wwPDB EM Validation Summary Report (i)

Mar 31, 2025 – 06:44 PM JST

PDB ID	:	6KAF / pdb_00006kaf
EMDB ID	:	EMD-9957
Title	:	C2S2M2N2-type PSII-LHCII
Authors	:	Chang, S.H.; Shen, L.L.; Huang, Z.H.; Wang, W.D.; Han, G.Y.; Shen, J.R.; Zhang, X.
Deposited on	:	2019-06-22
Resolution	:	3.73 Å(reported)

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

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

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

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

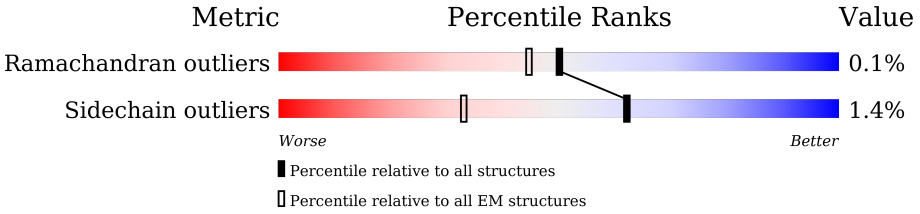
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.73 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	207382	16835
Sidechain outliers	206894	16415

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	R	280	16% 79% 20%
1	r	280	15% 79% • 20%
2	A	352	94% • 5%
2	a	352	• 94% 5%
3	D	352	95% • •
3	d	352	95% • •
4	F	44	5% 68% 32%
4	f	44	5% 68% 32%
5	H	88	• 73% 27%

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Mol	Chain	Length	Quality of chain
5	h	88	73% 27%
6	I	37	86% 5% 8%
6	i	37	86% 5% 8%
7	J	50	32% 62% 38%
7	j	50	32% 62% 38%
8	K	46	78% 22%
8	k	46	78% 22%
9	L	38	5% 97%
9	l	38	5% 97%
10	M	34	94% 6%
10	m	34	6% 94% 6%
11	O	291	7% 72% 28%
11	o	291	8% 71% 28%
12	T	31	97%
12	t	31	97%
13	W	115	47% 53%
13	w	115	47% 53%
14	X	101	35% 65%
14	x	101	35% 65%
15	Z	62	100%
15	z	62	100%
16	Y	33	9% 91% 9%
16	y	33	9% 91% 9%
17	E	82	82% 17%
17	e	82	82% 17%

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Mol	Chain	Length	Quality of chain
18	1	257	30% 82% 15%
18	2	257	63% 81% 15%
18	3	257	58% 82% 15%
18	4	257	30% 82% 15%
18	5	257	63% 82% 15%
18	6	257	57% 83% 15%
18	G	257	6% 83% 15%
18	N	257	81% 16%
18	P	257	61% 82% 15%
18	Q	257	80% 83% 15%
18	U	257	82% 15%
18	V	257	69% 82% 15%
18	g	257	7% 83% 15%
18	n	257	82% 15%
18	p	257	60% 81% 15%
18	q	257	80% 83% 15%
18	u	257	83% 15%
18	v	257	68% 82% 15%
19	S	289	81% 18%
19	s	289	81% 18%
20	C	461	97%
20	c	461	97%
21	B	508	98%
21	b	508	5% 98%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	301	X	-	-	-
22	CLA	1	302	X	-	-	-
22	CLA	1	303	X	-	-	-
22	CLA	1	304	X	-	-	-
22	CLA	1	305	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	2	301	X	-	-	-
22	CLA	2	302	X	-	-	-
22	CLA	2	303	X	-	-	-
22	CLA	2	304	X	-	-	-
22	CLA	2	305	X	-	-	-
22	CLA	2	306	X	-	-	-
22	CLA	2	307	X	-	-	-
22	CLA	2	308	X	-	-	-
22	CLA	3	301	X	-	-	-
22	CLA	3	302	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	3	306	X	-	-	-
22	CLA	3	307	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	4	301	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	305	X	-	-	-
22	CLA	4	306	X	-	-	-
22	CLA	4	307	X	-	-	-
22	CLA	4	308	X	-	-	-
22	CLA	5	301	X	-	-	-
22	CLA	5	302	X	-	-	-
22	CLA	5	303	X	-	-	-
22	CLA	5	304	X	-	-	-
22	CLA	5	305	X	-	-	-
22	CLA	5	306	X	-	-	-
22	CLA	5	307	X	-	-	-
22	CLA	5	308	X	-	-	-
22	CLA	6	302	X	-	-	-
22	CLA	6	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	6	304	X	-	-	-
22	CLA	6	305	X	-	-	-
22	CLA	6	306	X	-	-	-
22	CLA	6	307	X	-	-	-
22	CLA	6	308	X	-	-	-
22	CLA	6	309	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	408	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	C	515	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	G	301	X	-	-	-
22	CLA	G	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	G	303	X	-	-	-
22	CLA	G	304	X	-	-	-
22	CLA	G	305	X	-	-	-
22	CLA	G	306	X	-	-	-
22	CLA	G	307	X	-	-	-
22	CLA	G	308	X	-	-	-
22	CLA	N	301	X	-	-	-
22	CLA	N	302	X	-	-	-
22	CLA	N	303	X	-	-	-
22	CLA	N	304	X	-	-	-
22	CLA	N	305	X	-	-	-
22	CLA	N	306	X	-	-	-
22	CLA	N	307	X	-	-	-
22	CLA	N	308	X	-	-	-
22	CLA	P	302	X	-	-	-
22	CLA	P	303	X	-	-	-
22	CLA	P	304	X	-	-	-
22	CLA	P	305	X	-	-	-
22	CLA	P	306	X	-	-	-
22	CLA	P	307	X	-	-	-
22	CLA	P	308	X	-	-	-
22	CLA	P	309	X	-	-	-
22	CLA	Q	301	X	-	-	-
22	CLA	Q	302	X	-	-	-
22	CLA	Q	303	X	-	-	-
22	CLA	Q	304	X	-	-	-
22	CLA	Q	305	X	-	-	-
22	CLA	Q	306	X	-	-	-
22	CLA	Q	307	X	-	-	-
22	CLA	Q	308	X	-	-	-
22	CLA	R	302	X	-	-	-
22	CLA	R	303	X	-	-	-
22	CLA	R	304	X	-	-	-
22	CLA	R	305	X	-	-	-
22	CLA	R	306	X	-	-	-
22	CLA	R	307	X	-	-	-
22	CLA	R	308	X	-	-	-
22	CLA	R	309	X	-	-	-
22	CLA	R	310	X	-	-	-
22	CLA	R	311	X	-	-	-
22	CLA	S	301	X	-	-	-
22	CLA	S	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	S	303	X	-	-	-
22	CLA	S	304	X	-	-	-
22	CLA	S	305	X	-	-	-
22	CLA	S	306	X	-	-	-
22	CLA	S	307	X	-	-	-
22	CLA	S	308	X	-	-	-
22	CLA	S	309	X	-	-	-
22	CLA	U	302	X	-	-	-
22	CLA	U	303	X	-	-	-
22	CLA	U	304	X	-	-	-
22	CLA	U	305	X	-	-	-
22	CLA	U	306	X	-	-	-
22	CLA	U	307	X	-	-	-
22	CLA	U	308	X	-	-	-
22	CLA	V	302	X	-	-	-
22	CLA	V	303	X	-	-	-
22	CLA	V	304	X	-	-	-
22	CLA	V	305	X	-	-	-
22	CLA	V	306	X	-	-	-
22	CLA	V	307	X	-	-	-
22	CLA	V	308	X	-	-	-
22	CLA	X	202	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	g	301	X	-	-	-
22	CLA	g	302	X	-	-	-
22	CLA	g	303	X	-	-	-
22	CLA	g	304	X	-	-	-
22	CLA	g	305	X	-	-	-
22	CLA	g	306	X	-	-	-
22	CLA	g	307	X	-	-	-
22	CLA	g	308	X	-	-	-
22	CLA	n	301	X	-	-	-
22	CLA	n	302	X	-	-	-
22	CLA	n	303	X	-	-	-
22	CLA	n	304	X	-	-	-
22	CLA	n	305	X	-	-	-
22	CLA	n	306	X	-	-	-
22	CLA	n	307	X	-	-	-
22	CLA	n	308	X	-	-	-
22	CLA	p	302	X	-	-	-
22	CLA	p	303	X	-	-	-
22	CLA	p	304	X	-	-	-
22	CLA	p	305	X	-	-	-
22	CLA	p	306	X	-	-	-
22	CLA	p	307	X	-	-	-
22	CLA	p	308	X	-	-	-
22	CLA	p	309	X	-	-	-
22	CLA	q	302	X	-	-	-
22	CLA	q	303	X	-	-	-
22	CLA	q	304	X	-	-	-
22	CLA	q	305	X	-	-	-
22	CLA	q	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	q	307	X	-	-	-
22	CLA	q	308	X	-	-	-
22	CLA	r	601	X	-	-	-
22	CLA	r	602	X	-	-	-
22	CLA	r	603	X	-	-	-
22	CLA	r	604	X	-	-	-
22	CLA	r	605	X	-	-	-
22	CLA	r	606	X	-	-	-
22	CLA	r	607	X	-	-	-
22	CLA	r	608	X	-	-	-
22	CLA	r	609	X	-	-	-
22	CLA	r	610	X	-	-	-
22	CLA	s	301	X	-	-	-
22	CLA	s	302	X	-	-	-
22	CLA	s	303	X	-	-	-
22	CLA	s	304	X	-	-	-
22	CLA	s	305	X	-	-	-
22	CLA	s	306	X	-	-	-
22	CLA	s	307	X	-	-	-
22	CLA	s	308	X	-	-	-
22	CLA	s	309	X	-	-	-
22	CLA	u	302	X	-	-	-
22	CLA	u	303	X	-	-	-
22	CLA	u	304	X	-	-	-
22	CLA	u	305	X	-	-	-
22	CLA	u	306	X	-	-	-
22	CLA	u	307	X	-	-	-
22	CLA	u	308	X	-	-	-
22	CLA	v	302	X	-	-	-
22	CLA	v	303	X	-	-	-
22	CLA	v	304	X	-	-	-
22	CLA	v	305	X	-	-	-
22	CLA	v	306	X	-	-	-
22	CLA	v	307	X	-	-	-
22	CLA	v	308	X	-	-	-
22	CLA	x	201	X	-	-	-
26	CHL	1	313	X	-	-	-
26	CHL	1	314	X	-	-	-
26	CHL	1	315	X	-	-	-
26	CHL	1	316	X	-	-	-
26	CHL	1	317	X	-	-	-
26	CHL	1	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	2	313	X	-	-	-
26	CHL	2	314	X	-	-	-
26	CHL	2	315	X	-	-	-
26	CHL	2	316	X	-	-	-
26	CHL	2	317	X	-	-	-
26	CHL	2	318	X	-	-	-
26	CHL	3	311	X	-	-	-
26	CHL	3	312	X	-	-	-
26	CHL	3	313	X	-	-	-
26	CHL	3	314	X	-	-	-
26	CHL	3	315	X	-	-	-
26	CHL	3	316	X	-	-	-
26	CHL	4	313	X	-	-	-
26	CHL	4	314	X	-	-	-
26	CHL	4	315	X	-	-	-
26	CHL	4	316	X	-	-	-
26	CHL	4	317	X	-	-	-
26	CHL	5	313	X	-	-	-
26	CHL	5	314	X	-	-	-
26	CHL	5	315	X	-	-	-
26	CHL	5	316	X	-	-	-
26	CHL	5	317	X	-	-	-
26	CHL	5	318	X	-	-	-
26	CHL	6	301	X	-	-	-
26	CHL	6	312	X	-	-	-
26	CHL	6	313	X	-	-	-
26	CHL	6	314	X	-	-	-
26	CHL	6	315	X	-	-	-
26	CHL	6	316	X	-	-	-
26	CHL	6	317	X	-	-	-
26	CHL	G	311	X	-	-	-
26	CHL	G	312	X	-	-	-
26	CHL	G	313	X	-	-	-
26	CHL	G	314	X	-	-	-
26	CHL	G	315	X	-	-	-
26	CHL	G	316	X	-	-	-
26	CHL	N	313	X	-	-	-
26	CHL	N	314	X	-	-	-
26	CHL	N	315	X	-	-	-
26	CHL	N	316	X	-	-	-
26	CHL	N	317	X	-	-	-
26	CHL	P	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	P	315	X	-	-	-
26	CHL	P	316	X	-	-	-
26	CHL	P	317	X	-	-	-
26	CHL	P	318	X	-	-	-
26	CHL	P	319	X	-	-	-
26	CHL	Q	311	X	-	-	-
26	CHL	Q	312	X	-	-	-
26	CHL	Q	313	X	-	-	-
26	CHL	Q	314	X	-	-	-
26	CHL	Q	315	X	-	-	-
26	CHL	Q	316	X	-	-	-
26	CHL	R	315	X	-	-	-
26	CHL	R	316	X	-	-	-
26	CHL	R	317	X	-	-	-
26	CHL	S	313	X	-	-	-
26	CHL	S	314	X	-	-	-
26	CHL	S	315	X	-	-	-
26	CHL	S	316	X	-	-	-
26	CHL	U	313	X	-	-	-
26	CHL	U	314	X	-	-	-
26	CHL	U	315	X	-	-	-
26	CHL	U	316	X	-	-	-
26	CHL	U	317	X	-	-	-
26	CHL	U	319	X	-	-	-
26	CHL	V	313	X	-	-	-
26	CHL	V	314	X	-	-	-
26	CHL	V	315	X	-	-	-
26	CHL	V	316	X	-	-	-
26	CHL	V	317	X	-	-	-
26	CHL	V	318	X	-	-	-
26	CHL	g	311	X	-	-	-
26	CHL	g	312	X	-	-	-
26	CHL	g	313	X	-	-	-
26	CHL	g	314	X	-	-	-
26	CHL	g	315	X	-	-	-
26	CHL	g	316	X	-	-	-
26	CHL	n	313	X	-	-	-
26	CHL	n	314	X	-	-	-
26	CHL	n	315	X	-	-	-
26	CHL	n	316	X	-	-	-
26	CHL	n	317	X	-	-	-
26	CHL	n	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	p	314	X	-	-	-
26	CHL	p	315	X	-	-	-
26	CHL	p	316	X	-	-	-
26	CHL	p	317	X	-	-	-
26	CHL	p	318	X	-	-	-
26	CHL	p	319	X	-	-	-
26	CHL	p	320	X	-	-	-
26	CHL	q	311	X	-	-	-
26	CHL	q	312	X	-	-	-
26	CHL	q	313	X	-	-	-
26	CHL	q	314	X	-	-	-
26	CHL	q	315	X	-	-	-
26	CHL	r	614	X	-	-	-
26	CHL	r	615	X	-	-	-
26	CHL	r	616	X	-	-	-
26	CHL	r	619	X	-	-	-
26	CHL	s	313	X	-	-	-
26	CHL	s	314	X	-	-	-
26	CHL	s	315	X	-	-	-
26	CHL	s	316	X	-	-	-
26	CHL	u	313	X	-	-	-
26	CHL	u	314	X	-	-	-
26	CHL	u	315	X	-	-	-
26	CHL	u	316	X	-	-	-
26	CHL	u	317	X	-	-	-
26	CHL	u	318	X	-	-	-
26	CHL	v	313	X	-	-	-
26	CHL	v	314	X	-	-	-
26	CHL	v	315	X	-	-	-
26	CHL	v	316	X	-	-	-
26	CHL	v	317	X	-	-	-
26	CHL	v	318	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 104363 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 Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	r	223	1701	1081	286	329	5	0	0
1	R	223	1698	1080	285	328	5	0	0

- Molecule 2 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	a	333	2614	1707	430	462	15	0	0
2	A	333	2614	1707	430	462	15	0	0

- Molecule 3 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	341	2714	1791	447	464	12	0	0
3	D	341	2714	1791	447	464	12	0	0

- Molecule 4 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	f	30	243	165	41	36	1	0	0
4	F	30	243	165	41	36	1	0	0

- Molecule 5 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	h	64	488	327	72	87	2	0	0
5	H	64	488	327	72	87	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	i	34	275	189	41	43	2	0	0
6	I	34	275	189	41	43	2	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein J, PsbJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	j	31	245	168	36	39	2	0	0
7	J	31	245	168	36	39	2	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	k	36	288	203	41	44	0	0
8	K	36	288	203	41	44	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	l	37	306	205	50	51	0	0
9	L	37	306	205	50	51	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	m	32	248	168	35	45	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	M	32	248	168	35	45	0	0

- Molecule 11 is a protein called Oxygen-evolving enhancer protein 1 of photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	o	210	1592	1016	254	318	4	0	0
11	O	210	1592	1016	254	318	4	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	t	30	247	171	36	38	2	0	0
12	T	30	247	171	36	38	2	0	0

- Molecule 13 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	w	54	417	269	67	79	2	0	0
13	W	54	417	269	67	79	2	0	0

- Molecule 14 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	x	35	242	159	39	44	0	0
14	X	35	242	159	39	44	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	z	62	465	319	69	76	1	0	0
15	Z	62	465	319	69	76	1	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein 30, Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	Y	30	208	137	34	37	0	0
16	y	30	208	137	34	37	0	0

- Molecule 17 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	E	68	555	366	90	99	0	0
17	e	68	555	366	90	99	0	0

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	1	218	1669	1081	271	312	5	0	0
18	2	218	1669	1081	271	312	5	0	0
18	3	219	1675	1084	272	314	5	0	0
18	4	218	1669	1081	271	312	5	0	0
18	5	218	1669	1081	271	312	5	0	0
18	6	219	1675	1084	272	314	5	0	0
18	v	218	1669	1081	271	312	5	0	0
18	p	218	1669	1081	271	312	5	0	0
18	q	219	1675	1084	272	314	5	0	0
18	V	218	1669	1081	271	312	5	0	0
18	P	218	1669	1081	271	312	5	0	0
18	Q	219	1675	1084	272	314	5	0	0
18	U	218	1669	1081	271	312	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	217	1661	1075	270	311	5	0	0
18	G	219	1675	1084	272	314	5	0	0
18	u	218	1669	1081	271	312	5	0	0
18	n	218	1669	1081	271	312	5	0	0
18	g	219	1675	1084	272	314	5	0	0

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	236	1797	1166	290	337	4	0	0
19	s	236	1797	1166	290	337	4	0	0

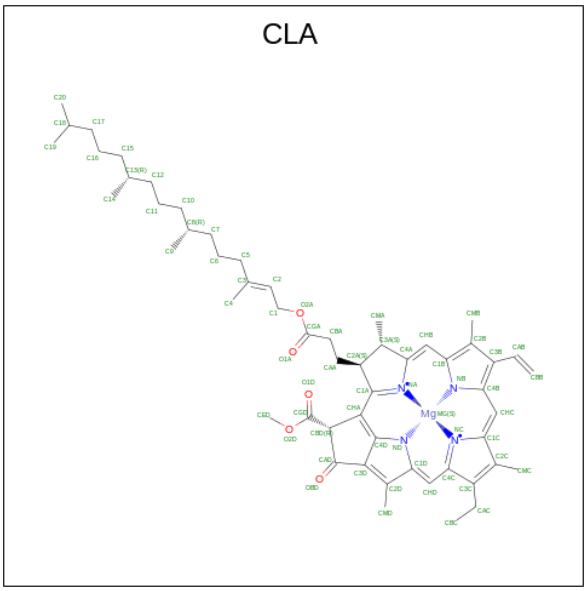
- Molecule 20 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	C	450	3502	2290	585	610	17	0	0
20	c	450	3502	2290	585	610	17	0	0

- Molecule 21 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	B	503	3937	2575	658	692	12	0	0
21	b	503	3937	2575	658	692	12	0	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	a	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	d	1	65	55	1	4	5	0
22	x	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	50	40	1	4	5	0
22	A	1	60	50	1	4	5	0
22	1	1	65	55	1	4	5	0
22	1	1	65	55	1	4	5	0
22	1	1	50	40	1	4	5	0
22	1	1	60	50	1	4	5	0
22	1	1	60	50	1	4	5	0
22	1	1	60	50	1	4	5	0
22	1	1	65	55	1	4	5	0
22	1	1	48	38	1	4	5	0
22	2	1	65	55	1	4	5	0
22	2	1	65	55	1	4	5	0
22	2	1	50	40	1	4	5	0
22	2	1	65	55	1	4	5	0
22	2	1	60	50	1	4	5	0
22	2	1	60	50	1	4	5	0
22	2	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	2	1	48	38	1	4	5	0
22	3	1	65	55	1	4	5	0
22	3	1	65	55	1	4	5	0
22	3	1	50	40	1	4	5	0
22	3	1	64	54	1	4	5	0
22	3	1	60	50	1	4	5	0
22	3	1	60	50	1	4	5	0
22	3	1	65	55	1	4	5	0
22	3	1	48	38	1	4	5	0
22	4	1	65	55	1	4	5	0
22	4	1	65	55	1	4	5	0
22	4	1	50	40	1	4	5	0
22	4	1	60	50	1	4	5	0
22	4	1	60	50	1	4	5	0
22	4	1	60	50	1	4	5	0
22	4	1	65	55	1	4	5	0
22	4	1	48	38	1	4	5	0
22	5	1	65	55	1	4	5	0
22	5	1	65	55	1	4	5	0
22	5	1	50	40	1	4	5	0
22	5	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	p	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	V	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	U	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	48	38	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	u	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	g	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms	AltConf
22	S	1	Total C Mg N O 49 39 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	D	1	Total C Mg N O 65 55 1 4 5	0
22	X	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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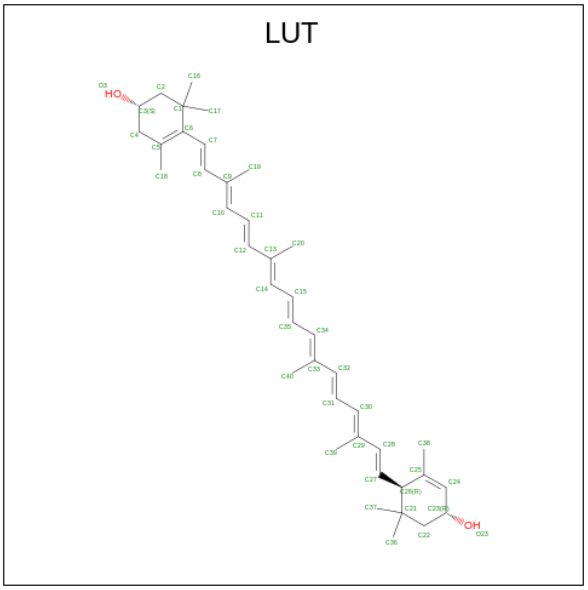
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	s	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	49	39	1	4	5	0

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	r	1	42	40	2	0
			Total	C	O	
23	1	1	42	40	2	0
			Total	C	O	
23	1	1	42	40	2	0
			Total	C	O	
23	2	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	2	1	42	40	2	0
23	4	1	42	40	2	0
23	4	1	42	40	2	0
23	5	1	42	40	2	0
23	5	1	42	40	2	0
23	v	1	42	40	2	0
23	v	1	42	40	2	0
23	p	1	42	40	2	0
23	p	1	42	40	2	0
23	V	1	42	40	2	0
23	V	1	42	40	2	0
23	P	1	42	40	2	0
23	P	1	42	40	2	0
23	U	1	42	40	2	0
23	U	1	42	40	2	0
23	N	1	42	40	2	0
23	N	1	42	40	2	0
23	u	1	42	40	2	0
23	u	1	42	40	2	0
23	n	1	42	40	2	0
23	n	1	42	40	2	0

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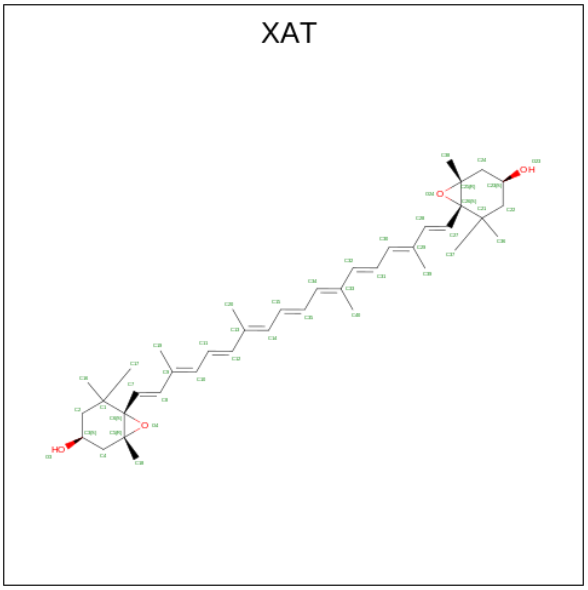
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	R	1	42	40	2	0
23	S	1	42	40	2	0
23	S	1	42	40	2	0
23	s	1	42	40	2	0
23	s	1	42	40	2	0

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	r	1	44	40	4	0
24	1	1	44	40	4	0
24	2	1	44	40	4	0
24	3	1	44	40	4	0
24	4	1	44	40	4	0
24	5	1	44	40	4	0

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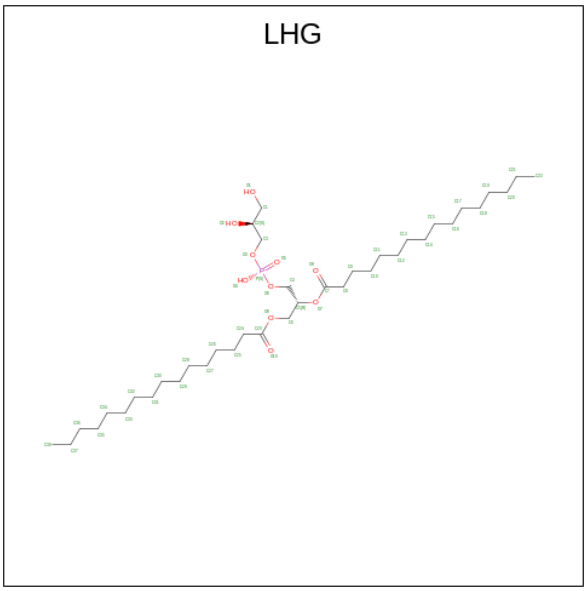
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	6	1	44	40	4	0
24	v	1	44	40	4	0
24	p	1	44	40	4	0
24	q	1	44	40	4	0
24	V	1	44	40	4	0
24	P	1	44	40	4	0
24	Q	1	44	40	4	0
24	U	1	44	40	4	0
24	N	1	44	40	4	0
24	G	1	44	40	4	0
24	u	1	44	40	4	0
24	n	1	44	40	4	0
24	g	1	44	40	4	0
24	R	1	44	40	4	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	r	1	42	31	10	1	0
25	a	1	43	32	10	1	0
25	d	1	46	35	10	1	0
25	d	1	49	38	10	1	0
25	l	1	49	38	10	1	0
25	A	1	43	32	10	1	0
25	L	1	49	38	10	1	0
25	1	1	49	38	10	1	0
25	2	1	49	38	10	1	0
25	3	1	49	38	10	1	0
25	4	1	49	38	10	1	0
25	5	1	49	38	10	1	0
25	6	1	49	38	10	1	0
25	v	1	49	38	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	p	1	49	38	10	1	0
25	q	1	49	38	10	1	0
25	V	1	49	38	10	1	0
25	P	1	49	38	10	1	0
25	Q	1	49	38	10	1	0
25	U	1	49	38	10	1	0
25	N	1	49	38	10	1	0
25	G	1	49	38	10	1	0
25	u	1	49	38	10	1	0
25	n	1	49	38	10	1	0
25	g	1	49	38	10	1	0
25	R	1	42	31	10	1	0
25	S	1	49	38	10	1	0
25	C	1	49	38	10	1	0
25	C	1	49	38	10	1	0
25	C	1	49	38	10	1	0
25	B	1	47	36	10	1	0
25	B	1	49	38	10	1	0
25	D	1	46	35	10	1	0
25	D	1	49	38	10	1	0
25	b	1	47	36	10	1	0

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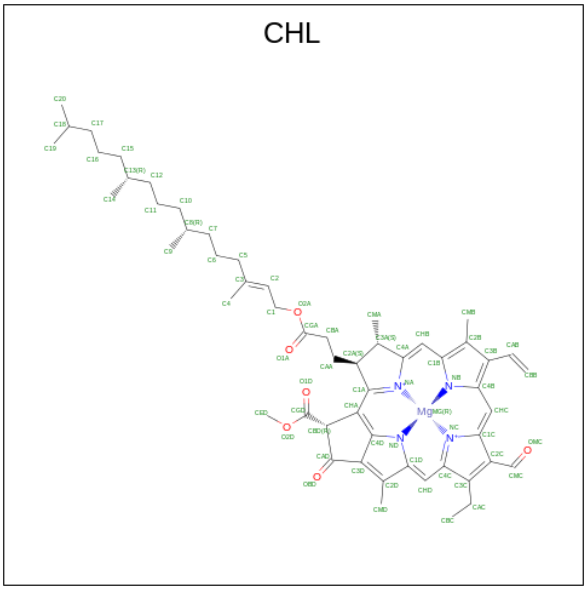
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	b	1	49	38	10	1	0
			Total	C	O	P	
25	c	1	49	38	10	1	0
			Total	C	O	P	
25	c	1	49	38	10	1	0
			Total	C	O	P	
25	c	1	49	38	10	1	0
			Total	C	O	P	
25	s	1	49	38	10	1	0

- Molecule 26 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	r	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	r	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
26	r	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	r	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	1	1	48	37	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	1	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	4	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	4	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	4	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	4	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	4	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	5	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	5	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	5	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	5	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	5	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	5	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	48	37	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	p	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	q	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	q	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	q	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	P	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	P	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	P	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	P	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	P	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	P	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	N	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	G	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	G	1	50	39	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	G	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	61	50	1	4	6	0

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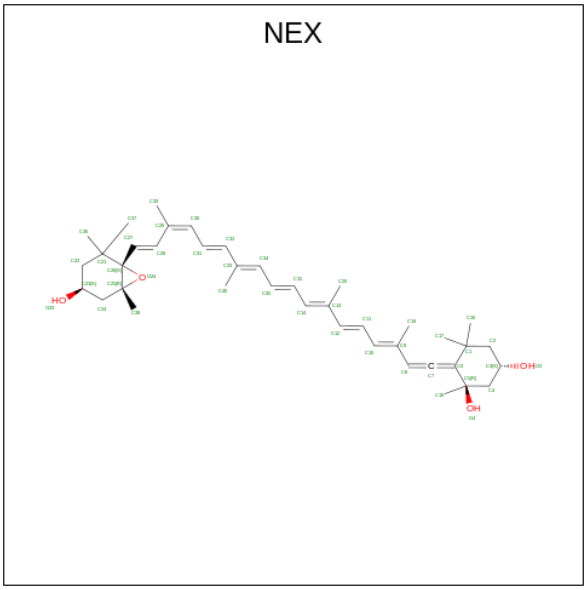
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	R	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	R	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
26	R	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
26	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
26	S	1	58	47	1	4	6	0
			Total	C	Mg	N	O	
26	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
26	s	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
26	s	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
26	s	1	58	47	1	4	6	0
			Total	C	Mg	N	O	
26	s	1	46	35	1	4	6	0

- Molecule 27 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	r	1	44	40	4	0
			Total	C	O	
27	r	1	44	40	4	0
			Total	C	O	
27	2	1	44	40	4	0
			Total	C	O	
27	5	1	44	40	4	0
			Total	C	O	
27	v	1	44	40	4	0
			Total	C	O	
27	p	1	44	40	4	0
			Total	C	O	
27	V	1	44	40	4	0
			Total	C	O	
27	P	1	44	40	4	0
			Total	C	O	
27	U	1	44	40	4	0
			Total	C	O	
27	N	1	44	40	4	0
			Total	C	O	
27	u	1	44	40	4	0
			Total	C	O	
27	u	1	44	40	4	0
			Total	C	O	
27	n	1	44	40	4	0
			Total	C	O	
27	R	1	44	40	4	0
			Total	C	O	
27	S	1	44	40	4	0
			Total	C	O	
27	s	1	44	40	4	0

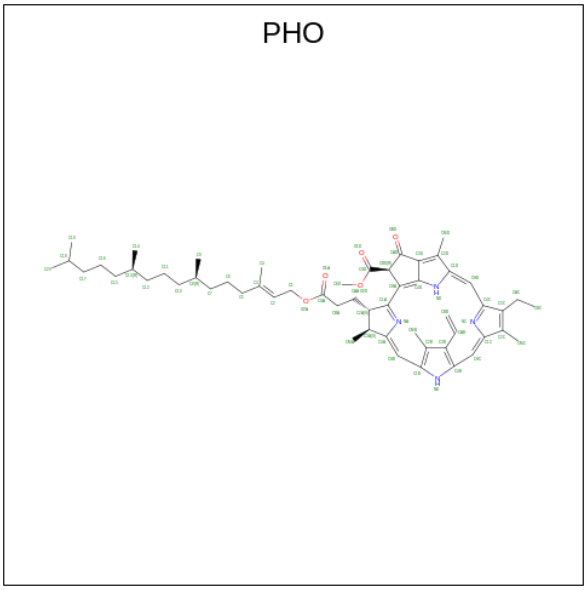
- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
28	a	1	1	1	0
			Total	Fe	
28	A	1	1	1	0

- Molecule 29 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

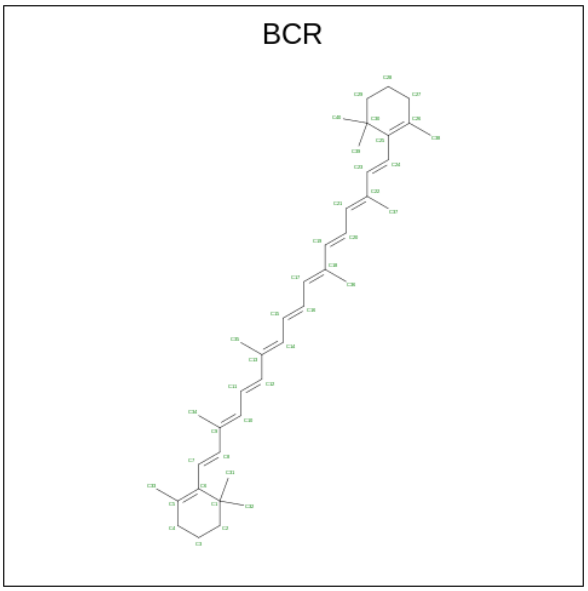
Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
29	a	2	2	2	0
			Total	Cl	
29	A	2	2	2	0

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	a	1	64	55	4	5	0
			Total	C	N	O	
30	d	1	64	55	4	5	0
			Total	C	N	O	
30	A	1	64	55	4	5	0
			Total	C	N	O	
30	D	1	64	55	4	5	0

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
31	a	1	40	40	0
31	d	1	40	40	0
31	k	1	40	40	0
31	t	1	40	40	0
31	x	1	40	40	0
31	z	1	40	40	0
31	A	1	40	40	0
31	K	1	40	40	0
31	T	1	40	40	0
31	C	1	40	40	0
31	C	1	40	40	0
31	C	1	40	40	0
31	B	1	40	40	0
31	B	1	40	40	0

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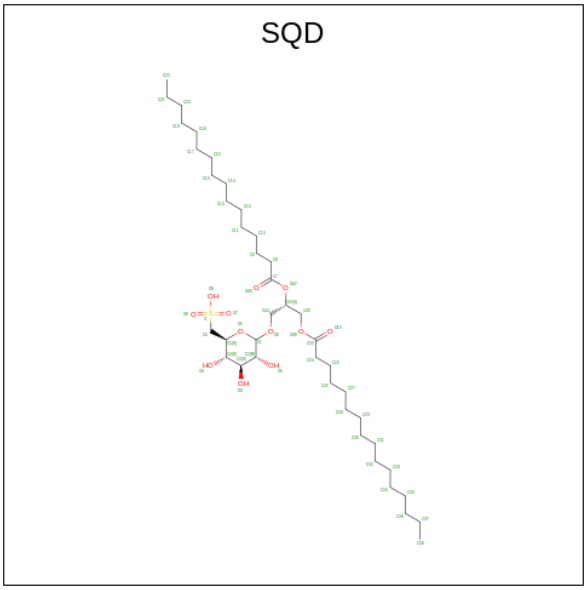
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
31	B	1	40	40	0
			Total	C	
31	D	1	40	40	0
			Total	C	
31	X	1	40	40	0
			Total	C	
31	b	1	40	40	0
			Total	C	
31	b	1	40	40	0
			Total	C	
31	b	1	40	40	0
			Total	C	
31	c	1	40	40	0
			Total	C	
31	c	1	40	40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	a	1	50	37	12	1	0
			Total	C	O	S	
32	a	1	54	41	12	1	0
			Total	C	O	S	
32	l	1	54	41	12	1	0

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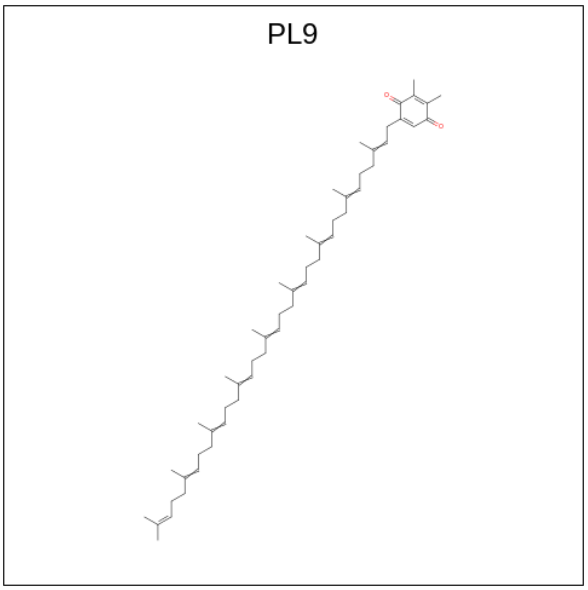
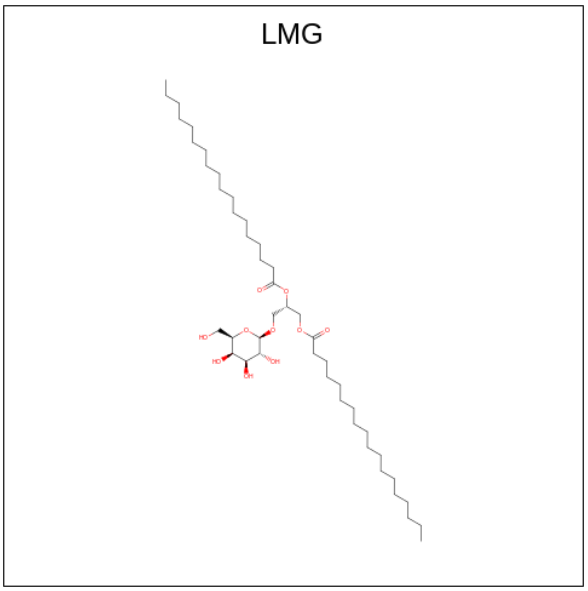
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	m	1	42	29	12	1	0
32	A	1	54	41	12	1	0
32	L	1	54	41	12	1	0
32	M	1	42	29	12	1	0
32	C	1	50	37	12	1	0

- Molecule 33 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



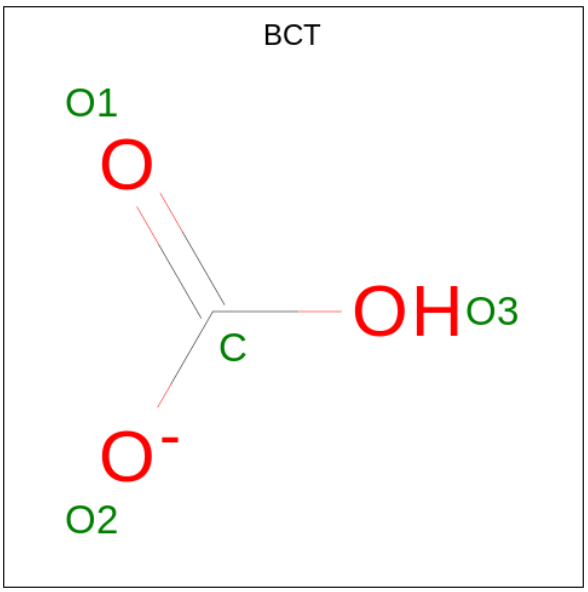
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	a	1	13	11	2	0
33	d	1	55	53	2	0
33	A	1	13	11	2	0
33	D	1	55	53	2	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



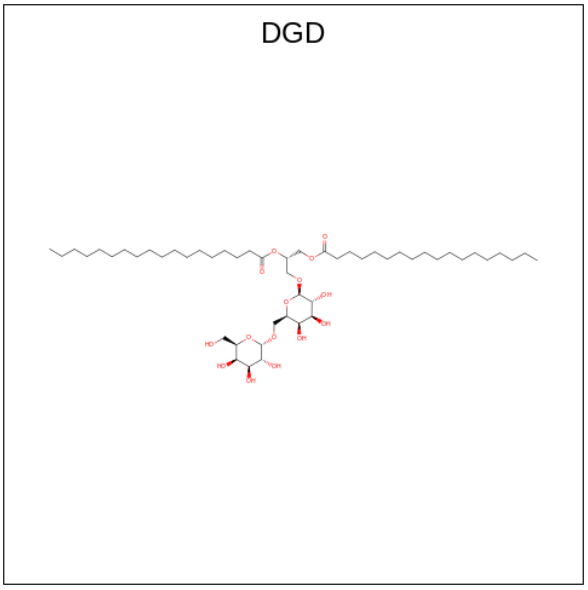
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	a	1	40	30	10	0
34	d	1	46	36	10	0
34	w	1	48	38	10	0
34	A	1	40	30	10	0
34	W	1	48	38	10	0
34	C	1	51	41	10	0
34	C	1	51	41	10	0
34	B	1	51	41	10	0
34	B	1	55	45	10	0
34	D	1	46	36	10	0
34	b	1	51	41	10	0
34	b	1	55	45	10	0
34	c	1	51	41	10	0
34	c	1	51	41	10	0

- Molecule 35 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



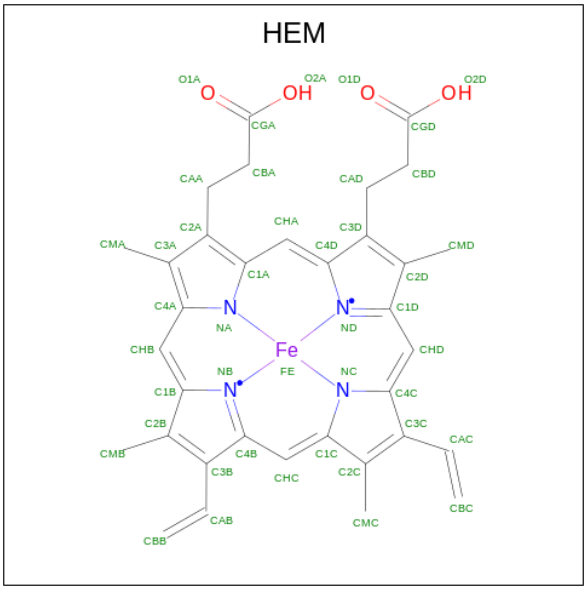
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	a	1	4	1	3	0
			Total	C	O	
35	D	1	4	1	3	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	a	1	59	44	15	0
36	A	1	59	44	15	0
36	J	1	60	45	15	0
36	C	1	55	40	15	0
36	C	1	62	47	15	0
36	B	1	62	47	15	0
36	b	1	62	47	15	0
36	c	1	55	40	15	0
36	c	1	62	47	15	0
36	c	1	60	45	15	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
37	E	1	43	34	1	4	4	0

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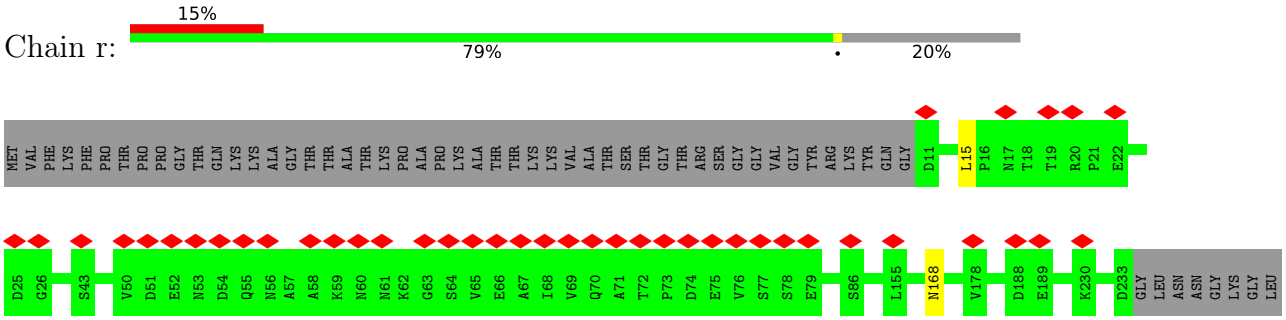
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
37	e	1	43	34	1	4	4	0

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.

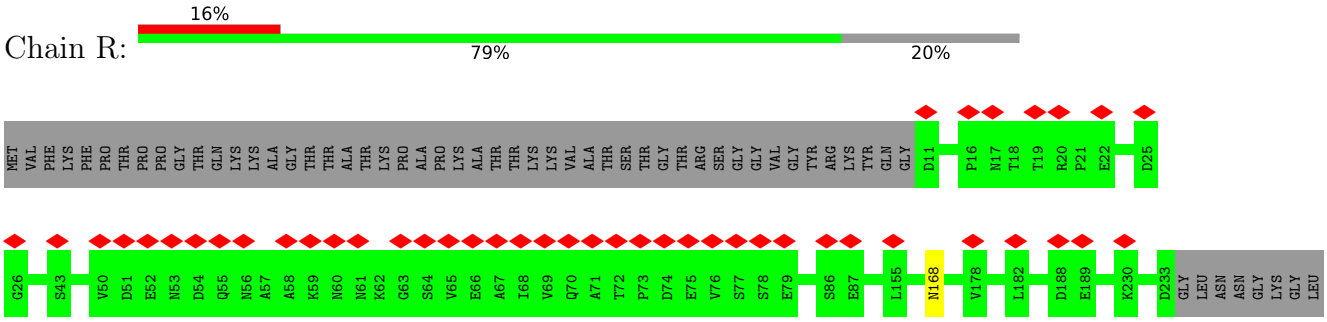
- Molecule 1: Chlorophyll a-b binding protein CP29

Chain r:



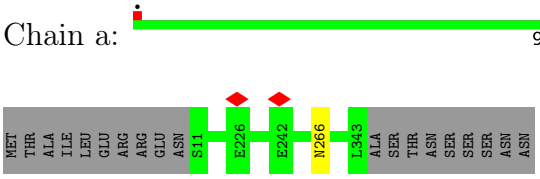
- Molecule 1: Chlorophyll a-b binding protein CP29

Chain R:



- Molecule 2: Photosystem II protein D1

Chain a:

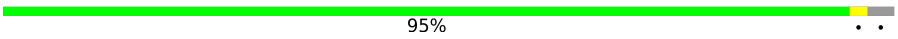


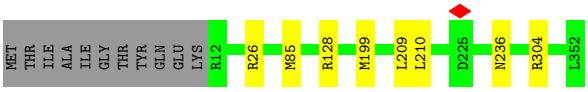
- Molecule 2: Photosystem II protein D1

Chain A:

• Molecule 3: Photosystem II D2 protein

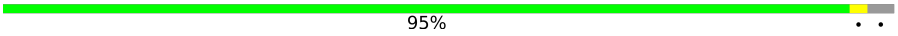
Chain d:

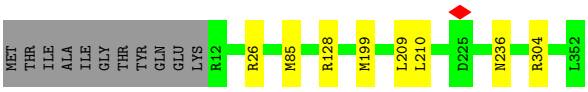




• Molecule 3: Photosystem II D2 protein

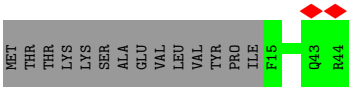
Chain D:





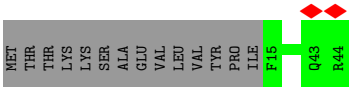
• Molecule 4: Cytochrome b559 subunit beta

Chain f:



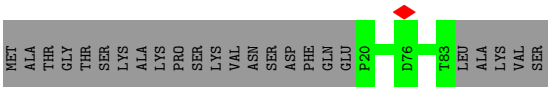
• Molecule 4: Cytochrome b559 subunit beta

Chain F:



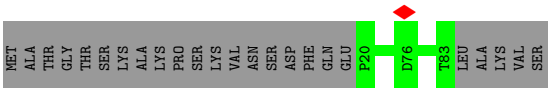
• Molecule 5: Photosystem II reaction center protein H

Chain h:



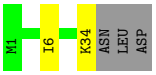
• Molecule 5: Photosystem II reaction center protein H

Chain H:



• Molecule 6: Photosystem II reaction center protein I

Chain i:

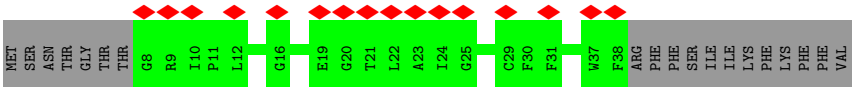


• Molecule 6: Photosystem II reaction center protein I

Chain I:

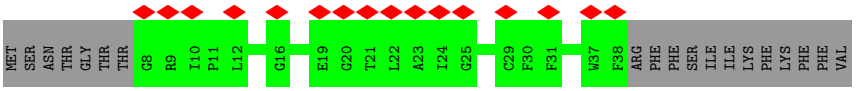
• Molecule 7: Photosystem II reaction center protein J, PsbJ

Chain j:



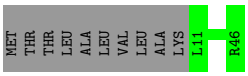
• Molecule 7: Photosystem II reaction center protein J, PsbJ

Chain J:



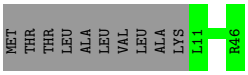
• Molecule 8: Photosystem II reaction center protein K

Chain k:



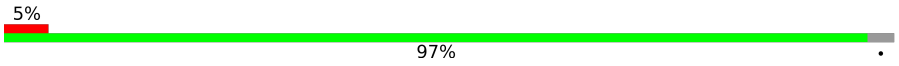
• Molecule 8: Photosystem II reaction center protein K

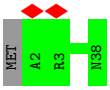
Chain K:



• Molecule 9: Photosystem II reaction center protein L

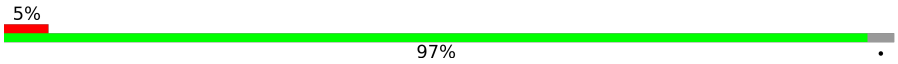
Chain l:

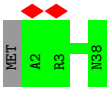




• Molecule 9: Photosystem II reaction center protein L

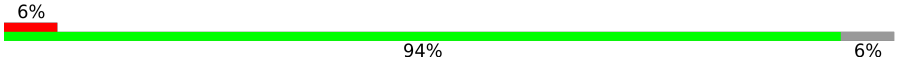
Chain L:

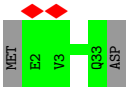




• Molecule 10: Photosystem II reaction center protein M

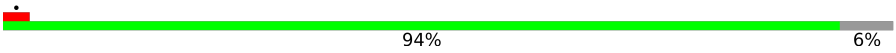
Chain m:

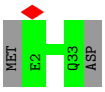




• Molecule 10: Photosystem II reaction center protein M

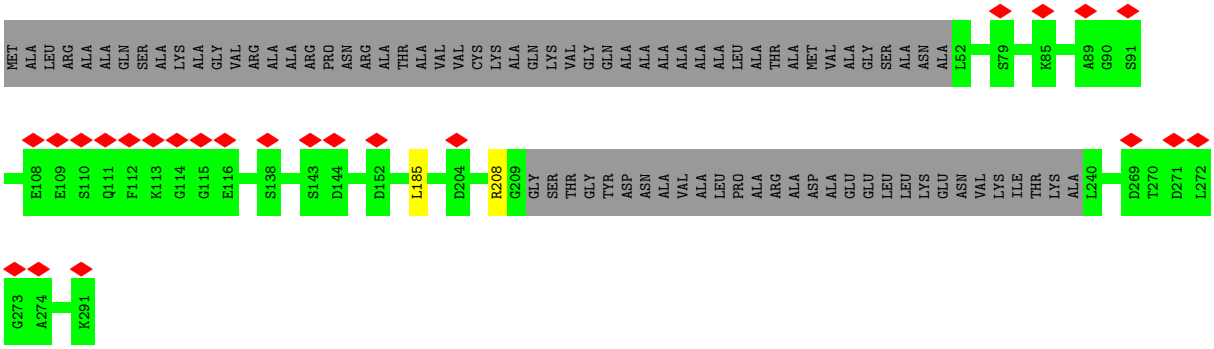
Chain M:





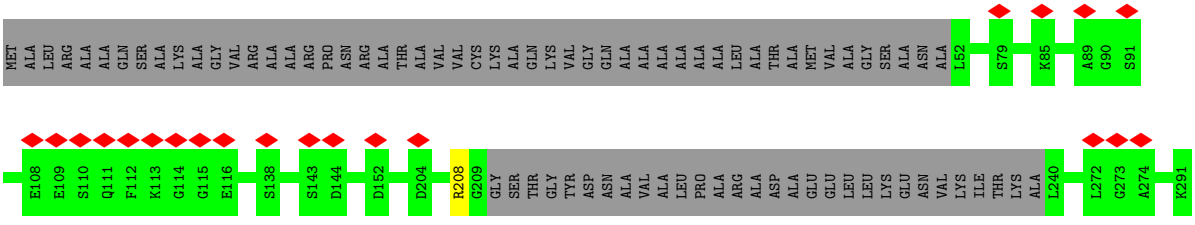
• Molecule 11: Oxygen-evolving enhancer protein 1 of photosystem II

Chain o:



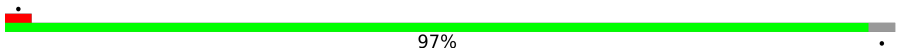
• Molecule 11: Oxygen-evolving enhancer protein 1 of photosystem II

Chain O:



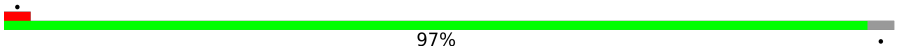
• Molecule 12: Photosystem II reaction center protein T

Chain t:



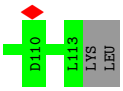
• Molecule 12: Photosystem II reaction center protein T

Chain T:



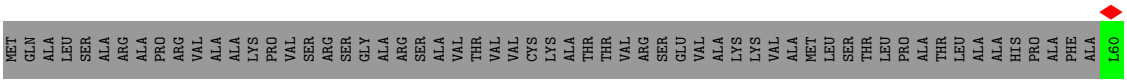
• Molecule 13: Photosystem II reaction center W protein, chloroplastic

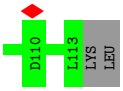
Chain w:



• Molecule 13: Photosystem II reaction center W protein, chloroplastic

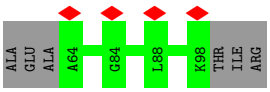
Chain W:





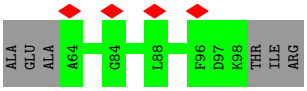
• Molecule 14: 4.1 kDa photosystem II subunit

Chain x:



• Molecule 14: 4.1 kDa photosystem II subunit

Chain X:



• Molecule 15: Photosystem II reaction center protein Z

Chain z: 100%

There are no outlier residues recorded for this chain.

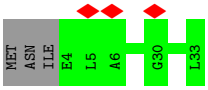
• Molecule 15: Photosystem II reaction center protein Z

Chain Z: 100%

There are no outlier residues recorded for this chain.

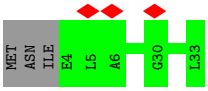
• Molecule 16: Photosystem II reaction center protein 30, Psb30

Chain Y: 9% 91% 9%



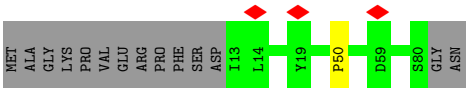
• Molecule 16: Photosystem II reaction center protein 30, Psb30

Chain y: 9% 91% 9%



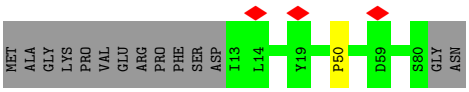
• Molecule 17: Cytochrome b559 subunit alpha

Chain E: 82% 17%



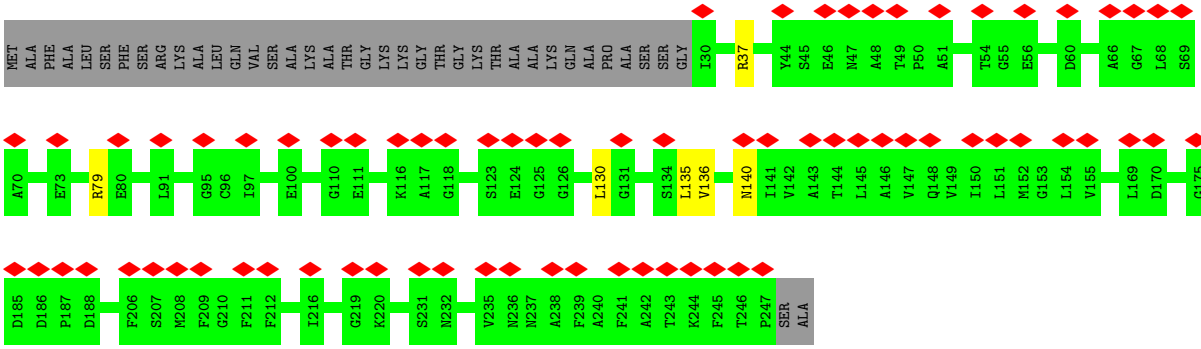
• Molecule 17: Cytochrome b559 subunit alpha

Chain e: 82% 17%



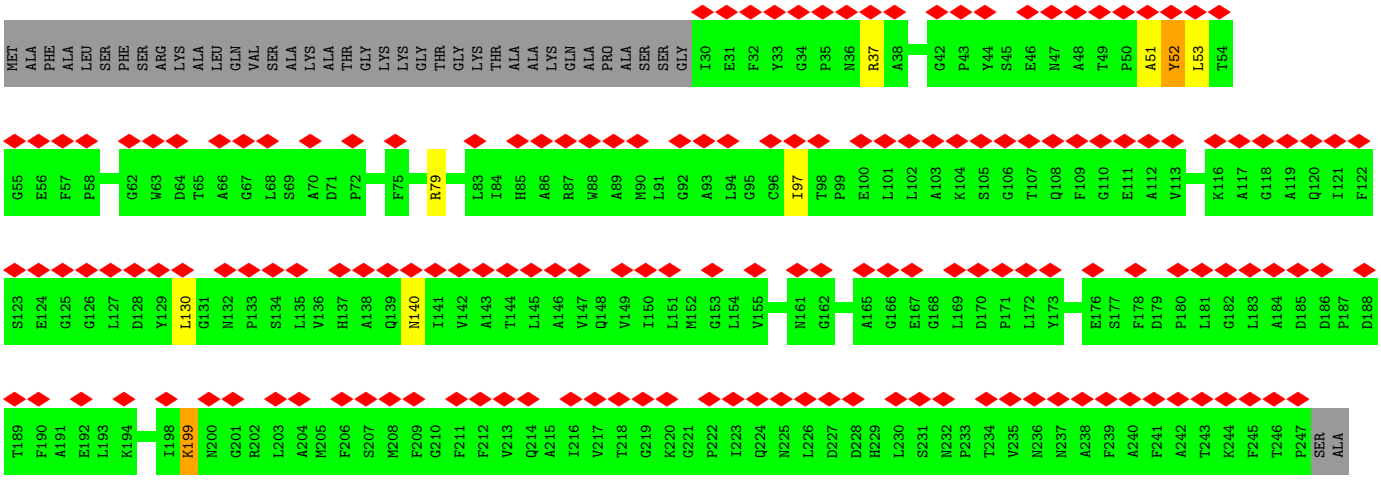
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 1: 30% 82% 15%



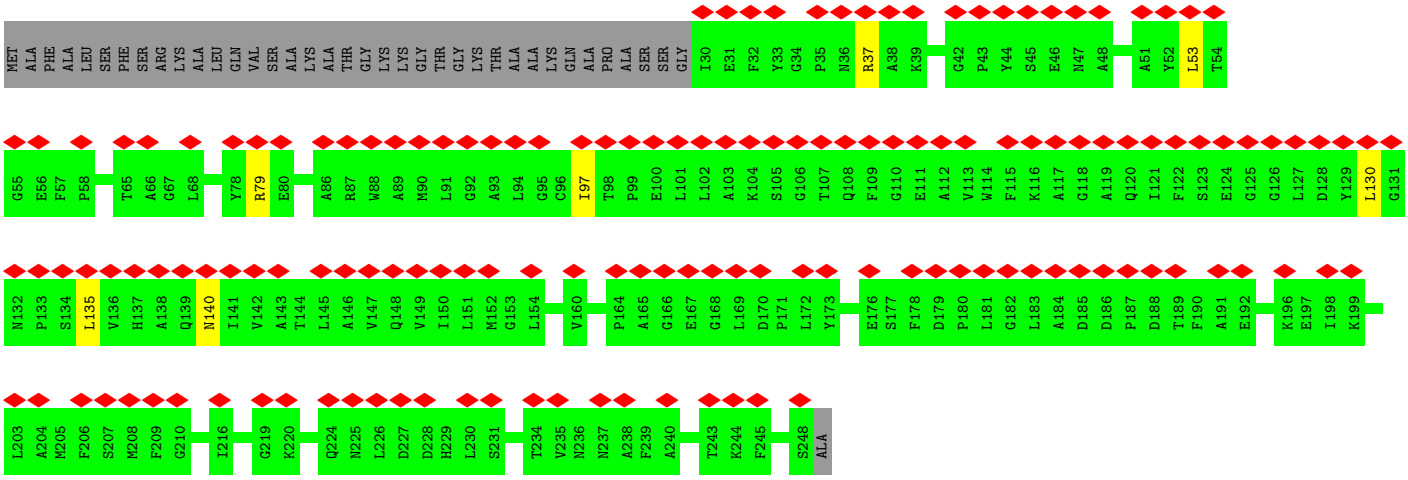
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



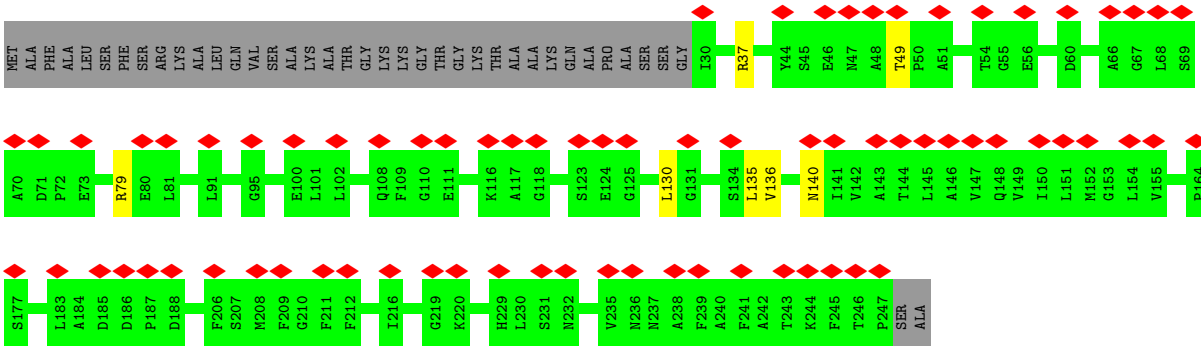
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



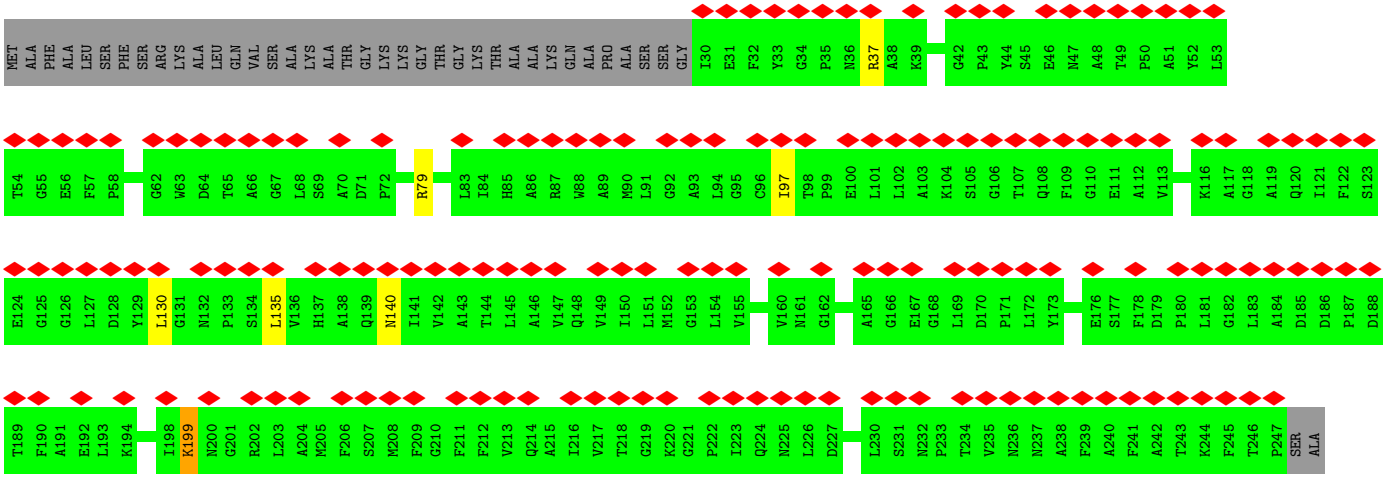
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



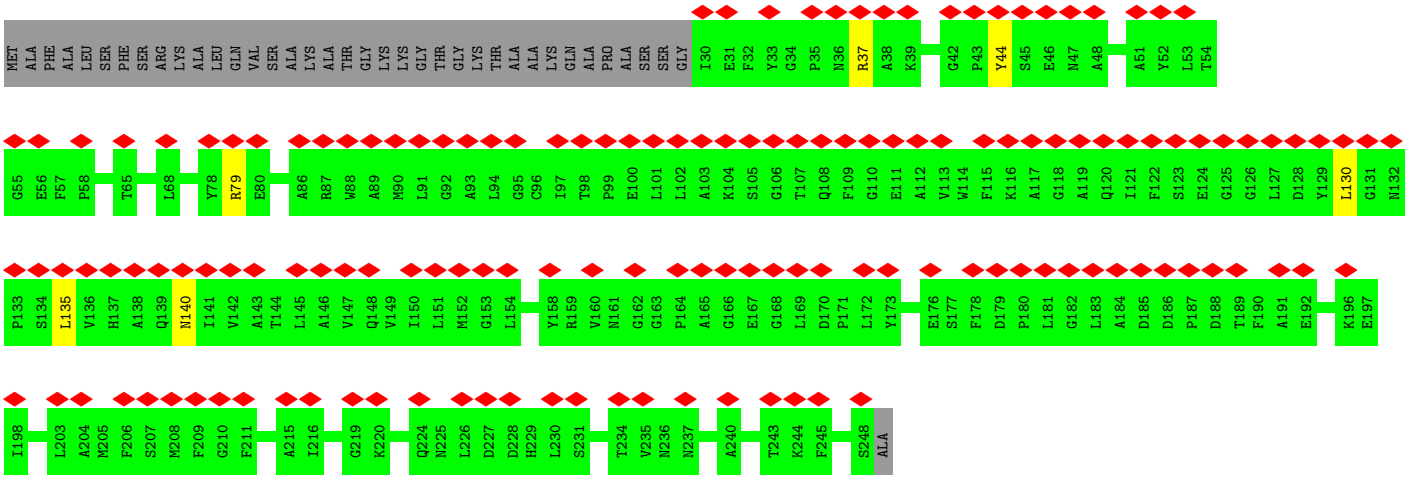
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



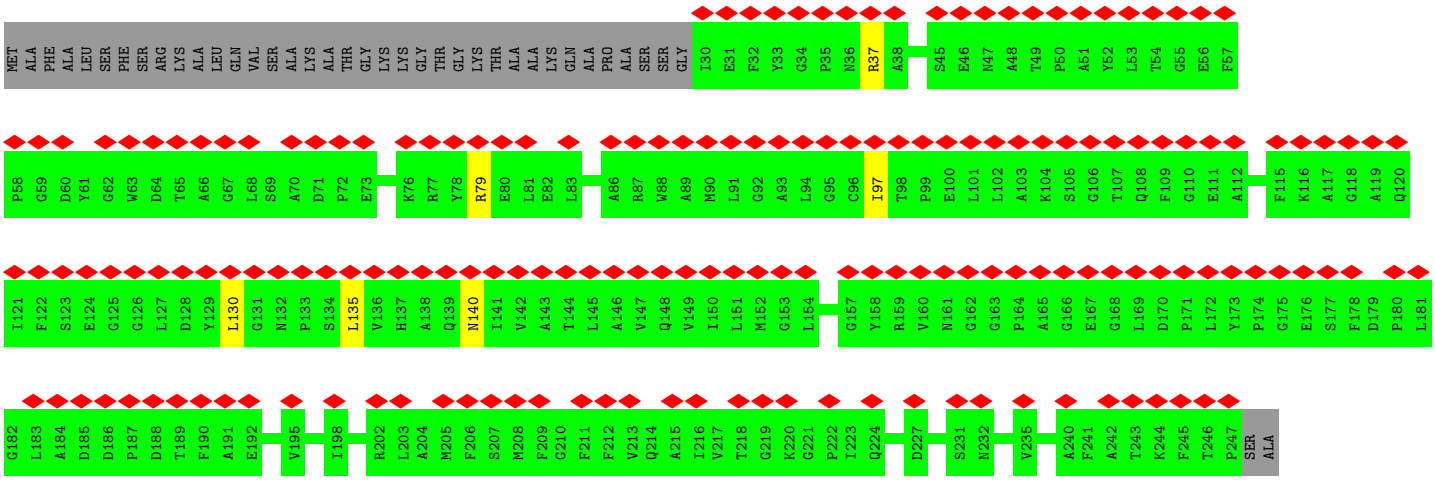
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



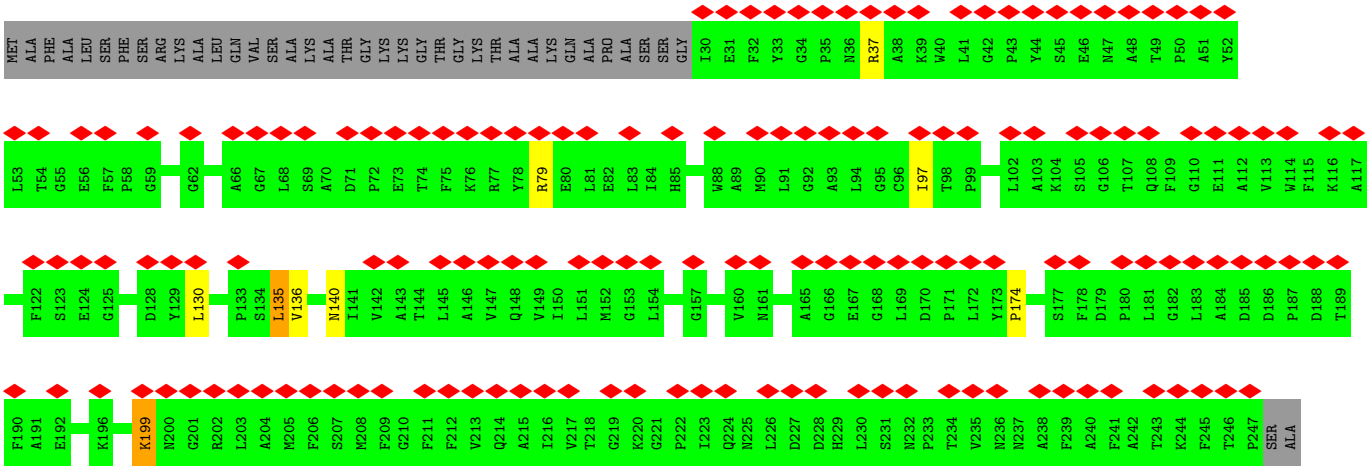
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain v:



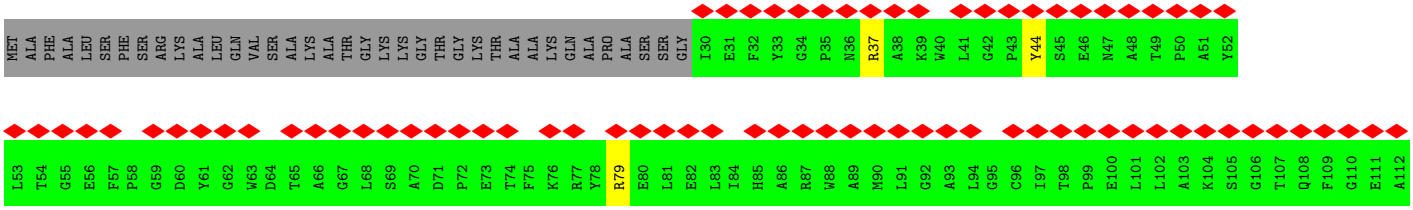
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain p:



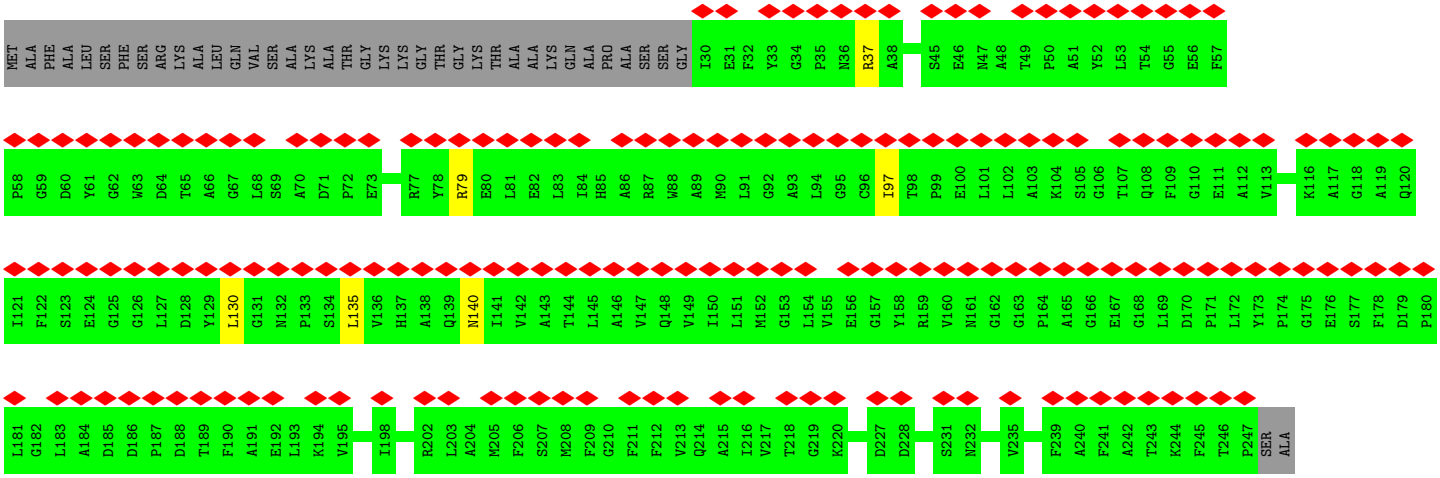
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain q:



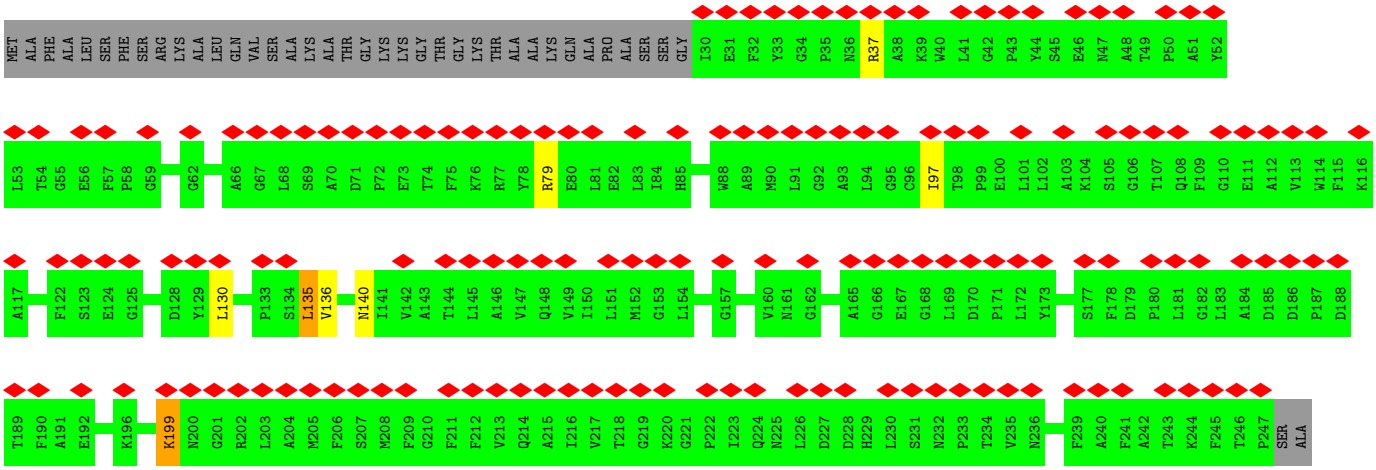
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain V: 69% 82% • 15%



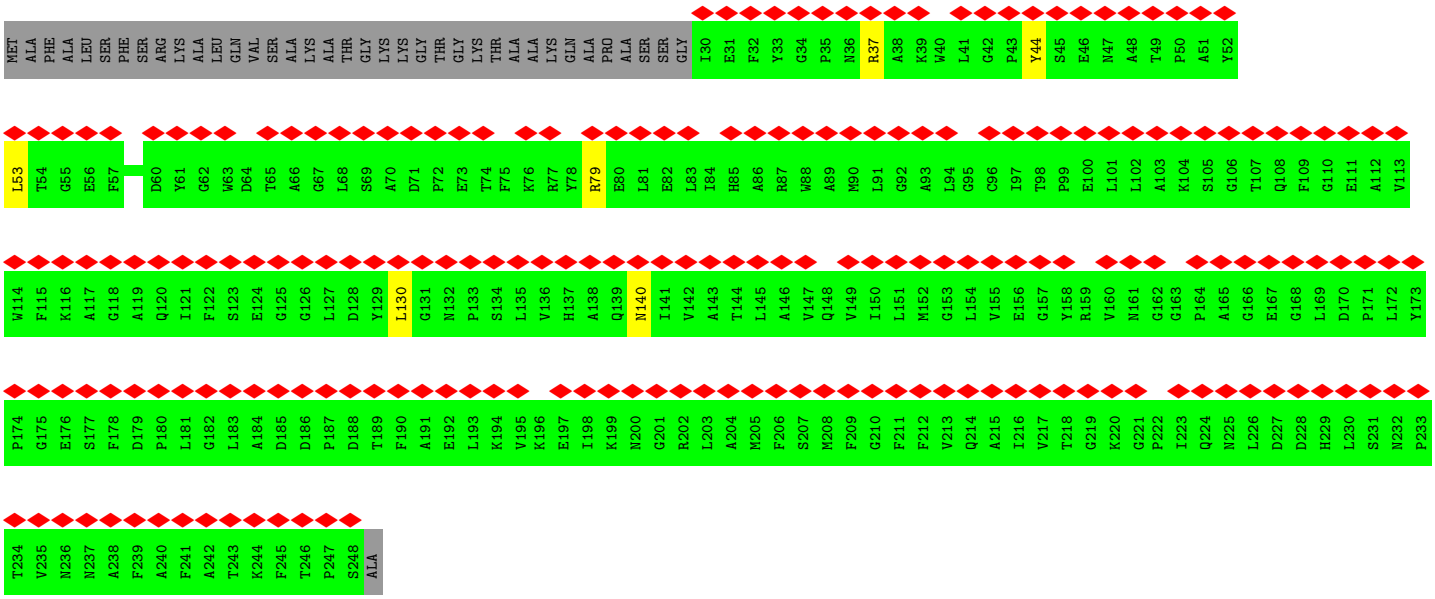
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain P: 61% 82% •• 15%



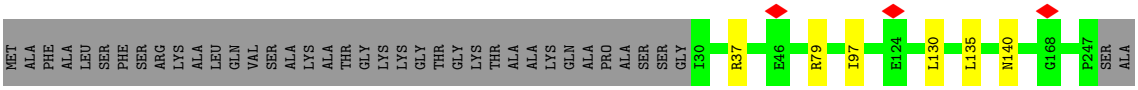
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain Q:



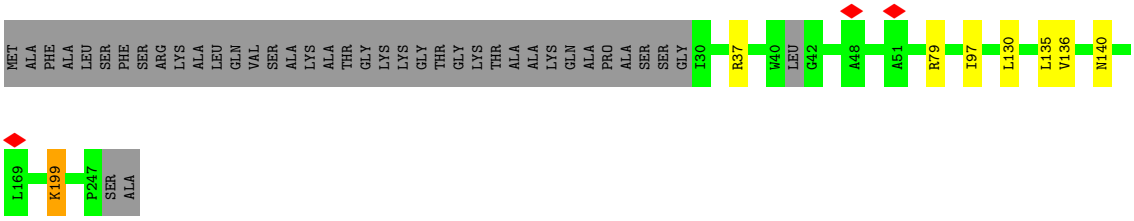
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain U:



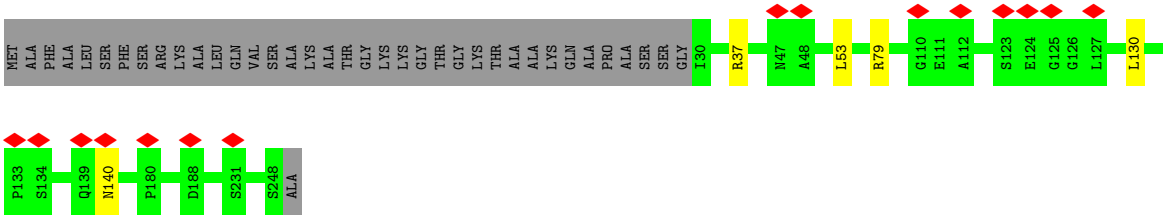
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain N:



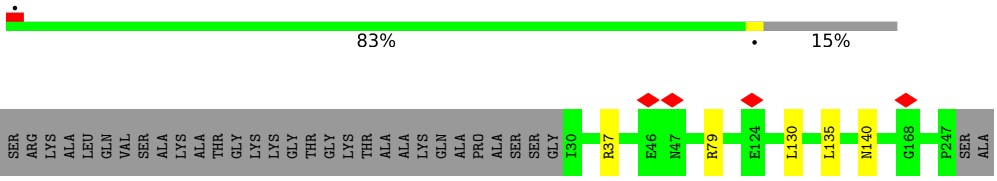
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain G:



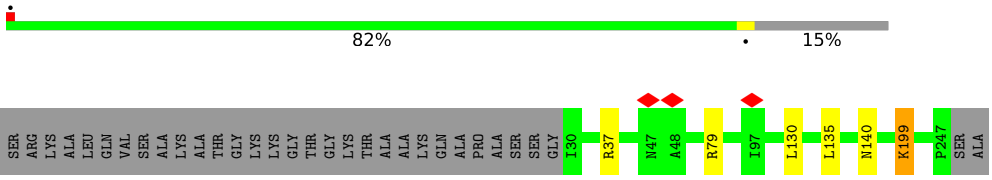
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain u:



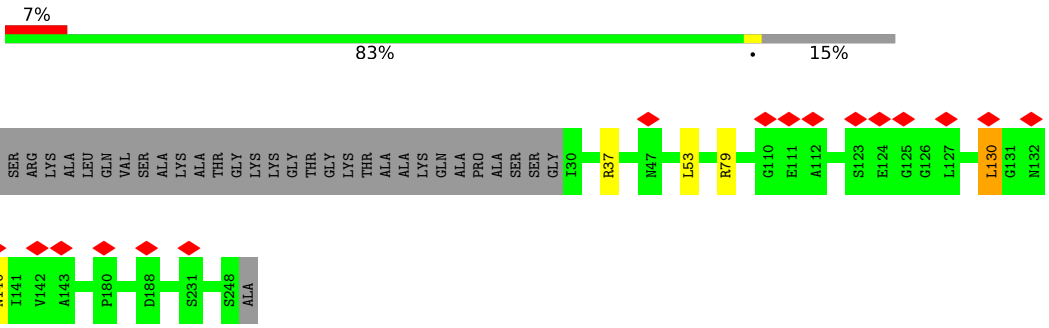
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain n:



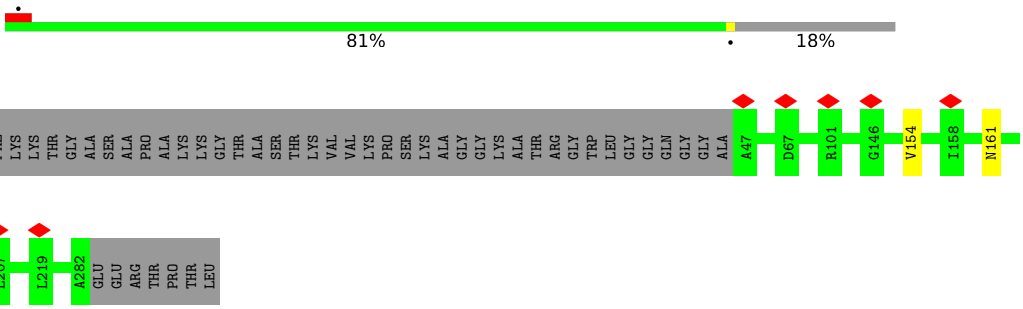
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain g:



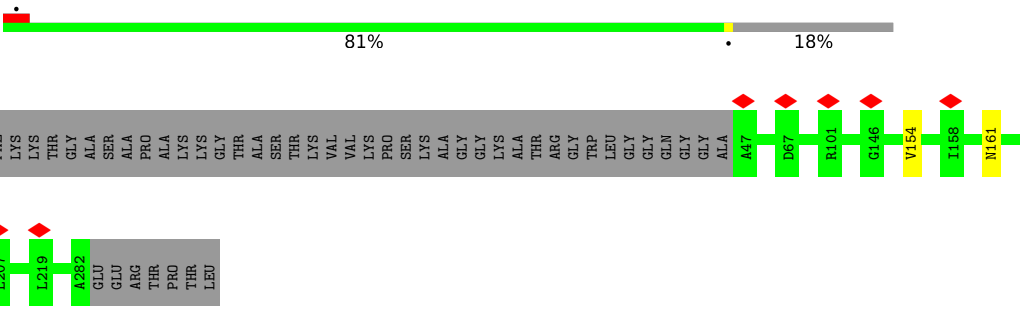
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain S:



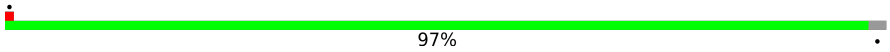
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

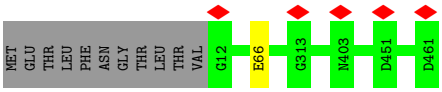
Chain s:



• Molecule 20: Photosystem II CP43 reaction center protein

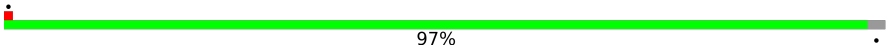
Chain C:

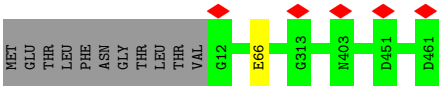




• Molecule 20: Photosystem II CP43 reaction center protein

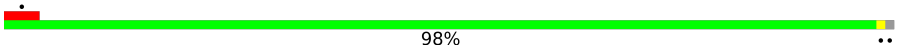
Chain c:

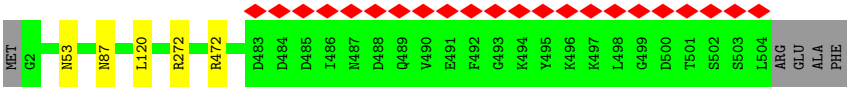




• Molecule 21: Photosystem II CP47 reaction center protein

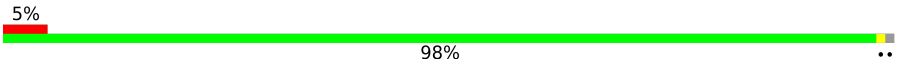
Chain B:

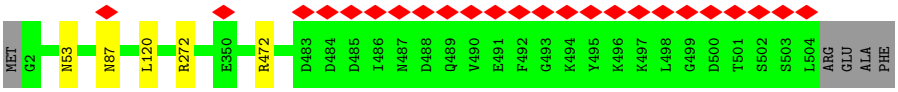




• Molecule 21: Photosystem II CP47 reaction center protein

Chain b:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89018	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.181	Depositor
Minimum map value	-1.592	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	392.1, 392.1, 392.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	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: CLA, PHO, XAT, LHG, LMG, HEM, PL9, BCR, DGD, SQD, BCT, CHL, CL, LUT, NEX, FE2

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	R	0.29	0/1736	0.55	0/2357
1	r	0.29	0/1739	0.55	0/2361
2	A	0.37	0/2696	0.55	1/3676 (0.0%)
2	a	0.37	0/2696	0.55	0/3676
3	D	0.38	0/2808	0.60	1/3830 (0.0%)
3	d	0.38	0/2808	0.60	1/3830 (0.0%)
4	F	0.31	0/250	0.51	0/338
4	f	0.32	0/250	0.52	0/338
5	H	0.33	0/499	0.55	0/683
5	h	0.32	0/499	0.55	0/683
6	I	0.42	0/283	0.58	0/383
6	i	0.42	0/283	0.58	0/383
7	J	0.28	0/254	0.49	0/345
7	j	0.27	0/254	0.48	0/345
8	K	0.40	0/300	0.65	0/414
8	k	0.40	0/300	0.64	0/414
9	L	0.33	0/314	0.51	0/427
9	l	0.33	0/314	0.51	0/427
10	M	0.30	0/252	0.53	0/345
10	m	0.30	0/252	0.54	0/345
11	O	0.30	0/1620	0.59	0/2184
11	o	0.30	0/1620	0.59	1/2184 (0.0%)
12	T	0.33	0/254	0.48	0/343
12	t	0.33	0/254	0.48	0/343
13	W	0.31	0/428	0.49	0/581
13	w	0.31	0/428	0.49	0/581
14	X	0.30	0/244	0.42	0/330
14	x	0.30	0/244	0.42	0/330
15	Z	0.29	0/476	0.49	0/654
15	z	0.29	0/476	0.49	0/654
16	Y	0.27	0/208	0.63	0/285
16	y	0.27	0/208	0.63	0/285

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	E	0.32	0/571	0.55	1/780 (0.1%)
17	e	0.32	0/571	0.56	1/780 (0.1%)
18	1	0.31	0/1717	0.56	1/2337 (0.0%)
18	2	0.33	0/1717	0.64	3/2337 (0.1%)
18	3	0.30	0/1723	0.57	2/2345 (0.1%)
18	4	0.31	0/1717	0.57	1/2337 (0.0%)
18	5	0.32	0/1717	0.60	2/2337 (0.1%)
18	6	0.31	0/1723	0.57	1/2345 (0.0%)
18	G	0.31	0/1723	0.59	2/2345 (0.1%)
18	N	0.33	0/1708	0.60	2/2323 (0.1%)
18	P	0.32	0/1717	0.60	3/2337 (0.1%)
18	Q	0.30	0/1723	0.58	2/2345 (0.1%)
18	U	0.33	0/1717	0.61	1/2337 (0.0%)
18	V	0.31	0/1717	0.57	1/2337 (0.0%)
18	g	0.31	0/1723	0.61	2/2345 (0.1%)
18	n	0.33	0/1717	0.62	2/2337 (0.1%)
18	p	0.32	0/1717	0.61	3/2337 (0.1%)
18	q	0.30	0/1723	0.58	1/2345 (0.0%)
18	u	0.33	0/1717	0.62	1/2337 (0.0%)
18	v	0.31	0/1717	0.58	1/2337 (0.0%)
19	S	0.33	0/1849	0.60	0/2521
19	s	0.33	0/1849	0.61	0/2521
20	C	0.34	0/3623	0.51	1/4936 (0.0%)
20	c	0.34	0/3623	0.51	1/4936 (0.0%)
21	B	0.33	0/4067	0.50	0/5533
21	b	0.33	0/4067	0.50	0/5533
All	All	0.33	0/76400	0.57	39/103994 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	r	0	1
18	1	0	1
18	2	0	2
18	3	0	1
18	4	0	2
18	5	0	1
18	6	0	2
18	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	P	0	1
18	Q	0	1
18	U	0	1
18	V	0	1
18	g	0	1
18	n	0	1
18	p	0	1
18	q	0	1
18	u	0	1
18	v	0	1
All	All	0	21

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	199	LYS	CD-CE-NZ	-8.78	91.50	111.70
18	5	199	LYS	CD-CE-NZ	-8.57	91.99	111.70
18	n	199	LYS	CD-CE-NZ	-8.17	92.92	111.70
18	p	199	LYS	CD-CE-NZ	-7.90	93.54	111.70
18	2	53	LEU	CA-CB-CG	7.88	133.43	115.30

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	1	135	LEU	Peptide
18	2	51	ALA	Peptide
18	2	52	TYR	Peptide
18	3	135	LEU	Peptide
1	r	15	LEU	Peptide

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	R	221/280 (79%)	201 (91%)	20 (9%)	0	100	100
1	r	221/280 (79%)	197 (89%)	24 (11%)	0	100	100
2	A	331/352 (94%)	314 (95%)	17 (5%)	0	100	100
2	a	331/352 (94%)	316 (96%)	15 (4%)	0	100	100
3	D	339/352 (96%)	304 (90%)	35 (10%)	0	100	100
3	d	339/352 (96%)	307 (91%)	32 (9%)	0	100	100
4	F	28/44 (64%)	27 (96%)	1 (4%)	0	100	100
4	f	28/44 (64%)	27 (96%)	1 (4%)	0	100	100
5	H	62/88 (70%)	61 (98%)	1 (2%)	0	100	100
5	h	62/88 (70%)	61 (98%)	1 (2%)	0	100	100
6	I	32/37 (86%)	29 (91%)	3 (9%)	0	100	100
6	i	32/37 (86%)	29 (91%)	3 (9%)	0	100	100
7	J	29/50 (58%)	27 (93%)	2 (7%)	0	100	100
7	j	29/50 (58%)	27 (93%)	2 (7%)	0	100	100
8	K	34/46 (74%)	30 (88%)	4 (12%)	0	100	100
8	k	34/46 (74%)	30 (88%)	4 (12%)	0	100	100
9	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
10	M	30/34 (88%)	30 (100%)	0	0	100	100
10	m	30/34 (88%)	30 (100%)	0	0	100	100
11	O	206/291 (71%)	176 (85%)	30 (15%)	0	100	100
11	o	206/291 (71%)	175 (85%)	31 (15%)	0	100	100
12	T	28/31 (90%)	25 (89%)	3 (11%)	0	100	100
12	t	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
13	W	52/115 (45%)	49 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	w	52/115 (45%)	49 (94%)	3 (6%)	0	100	100
14	X	33/101 (33%)	33 (100%)	0	0	100	100
14	x	33/101 (33%)	33 (100%)	0	0	100	100
15	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
15	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
16	Y	28/33 (85%)	26 (93%)	2 (7%)	0	100	100
16	y	28/33 (85%)	26 (93%)	2 (7%)	0	100	100
17	E	66/82 (80%)	58 (88%)	8 (12%)	0	100	100
17	e	66/82 (80%)	57 (86%)	9 (14%)	0	100	100
18	1	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	25	57
18	2	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	25	57
18	3	217/257 (84%)	191 (88%)	26 (12%)	0	100	100
18	4	216/257 (84%)	189 (88%)	26 (12%)	1 (0%)	25	57
18	5	216/257 (84%)	190 (88%)	26 (12%)	0	100	100
18	6	217/257 (84%)	190 (88%)	27 (12%)	0	100	100
18	G	217/257 (84%)	185 (85%)	32 (15%)	0	100	100
18	N	213/257 (83%)	188 (88%)	24 (11%)	1 (0%)	25	57
18	P	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	25	57
18	Q	217/257 (84%)	184 (85%)	33 (15%)	0	100	100
18	U	216/257 (84%)	187 (87%)	29 (13%)	0	100	100
18	V	216/257 (84%)	187 (87%)	29 (13%)	0	100	100
18	g	217/257 (84%)	183 (84%)	34 (16%)	0	100	100
18	n	216/257 (84%)	184 (85%)	32 (15%)	0	100	100
18	p	216/257 (84%)	186 (86%)	28 (13%)	2 (1%)	14	46
18	q	217/257 (84%)	186 (86%)	31 (14%)	0	100	100
18	u	216/257 (84%)	183 (85%)	33 (15%)	0	100	100
18	v	216/257 (84%)	186 (86%)	30 (14%)	0	100	100
19	S	234/289 (81%)	201 (86%)	33 (14%)	0	100	100
19	s	234/289 (81%)	202 (86%)	32 (14%)	0	100	100
20	C	448/461 (97%)	429 (96%)	19 (4%)	0	100	100
20	c	448/461 (97%)	430 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	B	501/508 (99%)	472 (94%)	29 (6%)	0	100	100
21	b	501/508 (99%)	470 (94%)	31 (6%)	0	100	100
All	All	9485/11214 (85%)	8533 (90%)	945 (10%)	7 (0%)	50	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	2	52	TYR
18	p	136	VAL
18	P	136	VAL
18	1	136	VAL
18	N	136	VAL

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	R	175/218 (80%)	174 (99%)	1 (1%)	84	90
1	r	176/218 (81%)	175 (99%)	1 (1%)	84	90
2	A	272/289 (94%)	271 (100%)	1 (0%)	89	93
2	a	272/289 (94%)	271 (100%)	1 (0%)	89	93
3	D	272/281 (97%)	265 (97%)	7 (3%)	41	62
3	d	272/281 (97%)	265 (97%)	7 (3%)	41	62
4	F	24/37 (65%)	24 (100%)	0	100	100
4	f	24/37 (65%)	24 (100%)	0	100	100
5	H	55/75 (73%)	55 (100%)	0	100	100
5	h	55/75 (73%)	55 (100%)	0	100	100
6	I	31/34 (91%)	29 (94%)	2 (6%)	14	41
6	i	31/34 (91%)	29 (94%)	2 (6%)	14	41
7	J	24/42 (57%)	24 (100%)	0	100	100
7	j	24/42 (57%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	30/38 (79%)	30 (100%)	0	100	100
8	k	30/38 (79%)	30 (100%)	0	100	100
9	L	34/35 (97%)	34 (100%)	0	100	100
9	l	34/35 (97%)	34 (100%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	100	100
10	m	28/30 (93%)	28 (100%)	0	100	100
11	O	174/223 (78%)	173 (99%)	1 (1%)	84	90
11	o	174/223 (78%)	173 (99%)	1 (1%)	84	90
12	T	27/28 (96%)	27 (100%)	0	100	100
12	t	27/28 (96%)	27 (100%)	0	100	100
13	W	42/87 (48%)	42 (100%)	0	100	100
13	w	42/87 (48%)	42 (100%)	0	100	100
14	X	25/67 (37%)	25 (100%)	0	100	100
14	x	25/67 (37%)	25 (100%)	0	100	100
15	Z	52/52 (100%)	52 (100%)	0	100	100
15	z	52/52 (100%)	52 (100%)	0	100	100
16	Y	24/27 (89%)	24 (100%)	0	100	100
16	y	24/27 (89%)	24 (100%)	0	100	100
17	E	60/71 (84%)	60 (100%)	0	100	100
17	e	60/71 (84%)	60 (100%)	0	100	100
18	1	169/194 (87%)	166 (98%)	3 (2%)	54	71
18	2	169/194 (87%)	164 (97%)	5 (3%)	36	59
18	3	170/194 (88%)	166 (98%)	4 (2%)	44	64
18	4	169/194 (87%)	166 (98%)	3 (2%)	54	71
18	5	169/194 (87%)	164 (97%)	5 (3%)	36	59
18	6	170/194 (88%)	167 (98%)	3 (2%)	54	71
18	G	170/194 (88%)	167 (98%)	3 (2%)	54	71
18	N	168/194 (87%)	163 (97%)	5 (3%)	36	59
18	P	169/194 (87%)	164 (97%)	5 (3%)	36	59
18	Q	170/194 (88%)	167 (98%)	3 (2%)	54	71
18	U	169/194 (87%)	165 (98%)	4 (2%)	44	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	V	169/194 (87%)	165 (98%)	4 (2%)	44	64
18	g	170/194 (88%)	166 (98%)	4 (2%)	44	64
18	n	169/194 (87%)	165 (98%)	4 (2%)	44	64
18	p	169/194 (87%)	164 (97%)	5 (3%)	36	59
18	q	170/194 (88%)	167 (98%)	3 (2%)	54	71
18	u	169/194 (87%)	166 (98%)	3 (2%)	54	71
18	v	169/194 (87%)	165 (98%)	4 (2%)	44	64
19	S	181/217 (83%)	179 (99%)	2 (1%)	70	80
19	s	181/217 (83%)	179 (99%)	2 (1%)	70	80
20	C	352/362 (97%)	352 (100%)	0	100	100
20	c	352/362 (97%)	352 (100%)	0	100	100
21	B	403/407 (99%)	398 (99%)	5 (1%)	67	79
21	b	403/407 (99%)	398 (99%)	5 (1%)	67	79
All	All	7618/8732 (87%)	7510 (99%)	108 (1%)	62	76

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	P	140	ASN
18	G	37	ARG
3	D	236	ASN
18	Q	37	ARG
18	U	140	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	229	HIS
1	R	56	ASN
21	b	114	HIS
18	U	140	ASN
18	u	140	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 552 ligands modelled in this entry, 6 are monoatomic - leaving 546 for Mogul analysis.

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	$\#\|Z\| > 2$
23	LUT	s	310	19	42,43,43	0.79	0	51,60,60	1.72	13 (25%)
22	CLA	U	306	-	60,68,73	1.57	9 (15%)	70,107,113	1.43	8 (11%)
22	CLA	u	302	-	65,73,73	1.48	8 (12%)	76,113,113	1.37	7 (9%)
26	CHL	U	314	-	50,58,74	2.15	14 (28%)	52,94,114	2.70	20 (38%)
31	BCR	X	201	-	41,41,41	4.79	24 (58%)	56,56,56	2.26	17 (30%)
26	CHL	6	301	-	66,74,74	1.91	16 (24%)	73,114,114	2.45	22 (30%)
22	CLA	c	511	20,8	65,73,73	1.48	9 (13%)	76,113,113	1.29	7 (9%)
26	CHL	u	317	18	66,74,74	1.86	15 (22%)	73,114,114	2.52	24 (32%)
26	CHL	G	316	-	61,69,74	1.95	15 (24%)	67,108,114	2.49	22 (32%)
26	CHL	2	314	-	48,56,74	2.38	17 (35%)	51,92,114	2.95	21 (41%)
22	CLA	g	305	22	60,68,73	1.52	8 (13%)	70,107,113	1.50	10 (14%)
22	CLA	n	306	-	60,68,73	1.49	6 (10%)	70,107,113	1.55	8 (11%)
37	HEM	e	101	4,17	41,50,50	1.59	5 (12%)	45,82,82	1.14	2 (4%)
22	CLA	C	512	20,8	65,73,73	1.48	9 (13%)	76,113,113	1.28	7 (9%)
23	LUT	2	310	-	42,43,43	0.78	0	51,60,60	1.64	12 (23%)
24	XAT	p	312	-	39,47,47	2.59	18 (46%)	54,74,74	11.83	18 (33%)
26	CHL	V	318	-	66,74,74	1.94	16 (24%)	73,114,114	2.32	21 (28%)
22	CLA	3	306	22	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	5	302	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
26	CHL	P	318	-	66,74,74	1.85	14 (21%)	73,114,114	2.42	22 (30%)
23	LUT	5	309	-	42,43,43	0.76	0	51,60,60	1.75	13 (25%)
23	LUT	u	309	-	42,43,43	0.75	0	51,60,60	1.52	10 (19%)
22	CLA	Q	301	-	65,73,73	1.49	7 (10%)	76,113,113	1.42	7 (9%)
22	CLA	c	509	-	65,73,73	1.53	9 (13%)	76,113,113	1.52	9 (11%)
25	LHG	D	407	3	48,48,48	0.90	4 (8%)	51,54,54	1.07	3 (5%)
26	CHL	U	315	-	66,74,74	1.85	14 (21%)	73,114,114	2.47	23 (31%)
25	LHG	s	312	19	48,48,48	0.89	4 (8%)	51,54,54	1.14	3 (5%)
22	CLA	3	305	22	60,68,73	1.51	6 (10%)	70,107,113	1.52	10 (14%)
22	CLA	p	303	-	65,73,73	1.47	8 (12%)	76,113,113	1.44	8 (10%)
26	CHL	3	315	18	66,74,74	1.89	16 (24%)	73,114,114	2.44	20 (27%)
26	CHL	N	315	-	50,58,74	2.17	16 (32%)	52,94,114	2.72	21 (40%)
22	CLA	s	309	-	49,57,73	1.67	8 (16%)	55,93,113	1.56	6 (10%)
22	CLA	c	507	-	65,73,73	1.52	9 (13%)	76,113,113	1.45	8 (10%)
23	LUT	4	309	-	42,43,43	0.73	0	51,60,60	1.60	11 (21%)
26	CHL	4	314	-	48,56,74	2.20	14 (29%)	51,92,114	2.87	21 (41%)
34	LMG	D	408	3	46,46,55	1.26	6 (13%)	54,54,63	1.02	2 (3%)
22	CLA	P	305	18	65,73,73	1.42	6 (9%)	76,113,113	1.45	8 (10%)
34	LMG	w	201	-	48,48,55	1.23	6 (12%)	56,56,63	1.12	4 (7%)
26	CHL	5	318	-	66,74,74	1.88	14 (21%)	73,114,114	2.37	23 (31%)
22	CLA	3	307	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
26	CHL	u	318	-	66,74,74	1.85	14 (21%)	73,114,114	2.38	21 (28%)
22	CLA	u	304	-	60,68,73	1.48	7 (11%)	70,107,113	1.55	7 (10%)
25	LHG	c	522	-	48,48,48	0.90	3 (6%)	51,54,54	1.07	2 (3%)
31	BCR	B	619	-	41,41,41	4.74	24 (58%)	56,56,56	2.26	22 (39%)
22	CLA	2	306	-	60,68,73	1.48	7 (11%)	70,107,113	1.56	8 (11%)
31	BCR	C	516	-	41,41,41	4.76	24 (58%)	56,56,56	2.30	20 (35%)
26	CHL	U	316	18	66,74,74	1.87	15 (22%)	73,114,114	2.56	24 (32%)
31	BCR	c	516	-	41,41,41	4.76	24 (58%)	56,56,56	2.30	21 (37%)
22	CLA	N	306	-	60,68,73	1.50	6 (10%)	70,107,113	1.55	8 (11%)
22	CLA	G	308	-	48,56,73	1.71	7 (14%)	55,92,113	1.58	7 (12%)
24	XAT	G	309	-	39,47,47	2.53	17 (43%)	54,74,74	11.82	19 (35%)
26	CHL	1	317	18	66,74,74	1.90	15 (22%)	73,114,114	2.52	26 (35%)
22	CLA	Q	305	22	60,68,73	1.52	7 (11%)	70,107,113	1.41	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	NEX	5	319	-	38,46,46	0.91	1 (2%)	50,70,70	2.43	16 (32%)
23	LUT	S	310	-	42,43,43	0.77	0	51,60,60	1.69	14 (27%)
22	CLA	B	616	21	65,73,73	1.42	9 (13%)	76,113,113	1.45	9 (11%)
22	CLA	u	307	-	65,73,73	1.44	8 (12%)	76,113,113	1.46	8 (10%)
22	CLA	Q	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.54	8 (14%)
26	CHL	2	316	-	66,74,74	1.94	16 (24%)	73,114,114	2.37	20 (27%)
22	CLA	q	303	-	50,58,73	1.69	6 (12%)	58,95,113	1.64	9 (15%)
26	CHL	n	317	-	66,74,74	1.92	17 (25%)	73,114,114	2.48	22 (30%)
22	CLA	B	606	-	65,73,73	1.46	9 (13%)	76,113,113	1.43	6 (7%)
27	NEX	V	319	-	38,46,46	0.91	1 (2%)	50,70,70	2.46	16 (32%)
31	BCR	B	620	-	41,41,41	4.75	24 (58%)	56,56,56	2.28	23 (41%)
26	CHL	U	317	-	66,74,74	1.86	14 (21%)	73,114,114	2.38	19 (26%)
22	CLA	C	504	-	65,73,73	1.49	10 (15%)	76,113,113	1.52	7 (9%)
22	CLA	6	302	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
22	CLA	B	610	-	65,73,73	1.48	8 (12%)	76,113,113	1.46	9 (11%)
31	BCR	C	518	-	41,41,41	4.75	24 (58%)	56,56,56	2.29	19 (33%)
34	LMG	d	407	3	46,46,55	1.26	6 (13%)	54,54,63	1.01	2 (3%)
26	CHL	2	317	-	66,74,74	1.86	13 (19%)	73,114,114	2.45	23 (31%)
26	CHL	g	311	-	66,74,74	1.89	15 (22%)	73,114,114	2.40	22 (30%)
31	BCR	A	409	-	41,41,41	4.74	24 (58%)	56,56,56	2.25	22 (39%)
23	LUT	P	310	-	42,43,43	0.73	0	51,60,60	1.67	14 (27%)
24	XAT	r	612	-	39,47,47	2.52	17 (43%)	54,74,74	11.45	25 (46%)
22	CLA	1	306	-	60,68,73	1.52	9 (15%)	70,107,113	1.45	9 (12%)
22	CLA	u	303	-	50,58,73	1.69	8 (16%)	58,95,113	1.59	8 (13%)
34	LMG	a	412	-	40,40,55	1.30	6 (15%)	48,48,63	1.16	2 (4%)
22	CLA	c	506	-	65,73,73	1.40	7 (10%)	76,113,113	1.65	9 (11%)
23	LUT	U	310	-	42,43,43	0.79	0	51,60,60	1.61	9 (17%)
25	LHG	N	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
26	CHL	g	313	-	50,58,74	2.19	14 (28%)	52,94,114	2.75	18 (34%)
25	LHG	v	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
25	LHG	p	313	-	48,48,48	0.90	4 (8%)	51,54,54	1.04	2 (3%)
22	CLA	b	605	21	65,73,73	1.46	9 (13%)	76,113,113	1.75	11 (14%)
22	CLA	N	305	18	60,68,73	1.49	6 (10%)	70,107,113	1.93	13 (18%)
27	NEX	N	318	-	38,46,46	0.93	2 (5%)	50,70,70	2.40	17 (34%)
26	CHL	4	316	18	66,74,74	1.91	15 (22%)	73,114,114	2.48	26 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	CLA	A	404	-	65,73,73	1.41	8 (12%)	76,113,113	1.59	8 (10%)
23	LUT	v	310	-	42,43,43	0.77	0	51,60,60	1.63	10 (19%)
27	NEX	u	319	-	38,46,46	0.93	1 (2%)	50,70,70	2.45	18 (36%)
32	SQD	l	102	9	53,54,54	0.93	4 (7%)	62,65,65	1.80	12 (19%)
22	CLA	3	301	-	65,73,73	1.47	7 (10%)	76,113,113	1.45	7 (9%)
26	CHL	S	314	-	46,54,74	2.28	16 (34%)	49,90,114	2.86	18 (36%)
26	CHL	n	315	-	50,58,74	2.22	16 (32%)	52,94,114	2.72	21 (40%)
35	BCT	a	414	-	2,3,3	1.35	0	2,3,3	0.20	0
30	PHO	A	407	-	51,69,69	1.09	5 (9%)	47,99,99	1.23	6 (12%)
22	CLA	a	405	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	8 (10%)
22	CLA	s	304	19	45,53,73	1.75	6 (13%)	52,89,113	1.58	6 (11%)
23	LUT	V	309	-	42,43,43	0.78	0	51,60,60	1.63	13 (25%)
26	CHL	4	317	-	66,74,74	1.88	15 (22%)	73,114,114	2.41	22 (30%)
26	CHL	V	313	-	66,74,74	1.95	16 (24%)	73,114,114	2.43	21 (28%)
33	PL9	A	410	-	13,13,55	3.64	7 (53%)	17,17,69	1.47	3 (17%)
33	PL9	D	405	-	55,55,55	1.54	6 (10%)	68,69,69	1.68	18 (26%)
26	CHL	6	317	-	61,69,74	1.99	13 (21%)	67,108,114	2.52	22 (32%)
22	CLA	r	602	-	60,68,73	1.53	6 (10%)	70,107,113	1.47	7 (10%)
22	CLA	6	303	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	7 (9%)
22	CLA	u	301	-	65,73,73	1.50	9 (13%)	76,113,113	1.41	6 (7%)
22	CLA	1	307	-	65,73,73	1.44	8 (12%)	76,113,113	1.47	9 (11%)
22	CLA	C	515	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	9 (11%)
22	CLA	G	307	-	65,73,73	1.47	7 (10%)	76,113,113	1.44	7 (9%)
22	CLA	R	311	-	45,53,73	1.78	6 (13%)	52,89,113	1.65	6 (11%)
24	XAT	N	311	-	39,47,47	2.53	17 (43%)	54,74,74	11.91	18 (33%)
26	CHL	S	315	19	58,66,74	2.14	16 (27%)	63,104,114	2.44	20 (31%)
22	CLA	q	301	-	65,73,73	1.50	7 (10%)	76,113,113	1.42	7 (9%)
31	BCR	t	101	-	41,41,41	4.79	24 (58%)	56,56,56	2.38	22 (39%)
22	CLA	p	308	-	60,68,73	1.53	7 (11%)	70,107,113	1.50	6 (8%)
26	CHL	r	614	-	66,74,74	1.88	13 (19%)	73,114,114	2.43	22 (30%)
31	BCR	a	409	-	41,41,41	4.73	24 (58%)	56,56,56	2.22	22 (39%)
27	NEX	s	317	19	38,46,46	0.87	1 (2%)	50,70,70	2.39	16 (32%)
22	CLA	6	307	22	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
30	PHO	D	401	-	51,69,69	1.03	4 (7%)	47,99,99	1.32	6 (12%)
22	CLA	1	305	-	60,68,73	1.49	6 (10%)	70,107,113	1.45	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	LHG	3	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.11	2 (3%)
22	CLA	c	510	-	65,73,73	1.38	7 (10%)	76,113,113	1.53	9 (11%)
22	CLA	U	305	-	60,68,73	1.52	7 (11%)	70,107,113	1.45	7 (10%)
22	CLA	n	305	18	60,68,73	1.51	7 (11%)	70,107,113	2.08	16 (22%)
22	CLA	R	307	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	6 (7%)
22	CLA	s	306	-	56,64,73	1.59	8 (14%)	65,102,113	1.51	10 (15%)
25	LHG	S	312	19	48,48,48	0.89	4 (8%)	51,54,54	1.13	3 (5%)
22	CLA	2	307	-	60,68,73	1.51	6 (10%)	70,107,113	1.50	7 (10%)
22	CLA	S	305	-	55,63,73	1.57	7 (12%)	64,101,113	1.49	7 (10%)
22	CLA	c	503	-	65,73,73	1.49	10 (15%)	76,113,113	1.51	7 (9%)
26	CHL	1	316	-	66,74,74	1.91	16 (24%)	73,114,114	2.45	22 (30%)
22	CLA	V	305	-	60,68,73	1.53	6 (10%)	70,107,113	1.48	7 (10%)
22	CLA	G	303	-	50,58,73	1.69	7 (14%)	58,95,113	1.62	7 (12%)
22	CLA	S	309	-	49,57,73	1.69	8 (16%)	55,93,113	1.55	6 (10%)
25	LHG	C	524	-	48,48,48	0.90	4 (8%)	51,54,54	1.13	2 (3%)
31	BCR	c	515	-	41,41,41	4.70	24 (58%)	56,56,56	2.67	23 (41%)
26	CHL	5	313	18	66,74,74	2.00	17 (25%)	73,114,114	2.39	21 (28%)
22	CLA	b	602	-	65,73,73	1.42	9 (13%)	76,113,113	1.44	7 (9%)
26	CHL	q	311	-	66,74,74	1.89	15 (22%)	73,114,114	2.43	22 (30%)
37	HEM	E	101	4,17	41,50,50	1.60	6 (14%)	45,82,82	1.15	2 (4%)
26	CHL	u	313	-	66,74,74	1.94	17 (25%)	73,114,114	2.37	23 (31%)
25	LHG	c	523	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
22	CLA	1	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.58	7 (12%)
31	BCR	T	101	-	41,41,41	4.79	24 (58%)	56,56,56	2.38	22 (39%)
26	CHL	g	312	-	48,56,74	2.27	14 (29%)	51,92,114	2.77	21 (41%)
31	BCR	b	620	-	41,41,41	4.77	24 (58%)	56,56,56	2.21	21 (37%)
22	CLA	4	308	-	48,56,73	1.69	6 (12%)	55,92,113	1.60	7 (12%)
33	PL9	d	404	-	55,55,55	1.54	6 (10%)	68,69,69	1.68	18 (26%)
22	CLA	q	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	8 (10%)
22	CLA	b	610	-	65,73,73	1.47	8 (12%)	76,113,113	1.45	9 (11%)
30	PHO	a	407	-	51,69,69	1.08	5 (9%)	47,99,99	1.23	6 (12%)
22	CLA	b	614	-	65,73,73	1.43	9 (13%)	76,113,113	1.42	7 (9%)
23	LUT	U	309	-	42,43,43	0.74	0	51,60,60	1.54	10 (19%)
22	CLA	6	309	-	48,56,73	1.70	6 (12%)	55,92,113	1.57	7 (12%)
22	CLA	3	303	-	50,58,73	1.68	7 (14%)	58,95,113	1.62	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	XAT	n	311	-	39,47,47	2.53	18 (46%)	54,74,74	11.76	23 (42%)
25	LHG	n	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.03	2 (3%)
22	CLA	V	303	-	50,58,73	1.66	8 (16%)	58,95,113	1.66	8 (13%)
26	CHL	p	319	-	66,74,74	1.90	15 (22%)	73,114,114	2.37	22 (30%)
27	NEX	U	318	-	38,46,46	0.96	1 (2%)	50,70,70	2.38	12 (24%)
22	CLA	s	305	-	55,63,73	1.58	7 (12%)	64,101,113	1.49	8 (12%)
22	CLA	3	304	18	64,72,73	1.47	8 (12%)	74,111,113	1.52	9 (12%)
22	CLA	x	201	14	65,73,73	1.40	7 (10%)	76,113,113	1.53	8 (10%)
22	CLA	u	308	-	48,56,73	1.70	8 (16%)	55,92,113	1.57	7 (12%)
22	CLA	g	304	18	64,72,73	1.48	7 (10%)	74,111,113	1.50	8 (10%)
22	CLA	v	304	-	60,68,73	1.50	6 (10%)	70,107,113	1.52	7 (10%)
22	CLA	G	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.51	6 (7%)
22	CLA	B	604	-	65,73,73	1.47	8 (12%)	76,113,113	1.44	7 (9%)
22	CLA	c	514	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	10 (13%)
25	LHG	2	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
22	CLA	q	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.58	8 (14%)
22	CLA	C	511	-	65,73,73	1.38	7 (10%)	76,113,113	1.53	11 (14%)
34	LMG	C	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.07	2 (3%)
22	CLA	b	615	-	65,73,73	1.43	8 (12%)	76,113,113	1.49	7 (9%)
22	CLA	b	606	-	65,73,73	1.46	9 (13%)	76,113,113	1.42	7 (9%)
22	CLA	6	305	18	64,72,73	1.47	7 (10%)	74,111,113	1.50	9 (12%)
22	CLA	v	306	-	60,68,73	1.55	8 (13%)	70,107,113	1.46	9 (12%)
22	CLA	C	507	-	65,73,73	1.39	7 (10%)	76,113,113	1.64	9 (11%)
30	PHO	d	401	-	51,69,69	1.03	4 (7%)	47,99,99	1.32	6 (12%)
22	CLA	C	509	20	65,73,73	1.46	9 (13%)	76,113,113	1.53	10 (13%)
22	CLA	b	613	-	65,73,73	1.44	8 (12%)	76,113,113	1.46	10 (13%)
26	CHL	r	616	-	61,69,74	2.02	17 (27%)	67,108,114	2.36	19 (28%)
26	CHL	s	313	-	46,54,74	2.34	16 (34%)	49,90,114	2.82	20 (40%)
22	CLA	B	602	-	65,73,73	1.43	9 (13%)	76,113,113	1.45	10 (13%)
26	CHL	u	314	-	48,56,74	2.22	16 (33%)	51,92,114	2.79	21 (41%)
22	CLA	R	305	-	48,56,73	1.73	6 (12%)	55,92,113	1.63	8 (14%)
26	CHL	s	316	-	46,54,74	2.37	16 (34%)	49,90,114	2.82	20 (40%)
34	LMG	A	411	-	40,40,55	1.30	6 (15%)	48,48,63	1.16	2 (4%)
22	CLA	b	611	-	65,73,73	1.48	8 (12%)	76,113,113	1.49	8 (10%)
26	CHL	P	317	-	66,74,74	1.93	17 (25%)	73,114,114	2.42	24 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	CHL	N	316	-	66,74,74	1.86	15 (22%)	73,114,114	2.48	21 (28%)
22	CLA	r	603	-	60,68,73	1.53	6 (10%)	70,107,113	1.46	6 (8%)
26	CHL	4	315	-	50,58,74	2.25	16 (32%)	52,94,114	2.67	19 (36%)
26	CHL	q	314	18	66,74,74	1.88	17 (25%)	73,114,114	2.48	20 (27%)
26	CHL	g	314	-	66,74,74	1.96	16 (24%)	73,114,114	2.41	23 (31%)
32	SQD	m	101	-	41,42,54	1.06	5 (12%)	50,53,65	1.75	11 (22%)
22	CLA	6	308	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
22	CLA	r	605	-	58,66,73	1.56	6 (10%)	67,104,113	1.53	6 (8%)
22	CLA	U	303	-	50,58,73	1.68	9 (18%)	58,95,113	1.56	7 (12%)
25	LHG	d	405	3	45,45,48	0.92	4 (8%)	48,51,54	1.07	2 (4%)
25	LHG	r	613	-	41,41,48	0.96	3 (7%)	44,47,54	1.09	2 (4%)
22	CLA	s	301	19	61,69,73	1.49	8 (13%)	71,108,113	1.53	11 (15%)
22	CLA	r	606	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
22	CLA	S	303	19	50,58,73	1.67	7 (14%)	58,95,113	1.63	8 (13%)
22	CLA	G	305	22	60,68,73	1.51	7 (11%)	70,107,113	1.53	8 (11%)
26	CHL	R	317	-	61,69,74	2.01	17 (27%)	67,108,114	2.38	20 (29%)
22	CLA	2	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.59	7 (12%)
22	CLA	b	607	-	65,73,73	1.48	9 (13%)	76,113,113	1.51	8 (10%)
26	CHL	n	314	-	48,56,74	2.35	17 (35%)	51,92,114	2.84	20 (39%)
23	LUT	N	310	-	42,43,43	0.78	0	51,60,60	1.69	15 (29%)
26	CHL	6	314	-	50,58,74	2.29	16 (32%)	52,94,114	2.62	22 (42%)
22	CLA	S	304	19	45,53,73	1.75	6 (13%)	52,89,113	1.58	6 (11%)
34	LMG	B	621	-	51,51,55	1.18	6 (11%)	59,59,63	1.44	6 (10%)
22	CLA	N	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	6 (7%)
22	CLA	1	302	-	65,73,73	1.50	6 (9%)	76,113,113	1.30	7 (9%)
22	CLA	R	304	-	60,68,73	1.53	5 (8%)	70,107,113	1.48	6 (8%)
22	CLA	n	302	-	65,73,73	1.52	7 (10%)	76,113,113	1.37	7 (9%)
32	SQD	A	412	-	53,54,54	0.95	5 (9%)	62,65,65	1.50	10 (16%)
34	LMG	W	201	-	48,48,55	1.23	6 (12%)	56,56,63	1.12	4 (7%)
25	LHG	P	313	-	48,48,48	0.90	4 (8%)	51,54,54	1.07	2 (3%)
26	CHL	p	317	-	66,74,74	1.91	16 (24%)	73,114,114	2.41	21 (28%)
26	CHL	v	316	-	66,74,74	1.89	16 (24%)	73,114,114	2.46	24 (32%)
26	CHL	q	313	-	50,58,74	2.18	16 (32%)	52,94,114	2.73	19 (36%)
22	CLA	v	305	-	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
22	CLA	s	307	-	49,57,73	1.66	7 (14%)	55,93,113	1.64	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	LHG	A	413	2	42,42,48	0.93	3 (7%)	45,48,54	1.11	2 (4%)
27	NEX	S	317	19	38,46,46	0.88	1 (2%)	50,70,70	2.45	17 (34%)
24	XAT	3	309	-	39,47,47	2.56	18 (46%)	54,74,74	11.80	17 (31%)
26	CHL	V	317	18	66,74,74	1.91	15 (22%)	73,114,114	2.51	25 (34%)
22	CLA	B	614	-	65,73,73	1.44	9 (13%)	76,113,113	1.43	7 (9%)
22	CLA	P	304	-	50,58,73	1.67	8 (16%)	58,95,113	1.58	8 (13%)
22	CLA	3	302	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
22	CLA	5	303	-	50,58,73	1.67	8 (16%)	58,95,113	1.58	8 (13%)
26	CHL	Q	311	-	66,74,74	1.90	16 (24%)	73,114,114	2.44	23 (31%)
22	CLA	S	306	-	56,64,73	1.59	8 (14%)	65,102,113	1.51	8 (12%)
26	CHL	G	314	-	66,74,74	1.94	16 (24%)	73,114,114	2.32	21 (28%)
22	CLA	V	302	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	7 (9%)
22	CLA	r	607	1	49,57,73	1.68	6 (12%)	55,93,113	1.66	9 (16%)
22	CLA	q	304	18	64,72,73	1.47	7 (10%)	74,111,113	1.63	8 (10%)
22	CLA	N	307	-	60,68,73	1.52	7 (11%)	70,107,113	1.48	7 (10%)
26	CHL	g	315	18	66,74,74	1.87	14 (21%)	73,114,114	2.44	20 (27%)
26	CHL	5	314	-	48,56,74	2.35	17 (35%)	51,92,114	2.83	20 (39%)
22	CLA	V	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	7 (9%)
22	CLA	X	202	14	65,73,73	1.40	7 (10%)	76,113,113	1.52	8 (10%)
27	NEX	P	301	18	38,46,46	0.94	1 (2%)	50,70,70	2.35	18 (36%)
22	CLA	P	307	-	60,68,73	1.48	6 (10%)	70,107,113	1.50	8 (11%)
26	CHL	r	615	-	56,64,74	2.05	15 (26%)	61,102,114	2.61	21 (34%)
26	CHL	S	316	-	46,54,74	2.36	16 (34%)	49,90,114	2.81	20 (40%)
23	LUT	5	310	-	42,43,43	0.77	0	51,60,60	1.64	12 (23%)
36	DGD	c	519	-	61,61,67	1.25	6 (9%)	75,75,81	1.17	3 (4%)
34	LMG	C	502	-	51,51,55	1.15	4 (7%)	59,59,63	1.16	3 (5%)
33	PL9	a	411	-	13,13,55	3.63	7 (53%)	17,17,69	1.48	3 (17%)
24	XAT	v	311	-	39,47,47	2.56	18 (46%)	54,74,74	12.01	19 (35%)
22	CLA	d	402	3	65,73,73	1.43	9 (13%)	76,113,113	1.39	8 (10%)
22	CLA	P	306	18	60,68,73	1.48	6 (10%)	70,107,113	2.01	12 (17%)
22	CLA	v	301	-	65,73,73	1.49	9 (13%)	76,113,113	1.35	6 (7%)
22	CLA	S	301	19	61,69,73	1.48	7 (11%)	71,108,113	1.52	10 (14%)
26	CHL	p	315	-	48,56,74	2.41	17 (35%)	51,92,114	2.76	19 (37%)
26	CHL	n	316	-	66,74,74	1.91	15 (22%)	73,114,114	2.35	21 (28%)
26	CHL	P	316	-	50,58,74	2.24	16 (32%)	52,94,114	2.70	20 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	P	302	-	65,73,73	1.44	7 (10%)	76,113,113	1.47	7 (9%)
22	CLA	g	306	22	60,68,73	1.56	7 (11%)	70,107,113	1.39	6 (8%)
22	CLA	R	310	-	60,68,73	1.54	5 (8%)	70,107,113	1.55	9 (12%)
22	CLA	B	605	21	65,73,73	1.46	9 (13%)	76,113,113	1.76	13 (17%)
26	CHL	G	315	18	66,74,74	1.87	16 (24%)	73,114,114	2.42	20 (27%)
32	SQD	a	413	-	53,54,54	0.95	5 (9%)	62,65,65	1.51	9 (14%)
24	XAT	P	312	-	39,47,47	2.59	18 (46%)	54,74,74	11.98	19 (35%)
26	CHL	v	315	-	50,58,74	2.23	16 (32%)	52,94,114	2.70	21 (40%)
25	LHG	5	312	-	48,48,48	0.90	3 (6%)	51,54,54	1.07	2 (3%)
22	CLA	5	307	-	60,68,73	1.51	7 (11%)	70,107,113	1.48	7 (10%)
34	LMG	b	621	-	51,51,55	1.18	6 (11%)	59,59,63	1.44	7 (11%)
26	CHL	U	313	-	66,74,74	1.95	16 (24%)	73,114,114	2.41	22 (30%)
25	LHG	q	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.05	2 (3%)
31	BCR	d	403	3	41,41,41	4.76	24 (58%)	56,56,56	2.26	23 (41%)
22	CLA	b	604	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	7 (9%)
24	XAT	4	311	-	39,47,47	2.54	17 (43%)	54,74,74	12.07	21 (38%)
26	CHL	g	316	-	61,69,74	1.97	16 (26%)	67,108,114	2.48	25 (37%)
22	CLA	b	609	-	65,73,73	1.45	8 (12%)	76,113,113	1.46	6 (7%)
22	CLA	U	307	-	65,73,73	1.45	9 (13%)	76,113,113	1.45	7 (9%)
22	CLA	3	308	-	48,56,73	1.71	6 (12%)	55,92,113	1.58	7 (12%)
22	CLA	R	302	27	49,57,73	1.73	7 (14%)	55,93,113	1.62	8 (14%)
22	CLA	5	306	-	60,68,73	1.47	7 (11%)	70,107,113	1.55	7 (10%)
22	CLA	R	303	-	60,68,73	1.52	6 (10%)	70,107,113	1.48	8 (11%)
22	CLA	S	307	-	49,57,73	1.66	7 (14%)	55,93,113	1.65	8 (14%)
22	CLA	U	301	-	65,73,73	1.49	9 (13%)	76,113,113	1.41	7 (9%)
22	CLA	n	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	7 (9%)
22	CLA	c	504	-	65,73,73	1.44	9 (13%)	76,113,113	1.43	7 (9%)
26	CHL	3	313	-	50,58,74	2.26	16 (32%)	52,94,114	2.63	21 (40%)
26	CHL	G	312	-	48,56,74	2.32	18 (37%)	51,92,114	2.82	20 (39%)
22	CLA	c	505	-	65,73,73	1.46	9 (13%)	76,113,113	1.45	7 (9%)
22	CLA	b	608	-	65,73,73	1.44	7 (10%)	76,113,113	1.52	7 (9%)
22	CLA	4	305	-	60,68,73	1.51	7 (11%)	70,107,113	1.42	8 (11%)
22	CLA	V	301	-	65,73,73	1.51	9 (13%)	76,113,113	1.33	6 (7%)
36	DGD	C	520	-	63,63,67	1.22	6 (9%)	77,77,81	1.16	4 (5%)
22	CLA	1	301	-	65,73,73	1.48	9 (13%)	76,113,113	1.41	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	CHL	5	316	-	66,74,74	1.94	16 (24%)	73,114,114	2.36	21 (28%)
26	CHL	n	318	-	66,74,74	1.95	16 (24%)	73,114,114	2.35	23 (31%)
31	BCR	x	202	-	41,41,41	4.78	24 (58%)	56,56,56	2.27	18 (32%)
26	CHL	3	314	-	66,74,74	1.96	17 (25%)	73,114,114	2.38	20 (27%)
22	CLA	r	604	-	48,56,73	1.72	6 (12%)	55,92,113	1.63	8 (14%)
26	CHL	1	318	-	66,74,74	1.89	15 (22%)	73,114,114	2.39	22 (30%)
27	NEX	p	301	18	38,46,46	0.98	2 (5%)	50,70,70	2.43	19 (38%)
27	NEX	n	319	-	38,46,46	0.96	2 (5%)	50,70,70	2.64	17 (34%)
22	CLA	N	308	-	48,56,73	1.74	6 (12%)	55,92,113	1.54	7 (12%)
22	CLA	v	302	-	65,73,73	1.48	8 (12%)	76,113,113	1.38	8 (10%)
22	CLA	B	613	-	65,73,73	1.43	8 (12%)	76,113,113	1.46	10 (13%)
22	CLA	n	307	-	60,68,73	1.51	7 (11%)	70,107,113	1.48	7 (10%)
22	CLA	V	308	-	48,56,73	1.69	6 (12%)	55,92,113	1.58	6 (10%)
24	XAT	g	309	-	39,47,47	2.53	17 (43%)	54,74,74	11.71	20 (37%)
25	LHG	6	311	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
25	LHG	V	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.10	2 (3%)
32	SQD	L	102	9	53,54,54	0.93	4 (7%)	62,65,65	1.80	12 (19%)
26	CHL	N	317	-	66,74,74	1.93	16 (24%)	73,114,114	2.33	22 (30%)
26	CHL	v	317	18	66,74,74	1.91	15 (22%)	73,114,114	2.52	25 (34%)
26	CHL	N	313	-	66,74,74	1.92	15 (22%)	73,114,114	2.41	22 (30%)
26	CHL	Q	313	-	50,58,74	2.20	16 (32%)	52,94,114	2.72	20 (38%)
25	LHG	G	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.10	2 (3%)
22	CLA	B	609	-	65,73,73	1.44	8 (12%)	76,113,113	1.45	6 (7%)
26	CHL	U	319	-	66,74,74	1.92	15 (22%)	73,114,114	2.39	21 (28%)
26	CHL	Q	314	-	66,74,74	1.93	16 (24%)	73,114,114	2.36	22 (30%)
24	XAT	U	311	-	39,47,47	2.51	17 (43%)	54,74,74	11.93	20 (37%)
36	DGD	c	518	-	63,63,67	1.22	6 (9%)	77,77,81	1.15	5 (6%)
23	LUT	v	309	-	42,43,43	0.79	0	51,60,60	1.65	12 (23%)
22	CLA	R	309	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	9 (16%)
22	CLA	s	302	-	45,53,73	1.81	6 (13%)	52,89,113	1.61	7 (13%)
22	CLA	s	303	19	50,58,73	1.67	7 (14%)	58,95,113	1.64	8 (13%)
24	XAT	2	311	-	39,47,47	2.58	18 (46%)	54,74,74	11.93	19 (35%)
36	DGD	A	414	-	60,60,67	1.27	7 (11%)	74,74,81	1.25	6 (8%)
26	CHL	Q	312	-	48,56,74	2.29	15 (31%)	51,92,114	2.76	21 (41%)
27	NEX	r	617	-	38,46,46	1.01	3 (7%)	50,70,70	2.42	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	5	308	-	48,56,73	1.70	6 (12%)	55,92,113	1.57	7 (12%)
34	LMG	c	501	-	51,51,55	1.15	5 (9%)	59,59,63	1.16	3 (5%)
23	LUT	P	311	-	42,43,43	0.76	0	51,60,60	1.58	12 (23%)
22	CLA	B	608	-	65,73,73	1.43	7 (10%)	76,113,113	1.52	7 (9%)
22	CLA	U	308	-	48,56,73	1.71	8 (16%)	55,92,113	1.58	7 (12%)
22	CLA	N	302	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	7 (9%)
26	CHL	3	316	-	61,69,74	2.00	14 (22%)	67,108,114	2.48	23 (34%)
26	CHL	2	315	-	50,58,74	2.18	15 (30%)	52,94,114	2.77	19 (36%)
26	CHL	1	313	-	66,74,74	1.94	15 (22%)	73,114,114	2.37	23 (31%)
31	BCR	z	101	-	41,41,41	4.76	24 (58%)	56,56,56	2.32	20 (35%)
24	XAT	q	309	-	39,47,47	2.58	18 (46%)	54,74,74	11.94	18 (33%)
22	CLA	G	304	18	64,72,73	1.48	7 (10%)	74,111,113	1.53	9 (12%)
26	CHL	v	318	-	66,74,74	1.92	16 (24%)	73,114,114	2.32	21 (28%)
22	CLA	N	304	18	65,73,73	1.43	7 (10%)	76,113,113	1.53	9 (11%)
23	LUT	n	309	-	42,43,43	0.74	0	51,60,60	1.62	11 (21%)
27	NEX	v	319	-	38,46,46	0.89	1 (2%)	50,70,70	2.45	14 (28%)
26	CHL	5	315	-	50,58,74	2.17	15 (30%)	52,94,114	2.79	20 (38%)
26	CHL	V	314	-	48,56,74	2.30	17 (35%)	51,92,114	2.79	21 (41%)
25	LHG	b	622	-	46,46,48	0.91	4 (8%)	49,52,54	1.04	2 (4%)
22	CLA	A	406	-	50,58,73	1.65	10 (20%)	58,95,113	1.56	7 (12%)
25	LHG	B	622	-	46,46,48	0.91	4 (8%)	49,52,54	1.06	2 (4%)
26	CHL	1	314	22	48,56,74	2.25	14 (29%)	51,92,114	2.82	20 (39%)
26	CHL	S	313	-	46,54,74	2.33	16 (34%)	49,90,114	2.84	20 (40%)
22	CLA	b	612	-	65,73,73	1.48	7 (10%)	76,113,113	1.54	7 (9%)
22	CLA	6	304	-	50,58,73	1.68	7 (14%)	58,95,113	1.60	8 (13%)
22	CLA	g	302	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	7 (9%)
22	CLA	g	303	-	50,58,73	1.69	7 (14%)	58,95,113	1.62	7 (12%)
23	LUT	1	309	-	42,43,43	0.72	0	51,60,60	1.57	10 (19%)
25	LHG	1	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
22	CLA	v	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
34	LMG	B	624	21	55,55,55	1.16	6 (10%)	63,63,63	1.07	2 (3%)
32	SQD	C	501	-	49,50,54	1.00	5 (10%)	58,61,65	1.75	11 (18%)
26	CHL	G	311	-	66,74,74	1.87	15 (22%)	73,114,114	2.46	23 (31%)
22	CLA	B	603	-	65,73,73	1.45	9 (13%)	76,113,113	1.42	6 (7%)
22	CLA	G	306	22	60,68,73	1.54	6 (10%)	70,107,113	1.39	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	n	308	-	48,56,73	1.75	6 (12%)	55,92,113	1.65	9 (16%)
23	LUT	p	311	-	42,43,43	0.76	0	51,60,60	1.54	12 (23%)
22	CLA	s	308	-	55,63,73	1.58	8 (14%)	64,101,113	1.51	7 (10%)
22	CLA	r	609	26	60,68,73	1.54	6 (10%)	70,107,113	1.58	11 (15%)
22	CLA	A	408	-	60,68,73	1.45	8 (13%)	70,107,113	1.67	8 (11%)
22	CLA	2	305	18	60,68,73	1.50	7 (11%)	70,107,113	2.03	15 (21%)
25	LHG	C	523	-	48,48,48	0.89	3 (6%)	51,54,54	1.07	2 (3%)
36	DGD	c	517	-	56,56,67	1.30	8 (14%)	70,70,81	1.19	5 (7%)
31	BCR	b	618	-	41,41,41	4.74	24 (58%)	56,56,56	2.46	23 (41%)
22	CLA	U	302	-	65,73,73	1.47	8 (12%)	76,113,113	1.39	6 (7%)
26	CHL	n	313	18	66,74,74	1.94	16 (24%)	73,114,114	2.40	24 (32%)
22	CLA	4	303	-	50,58,73	1.68	8 (16%)	58,95,113	1.56	8 (13%)
22	CLA	R	308	1	49,57,73	1.68	6 (12%)	55,93,113	1.66	8 (14%)
22	CLA	2	302	-	65,73,73	1.48	8 (12%)	76,113,113	1.38	7 (9%)
25	LHG	b	623	21	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
22	CLA	n	304	18	65,73,73	1.42	7 (10%)	76,113,113	1.54	9 (11%)
23	LUT	2	309	-	42,43,43	0.76	0	51,60,60	1.68	14 (27%)
35	BCT	D	402	-	2,3,3	1.35	0	2,3,3	0.19	0
23	LUT	1	310	-	42,43,43	0.80	0	51,60,60	1.74	14 (27%)
22	CLA	B	611	-	65,73,73	1.47	8 (12%)	76,113,113	1.49	8 (10%)
22	CLA	V	306	-	60,68,73	1.56	7 (11%)	70,107,113	1.43	8 (11%)
36	DGD	b	601	21	63,63,67	1.23	7 (11%)	77,77,81	1.06	3 (3%)
22	CLA	g	307	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
22	CLA	4	306	-	60,68,73	1.56	8 (13%)	70,107,113	1.42	8 (11%)
22	CLA	c	508	20	65,73,73	1.47	9 (13%)	76,113,113	1.52	10 (13%)
24	XAT	1	311	-	39,47,47	2.54	17 (43%)	54,74,74	12.16	18 (33%)
22	CLA	Q	303	-	50,58,73	1.70	6 (12%)	58,95,113	1.58	8 (13%)
22	CLA	D	403	3	65,73,73	1.43	9 (13%)	76,113,113	1.39	8 (10%)
26	CHL	r	619	1	48,56,74	2.20	15 (31%)	51,92,114	2.82	19 (37%)
31	BCR	b	619	-	41,41,41	4.74	24 (58%)	56,56,56	2.27	20 (35%)
26	CHL	P	319	-	66,74,74	1.88	14 (21%)	73,114,114	2.40	20 (27%)
26	CHL	V	316	-	66,74,74	1.94	16 (24%)	73,114,114	2.38	22 (30%)
36	DGD	C	519	-	56,56,67	1.30	8 (14%)	70,70,81	1.19	5 (7%)
26	CHL	N	314	-	48,56,74	2.33	16 (33%)	51,92,114	2.82	20 (39%)
22	CLA	c	512	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	LUT	n	310	-	42,43,43	0.79	0	51,60,60	1.75	14 (27%)
23	LUT	r	611	1	42,43,43	0.75	0	51,60,60	1.66	10 (19%)
26	CHL	P	315	-	48,56,74	2.46	16 (33%)	51,92,114	2.76	19 (37%)
22	CLA	Q	306	22	60,68,73	1.54	5 (8%)	70,107,113	1.40	6 (8%)
22	CLA	5	304	18	65,73,73	1.45	9 (13%)	76,113,113	1.51	10 (13%)
22	CLA	B	615	-	65,73,73	1.42	9 (13%)	76,113,113	1.48	7 (9%)
22	CLA	C	513	-	65,73,73	1.47	9 (13%)	76,113,113	1.53	9 (11%)
22	CLA	C	506	-	65,73,73	1.46	9 (13%)	76,113,113	1.43	7 (9%)
23	LUT	S	311	-	42,43,43	0.77	0	51,60,60	1.64	17 (33%)
26	CHL	G	313	-	50,58,74	2.19	15 (30%)	52,94,114	2.72	18 (34%)
22	CLA	4	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.49	9 (11%)
22	CLA	r	610	-	45,53,73	1.79	6 (13%)	52,89,113	1.65	6 (11%)
22	CLA	C	514	-	65,73,73	1.44	10 (15%)	76,113,113	1.41	7 (9%)
26	CHL	R	315	-	66,74,74	1.88	13 (19%)	73,114,114	2.43	22 (30%)
26	CHL	6	313	-	48,56,74	2.37	17 (35%)	51,92,114	2.83	23 (45%)
26	CHL	Q	315	18	66,74,74	1.87	16 (24%)	73,114,114	2.47	21 (28%)
22	CLA	S	302	-	45,53,73	1.81	6 (13%)	52,89,113	1.61	7 (13%)
26	CHL	3	311	-	66,74,74	1.89	14 (21%)	73,114,114	2.46	23 (31%)
25	LHG	B	623	21	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
27	NEX	u	320	-	38,46,46	0.89	2 (5%)	50,70,70	2.32	18 (36%)
24	XAT	V	311	-	39,47,47	2.58	18 (46%)	54,74,74	12.00	18 (33%)
22	CLA	v	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.58	6 (10%)
22	CLA	N	303	-	50,58,73	1.65	7 (14%)	58,95,113	1.69	7 (12%)
22	CLA	2	304	18	65,73,73	1.45	9 (13%)	76,113,113	1.48	9 (11%)
22	CLA	p	306	18	60,68,73	1.49	6 (10%)	70,107,113	2.10	16 (22%)
22	CLA	S	308	-	55,63,73	1.59	7 (12%)	64,101,113	1.50	7 (10%)
22	CLA	c	502	-	65,73,73	1.48	9 (13%)	76,113,113	1.41	8 (10%)
36	DGD	B	601	21	63,63,67	1.22	7 (11%)	77,77,81	1.07	3 (3%)
22	CLA	4	301	-	65,73,73	1.47	9 (13%)	76,113,113	1.44	7 (9%)
32	SQD	M	101	-	41,42,54	1.06	5 (12%)	50,53,65	1.74	11 (22%)
26	CHL	q	312	-	48,56,74	2.36	17 (35%)	51,92,114	2.82	21 (41%)
26	CHL	v	313	-	66,74,74	1.92	16 (24%)	73,114,114	2.45	23 (31%)
22	CLA	2	303	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)
26	CHL	p	318	-	66,74,74	1.84	14 (21%)	73,114,114	2.44	20 (27%)
22	CLA	q	306	22	60,68,73	1.53	5 (8%)	70,107,113	1.44	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	XAT	R	313	-	39,47,47	2.54	17 (43%)	54,74,74	11.48	22 (40%)
26	CHL	v	314	-	48,56,74	2.23	15 (31%)	51,92,114	2.84	21 (41%)
23	LUT	4	310	-	42,43,43	0.83	1 (2%)	51,60,60	1.79	14 (27%)
26	CHL	V	315	-	50,58,74	2.29	16 (32%)	52,94,114	2.69	20 (38%)
36	DGD	J	101	-	61,61,67	1.26	6 (9%)	75,75,81	1.17	3 (4%)
22	CLA	R	306	-	58,66,73	1.56	6 (10%)	67,104,113	1.53	6 (8%)
22	CLA	q	302	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	7 (9%)
22	CLA	p	307	-	60,68,73	1.52	5 (8%)	70,107,113	1.46	8 (11%)
22	CLA	C	503	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	9 (11%)
26	CHL	Q	316	-	61,69,74	2.00	16 (26%)	67,108,114	2.48	22 (32%)
22	CLA	g	308	-	48,56,73	1.70	6 (12%)	55,92,113	1.56	7 (12%)
25	LHG	a	415	2	42,42,48	0.93	3 (7%)	45,48,54	1.10	2 (4%)
25	LHG	l	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	3 (5%)
31	BCR	K	101	-	41,41,41	4.72	24 (58%)	56,56,56	2.53	19 (33%)
31	BCR	D	404	3	41,41,41	4.77	24 (58%)	56,56,56	2.26	23 (41%)
22	CLA	P	309	-	48,56,73	1.69	6 (12%)	55,92,113	1.57	7 (12%)
22	CLA	p	309	-	48,56,73	1.70	6 (12%)	55,92,113	1.57	7 (12%)
25	LHG	U	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.17	3 (5%)
22	CLA	n	303	-	50,58,73	1.69	6 (12%)	58,95,113	1.61	8 (13%)
25	LHG	4	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.07	2 (3%)
22	CLA	5	305	18	60,68,73	1.52	7 (11%)	70,107,113	2.04	13 (18%)
27	NEX	2	319	-	38,46,46	0.93	1 (2%)	50,70,70	2.45	14 (28%)
27	NEX	r	618	1,22	38,46,46	1.04	2 (5%)	50,70,70	2.49	16 (32%)
31	BCR	C	517	-	41,41,41	4.69	24 (58%)	56,56,56	2.67	24 (42%)
34	LMG	c	520	-	51,51,55	1.20	6 (11%)	59,59,63	1.08	2 (3%)
22	CLA	B	607	-	65,73,73	1.48	9 (13%)	76,113,113	1.50	9 (11%)
22	CLA	C	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.43	7 (9%)
32	SQD	a	410	-	49,50,54	1.01	5 (10%)	58,61,65	1.74	11 (18%)
22	CLA	P	308	-	60,68,73	1.53	7 (11%)	70,107,113	1.47	6 (8%)
22	CLA	2	301	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
22	CLA	a	406	-	50,58,73	1.65	10 (20%)	58,95,113	1.56	8 (13%)
26	CHL	p	320	-	66,74,74	1.87	14 (21%)	73,114,114	2.42	21 (28%)
22	CLA	u	306	-	60,68,73	1.54	10 (16%)	70,107,113	1.44	7 (10%)
22	CLA	p	304	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	8 (13%)
24	XAT	Q	309	-	39,47,47	2.60	18 (46%)	54,74,74	11.94	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	G	302	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	7 (9%)
26	CHL	1	315	-	50,58,74	2.23	16 (32%)	52,94,114	2.67	19 (36%)
26	CHL	R	316	-	56,64,74	2.05	14 (25%)	61,102,114	2.62	21 (34%)
22	CLA	1	304	-	60,68,73	1.49	8 (13%)	70,107,113	1.45	6 (8%)
26	CHL	2	313	18	66,74,74	1.99	17 (25%)	73,114,114	2.38	22 (30%)
26	CHL	2	318	-	66,74,74	1.88	14 (21%)	73,114,114	2.37	23 (31%)
31	BCR	B	618	-	41,41,41	4.74	24 (58%)	56,56,56	2.45	22 (39%)
22	CLA	u	305	-	60,68,73	1.52	7 (11%)	70,107,113	1.45	7 (10%)
22	CLA	1	303	-	50,58,73	1.66	9 (18%)	58,95,113	1.58	8 (13%)
22	CLA	Q	304	18	64,72,73	1.47	7 (10%)	74,111,113	1.53	9 (12%)
22	CLA	a	408	-	60,68,73	1.46	8 (13%)	70,107,113	1.68	8 (11%)
23	LUT	p	310	-	42,43,43	0.74	0	51,60,60	1.72	14 (27%)
26	CHL	6	312	-	66,74,74	1.90	15 (22%)	73,114,114	2.48	23 (31%)
26	CHL	s	315	19	58,66,74	2.14	16 (27%)	63,104,114	2.45	20 (31%)
26	CHL	p	316	-	50,58,74	2.23	16 (32%)	52,94,114	2.72	22 (42%)
26	CHL	q	315	-	61,69,74	2.01	16 (26%)	67,108,114	2.49	23 (34%)
23	LUT	N	309	-	42,43,43	0.72	0	51,60,60	1.55	11 (21%)
26	CHL	P	314	18	66,74,74	1.98	16 (24%)	73,114,114	2.40	22 (30%)
26	CHL	p	314	18	66,74,74	1.93	16 (24%)	73,114,114	2.42	23 (31%)
23	LUT	s	311	-	42,43,43	0.76	0	51,60,60	1.65	16 (31%)
22	CLA	6	306	22	60,68,73	1.51	6 (10%)	70,107,113	1.51	10 (14%)
22	CLA	B	612	-	65,73,73	1.49	7 (10%)	76,113,113	1.55	7 (9%)
22	CLA	b	617	21	65,73,73	1.51	10 (15%)	76,113,113	1.56	12 (15%)
22	CLA	r	601	27	49,57,73	1.73	7 (14%)	55,93,113	1.63	8 (14%)
26	CHL	5	317	-	66,74,74	1.86	12 (18%)	73,114,114	2.45	22 (30%)
25	LHG	g	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
24	XAT	u	311	-	39,47,47	2.54	18 (46%)	54,74,74	11.77	18 (33%)
23	LUT	R	312	-	42,43,43	0.73	0	51,60,60	1.52	11 (21%)
25	LHG	C	522	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
26	CHL	4	313	-	66,74,74	1.95	16 (24%)	73,114,114	2.33	22 (30%)
22	CLA	a	404	-	65,73,73	1.40	8 (12%)	76,113,113	1.60	8 (10%)
22	CLA	V	304	-	60,68,73	1.50	6 (10%)	70,107,113	1.52	8 (11%)
25	LHG	u	312	-	48,48,48	0.88	4 (8%)	51,54,54	1.13	3 (5%)
26	CHL	6	315	-	66,74,74	1.96	17 (25%)	73,114,114	2.39	22 (30%)
22	CLA	5	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	Q	302	-	65,73,73	1.45	6 (9%)	76,113,113	1.36	7 (9%)
36	DGD	a	416	-	60,60,67	1.27	7 (11%)	74,74,81	1.25	6 (8%)
26	CHL	u	316	-	66,74,74	1.90	14 (21%)	73,114,114	2.52	27 (36%)
24	XAT	5	311	-	39,47,47	2.58	18 (46%)	54,74,74	11.93	19 (35%)
22	CLA	4	304	-	60,68,73	1.50	8 (13%)	70,107,113	1.46	6 (8%)
26	CHL	u	315	-	50,58,74	2.14	13 (26%)	52,94,114	2.65	20 (38%)
25	LHG	L	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	3 (5%)
22	CLA	A	405	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	10 (13%)
23	LUT	V	310	-	42,43,43	0.78	0	51,60,60	1.62	12 (23%)
22	CLA	p	305	18	65,73,73	1.42	6 (9%)	76,113,113	1.46	8 (10%)
25	LHG	Q	310	-	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
25	LHG	R	314	-	41,41,48	0.96	3 (7%)	44,47,54	1.09	2 (4%)
22	CLA	q	305	22	60,68,73	1.51	7 (11%)	70,107,113	1.44	6 (8%)
25	LHG	c	521	-	48,48,48	0.90	4 (8%)	51,54,54	1.08	2 (3%)
27	NEX	R	301	1,22	38,46,46	1.03	2 (5%)	50,70,70	2.42	13 (26%)
22	CLA	C	508	-	65,73,73	1.51	9 (13%)	76,113,113	1.43	7 (9%)
22	CLA	v	303	-	50,58,73	1.67	7 (14%)	58,95,113	1.62	6 (10%)
22	CLA	p	302	-	65,73,73	1.43	7 (10%)	76,113,113	1.47	7 (9%)
22	CLA	B	617	-	65,73,73	1.41	8 (12%)	76,113,113	1.51	8 (10%)
23	LUT	u	310	-	42,43,43	0.78	0	51,60,60	1.60	10 (19%)
22	CLA	g	301	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	7 (9%)
26	CHL	3	312	-	48,56,74	2.38	17 (35%)	51,92,114	2.80	23 (45%)
31	BCR	k	101	-	41,41,41	4.73	25 (60%)	56,56,56	2.52	19 (33%)
22	CLA	U	304	-	60,68,73	1.50	9 (15%)	70,107,113	1.48	8 (11%)
25	LHG	D	406	3	45,45,48	0.92	4 (8%)	48,51,54	1.08	2 (4%)
22	CLA	P	303	-	65,73,73	1.45	8 (12%)	76,113,113	1.42	7 (9%)
22	CLA	b	603	-	65,73,73	1.45	9 (13%)	76,113,113	1.42	6 (7%)
26	CHL	6	316	18	66,74,74	1.89	17 (25%)	73,114,114	2.47	19 (26%)
25	LHG	d	406	3	48,48,48	0.90	4 (8%)	51,54,54	1.07	3 (5%)
22	CLA	r	608	-	49,57,73	1.68	6 (12%)	55,93,113	1.65	8 (14%)
22	CLA	C	510	-	65,73,73	1.53	9 (13%)	76,113,113	1.52	9 (11%)
22	CLA	4	302	-	65,73,73	1.50	7 (10%)	76,113,113	1.34	7 (9%)
22	CLA	Q	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
24	XAT	6	310	-	39,47,47	2.56	18 (46%)	54,74,74	11.74	17 (31%)
34	LMG	b	624	21	55,55,55	1.17	6 (10%)	63,63,63	1.07	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	CHL	s	314	-	46,54,74	2.29	16 (34%)	49,90,114	2.86	19 (38%)
22	CLA	c	513	-	65,73,73	1.43	9 (13%)	76,113,113	1.42	8 (10%)
22	CLA	b	616	21	65,73,73	1.43	9 (13%)	76,113,113	1.46	9 (11%)

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
23	LUT	s	310	19	-	2/29/67/67	0/2/2/2
22	CLA	U	306	-	1/1/14/20	10/31/109/115	-
22	CLA	u	302	-	1/1/15/20	14/37/115/115	-
26	CHL	U	314	-	3/3/16/26	10/20/118/137	-
31	BCR	X	201	-	-	9/29/63/63	0/2/2/2
26	CHL	6	301	-	3/3/20/26	20/39/137/137	-
22	CLA	c	511	20,8	1/1/15/20	18/37/115/115	-
26	CHL	u	317	18	3/3/20/26	11/39/137/137	-
26	CHL	G	316	-	3/3/19/26	13/33/131/137	-
26	CHL	2	314	-	3/3/16/26	9/18/116/137	-
22	CLA	g	305	22	1/1/14/20	10/31/109/115	-
22	CLA	n	306	-	1/1/14/20	9/31/109/115	-
37	HEM	e	101	4,17	-	3/12/54/54	-
22	CLA	C	512	20,8	1/1/15/20	20/37/115/115	-
23	LUT	2	310	-	-	1/29/67/67	0/2/2/2
24	XAT	p	312	-	-	7/31/93/93	0/4/4/4
26	CHL	V	318	-	3/3/20/26	17/39/137/137	-
22	CLA	3	306	22	1/1/14/20	16/31/109/115	-
22	CLA	5	302	-	1/1/15/20	16/37/115/115	-
26	CHL	P	318	-	3/3/20/26	17/39/137/137	-
23	LUT	5	309	-	-	4/29/67/67	0/2/2/2
23	LUT	u	309	-	-	2/29/67/67	0/2/2/2
22	CLA	Q	301	-	1/1/15/20	14/37/115/115	-
22	CLA	c	509	-	1/1/15/20	9/37/115/115	-
25	LHG	D	407	3	-	18/53/53/53	-
26	CHL	U	315	-	3/3/20/26	14/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	s	312	19	-	17/53/53/53	-
22	CLA	3	305	22	1/1/14/20	9/31/109/115	-
22	CLA	p	303	-	1/1/15/20	6/37/115/115	-
26	CHL	3	315	18	3/3/20/26	21/39/137/137	-
26	CHL	N	315	-	3/3/16/26	7/20/118/137	-
22	CLA	s	309	-	1/1/11/20	2/18/96/115	-
22	CLA	c	507	-	1/1/15/20	20/37/115/115	-
23	LUT	4	309	-	-	2/29/67/67	0/2/2/2
26	CHL	4	314	-	3/3/16/26	10/18/116/137	-
34	LMG	D	408	3	-	17/41/61/70	0/1/1/1
22	CLA	P	305	18	1/1/15/20	10/37/115/115	-
34	LMG	w	201	-	-	22/43/63/70	0/1/1/1
26	CHL	5	318	-	3/3/20/26	16/39/137/137	-
22	CLA	3	307	-	1/1/15/20	10/37/115/115	-
26	CHL	u	318	-	3/3/20/26	20/39/137/137	-
22	CLA	u	304	-	1/1/14/20	5/31/109/115	-
25	LHG	c	522	-	-	24/53/53/53	-
31	BCR	B	619	-	-	14/29/63/63	0/2/2/2
22	CLA	2	306	-	1/1/14/20	11/31/109/115	-
31	BCR	C	516	-	-	8/29/63/63	0/2/2/2
26	CHL	U	316	18	3/3/20/26	11/39/137/137	-
31	BCR	c	516	-	-	11/29/63/63	0/2/2/2
22	CLA	N	306	-	1/1/14/20	9/31/109/115	-
22	CLA	G	308	-	1/1/11/20	9/17/95/115	-
26	CHL	1	317	18	3/3/20/26	19/39/137/137	-
24	XAT	G	309	-	-	10/31/93/93	0/4/4/4
22	CLA	Q	305	22	1/1/14/20	16/31/109/115	-
27	NEX	5	319	-	-	8/27/83/83	0/3/3/3
23	LUT	S	310	-	-	2/29/67/67	0/2/2/2
22	CLA	B	616	21	1/1/15/20	6/37/115/115	-
22	CLA	u	307	-	1/1/15/20	14/37/115/115	-
22	CLA	Q	308	-	1/1/11/20	9/17/95/115	-
26	CHL	2	316	-	3/3/20/26	17/39/137/137	-
22	CLA	q	303	-	1/1/12/20	8/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	n	317	-	3/3/20/26	17/39/137/137	-
22	CLA	B	606	-	1/1/15/20	18/37/115/115	-
27	NEX	V	319	-	-	6/27/83/83	0/3/3/3
31	BCR	B	620	-	-	12/29/63/63	0/2/2/2
26	CHL	U	317	-	3/3/20/26	18/39/137/137	-
22	CLA	C	504	-	1/1/15/20	21/37/115/115	-
22	CLA	6	302	-	1/1/15/20	17/37/115/115	-
22	CLA	B	610	-	1/1/15/20	16/37/115/115	-
31	BCR	C	518	-	-	11/29/63/63	0/2/2/2
34	LMG	d	407	3	-	17/41/61/70	0/1/1/1
26	CHL	2	317	-	3/3/20/26	11/39/137/137	-
26	CHL	g	311	-	3/3/20/26	21/39/137/137	-
31	BCR	A	409	-	-	3/29/63/63	0/2/2/2
23	LUT	P	310	-	-	2/29/67/67	0/2/2/2
24	XAT	r	612	-	-	7/31/93/93	0/4/4/4
22	CLA	1	306	-	1/1/14/20	14/31/109/115	-
22	CLA	u	303	-	1/1/12/20	6/19/97/115	-
34	LMG	a	412	-	-	8/35/55/70	0/1/1/1
22	CLA	c	506	-	1/1/15/20	19/37/115/115	-
26	CHL	g	313	-	3/3/16/26	8/20/118/137	-
23	LUT	U	310	-	-	3/29/67/67	0/2/2/2
25	LHG	N	312	-	-	16/53/53/53	-
25	LHG	v	312	-	-	19/53/53/53	-
25	LHG	p	313	-	-	22/53/53/53	-
22	CLA	b	605	21	1/1/15/20	16/37/115/115	-
22	CLA	N	305	18	1/1/14/20	12/31/109/115	-
27	NEX	N	318	-	-	9/27/83/83	0/3/3/3
26	CHL	4	316	18	3/3/20/26	14/39/137/137	-
22	CLA	A	404	-	1/1/15/20	15/37/115/115	-
23	LUT	v	310	-	-	0/29/67/67	0/2/2/2
27	NEX	u	319	-	-	7/27/83/83	0/3/3/3
32	SQD	l	102	9	-	21/49/69/69	0/1/1/1
22	CLA	3	301	-	1/1/15/20	14/37/115/115	-
26	CHL	S	314	-	3/3/16/26	7/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	n	315	-	3/3/16/26	10/20/118/137	-
30	PHO	A	407	-	-	10/37/103/103	0/5/6/6
22	CLA	a	405	-	1/1/15/20	10/37/115/115	-
22	CLA	s	304	19	1/1/11/20	9/13/91/115	-
23	LUT	V	309	-	-	2/29/67/67	0/2/2/2
26	CHL	4	317	-	3/3/20/26	14/39/137/137	-
26	CHL	V	313	-	3/3/20/26	19/39/137/137	-
33	PL9	A	410	-	-	0/5/18/73	0/1/1/1
33	PL9	D	405	-	-	9/53/73/73	0/1/1/1
26	CHL	6	317	-	3/3/19/26	16/33/131/137	-
22	CLA	r	602	-	1/1/14/20	7/31/109/115	-
22	CLA	6	303	-	1/1/15/20	12/37/115/115	-
22	CLA	u	301	-	-	7/37/115/115	-
22	CLA	1	307	-	1/1/15/20	11/37/115/115	-
22	CLA	C	515	-	1/1/15/20	10/37/115/115	-
22	CLA	G	307	-	1/1/15/20	12/37/115/115	-
22	CLA	R	311	-	1/1/11/20	8/13/91/115	-
24	XAT	N	311	-	-	8/31/93/93	0/4/4/4
26	CHL	S	315	19	3/3/18/26	15/30/128/137	-
22	CLA	q	301	-	-	15/37/115/115	-
31	BCR	t	101	-	-	12/29/63/63	0/2/2/2
22	CLA	p	308	-	1/1/14/20	11/31/109/115	-
26	CHL	r	614	-	3/3/20/26	20/39/137/137	-
31	BCR	a	409	-	-	2/29/63/63	0/2/2/2
27	NEX	s	317	19	-	4/27/83/83	0/3/3/3
22	CLA	6	307	22	1/1/14/20	16/31/109/115	-
30	PHO	D	401	-	-	11/37/103/103	0/5/6/6
22	CLA	1	305	-	1/1/14/20	8/31/109/115	-
25	LHG	3	310	-	-	18/53/53/53	-
22	CLA	c	510	-	1/1/15/20	15/37/115/115	-
22	CLA	U	305	-	1/1/14/20	10/31/109/115	-
22	CLA	n	305	18	1/1/14/20	11/31/109/115	-
22	CLA	R	307	-	1/1/15/20	16/37/115/115	-
22	CLA	s	306	-	1/1/13/20	5/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	S	312	19	-	17/53/53/53	-
22	CLA	2	307	-	1/1/14/20	8/31/109/115	-
22	CLA	S	305	-	1/1/13/20	6/25/103/115	-
22	CLA	c	503	-	1/1/15/20	20/37/115/115	-
26	CHL	1	316	-	3/3/20/26	21/39/137/137	-
22	CLA	V	305	-	1/1/14/20	8/31/109/115	-
22	CLA	G	303	-	1/1/12/20	10/19/97/115	-
22	CLA	S	309	-	1/1/11/20	2/18/96/115	-
25	LHG	C	524	-	-	13/53/53/53	-
31	BCR	c	515	-	-	14/29/63/63	0/2/2/2
26	CHL	5	313	18	3/3/20/26	21/39/137/137	-
22	CLA	b	602	-	1/1/15/20	17/37/115/115	-
26	CHL	q	311	-	3/3/20/26	17/39/137/137	-
37	HEM	E	101	4,17	-	2/12/54/54	-
26	CHL	u	313	-	3/3/20/26	14/39/137/137	-
25	LHG	c	523	-	-	17/53/53/53	-
22	CLA	1	308	-	1/1/11/20	11/17/95/115	-
31	BCR	T	101	-	-	12/29/63/63	0/2/2/2
26	CHL	g	312	-	3/3/16/26	10/18/116/137	-
31	BCR	b	620	-	-	12/29/63/63	0/2/2/2
22	CLA	4	308	-	1/1/11/20	11/17/95/115	-
33	PL9	d	404	-	-	9/53/73/73	0/1/1/1
22	CLA	q	307	-	1/1/15/20	15/37/115/115	-
22	CLA	b	610	-	1/1/15/20	16/37/115/115	-
30	PHO	a	407	-	-	10/37/103/103	0/5/6/6
22	CLA	b	614	-	1/1/15/20	16/37/115/115	-
23	LUT	U	309	-	-	4/29/67/67	0/2/2/2
22	CLA	6	309	-	1/1/11/20	10/17/95/115	-
22	CLA	3	303	-	1/1/12/20	10/19/97/115	-
24	XAT	n	311	-	-	9/31/93/93	0/4/4/4
25	LHG	n	312	-	-	19/53/53/53	-
22	CLA	V	303	-	1/1/12/20	6/19/97/115	-
26	CHL	p	319	-	3/3/20/26	15/39/137/137	-
27	NEX	U	318	-	-	3/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	s	305	-	1/1/13/20	5/25/103/115	-
22	CLA	3	304	18	1/1/14/20	15/36/114/115	-
22	CLA	x	201	14	1/1/15/20	10/37/115/115	-
22	CLA	u	308	-	1/1/11/20	10/17/95/115	-
22	CLA	g	304	18	1/1/14/20	8/36/114/115	-
22	CLA	v	304	-	1/1/14/20	14/31/109/115	-
22	CLA	G	301	-	1/1/15/20	19/37/115/115	-
22	CLA	B	604	-	1/1/15/20	15/37/115/115	-
22	CLA	c	514	-	1/1/15/20	9/37/115/115	-
25	LHG	2	312	-	-	24/53/53/53	-
22	CLA	q	308	-	1/1/11/20	11/17/95/115	-
22	CLA	C	511	-	1/1/15/20	14/37/115/115	-
34	LMG	C	521	-	-	19/46/66/70	0/1/1/1
22	CLA	b	615	-	1/1/15/20	18/37/115/115	-
22	CLA	b	606	-	1/1/15/20	18/37/115/115	-
22	CLA	6	305	18	1/1/14/20	19/36/114/115	-
22	CLA	v	306	-	1/1/14/20	13/31/109/115	-
22	CLA	C	507	-	1/1/15/20	19/37/115/115	-
30	PHO	d	401	-	-	11/37/103/103	0/5/6/6
22	CLA	C	509	20	1/1/15/20	14/37/115/115	-
22	CLA	b	613	-	1/1/15/20	16/37/115/115	-
26	CHL	r	616	-	3/3/19/26	16/33/131/137	-
26	CHL	s	313	-	3/3/16/26	7/15/113/137	-
22	CLA	B	602	-	1/1/15/20	19/37/115/115	-
26	CHL	u	314	-	3/3/16/26	11/18/116/137	-
22	CLA	R	305	-	1/1/11/20	7/17/95/115	-
26	CHL	s	316	-	3/3/16/26	11/15/113/137	-
34	LMG	A	411	-	-	11/35/55/70	0/1/1/1
22	CLA	b	611	-	1/1/15/20	14/37/115/115	-
26	CHL	P	317	-	3/3/20/26	15/39/137/137	-
26	CHL	N	316	-	3/3/20/26	17/39/137/137	-
22	CLA	r	603	-	1/1/14/20	11/31/109/115	-
26	CHL	4	315	-	3/3/16/26	6/20/118/137	-
26	CHL	q	314	18	3/3/20/26	23/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	g	314	-	3/3/20/26	20/39/137/137	-
32	SQD	m	101	-	-	21/37/57/69	0/1/1/1
22	CLA	6	308	-	1/1/15/20	10/37/115/115	-
22	CLA	r	605	-	1/1/13/20	7/29/107/115	-
22	CLA	U	303	-	1/1/12/20	5/19/97/115	-
25	LHG	d	405	3	-	26/50/50/53	-
25	LHG	r	613	-	-	19/46/46/53	-
22	CLA	s	301	19	1/1/14/20	16/33/111/115	-
22	CLA	r	606	-	1/1/15/20	16/37/115/115	-
22	CLA	S	303	19	1/1/12/20	6/19/97/115	-
22	CLA	G	305	22	1/1/14/20	10/31/109/115	-
26	CHL	R	317	-	3/3/19/26	16/33/131/137	-
22	CLA	2	308	-	1/1/11/20	6/17/95/115	-
22	CLA	b	607	-	-	13/37/115/115	-
26	CHL	n	314	-	3/3/16/26	10/18/116/137	-
23	LUT	N	310	-	-	1/29/67/67	0/2/2/2
26	CHL	6	314	-	3/3/16/26	11/20/118/137	-
22	CLA	S	304	19	1/1/11/20	9/13/91/115	-
34	LMG	B	621	-	-	20/46/66/70	0/1/1/1
22	CLA	N	301	-	1/1/15/20	13/37/115/115	-
22	CLA	1	302	-	1/1/15/20	14/37/115/115	-
22	CLA	R	304	-	1/1/14/20	11/31/109/115	-
22	CLA	n	302	-	1/1/15/20	16/37/115/115	-
32	SQD	A	412	-	-	21/49/69/69	0/1/1/1
34	LMG	W	201	-	-	21/43/63/70	0/1/1/1
25	LHG	P	313	-	-	24/53/53/53	-
26	CHL	p	317	-	3/3/20/26	14/39/137/137	-
26	CHL	v	316	-	3/3/20/26	15/39/137/137	-
26	CHL	q	313	-	3/3/16/26	9/20/118/137	-
22	CLA	v	305	-	1/1/14/20	7/31/109/115	-
22	CLA	s	307	-	1/1/11/20	6/18/96/115	-
25	LHG	A	413	2	-	27/47/47/53	-
27	NEX	S	317	19	-	4/27/83/83	0/3/3/3
24	XAT	3	309	-	-	8/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	V	317	18	3/3/20/26	14/39/137/137	-
22	CLA	B	614	-	1/1/15/20	14/37/115/115	-
22	CLA	P	304	-	1/1/12/20	10/19/97/115	-
22	CLA	3	302	-	1/1/15/20	13/37/115/115	-
22	CLA	5	303	-	1/1/12/20	5/19/97/115	-
26	CHL	Q	311	-	3/3/20/26	19/39/137/137	-
22	CLA	S	306	-	1/1/13/20	6/27/105/115	-
26	CHL	G	314	-	3/3/20/26	15/39/137/137	-
22	CLA	V	302	-	1/1/15/20	12/37/115/115	-
22	CLA	r	607	1	1/1/11/20	9/18/96/115	-
22	CLA	q	304	18	1/1/14/20	15/36/114/115	-
22	CLA	N	307	-	1/1/14/20	13/31/109/115	-
26	CHL	g	315	18	3/3/20/26	23/39/137/137	-
26	CHL	5	314	-	3/3/16/26	11/18/116/137	-
22	CLA	V	307	-	1/1/15/20	8/37/115/115	-
22	CLA	X	202	14	1/1/15/20	9/37/115/115	-
27	NEX	P	301	18	-	3/27/83/83	0/3/3/3
22	CLA	P	307	-	1/1/14/20	12/31/109/115	-
26	CHL	r	615	-	3/3/18/26	10/27/125/137	-
26	CHL	S	316	-	3/3/16/26	11/15/113/137	-
23	LUT	5	310	-	-	1/29/67/67	0/2/2/2
36	DGD	c	519	-	-	21/49/89/95	0/2/2/2
34	LMG	C	502	-	-	26/46/66/70	0/1/1/1
33	PL9	a	411	-	-	0/5/18/73	0/1/1/1
24	XAT	v	311	-	-	11/31/93/93	0/4/4/4
22	CLA	d	402	3	1/1/15/20	13/37/115/115	-
22	CLA	P	306	18	1/1/14/20	10/31/109/115	-
22	CLA	v	301	-	-	11/37/115/115	-
22	CLA	S	301	19	1/1/14/20	16/33/111/115	-
26	CHL	p	315	-	3/3/16/26	8/18/116/137	-
26	CHL	n	316	-	3/3/20/26	25/39/137/137	-
26	CHL	P	316	-	3/3/16/26	7/20/118/137	-
22	CLA	P	302	-	1/1/15/20	16/37/115/115	-
22	CLA	g	306	22	1/1/14/20	13/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	R	310	-	1/1/14/20	10/31/109/115	-
22	CLA	B	605	21	1/1/15/20	18/37/115/115	-
26	CHL	G	315	18	3/3/20/26	19/39/137/137	-
32	SQD	a	413	-	-	22/49/69/69	0/1/1/1
24	XAT	P	312	-	-	8/31/93/93	0/4/4/4
26	CHL	v	315	-	3/3/16/26	8/20/118/137	-
25	LHG	5	312	-	-	23/53/53/53	-
22	CLA	5	307	-	1/1/14/20	10/31/109/115	-
34	LMG	b	621	-	-	24/46/66/70	0/1/1/1
26	CHL	U	313	-	3/3/20/26	15/39/137/137	-
25	LHG	q	310	-	-	22/53/53/53	-
31	BCR	d	403	3	-	12/29/63/63	0/2/2/2
22	CLA	b	604	-	1/1/15/20	16/37/115/115	-
26	CHL	g	316	-	3/3/19/26	15/33/131/137	-
24	XAT	4	311	-	-	8/31/93/93	0/4/4/4
22	CLA	b	609	-	1/1/15/20	12/37/115/115	-
22	CLA	U	307	-	1/1/15/20	15/37/115/115	-
22	CLA	3	308	-	1/1/11/20	10/17/95/115	-
22	CLA	R	302	27	1/1/11/20	8/18/96/115	-
22	CLA	5	306	-	1/1/14/20	13/31/109/115	-
22	CLA	R	303	-	1/1/14/20	7/31/109/115	-
22	CLA	S	307	-	1/1/11/20	6/18/96/115	-
22	CLA	U	301	-	-	8/37/115/115	-
22	CLA	n	301	-	1/1/15/20	13/37/115/115	-
22	CLA	c	504	-	1/1/15/20	17/37/115/115	-
26	CHL	3	313	-	3/3/16/26	14/20/118/137	-
26	CHL	G	312	-	3/3/16/26	6/18/116/137	-
22	CLA	c	505	-	1/1/15/20	9/37/115/115	-
22	CLA	b	608	-	1/1/15/20	11/37/115/115	-
22	CLA	4	305	-	1/1/14/20	6/31/109/115	-
22	CLA	V	301	-	-	12/37/115/115	-
36	DGD	C	520	-	-	31/51/91/95	0/2/2/2
22	CLA	1	301	-	1/1/15/20	7/37/115/115	-
26	CHL	5	316	-	3/3/20/26	18/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	n	318	-	3/3/20/26	23/39/137/137	-
31	BCR	x	202	-	-	9/29/63/63	0/2/2/2
26	CHL	3	314	-	3/3/20/26	16/39/137/137	-
22	CLA	r	604	-	1/1/11/20	7/17/95/115	-
26	CHL	1	318	-	3/3/20/26	14/39/137/137	-
27	NEX	p	301	18	-	3/27/83/83	0/3/3/3
27	NEX	n	319	-	-	7/27/83/83	0/3/3/3
22	CLA	N	308	-	1/1/11/20	14/17/95/115	-
22	CLA	v	302	-	1/1/15/20	12/37/115/115	-
22	CLA	B	613	-	1/1/15/20	16/37/115/115	-
22	CLA	n	307	-	1/1/14/20	11/31/109/115	-
22	CLA	V	308	-	1/1/11/20	9/17/95/115	-
24	XAT	g	309	-	-	10/31/93/93	0/4/4/4
25	LHG	6	311	-	-	19/53/53/53	-
25	LHG	V	312	-	-	18/53/53/53	-
32	SQD	L	102	9	-	21/49/69/69	0/1/1/1
26	CHL	N	317	-	3/3/20/26	20/39/137/137	-
26	CHL	v	317	18	3/3/20/26	12/39/137/137	-
26	CHL	N	313	-	3/3/20/26	13/39/137/137	-
26	CHL	Q	313	-	3/3/16/26	9/20/118/137	-
25	LHG	G	310	-	-	19/53/53/53	-
22	CLA	B	609	-	1/1/15/20	12/37/115/115	-
26	CHL	U	319	-	3/3/20/26	20/39/137/137	-
26	CHL	Q	314	-	3/3/20/26	20/39/137/137	-
24	XAT	U	311	-	-	7/31/93/93	0/4/4/4
36	DGD	c	518	-	-	31/51/91/95	0/2/2/2
23	LUT	v	309	-	-	2/29/67/67	0/2/2/2
22	CLA	R	309	-	1/1/11/20	7/18/96/115	-
22	CLA	s	302	-	1/1/11/20	6/13/91/115	-
22	CLA	s	303	19	1/1/12/20	6/19/97/115	-
24	XAT	2	311	-	-	6/31/93/93	0/4/4/4
36	DGD	A	414	-	-	22/48/88/95	0/2/2/2
26	CHL	Q	312	-	3/3/16/26	14/18/116/137	-
27	NEX	r	617	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	308	-	1/1/11/20	3/17/95/115	-
34	LMG	c	501	-	-	25/46/66/70	0/1/1/1
23	LUT	P	311	-	-	3/29/67/67	0/2/2/2
22	CLA	B	608	-	1/1/15/20	14/37/115/115	-
22	CLA	U	308	-	1/1/11/20	10/17/95/115	-
22	CLA	N	302	-	1/1/15/20	20/37/115/115	-
26	CHL	3	316	-	3/3/19/26	16/33/131/137	-
26	CHL	2	315	-	3/3/16/26	5/20/118/137	-
26	CHL	1	313	-	3/3/20/26	12/39/137/137	-
31	BCR	z	101	-	-	8/29/63/63	0/2/2/2
24	XAT	q	309	-	-	12/31/93/93	0/4/4/4
22	CLA	G	304	18	1/1/14/20	10/36/114/115	-
26	CHL	v	318	-	3/3/20/26	20/39/137/137	-
22	CLA	N	304	18	1/1/15/20	17/37/115/115	-
23	LUT	n	309	-	-	0/29/67/67	0/2/2/2
27	NEX	v	319	-	-	4/27/83/83	0/3/3/3
26	CHL	5	315	-	3/3/16/26	6/20/118/137	-
26	CHL	V	314	-	3/3/16/26	11/18/116/137	-
26	CHL	S	313	-	3/3/16/26	7/15/113/137	-
22	CLA	A	406	-	1/1/12/20	7/19/97/115	-
26	CHL	1	314	22	3/3/16/26	14/18/116/137	-
25	LHG	B	622	-	-	21/51/51/53	-
25	LHG	b	622	-	-	22/51/51/53	-
22	CLA	b	612	-	1/1/15/20	13/37/115/115	-
22	CLA	6	304	-	1/1/12/20	11/19/97/115	-
22	CLA	g	302	-	1/1/15/20	13/37/115/115	-
22	CLA	g	303	-	1/1/12/20	11/19/97/115	-
23	LUT	1	309	-	-	2/29/67/67	0/2/2/2
25	LHG	1	312	-	-	14/53/53/53	-
22	CLA	v	307	-	1/1/15/20	10/37/115/115	-
34	LMG	B	624	21	-	21/50/70/70	0/1/1/1
32	SQD	C	501	-	-	27/45/65/69	0/1/1/1
26	CHL	G	311	-	3/3/20/26	18/39/137/137	-
22	CLA	B	603	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	G	306	22	1/1/14/20	9/31/109/115	-
22	CLA	n	308	-	1/1/11/20	11/17/95/115	-
23	LUT	p	311	-	-	3/29/67/67	0/2/2/2
22	CLA	s	308	-	1/1/13/20	7/25/103/115	-
22	CLA	r	609	26	1/1/14/20	10/31/109/115	-
22	CLA	A	408	-	1/1/14/20	12/31/109/115	-
22	CLA	2	305	18	1/1/14/20	11/31/109/115	-
25	LHG	C	523	-	-	24/53/53/53	-
36	DGD	c	517	-	-	22/44/84/95	0/2/2/2
31	BCR	b	618	-	-	8/29/63/63	0/2/2/2
22	CLA	U	302	-	1/1/15/20	12/37/115/115	-
26	CHL	n	313	18	3/3/20/26	19/39/137/137	-
22	CLA	4	303	-	1/1/12/20	9/19/97/115	-
22	CLA	R	308	1	1/1/11/20	10/18/96/115	-
22	CLA	2	302	-	1/1/15/20	14/37/115/115	-
25	LHG	b	623	21	-	24/53/53/53	-
22	CLA	n	304	18	1/1/15/20	14/37/115/115	-
23	LUT	2	309	-	-	4/29/67/67	0/2/2/2
23	LUT	1	310	-	-	0/29/67/67	0/2/2/2
22	CLA	B	611	-	1/1/15/20	14/37/115/115	-
22	CLA	V	306	-	1/1/14/20	7/31/109/115	-
36	DGD	b	601	21	-	21/51/91/95	0/2/2/2
22	CLA	g	307	-	1/1/15/20	12/37/115/115	-
22	CLA	4	306	-	1/1/14/20	16/31/109/115	-
22	CLA	c	508	20	1/1/15/20	14/37/115/115	-
24	XAT	1	311	-	-	7/31/93/93	0/4/4/4
22	CLA	Q	303	-	1/1/12/20	10/19/97/115	-
22	CLA	D	403	3	1/1/15/20	15/37/115/115	-
26	CHL	r	619	1	3/3/16/26	8/18/116/137	-
31	BCR	b	619	-	-	14/29/63/63	0/2/2/2
26	CHL	P	319	-	3/3/20/26	20/39/137/137	-
26	CHL	V	316	-	3/3/20/26	17/39/137/137	-
36	DGD	C	519	-	-	23/44/84/95	0/2/2/2
26	CHL	N	314	-	3/3/16/26	10/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	512	-	1/1/15/20	9/37/115/115	-
23	LUT	n	310	-	-	3/29/67/67	0/2/2/2
23	LUT	r	611	1	-	2/29/67/67	0/2/2/2
26	CHL	P	315	-	3/3/16/26	9/18/116/137	-
22	CLA	Q	306	22	1/1/14/20	11/31/109/115	-
22	CLA	5	304	18	1/1/15/20	12/37/115/115	-
22	CLA	B	615	-	1/1/15/20	17/37/115/115	-
22	CLA	C	513	-	1/1/15/20	10/37/115/115	-
22	CLA	C	506	-	1/1/15/20	13/37/115/115	-
23	LUT	S	311	-	-	8/29/67/67	0/2/2/2
26	CHL	G	313	-	3/3/16/26	7/20/118/137	-
22	CLA	4	307	-	1/1/15/20	7/37/115/115	-
22	CLA	r	610	-	1/1/11/20	8/13/91/115	-
22	CLA	C	514	-	1/1/15/20	12/37/115/115	-
26	CHL	R	315	-	3/3/20/26	20/39/137/137	-
26	CHL	6	313	-	3/3/16/26	8/18/116/137	-
26	CHL	Q	315	18	3/3/20/26	20/39/137/137	-
22	CLA	S	302	-	1/1/11/20	6/13/91/115	-
26	CHL	3	311	-	3/3/20/26	16/39/137/137	-
25	LHG	B	623	21	-	21/53/53/53	-
27	NEX	u	320	-	-	2/27/83/83	0/3/3/3
24	XAT	V	311	-	-	11/31/93/93	0/4/4/4
22	CLA	v	308	-	1/1/11/20	9/17/95/115	-
22	CLA	N	303	-	1/1/12/20	5/19/97/115	-
22	CLA	2	304	18	1/1/15/20	9/37/115/115	-
22	CLA	p	306	18	1/1/14/20	11/31/109/115	-
22	CLA	S	308	-	1/1/13/20	7/25/103/115	-
22	CLA	c	502	-	1/1/15/20	8/37/115/115	-
36	DGD	B	601	21	-	22/51/91/95	0/2/2/2
22	CLA	4	301	-	1/1/15/20	7/37/115/115	-
32	SQD	M	101	-	-	22/37/57/69	0/1/1/1
26	CHL	q	312	-	3/3/16/26	12/18/116/137	-
26	CHL	v	313	-	3/3/20/26	16/39/137/137	-
22	CLA	2	303	-	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	p	318	-	3/3/20/26	17/39/137/137	-
22	CLA	q	306	22	1/1/14/20	12/31/109/115	-
24	XAT	R	313	-	-	8/31/93/93	0/4/4/4
26	CHL	v	314	-	3/3/16/26	12/18/116/137	-
26	CHL	V	315	-	3/3/16/26	6/20/118/137	-
23	LUT	4	310	-	-	0/29/67/67	0/2/2/2
36	DGD	J	101	-	-	21/49/89/95	0/2/2/2
22	CLA	R	306	-	1/1/13/20	7/29/107/115	-
22	CLA	q	302	-	1/1/15/20	11/37/115/115	-
22	CLA	p	307	-	1/1/14/20	7/31/109/115	-
22	CLA	C	503	-	1/1/15/20	7/37/115/115	-
26	CHL	Q	316	-	3/3/19/26	12/33/131/137	-
22	CLA	g	308	-	1/1/11/20	8/17/95/115	-
25	LHG	a	415	2	-	26/47/47/53	-
25	LHG	l	101	-	-	27/53/53/53	-
31	BCR	K	101	-	-	13/29/63/63	0/2/2/2
31	BCR	D	404	3	-	13/29/63/63	0/2/2/2
22	CLA	P	309	-	1/1/11/20	10/17/95/115	-
22	CLA	p	309	-	1/1/11/20	6/17/95/115	-
25	LHG	U	312	-	-	29/53/53/53	-
22	CLA	n	303	-	1/1/12/20	7/19/97/115	-
25	LHG	4	312	-	-	18/53/53/53	-
22	CLA	5	305	18	1/1/14/20	11/31/109/115	-
27	NEX	2	319	-	-	7/27/83/83	0/3/3/3
27	NEX	r	618	1,22	-	7/27/83/83	0/3/3/3
31	BCR	C	517	-	-	14/29/63/63	0/2/2/2
34	LMG	c	520	-	-	21/46/66/70	0/1/1/1
22	CLA	B	607	-	1/1/15/20	13/37/115/115	-
22	CLA	C	505	-	1/1/15/20	17/37/115/115	-
32	SQD	a	410	-	-	25/45/65/69	0/1/1/1
22	CLA	P	308	-	1/1/14/20	13/31/109/115	-
22	CLA	2	301	-	1/1/15/20	11/37/115/115	-
22	CLA	a	406	-	1/1/12/20	8/19/97/115	-
26	CHL	p	320	-	3/3/20/26	18/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	u	306	-	1/1/14/20	10/31/109/115	-
22	CLA	p	304	-	1/1/12/20	10/19/97/115	-
24	XAT	Q	309	-	-	10/31/93/93	0/4/4/4
22	CLA	G	302	-	1/1/15/20	17/37/115/115	-
26	CHL	1	315	-	3/3/16/26	6/20/118/137	-
26	CHL	R	316	-	3/3/18/26	11/27/125/137	-
22	CLA	1	304	-	1/1/14/20	7/31/109/115	-
26	CHL	2	313	18	3/3/20/26	20/39/137/137	-
26	CHL	2	318	-	3/3/20/26	18/39/137/137	-
31	BCR	B	618	-	-	8/29/63/63	0/2/2/2
22	CLA	u	305	-	1/1/14/20	12/31/109/115	-
22	CLA	1	303	-	1/1/12/20	8/19/97/115	-
22	CLA	Q	304	18	1/1/14/20	14/36/114/115	-
22	CLA	a	408	-	1/1/14/20	11/31/109/115	-
26	CHL	6	312	-	3/3/20/26	16/39/137/137	-
26	CHL	s	315	19	3/3/18/26	15/30/128/137	-
23	LUT	p	310	-	-	2/29/67/67	0/2/2/2
26	CHL	p	316	-	3/3/16/26	7/20/118/137	-
26	CHL	q	315	-	3/3/19/26	12/33/131/137	-
23	LUT	N	309	-	-	2/29/67/67	0/2/2/2
26	CHL	P	314	18	3/3/20/26	14/39/137/137	-
26	CHL	p	314	18	3/3/20/26	13/39/137/137	-
23	LUT	s	311	-	-	7/29/67/67	0/2/2/2
22	CLA	6	306	22	1/1/14/20	13/31/109/115	-
22	CLA	B	612	-	1/1/15/20	15/37/115/115	-
22	CLA	b	617	21	1/1/15/20	12/37/115/115	-
22	CLA	r	601	27	1/1/11/20	7/18/96/115	-
26	CHL	5	317	-	3/3/20/26	15/39/137/137	-
25	LHG	g	310	-	-	20/53/53/53	-
24	XAT	u	311	-	-	7/31/93/93	0/4/4/4
23	LUT	R	312	-	-	4/29/67/67	0/2/2/2
25	LHG	C	522	-	-	16/53/53/53	-
26	CHL	4	313	-	3/3/20/26	16/39/137/137	-
22	CLA	a	404	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	V	304	-	1/1/14/20	12/31/109/115	-
25	LHG	u	312	-	-	25/53/53/53	-
26	CHL	6	315	-	3/3/20/26	15/39/137/137	-
22	CLA	5	301	-	1/1/15/20	10/37/115/115	-
22	CLA	Q	302	-	1/1/15/20	11/37/115/115	-
36	DGD	a	416	-	-	24/48/88/95	0/2/2/2
26	CHL	u	316	-	3/3/20/26	23/39/137/137	-
24	XAT	5	311	-	-	6/31/93/93	0/4/4/4
22	CLA	4	304	-	1/1/14/20	9/31/109/115	-
26	CHL	u	315	-	3/3/16/26	8/20/118/137	-
25	LHG	L	101	-	-	28/53/53/53	-
22	CLA	A	405	-	1/1/15/20	10/37/115/115	-
23	LUT	V	310	-	-	0/29/67/67	0/2/2/2
22	CLA	p	305	18	1/1/15/20	11/37/115/115	-
25	LHG	Q	310	-	-	19/53/53/53	-
25	LHG	R	314	-	-	24/46/46/53	-
22	CLA	q	305	22	1/1/14/20	12/31/109/115	-
25	LHG	c	521	-	-	14/53/53/53	-
27	NEX	R	301	1,22	-	10/27/83/83	0/3/3/3
22	CLA	C	508	-	1/1/15/20	20/37/115/115	-
22	CLA	v	303	-	1/1/12/20	7/19/97/115	-
22	CLA	p	302	-	1/1/15/20	15/37/115/115	-
22	CLA	B	617	-	1/1/15/20	11/37/115/115	-
23	LUT	u	310	-	-	2/29/67/67	0/2/2/2
22	CLA	g	301	-	1/1/15/20	14/37/115/115	-
26	CHL	3	312	-	3/3/16/26	8/18/116/137	-
31	BCR	k	101	-	-	13/29/63/63	0/2/2/2
22	CLA	U	304	-	1/1/14/20	5/31/109/115	-
25	LHG	D	406	3	-	28/50/50/53	-
22	CLA	P	303	-	1/1/15/20	13/37/115/115	-
22	CLA	b	603	-	1/1/15/20	12/37/115/115	-
26	CHL	6	316	18	3/3/20/26	23/39/137/137	-
25	LHG	d	406	3	-	19/53/53/53	-
22	CLA	r	608	-	1/1/11/20	7/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	510	-	1/1/15/20	8/37/115/115	-
22	CLA	4	302	-	1/1/15/20	15/37/115/115	-
22	CLA	Q	307	-	1/1/15/20	10/37/115/115	-
24	XAT	6	310	-	-	8/31/93/93	0/4/4/4
34	LMG	b	624	21	-	22/50/70/70	0/1/1/1
26	CHL	s	314	-	3/3/16/26	6/15/113/137	-
22	CLA	c	513	-	1/1/15/20	8/37/115/115	-
22	CLA	b	616	21	1/1/15/20	9/37/115/115	-

The worst 5 of 5049 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	409	BCR	C26-C25	15.51	1.61	1.34
31	a	409	BCR	C26-C25	15.51	1.61	1.34
31	b	619	BCR	C5-C6	15.49	1.61	1.34
31	B	619	BCR	C5-C6	15.47	1.61	1.34
31	x	202	BCR	C5-C6	15.45	1.61	1.34

The worst 5 of 6389 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	311	XAT	O4-C5-C4	60.27	158.66	113.38
24	2	311	XAT	O4-C5-C4	60.01	158.46	113.38
24	n	311	XAT	O24-C25-C24	59.81	158.31	113.38
24	N	311	XAT	O24-C25-C24	59.80	158.31	113.38
24	4	311	XAT	O4-C5-C4	59.80	158.31	113.38

5 of 612 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	r	601	CLA	ND
22	r	602	CLA	ND
22	r	603	CLA	ND
22	r	604	CLA	ND
22	r	605	CLA	ND

5 of 6713 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	r	604	CLA	C1A-C2A-CAA-CBA

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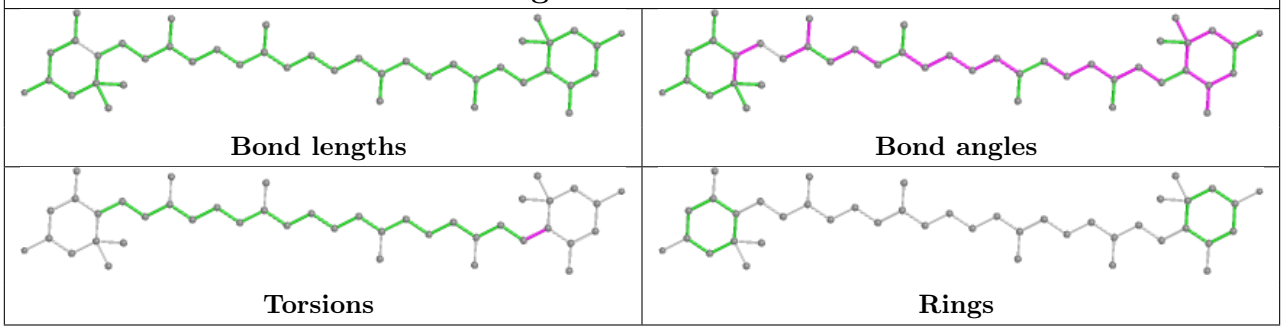
Mol	Chain	Res	Type	Atoms
22	r	606	CLA	CBD-CGD-O2D-CED
22	r	606	CLA	C2-C3-C5-C6
22	r	606	CLA	C4-C3-C5-C6
22	r	607	CLA	C1A-C2A-CAA-CBA

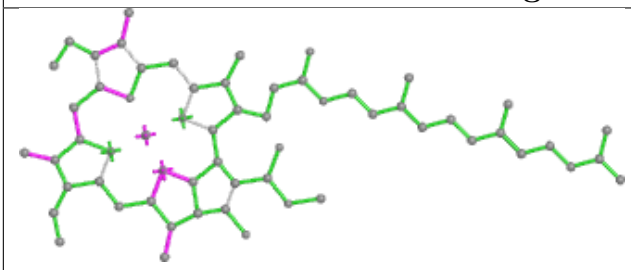
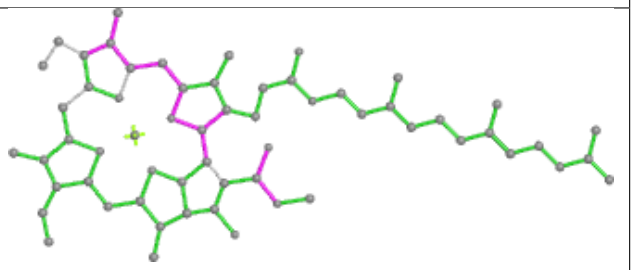
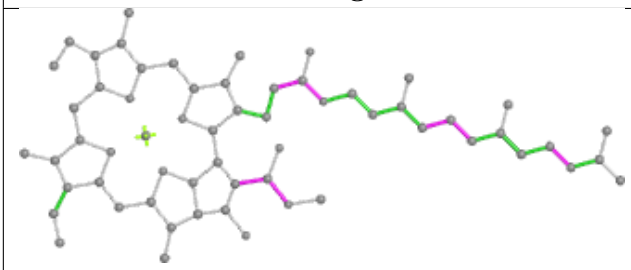
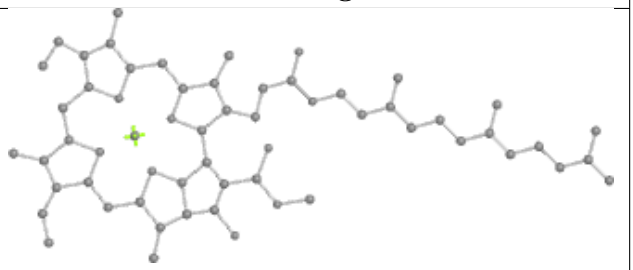
There are no ring outliers.

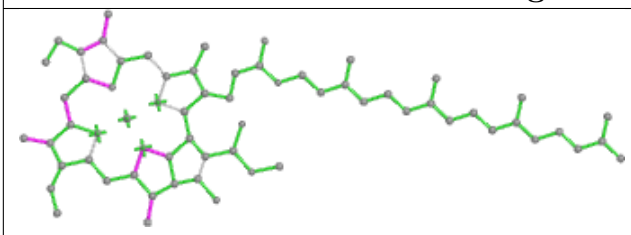
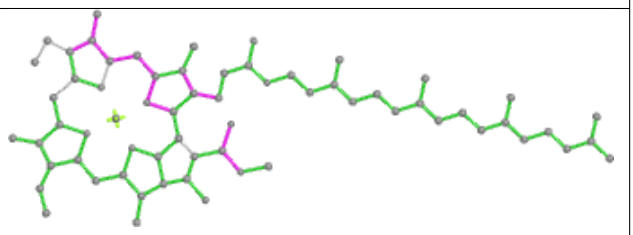
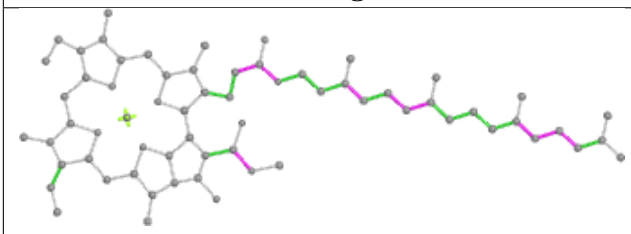
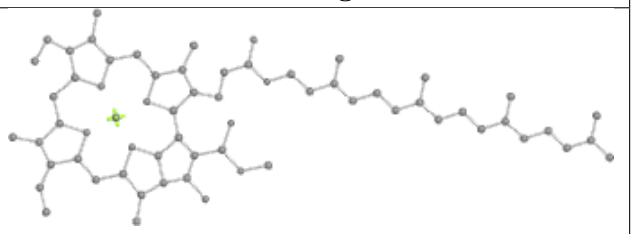
No monomer is involved in short contacts.

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.

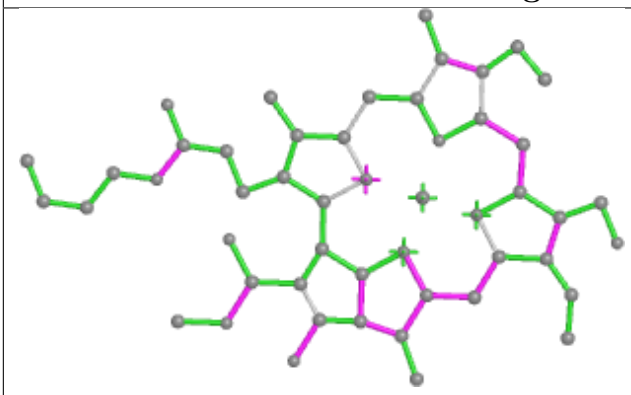
Ligand LUT s 310



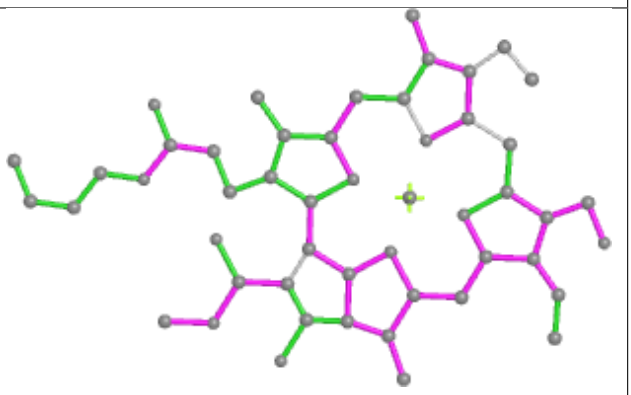
Ligand CLA U 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA u 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

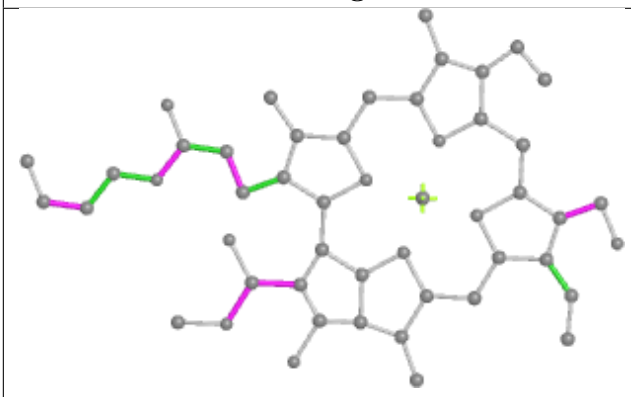
Ligand CHL U 314



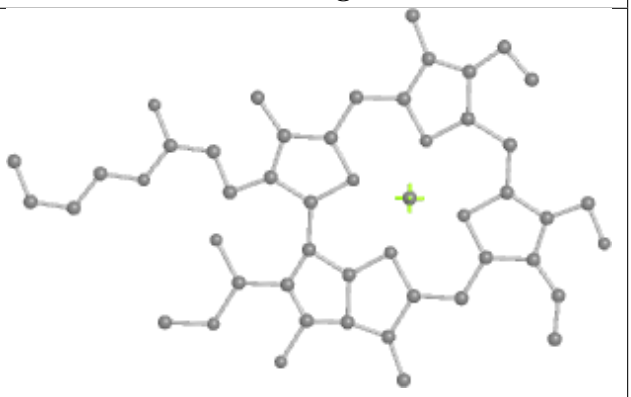
Bond lengths



Bond angles

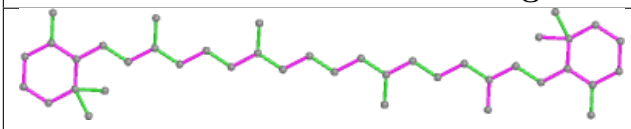


Torsions

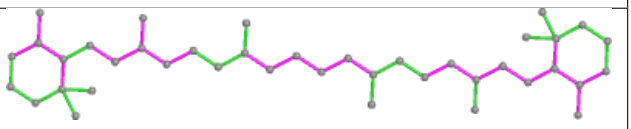


Rings

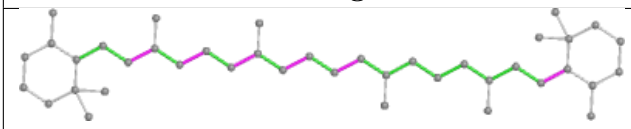
Ligand BCR X 201



Bond lengths



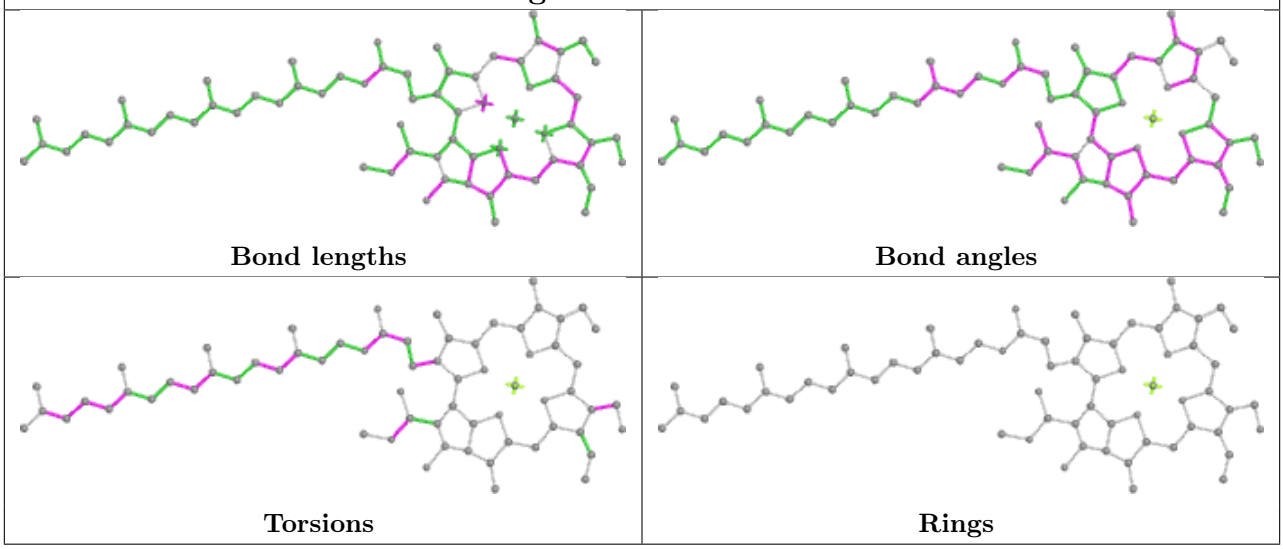
Bond angles



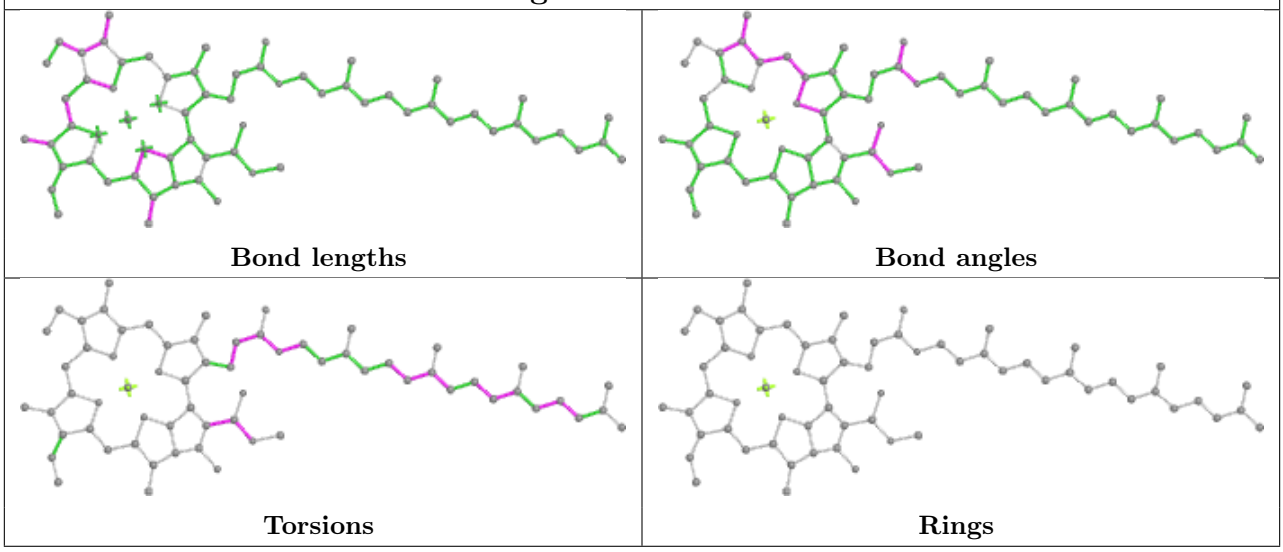
Torsions

Rings

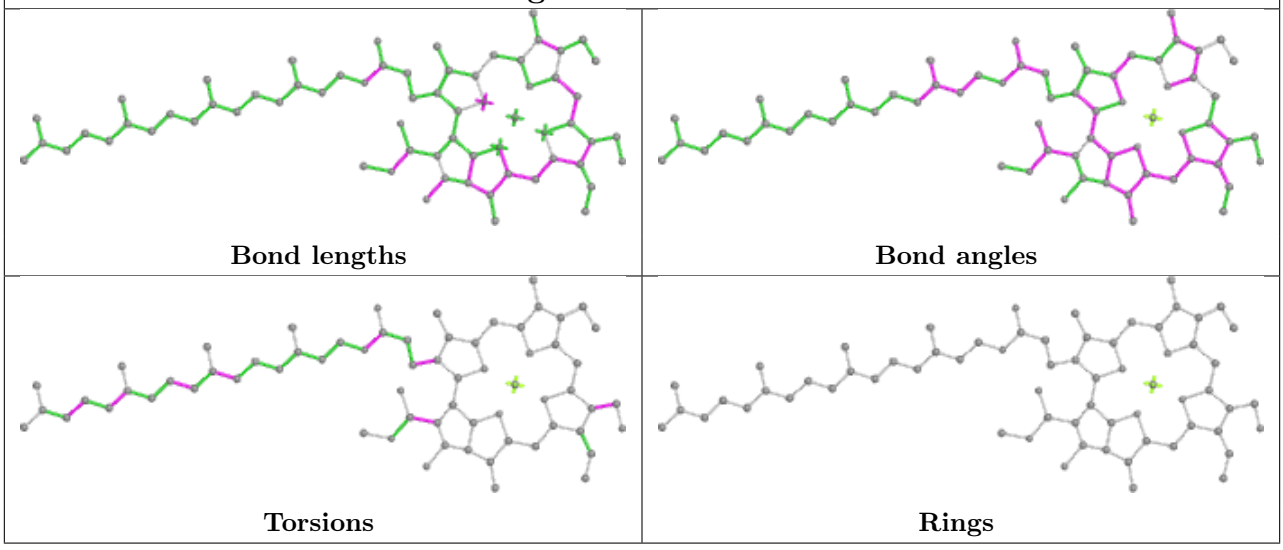
Ligand CHL 6 301



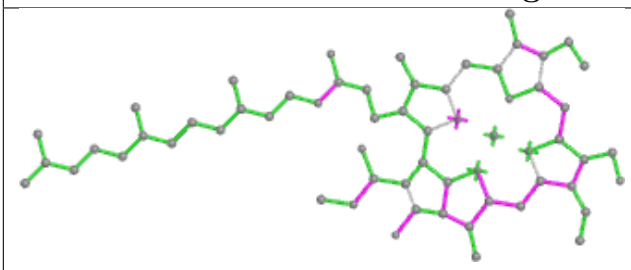
Ligand CLA c 511



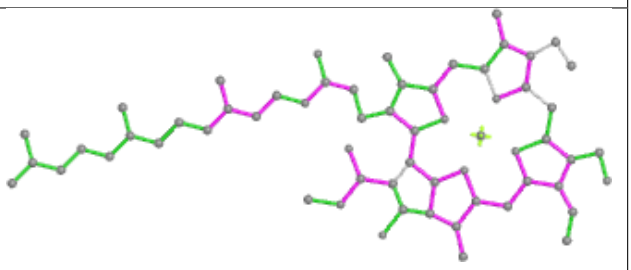
Ligand CHL u 317



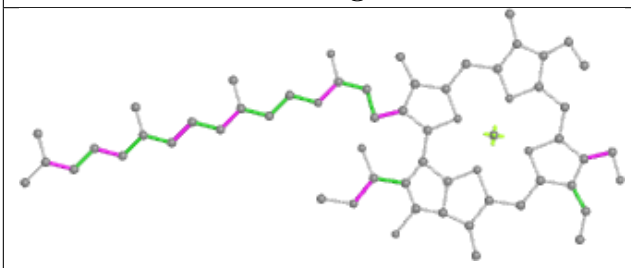
Ligand CHL G 316



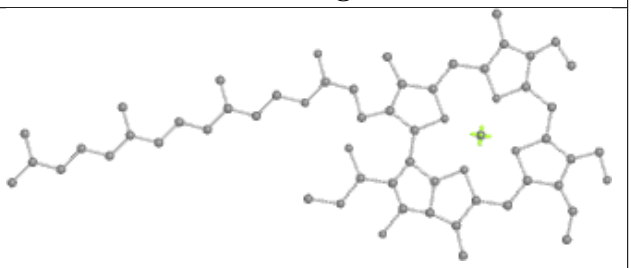
Bond lengths



Bond angles

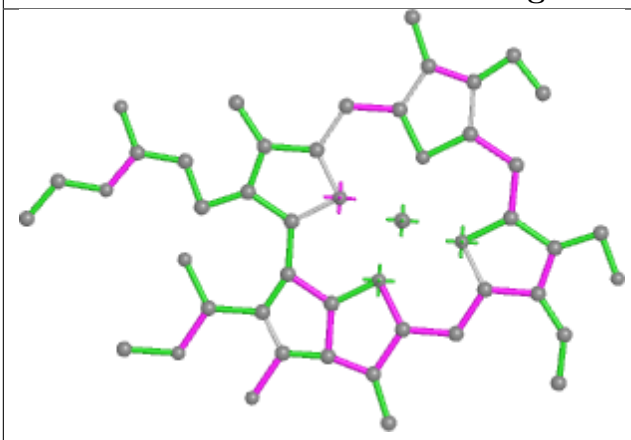


Torsions



Rings

Ligand CHL 2 314



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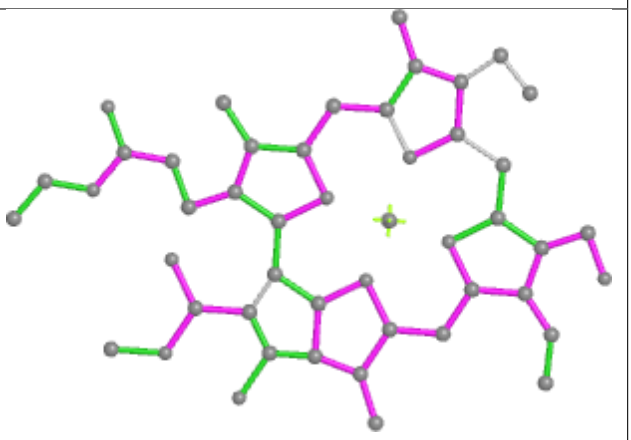
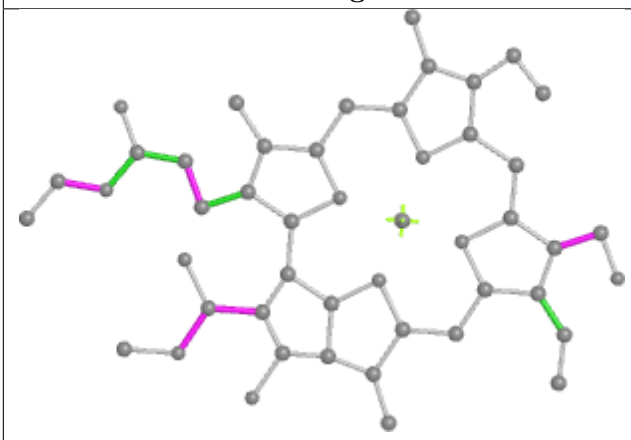


Bond angles



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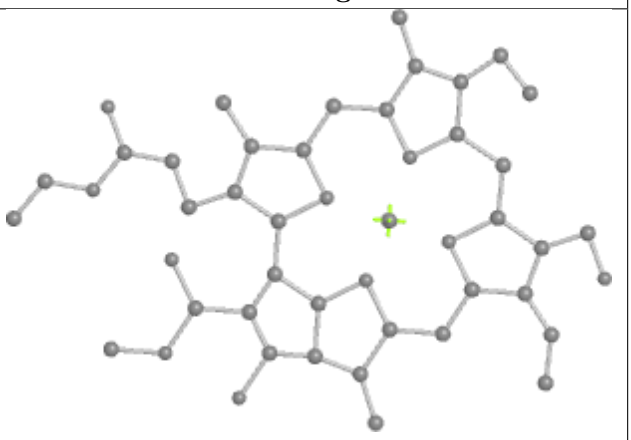
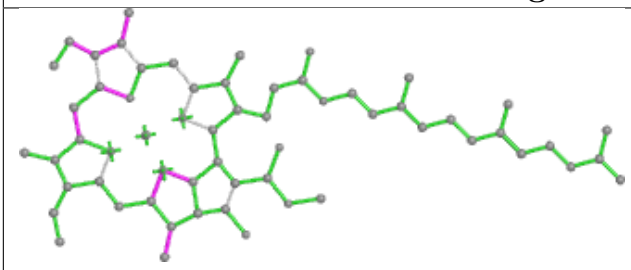
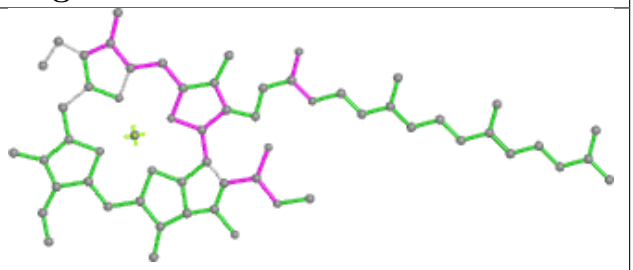
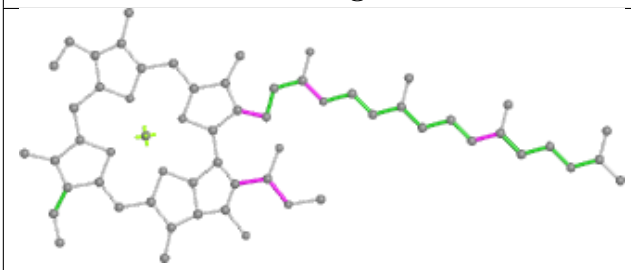
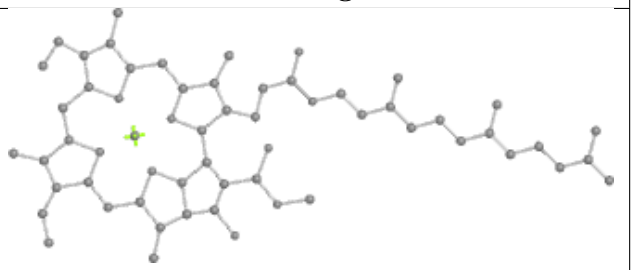
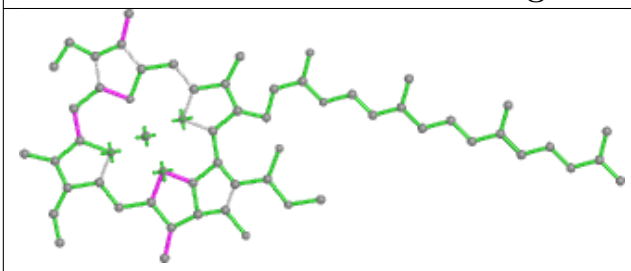
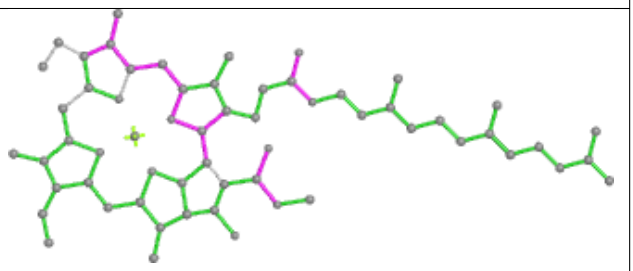
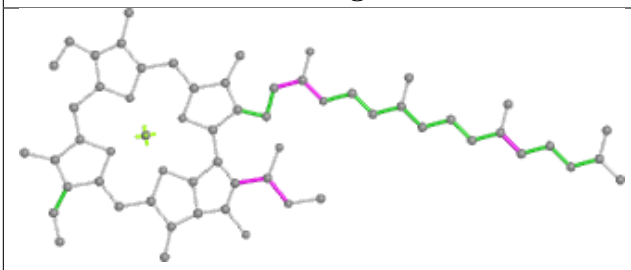
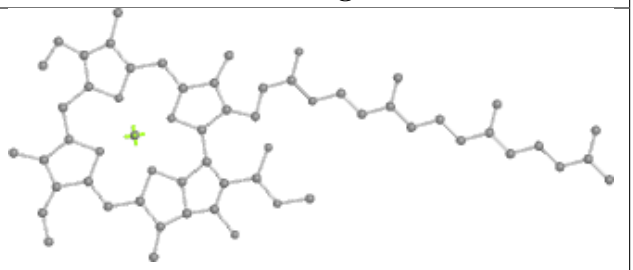
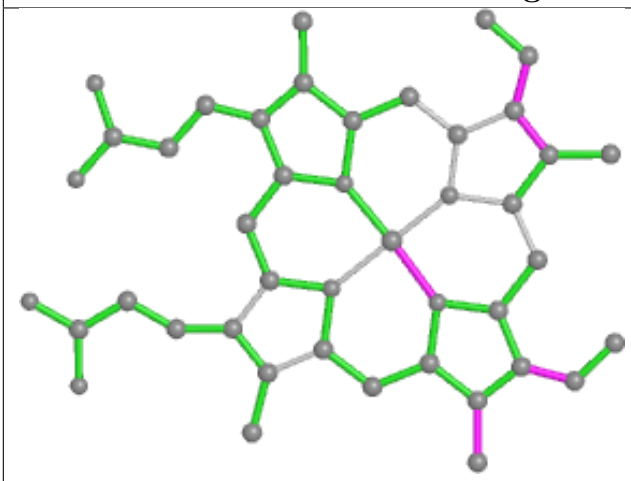


Rings

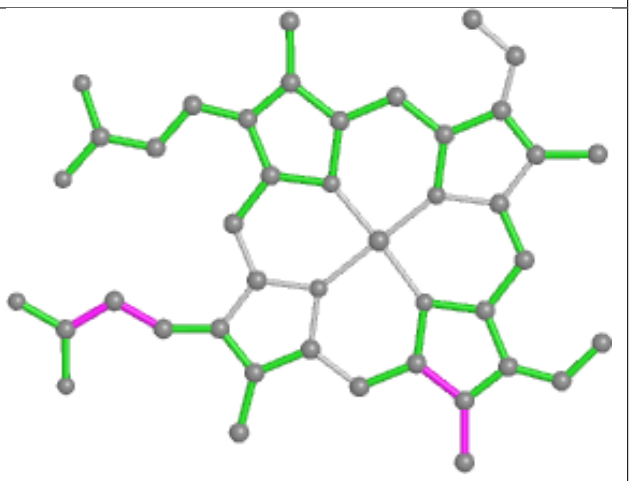
Ligand CLA g 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

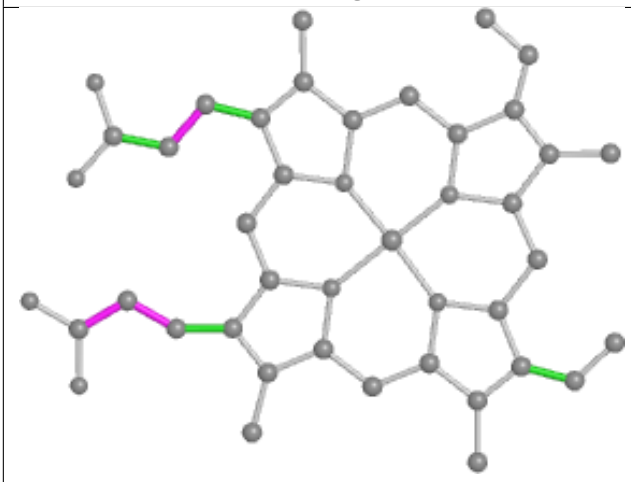
Ligand HEM e 101



Bond lengths



Bond angles



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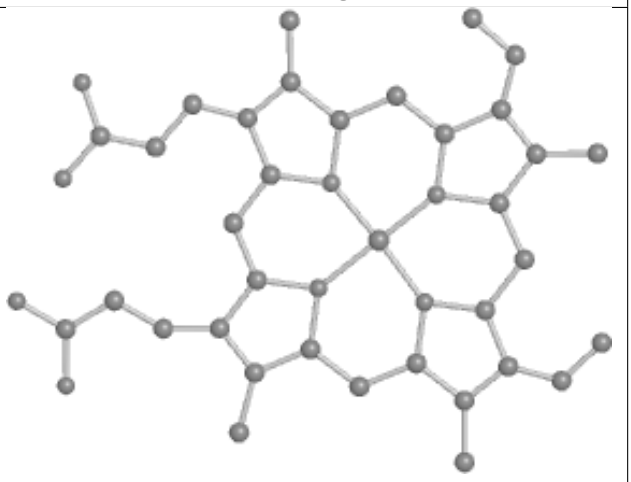
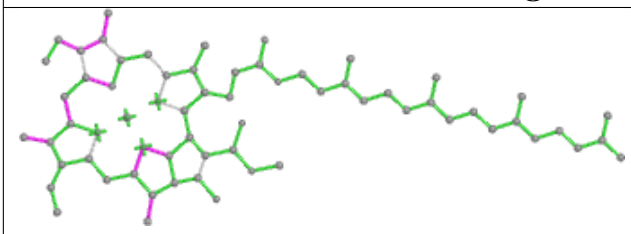
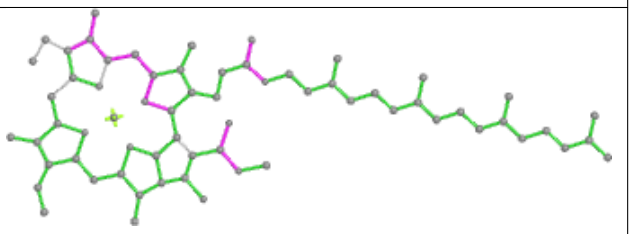


Rings

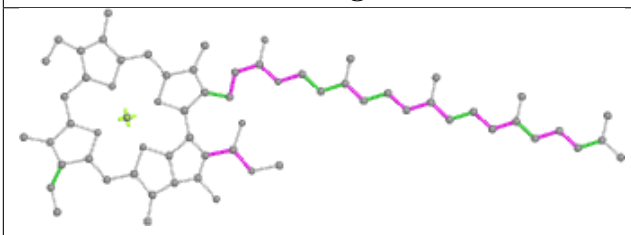
Ligand CLA C 512



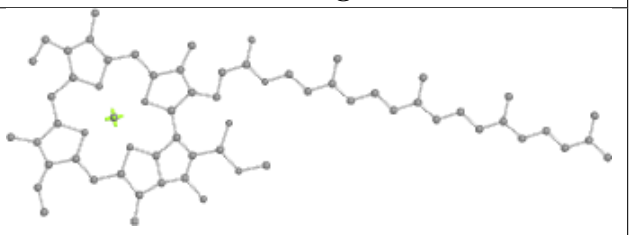
Bond lengths



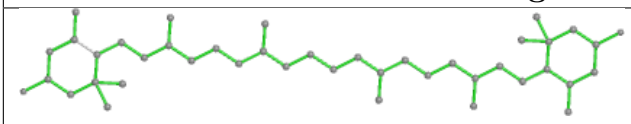
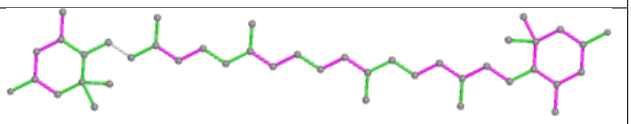
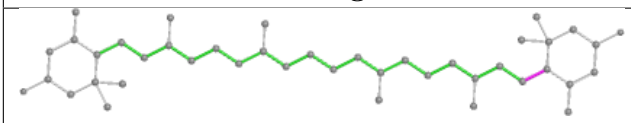
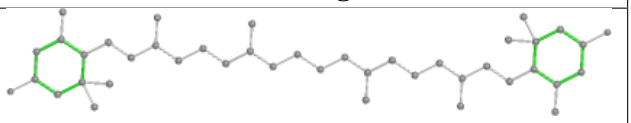
Bond angles



Torsions



Rings

Ligand LUT 2 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

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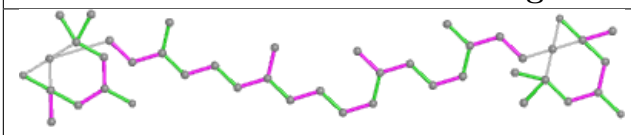
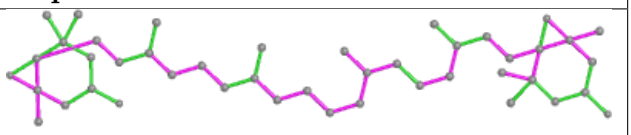
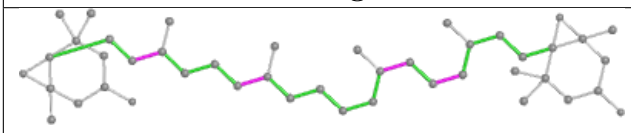
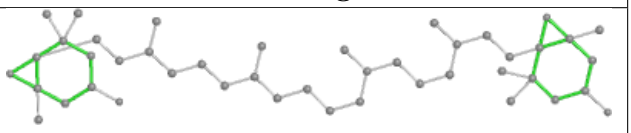
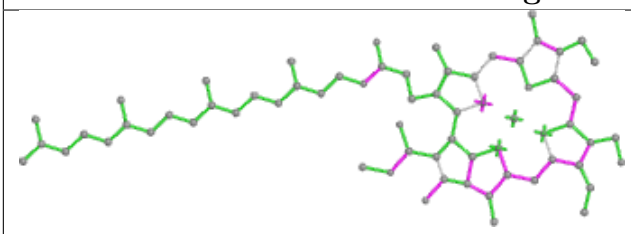
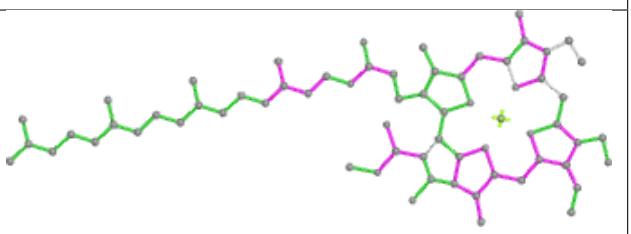
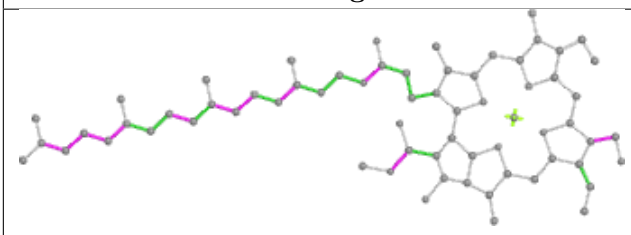
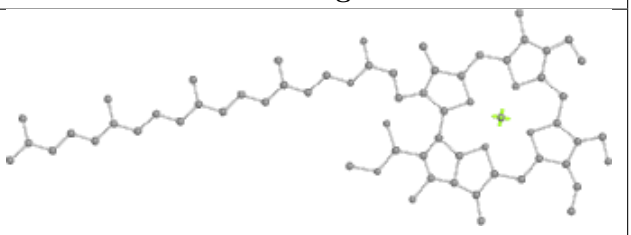
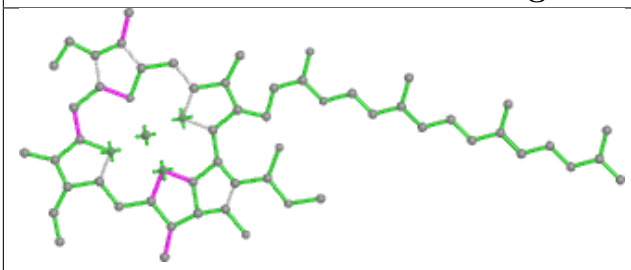
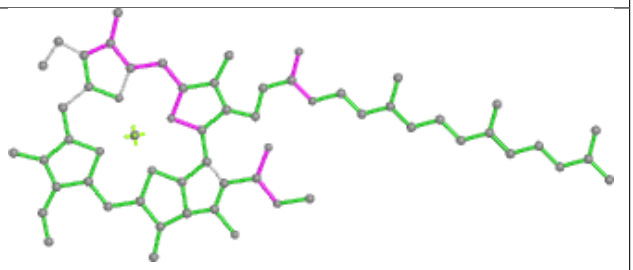
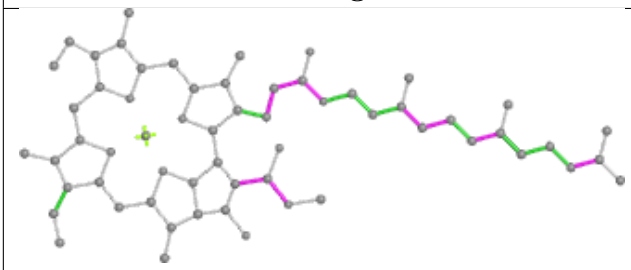
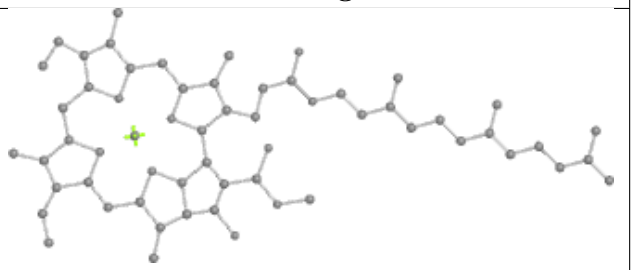
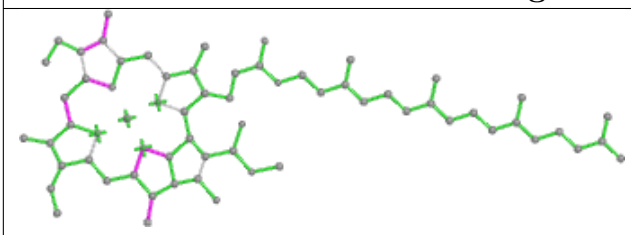
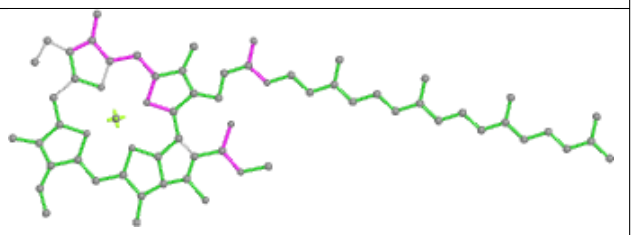
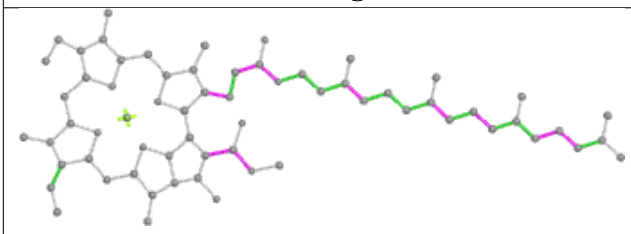
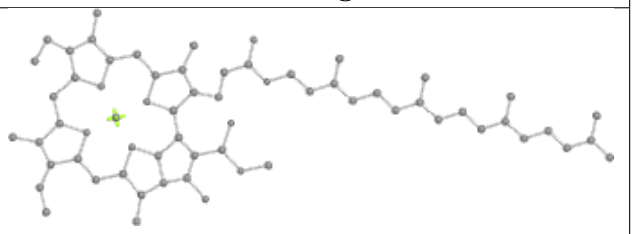
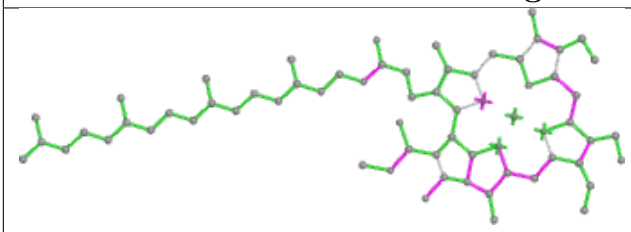
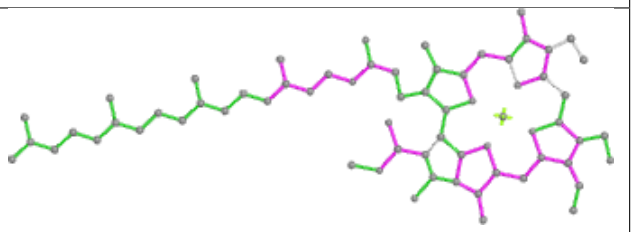
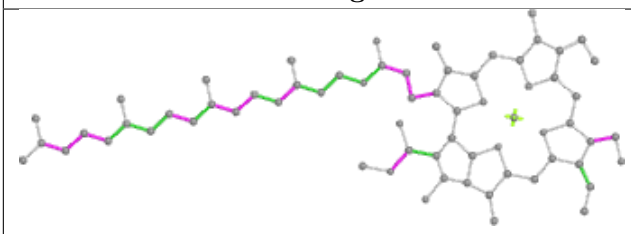
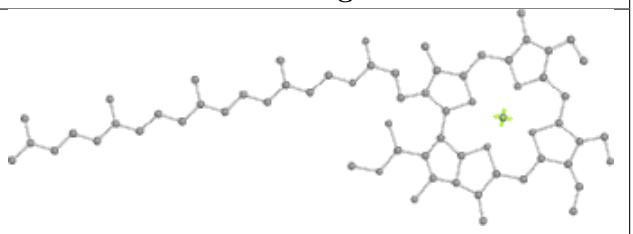
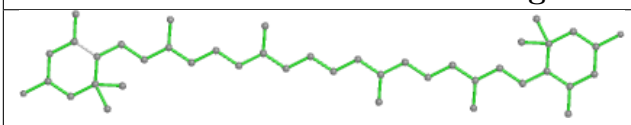
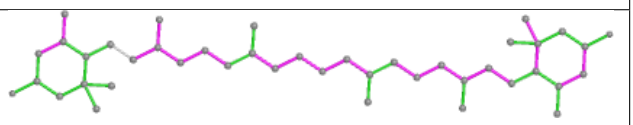
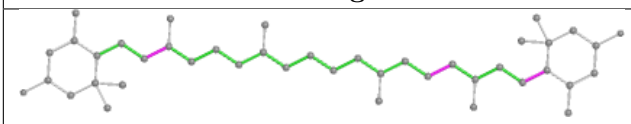
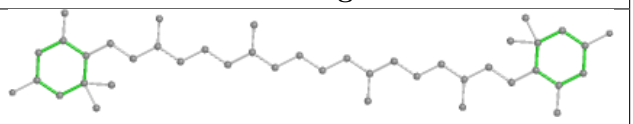
 Bond lengths	 Bond angles
 Torsions	 Rings

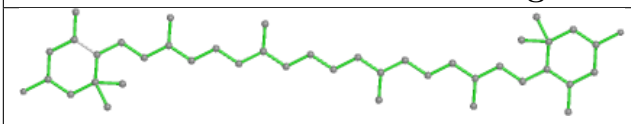
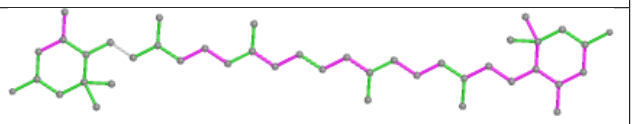
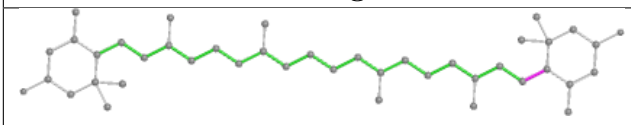
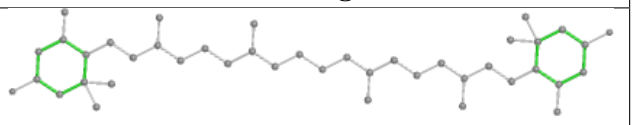
Ligand CHL V 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

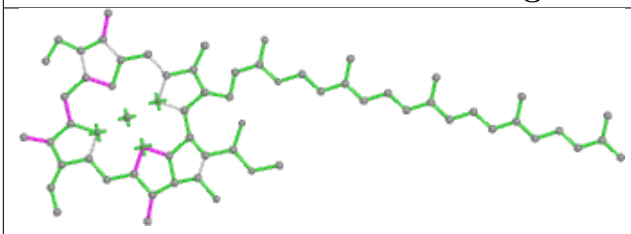
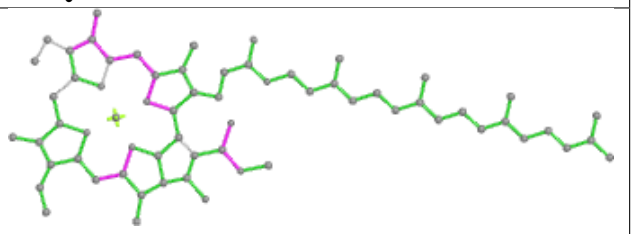
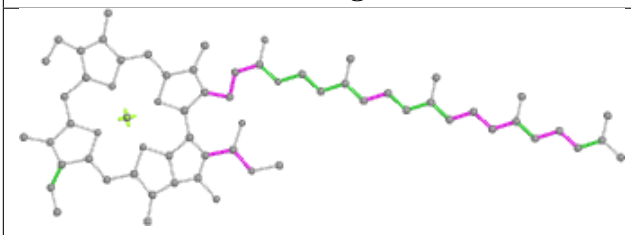
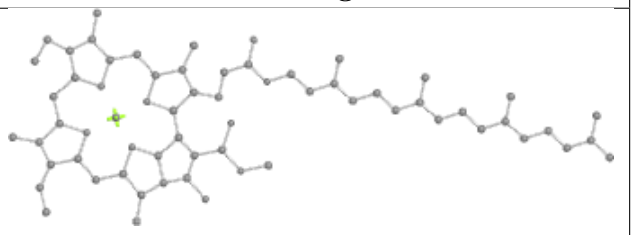
Ligand CLA 3 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

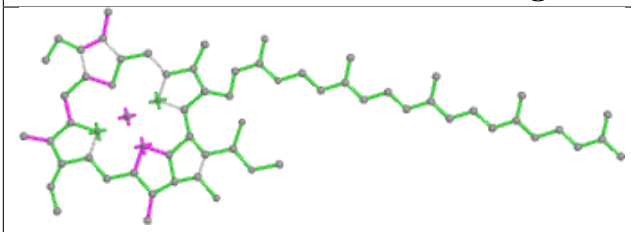
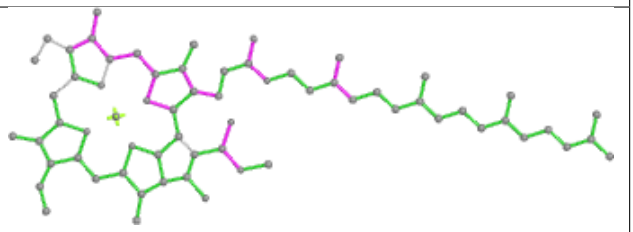
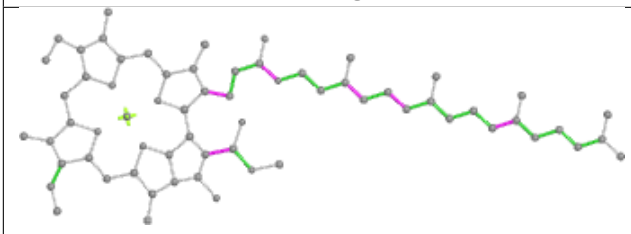
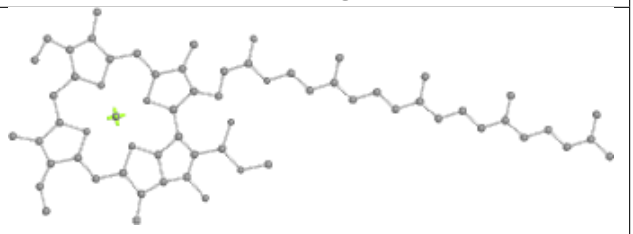
Ligand CLA 5 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL P 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

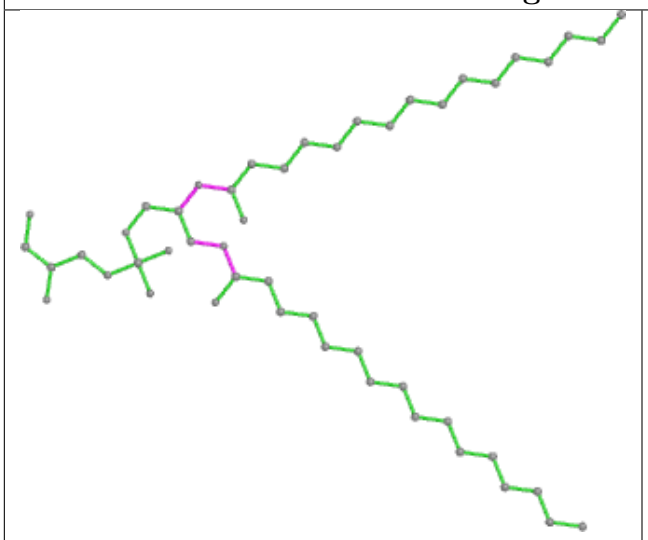
Ligand LUT 5 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT u 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

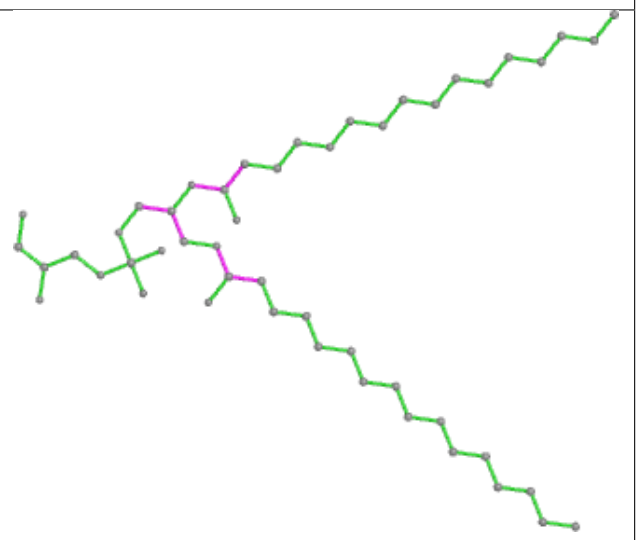
Ligand CLA Q 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

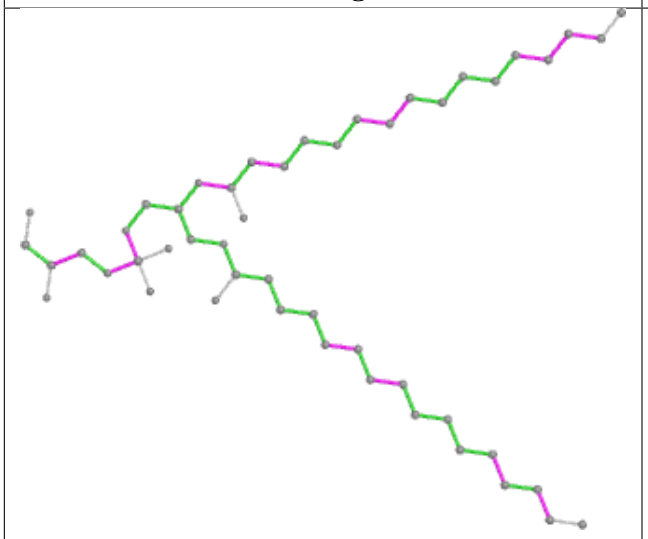
Ligand LHG D 407



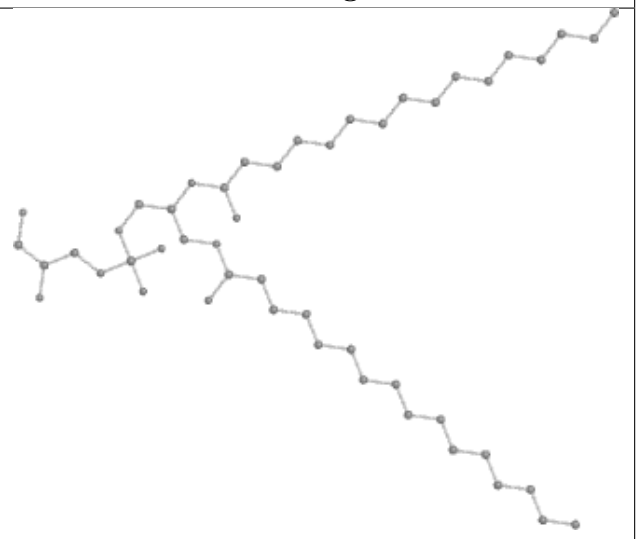
Bond lengths



Bond angles

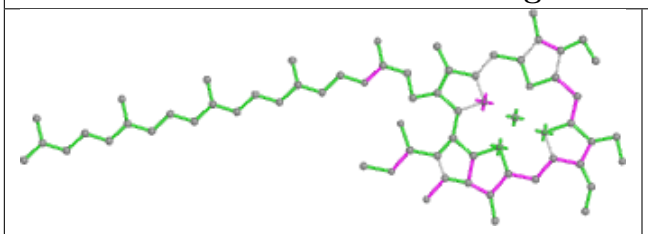


Torsions

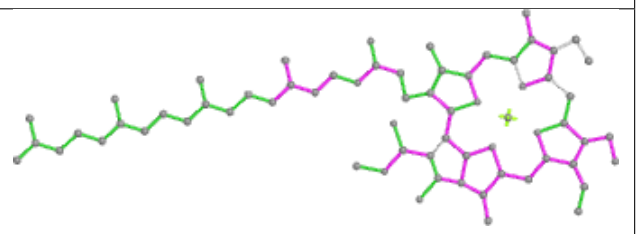


Rings

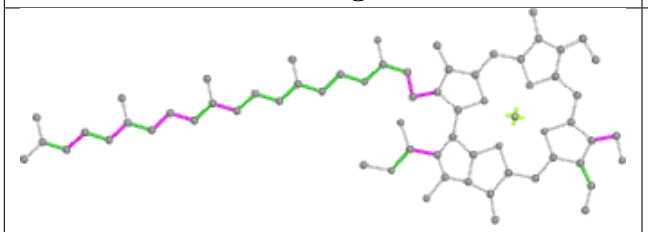
Ligand CHL U 315



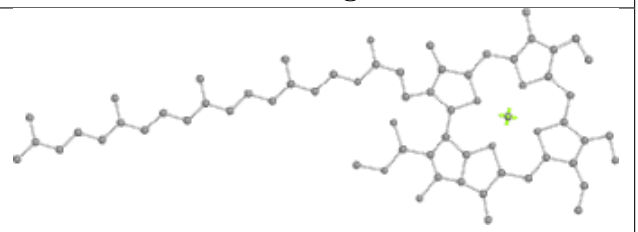
Bond lengths



Bond angles

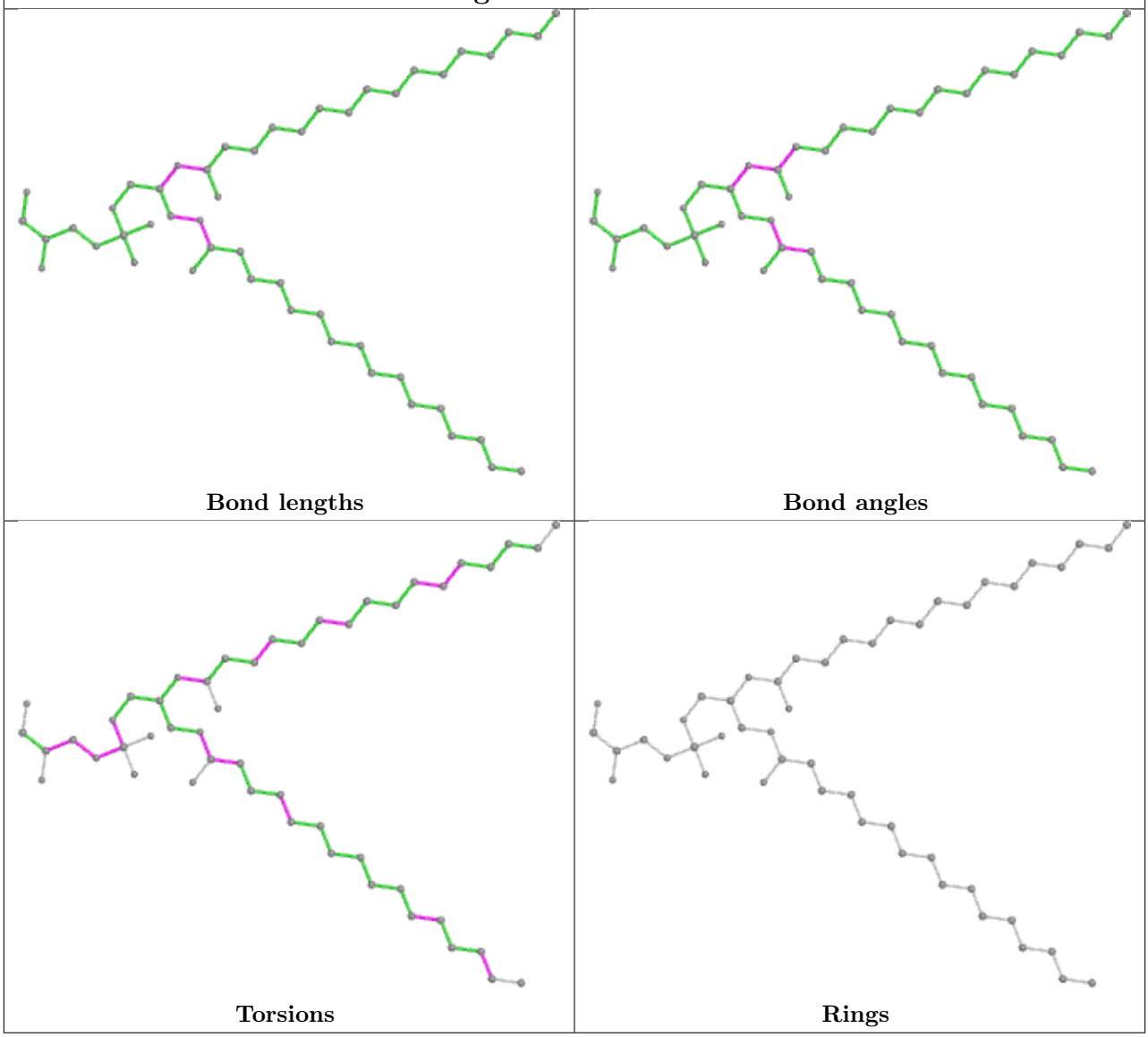


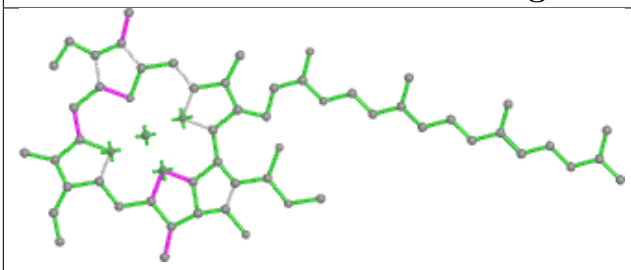
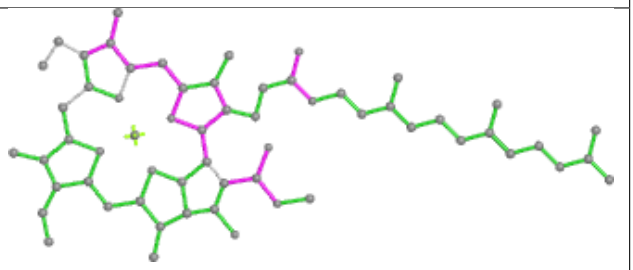
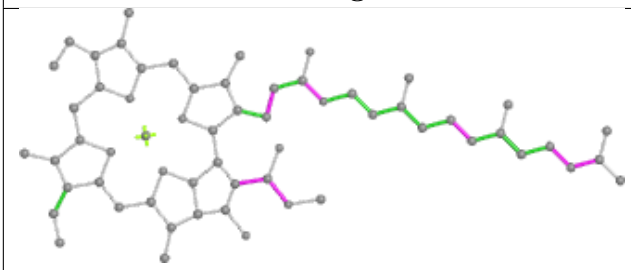
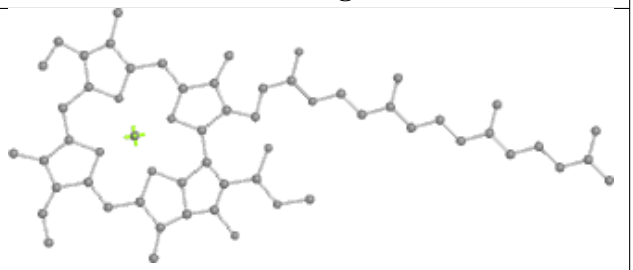
Torsions

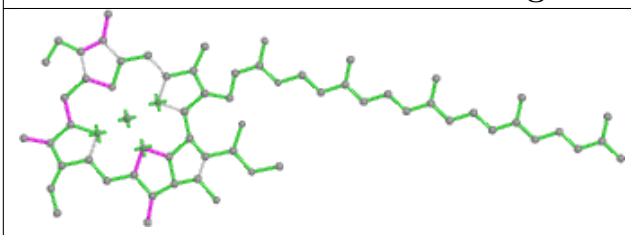
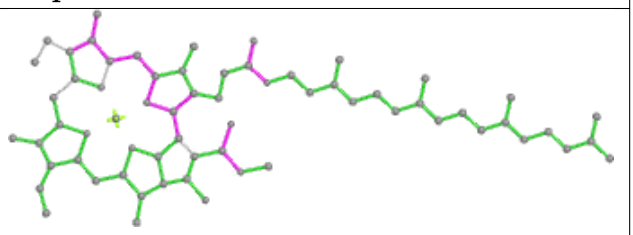
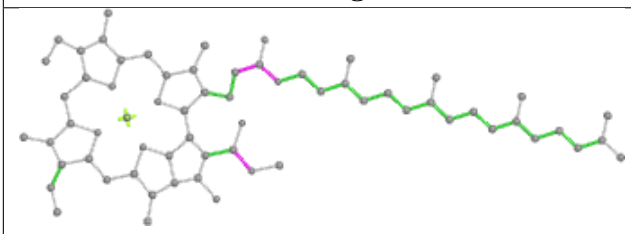
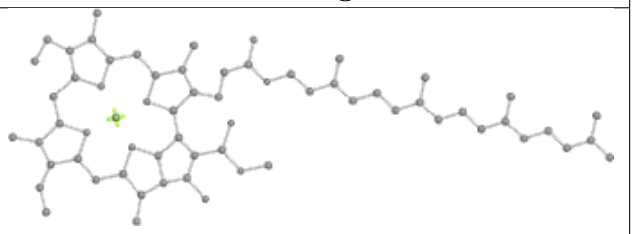


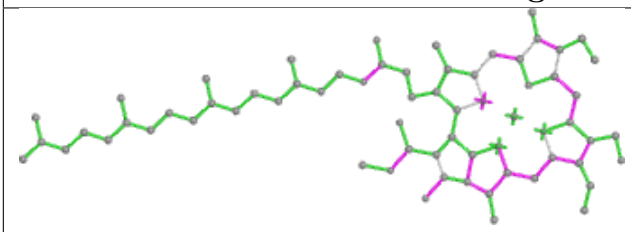
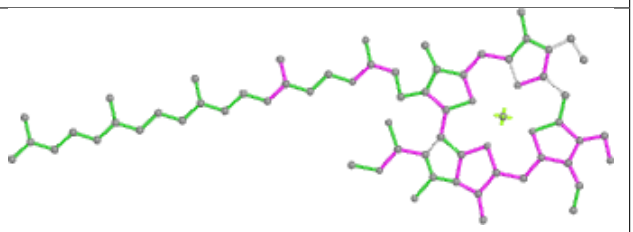
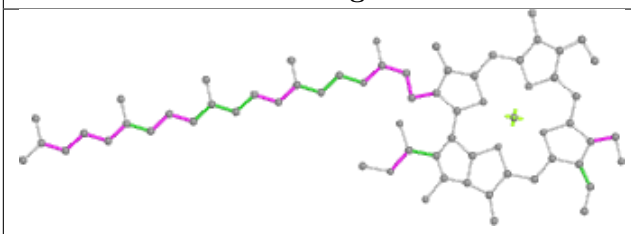
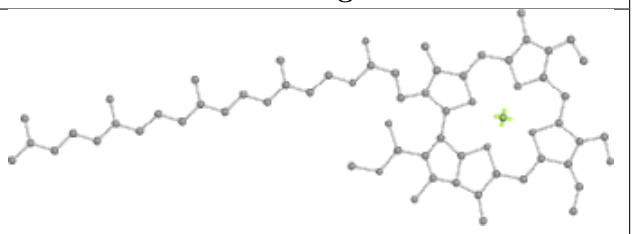
Rings

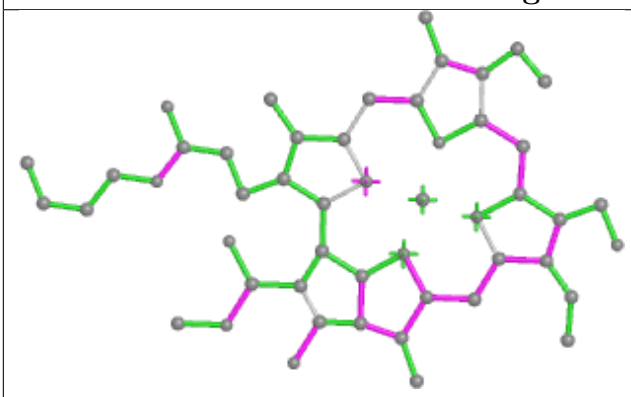
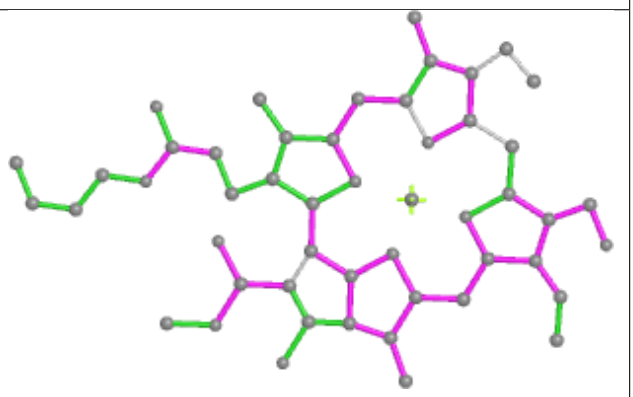
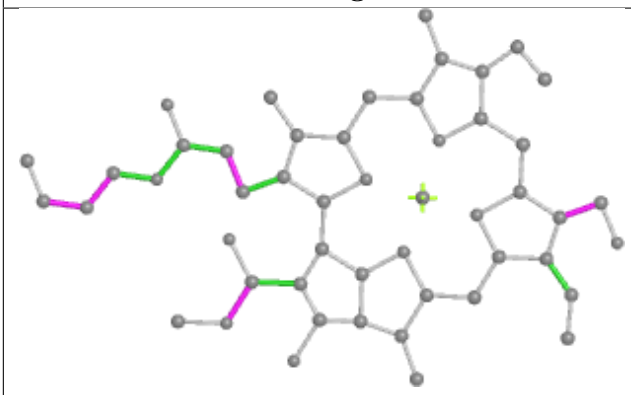
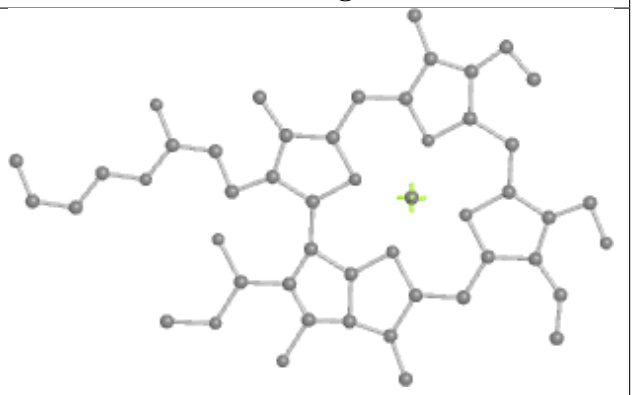
Ligand LHG s 312

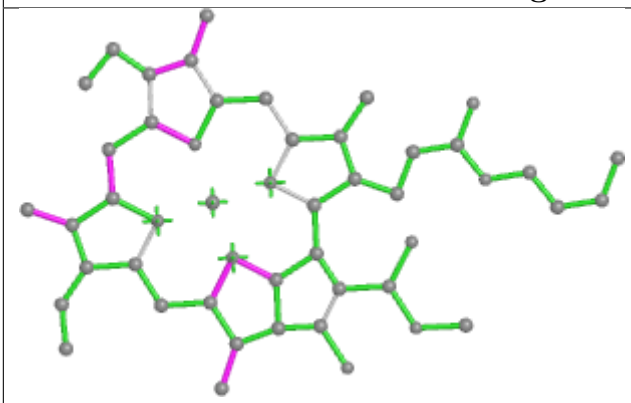
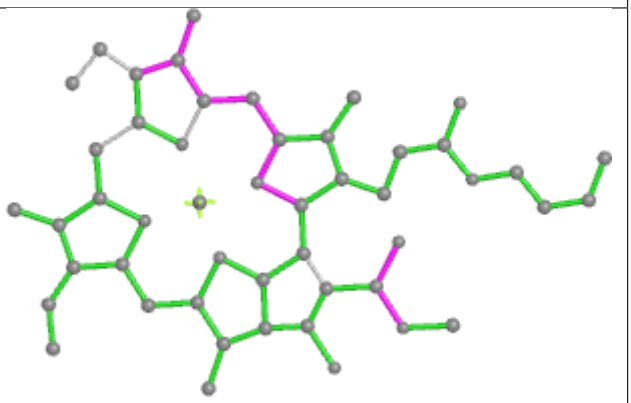
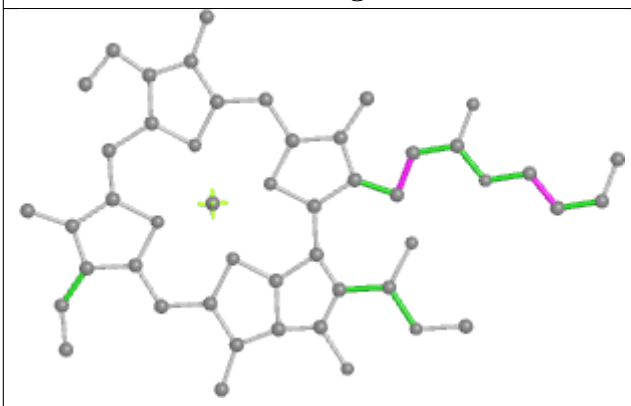
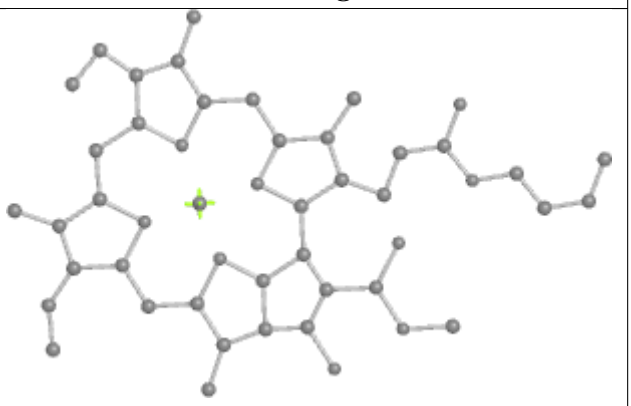


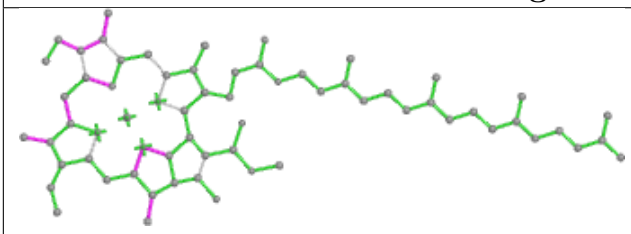
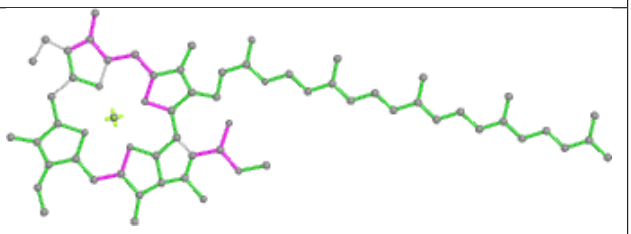
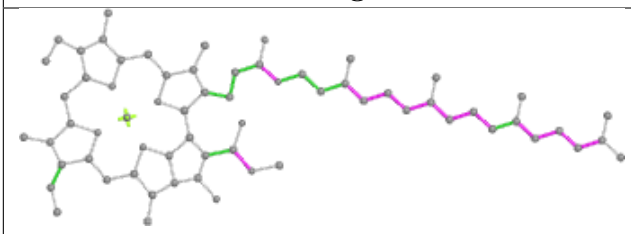
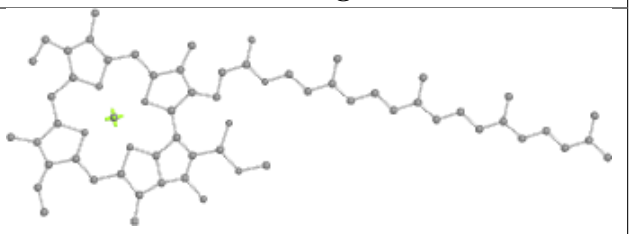
Ligand CLA 3 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

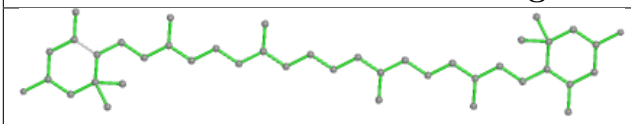
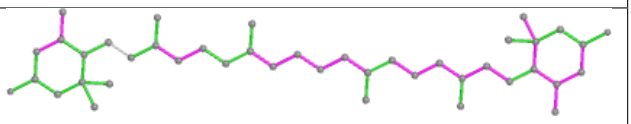
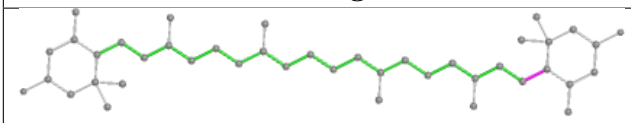
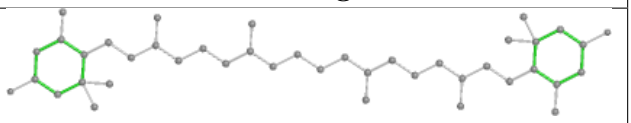
Ligand CLA p 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

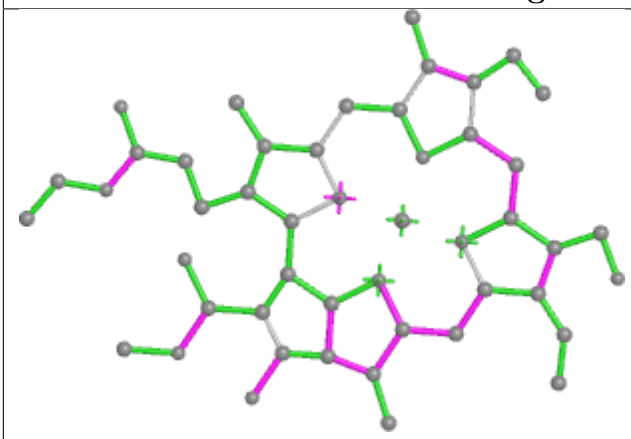
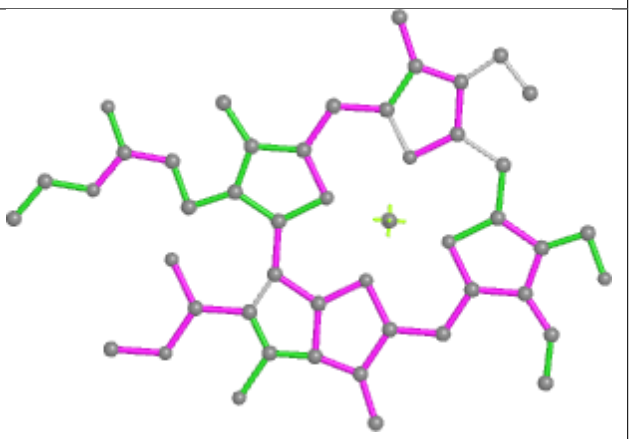
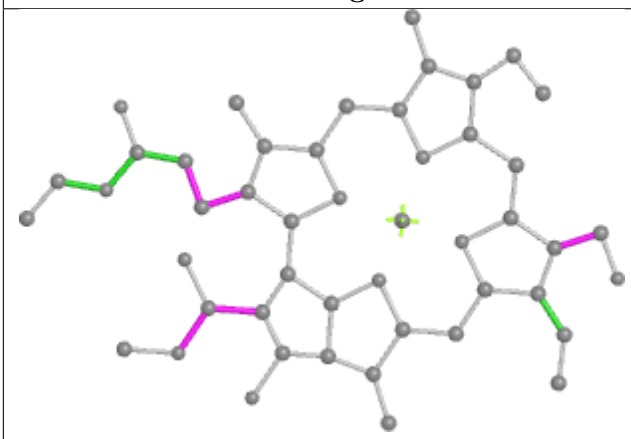
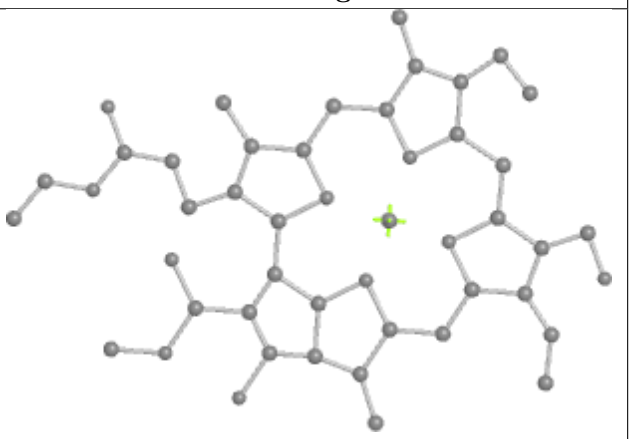
Ligand CHL 3 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

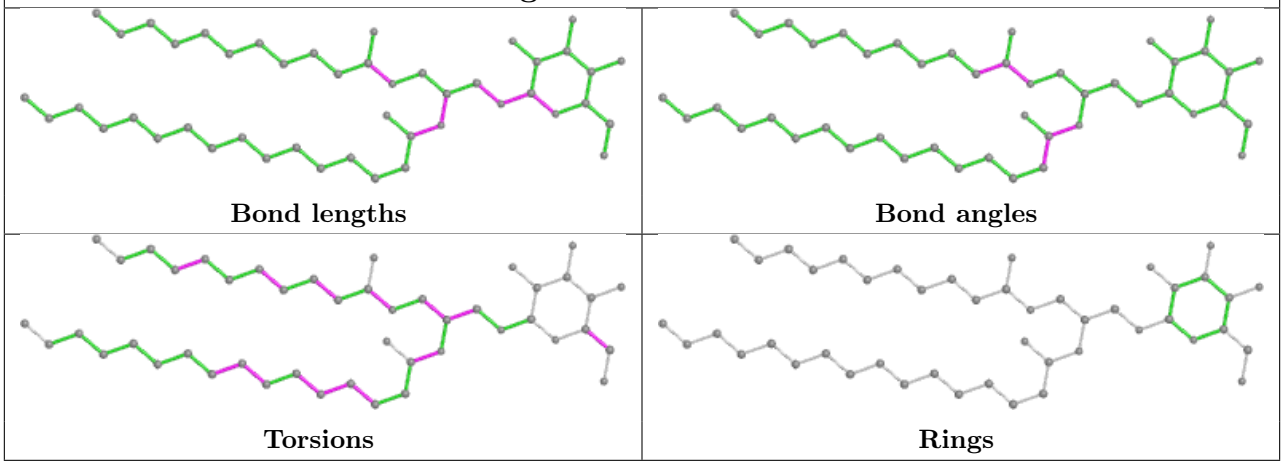
Ligand CLA s 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

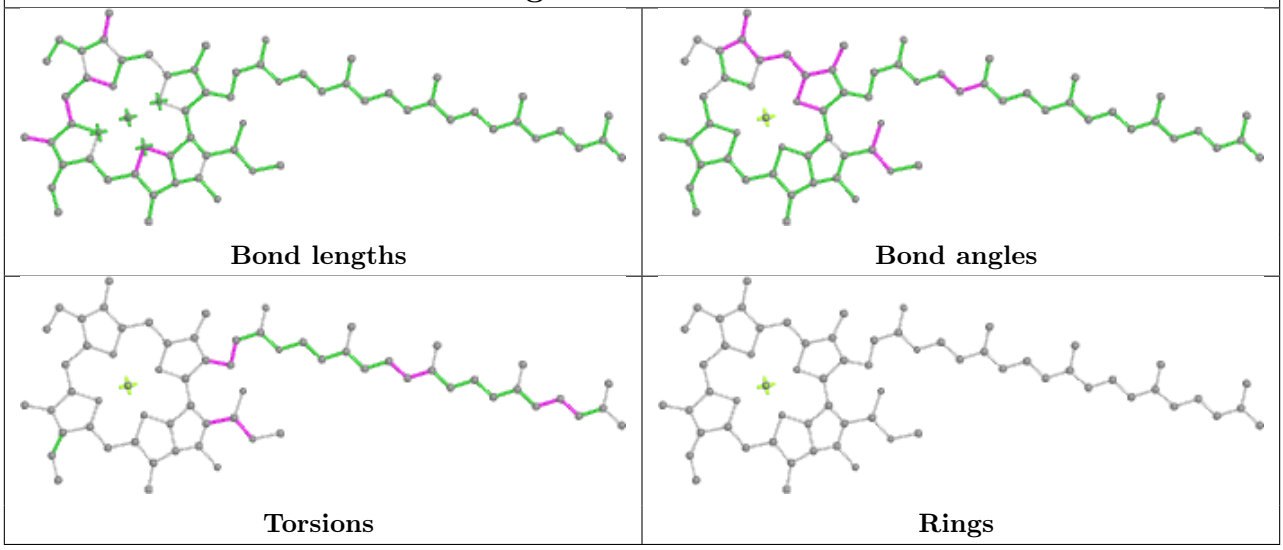
Ligand LUT 4 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 4 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

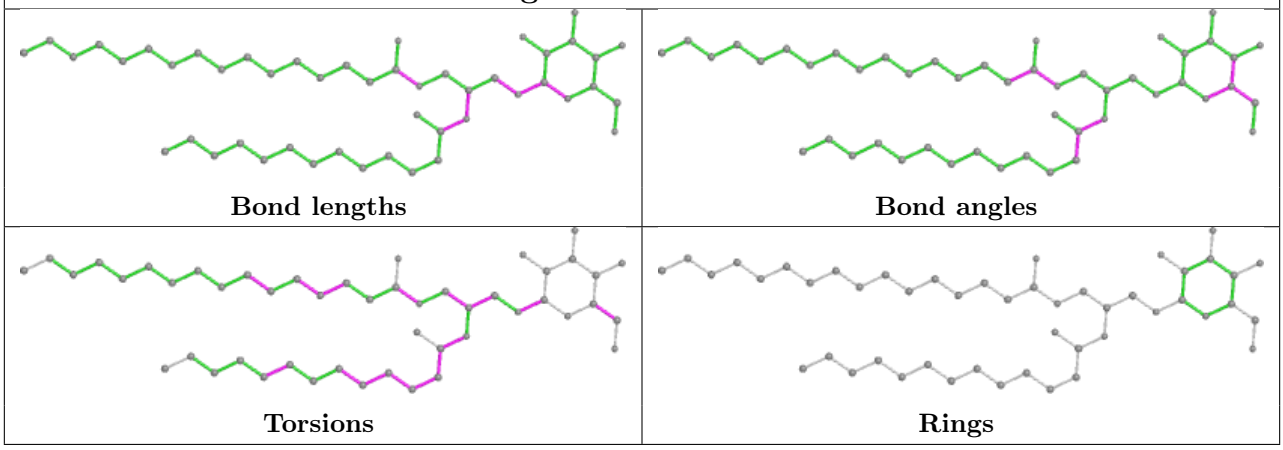
Ligand LMG D 408



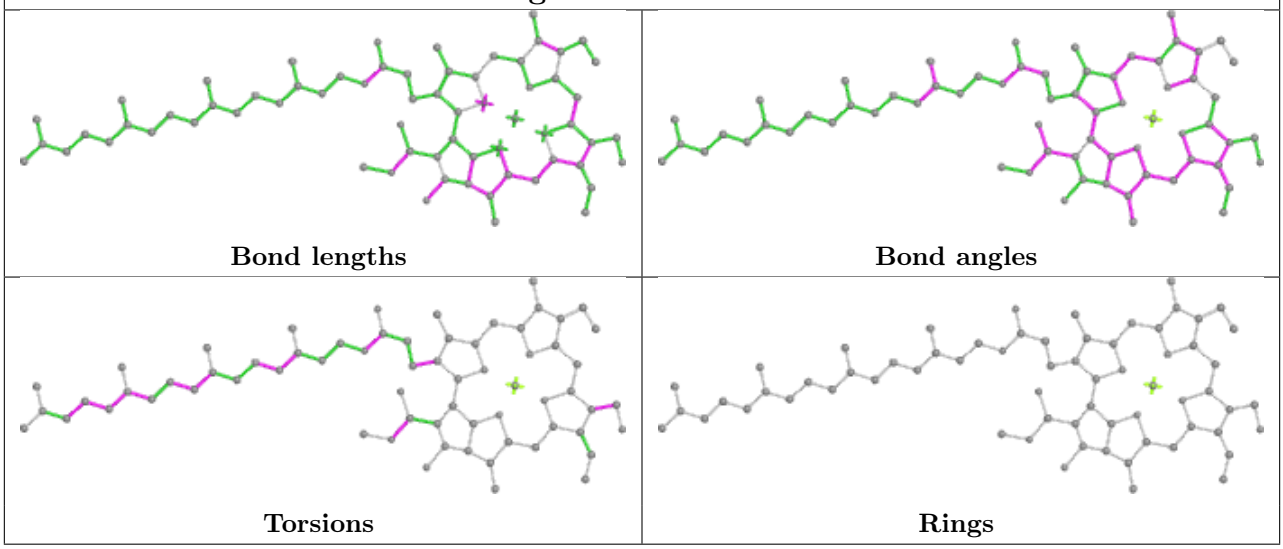
Ligand CLA P 305



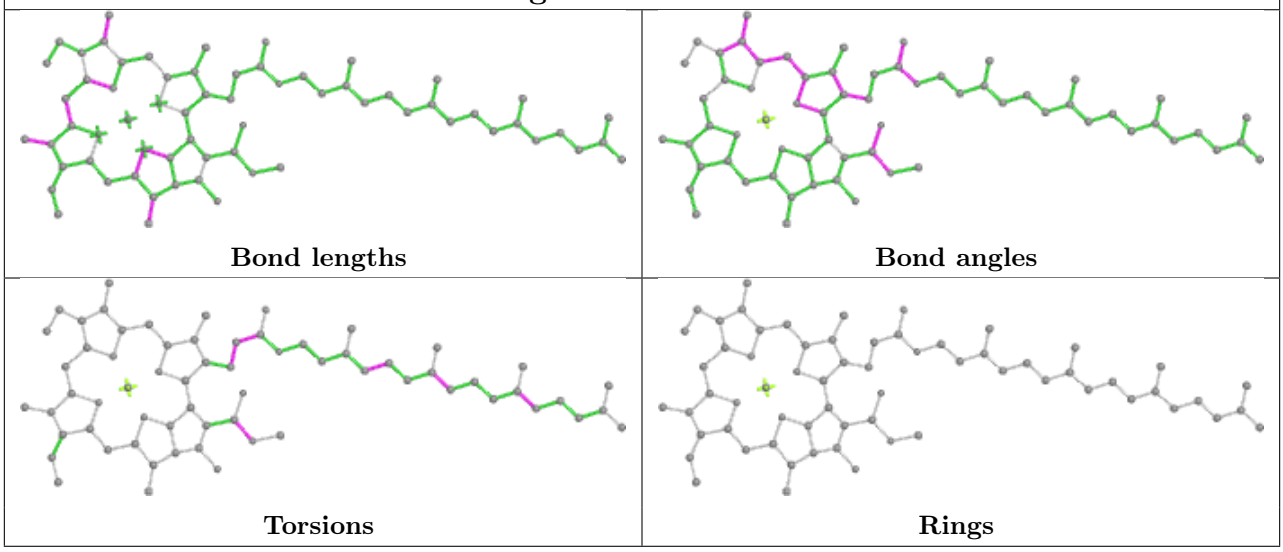
Ligand LMG w 201



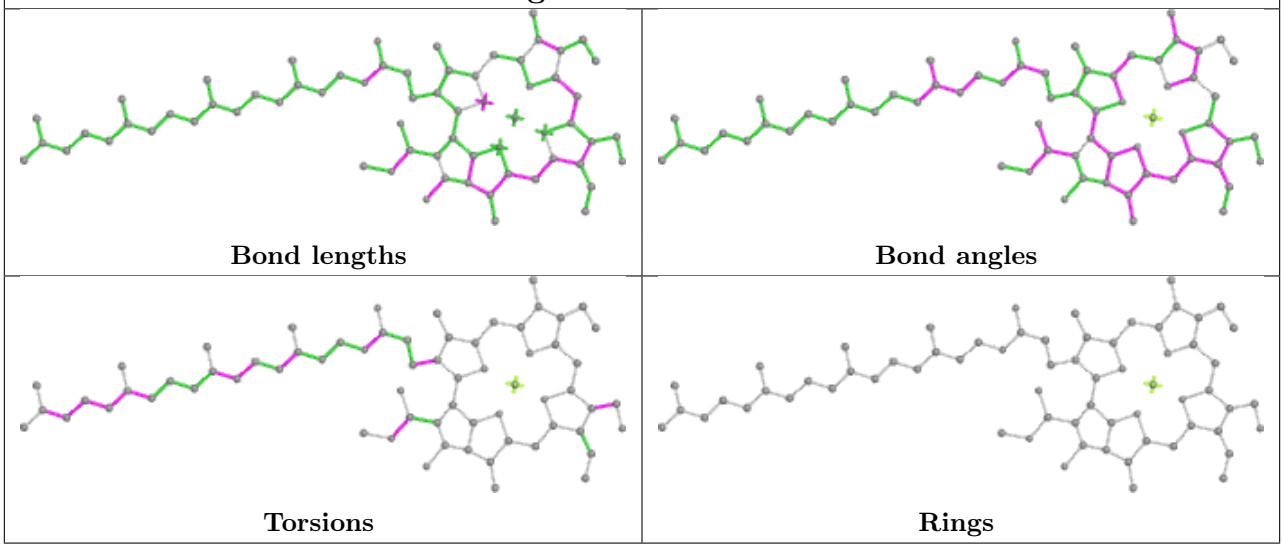
Ligand CHL 5 318

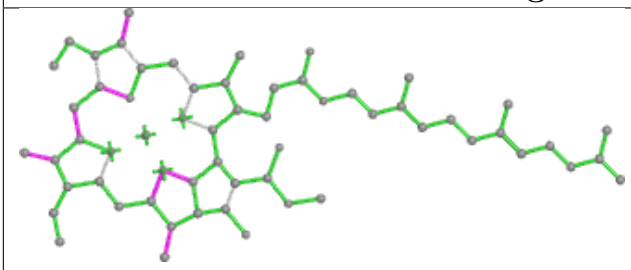
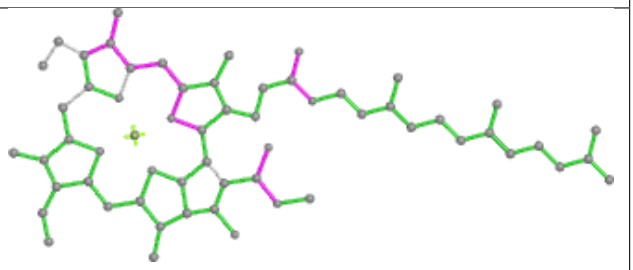
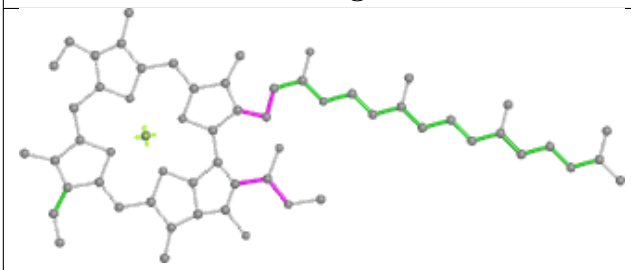
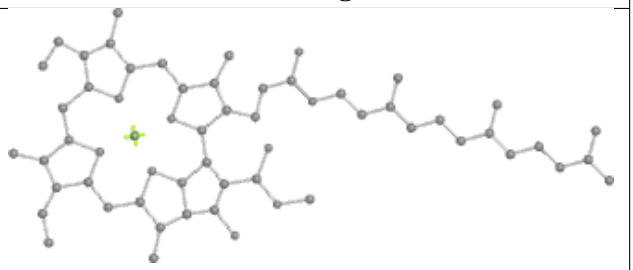


Ligand CLA 3 307

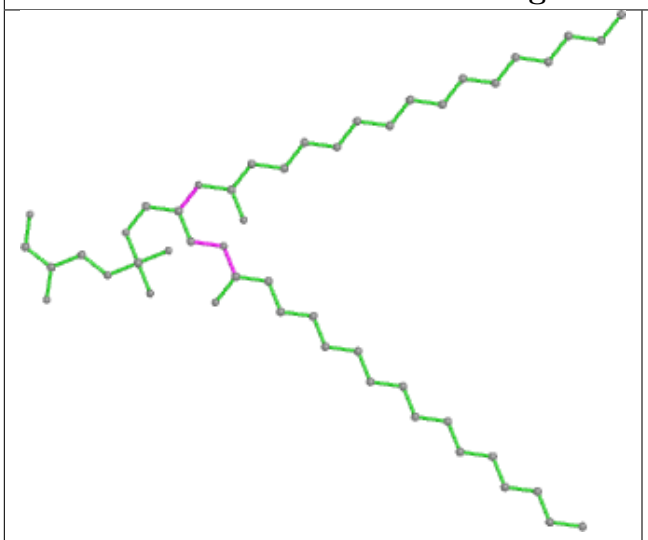


Ligand CHL u 318

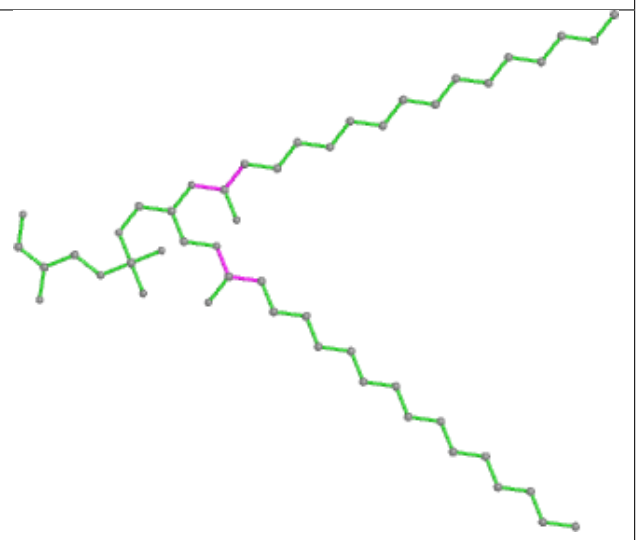


Ligand CLA u 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

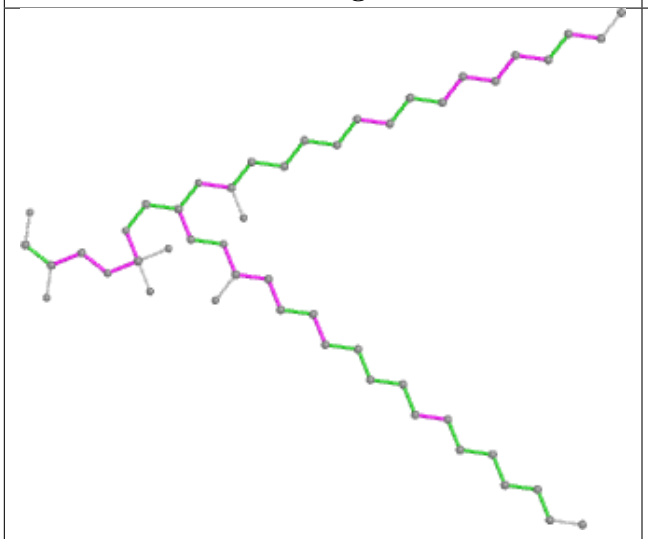
Ligand LHG c 522



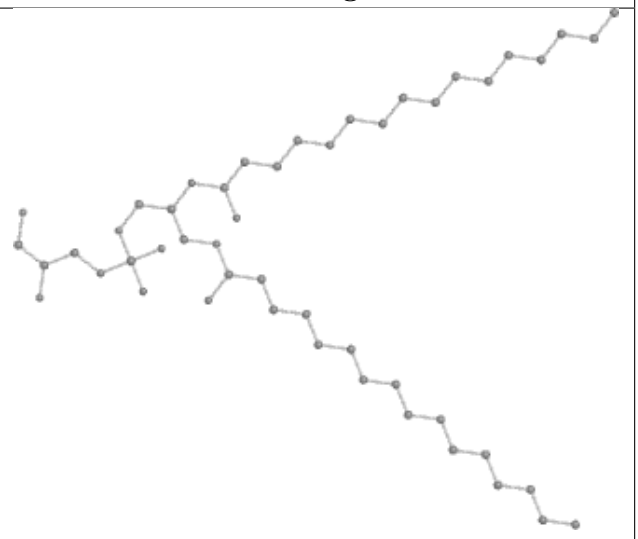
Bond lengths



Bond angles

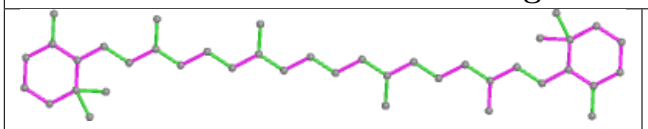


Torsions

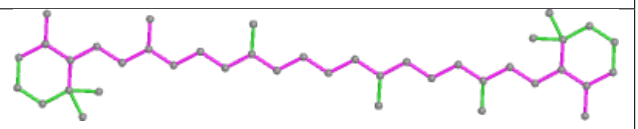


Rings

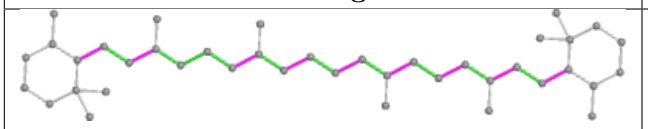
Ligand BCR B 619



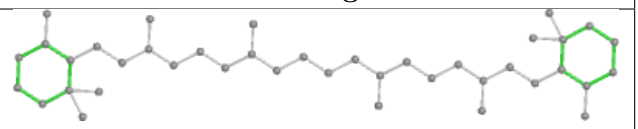
Bond lengths



Bond angles

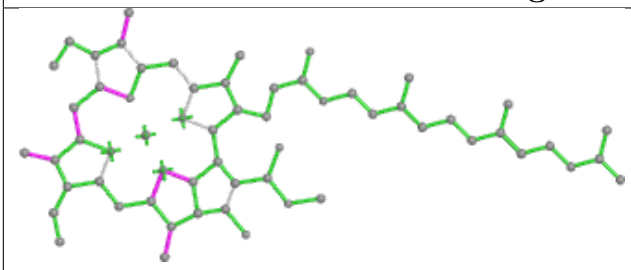


Torsions



Rings

Ligand CLA 2 306



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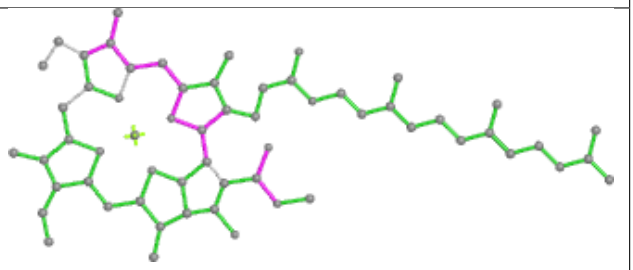
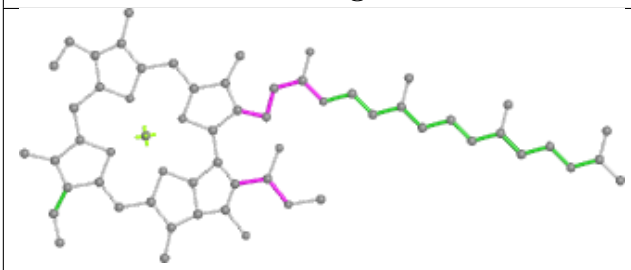
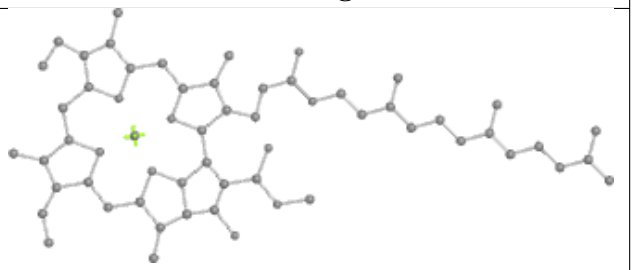


Bond angles

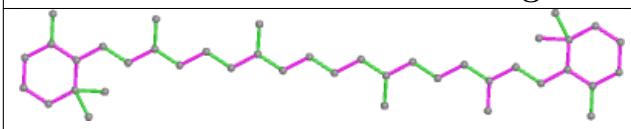


Torsions

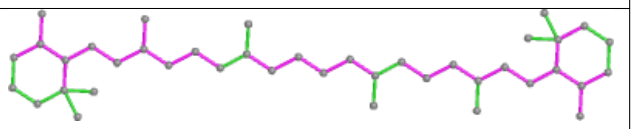


Rings

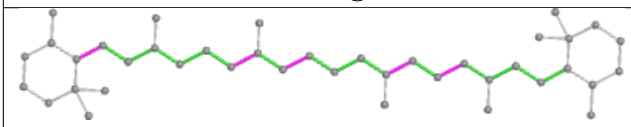
Ligand BCR C 516



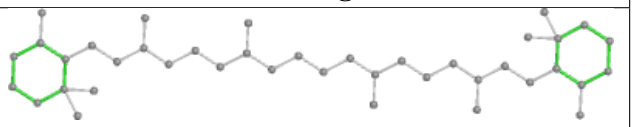
Bond lengths



Bond angles

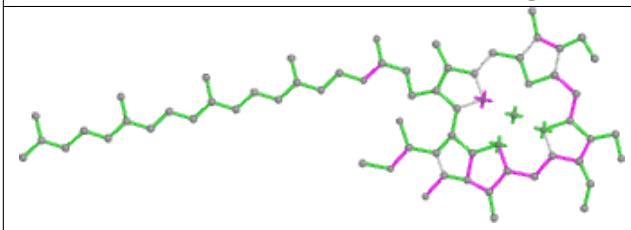


Torsions

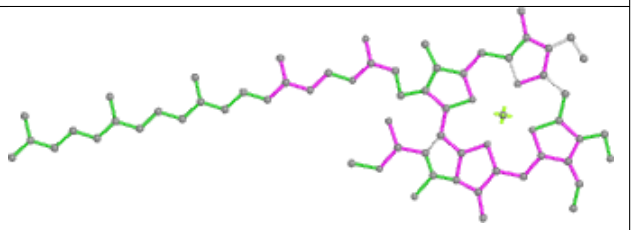


Rings

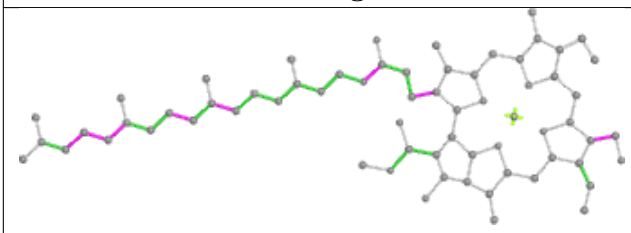
Ligand CHL U 316



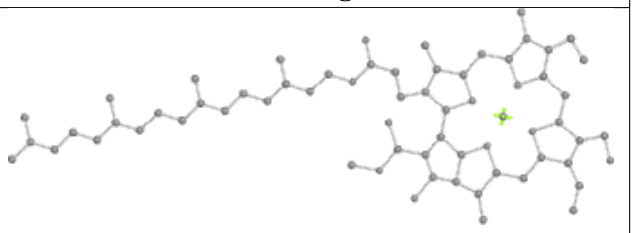
Bond lengths



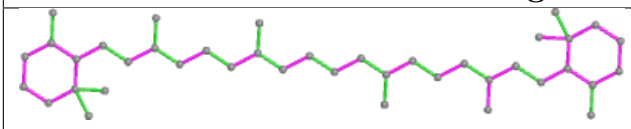
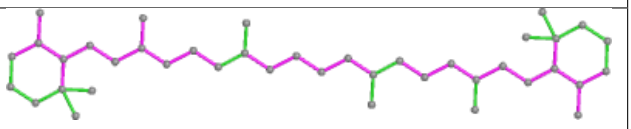
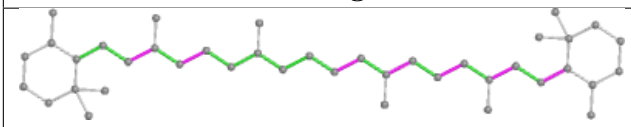
Bond angles

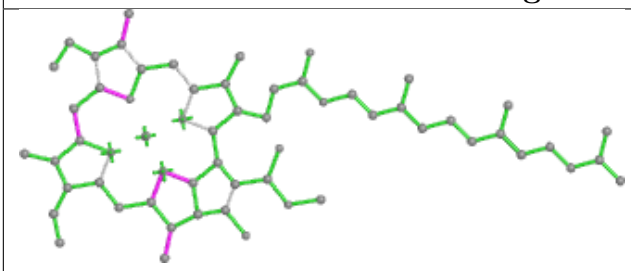
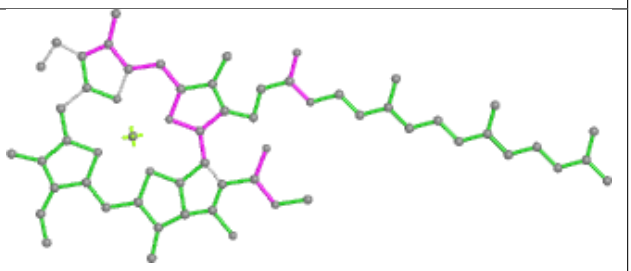
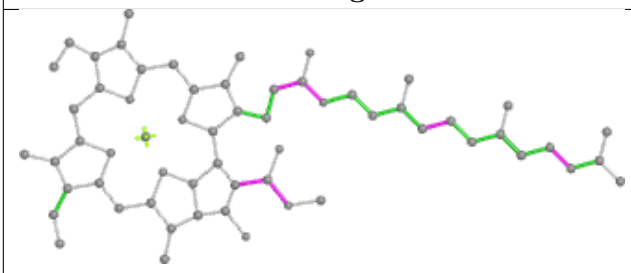
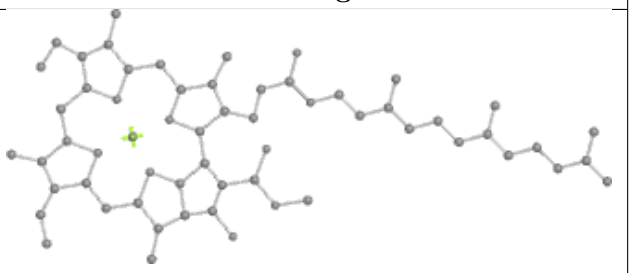


Torsions

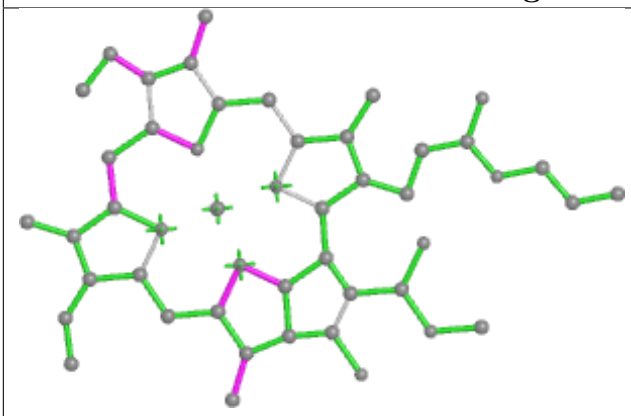


Rings

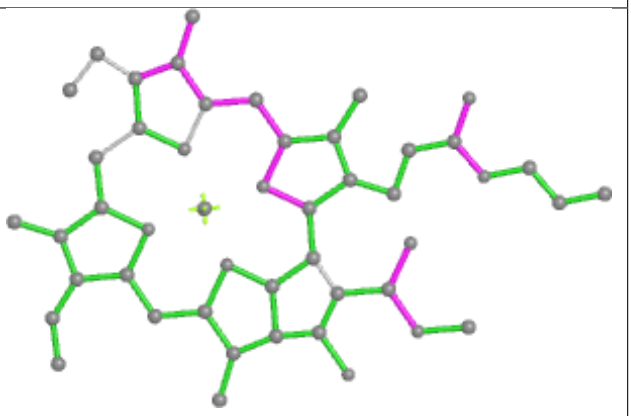
Ligand BCR c 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

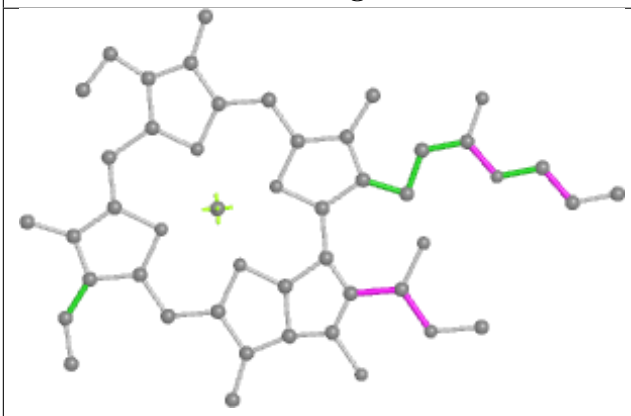
Ligand CLA G 308



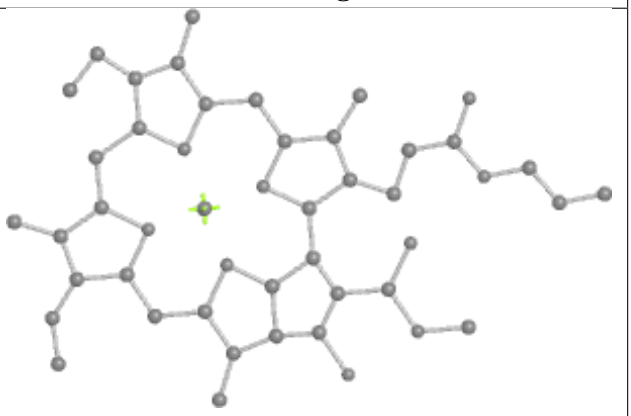
Bond lengths



Bond angles

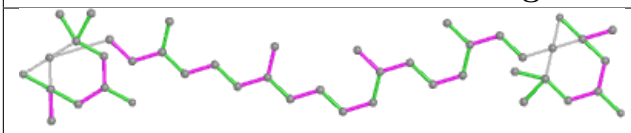


Torsions

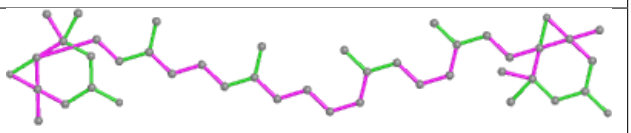


Rings

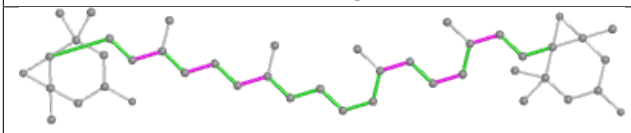
Ligand XAT G 309



Bond lengths



Bond angles



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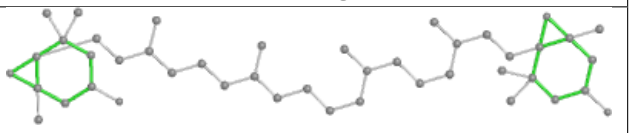
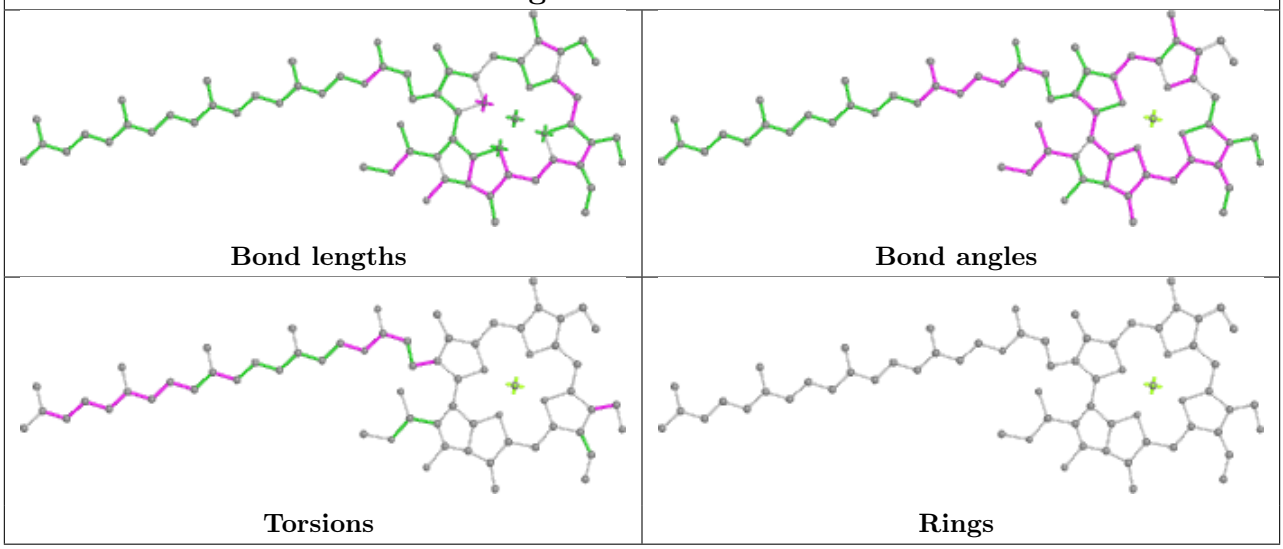
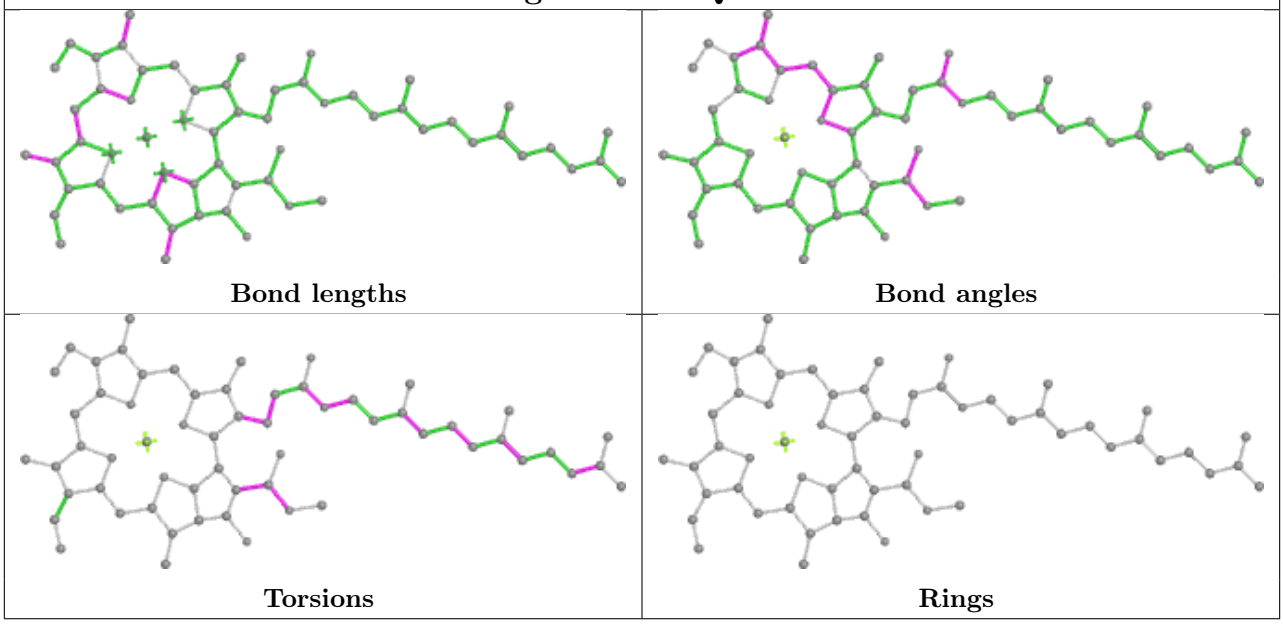


Rings

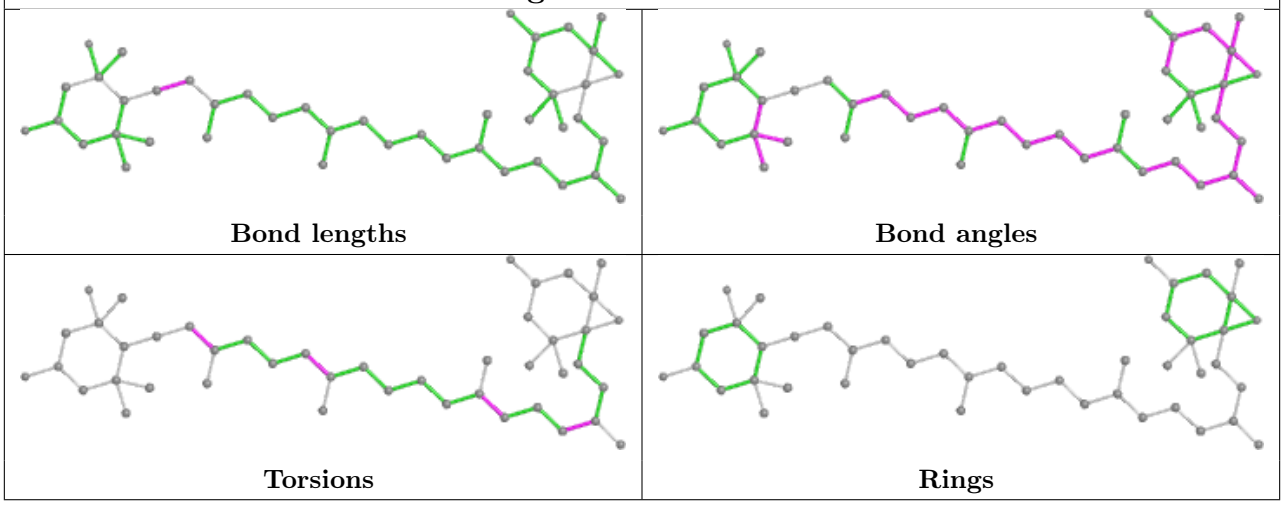
Ligand CHL 1 317



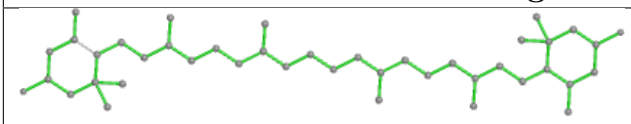
Ligand CLA Q 305



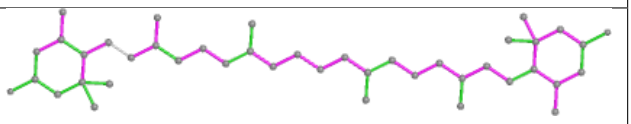
Ligand NEX 5 319



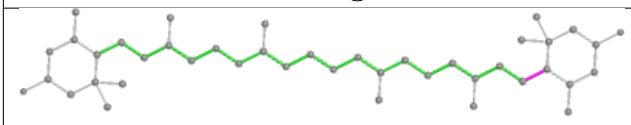
Ligand LUT S 310



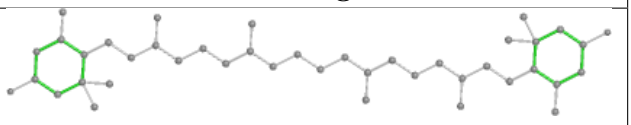
Bond lengths



Bond angles

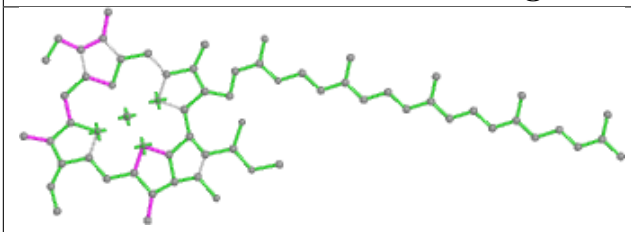


Torsions

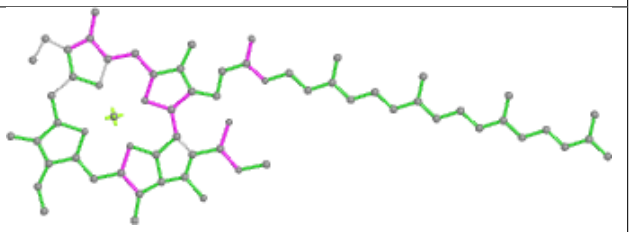


Rings

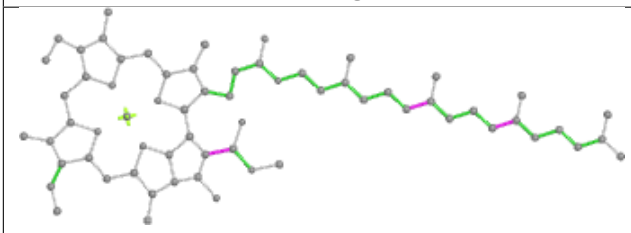
Ligand CLA B 616



Bond lengths



Bond angles



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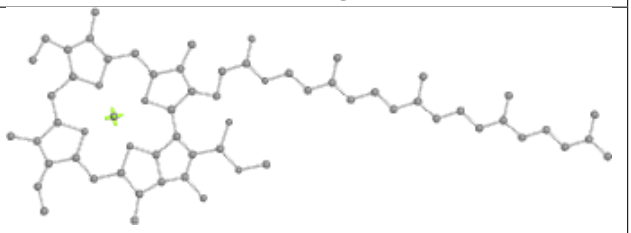
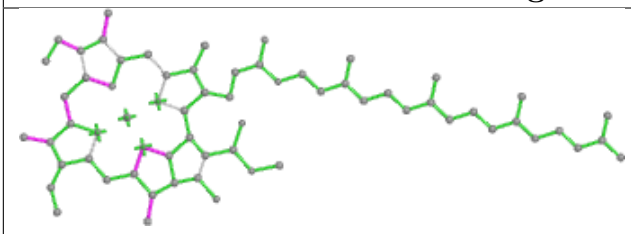


Rings

Ligand CLA u 307



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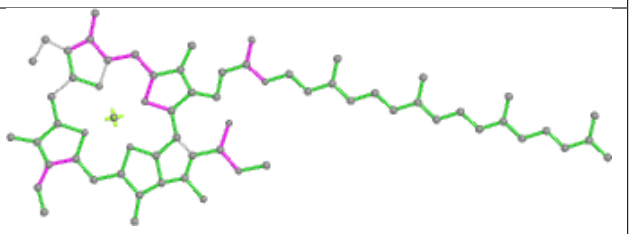
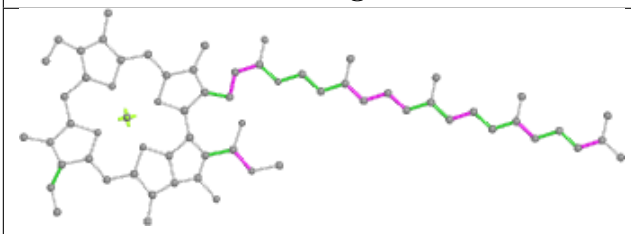
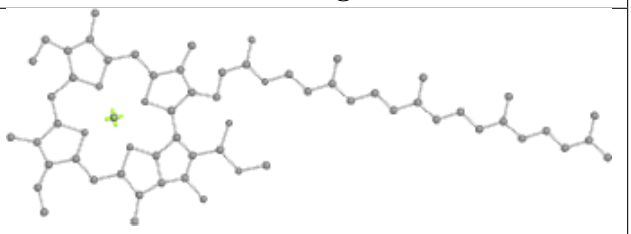


Bond angles

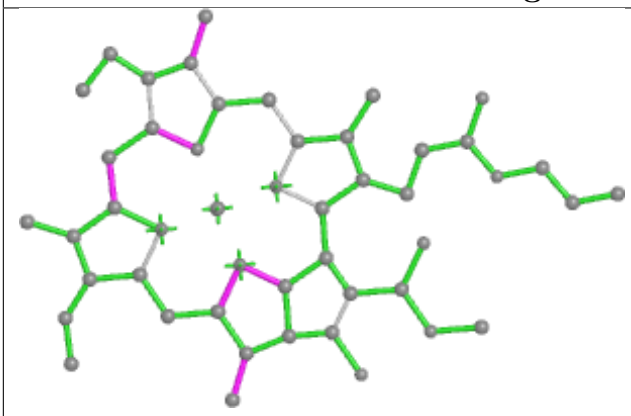


Torsions



Rings

Ligand CLA Q 308



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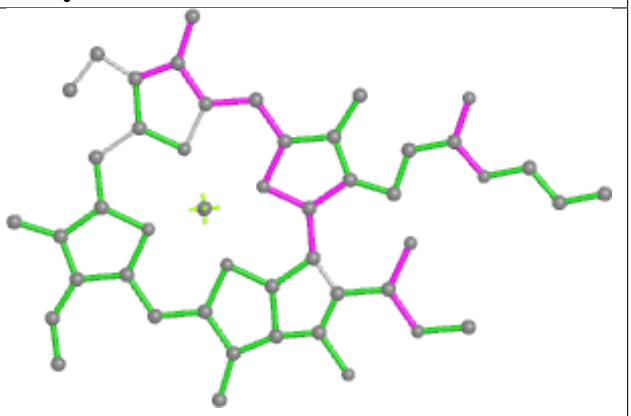
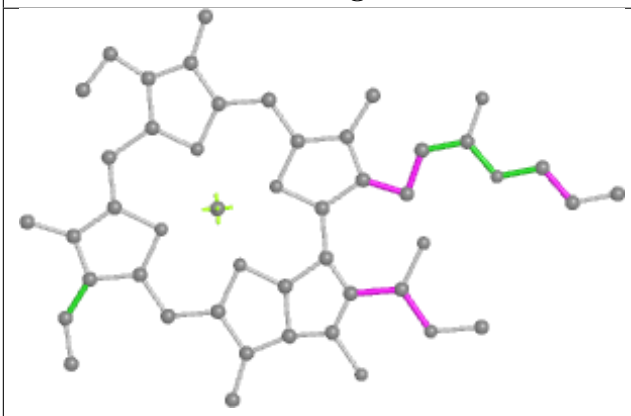
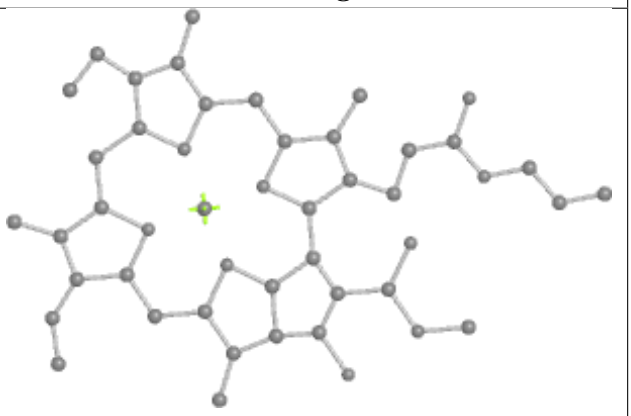


Bond angles

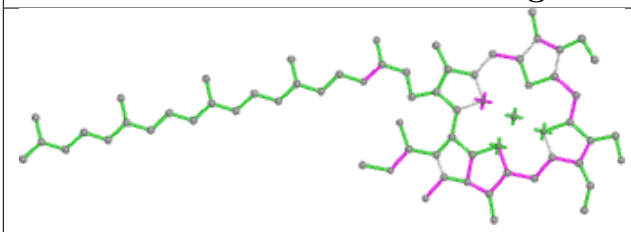


Torsions



Rings

Ligand CHL 2 316



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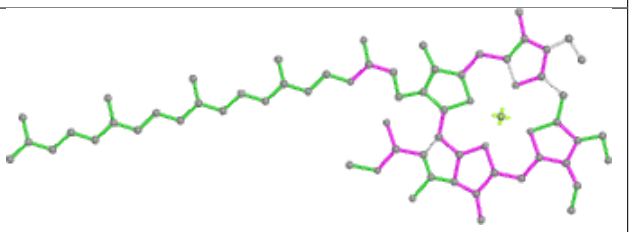
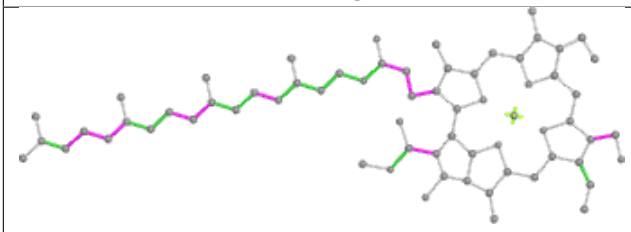
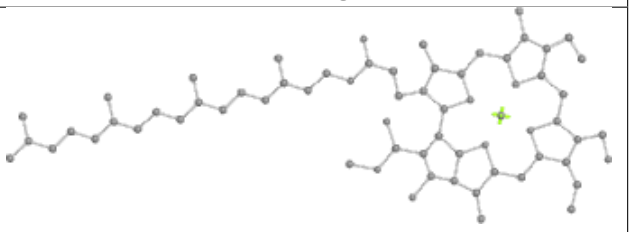


Bond angles

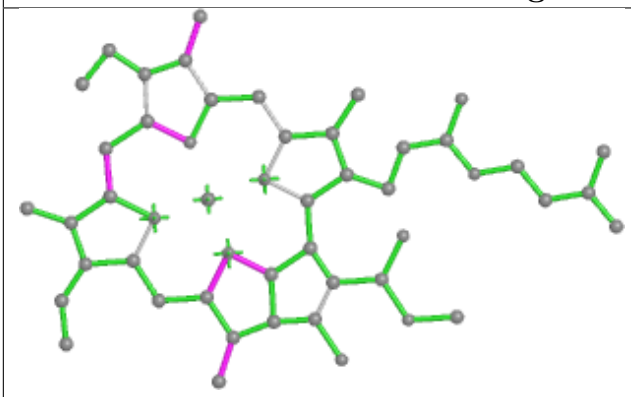


Torsions

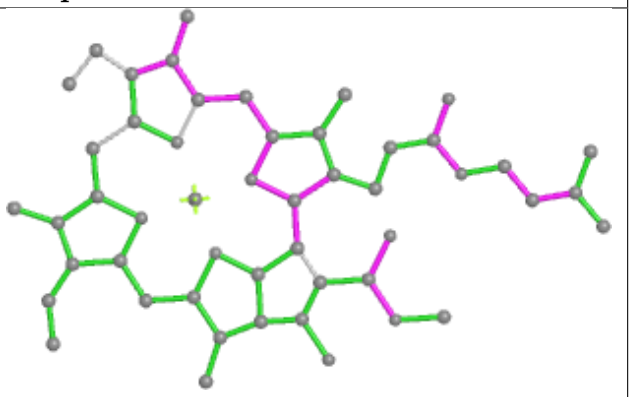


Rings

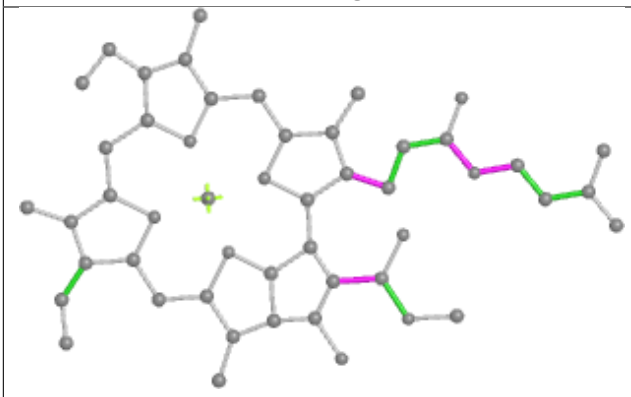
Ligand CLA q 303



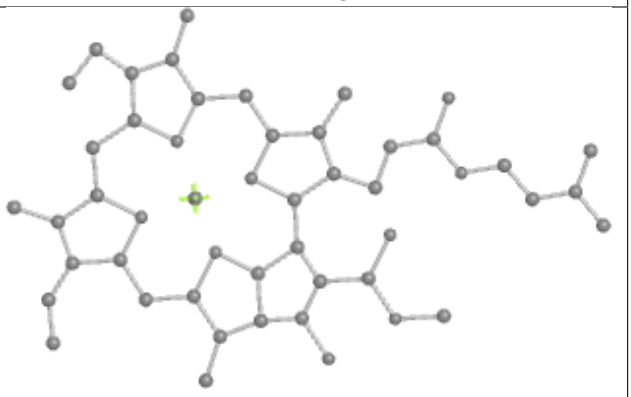
Bond lengths



Bond angles

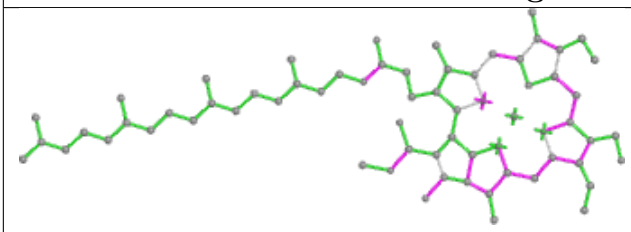


Torsions

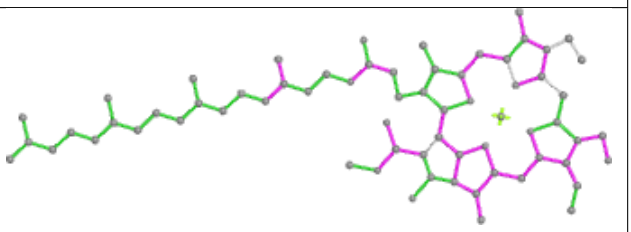


Rings

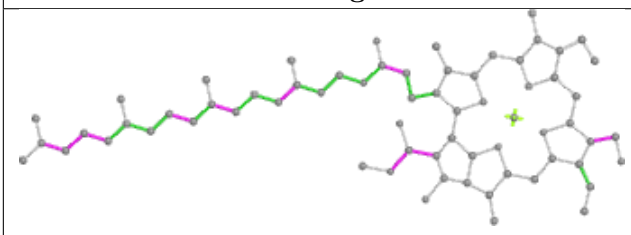
Ligand CHL n 317



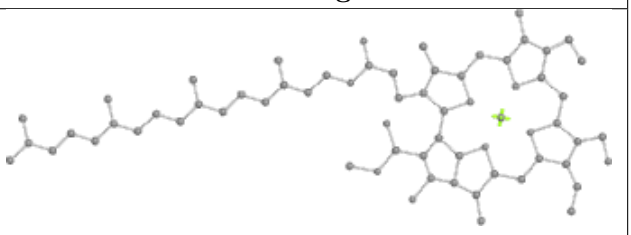
Bond lengths



Bond angles

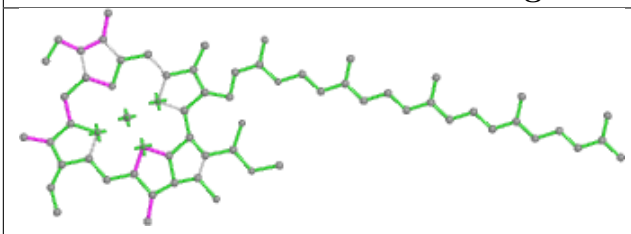


Torsions

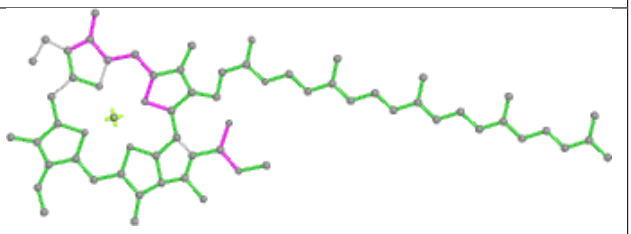


Rings

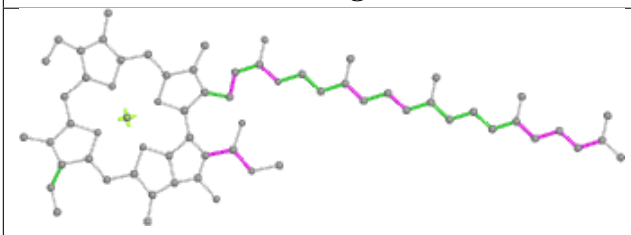
Ligand CLA B 606



Bond lengths



Bond angles



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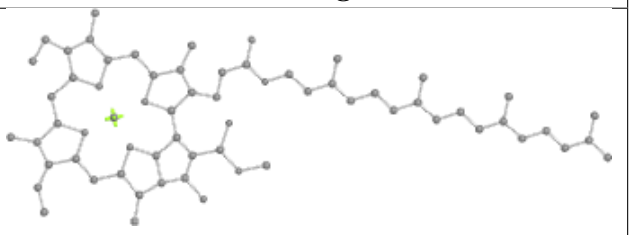
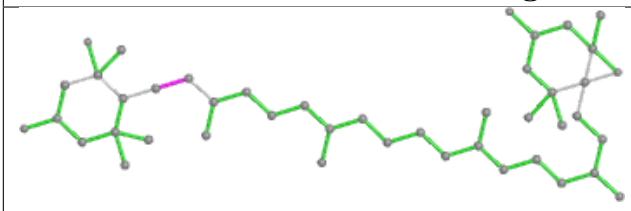


Rings

Ligand NEX V 319



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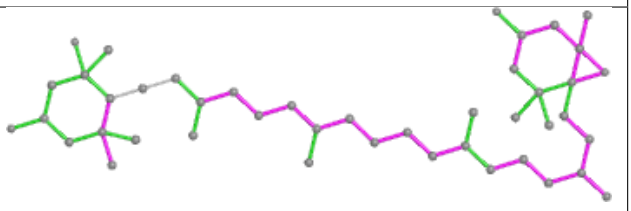

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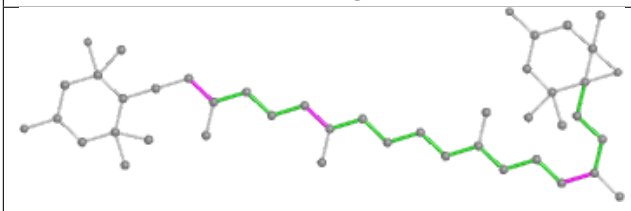

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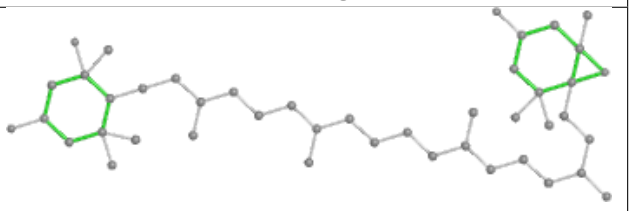
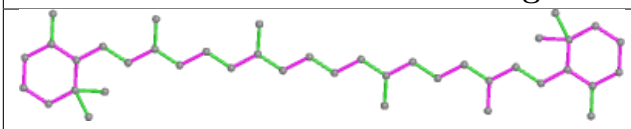


Rings

Ligand BCR B 620



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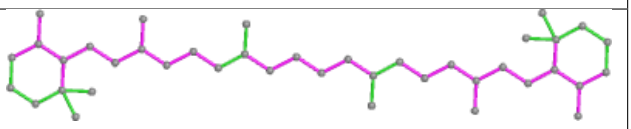
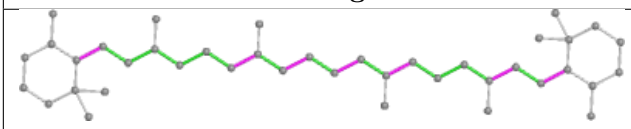


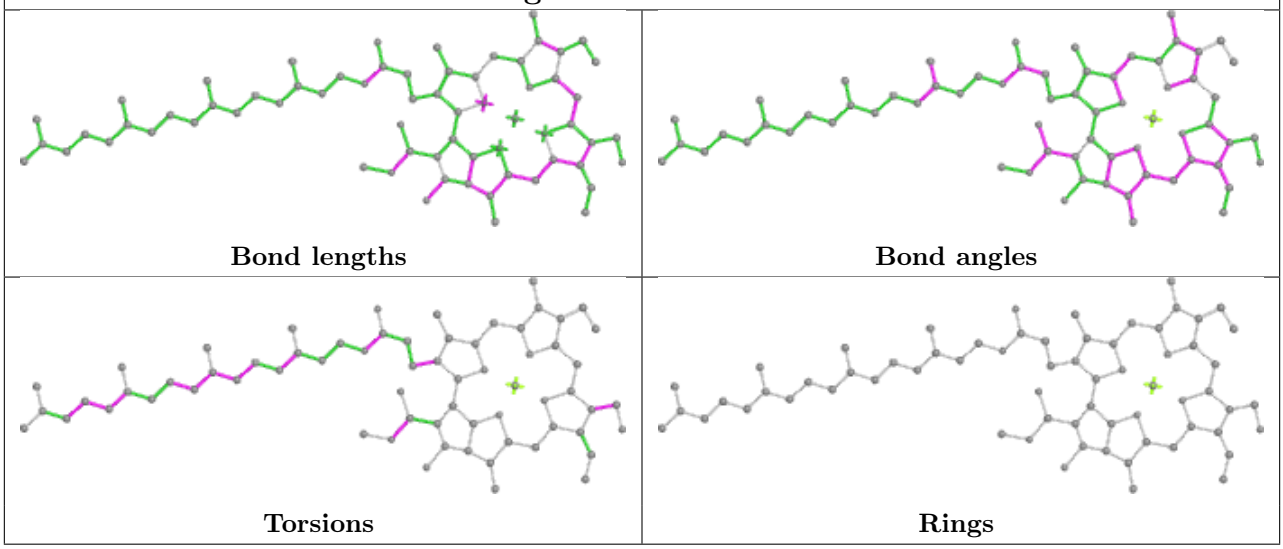
Bond angles



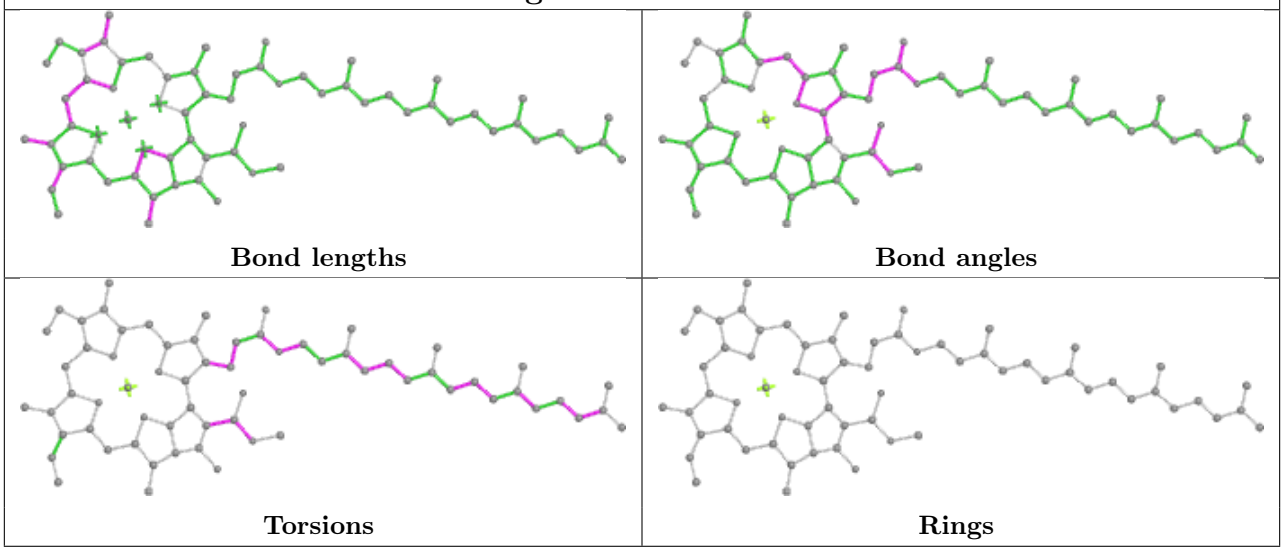
Torsions

Rings

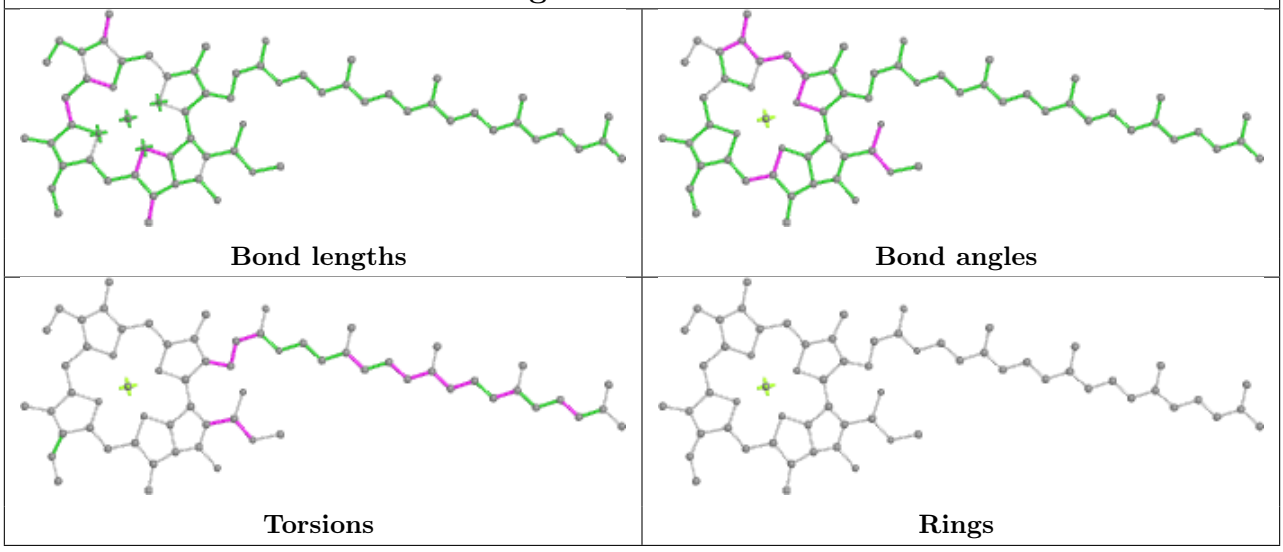
Ligand CHL U 317



Ligand CLA C 504



Ligand CLA 6 302



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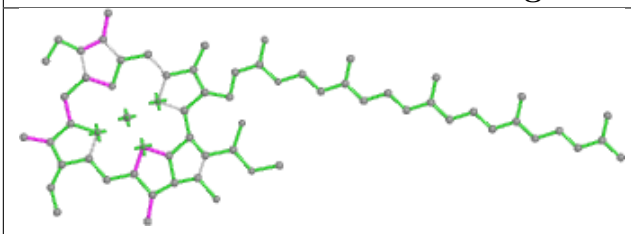

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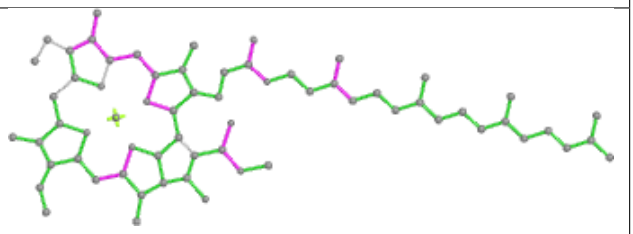
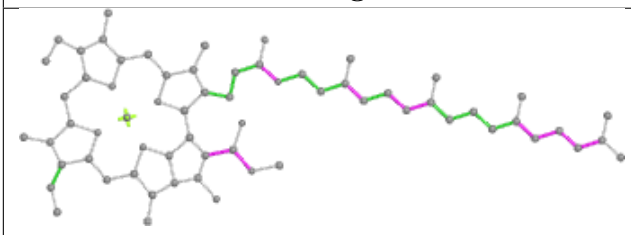


Bond angles



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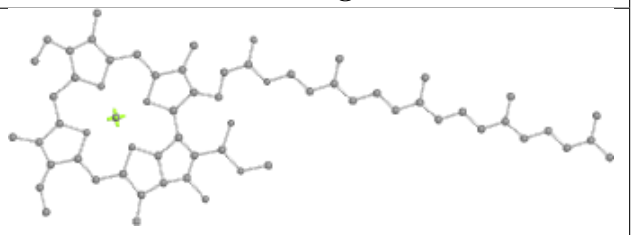
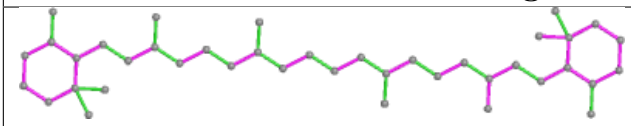


Rings

Ligand BCR C 518



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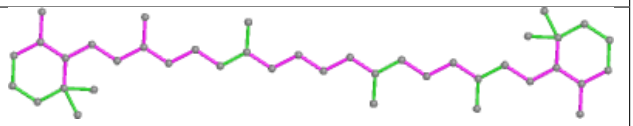
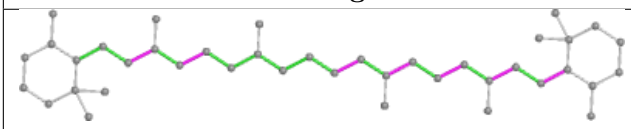


Bond angles



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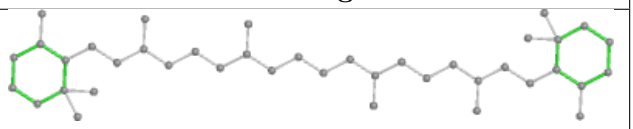
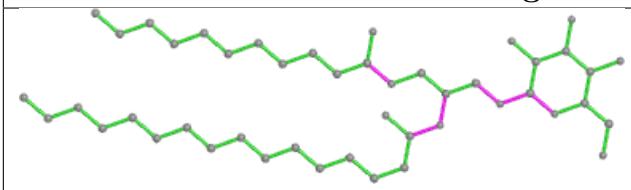


Rings

Ligand LMG d 407



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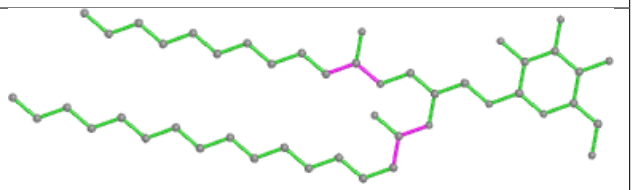
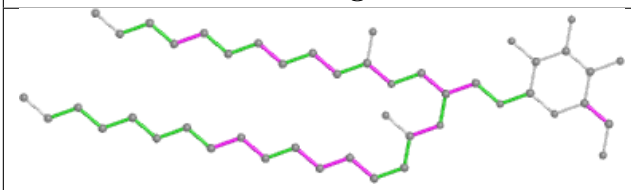


Bond angles



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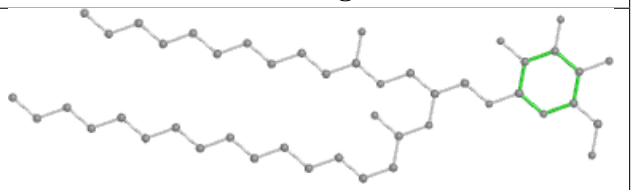
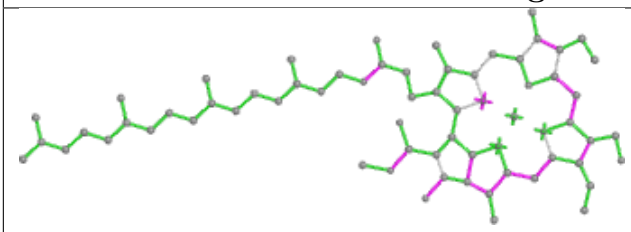
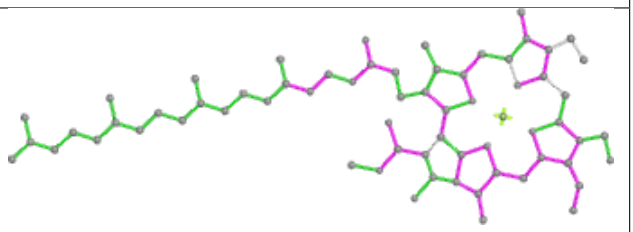
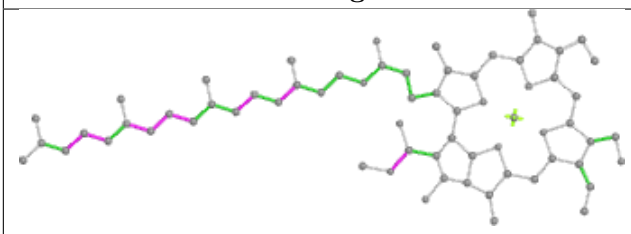
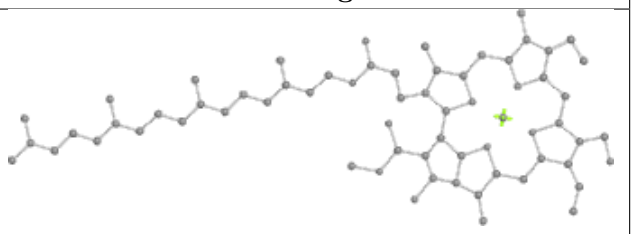
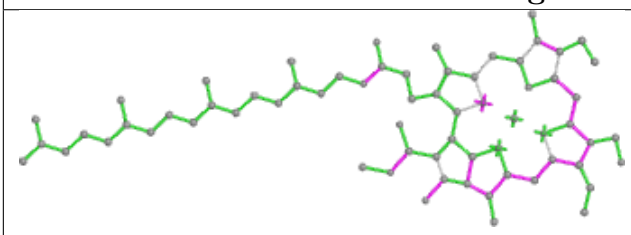
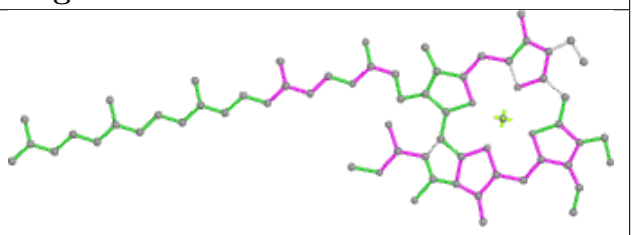
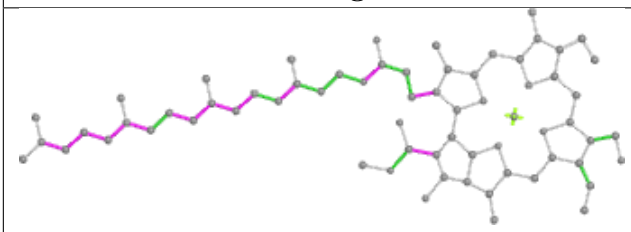
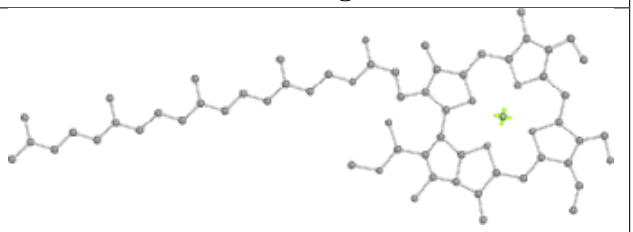
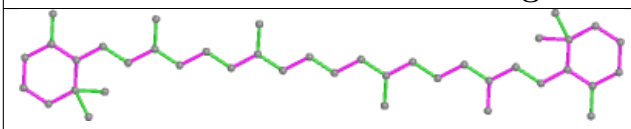
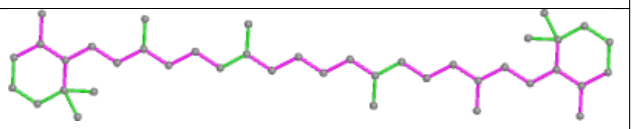
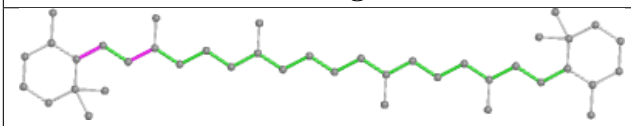
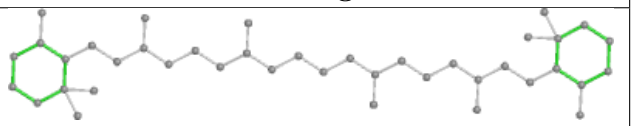


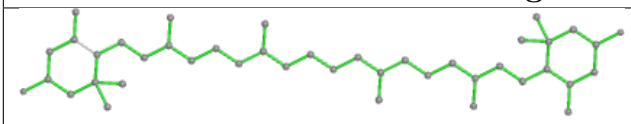
Rings

Ligand CHL 2 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

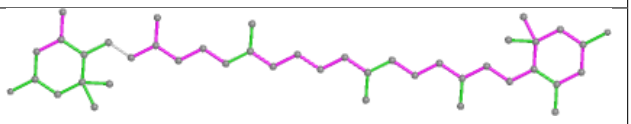
Ligand CHL g 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

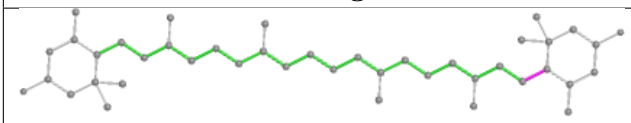
Ligand LUT P 310



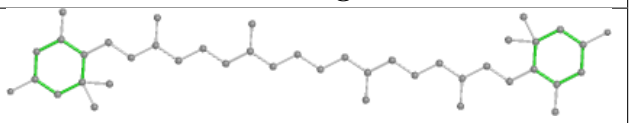
Bond lengths



Bond angles

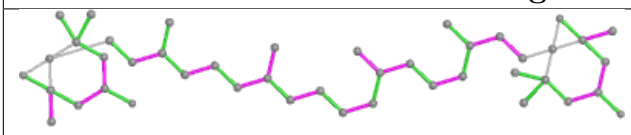


Torsions

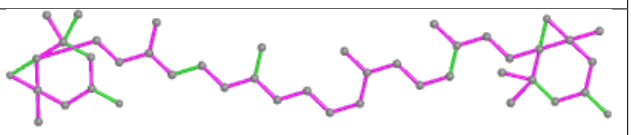


Rings

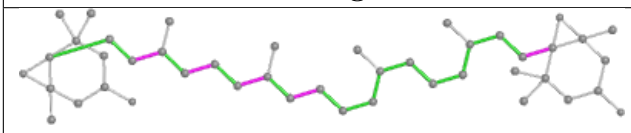
Ligand XAT r 612



Bond lengths



Bond angles



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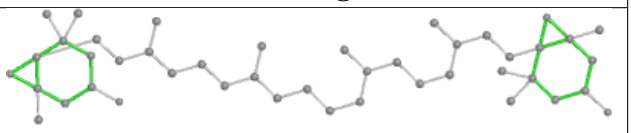
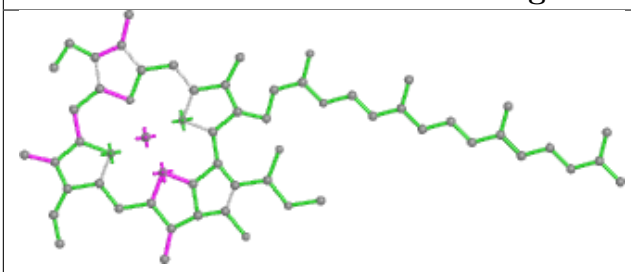
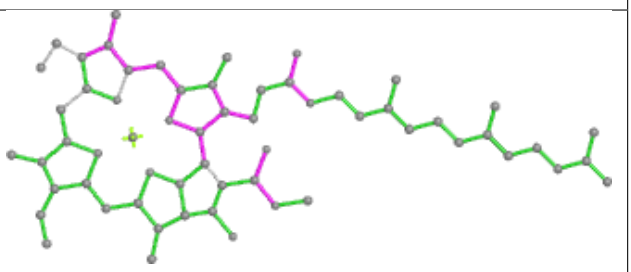


Rings

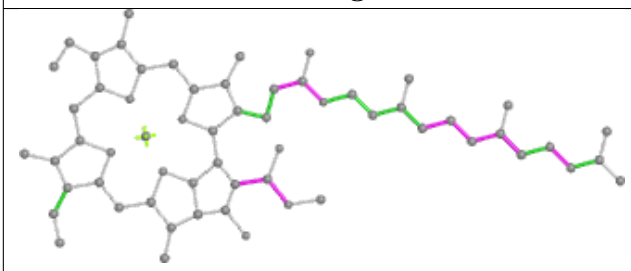
Ligand CLA 1 306



Bond lengths



Bond angles



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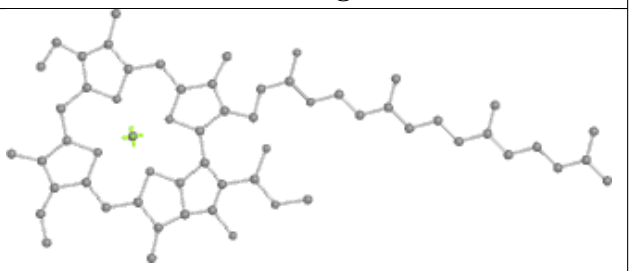
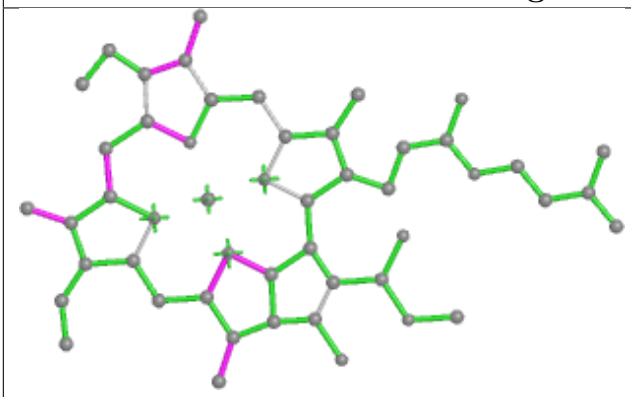
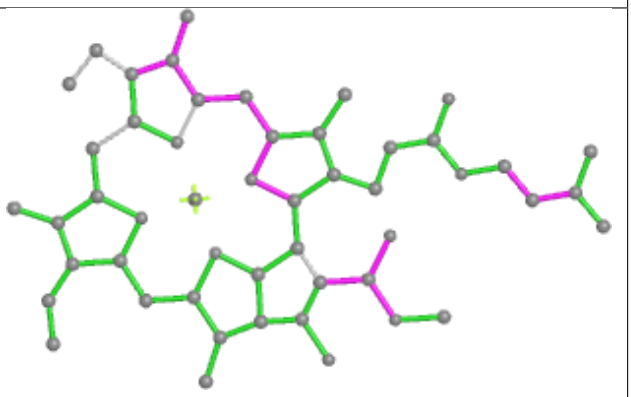
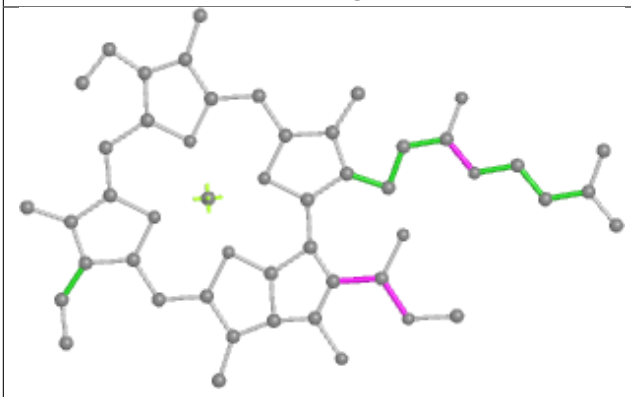
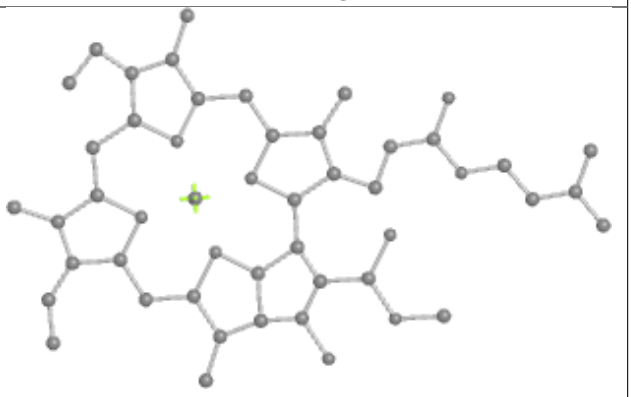
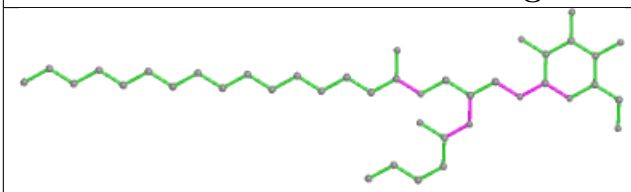
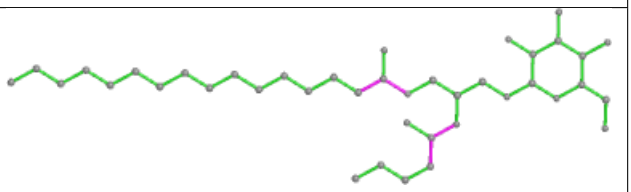
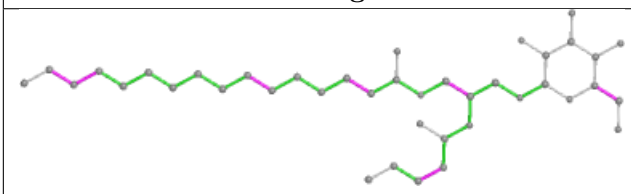
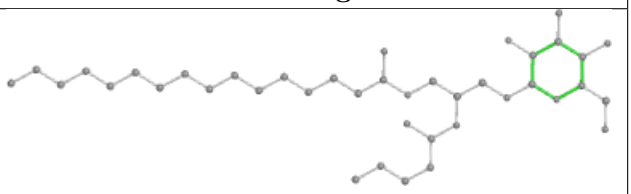
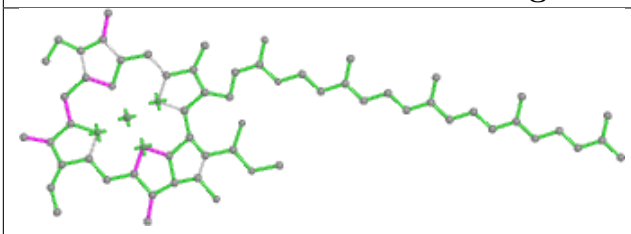
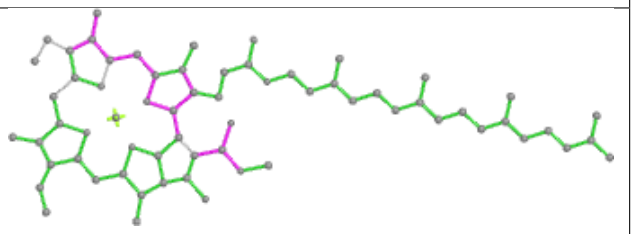
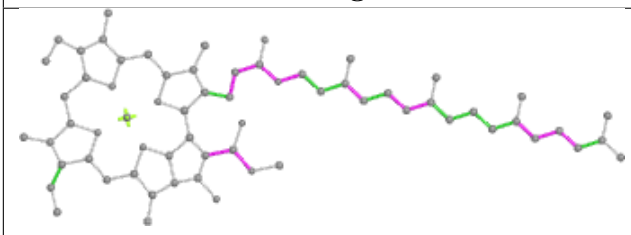
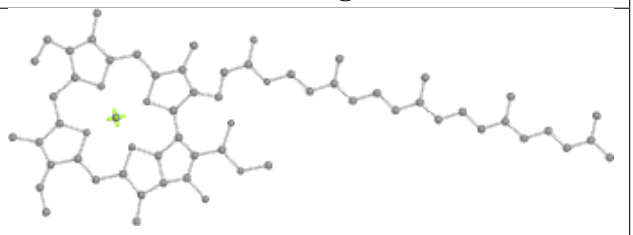
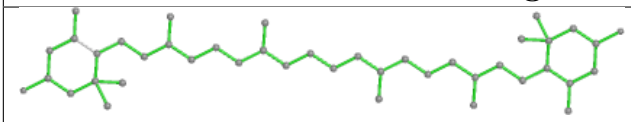
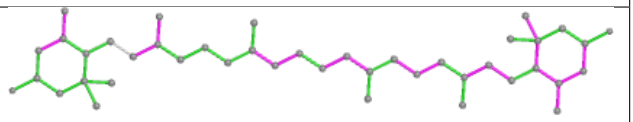
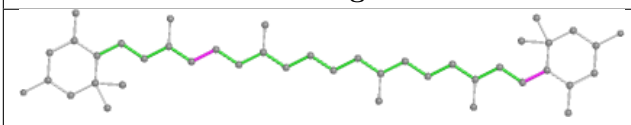
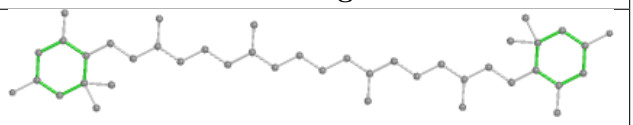


Rings

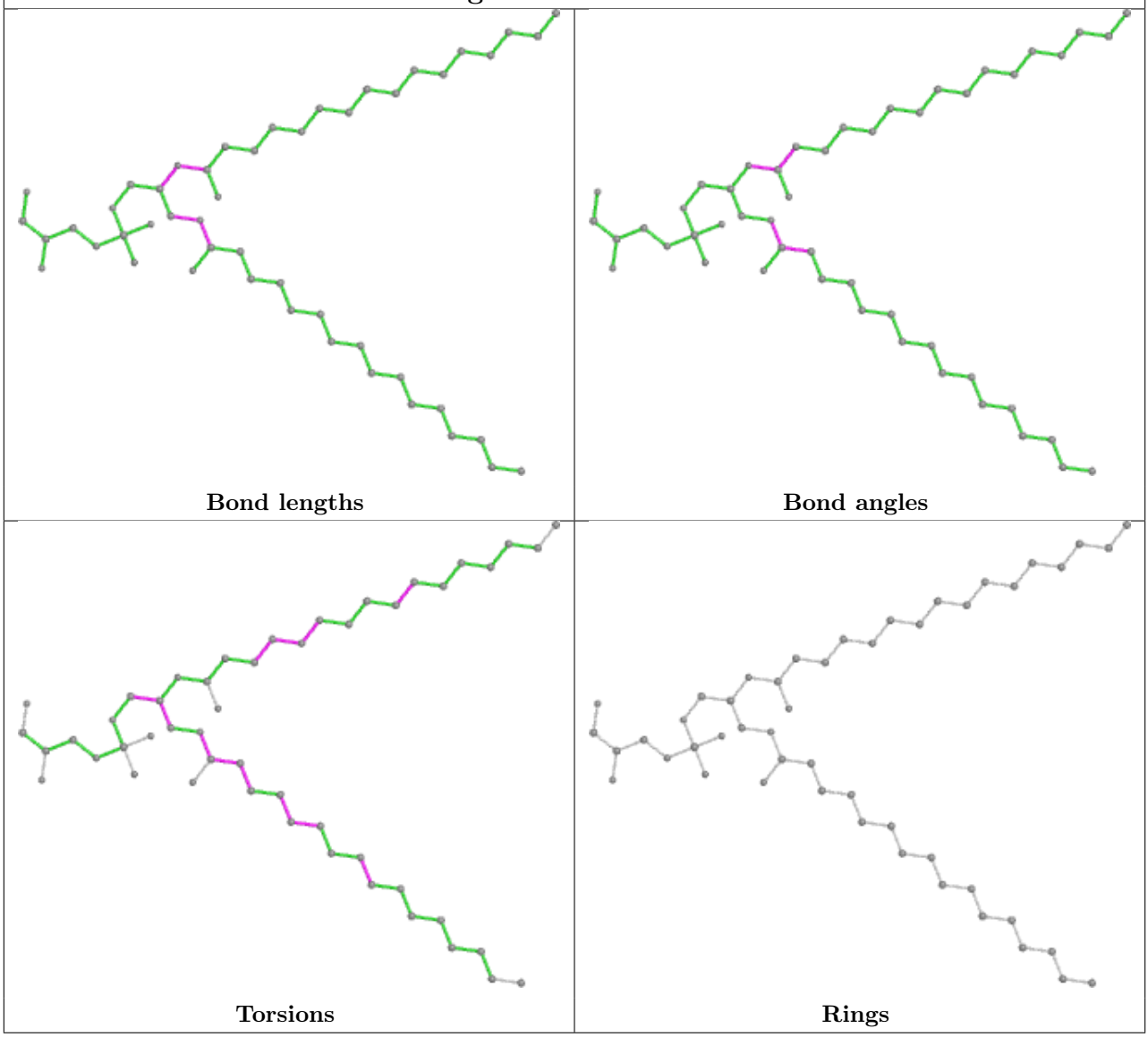
Ligand CLA u 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

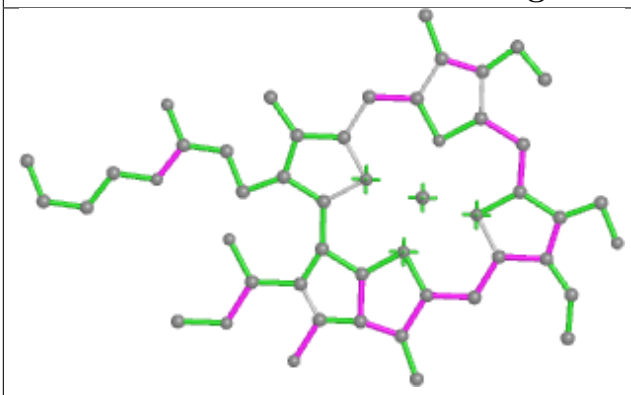
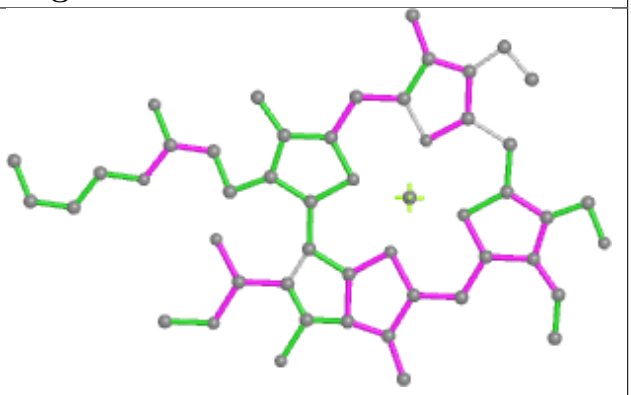
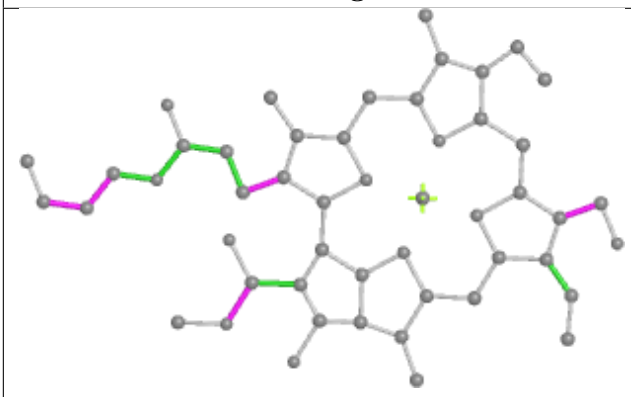
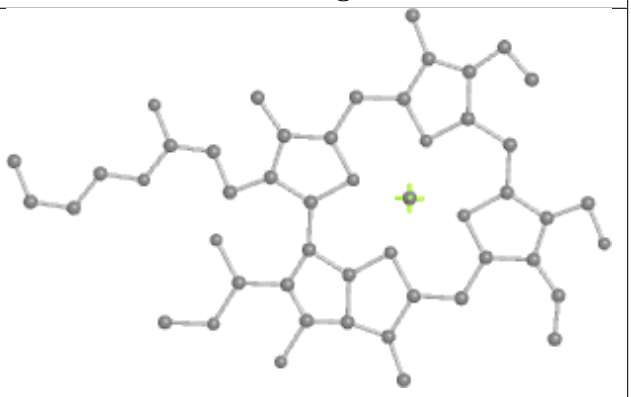
Ligand LMG a 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

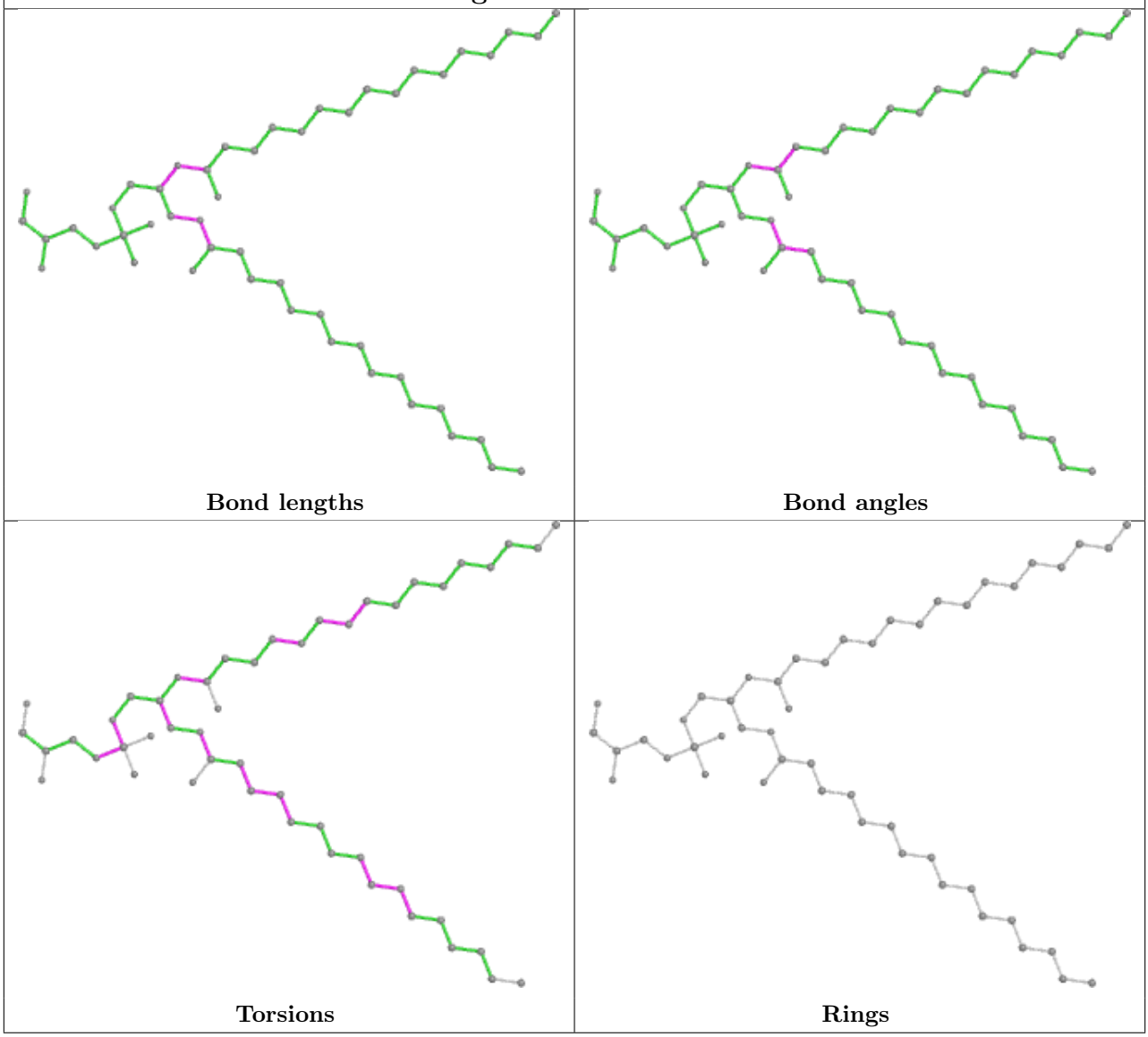
Ligand LUT U 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG N 312

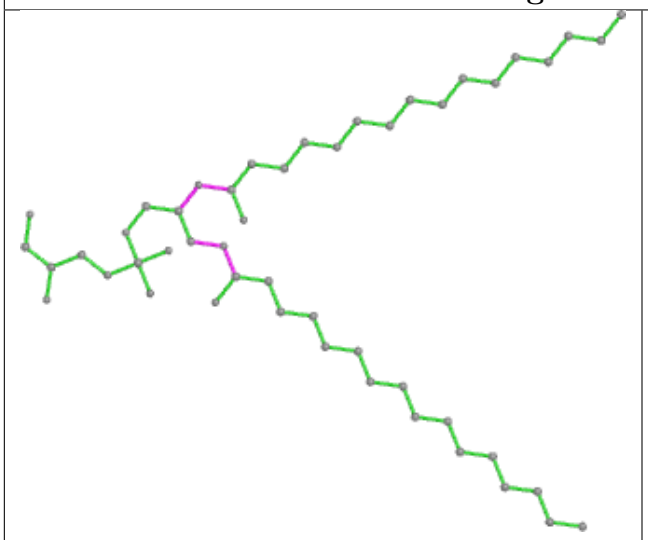


Ligand CHL g 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

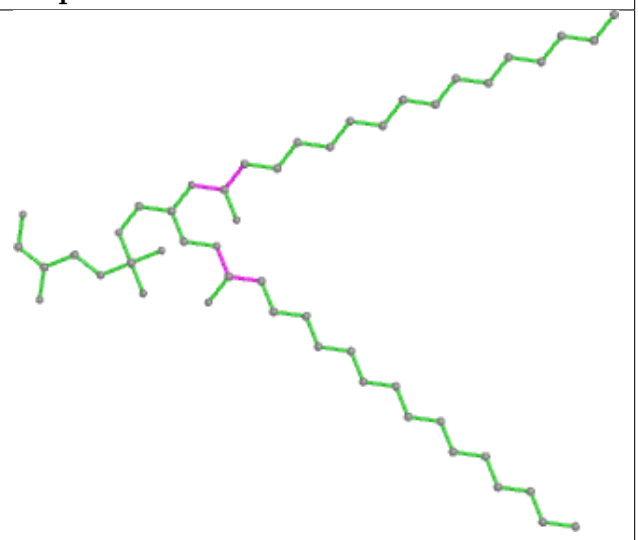
Ligand LHG v 312



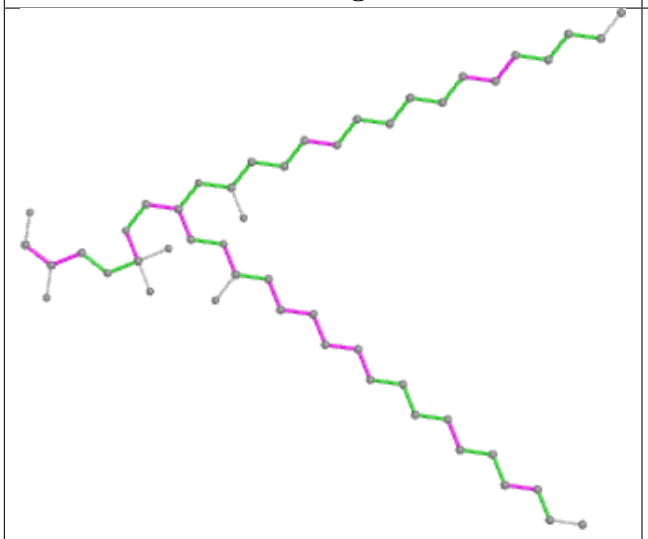
Ligand LHG p 313



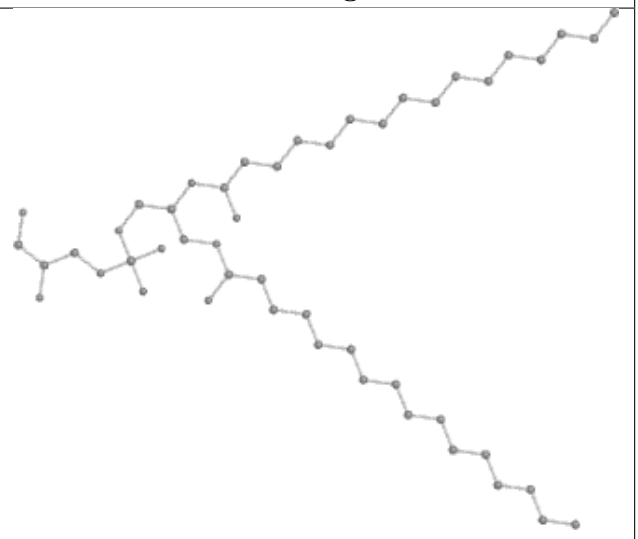
Bond lengths



Bond angles

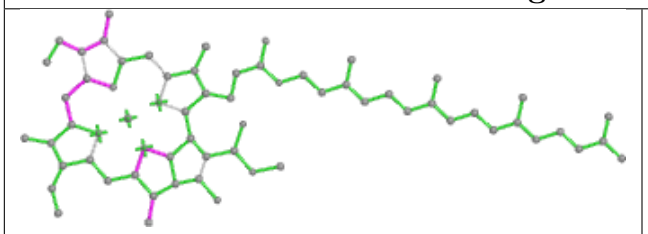


Torsions

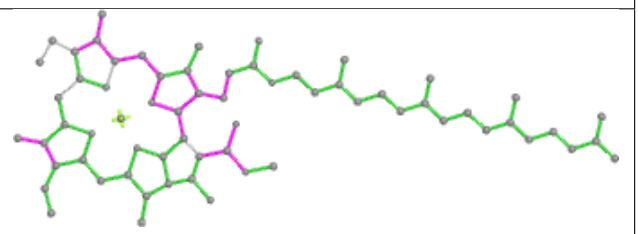


Rings

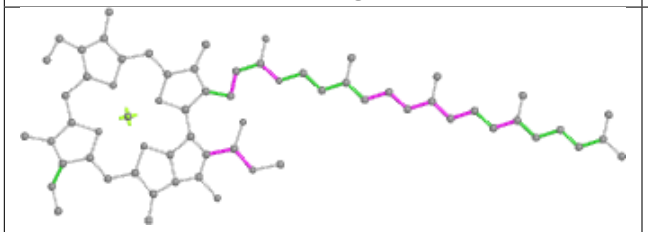
Ligand CLA b 605



Bond lengths



Bond angles



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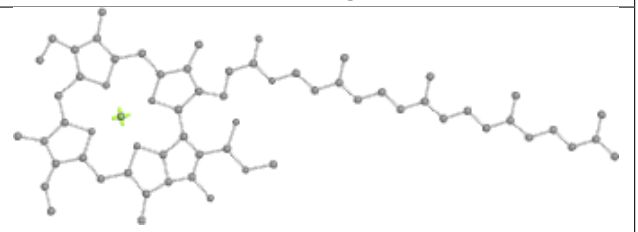
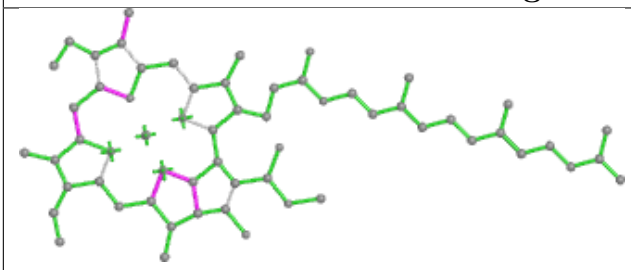
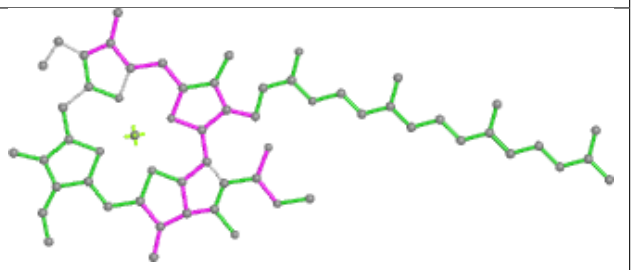


Rings

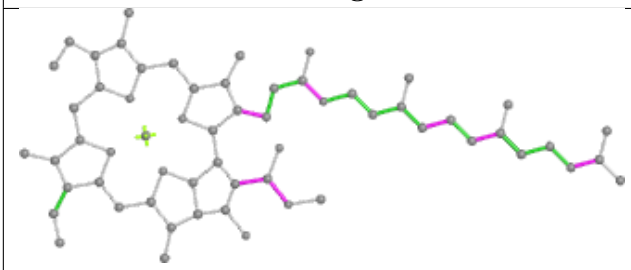
Ligand CLA N 305



Bond lengths



Bond angles



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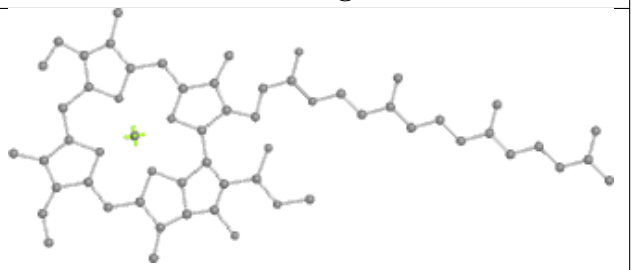
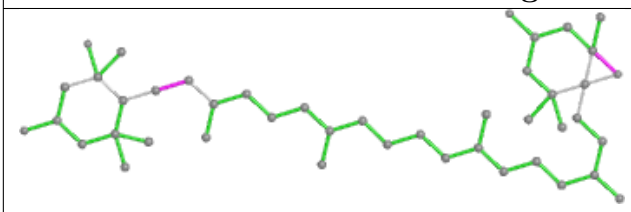
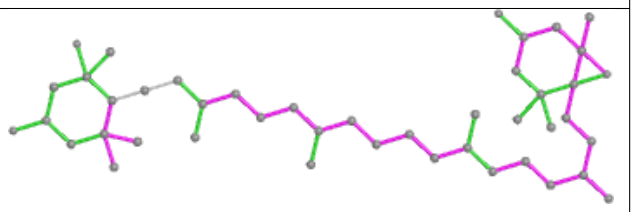


Rings

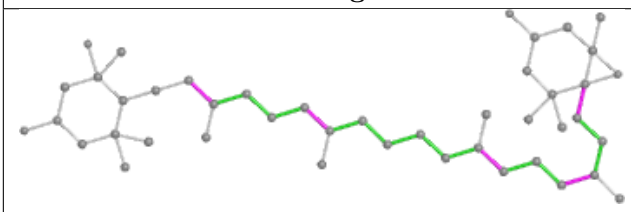
Ligand NEX N 318



Bond lengths



Bond angles



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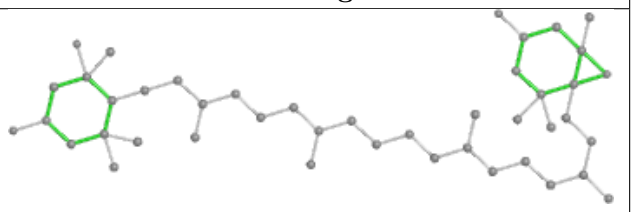
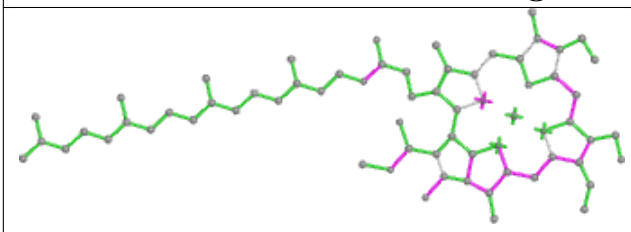
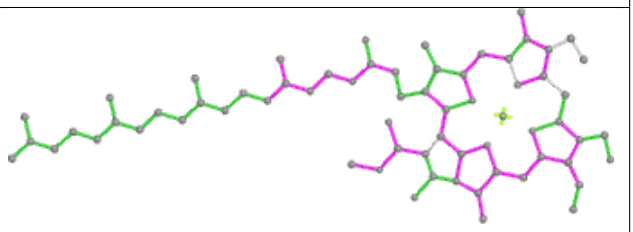


Rings

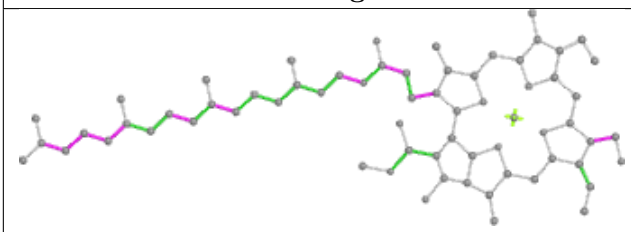
Ligand CHL 4 316



Bond lengths



Bond angles



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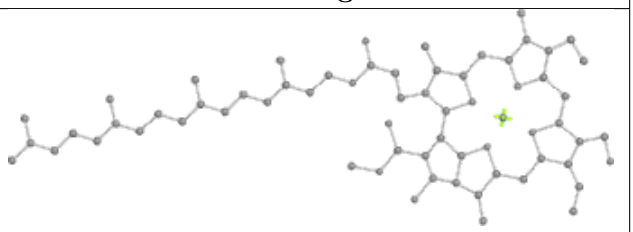
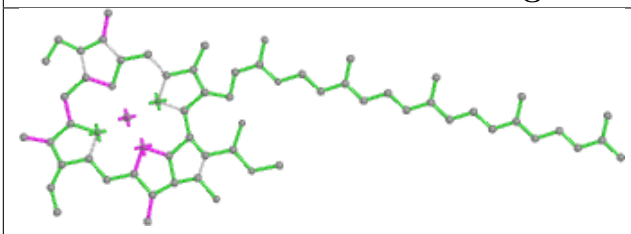
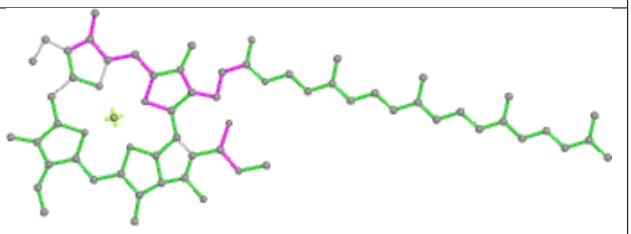


Rings

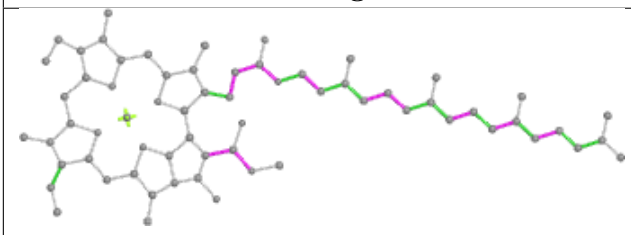
Ligand CLA A 404



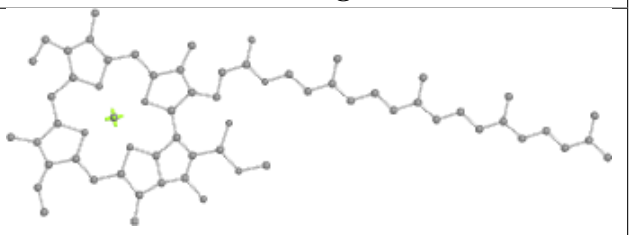
Bond lengths



Bond angles

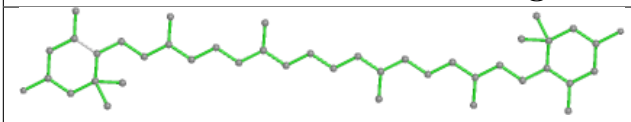


Torsions

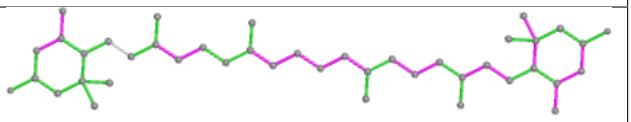


Rings

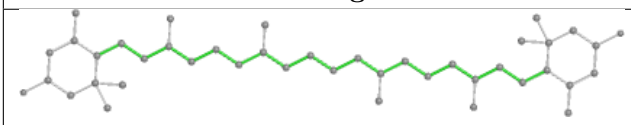
Ligand LUT v 310



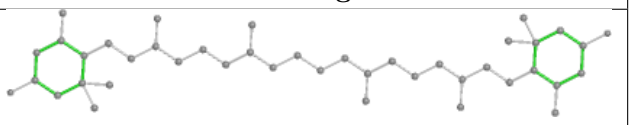
Bond lengths



Bond angles

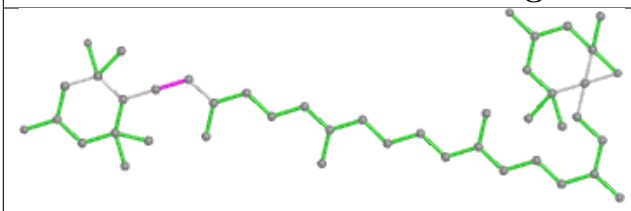


Torsions

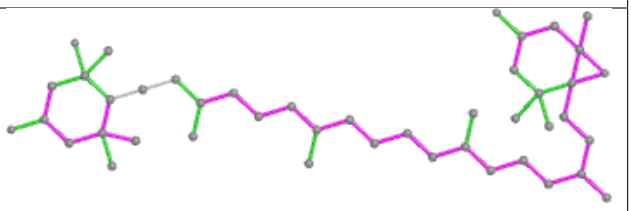


Rings

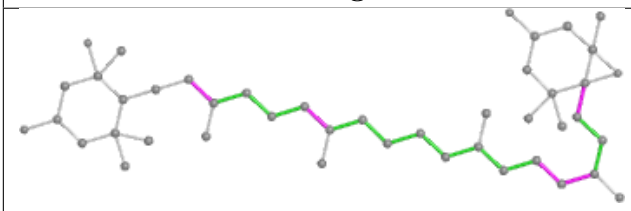
Ligand NEX u 319



Bond lengths



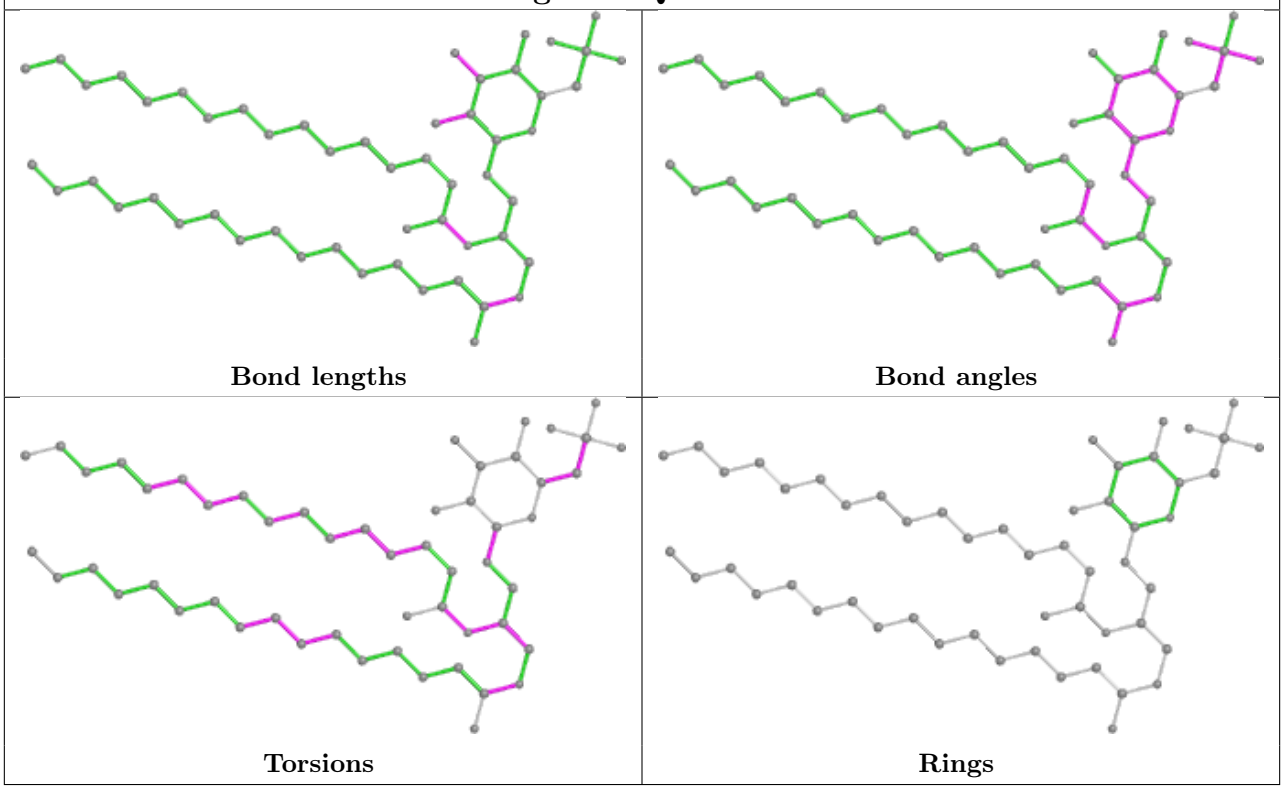
Bond angles



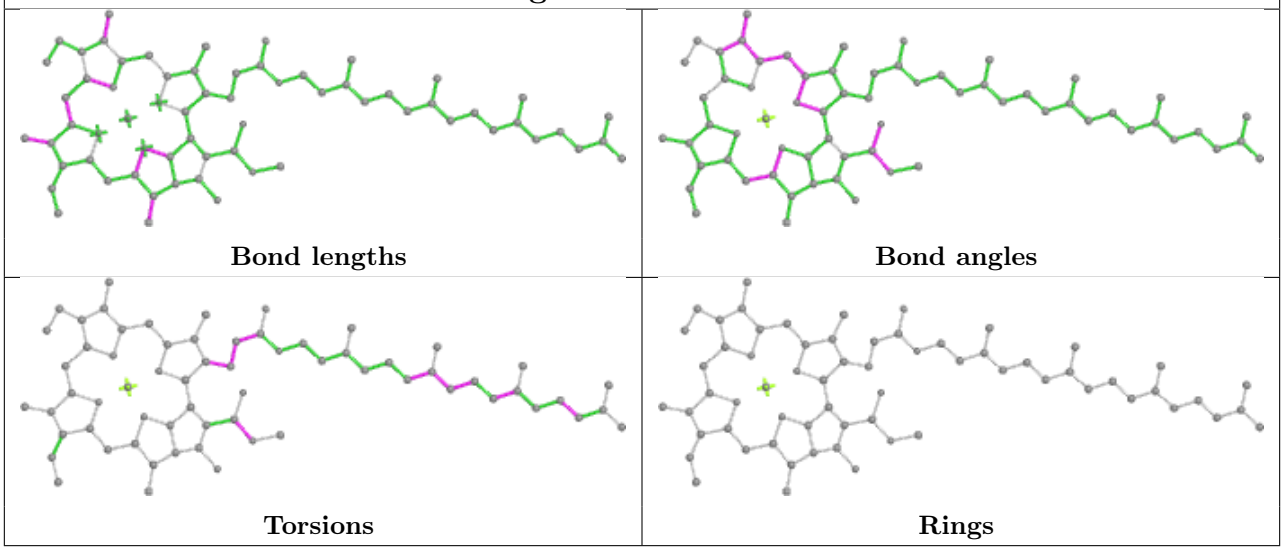
Torsions

Rings

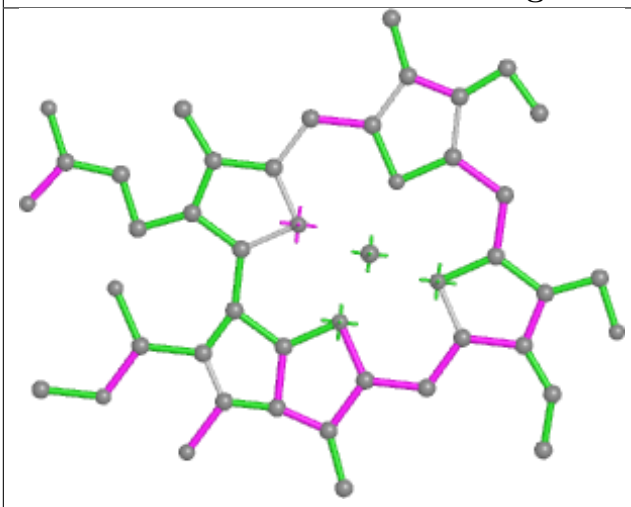
Ligand SQD l 102



Ligand CLA 3 301



Ligand CHL S 314



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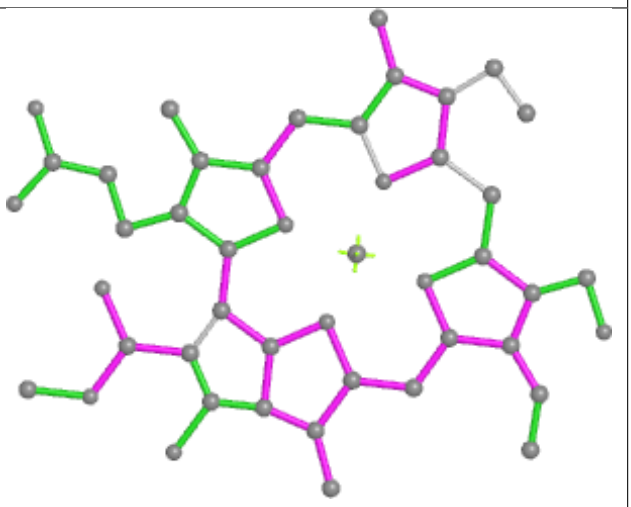
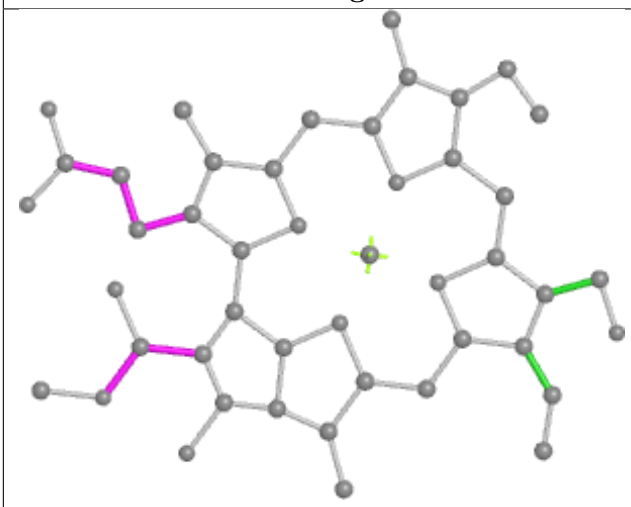
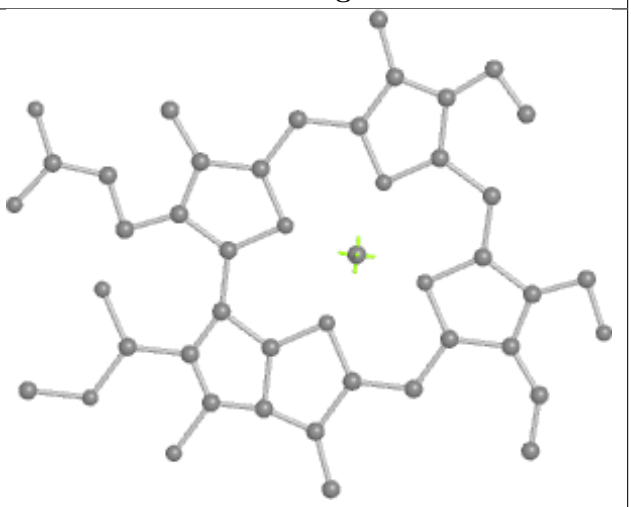


Bond angles

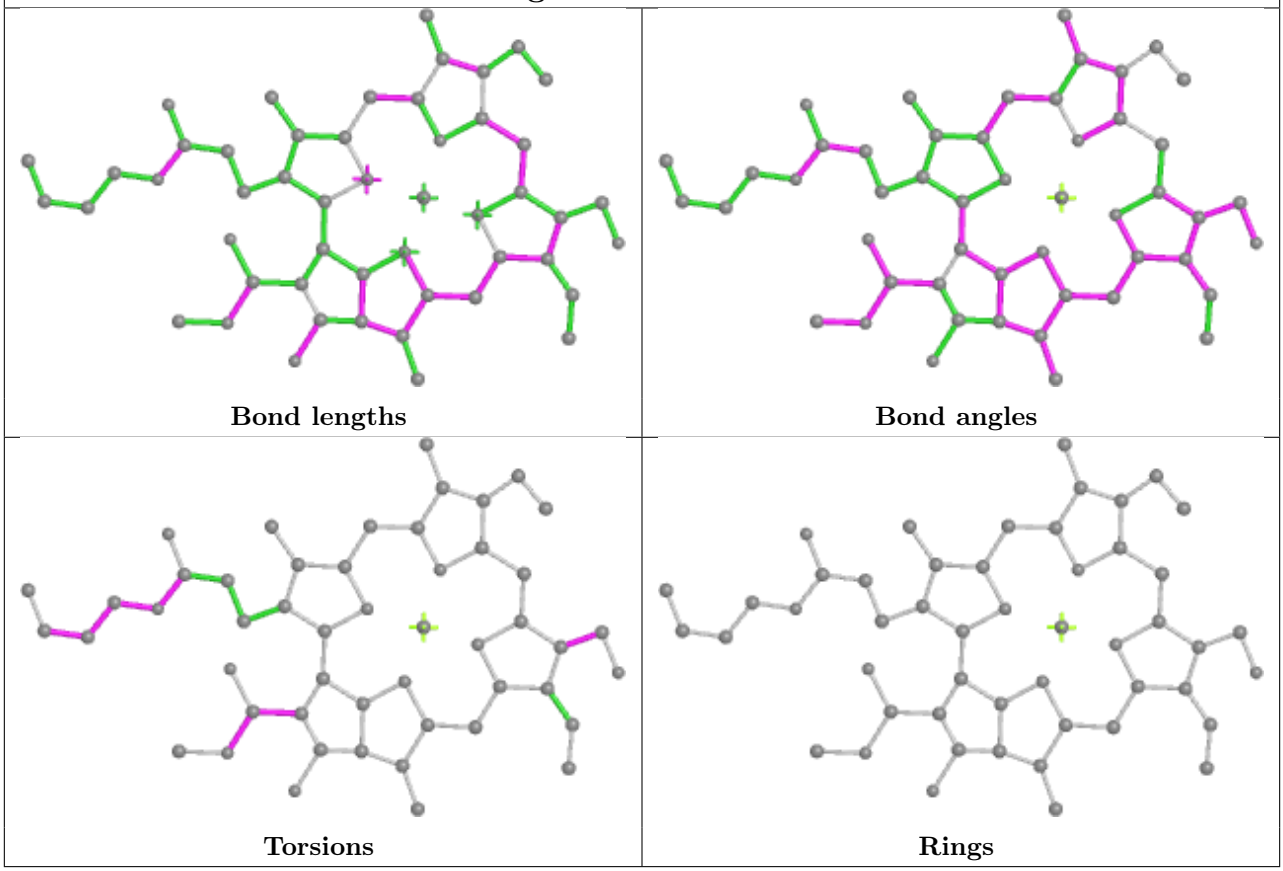


Torsions

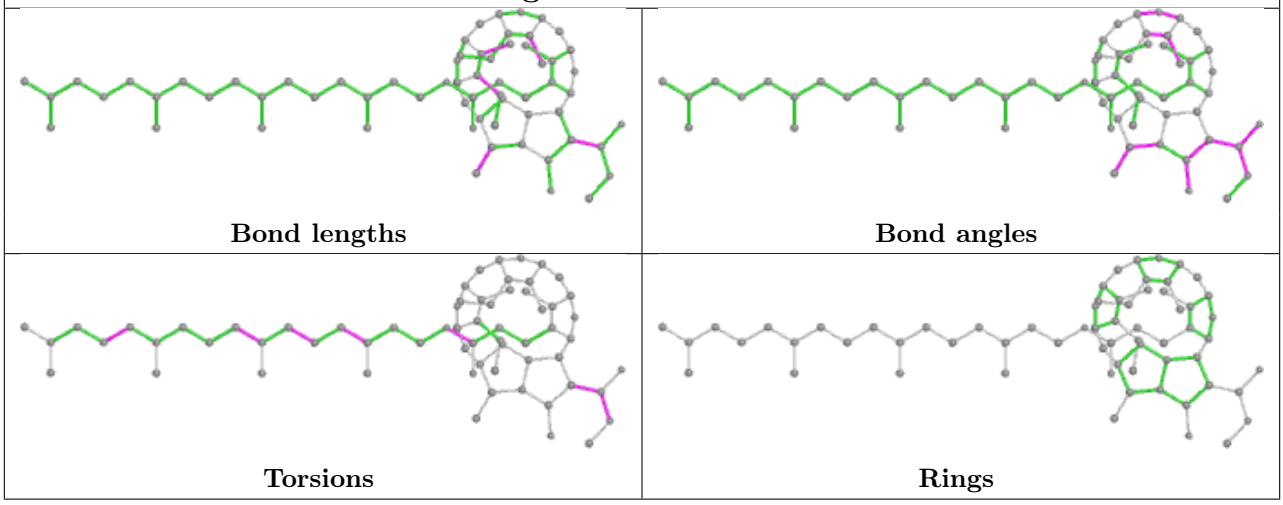


Rings

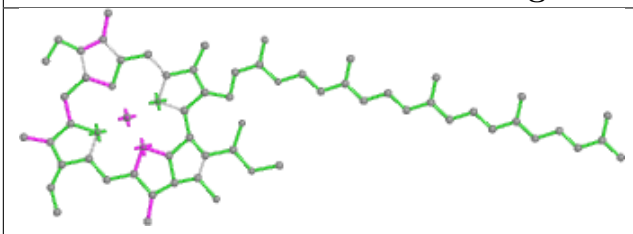
Ligand CHL n 315



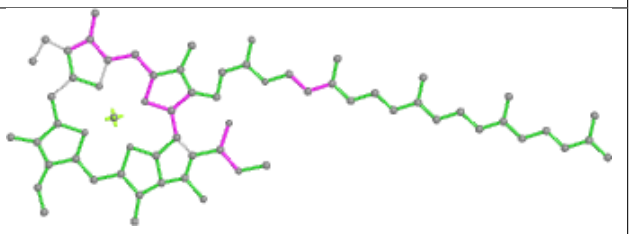
Ligand PHO A 407



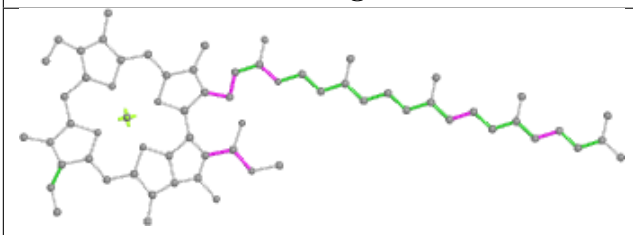
Ligand CLA a 405



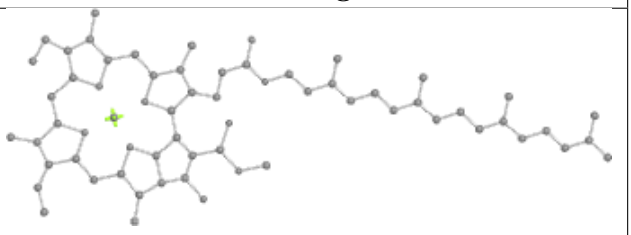
Bond lengths



Bond angles

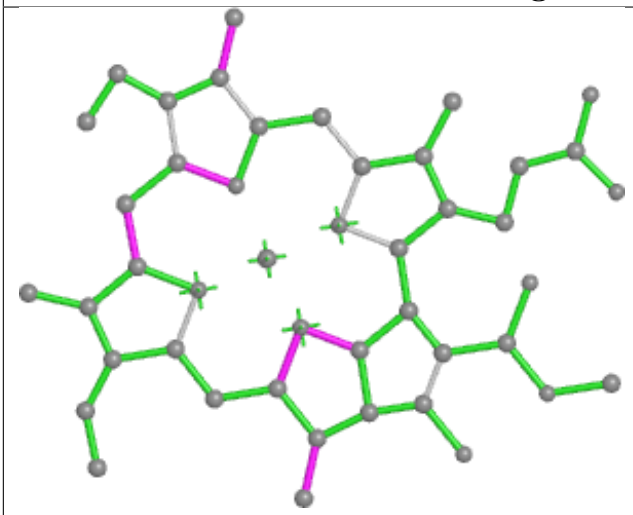


Torsions

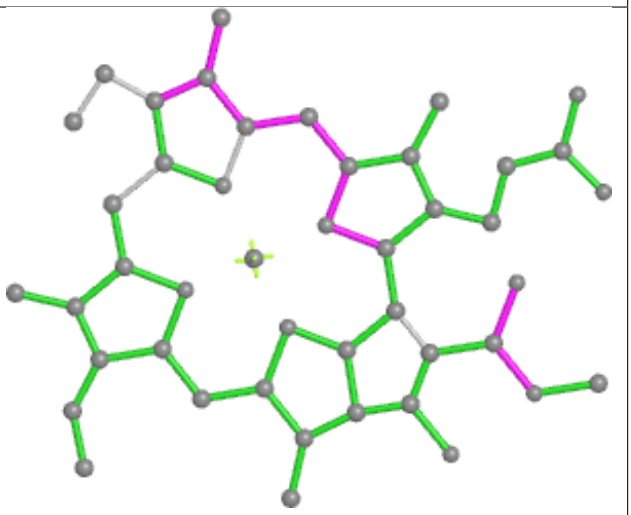


Rings

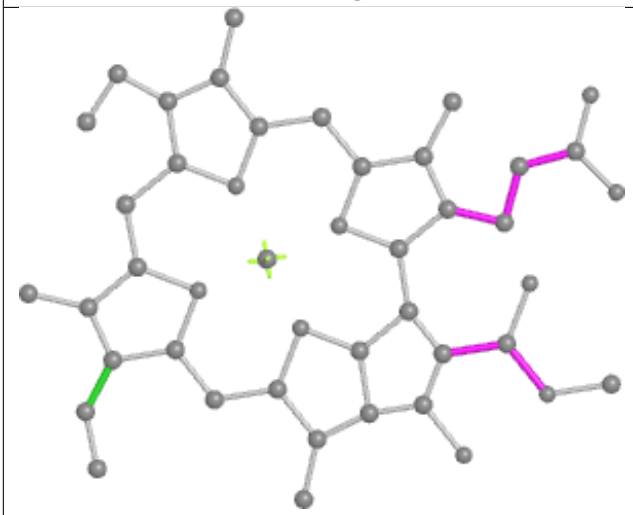
Ligand CLA s 304



Bond lengths



Bond angles



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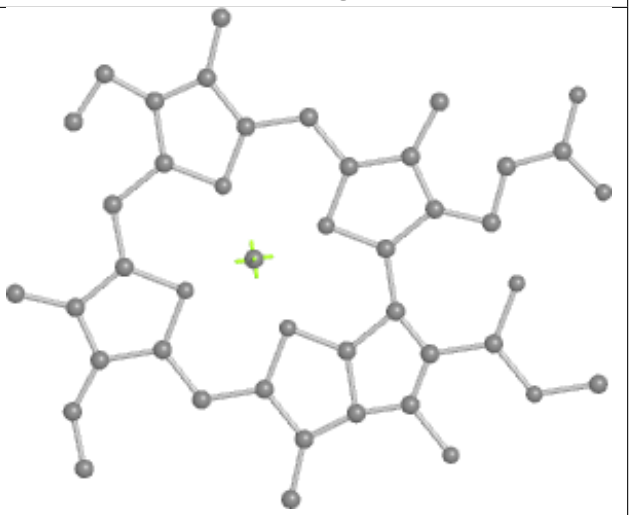
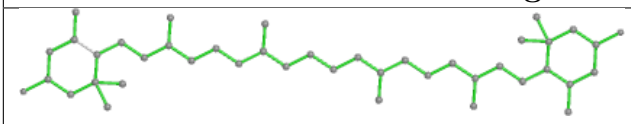


Rings

Ligand LUT V 309



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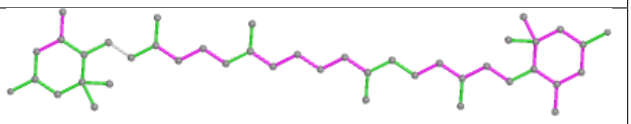
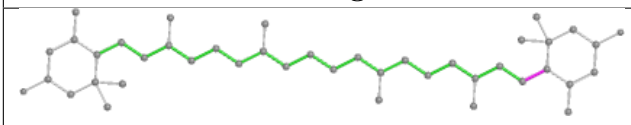


Bond angles



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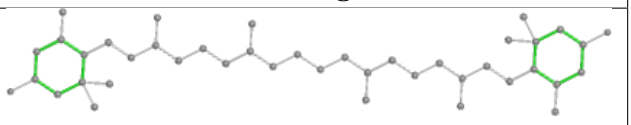
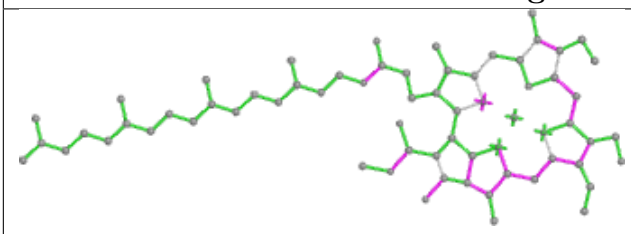


Rings

Ligand CHL 4 317



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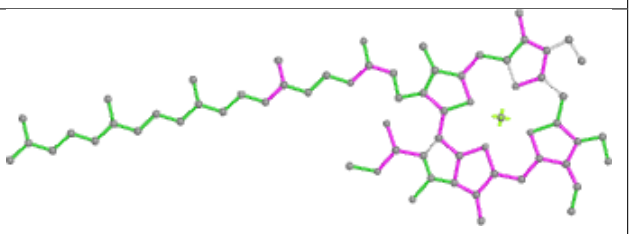
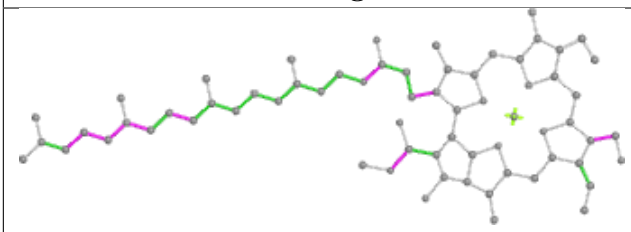
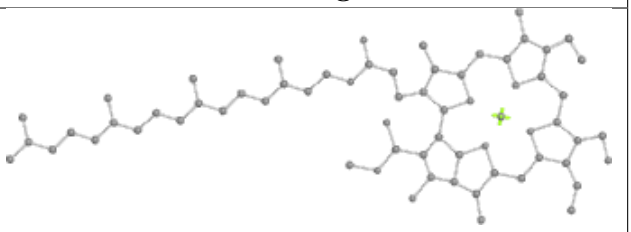


Bond angles

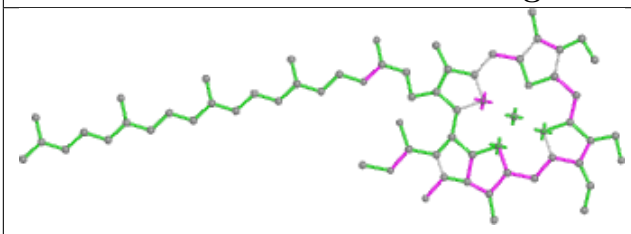


Torsions



Rings

Ligand CHL V 313



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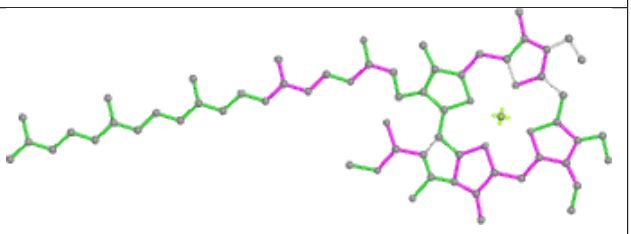
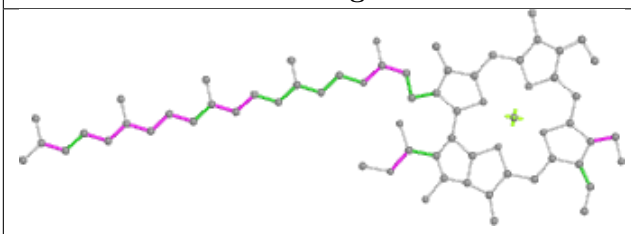


Bond angles



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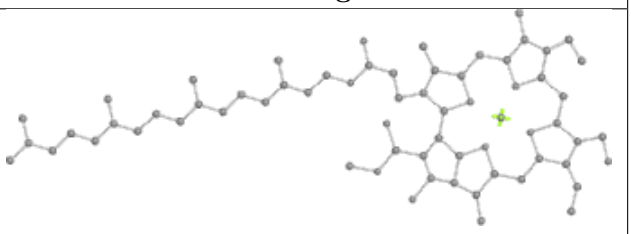
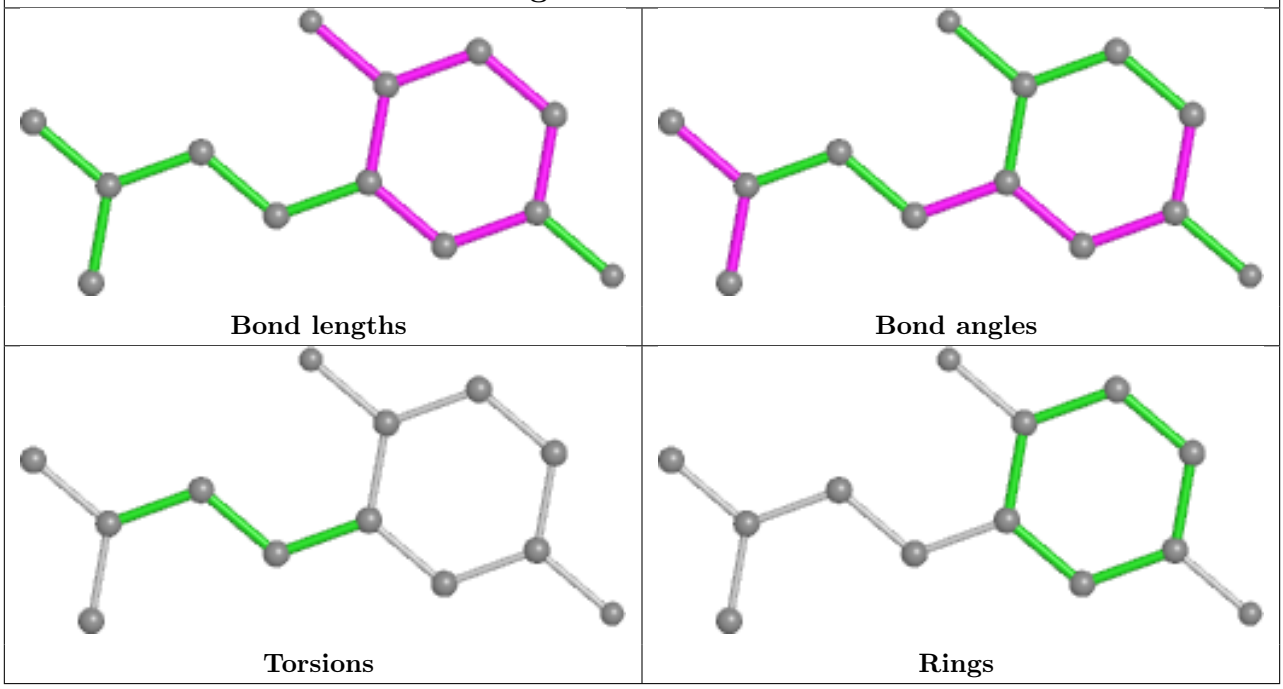
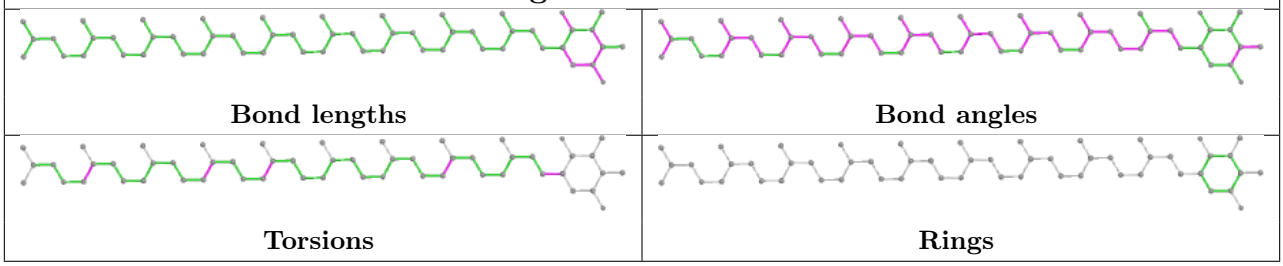


Rings

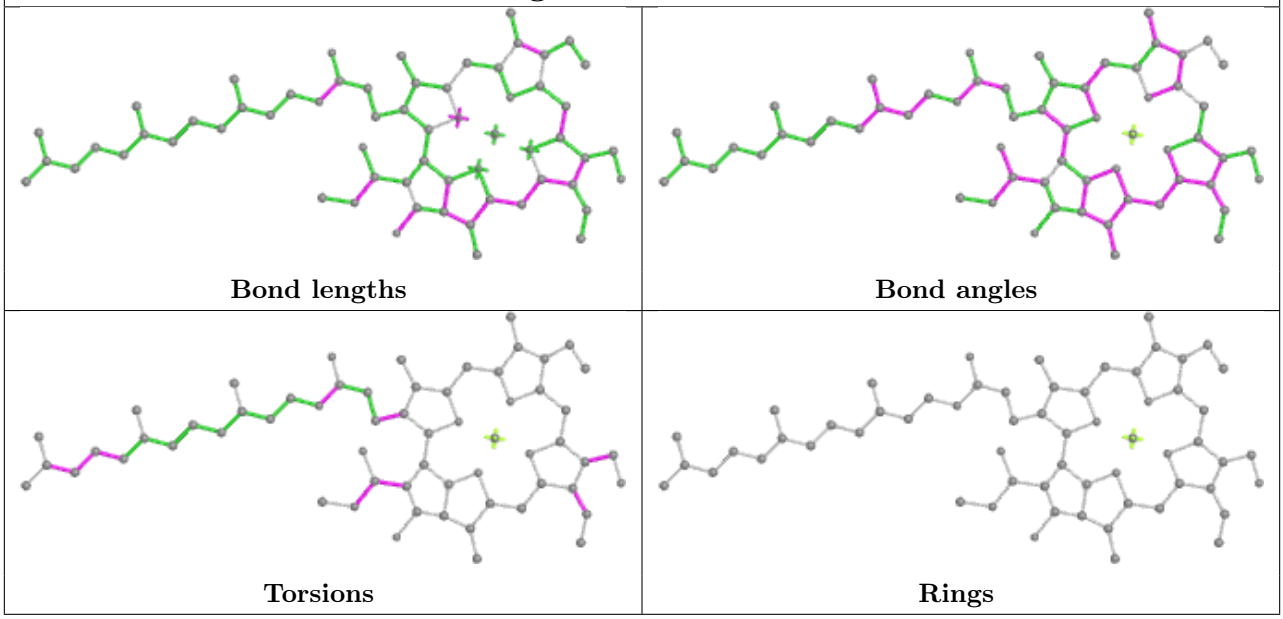
Ligand PL9 A 410

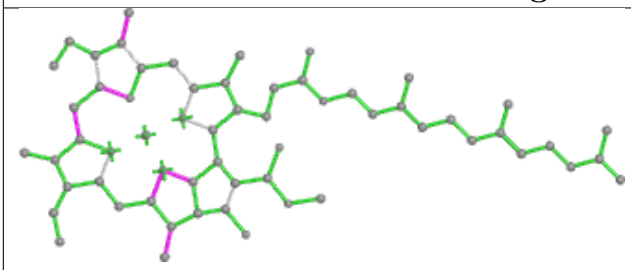
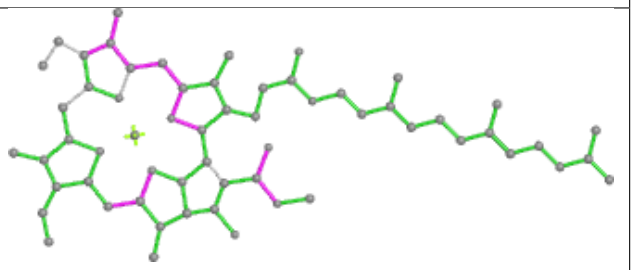
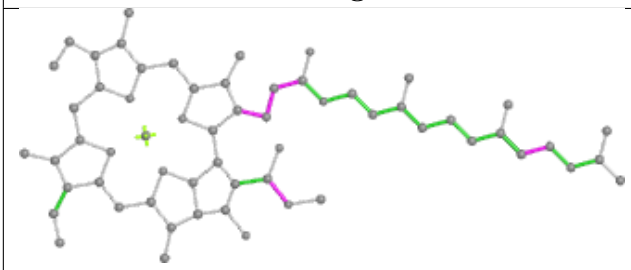
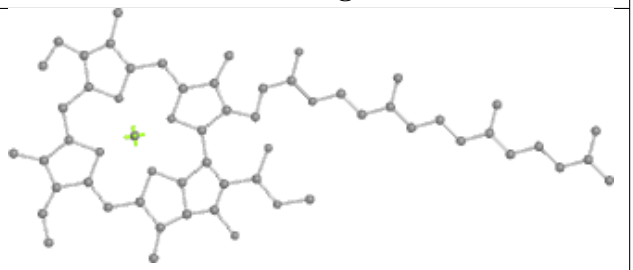


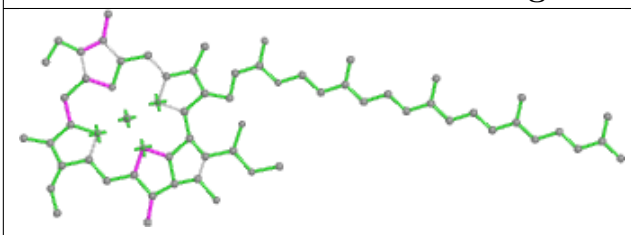
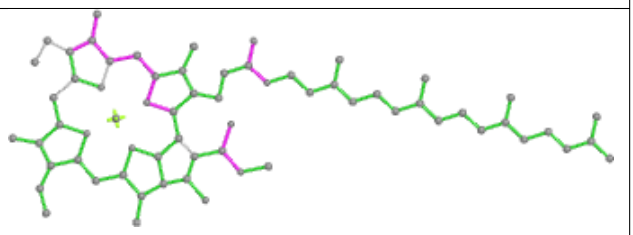
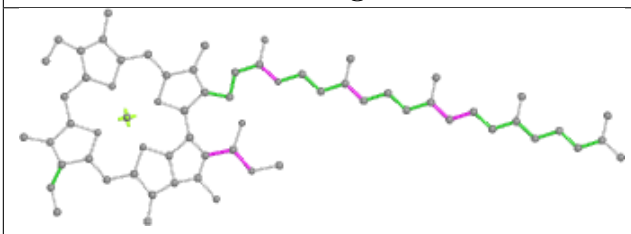
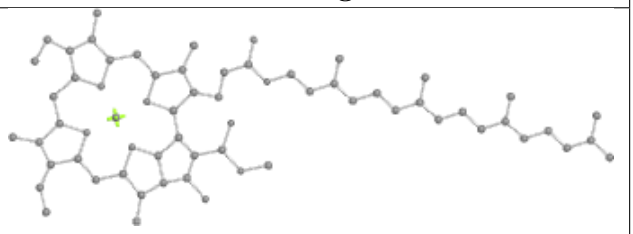
Ligand PL9 D 405

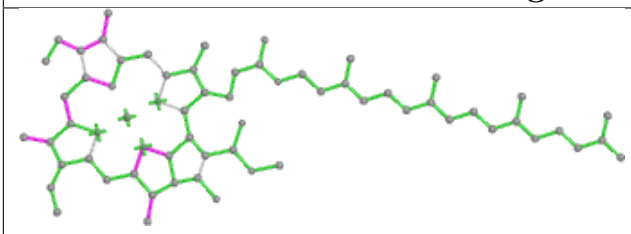
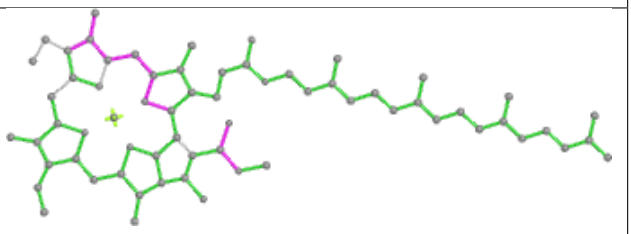
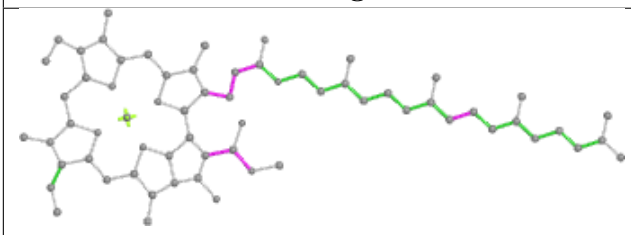
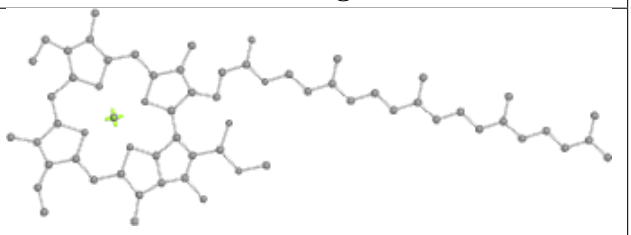


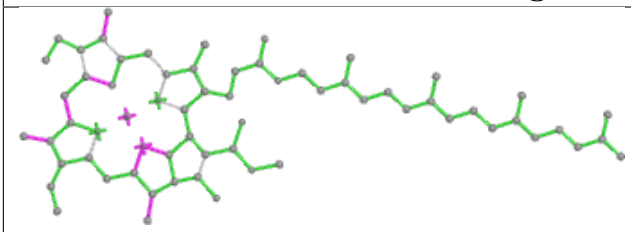
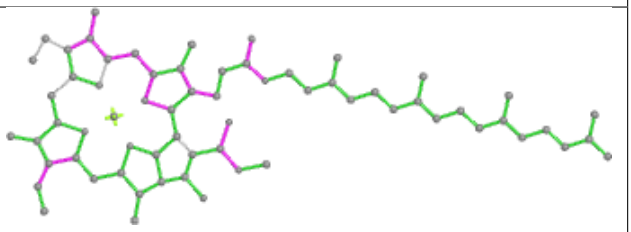
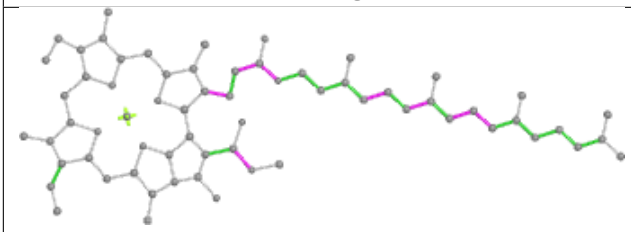
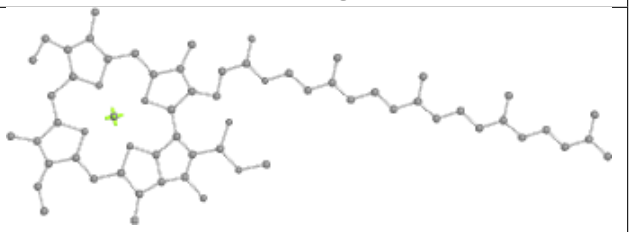
Ligand CHL 6 317



Ligand CLA r 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA u 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

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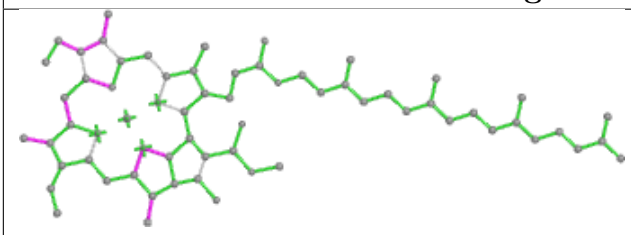
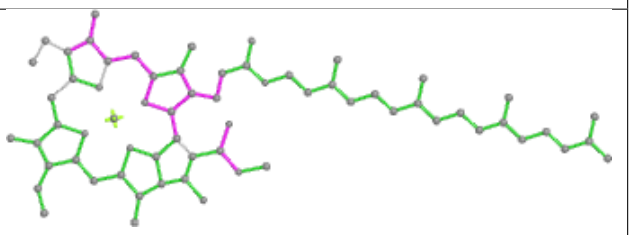
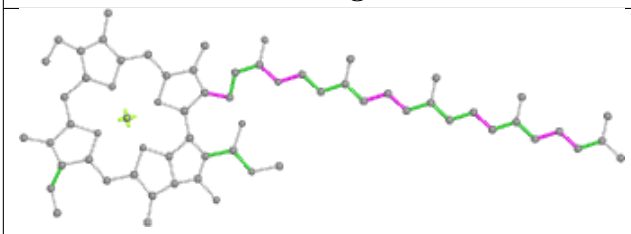
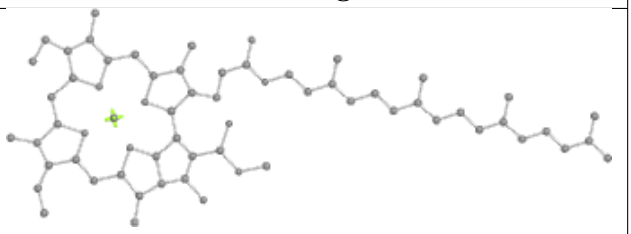
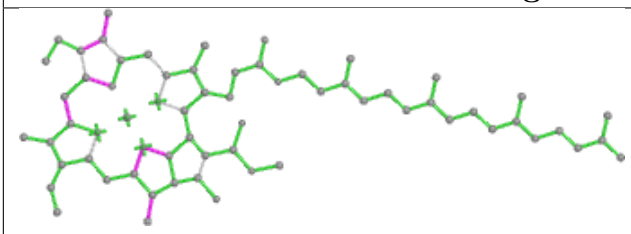
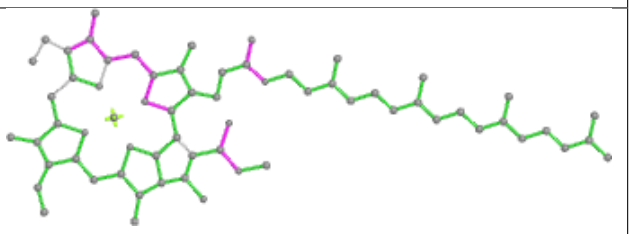
 Bond lengths	 Bond angles
 Torsions	 Rings

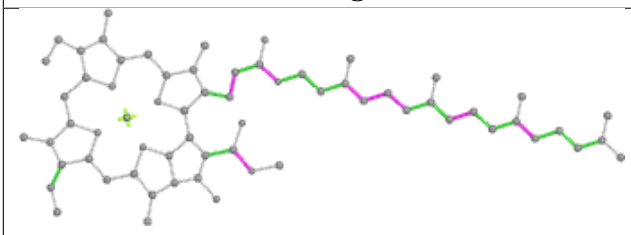
Ligand CLA G 307



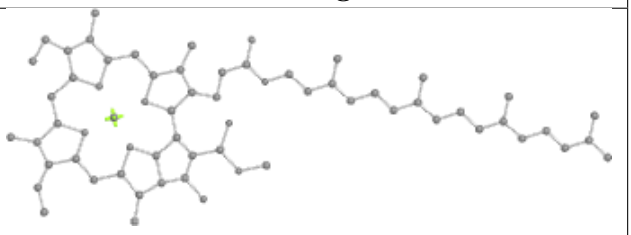
Bond lengths



Bond angles

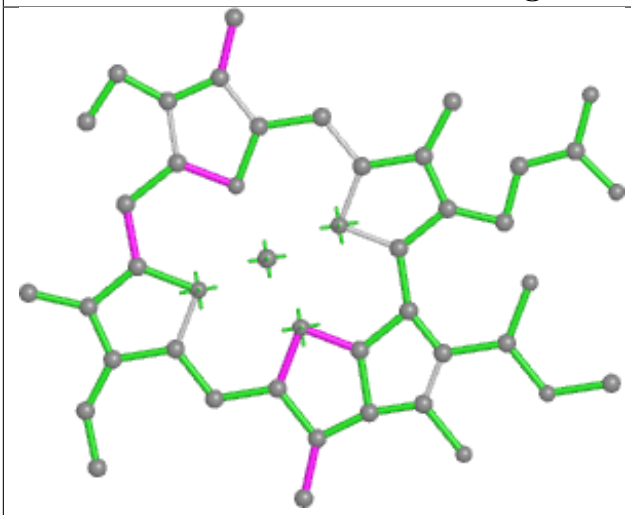


Torsions



Rings

Ligand CLA R 311



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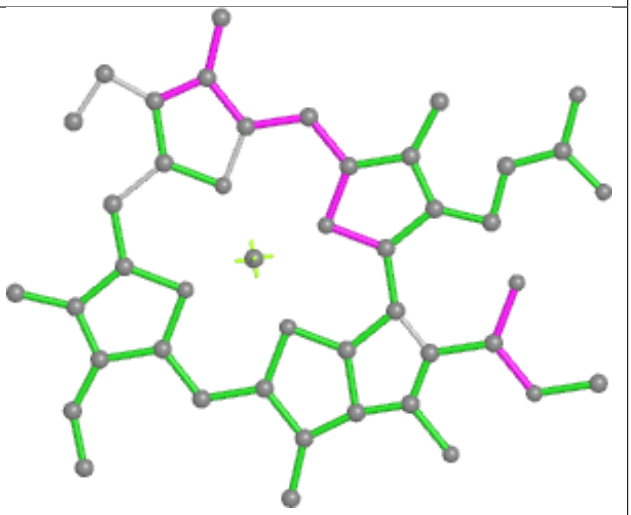
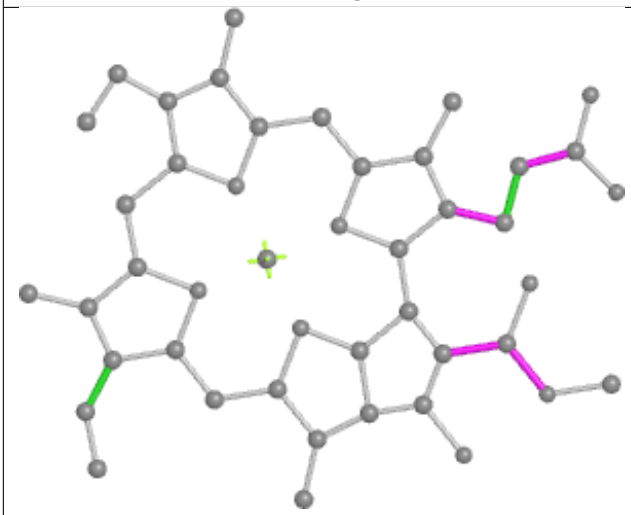


Bond angles



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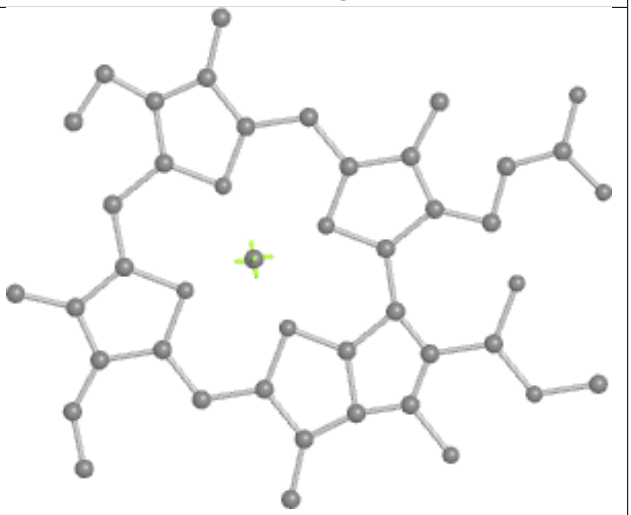
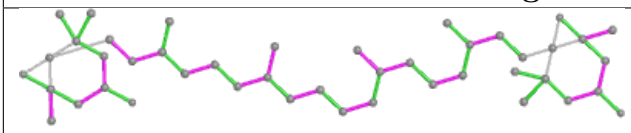
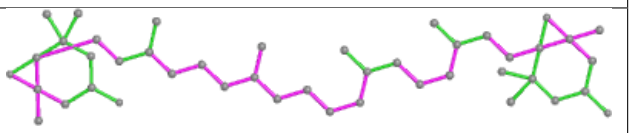


Rings

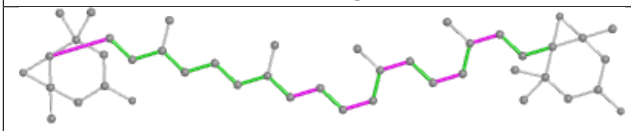
Ligand XAT N 311



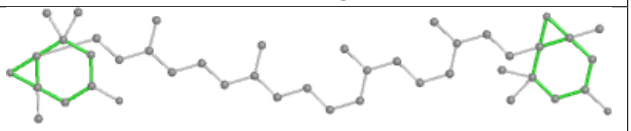
Bond lengths



Bond angles

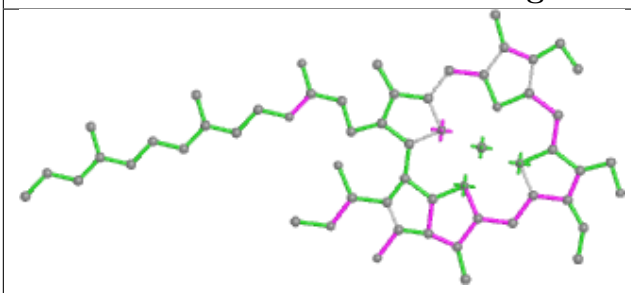


Torsions



Rings

Ligand CHL S 315



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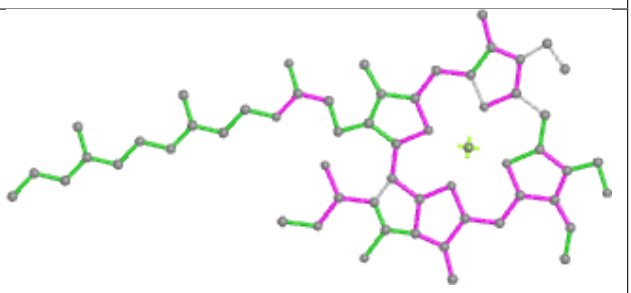
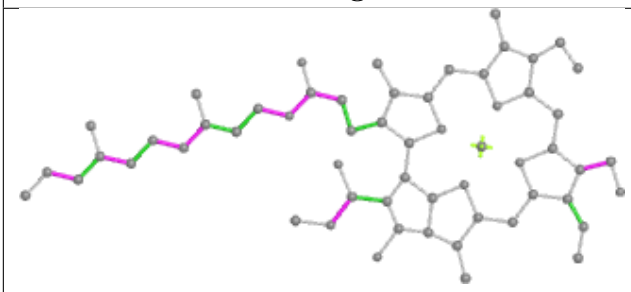
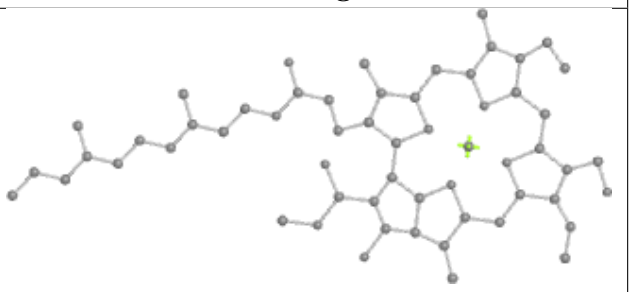


Bond angles

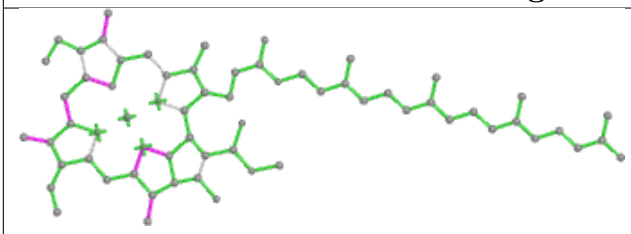


Torsions

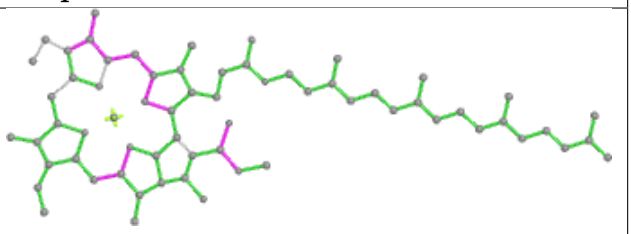


Rings

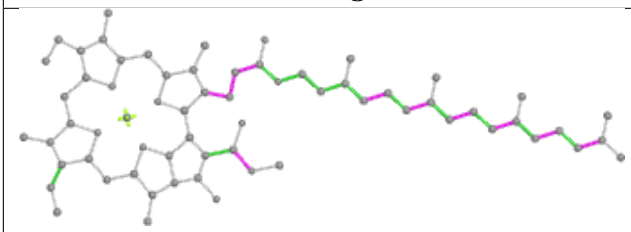
Ligand CLA q 301



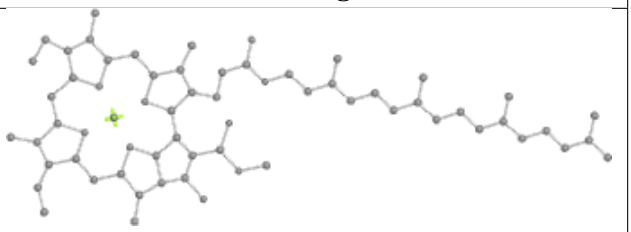
Bond lengths



Bond angles

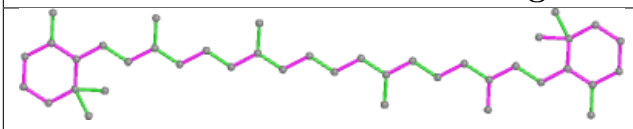


Torsions

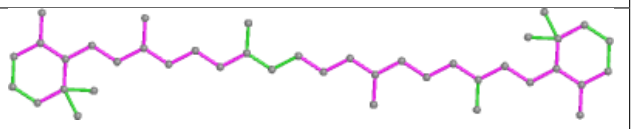


Rings

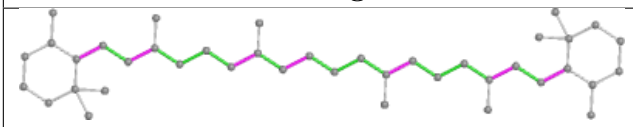
Ligand BCR t 101



Bond lengths



Bond angles



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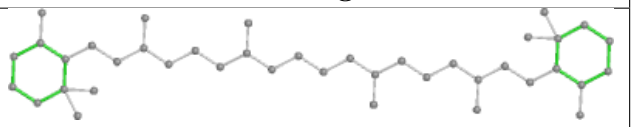
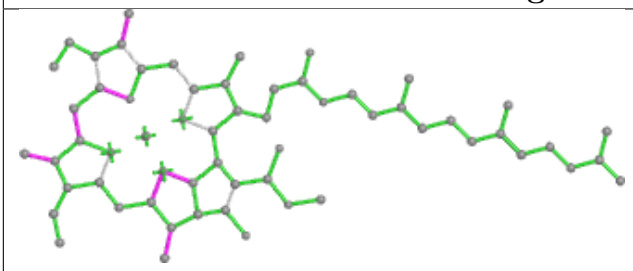


Rings

Ligand CLA p 308



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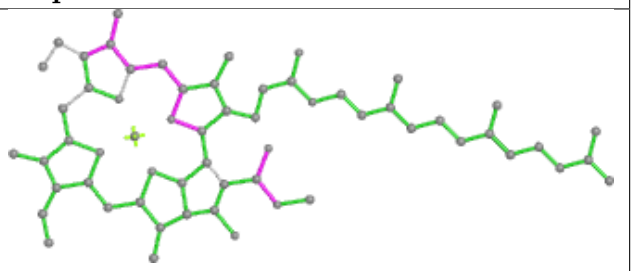

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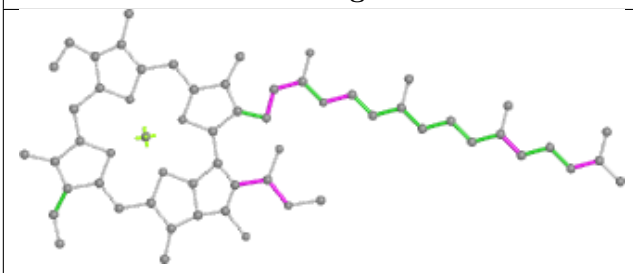

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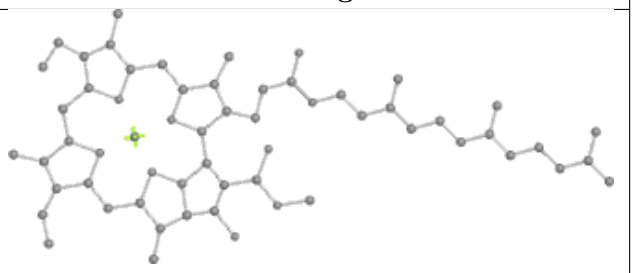
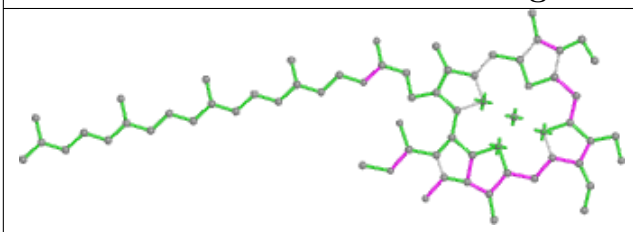


Rings

Ligand CHL r 614



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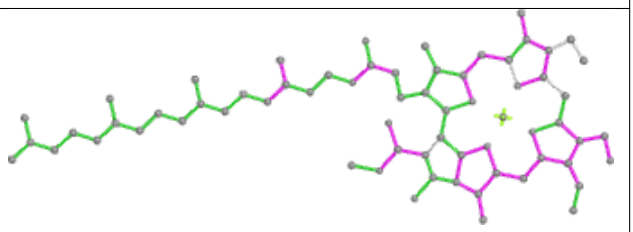

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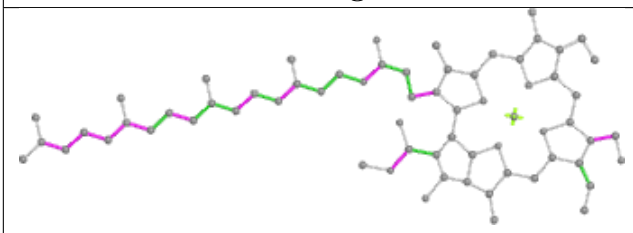

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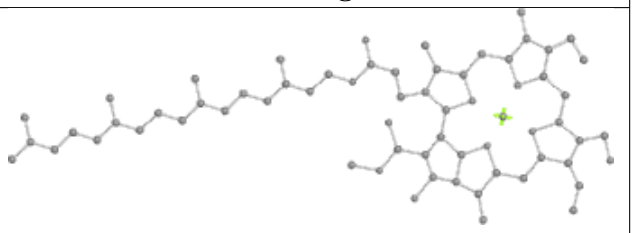
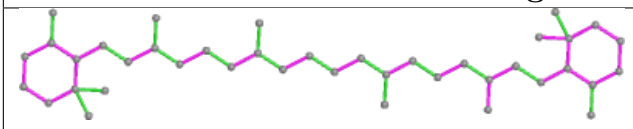


Rings

Ligand BCR a 409



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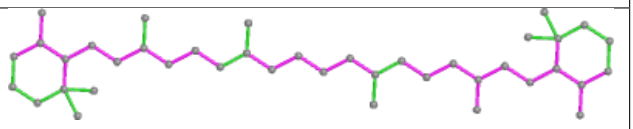
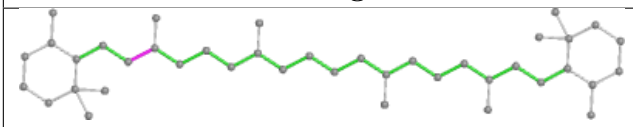


Bond angles



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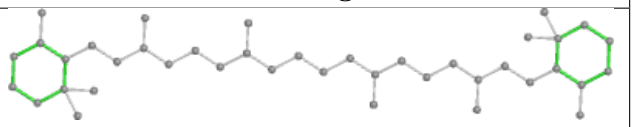
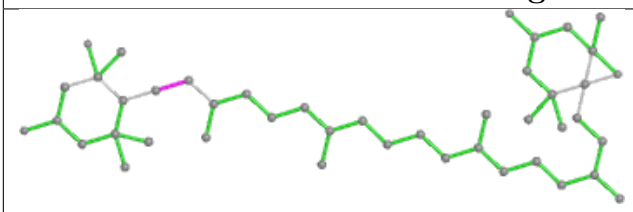


Rings

Ligand NEX s 317



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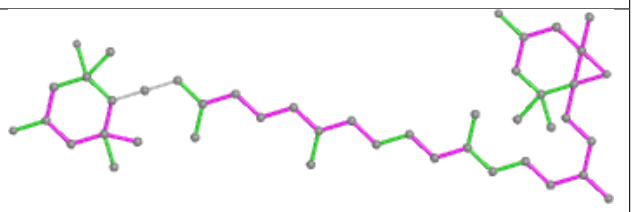

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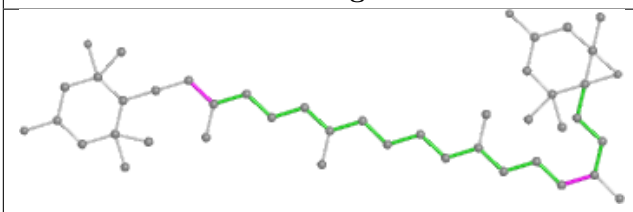
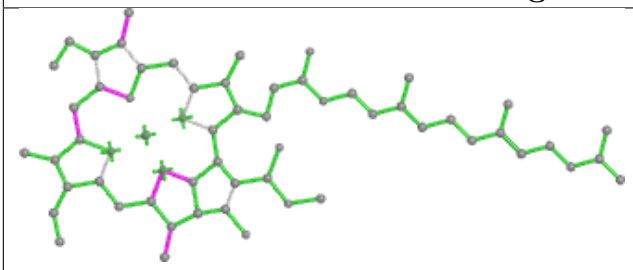


Torsions

Rings

Ligand CLA 6 307



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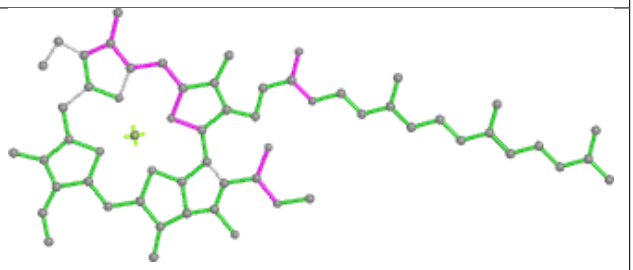
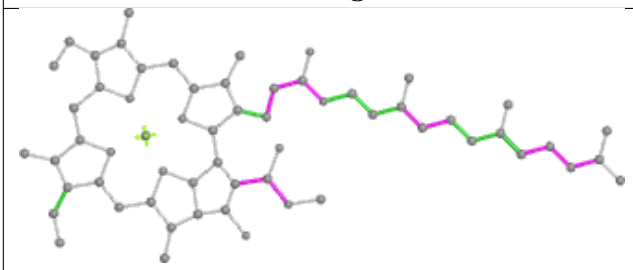


Bond angles



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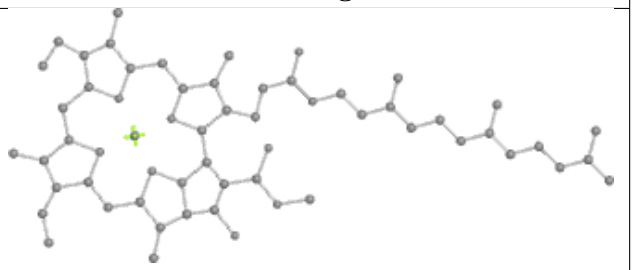
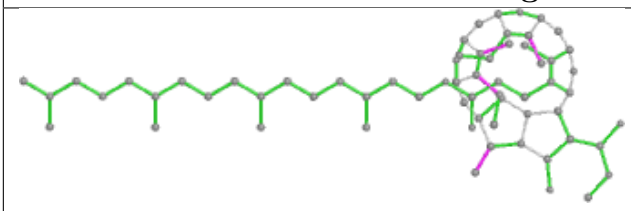


Rings

Ligand PHO D 401



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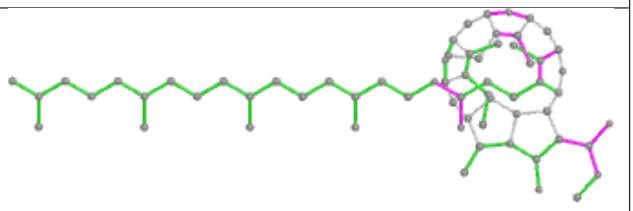

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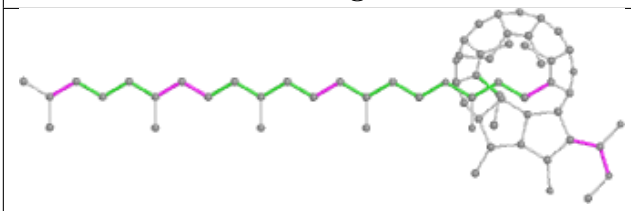

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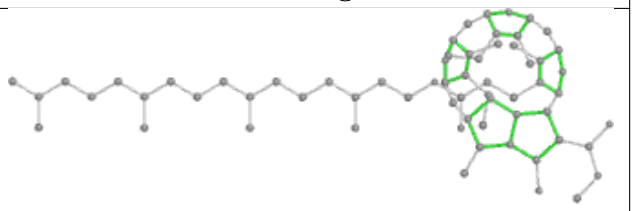
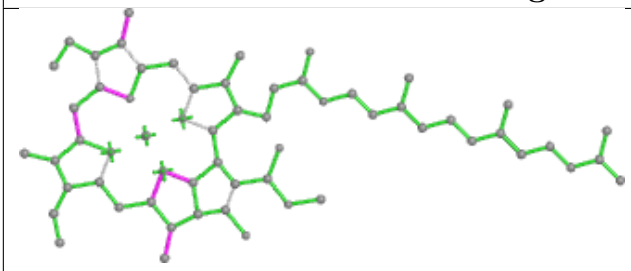


Rings

Ligand CLA 1 305



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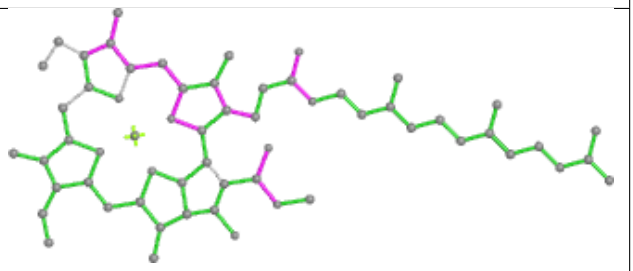

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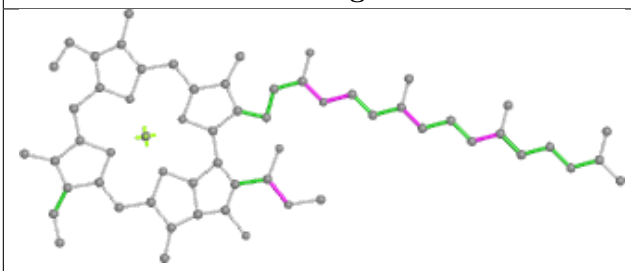

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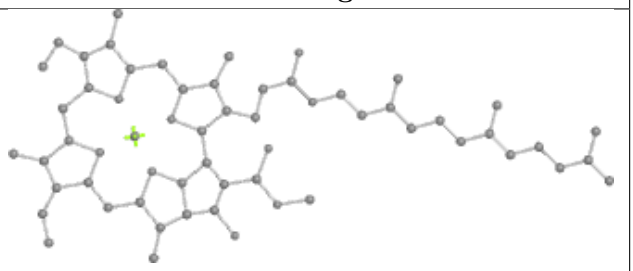
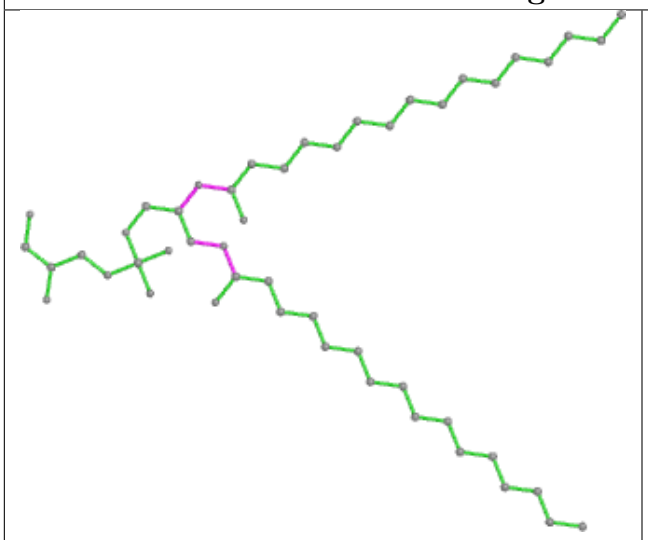


Rings

Ligand LHG 3 310



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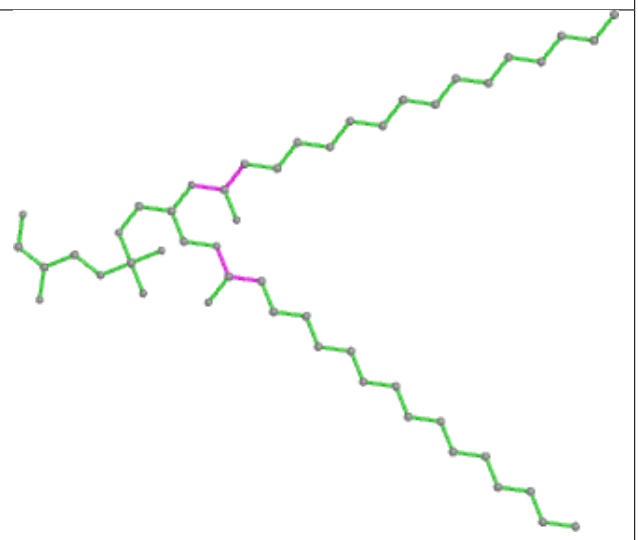
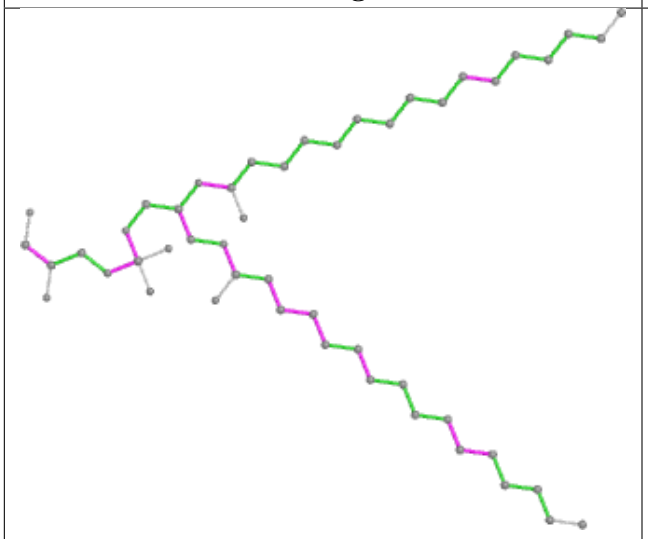


Bond angles



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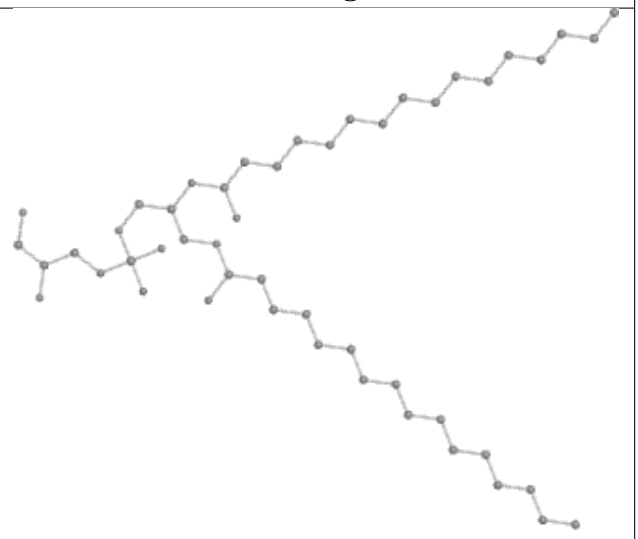
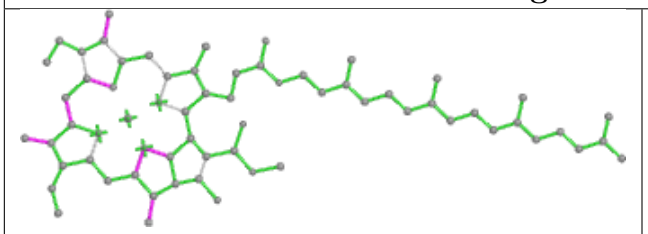
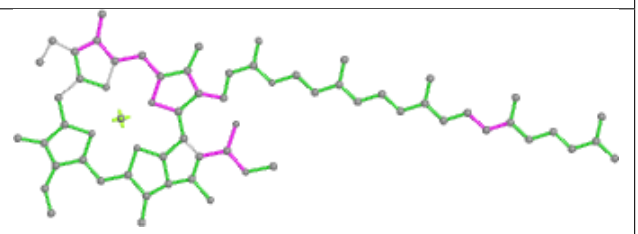


Rings

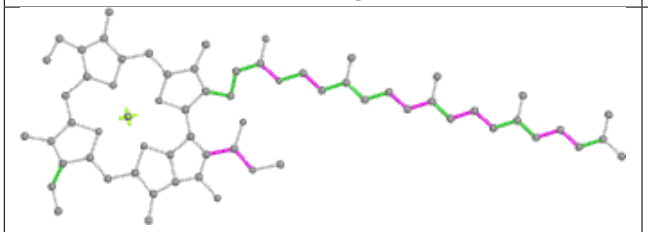
Ligand CLA c 510



Bond lengths



Bond angles



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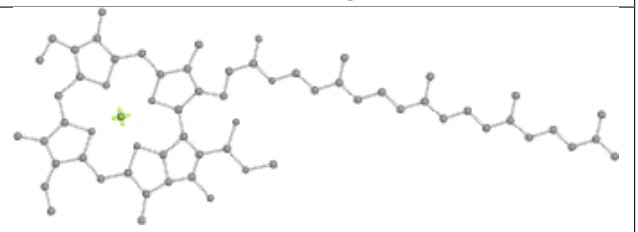
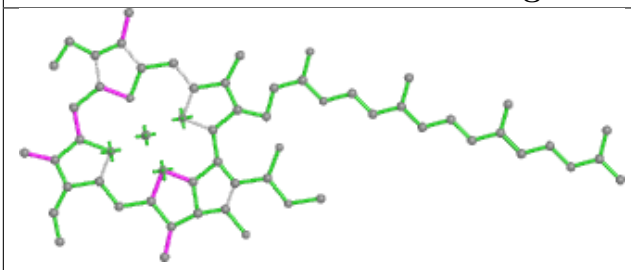
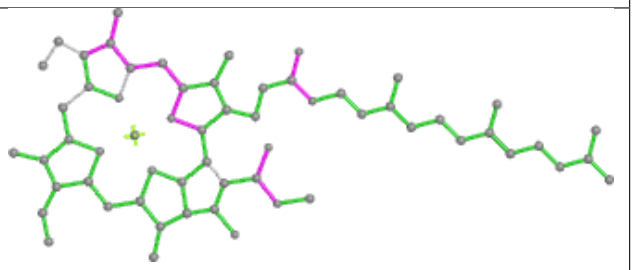
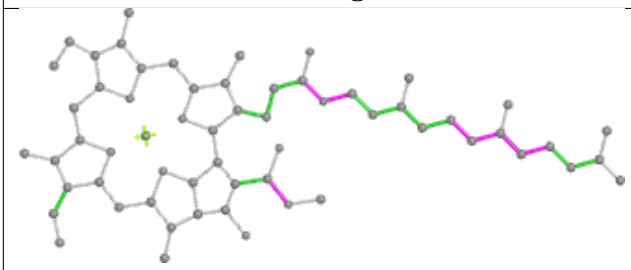
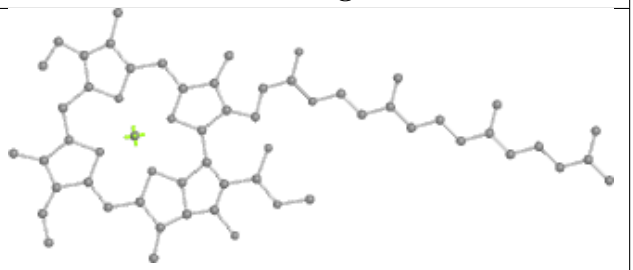


Rings

Ligand CLA U 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

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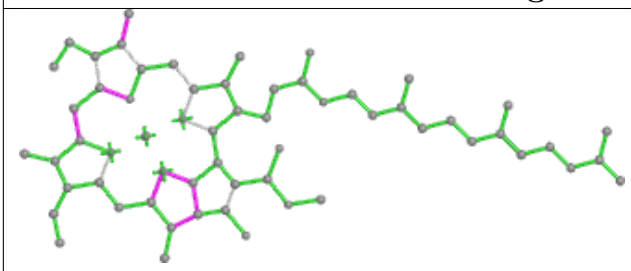
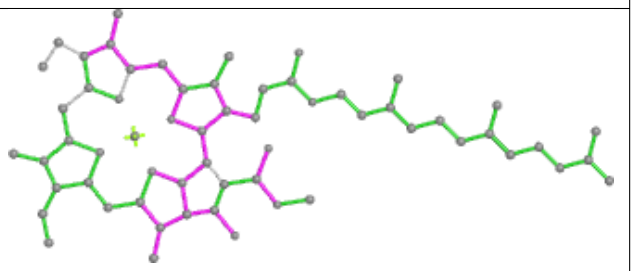
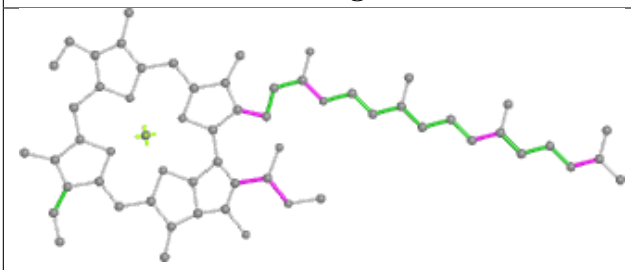
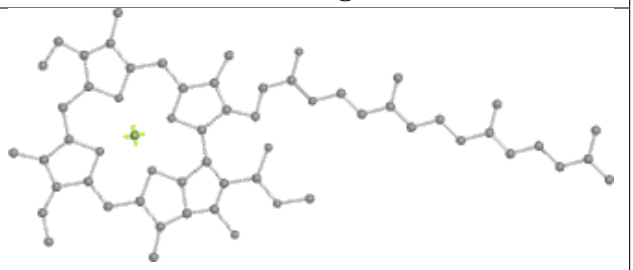
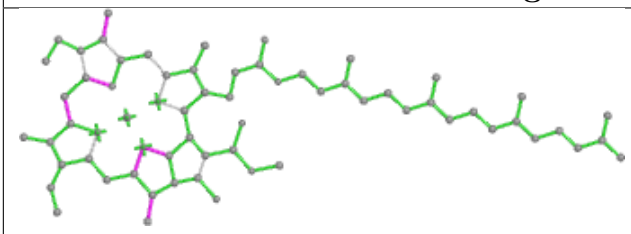
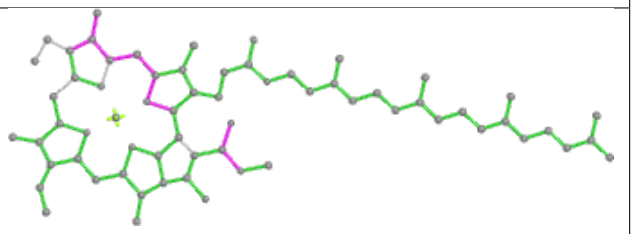
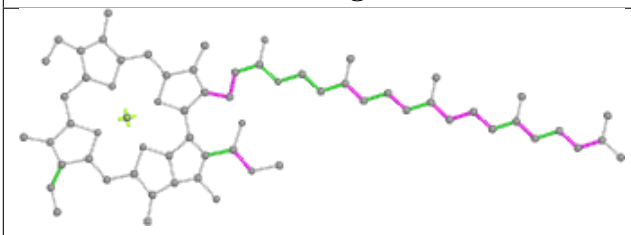
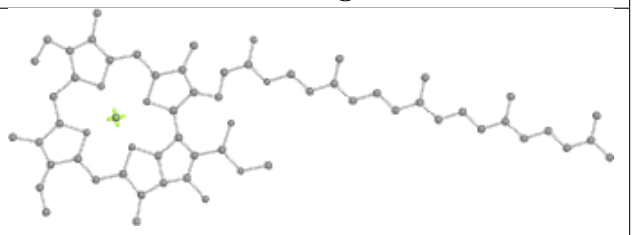
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

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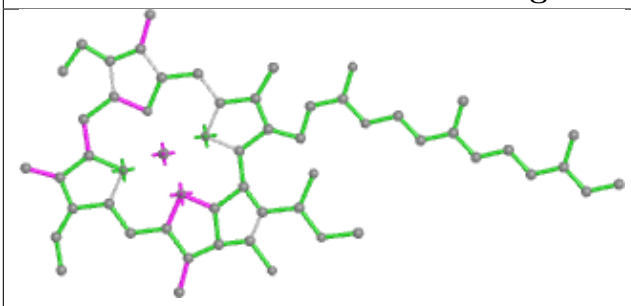
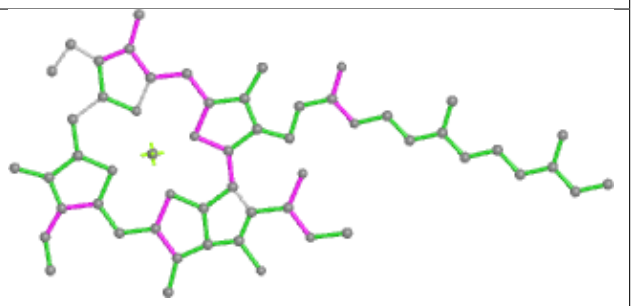
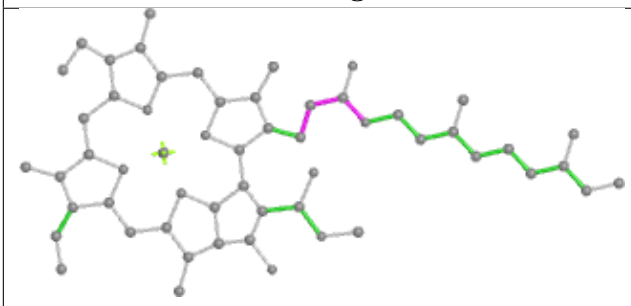
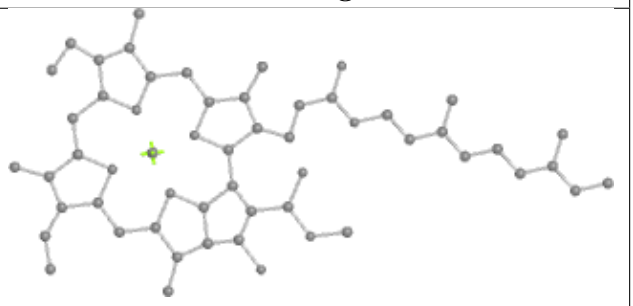
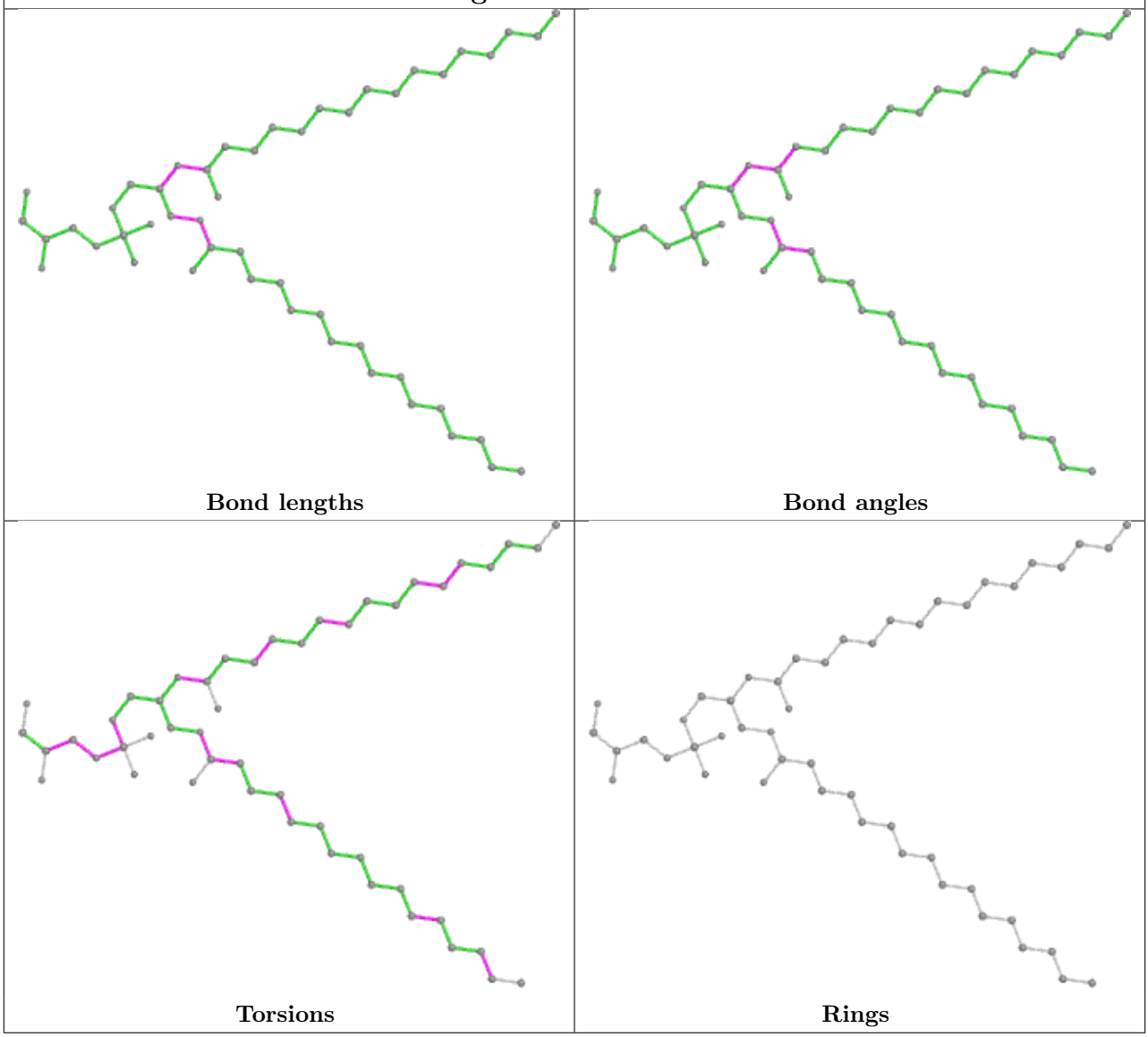
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG S 312



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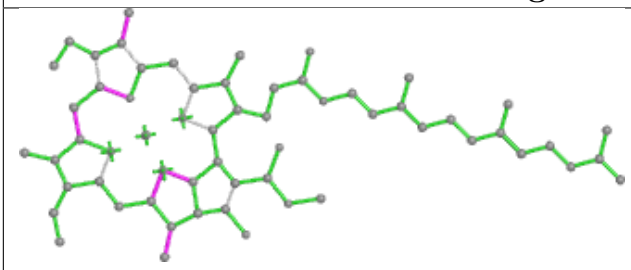
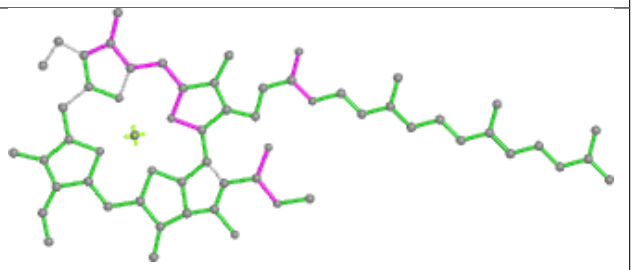
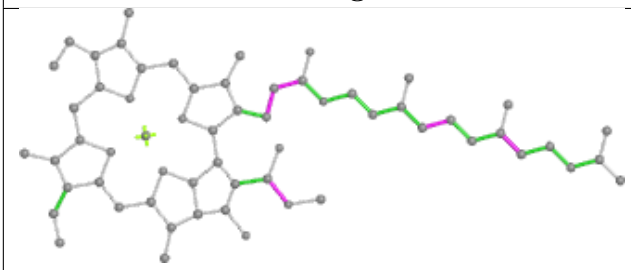
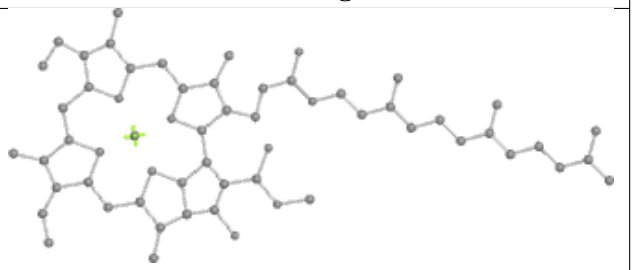
 Bond lengths	 Bond angles
 Torsions	 Rings

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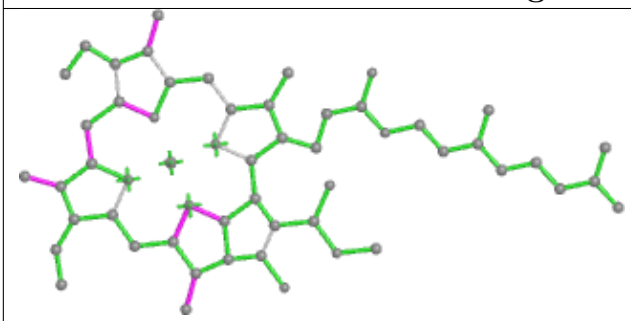
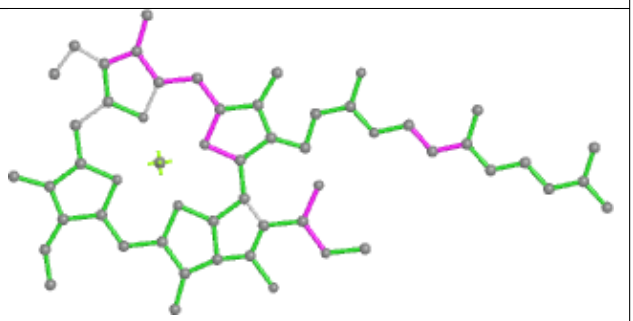
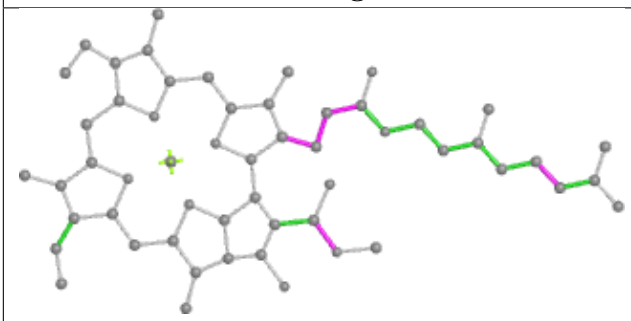
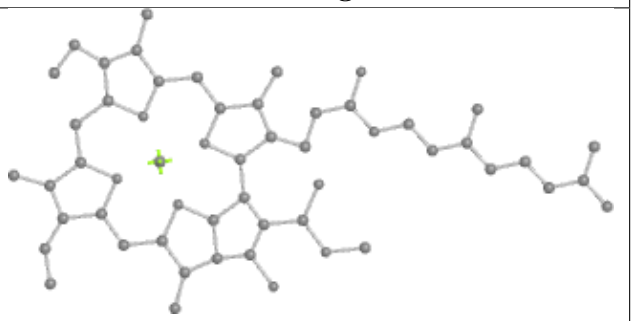
 Bond lengths	 Bond angles
 Torsions	 Rings

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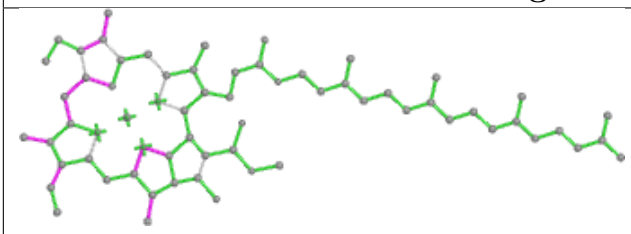
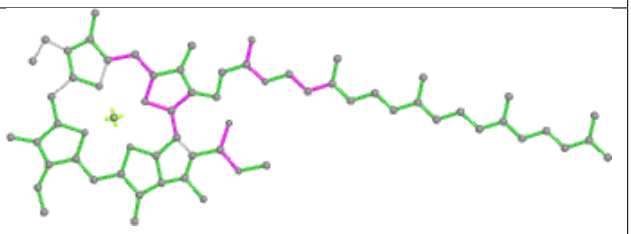
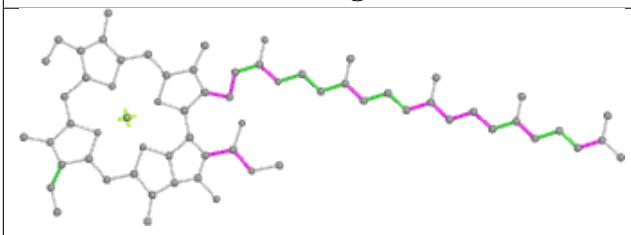
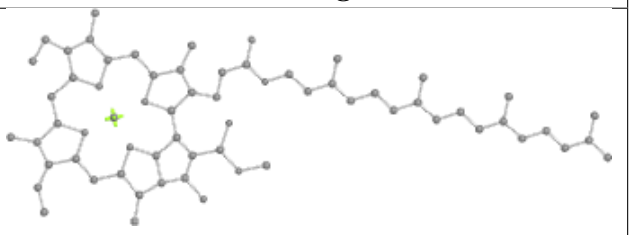
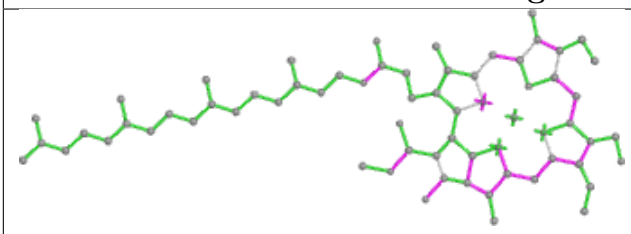
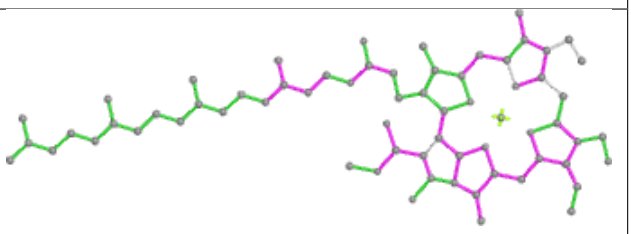
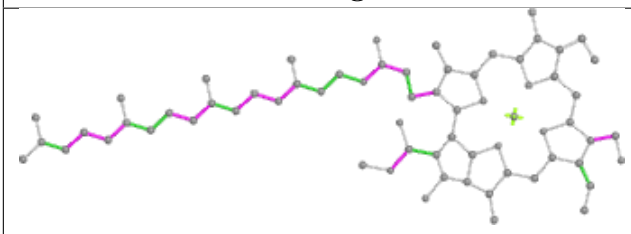
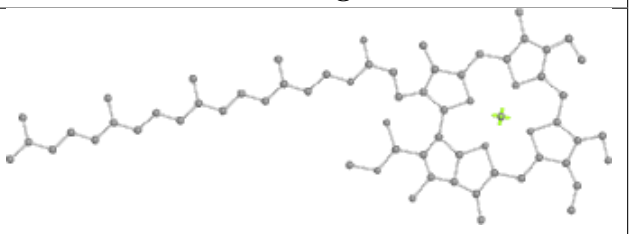
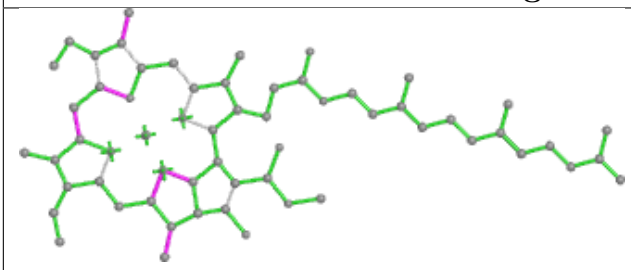
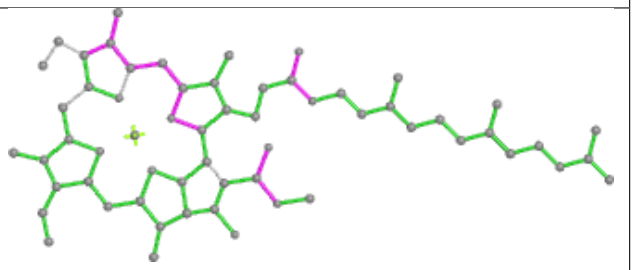
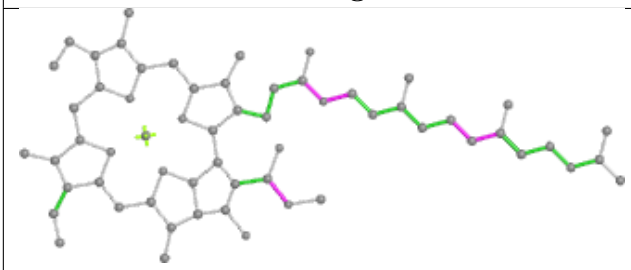
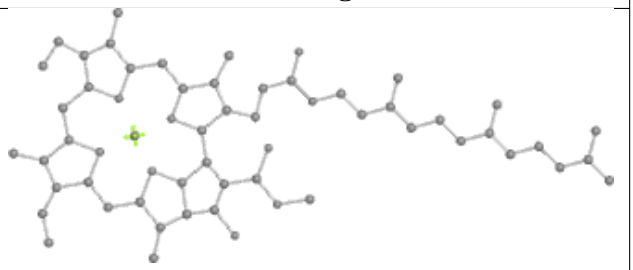
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 1 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

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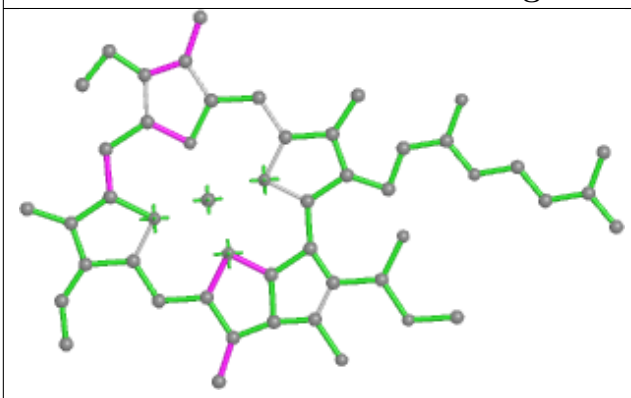
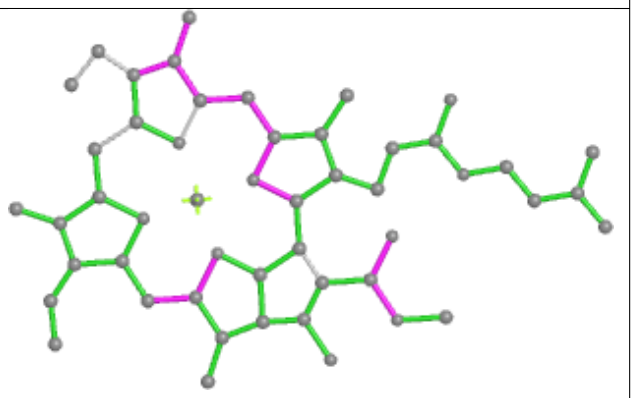
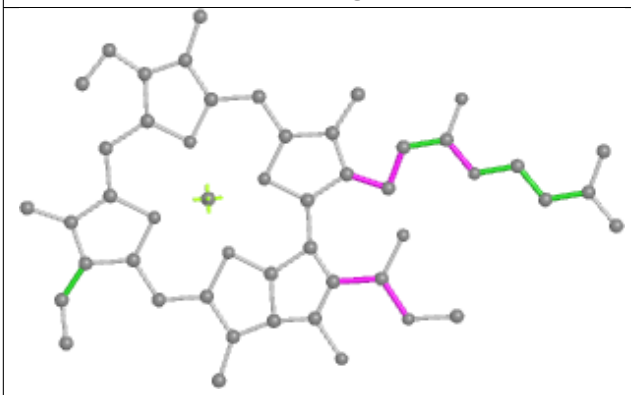
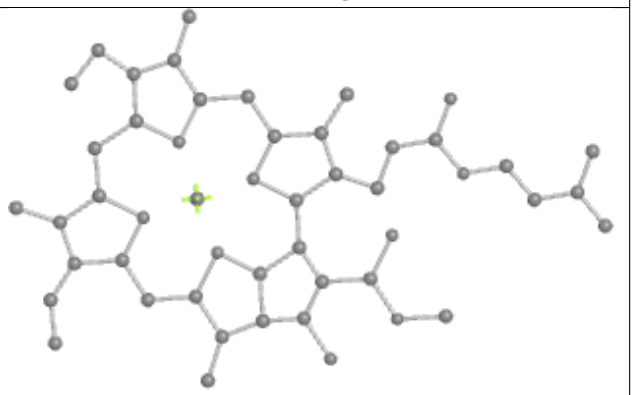
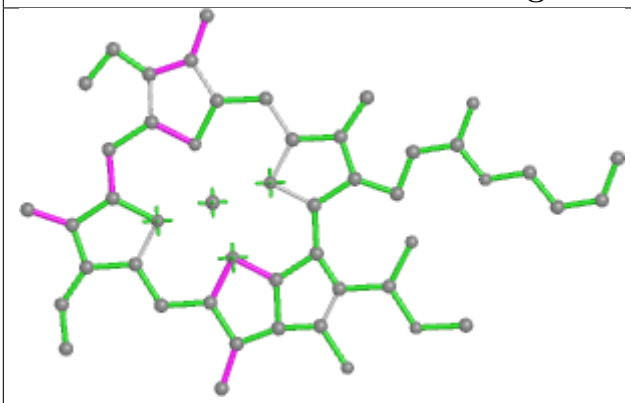
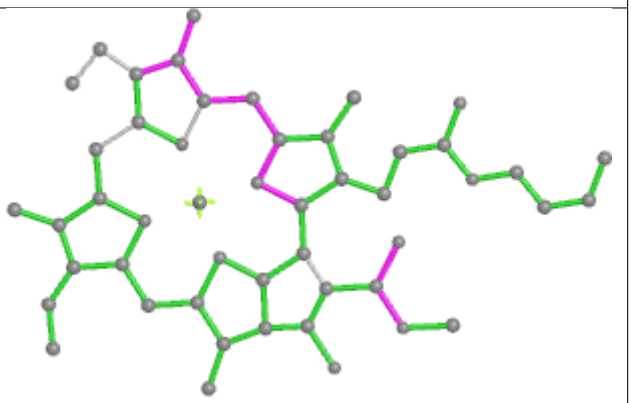
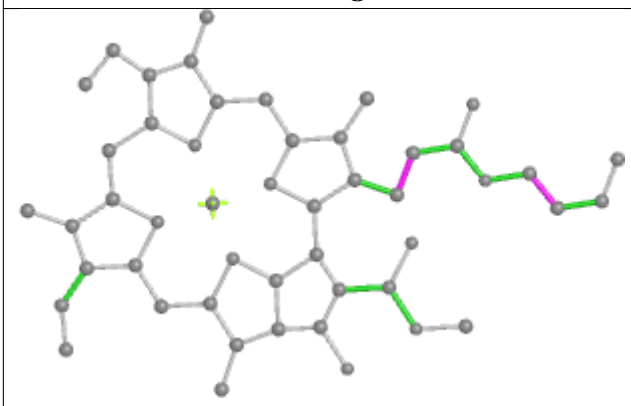
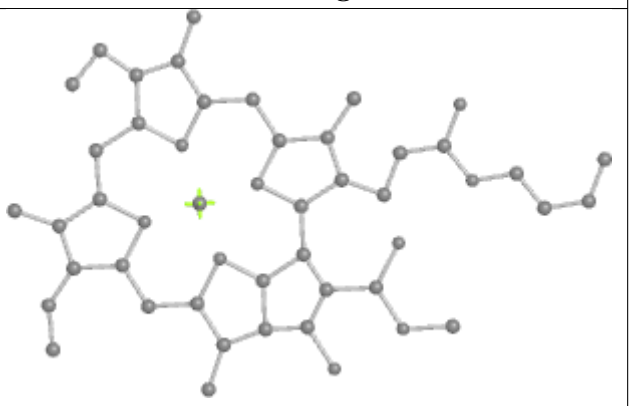
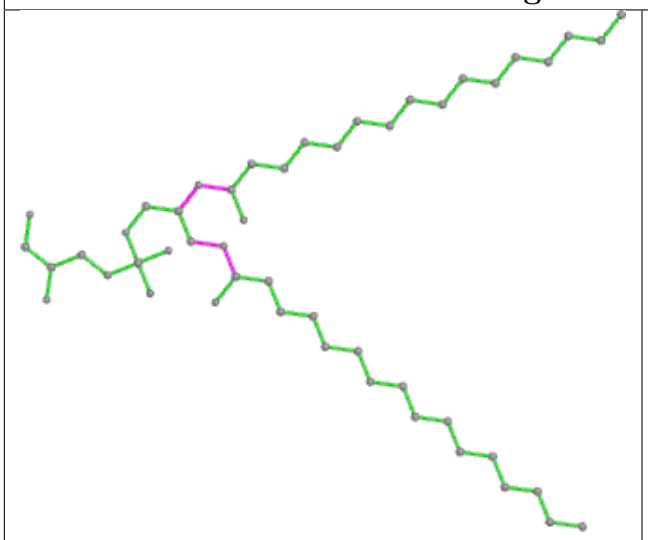
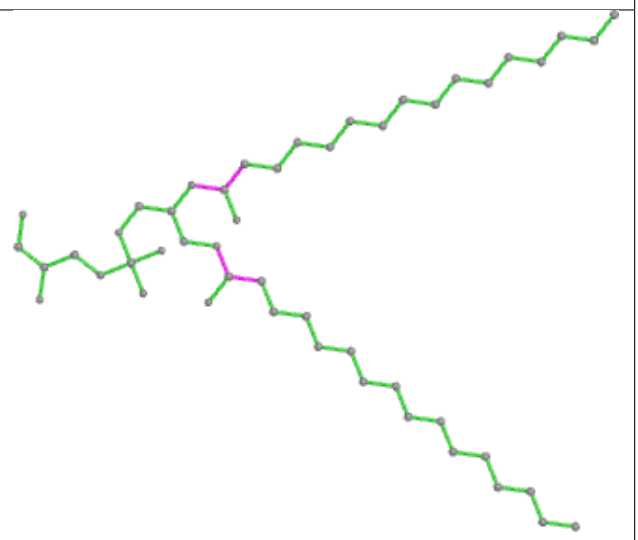
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

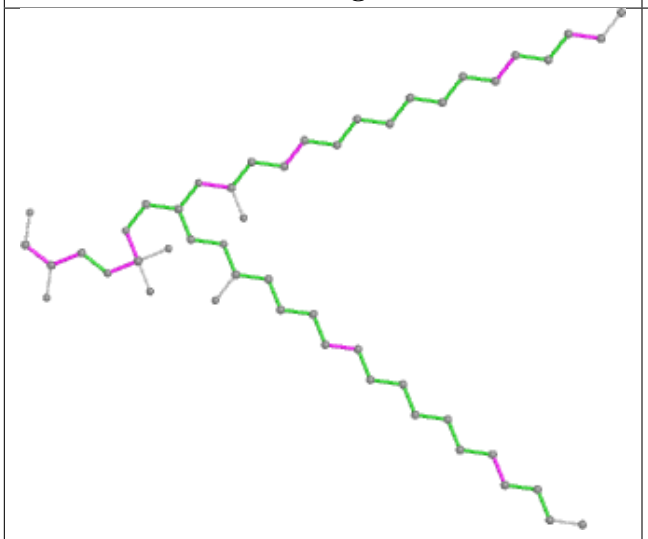
Ligand LHG C 524



Bond lengths



Bond angles



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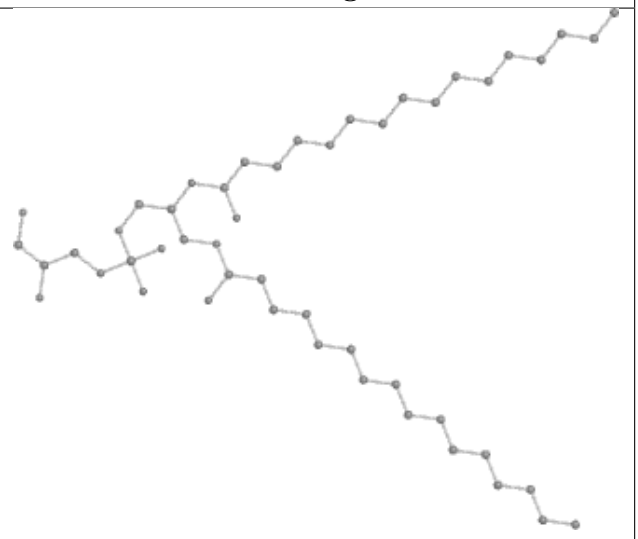
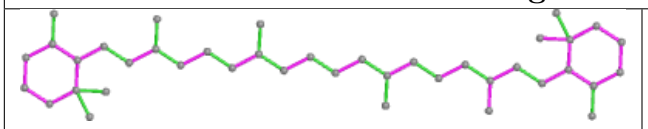


Rings

Ligand BCR c 515



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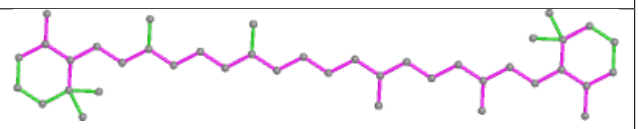

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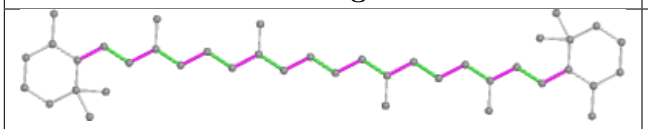

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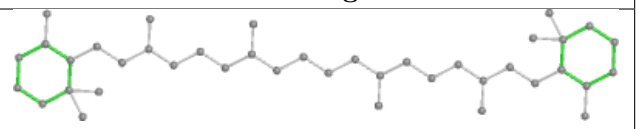
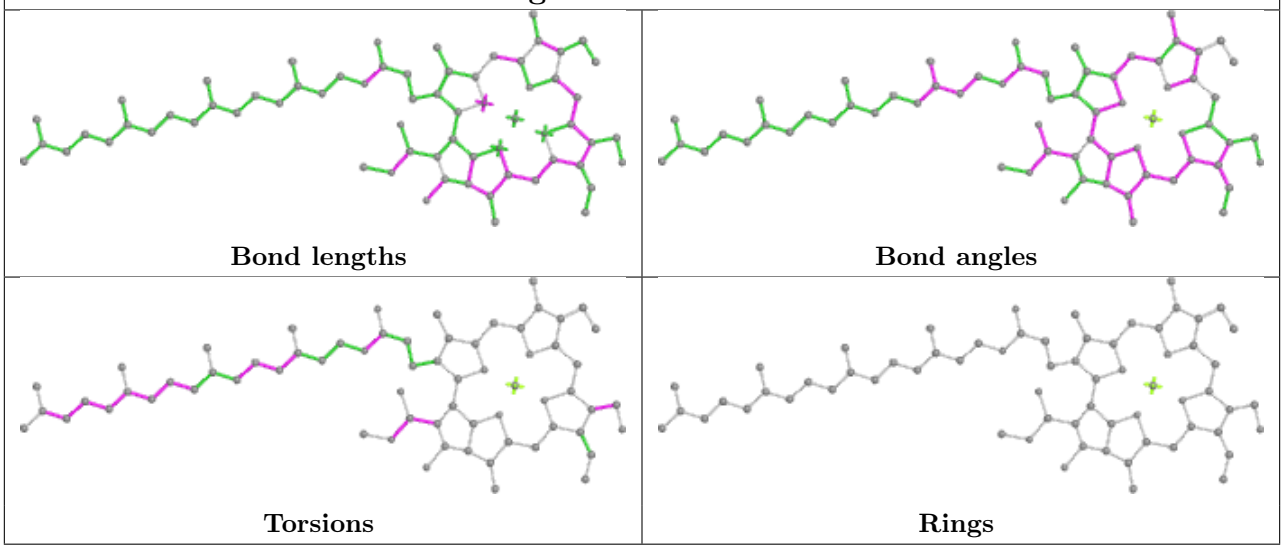
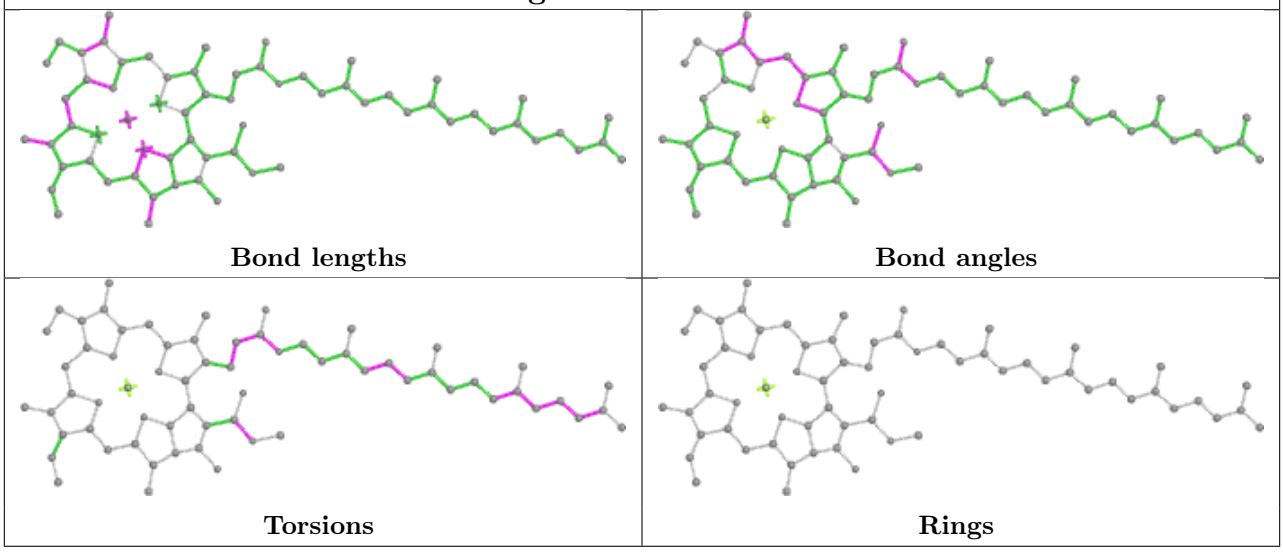


Rings

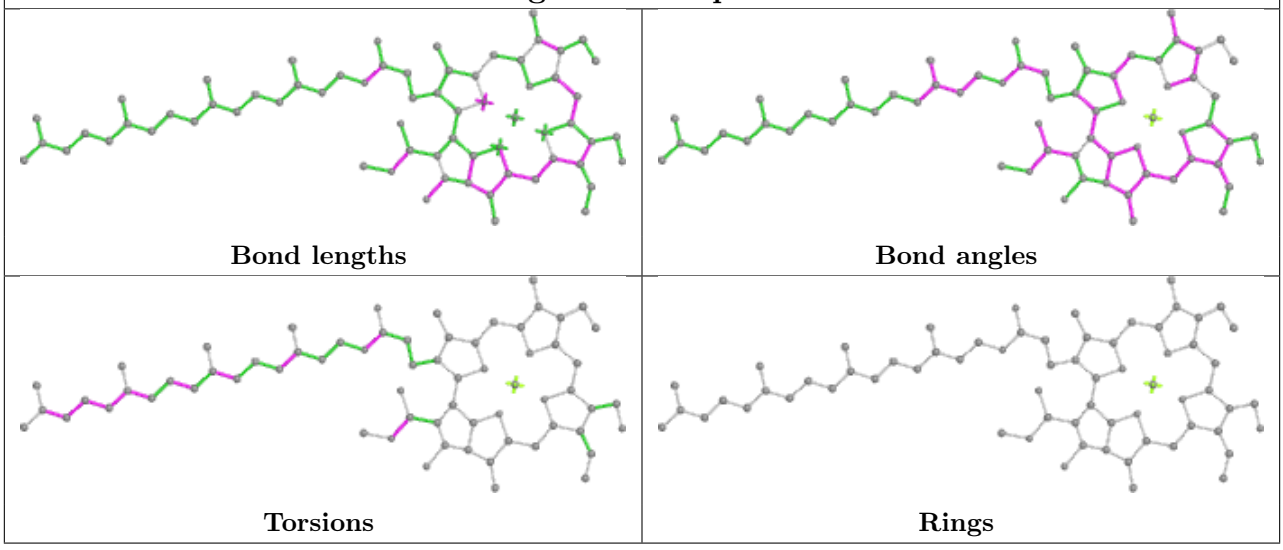
Ligand CHL 5 313



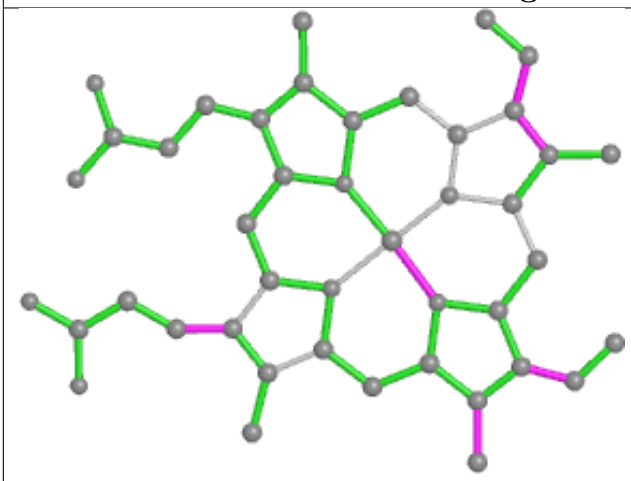
Ligand CLA b 602



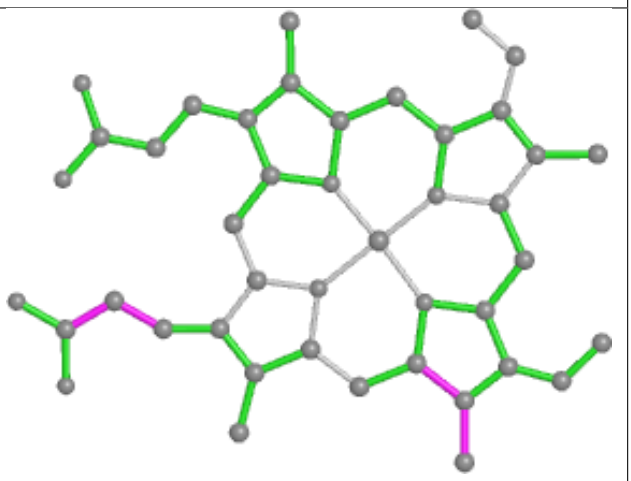
Ligand CHL q 311



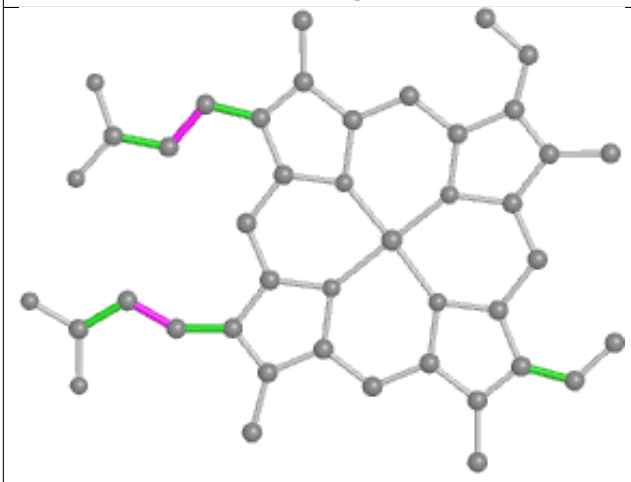
Ligand HEM E 101



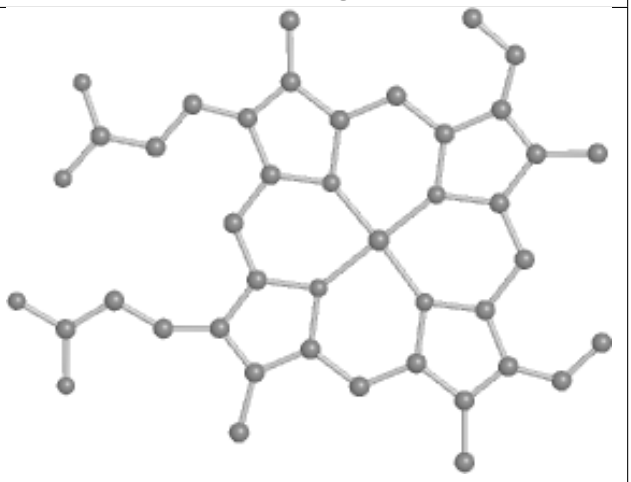
Bond lengths



Bond angles

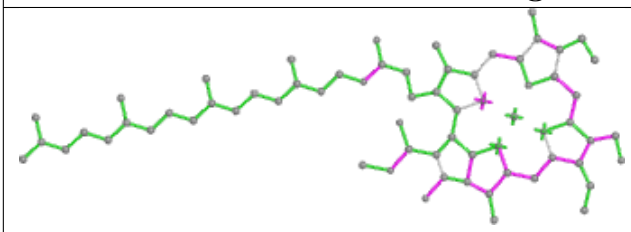


Torsions



Rings

Ligand CHL u 313



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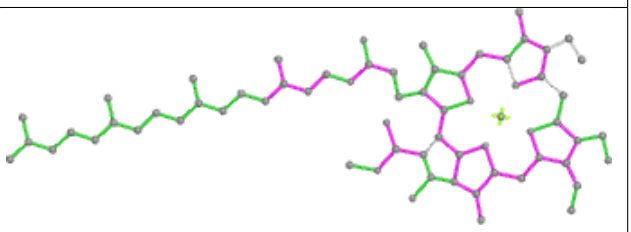
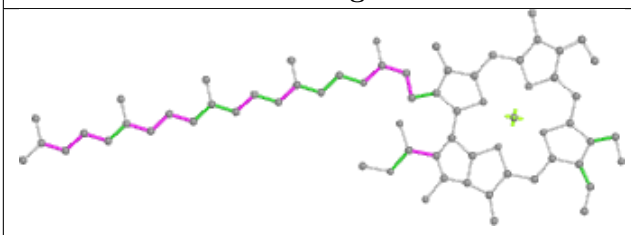


Bond angles



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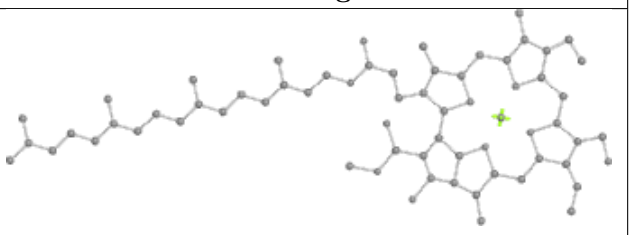
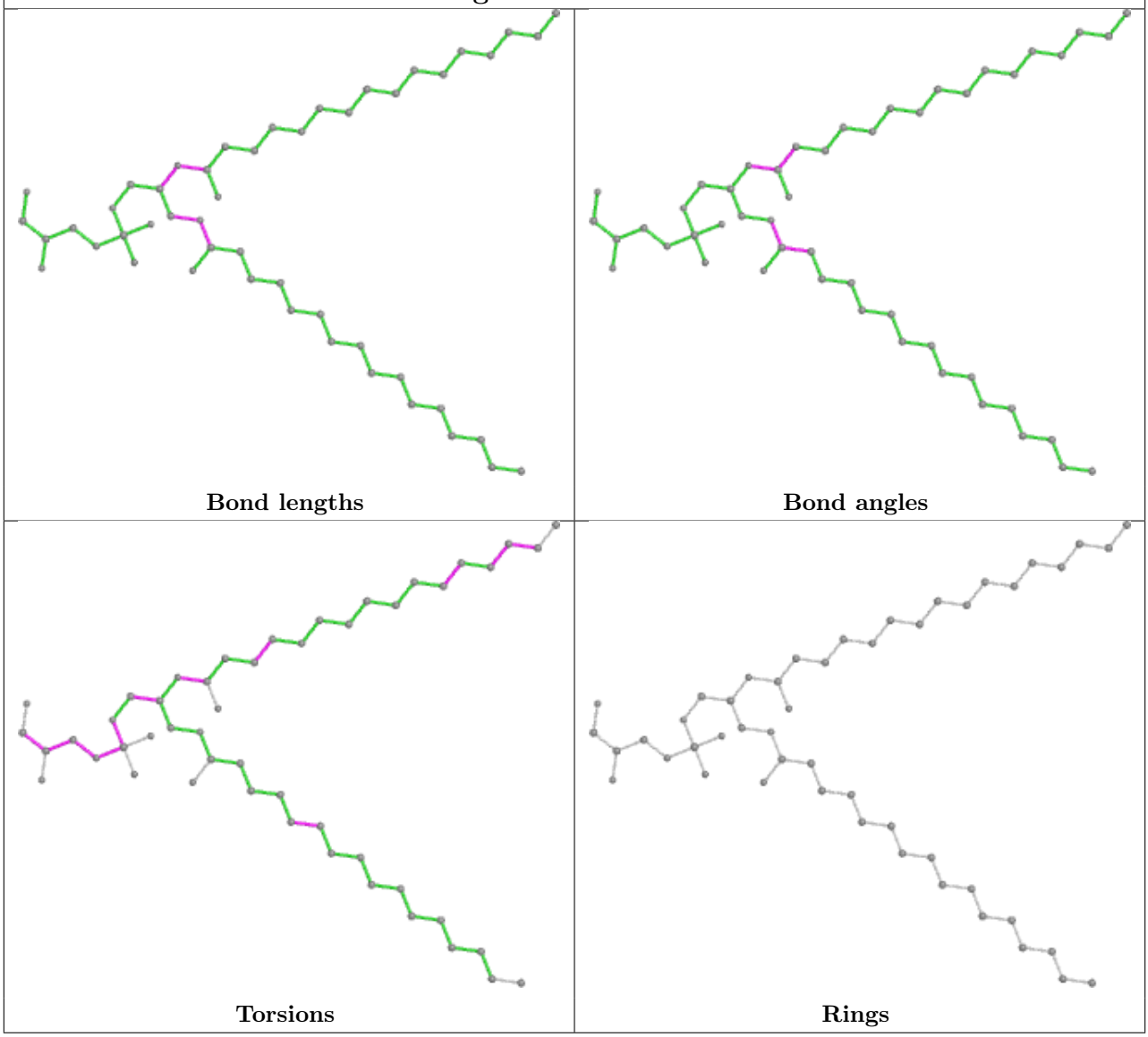
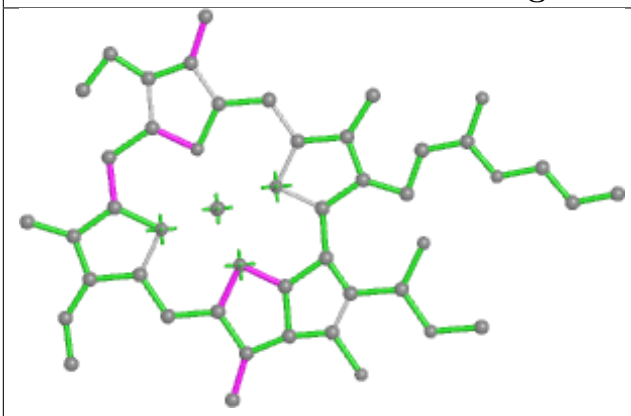


Rings

Ligand LHG c 523



Ligand CLA 1 308



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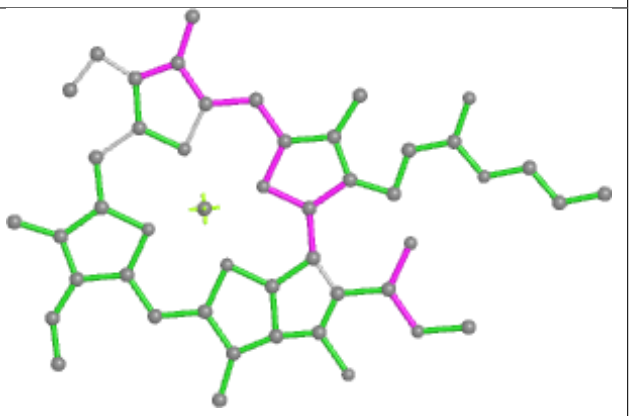

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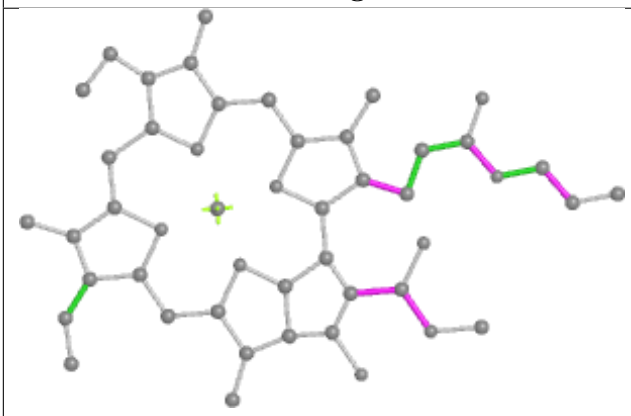

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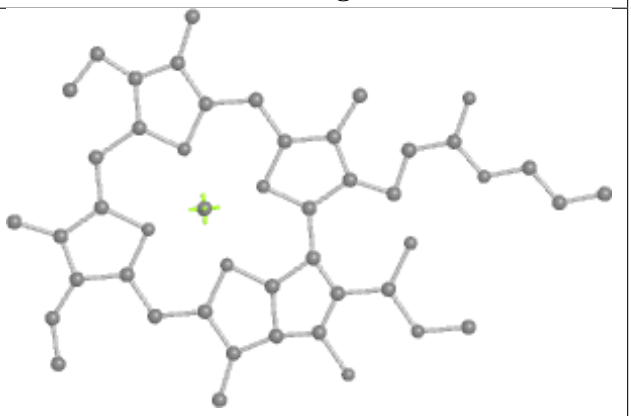
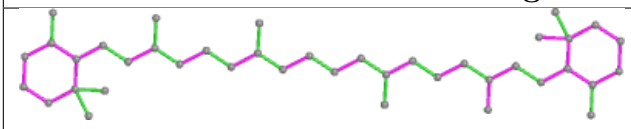
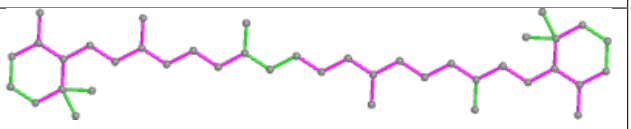


Rings

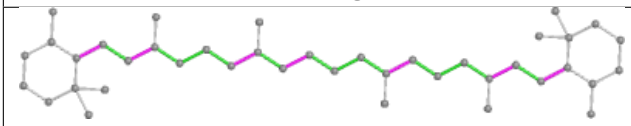
Ligand BCR T 101



Bond lengths



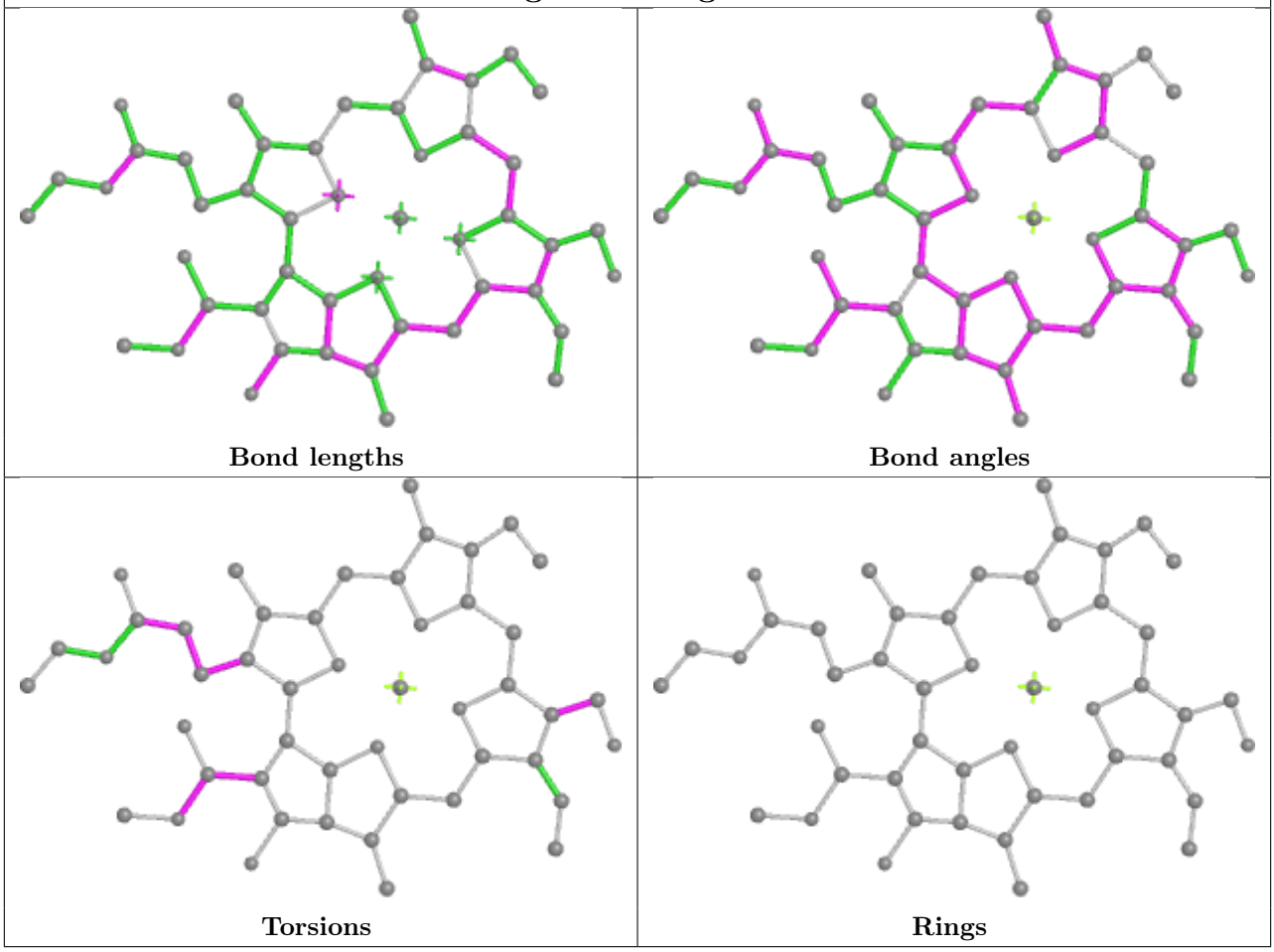
Bond angles



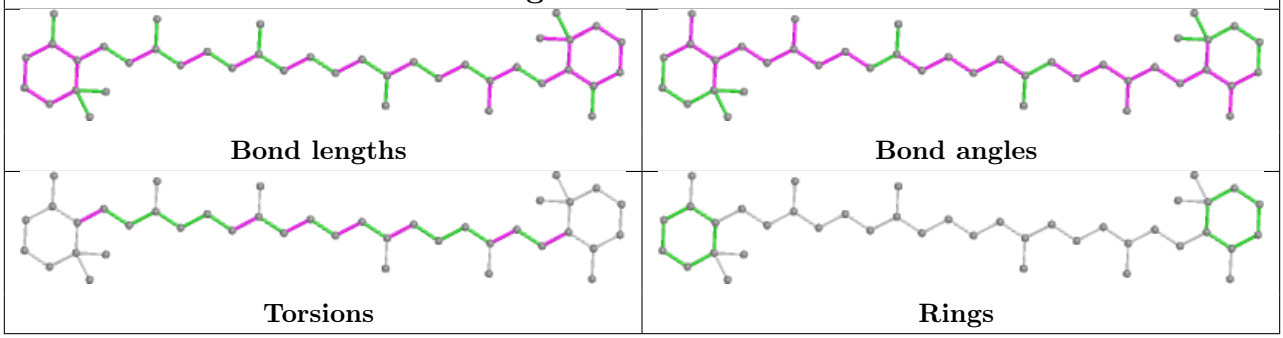
Torsions

Rings

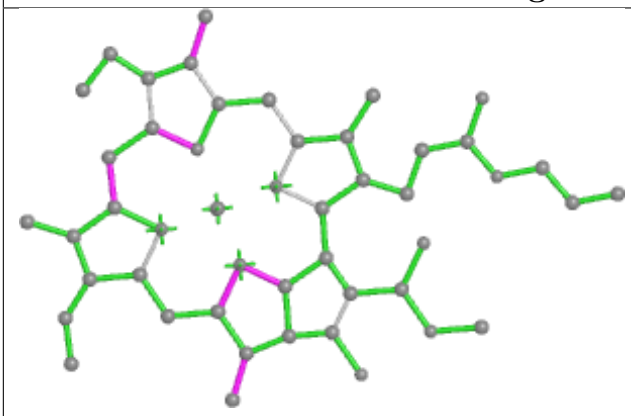
Ligand CHL g 312



Ligand BCR b 620



Ligand CLA 4 308



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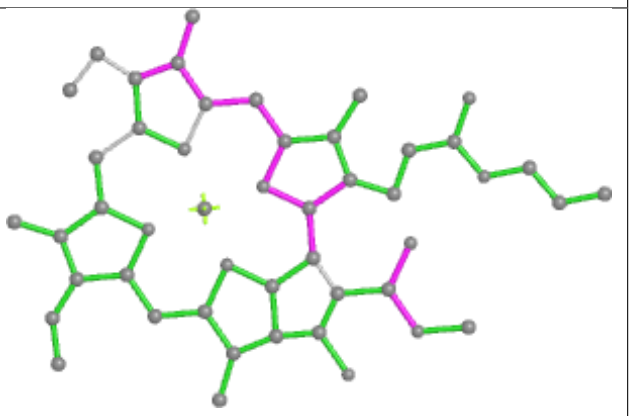
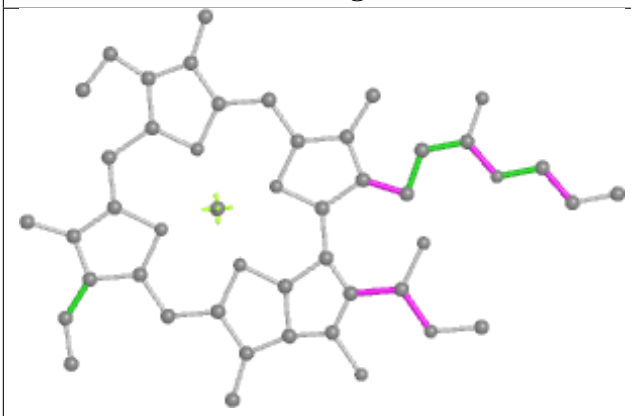


Bond angles



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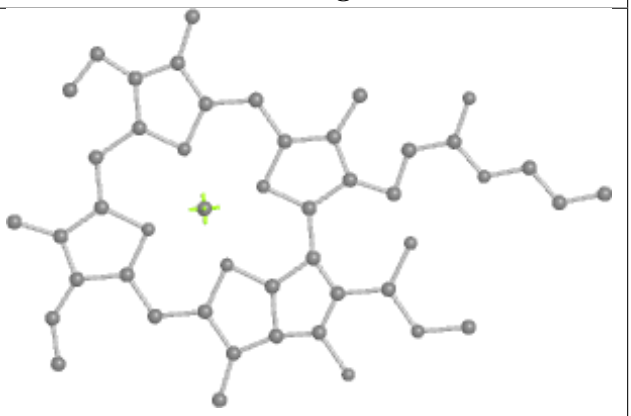
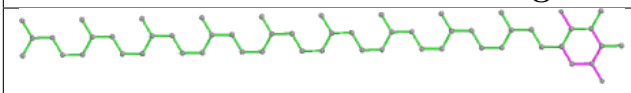
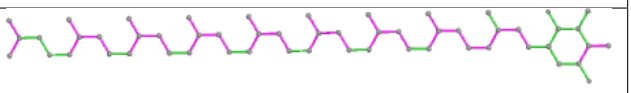


Rings

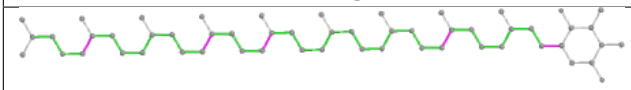
Ligand PL9 d 404



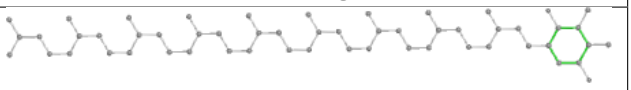
Bond lengths



Bond angles

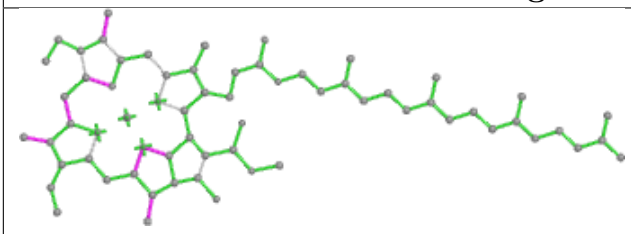


Torsions

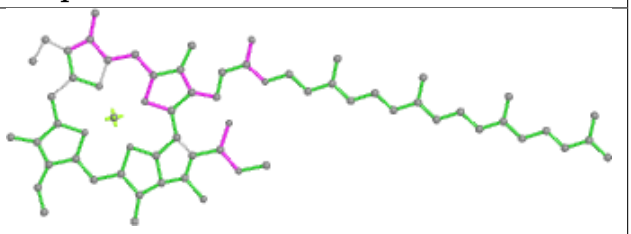


Rings

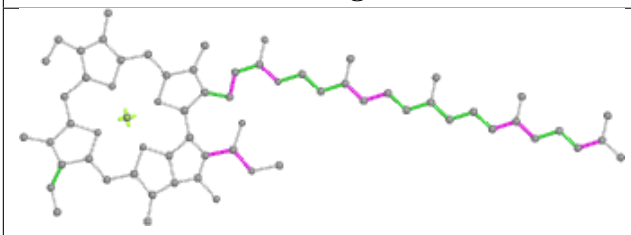
Ligand CLA q 307



Bond lengths



Bond angles



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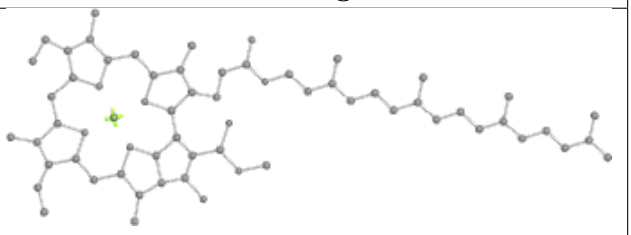
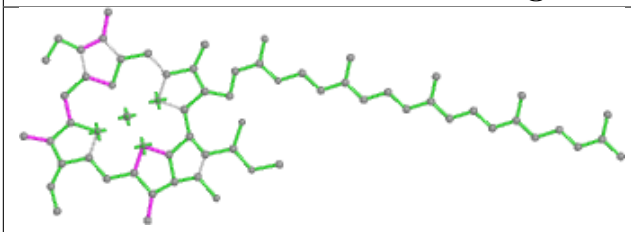
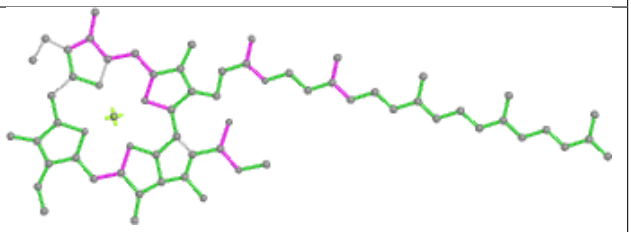


Rings

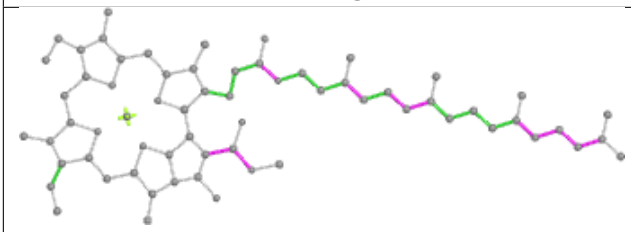
Ligand CLA b 610



Bond lengths



Bond angles



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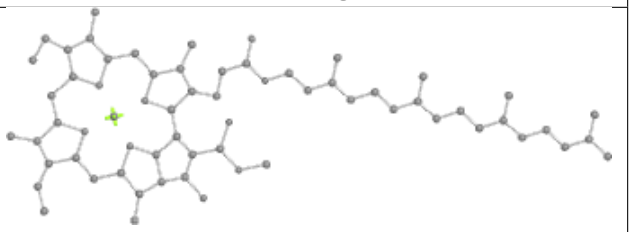
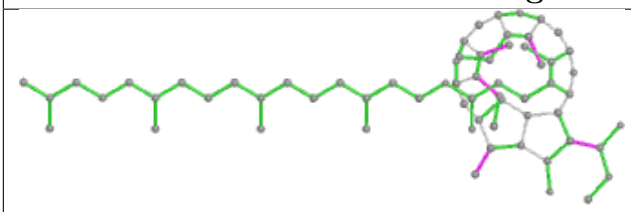
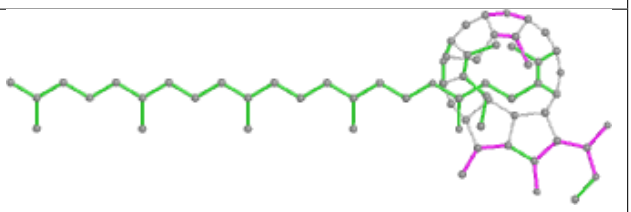


Rings

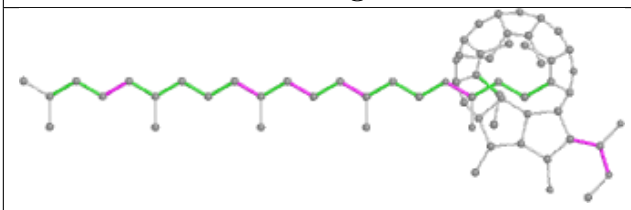
Ligand PHO a 407



Bond lengths



Bond angles



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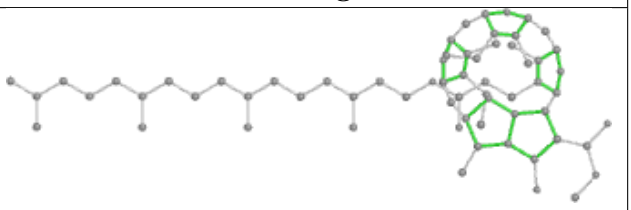
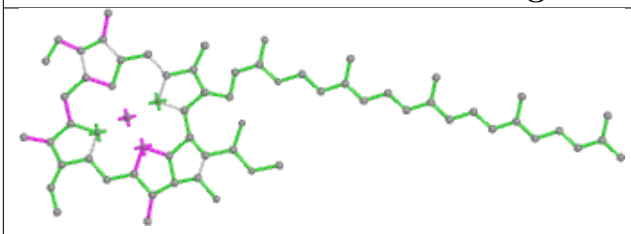
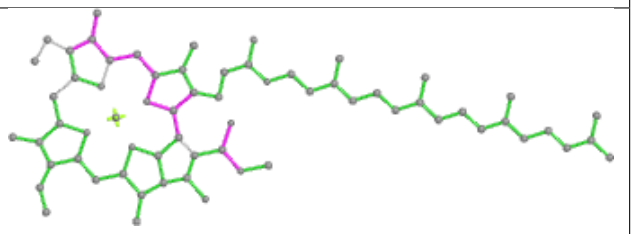
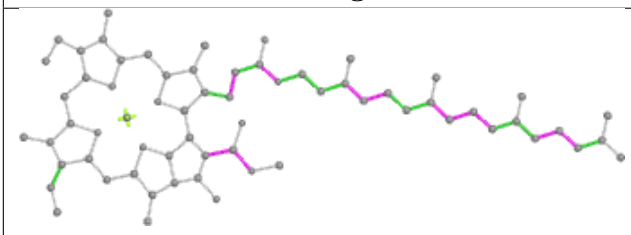
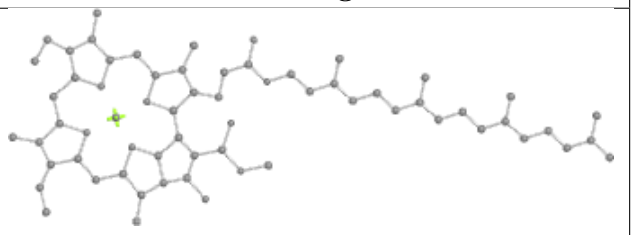
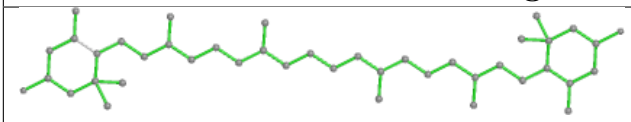
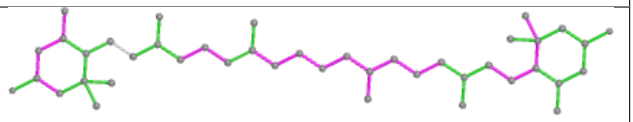
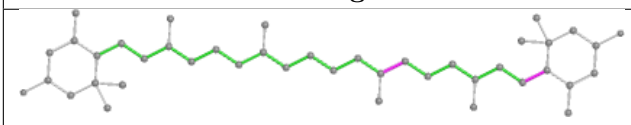
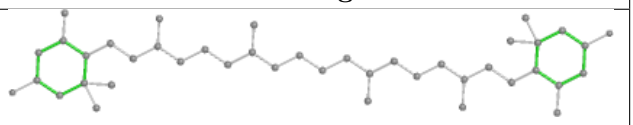
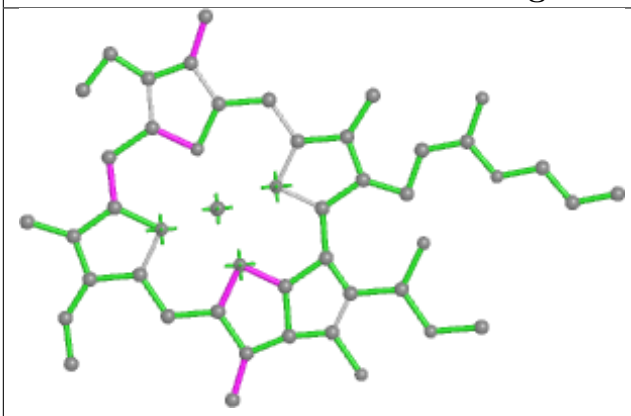


Rings

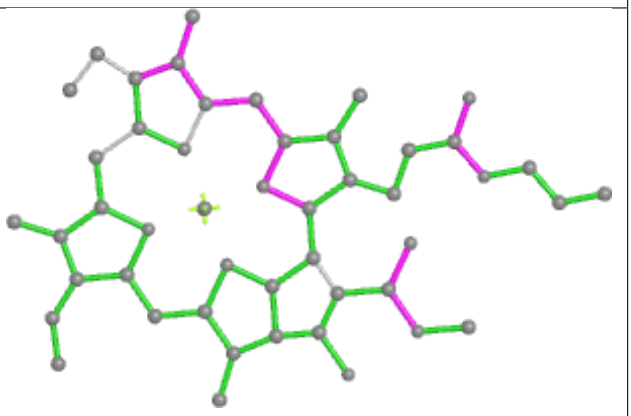
Ligand CLA b 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT U 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

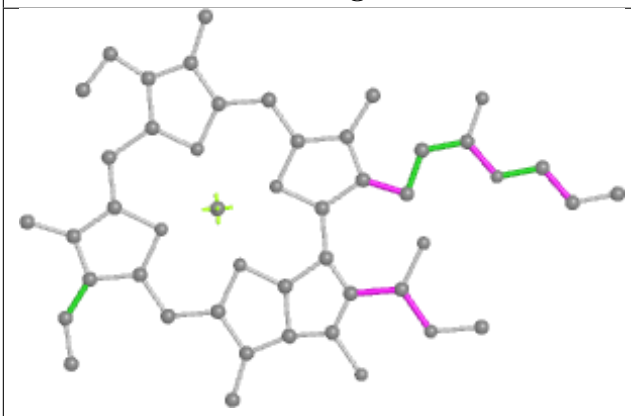
Ligand CLA 6 309



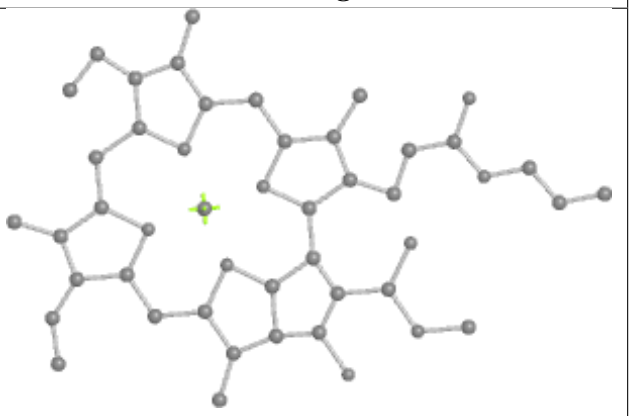
Bond lengths



Bond angles

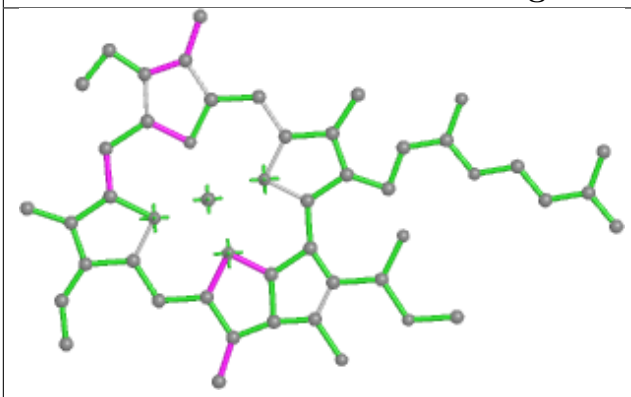


Torsions

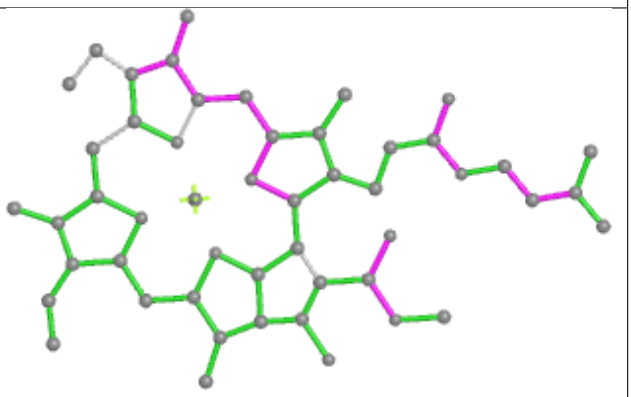


Rings

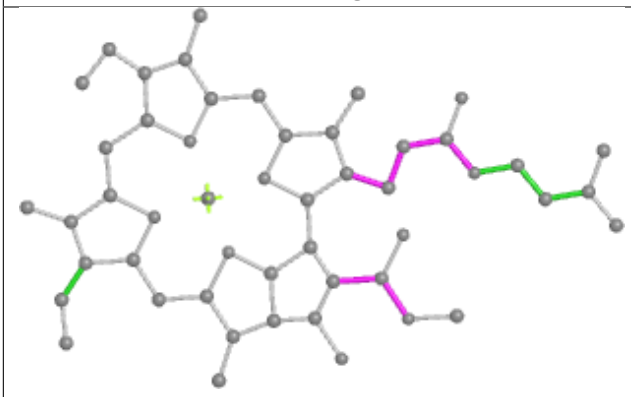
Ligand CLA 3 303



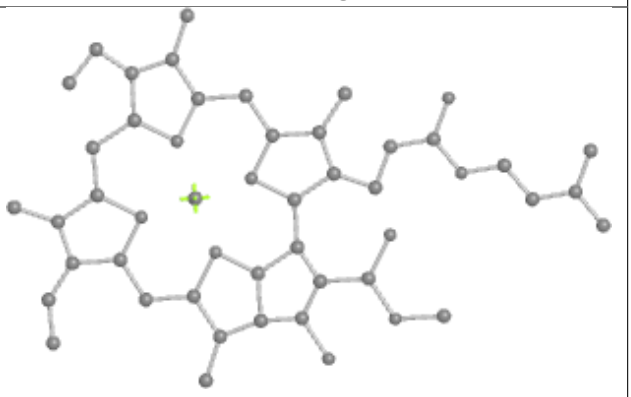
Bond lengths



Bond angles

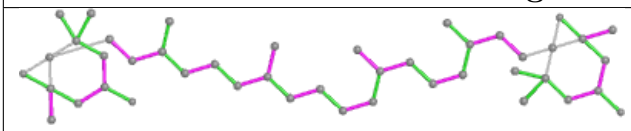


Torsions

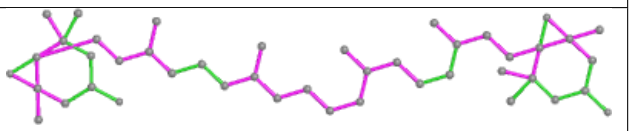


Rings

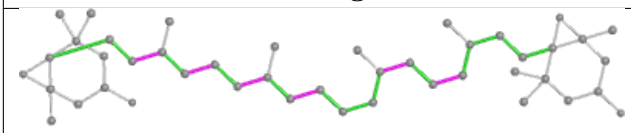
Ligand XAT n 311



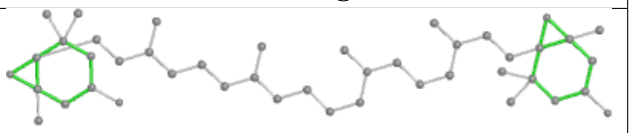
Bond lengths



Bond angles

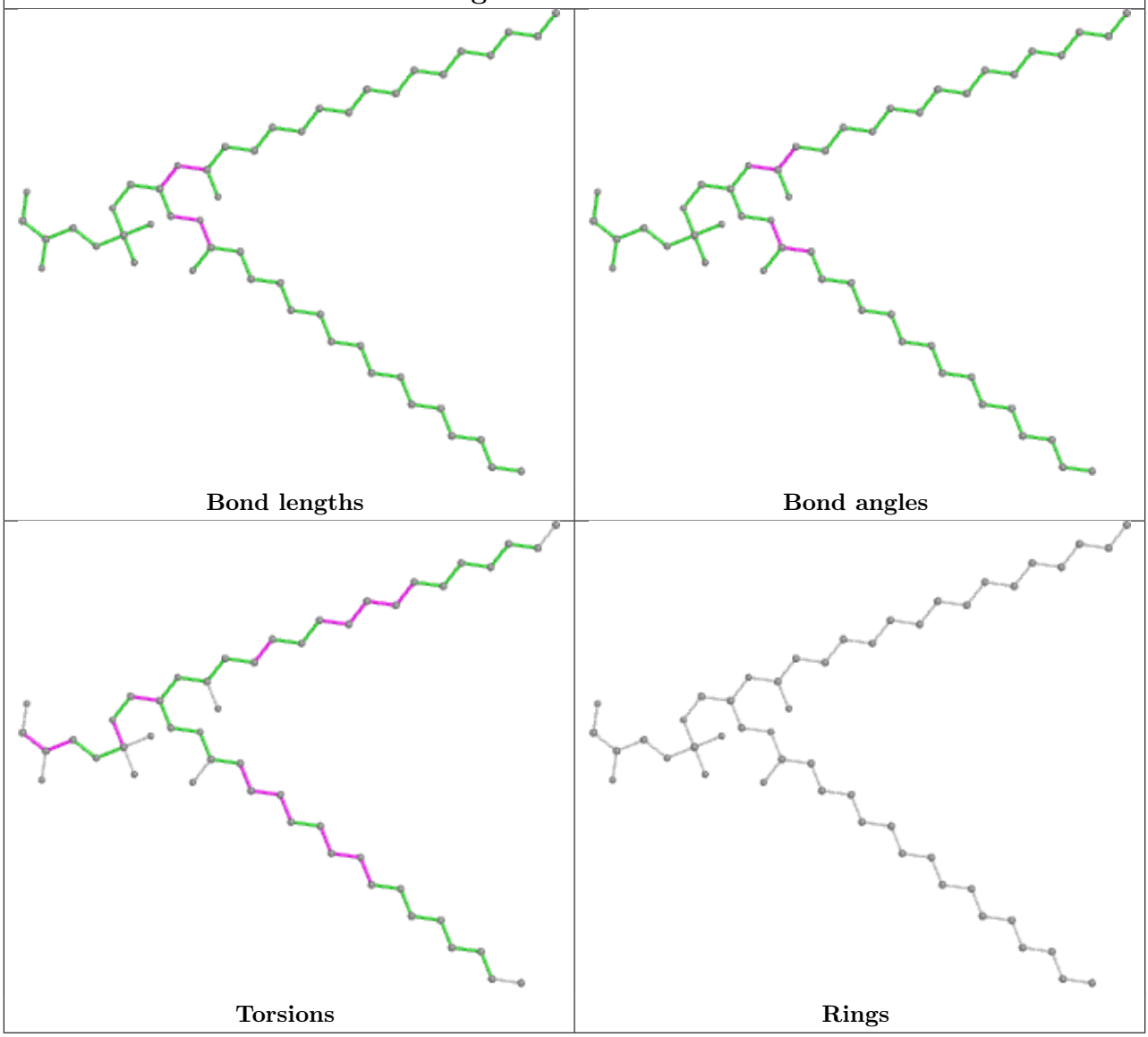


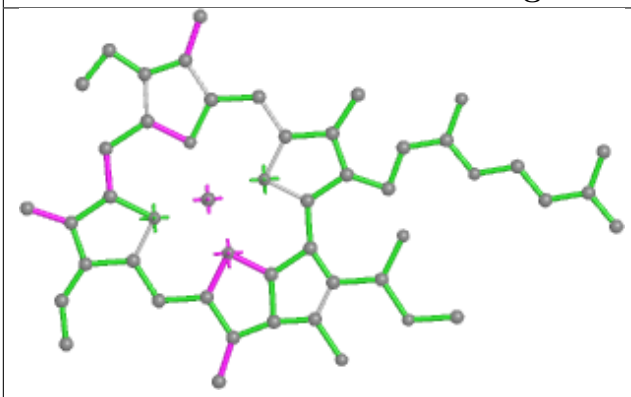
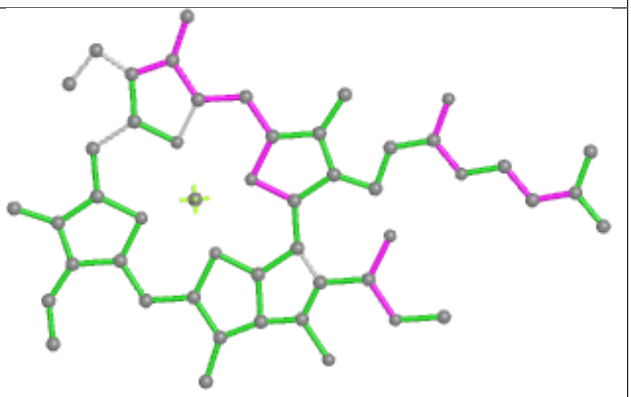
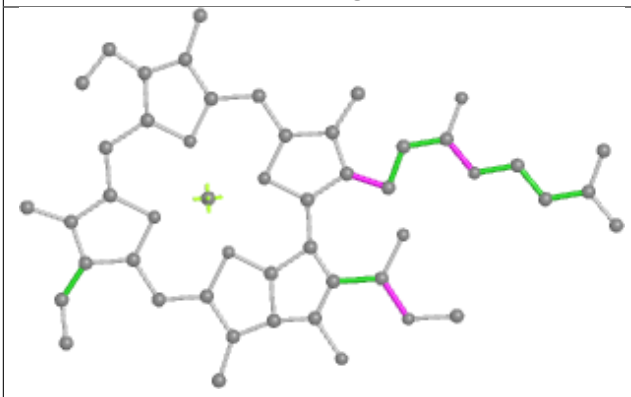
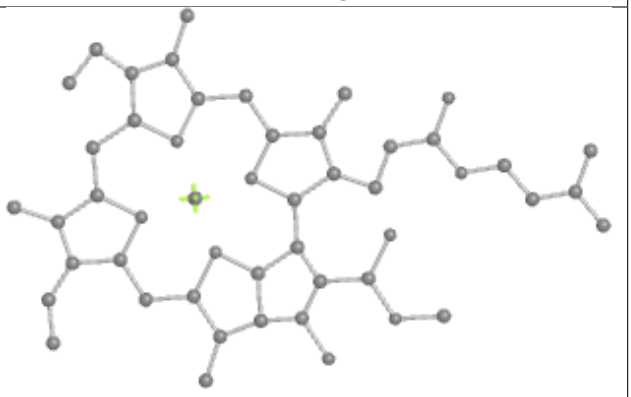
Torsions

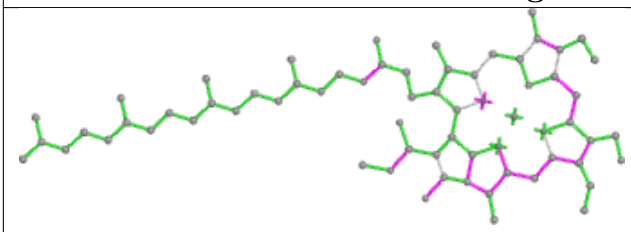
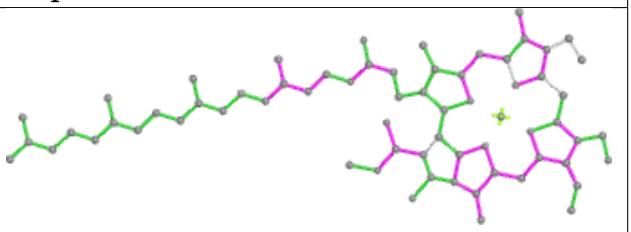
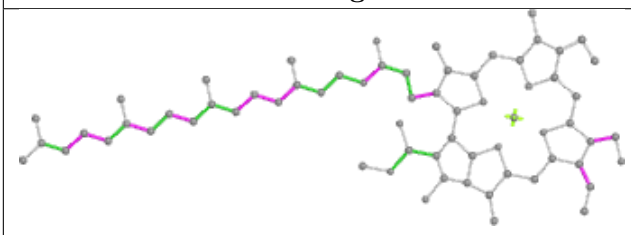
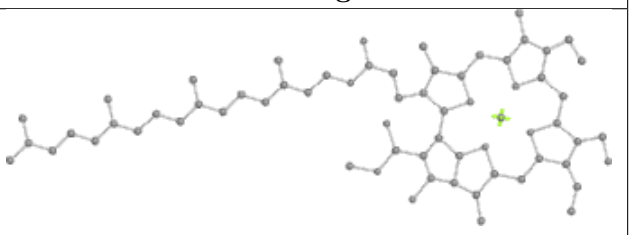


Rings

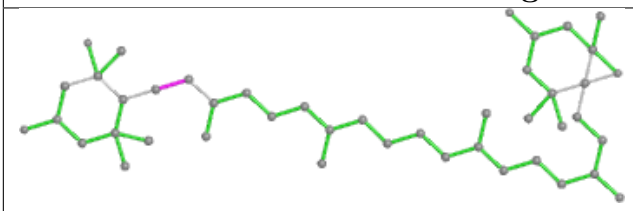
Ligand LHG n 312



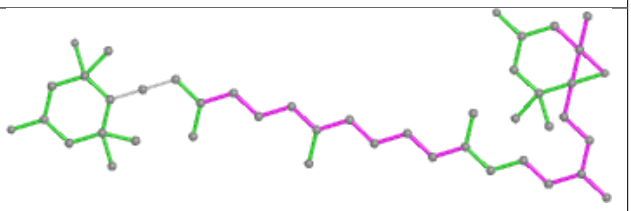
Ligand CLA V 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL p 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

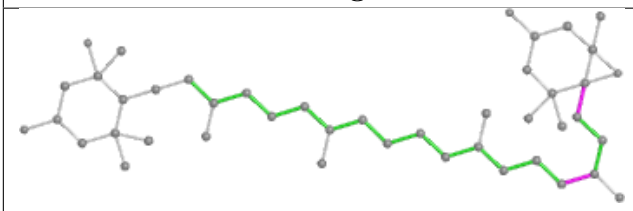
Ligand NEX U 318



Bond lengths



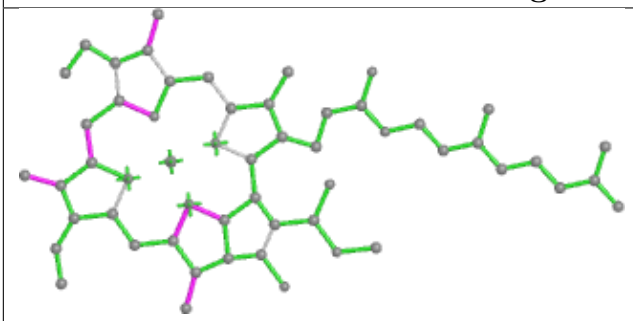
Bond angles



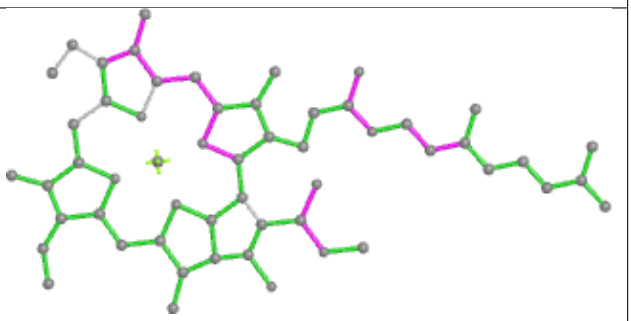
Torsions

Rings

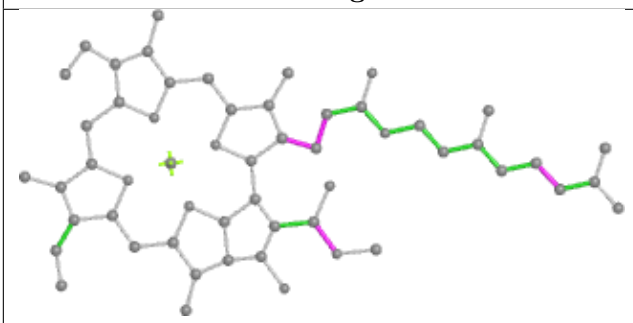
Ligand CLA s 305



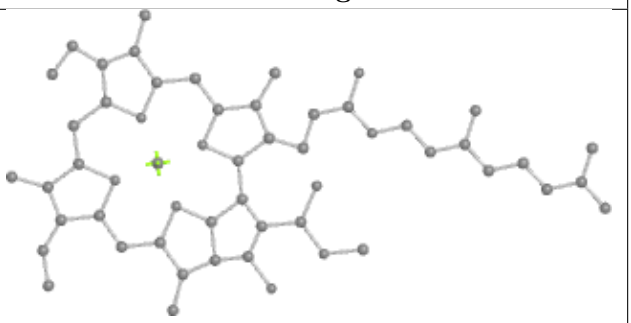
Bond lengths



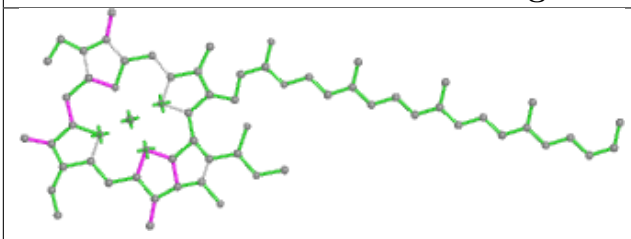
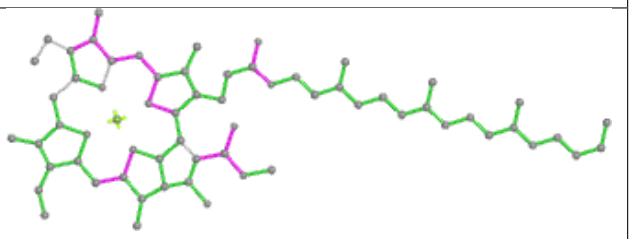
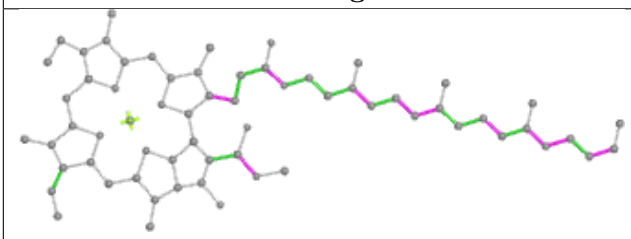
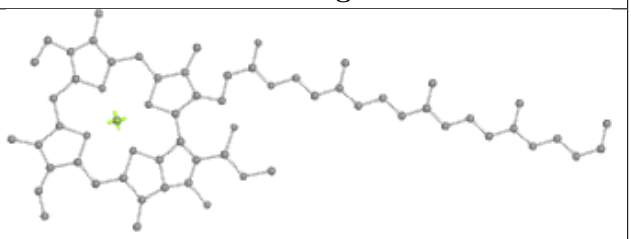
Bond angles

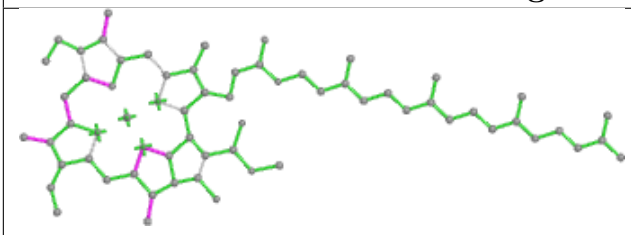
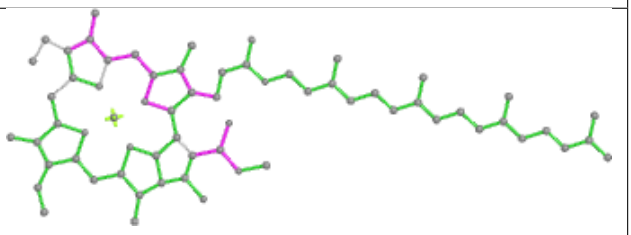
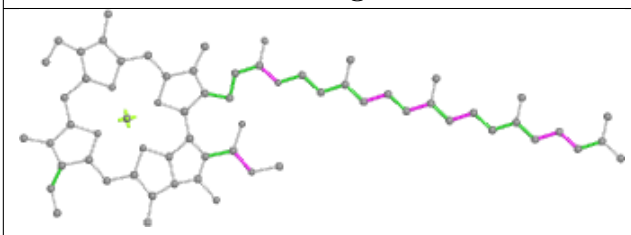
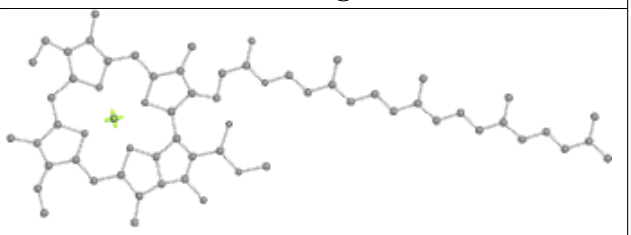


Torsions

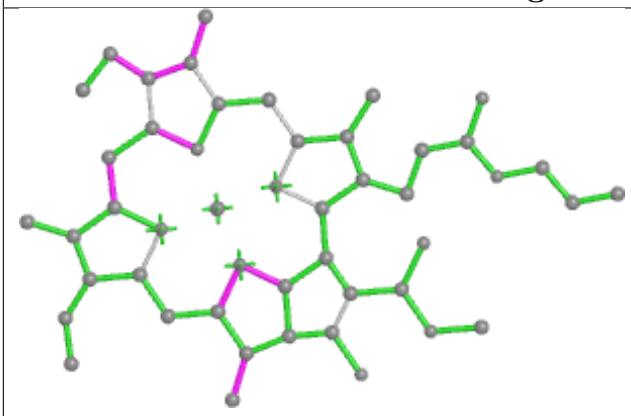


Rings

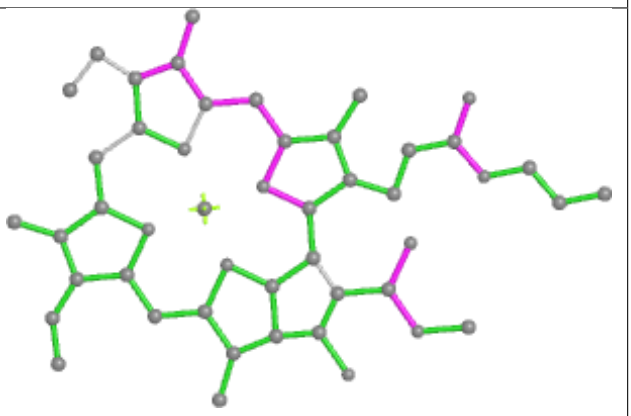
Ligand CLA 3 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA x 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

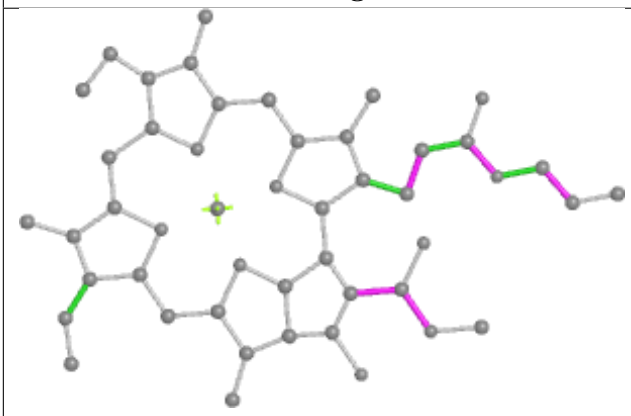
Ligand CLA u 308



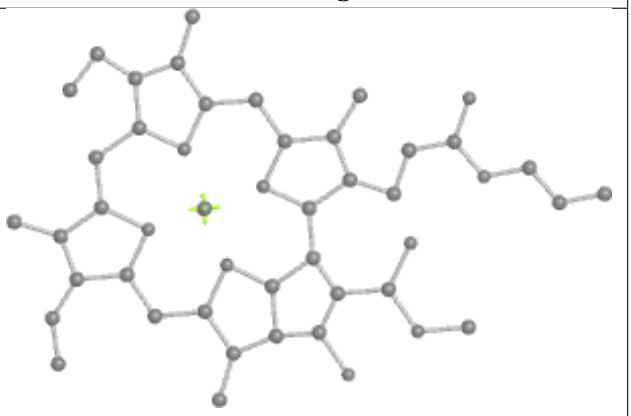
Bond lengths



Bond angles

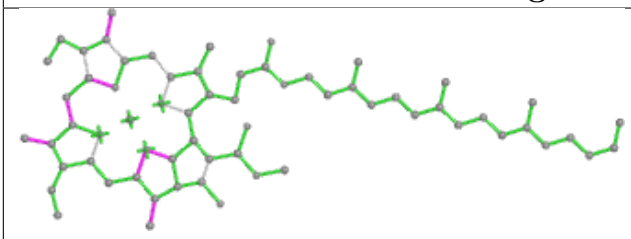


Torsions

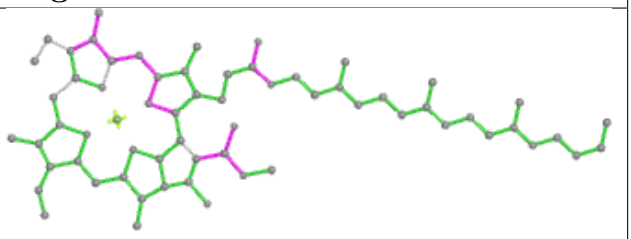


Rings

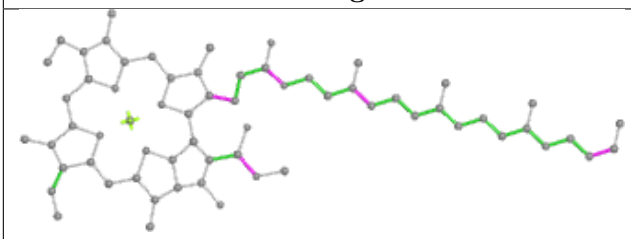
Ligand CLA g 304



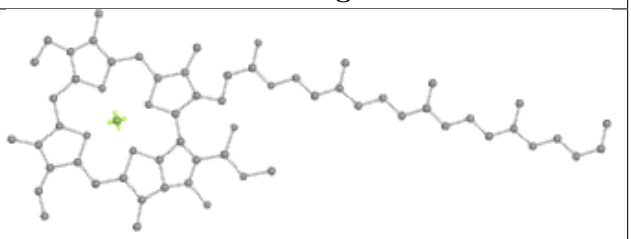
Bond lengths



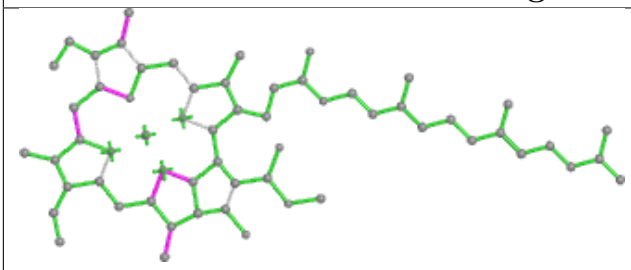
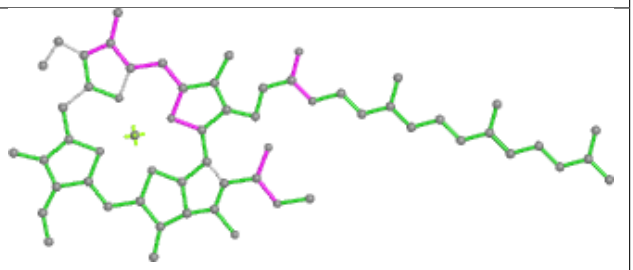
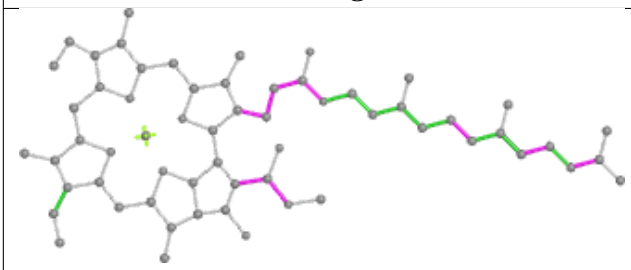
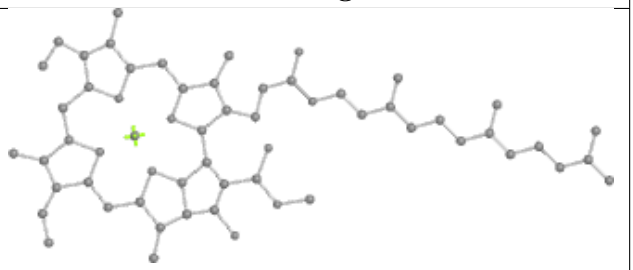
Bond angles

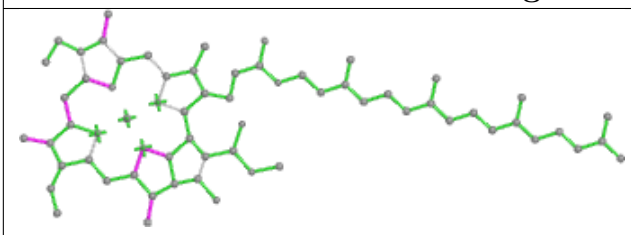
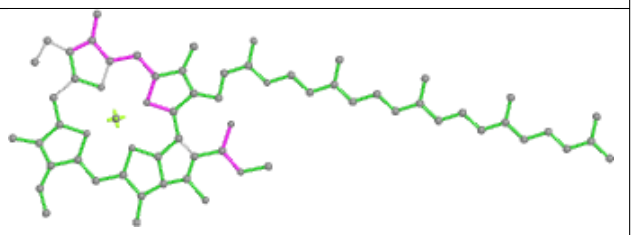
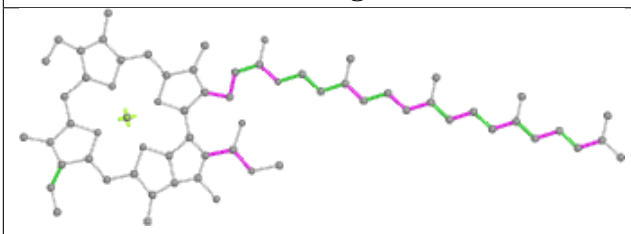
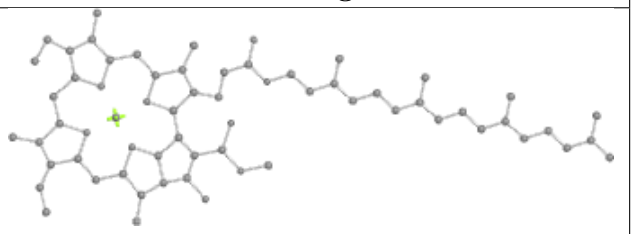


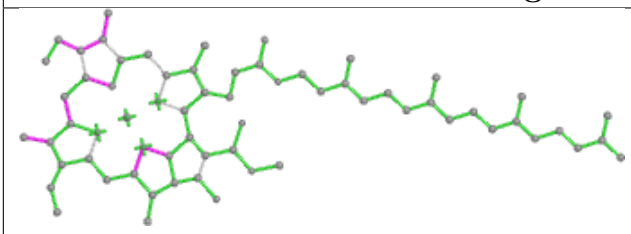
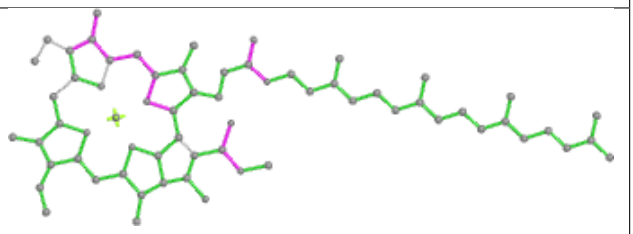
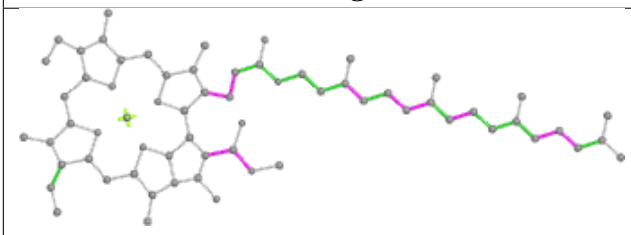
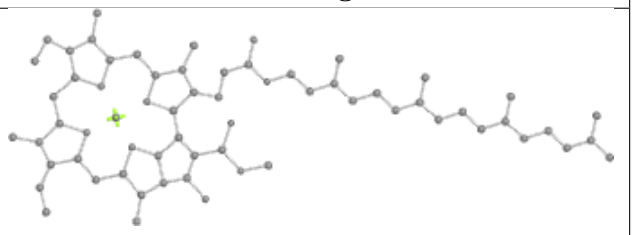
Torsions

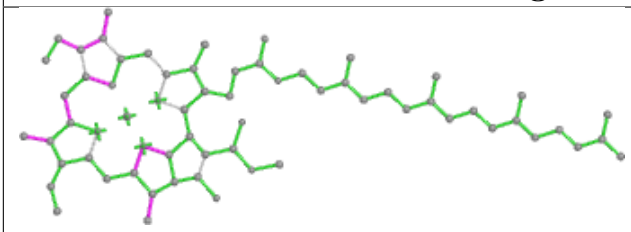
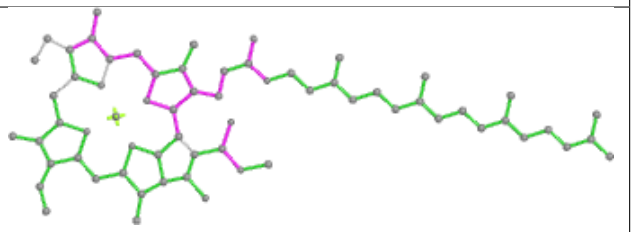
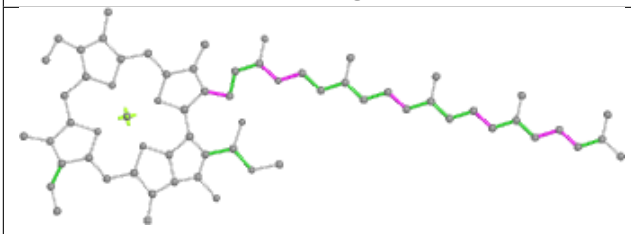
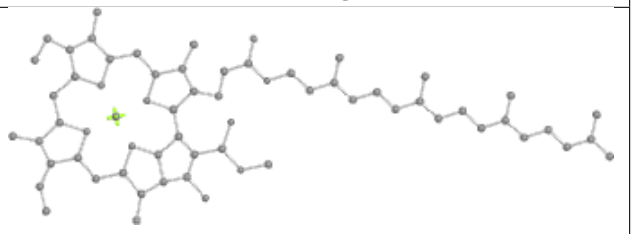


Rings

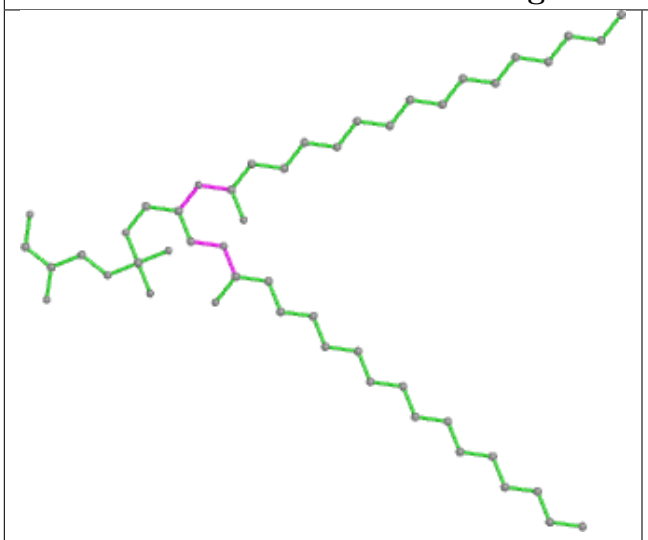
Ligand CLA v 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

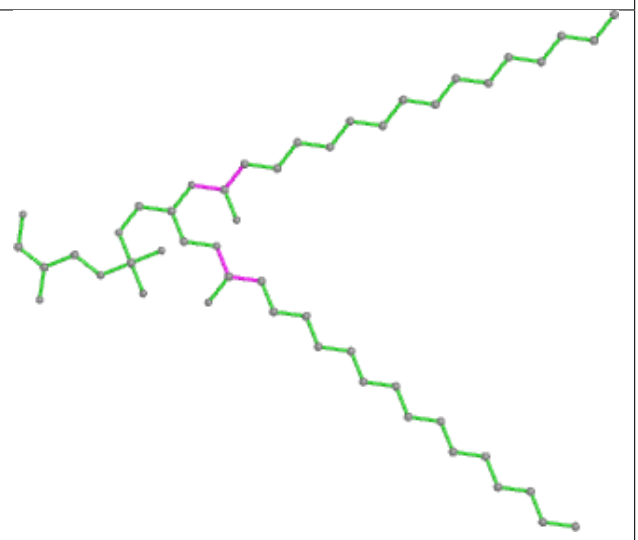
Ligand CLA B 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

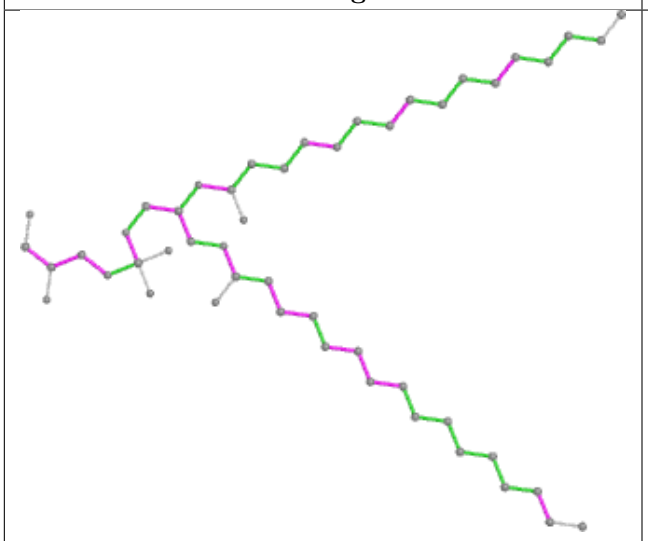
Ligand LHG 2 312



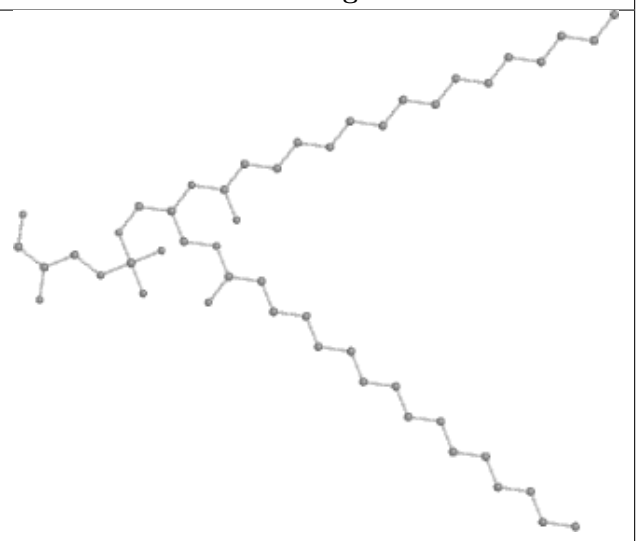
Bond lengths



Bond angles

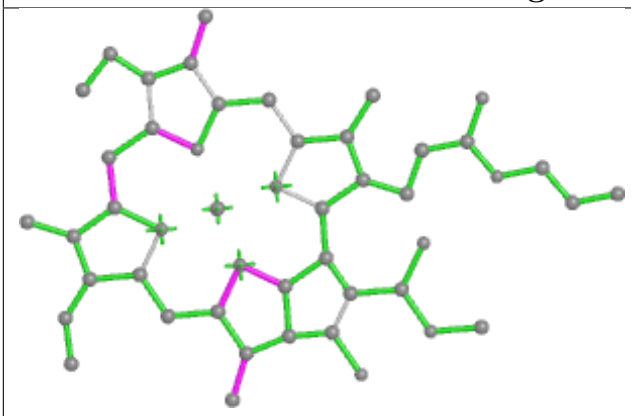


Torsions

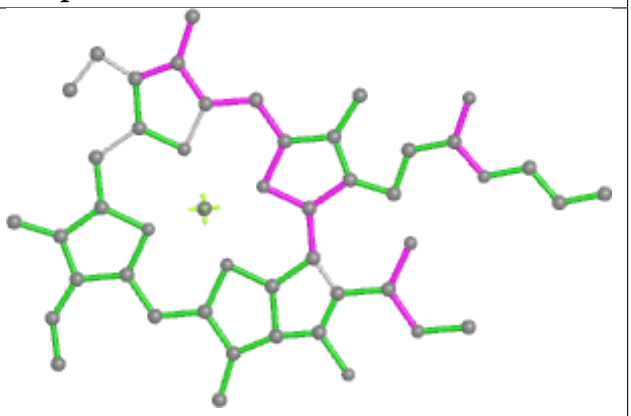


Rings

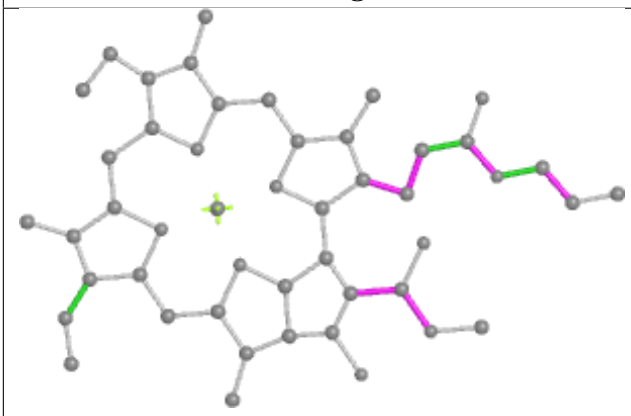
Ligand CLA q 308



Bond lengths



Bond angles



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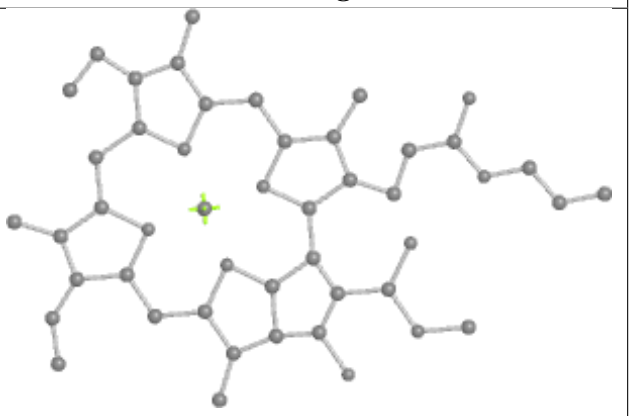
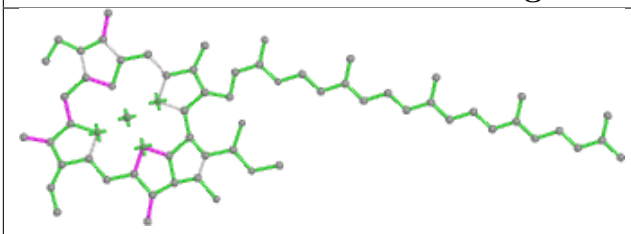


Rings

Ligand CLA C 511



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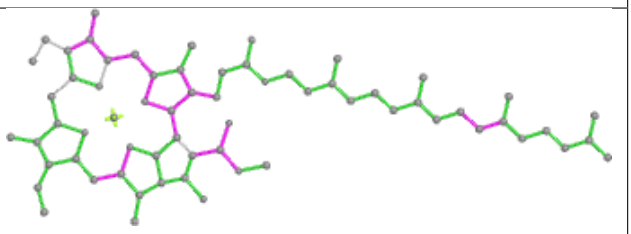
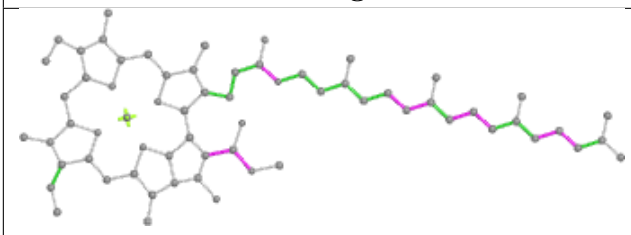
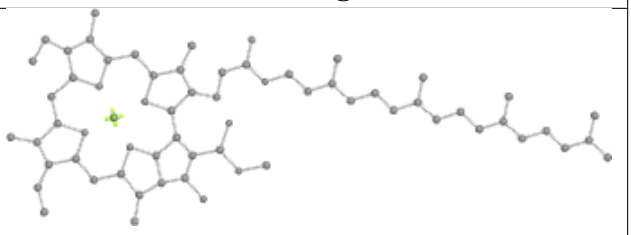


Bond angles

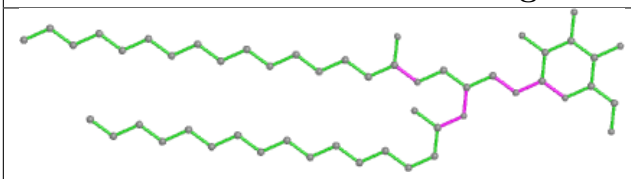


Torsions

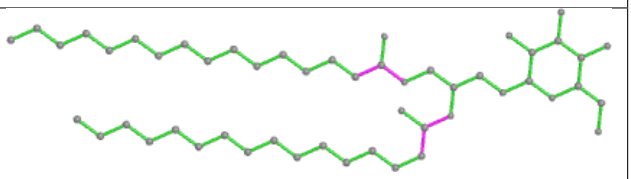


Rings

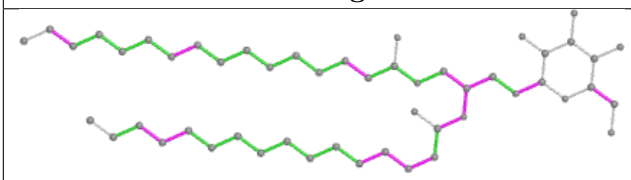
Ligand LMG C 521



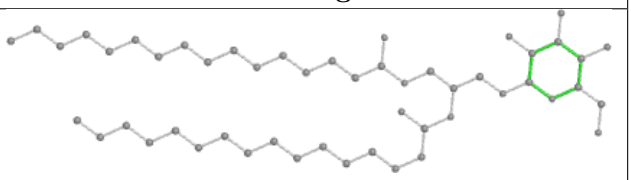
Bond lengths



Bond angles

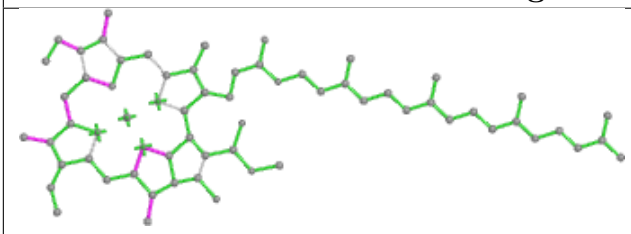


Torsions

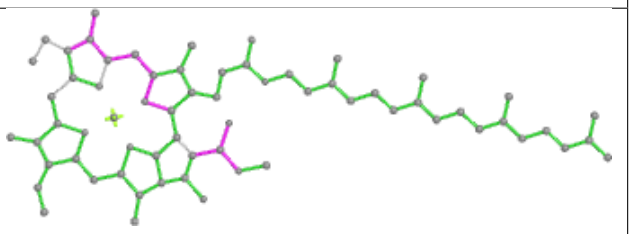


Rings

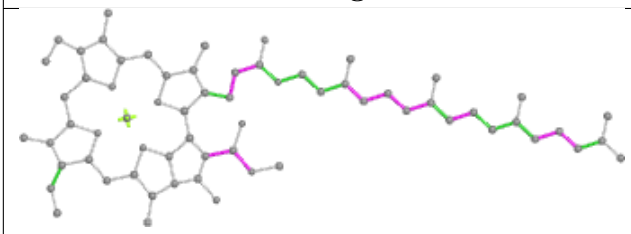
Ligand CLA b 615



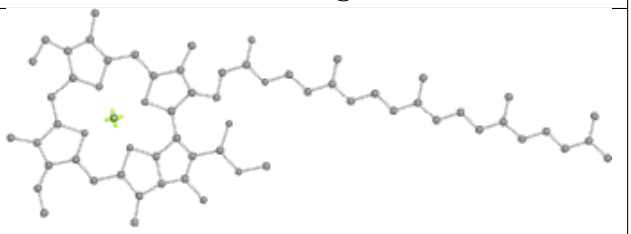
Bond lengths



Bond angles

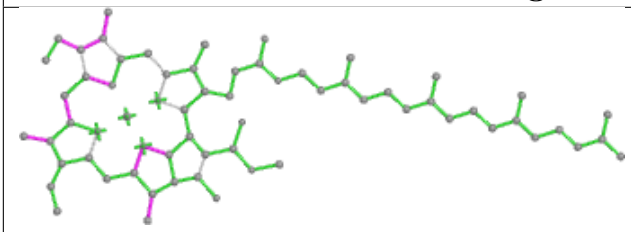


Torsions



Rings

Ligand CLA b 606



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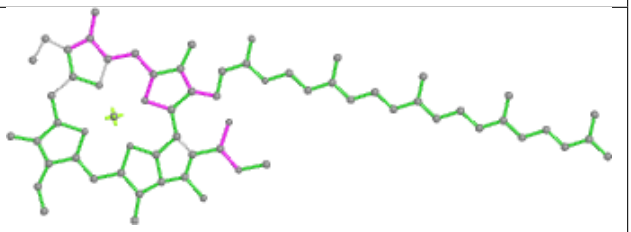
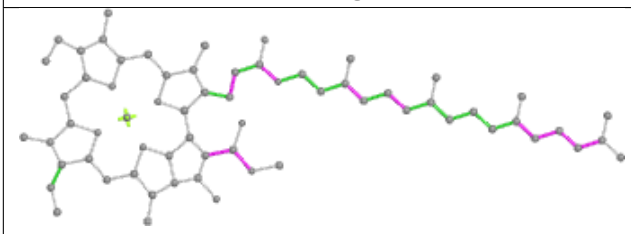


Bond angles



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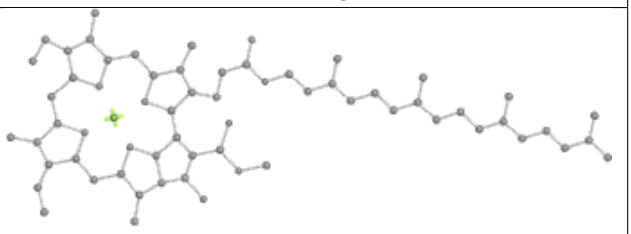
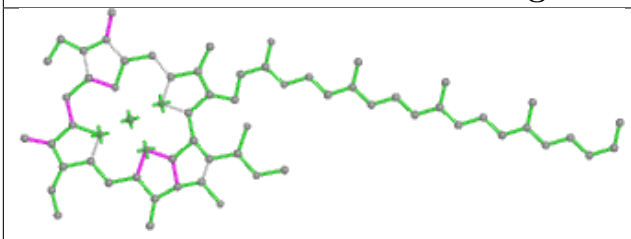
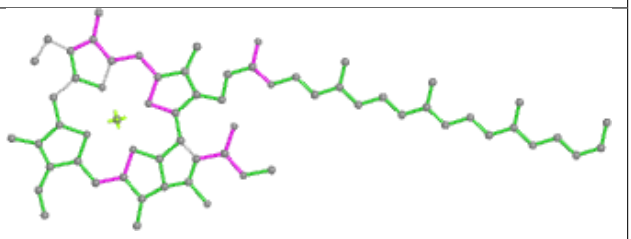
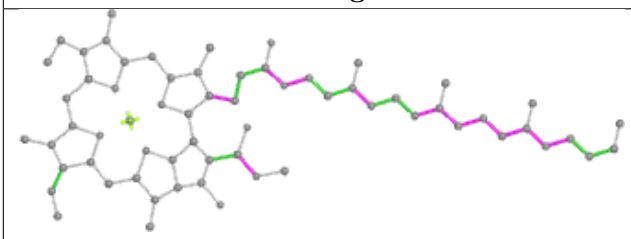
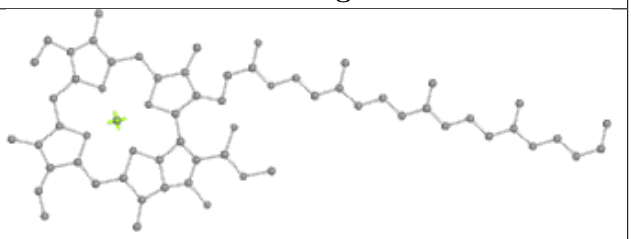
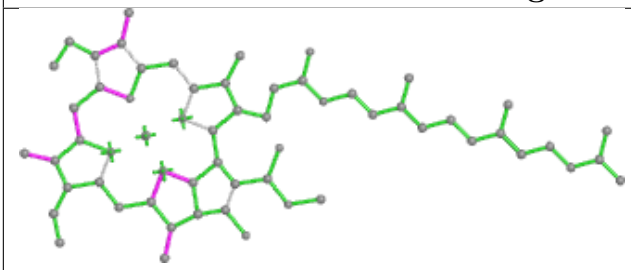
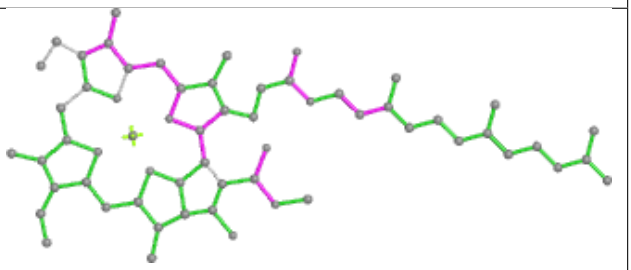
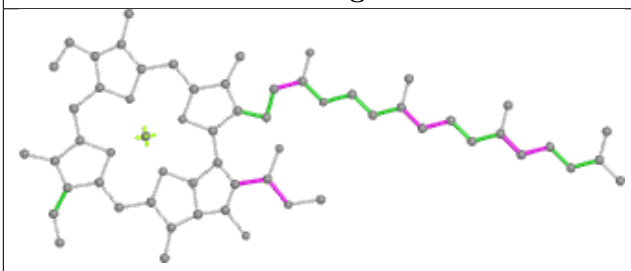
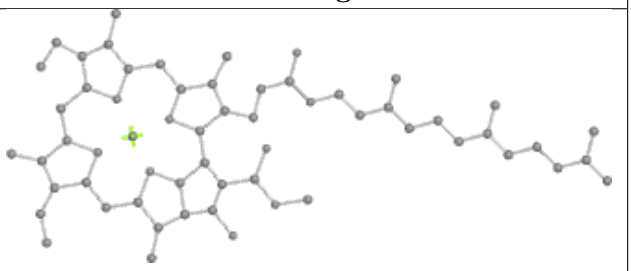
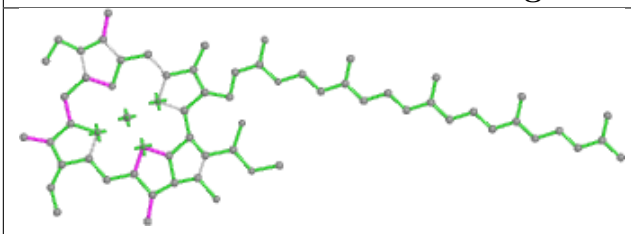


Rings

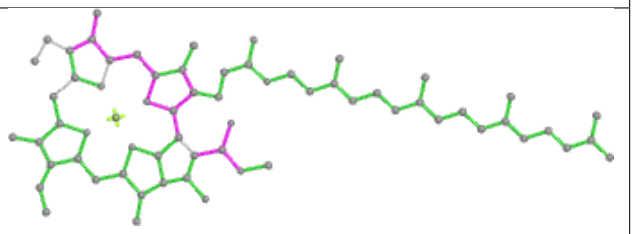
Ligand CLA 6 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

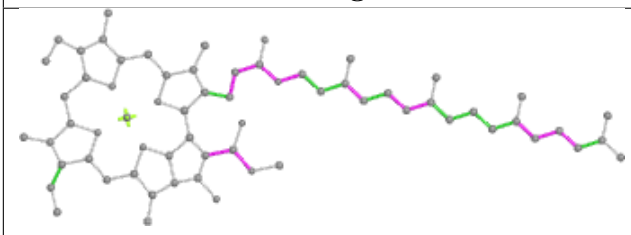
Ligand CLA C 507



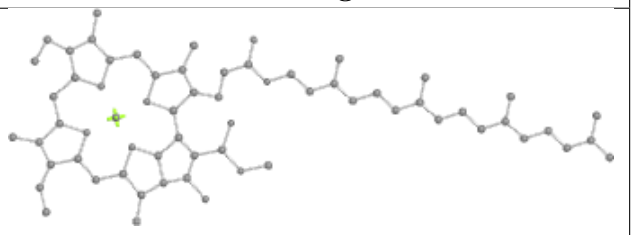
Bond lengths



Bond angles

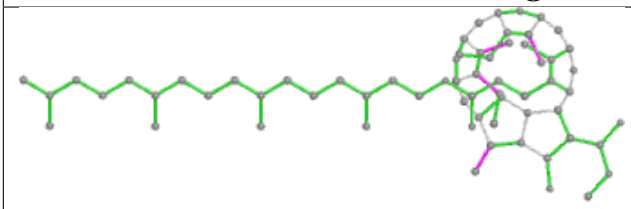


Torsions

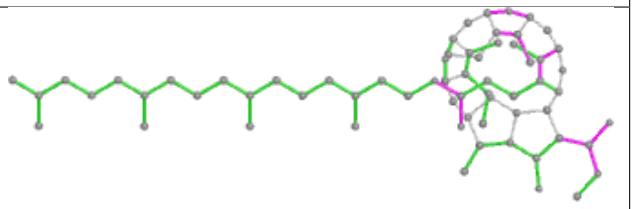


Rings

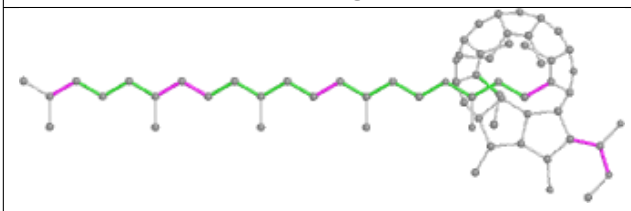
Ligand PHO d 401



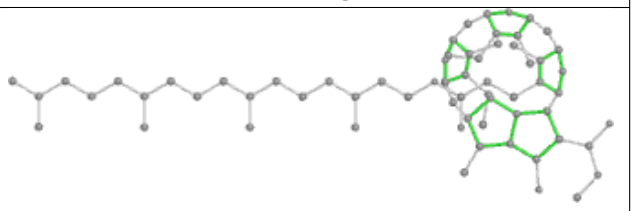
Bond lengths



Bond angles

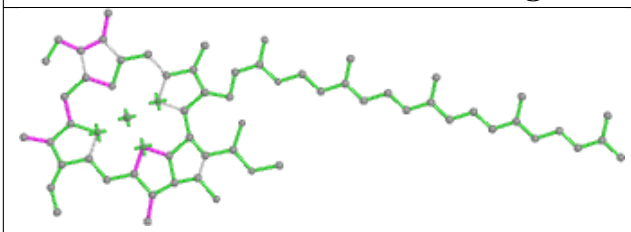


Torsions

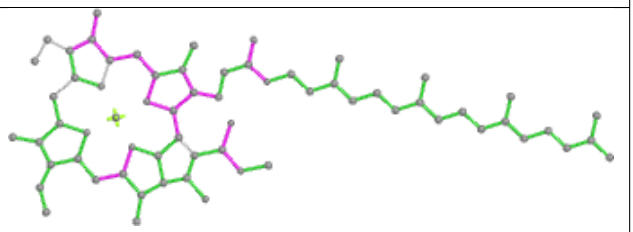


Rings

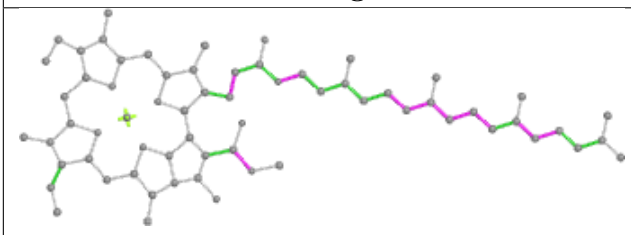
Ligand CLA C 509



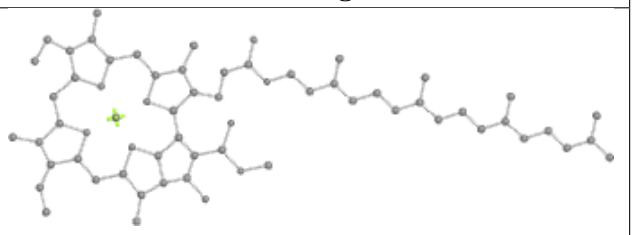
Bond lengths



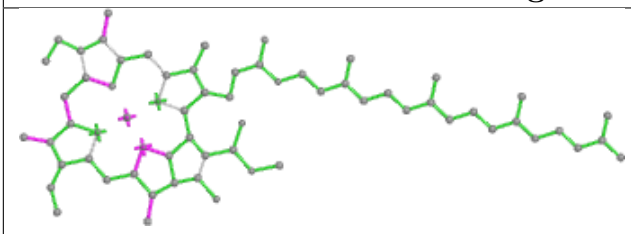
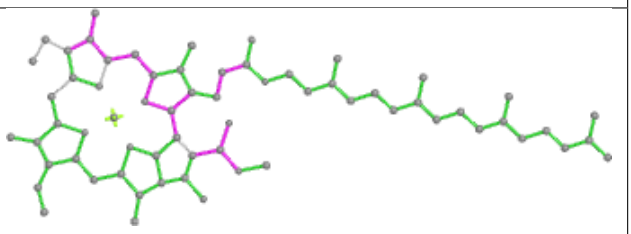
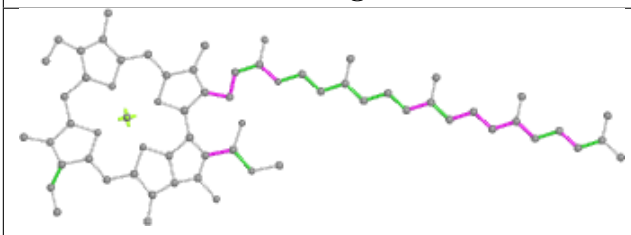
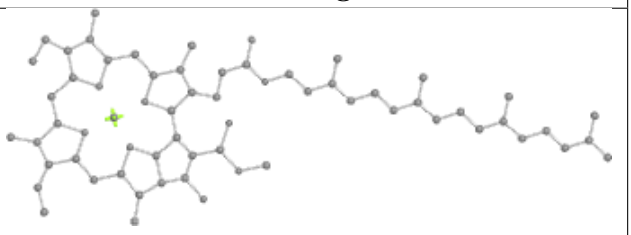
Bond angles

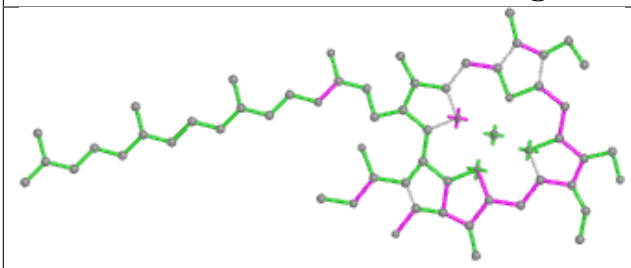
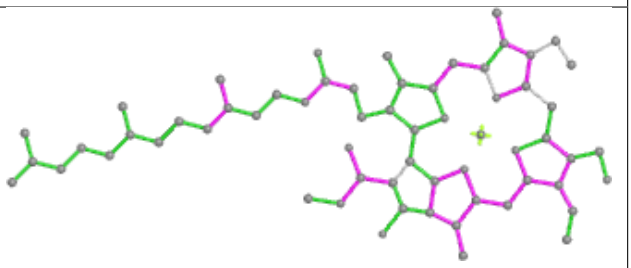
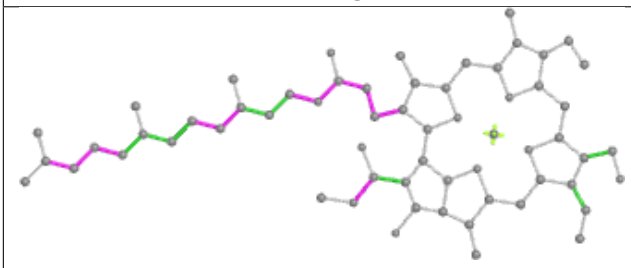
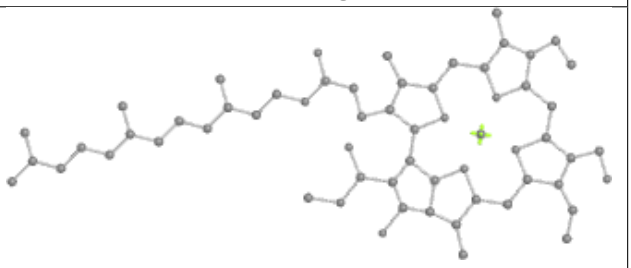


Torsions

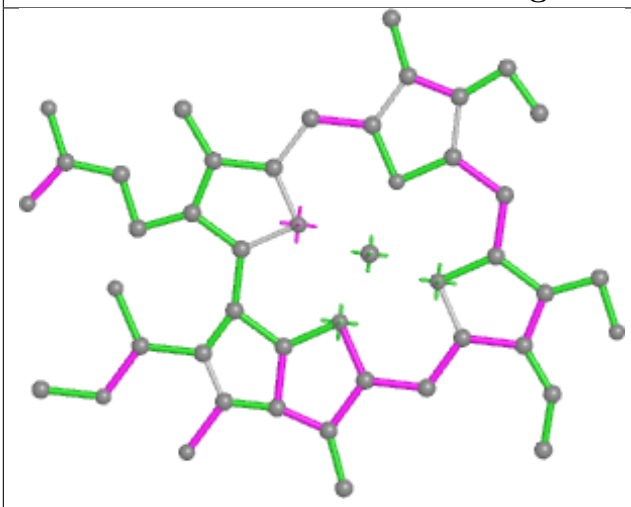


Rings

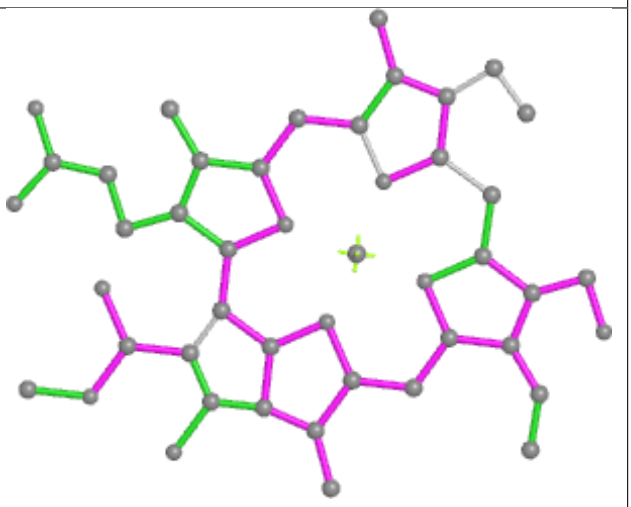
Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL r 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

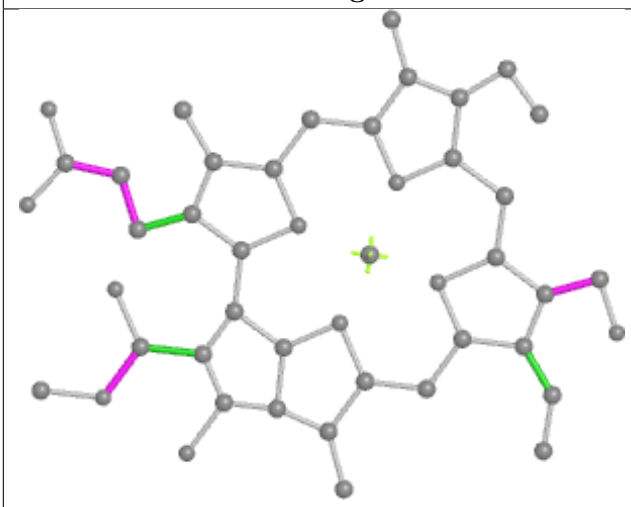
Ligand CHL s 313



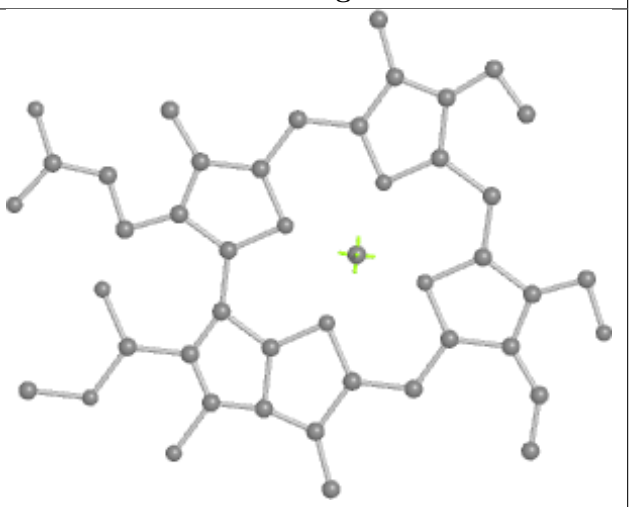
Bond lengths



Bond angles

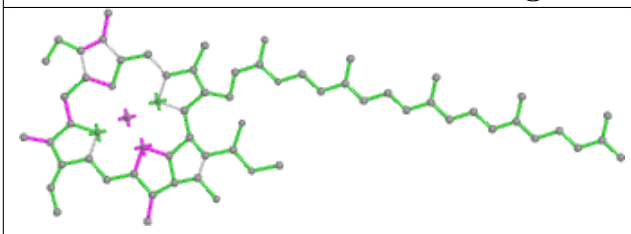


Torsions

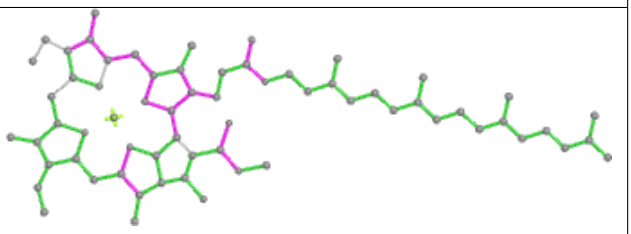


Rings

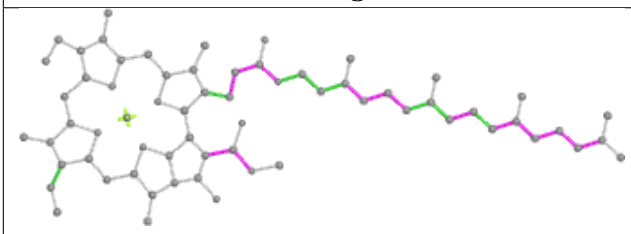
Ligand CLA B 602



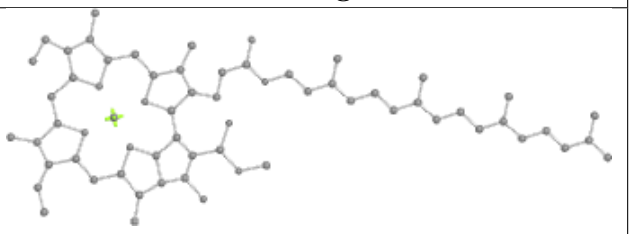
Bond lengths



Bond angles

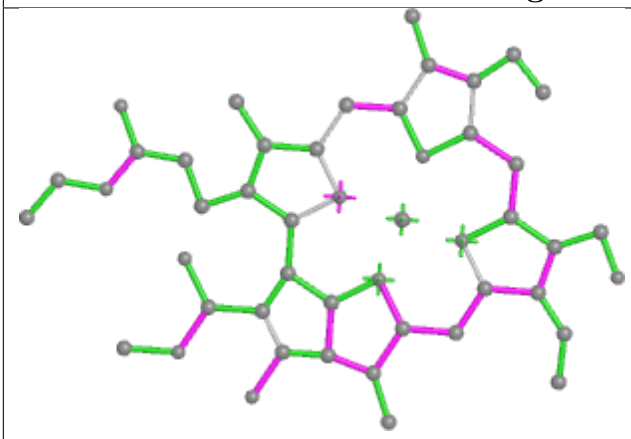


Torsions



Rings

Ligand CHL u 314



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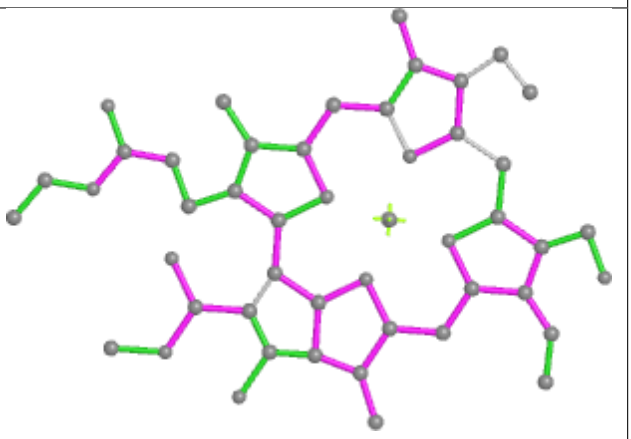
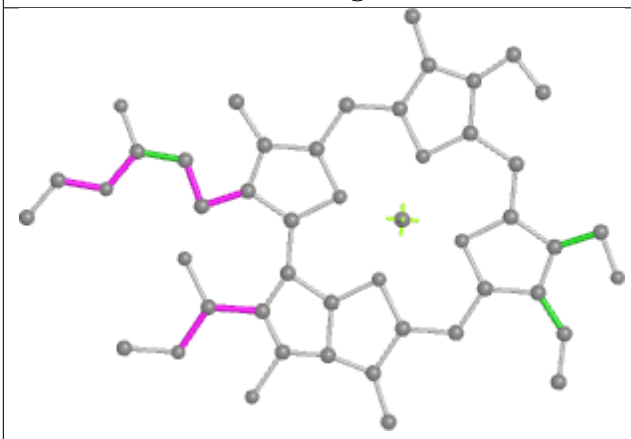
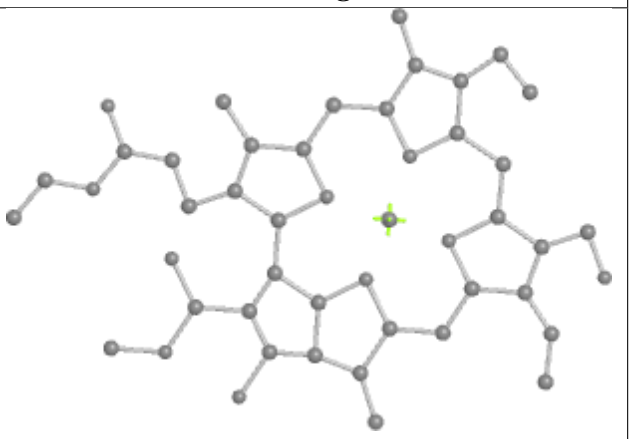


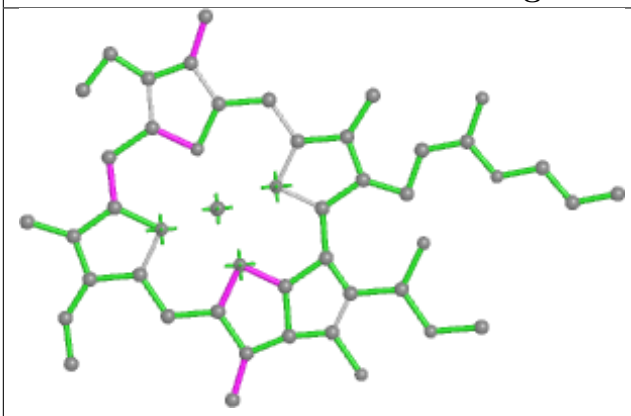
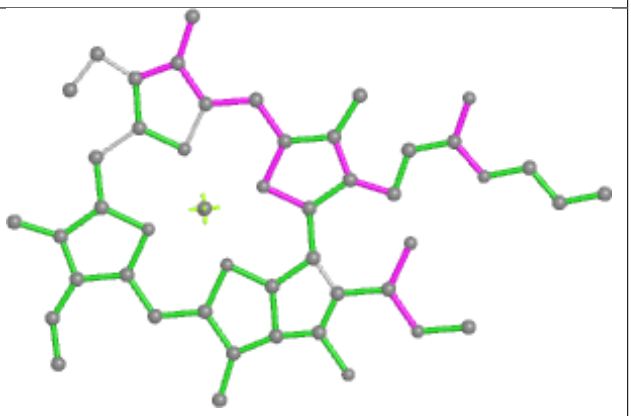
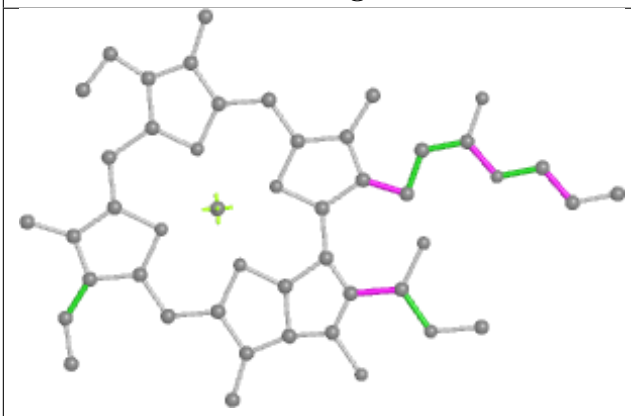
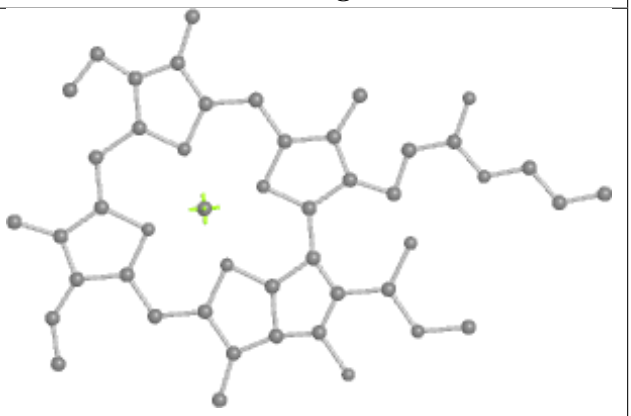
Bond angles



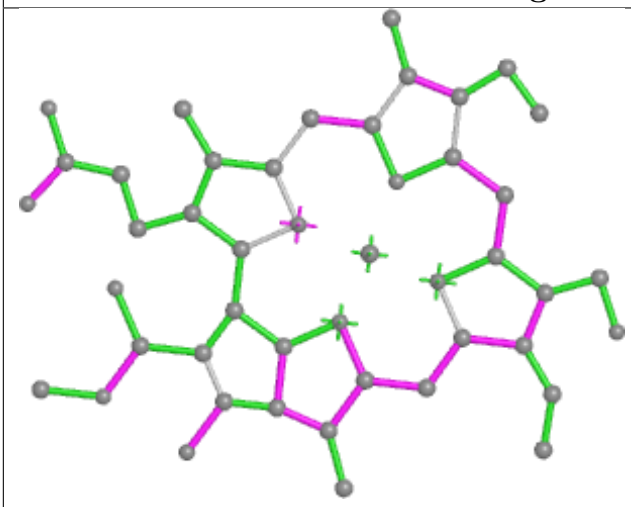
Torsions



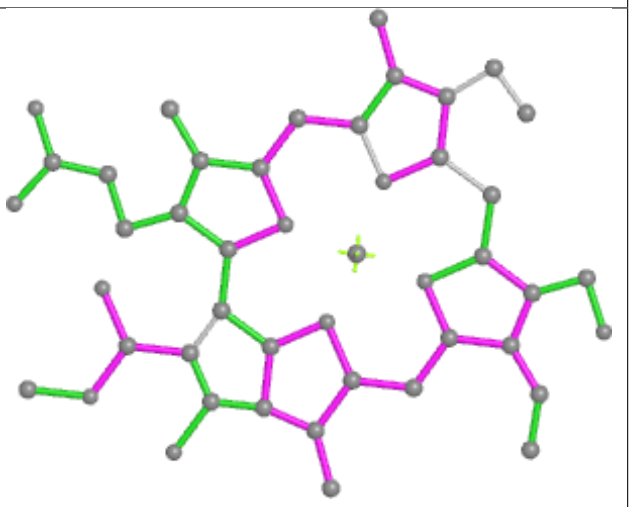
Rings

Ligand CLA R 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

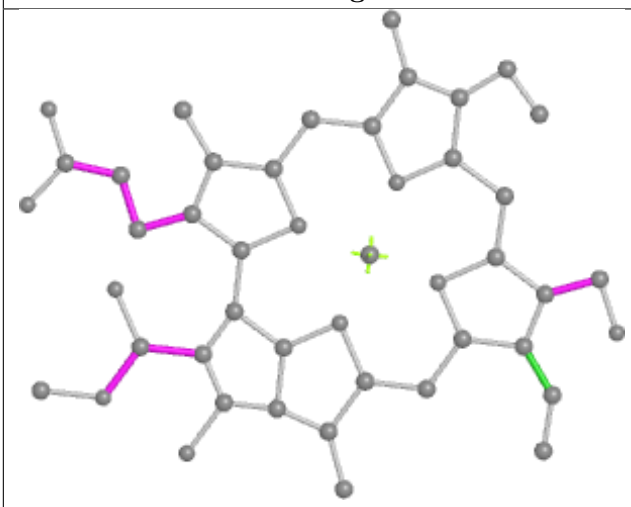
Ligand CHL s 316



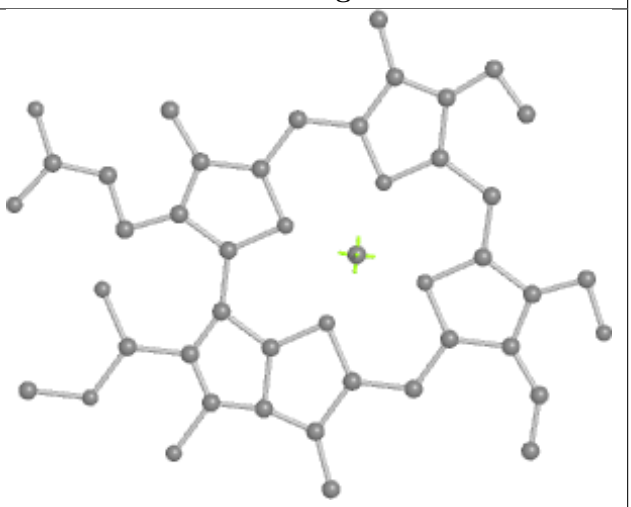
Bond lengths



Bond angles

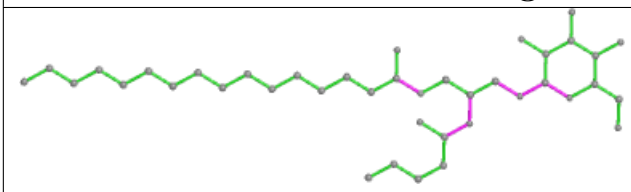


Torsions

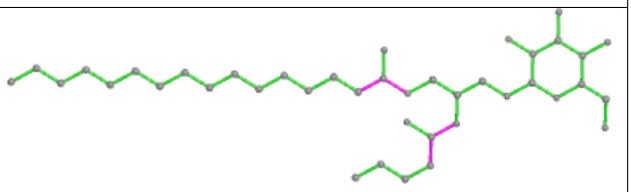


Rings

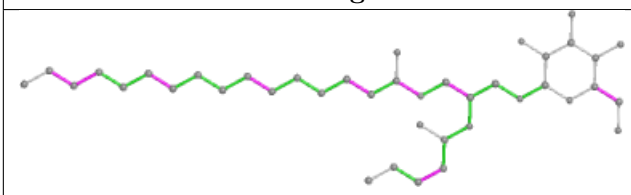
Ligand LMG A 411



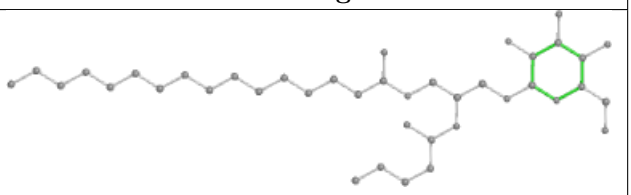
Bond lengths



Bond angles

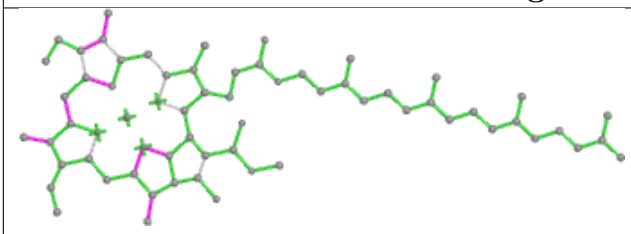


Torsions

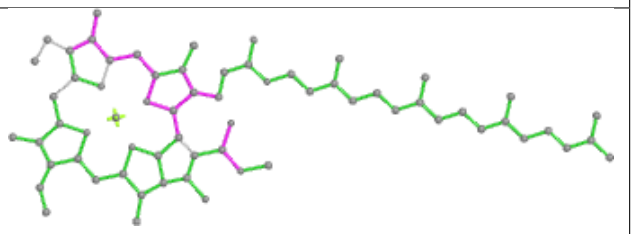


Rings

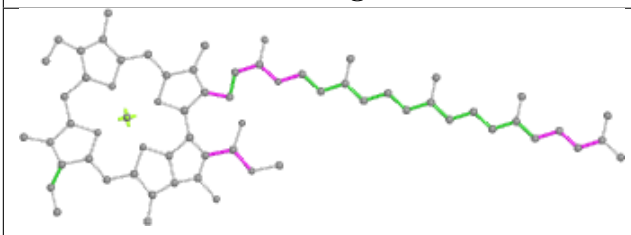
Ligand CLA b 611



Bond lengths



Bond angles



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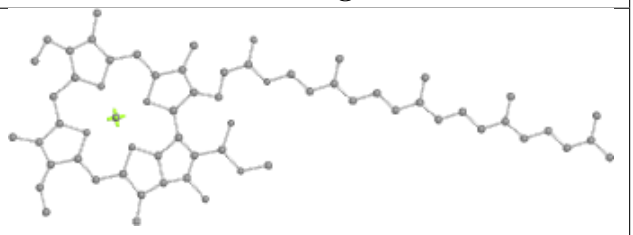
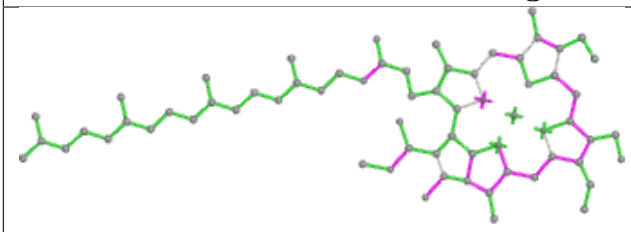
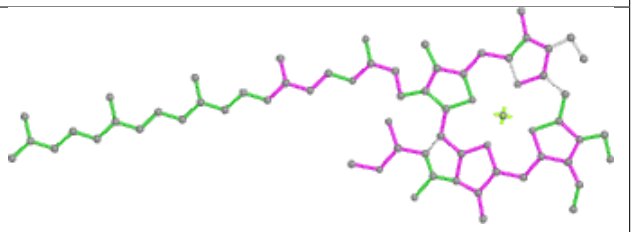


Rings

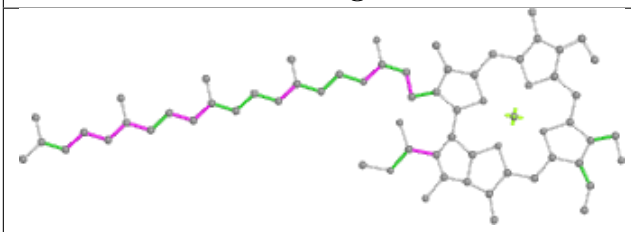
Ligand CHL P 317



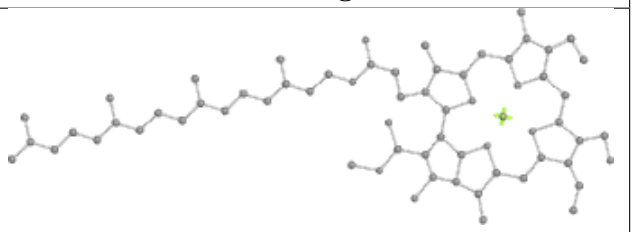
Bond lengths



Bond angles

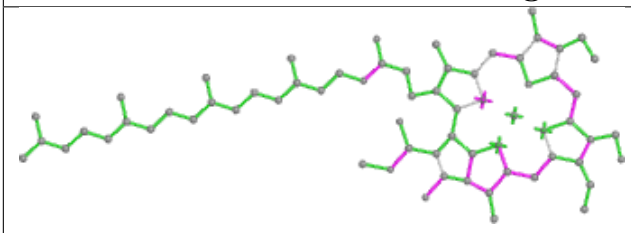


Torsions

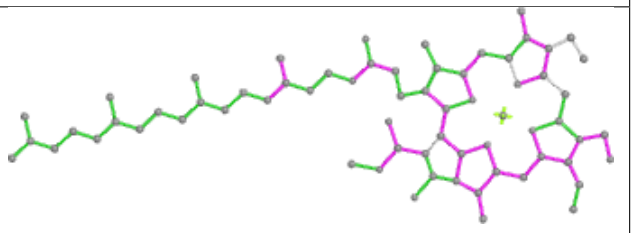


Rings

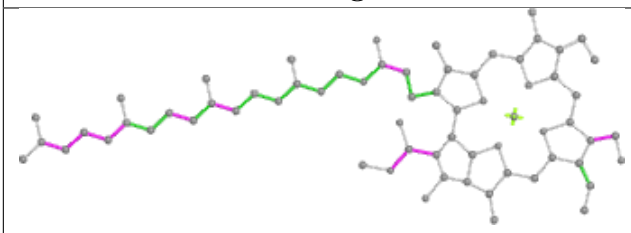
Ligand CHL N 316



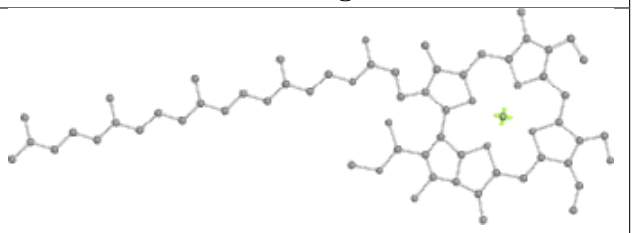
Bond lengths



Bond angles

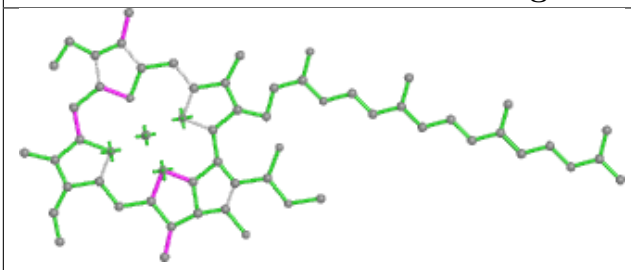


Torsions

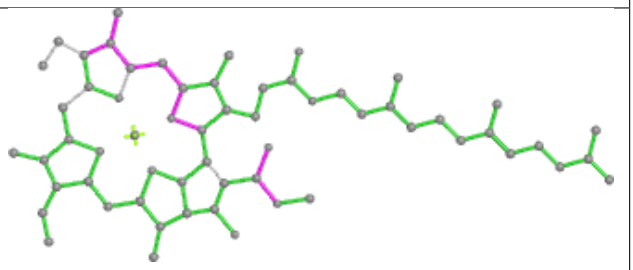


Rings

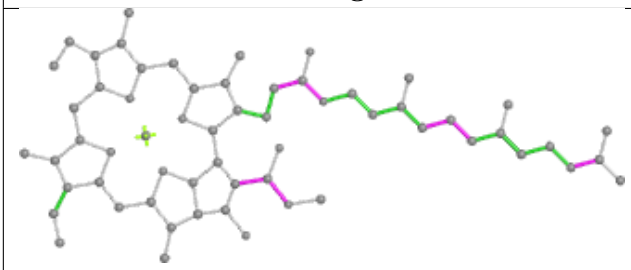
Ligand CLA r 603



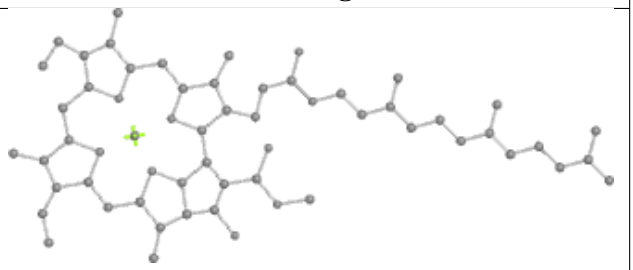
Bond lengths



Bond angles

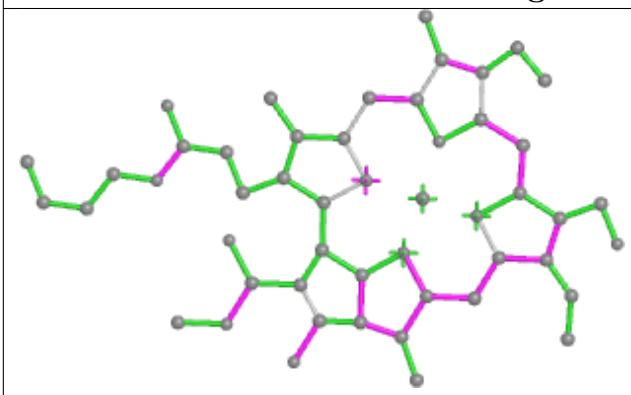


Torsions

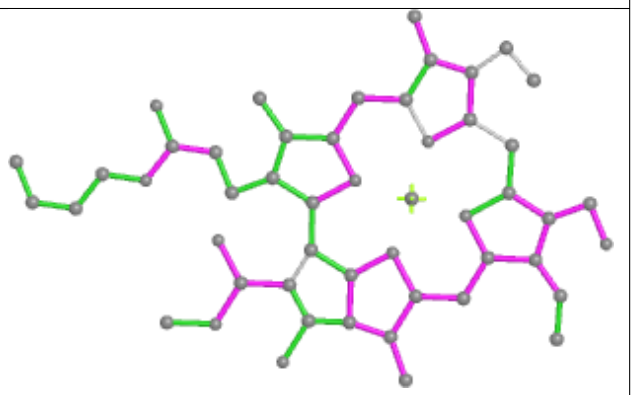


Rings

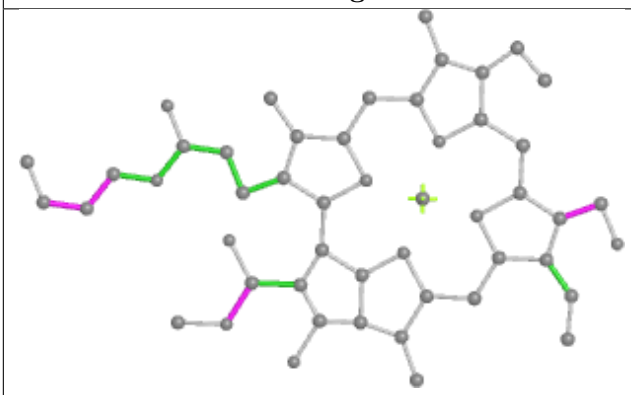
Ligand CHL 4 315



Bond lengths



Bond angles



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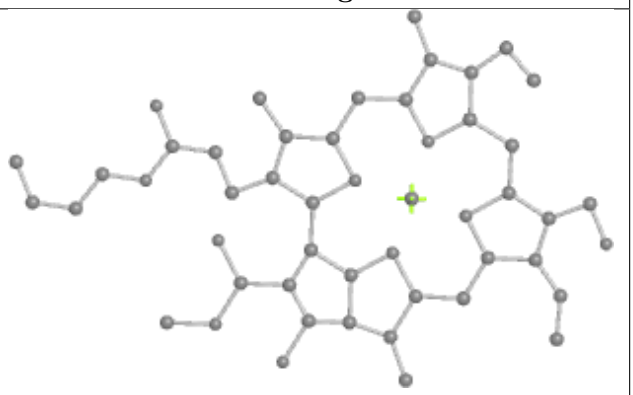
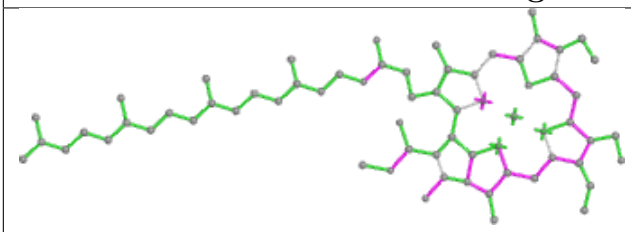
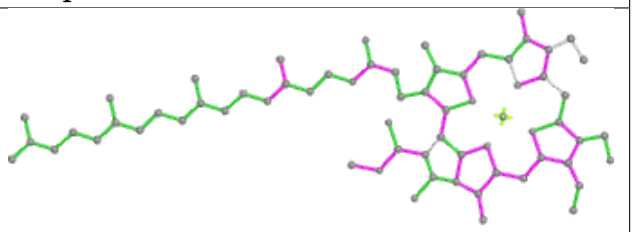
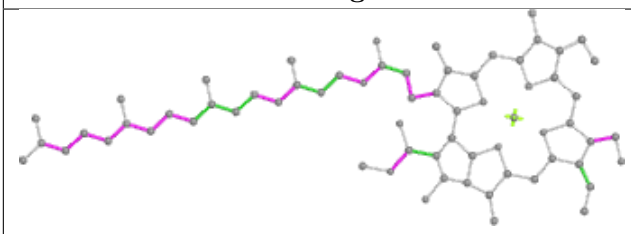
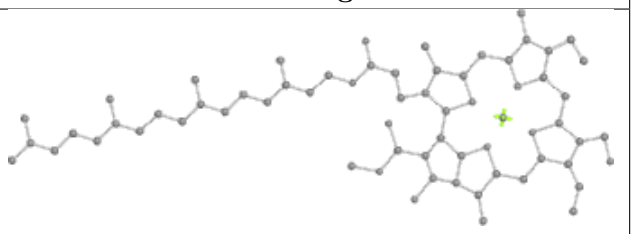
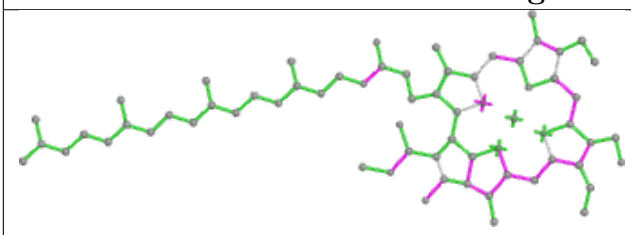
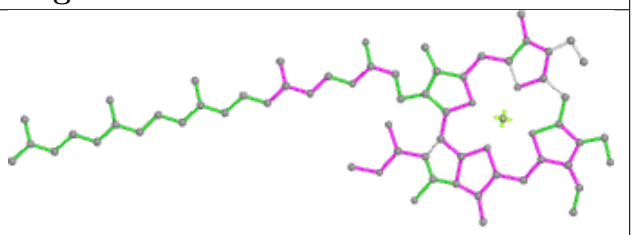
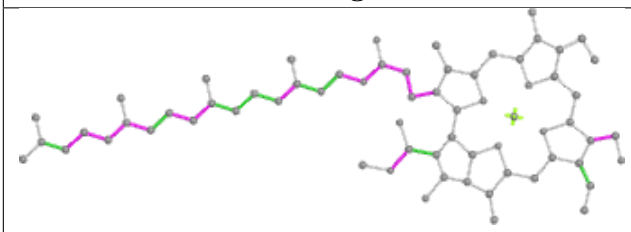
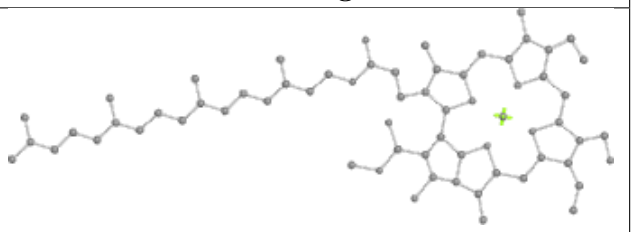
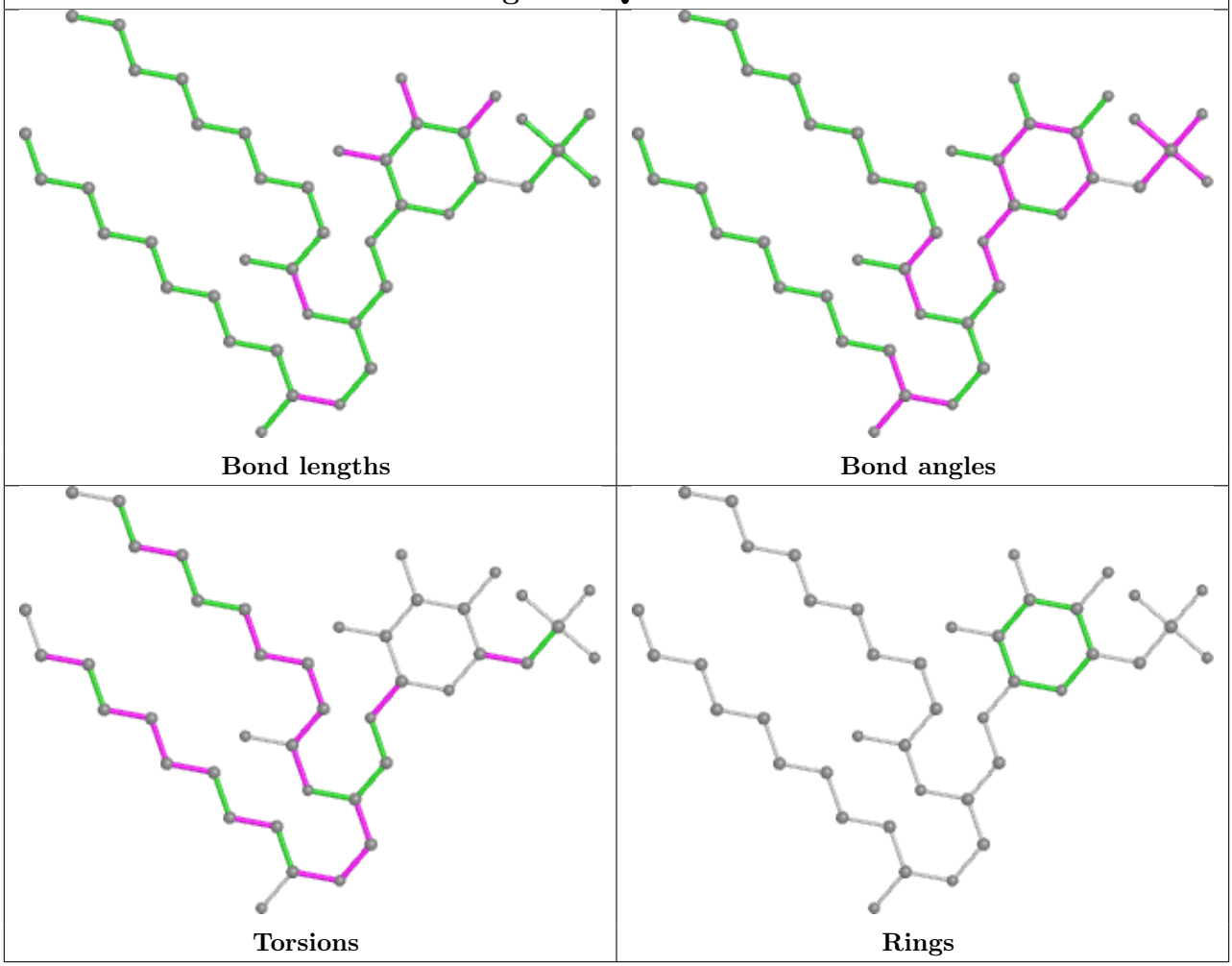


Rings

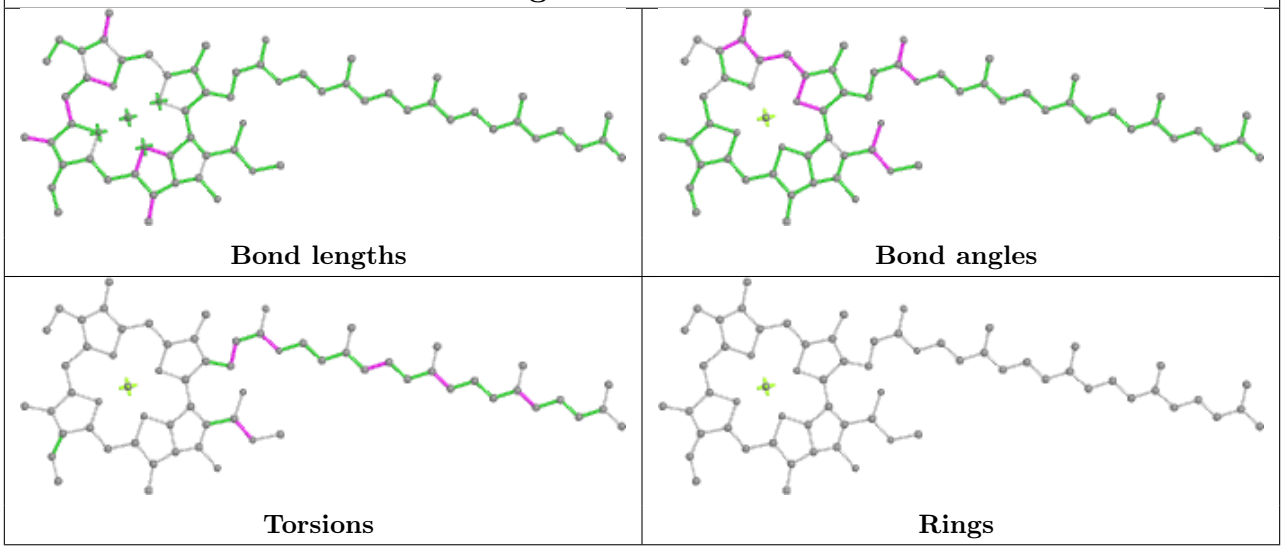
Ligand CHL q 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL g 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD m 101



Ligand CLA 6 308



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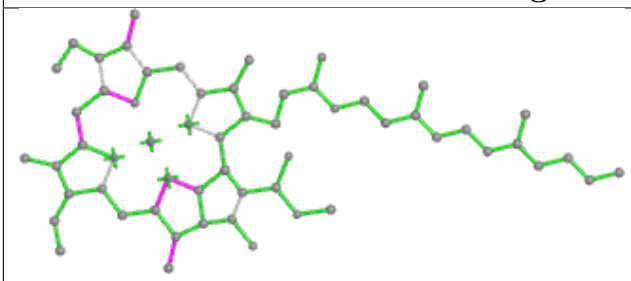
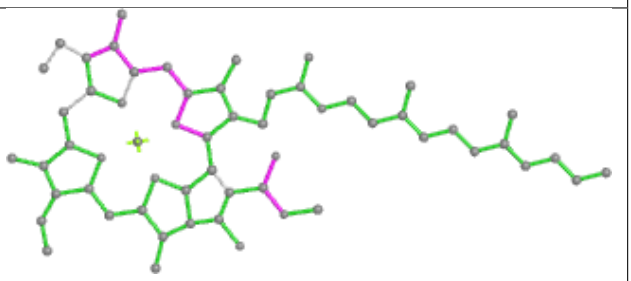
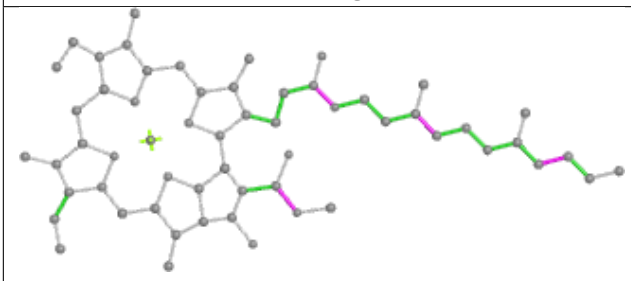
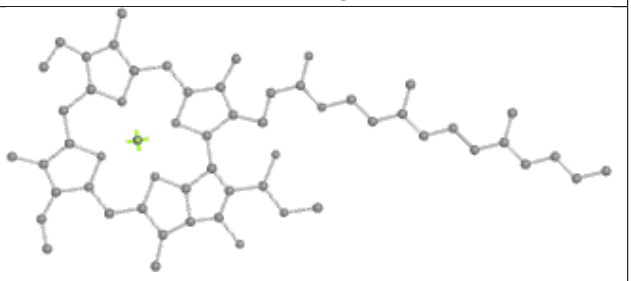
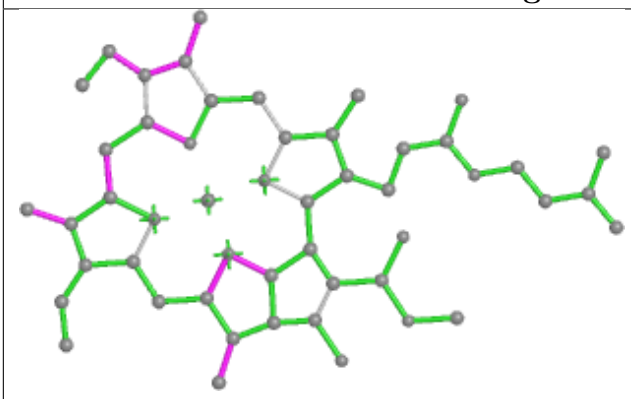
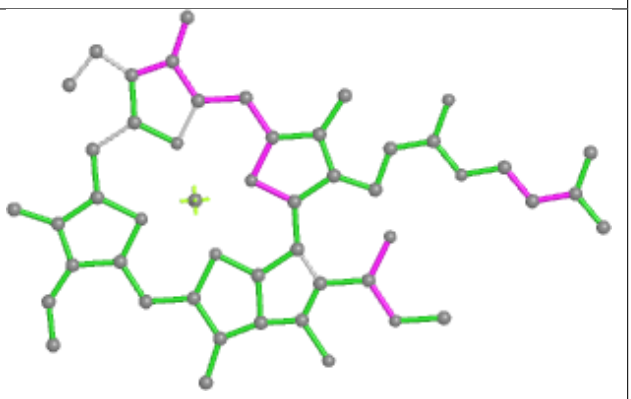
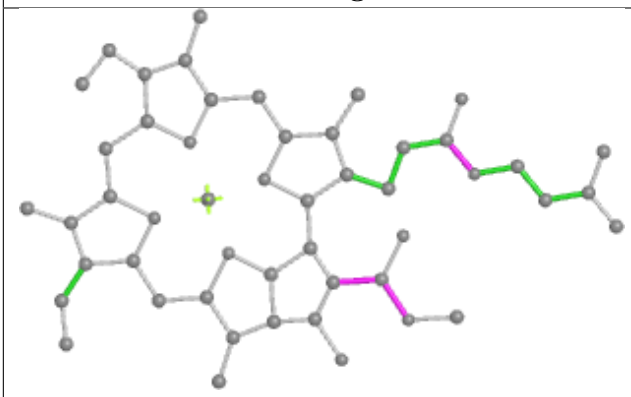
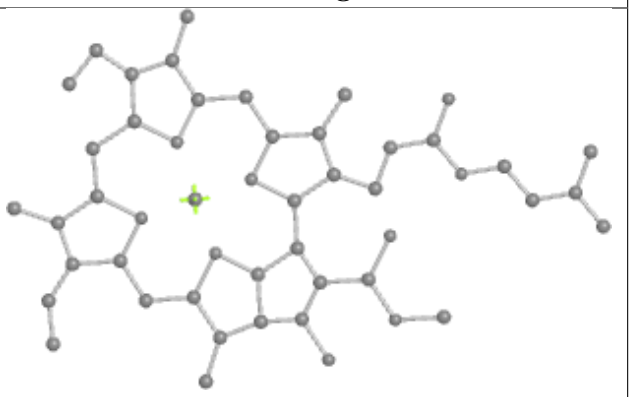
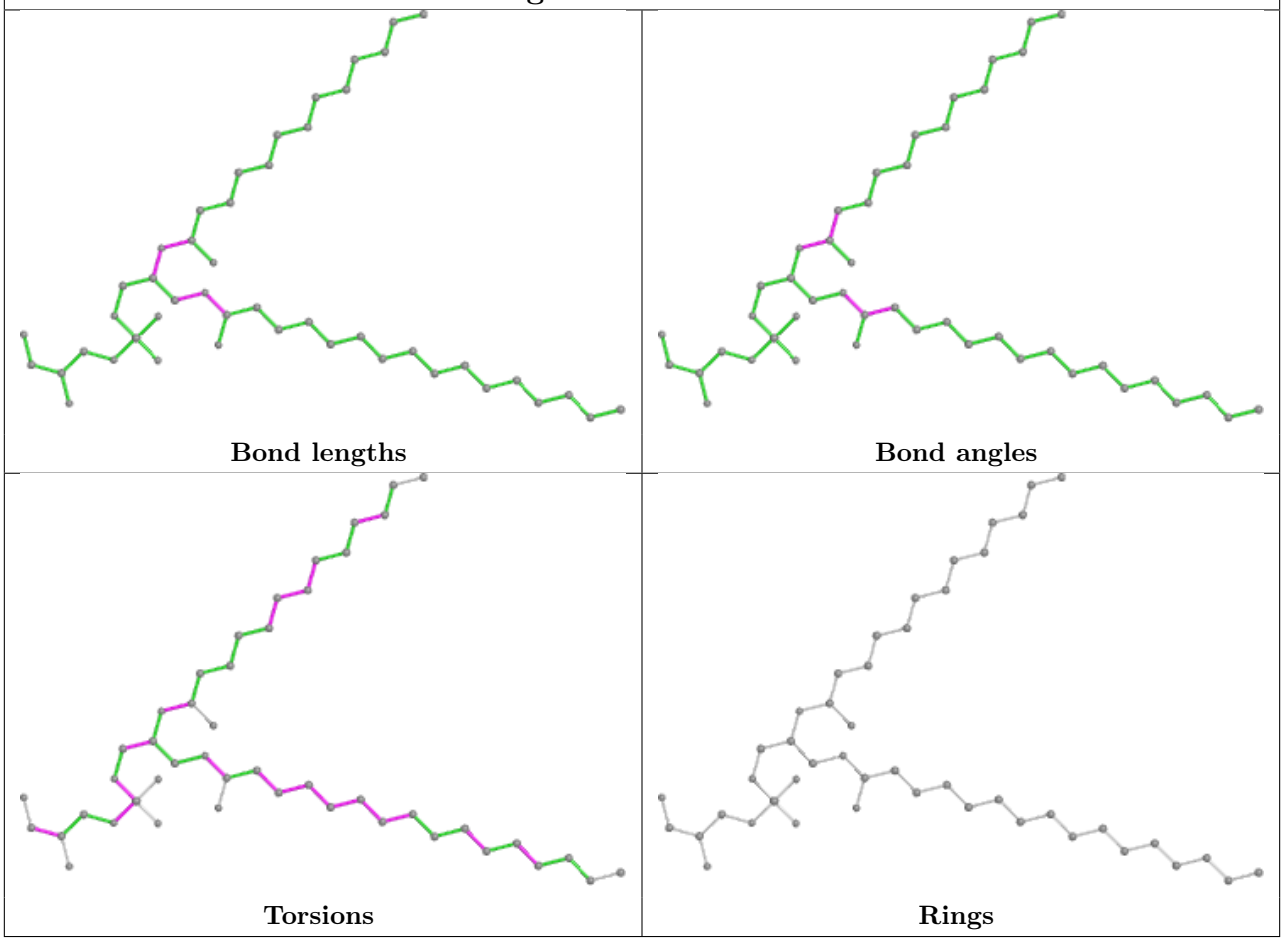
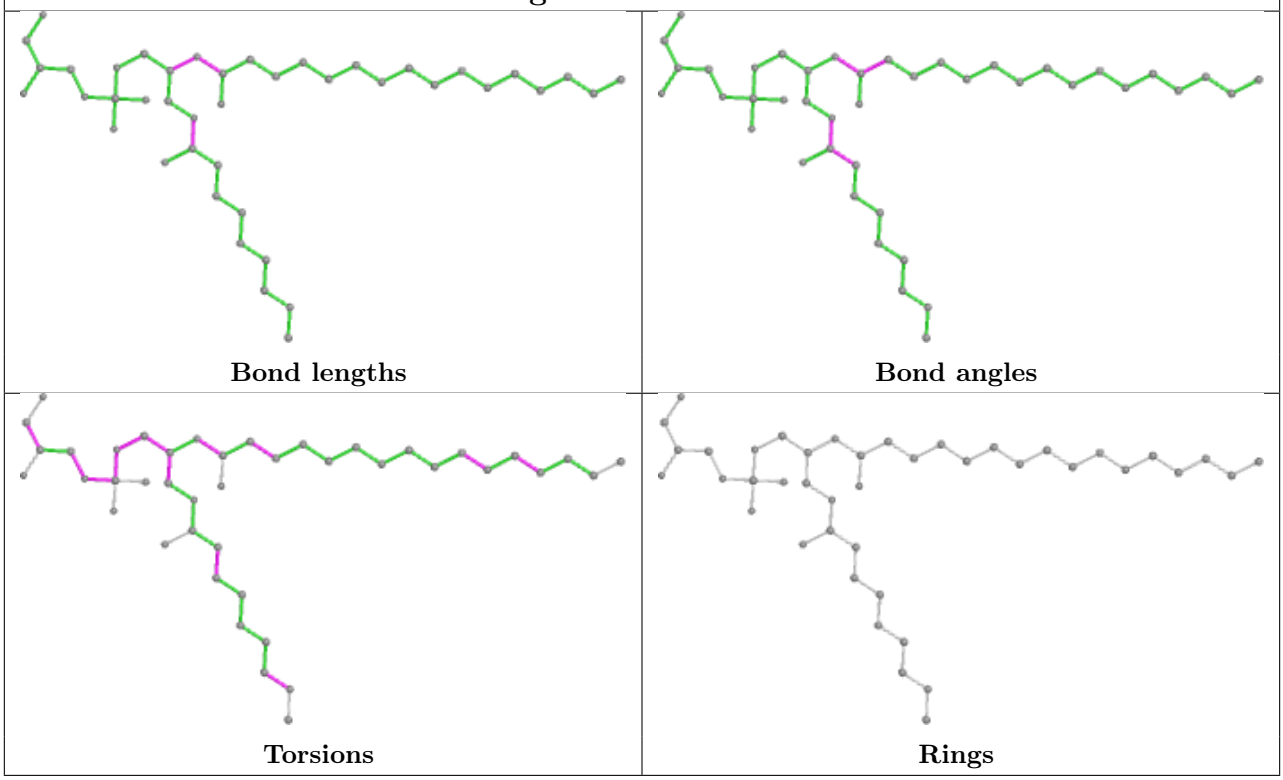
 Bond lengths	 Bond angles
 Torsions	 Rings

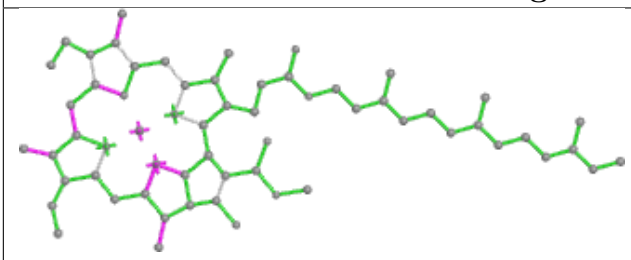
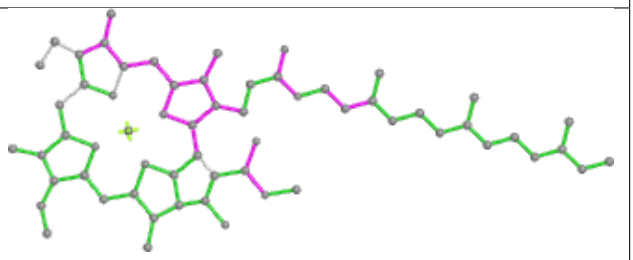
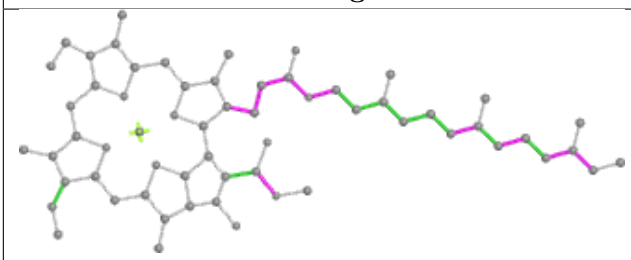
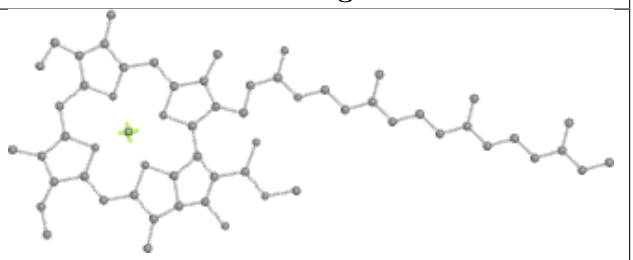
Ligand CLA U 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

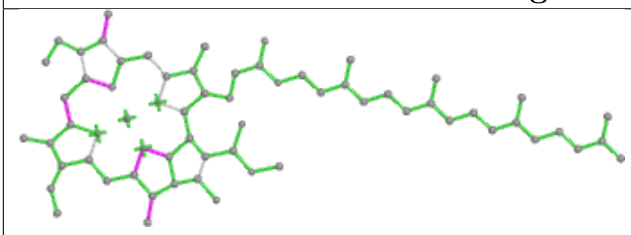
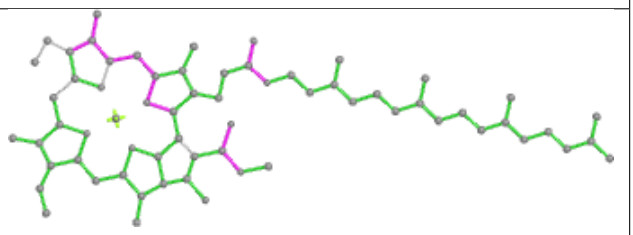
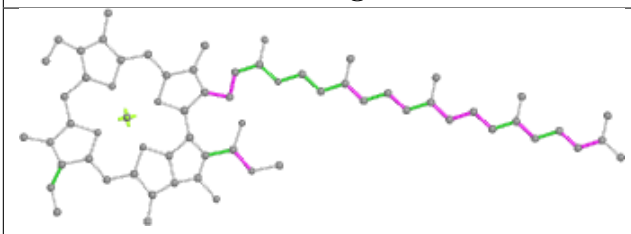
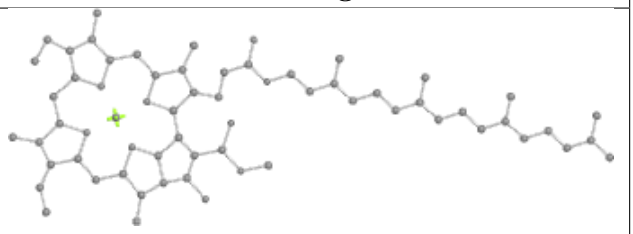
Ligand LHG d 405



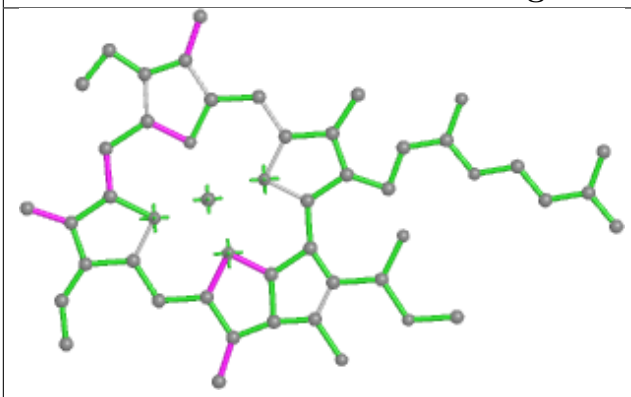
Ligand LHG r 613



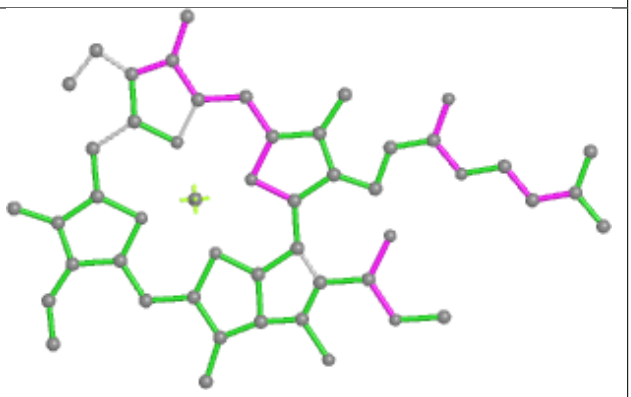
Ligand CLA s 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

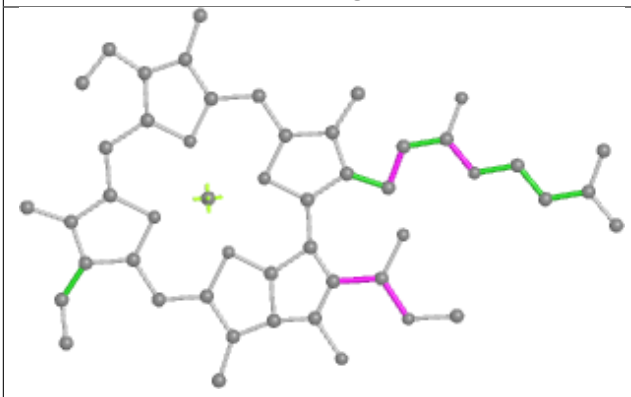
Ligand CLA S 303



Bond lengths



Bond angles



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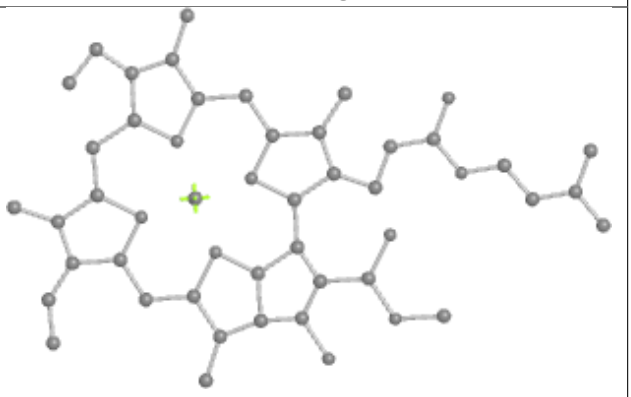
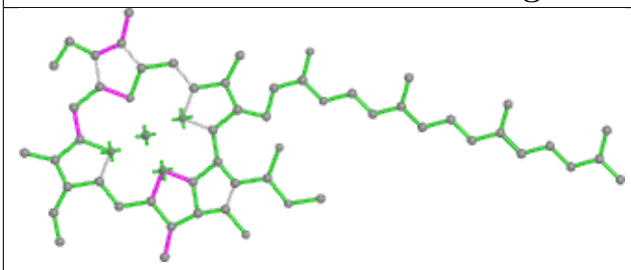


Rings

Ligand CLA G 305



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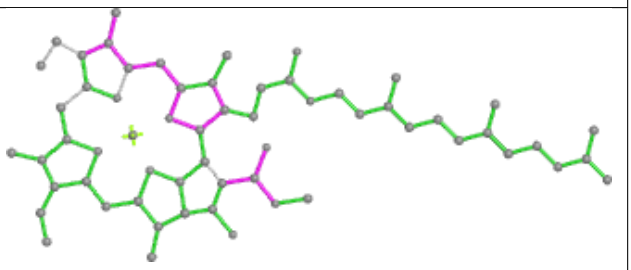
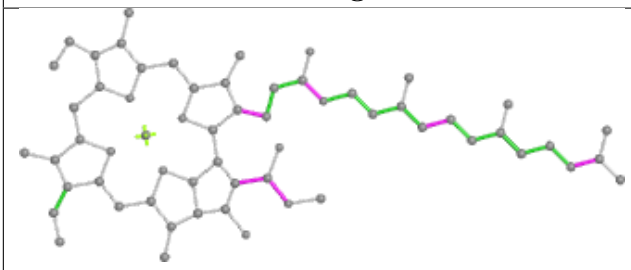


Bond angles



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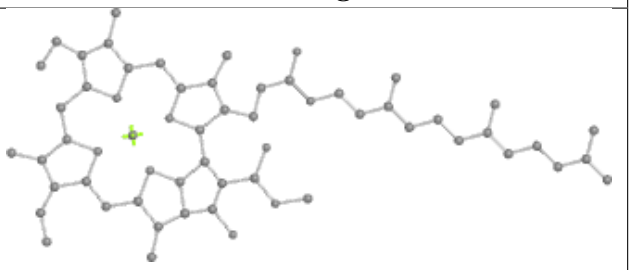
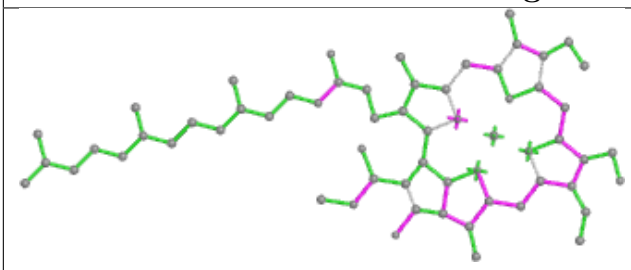
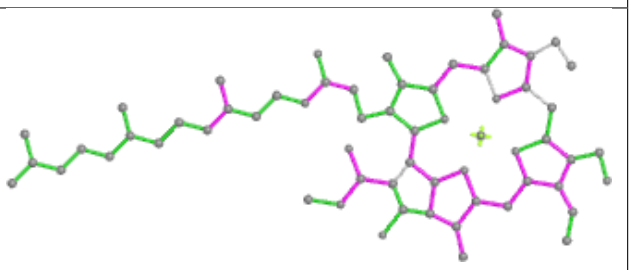


Rings

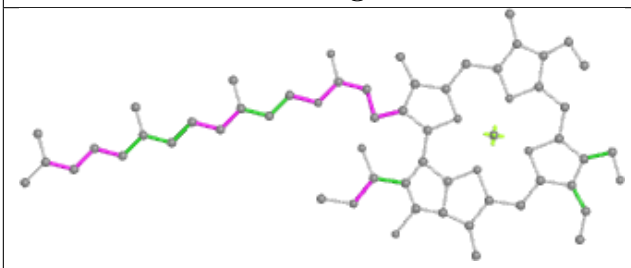
Ligand CHL R 317



Bond lengths



Bond angles



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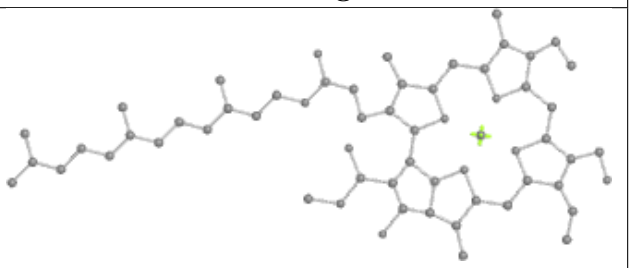
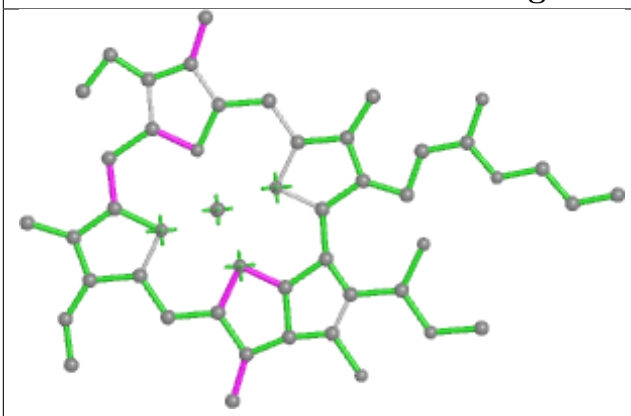
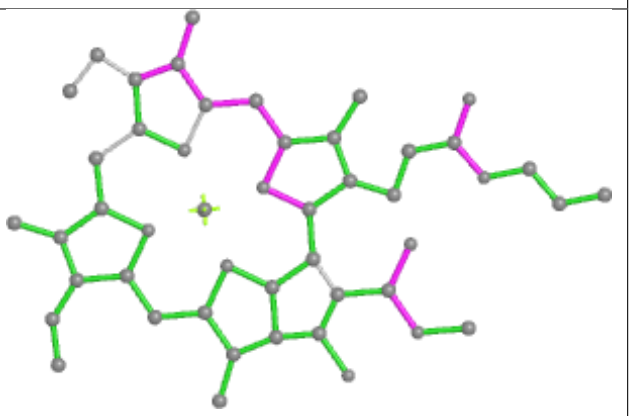


Rings

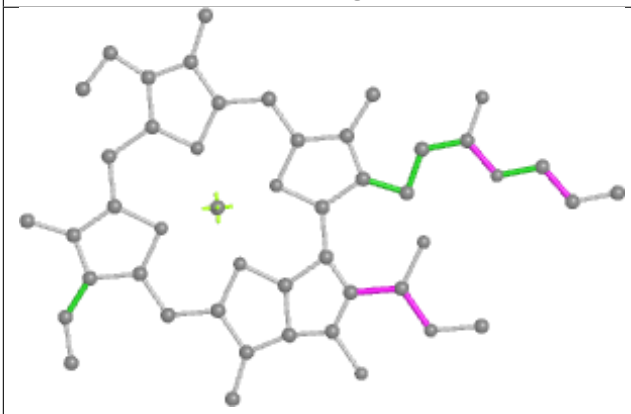
Ligand CLA 2 308



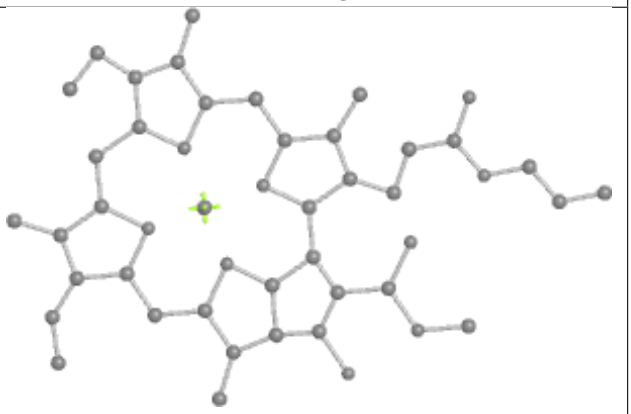
Bond lengths



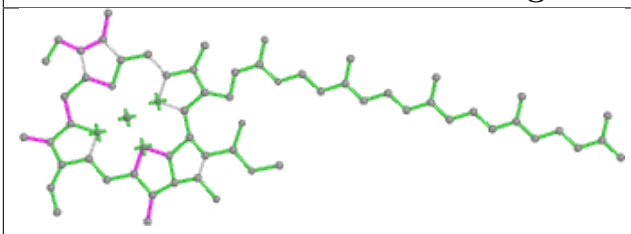
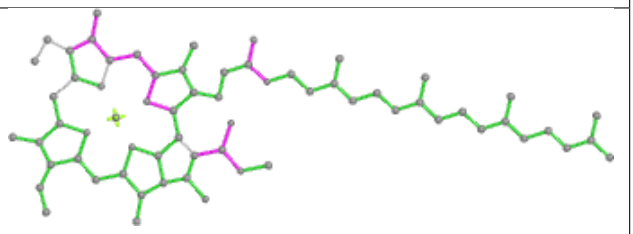
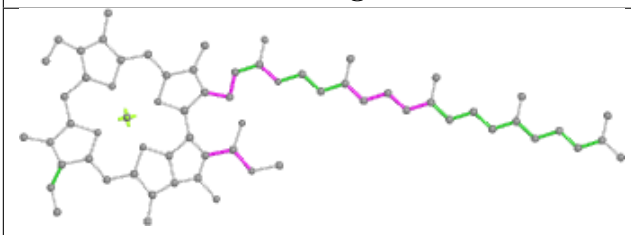
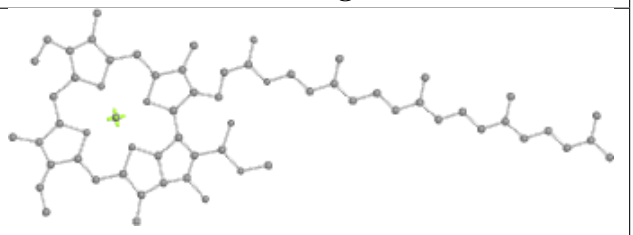
Bond angles

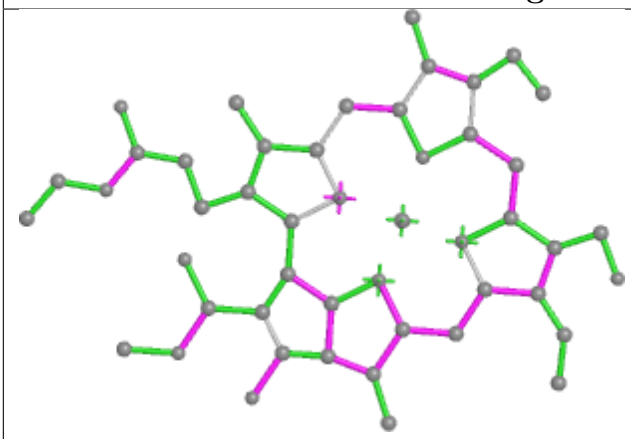
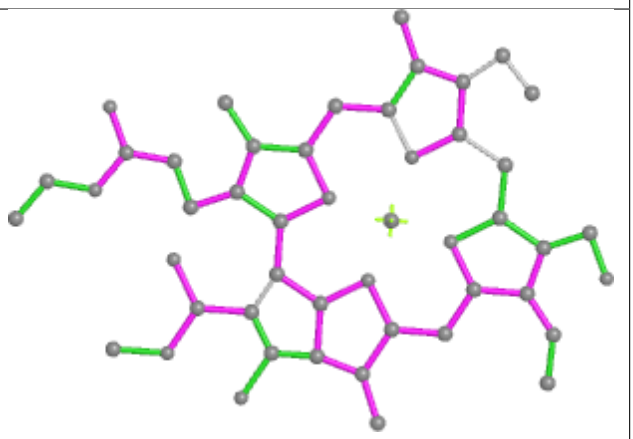
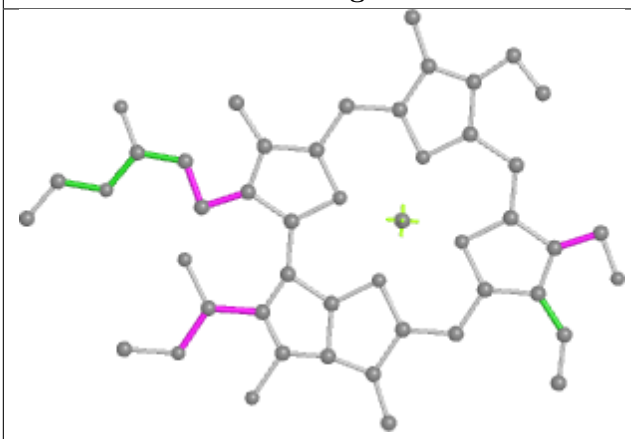
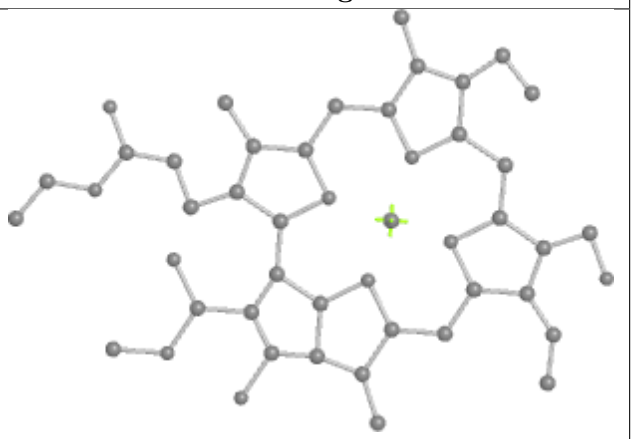


Torsions

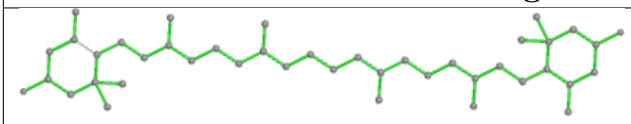


Rings

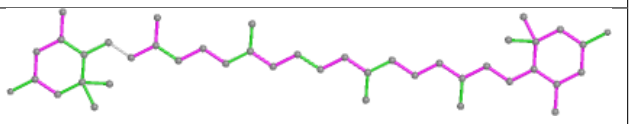
Ligand CLA b 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL n 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

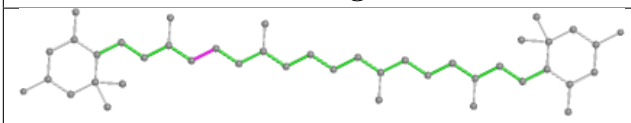
Ligand LUT N 310



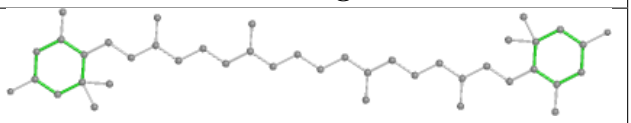
Bond lengths



Bond angles

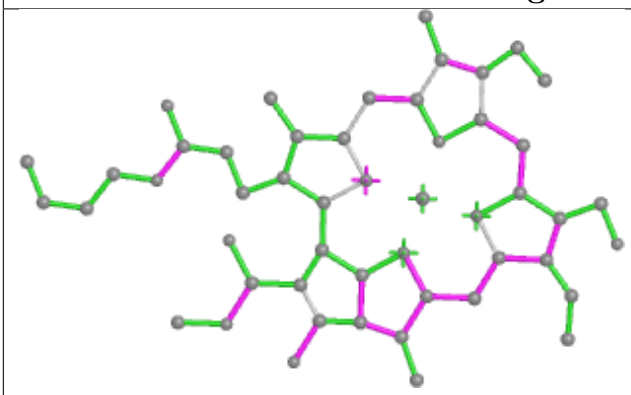


Torsions

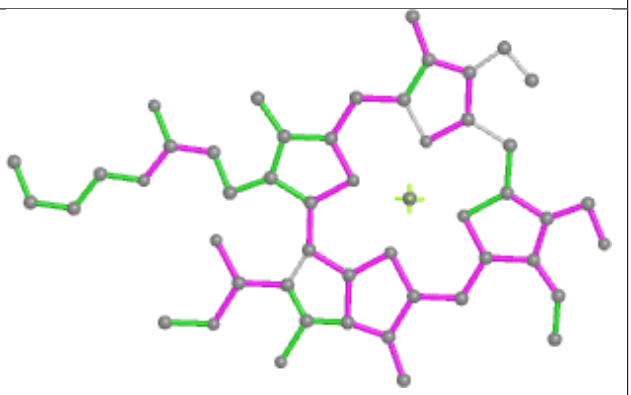


Rings

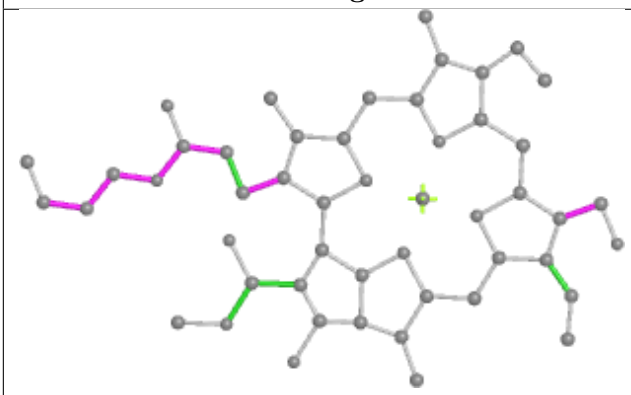
Ligand CHL 6 314



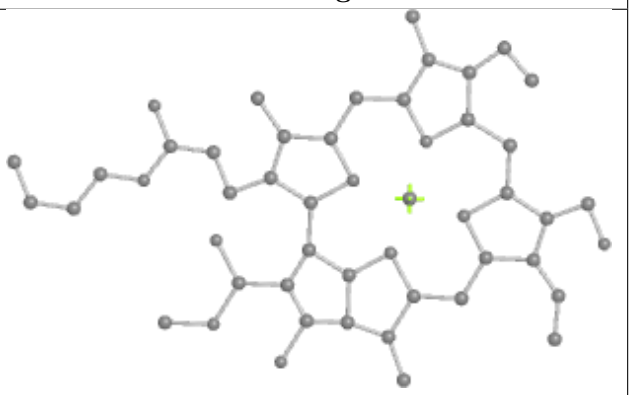
Bond lengths



Bond angles

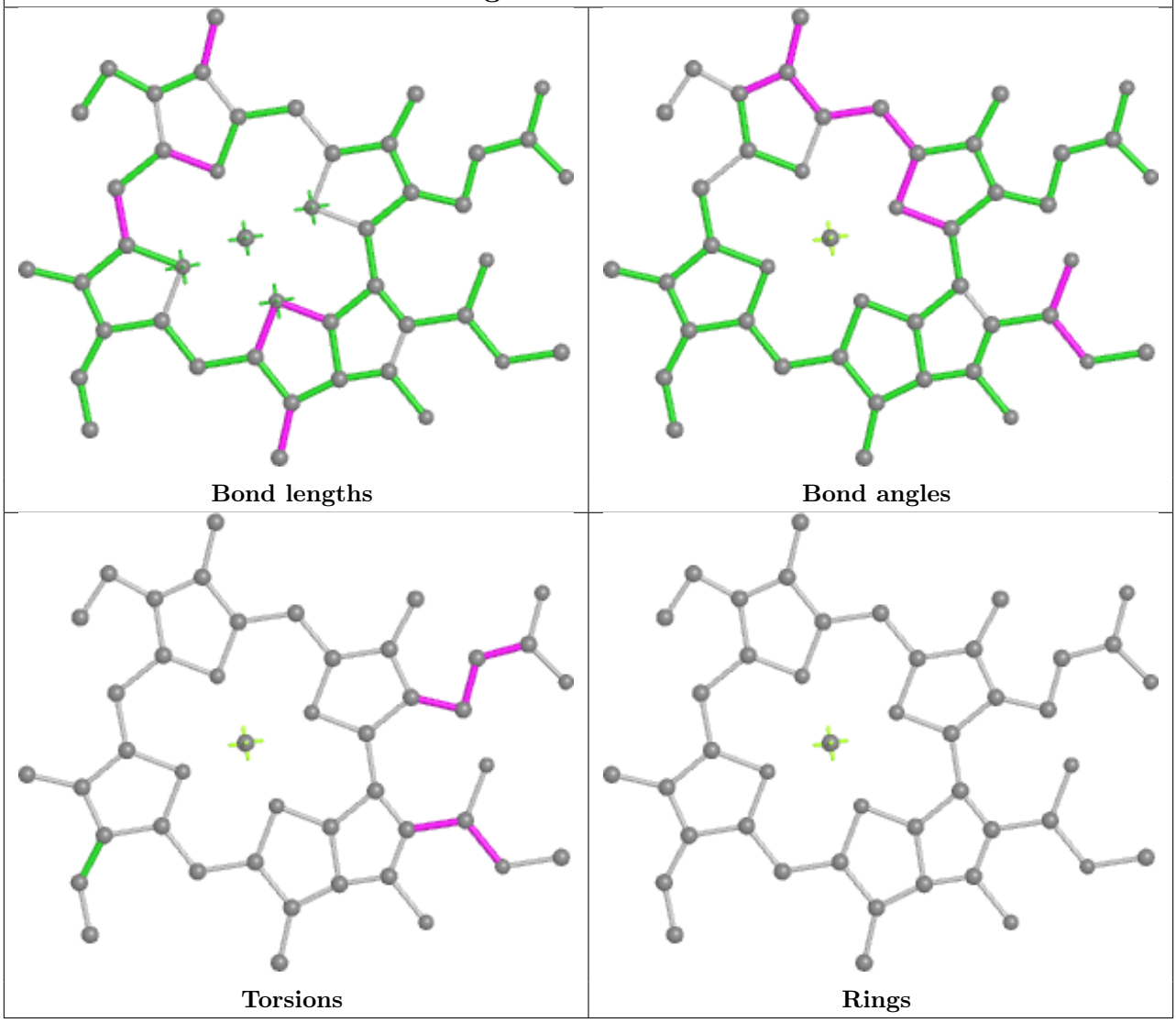


Torsions

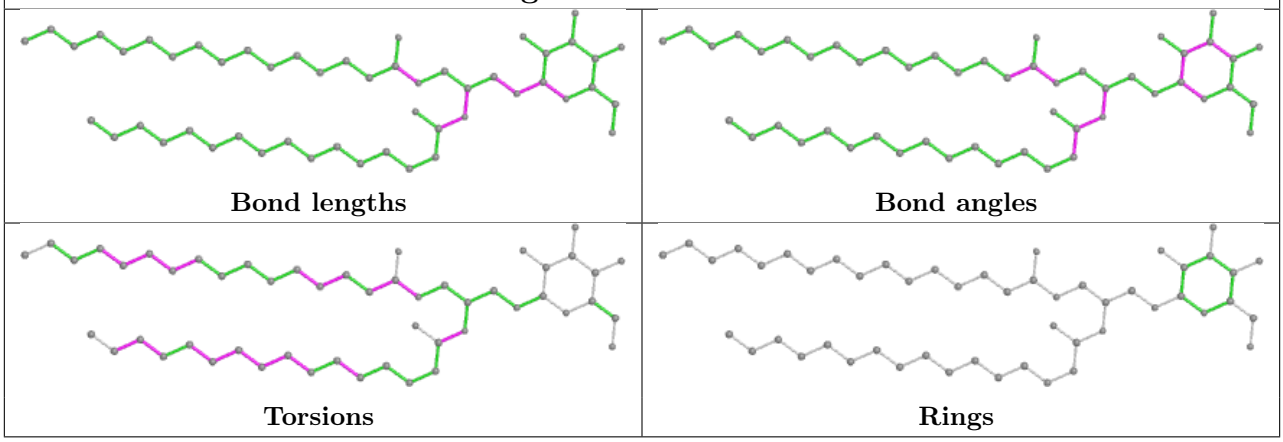


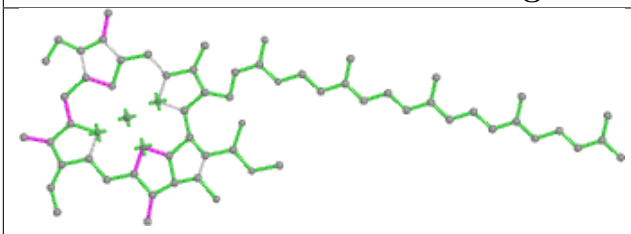
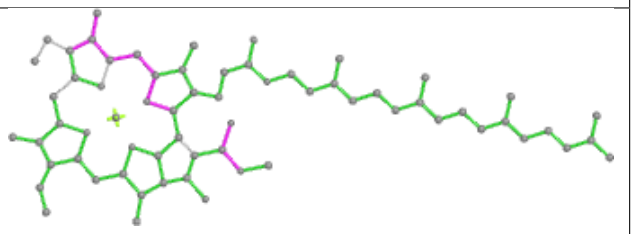
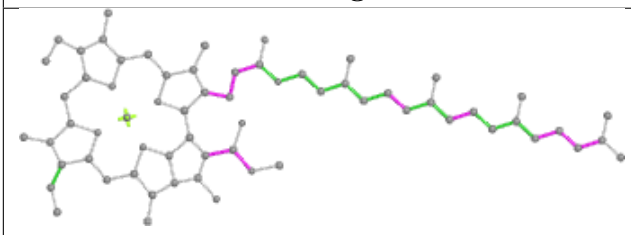
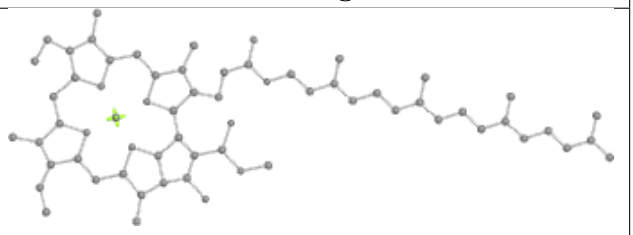
Rings

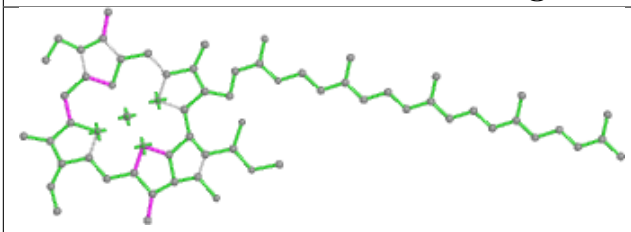
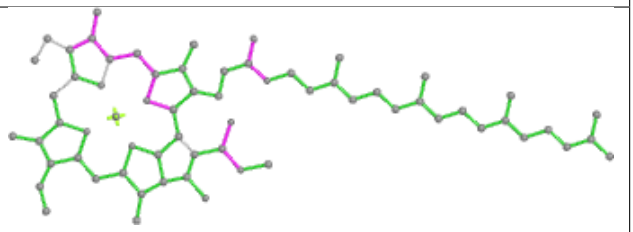
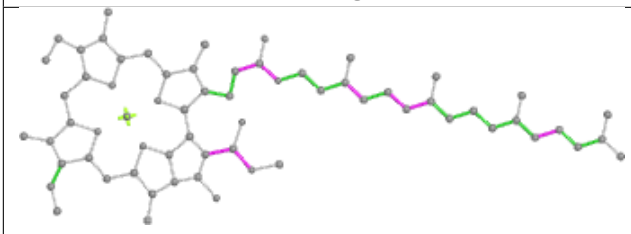
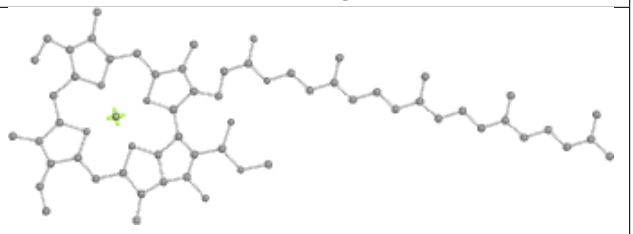
Ligand CLA S 304

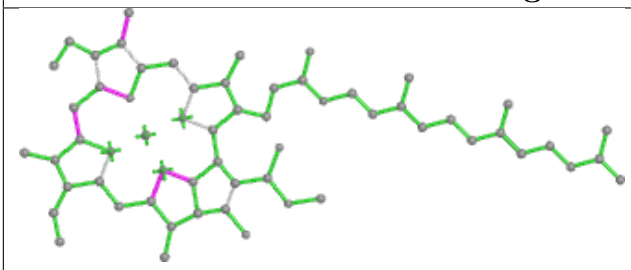
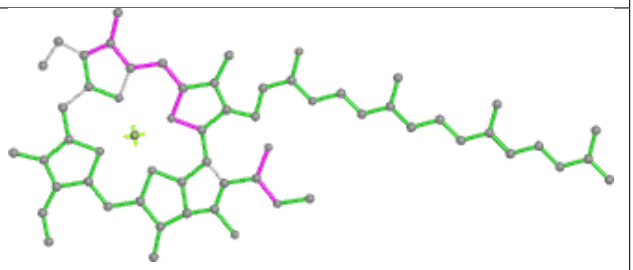
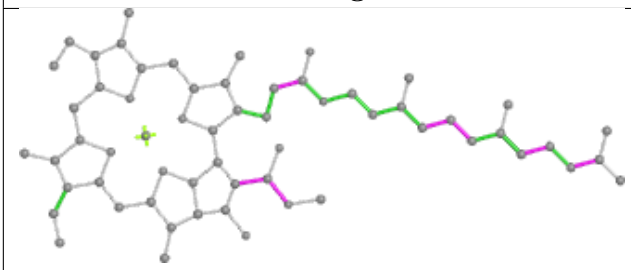
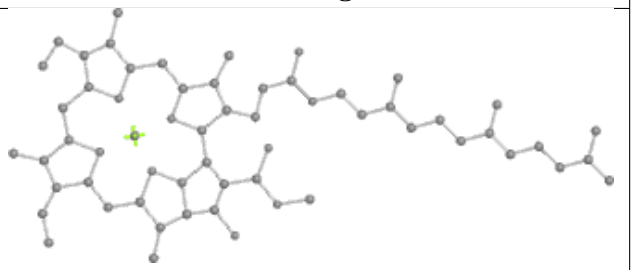


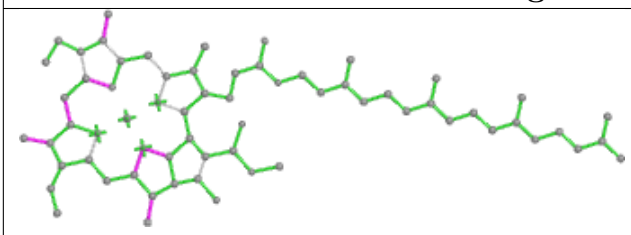
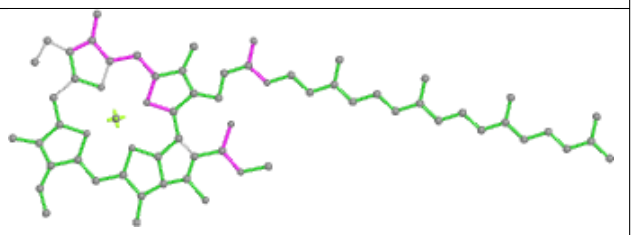
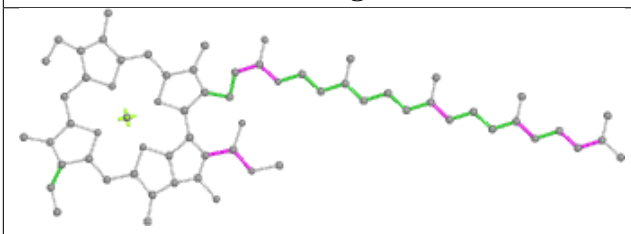
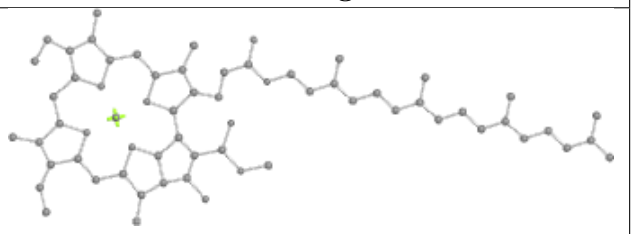
Ligand LMG B 621



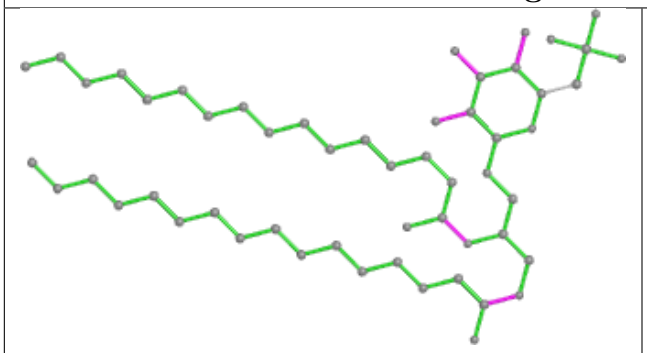
Ligand CLA N 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

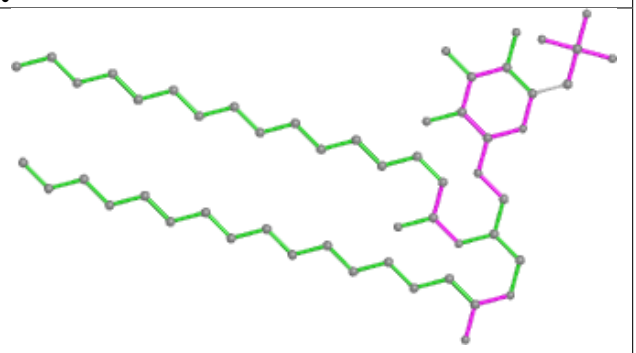
Ligand CLA R 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

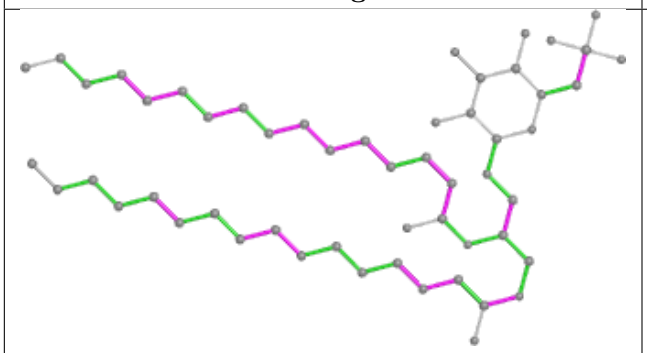
Ligand SQD A 412



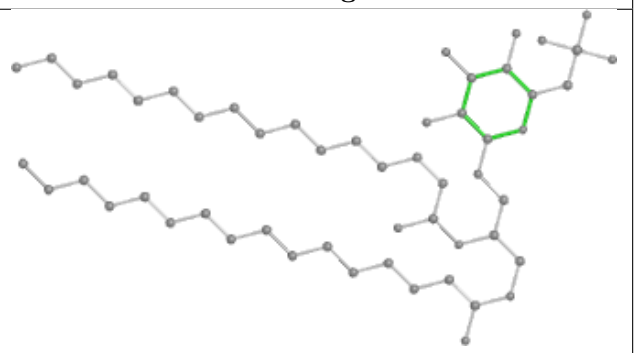
Bond lengths



Bond angles

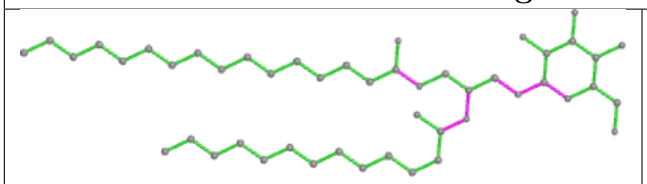


Torsions



Rings

Ligand LMG W 201



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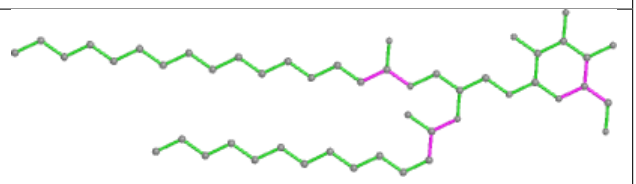
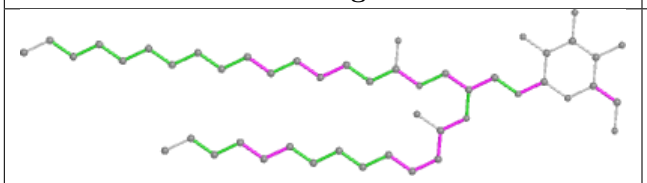


Bond angles



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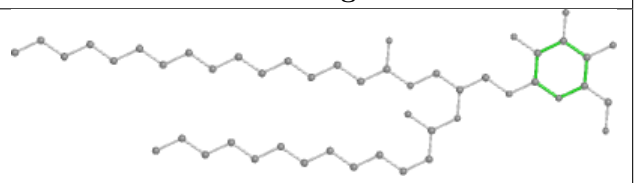
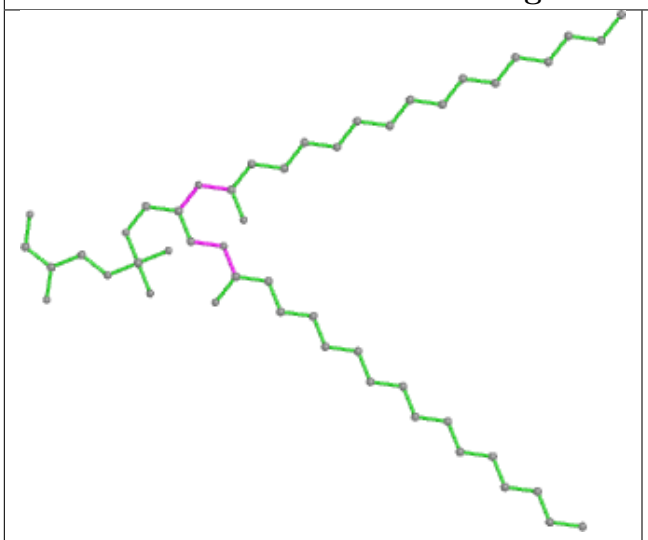


Rings

Ligand LHG P 313



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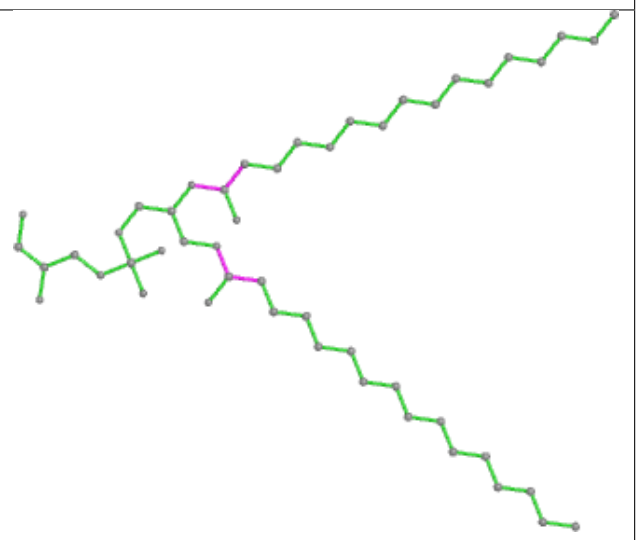
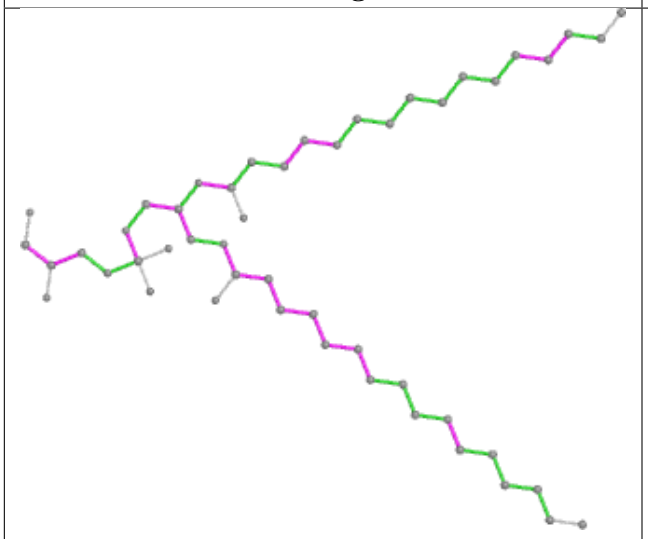


Bond angles



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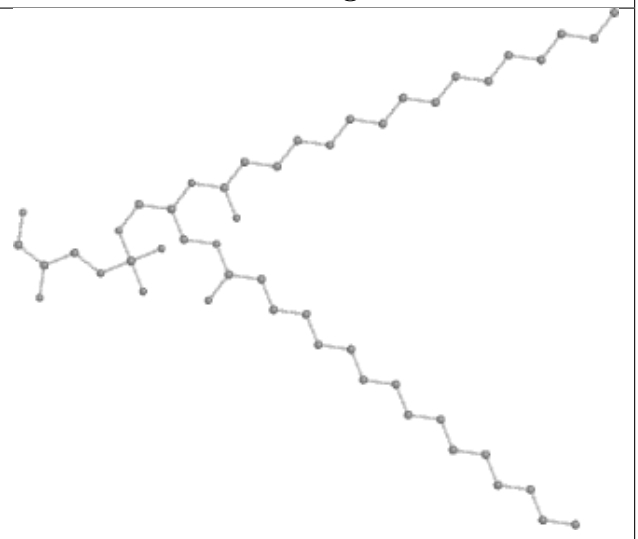
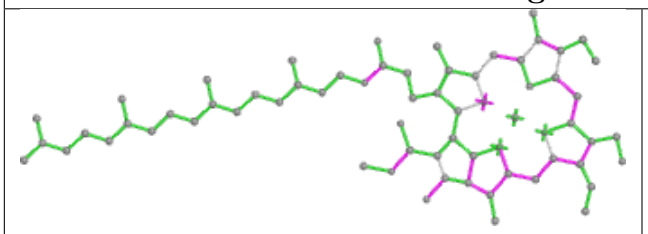


Rings

Ligand CHL p 317



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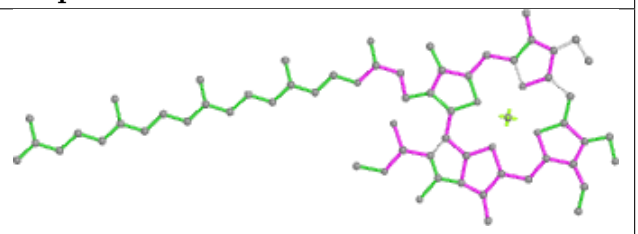
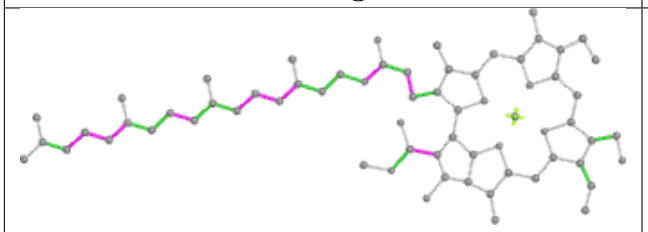


Bond angles



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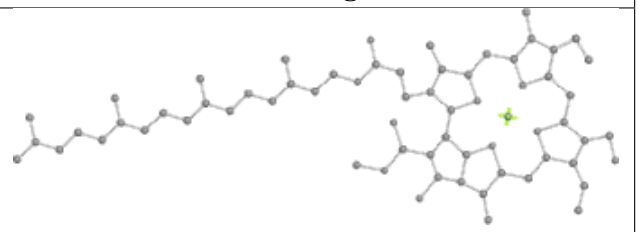
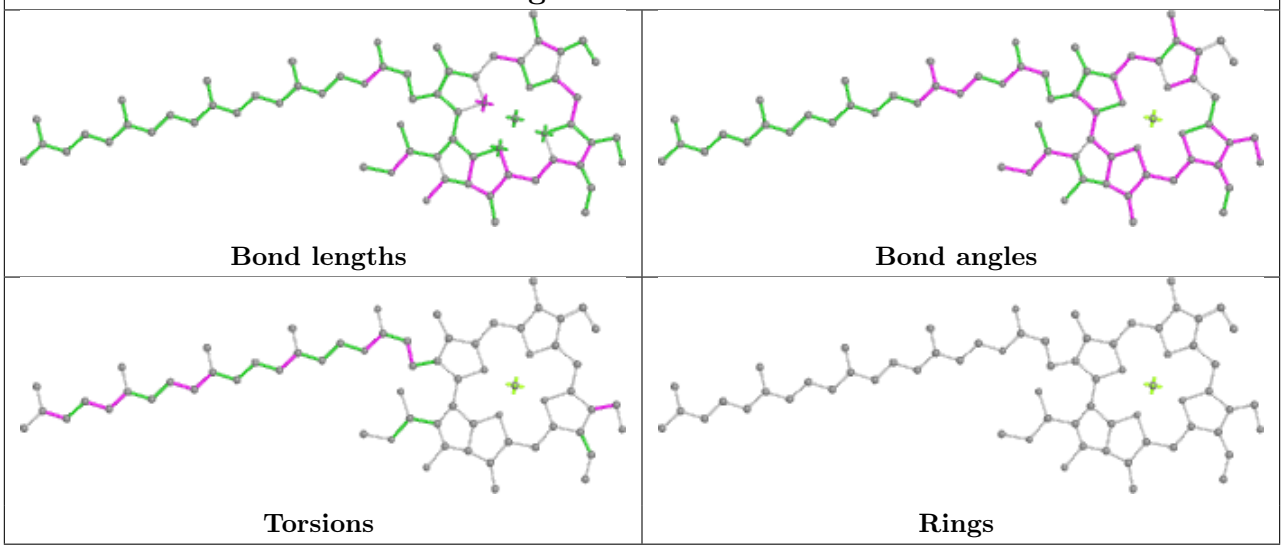
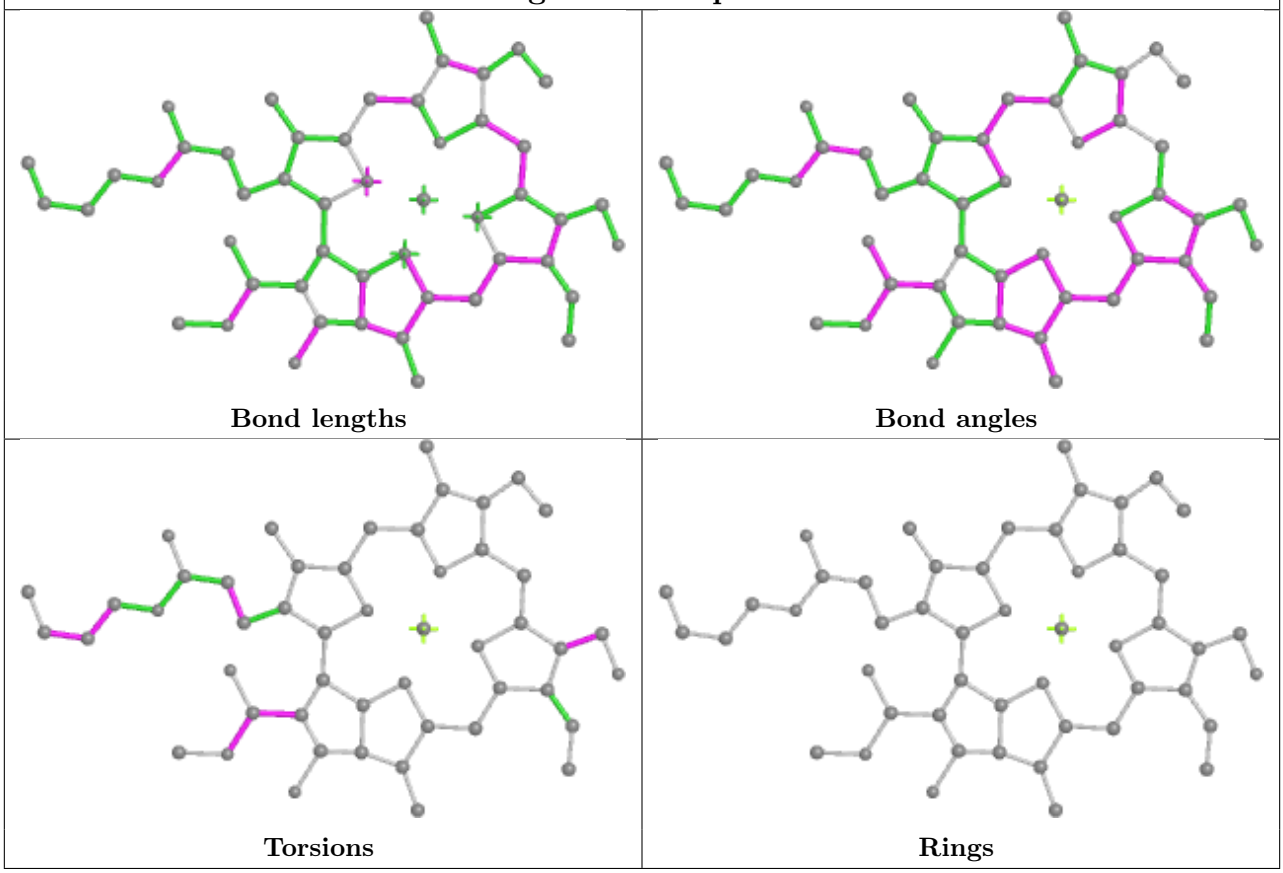


Rings

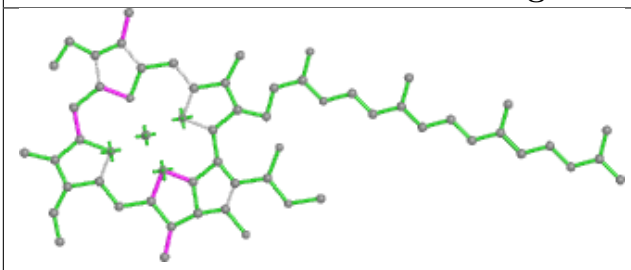
Ligand CHL v 316



Ligand CHL q 313



Ligand CLA v 305



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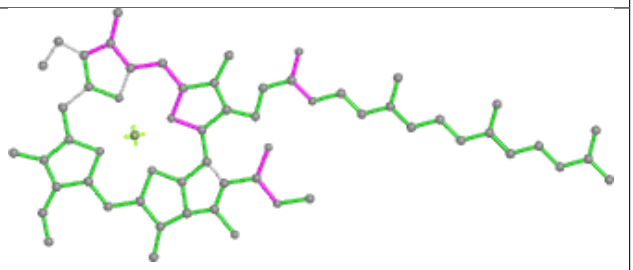
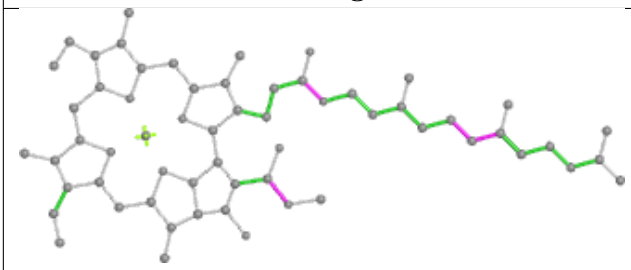


Bond angles



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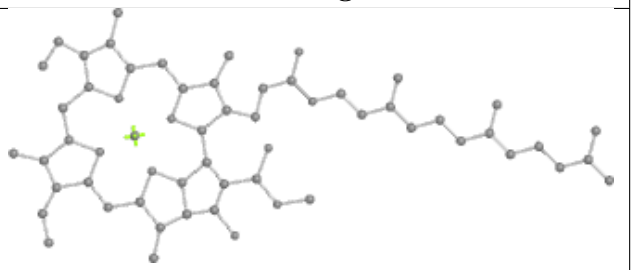
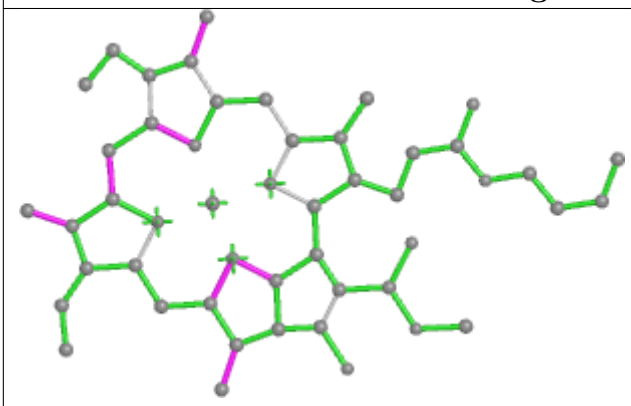


Rings

Ligand CLA s 307



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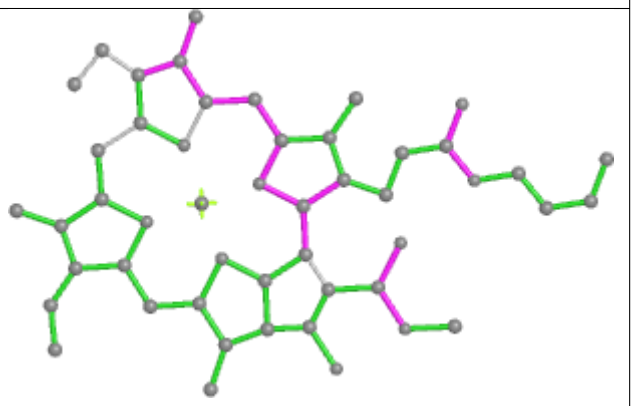
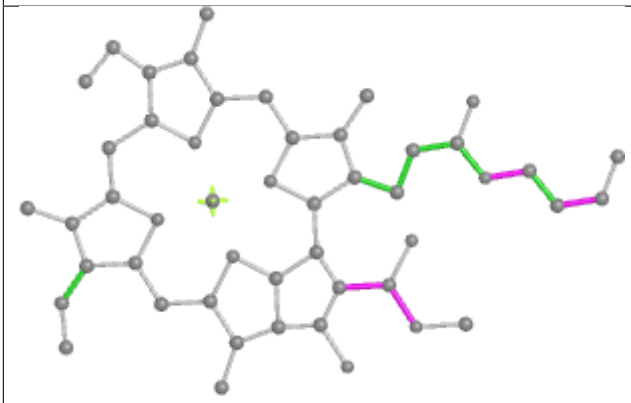
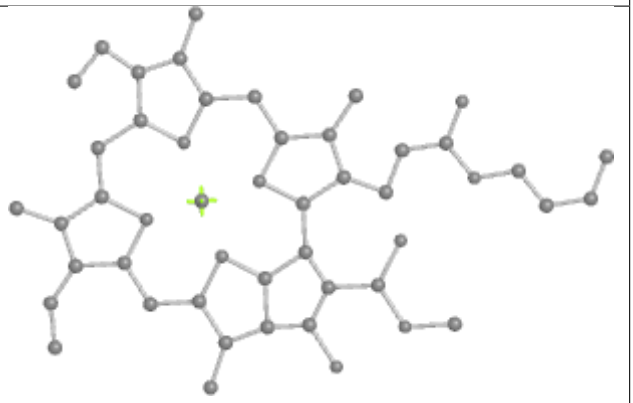


Bond angles

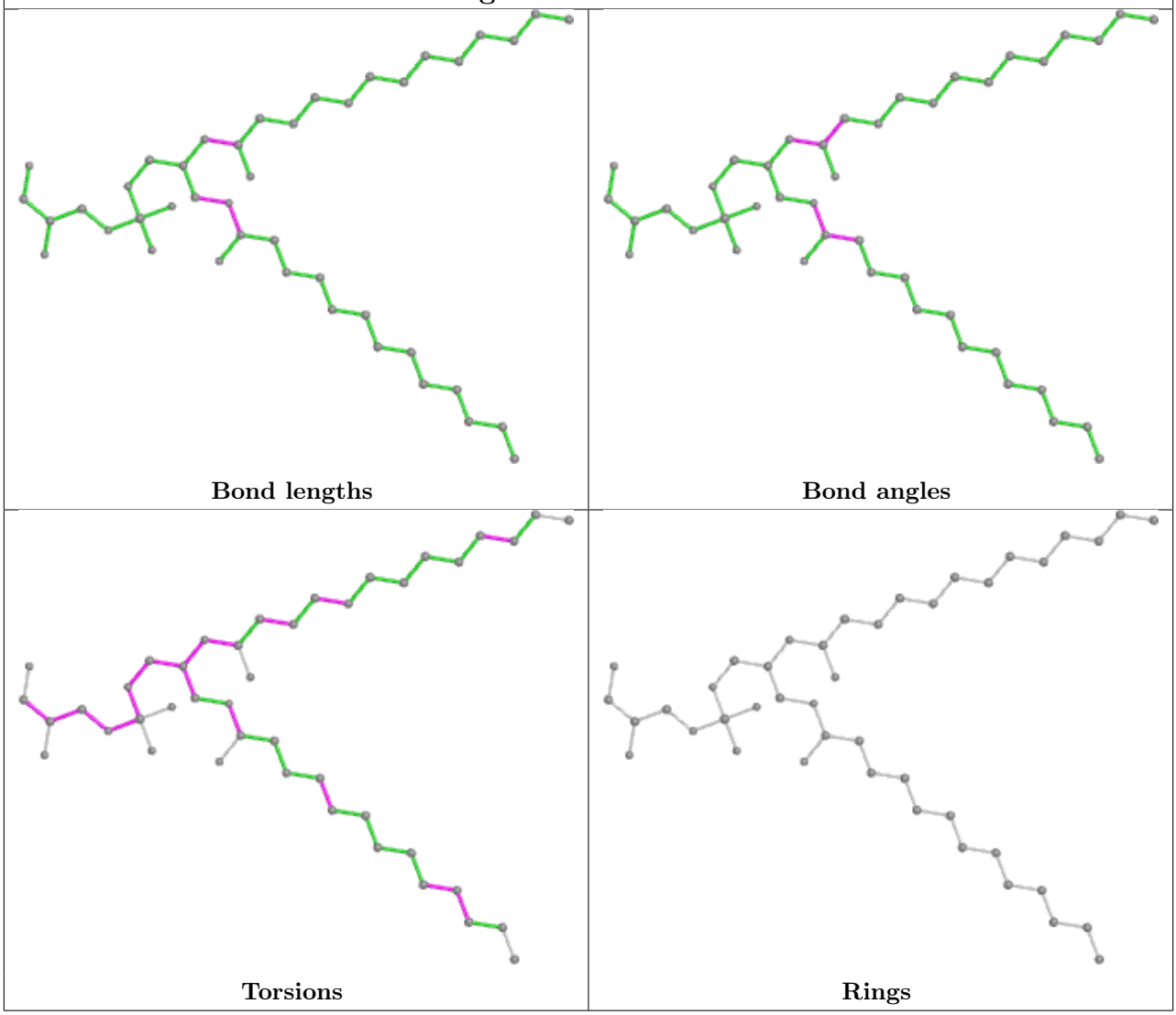


Torsions

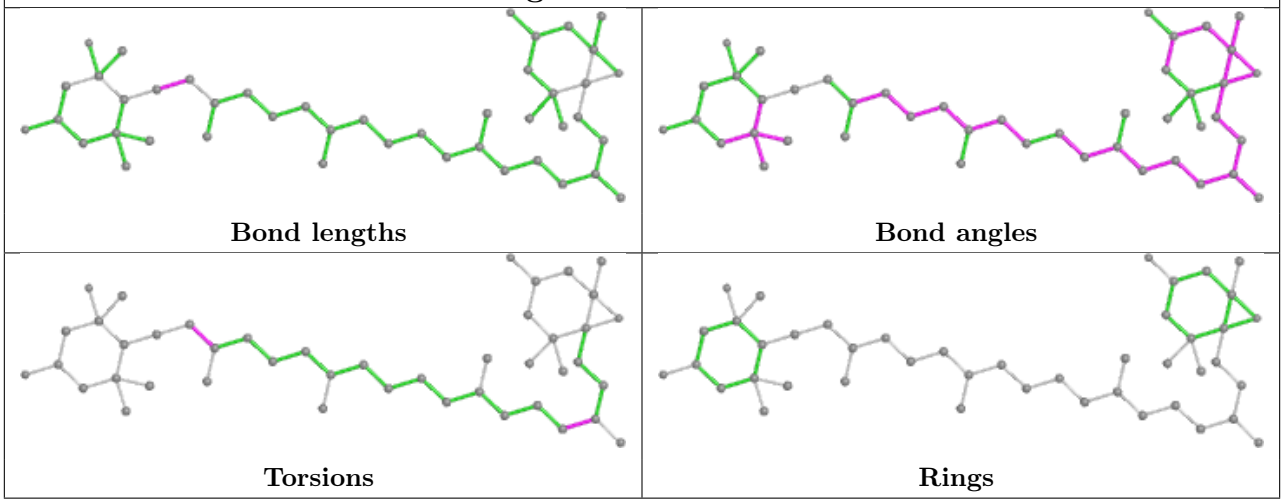


Rings

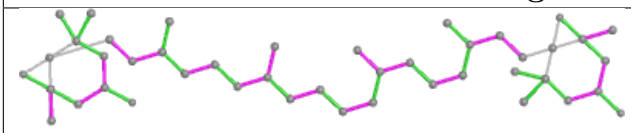
Ligand LHG A 413



Ligand NEX S 317



Ligand XAT 3 309



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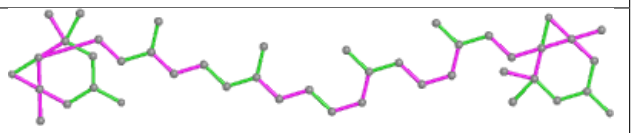
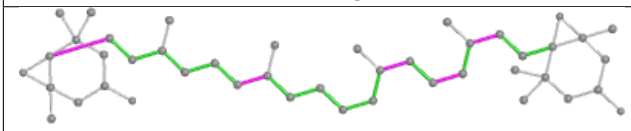


Bond angles



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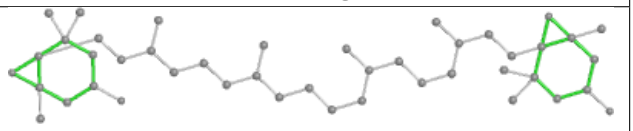
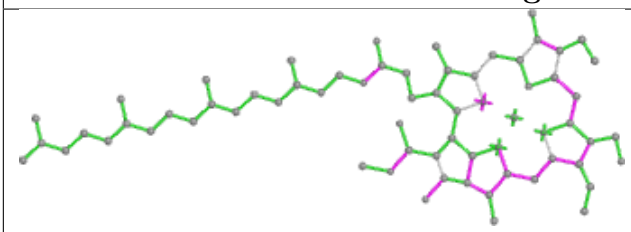


Rings

Ligand CHL V 317



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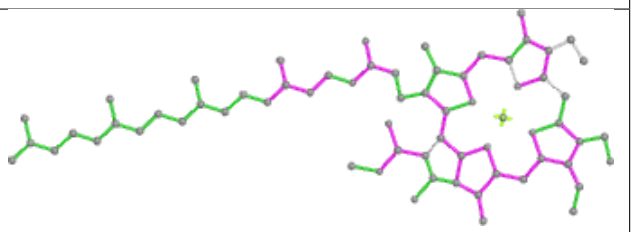
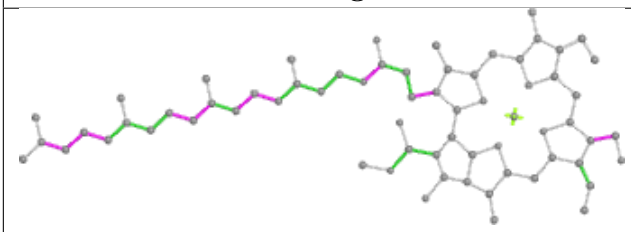


Bond angles



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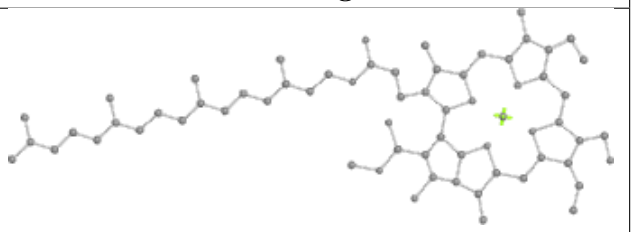
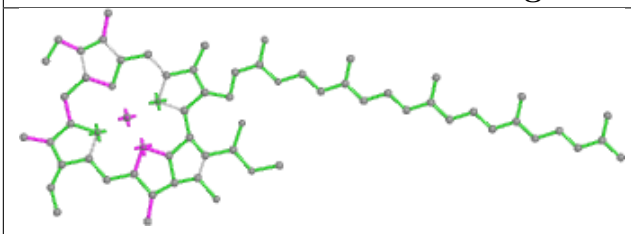
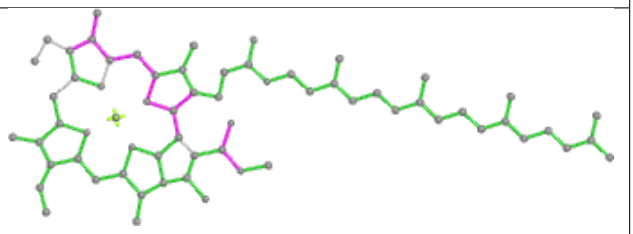


Rings

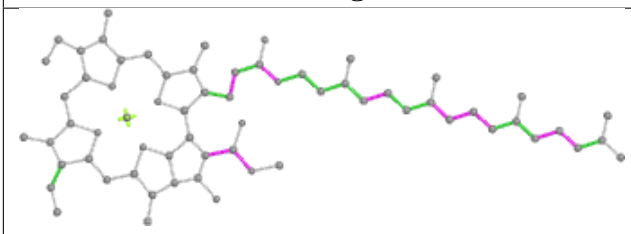
Ligand CLA B 614



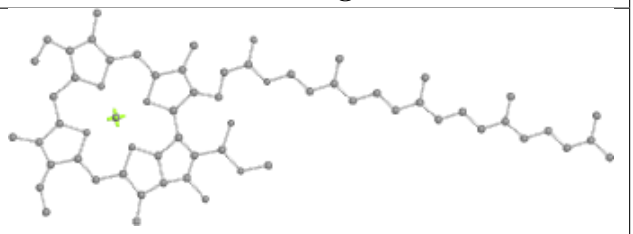
Bond lengths



Bond angles

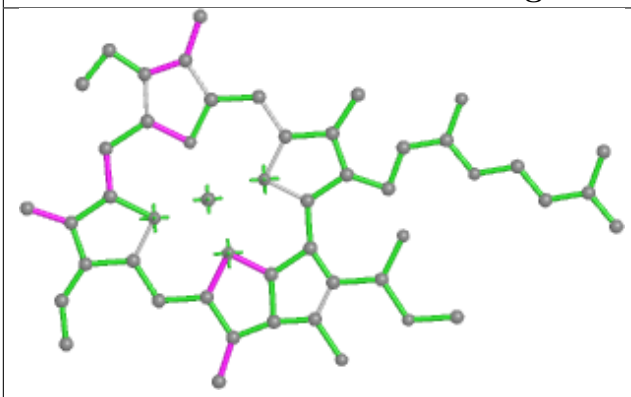


Torsions

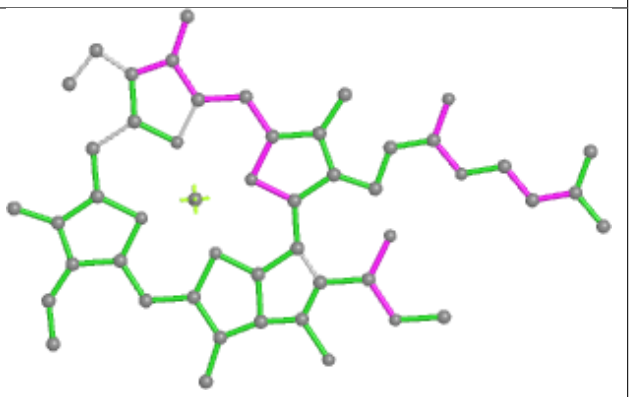


Rings

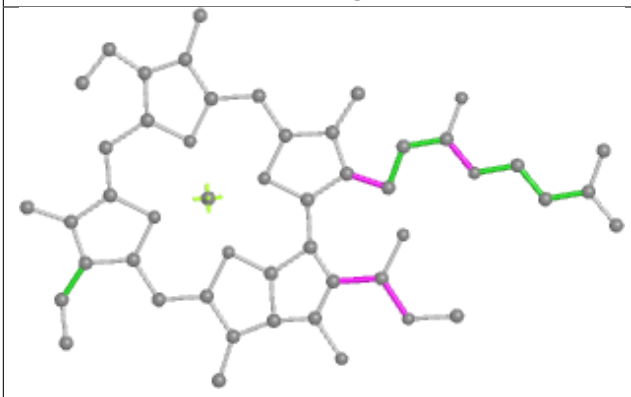
Ligand CLA P 304



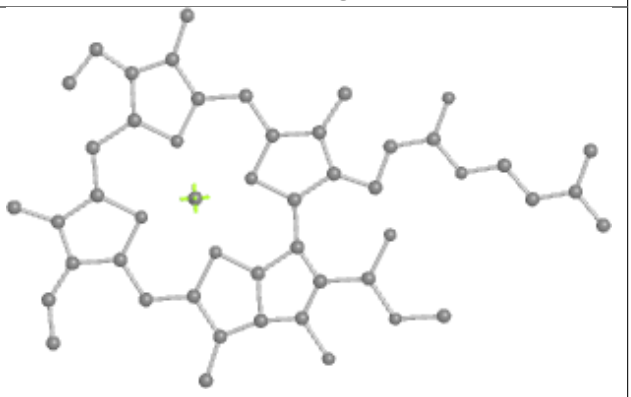
Bond lengths



Bond angles

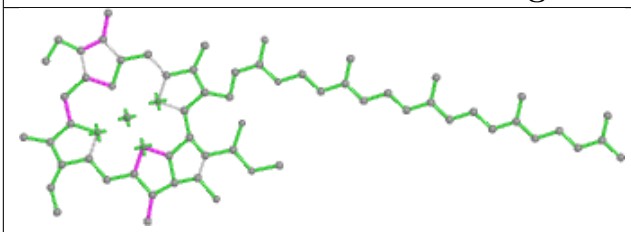


Torsions

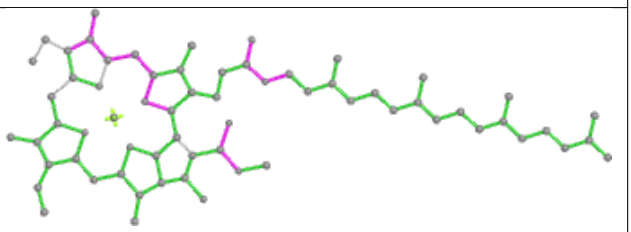


Rings

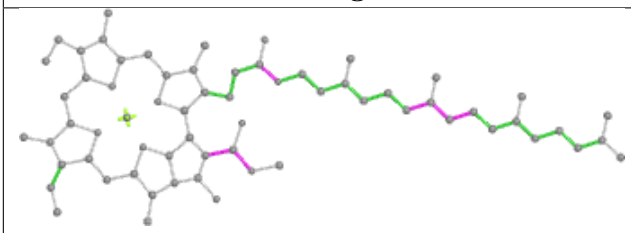
Ligand CLA 3 302



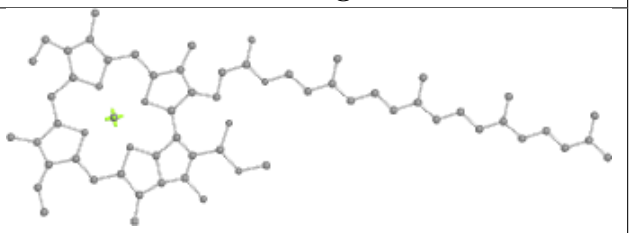
Bond lengths



Bond angles

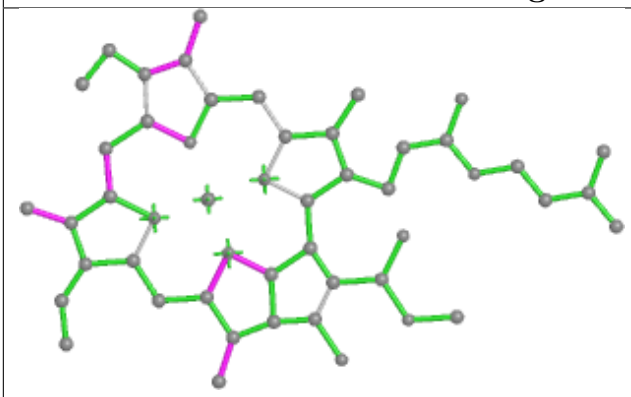


Torsions

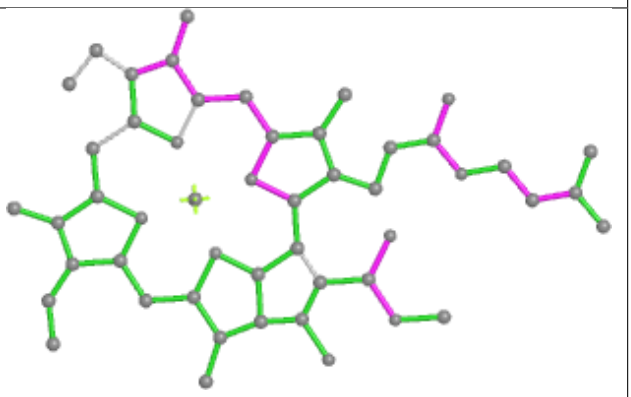


Rings

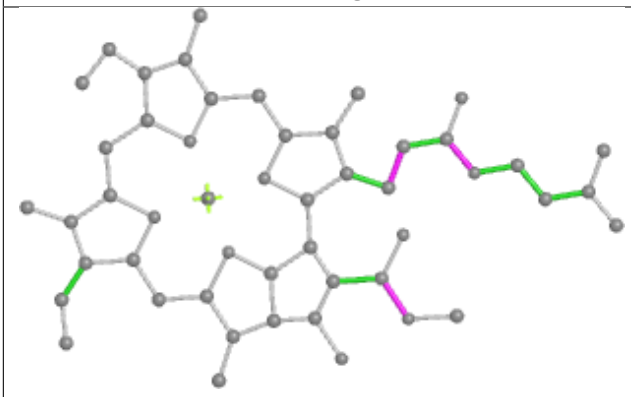
Ligand CLA 5 303



Bond lengths



Bond angles



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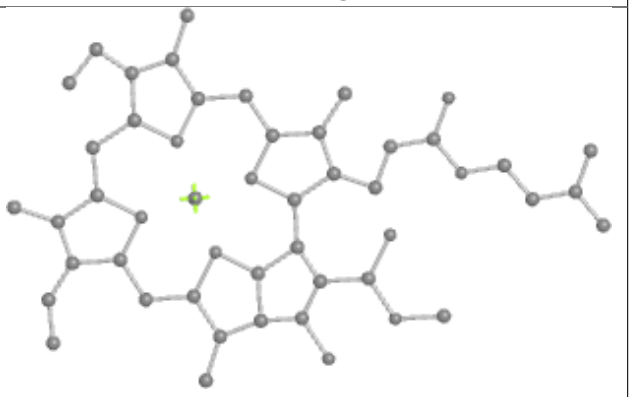
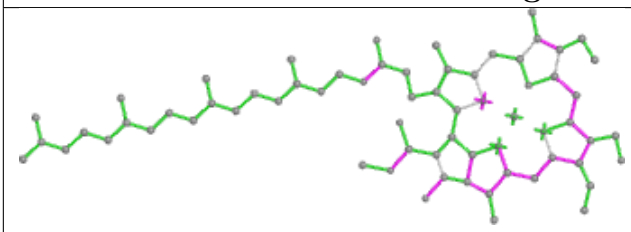
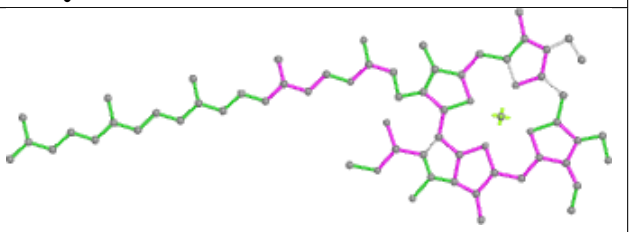


Rings

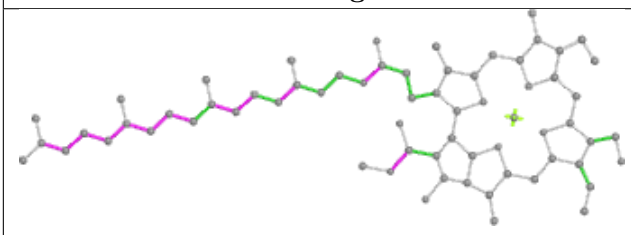
Ligand CHL Q 311



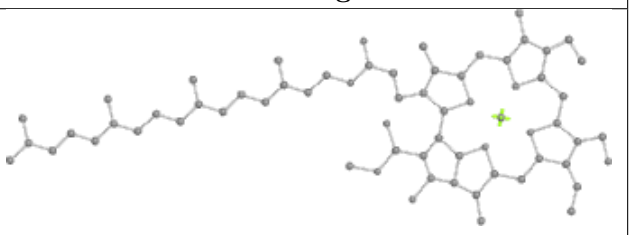
Bond lengths



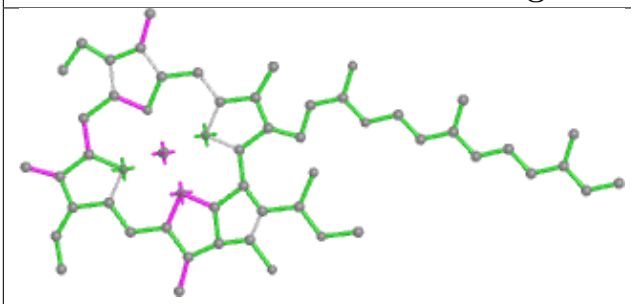
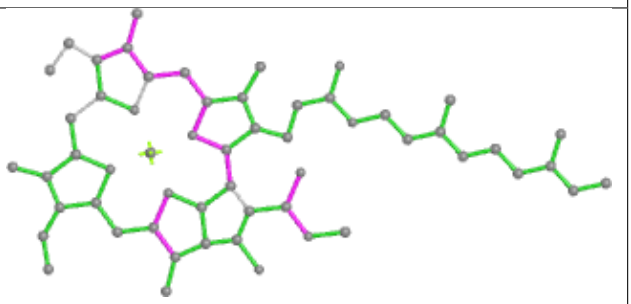
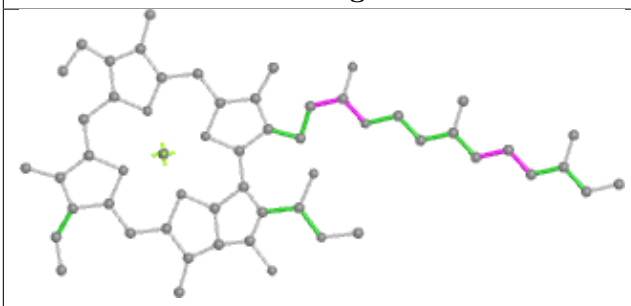
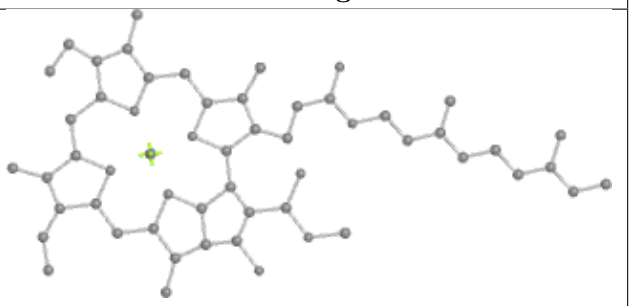
Bond angles

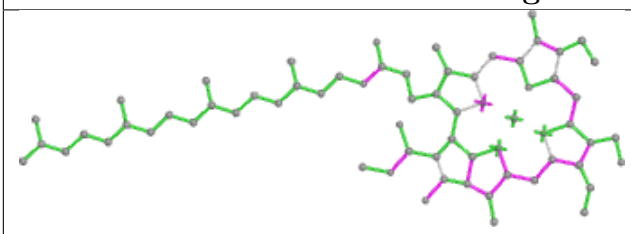
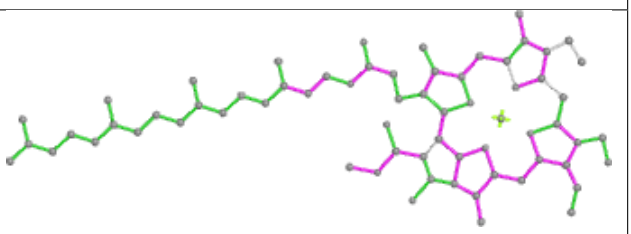
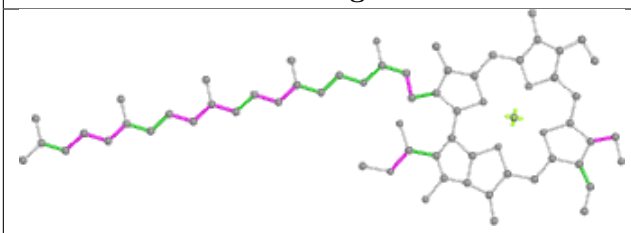
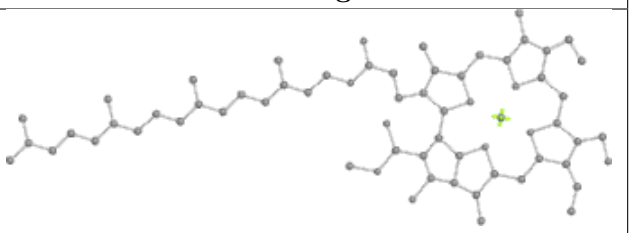


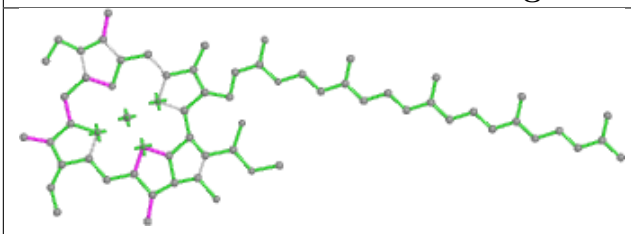
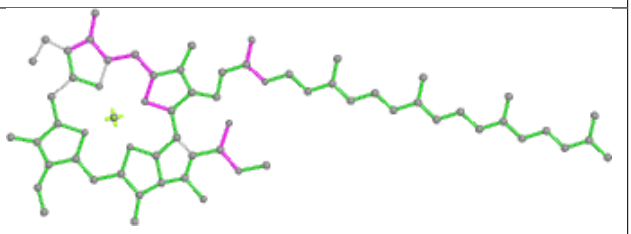
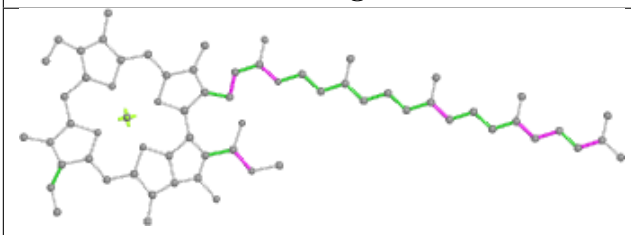
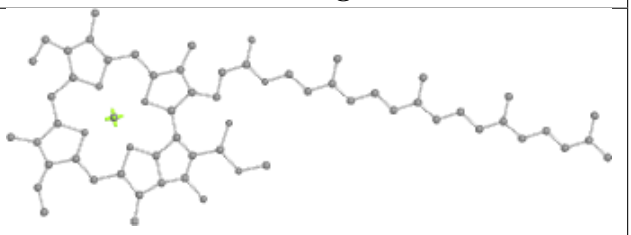
Torsions

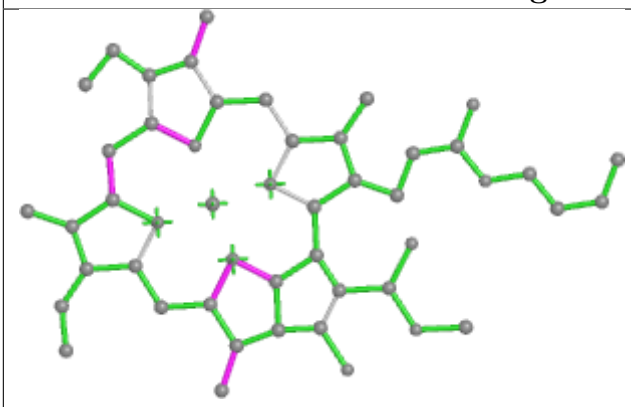
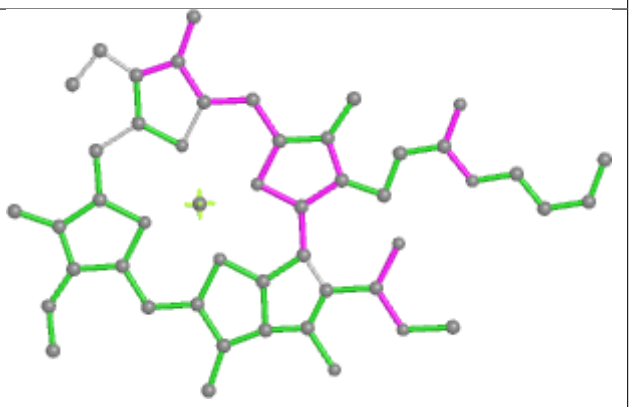
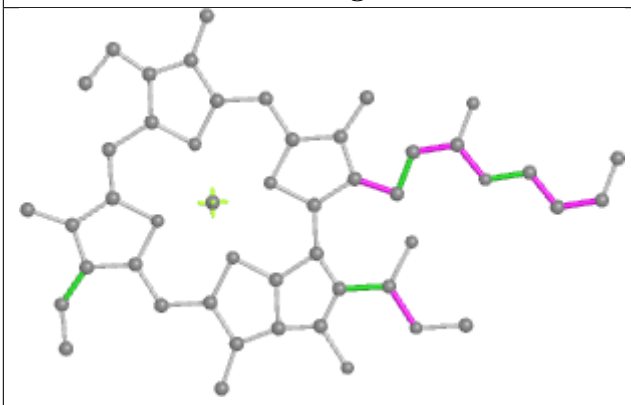
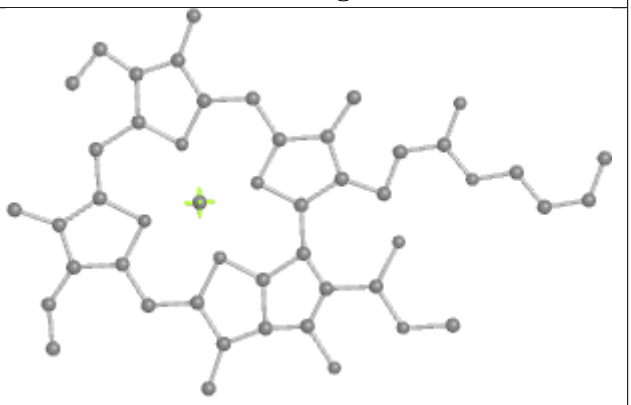


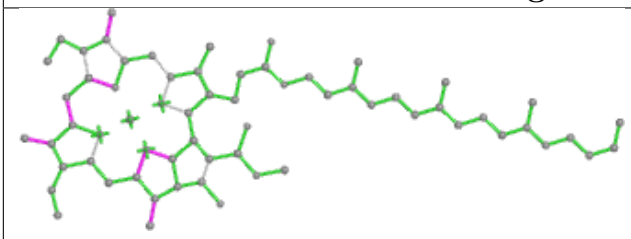
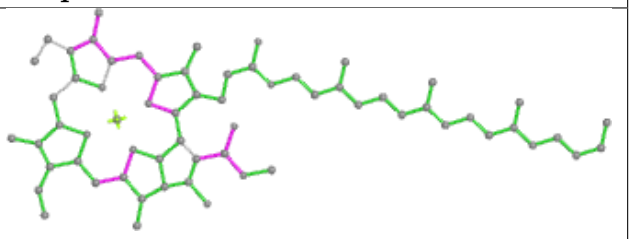
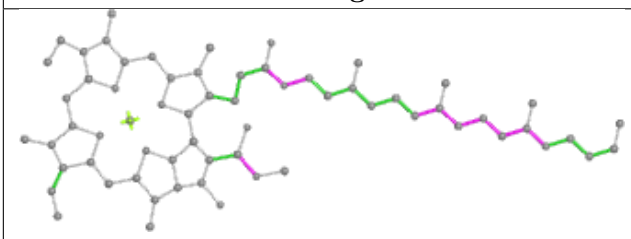
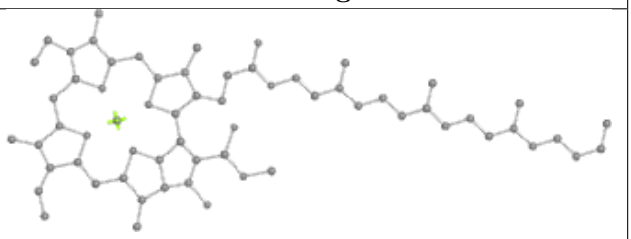
Rings

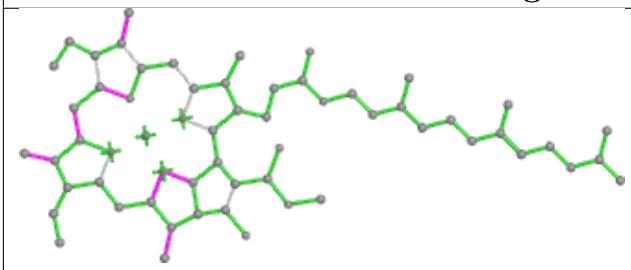
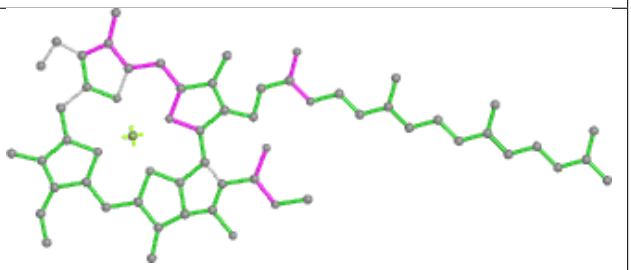
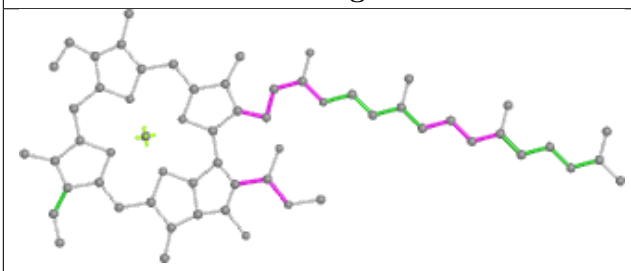
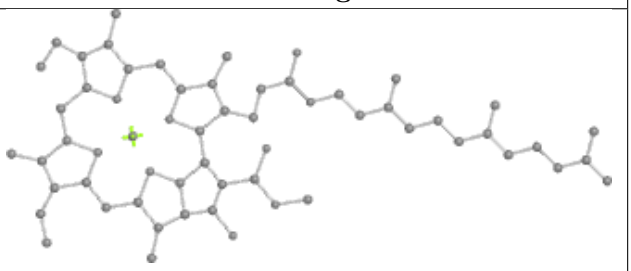
Ligand CLA S 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

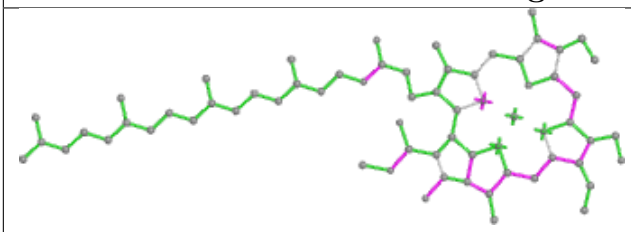
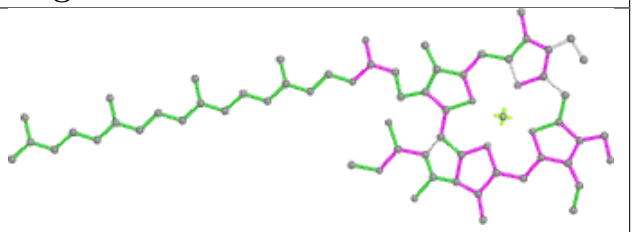
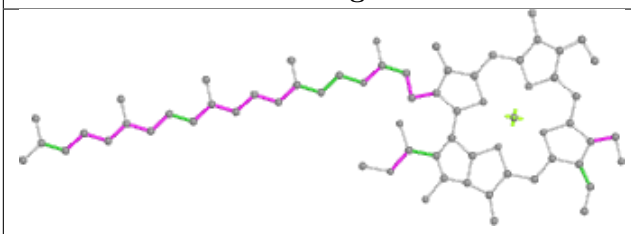
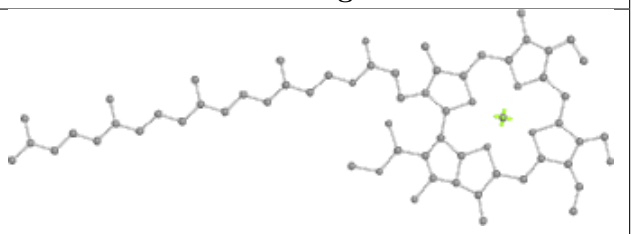
Ligand CHL G 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

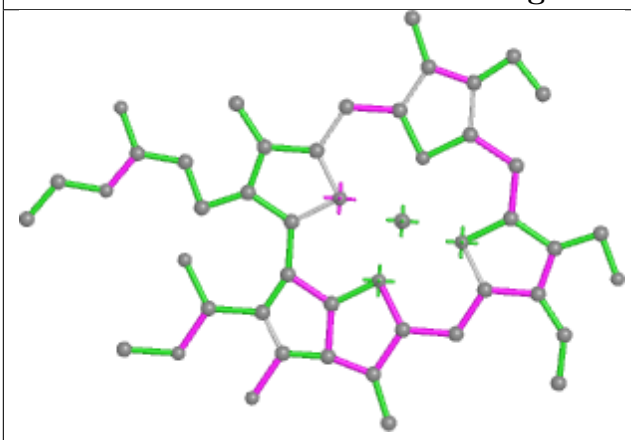
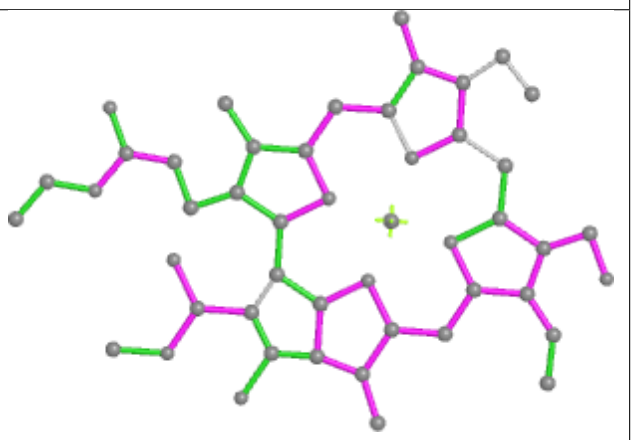
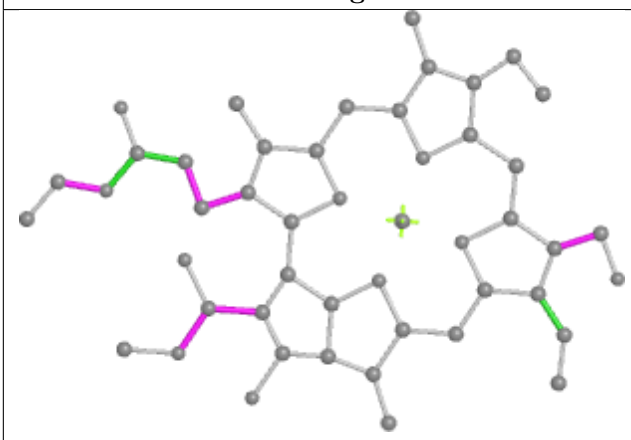
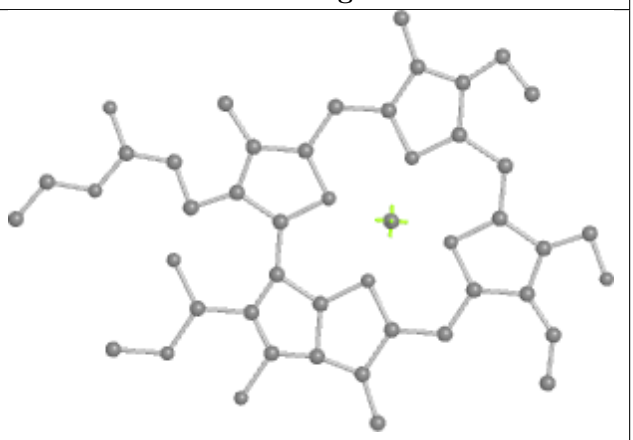
Ligand CLA V 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

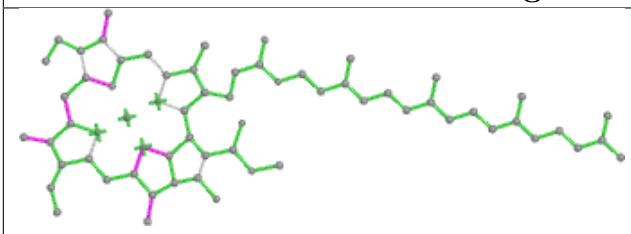
Ligand CLA q 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

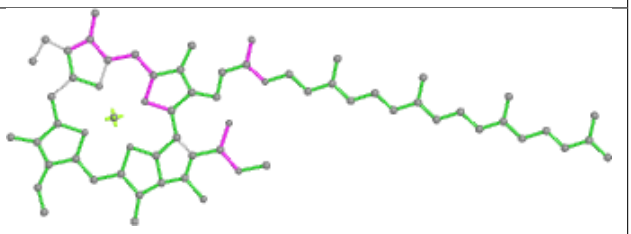
Ligand CHL g 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 5 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

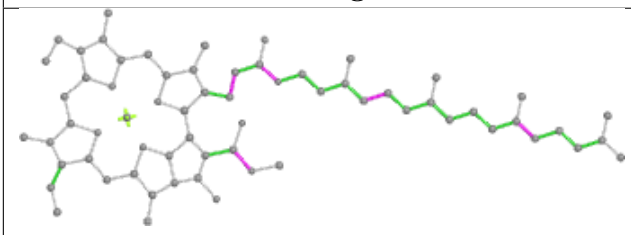
Ligand CLA V 307



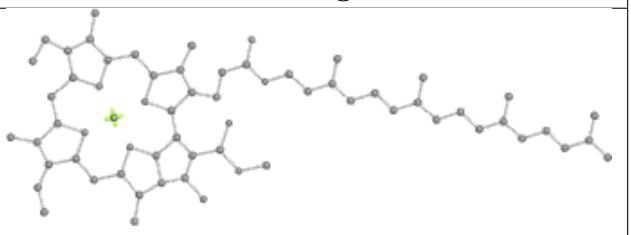
Bond lengths



Bond angles

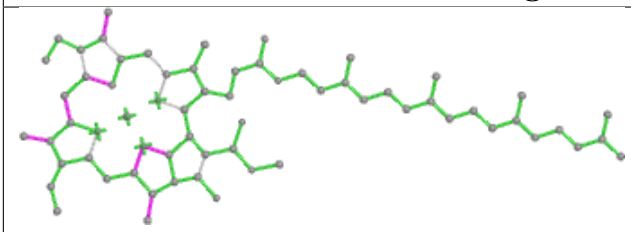


Torsions

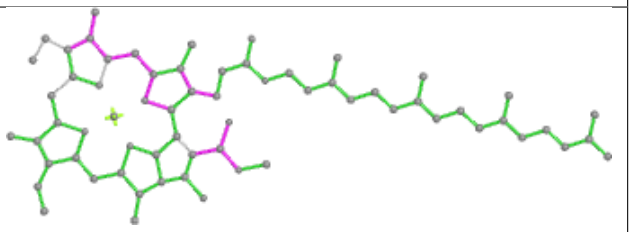


Rings

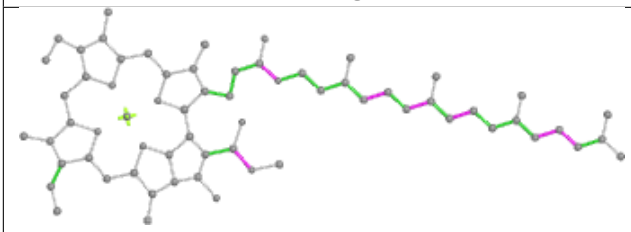
Ligand CLA X 202



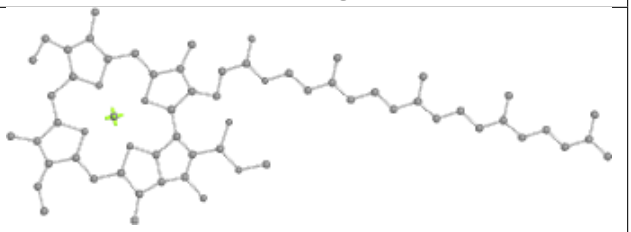
Bond lengths



Bond angles

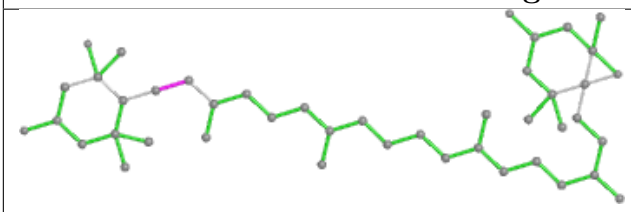


Torsions

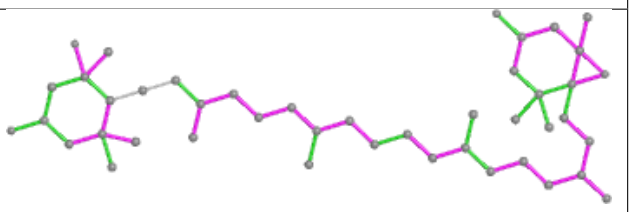


Rings

Ligand NEX P 301



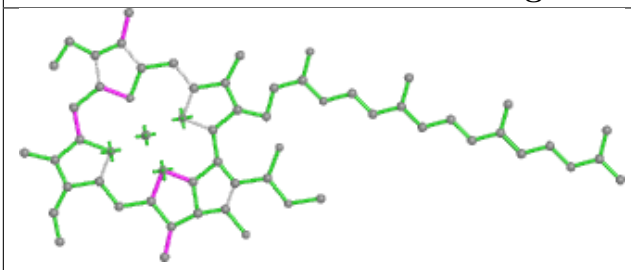
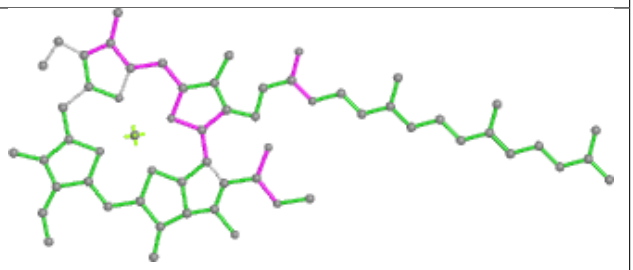
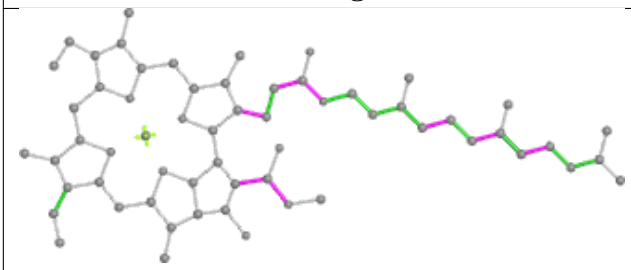
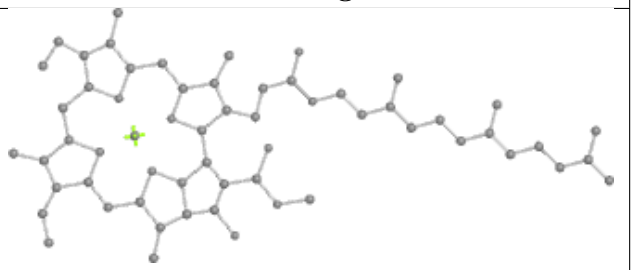
Bond lengths

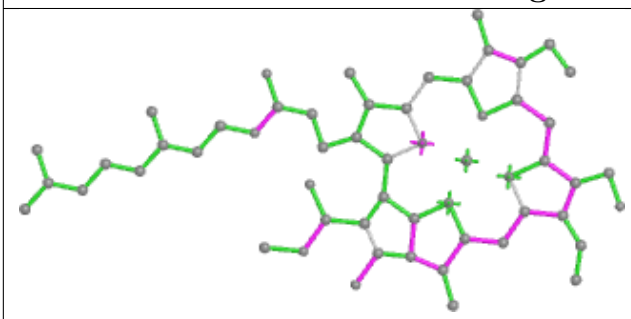
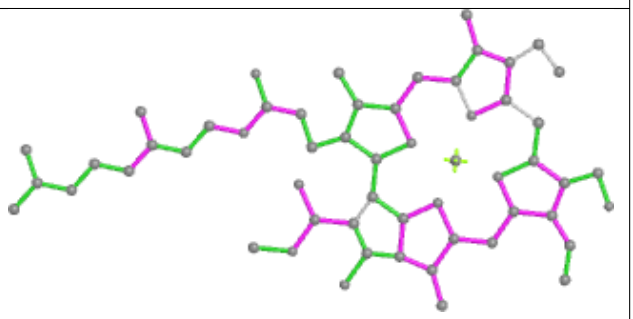
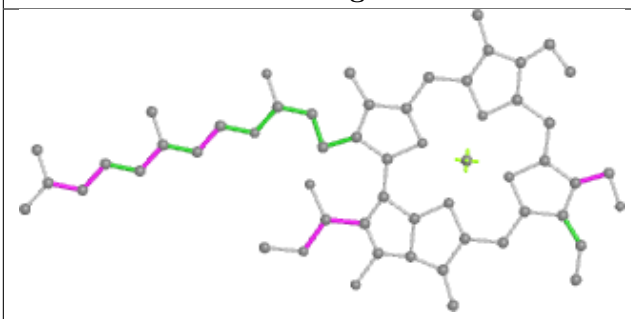
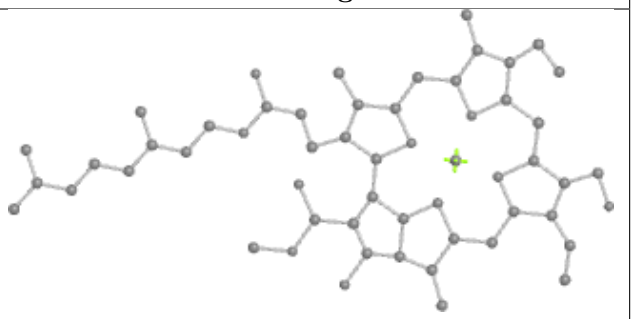


Bond angles

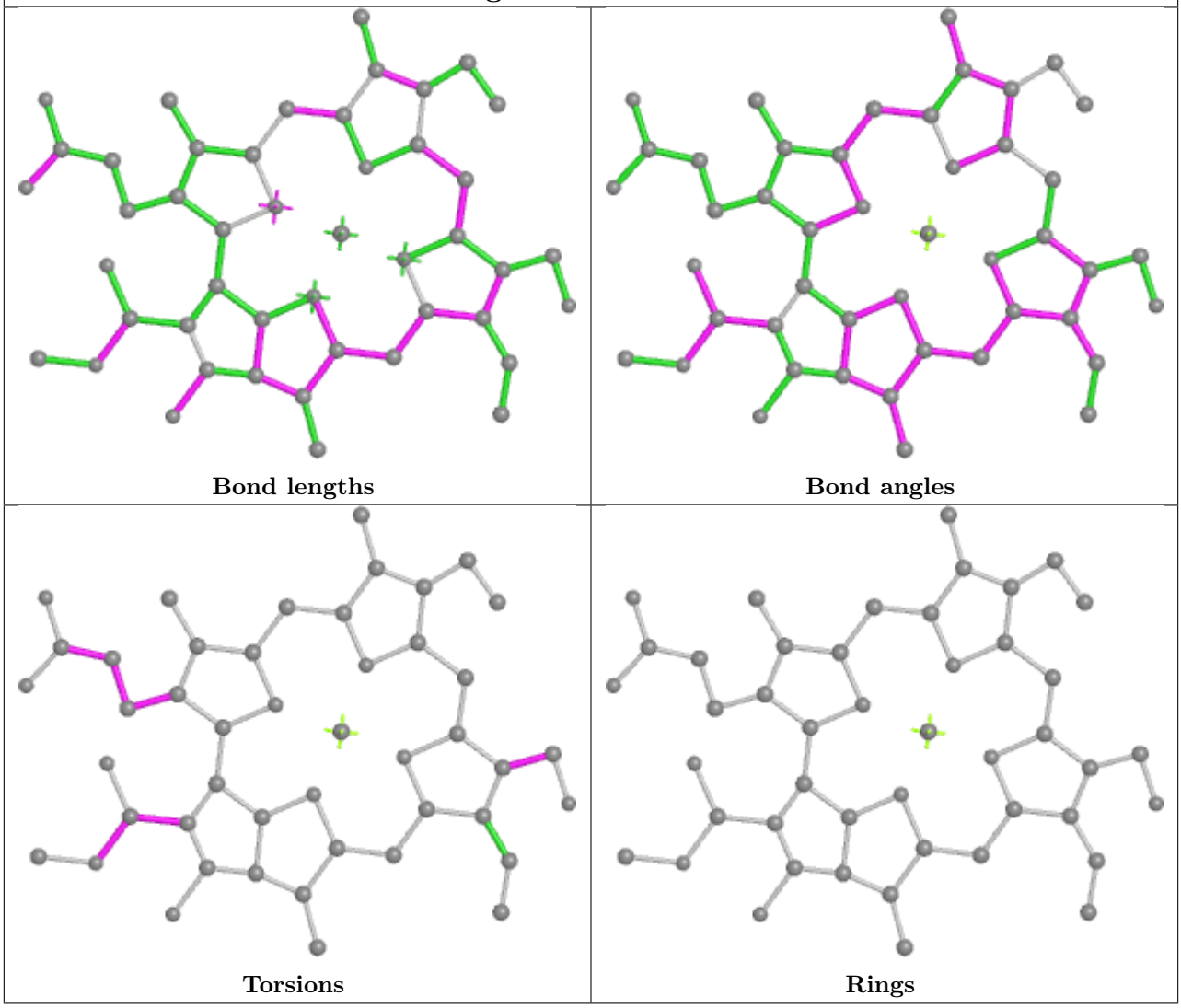
Torsions

Rings

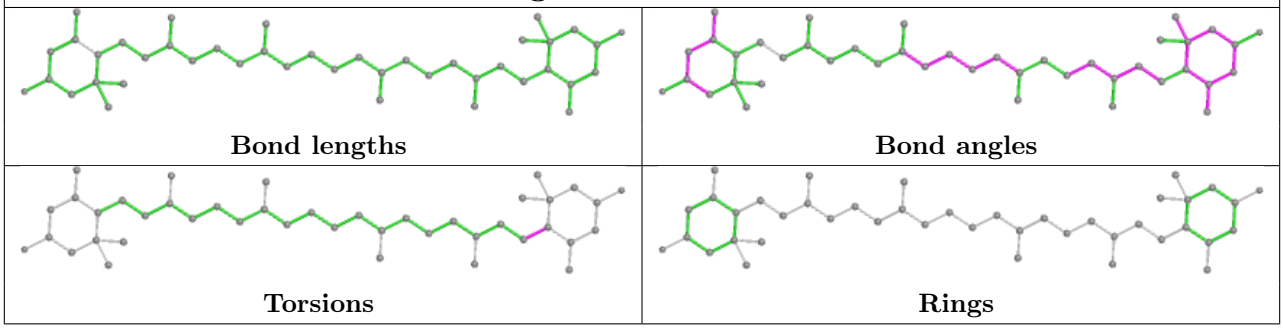
Ligand CLA P 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL r 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

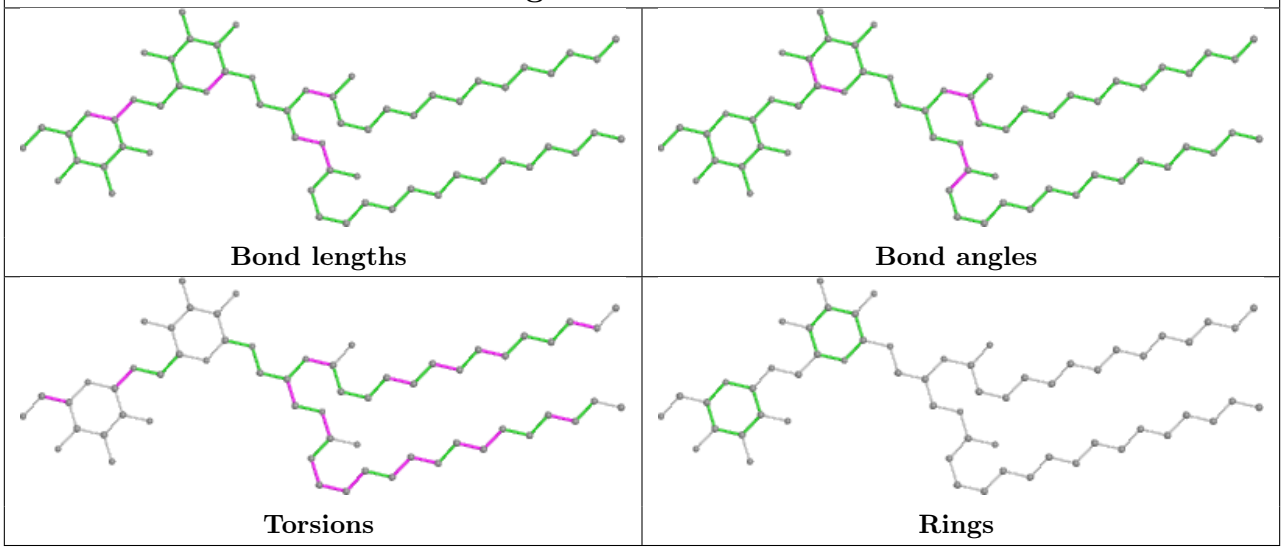
Ligand CHL S 316



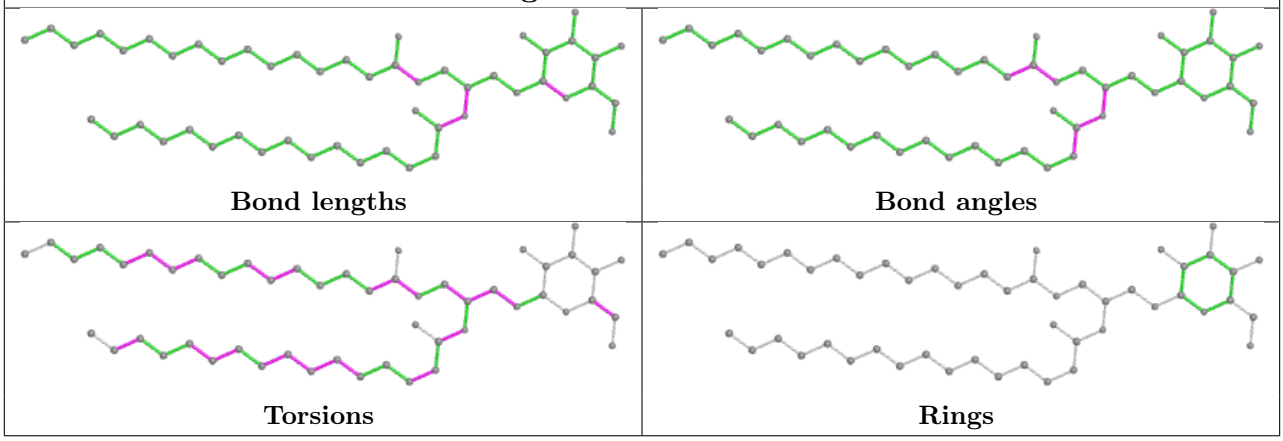
Ligand LUT 5 310



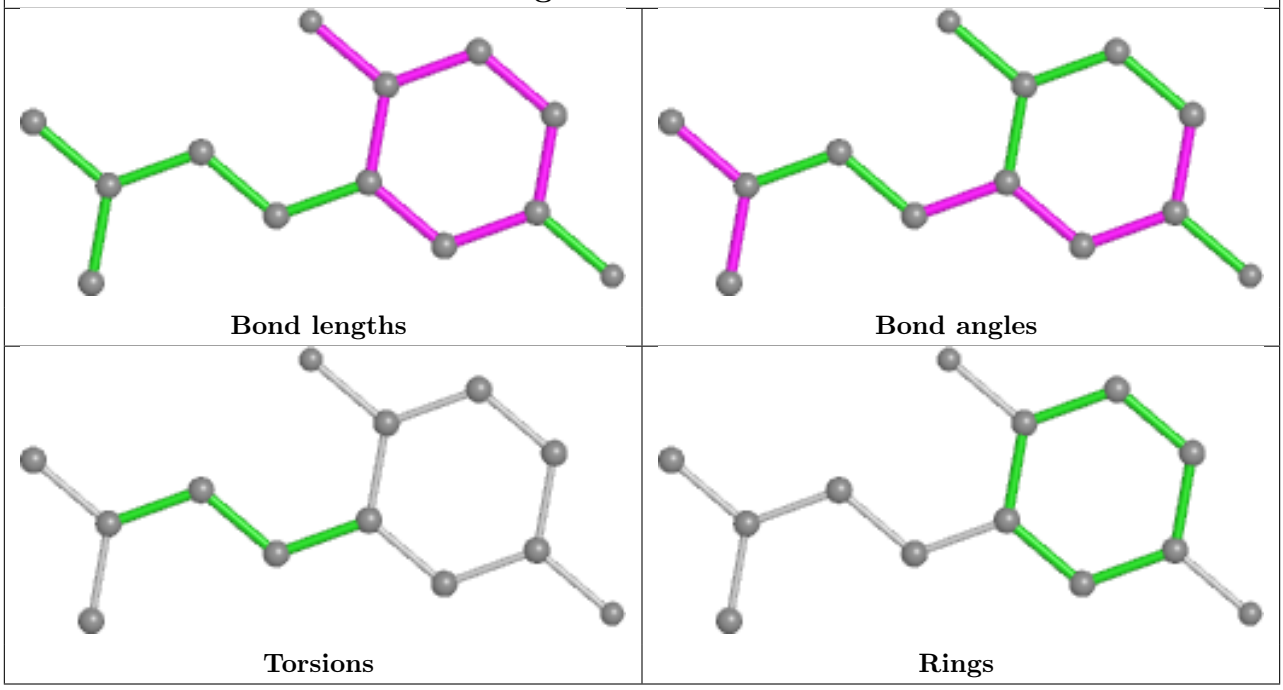
Ligand DGD c 519



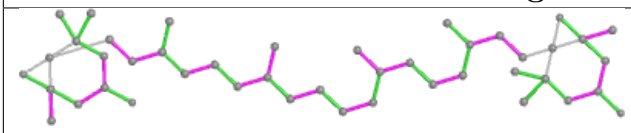
Ligand LMG C 502



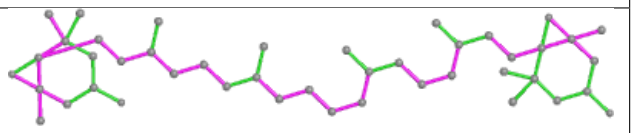
Ligand PL9 a 411



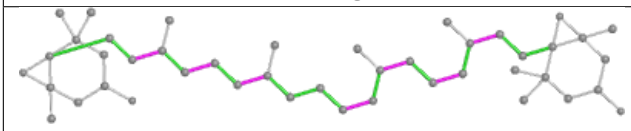
Ligand XAT v 311



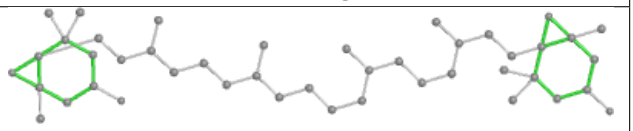
Bond lengths



Bond angles

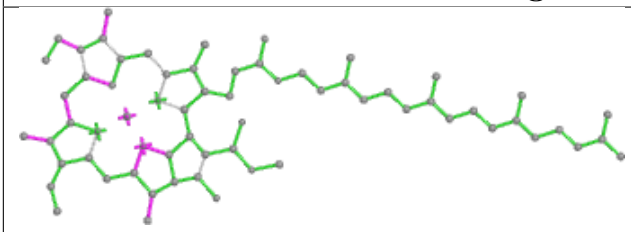


Torsions

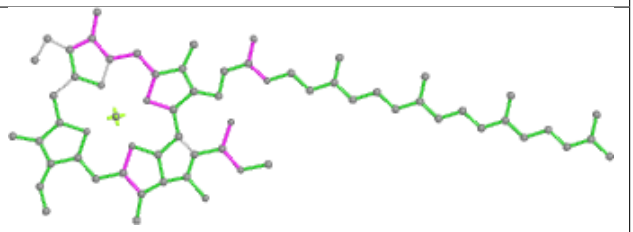


Rings

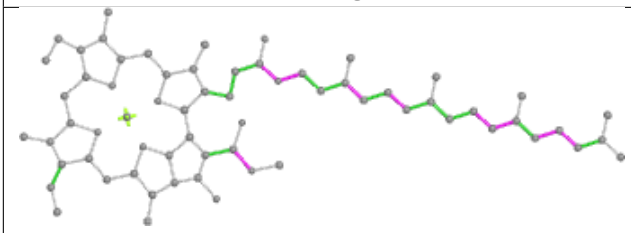
Ligand CLA d 402



Bond lengths



Bond angles



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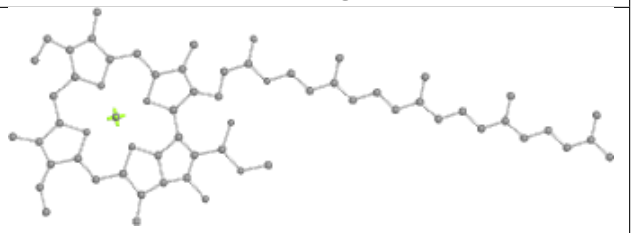
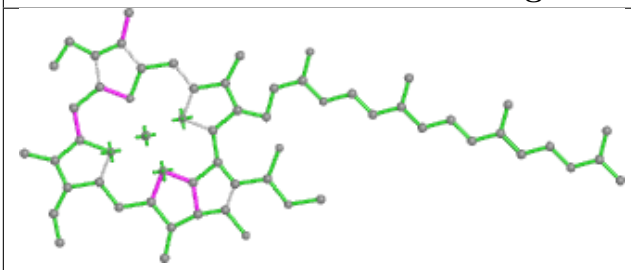


Rings

Ligand CLA P 306



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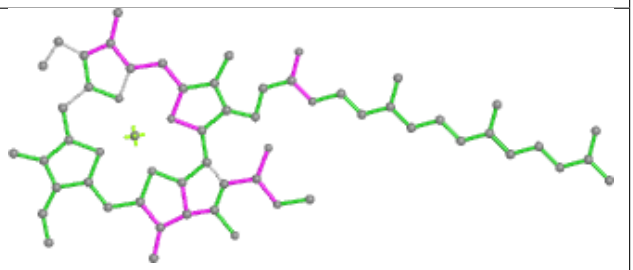
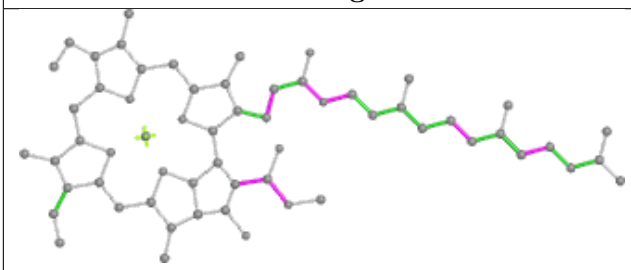


Bond angles



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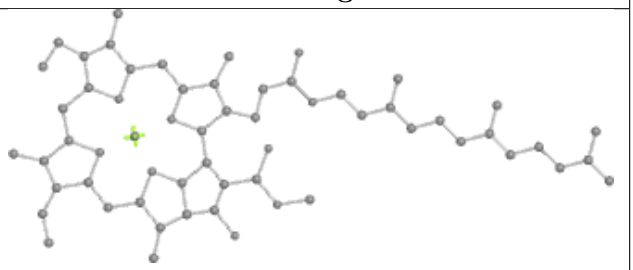
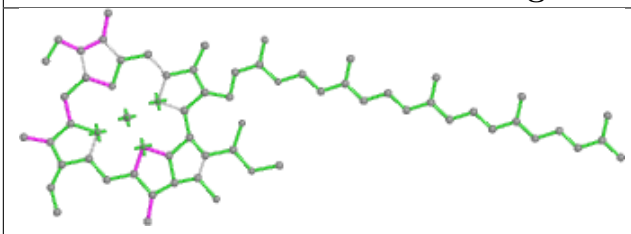
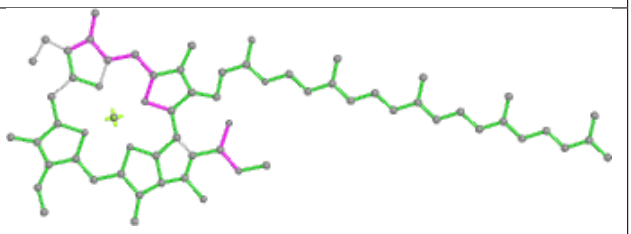
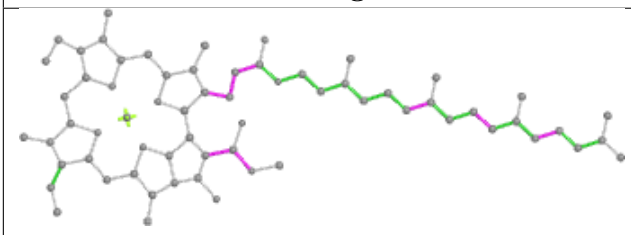
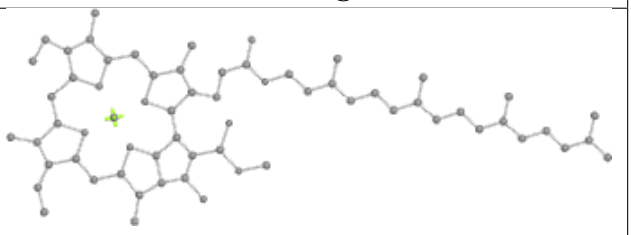
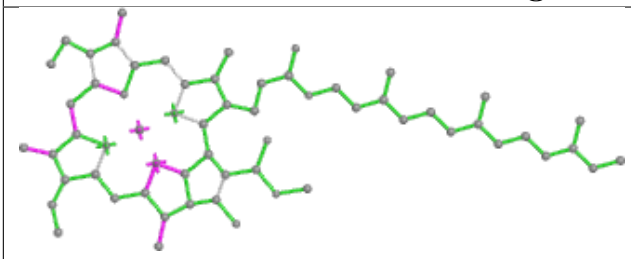
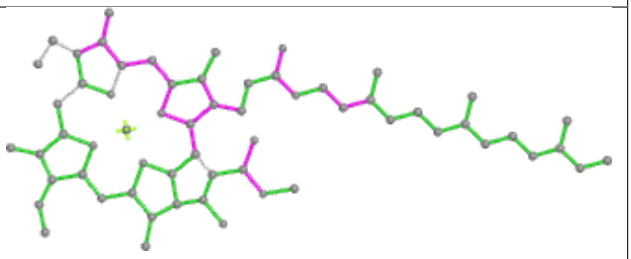
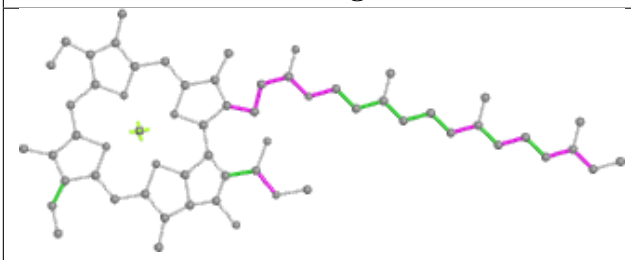
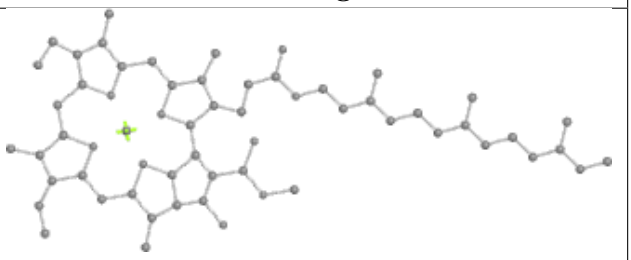
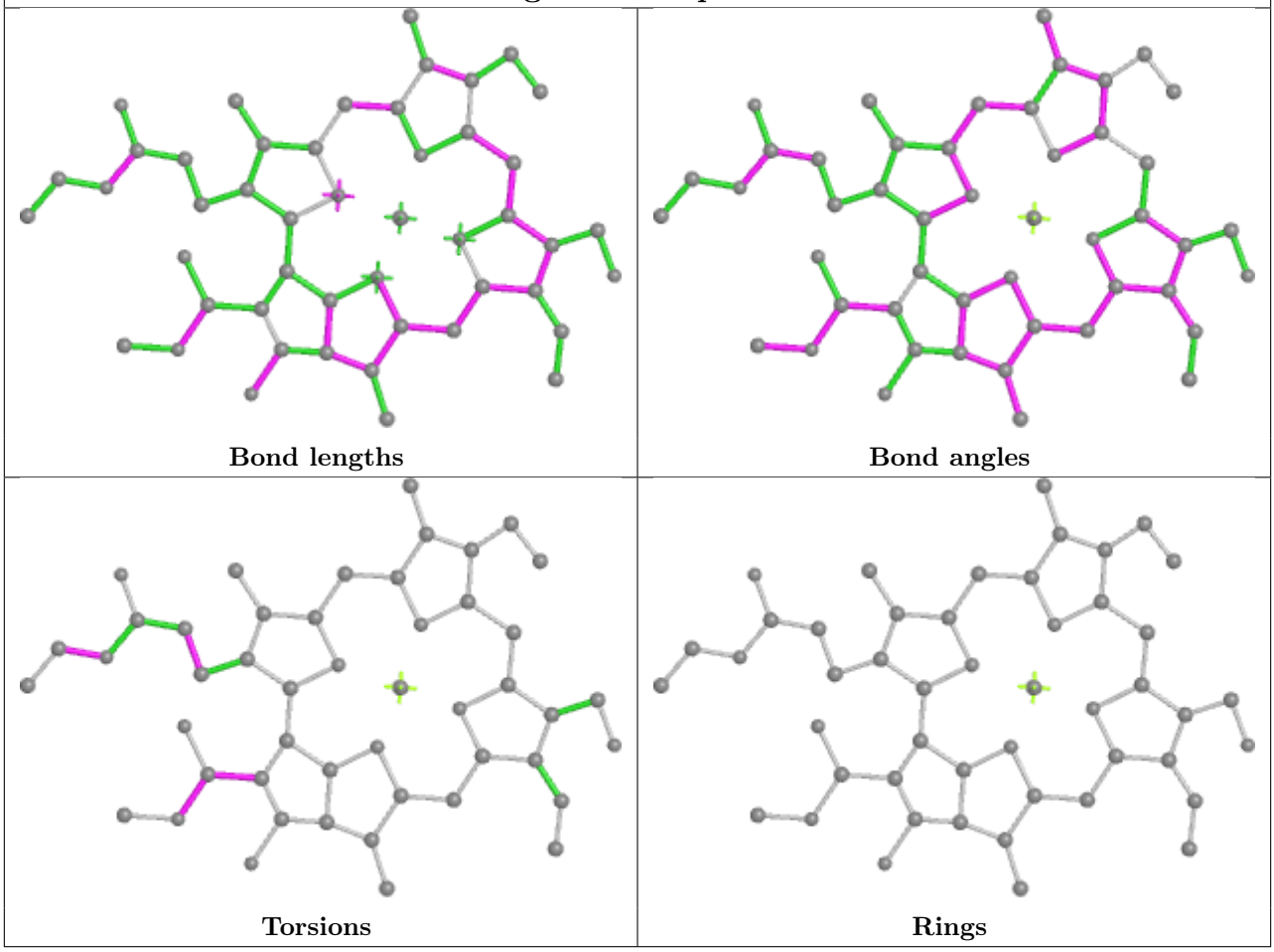


Rings

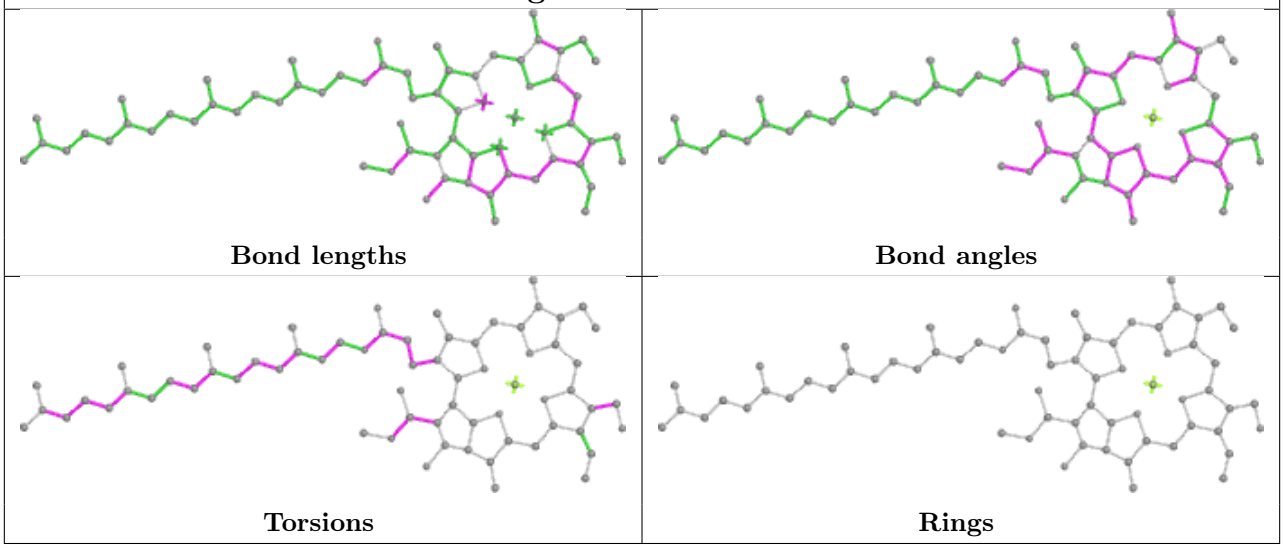
Ligand CLA v 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

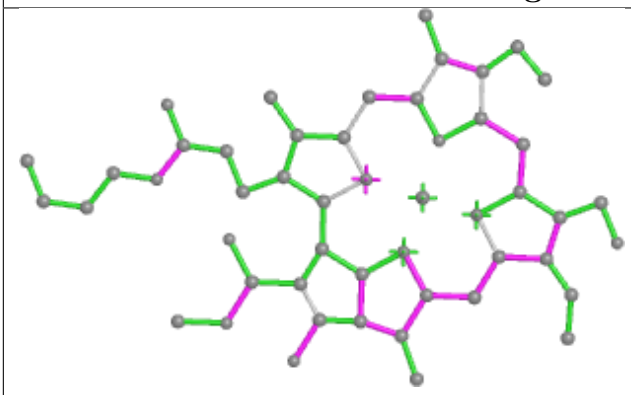
Ligand CHL p 315



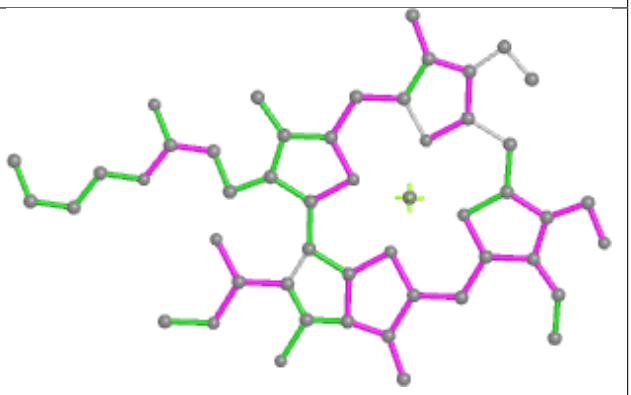
Ligand CHL n 316



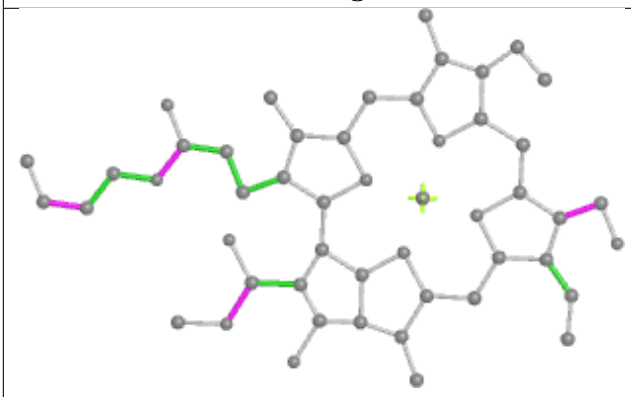
Ligand CHL P 316



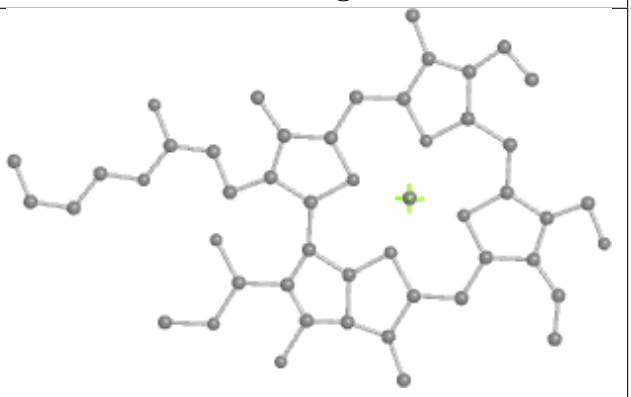
Bond lengths



Bond angles

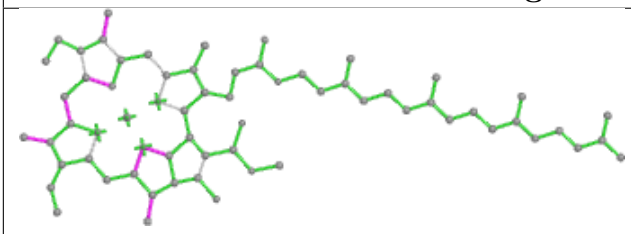


Torsions

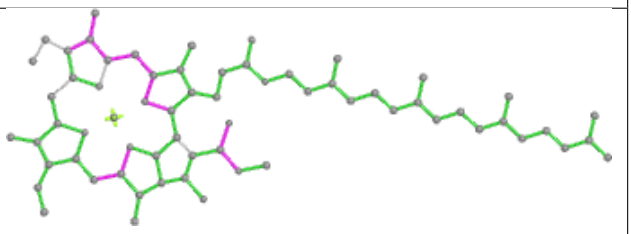


Rings

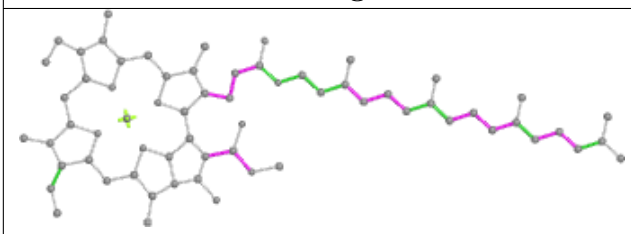
Ligand CLA P 302



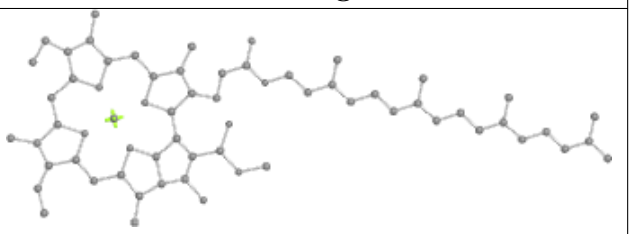
Bond lengths



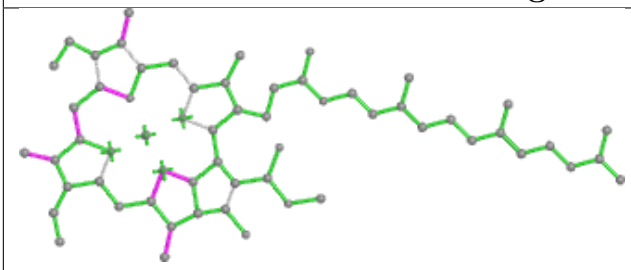
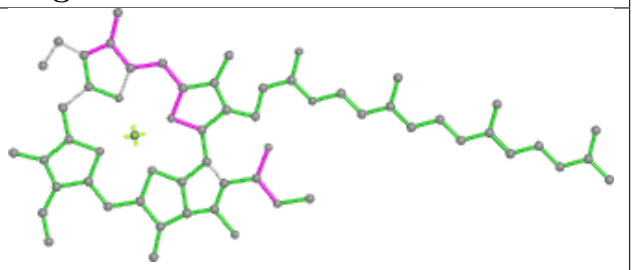
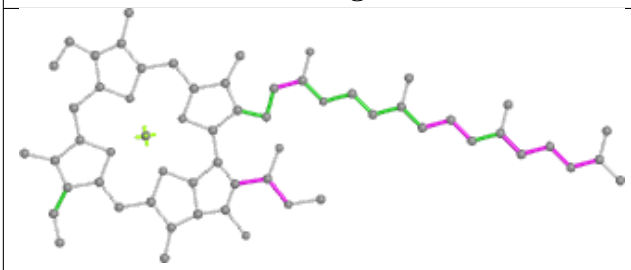
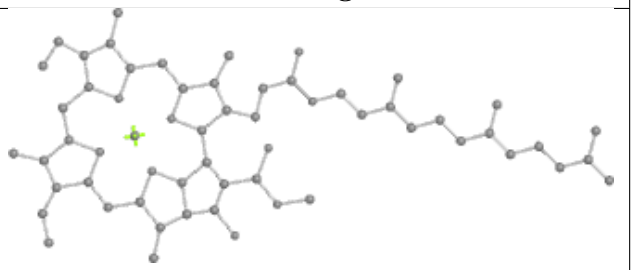
Bond angles

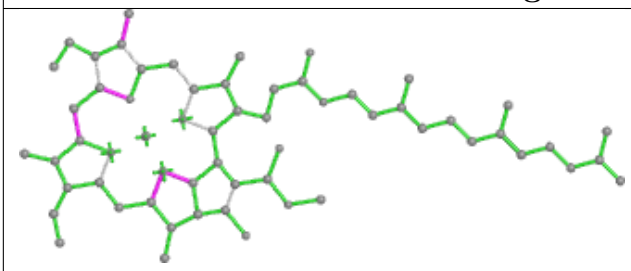
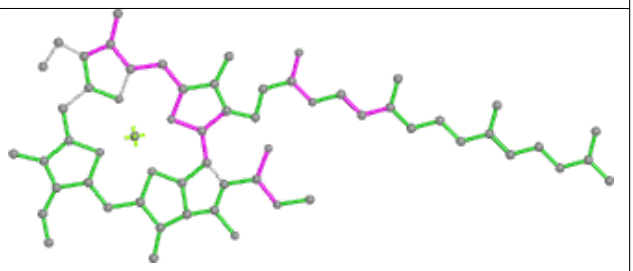
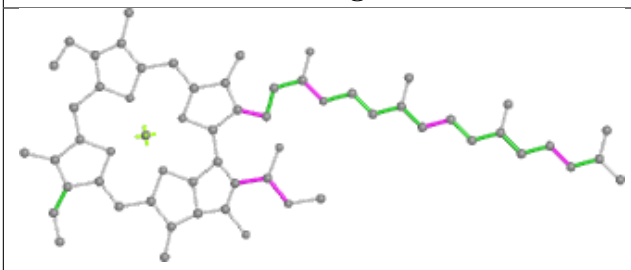
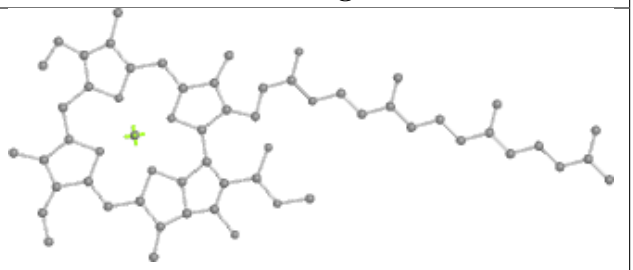


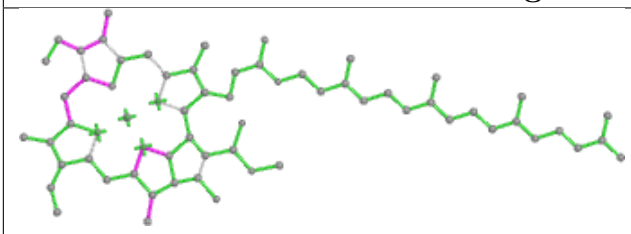
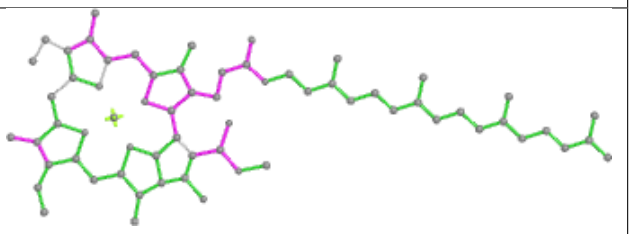
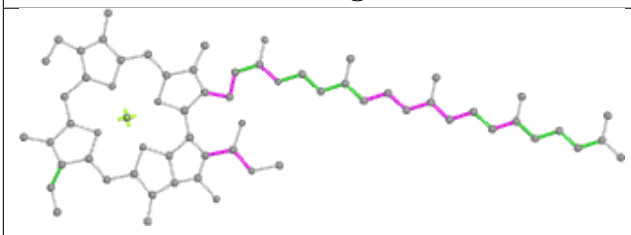
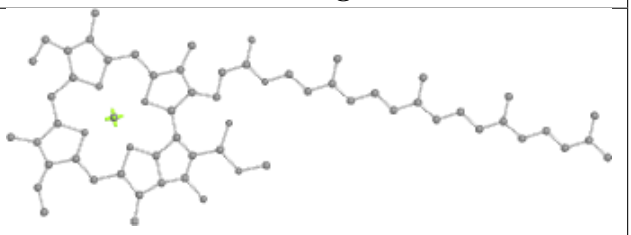
Torsions

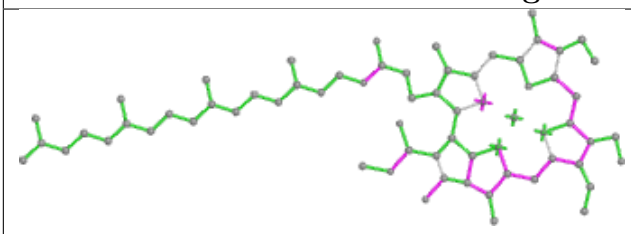
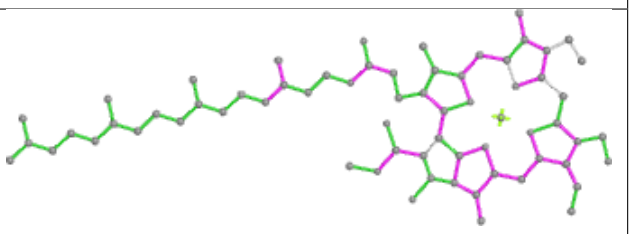
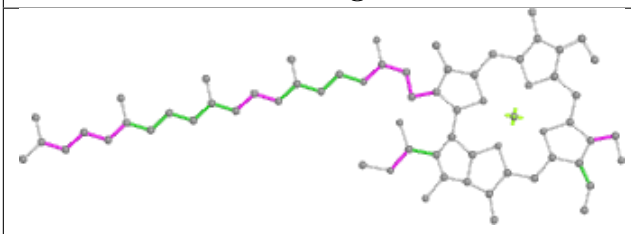
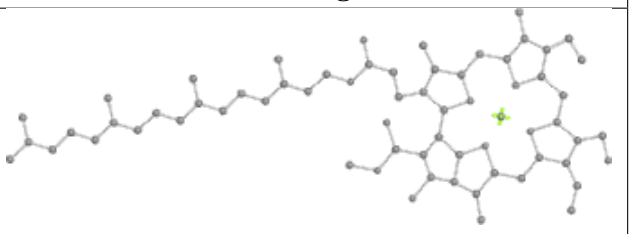


Rings

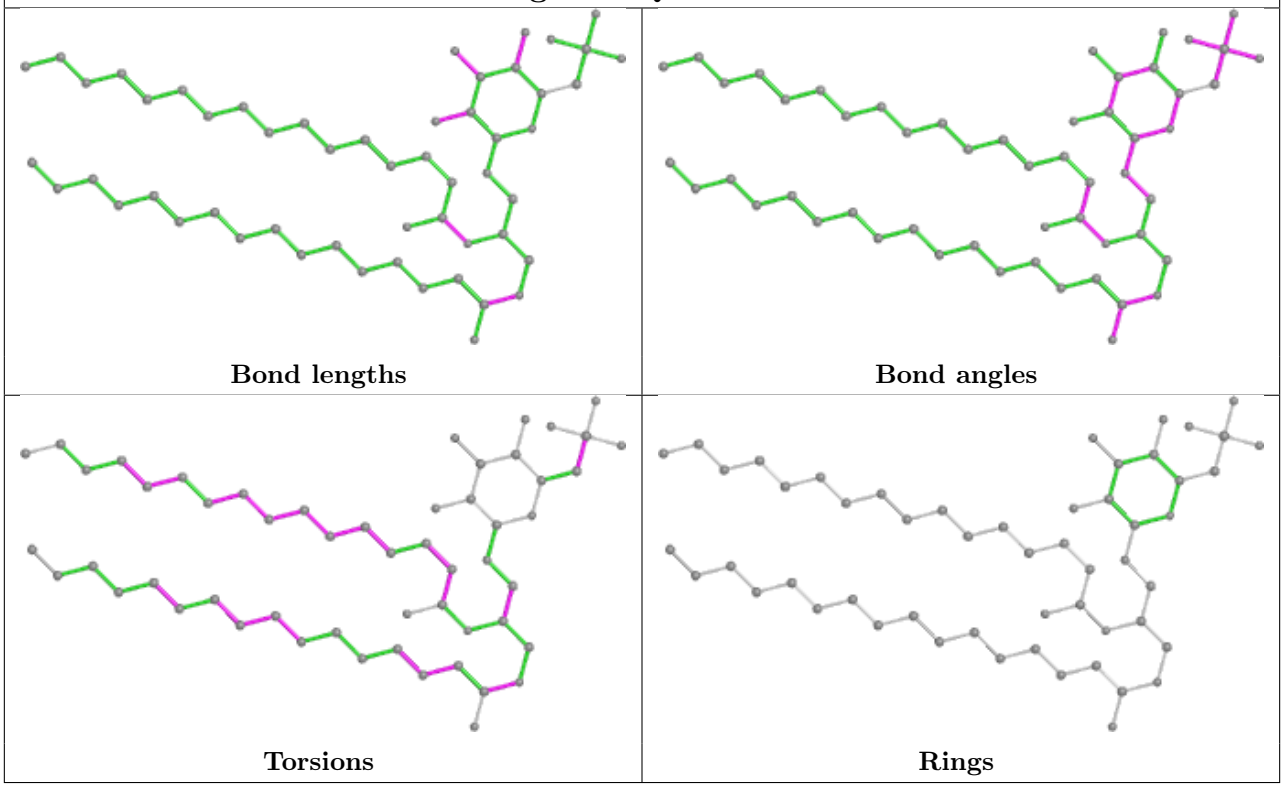
Ligand CLA g 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

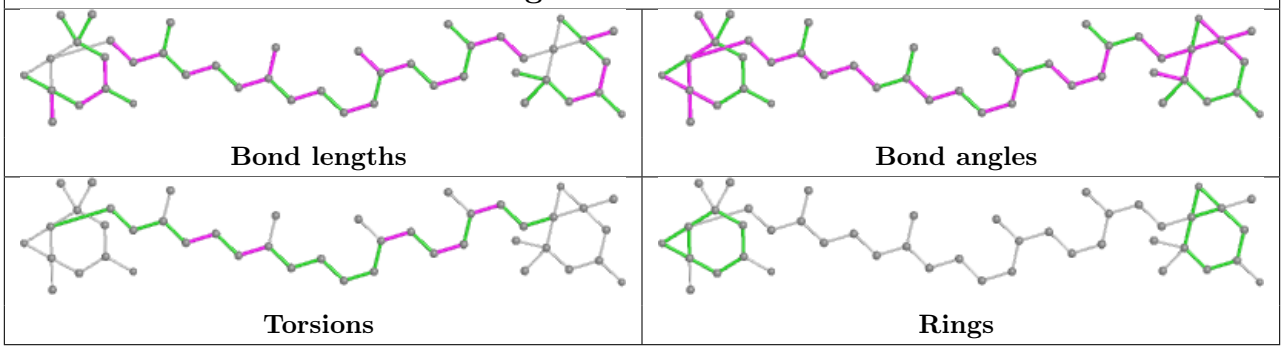
Ligand CLA B 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

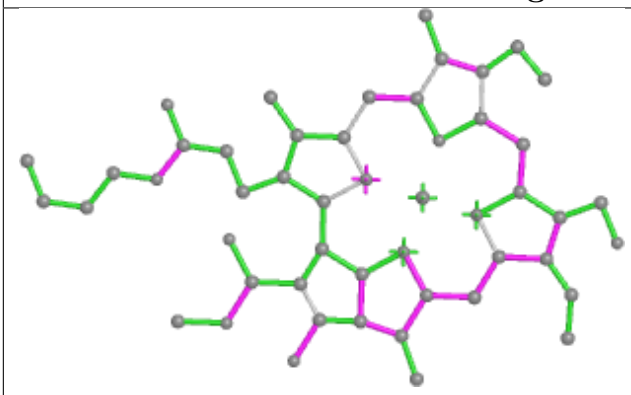
Ligand SQD a 413



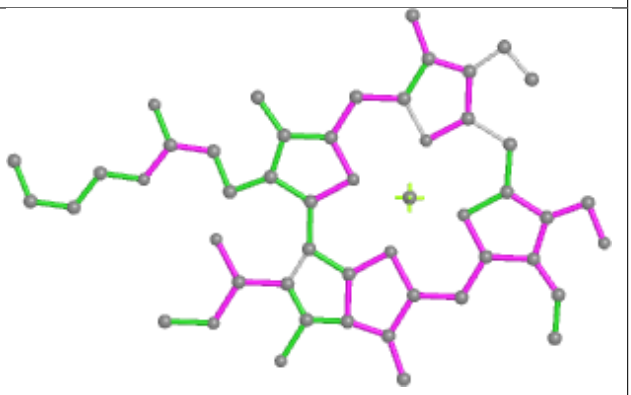
Ligand XAT P 312



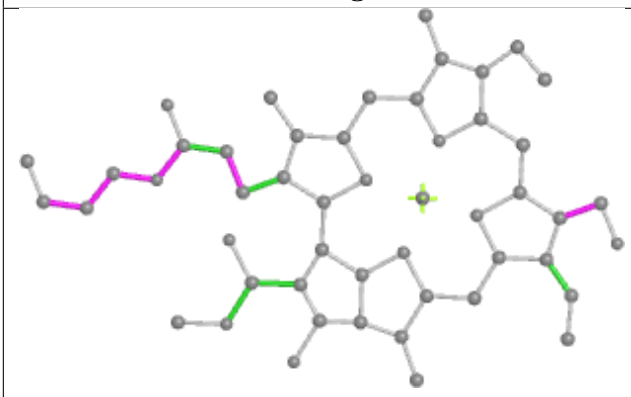
Ligand CHL v 315



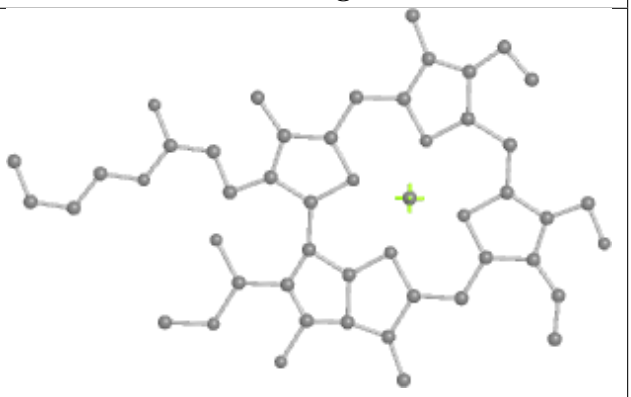
Bond lengths



Bond angles

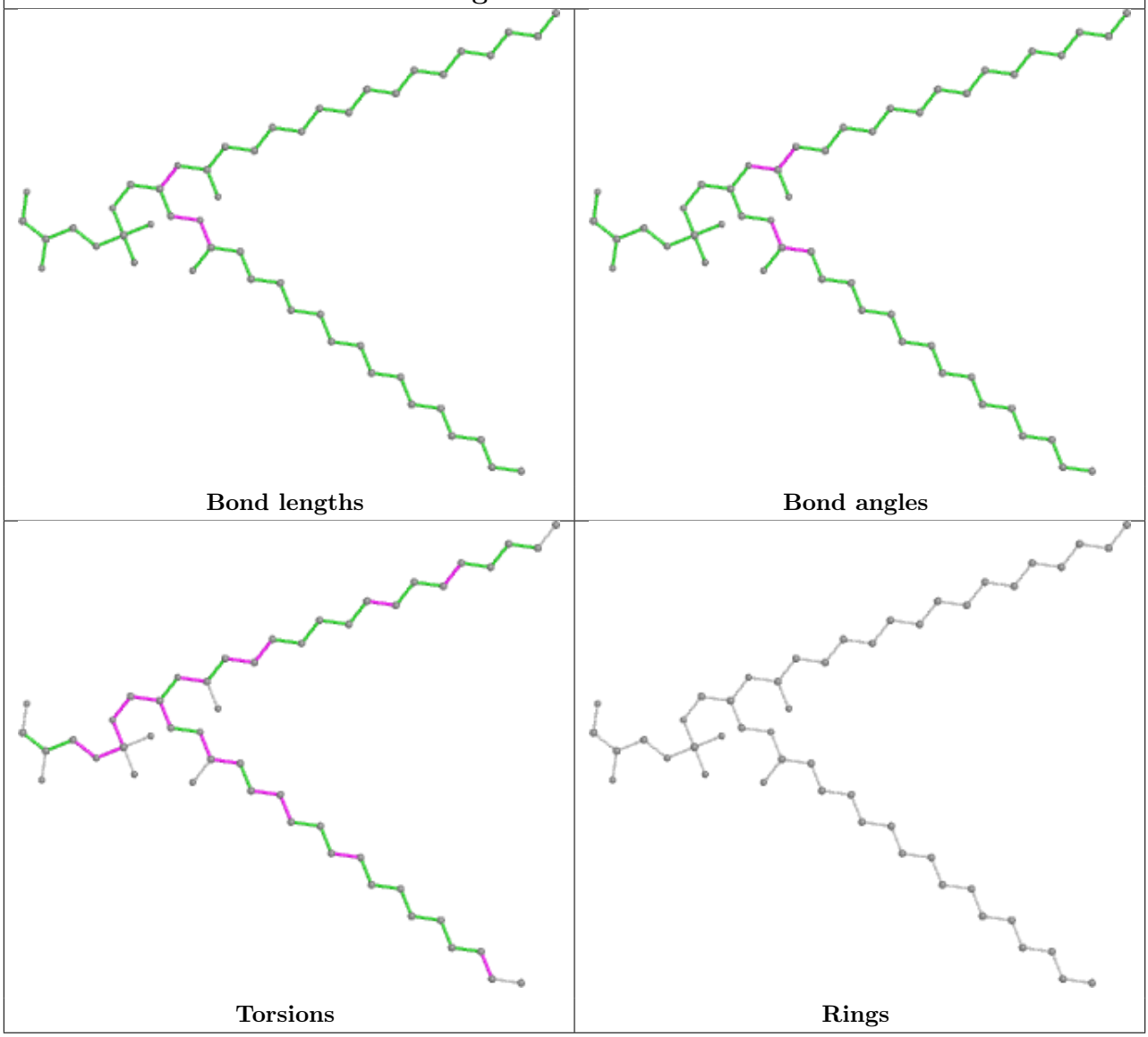


Torsions

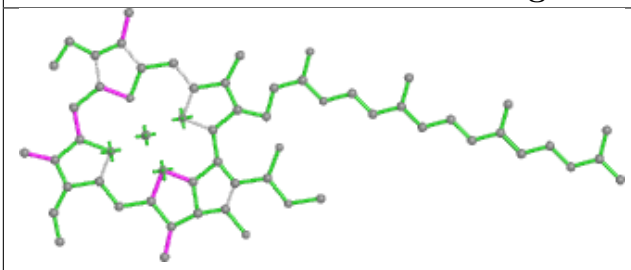


Rings

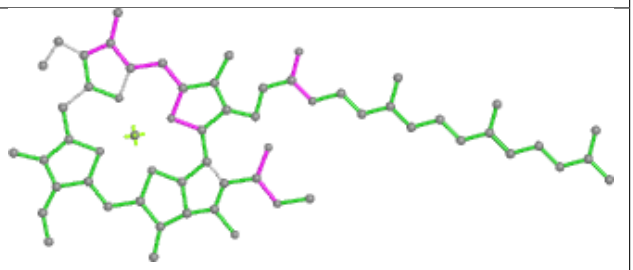
Ligand LHG 5 312



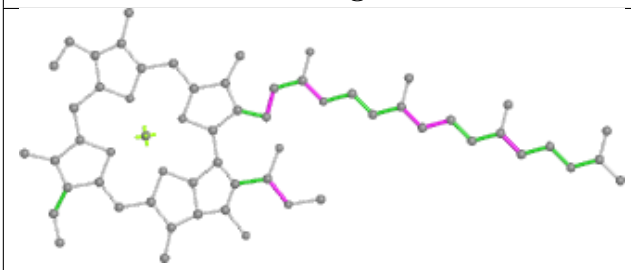
Ligand CLA 5 307



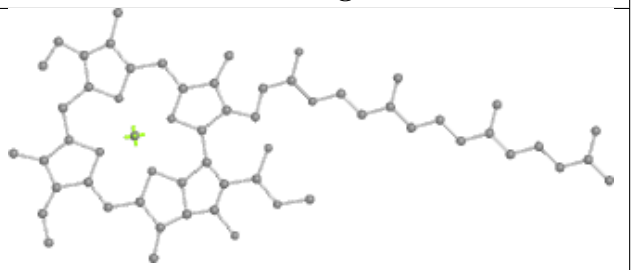
Bond lengths



Bond angles

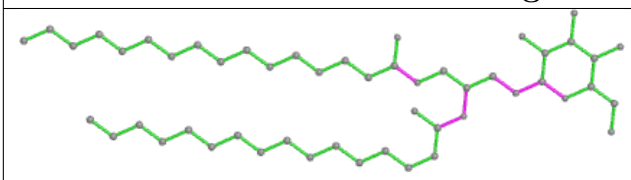


Torsions



Rings

Ligand LMG b 621



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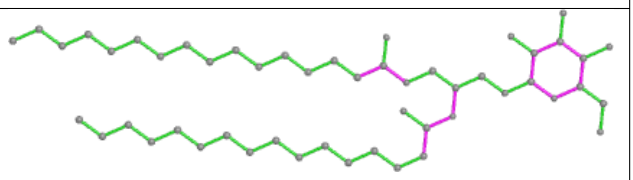
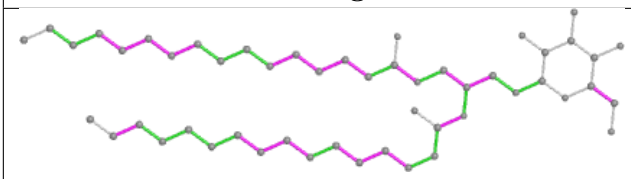


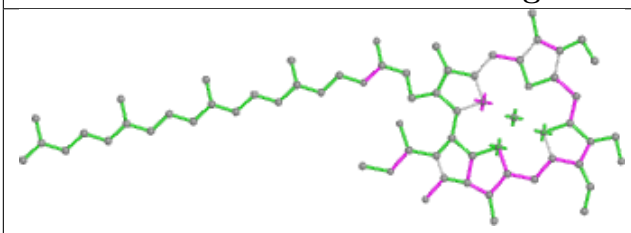
Bond angles



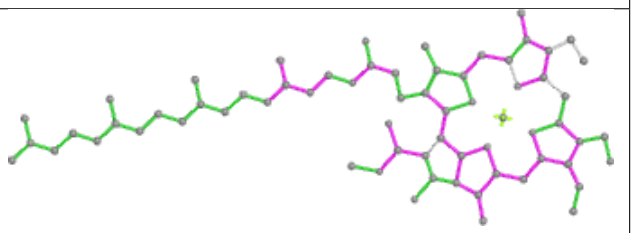
Torsions

Rings

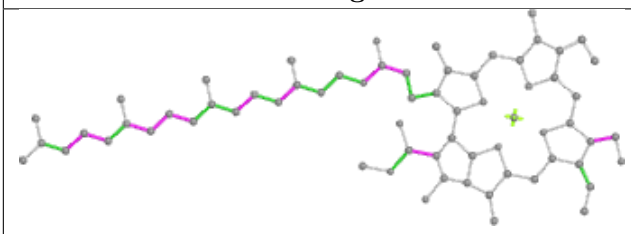
Ligand CHL U 313



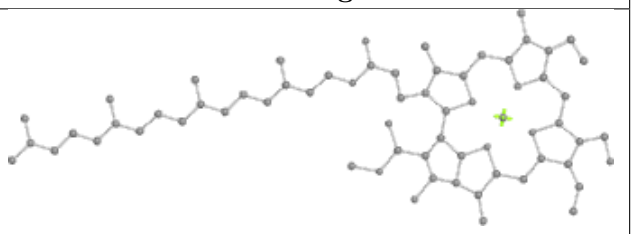
Bond lengths



Bond angles

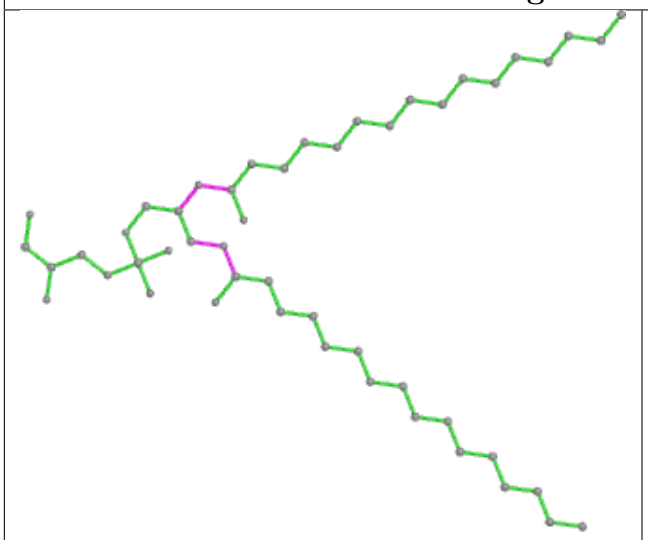


Torsions

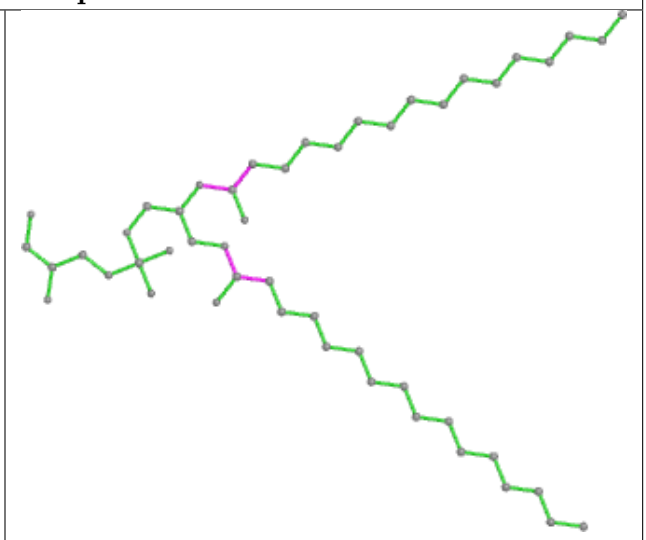


Rings

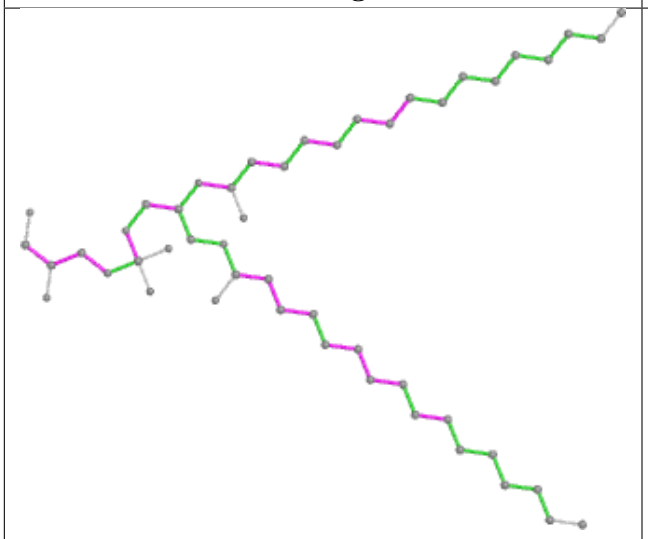
Ligand LHG q 310



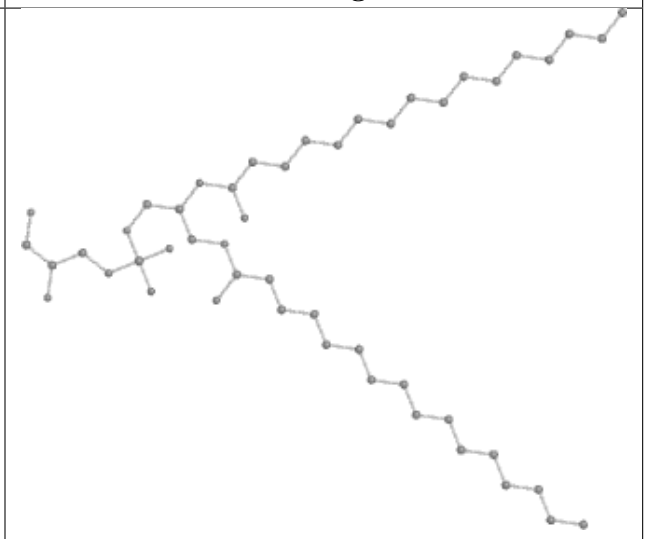
Bond lengths



Bond angles

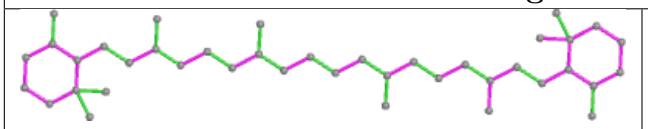


Torsions

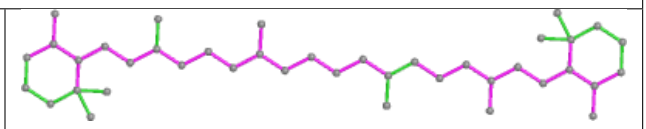


Rings

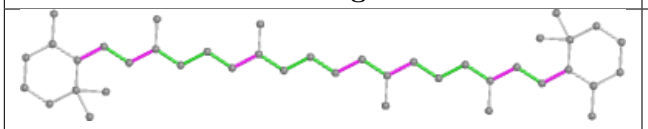
Ligand BCR d 403



Bond lengths



Bond angles



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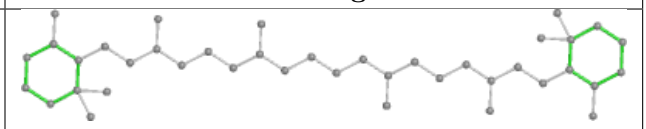
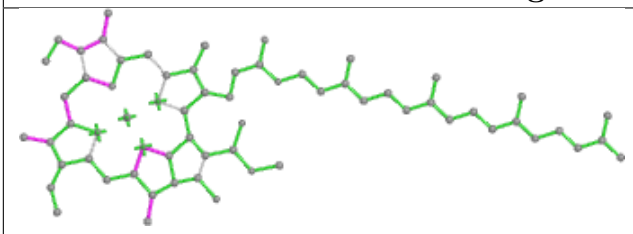
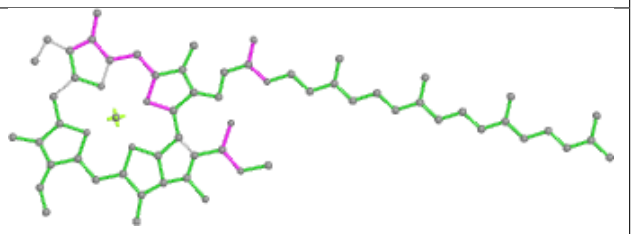


Rings

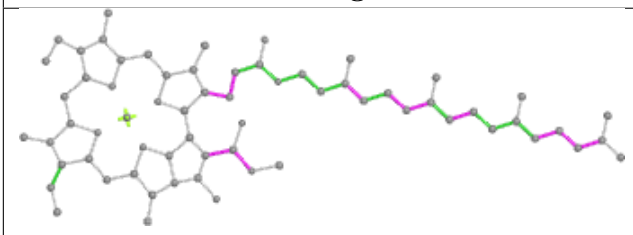
Ligand CLA b 604



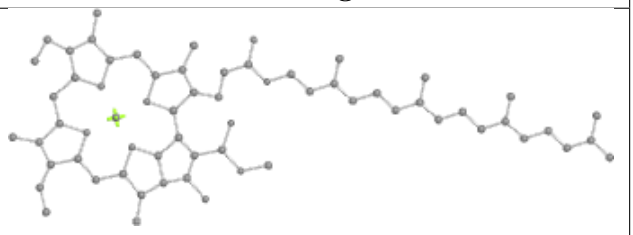
Bond lengths



Bond angles

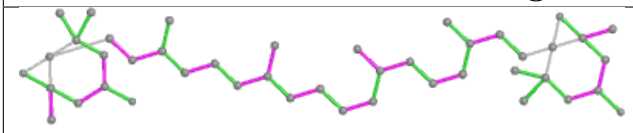


Torsions



Rings

Ligand XAT 4 311



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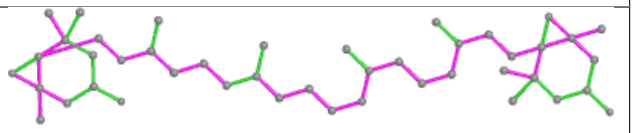
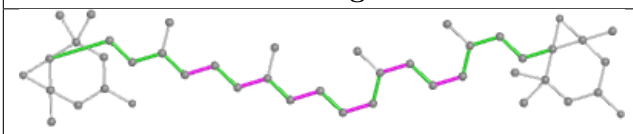


Bond angles



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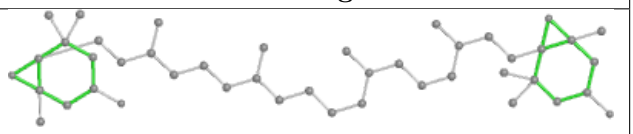
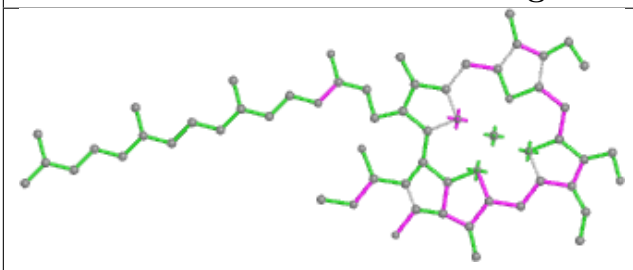


Rings

Ligand CHL g 316



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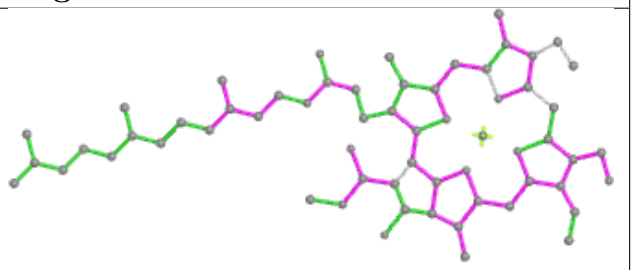
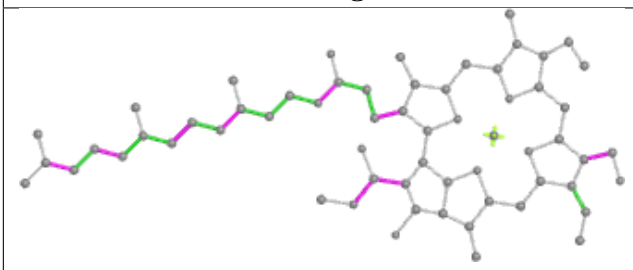
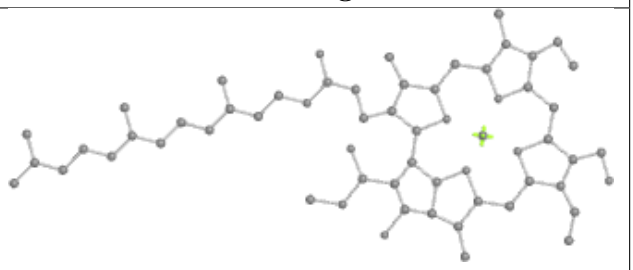


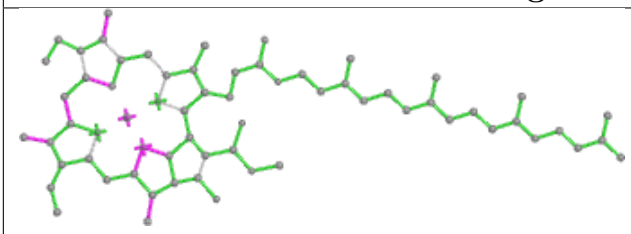
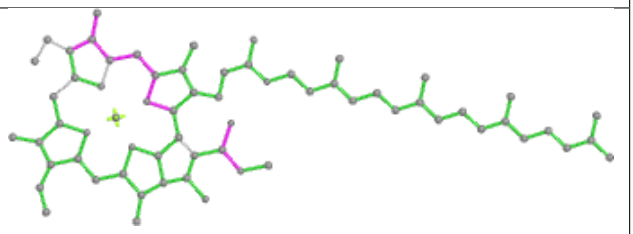
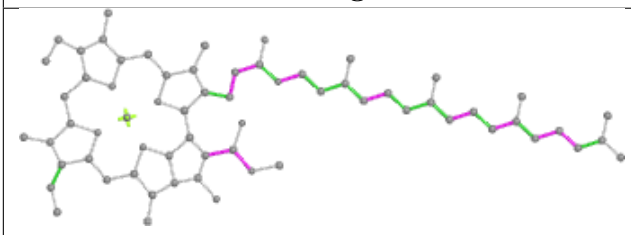
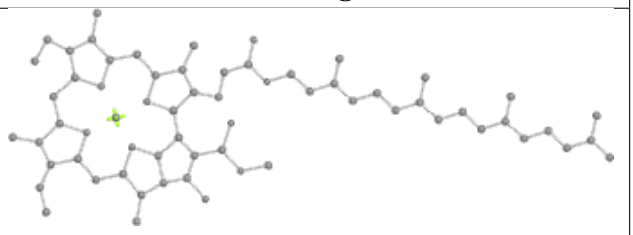
Bond angles

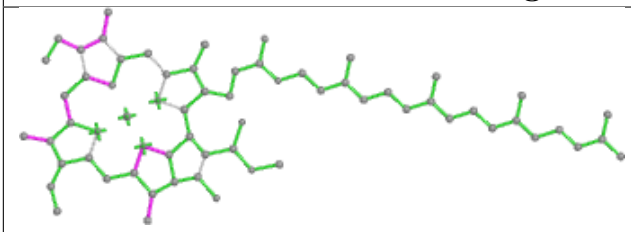
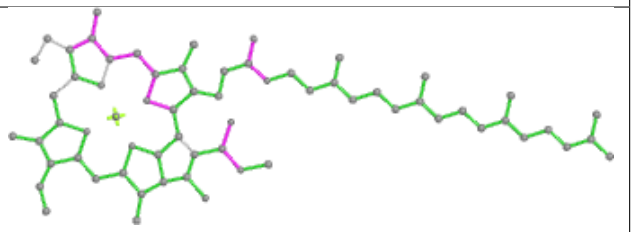
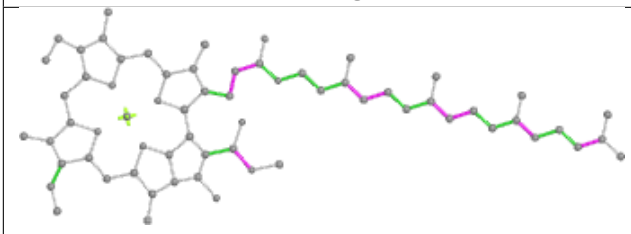
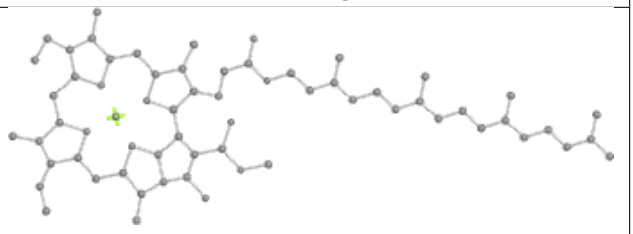


Torsions

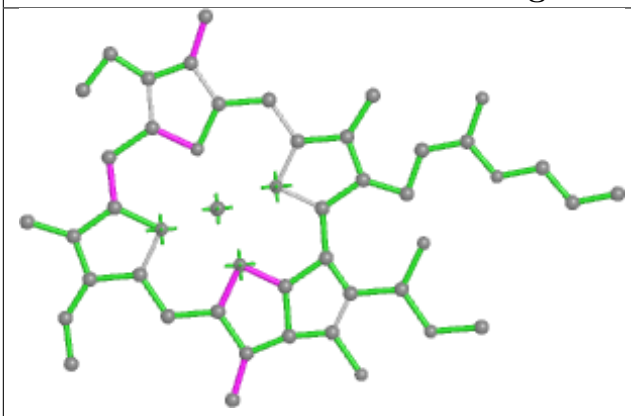


Rings

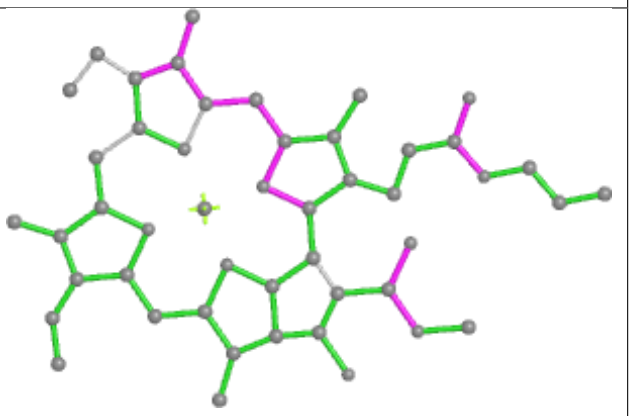
Ligand CLA b 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

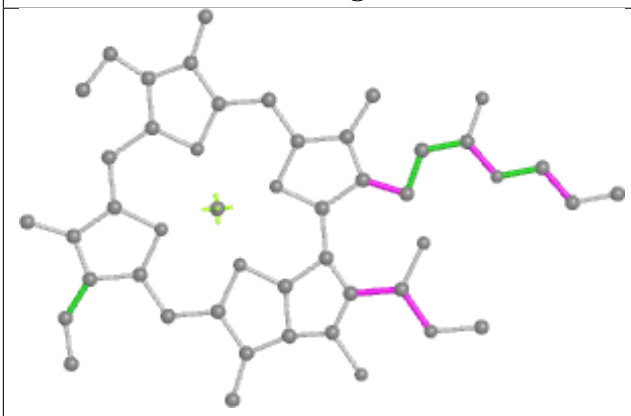
Ligand CLA 3 308



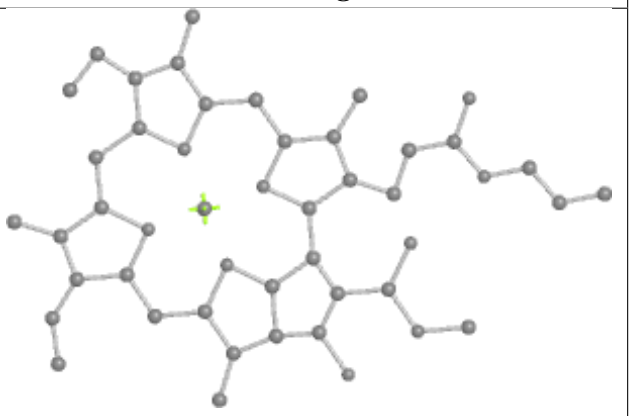
Bond lengths



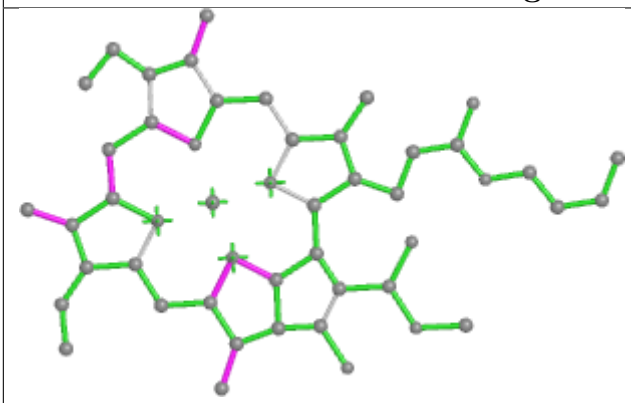
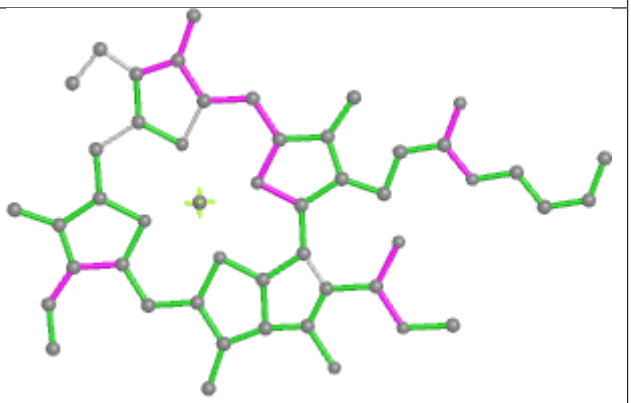
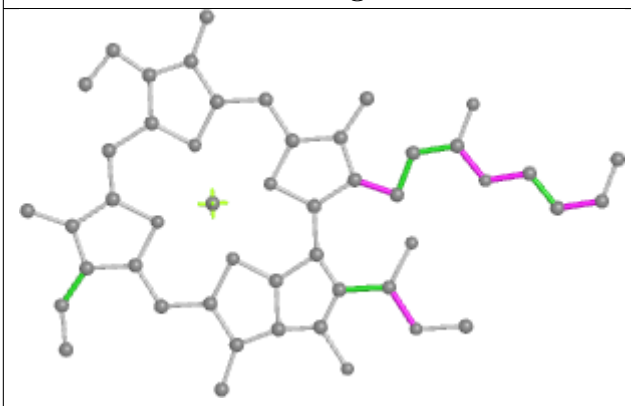
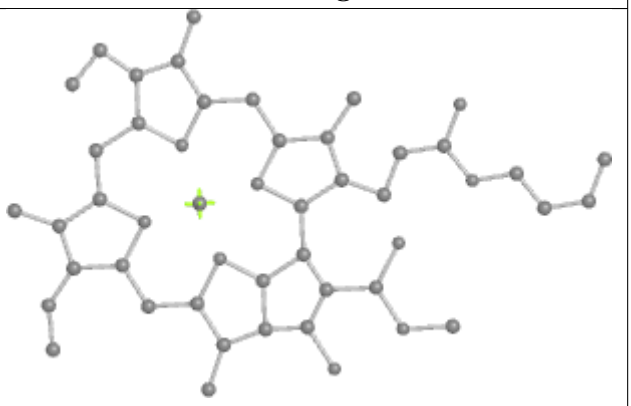
Bond angles

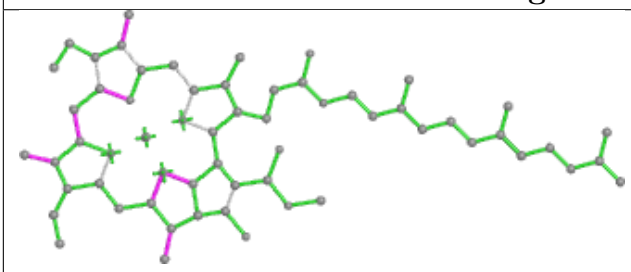
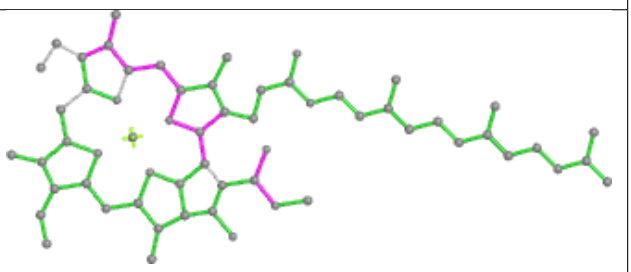
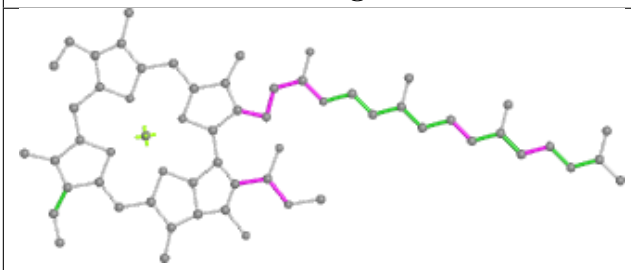
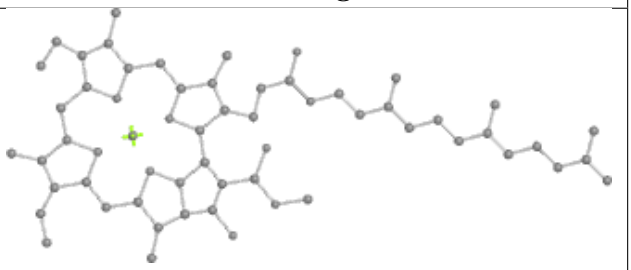


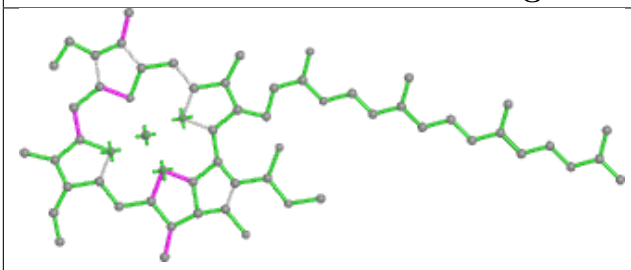
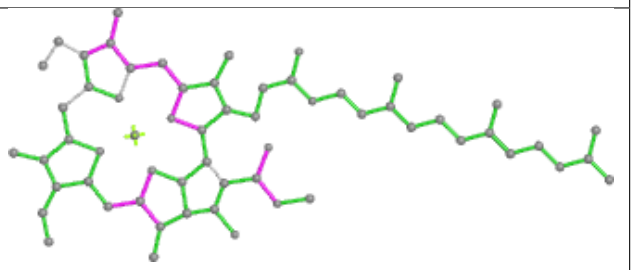
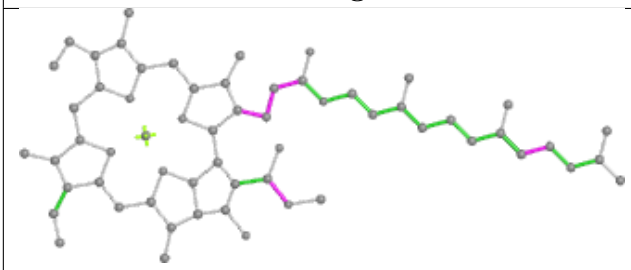
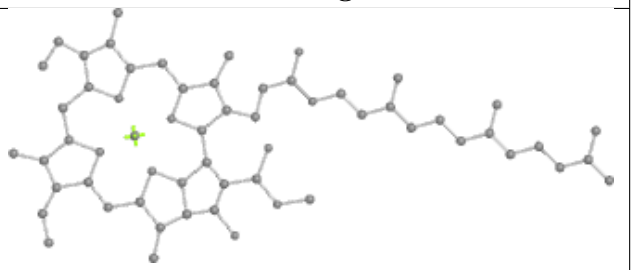
Torsions

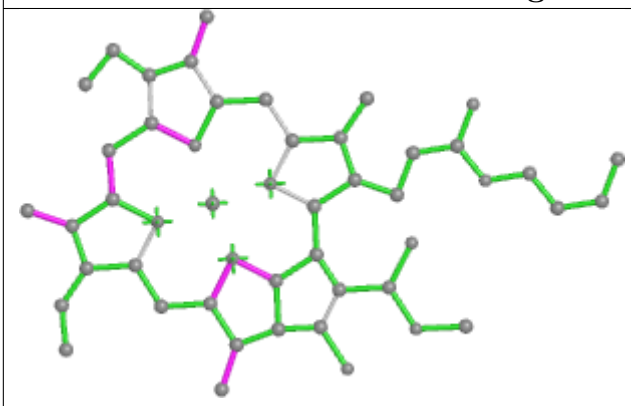
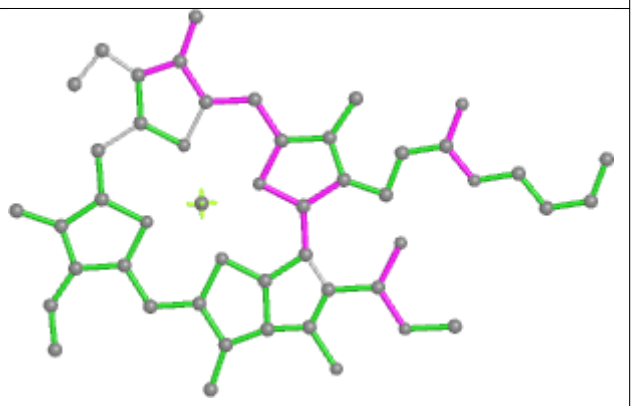
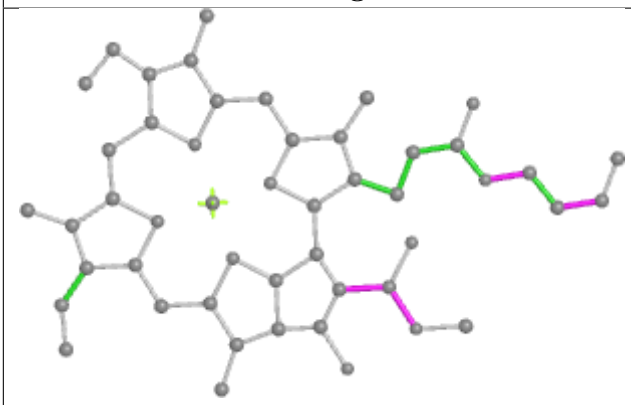
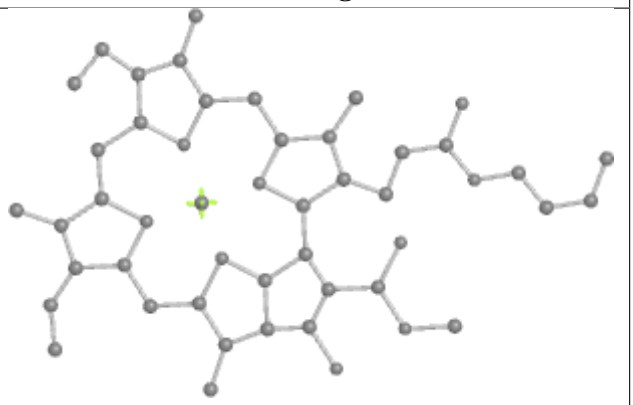


Rings

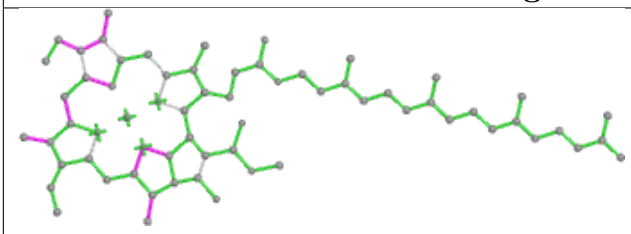
Ligand CLA R 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 301



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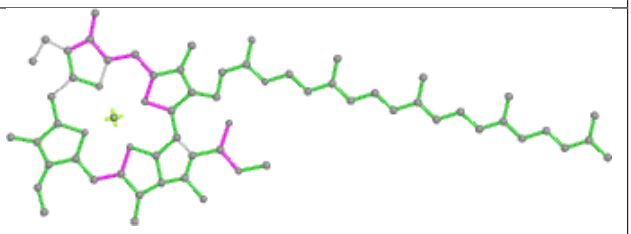
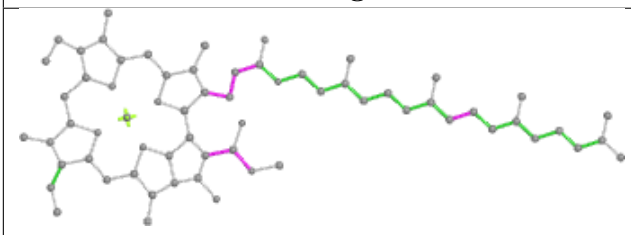


Bond angles



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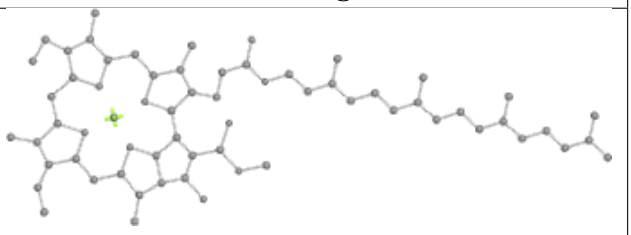
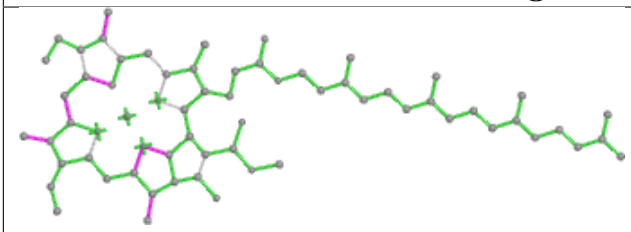


Rings

Ligand CLA n 301



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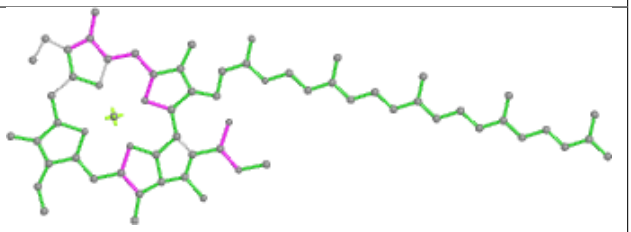
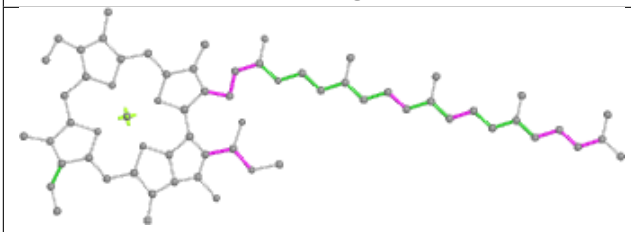


Bond angles



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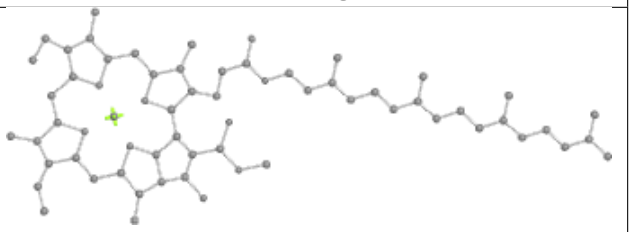
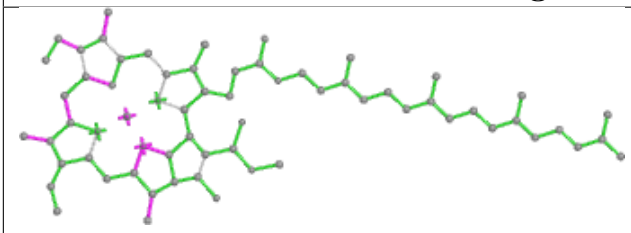


Rings

Ligand CLA c 504



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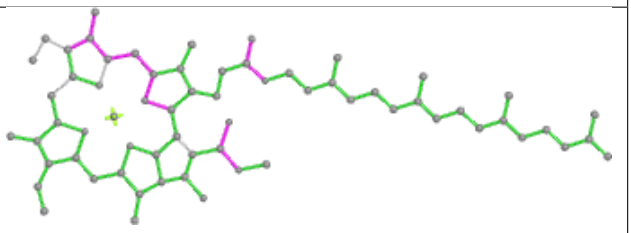

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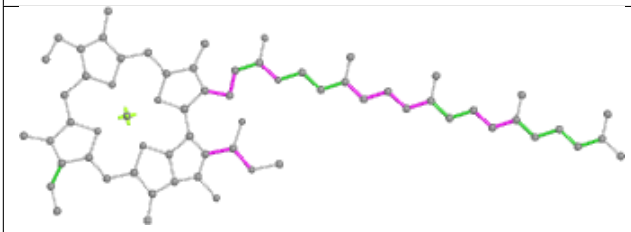

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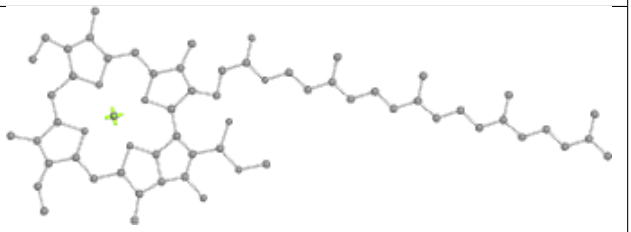
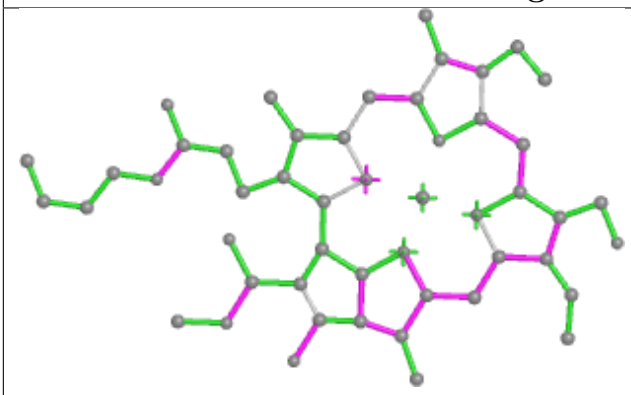
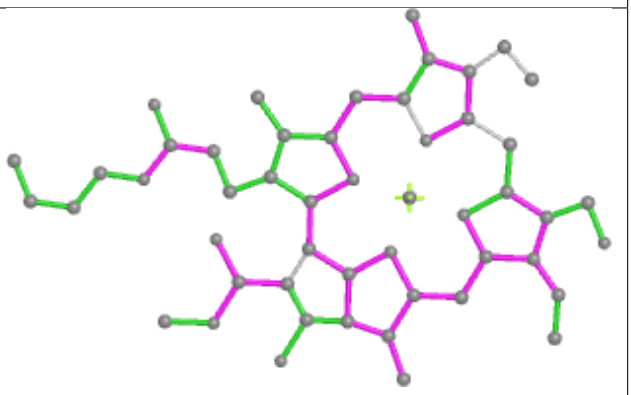
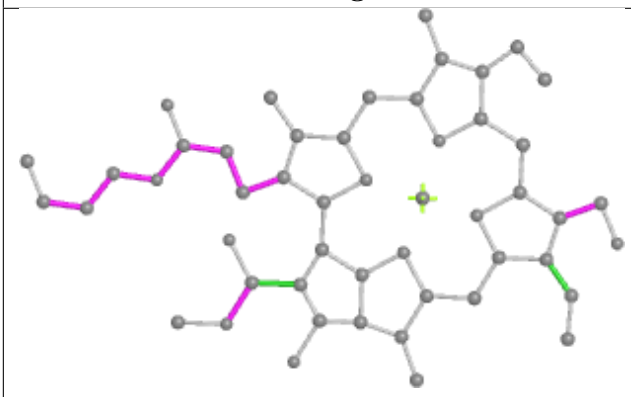
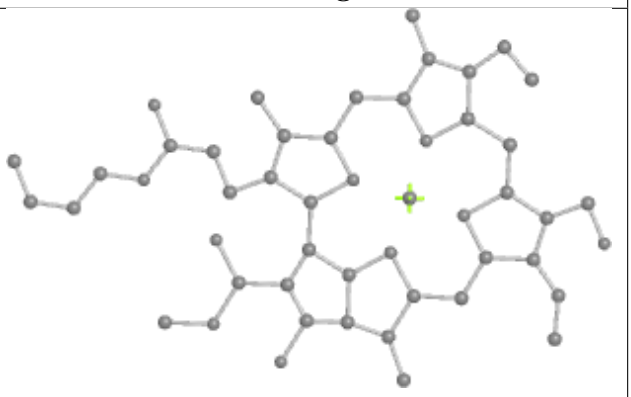
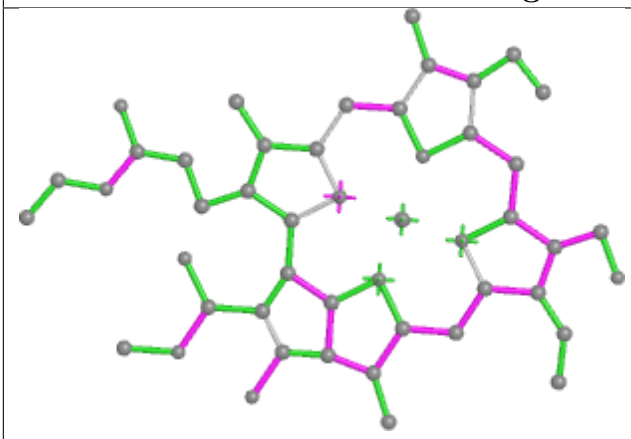


Rings

Ligand CHL 3 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 312



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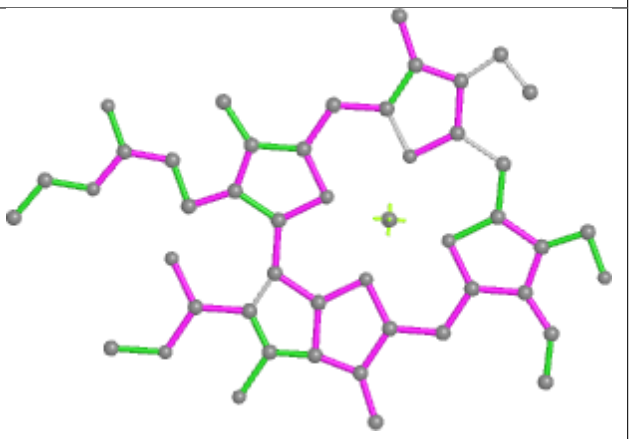
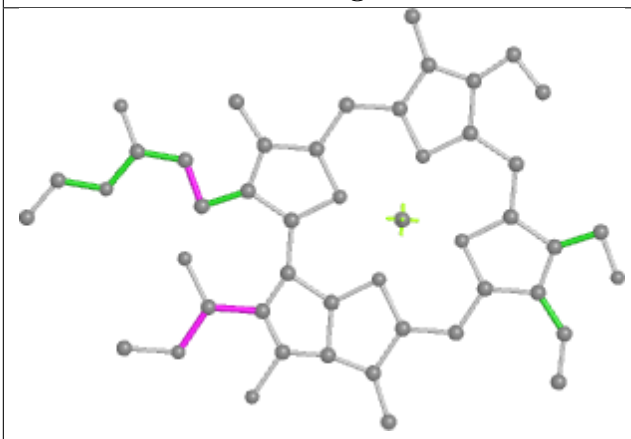


Bond angles



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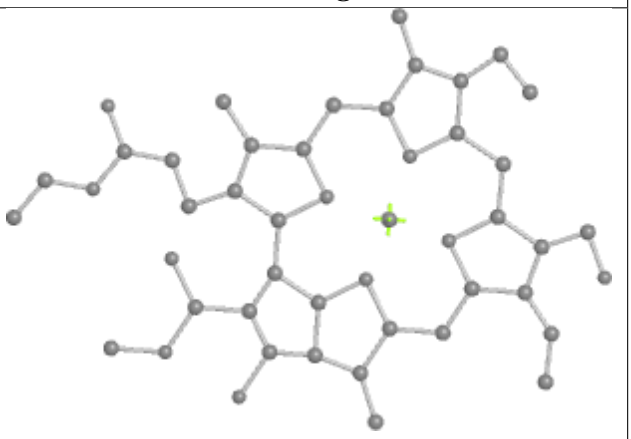
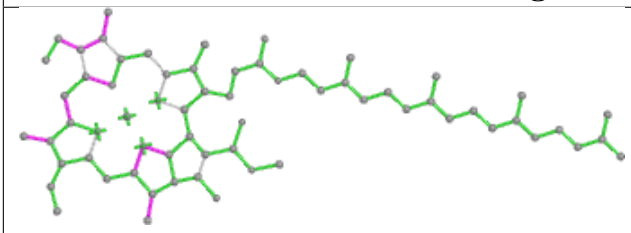


Rings

Ligand CLA c 505



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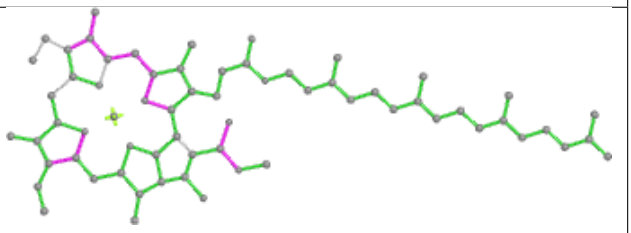
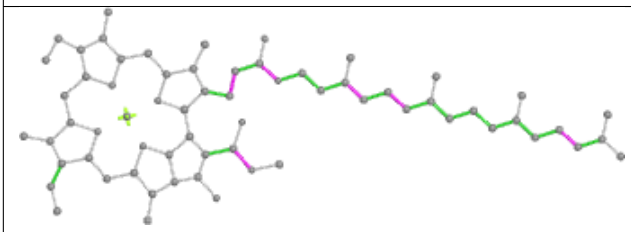


Bond angles



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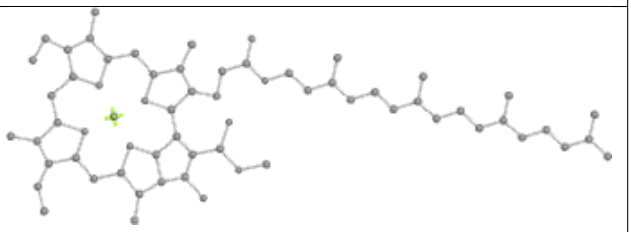

Rings

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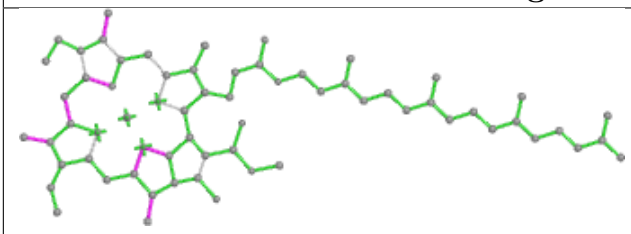
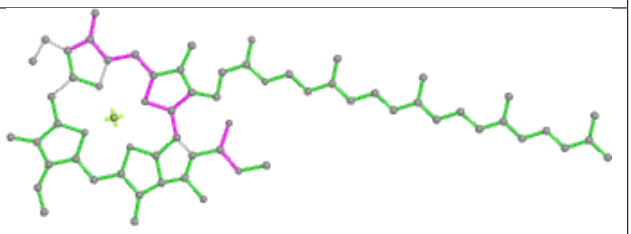
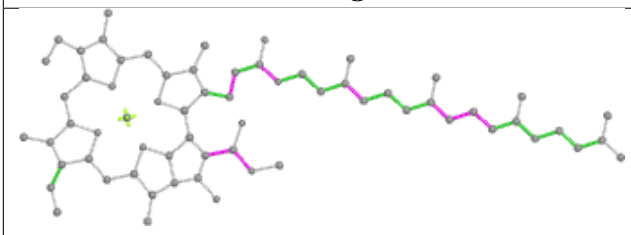
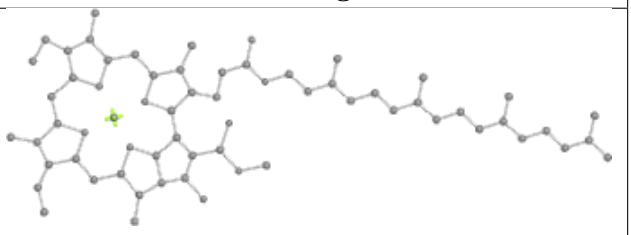
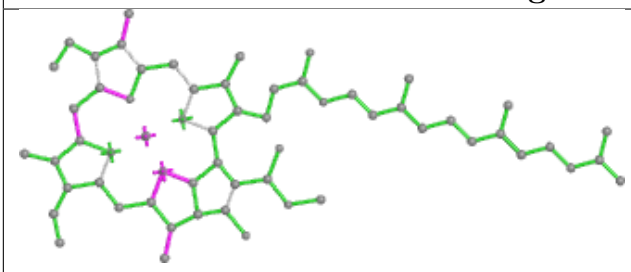
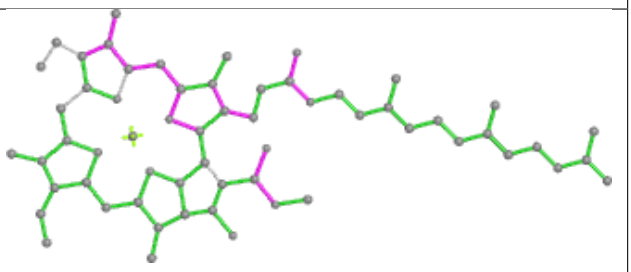
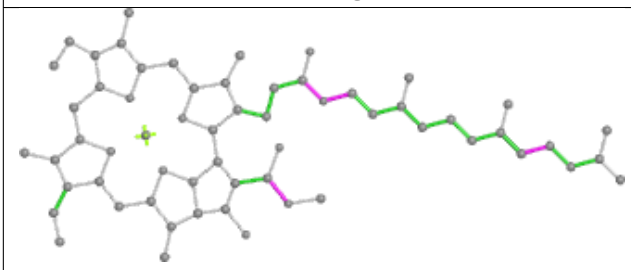
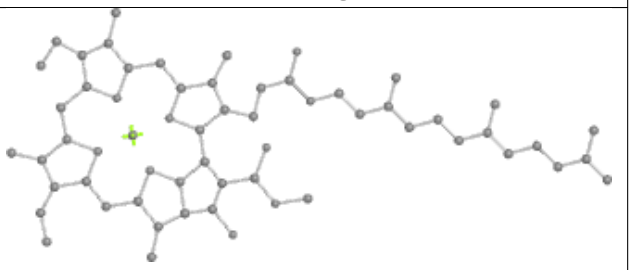
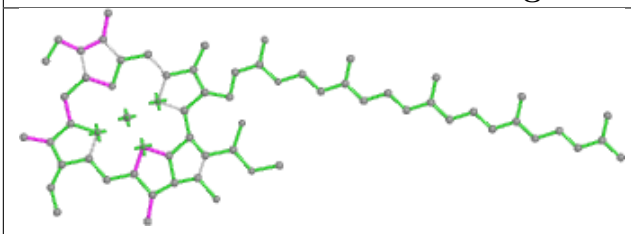
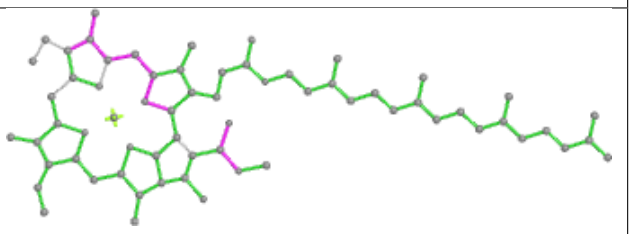
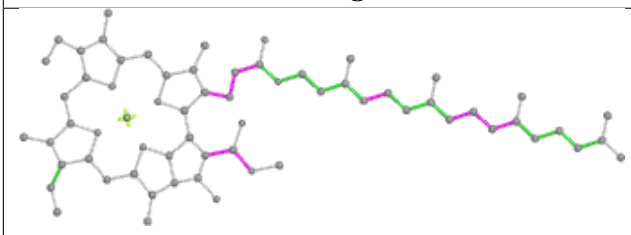
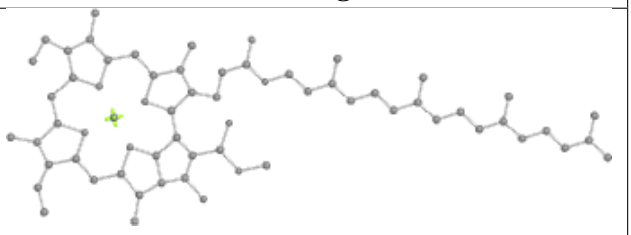
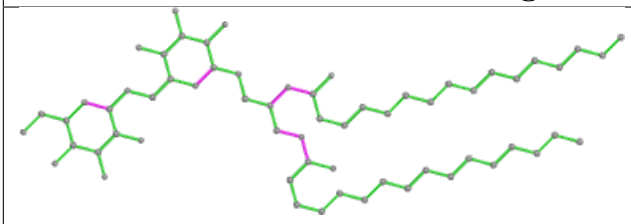
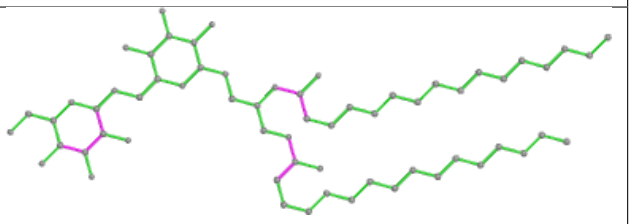
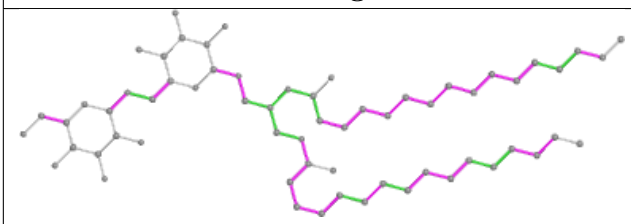
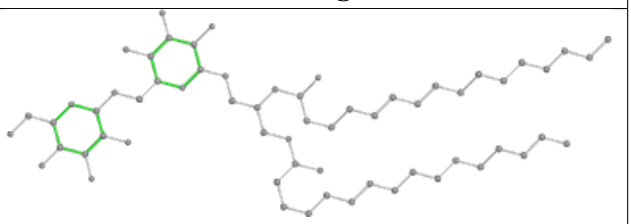
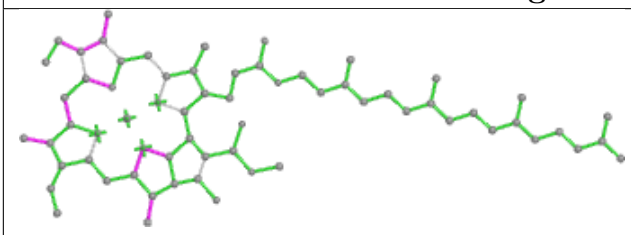
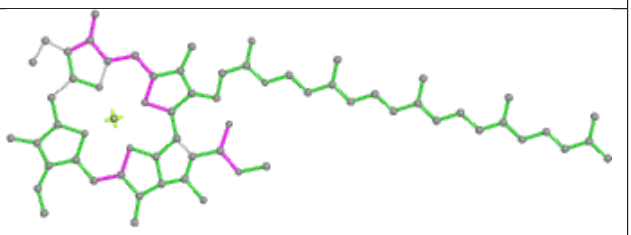
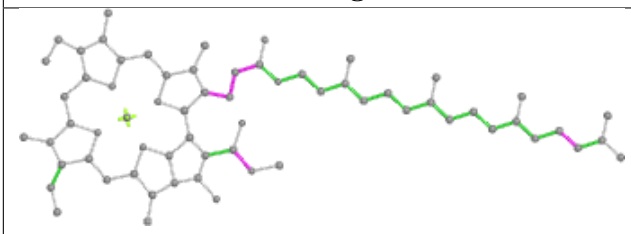
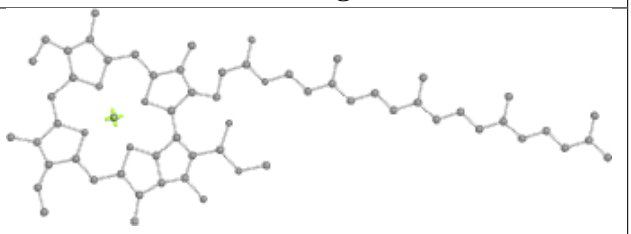
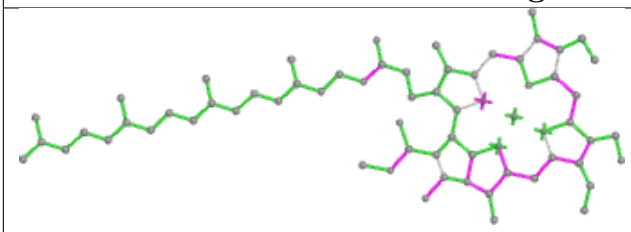
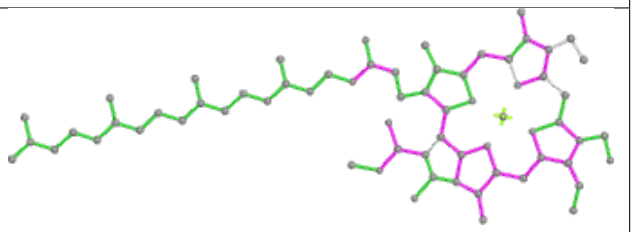
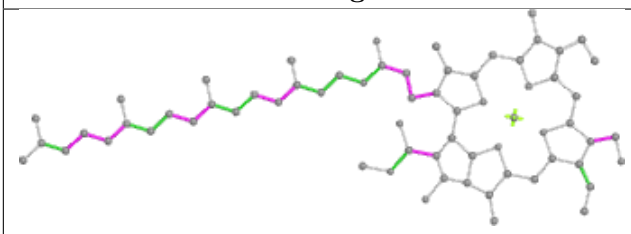
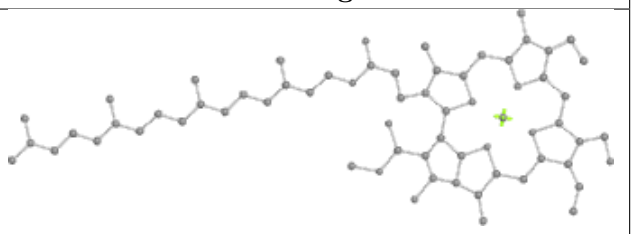
 Bond lengths	 Bond angles
 Torsions	 Rings

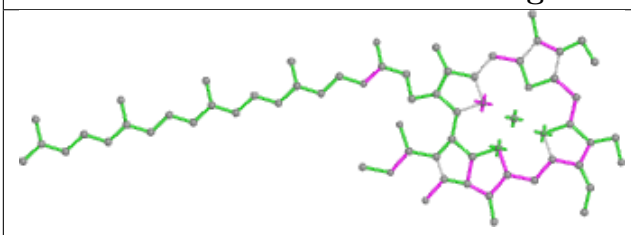
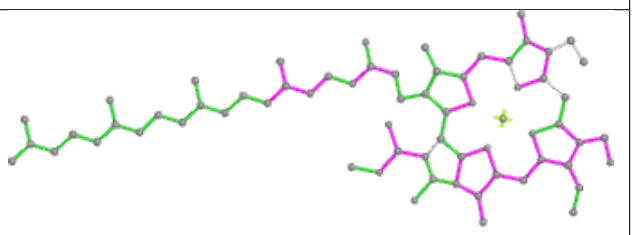
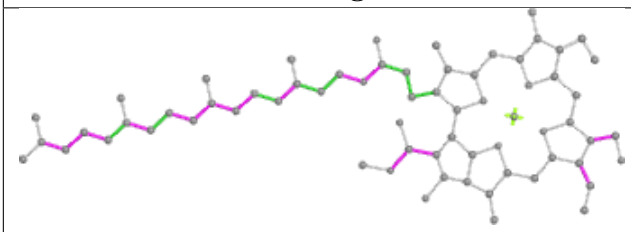
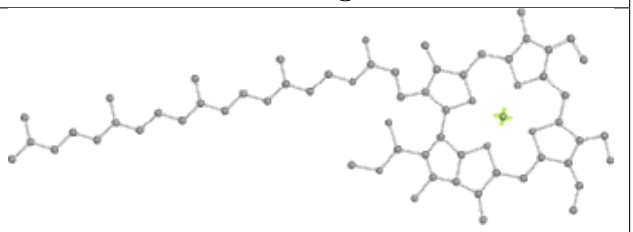
Ligand CLA 4 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

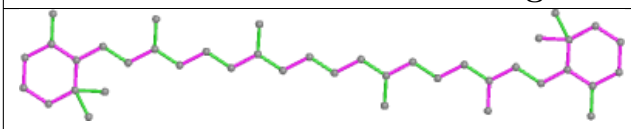
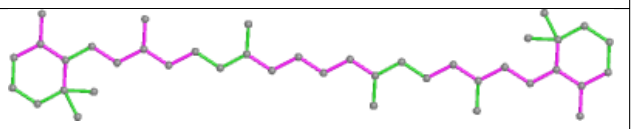
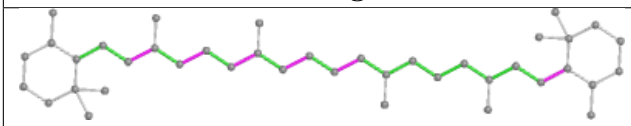
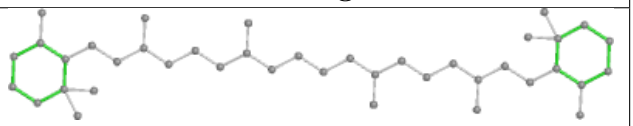
Ligand CLA V 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

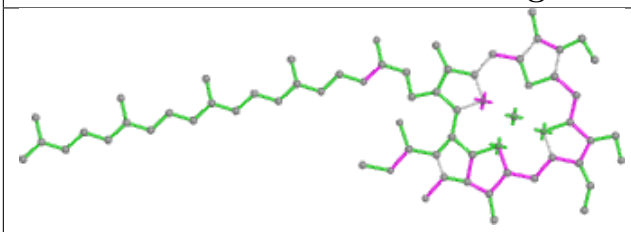
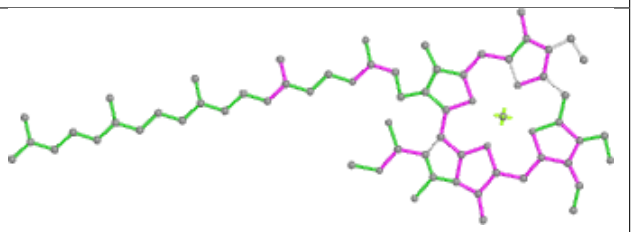
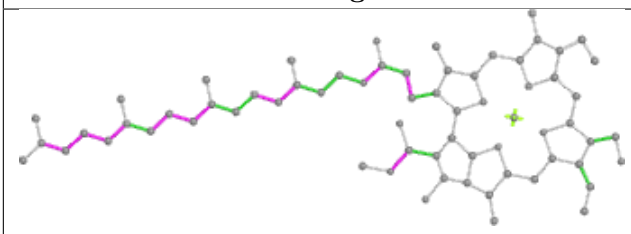
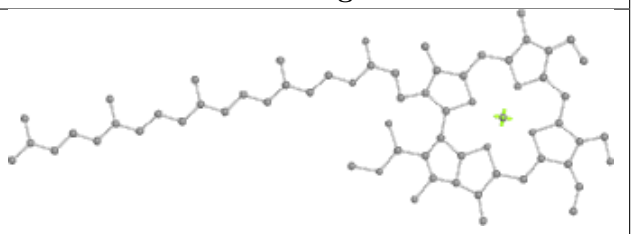
Ligand DGD C 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

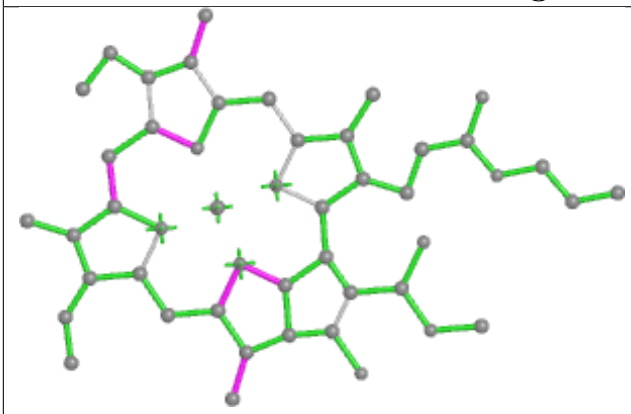
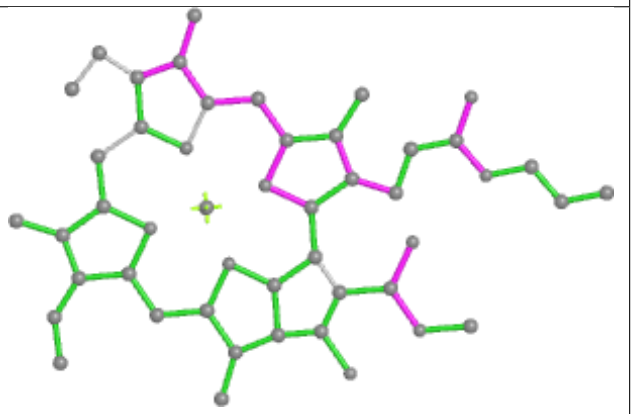
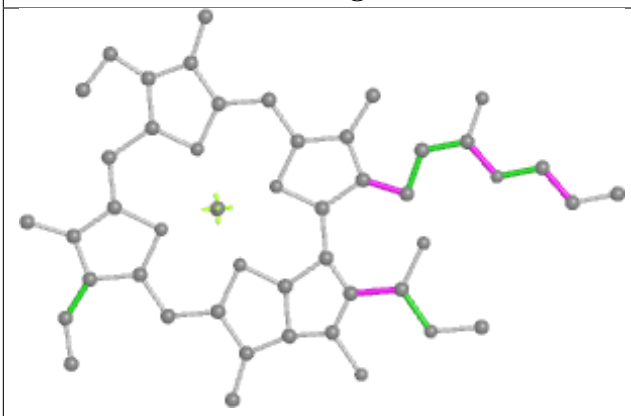
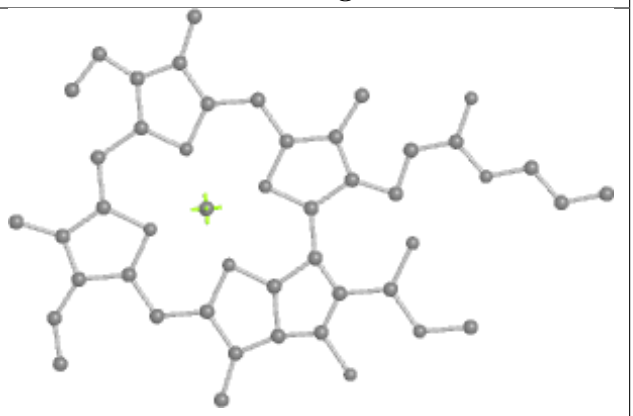
Ligand CLA 1 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 5 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

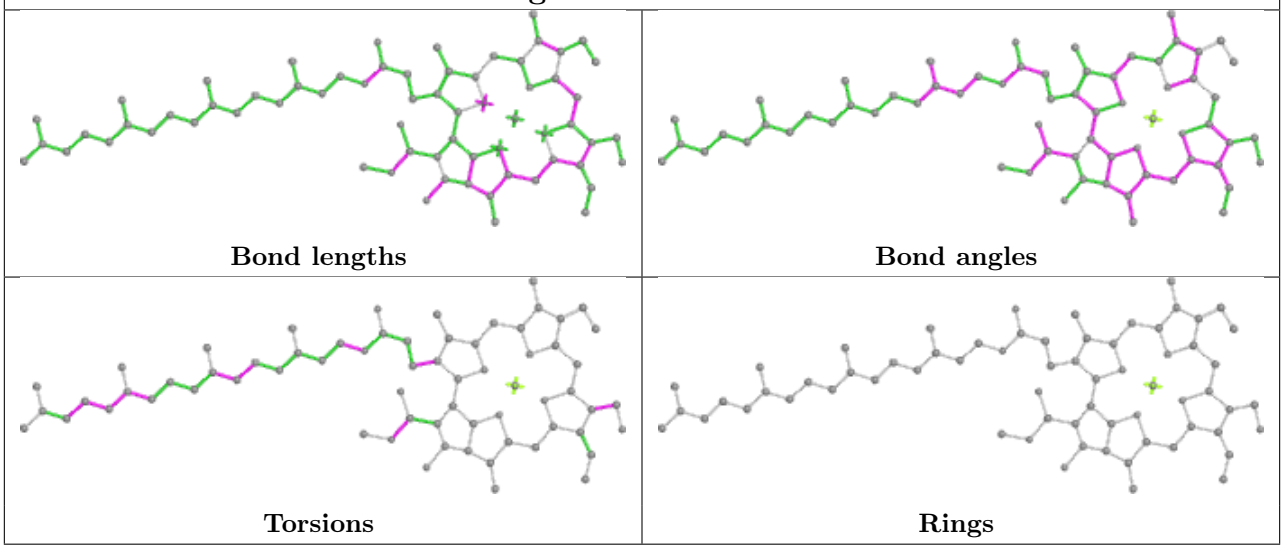
Ligand CHL n 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR x 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

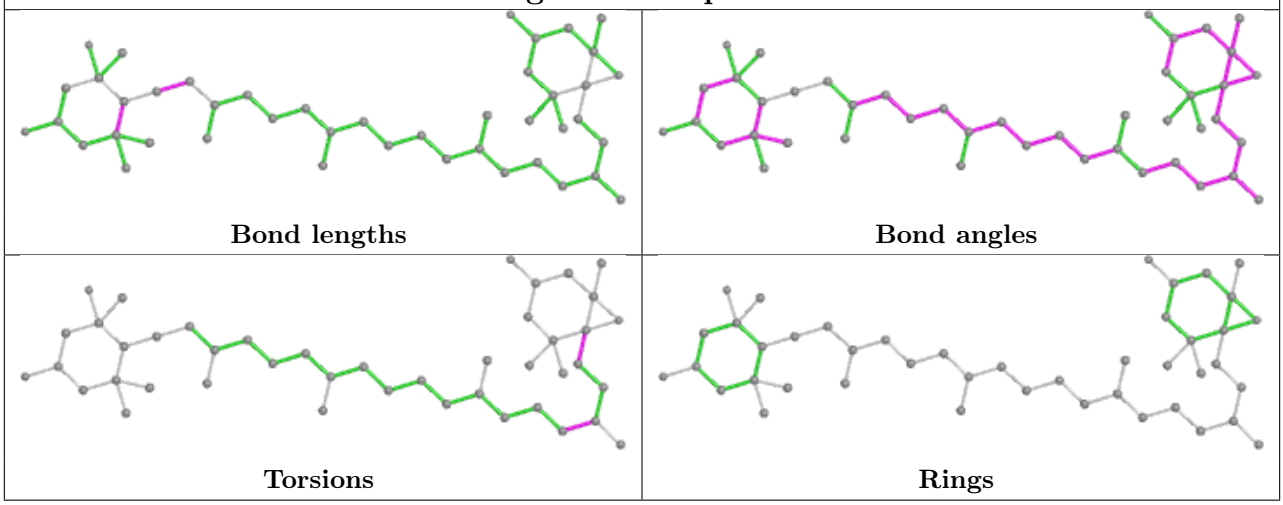
Ligand CHL 3 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

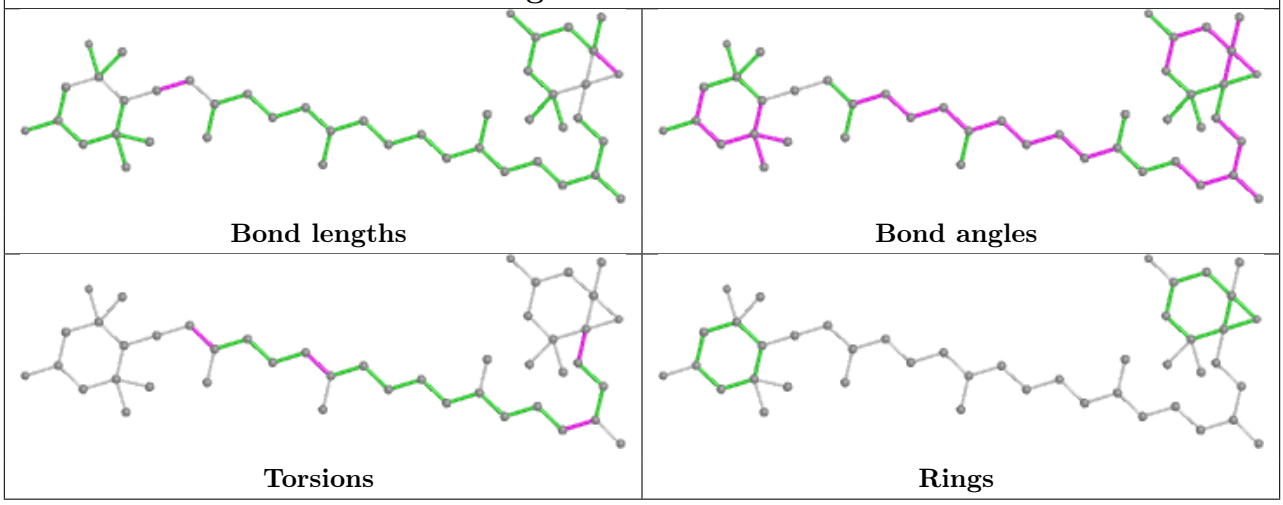
Ligand CHL 1 318



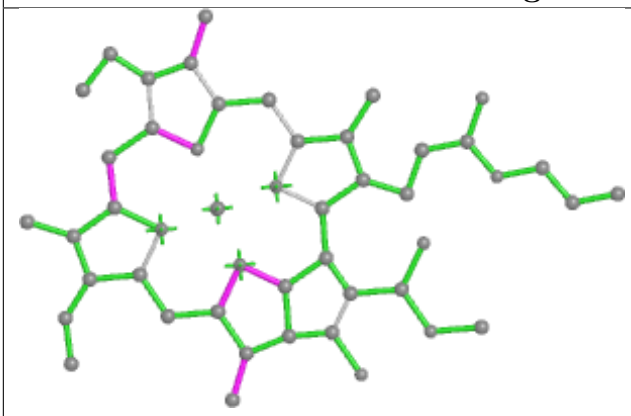
Ligand NEX p 301



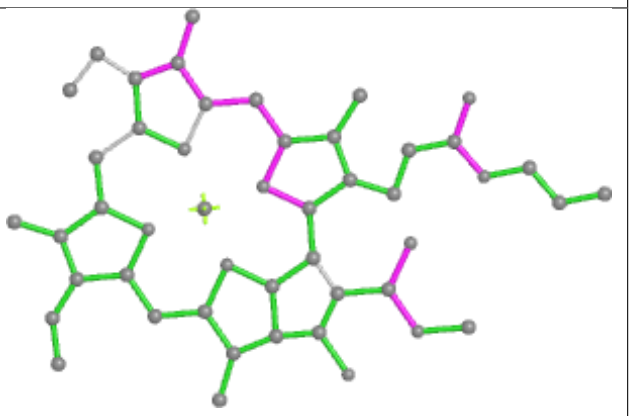
Ligand NEX n 319



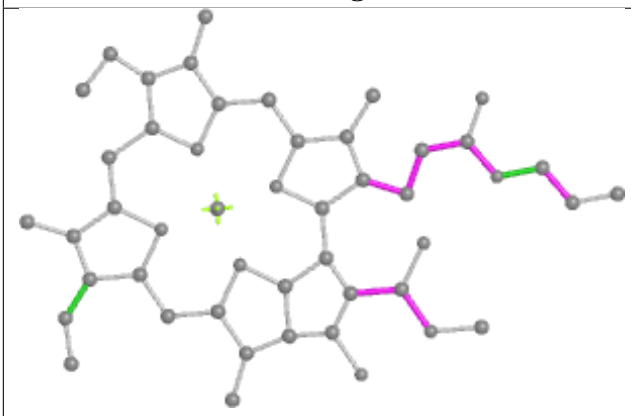
Ligand CLA N 308



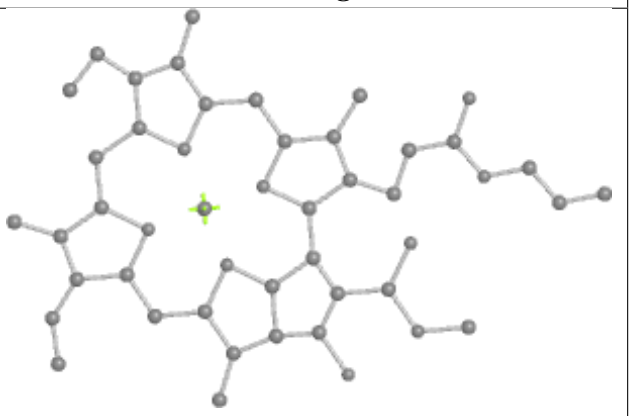
Bond lengths



Bond angles

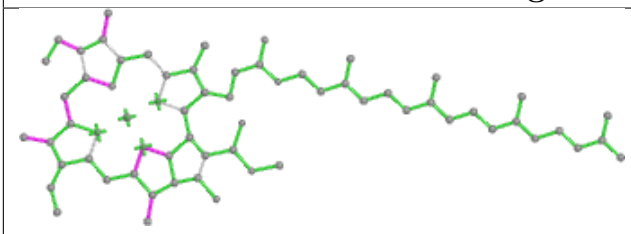


Torsions

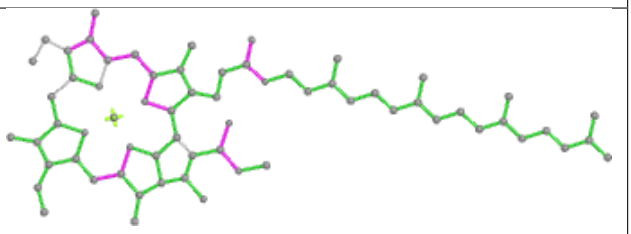


Rings

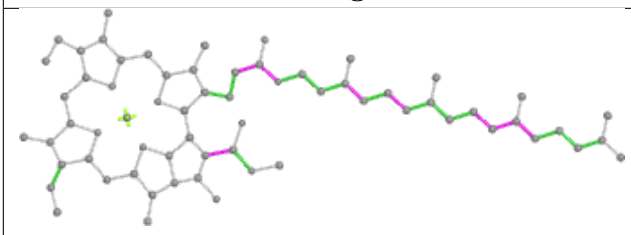
Ligand CLA v 302



Bond lengths



Bond angles



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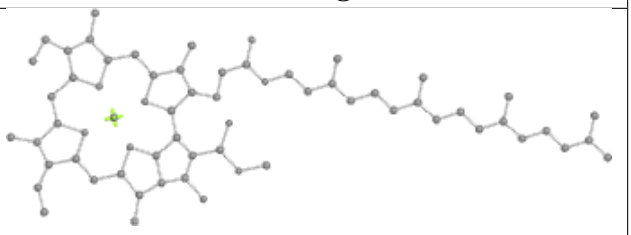
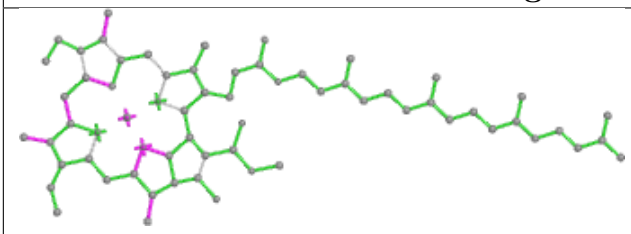
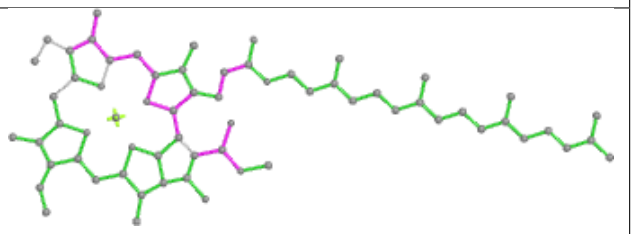
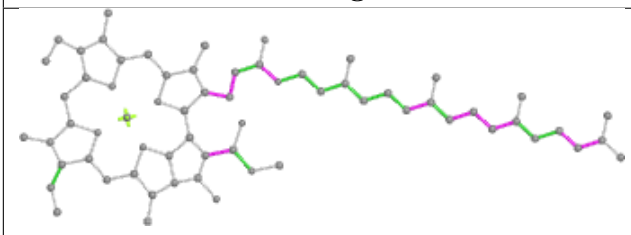
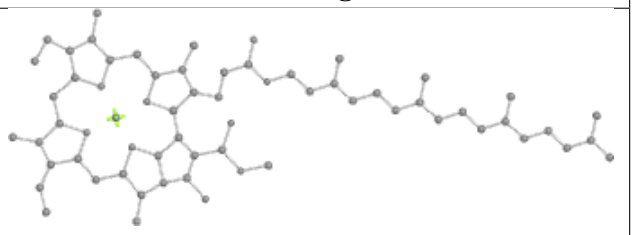
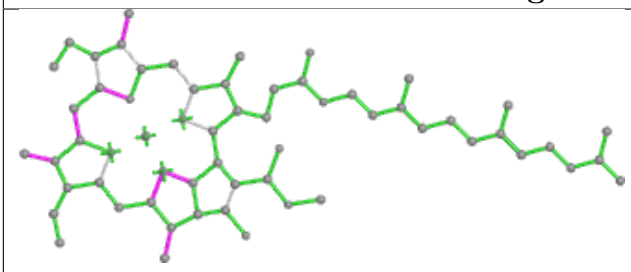
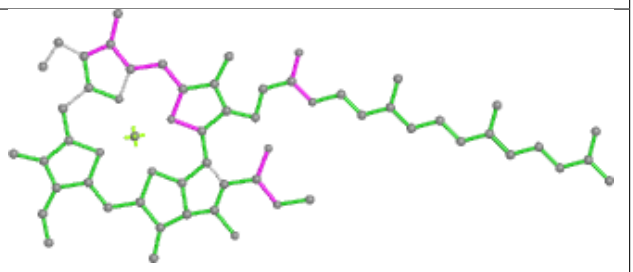
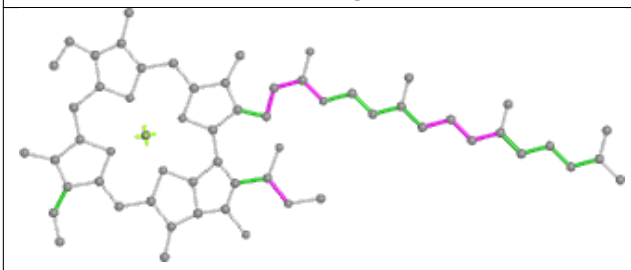
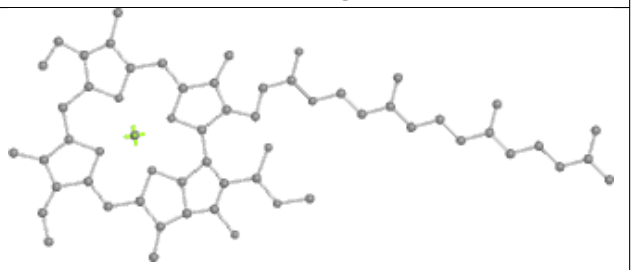
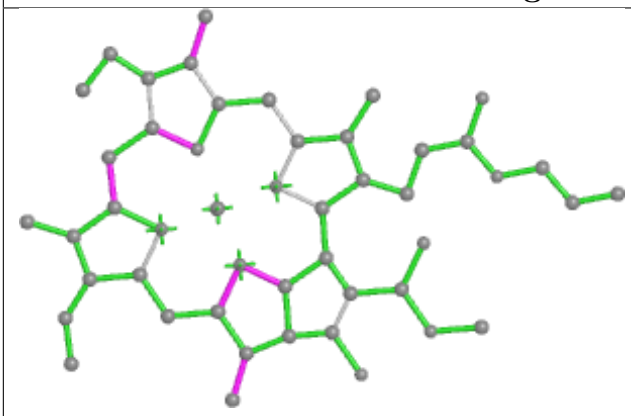


Rings

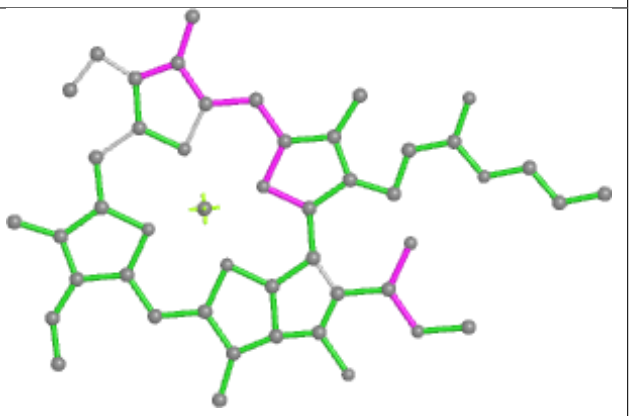
Ligand CLA B 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

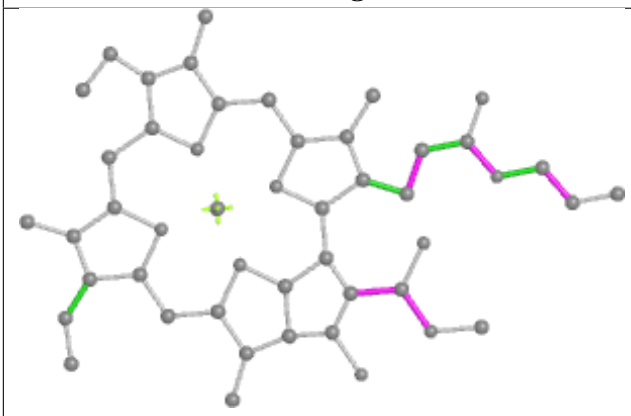
Ligand CLA V 308



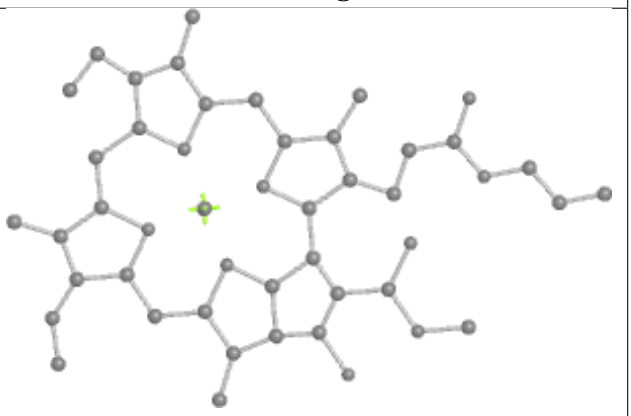
Bond lengths



Bond angles

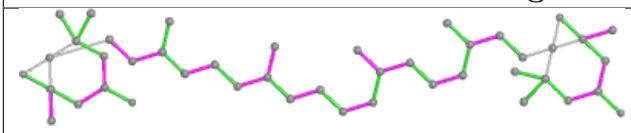


Torsions

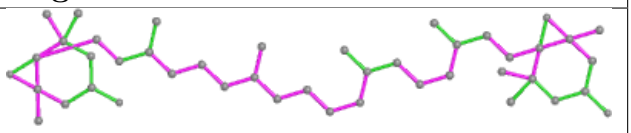


Rings

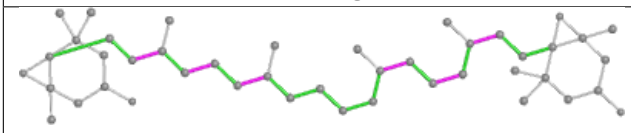
Ligand XAT g 309



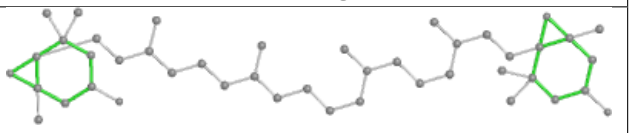
Bond lengths



Bond angles

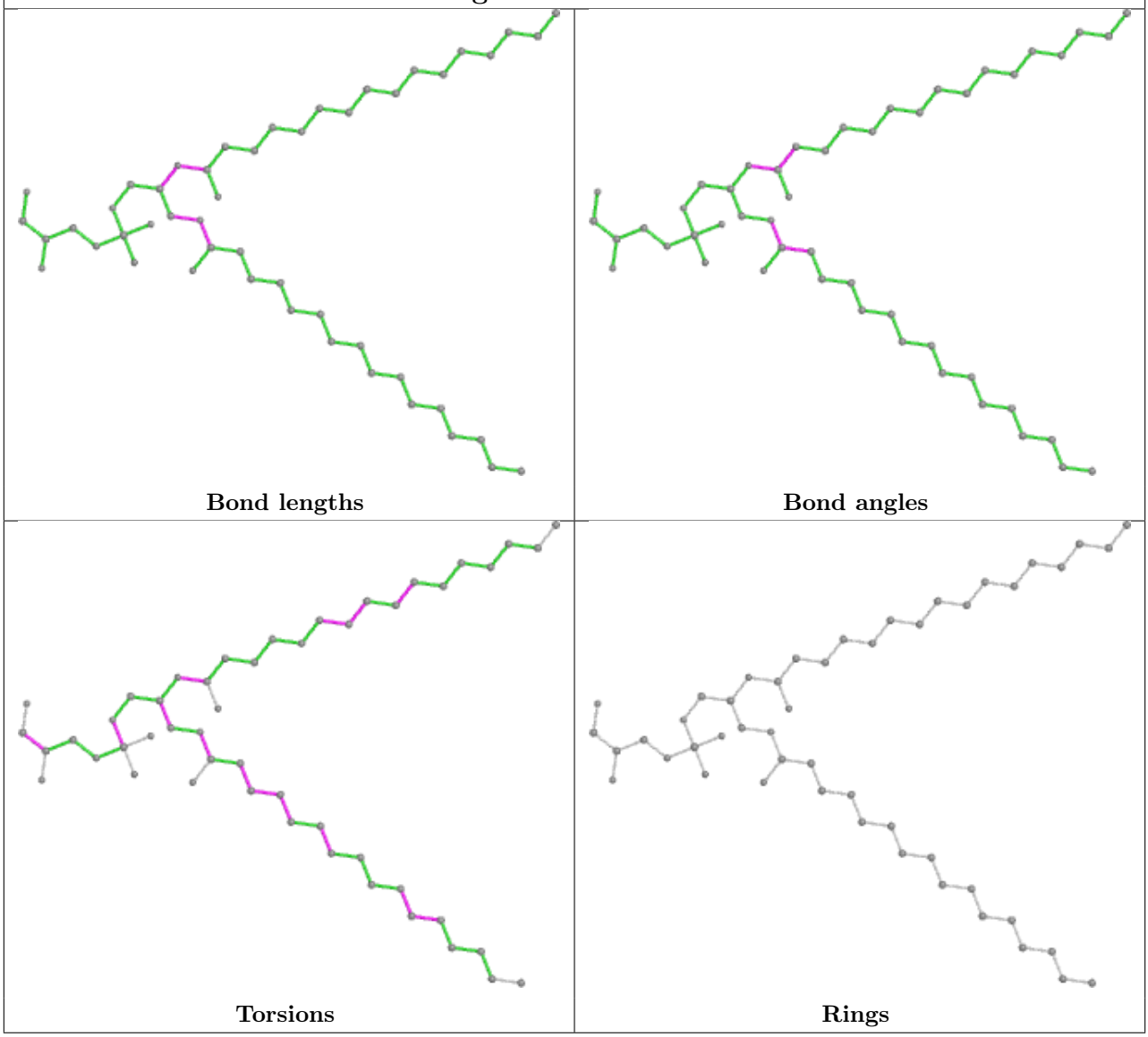


Torsions

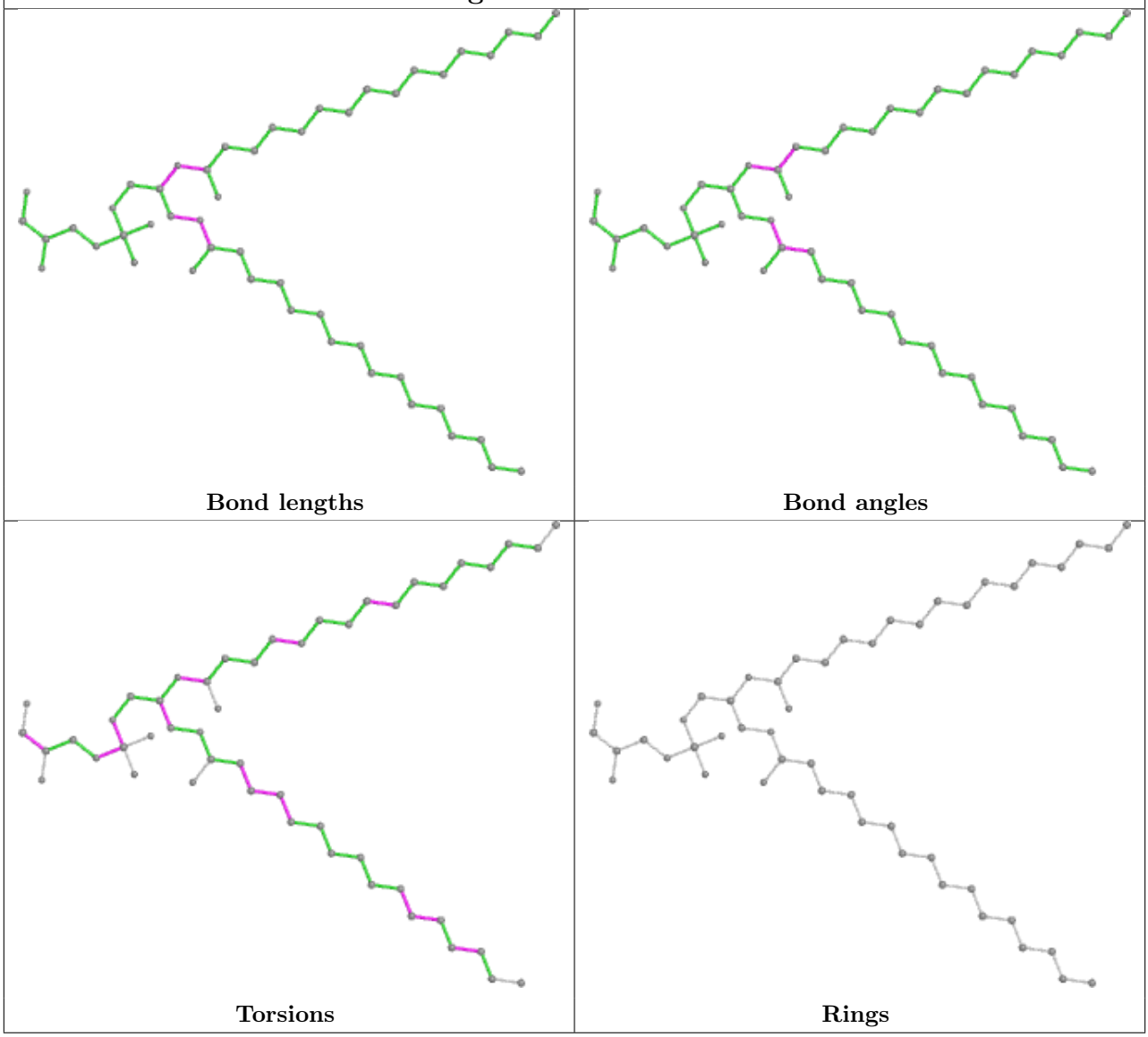


Rings

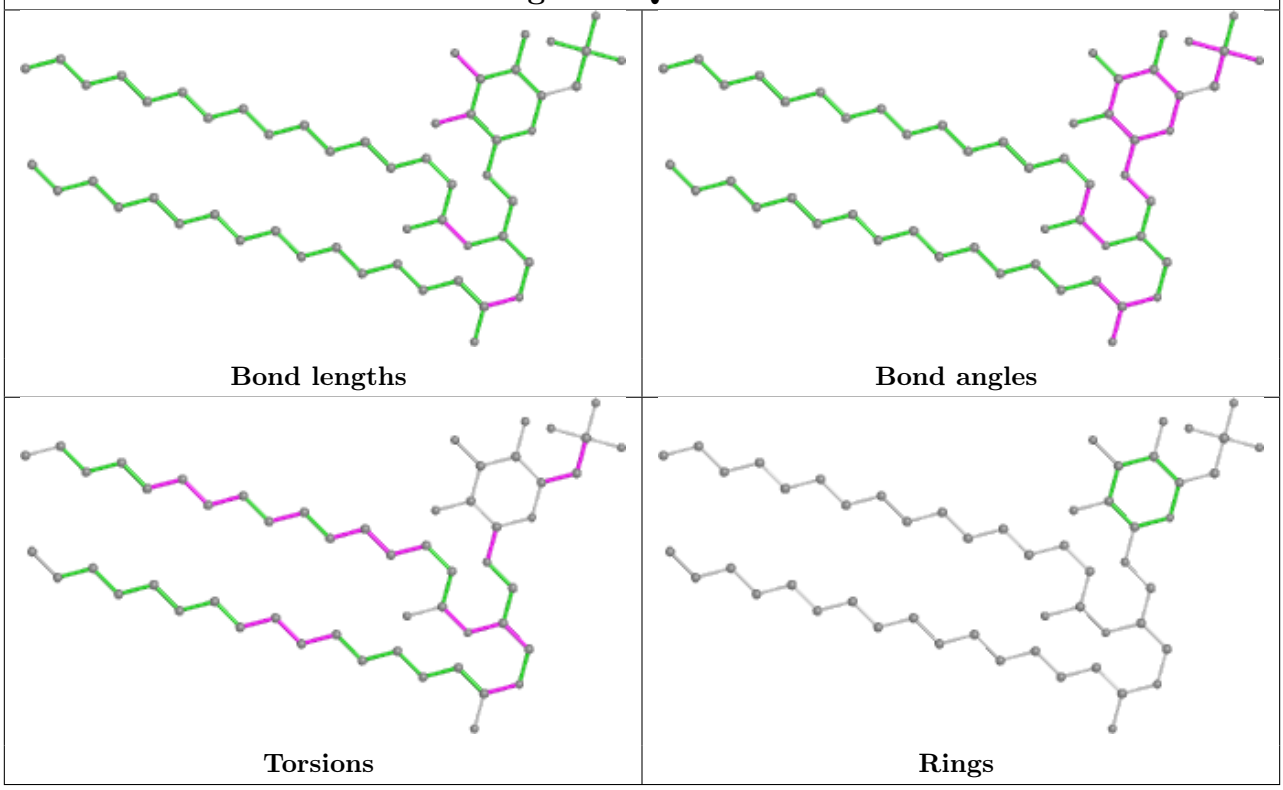
Ligand LHG 6 311



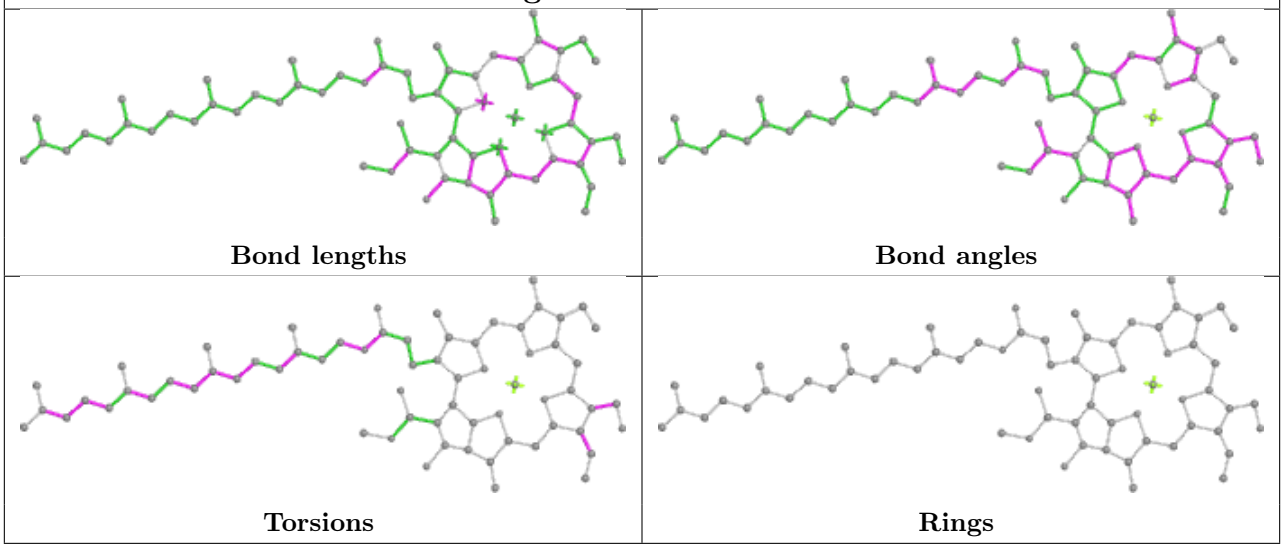
Ligand LHG V 312

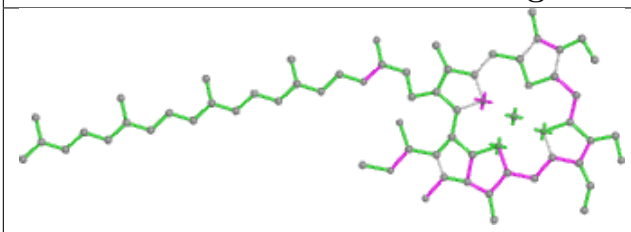
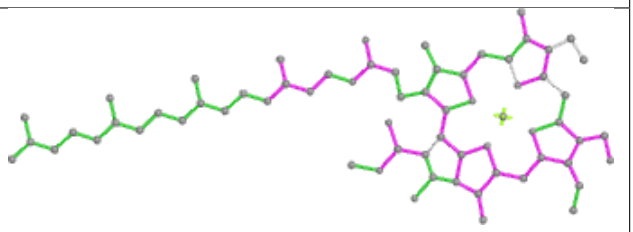
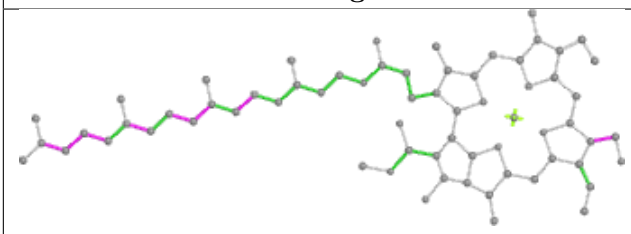
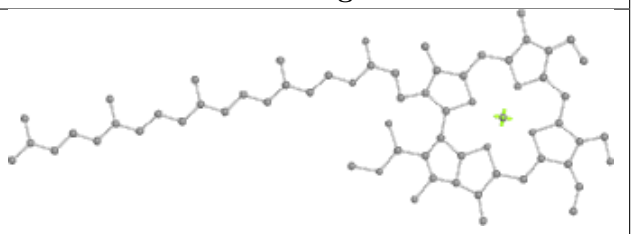


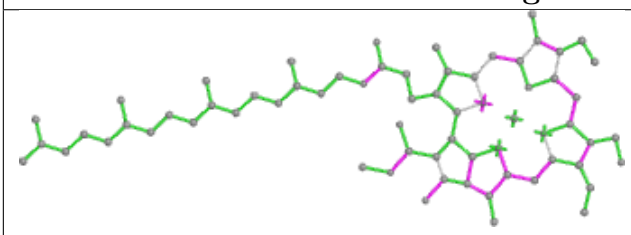
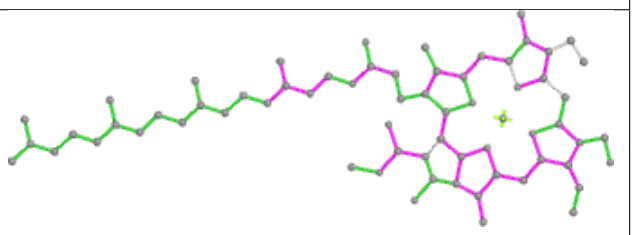
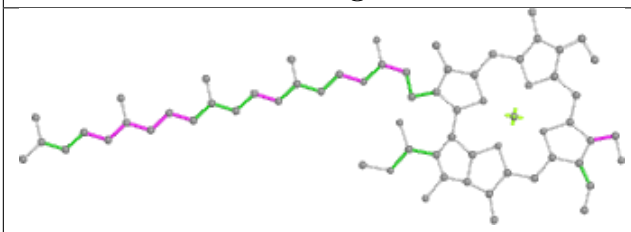
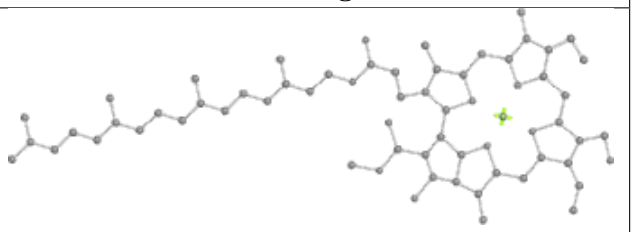
Ligand SQD L 102

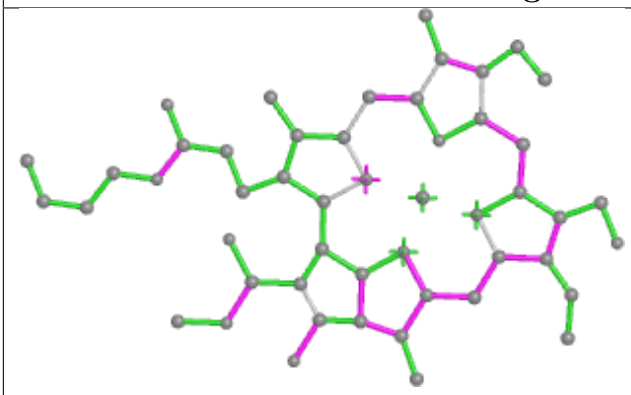
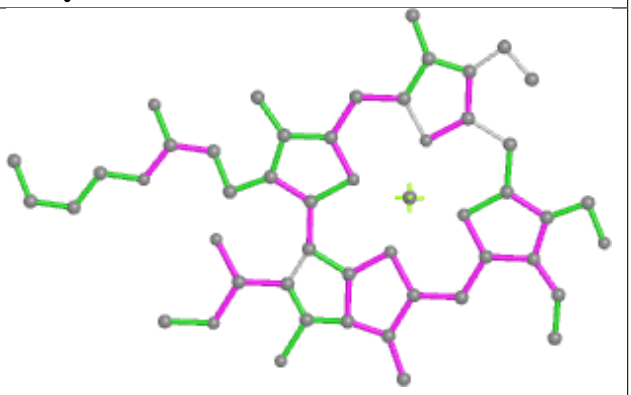
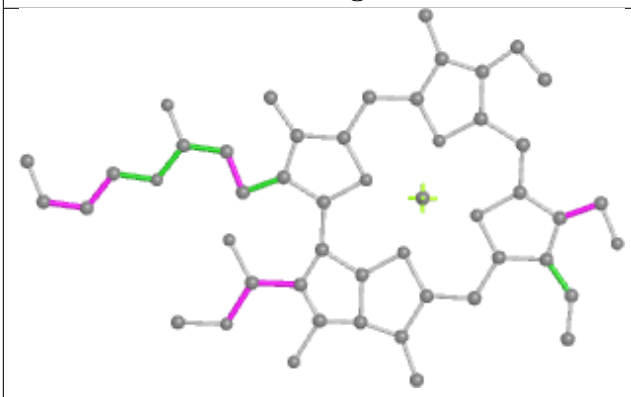
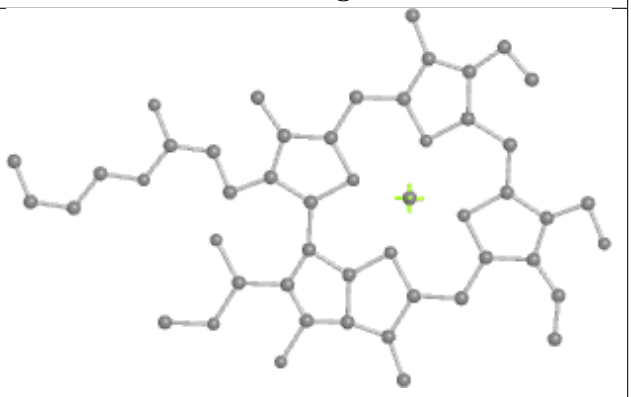


Ligand CHL N 317

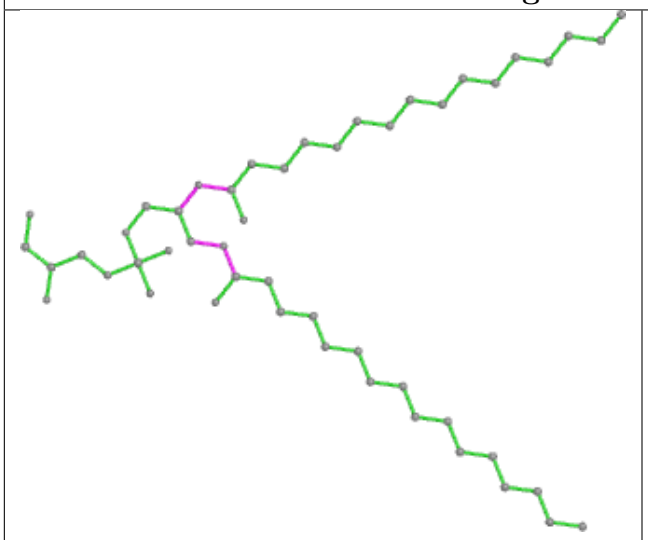


Ligand CHL v 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

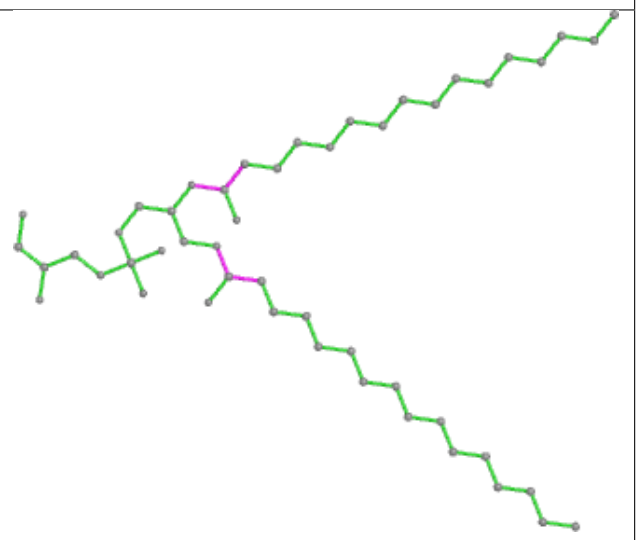
Ligand CHL N 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL Q 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

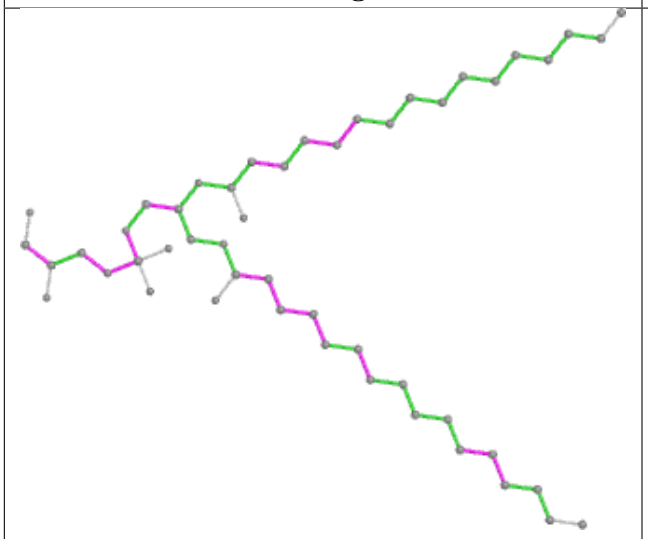
Ligand LHG G 310



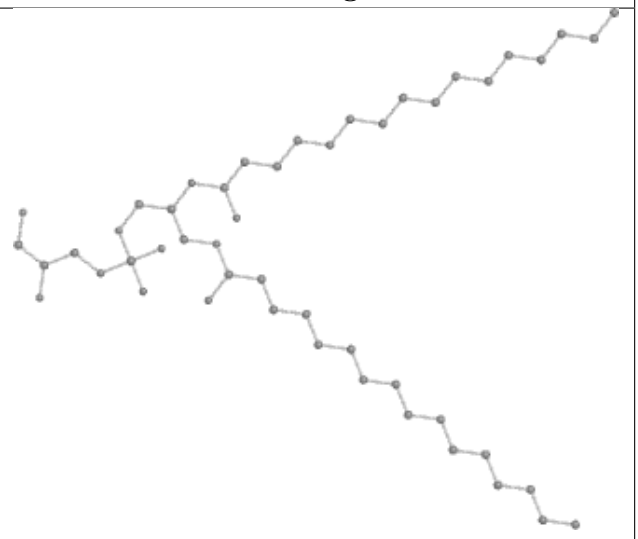
Bond lengths



Bond angles

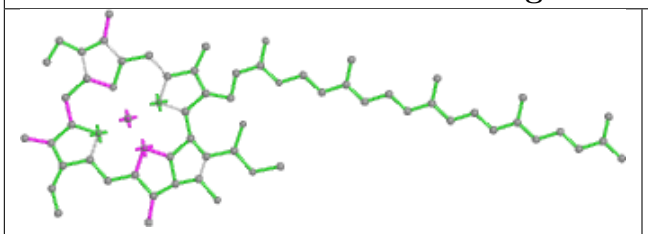


Torsions

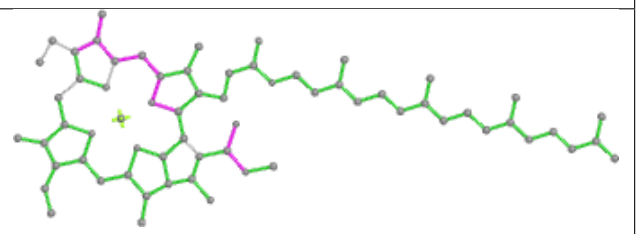


Rings

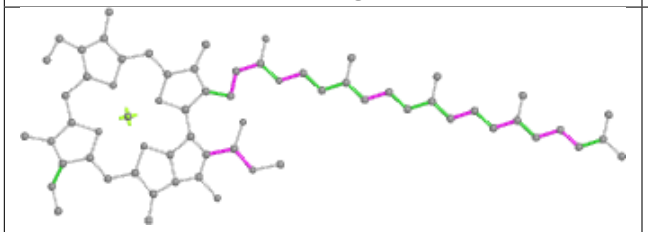
Ligand CLA B 609



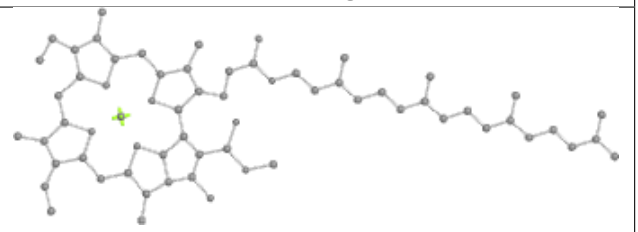
Bond lengths



Bond angles

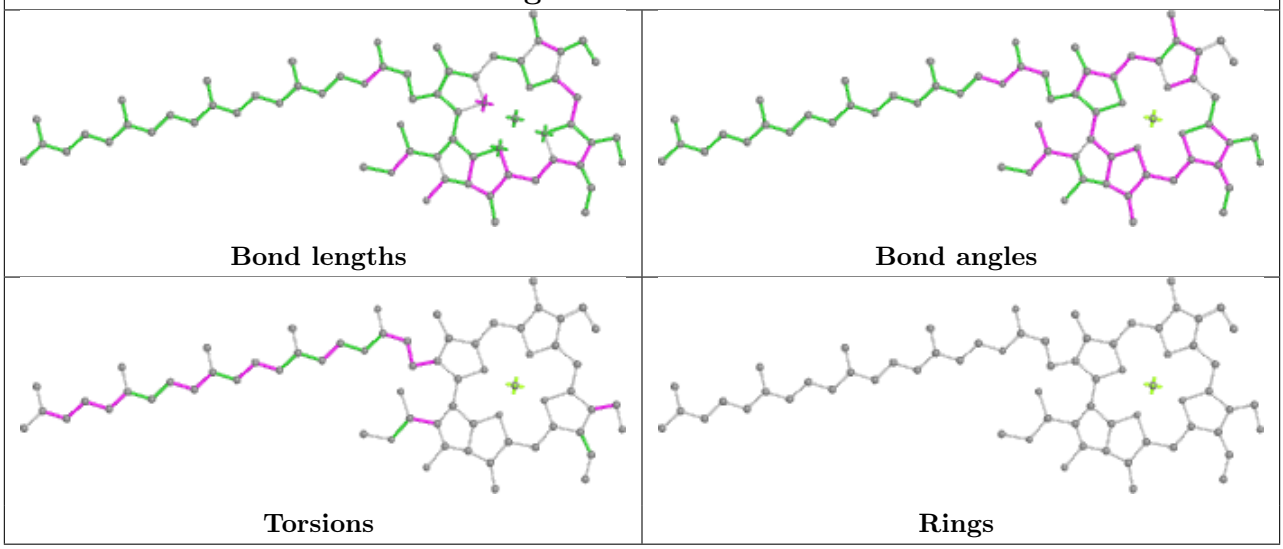


Torsions

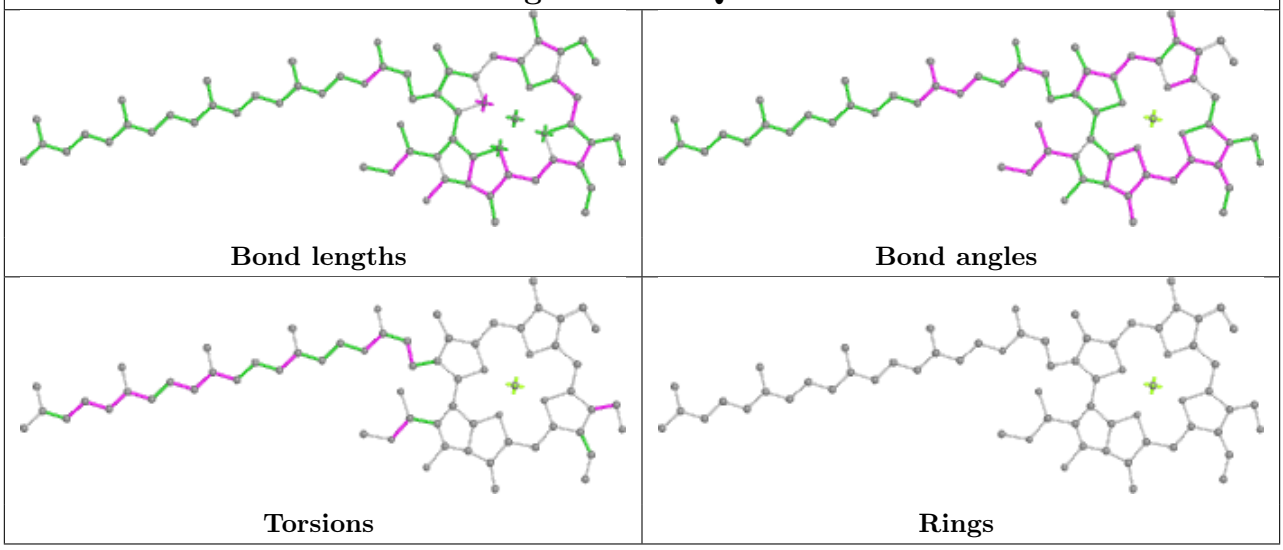


Rings

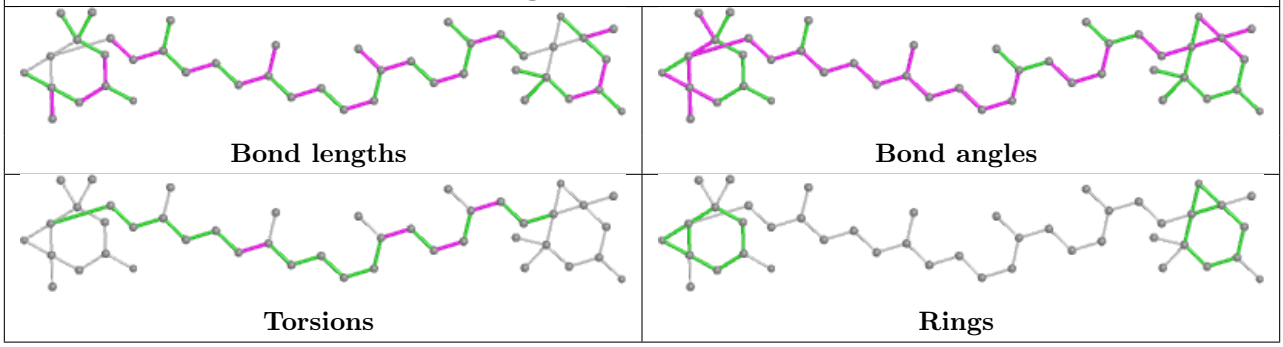
Ligand CHL U 319

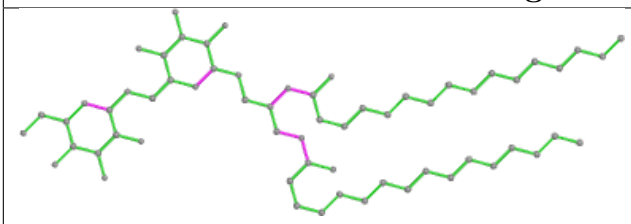
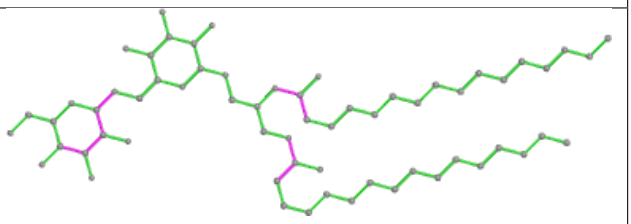
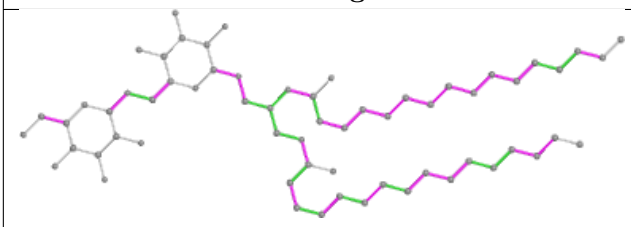
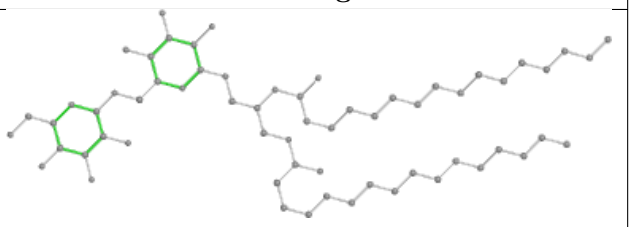


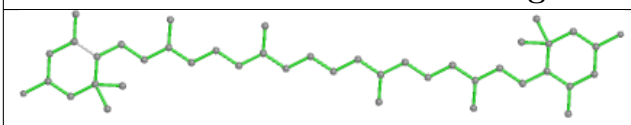
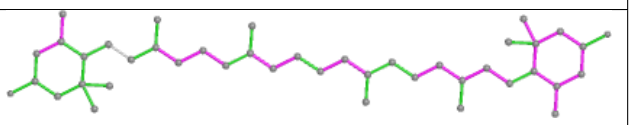
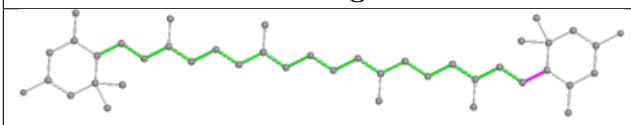
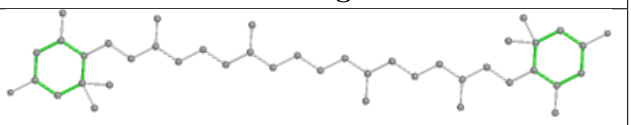
Ligand CHL Q 314

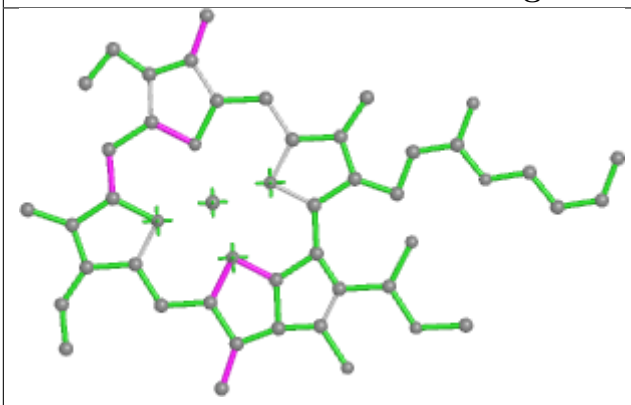
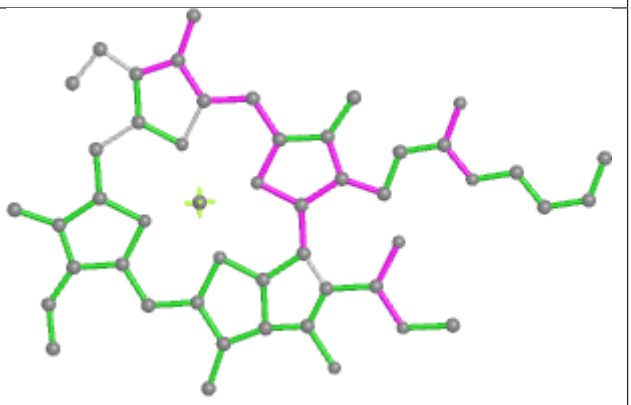
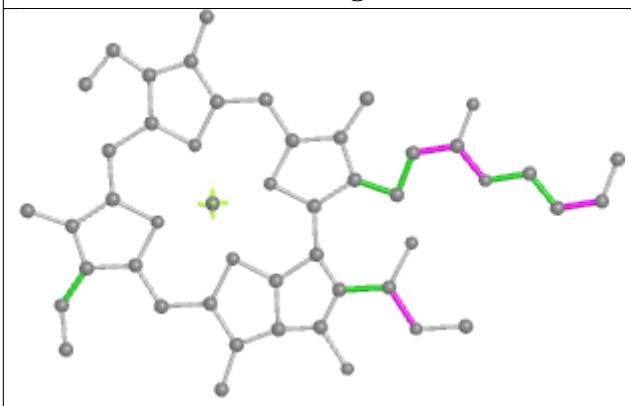
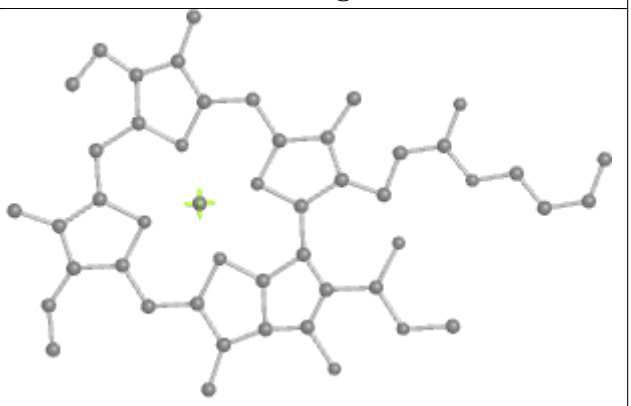


Ligand XAT U 311

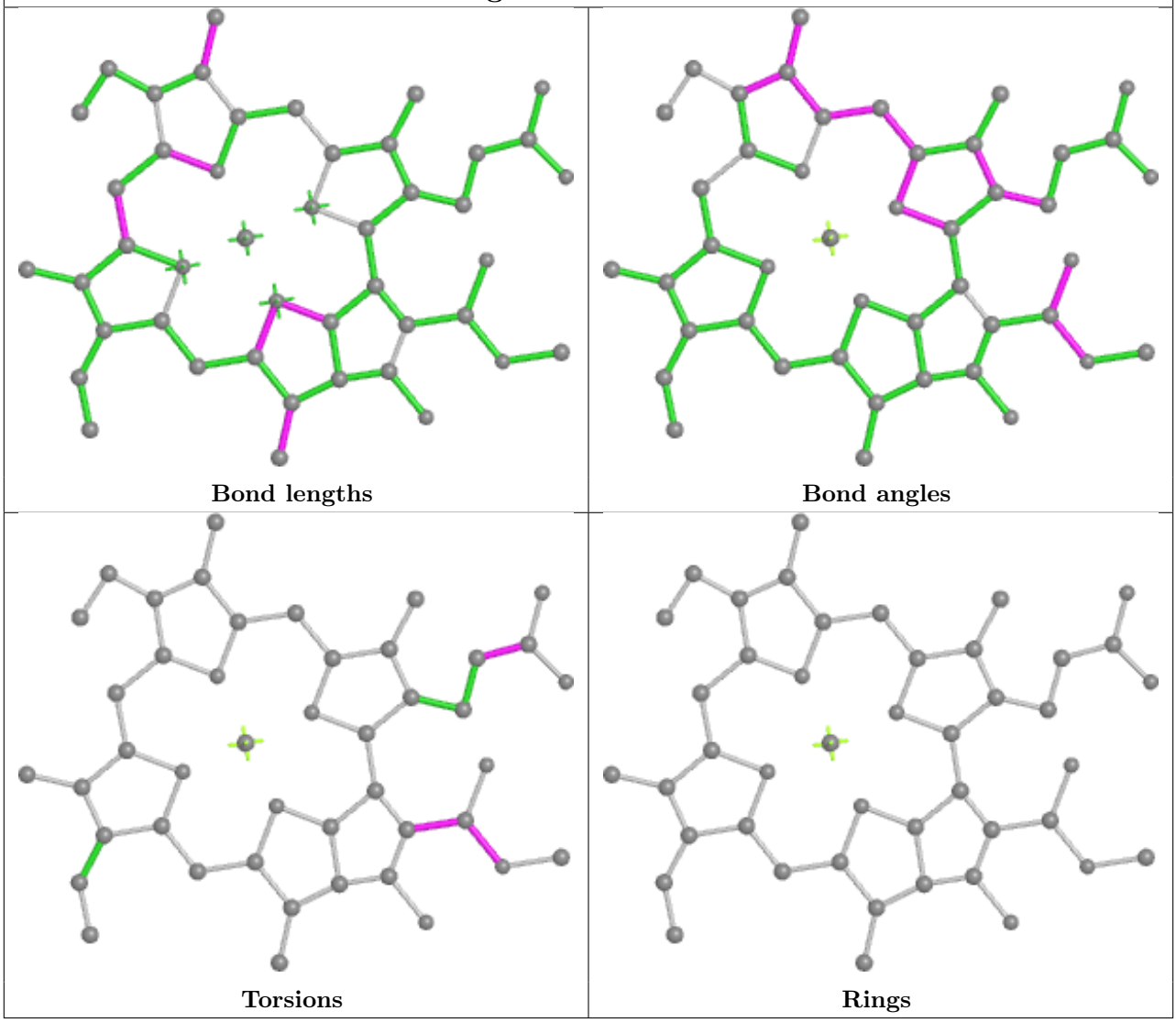


Ligand DGD c 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT v 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 302



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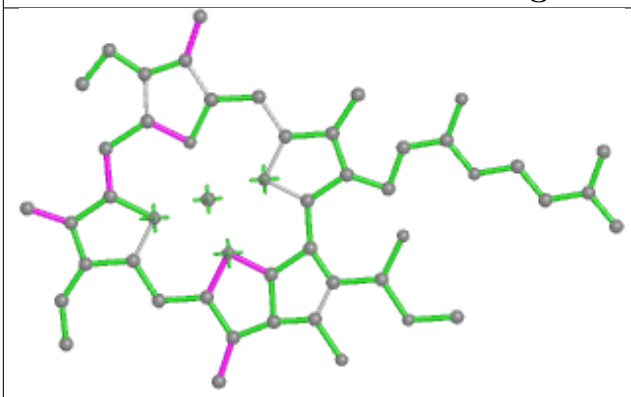
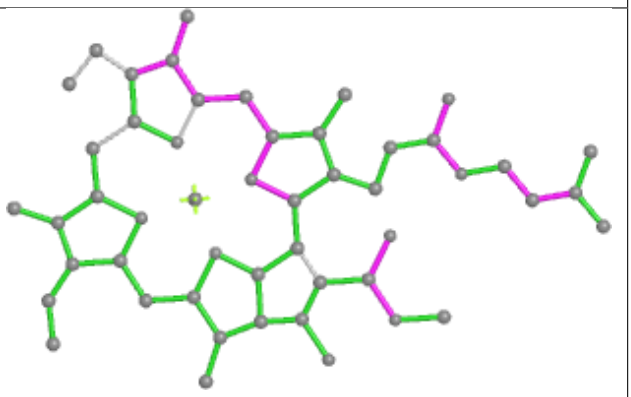
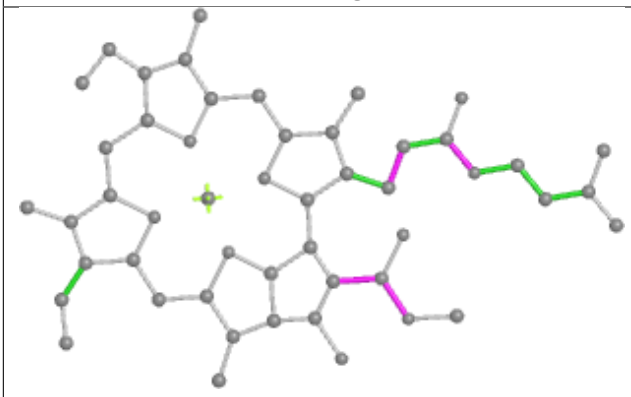


Bond lengths



Bond angles



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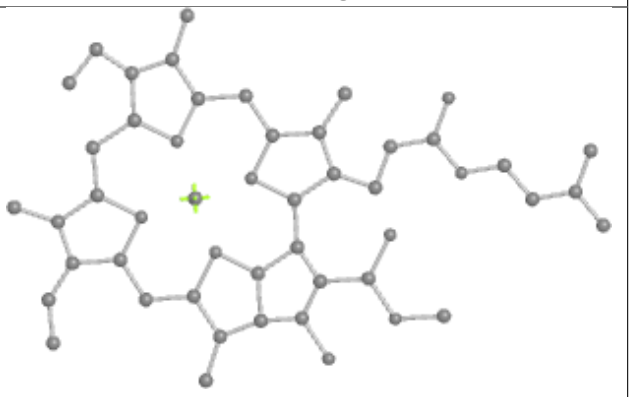
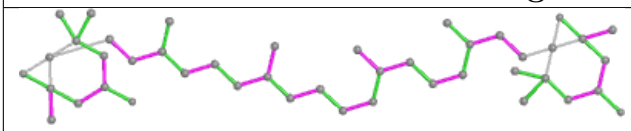


Rings

Ligand XAT 2 311



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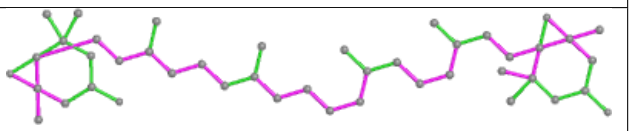
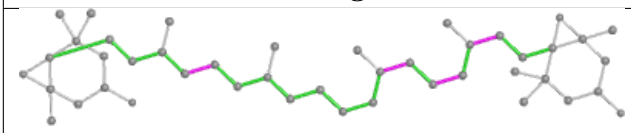


Bond angles



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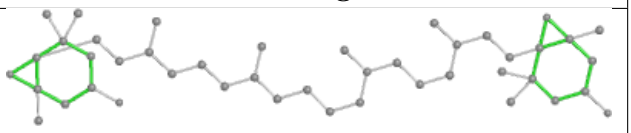
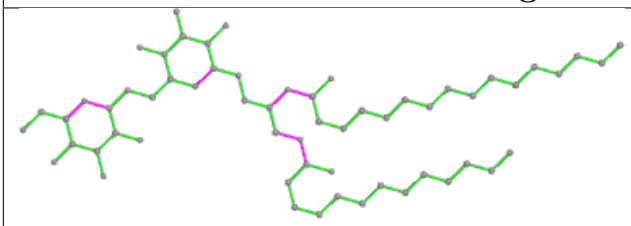


Rings

Ligand DGD A 414



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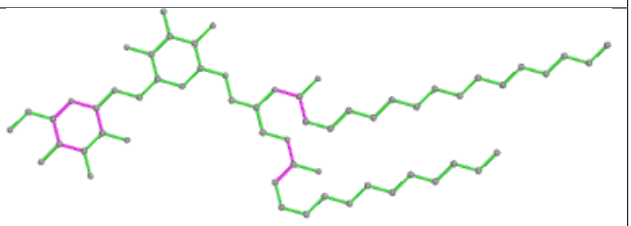

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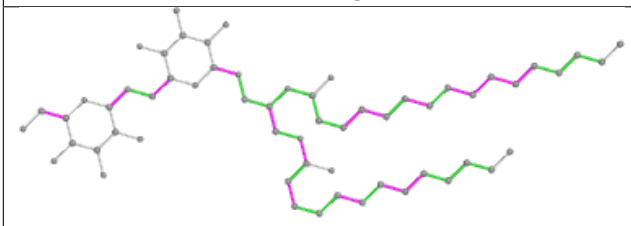

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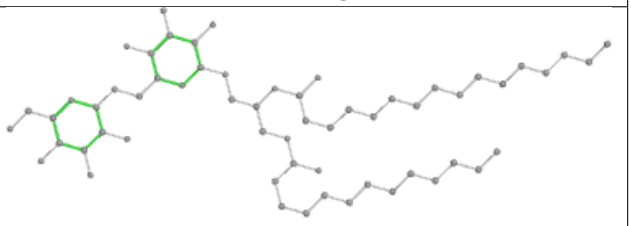
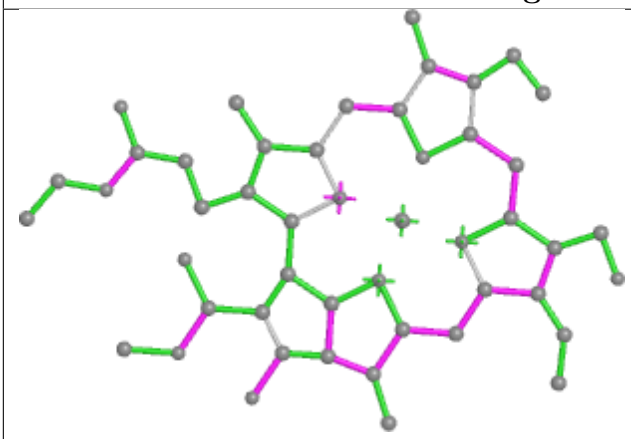


Rings

Ligand CHL Q 312



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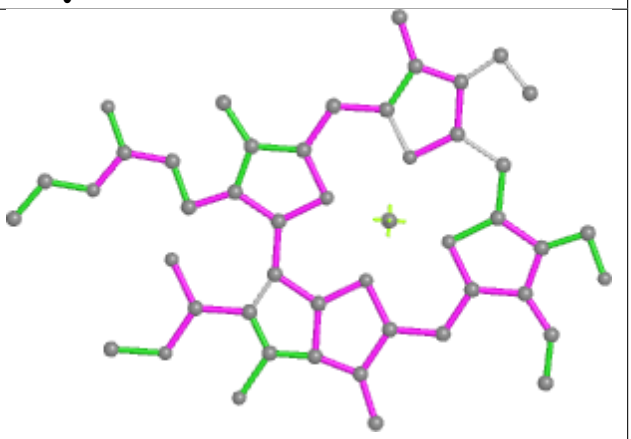

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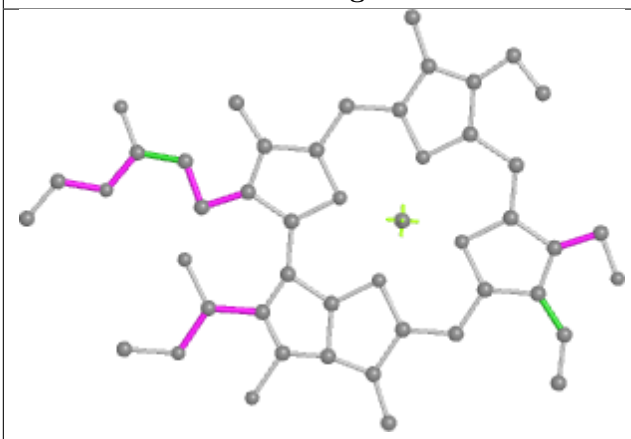

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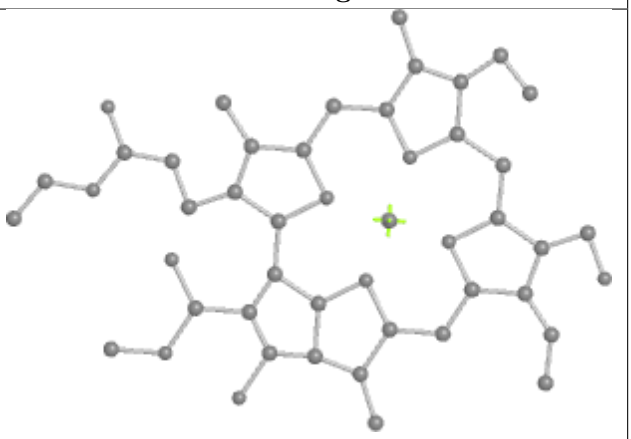
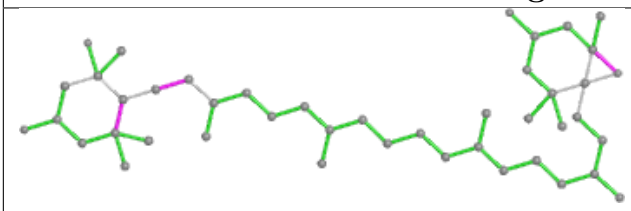


Rings

Ligand NEX r 617



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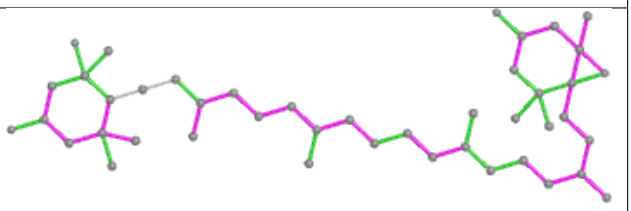
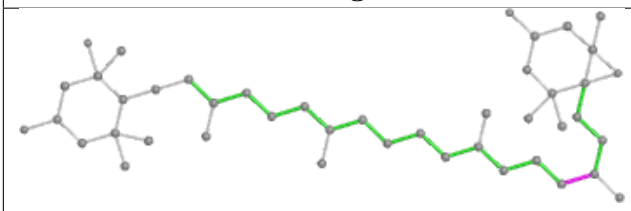


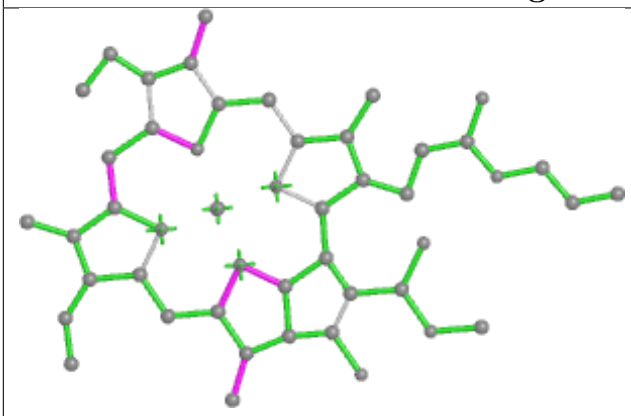
Bond angles



Torsions

Rings

Ligand CLA 5 308



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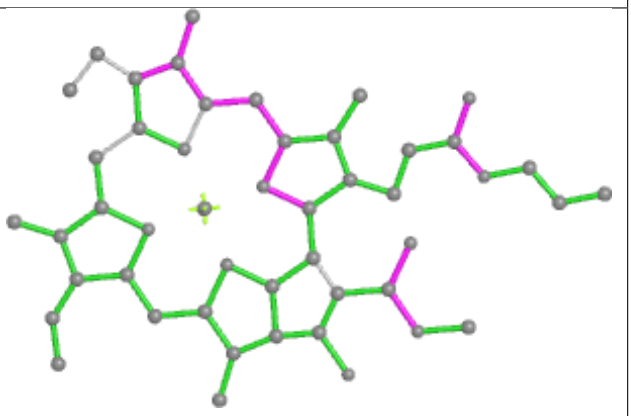

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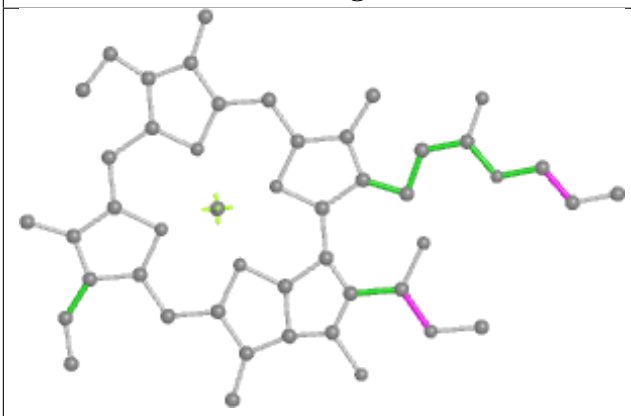
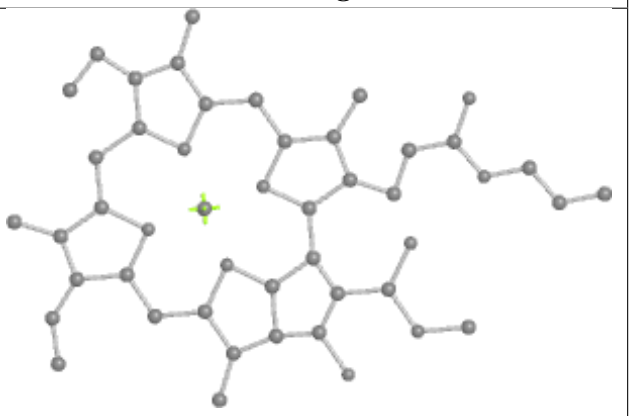
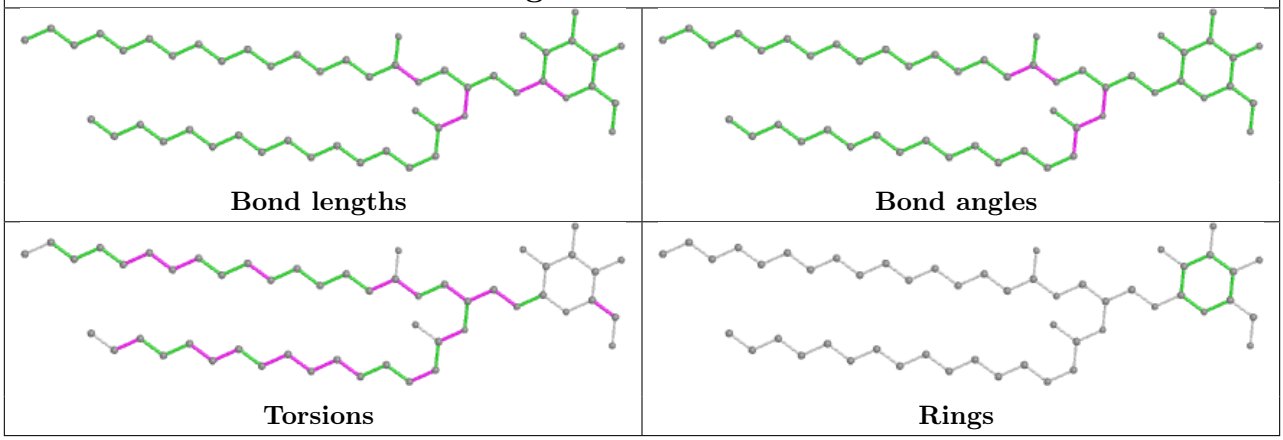


Torsions



Rings

Ligand LMG c 501



Ligand LUT P 311

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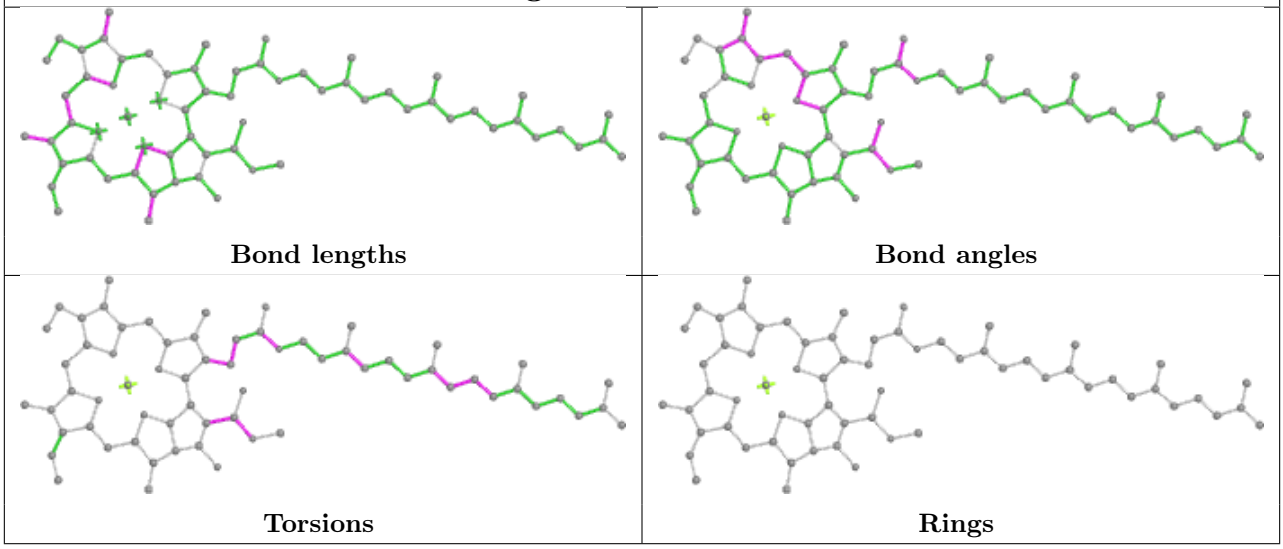
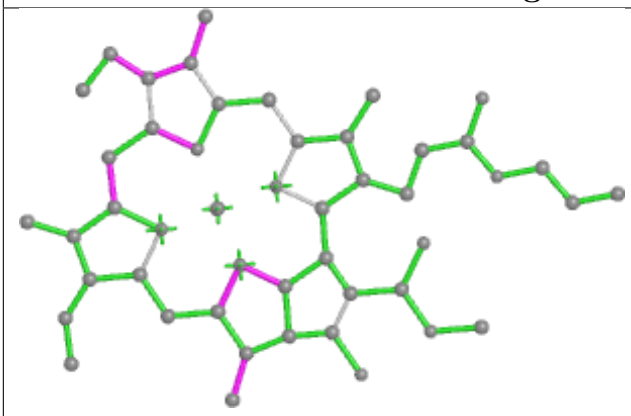


Ligand CLA U 308



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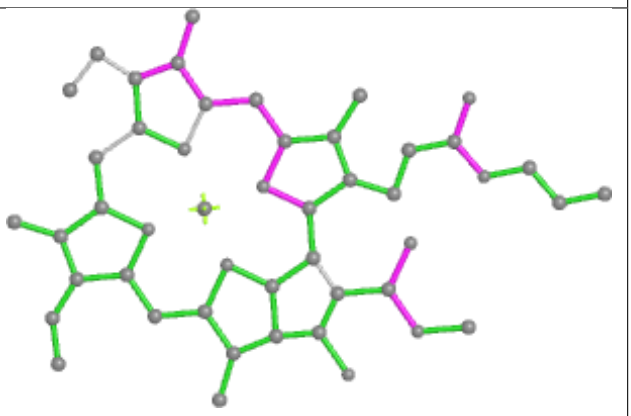

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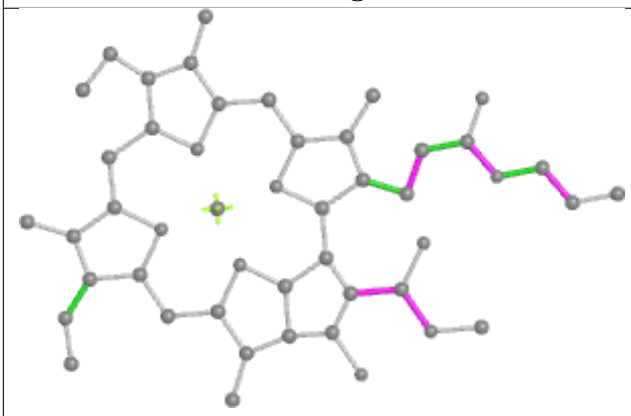

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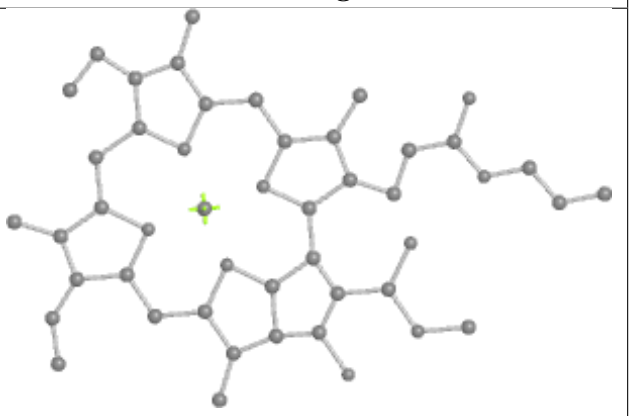
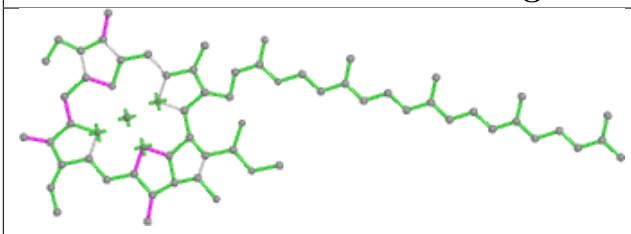


Rings

Ligand CLA N 302



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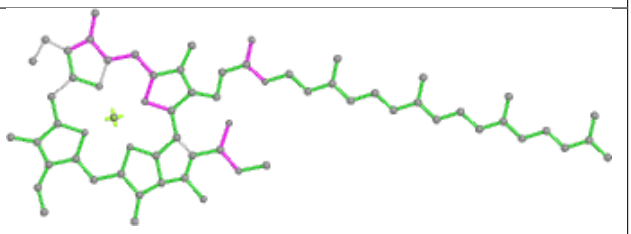
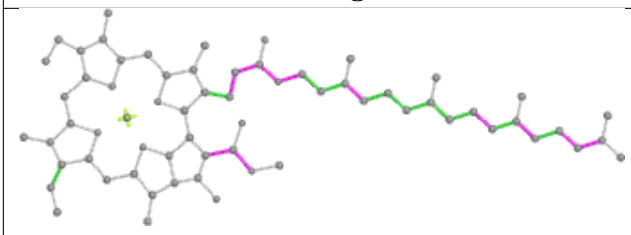
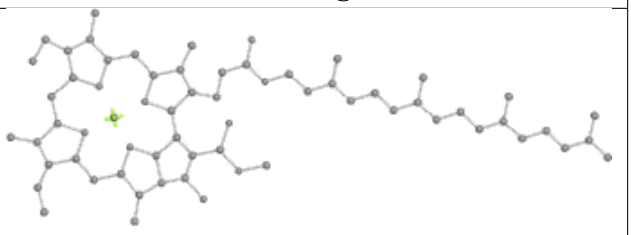


Bond angles

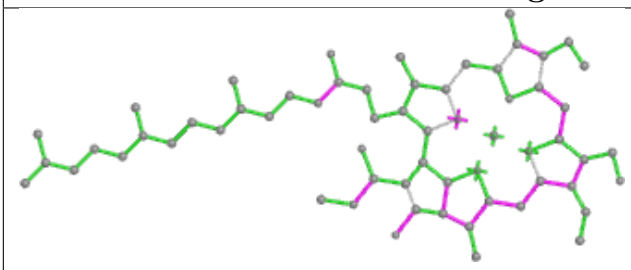


Torsions



Rings

Ligand CHL 3 316



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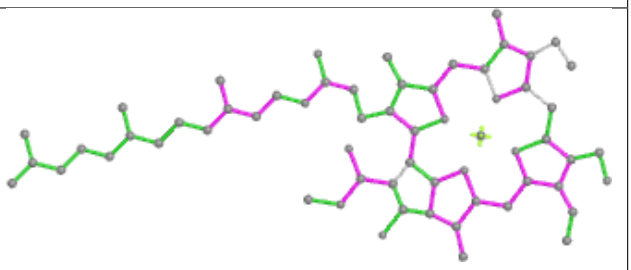
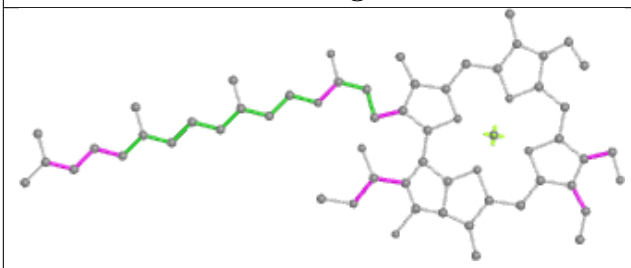


Bond angles



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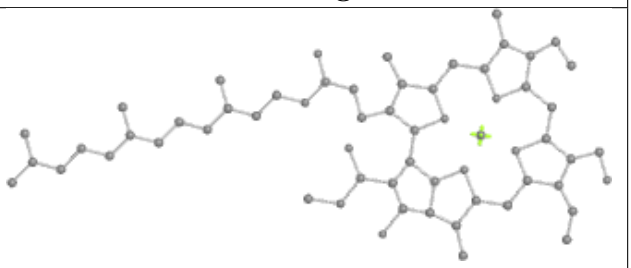
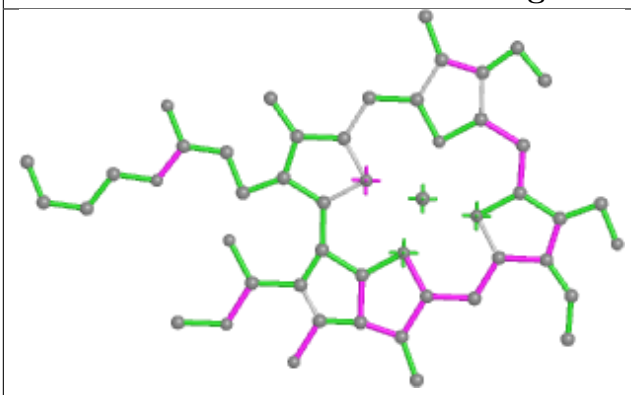
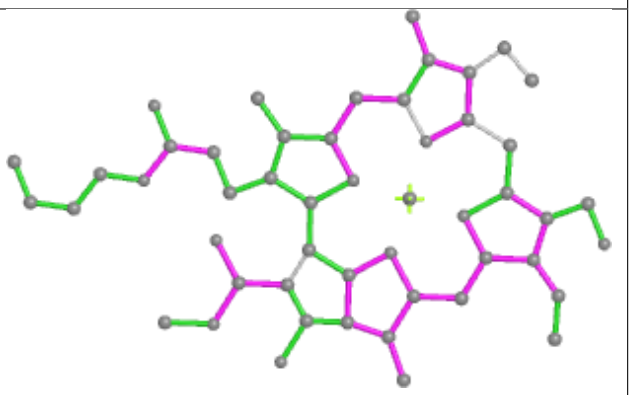


Rings

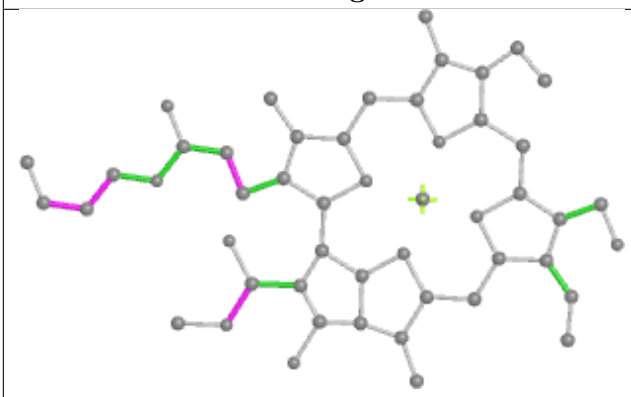
Ligand CHL 2 315



Bond lengths



Bond angles



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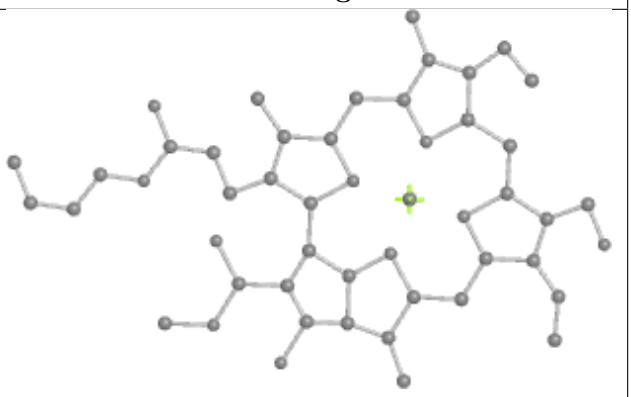
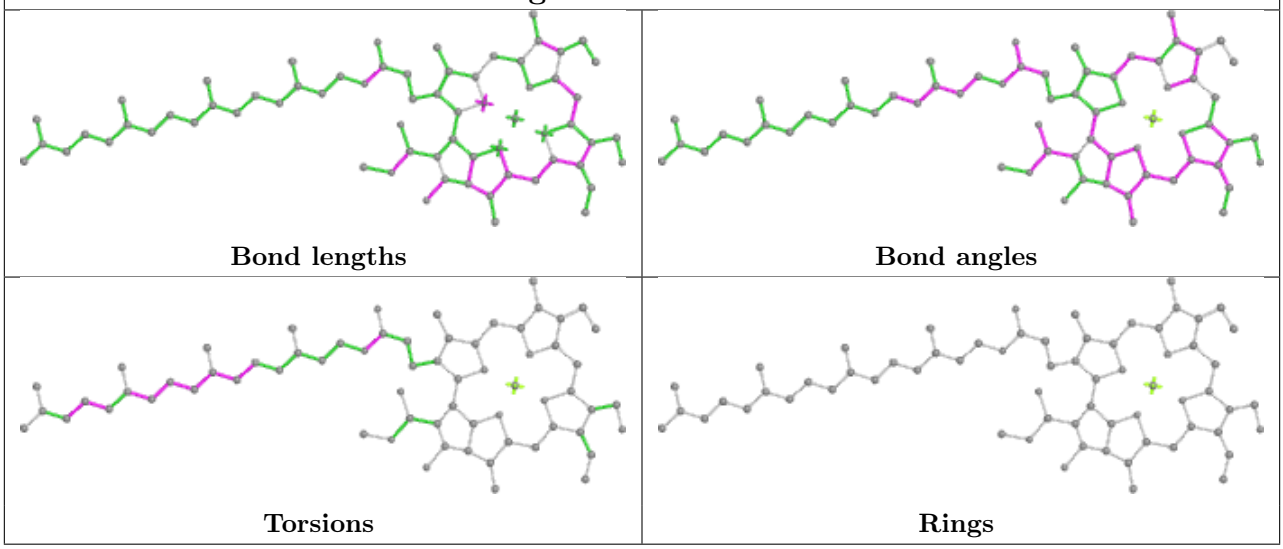
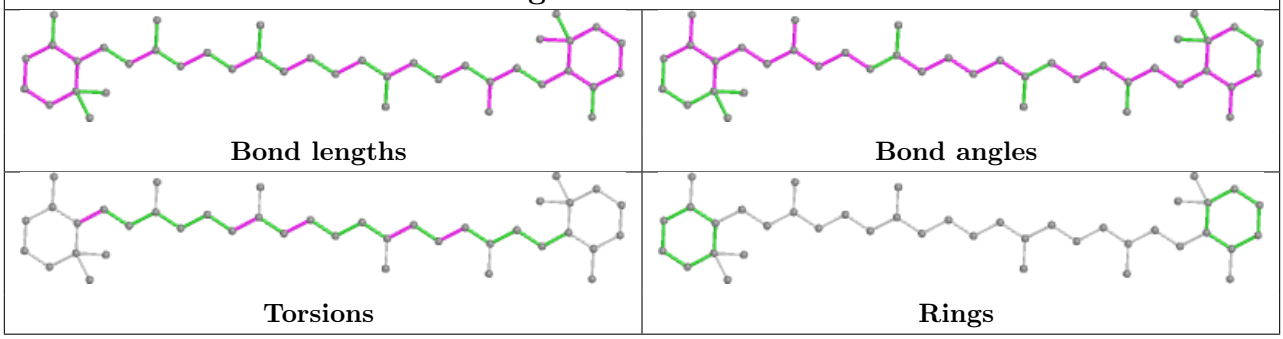


Rings

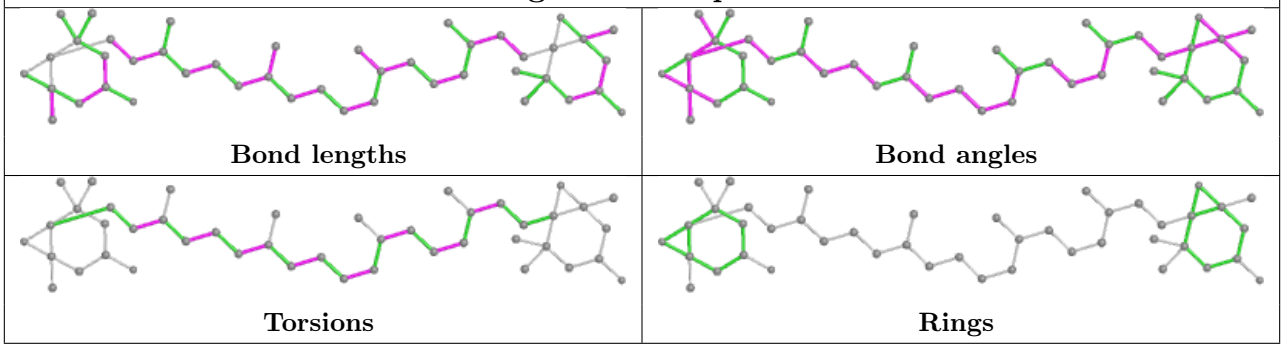
Ligand CHL 1 313



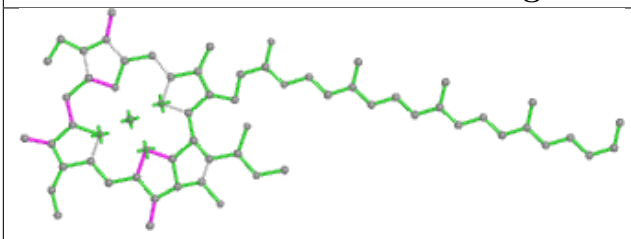
Ligand BCR z 101



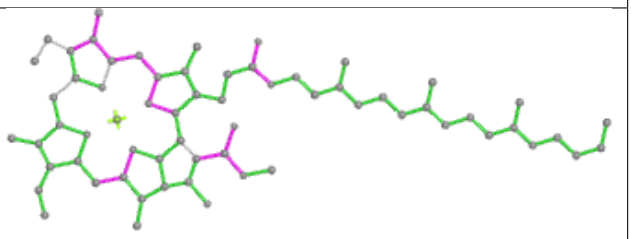
Ligand XAT q 309



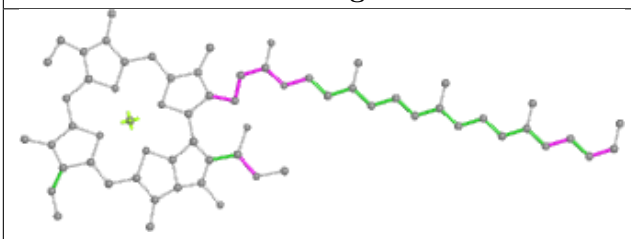
Ligand CLA G 304



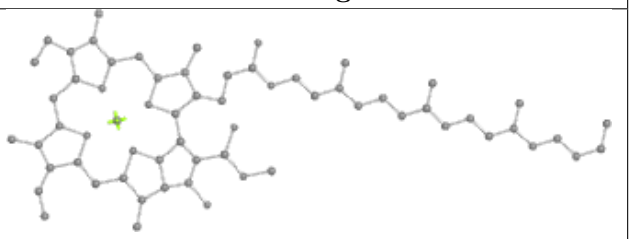
Bond lengths



Bond angles

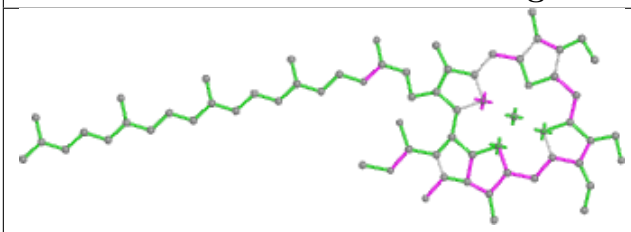


Torsions

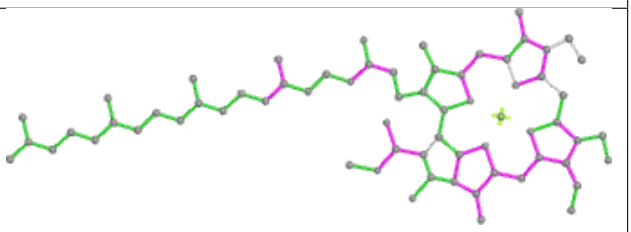


Rings

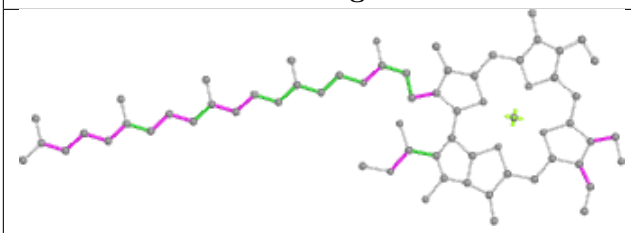
Ligand CHL v 318



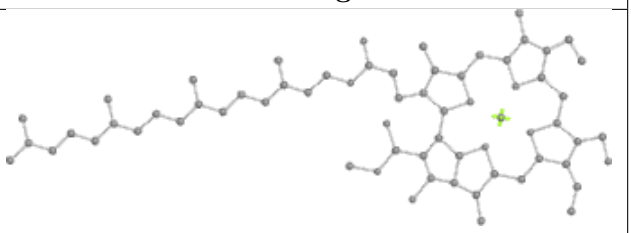
Bond lengths



Bond angles

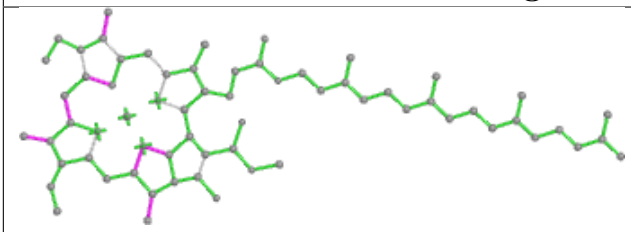


Torsions

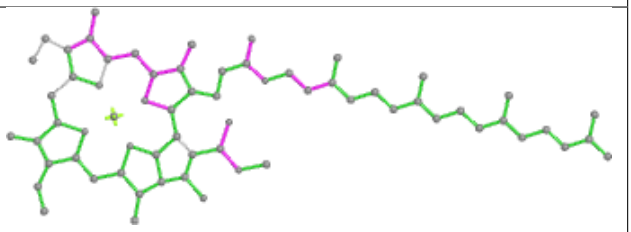


Rings

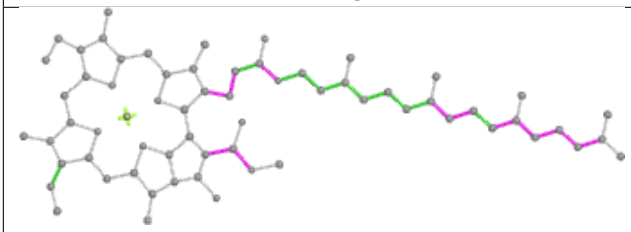
Ligand CLA N 304



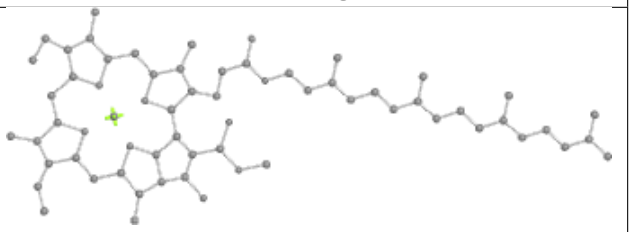
Bond lengths



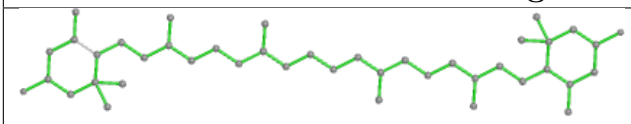
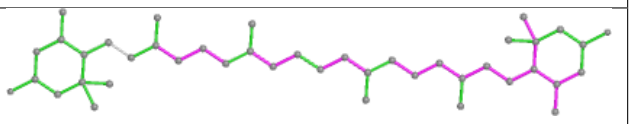
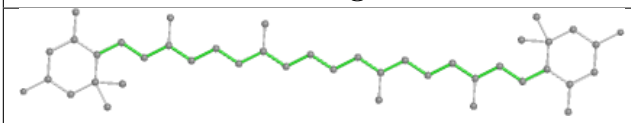
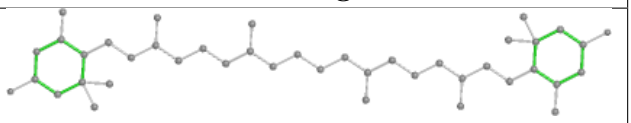
Bond angles

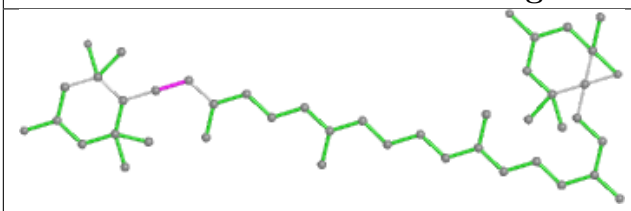
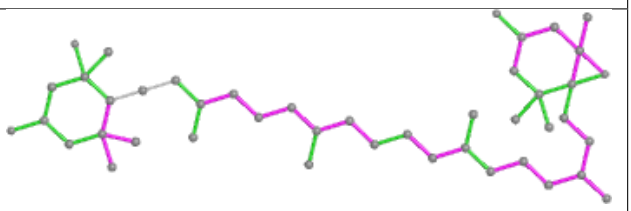
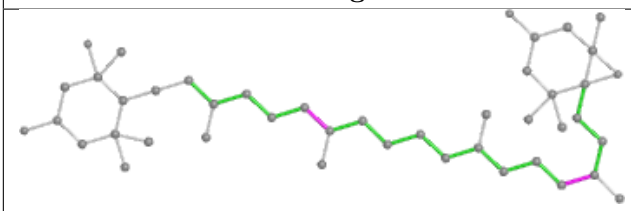


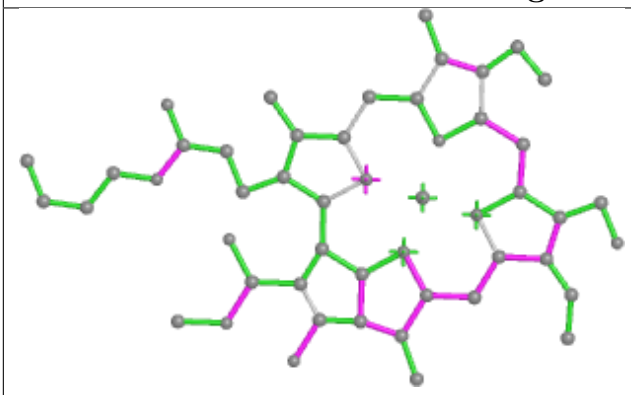
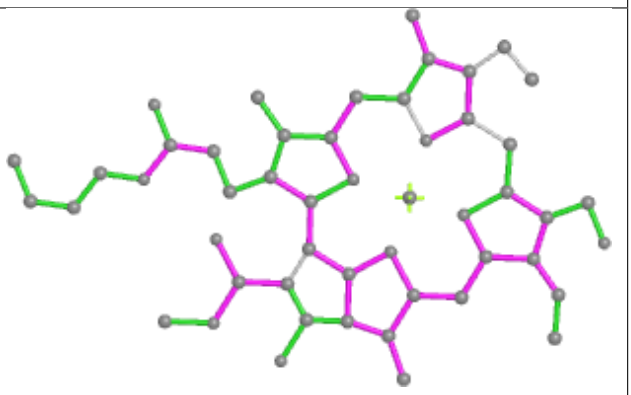
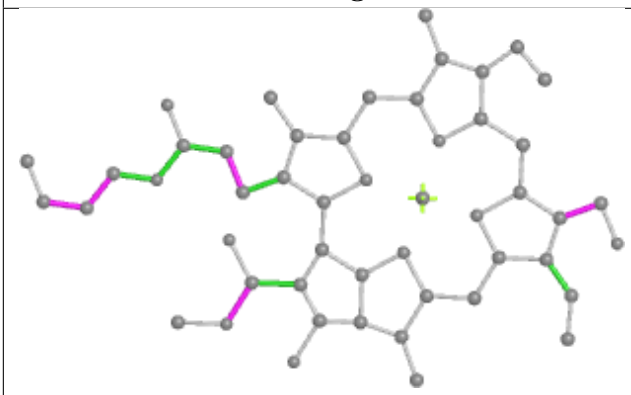
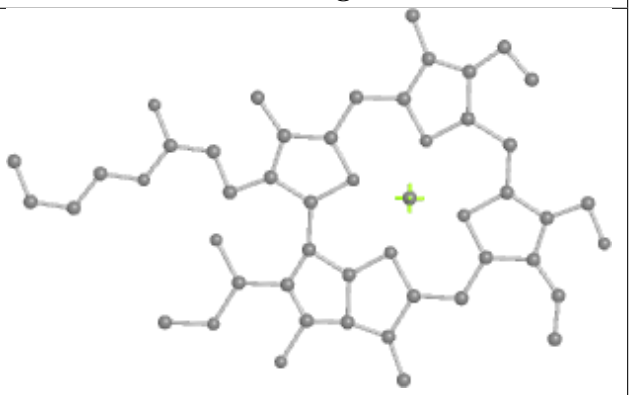
Torsions

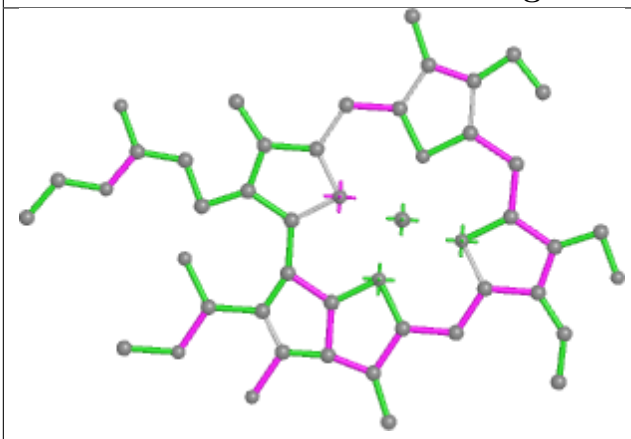
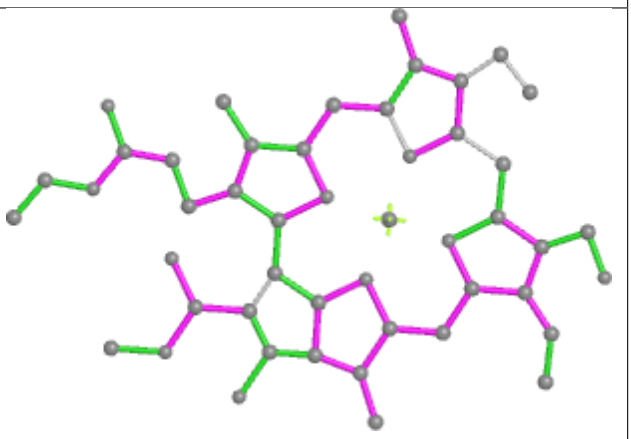
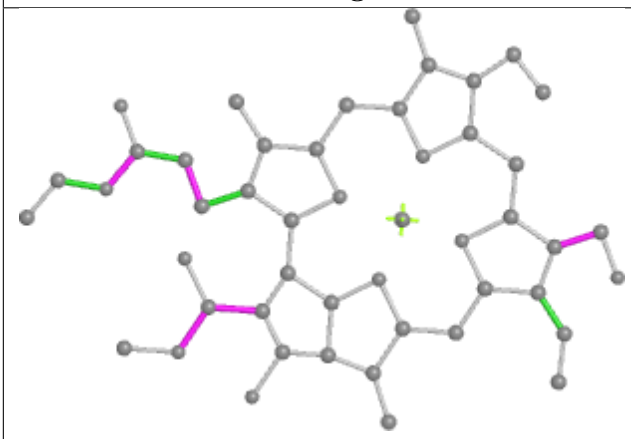
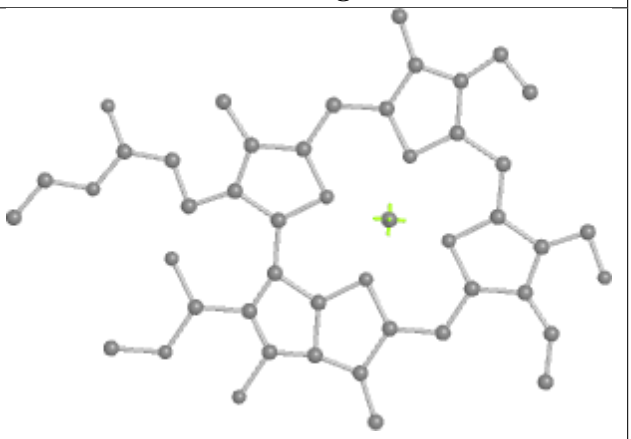


Rings

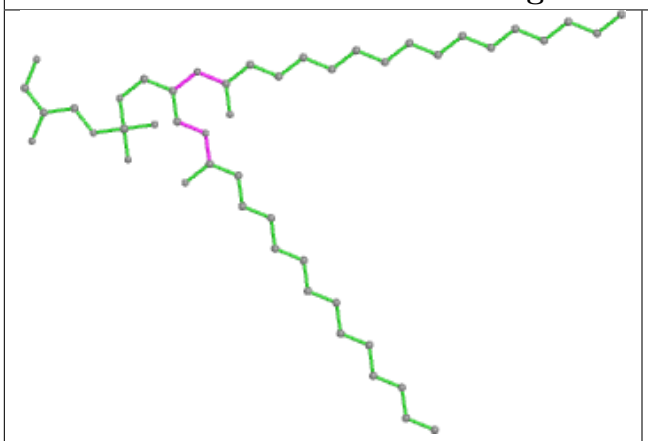
Ligand LUT n 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX v 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

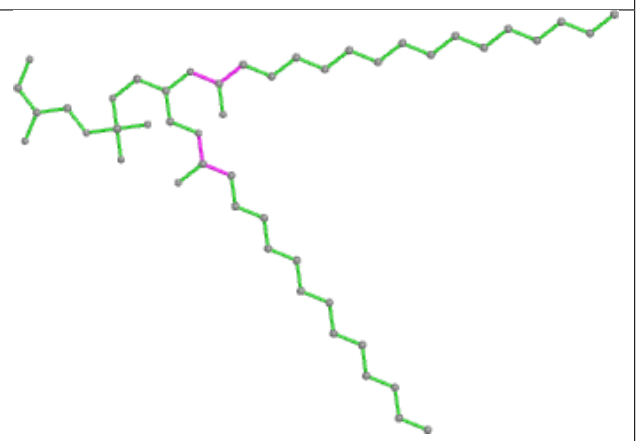
Ligand CHL 5 315	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CHL V 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

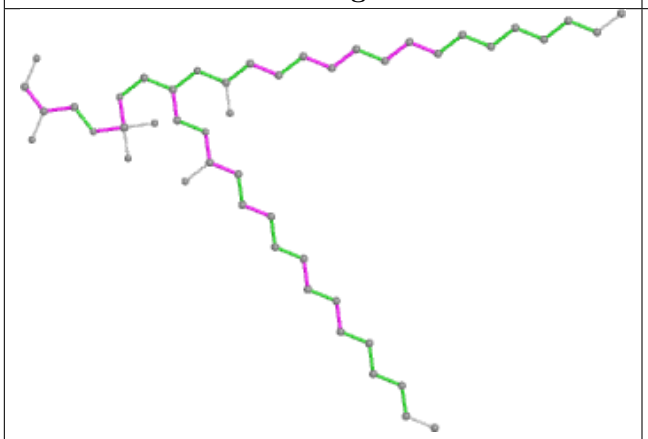
Ligand LHG b 622



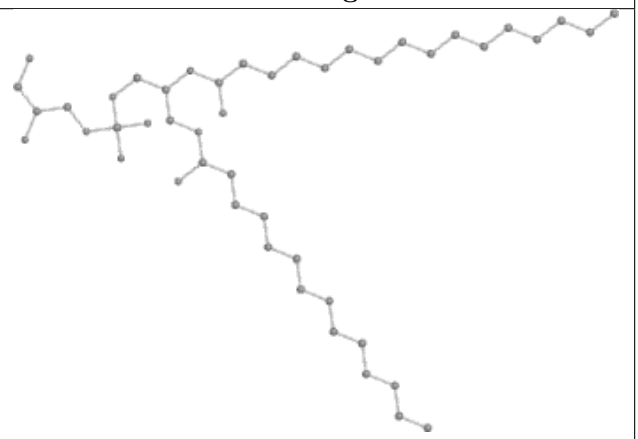
Bond lengths



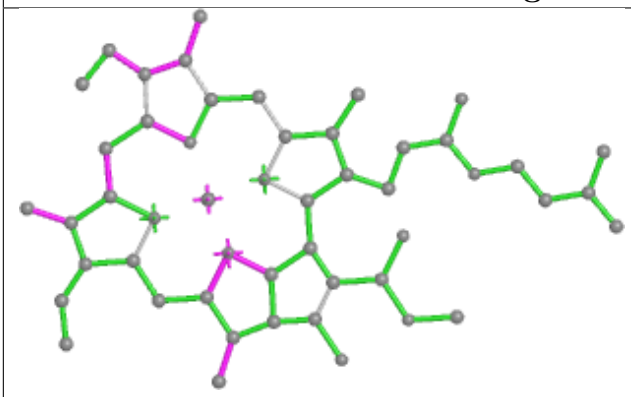
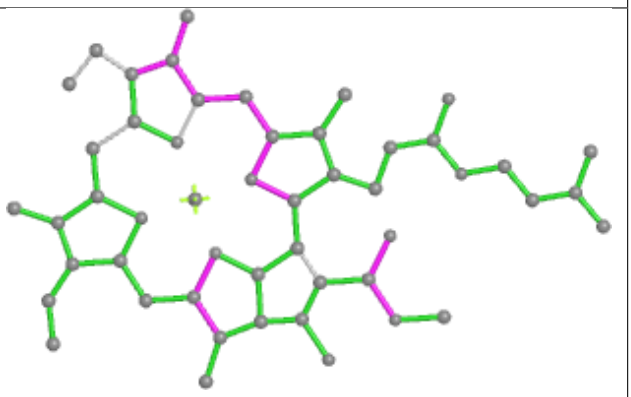
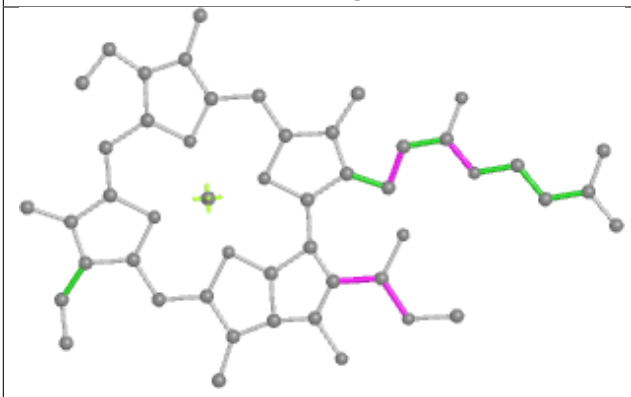
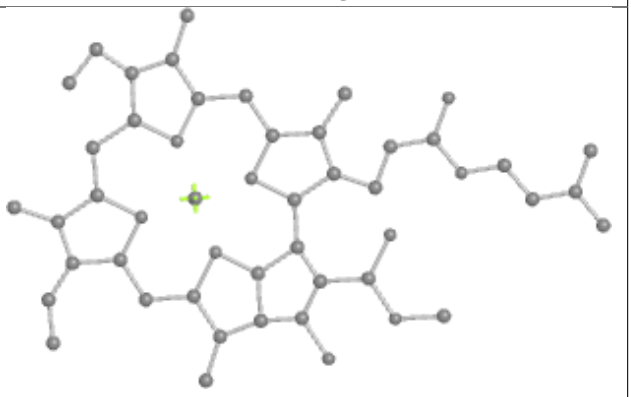
Bond angles

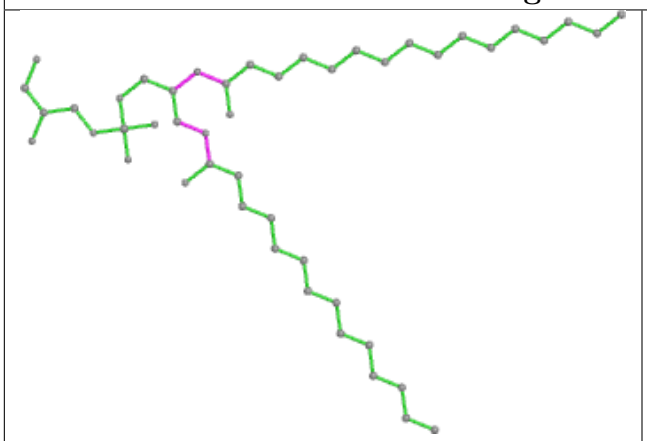
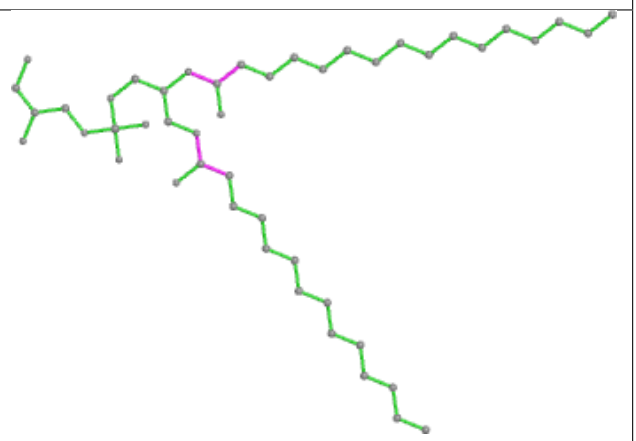
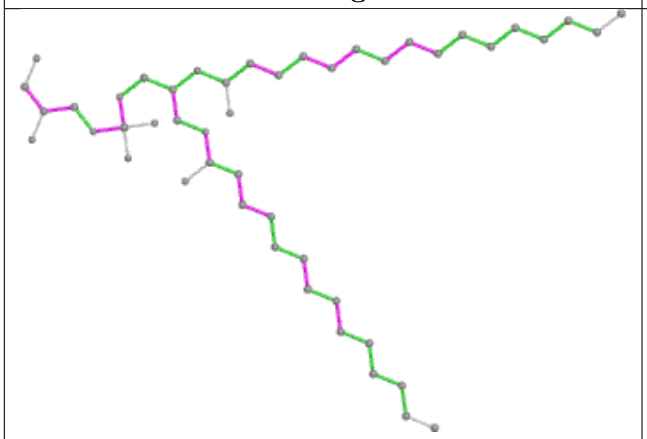
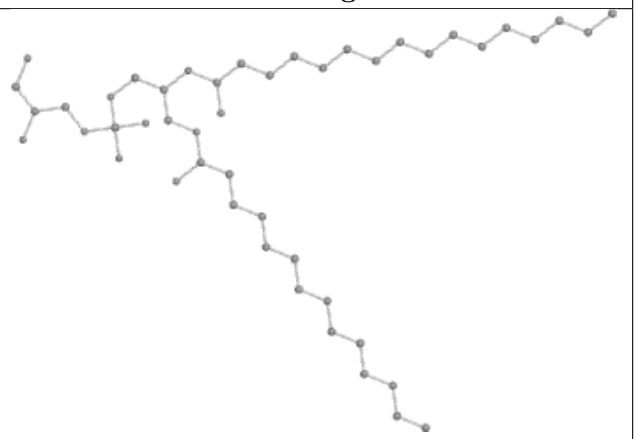


Torsions

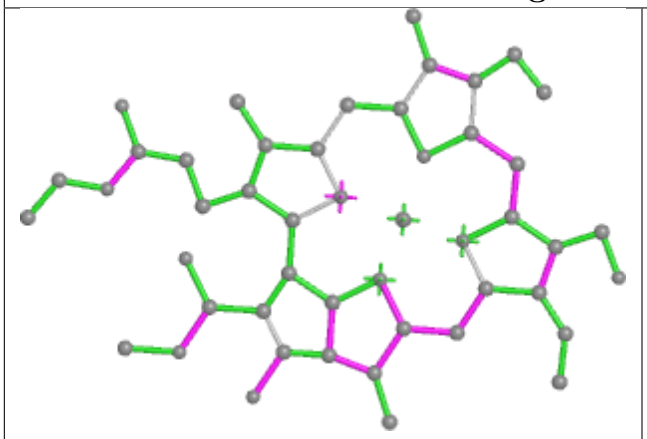


Rings

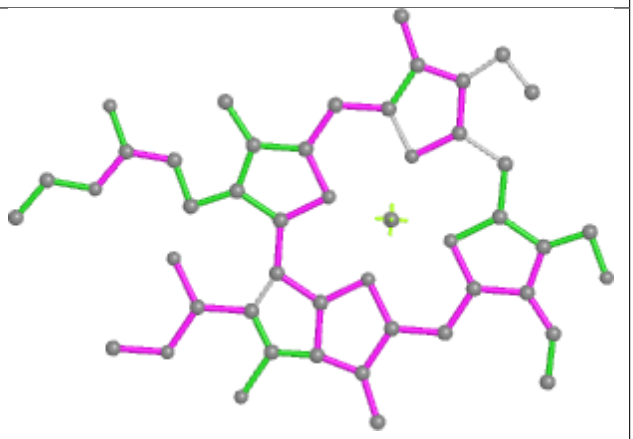
Ligand CLA A 406	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand LHG B 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

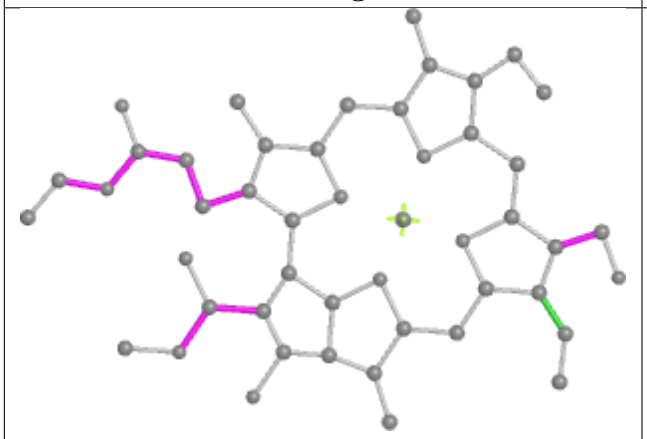
Ligand CHL 1 314



Bond lengths



Bond angles



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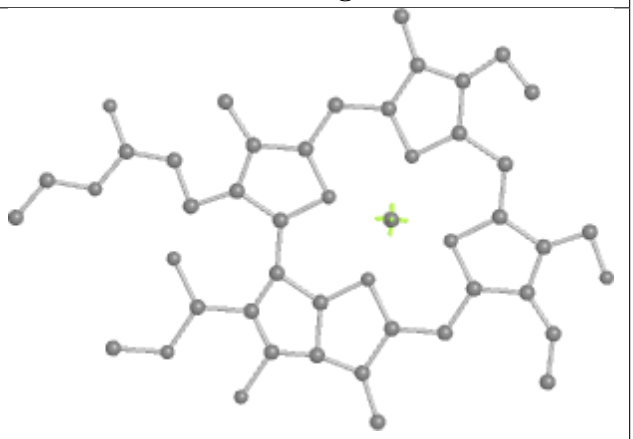
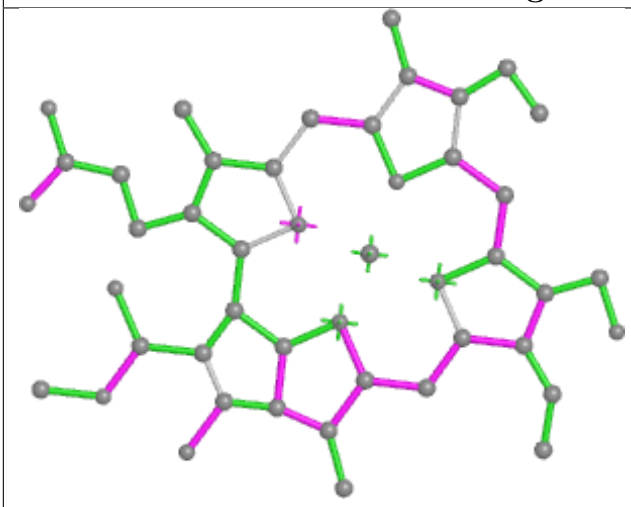
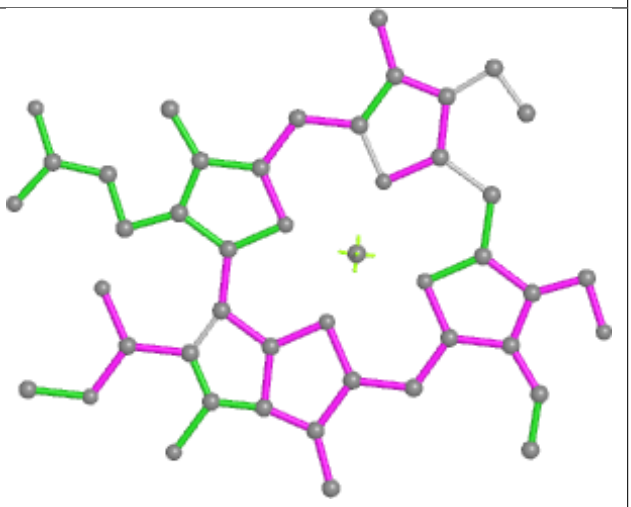


Rings

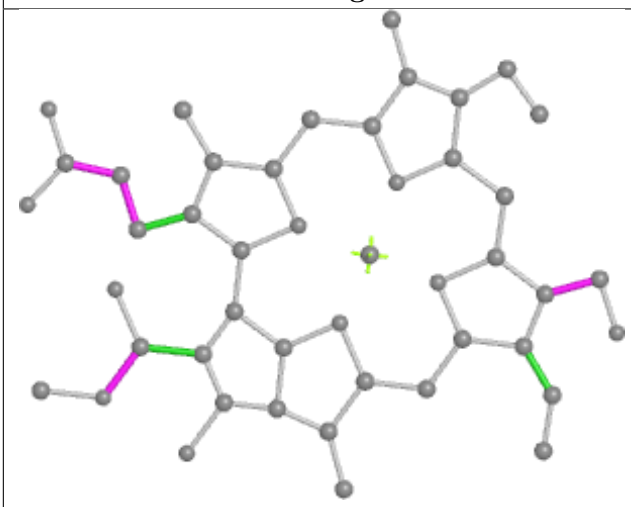
Ligand CHL S 313



Bond lengths



Bond angles



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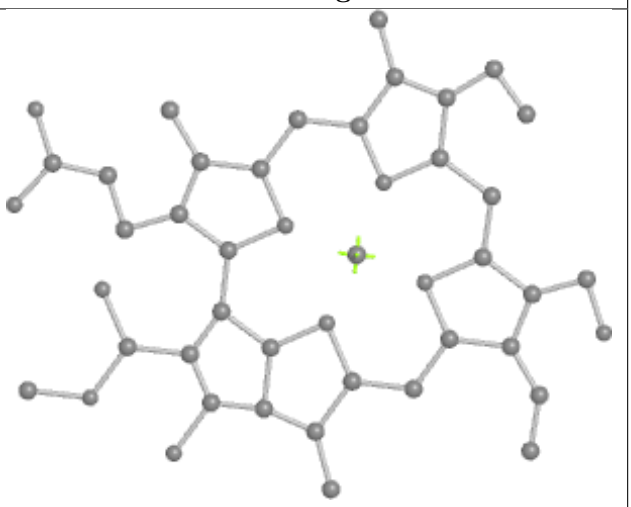
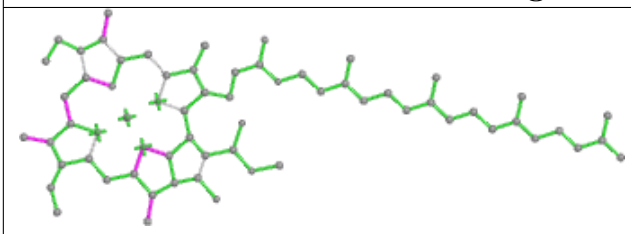
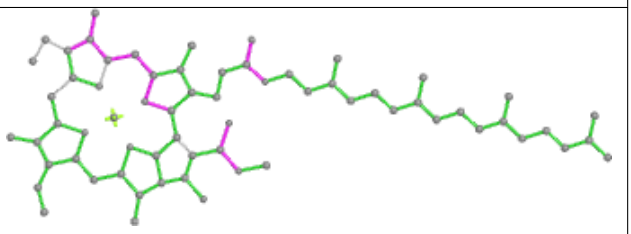


Rings

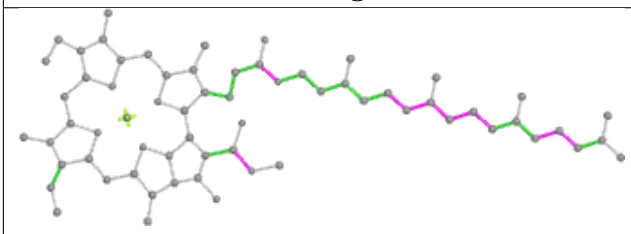
Ligand CLA b 612



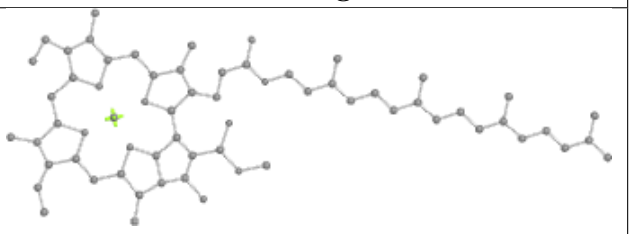
Bond lengths



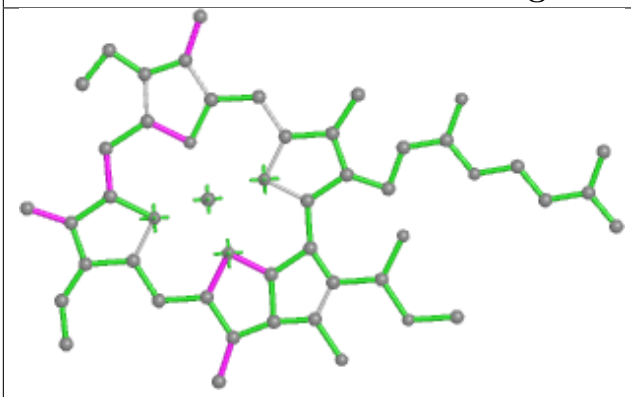
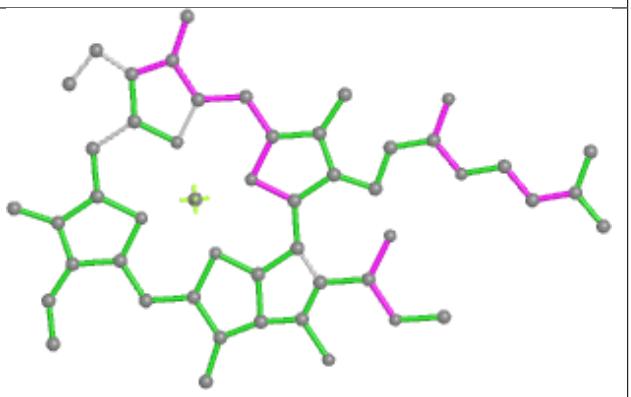
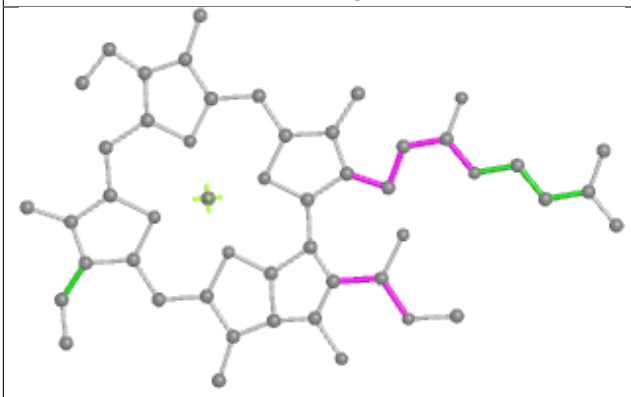
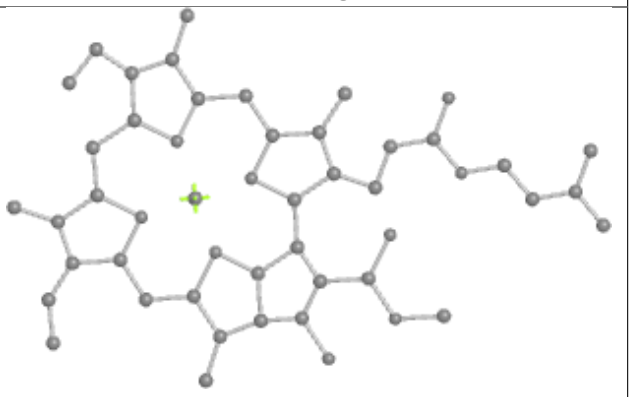
Bond angles

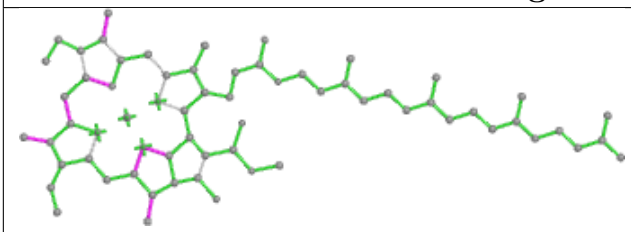
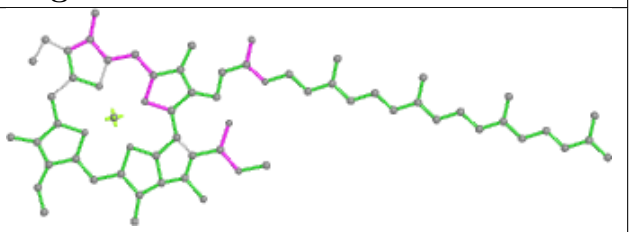
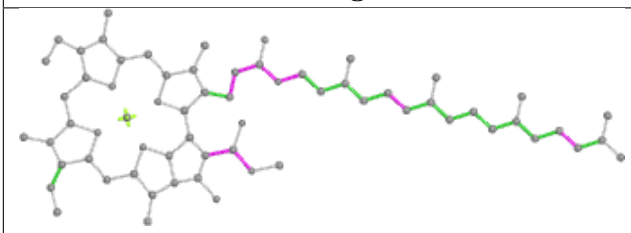
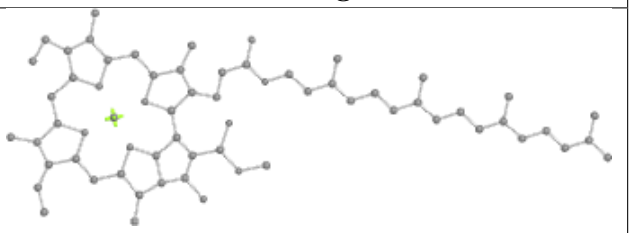


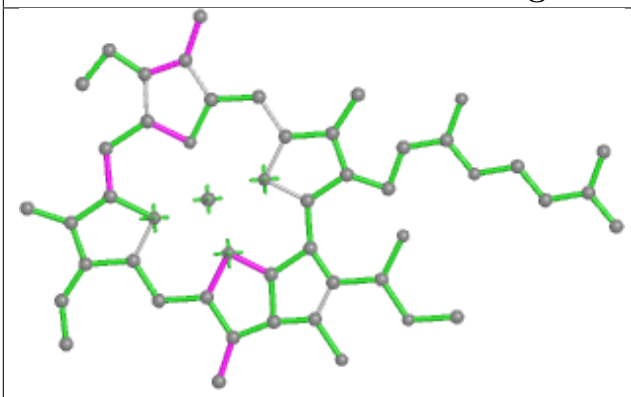
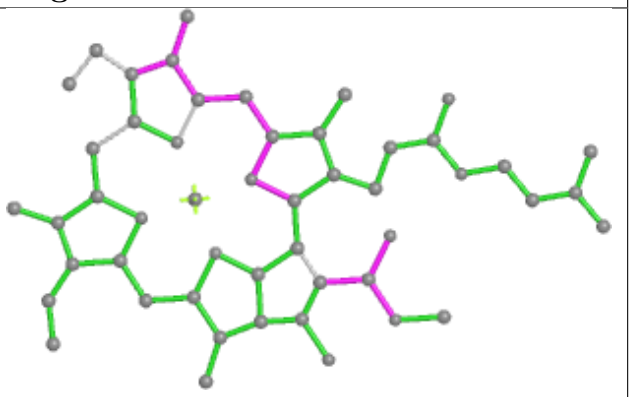
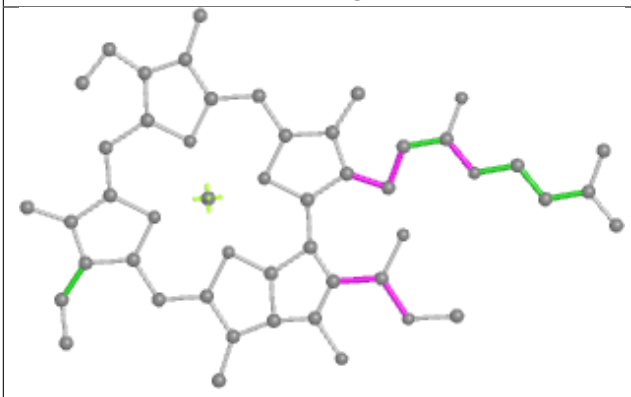
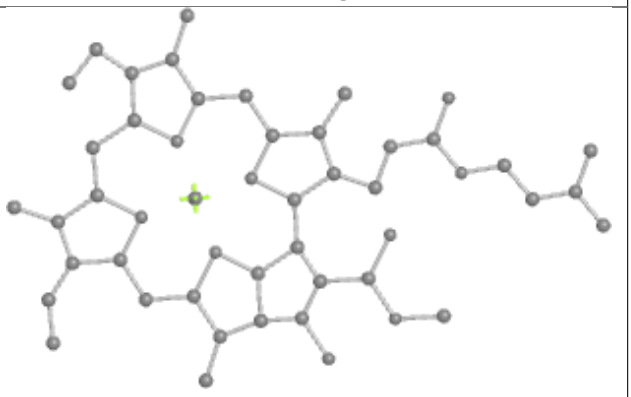
Torsions

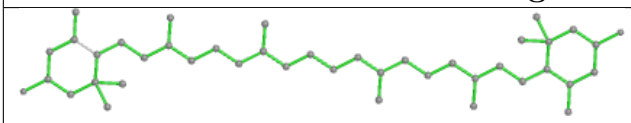
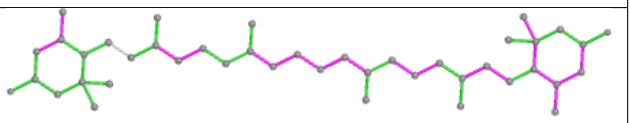
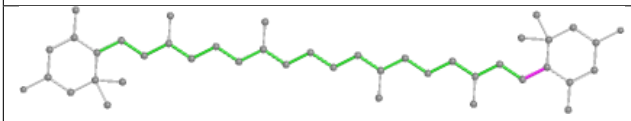
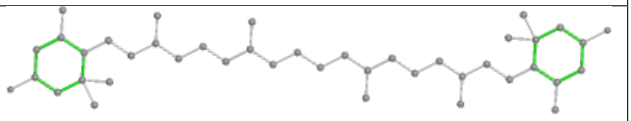


Rings

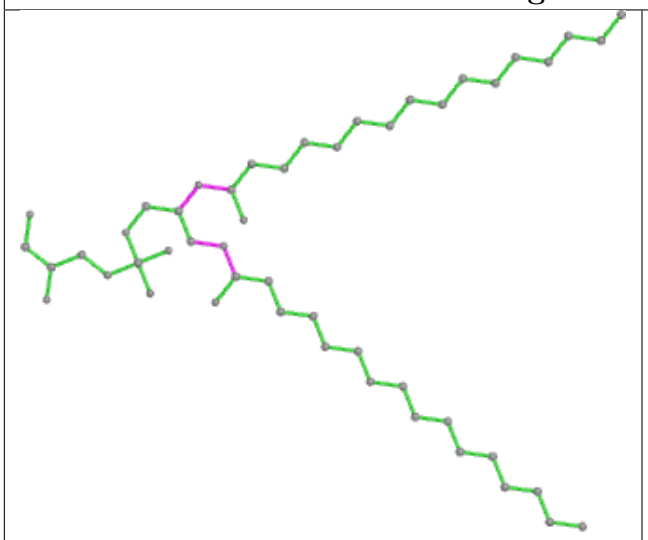
Ligand CLA 6 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

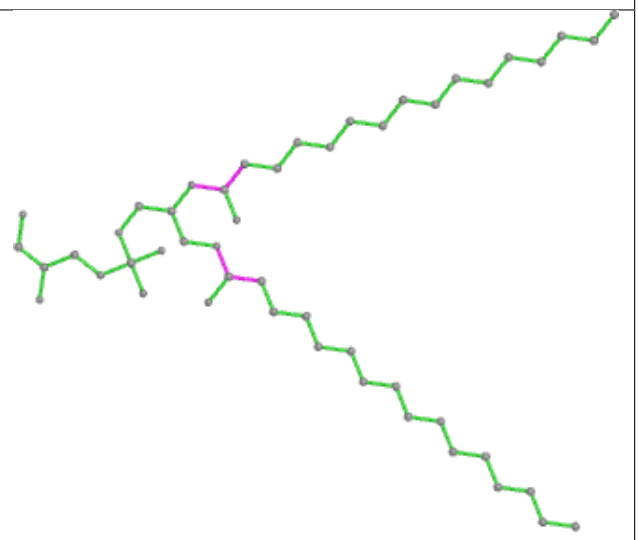
Ligand CLA g 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 1 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

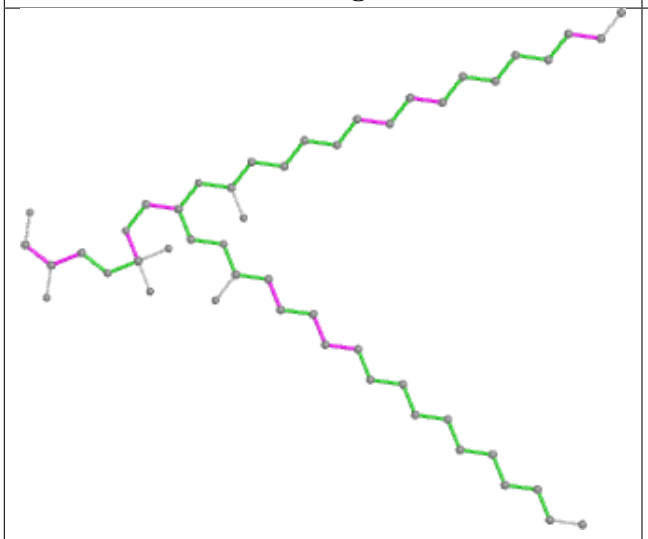
Ligand LHG 1 312



Bond lengths



Bond angles



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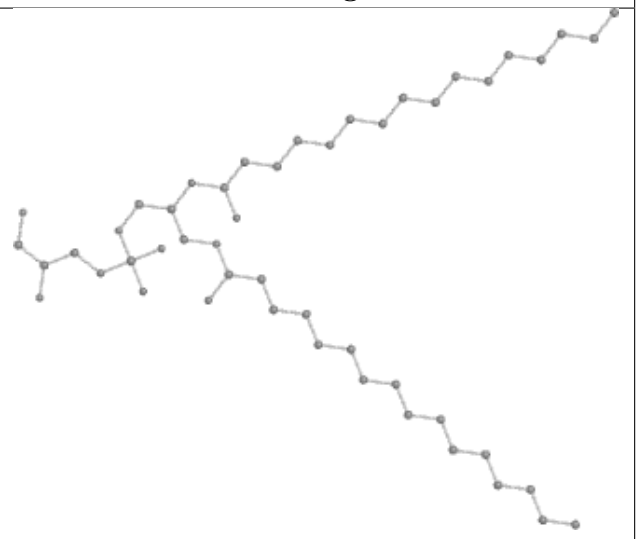
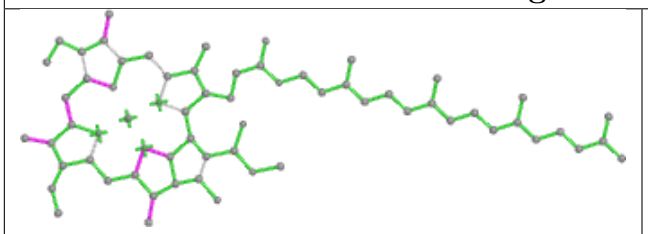
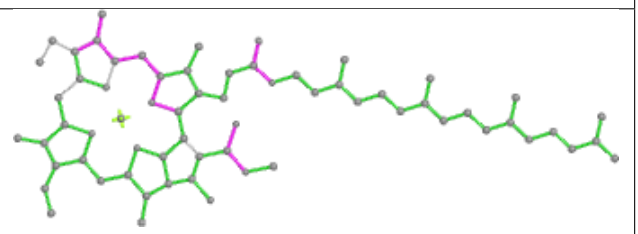


Rings

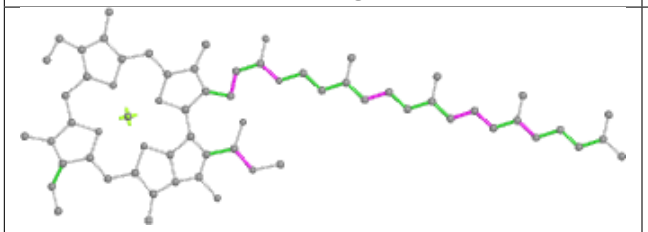
Ligand CLA v 307



Bond lengths



Bond angles



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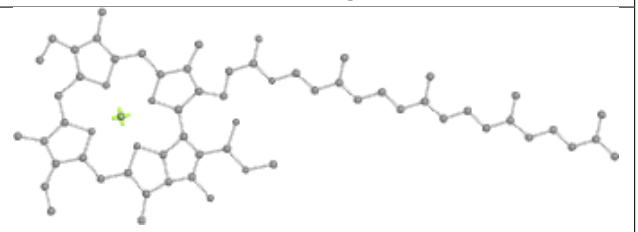
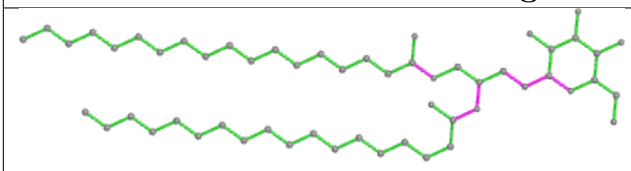
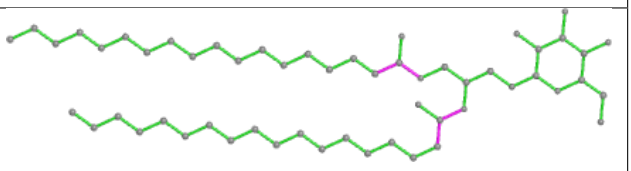
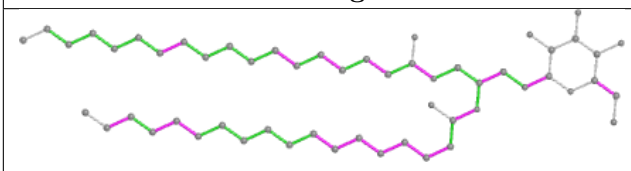
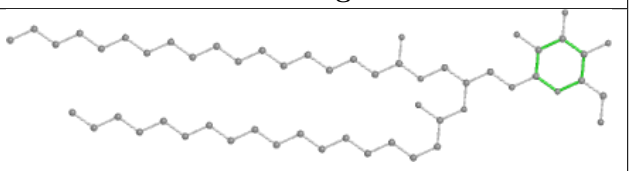


Rings

Ligand LMG B 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

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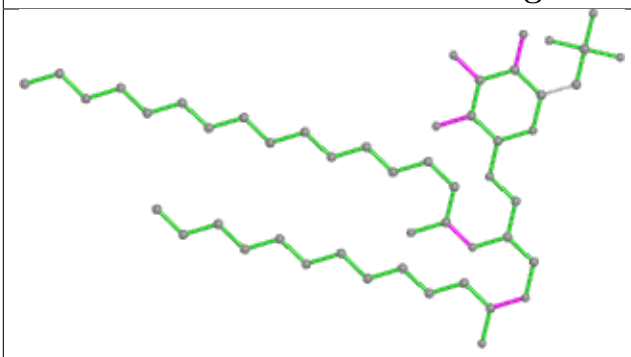
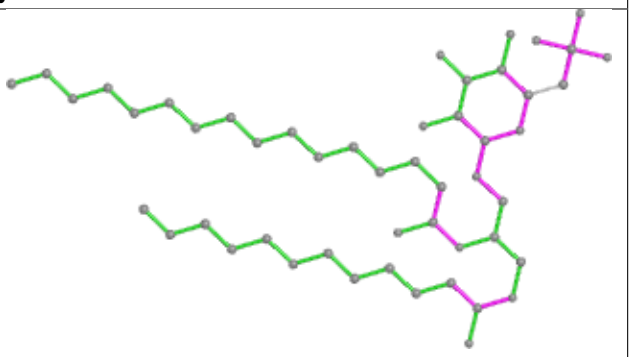
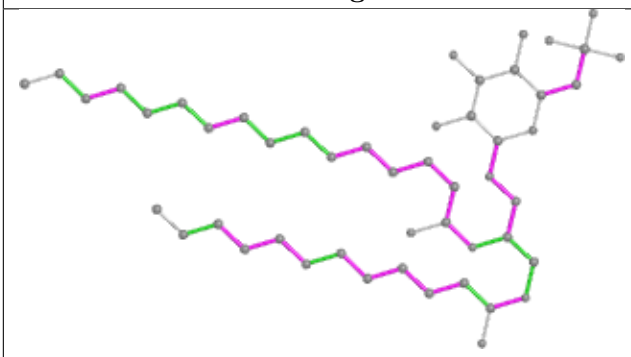
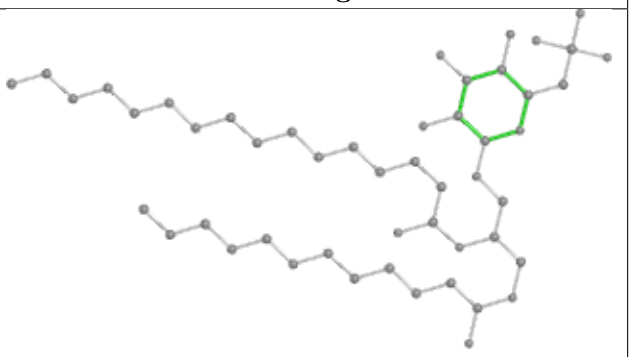
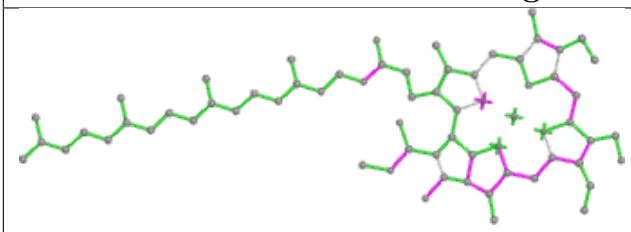
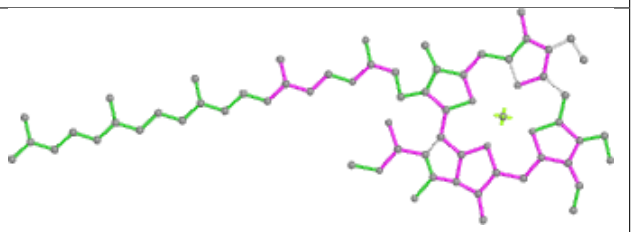
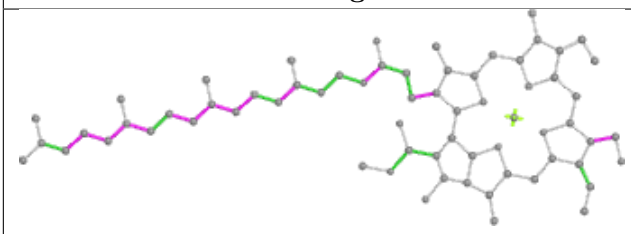
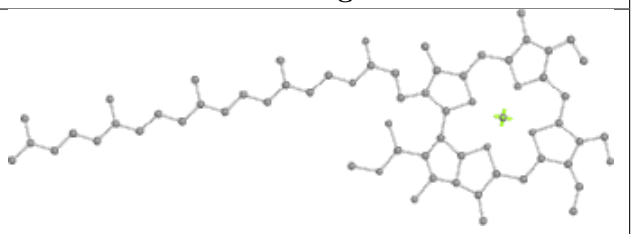
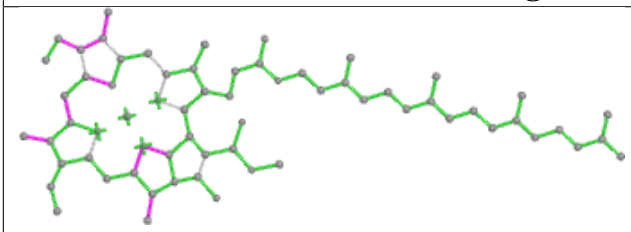
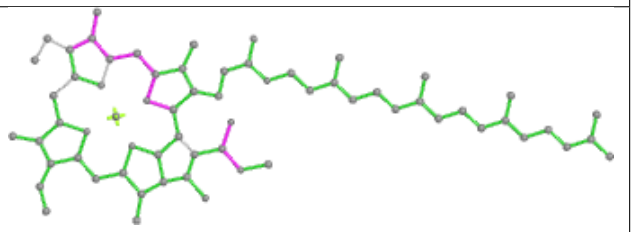
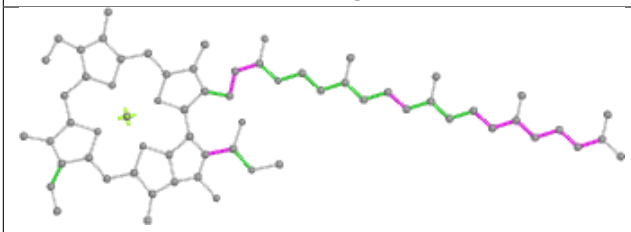
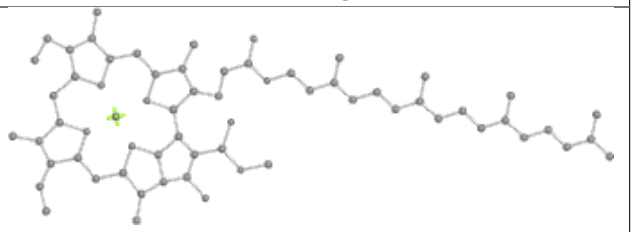
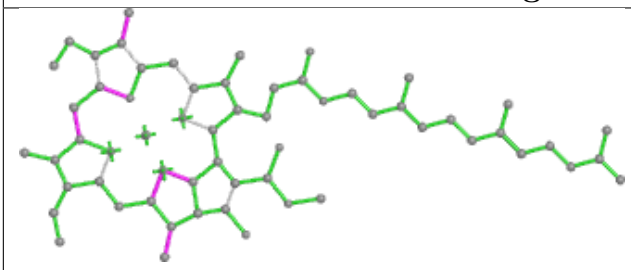
 Bond lengths	 Bond angles
 Torsions	 Rings

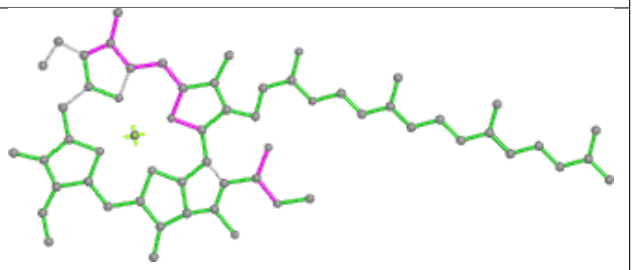
Ligand CHL G 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

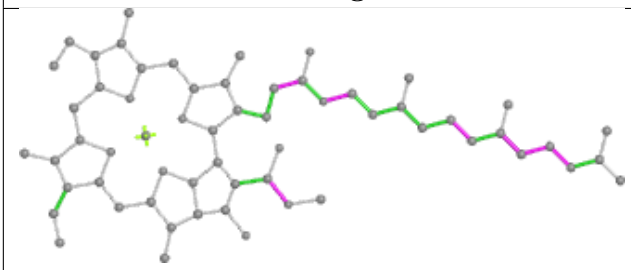
Ligand CLA G 306



Bond lengths



Bond angles



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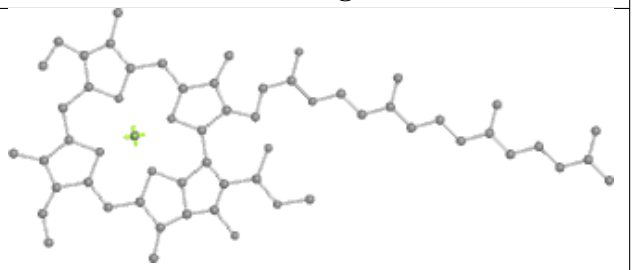
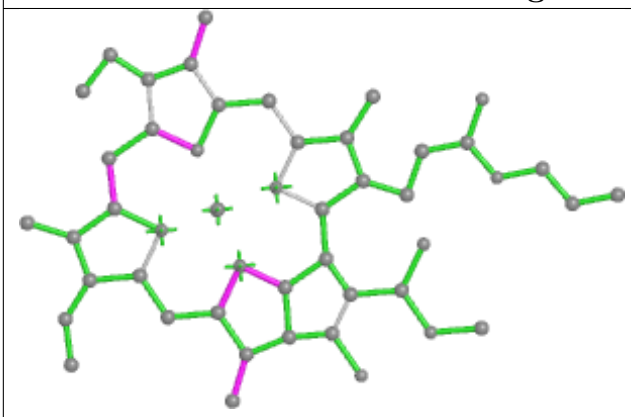


Rings

Ligand CLA n 308



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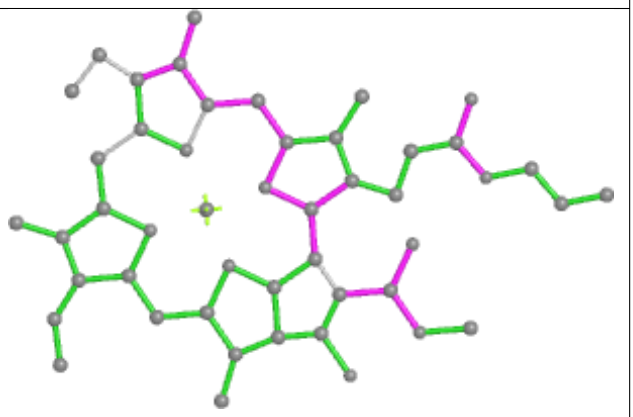
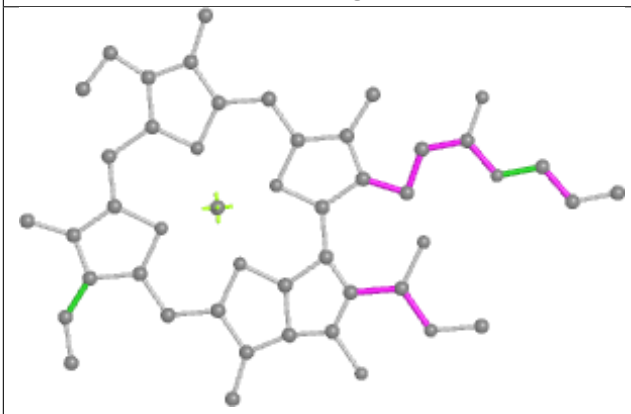


Bond angles



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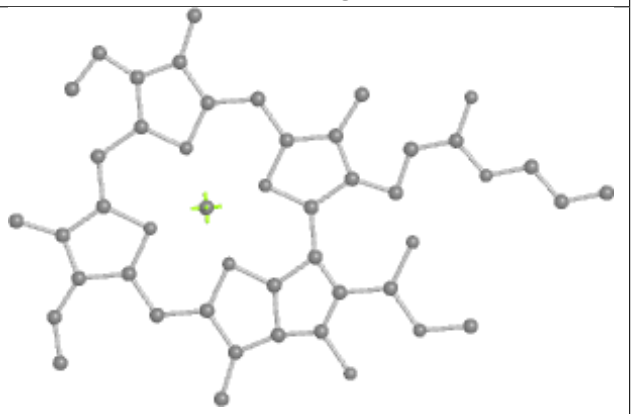
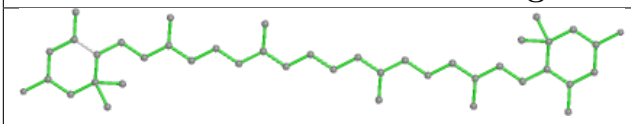


Rings

Ligand LUT p 311



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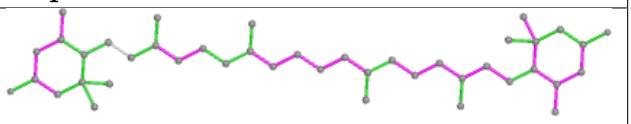

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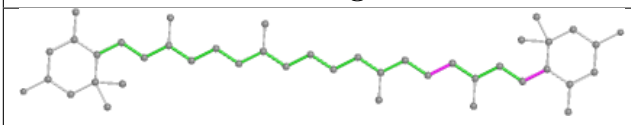

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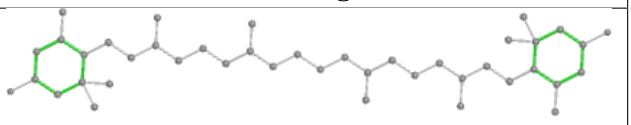
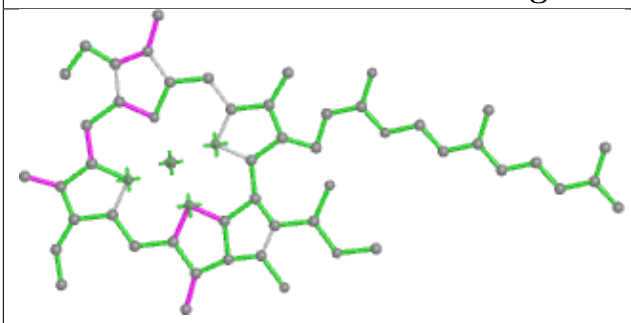


Rings

Ligand CLA s 308



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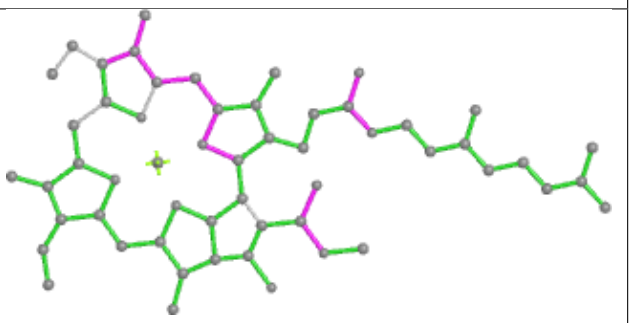
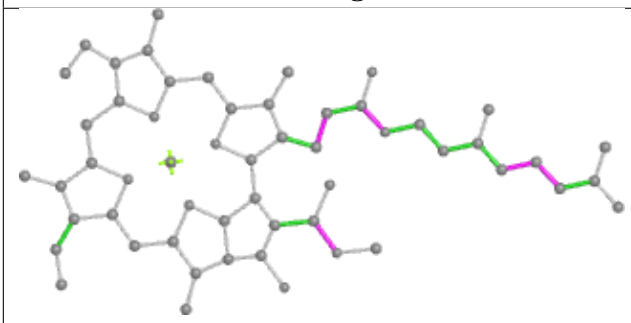


Bond angles



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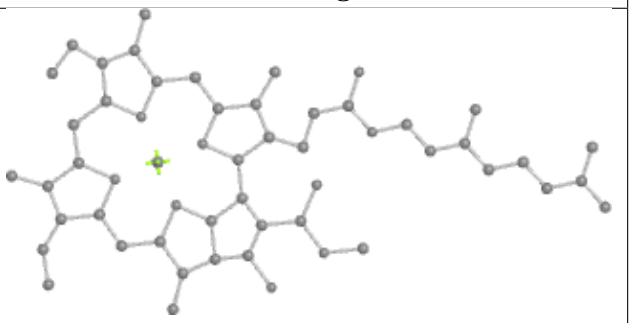
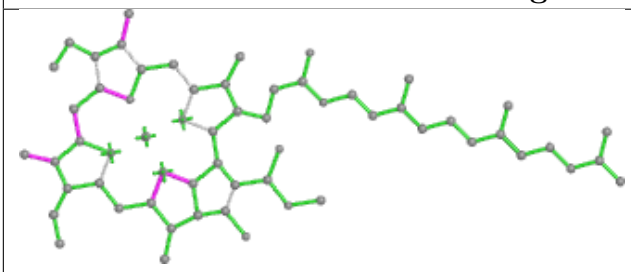


Rings

Ligand CLA r 609



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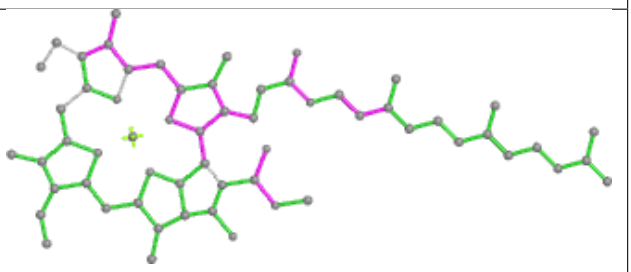
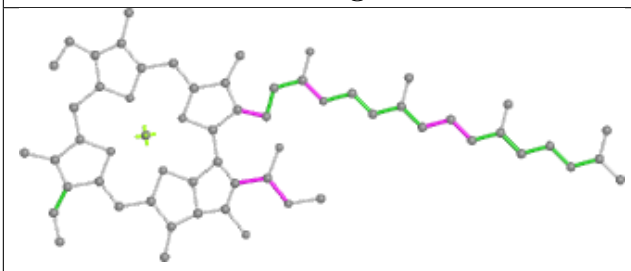


Bond angles



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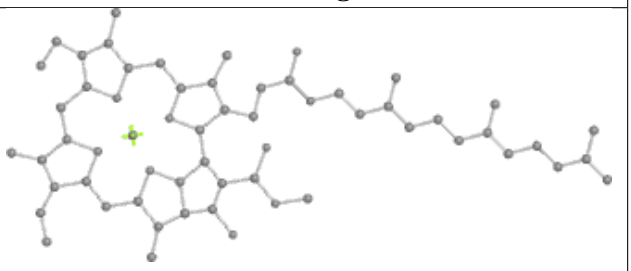
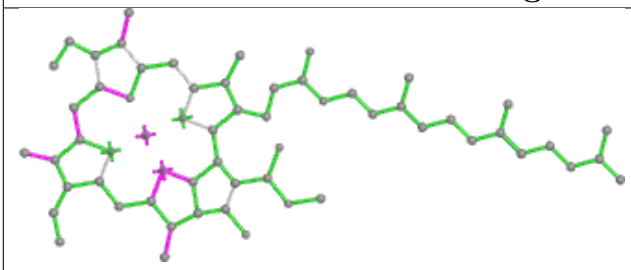
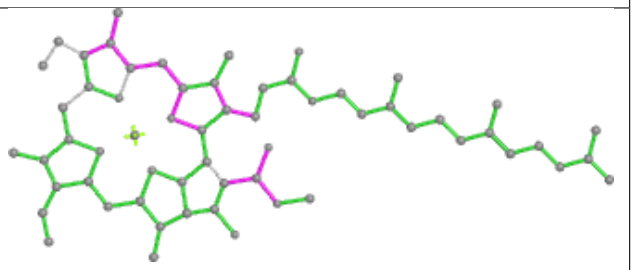
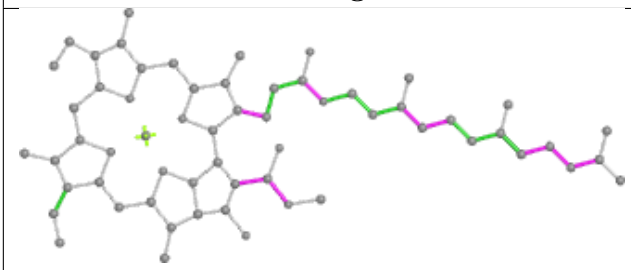
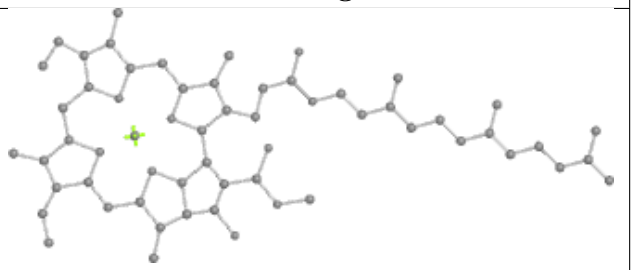
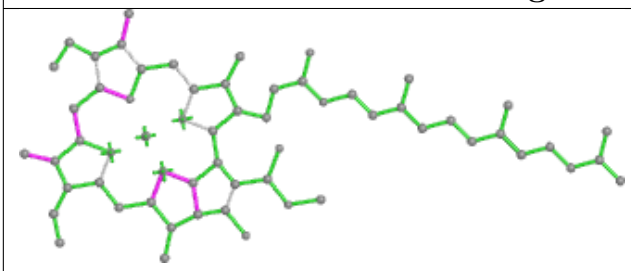
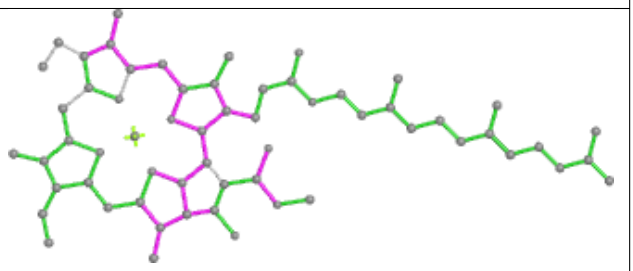
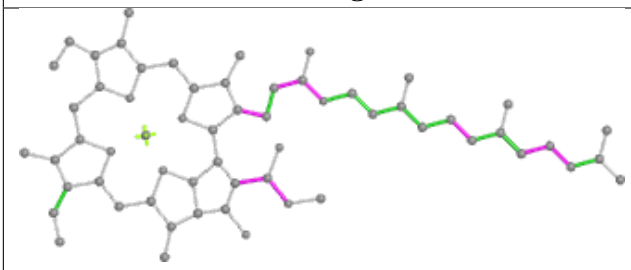
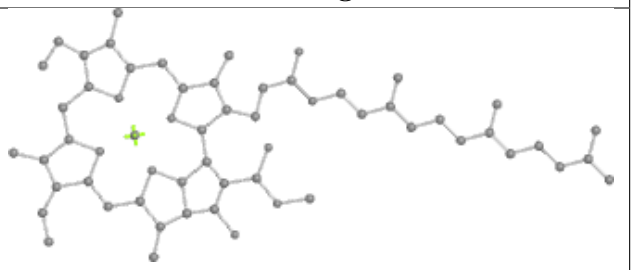
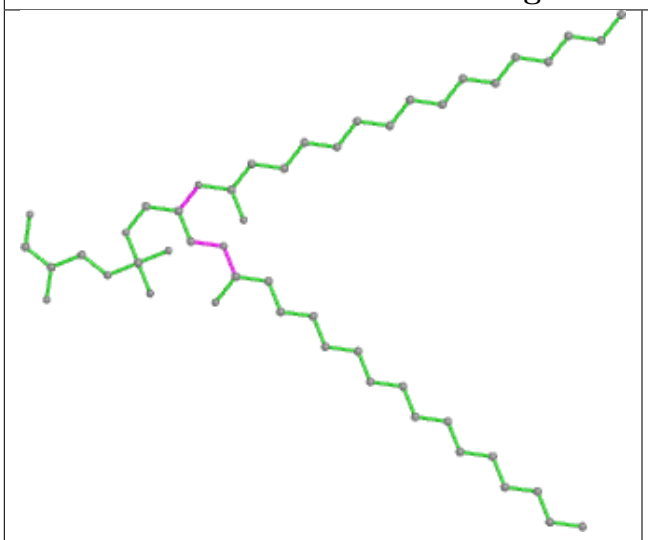


Rings

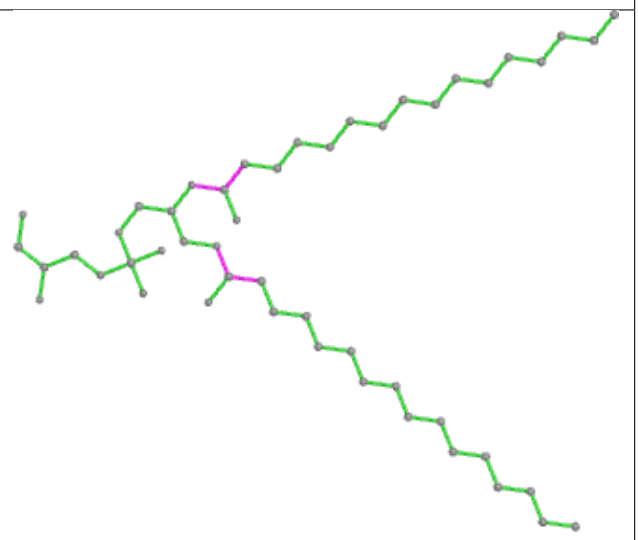
Ligand CLA A 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

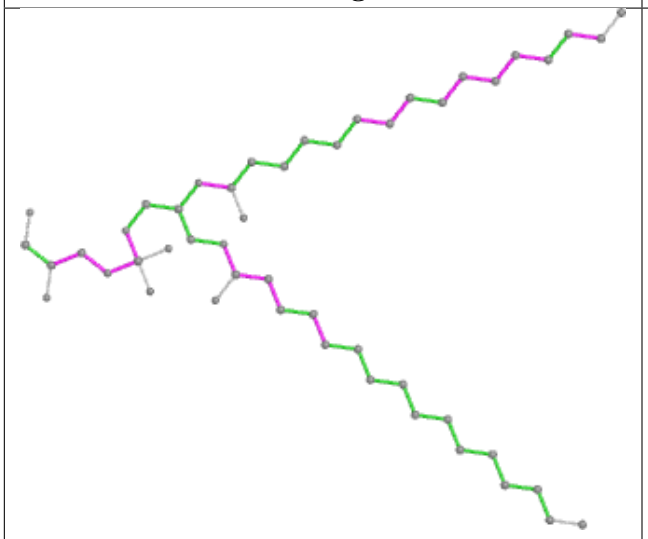
Ligand LHG C 523



Bond lengths



Bond angles



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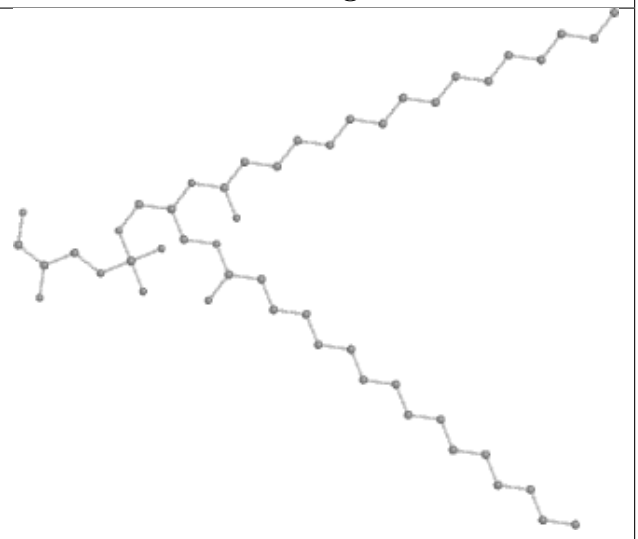
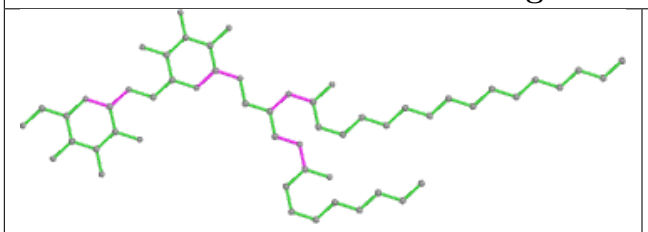


Rings

Ligand DGD c 517



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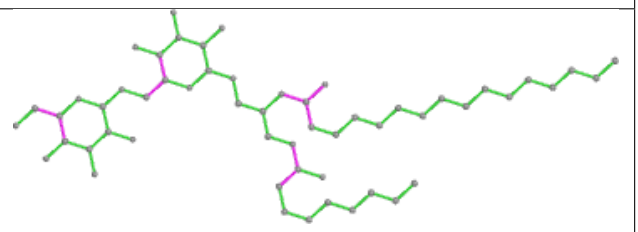

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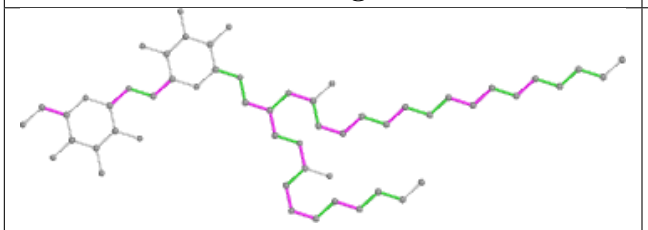

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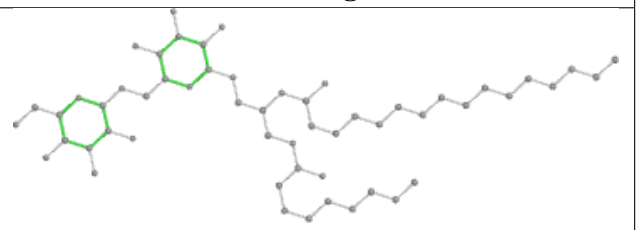
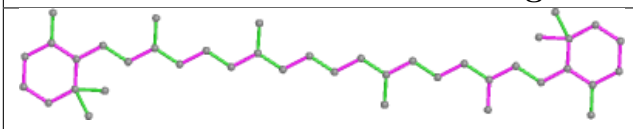


Rings

Ligand BCR b 618



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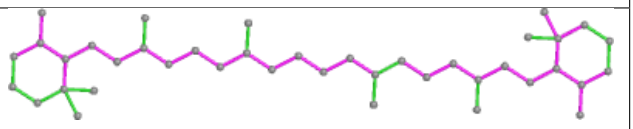

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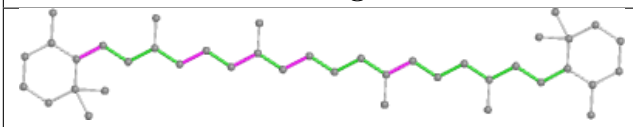

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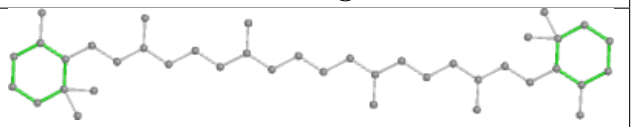
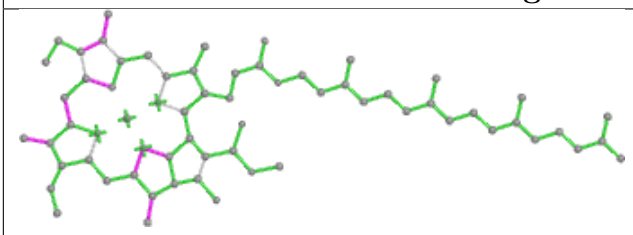


Rings

Ligand CLA U 302



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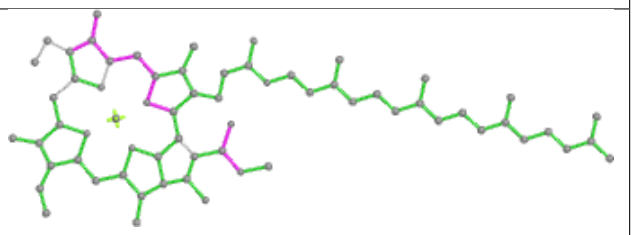
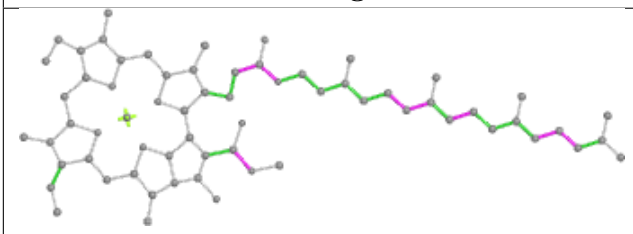


Bond angles



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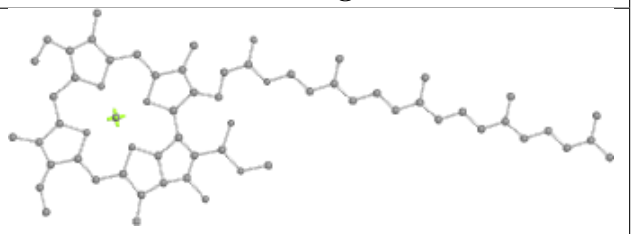
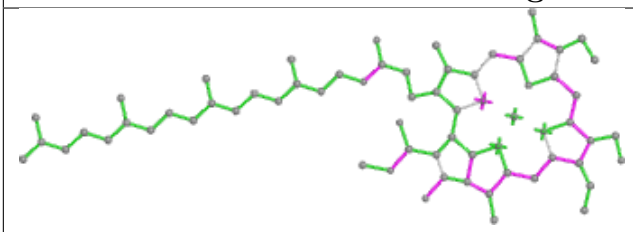


Rings

Ligand CHL n 313



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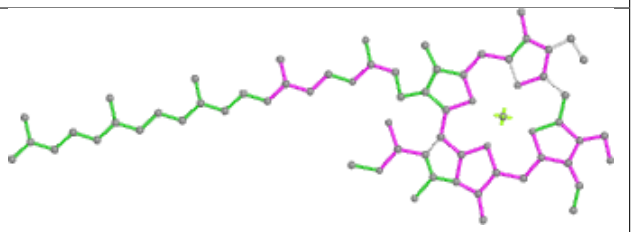

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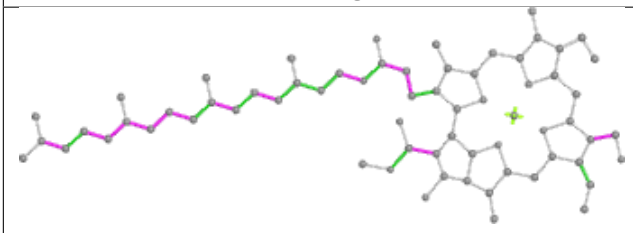

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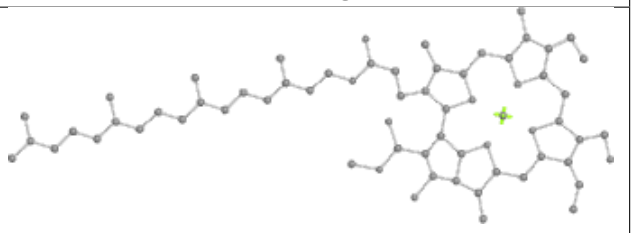
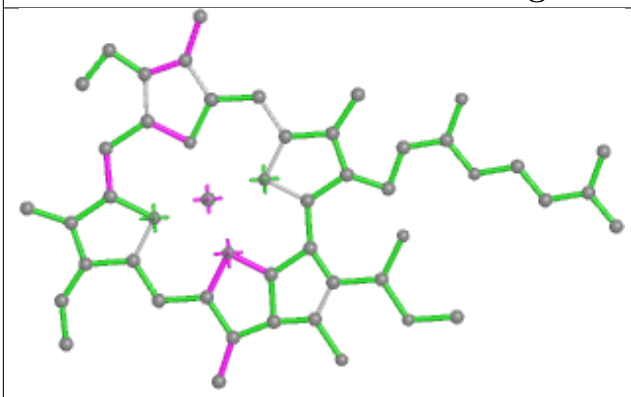
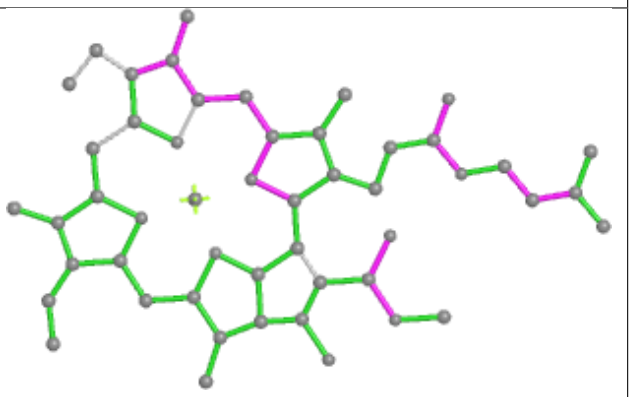
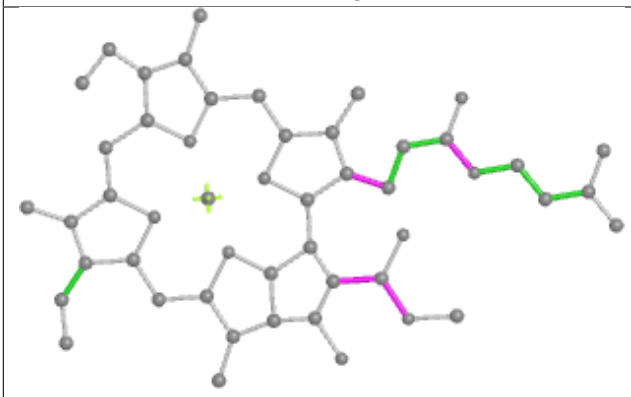
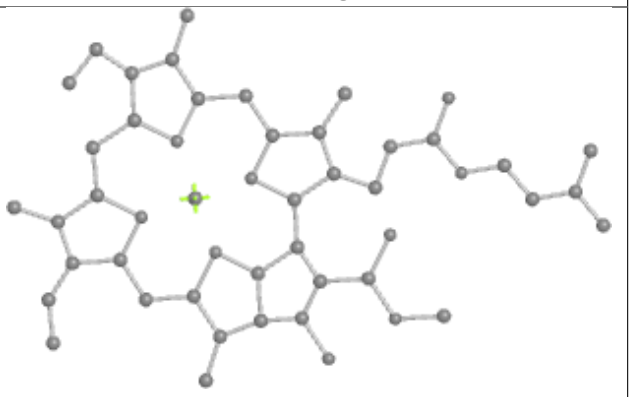
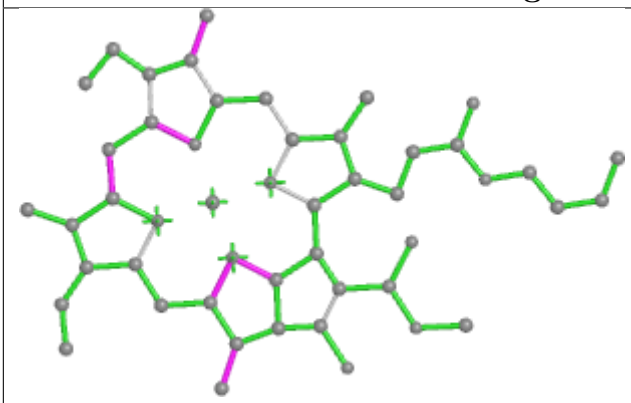


Rings

Ligand CLA 4 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 308



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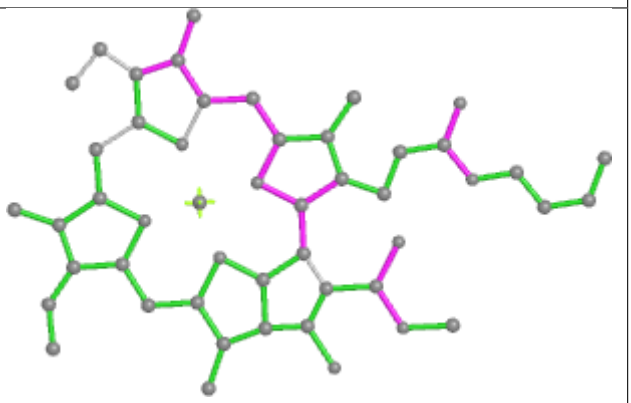
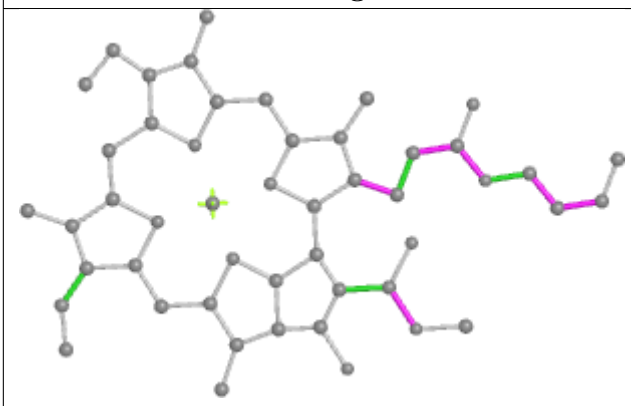


Bond angles



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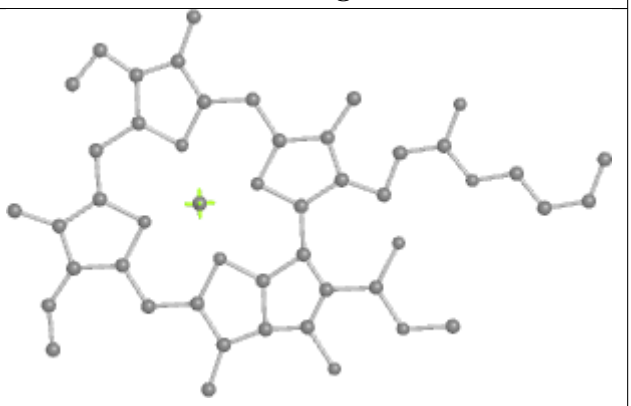
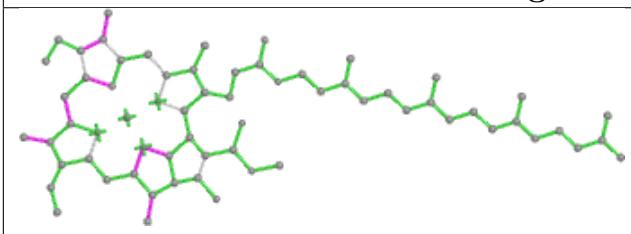


Rings

Ligand CLA 2 302



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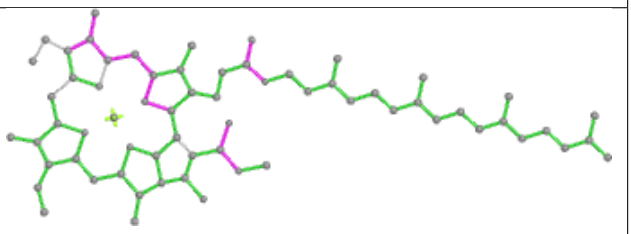

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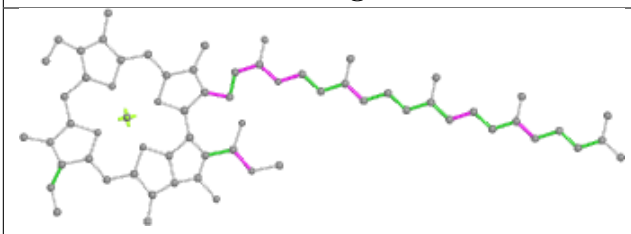

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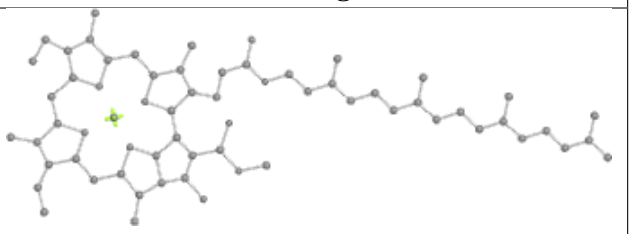
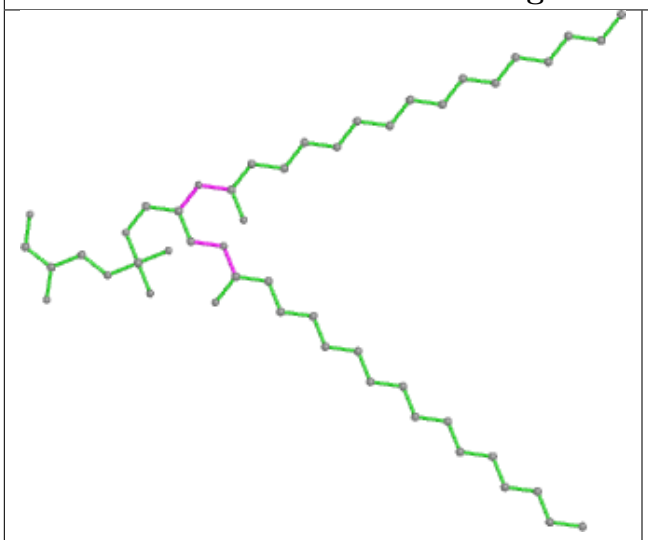


Rings

Ligand LHG b 623



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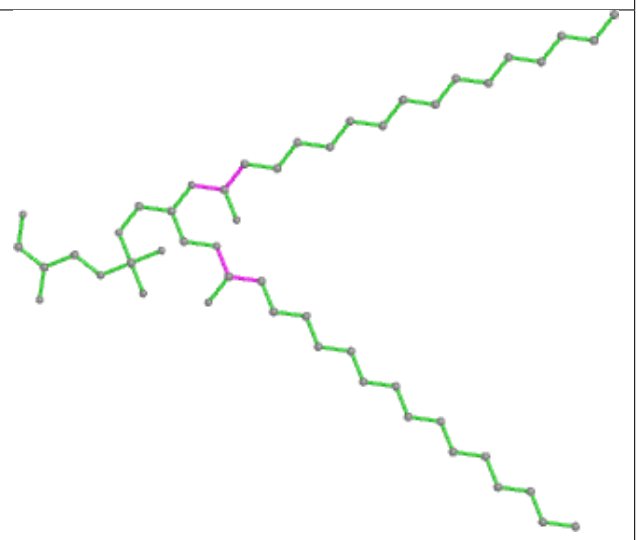
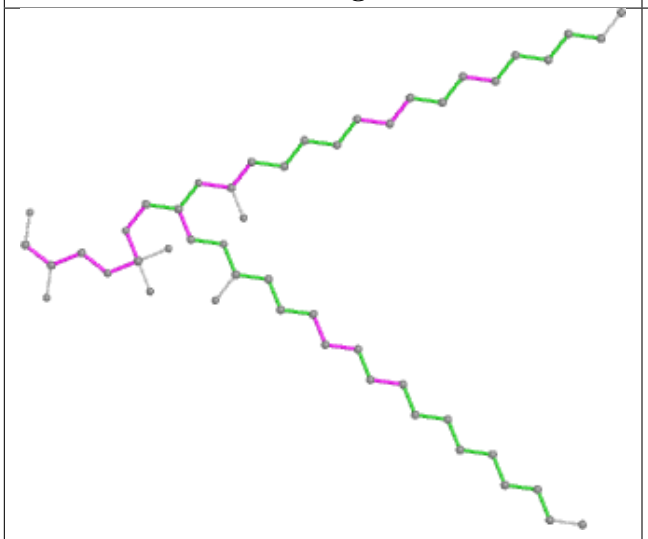


Bond angles



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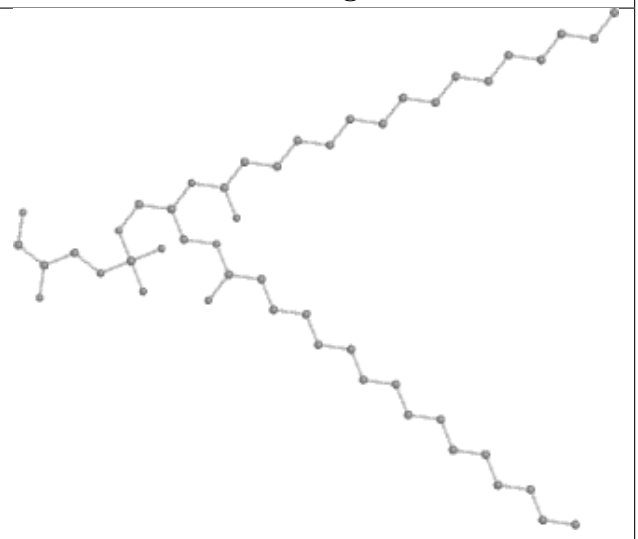
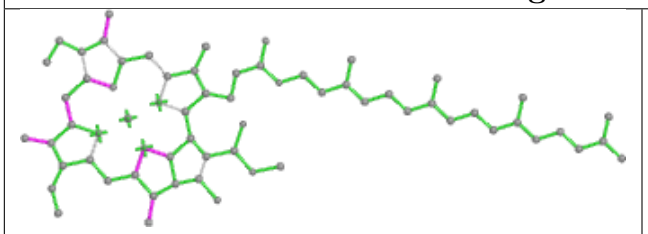


Rings

Ligand CLA n 304



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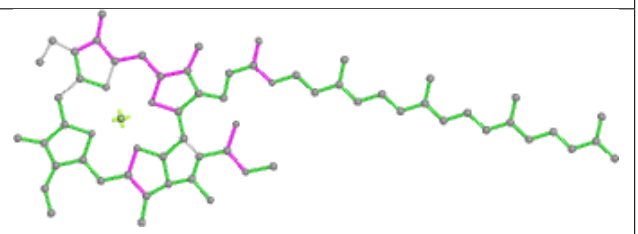
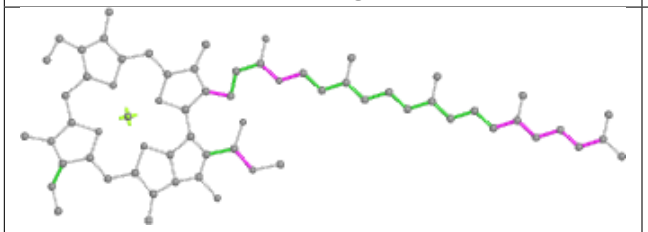


Bond angles



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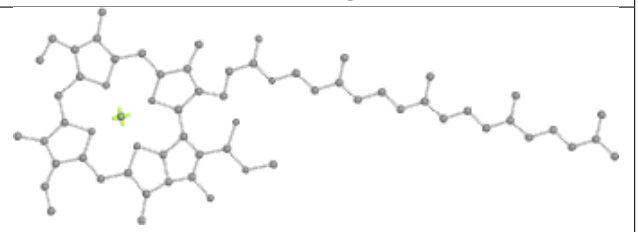
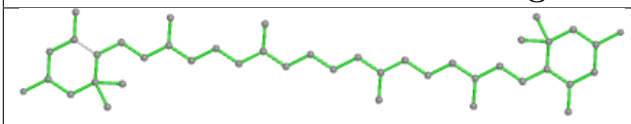
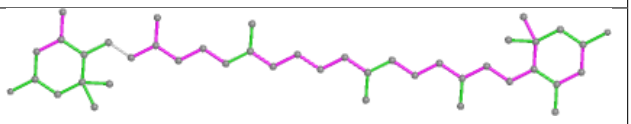
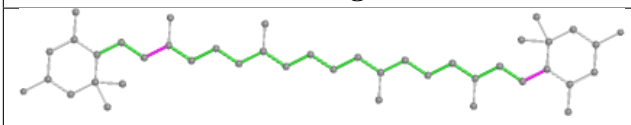
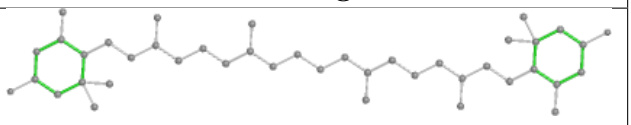
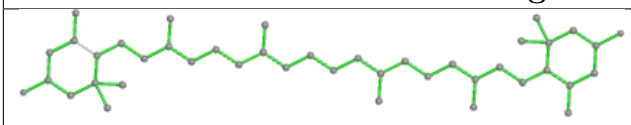
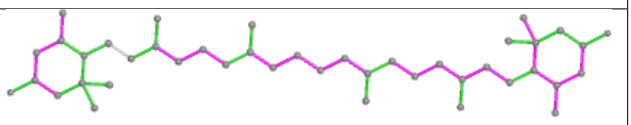
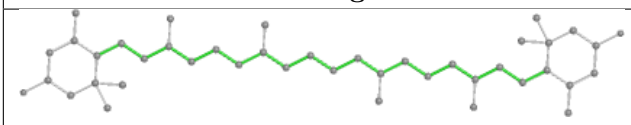
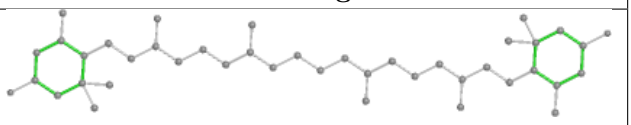
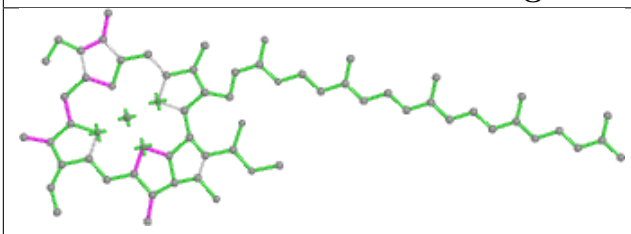
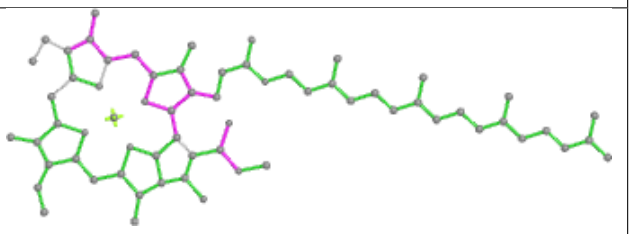
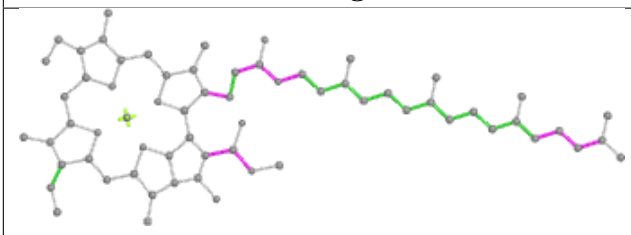
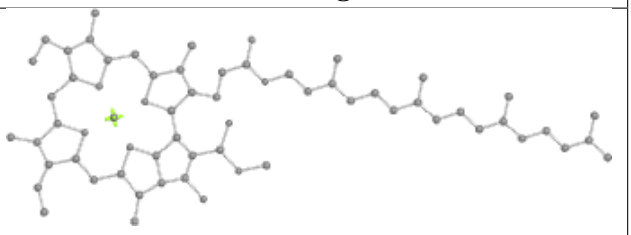
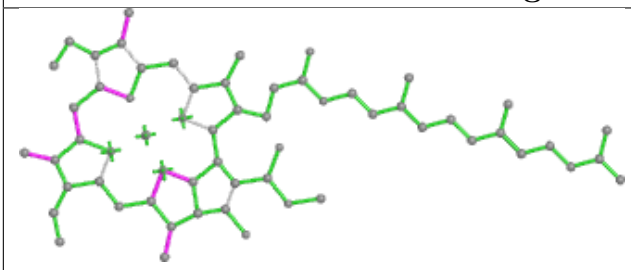
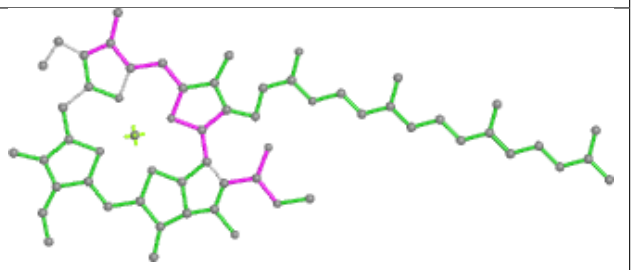
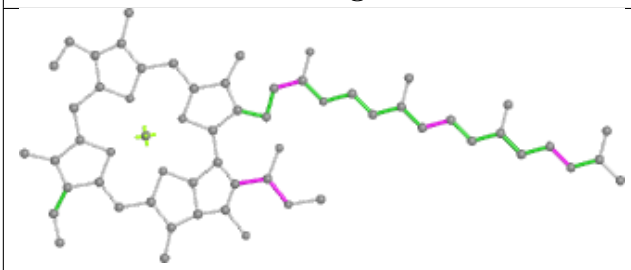
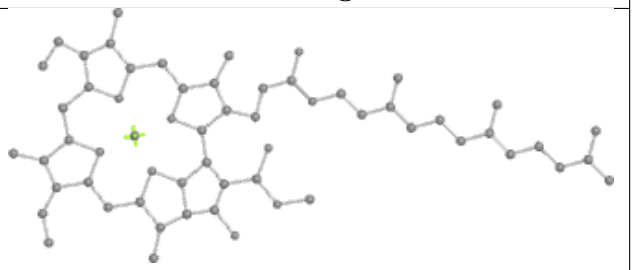


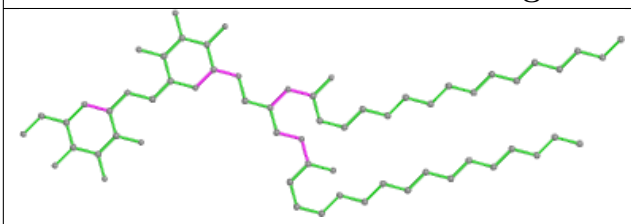
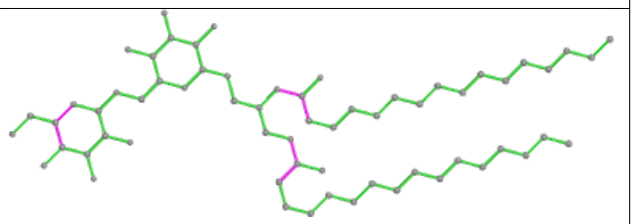
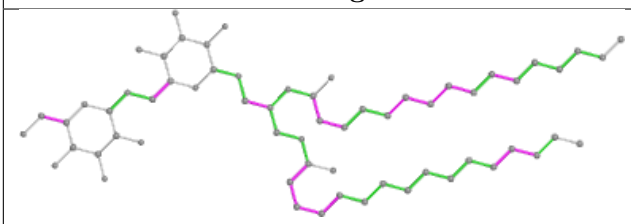
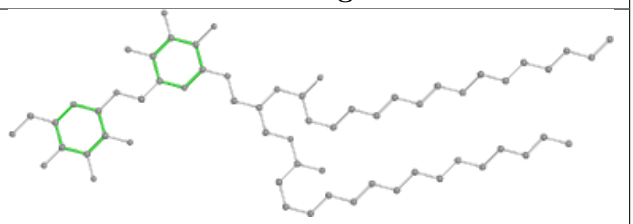
Rings

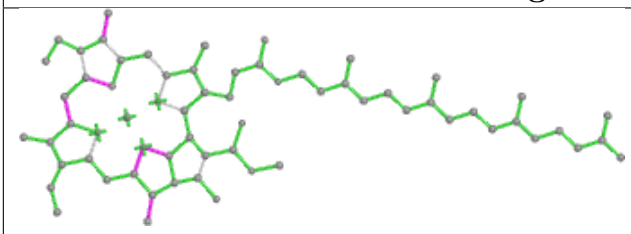
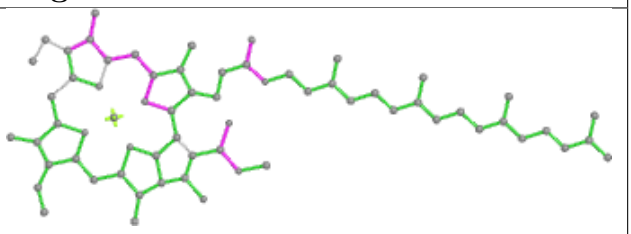
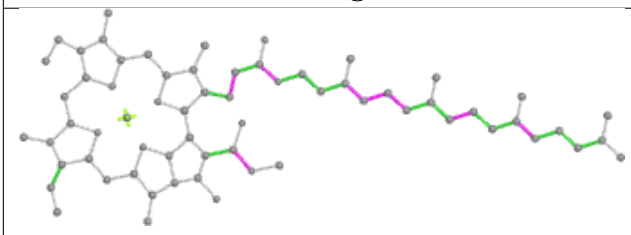
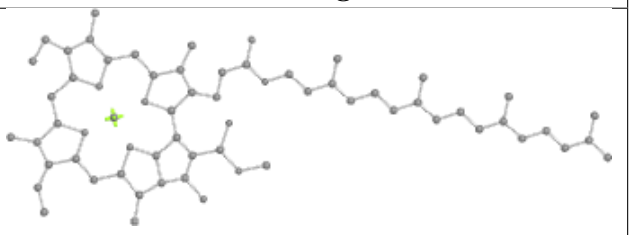
Ligand LUT 2 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

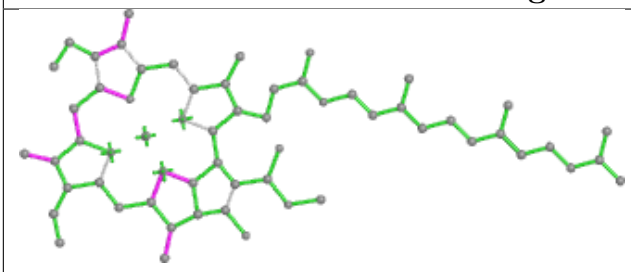
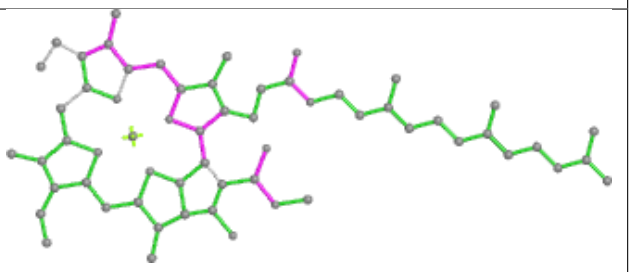
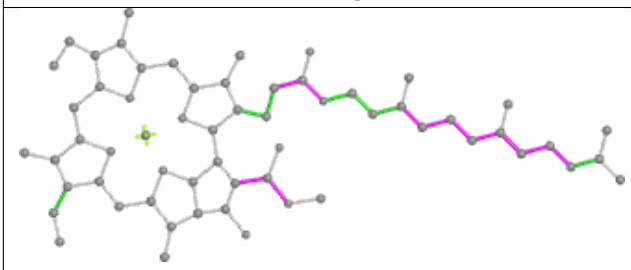
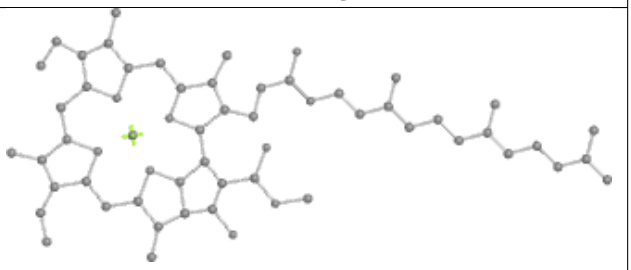
Ligand LUT 1 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

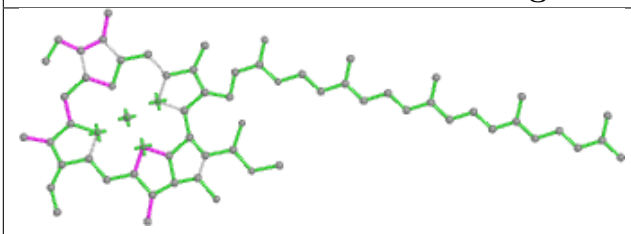
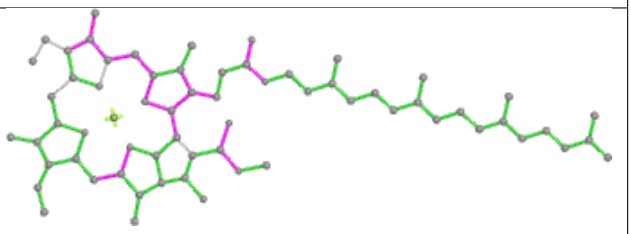
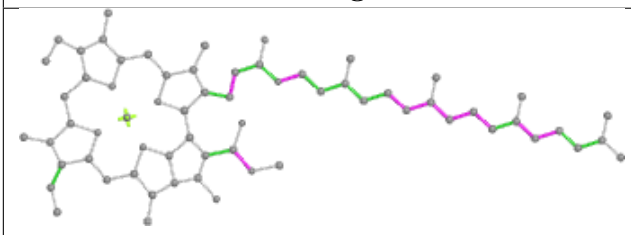
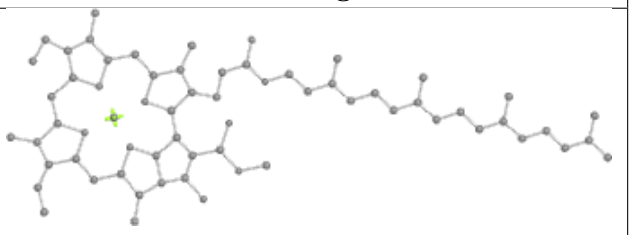
Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

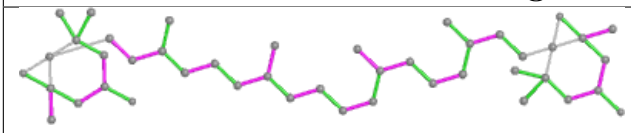
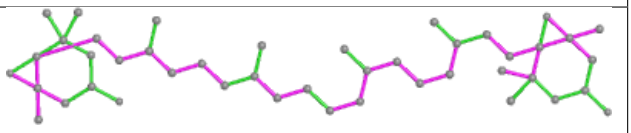
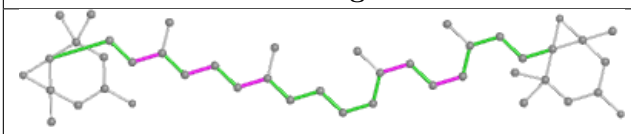
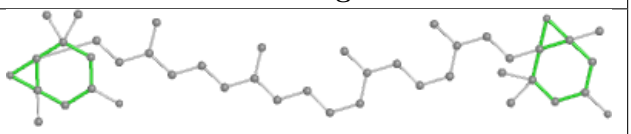
Ligand CLA V 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD b 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

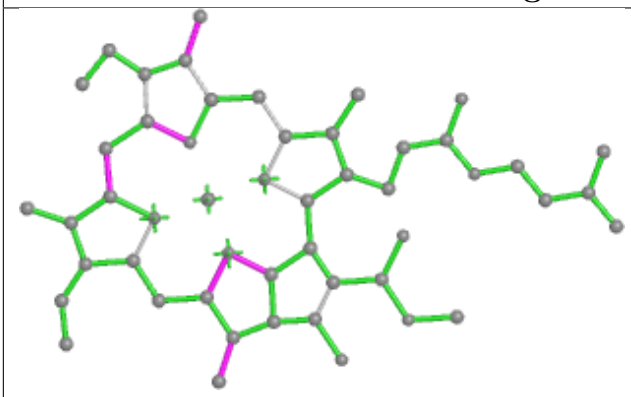
Ligand CLA g 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT 1 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 303



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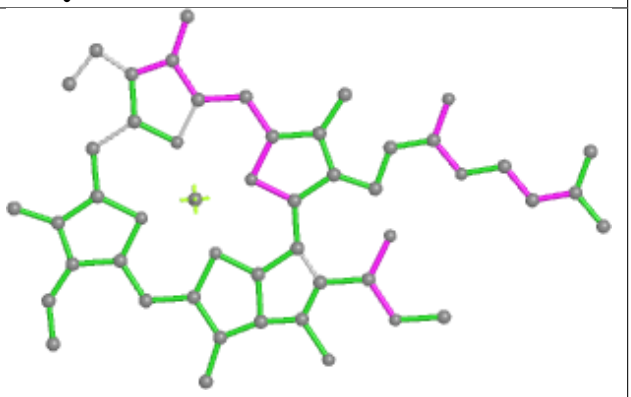
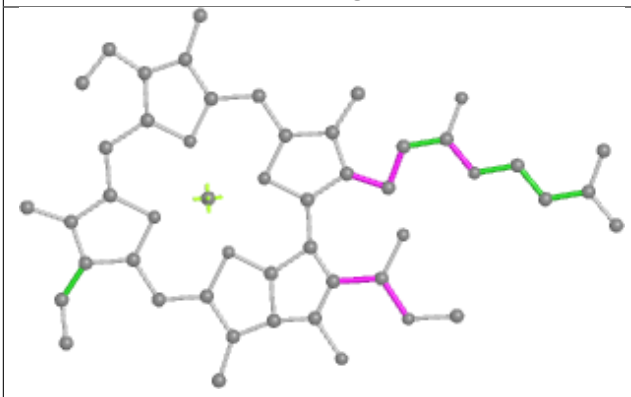


Bond angles



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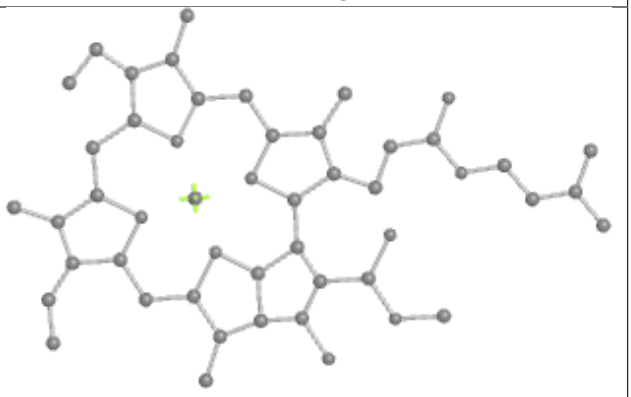
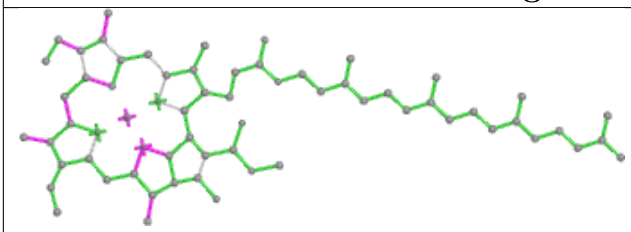
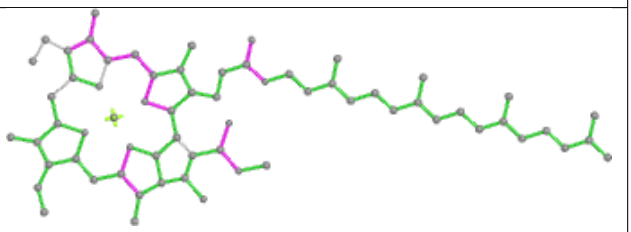


Rings

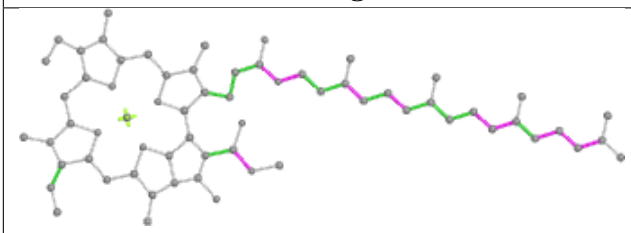
Ligand CLA D 403



Bond lengths



Bond angles



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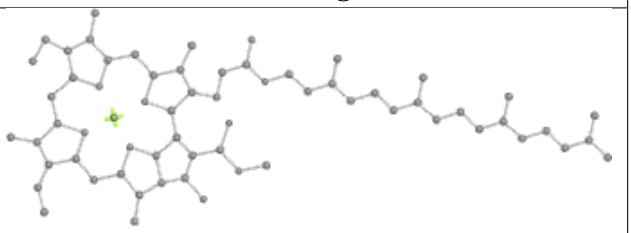
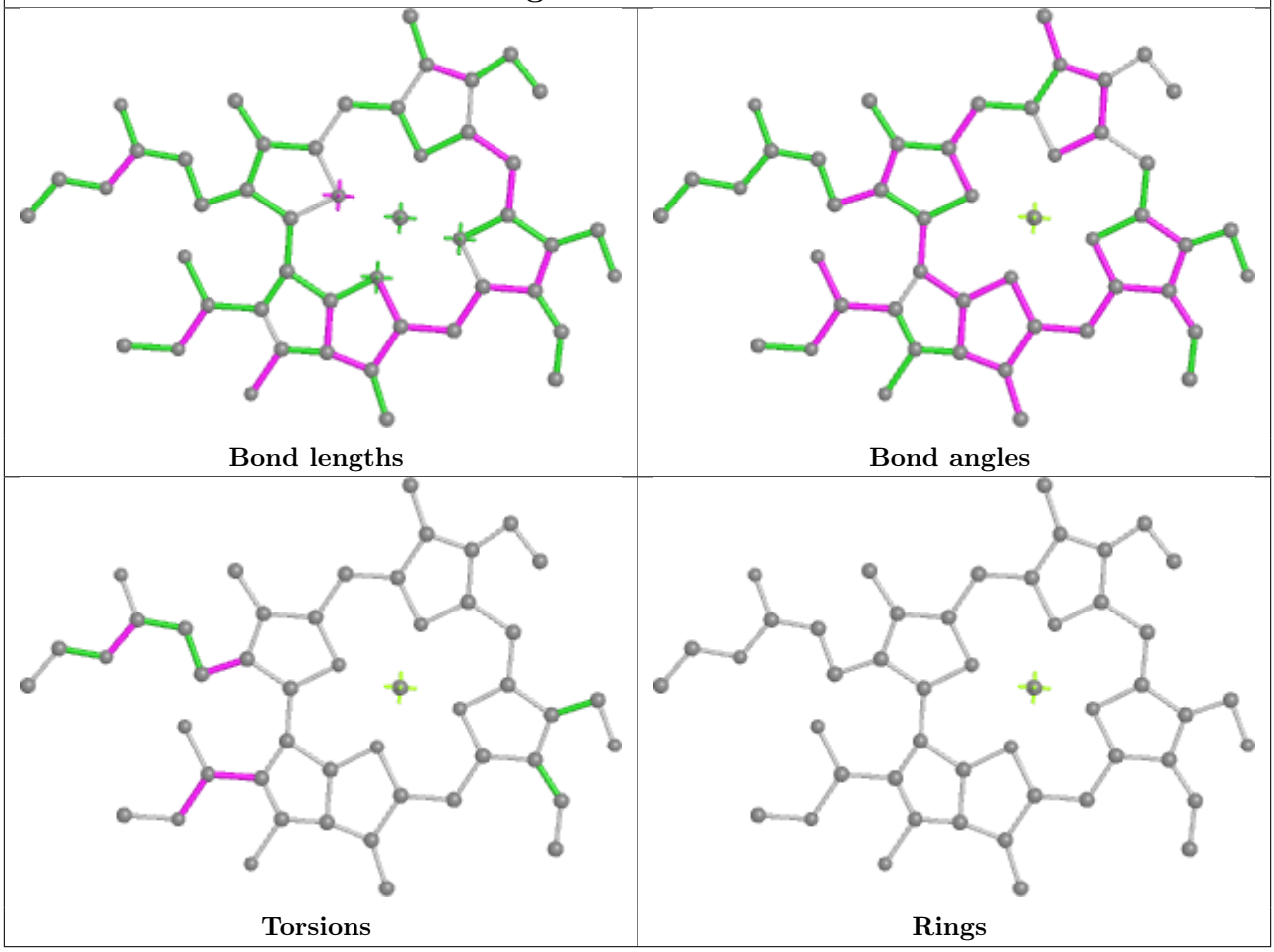
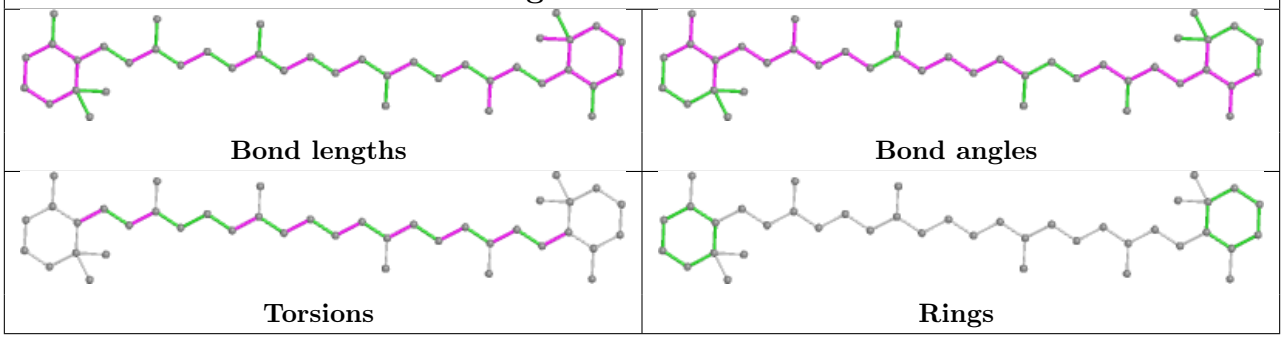


Rings

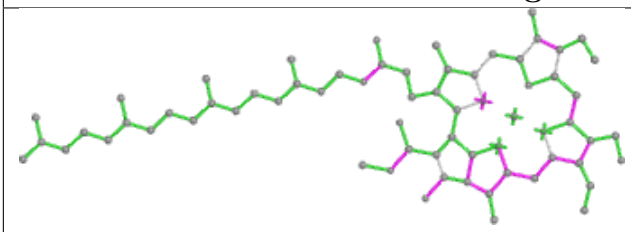
Ligand CHL r 619



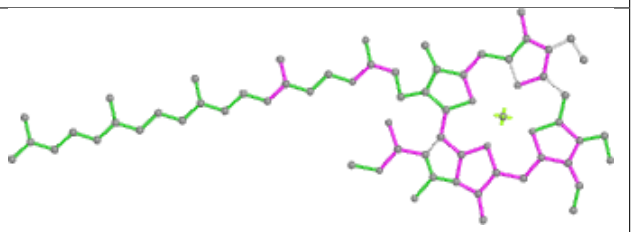
Ligand BCR b 619



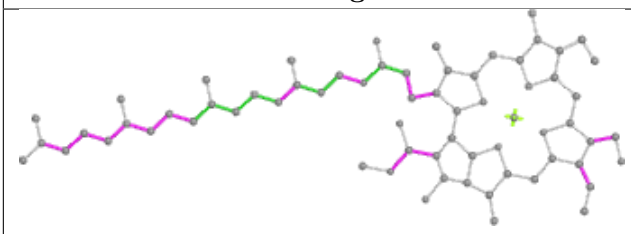
Ligand CHL P 319



Bond lengths



Bond angles



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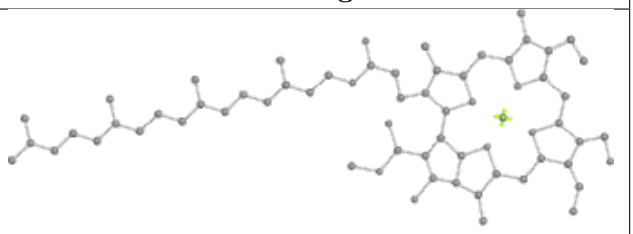
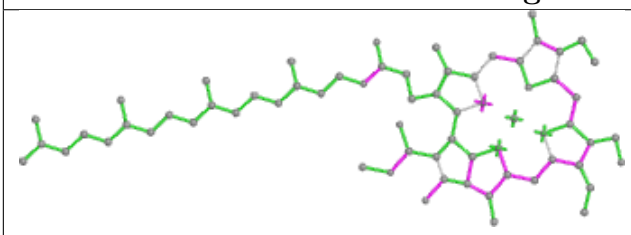
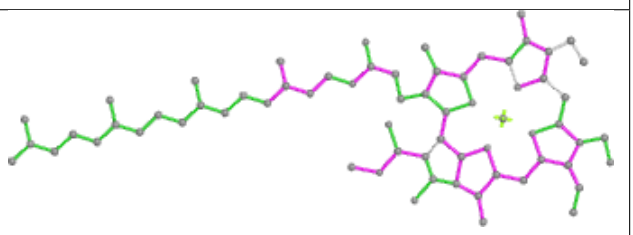


Rings

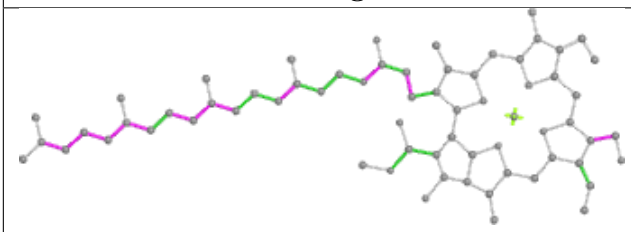
Ligand CHL V 316



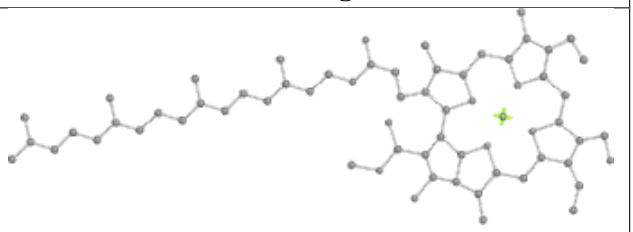
Bond lengths



Bond angles

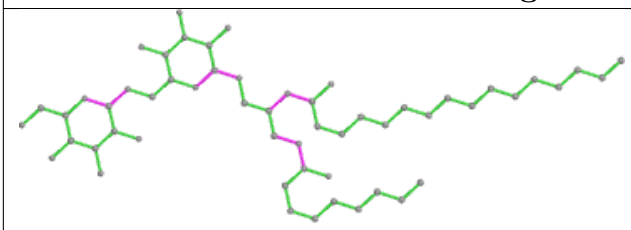


Torsions

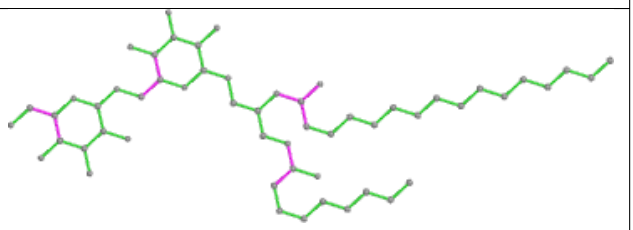


Rings

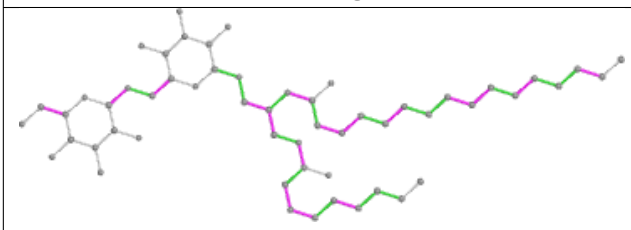
Ligand DGD C 519



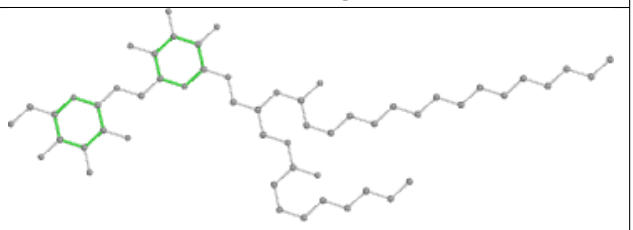
Bond lengths



Bond angles

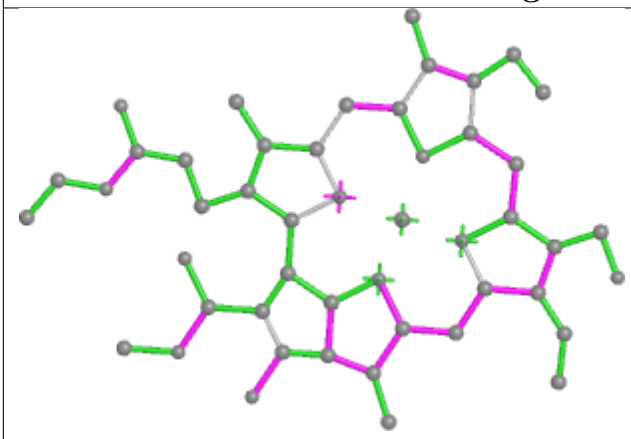


Torsions



Rings

Ligand CHL N 314



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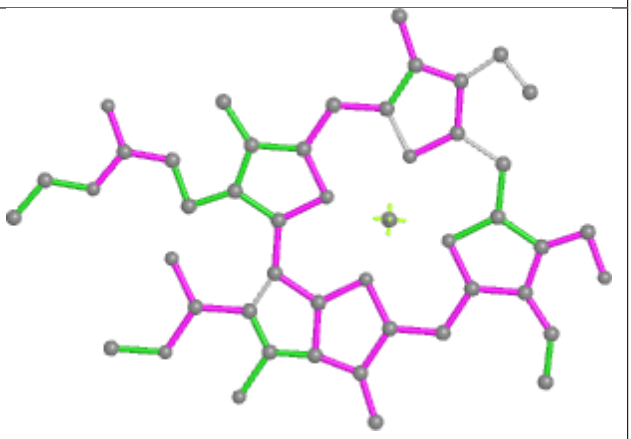
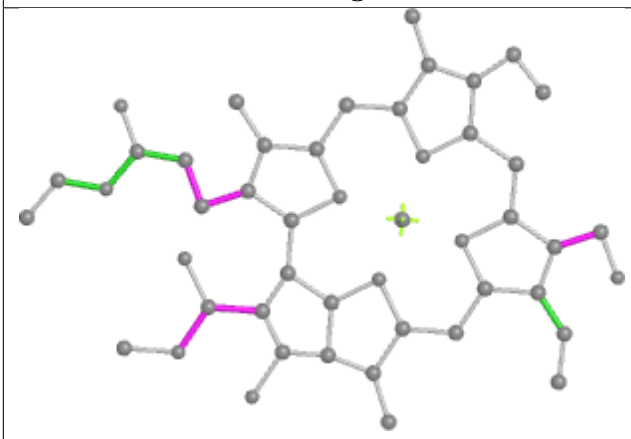


Bond angles



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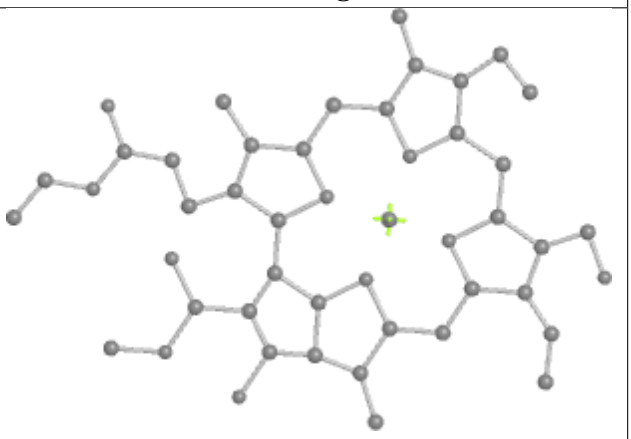
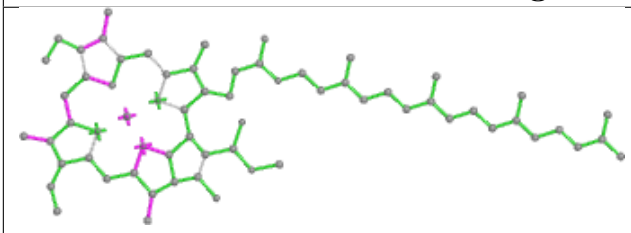


Rings

Ligand CLA c 512



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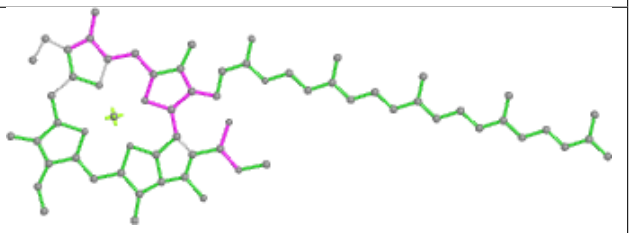
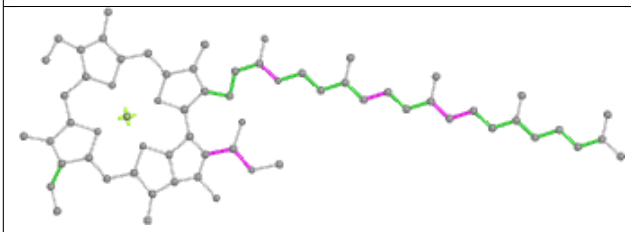


Bond angles



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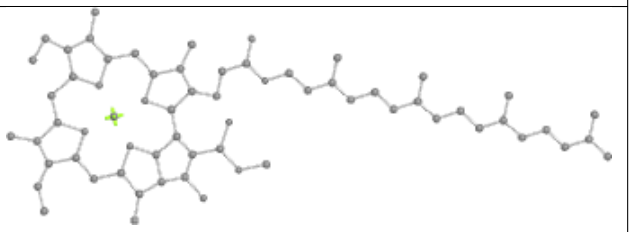
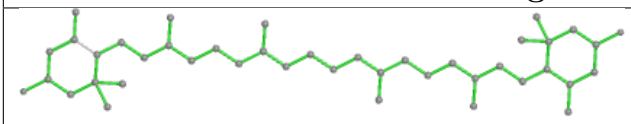


Rings

Ligand LUT n 310



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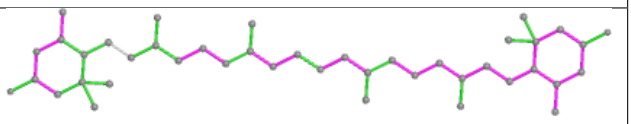
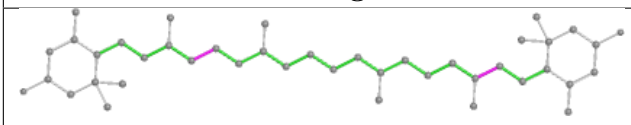


Bond angles



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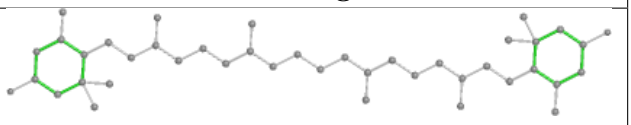
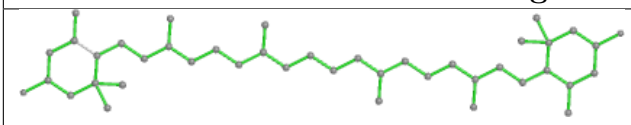
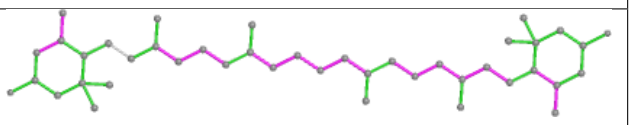


Rings

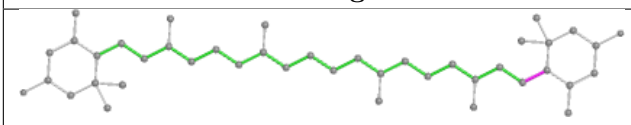
Ligand LUT r 611



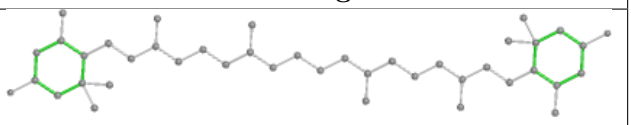
Bond lengths



Bond angles

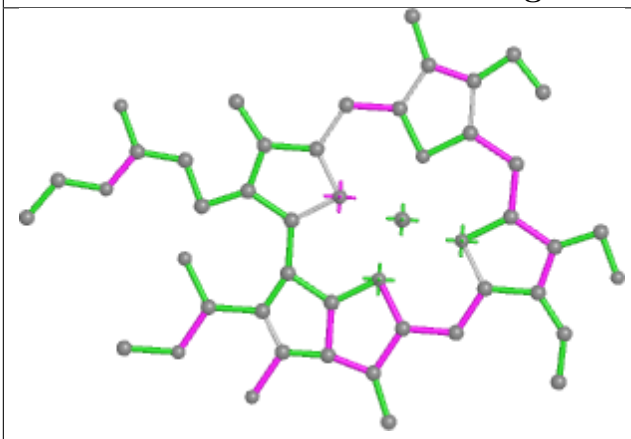


Torsions

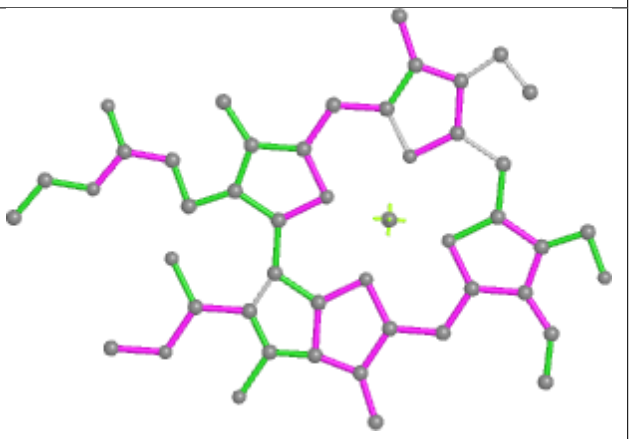


Rings

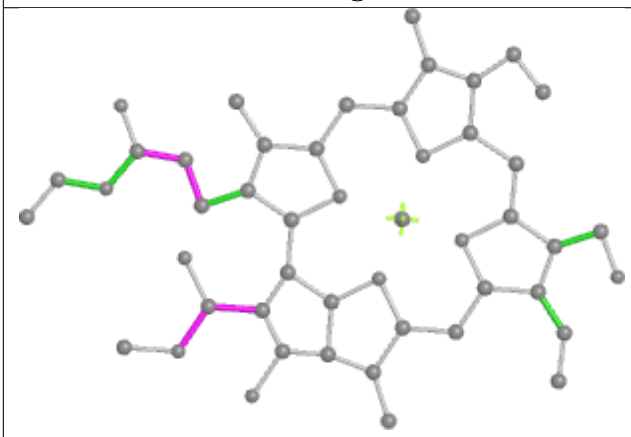
Ligand CHL P 315



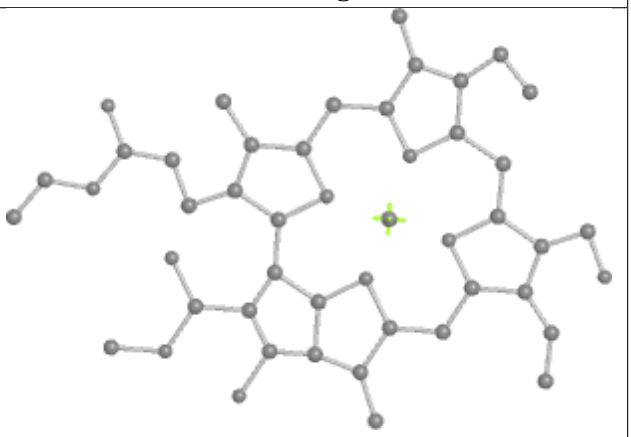
Bond lengths



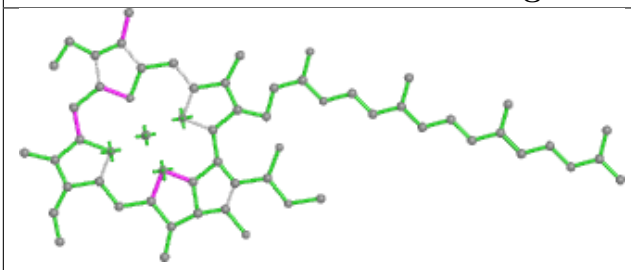
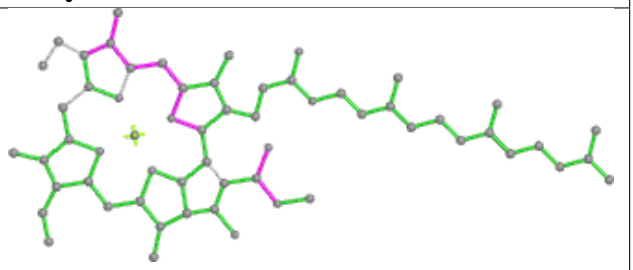
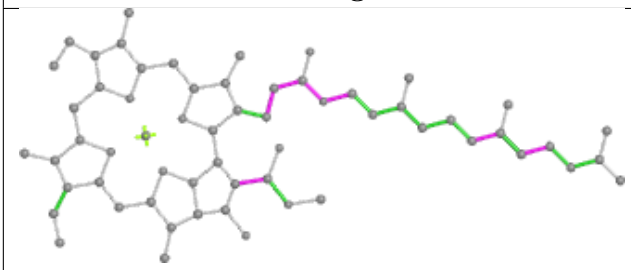
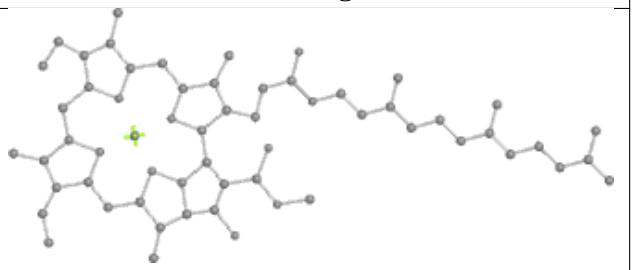
Bond angles

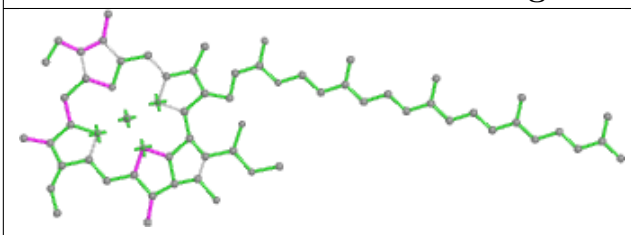
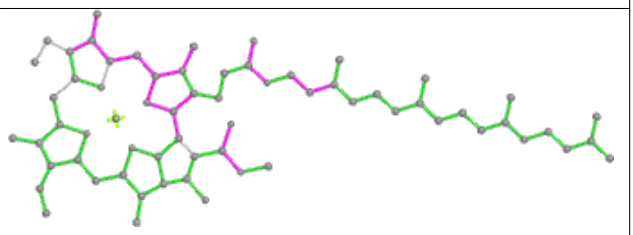
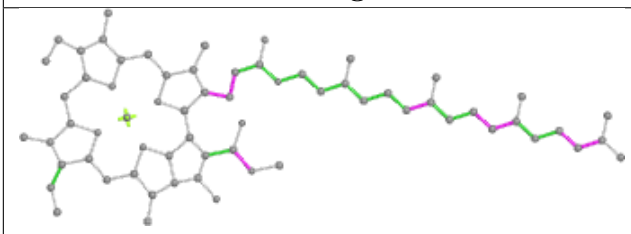
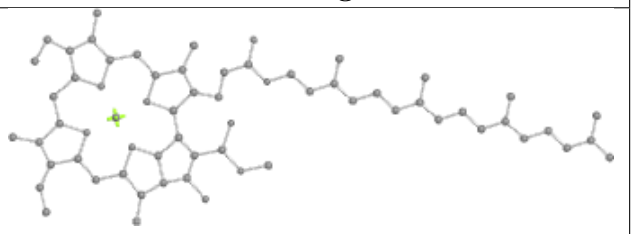


Torsions

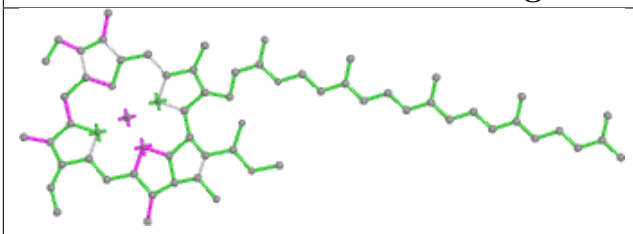


Rings

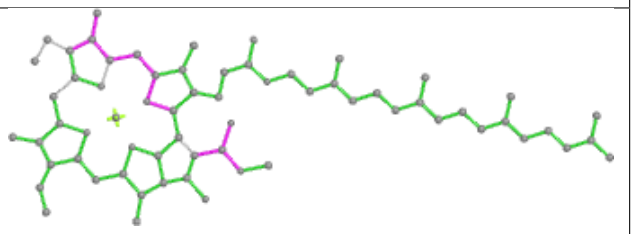
Ligand CLA Q 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

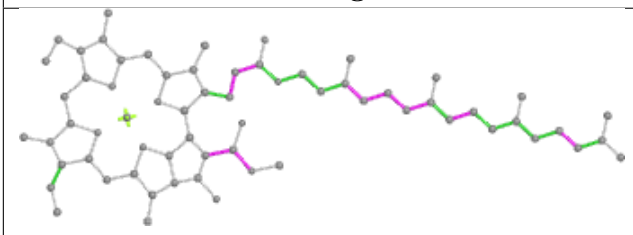
Ligand CLA B 615



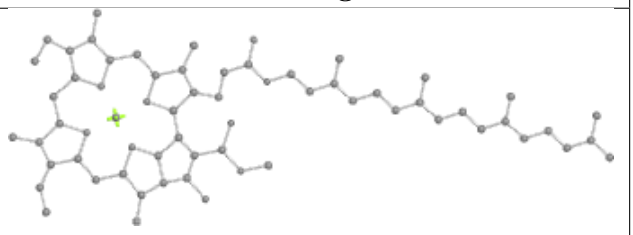
Bond lengths



Bond angles

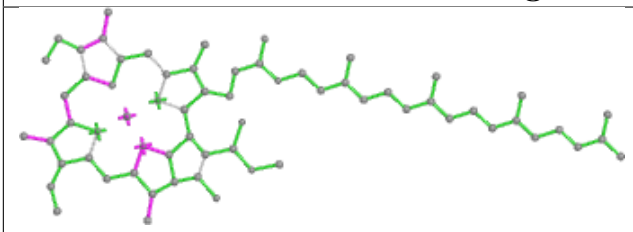


Torsions

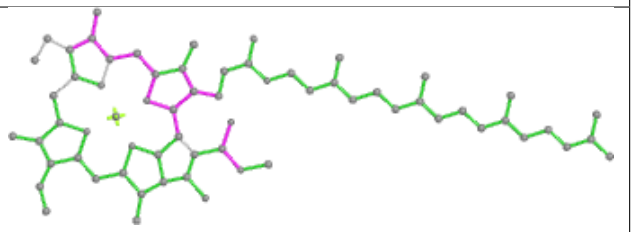


Rings

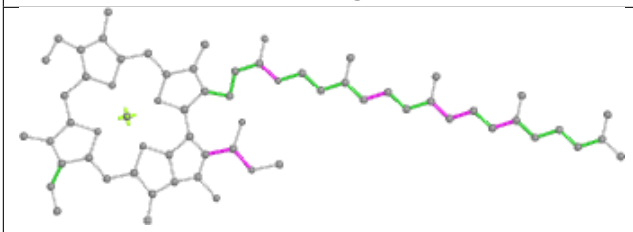
Ligand CLA C 513



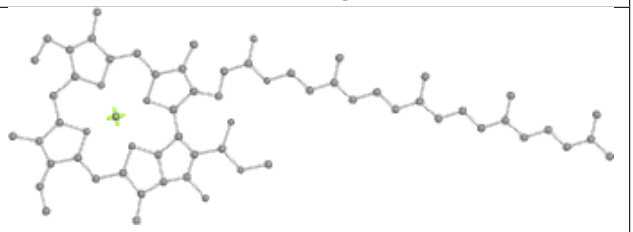
Bond lengths



Bond angles

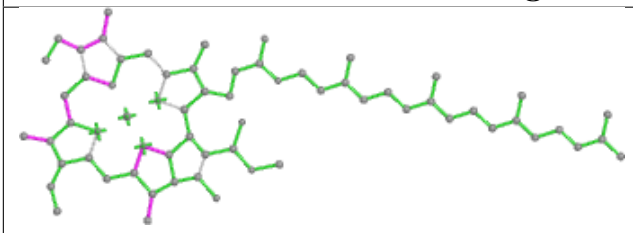


Torsions

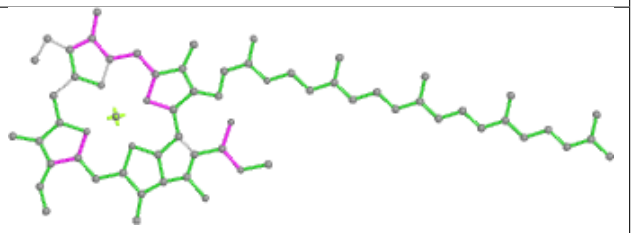


Rings

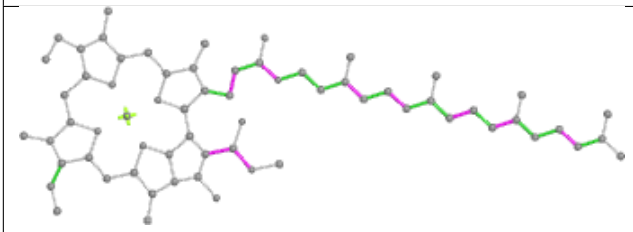
Ligand CLA C 506



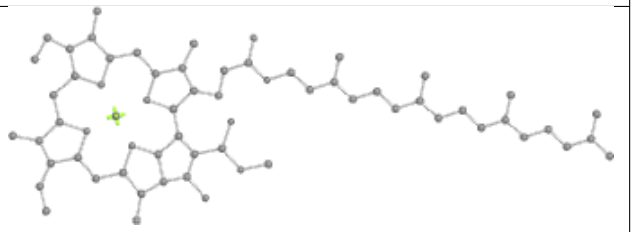
Bond lengths



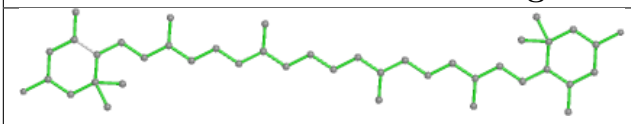
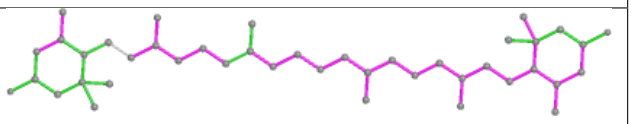
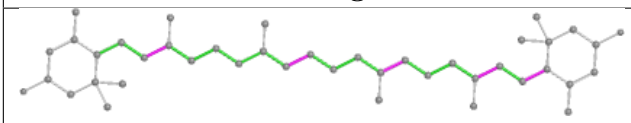
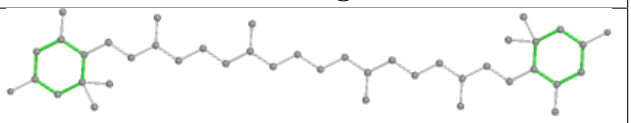
Bond angles

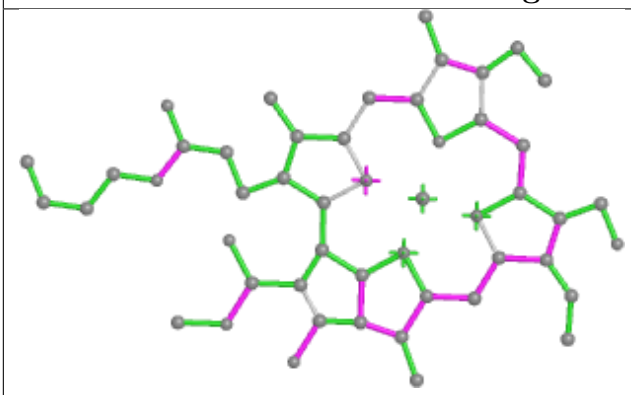
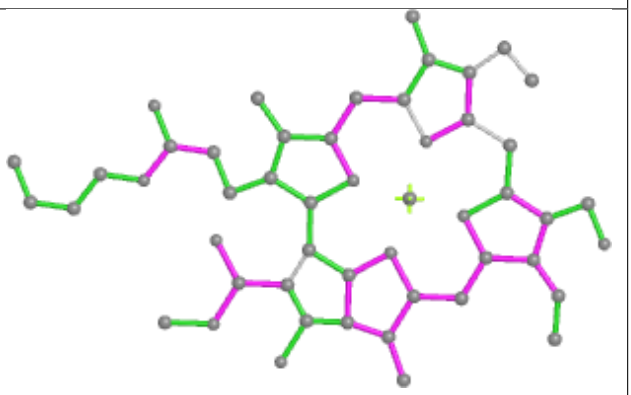
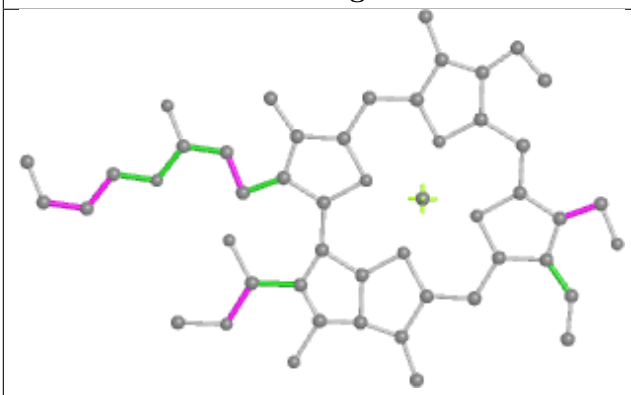
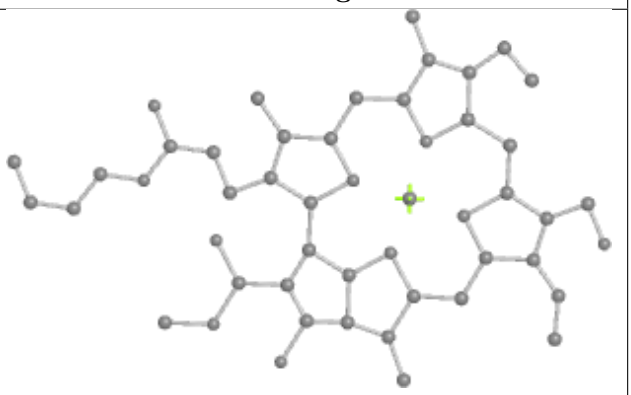


Torsions

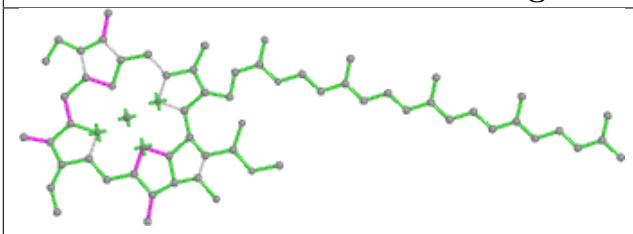


Rings

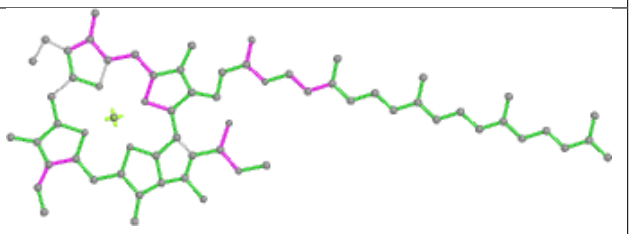
Ligand LUT S 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

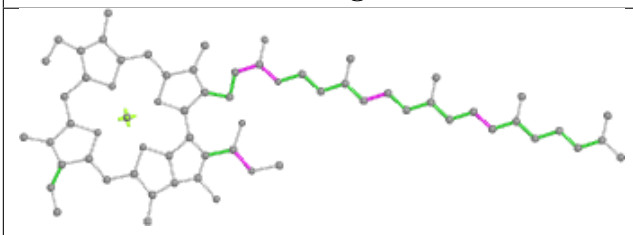
Ligand CLA 4 307



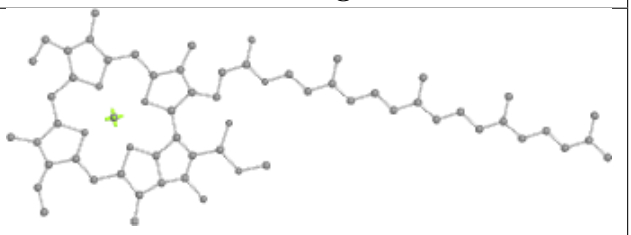
Bond lengths



Bond angles

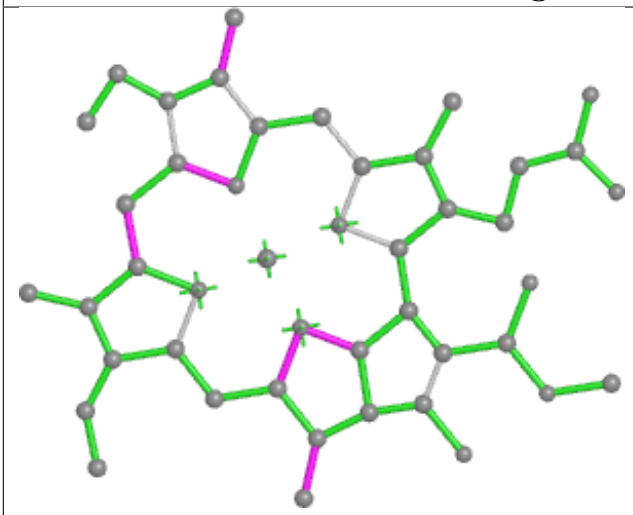


Torsions

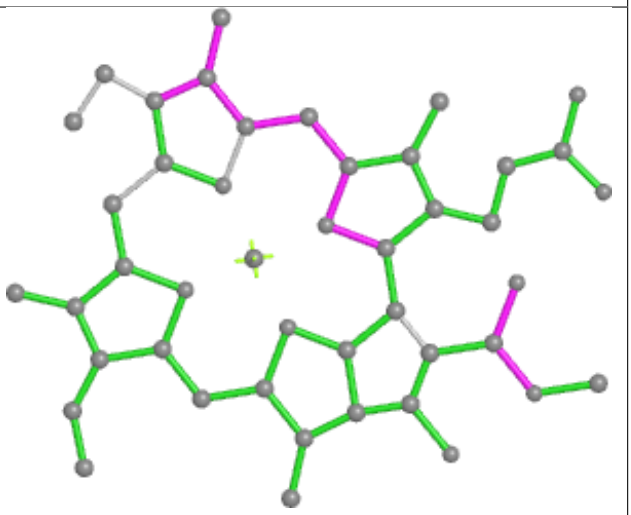


Rings

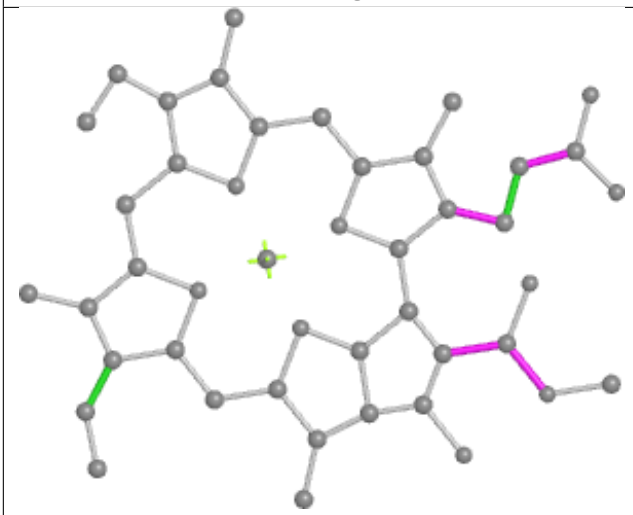
Ligand CLA r 610



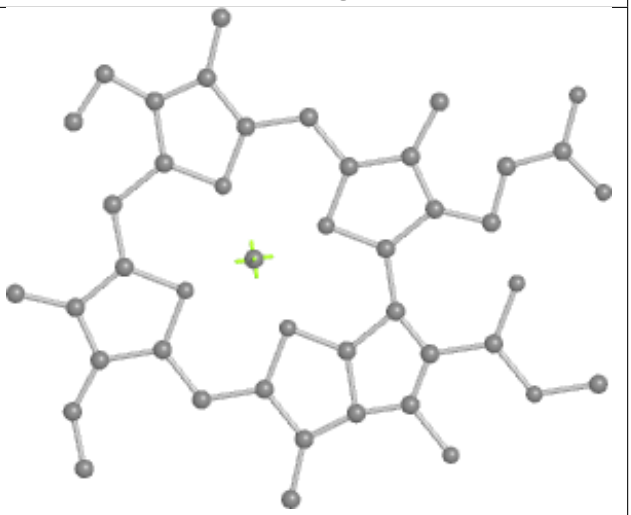
Bond lengths



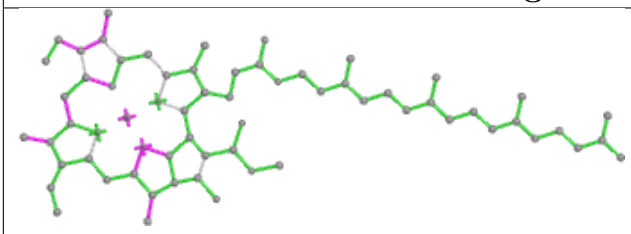
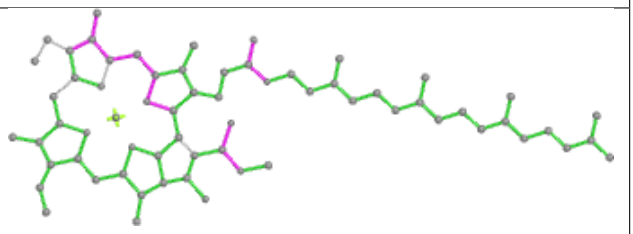
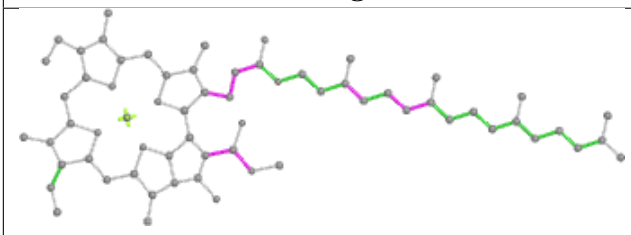
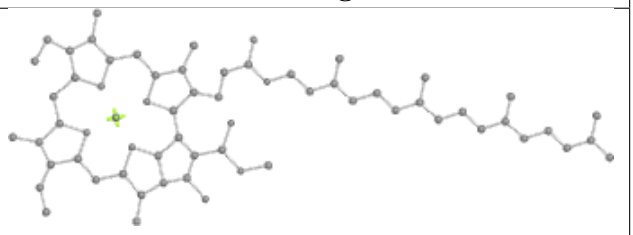
Bond angles

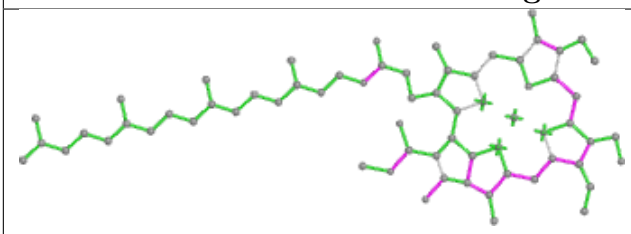
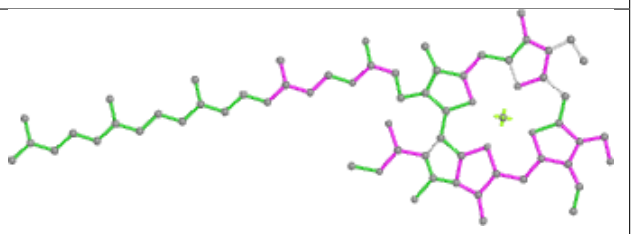
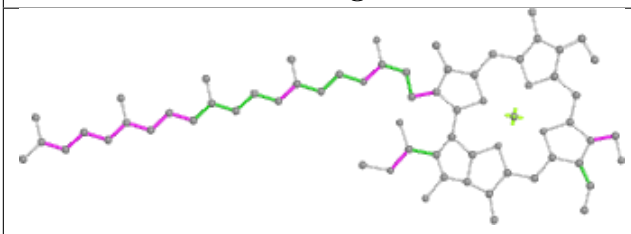
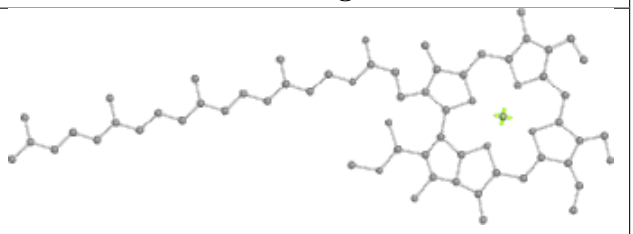


Torsions

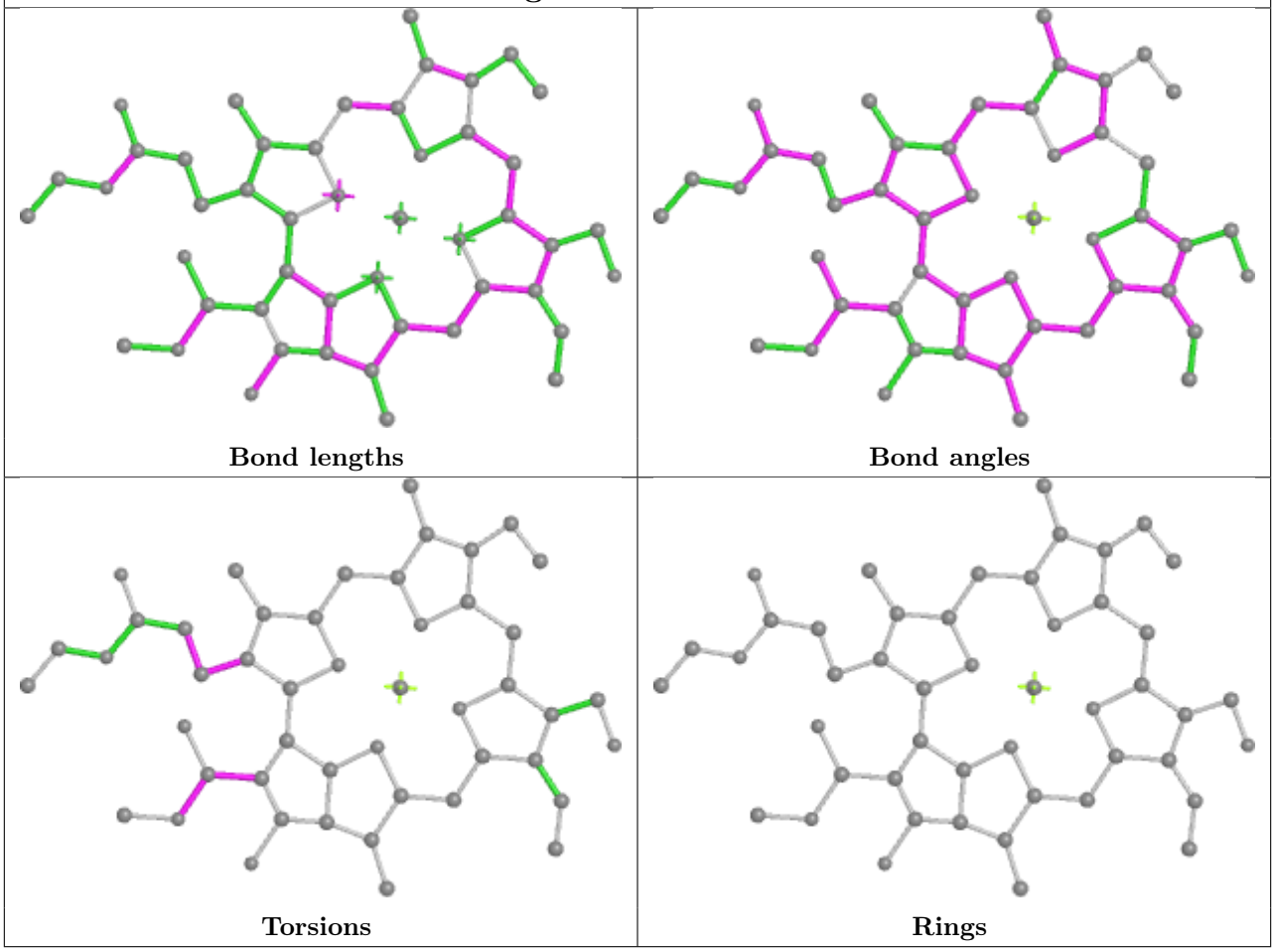


Rings

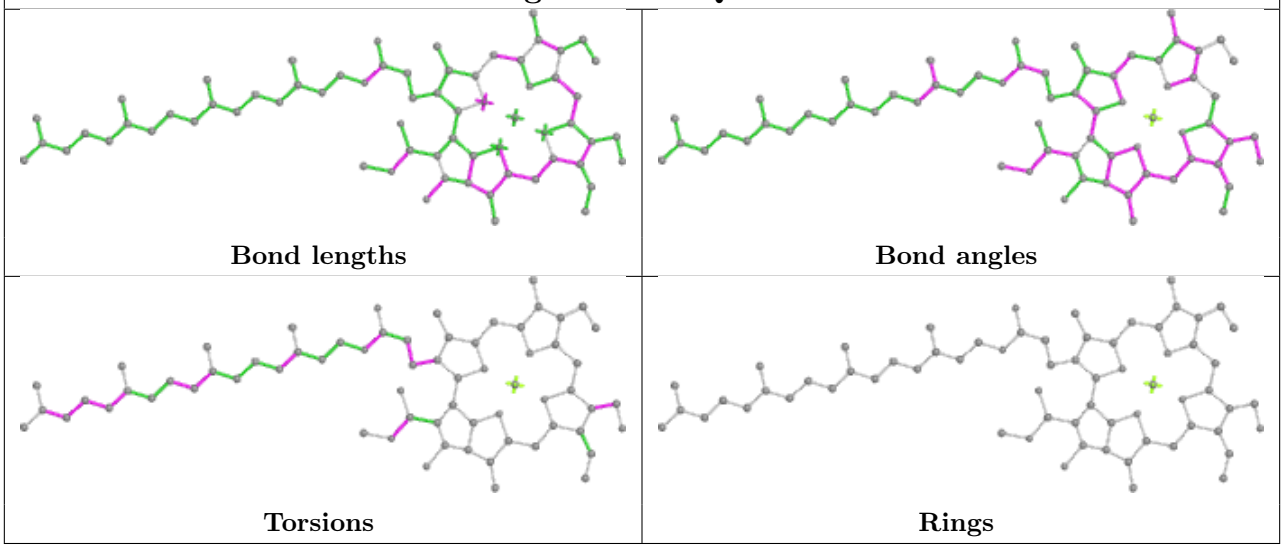
Ligand CLA C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL R 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

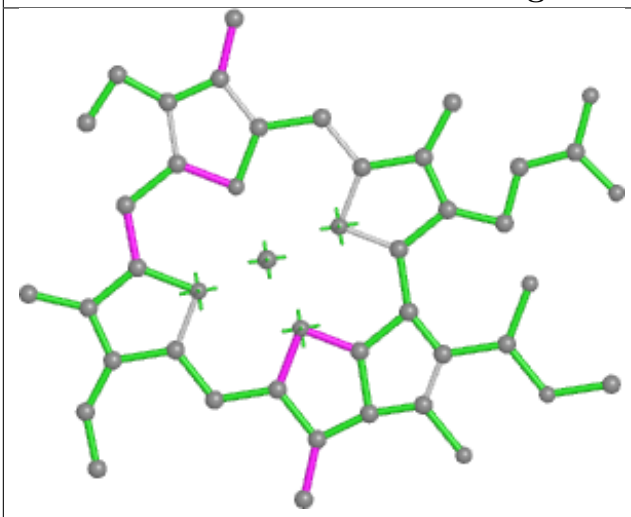
Ligand CHL 6 313



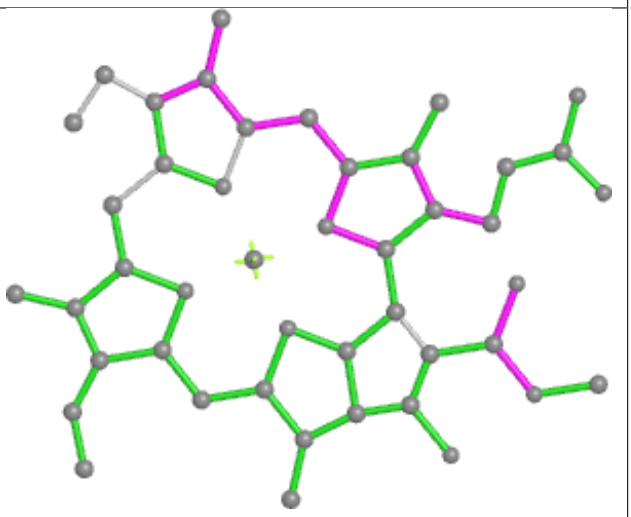
Ligand CHL Q 315



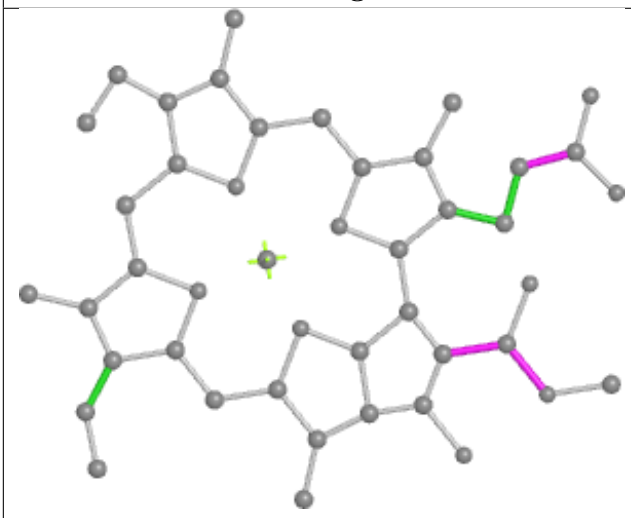
Ligand CLA S 302



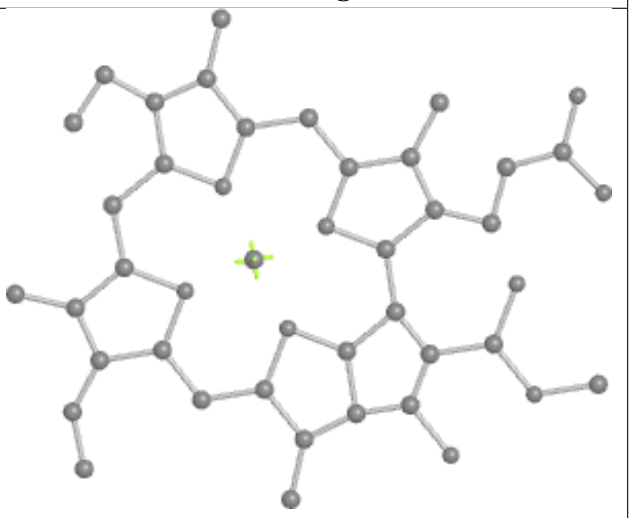
Bond lengths



Bond angles

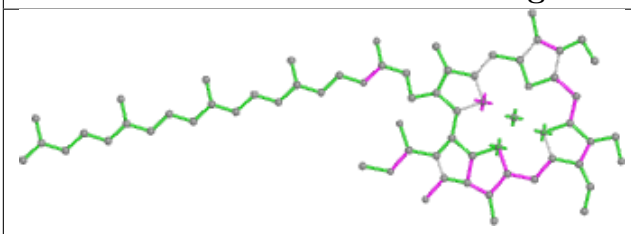


Torsions

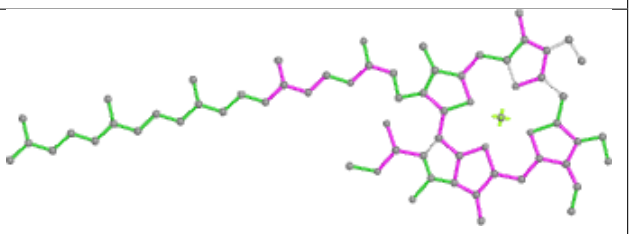


Rings

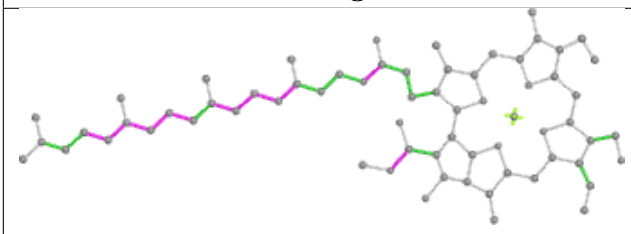
Ligand CHL 3 311



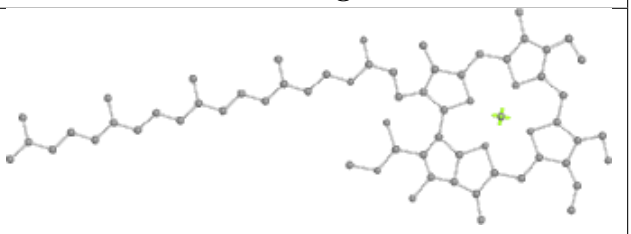
Bond lengths



Bond angles

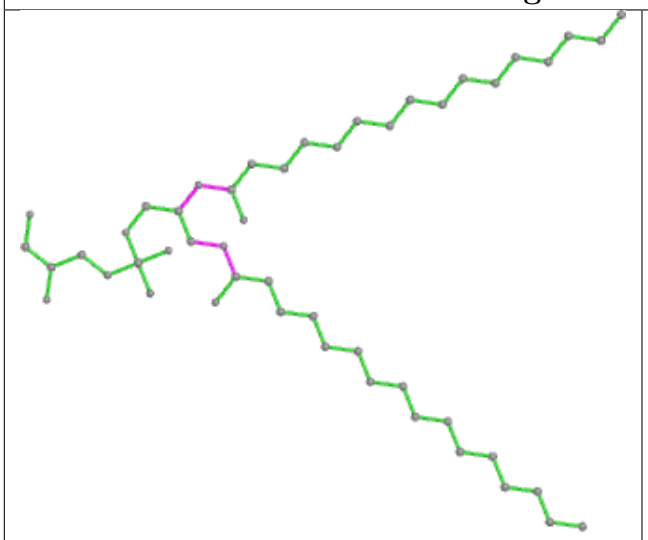


Torsions

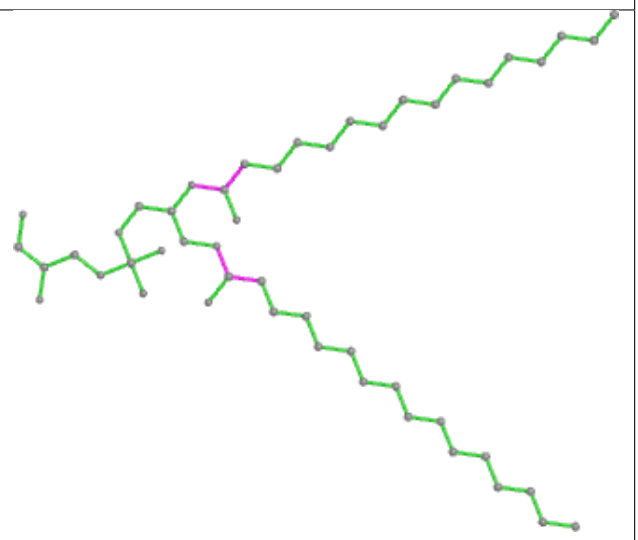


Rings

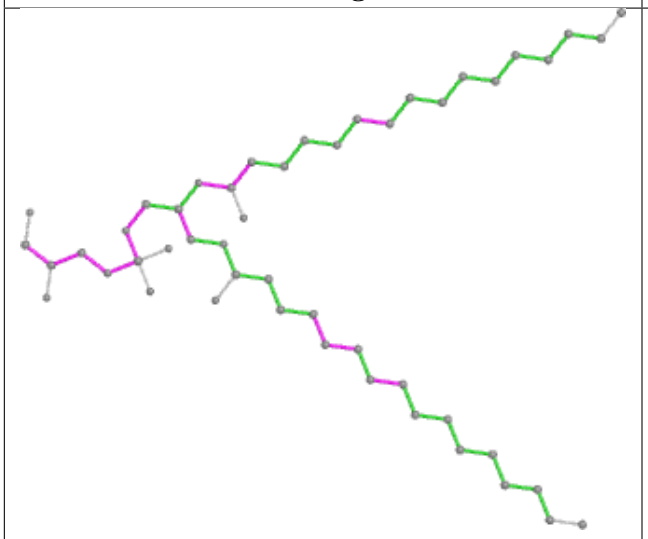
Ligand LHG B 623



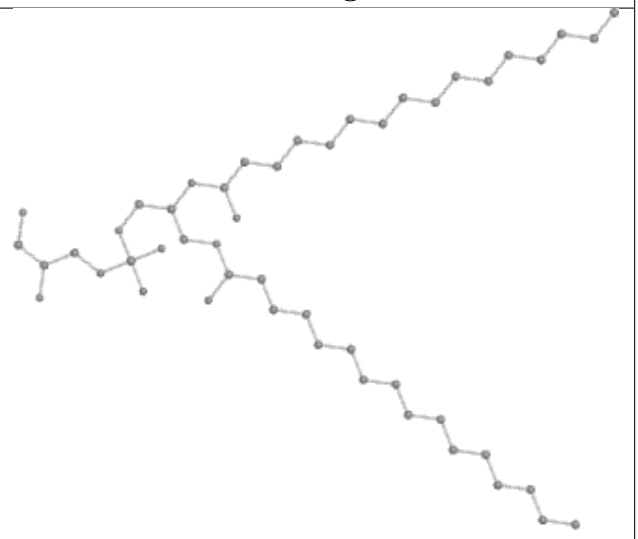
Bond lengths



Bond angles

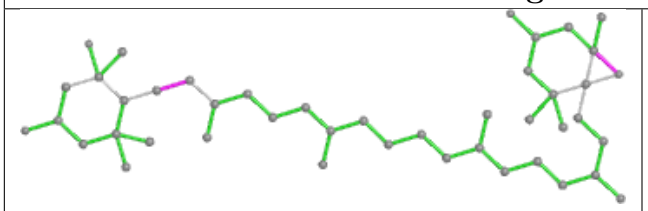


Torsions

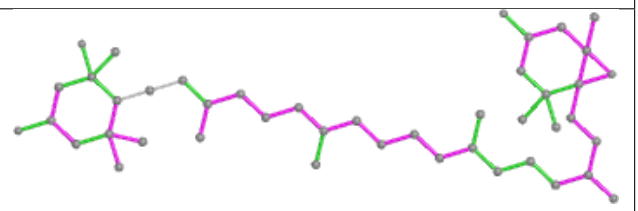


Rings

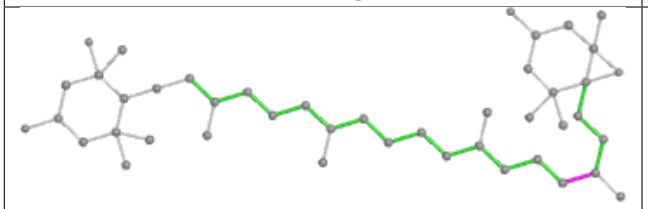
Ligand NEX u 320



Bond lengths

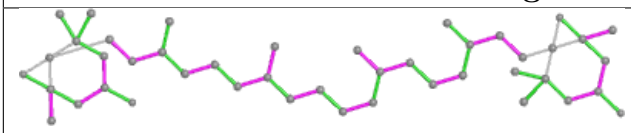
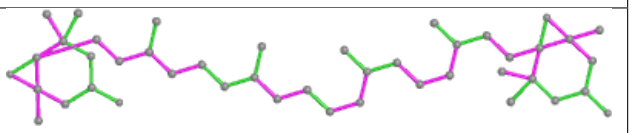
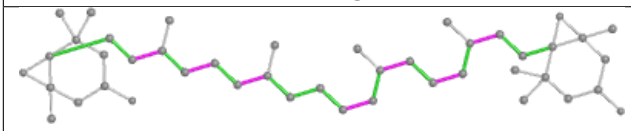
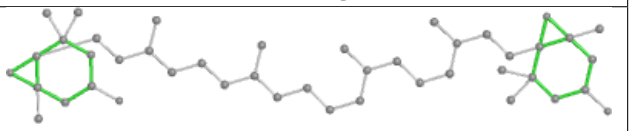


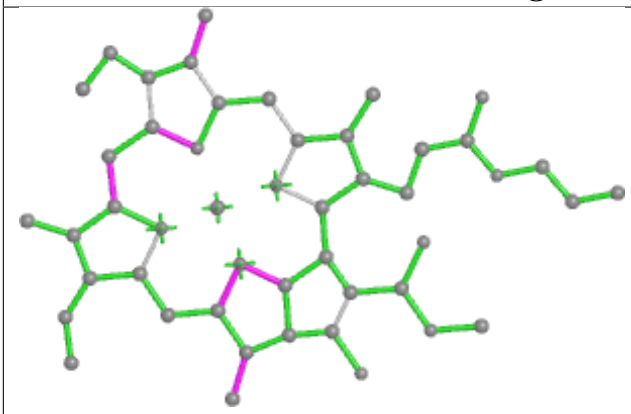
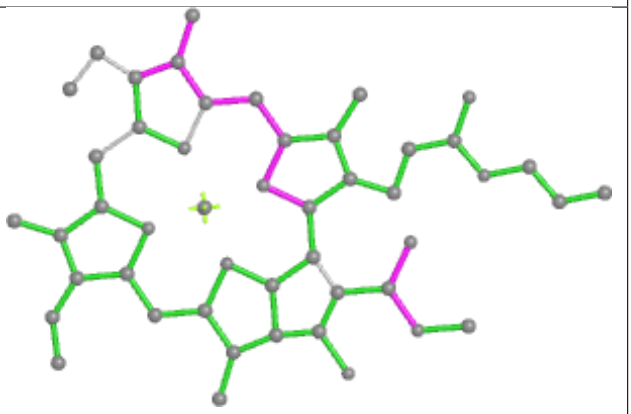
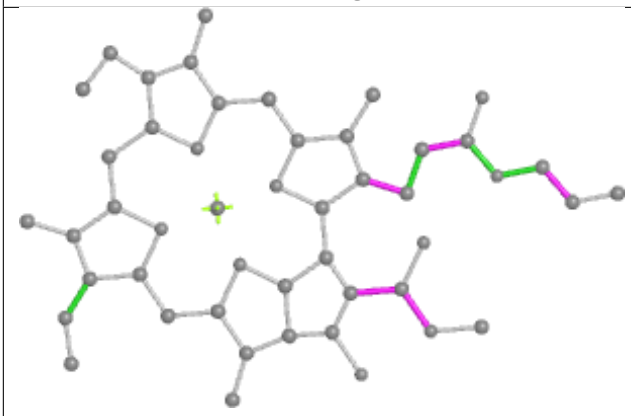
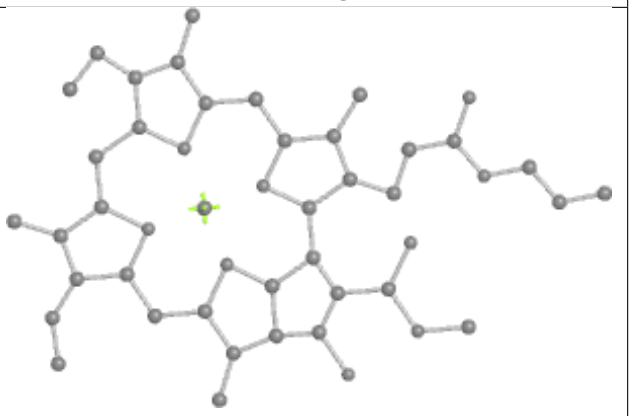
Bond angles

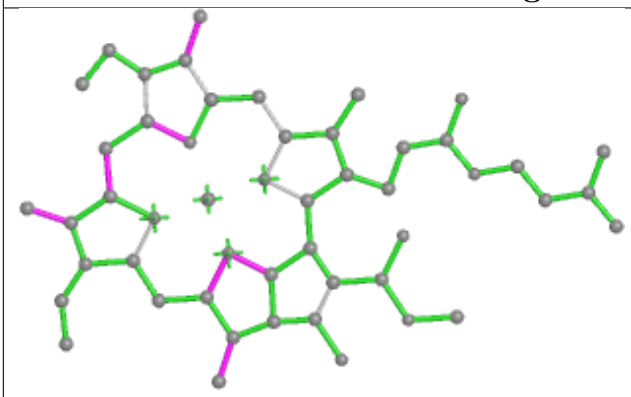
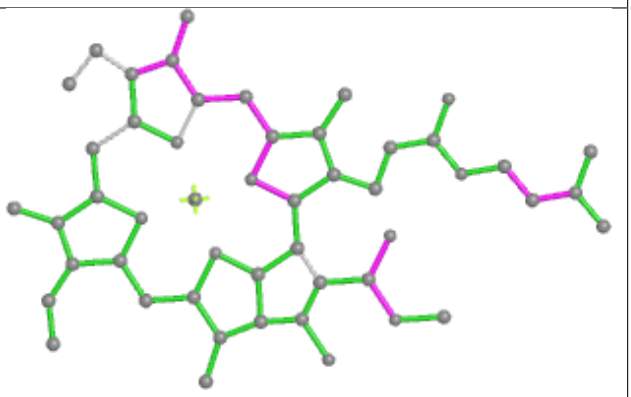
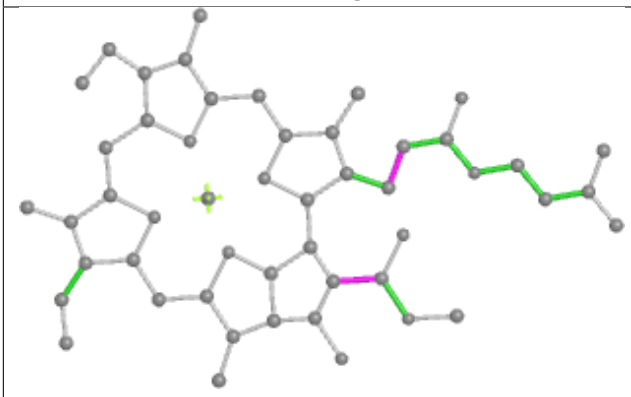
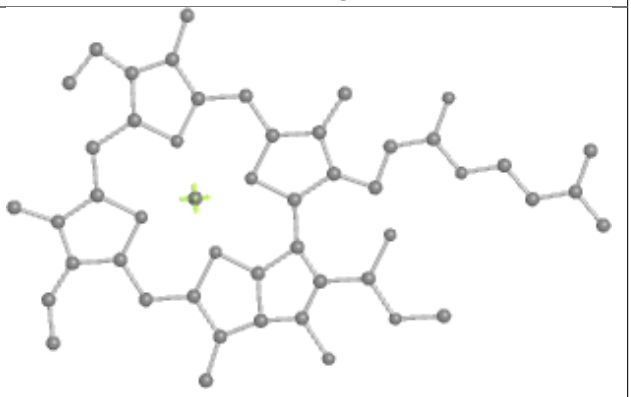


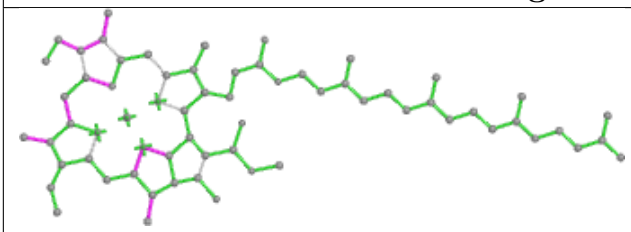
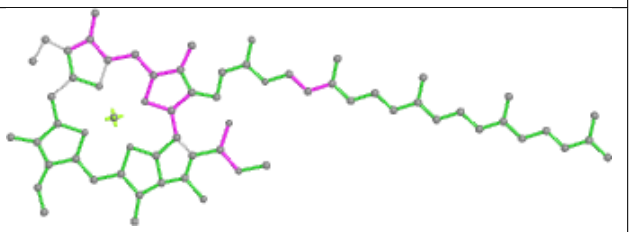
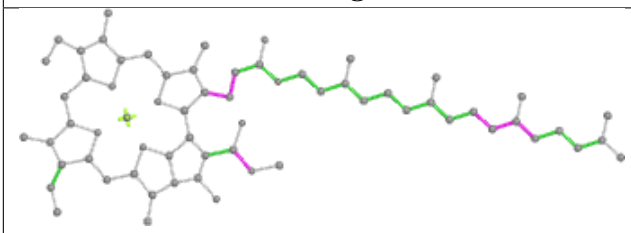
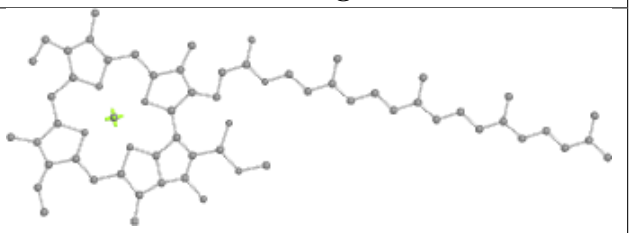
Torsions

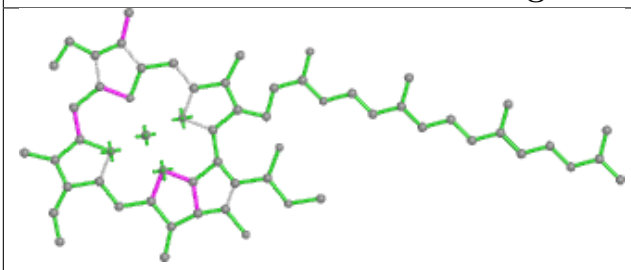
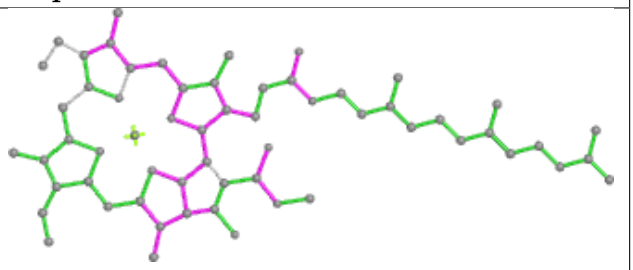
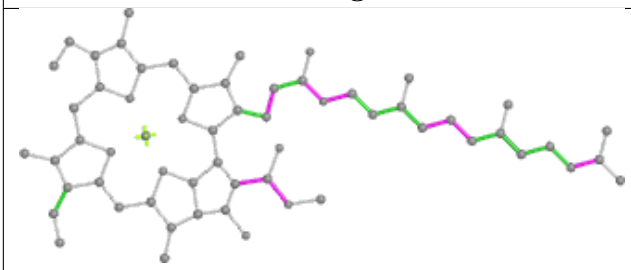
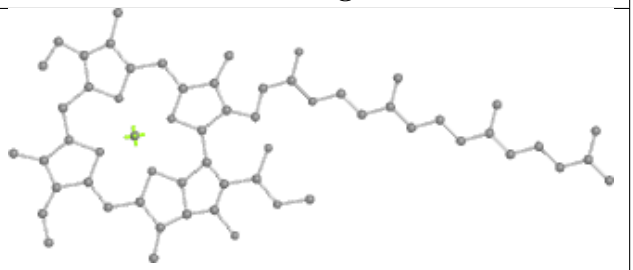
Rings

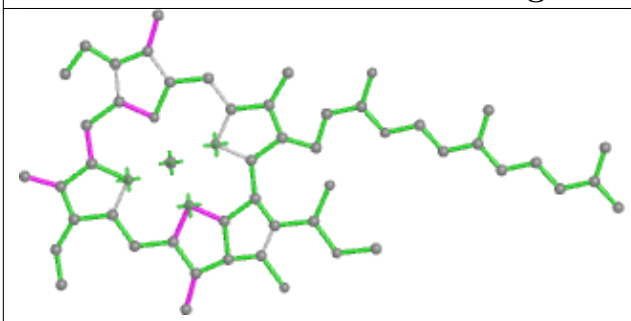
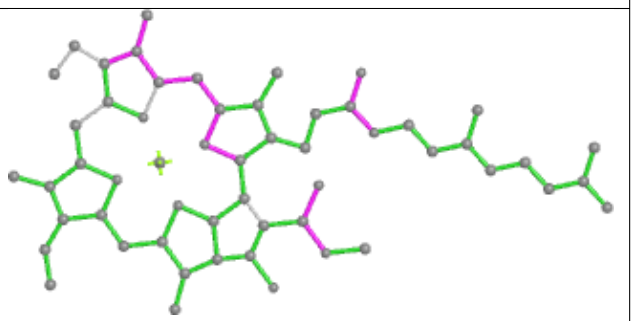
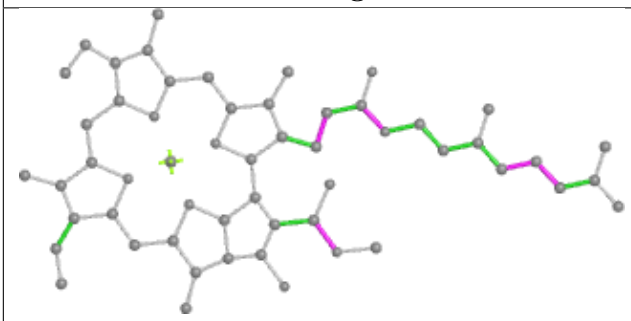
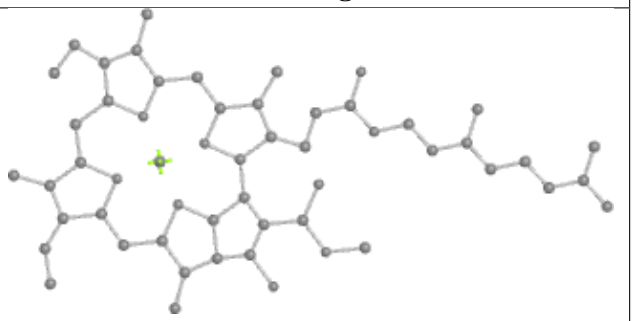
Ligand XAT V 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

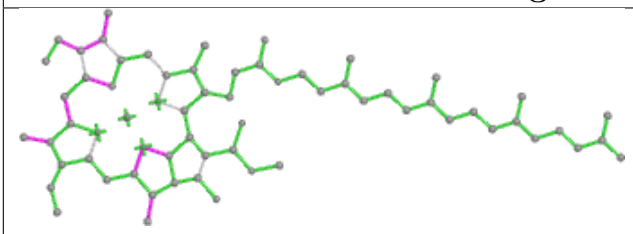
Ligand CLA N 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

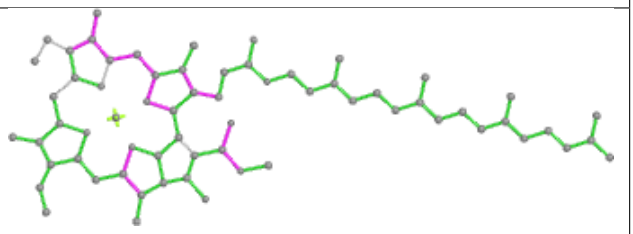
Ligand CLA p 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

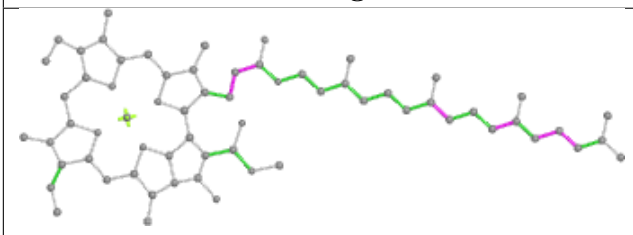
Ligand CLA c 502



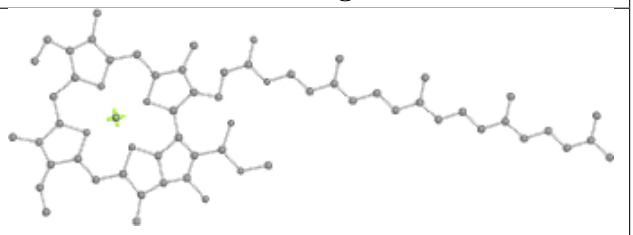
Bond lengths



Bond angles

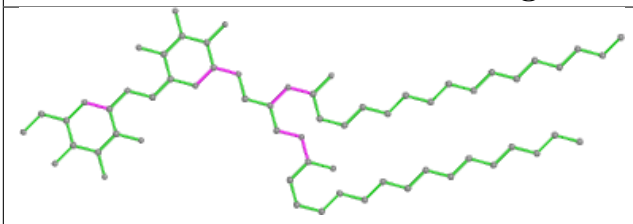


Torsions

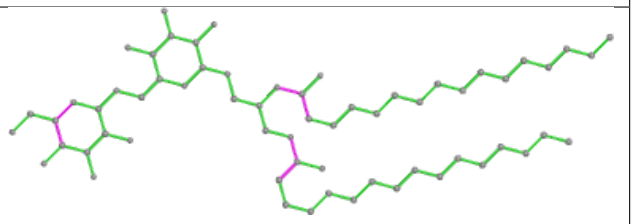


Rings

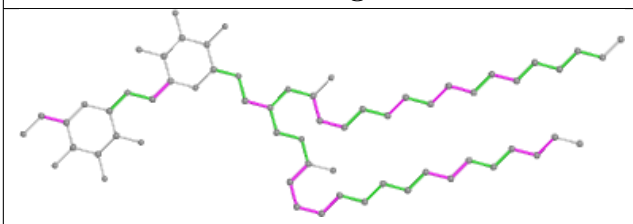
Ligand DGD B 601



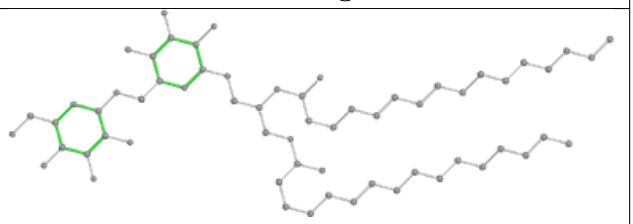
Bond lengths



Bond angles

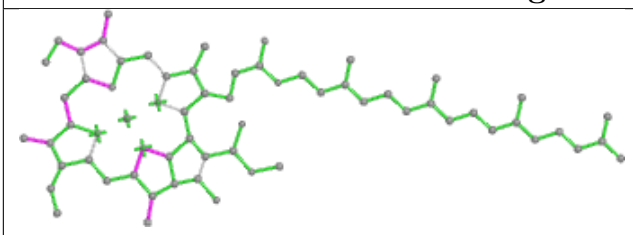


Torsions

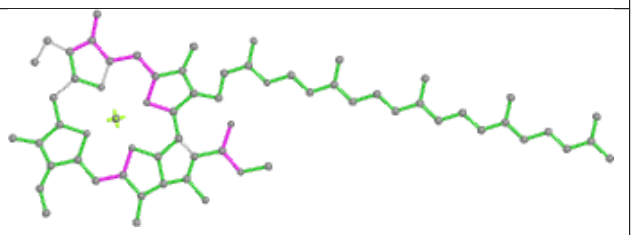


Rings

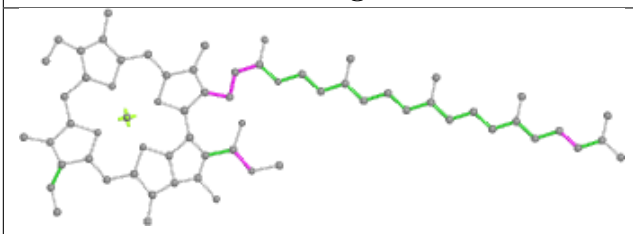
Ligand CLA 4 301



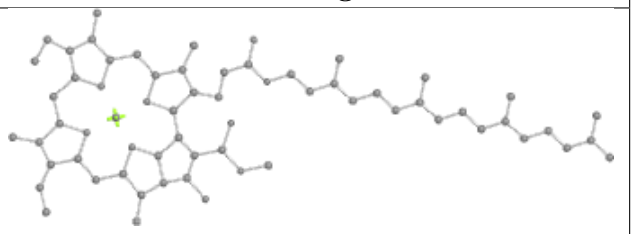
Bond lengths



Bond angles

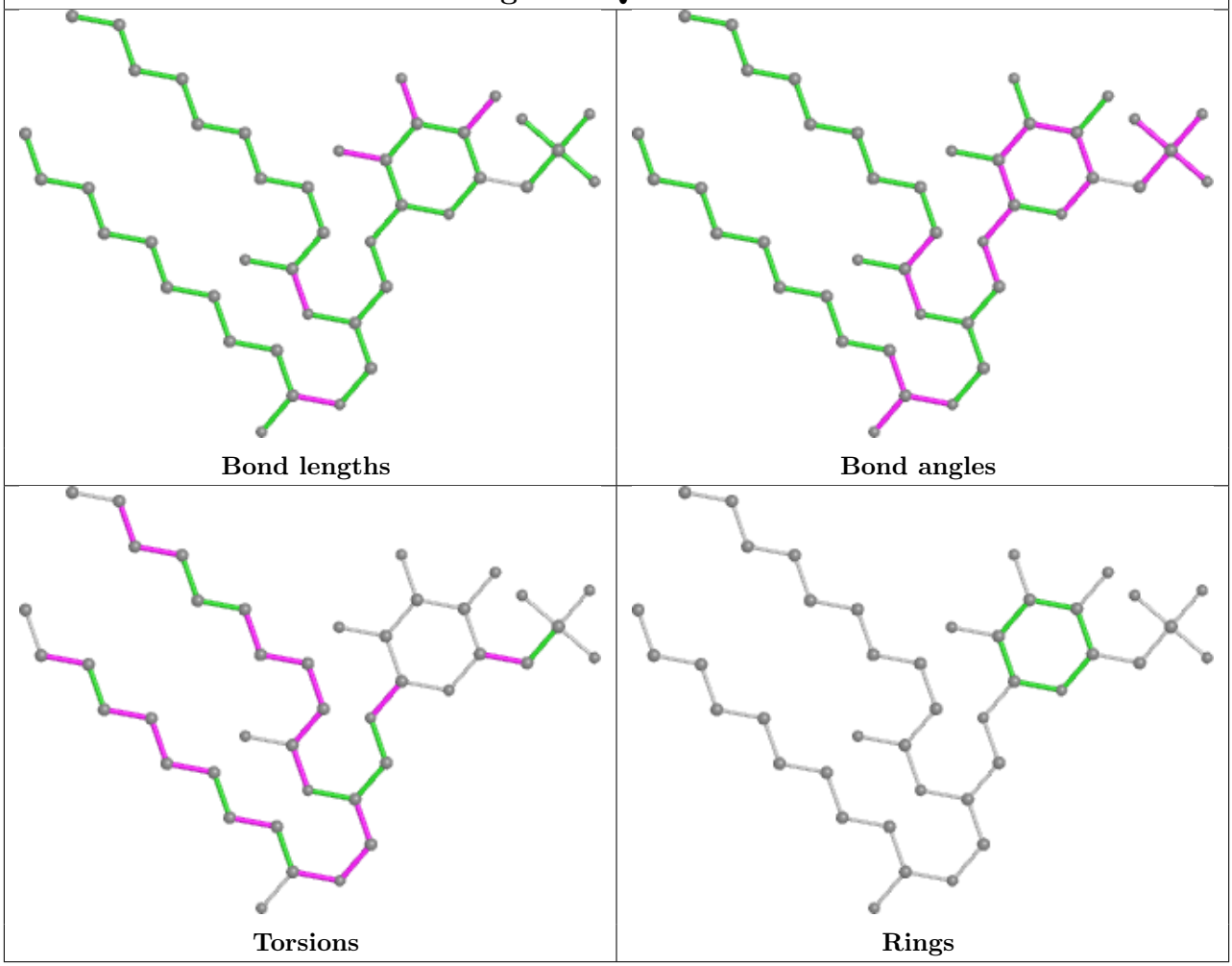


Torsions

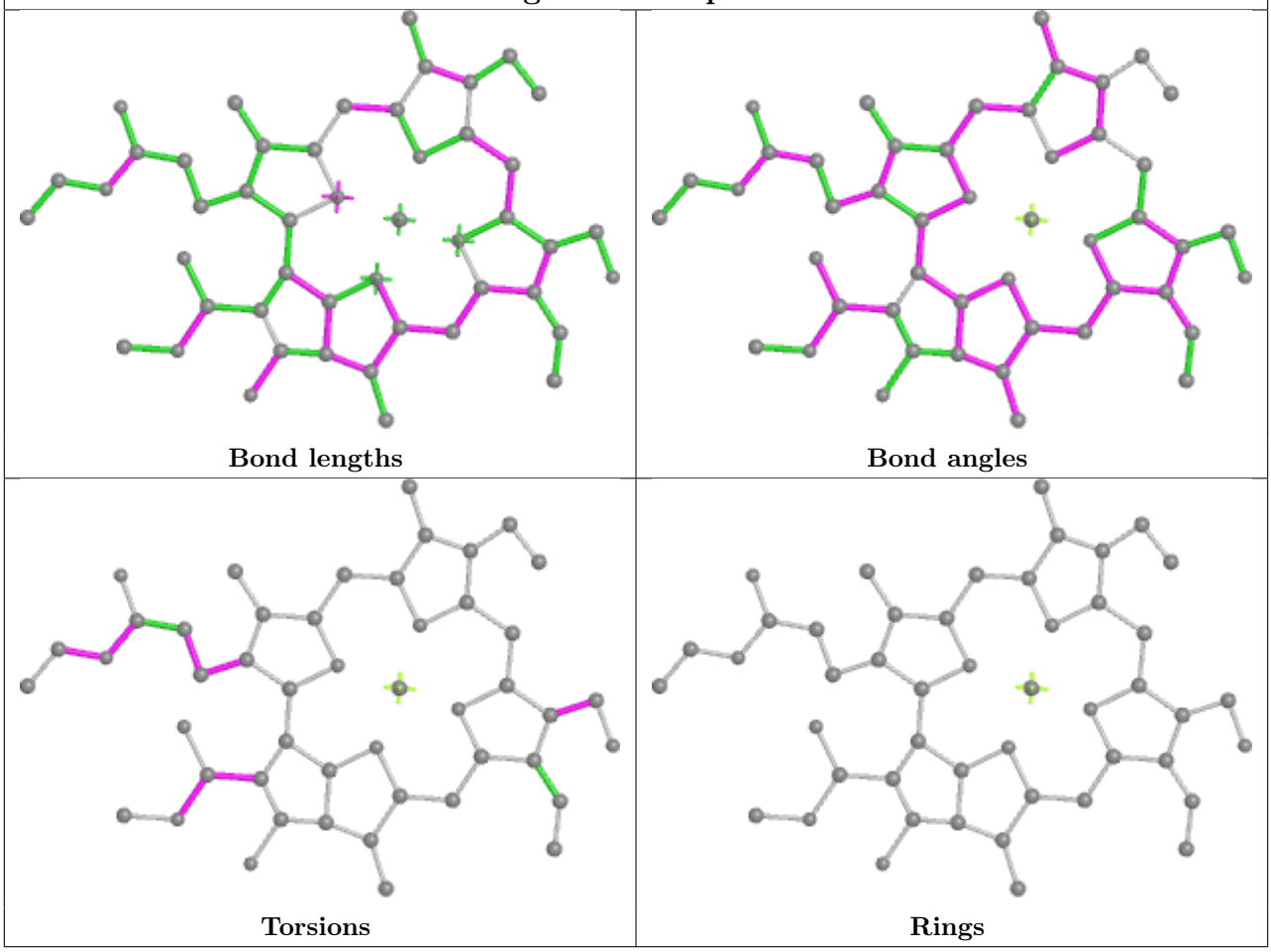


Rings

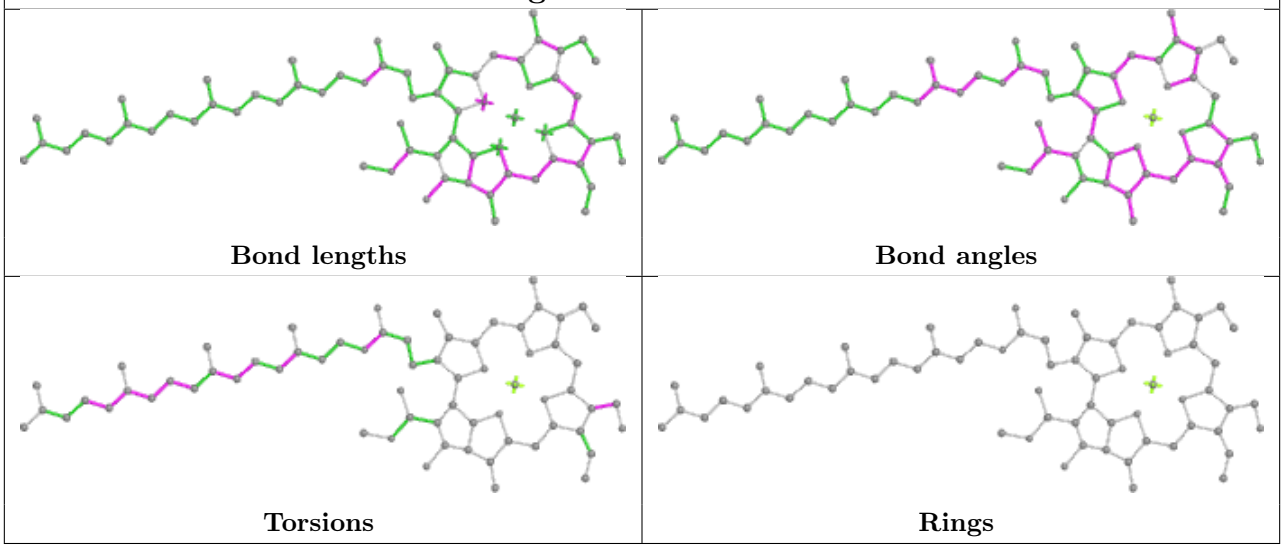
Ligand SQD M 101



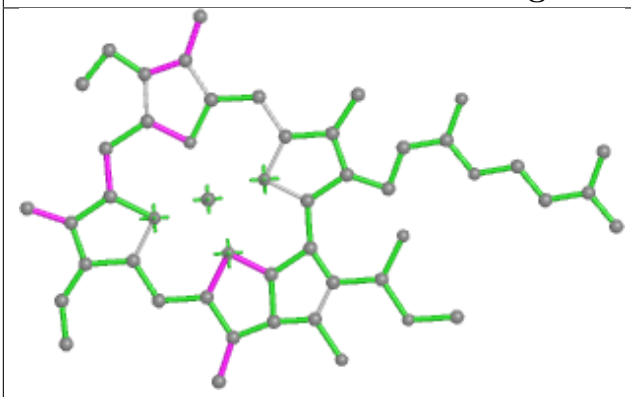
Ligand CHL q 312



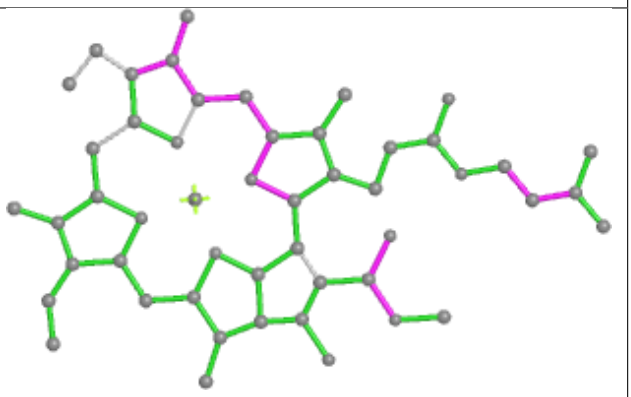
Ligand CHL v 313



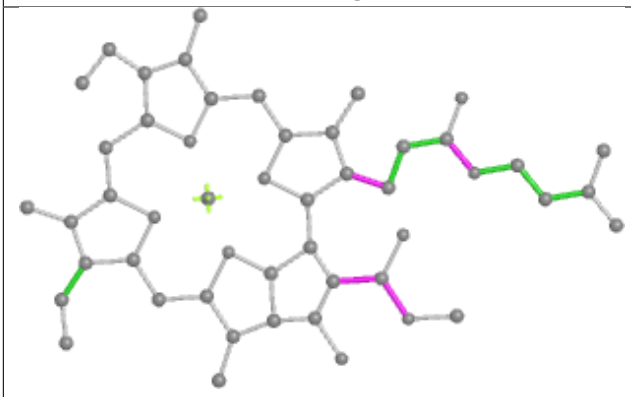
Ligand CLA 2 303



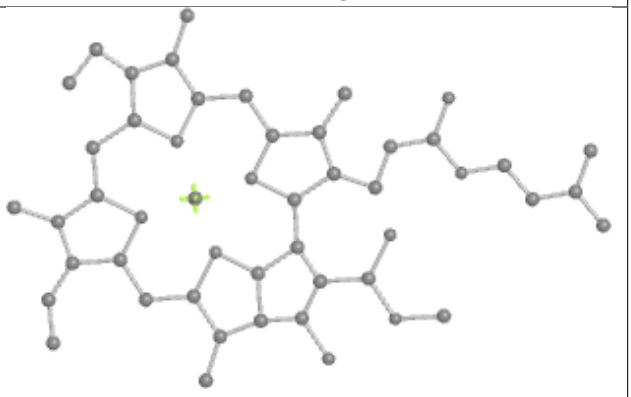
Bond lengths



Bond angles

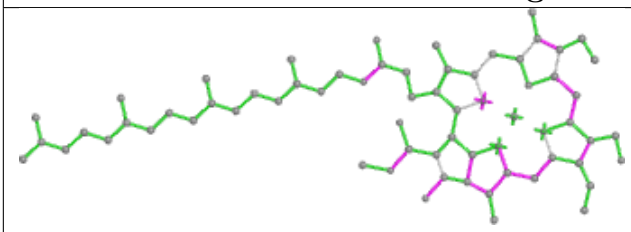


Torsions

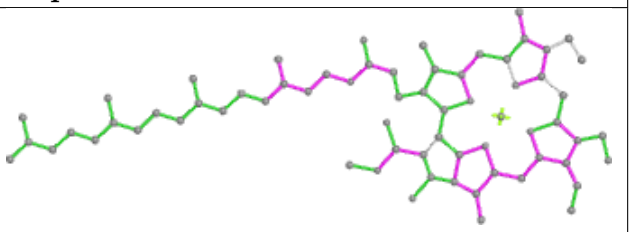


Rings

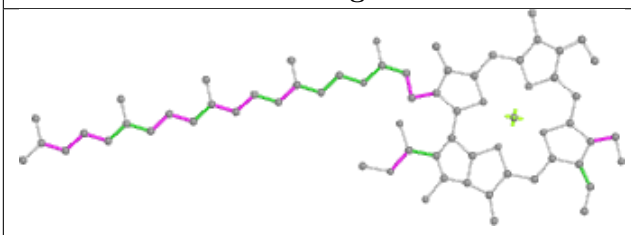
Ligand CHL p 318



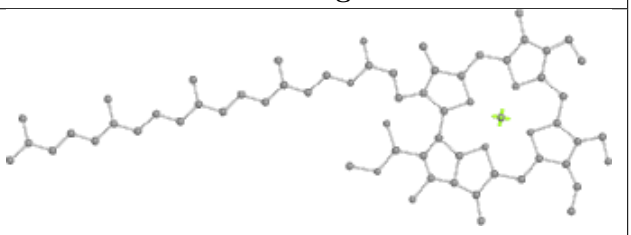
Bond lengths



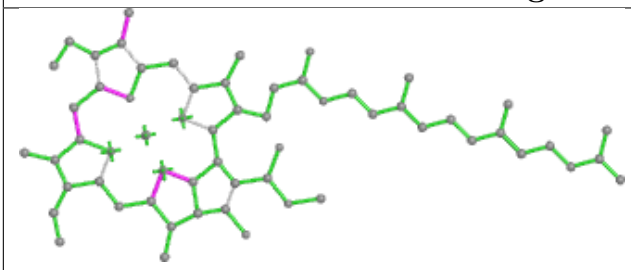
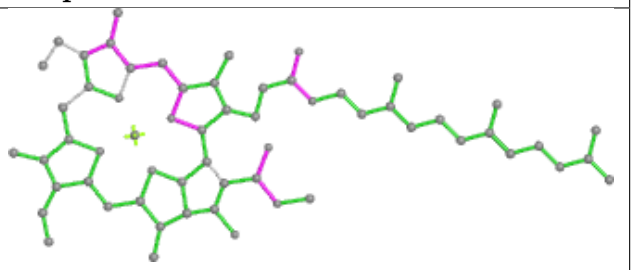
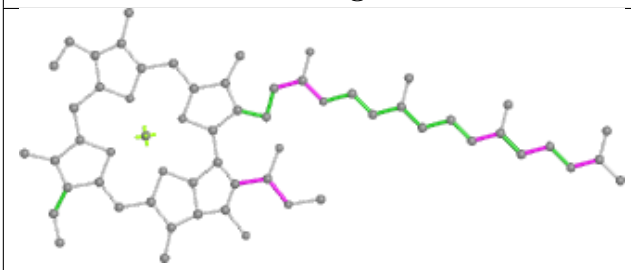
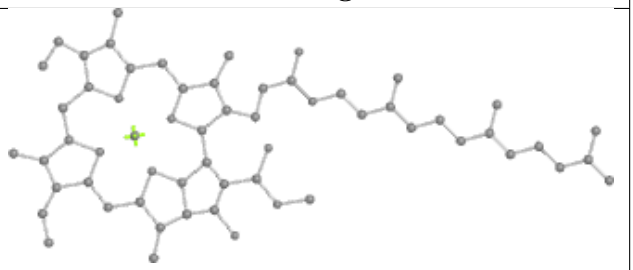
Bond angles

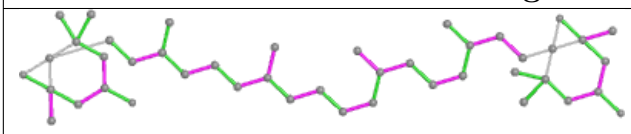
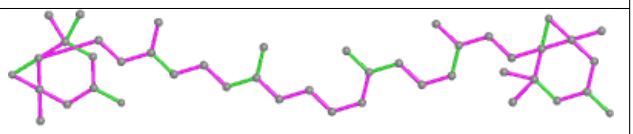
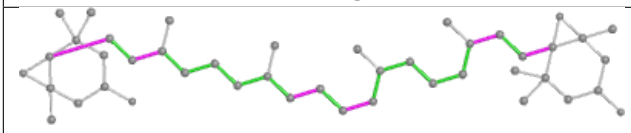
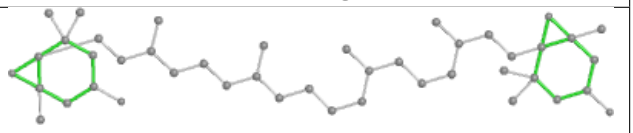


Torsions

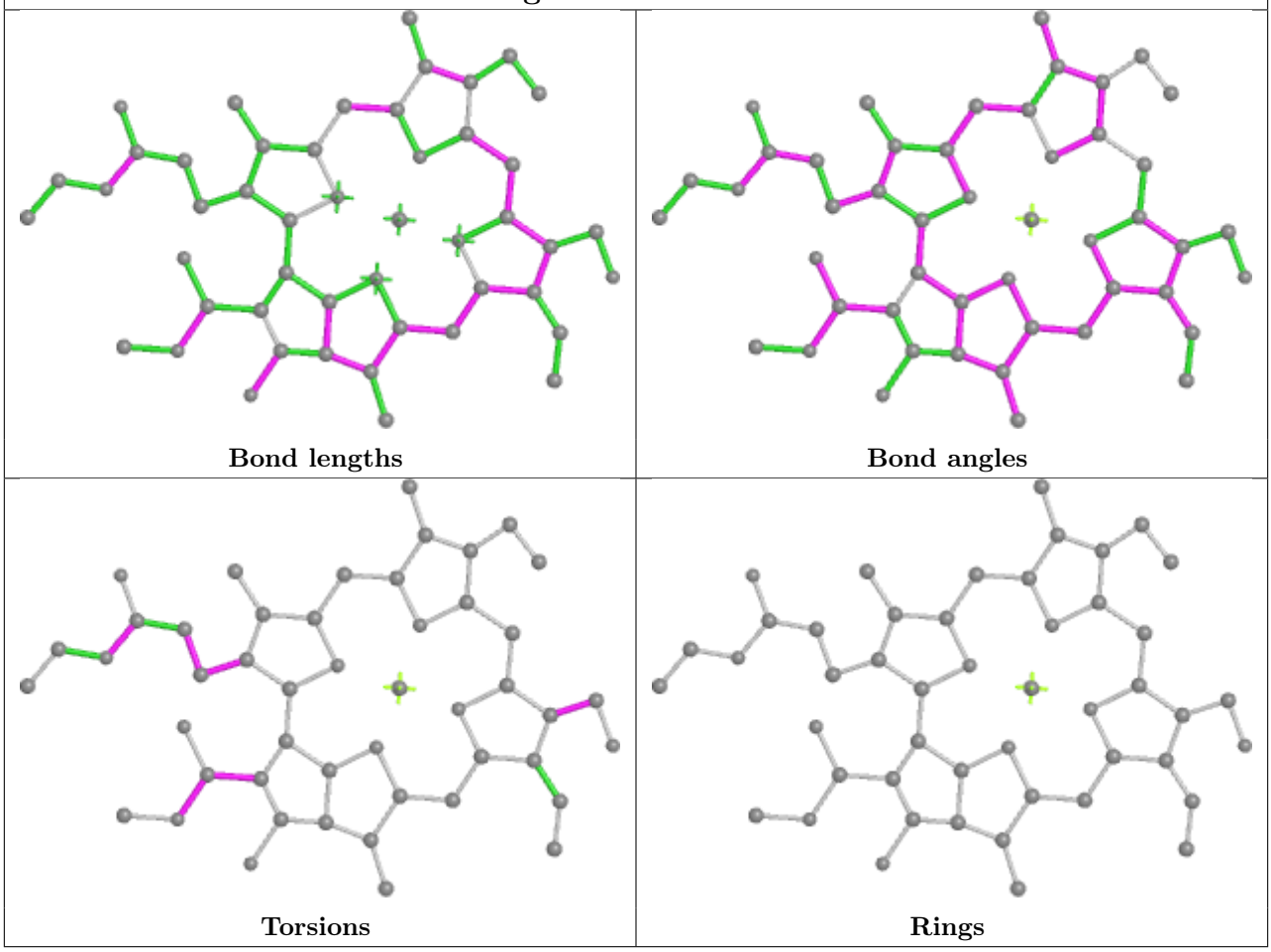


Rings

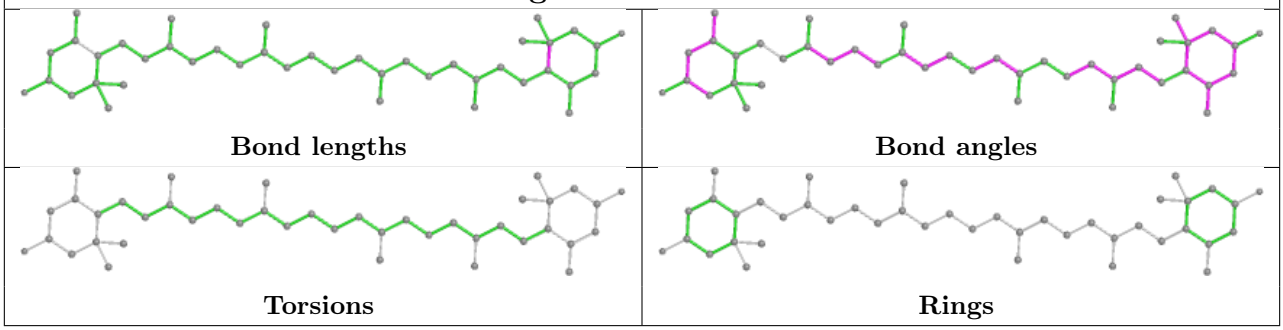
Ligand CLA q 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT R 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

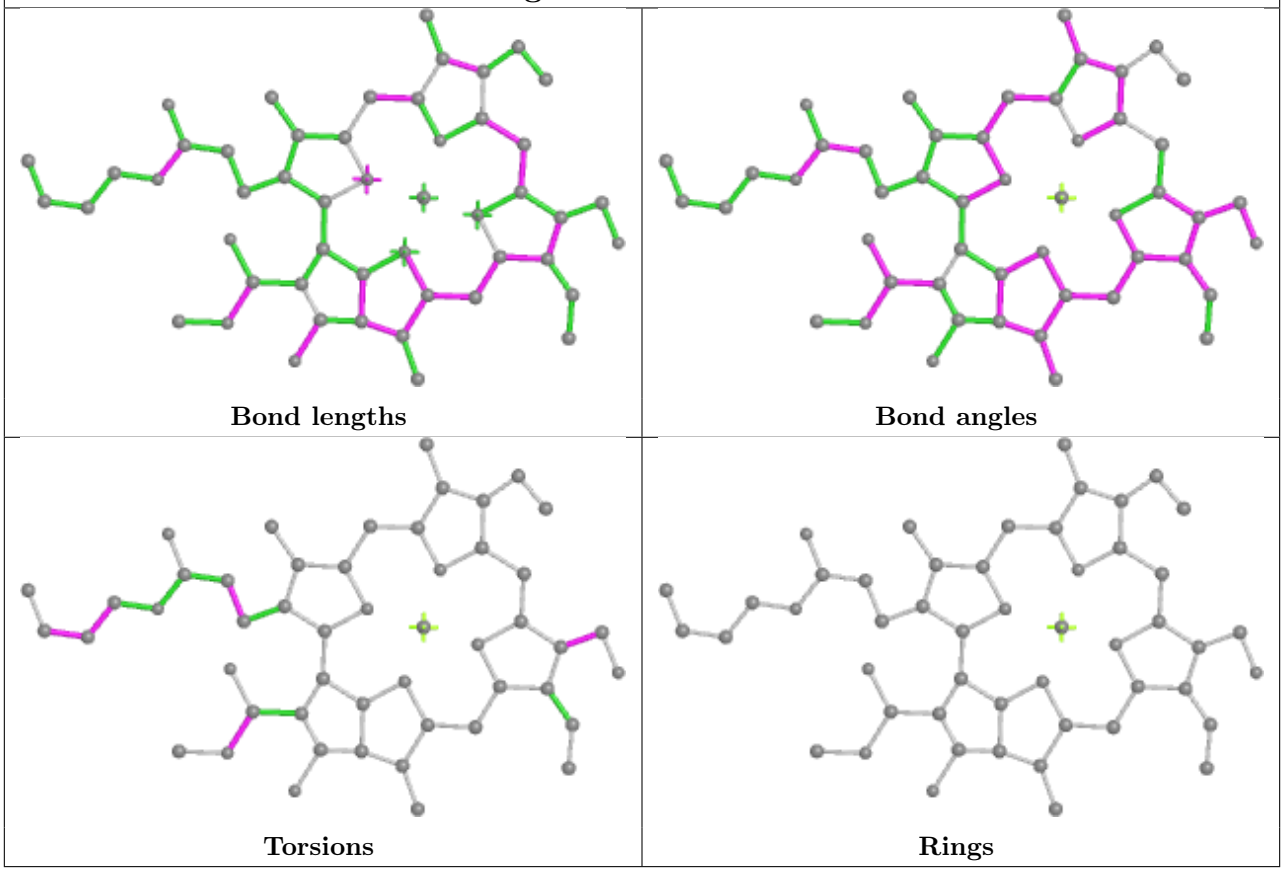
Ligand CHL v 314



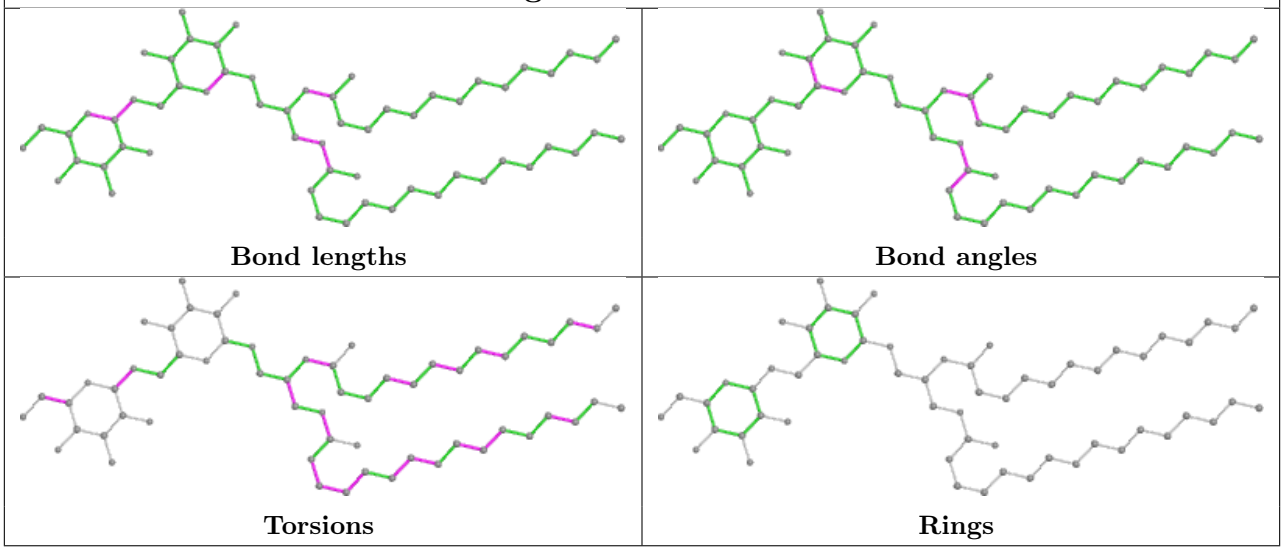
Ligand LUT 4 310

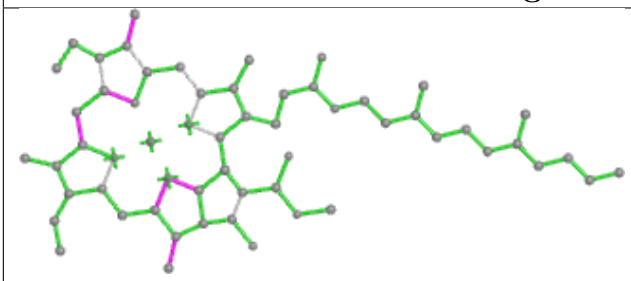
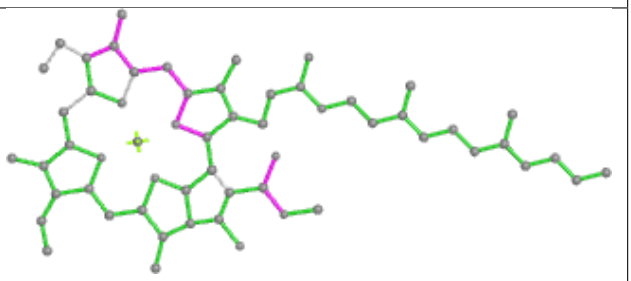
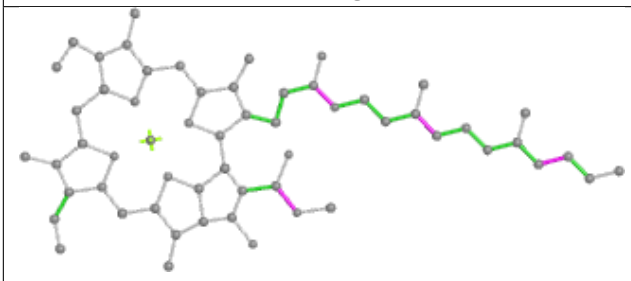
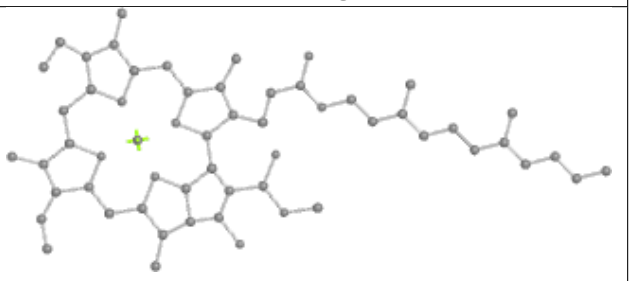


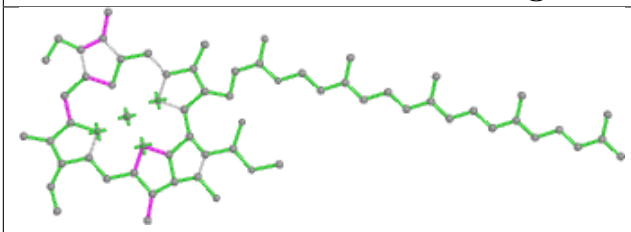
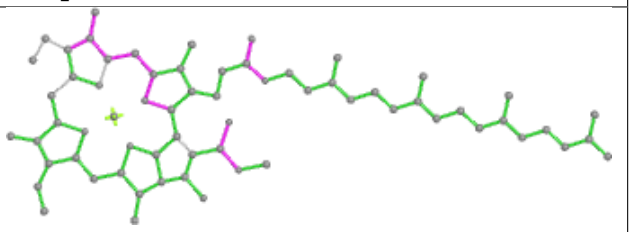
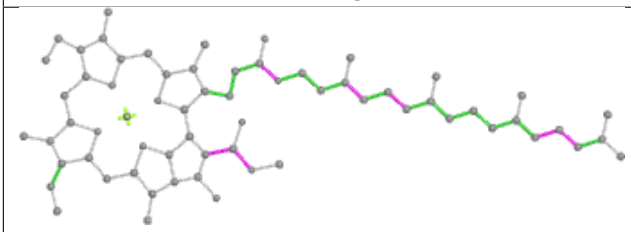
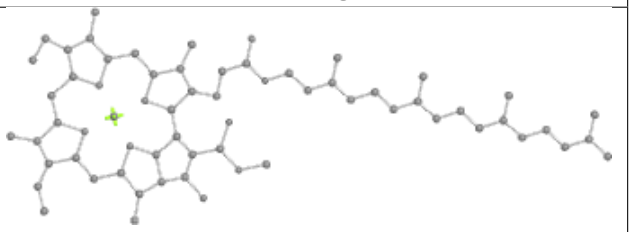
Ligand CHL V 315

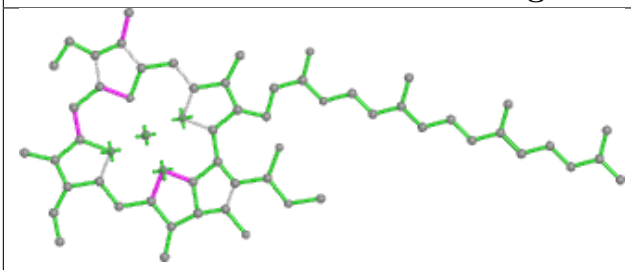
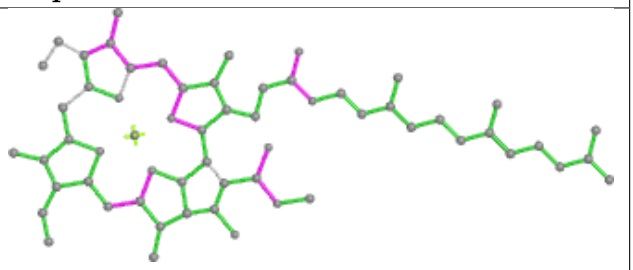
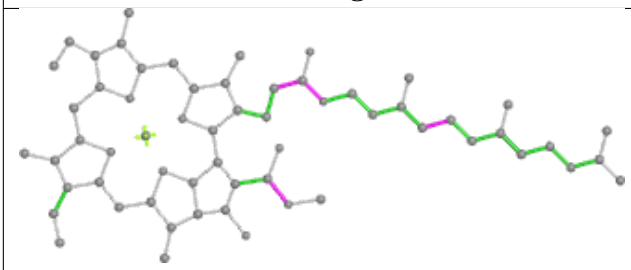
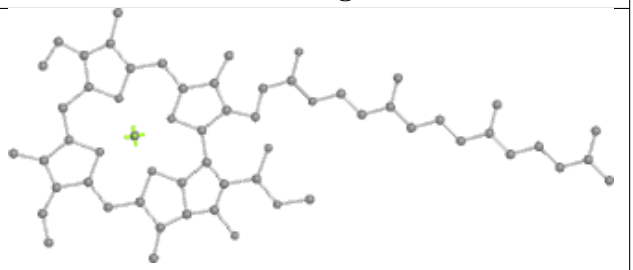


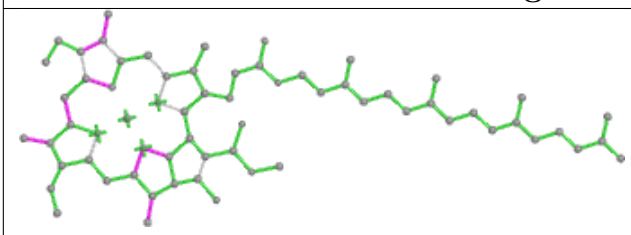
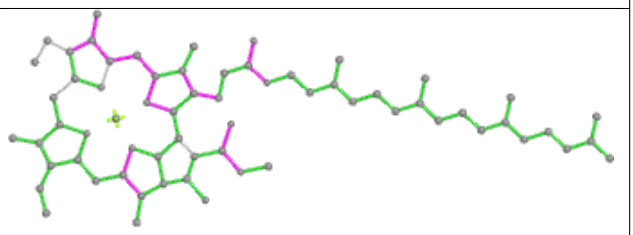
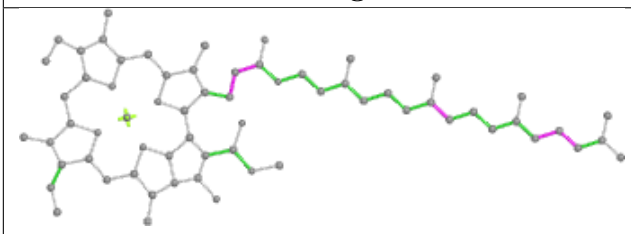
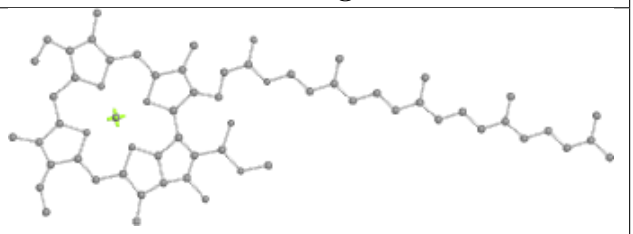
Ligand DGD J 101



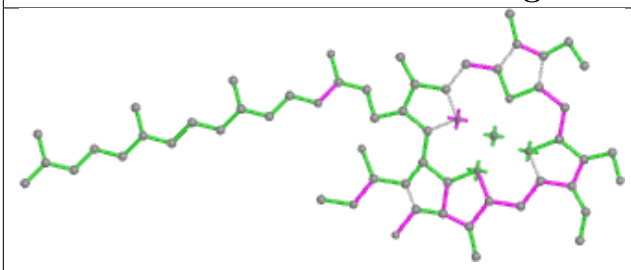
Ligand CLA R 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

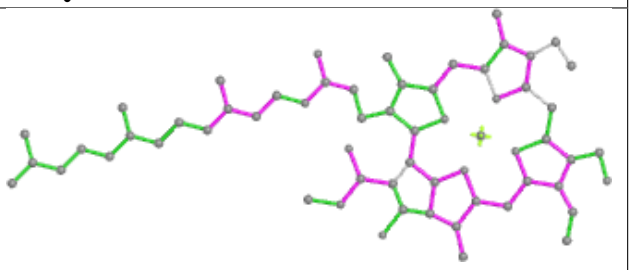
Ligand CLA p 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

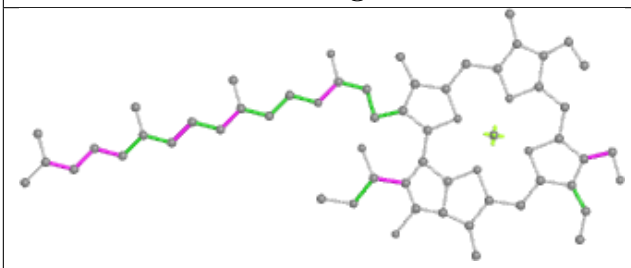
Ligand CHL Q 316



Bond lengths



Bond angles



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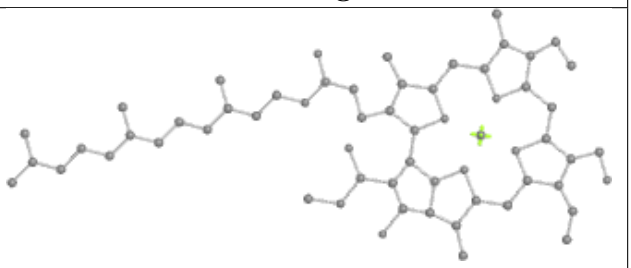
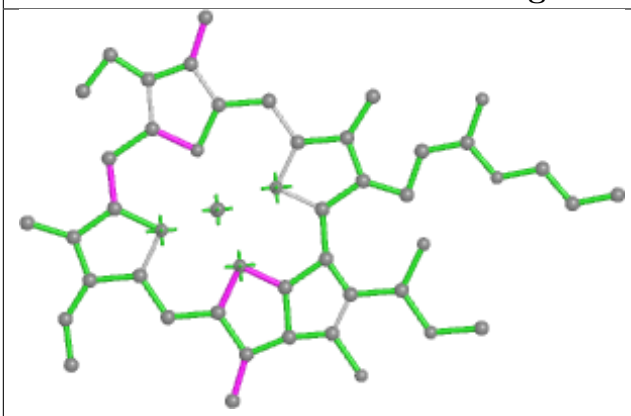


Rings

Ligand CLA g 308



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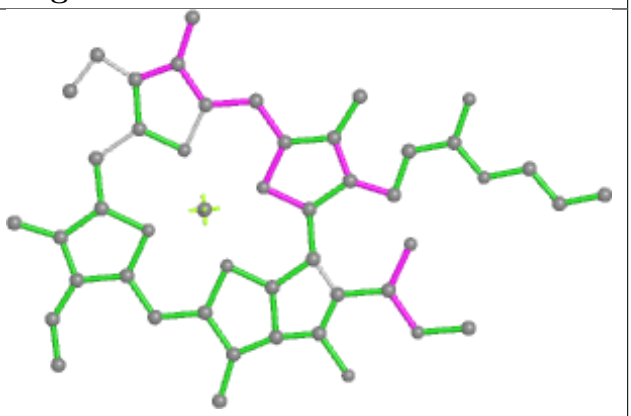
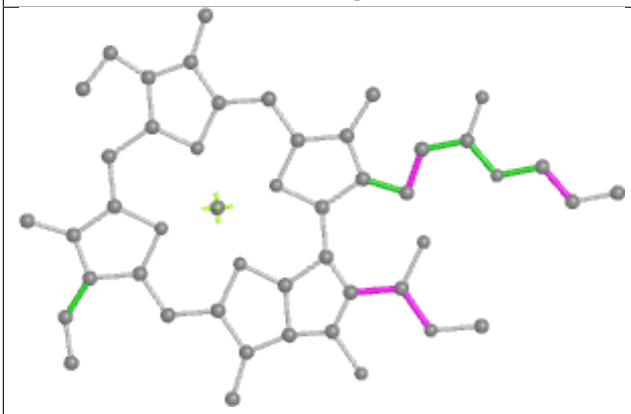


Bond angles



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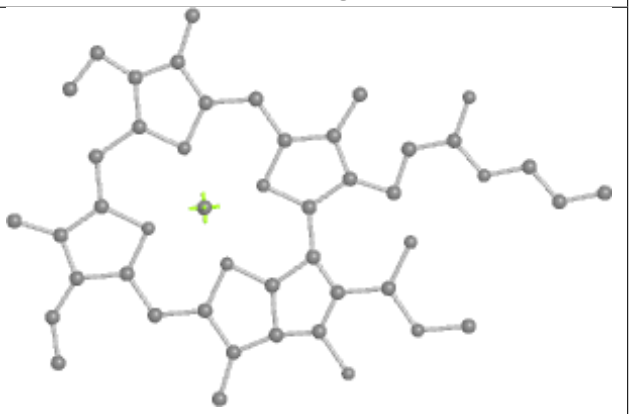
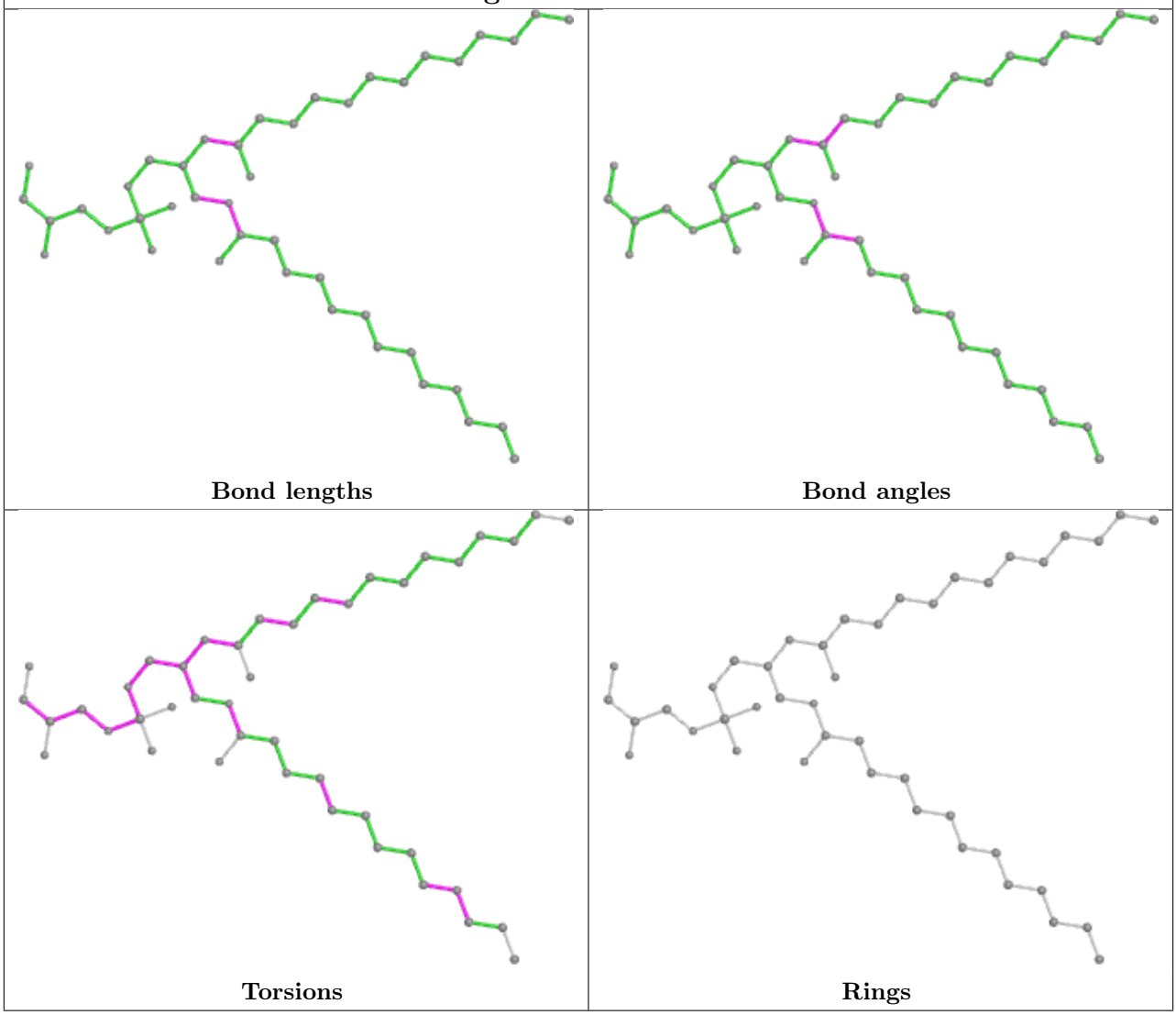
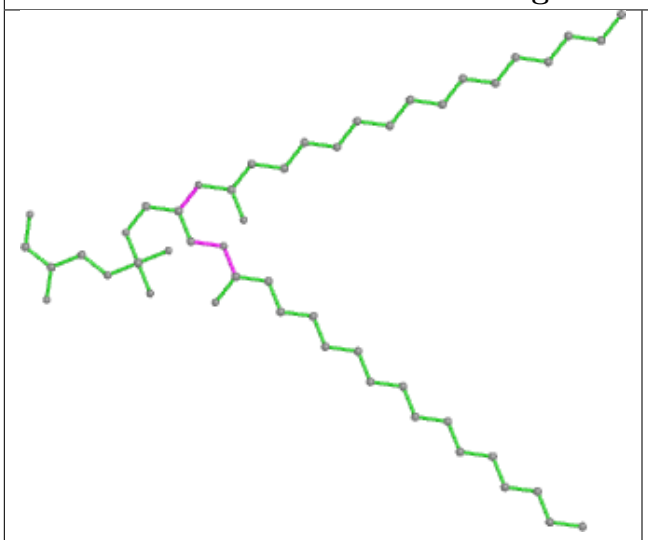


Rings

Ligand LHG a 415



Ligand LHG l 101



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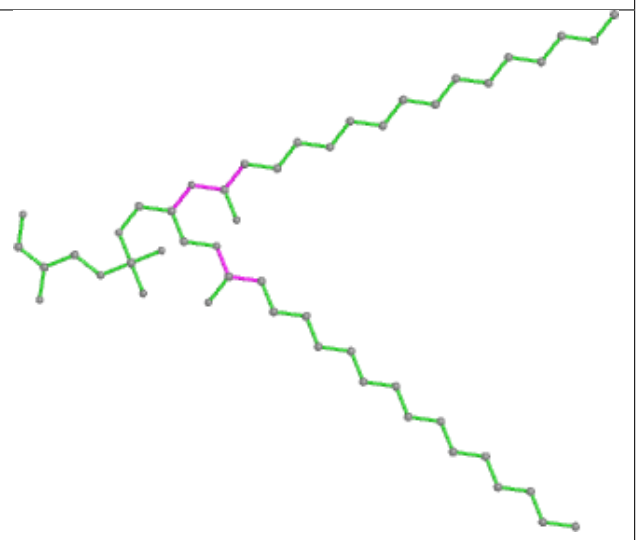

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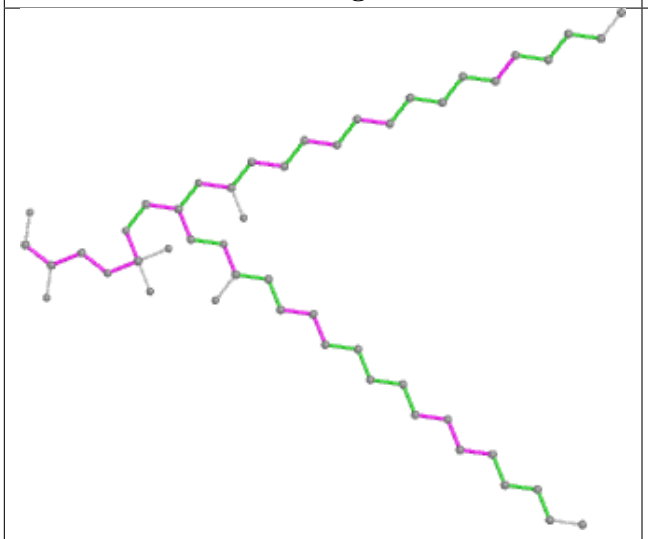

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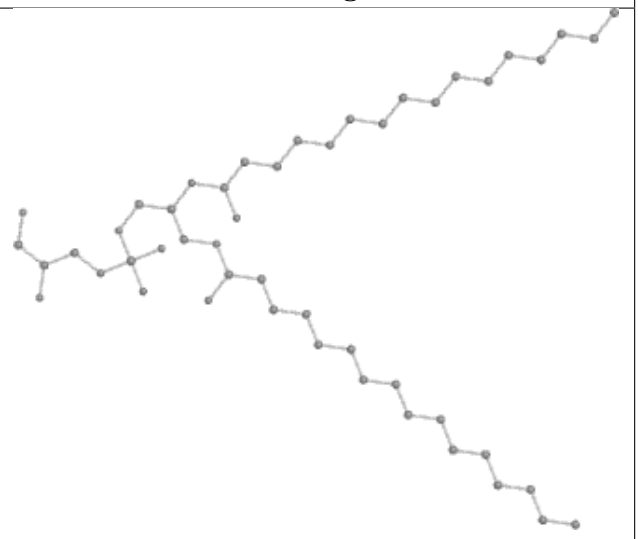
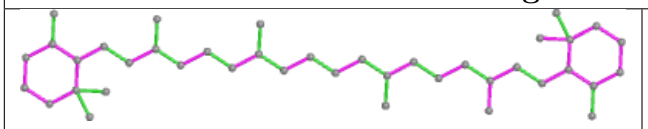


Rings

Ligand BCR K 101



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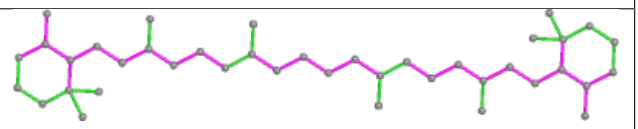
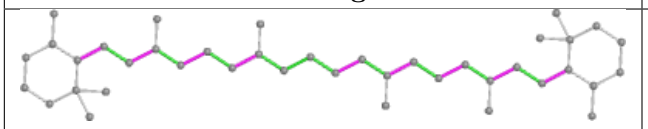


Bond angles



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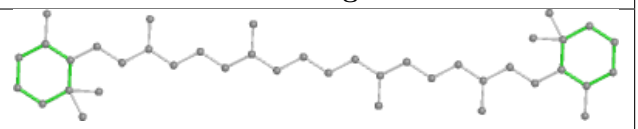
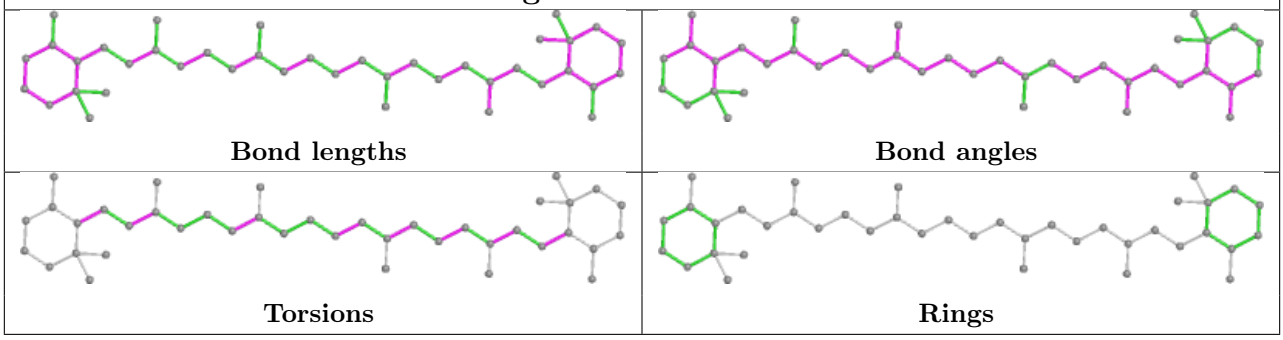
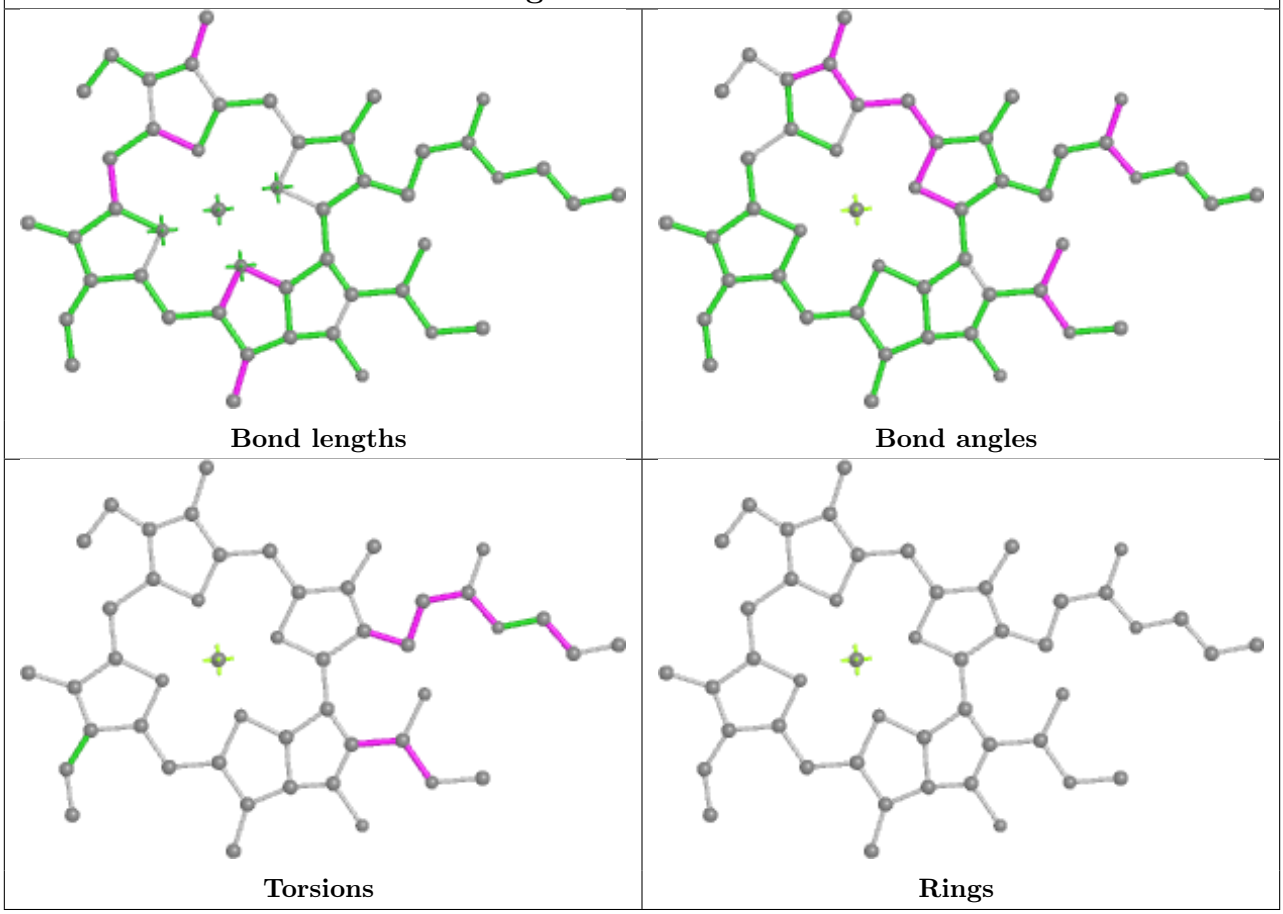


Rings

Ligand BCR D 404



Ligand CLA P 309



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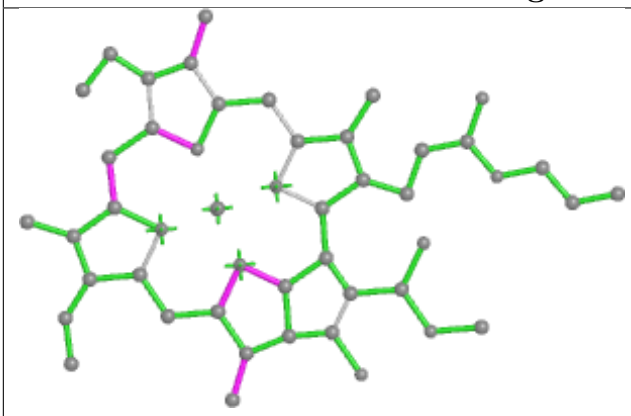

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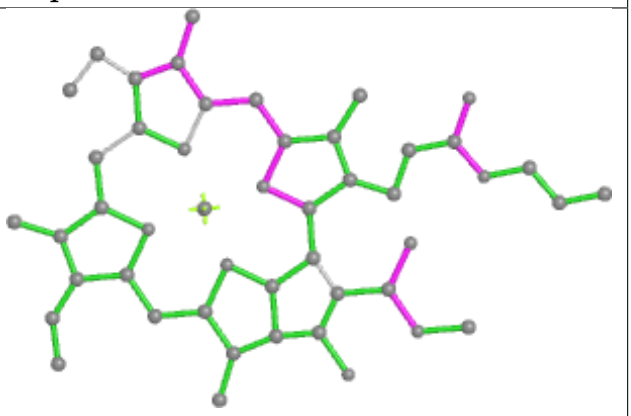

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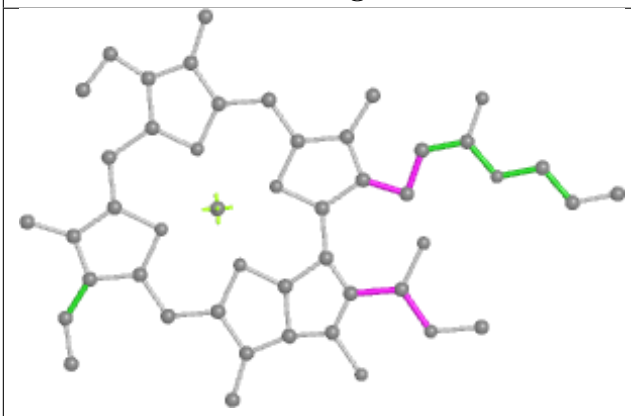

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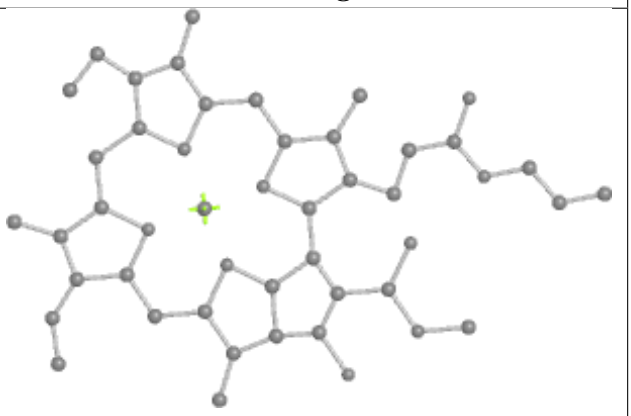
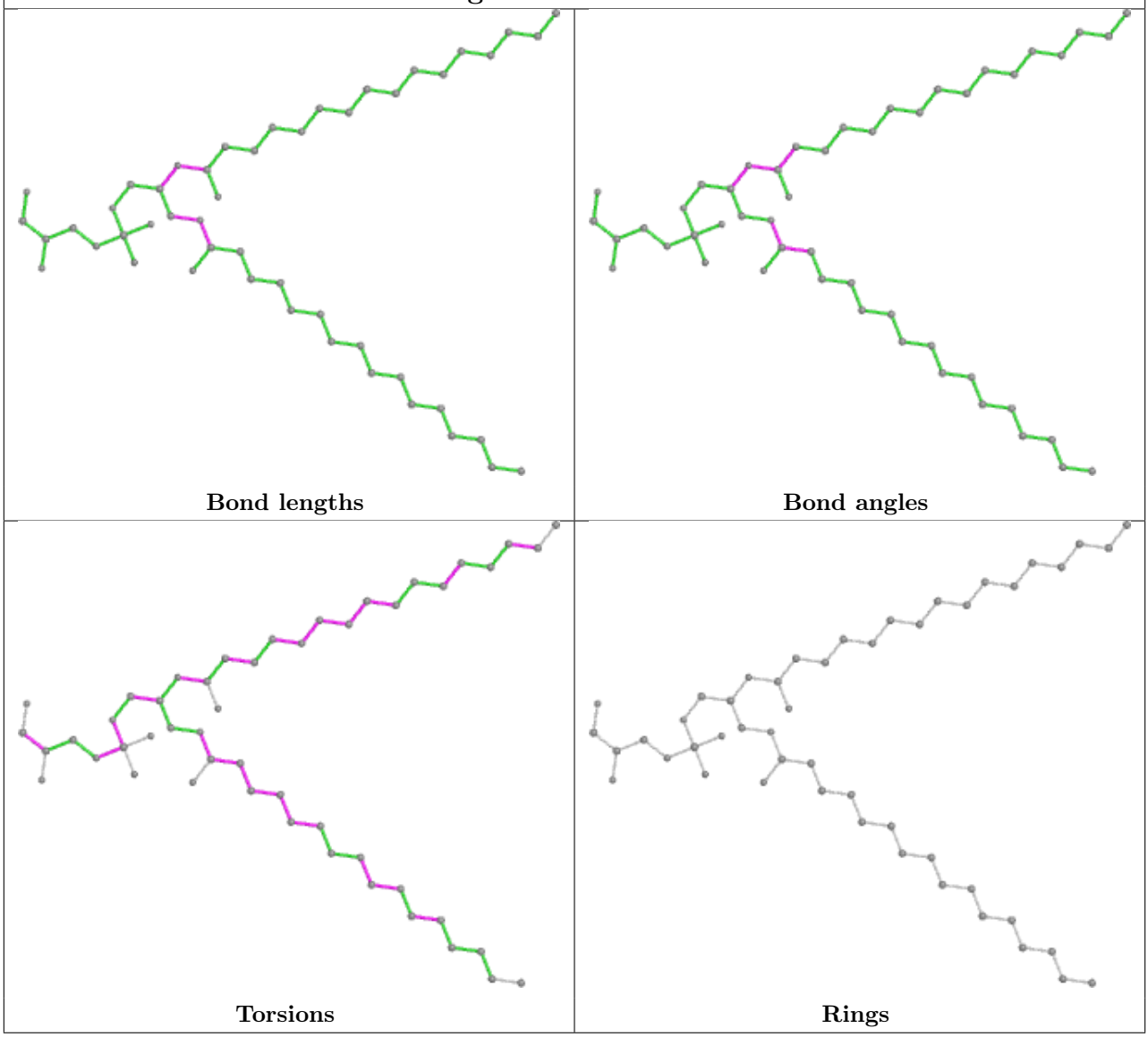
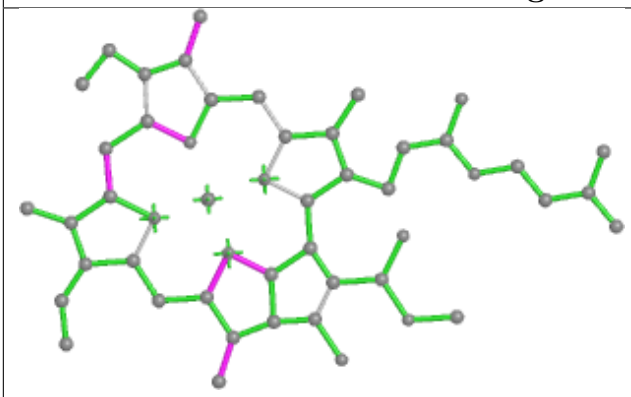
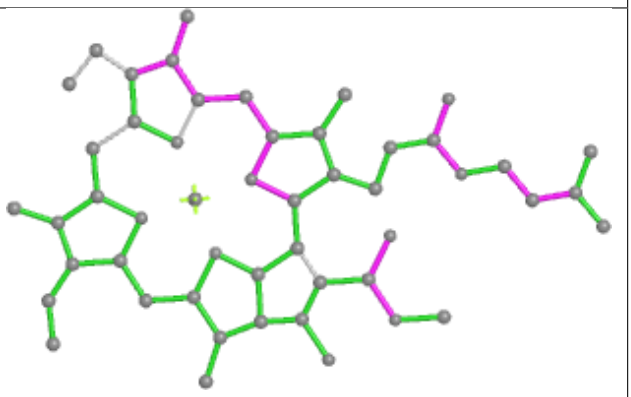
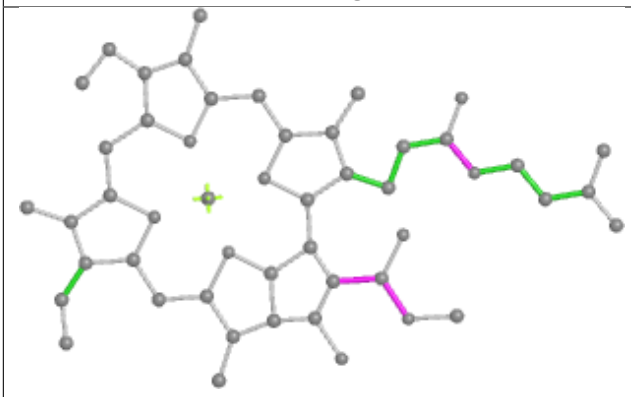
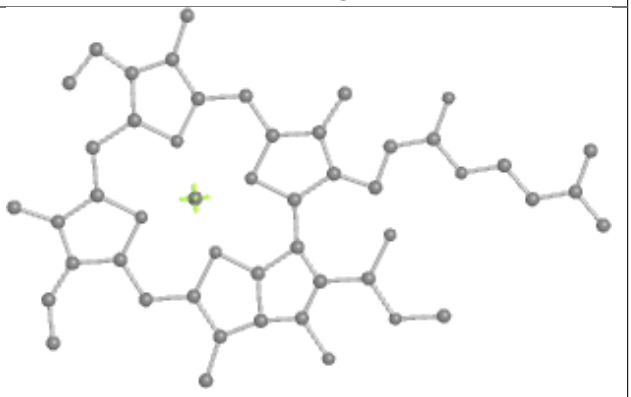


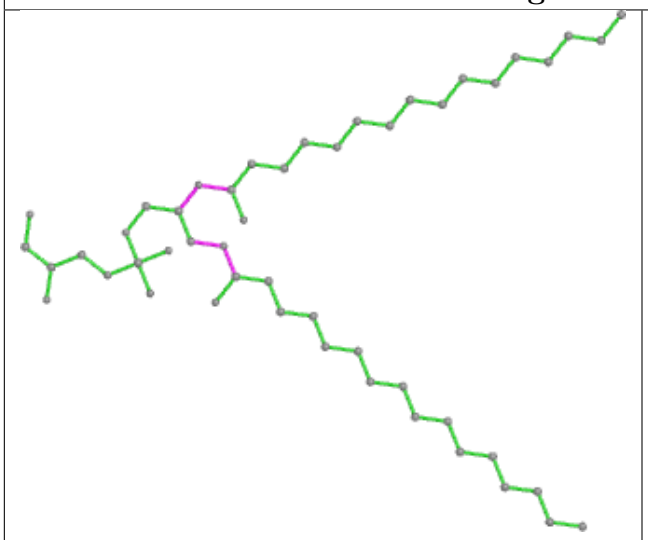
Rings

Ligand LHG U 312

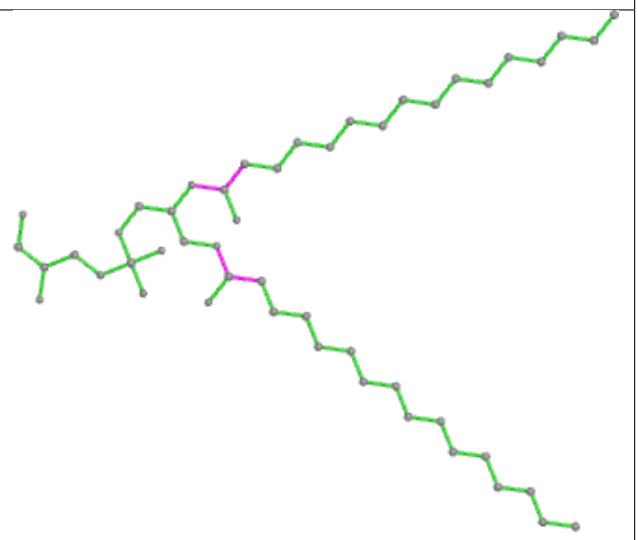


Ligand CLA n 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 4 312



Bond lengths



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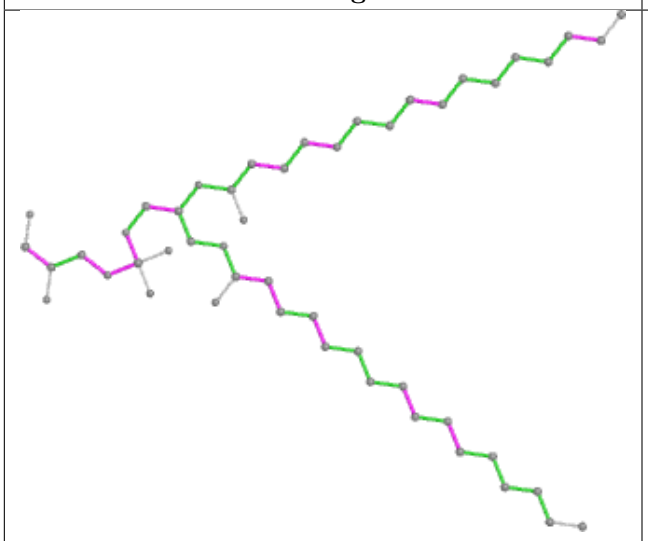

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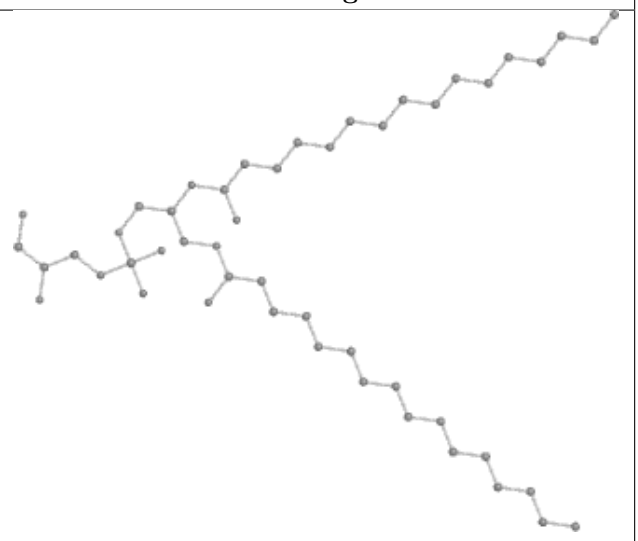
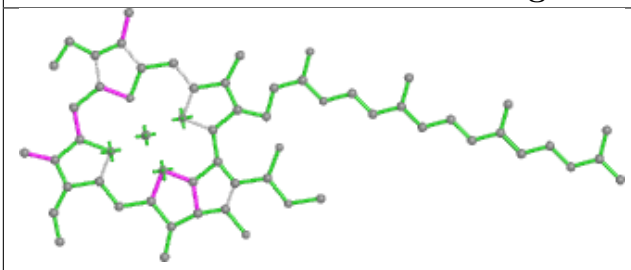


Rings

Ligand CLA 5 305



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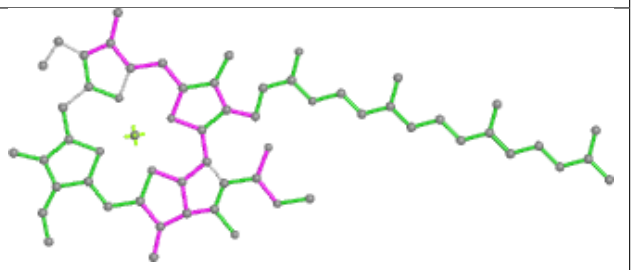
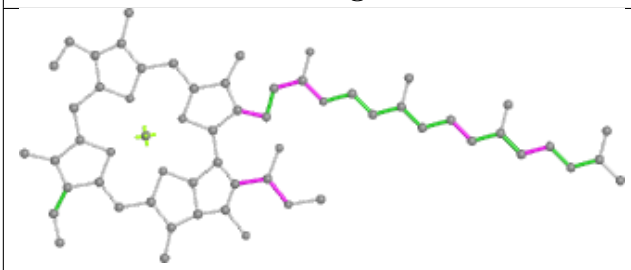
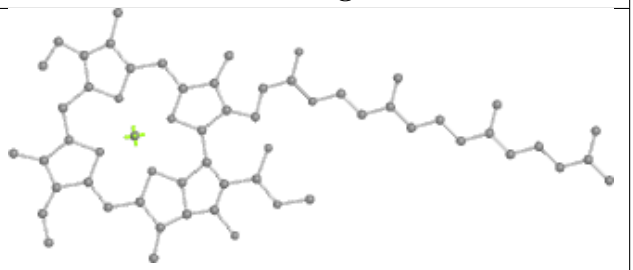


Bond angles

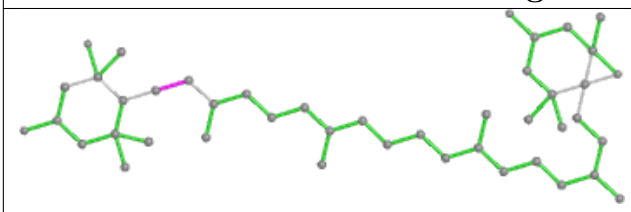


Torsions

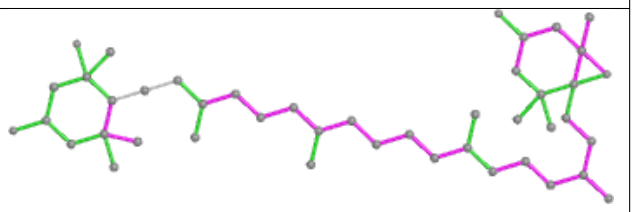


Rings

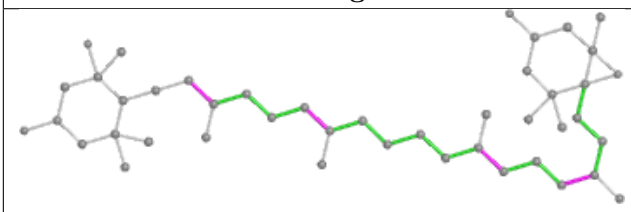
Ligand NEX 2 319



Bond lengths



Bond angles



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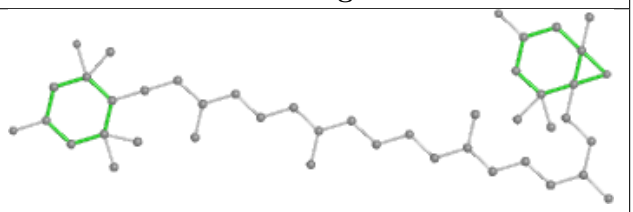
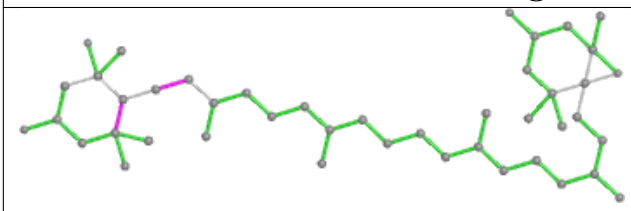
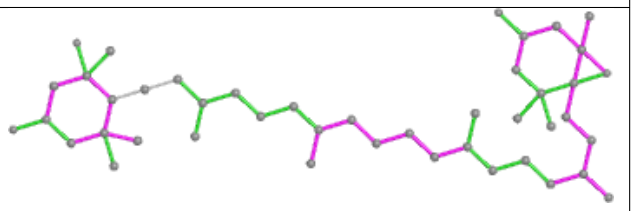


Rings

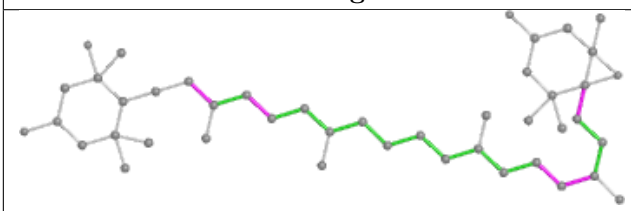
Ligand NEX r 618



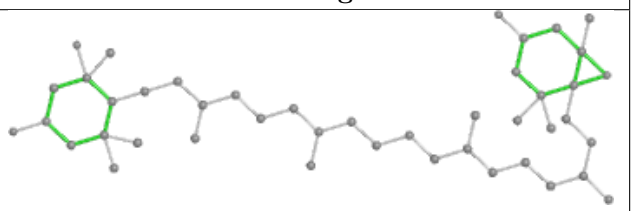
Bond lengths



Bond angles

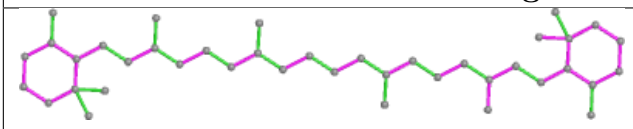


Torsions

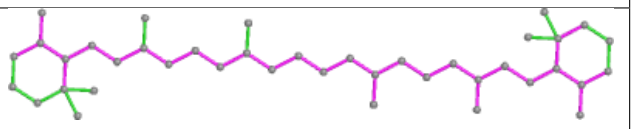


Rings

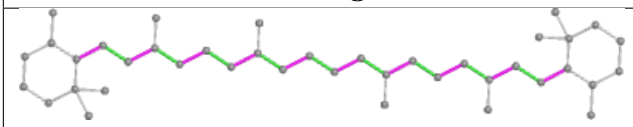
Ligand BCR C 517



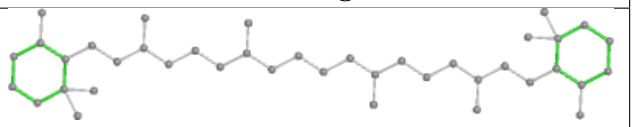
Bond lengths



Bond angles

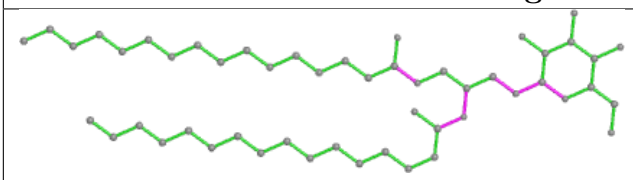


Torsions

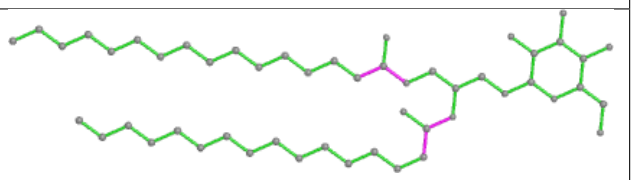


Rings

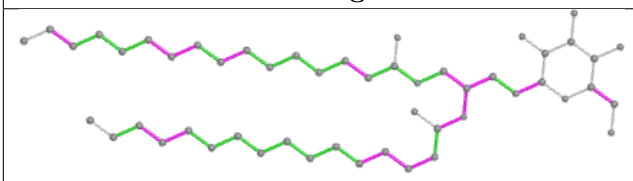
Ligand LMG c 520



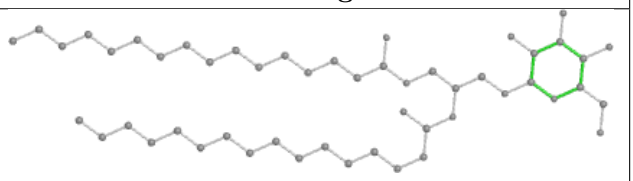
Bond lengths



Bond angles

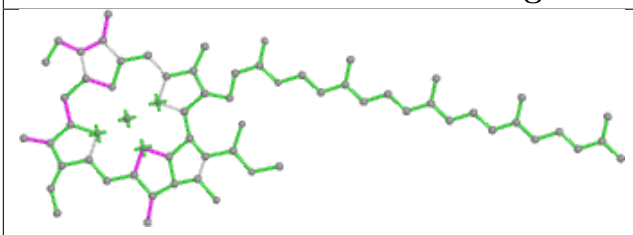


Torsions

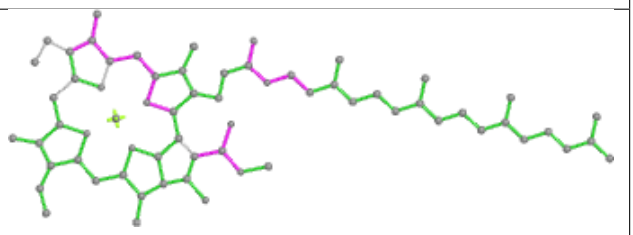


Rings

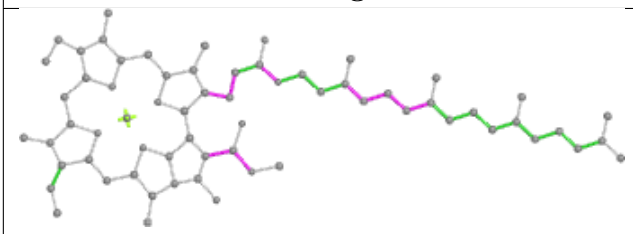
Ligand CLA B 607



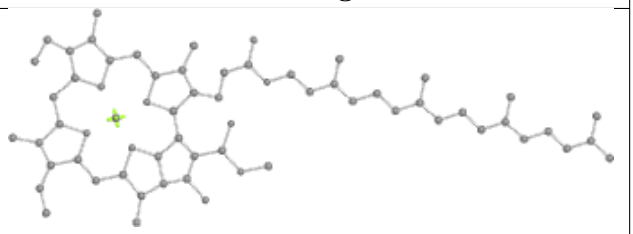
Bond lengths



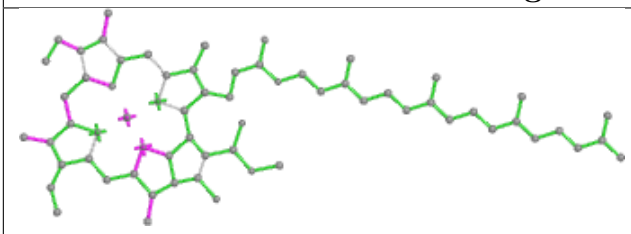
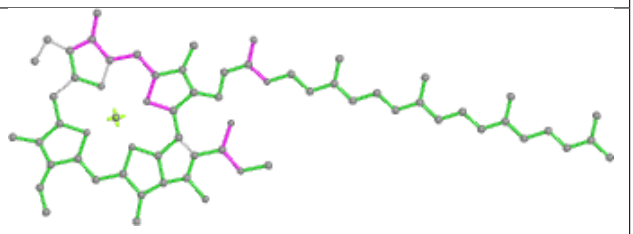
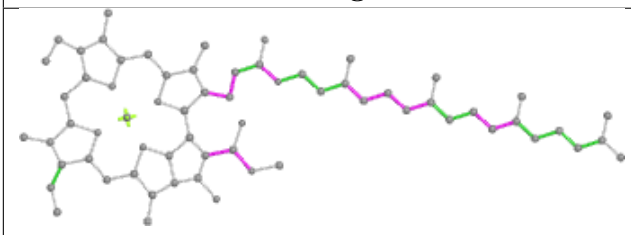
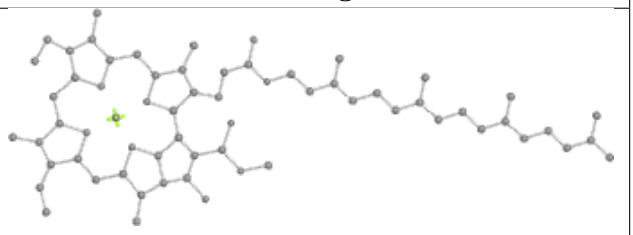
Bond angles

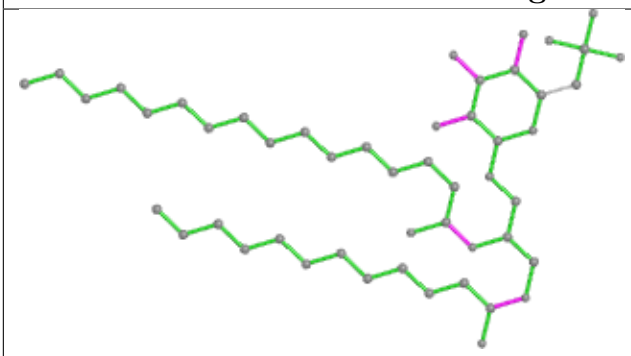
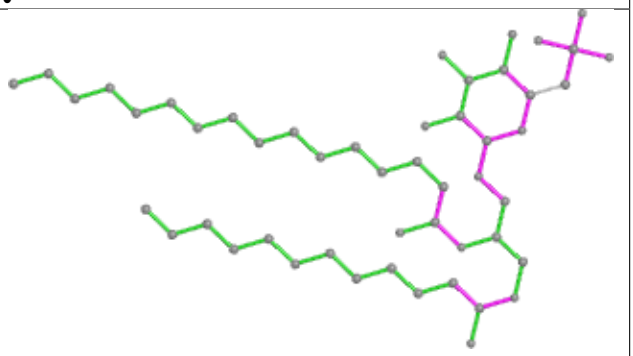
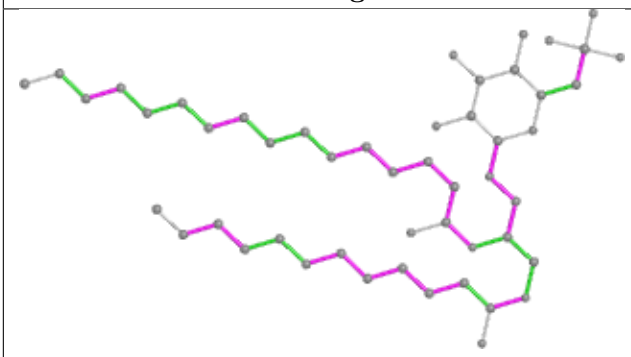
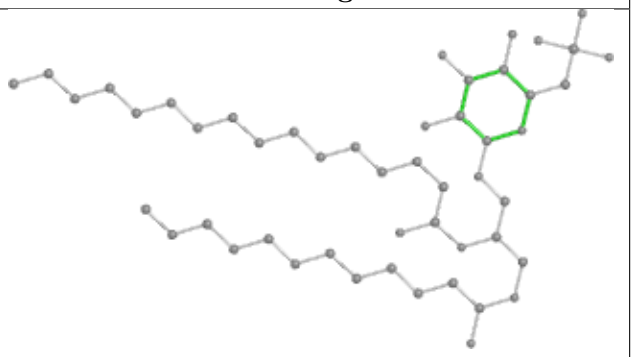


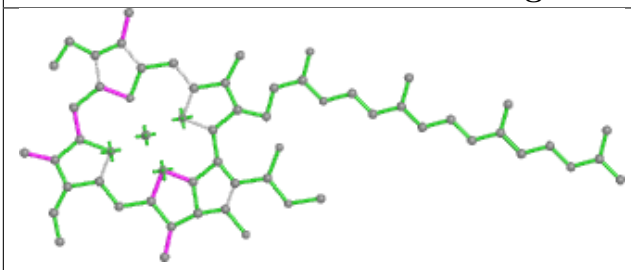
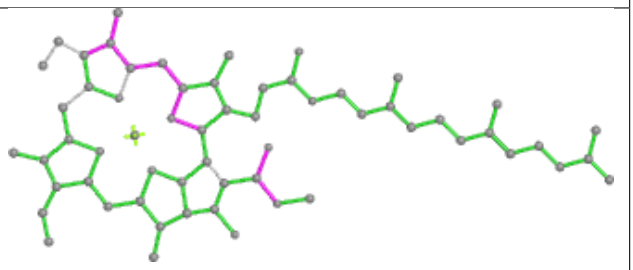
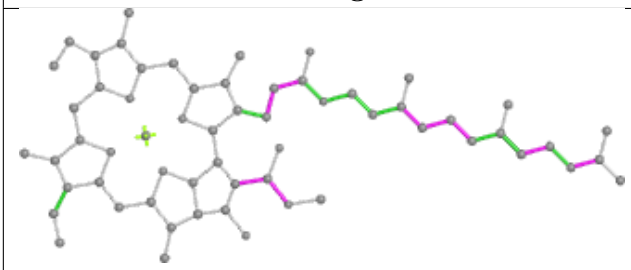
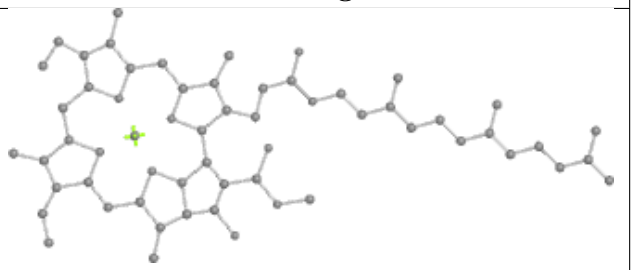
Torsions

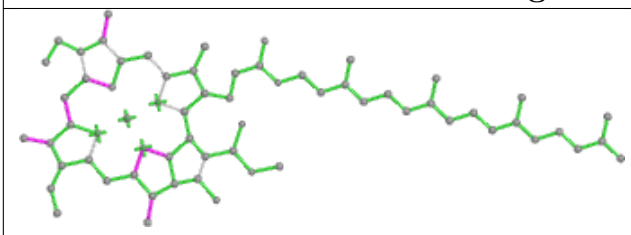
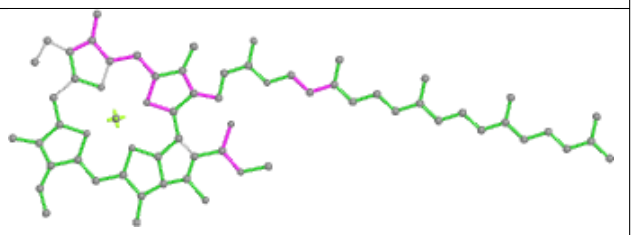
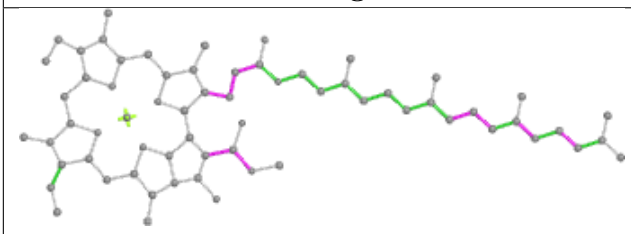
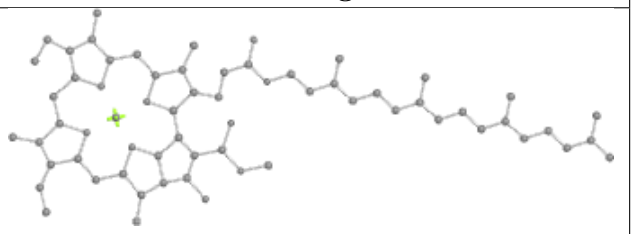


Rings

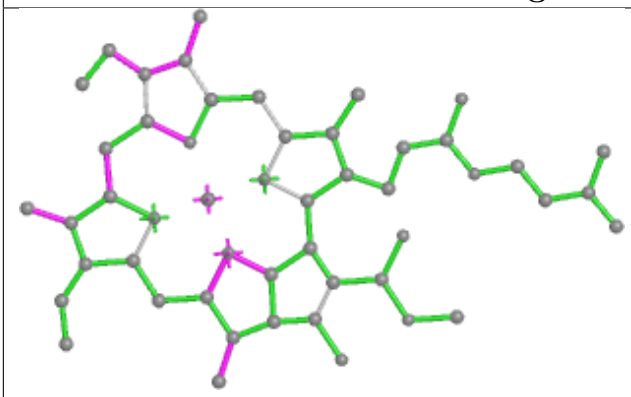
Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD a 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

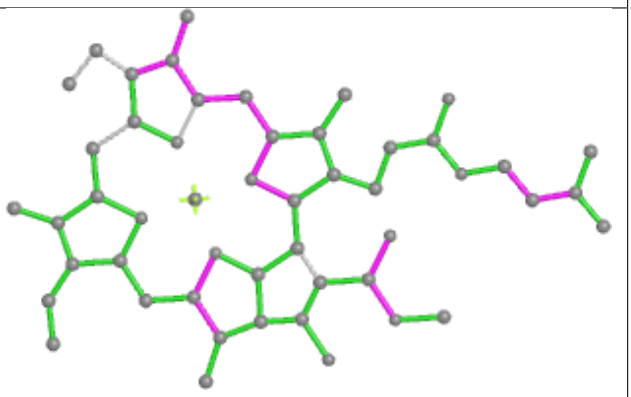
Ligand CLA P 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

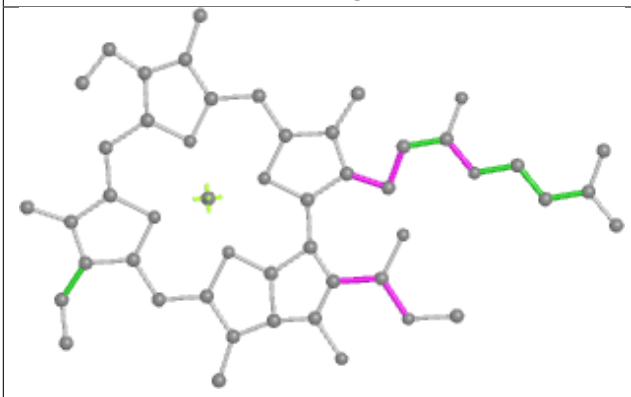
Ligand CLA a 406



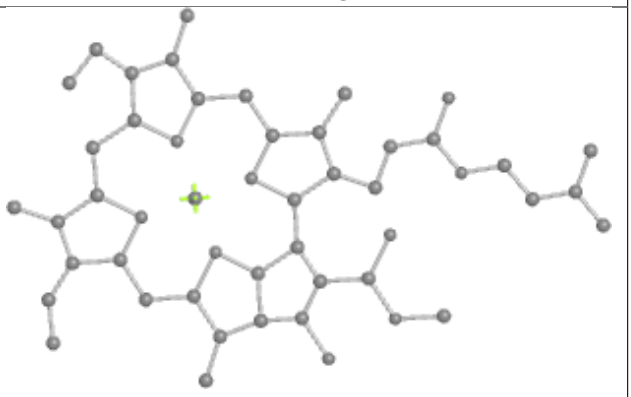
Bond lengths



Bond angles

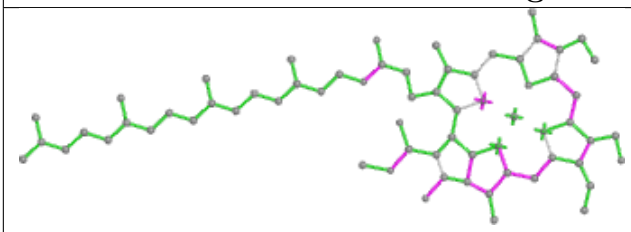


Torsions

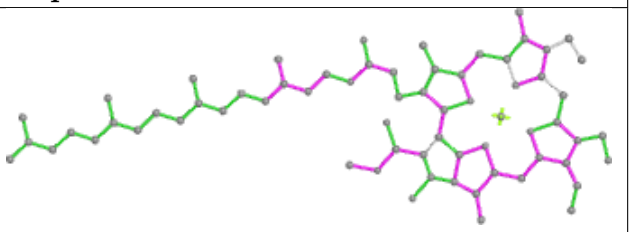


Rings

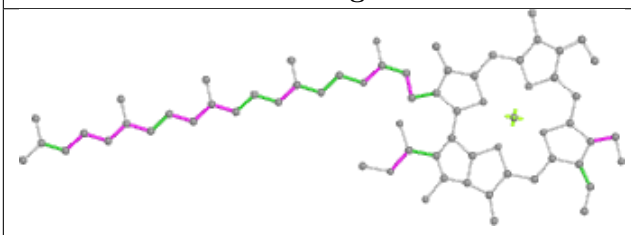
Ligand CHL p 320



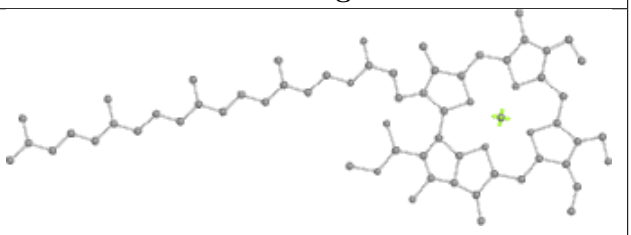
Bond lengths



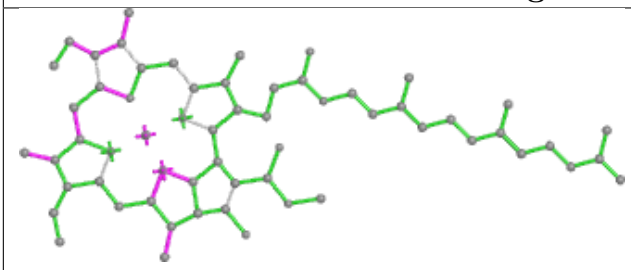
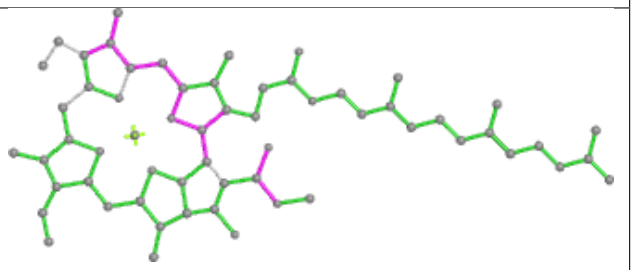
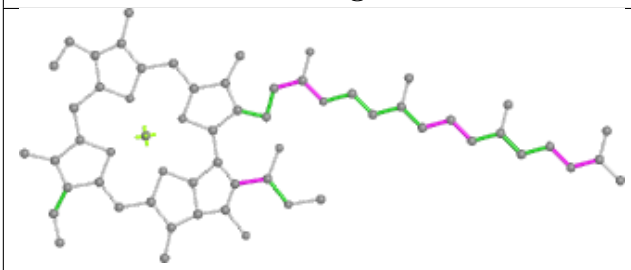
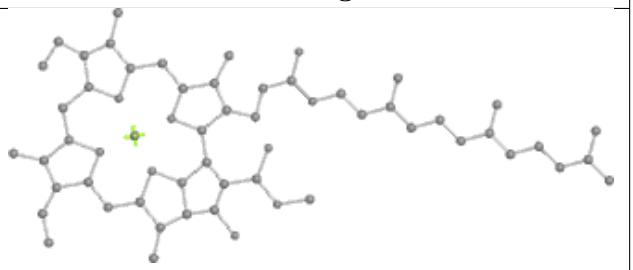
Bond angles

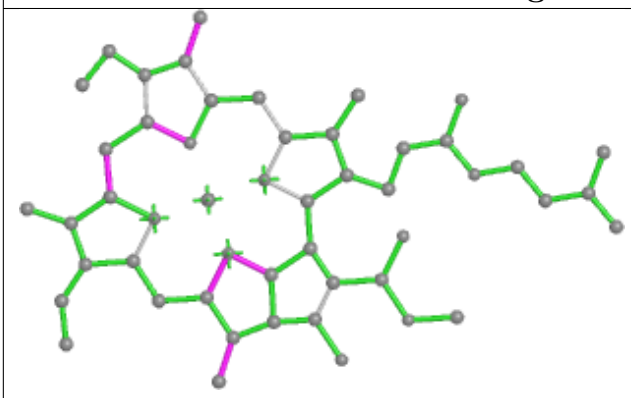
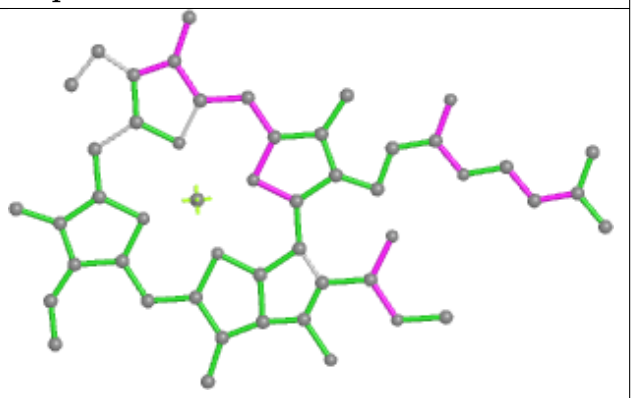
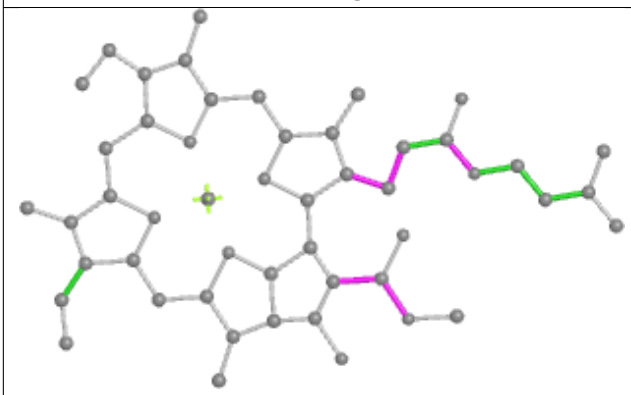
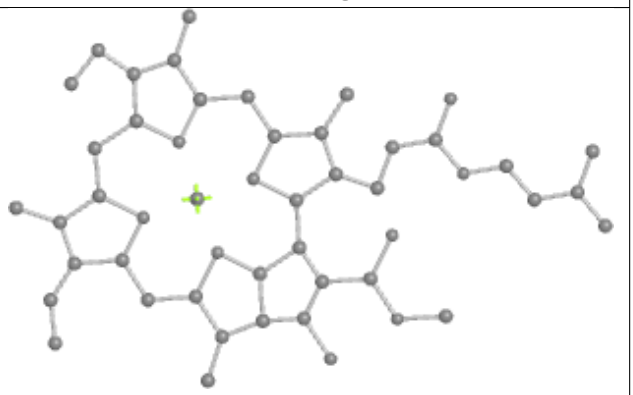


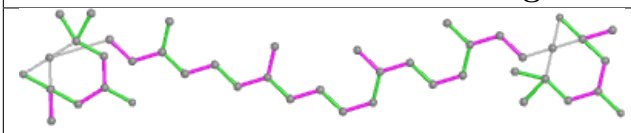
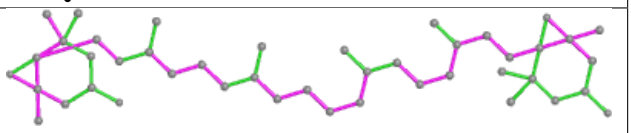
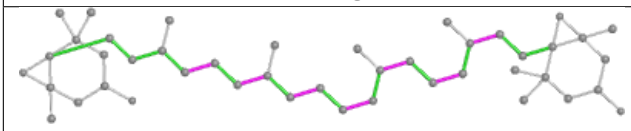
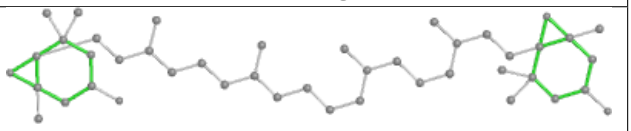
Torsions

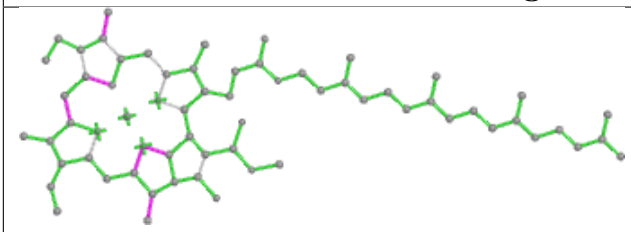
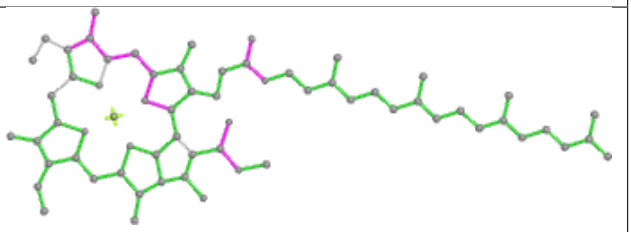
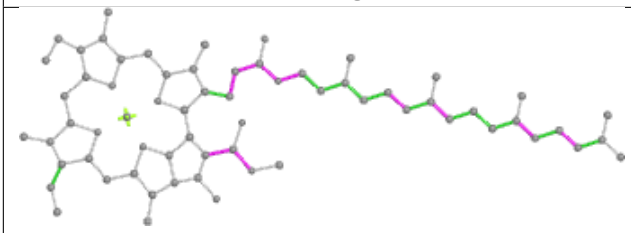
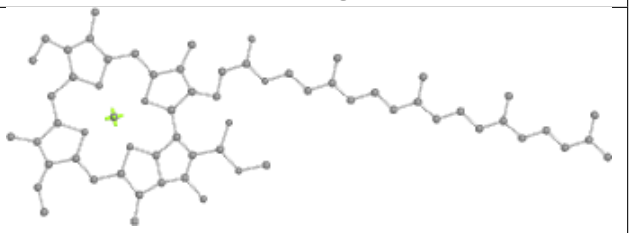


Rings

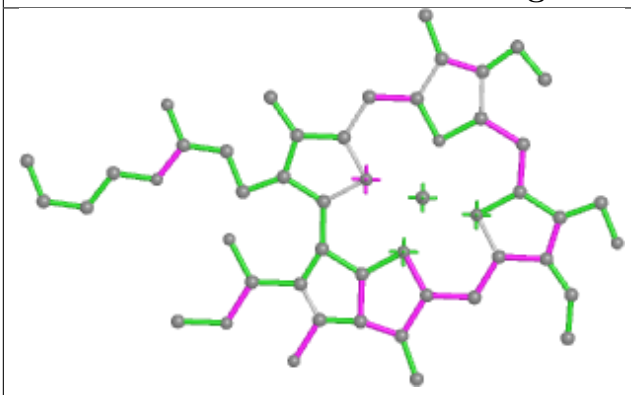
Ligand CLA u 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

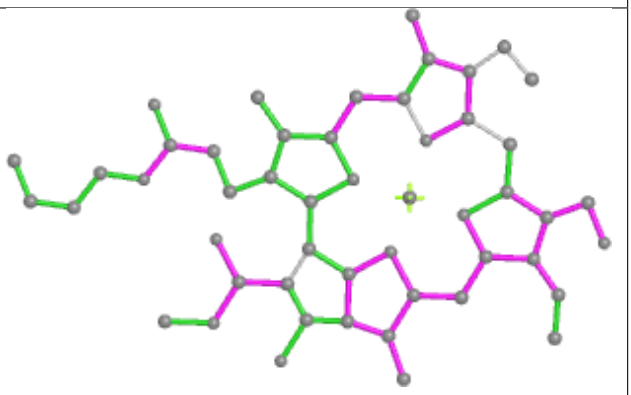
Ligand XAT Q 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

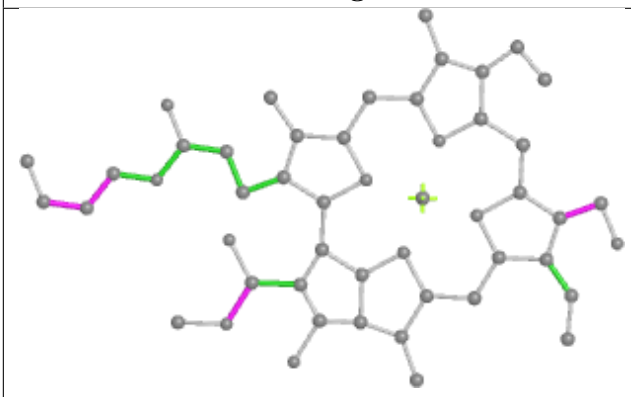
Ligand CHL 1 315



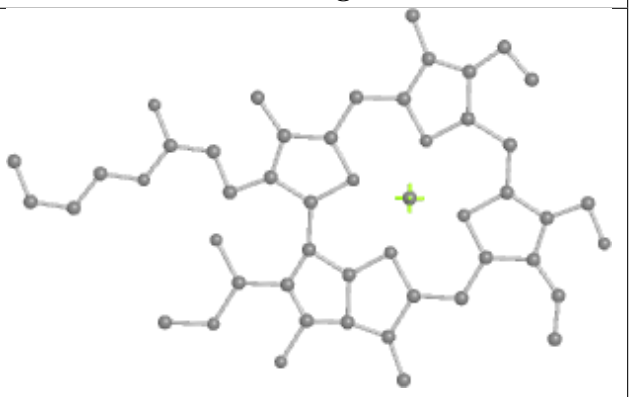
Bond lengths



Bond angles

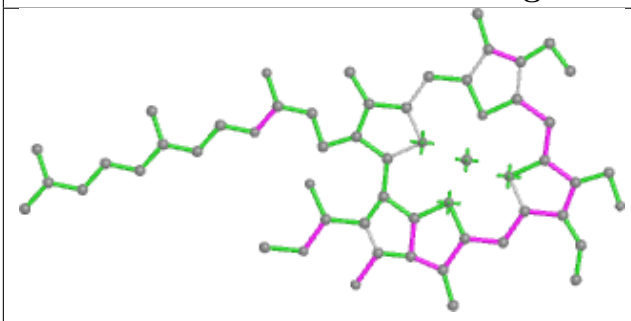


Torsions

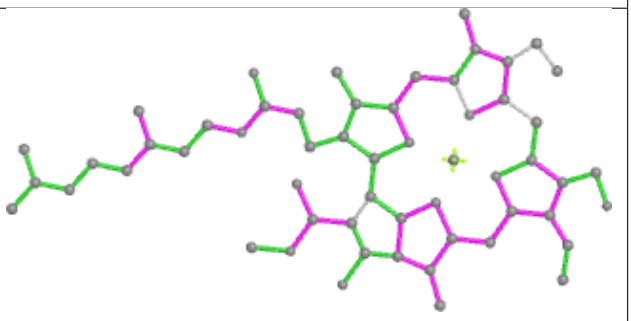


Rings

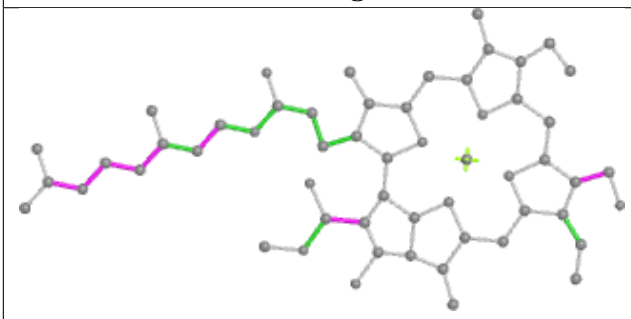
Ligand CHL R 316



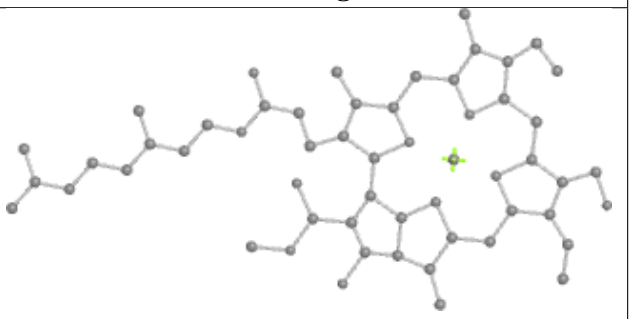
Bond lengths



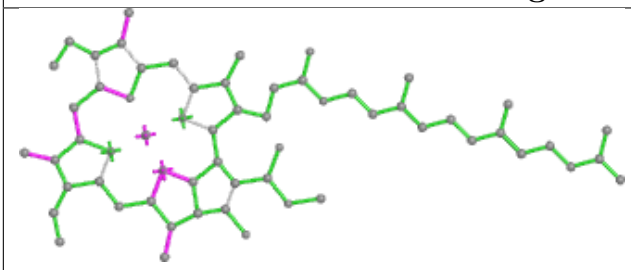
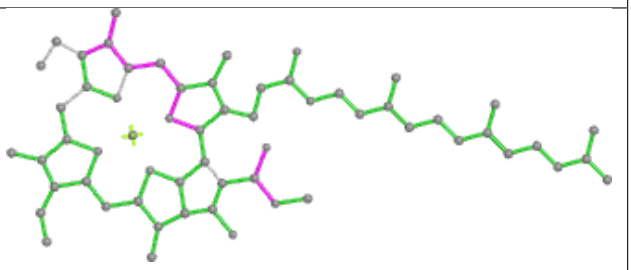
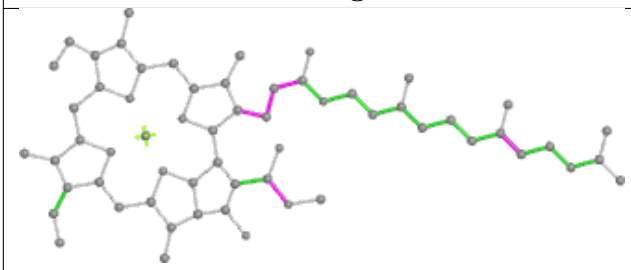
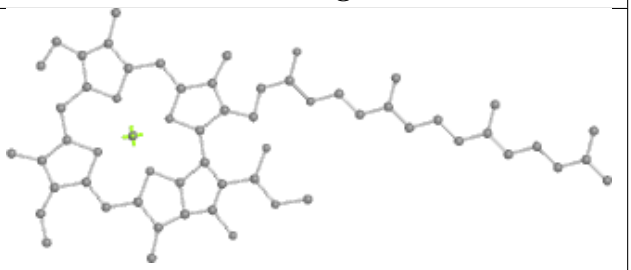
Bond angles

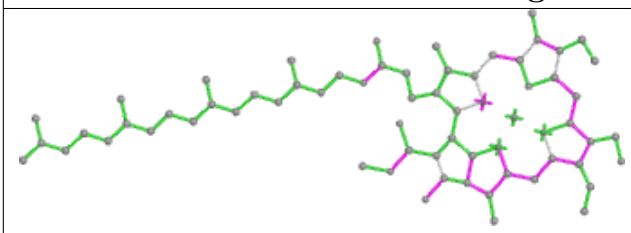
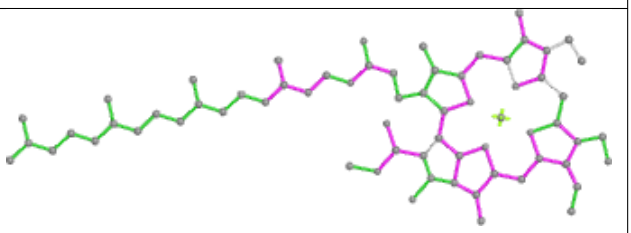
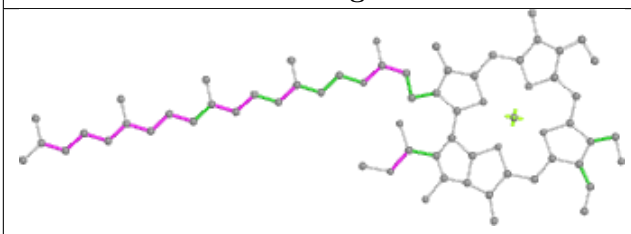
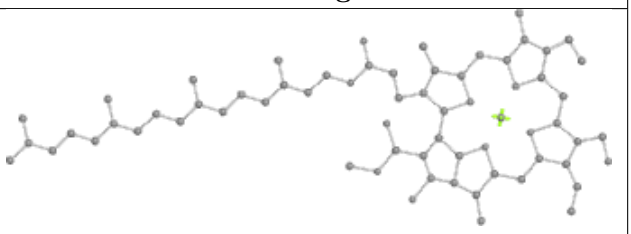


Torsions

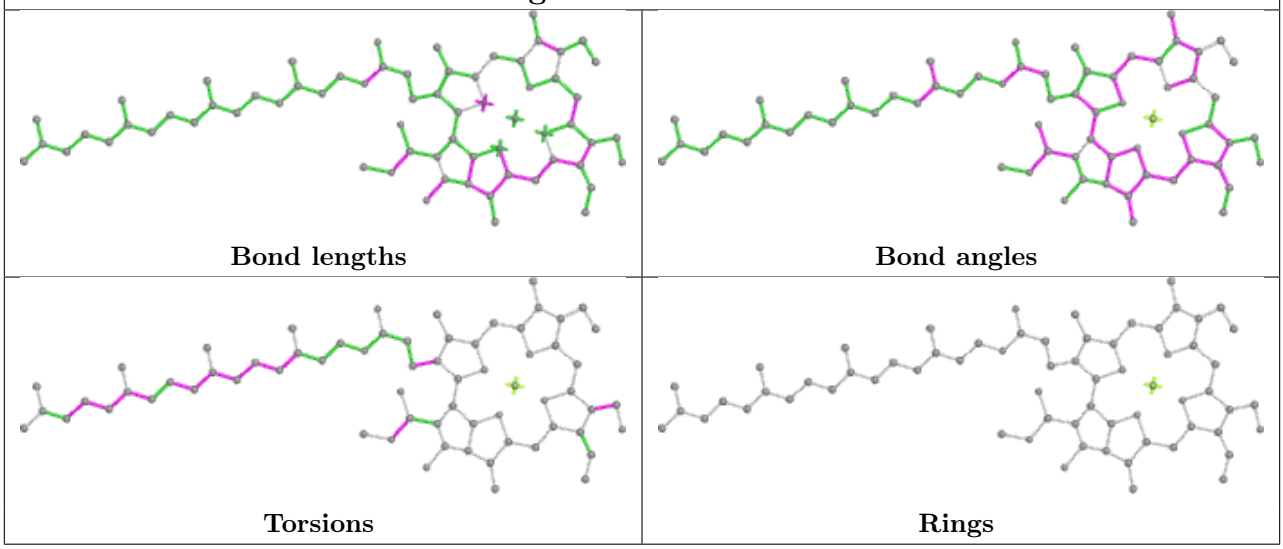


Rings

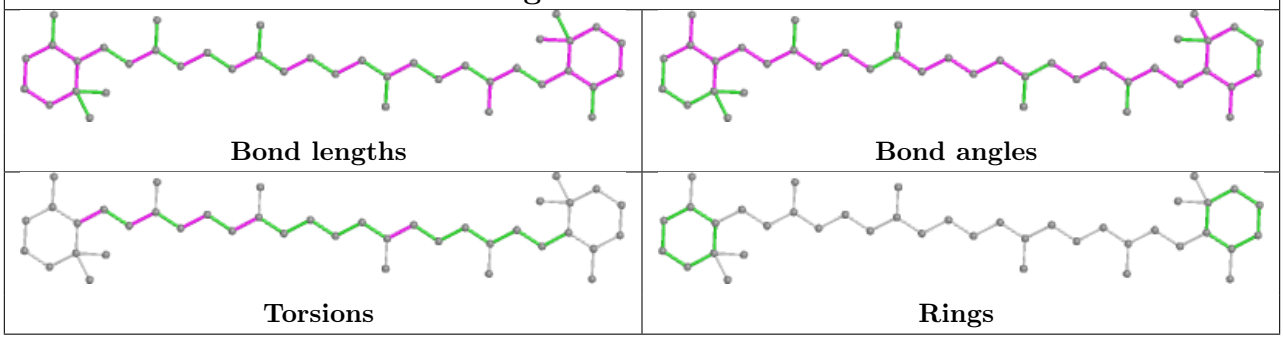
Ligand CLA 1 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 2 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

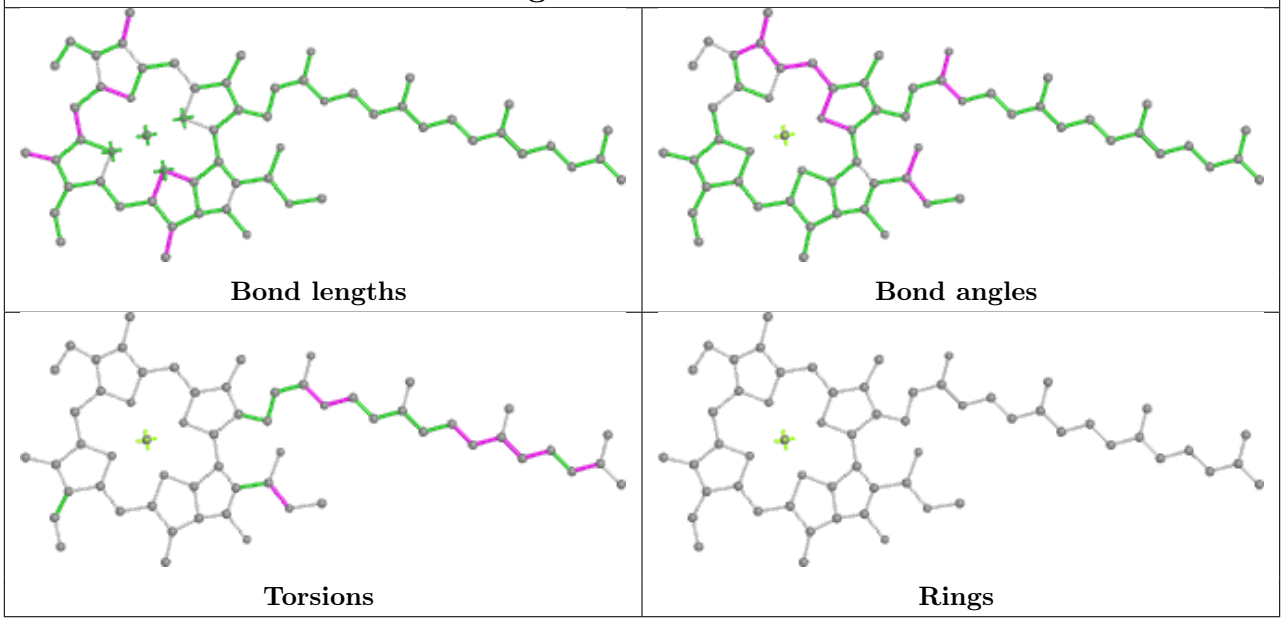
Ligand CHL 2 318



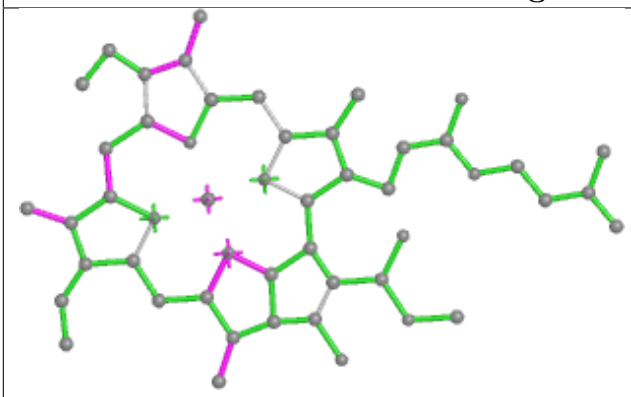
Ligand BCR B 618



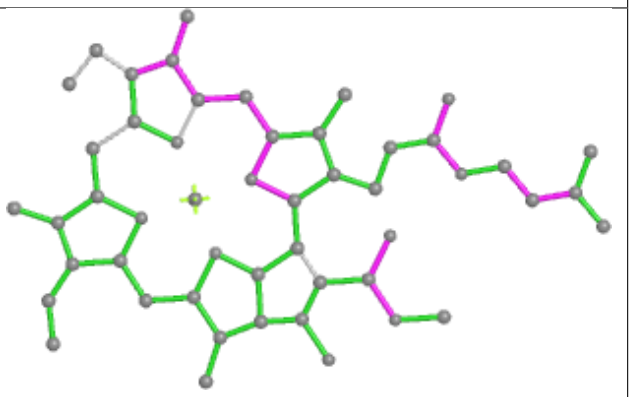
Ligand CLA u 305



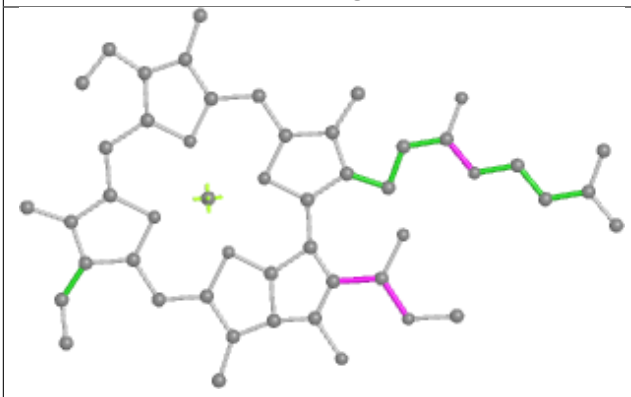
Ligand CLA 1 303



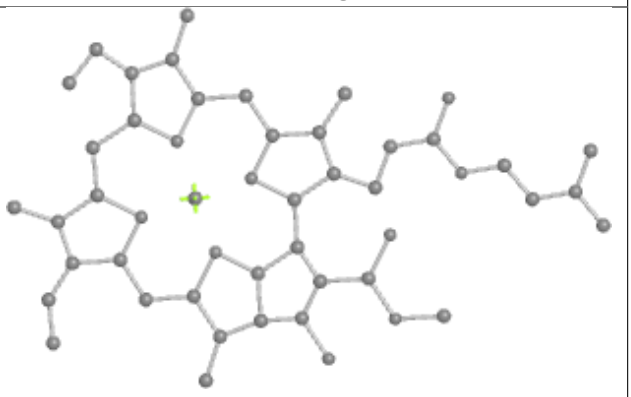
Bond lengths



Bond angles

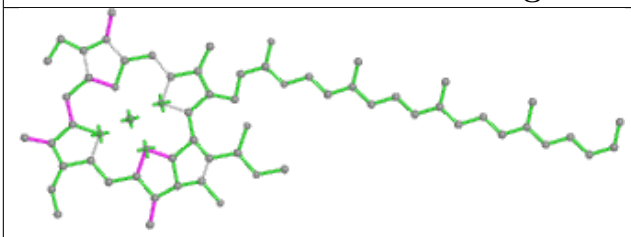


Torsions

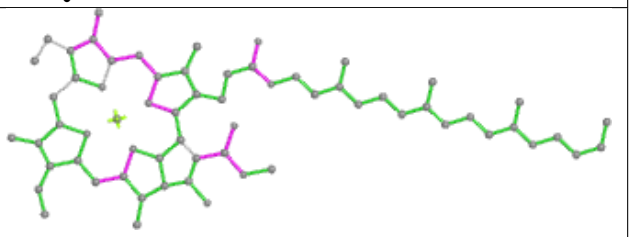


Rings

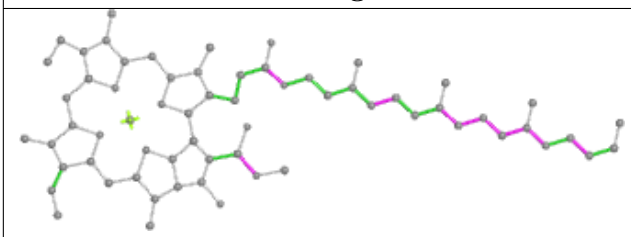
Ligand CLA Q 304



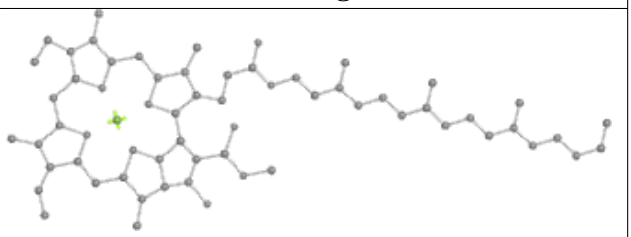
Bond lengths



Bond angles

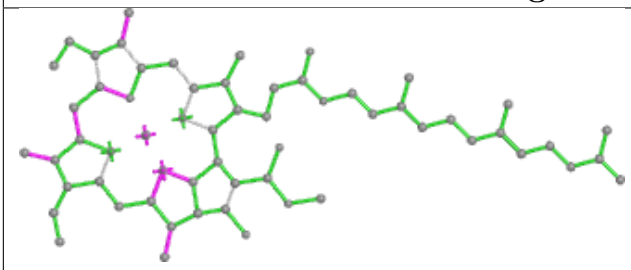


Torsions

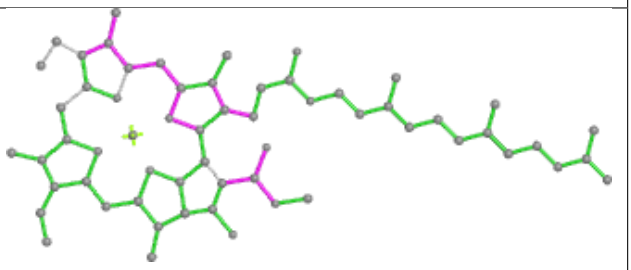


Rings

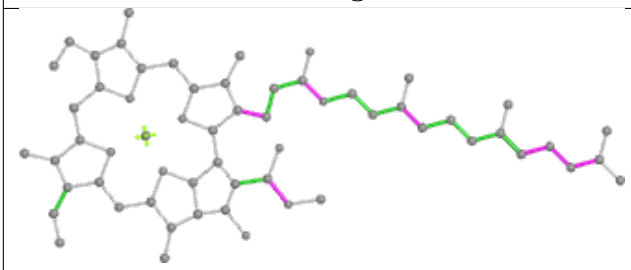
Ligand CLA a 408



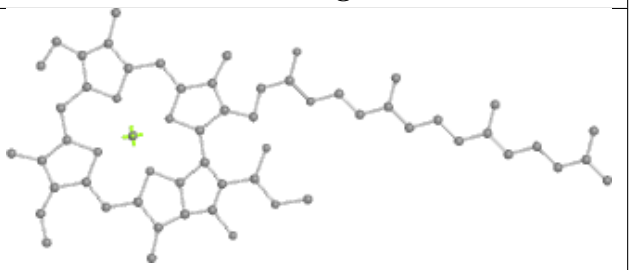
Bond lengths



Bond angles

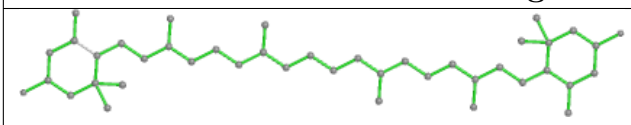


Torsions

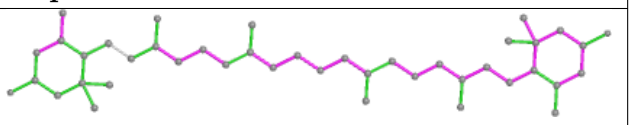


Rings

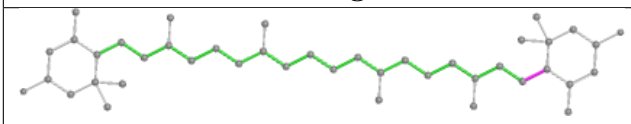
Ligand LUT p 310



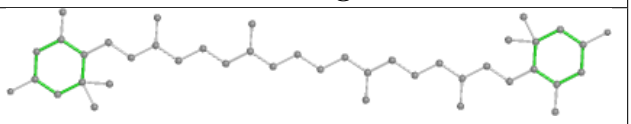
Bond lengths



Bond angles

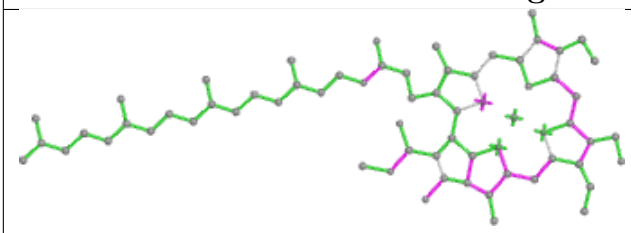


Torsions

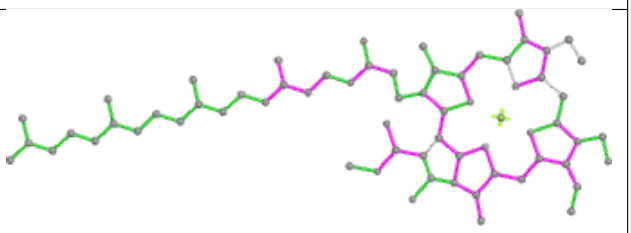


Rings

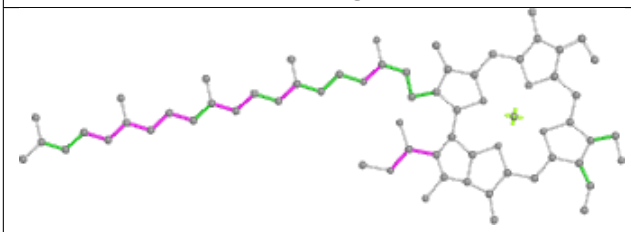
Ligand CHL 6 312



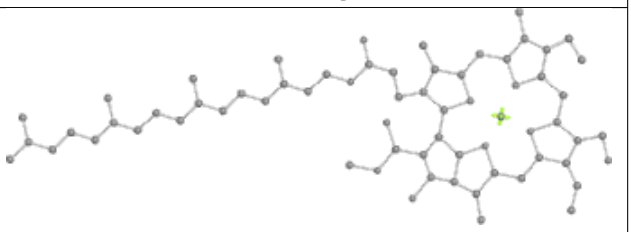
Bond lengths



Bond angles

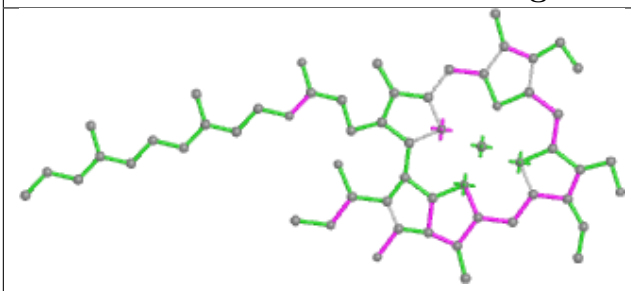


Torsions

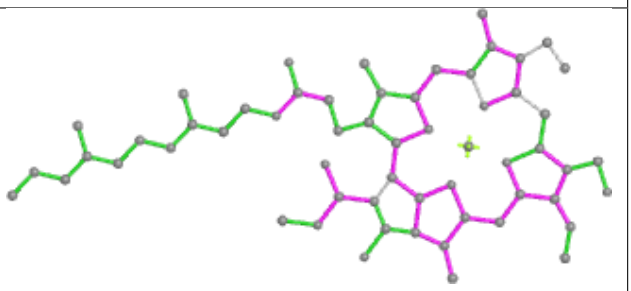


Rings

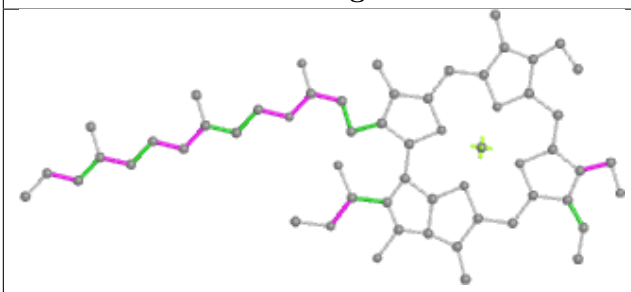
Ligand CHL s 315



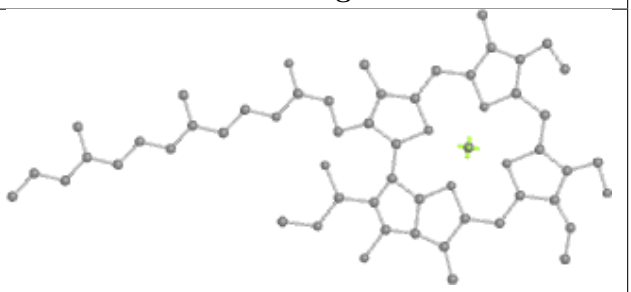
Bond lengths



Bond angles

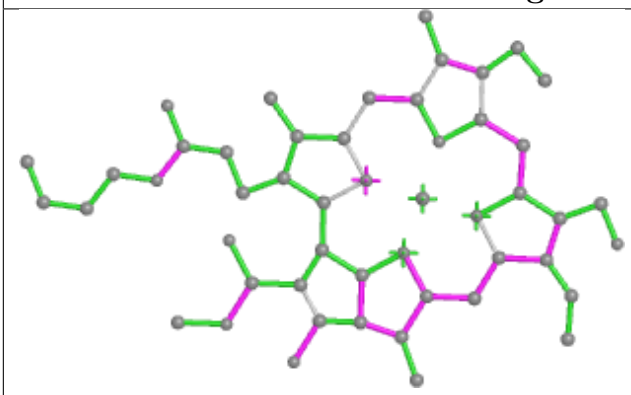


Torsions

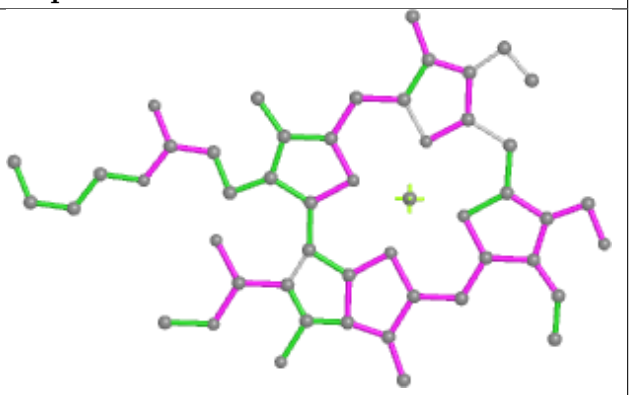


Rings

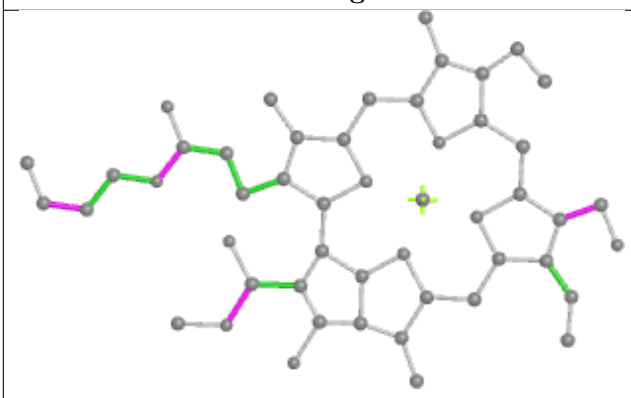
Ligand CHL p 316



Bond lengths



Bond angles



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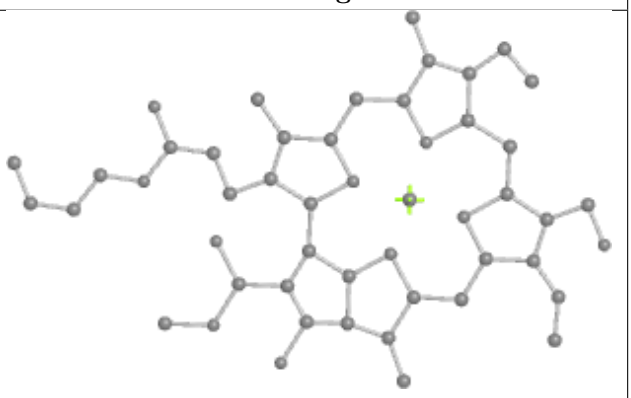
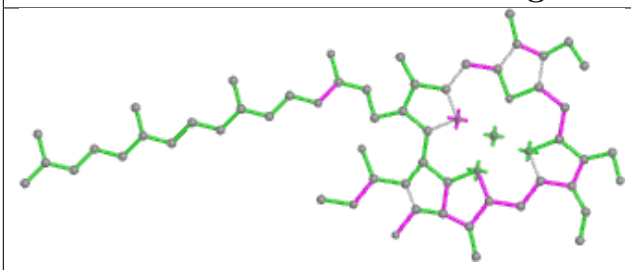


Rings

Ligand CHL q 315



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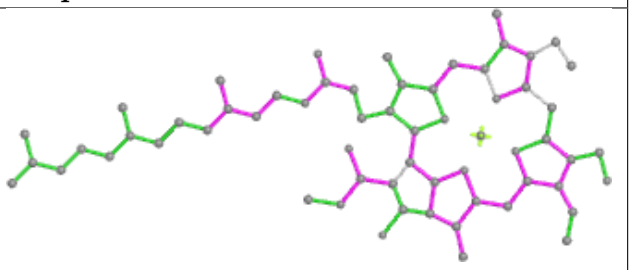
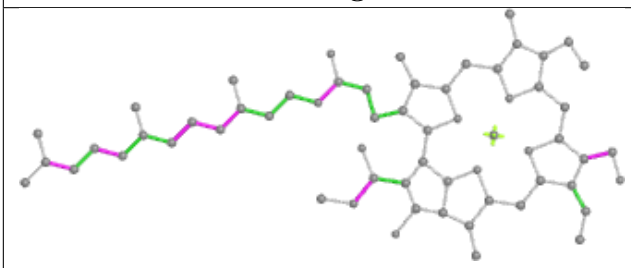


Bond angles



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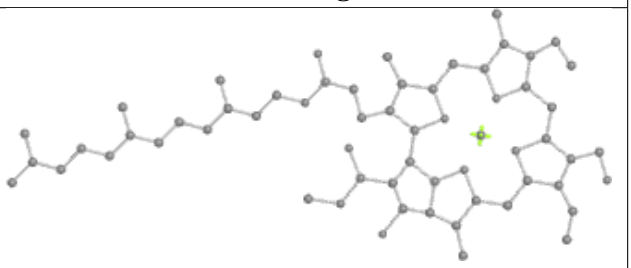
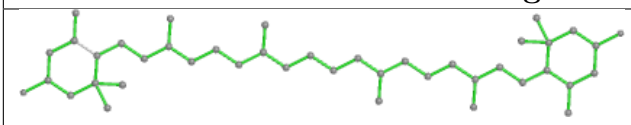
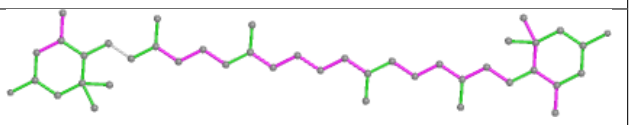


Rings

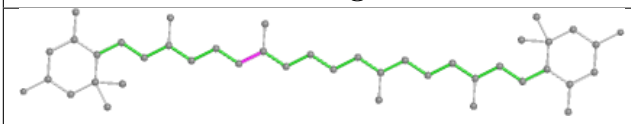
Ligand LUT N 309



Bond lengths



Bond angles



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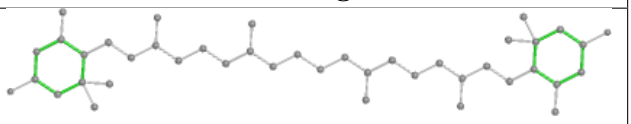
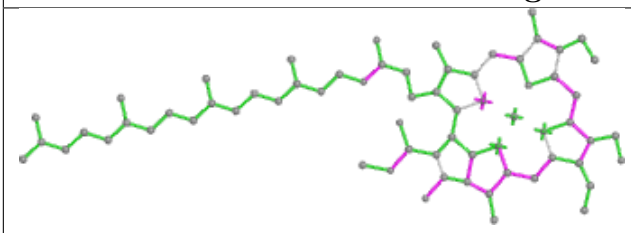
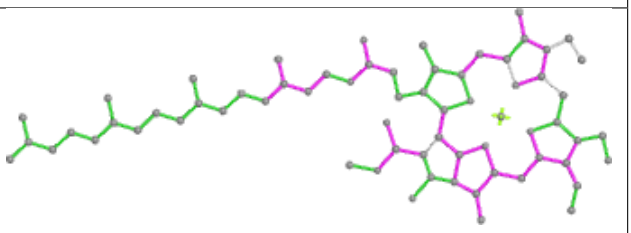


Rings

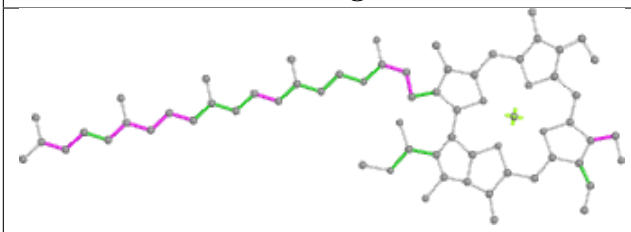
Ligand CHL P 314



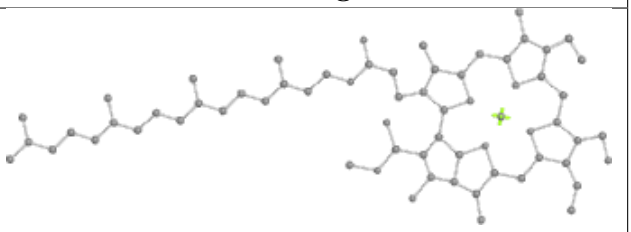
Bond lengths



Bond angles

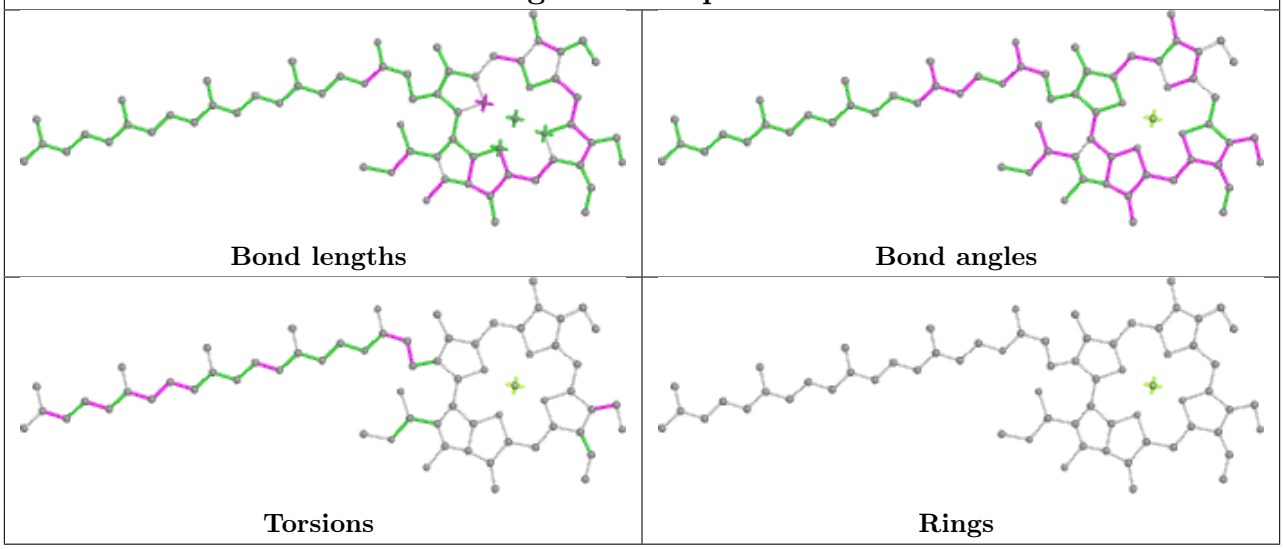


Torsions

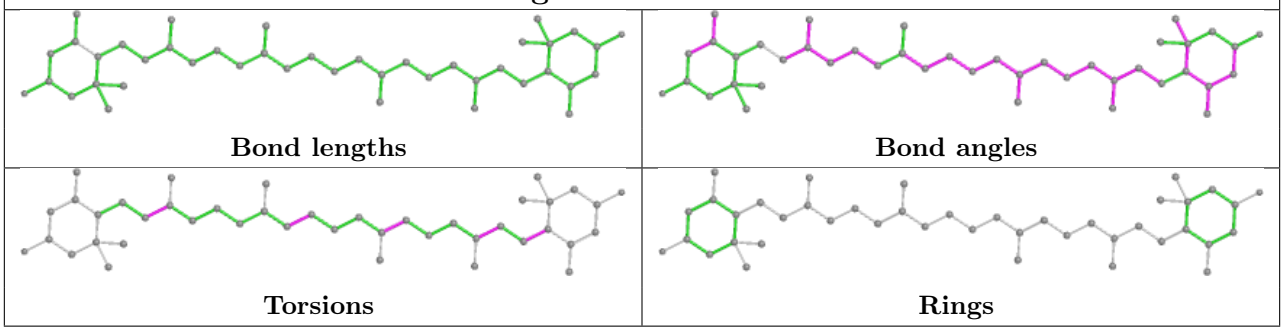


Rings

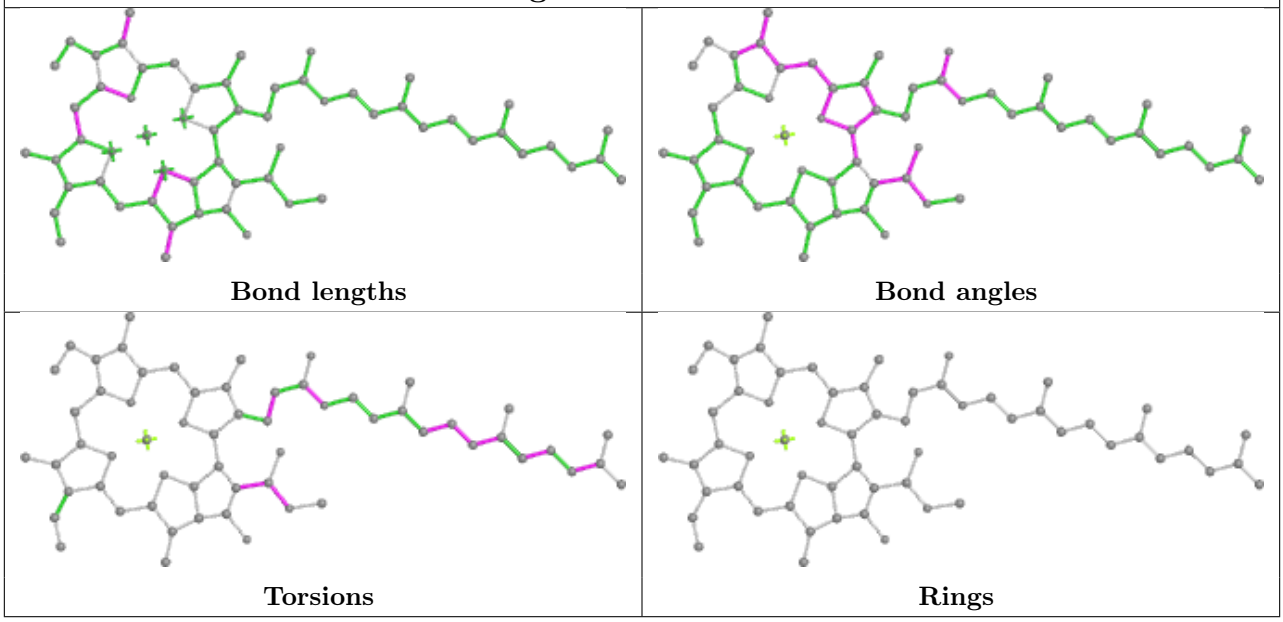
Ligand CHL p 314

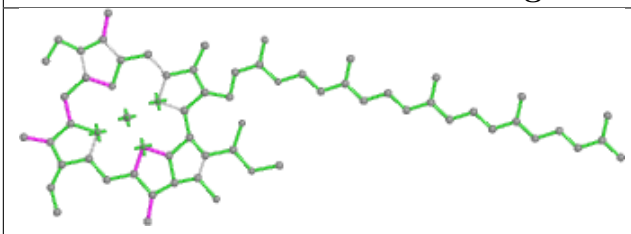
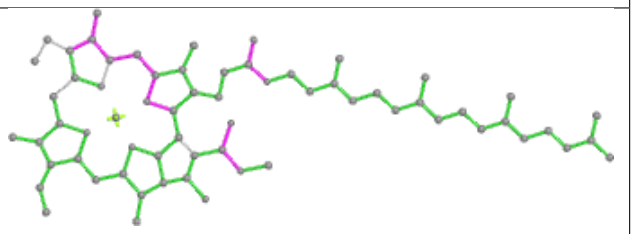
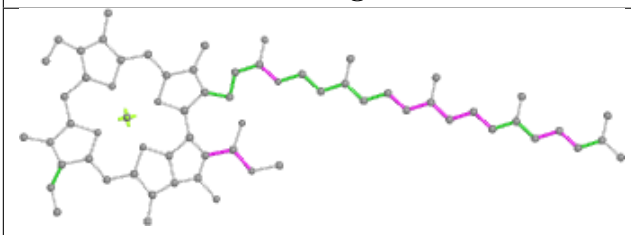
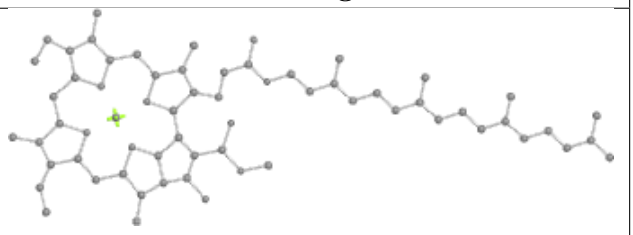


Ligand LUT s 311



Ligand CLA 6 306



Ligand CLA B 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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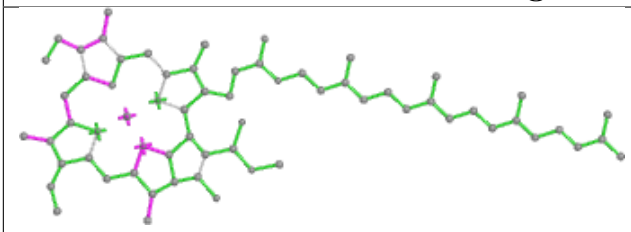
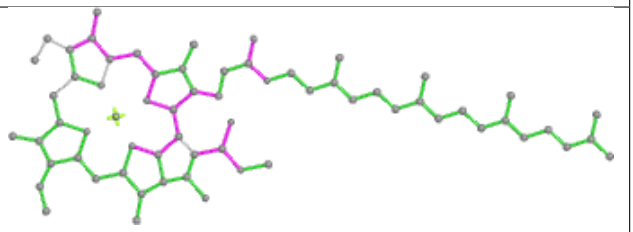
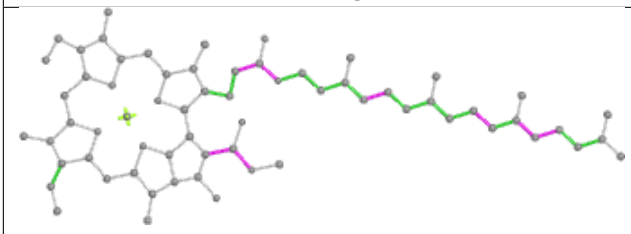
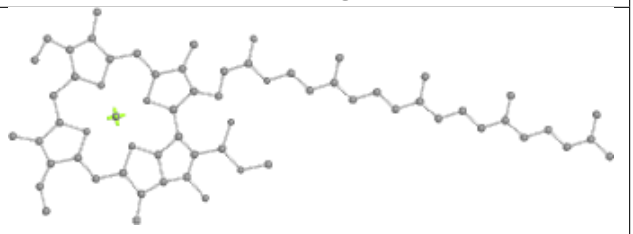
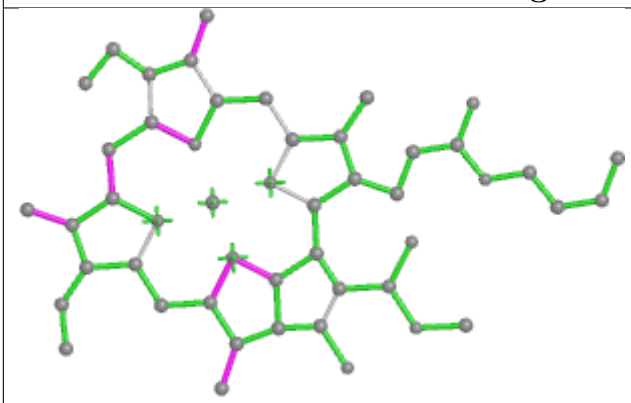
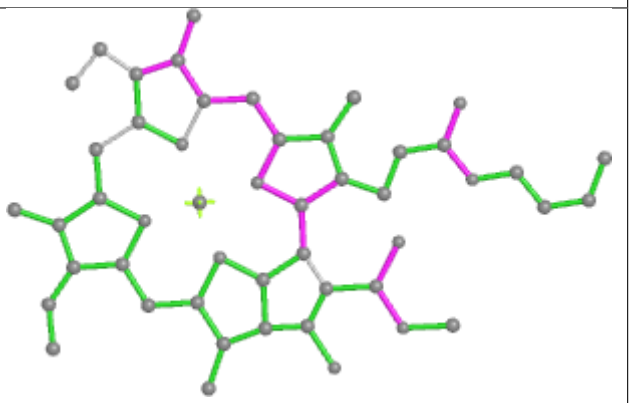
 Bond lengths	 Bond angles
 Torsions	 Rings

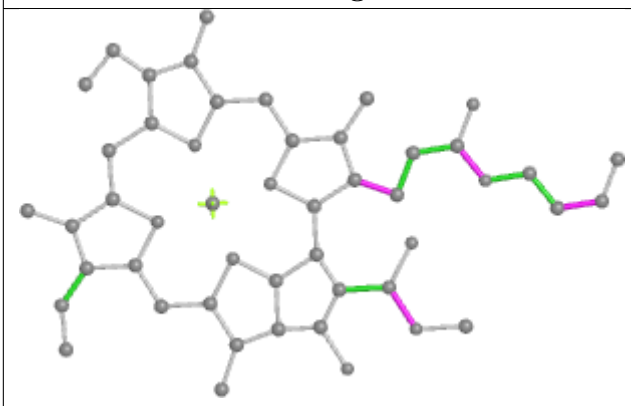
Ligand CLA r 601



Bond lengths



Bond angles



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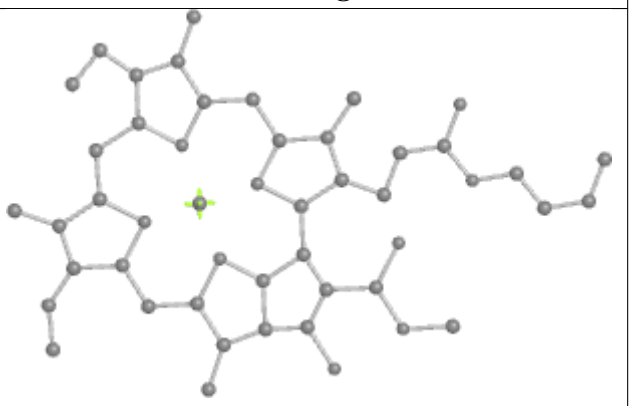
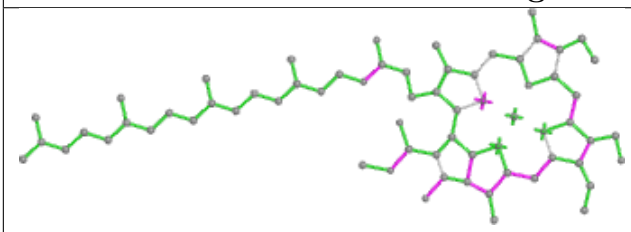


Rings

Ligand CHL 5 317



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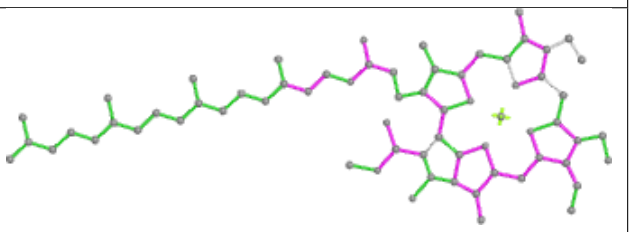

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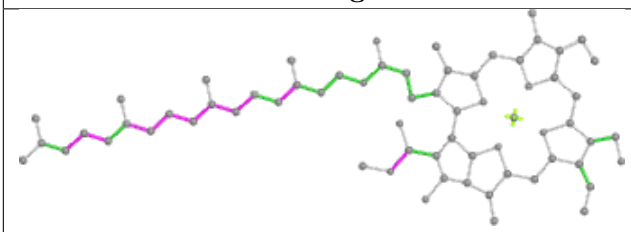

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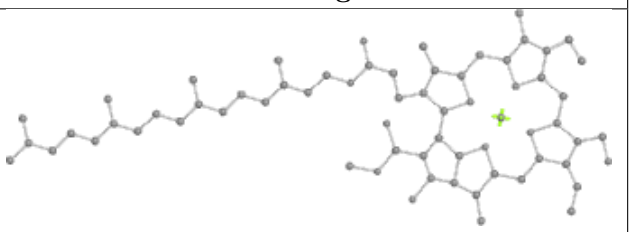
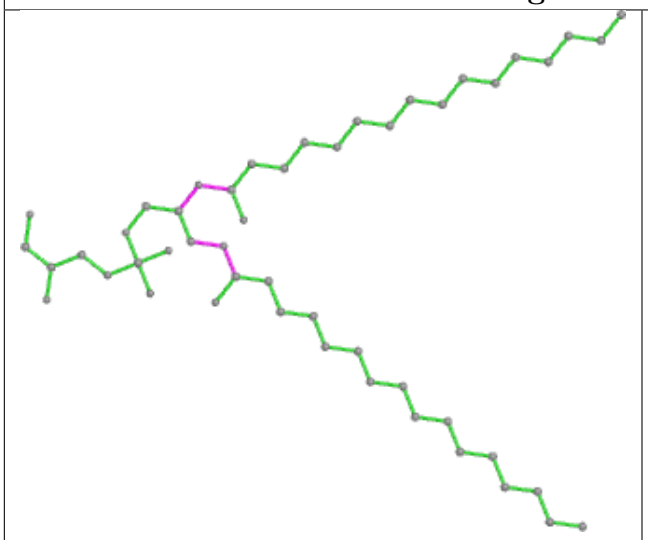


Rings

Ligand LHG g 310



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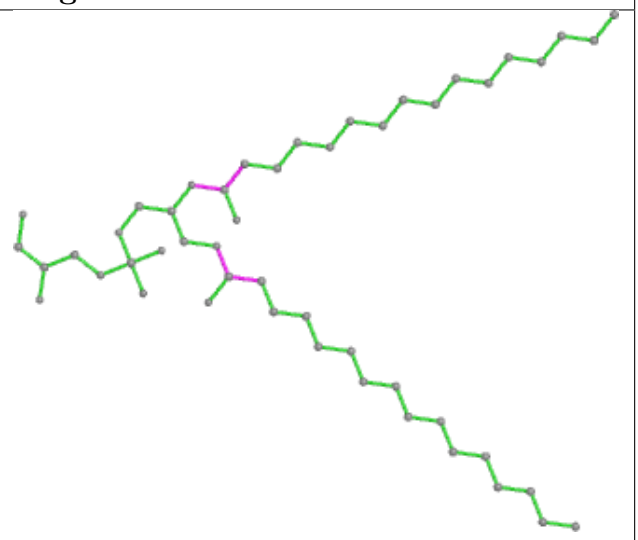
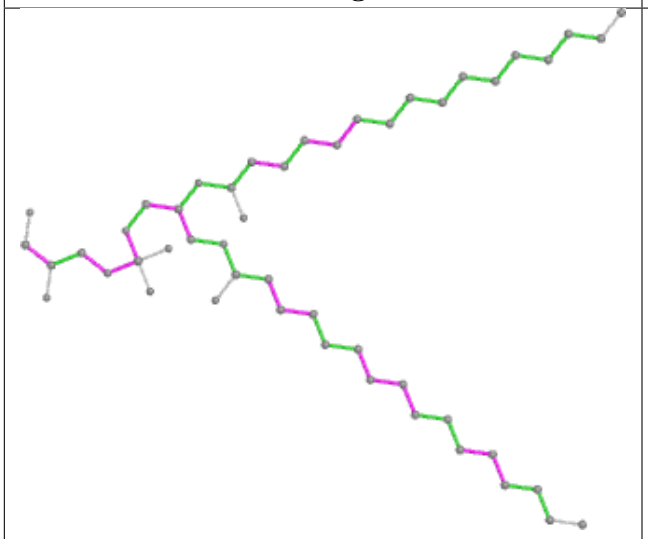


Bond angles



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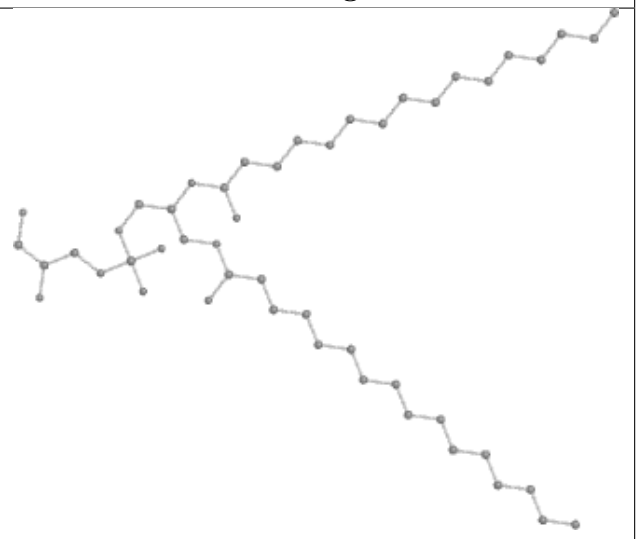
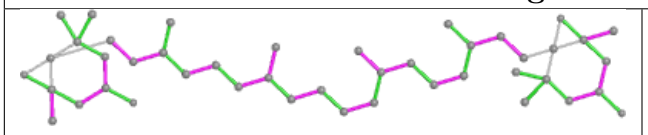


Rings

Ligand XAT u 311



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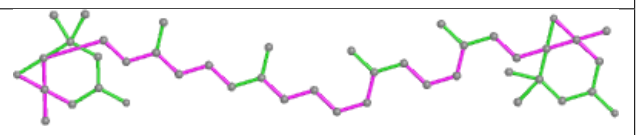

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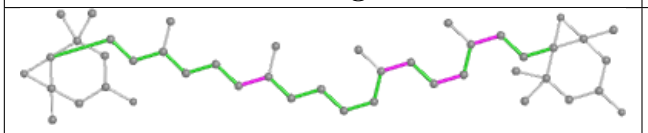

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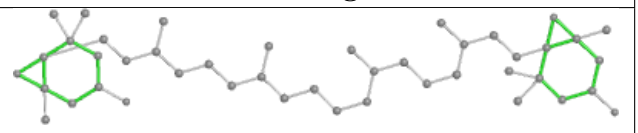
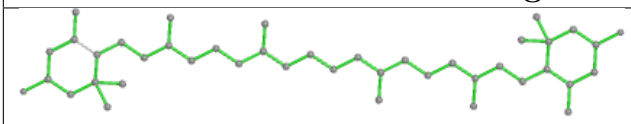


Rings

Ligand LUT R 312



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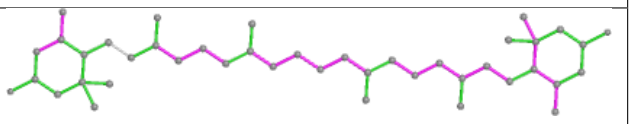
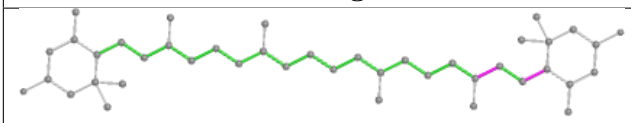


Bond angles



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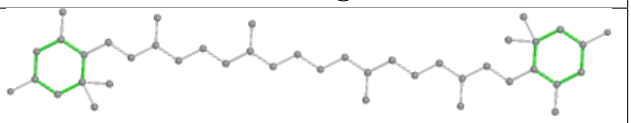
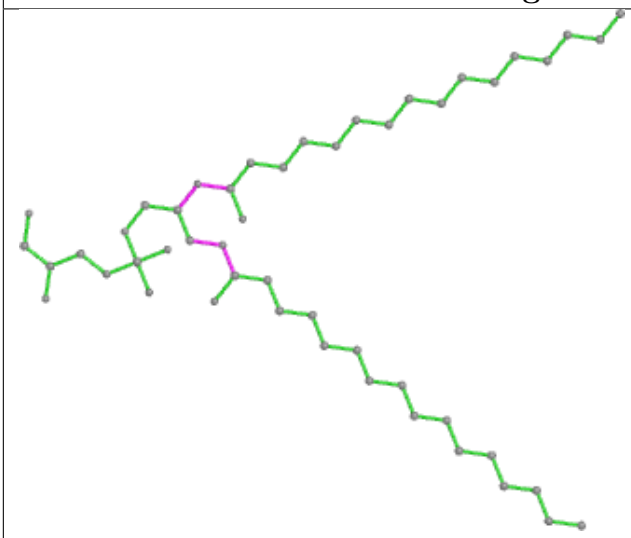
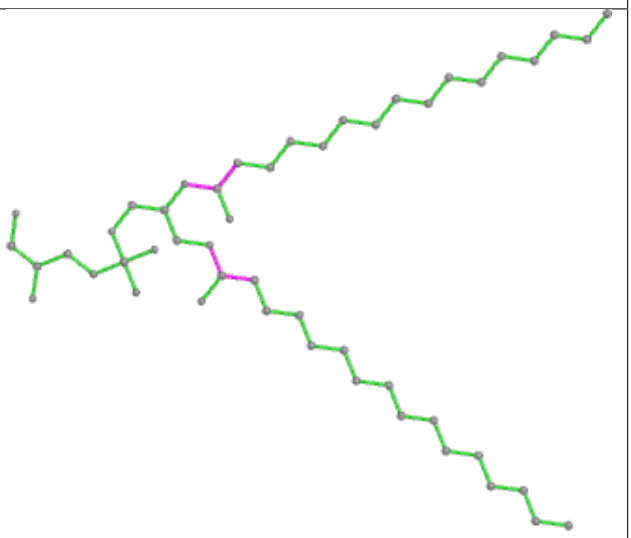


Rings

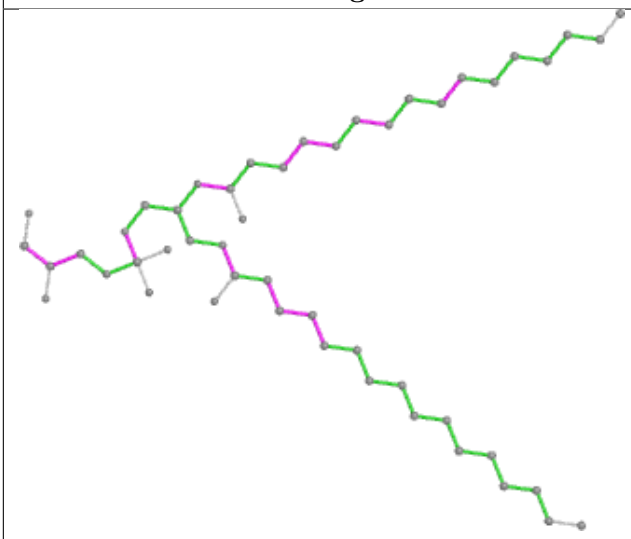
Ligand LHG C 522



Bond lengths



Bond angles



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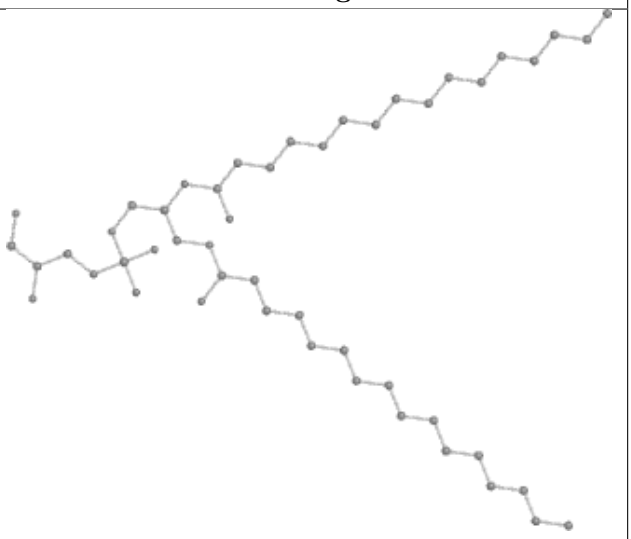
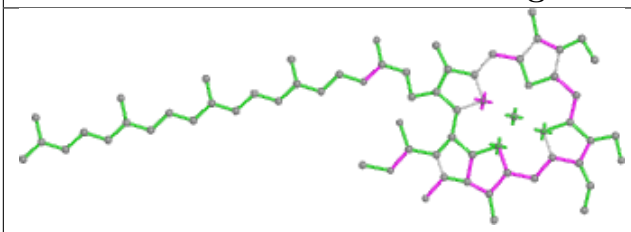
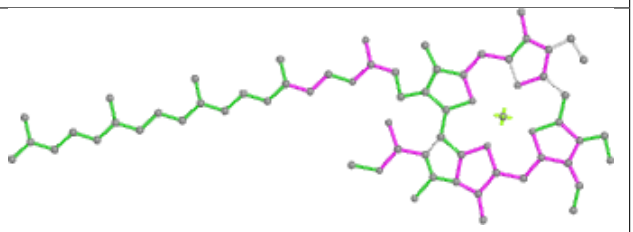
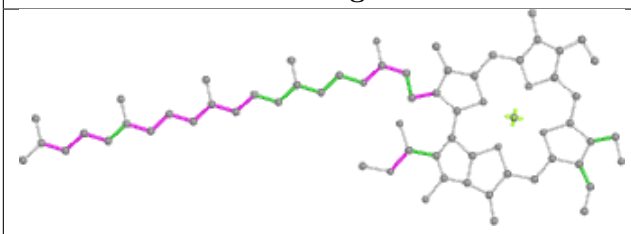
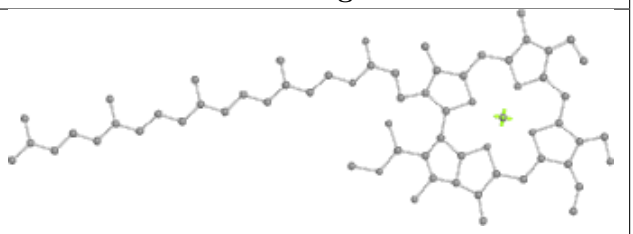
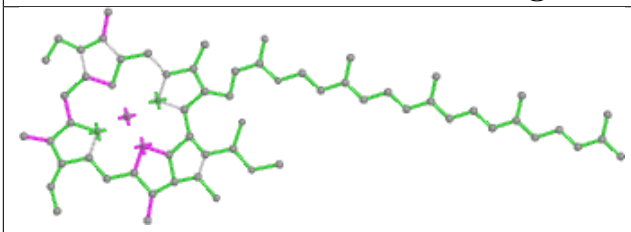
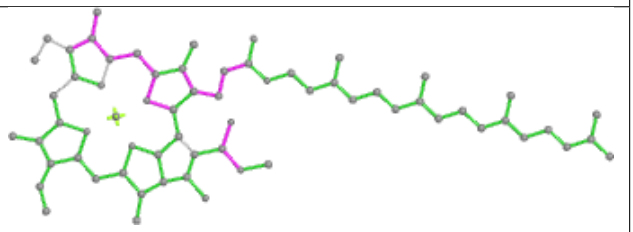
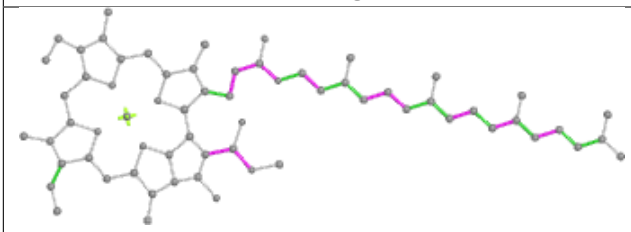
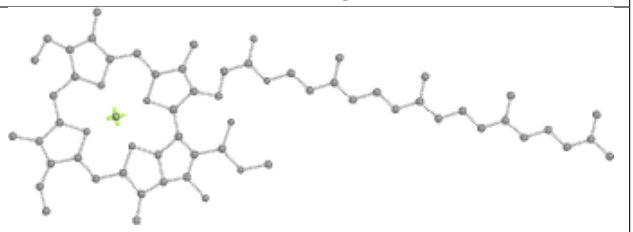
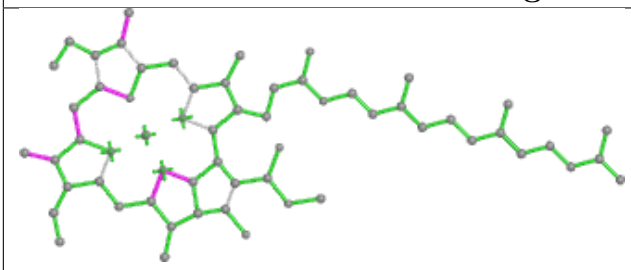
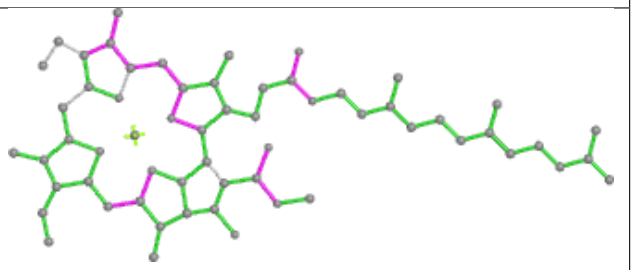
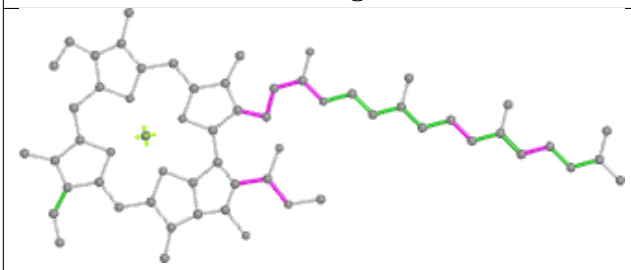
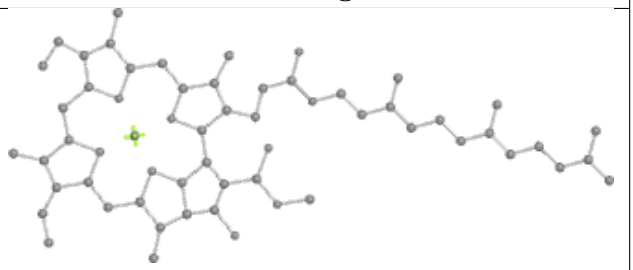


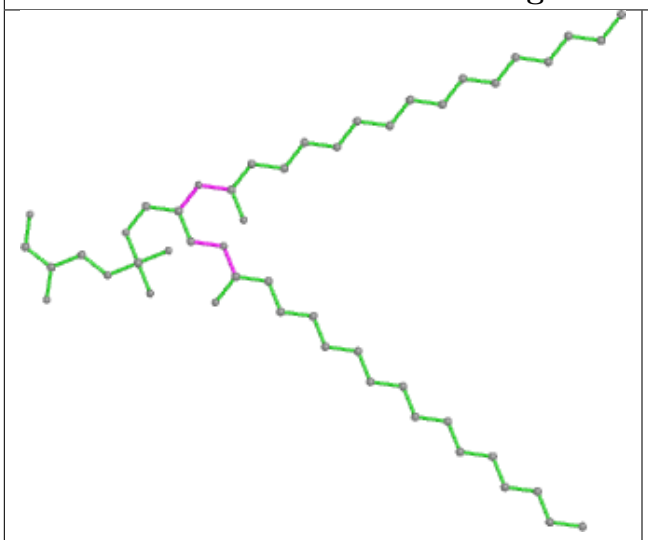
Rings

Ligand CHL 4 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

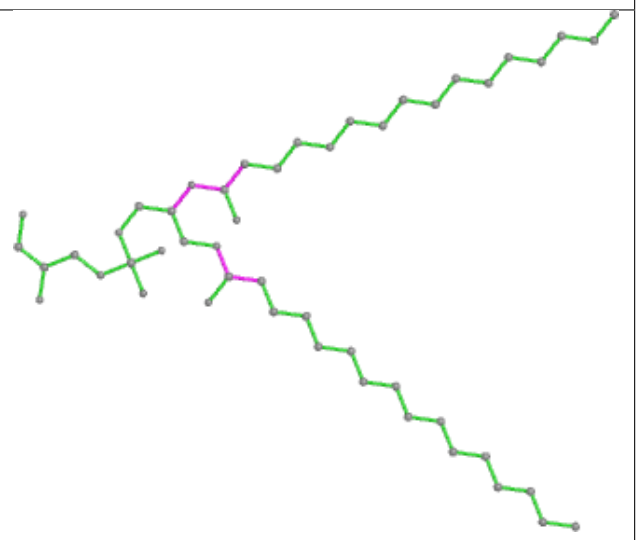
Ligand CLA a 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

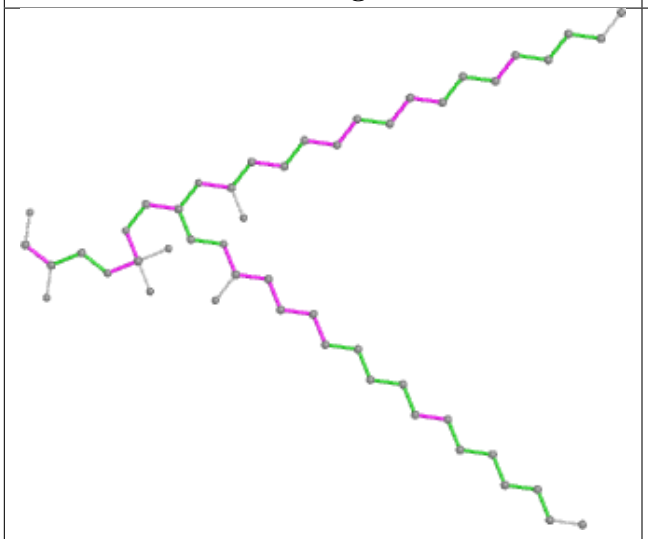
Ligand LHG u 312



Bond lengths



Bond angles



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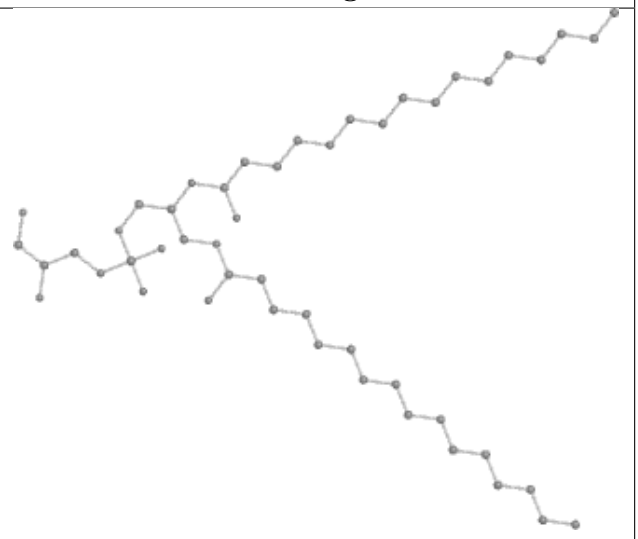
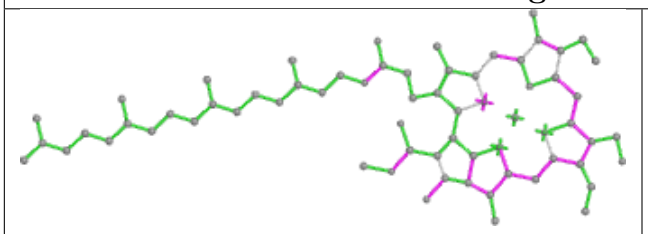


Rings

Ligand CHL 6 315



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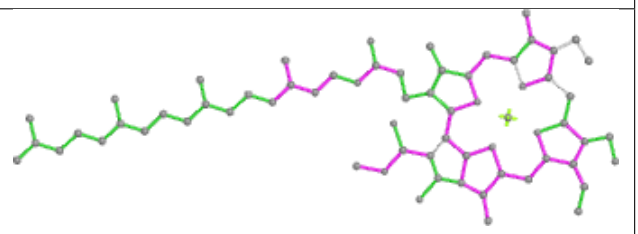
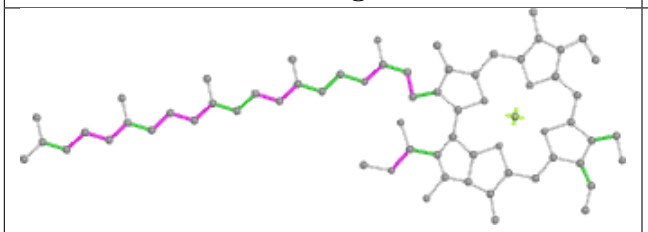


Bond angles



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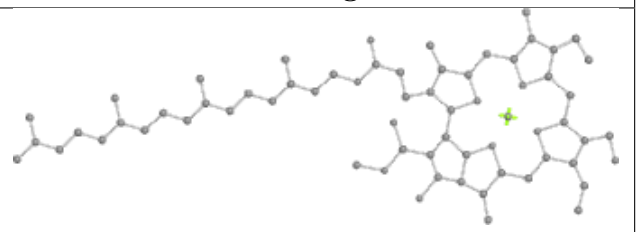
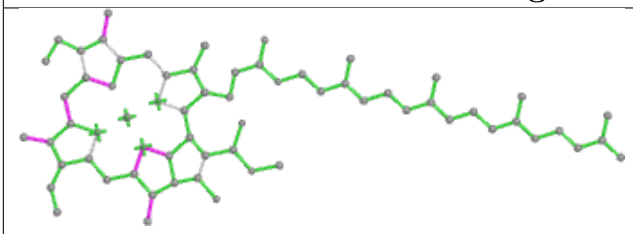
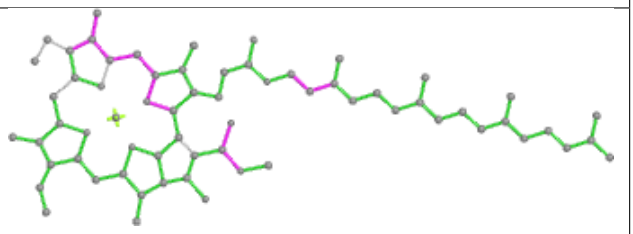


Rings

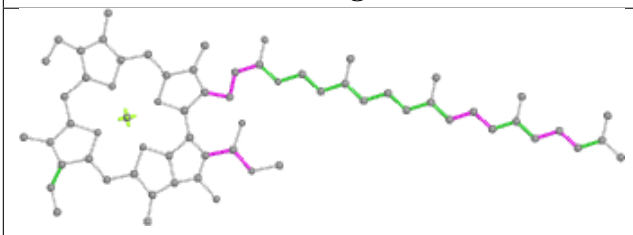
Ligand CLA 5 301



Bond lengths



Bond angles



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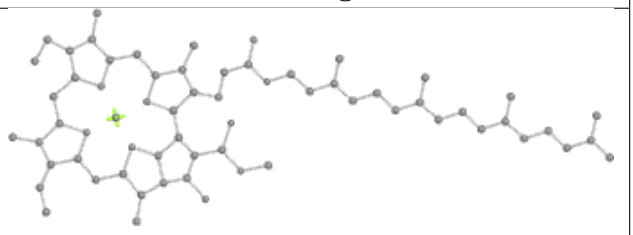
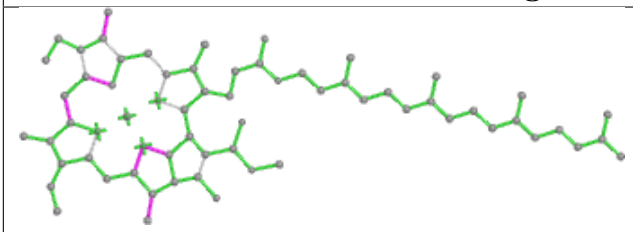
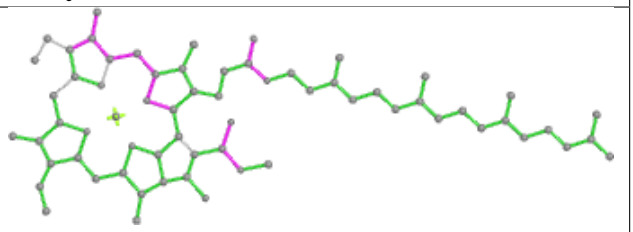


Rings

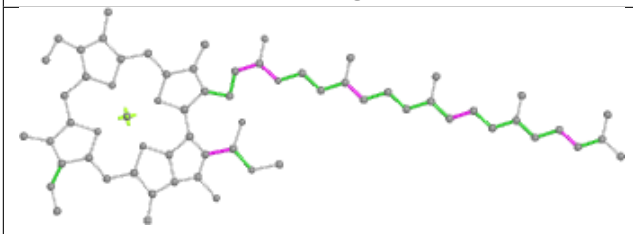
Ligand CLA Q 302



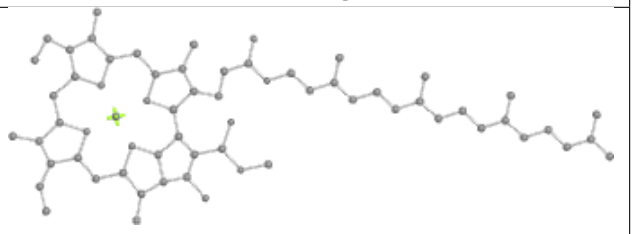
Bond lengths



Bond angles

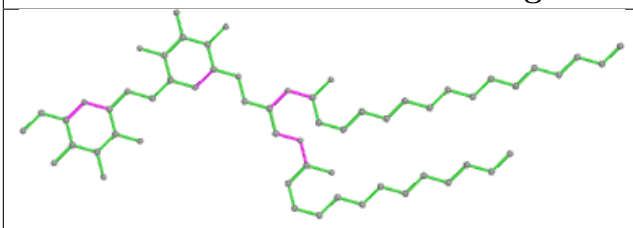


Torsions

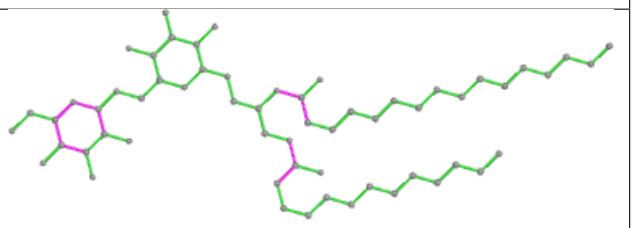


Rings

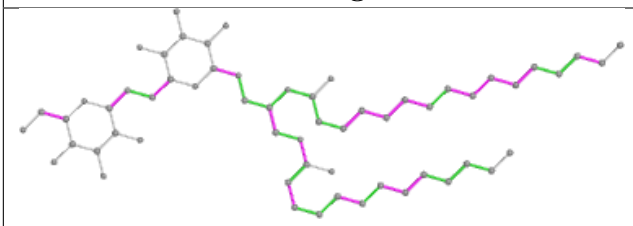
Ligand DGD a 416



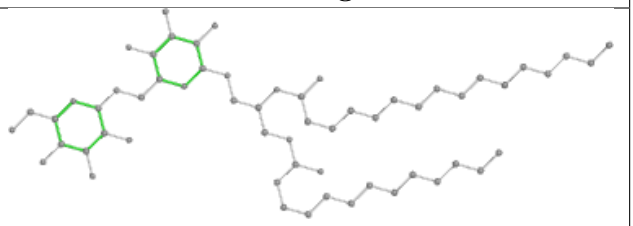
Bond lengths



Bond angles

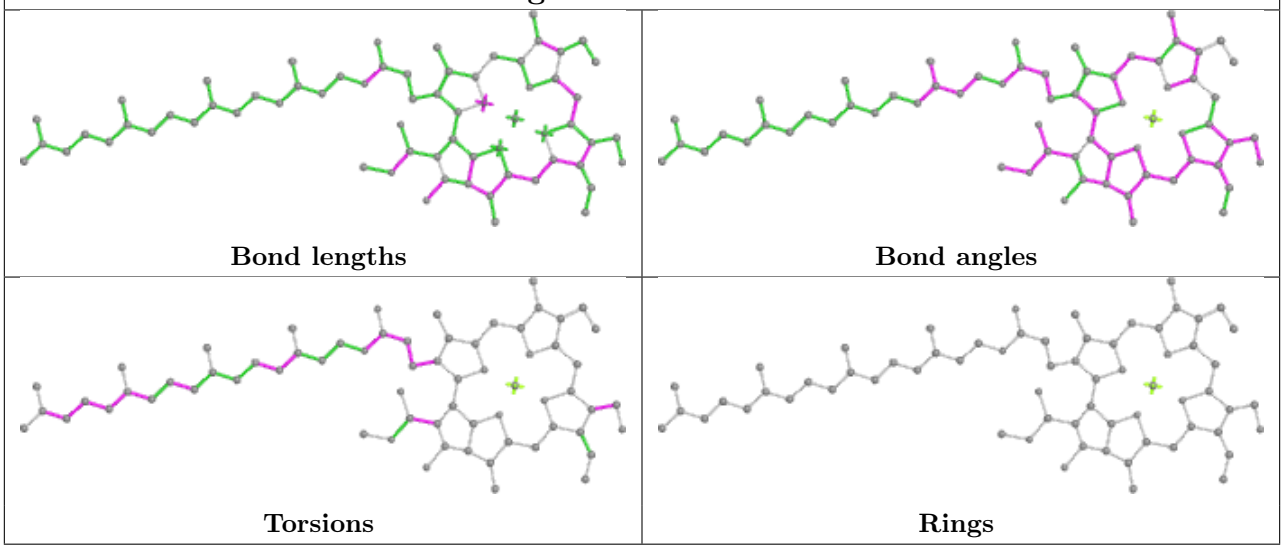


Torsions

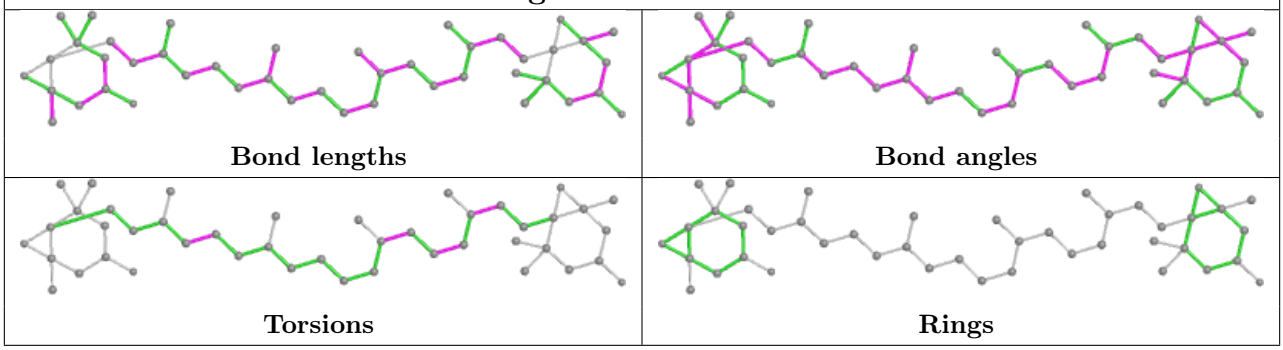


Rings

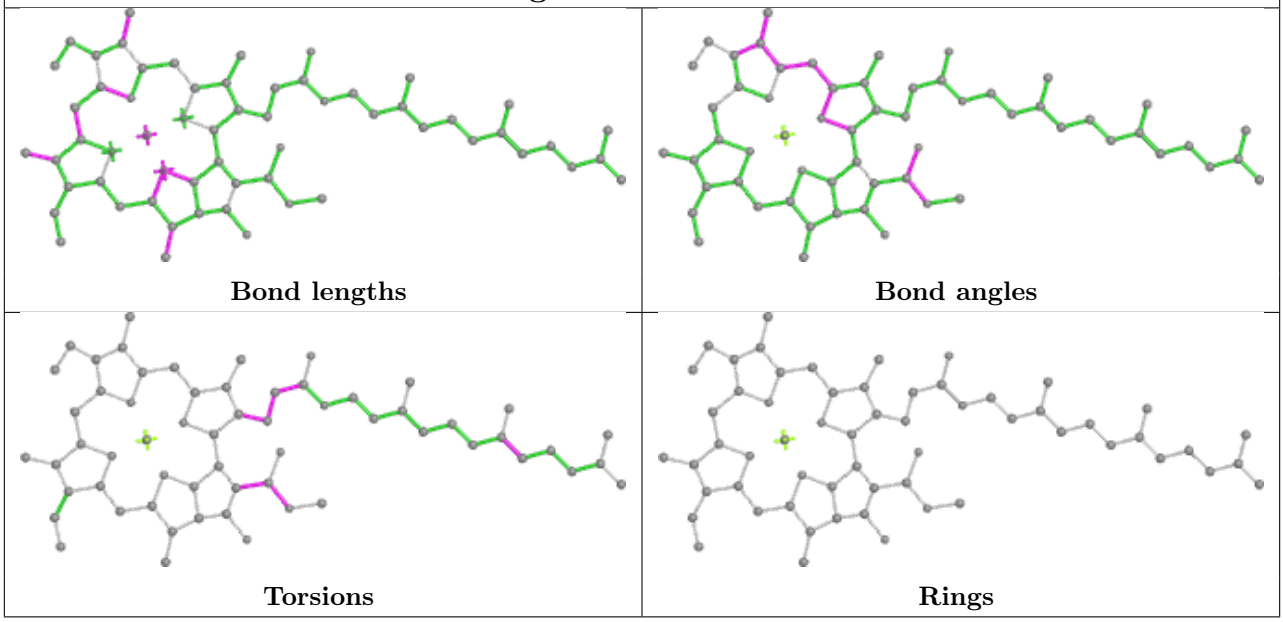
Ligand CHL u 316



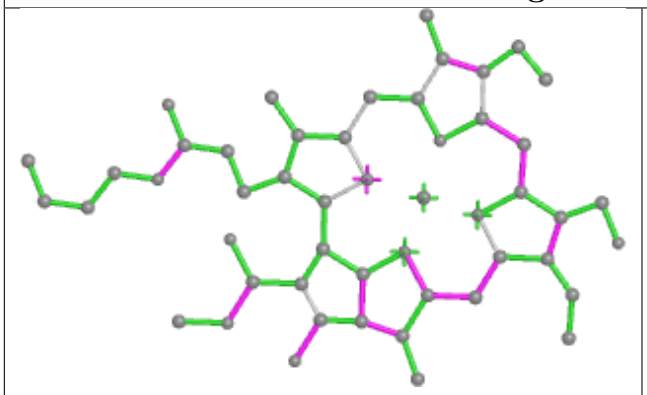
Ligand XAT 5 311



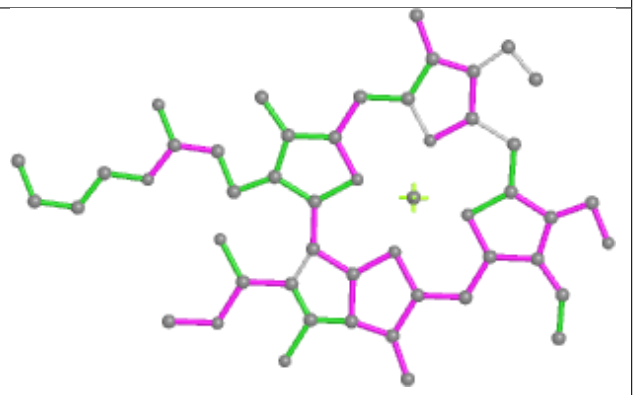
Ligand CLA 4 304



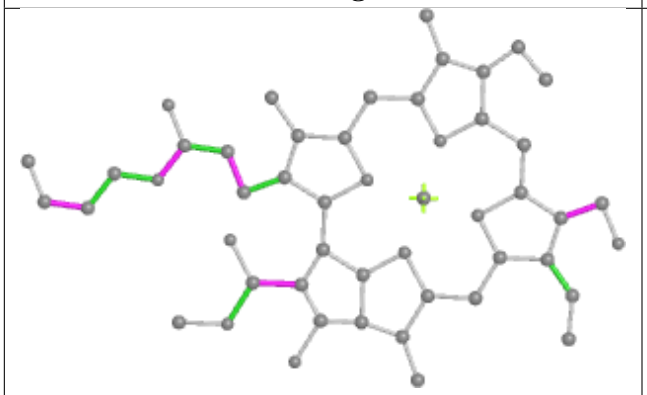
Ligand CHL u 315



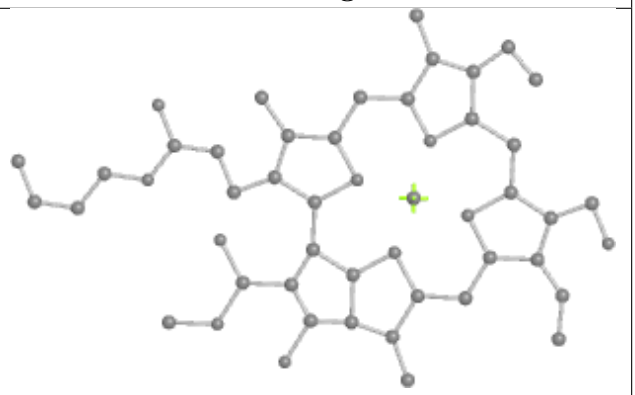
Bond lengths



Bond angles

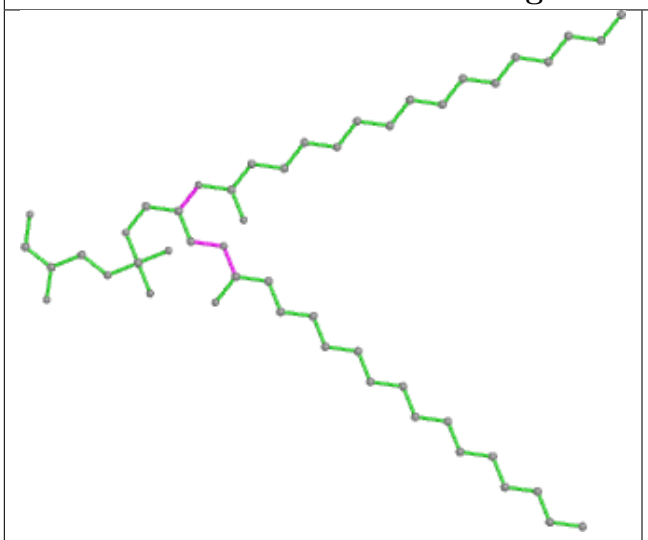


Torsions

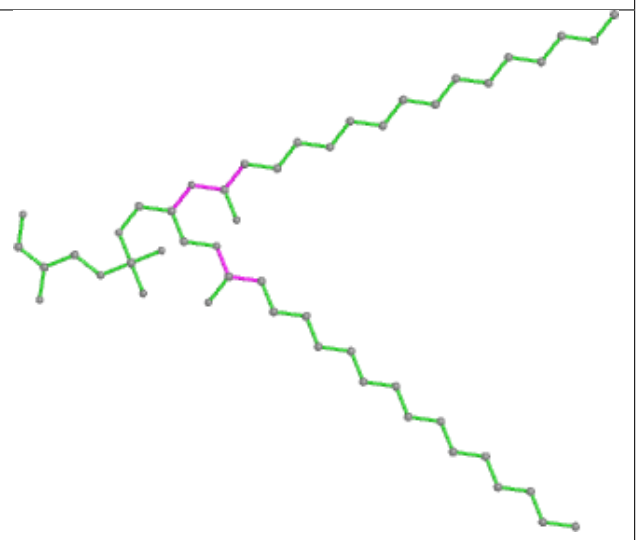


Rings

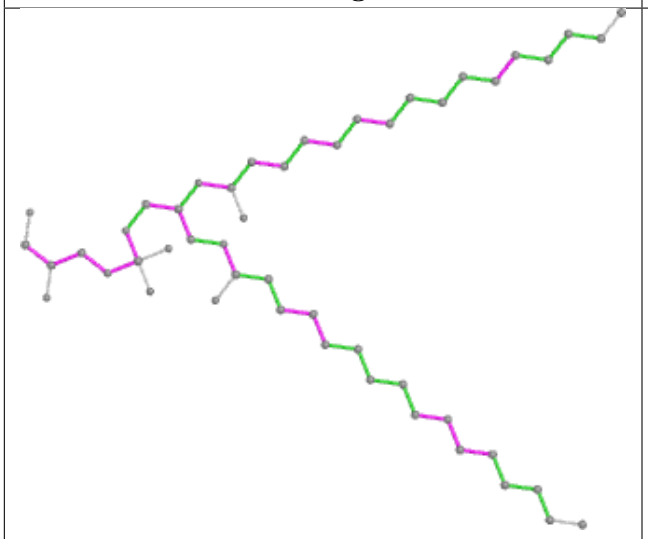
Ligand LHG L 101



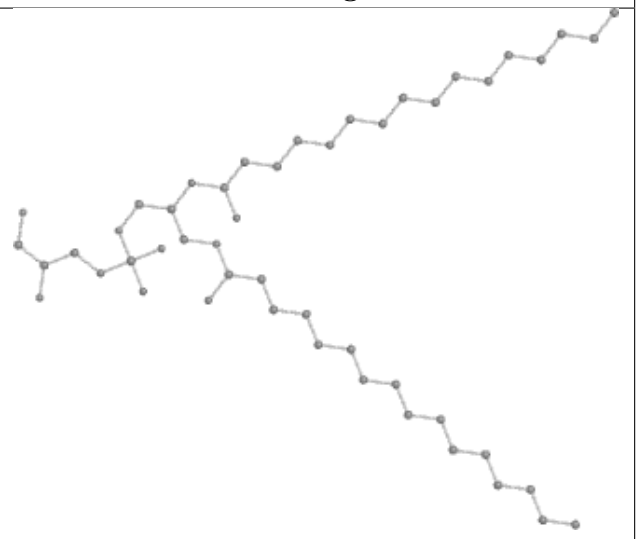
Bond lengths



Bond angles

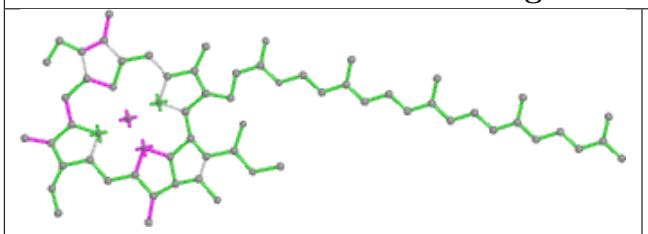


Torsions

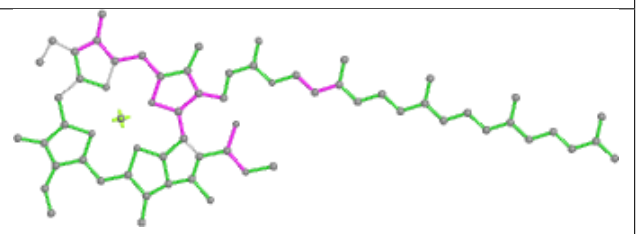


Rings

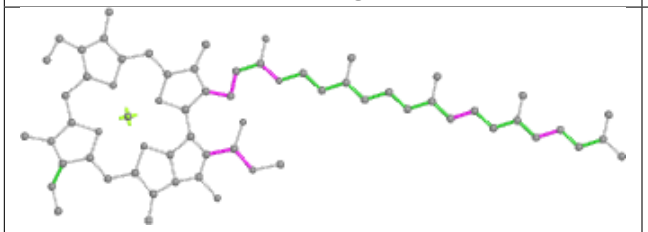
Ligand CLA A 405



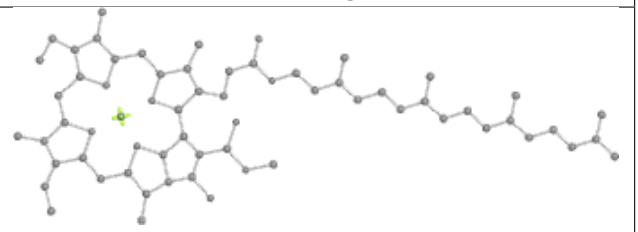
Bond lengths



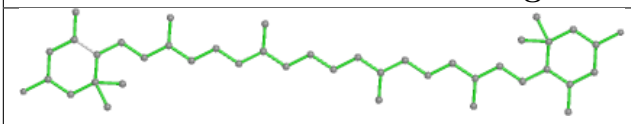
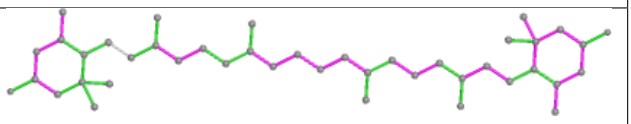
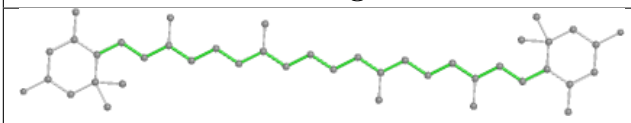
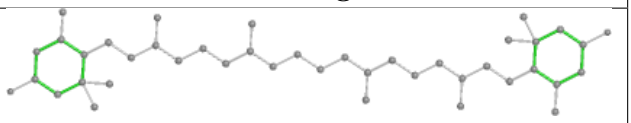
Bond angles

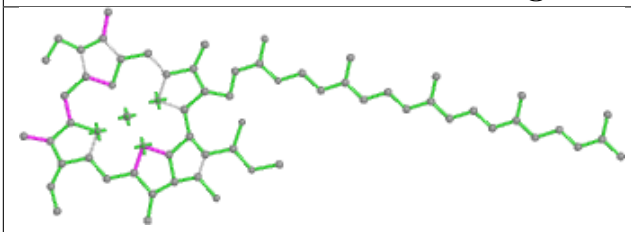
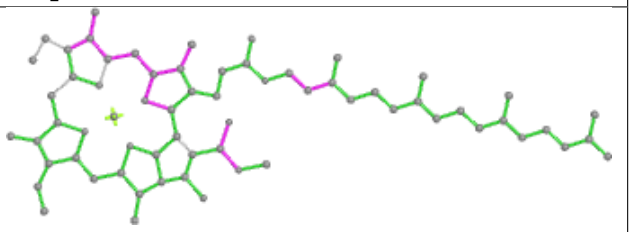
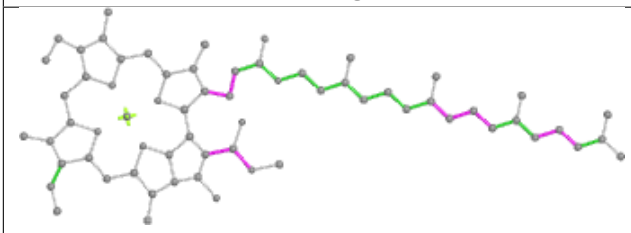
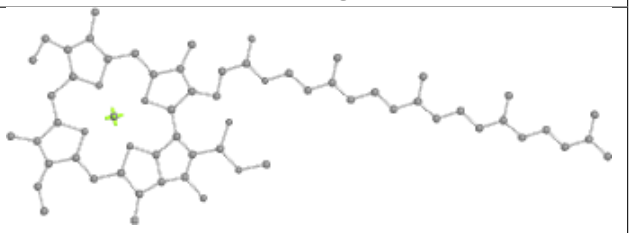


Torsions

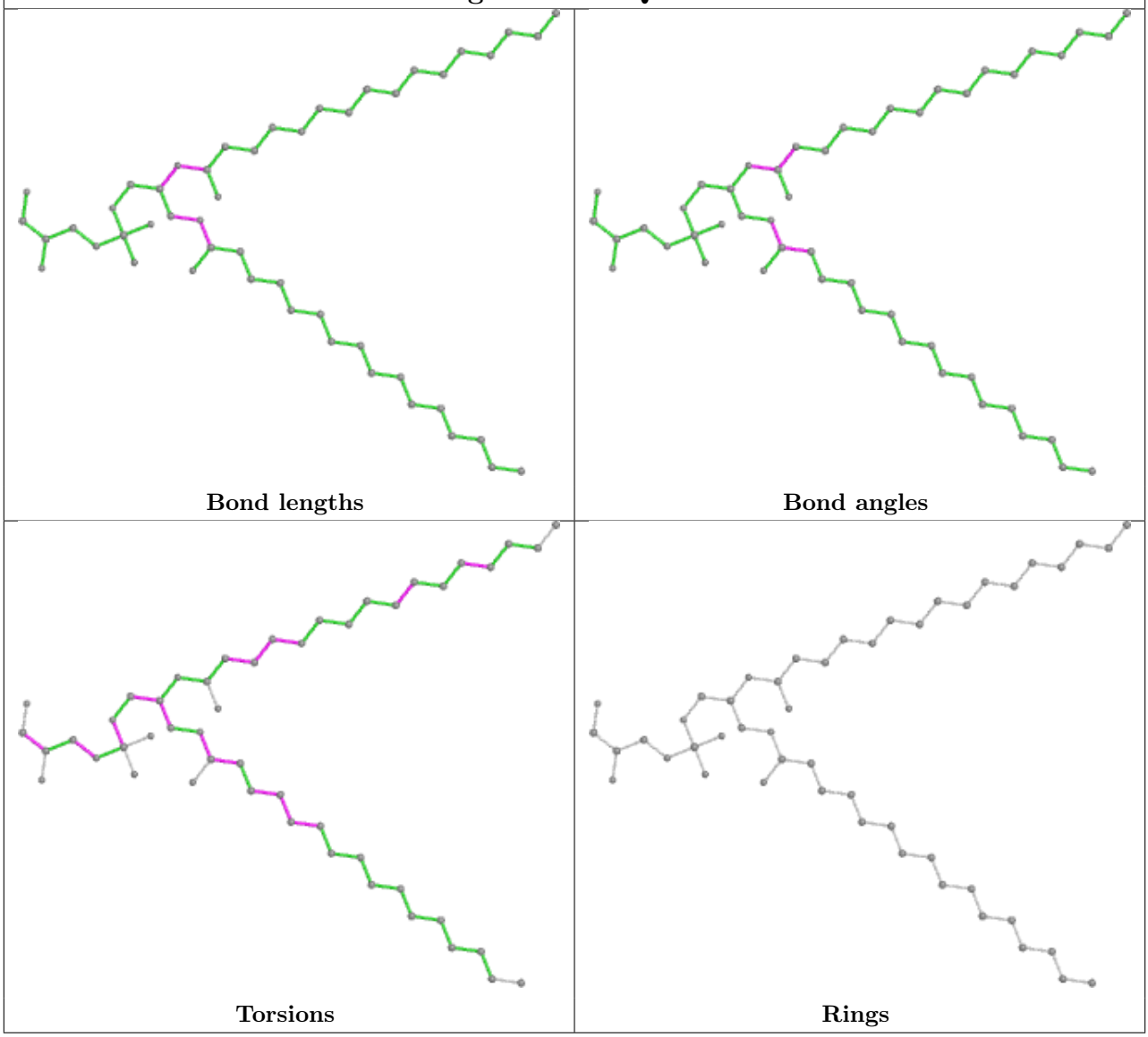


Rings

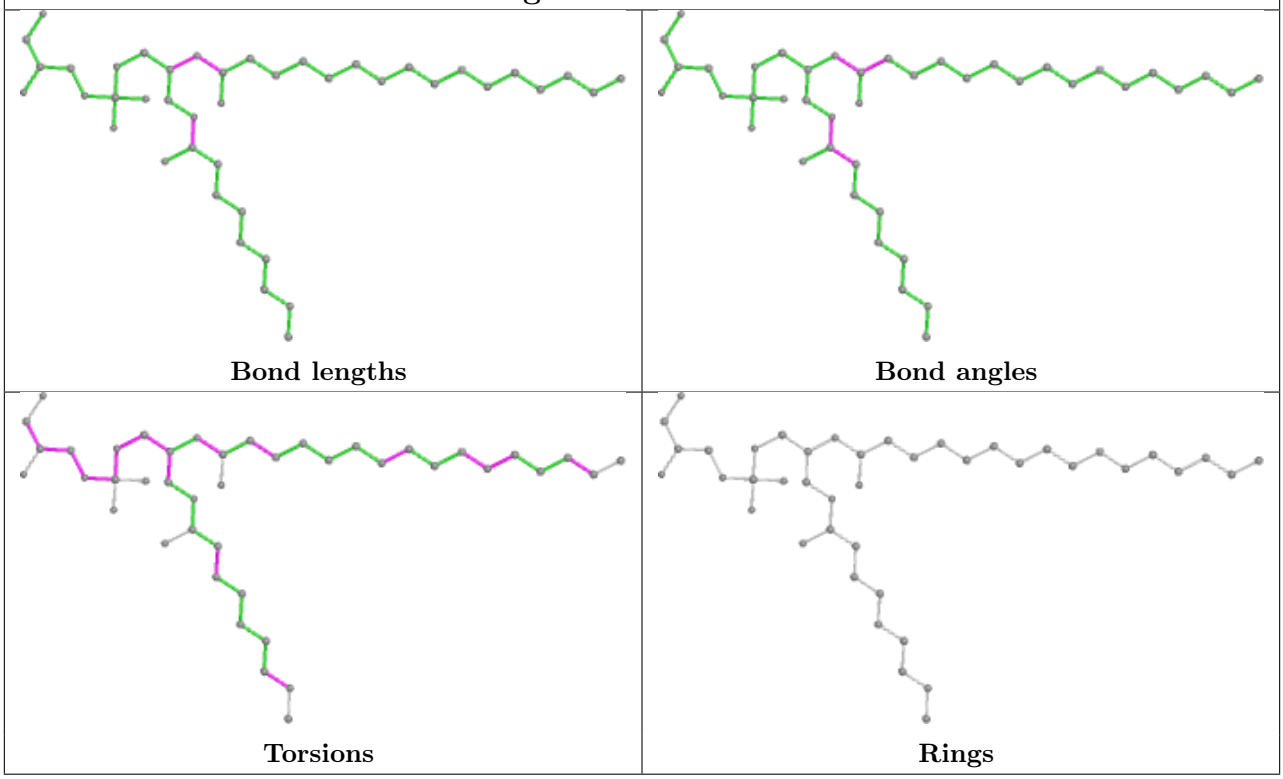
Ligand LUT V 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

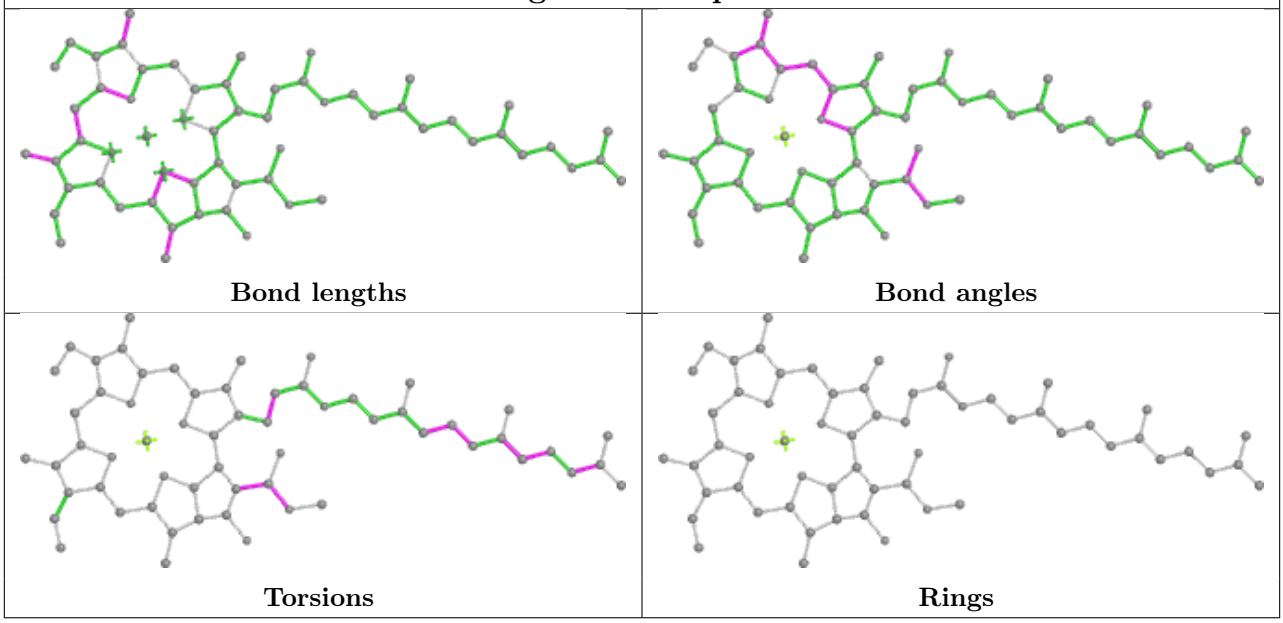
Ligand LHG Q 310



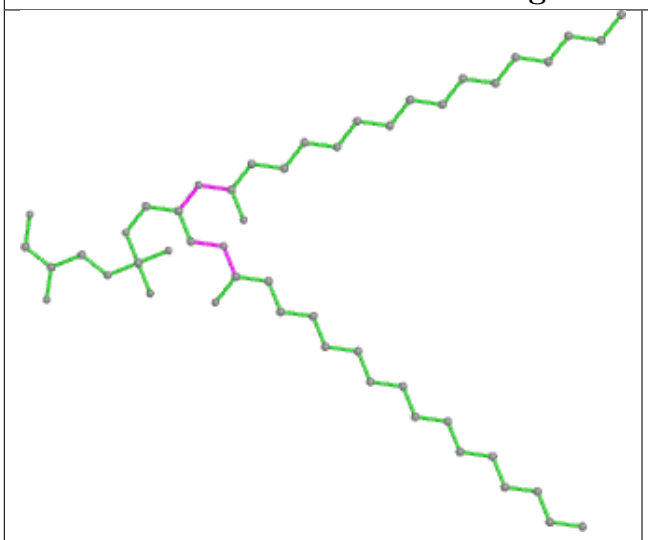
Ligand LHG R 314



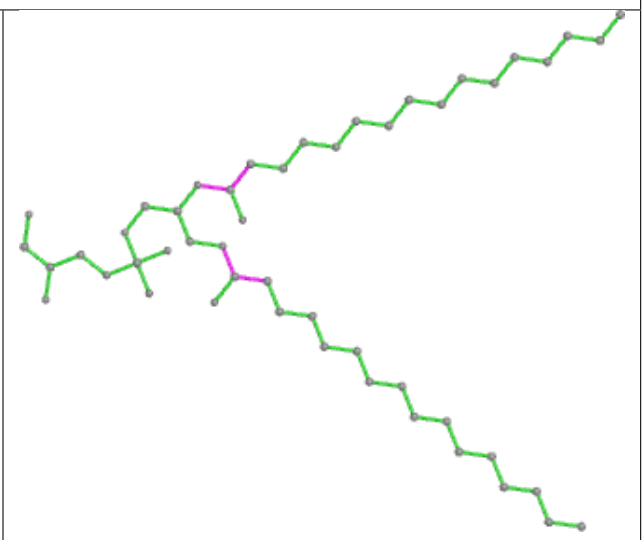
Ligand CLA q 305



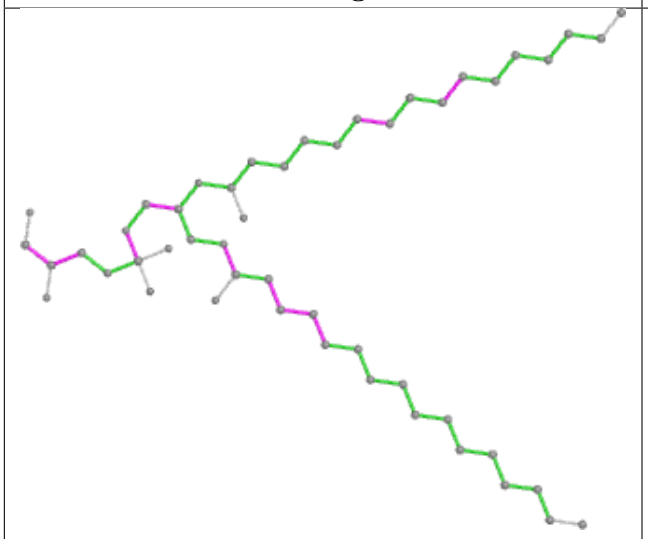
Ligand LHG c 521



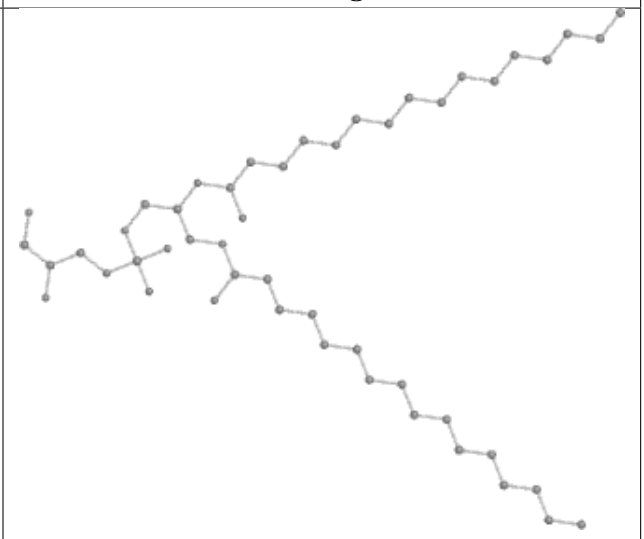
Bond lengths



Bond angles

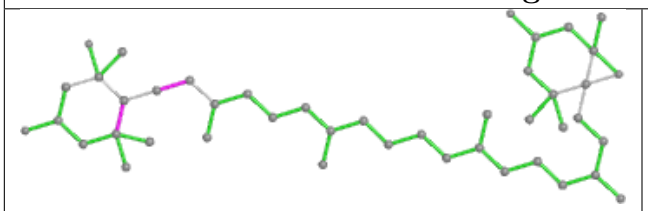


Torsions

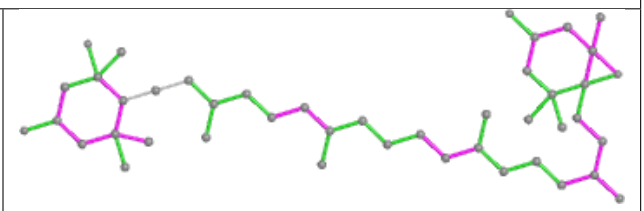


Rings

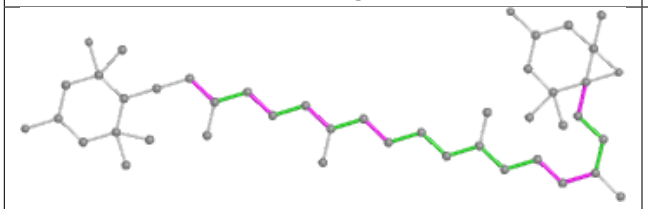
Ligand NEX R 301



Bond lengths

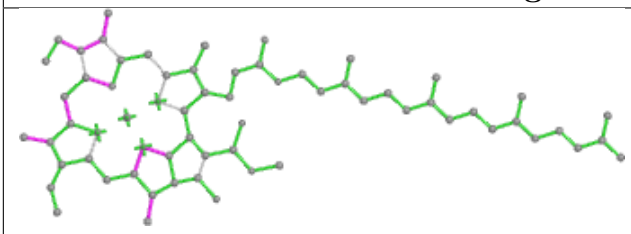
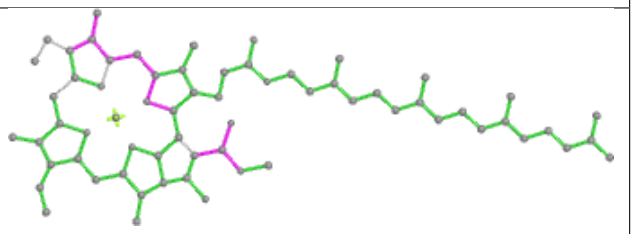
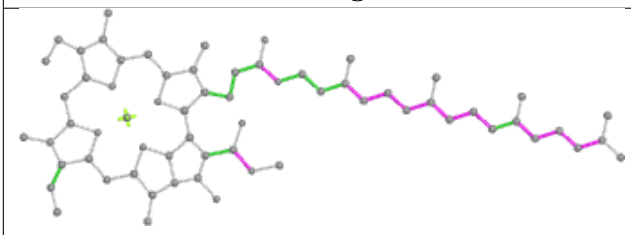
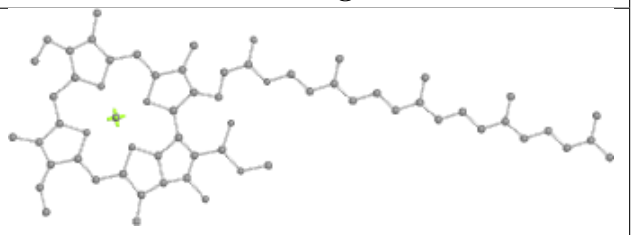


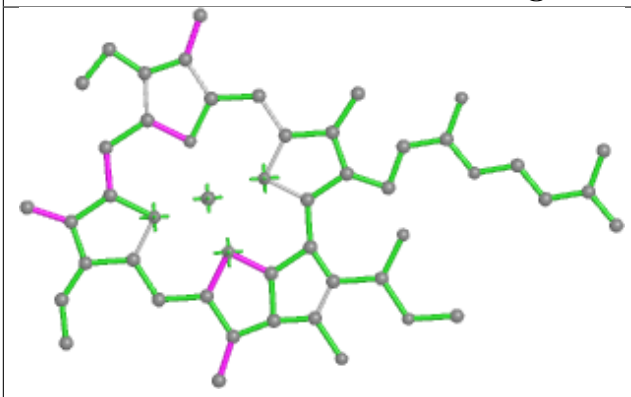
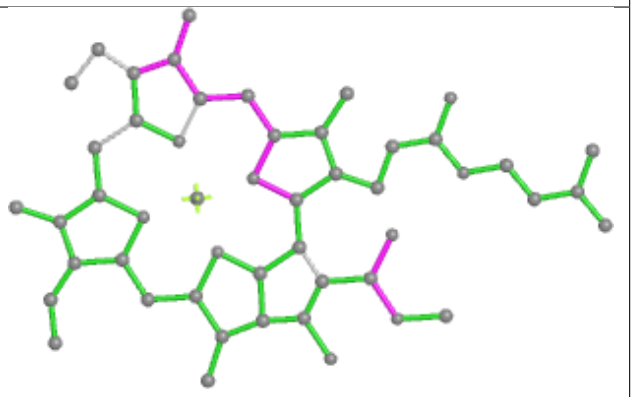
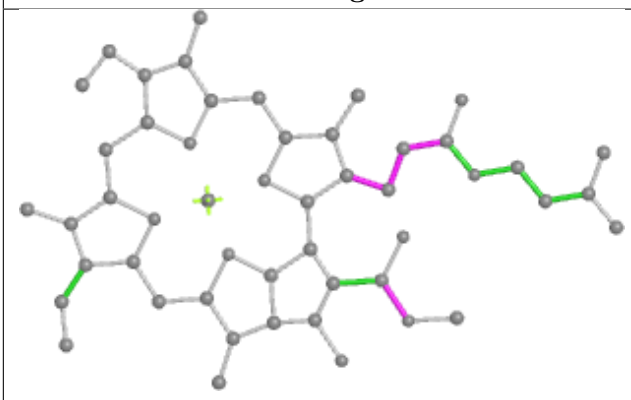
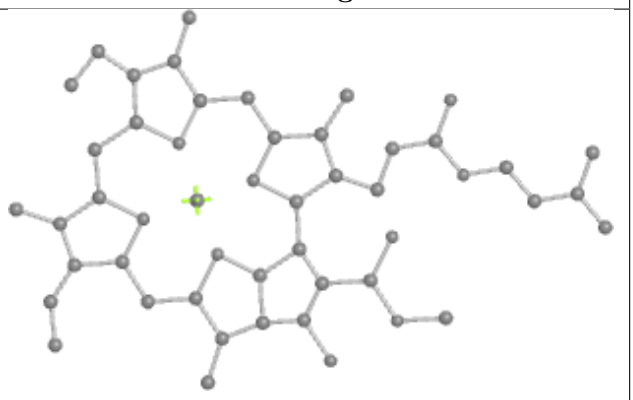
Bond angles



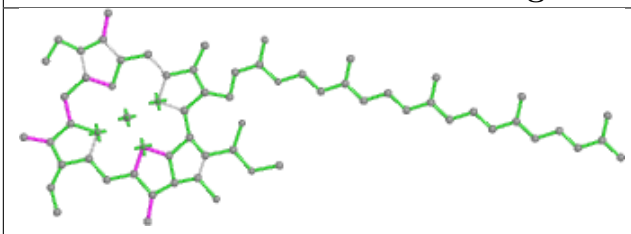
Torsions

Rings

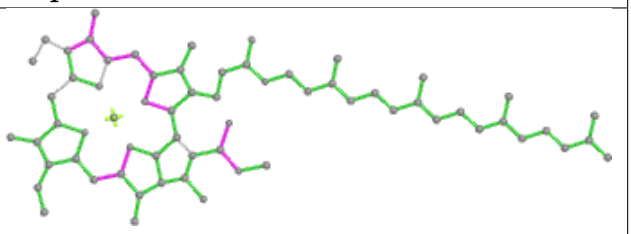
Ligand CLA C 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

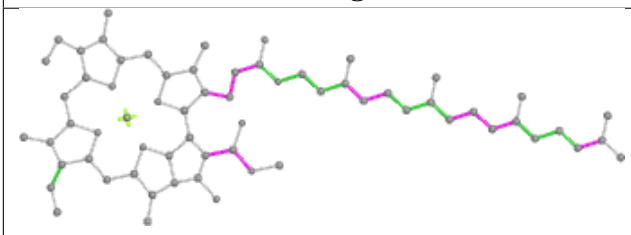
Ligand CLA p 302



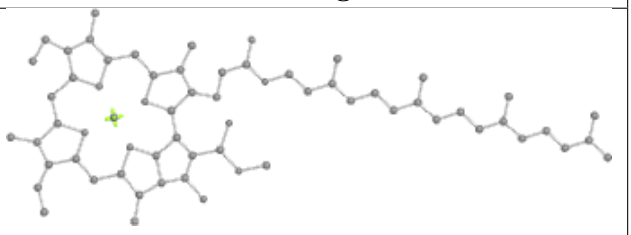
Bond lengths



Bond angles

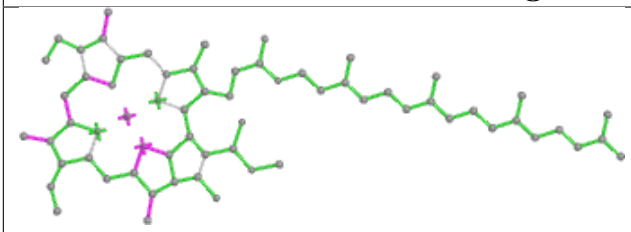


Torsions

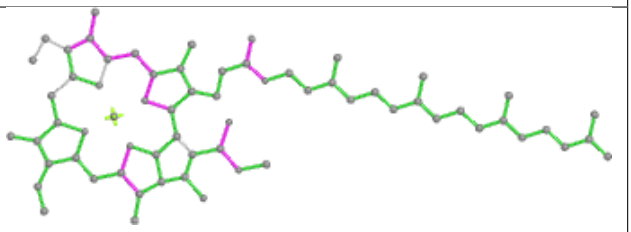


Rings

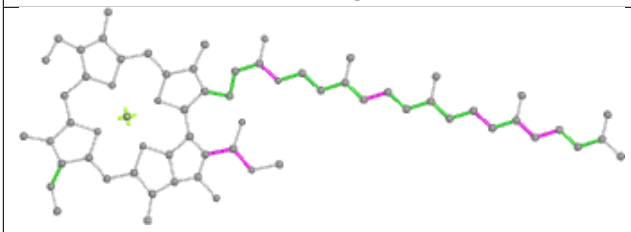
Ligand CLA B 617



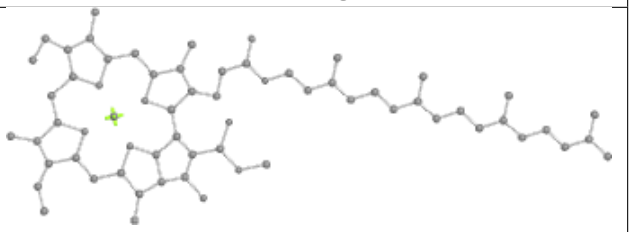
Bond lengths



Bond angles

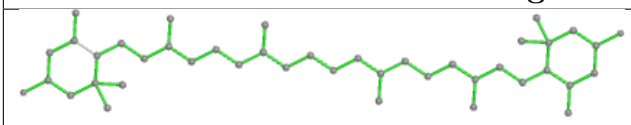


Torsions

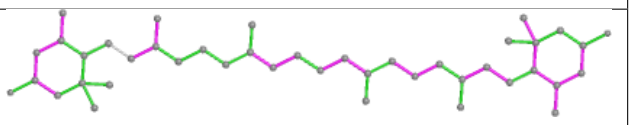


Rings

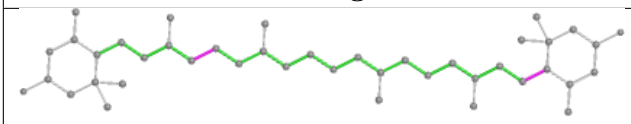
Ligand LUT u 310



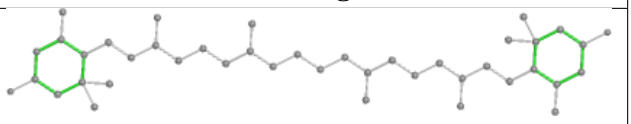
Bond lengths



Bond angles

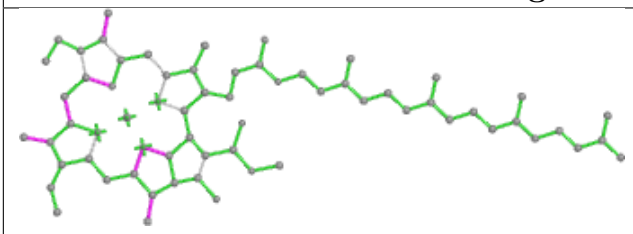


Torsions

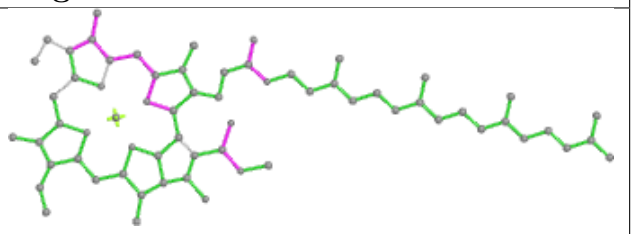


Rings

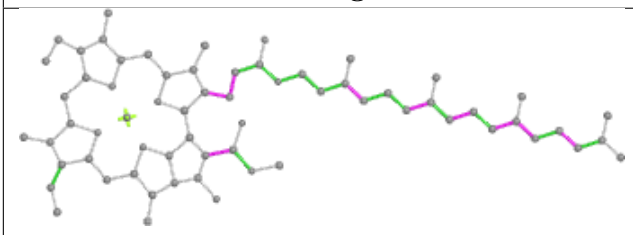
Ligand CLA g 301



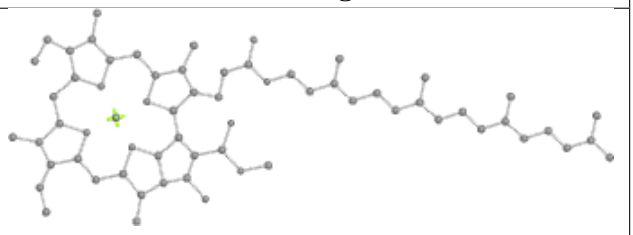
Bond lengths



Bond angles

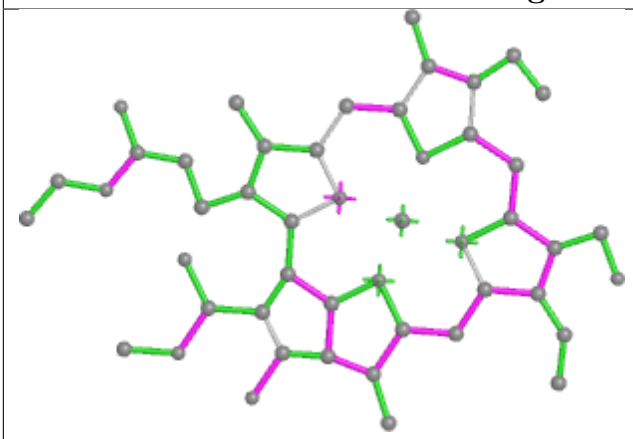


Torsions

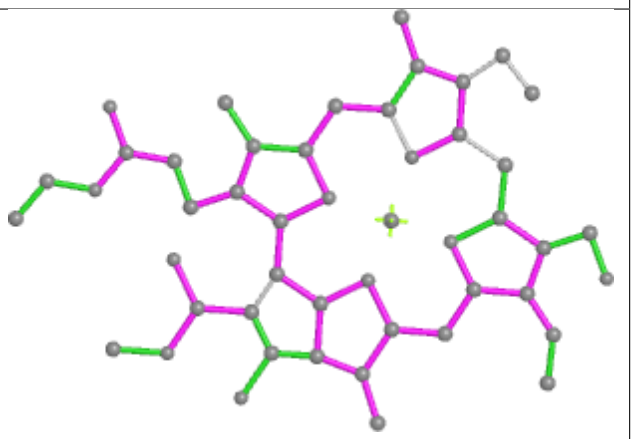


Rings

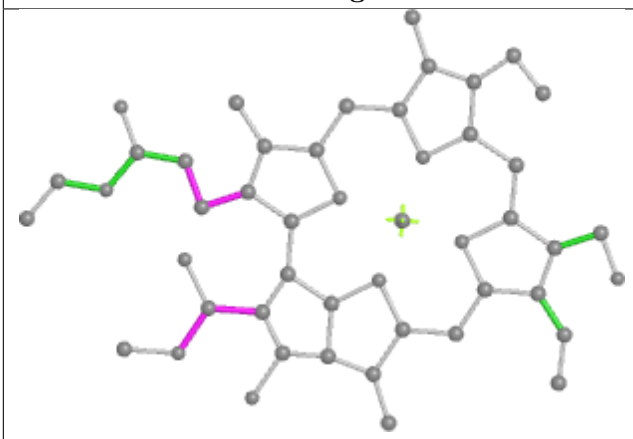
Ligand CHL 3 312



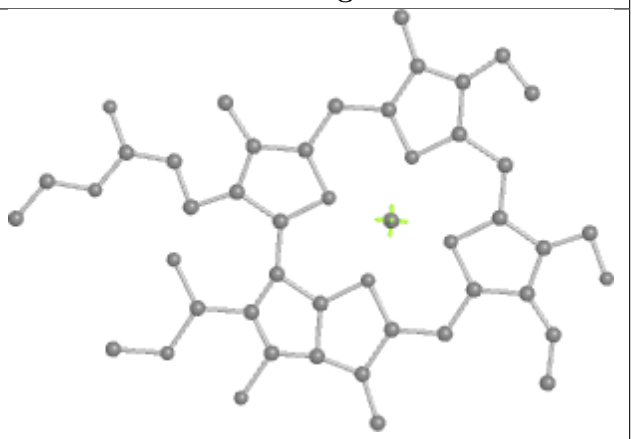
Bond lengths



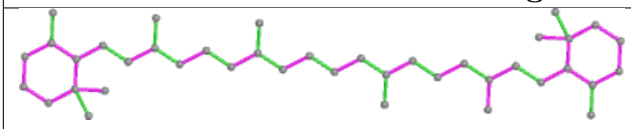
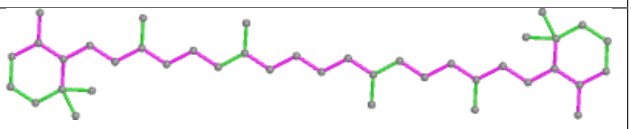
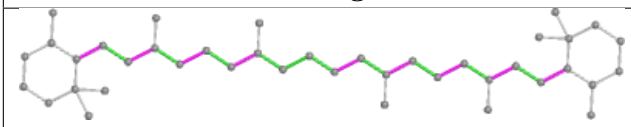
Bond angles

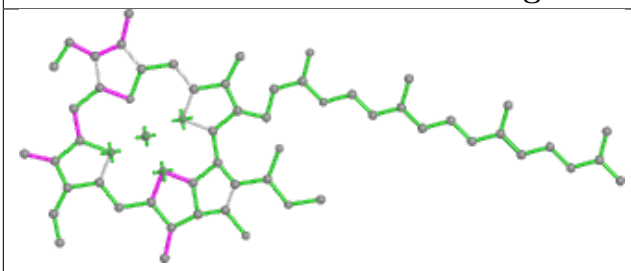
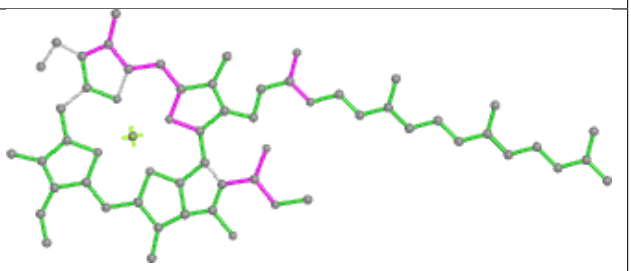
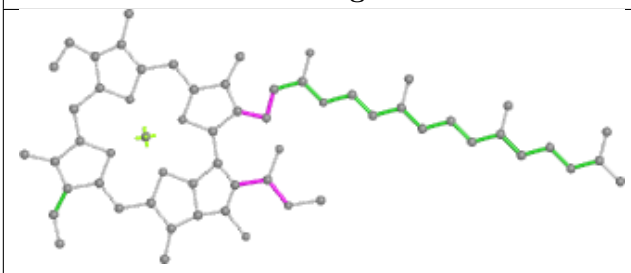
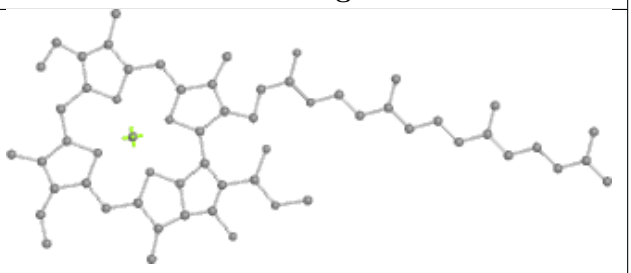


Torsions

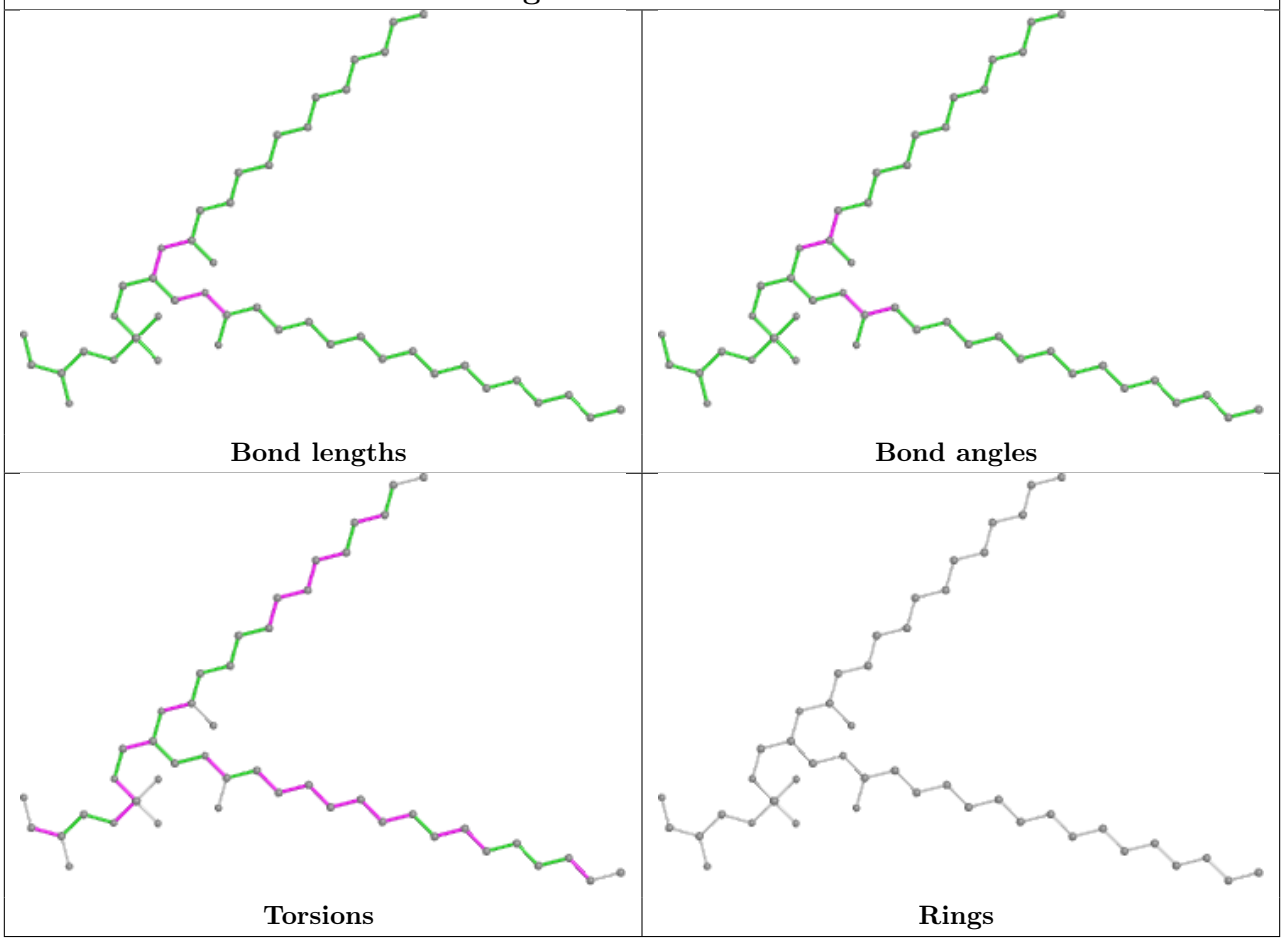


Rings

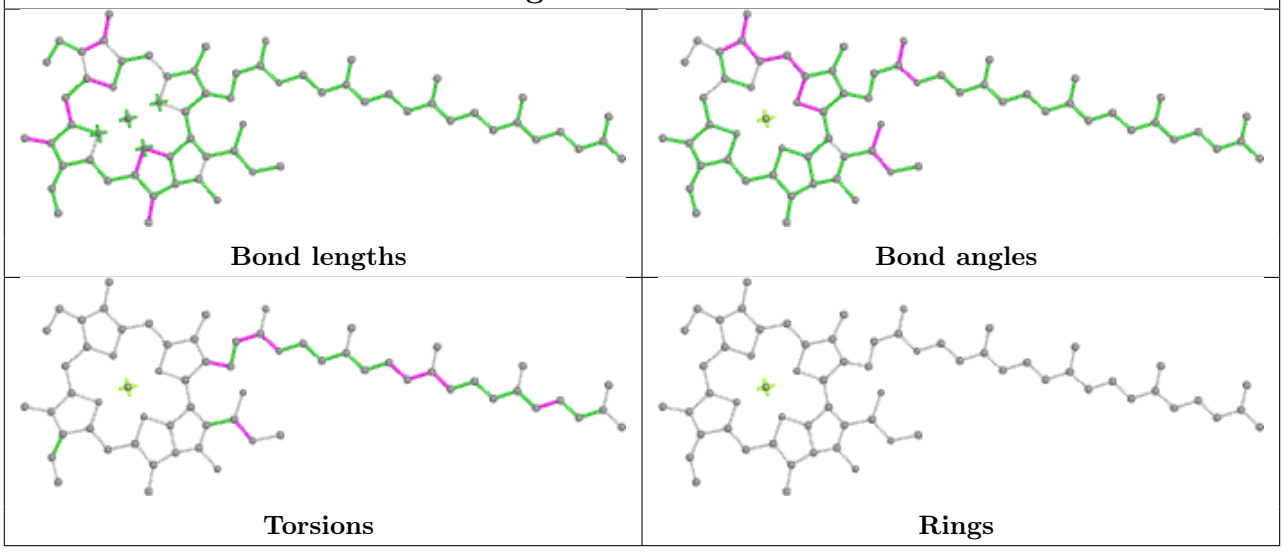
Ligand BCR k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

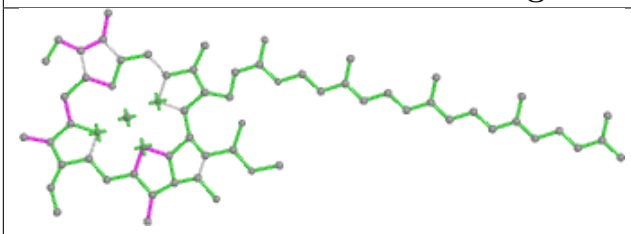
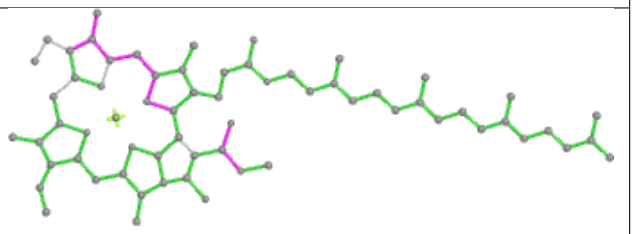
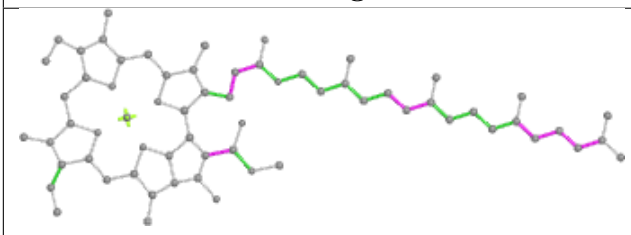
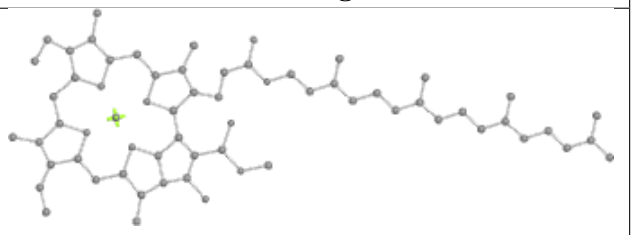
Ligand CLA U 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

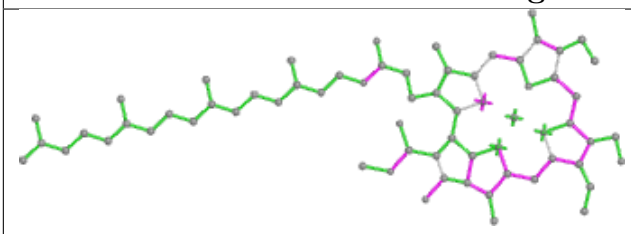
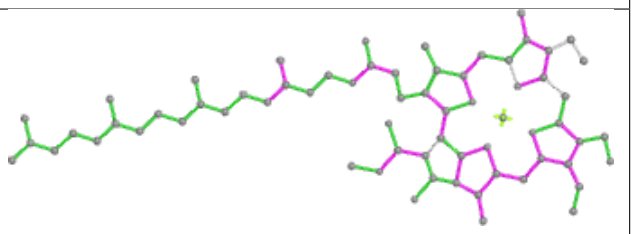
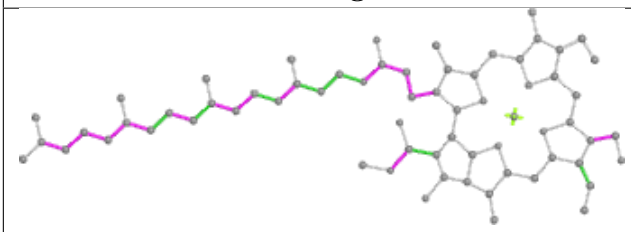
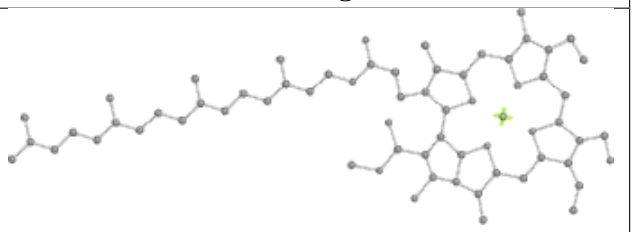
Ligand LHG D 406



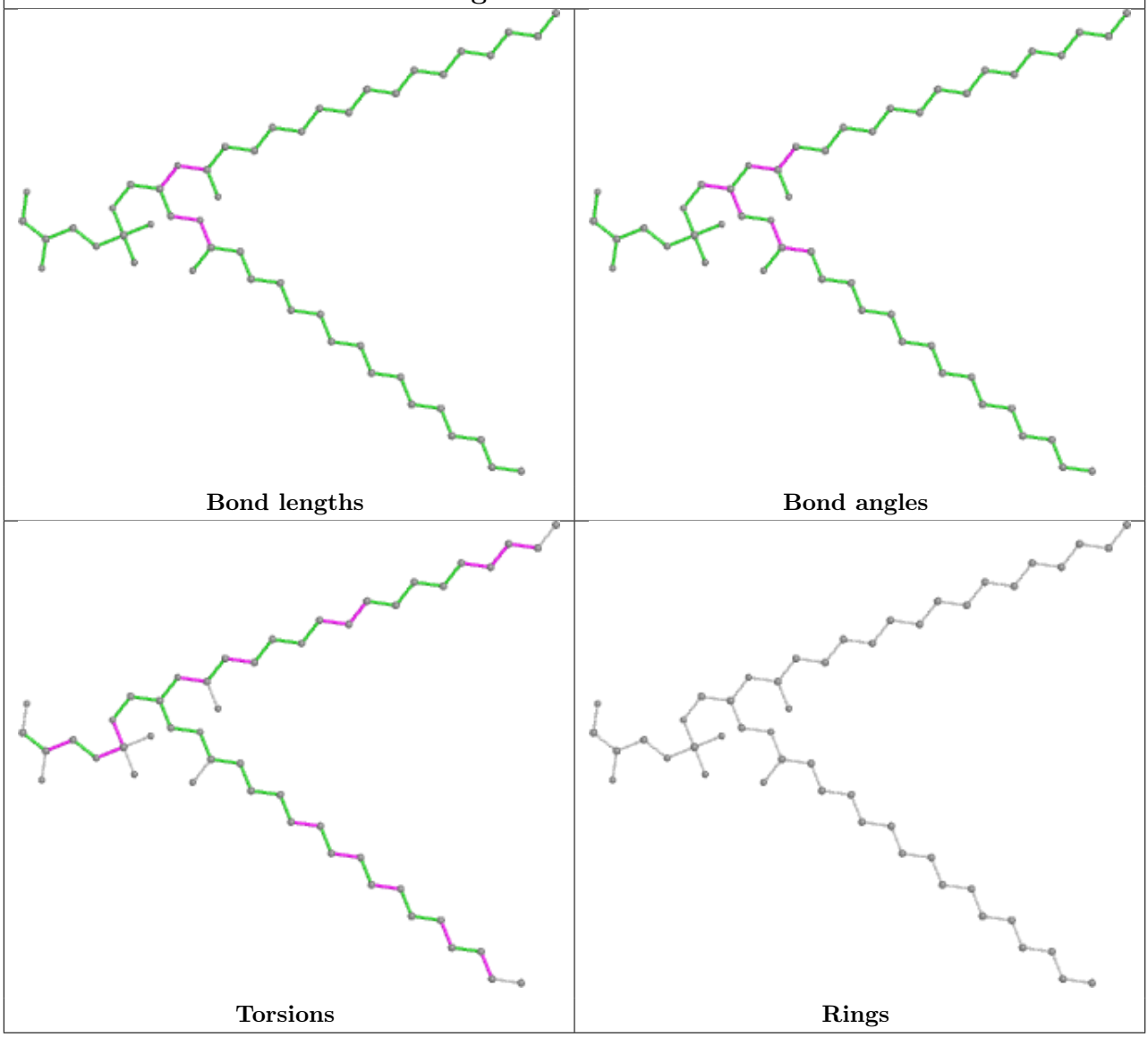
Ligand CLA P 303



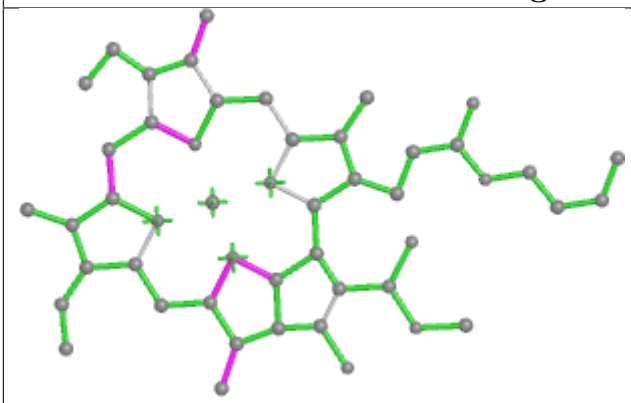
Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 6 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

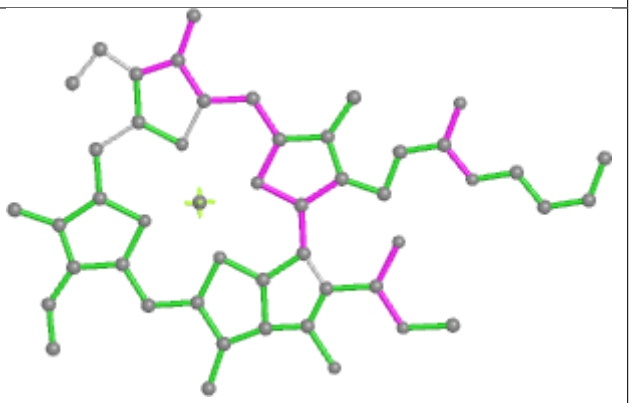
Ligand LHG d 406



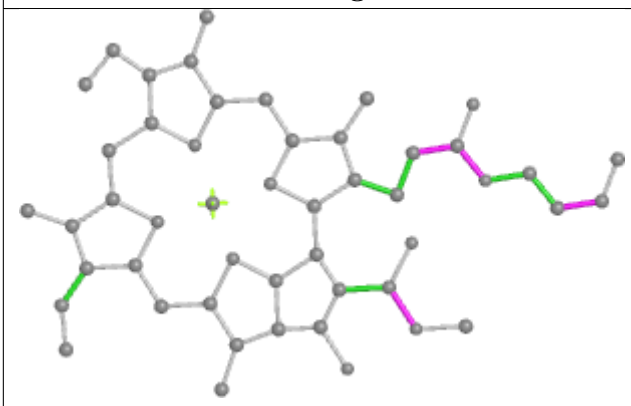
Ligand CLA r 608



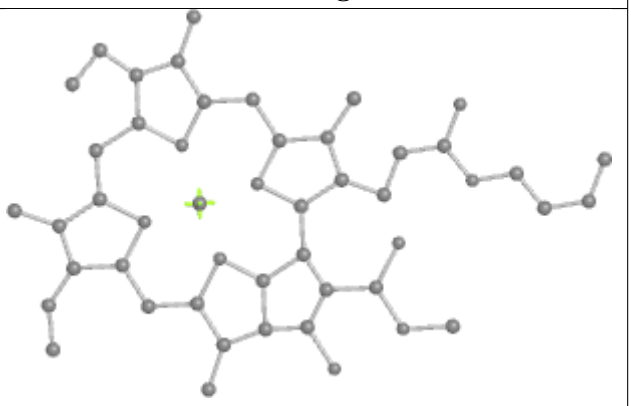
Bond lengths



Bond angles

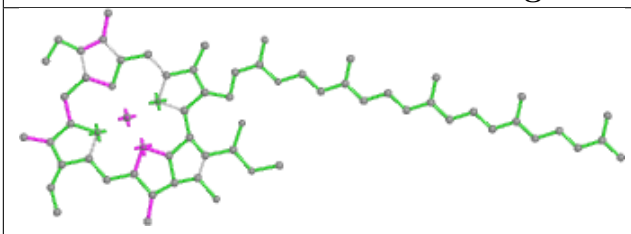


Torsions

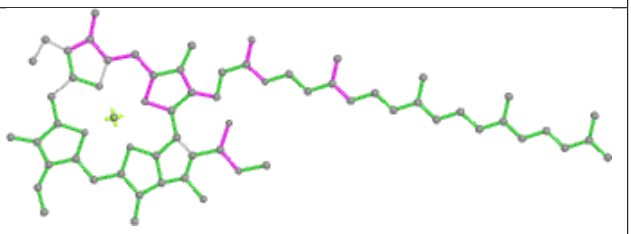


Rings

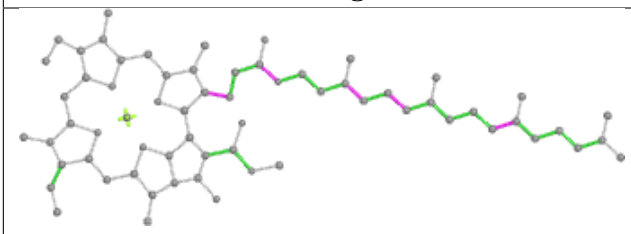
Ligand CLA C 510



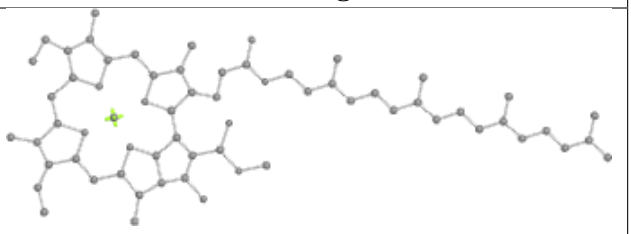
Bond lengths



Bond angles

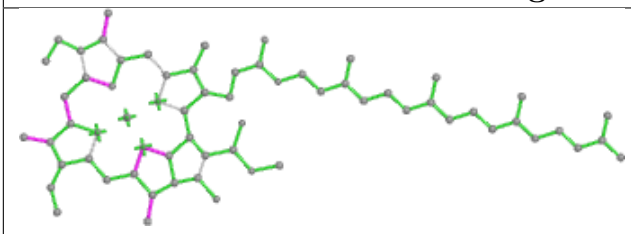


Torsions

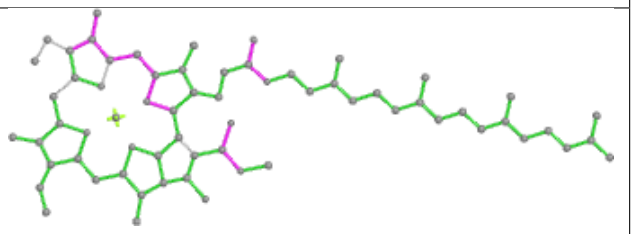


Rings

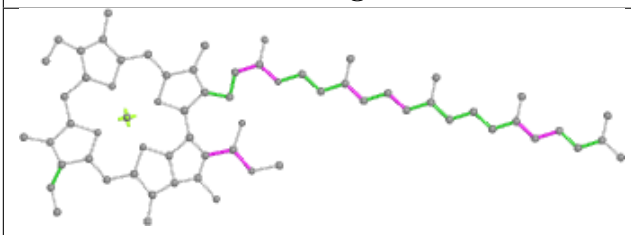
Ligand CLA 4 302



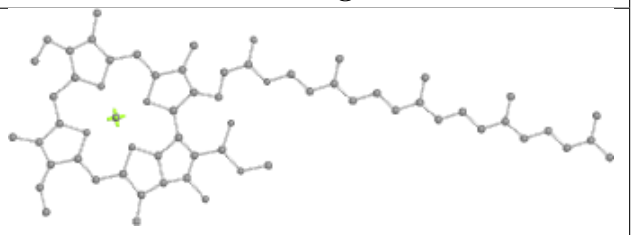
Bond lengths



Bond angles

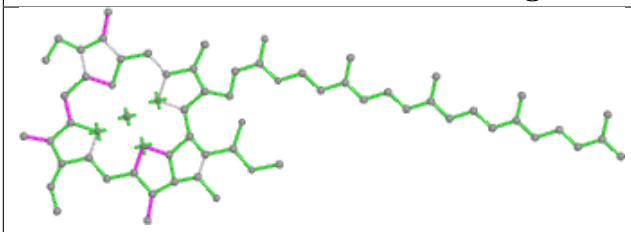


Torsions

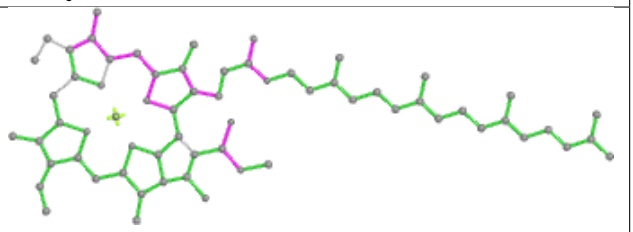


Rings

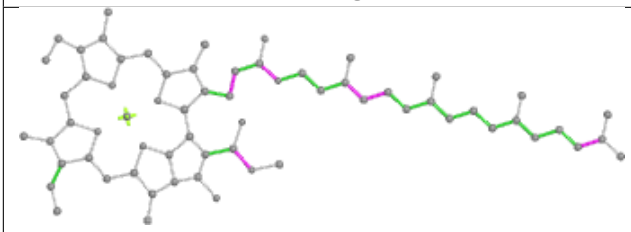
Ligand CLA Q 307



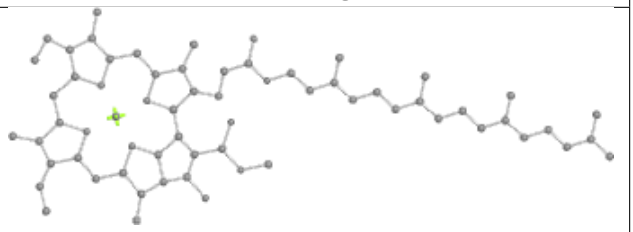
Bond lengths



Bond angles

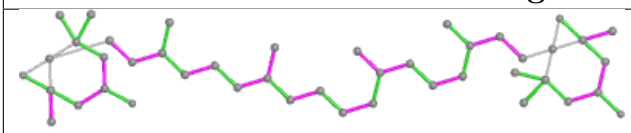


Torsions

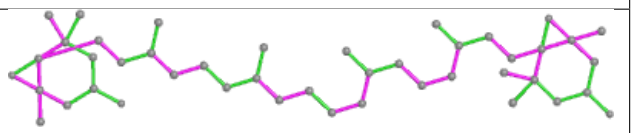


Rings

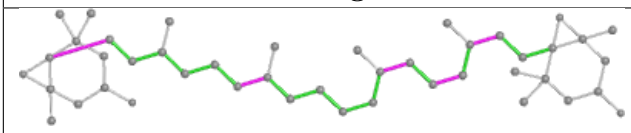
Ligand XAT 6 310



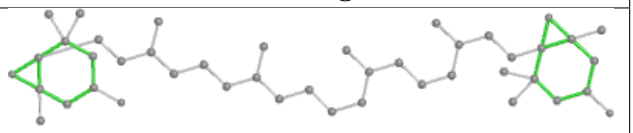
Bond lengths



Bond angles

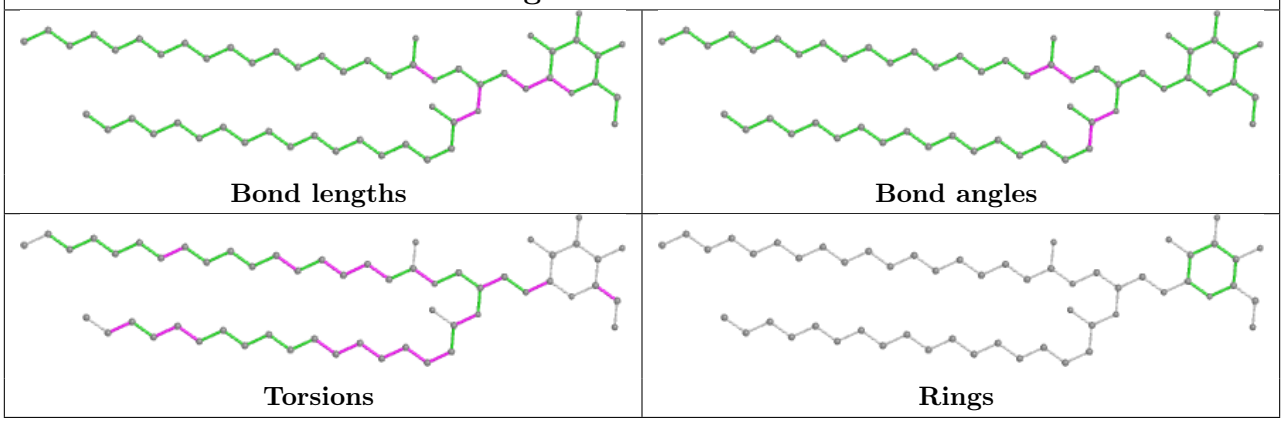


Torsions

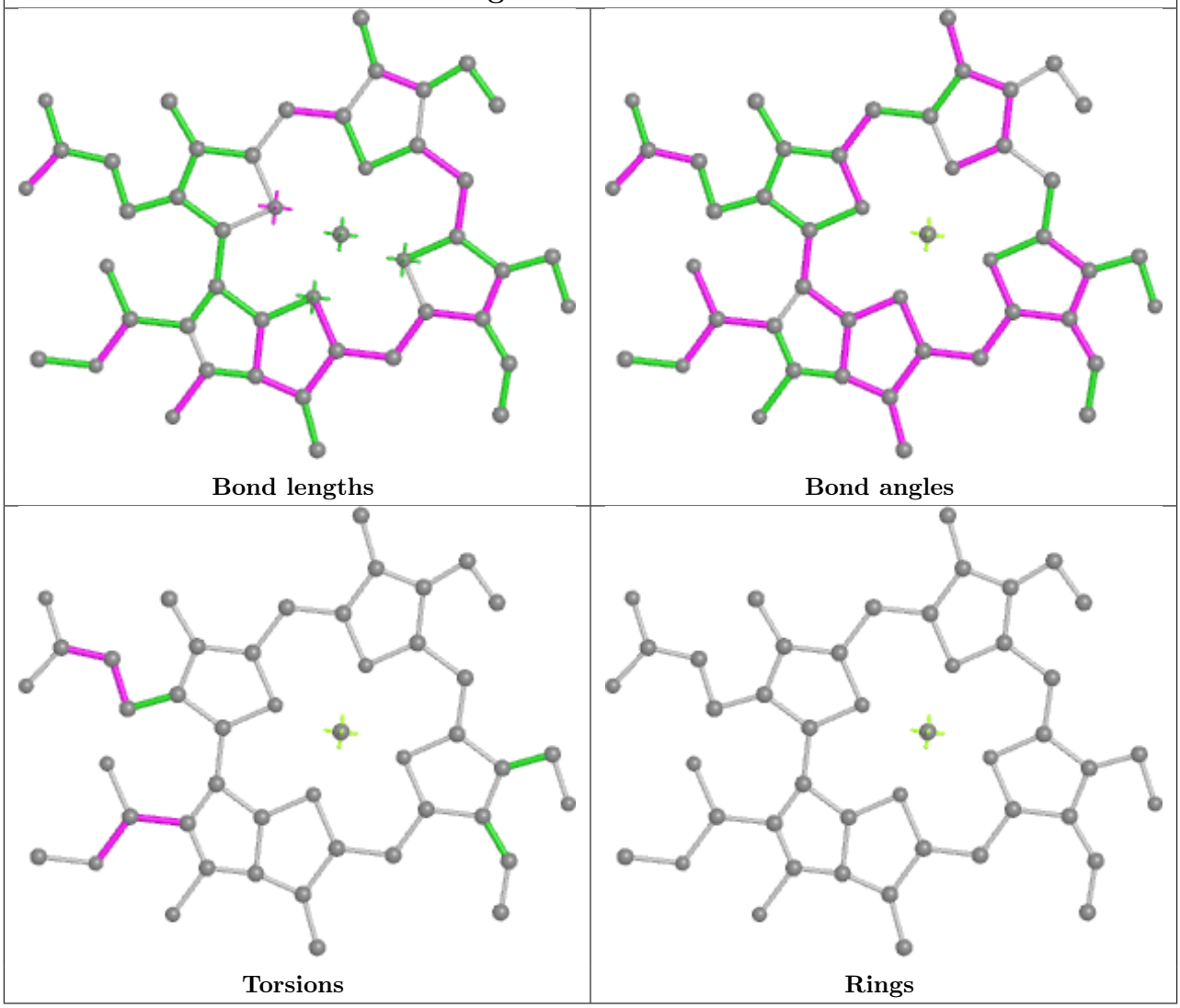


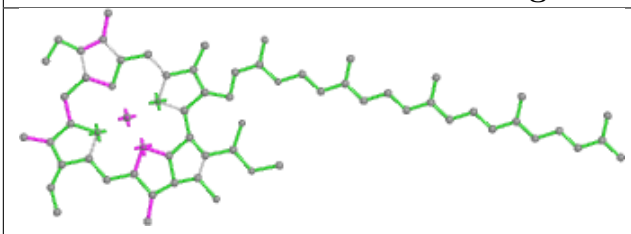
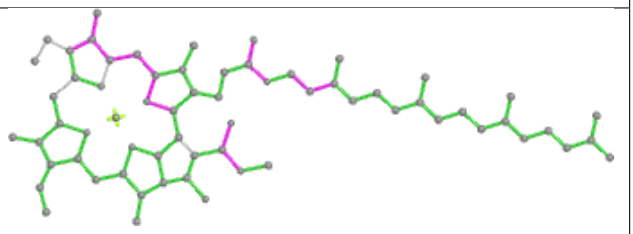
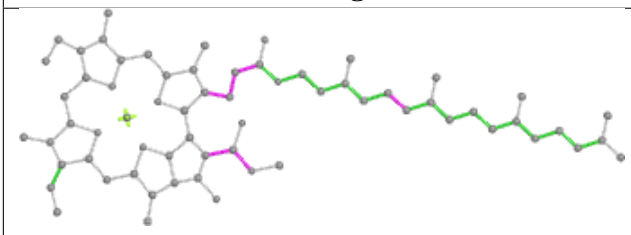
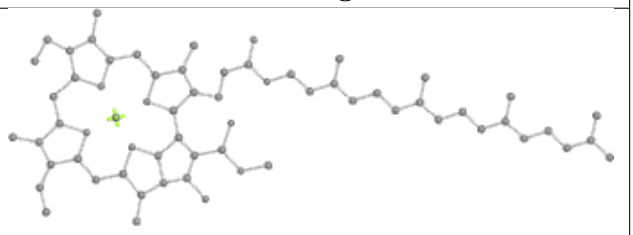
Rings

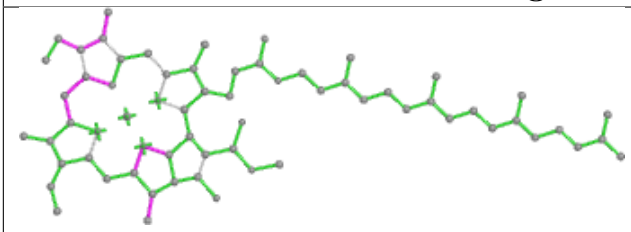
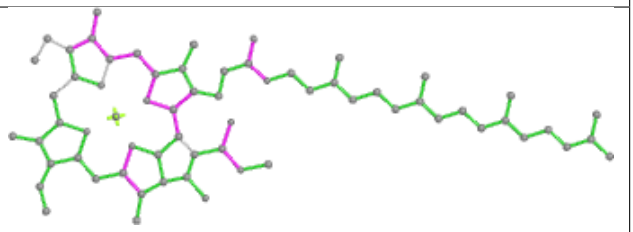
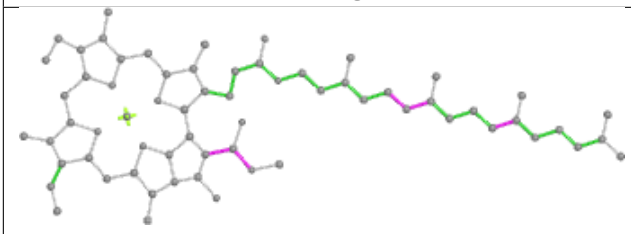
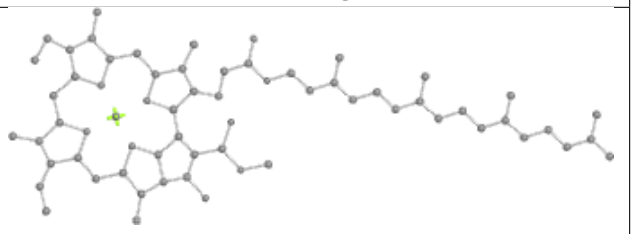
Ligand LMG b 624



Ligand CHL s 314



Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

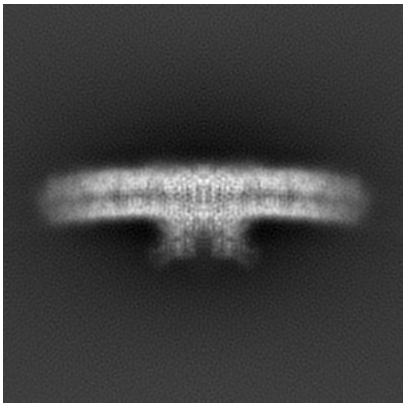
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9957. These allow visual inspection of the internal detail of the map and identification of artifacts.

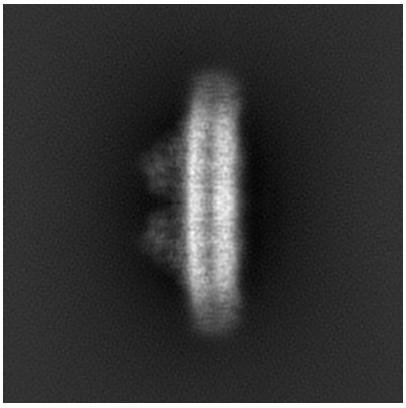
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

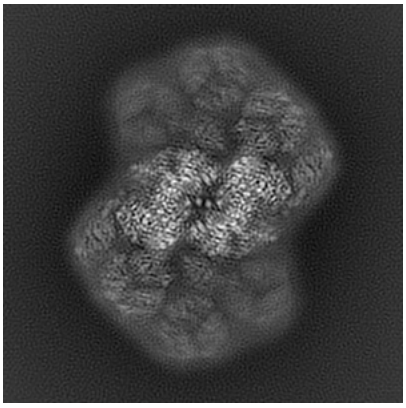
6.1.1 Primary map



X



Y

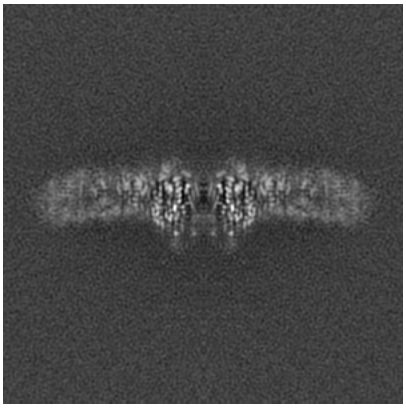


Z

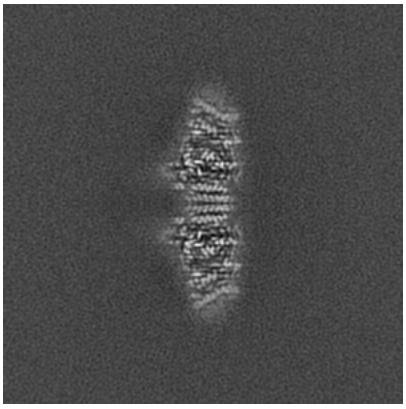
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

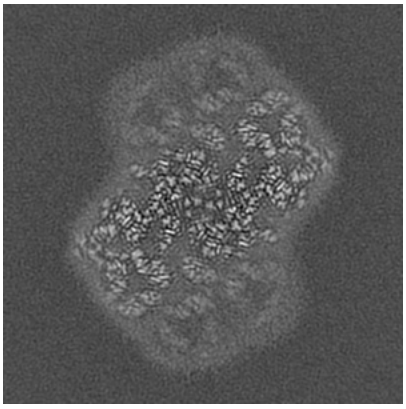
6.2.1 Primary map



X Index: 150



Y Index: 150

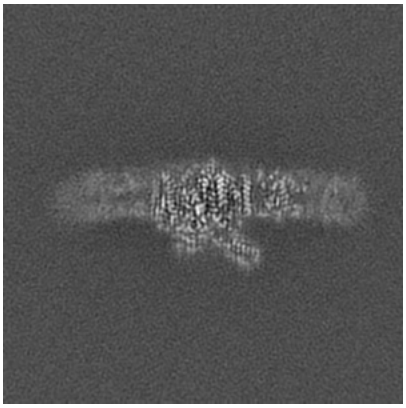


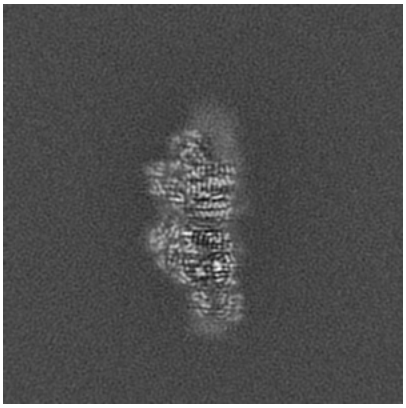
Z Index: 150

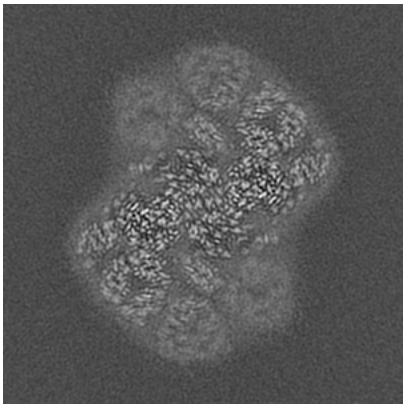
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 180

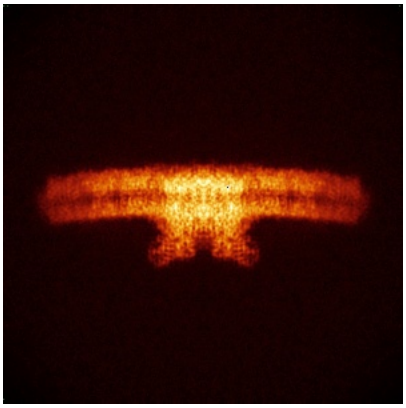

Y Index: 131

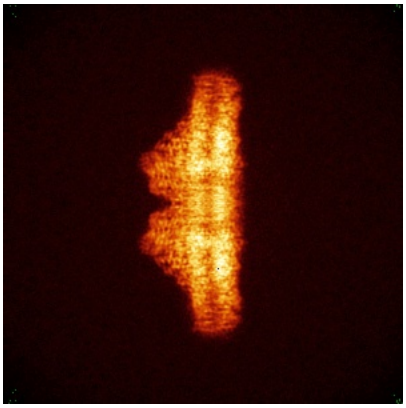

Z Index: 164

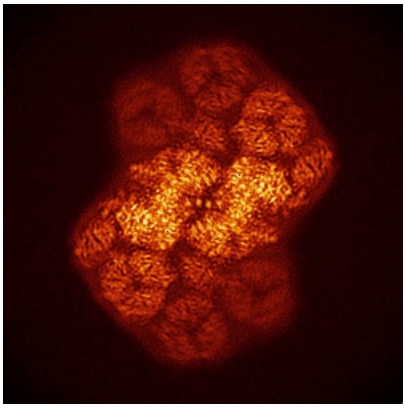
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

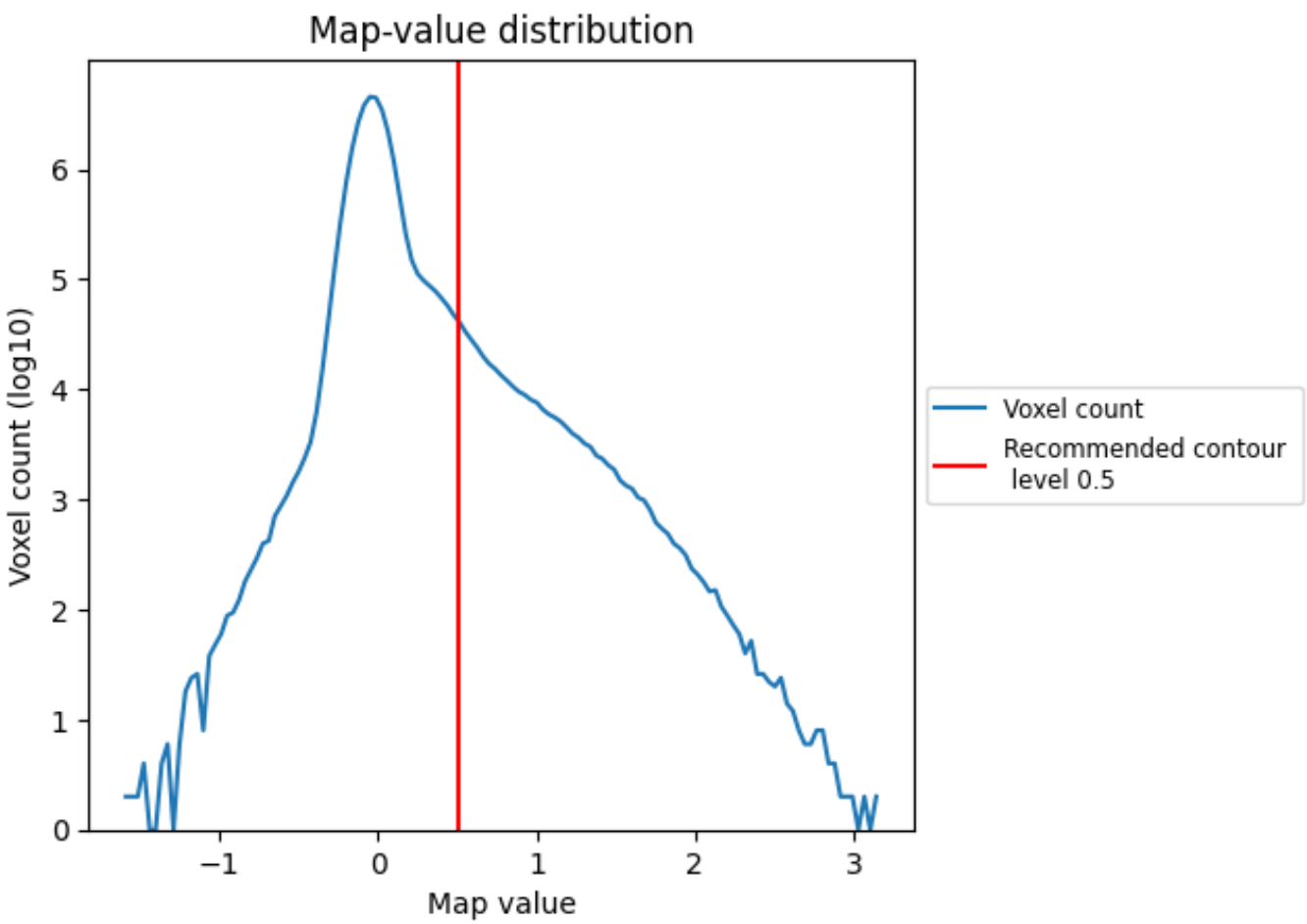
6.6 Mask visualisation (i)

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

7 Map analysis (i)

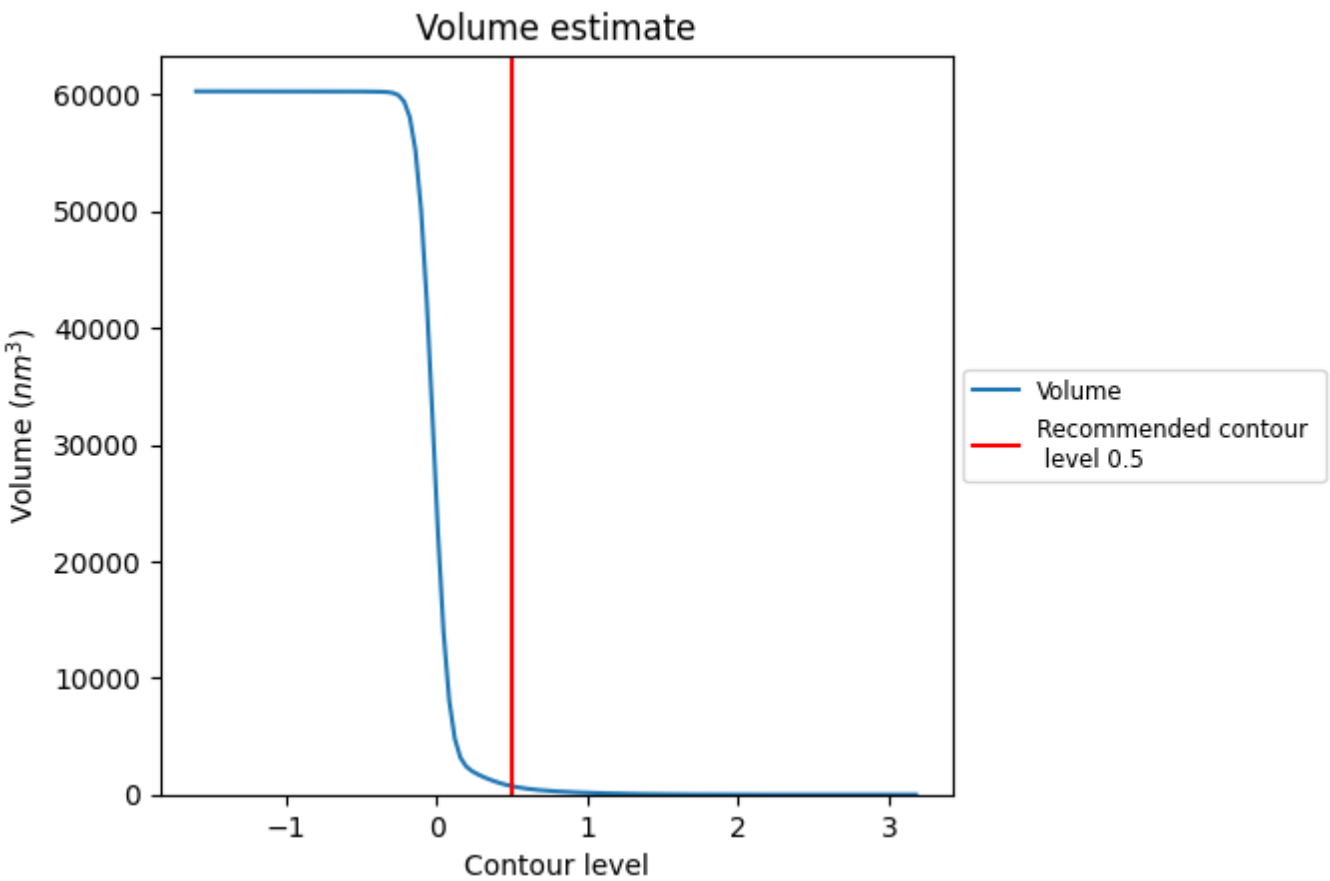
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

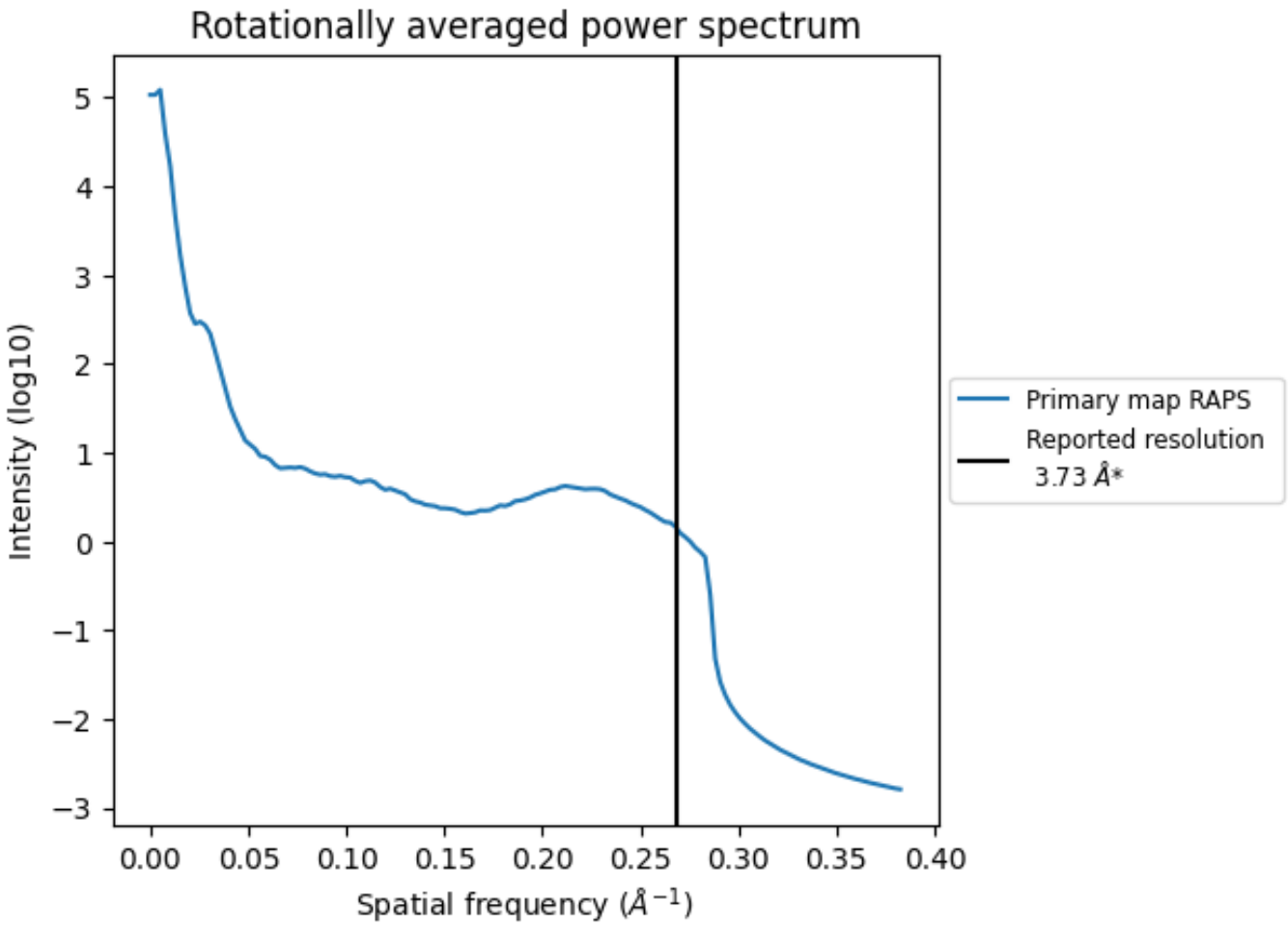
7.2 Volume estimate (i)



The volume at the recommended contour level is 727 nm^3; this corresponds to an approximate mass of 657 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 0.268 Å^{-1}

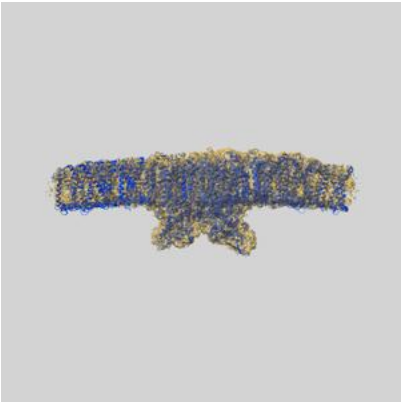
8 Fourier-Shell correlation (i)

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

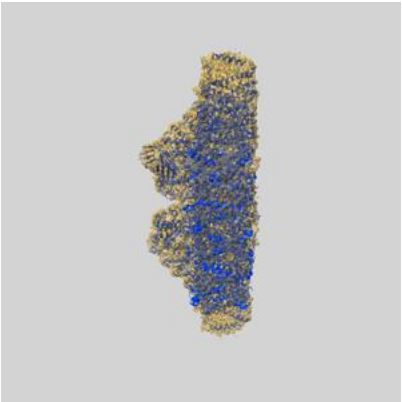
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9957 and PDB model 6KAF. Per-residue inclusion information can be found in section 3 on page 53.

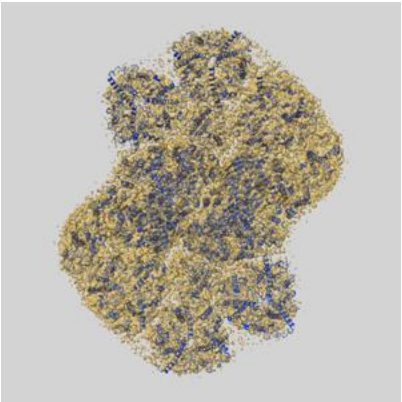
9.1 Map-model overlay (i)



X



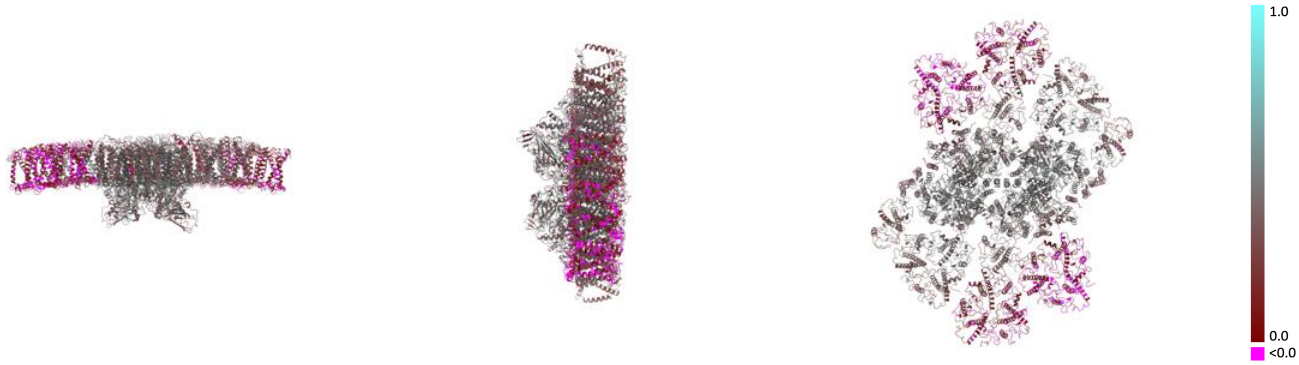
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

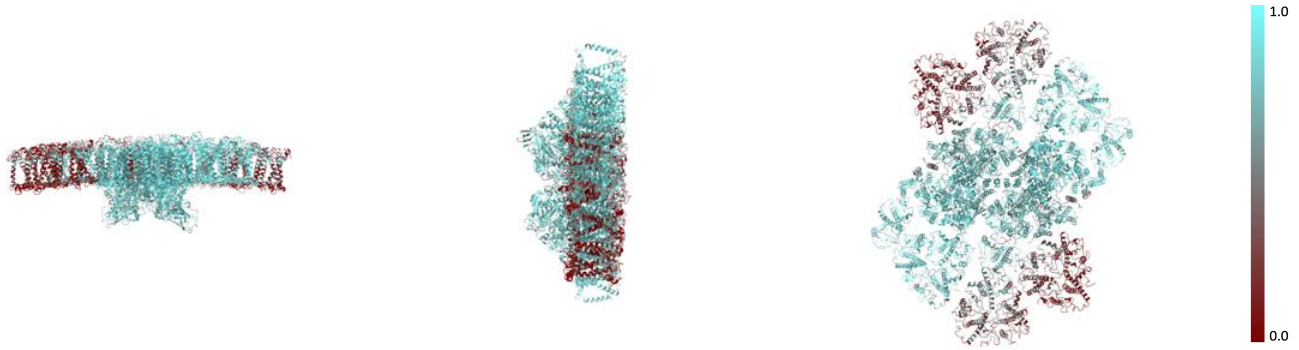
9.2 Q-score mapped to coordinate model (i)



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.

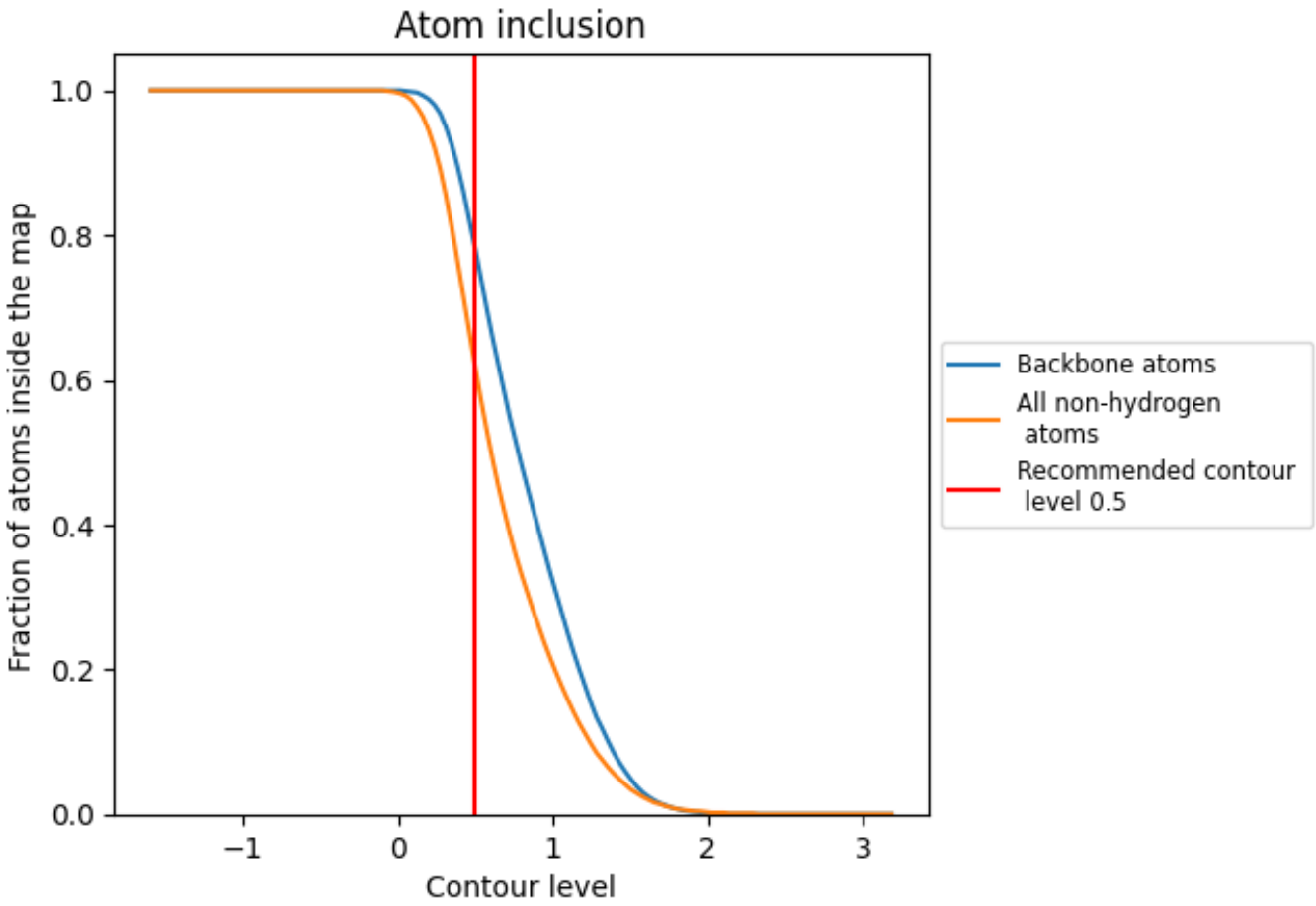
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6150	0.3260
1	0.4690	0.2180
2	0.2680	0.1130
3	0.2680	0.1030
4	0.4800	0.2330
5	0.2690	0.1100
6	0.2770	0.1120
A	0.8490	0.4710
B	0.7780	0.4420
C	0.8260	0.4680
D	0.8310	0.4580
E	0.7560	0.3920
F	0.7560	0.3190
G	0.7130	0.3870
H	0.8090	0.4290
I	0.9010	0.4840
J	0.4170	0.2730
K	0.8150	0.4280
L	0.7390	0.4530
M	0.7010	0.4110
N	0.7720	0.4060
O	0.7120	0.3810
P	0.2560	0.0890
Q	0.1050	0.0300
R	0.6320	0.3760
S	0.7690	0.3680
T	0.6880	0.4350
U	0.7830	0.4490
V	0.2130	0.0700
W	0.7840	0.4360
X	0.6850	0.3900
Y	0.6120	0.3520
Z	0.7730	0.3730
a	0.8460	0.4710
b	0.7770	0.4400

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Chain	Atom inclusion	Q-score
c	0.8220	0.4660
d	0.8320	0.4570
e	0.7540	0.3870
f	0.7600	0.3190
g	0.7080	0.3760
h	0.8160	0.4260
i	0.9010	0.4870
j	0.4120	0.2370
k	0.8150	0.4320
l	0.7360	0.4490
m	0.7010	0.4070
n	0.7640	0.3960
o	0.7120	0.3830
p	0.2400	0.0800
q	0.1080	0.0270
r	0.6390	0.3800
s	0.7680	0.3660
t	0.6880	0.4350
u	0.7850	0.4490
v	0.2150	0.0810
w	0.7790	0.4330
x	0.6850	0.3930
y	0.6120	0.3550
z	0.7630	0.3830