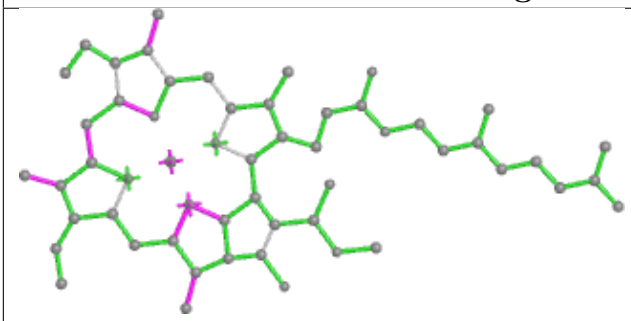


Rings

Ligand CLA H 1212



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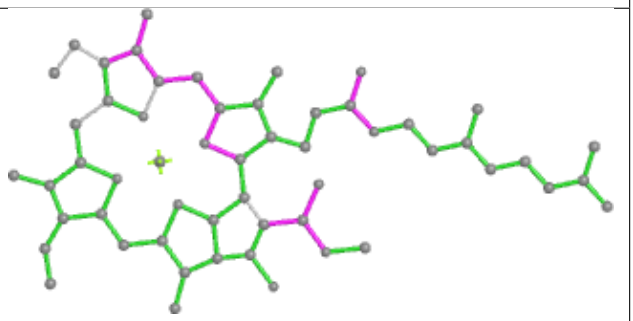

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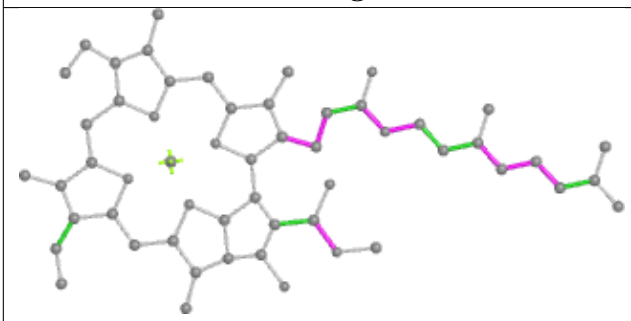

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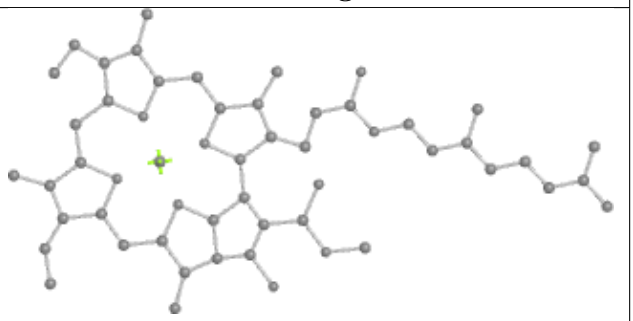
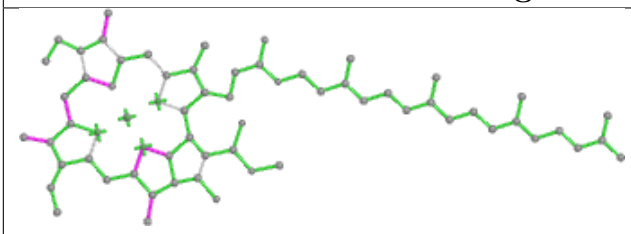


Rings

Ligand CLA A 1103



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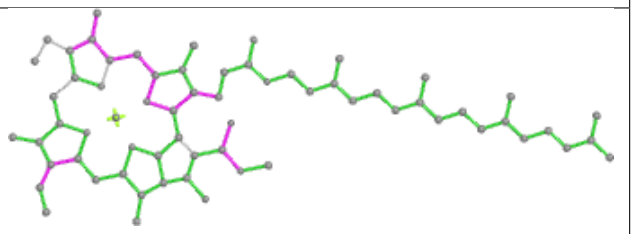
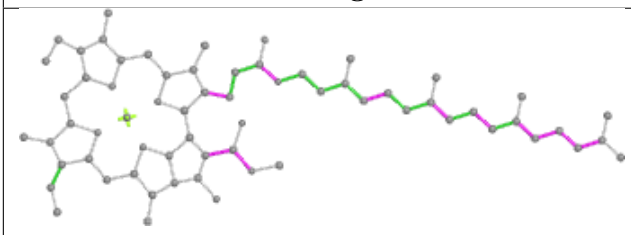


Bond angles



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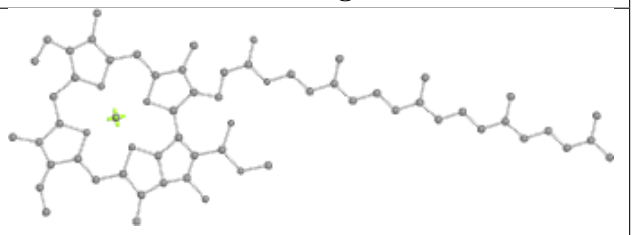
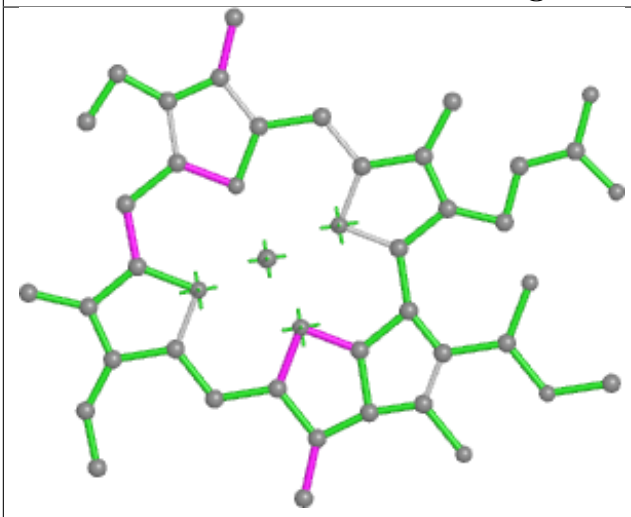
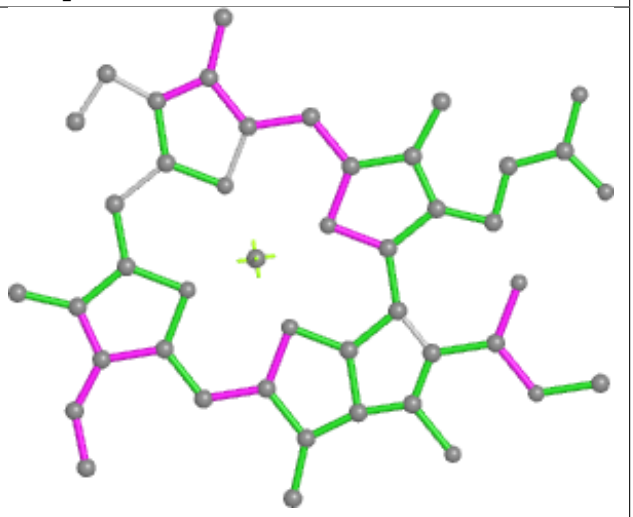


Rings

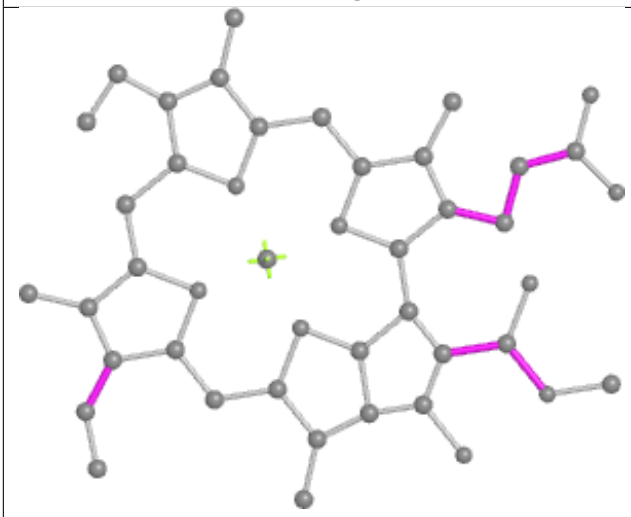
Ligand CLA q 516



Bond lengths



Bond angles



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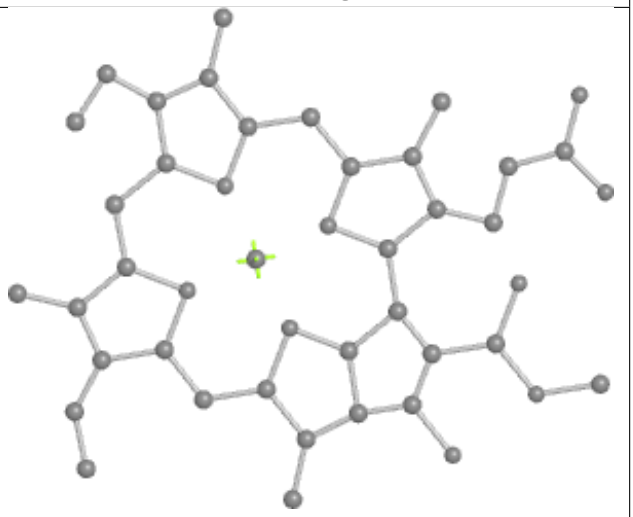
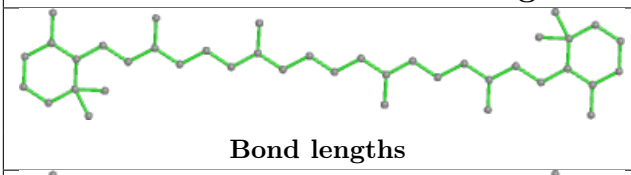
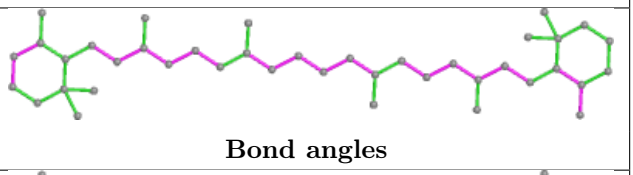


Rings

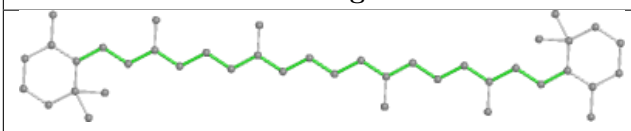
Ligand BCR e 4003



Bond lengths



Bond angles



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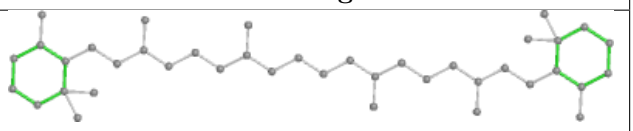
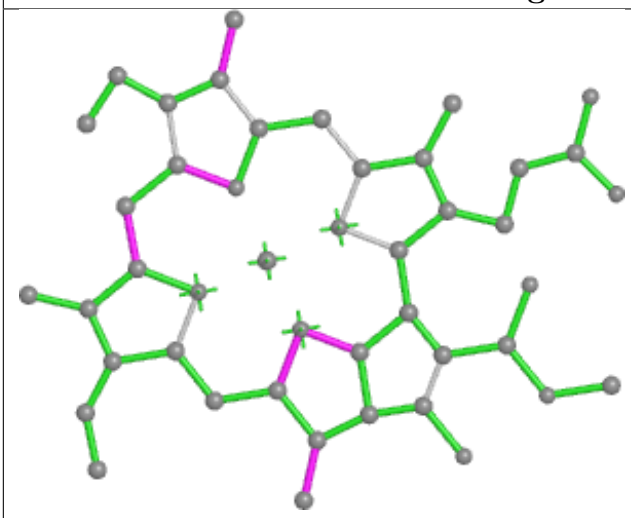
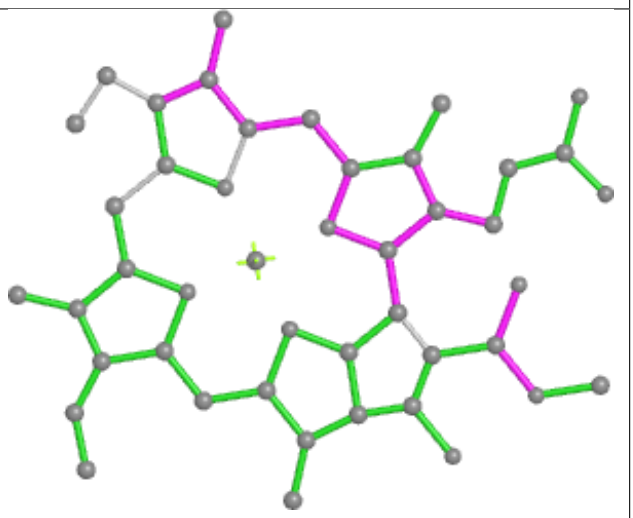


Rings

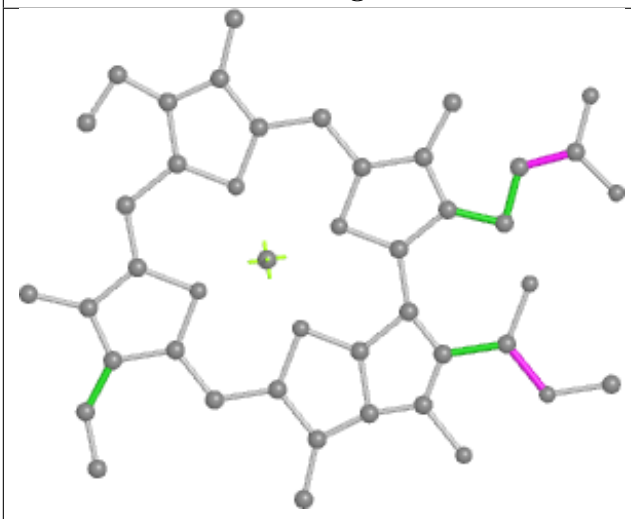
Ligand CLA v 507



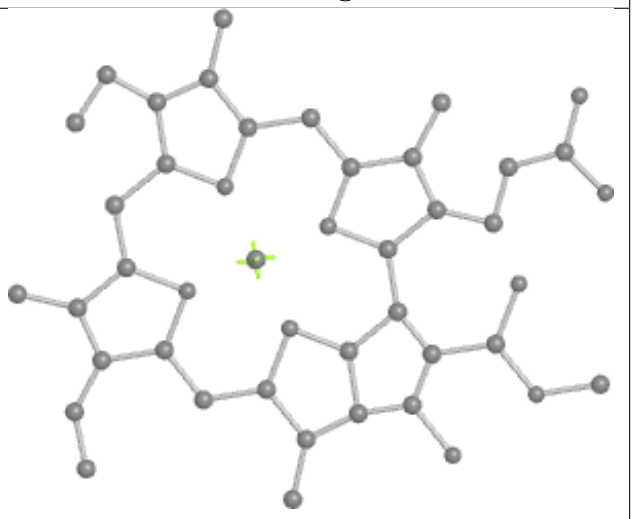
Bond lengths



Bond angles

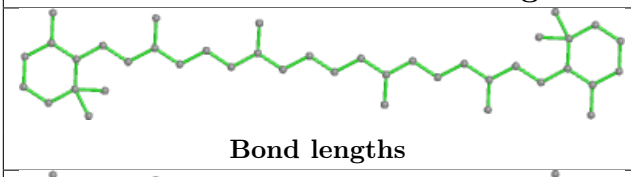


Torsions



Rings

Ligand BCR f 4017



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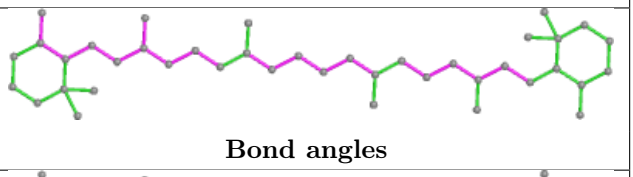

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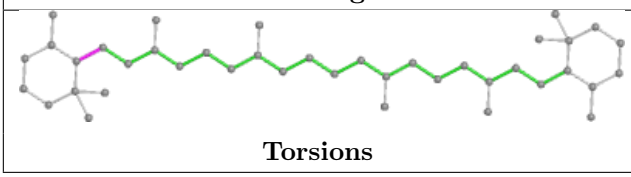

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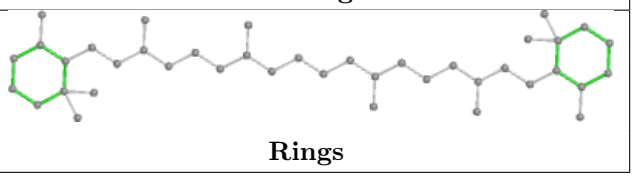
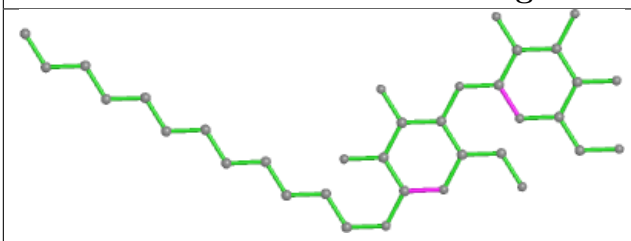


Rings

Ligand LMU e 1848



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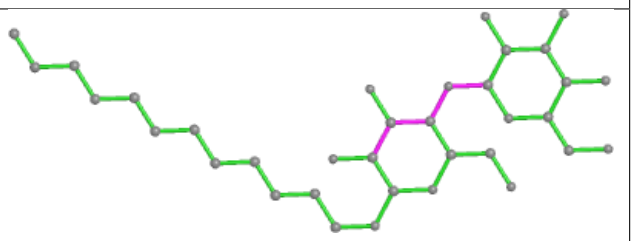
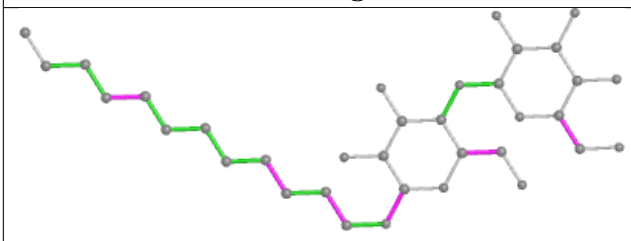


Bond angles



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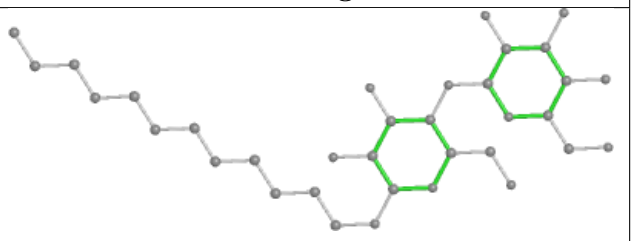
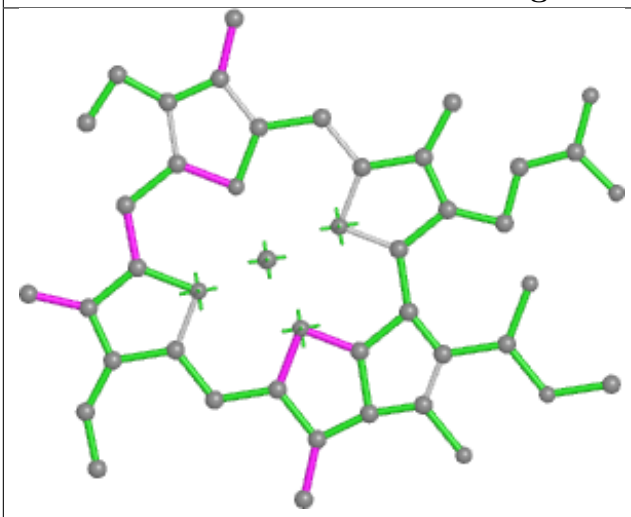


Rings

Ligand CLA t 513



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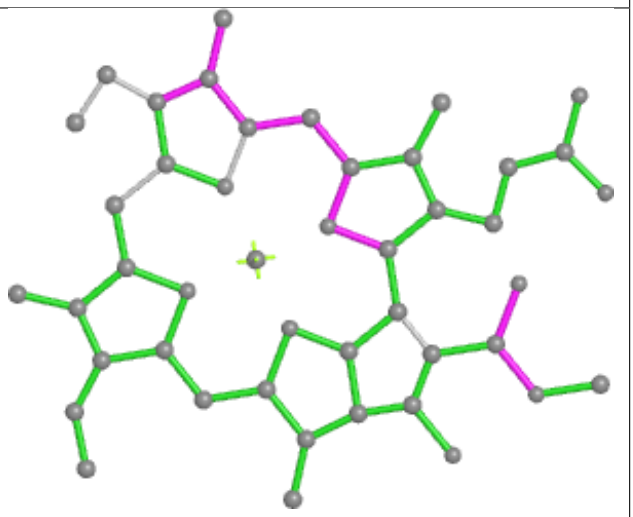

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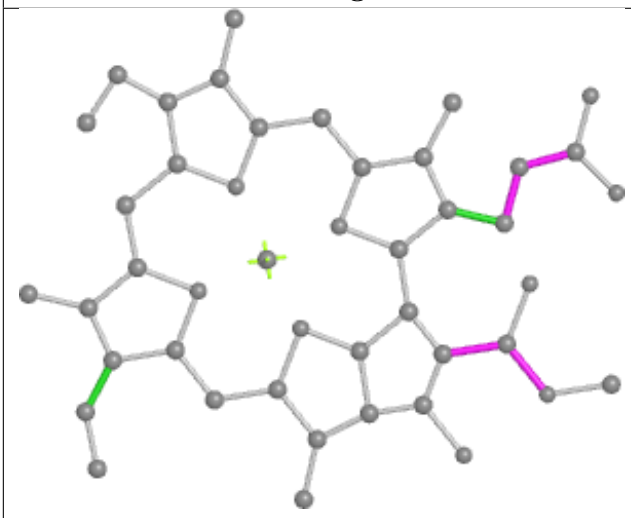

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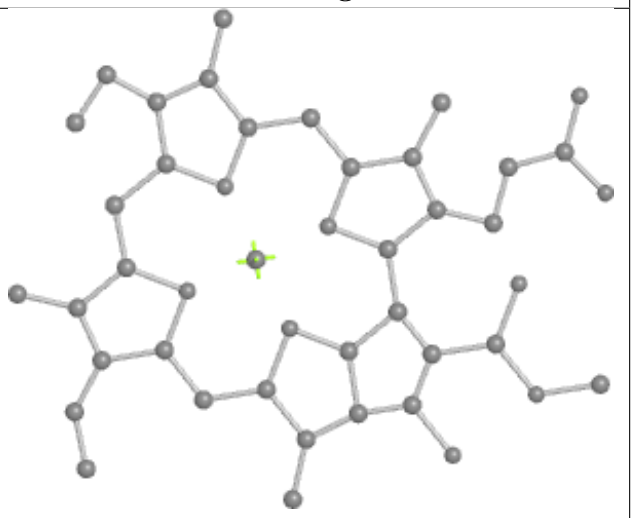
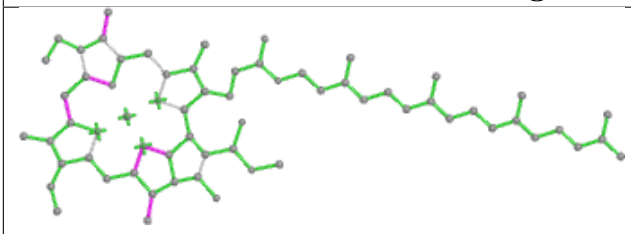


Rings

Ligand CLA a 510



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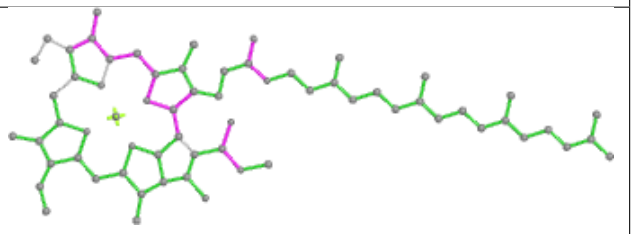
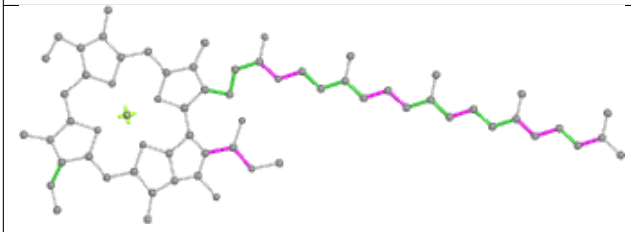


Bond angles



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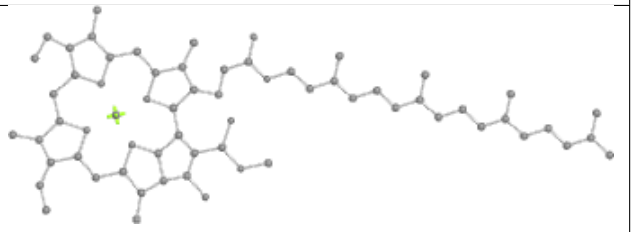
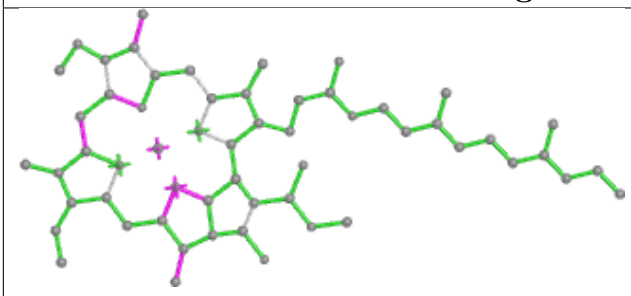


Rings

Ligand CLA B 1217



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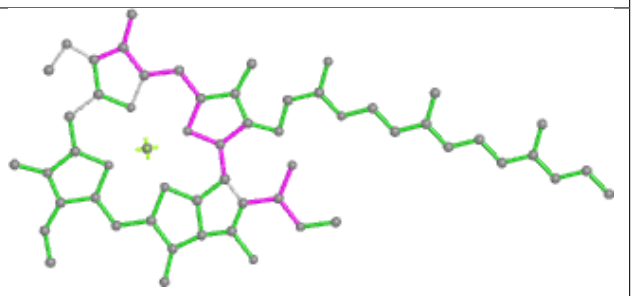
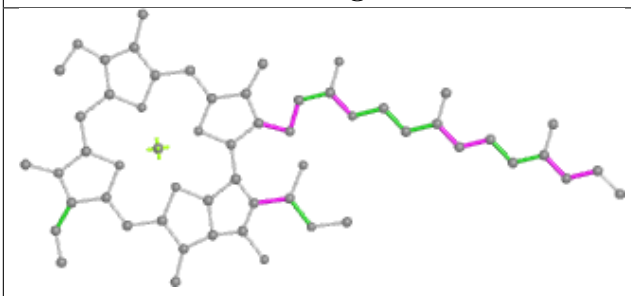


Bond angles



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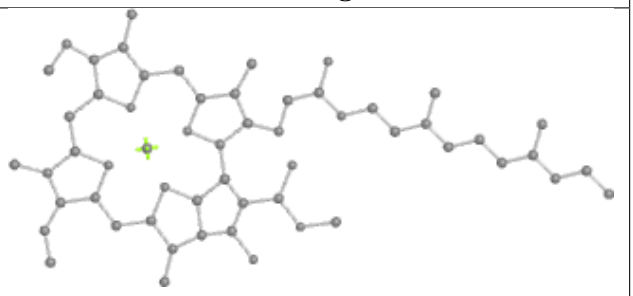
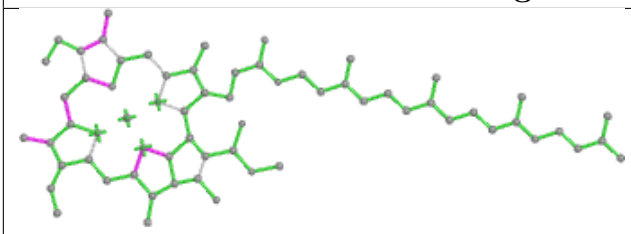


Rings

Ligand CLA G 1137



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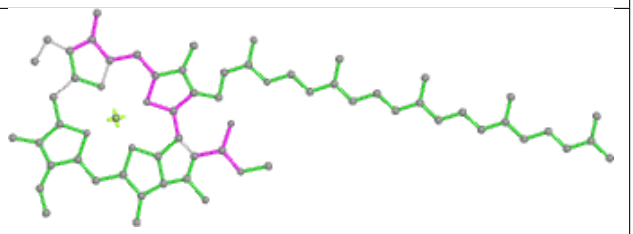
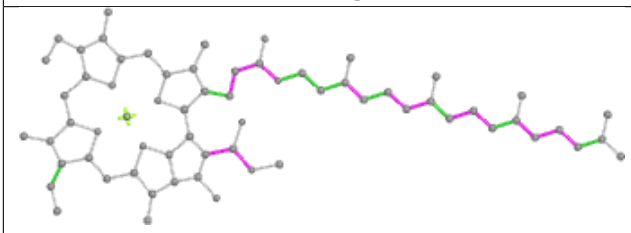


Bond angles



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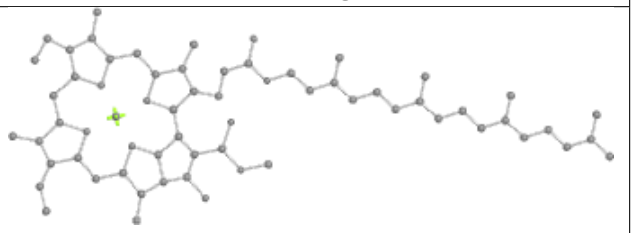
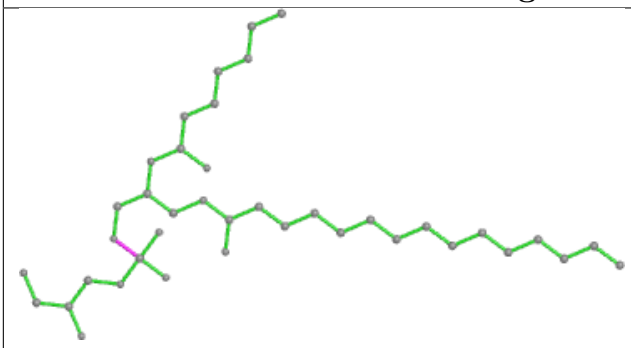


Rings

Ligand LHG e 5002



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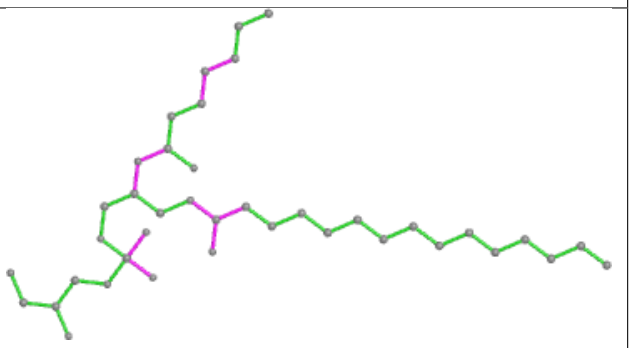
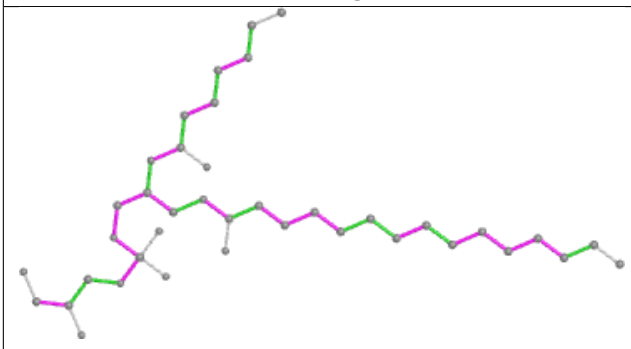


Bond angles



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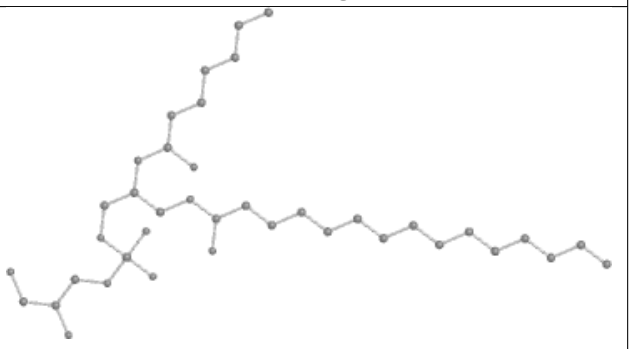
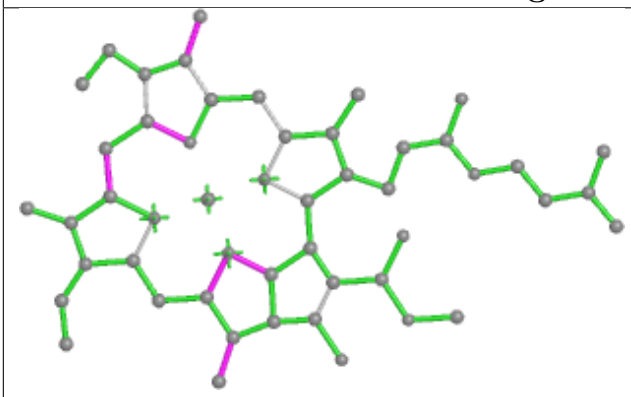


Rings

Ligand CLA 3 511



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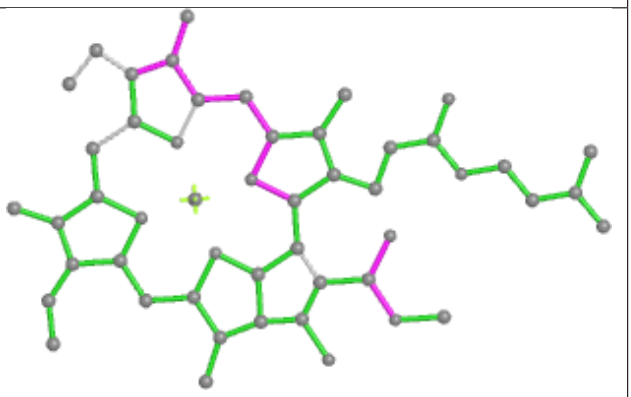
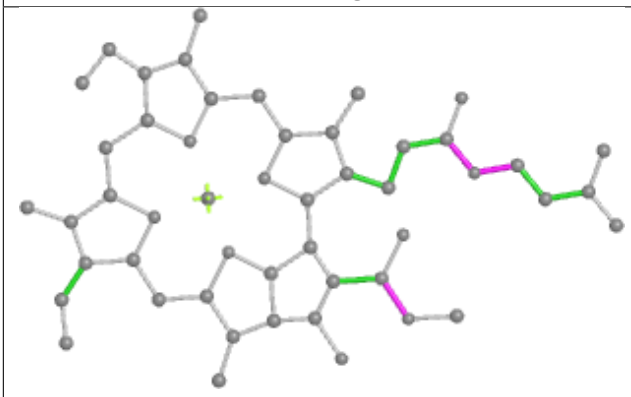


Bond angles



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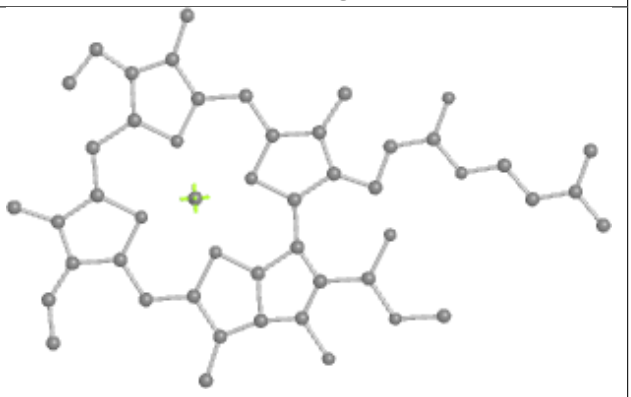
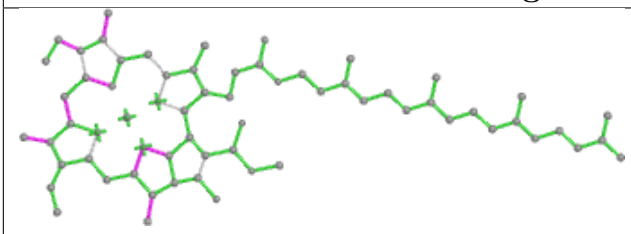


Rings

Ligand CLA f 1235



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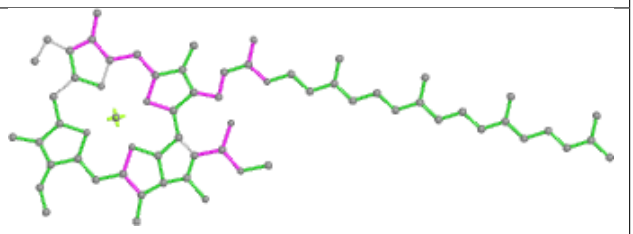
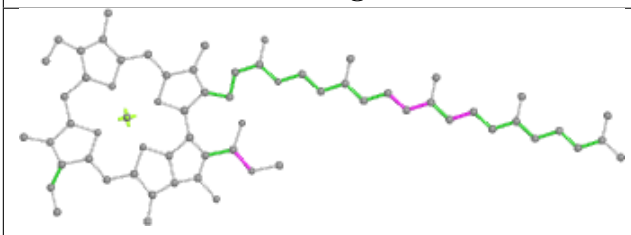


Bond angles



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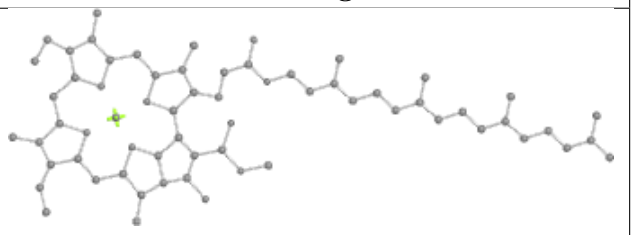
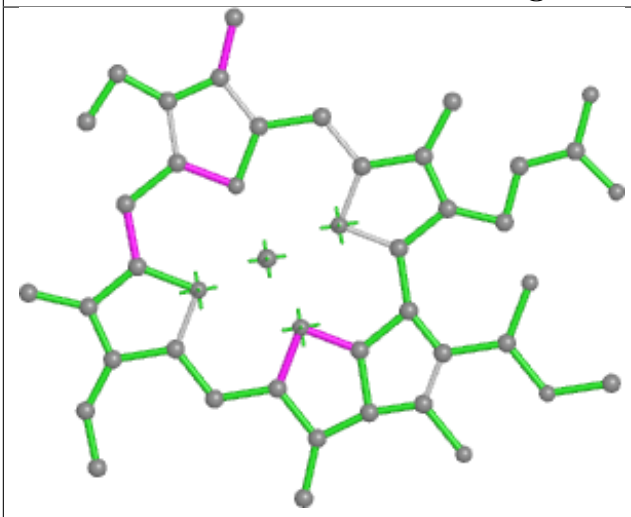


Rings

Ligand CLA v 504



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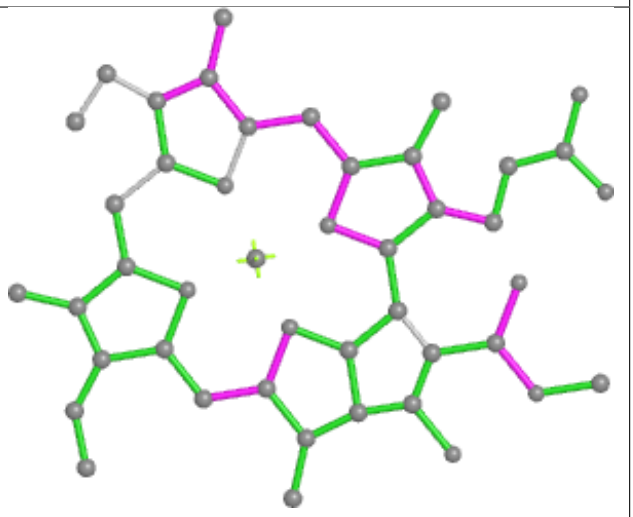
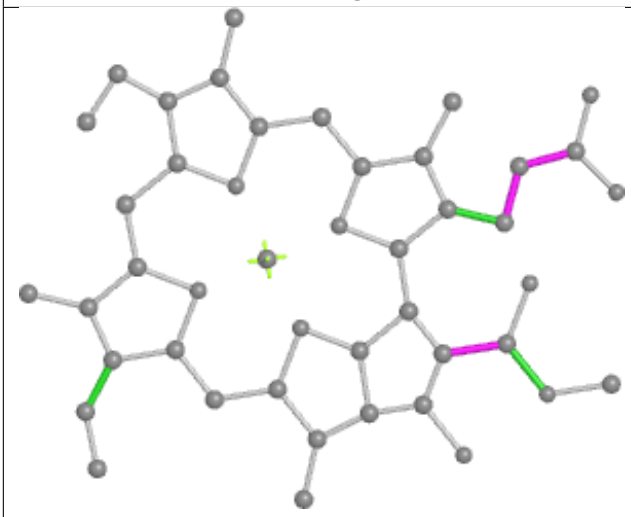


Bond angles



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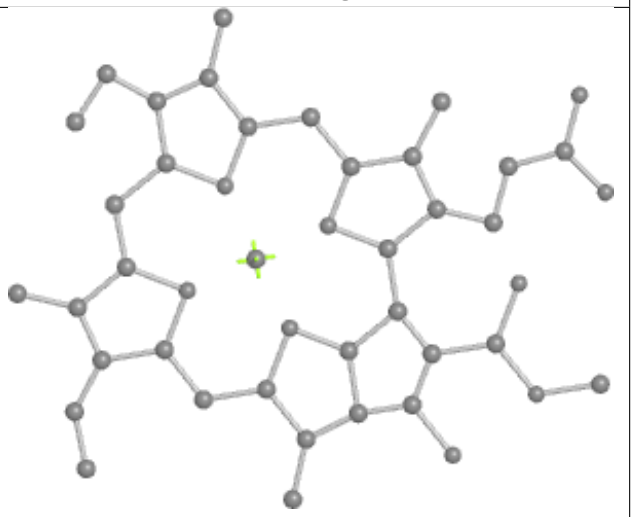
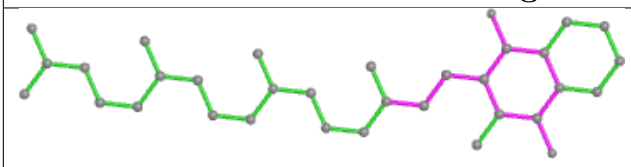


Rings

Ligand PQN f 2002



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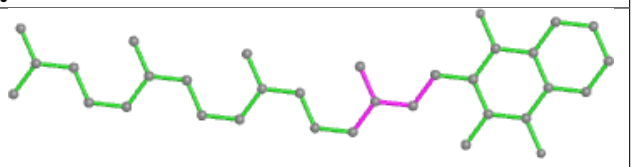
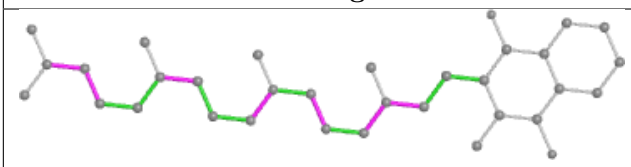


Bond angles



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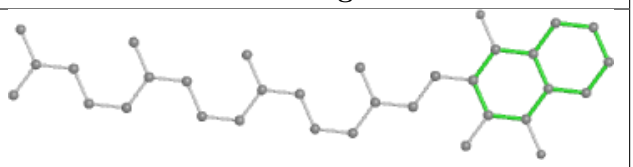
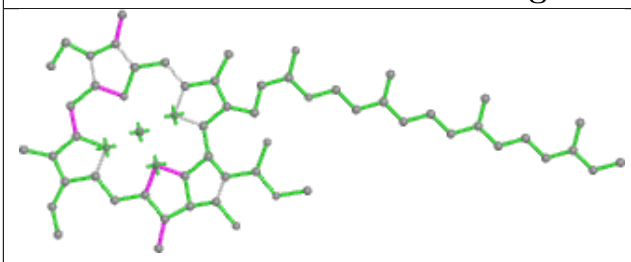


Rings

Ligand CLA c 505



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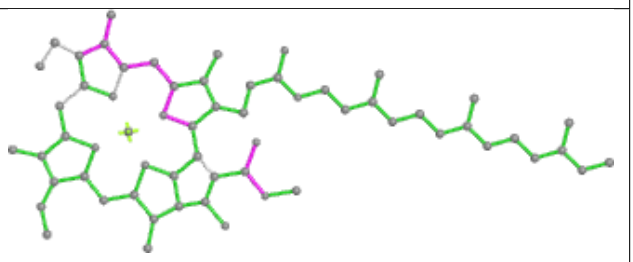
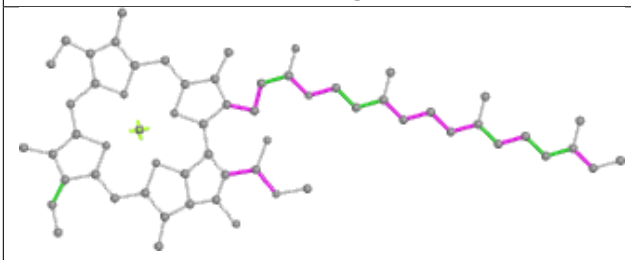


Bond angles



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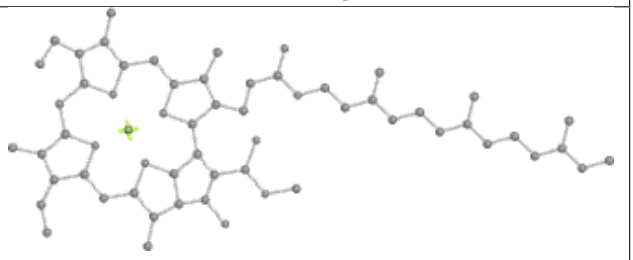
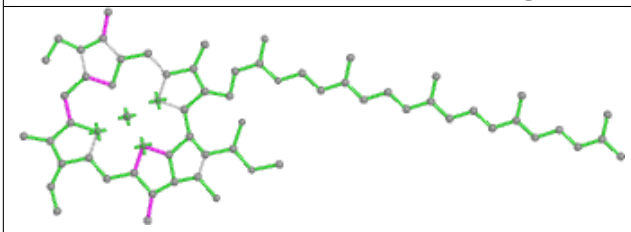
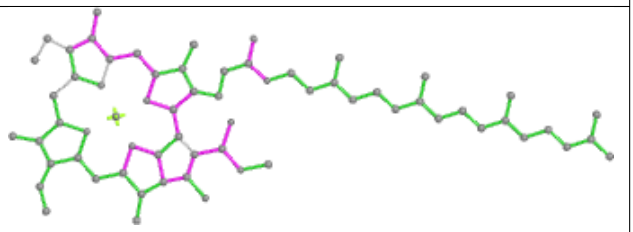


Rings

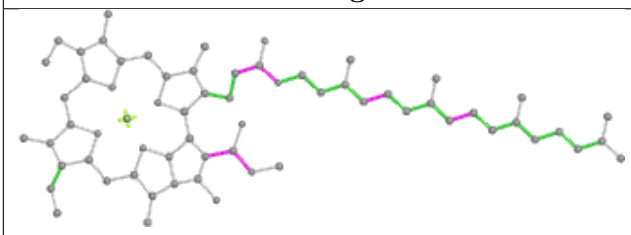
Ligand CLA e 1011



Bond lengths



Bond angles



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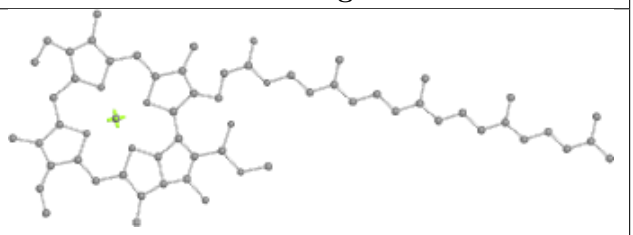
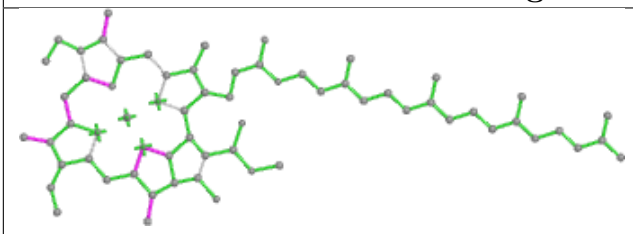
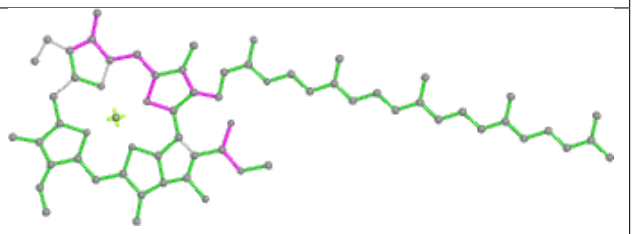


Rings

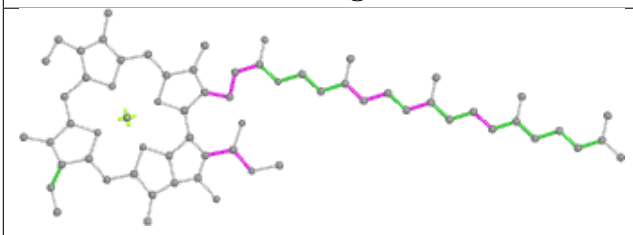
Ligand CLA Z 501



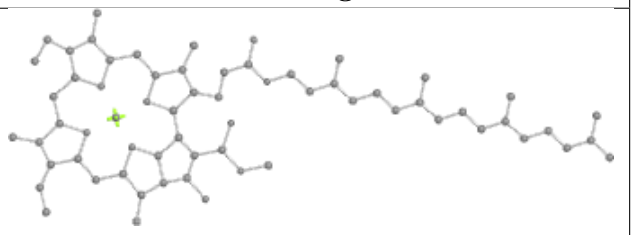
Bond lengths



Bond angles

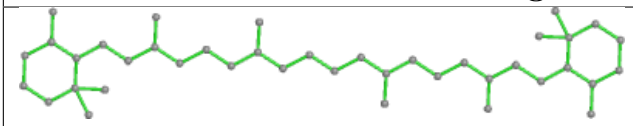


Torsions

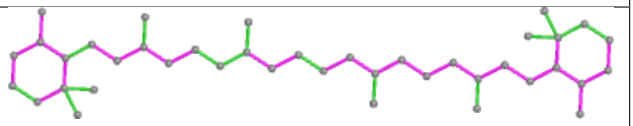


Rings

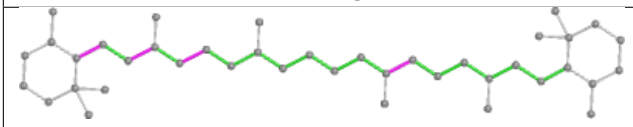
Ligand BCR c 521



Bond lengths



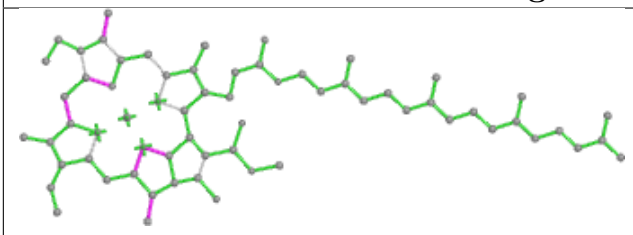
Bond angles



Torsions

Rings

Ligand CLA 3 513



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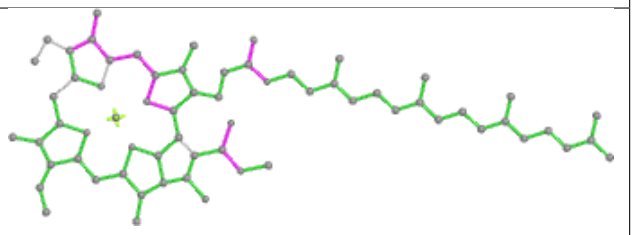
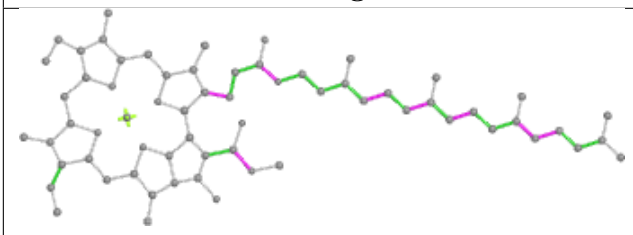
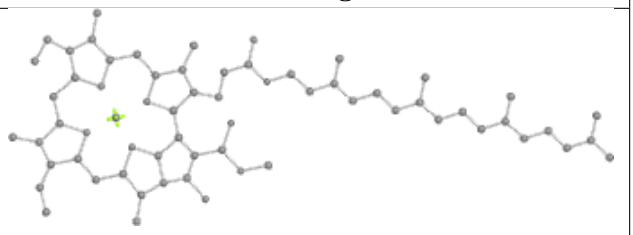


Bond angles

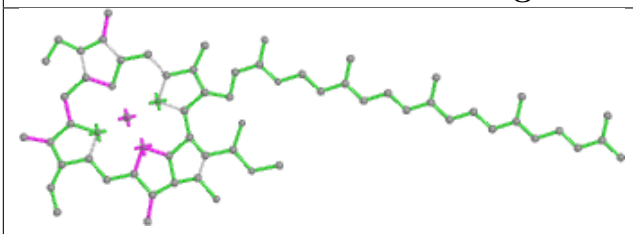


Torsions

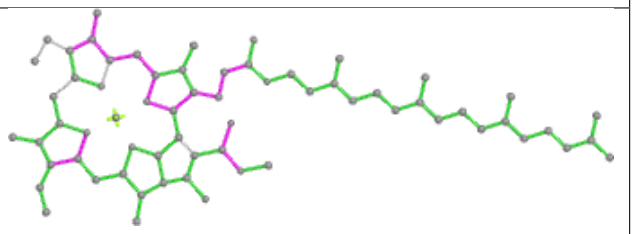


Rings

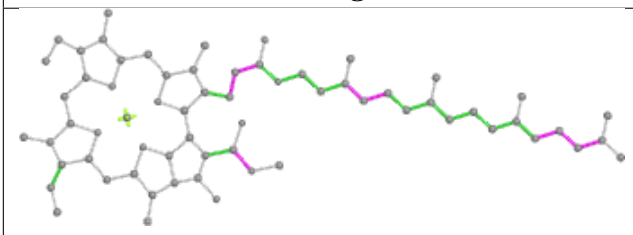
Ligand CLA G 1013



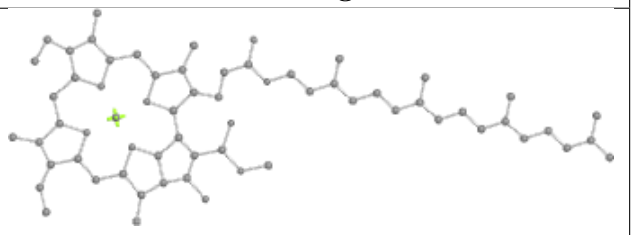
Bond lengths



Bond angles

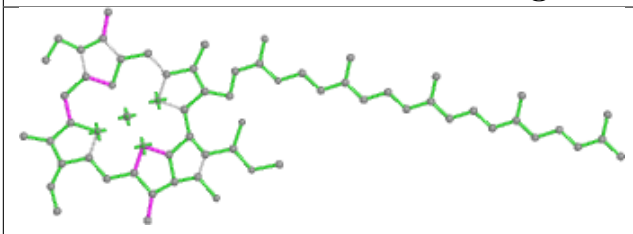


Torsions



Rings

Ligand CLA t 509



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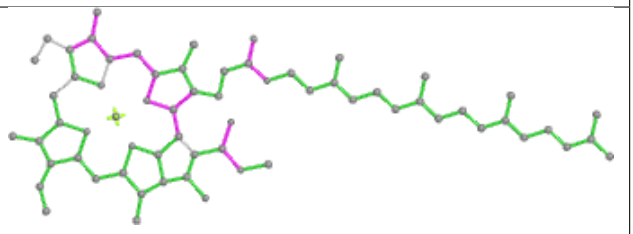
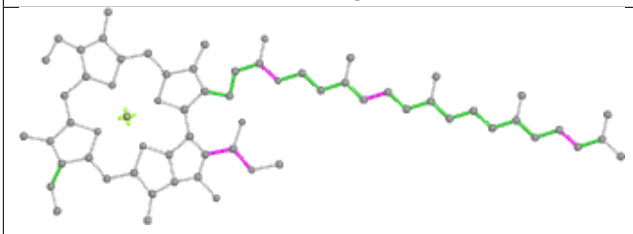
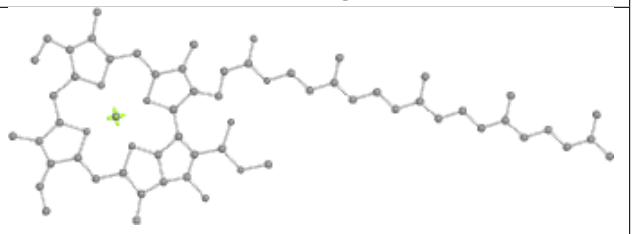


Bond angles

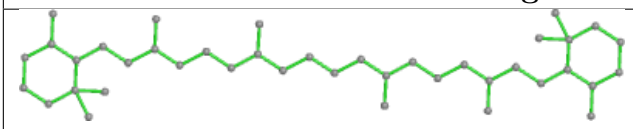


Torsions



Rings

Ligand BCR l 4013



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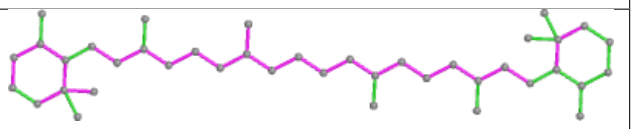
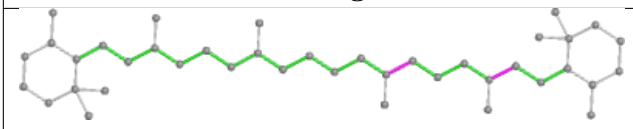


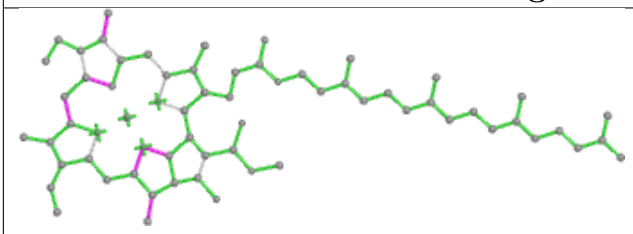
Bond angles



Torsions

Rings

Ligand CLA 3 505



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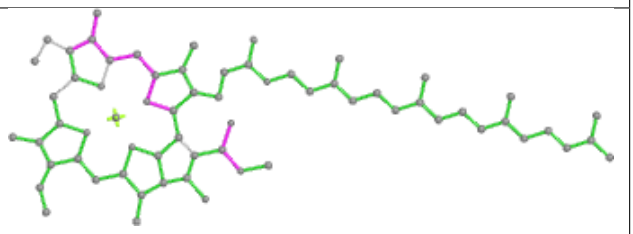
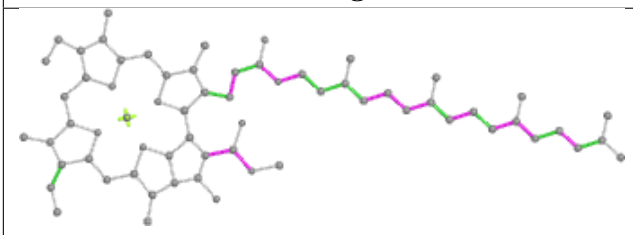


Bond angles



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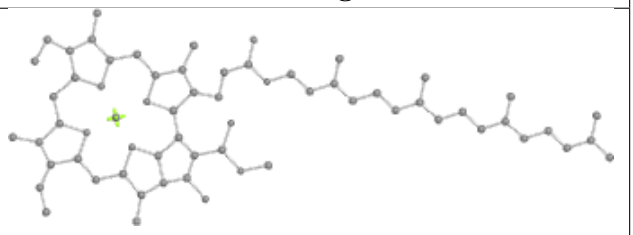
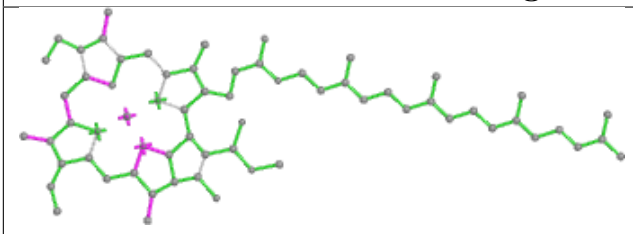


Rings

Ligand CLA f 1023



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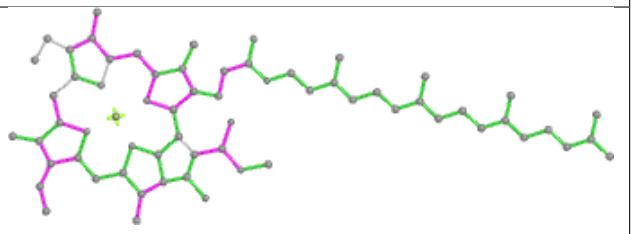
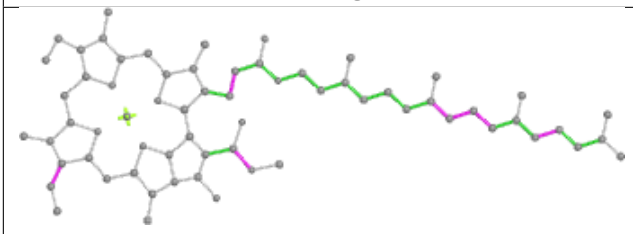


Bond angles



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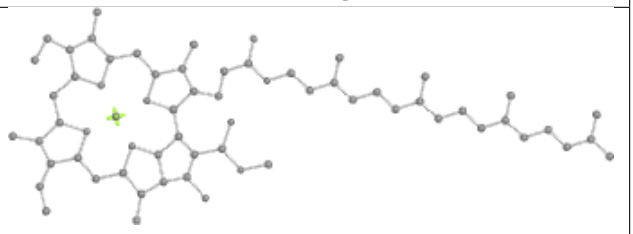
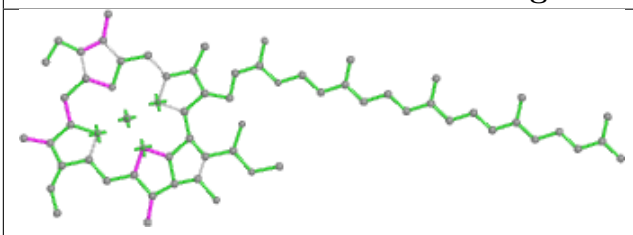


Rings

Ligand CLA r 513



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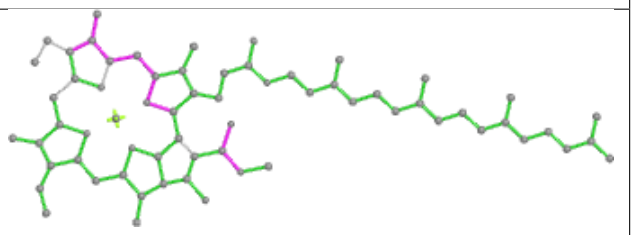

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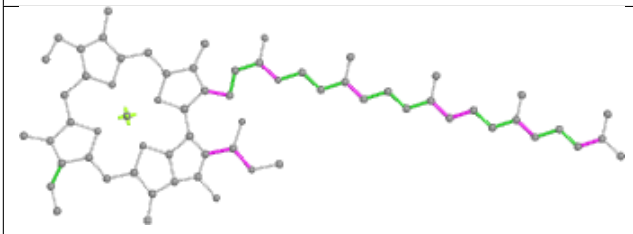

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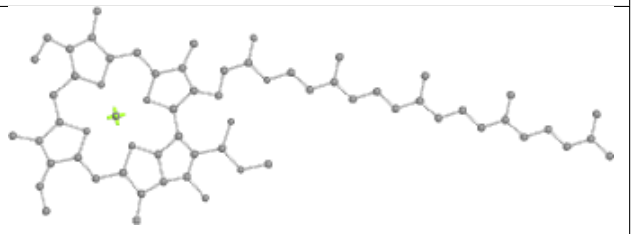
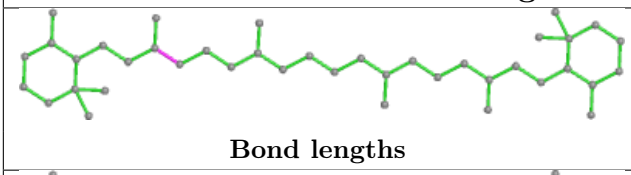


Rings

Ligand BCR e 4008



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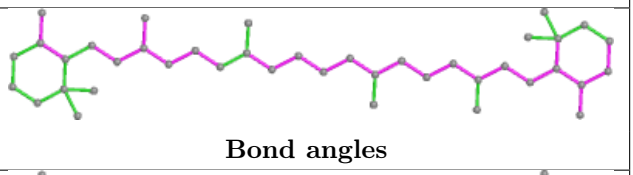
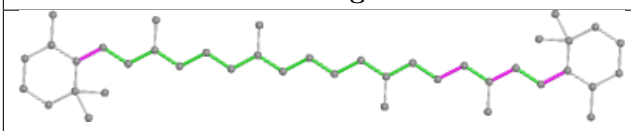
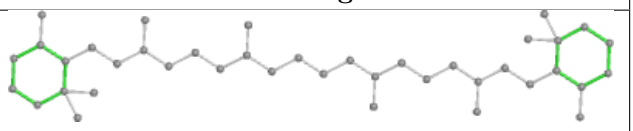


Bond angles

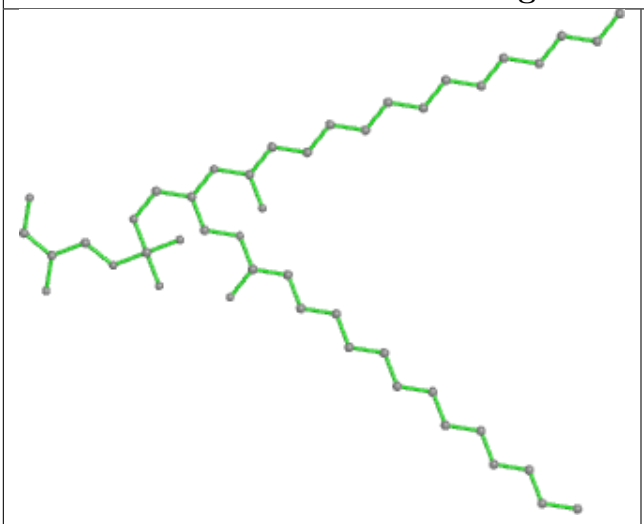


Torsions



Rings

Ligand LHG e 5006



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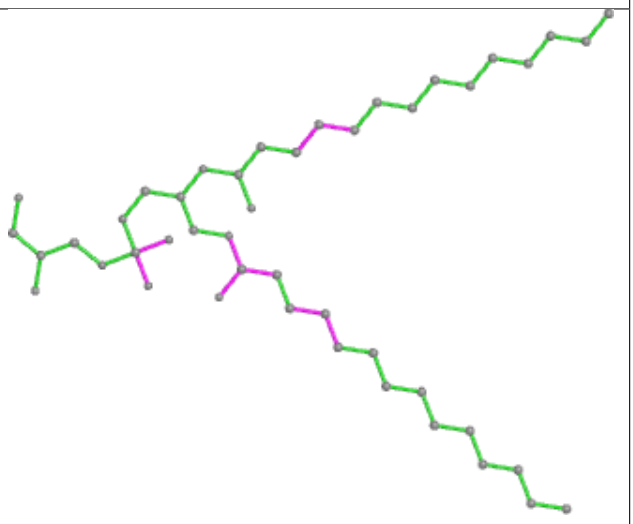
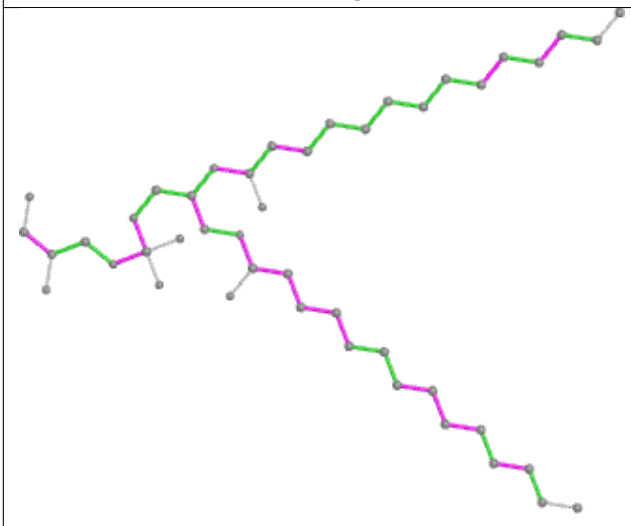


Bond angles



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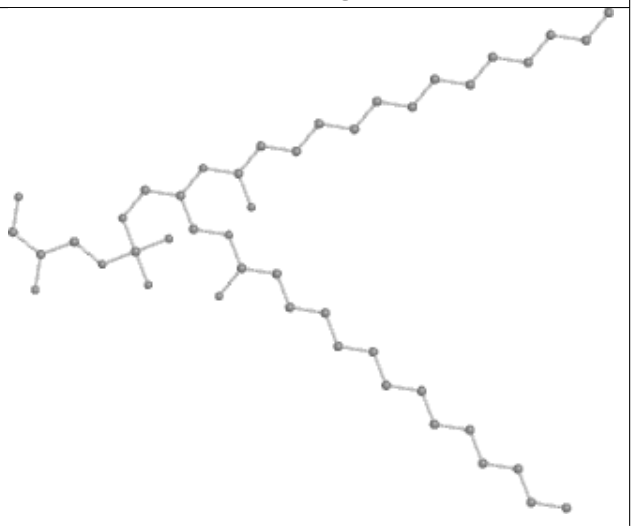
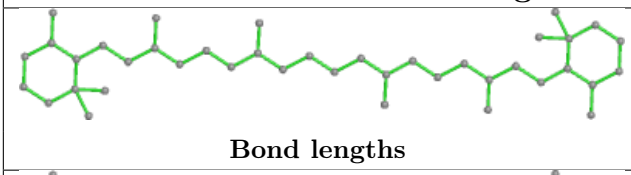


Rings

Ligand BCR T 4012



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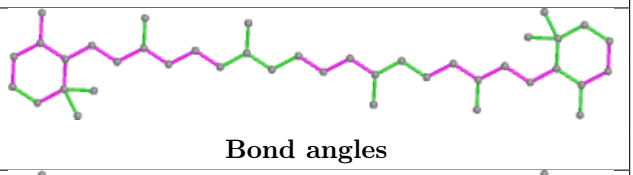
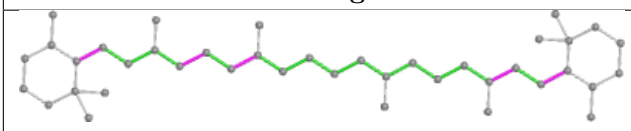
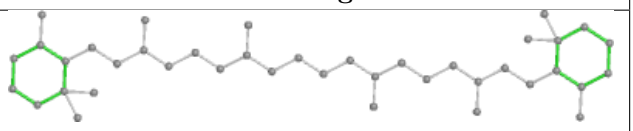


Bond angles

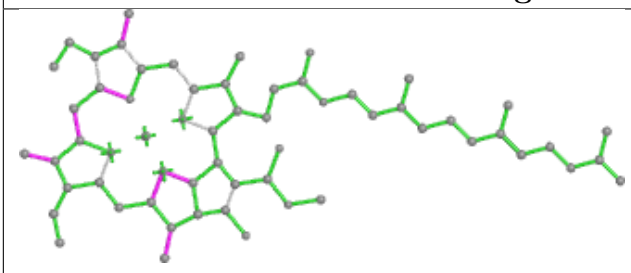


Torsions



Rings

Ligand CLA H 1218



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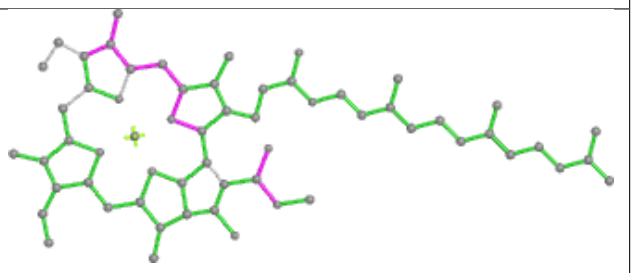
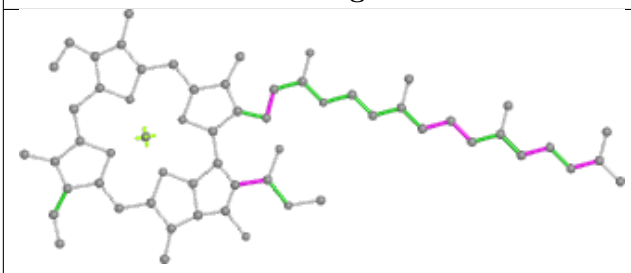


Bond angles



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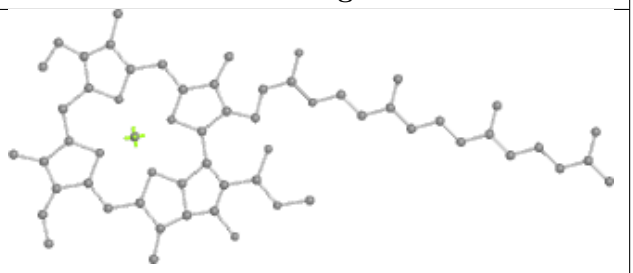
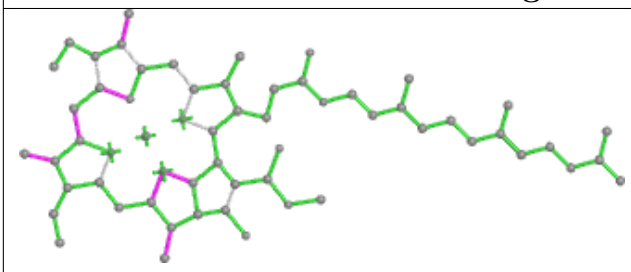


Rings

Ligand CLA f 1218



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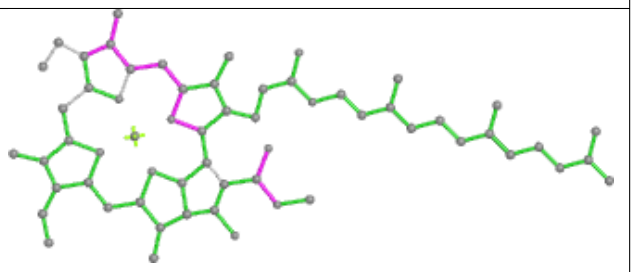
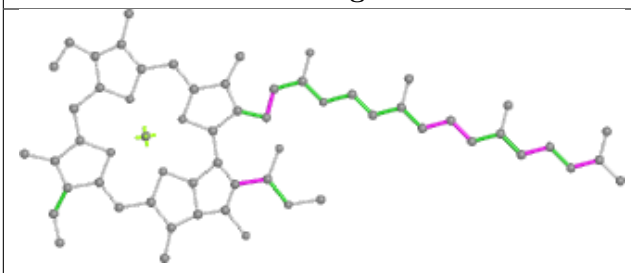


Bond angles



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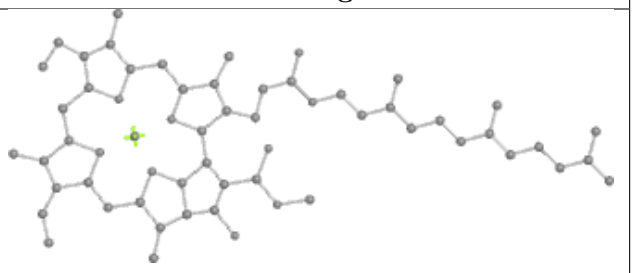
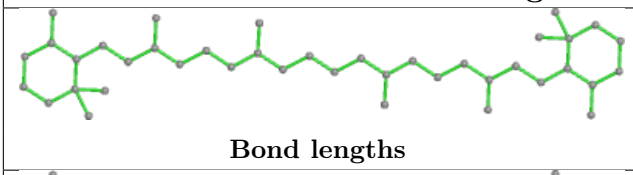
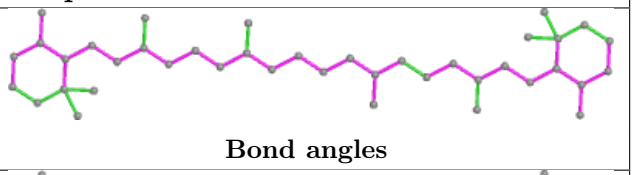


Rings

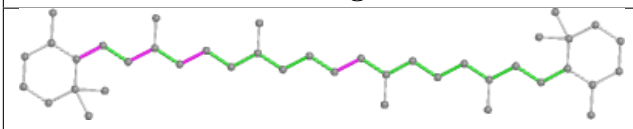
Ligand BCR q 522



Bond lengths



Bond angles



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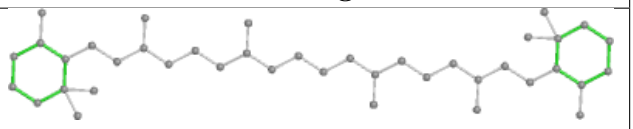
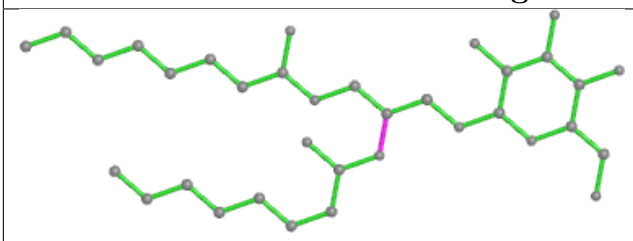
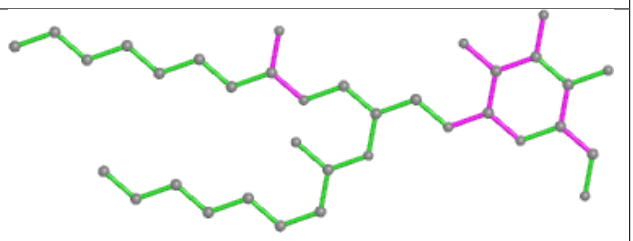


Rings

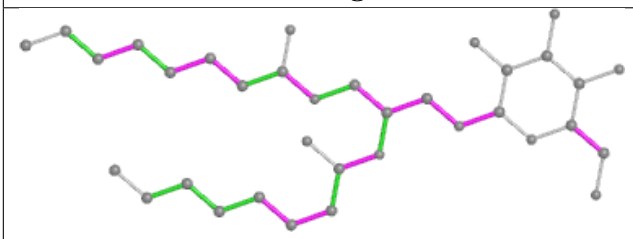
Ligand LMG T 5104



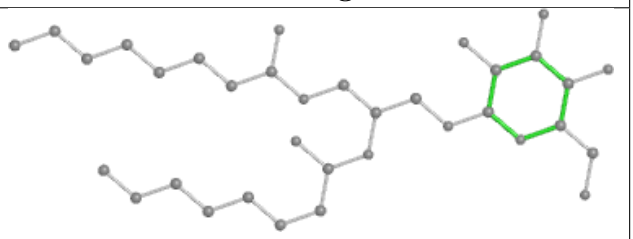
Bond lengths



Bond angles

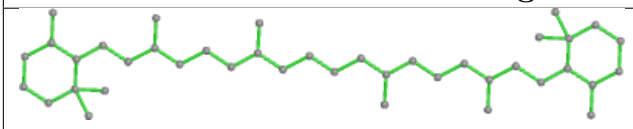


Torsions



Rings

Ligand BCR J 4012



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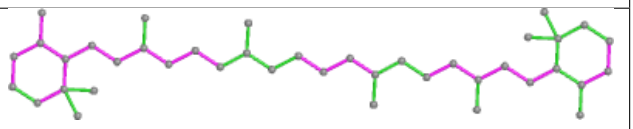
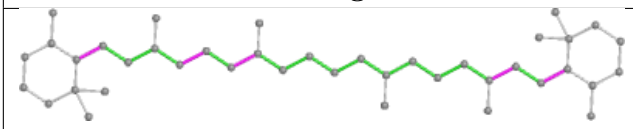


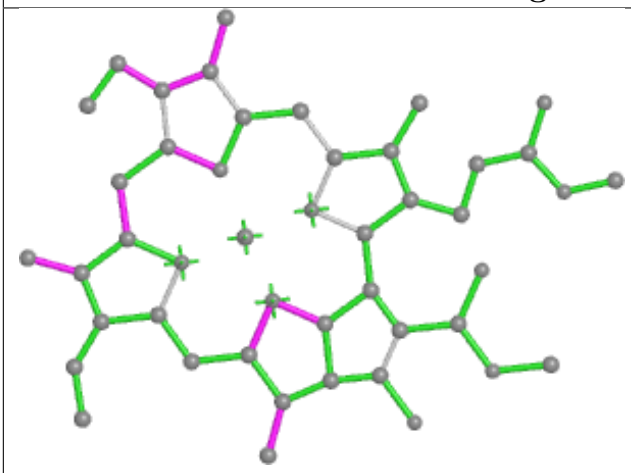
Bond angles



Torsions

Rings

Ligand CLA c 519



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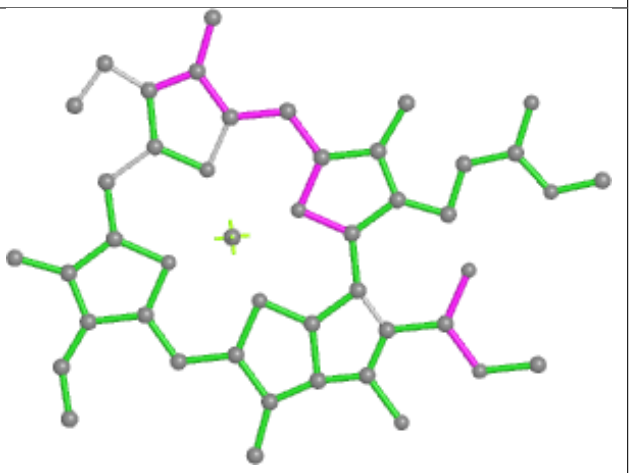
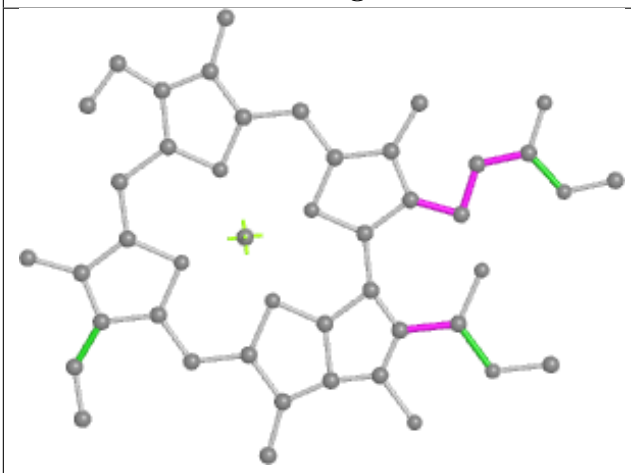
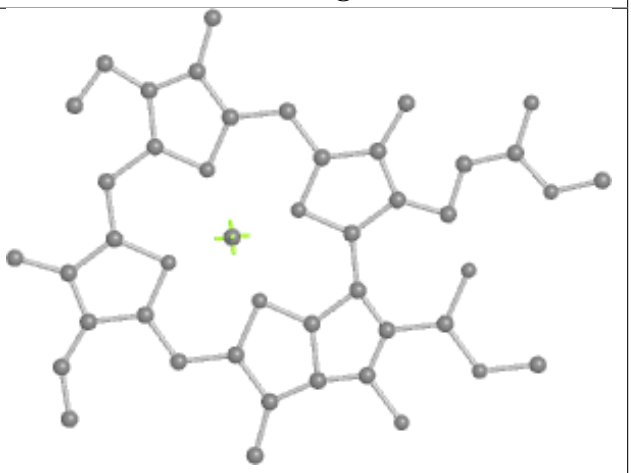


Bond angles

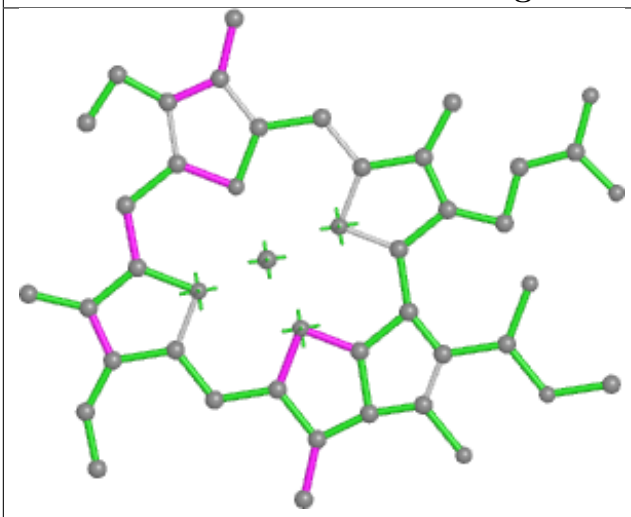


Torsions



Rings

Ligand CLA U 1105



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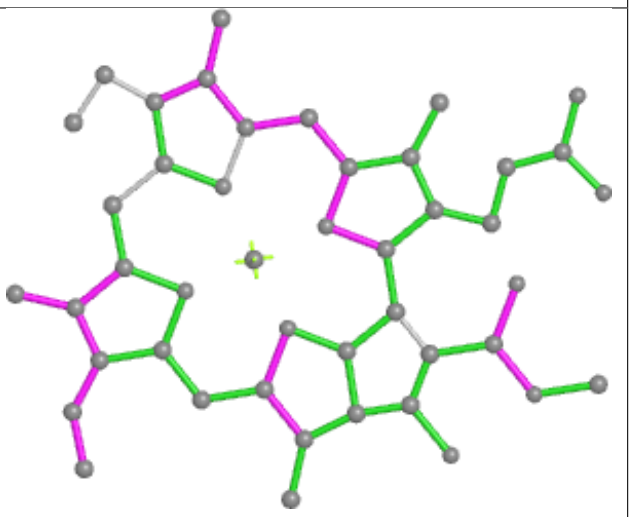
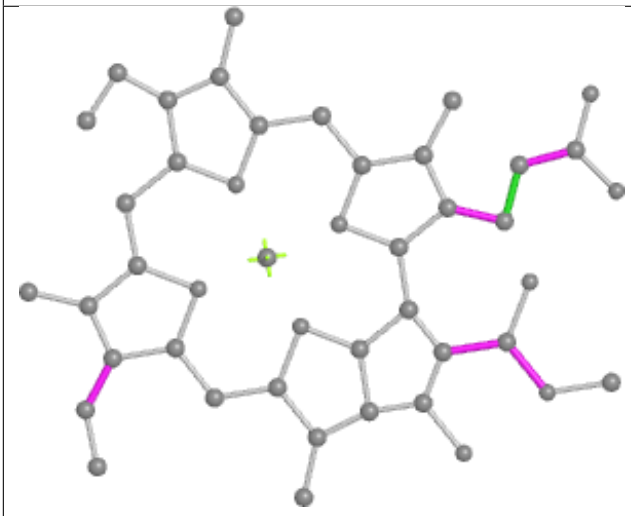


Bond angles



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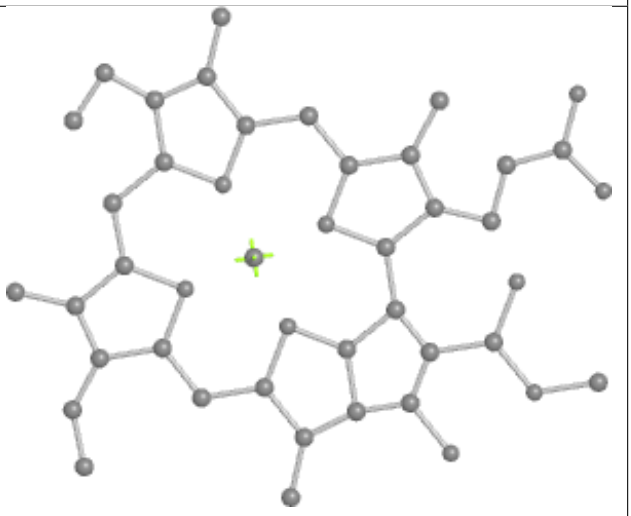
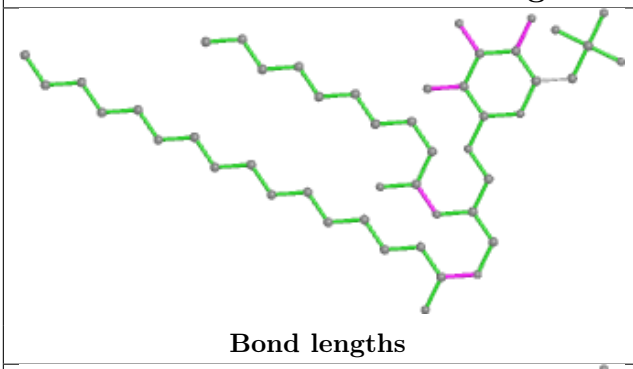


Rings

Ligand SQD q 822



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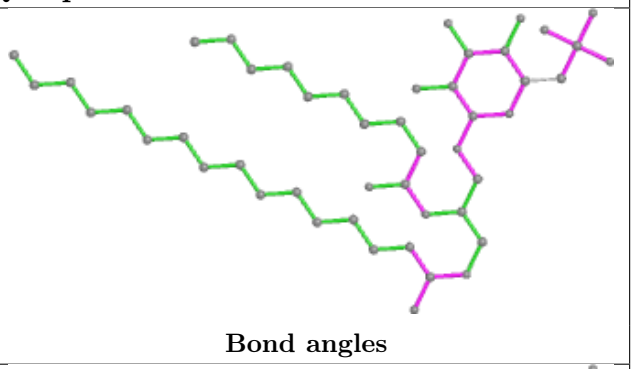
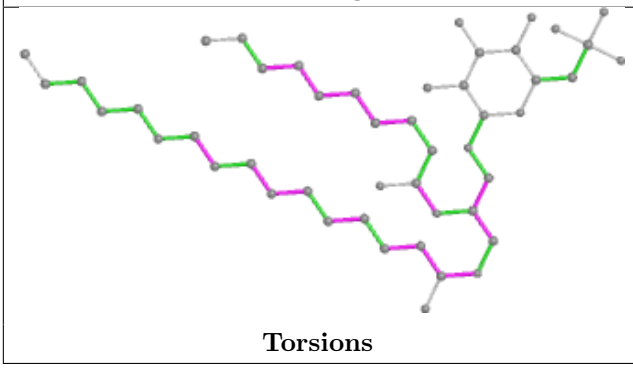


Bond angles



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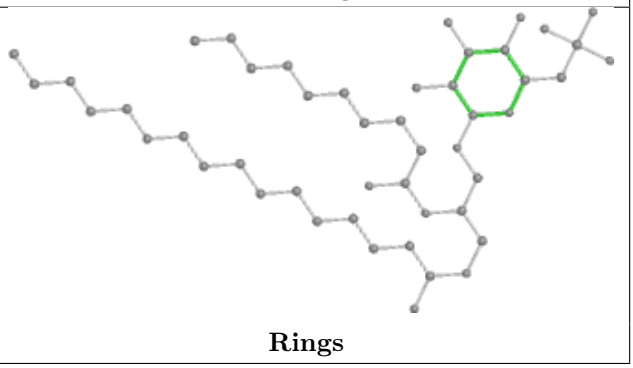
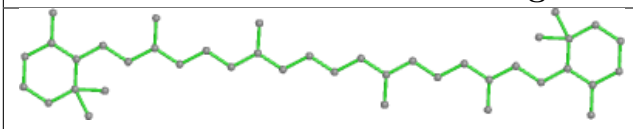


Rings

Ligand BCR t 523



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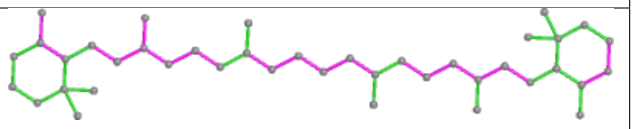

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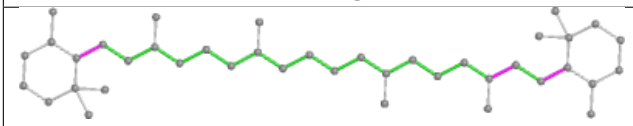
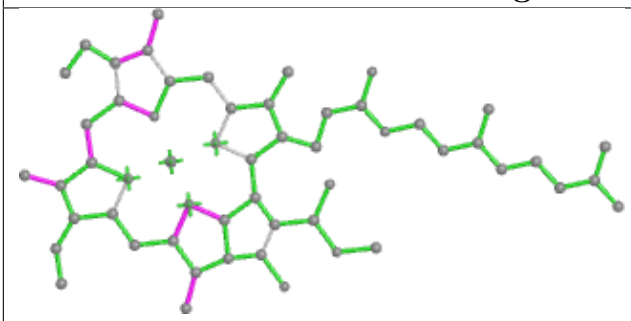


Torsions

Rings

Ligand CLA m 1401



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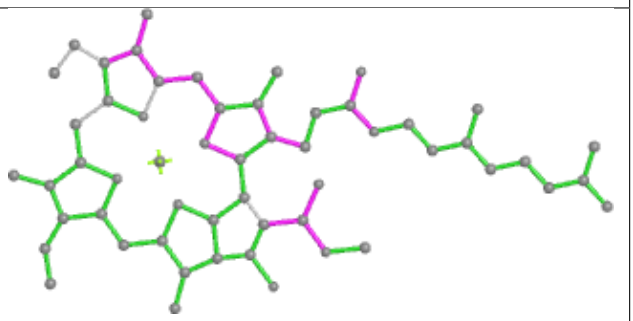
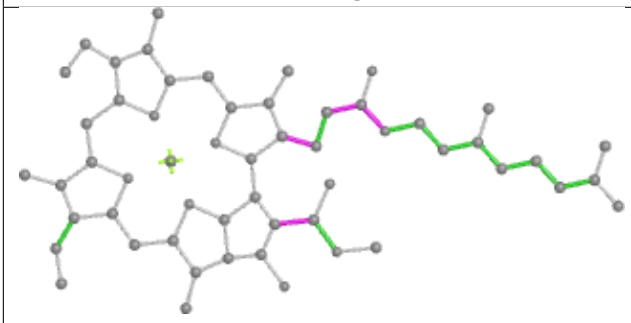
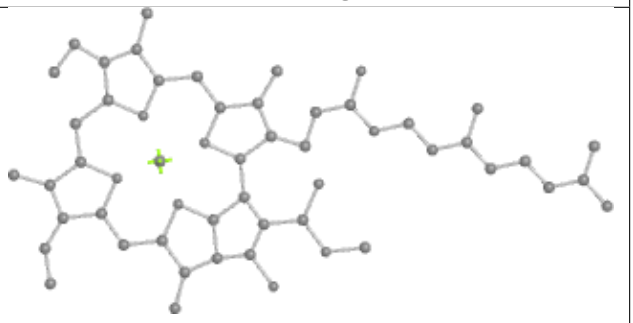


Bond angles

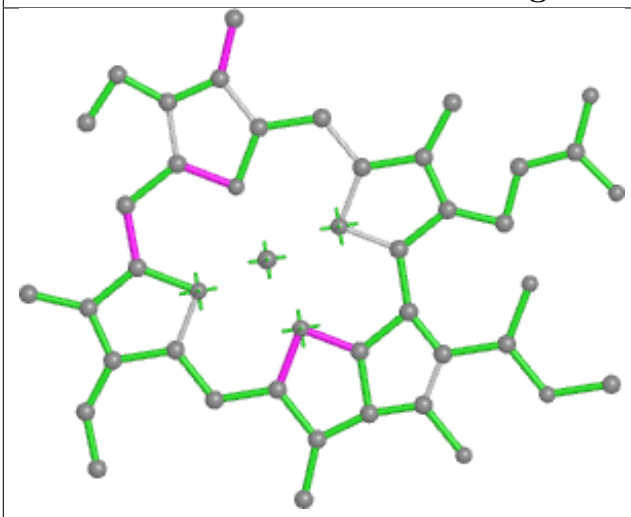


Torsions

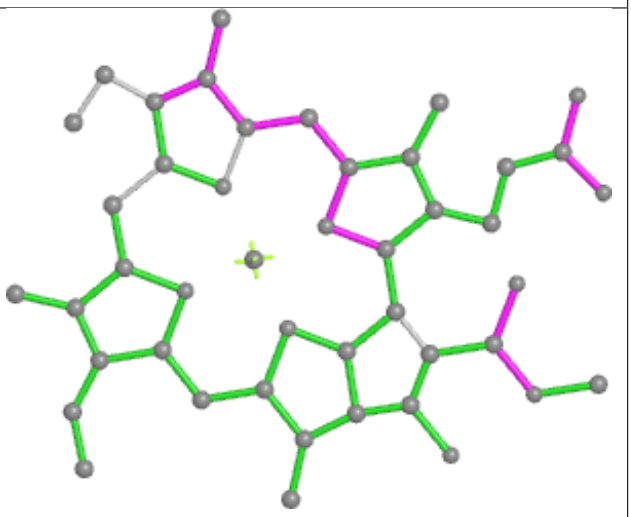


Rings

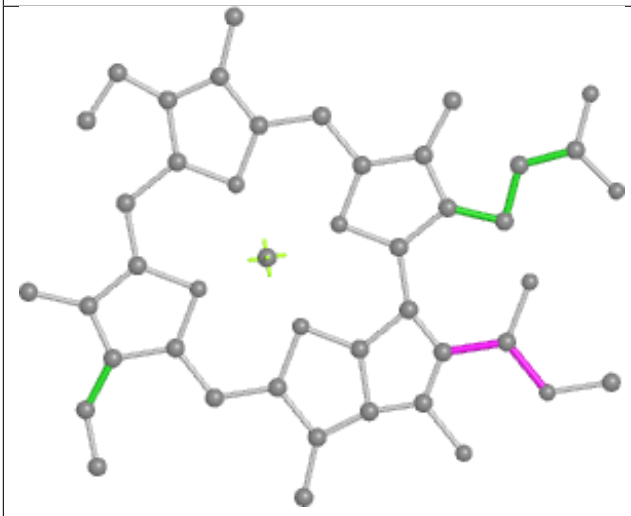
Ligand CLA c 506



Bond lengths



Bond angles



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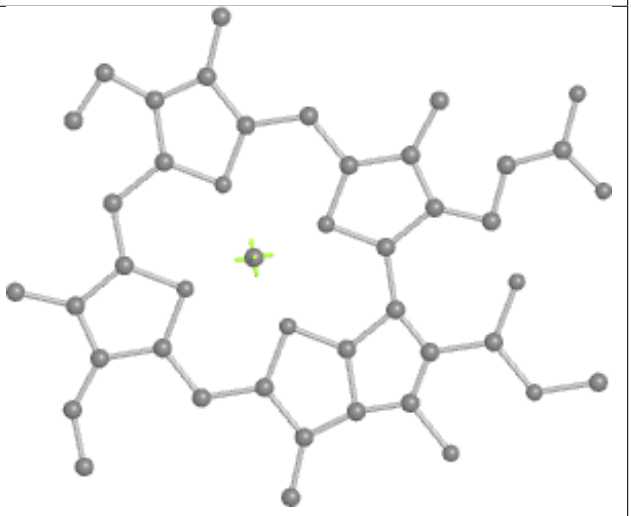
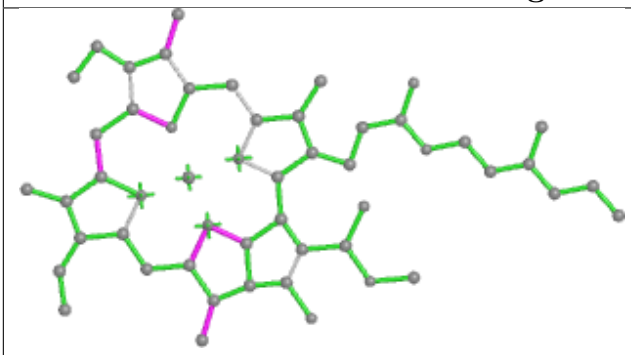
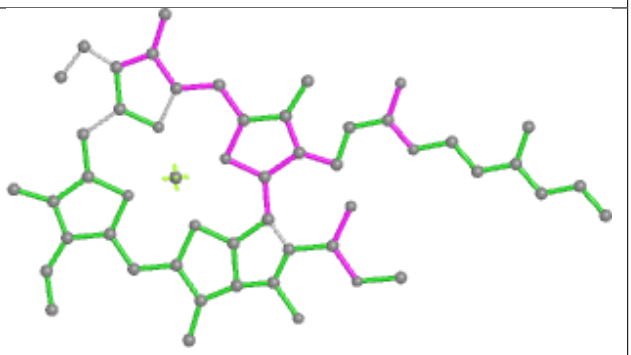
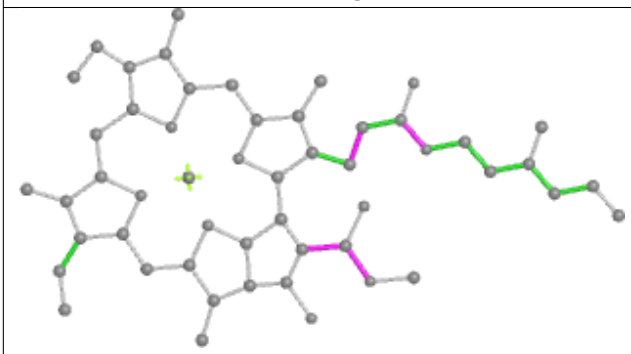
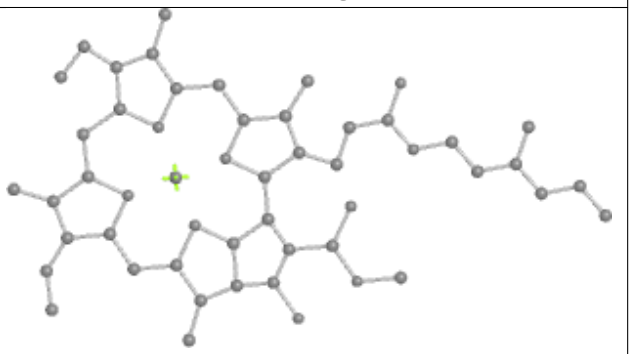
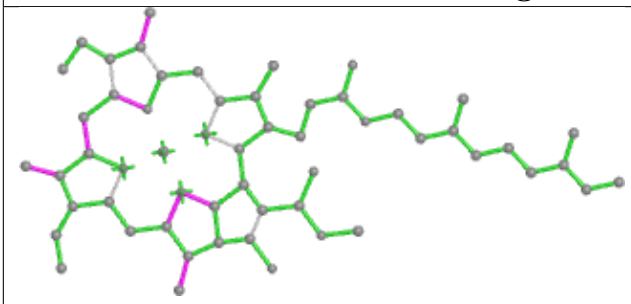
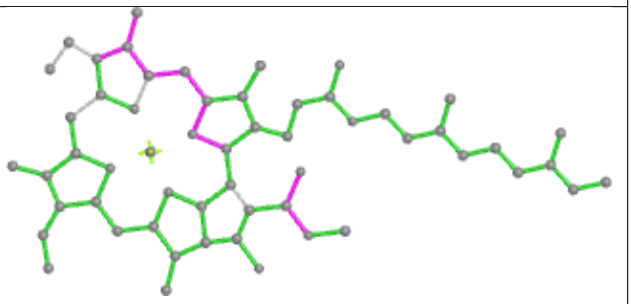
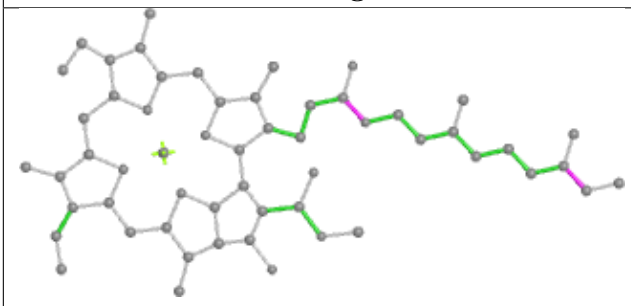
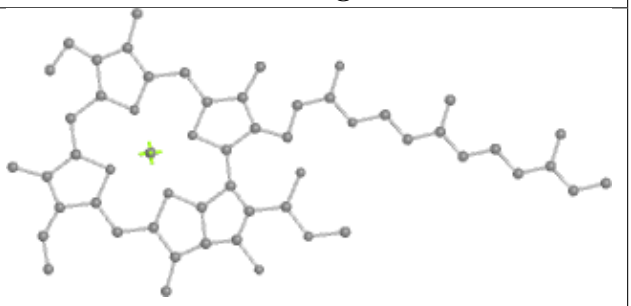
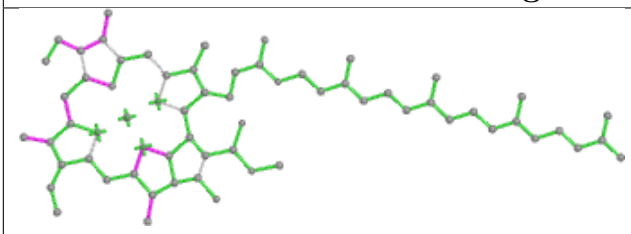


Rings

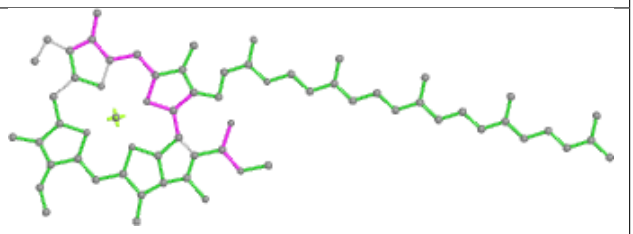
Ligand CLA d 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1211	
 Bond lengths	 Bond angles
 Torsions	 Rings

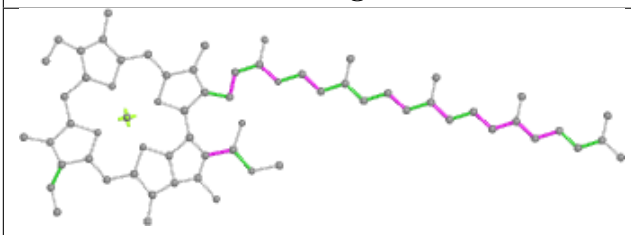
Ligand CLA f 1214



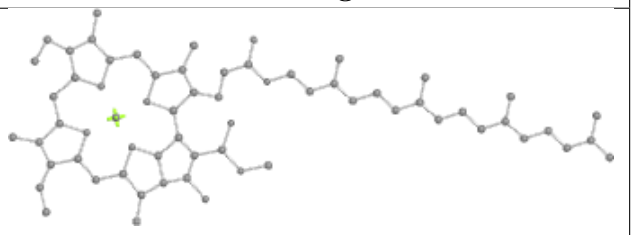
Bond lengths



Bond angles

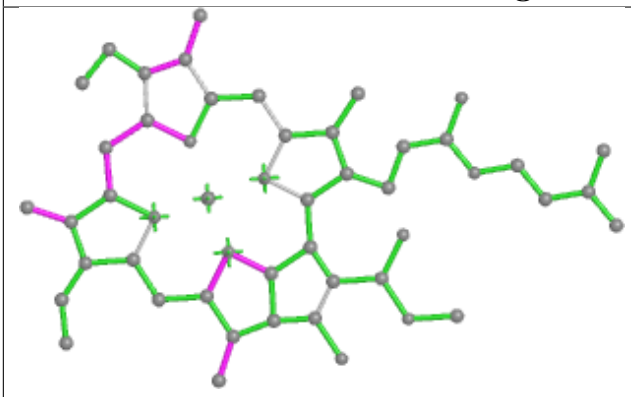


Torsions



Rings

Ligand CLA K 1103



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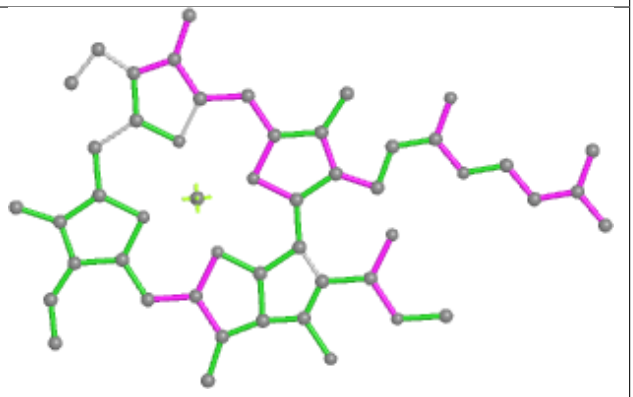
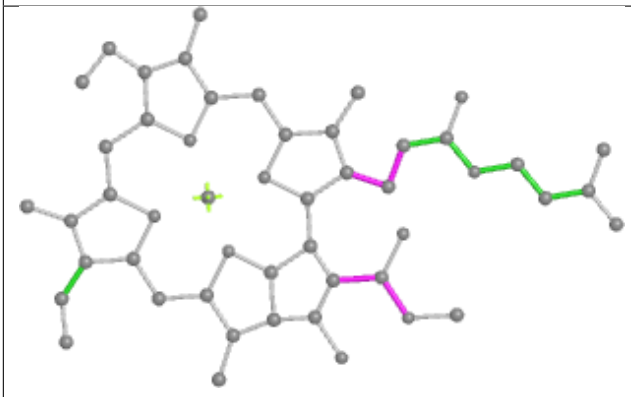


Bond angles



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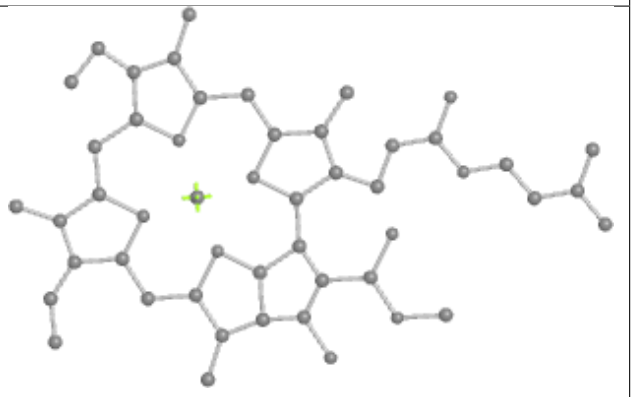
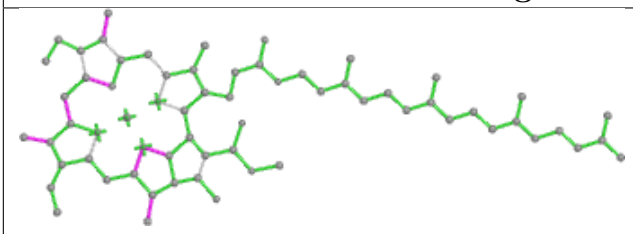
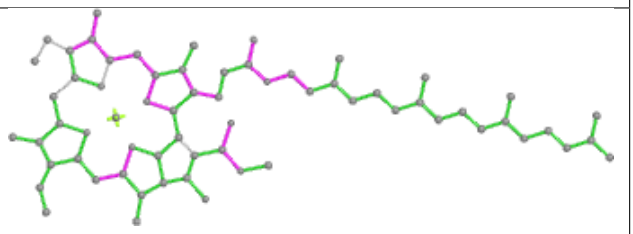


Rings

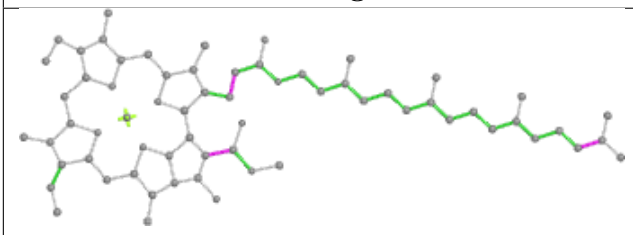
Ligand CLA H 1238



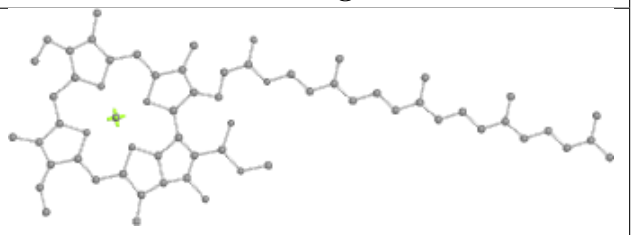
Bond lengths



Bond angles

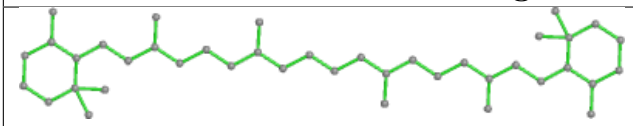


Torsions

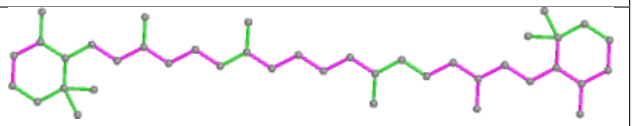


Rings

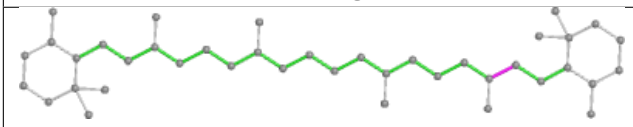
Ligand BCR U 4104



Bond lengths



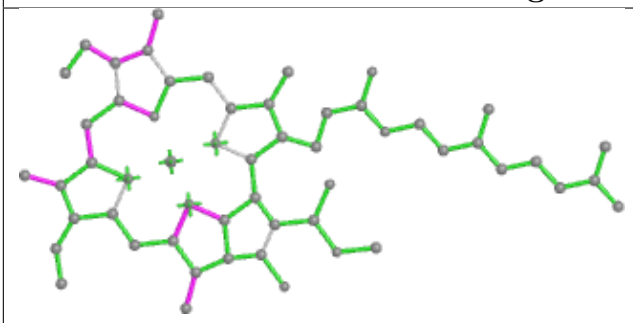
Bond angles



Torsions

Rings

Ligand CLA b 519



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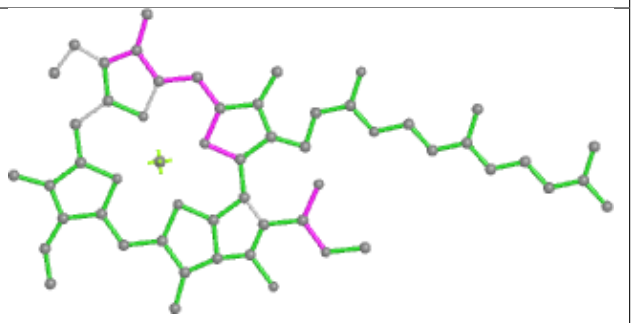
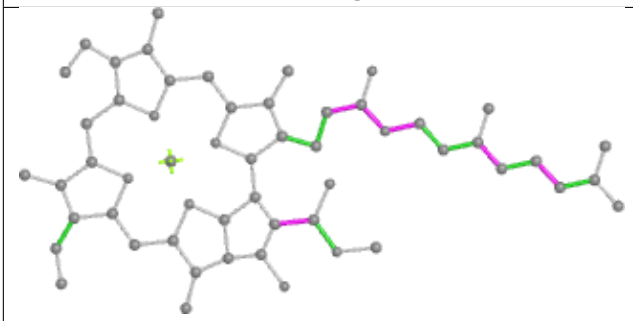
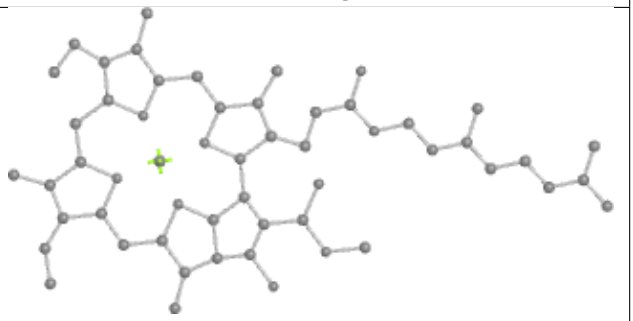


Bond angles

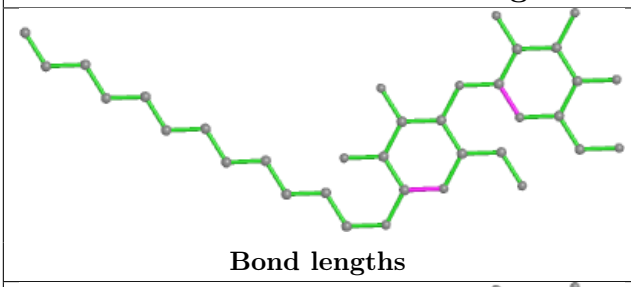


Torsions

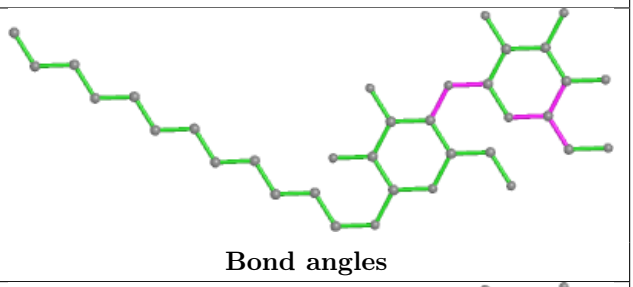


Rings

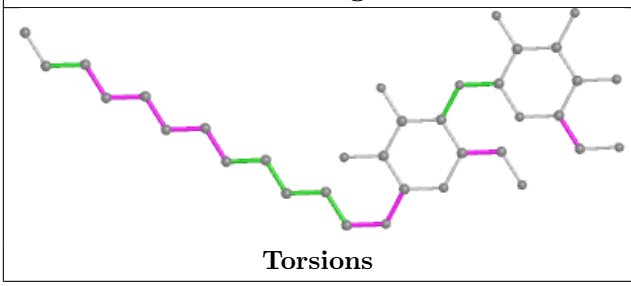
Ligand LMU H 1843



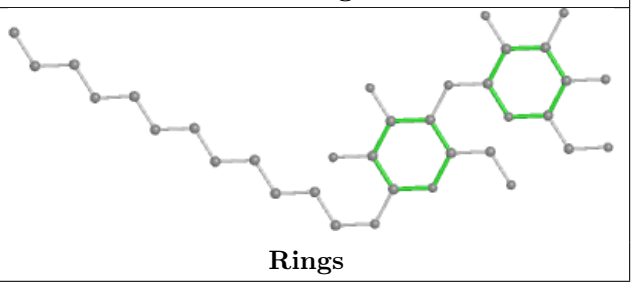
Bond lengths



Bond angles

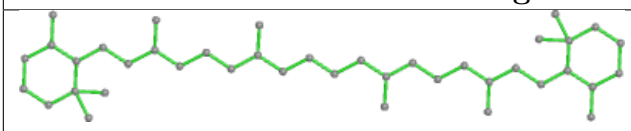


Torsions



Rings

Ligand BCR V 4022



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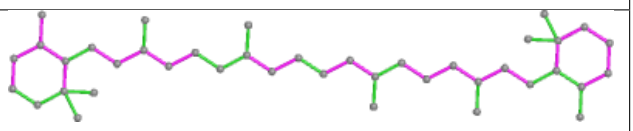

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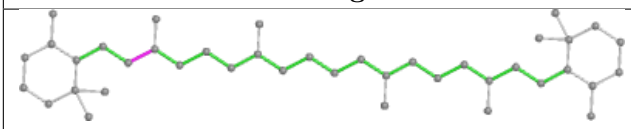

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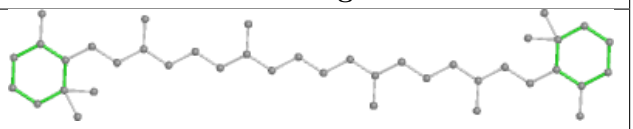
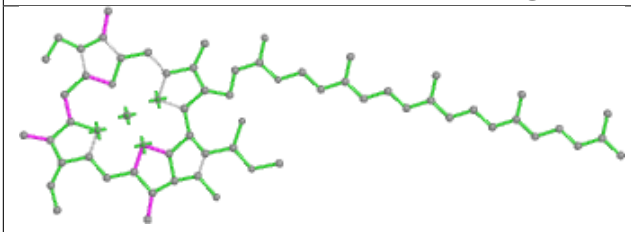


Rings

Ligand CLA Y 509



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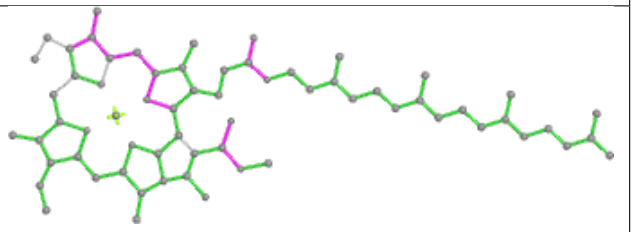

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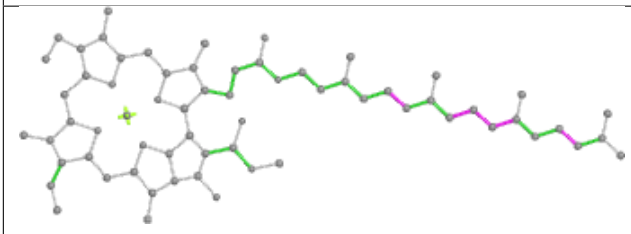

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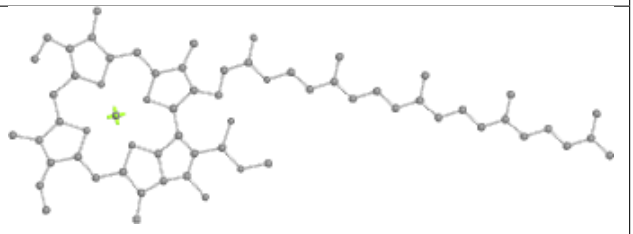
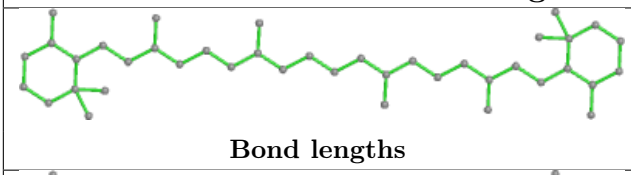


Rings

Ligand BCR t 524



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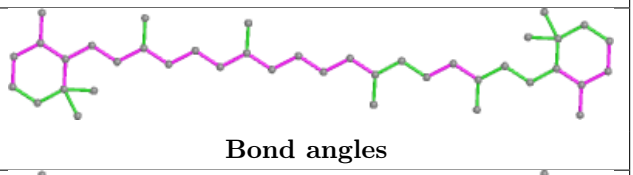

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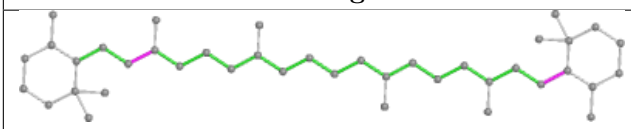

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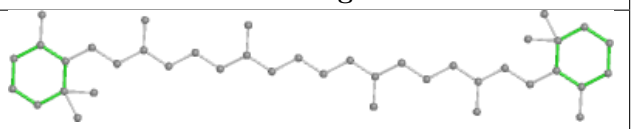
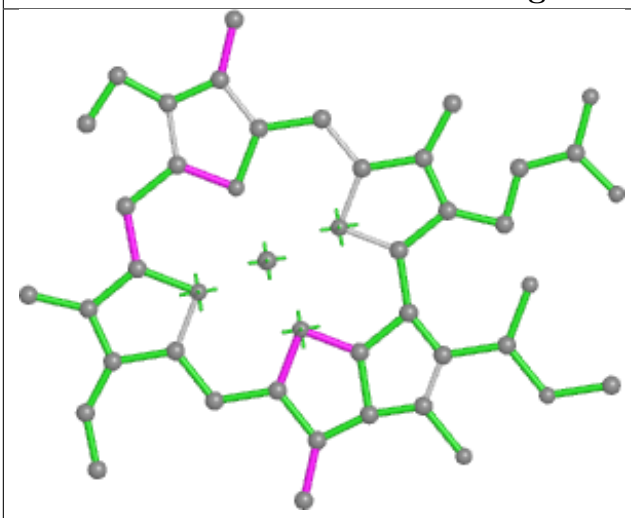


Rings

Ligand CLA 6 509



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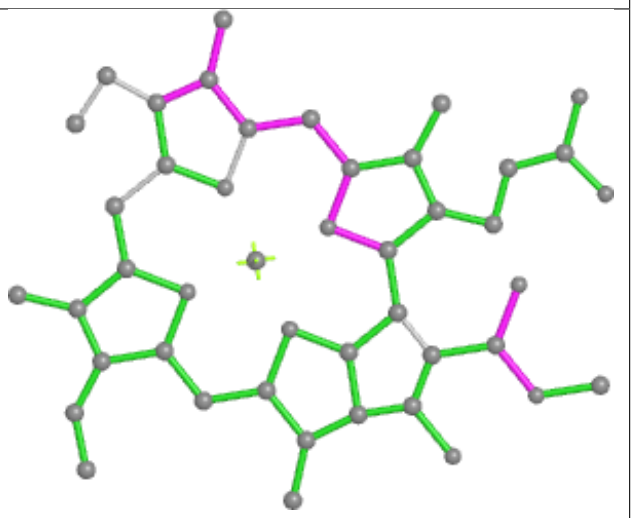

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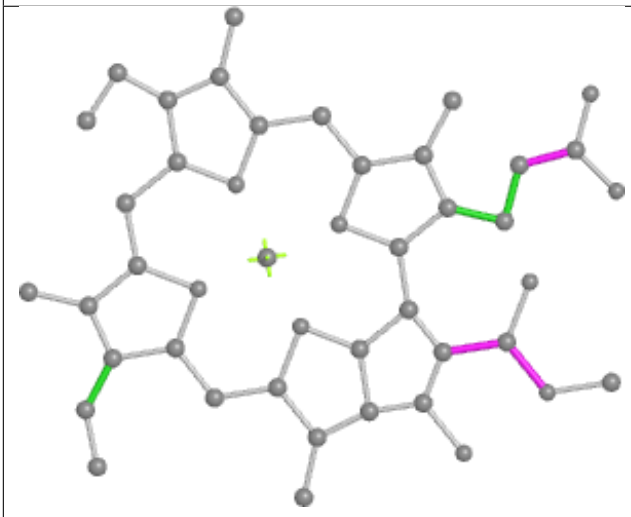

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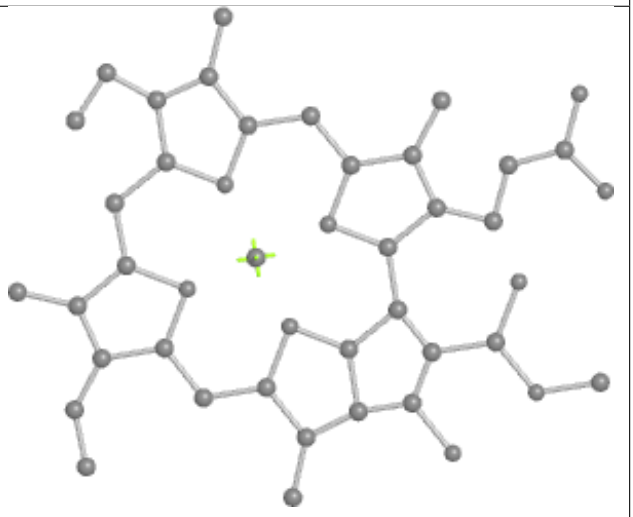
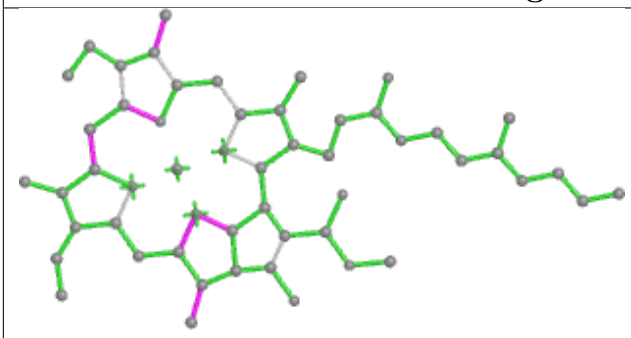


Rings

Ligand CLA Z 512



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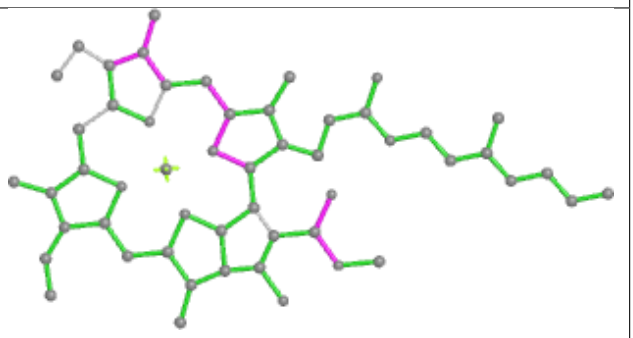

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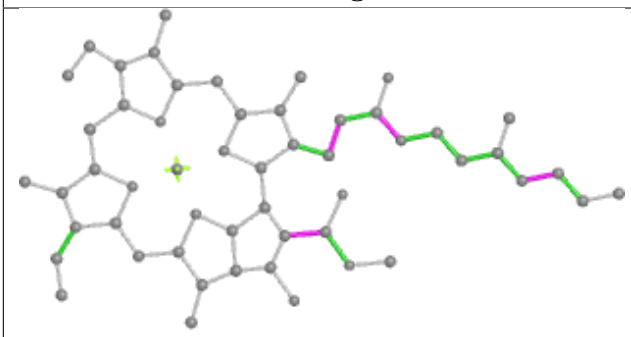

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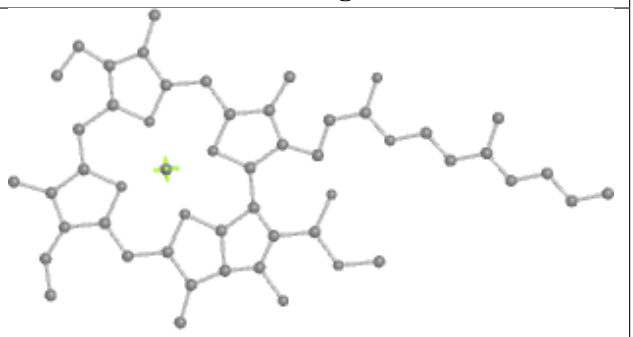
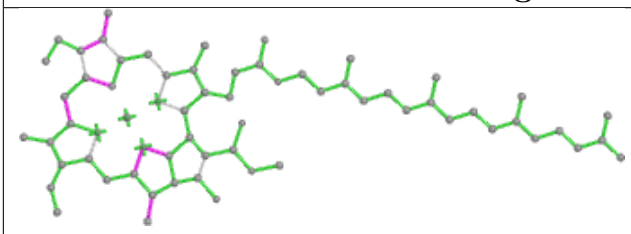


Rings

Ligand CLA H 1208



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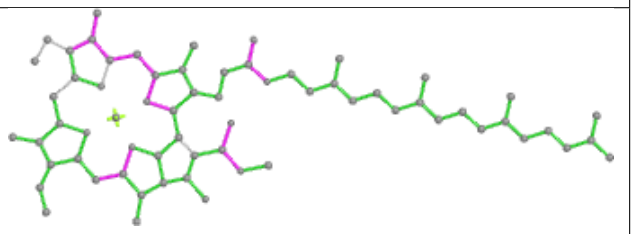

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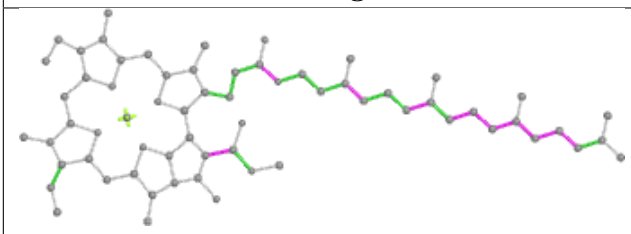

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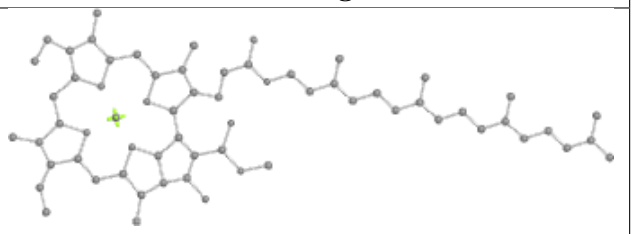
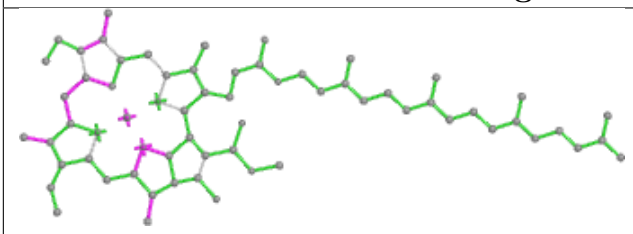


Rings

Ligand CLA A 1117



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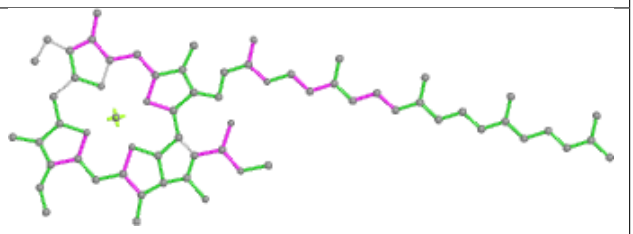

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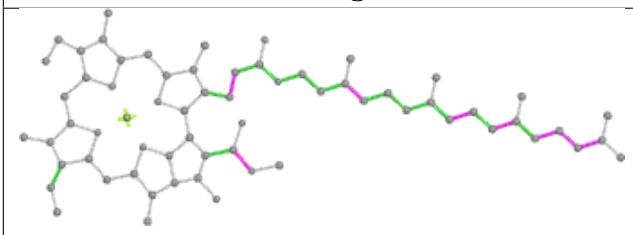

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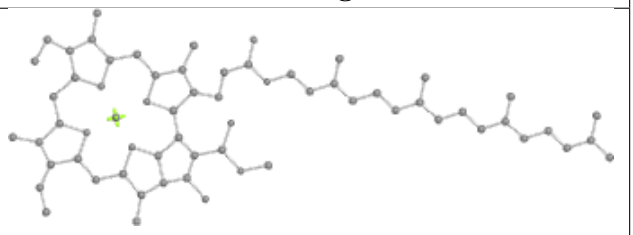

Rings

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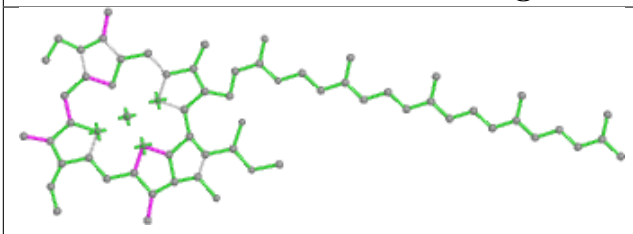

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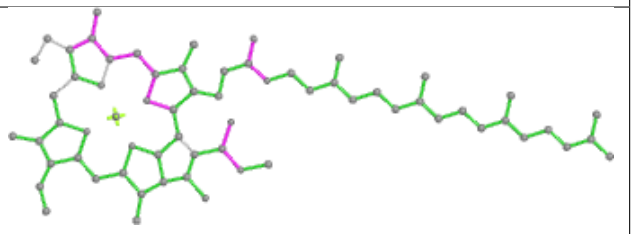

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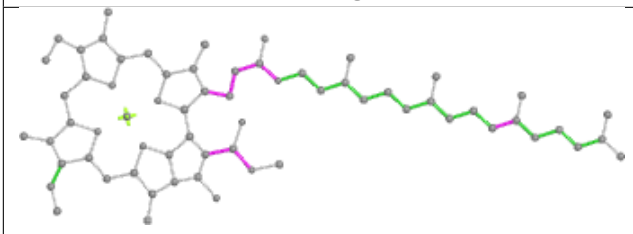

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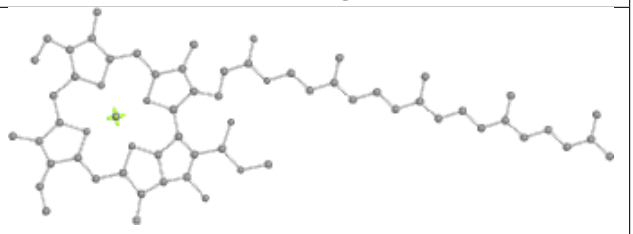
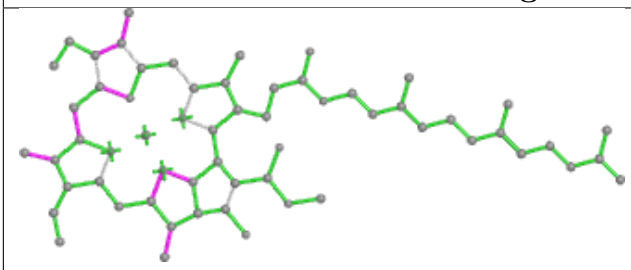


Rings

Ligand CLA e 1136



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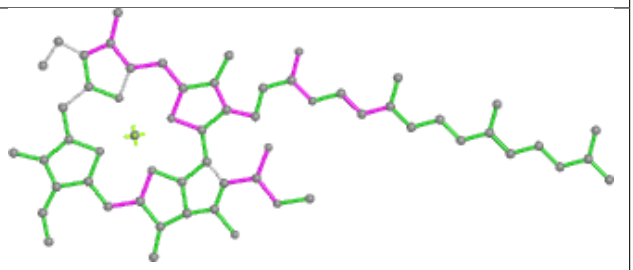

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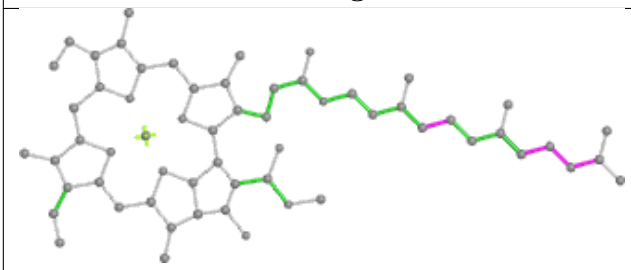

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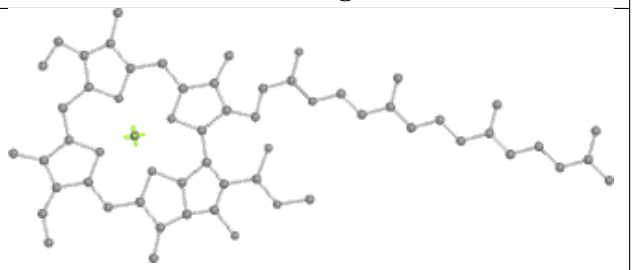
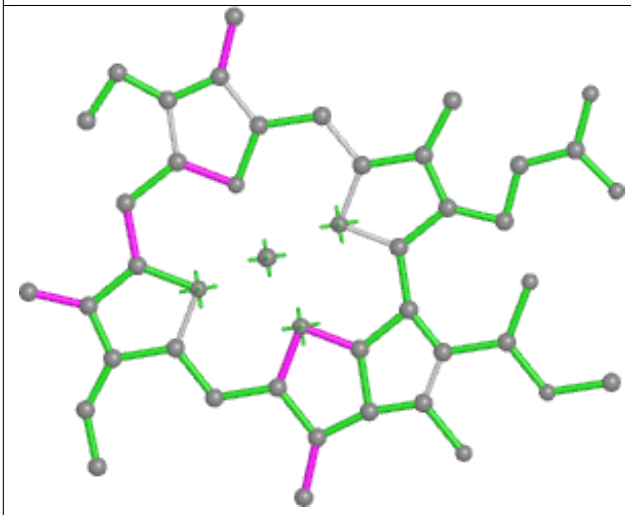


Rings

Ligand CLA c 508



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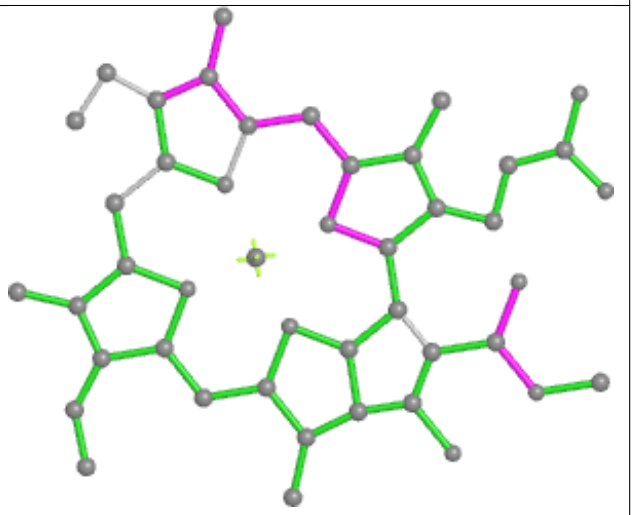
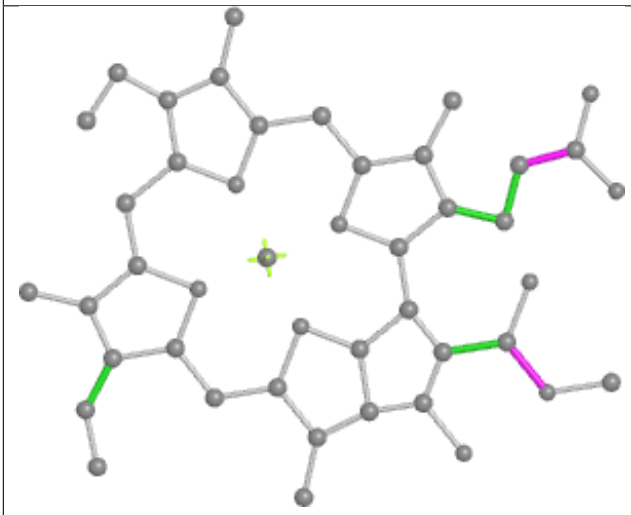


Bond angles



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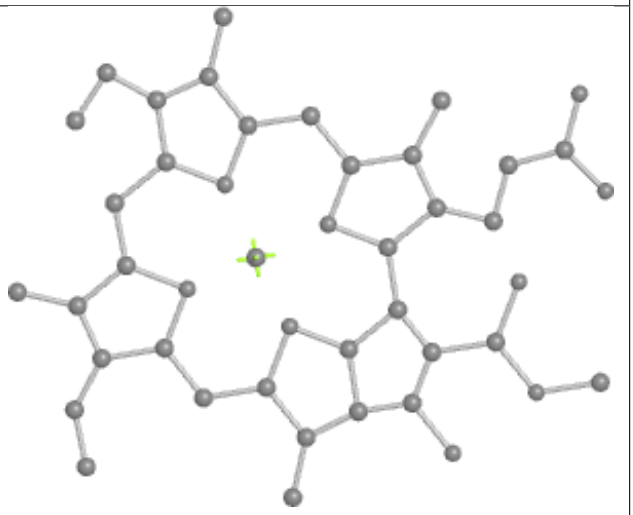
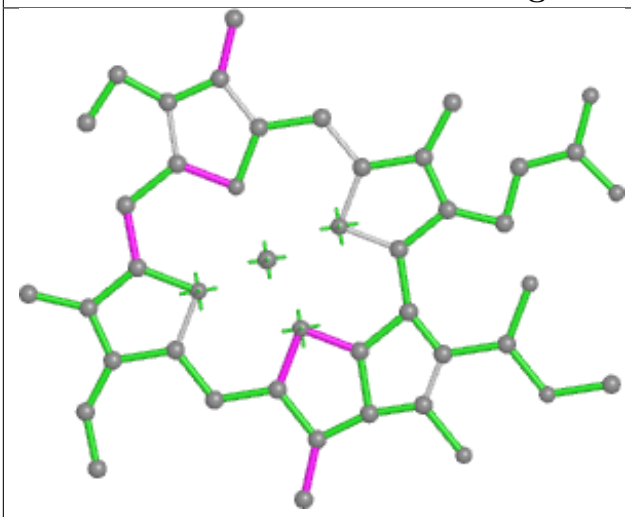


Rings

Ligand CLA 5 507



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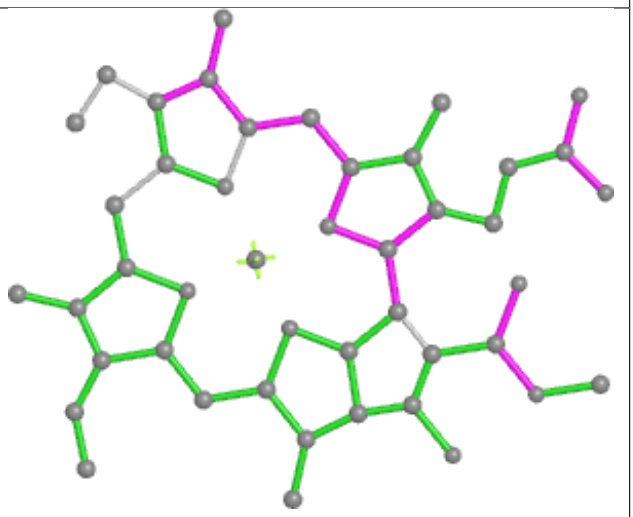
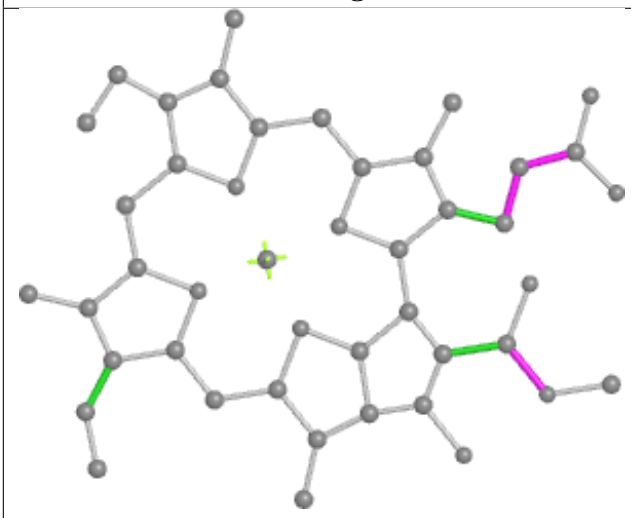


Bond angles



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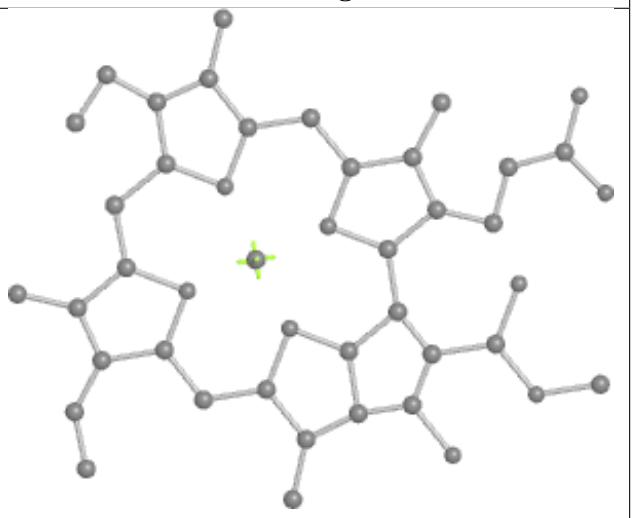
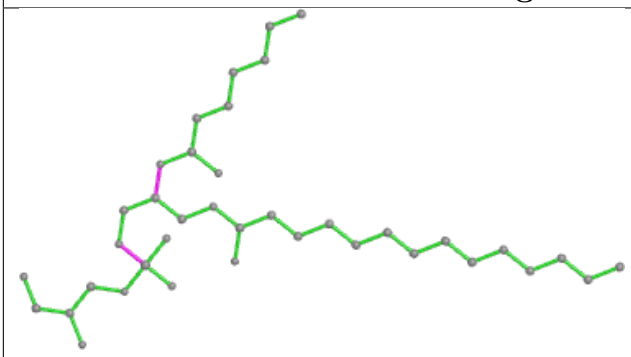


Rings

Ligand LHG L 5218



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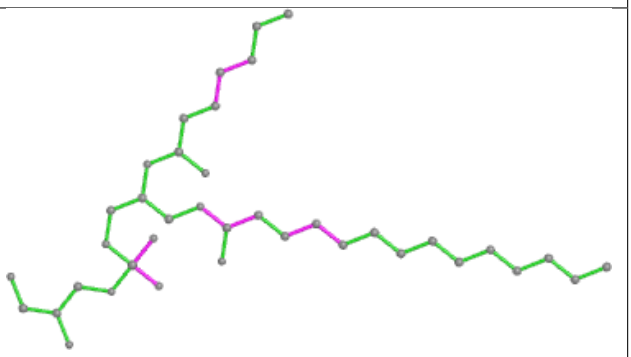

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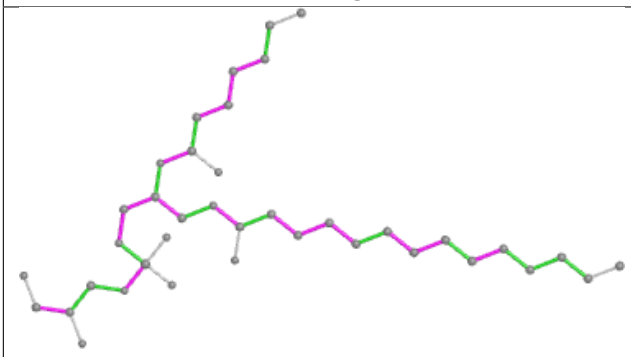

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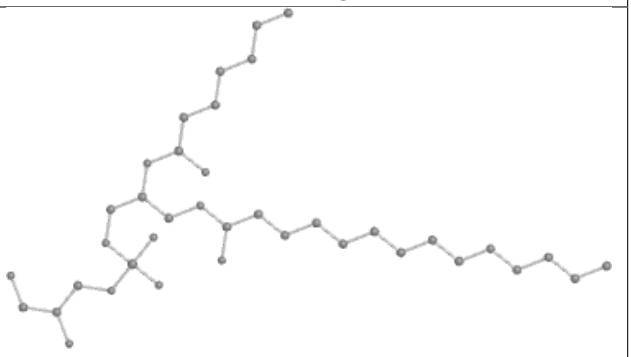
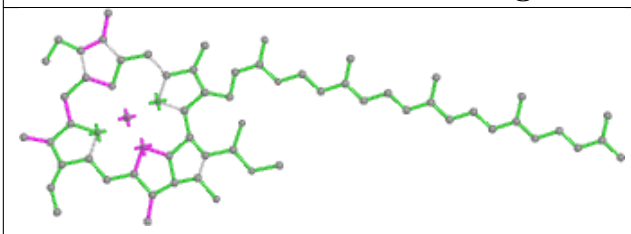


Rings

Ligand CLA H 1205



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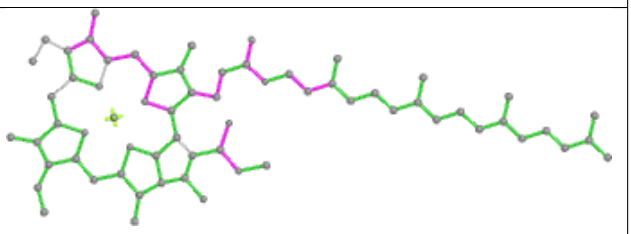
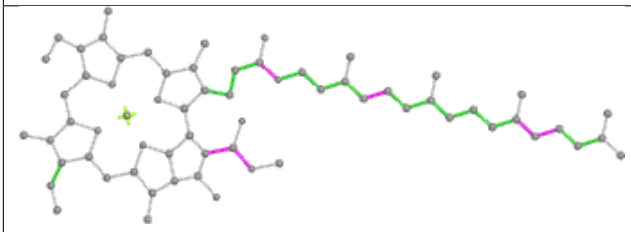


Bond angles



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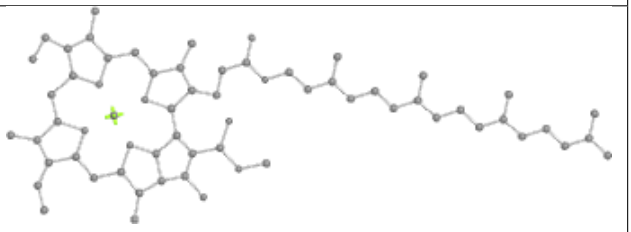
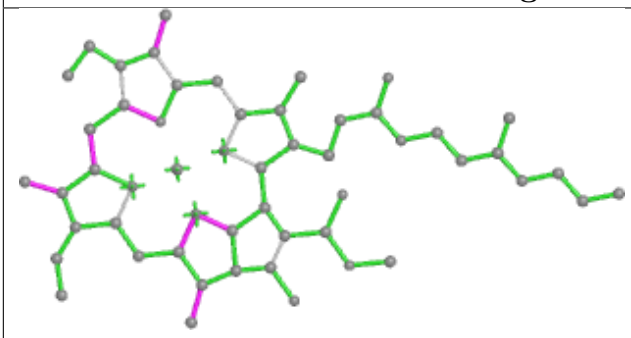


Rings

Ligand CLA e 1120



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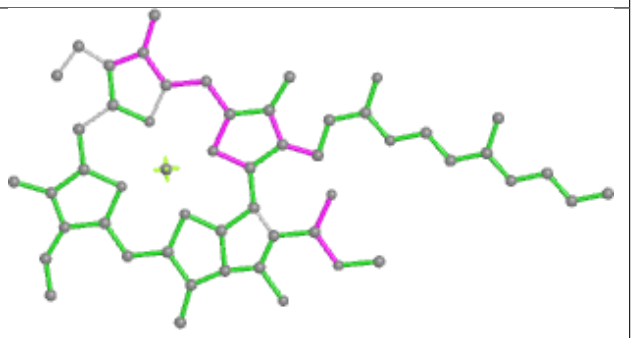
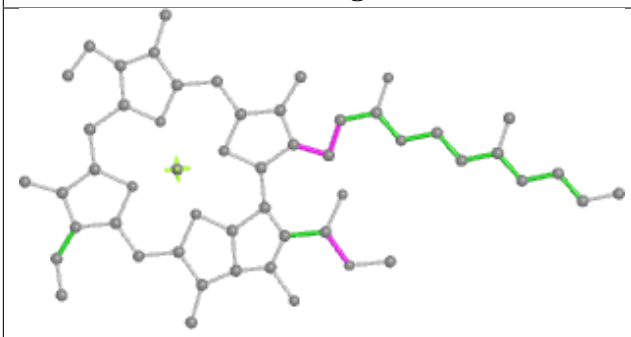
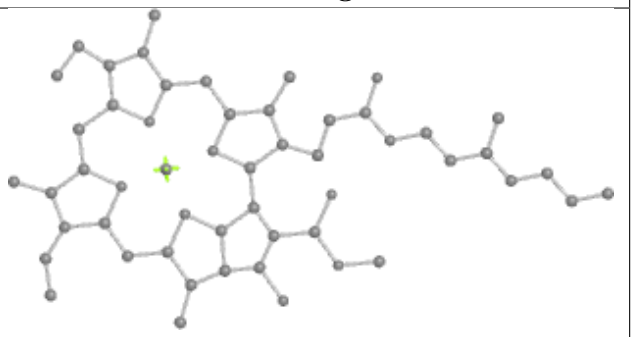


Bond angles

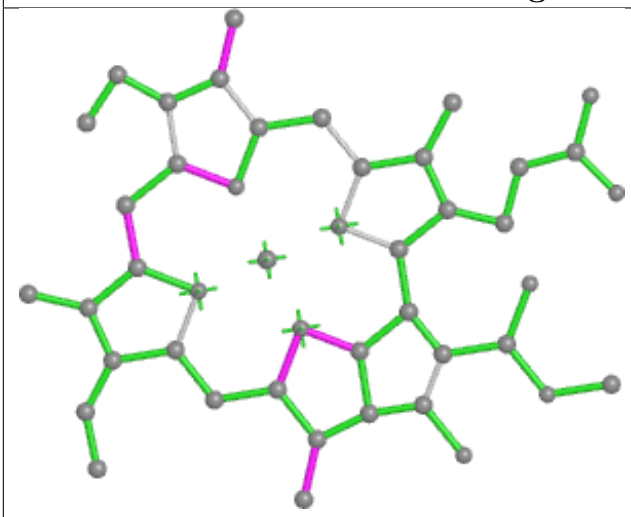


Torsions

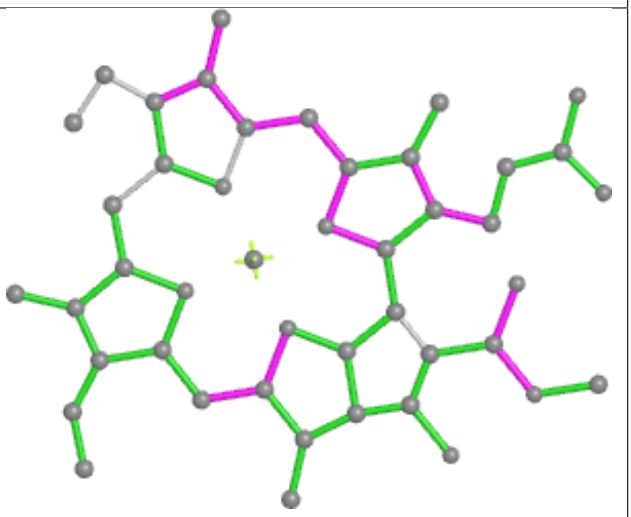


Rings

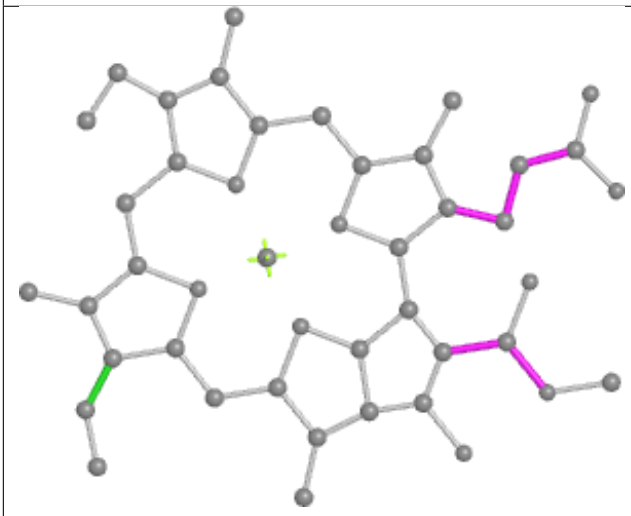
Ligand CLA 6 516



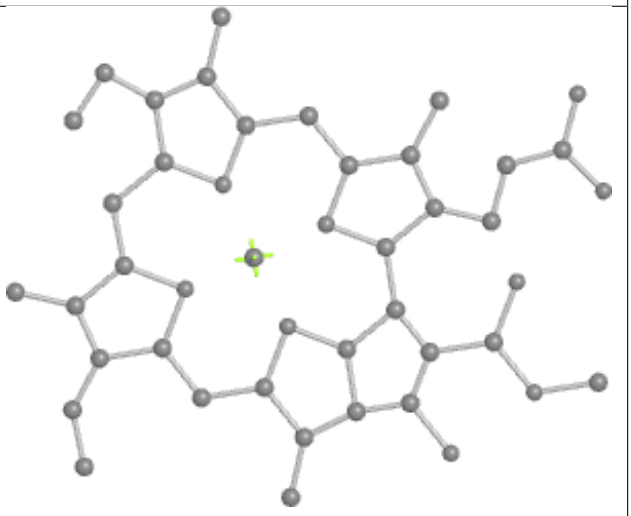
Bond lengths



Bond angles

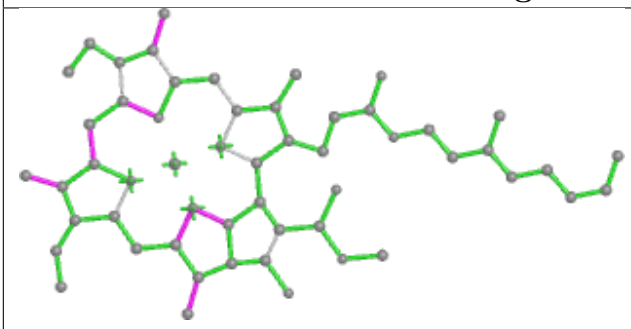


Torsions



Rings

Ligand CLA A 1108



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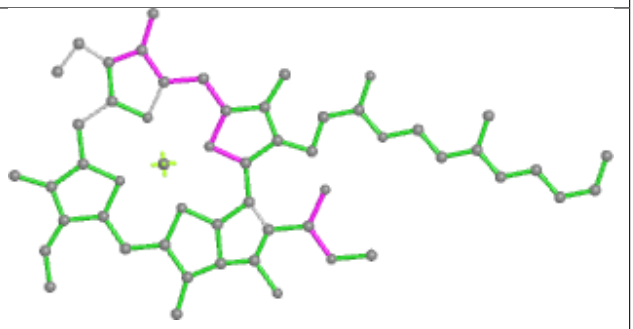

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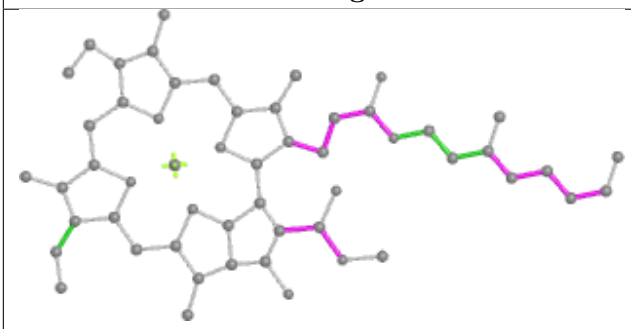

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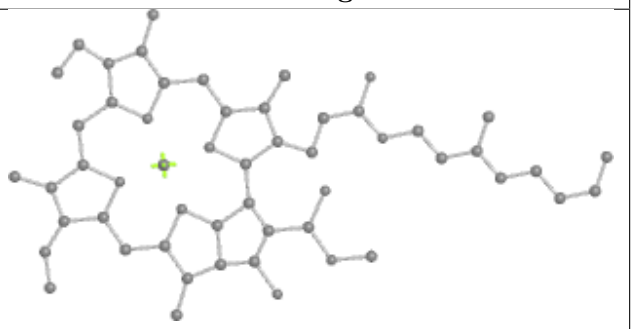
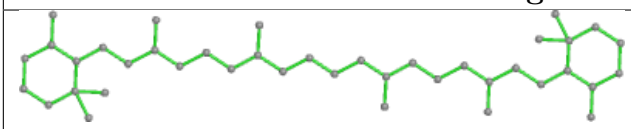


Rings

Ligand BCR 6 523



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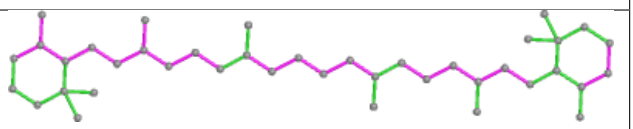

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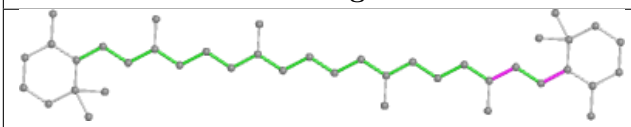

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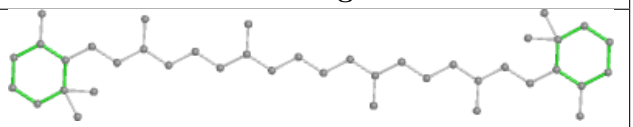
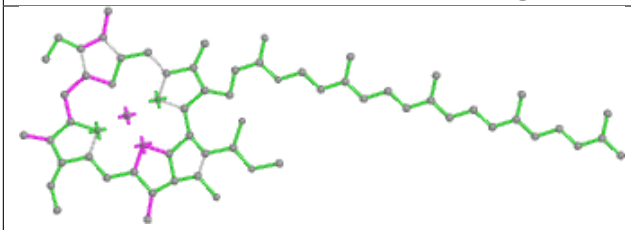


Rings

Ligand CLA G 1128



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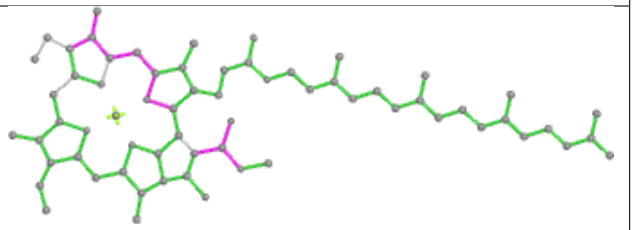
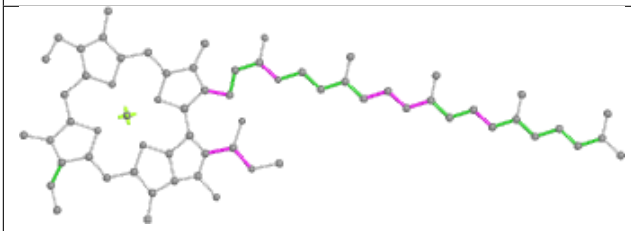


Bond angles



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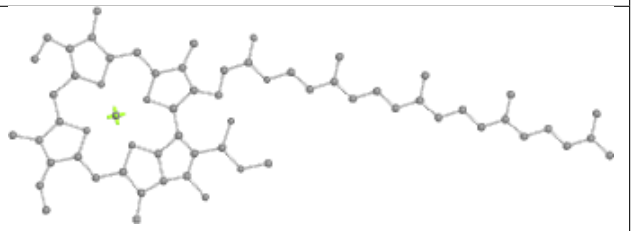
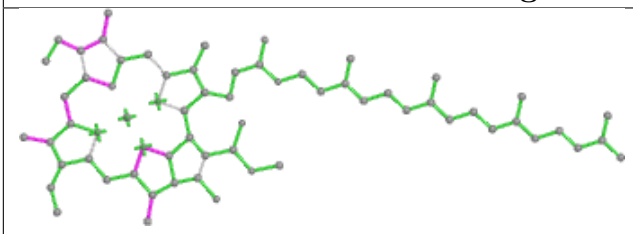


Rings

Ligand CLA e 1131



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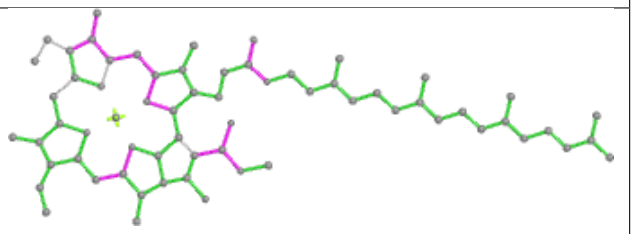

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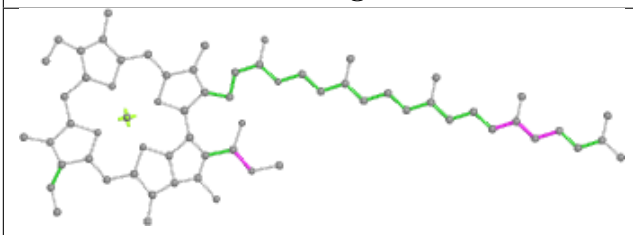

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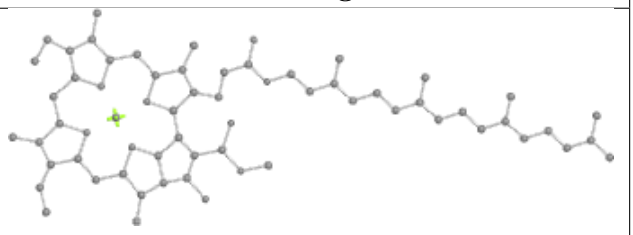
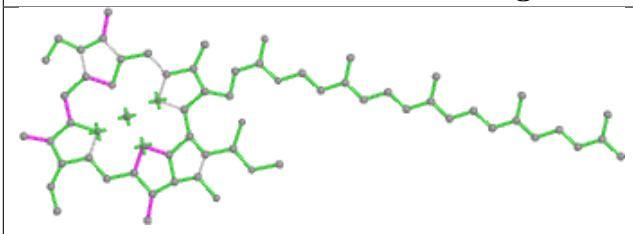


Rings

Ligand CLA A 1130



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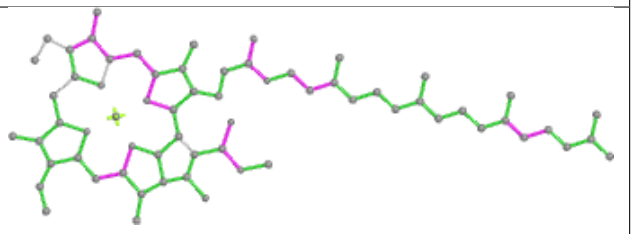
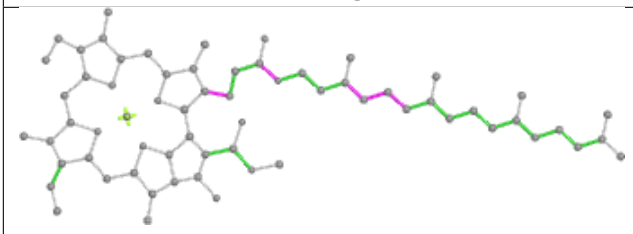


Bond angles



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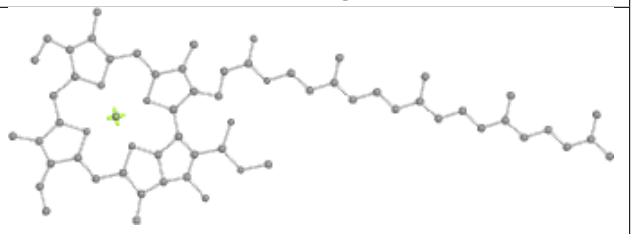
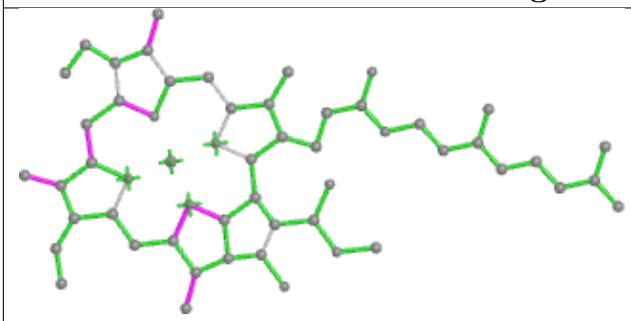


Rings

Ligand CLA s 508



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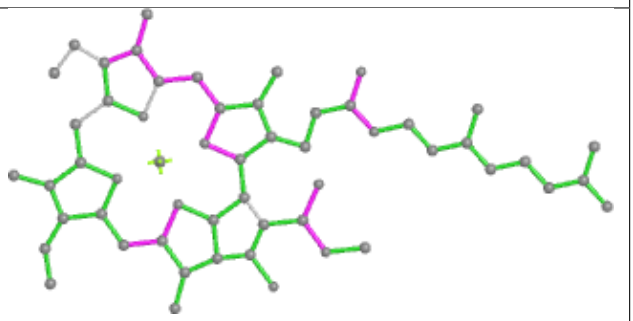
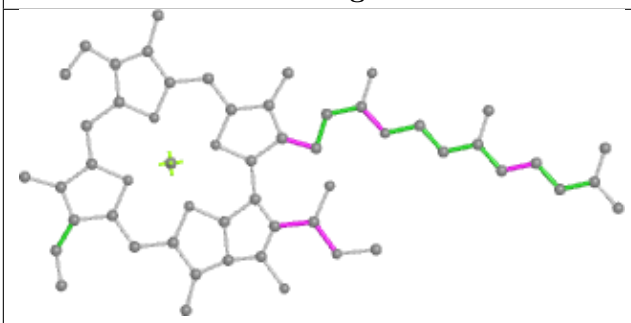


Bond angles



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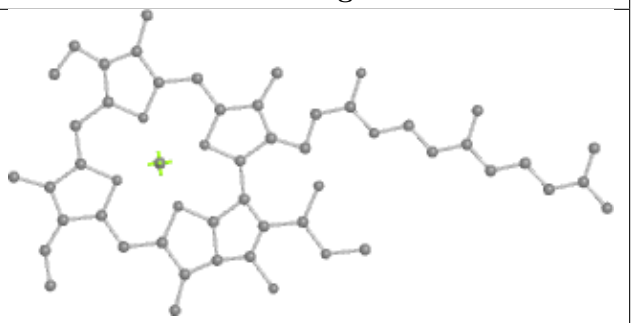
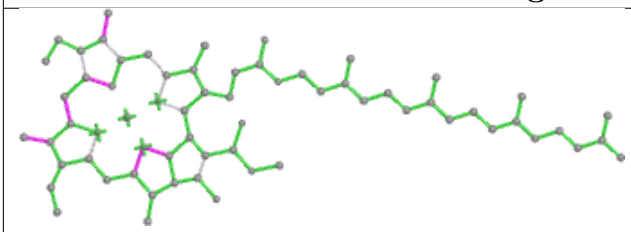


Rings

Ligand CLA u 501



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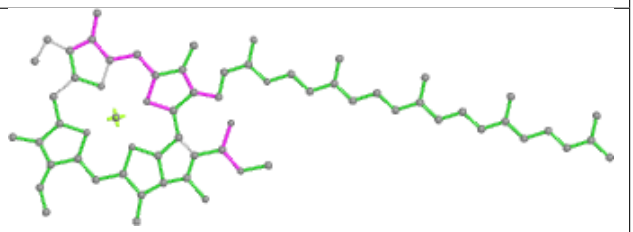
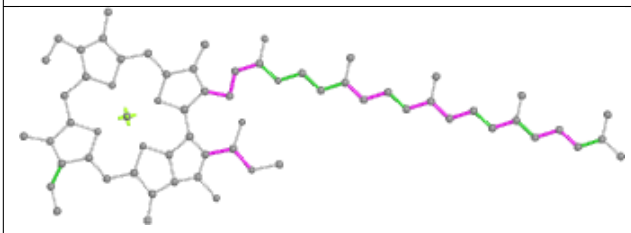


Bond angles



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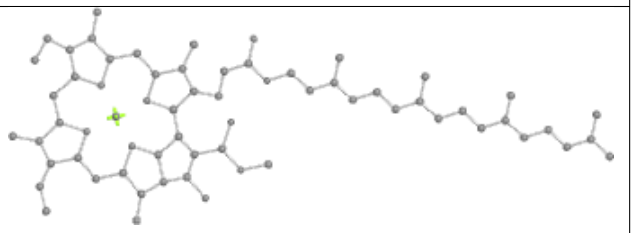
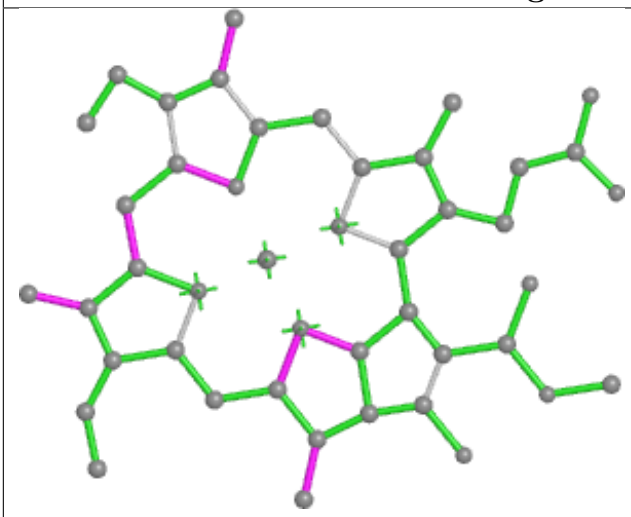


Rings

Ligand CLA u 517



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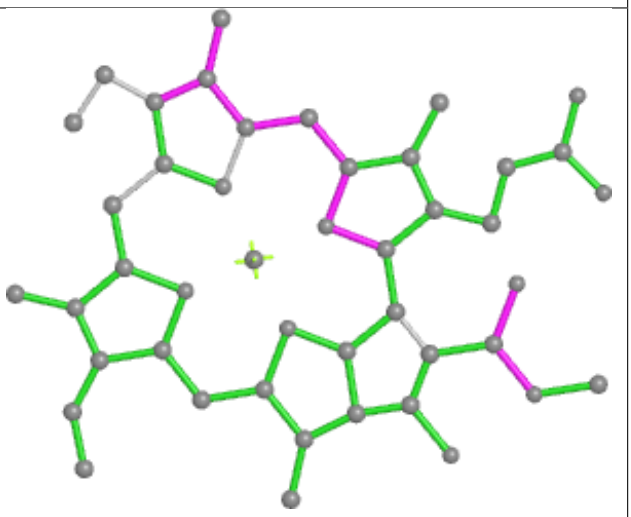
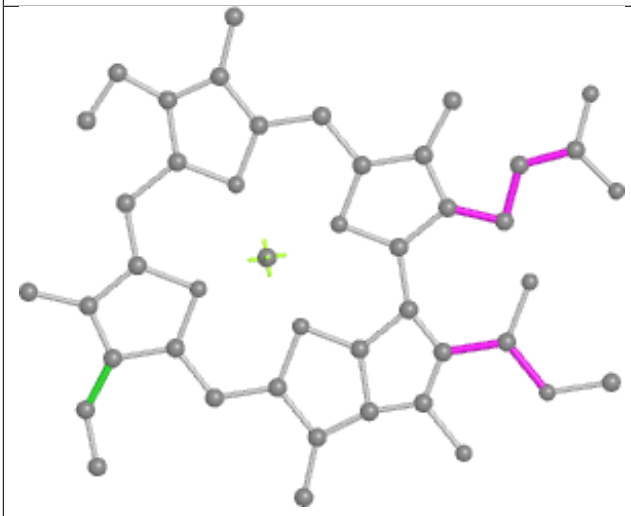


Bond angles



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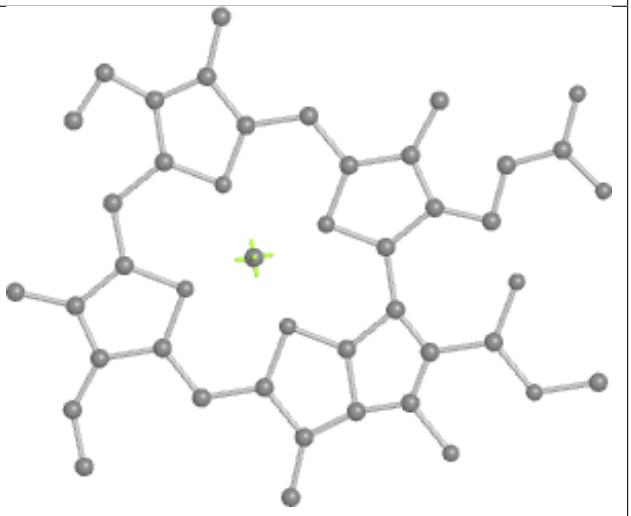
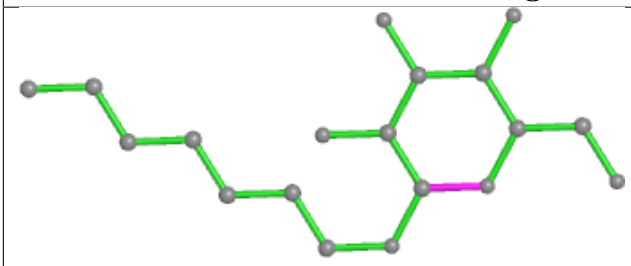


Rings

Ligand LMU 1 902



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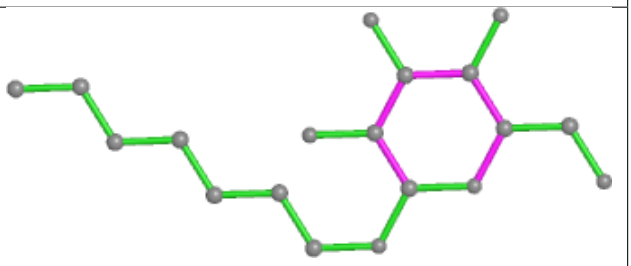
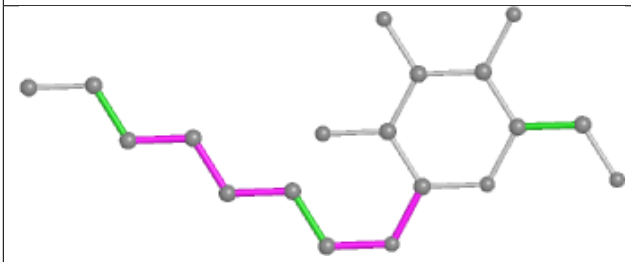


Bond angles



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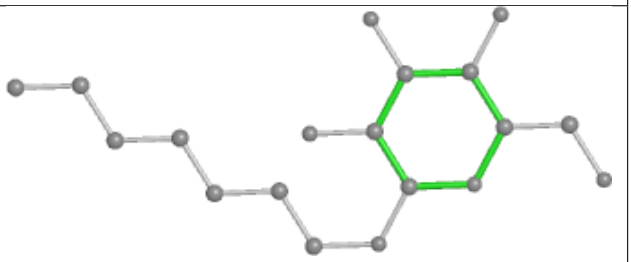
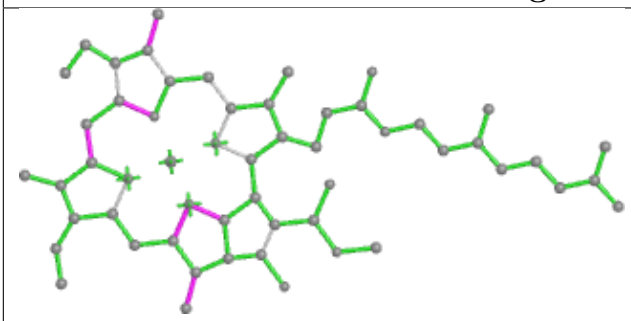


Rings

Ligand CLA c 503



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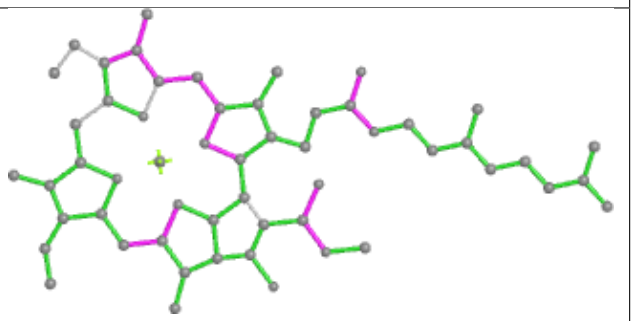
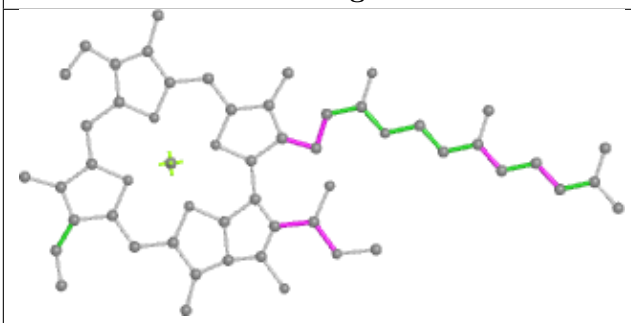


Bond angles



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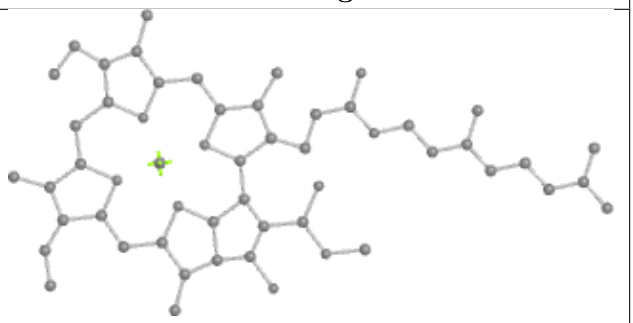
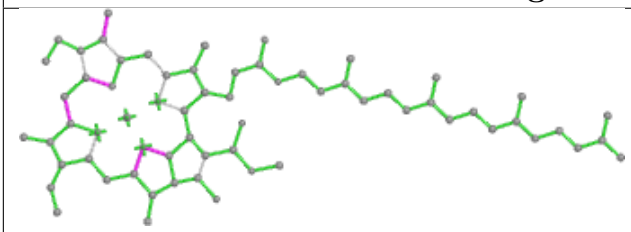


Rings

Ligand CLA q 510



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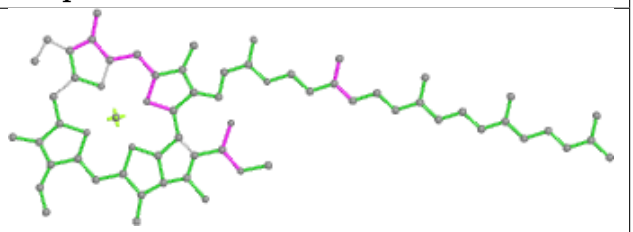
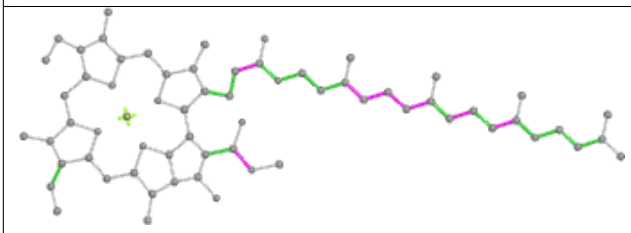


Bond angles



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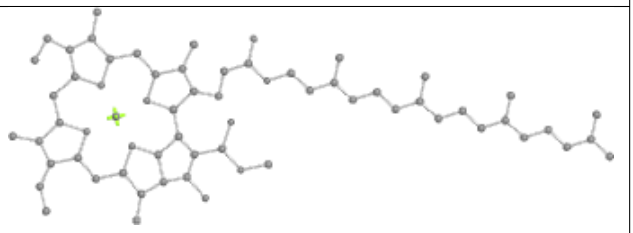
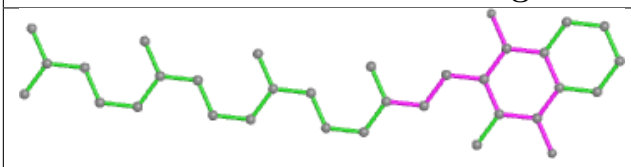


Rings

Ligand PQN H 2002



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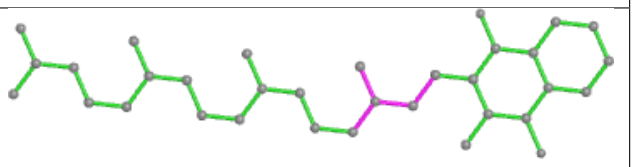
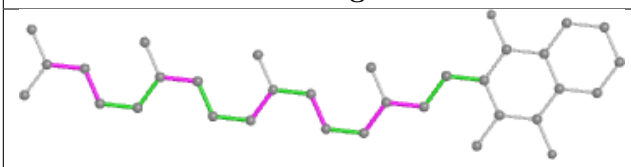


Bond angles



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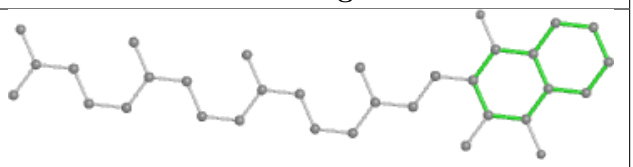
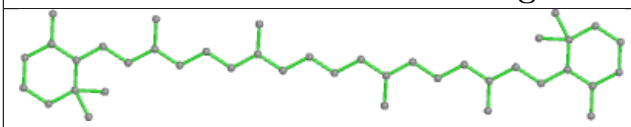


Rings

Ligand BCR e 4011



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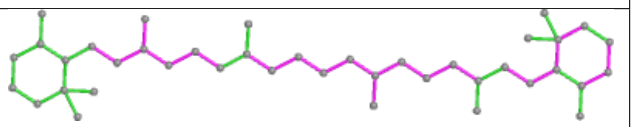
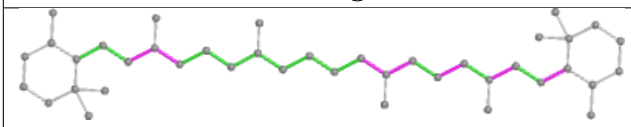


Bond angles



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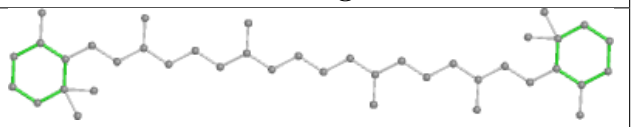
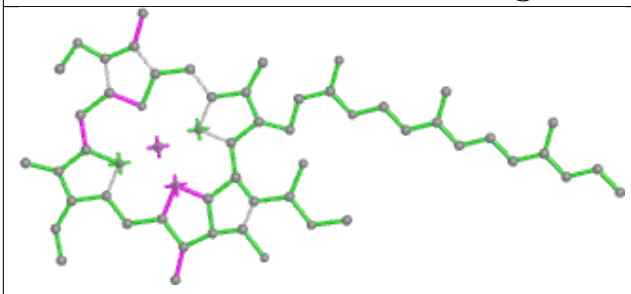
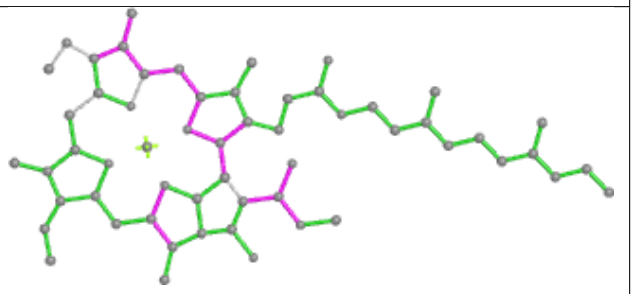


Rings

Ligand CLA H 1217



Bond lengths



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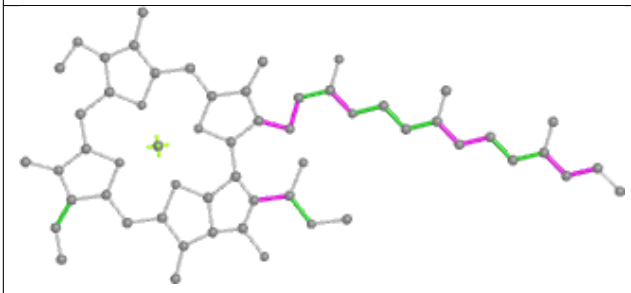
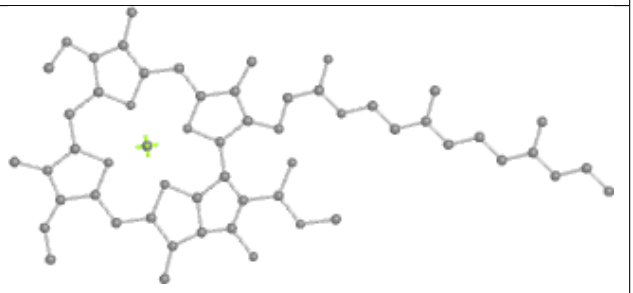
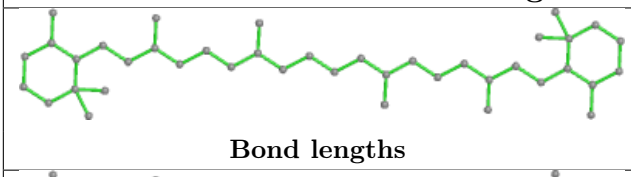


Torsions



Rings

Ligand BCR q 523



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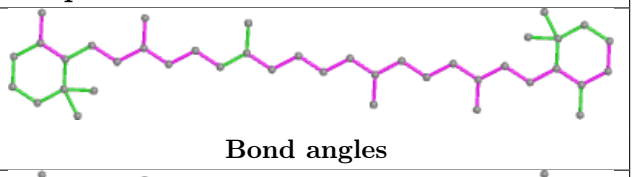

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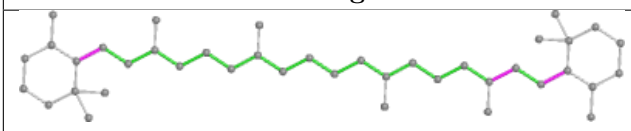

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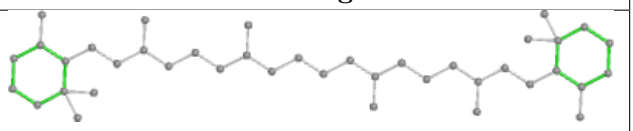
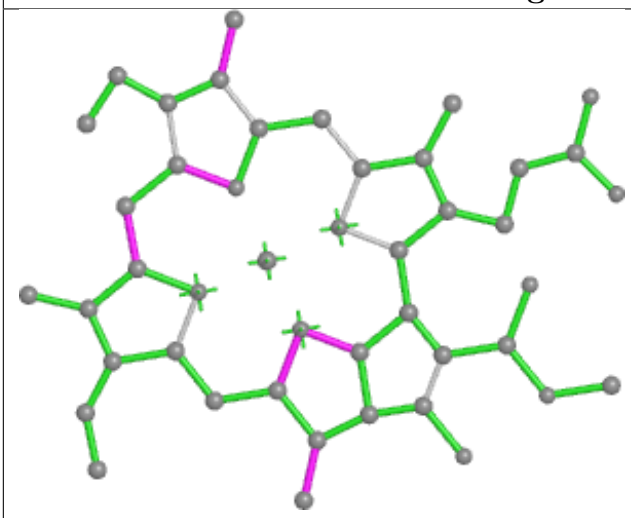


Rings

Ligand CLA d 511



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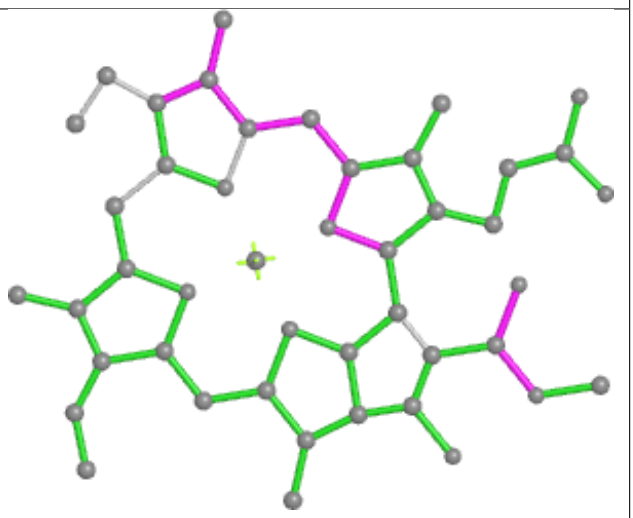

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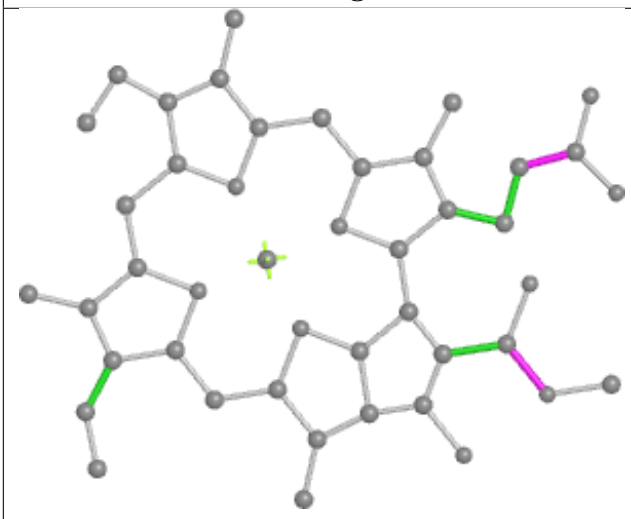

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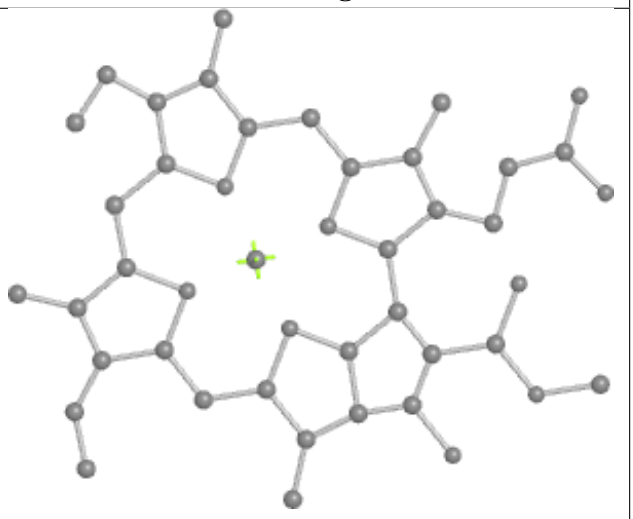
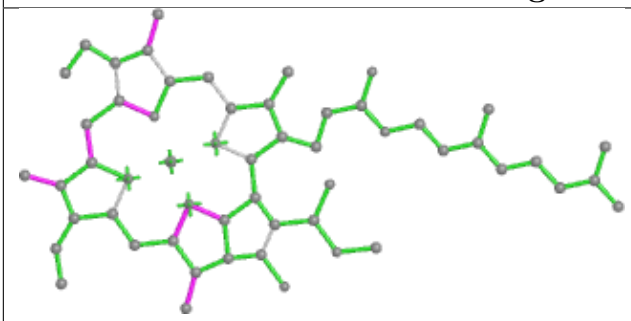


Rings

Ligand CLA a 518



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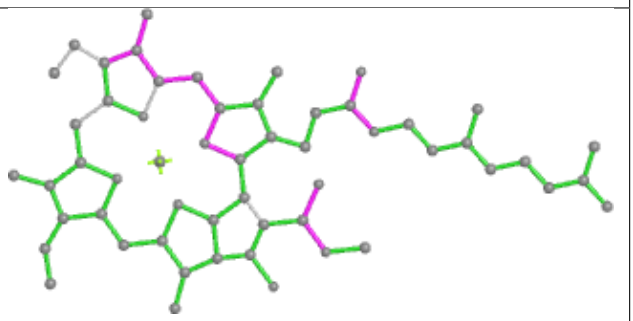

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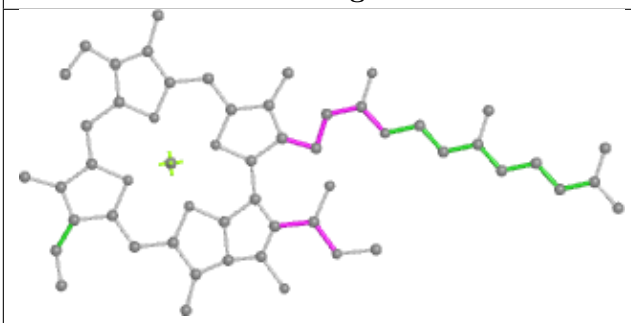

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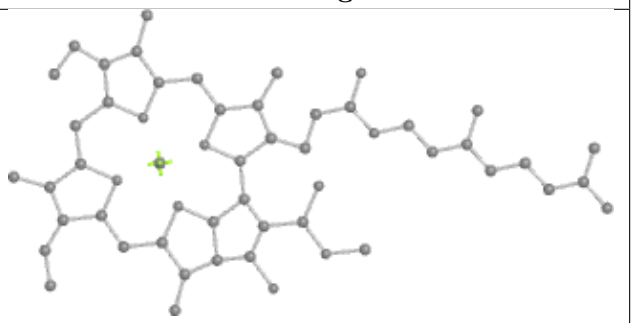
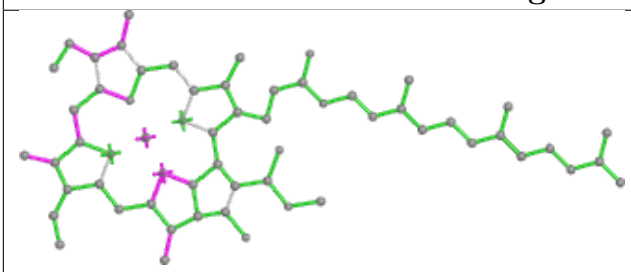


Rings

Ligand CLA 1 518



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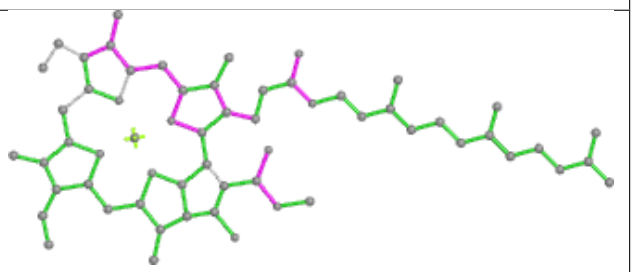

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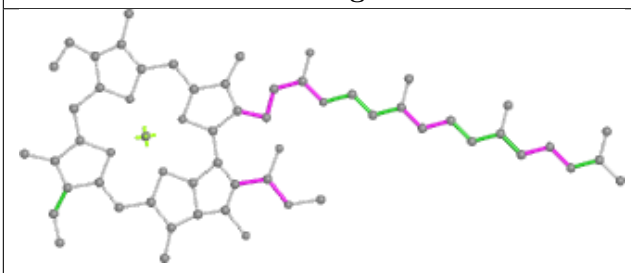

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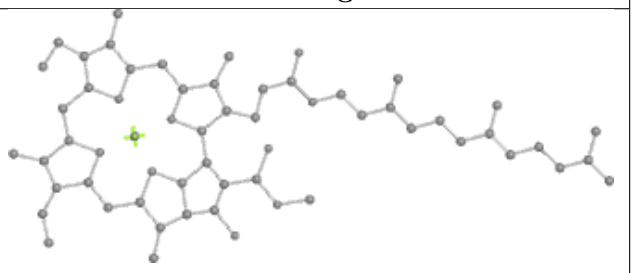
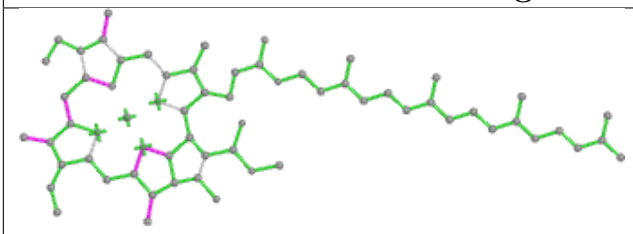


Rings

Ligand CLA V 1502



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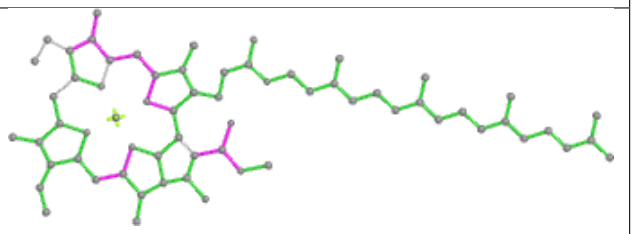
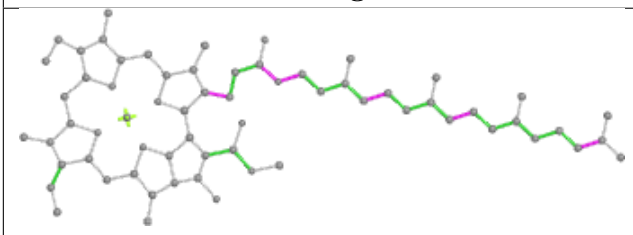


Bond angles



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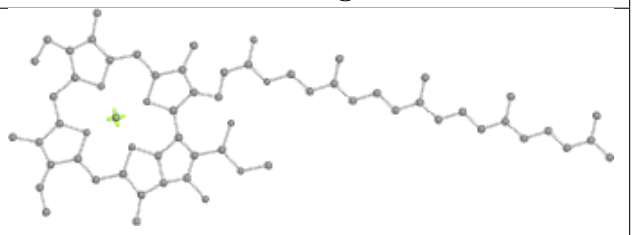
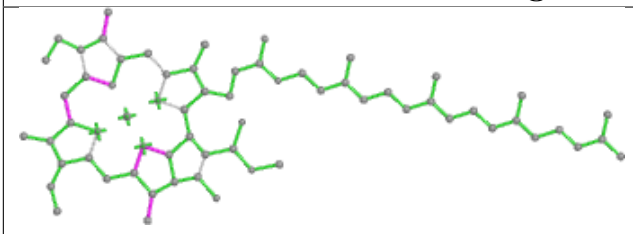


Rings

Ligand CLA v 505



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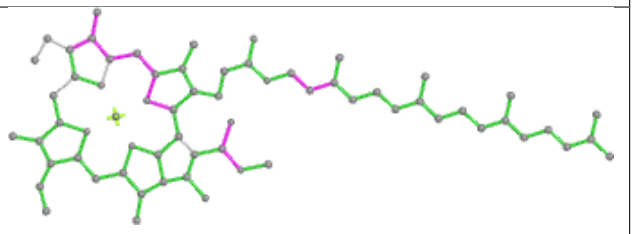

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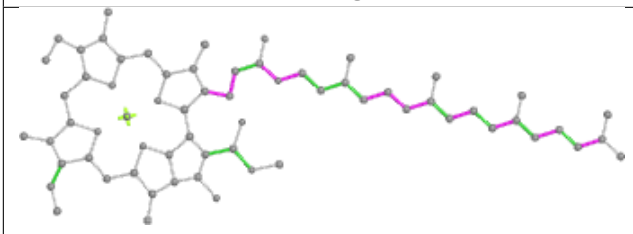

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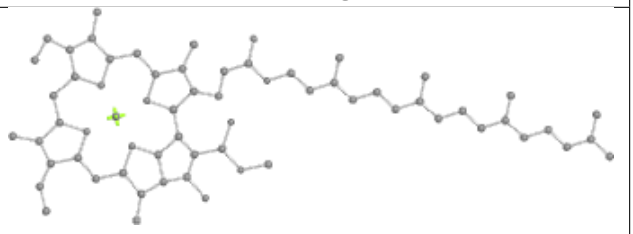
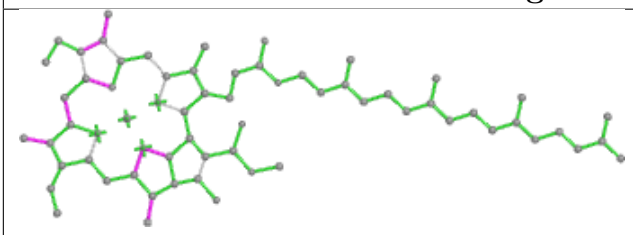


Rings

Ligand CLA Z 513



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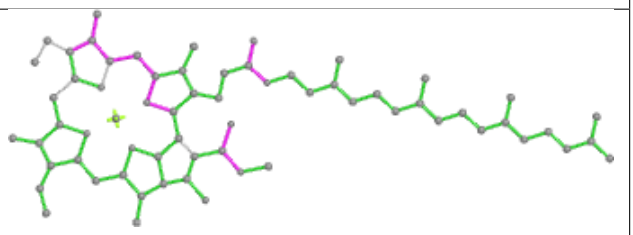
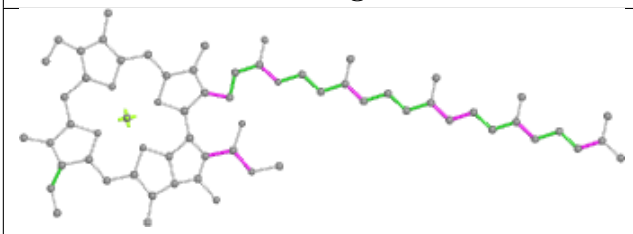


Bond angles



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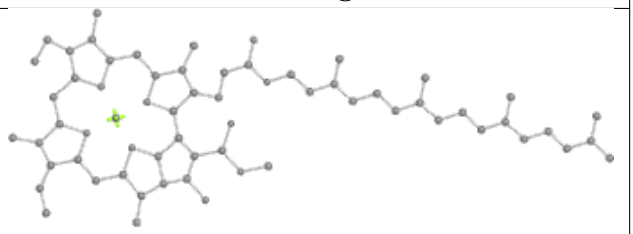
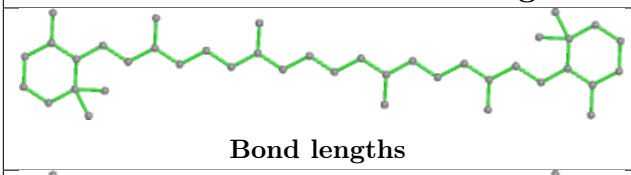


Rings

Ligand BCR e 4001



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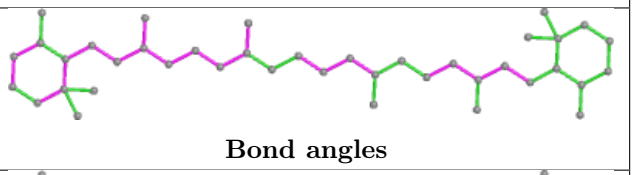
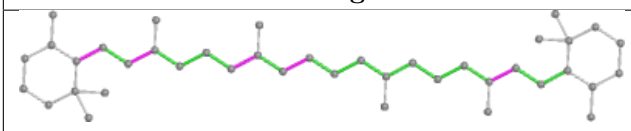


Bond angles



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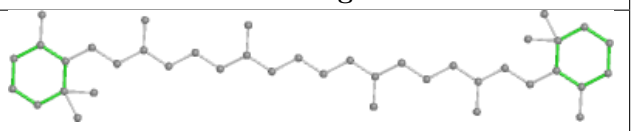
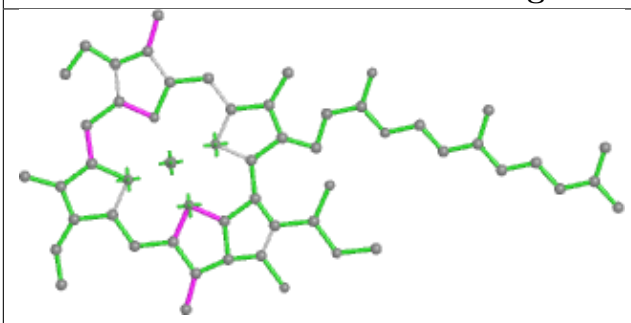


Rings

Ligand CLA b 503



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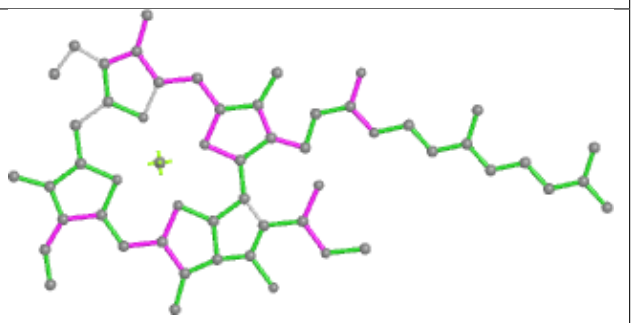

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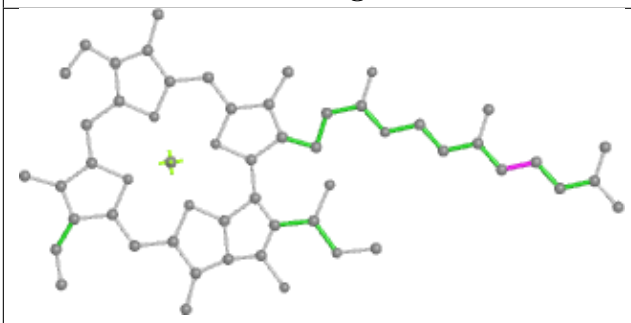

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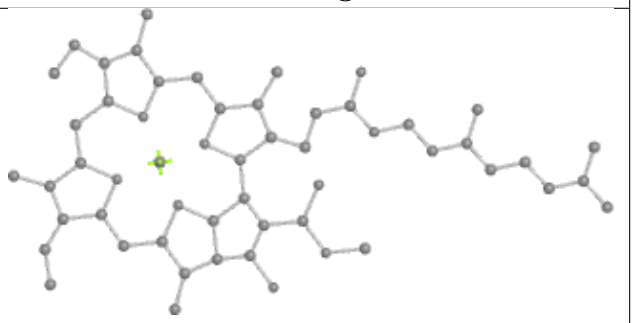
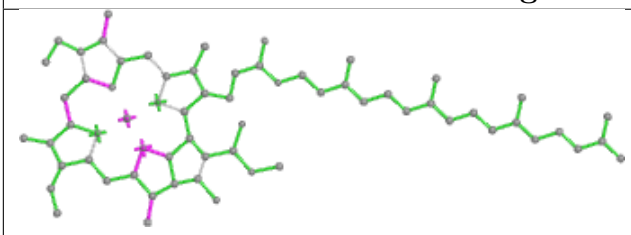


Rings

Ligand CLA e 1139



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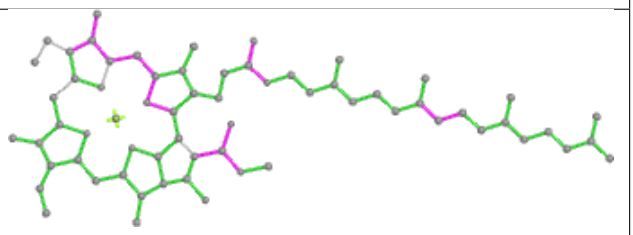
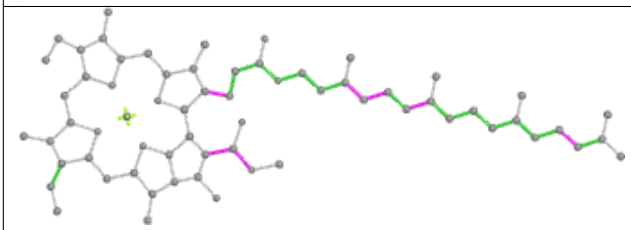


Bond angles



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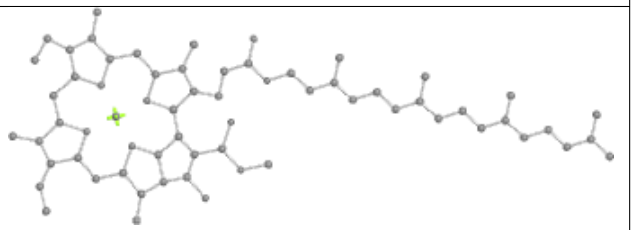
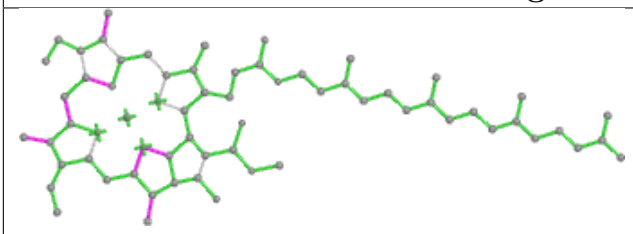


Rings

Ligand CLA u 509



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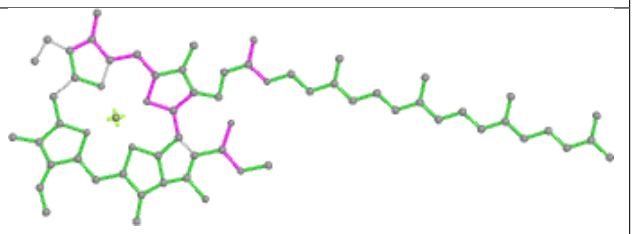

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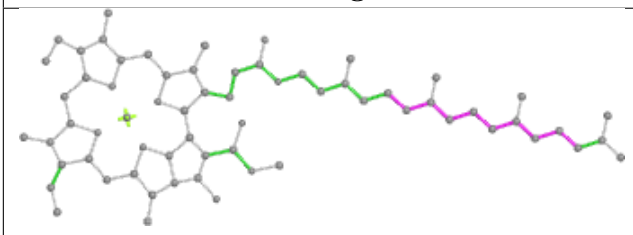

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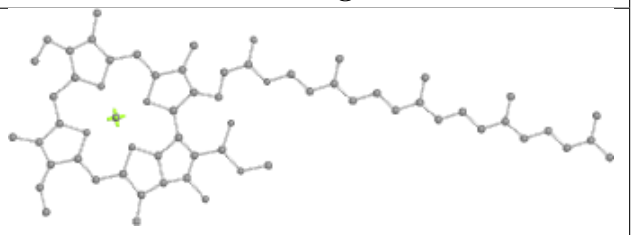
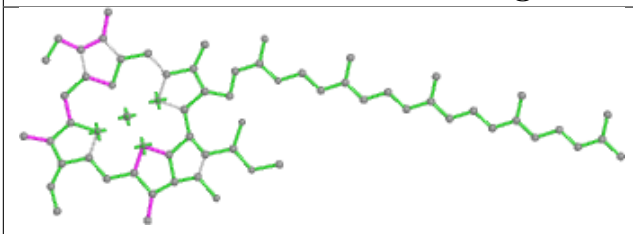


Rings

Ligand CLA G 1131



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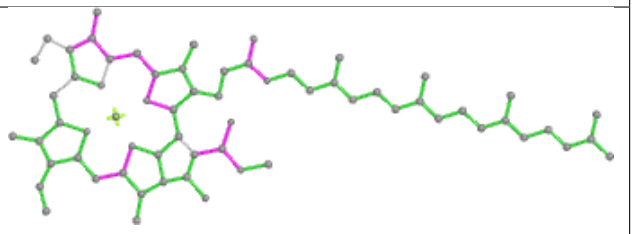
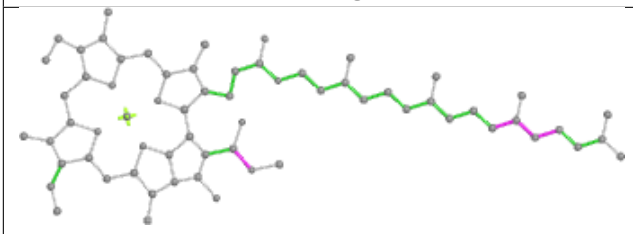


Bond angles



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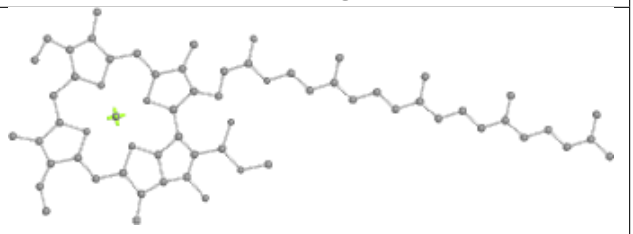
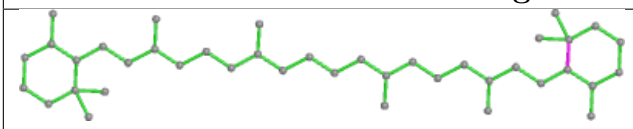


Rings

Ligand BCR A 4002



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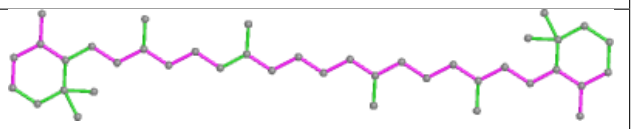
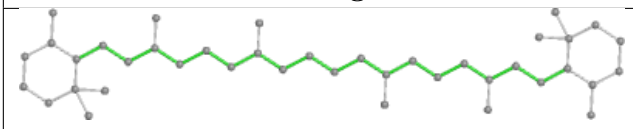


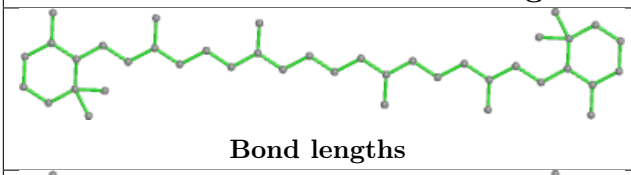
Bond angles



Torsions

Rings

Ligand BCR d 521



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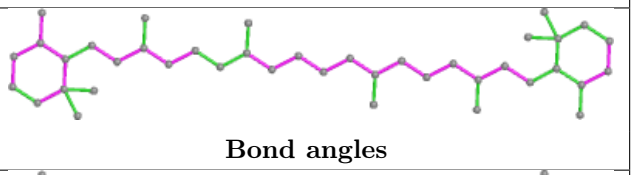
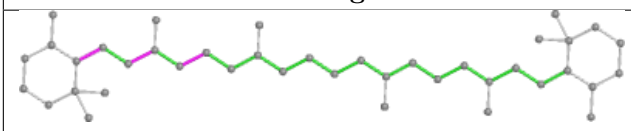


Bond angles



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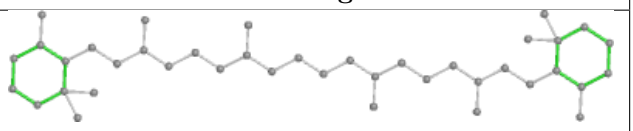
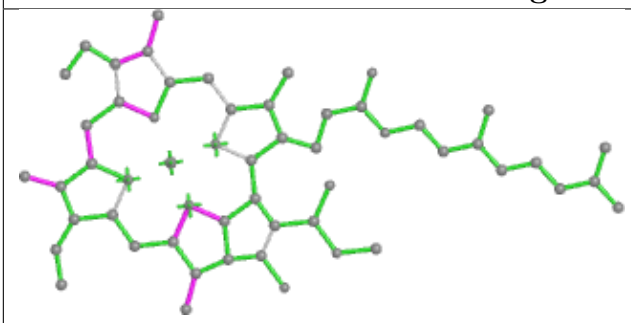
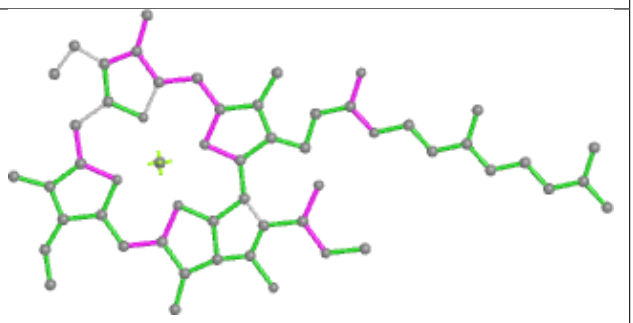


Rings

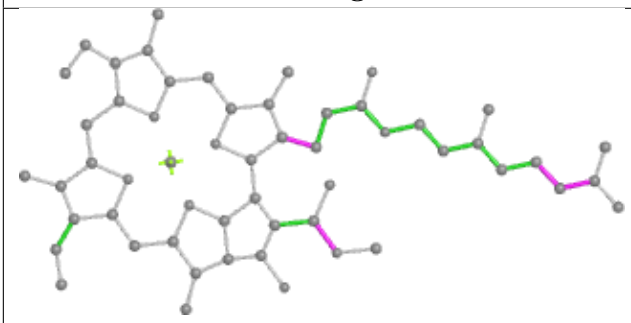
Ligand CLA r 508



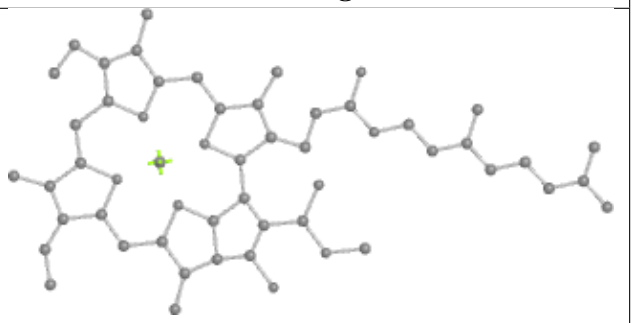
Bond lengths



Bond angles

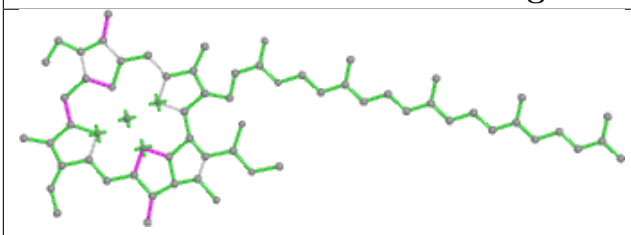


Torsions



Rings

Ligand CLA d 505



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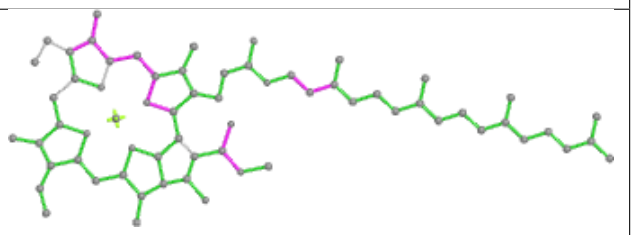
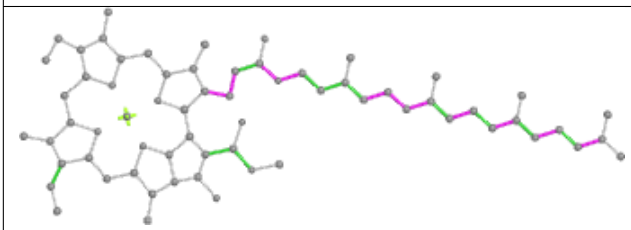
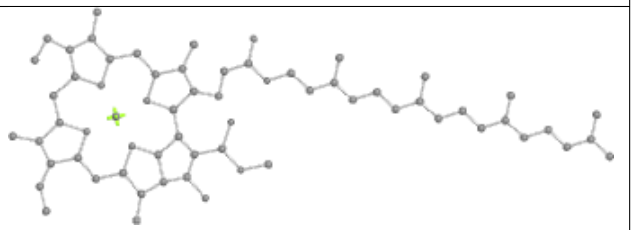


Bond angles

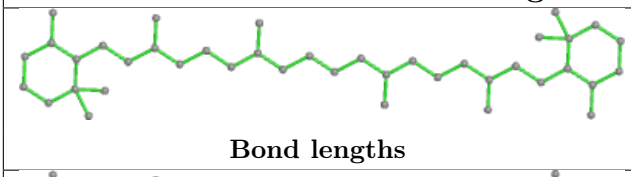


Torsions



Rings

Ligand BCR a 524



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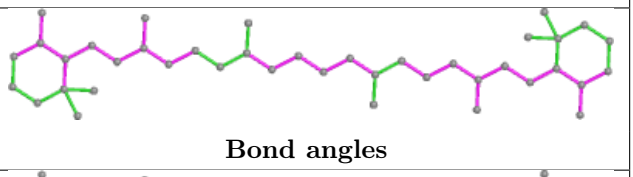
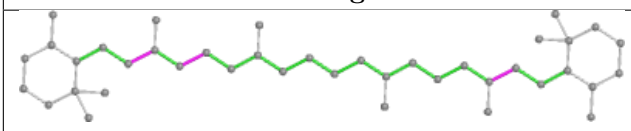


Bond angles



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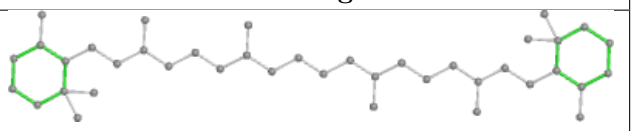
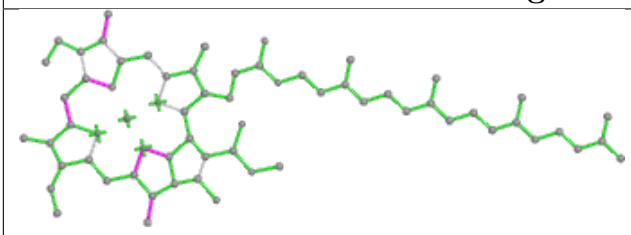


Rings

Ligand CLA q 505



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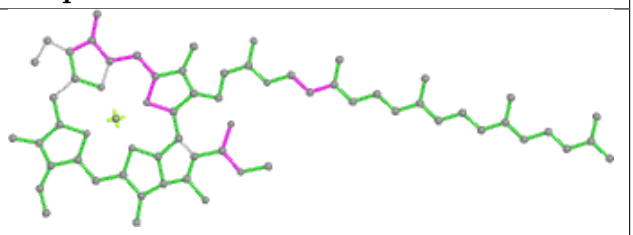

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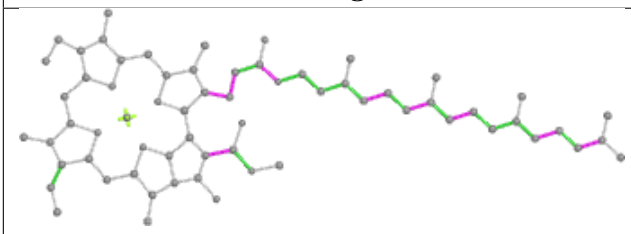

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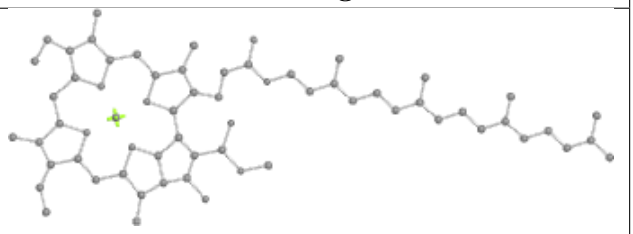
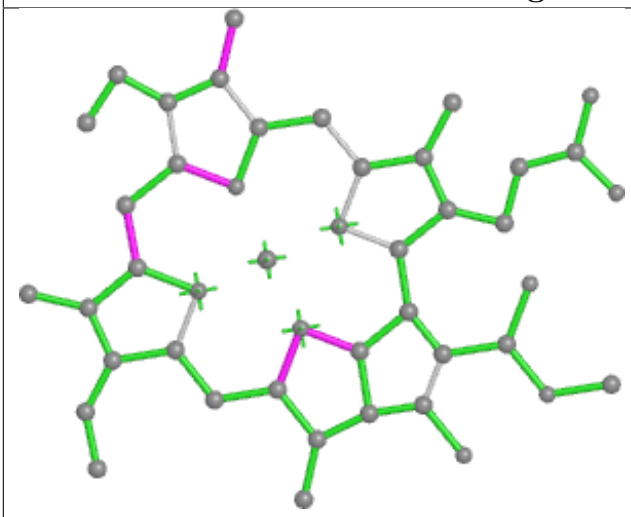


Rings

Ligand CLA d 510



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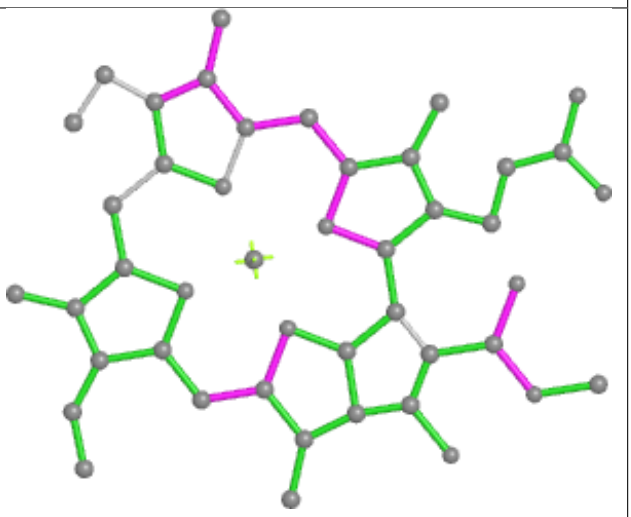
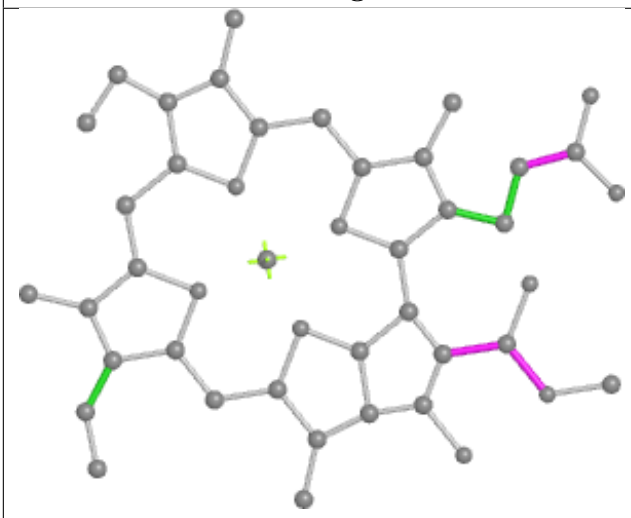


Bond angles



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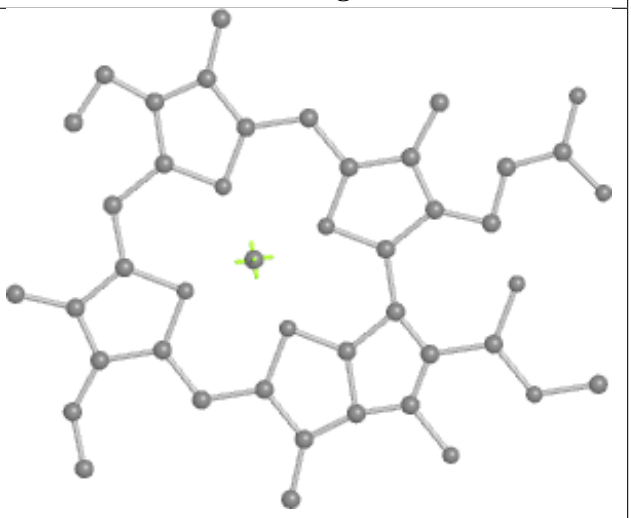
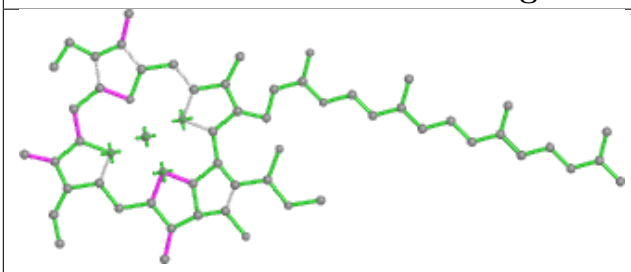


Rings

Ligand CLA e 1115



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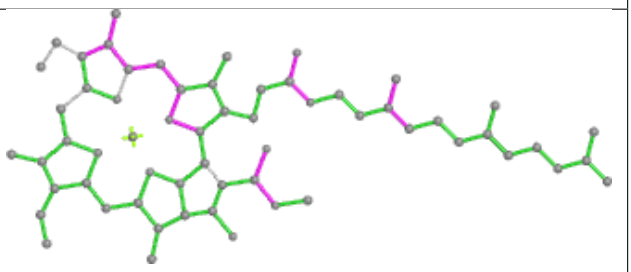
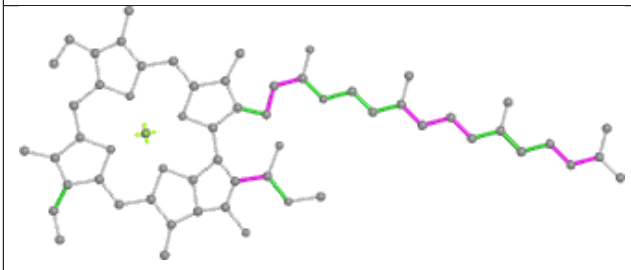


Bond angles



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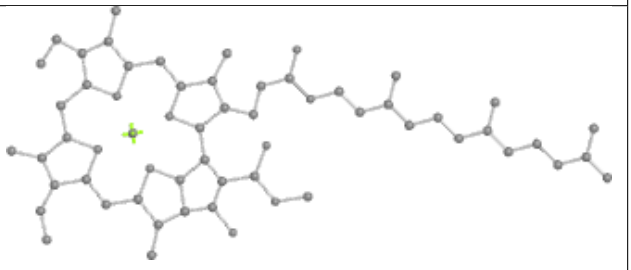
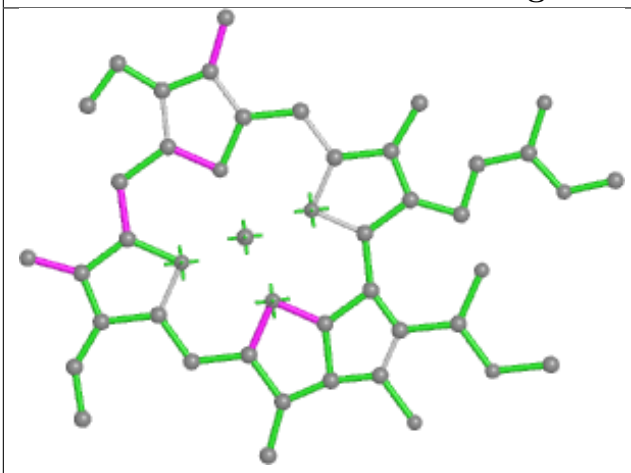


Rings

Ligand CLA v 519



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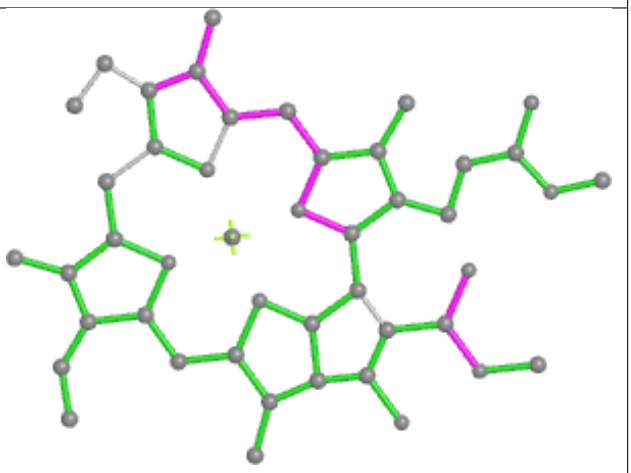
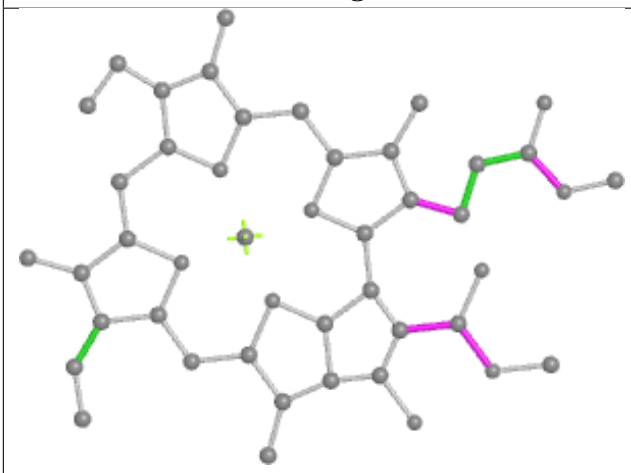


Bond angles



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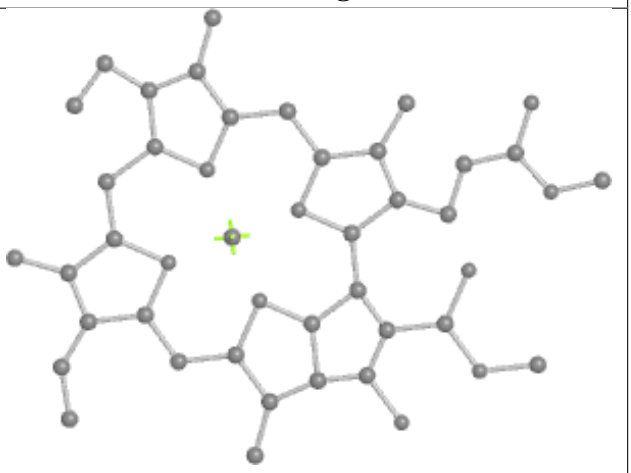
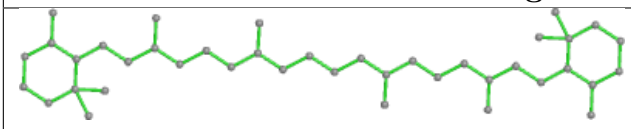


Rings

Ligand BCR b 524



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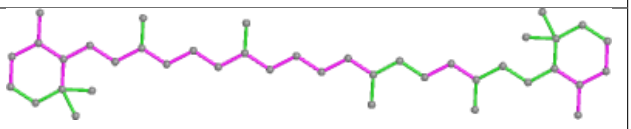

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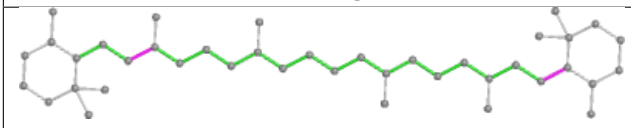

Torsions

Rings

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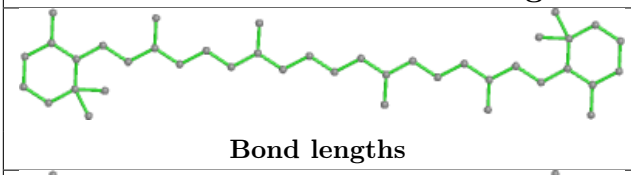

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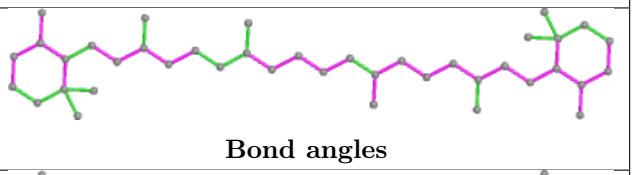
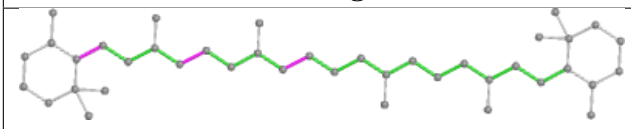


Bond angles



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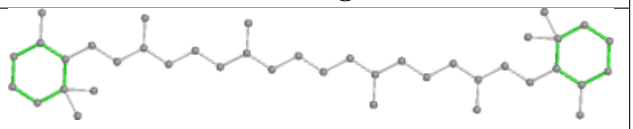
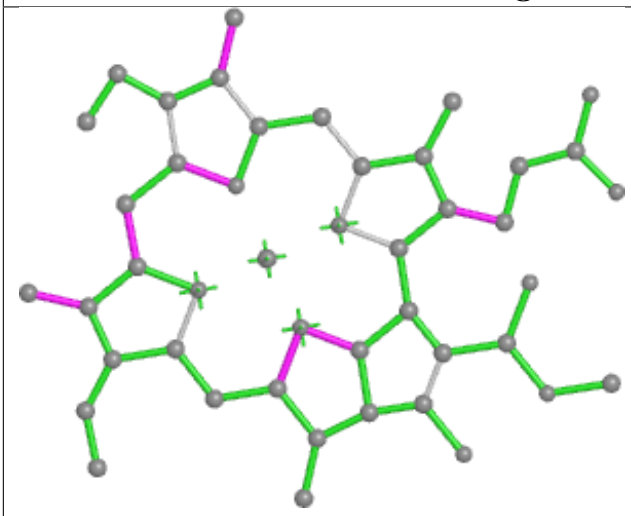


Rings

Ligand CLA A 1801



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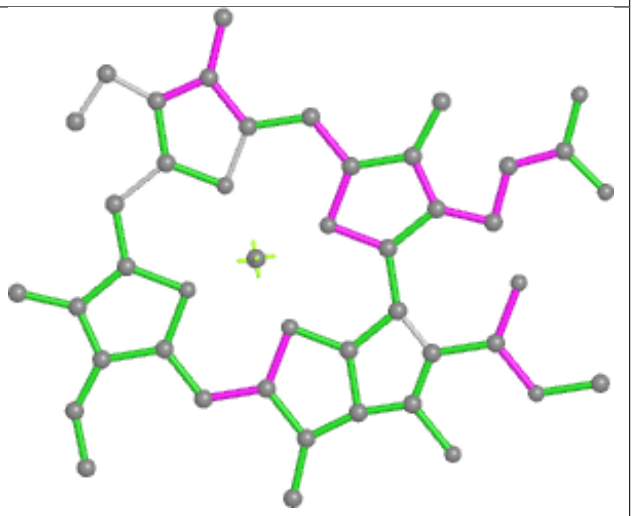
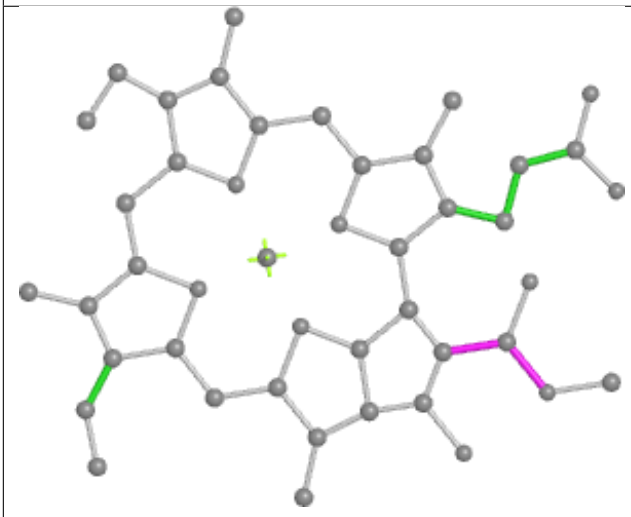


Bond angles



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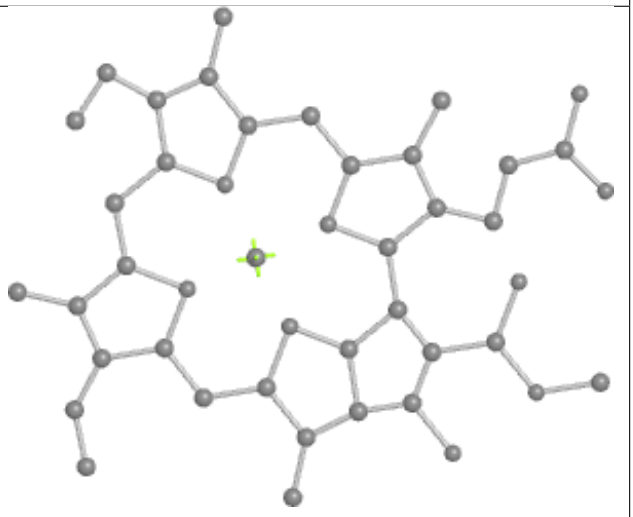
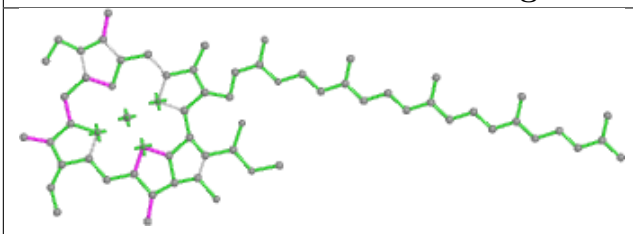


Rings

Ligand CLA e 1126



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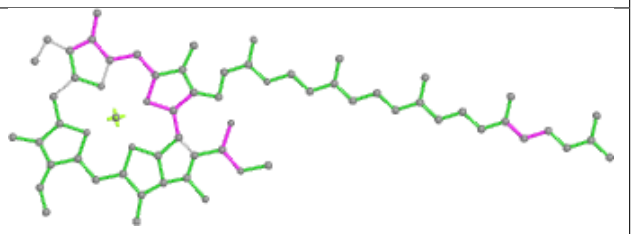
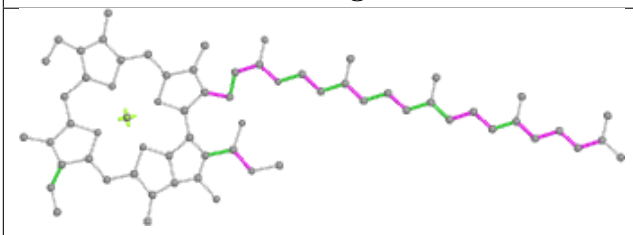


Bond angles



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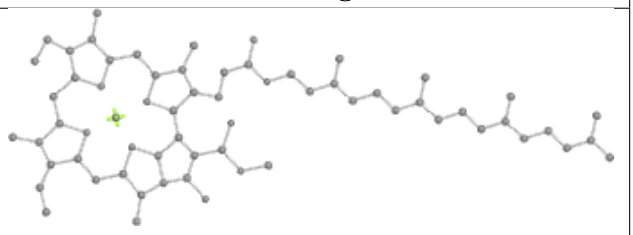
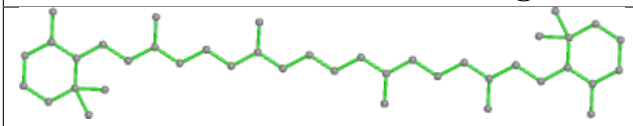


Rings

Ligand BCR F 4016



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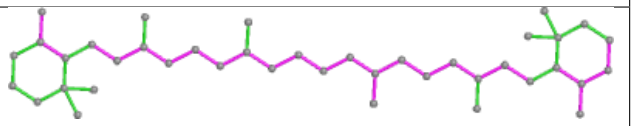
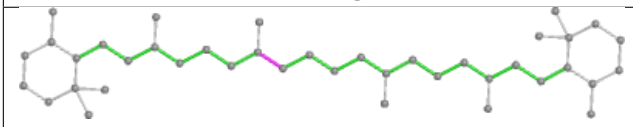


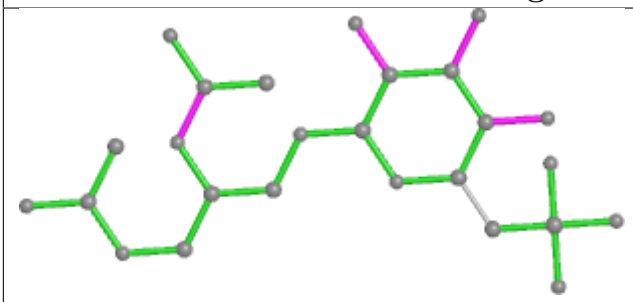
Bond angles



Torsions

Rings

Ligand SQD b 822



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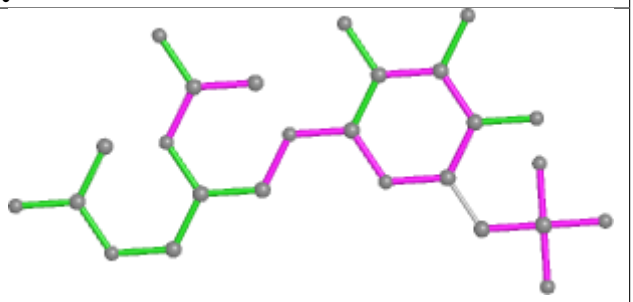
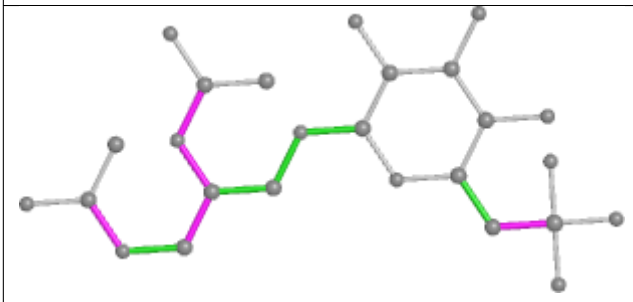
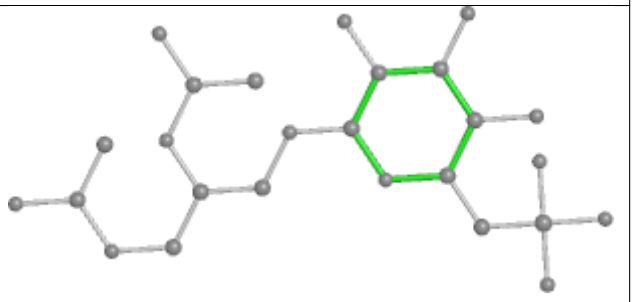


Bond angles

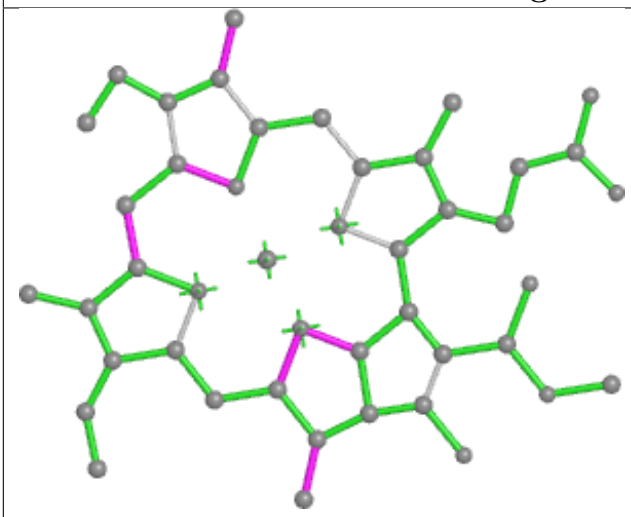


Torsions



Rings

Ligand CLA t 507



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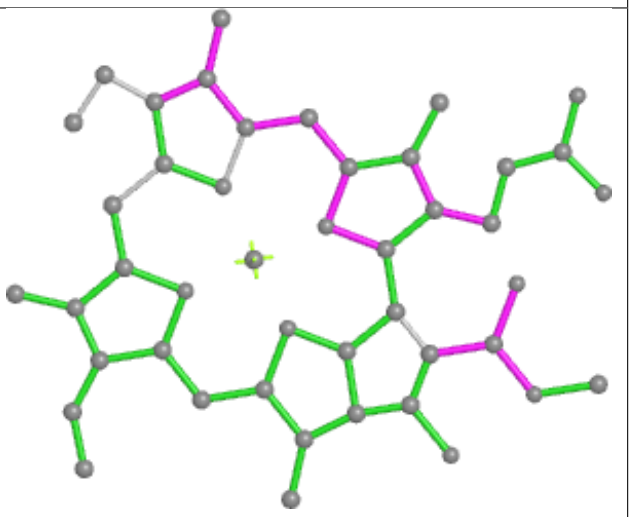
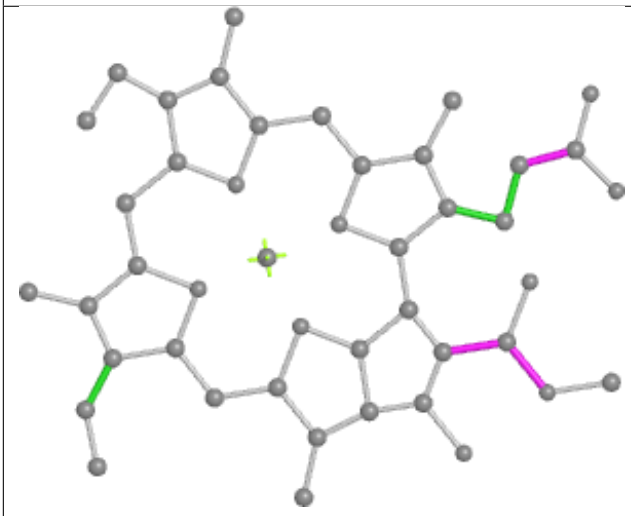


Bond angles



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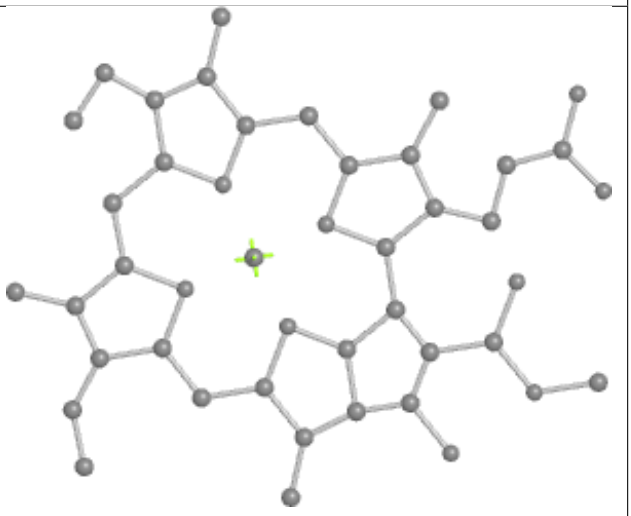
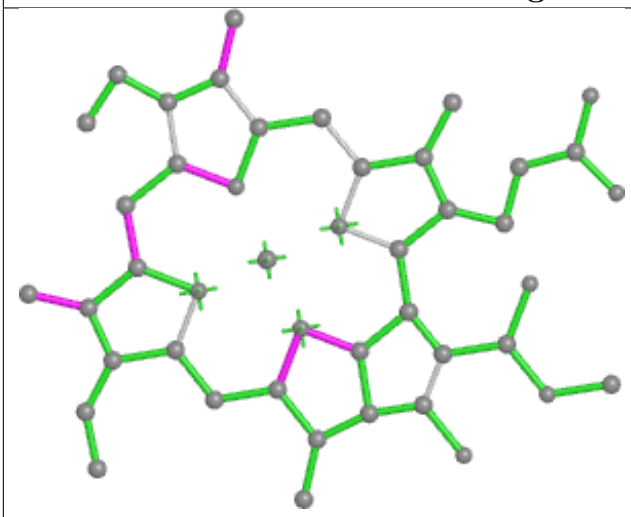


Rings

Ligand CLA d 506



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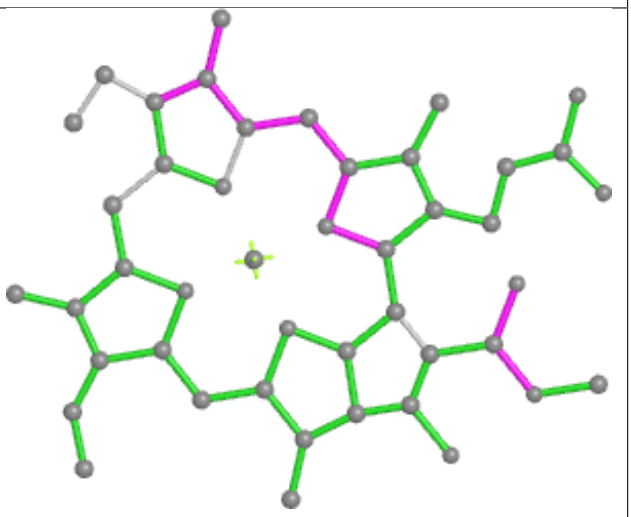
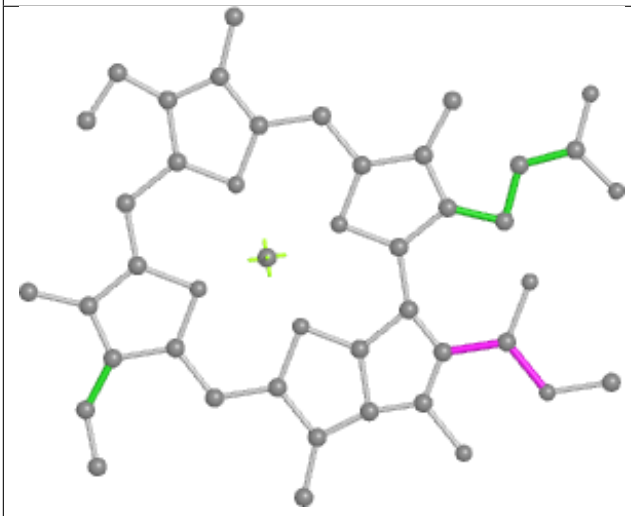


Bond angles



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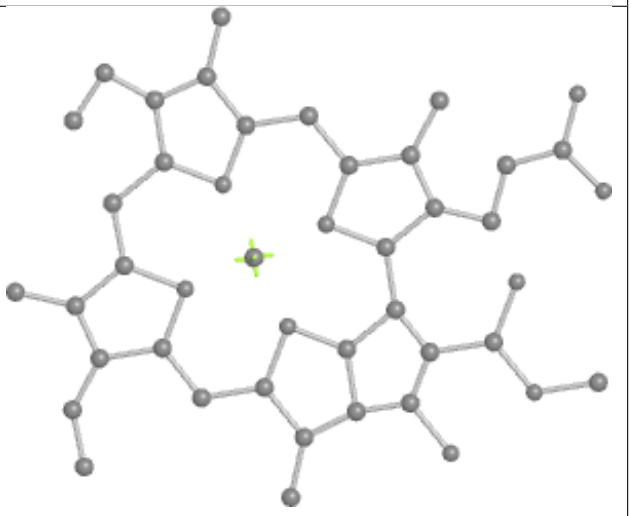
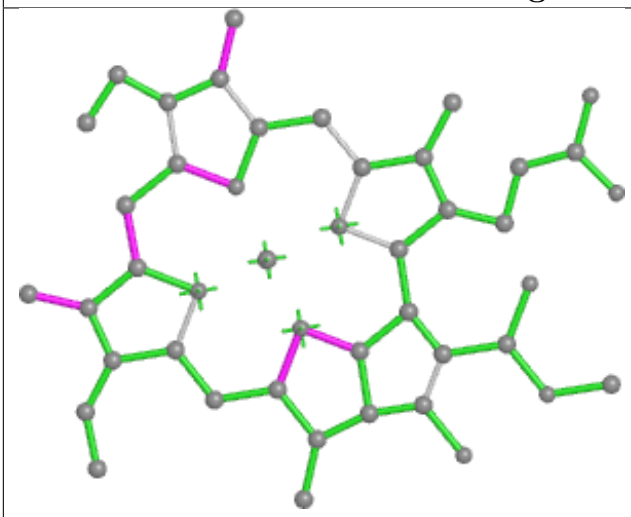
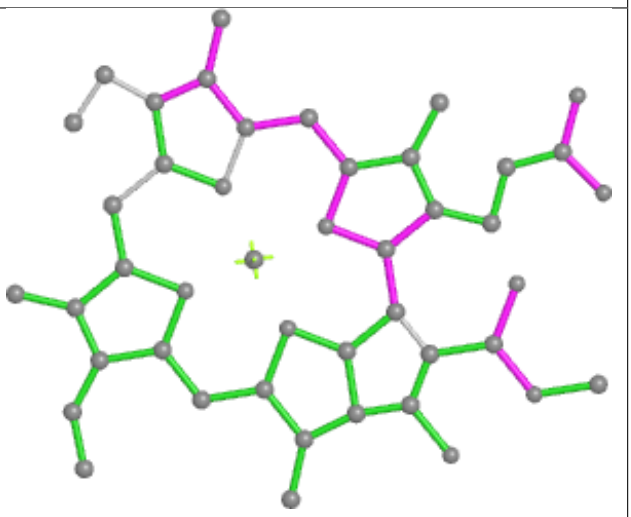


Rings

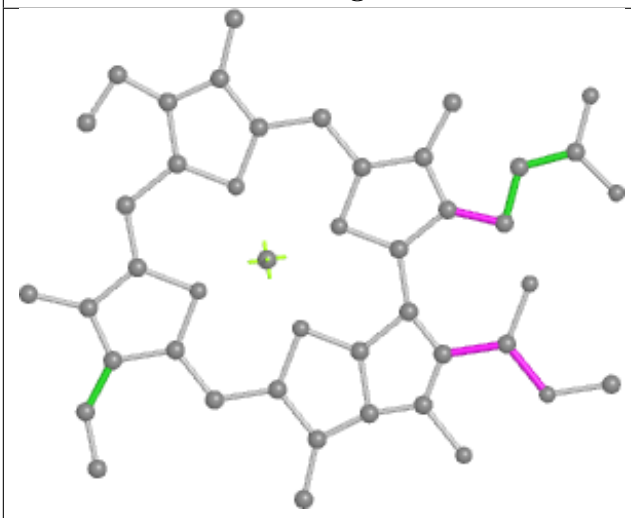
Ligand CLA 4 517



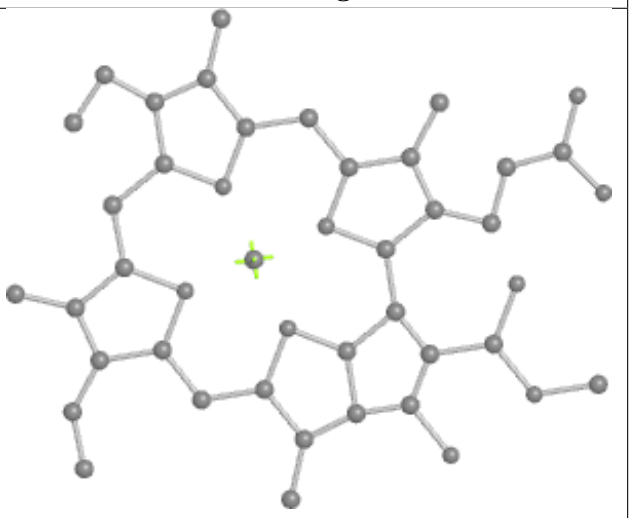
Bond lengths



Bond angles

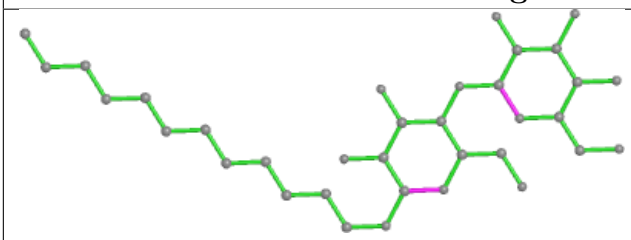


Torsions



Rings

Ligand LMU G 1848



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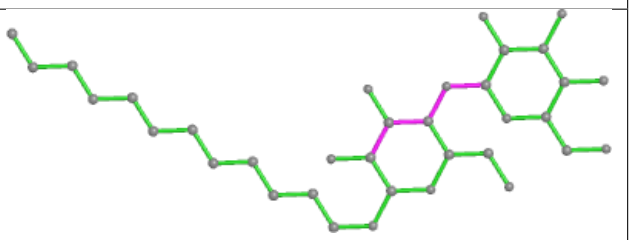

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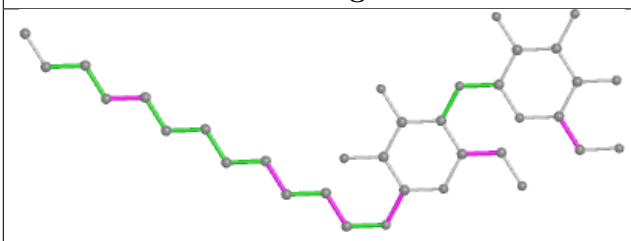

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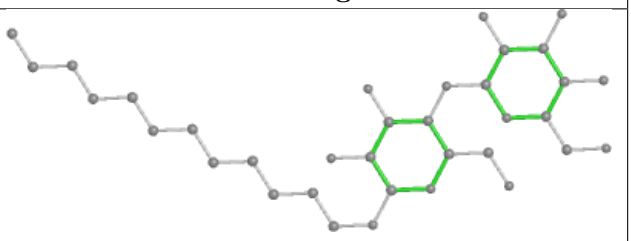
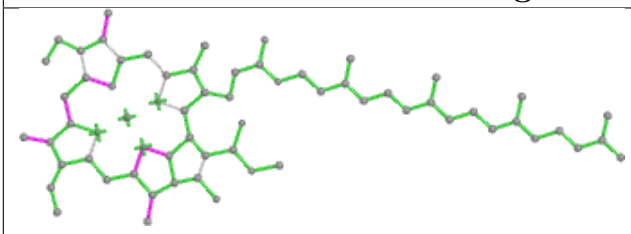


Rings

Ligand CLA G 1109



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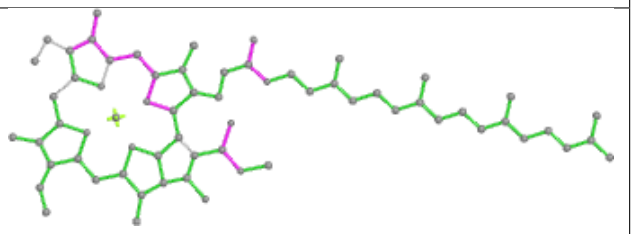

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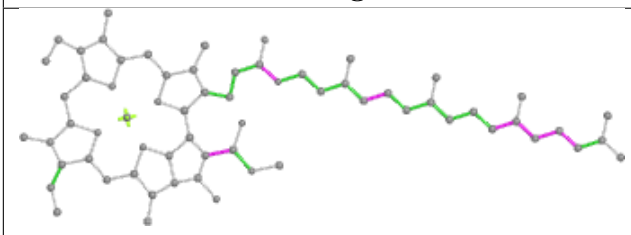

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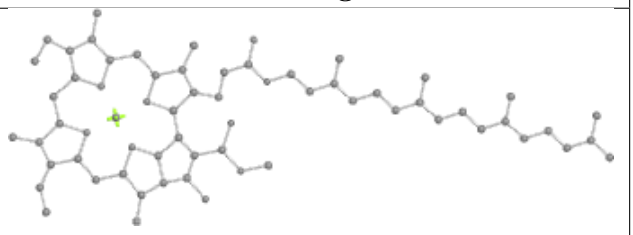
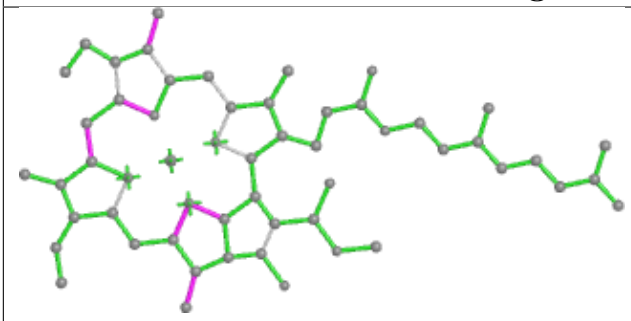


Rings

Ligand CLA 5 518



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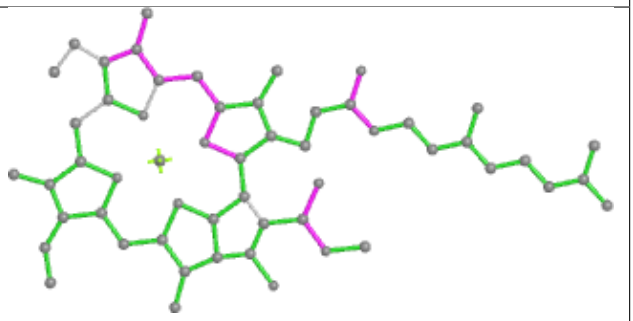

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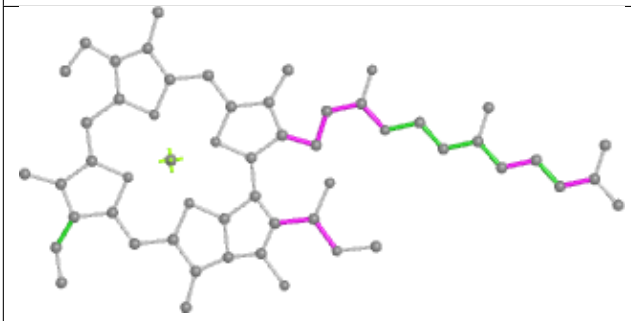

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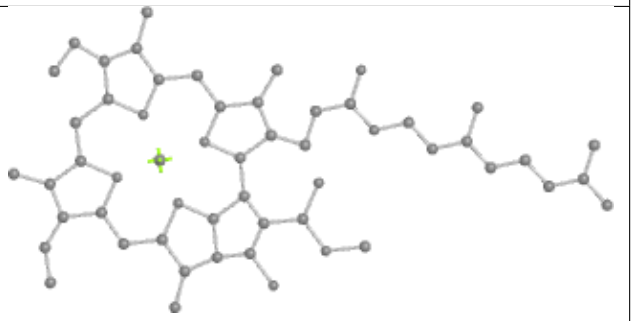
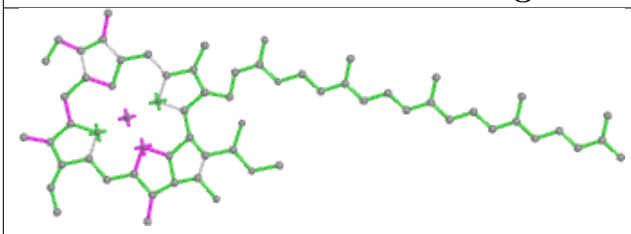


Rings

Ligand CLA H 1225



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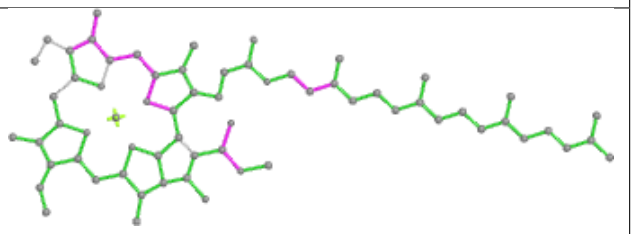

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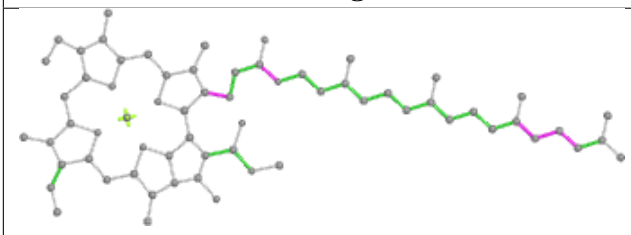

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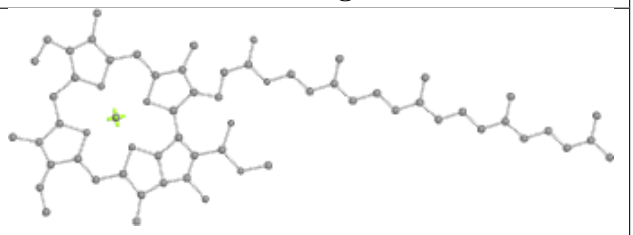
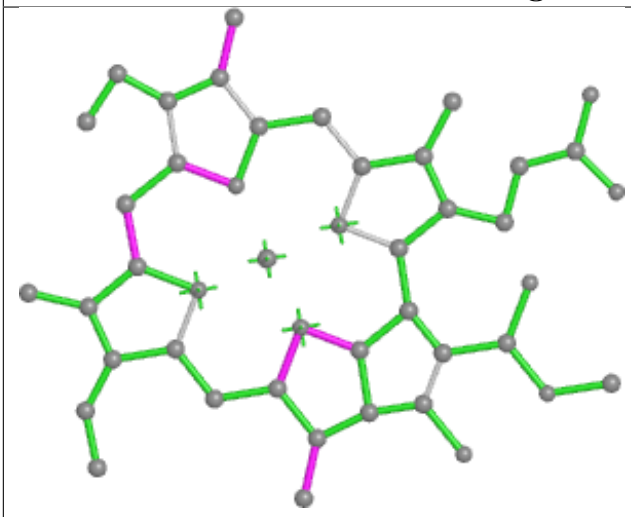


Rings

Ligand CLA d 512



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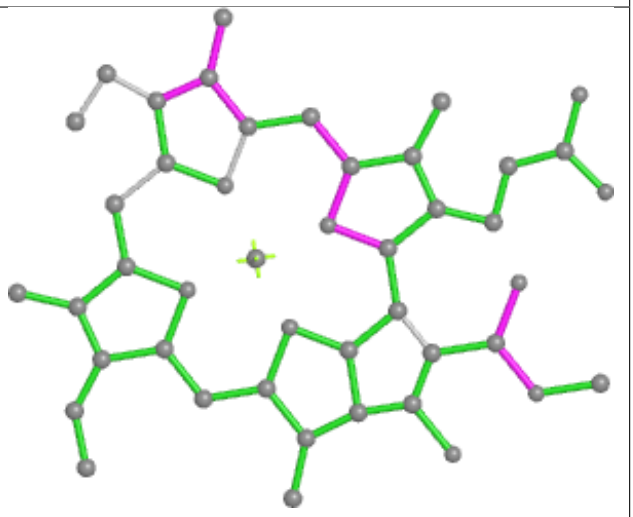

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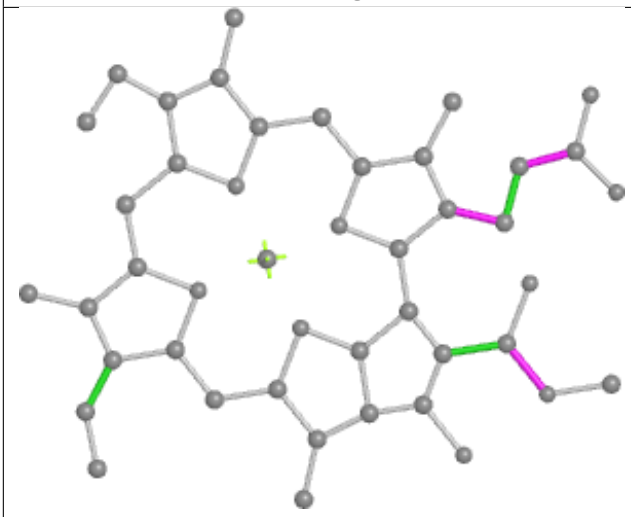

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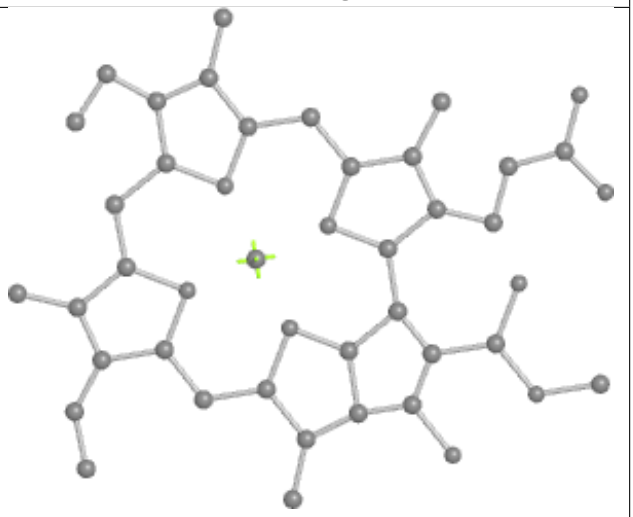
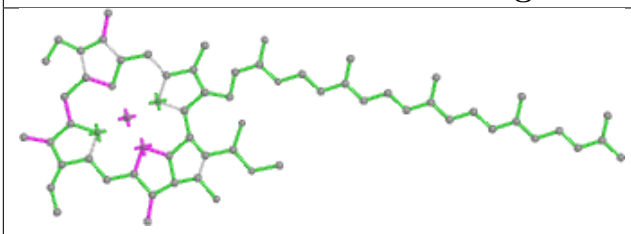


Rings

Ligand CLA A 1013



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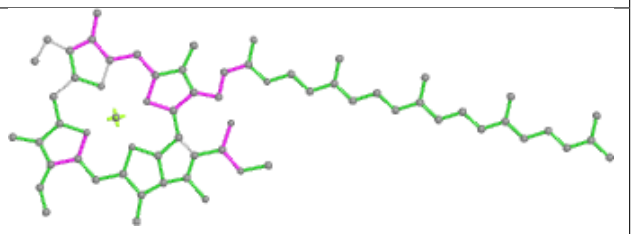

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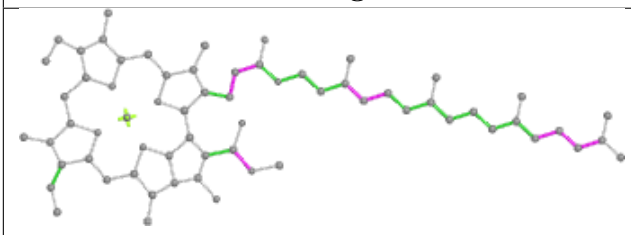

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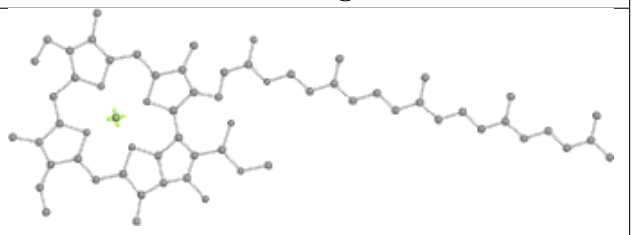
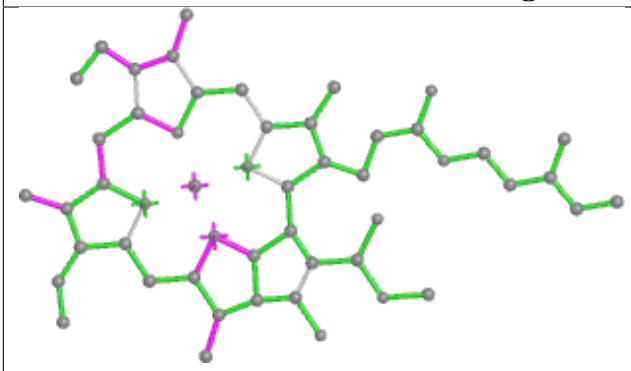


Rings

Ligand CLA e 1129



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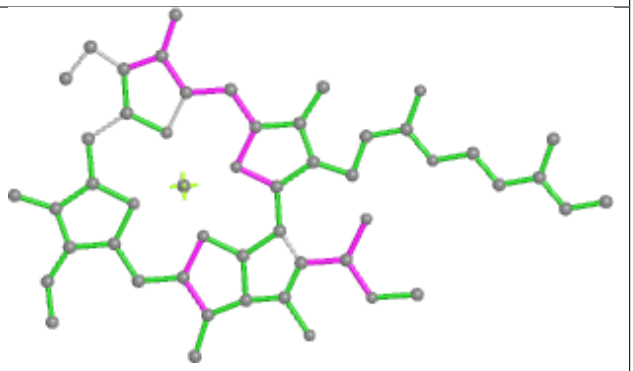

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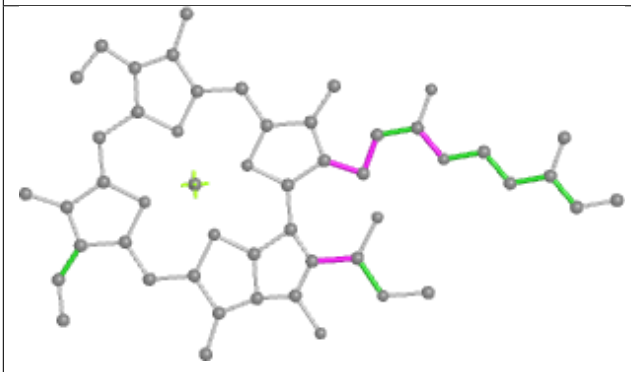

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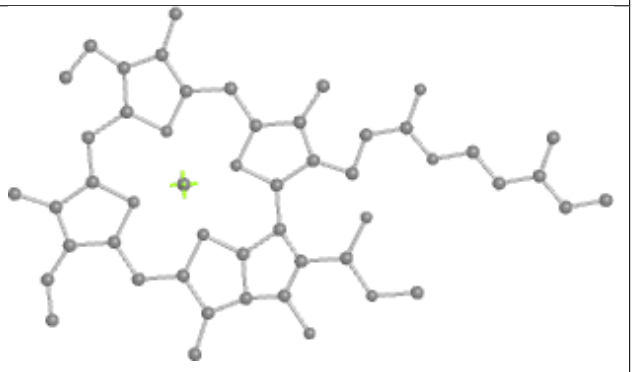
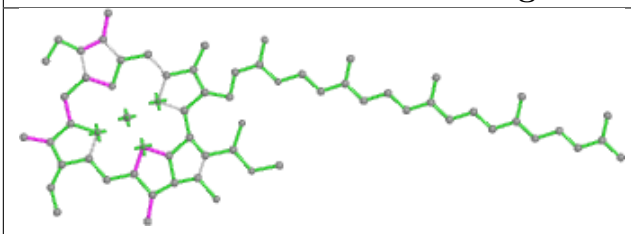


Rings

Ligand CLA n 1501



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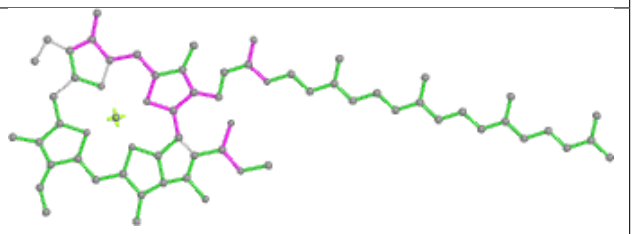
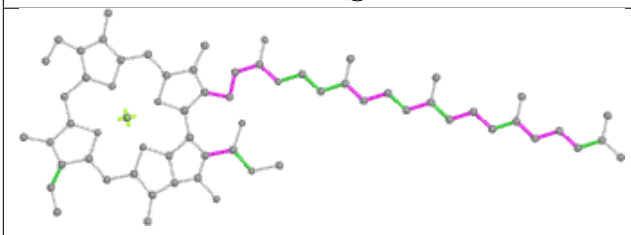


Bond angles



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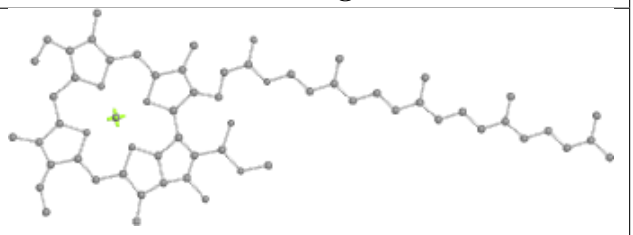
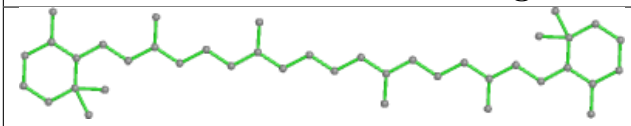


Rings

Ligand BCR V 4219



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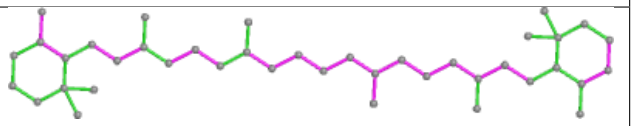

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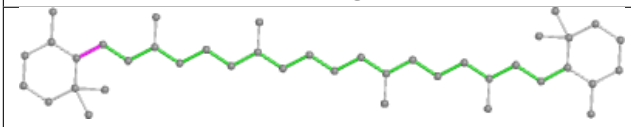
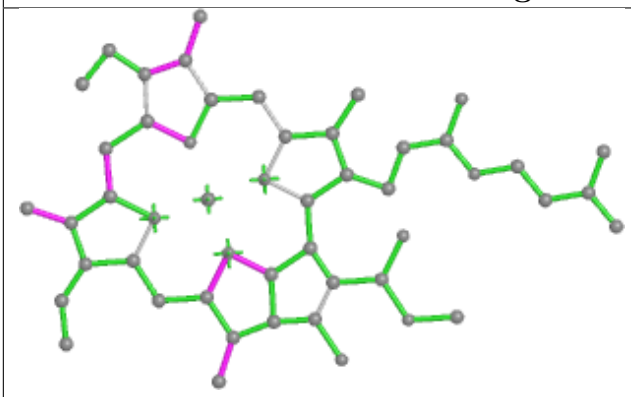
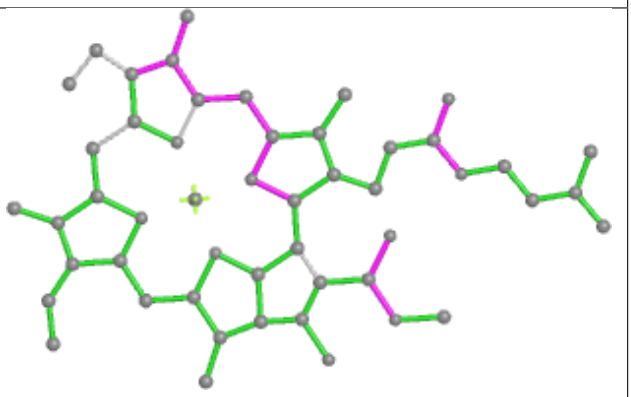
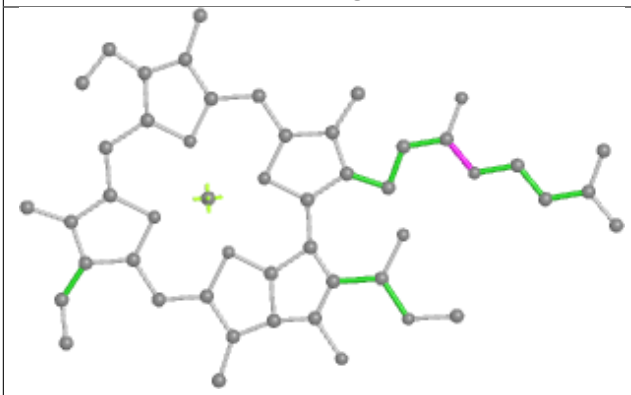
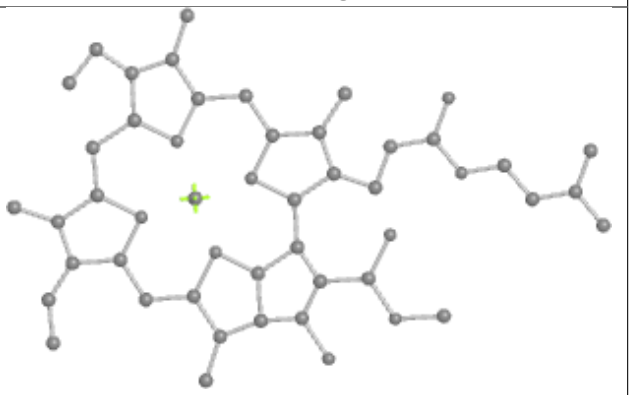
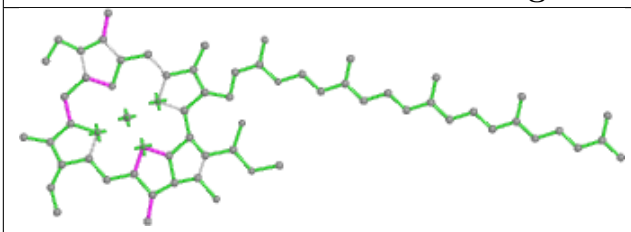
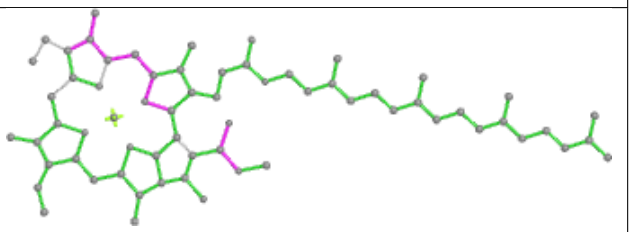
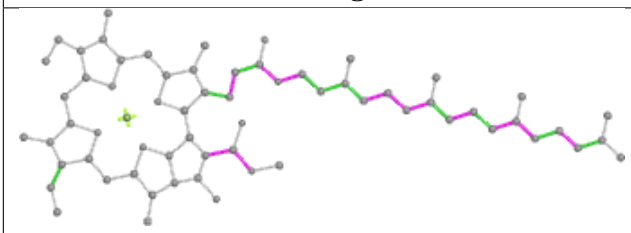
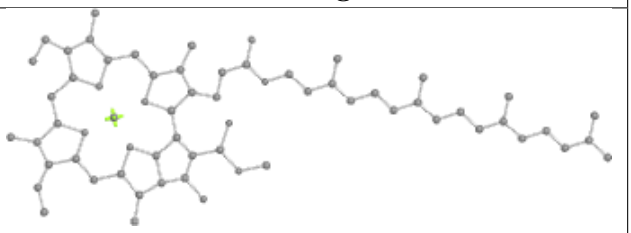


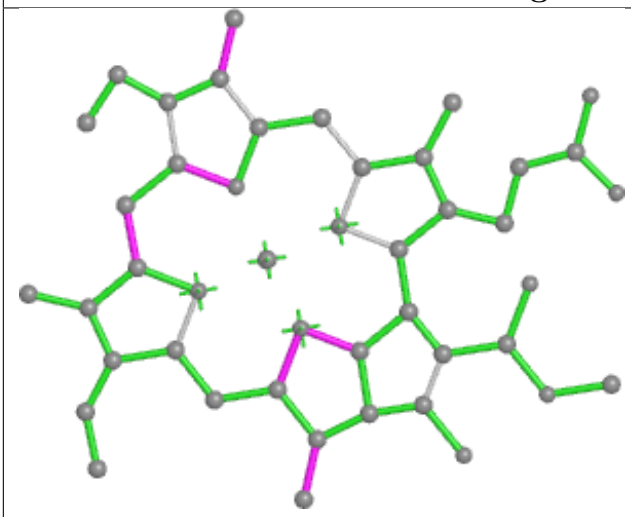
Torsions

Rings

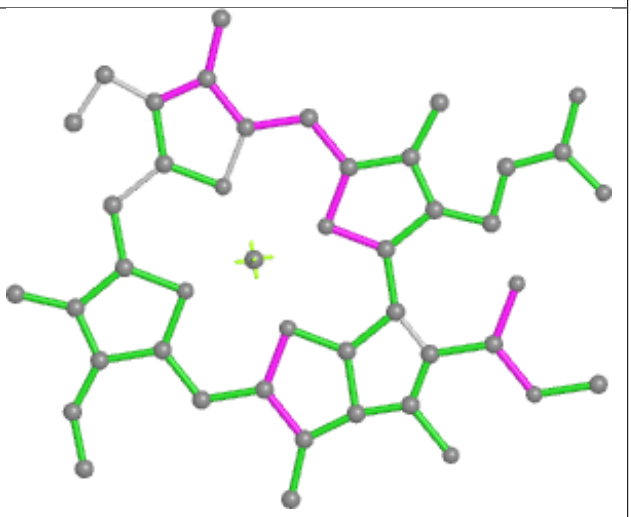
Ligand CLA G 1114	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

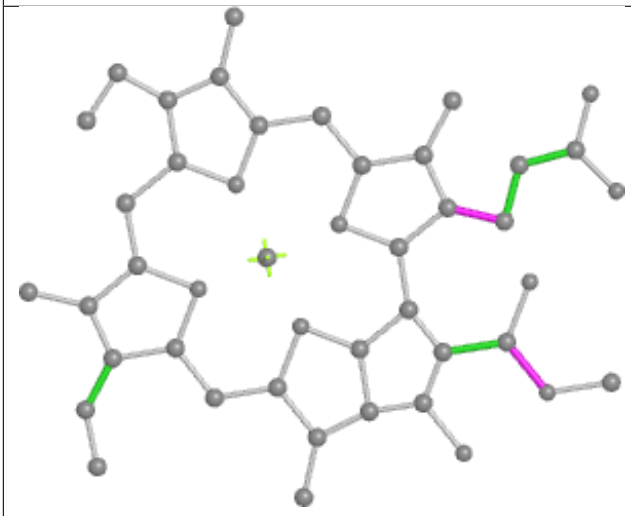
Ligand CLA t 511



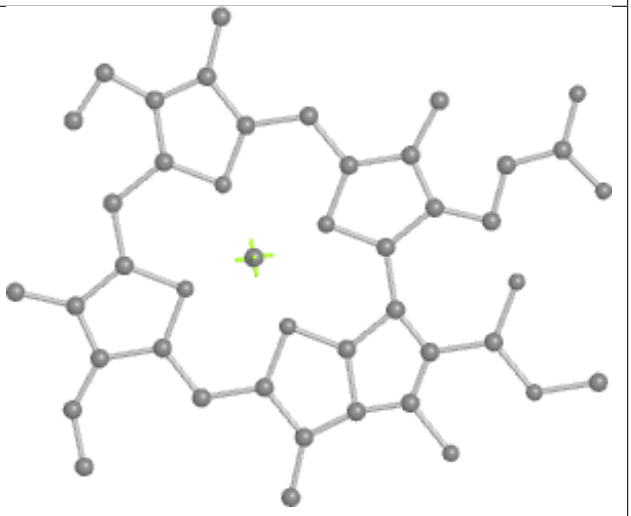
Bond lengths



Bond angles

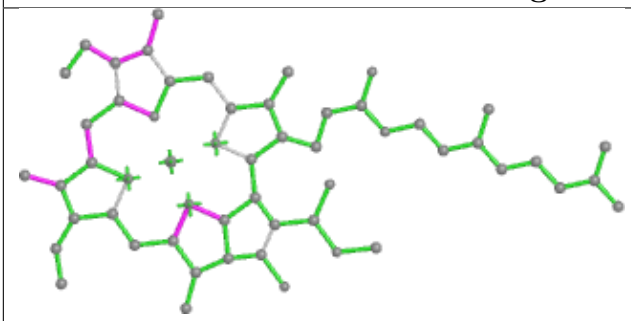


Torsions



Rings

Ligand CLA r 519



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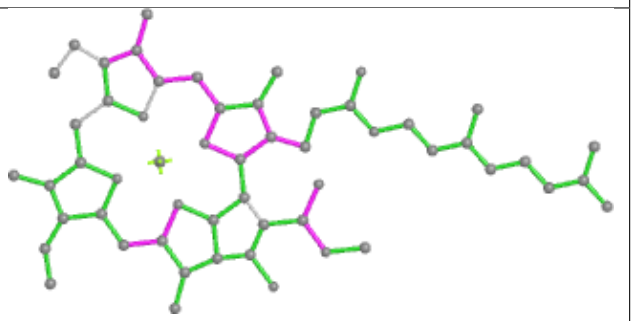
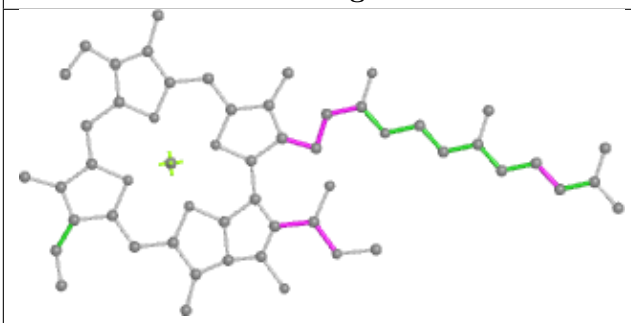


Bond angles



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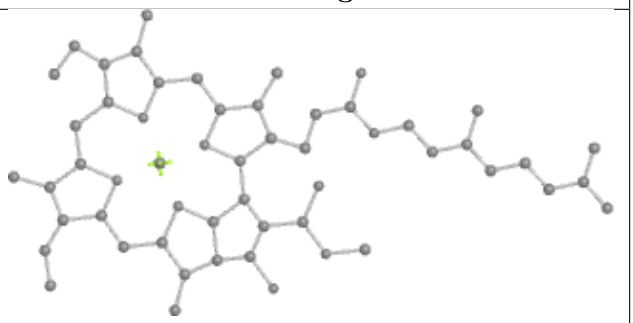
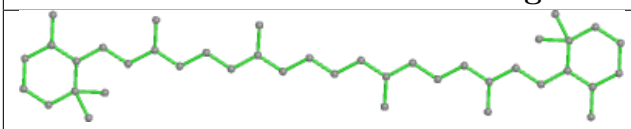


Rings

Ligand BCR Z 524



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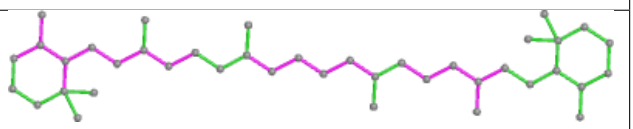
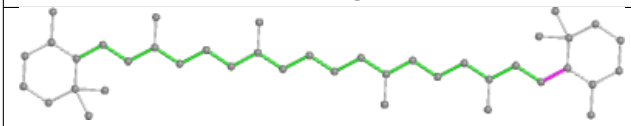


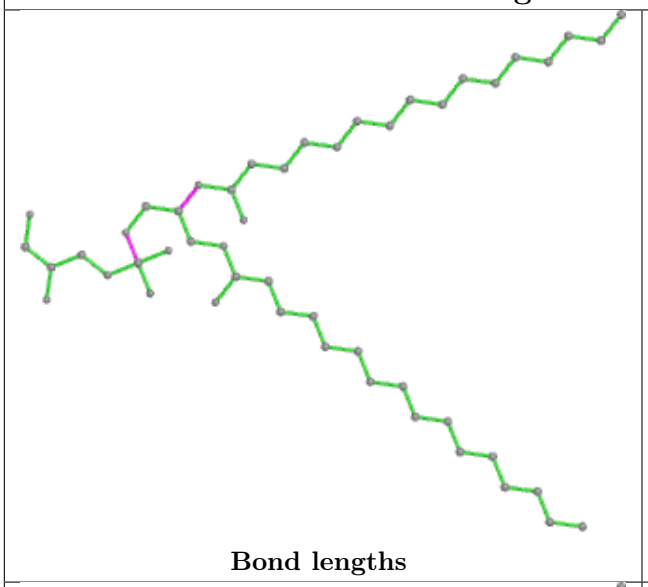
Bond angles



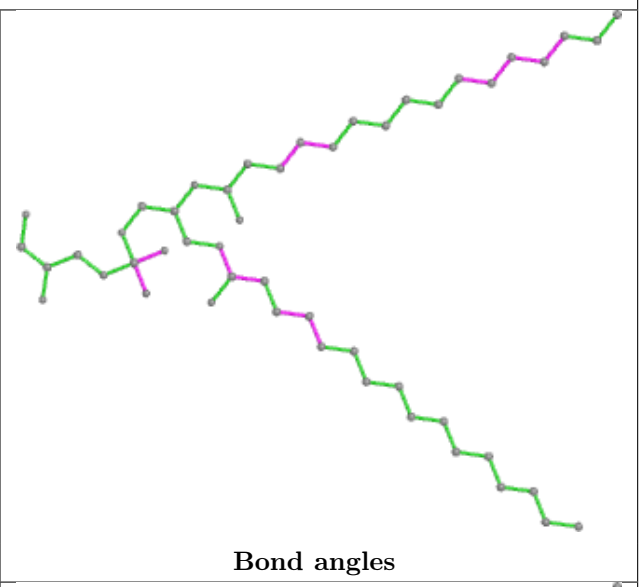
Torsions

Rings

Ligand LHG V 5221



Bond lengths



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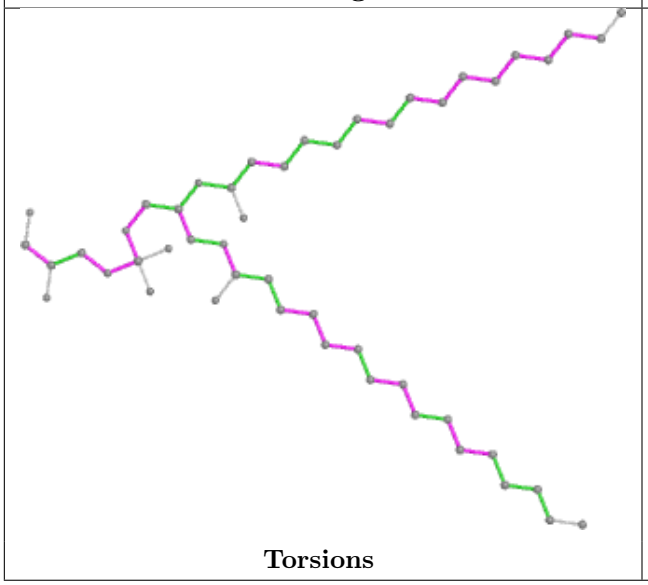
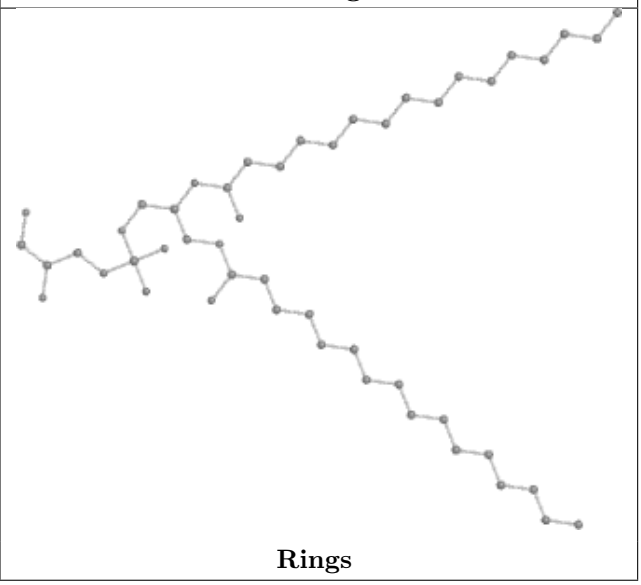
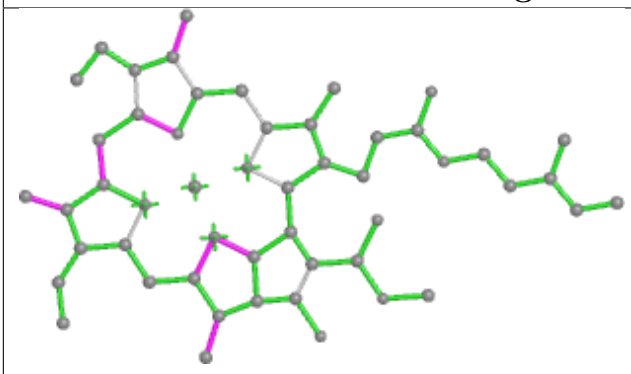


Torsions



Rings

Ligand CLA A 1110



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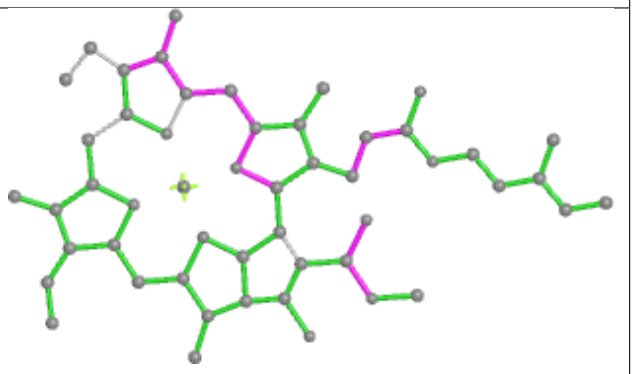
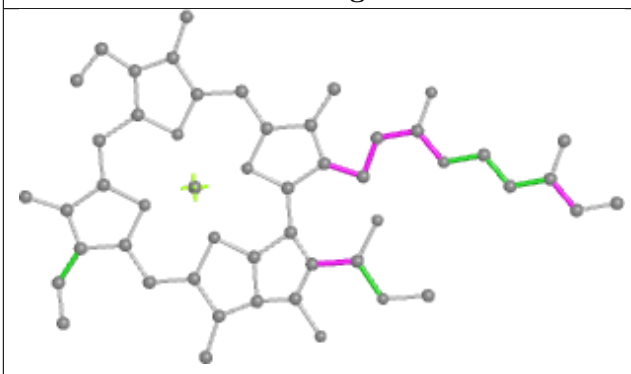
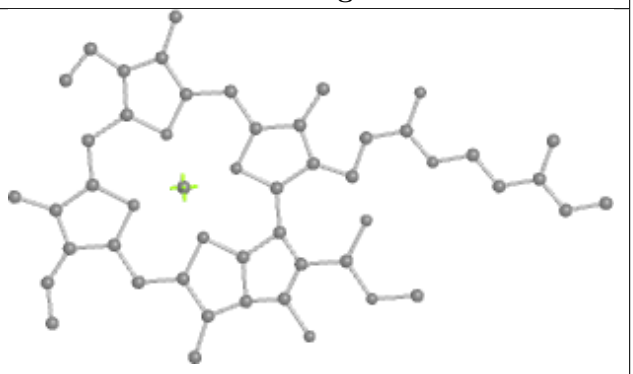


Bond angles

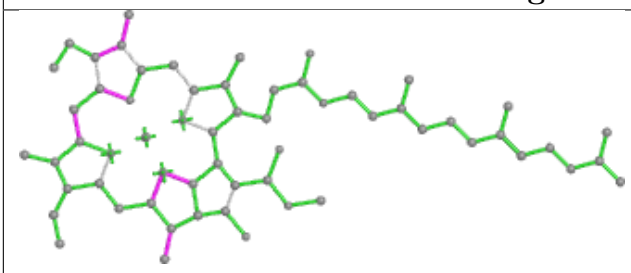


Torsions



Rings

Ligand CLA q 502



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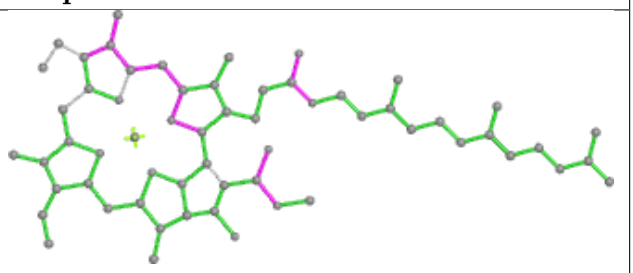
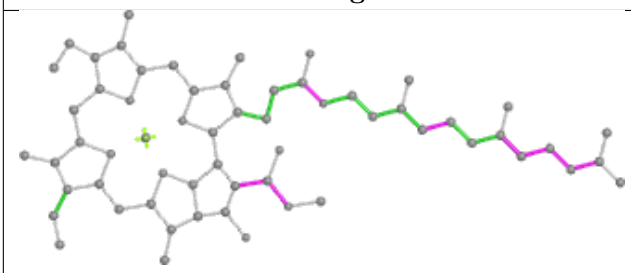
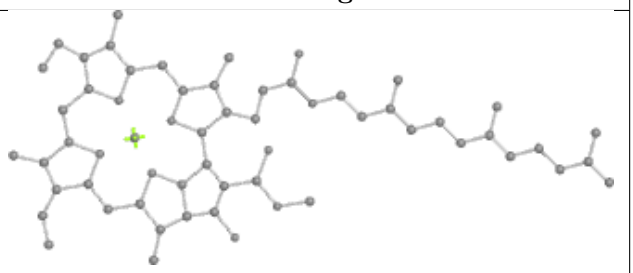


Bond angles

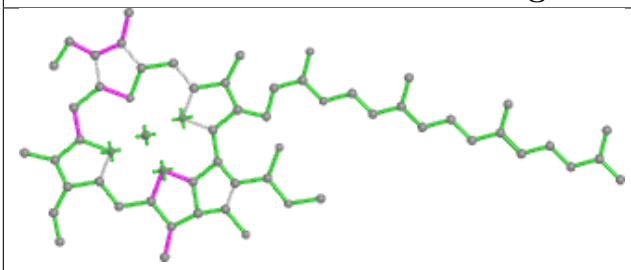


Torsions



Rings

Ligand CLA 2 502



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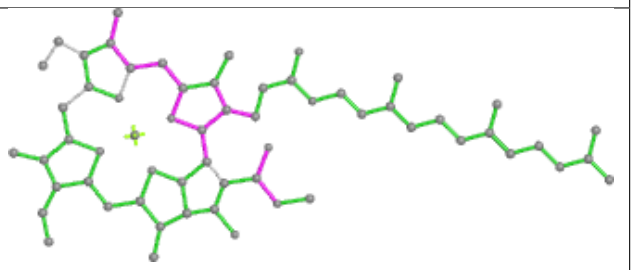
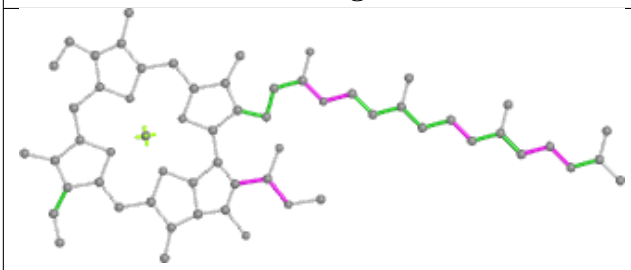
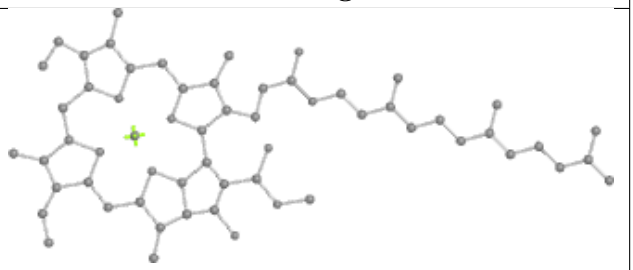


Bond angles

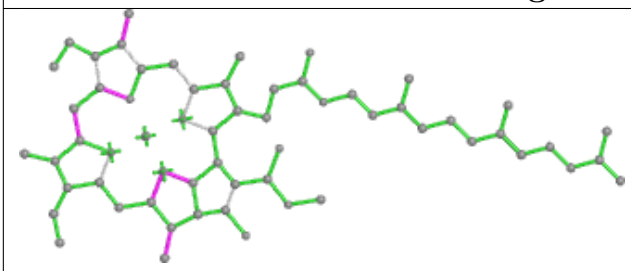


Torsions



Rings

Ligand CLA 1 507



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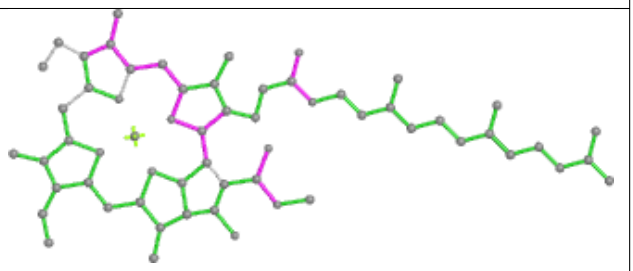

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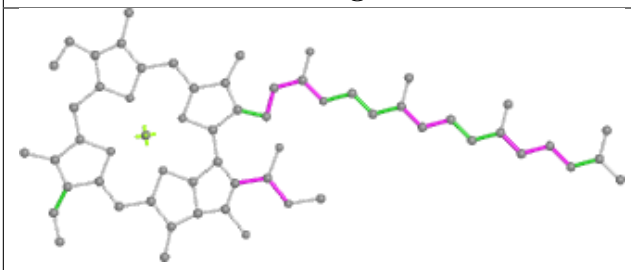

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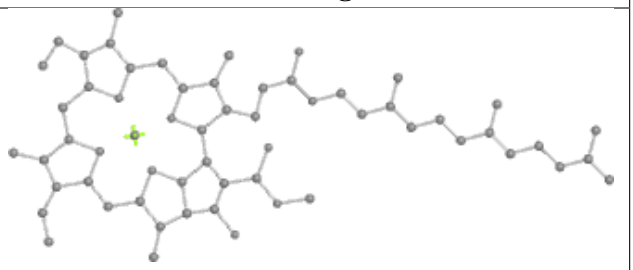
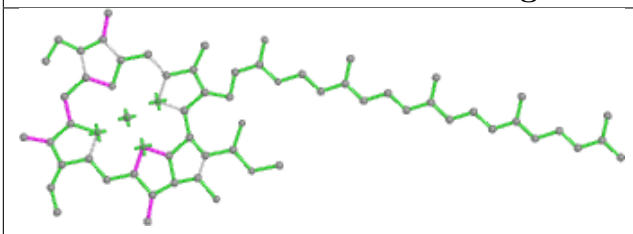


Rings

Ligand CLA e 1102



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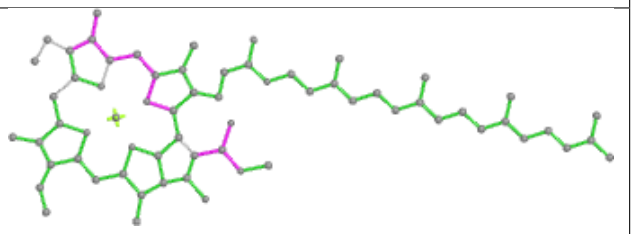
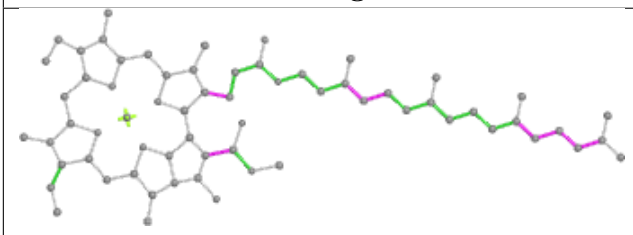


Bond angles



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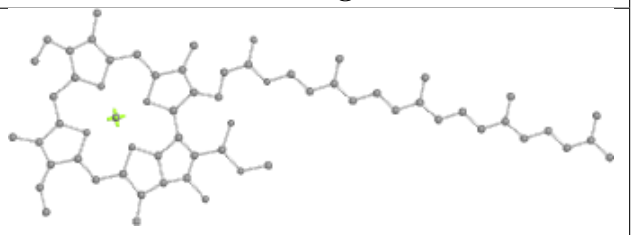
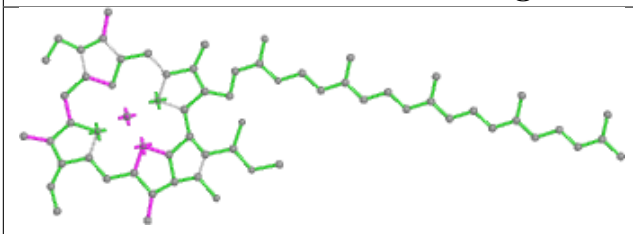


Rings

Ligand CLA H 1215



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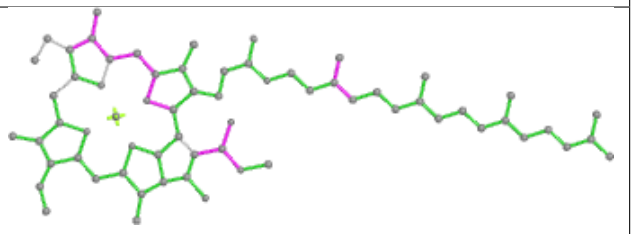
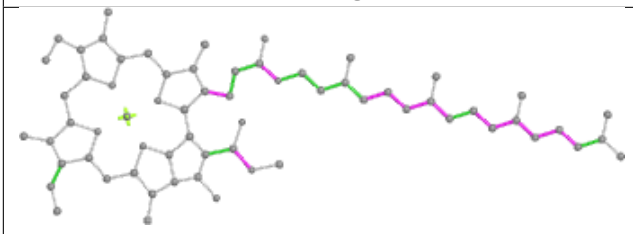


Bond angles



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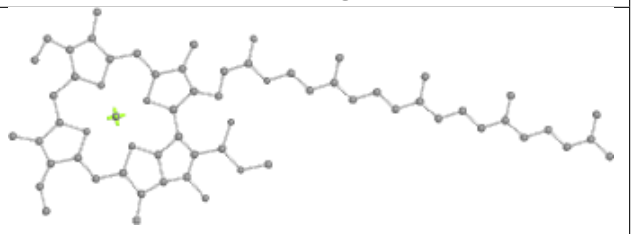
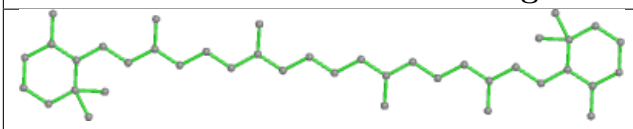


Rings

Ligand BCR f 4005



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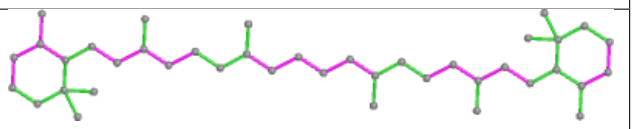
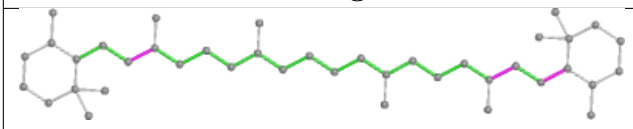


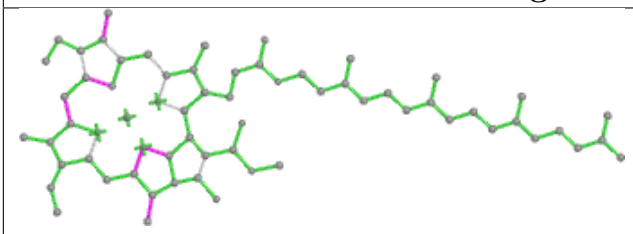
Bond angles



Torsions

Rings

Ligand CLA s 507



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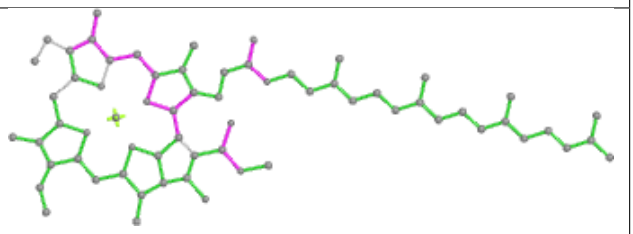
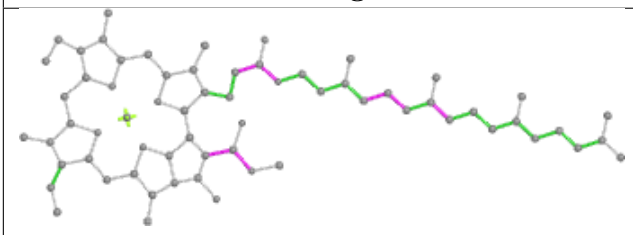
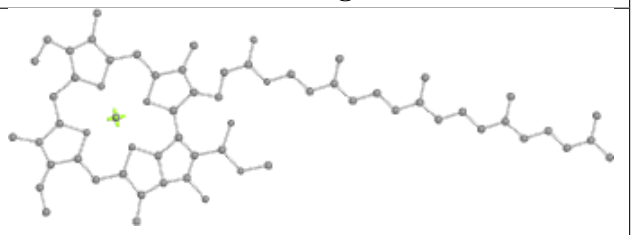


Bond angles

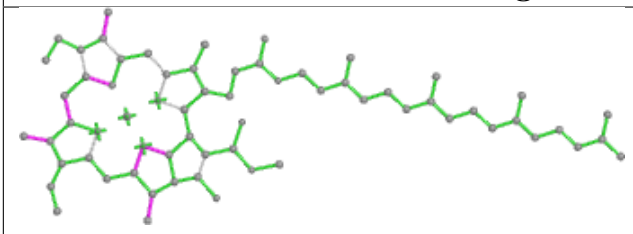


Torsions



Rings

Ligand CLA A 1127



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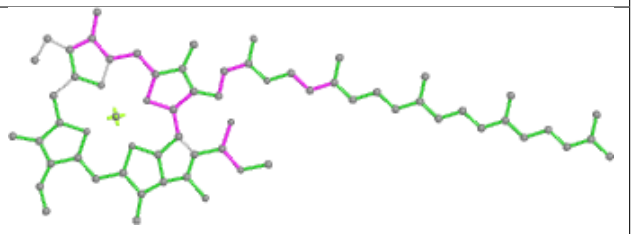
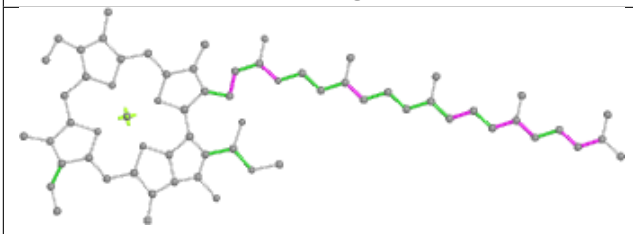
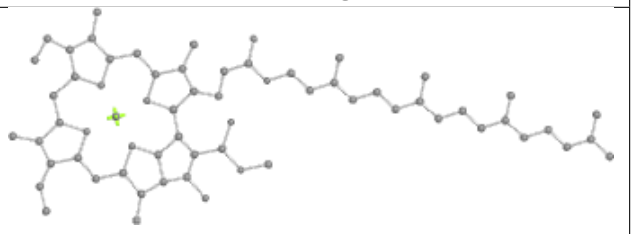


Bond angles

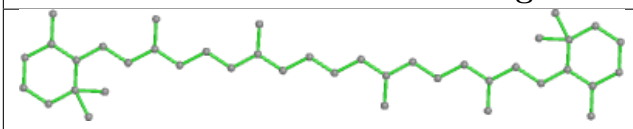


Torsions



Rings

Ligand BCR L 4019



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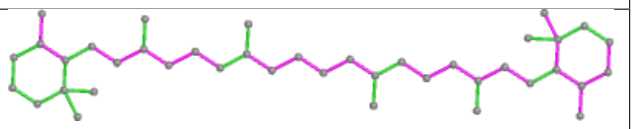
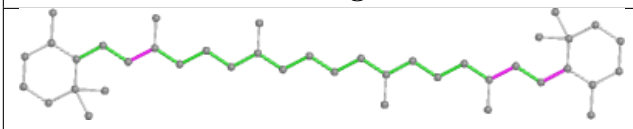


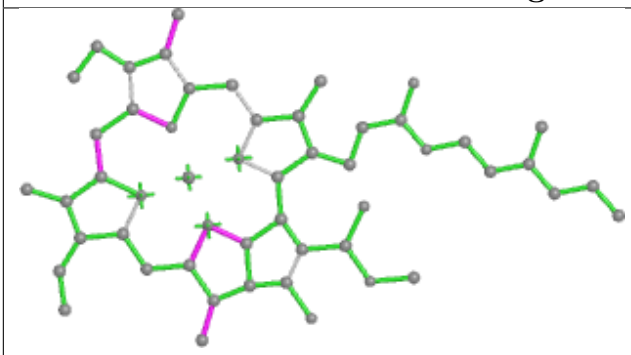
Bond angles



Torsions

Rings

Ligand CLA v 503



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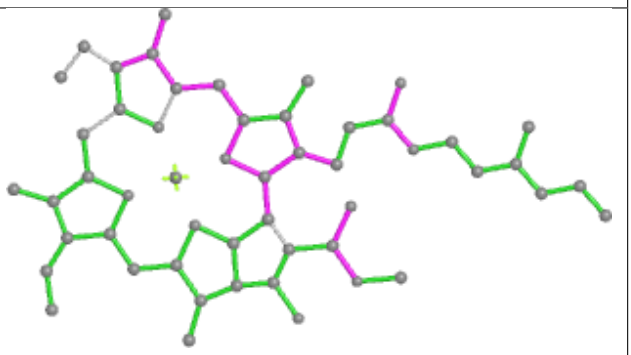
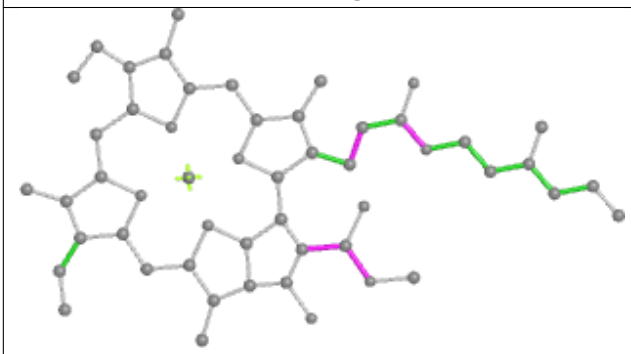


Bond angles



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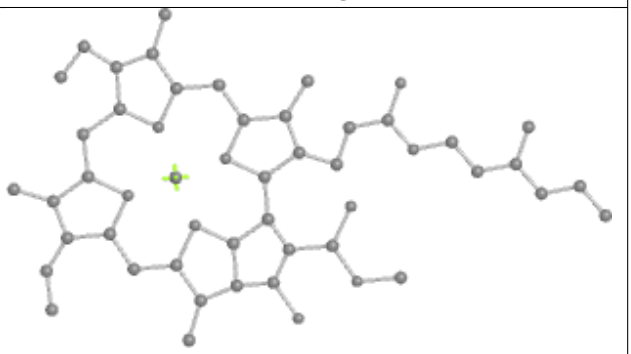
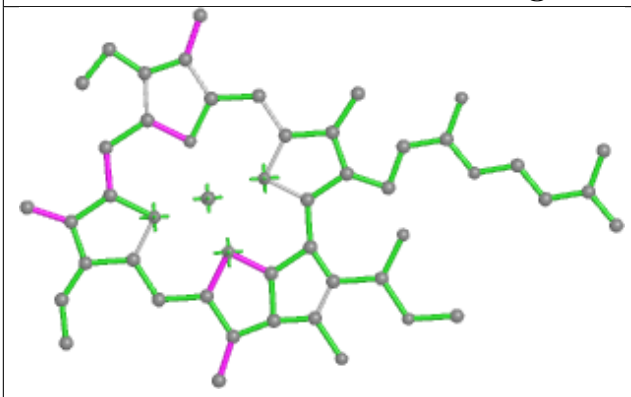


Rings

Ligand CLA 2 504



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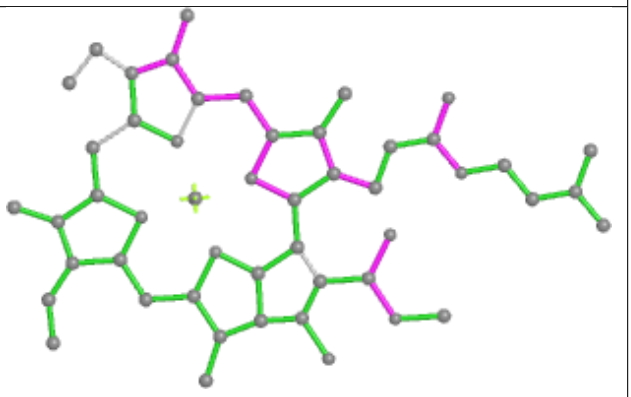
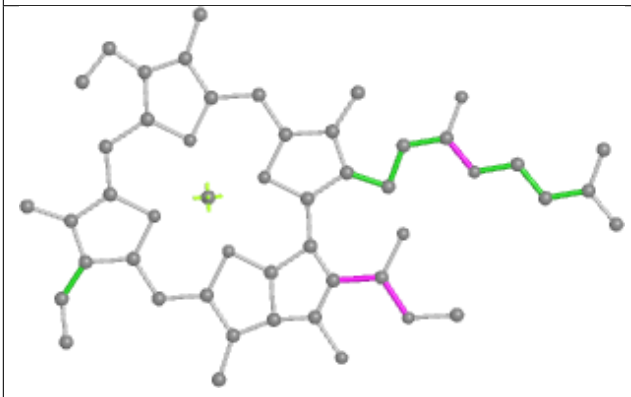
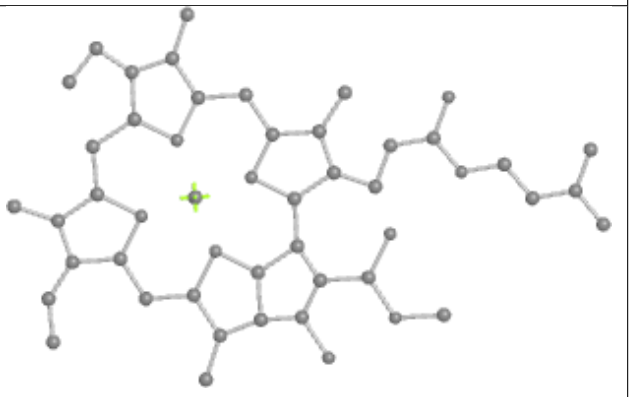


Bond angles

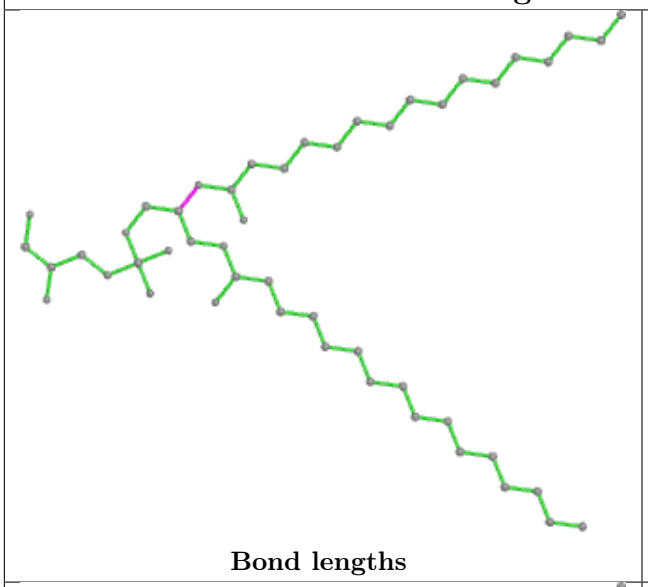


Torsions



Rings

Ligand LHG G 5001



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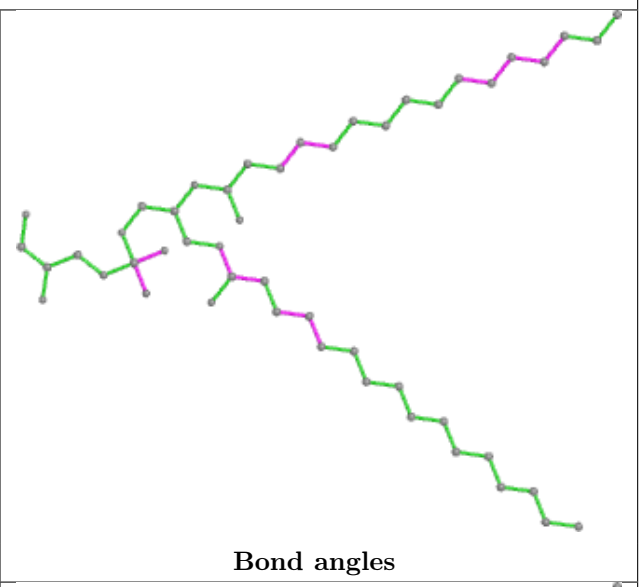
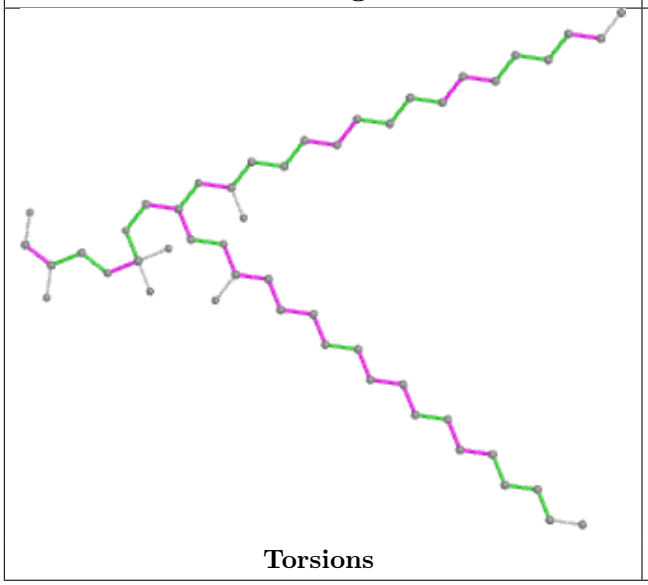
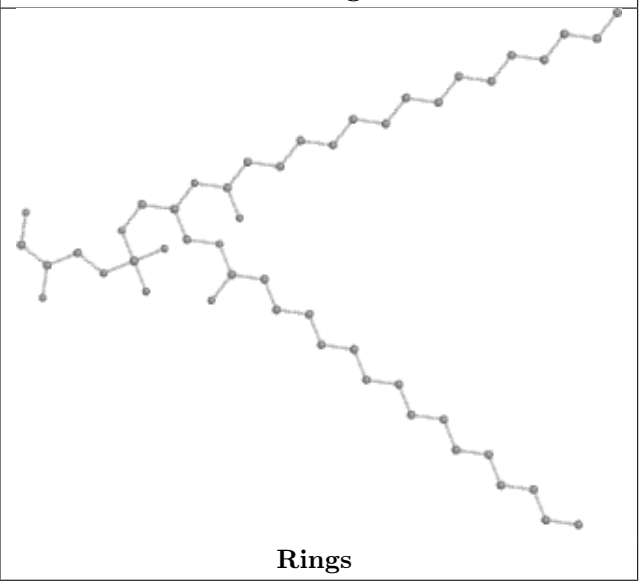


Bond angles

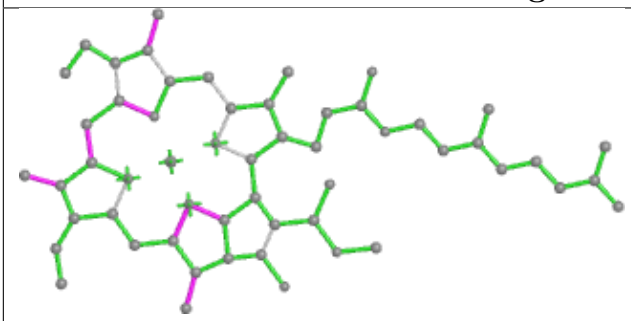


Torsions

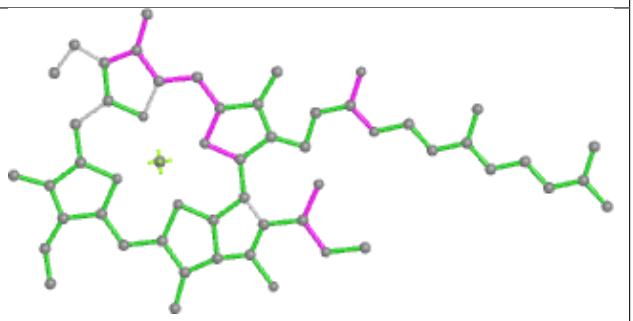


Rings

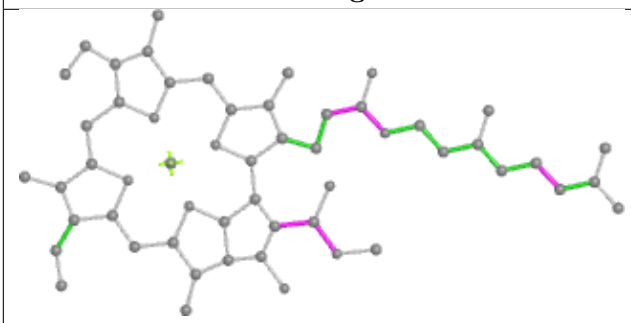
Ligand CLA a 519



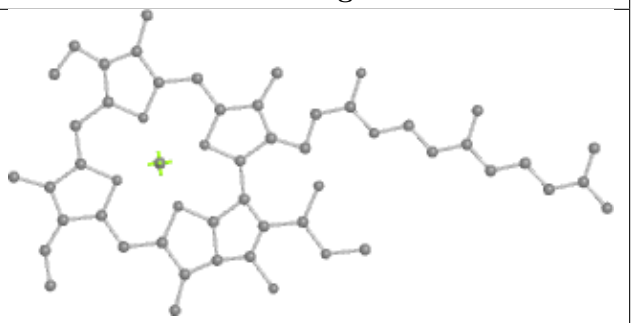
Bond lengths



Bond angles

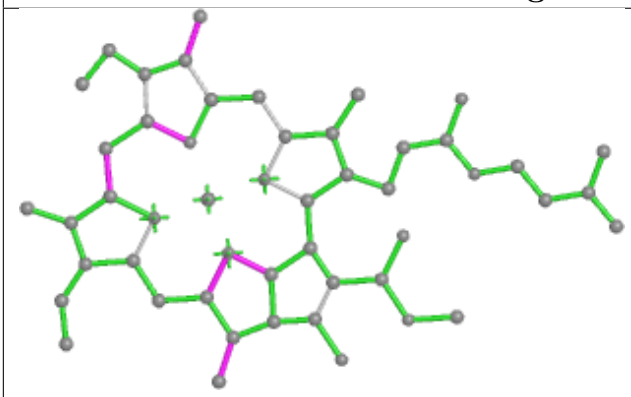


Torsions



Rings

Ligand CLA b 510



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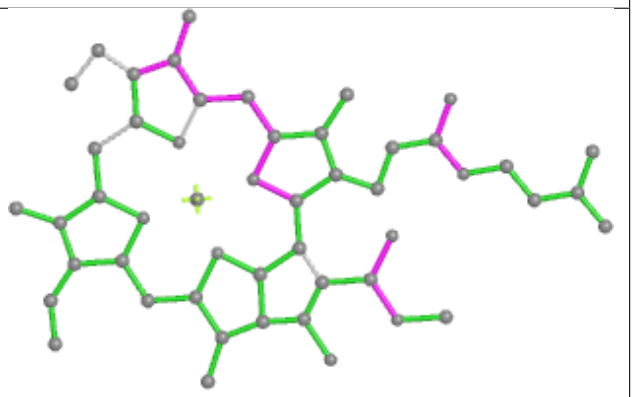

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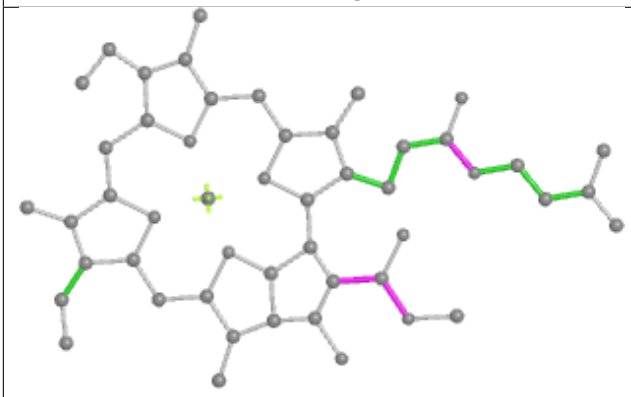

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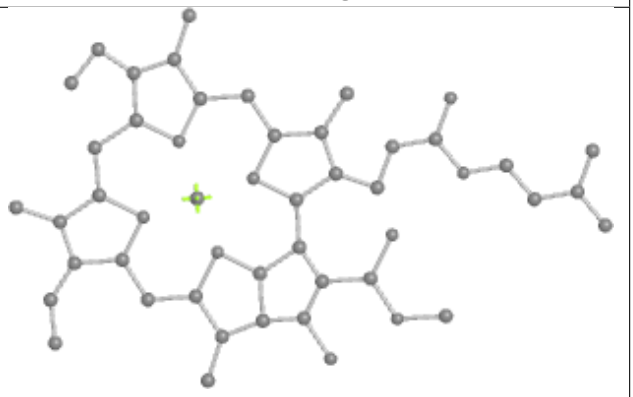
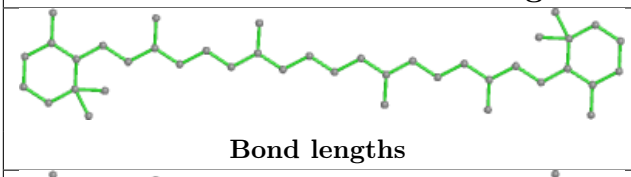


Rings

Ligand BCR d 522



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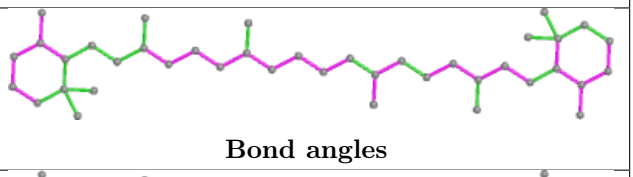

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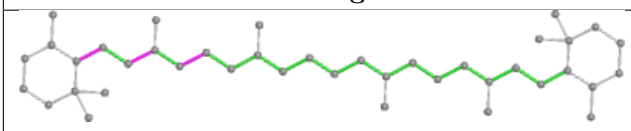

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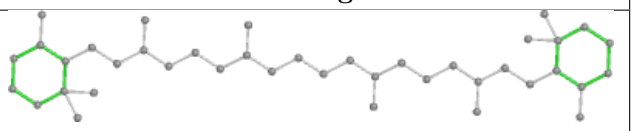
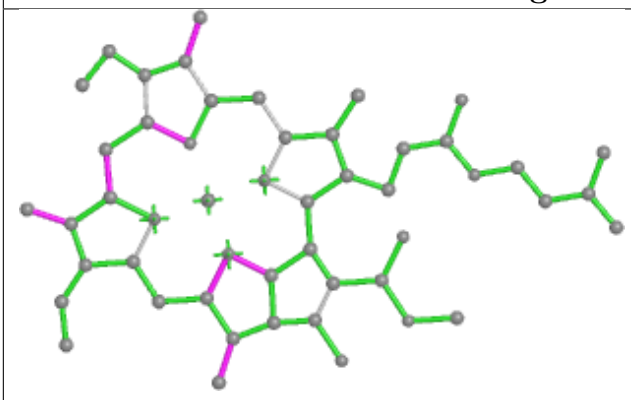


Rings

Ligand CLA r 504



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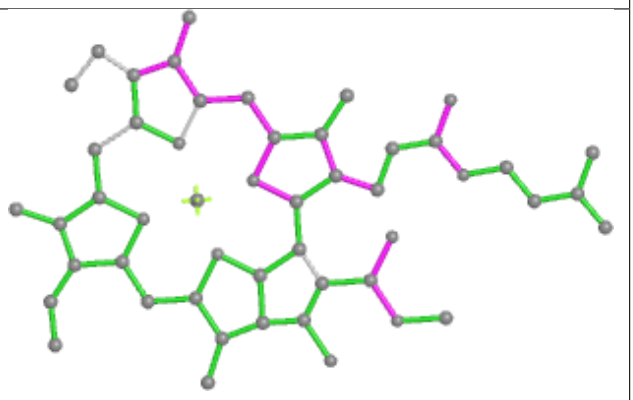

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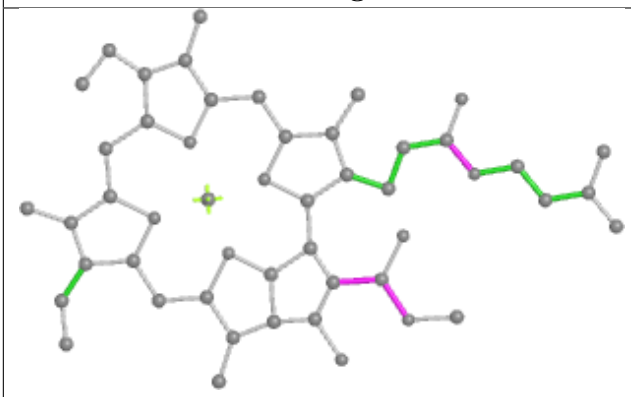

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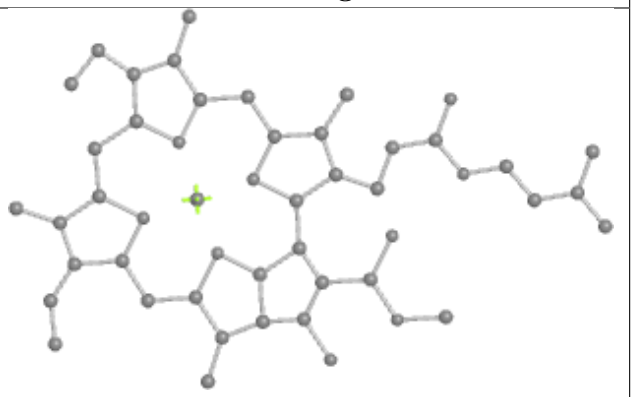
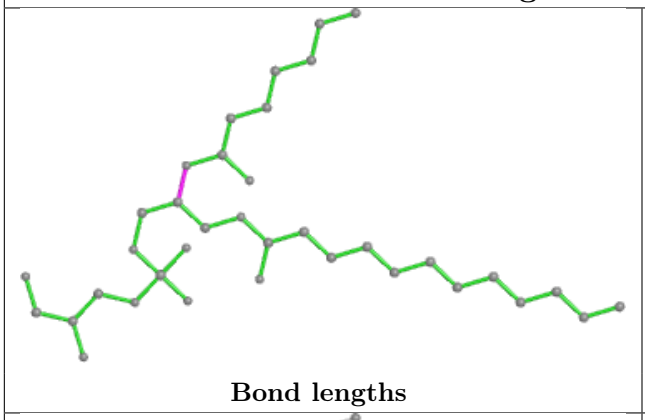


Rings

Ligand LHG e 5004



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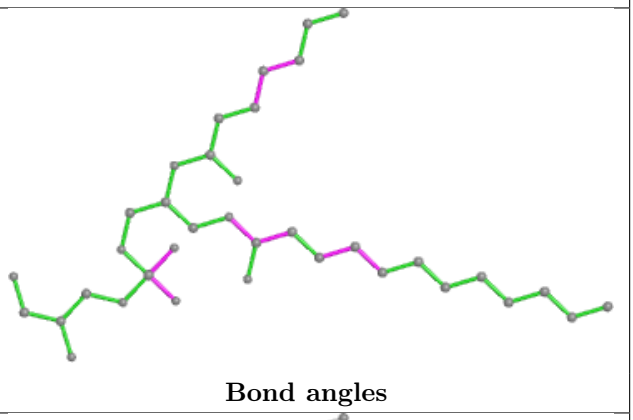

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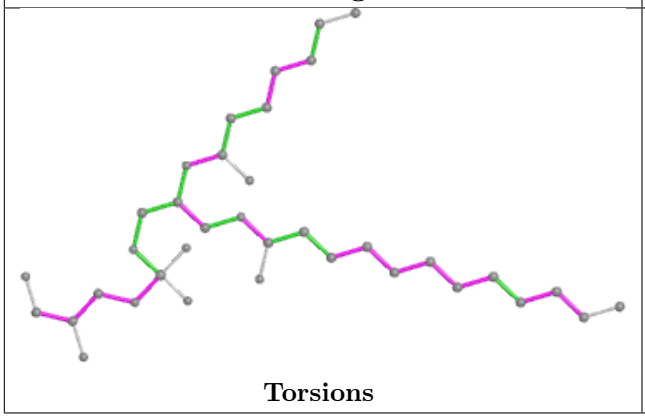

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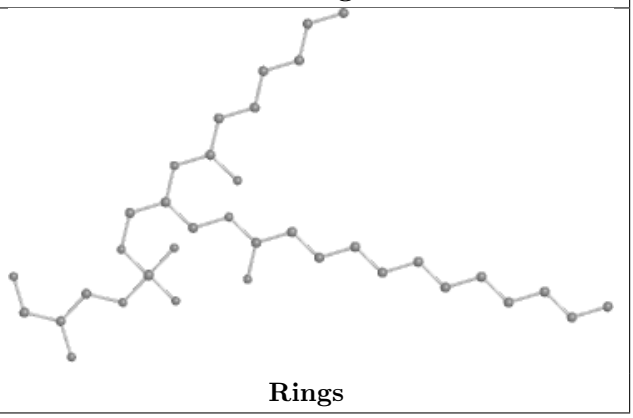
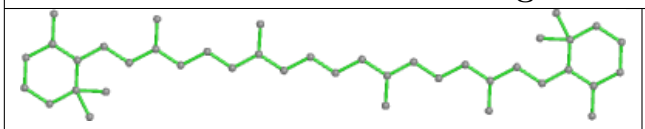


Rings

Ligand BCR L 4020



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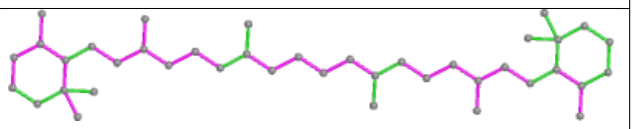

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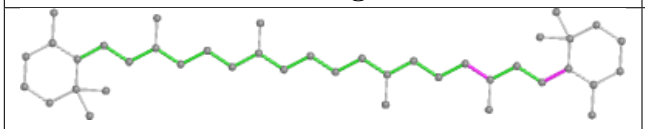

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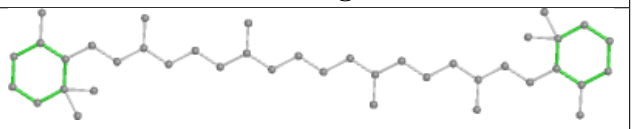
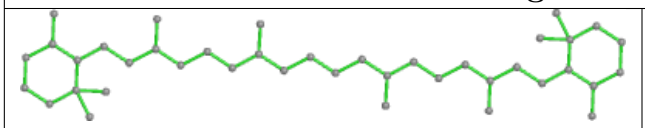


Rings

Ligand BCR v 522



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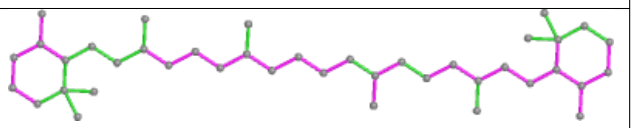

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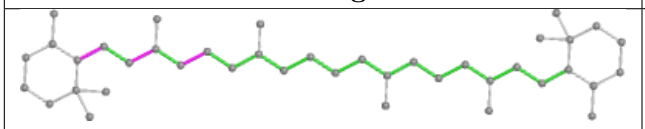

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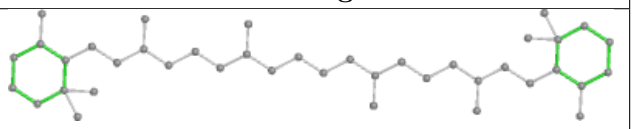
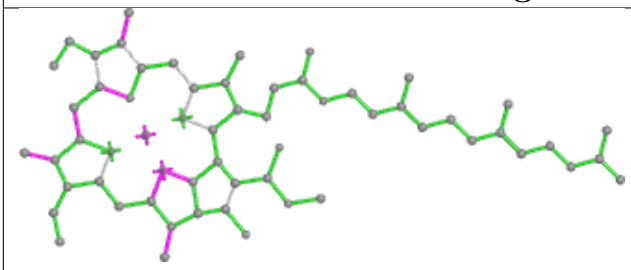


Rings

Ligand CLA G 1116



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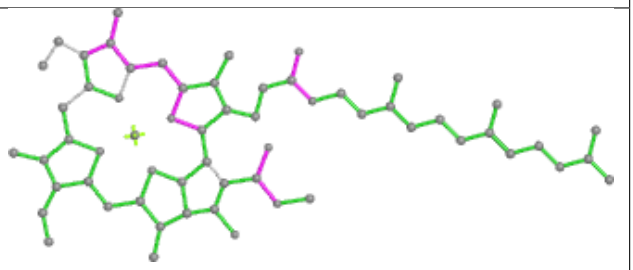

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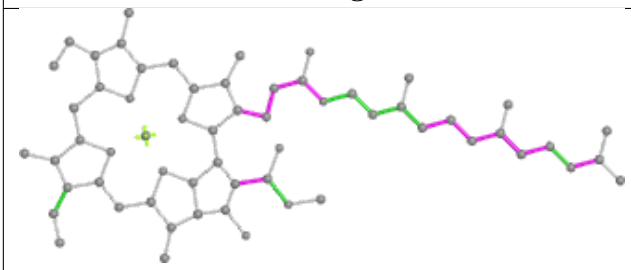

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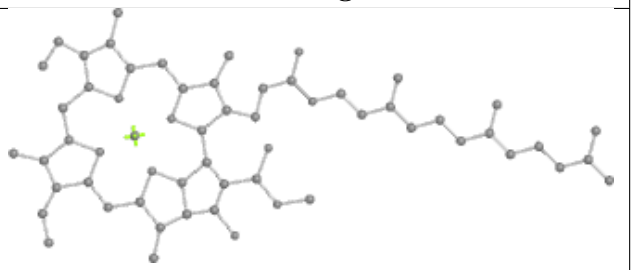
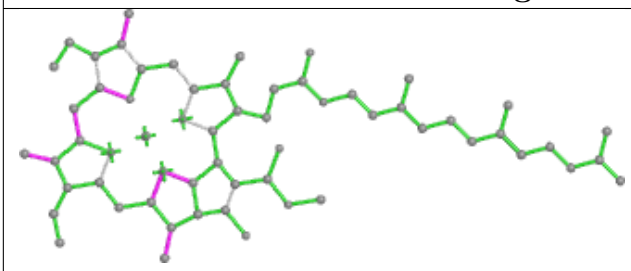


Rings

Ligand CLA G 1115



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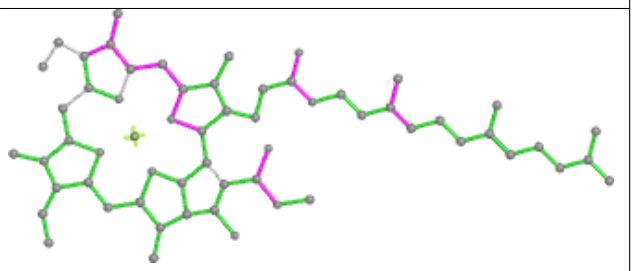
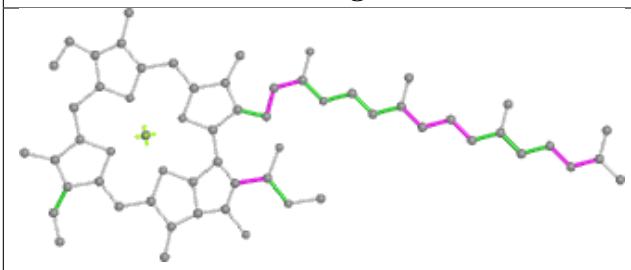


Bond angles



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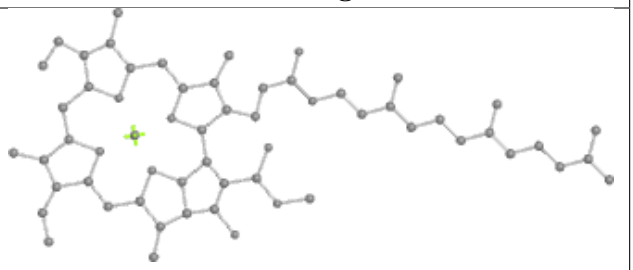
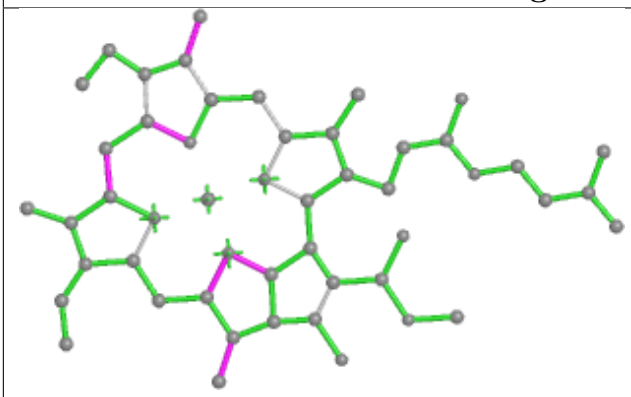


Rings

Ligand CLA s 511



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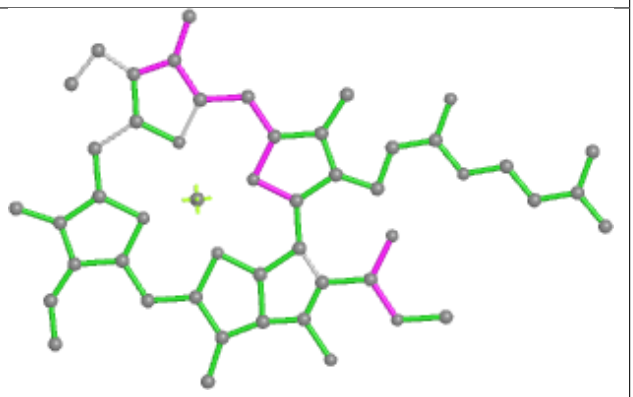

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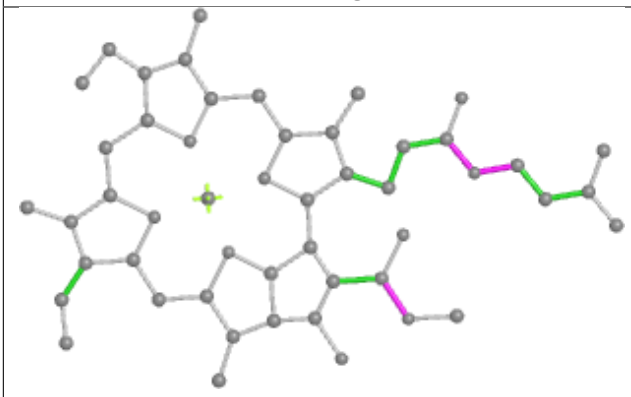

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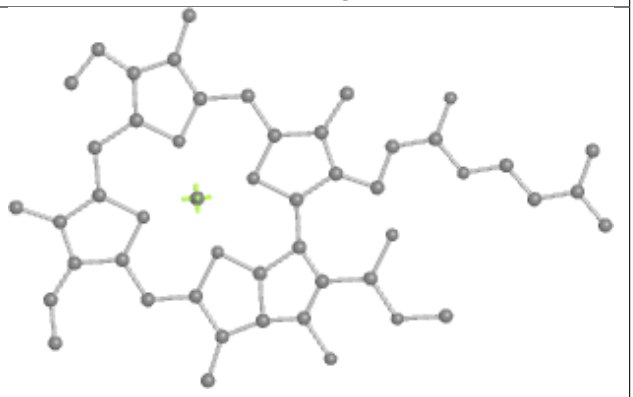
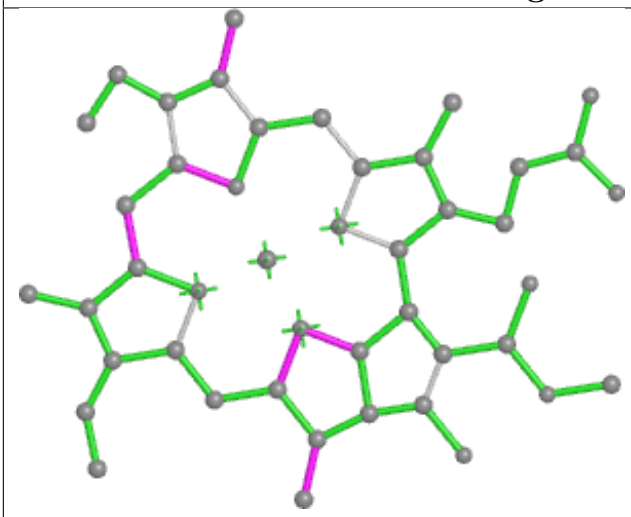


Rings

Ligand CLA b 506



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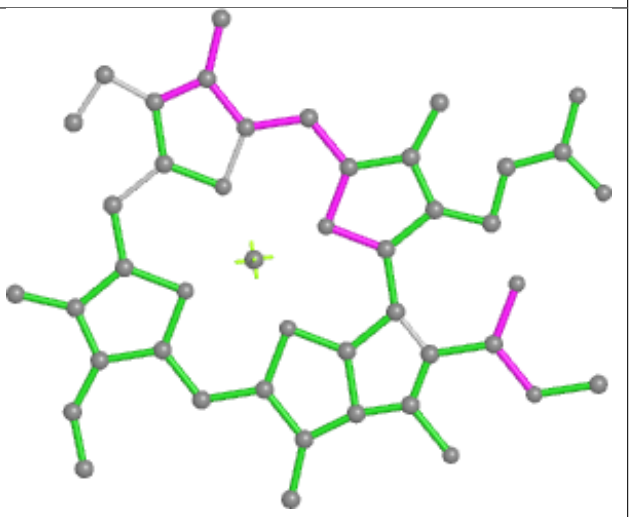

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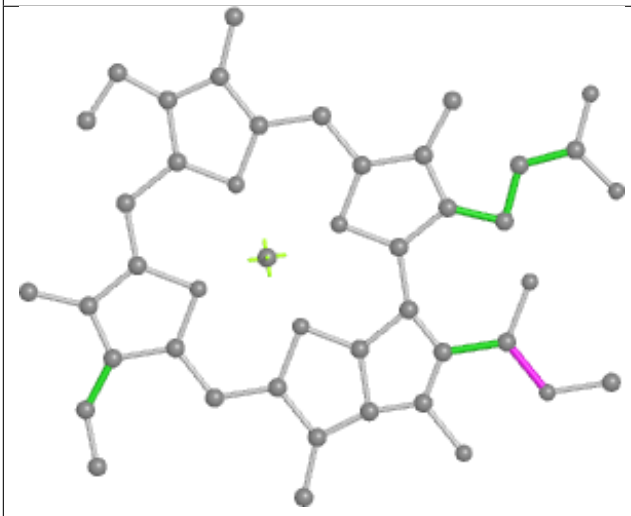

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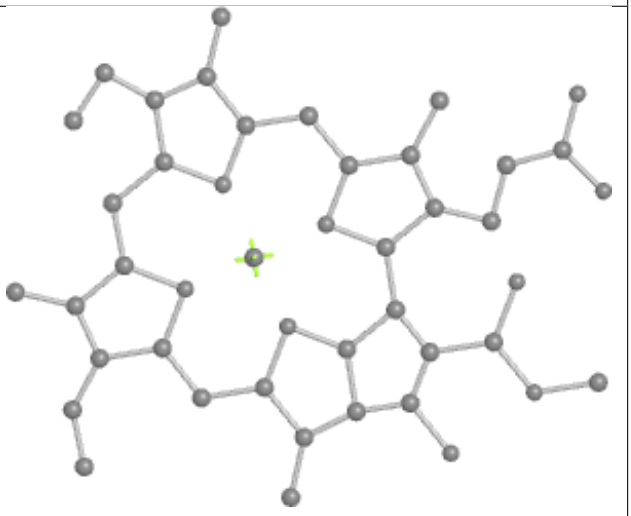
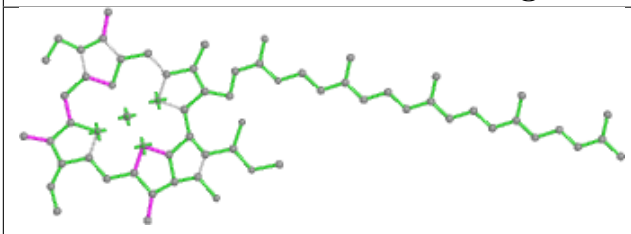


Rings

Ligand CLA e 1111



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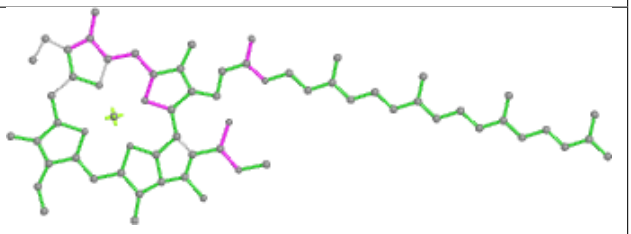

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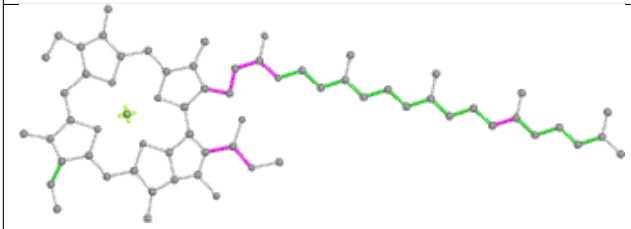

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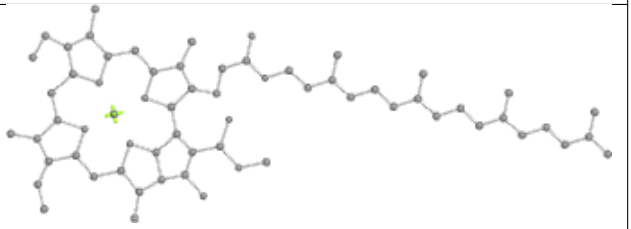
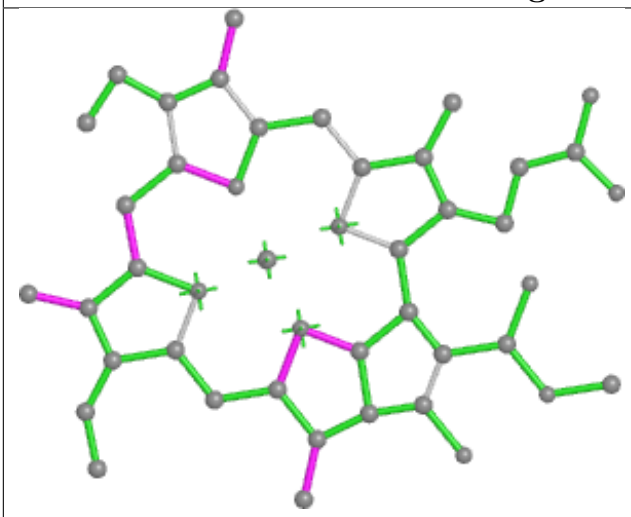


Rings

Ligand CLA 1 517



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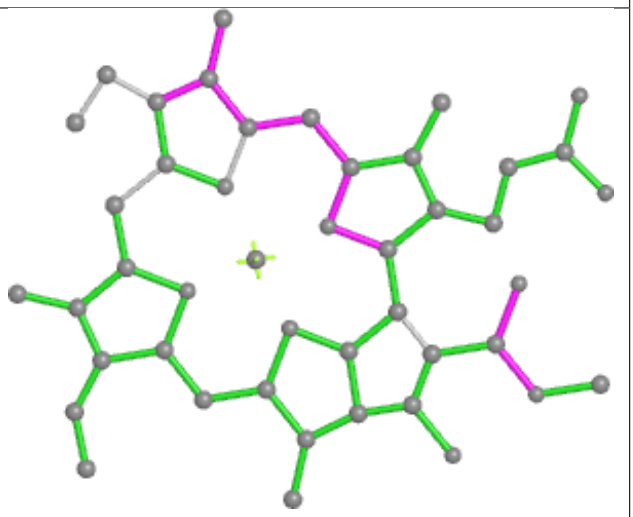
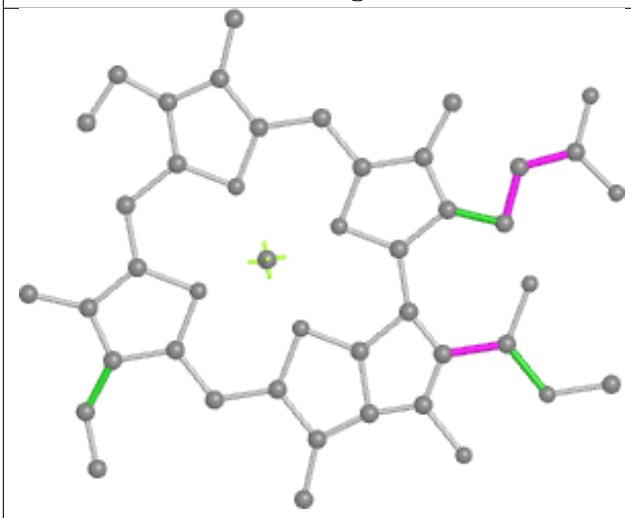


Bond angles



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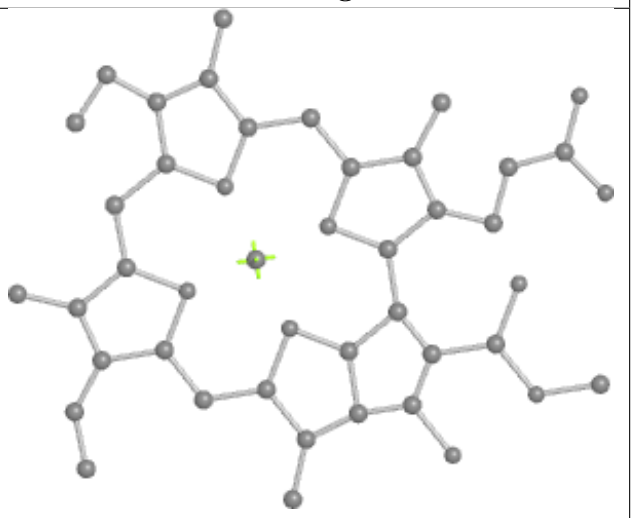
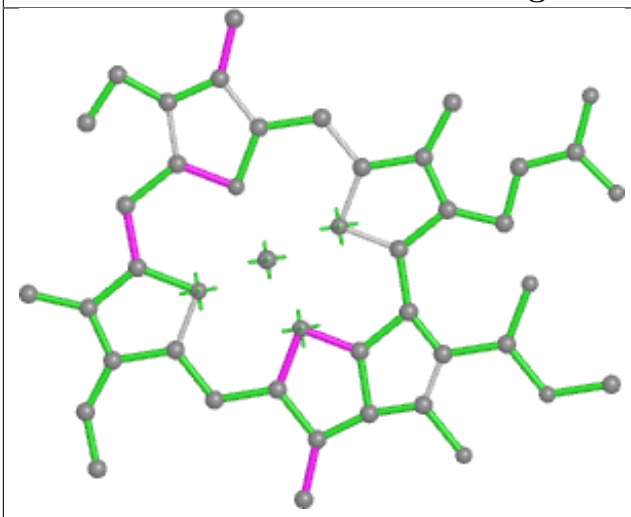


Rings

Ligand CLA a 516



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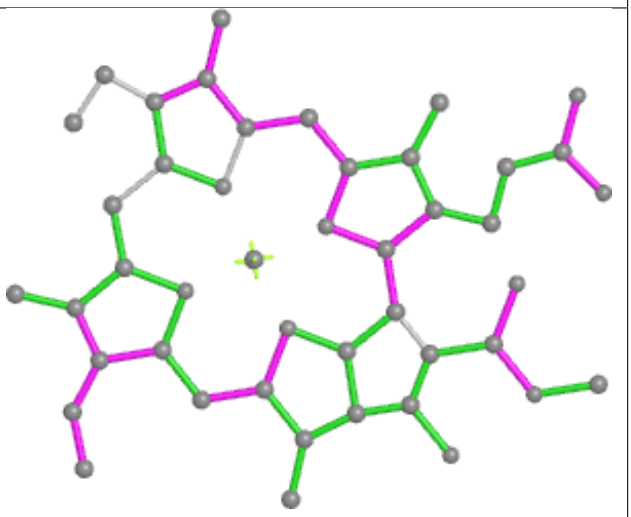
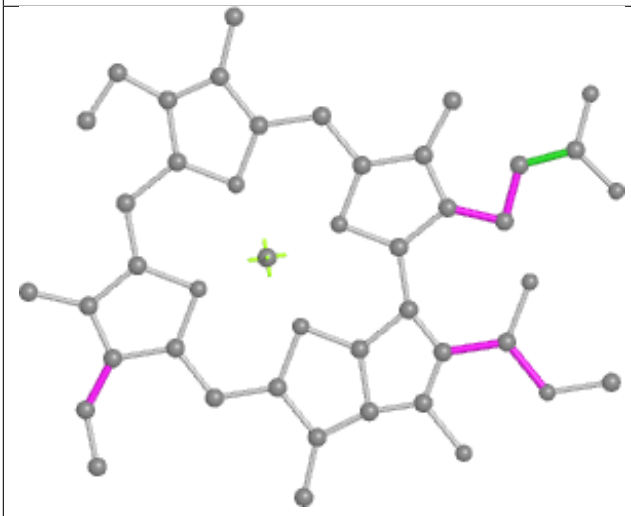


Bond angles



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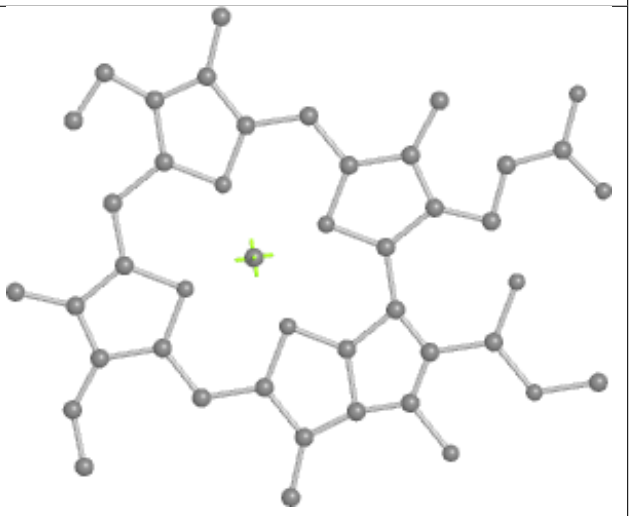
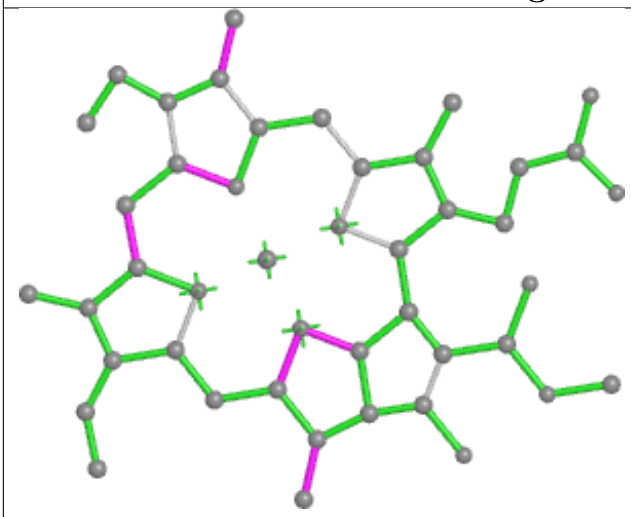


Rings

Ligand CLA 4 504



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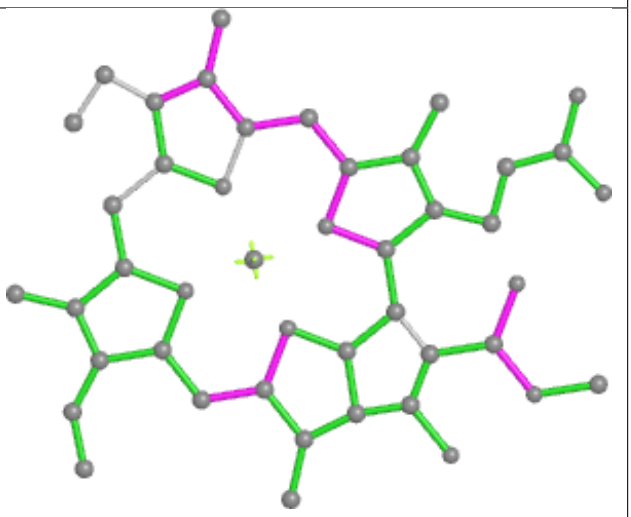
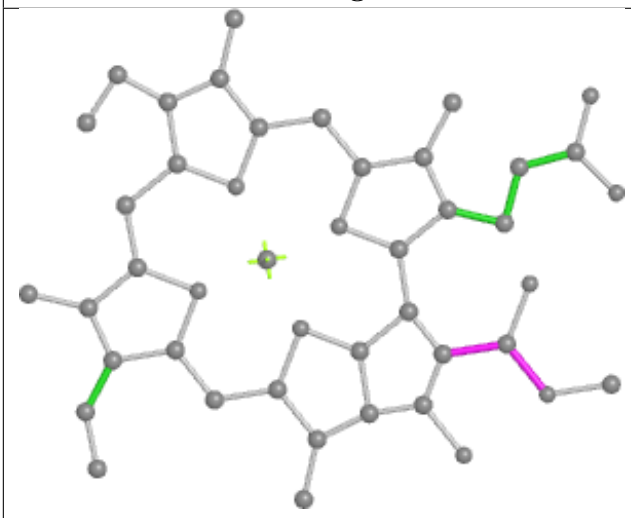


Bond angles



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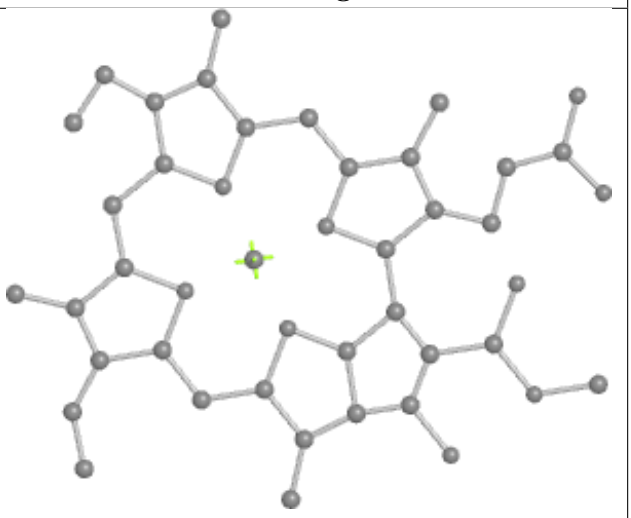
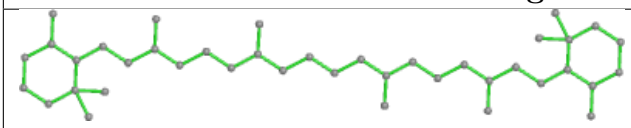
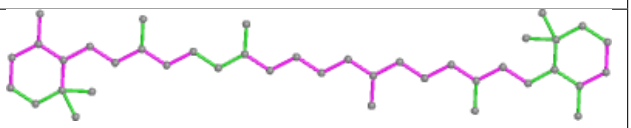


Rings

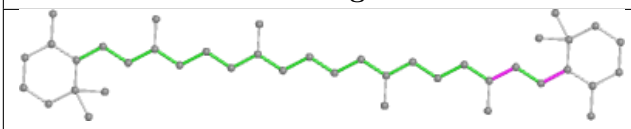
Ligand BCR a 523



Bond lengths

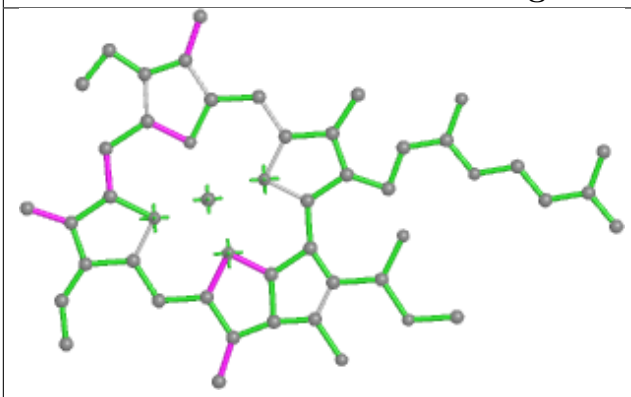
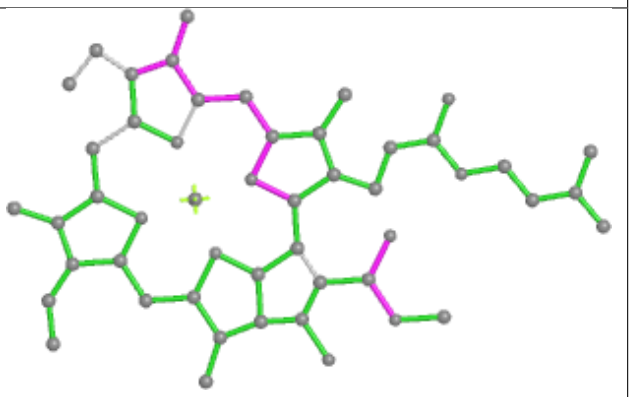
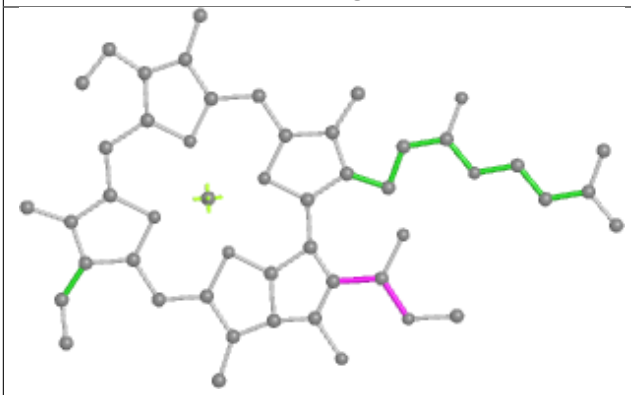
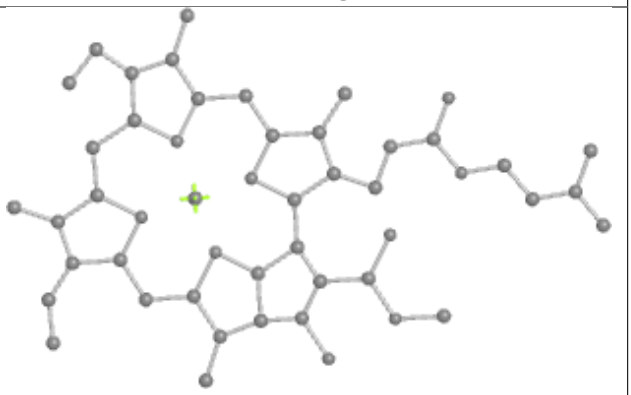


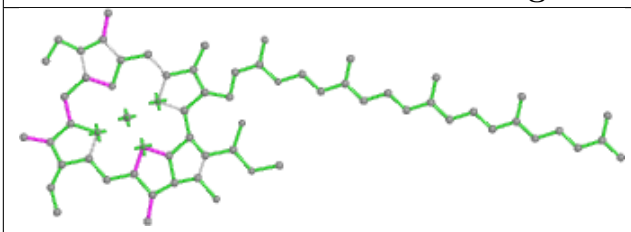
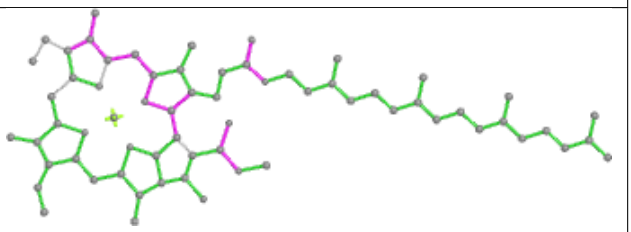
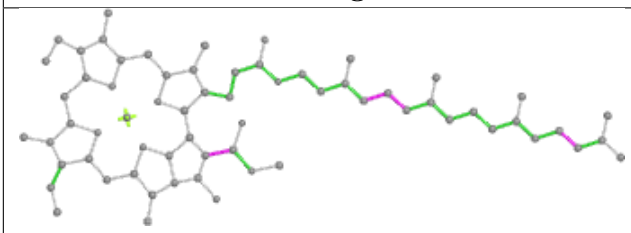
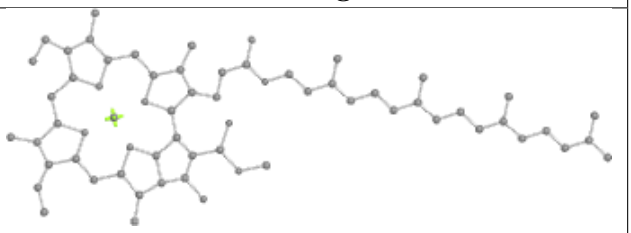
Bond angles



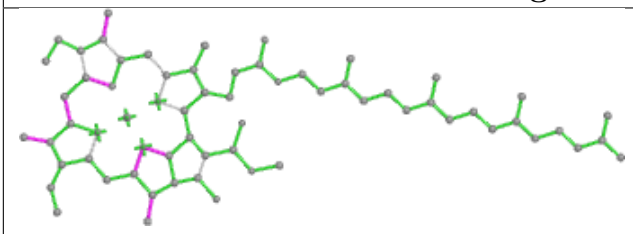
Torsions

Rings

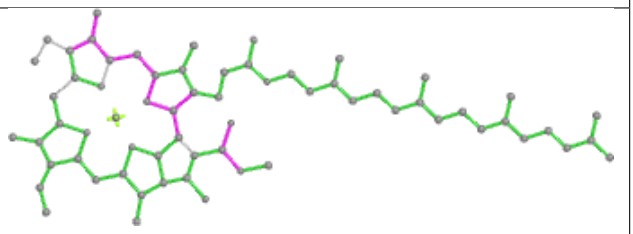
Ligand CLA 3 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 503



Bond lengths



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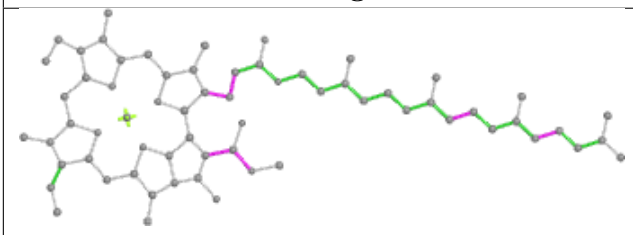
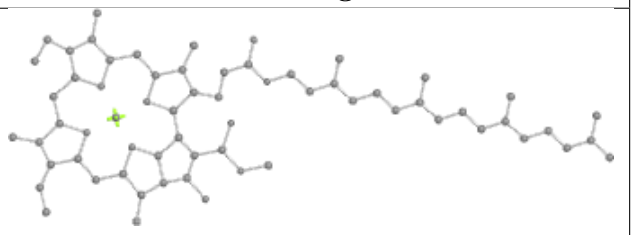
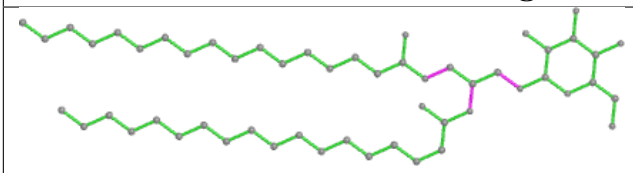


Torsions



Rings

Ligand LMG f 5002



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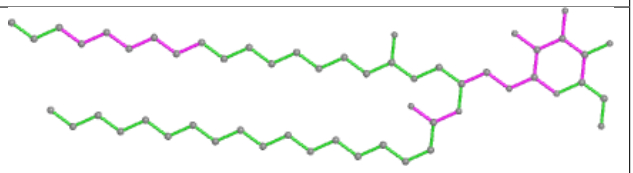
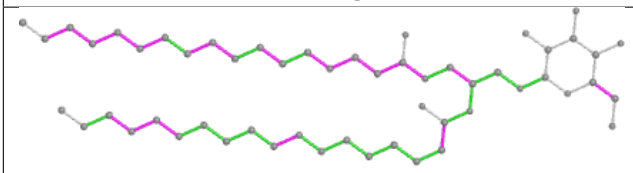


Bond angles



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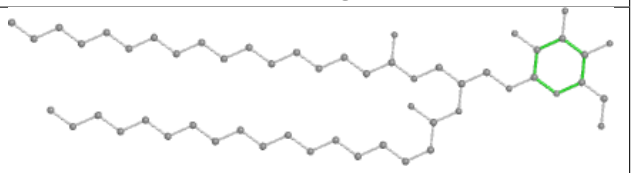
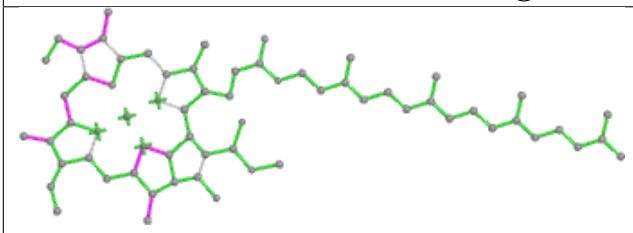


Rings

Ligand CLA B 1227



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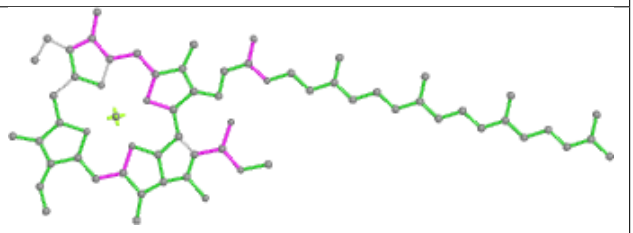
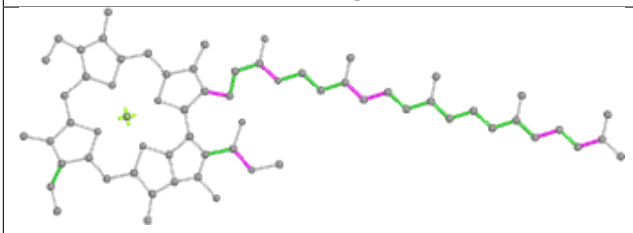


Bond angles



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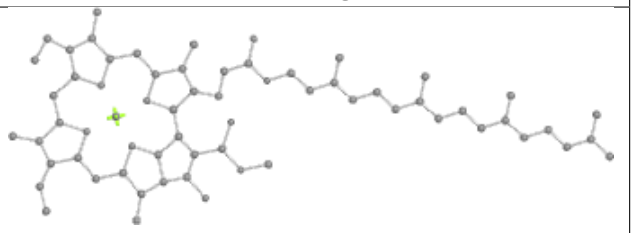
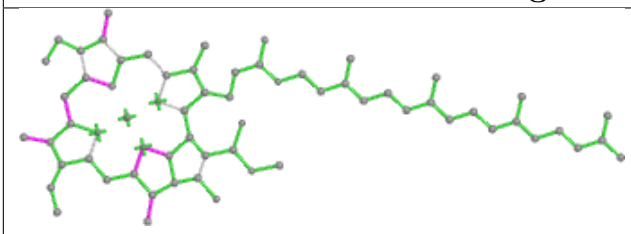


Rings

Ligand CLA c 501



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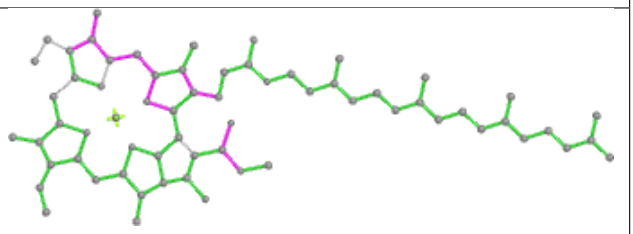
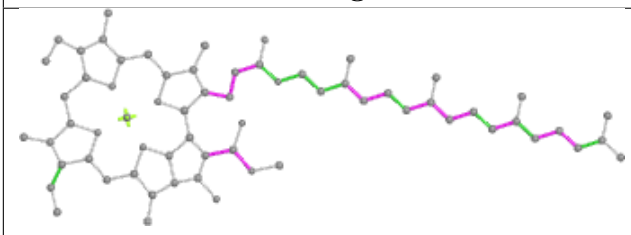


Bond angles



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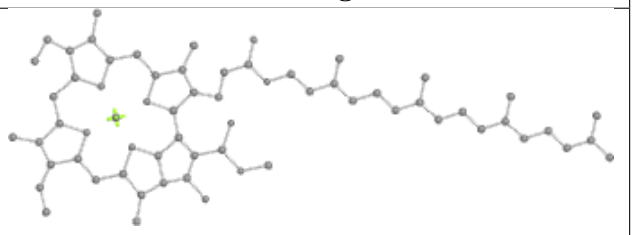
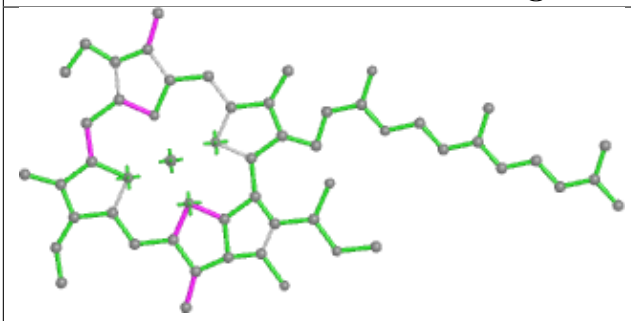


Rings

Ligand CLA u 518



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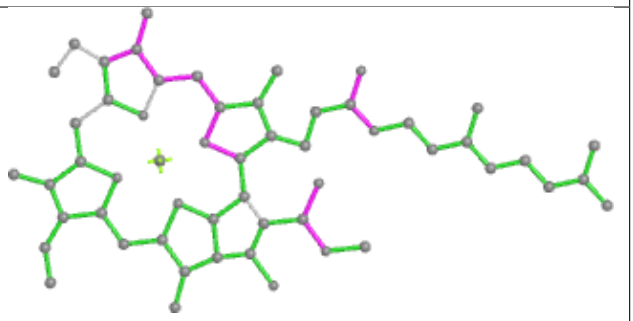

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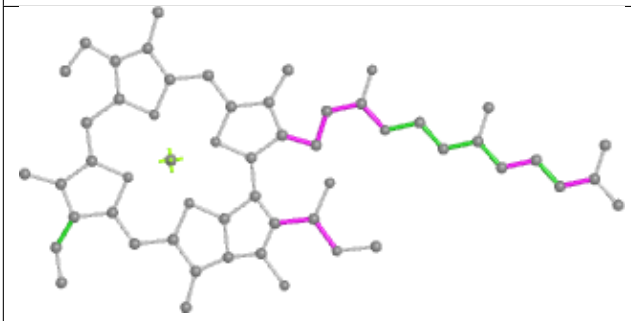

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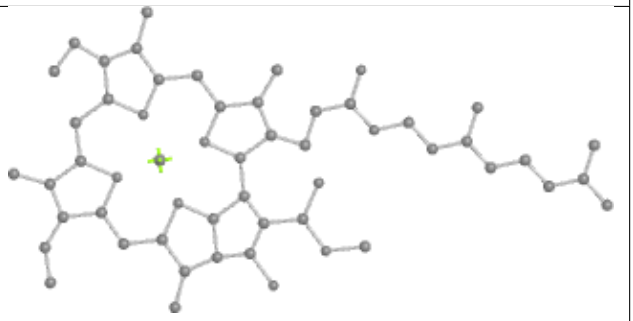
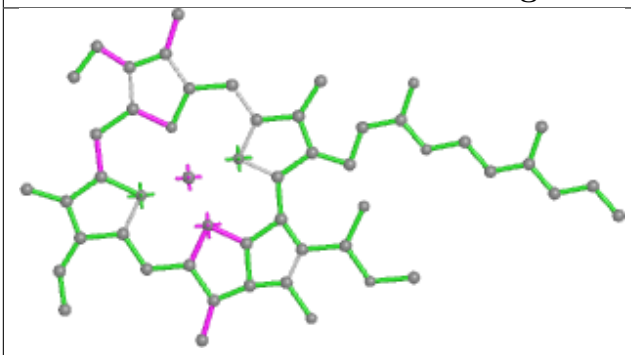
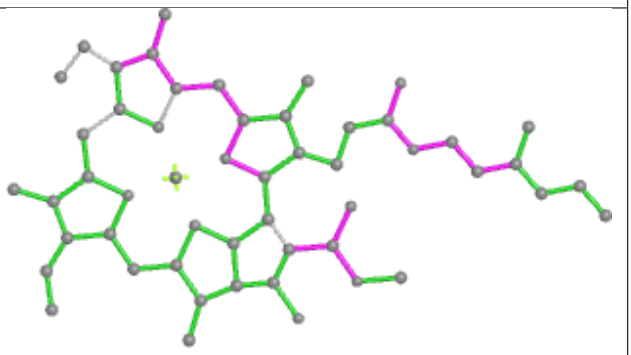
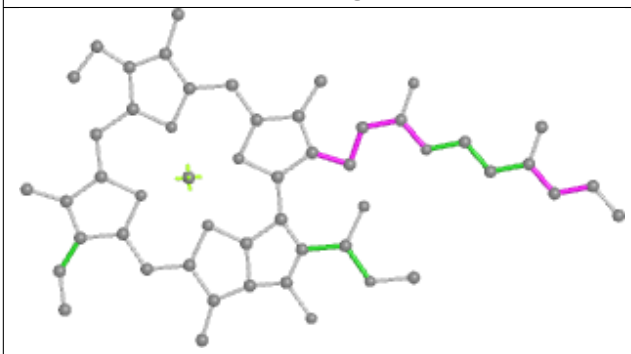
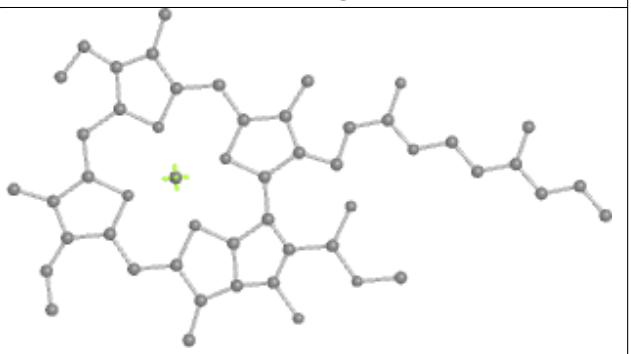
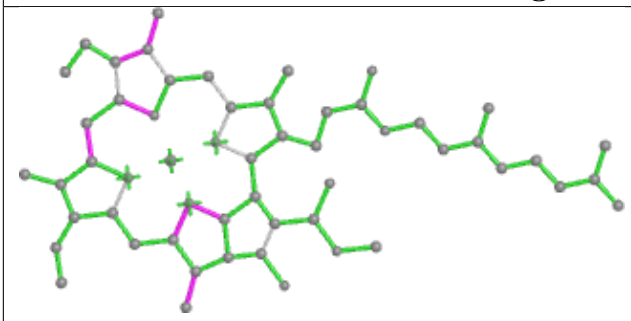
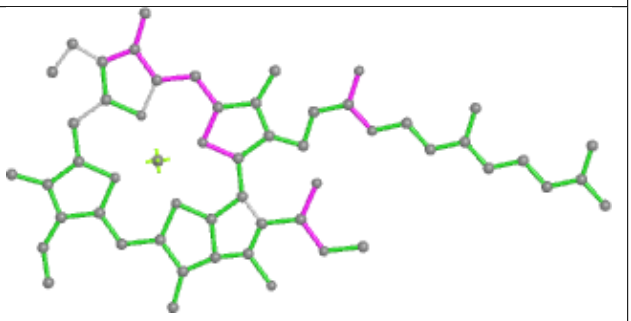
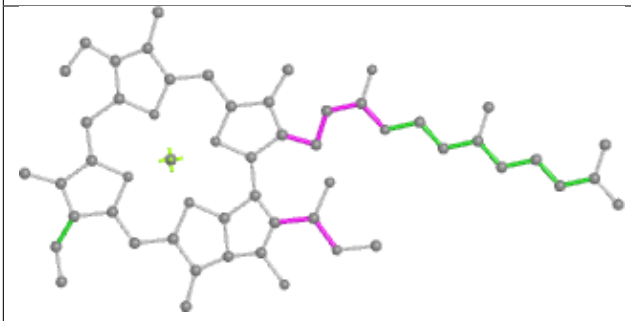
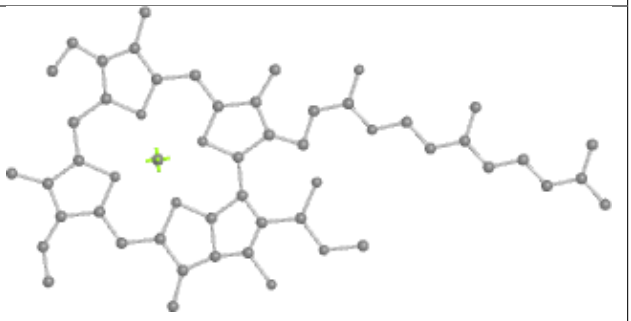
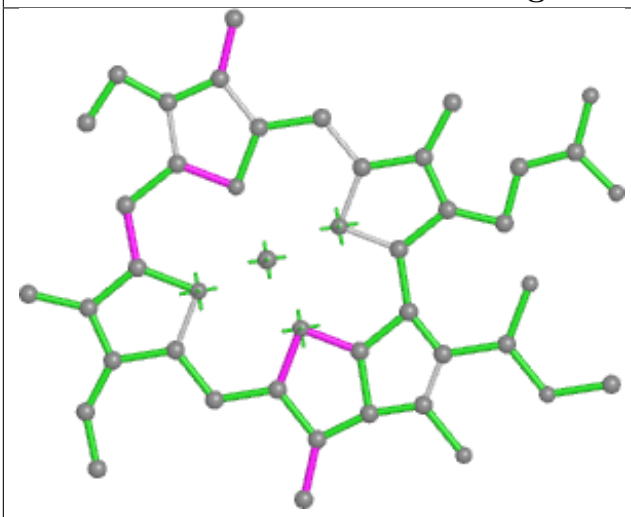


Rings

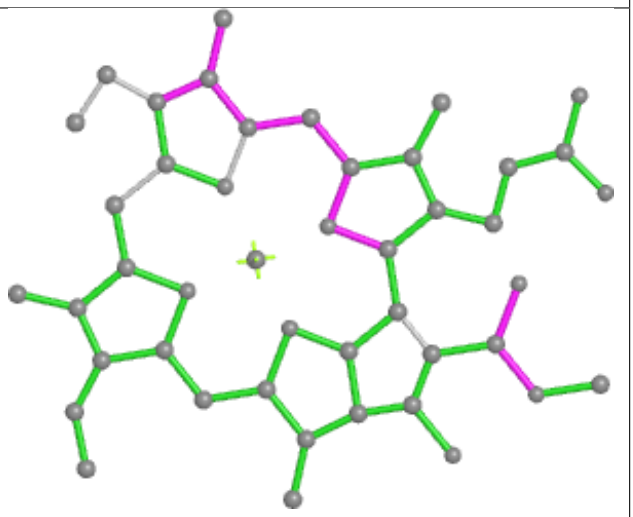
Ligand CLA e 1135	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA t 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

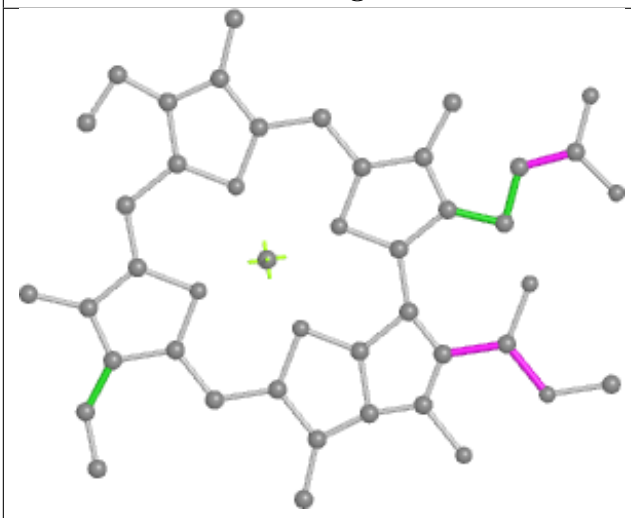
Ligand CLA v 509



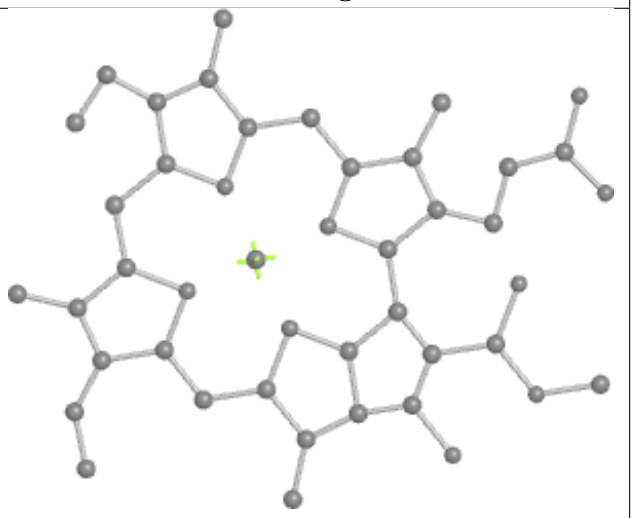
Bond lengths



Bond angles

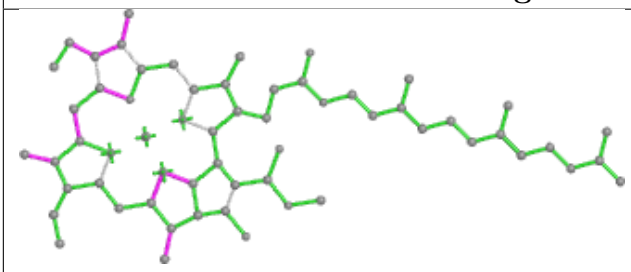


Torsions



Rings

Ligand CLA G 1122



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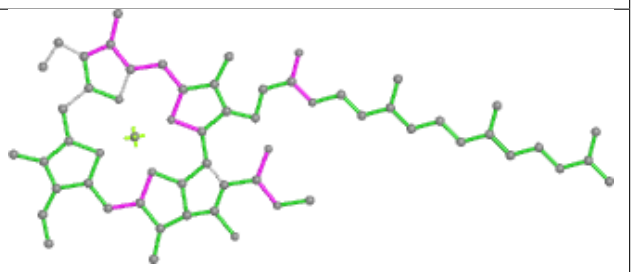

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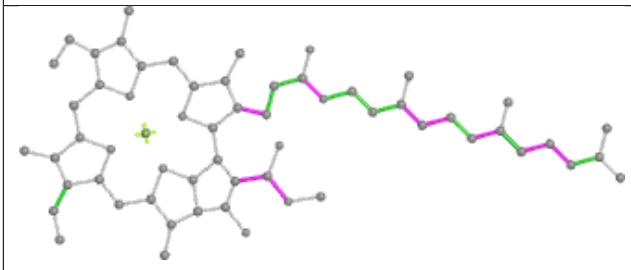

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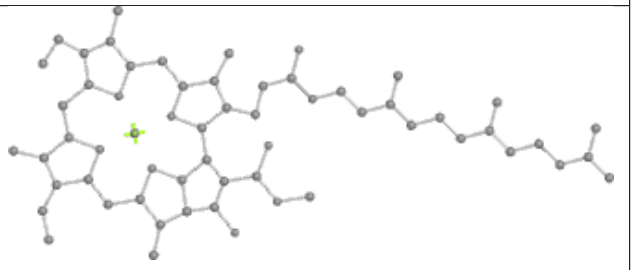
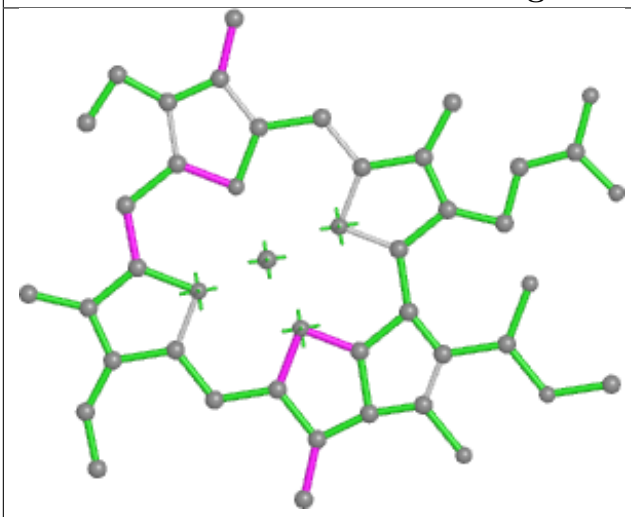


Rings

Ligand CLA u 507



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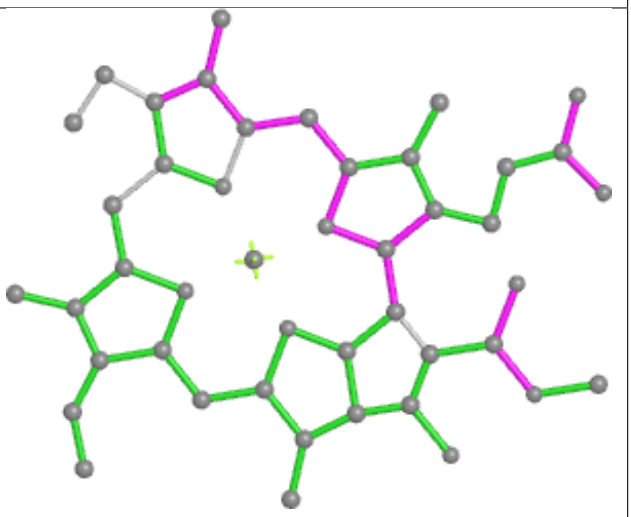
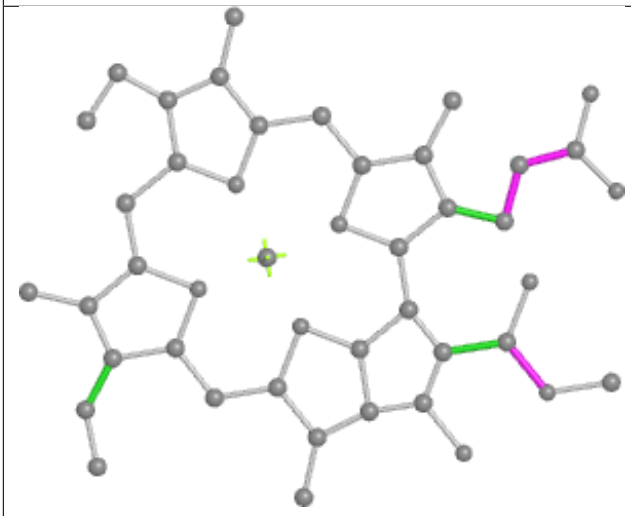


Bond angles



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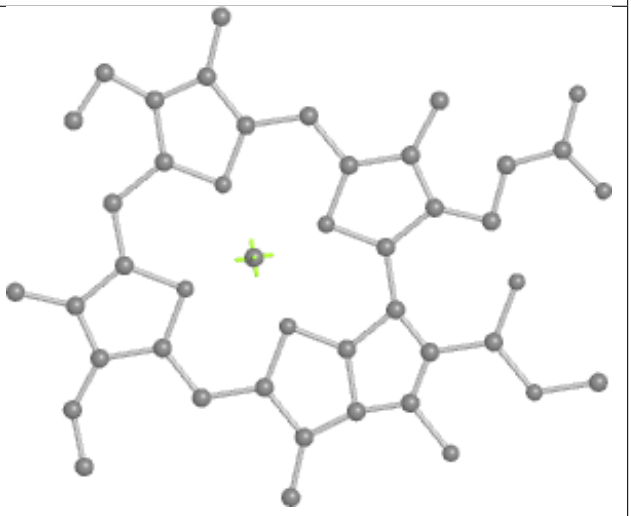
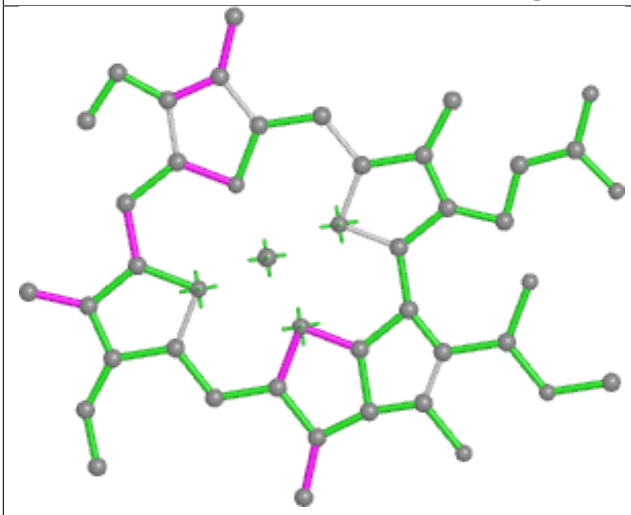


Rings

Ligand CLA 4 508



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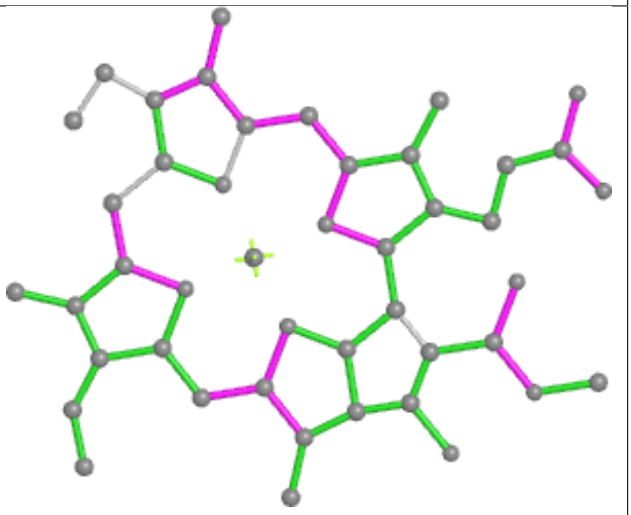
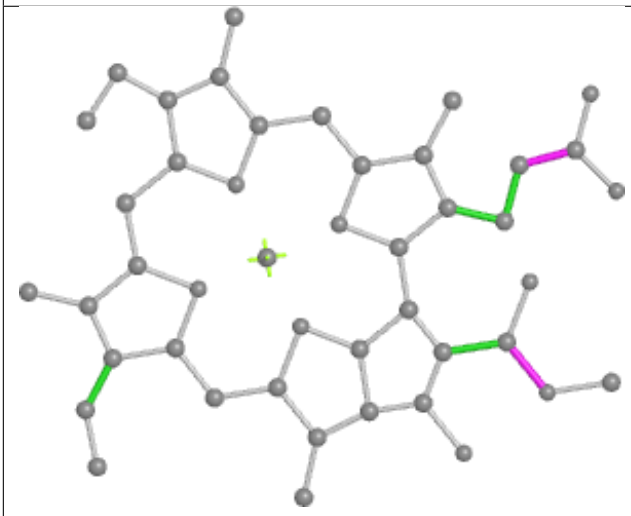


Bond angles



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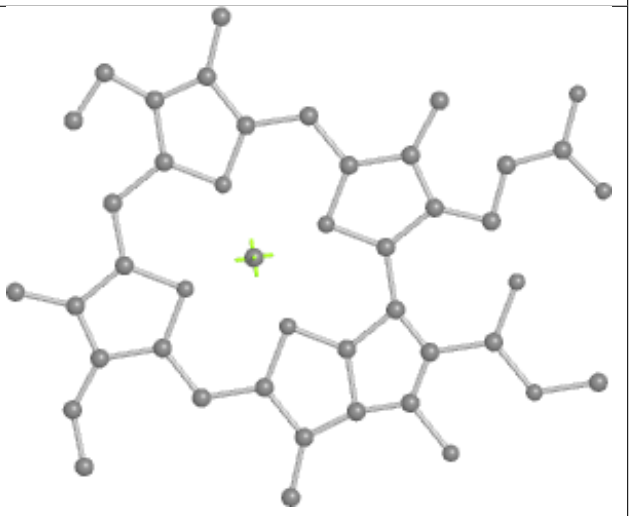
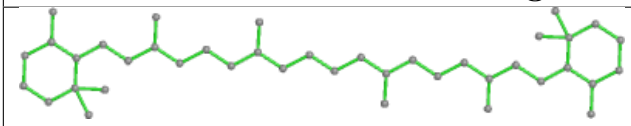


Rings

Ligand BCR 3 523



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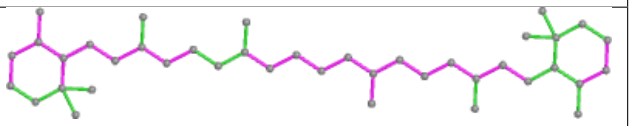
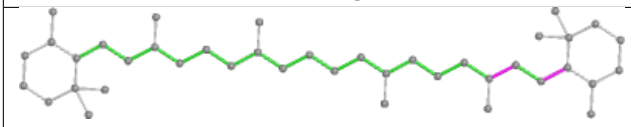


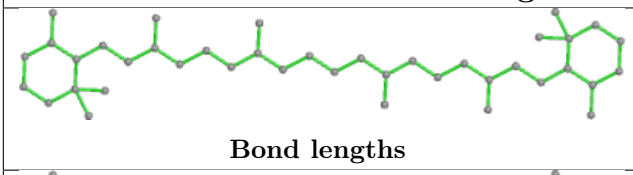
Bond angles



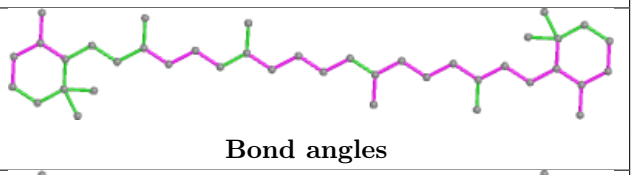
Torsions

Rings

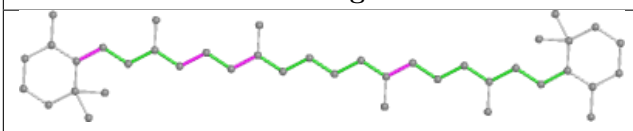
Ligand BCR o 4021



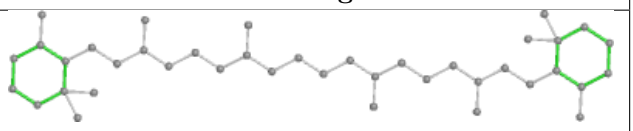
Bond lengths



Bond angles

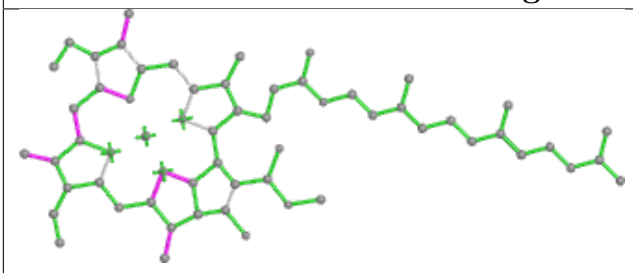


Torsions

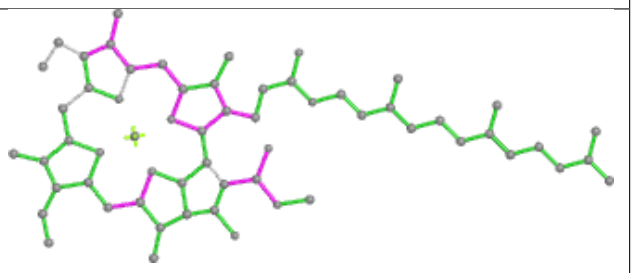


Rings

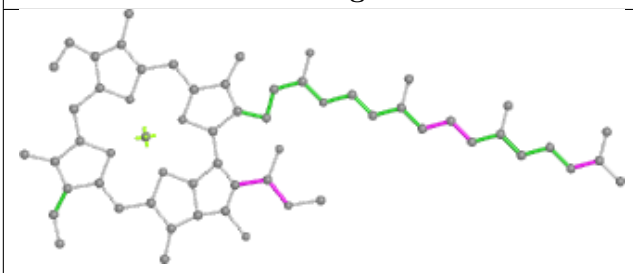
Ligand CLA f 1222



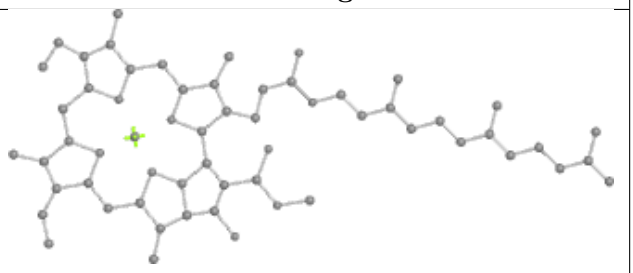
Bond lengths



Bond angles

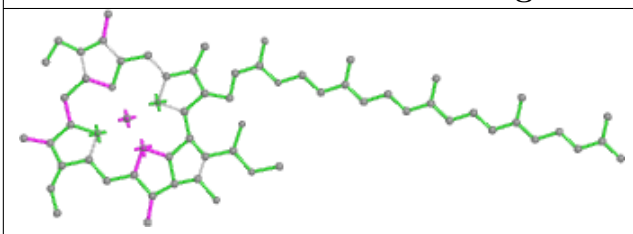


Torsions

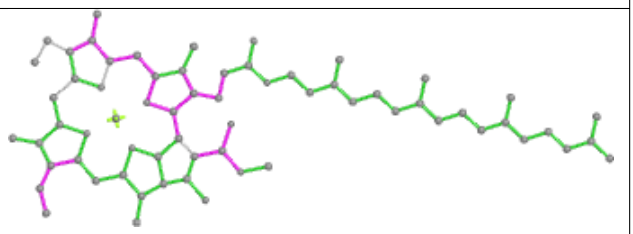


Rings

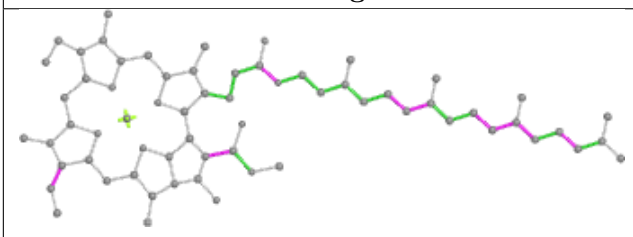
Ligand CLA B 1234



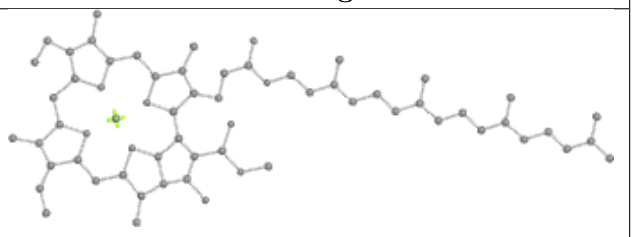
Bond lengths



Bond angles

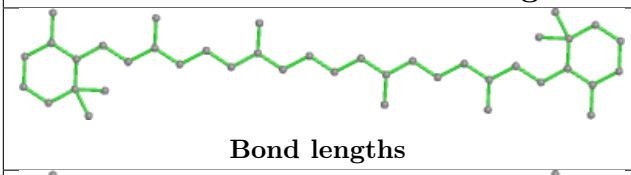


Torsions

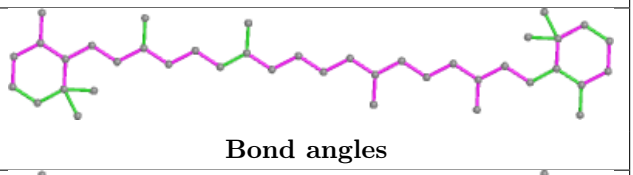


Rings

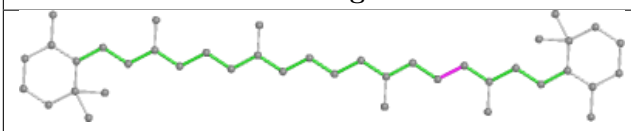
Ligand BCR f 4009



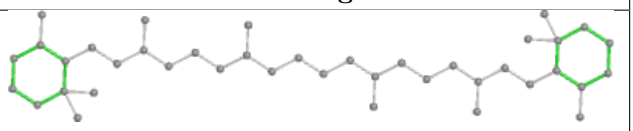
Bond lengths



Bond angles

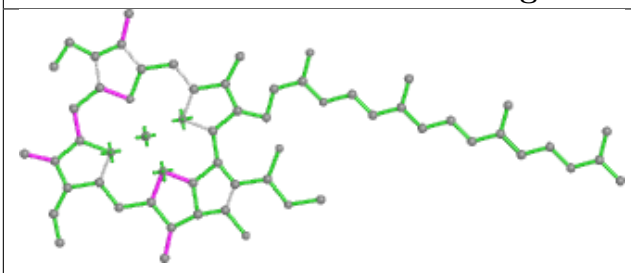


Torsions

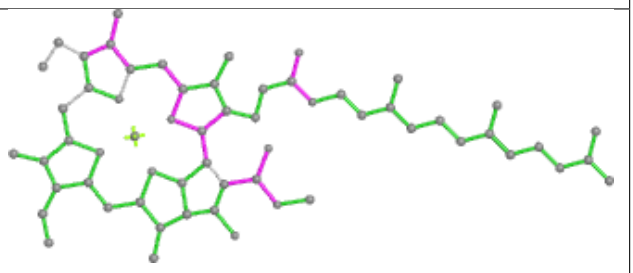


Rings

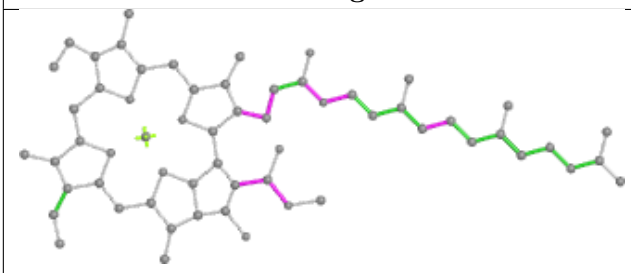
Ligand CLA e 1118



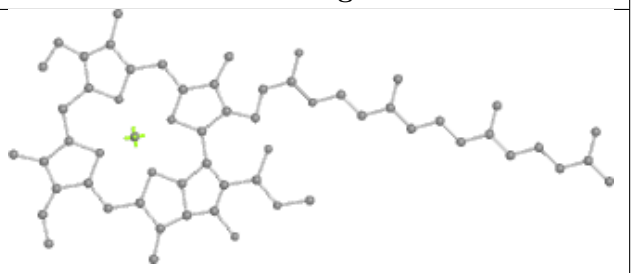
Bond lengths



Bond angles

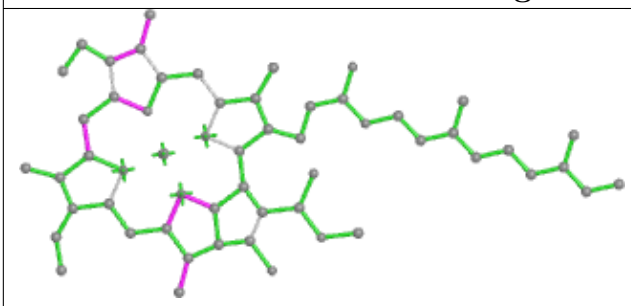


Torsions

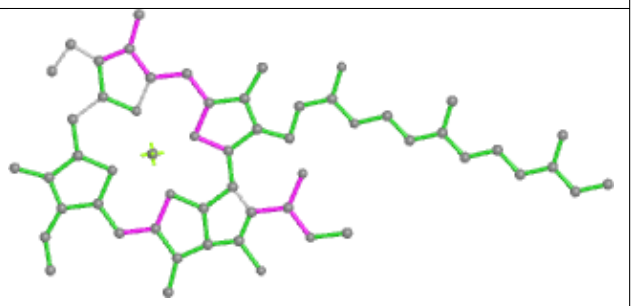


Rings

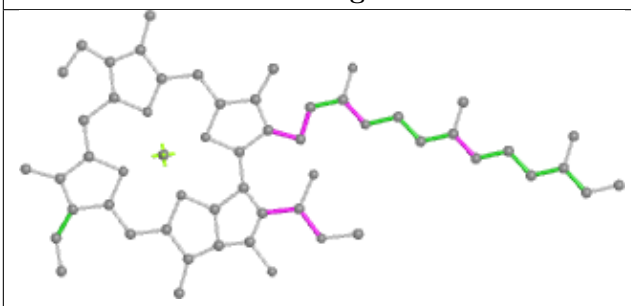
Ligand CLA G 1134



Bond lengths



Bond angles



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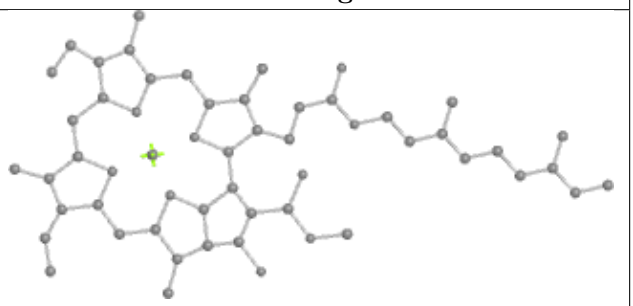
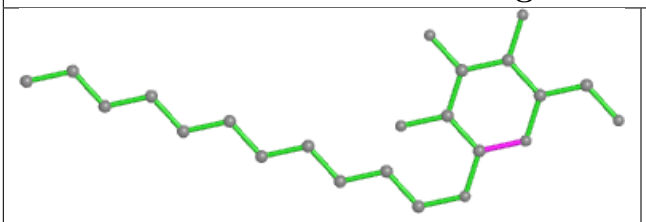
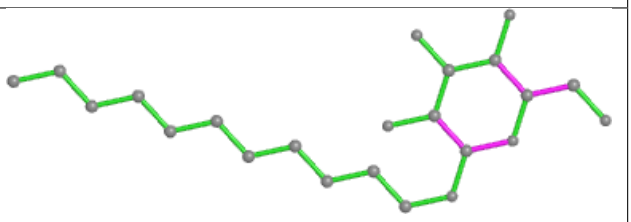


Rings

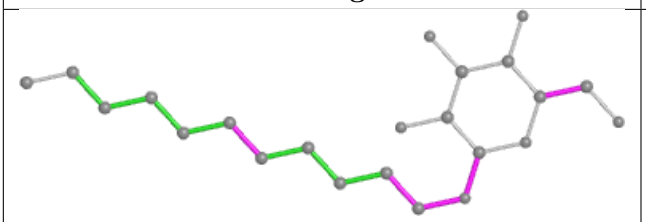
Ligand LMU e 1849



Bond lengths



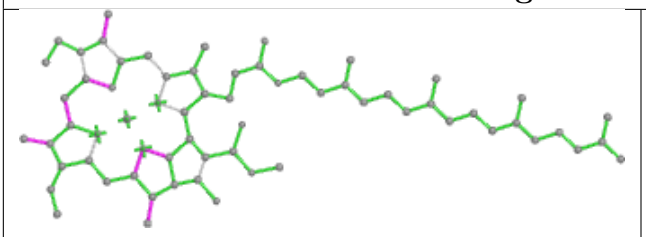
Bond angles



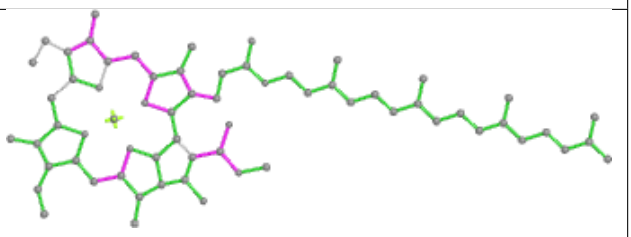
Torsions

Rings

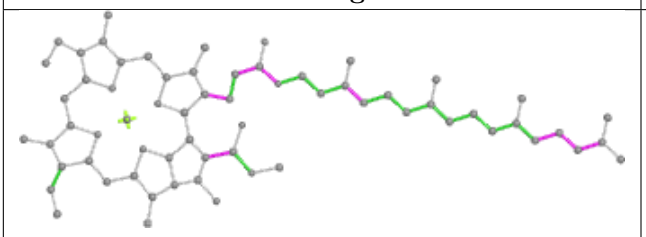
Ligand CLA B 1202



Bond lengths



Bond angles



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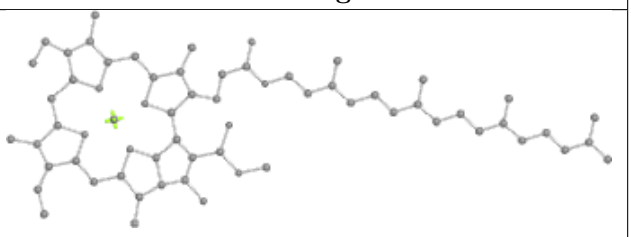
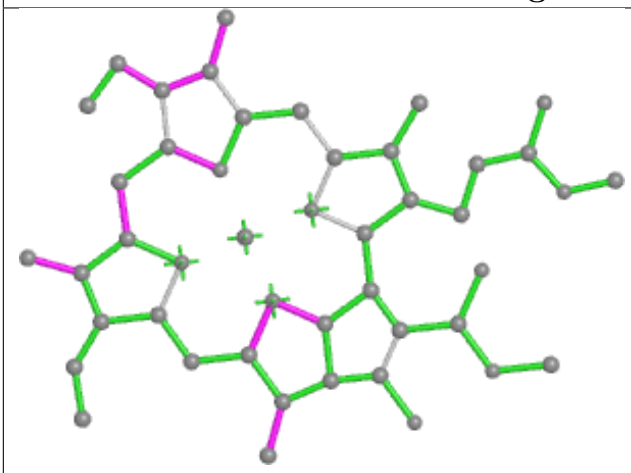


Rings

Ligand CLA 5 519



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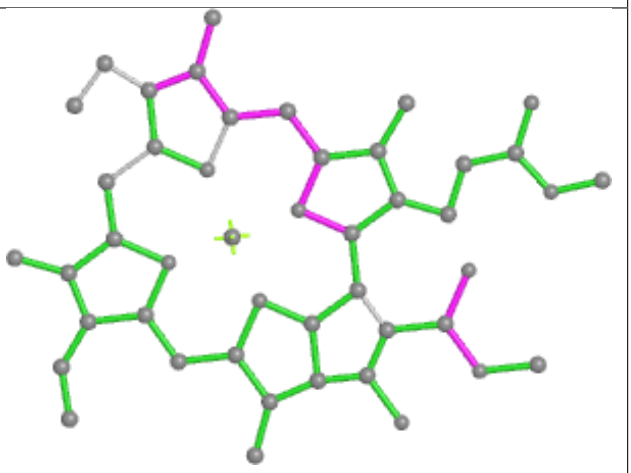
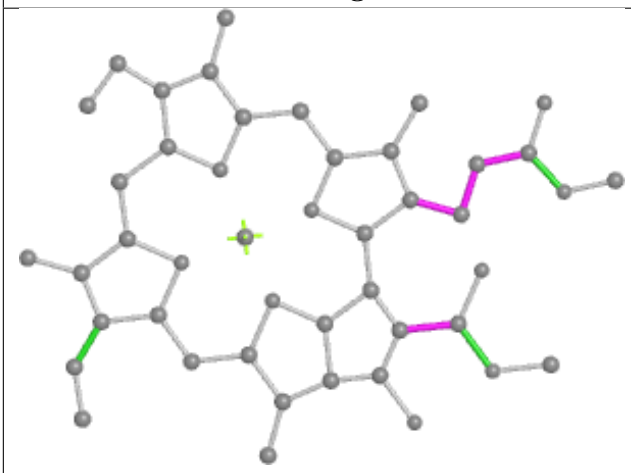
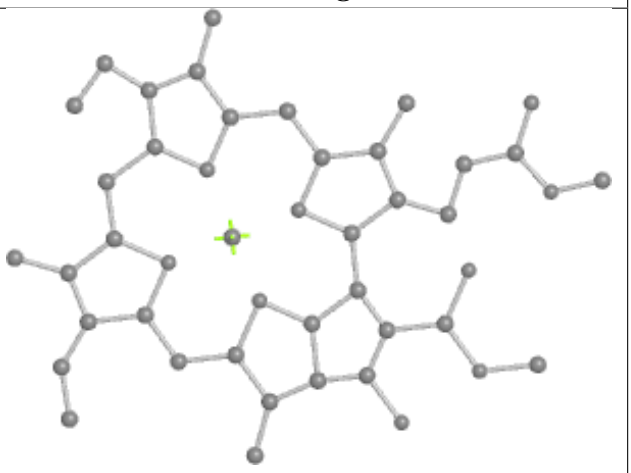


Bond angles

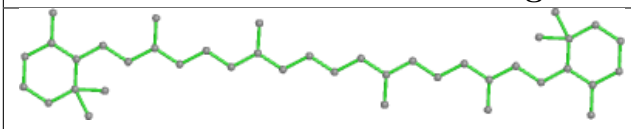


Torsions

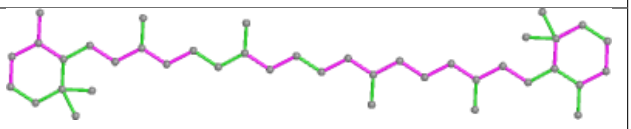


Rings

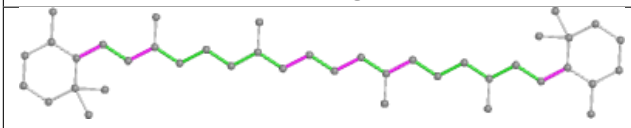
Ligand BCR b 521



Bond lengths



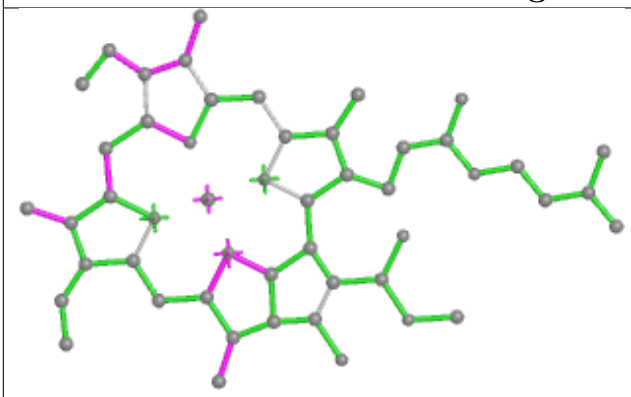
Bond angles



Torsions

Rings

Ligand CLA 1 519



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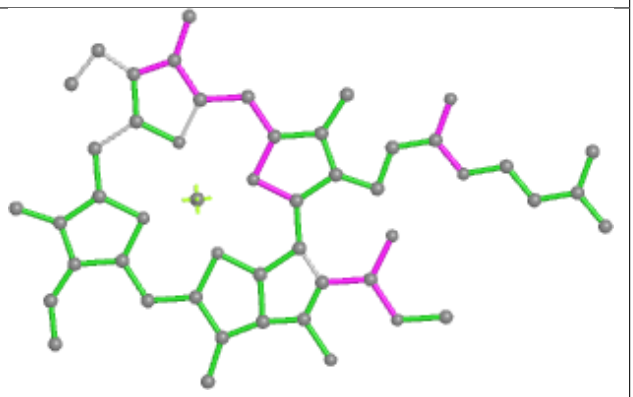
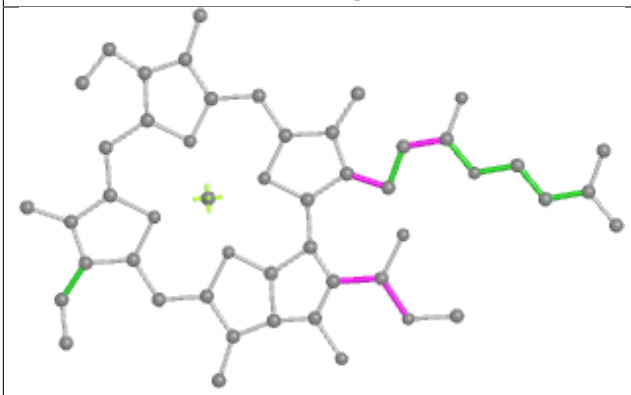
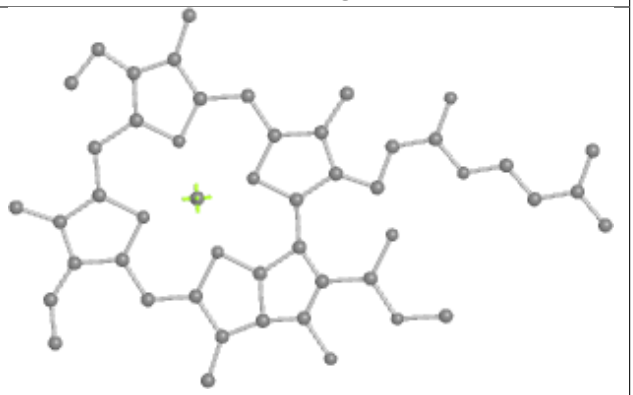


Bond angles

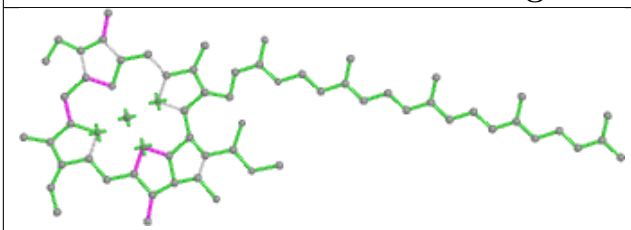


Torsions



Rings

Ligand CLA Z 507



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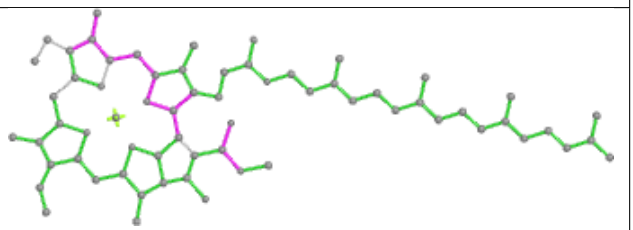
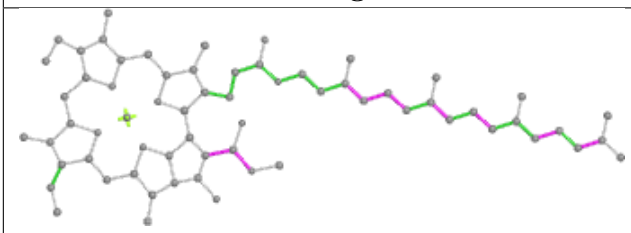
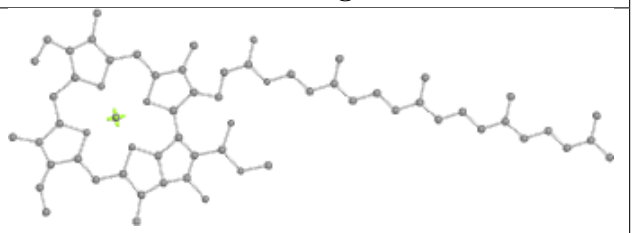


Bond angles

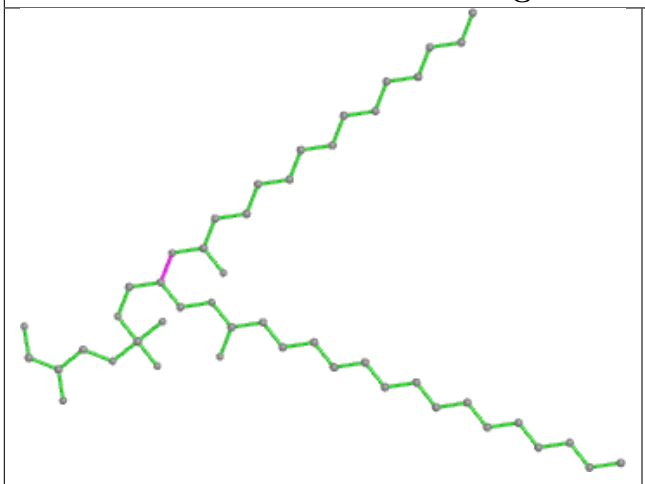


Torsions

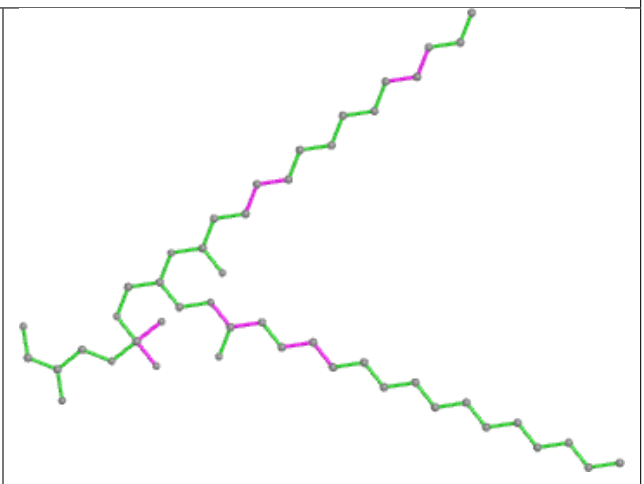


Rings

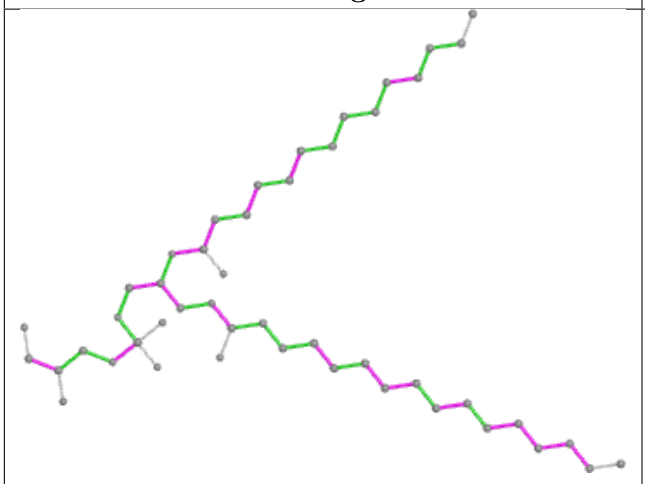
Ligand LHG G 5007



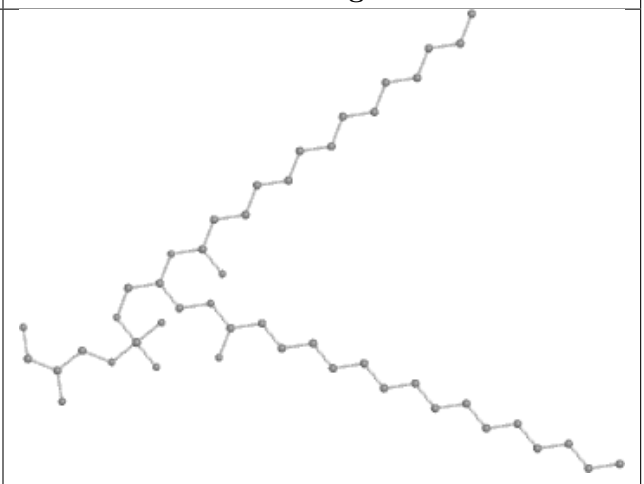
Bond lengths



Bond angles

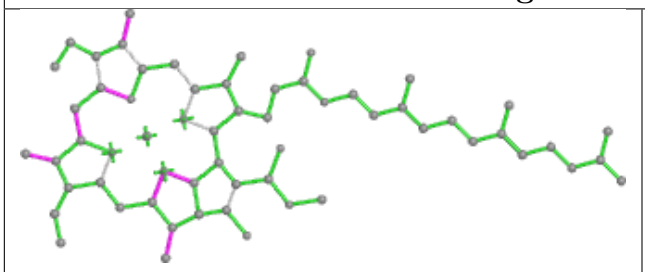


Torsions

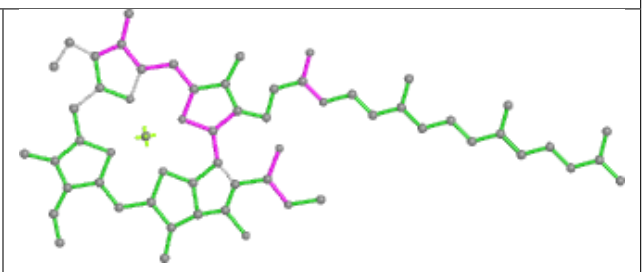


Rings

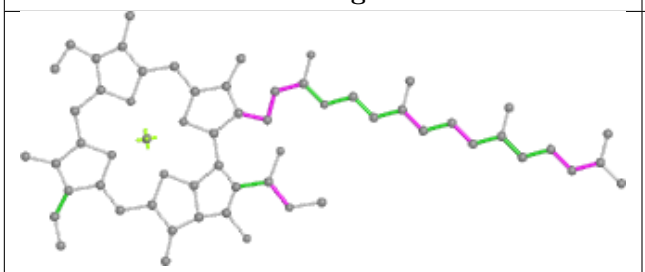
Ligand CLA B 1224



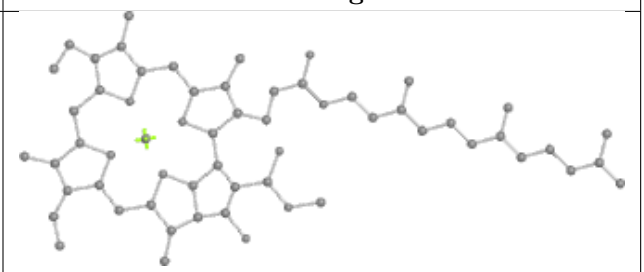
Bond lengths



Bond angles

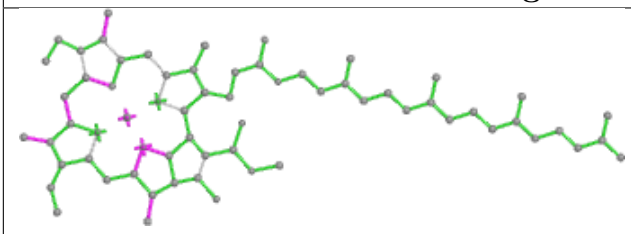


Torsions

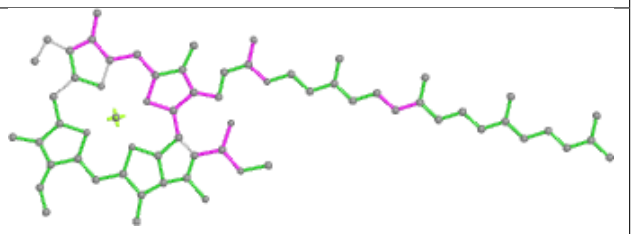


Rings

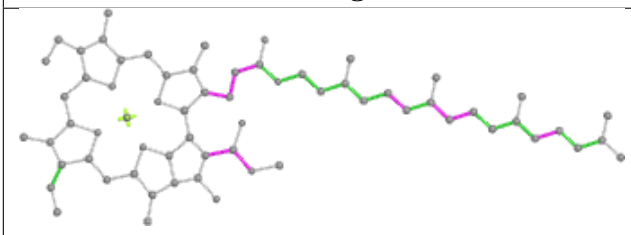
Ligand CLA f 1221



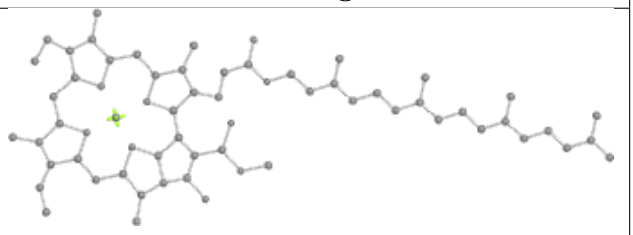
Bond lengths



Bond angles

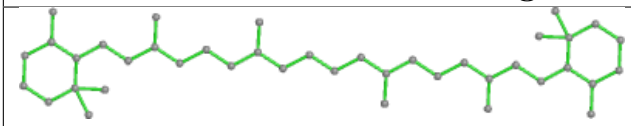


Torsions

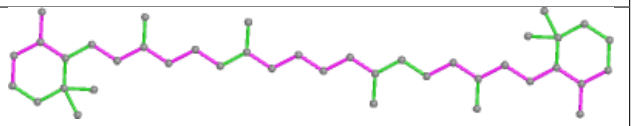


Rings

Ligand BCR e 4002



Bond lengths



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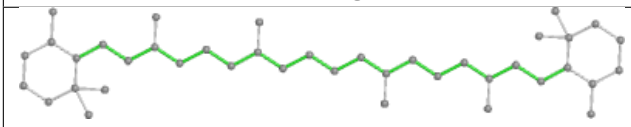
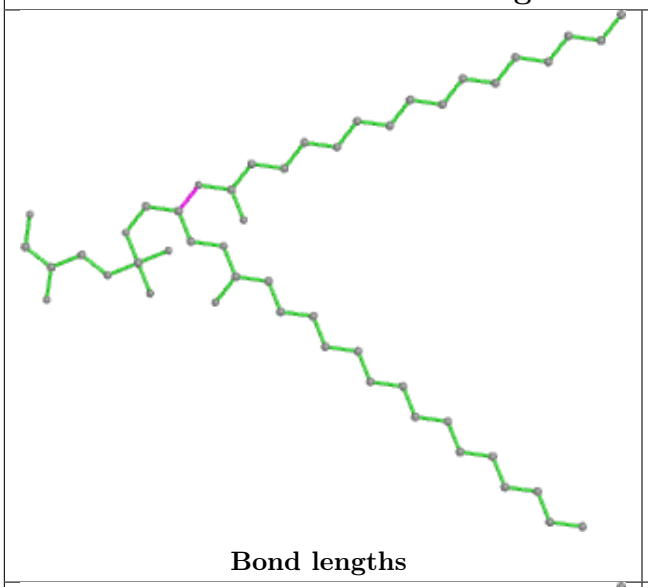


Torsions

Rings

Ligand LHG A 5001



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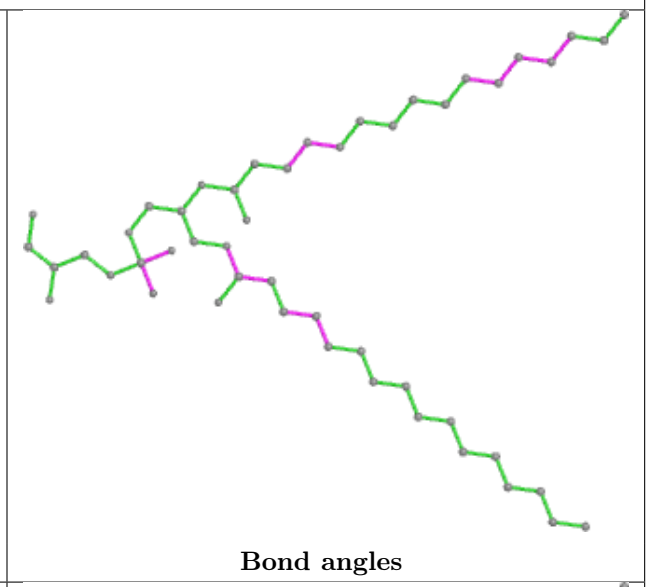

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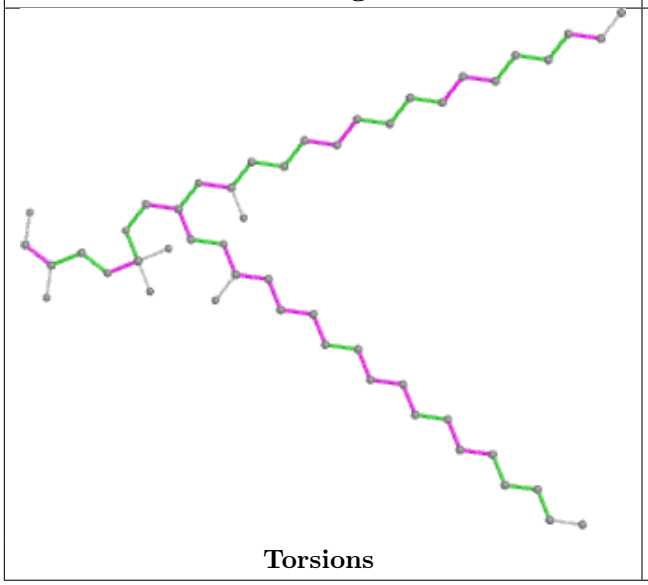

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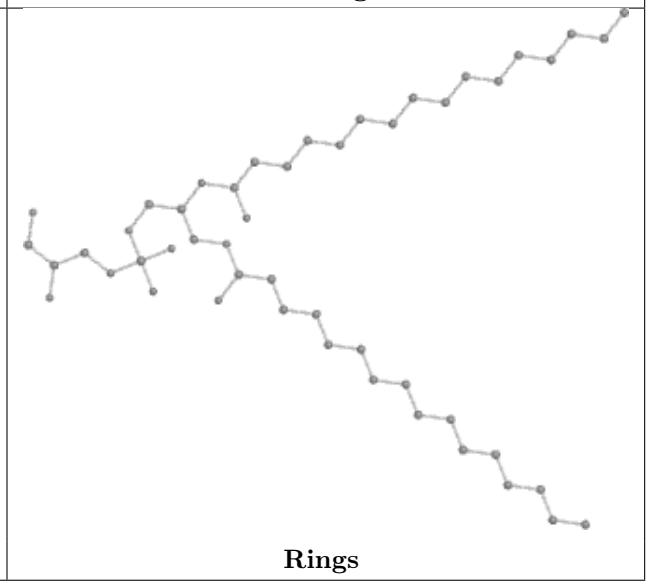
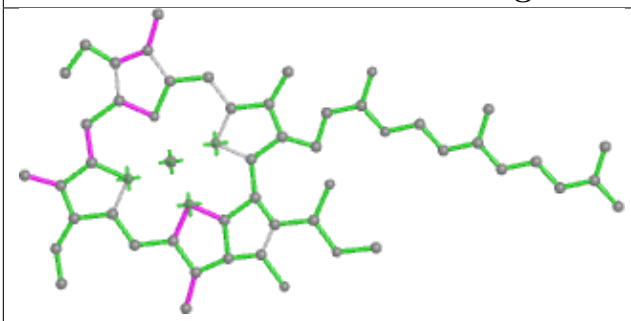


Rings

Ligand CLA K 1401



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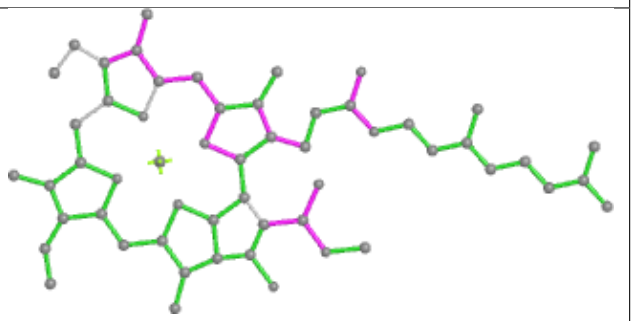

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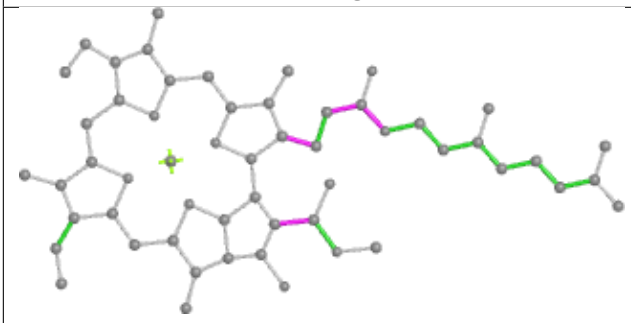

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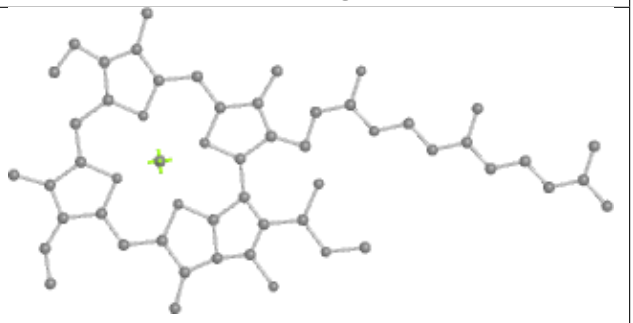
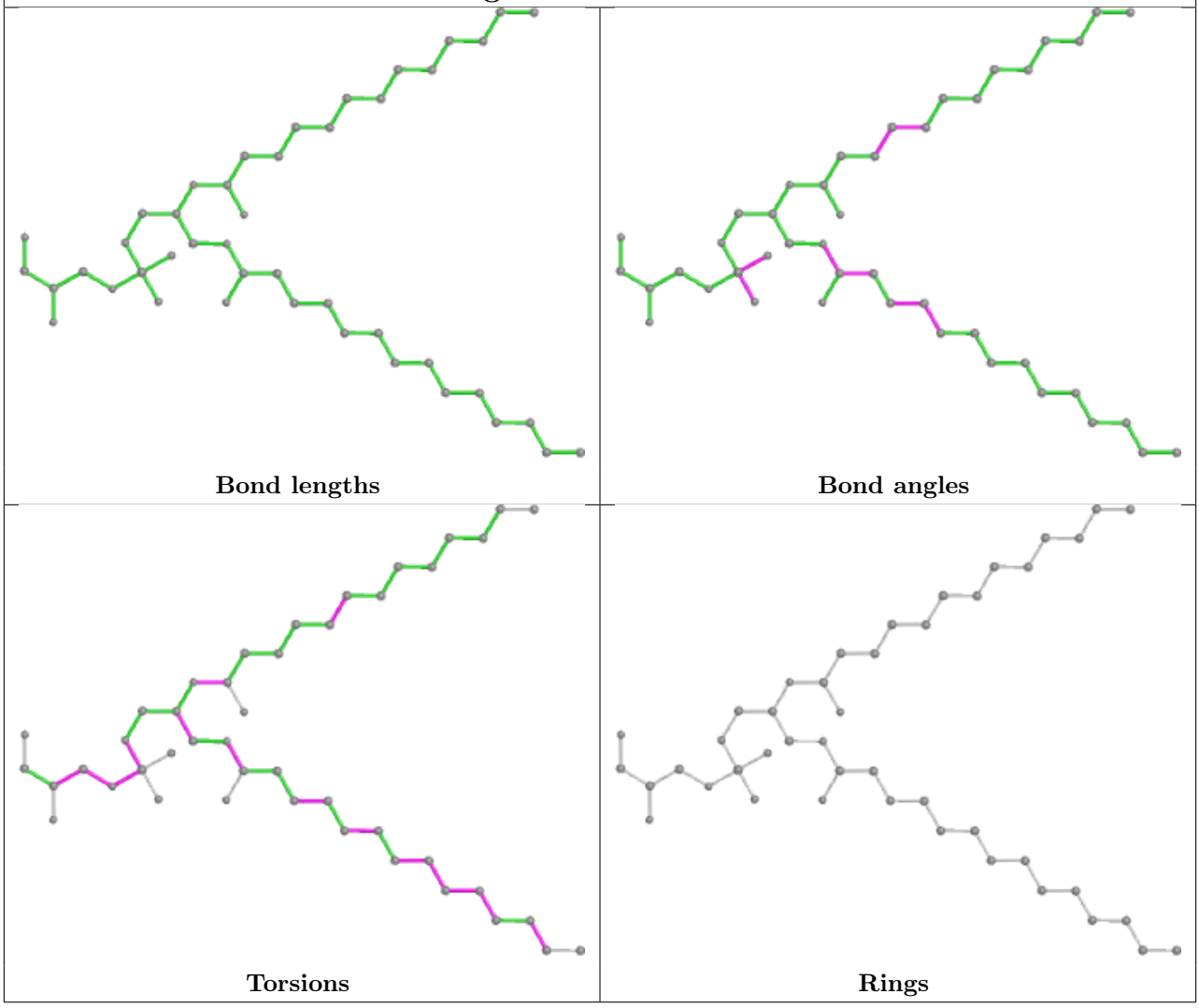
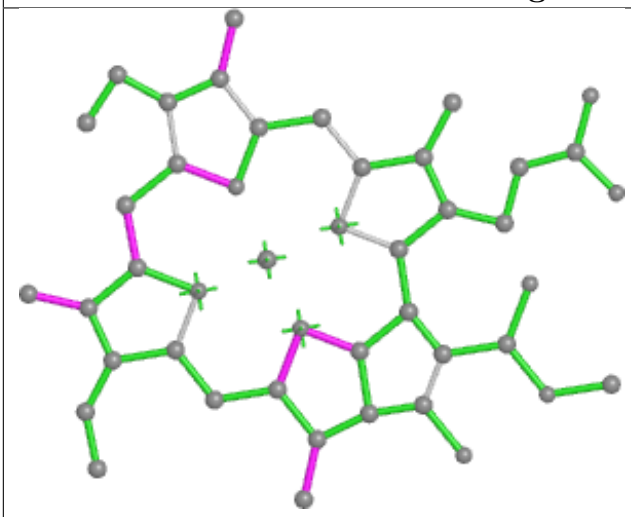


Rings

Ligand LHG S 5001



Ligand CLA 6 517



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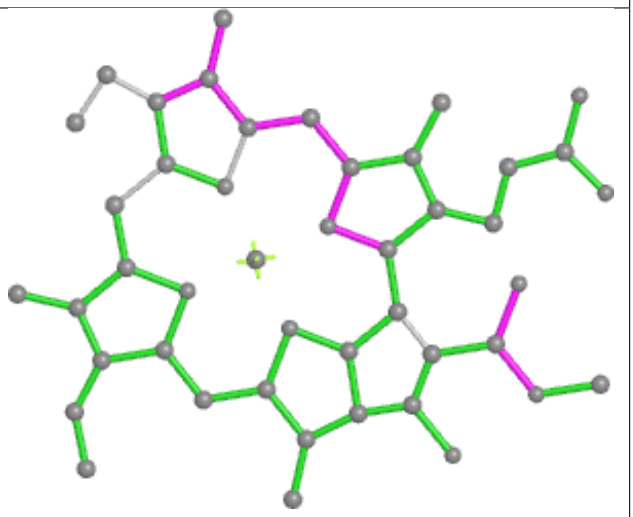

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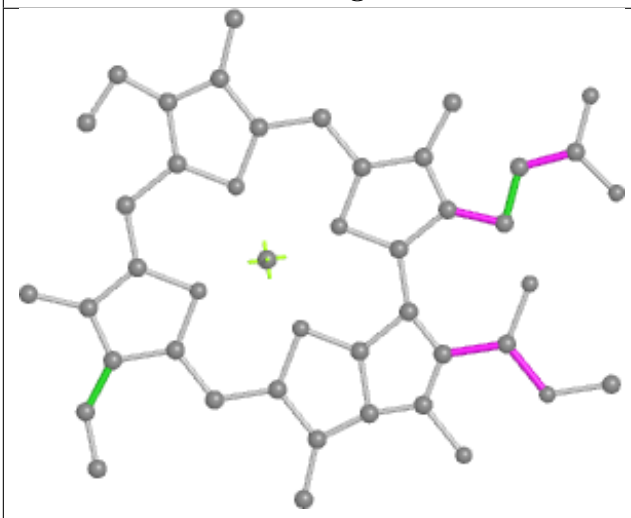

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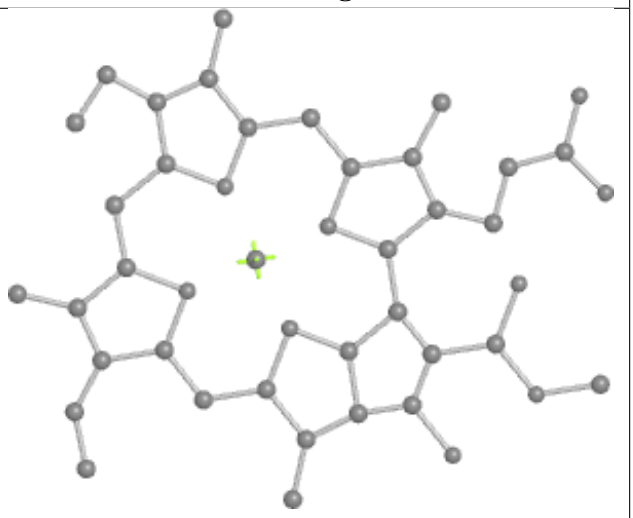
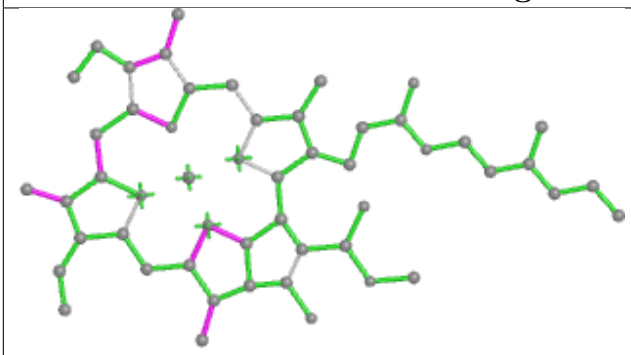


Rings

Ligand CLA H 1209



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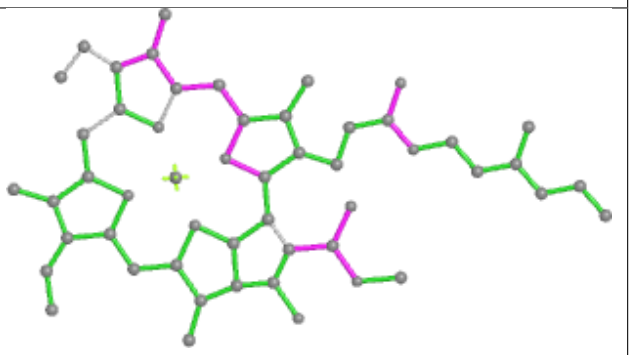
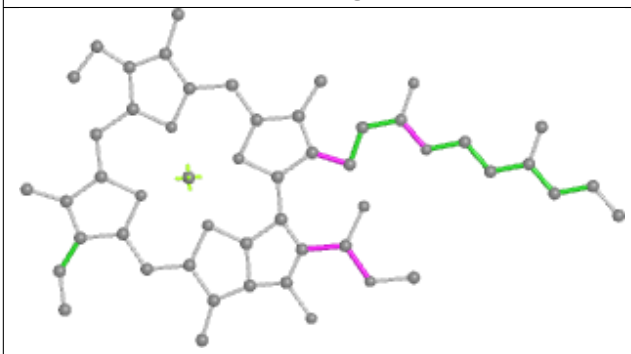


Bond angles



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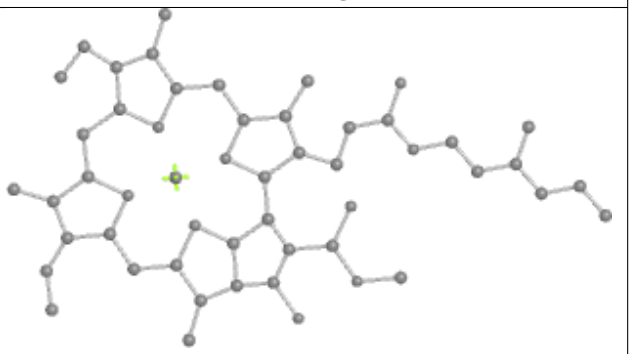
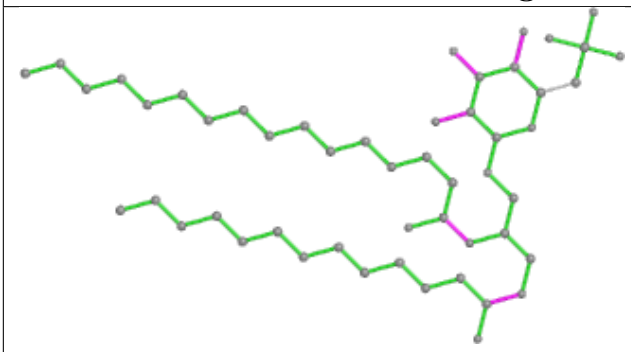


Rings

Ligand SQD L 5216



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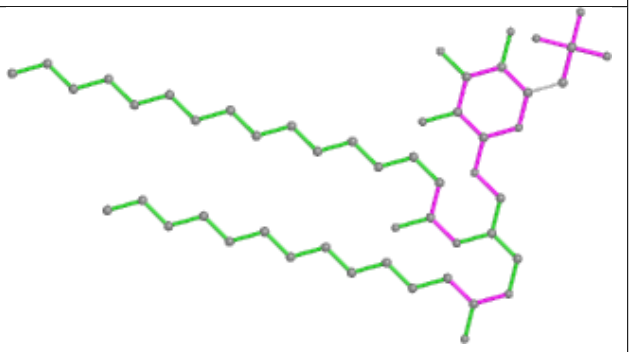

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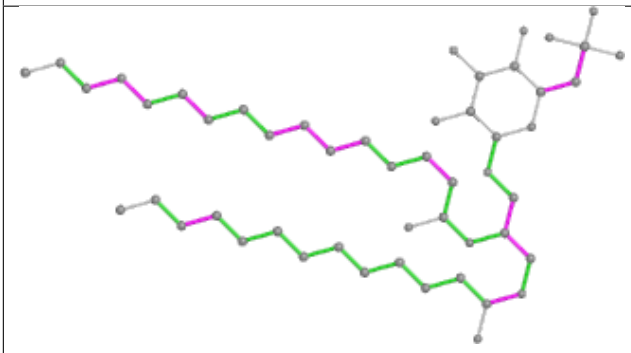

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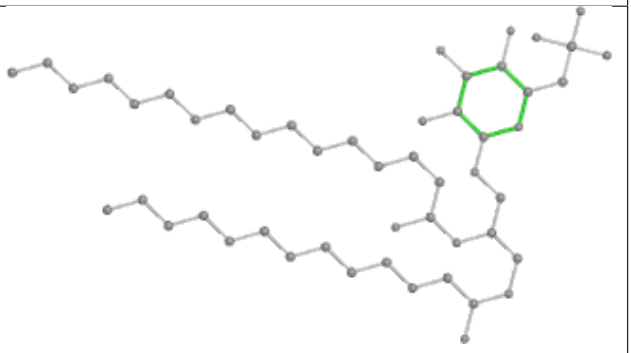
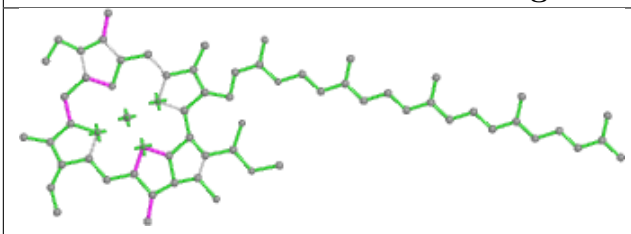


Rings

Ligand CLA t 505



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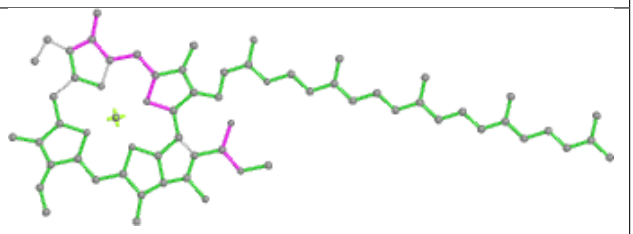

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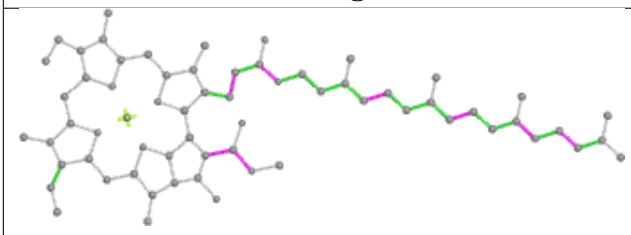

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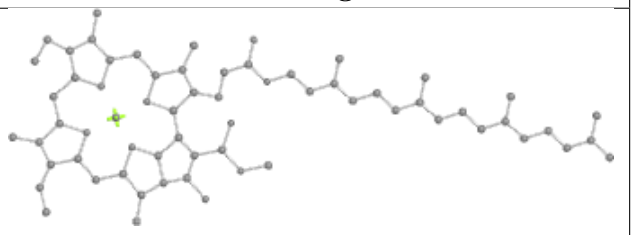
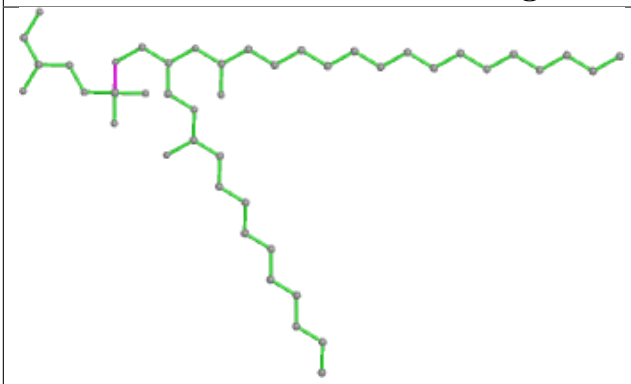


Rings

Ligand LHG f 1855



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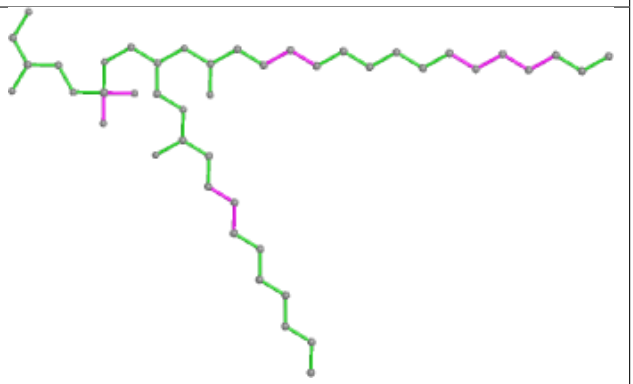

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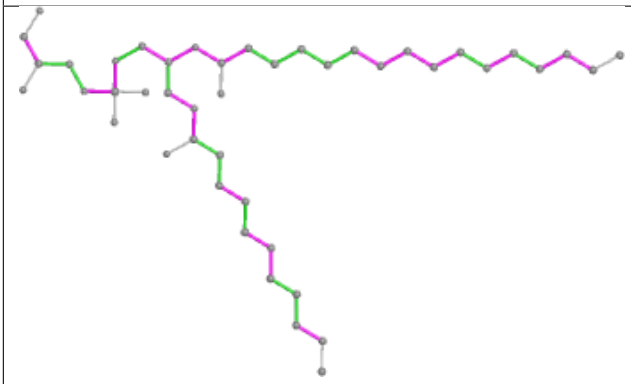

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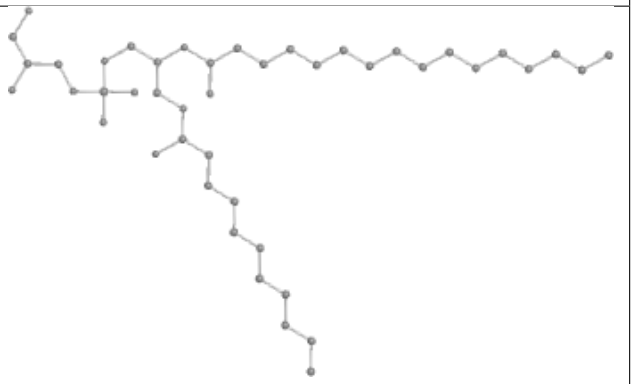
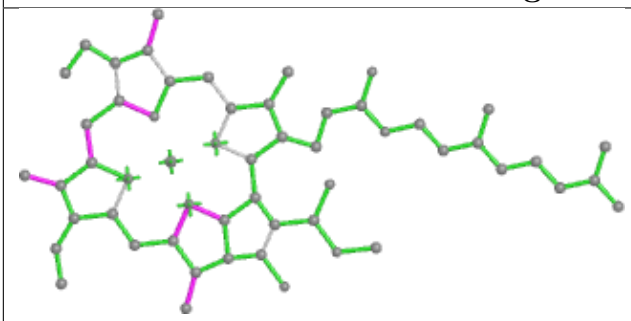


Rings

Ligand CLA Y 513



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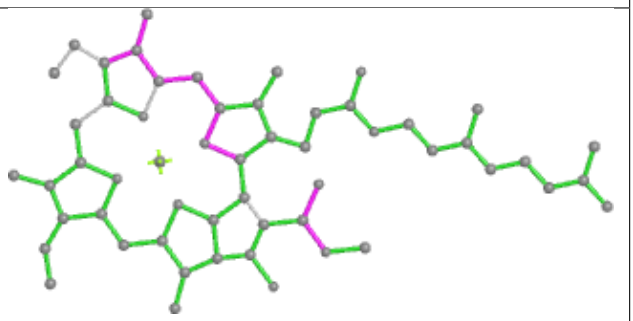
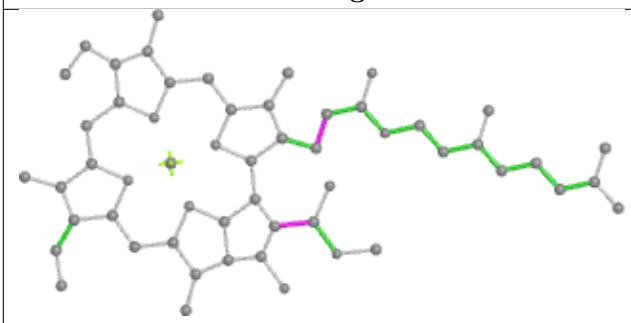


Bond angles



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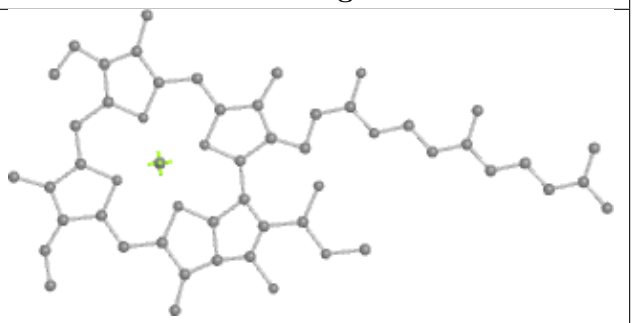
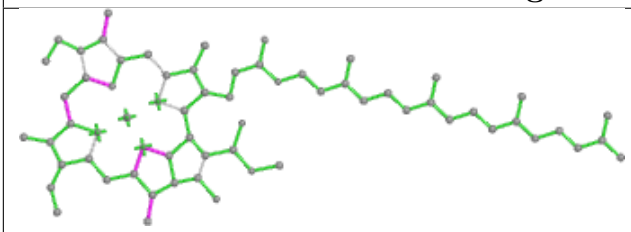


Rings

Ligand CLA Z 518



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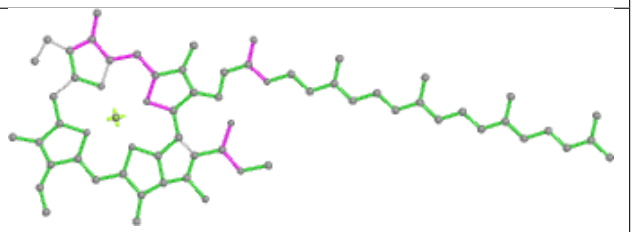

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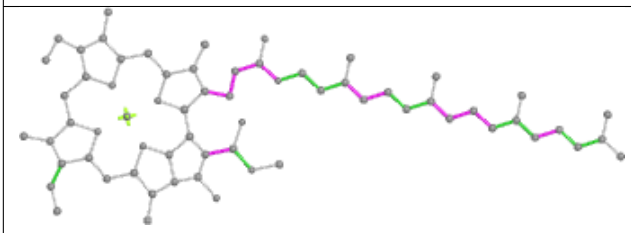

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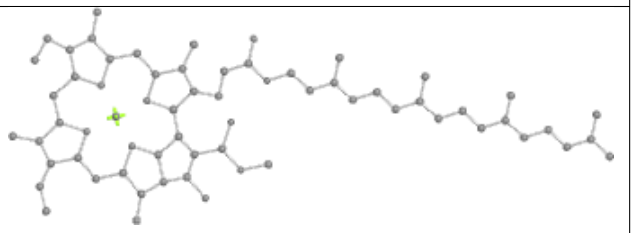
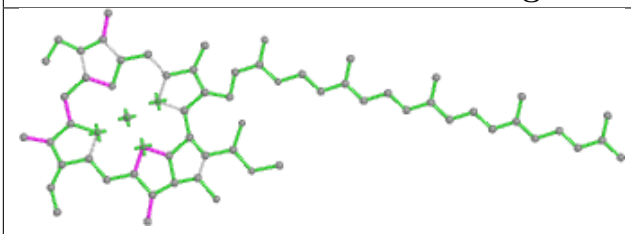


Rings

Ligand CLA f 1223



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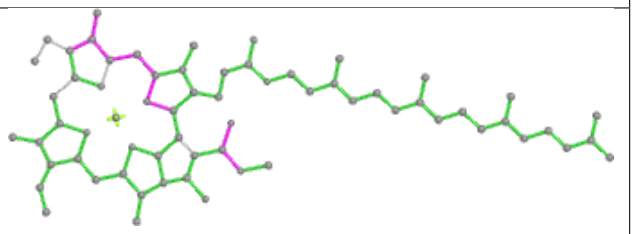
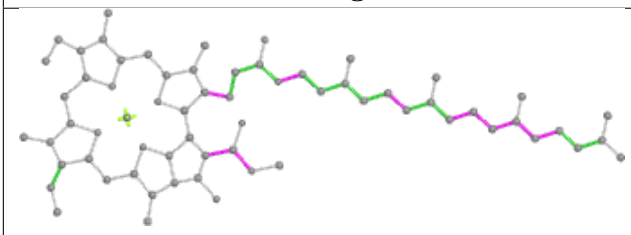


Bond angles



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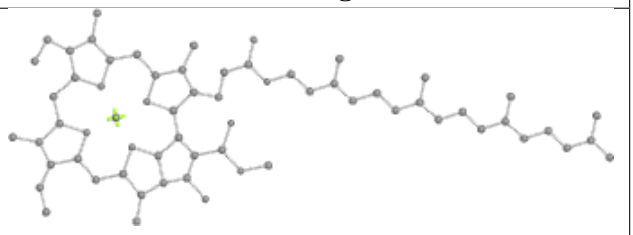
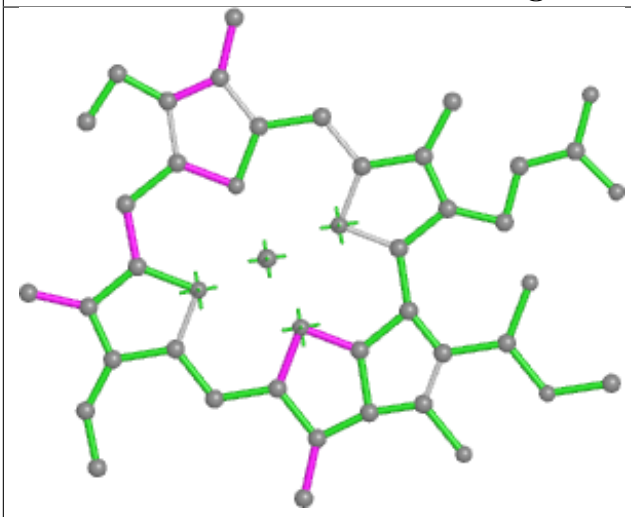


Rings

Ligand CLA u 513



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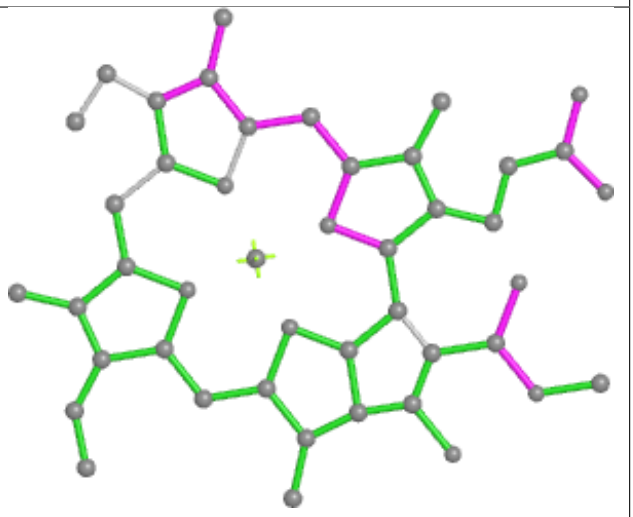
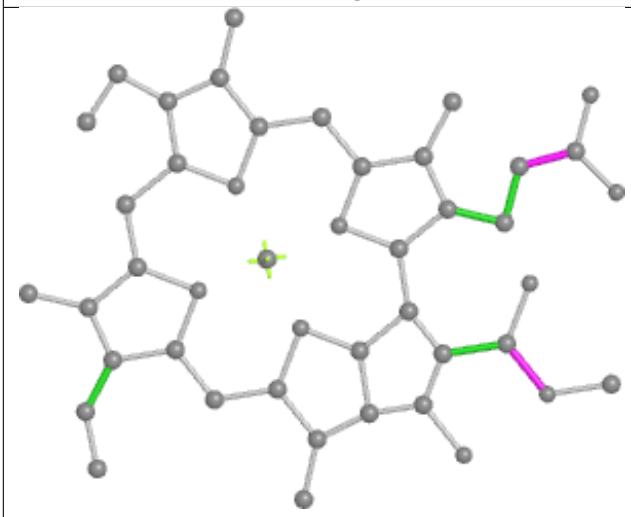


Bond angles



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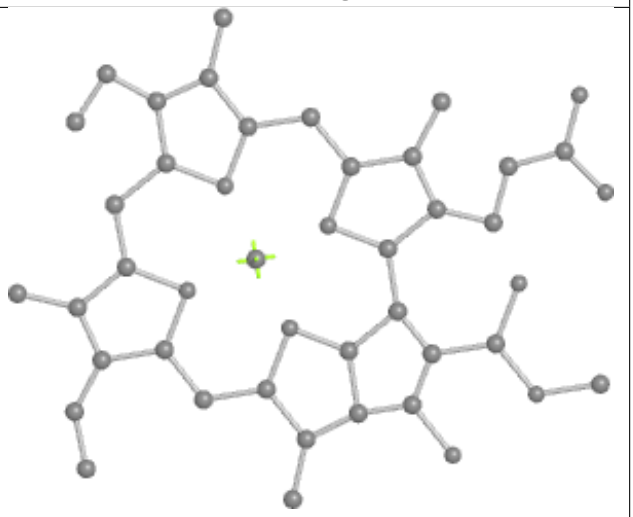
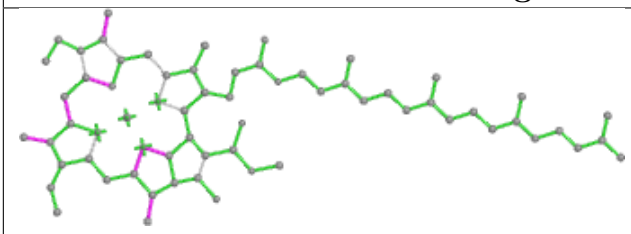


Rings

Ligand CLA G 1138



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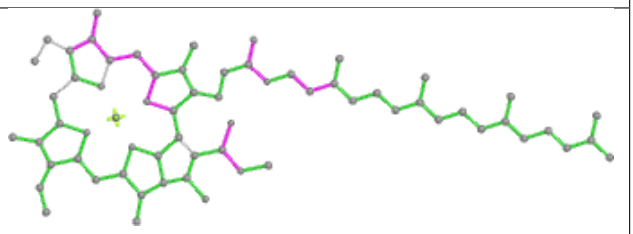
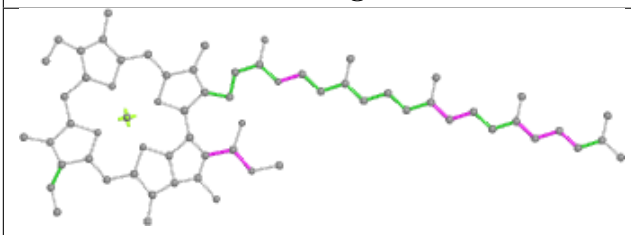


Bond angles



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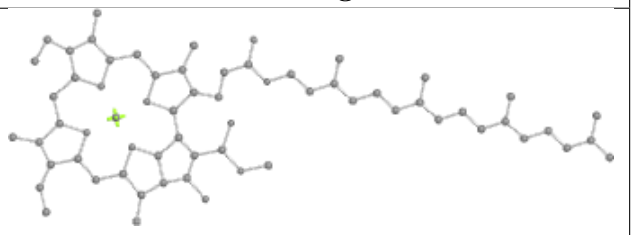
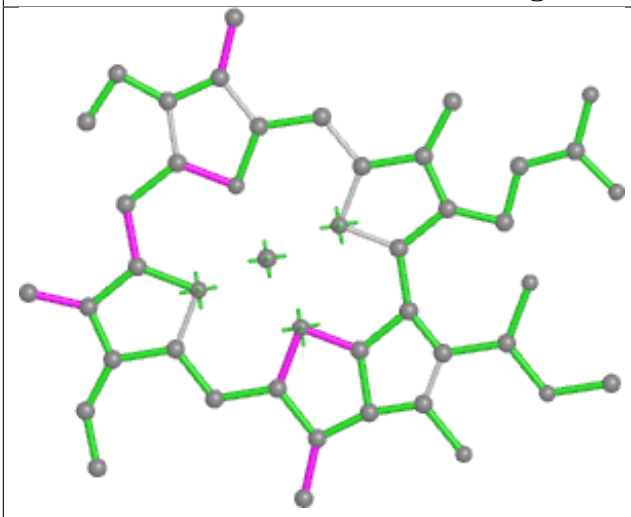


Rings

Ligand CLA 2 517



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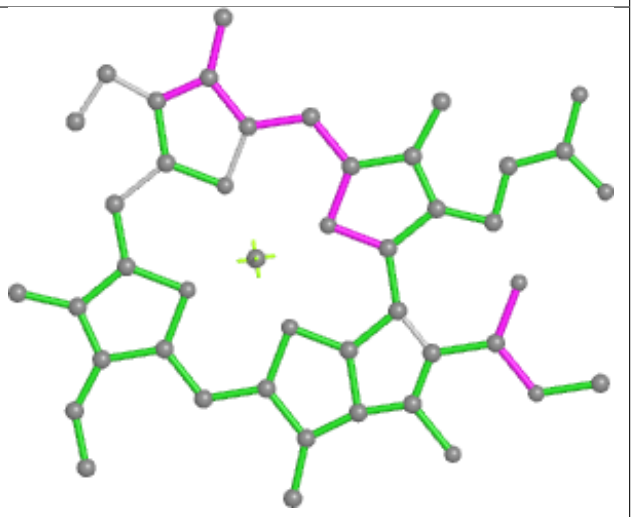
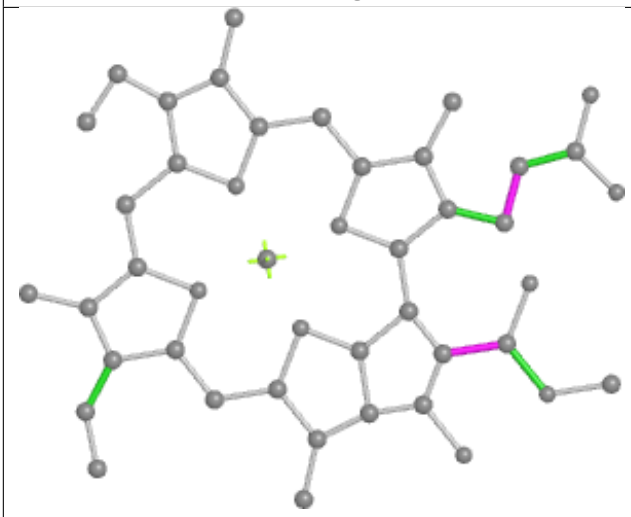
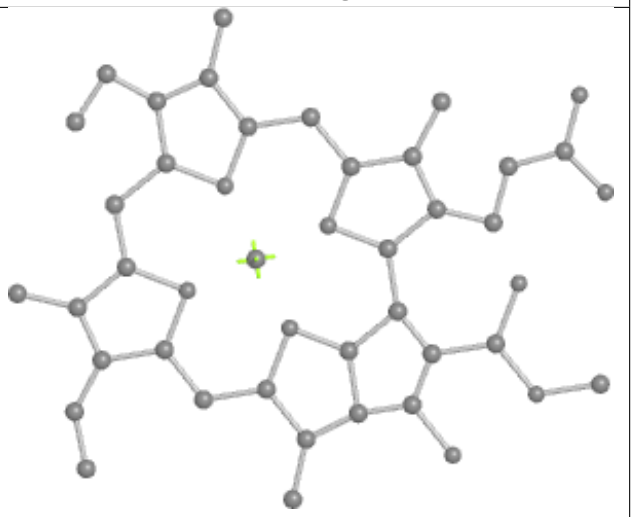


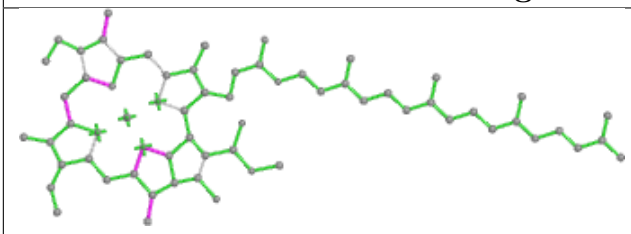
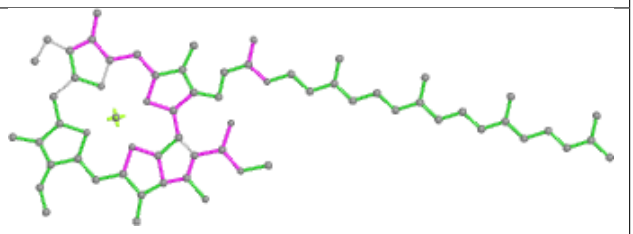
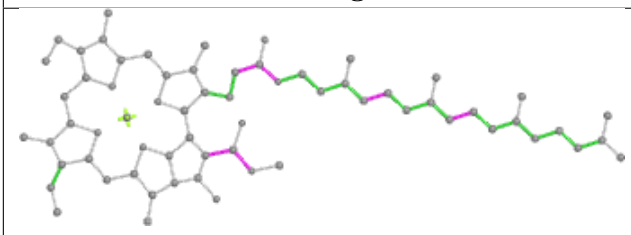
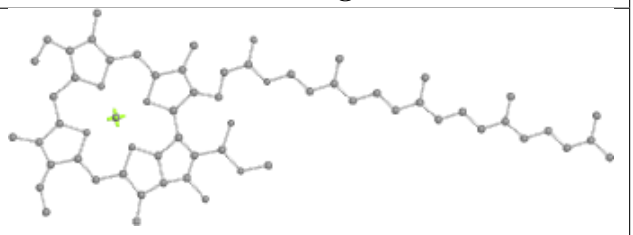
Bond angles



Torsions



Rings

Ligand CLA A 1011	
 Bond lengths	 Bond angles
 Torsions	 Rings

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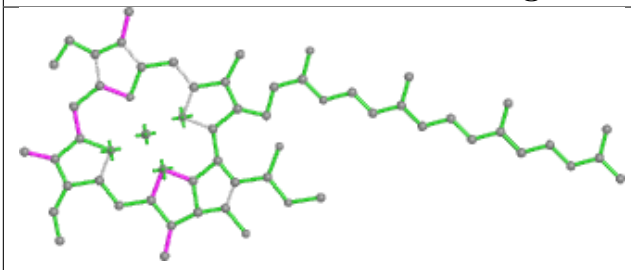
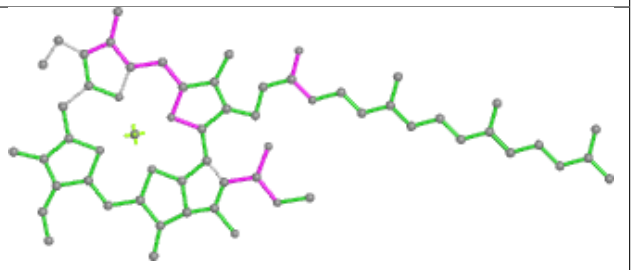
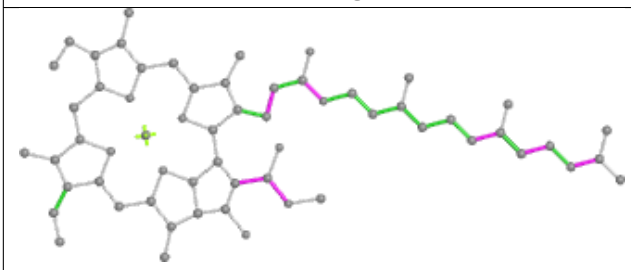
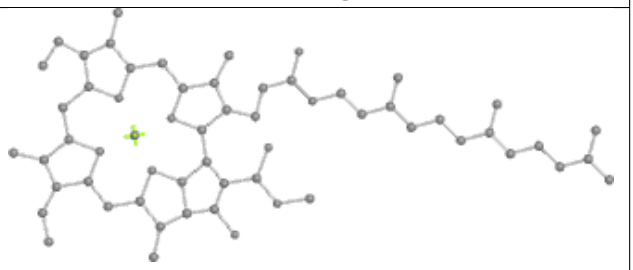
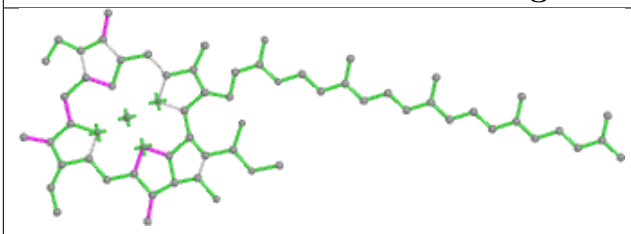
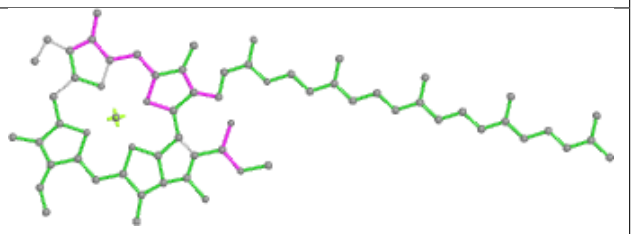
 Bond lengths	 Bond angles
 Torsions	 Rings

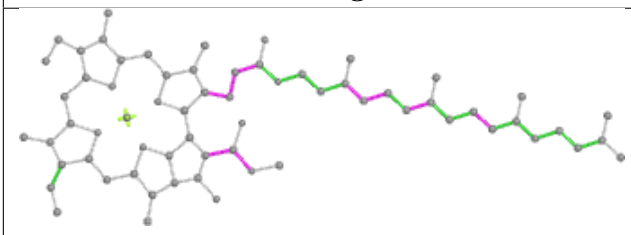
Ligand CLA r 501



Bond lengths



Bond angles



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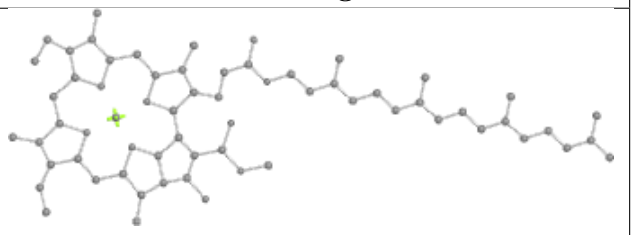
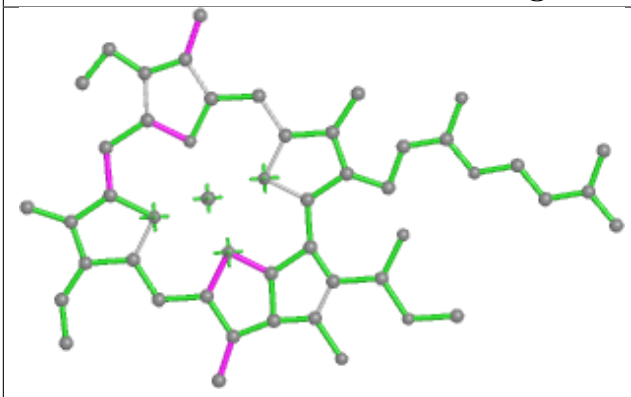


Rings

Ligand CLA 4 510



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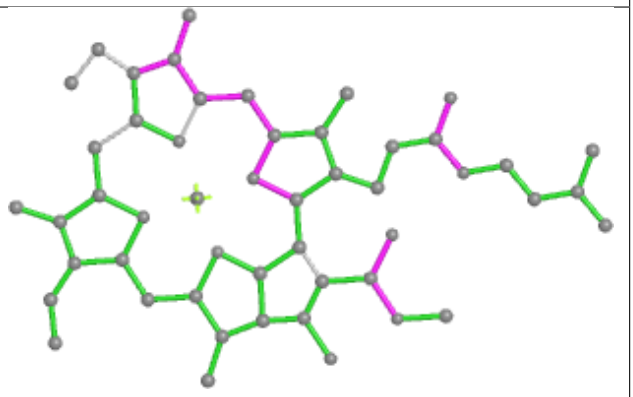

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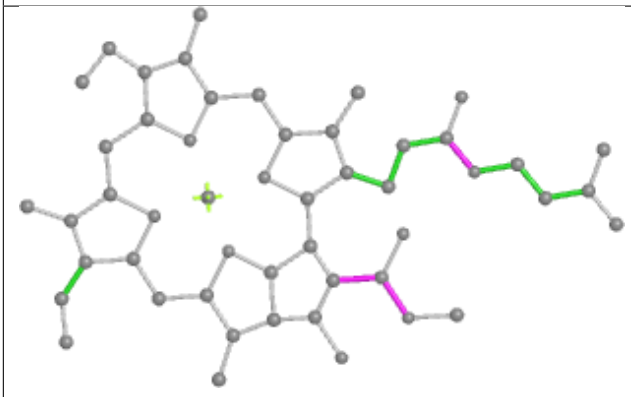

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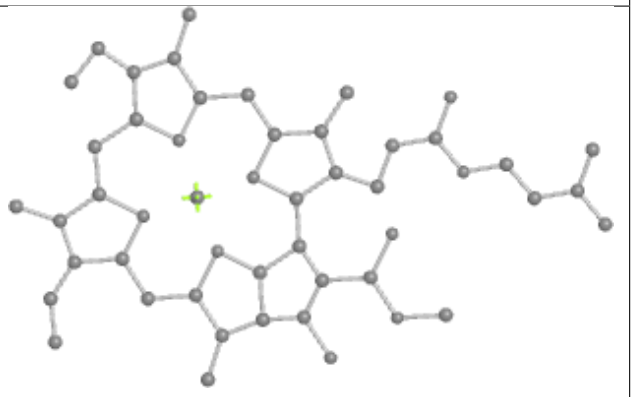
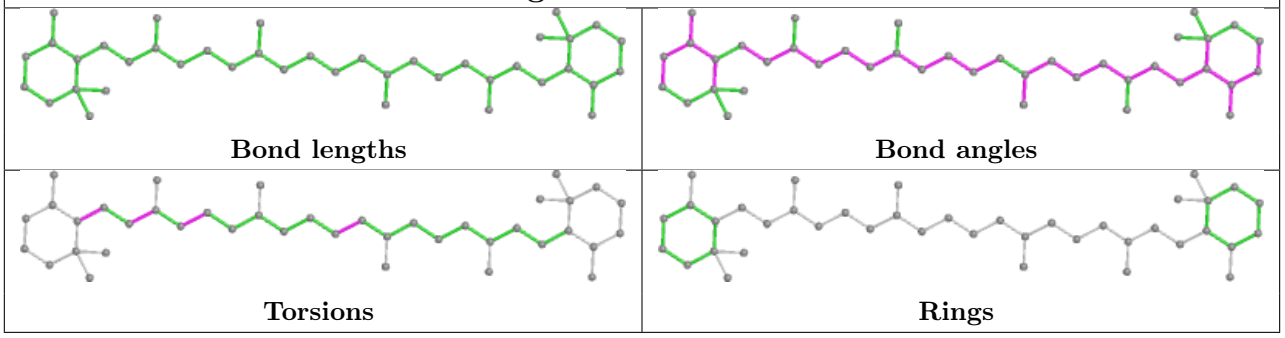


Rings

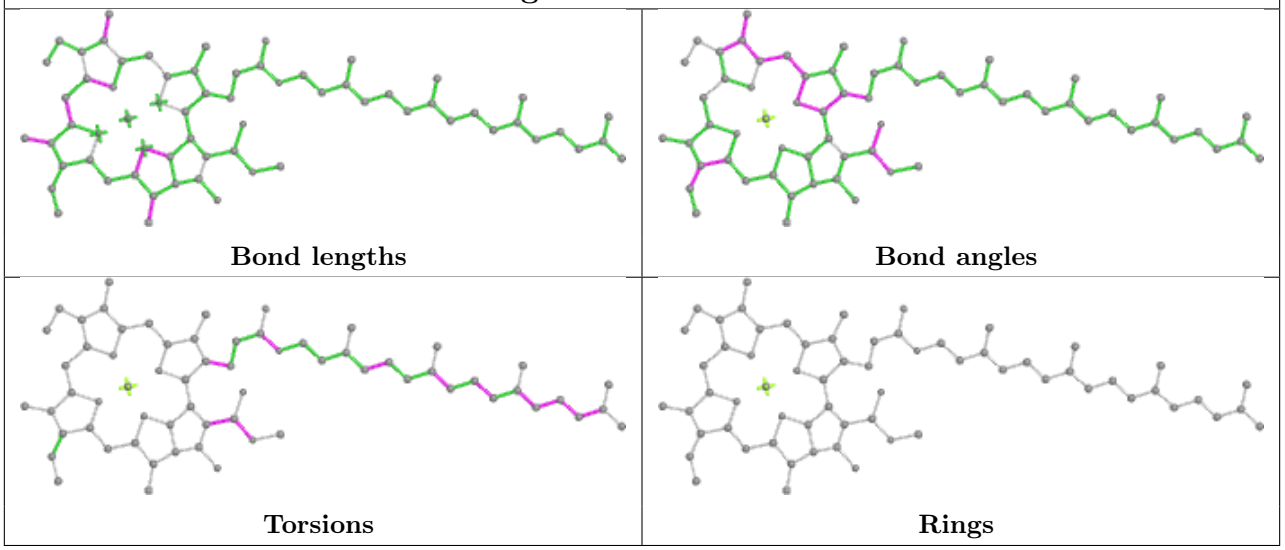
Ligand BCR 2 522



Bond lengths | Bond angles

Torsions | Rings

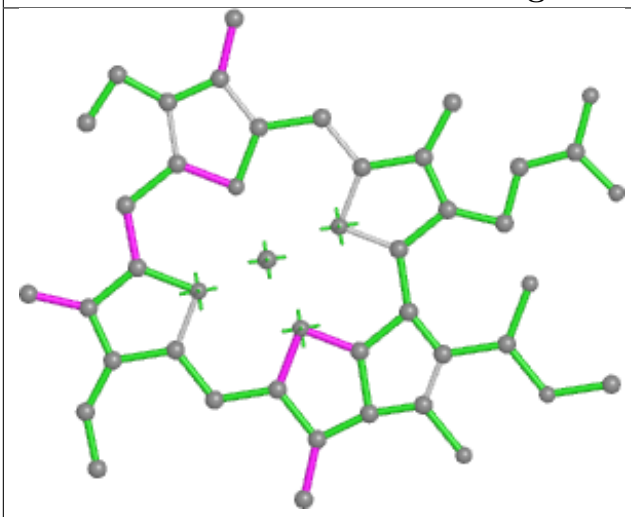
Ligand CLA e 1103



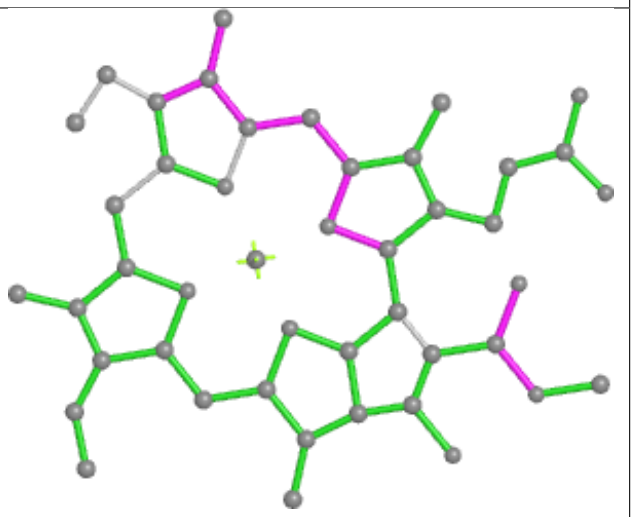
Bond lengths | Bond angles

Torsions | Rings

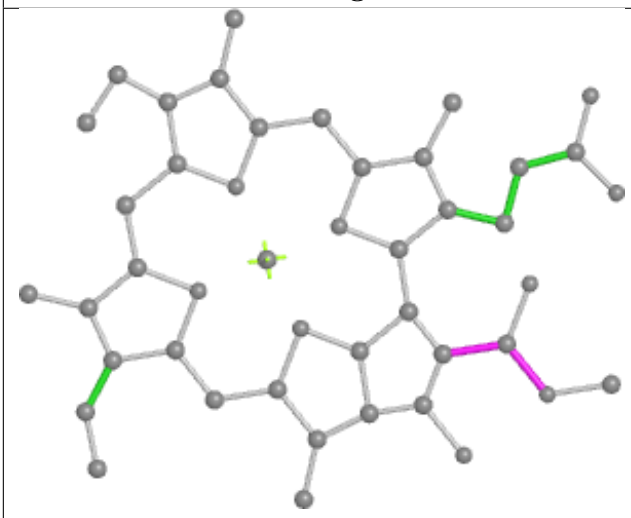
Ligand CLA v 506



Bond lengths



Bond angles



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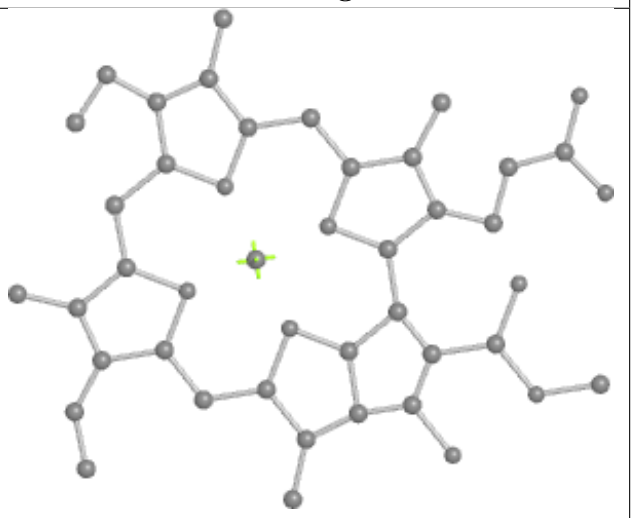

Rings

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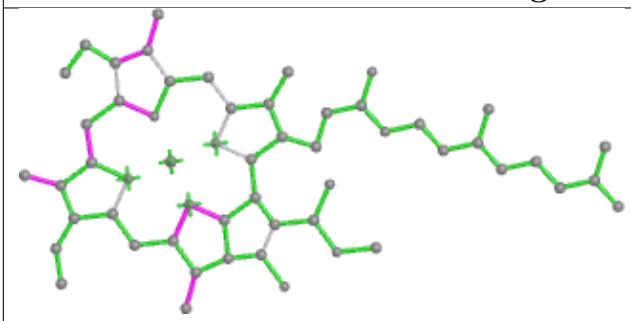

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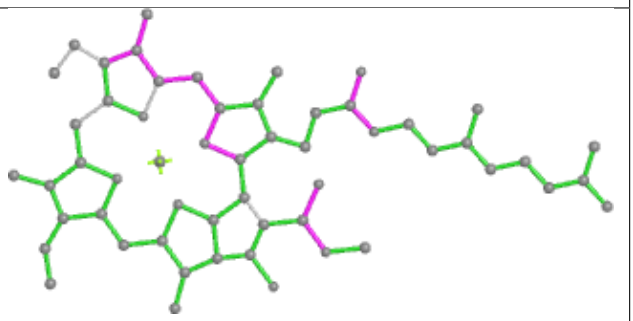

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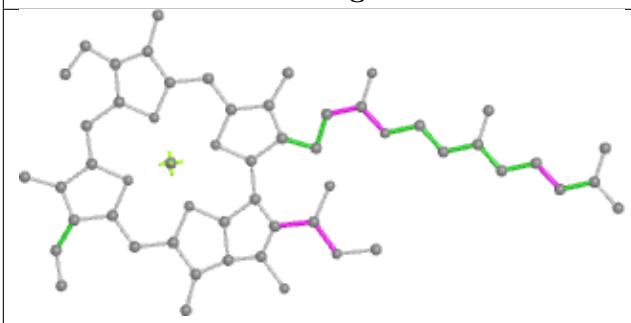

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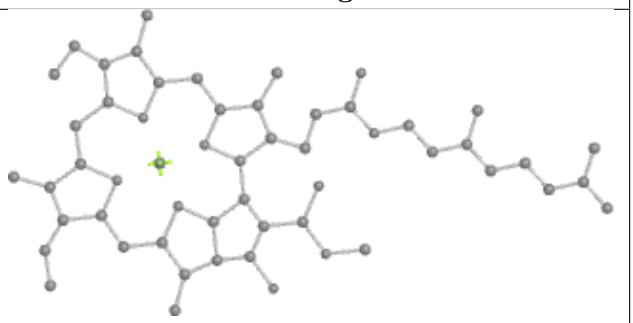
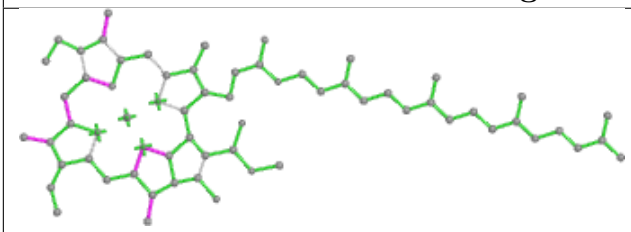


Rings

Ligand CLA e 1123



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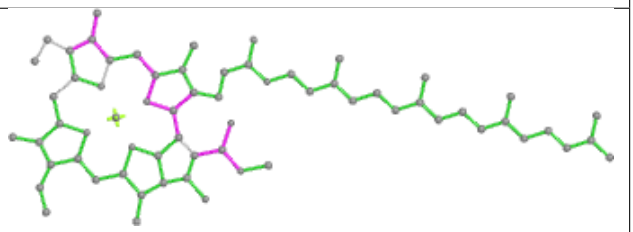
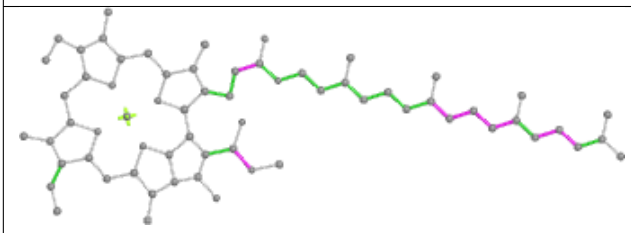


Bond angles



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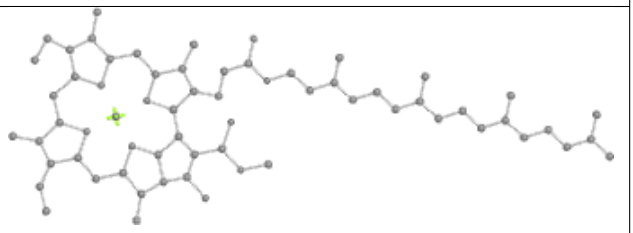
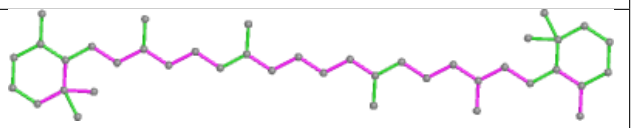


Rings

Ligand BCR T 4015

Bond lengths



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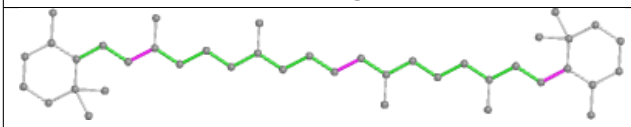

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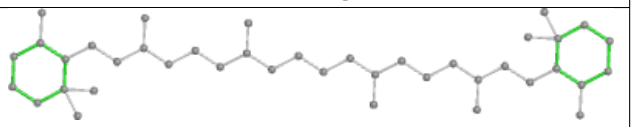
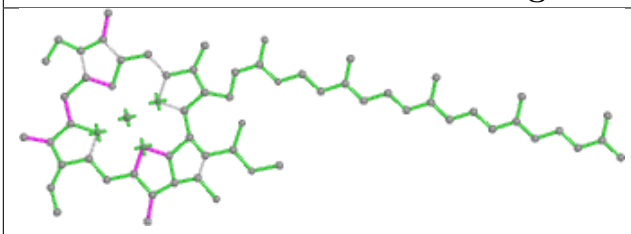


Rings

Ligand CLA 3 501



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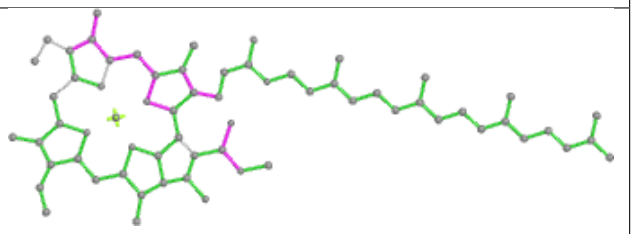
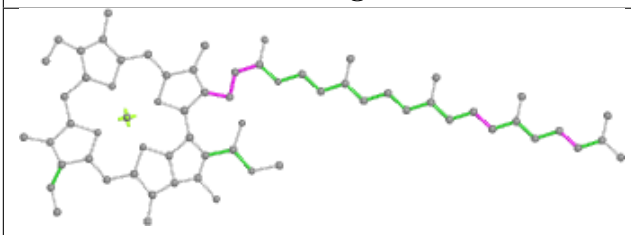


Bond angles



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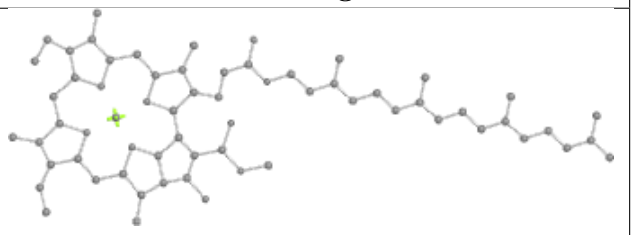
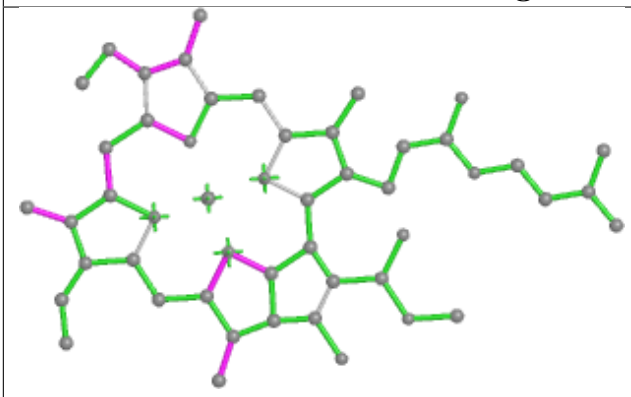


Rings

Ligand CLA A 1112



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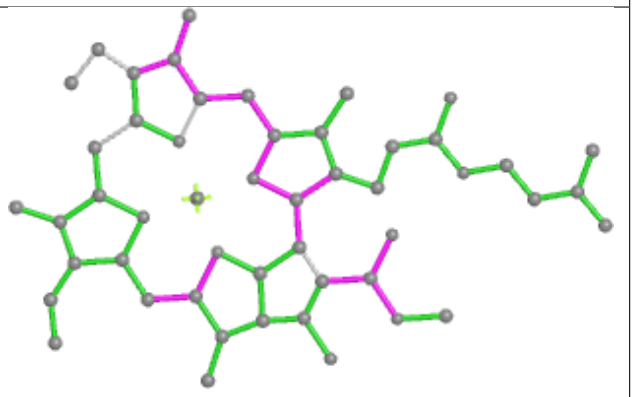

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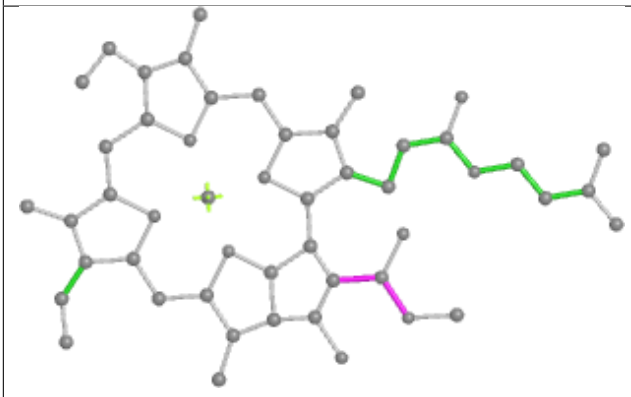

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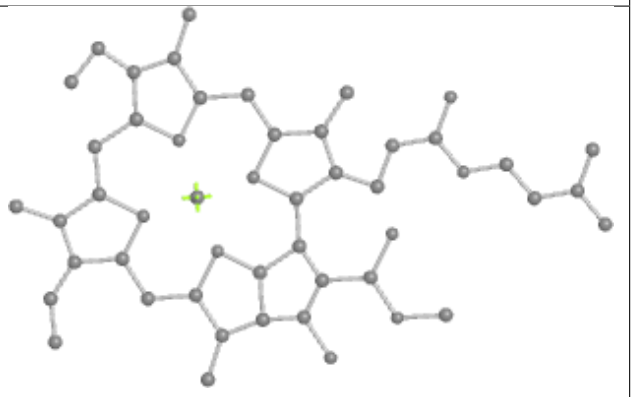
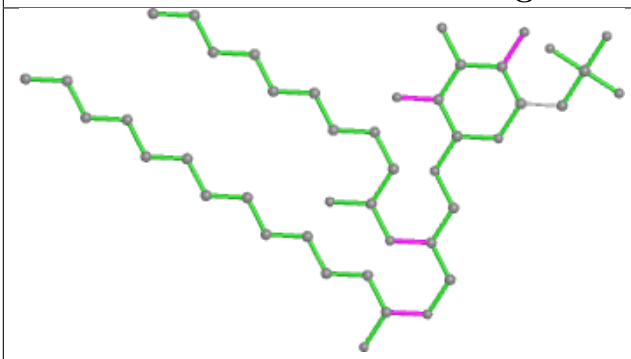


Rings

Ligand SQD B 1852



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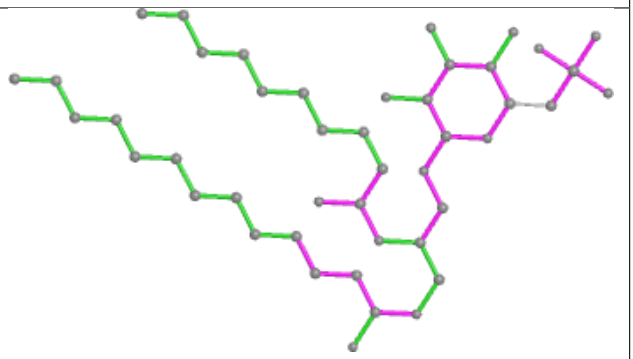

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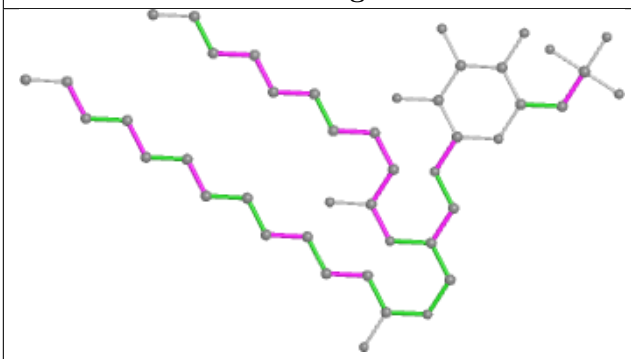

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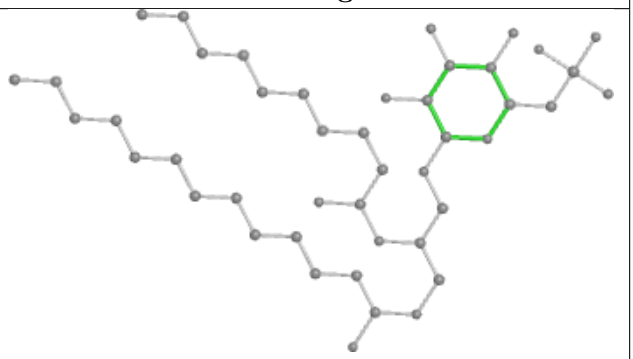
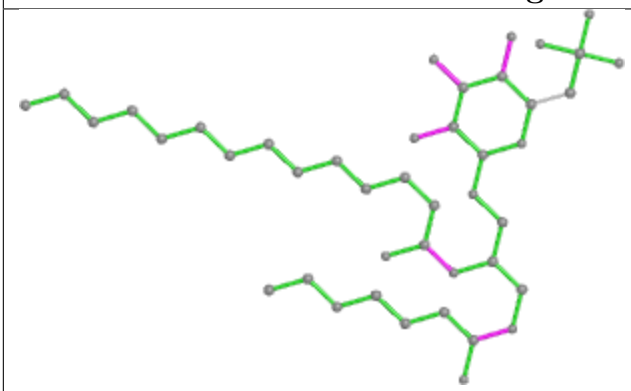


Rings

Ligand SQD Z 822



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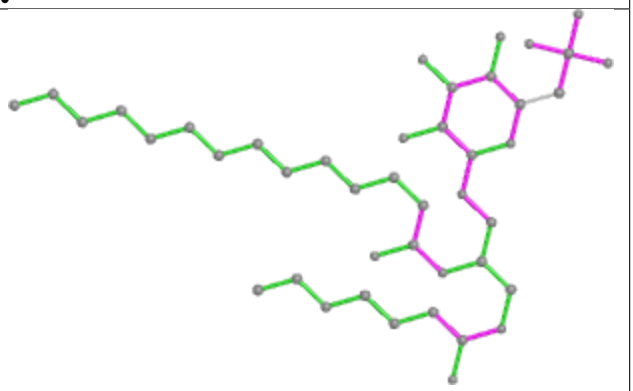
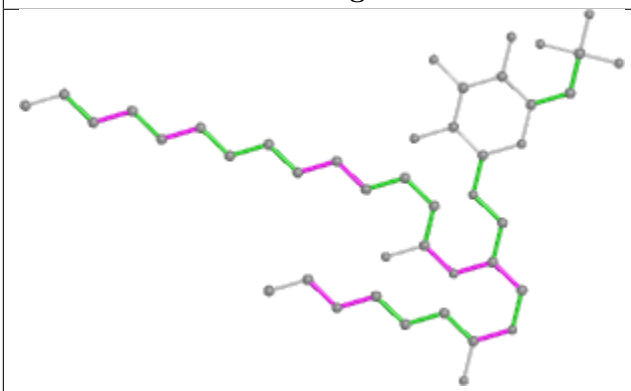


Bond angles



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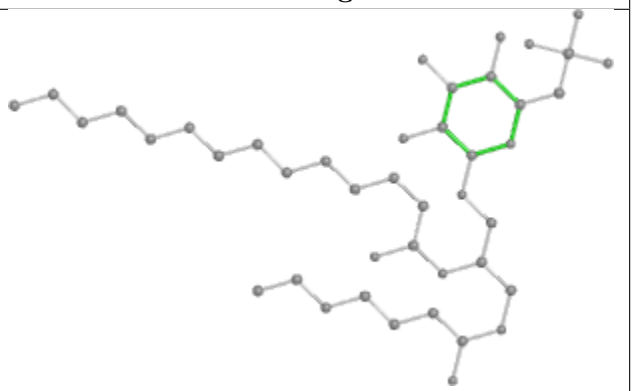
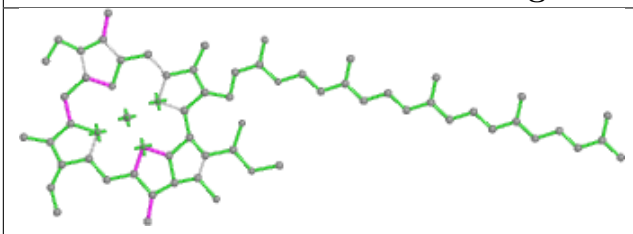


Rings

Ligand CLA 3 510



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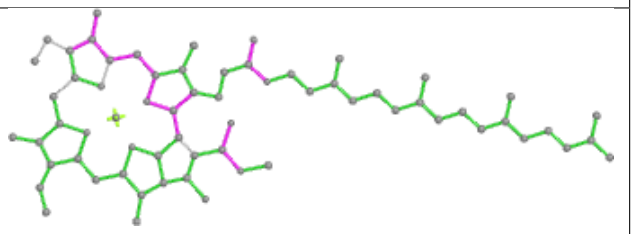
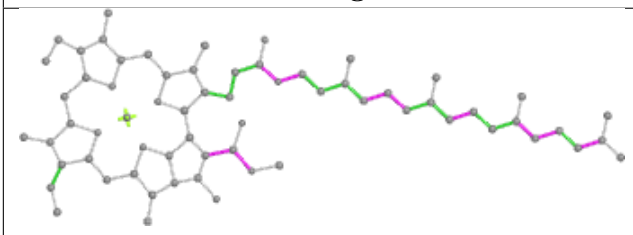


Bond angles



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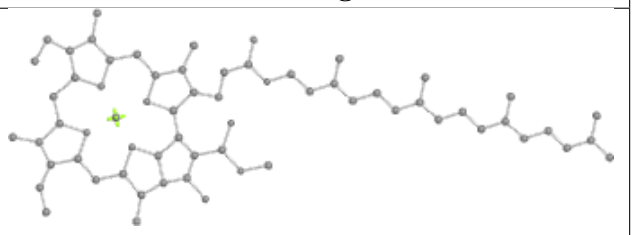
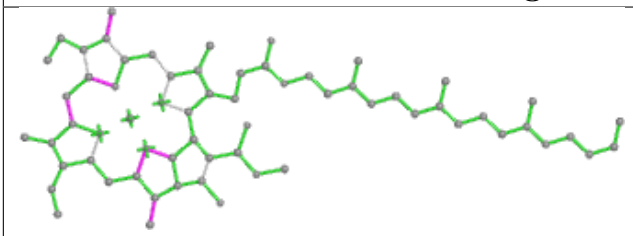


Rings

Ligand CLA Y 503



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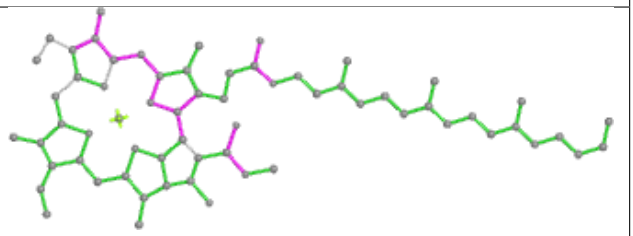
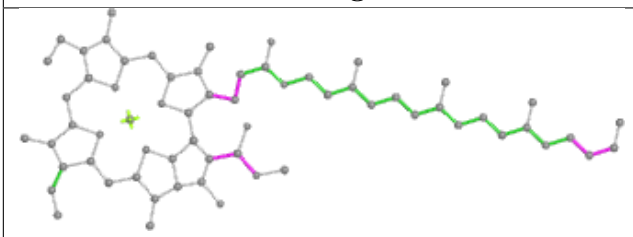


Bond angles



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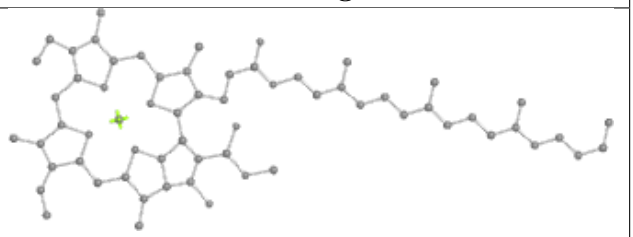
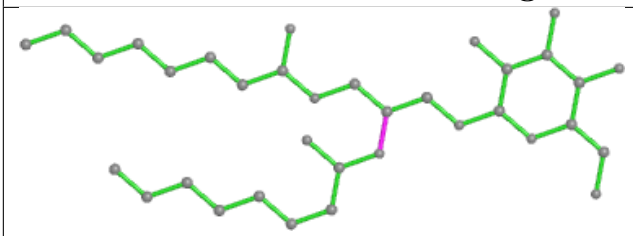
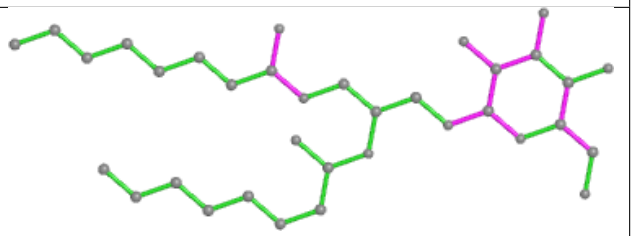


Rings

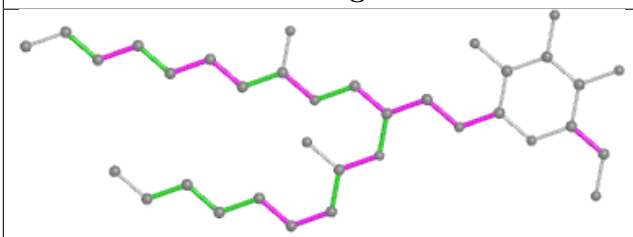
Ligand LMG l 5104



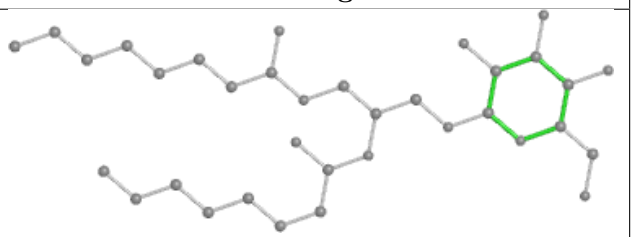
Bond lengths



Bond angles

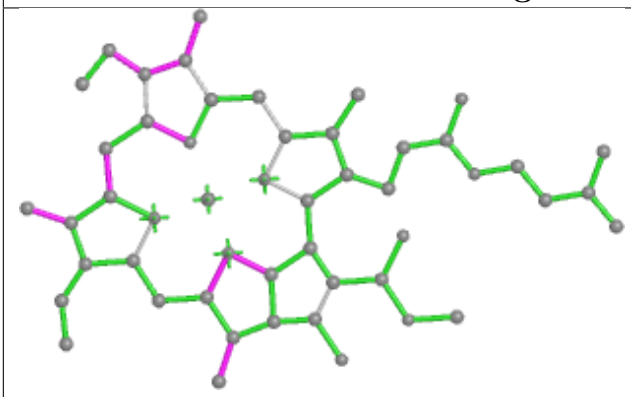


Torsions



Rings

Ligand CLA G 1112



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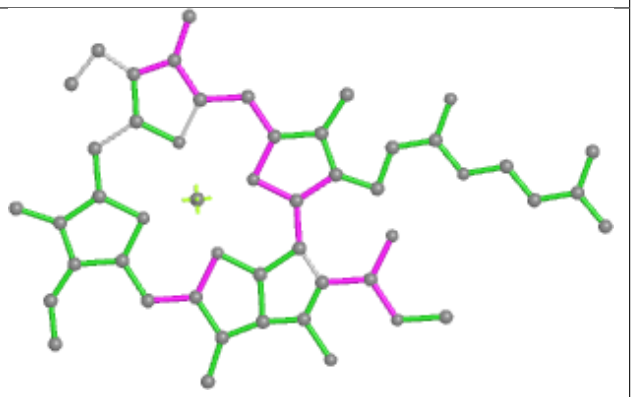
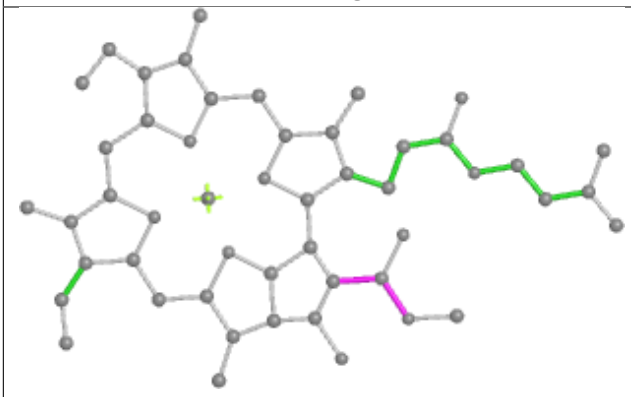
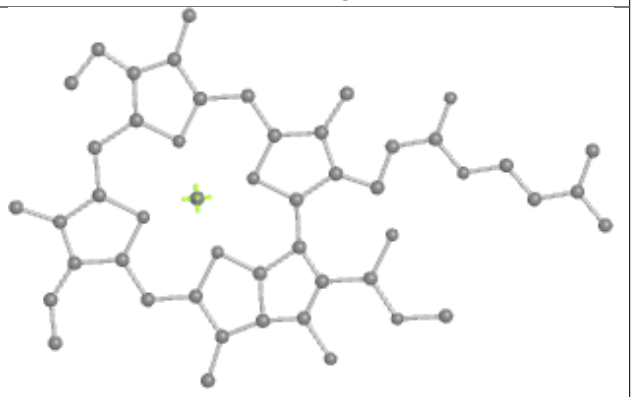


Bond angles

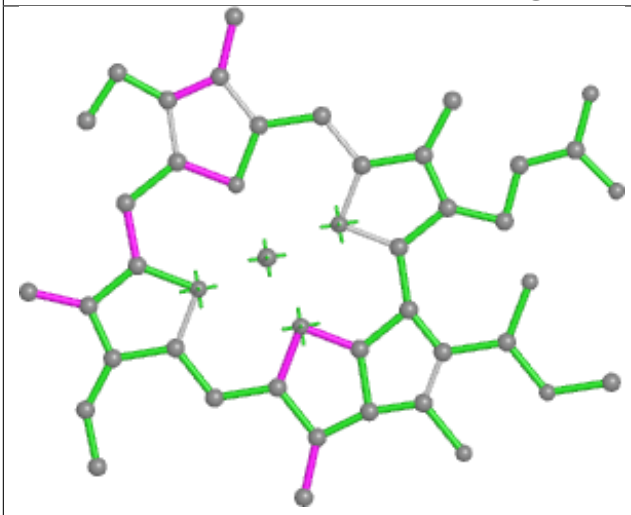


Torsions

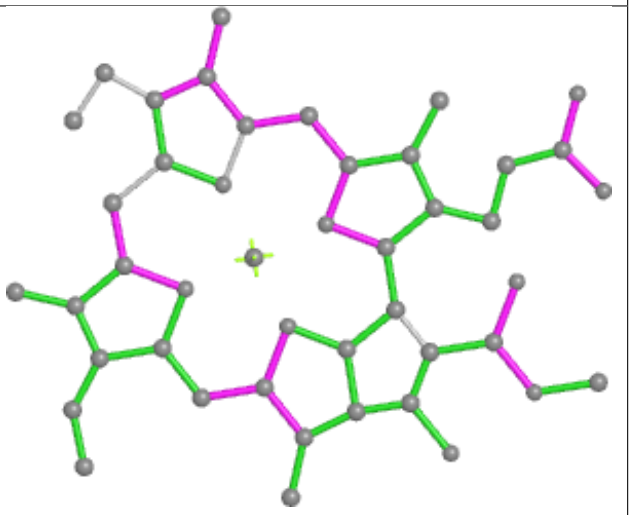


Rings

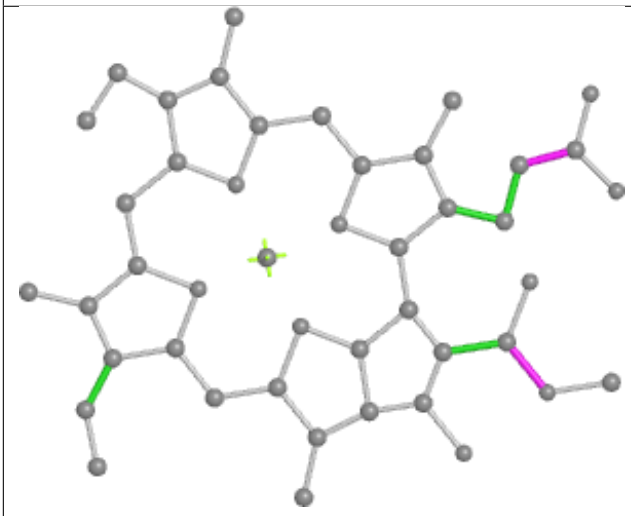
Ligand CLA b 508



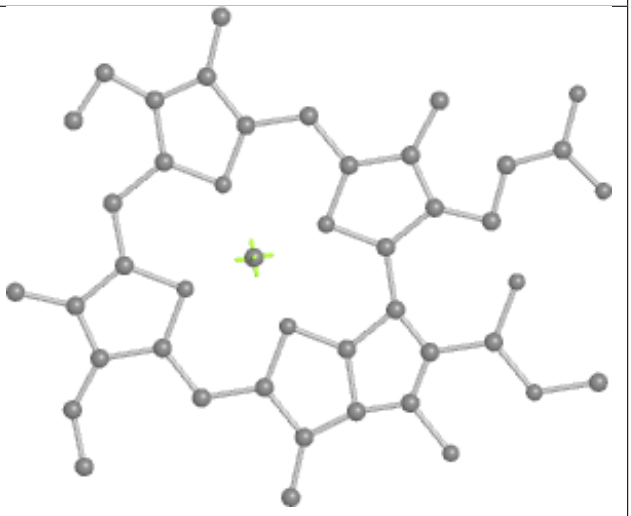
Bond lengths



Bond angles

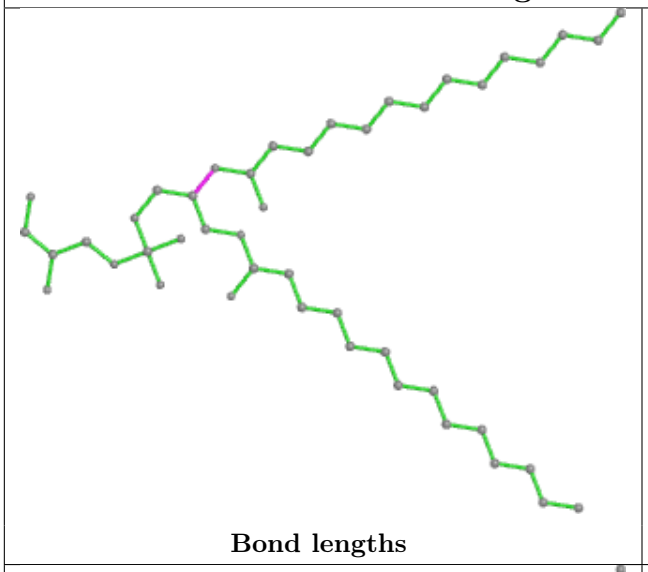


Torsions

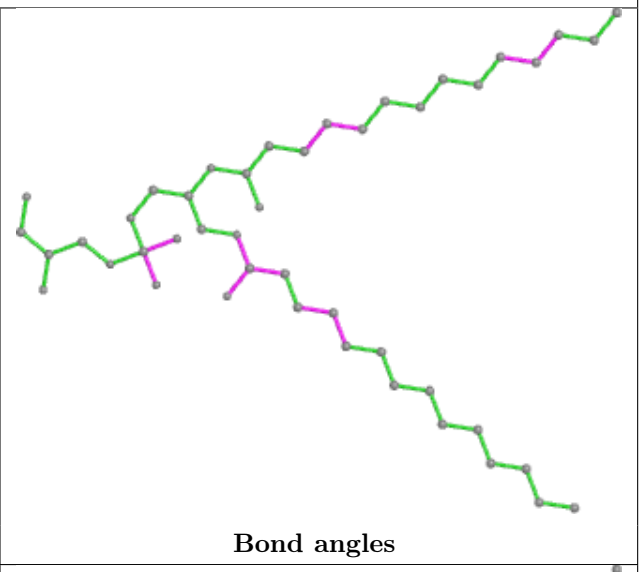


Rings

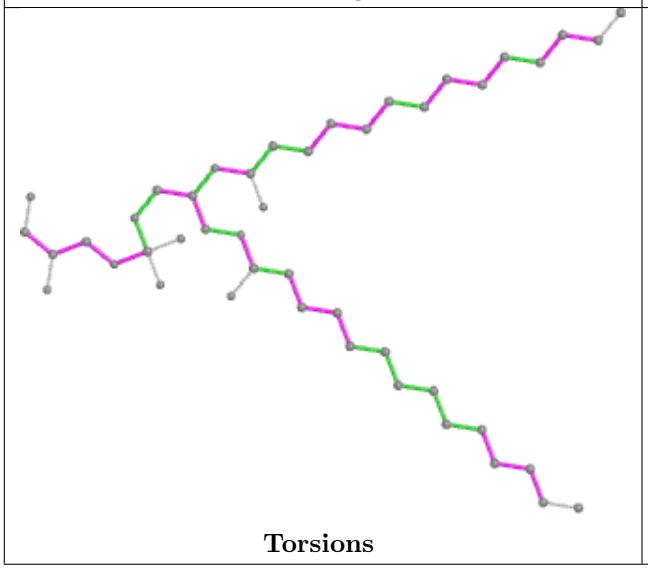
Ligand LHG A 5005



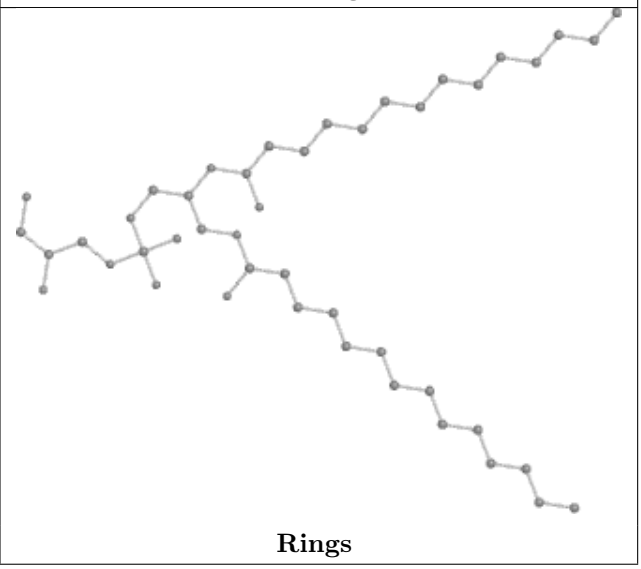
Bond lengths



Bond angles

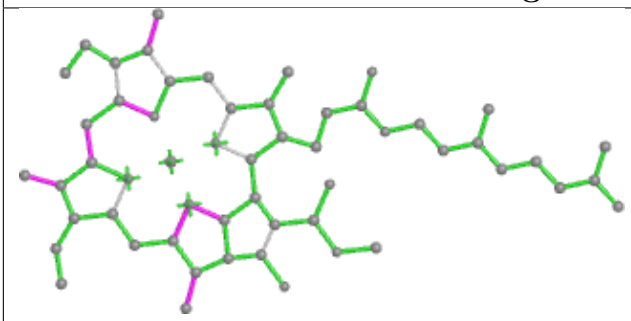


Torsions

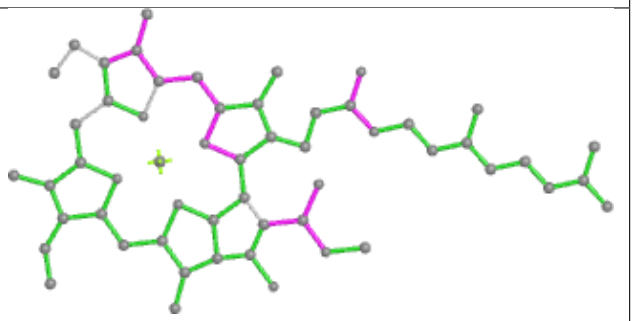


Rings

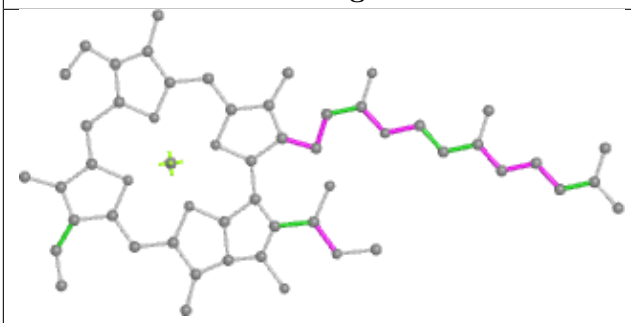
Ligand CLA f 1212



Bond lengths



Bond angles



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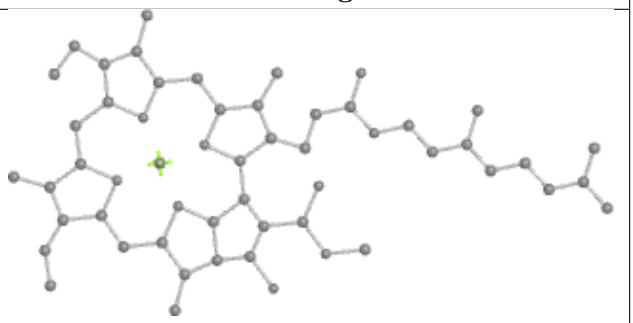
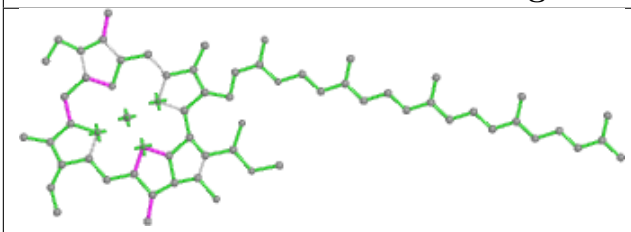
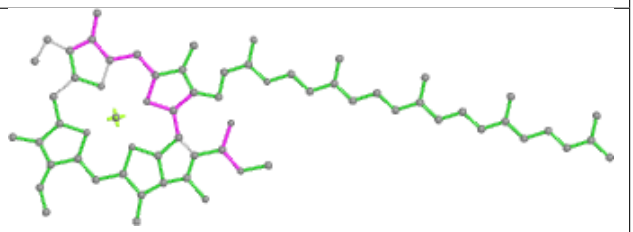


Rings

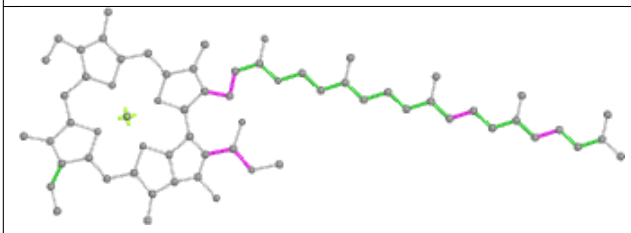
Ligand CLA 2 503



Bond lengths



Bond angles



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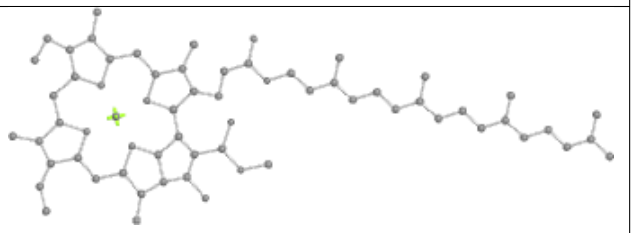
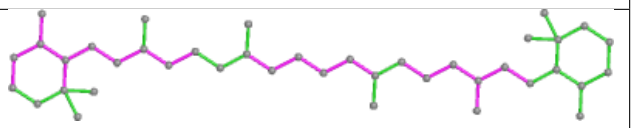


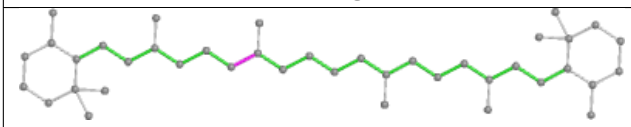
Rings

Ligand BCR Y 524

Bond lengths



Bond angles



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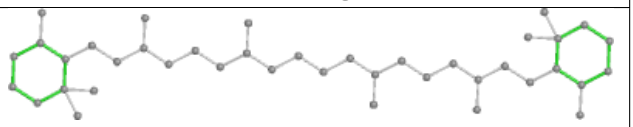
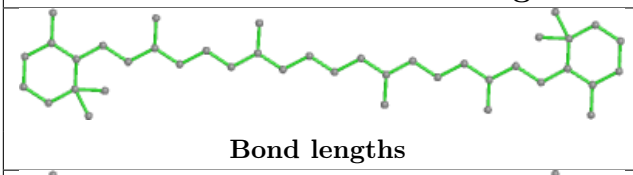
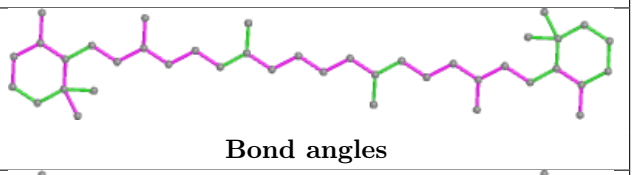


Rings

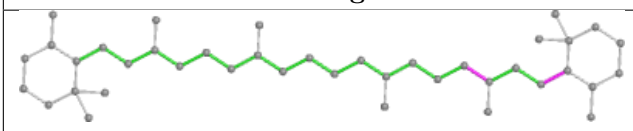
Ligand BCR V 4020



Bond lengths



Bond angles



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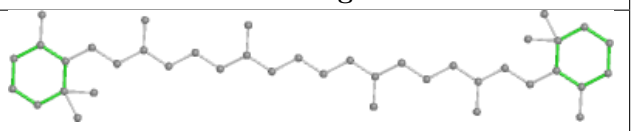
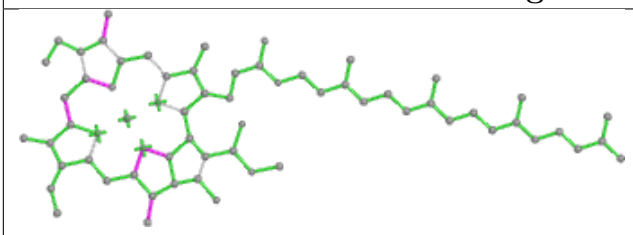


Rings

Ligand CLA Z 503



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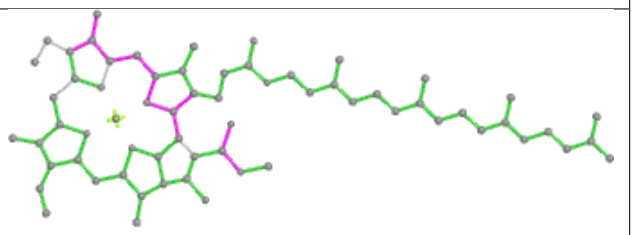
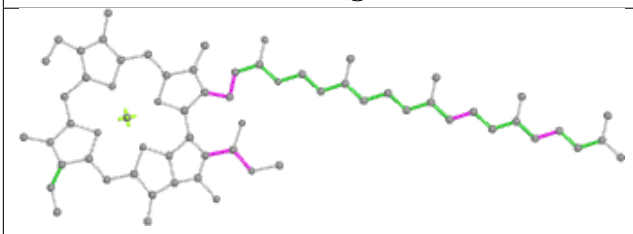
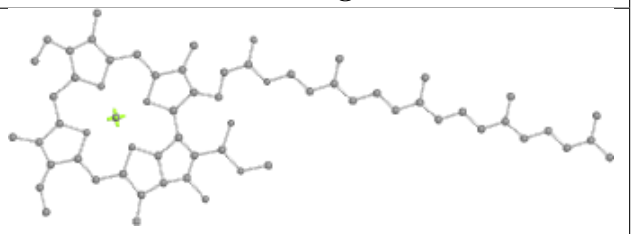


Bond angles

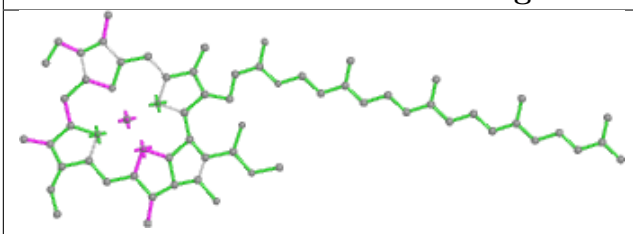


Torsions

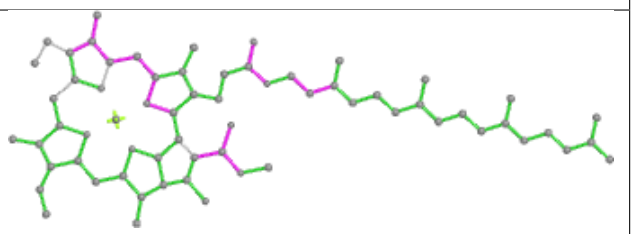


Rings

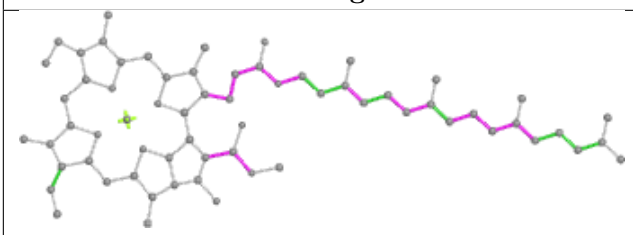
Ligand CLA G 1106



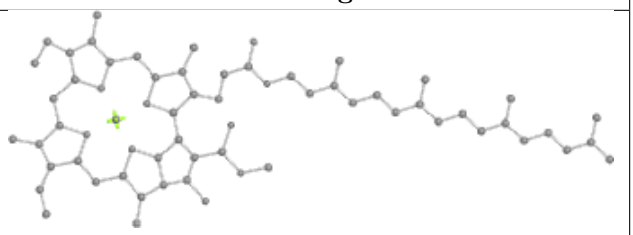
Bond lengths



Bond angles

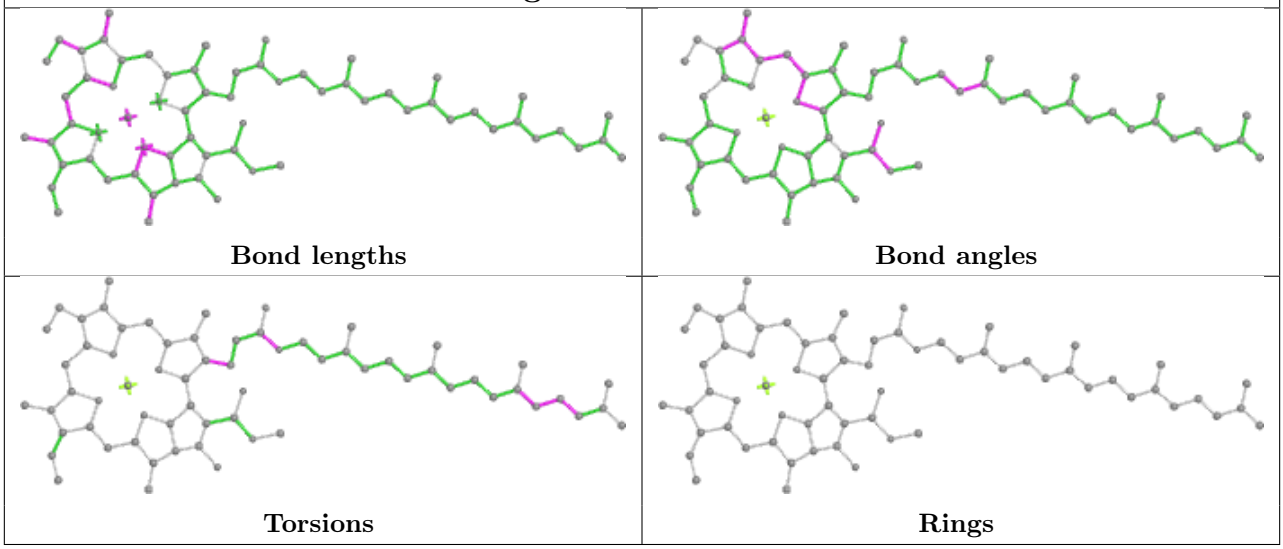


Torsions

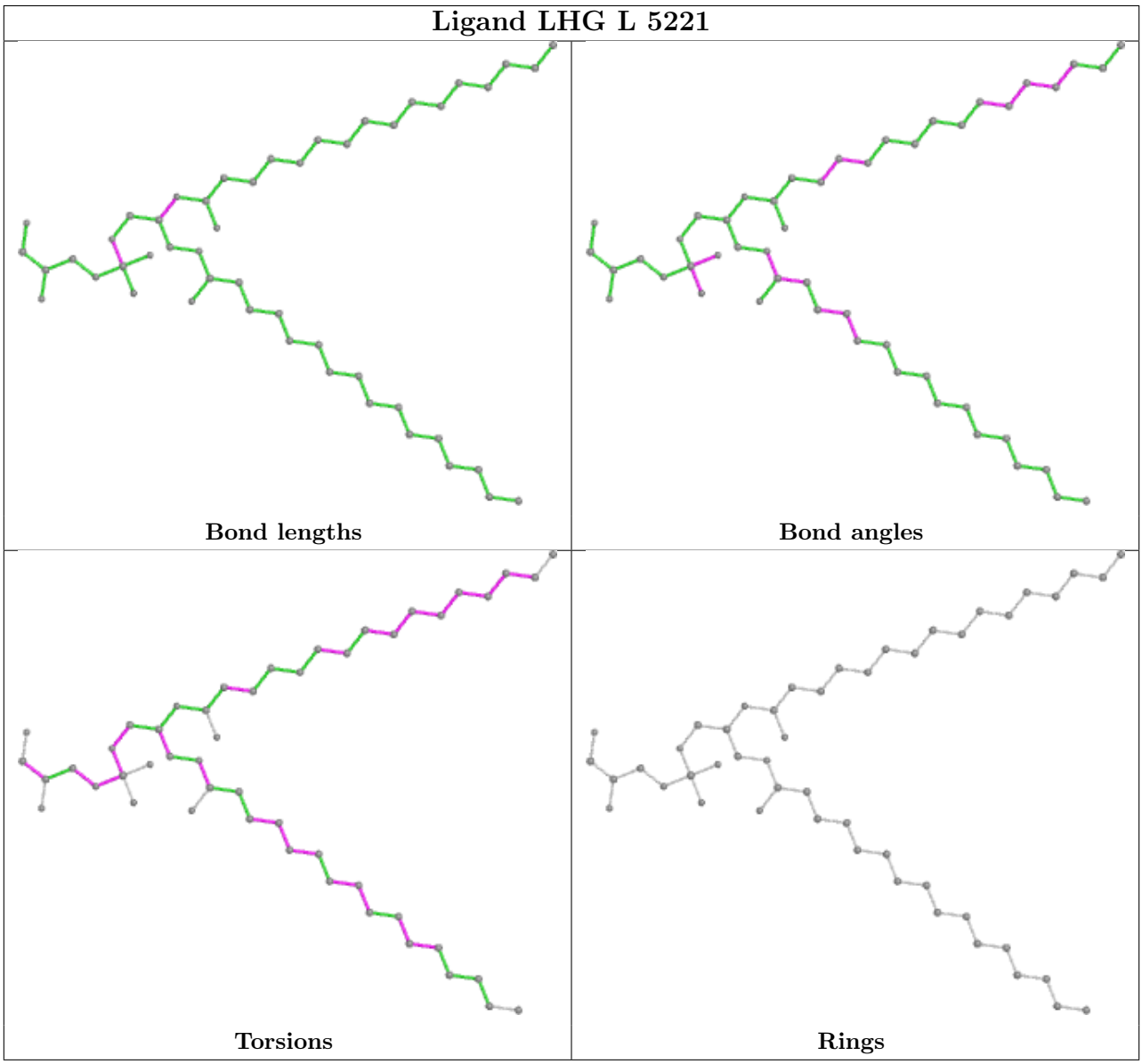


Rings

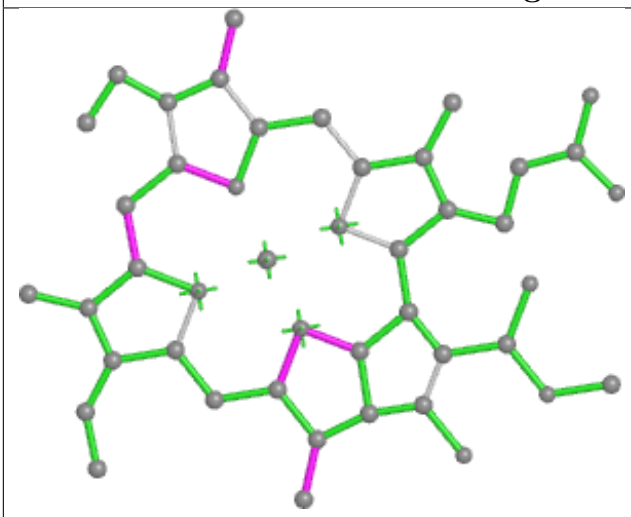
Ligand CLA f 1225



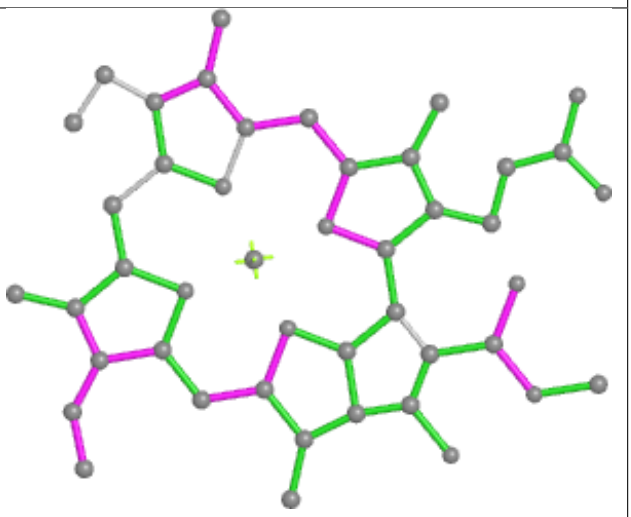
Ligand LHG L 5221



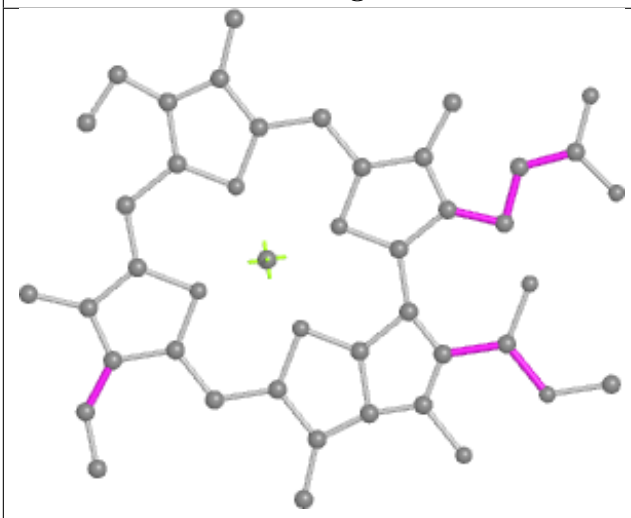
Ligand CLA Y 516



Bond lengths



Bond angles



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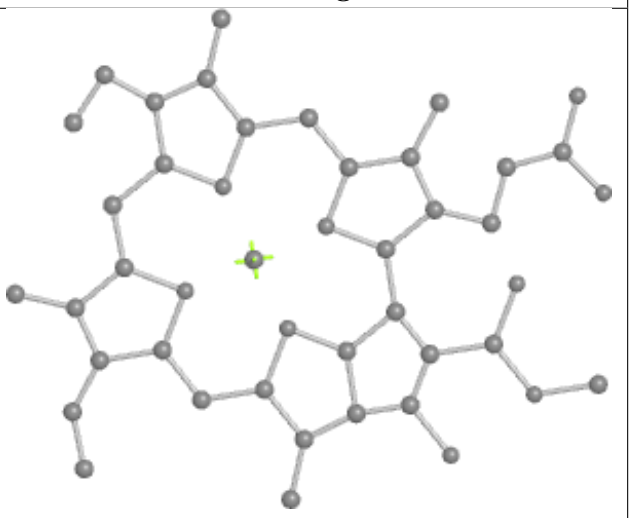
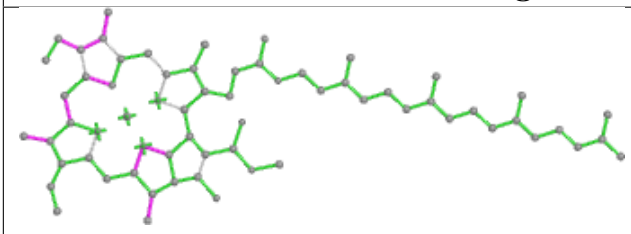


Rings

Ligand CLA H 1227



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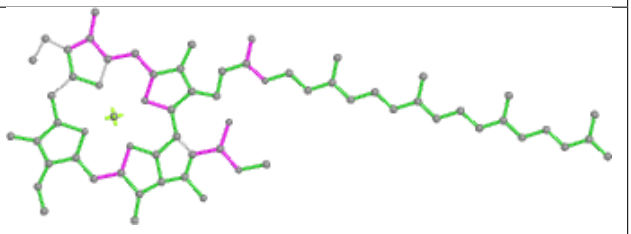
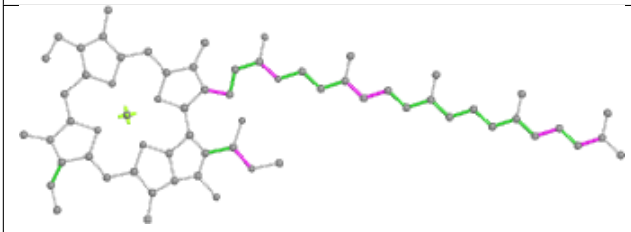


Bond angles



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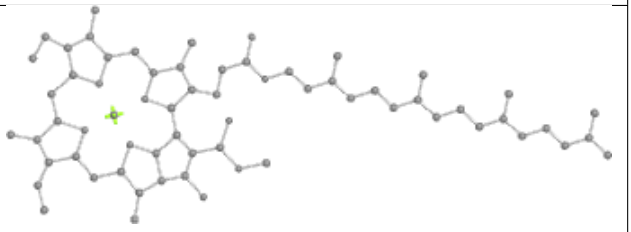
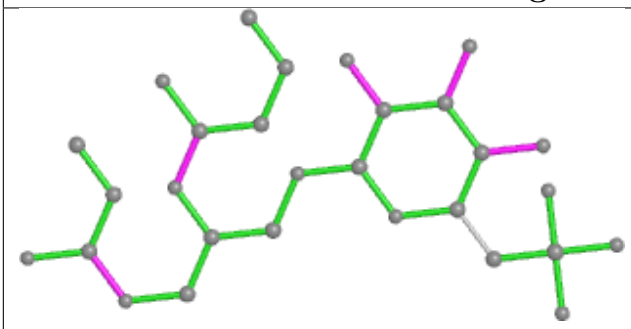
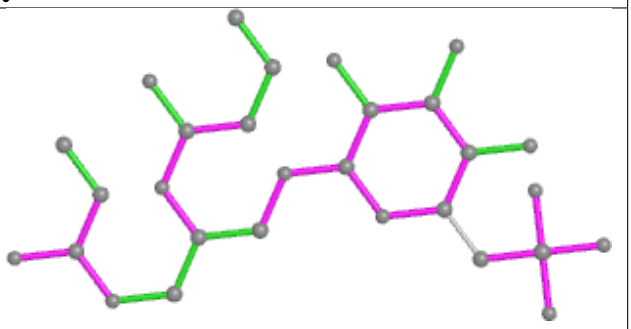


Rings

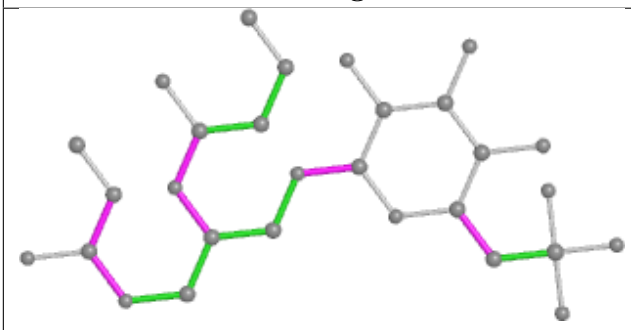
Ligand SQD c 822



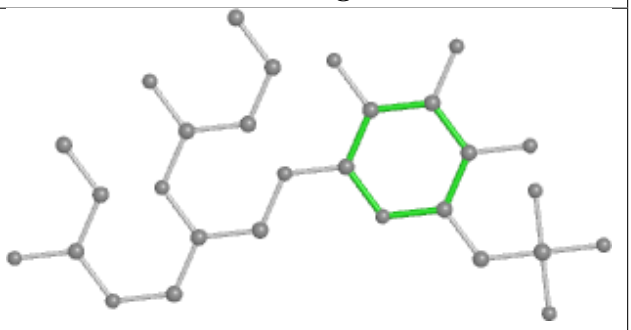
Bond lengths



Bond angles

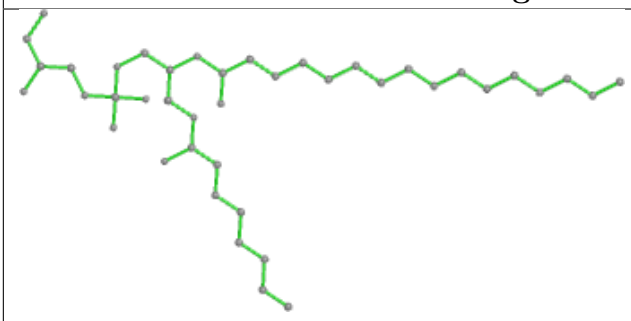


Torsions

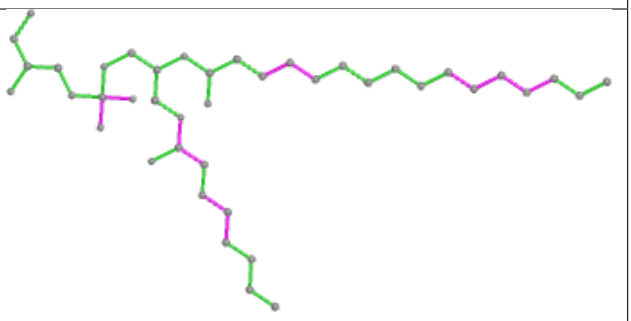


Rings

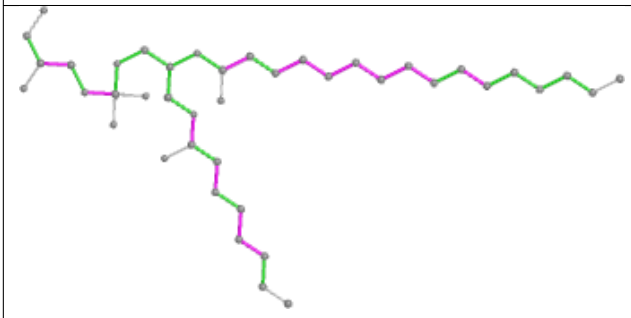
Ligand LHG G 5003



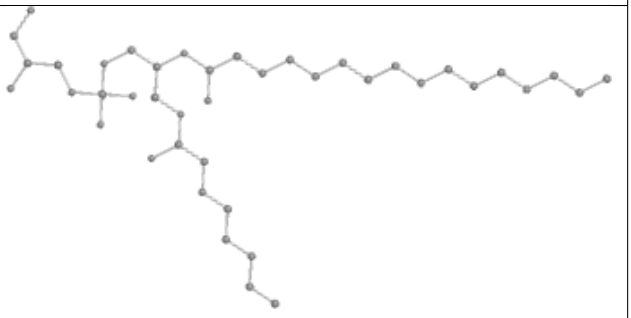
Bond lengths



Bond angles

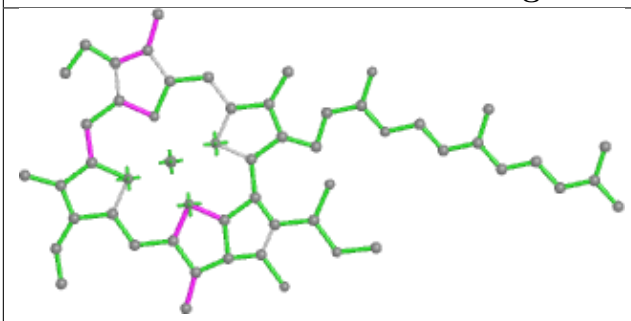


Torsions

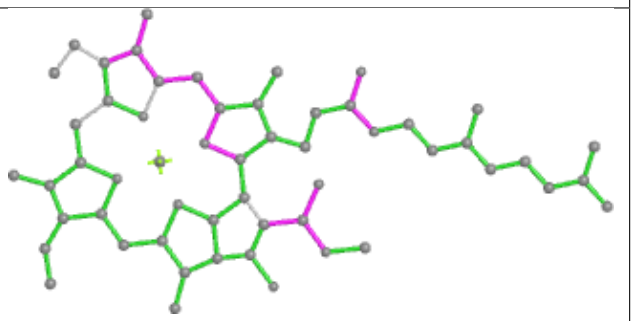


Rings

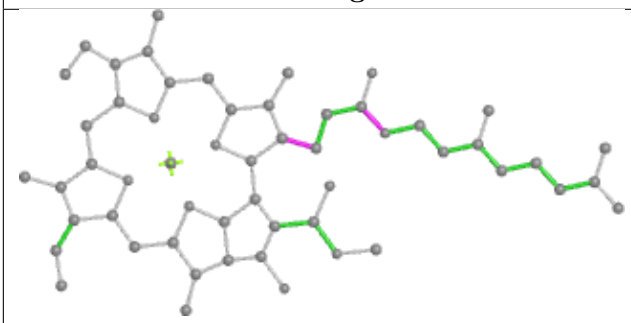
Ligand CLA f 1236



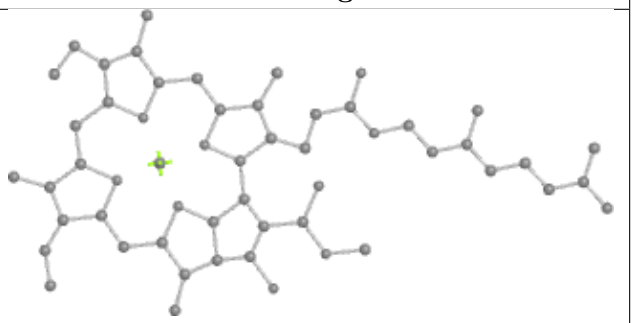
Bond lengths



Bond angles

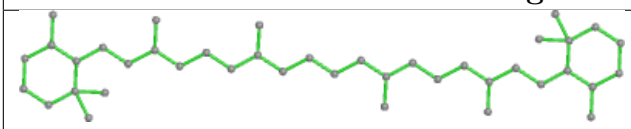


Torsions

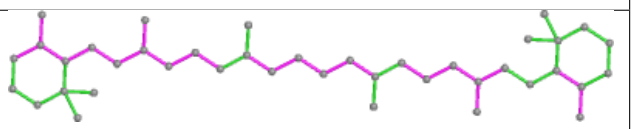


Rings

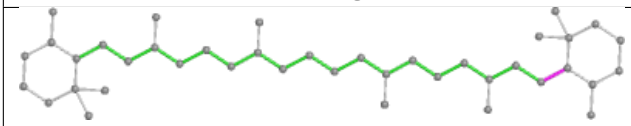
Ligand BCR 5 524



Bond lengths



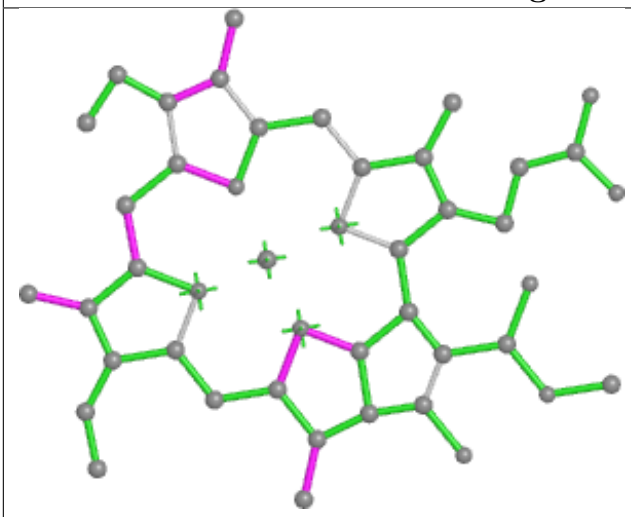
Bond angles



Torsions

Rings

Ligand CLA c 513



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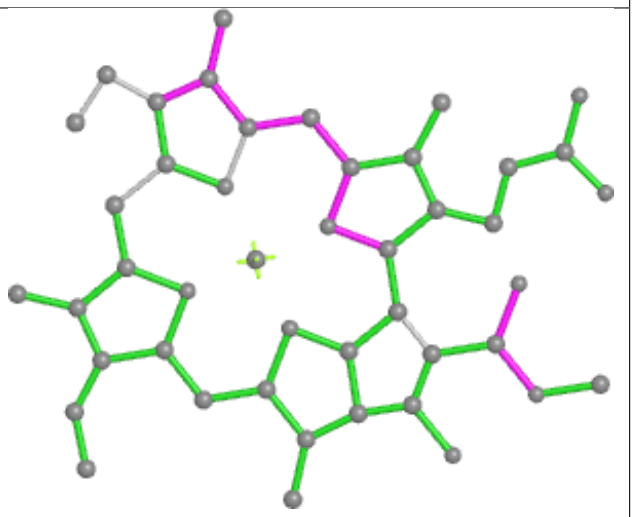
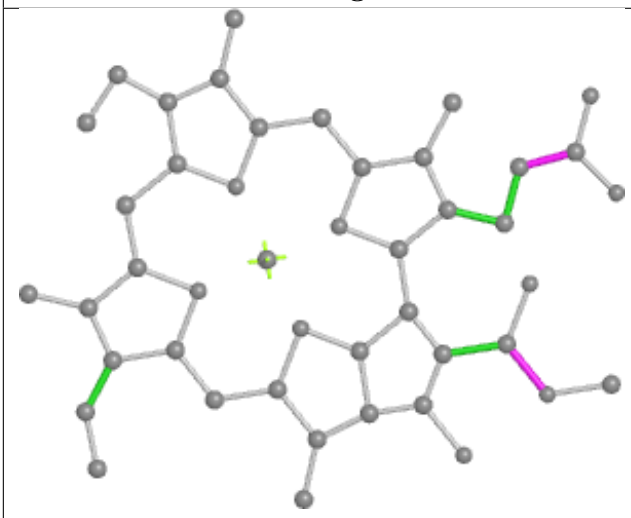


Bond angles



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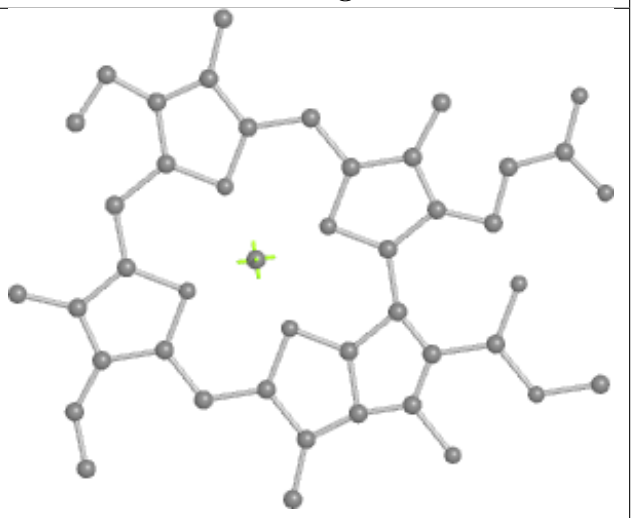
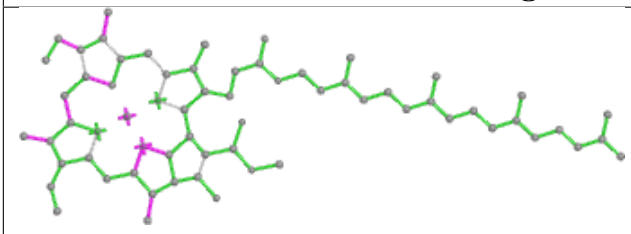


Rings

Ligand CLA e 1022



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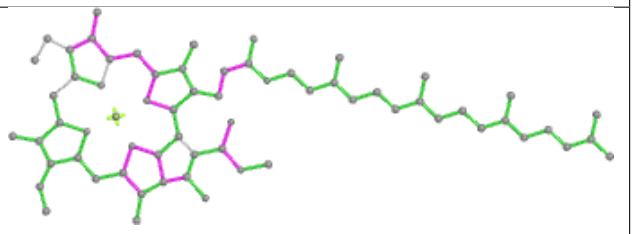
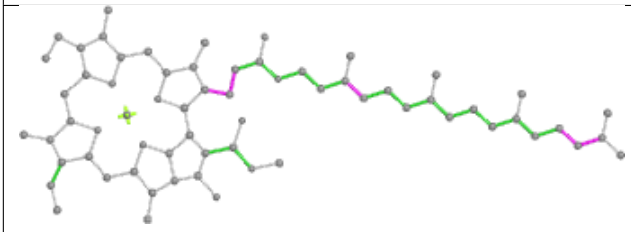
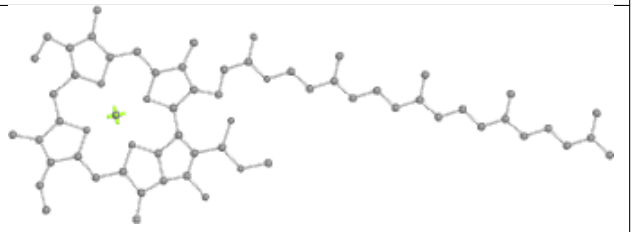


Bond angles

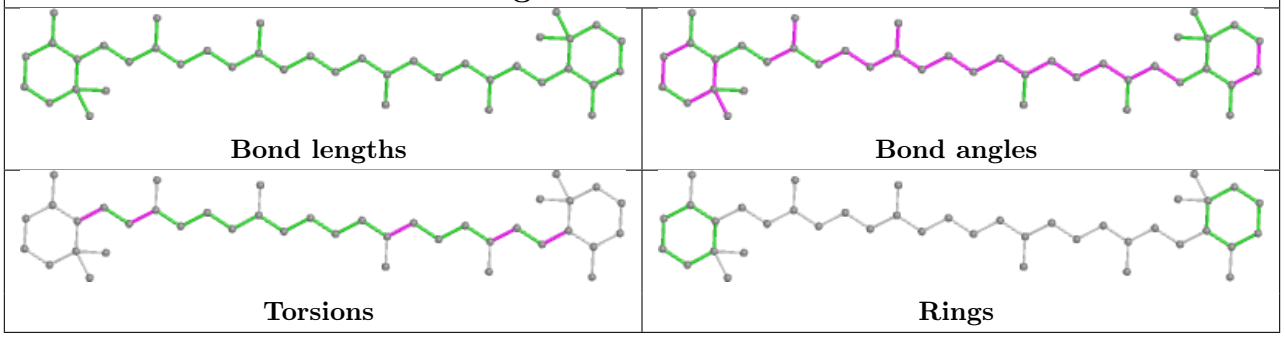


Torsions

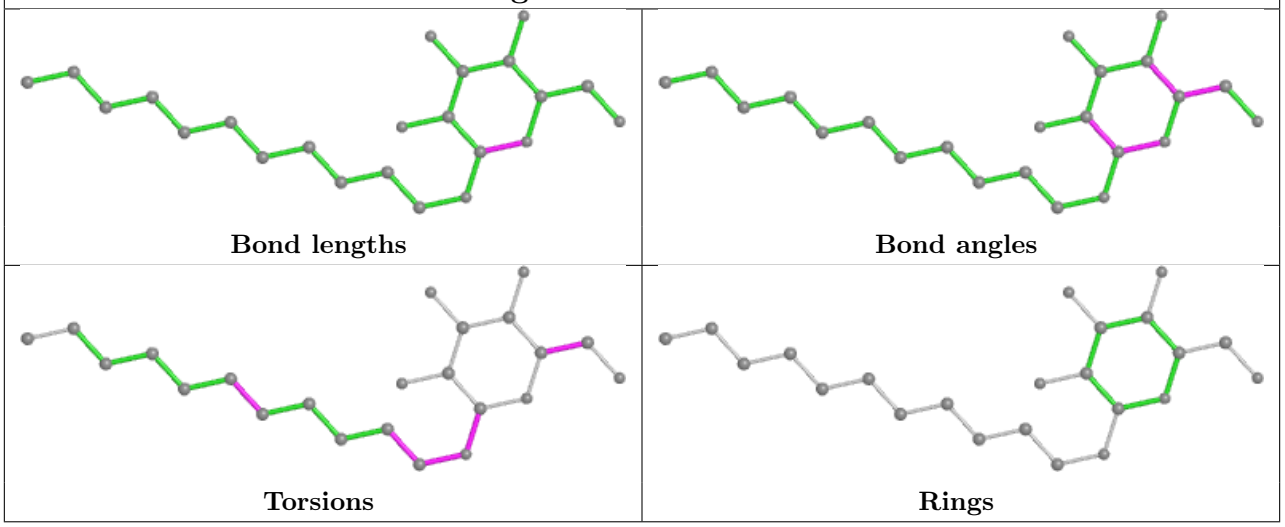


Rings

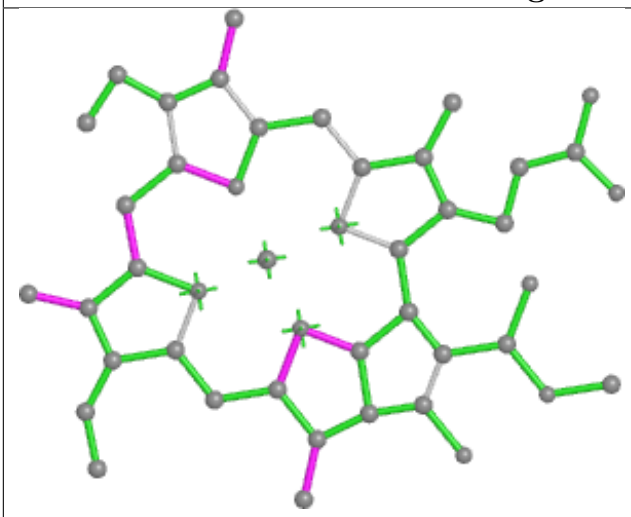
Ligand BCR H 4014



Ligand LMU G 1849



Ligand CLA q 517



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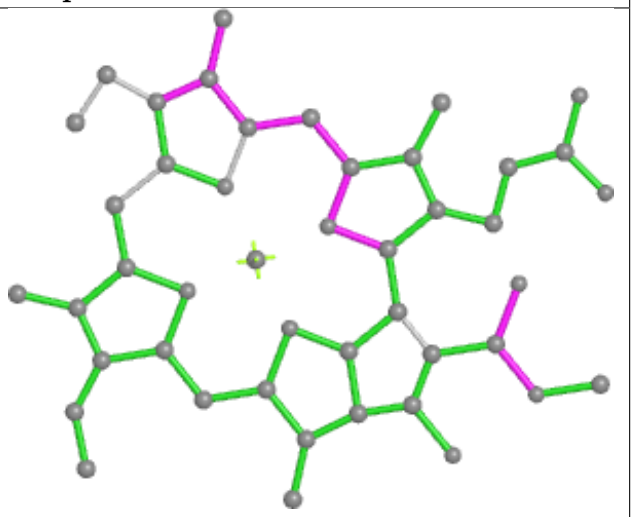
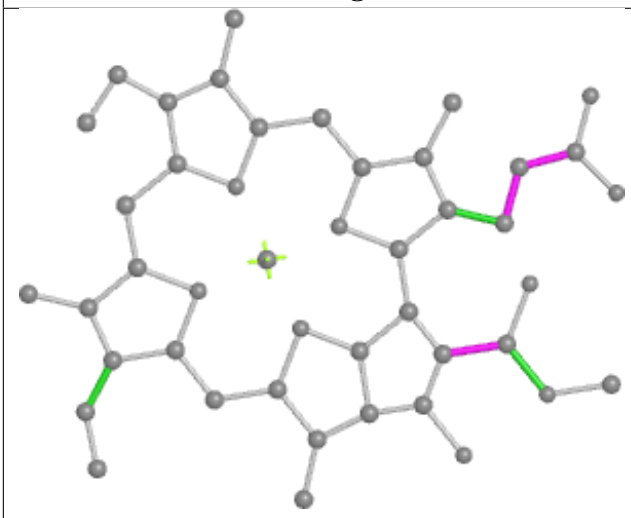


Bond angles



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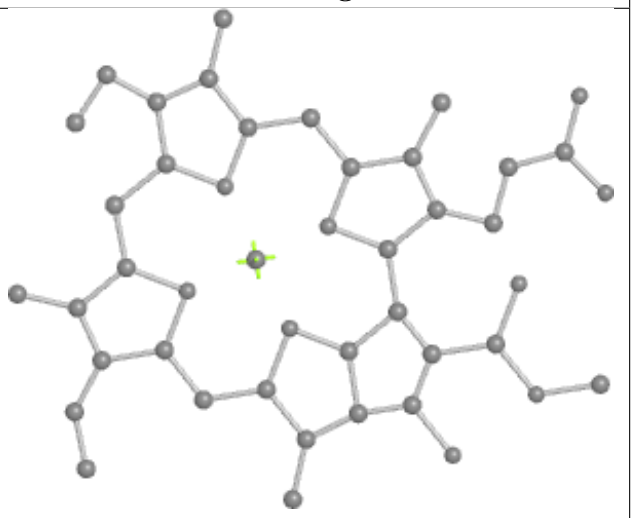
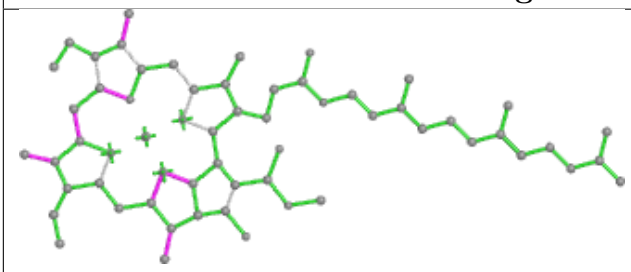


Rings

Ligand CLA B 1201



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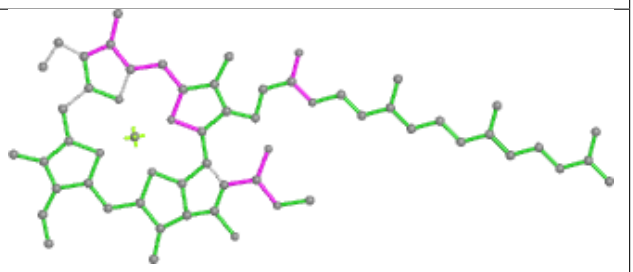
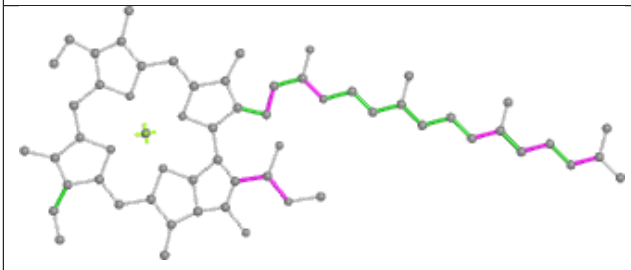


Bond angles



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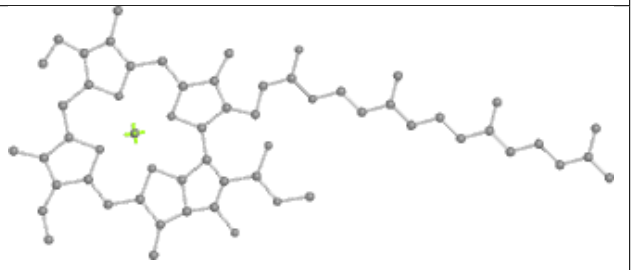
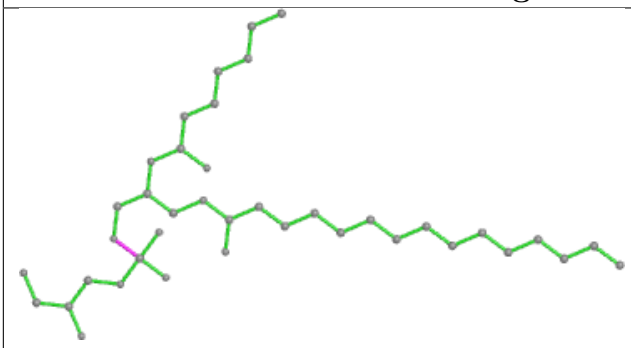
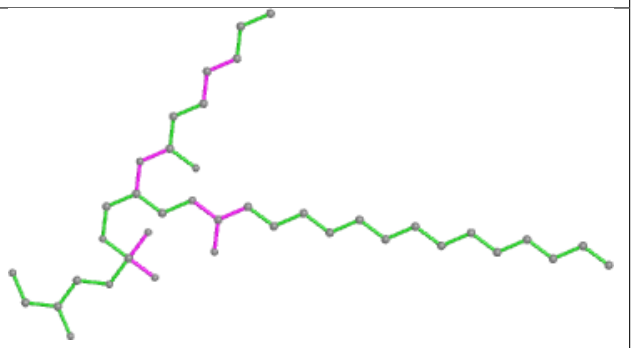


Rings

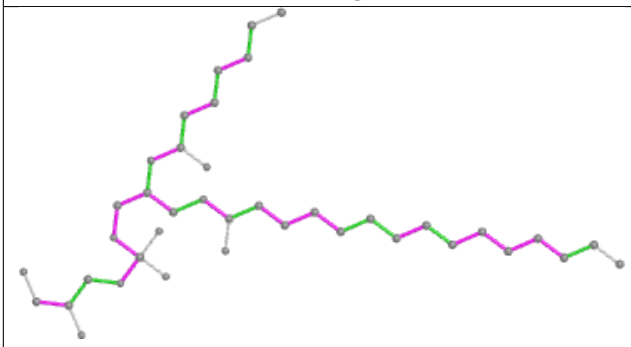
Ligand LHG G 5002



Bond lengths



Bond angles



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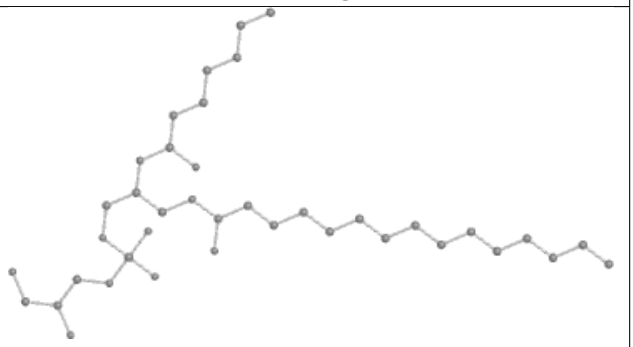
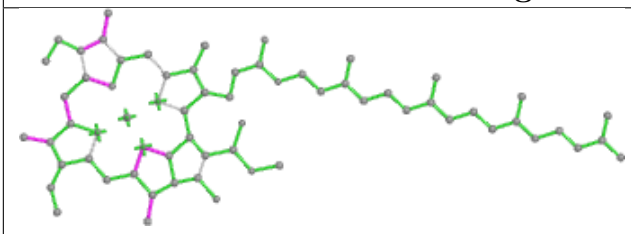


Rings

Ligand CLA A 1101



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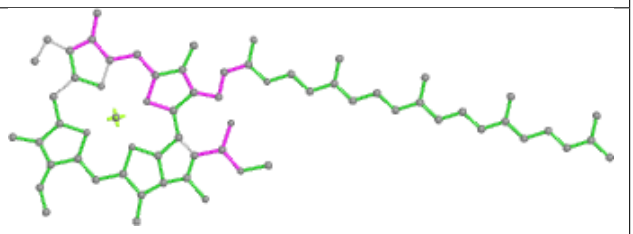
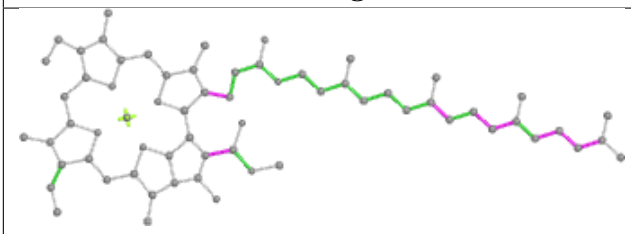


Bond angles



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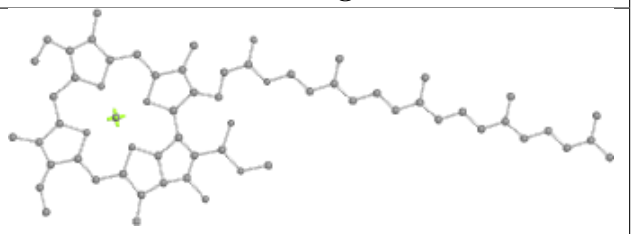
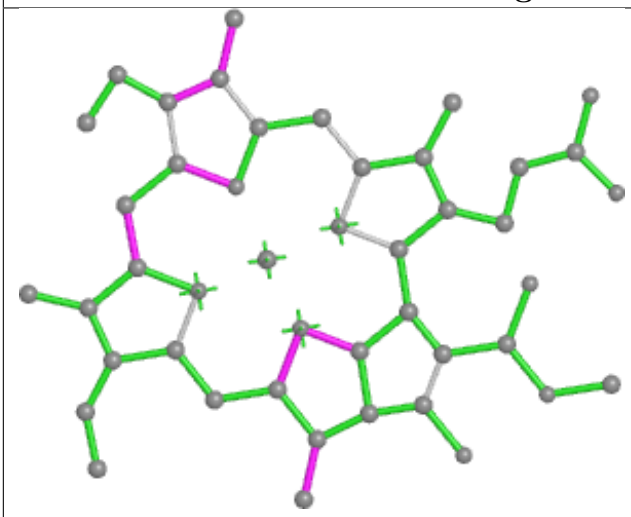
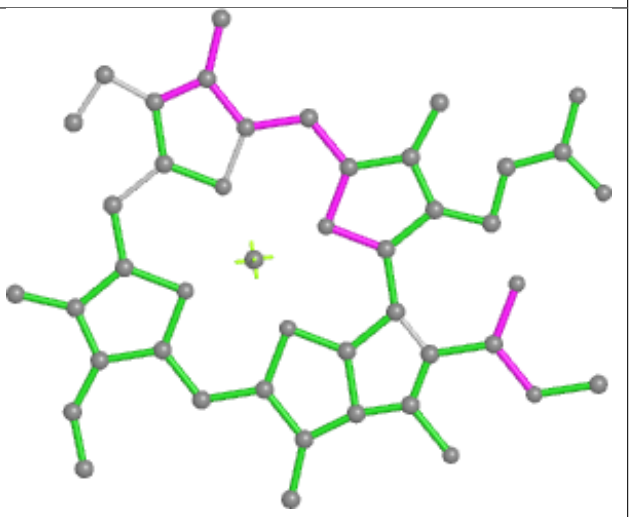


Rings

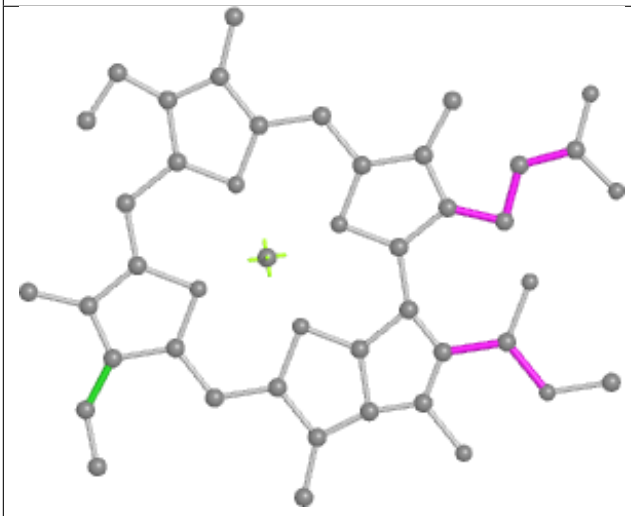
Ligand CLA R 1302



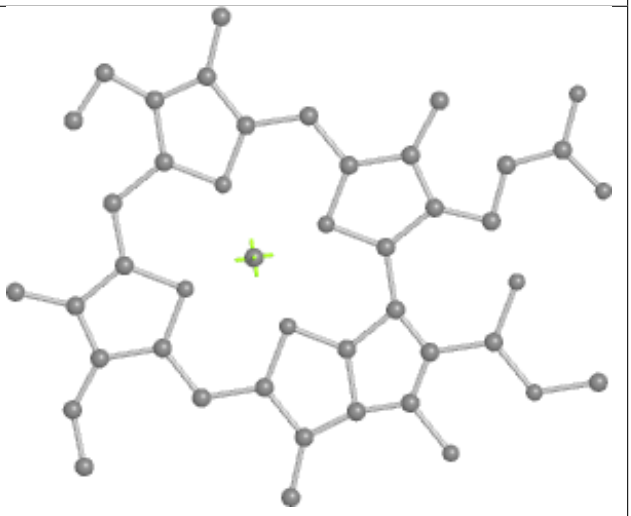
Bond lengths



Bond angles

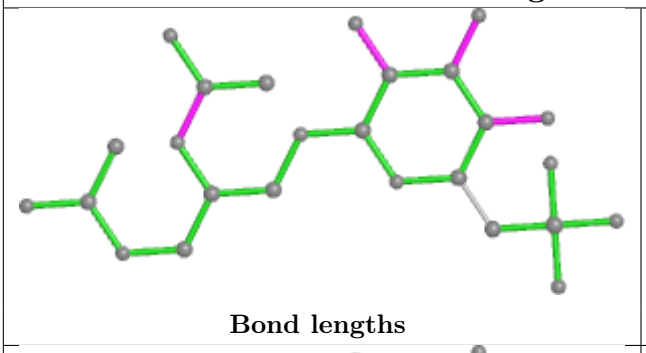


Torsions



Rings

Ligand SQD v 822



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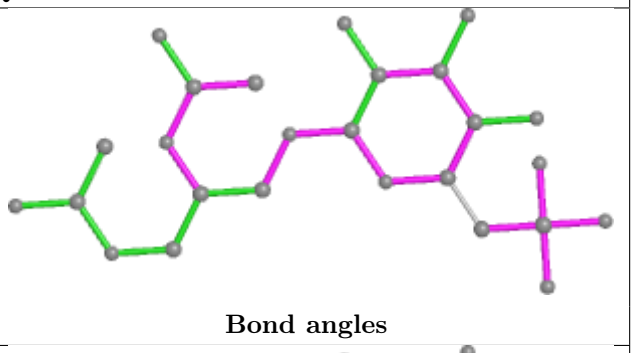
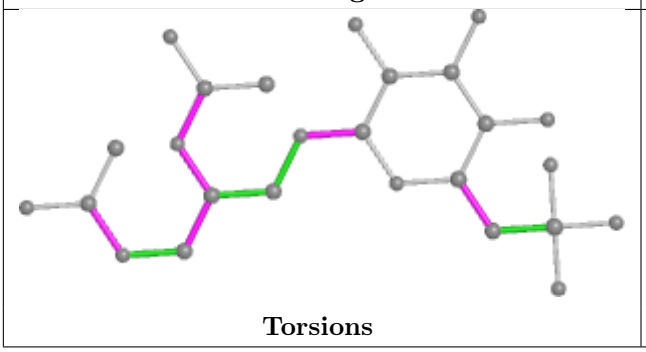


Bond angles



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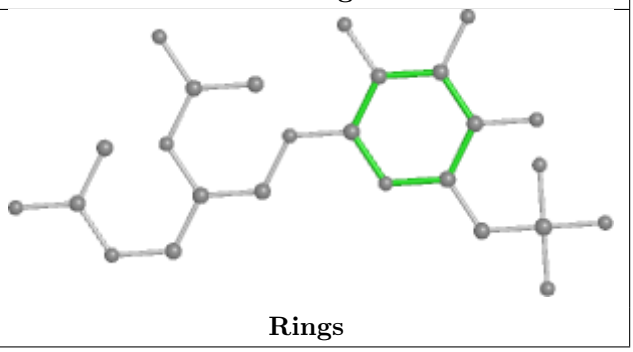
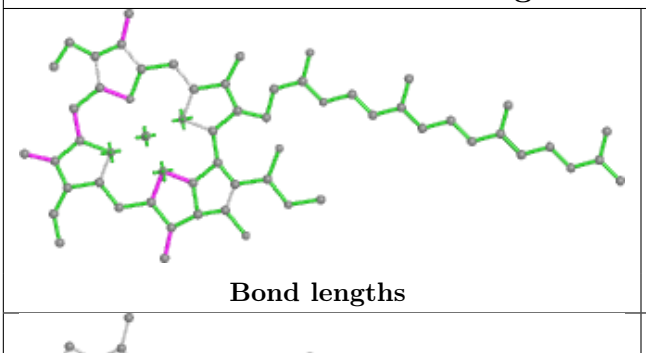


Rings

Ligand CLA H 1224



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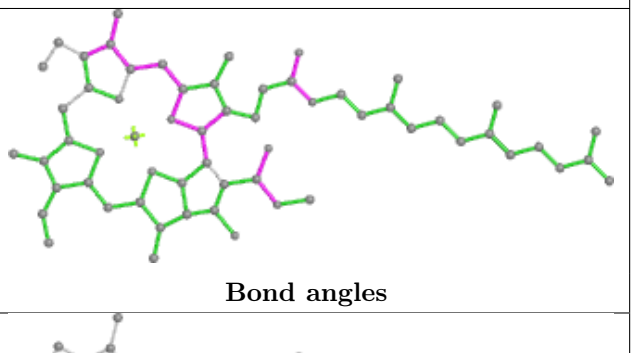
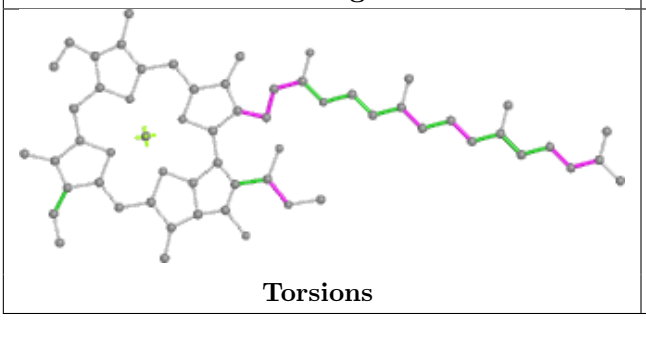


Bond angles



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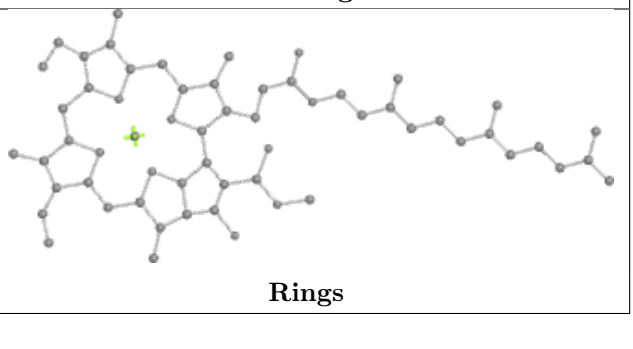
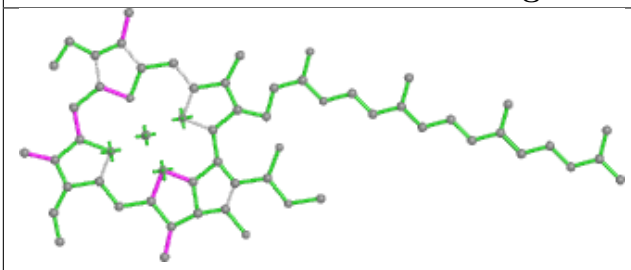
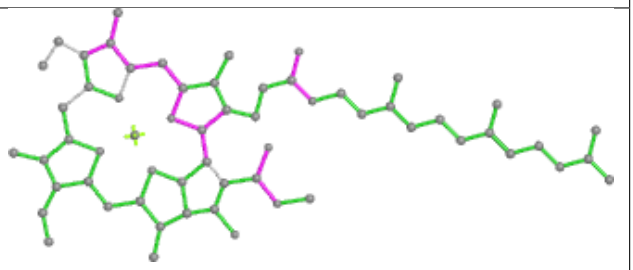
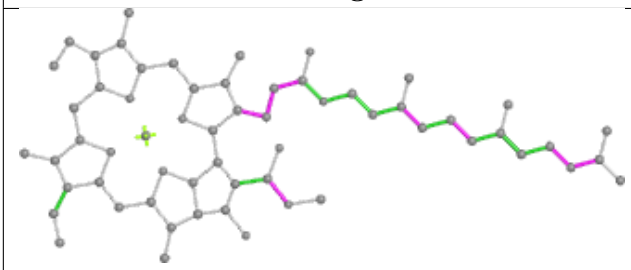
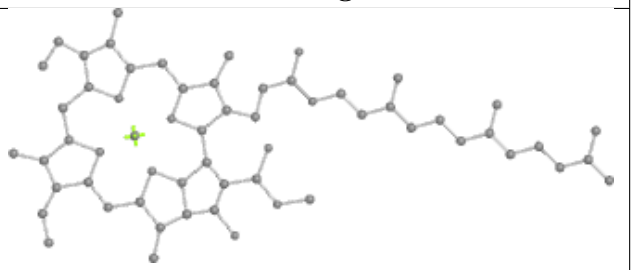
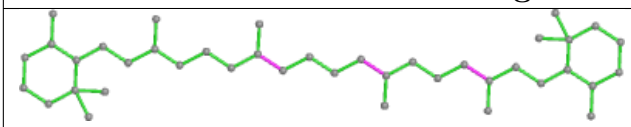
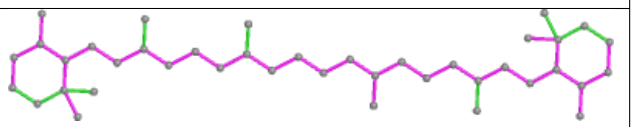
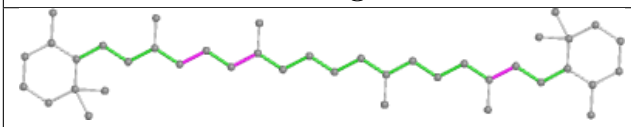
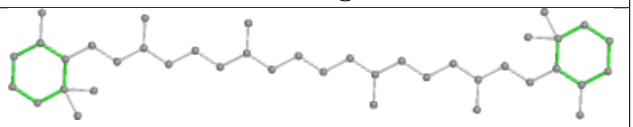
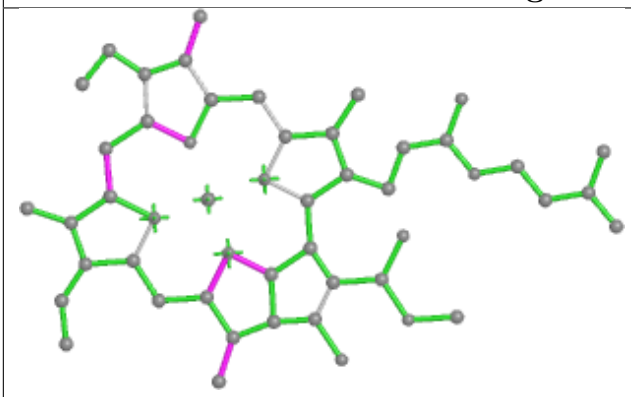


Rings

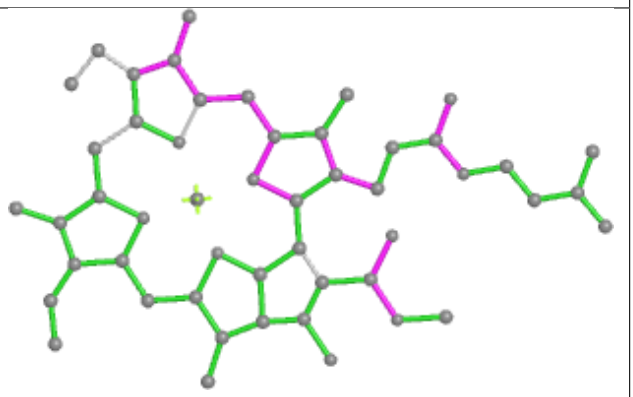
Ligand CLA f 1224	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 4010	
	
Bond lengths	Bond angles
	
Torsions	Rings

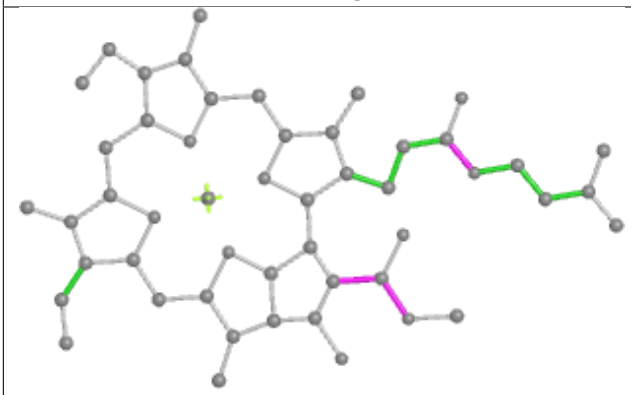
Ligand CLA Z 504



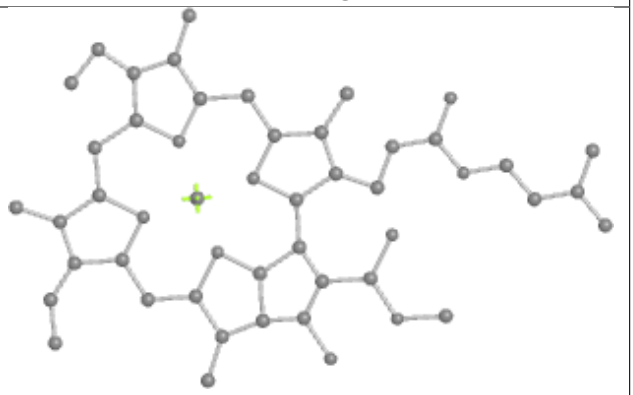
Bond lengths



Bond angles

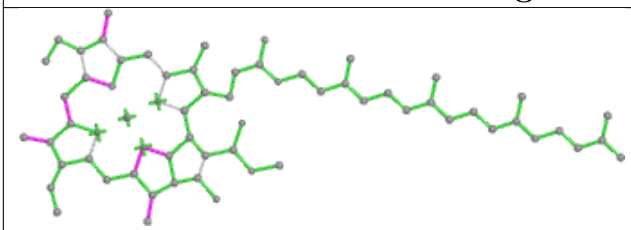


Torsions

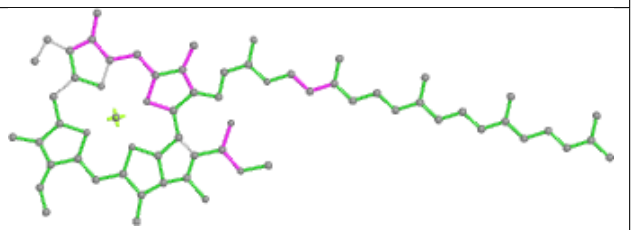


Rings

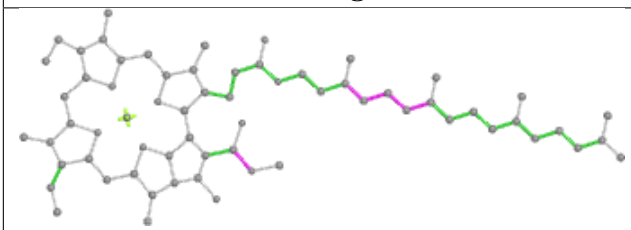
Ligand CLA B 1231



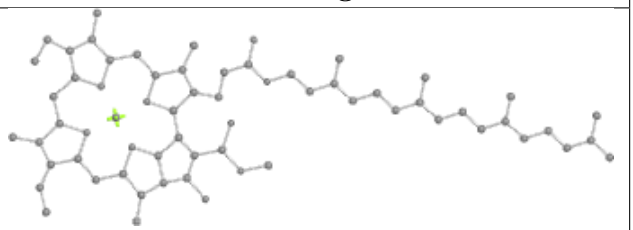
Bond lengths



Bond angles

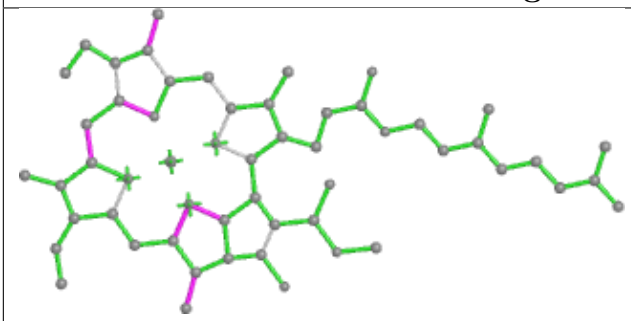


Torsions



Rings

Ligand CLA Y 511



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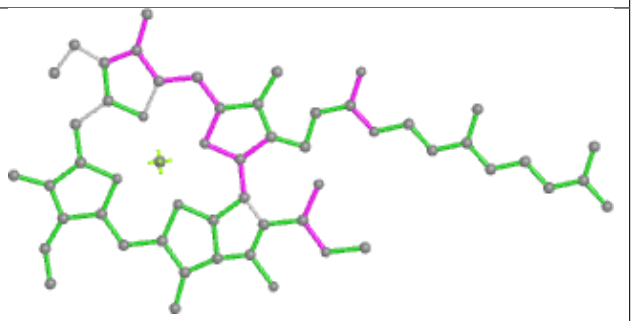
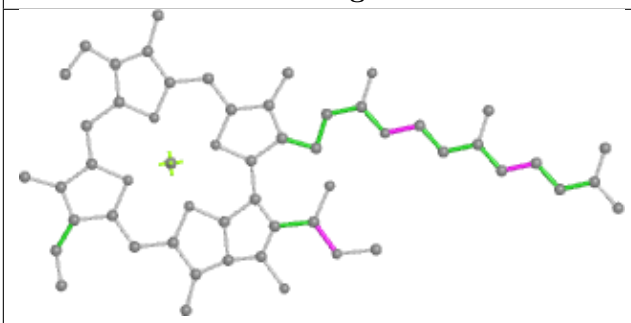


Bond angles



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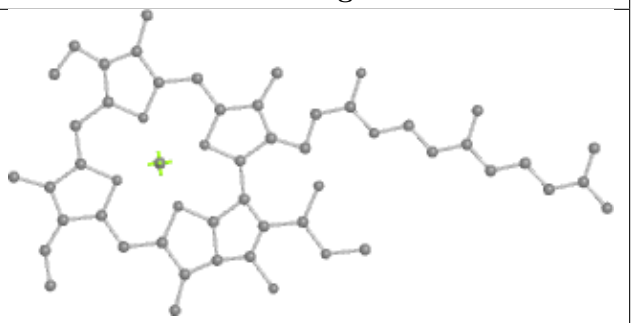
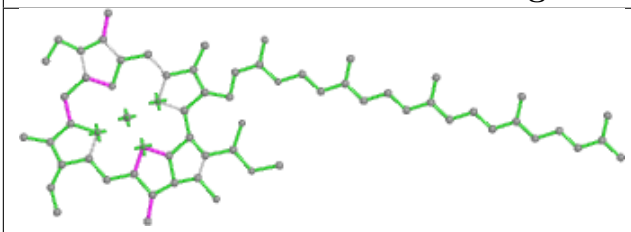


Rings

Ligand CLA 4 505



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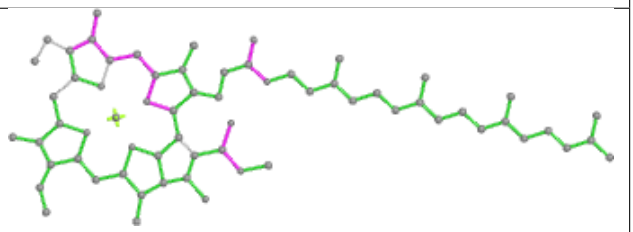
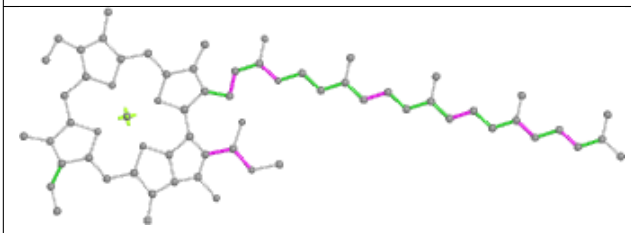
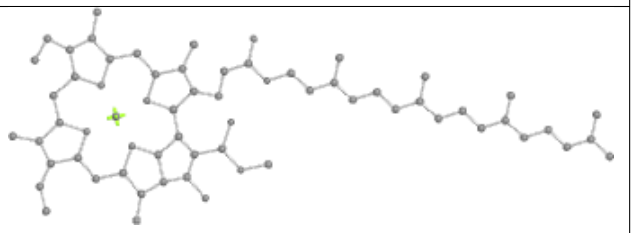


Bond angles

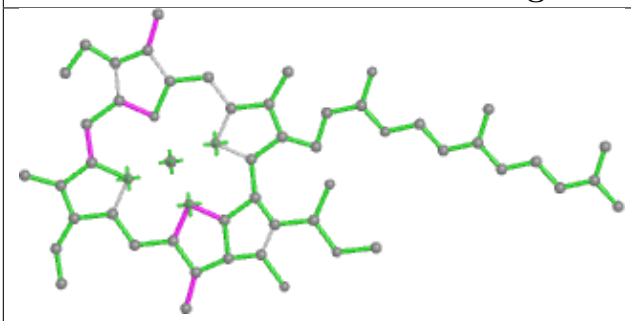


Torsions



Rings

Ligand CLA u 511



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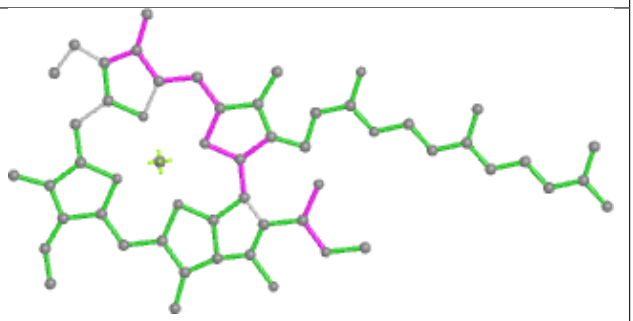
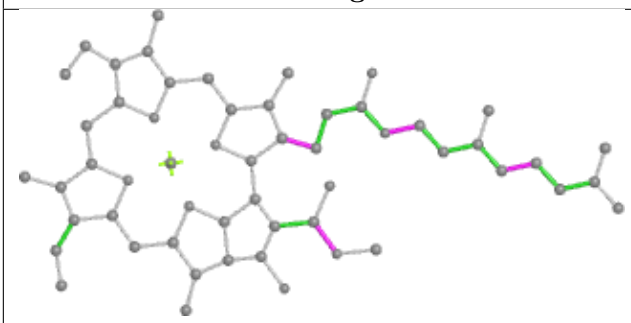
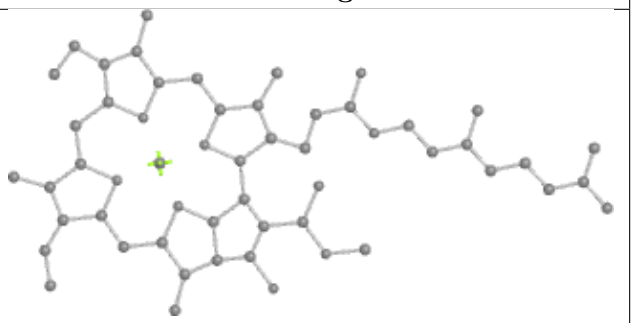


Bond angles

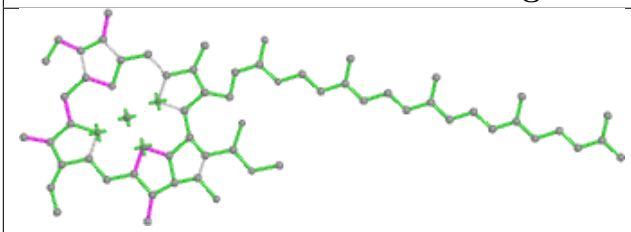


Torsions



Rings

Ligand CLA f 1210



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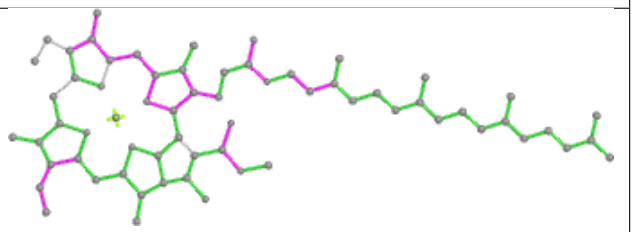

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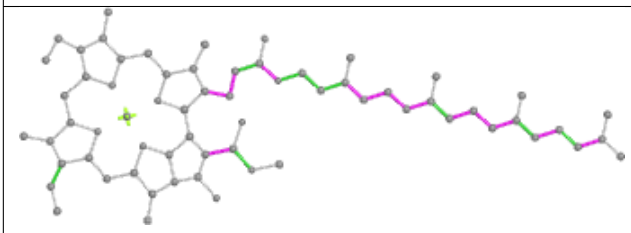

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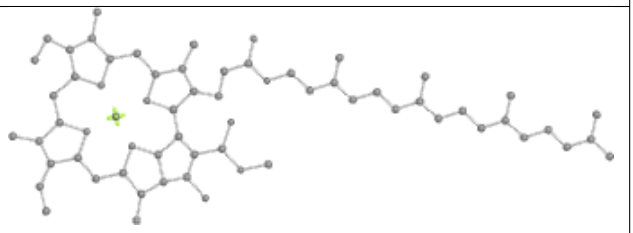
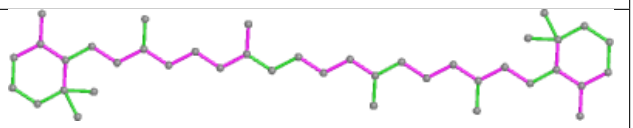


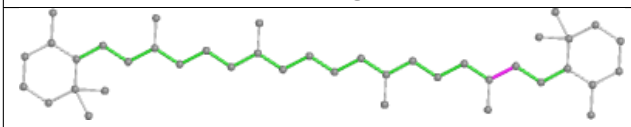
Rings

Ligand BCR I 4018

Bond lengths



Bond angles



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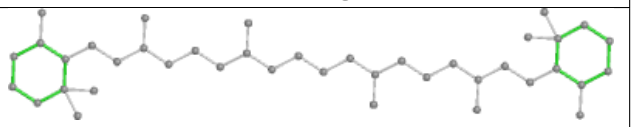
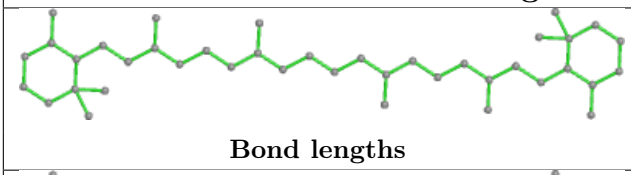


Rings

Ligand BCR l 4012



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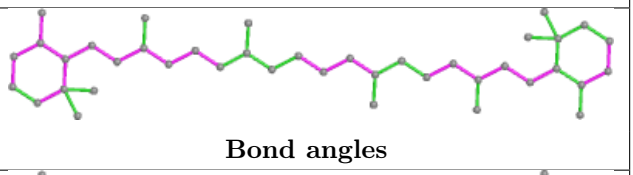

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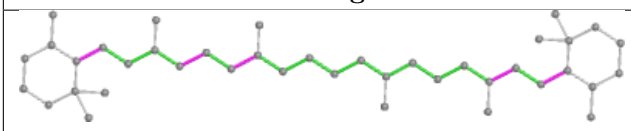

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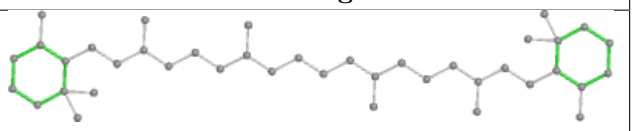
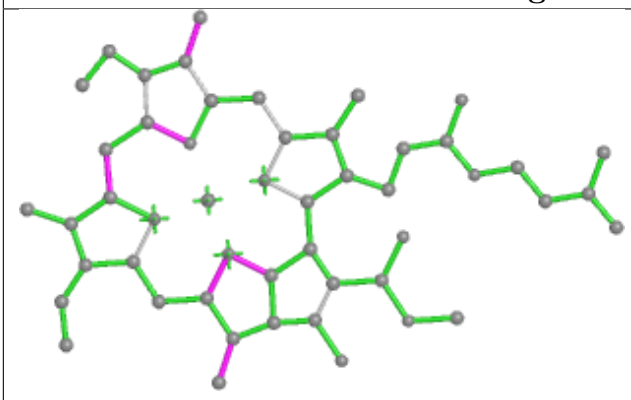


Rings

Ligand CLA 4 502



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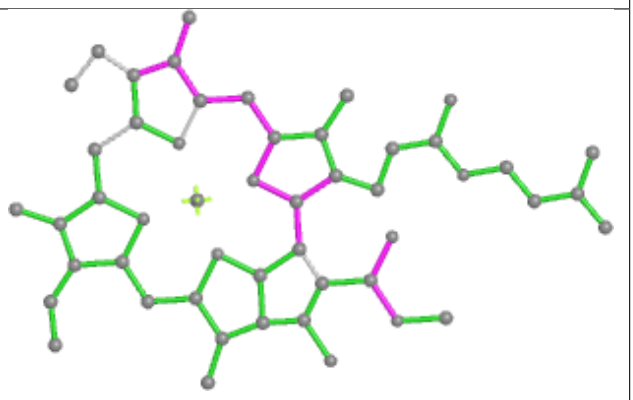
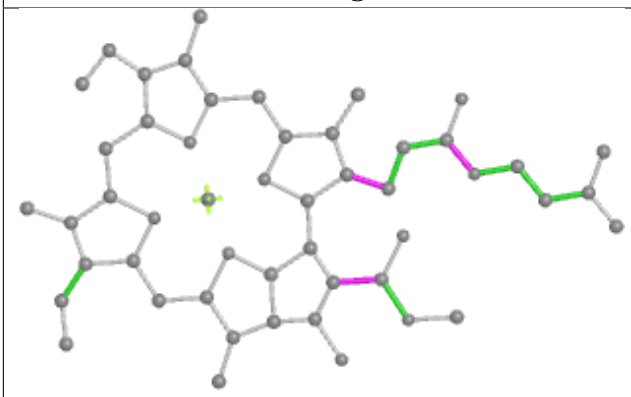


Bond angles



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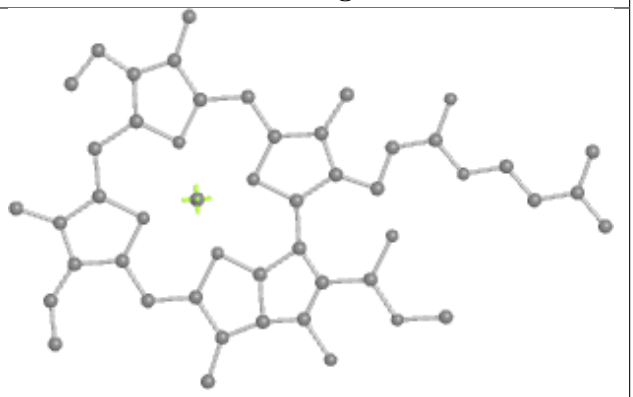
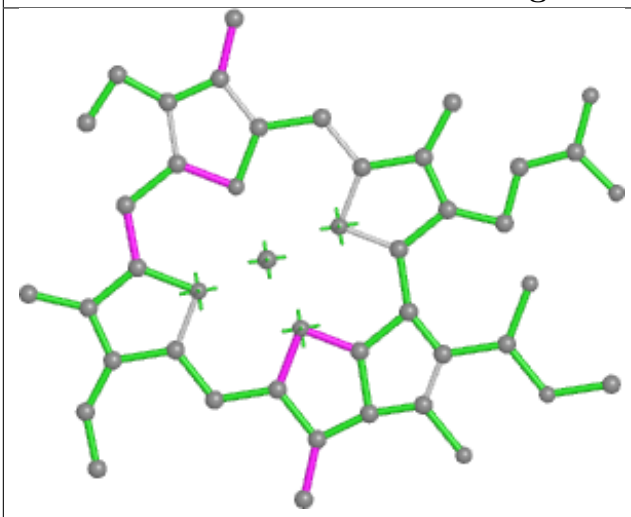


Rings

Ligand CLA c 512



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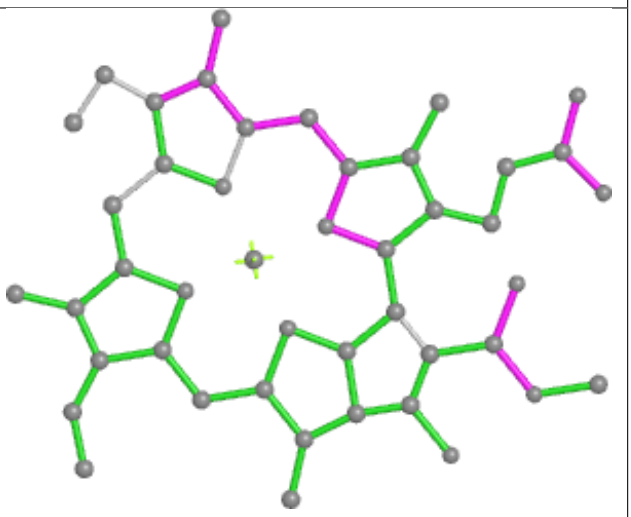
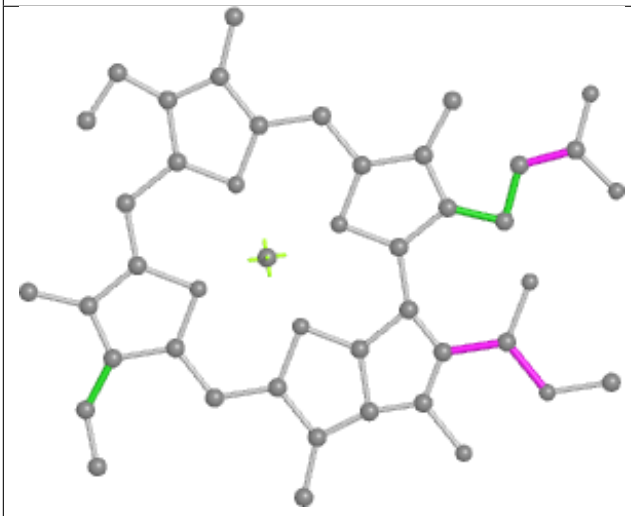


Bond angles



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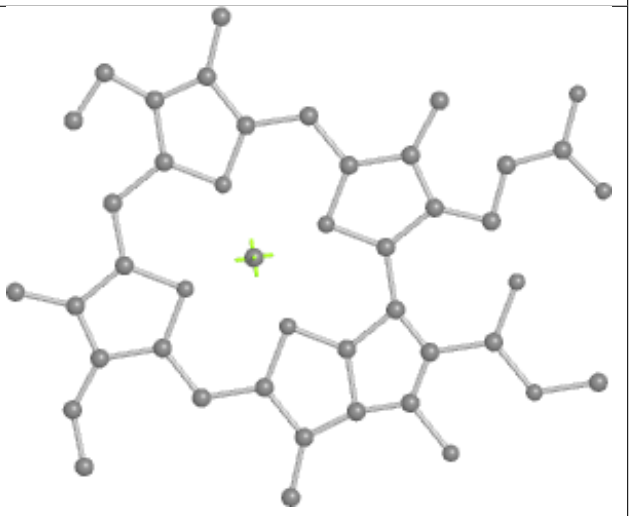
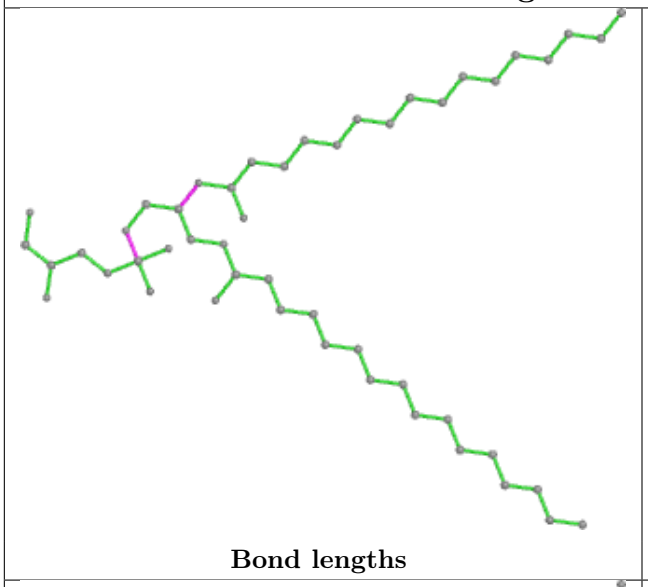


Rings

Ligand LHG n 5221



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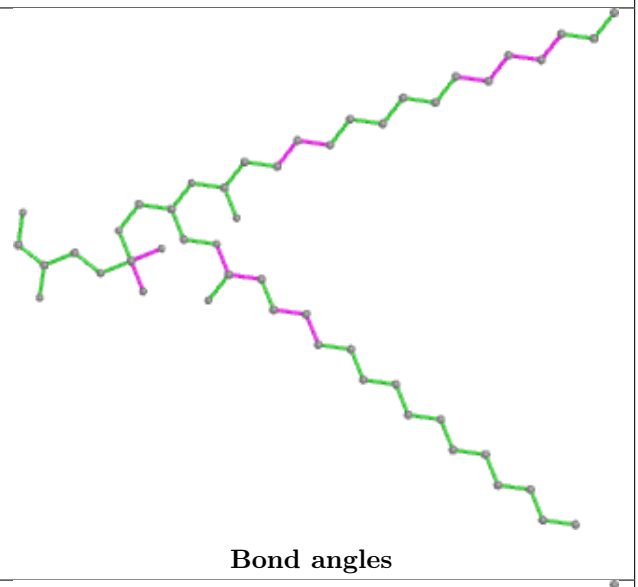
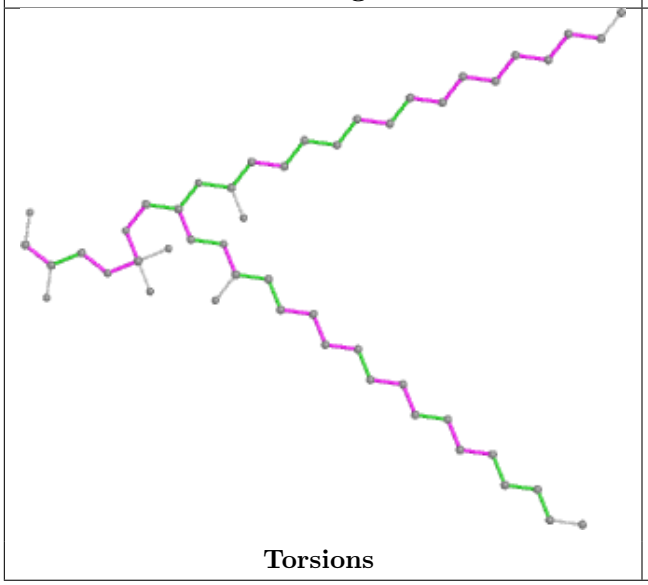


Bond angles



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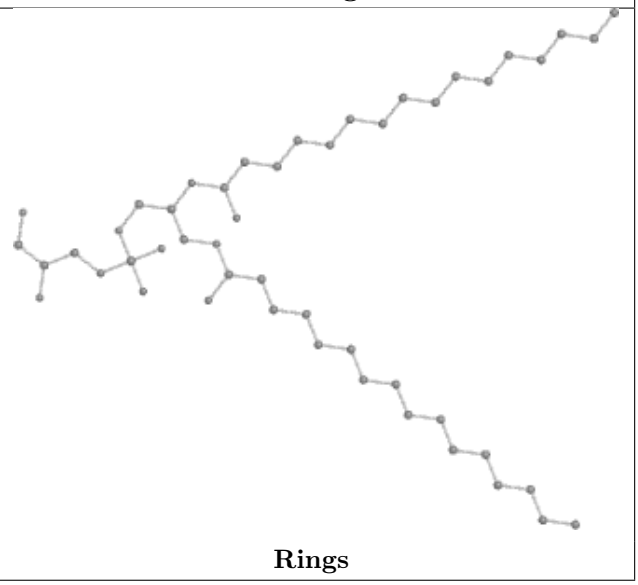
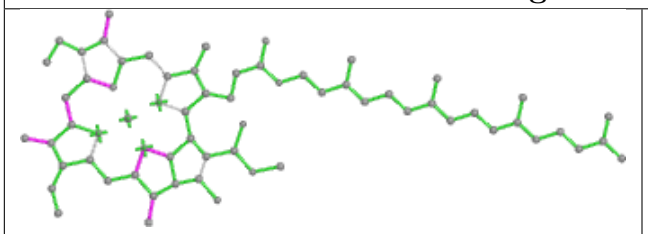


Rings

Ligand CLA 2 501



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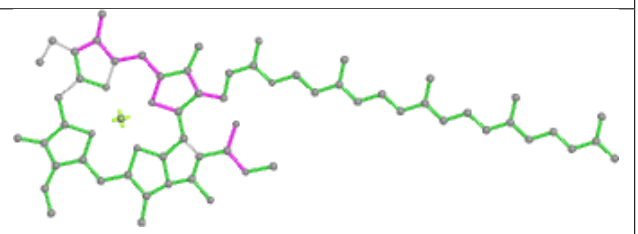

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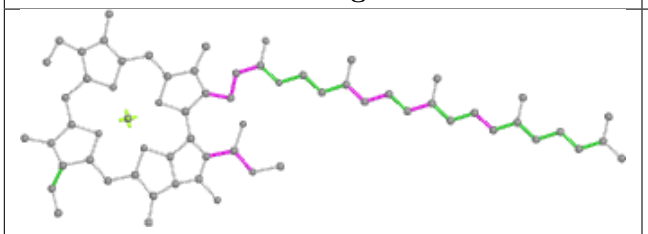

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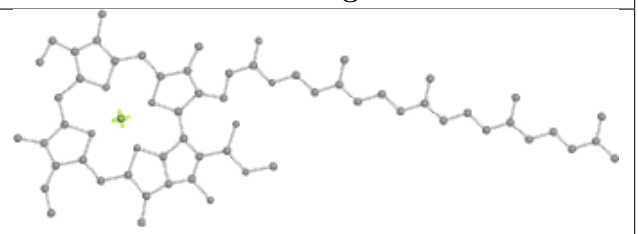
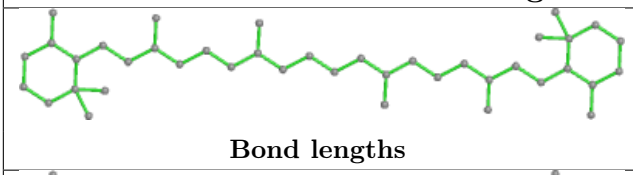


Rings

Ligand BCR 6 522



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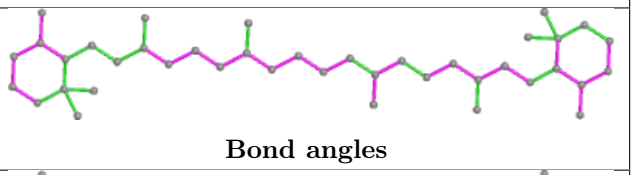

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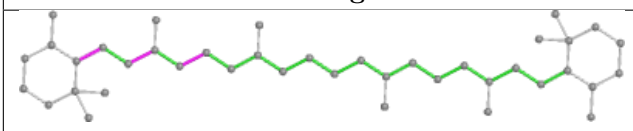

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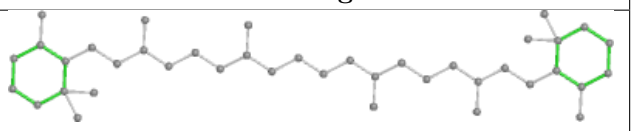
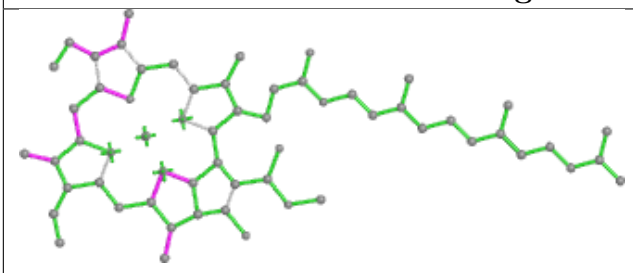


Rings

Ligand CLA A 1122



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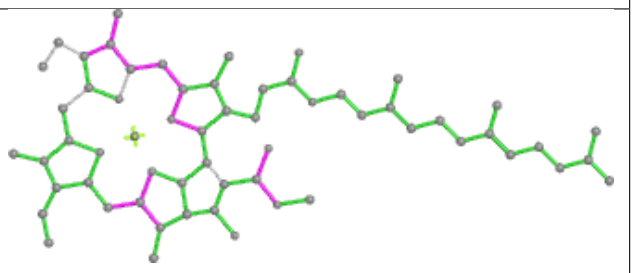

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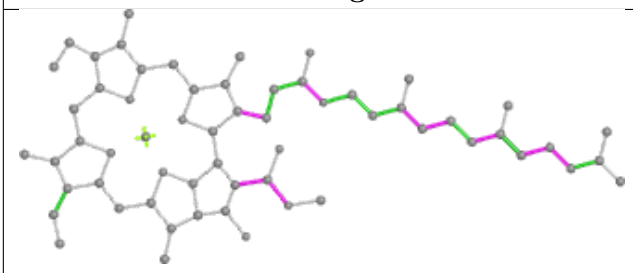

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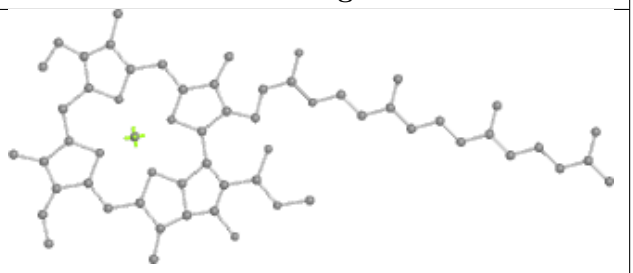
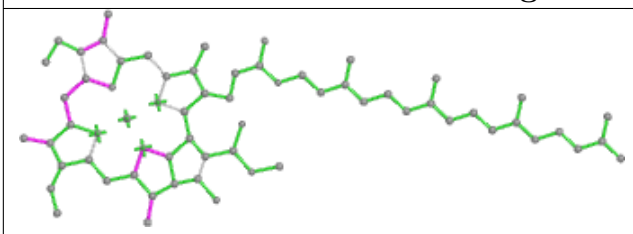


Rings

Ligand CLA e 1237



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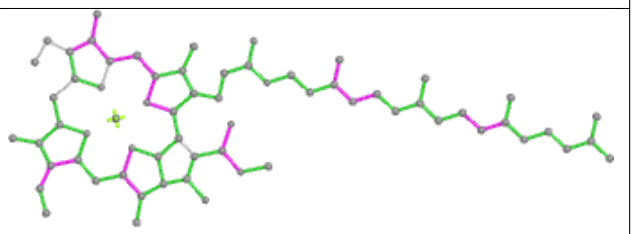
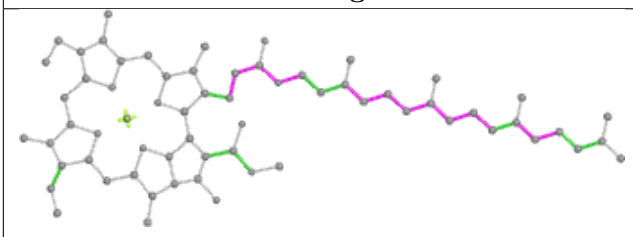


Bond angles



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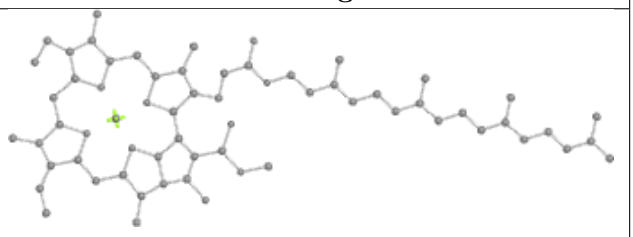
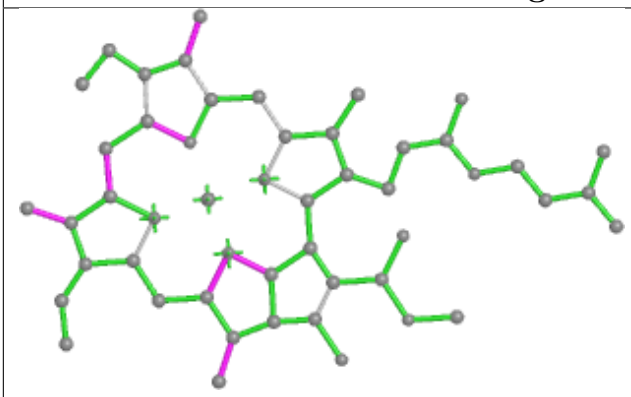
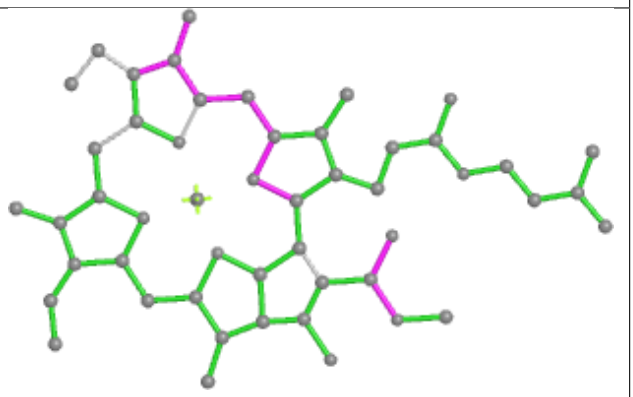


Rings

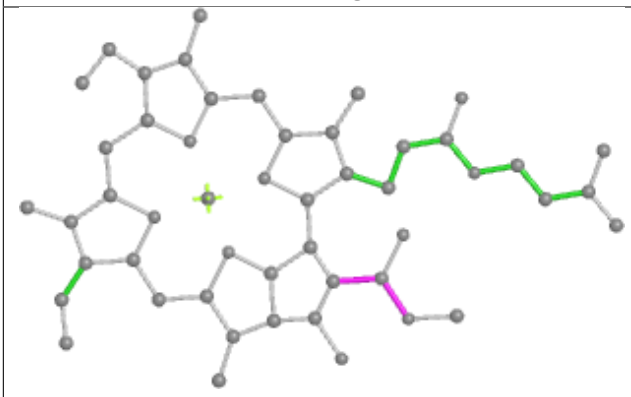
Ligand CLA a 506



Bond lengths



Bond angles



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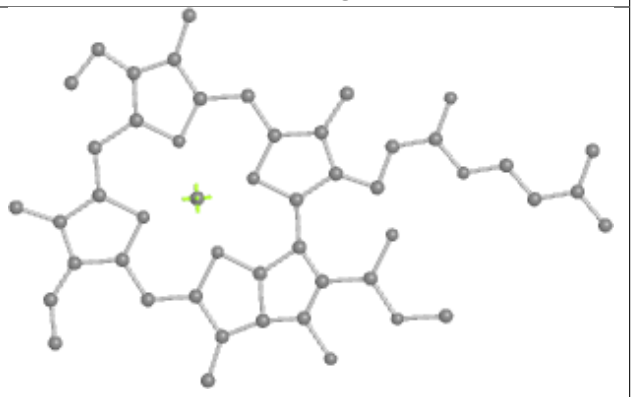
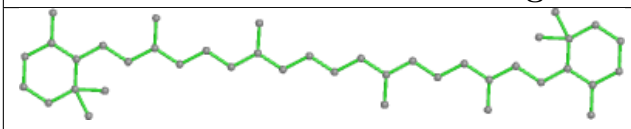
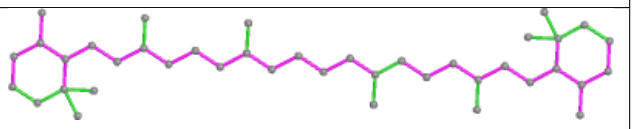


Rings

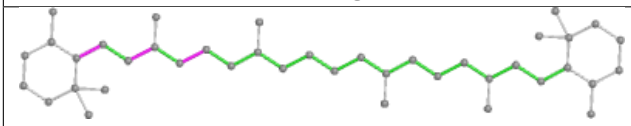
Ligand BCR 5 522



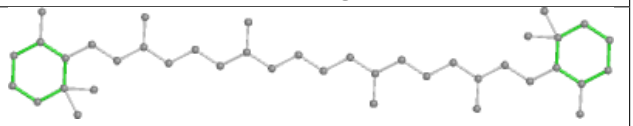
Bond lengths



Bond angles

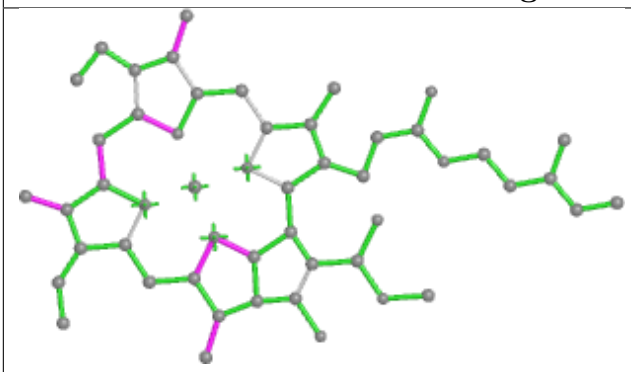


Torsions



Rings

Ligand CLA e 1110



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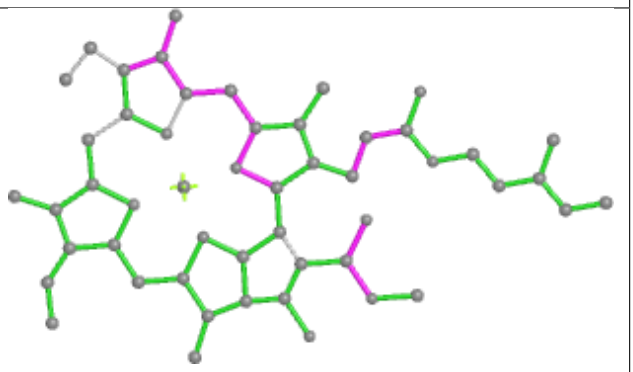
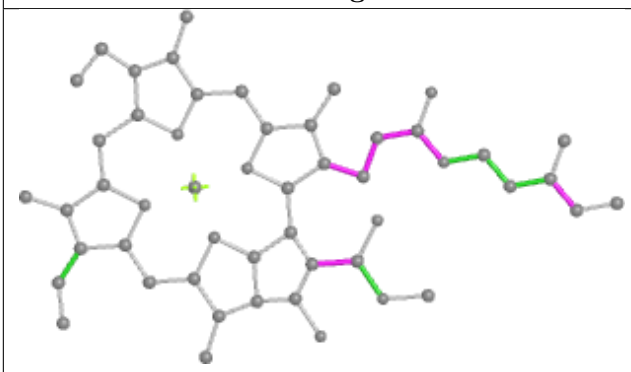


Bond angles



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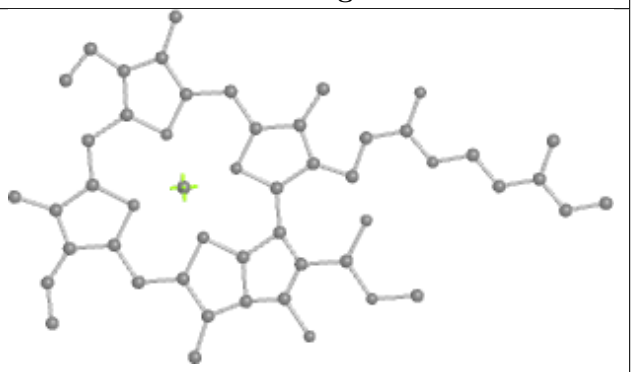
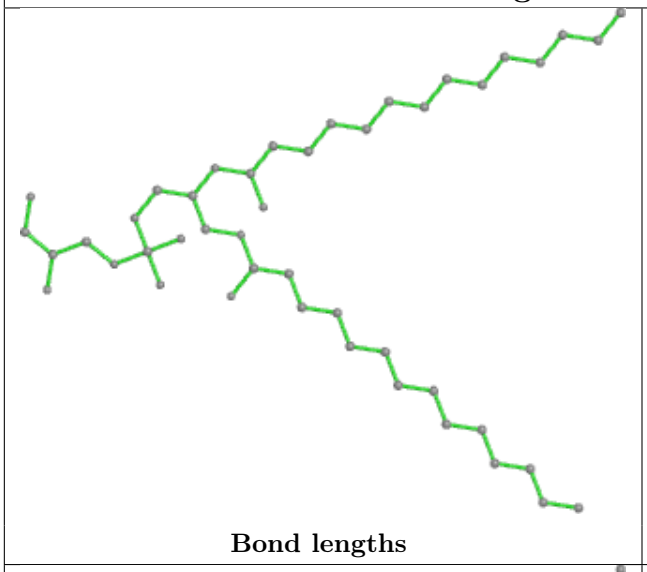


Rings

Ligand LHG G 5006



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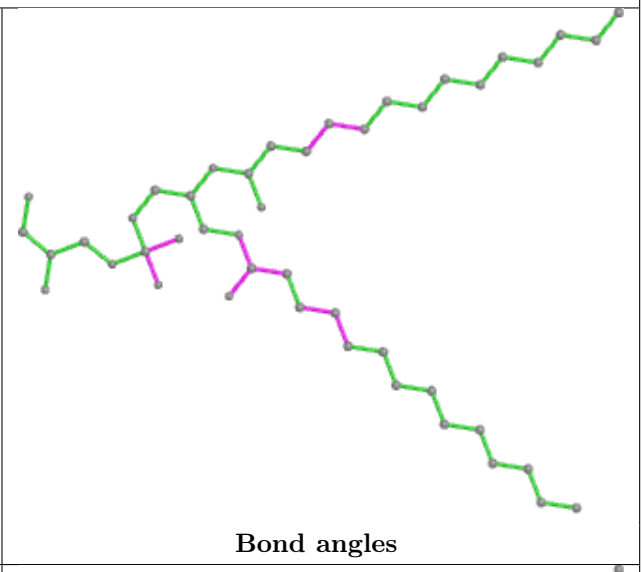
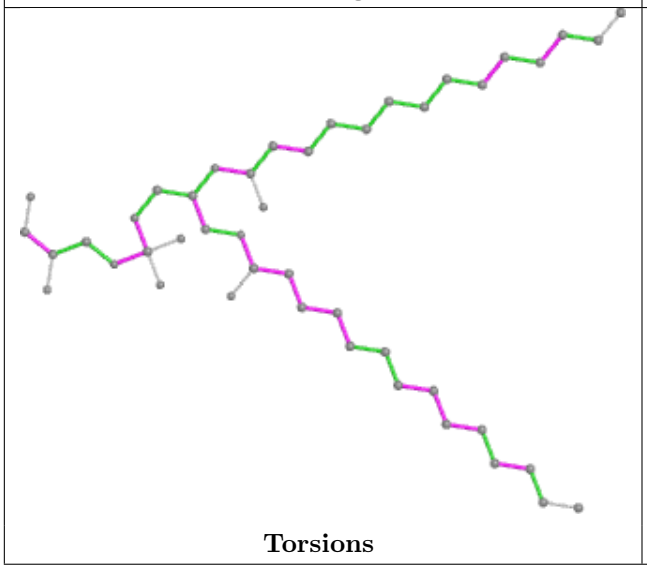
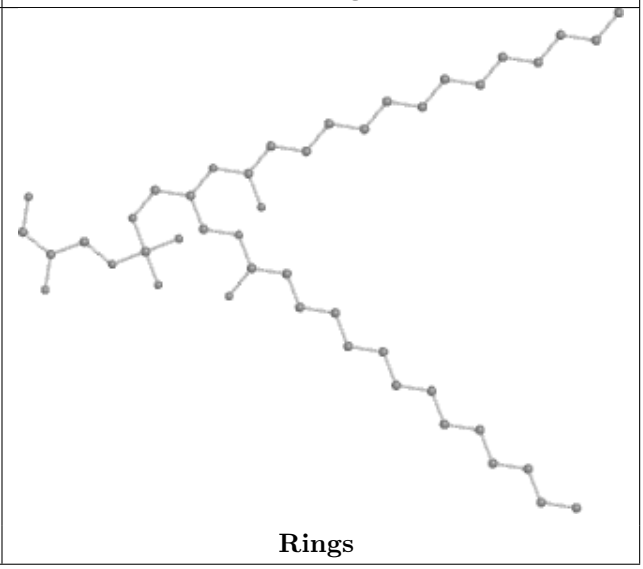


Bond angles

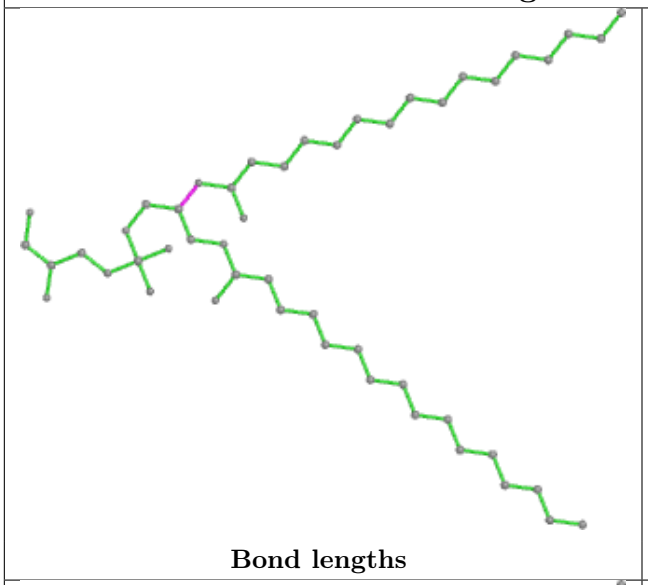


Torsions



Rings

Ligand LHG e 5001



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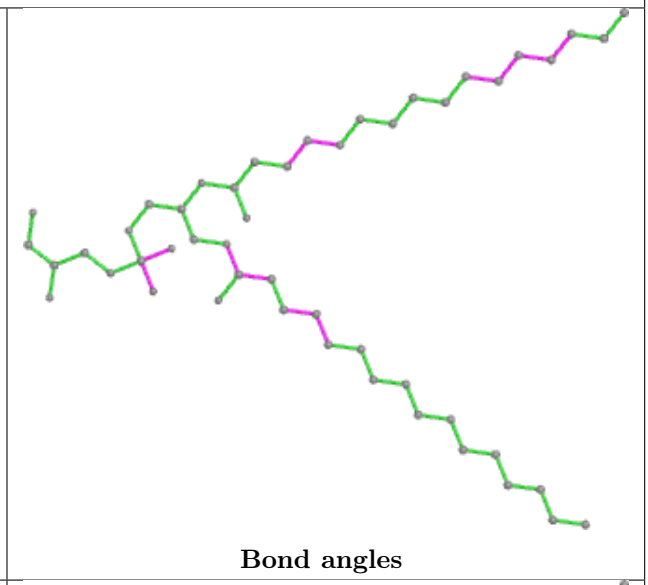
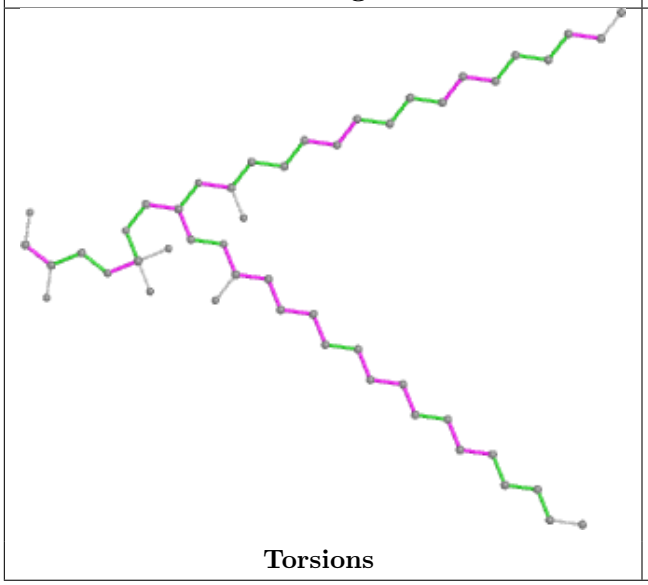
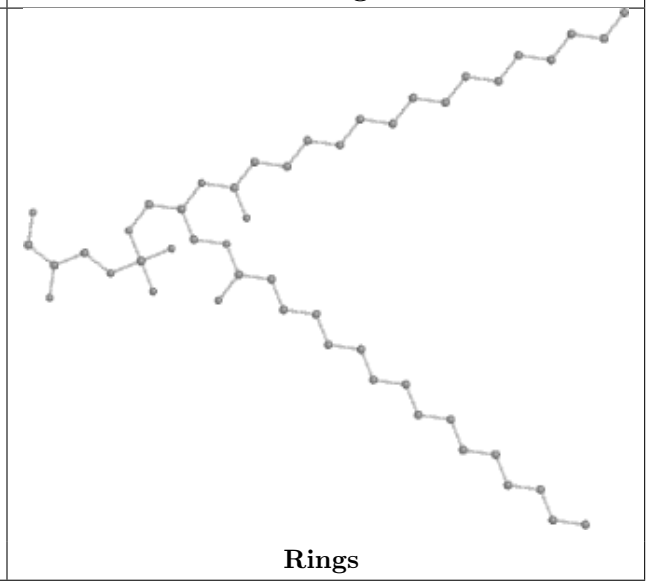


Bond angles

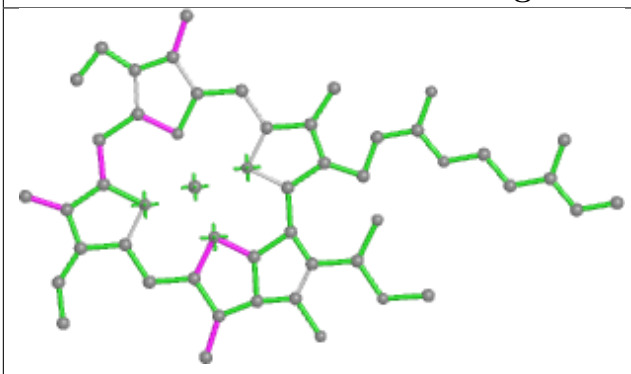


Torsions

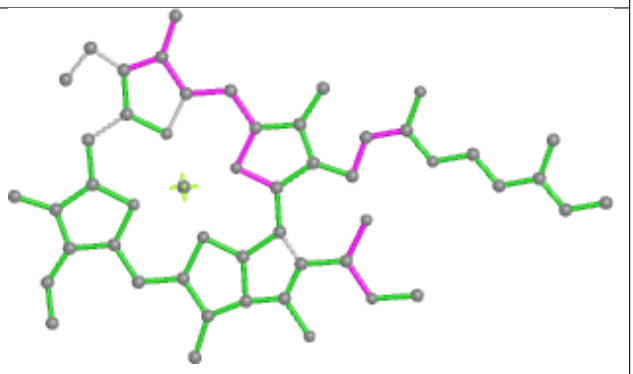


Rings

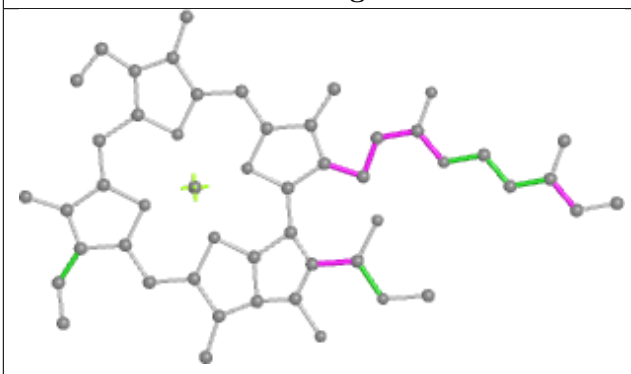
Ligand CLA G 1110



Bond lengths



Bond angles



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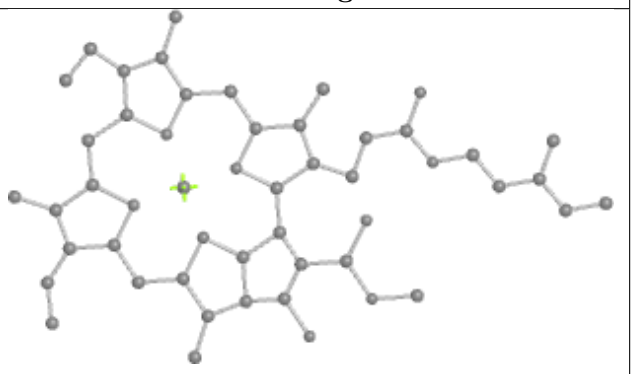
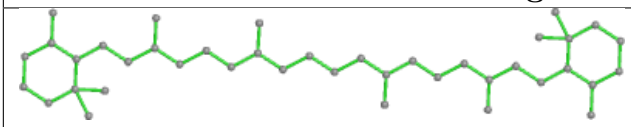


Rings

Ligand BCR 5 521



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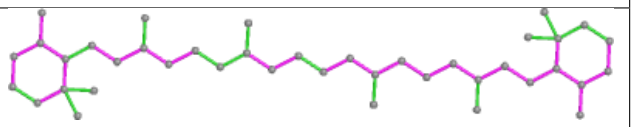
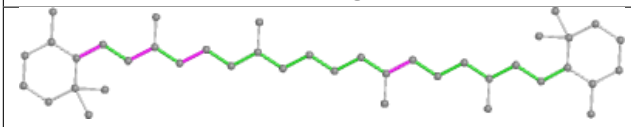


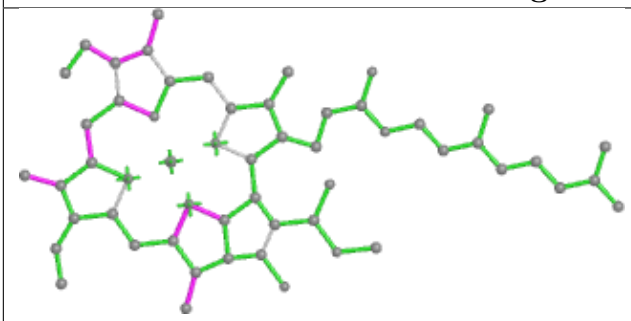
Bond angles



Torsions

Rings

Ligand CLA t 519



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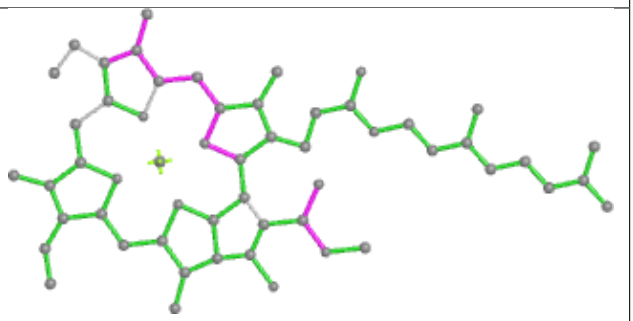
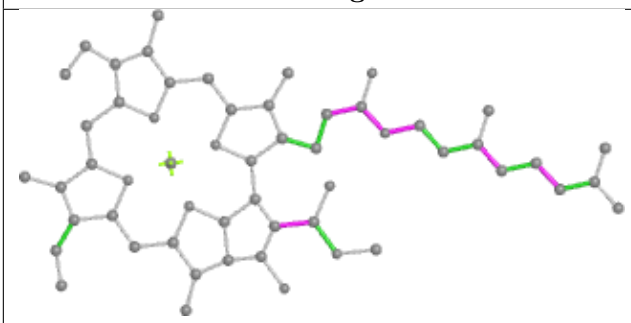
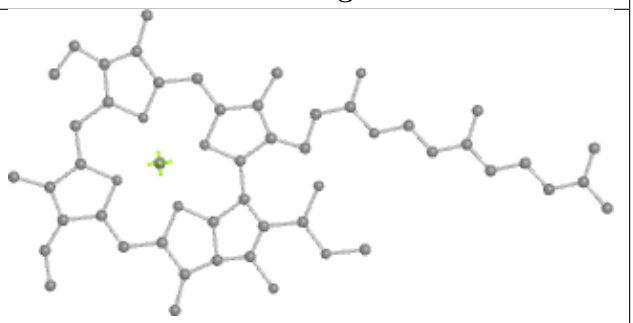


Bond angles

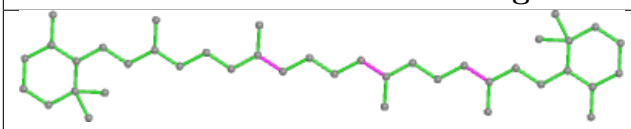


Torsions



Rings

Ligand BCR H 4010



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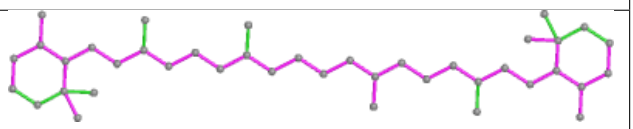
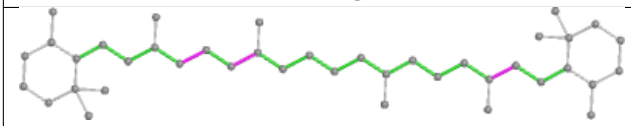


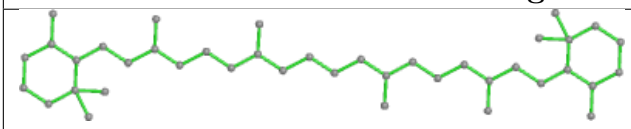
Bond angles



Torsions

Rings

Ligand BCR c 523



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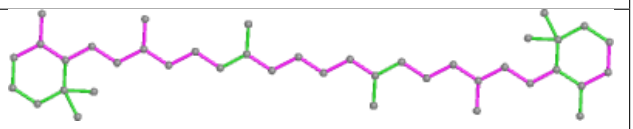

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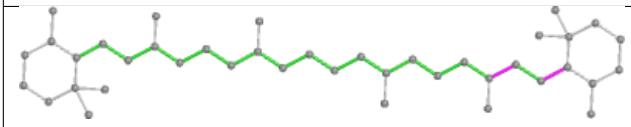
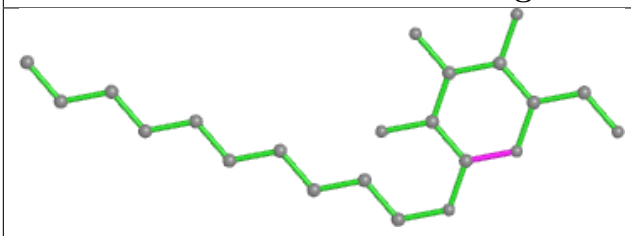


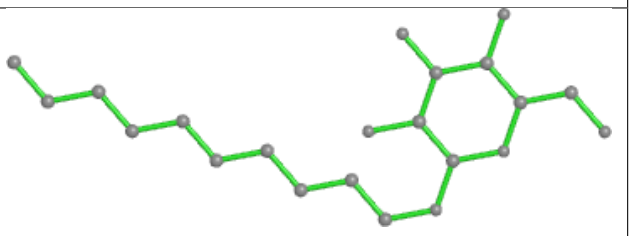
Torsions

Rings

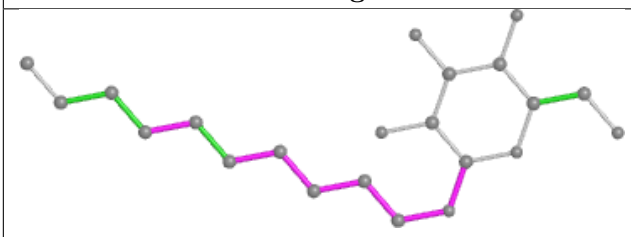
Ligand LMU J 5105



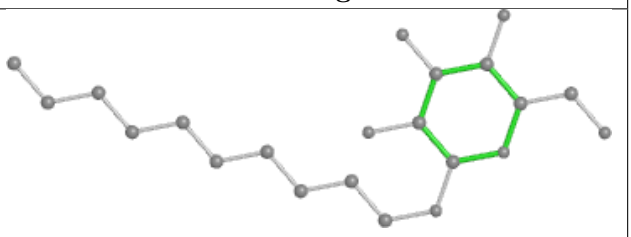
Bond lengths



Bond angles

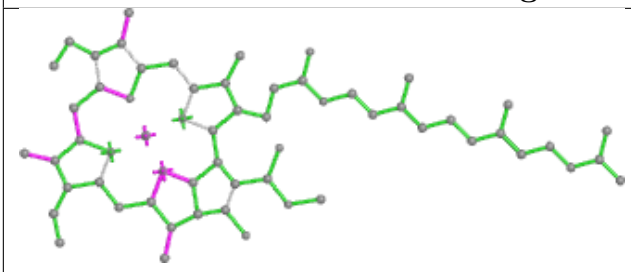


Torsions



Rings

Ligand CLA e 1116



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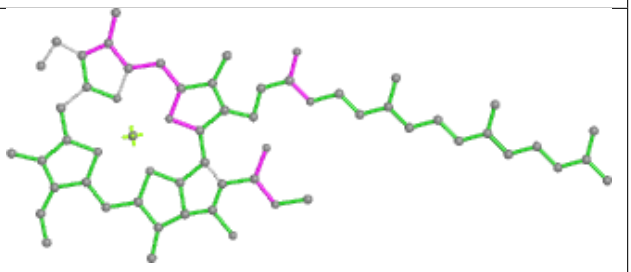
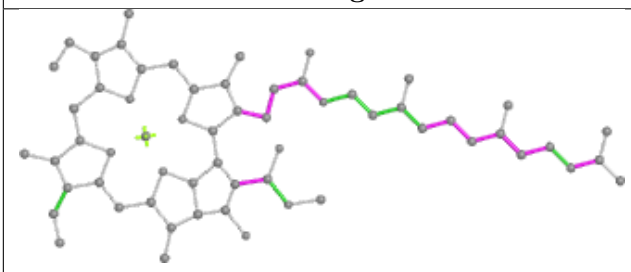


Bond angles



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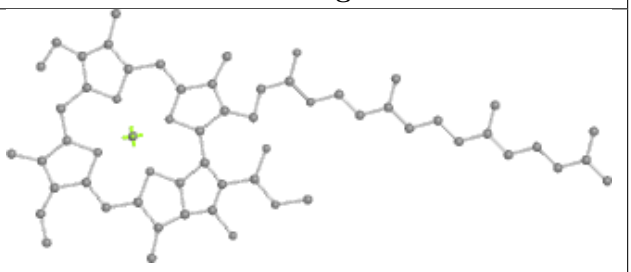
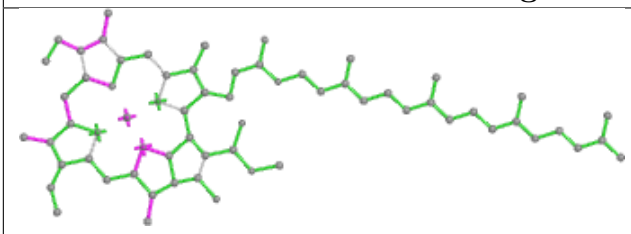


Rings

Ligand CLA e 1107



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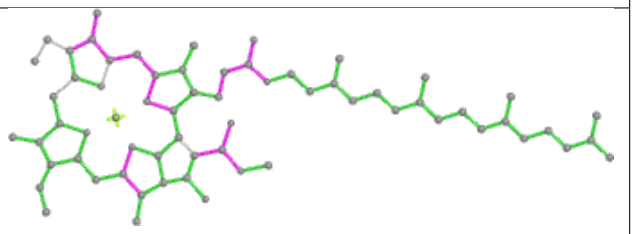
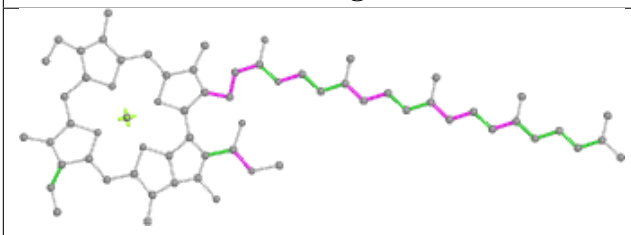


Bond angles



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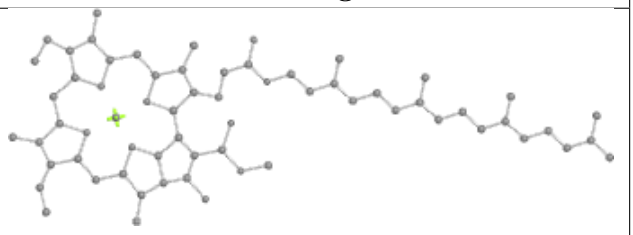
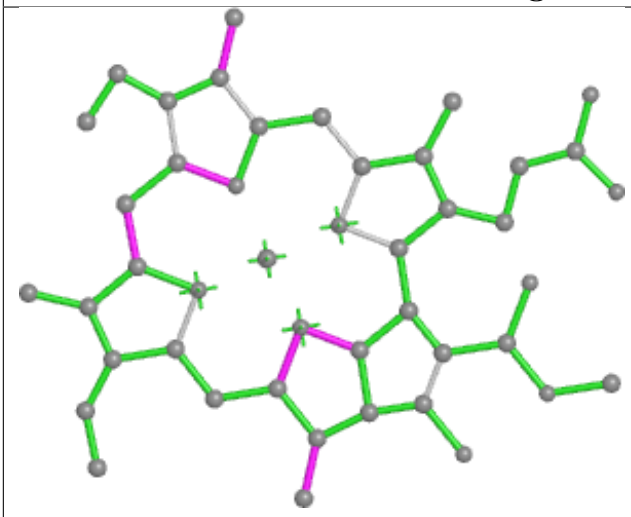


Rings

Ligand CLA v 512



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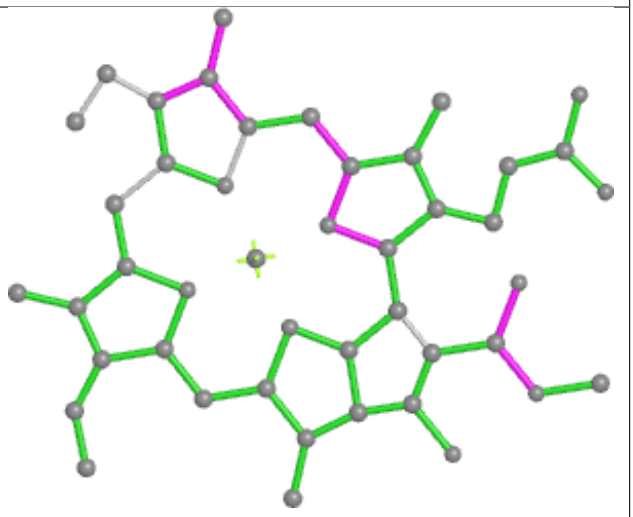
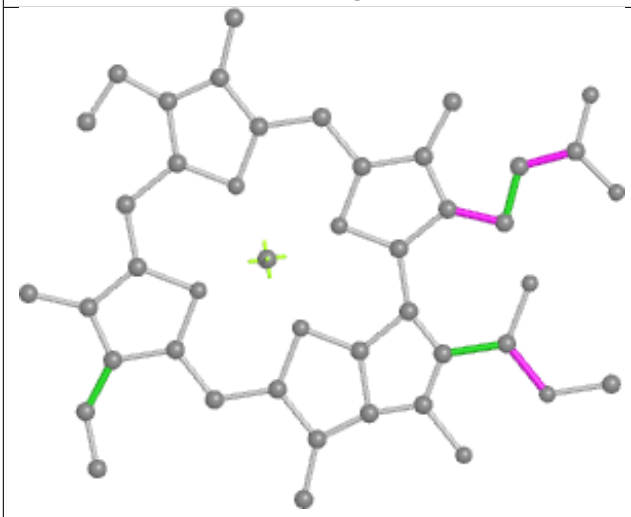
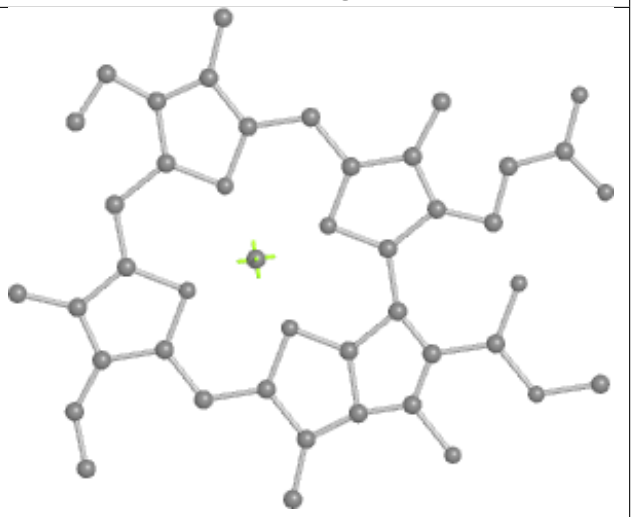


Bond angles

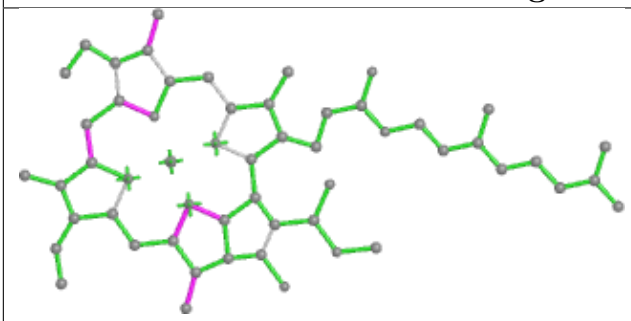


Torsions

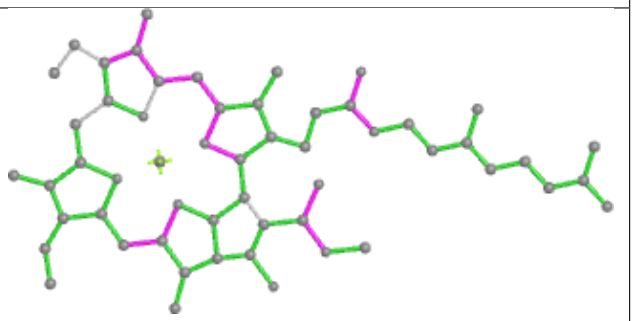


Rings

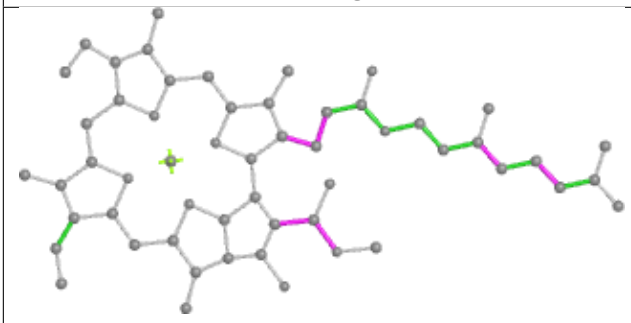
Ligand CLA 5 503



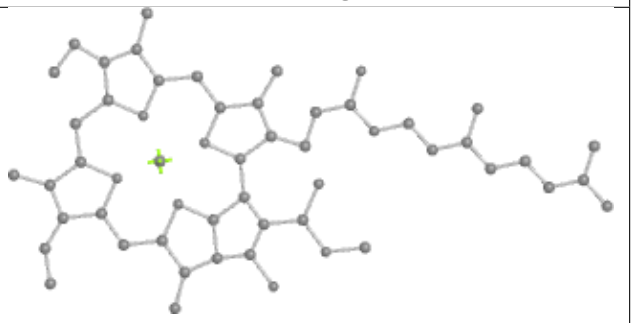
Bond lengths



Bond angles

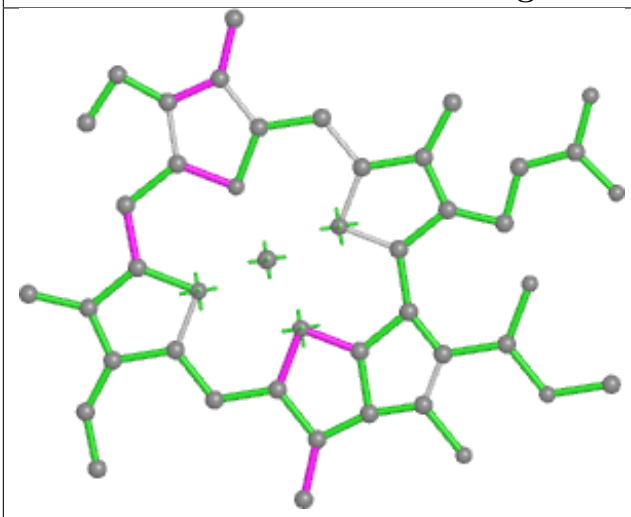


Torsions

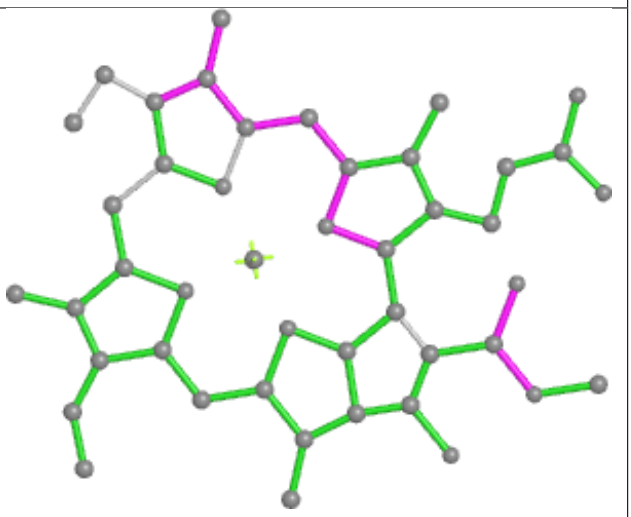


Rings

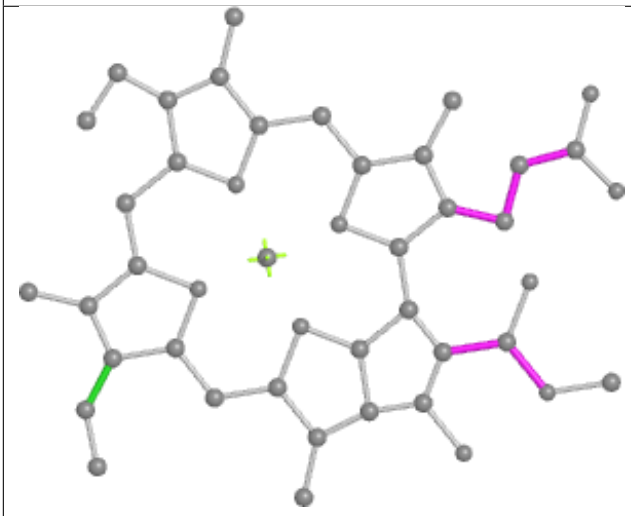
Ligand CLA F 1302



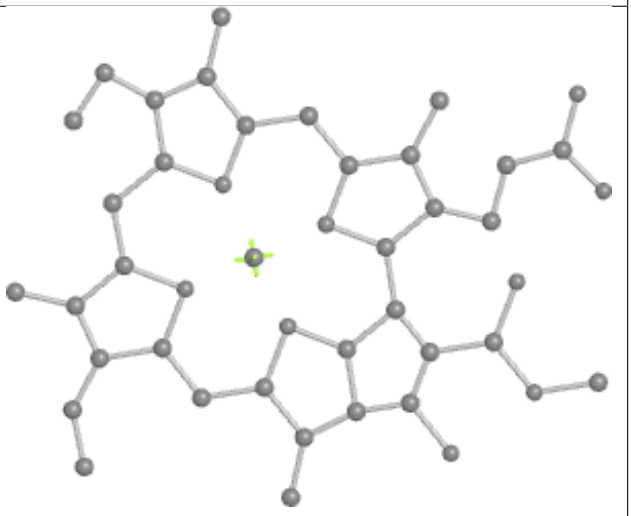
Bond lengths



Bond angles

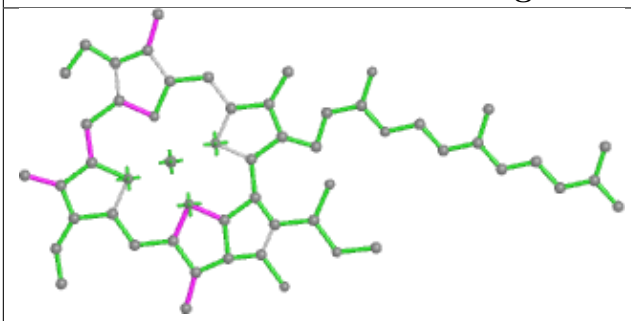


Torsions

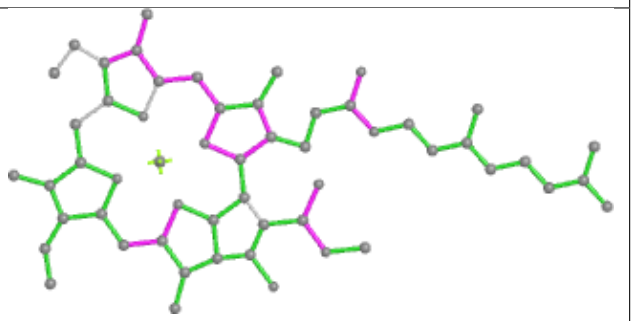


Rings

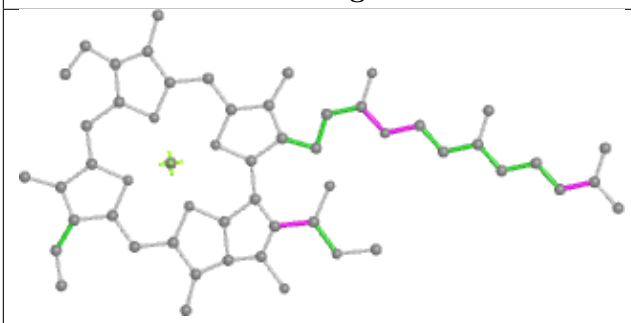
Ligand CLA A 1105



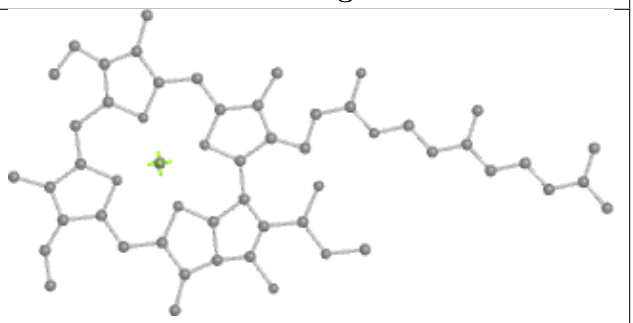
Bond lengths



Bond angles

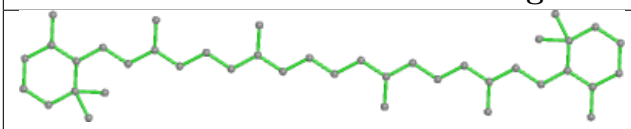


Torsions

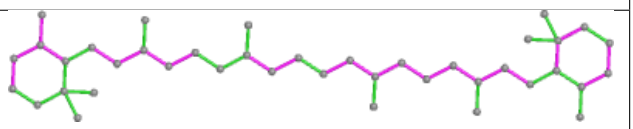


Rings

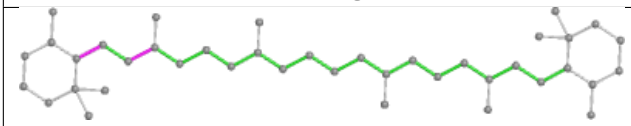
Ligand BCR 2 521



Bond lengths



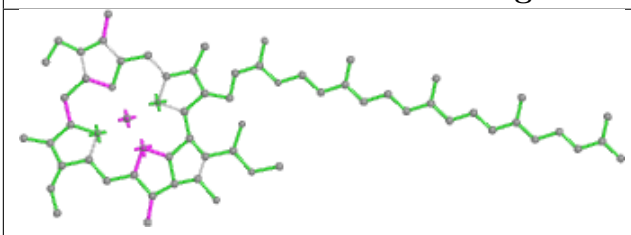
Bond angles



Torsions

Rings

Ligand CLA A 1139



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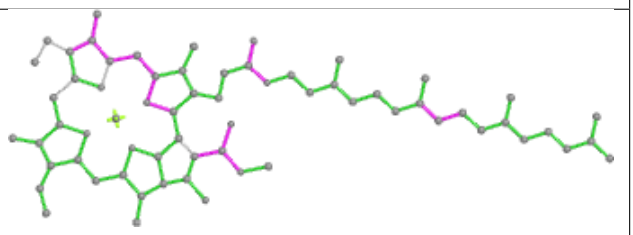
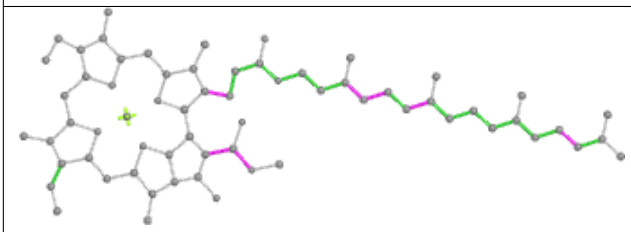


Bond angles



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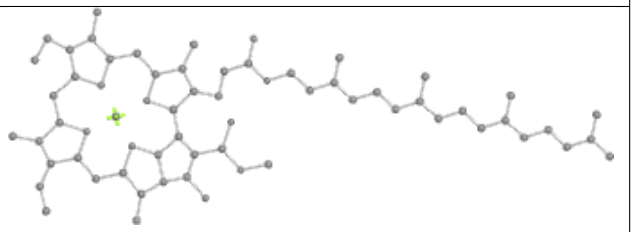
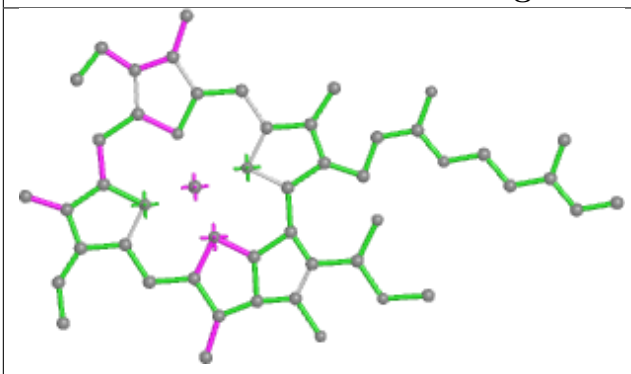


Rings

Ligand CLA G 1129



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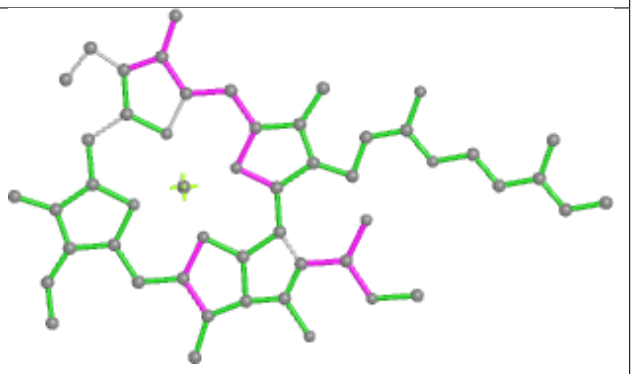
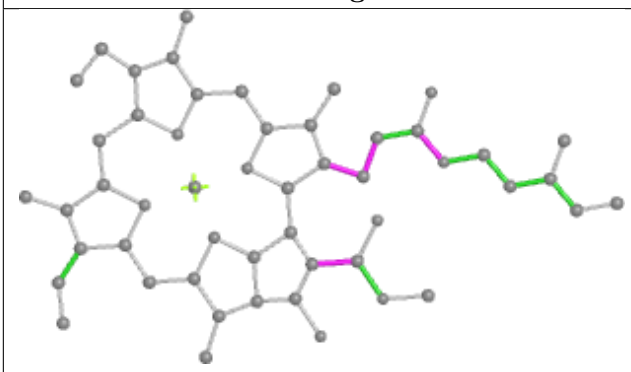
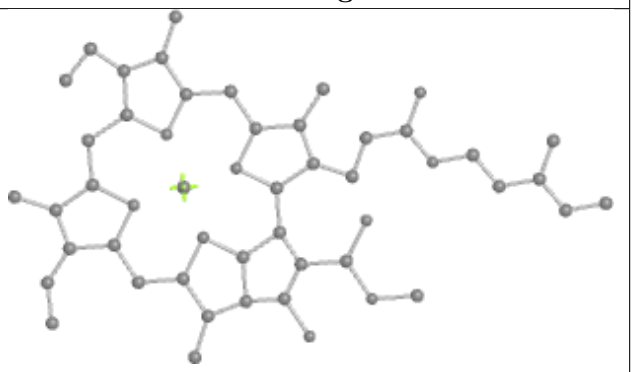


Bond angles

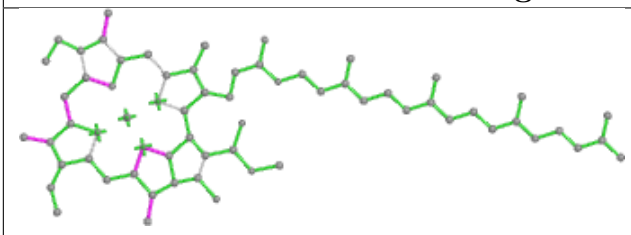


Torsions



Rings

Ligand CLA A 1104



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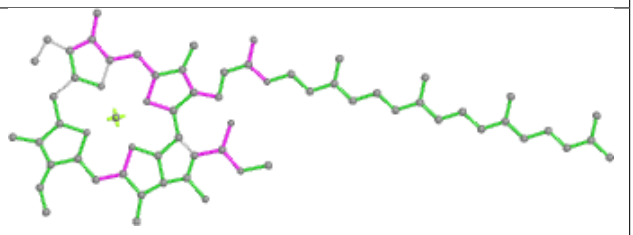
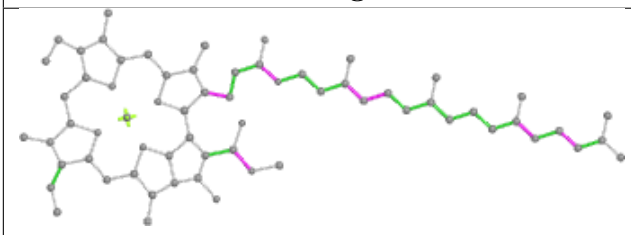


Bond angles



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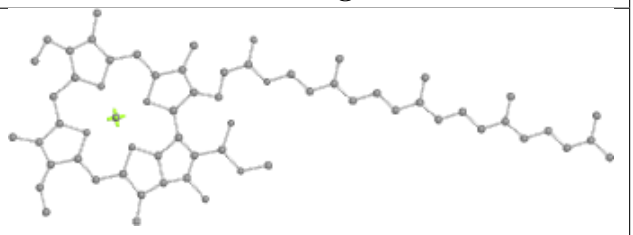
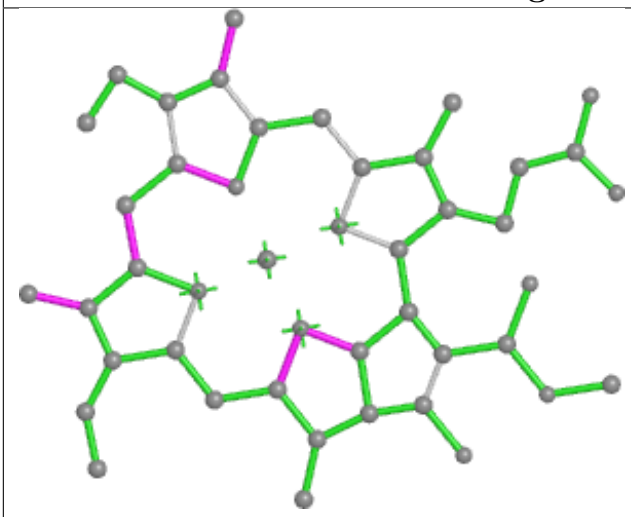
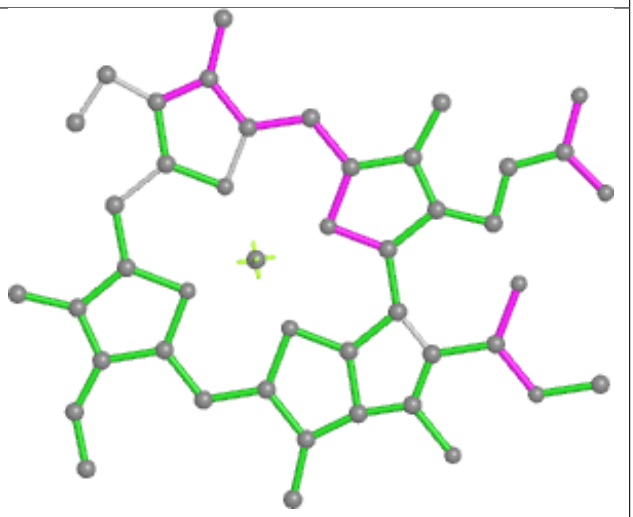


Rings

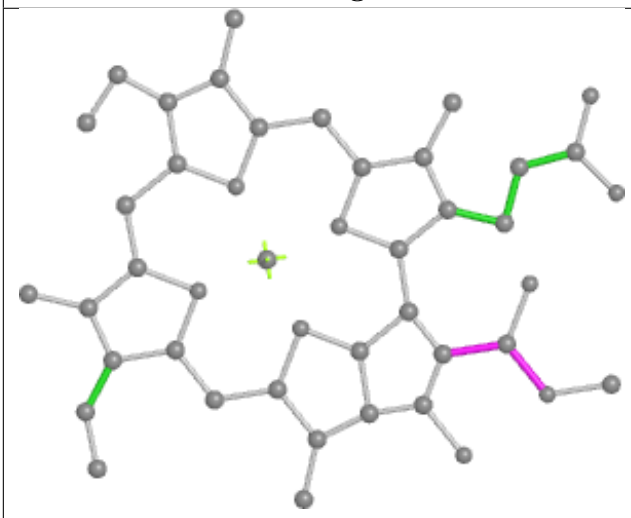
Ligand CLA 5 506



Bond lengths



Bond angles



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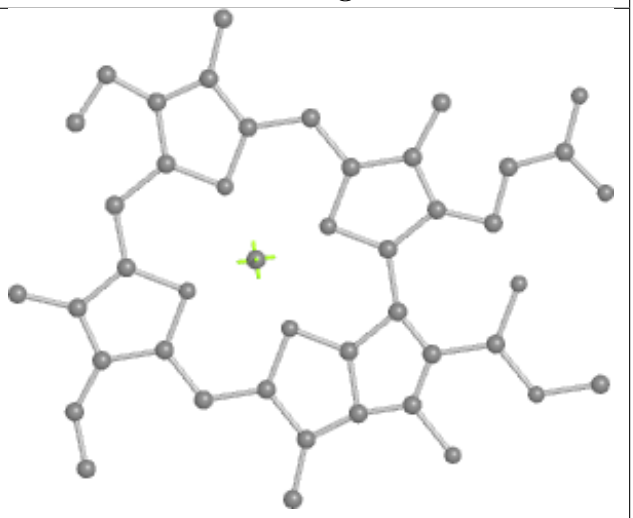
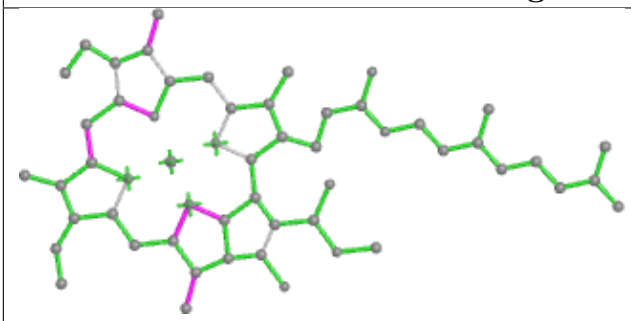
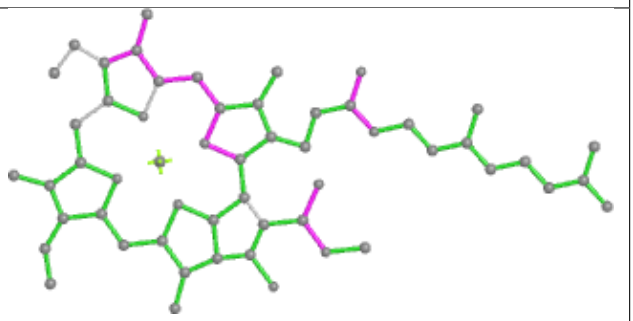


Rings

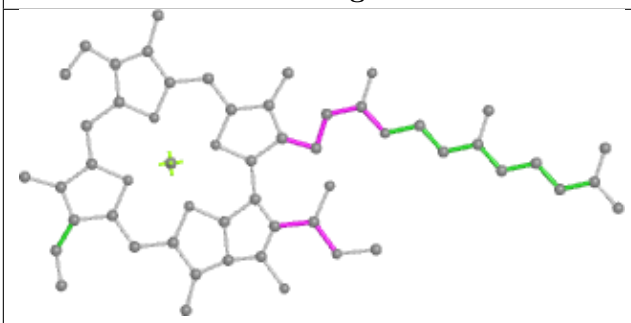
Ligand CLA d 518



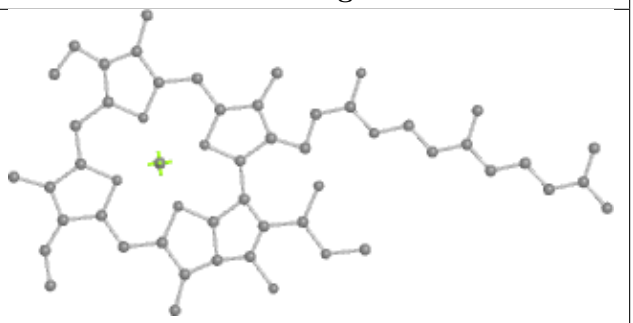
Bond lengths



Bond angles

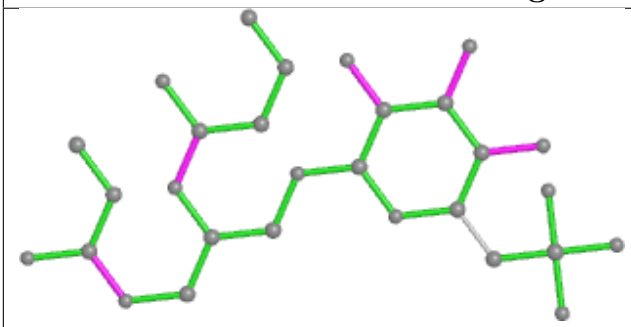


Torsions

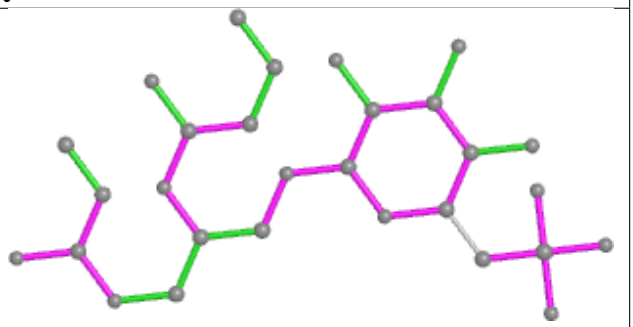


Rings

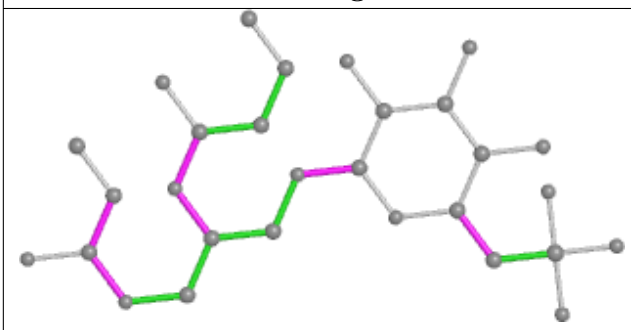
Ligand SQD 5 822



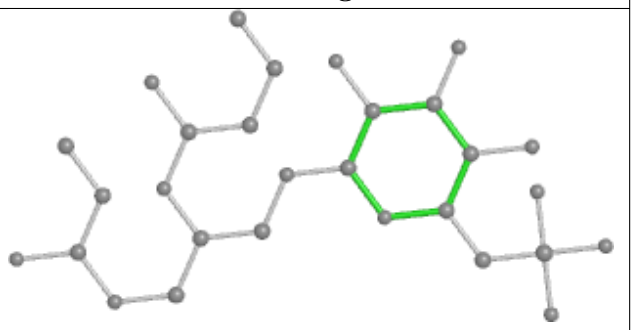
Bond lengths



Bond angles

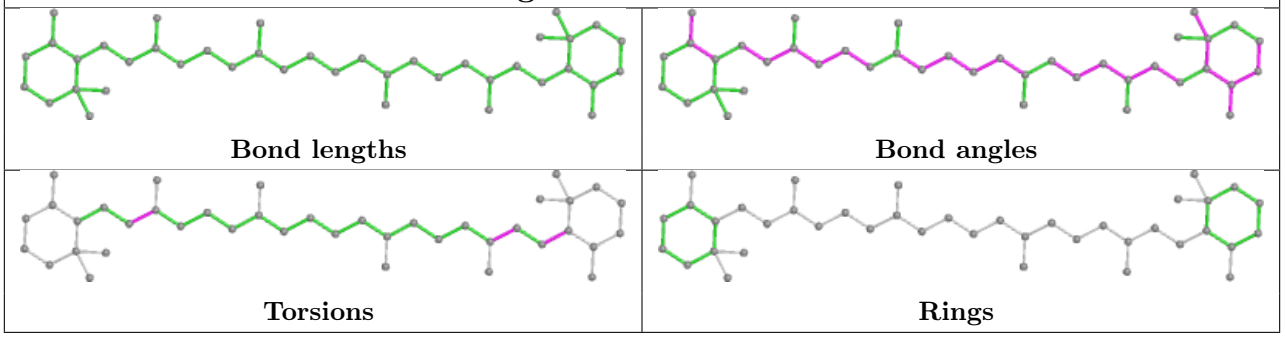


Torsions

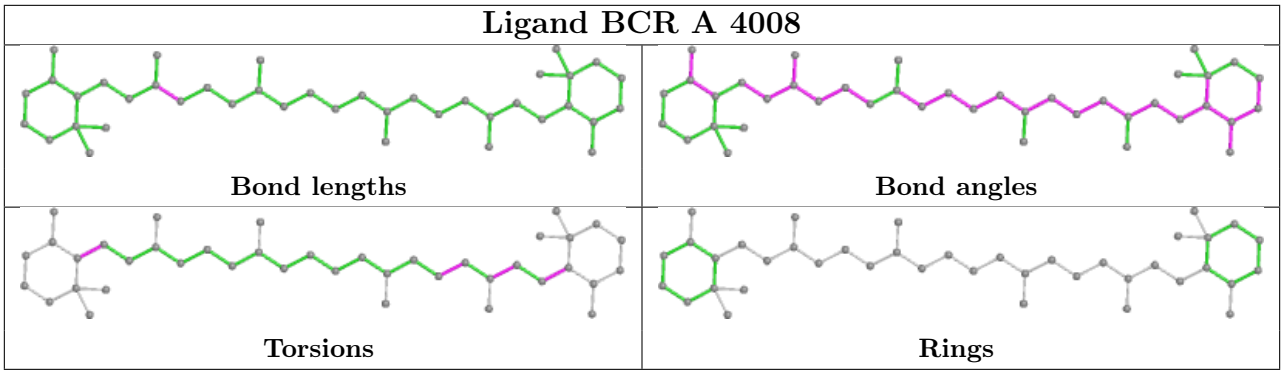


Rings

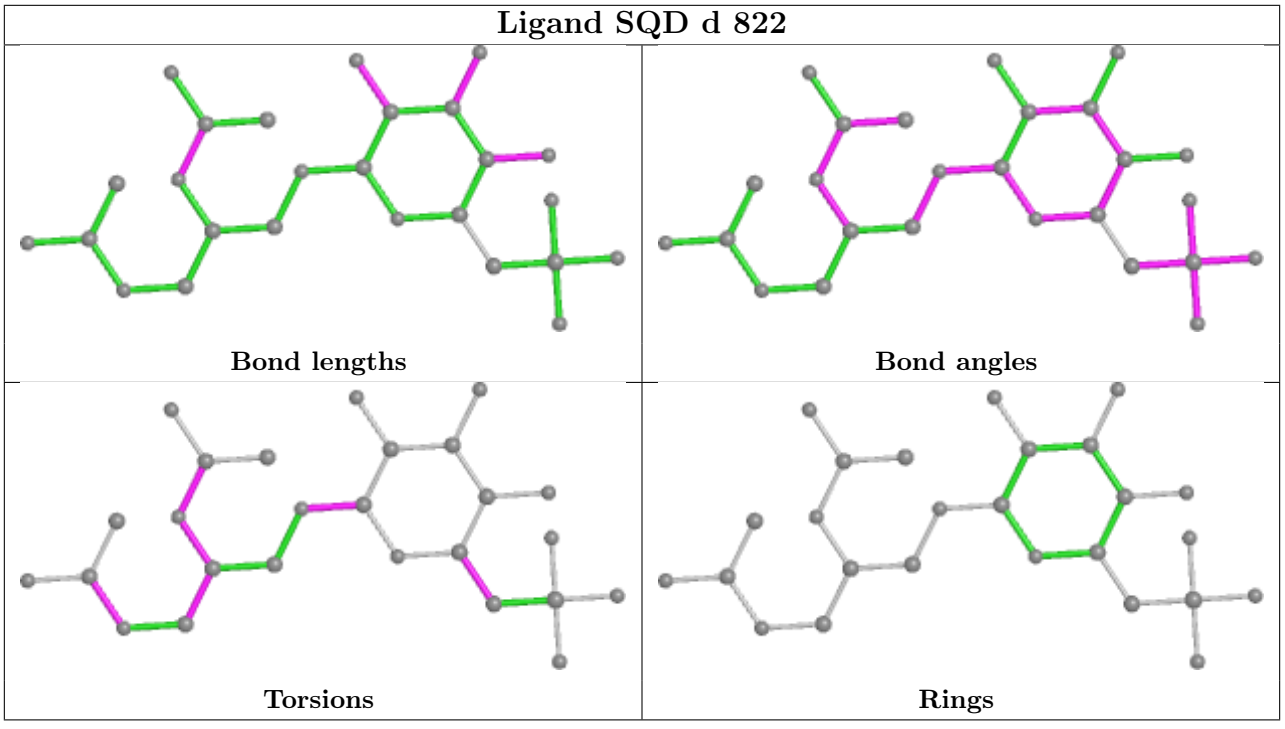
Ligand BCR n 4019



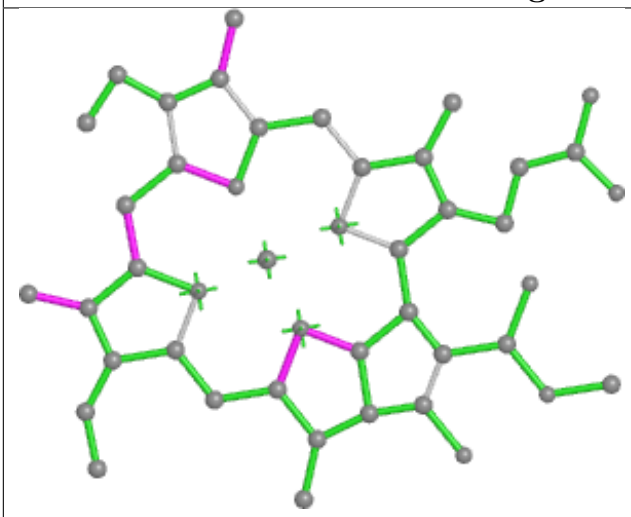
Ligand BCR A 4008



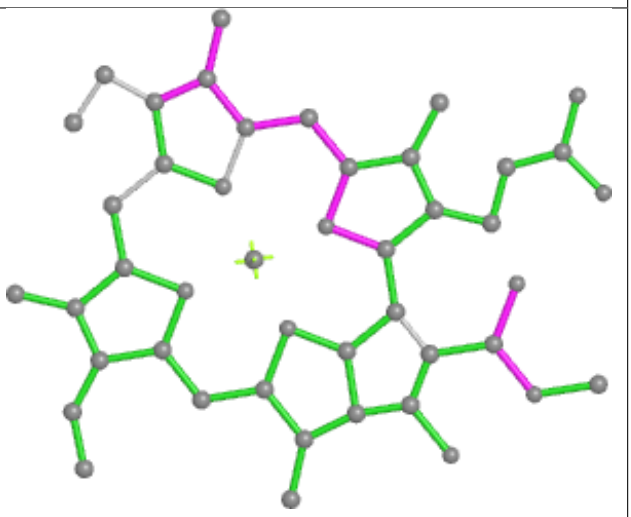
Ligand SQD d 822



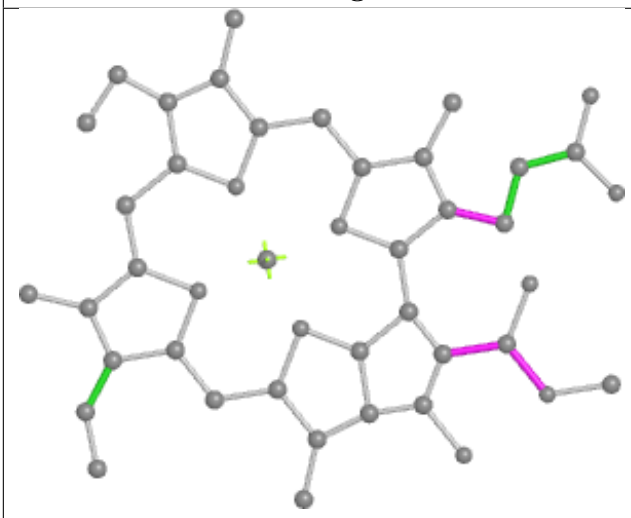
Ligand CLA 1 506



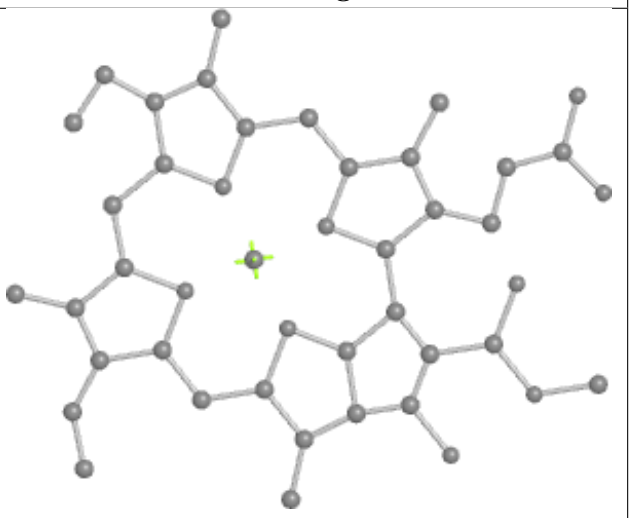
Bond lengths



Bond angles

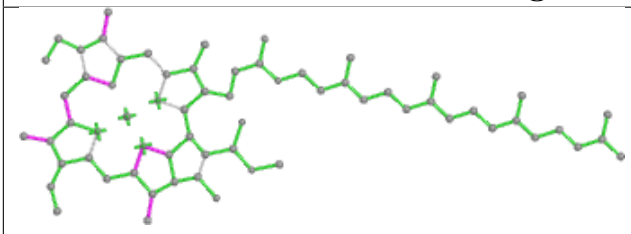


Torsions



Rings

Ligand CLA 1 509



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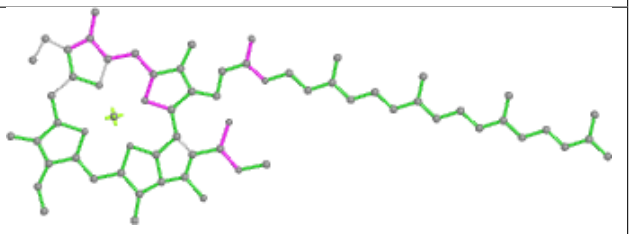
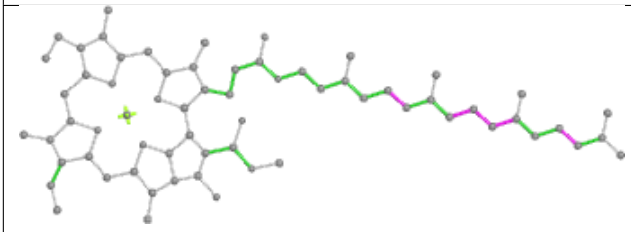
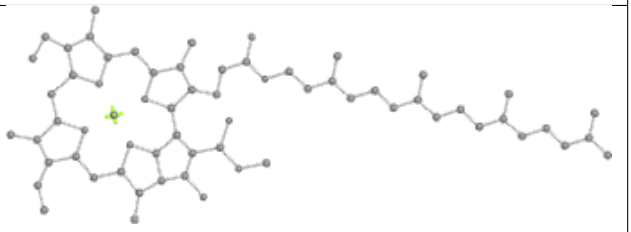


Bond angles

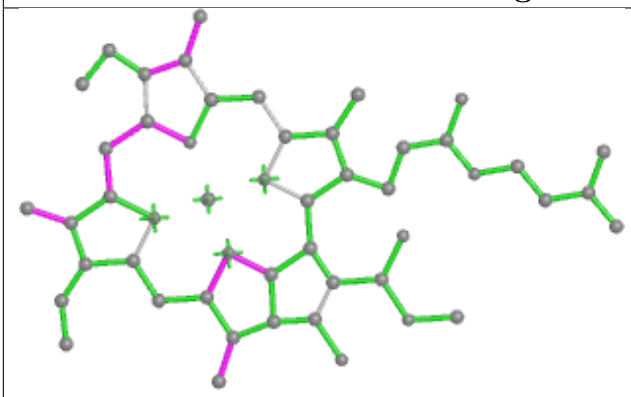


Torsions

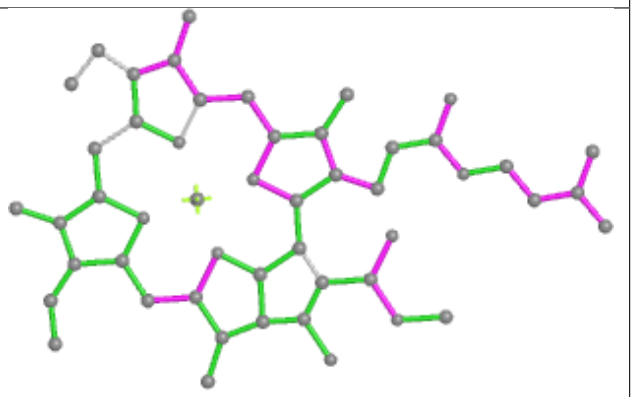


Rings

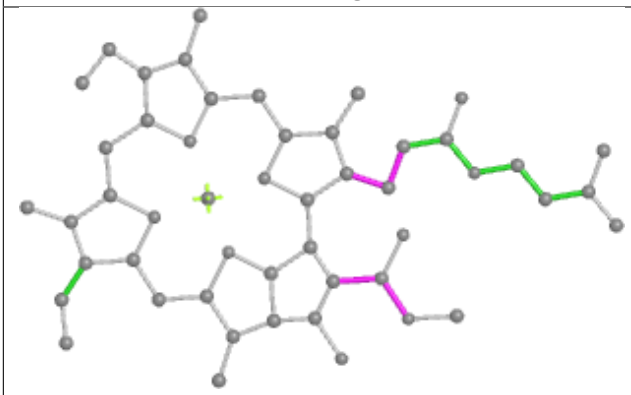
Ligand CLA U 1103



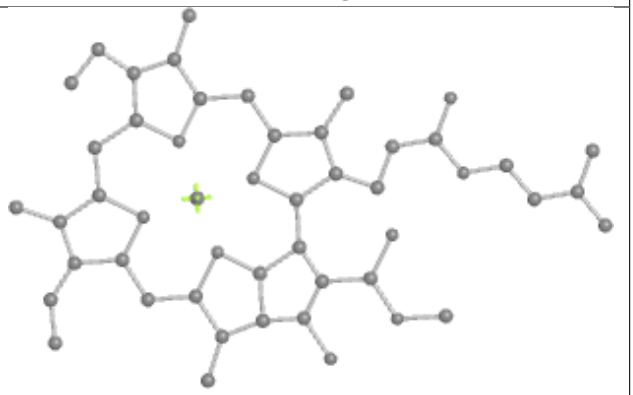
Bond lengths



Bond angles

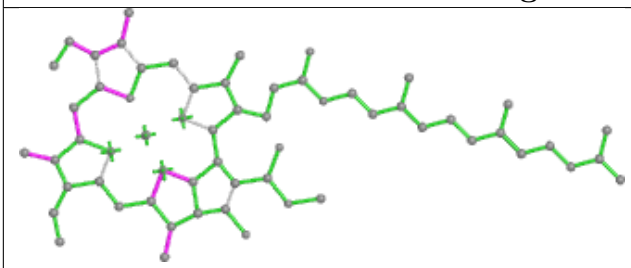


Torsions

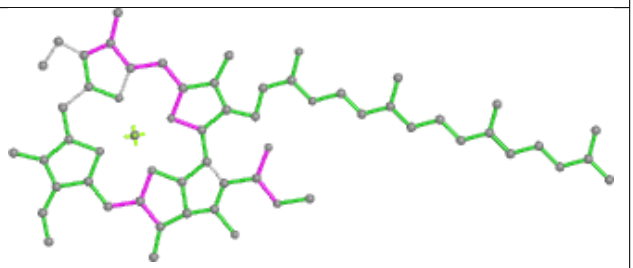


Rings

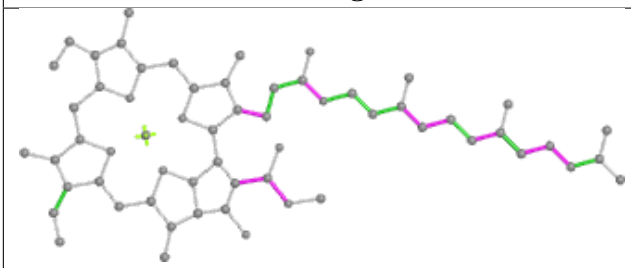
Ligand CLA e 1122



Bond lengths



Bond angles



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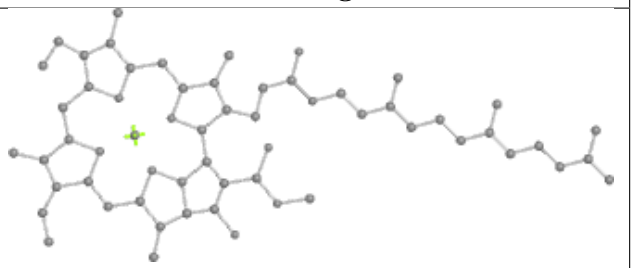
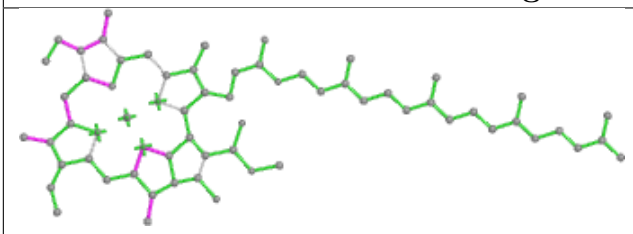
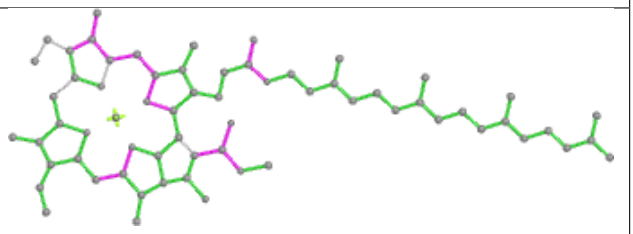


Rings

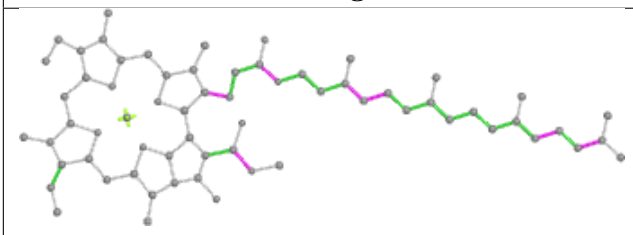
Ligand CLA f 1227



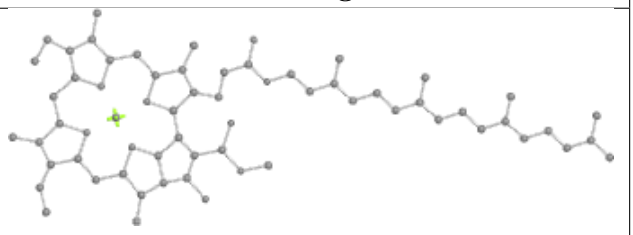
Bond lengths



Bond angles

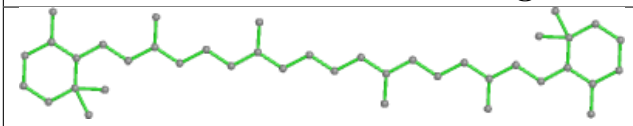


Torsions

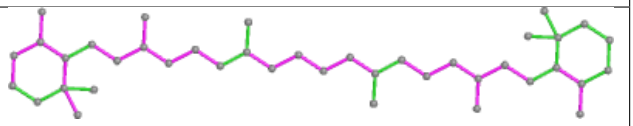


Rings

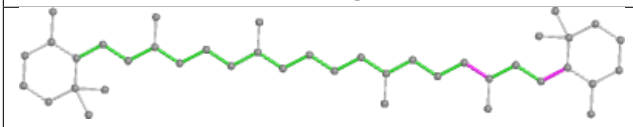
Ligand BCR n 4020



Bond lengths



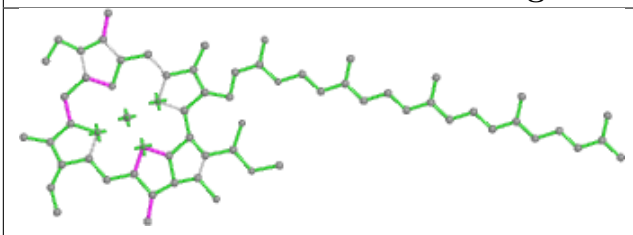
Bond angles



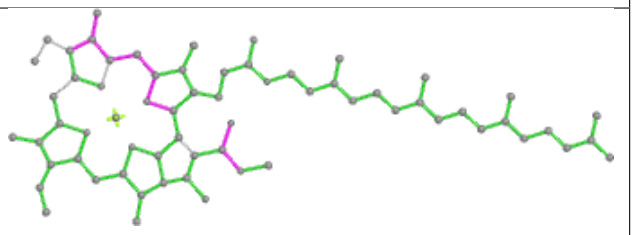
Torsions

Rings

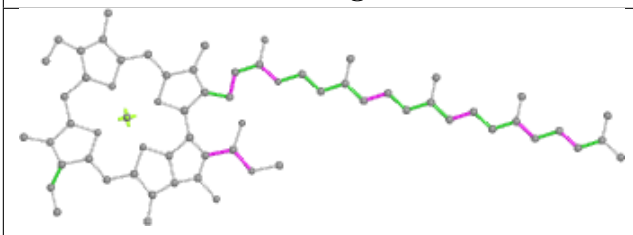
Ligand CLA b 505



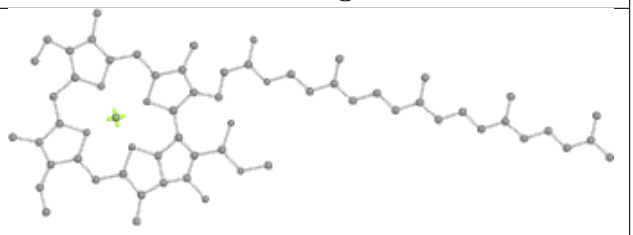
Bond lengths



Bond angles

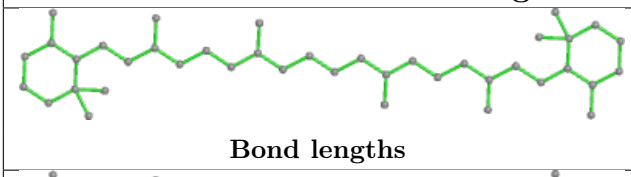


Torsions



Rings

Ligand BCR G 4003



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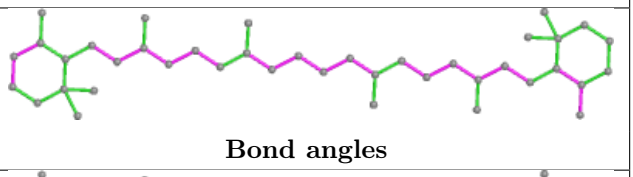
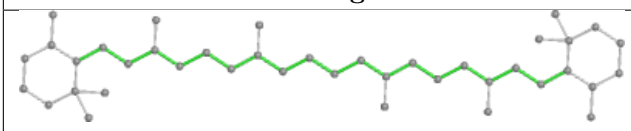
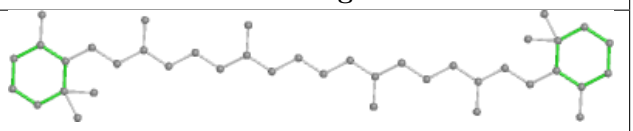


Bond angles

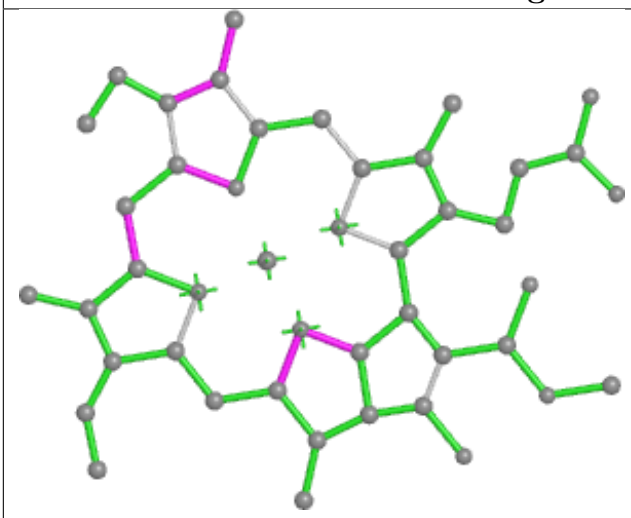


Torsions



Rings

Ligand CLA v 513



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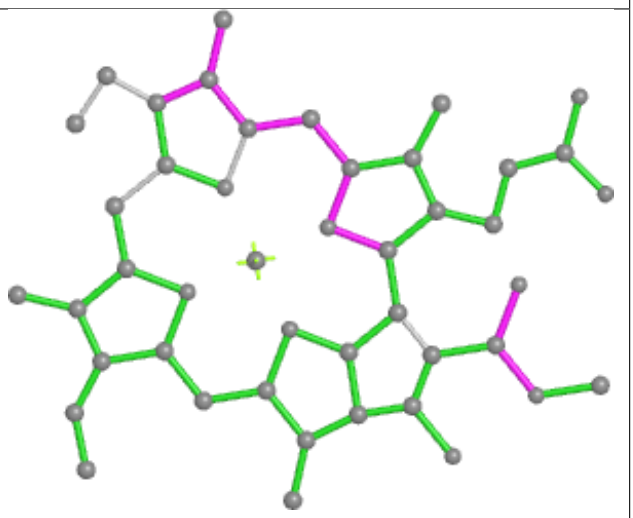

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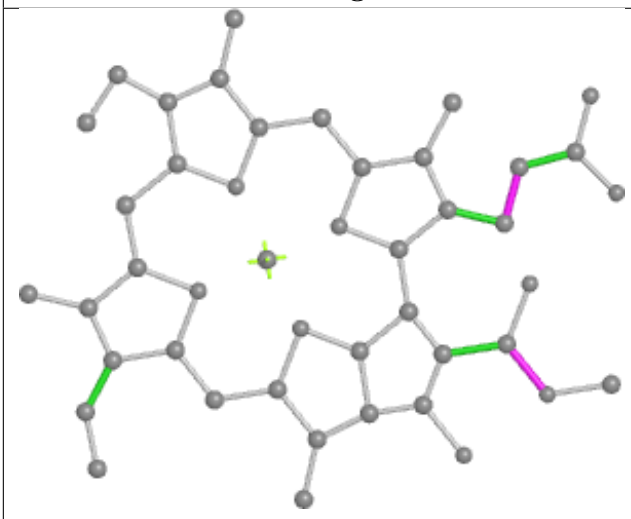

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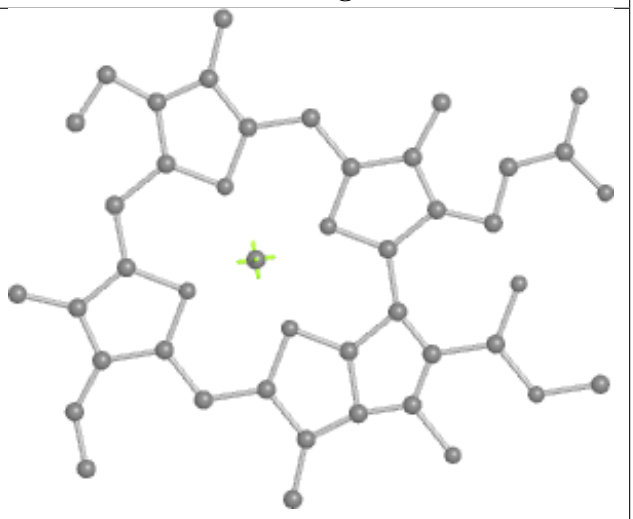
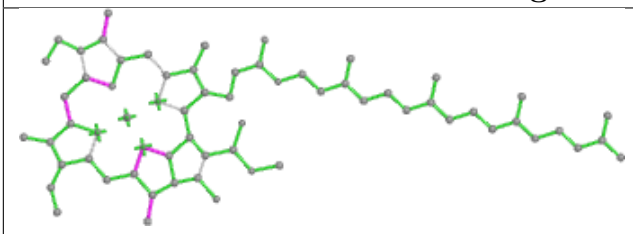


Rings

Ligand CLA s 503



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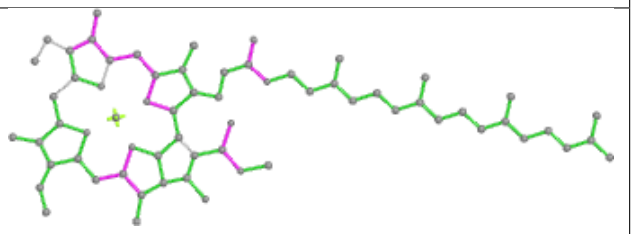
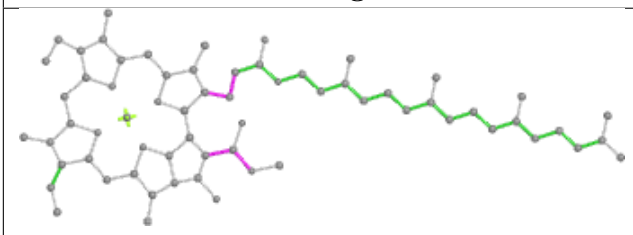


Bond angles



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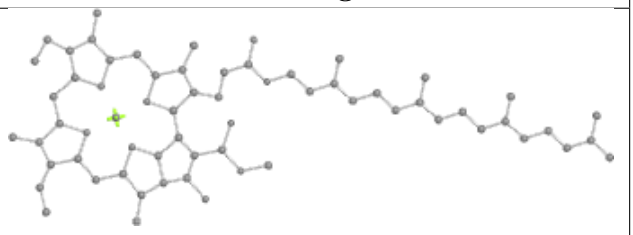
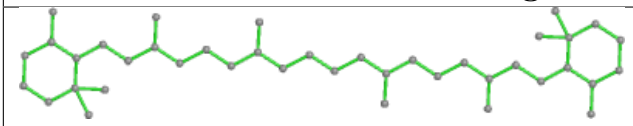


Rings

Ligand BCR Y 522



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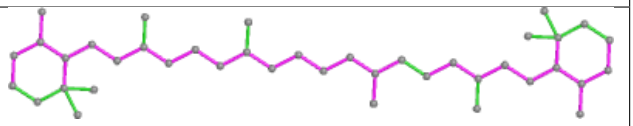
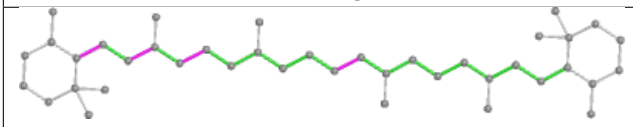


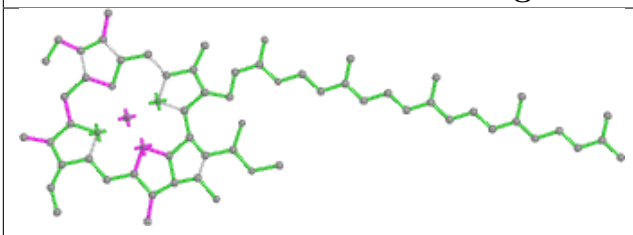
Bond angles



Torsions

Rings

Ligand CLA G 1022



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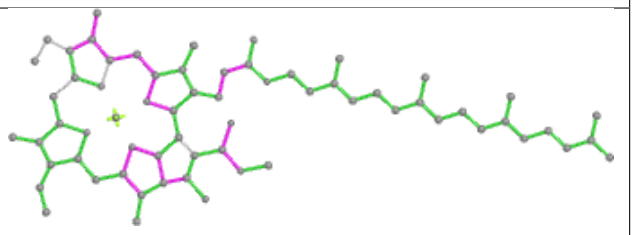
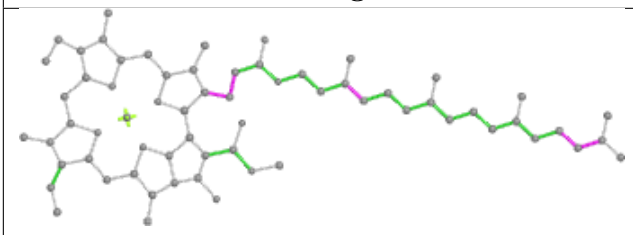


Bond angles



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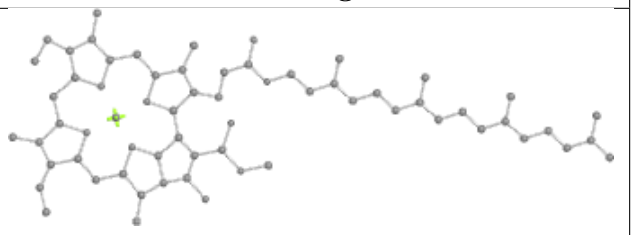
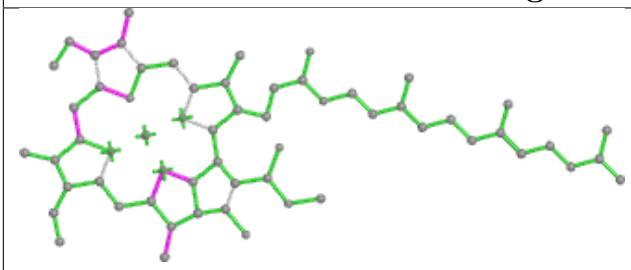


Rings

Ligand CLA Z 502



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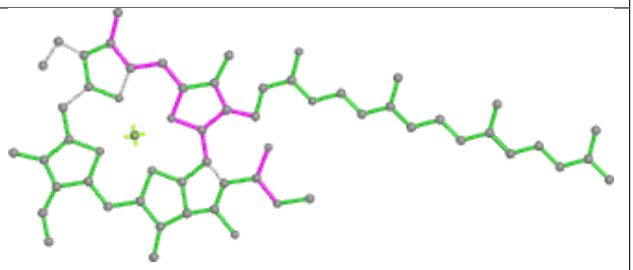
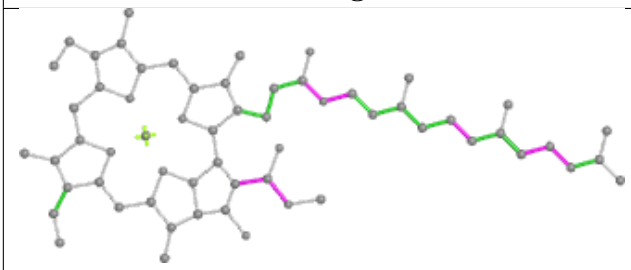


Bond angles



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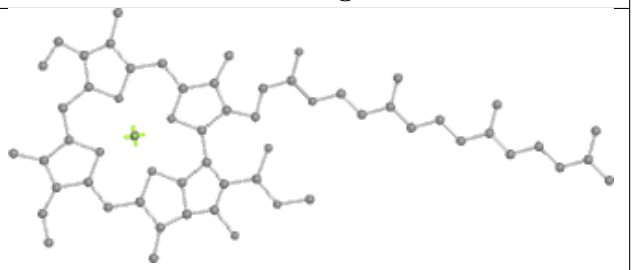
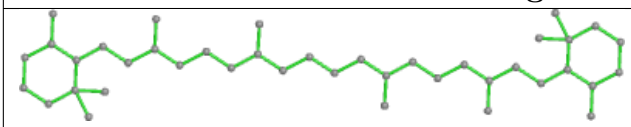


Rings

Ligand BCR 1 523



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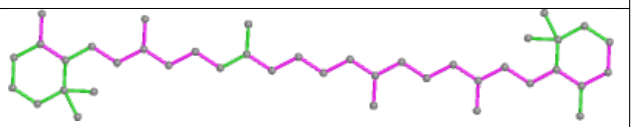

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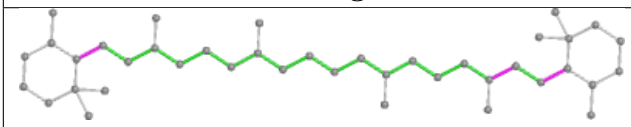

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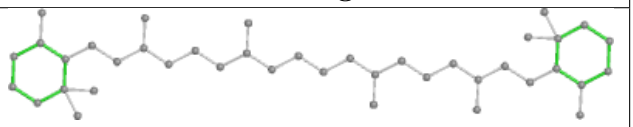
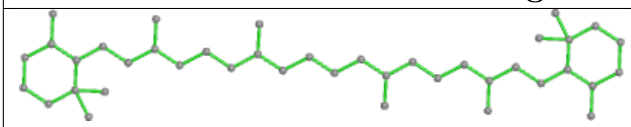


Rings

Ligand BCR 6 524



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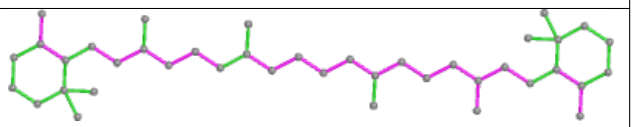
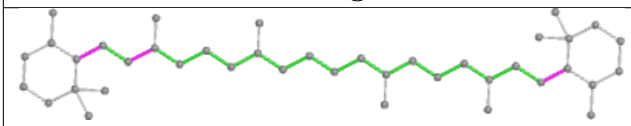


Bond angles



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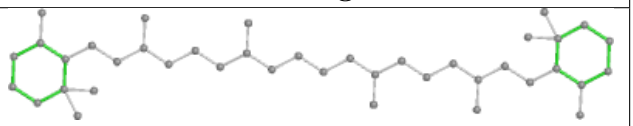
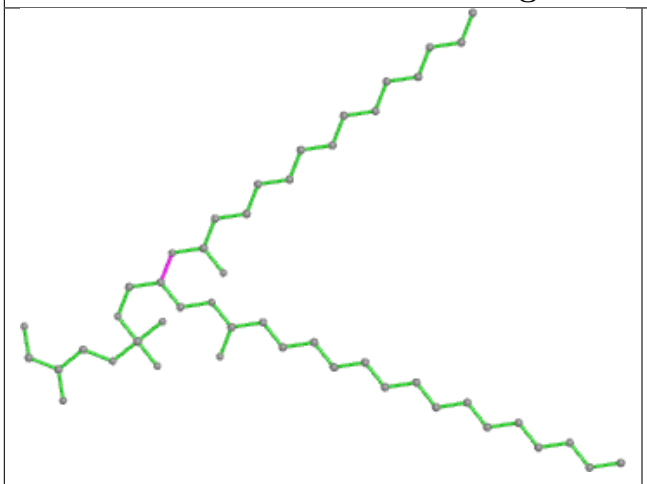


Rings

Ligand LHG e 5007



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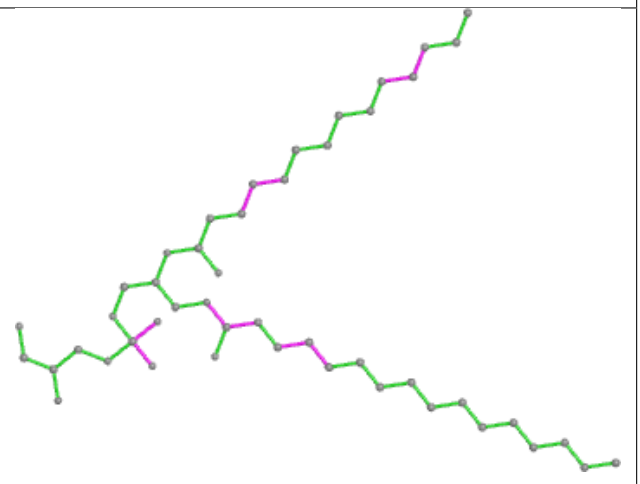
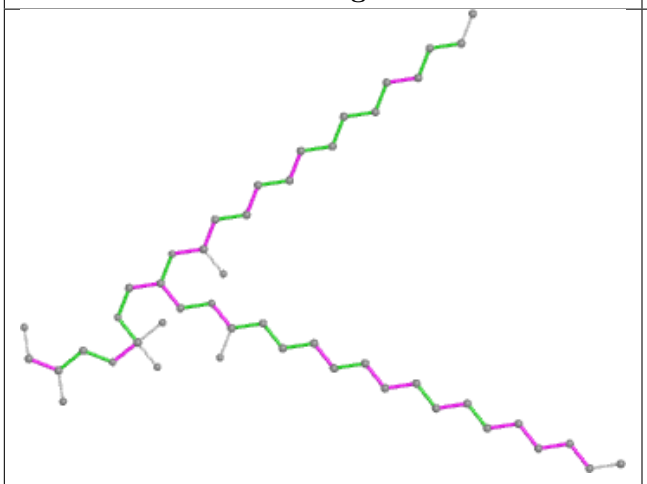


Bond angles



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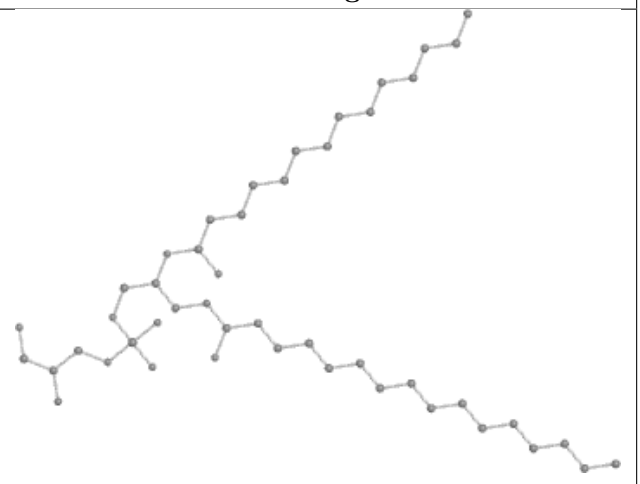
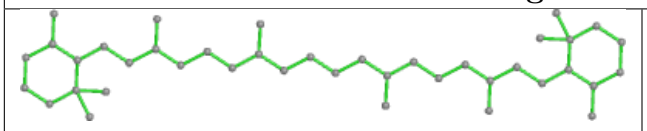


Rings

Ligand BCR u 522



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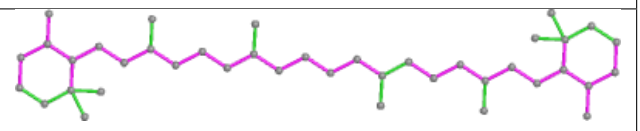
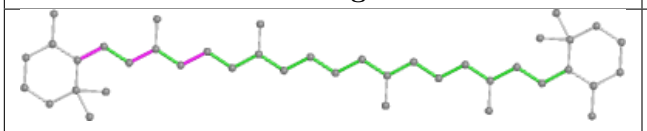


Bond angles



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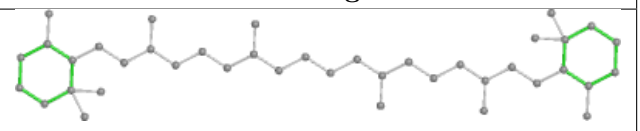
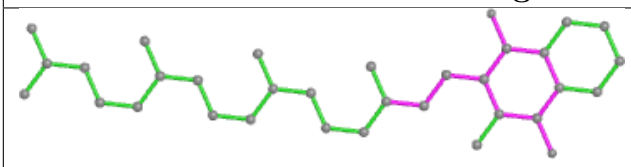


Rings

Ligand PQN B 2002



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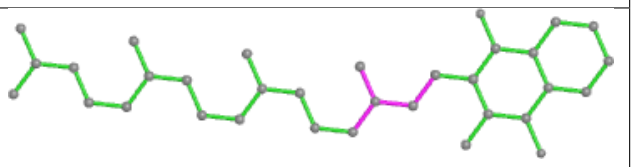
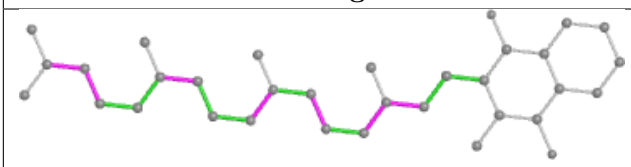


Bond angles



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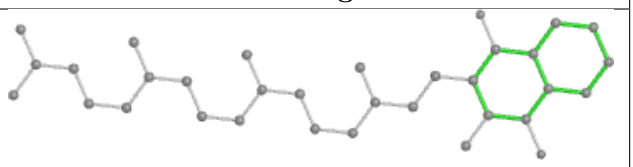
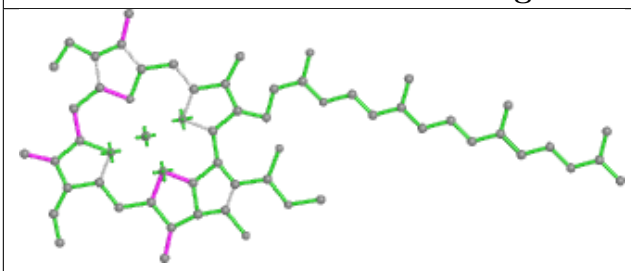


Rings

Ligand CLA H 1201



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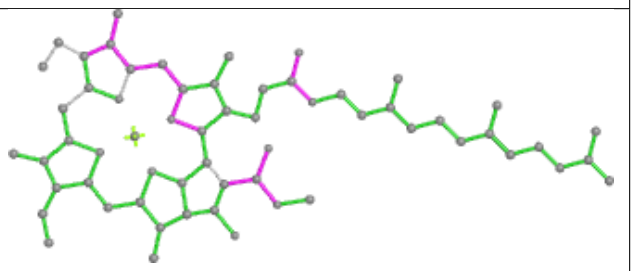
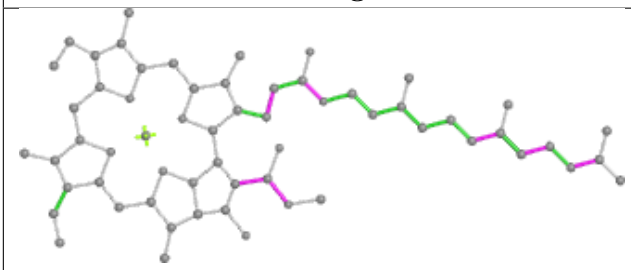


Bond angles



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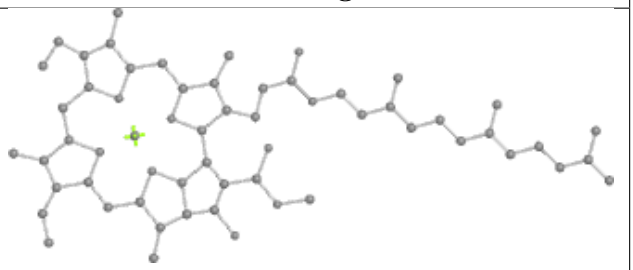
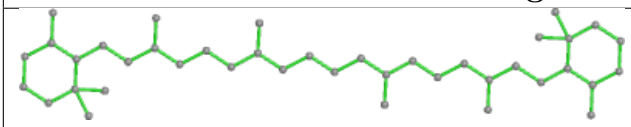
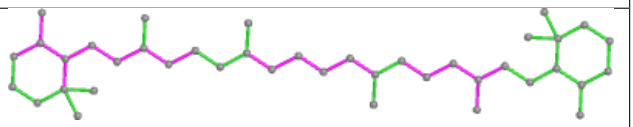


Rings

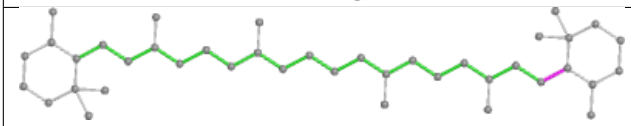
Ligand BCR 2 524



Bond lengths



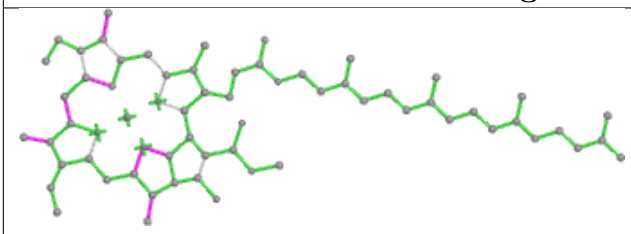
Bond angles



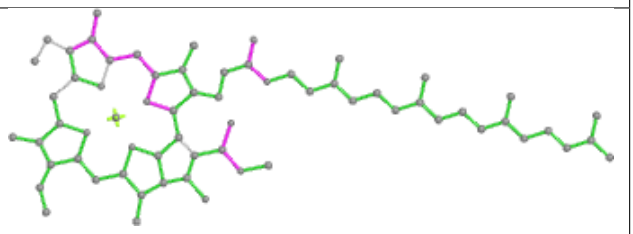
Torsions

Rings

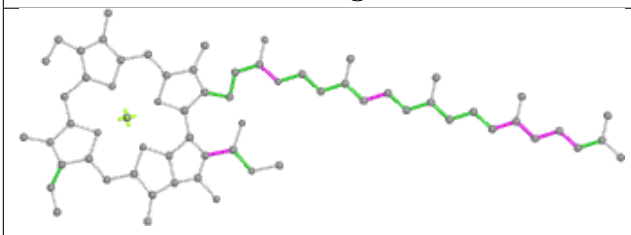
Ligand CLA e 1109



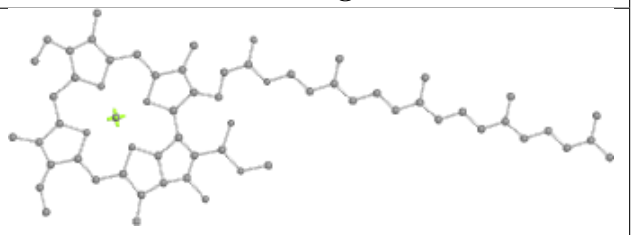
Bond lengths



Bond angles

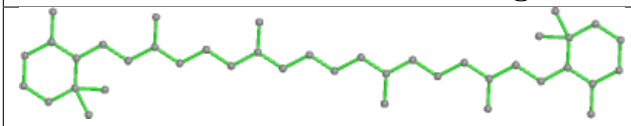


Torsions

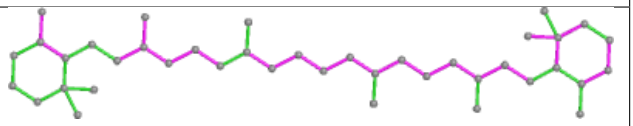


Rings

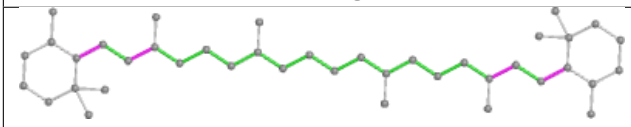
Ligand BCR H 4004



Bond lengths



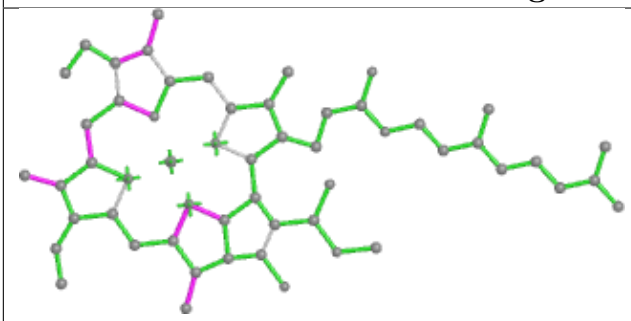
Bond angles



Torsions

Rings

Ligand CLA 2 508



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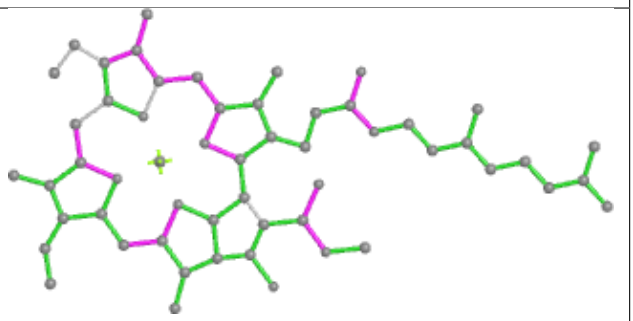

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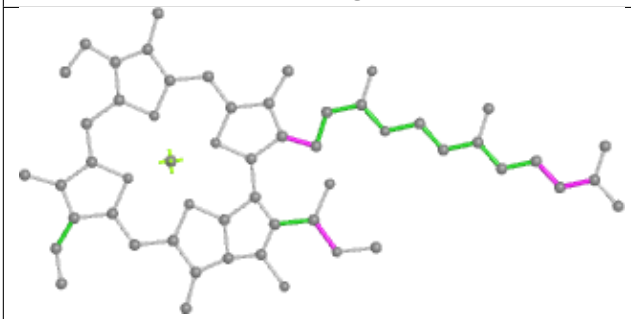
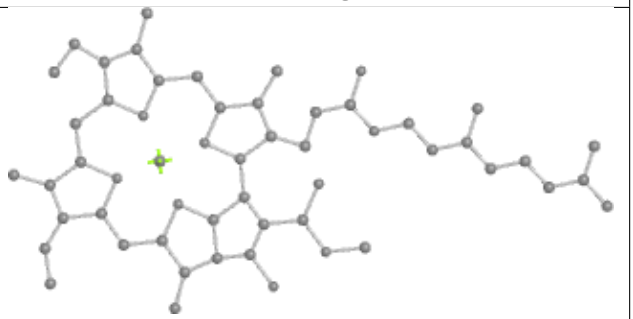
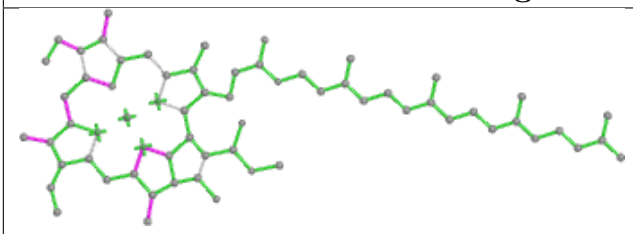


Torsions



Rings

Ligand CLA H 1210



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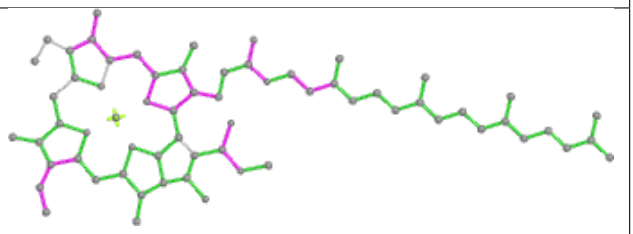
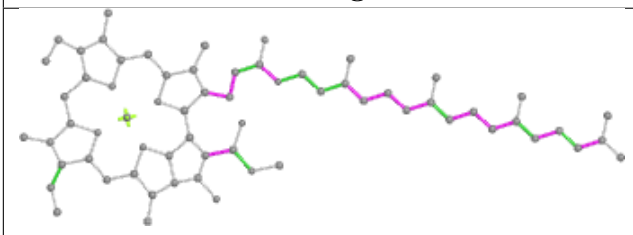
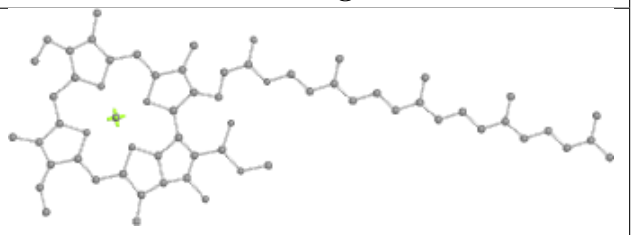


Bond angles

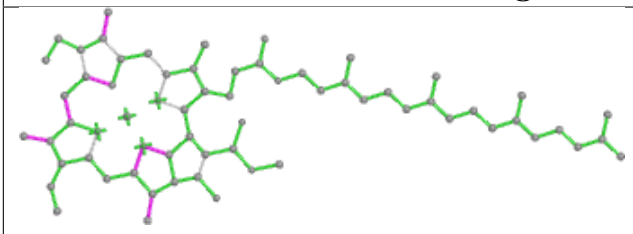


Torsions



Rings

Ligand CLA H 1231



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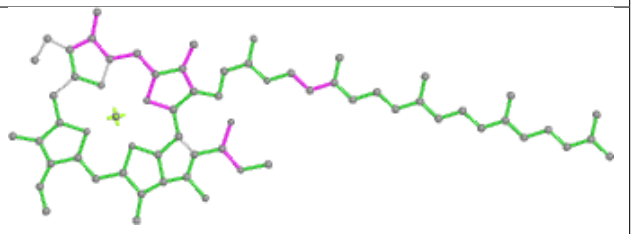
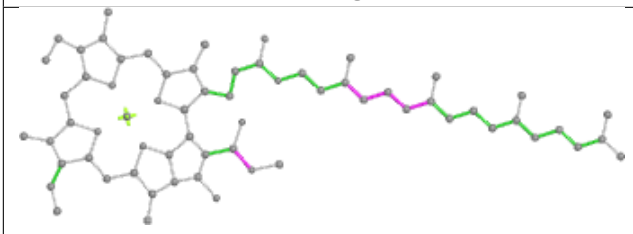


Bond angles



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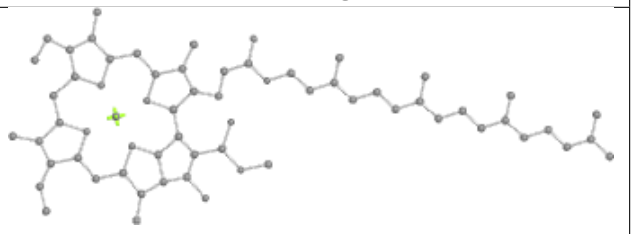
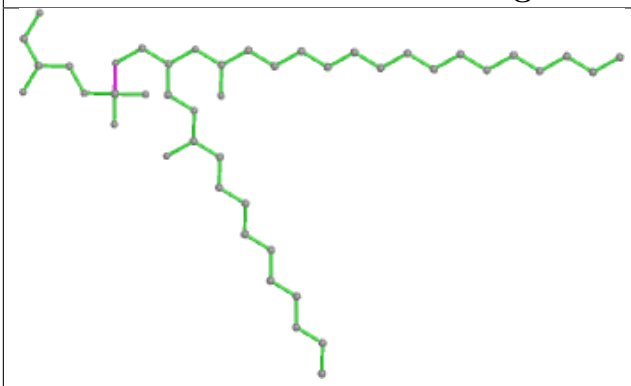
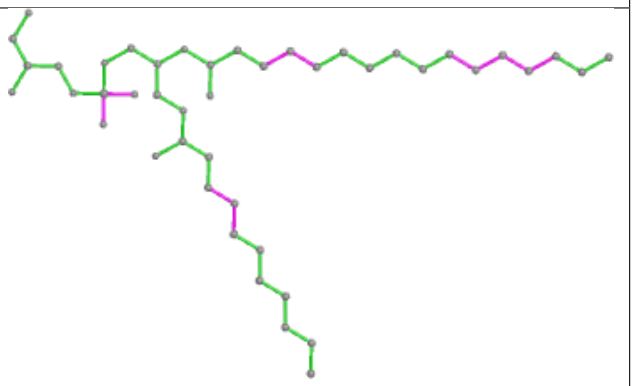


Rings

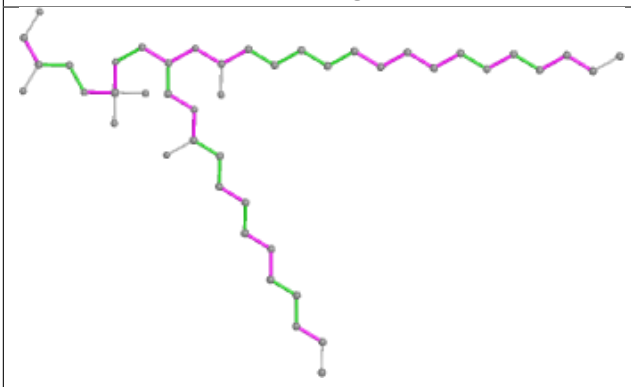
Ligand LHG B 1855



Bond lengths



Bond angles



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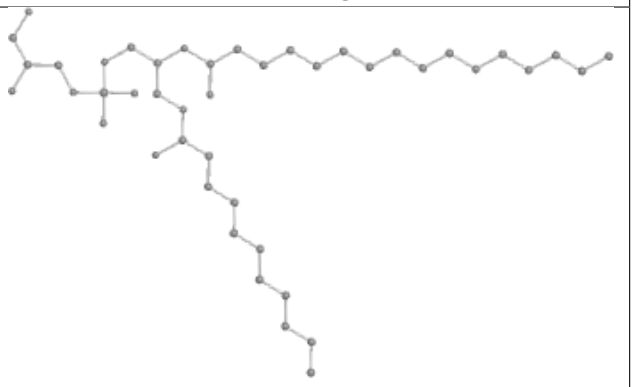
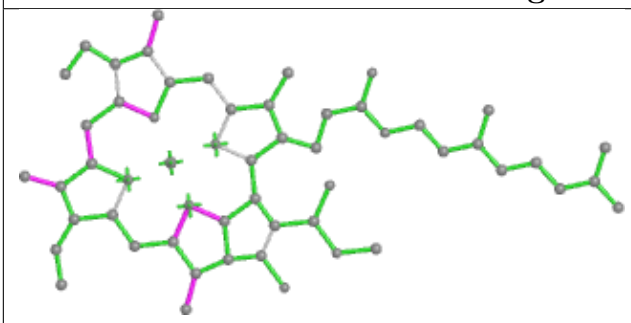


Rings

Ligand CLA q 513



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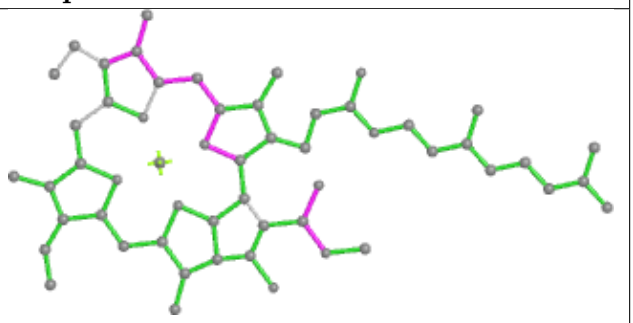
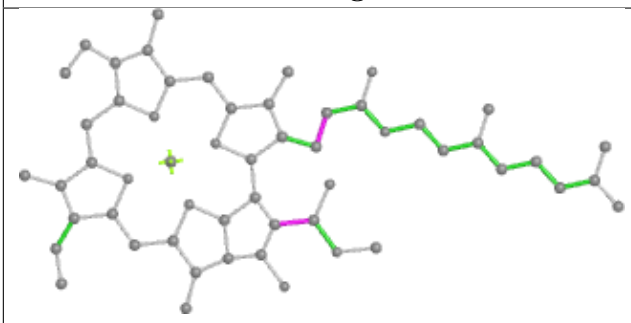


Bond angles



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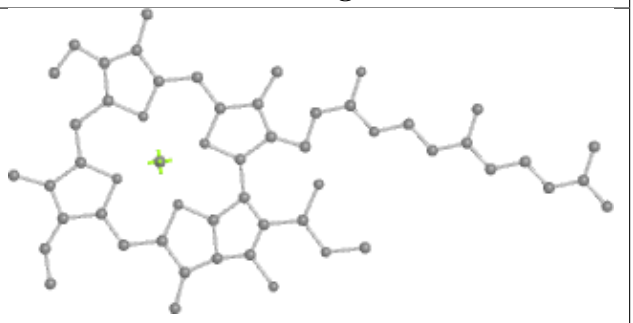
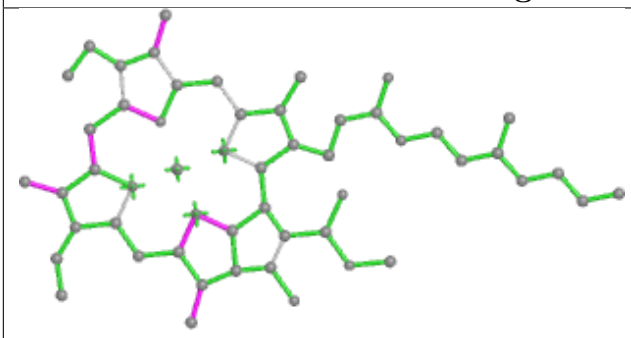


Rings

Ligand CLA A 1120



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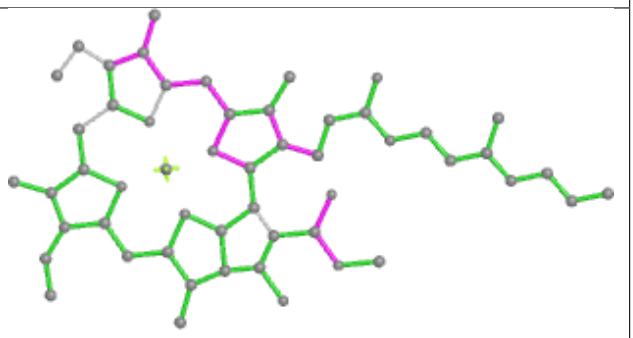
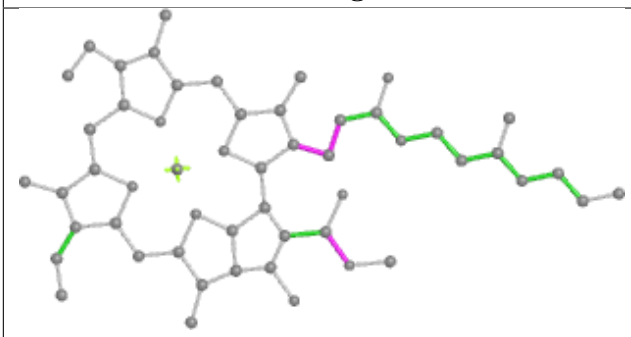


Bond angles



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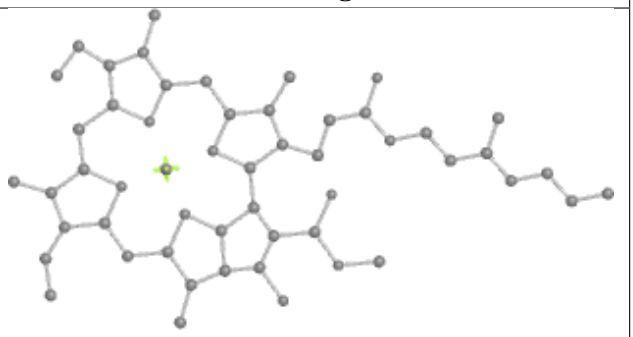
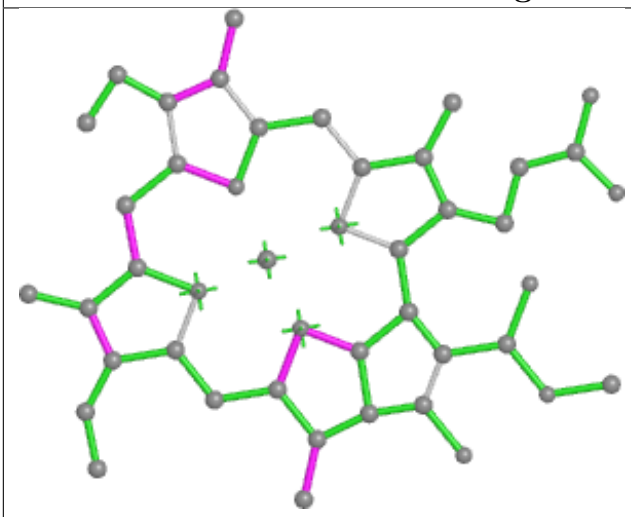


Rings

Ligand CLA K 1105



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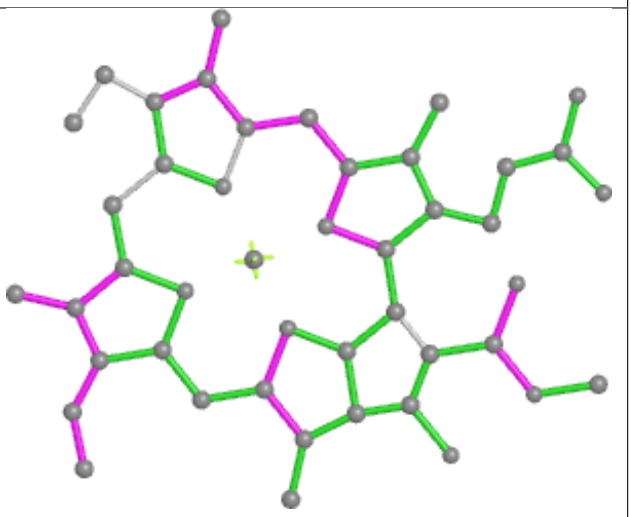

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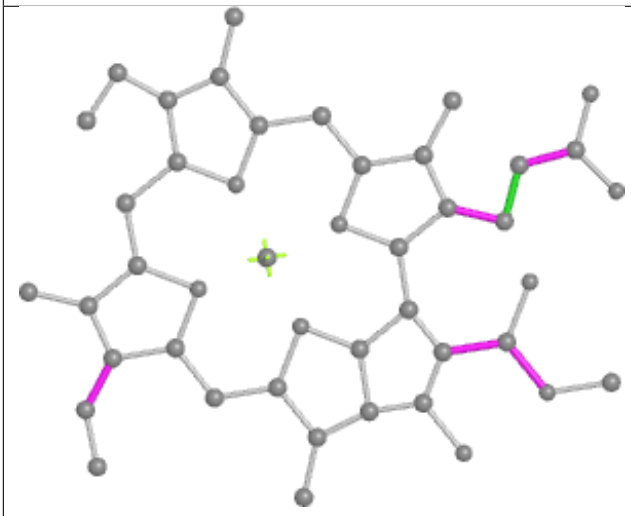

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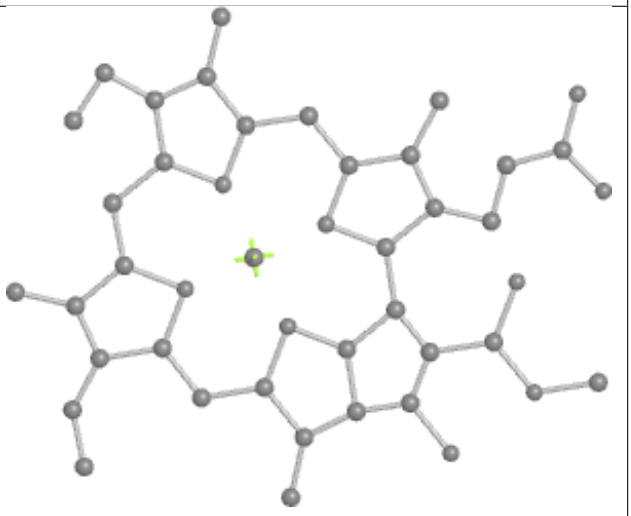
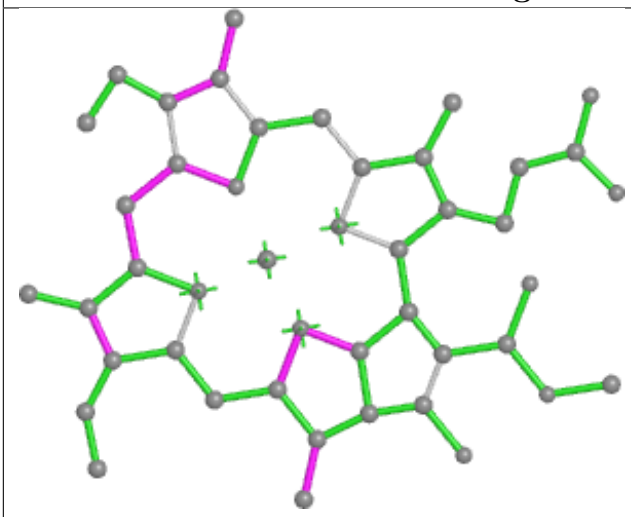


Rings

Ligand CLA m 1105



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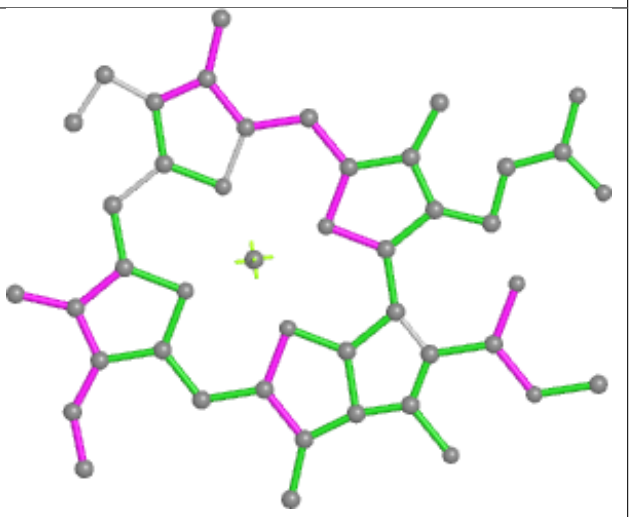
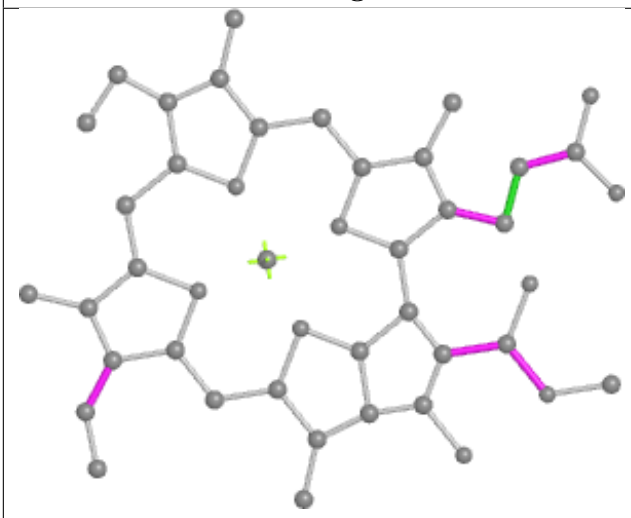


Bond angles



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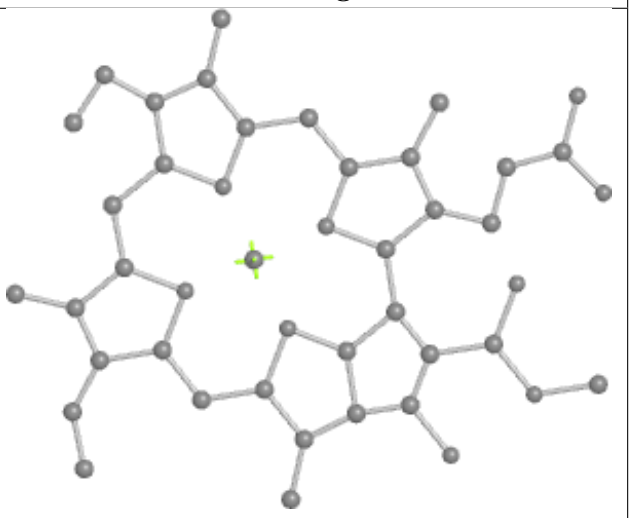
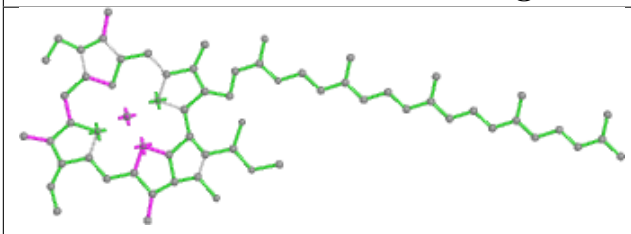


Rings

Ligand CLA B 1204



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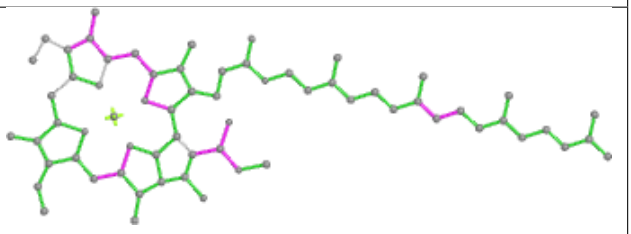

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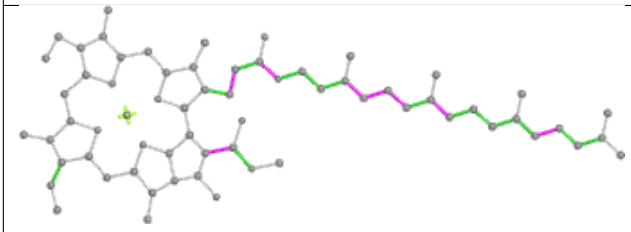

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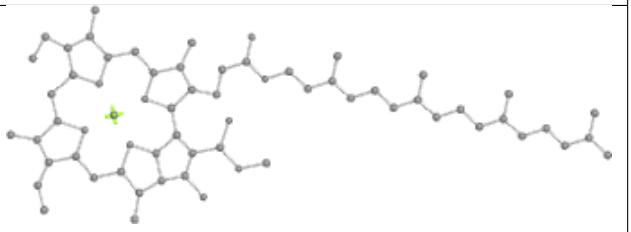
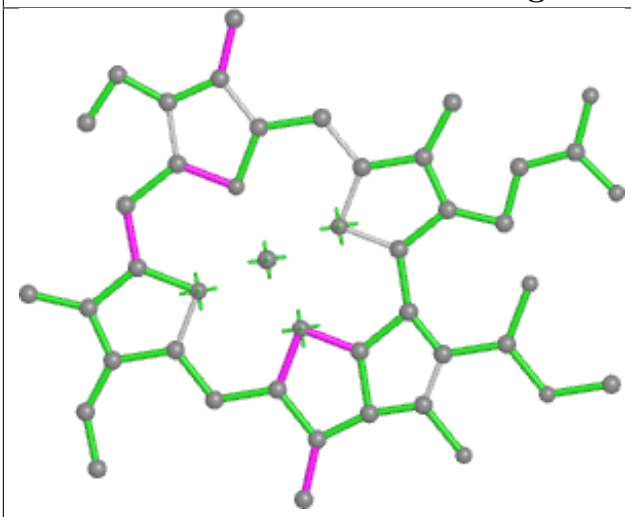


Rings

Ligand CLA v 510



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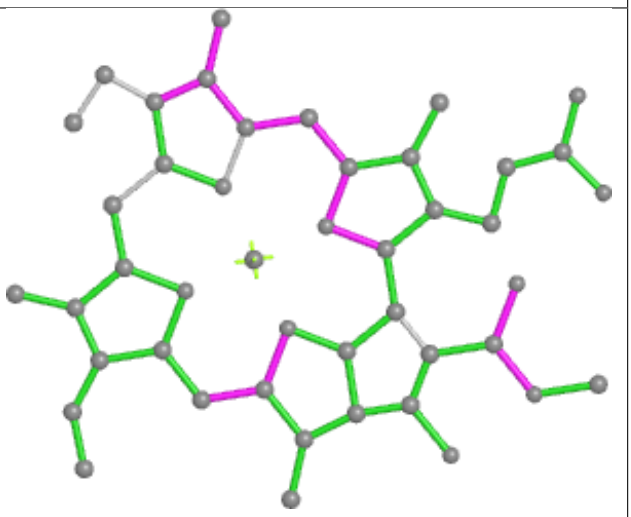

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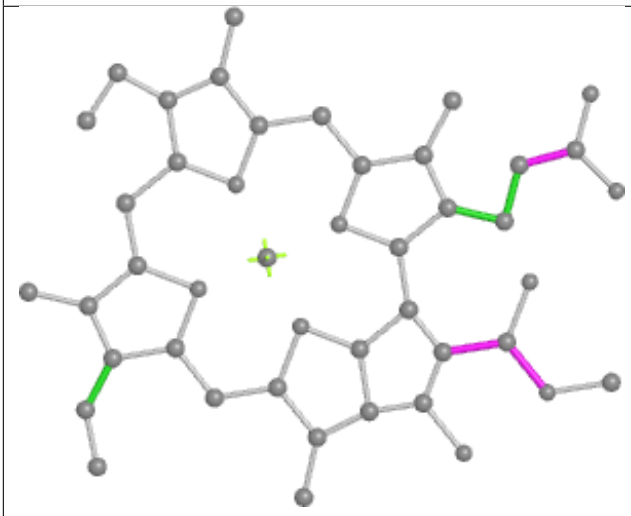

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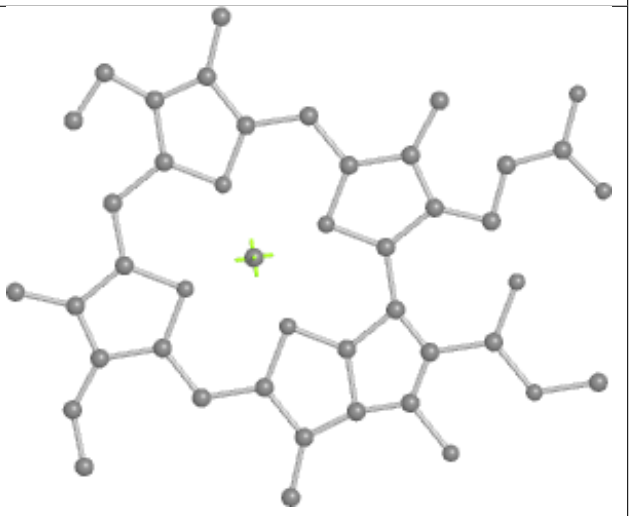
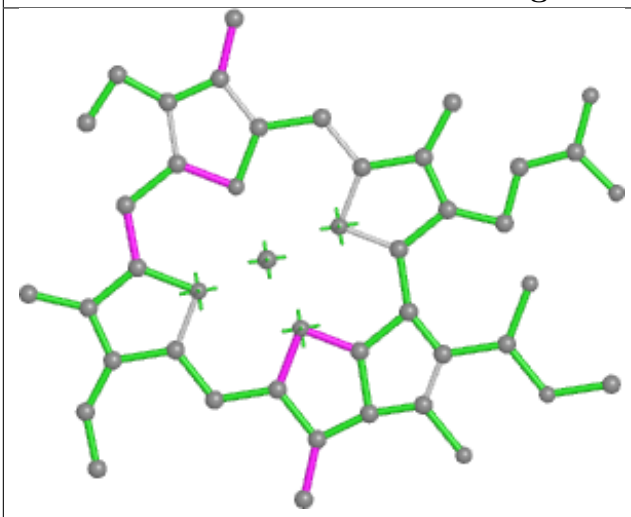


Rings

Ligand CLA t 506



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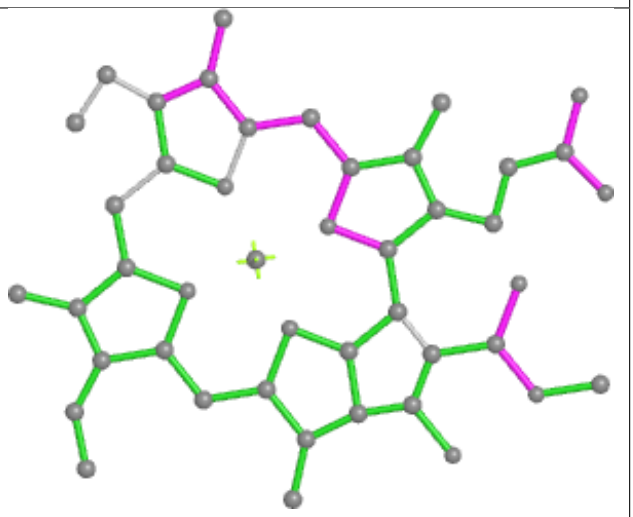
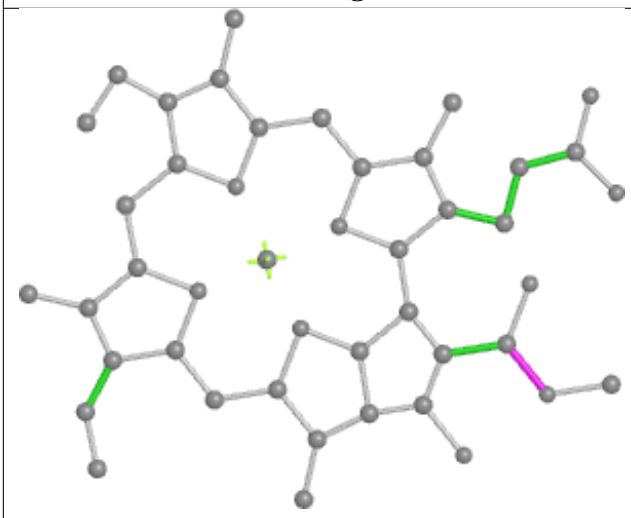


Bond angles



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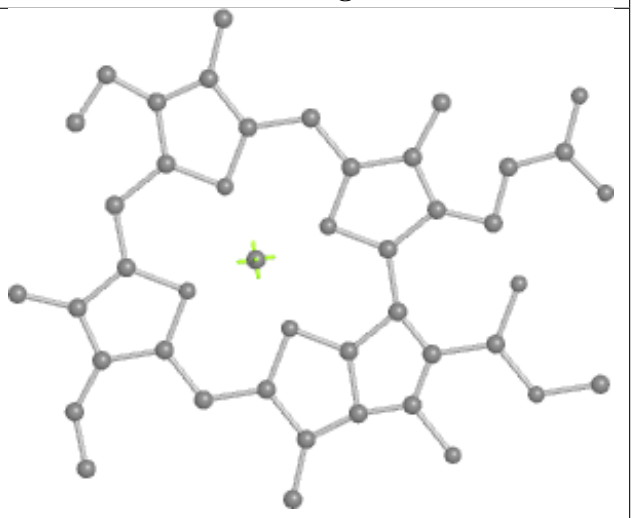
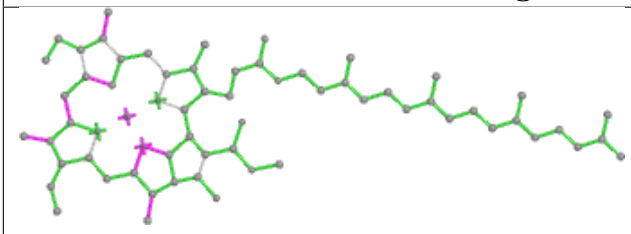


Rings

Ligand CLA H 1204



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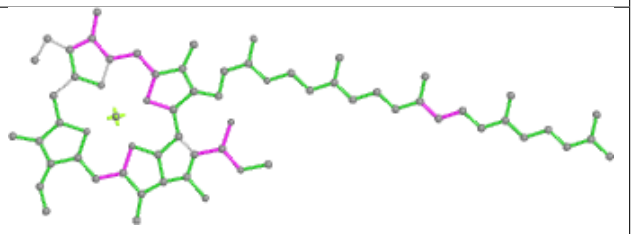
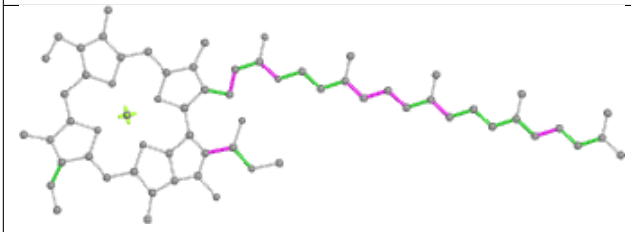


Bond angles



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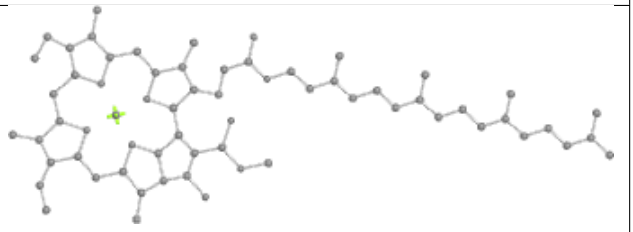
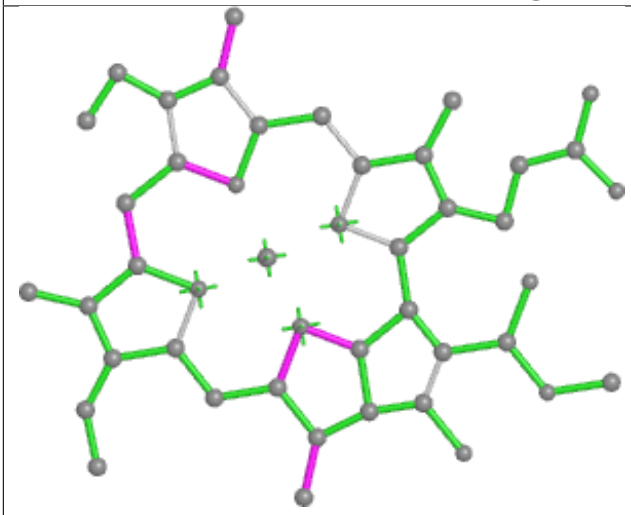


Rings

Ligand CLA b 516



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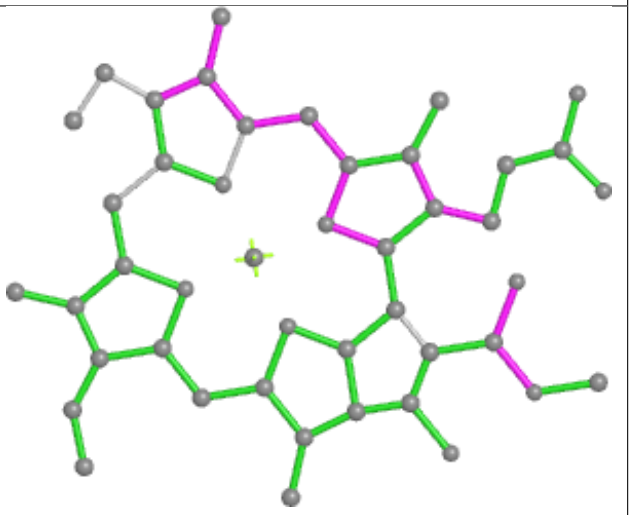
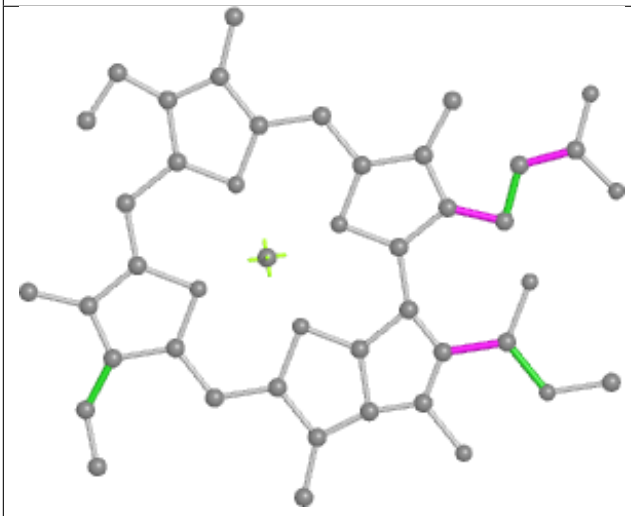
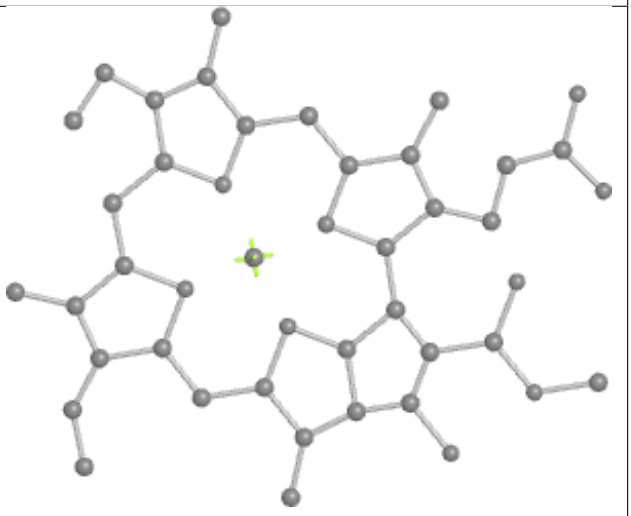


Bond angles

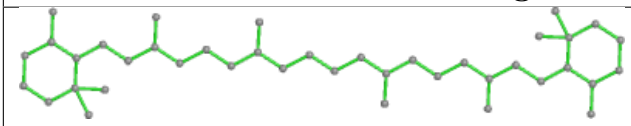


Torsions



Rings

Ligand BCR A 4011



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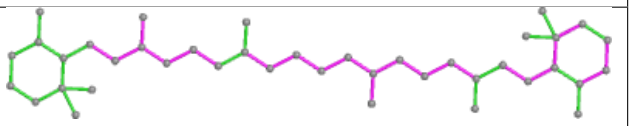
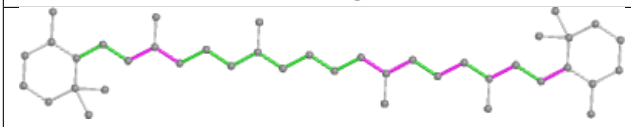


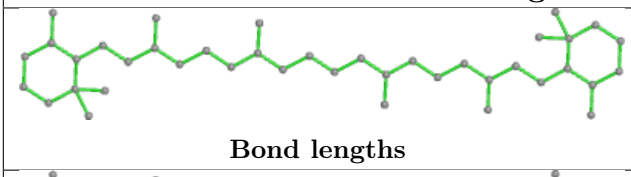
Bond angles



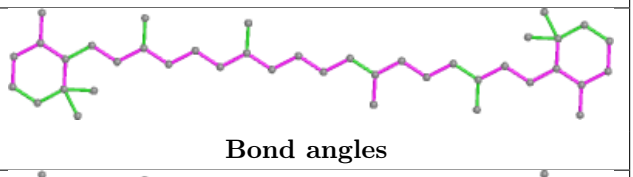
Torsions

Rings

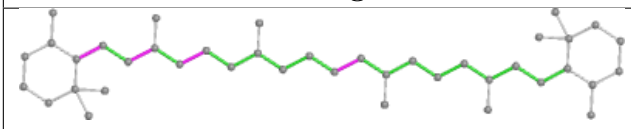
Ligand BCR r 522



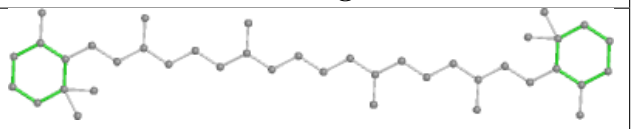
Bond lengths



Bond angles

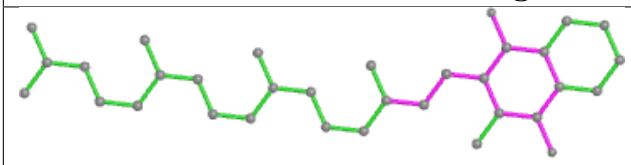


Torsions



Rings

Ligand PQN A 2001



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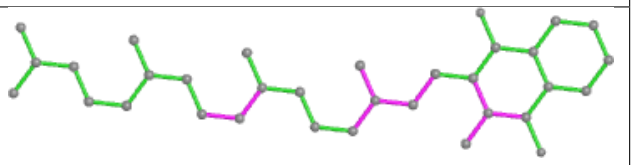
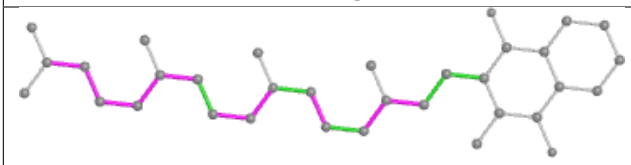
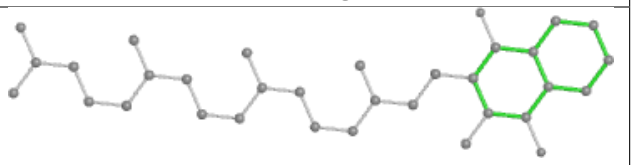


Bond angles

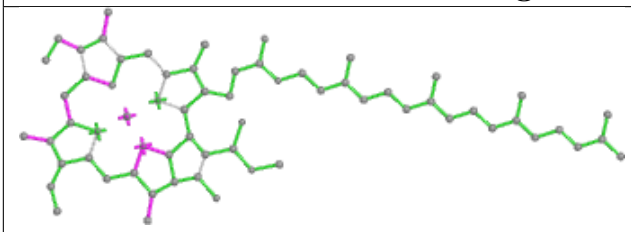


Torsions

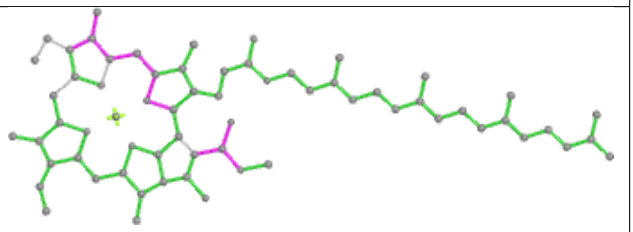


Rings

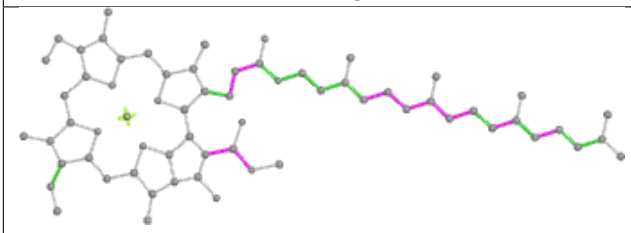
Ligand CLA B 1203



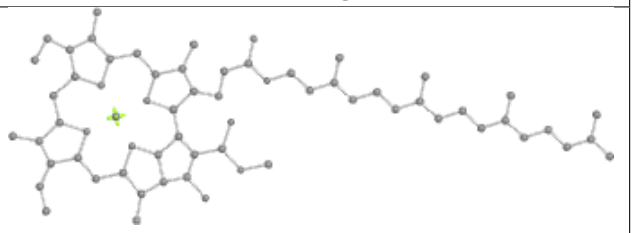
Bond lengths



Bond angles

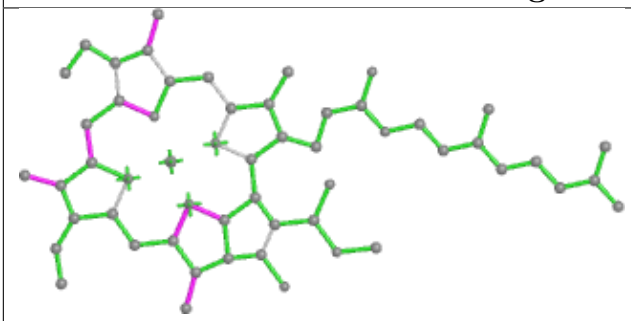


Torsions



Rings

Ligand CLA a 508



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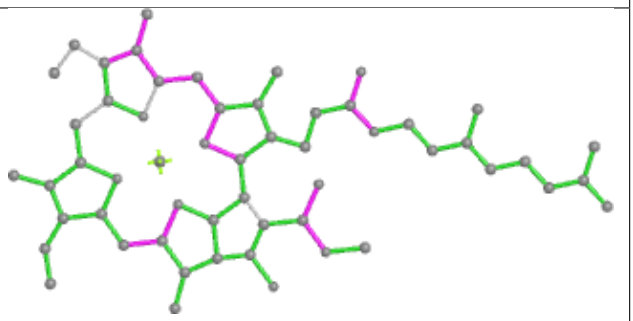
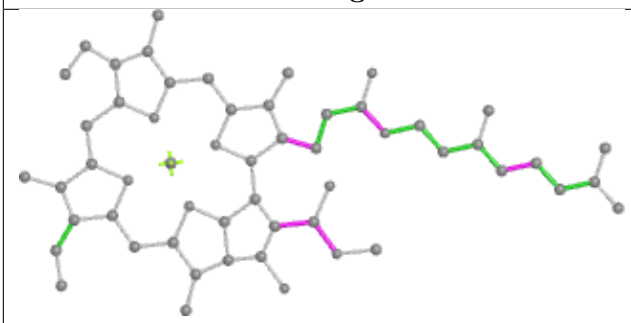


Bond angles



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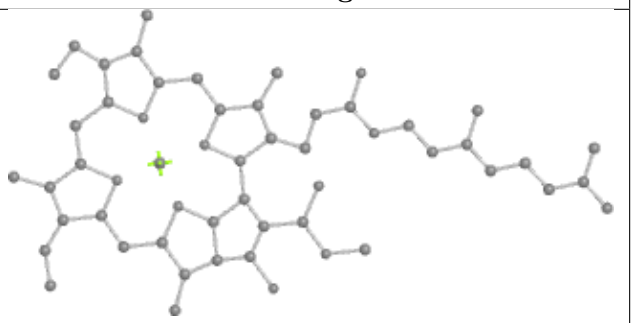
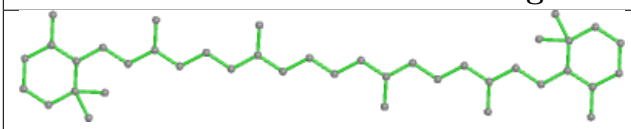


Rings

Ligand BCR 6 521



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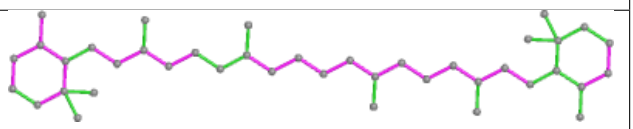
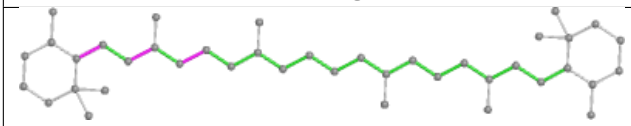


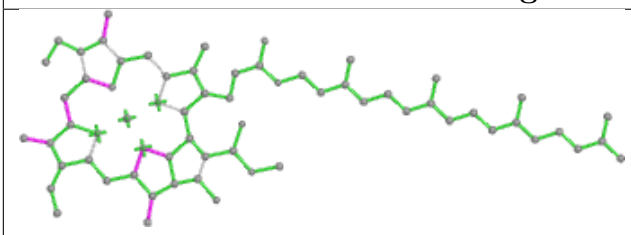
Bond angles



Torsions

Rings

Ligand CLA e 1127



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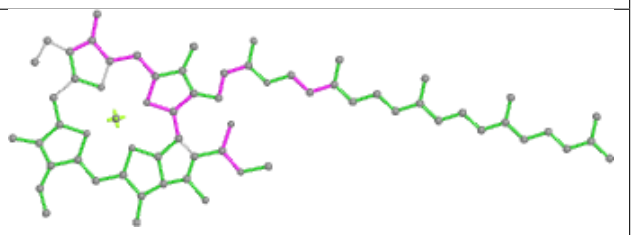
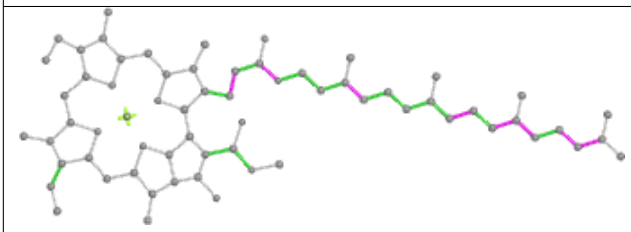


Bond angles



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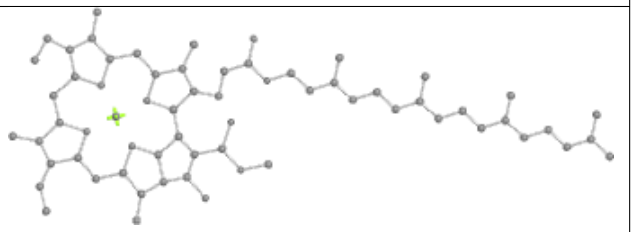
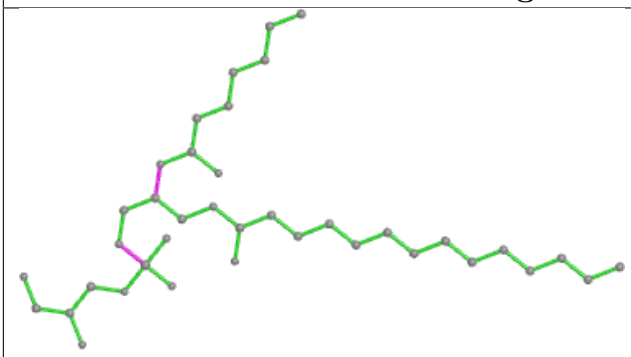


Rings

Ligand LHG n 5218



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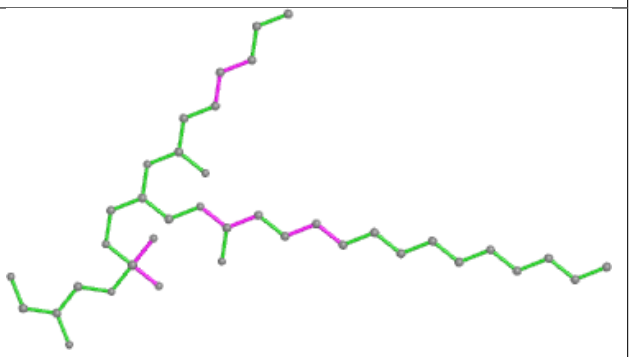
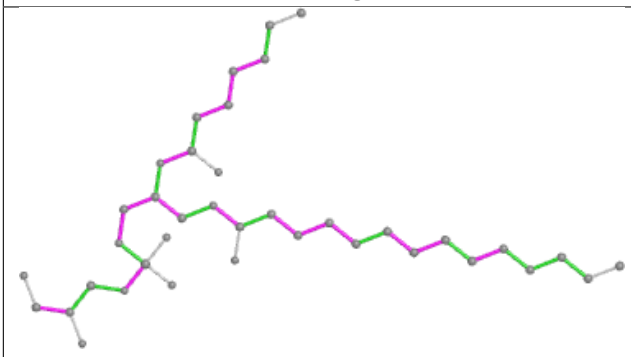


Bond angles



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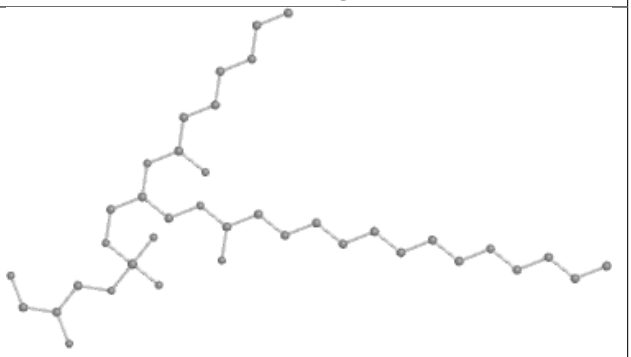
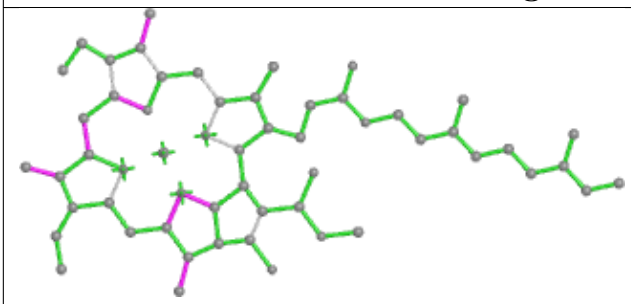


Rings

Ligand CLA f 1211



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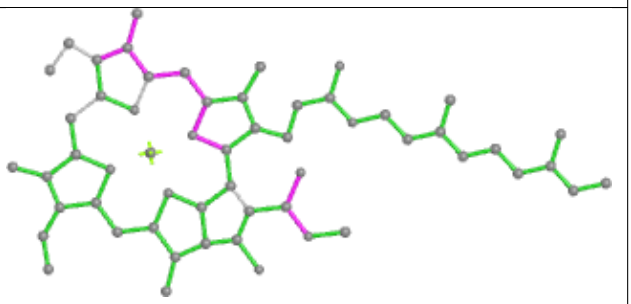
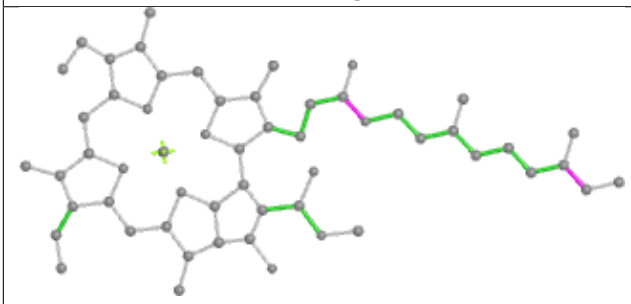
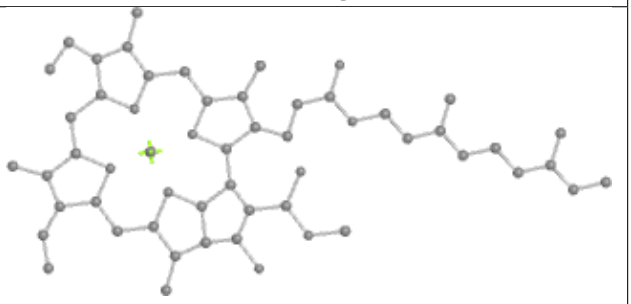


Bond angles

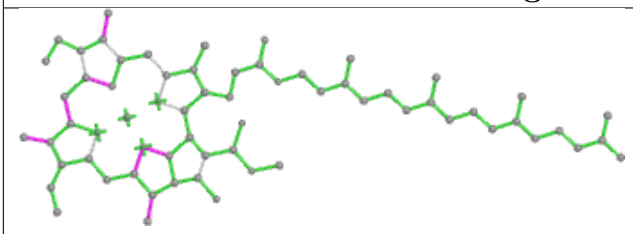


Torsions

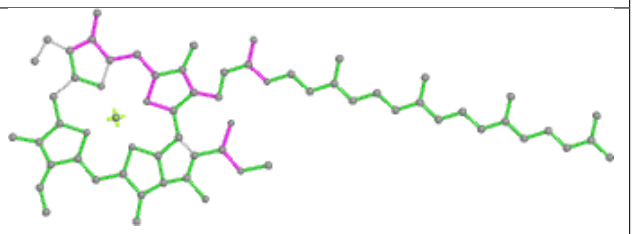


Rings

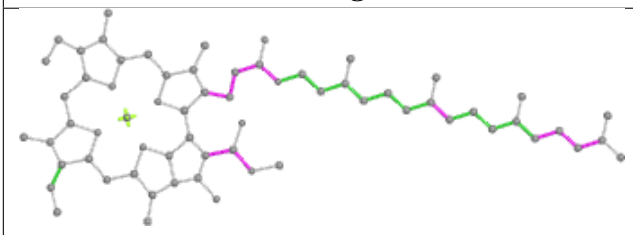
Ligand CLA Y 501



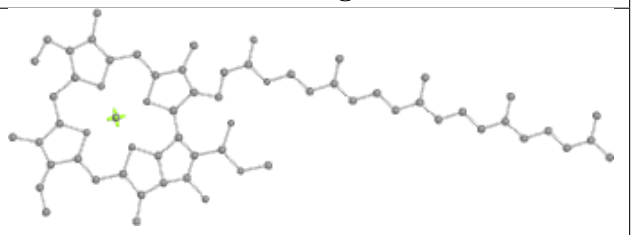
Bond lengths



Bond angles

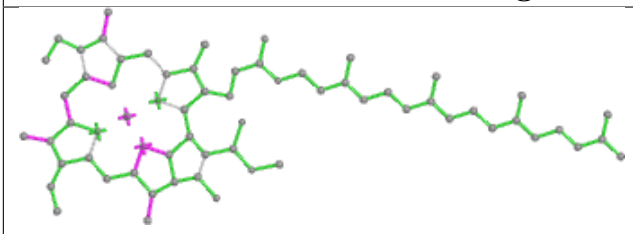


Torsions



Rings

Ligand CLA B 1021



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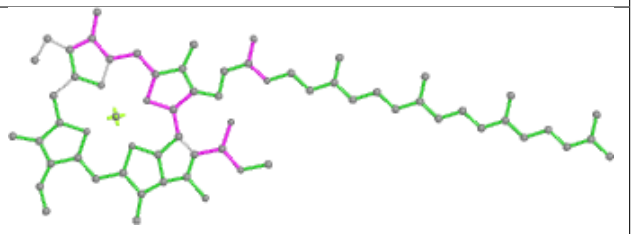
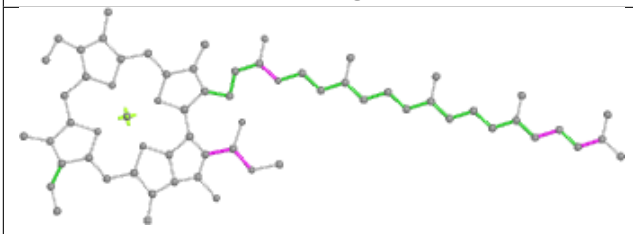


Bond angles



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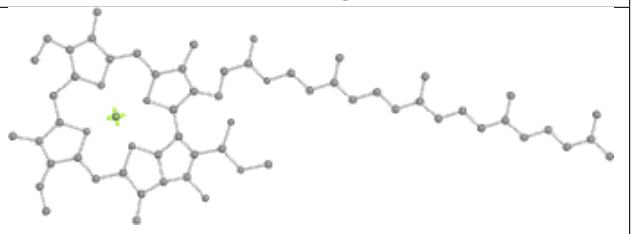
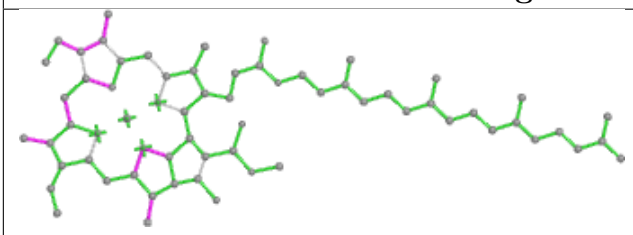


Rings

Ligand CLA B 1214



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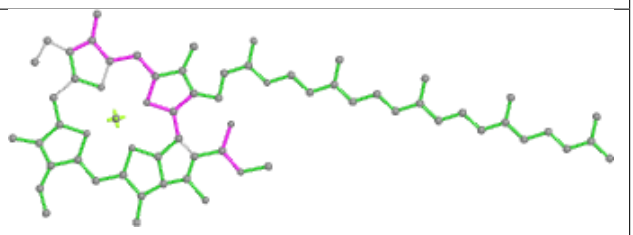
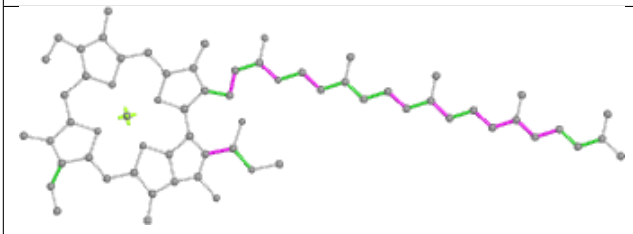
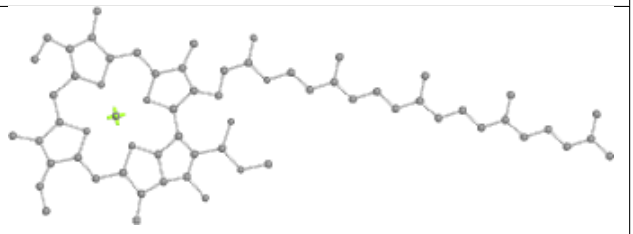


Bond angles

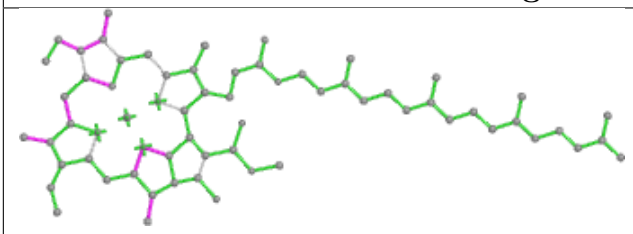


Torsions



Rings

Ligand CLA f 1207



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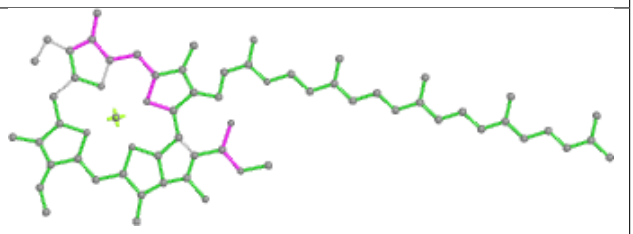
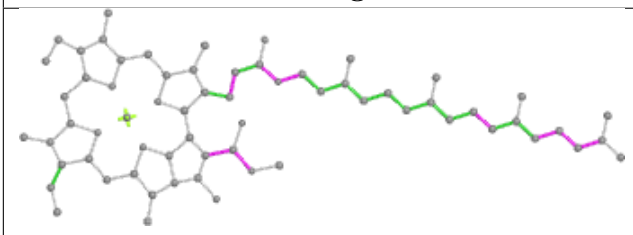


Bond angles



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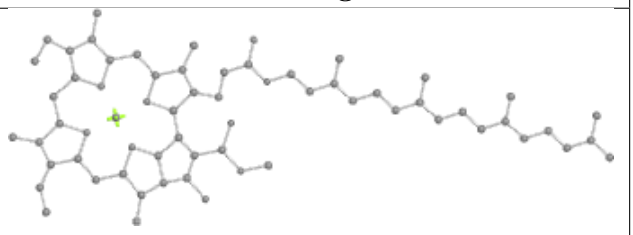
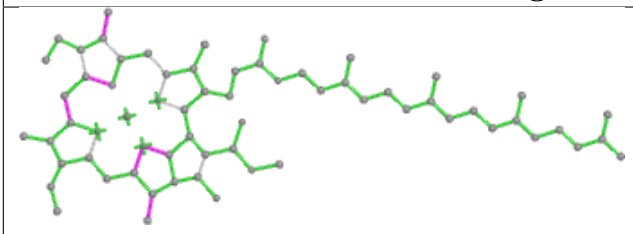


Rings

Ligand CLA a 513



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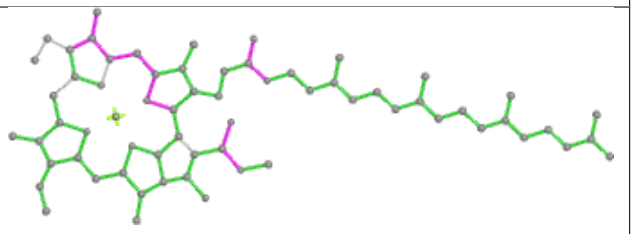
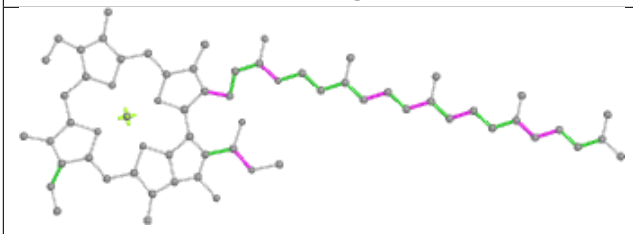
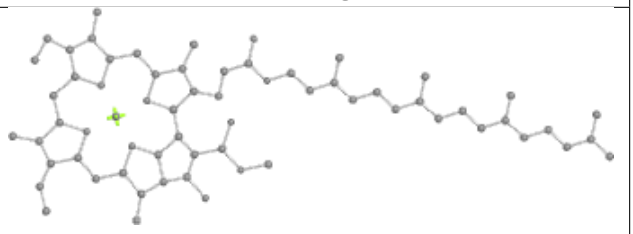


Bond angles

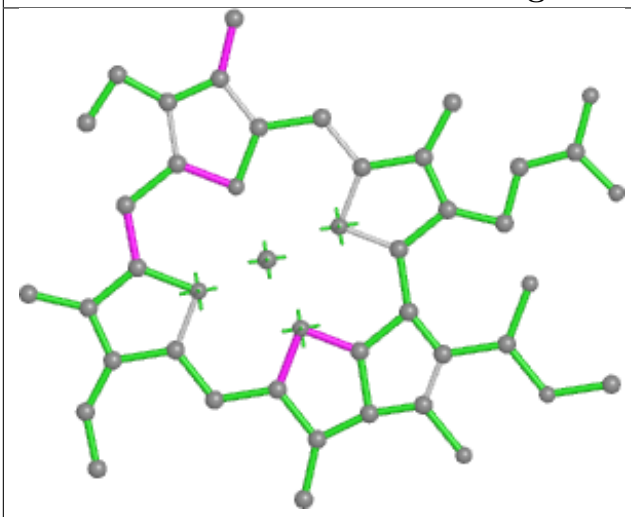


Torsions

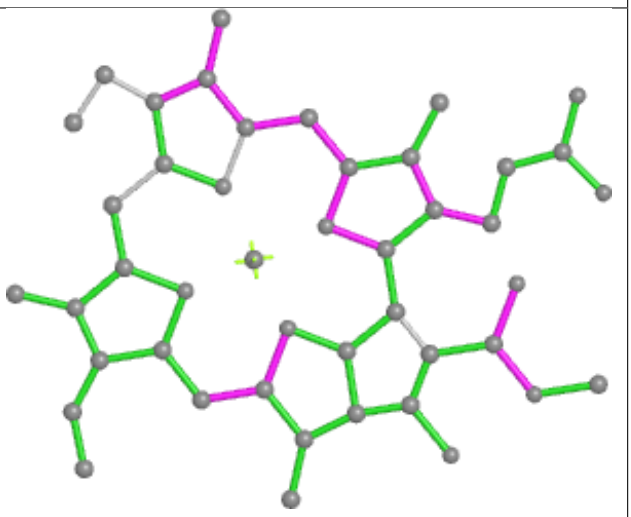


Rings

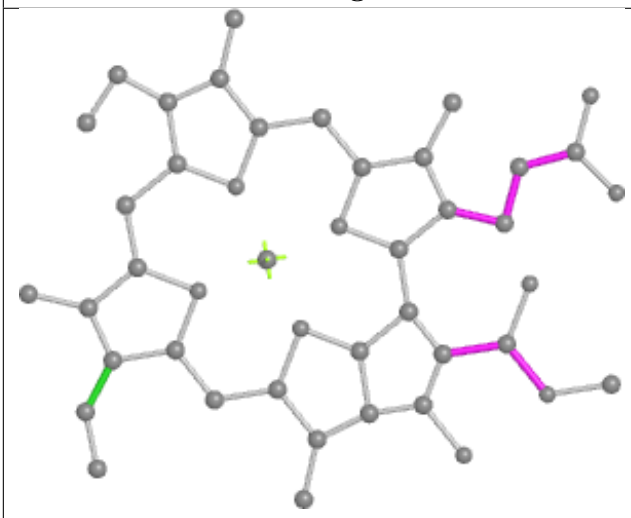
Ligand CLA v 516



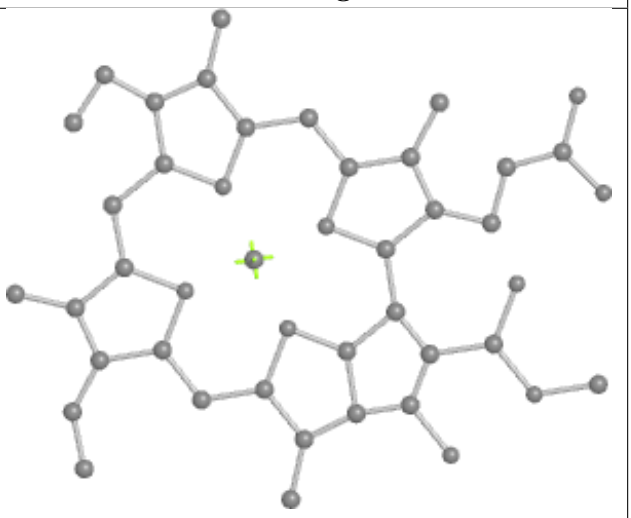
Bond lengths



Bond angles

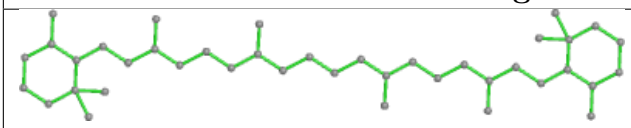


Torsions

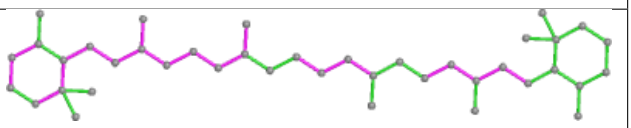


Rings

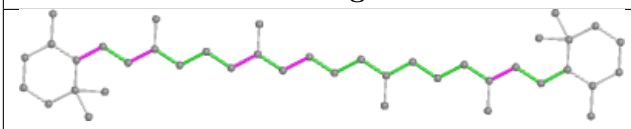
Ligand BCR A 4001



Bond lengths



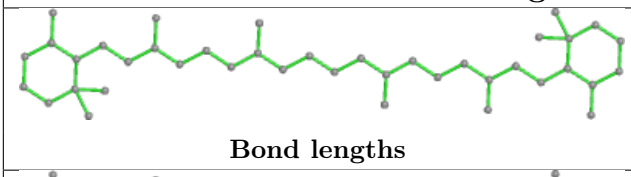
Bond angles



Torsions

Rings

Ligand BCR s 521



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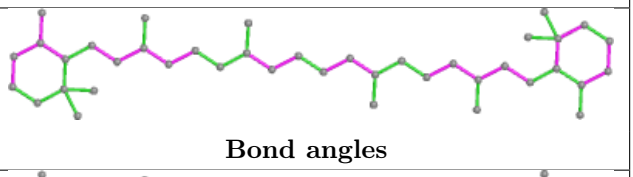
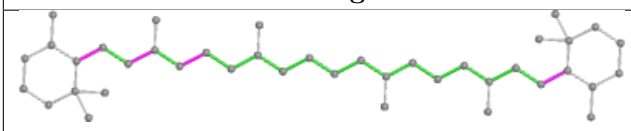
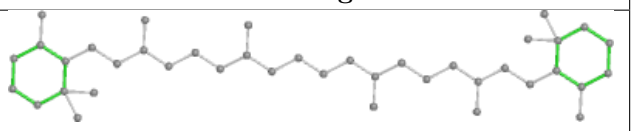


Bond angles

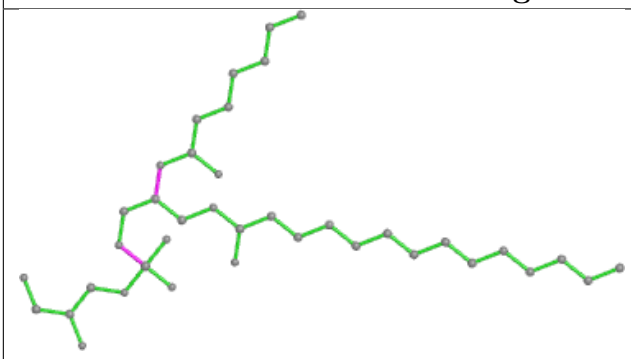


Torsions



Rings

Ligand LHG V 5218



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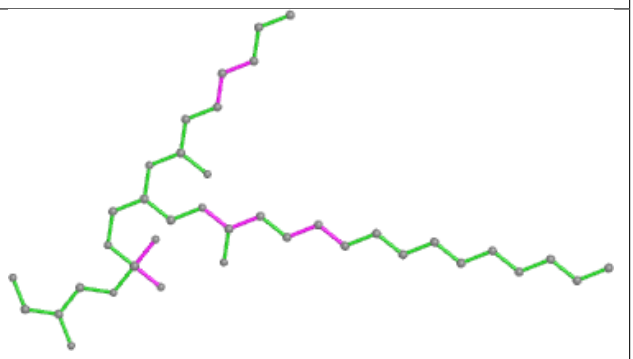

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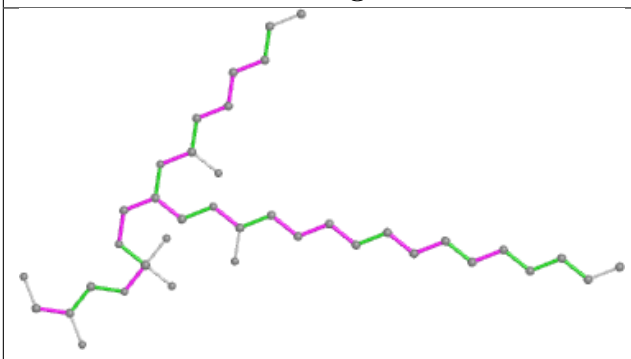

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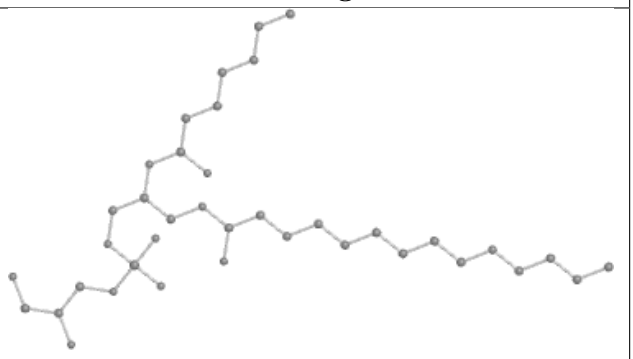
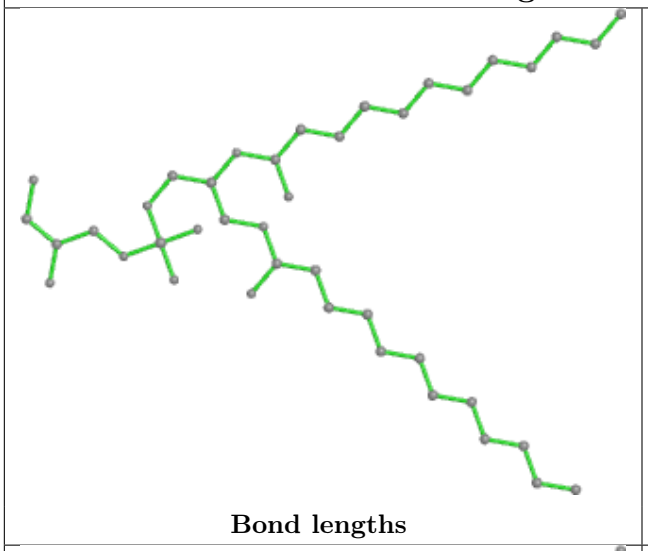


Rings

Ligand LHG n 5220



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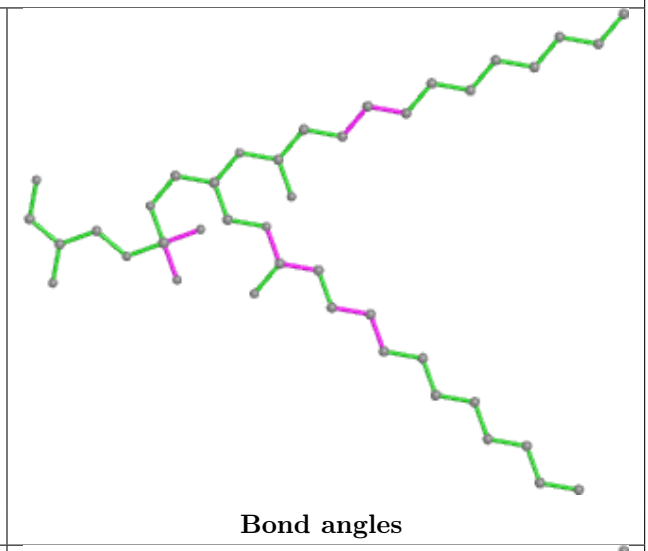

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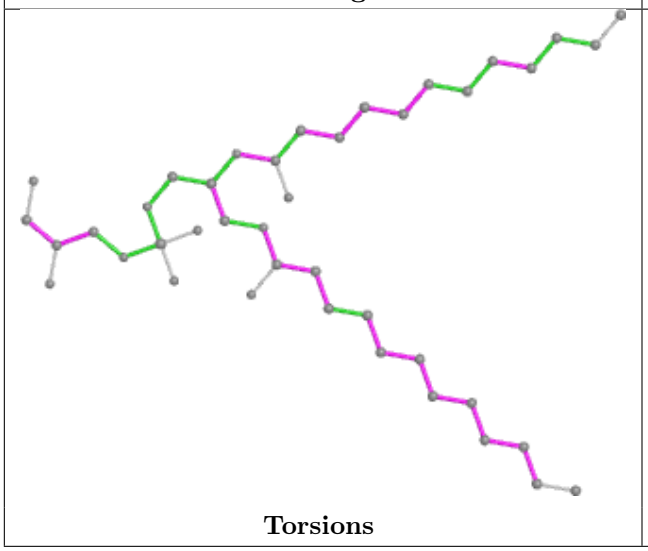

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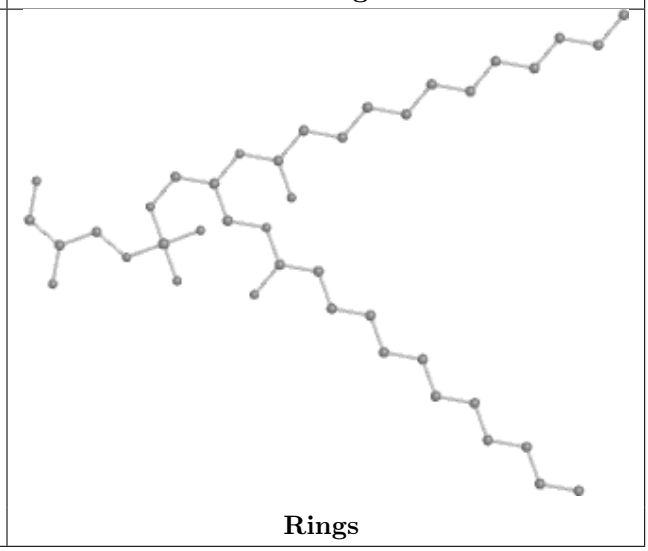
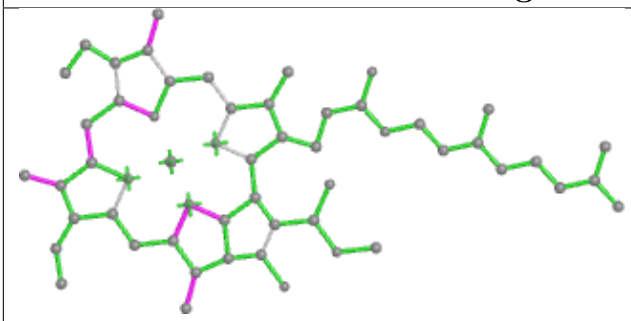


Rings

Ligand CLA B 1228



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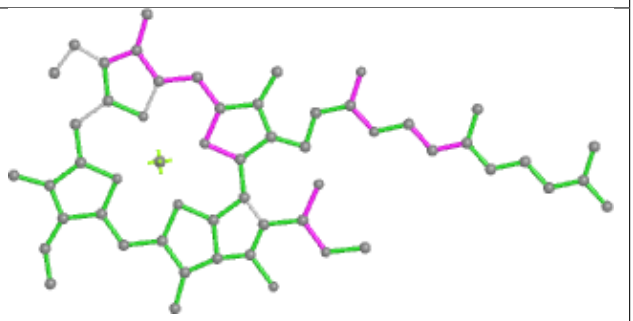

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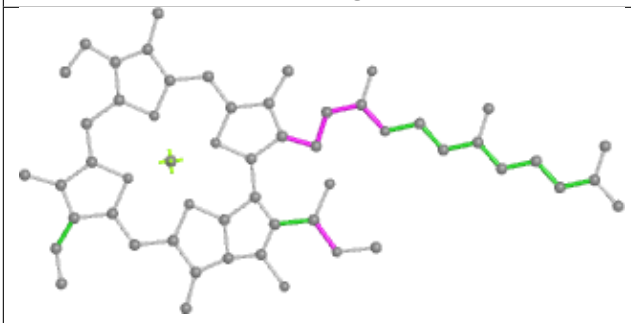

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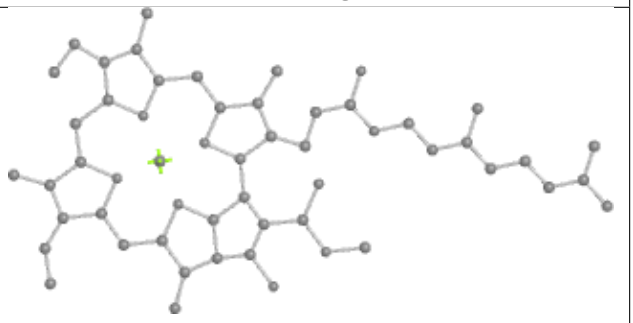
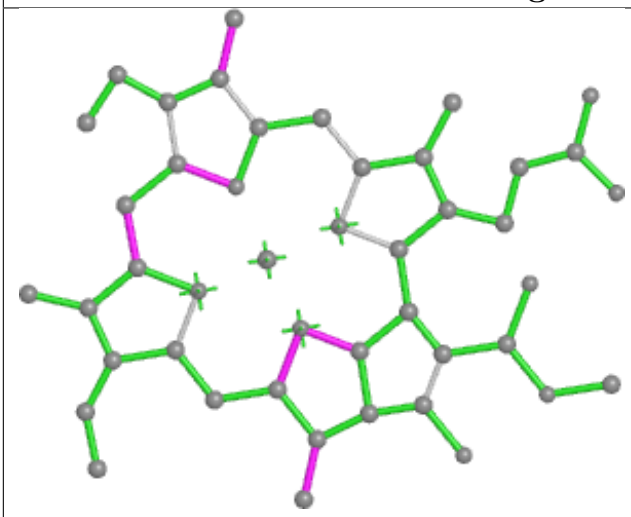


Rings

Ligand CLA 6 510



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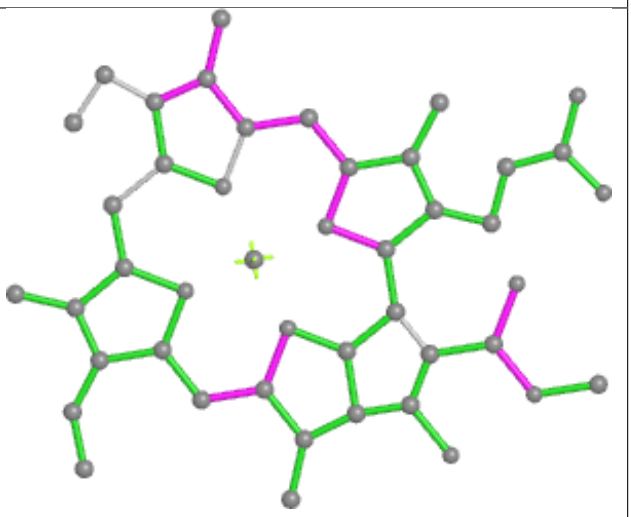

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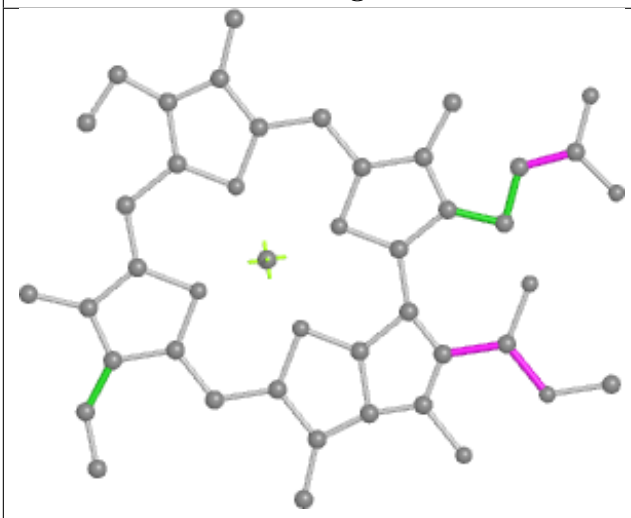

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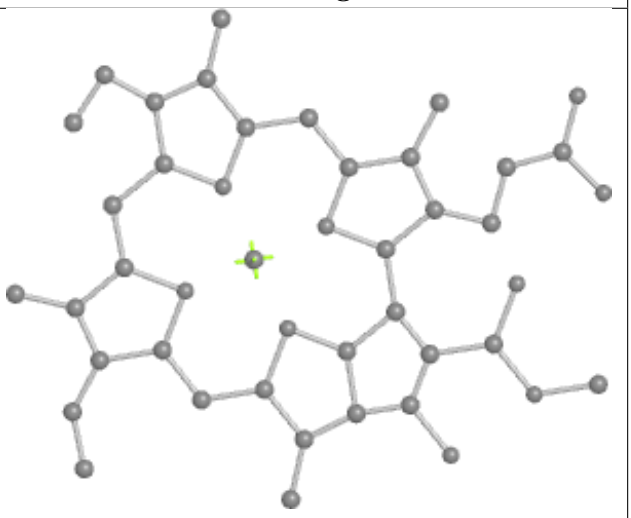
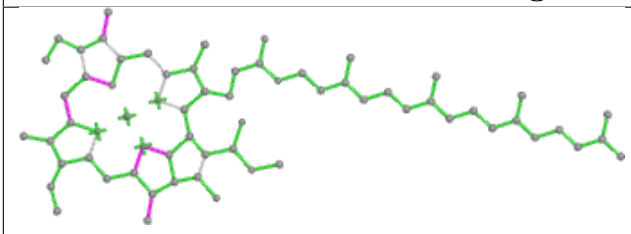


Rings

Ligand CLA 1 510



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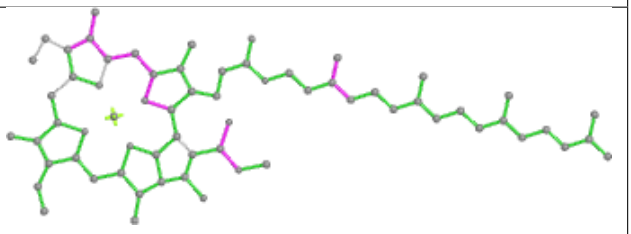
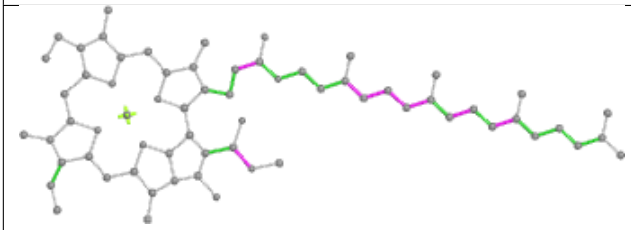


Bond angles



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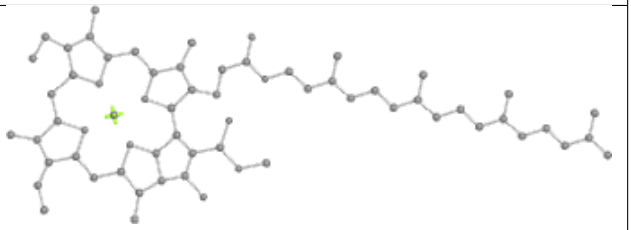
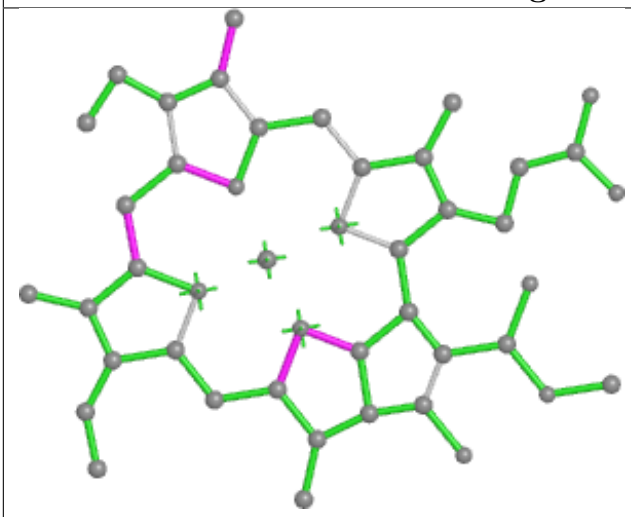


Rings

Ligand CLA c 504



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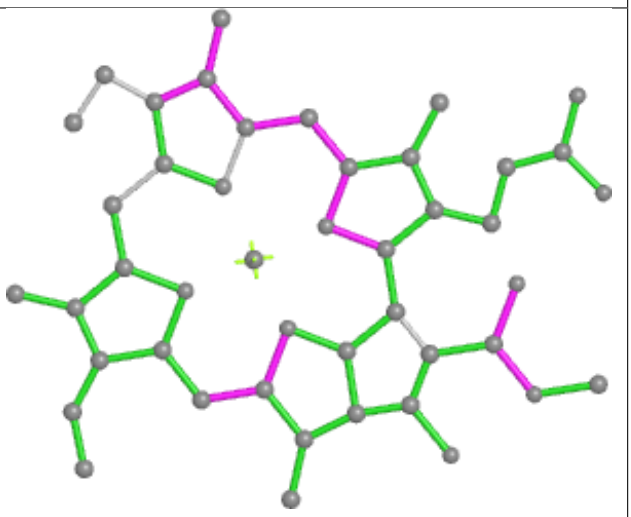

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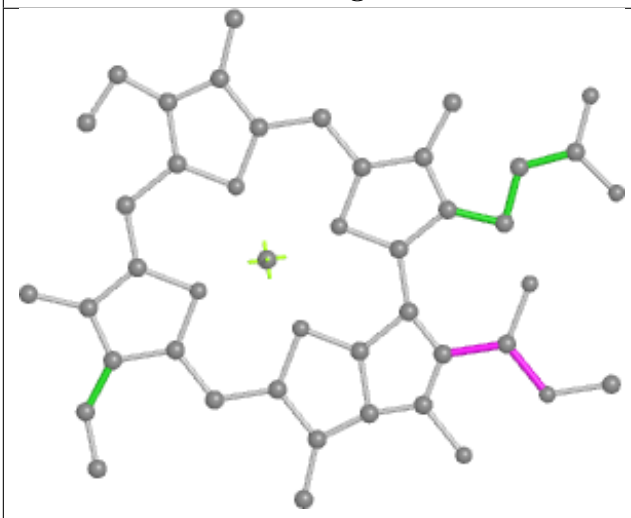

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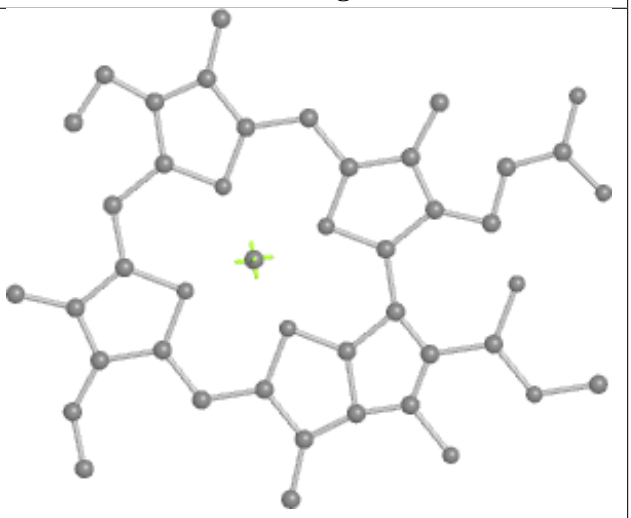
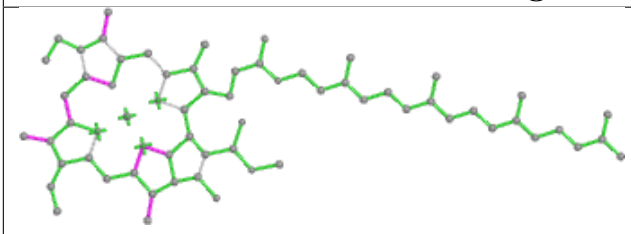


Rings

Ligand CLA q 509



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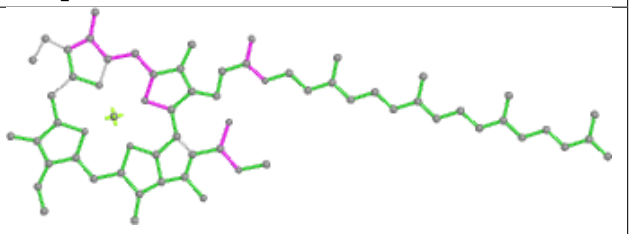

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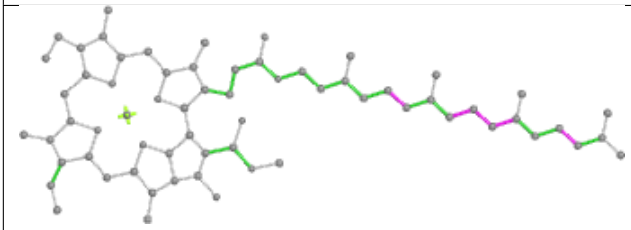

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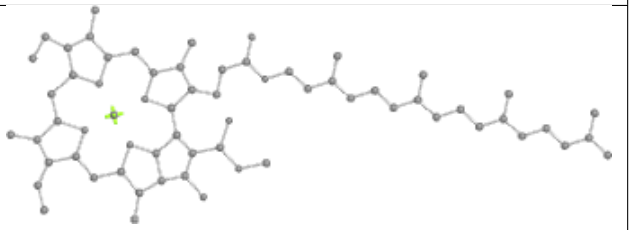
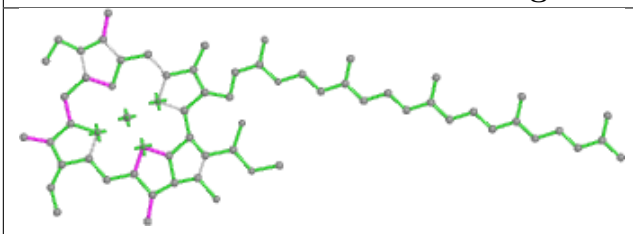


Rings

Ligand CLA s 501



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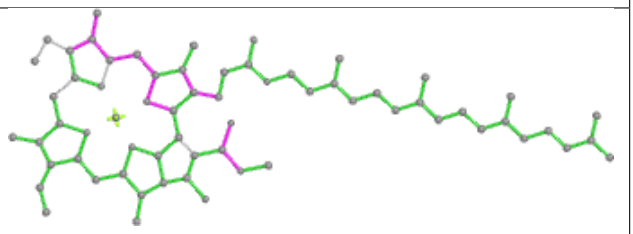

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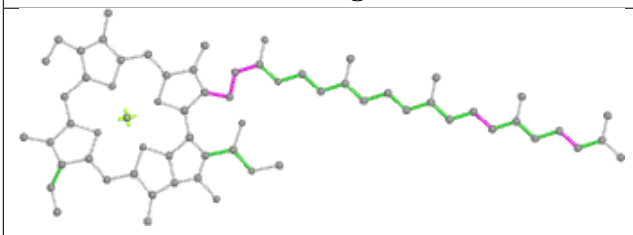

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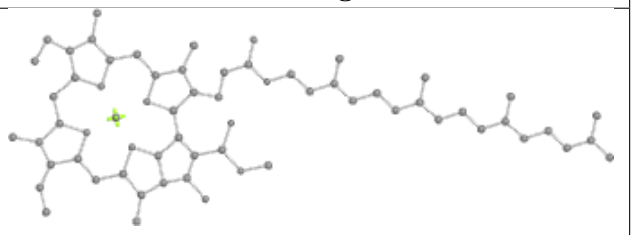
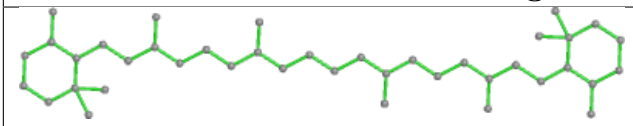


Rings

Ligand BCR v 524



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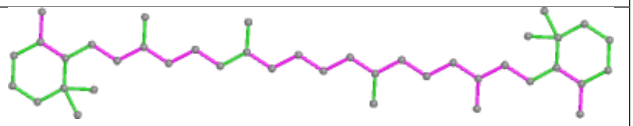

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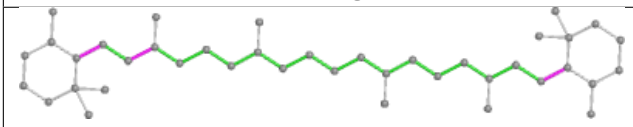
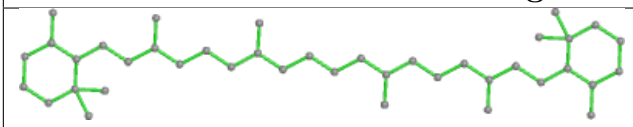


Torsions

Rings

Ligand BCR 4 522



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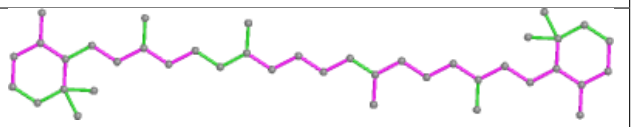

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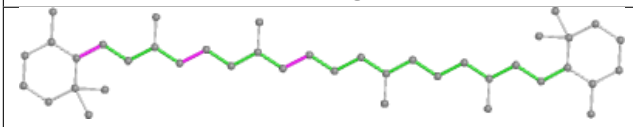
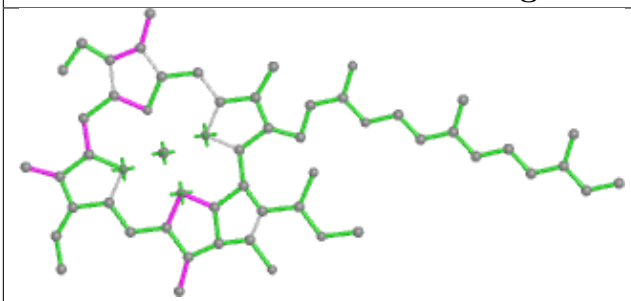


Torsions

Rings

Ligand CLA e 1134



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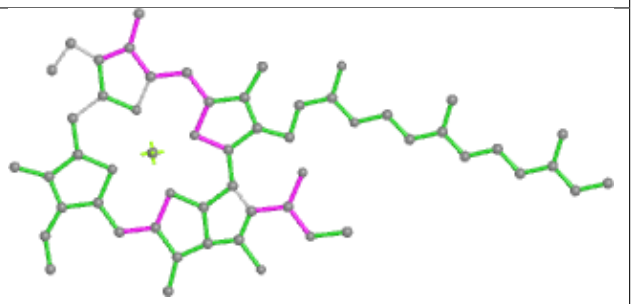

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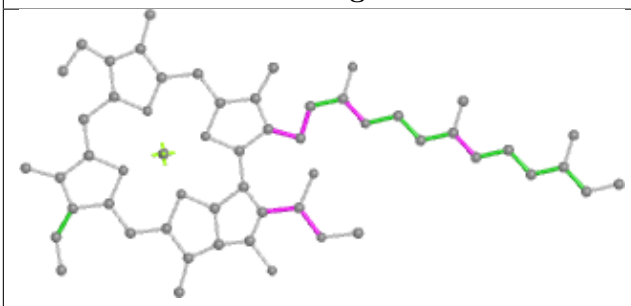

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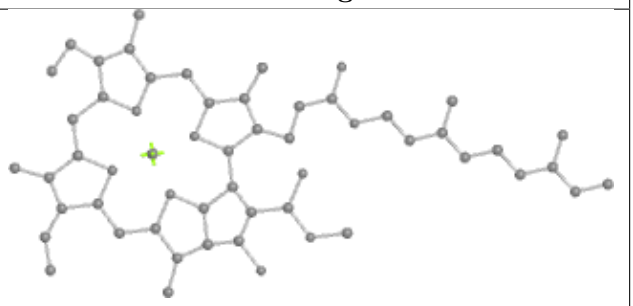
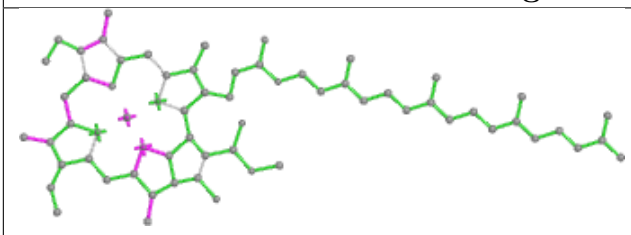


Rings

Ligand CLA f 1205



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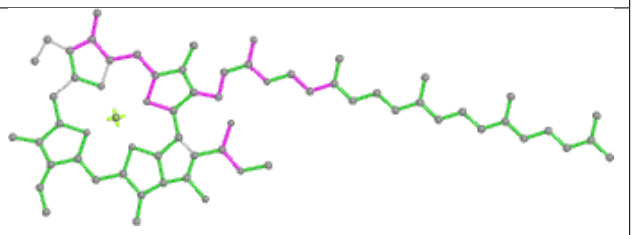
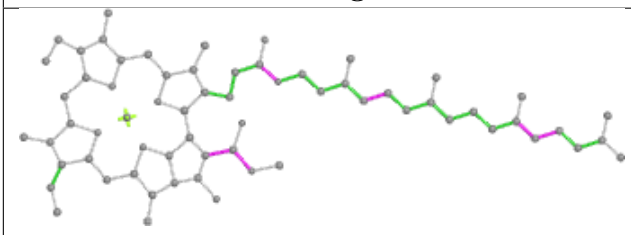


Bond angles



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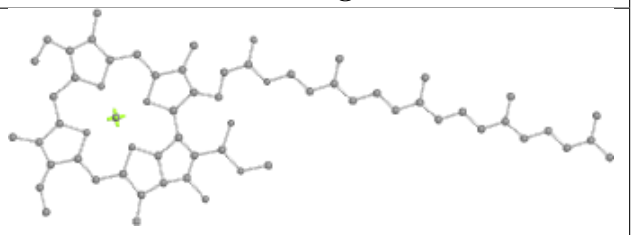
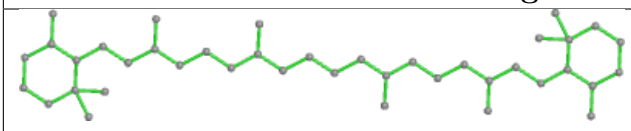


Rings

Ligand BCR f 4014



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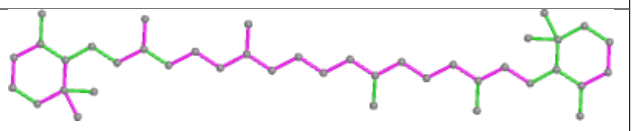
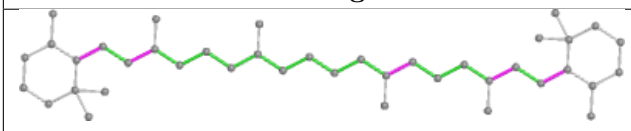


Bond angles



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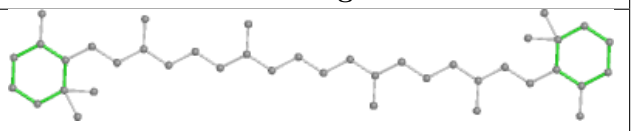
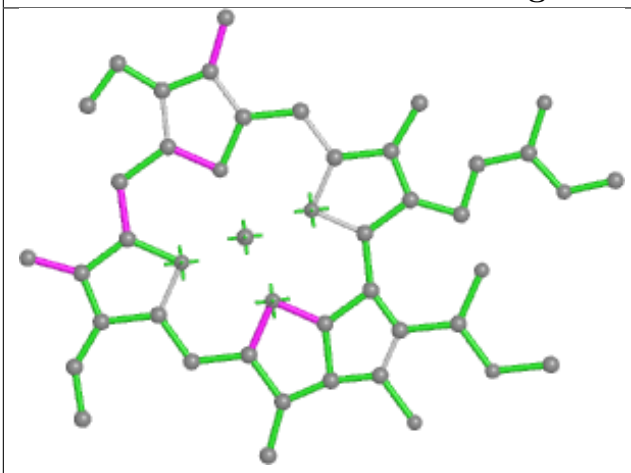


Rings

Ligand CLA 6 519



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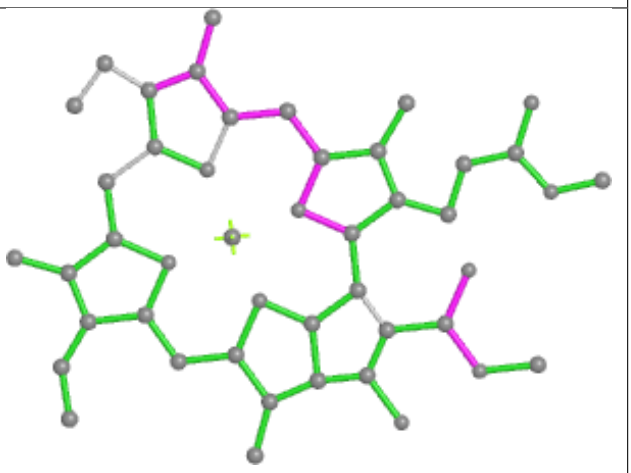
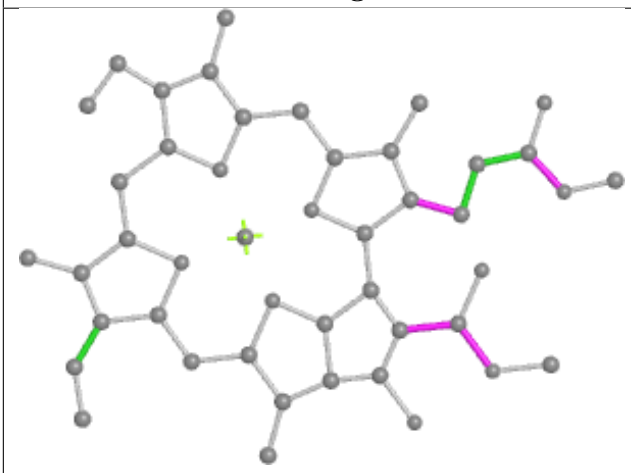


Bond angles



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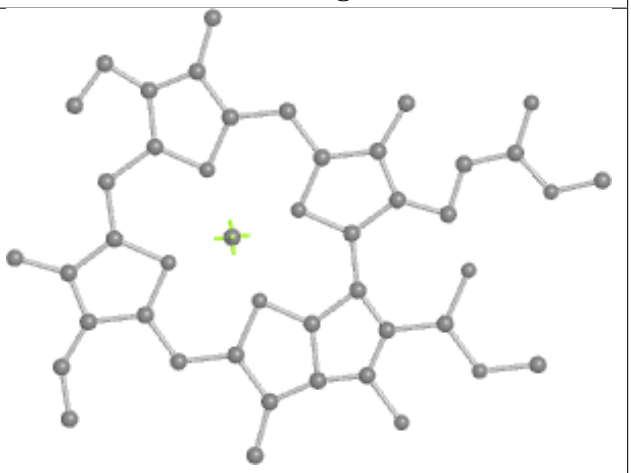
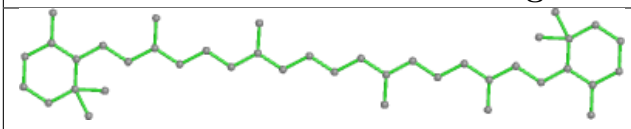
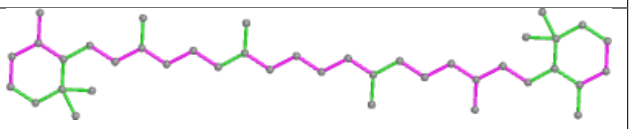


Rings

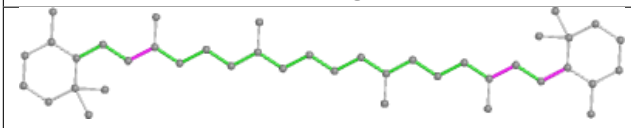
Ligand BCR 2 523



Bond lengths



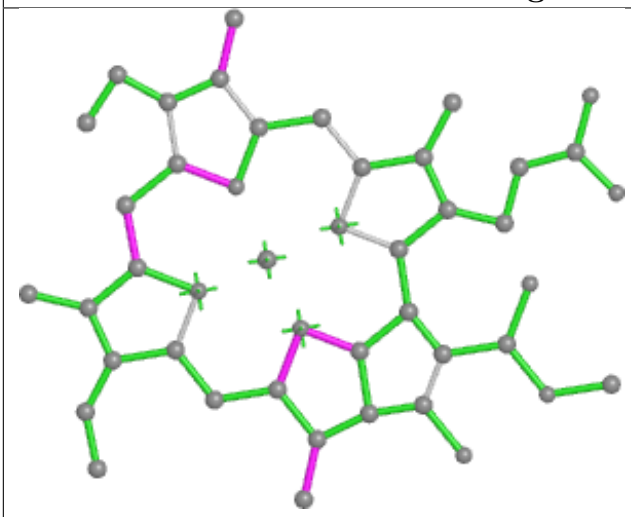
Bond angles



Torsions

Rings

Ligand CLA b 512



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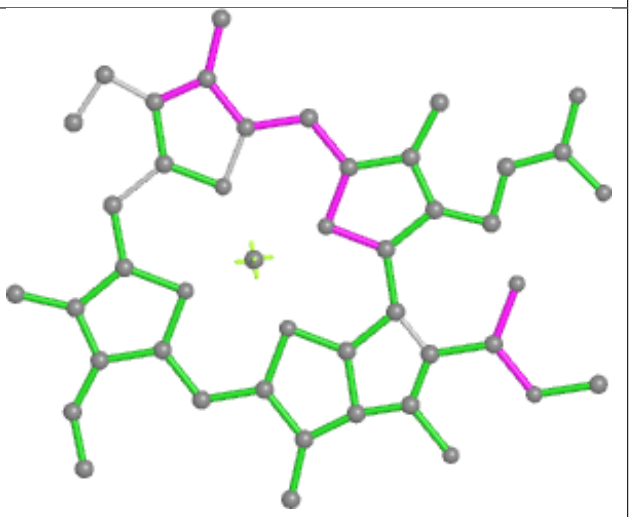

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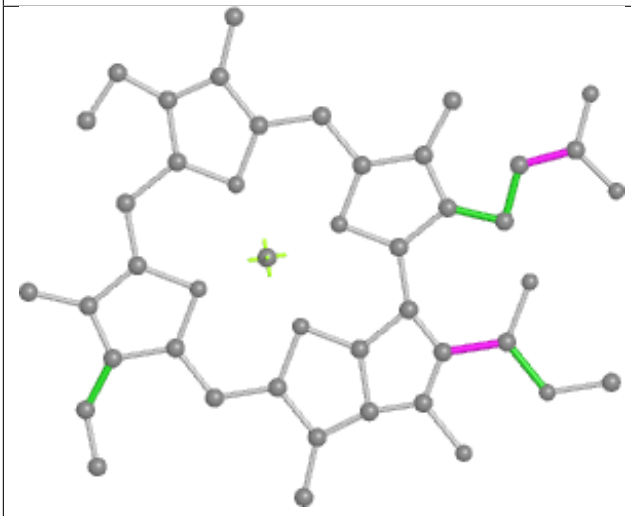

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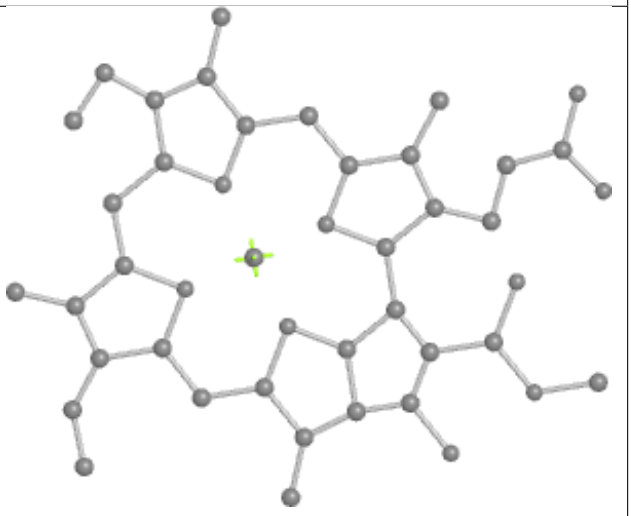
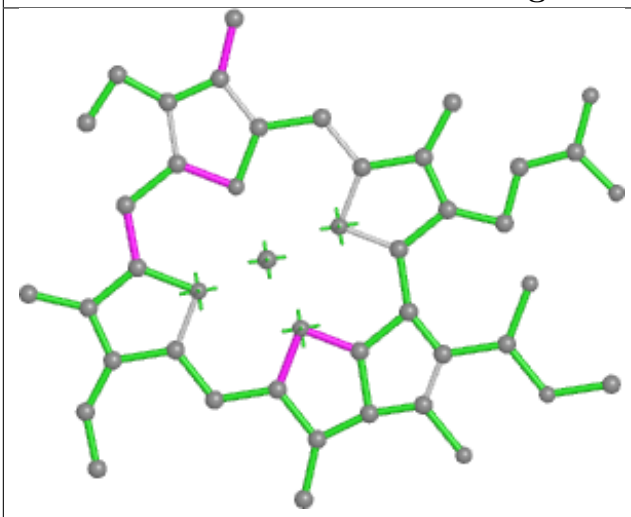


Rings

Ligand CLA 6 506



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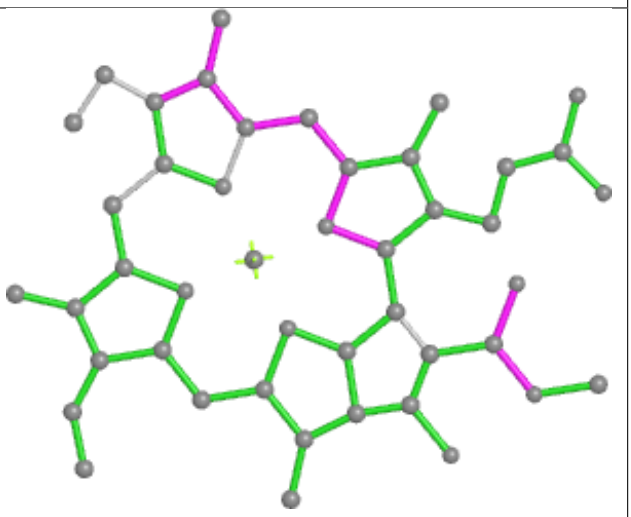

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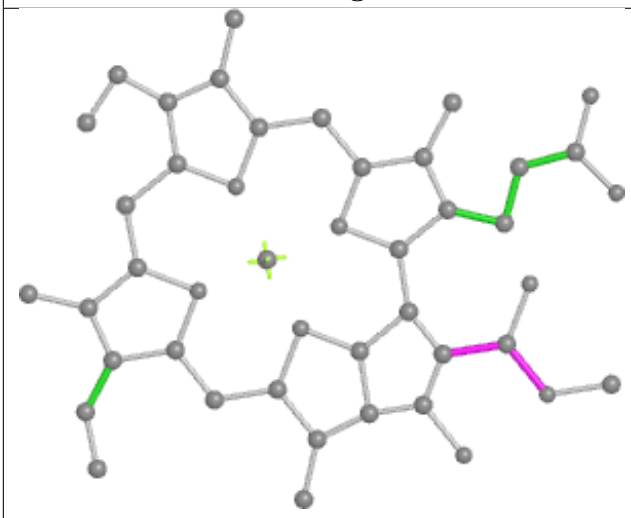

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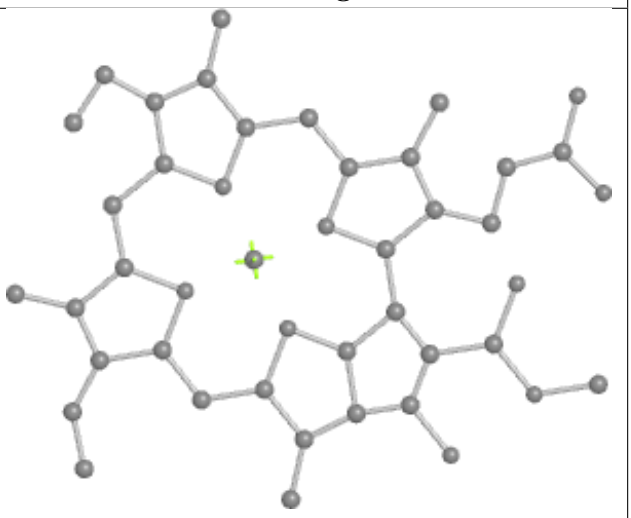
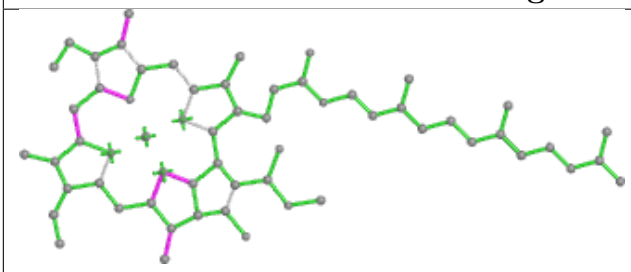


Rings

Ligand CLA d 501



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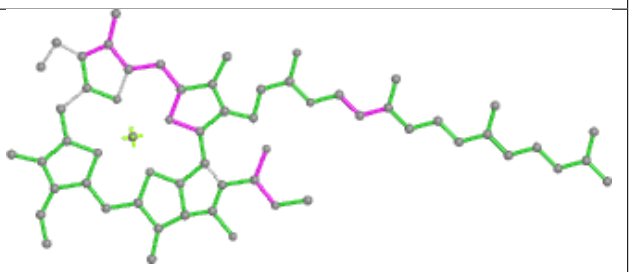

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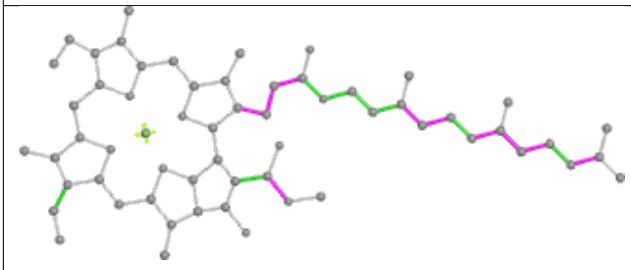

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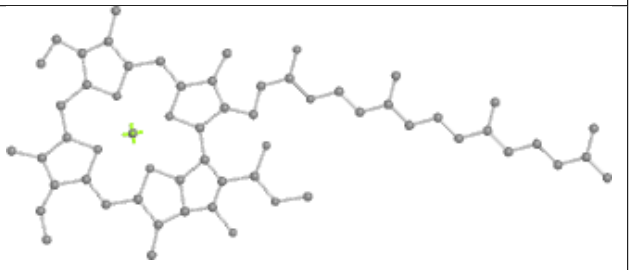
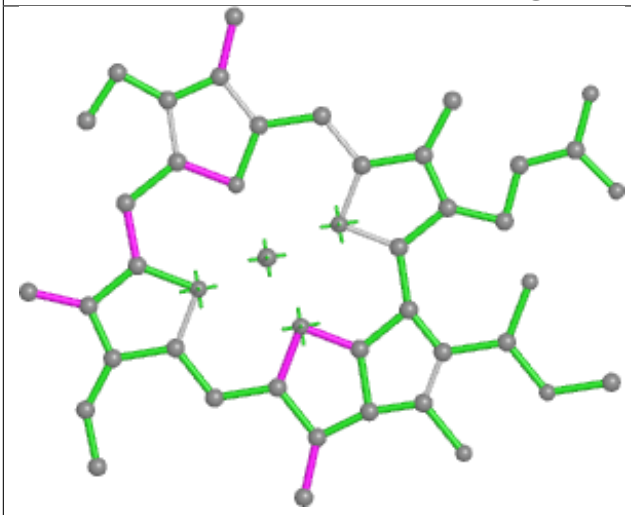


Rings

Ligand CLA d 517



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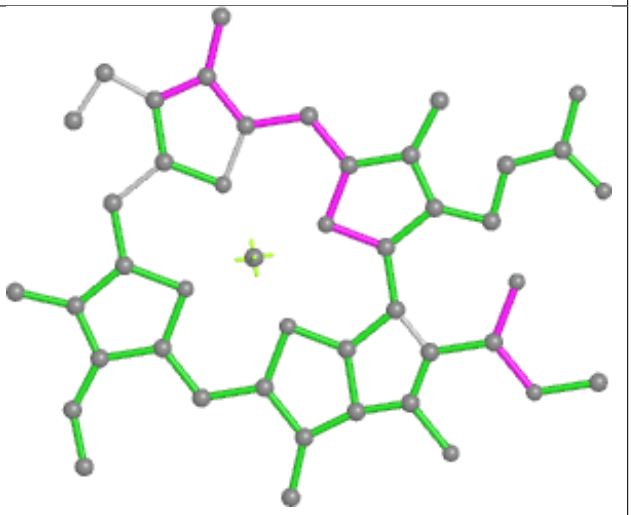
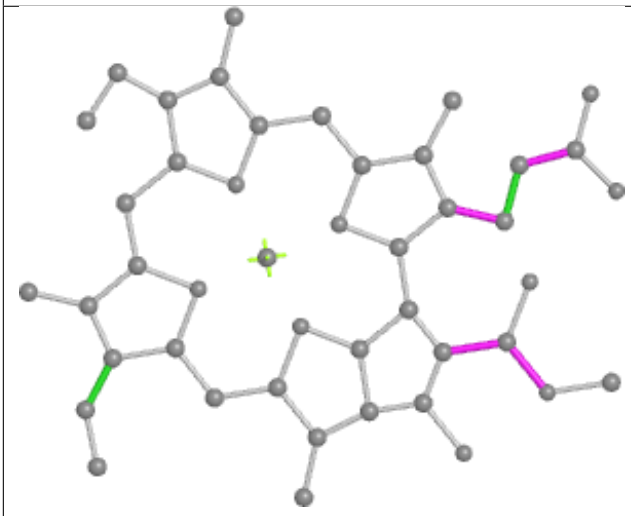


Bond angles



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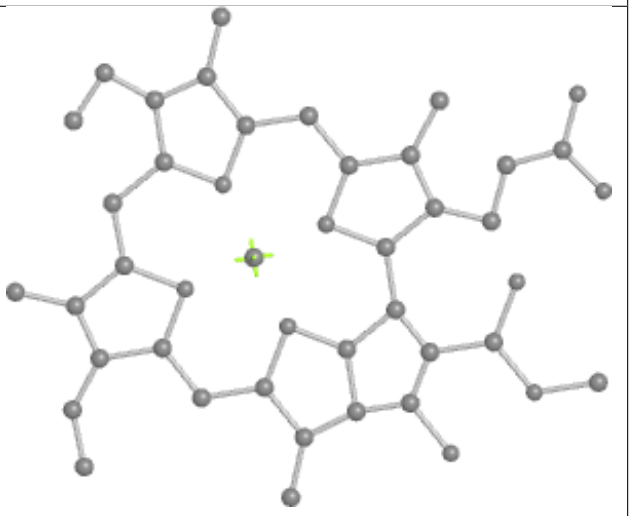
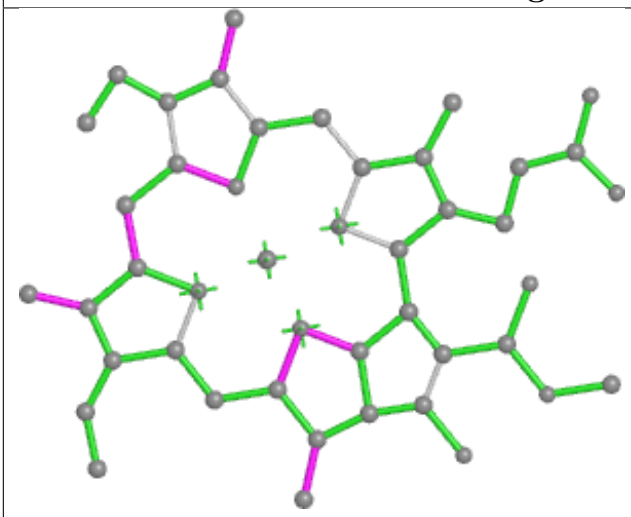


Rings

Ligand CLA v 508



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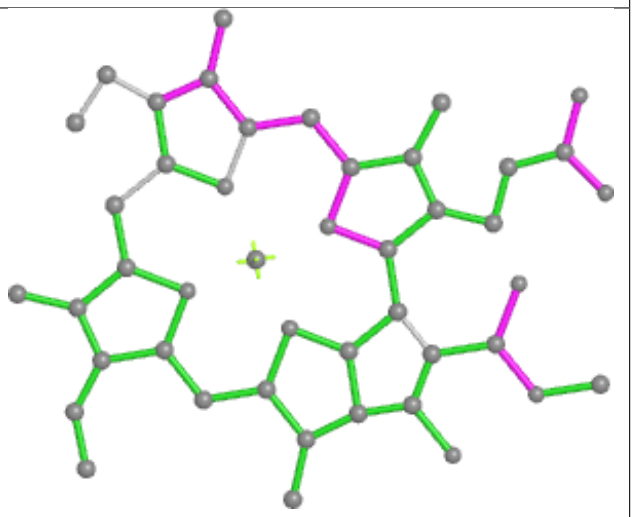
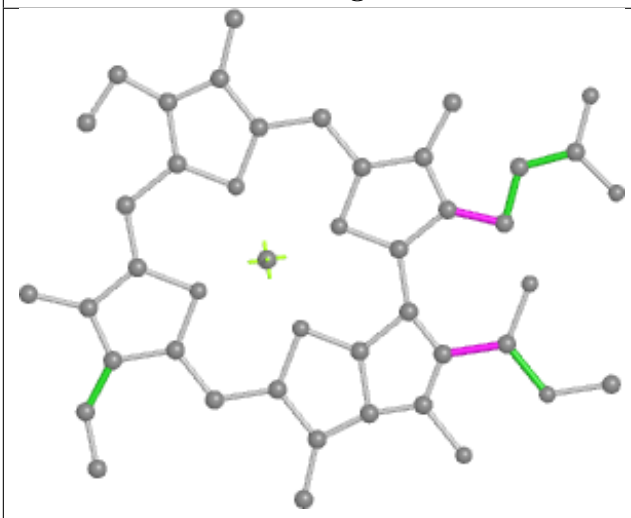


Bond angles



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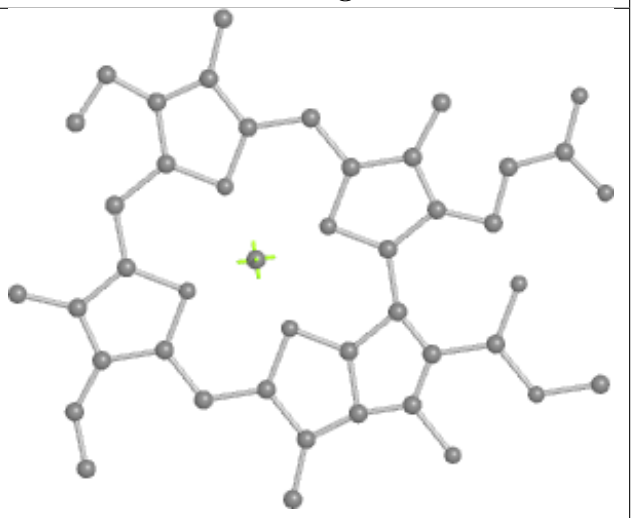
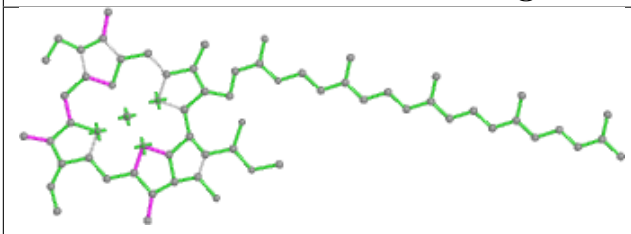


Rings

Ligand CLA L 1501



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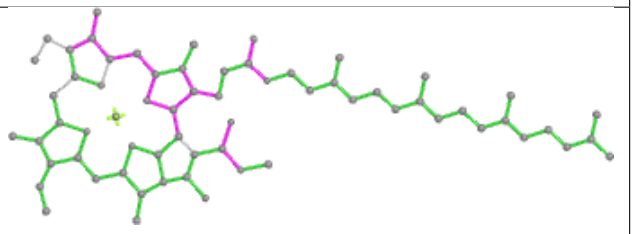

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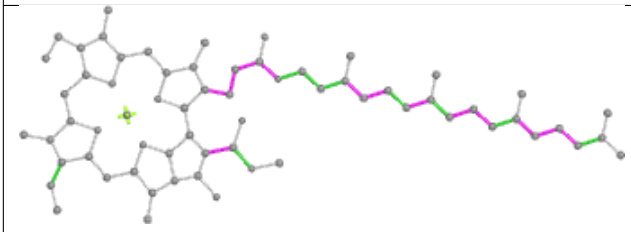

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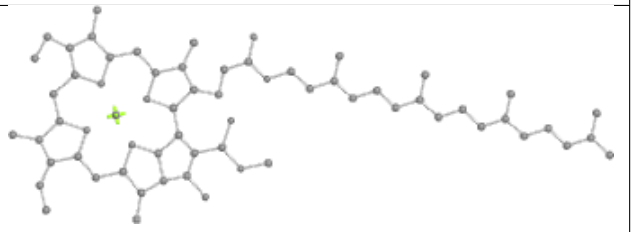
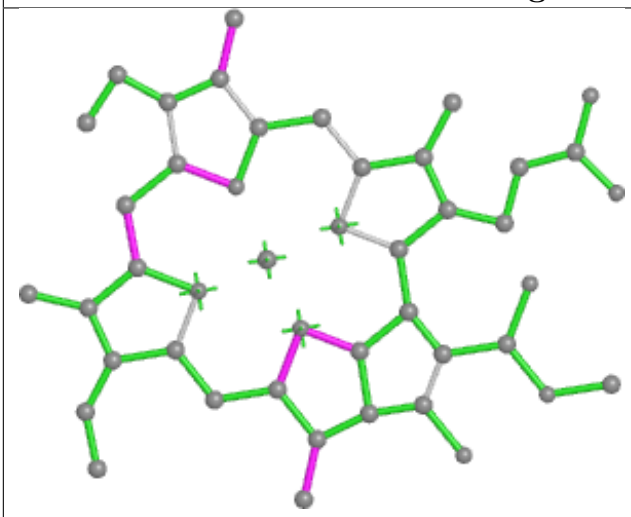


Rings

Ligand CLA 1 516



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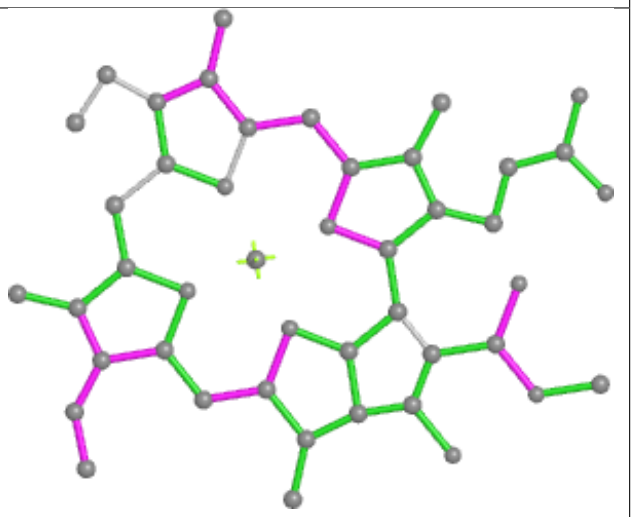

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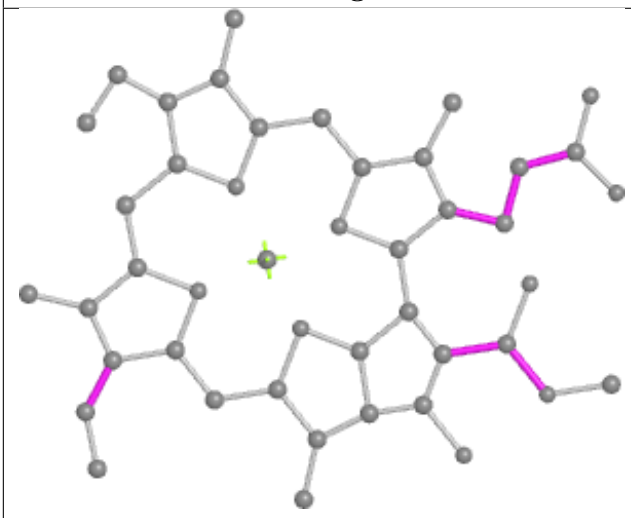

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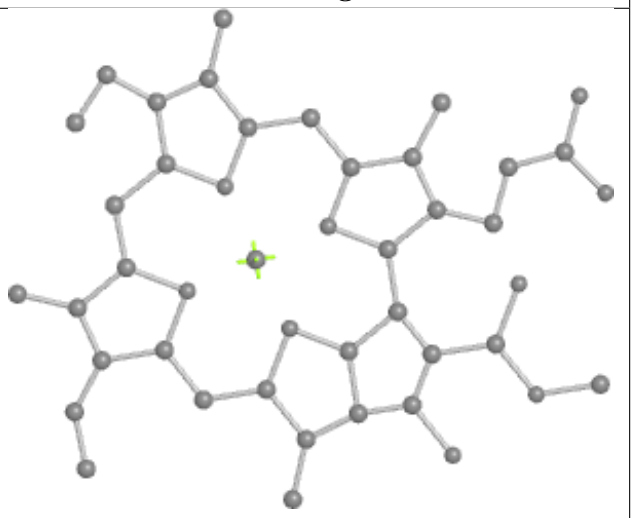
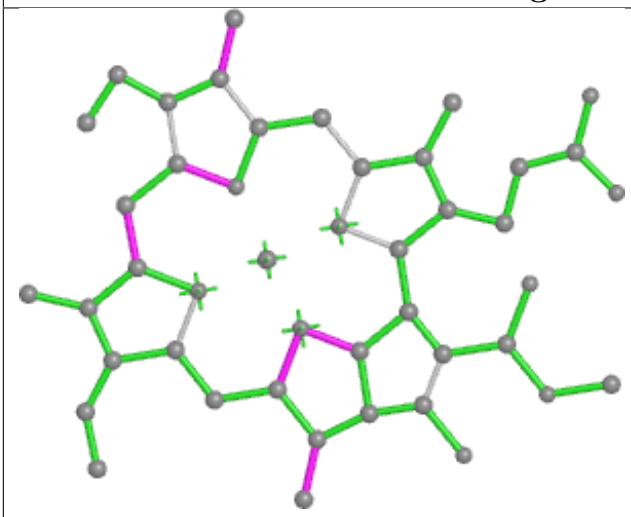


Rings

Ligand CLA r 516



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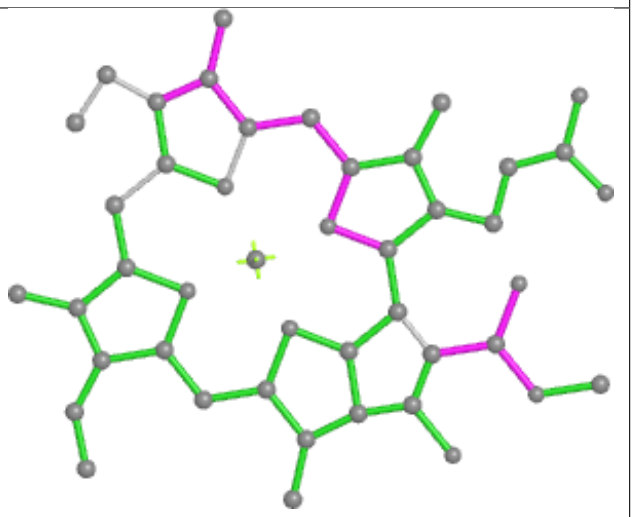
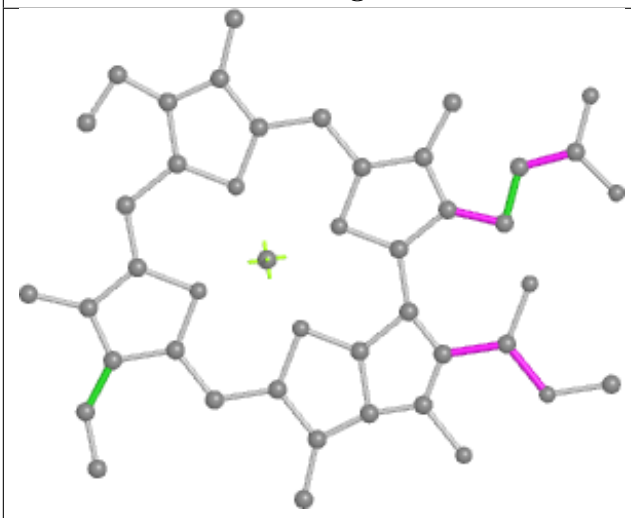


Bond angles



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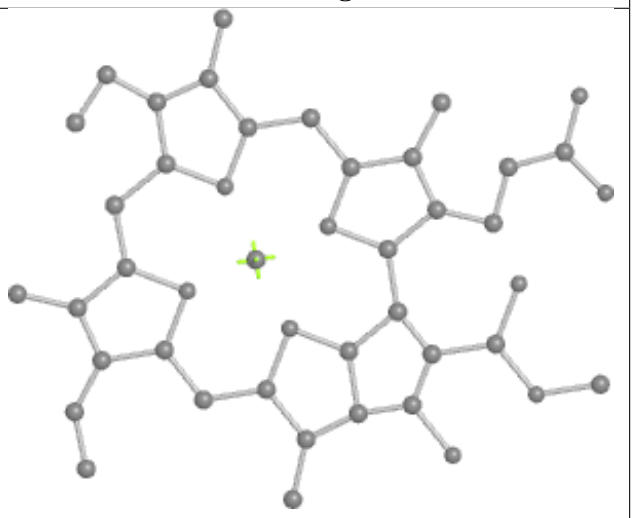
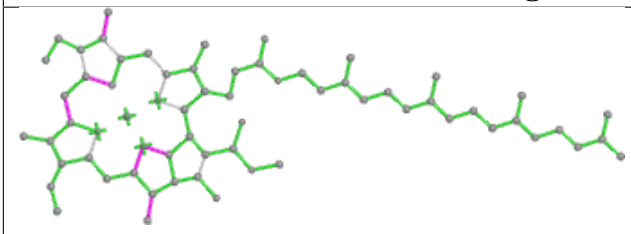


Rings

Ligand CLA Y 505



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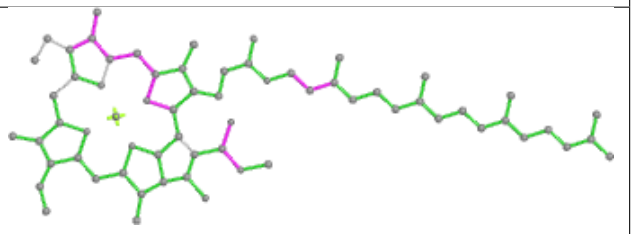

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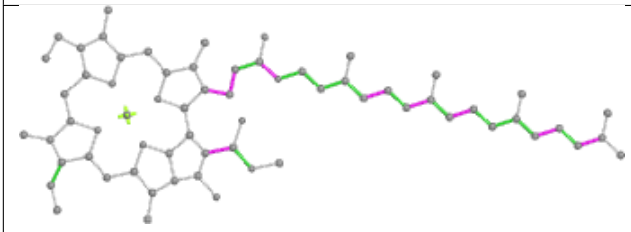

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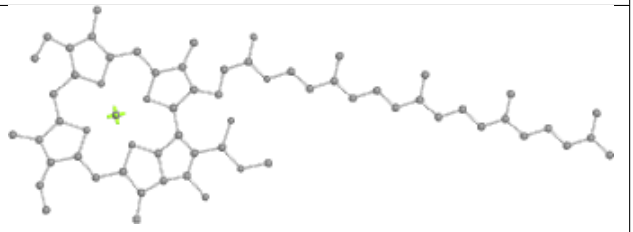
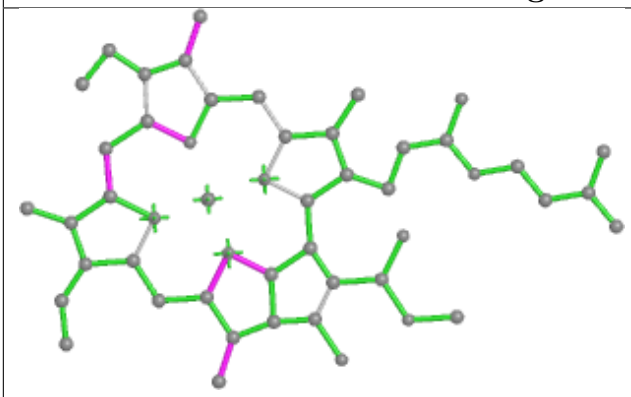


Rings

Ligand CLA d 502



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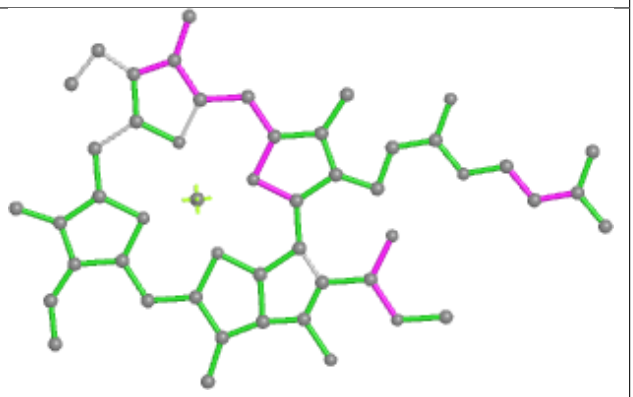
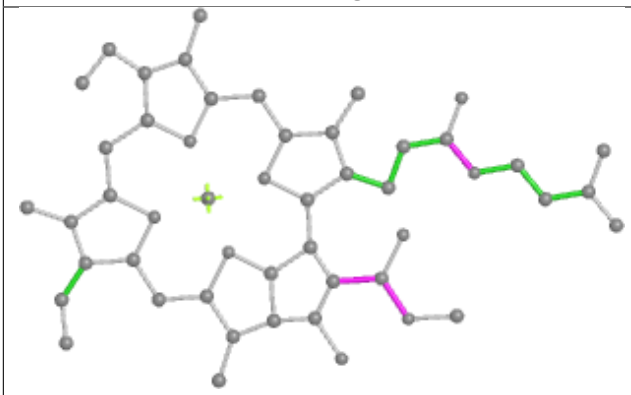


Bond angles



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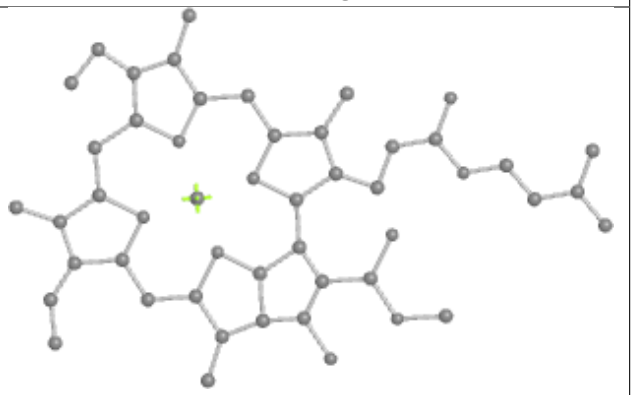
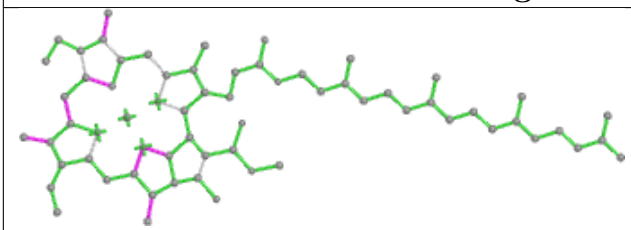


Rings

Ligand CLA G 1103



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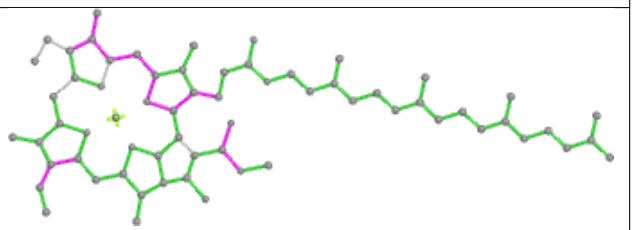
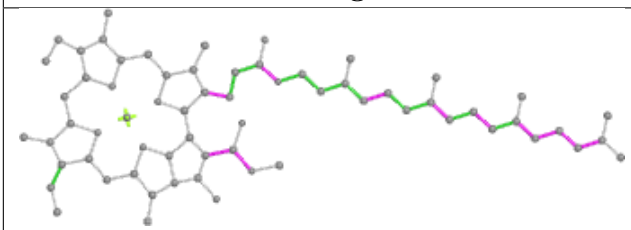


Bond angles



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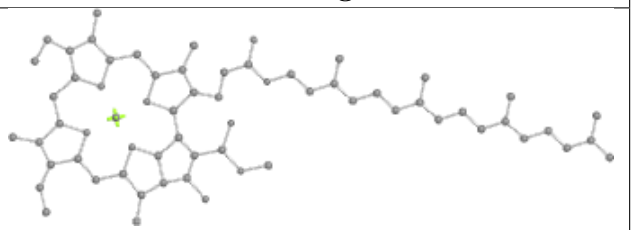
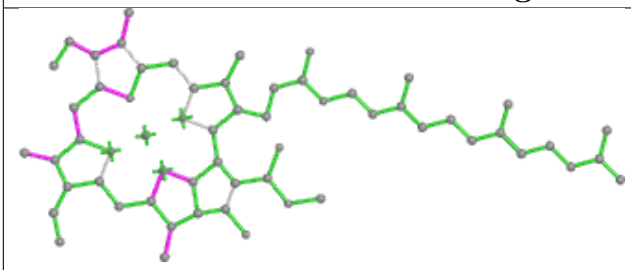


Rings

Ligand CLA H 1230



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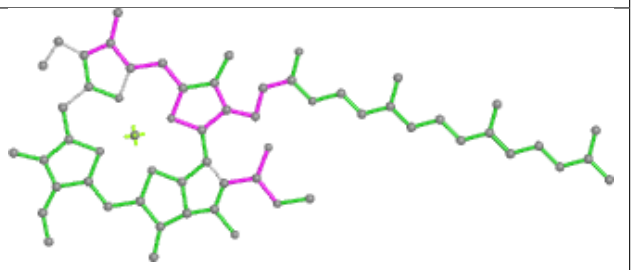
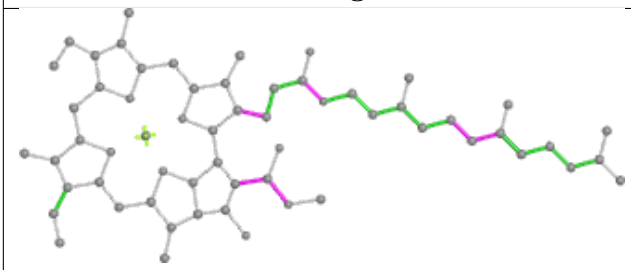


Bond angles



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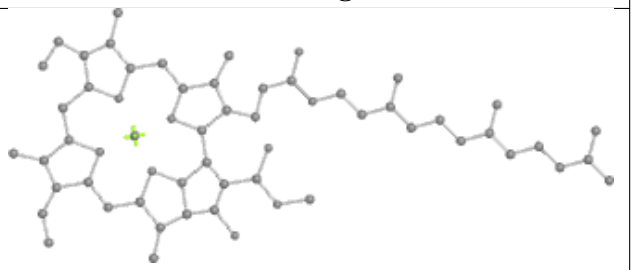
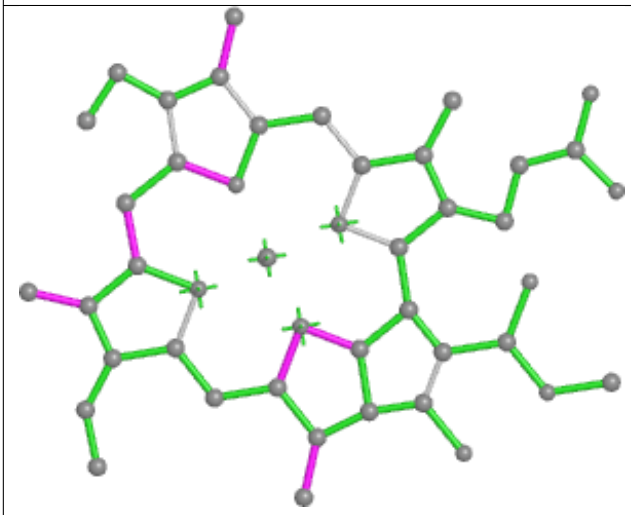


Rings

Ligand CLA 6 508



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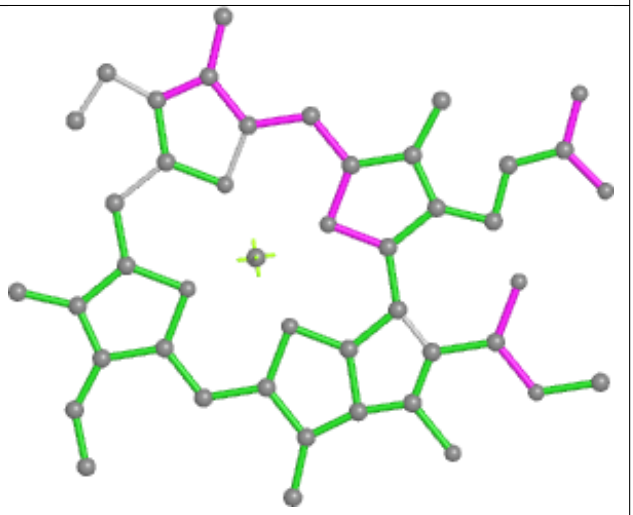
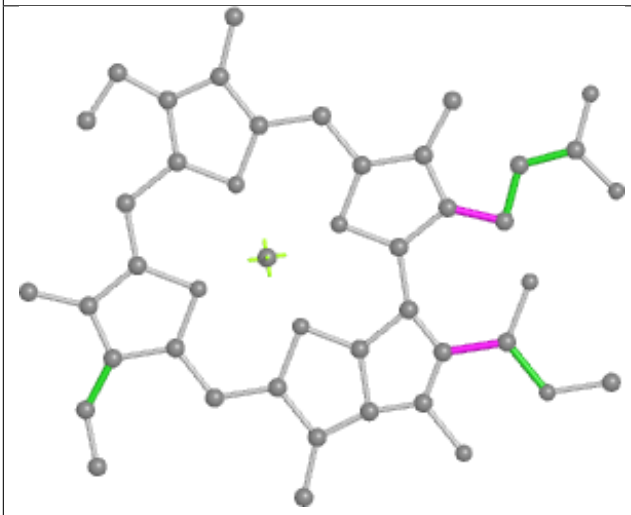
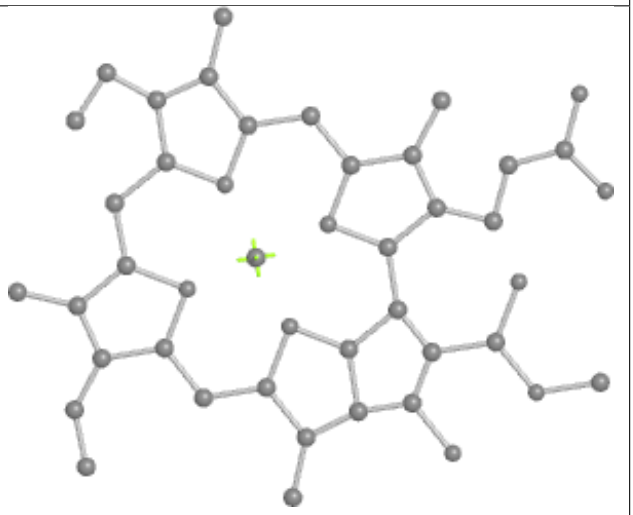


Bond angles

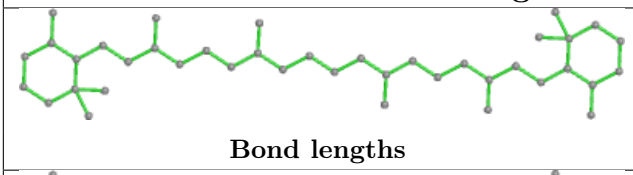


Torsions

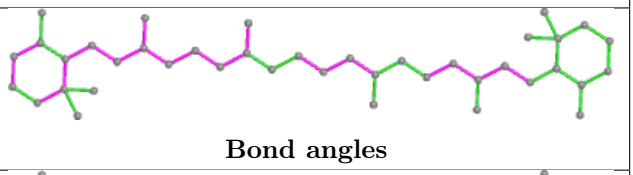


Rings

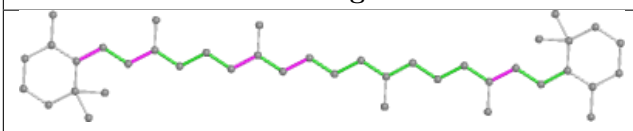
Ligand BCR G 4001



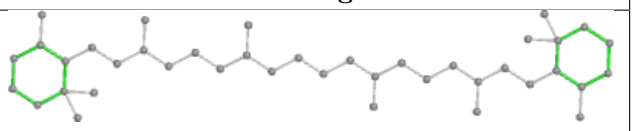
Bond lengths



Bond angles

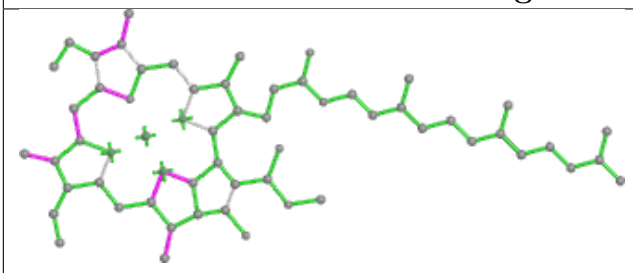


Torsions

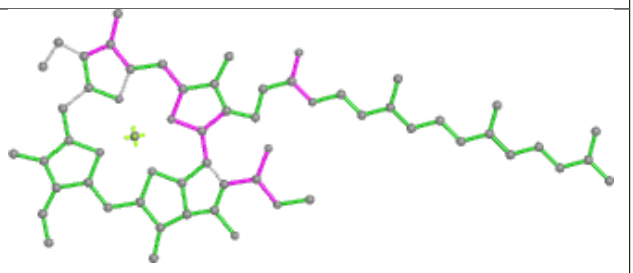


Rings

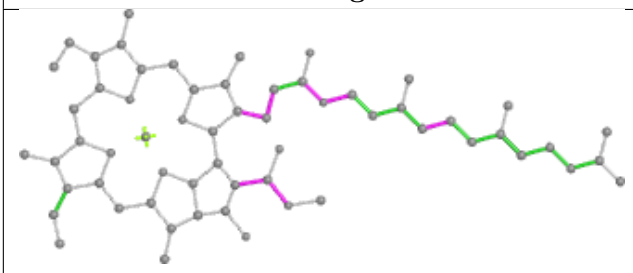
Ligand CLA A 1118



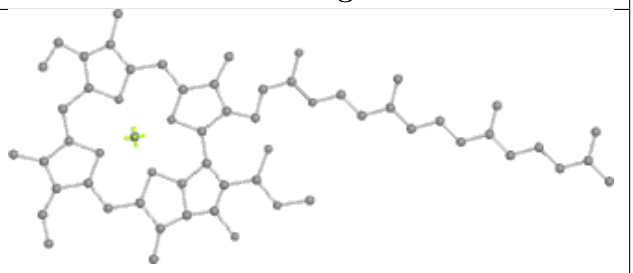
Bond lengths



Bond angles

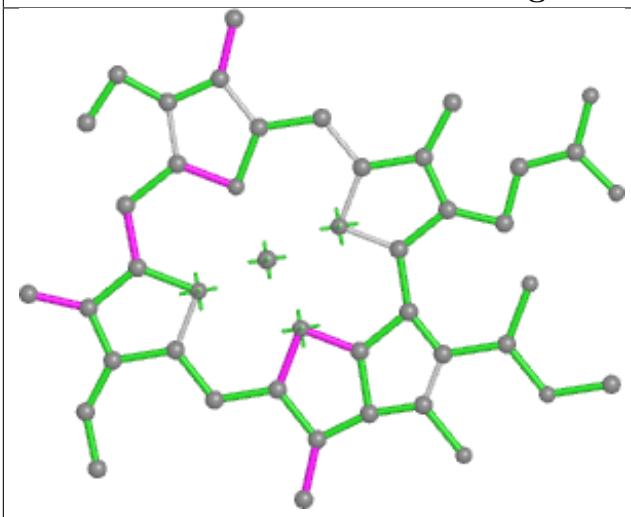


Torsions



Rings

Ligand CLA 5 508



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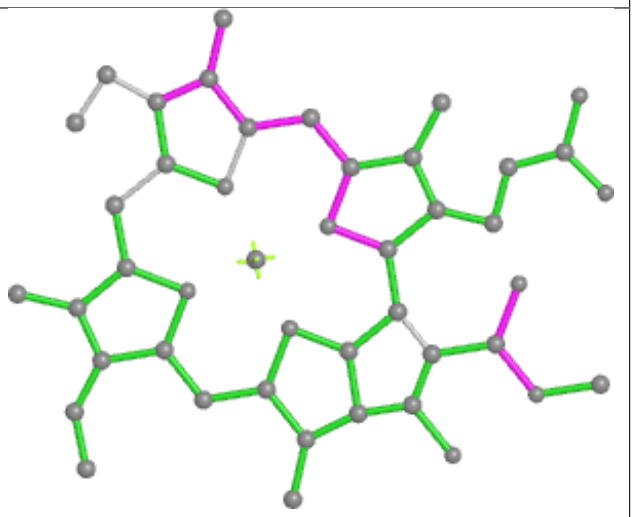
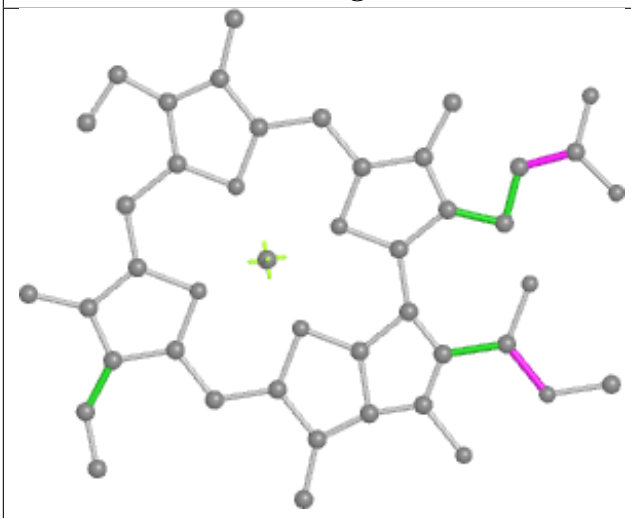


Bond angles



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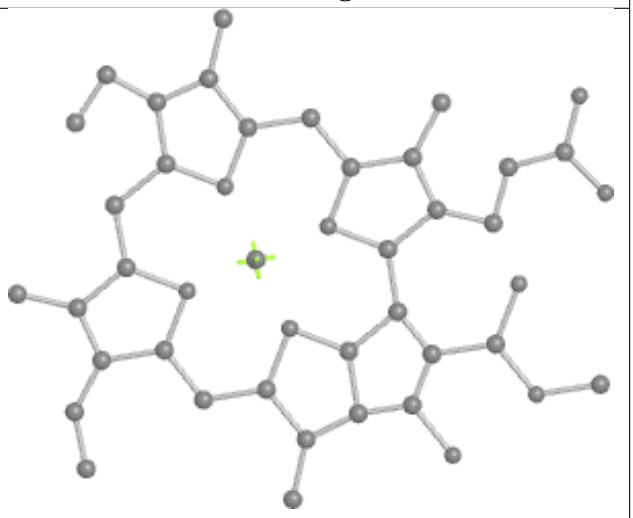
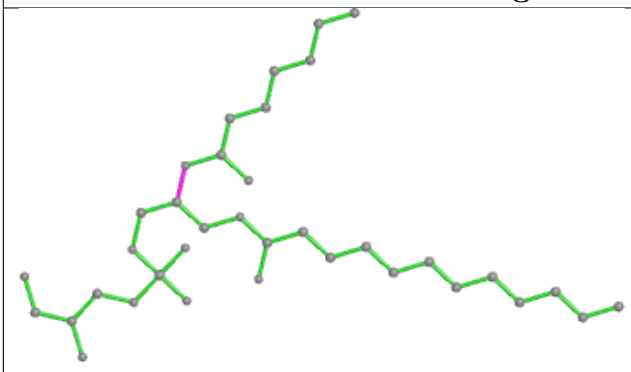


Rings

Ligand LHG G 5004



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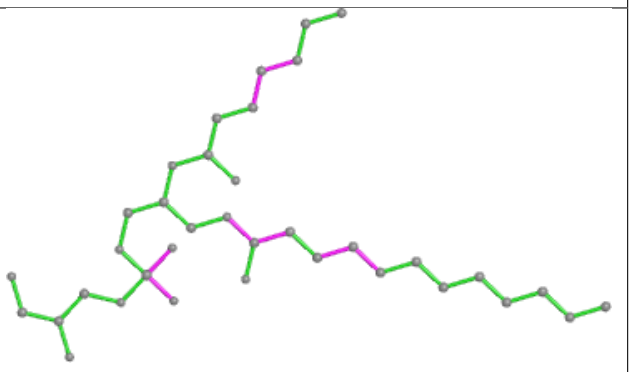

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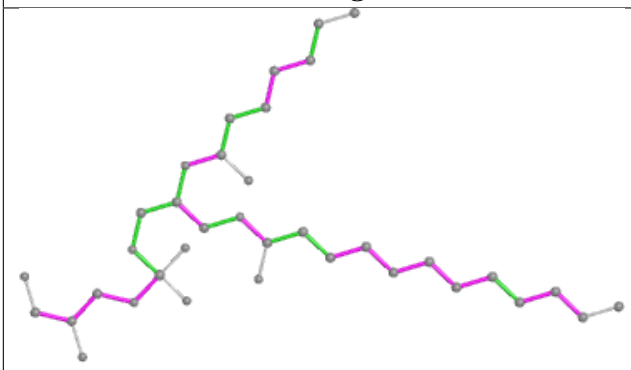
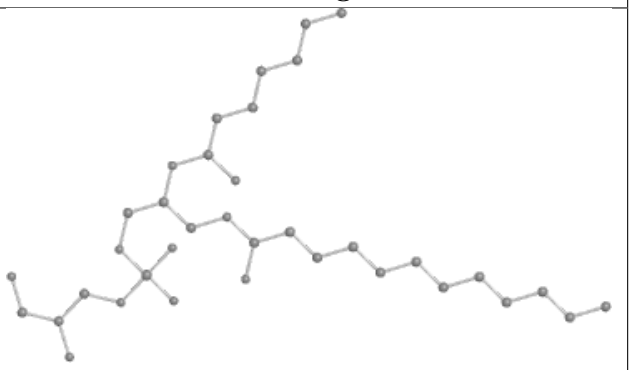
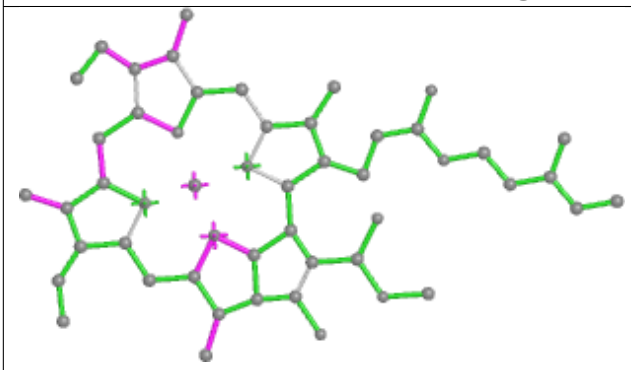


Torsions



Rings

Ligand CLA A 1129



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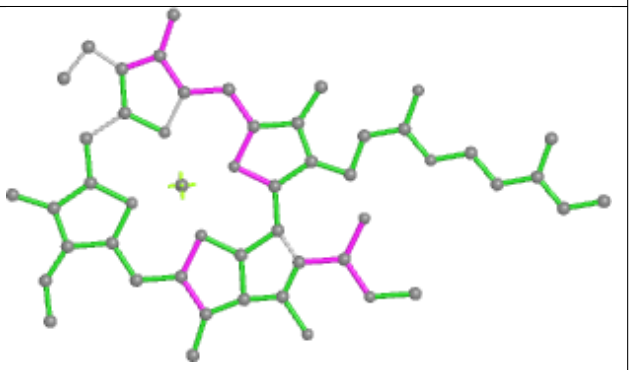
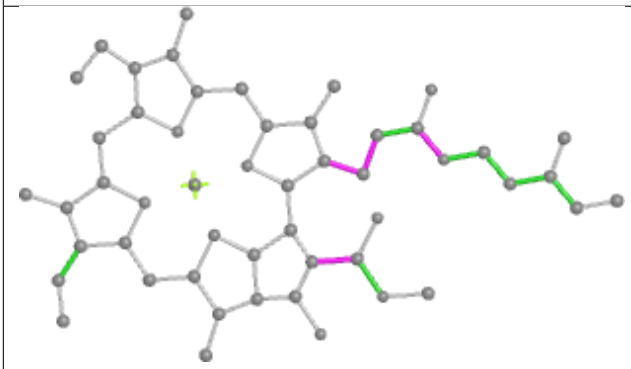


Bond angles



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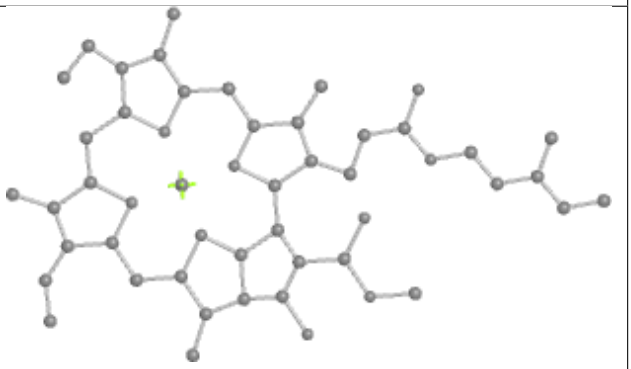
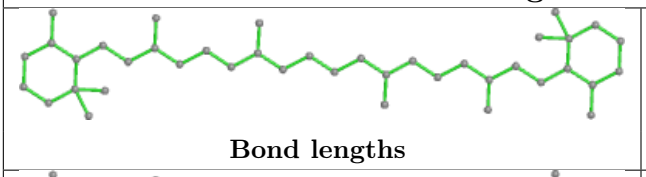


Rings

Ligand BCR 4 524



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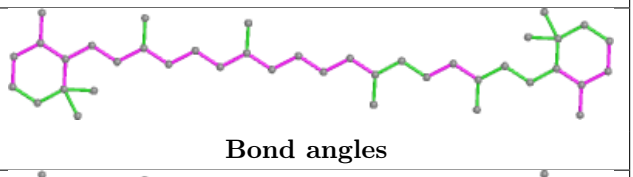

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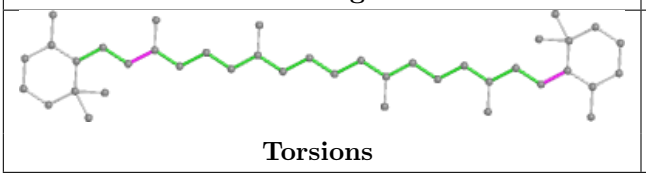

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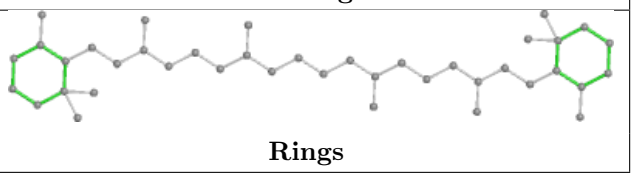
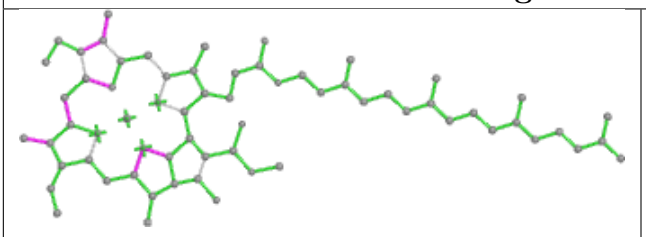


Rings

Ligand CLA A 1137



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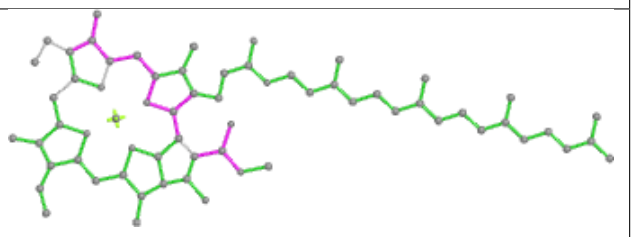

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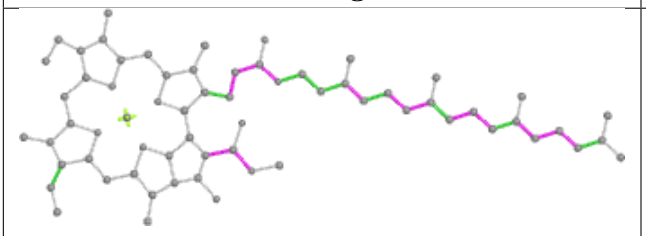

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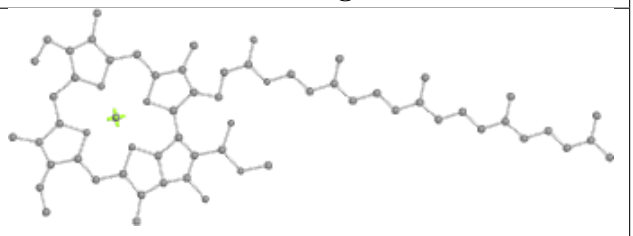
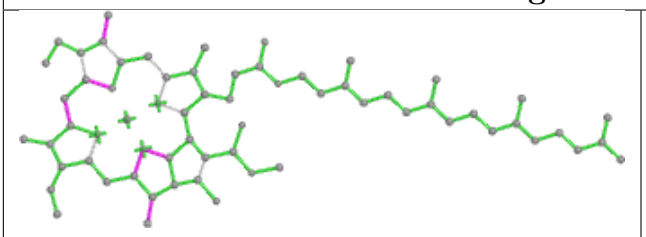


Rings

Ligand CLA 3 503



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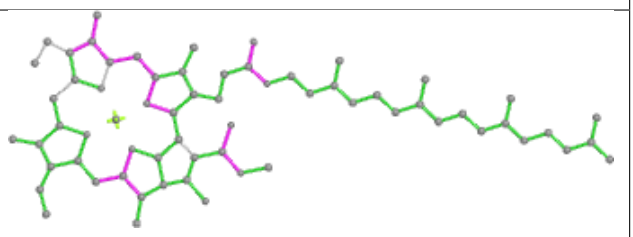

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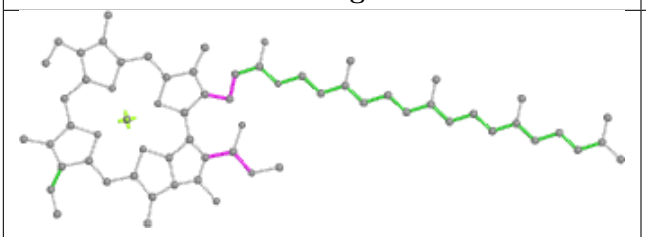

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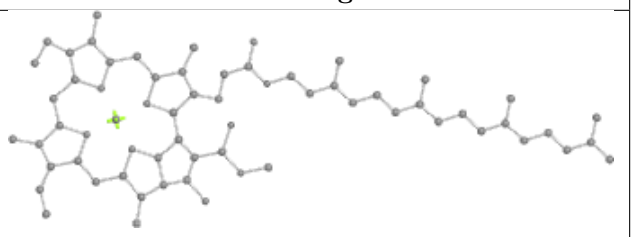
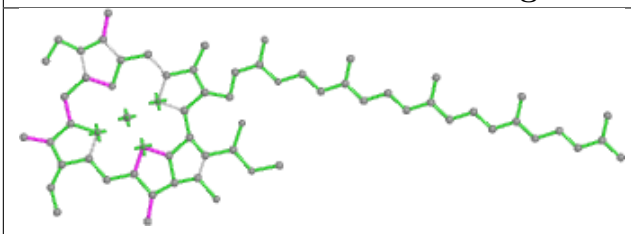


Rings

Ligand CLA e 1130



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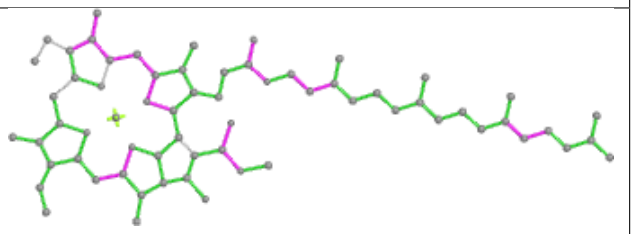
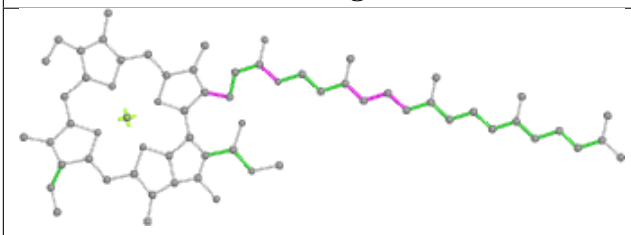


Bond angles



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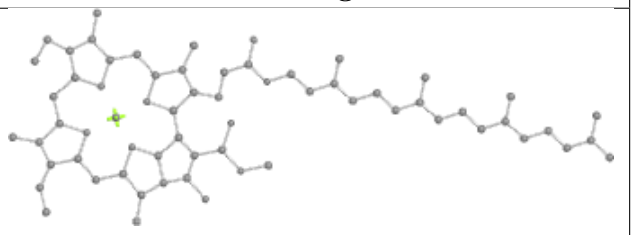
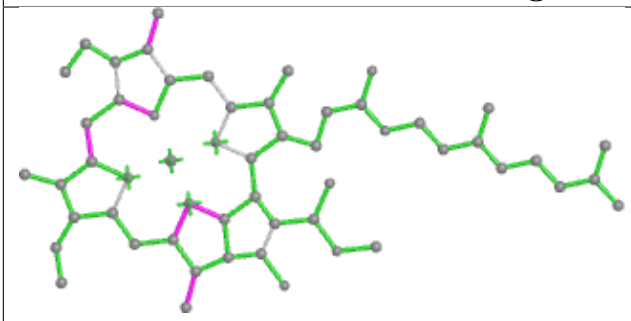


Rings

Ligand CLA q 511



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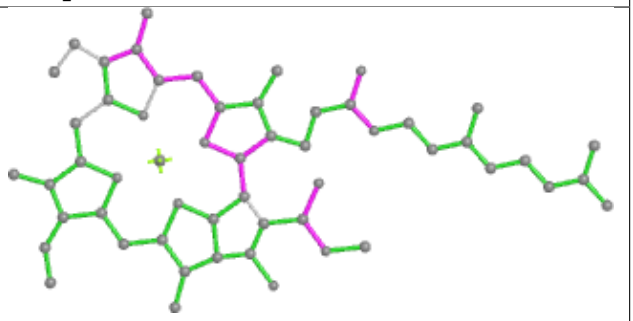
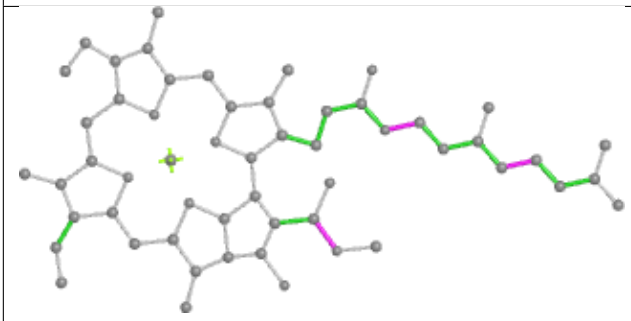


Bond angles



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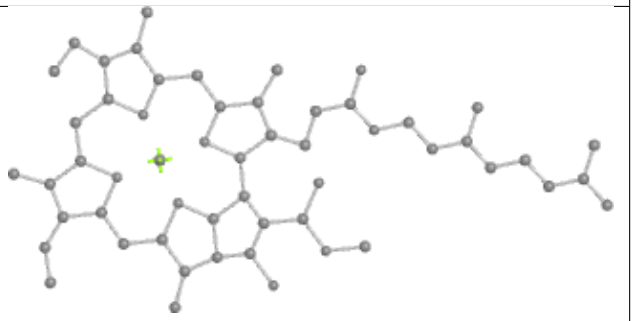
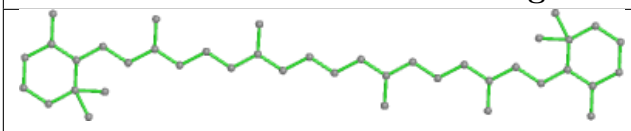


Rings

Ligand BCR r 524



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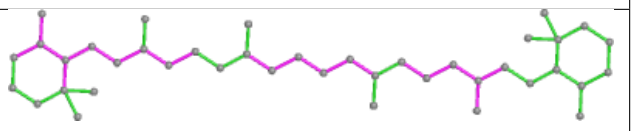
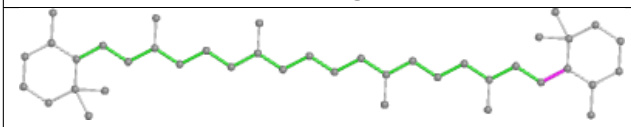


Bond angles



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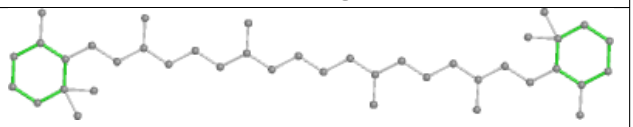
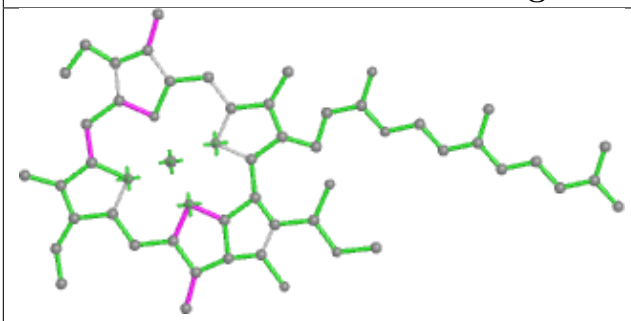


Rings

Ligand CLA 2 511



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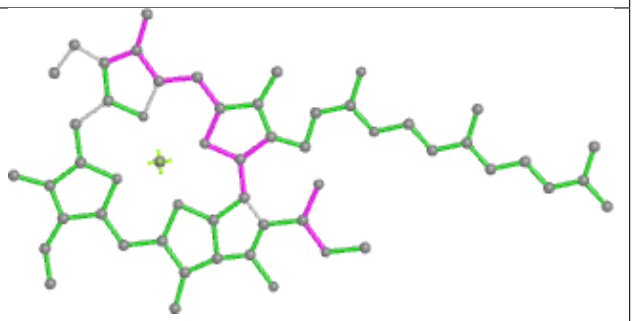
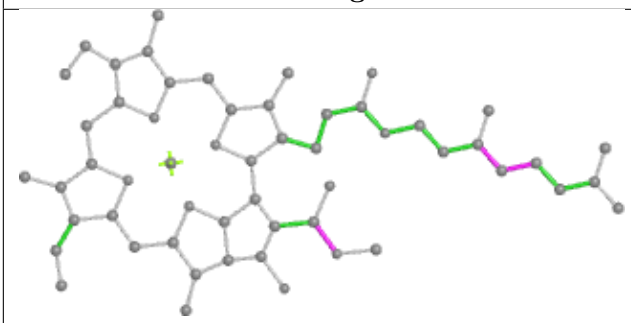


Bond angles



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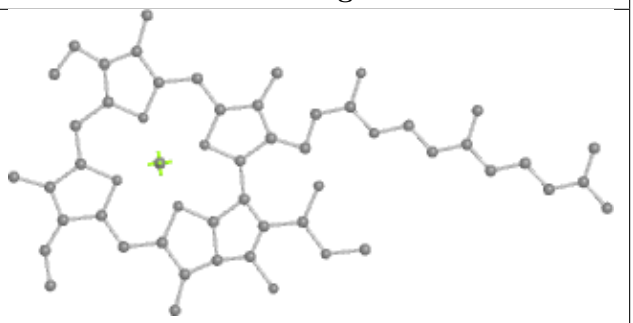
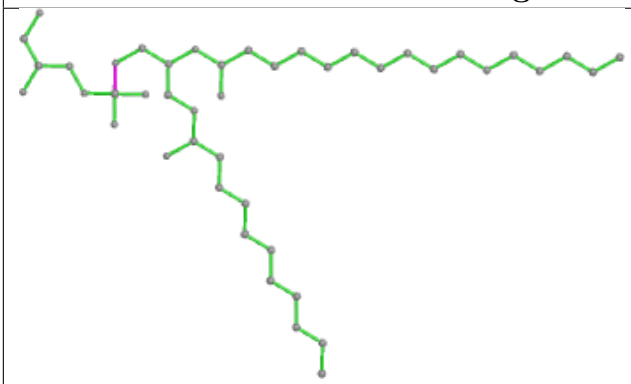


Rings

Ligand LHG H 1855



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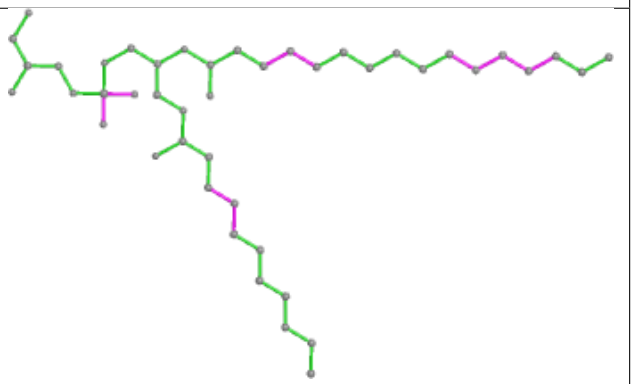
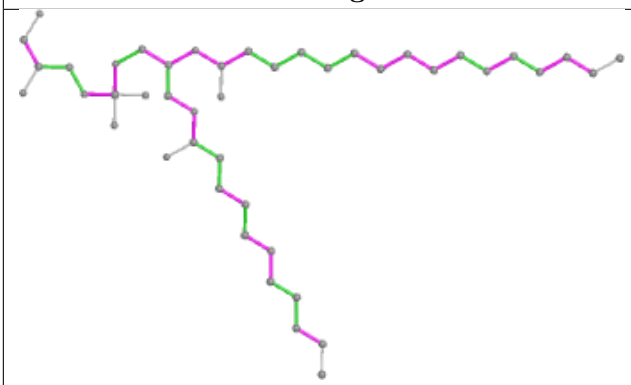
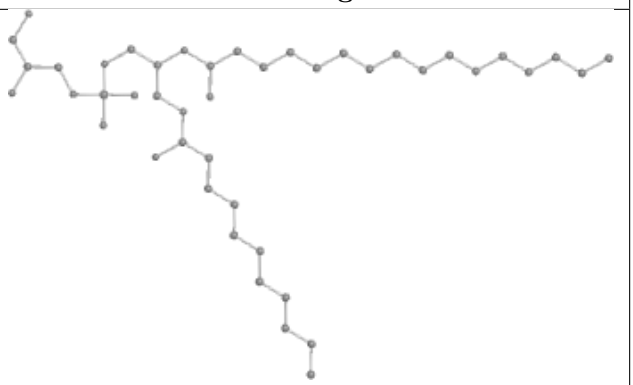


Bond angles

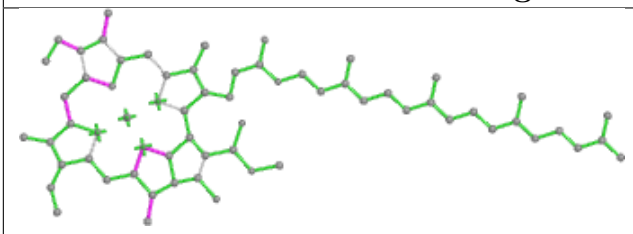


Torsions



Rings

Ligand CLA G 1133



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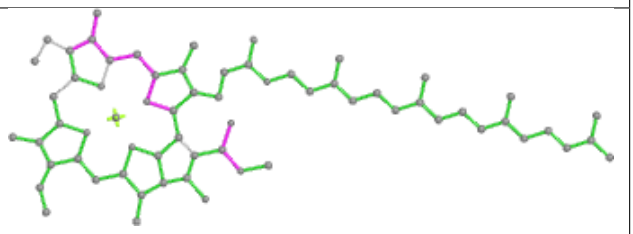
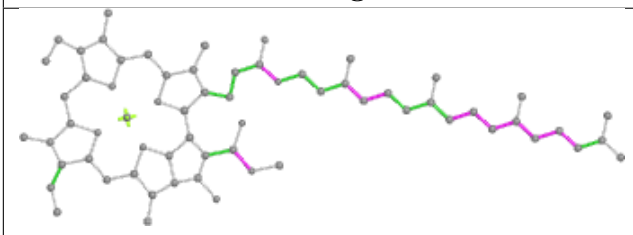
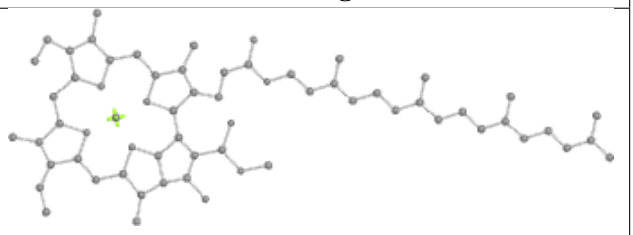


Bond angles

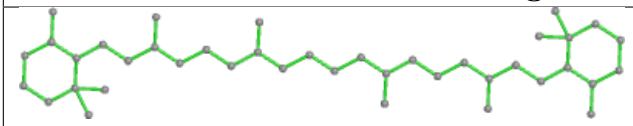


Torsions



Rings

Ligand BCR u 521



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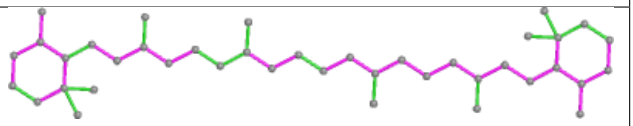
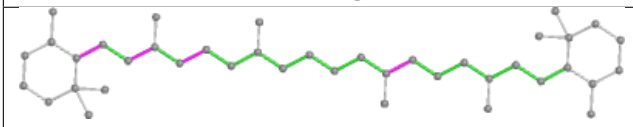


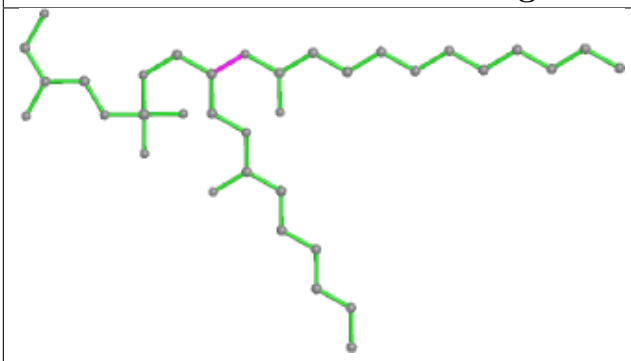
Bond angles



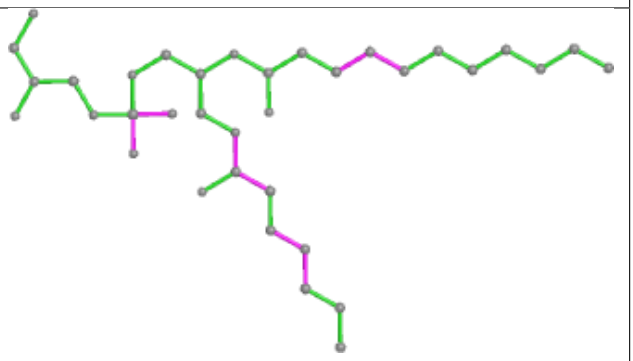
Torsions

Rings

Ligand LHG e 5008



Bond lengths



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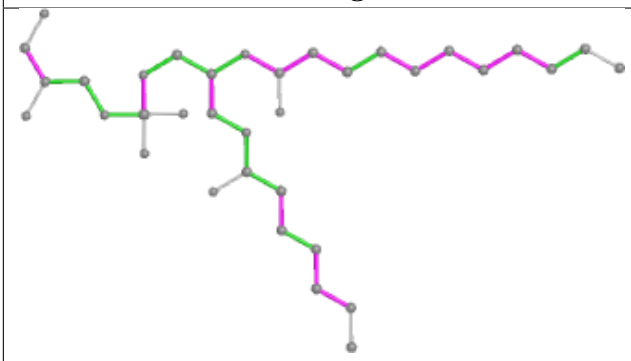
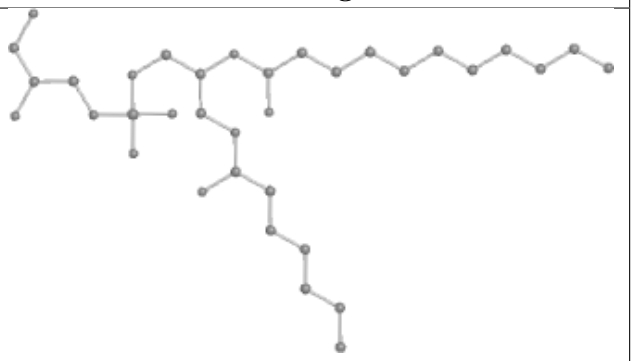
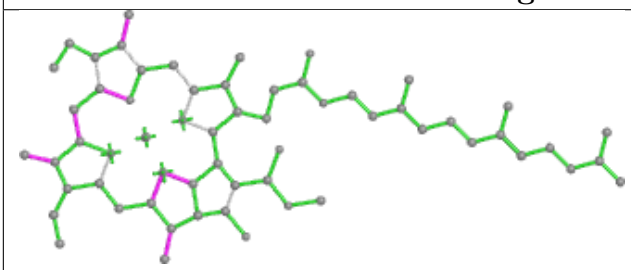


Torsions



Rings

Ligand CLA L 1503



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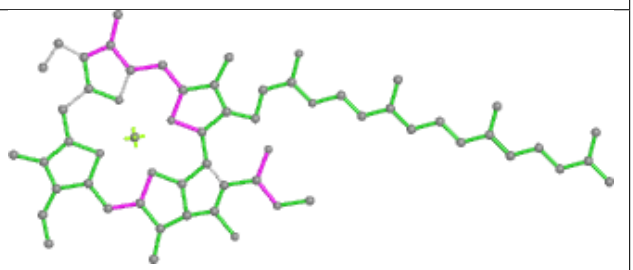

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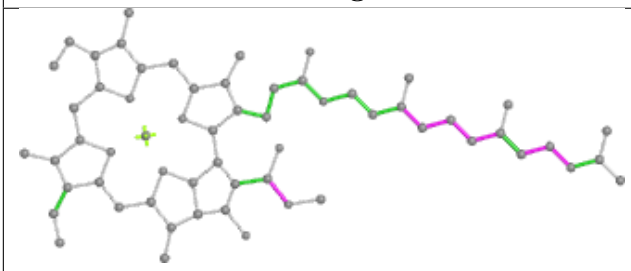

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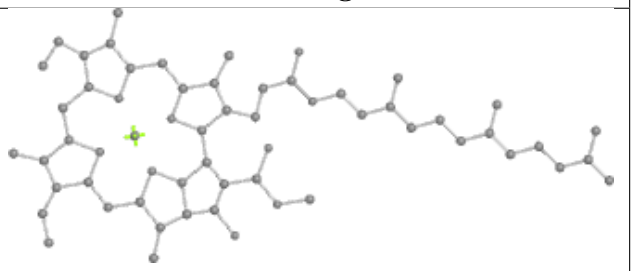
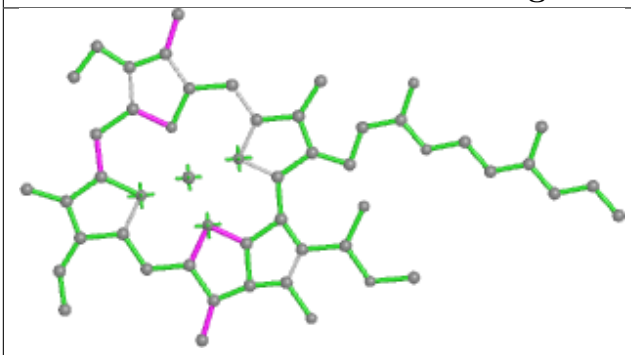


Rings

Ligand CLA 6 503



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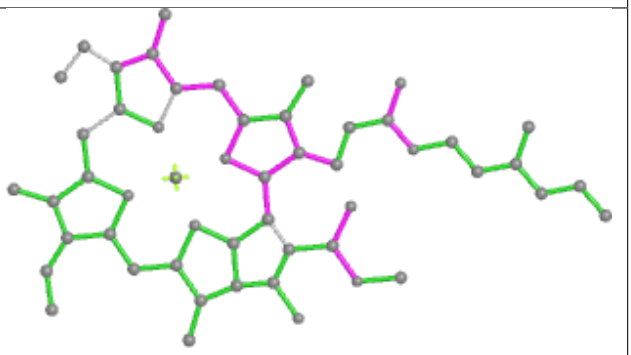

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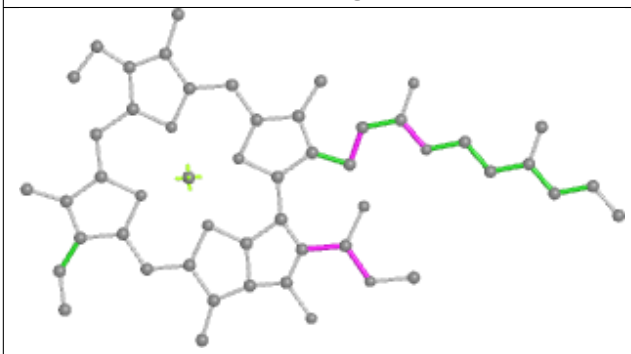

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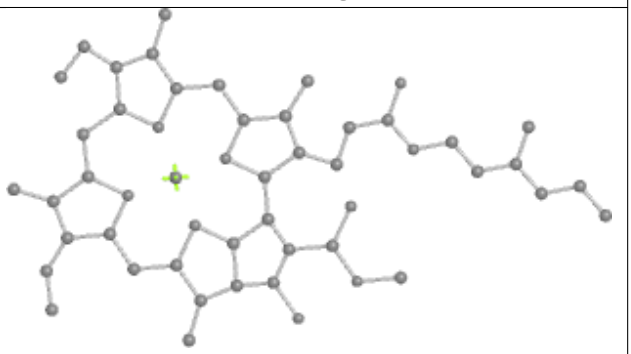
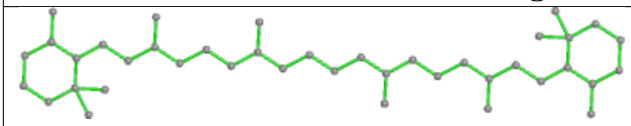


Rings

Ligand BCR s 523



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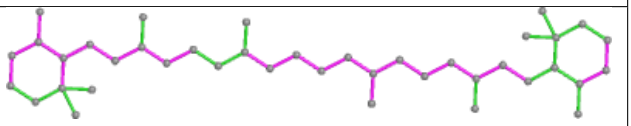
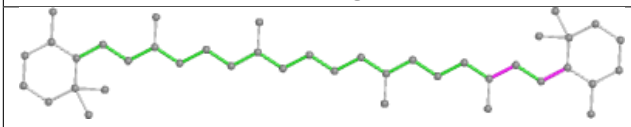


Bond angles



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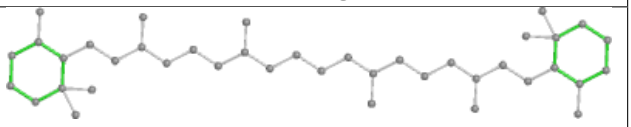
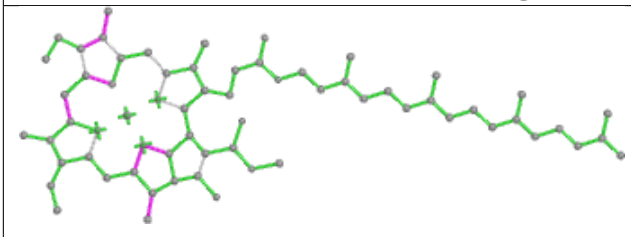


Rings

Ligand CLA R 1301



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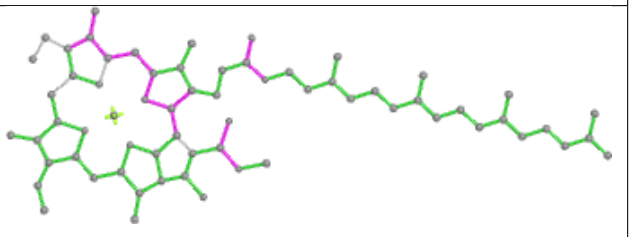
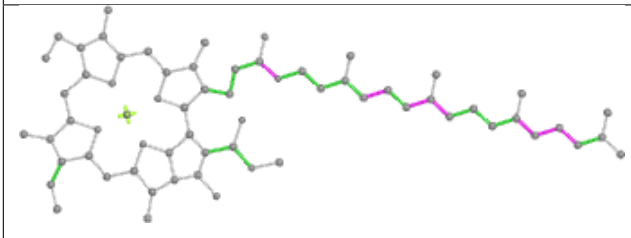


Bond angles



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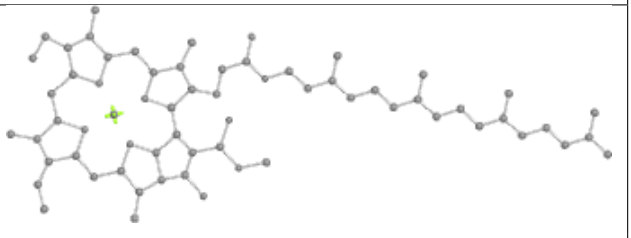
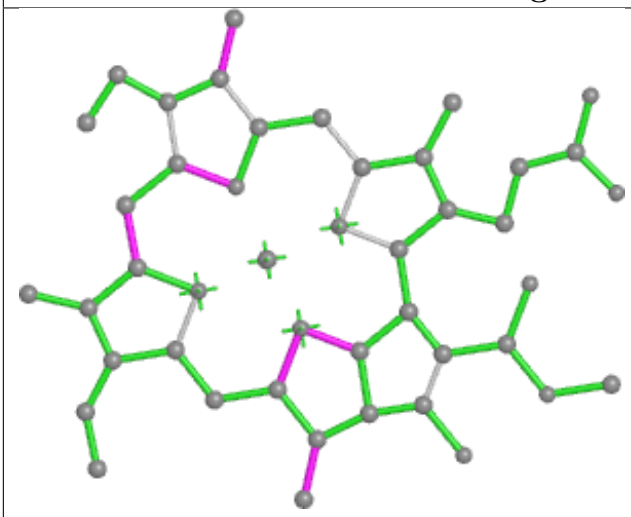


Rings

Ligand CLA t 504



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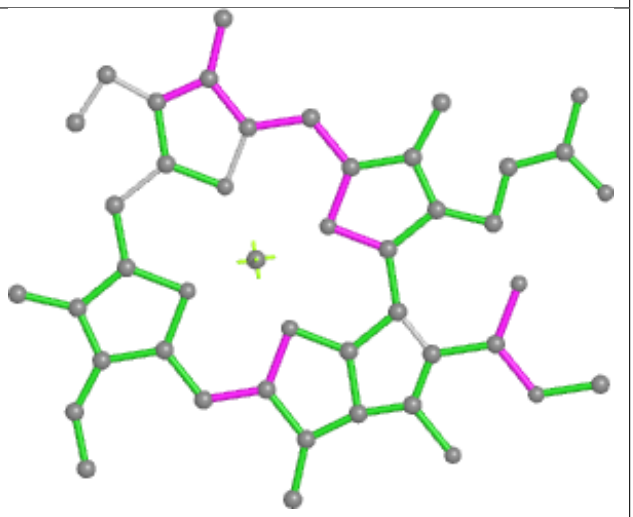

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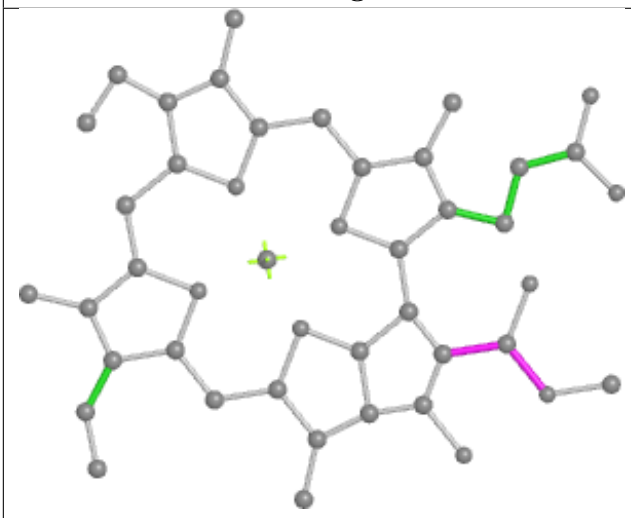

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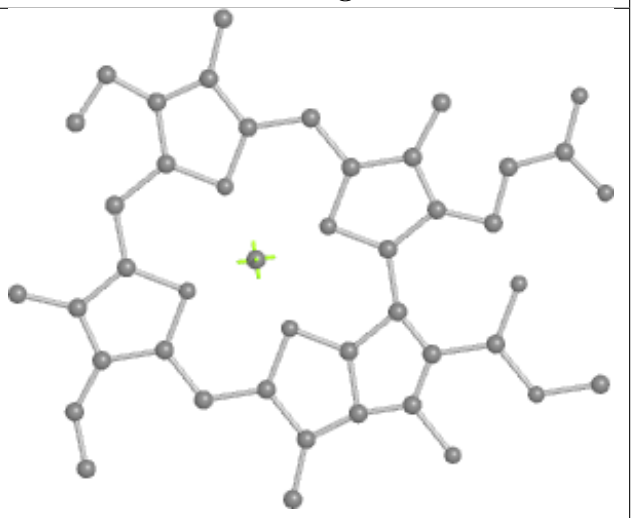
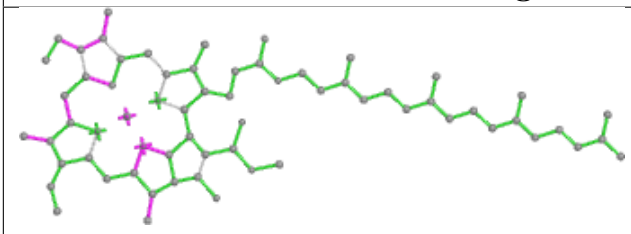


Rings

Ligand CLA A 1132



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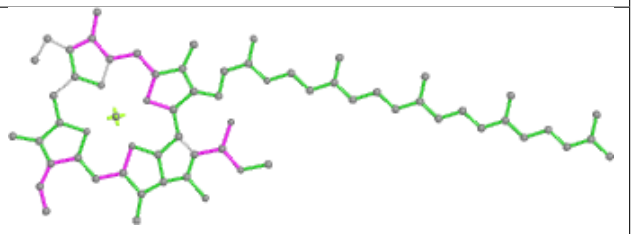

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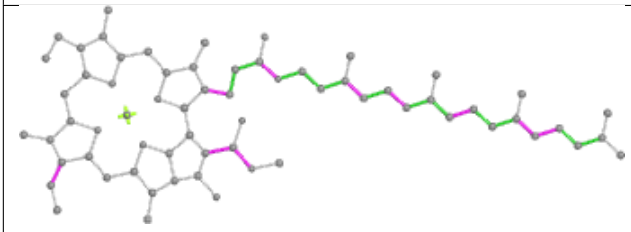

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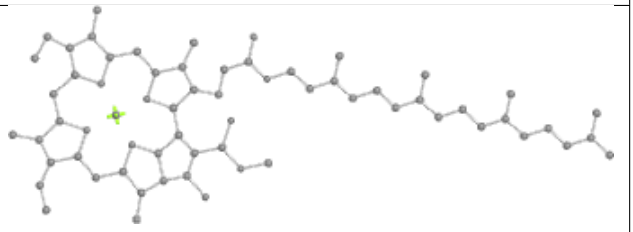
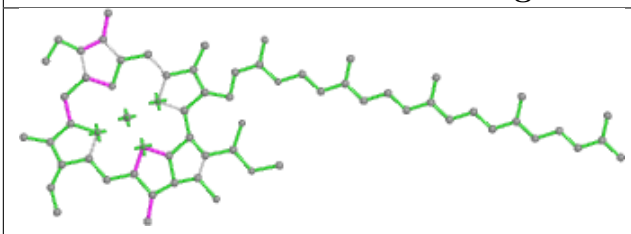


Rings

Ligand CLA H 1219



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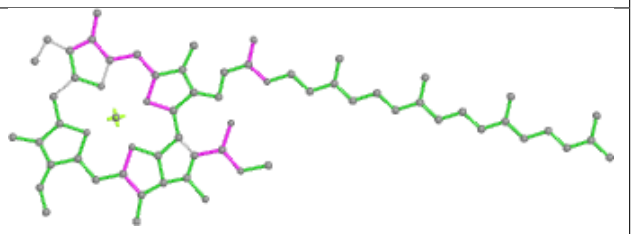

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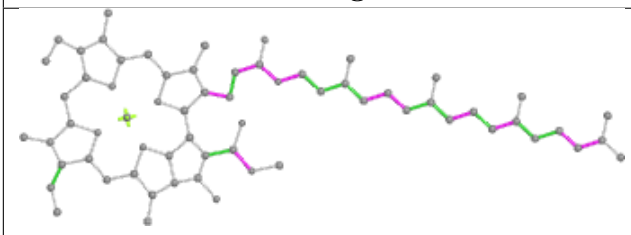

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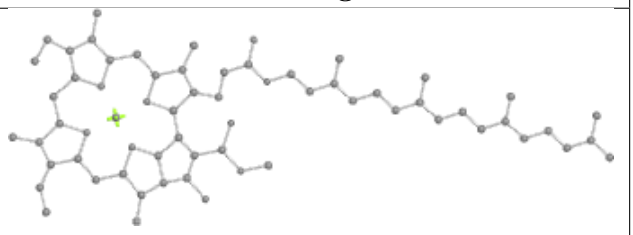
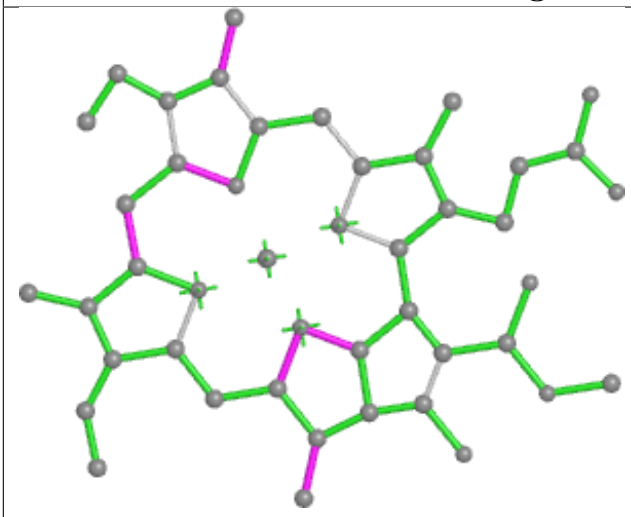


Rings

Ligand CLA 4 506



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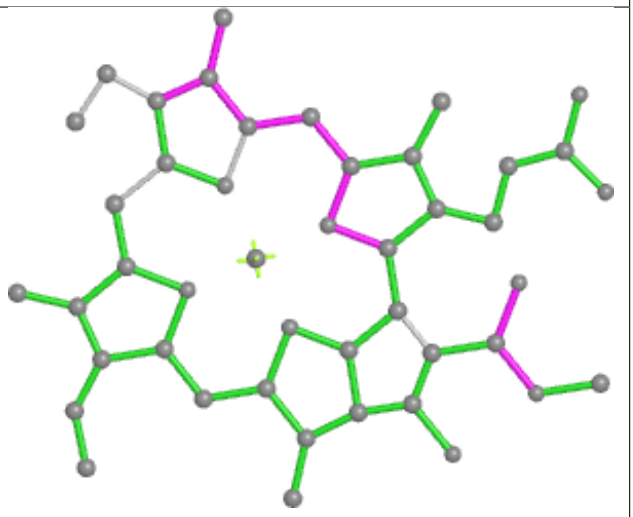

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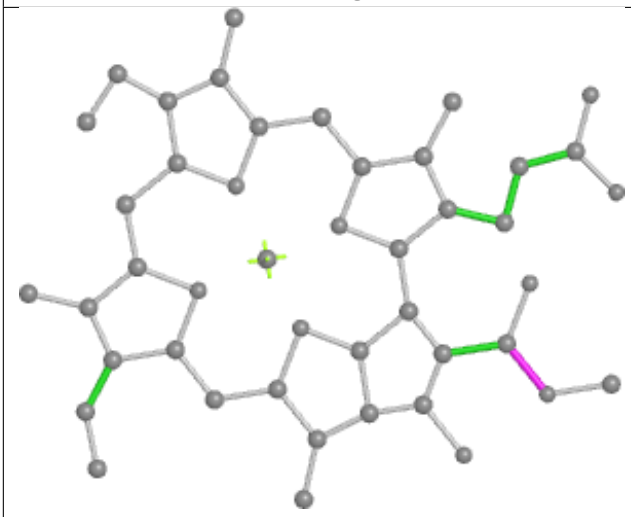

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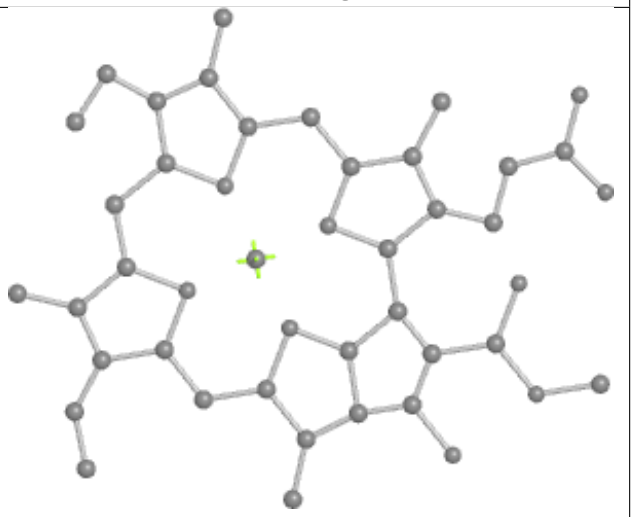
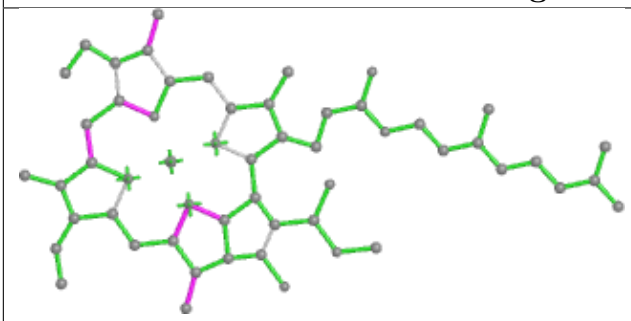


Rings

Ligand CLA c 518



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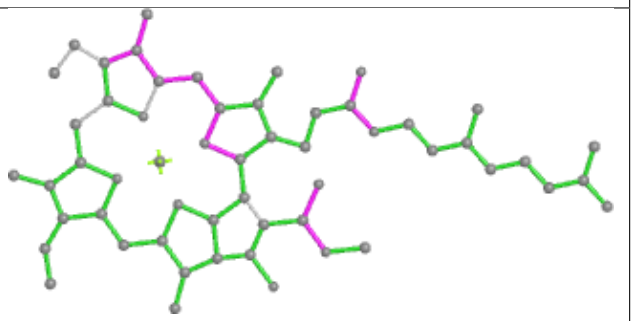

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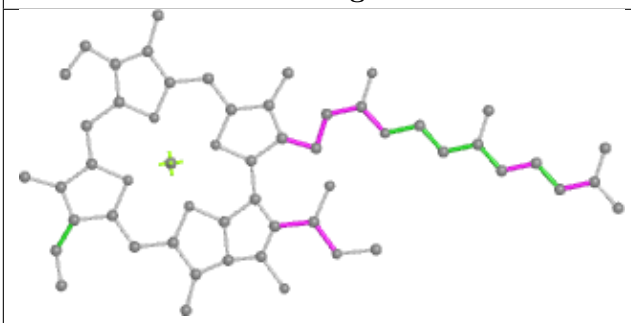

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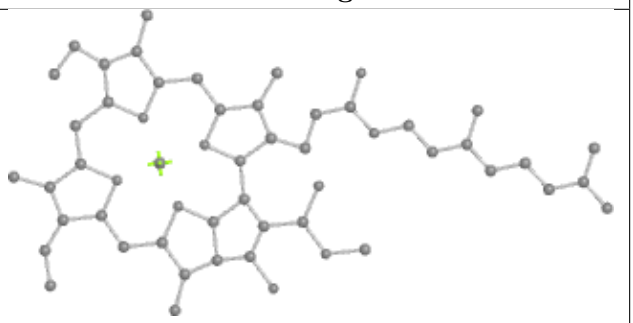
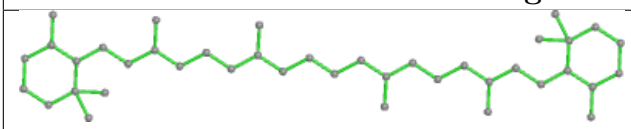


Rings

Ligand BCR Z 522



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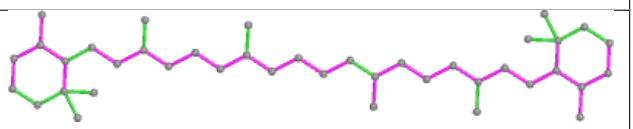

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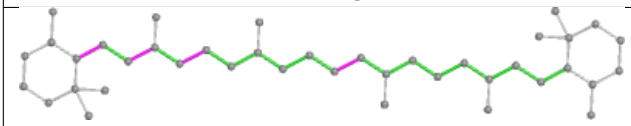
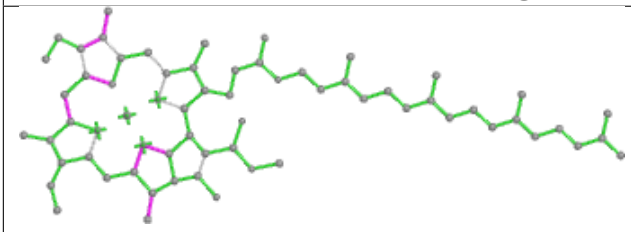


Torsions

Rings

Ligand CLA B 1208



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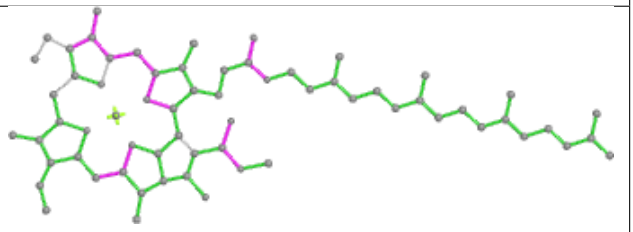

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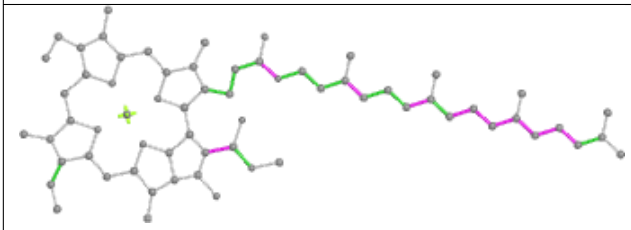

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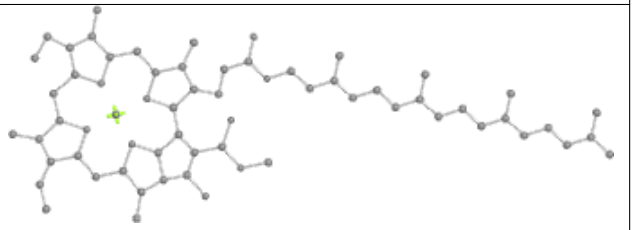
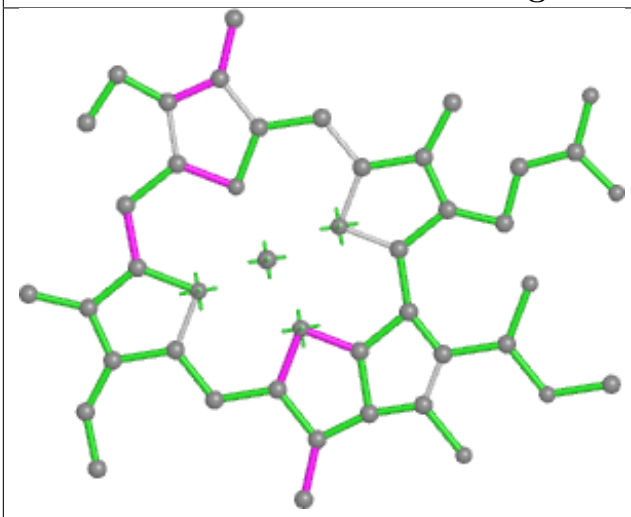


Rings

Ligand CLA 5 512



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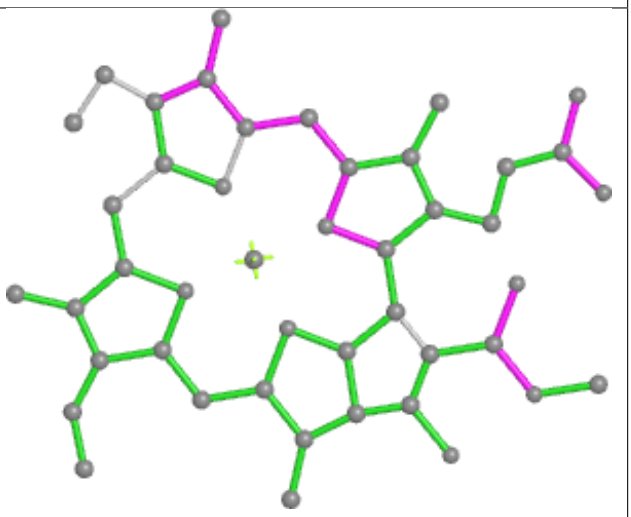
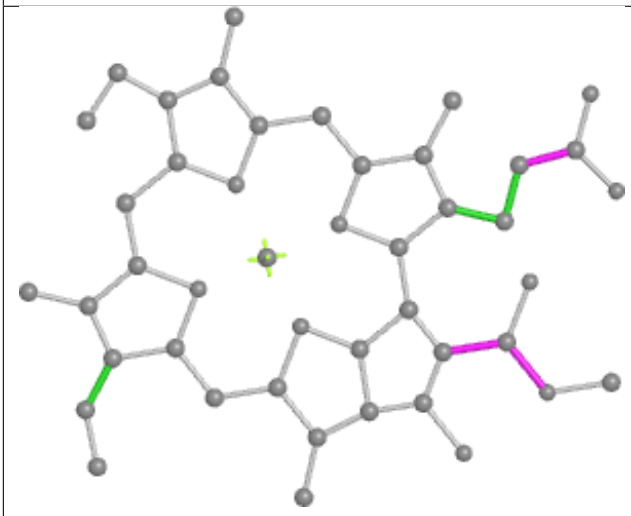


Bond angles



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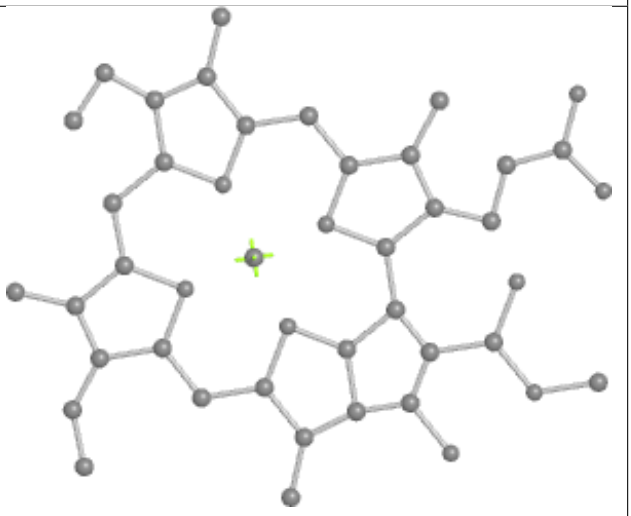
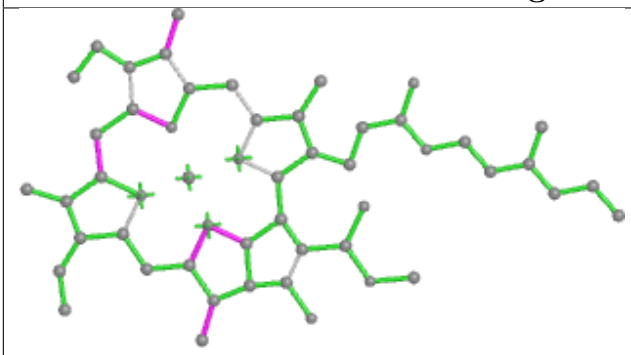
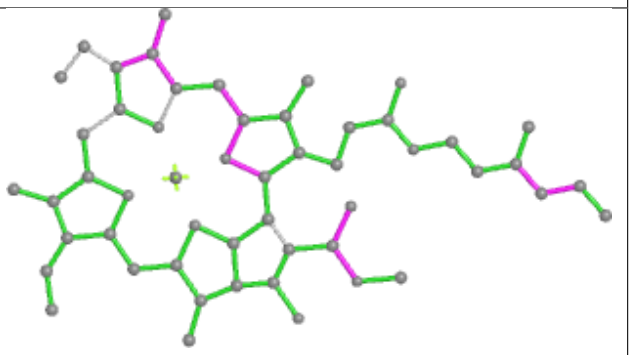
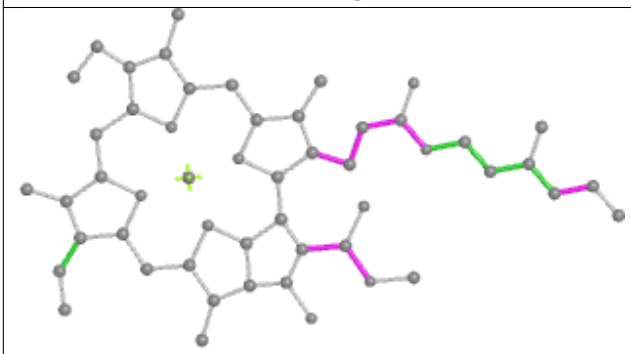
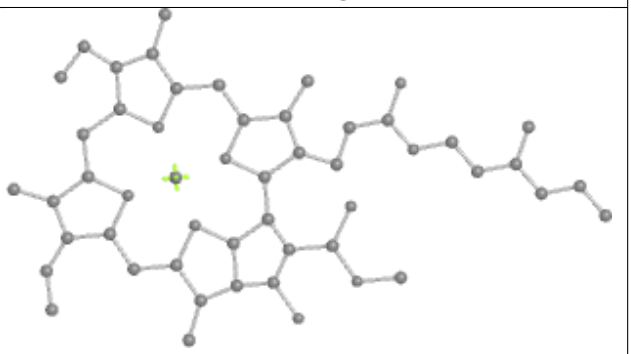
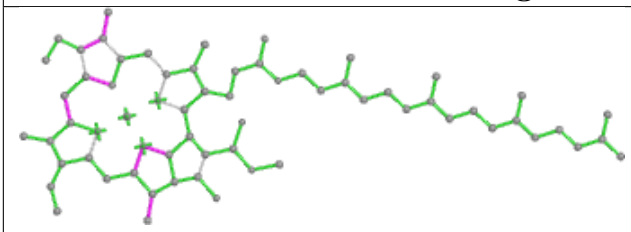
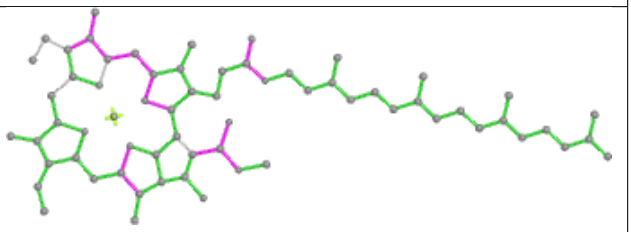
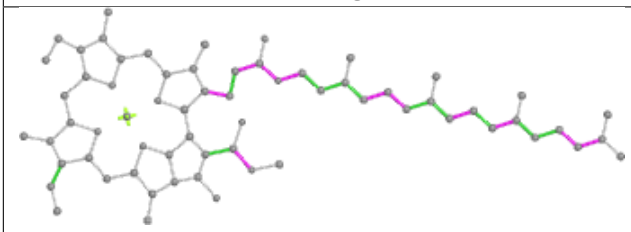
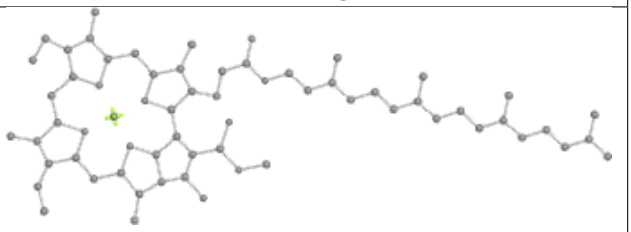
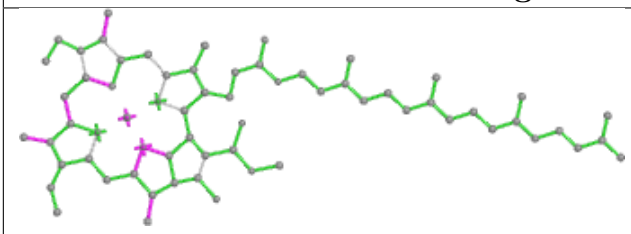


Rings

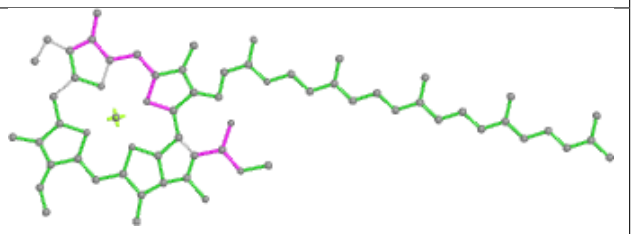
Ligand CLA 1 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1219	
	
Bond lengths	Bond angles
	
Torsions	Rings

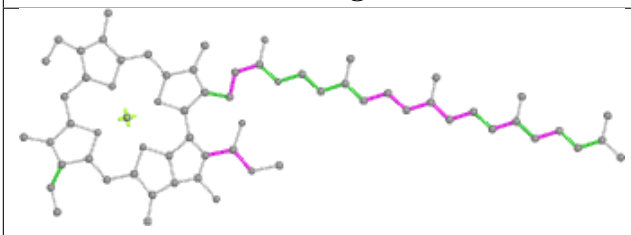
Ligand CLA H 1203



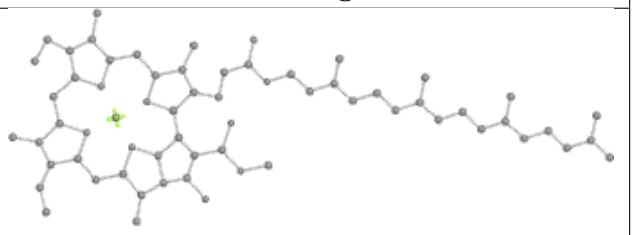
Bond lengths



Bond angles

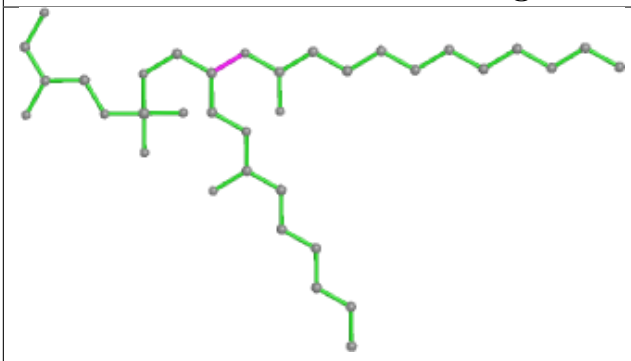


Torsions

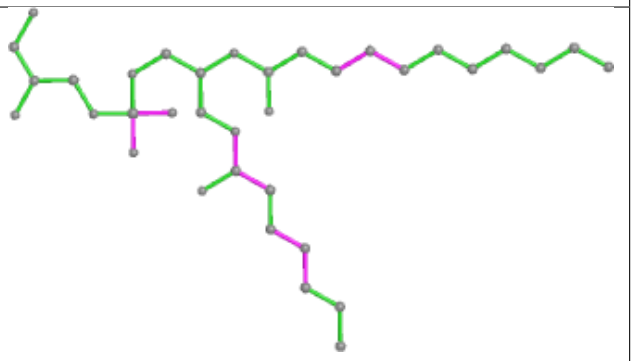


Rings

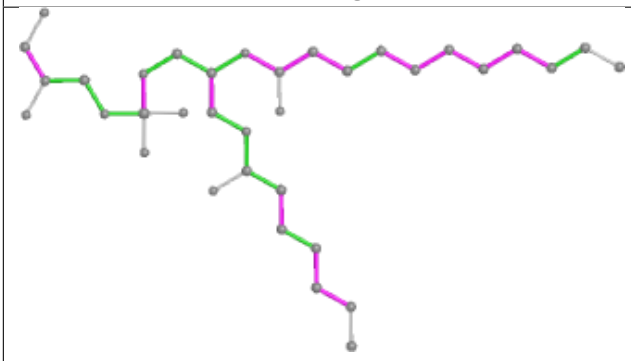
Ligand LHG G 5008



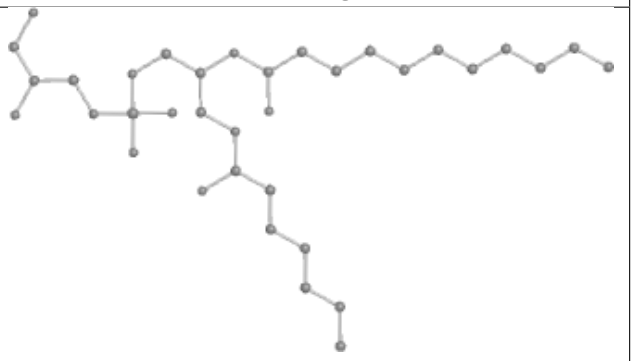
Bond lengths



Bond angles

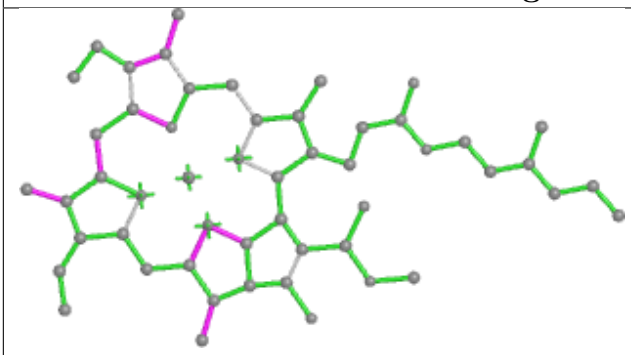


Torsions



Rings

Ligand CLA f 1209



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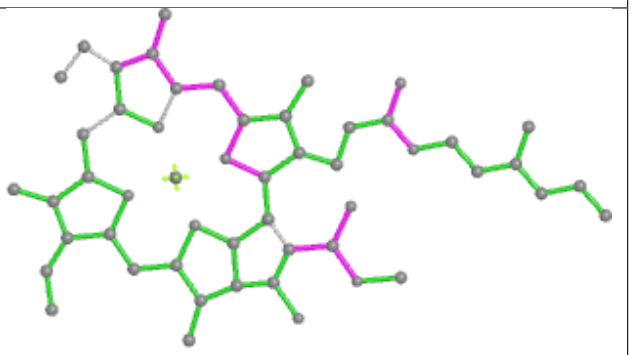
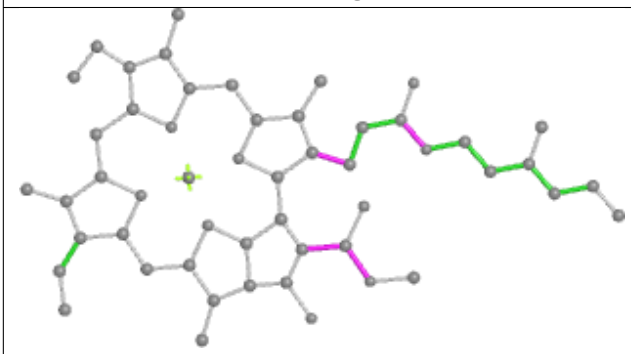
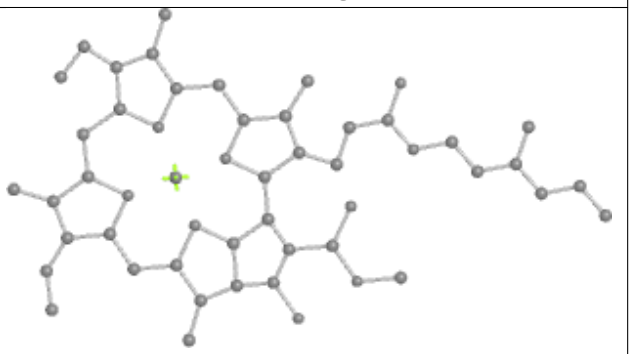


Bond angles

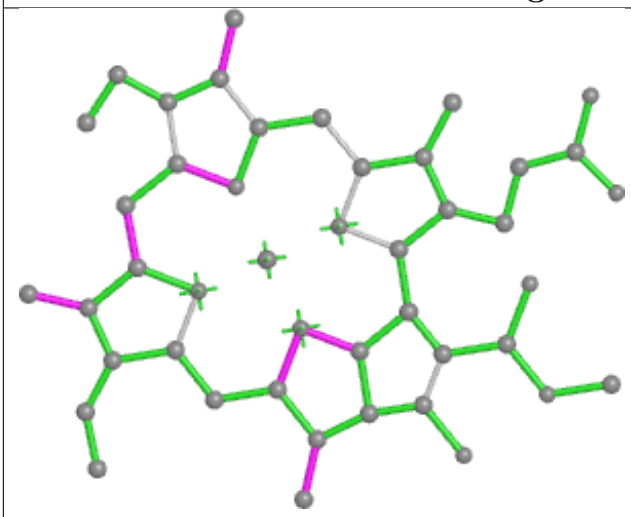


Torsions



Rings

Ligand CLA u 508



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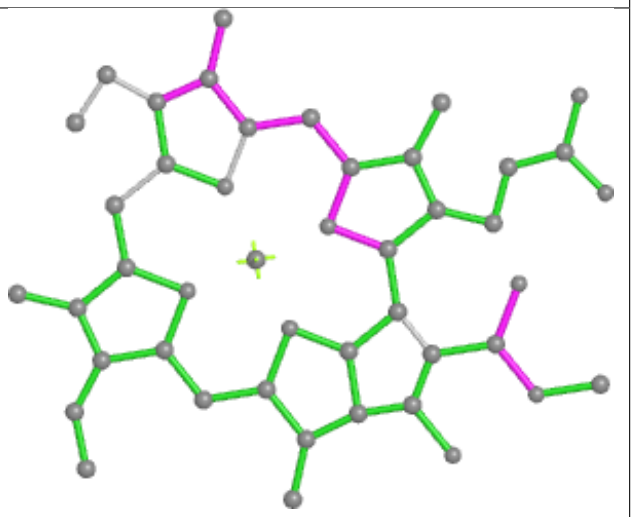
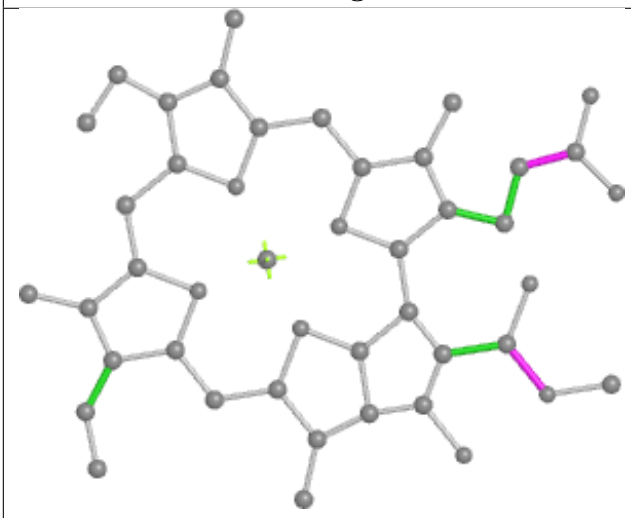


Bond angles



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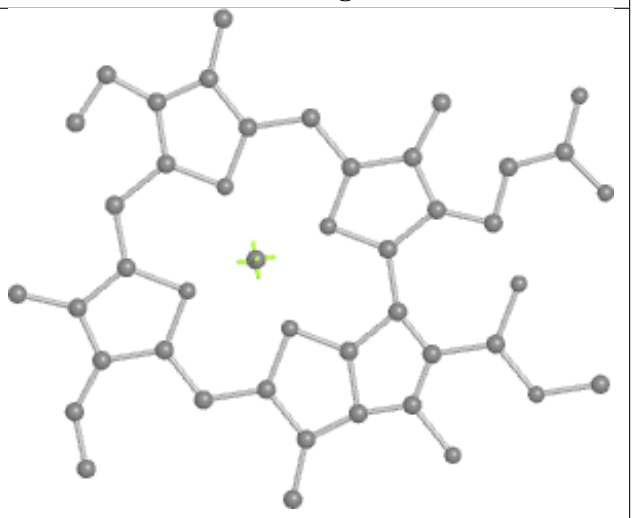
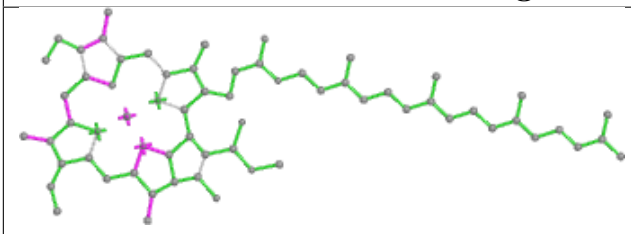


Rings

Ligand CLA B 1205



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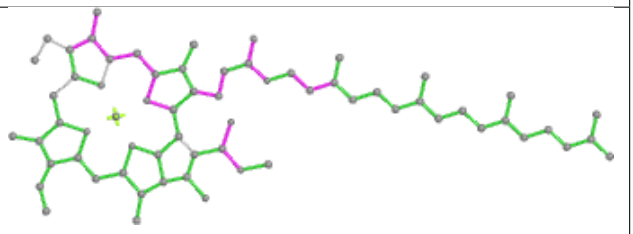
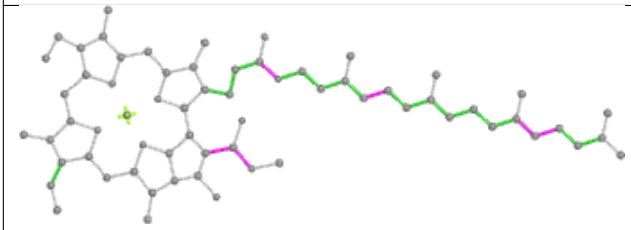


Bond angles



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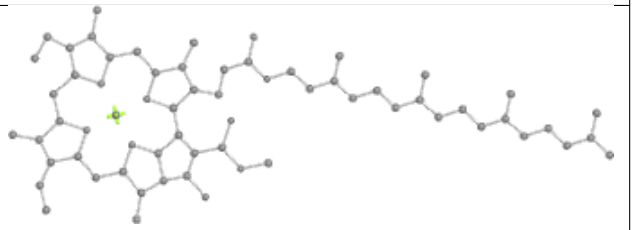
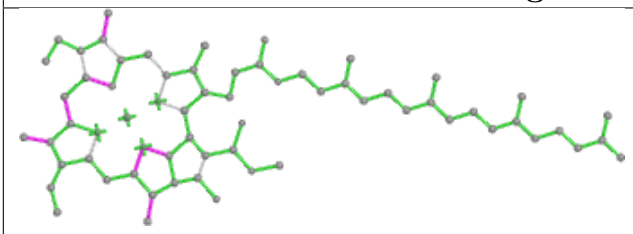


Rings

Ligand CLA Z 509



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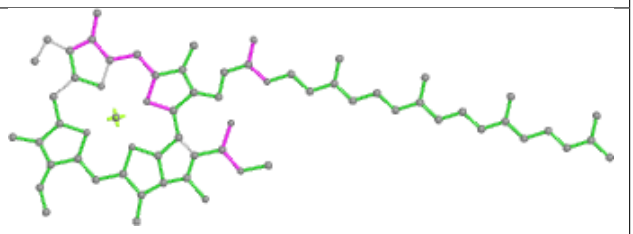
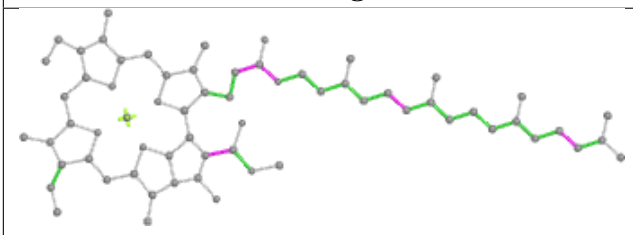


Bond angles



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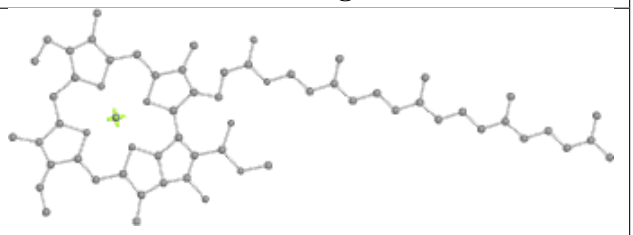
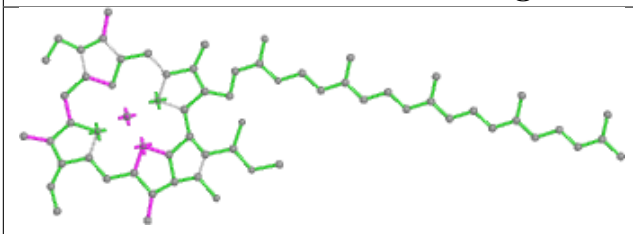


Rings

Ligand CLA H 1021



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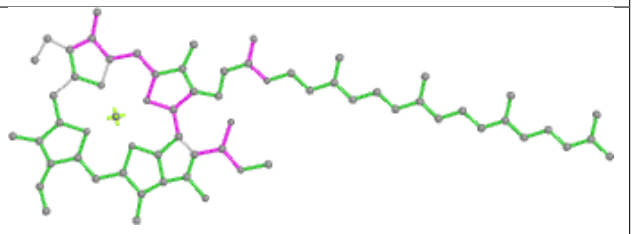
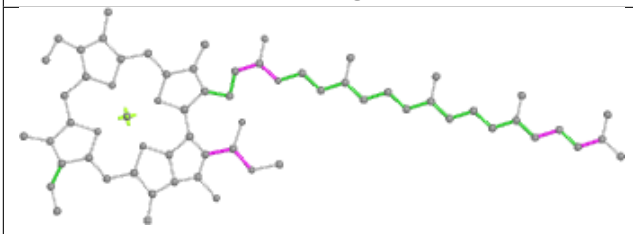


Bond angles



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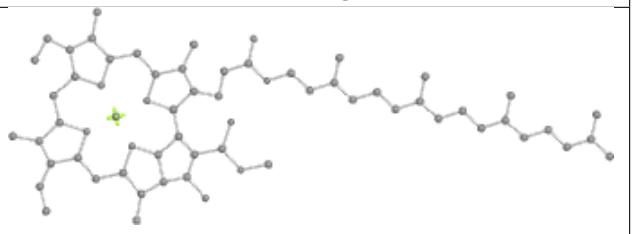
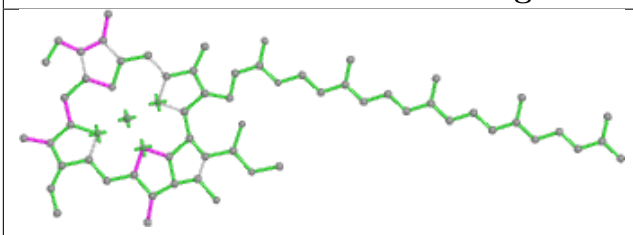


Rings

Ligand CLA H 1214



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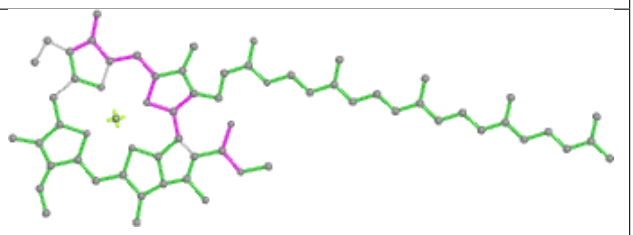
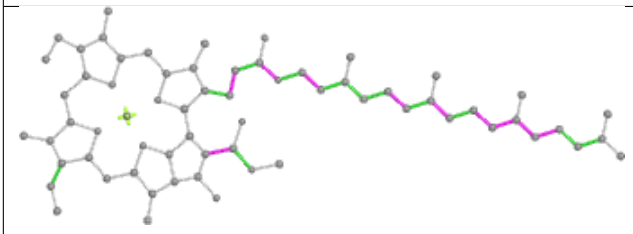


Bond angles



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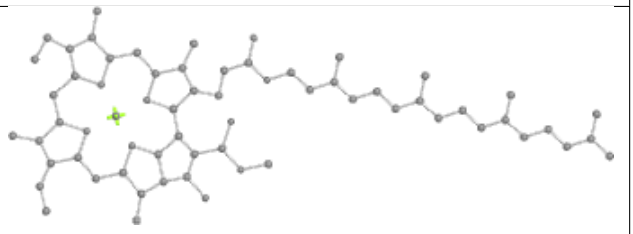
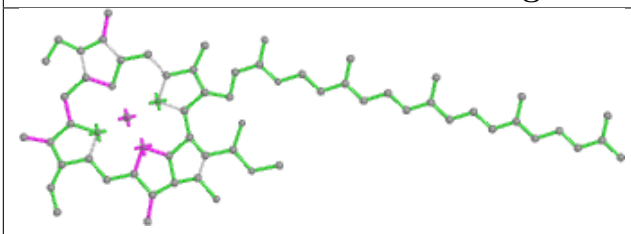


Rings

Ligand CLA f 1021



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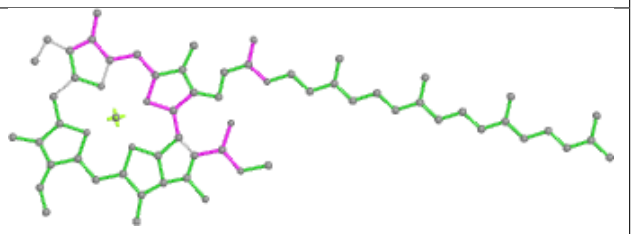

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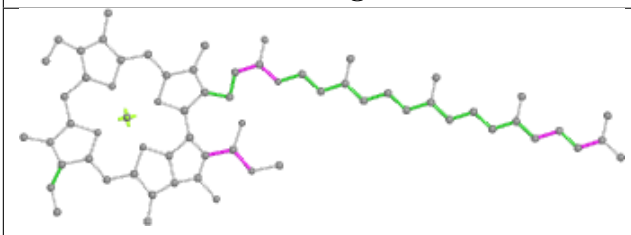

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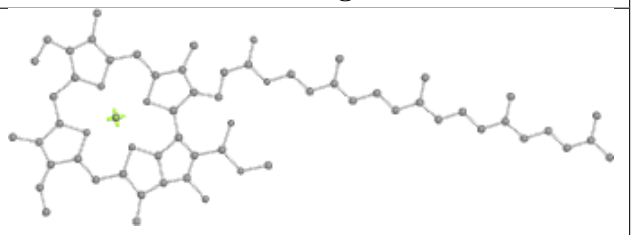
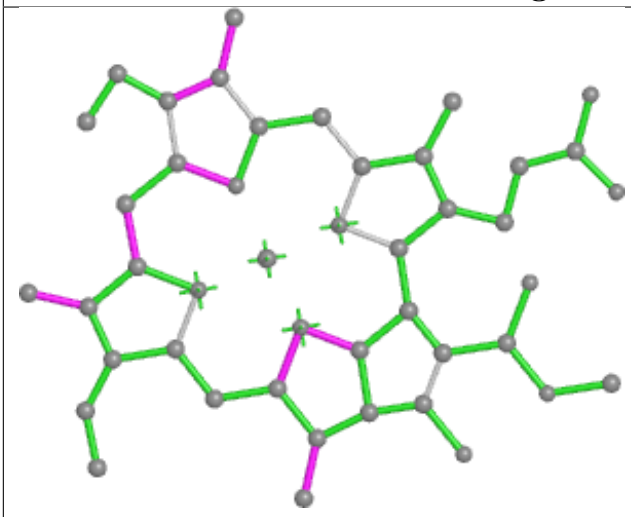


Rings

Ligand CLA t 508



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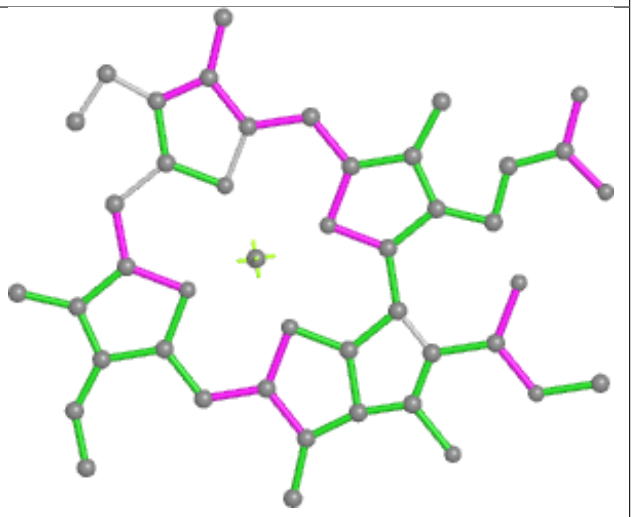
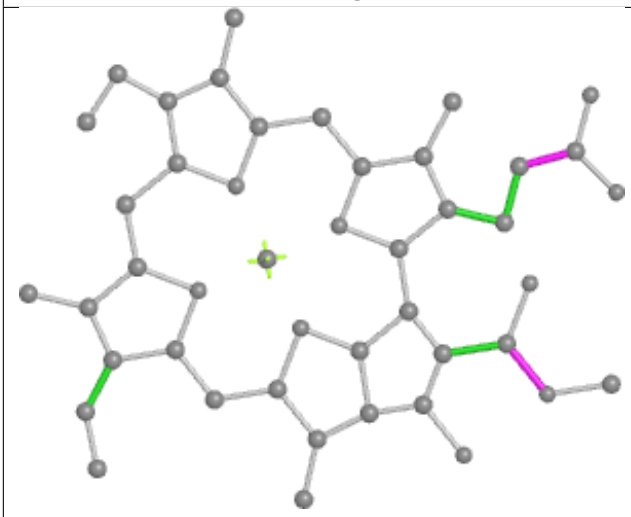


Bond angles



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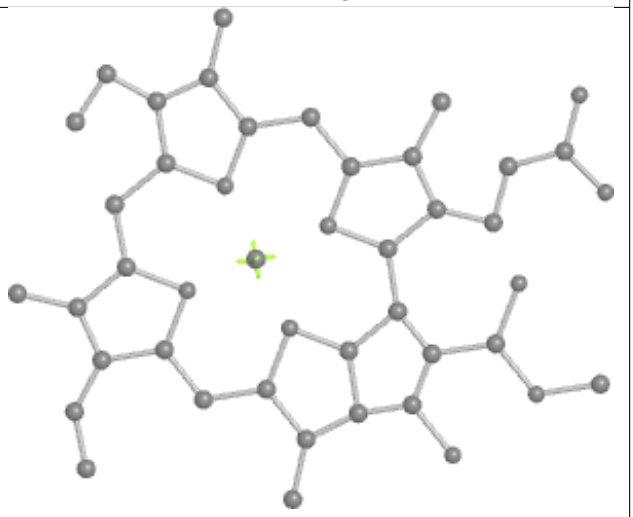
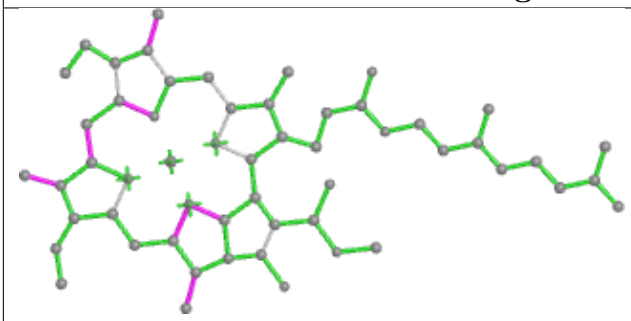


Rings

Ligand CLA H 1228



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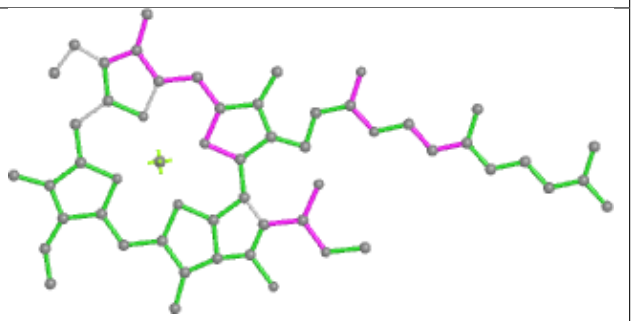
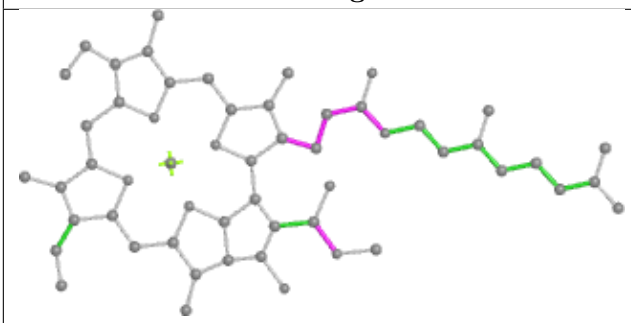


Bond angles



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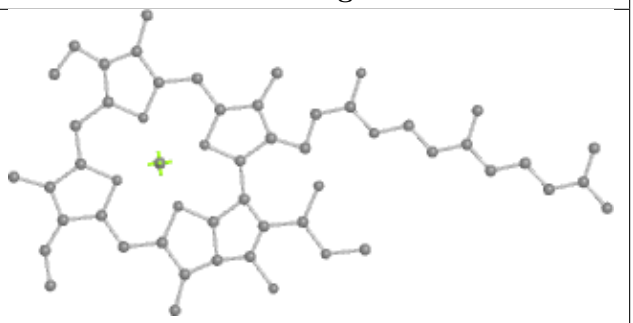
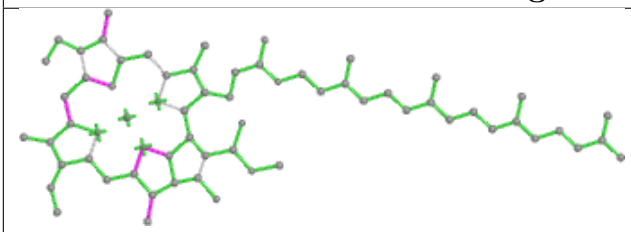


Rings

Ligand CLA 2 510



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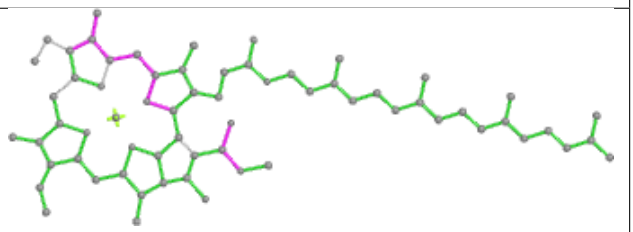
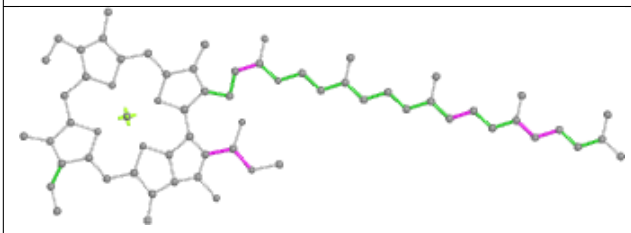


Bond angles



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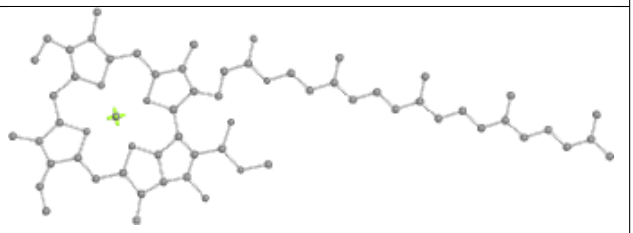
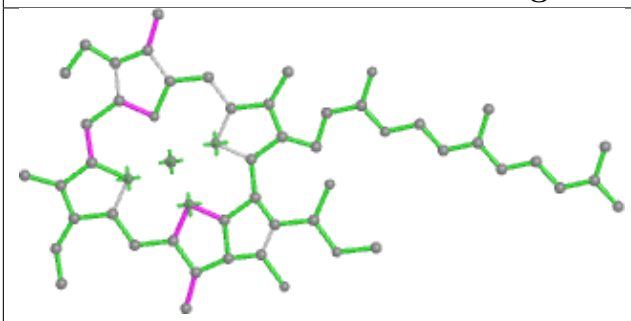


Rings

Ligand CLA t 503



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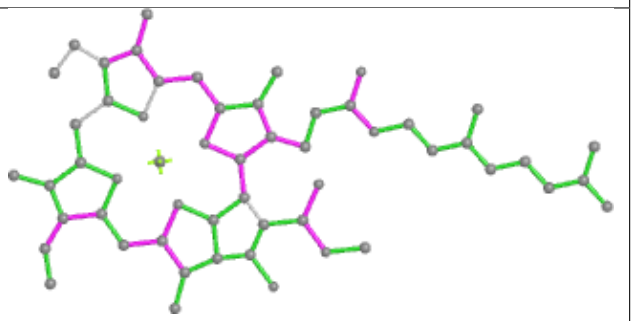
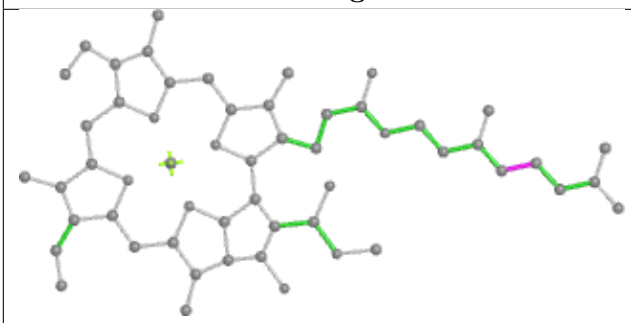
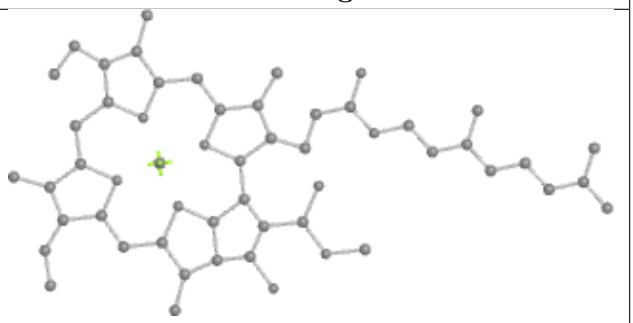


Bond angles

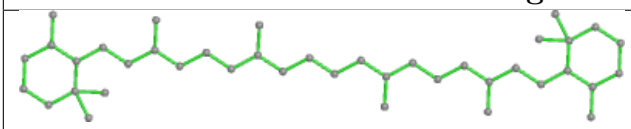


Torsions



Rings

Ligand BCR 5 523



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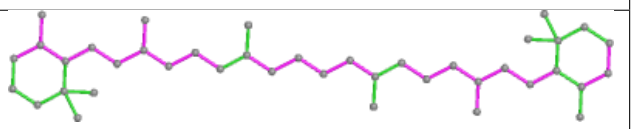
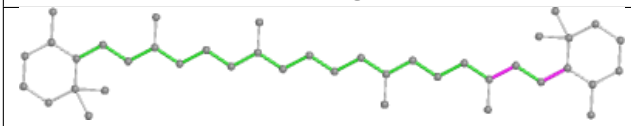


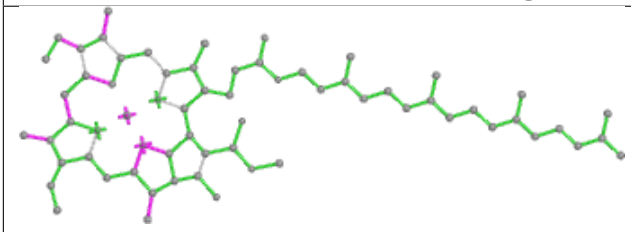
Bond angles



Torsions

Rings

Ligand CLA e 1106



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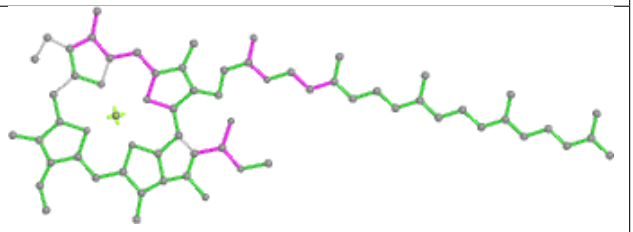
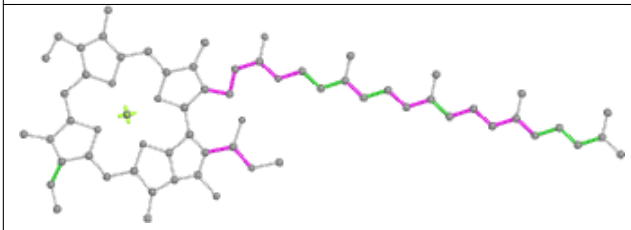
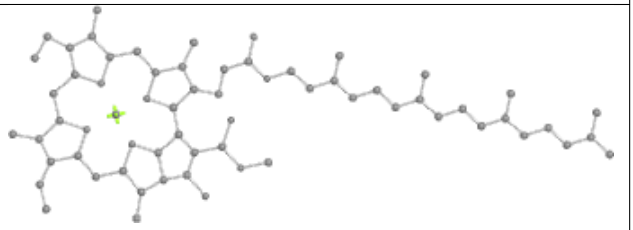


Bond angles

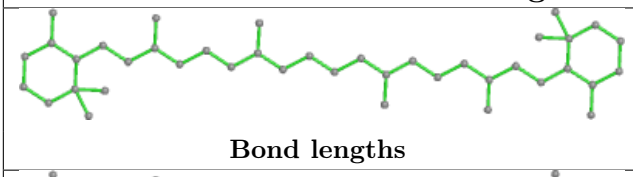


Torsions



Rings

Ligand BCR r 521



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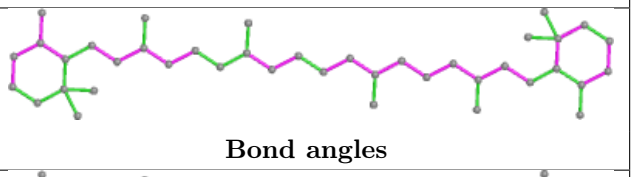

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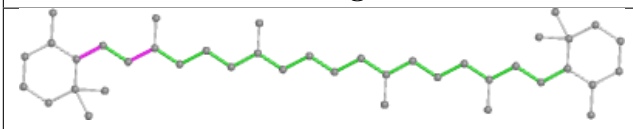

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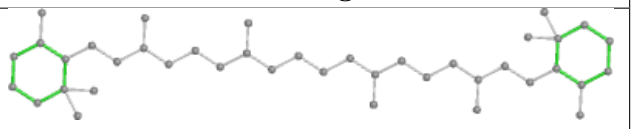

Rings

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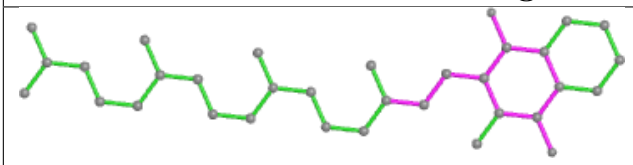

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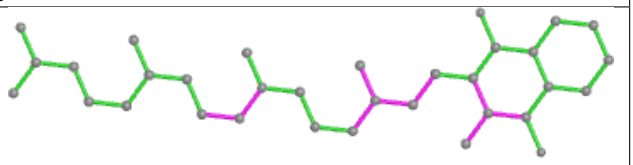

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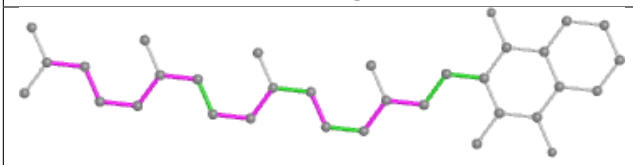

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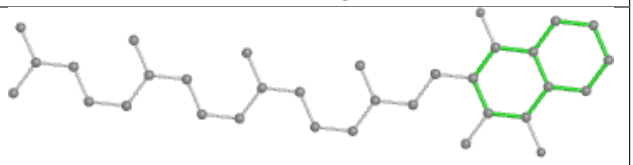
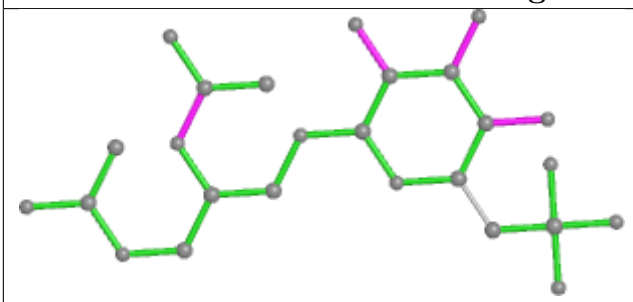


Rings

Ligand SQD 6 822



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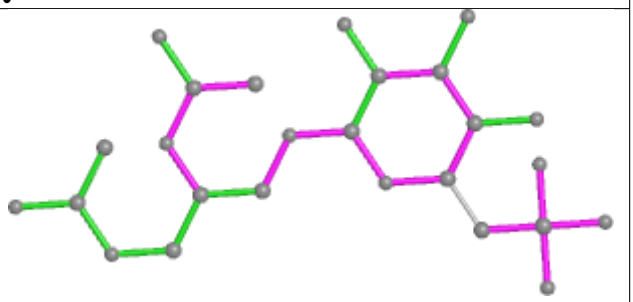

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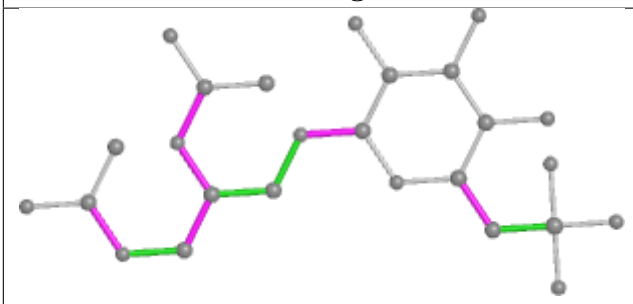

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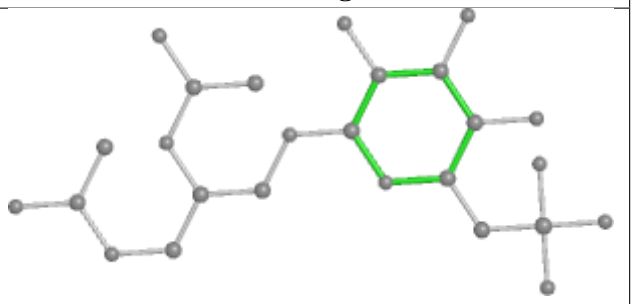
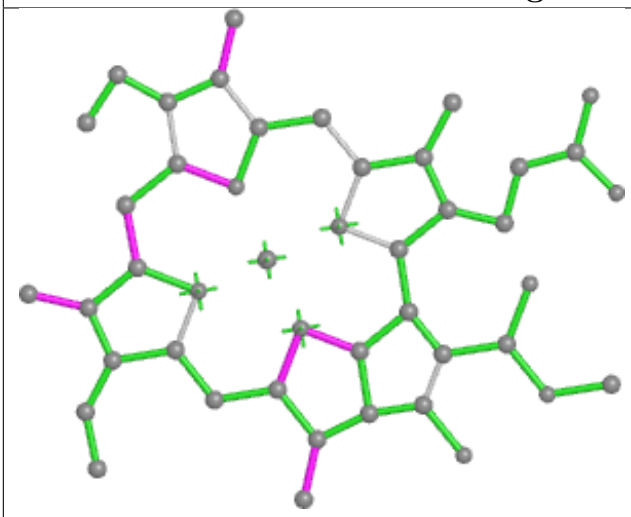


Rings

Ligand CLA Z 516



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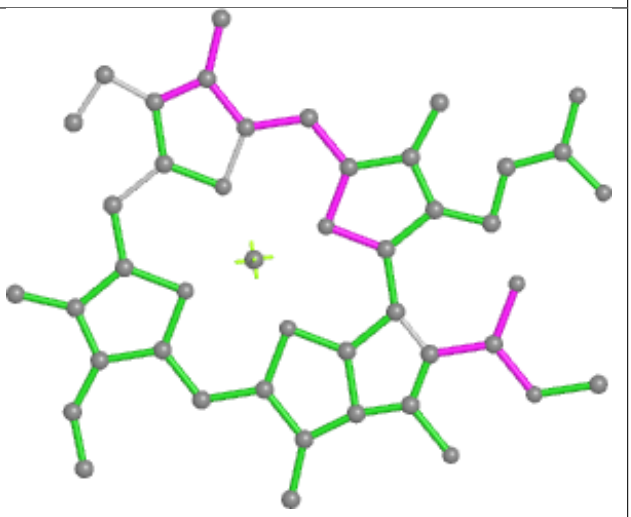

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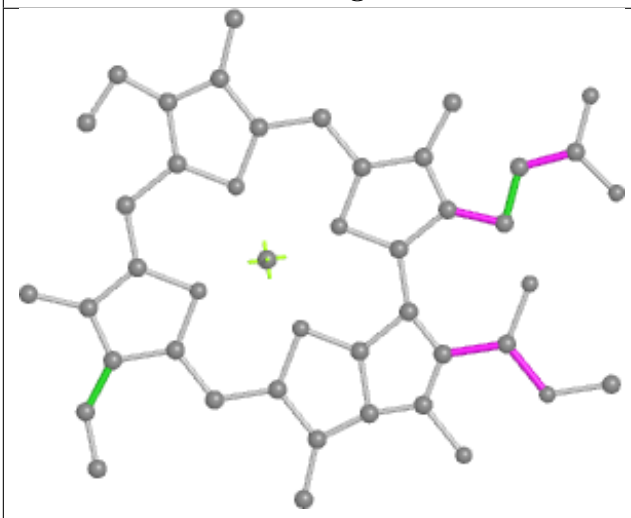

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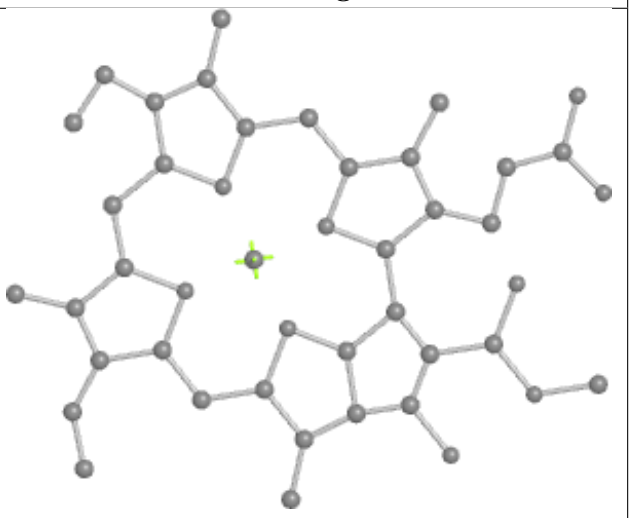
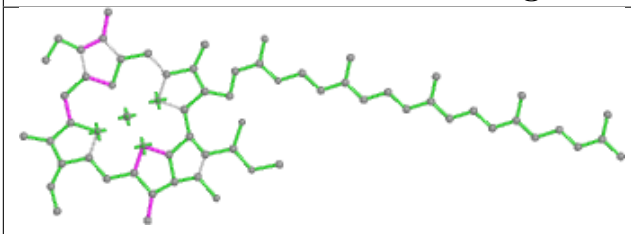


Rings

Ligand CLA j 1301



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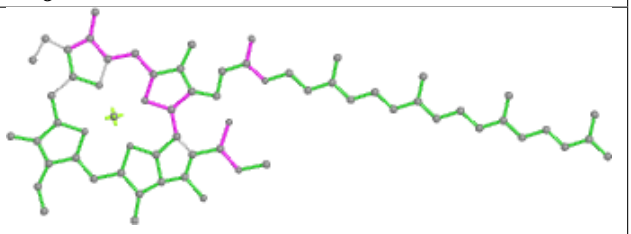

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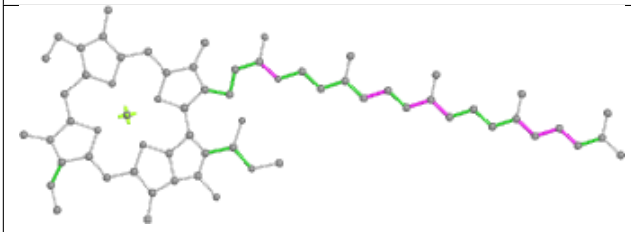

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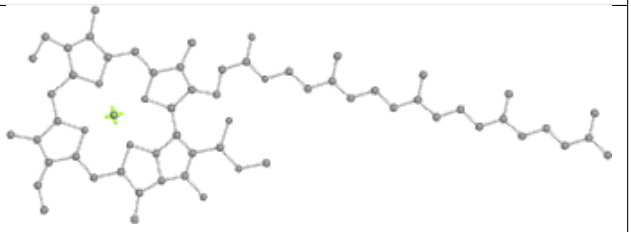

Rings

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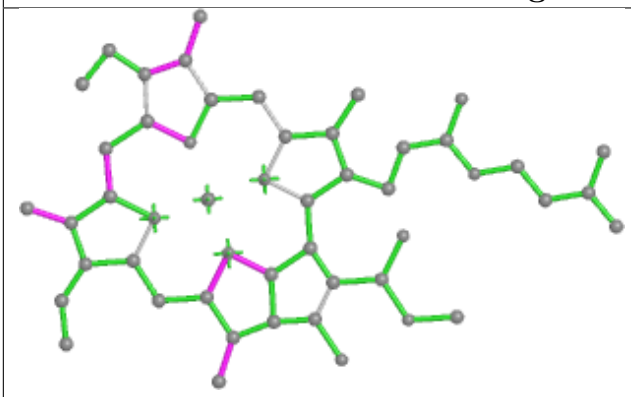

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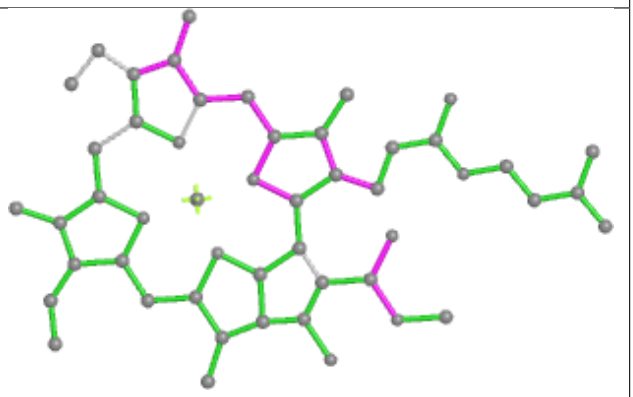

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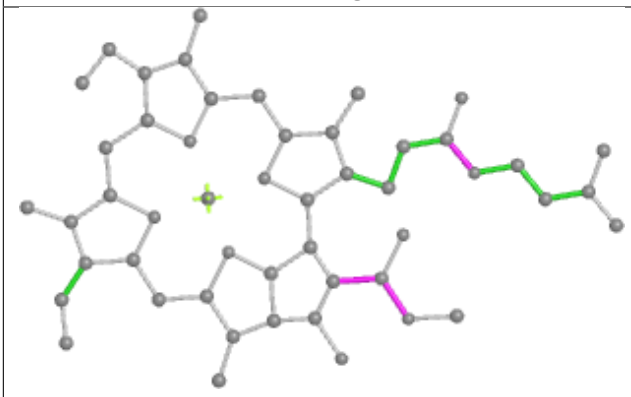

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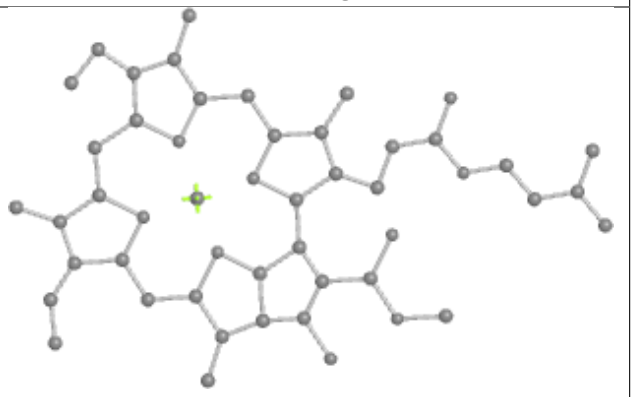

Rings

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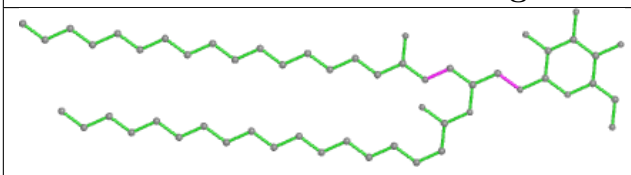

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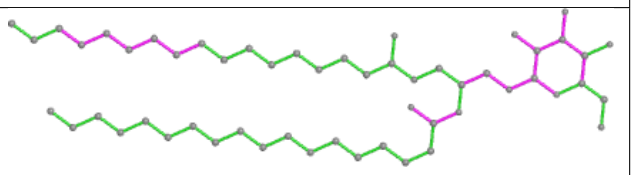

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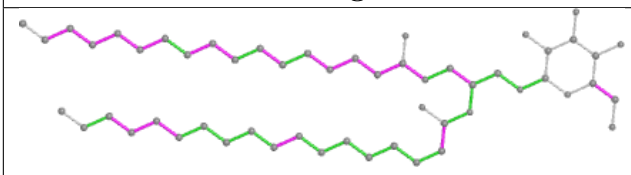

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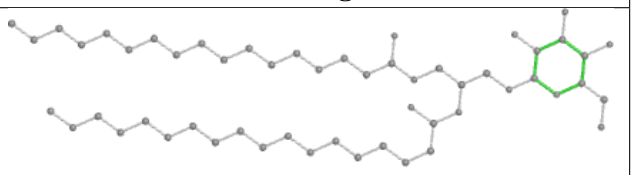
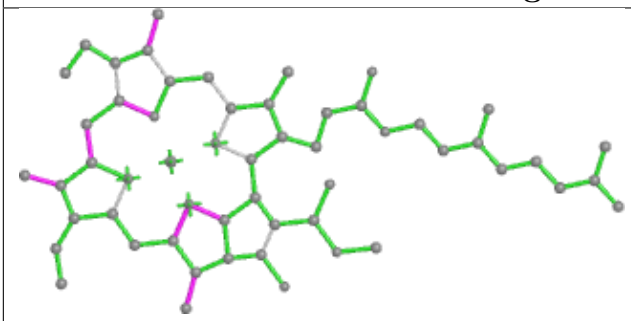


Rings

Ligand CLA Y 508



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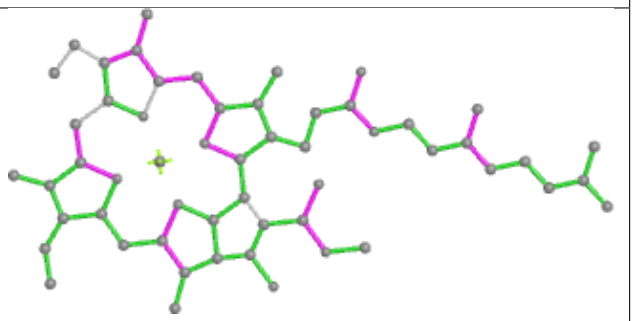

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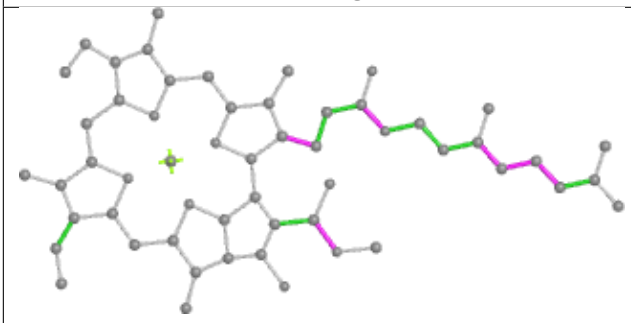

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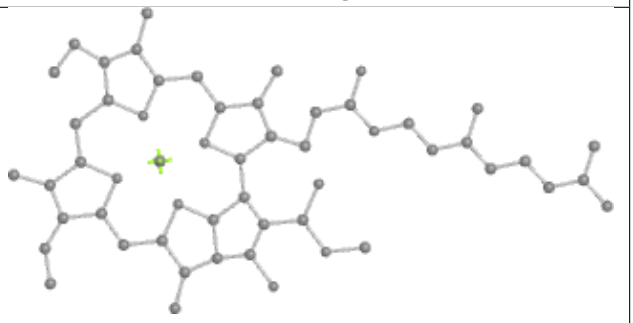

Rings

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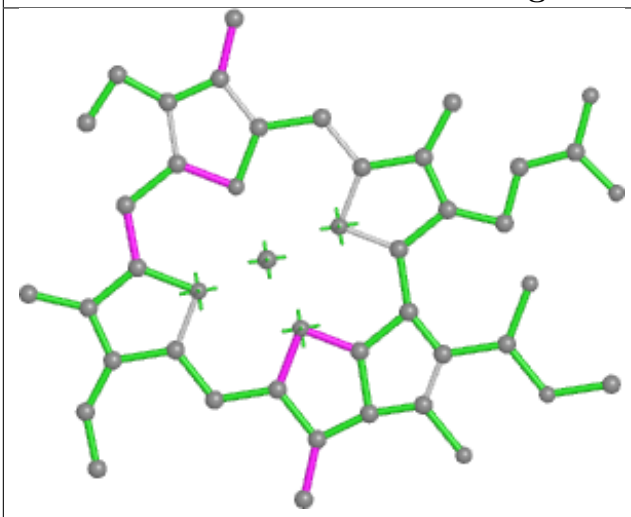

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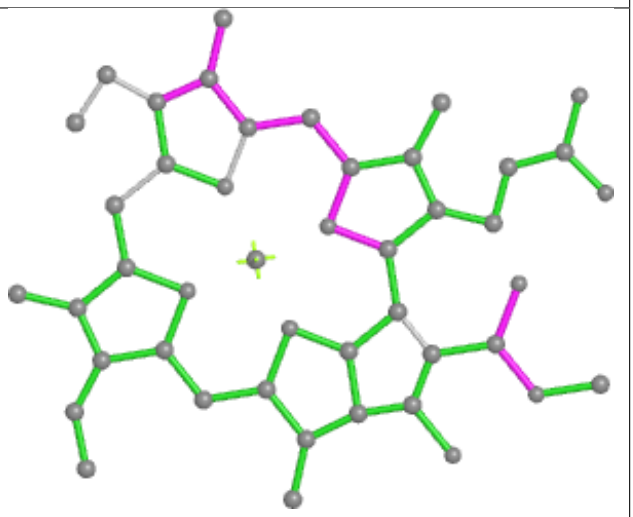

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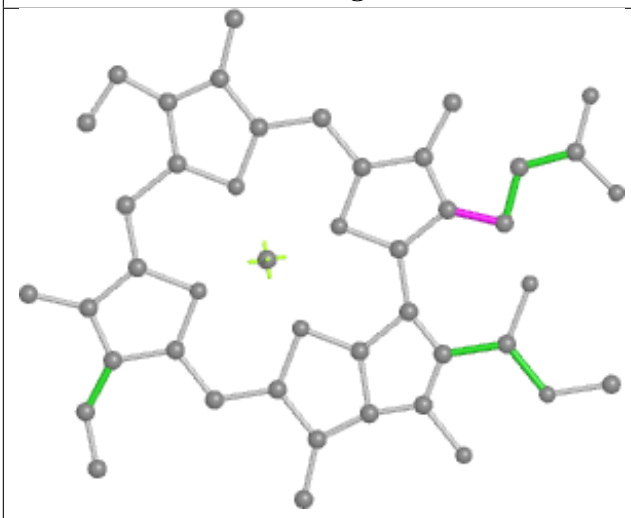

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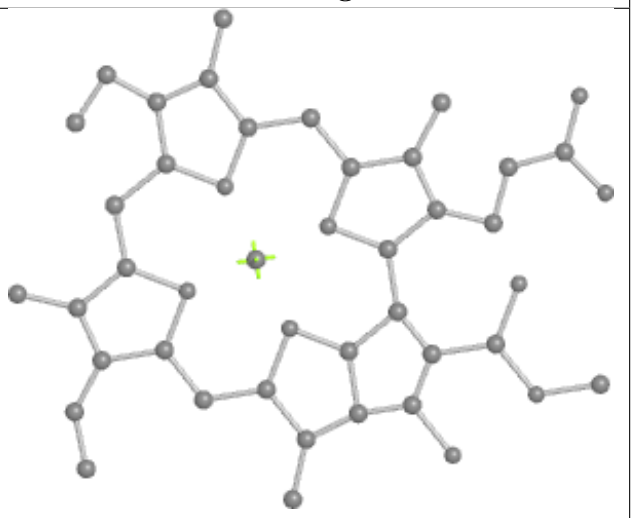

Rings

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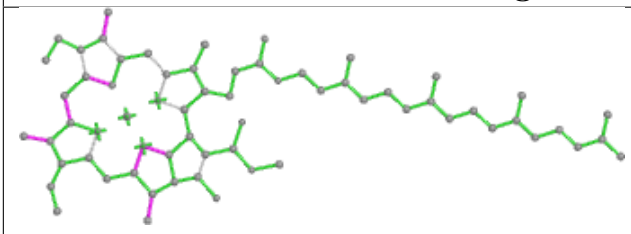

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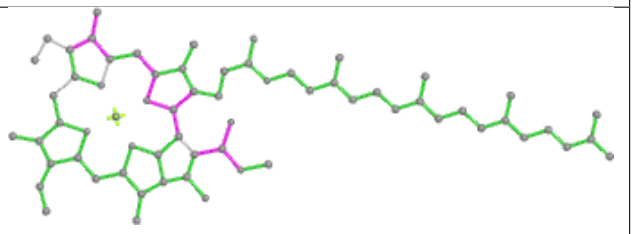

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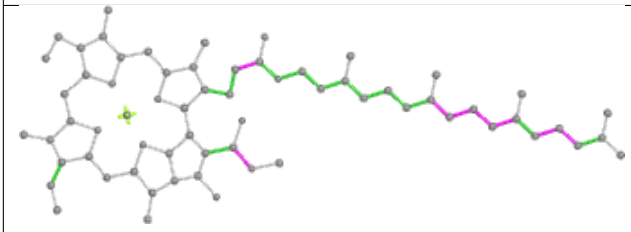

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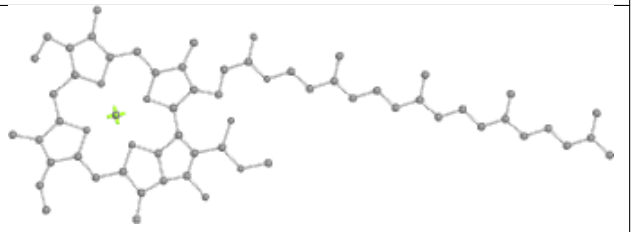
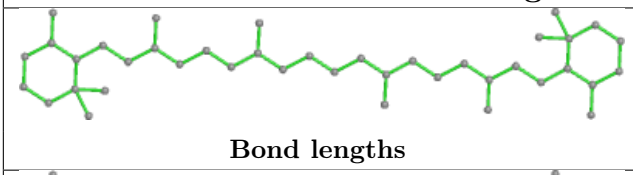


Rings

Ligand BCR Z 523



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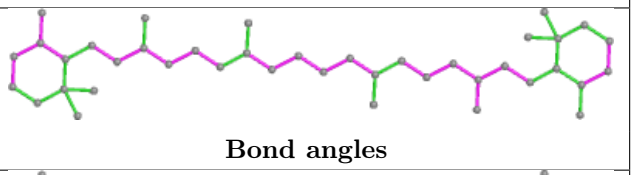

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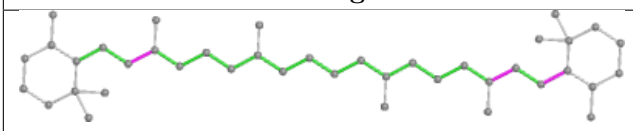

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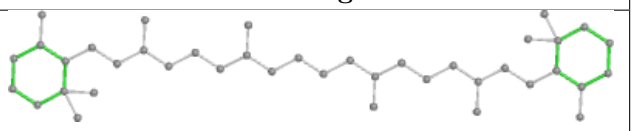

Rings

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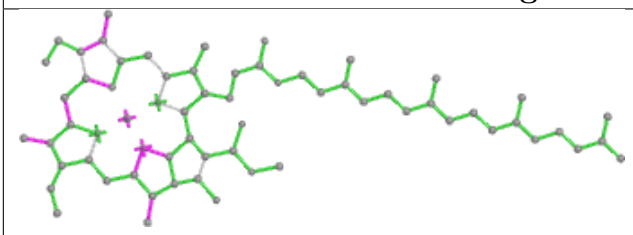

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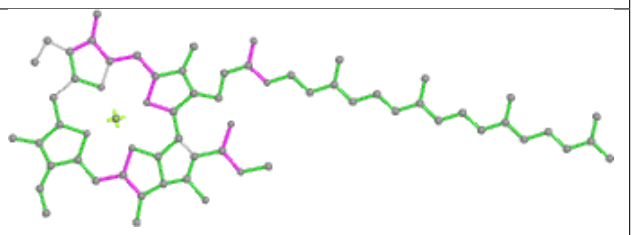
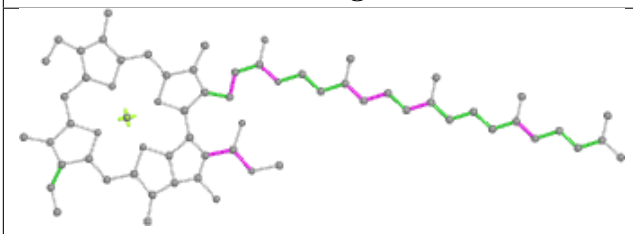


Bond angles



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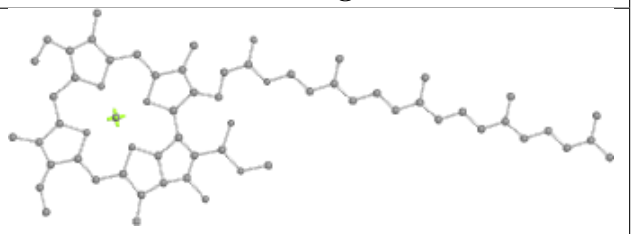

Rings

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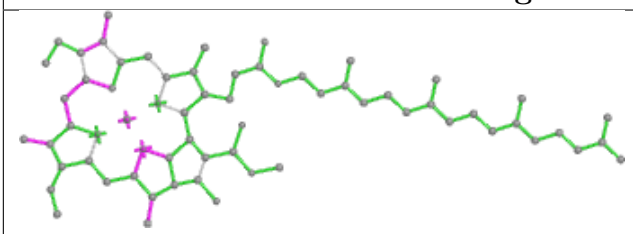

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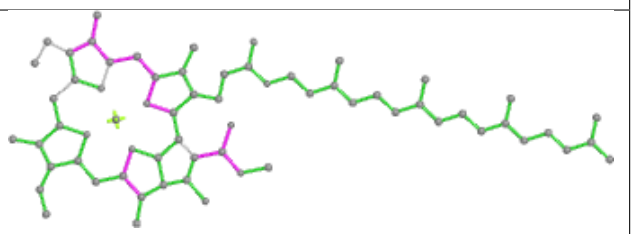
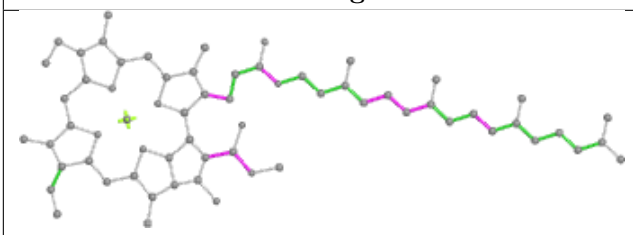


Bond angles



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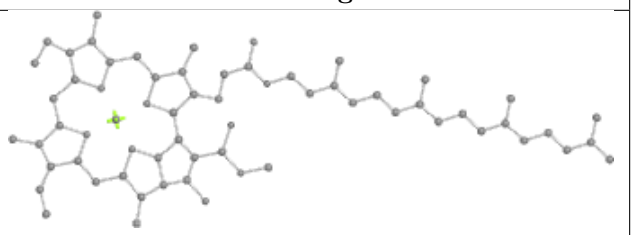
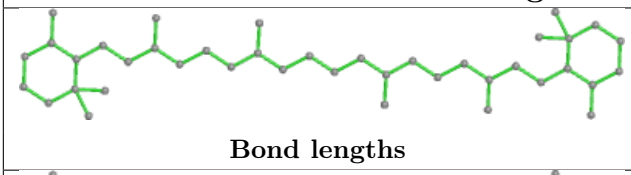


Rings

Ligand BCR 4 521



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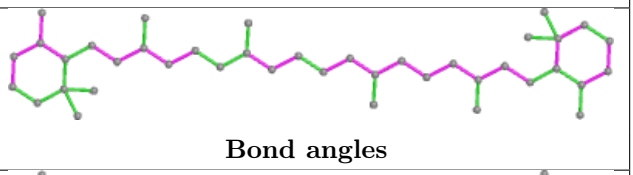
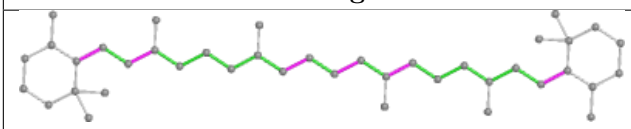


Bond angles



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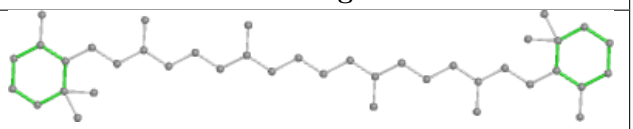
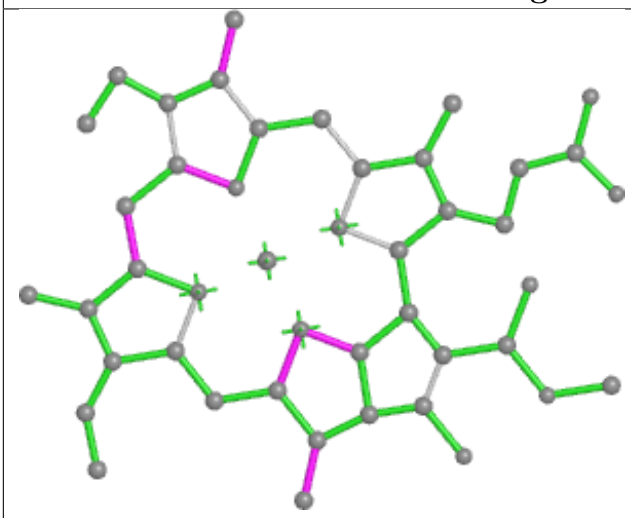
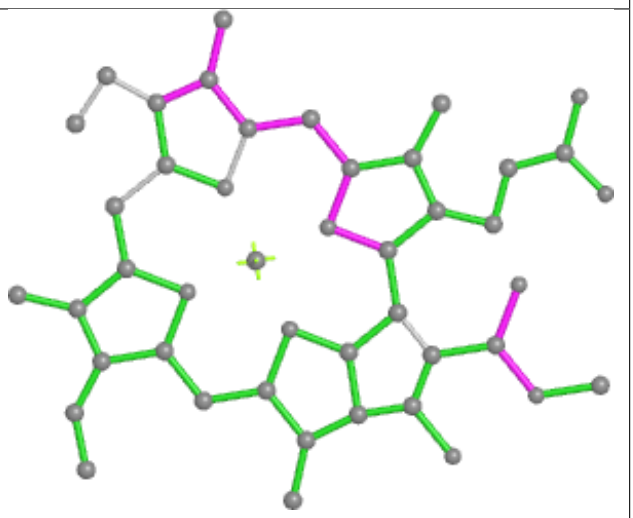


Rings

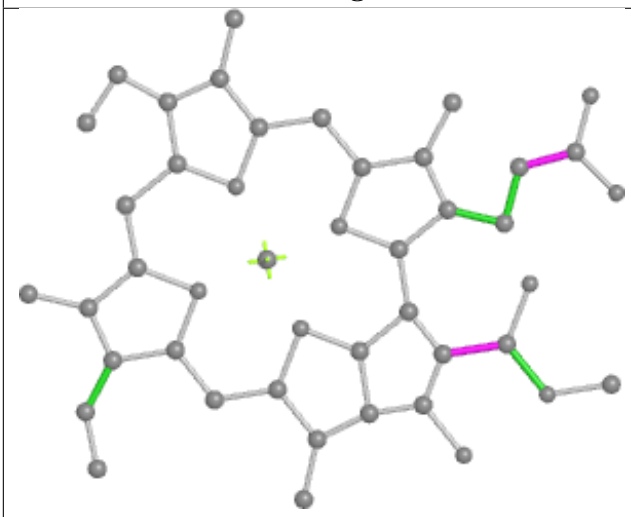
Ligand CLA t 512



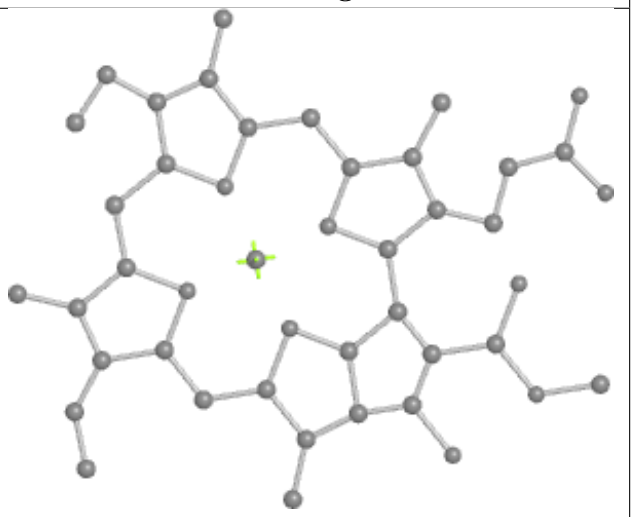
Bond lengths



Bond angles

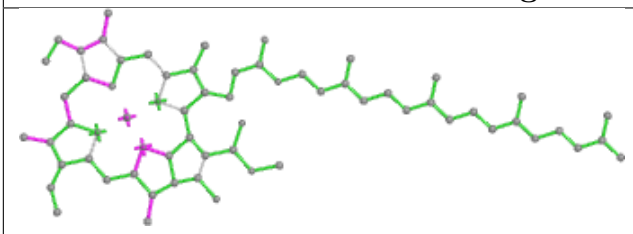


Torsions



Rings

Ligand CLA e 1132



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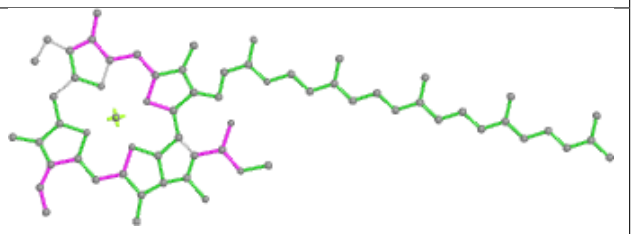

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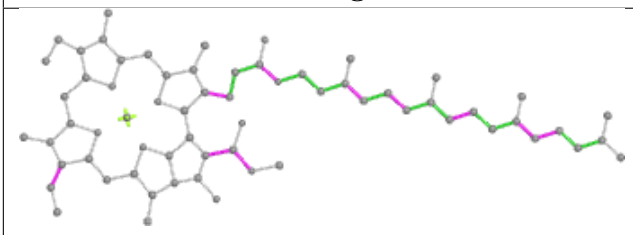
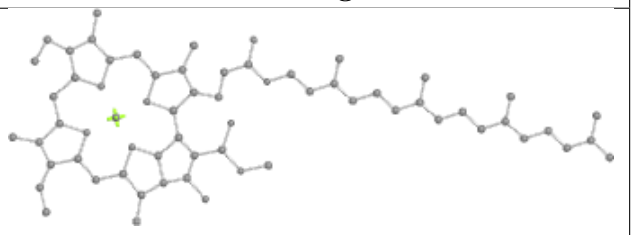
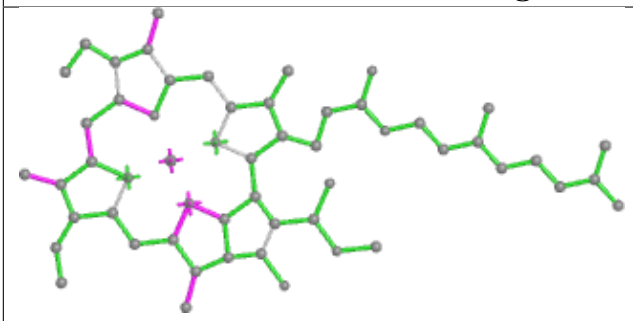


Torsions



Rings

Ligand CLA G 1121



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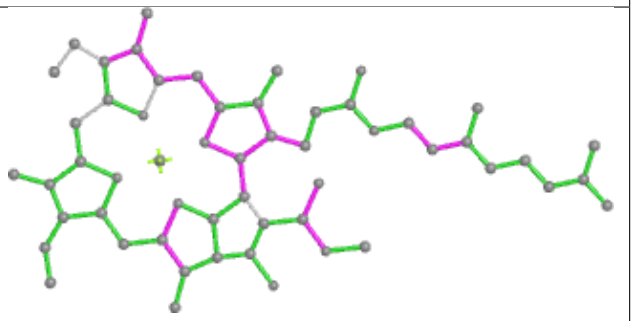
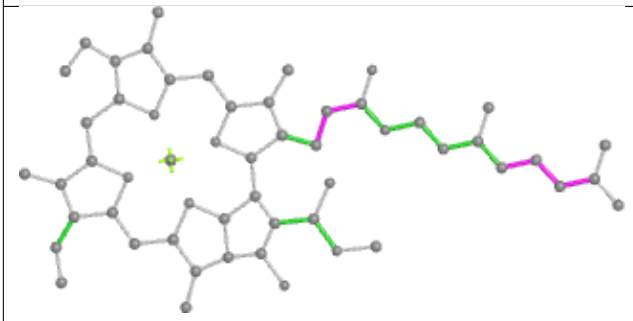
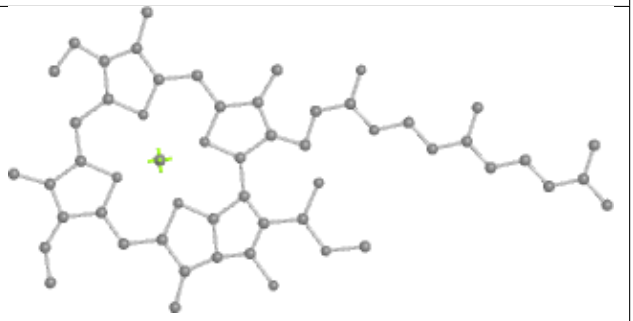


Bond angles

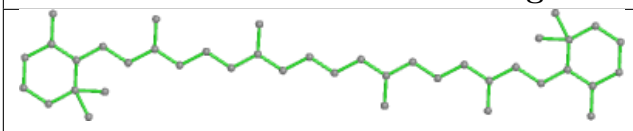


Torsions



Rings

Ligand BCR 3 522



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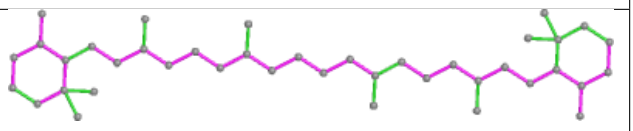
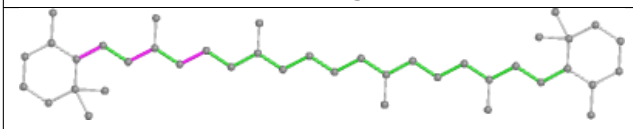


Bond angles



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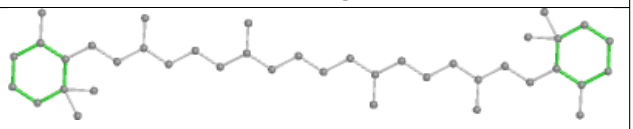
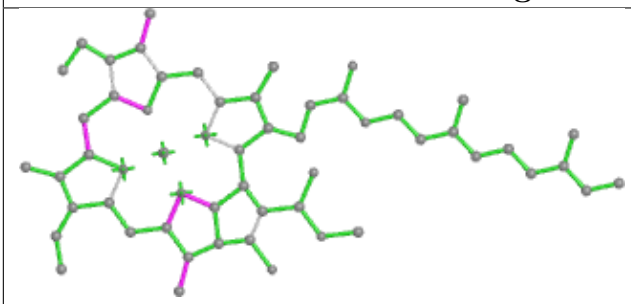


Rings

Ligand CLA G 1124



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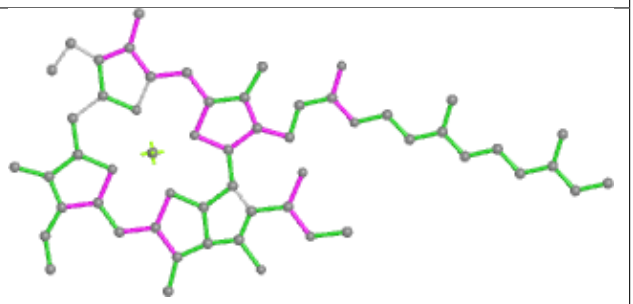
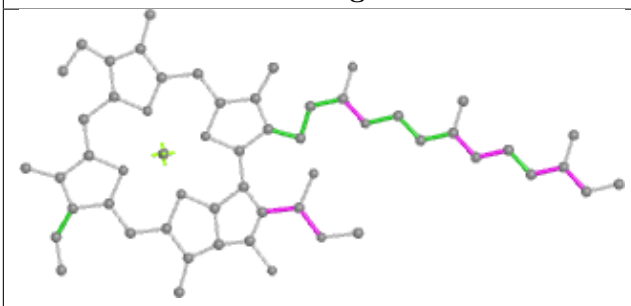


Bond angles



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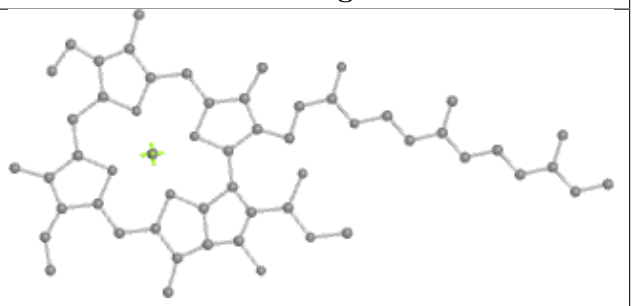
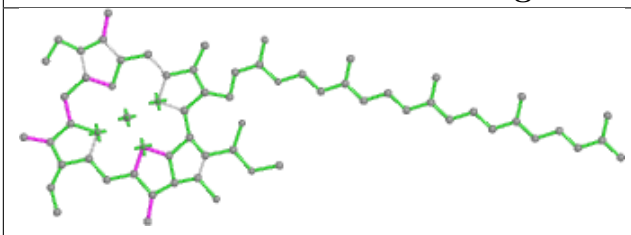


Rings

Ligand CLA H 1202



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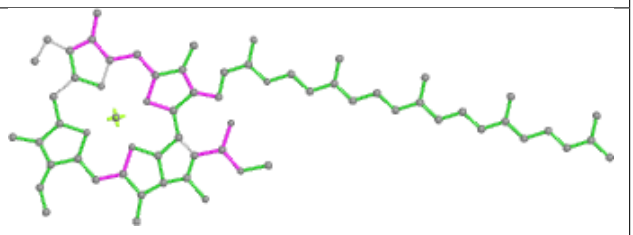
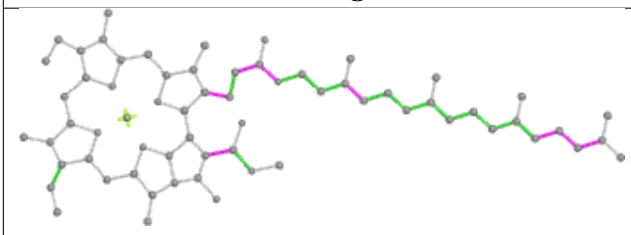


Bond angles



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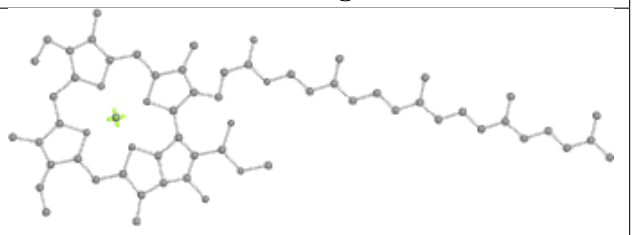
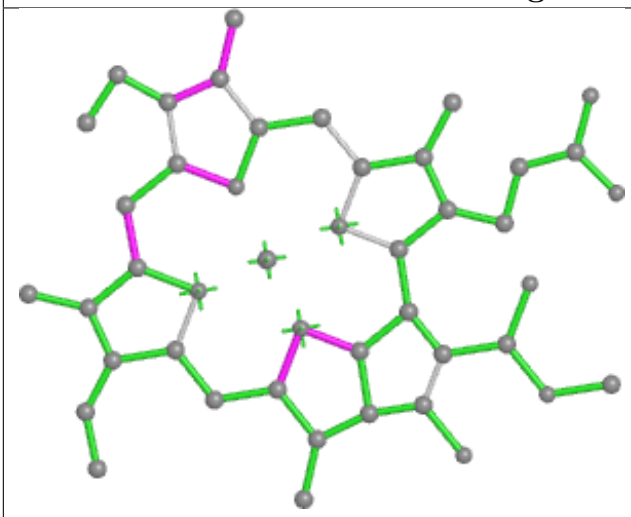


Rings

Ligand CLA d 513



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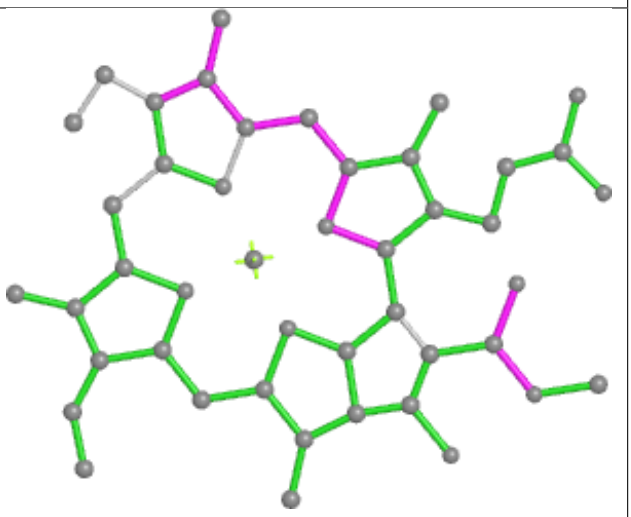
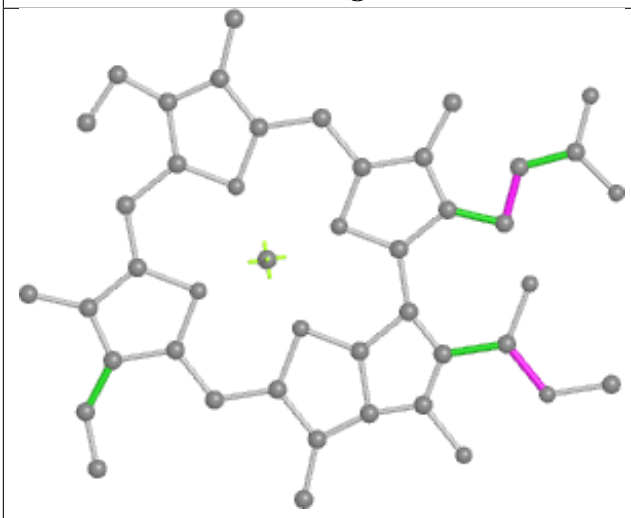


Bond angles



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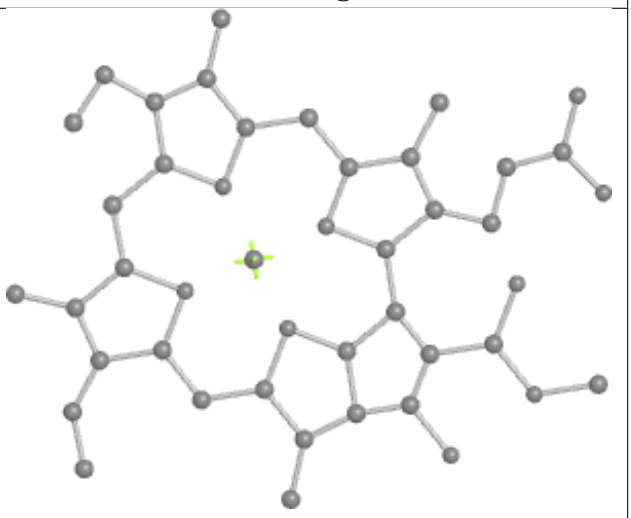
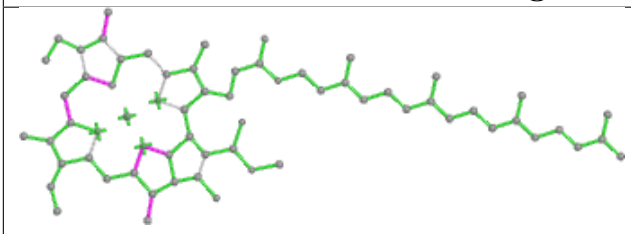


Rings

Ligand CLA 1 505



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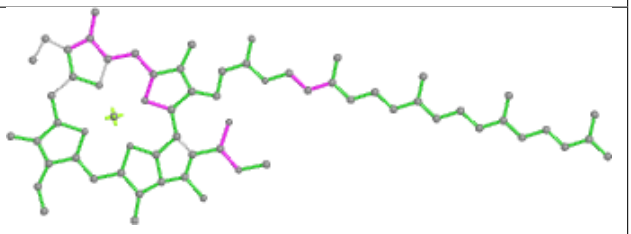
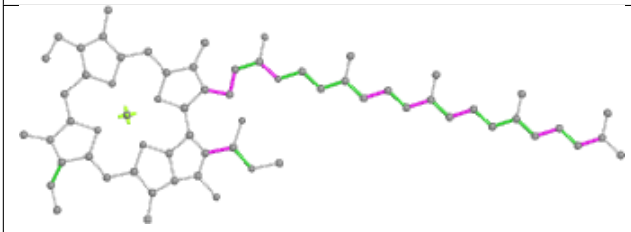


Bond angles



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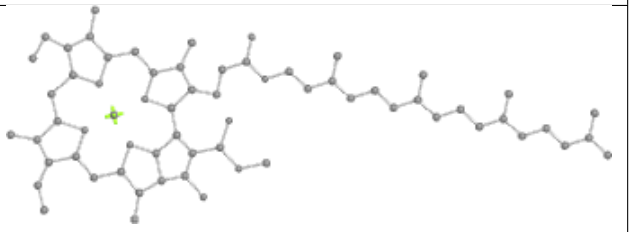
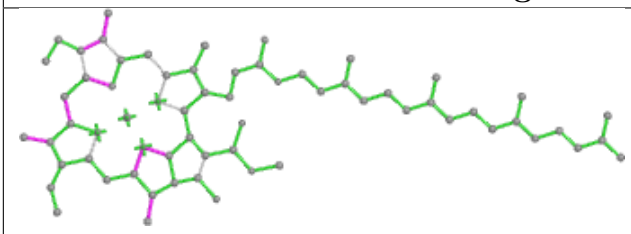


Rings

Ligand CLA G 1140



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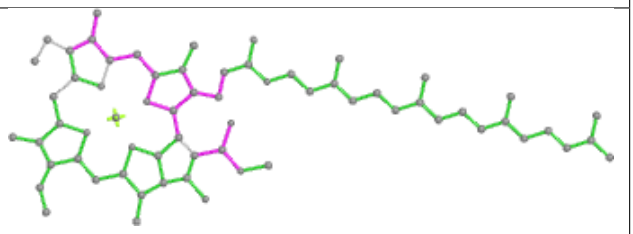
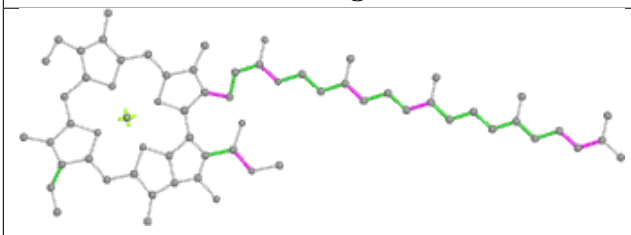
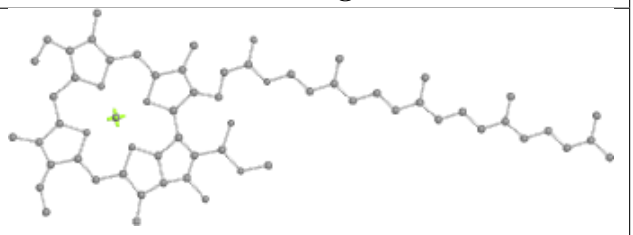


Bond angles

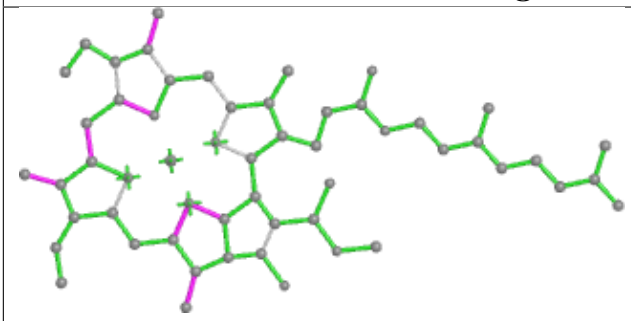


Torsions



Rings

Ligand CLA U 1401



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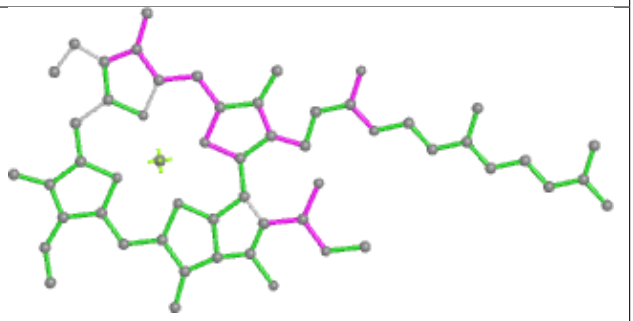
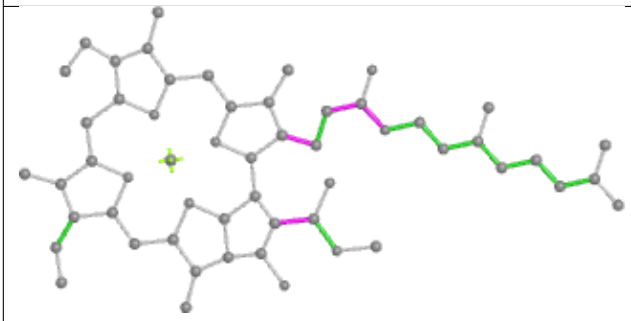
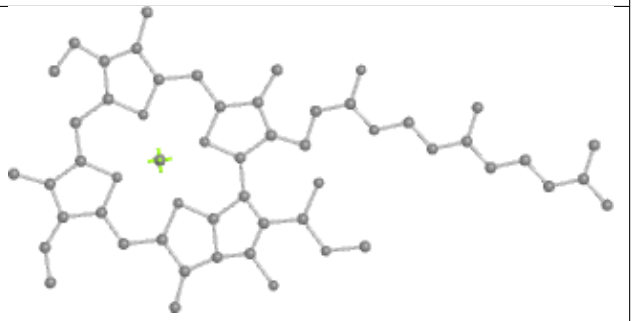


Bond angles

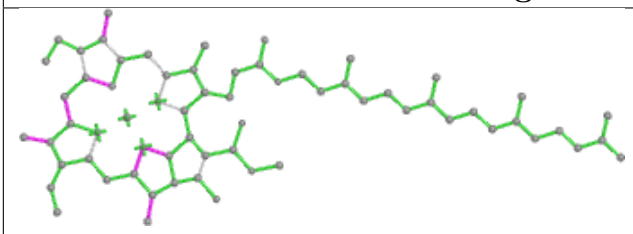


Torsions



Rings

Ligand CLA A 1138



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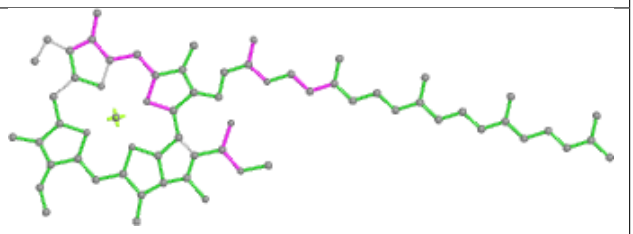
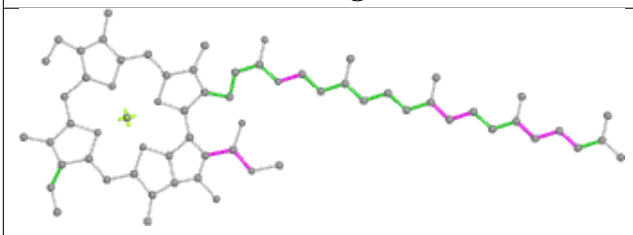


Bond angles



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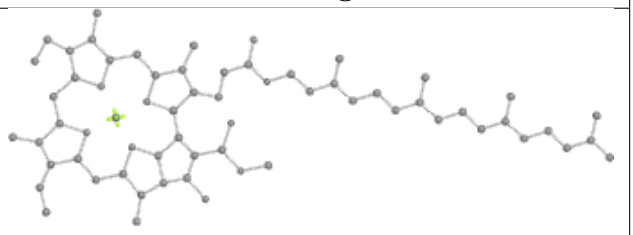
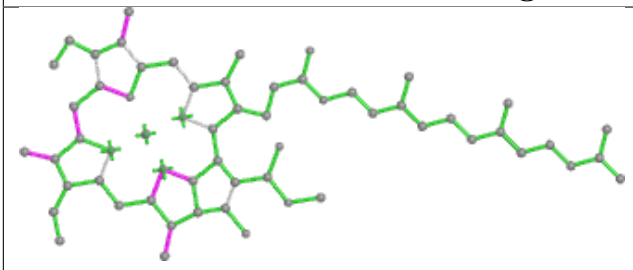


Rings

Ligand CLA n 1503



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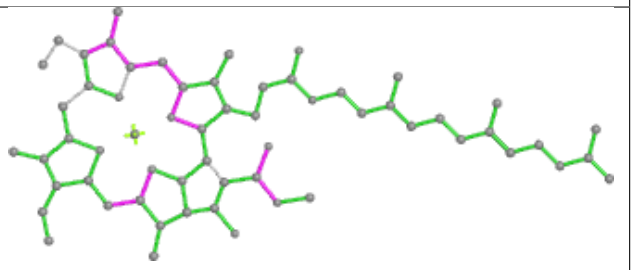
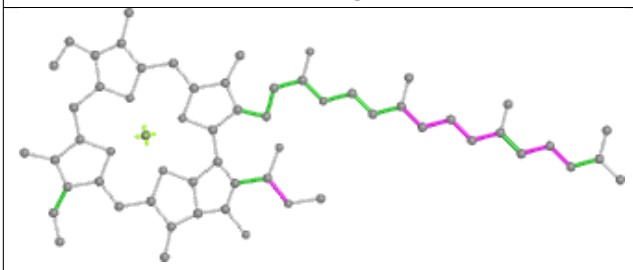


Bond angles



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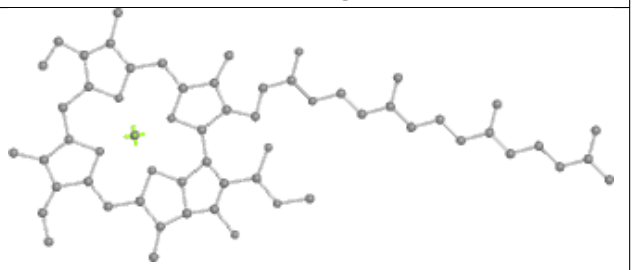
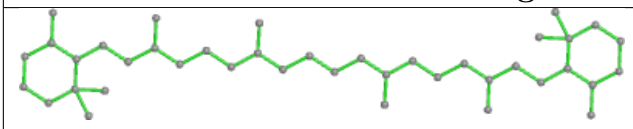


Rings

Ligand BCR J 4015



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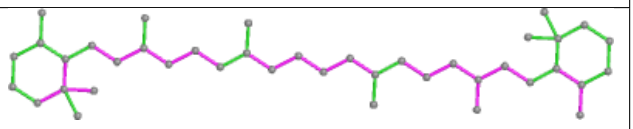
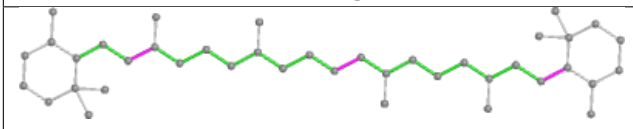


Bond angles



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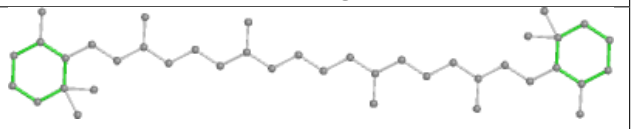
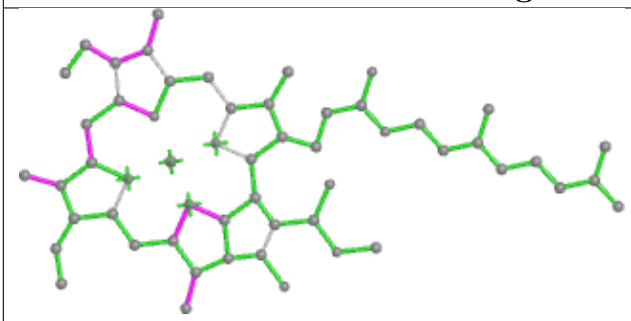
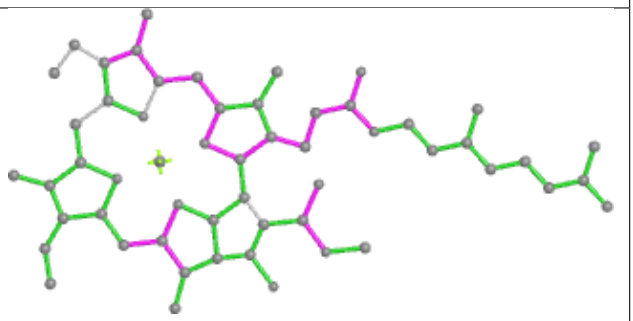


Rings

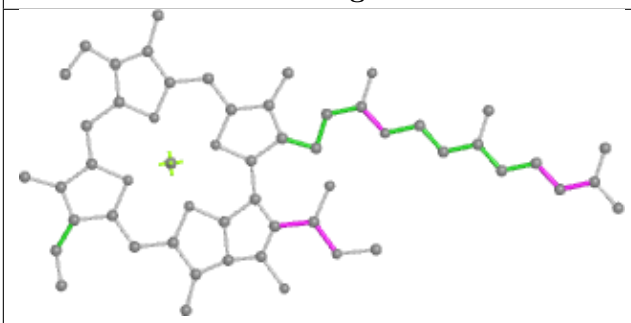
Ligand CLA B 1220



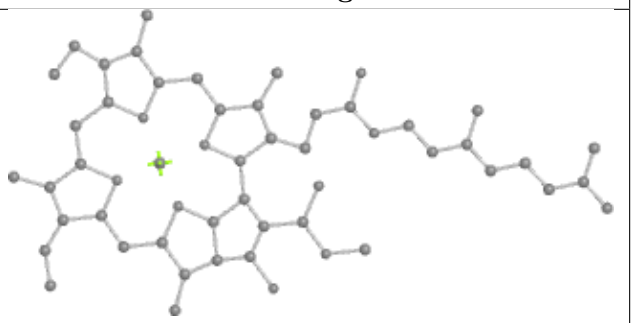
Bond lengths



Bond angles

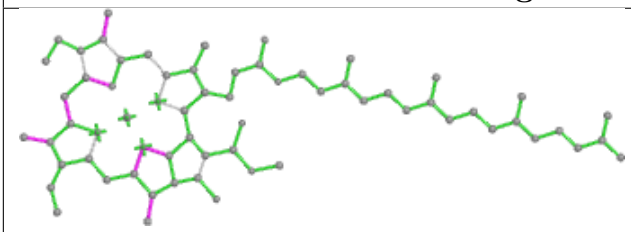


Torsions

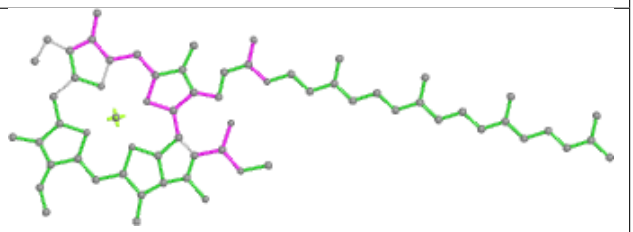


Rings

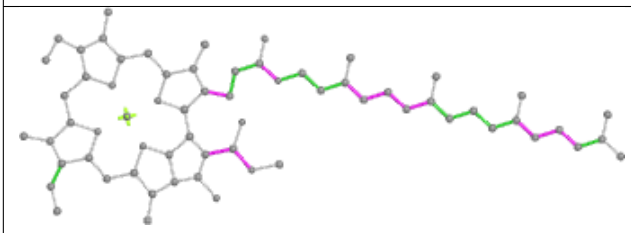
Ligand CLA T 1303



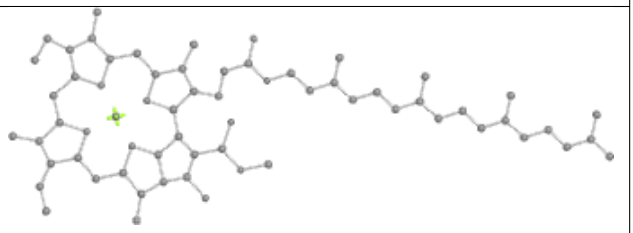
Bond lengths



Bond angles



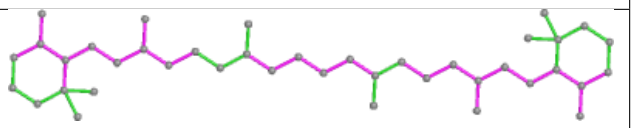
Torsions



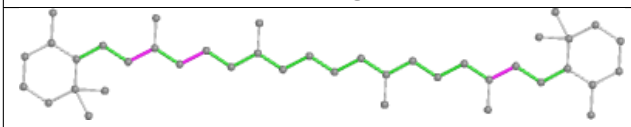
Rings

Ligand BCR 3 524

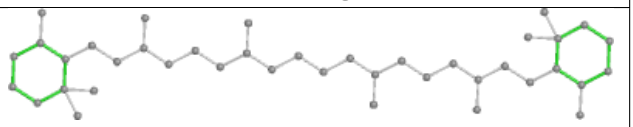
Bond lengths



Bond angles

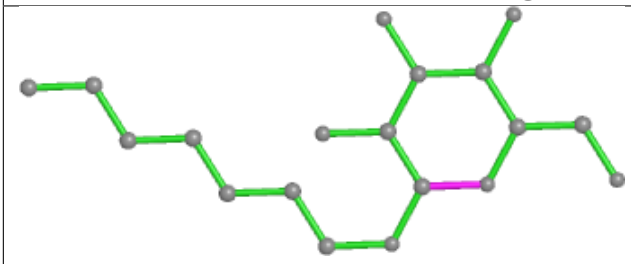


Torsions



Rings

Ligand LMU Y 902



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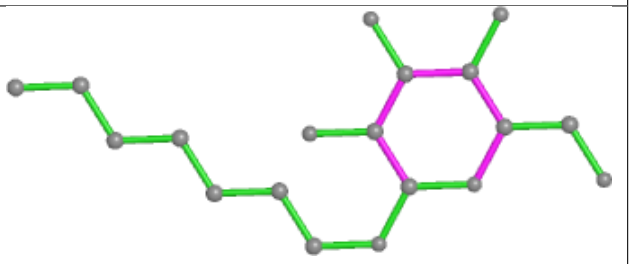
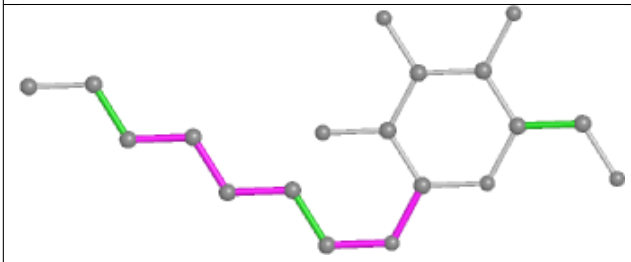


Bond angles



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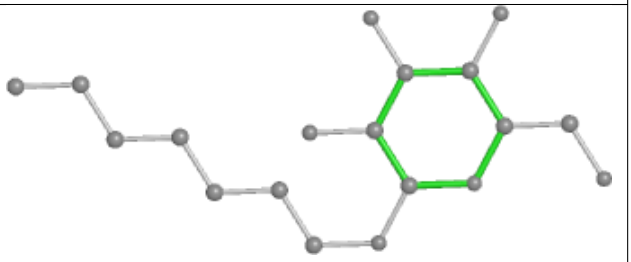
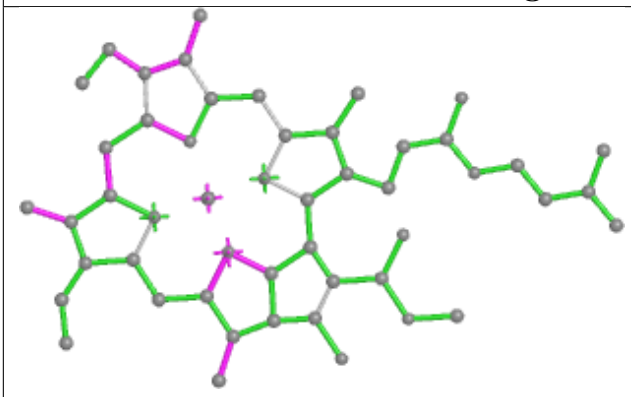


Rings

Ligand CLA Y 519



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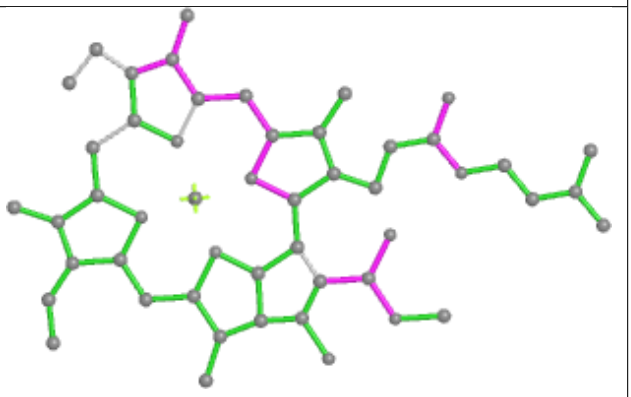
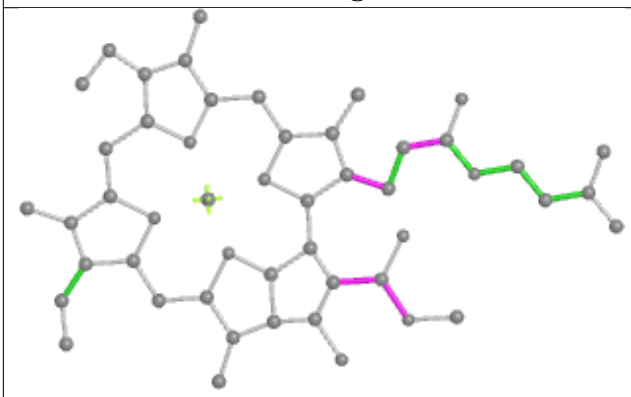
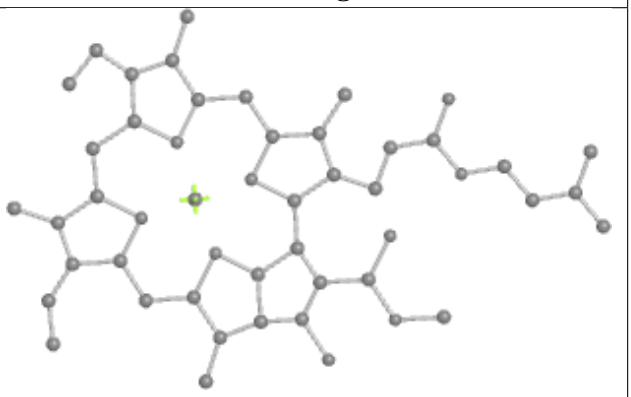


Bond angles

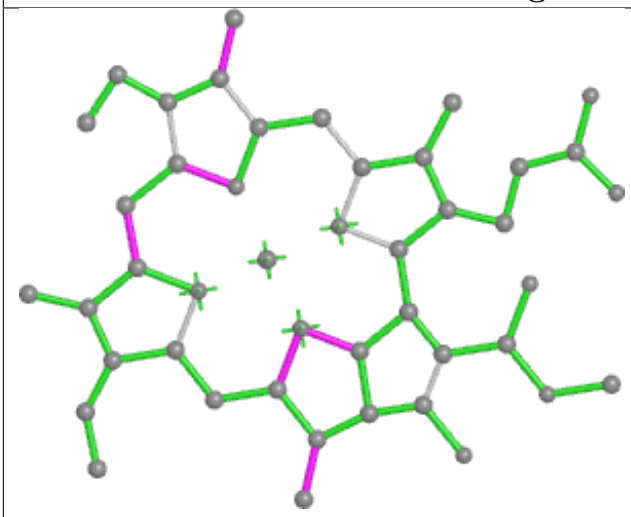


Torsions



Rings

Ligand CLA a 504



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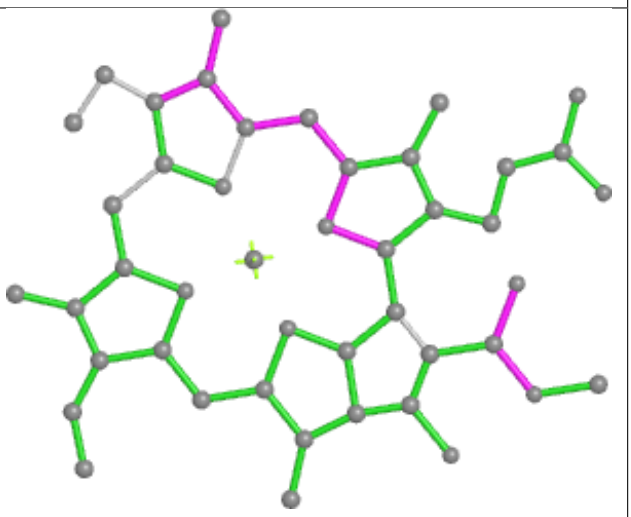
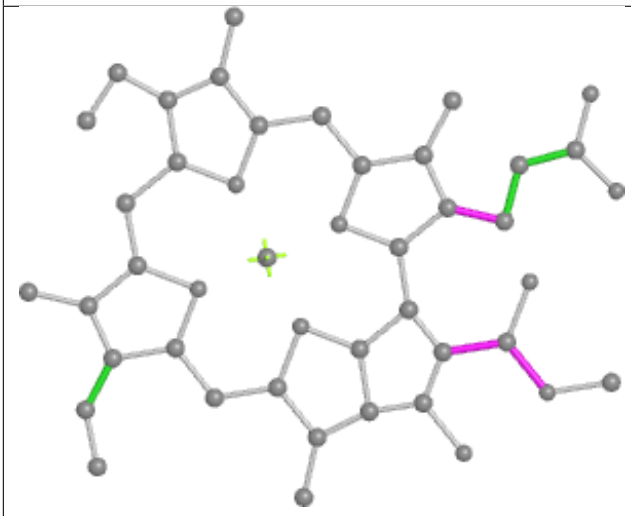
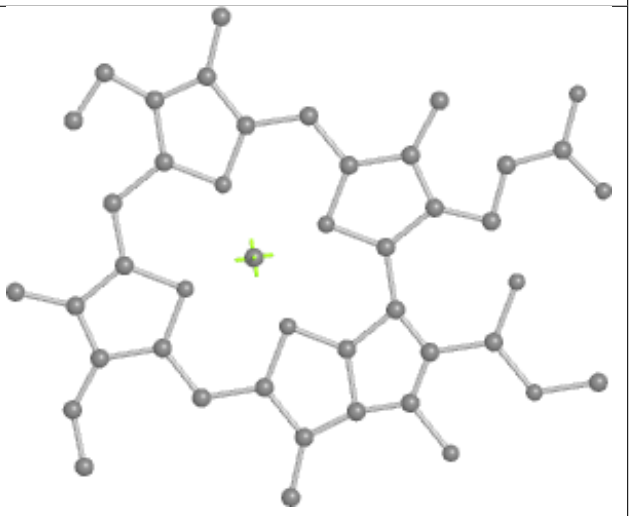


Bond angles

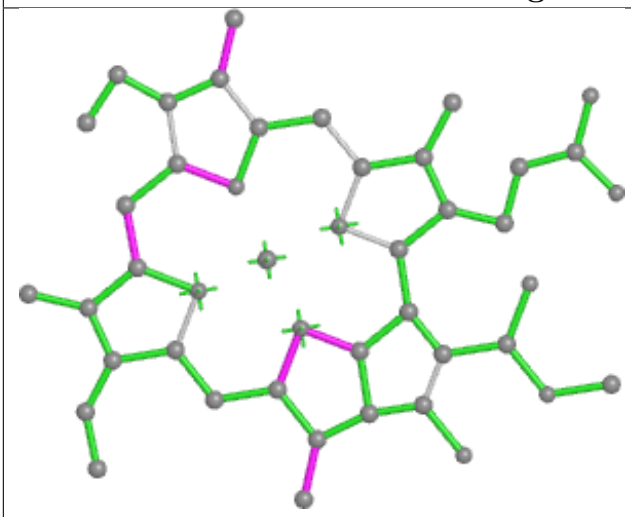


Torsions

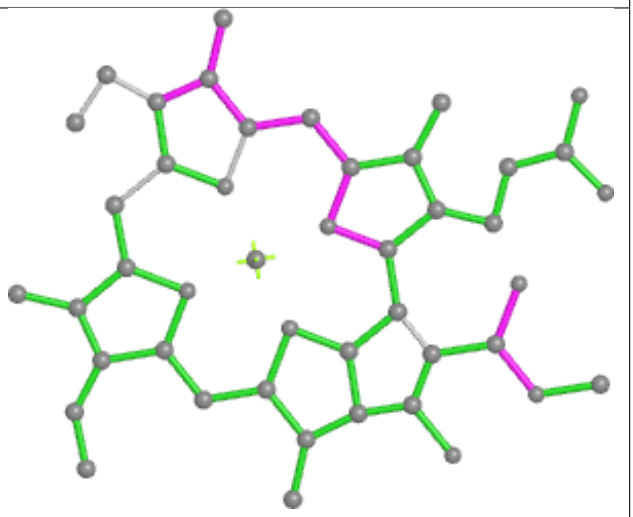


Rings

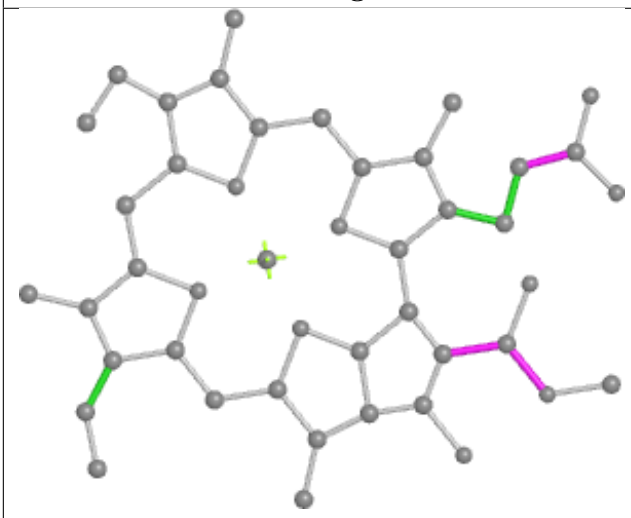
Ligand CLA d 509



Bond lengths



Bond angles



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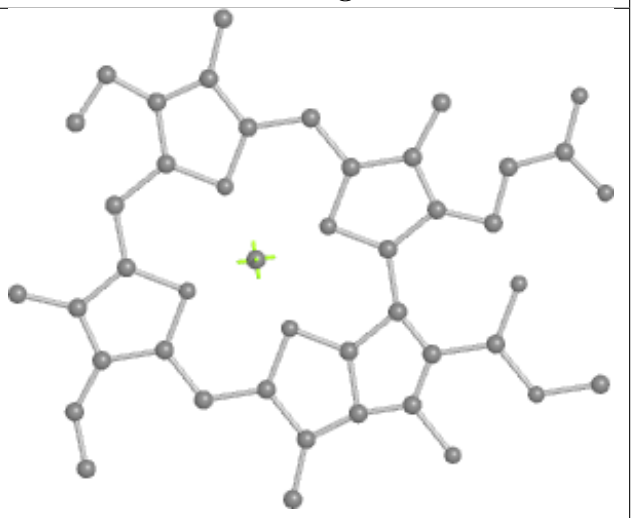
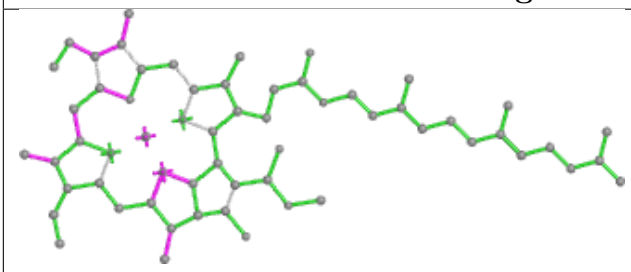


Rings

Ligand CLA B 1216



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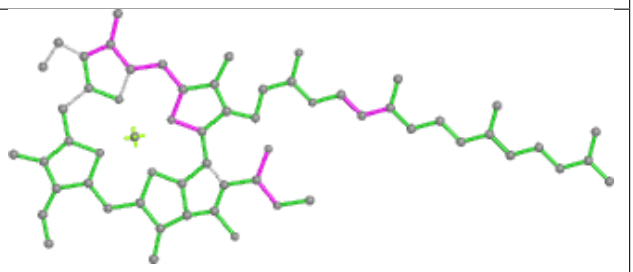
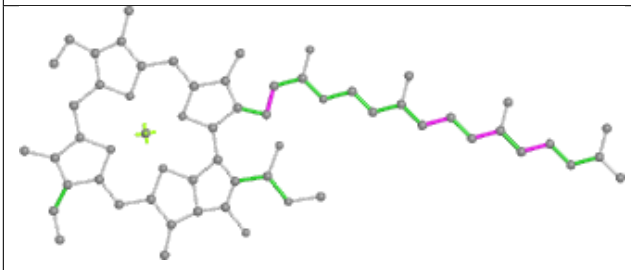


Bond angles



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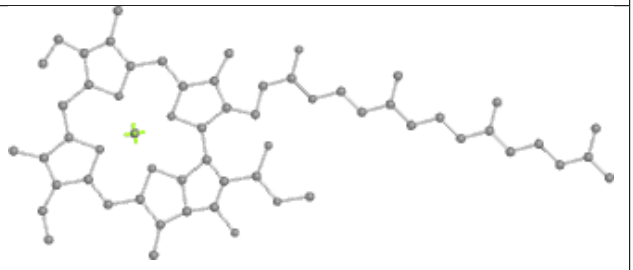
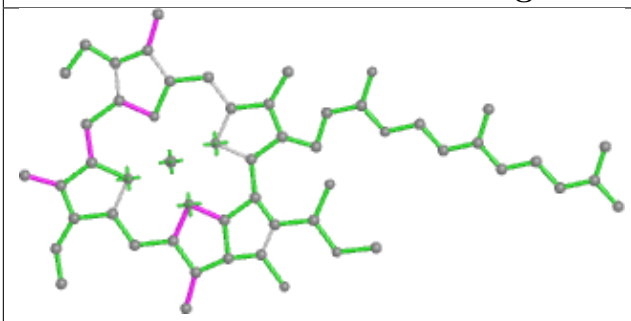


Rings

Ligand CLA B 1212



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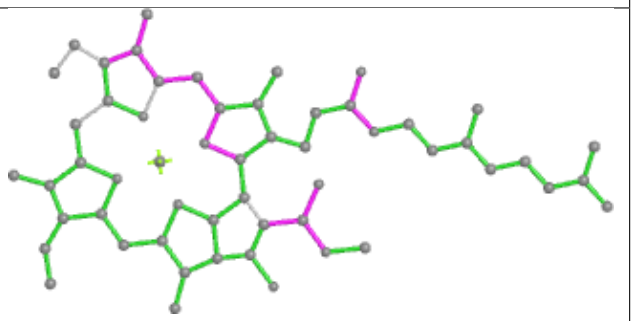
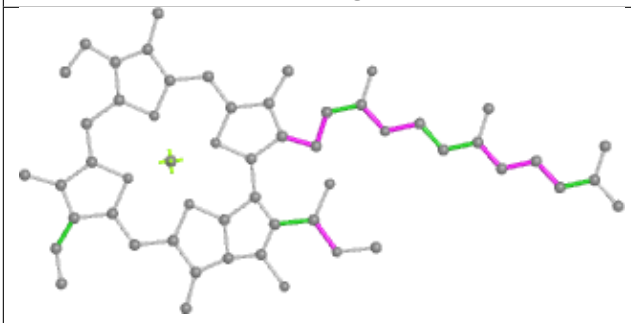


Bond angles



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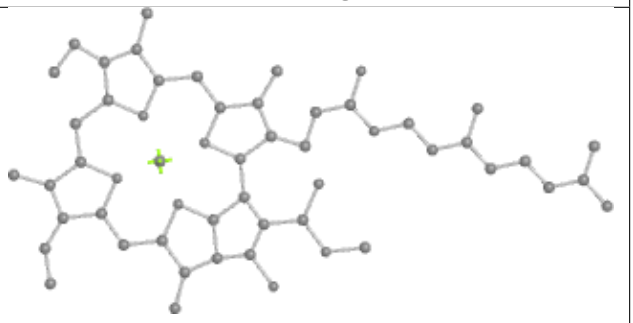
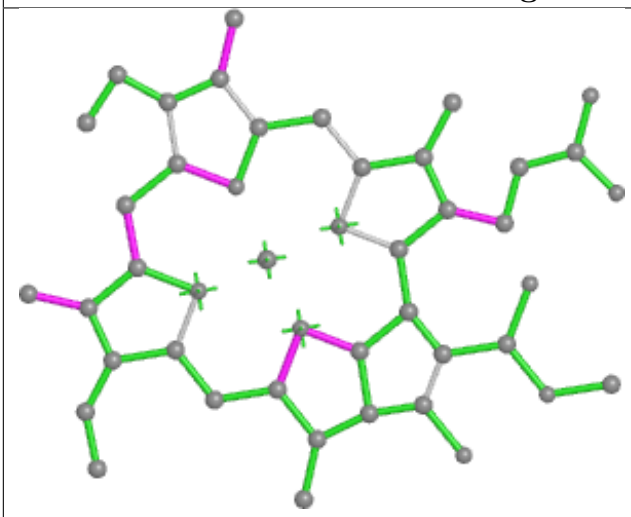


Rings

Ligand CLA e 1801



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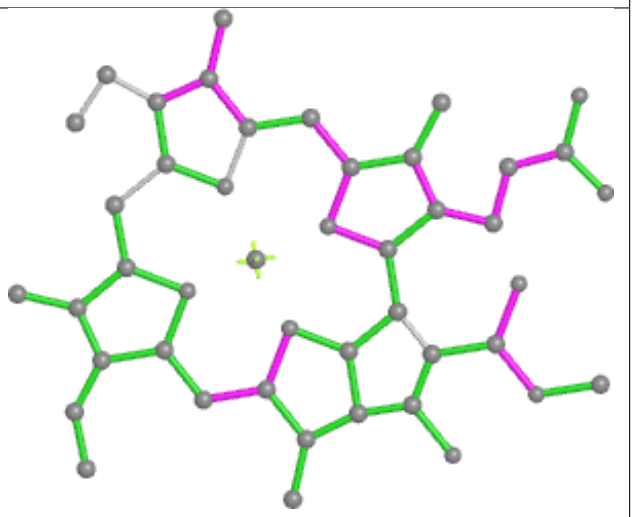
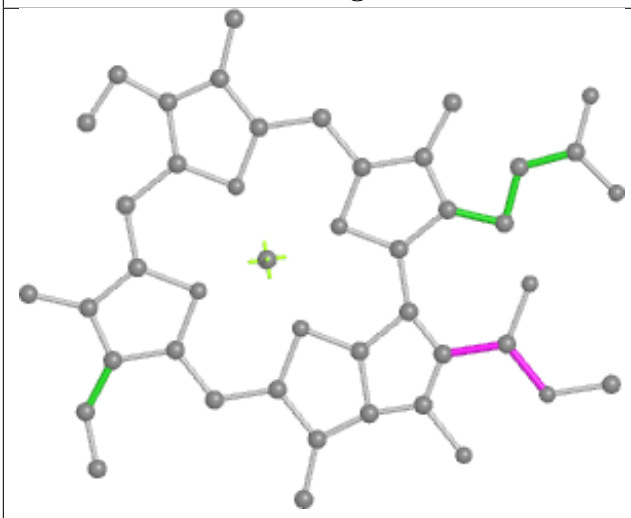


Bond angles



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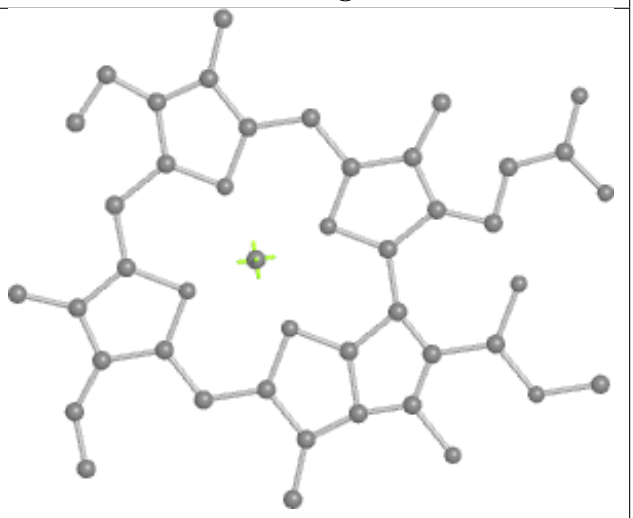
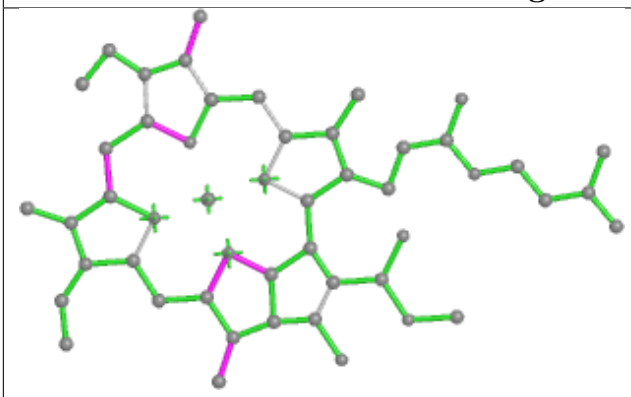


Rings

Ligand CLA 6 502



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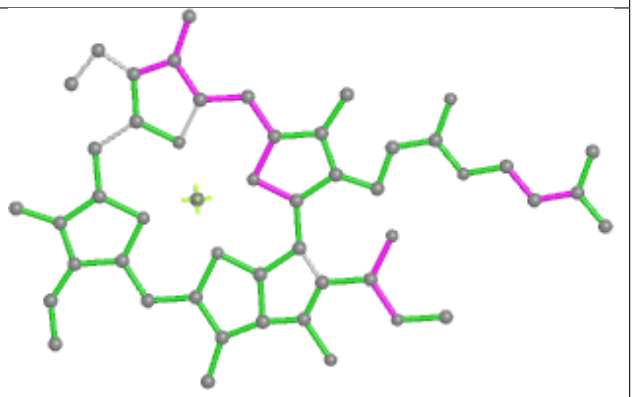
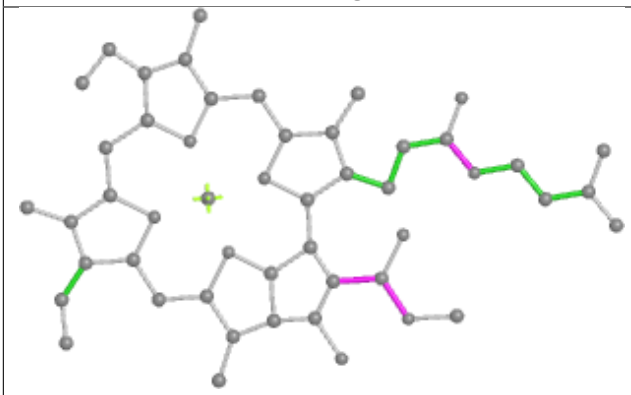


Bond angles



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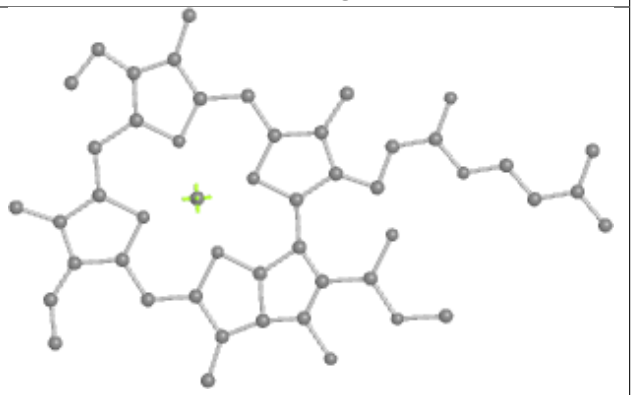
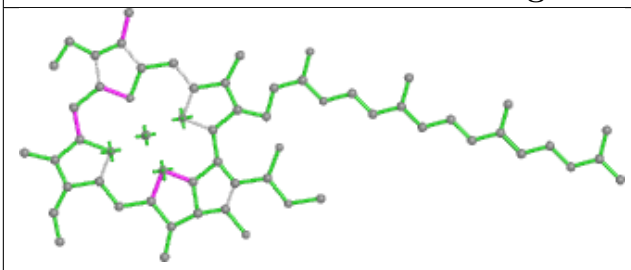


Rings

Ligand CLA b 501



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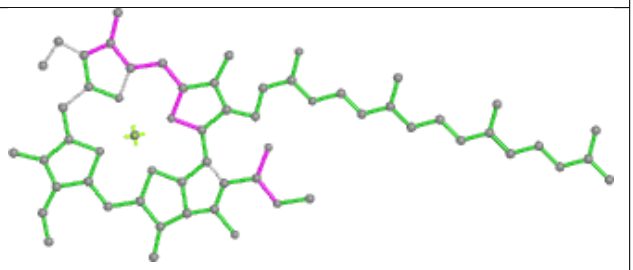
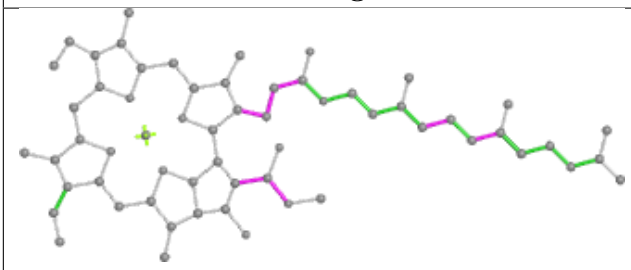


Bond angles



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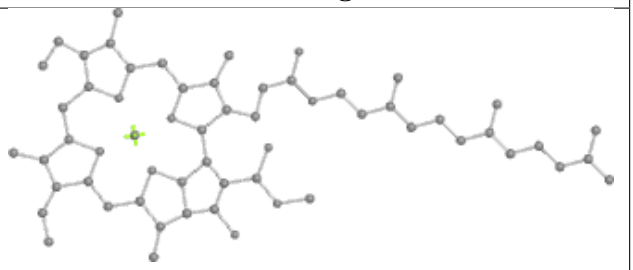
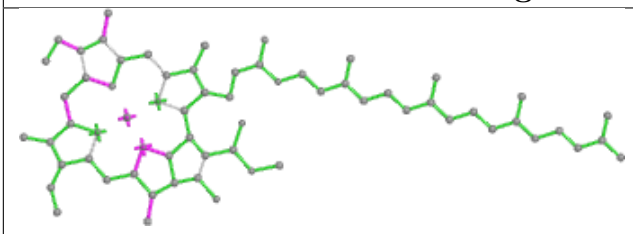


Rings

Ligand CLA A 1133



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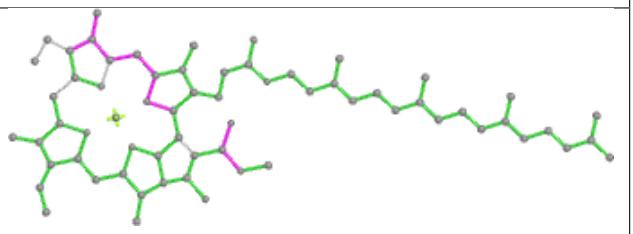
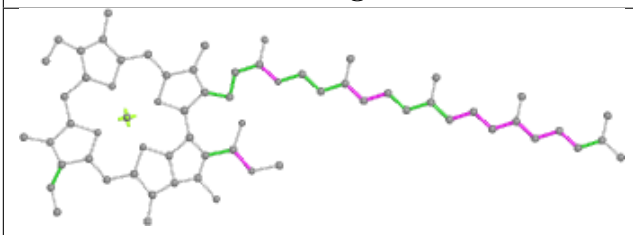


Bond angles



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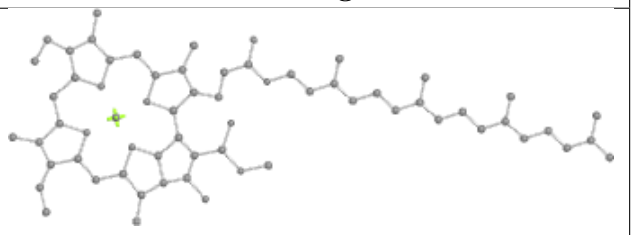
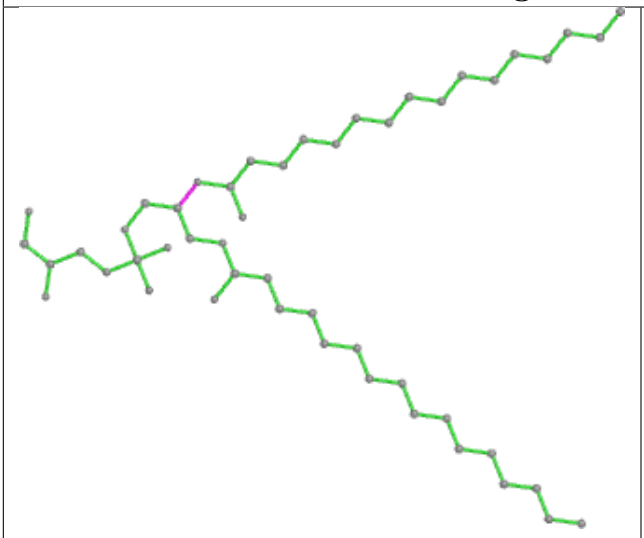
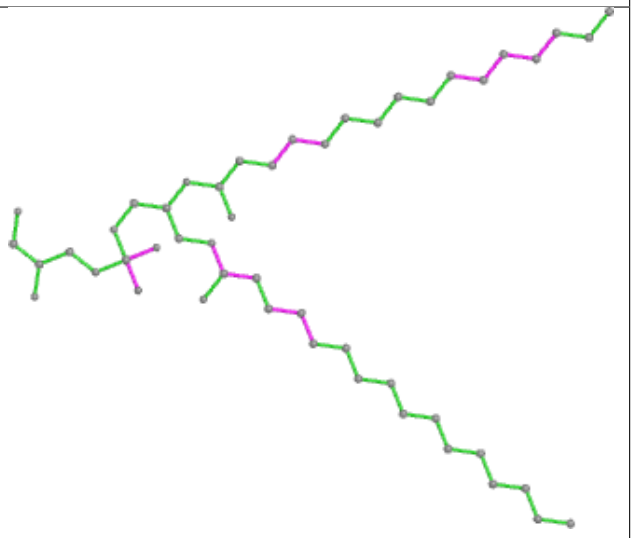


Rings

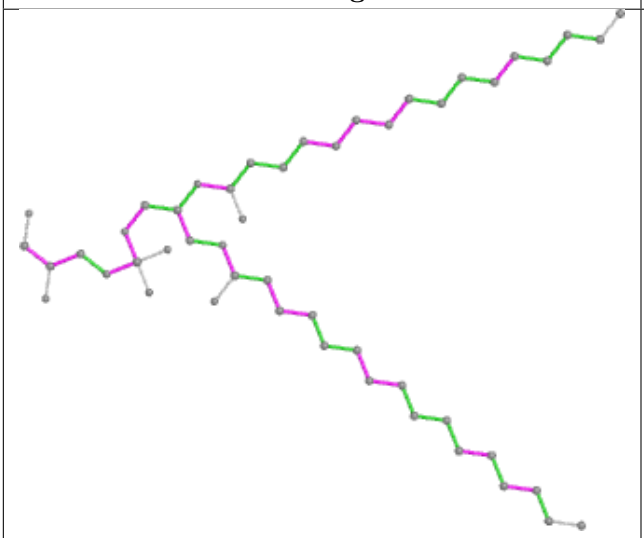
Ligand LHG A 5009



Bond lengths



Bond angles



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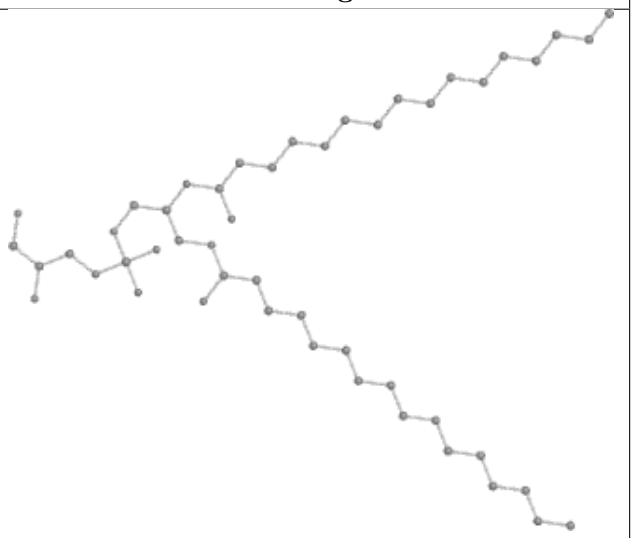
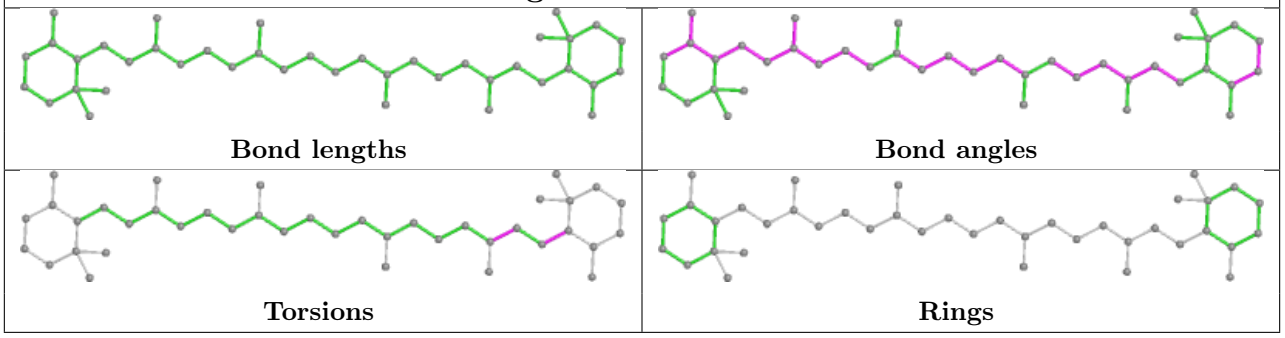
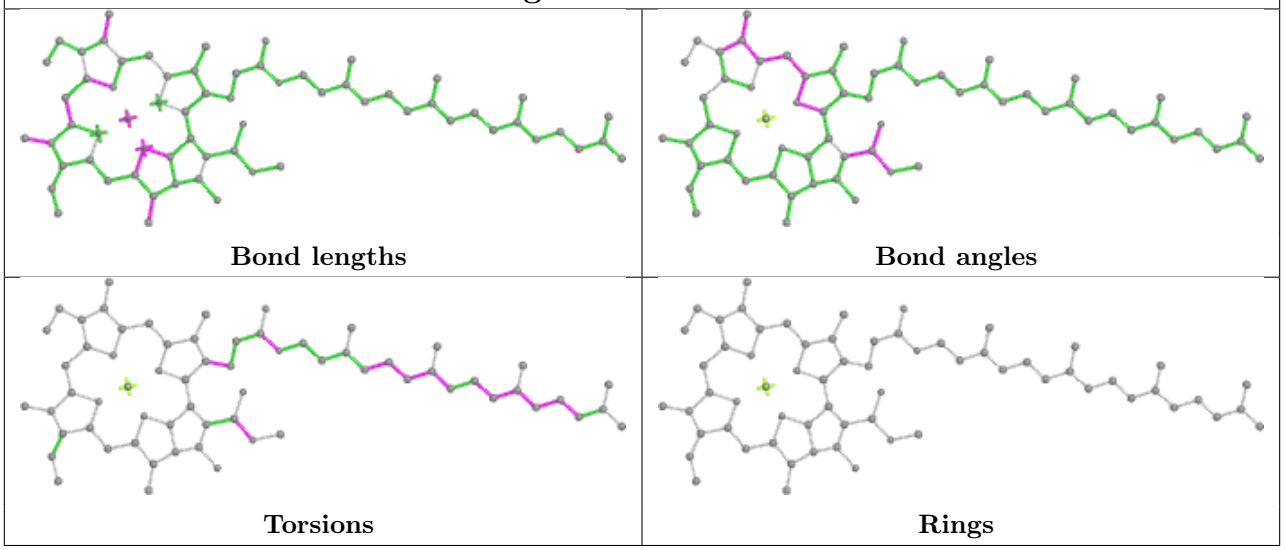


Rings

Ligand BCR d 523



Ligand CLA f 1215



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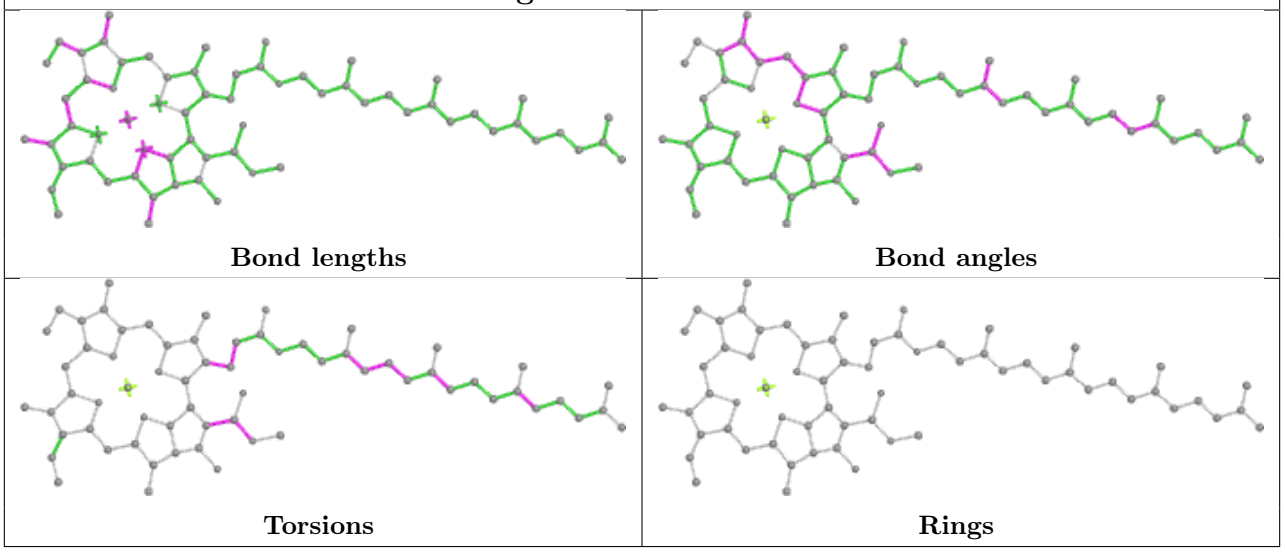
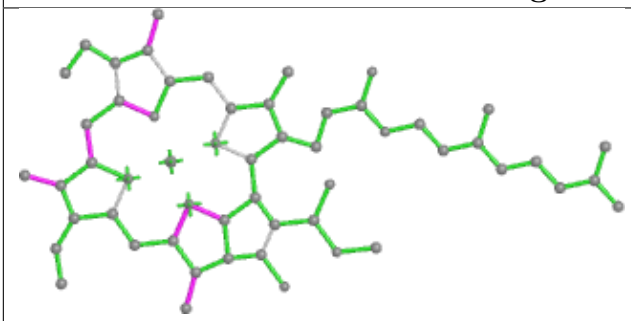
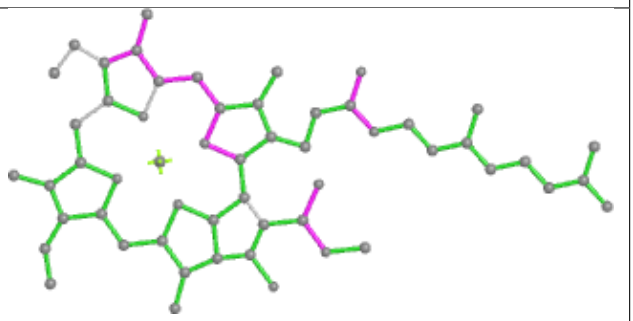


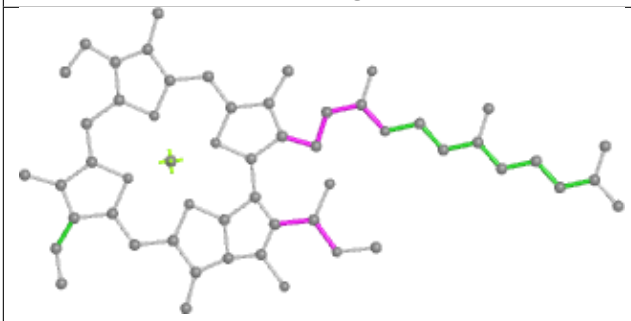
Ligand CLA s 518



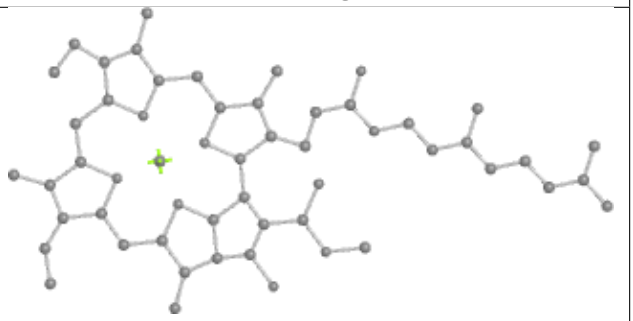
Bond lengths



Bond angles

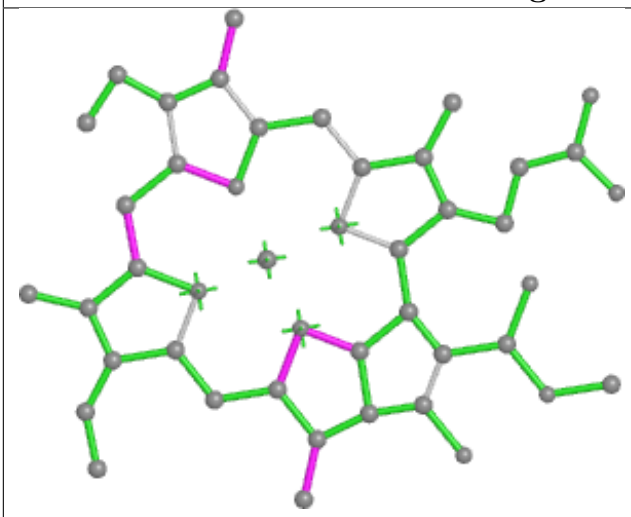


Torsions

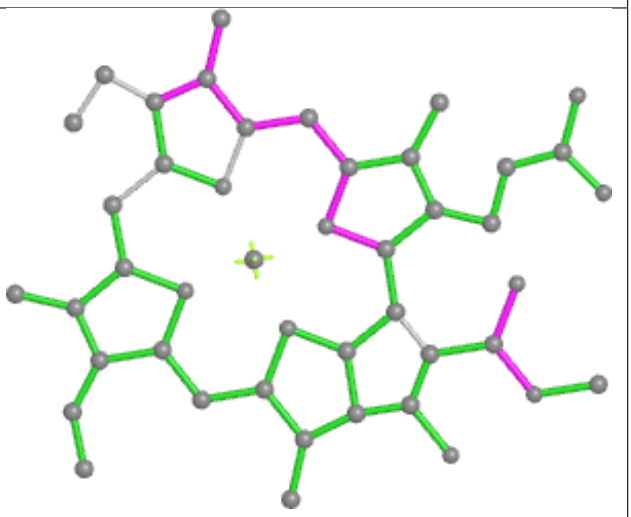


Rings

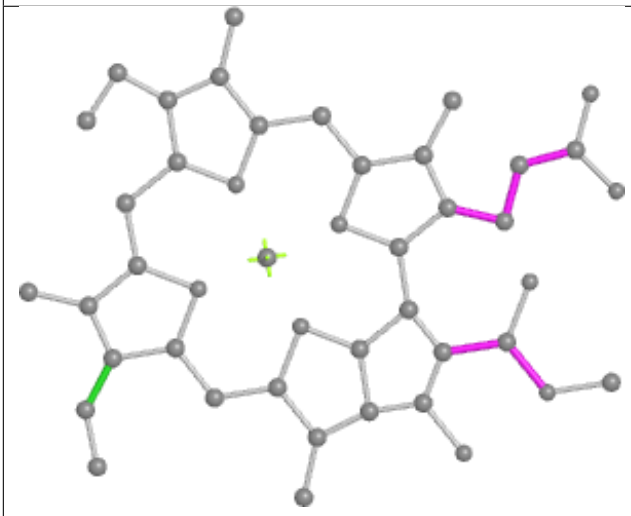
Ligand CLA c 517



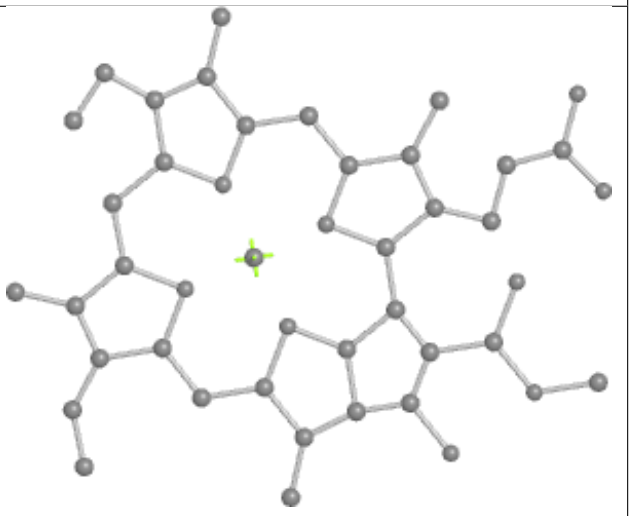
Bond lengths



Bond angles

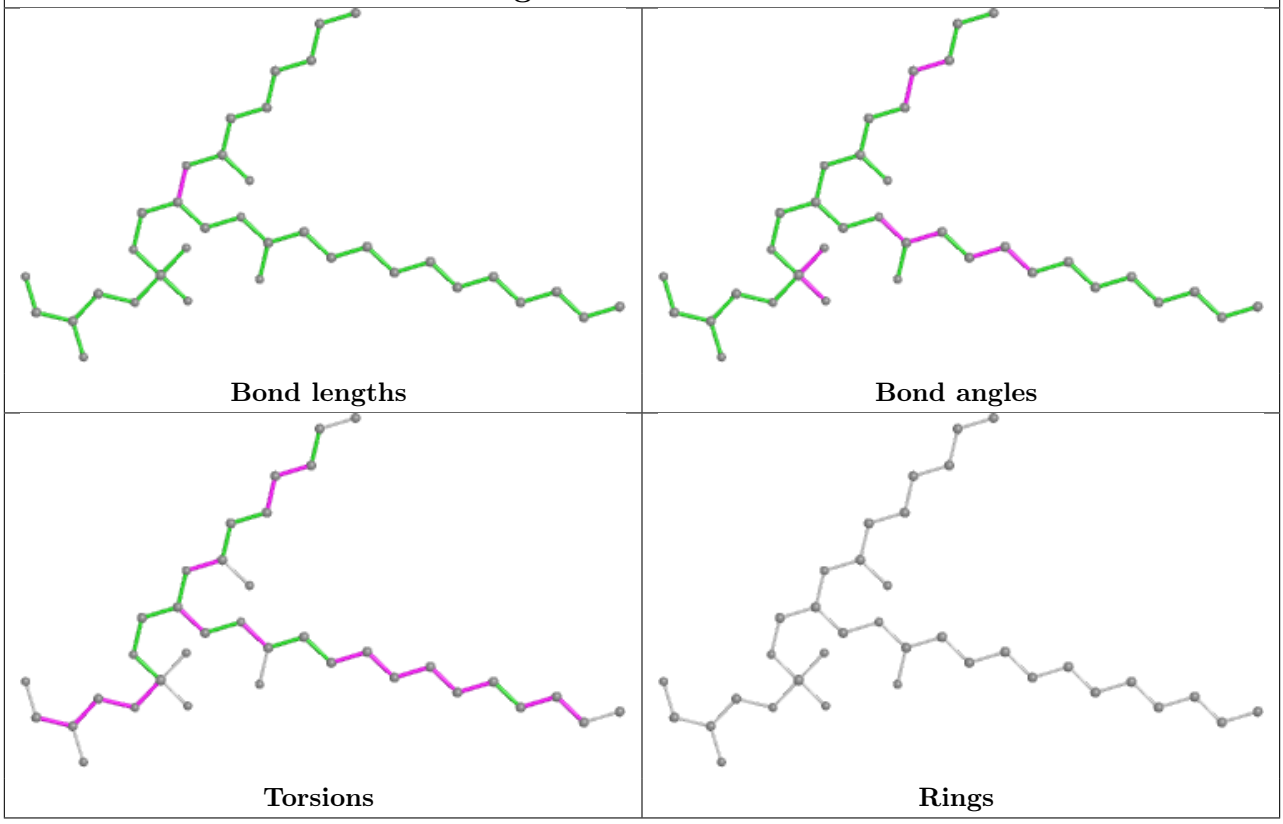


Torsions

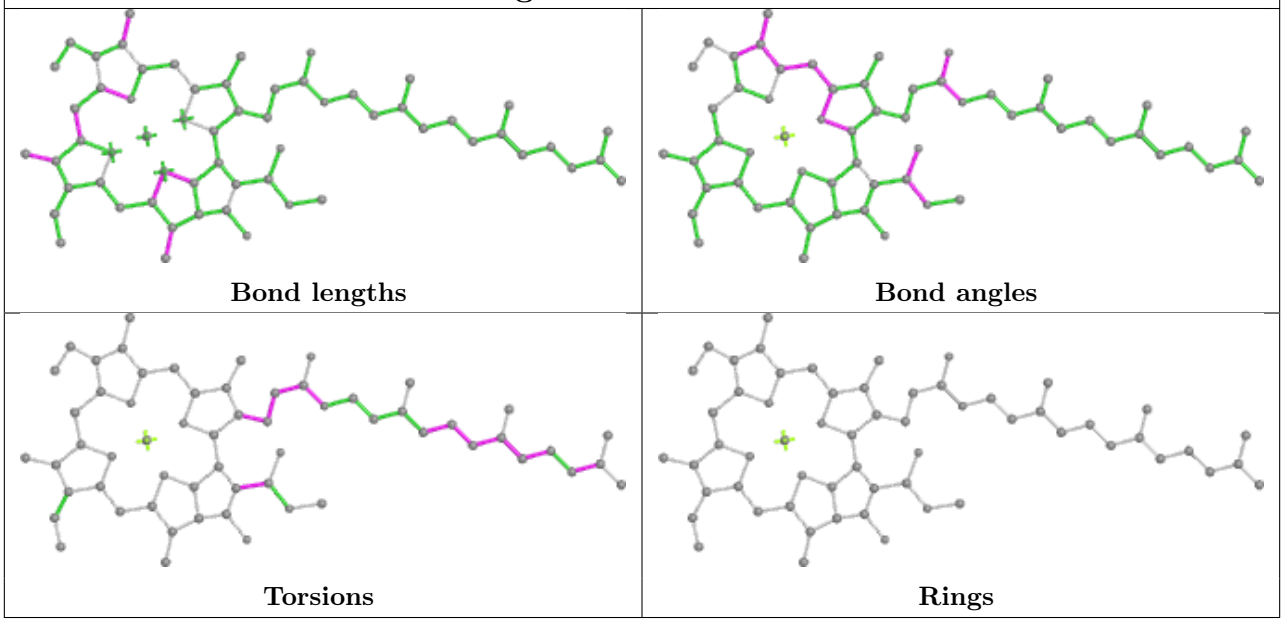


Rings

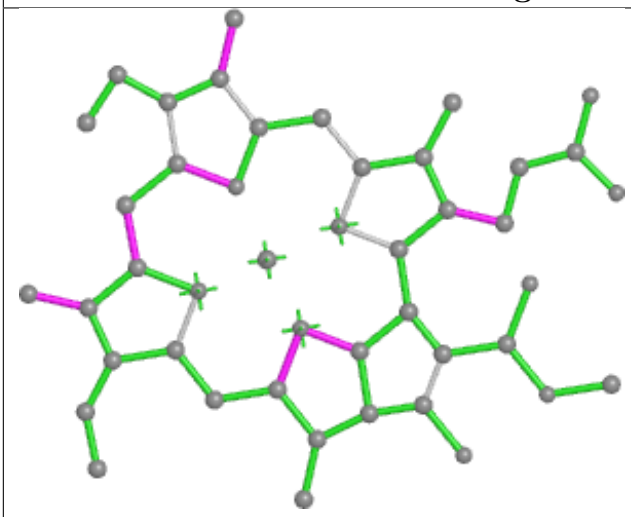
Ligand LHG A 5004



Ligand CLA A 1116



Ligand CLA G 1801



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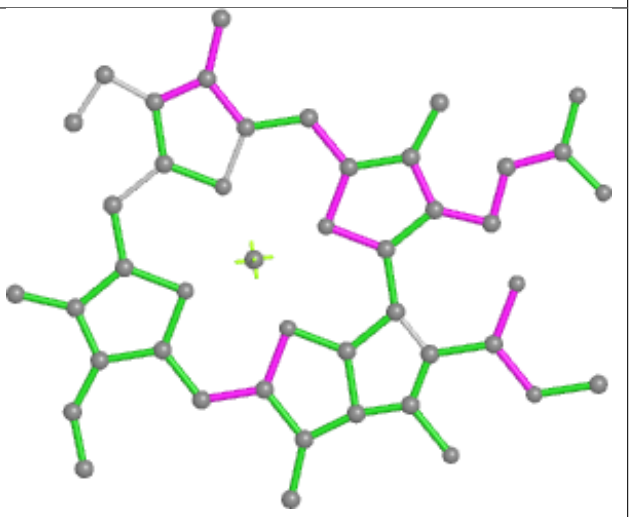
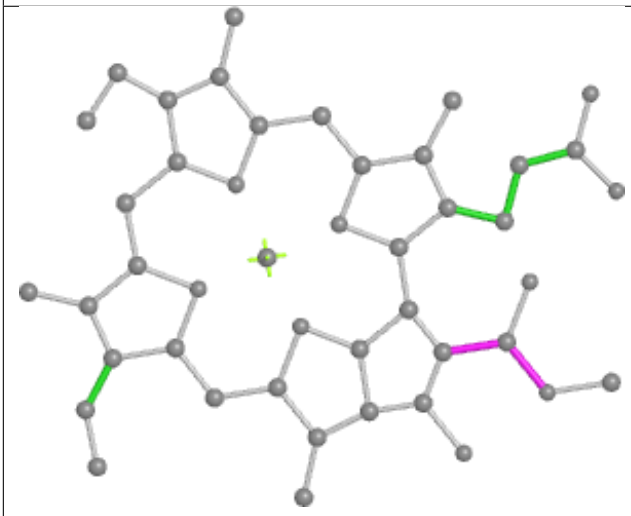
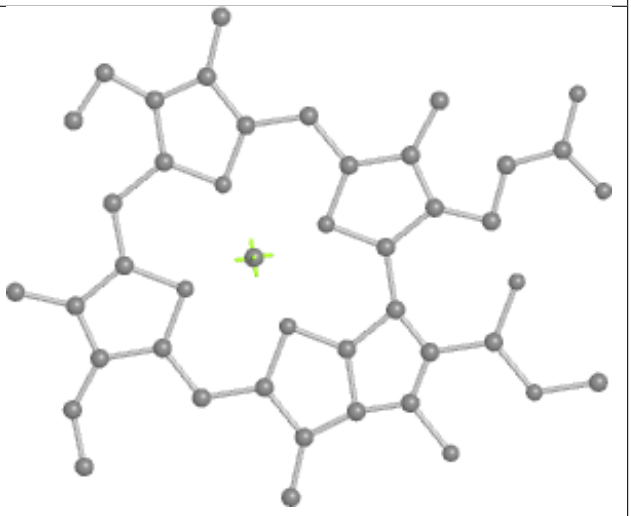


Bond angles

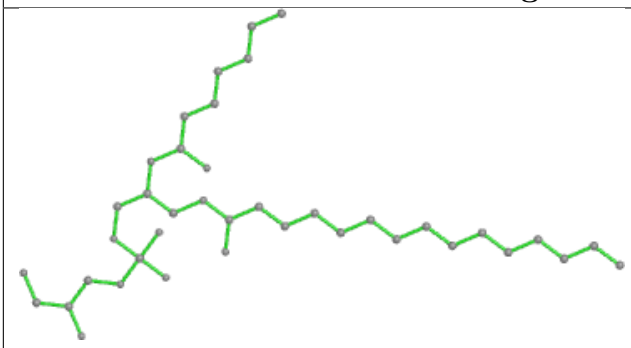


Torsions

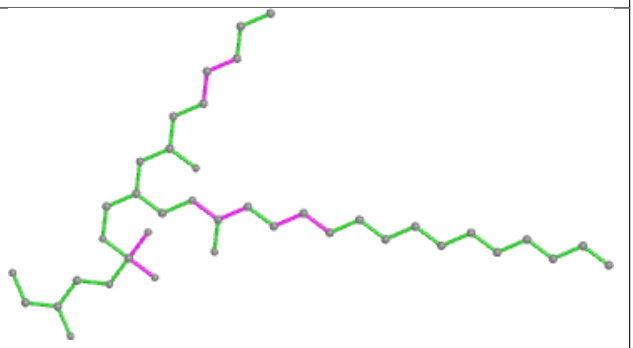


Rings

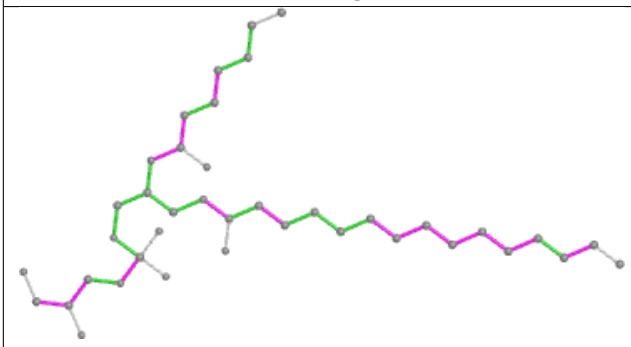
Ligand LHG f 1842



Bond lengths



Bond angles



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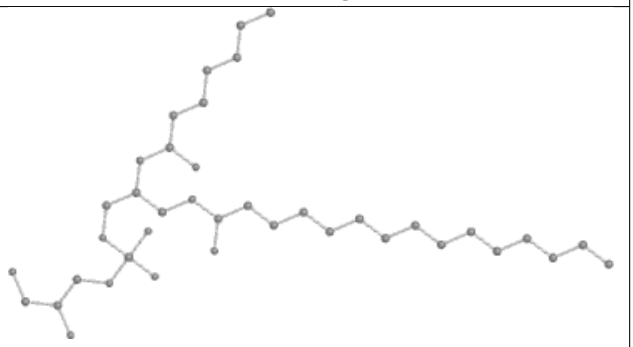
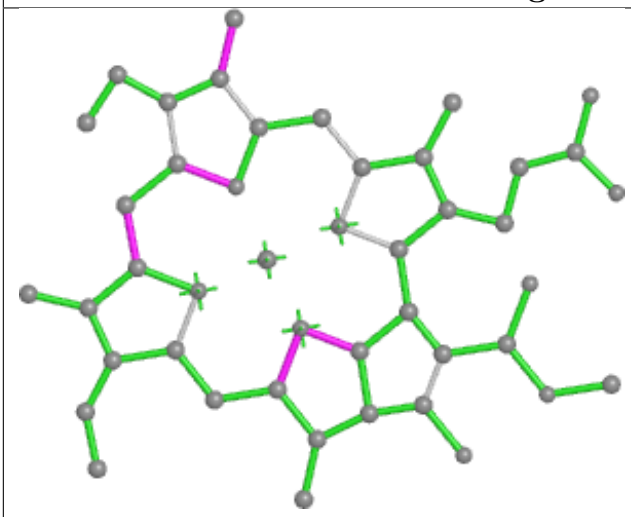
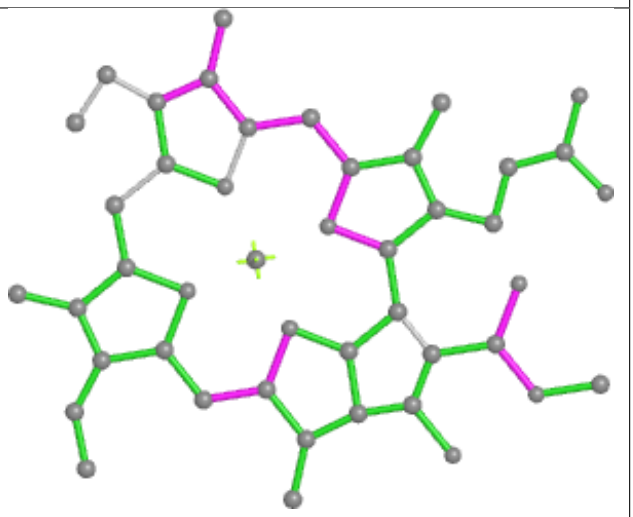


Rings

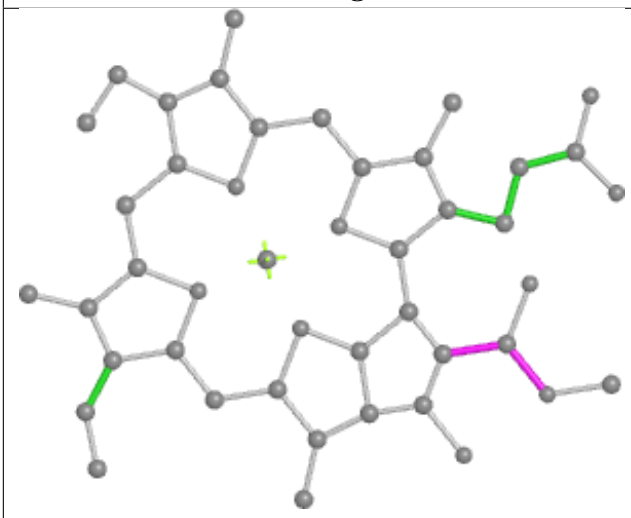
Ligand CLA 5 504



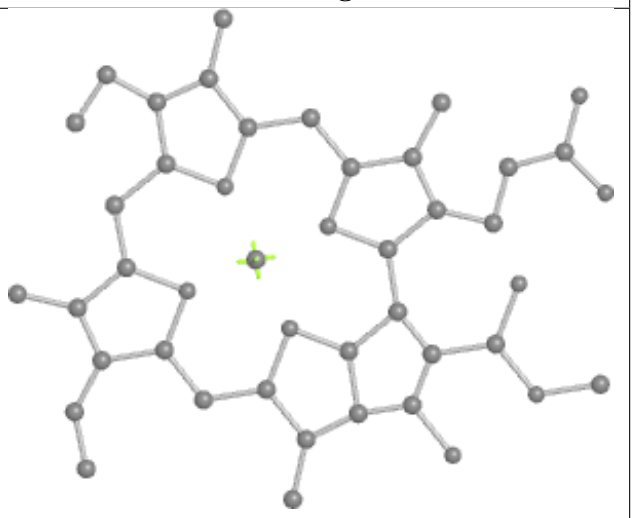
Bond lengths



Bond angles

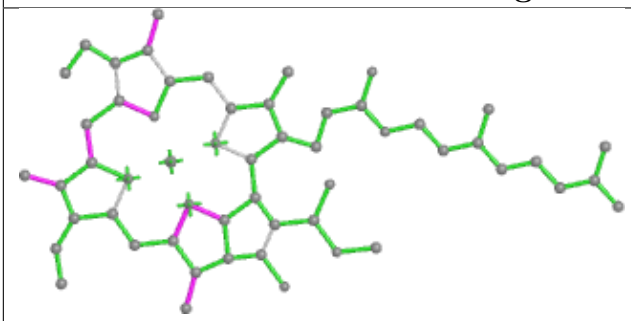


Torsions



Rings

Ligand CLA A 1121



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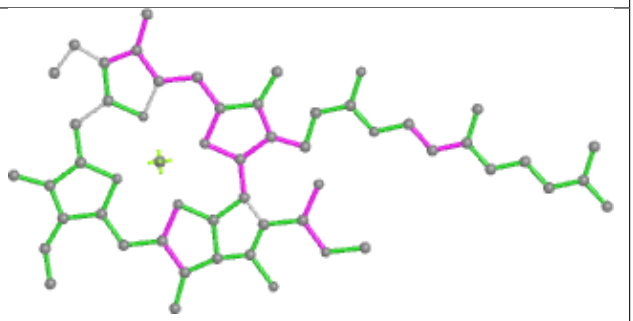
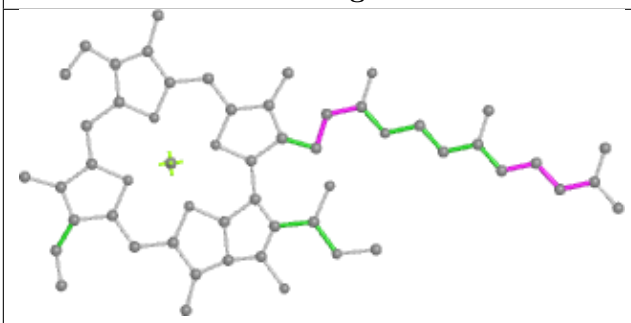


Bond angles



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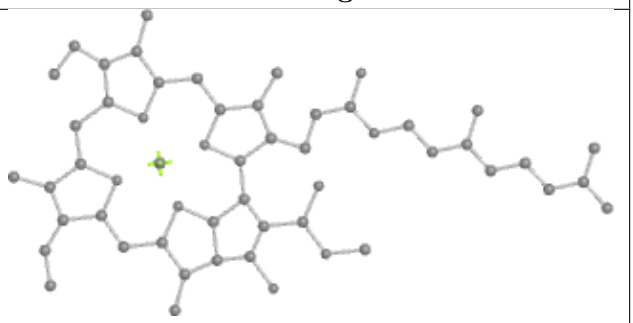
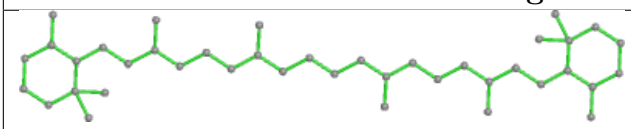


Rings

Ligand BCR 1 524



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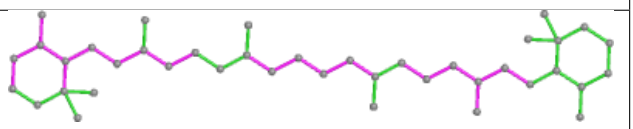
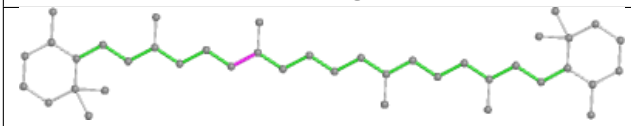


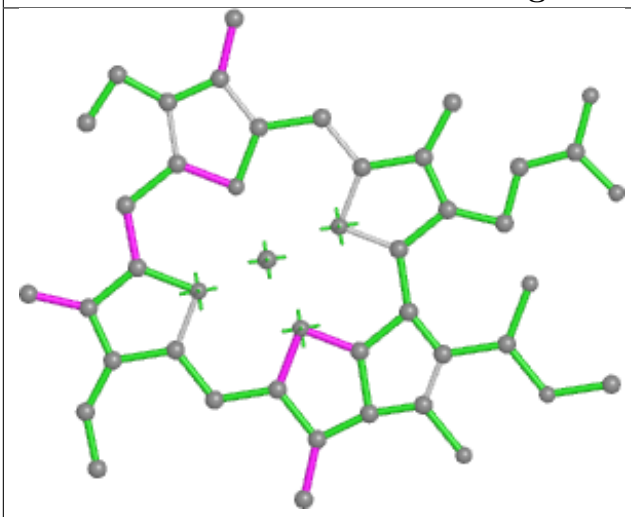
Bond angles



Torsions

Rings

Ligand CLA 4 513



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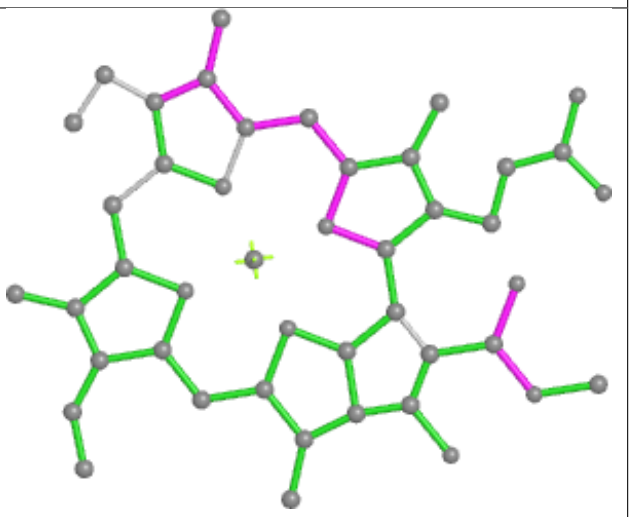
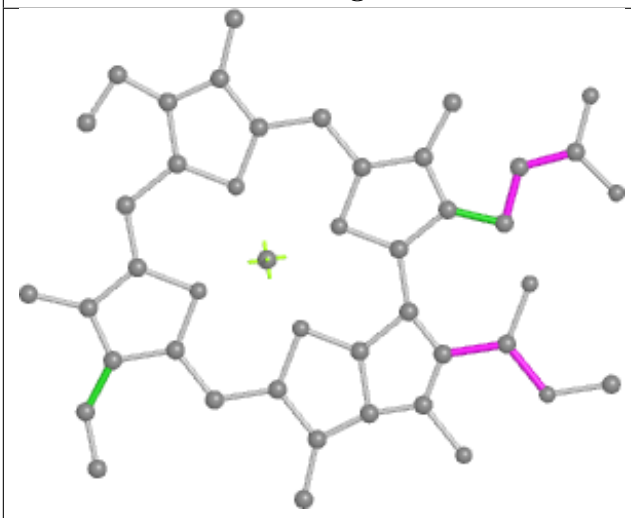


Bond angles



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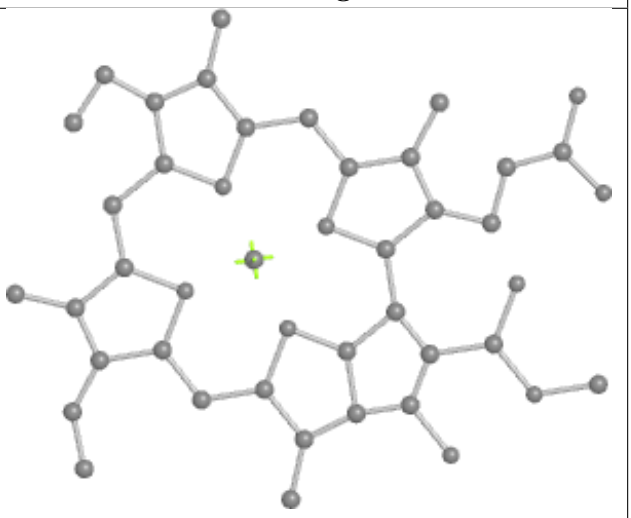
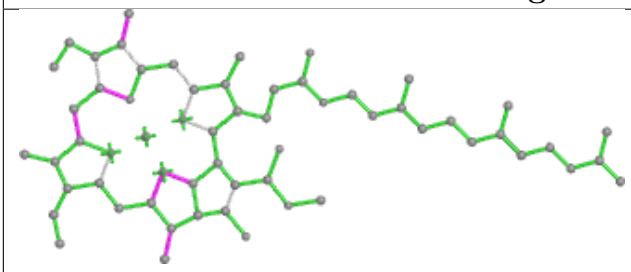


Rings

Ligand CLA 6 501



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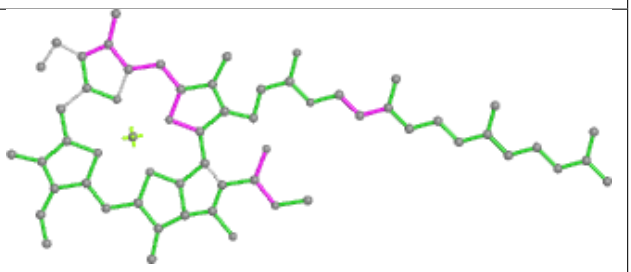

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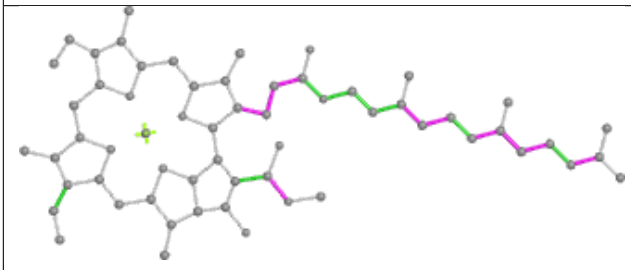

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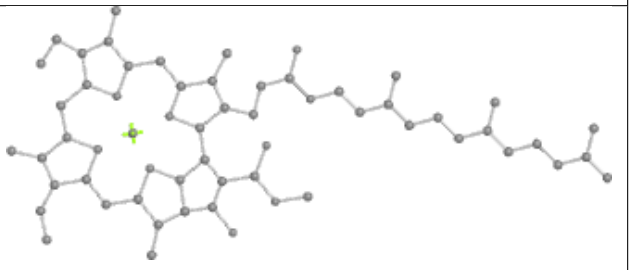
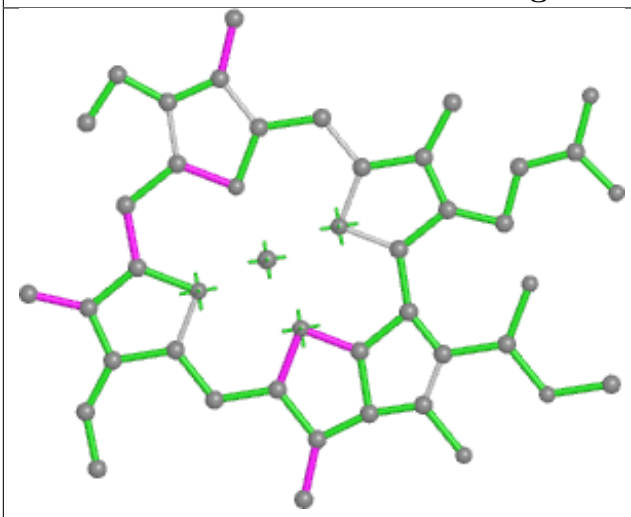
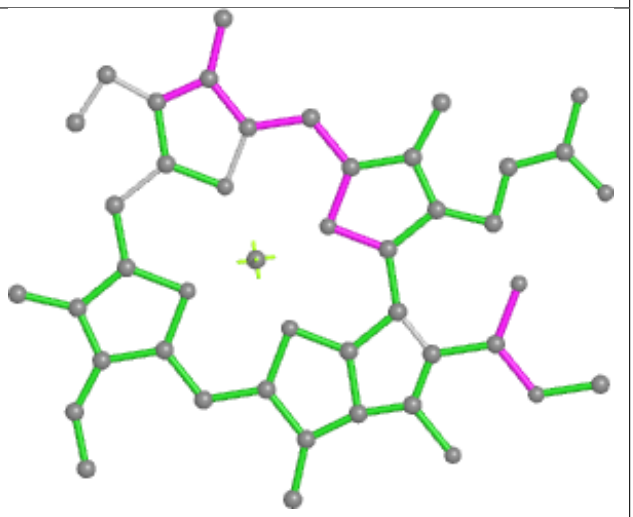


Rings

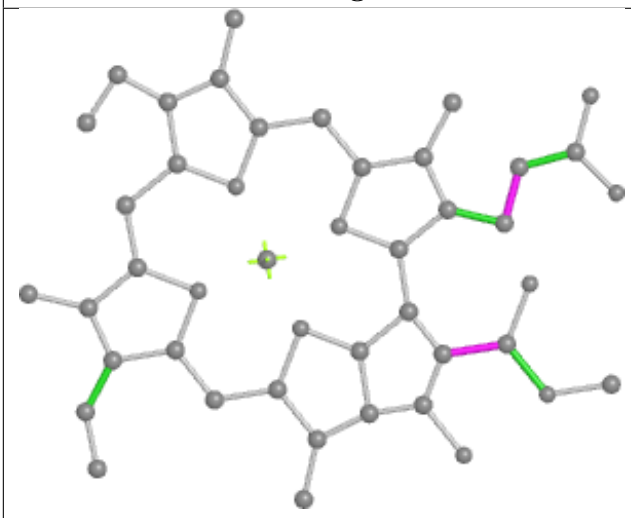
Ligand CLA r 517



Bond lengths



Bond angles



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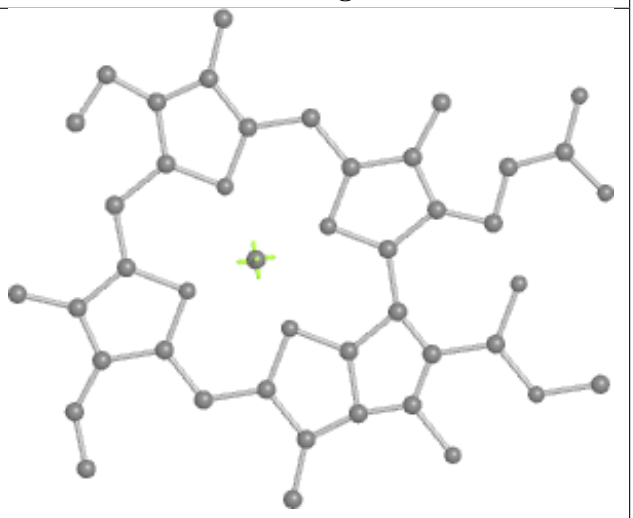
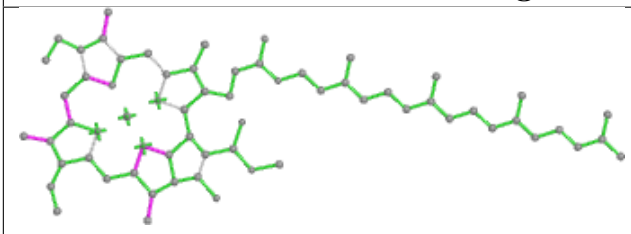


Rings

Ligand CLA B 1213



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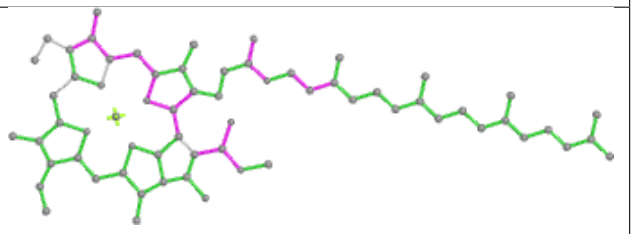
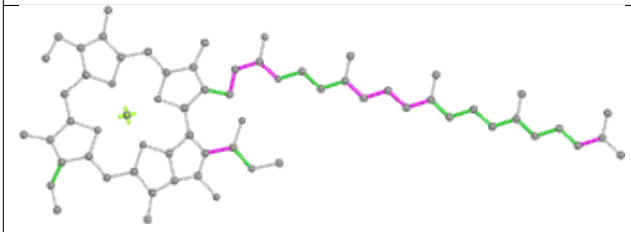


Bond angles



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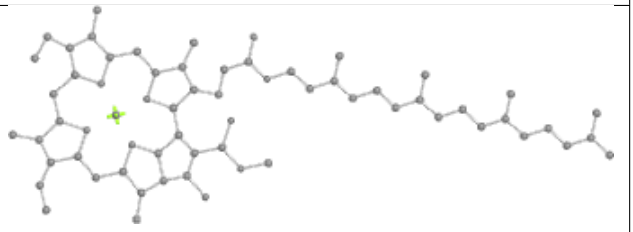
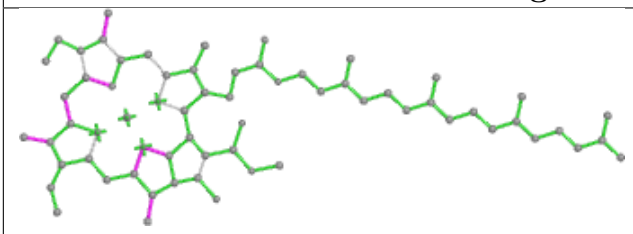


Rings

Ligand CLA r 510



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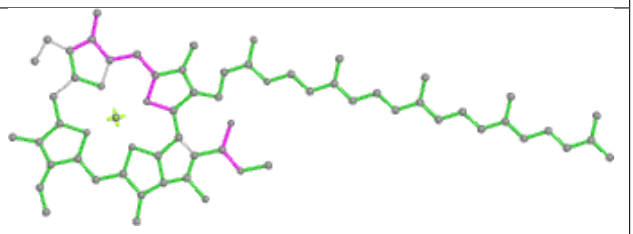
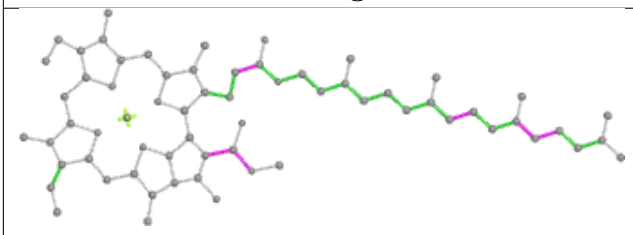


Bond angles



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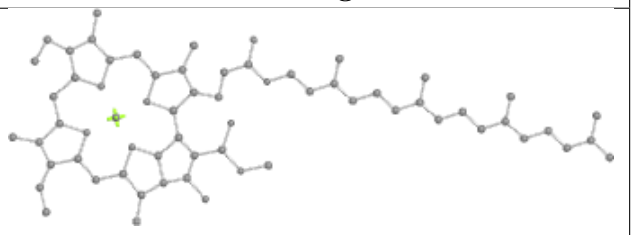
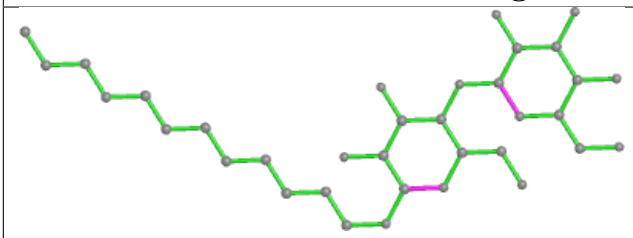


Rings

Ligand LMU A 1848



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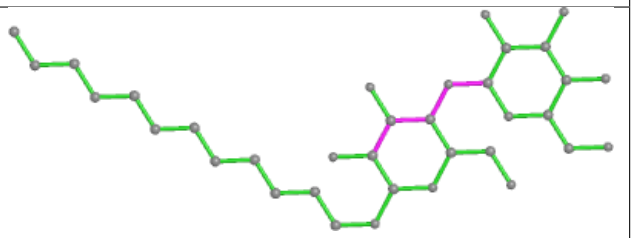
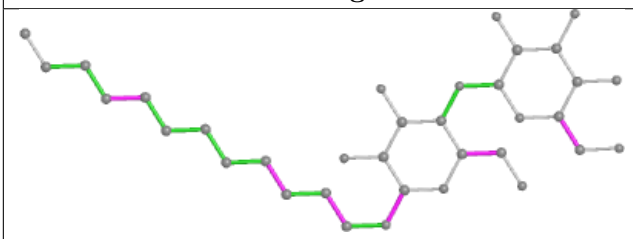


Bond angles



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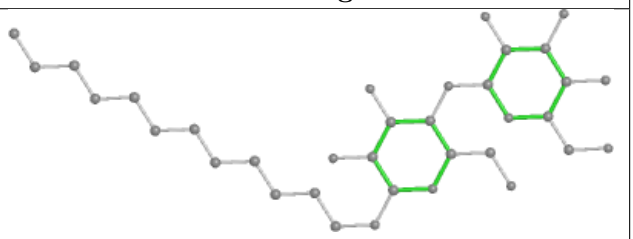
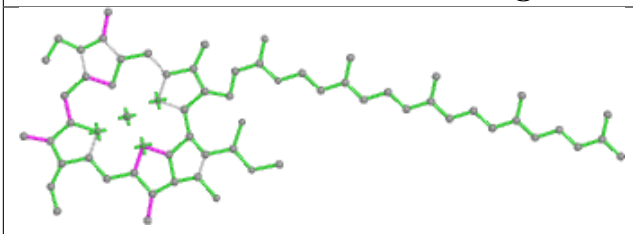
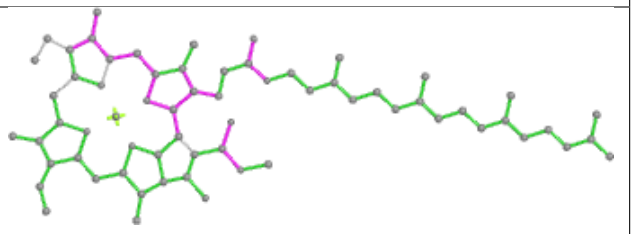


Rings

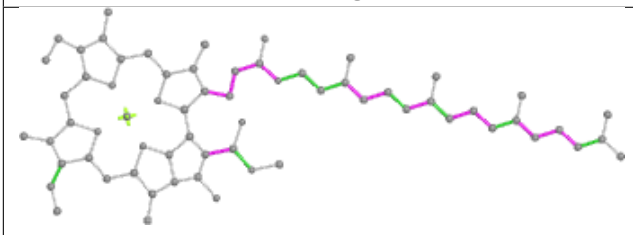
Ligand CLA V 1501



Bond lengths



Bond angles



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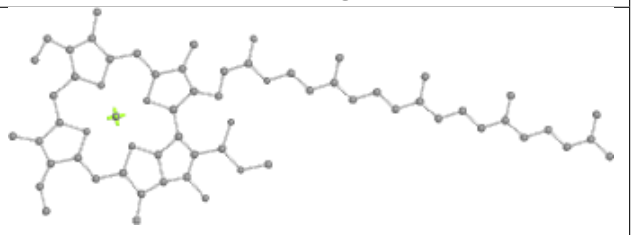
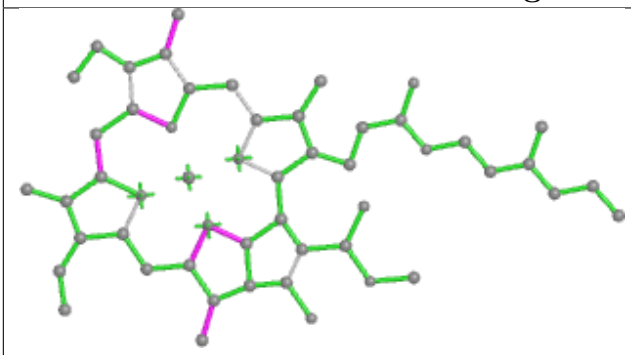
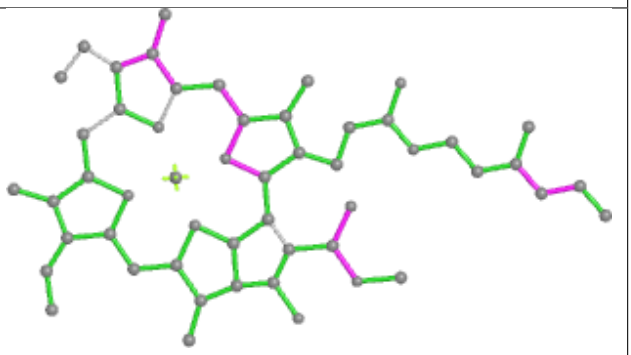


Rings

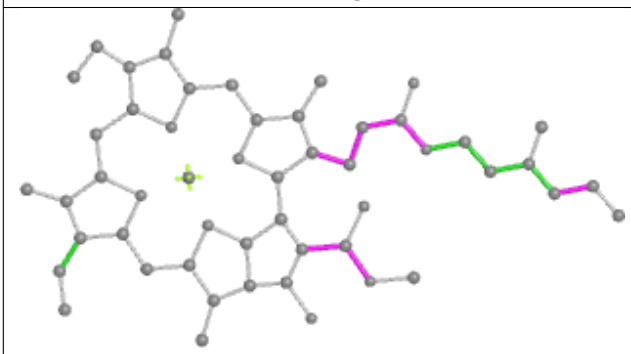
Ligand CLA Y 512



Bond lengths



Bond angles



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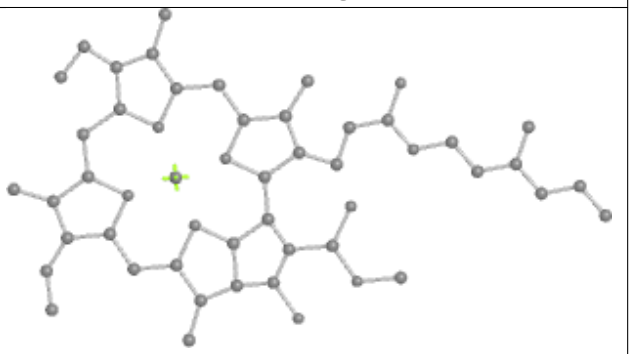
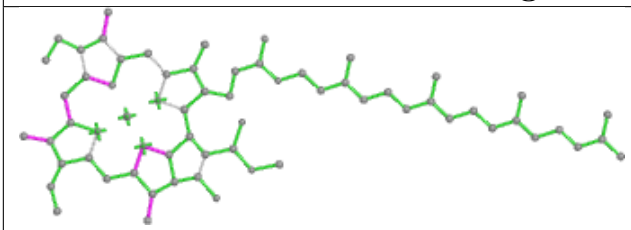
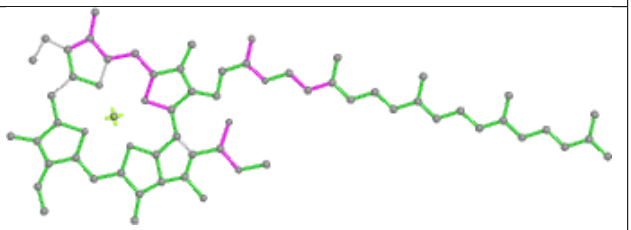


Rings

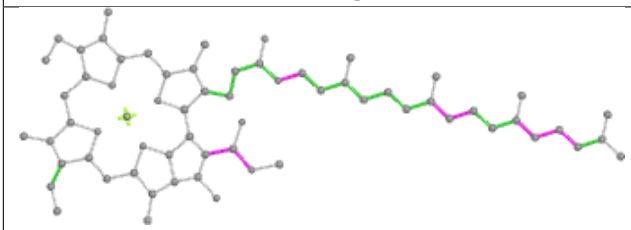
Ligand CLA e 1138



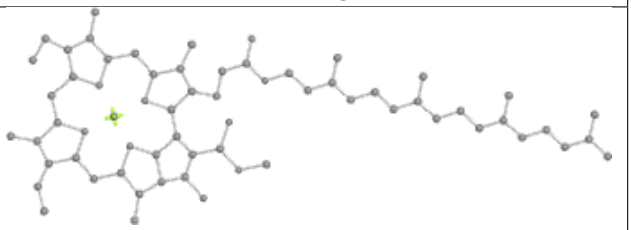
Bond lengths



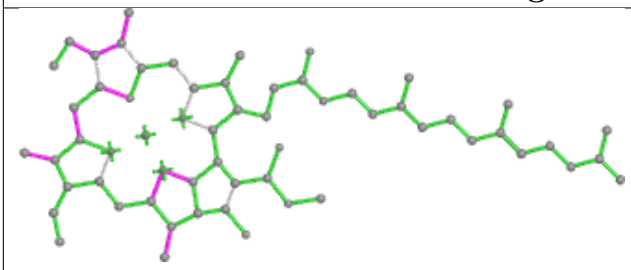
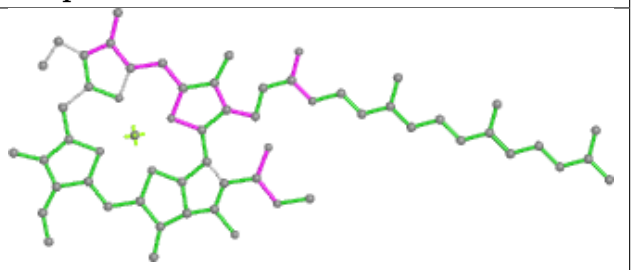
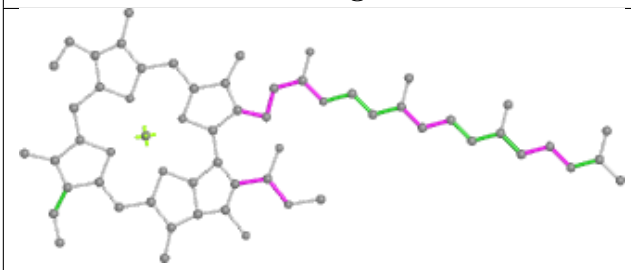
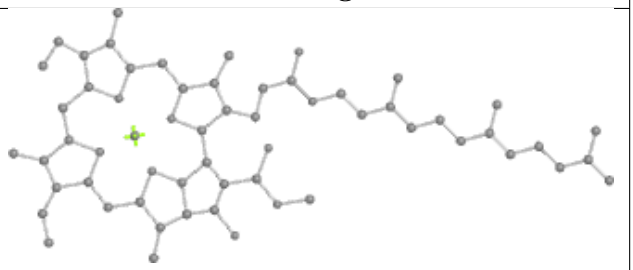
Bond angles

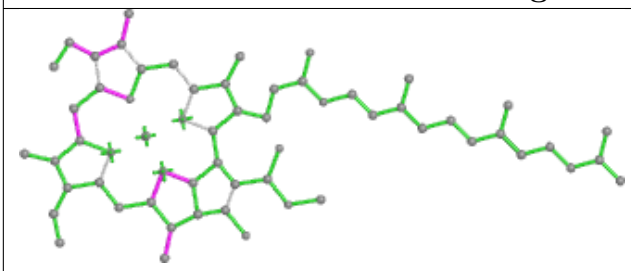
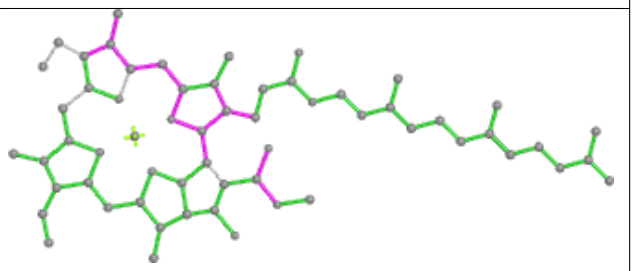
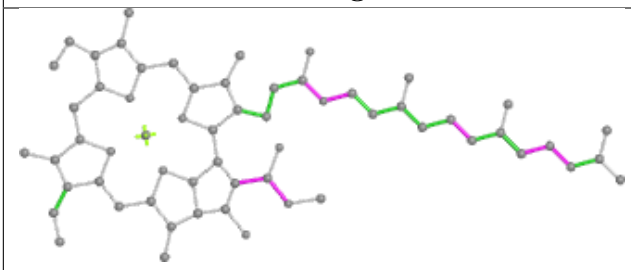
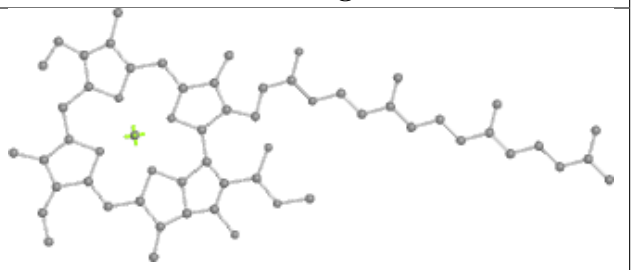


Torsions

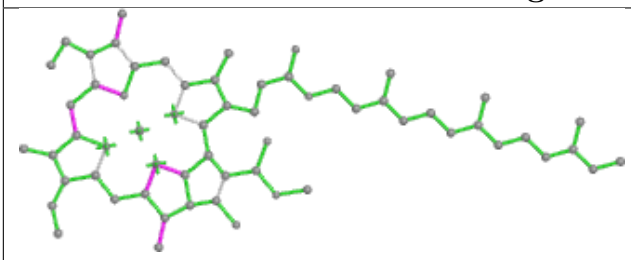


Rings

Ligand CLA q 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA u 505



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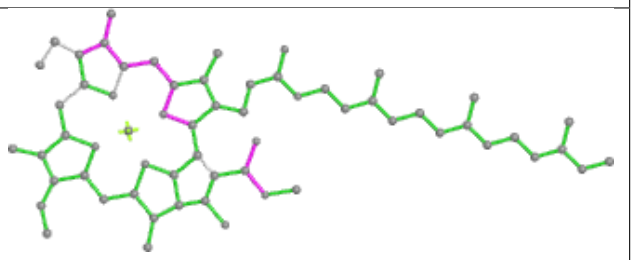
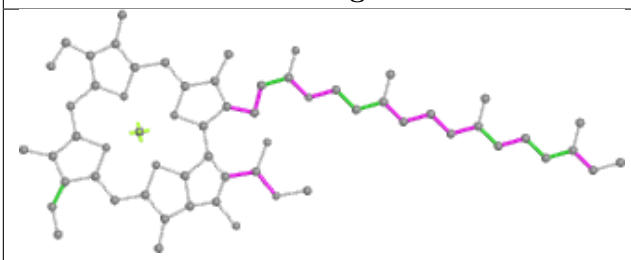


Bond angles



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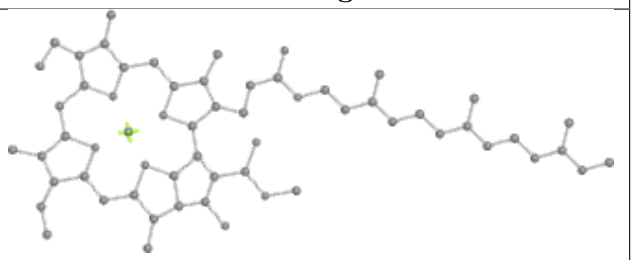
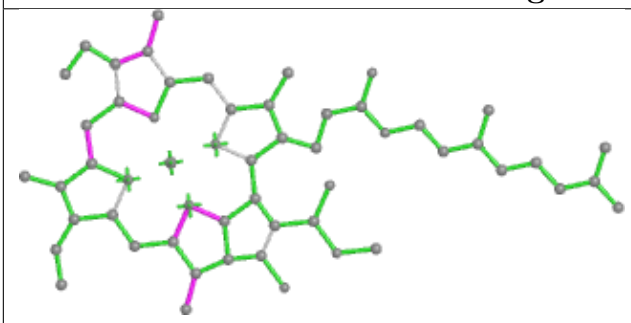


Rings

Ligand CLA b 518



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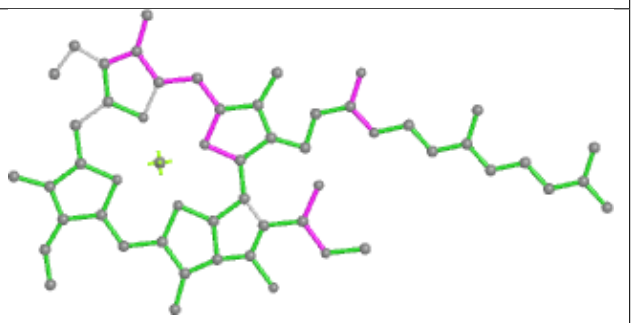

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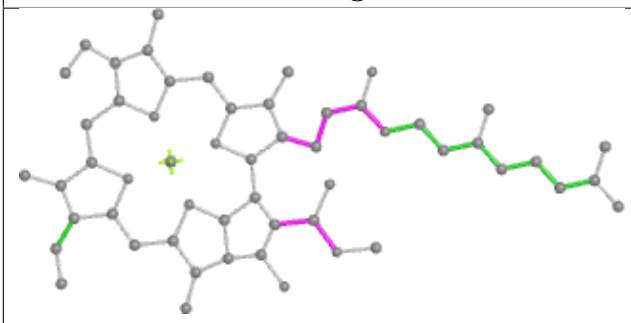

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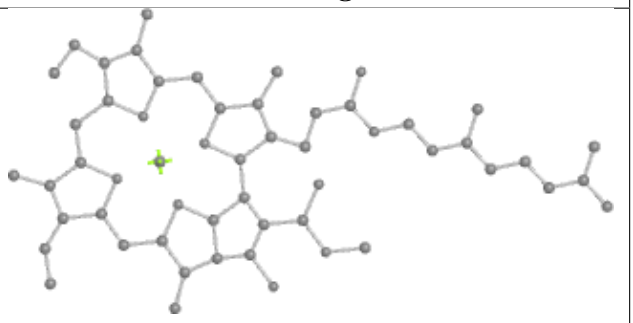
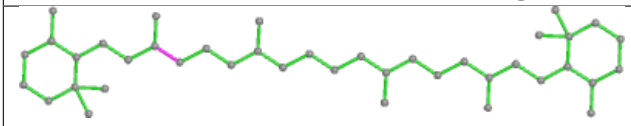


Rings

Ligand BCR G 4008



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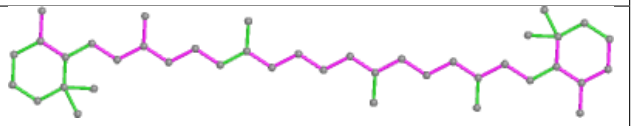

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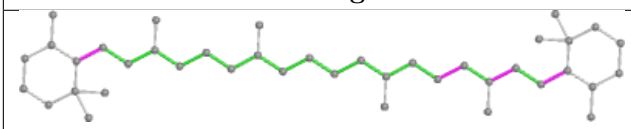

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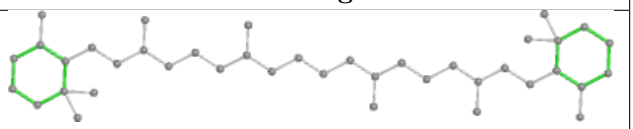
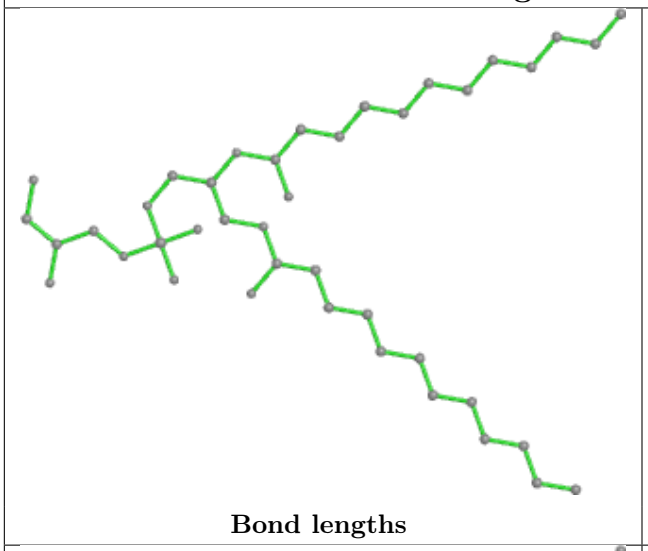


Rings

Ligand LHG V 5220



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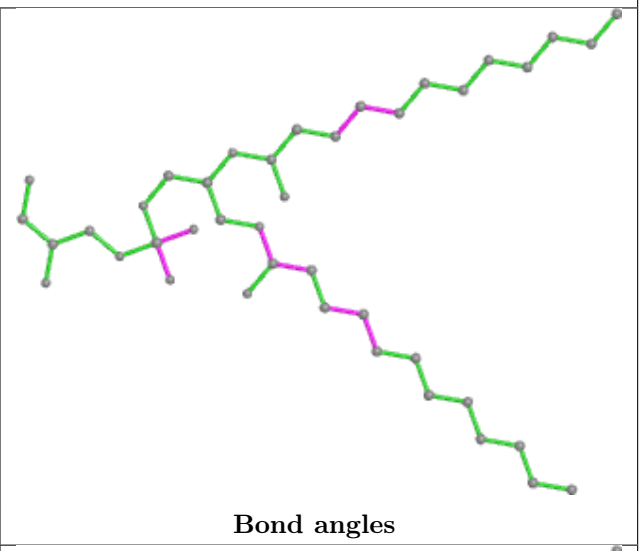
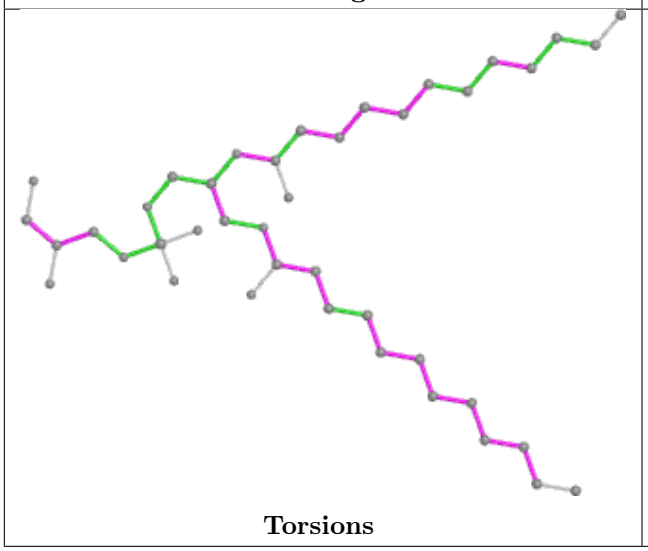


Bond angles



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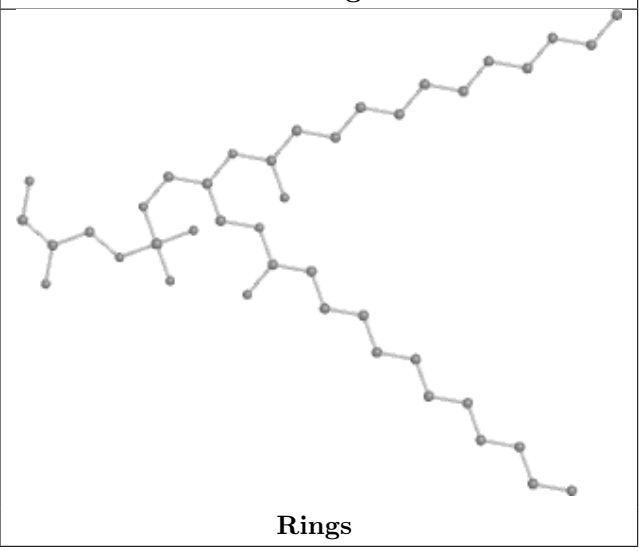
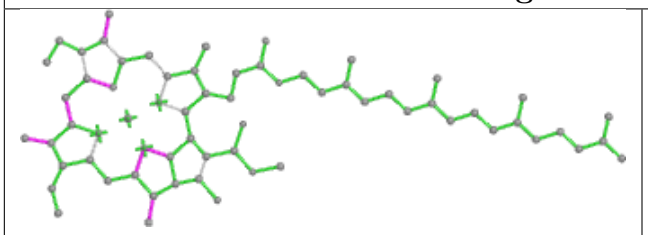


Rings

Ligand CLA A 1123



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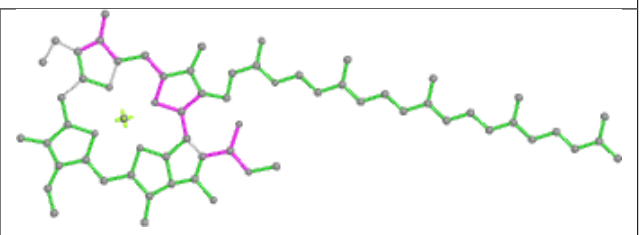

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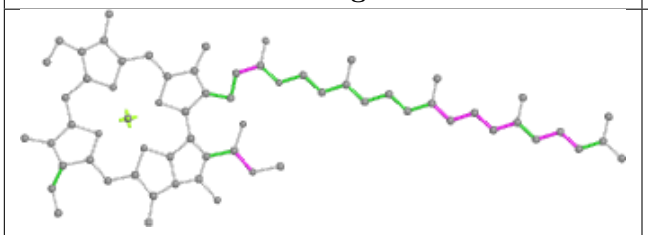

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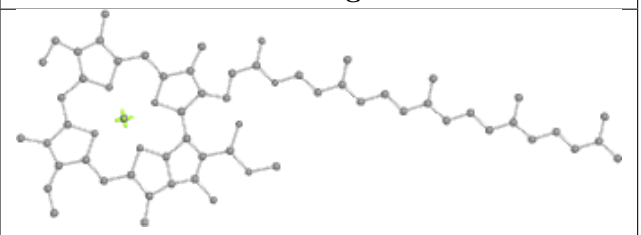
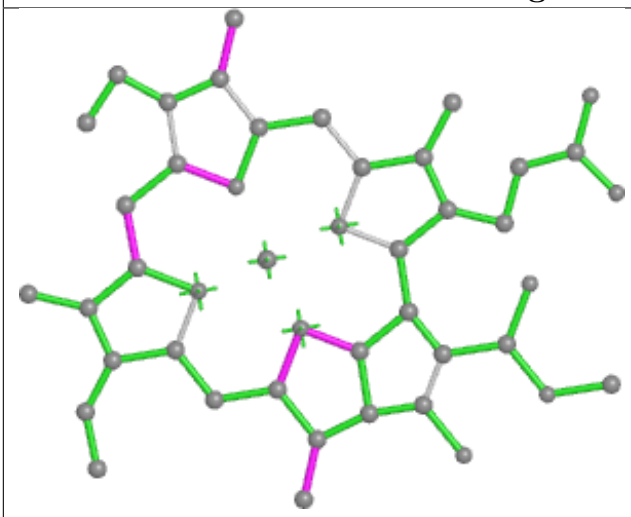


Rings

Ligand CLA 4 507



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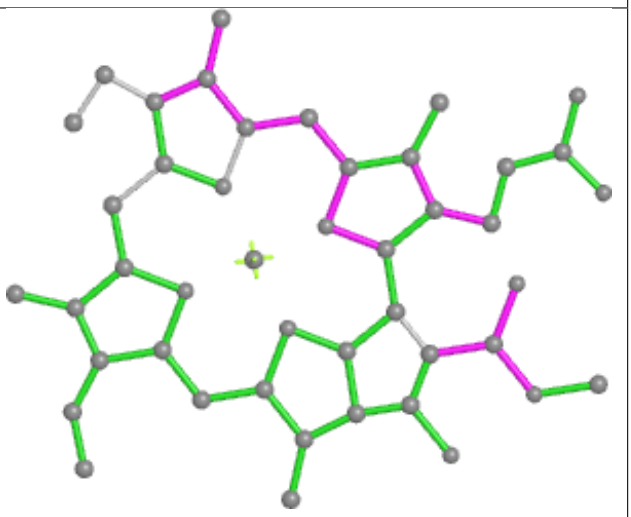
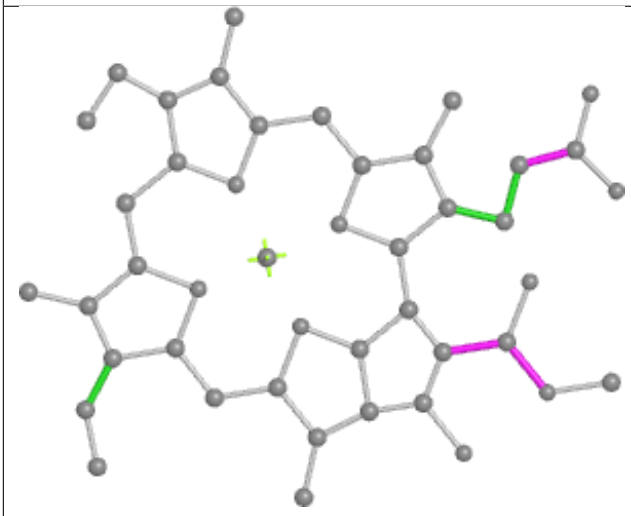


Bond angles



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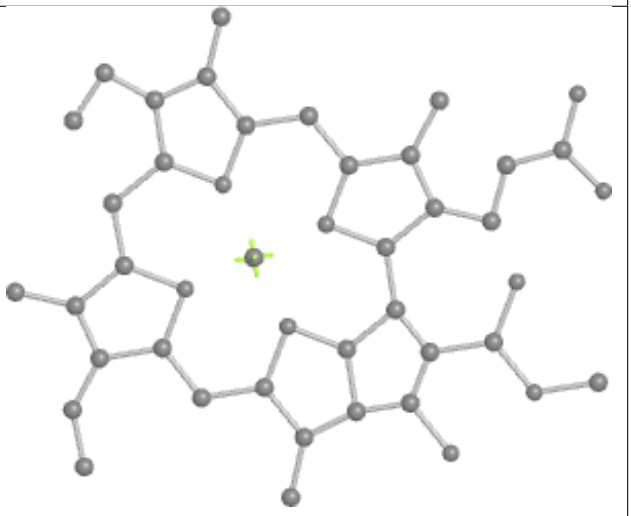
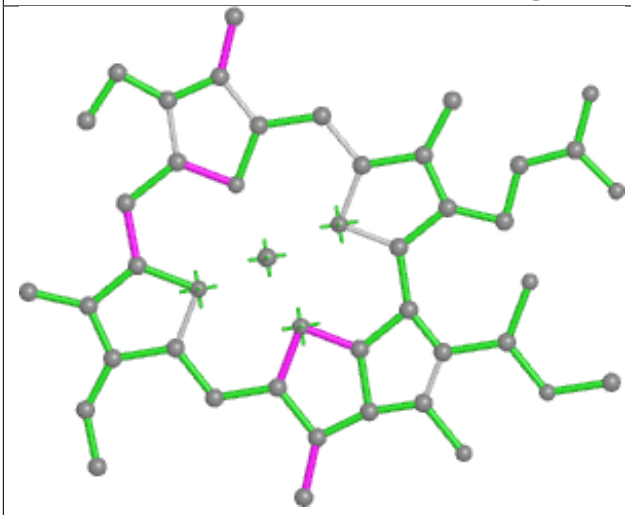


Rings

Ligand CLA b 507



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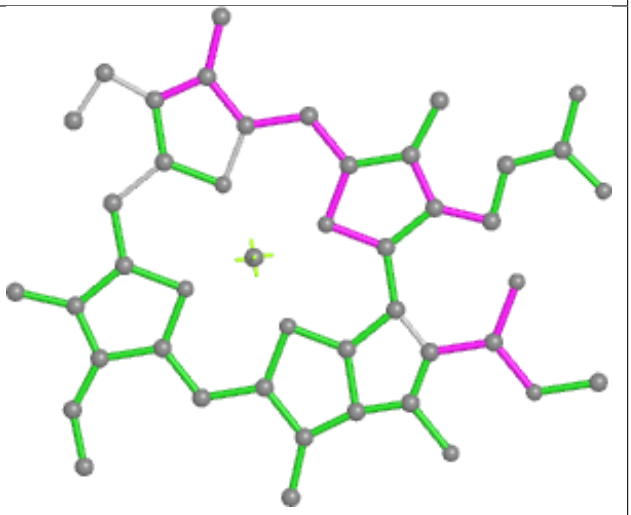
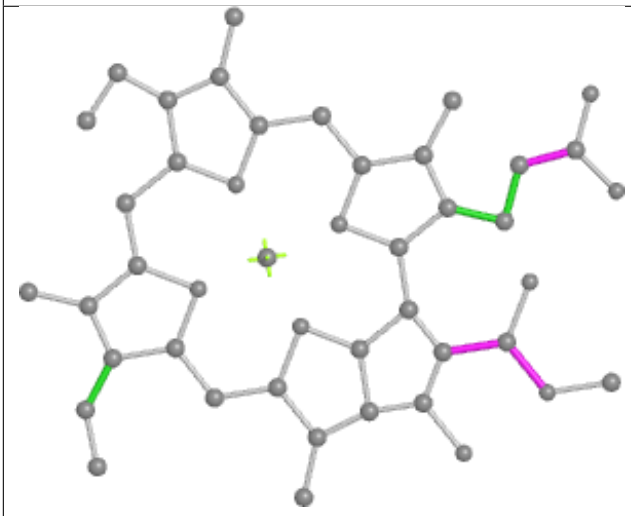


Bond angles



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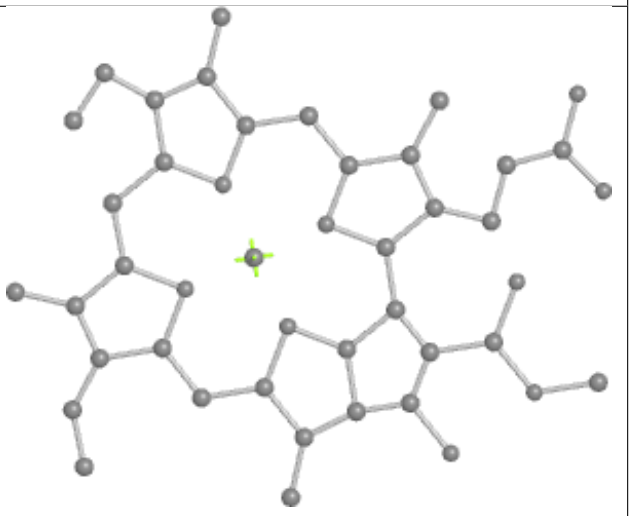
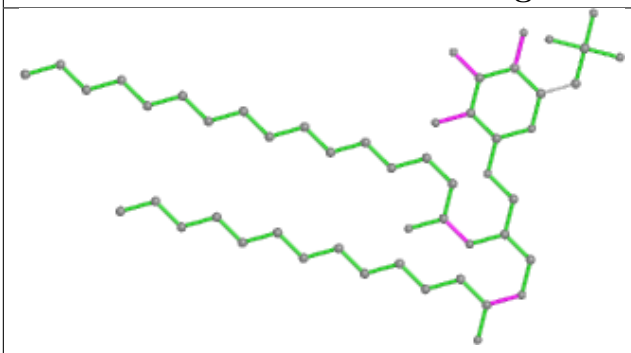


Rings

Ligand SQD V 5216



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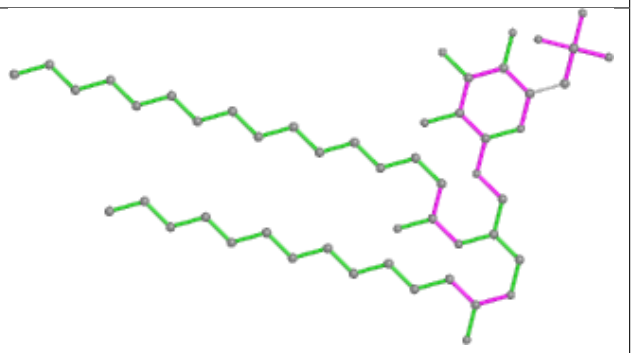

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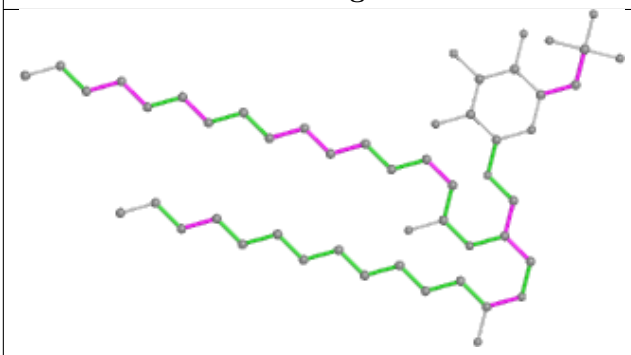

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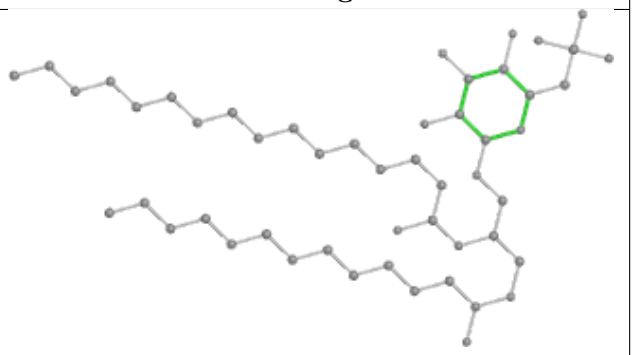
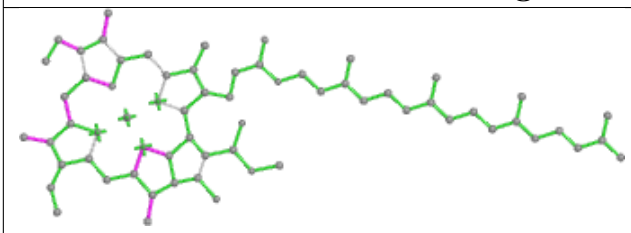


Rings

Ligand CLA A 1125



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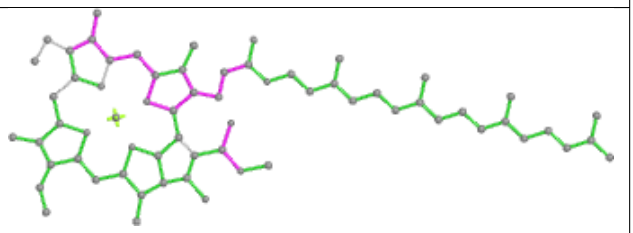
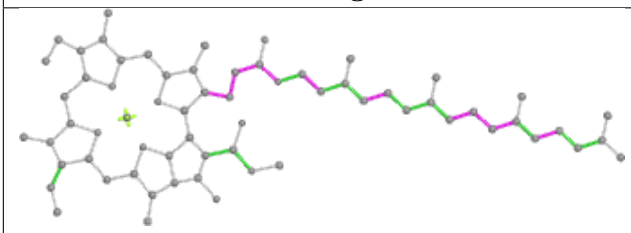


Bond angles



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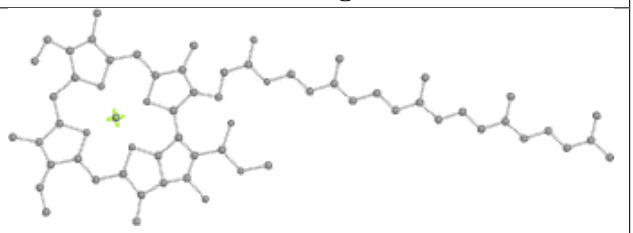
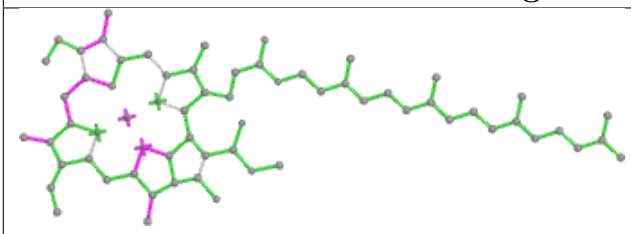


Rings

Ligand CLA f 1226



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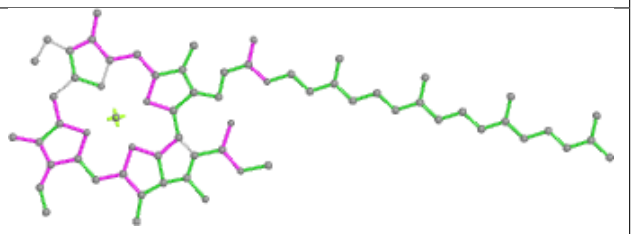
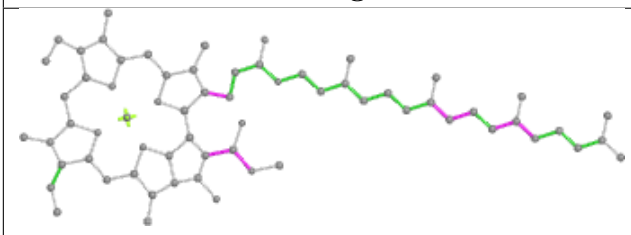


Bond angles



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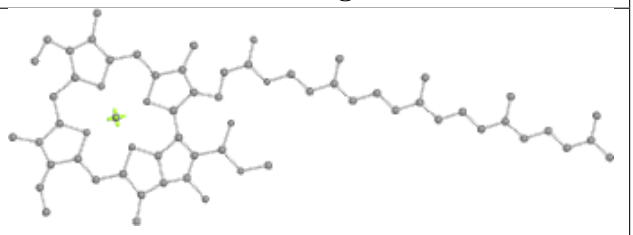
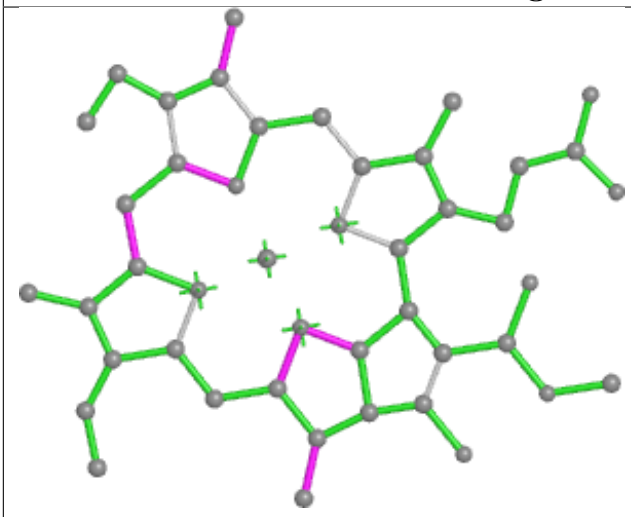


Rings

Ligand CLA b 504



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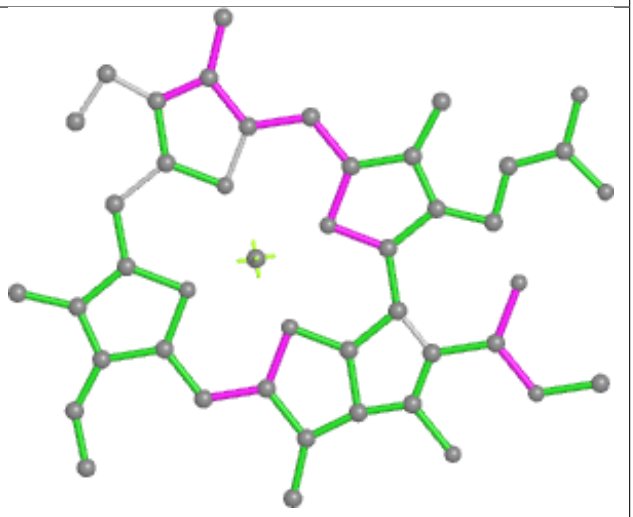
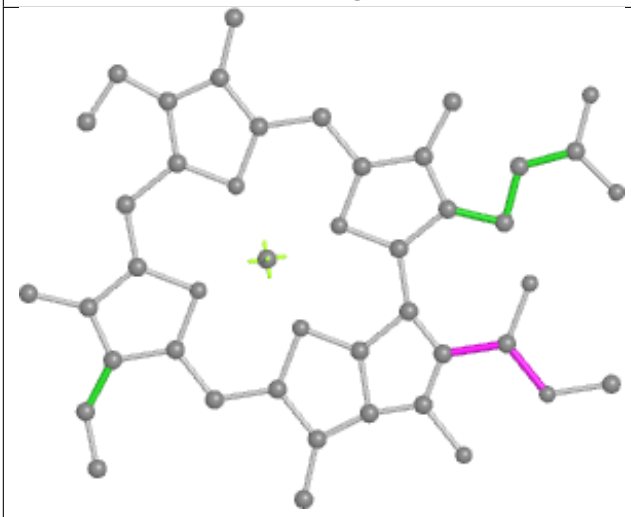


Bond angles



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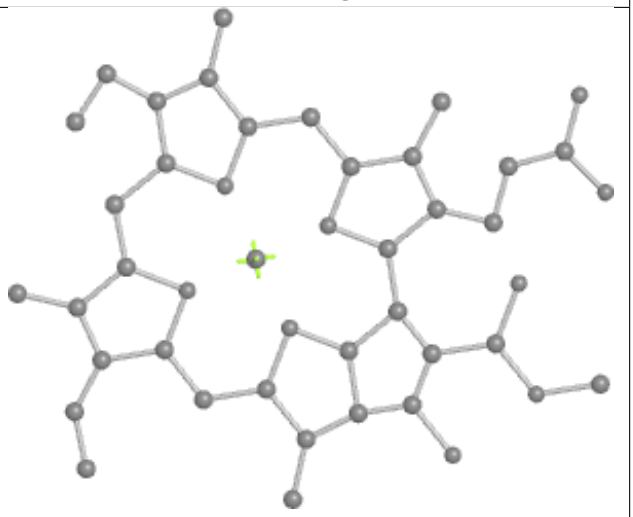
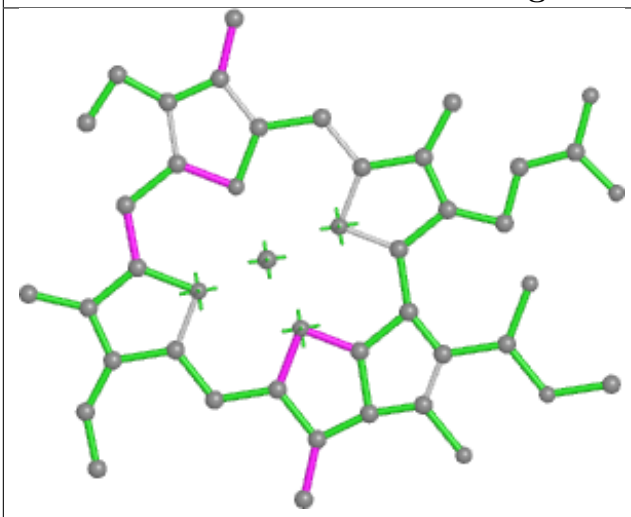
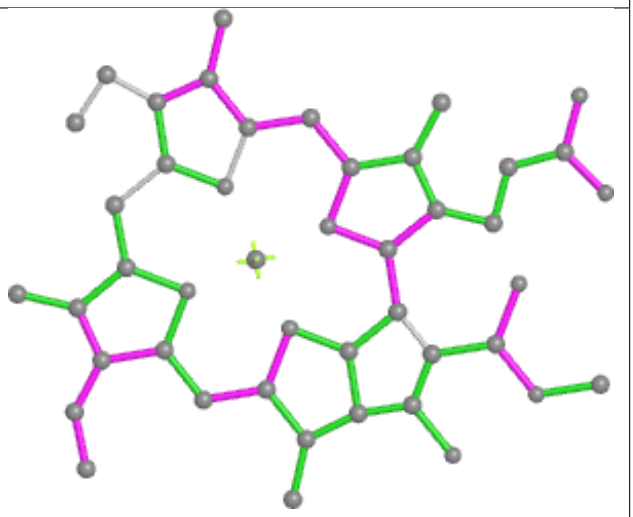


Rings

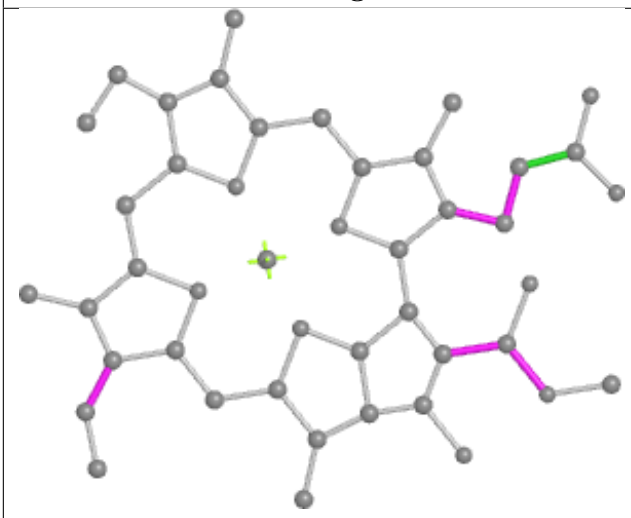
Ligand CLA 3 516



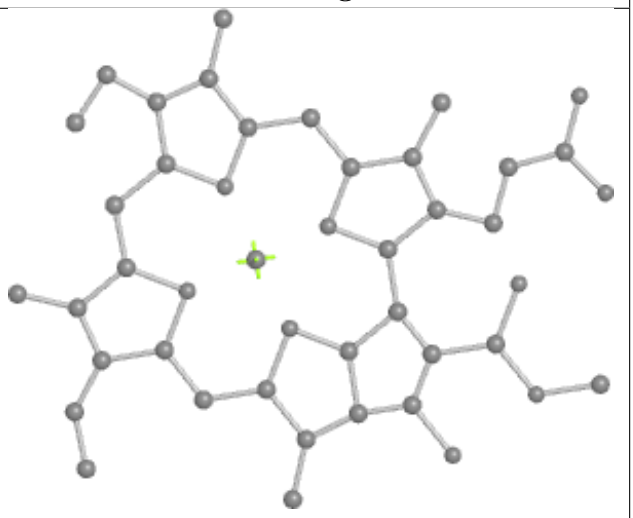
Bond lengths



Bond angles

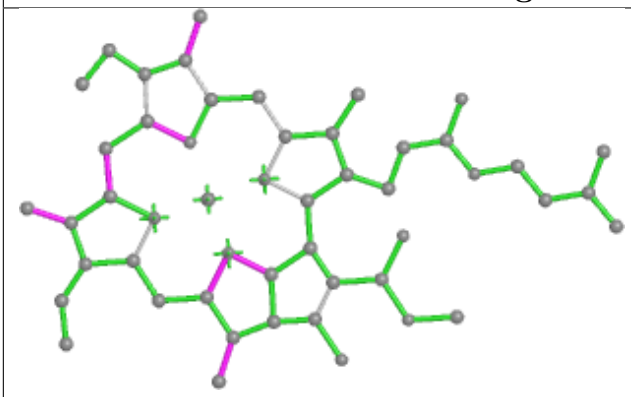


Torsions

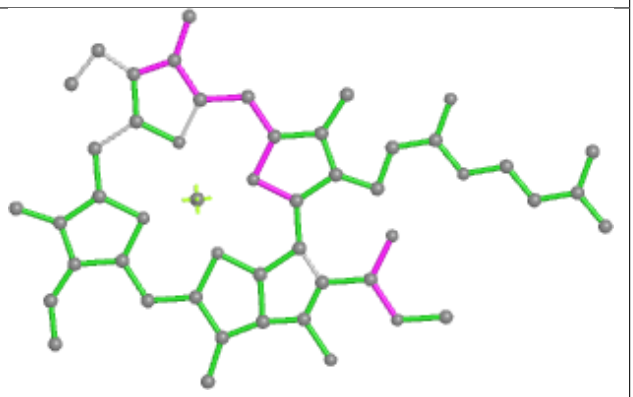


Rings

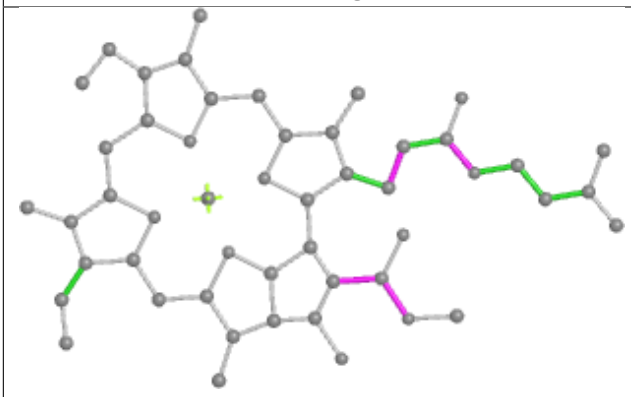
Ligand CLA B 1232



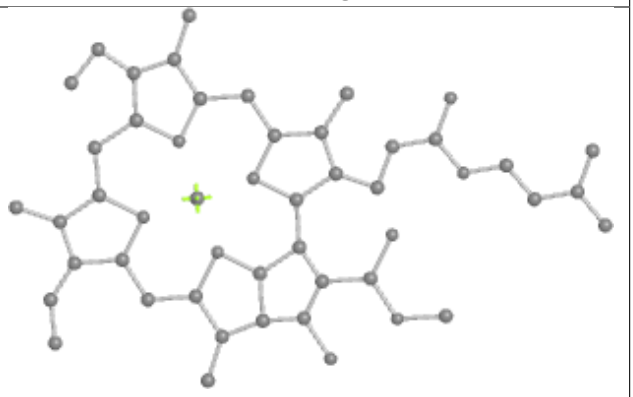
Bond lengths



Bond angles

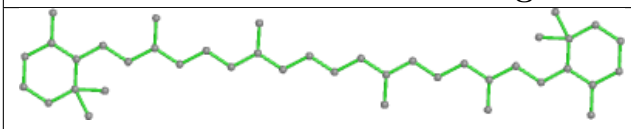


Torsions



Rings

Ligand BCR L 4022



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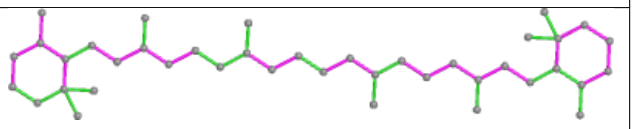
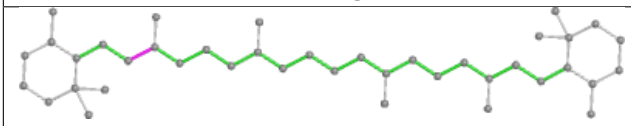
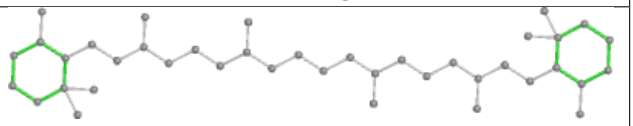


Bond angles

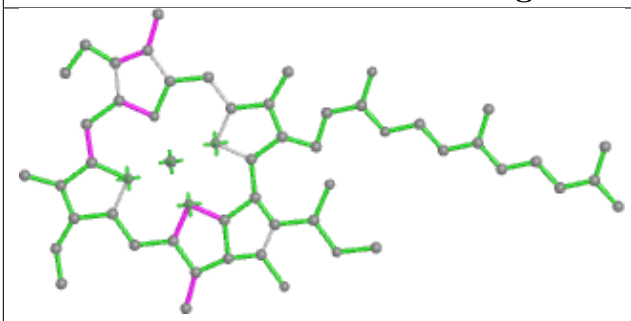


Torsions



Rings

Ligand CLA B 1236



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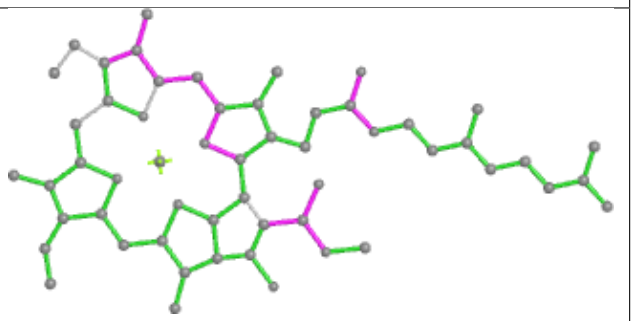
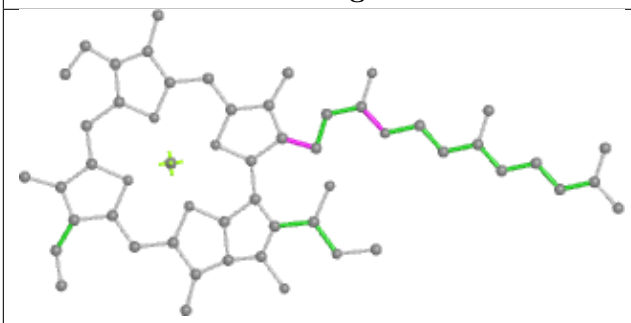
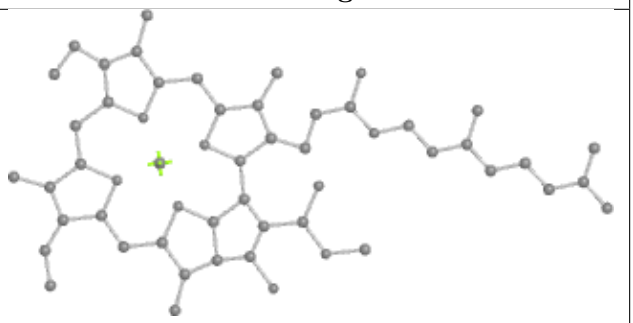


Bond angles

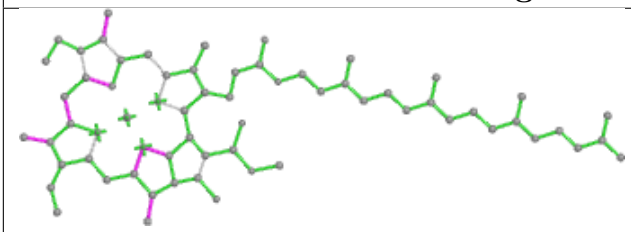


Torsions

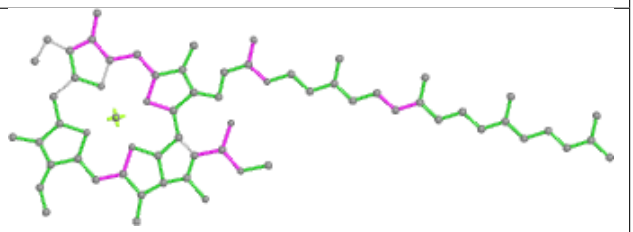


Rings

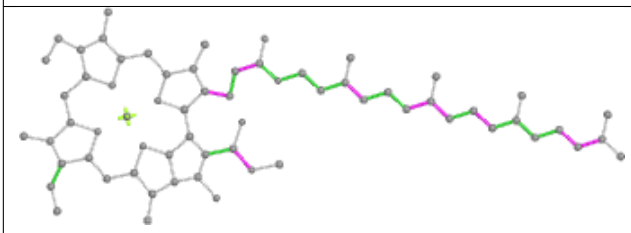
Ligand CLA B 1229



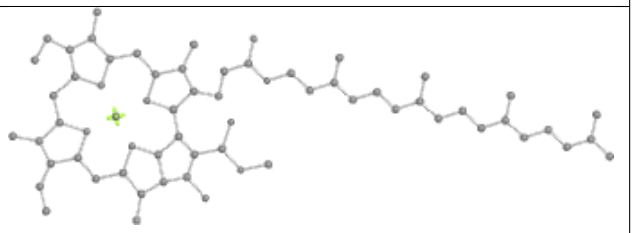
Bond lengths



Bond angles

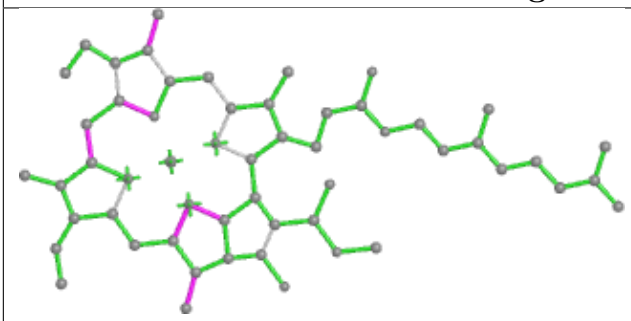


Torsions

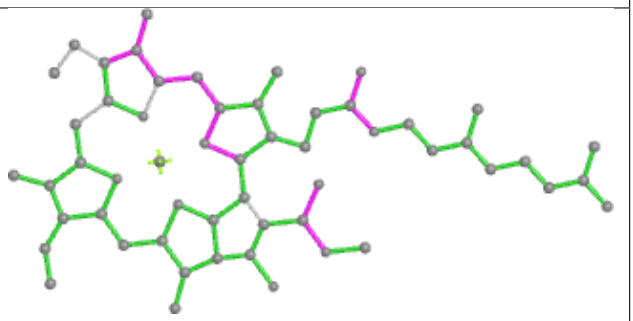


Rings

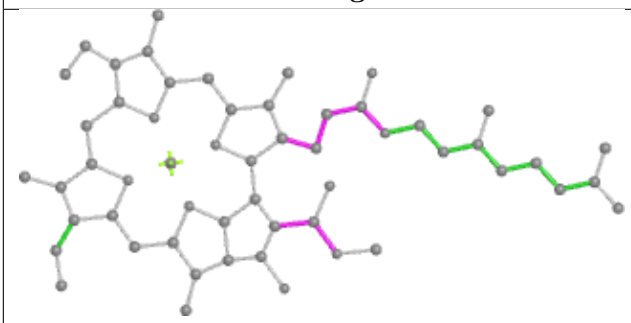
Ligand CLA 4 518



Bond lengths



Bond angles



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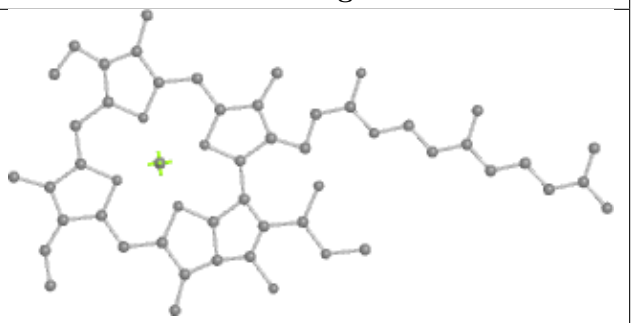
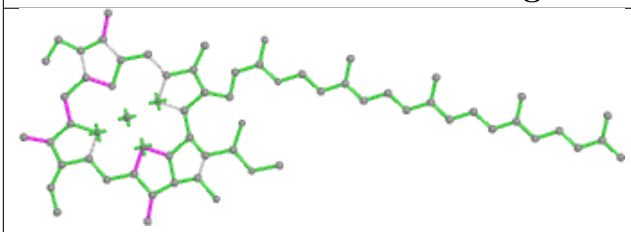


Rings

Ligand CLA l 1303



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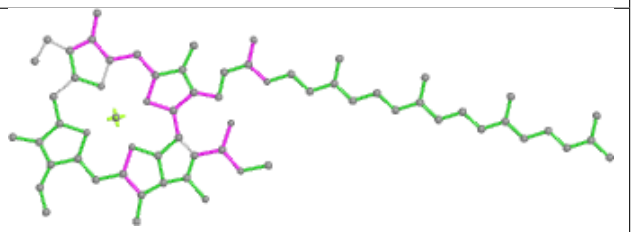
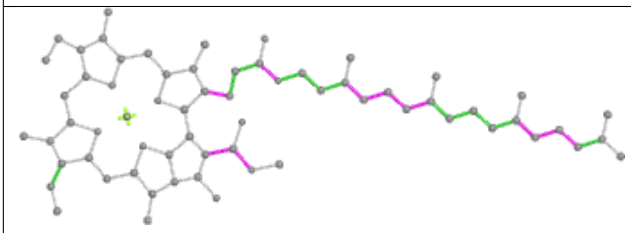
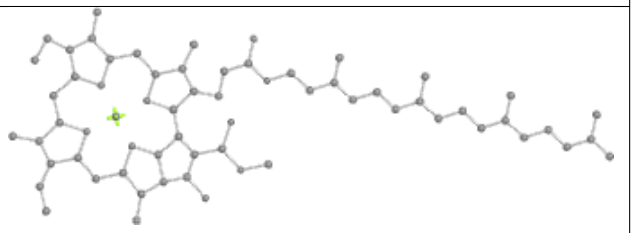


Bond angles

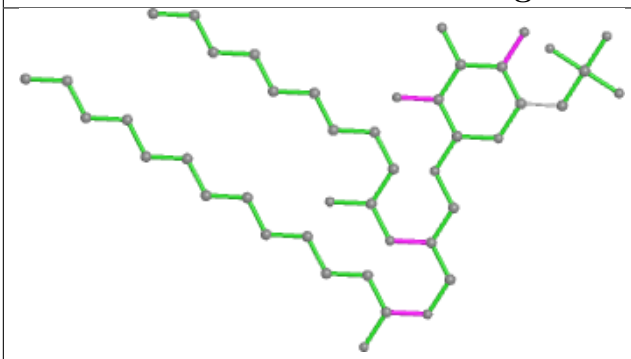


Torsions



Rings

Ligand SQD H 1852



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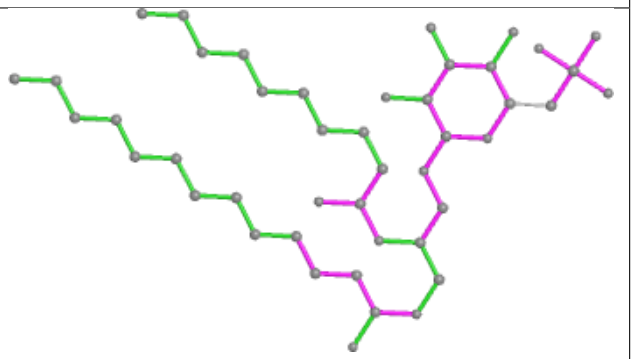
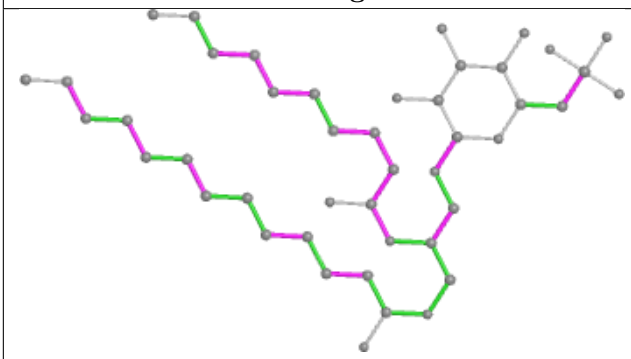


Bond angles



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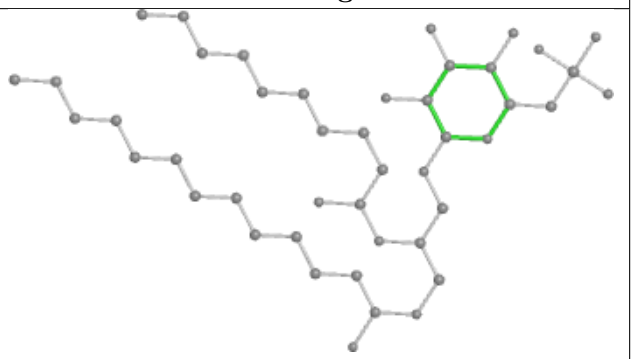
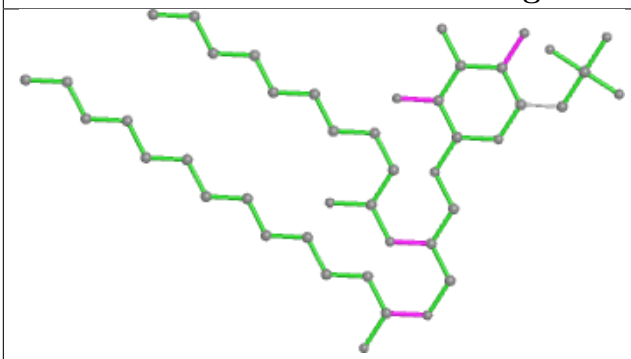


Rings

Ligand SQD f 1852



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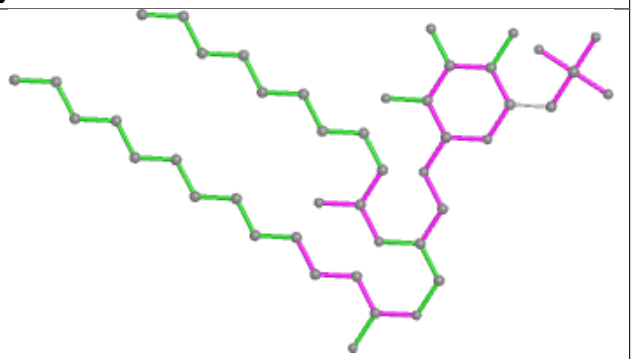
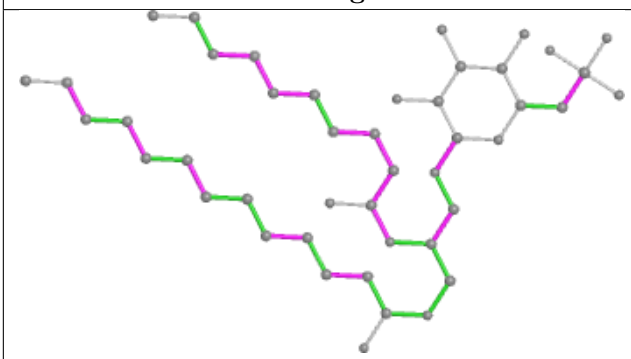


Bond angles



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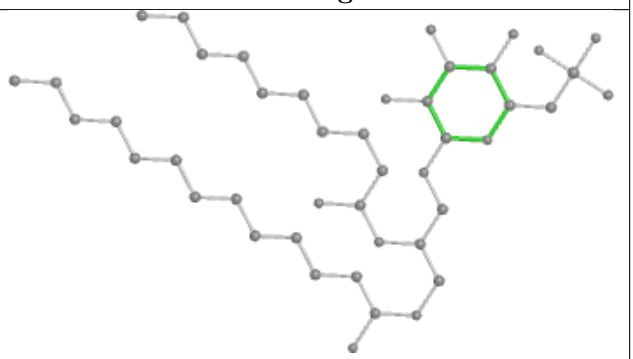
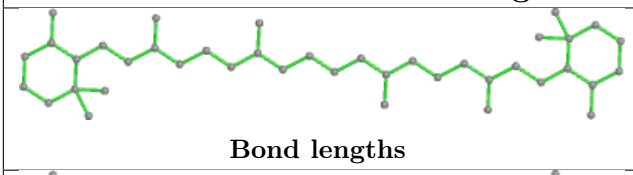


Rings

Ligand BCR K 4104



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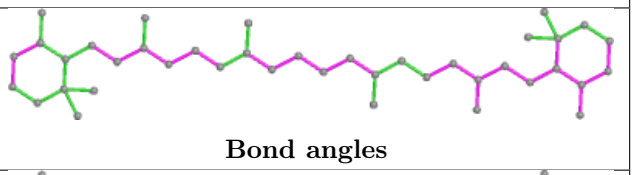
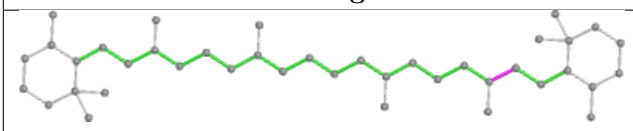


Bond angles



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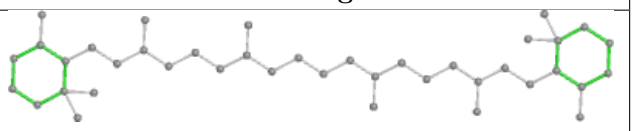
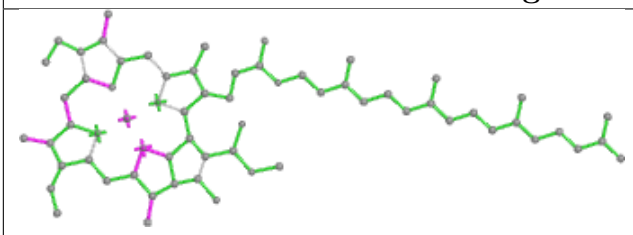


Rings

Ligand CLA f 1204



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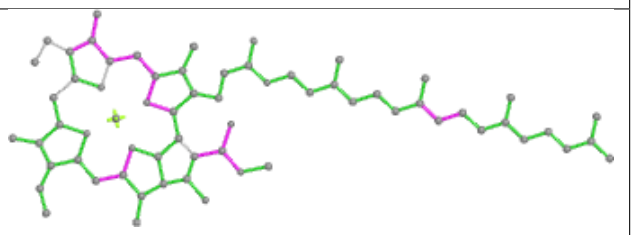
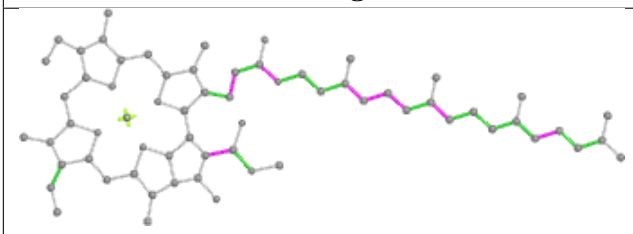


Bond angles



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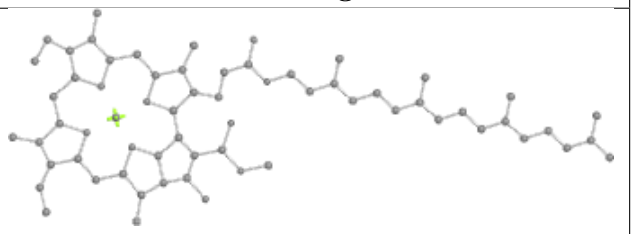
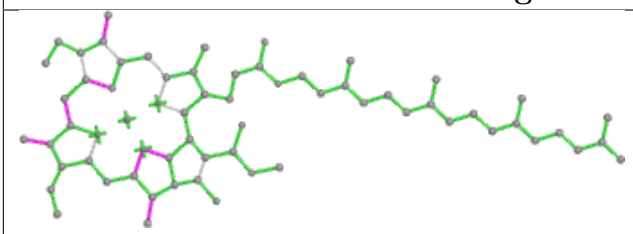


Rings

Ligand CLA A 1109



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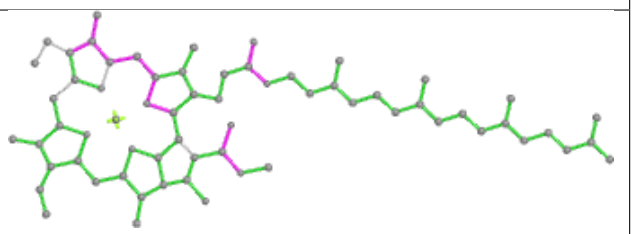
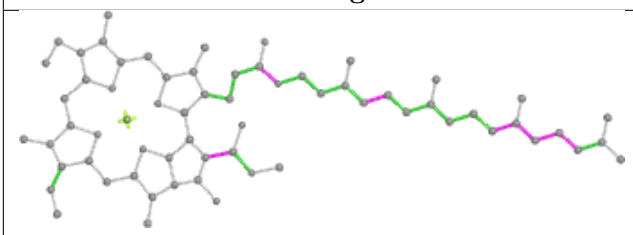


Bond angles



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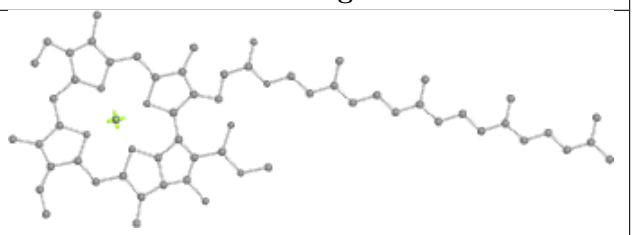
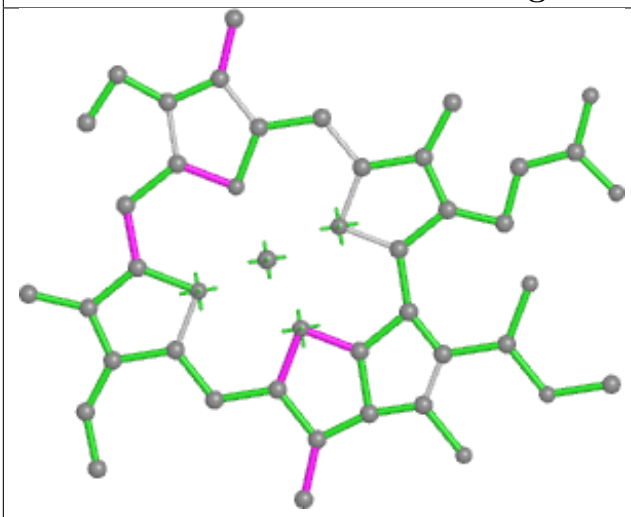


Rings

Ligand CLA 4 511



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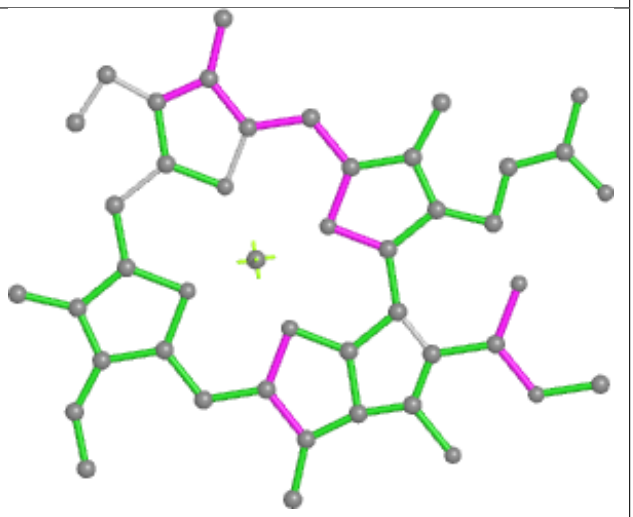
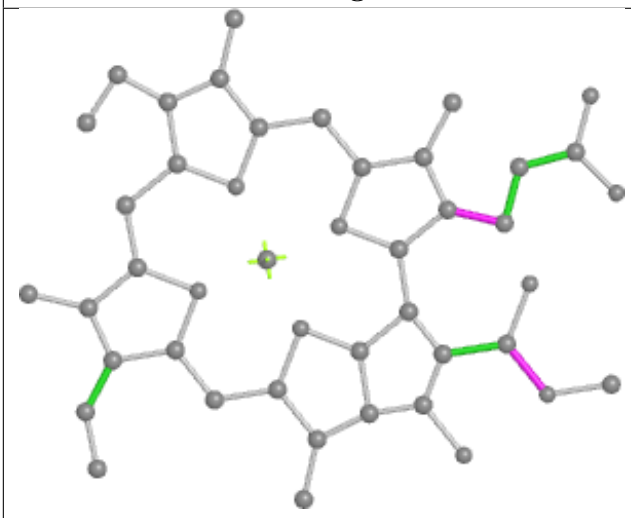


Bond angles



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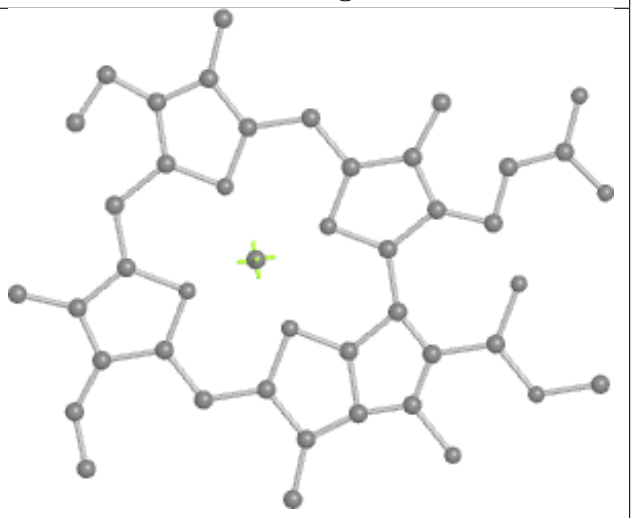
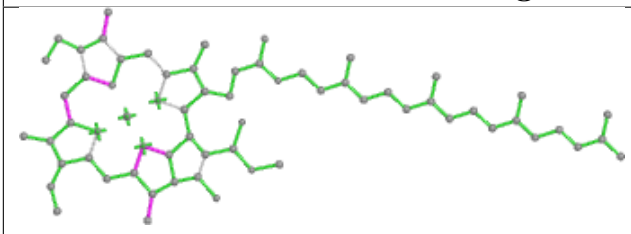


Rings

Ligand CLA B 1240



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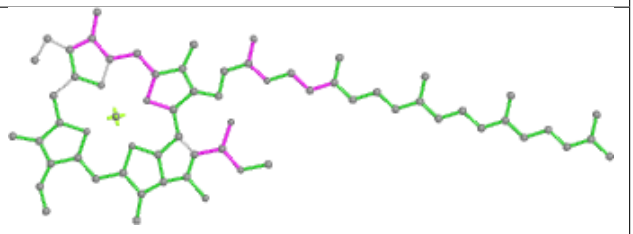
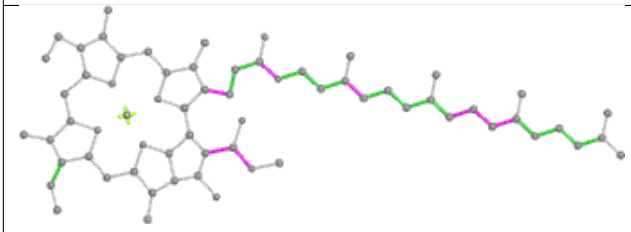


Bond angles



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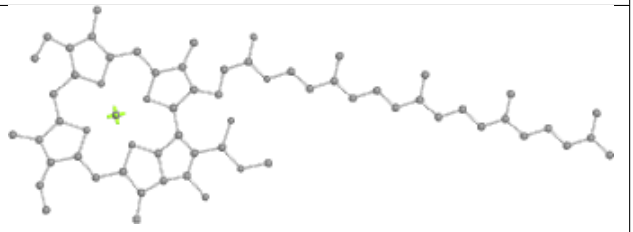
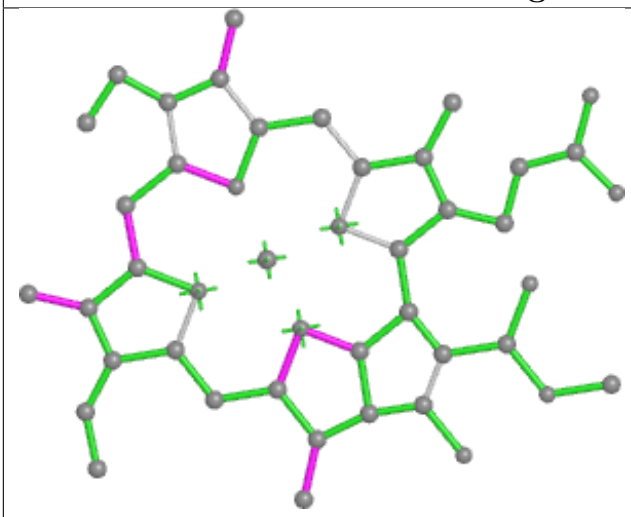
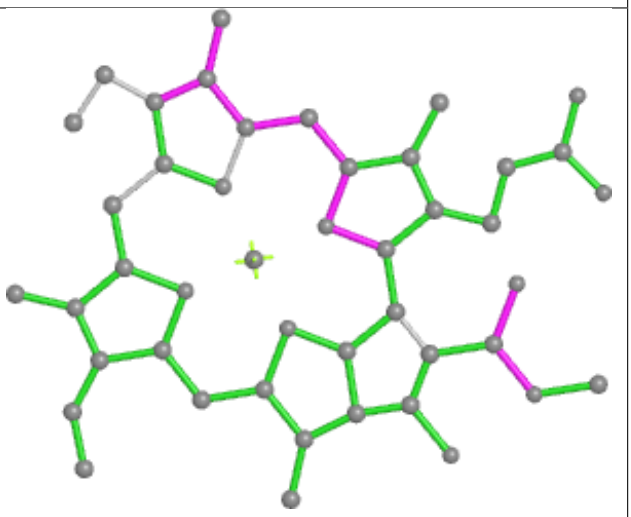


Rings

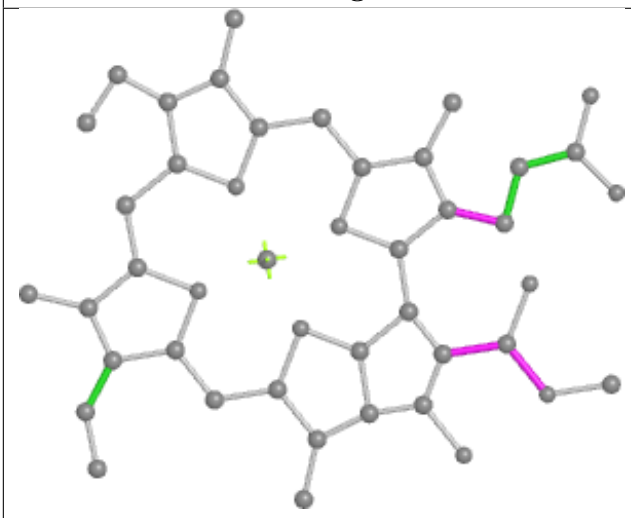
Ligand CLA a 517



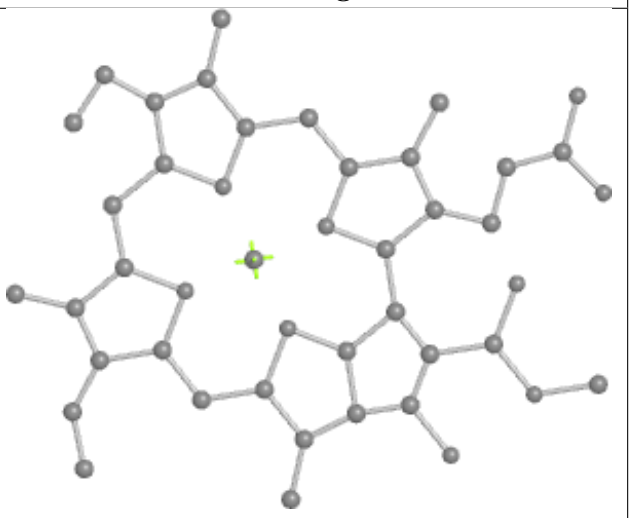
Bond lengths



Bond angles

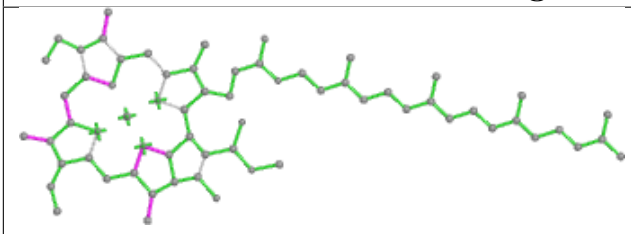


Torsions

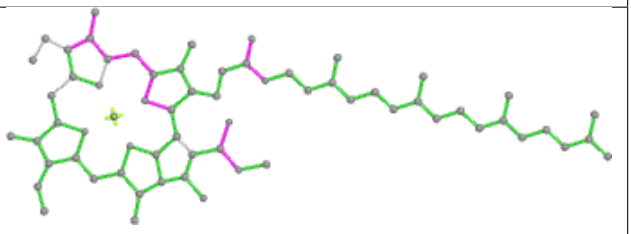


Rings

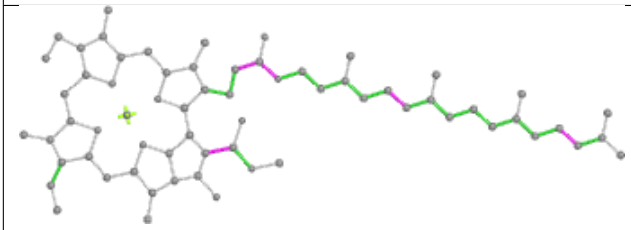
Ligand CLA 2 509



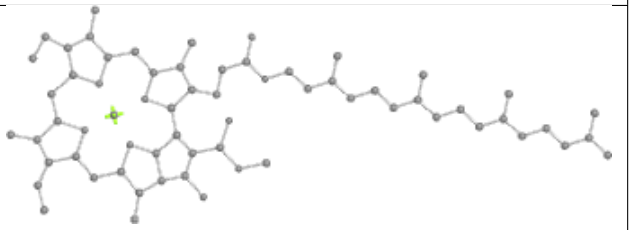
Bond lengths



Bond angles

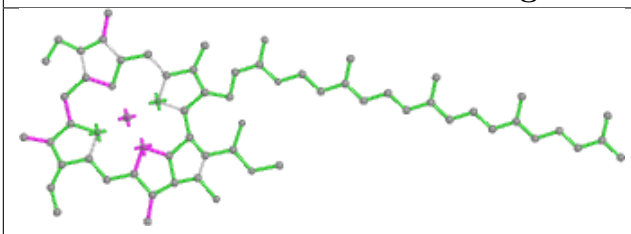


Torsions



Rings

Ligand CLA e 1013



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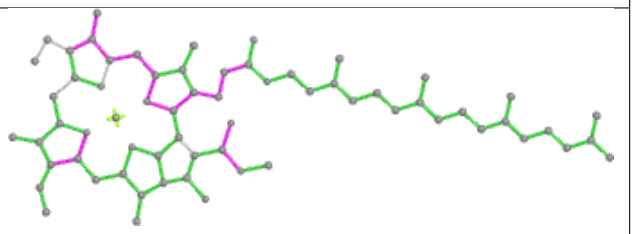

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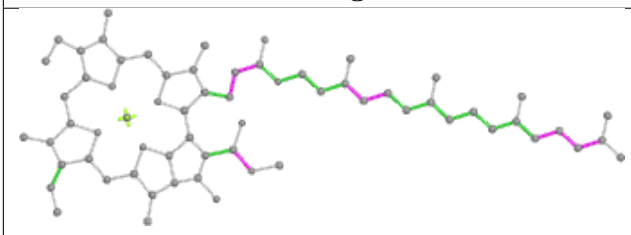

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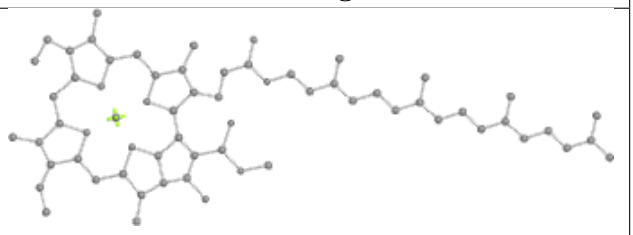
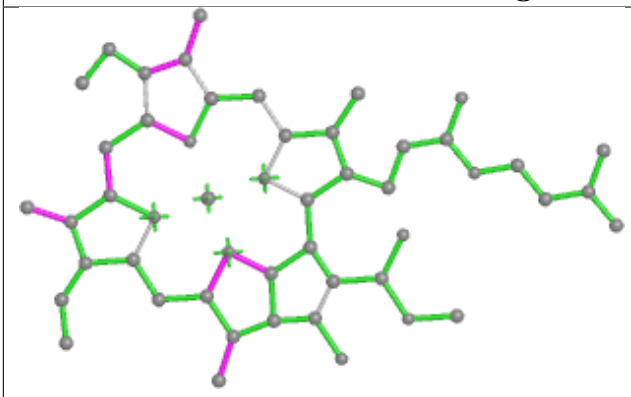


Rings

Ligand CLA A 1114



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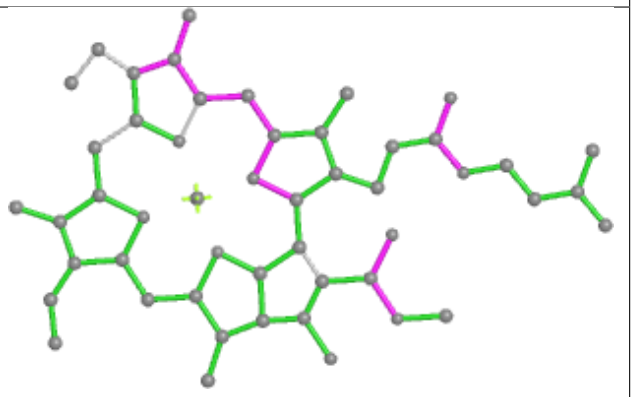

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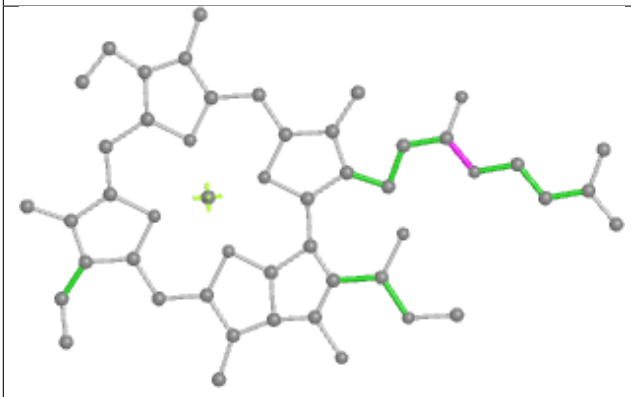

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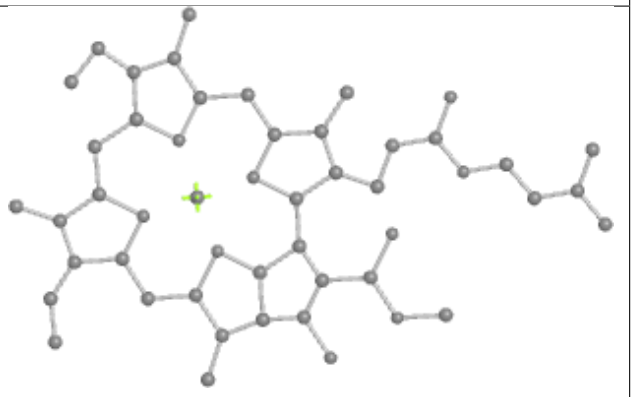
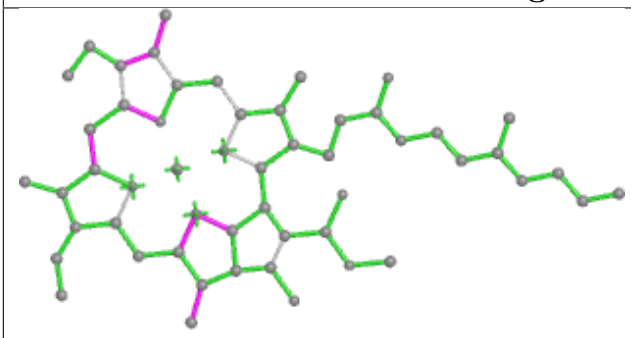


Rings

Ligand CLA 2 512



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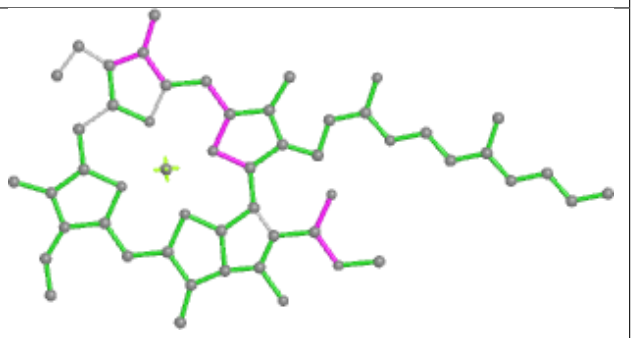
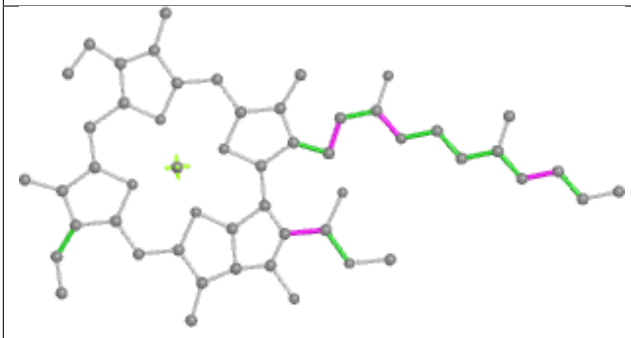


Bond angles



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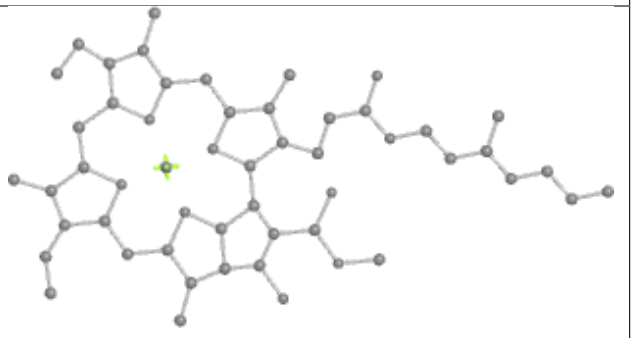
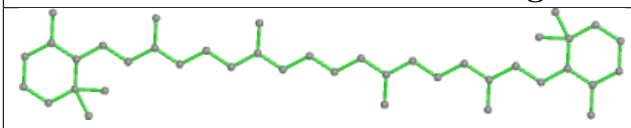


Rings

Ligand BCR a 522



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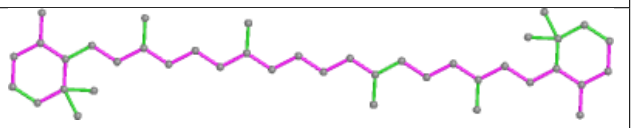

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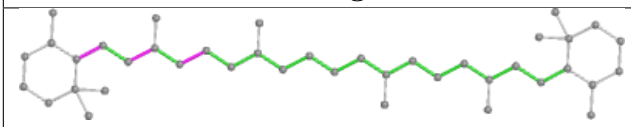

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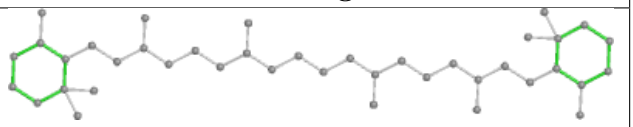
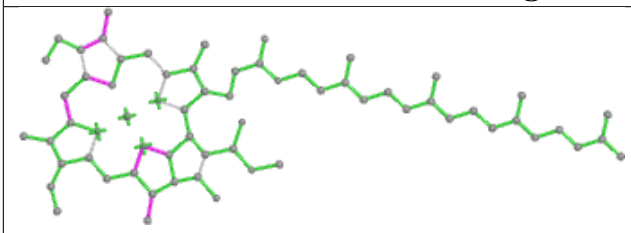


Rings

Ligand CLA f 1208



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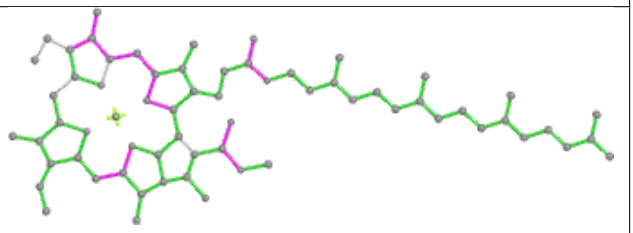
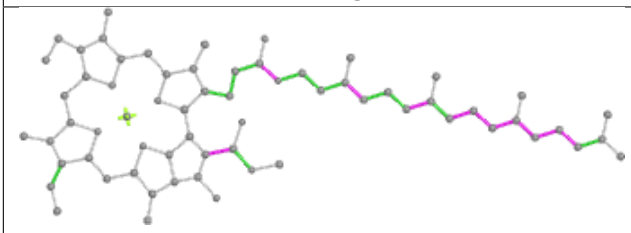


Bond angles



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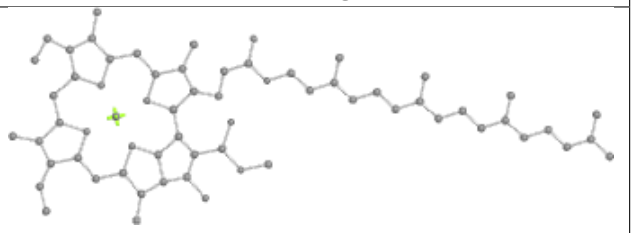
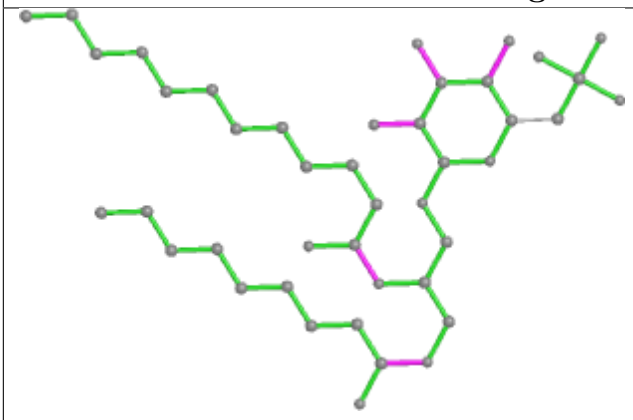


Rings

Ligand SQD 3 822



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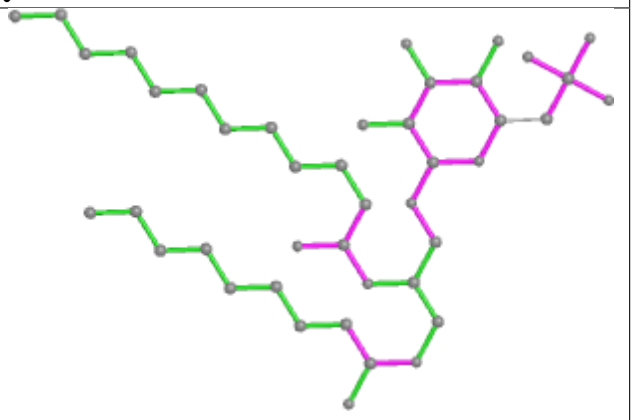

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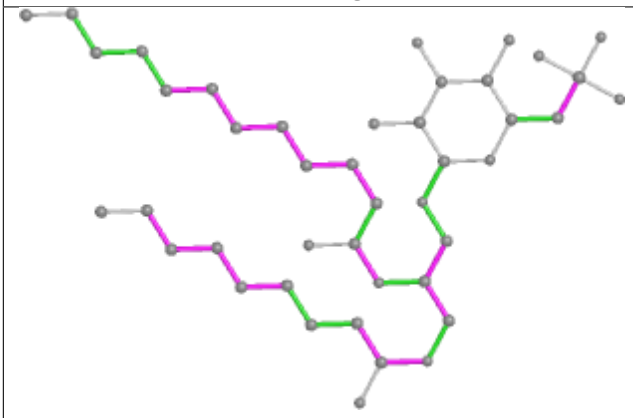

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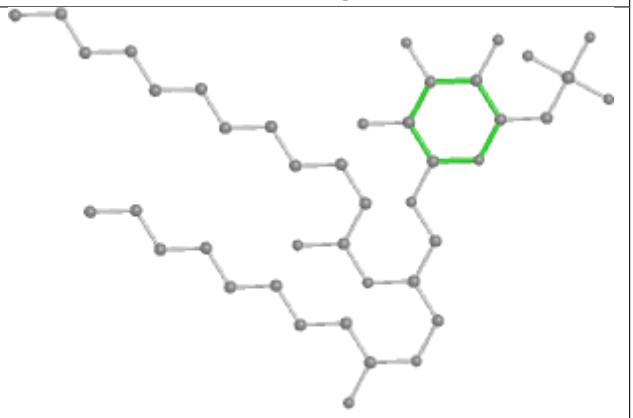
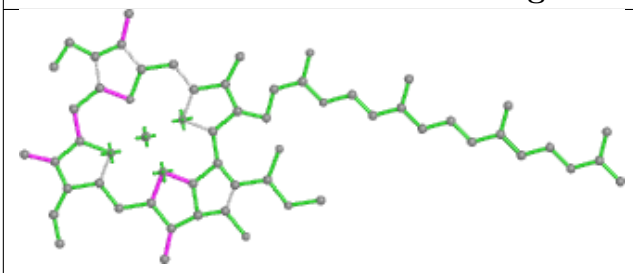


Rings

Ligand CLA v 501



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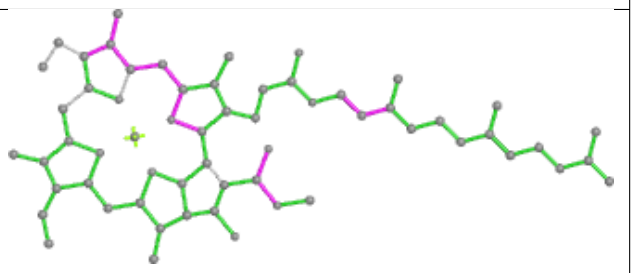

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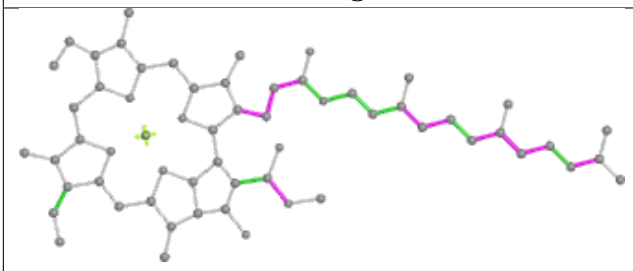

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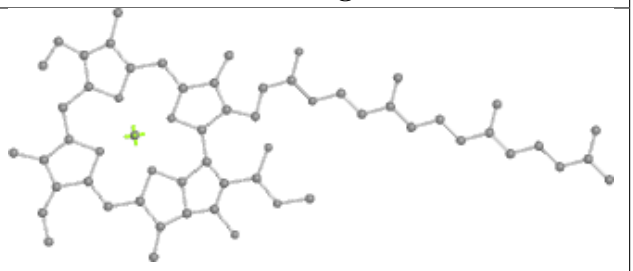
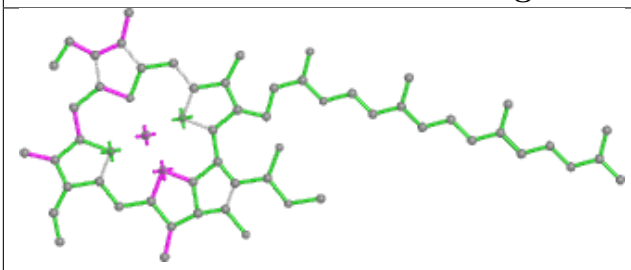


Rings

Ligand CLA H 1216



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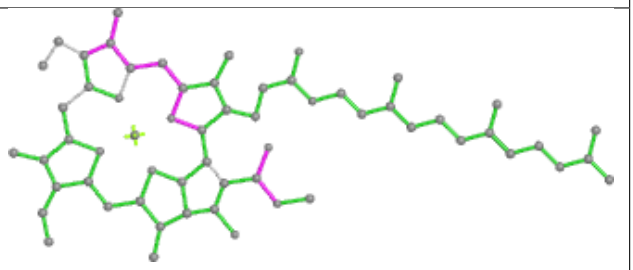
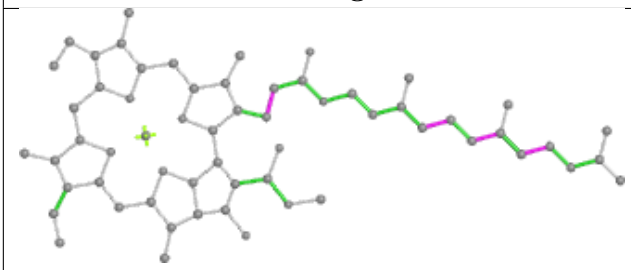


Bond angles



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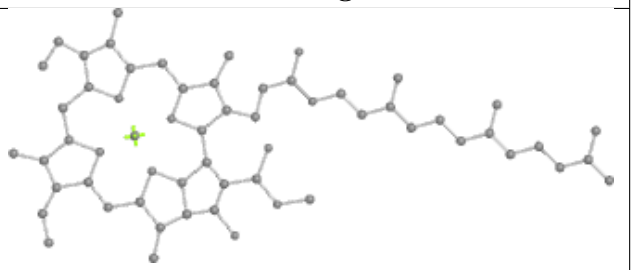
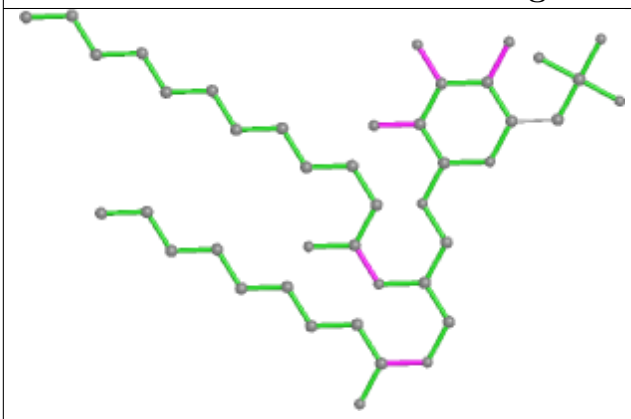


Rings

Ligand SQD a 822



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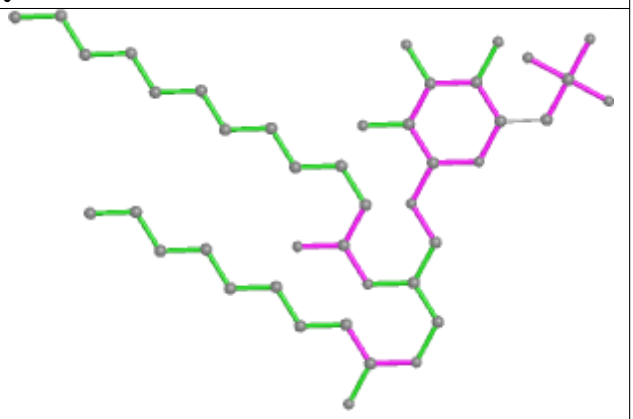

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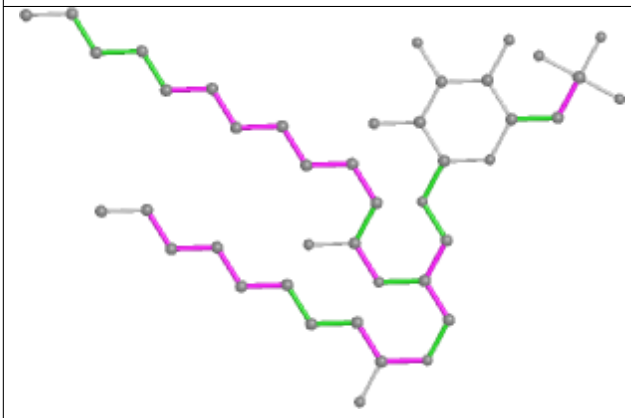

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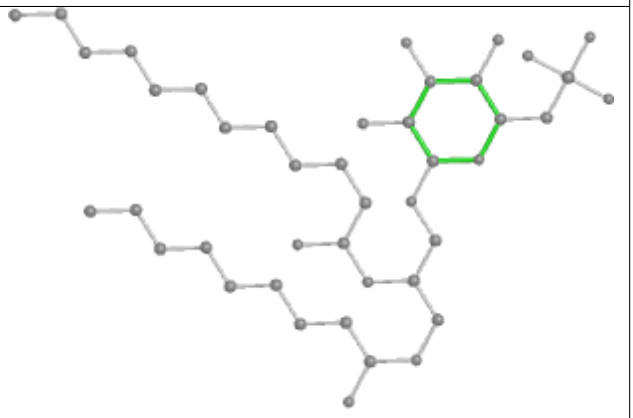
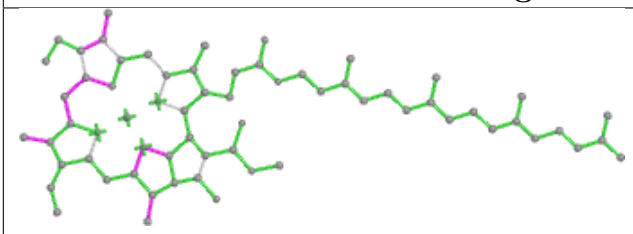


Rings

Ligand CLA A 1237



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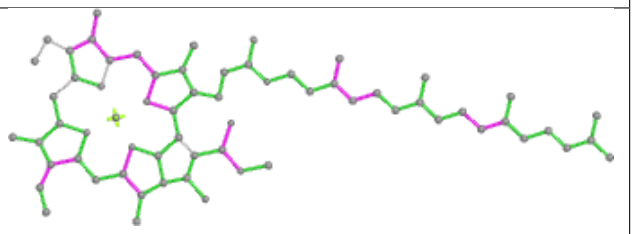

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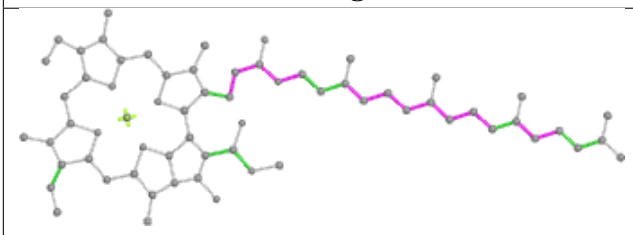

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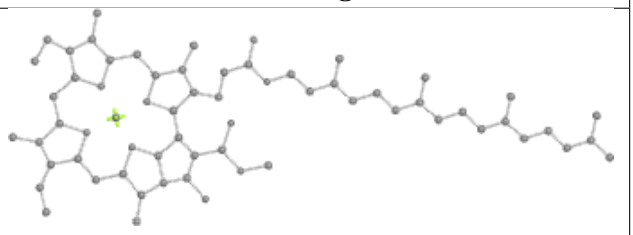
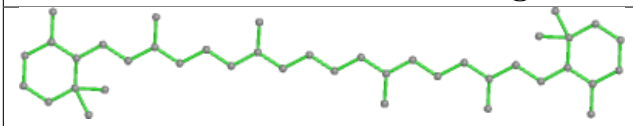


Rings

Ligand BCR m 4104



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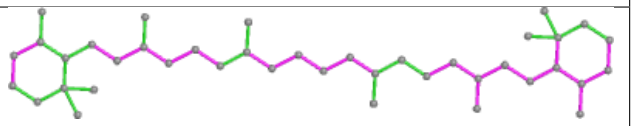

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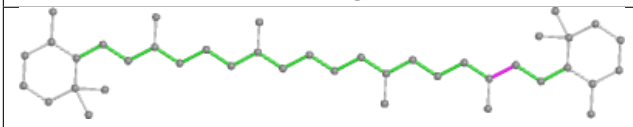
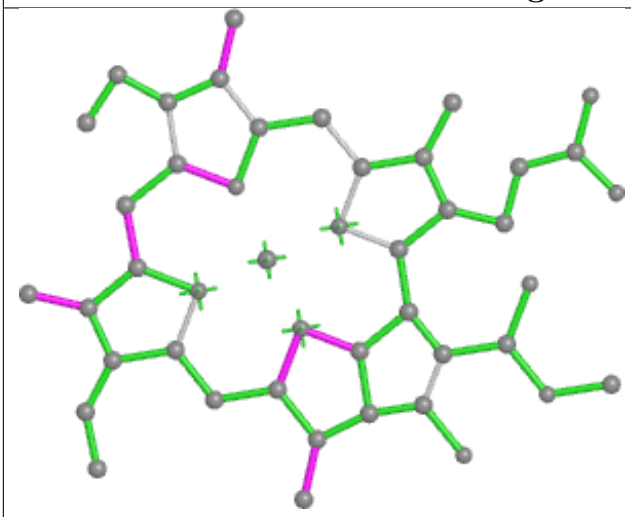


Torsions

Rings

Ligand CLA b 513



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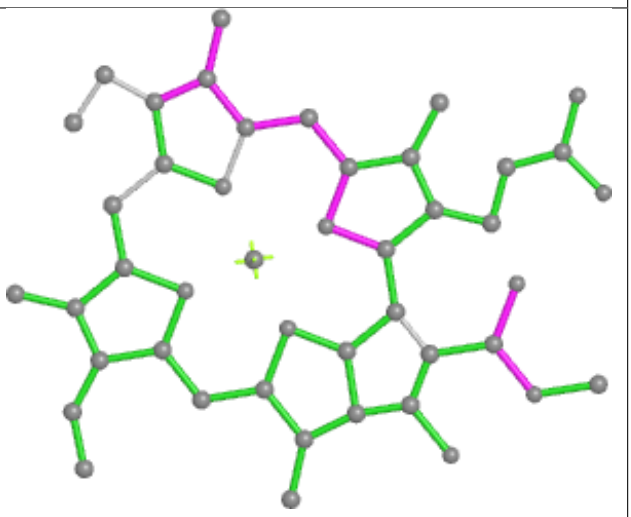
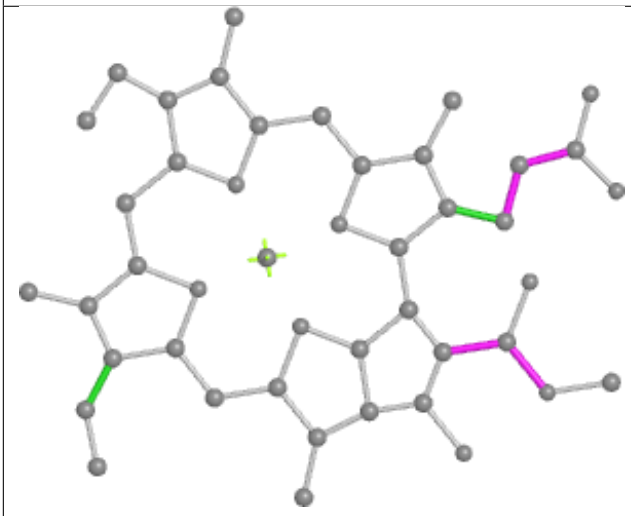


Bond angles



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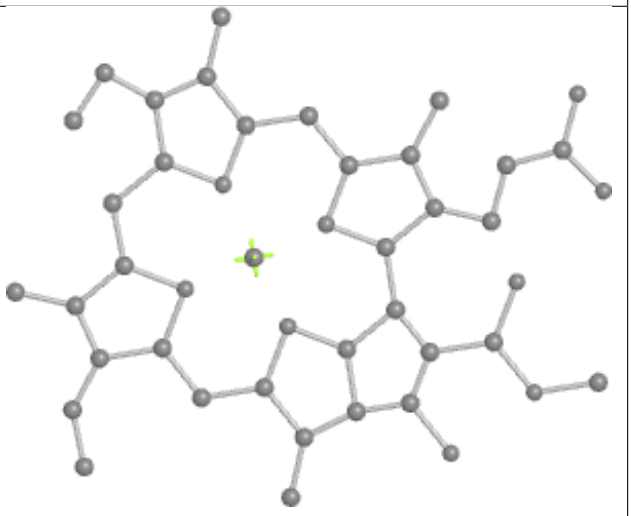
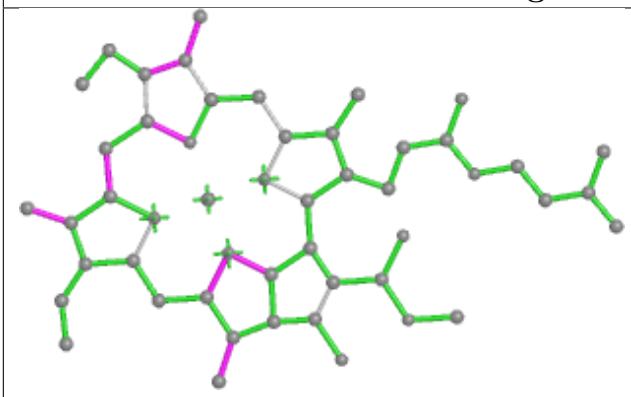
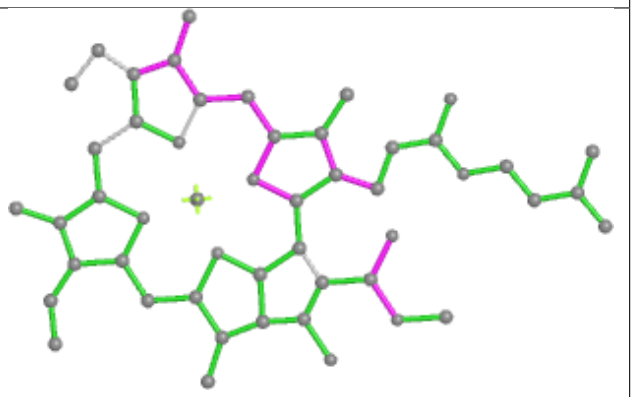


Rings

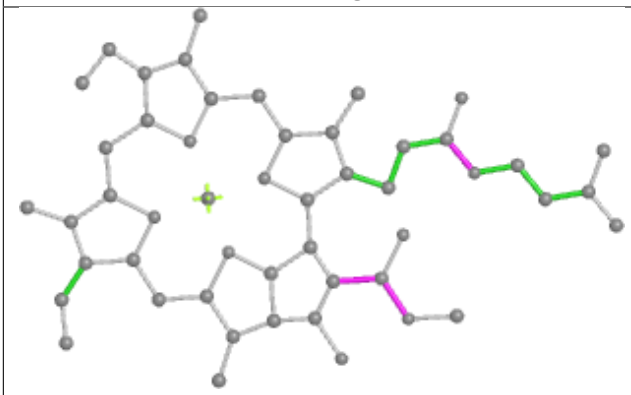
Ligand CLA u 502



Bond lengths



Bond angles



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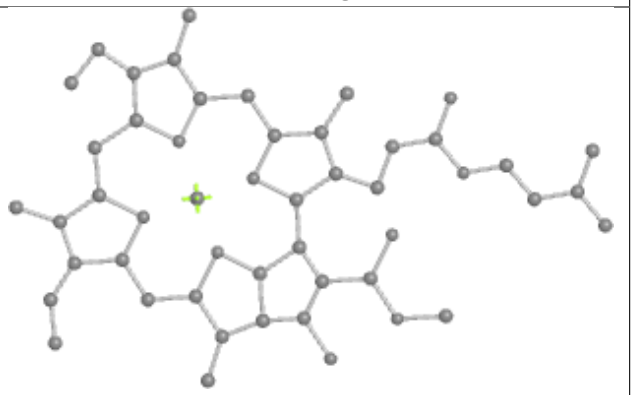
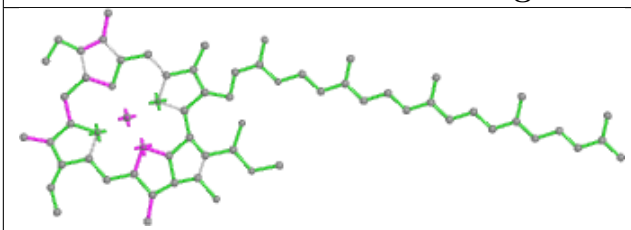
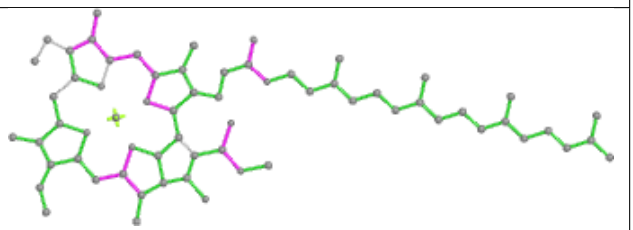


Rings

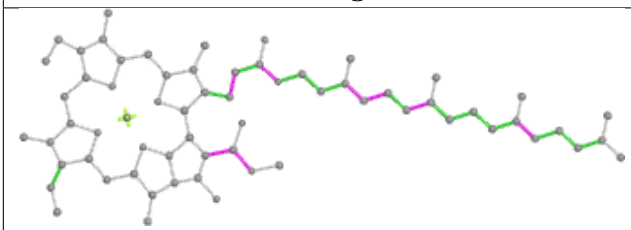
Ligand CLA G 1119



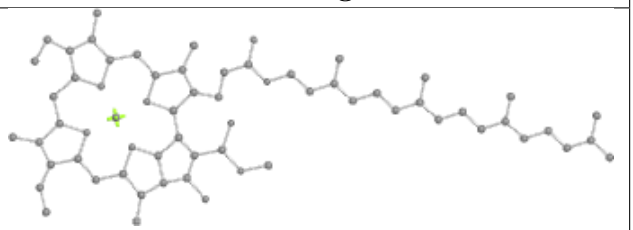
Bond lengths



Bond angles

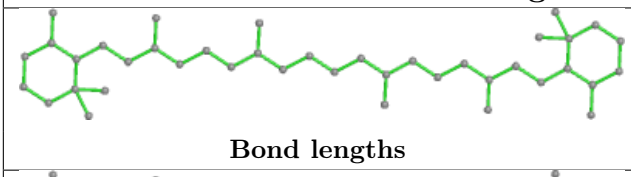


Torsions

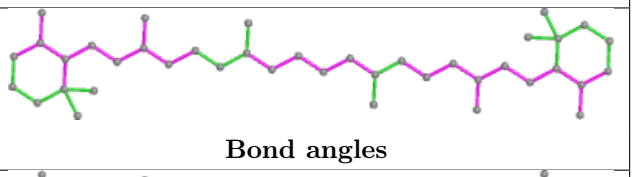


Rings

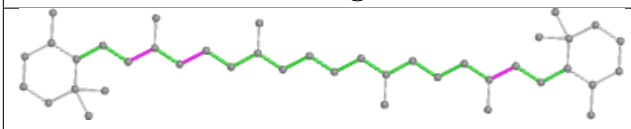
Ligand BCR s 524



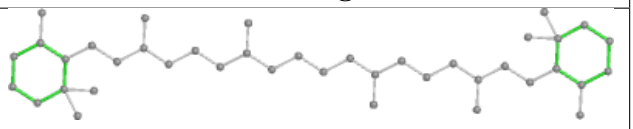
Bond lengths



Bond angles

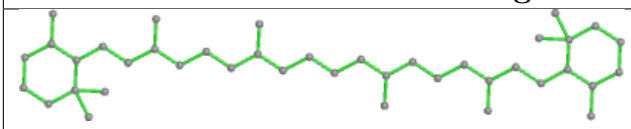


Torsions



Rings

Ligand BCR B 4006



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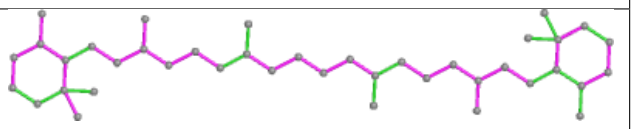

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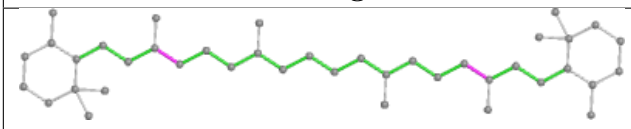
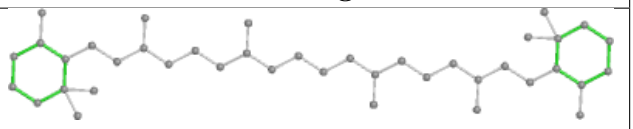
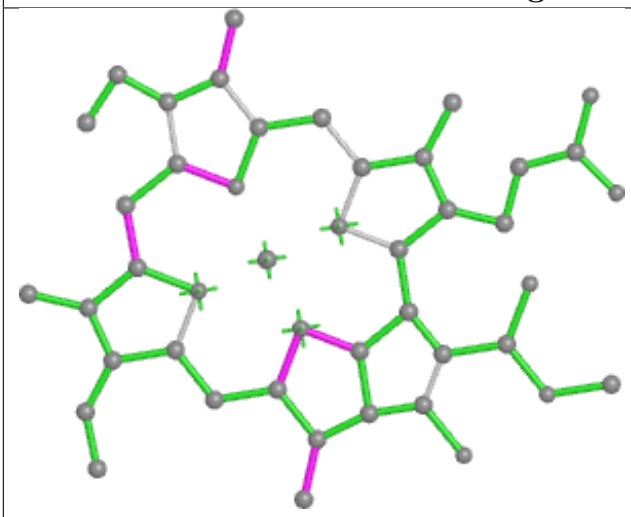


Torsions



Rings

Ligand CLA u 516



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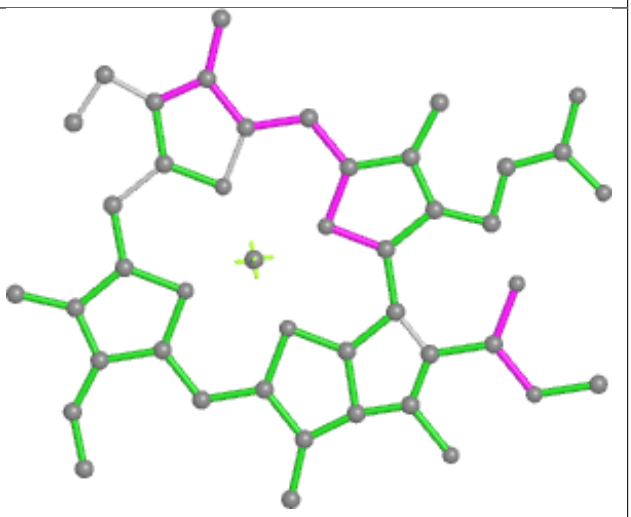
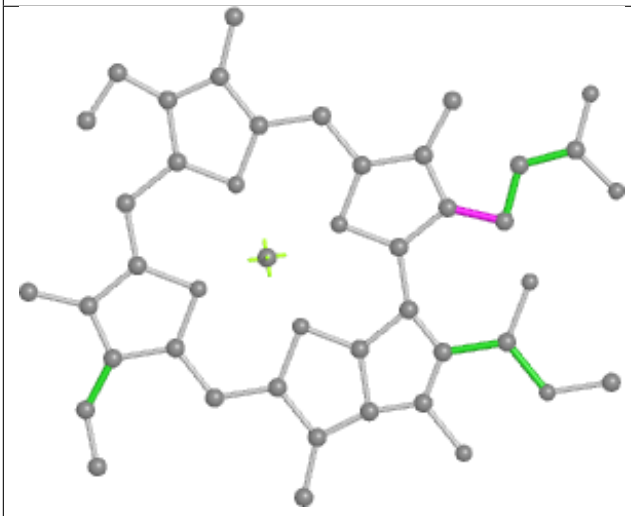
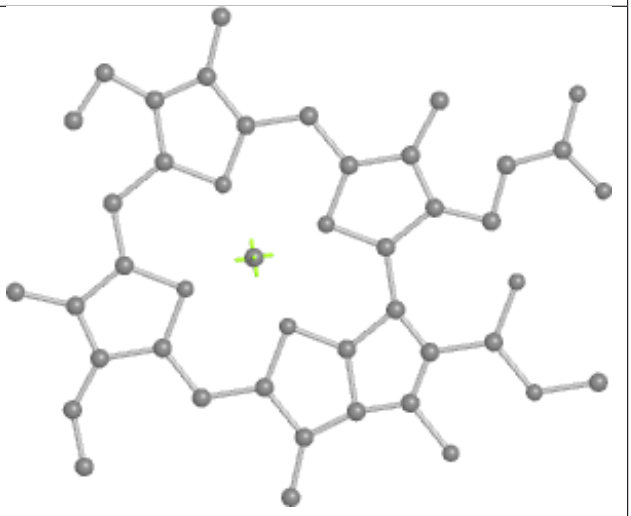


Bond angles

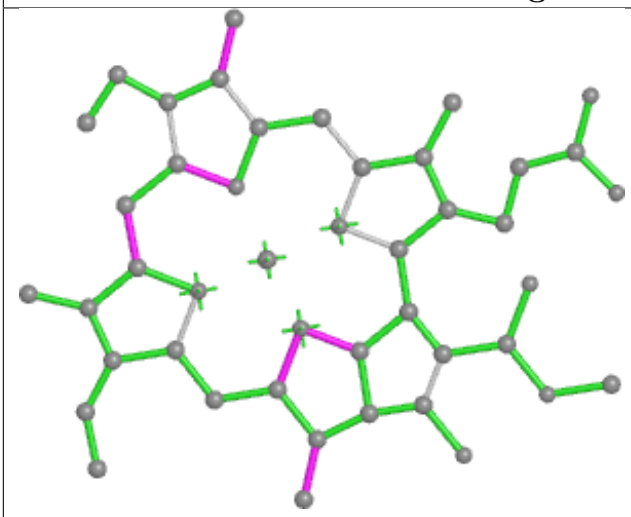


Torsions



Rings

Ligand CLA 3 504



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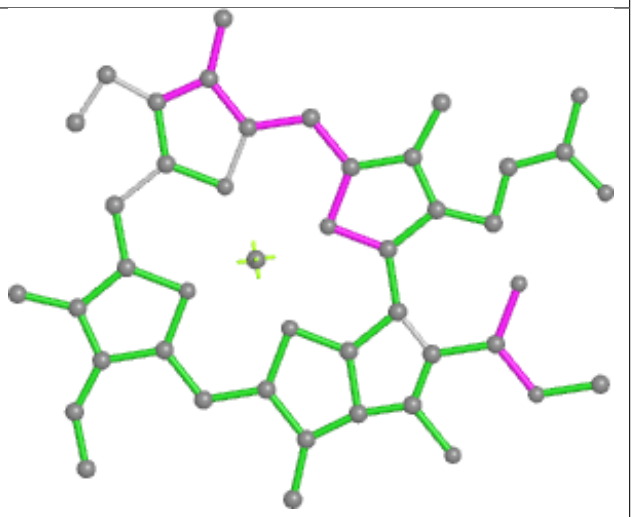

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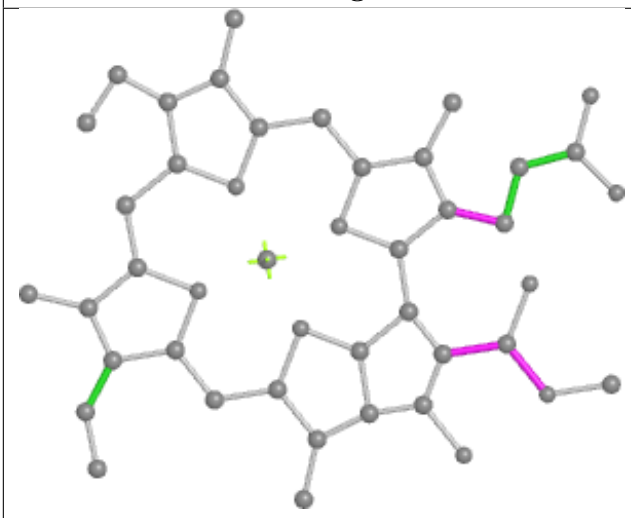

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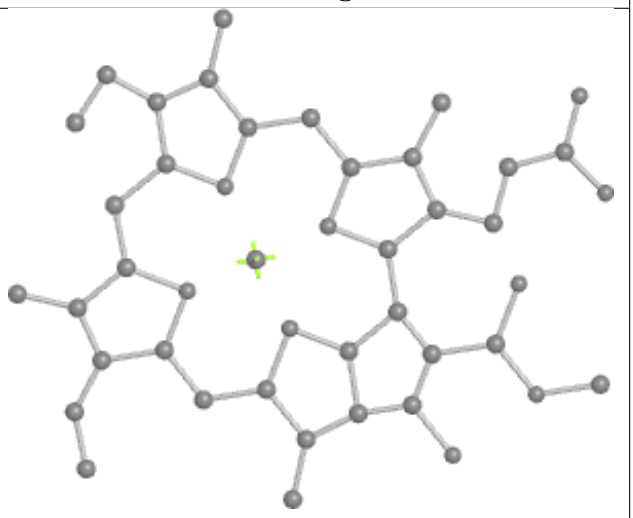
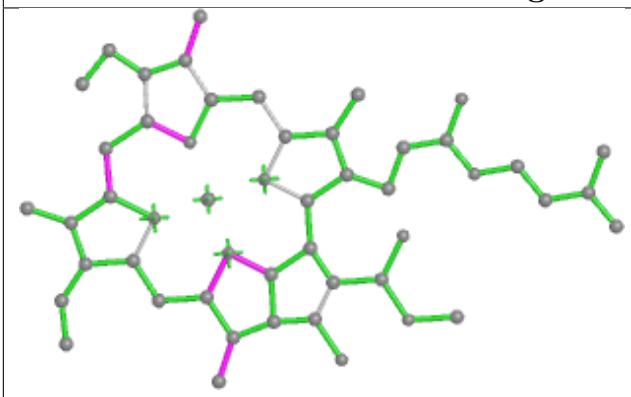


Rings

Ligand CLA v 502



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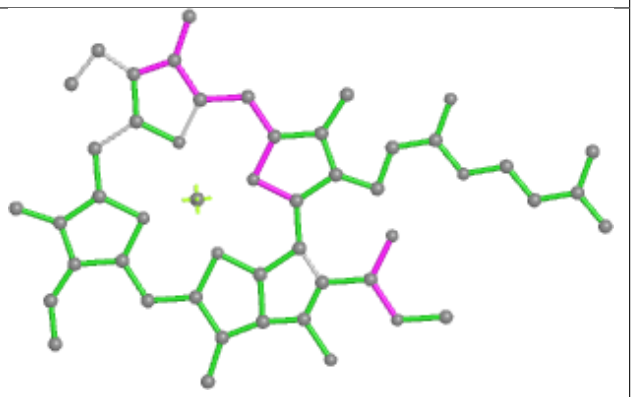

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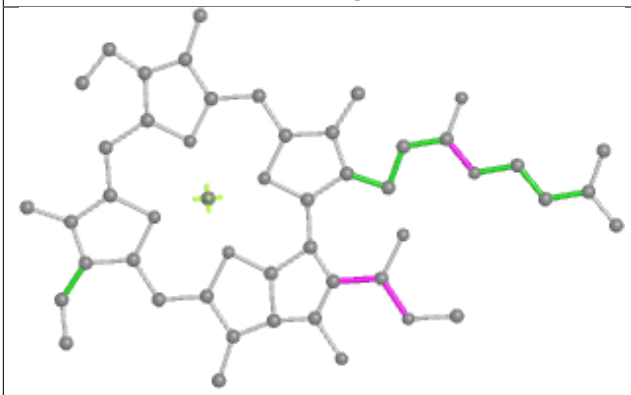

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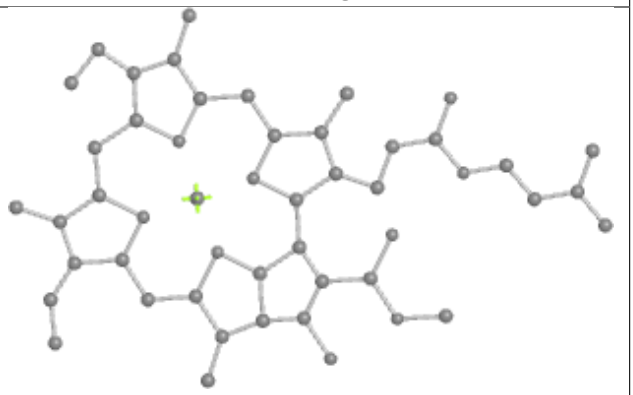
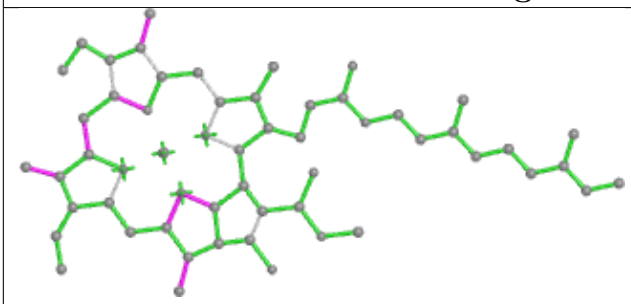


Rings

Ligand CLA H 1211



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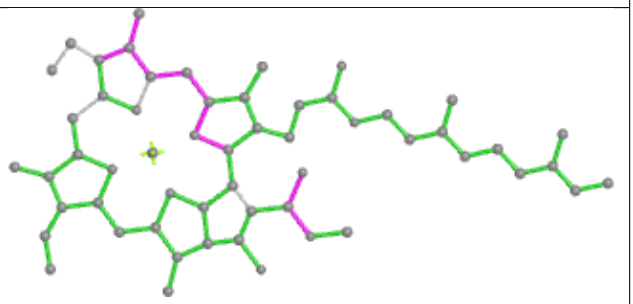

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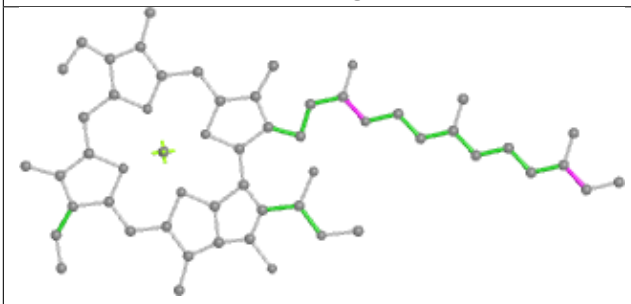

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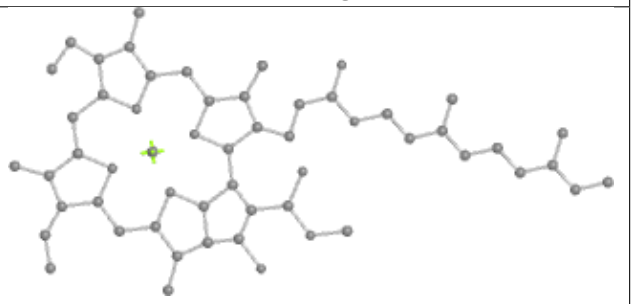
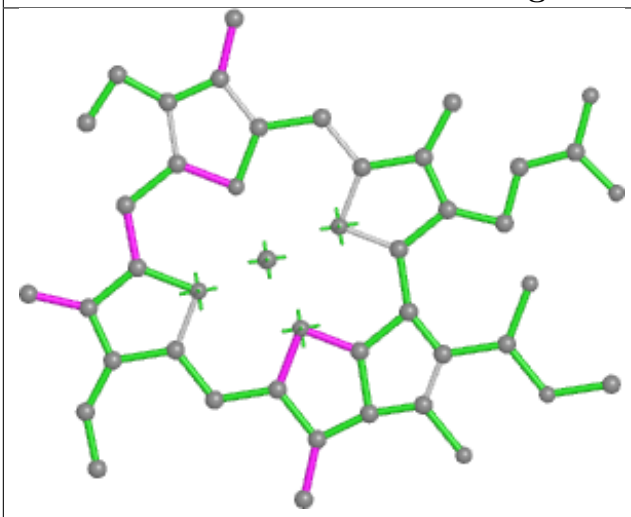


Rings

Ligand CLA 3 517



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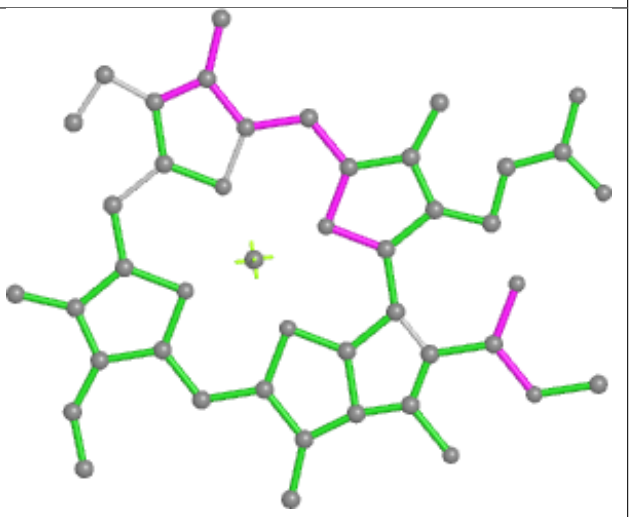

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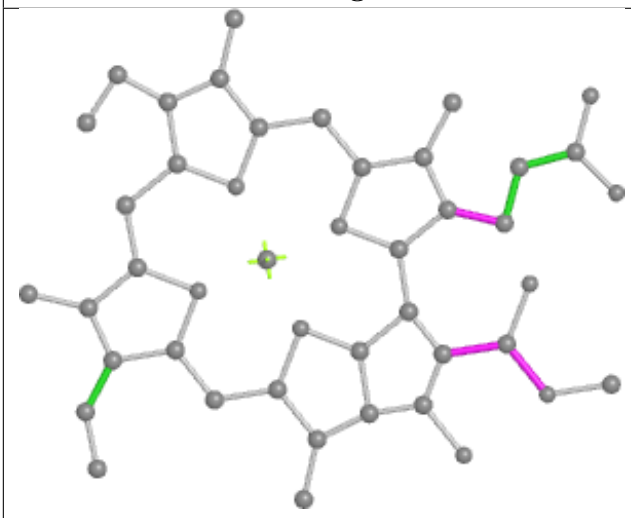

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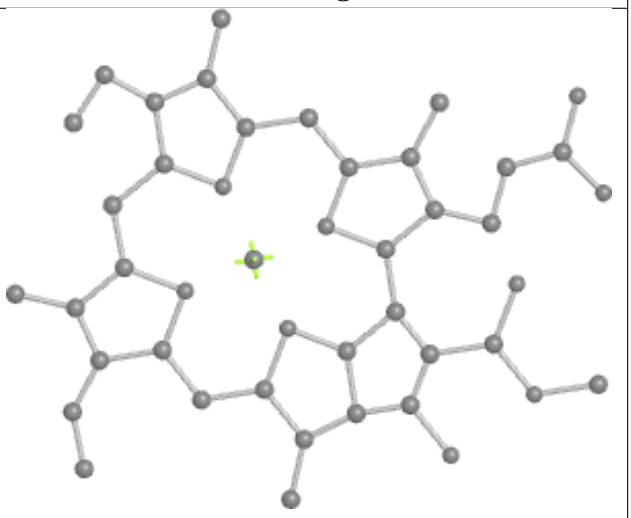
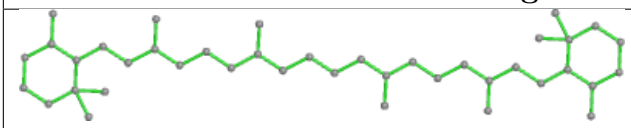


Rings

Ligand BCR f 4004



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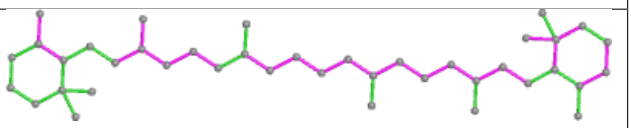
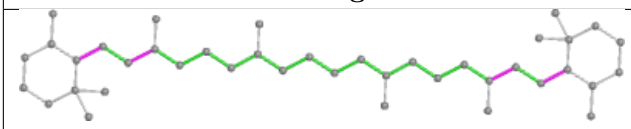


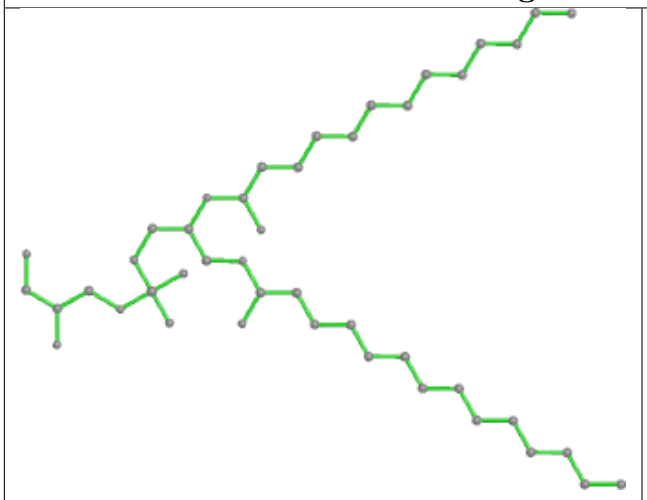
Bond angles



Torsions

Rings

Ligand LHG k 5001



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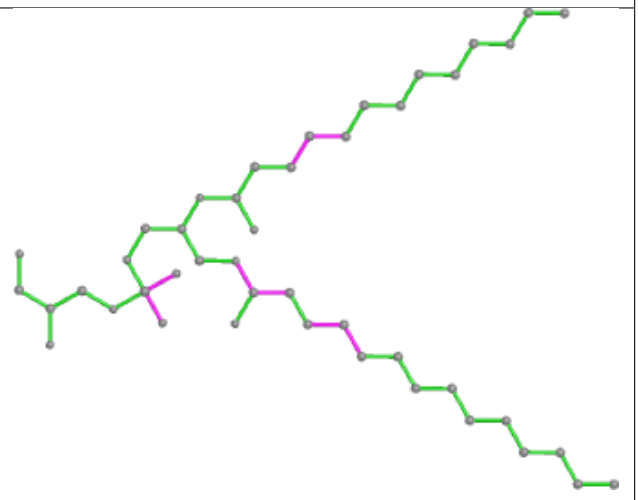

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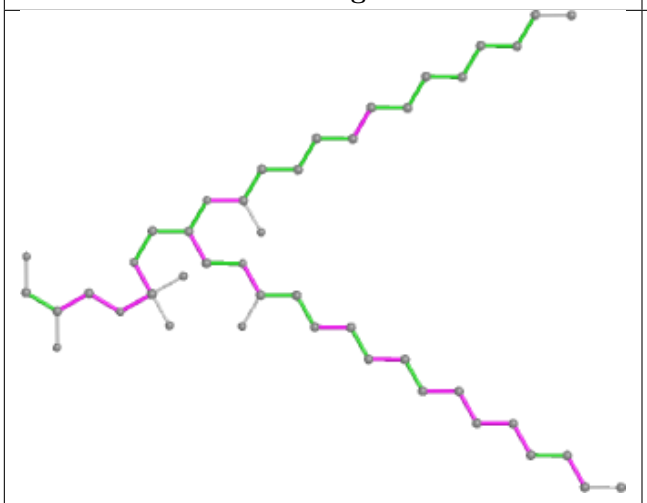

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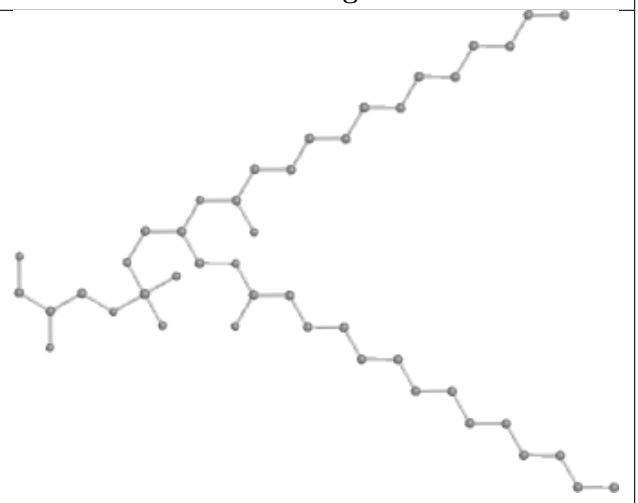
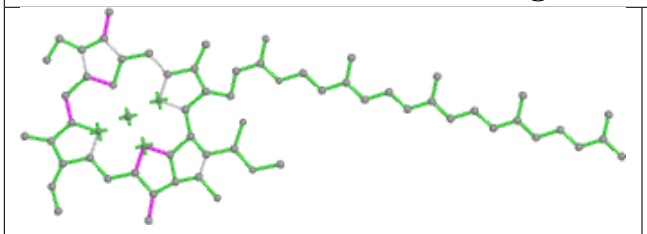


Rings

Ligand CLA a 503



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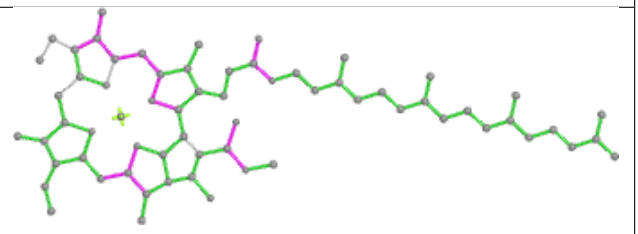
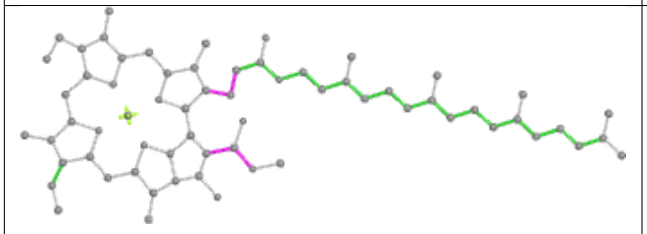


Bond angles



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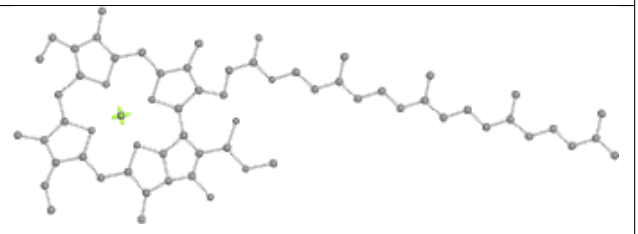
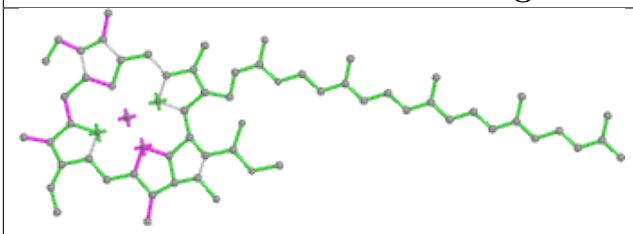


Rings

Ligand CLA H 1012



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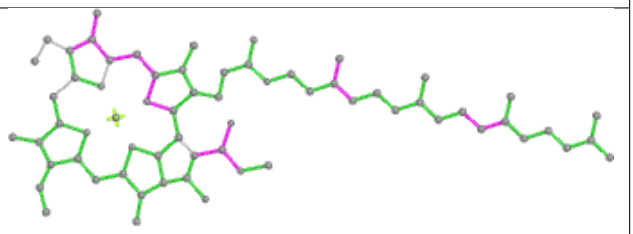
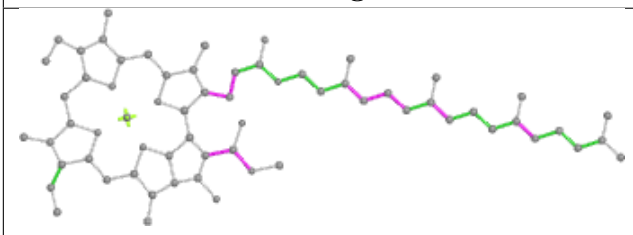


Bond angles



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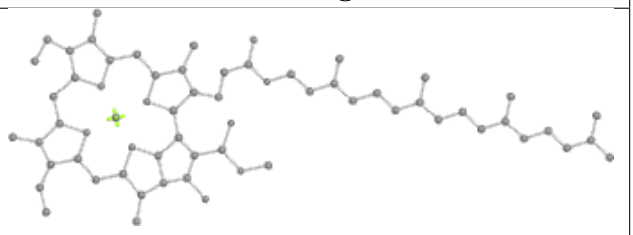
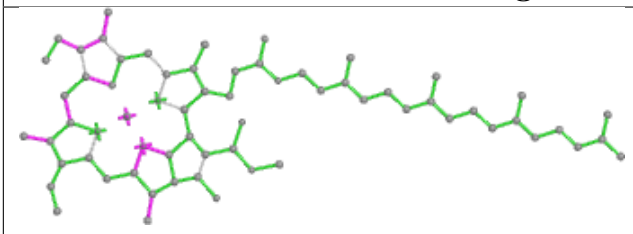


Rings

Ligand CLA A 1107



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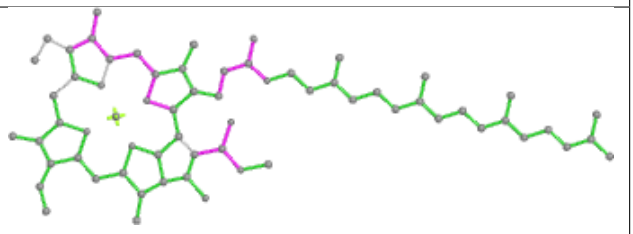
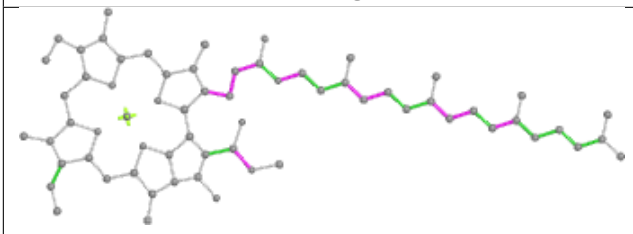


Bond angles



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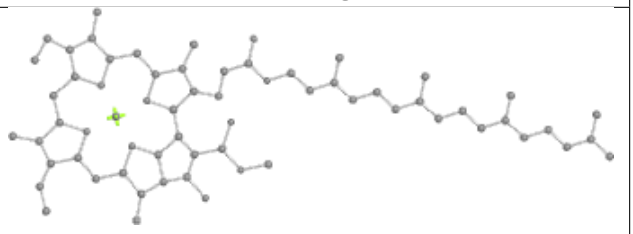
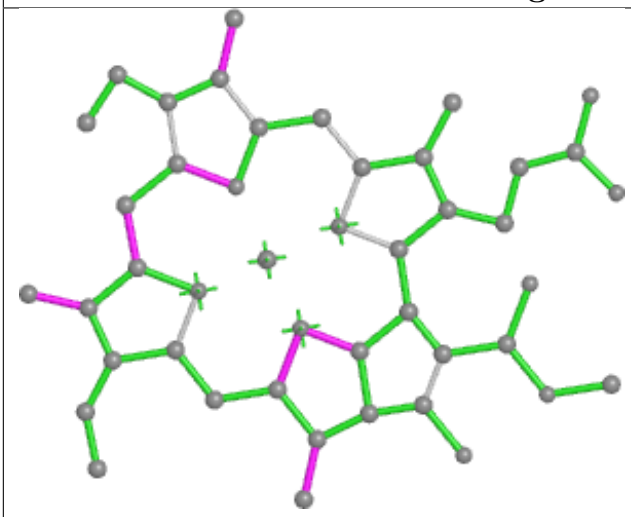


Rings

Ligand CLA 5 517



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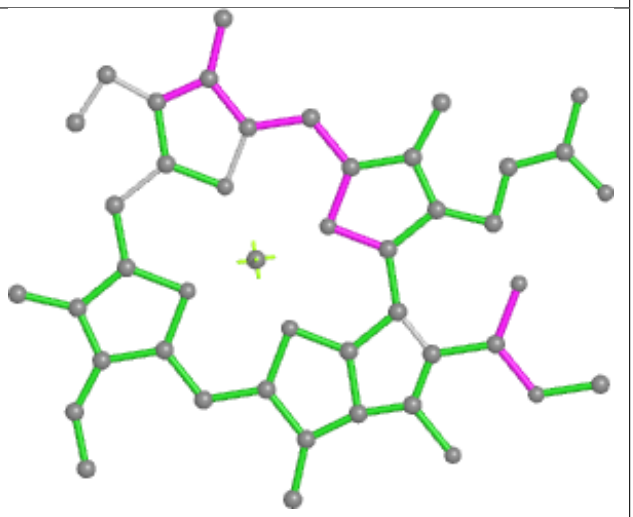
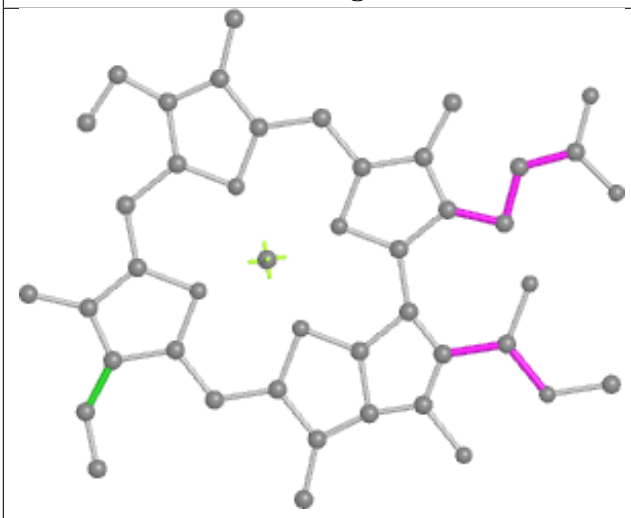


Bond angles



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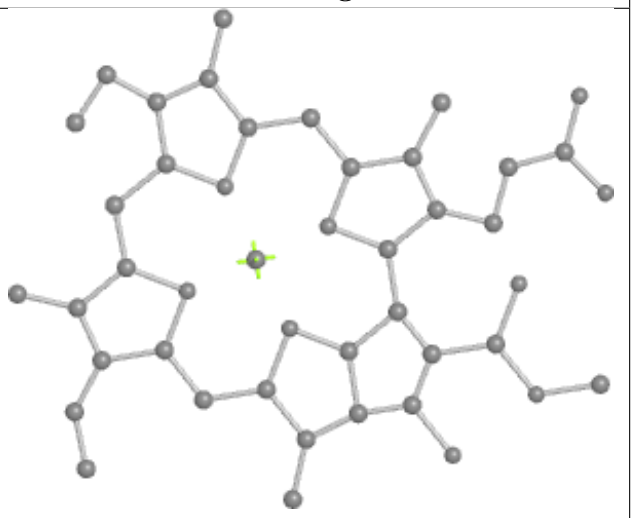
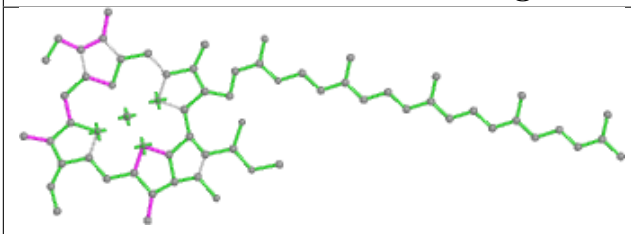


Rings

Ligand CLA G 1132



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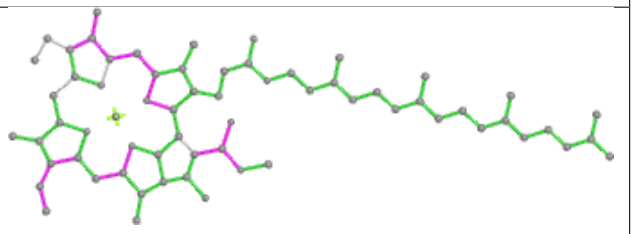
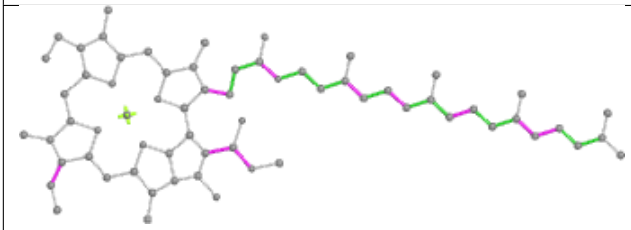


Bond angles



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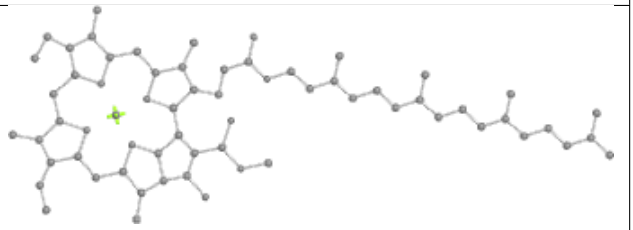
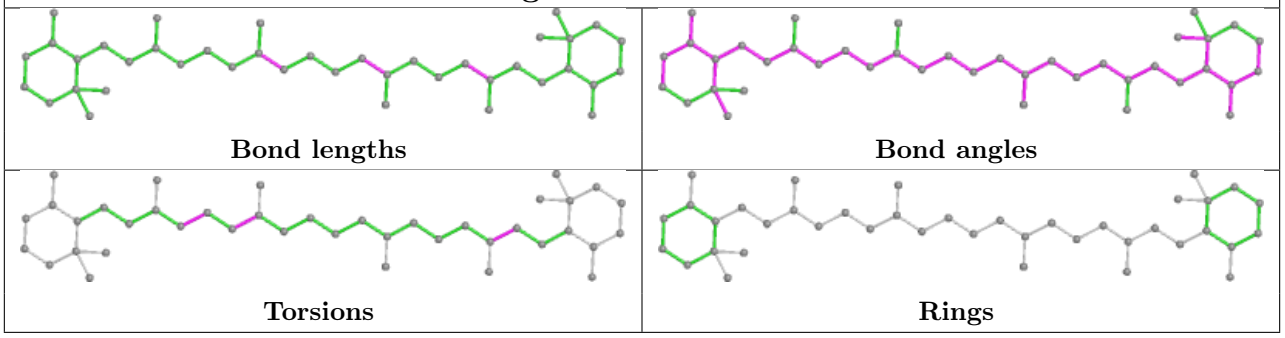
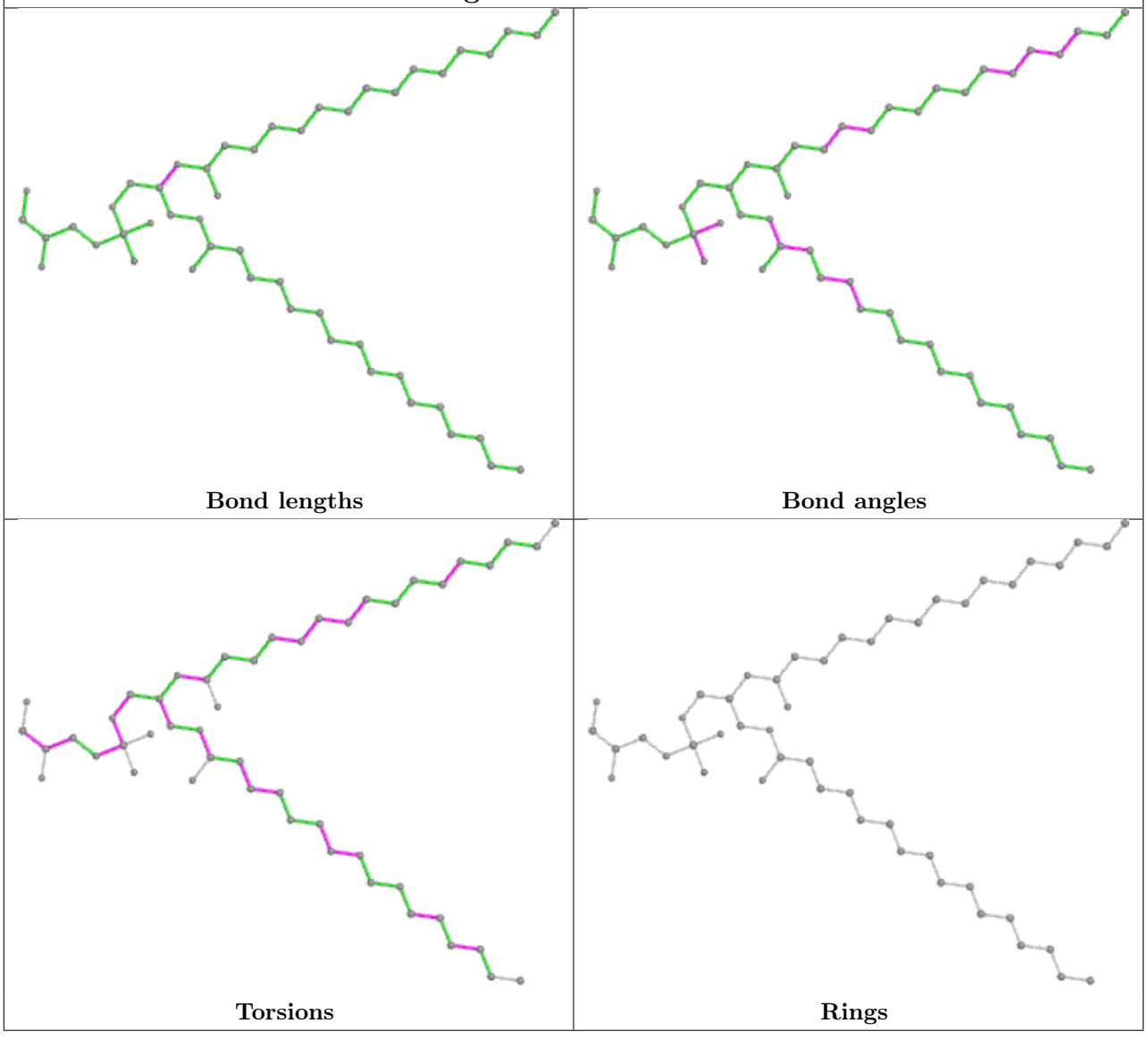


Rings

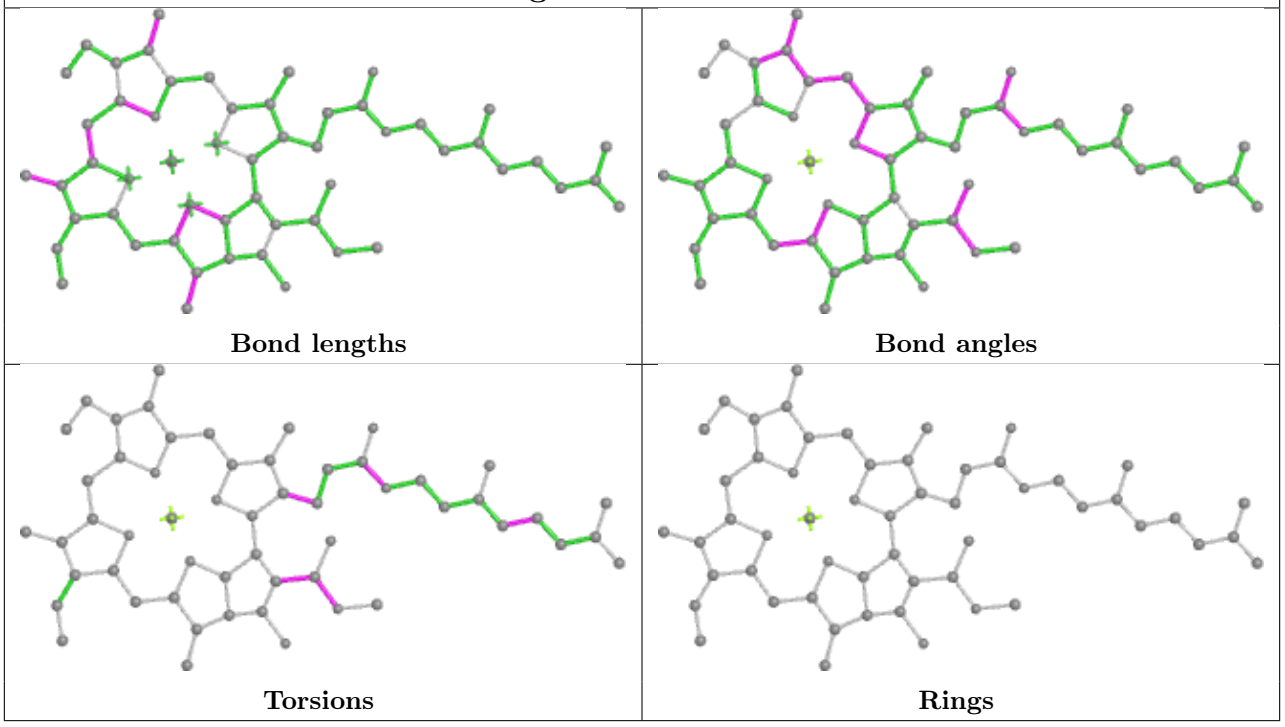
Ligand BCR f 4010



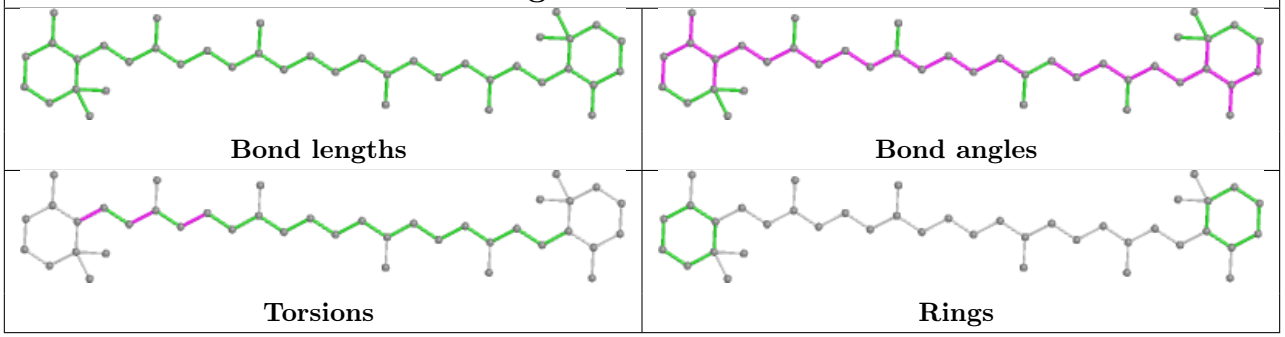
Ligand LHG e 5009



Ligand CLA 3 508



Ligand BCR c 522



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

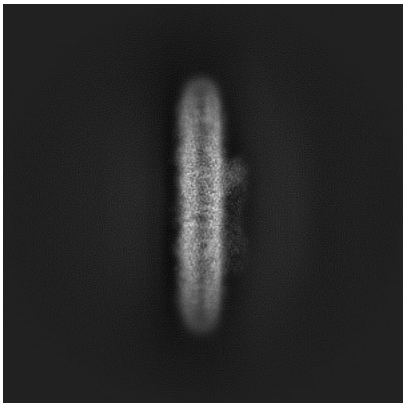
This section contains visualisations of the EMDB entry EMD-9995. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

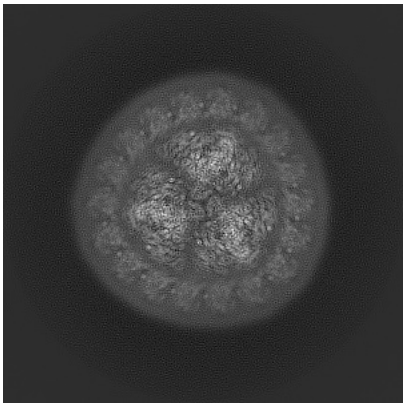
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

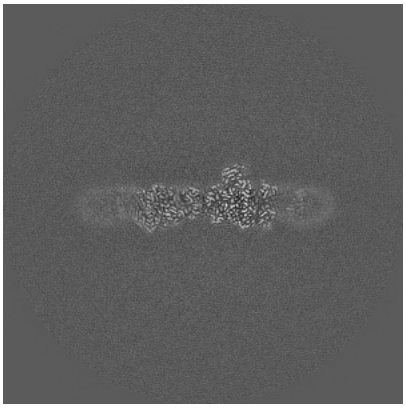


Z

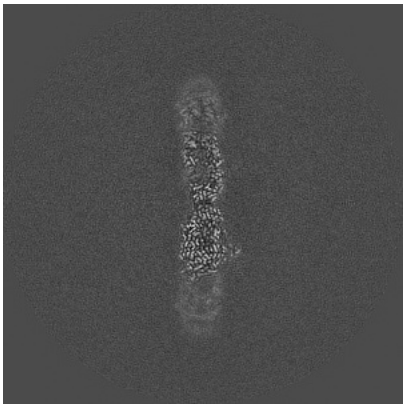
The images above show the map projected in three orthogonal directions.

6.2 Central slices

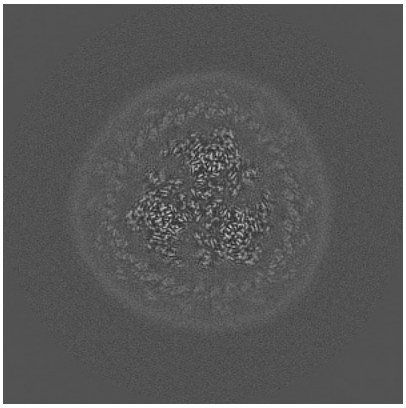
6.2.1 Primary map



X Index: 240



Y Index: 240

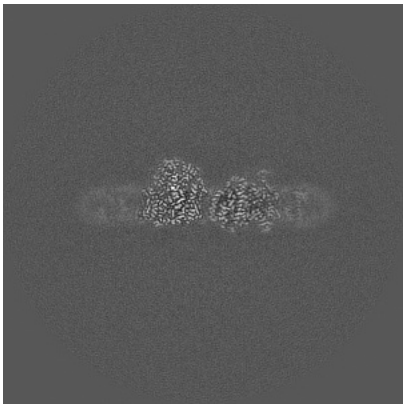


Z Index: 240

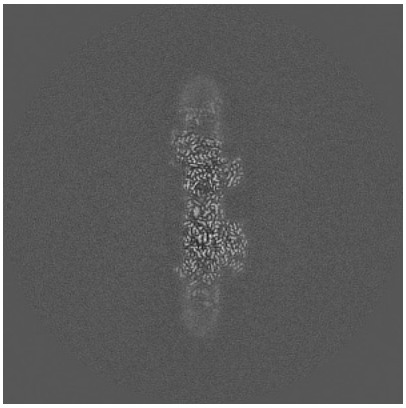
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

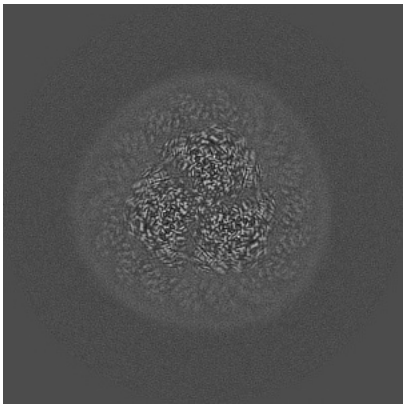
6.3.1 Primary map



X Index: 276



Y Index: 224



Z Index: 229

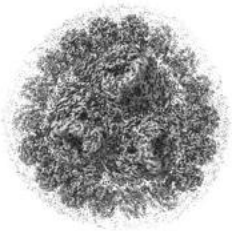
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

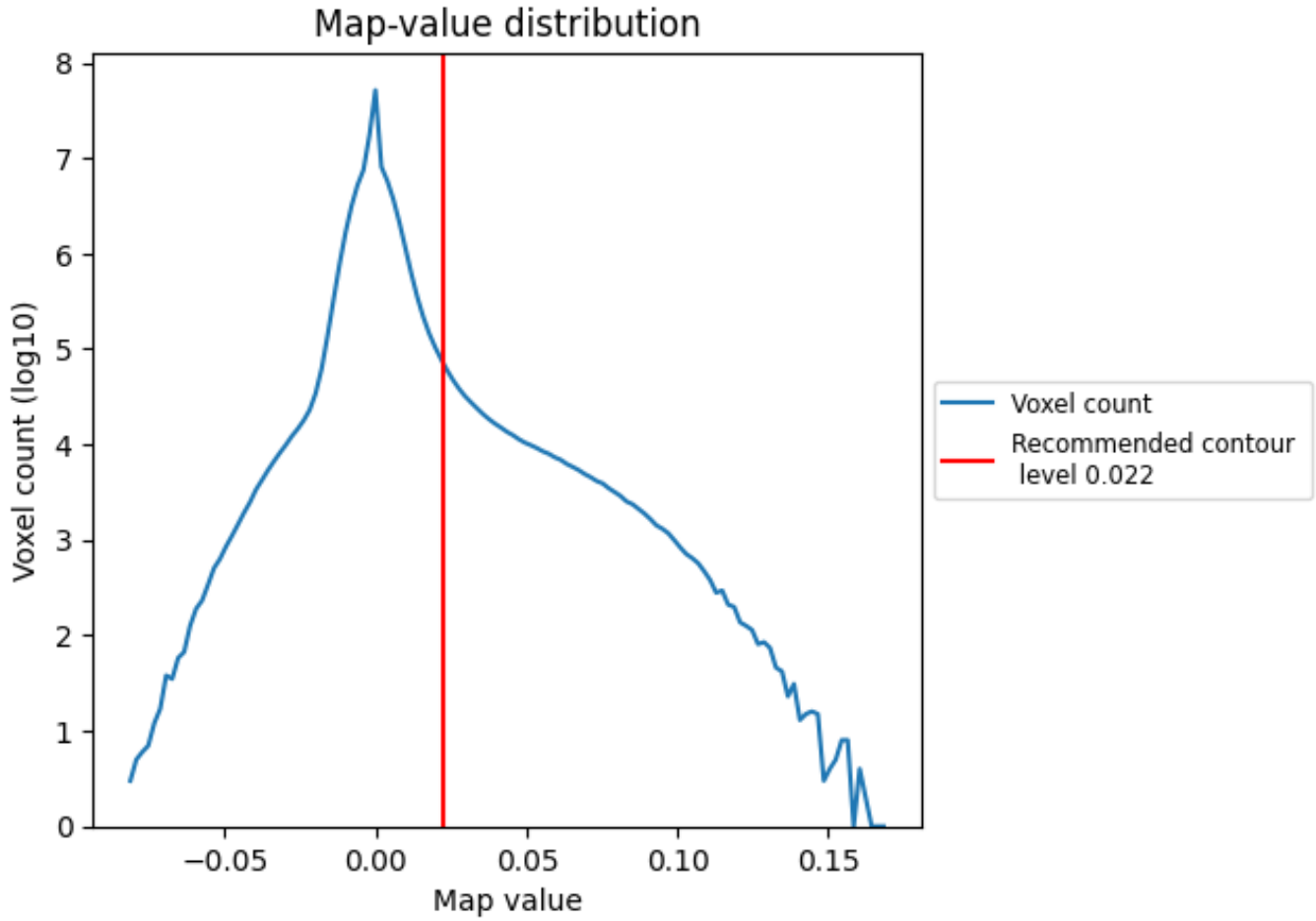
6.5 Mask visualisation (i)

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

7 Map analysis

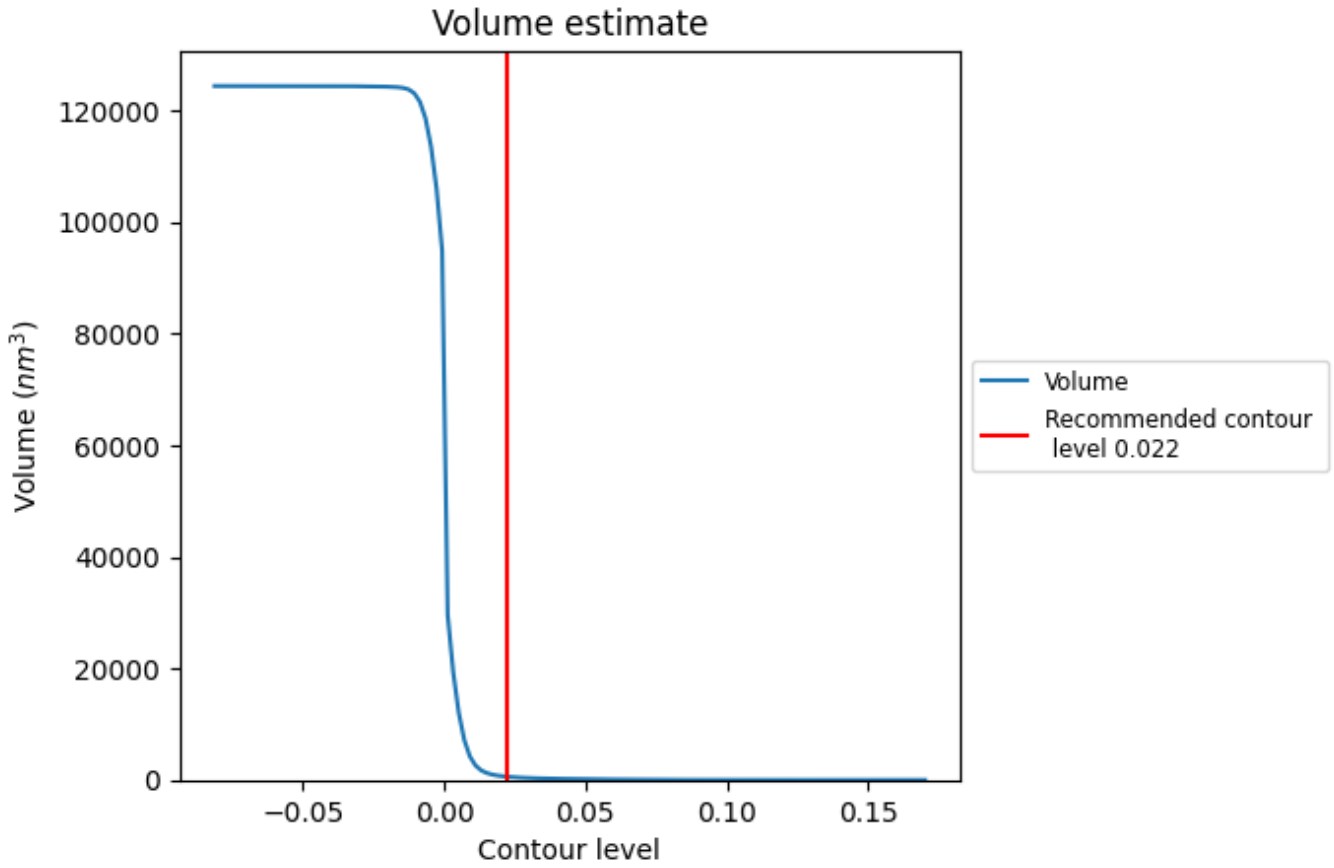
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

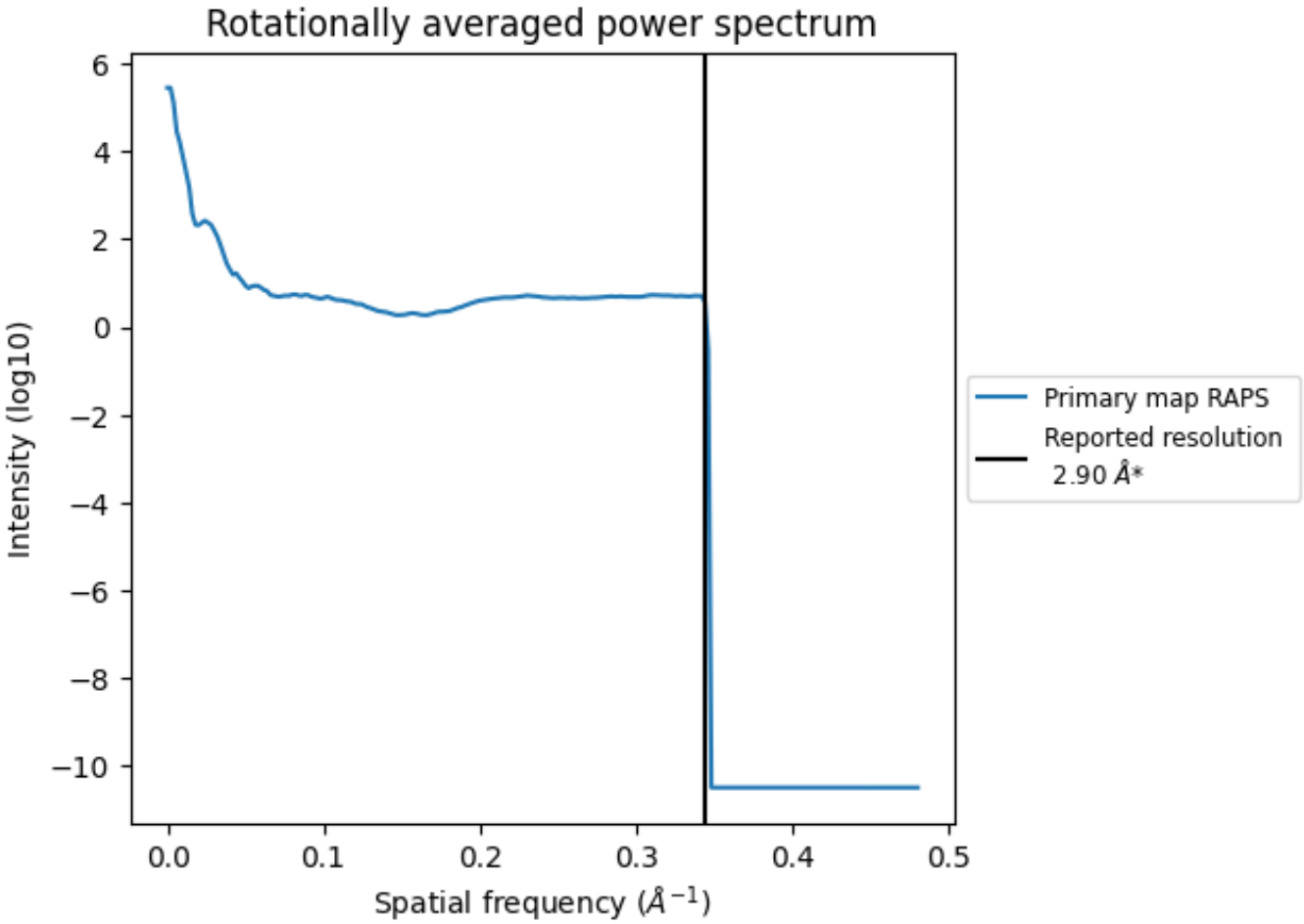
7.2 Volume estimate (i)



The volume at the recommended contour level is 595 nm^3; this corresponds to an approximate mass of 538 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 0.345 $Å^{-1}$

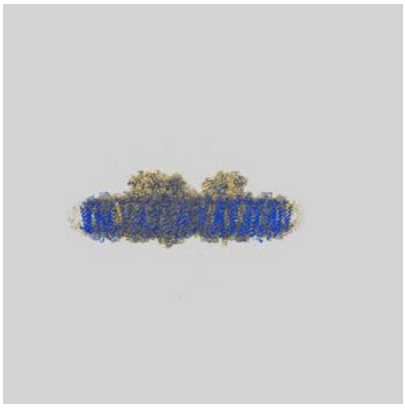
8 Fourier-Shell correlation

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

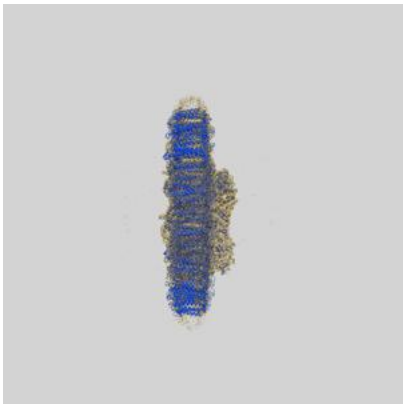
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9995 and PDB model 6KIG. Per-residue inclusion information can be found in section 3 on page 69.

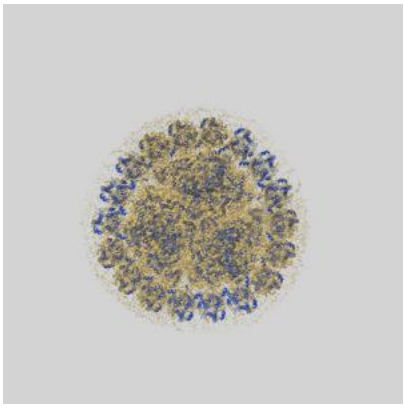
9.1 Map-model overlay



X



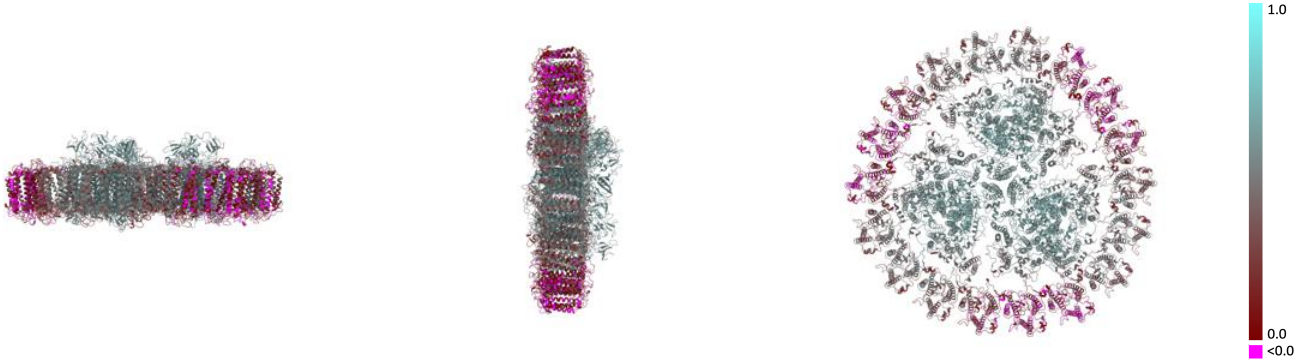
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 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.

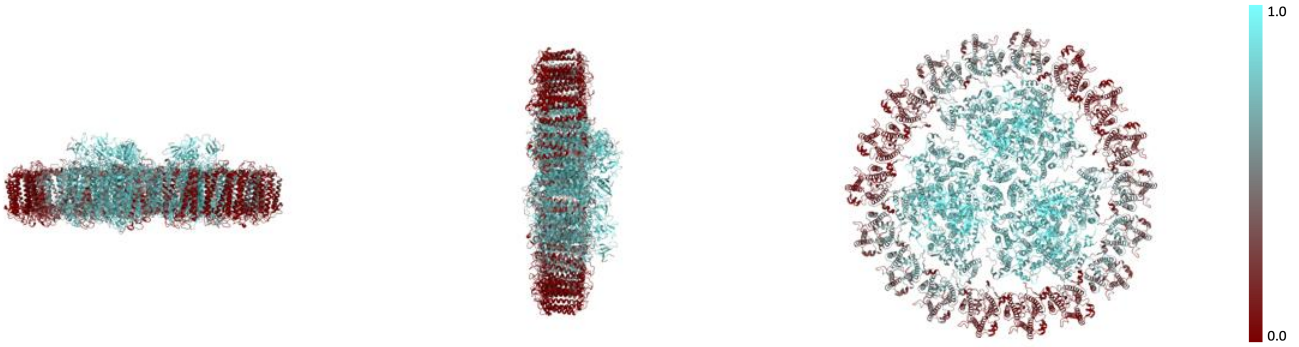
9.2 Q-score mapped to coordinate model



X Y Z

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.

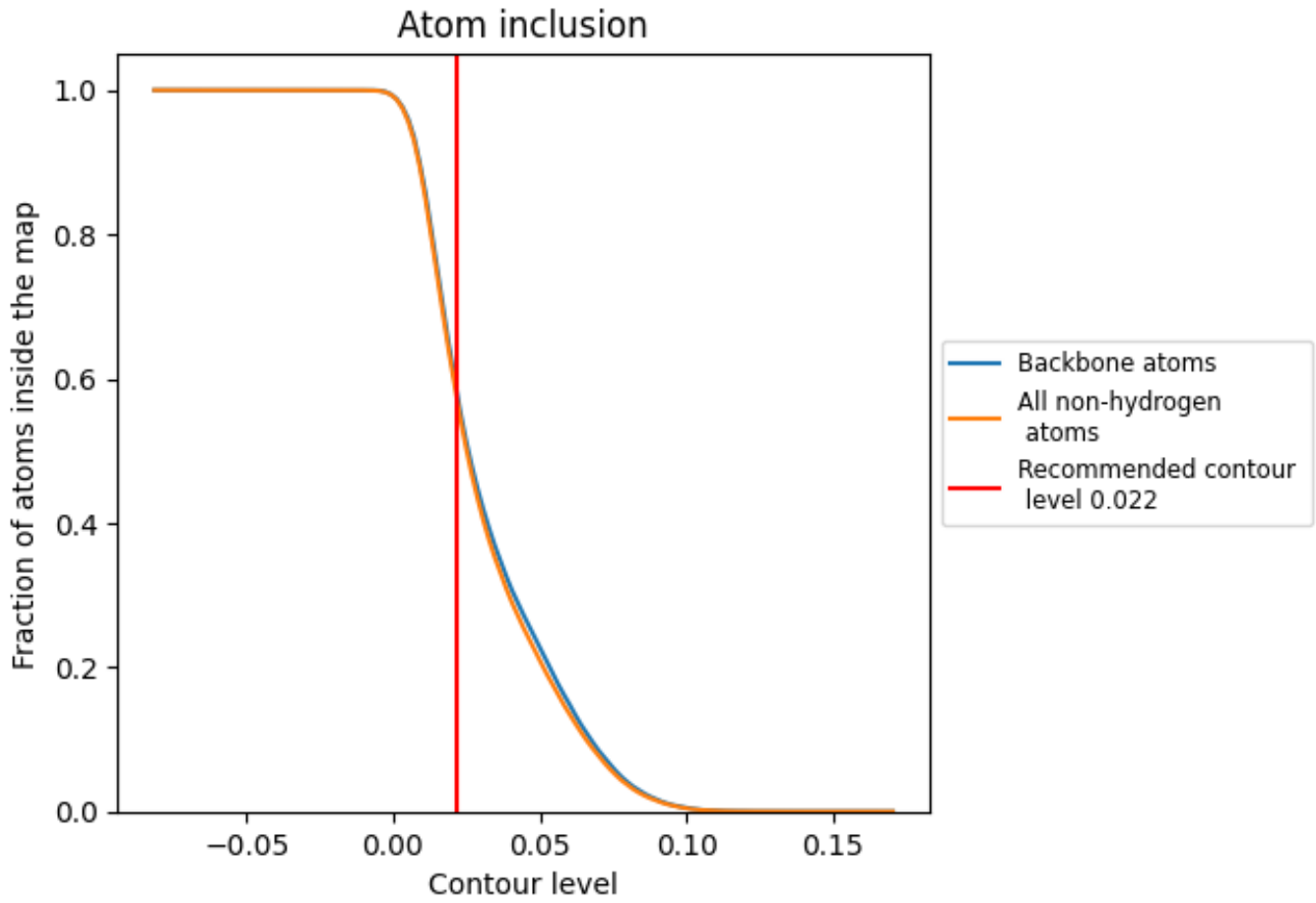
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5647	0.4190
1	0.4068	0.3640
2	0.4699	0.4180
3	0.3896	0.3830
4	0.1067	0.1410
5	0.0559	0.0860
6	0.1523	0.1850
A	0.8491	0.5780
B	0.8269	0.5450
C	0.9417	0.6070
D	0.8582	0.5770
E	0.7872	0.5410
F	0.7466	0.5290
G	0.8453	0.5770
H	0.8162	0.5370
I	0.8329	0.5720
J	0.7552	0.5460
K	0.5868	0.3890
L	0.8653	0.5930
M	0.7977	0.5290
N	0.9450	0.6070
O	0.8591	0.5780
Q	0.7815	0.5500
R	0.7440	0.5230
S	0.8247	0.5780
T	0.7359	0.5460
U	0.5813	0.3860
V	0.8689	0.5940
W	0.7786	0.5320
Y	0.4057	0.3660
Z	0.4669	0.4160
a	0.3874	0.3780
b	0.1036	0.1380
c	0.0531	0.0780
d	0.1449	0.1710

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	0.8419	0.5750
f	0.8211	0.5420
g	0.9417	0.6070
h	0.8693	0.5800
i	0.7947	0.5480
j	0.7500	0.5280
k	0.8411	0.5750
l	0.7472	0.5450
m	0.5785	0.3770
n	0.8665	0.5940
o	0.7824	0.5300
q	0.3921	0.3580
r	0.4580	0.4140
s	0.3907	0.3860
t	0.1104	0.1390
u	0.0559	0.0810
v	0.1543	0.1840