wwPDB EM Validation Summary Report

Mar 25, 2026 – 01:04 PM UTC

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 ⓘ symbol.

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

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

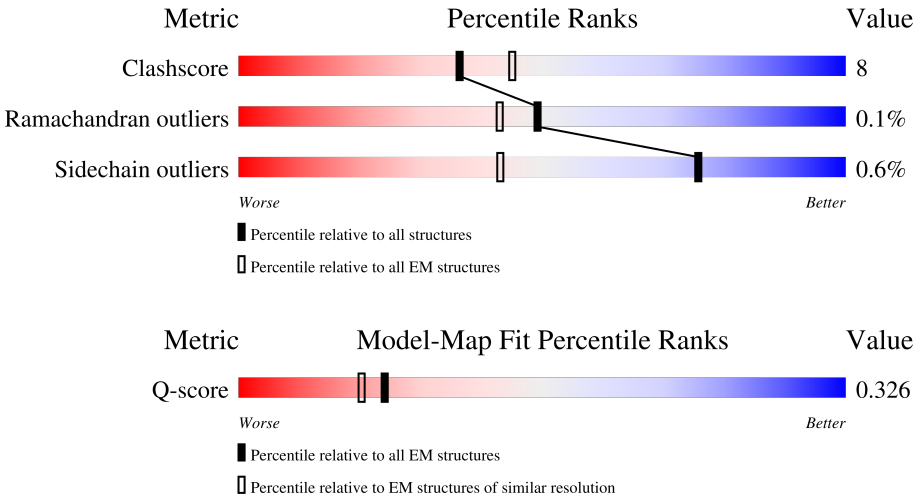
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10415 (3.23 - 4.23)

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% 64% 16% 20%
1	r	280	15% 64% 15% 20%
2	A	352	80% 14% 5%
2	a	352	82% 13% 5%

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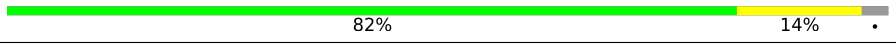
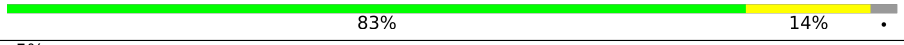
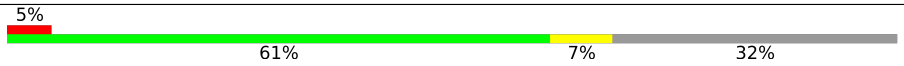
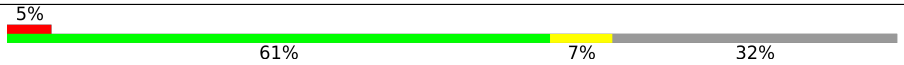
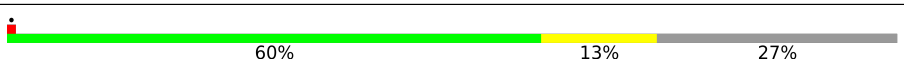
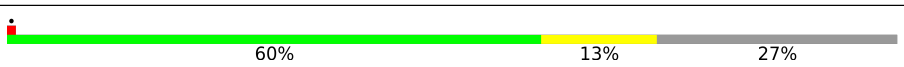
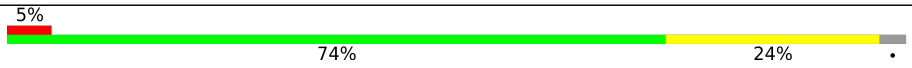
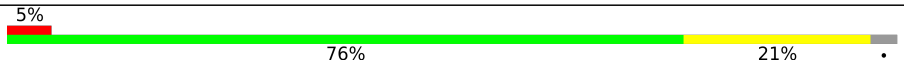
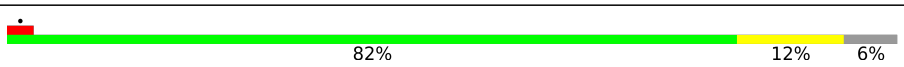
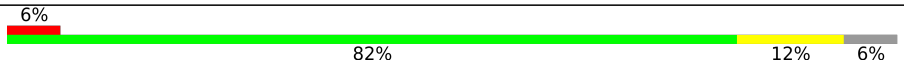
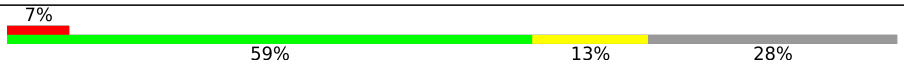
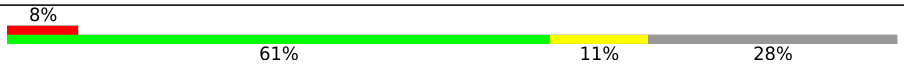
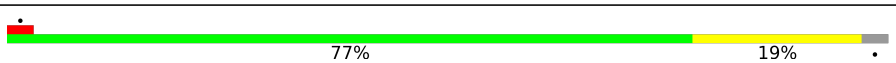
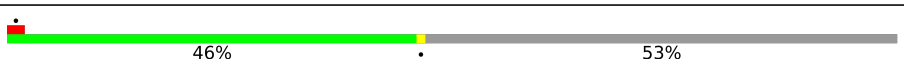
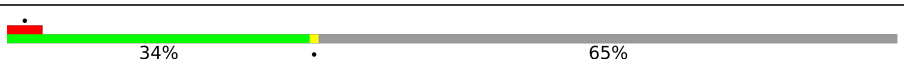
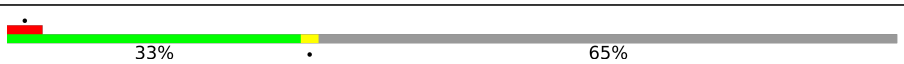
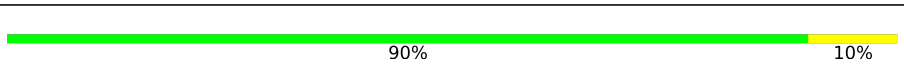
Mol	Chain	Length	Quality of chain
3	D	352	
3	d	352	
4	F	44	
4	f	44	
5	H	88	
5	h	88	
6	I	37	
6	i	37	
7	J	50	
7	j	50	
8	K	46	
8	k	46	
9	L	38	
9	l	38	
10	M	34	
10	m	34	
11	O	291	
11	o	291	
12	T	31	
12	t	31	
13	W	115	
13	w	115	
14	X	101	
14	x	101	
15	Z	62	

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Mol	Chain	Length	Quality of chain
15	z	62	85% 15%
16	Y	33	9% 85% 6% 9%
16	y	33	9% 85% 6% 9%
17	E	82	72% 11% 17%
17	e	82	72% 11% 17%
18	1	257	30% 73% 12% 15%
18	2	257	63% 74% 10% 15%
18	3	257	58% 73% 12% 15%
18	4	257	30% 68% 16% 15%
18	5	257	63% 72% 12% 15%
18	6	257	57% 73% 12% 15%
18	G	257	6% 70% 15% 15%
18	N	257	73% 11% 16%
18	P	257	61% 72% 12% 15%
18	Q	257	80% 72% 13% 15%
18	U	257	67% 17% 15%
18	V	257	69% 70% 14% 15%
18	g	257	7% 73% 11% 15%
18	n	257	76% 9% 15%
18	p	257	60% 71% 12% 15%
18	q	257	80% 72% 13% 15%
18	u	257	65% 20% 15%
18	v	257	68% 73% 12% 15%
19	S	289	68% 13% 18%
19	s	289	69% 12% 18%

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Mol	Chain	Length	Quality of chain
20	C	461	84% 14%
20	c	461	85% 13%
21	B	508	85% 14%
21	b	508	5% 84% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	v	317	X	-	-	-
26	CHL	v	318	X	-	-	-
29	CL	A	402	-	-	X	-
29	CL	a	402	-	-	X	-
29	CL	a	403	-	-	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
1	r	223	Total	C	N	O	S	0	0
			1701	1081	286	329	5		
1	R	223	Total	C	N	O	S	0	0
			1698	1080	285	328	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

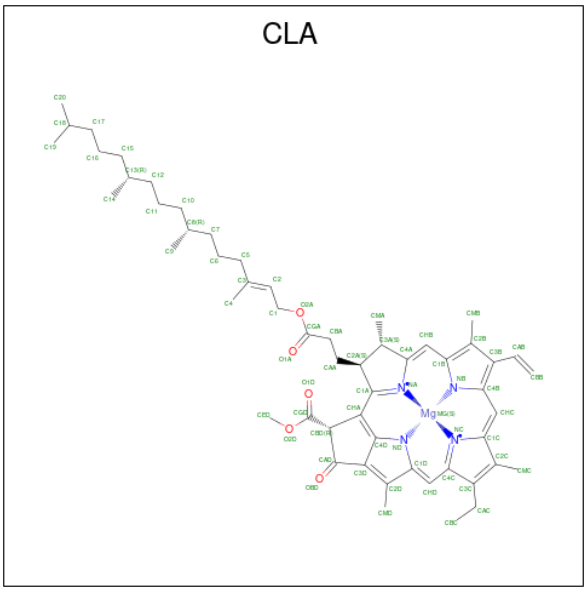
- Molecule 20 is a protein called Photosystem II CP43 reaction center protein.

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

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

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

- 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
22	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
22	S	1	Total	C	Mg	N	O	0
			49	39	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	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	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	

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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	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	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	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	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	

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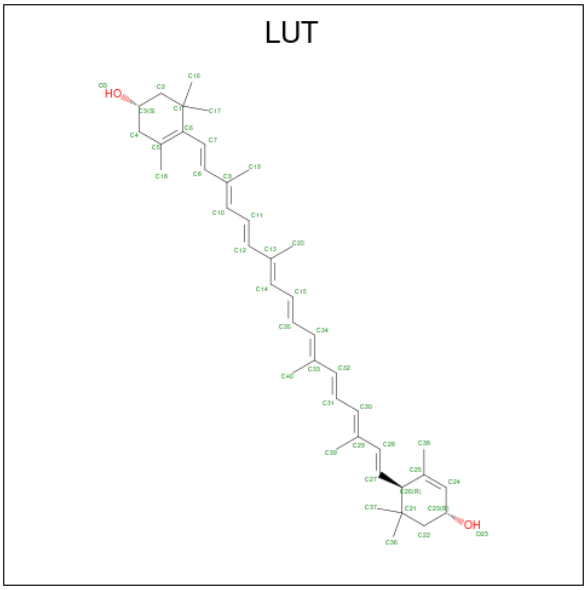
Mol	Chain	Residues	Atoms					AltConf
22	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	s	1	Total	C	Mg	N	O	0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

- 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
23	r	1	Total	C	O	0
			42	40	2	
23	1	1	Total	C	O	0
			42	40	2	
23	1	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	

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

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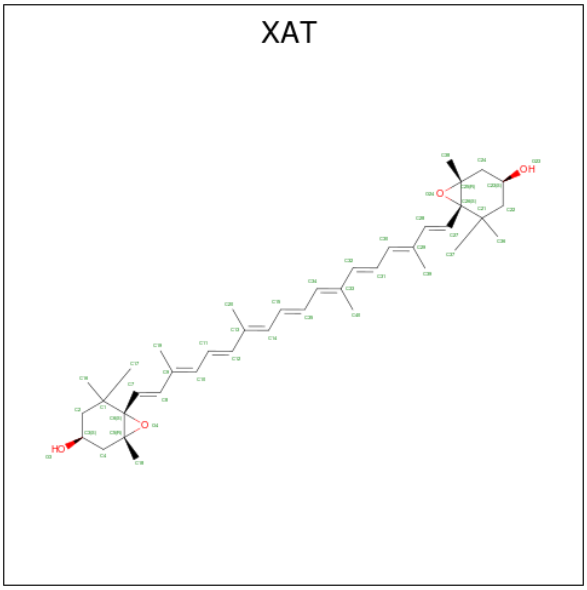
Mol	Chain	Residues	Atoms	AltConf
23	R	1	Total C O 42 40 2	0
23	S	1	Total C O 42 40 2	0
23	S	1	Total C O 42 40 2	0
23	s	1	Total C O 42 40 2	0
23	s	1	Total C O 42 40 2	0

- 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
24	r	1	Total C O 44 40 4	0
24	1	1	Total C O 44 40 4	0
24	2	1	Total C O 44 40 4	0
24	3	1	Total C O 44 40 4	0
24	4	1	Total C O 44 40 4	0
24	5	1	Total C O 44 40 4	0

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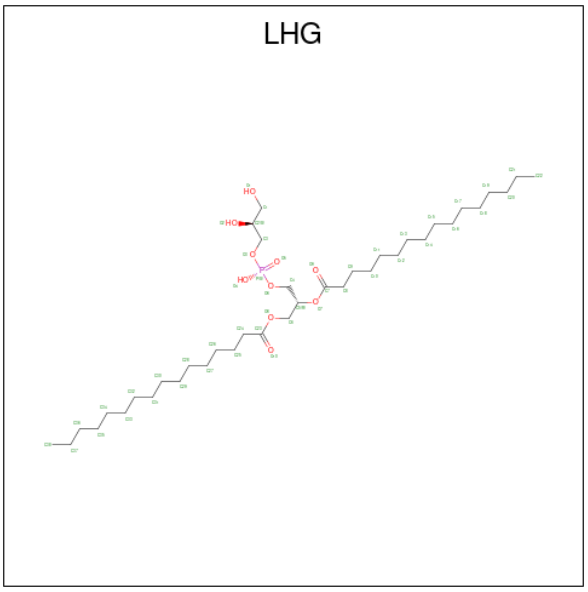
Mol	Chain	Residues	Atoms	AltConf
24	6	1	Total C O 44 40 4	0
24	v	1	Total C O 44 40 4	0
24	p	1	Total C O 44 40 4	0
24	q	1	Total C O 44 40 4	0
24	V	1	Total C O 44 40 4	0
24	P	1	Total C O 44 40 4	0
24	Q	1	Total C O 44 40 4	0
24	U	1	Total C O 44 40 4	0
24	N	1	Total C O 44 40 4	0
24	G	1	Total C O 44 40 4	0
24	u	1	Total C O 44 40 4	0
24	n	1	Total C O 44 40 4	0
24	g	1	Total C O 44 40 4	0
24	R	1	Total C O 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
25	r	1	Total	C	O	P	0
			42	31	10	1	
25	a	1	Total	C	O	P	0
			43	32	10	1	
25	d	1	Total	C	O	P	0
			46	35	10	1	
25	d	1	Total	C	O	P	0
			49	38	10	1	
25	l	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			43	32	10	1	
25	L	1	Total	C	O	P	0
			49	38	10	1	
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	2	1	Total	C	O	P	0
			49	38	10	1	
25	3	1	Total	C	O	P	0
			49	38	10	1	
25	4	1	Total	C	O	P	0
			49	38	10	1	
25	5	1	Total	C	O	P	0
			49	38	10	1	
25	6	1	Total	C	O	P	0
			49	38	10	1	
25	v	1	Total	C	O	P	0
			49	38	10	1	

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

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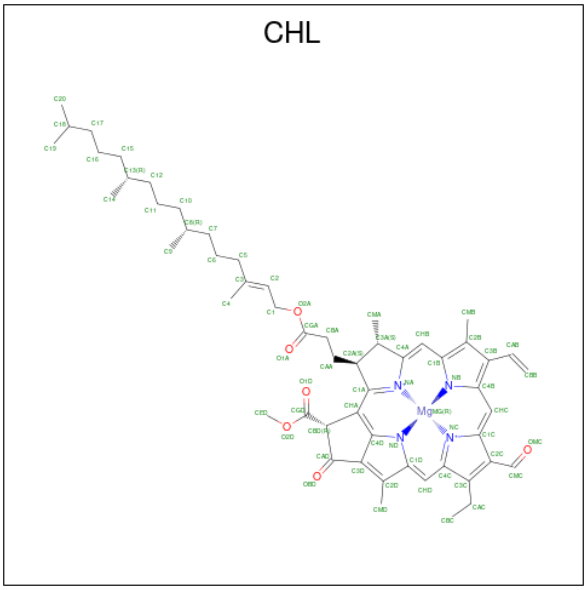
Mol	Chain	Residues	Atoms				AltConf
25	b	1	Total	C	O	P	0
			49	38	10	1	
25	c	1	Total	C	O	P	0
			49	38	10	1	
25	c	1	Total	C	O	P	0
			49	38	10	1	
25	c	1	Total	C	O	P	0
			49	38	10	1	
25	s	1	Total	C	O	P	0
			49	38	10	1	

- 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
26	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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

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

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

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

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

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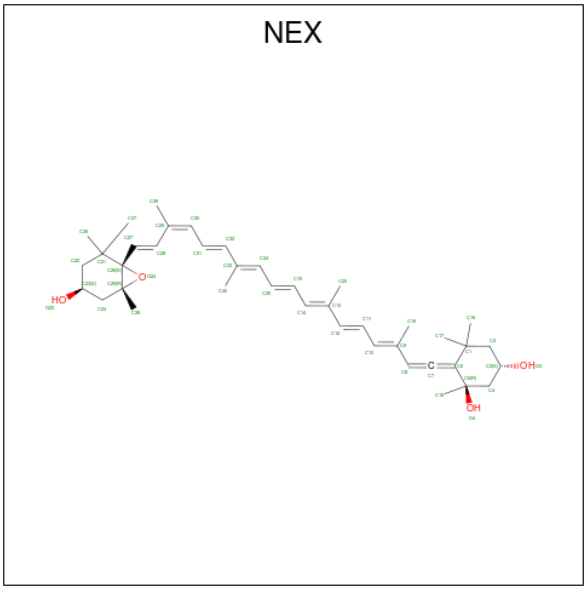
Mol	Chain	Residues	Atoms					AltConf
26	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	R	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	S	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
26	S	1	Total	C	Mg	N	O	0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

- 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
27	r	1	Total	C	O	0
			44	40	4	
27	r	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	v	1	Total	C	O	0
			44	40	4	
27	p	1	Total	C	O	0
			44	40	4	
27	V	1	Total	C	O	0
			44	40	4	
27	P	1	Total	C	O	0
			44	40	4	
27	U	1	Total	C	O	0
			44	40	4	
27	N	1	Total	C	O	0
			44	40	4	
27	u	1	Total	C	O	0
			44	40	4	
27	u	1	Total	C	O	0
			44	40	4	
27	n	1	Total	C	O	0
			44	40	4	
27	R	1	Total	C	O	0
			44	40	4	
27	S	1	Total	C	O	0
			44	40	4	
27	s	1	Total	C	O	0
			44	40	4	

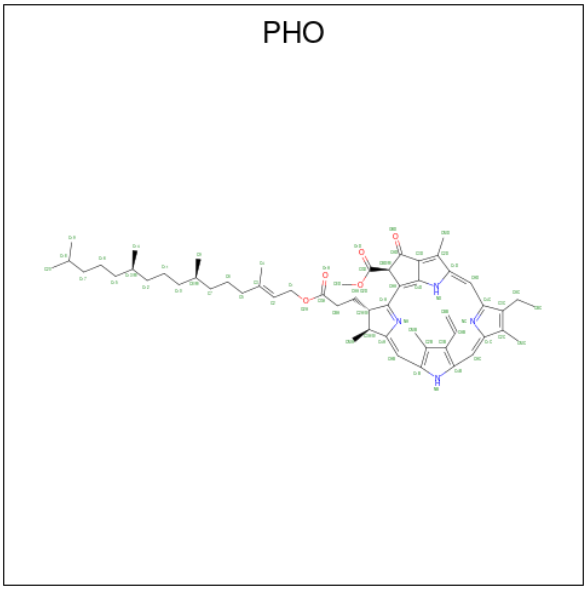
- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

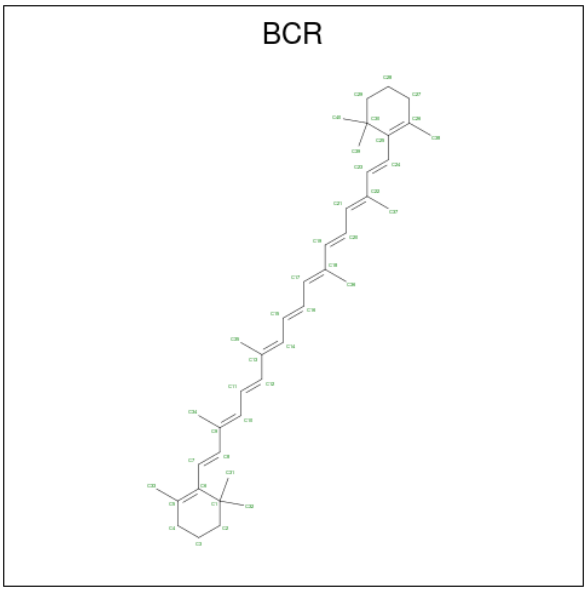
Mol	Chain	Residues	Atoms	AltConf
29	a	2	Total Cl 2 2	0
29	A	2	Total Cl 2 2	0

- 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
30	a	1	Total C N O 64 55 4 5	0
30	d	1	Total C N O 64 55 4 5	0
30	A	1	Total C N O 64 55 4 5	0
30	D	1	Total C N O 64 55 4 5	0

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



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

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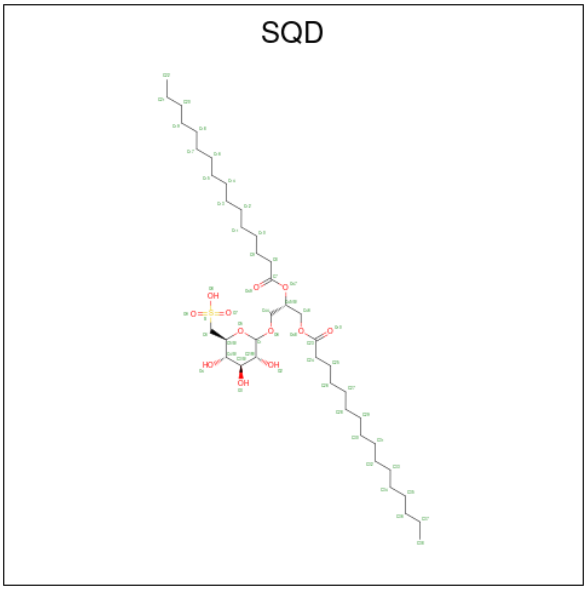
Mol	Chain	Residues	Atoms	AltConf
31	B	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	X	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0

- 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
32	a	1	Total C O S 50 37 12 1	0
32	a	1	Total C O S 54 41 12 1	0
32	l	1	Total C O S 54 41 12 1	0

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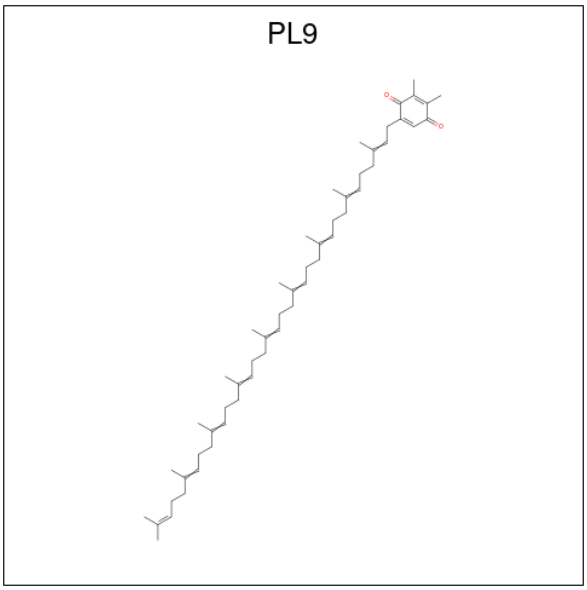
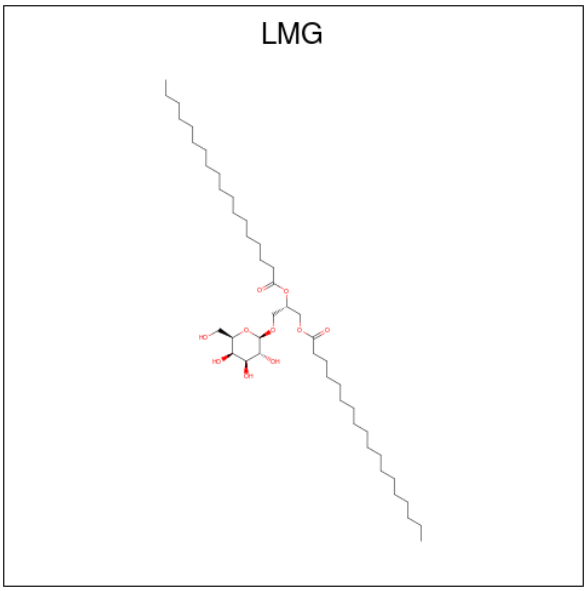
Mol	Chain	Residues	Atoms				AltConf
32	m	1	Total	C	O	S	0
			42	29	12	1	
32	A	1	Total	C	O	S	0
			54	41	12	1	
32	L	1	Total	C	O	S	0
			54	41	12	1	
32	M	1	Total	C	O	S	0
			42	29	12	1	
32	C	1	Total	C	O	S	0
			50	37	12	1	

- 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: $C_{53}H_{80}O_2$).



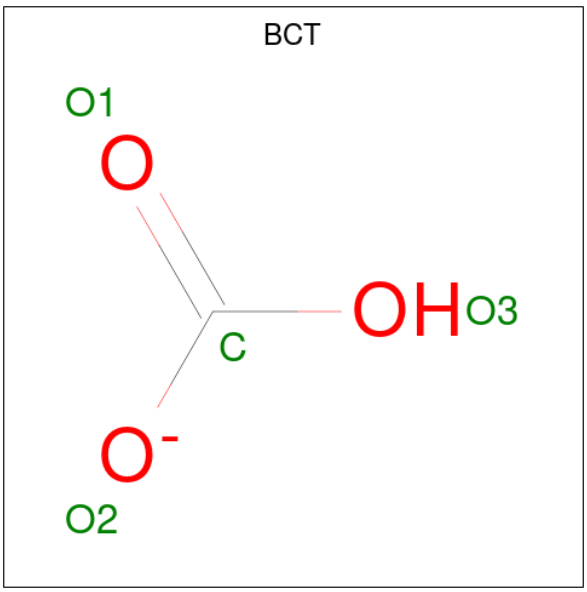
Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total	C	O	0
			13	11	2	
33	d	1	Total	C	O	0
			55	53	2	
33	A	1	Total	C	O	0
			13	11	2	
33	D	1	Total	C	O	0
			55	53	2	

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



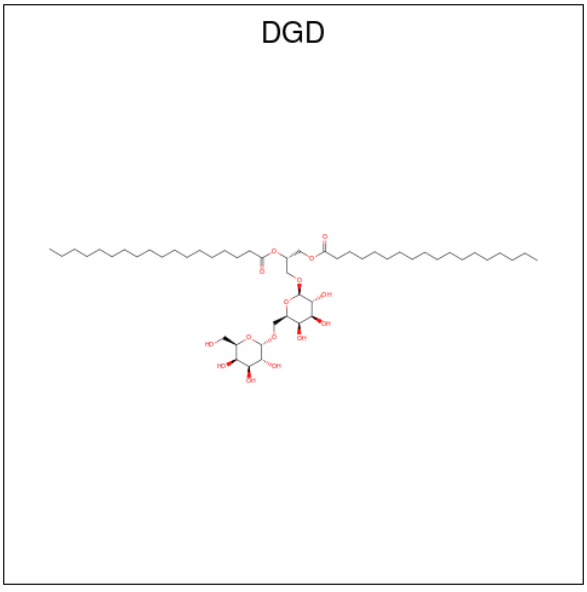
Mol	Chain	Residues	Atoms	AltConf
34	a	1	Total C O 40 30 10	0
34	d	1	Total C O 46 36 10	0
34	w	1	Total C O 48 38 10	0
34	A	1	Total C O 40 30 10	0
34	W	1	Total C O 48 38 10	0
34	C	1	Total C O 51 41 10	0
34	C	1	Total C O 51 41 10	0
34	B	1	Total C O 51 41 10	0
34	B	1	Total C O 55 45 10	0
34	D	1	Total C O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

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



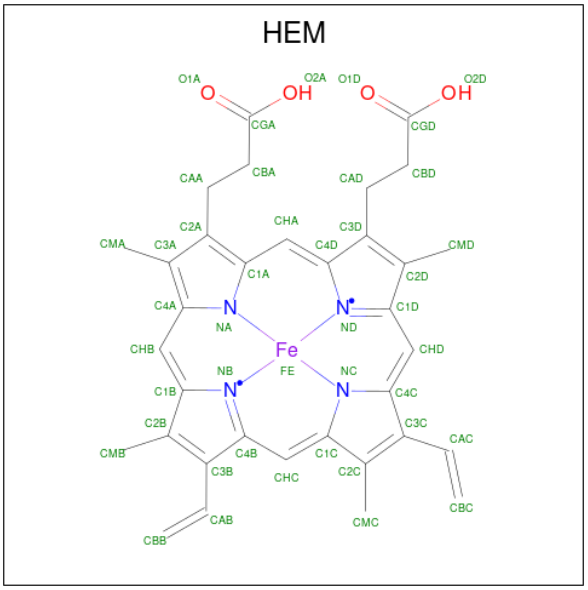
Mol	Chain	Residues	Atoms			AltConf
35	a	1	Total	C	O	0
			4	1	3	
35	D	1	Total	C	O	0
			4	1	3	

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



Mol	Chain	Residues	Atoms	AltConf
36	a	1	Total C O 59 44 15	0
36	A	1	Total C O 59 44 15	0
36	J	1	Total C O 60 45 15	0
36	C	1	Total C O 55 40 15	0
36	C	1	Total C O 62 47 15	0
36	B	1	Total C O 62 47 15	0
36	b	1	Total C O 62 47 15	0
36	c	1	Total C O 55 40 15	0
36	c	1	Total C O 62 47 15	0
36	c	1	Total C O 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
37	E	1	Total C Fe N O 43 34 1 4 4	0

Continued on next page...

Continued from previous page...

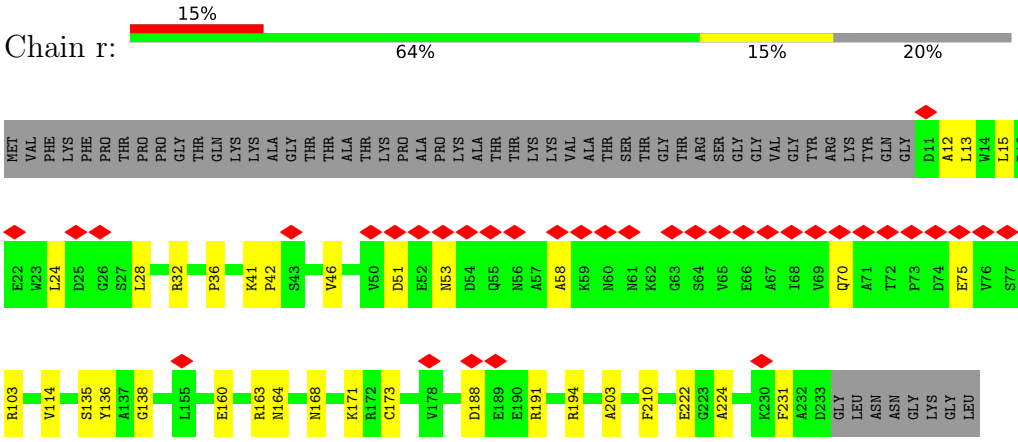
Mol	Chain	Residues	Atoms					AltConf
37	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots

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.

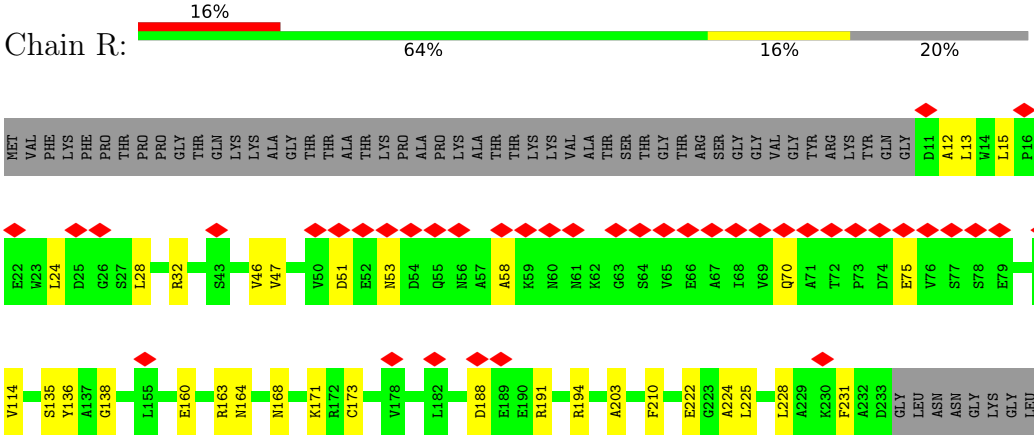
• Molecule 1: Chlorophyll a-b binding protein CP29

Chain r:



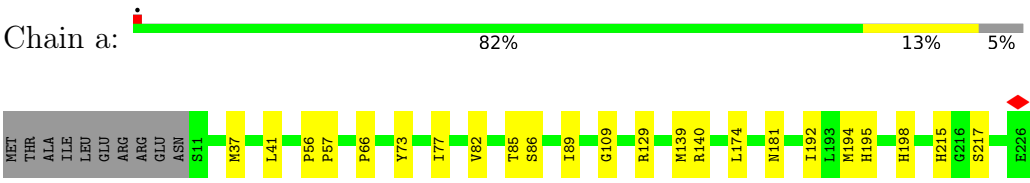
• Molecule 1: Chlorophyll a-b binding protein CP29

Chain R:

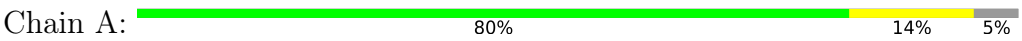


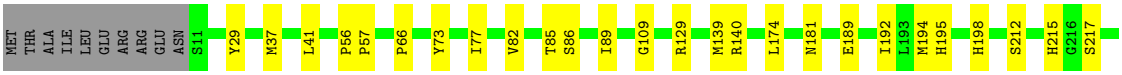
• Molecule 2: Photosystem II protein D1

Chain a:

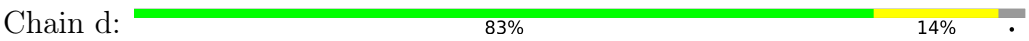


• Molecule 2: Photosystem II protein D1

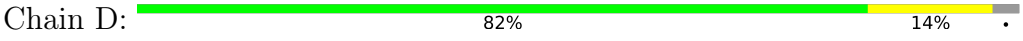


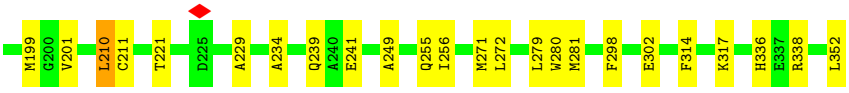


• Molecule 3: Photosystem II D2 protein

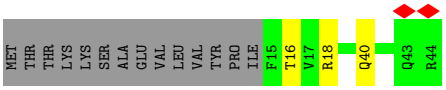


• Molecule 3: Photosystem II D2 protein

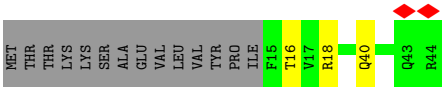




• Molecule 4: Cytochrome b559 subunit beta

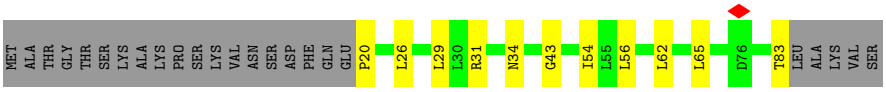


• Molecule 4: Cytochrome b559 subunit beta



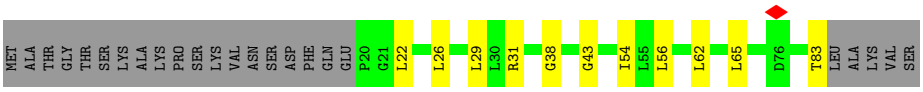
• Molecule 5: Photosystem II reaction center protein H

Chain h:



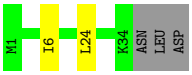
• Molecule 5: Photosystem II reaction center protein H

Chain H:



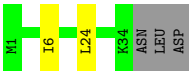
• Molecule 6: Photosystem II reaction center protein I

Chain i:



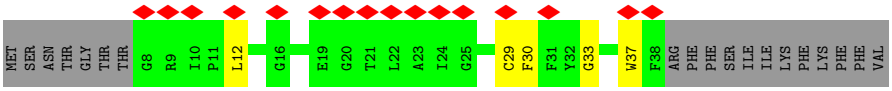
• Molecule 6: Photosystem II reaction center protein I

Chain I:



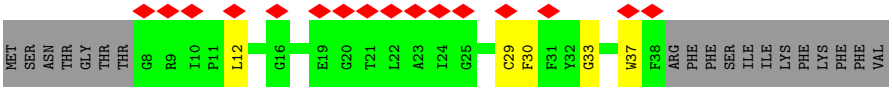
• Molecule 7: Photosystem II reaction center protein J, PsbJ

Chain j:



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

Chain J:

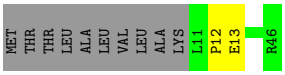


• Molecule 8: Photosystem II reaction center protein K

Chain k:

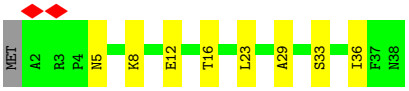
• Molecule 8: Photosystem II reaction center protein K

Chain K:



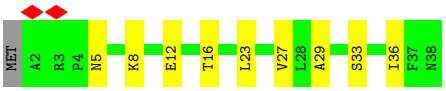
• Molecule 9: Photosystem II reaction center protein L

Chain l:



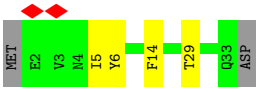
• Molecule 9: Photosystem II reaction center protein L

Chain L:



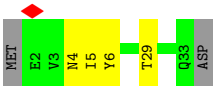
• Molecule 10: Photosystem II reaction center protein M

Chain m:



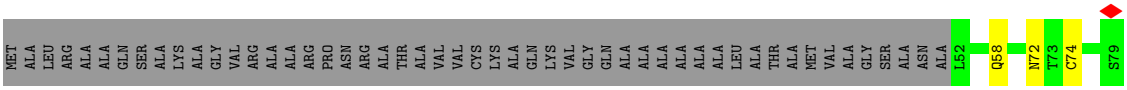
• Molecule 10: Photosystem II reaction center protein M

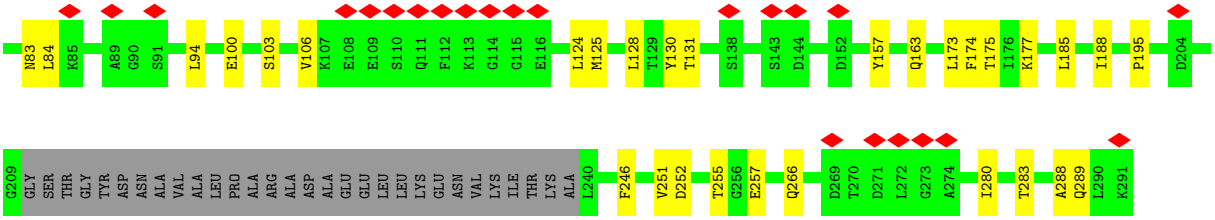
Chain M:



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

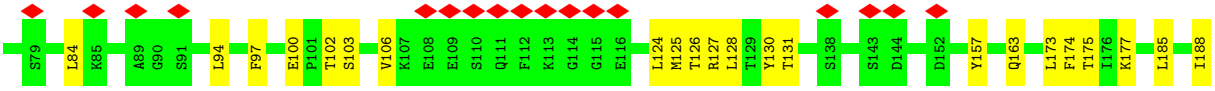
Chain o:

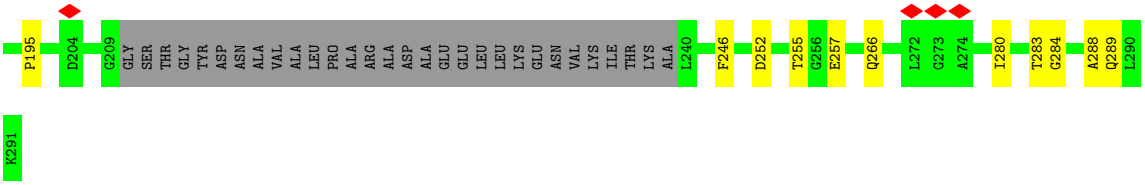




• Molecule 11: Oxygen-evolving enhancer protein 1 of photosystem II

Chain O:





• Molecule 12: Photosystem II reaction center protein T

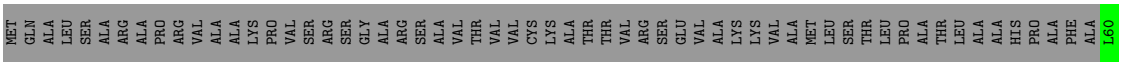
Chain t:

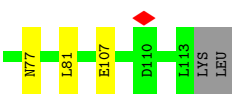
• Molecule 12: Photosystem II reaction center protein T

Chain T:

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

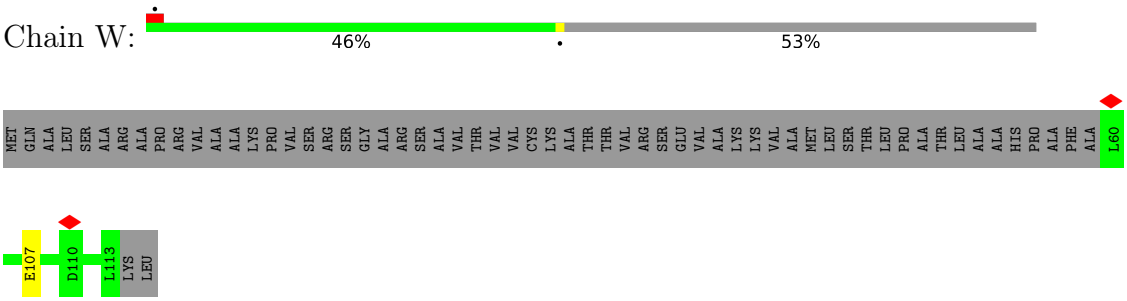
Chain w:





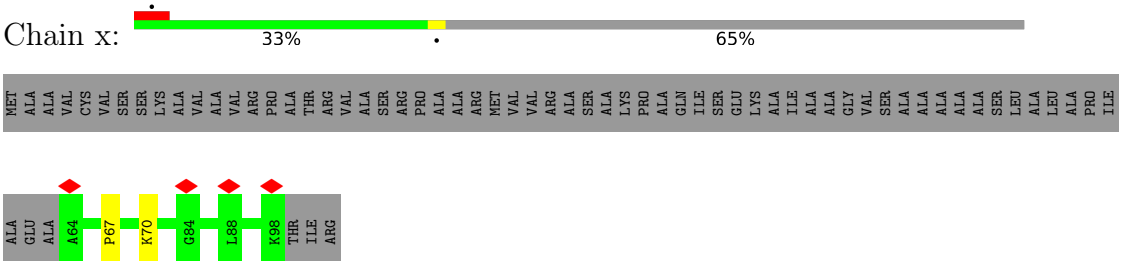
• Molecule 13: Photosystem II reaction center W protein, chloroplastic

Chain W:



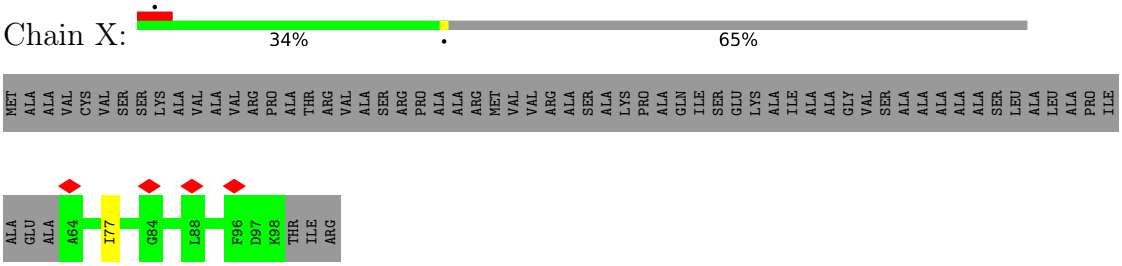
• Molecule 14: 4.1 kDa photosystem II subunit

Chain x:



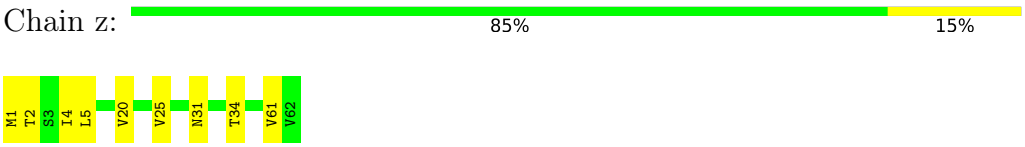
• Molecule 14: 4.1 kDa photosystem II subunit

Chain X:



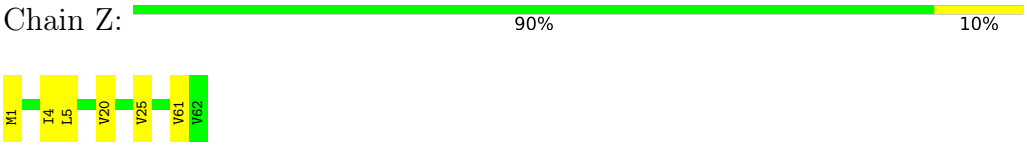
• Molecule 15: Photosystem II reaction center protein Z

Chain z:



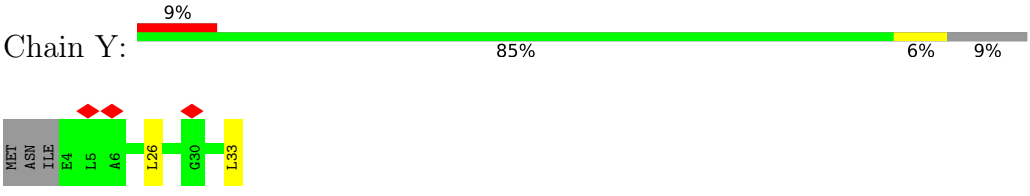
• Molecule 15: Photosystem II reaction center protein Z

Chain Z:



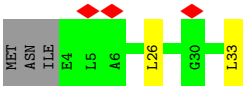
• Molecule 16: Photosystem II reaction center protein 30, Psb30

Chain Y:



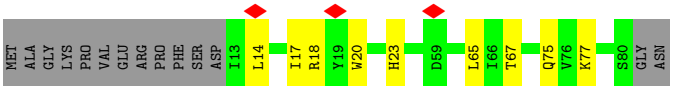
• Molecule 16: Photosystem II reaction center protein 30, Psb30

Chain y:



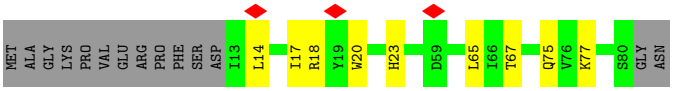
• Molecule 17: Cytochrome b559 subunit alpha

Chain E:



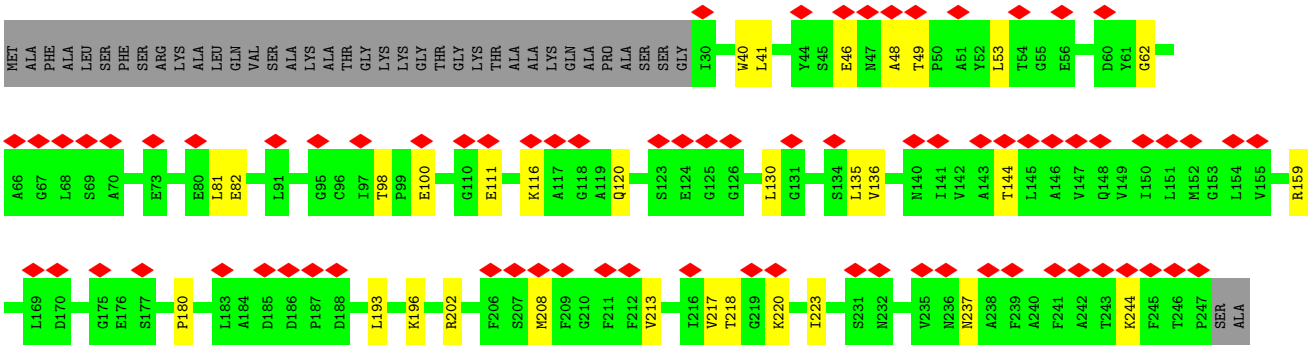
• Molecule 17: Cytochrome b559 subunit alpha

Chain e:



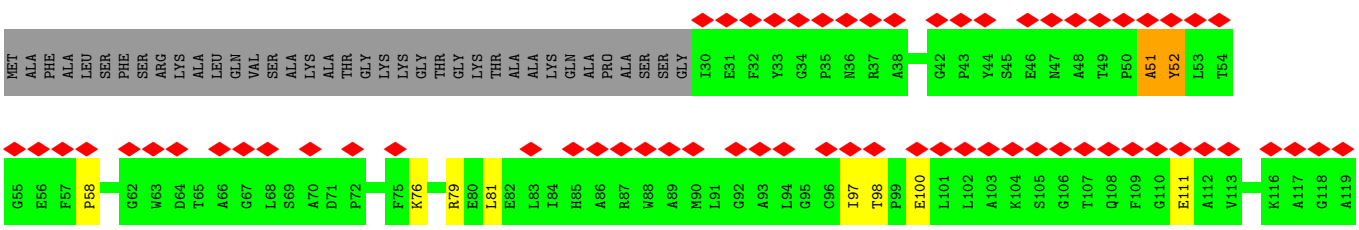
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



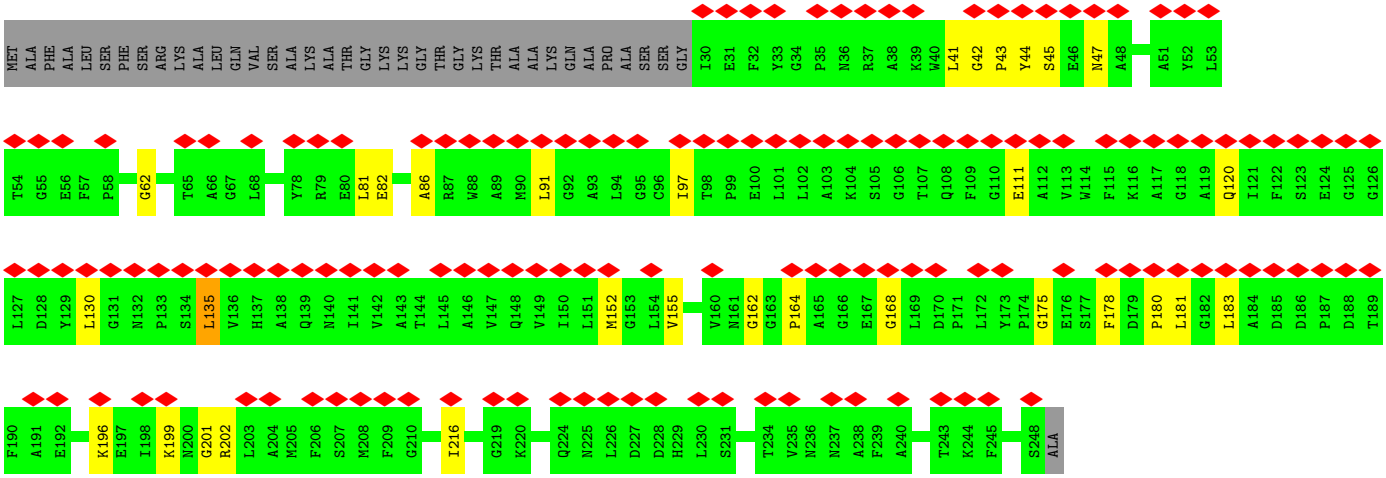
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



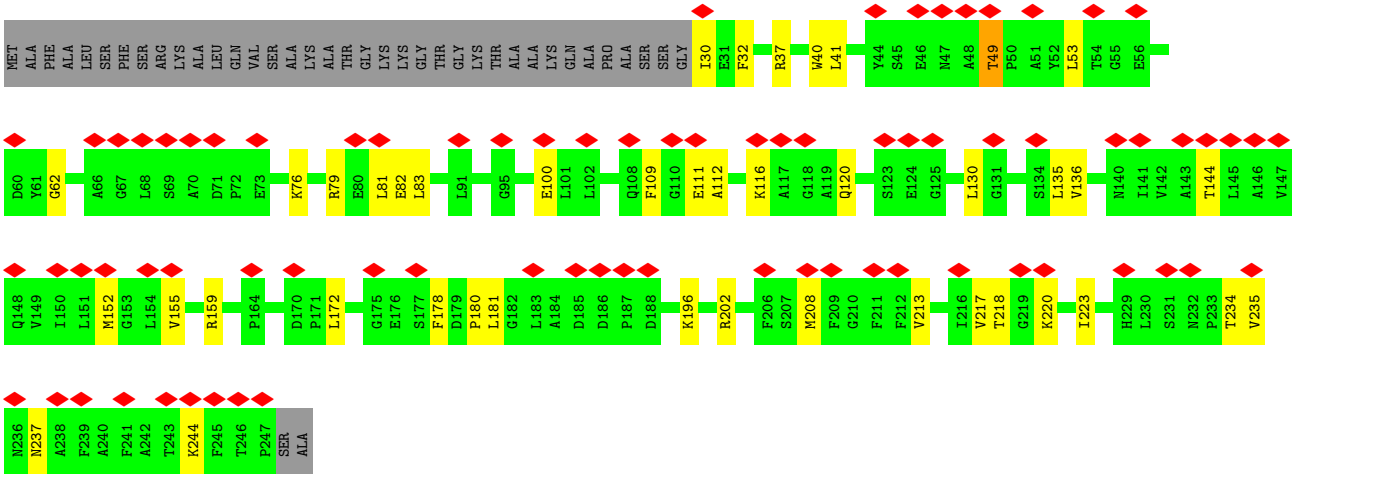
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



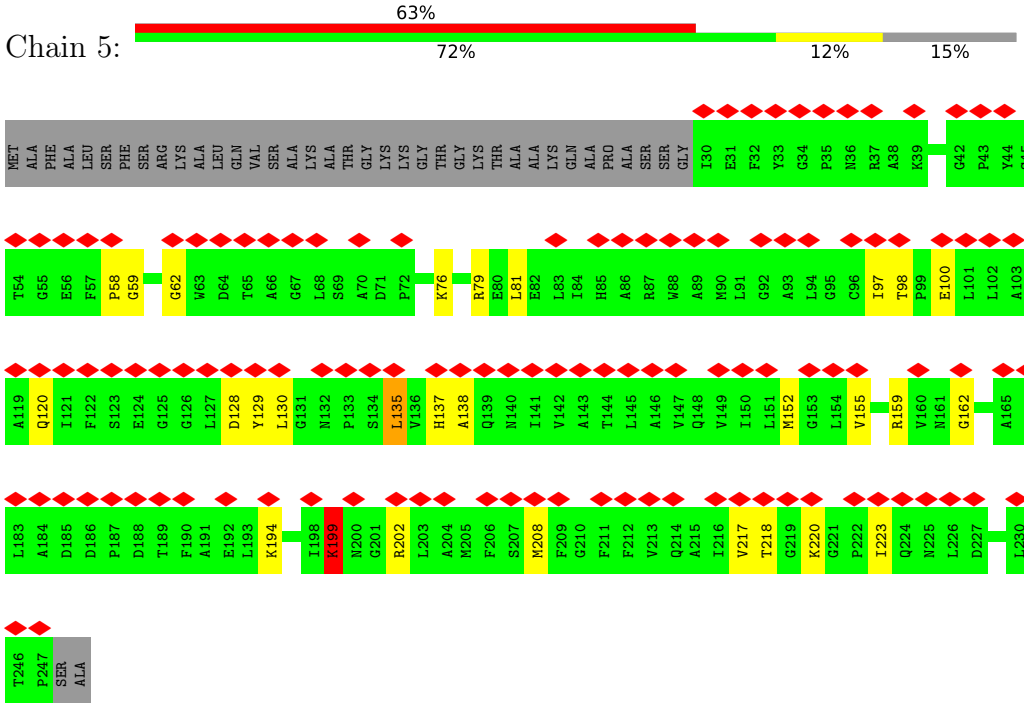
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



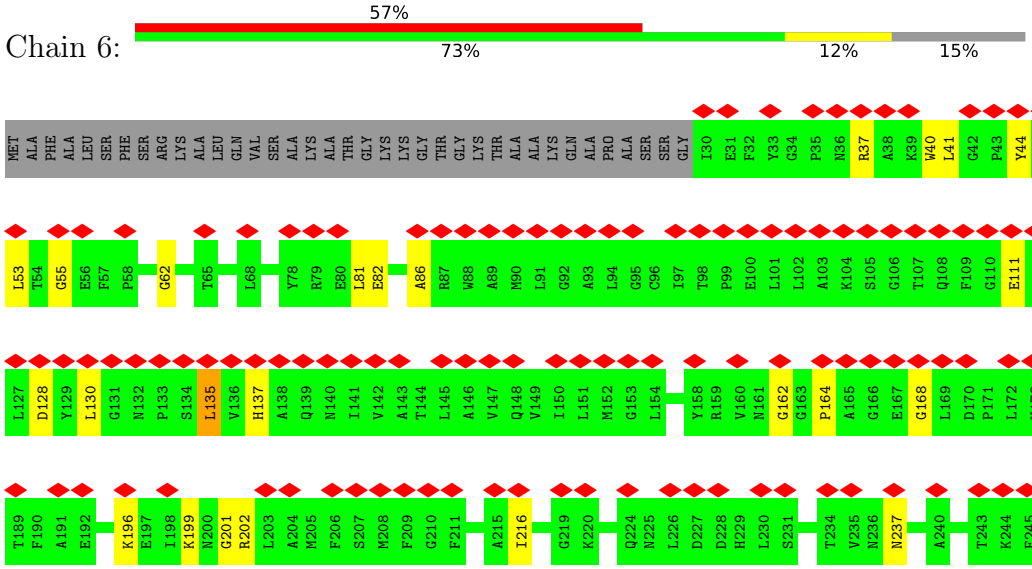
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



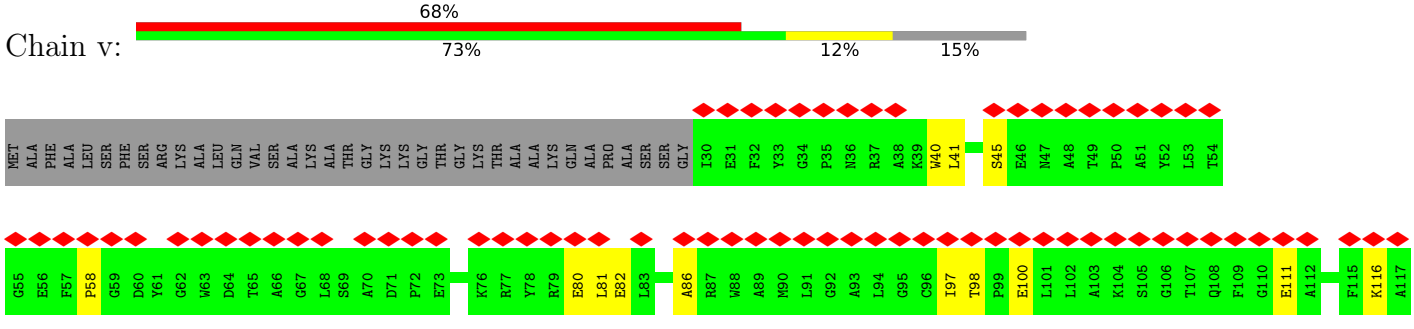
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

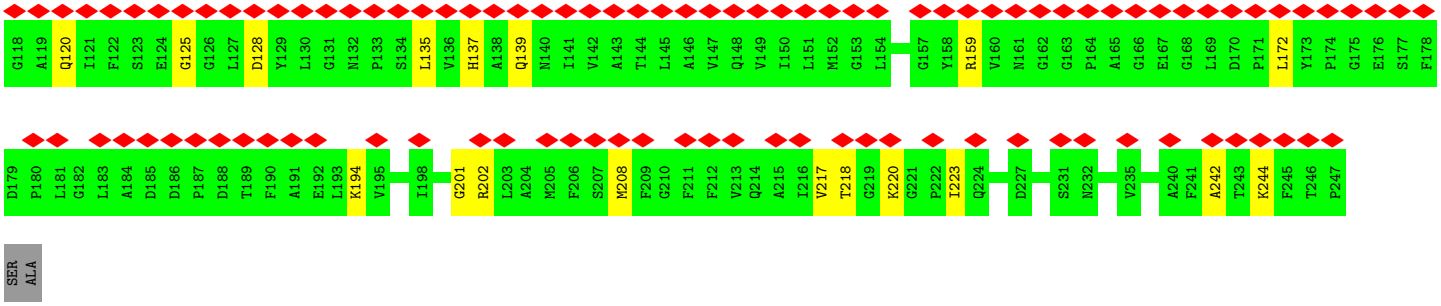
Chain 6:



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

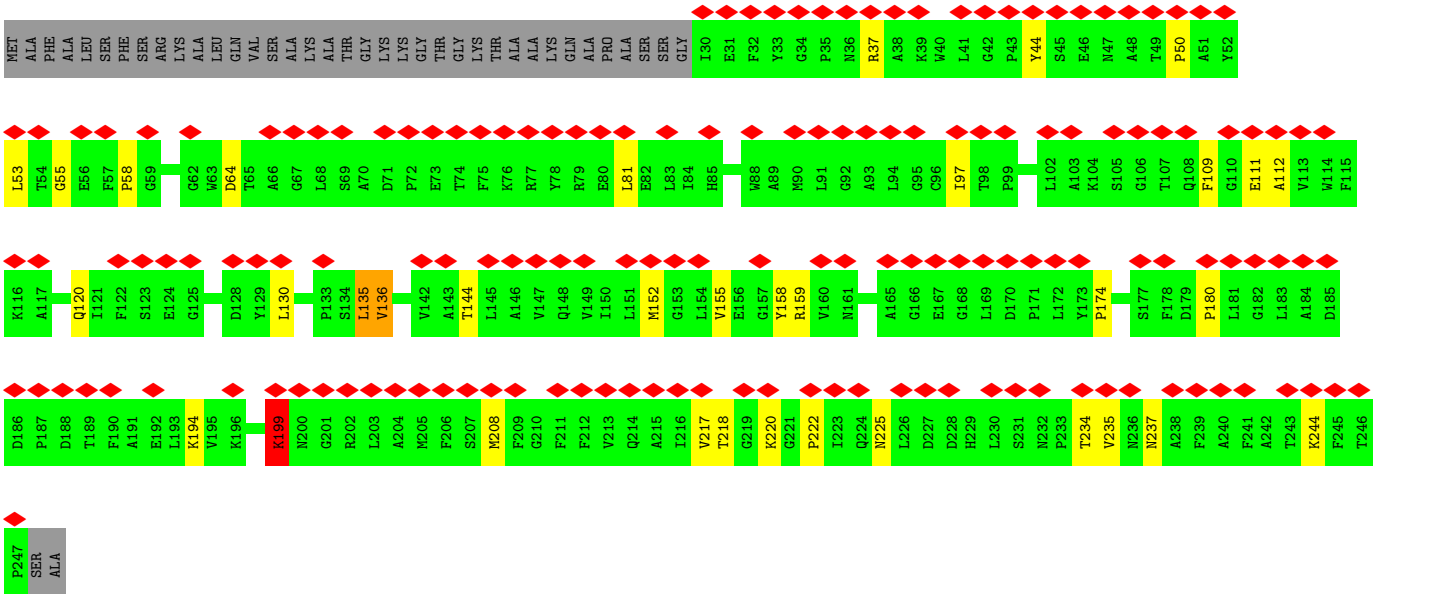
Chain v:





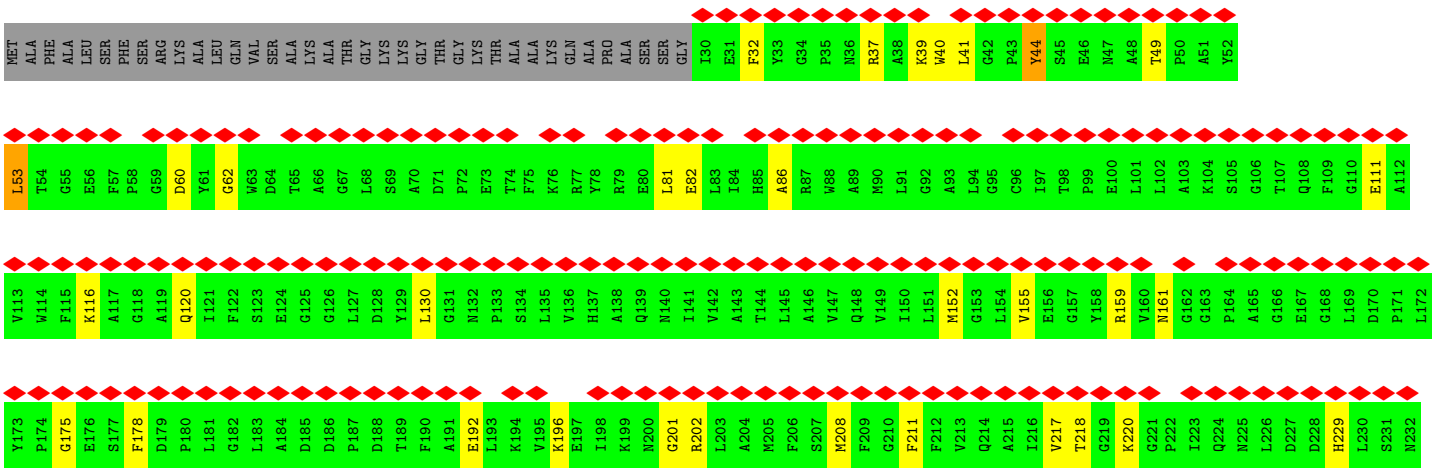
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

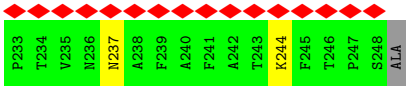
Chain p:



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

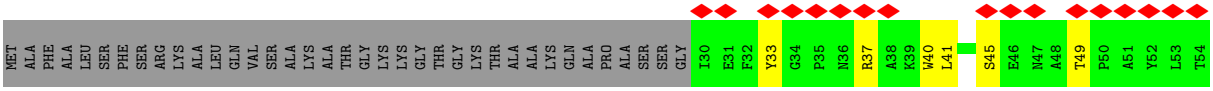
Chain q:

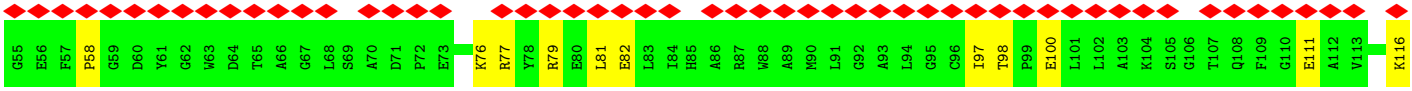


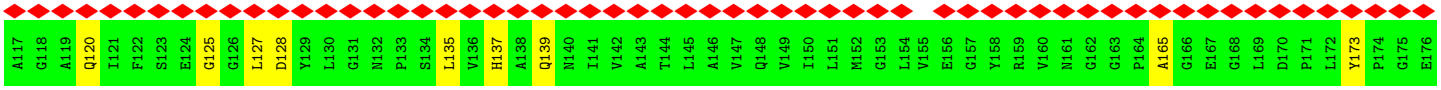


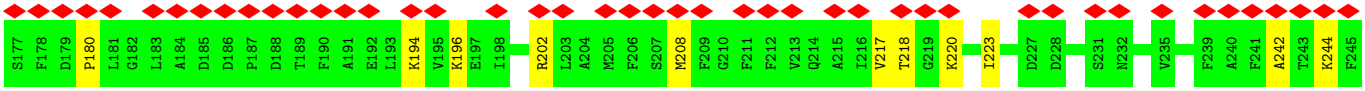
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain V:



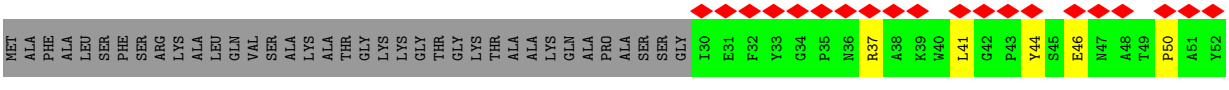


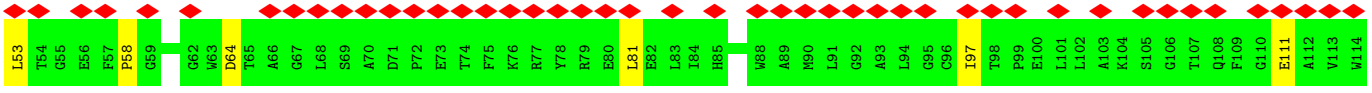


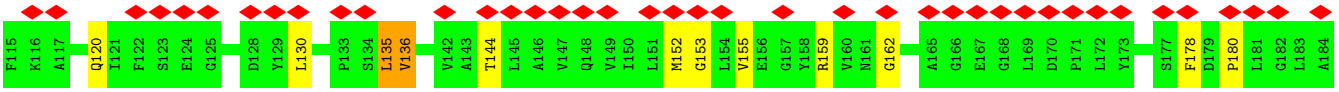


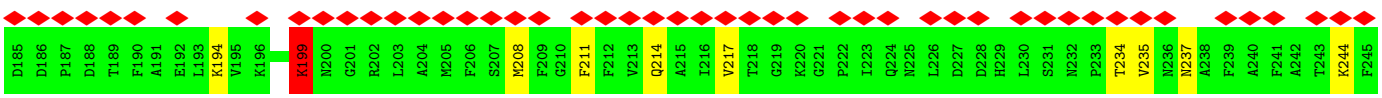
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain P:



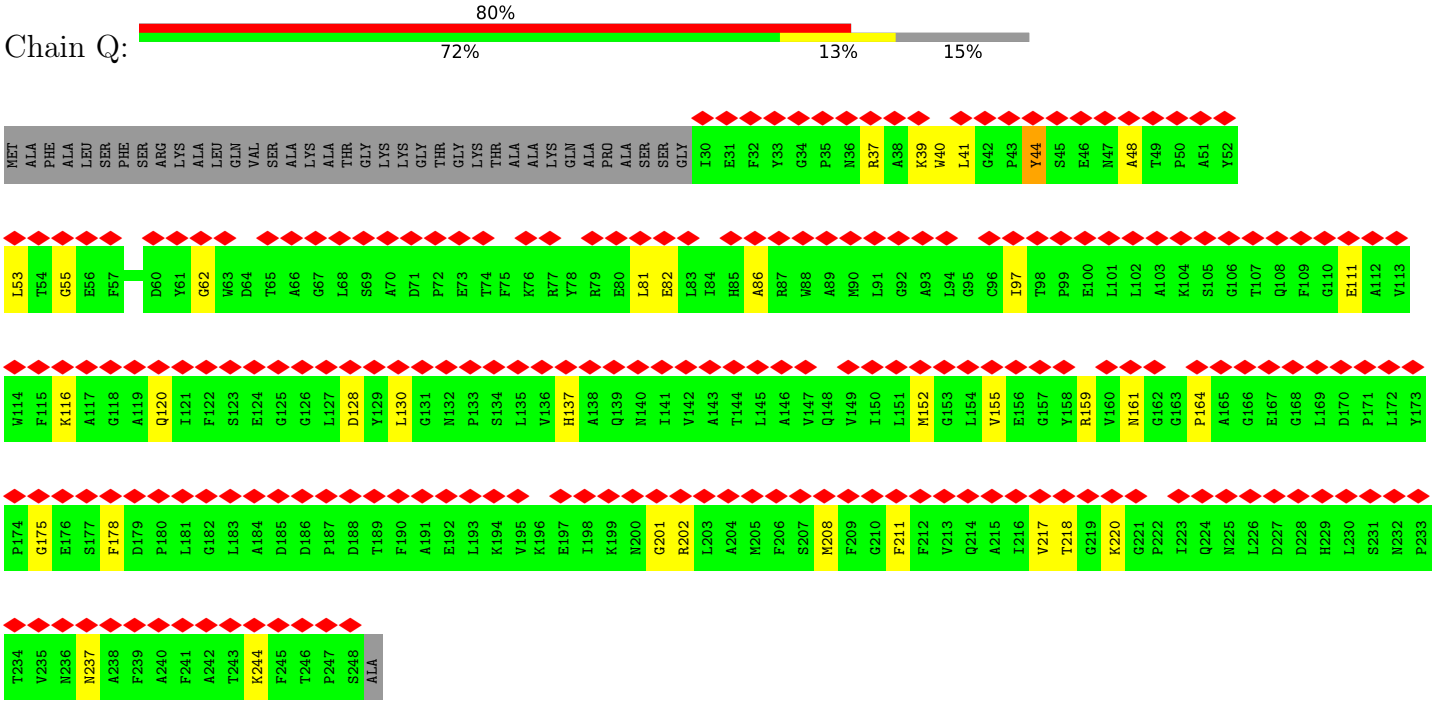






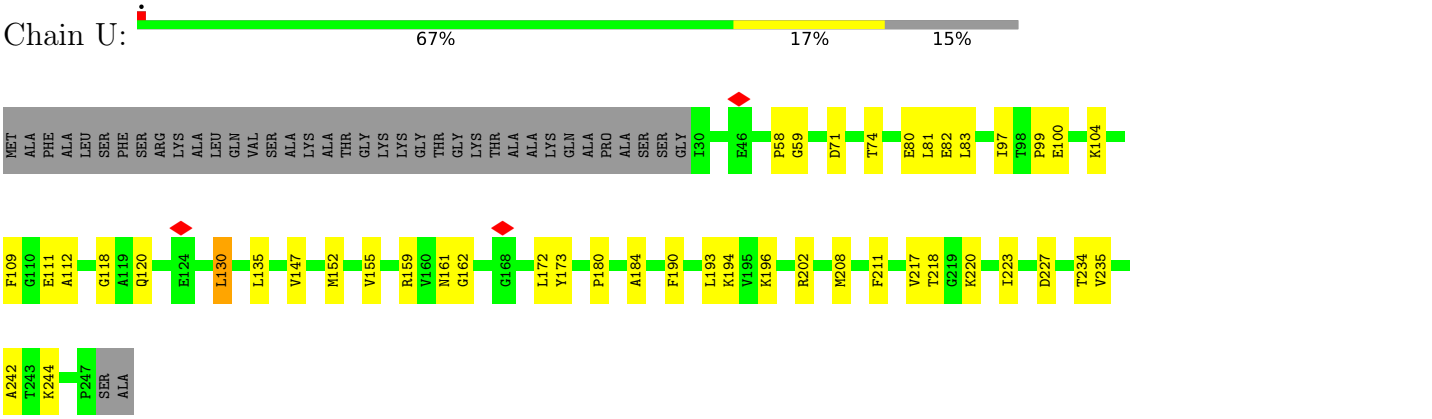
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain Q:



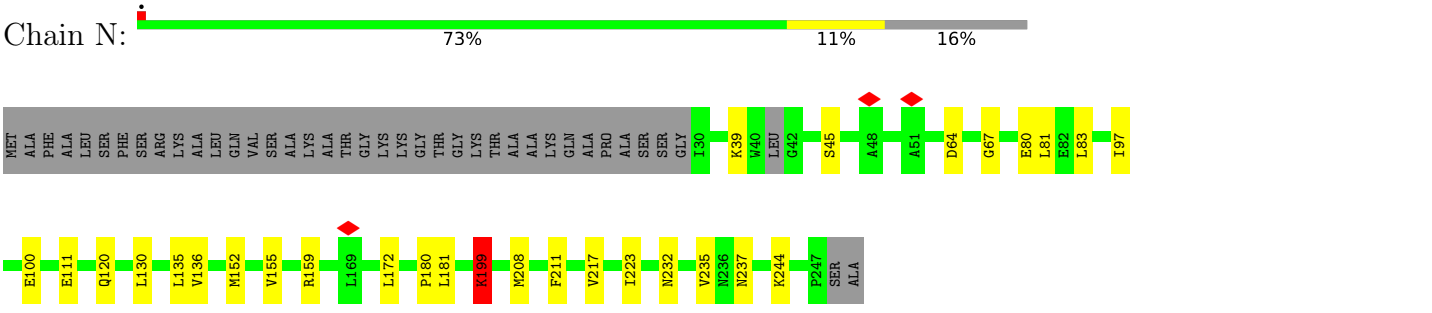
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain U:



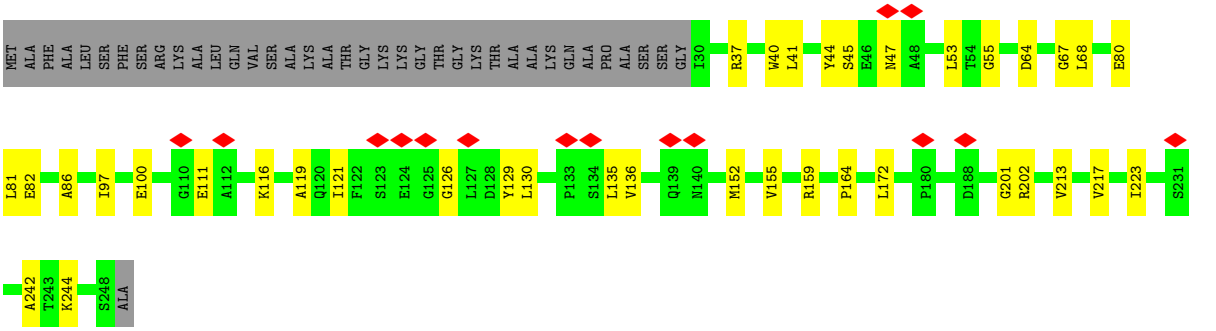
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain N:

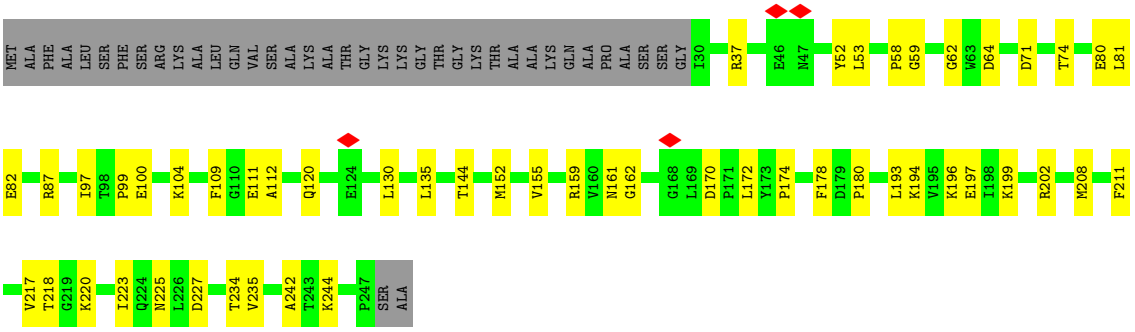


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

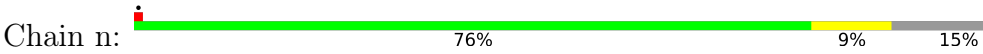
Chain G:

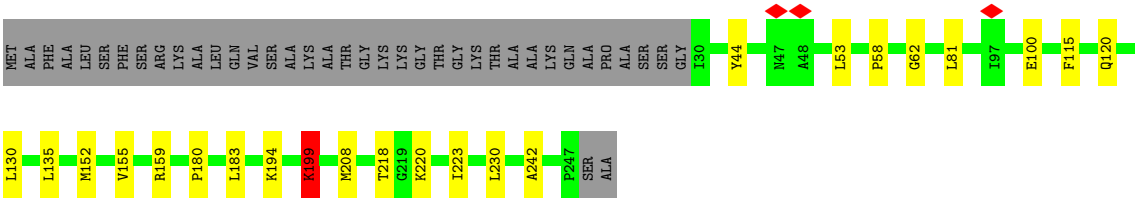


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

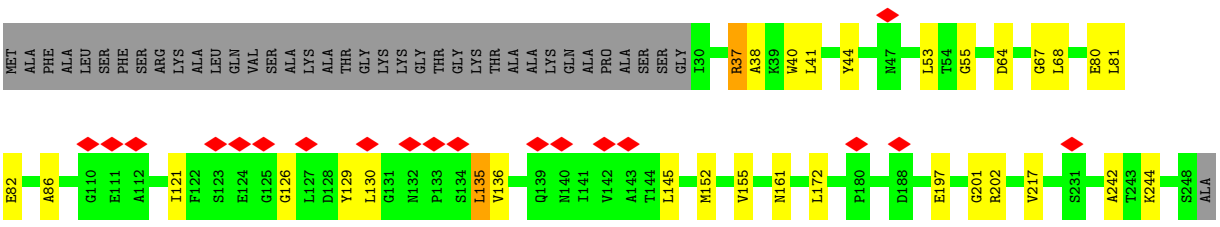


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

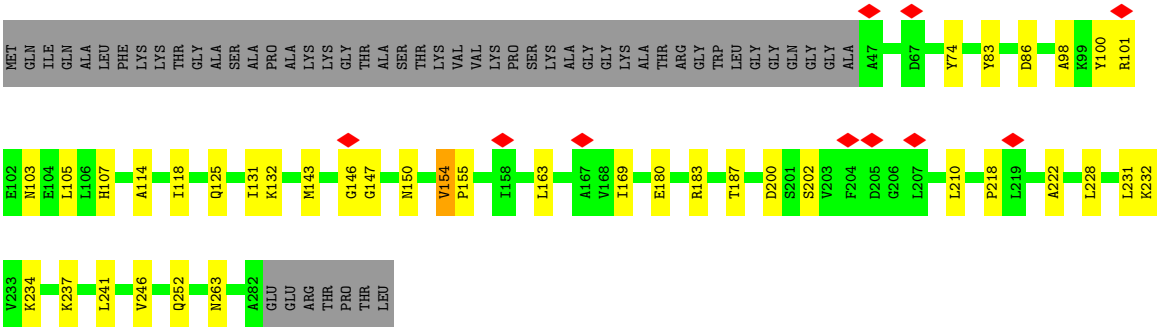




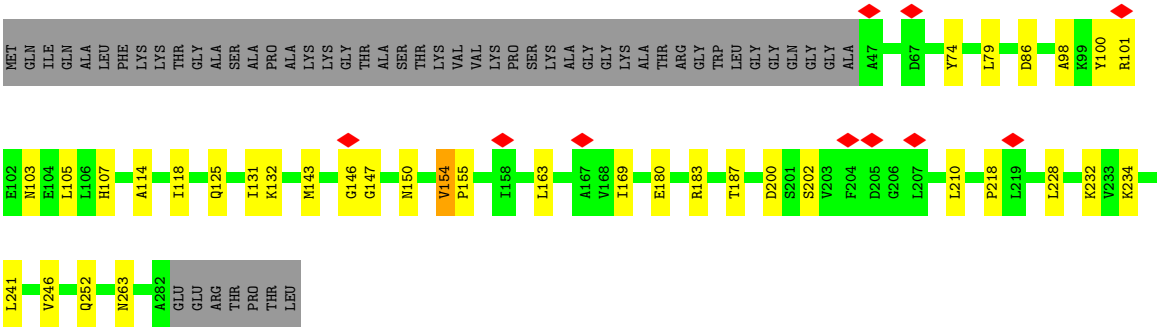
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



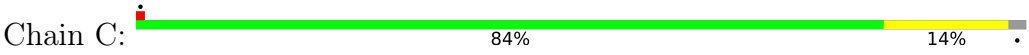
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

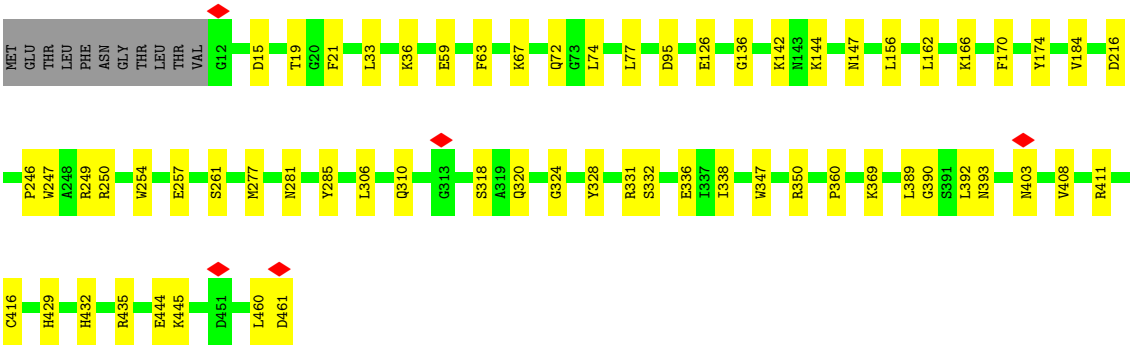


• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

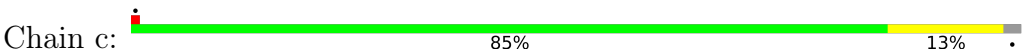


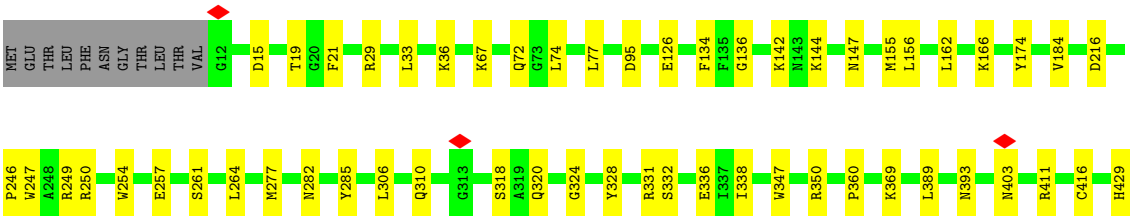
• Molecule 20: Photosystem II CP43 reaction center protein

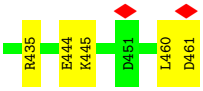




• Molecule 20: Photosystem II CP43 reaction center protein

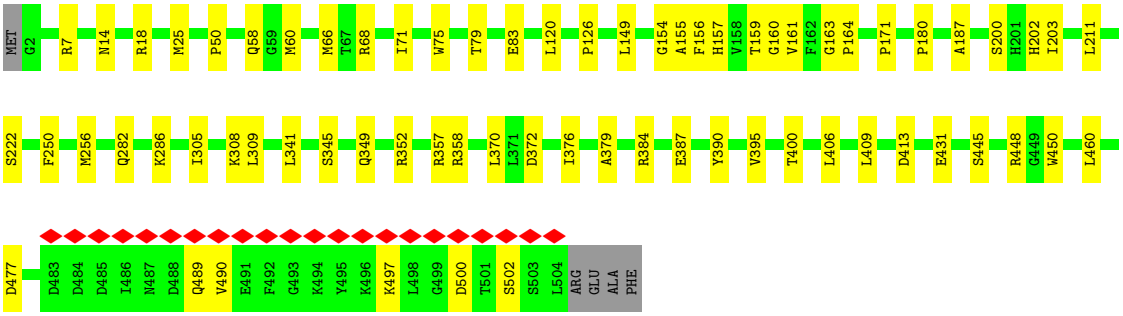






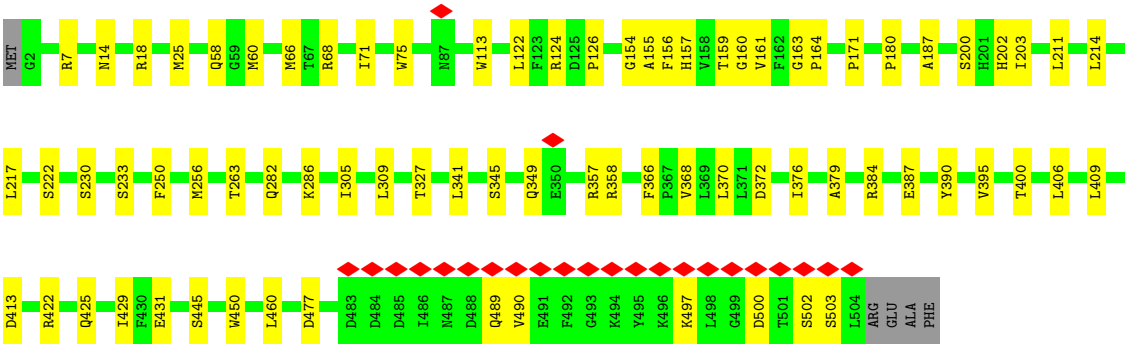
• Molecule 21: Photosystem II CP47 reaction center protein

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: HEM, PL9, SQD, PHO, NEX, XAT, BCT, LUT, CHL, DGD, LMG, BCR, CLA, LHG, FE2, CL

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	0.21	0/1736	0.56	0/2357
1	r	0.21	0/1739	0.57	0/2361
2	A	0.28	0/2696	0.51	0/3676
2	a	0.29	0/2696	0.53	0/3676
3	D	0.29	0/2808	0.61	0/3830
3	d	0.29	0/2808	0.61	0/3830
4	F	0.25	0/250	0.56	0/338
4	f	0.26	0/250	0.56	0/338
5	H	0.25	0/499	0.51	0/683
5	h	0.25	0/499	0.52	0/683
6	I	0.31	0/283	0.57	0/383
6	i	0.31	0/283	0.57	0/383
7	J	0.18	0/254	0.47	0/345
7	j	0.17	0/254	0.47	0/345
8	K	0.33	0/300	0.74	0/414
8	k	0.35	0/300	0.73	0/414
9	L	0.26	0/314	0.52	0/427
9	l	0.26	0/314	0.55	0/427
10	M	0.24	0/252	0.48	0/345
10	m	0.24	0/252	0.48	0/345
11	O	0.21	0/1620	0.53	0/2184
11	o	0.21	0/1620	0.53	0/2184
12	T	0.22	0/254	0.54	0/343
12	t	0.21	0/254	0.54	0/343
13	W	0.24	0/428	0.48	0/581
13	w	0.24	0/428	0.48	0/581
14	X	0.21	0/244	0.40	0/330
14	x	0.21	0/244	0.40	0/330
15	Z	0.19	0/476	0.41	0/654
15	z	0.19	0/476	0.41	0/654
16	Y	0.19	0/208	0.48	0/285
16	y	0.19	0/208	0.48	0/285

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	E	0.22	0/571	0.54	0/780
17	e	0.22	0/571	0.51	0/780
18	1	0.22	0/1717	0.55	0/2337
18	2	0.25	0/1717	0.63	3/2337 (0.1%)
18	3	0.20	0/1723	0.52	0/2345
18	4	0.22	0/1717	0.56	0/2337
18	5	0.24	0/1717	0.56	1/2337 (0.0%)
18	6	0.21	0/1723	0.54	0/2345
18	G	0.23	0/1723	0.56	0/2345
18	N	0.24	0/1708	0.55	1/2323 (0.0%)
18	P	0.22	0/1717	0.55	1/2337 (0.0%)
18	Q	0.20	0/1723	0.57	0/2345
18	U	0.25	0/1717	0.56	0/2337
18	V	0.21	0/1717	0.53	0/2337
18	g	0.23	0/1723	0.61	0/2345
18	n	0.23	0/1717	0.59	1/2337 (0.0%)
18	p	0.23	0/1717	0.57	1/2337 (0.0%)
18	q	0.21	0/1723	0.57	0/2345
18	u	0.26	0/1717	0.59	0/2337
18	v	0.22	0/1717	0.55	0/2337
19	S	0.25	0/1849	0.65	2/2521 (0.1%)
19	s	0.25	0/1849	0.66	2/2521 (0.1%)
20	C	0.26	0/3623	0.47	0/4936
20	c	0.26	0/3623	0.47	0/4936
21	B	0.23	0/4067	0.45	0/5533
21	b	0.23	0/4067	0.46	0/5533
All	All	0.24	0/76400	0.54	12/103994 (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 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	199	LYS	CD-CE-NZ	-6.37	91.50	111.90
18	5	199	LYS	CD-CE-NZ	-6.22	91.99	111.90
18	n	199	LYS	CD-CE-NZ	-5.93	92.92	111.90
18	p	199	LYS	CD-CE-NZ	-5.74	93.54	111.90
18	2	51	ALA	CA-C-N	5.30	131.65	121.54

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)

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1698	0	1653	34	0
1	r	1701	0	1656	31	0
2	A	2614	0	2516	41	0
2	a	2614	0	2516	38	0
3	D	2714	0	2596	40	0
3	d	2714	0	2596	38	0
4	F	243	0	252	4	0
4	f	243	0	252	4	0
5	H	488	0	515	9	0
5	h	488	0	515	9	0
6	I	275	0	287	1	0
6	i	275	0	287	1	0
7	J	245	0	236	5	0
7	j	245	0	236	5	0
8	K	288	0	295	1	0
8	k	288	0	295	2	0
9	L	306	0	313	7	0
9	l	306	0	313	6	0
10	M	248	0	266	4	0
10	m	248	0	266	4	0
11	O	1592	0	1592	25	0
11	o	1592	0	1592	22	0
12	T	247	0	260	6	0
12	t	247	0	260	7	0
13	W	417	0	387	1	0
13	w	417	0	387	2	0
14	X	242	0	266	1	0
14	x	242	0	266	1	0
15	Z	465	0	499	4	0
15	z	465	0	499	6	0
16	Y	208	0	239	2	0
16	y	208	0	239	2	0
17	E	555	0	550	6	0
17	e	555	0	550	7	0
18	1	1669	0	1612	21	0
18	2	1669	0	1612	16	0
18	3	1675	0	1616	22	0
18	4	1669	0	1612	28	0
18	5	1669	0	1612	22	0
18	6	1675	0	1616	23	0
18	G	1675	0	1617	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	1661	0	1600	19	0
18	P	1669	0	1612	26	0
18	Q	1675	0	1617	24	0
18	U	1669	0	1612	27	0
18	V	1669	0	1612	24	0
18	g	1675	0	1617	21	0
18	n	1669	0	1612	16	0
18	p	1669	0	1612	23	0
18	q	1675	0	1617	24	0
18	u	1669	0	1612	32	0
18	v	1669	0	1612	18	0
19	S	1797	0	1744	25	0
19	s	1797	0	1743	24	0
20	C	3502	0	3373	46	0
20	c	3502	0	3373	44	0
21	B	3937	0	3814	50	0
21	b	3937	0	3814	55	0
22	1	473	0	468	16	0
22	2	473	0	466	22	0
22	3	477	0	475	15	0
22	4	473	0	468	19	0
22	5	473	0	466	19	0
22	6	477	0	474	12	0
22	A	240	0	242	8	0
22	B	1040	0	1150	29	0
22	C	845	0	933	25	0
22	D	65	0	71	3	0
22	G	477	0	475	9	0
22	N	473	0	466	15	0
22	P	473	0	466	17	0
22	Q	477	0	475	14	0
22	R	543	0	489	14	0
22	S	465	0	391	10	0
22	U	473	0	468	11	0
22	V	473	0	468	16	0
22	X	65	0	70	1	0
22	a	240	0	242	6	0
22	b	1040	0	1149	33	0
22	c	845	0	933	23	0
22	d	65	0	71	2	0
22	g	477	0	474	5	0
22	n	473	0	466	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	p	473	0	466	14	0
22	q	477	0	474	10	0
22	r	543	0	487	19	0
22	s	465	0	391	13	0
22	u	473	0	468	14	0
22	v	473	0	468	14	0
22	x	65	0	70	0	0
23	1	84	0	112	5	0
23	2	84	0	112	8	0
23	4	84	0	112	9	0
23	5	84	0	112	14	0
23	N	84	0	112	9	0
23	P	84	0	112	7	0
23	R	42	0	56	2	0
23	S	84	0	112	9	0
23	U	84	0	112	4	0
23	V	84	0	112	11	0
23	n	84	0	112	7	0
23	p	84	0	112	5	0
23	r	42	0	55	4	0
23	s	84	0	111	10	0
23	u	84	0	112	6	0
23	v	84	0	112	7	0
24	1	44	0	56	2	0
24	2	44	0	56	5	0
24	3	44	0	56	2	0
24	4	44	0	56	1	0
24	5	44	0	56	3	0
24	6	44	0	56	4	0
24	G	44	0	56	3	0
24	N	44	0	56	2	0
24	P	44	0	56	4	0
24	Q	44	0	56	0	0
24	R	44	0	56	3	0
24	U	44	0	56	5	0
24	V	44	0	56	4	0
24	g	44	0	56	5	0
24	n	44	0	56	1	0
24	p	44	0	56	3	0
24	q	44	0	56	1	0
24	r	44	0	56	4	0
24	u	44	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	v	44	0	56	3	0
25	1	49	0	74	0	0
25	2	49	0	74	3	0
25	3	49	0	74	3	0
25	4	49	0	74	1	0
25	5	49	0	74	1	0
25	6	49	0	74	3	0
25	A	43	0	56	3	0
25	B	96	0	139	0	0
25	C	147	0	222	5	0
25	D	95	0	138	11	0
25	G	49	0	74	0	0
25	L	49	0	74	2	0
25	N	49	0	74	4	0
25	P	49	0	74	1	0
25	Q	49	0	74	4	0
25	R	42	0	57	0	0
25	S	49	0	71	5	0
25	U	49	0	74	4	0
25	V	49	0	74	6	0
25	a	43	0	56	1	0
25	b	96	0	139	0	0
25	c	147	0	222	7	0
25	d	95	0	138	12	0
25	g	49	0	74	2	0
25	l	49	0	74	1	0
25	n	49	0	74	1	0
25	p	49	0	74	2	0
25	q	49	0	74	2	0
25	r	42	0	57	1	0
25	s	49	0	71	3	0
25	u	49	0	74	2	0
25	v	49	0	74	4	0
26	1	362	0	347	10	0
26	2	362	0	349	12	0
26	3	357	0	335	16	0
26	4	296	0	277	11	0
26	5	362	0	349	12	0
26	6	423	0	405	20	0
26	G	357	0	335	13	0
26	N	296	0	280	12	0
26	P	362	0	349	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Q	357	0	335	9	0
26	R	183	0	174	5	0
26	S	196	0	141	4	0
26	U	380	0	384	17	0
26	V	362	0	347	15	0
26	g	357	0	335	12	0
26	n	362	0	349	13	0
26	p	428	0	419	12	0
26	q	291	0	265	13	0
26	r	231	0	207	7	0
26	s	196	0	141	2	0
26	u	362	0	347	11	0
26	v	362	0	347	14	0
27	2	44	0	56	1	0
27	5	44	0	56	2	0
27	N	44	0	56	2	0
27	P	44	0	54	1	0
27	R	44	0	54	3	0
27	S	44	0	55	3	0
27	U	44	0	56	0	0
27	V	44	0	56	3	0
27	n	44	0	56	2	0
27	p	44	0	54	4	0
27	r	88	0	110	7	0
27	s	44	0	55	4	0
27	u	88	0	112	3	0
27	v	44	0	56	2	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	2	0	0	2	0
29	a	2	0	0	4	0
30	A	64	0	74	4	0
30	D	64	0	74	1	0
30	a	64	0	74	2	0
30	d	64	0	74	1	0
31	A	40	0	56	4	0
31	B	120	0	168	11	0
31	C	120	0	168	4	0
31	D	40	0	55	1	0
31	K	40	0	56	2	0
31	T	40	0	56	5	0
31	X	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	a	40	0	56	3	0
31	b	120	0	168	12	0
31	c	80	0	112	1	0
31	d	40	0	55	0	0
31	k	40	0	56	2	0
31	t	40	0	56	6	0
31	x	40	0	56	3	0
31	z	40	0	56	2	0
32	A	54	0	77	3	0
32	C	50	0	66	2	0
32	L	54	0	76	2	0
32	M	42	0	48	1	0
32	a	104	0	143	6	0
32	l	54	0	76	3	0
32	m	42	0	48	1	0
33	A	13	0	7	0	0
33	D	55	0	80	3	0
33	a	13	0	7	0	0
33	d	55	0	80	3	0
34	A	40	0	50	1	0
34	B	106	0	157	4	0
34	C	102	0	144	4	0
34	D	46	0	61	0	0
34	W	48	0	66	2	0
34	a	40	0	50	1	0
34	b	106	0	157	5	0
34	c	102	0	144	3	0
34	d	46	0	61	0	0
34	w	48	0	66	2	0
35	D	4	0	1	1	0
35	a	4	0	1	1	0
36	A	59	0	76	2	0
36	B	62	0	80	6	0
36	C	117	0	150	7	0
36	J	60	0	78	2	0
36	a	59	0	76	2	0
36	b	62	0	80	7	0
36	c	177	0	228	8	0
37	E	43	0	30	1	0
37	e	43	0	30	1	0
All	All	104363	0	104847	1605	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1605 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:v:208:MET:HE2	23:v:310:LUT:H10	1.67	0.74
11:o:125:MET:SD	11:o:163:GLN:NE2	2.61	0.73
11:O:125:MET:SD	11:O:163:GLN:NE2	2.62	0.73
18:V:208:MET:HE2	23:V:310:LUT:H10	1.72	0.72
22:2:304:CLA:H52	23:2:309:LUT:H30	1.71	0.71

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	24	56
18	2	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	24	56
18	3	217/257 (84%)	191 (88%)	26 (12%)	0	100	100
18	4	216/257 (84%)	189 (88%)	26 (12%)	1 (0%)	24	56
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%)	24	56
18	P	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	24	56
18	Q	217/257 (84%)	184 (85%)	33 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	45
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
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%)	49	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%)	175 (100%)	0	100	100
1	r	176/218 (81%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	272/289 (94%)	272 (100%)	0	100	100
2	a	272/289 (94%)	272 (100%)	0	100	100
3	D	272/281 (97%)	270 (99%)	2 (1%)	76	77
3	d	272/281 (97%)	270 (99%)	2 (1%)	76	77
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%)	54 (98%)	1 (2%)	51	66
5	h	55/75 (73%)	54 (98%)	1 (2%)	51	66
6	I	31/34 (91%)	30 (97%)	1 (3%)	34	56
6	i	31/34 (91%)	30 (97%)	1 (3%)	34	56
7	J	24/42 (57%)	24 (100%)	0	100	100
7	j	24/42 (57%)	24 (100%)	0	100	100
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%)	174 (100%)	0	100	100
11	o	174/223 (78%)	174 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	e	60/71 (84%)	60 (100%)	0	100	100
18	1	169/194 (87%)	168 (99%)	1 (1%)	78	79
18	2	169/194 (87%)	166 (98%)	3 (2%)	51	66
18	3	170/194 (88%)	168 (99%)	2 (1%)	63	71
18	4	169/194 (87%)	168 (99%)	1 (1%)	78	79
18	5	169/194 (87%)	166 (98%)	3 (2%)	51	66
18	6	170/194 (88%)	169 (99%)	1 (1%)	78	79
18	G	170/194 (88%)	168 (99%)	2 (1%)	63	71
18	N	168/194 (87%)	165 (98%)	3 (2%)	51	66
18	P	169/194 (87%)	166 (98%)	3 (2%)	51	66
18	Q	170/194 (88%)	168 (99%)	2 (1%)	63	71
18	U	169/194 (87%)	167 (99%)	2 (1%)	63	71
18	V	169/194 (87%)	168 (99%)	1 (1%)	78	79
18	g	170/194 (88%)	167 (98%)	3 (2%)	51	66
18	n	169/194 (87%)	167 (99%)	2 (1%)	63	71
18	p	169/194 (87%)	166 (98%)	3 (2%)	51	66
18	q	170/194 (88%)	168 (99%)	2 (1%)	63	71
18	u	169/194 (87%)	167 (99%)	2 (1%)	63	71
18	v	169/194 (87%)	168 (99%)	1 (1%)	78	79
19	S	181/217 (83%)	180 (99%)	1 (1%)	78	79
19	s	181/217 (83%)	180 (99%)	1 (1%)	78	79
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%)	403 (100%)	0	100	100
21	b	403/407 (99%)	403 (100%)	0	100	100
All	All	7618/8732 (87%)	7571 (99%)	47 (1%)	76	79

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	Q	130	LEU
18	G	130	LEU
18	U	97	ILE

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Mol	Chain	Res	Type
18	N	130	LEU
18	u	130	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	239	GLN
3	D	350	ASN
20	c	320	GLN
18	6	236	ASN
18	6	120	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
22	CLA	b	614	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	5	308	-	52,56,73	1.32	7 (13%)	61,92,113	1.42	5 (8%)
26	CHL	V	315	-	44,58,74	3.99	19 (43%)	37,94,114	2.19	10 (27%)
26	CHL	V	313	-	60,74,74	3.41	19 (31%)	58,114,114	2.08	13 (22%)
26	CHL	N	317	-	60,74,74	3.36	19 (31%)	58,114,114	1.94	14 (24%)
25	LHG	s	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.15	3 (5%)
31	BCR	z	101	-	41,41,41	4.90	24 (58%)	56,56,56	2.37	19 (33%)
22	CLA	B	616	-	69,73,73	1.17	7 (10%)	82,113,113	1.35	6 (7%)
22	CLA	6	307	22	64,68,73	1.21	7 (10%)	76,107,113	1.32	5 (6%)
22	CLA	V	304	-	64,68,73	1.19	8 (12%)	76,107,113	1.37	8 (10%)
26	CHL	G	311	-	60,74,74	3.35	20 (33%)	58,114,114	2.31	15 (25%)
22	CLA	4	302	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	n	302	-	69,73,73	1.19	8 (11%)	82,113,113	1.29	6 (7%)
23	LUT	p	311	-	42,43,43	0.75	0	51,60,60	1.58	12 (23%)
25	LHG	b	623	-	48,48,48	0.91	4 (8%)	51,54,54	1.07	2 (3%)
26	CHL	v	317	-	60,74,74	3.39	18 (30%)	58,114,114	2.56	16 (27%)
26	CHL	g	311	-	60,74,74	3.38	20 (33%)	58,114,114	2.03	14 (24%)
22	CLA	b	612	-	69,73,73	1.16	9 (13%)	82,113,113	1.42	7 (8%)
25	LHG	q	310	-	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
22	CLA	b	608	-	69,73,73	1.15	8 (11%)	82,113,113	1.38	7 (8%)
22	CLA	G	308	-	52,56,73	1.33	8 (15%)	61,92,113	1.45	6 (9%)
22	CLA	4	308	-	52,56,73	1.32	9 (17%)	61,92,113	1.44	5 (8%)
22	CLA	U	305	-	64,68,73	1.19	9 (14%)	76,107,113	1.30	4 (5%)
26	CHL	v	315	-	44,58,74	3.97	19 (43%)	37,94,114	2.33	10 (27%)
26	CHL	R	316	-	50,64,74	3.71	19 (38%)	46,102,114	2.28	13 (28%)
22	CLA	1	308	-	52,56,73	1.31	9 (17%)	61,92,113	1.43	5 (8%)
25	LHG	c	523	-	48,48,48	0.91	4 (8%)	51,54,54	1.13	2 (3%)
23	LUT	v	309	-	42,43,43	0.78	0	51,60,60	1.69	12 (23%)
26	CHL	P	318	-	60,74,74	3.26	19 (31%)	58,114,114	2.08	14 (24%)
22	CLA	b	602	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
26	CHL	6	314	-	44,58,74	3.98	19 (43%)	37,94,114	2.25	12 (32%)
22	CLA	v	302	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
26	CHL	r	619	-	42,56,74	3.95	19 (45%)	36,92,114	2.62	13 (36%)
22	CLA	v	307	-	69,73,73	1.14	9 (13%)	82,113,113	1.34	6 (7%)
26	CHL	P	314	18	60,74,74	3.41	19 (31%)	58,114,114	1.98	14 (24%)
22	CLA	B	612	-	69,73,73	1.17	9 (13%)	82,113,113	1.42	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	1	304	-	64,68,73	1.19	10 (15%)	76,107,113	1.35	5 (6%)
31	BCR	k	101	-	41,41,41	4.86	25 (60%)	56,56,56	2.57	20 (35%)
22	CLA	P	309	-	52,56,73	1.32	8 (15%)	61,92,113	1.43	5 (8%)
22	CLA	B	608	-	69,73,73	1.14	8 (11%)	82,113,113	1.37	7 (8%)
23	LUT	S	311	-	42,43,43	0.71	0	51,60,60	1.79	20 (39%)
24	XAT	U	311	-	41,47,47	2.65	19 (46%)	54,74,74	9.91	22 (40%)
27	NEX	s	317	-	40,46,46	0.98	3 (7%)	50,70,70	2.26	17 (34%)
22	CLA	5	304	-	69,73,73	1.15	9 (13%)	82,113,113	1.39	8 (9%)
26	CHL	N	314	-	42,56,74	4.12	18 (42%)	36,92,114	2.33	14 (38%)
22	CLA	4	306	-	64,68,73	1.22	8 (12%)	76,107,113	1.32	6 (7%)
22	CLA	C	514	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	5 (6%)
26	CHL	6	301	-	60,74,74	3.35	19 (31%)	58,114,114	1.98	17 (29%)
36	DGD	B	601	-	63,63,67	1.24	7 (11%)	77,77,81	1.08	3 (3%)
23	LUT	U	310	-	42,43,43	0.77	0	51,60,60	1.68	10 (19%)
22	CLA	r	608	-	53,57,73	1.31	8 (15%)	61,93,113	1.45	7 (11%)
22	CLA	N	307	-	64,68,73	1.20	9 (14%)	76,107,113	1.36	5 (6%)
22	CLA	C	506	-	69,73,73	1.15	8 (11%)	82,113,113	1.33	4 (4%)
36	DGD	c	519	-	61,61,67	1.26	6 (9%)	75,75,81	1.18	3 (4%)
26	CHL	4	316	-	60,74,74	3.35	18 (30%)	58,114,114	2.35	16 (27%)
22	CLA	P	302	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
22	CLA	R	308	-	53,57,73	1.30	7 (13%)	61,93,113	1.52	6 (9%)
22	CLA	S	301	-	65,69,73	1.16	9 (13%)	77,108,113	1.36	10 (12%)
22	CLA	d	402	-	69,73,73	1.16	10 (14%)	82,113,113	1.27	5 (6%)
22	CLA	g	302	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
22	CLA	B	606	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	5 (6%)
25	LHG	d	406	-	48,48,48	0.91	4 (8%)	51,54,54	1.08	3 (5%)
22	CLA	4	304	-	64,68,73	1.19	10 (15%)	76,107,113	1.35	5 (6%)
22	CLA	1	305	-	64,68,73	1.19	7 (10%)	76,107,113	1.36	7 (9%)
22	CLA	u	304	-	64,68,73	1.19	9 (14%)	76,107,113	1.38	7 (9%)
22	CLA	G	302	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
31	BCR	x	202	-	41,41,41	4.92	24 (58%)	56,56,56	2.28	17 (30%)
23	LUT	u	310	-	42,43,43	0.76	0	51,60,60	1.67	11 (21%)
22	CLA	R	302	27	53,57,73	1.35	8 (15%)	61,93,113	1.48	6 (9%)
22	CLA	4	305	-	64,68,73	1.20	10 (15%)	76,107,113	1.32	6 (7%)
22	CLA	b	607	-	69,73,73	1.16	8 (11%)	82,113,113	1.39	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	BCR	C	516	-	41,41,41	4.90	24 (58%)	56,56,56	2.34	19 (33%)
26	CHL	p	314	18	60,74,74	3.38	19 (31%)	58,114,114	2.12	16 (27%)
26	CHL	u	318	-	60,74,74	3.35	19 (31%)	58,114,114	2.20	14 (24%)
25	LHG	5	312	-	48,48,48	0.91	4 (8%)	51,54,54	1.08	3 (5%)
22	CLA	a	405	-	69,73,73	1.17	9 (13%)	82,113,113	1.37	8 (9%)
26	CHL	n	317	-	60,74,74	3.35	19 (31%)	58,114,114	2.10	15 (25%)
22	CLA	3	304	-	68,72,73	1.17	9 (13%)	80,111,113	1.36	8 (10%)
26	CHL	g	314	-	60,74,74	3.45	19 (31%)	58,114,114	1.78	13 (22%)
26	CHL	2	317	-	60,74,74	3.31	19 (31%)	58,114,114	2.26	16 (27%)
26	CHL	S	315	-	52,66,74	3.72	20 (38%)	48,104,114	2.02	11 (22%)
22	CLA	B	613	-	69,73,73	1.17	10 (14%)	82,113,113	1.34	10 (12%)
35	BCT	a	414	-	3,3,3	2.66	1 (33%)	2,3,3	0.15	0
22	CLA	V	305	-	64,68,73	1.20	9 (14%)	76,107,113	1.37	6 (7%)
26	CHL	S	316	-	40,54,74	4.19	19 (47%)	34,90,114	2.29	9 (26%)
22	CLA	u	305	-	64,68,73	1.19	9 (14%)	76,107,113	1.29	5 (6%)
22	CLA	b	610	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
22	CLA	D	403	-	69,73,73	1.16	10 (14%)	82,113,113	1.27	5 (6%)
23	LUT	r	611	-	42,43,43	0.70	0	51,60,60	1.77	13 (25%)
22	CLA	U	303	-	54,58,73	1.31	8 (14%)	64,95,113	1.40	6 (9%)
22	CLA	6	306	22	64,68,73	1.20	8 (12%)	76,107,113	1.40	9 (11%)
26	CHL	g	313	-	44,58,74	3.97	19 (43%)	37,94,114	2.40	12 (32%)
36	DGD	b	601	-	63,63,67	1.24	8 (12%)	77,77,81	1.06	3 (3%)
23	LUT	n	309	-	42,43,43	0.70	0	51,60,60	1.81	13 (25%)
22	CLA	r	607	-	53,57,73	1.31	7 (13%)	61,93,113	1.51	7 (11%)
24	XAT	G	309	-	41,47,47	2.67	19 (46%)	54,74,74	9.83	23 (42%)
22	CLA	n	306	-	64,68,73	1.19	6 (9%)	76,107,113	1.38	7 (9%)
25	LHG	2	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.10	2 (3%)
25	LHG	C	523	-	48,48,48	0.91	3 (6%)	51,54,54	1.08	2 (3%)
22	CLA	B	614	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	7 (8%)
22	CLA	r	610	-	49,53,73	1.39	9 (18%)	58,89,113	1.49	4 (6%)
22	CLA	c	506	-	69,73,73	1.14	8 (11%)	82,113,113	1.48	9 (10%)
22	CLA	4	303	-	54,58,73	1.30	10 (18%)	64,95,113	1.40	7 (10%)
25	LHG	p	313	-	48,48,48	0.91	4 (8%)	51,54,54	1.04	2 (3%)
26	CHL	s	314	-	40,54,74	4.13	18 (45%)	34,90,114	2.68	11 (32%)
22	CLA	C	509	-	69,73,73	1.15	7 (10%)	82,113,113	1.41	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	HEM	e	101	4	50,50,50	1.46	8 (16%)	67,82,82	1.12	3 (4%)
22	CLA	n	307	-	64,68,73	1.20	9 (14%)	76,107,113	1.35	5 (6%)
23	LUT	s	310	-	42,43,43	0.75	0	51,60,60	1.90	15 (29%)
22	CLA	G	301	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	7 (8%)
22	CLA	s	302	-	49,53,73	1.39	7 (14%)	58,89,113	1.48	5 (8%)
22	CLA	C	508	-	69,73,73	1.17	7 (10%)	82,113,113	1.34	5 (6%)
26	CHL	V	316	-	60,74,74	3.38	19 (31%)	58,114,114	1.73	14 (24%)
22	CLA	x	201	-	69,73,73	1.14	10 (14%)	82,113,113	1.37	8 (9%)
22	CLA	3	305	22	64,68,73	1.19	9 (14%)	76,107,113	1.41	8 (10%)
22	CLA	v	306	-	64,68,73	1.21	8 (12%)	76,107,113	1.35	8 (10%)
31	BCR	C	517	-	41,41,41	4.83	24 (58%)	56,56,56	2.72	24 (42%)
26	CHL	4	315	-	44,58,74	3.92	19 (43%)	37,94,114	2.27	11 (29%)
22	CLA	6	308	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	6 (7%)
22	CLA	b	604	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
34	LMG	C	521	-	51,51,55	1.22	6 (11%)	59,59,63	1.08	2 (3%)
22	CLA	R	307	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
22	CLA	v	303	-	54,58,73	1.31	8 (14%)	64,95,113	1.46	4 (6%)
24	XAT	r	612	-	41,47,47	2.67	18 (43%)	54,74,74	9.55	27 (50%)
22	CLA	S	305	-	59,63,73	1.25	8 (13%)	70,101,113	1.36	7 (10%)
26	CHL	1	315	-	44,58,74	3.91	19 (43%)	37,94,114	2.32	11 (29%)
27	NEX	v	319	-	40,46,46	1.01	3 (7%)	50,70,70	2.31	15 (30%)
22	CLA	P	306	-	64,68,73	1.18	8 (12%)	76,107,113	1.88	10 (13%)
22	CLA	2	307	-	64,68,73	1.19	9 (14%)	76,107,113	1.38	5 (6%)
34	LMG	d	407	-	46,46,55	1.27	6 (13%)	54,54,63	1.01	2 (3%)
36	DGD	c	517	-	56,56,67	1.32	9 (16%)	70,70,81	1.20	5 (7%)
32	SQD	m	101	-	40,42,54	1.07	3 (7%)	50,53,65	1.67	10 (20%)
31	BCR	B	619	-	41,41,41	4.88	25 (60%)	56,56,56	2.30	22 (39%)
26	CHL	5	317	-	60,74,74	3.31	19 (31%)	58,114,114	2.23	15 (25%)
22	CLA	p	309	-	52,56,73	1.32	8 (15%)	61,92,113	1.43	5 (8%)
22	CLA	G	305	22	64,68,73	1.19	8 (12%)	76,107,113	1.43	7 (9%)
22	CLA	B	617	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	8 (9%)
25	LHG	3	310	-	48,48,48	0.91	4 (8%)	51,54,54	1.11	2 (3%)
22	CLA	C	513	-	69,73,73	1.18	10 (14%)	82,113,113	1.40	8 (9%)
25	LHG	b	622	-	46,46,48	0.92	4 (8%)	49,52,54	1.05	2 (4%)
22	CLA	r	606	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CHL	s	315	-	52,66,74	3.72	20 (38%)	48,104,114	2.01	11 (22%)
26	CHL	5	315	-	44,58,74	3.93	19 (43%)	37,94,114	2.55	10 (27%)
22	CLA	B	604	-	69,73,73	1.14	9 (13%)	82,113,113	1.30	6 (7%)
22	CLA	g	306	22	64,68,73	1.21	7 (10%)	76,107,113	1.26	4 (5%)
22	CLA	Q	304	-	68,72,73	1.18	8 (11%)	80,111,113	1.38	8 (10%)
26	CHL	r	615	-	50,64,74	3.70	19 (38%)	46,102,114	2.24	12 (26%)
36	DGD	c	518	-	63,63,67	1.24	6 (9%)	77,77,81	1.15	5 (6%)
26	CHL	p	317	-	60,74,74	3.36	19 (31%)	58,114,114	1.93	13 (22%)
22	CLA	R	306	-	62,66,73	1.22	8 (12%)	73,104,113	1.40	5 (6%)
26	CHL	4	317	-	60,74,74	3.34	19 (31%)	58,114,114	2.22	14 (24%)
22	CLA	c	513	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
24	XAT	R	313	-	41,47,47	2.68	18 (43%)	54,74,74	9.58	24 (44%)
26	CHL	n	313	18	60,74,74	3.37	19 (31%)	58,114,114	2.09	14 (24%)
36	DGD	a	416	-	60,60,67	1.28	7 (11%)	74,74,81	1.25	6 (8%)
22	CLA	r	601	27	53,57,73	1.35	9 (16%)	61,93,113	1.49	6 (9%)
22	CLA	s	303	-	54,58,73	1.31	8 (14%)	64,95,113	1.45	8 (12%)
26	CHL	6	316	-	60,74,74	3.37	19 (31%)	58,114,114	2.08	13 (22%)
26	CHL	1	317	-	60,74,74	3.33	18 (30%)	58,114,114	2.47	16 (27%)
26	CHL	P	316	-	44,58,74	3.97	19 (43%)	37,94,114	2.31	10 (27%)
31	BCR	t	101	-	41,41,41	4.92	25 (60%)	56,56,56	2.40	21 (37%)
22	CLA	R	311	-	49,53,73	1.38	9 (18%)	58,89,113	1.49	4 (6%)
22	CLA	q	301	-	69,73,73	1.18	9 (13%)	82,113,113	1.28	6 (7%)
26	CHL	N	316	-	60,74,74	3.29	19 (31%)	58,114,114	2.20	15 (25%)
31	BCR	B	618	-	41,41,41	4.88	24 (58%)	56,56,56	2.49	23 (41%)
26	CHL	q	315	-	55,69,74	3.54	19 (34%)	52,108,114	2.08	15 (28%)
31	BCR	K	101	-	41,41,41	4.86	25 (60%)	56,56,56	2.58	20 (35%)
22	CLA	g	308	-	52,56,73	1.33	9 (17%)	61,92,113	1.43	5 (8%)
22	CLA	a	406	-	54,58,73	1.31	9 (16%)	64,95,113	1.42	5 (7%)
22	CLA	U	302	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	5 (6%)
24	XAT	5	311	-	41,47,47	2.72	19 (46%)	54,74,74	9.91	21 (38%)
26	CHL	3	312	-	42,56,74	4.26	19 (45%)	36,92,114	2.20	12 (33%)
23	LUT	1	309	-	42,43,43	0.70	0	51,60,60	1.65	13 (25%)
22	CLA	C	511	-	69,73,73	1.13	8 (11%)	82,113,113	1.37	10 (12%)
26	CHL	3	313	-	44,58,74	3.97	19 (43%)	37,94,114	2.25	12 (32%)
22	CLA	r	604	-	52,56,73	1.33	9 (17%)	61,92,113	1.49	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	q	303	-	54,58,73	1.30	9 (16%)	64,95,113	1.46	8 (12%)
22	CLA	V	301	-	69,73,73	1.17	9 (13%)	82,113,113	1.21	5 (6%)
22	CLA	G	306	22	64,68,73	1.20	8 (12%)	76,107,113	1.27	4 (5%)
22	CLA	2	301	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	9 (10%)
26	CHL	P	319	-	60,74,74	3.32	20 (33%)	58,114,114	2.11	12 (20%)
22	CLA	b	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.38	6 (7%)
32	SQD	A	412	-	52,54,54	0.95	4 (7%)	62,65,65	1.45	10 (16%)
24	XAT	4	311	-	41,47,47	2.67	19 (46%)	54,74,74	10.02	23 (42%)
22	CLA	c	505	-	69,73,73	1.14	8 (11%)	82,113,113	1.35	4 (4%)
26	CHL	G	312	-	42,56,74	4.21	19 (45%)	36,92,114	2.21	9 (25%)
26	CHL	3	316	-	55,69,74	3.53	19 (34%)	52,108,114	2.21	13 (25%)
26	CHL	p	315	-	42,56,74	4.19	21 (50%)	36,92,114	2.00	9 (25%)
22	CLA	R	310	-	64,68,73	1.23	8 (12%)	76,107,113	1.42	7 (9%)
24	XAT	1	311	-	41,47,47	2.67	20 (48%)	54,74,74	10.09	20 (37%)
34	LMG	a	412	-	40,40,55	1.32	6 (15%)	48,48,63	1.17	2 (4%)
25	LHG	D	407	-	48,48,48	0.91	4 (8%)	51,54,54	1.08	3 (5%)
26	CHL	G	315	-	60,74,74	3.36	19 (31%)	58,114,114	1.99	10 (17%)
22	CLA	c	507	-	69,73,73	1.17	8 (11%)	82,113,113	1.36	6 (7%)
22	CLA	R	304	-	64,68,73	1.20	9 (14%)	76,107,113	1.34	5 (6%)
22	CLA	u	302	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
22	CLA	G	304	-	68,72,73	1.17	8 (11%)	80,111,113	1.37	8 (10%)
26	CHL	g	316	-	55,69,74	3.48	19 (34%)	52,108,114	2.25	15 (28%)
34	LMG	c	520	-	51,51,55	1.22	6 (11%)	59,59,63	1.08	2 (3%)
22	CLA	X	202	-	69,73,73	1.14	9 (13%)	82,113,113	1.36	8 (9%)
22	CLA	R	305	-	52,56,73	1.33	9 (17%)	61,92,113	1.49	6 (9%)
25	LHG	R	314	-	41,41,48	0.97	3 (7%)	44,47,54	1.10	2 (4%)
34	LMG	b	621	-	51,51,55	1.20	6 (11%)	59,59,63	1.44	8 (13%)
22	CLA	c	509	-	69,73,73	1.19	11 (15%)	82,113,113	1.43	9 (10%)
23	LUT	v	310	-	42,43,43	0.75	0	51,60,60	1.67	10 (19%)
22	CLA	4	301	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
22	CLA	c	511	-	69,73,73	1.18	9 (13%)	82,113,113	1.20	5 (6%)
24	XAT	6	310	-	41,47,47	2.70	19 (46%)	54,74,74	9.77	20 (37%)
30	PHO	d	401	-	58,69,69	2.08	9 (15%)	55,99,99	1.80	10 (18%)
22	CLA	r	609	26	64,68,73	1.22	9 (14%)	76,107,113	1.46	9 (11%)
24	XAT	Q	309	-	41,47,47	2.73	20 (48%)	54,74,74	9.93	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	SQD	a	410	-	48,50,54	1.01	5 (10%)	58,61,65	1.69	11 (18%)
26	CHL	n	318	-	60,74,74	3.36	19 (31%)	58,114,114	1.99	14 (24%)
22	CLA	3	307	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	6 (7%)
22	CLA	C	503	-	69,73,73	1.17	8 (11%)	82,113,113	1.33	6 (7%)
22	CLA	5	303	-	54,58,73	1.30	8 (14%)	64,95,113	1.43	6 (9%)
22	CLA	S	309	-	53,57,73	1.32	9 (16%)	61,93,113	1.41	4 (6%)
22	CLA	r	605	-	62,66,73	1.22	8 (12%)	73,104,113	1.40	5 (6%)
36	DGD	A	414	-	60,60,67	1.28	7 (11%)	74,74,81	1.25	6 (8%)
26	CHL	u	313	-	60,74,74	3.36	20 (33%)	58,114,114	2.00	14 (24%)
22	CLA	U	307	-	69,73,73	1.15	7 (10%)	82,113,113	1.35	5 (6%)
26	CHL	s	316	-	40,54,74	4.19	19 (47%)	34,90,114	2.28	8 (23%)
24	XAT	u	311	-	41,47,47	2.68	19 (46%)	54,74,74	9.78	20 (37%)
22	CLA	3	302	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	6 (7%)
26	CHL	g	312	-	42,56,74	4.11	18 (42%)	36,92,114	2.31	12 (33%)
22	CLA	Q	301	-	69,73,73	1.18	9 (13%)	82,113,113	1.29	7 (8%)
34	LMG	B	621	-	51,51,55	1.20	6 (11%)	59,59,63	1.44	6 (10%)
22	CLA	s	306	-	60,64,73	1.26	9 (15%)	71,102,113	1.38	7 (9%)
22	CLA	p	304	-	54,58,73	1.31	8 (14%)	64,95,113	1.40	5 (7%)
25	LHG	Q	310	-	48,48,48	0.92	4 (8%)	51,54,54	1.07	2 (3%)
27	NEX	U	318	-	40,46,46	1.05	3 (7%)	50,70,70	2.24	15 (30%)
22	CLA	6	302	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
24	XAT	N	311	-	41,47,47	2.67	19 (46%)	54,74,74	9.91	21 (38%)
22	CLA	p	303	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	6 (7%)
22	CLA	1	303	-	54,58,73	1.30	9 (16%)	64,95,113	1.42	7 (10%)
26	CHL	u	314	-	42,56,74	3.96	18 (42%)	36,92,114	2.49	12 (33%)
26	CHL	q	311	-	60,74,74	3.35	20 (33%)	58,114,114	2.24	15 (25%)
25	LHG	N	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.10	2 (3%)
23	LUT	N	309	-	42,43,43	0.68	0	51,60,60	1.71	11 (21%)
25	LHG	P	313	-	48,48,48	0.91	4 (8%)	51,54,54	1.08	2 (3%)
22	CLA	N	306	-	64,68,73	1.20	7 (10%)	76,107,113	1.38	7 (9%)
22	CLA	g	303	-	54,58,73	1.31	9 (16%)	64,95,113	1.49	6 (9%)
23	LUT	U	309	-	42,43,43	0.71	0	51,60,60	1.74	12 (23%)
31	BCR	c	515	-	41,41,41	4.84	24 (58%)	56,56,56	2.73	23 (41%)
22	CLA	v	301	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	5 (6%)
22	CLA	2	304	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CHL	G	314	-	60,74,74	3.41	19 (31%)	58,114,114	1.72	12 (20%)
22	CLA	s	307	-	53,57,73	1.31	8 (15%)	61,93,113	1.48	7 (11%)
26	CHL	4	314	-	42,56,74	3.98	18 (42%)	36,92,114	2.44	13 (36%)
22	CLA	v	308	-	52,56,73	1.32	8 (15%)	61,92,113	1.41	4 (6%)
24	XAT	V	311	-	41,47,47	2.72	19 (46%)	54,74,74	9.97	22 (40%)
26	CHL	Q	316	-	55,69,74	3.54	19 (34%)	52,108,114	2.10	15 (28%)
23	LUT	P	310	-	42,43,43	0.68	0	51,60,60	1.82	16 (31%)
27	NEX	u	319	-	40,46,46	1.03	3 (7%)	50,70,70	2.44	18 (36%)
22	CLA	c	514	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	8 (9%)
23	LUT	P	311	-	42,43,43	0.75	0	51,60,60	1.62	12 (23%)
26	CHL	R	317	-	55,69,74	3.51	20 (36%)	52,108,114	1.92	13 (25%)
22	CLA	A	405	-	69,73,73	1.17	9 (13%)	82,113,113	1.37	8 (9%)
26	CHL	p	320	-	60,74,74	3.32	19 (31%)	58,114,114	2.15	15 (25%)
25	LHG	V	312	-	48,48,48	0.91	4 (8%)	51,54,54	1.10	2 (3%)
26	CHL	U	315	-	60,74,74	3.32	19 (31%)	58,114,114	2.22	14 (24%)
27	NEX	S	317	-	40,46,46	0.96	3 (7%)	50,70,70	2.37	18 (36%)
22	CLA	C	515	-	69,73,73	1.15	9 (13%)	82,113,113	1.37	8 (9%)
23	LUT	N	310	-	42,43,43	0.76	0	51,60,60	1.72	14 (27%)
31	BCR	b	619	-	41,41,41	4.89	24 (58%)	56,56,56	2.31	20 (35%)
22	CLA	3	303	-	54,58,73	1.31	9 (16%)	64,95,113	1.44	7 (10%)
22	CLA	S	304	-	49,53,73	1.37	8 (16%)	58,89,113	1.42	4 (6%)
31	BCR	a	409	-	41,41,41	4.87	24 (58%)	56,56,56	2.26	22 (39%)
26	CHL	Q	314	-	60,74,74	3.40	19 (31%)	58,114,114	1.79	13 (22%)
26	CHL	N	313	-	60,74,74	3.36	19 (31%)	58,114,114	1.95	12 (20%)
34	LMG	b	624	-	55,55,55	1.19	6 (10%)	63,63,63	1.07	2 (3%)
22	CLA	R	309	-	53,57,73	1.31	7 (13%)	61,93,113	1.45	8 (13%)
26	CHL	5	314	-	42,56,74	4.18	19 (45%)	36,92,114	2.22	13 (36%)
22	CLA	Q	302	-	69,73,73	1.15	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	q	302	-	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	u	303	-	54,58,73	1.31	8 (14%)	64,95,113	1.44	6 (9%)
34	LMG	A	411	-	40,40,55	1.32	6 (15%)	48,48,63	1.17	2 (4%)
22	CLA	Q	307	-	69,73,73	1.14	8 (11%)	82,113,113	1.32	6 (7%)
25	LHG	c	521	-	48,48,48	0.91	4 (8%)	51,54,54	1.09	2 (3%)
22	CLA	B	607	-	69,73,73	1.16	8 (11%)	82,113,113	1.39	6 (7%)
31	BCR	T	101	-	41,41,41	4.92	25 (60%)	56,56,56	2.40	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CHL	p	318	-	60,74,74	3.27	19 (31%)	58,114,114	2.15	14 (24%)
26	CHL	G	313	-	44,58,74	3.91	19 (43%)	37,94,114	2.50	11 (29%)
25	LHG	1	312	-	48,48,48	0.91	4 (8%)	51,54,54	1.10	2 (3%)
22	CLA	c	510	-	69,73,73	1.13	8 (11%)	82,113,113	1.37	9 (10%)
27	NEX	V	319	-	40,46,46	1.00	2 (5%)	50,70,70	2.34	16 (32%)
34	LMG	w	201	-	48,48,55	1.25	6 (12%)	56,56,63	1.12	4 (7%)
34	LMG	C	502	-	51,51,55	1.17	5 (9%)	59,59,63	1.17	3 (5%)
22	CLA	u	307	-	69,73,73	1.14	7 (10%)	82,113,113	1.35	6 (7%)
22	CLA	C	504	-	69,73,73	1.18	9 (13%)	82,113,113	1.46	8 (9%)
22	CLA	c	508	-	69,73,73	1.15	8 (11%)	82,113,113	1.39	7 (8%)
27	NEX	p	301	-	40,46,46	1.06	4 (10%)	50,70,70	2.30	18 (36%)
22	CLA	Q	305	22	64,68,73	1.20	9 (14%)	76,107,113	1.29	5 (6%)
34	LMG	W	201	-	48,48,55	1.25	6 (12%)	56,56,63	1.12	4 (7%)
22	CLA	n	304	-	69,73,73	1.14	9 (13%)	82,113,113	1.39	8 (9%)
26	CHL	1	314	22	42,56,74	4.04	18 (42%)	36,92,114	2.18	11 (30%)
26	CHL	g	315	-	60,74,74	3.36	19 (31%)	58,114,114	2.04	11 (18%)
22	CLA	3	306	22	64,68,73	1.20	8 (12%)	76,107,113	1.31	5 (6%)
31	BCR	X	201	-	41,41,41	4.92	24 (58%)	56,56,56	2.28	18 (32%)
26	CHL	q	314	-	60,74,74	3.36	19 (31%)	58,114,114	2.03	12 (20%)
22	CLA	P	308	-	64,68,73	1.20	9 (14%)	76,107,113	1.35	5 (6%)
25	LHG	S	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.14	3 (5%)
26	CHL	v	314	-	42,56,74	4.09	19 (45%)	36,92,114	2.59	12 (33%)
25	LHG	A	413	-	42,42,48	0.93	3 (7%)	45,48,54	1.12	2 (4%)
22	CLA	6	304	-	54,58,73	1.31	9 (16%)	64,95,113	1.41	8 (12%)
22	CLA	N	308	-	52,56,73	1.34	8 (15%)	61,92,113	1.40	6 (9%)
22	CLA	P	304	-	54,58,73	1.31	8 (14%)	64,95,113	1.42	5 (7%)
25	LHG	u	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.14	3 (5%)
22	CLA	n	301	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
22	CLA	G	303	-	54,58,73	1.31	8 (14%)	64,95,113	1.46	6 (9%)
26	CHL	V	317	-	60,74,74	3.38	19 (31%)	58,114,114	2.46	16 (27%)
22	CLA	A	406	-	54,58,73	1.31	9 (16%)	64,95,113	1.42	4 (6%)
22	CLA	B	602	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	8 (9%)
22	CLA	5	302	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	5 (6%)
22	CLA	q	307	-	69,73,73	1.14	8 (11%)	82,113,113	1.35	6 (7%)
22	CLA	N	303	-	54,58,73	1.30	9 (16%)	64,95,113	1.50	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	XAT	P	312	-	41,47,47	2.73	20 (48%)	54,74,74	9.95	21 (38%)
22	CLA	5	307	-	64,68,73	1.18	9 (14%)	76,107,113	1.36	5 (6%)
22	CLA	V	307	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	5 (6%)
26	CHL	V	314	-	42,56,74	4.20	19 (45%)	36,92,114	2.26	11 (30%)
26	CHL	U	319	-	60,74,74	3.37	19 (31%)	58,114,114	1.82	13 (22%)
26	CHL	v	316	-	60,74,74	3.33	19 (31%)	58,114,114	2.03	15 (25%)
26	CHL	2	314	-	42,56,74	4.24	19 (45%)	36,92,114	2.29	13 (36%)
22	CLA	6	305	-	68,72,73	1.17	9 (13%)	80,111,113	1.35	8 (10%)
25	LHG	r	613	-	41,41,48	0.97	3 (7%)	44,47,54	1.10	2 (4%)
25	LHG	g	310	-	48,48,48	0.90	4 (8%)	51,54,54	1.10	2 (3%)
27	NEX	r	618	22	40,46,46	1.17	4 (10%)	50,70,70	2.27	14 (28%)
33	PL9	D	405	-	55,55,55	1.60	6 (10%)	68,69,69	1.68	18 (26%)
26	CHL	s	313	-	40,54,74	4.17	19 (47%)	34,90,114	2.43	12 (35%)
22	CLA	C	505	-	69,73,73	1.16	10 (14%)	82,113,113	1.33	5 (6%)
22	CLA	n	305	-	64,68,73	1.20	6 (9%)	76,107,113	1.95	13 (17%)
22	CLA	6	309	-	52,56,73	1.32	8 (15%)	61,92,113	1.40	5 (8%)
22	CLA	G	307	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	5 (6%)
22	CLA	b	605	-	69,73,73	1.17	7 (10%)	82,113,113	1.65	10 (12%)
23	LUT	n	310	-	42,43,43	0.77	0	51,60,60	1.80	14 (27%)
22	CLA	4	307	-	69,73,73	1.15	9 (13%)	82,113,113	1.38	8 (9%)
30	PHO	a	407	-	58,69,69	2.11	11 (18%)	55,99,99	1.60	9 (16%)
22	CLA	p	307	-	64,68,73	1.20	6 (9%)	76,107,113	1.34	5 (6%)
22	CLA	1	302	-	69,73,73	1.18	8 (11%)	82,113,113	1.22	5 (6%)
34	LMG	B	624	-	55,55,55	1.18	6 (10%)	63,63,63	1.07	2 (3%)
22	CLA	u	308	-	52,56,73	1.32	9 (17%)	61,92,113	1.43	5 (8%)
24	XAT	g	309	-	41,47,47	2.67	19 (46%)	54,74,74	9.74	23 (42%)
25	LHG	L	101	-	48,48,48	0.91	3 (6%)	51,54,54	1.12	3 (5%)
22	CLA	a	404	-	69,73,73	1.16	10 (14%)	82,113,113	1.44	8 (9%)
22	CLA	1	307	-	69,73,73	1.15	10 (14%)	82,113,113	1.36	8 (9%)
22	CLA	g	304	-	68,72,73	1.17	8 (11%)	80,111,113	1.36	8 (10%)
22	CLA	C	512	-	69,73,73	1.17	9 (13%)	82,113,113	1.19	5 (6%)
24	XAT	p	312	-	41,47,47	2.73	19 (46%)	54,74,74	9.83	20 (37%)
22	CLA	V	306	-	64,68,73	1.22	8 (12%)	76,107,113	1.34	7 (9%)
27	NEX	R	301	22	40,46,46	1.18	4 (10%)	50,70,70	2.24	14 (28%)
26	CHL	p	319	-	60,74,74	3.35	19 (31%)	58,114,114	2.03	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	LHG	d	405	-	45,45,48	0.94	4 (8%)	48,51,54	1.08	3 (6%)
26	CHL	3	314	-	60,74,74	3.42	19 (31%)	58,114,114	1.76	11 (18%)
26	CHL	6	317	-	55,69,74	3.53	19 (34%)	52,108,114	2.27	16 (30%)
26	CHL	3	311	-	60,74,74	3.36	19 (31%)	58,114,114	2.29	15 (25%)
22	CLA	g	301	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	8 (9%)
26	CHL	S	313	-	40,54,74	4.16	19 (47%)	34,90,114	2.51	13 (38%)
22	CLA	c	512	-	69,73,73	1.18	10 (14%)	82,113,113	1.38	8 (9%)
22	CLA	B	605	-	69,73,73	1.17	6 (8%)	82,113,113	1.65	11 (13%)
22	CLA	1	306	-	64,68,73	1.21	9 (14%)	76,107,113	1.35	7 (9%)
23	LUT	5	309	-	42,43,43	0.69	0	51,60,60	1.86	16 (31%)
22	CLA	5	306	-	64,68,73	1.18	7 (10%)	76,107,113	1.38	9 (11%)
22	CLA	P	305	-	69,73,73	1.14	8 (11%)	82,113,113	1.32	6 (7%)
23	LUT	V	310	-	42,43,43	0.76	0	51,60,60	1.65	14 (27%)
22	CLA	5	301	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	8 (9%)
22	CLA	P	307	-	64,68,73	1.19	6 (9%)	76,107,113	1.35	9 (11%)
25	LHG	G	310	-	48,48,48	0.90	4 (8%)	51,54,54	1.11	2 (3%)
22	CLA	Q	303	-	54,58,73	1.31	8 (14%)	64,95,113	1.39	5 (7%)
23	LUT	p	310	-	42,43,43	0.69	0	51,60,60	1.86	16 (31%)
22	CLA	p	302	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
23	LUT	2	310	-	42,43,43	0.77	0	51,60,60	1.65	12 (23%)
22	CLA	s	308	-	59,63,73	1.24	9 (15%)	70,101,113	1.39	5 (7%)
36	DGD	C	519	-	56,56,67	1.32	8 (14%)	70,70,81	1.19	5 (7%)
22	CLA	N	305	-	64,68,73	1.18	8 (12%)	76,107,113	1.80	10 (13%)
33	PL9	A	410	-	13,13,55	3.64	7 (53%)	17,17,69	1.56	3 (17%)
22	CLA	C	507	-	69,73,73	1.14	7 (10%)	82,113,113	1.48	9 (10%)
25	LHG	B	622	-	46,46,48	0.92	4 (8%)	49,52,54	1.07	2 (4%)
26	CHL	2	315	-	44,58,74	3.96	19 (43%)	37,94,114	2.34	10 (27%)
27	NEX	2	319	-	40,46,46	1.04	3 (7%)	50,70,70	2.34	14 (28%)
26	CHL	2	313	18	60,74,74	3.43	19 (31%)	58,114,114	1.92	12 (20%)
30	PHO	D	401	-	58,69,69	2.08	9 (15%)	55,99,99	1.80	10 (18%)
25	LHG	n	312	-	48,48,48	0.92	4 (8%)	51,54,54	1.04	2 (3%)
22	CLA	g	305	22	64,68,73	1.20	7 (10%)	76,107,113	1.41	8 (10%)
32	SQD	l	102	-	52,54,54	0.93	3 (5%)	62,65,65	1.74	12 (19%)
23	LUT	4	309	-	42,43,43	0.72	0	51,60,60	1.69	13 (25%)
25	LHG	c	522	-	48,48,48	0.91	3 (6%)	51,54,54	1.08	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	s	301	-	65,69,73	1.17	10 (15%)	77,108,113	1.37	11 (14%)
33	PL9	a	411	-	13,13,55	3.63	7 (53%)	17,17,69	1.57	3 (17%)
26	CHL	r	616	-	55,69,74	3.51	19 (34%)	52,108,114	1.91	13 (25%)
22	CLA	R	303	-	64,68,73	1.21	8 (12%)	76,107,113	1.33	6 (7%)
26	CHL	Q	311	-	60,74,74	3.37	20 (33%)	58,114,114	2.29	16 (27%)
22	CLA	b	615	-	69,73,73	1.13	9 (13%)	82,113,113	1.37	6 (7%)
26	CHL	6	312	-	60,74,74	3.35	19 (31%)	58,114,114	2.30	15 (25%)
22	CLA	1	301	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
26	CHL	5	316	-	60,74,74	3.36	19 (31%)	58,114,114	2.03	15 (25%)
22	CLA	B	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.33	5 (6%)
31	BCR	A	409	-	41,41,41	4.88	24 (58%)	56,56,56	2.29	23 (41%)
24	XAT	q	309	-	41,47,47	2.72	20 (48%)	54,74,74	9.93	20 (37%)
26	CHL	6	313	-	42,56,74	4.25	19 (45%)	36,92,114	2.21	12 (33%)
22	CLA	q	308	-	52,56,73	1.32	8 (15%)	61,92,113	1.44	6 (9%)
26	CHL	r	614	-	60,74,74	3.37	19 (31%)	58,114,114	2.17	14 (24%)
22	CLA	Q	306	22	64,68,73	1.20	8 (12%)	76,107,113	1.26	3 (3%)
22	CLA	q	306	22	64,68,73	1.20	8 (12%)	76,107,113	1.30	5 (6%)
22	CLA	c	503	-	69,73,73	1.18	8 (11%)	82,113,113	1.46	7 (8%)
26	CHL	n	315	-	44,58,74	3.92	19 (43%)	37,94,114	2.17	13 (35%)
26	CHL	p	316	-	44,58,74	3.96	19 (43%)	37,94,114	2.34	11 (29%)
26	CHL	U	314	-	44,58,74	3.82	19 (43%)	37,94,114	2.43	11 (29%)
24	XAT	n	311	-	41,47,47	2.66	19 (46%)	54,74,74	9.78	26 (48%)
31	BCR	B	620	-	41,41,41	4.89	24 (58%)	56,56,56	2.31	23 (41%)
26	CHL	q	312	-	42,56,74	4.21	19 (45%)	36,92,114	2.24	11 (30%)
23	LUT	S	310	-	42,43,43	0.74	0	51,60,60	1.85	14 (27%)
22	CLA	2	303	-	54,58,73	1.29	8 (14%)	64,95,113	1.41	5 (7%)
22	CLA	S	302	-	49,53,73	1.40	7 (14%)	58,89,113	1.48	5 (8%)
26	CHL	2	318	-	60,74,74	3.31	20 (33%)	58,114,114	2.14	13 (22%)
22	CLA	a	408	-	64,68,73	1.19	11 (17%)	76,107,113	1.49	8 (10%)
22	CLA	S	307	-	53,57,73	1.31	9 (16%)	61,93,113	1.48	8 (13%)
22	CLA	V	303	-	54,58,73	1.31	10 (18%)	64,95,113	1.48	8 (12%)
22	CLA	V	308	-	52,56,73	1.32	8 (15%)	61,92,113	1.43	6 (9%)
22	CLA	n	308	-	52,56,73	1.36	9 (17%)	61,92,113	1.51	7 (11%)
26	CHL	Q	312	-	42,56,74	4.12	19 (45%)	36,92,114	2.25	10 (27%)
25	LHG	C	522	-	48,48,48	0.91	4 (8%)	51,54,54	1.10	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	2	308	-	52,56,73	1.32	9 (17%)	61,92,113	1.45	5 (8%)
27	NEX	N	318	-	40,46,46	1.01	3 (7%)	50,70,70	2.29	18 (36%)
26	CHL	n	316	-	60,74,74	3.35	19 (31%)	58,114,114	1.85	11 (18%)
22	CLA	A	408	-	64,68,73	1.19	11 (17%)	76,107,113	1.48	8 (10%)
35	BCT	D	402	-	3,3,3	2.67	1 (33%)	2,3,3	0.14	0
26	CHL	2	316	-	60,74,74	3.36	19 (31%)	58,114,114	2.05	13 (22%)
22	CLA	N	302	-	69,73,73	1.19	8 (11%)	82,113,113	1.29	5 (6%)
26	CHL	1	316	-	60,74,74	3.35	19 (31%)	58,114,114	2.00	15 (25%)
24	XAT	v	311	-	41,47,47	2.70	19 (46%)	54,74,74	9.98	21 (38%)
32	SQD	a	413	-	52,54,54	0.95	3 (5%)	62,65,65	1.45	9 (14%)
27	NEX	5	319	-	40,46,46	1.03	3 (7%)	50,70,70	2.32	18 (36%)
25	LHG	l	101	-	48,48,48	0.91	3 (6%)	51,54,54	1.12	3 (5%)
34	LMG	c	501	-	51,51,55	1.17	5 (9%)	59,59,63	1.16	3 (5%)
22	CLA	N	301	-	69,73,73	1.17	9 (13%)	82,113,113	1.32	7 (8%)
26	CHL	P	317	-	60,74,74	3.40	19 (31%)	58,114,114	1.90	14 (24%)
26	CHL	n	314	-	42,56,74	4.16	18 (42%)	36,92,114	2.39	16 (44%)
22	CLA	q	305	22	64,68,73	1.20	9 (14%)	76,107,113	1.32	5 (6%)
31	BCR	d	403	-	41,41,41	4.90	24 (58%)	56,56,56	2.30	23 (41%)
31	BCR	c	516	-	41,41,41	4.90	25 (60%)	56,56,56	2.33	20 (35%)
22	CLA	s	305	-	59,63,73	1.25	9 (15%)	70,101,113	1.37	7 (10%)
22	CLA	5	305	-	64,68,73	1.20	7 (10%)	76,107,113	1.91	10 (13%)
26	CHL	6	315	-	60,74,74	3.42	19 (31%)	58,114,114	1.78	13 (22%)
22	CLA	v	304	-	64,68,73	1.19	9 (14%)	76,107,113	1.37	9 (11%)
22	CLA	B	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.37	7 (8%)
27	NEX	n	319	-	40,46,46	1.04	3 (7%)	50,70,70	2.50	17 (34%)
22	CLA	b	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
22	CLA	U	306	-	64,68,73	1.22	9 (14%)	76,107,113	1.32	6 (7%)
26	CHL	P	315	-	42,56,74	4.24	21 (50%)	36,92,114	1.99	9 (25%)
22	CLA	C	510	-	69,73,73	1.19	11 (15%)	82,113,113	1.43	9 (10%)
22	CLA	U	301	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	7 (8%)
22	CLA	p	305	-	69,73,73	1.13	9 (13%)	82,113,113	1.34	6 (7%)
26	CHL	u	315	-	44,58,74	3.78	19 (43%)	37,94,114	2.41	11 (29%)
26	CHL	u	316	-	60,74,74	3.38	19 (31%)	58,114,114	2.10	19 (32%)
26	CHL	U	313	-	60,74,74	3.37	19 (31%)	58,114,114	2.03	15 (25%)
22	CLA	B	615	-	69,73,73	1.13	9 (13%)	82,113,113	1.36	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	V	302	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
32	SQD	M	101	-	40,42,54	1.07	3 (7%)	50,53,65	1.66	10 (20%)
22	CLA	S	303	-	54,58,73	1.30	8 (14%)	64,95,113	1.44	7 (10%)
27	NEX	r	617	-	40,46,46	1.15	4 (10%)	50,70,70	2.31	19 (38%)
27	NEX	u	320	-	40,46,46	0.99	3 (7%)	50,70,70	2.23	19 (38%)
22	CLA	p	308	-	64,68,73	1.20	9 (14%)	76,107,113	1.37	4 (5%)
26	CHL	R	315	-	60,74,74	3.36	19 (31%)	58,114,114	2.22	14 (24%)
22	CLA	U	304	-	64,68,73	1.19	9 (14%)	76,107,113	1.38	6 (7%)
22	CLA	n	303	-	54,58,73	1.30	9 (16%)	64,95,113	1.40	8 (12%)
22	CLA	p	306	-	64,68,73	1.19	8 (12%)	76,107,113	1.97	14 (18%)
22	CLA	2	305	-	64,68,73	1.18	7 (10%)	76,107,113	1.91	13 (17%)
26	CHL	5	318	-	60,74,74	3.31	19 (31%)	58,114,114	2.15	12 (20%)
22	CLA	B	610	-	69,73,73	1.14	9 (13%)	82,113,113	1.33	7 (8%)
22	CLA	s	309	-	53,57,73	1.29	8 (15%)	61,93,113	1.39	3 (4%)
25	LHG	6	311	-	48,48,48	0.91	4 (8%)	51,54,54	1.12	2 (3%)
37	HEM	E	101	4	50,50,50	1.45	6 (12%)	67,82,82	1.13	3 (4%)
25	LHG	D	406	-	45,45,48	0.94	4 (8%)	48,51,54	1.09	3 (6%)
22	CLA	v	305	-	64,68,73	1.20	9 (14%)	76,107,113	1.32	5 (6%)
26	CHL	3	315	-	60,74,74	3.36	19 (31%)	58,114,114	1.98	12 (20%)
22	CLA	g	307	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	5 (6%)
26	CHL	V	318	-	60,74,74	3.39	20 (33%)	58,114,114	1.94	12 (20%)
26	CHL	u	317	-	60,74,74	3.28	19 (31%)	58,114,114	2.47	16 (27%)
36	DGD	J	101	-	61,61,67	1.28	6 (9%)	75,75,81	1.18	4 (5%)
25	LHG	B	623	-	48,48,48	0.91	4 (8%)	51,54,54	1.07	2 (3%)
23	LUT	4	310	-	42,43,43	0.82	1 (2%)	51,60,60	1.77	15 (29%)
25	LHG	C	524	-	48,48,48	0.91	4 (8%)	51,54,54	1.14	2 (3%)
26	CHL	1	318	-	60,74,74	3.34	20 (33%)	58,114,114	2.14	15 (25%)
27	NEX	P	301	-	40,46,46	1.04	3 (7%)	50,70,70	2.23	16 (32%)
22	CLA	c	502	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	6 (7%)
31	BCR	b	620	-	41,41,41	4.90	24 (58%)	56,56,56	2.25	22 (39%)
25	LHG	U	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.18	3 (5%)
26	CHL	4	313	-	60,74,74	3.35	19 (31%)	58,114,114	1.98	13 (22%)
24	XAT	3	309	-	41,47,47	2.70	19 (46%)	54,74,74	9.81	19 (35%)
24	XAT	2	311	-	41,47,47	2.71	19 (46%)	54,74,74	9.91	21 (38%)
23	LUT	u	309	-	42,43,43	0.73	0	51,60,60	1.67	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	S	306	-	60,64,73	1.26	9 (15%)	71,102,113	1.38	6 (8%)
22	CLA	u	306	-	64,68,73	1.22	9 (14%)	76,107,113	1.34	5 (6%)
26	CHL	G	316	-	55,69,74	3.46	19 (34%)	52,108,114	2.27	14 (26%)
34	LMG	D	408	-	46,46,55	1.28	6 (13%)	54,54,63	1.02	2 (3%)
22	CLA	r	602	-	64,68,73	1.21	9 (14%)	76,107,113	1.32	4 (5%)
25	LHG	4	312	-	48,48,48	0.91	4 (8%)	51,54,54	1.08	2 (3%)
22	CLA	r	603	-	64,68,73	1.21	8 (12%)	76,107,113	1.34	4 (5%)
22	CLA	U	308	-	52,56,73	1.32	9 (17%)	61,92,113	1.44	5 (8%)
22	CLA	b	606	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	5 (6%)
23	LUT	5	310	-	42,43,43	0.75	0	51,60,60	1.66	11 (21%)
22	CLA	b	617	-	69,73,73	1.21	9 (13%)	82,113,113	1.48	10 (12%)
22	CLA	u	301	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	7 (8%)
23	LUT	s	311	-	42,43,43	0.71	0	51,60,60	1.80	19 (37%)
31	BCR	b	618	-	41,41,41	4.88	24 (58%)	56,56,56	2.50	26 (46%)
26	CHL	Q	315	-	60,74,74	3.35	19 (31%)	58,114,114	2.06	13 (22%)
26	CHL	Q	313	-	44,58,74	3.91	20 (45%)	37,94,114	2.63	11 (29%)
23	LUT	2	309	-	42,43,43	0.69	0	51,60,60	1.78	17 (33%)
22	CLA	2	302	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
22	CLA	2	306	-	64,68,73	1.19	7 (10%)	76,107,113	1.38	8 (10%)
26	CHL	5	313	18	60,74,74	3.46	19 (31%)	58,114,114	1.90	13 (22%)
22	CLA	3	308	-	52,56,73	1.32	7 (13%)	61,92,113	1.40	5 (8%)
36	DGD	C	520	-	63,63,67	1.24	6 (9%)	77,77,81	1.16	5 (6%)
22	CLA	c	504	-	69,73,73	1.16	10 (14%)	82,113,113	1.33	5 (6%)
22	CLA	q	304	-	68,72,73	1.17	8 (11%)	80,111,113	1.45	7 (8%)
22	CLA	b	613	-	69,73,73	1.17	11 (15%)	82,113,113	1.33	10 (12%)
22	CLA	s	304	-	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
22	CLA	b	609	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
22	CLA	6	303	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
22	CLA	S	308	-	59,63,73	1.24	9 (15%)	70,101,113	1.38	5 (7%)
25	LHG	v	312	-	48,48,48	0.91	4 (8%)	51,54,54	1.13	2 (3%)
22	CLA	P	303	-	69,73,73	1.15	8 (11%)	82,113,113	1.32	5 (6%)
33	PL9	d	404	-	55,55,55	1.60	6 (10%)	68,69,69	1.69	18 (26%)
26	CHL	U	316	-	60,74,74	3.30	19 (31%)	58,114,114	2.59	16 (27%)
31	BCR	D	404	-	41,41,41	4.90	24 (58%)	56,56,56	2.30	23 (41%)
22	CLA	A	404	-	69,73,73	1.17	9 (13%)	82,113,113	1.43	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	LUT	1	310	-	42,43,43	0.76	0	51,60,60	1.79	15 (29%)
26	CHL	v	318	-	60,74,74	3.36	20 (33%)	58,114,114	1.99	12 (20%)
26	CHL	N	315	-	44,58,74	3.85	19 (43%)	37,94,114	2.50	11 (29%)
32	SQD	L	102	-	52,54,54	0.93	3 (5%)	62,65,65	1.73	12 (19%)
31	BCR	C	518	-	41,41,41	4.89	24 (58%)	56,56,56	2.33	20 (35%)
22	CLA	b	616	-	69,73,73	1.17	7 (10%)	82,113,113	1.36	6 (7%)
22	CLA	3	301	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
23	LUT	V	309	-	42,43,43	0.77	0	51,60,60	1.68	14 (27%)
30	PHO	A	407	-	58,69,69	2.12	11 (18%)	55,99,99	1.60	9 (16%)
26	CHL	1	313	-	60,74,74	3.38	19 (31%)	58,114,114	2.01	13 (22%)
32	SQD	C	501	-	48,50,54	1.00	5 (10%)	58,61,65	1.69	11 (18%)
25	LHG	a	415	-	42,42,48	0.93	3 (7%)	45,48,54	1.11	2 (4%)
26	CHL	q	313	-	44,58,74	3.90	20 (45%)	37,94,114	2.62	11 (29%)
26	CHL	S	314	-	40,54,74	4.14	18 (45%)	34,90,114	2.68	11 (32%)
26	CHL	v	313	-	60,74,74	3.38	19 (31%)	58,114,114	2.18	13 (22%)
22	CLA	N	304	-	69,73,73	1.13	9 (13%)	82,113,113	1.38	9 (10%)
26	CHL	U	317	-	60,74,74	3.32	19 (31%)	58,114,114	2.13	14 (24%)
22	CLA	Q	308	-	52,56,73	1.32	8 (15%)	61,92,113	1.41	7 (11%)
22	CLA	B	609	-	69,73,73	1.15	10 (14%)	82,113,113	1.30	6 (7%)
23	LUT	R	312	-	42,43,43	0.69	0	51,60,60	1.62	14 (27%)

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
22	CLA	b	614	-	1/1/15/20	13/39/115/115	-
22	CLA	5	308	-	1/1/11/20	6/19/95/115	-
26	CHL	V	315	-	3/3/16/26	6/20/118/137	-
26	CHL	V	313	-	3/3/20/26	20/39/137/137	-
26	CHL	N	317	-	3/3/20/26	21/39/137/137	-
25	LHG	s	312	-	-	16/53/53/53	-
31	BCR	z	101	-	-	8/29/63/63	0/2/2/2
22	CLA	B	616	-	1/1/15/20	6/39/115/115	-
22	CLA	6	307	22	1/1/14/20	18/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	V	304	-	1/1/14/20	11/33/109/115	-
26	CHL	G	311	-	3/3/20/26	19/39/137/137	-
22	CLA	4	302	-	1/1/15/20	14/39/115/115	-
22	CLA	n	302	-	1/1/15/20	13/39/115/115	-
26	CHL	v	317	-	3/3/20/26	12/39/137/137	-
26	CHL	g	311	-	3/3/20/26	20/39/137/137	-
23	LUT	p	311	-	-	1/29/67/67	0/2/2/2
25	LHG	b	623	-	-	24/53/53/53	-
22	CLA	b	612	-	1/1/15/20	15/39/115/115	-
25	LHG	q	310	-	-	21/53/53/53	-
22	CLA	b	608	-	1/1/15/20	12/39/115/115	-
22	CLA	G	308	-	1/1/11/20	9/19/95/115	-
22	CLA	4	308	-	1/1/11/20	11/19/95/115	-
22	CLA	U	305	-	1/1/14/20	12/33/109/115	-
26	CHL	v	315	-	3/3/16/26	8/20/118/137	-
26	CHL	R	316	-	3/3/18/26	9/27/125/137	-
22	CLA	1	308	-	1/1/11/20	11/19/95/115	-
25	LHG	c	523	-	-	16/53/53/53	-
26	CHL	P	318	-	3/3/20/26	18/39/137/137	-
23	LUT	v	309	-	-	2/29/67/67	0/2/2/2
22	CLA	b	602	-	1/1/15/20	19/39/115/115	-
26	CHL	6	314	-	3/3/16/26	11/20/118/137	-
22	CLA	v	302	-	1/1/15/20	13/39/115/115	-
26	CHL	r	619	-	3/3/16/26	7/18/116/137	-
22	CLA	v	307	-	1/1/15/20	12/39/115/115	-
26	CHL	P	314	18	3/3/20/26	13/39/137/137	-
22	CLA	B	612	-	1/1/15/20	15/39/115/115	-
22	CLA	1	304	-	1/1/14/20	8/33/109/115	-
31	BCR	k	101	-	-	13/29/63/63	0/2/2/2
22	CLA	P	309	-	1/1/11/20	11/19/95/115	-
22	CLA	B	608	-	1/1/15/20	15/39/115/115	-
23	LUT	S	311	-	-	5/29/67/67	0/2/2/2
24	XAT	U	311	-	-	7/31/93/93	0/4/4/4
27	NEX	s	317	-	-	4/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	304	-	1/1/15/20	14/39/115/115	-
26	CHL	N	314	-	3/3/16/26	8/18/116/137	-
22	CLA	4	306	-	1/1/14/20	17/33/109/115	-
22	CLA	C	514	-	1/1/15/20	15/39/115/115	-
26	CHL	6	301	-	3/3/20/26	22/39/137/137	-
36	DGD	B	601	-	-	22/51/91/95	0/2/2/2
23	LUT	U	310	-	-	1/29/67/67	0/2/2/2
22	CLA	r	608	-	1/1/11/20	7/20/96/115	-
22	CLA	N	307	-	1/1/14/20	13/33/109/115	-
22	CLA	C	506	-	1/1/15/20	15/39/115/115	-
36	DGD	c	519	-	-	21/49/89/95	0/2/2/2
26	CHL	4	316	-	3/3/20/26	14/39/137/137	-
22	CLA	P	302	-	1/1/15/20	16/39/115/115	-
22	CLA	R	308	-	1/1/11/20	11/20/96/115	-
22	CLA	S	301	-	1/1/14/20	17/35/111/115	-
22	CLA	d	402	-	1/1/15/20	15/39/115/115	-
22	CLA	g	302	-	1/1/15/20	14/39/115/115	-
22	CLA	B	606	-	1/1/15/20	18/39/115/115	-
25	LHG	d	406	-	-	18/53/53/53	-
22	CLA	4	304	-	1/1/14/20	9/33/109/115	-
22	CLA	1	305	-	1/1/14/20	10/33/109/115	-
22	CLA	u	304	-	1/1/14/20	4/33/109/115	-
22	CLA	G	302	-	1/1/15/20	18/39/115/115	-
31	BCR	x	202	-	-	9/29/63/63	0/2/2/2
23	LUT	u	310	-	-	1/29/67/67	0/2/2/2
22	CLA	R	302	27	1/1/11/20	10/20/96/115	-
22	CLA	4	305	-	1/1/14/20	8/33/109/115	-
22	CLA	b	607	-	-	16/39/115/115	-
31	BCR	C	516	-	-	8/29/63/63	0/2/2/2
26	CHL	p	314	18	3/3/20/26	10/39/137/137	-
26	CHL	u	318	-	3/3/20/26	20/39/137/137	-
25	LHG	5	312	-	-	21/53/53/53	-
22	CLA	a	405	-	1/1/15/20	10/39/115/115	-
26	CHL	n	317	-	3/3/20/26	15/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	304	-	1/1/14/20	15/38/114/115	-
26	CHL	g	314	-	3/3/20/26	19/39/137/137	-
26	CHL	2	317	-	3/3/20/26	11/39/137/137	-
26	CHL	S	315	-	3/3/18/26	15/30/128/137	-
22	CLA	B	613	-	1/1/15/20	14/39/115/115	-
22	CLA	V	305	-	1/1/14/20	10/33/109/115	-
26	CHL	S	316	-	3/3/16/26	8/15/113/137	-
22	CLA	u	305	-	1/1/14/20	14/33/109/115	-
22	CLA	b	610	-	1/1/15/20	18/39/115/115	-
22	CLA	D	403	-	1/1/15/20	17/39/115/115	-
26	CHL	g	313	-	3/3/16/26	8/20/118/137	-
22	CLA	U	303	-	1/1/12/20	8/21/97/115	-
22	CLA	6	306	22	1/1/14/20	14/33/109/115	-
23	LUT	r	611	-	-	2/29/67/67	0/2/2/2
36	DGD	b	601	-	-	21/51/91/95	0/2/2/2
23	LUT	n	309	-	-	0/29/67/67	0/2/2/2
22	CLA	r	607	-	1/1/11/20	11/20/96/115	-
24	XAT	G	309	-	-	10/31/93/93	0/4/4/4
22	CLA	n	306	-	1/1/14/20	8/33/109/115	-
25	LHG	2	312	-	-	24/53/53/53	-
25	LHG	C	523	-	-	24/53/53/53	-
22	CLA	B	614	-	1/1/15/20	12/39/115/115	-
22	CLA	r	610	-	1/1/11/20	8/15/91/115	-
22	CLA	c	506	-	1/1/15/20	18/39/115/115	-
22	CLA	4	303	-	1/1/12/20	9/21/97/115	-
26	CHL	s	314	-	3/3/16/26	5/15/113/137	-
25	LHG	p	313	-	-	21/53/53/53	-
22	CLA	C	509	-	1/1/15/20	17/39/115/115	-
37	HEM	e	101	4	-	2/14/54/54	-
22	CLA	n	307	-	1/1/14/20	12/33/109/115	-
23	LUT	s	310	-	-	0/29/67/67	0/2/2/2
22	CLA	G	301	-	1/1/15/20	19/39/115/115	-
22	CLA	s	302	-	1/1/11/20	6/15/91/115	-
22	CLA	C	508	-	1/1/15/20	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	V	316	-	3/3/20/26	19/39/137/137	-
22	CLA	x	201	-	1/1/15/20	8/39/115/115	-
22	CLA	3	305	22	1/1/14/20	10/33/109/115	-
22	CLA	v	306	-	1/1/14/20	14/33/109/115	-
31	BCR	C	517	-	-	14/29/63/63	0/2/2/2
26	CHL	4	315	-	3/3/16/26	6/20/118/137	-
22	CLA	6	308	-	1/1/15/20	12/39/115/115	-
22	CLA	b	604	-	1/1/15/20	17/39/115/115	-
34	LMG	C	521	-	-	19/46/66/70	0/1/1/1
22	CLA	R	307	-	1/1/15/20	18/39/115/115	-
22	CLA	v	303	-	1/1/12/20	10/21/97/115	-
24	XAT	r	612	-	-	7/31/93/93	0/4/4/4
22	CLA	S	305	-	1/1/13/20	7/27/103/115	-
26	CHL	1	315	-	3/3/16/26	6/20/118/137	-
27	NEX	v	319	-	-	4/27/83/83	0/3/3/3
22	CLA	P	306	-	1/1/14/20	10/33/109/115	-
22	CLA	2	307	-	1/1/14/20	10/33/109/115	-
34	LMG	d	407	-	-	17/41/61/70	0/1/1/1
36	DGD	c	517	-	-	21/44/84/95	0/2/2/2
32	SQD	m	101	-	-	20/37/57/69	0/1/1/1
31	BCR	B	619	-	-	14/29/63/63	0/2/2/2
26	CHL	5	317	-	3/3/20/26	15/39/137/137	-
22	CLA	p	309	-	1/1/11/20	7/19/95/115	-
22	CLA	G	305	22	1/1/14/20	10/33/109/115	-
22	CLA	B	617	-	1/1/15/20	11/39/115/115	-
25	LHG	3	310	-	-	16/53/53/53	-
22	CLA	C	513	-	1/1/15/20	8/39/115/115	-
25	LHG	b	622	-	-	20/51/51/53	-
22	CLA	r	606	-	1/1/15/20	18/39/115/115	-
26	CHL	s	315	-	3/3/18/26	15/30/128/137	-
26	CHL	5	315	-	3/3/16/26	9/20/118/137	-
22	CLA	B	604	-	1/1/15/20	16/39/115/115	-
22	CLA	g	306	22	1/1/14/20	14/33/109/115	-
22	CLA	Q	304	-	1/1/14/20	14/38/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	r	615	-	3/3/18/26	11/27/125/137	-
36	DGD	c	518	-	-	31/51/91/95	0/2/2/2
26	CHL	p	317	-	3/3/20/26	12/39/137/137	-
22	CLA	R	306	-	1/1/13/20	7/31/107/115	-
26	CHL	4	317	-	3/3/20/26	17/39/137/137	-
22	CLA	c	513	-	1/1/15/20	11/39/115/115	-
24	XAT	R	313	-	-	8/31/93/93	0/4/4/4
26	CHL	n	313	18	3/3/20/26	14/39/137/137	-
36	DGD	a	416	-	-	23/48/88/95	0/2/2/2
22	CLA	r	601	27	1/1/11/20	9/20/96/115	-
22	CLA	s	303	-	1/1/12/20	5/21/97/115	-
26	CHL	6	316	-	3/3/20/26	23/39/137/137	-
26	CHL	1	317	-	3/3/20/26	18/39/137/137	-
26	CHL	P	316	-	3/3/16/26	7/20/118/137	-
31	BCR	t	101	-	-	12/29/63/63	0/2/2/2
22	CLA	R	311	-	1/1/11/20	8/15/91/115	-
22	CLA	q	301	-	-	19/39/115/115	-
26	CHL	N	316	-	3/3/20/26	13/39/137/137	-
31	BCR	B	618	-	-	6/29/63/63	0/2/2/2
26	CHL	q	315	-	3/3/19/26	12/33/131/137	-
31	BCR	K	101	-	-	13/29/63/63	0/2/2/2
22	CLA	g	308	-	1/1/11/20	8/19/95/115	-
22	CLA	a	406	-	1/1/12/20	8/21/97/115	-
22	CLA	U	302	-	1/1/15/20	14/39/115/115	-
24	XAT	5	311	-	-	6/31/93/93	0/4/4/4
26	CHL	3	312	-	3/3/16/26	6/18/116/137	-
23	LUT	1	309	-	-	2/29/67/67	0/2/2/2
22	CLA	C	511	-	1/1/15/20	13/39/115/115	-
26	CHL	3	313	-	3/3/16/26	15/20/118/137	-
22	CLA	r	604	-	1/1/11/20	9/19/95/115	-
22	CLA	q	303	-	1/1/12/20	8/21/97/115	-
22	CLA	V	301	-	-	14/39/115/115	-
22	CLA	G	306	22	1/1/14/20	12/33/109/115	-
22	CLA	2	301	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	P	319	-	3/3/20/26	20/39/137/137	-
22	CLA	b	611	-	1/1/15/20	16/39/115/115	-
32	SQD	A	412	-	-	21/49/69/69	0/1/1/1
24	XAT	4	311	-	-	8/31/93/93	0/4/4/4
22	CLA	c	505	-	1/1/15/20	13/39/115/115	-
26	CHL	G	312	-	3/3/16/26	4/18/116/137	-
26	CHL	3	316	-	3/3/19/26	15/33/131/137	-
26	CHL	p	315	-	3/3/16/26	6/18/116/137	-
22	CLA	R	310	-	1/1/14/20	10/33/109/115	-
24	XAT	1	311	-	-	6/31/93/93	0/4/4/4
34	LMG	a	412	-	-	8/35/55/70	0/1/1/1
25	LHG	D	407	-	-	17/53/53/53	-
26	CHL	G	315	-	3/3/20/26	19/39/137/137	-
22	CLA	c	507	-	1/1/15/20	22/39/115/115	-
22	CLA	R	304	-	1/1/14/20	11/33/109/115	-
22	CLA	u	302	-	1/1/15/20	18/39/115/115	-
22	CLA	G	304	-	1/1/14/20	9/38/114/115	-
26	CHL	g	316	-	3/3/19/26	13/33/131/137	-
34	LMG	c	520	-	-	21/46/66/70	0/1/1/1
22	CLA	X	202	-	1/1/15/20	8/39/115/115	-
22	CLA	R	305	-	1/1/11/20	9/19/95/115	-
25	LHG	R	314	-	-	24/46/46/53	-
34	LMG	b	621	-	-	25/46/66/70	0/1/1/1
22	CLA	c	509	-	1/1/15/20	11/39/115/115	-
23	LUT	v	310	-	-	0/29/67/67	0/2/2/2
22	CLA	4	301	-	1/1/15/20	9/39/115/115	-
22	CLA	c	511	-	1/1/15/20	18/39/115/115	-
24	XAT	6	310	-	-	8/31/93/93	0/4/4/4
30	PHO	d	401	-	-	12/37/103/103	0/5/6/6
22	CLA	r	609	26	1/1/14/20	10/33/109/115	-
24	XAT	Q	309	-	-	10/31/93/93	0/4/4/4
32	SQD	a	410	-	-	25/45/65/69	0/1/1/1
26	CHL	n	318	-	3/3/20/26	24/39/137/137	-
22	CLA	3	307	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	503	-	1/1/15/20	9/39/115/115	-
22	CLA	5	303	-	1/1/12/20	7/21/97/115	-
22	CLA	S	309	-	1/1/11/20	4/20/96/115	-
22	CLA	r	605	-	1/1/13/20	9/31/107/115	-
36	DGD	A	414	-	-	22/48/88/95	0/2/2/2
26	CHL	u	313	-	3/3/20/26	12/39/137/137	-
22	CLA	U	307	-	1/1/15/20	16/39/115/115	-
26	CHL	s	316	-	3/3/16/26	8/15/113/137	-
24	XAT	u	311	-	-	7/31/93/93	0/4/4/4
22	CLA	3	302	-	1/1/15/20	13/39/115/115	-
26	CHL	g	312	-	3/3/16/26	8/18/116/137	-
22	CLA	Q	301	-	1/1/15/20	14/39/115/115	-
34	LMG	B	621	-	-	20/46/66/70	0/1/1/1
22	CLA	s	306	-	1/1/13/20	6/29/105/115	-
22	CLA	p	304	-	1/1/12/20	11/21/97/115	-
25	LHG	Q	310	-	-	20/53/53/53	-
27	NEX	U	318	-	-	3/27/83/83	0/3/3/3
22	CLA	6	302	-	1/1/15/20	15/39/115/115	-
24	XAT	N	311	-	-	8/31/93/93	0/4/4/4
22	CLA	p	303	-	1/1/15/20	8/39/115/115	-
22	CLA	1	303	-	1/1/12/20	8/21/97/115	-
26	CHL	u	314	-	3/3/16/26	10/18/116/137	-
26	CHL	q	311	-	3/3/20/26	17/39/137/137	-
25	LHG	N	312	-	-	16/53/53/53	-
23	LUT	N	309	-	-	2/29/67/67	0/2/2/2
25	LHG	P	313	-	-	24/53/53/53	-
22	CLA	N	306	-	1/1/14/20	8/33/109/115	-
22	CLA	g	303	-	1/1/12/20	11/21/97/115	-
23	LUT	U	309	-	-	4/29/67/67	0/2/2/2
31	BCR	c	515	-	-	14/29/63/63	0/2/2/2
22	CLA	v	301	-	-	13/39/115/115	-
22	CLA	2	304	-	1/1/15/20	11/39/115/115	-
26	CHL	G	314	-	3/3/20/26	16/39/137/137	-
22	CLA	s	307	-	1/1/11/20	5/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	4	314	-	3/3/16/26	8/18/116/137	-
22	CLA	v	308	-	1/1/11/20	9/19/95/115	-
24	XAT	V	311	-	-	11/31/93/93	0/4/4/4
26	CHL	Q	316	-	3/3/19/26	11/33/131/137	-
23	LUT	P	310	-	-	0/29/67/67	0/2/2/2
27	NEX	u	319	-	-	7/27/83/83	0/3/3/3
22	CLA	c	514	-	1/1/15/20	11/39/115/115	-
23	LUT	P	311	-	-	2/29/67/67	0/2/2/2
26	CHL	R	317	-	3/3/19/26	17/33/131/137	-
22	CLA	A	405	-	1/1/15/20	10/39/115/115	-
26	CHL	p	320	-	3/3/20/26	19/39/137/137	-
25	LHG	V	312	-	-	18/53/53/53	-
26	CHL	U	315	-	3/3/20/26	11/39/137/137	-
27	NEX	S	317	-	-	4/27/83/83	0/3/3/3
22	CLA	C	515	-	1/1/15/20	12/39/115/115	-
23	LUT	N	310	-	-	1/29/67/67	0/2/2/2
31	BCR	b	619	-	-	14/29/63/63	0/2/2/2
22	CLA	3	303	-	1/1/12/20	12/21/97/115	-
22	CLA	S	304	-	1/1/11/20	9/15/91/115	-
31	BCR	a	409	-	-	2/29/63/63	0/2/2/2
26	CHL	Q	314	-	3/3/20/26	20/39/137/137	-
26	CHL	N	313	-	3/3/20/26	13/39/137/137	-
34	LMG	b	624	-	-	22/50/70/70	0/1/1/1
22	CLA	R	309	-	1/1/11/20	7/20/96/115	-
26	CHL	5	314	-	3/3/16/26	9/18/116/137	-
22	CLA	Q	302	-	1/1/15/20	12/39/115/115	-
22	CLA	q	302	-	1/1/15/20	12/39/115/115	-
22	CLA	u	303	-	1/1/12/20	8/21/97/115	-
34	LMG	A	411	-	-	11/35/55/70	0/1/1/1
22	CLA	Q	307	-	1/1/15/20	12/39/115/115	-
25	LHG	c	521	-	-	13/53/53/53	-
22	CLA	B	607	-	1/1/15/20	16/39/115/115	-
31	BCR	T	101	-	-	12/29/63/63	0/2/2/2
26	CHL	p	318	-	3/3/20/26	16/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	G	313	-	3/3/16/26	9/20/118/137	-
25	LHG	1	312	-	-	13/53/53/53	-
22	CLA	c	510	-	1/1/15/20	13/39/115/115	-
27	NEX	V	319	-	-	6/27/83/83	0/3/3/3
34	LMG	w	201	-	-	22/43/63/70	0/1/1/1
34	LMG	C	502	-	-	26/46/66/70	0/1/1/1
22	CLA	u	307	-	1/1/15/20	15/39/115/115	-
22	CLA	C	504	-	1/1/15/20	20/39/115/115	-
22	CLA	c	508	-	1/1/15/20	16/39/115/115	-
27	NEX	p	301	-	-	3/27/83/83	0/3/3/3
22	CLA	Q	305	22	1/1/14/20	15/33/109/115	-
34	LMG	W	201	-	-	21/43/63/70	0/1/1/1
22	CLA	n	304	-	1/1/15/20	15/39/115/115	-
26	CHL	1	314	22	3/3/16/26	12/18/116/137	-
26	CHL	g	315	-	3/3/20/26	23/39/137/137	-
22	CLA	3	306	22	1/1/14/20	18/33/109/115	-
31	BCR	X	201	-	-	9/29/63/63	0/2/2/2
26	CHL	q	314	-	3/3/20/26	23/39/137/137	-
22	CLA	P	308	-	1/1/14/20	12/33/109/115	-
25	LHG	S	312	-	-	16/53/53/53	-
26	CHL	v	314	-	3/3/16/26	10/18/116/137	-
25	LHG	A	413	-	-	27/47/47/53	-
22	CLA	6	304	-	1/1/12/20	11/21/97/115	-
22	CLA	N	308	-	1/1/11/20	14/19/95/115	-
22	CLA	P	304	-	1/1/12/20	10/21/97/115	-
25	LHG	u	312	-	-	25/53/53/53	-
22	CLA	n	301	-	1/1/15/20	12/39/115/115	-
22	CLA	G	303	-	1/1/12/20	11/21/97/115	-
26	CHL	V	317	-	3/3/20/26	14/39/137/137	-
22	CLA	A	406	-	1/1/12/20	7/21/97/115	-
22	CLA	B	602	-	1/1/15/20	20/39/115/115	-
22	CLA	5	302	-	1/1/15/20	17/39/115/115	-
22	CLA	q	307	-	1/1/15/20	16/39/115/115	-
22	CLA	N	303	-	1/1/12/20	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	XAT	P	312	-	-	8/31/93/93	0/4/4/4
22	CLA	5	307	-	1/1/14/20	12/33/109/115	-
22	CLA	V	307	-	1/1/15/20	10/39/115/115	-
26	CHL	V	314	-	3/3/16/26	10/18/116/137	-
26	CHL	U	319	-	3/3/20/26	16/39/137/137	-
26	CHL	v	316	-	3/3/20/26	14/39/137/137	-
26	CHL	2	314	-	3/3/16/26	8/18/116/137	-
22	CLA	6	305	-	1/1/14/20	17/38/114/115	-
25	LHG	r	613	-	-	19/46/46/53	-
25	LHG	g	310	-	-	18/53/53/53	-
27	NEX	r	618	22	-	7/27/83/83	0/3/3/3
33	PL9	D	405	-	-	9/53/73/73	0/1/1/1
26	CHL	s	313	-	3/3/16/26	8/15/113/137	-
22	CLA	C	505	-	1/1/15/20	18/39/115/115	-
22	CLA	n	305	-	1/1/14/20	11/33/109/115	-
22	CLA	6	309	-	1/1/11/20	10/19/95/115	-
22	CLA	G	307	-	1/1/15/20	12/39/115/115	-
22	CLA	b	605	-	1/1/15/20	17/39/115/115	-
23	LUT	n	310	-	-	3/29/67/67	0/2/2/2
22	CLA	4	307	-	1/1/15/20	9/39/115/115	-
30	PHO	a	407	-	-	11/37/103/103	0/5/6/6
22	CLA	p	307	-	1/1/14/20	11/33/109/115	-
22	CLA	1	302	-	1/1/15/20	13/39/115/115	-
34	LMG	B	624	-	-	21/50/70/70	0/1/1/1
22	CLA	u	308	-	1/1/11/20	10/19/95/115	-
24	XAT	g	309	-	-	10/31/93/93	0/4/4/4
25	LHG	L	101	-	-	28/53/53/53	-
22	CLA	a	404	-	1/1/15/20	11/39/115/115	-
22	CLA	1	307	-	1/1/15/20	11/39/115/115	-
22	CLA	g	304	-	1/1/14/20	8/38/114/115	-
22	CLA	C	512	-	1/1/15/20	18/39/115/115	-
24	XAT	p	312	-	-	7/31/93/93	0/4/4/4
22	CLA	V	306	-	1/1/14/20	6/33/109/115	-
27	NEX	R	301	22	-	10/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	p	319	-	3/3/20/26	18/39/137/137	-
25	LHG	d	405	-	-	26/50/50/53	-
26	CHL	3	314	-	3/3/20/26	18/39/137/137	-
26	CHL	6	317	-	3/3/19/26	15/33/131/137	-
26	CHL	3	311	-	3/3/20/26	19/39/137/137	-
22	CLA	g	301	-	1/1/15/20	14/39/115/115	-
26	CHL	S	313	-	3/3/16/26	9/15/113/137	-
22	CLA	c	512	-	1/1/15/20	7/39/115/115	-
22	CLA	B	605	-	1/1/15/20	17/39/115/115	-
22	CLA	1	306	-	1/1/14/20	16/33/109/115	-
23	LUT	5	309	-	-	3/29/67/67	0/2/2/2
22	CLA	5	306	-	1/1/14/20	13/33/109/115	-
22	CLA	P	305	-	1/1/15/20	11/39/115/115	-
23	LUT	V	310	-	-	0/29/67/67	0/2/2/2
22	CLA	5	301	-	1/1/15/20	8/39/115/115	-
22	CLA	P	307	-	1/1/14/20	12/33/109/115	-
25	LHG	G	310	-	-	18/53/53/53	-
22	CLA	Q	303	-	1/1/12/20	11/21/97/115	-
23	LUT	p	310	-	-	0/29/67/67	0/2/2/2
22	CLA	p	302	-	1/1/15/20	15/39/115/115	-
23	LUT	2	310	-	-	0/29/67/67	0/2/2/2
22	CLA	s	308	-	1/1/13/20	9/27/103/115	-
36	DGD	C	519	-	-	22/44/84/95	0/2/2/2
22	CLA	N	305	-	1/1/14/20	10/33/109/115	-
33	PL9	A	410	-	-	0/5/18/73	0/1/1/1
22	CLA	C	507	-	1/1/15/20	18/39/115/115	-
25	LHG	B	622	-	-	21/51/51/53	-
26	CHL	2	315	-	3/3/16/26	7/20/118/137	-
27	NEX	2	319	-	-	7/27/83/83	0/3/3/3
26	CHL	2	313	18	3/3/20/26	19/39/137/137	-
30	PHO	D	401	-	-	12/37/103/103	0/5/6/6
25	LHG	n	312	-	-	18/53/53/53	-
22	CLA	g	305	22	1/1/14/20	10/33/109/115	-
32	SQD	l	102	-	-	21/49/69/69	0/1/1/1
23	LUT	4	309	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	c	522	-	-	22/53/53/53	-
22	CLA	s	301	-	1/1/14/20	17/35/111/115	-
33	PL9	a	411	-	-	0/5/18/73	0/1/1/1
26	CHL	r	616	-	3/3/19/26	17/33/131/137	-
22	CLA	R	303	-	1/1/14/20	9/33/109/115	-
26	CHL	Q	311	-	3/3/20/26	21/39/137/137	-
22	CLA	b	615	-	1/1/15/20	17/39/115/115	-
26	CHL	6	312	-	3/3/20/26	17/39/137/137	-
22	CLA	1	301	-	1/1/15/20	11/39/115/115	-
26	CHL	5	316	-	3/3/20/26	15/39/137/137	-
22	CLA	B	603	-	1/1/15/20	14/39/115/115	-
31	BCR	A	409	-	-	2/29/63/63	0/2/2/2
24	XAT	q	309	-	-	11/31/93/93	0/4/4/4
26	CHL	6	313	-	3/3/16/26	6/18/116/137	-
22	CLA	q	308	-	1/1/11/20	12/19/95/115	-
26	CHL	r	614	-	3/3/20/26	21/39/137/137	-
22	CLA	Q	306	22	1/1/14/20	12/33/109/115	-
22	CLA	q	306	22	1/1/14/20	13/33/109/115	-
22	CLA	c	503	-	1/1/15/20	21/39/115/115	-
26	CHL	n	315	-	3/3/16/26	9/20/118/137	-
26	CHL	p	316	-	3/3/16/26	7/20/118/137	-
26	CHL	U	314	-	3/3/16/26	8/20/118/137	-
24	XAT	n	311	-	-	9/31/93/93	0/4/4/4
31	BCR	B	620	-	-	12/29/63/63	0/2/2/2
26	CHL	q	312	-	3/3/16/26	10/18/116/137	-
23	LUT	S	310	-	-	0/29/67/67	0/2/2/2
22	CLA	2	303	-	1/1/12/20	9/21/97/115	-
22	CLA	S	302	-	1/1/11/20	6/15/91/115	-
26	CHL	2	318	-	3/3/20/26	21/39/137/137	-
22	CLA	a	408	-	1/1/14/20	12/33/109/115	-
22	CLA	S	307	-	1/1/11/20	6/20/96/115	-
22	CLA	V	303	-	1/1/12/20	10/21/97/115	-
22	CLA	V	308	-	1/1/11/20	10/19/95/115	-
22	CLA	n	308	-	1/1/11/20	12/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	Q	312	-	3/3/16/26	11/18/116/137	-
25	LHG	C	522	-	-	16/53/53/53	-
22	CLA	2	308	-	1/1/11/20	7/19/95/115	-
27	NEX	N	318	-	-	9/27/83/83	0/3/3/3
26	CHL	n	316	-	3/3/20/26	22/39/137/137	-
22	CLA	A	408	-	1/1/14/20	11/33/109/115	-
26	CHL	2	316	-	3/3/20/26	15/39/137/137	-
22	CLA	N	302	-	1/1/15/20	17/39/115/115	-
26	CHL	1	316	-	3/3/20/26	22/39/137/137	-
24	XAT	v	311	-	-	11/31/93/93	0/4/4/4
32	SQD	a	413	-	-	23/49/69/69	0/1/1/1
27	NEX	5	319	-	-	7/27/83/83	0/3/3/3
25	LHG	l	101	-	-	27/53/53/53	-
34	LMG	c	501	-	-	25/46/66/70	0/1/1/1
22	CLA	N	301	-	1/1/15/20	13/39/115/115	-
26	CHL	P	317	-	3/3/20/26	13/39/137/137	-
26	CHL	n	314	-	3/3/16/26	8/18/116/137	-
22	CLA	q	305	22	1/1/14/20	12/33/109/115	-
31	BCR	d	403	-	-	13/29/63/63	0/2/2/2
31	BCR	c	516	-	-	11/29/63/63	0/2/2/2
22	CLA	s	305	-	1/1/13/20	7/27/103/115	-
22	CLA	5	305	-	1/1/14/20	11/33/109/115	-
26	CHL	6	315	-	3/3/20/26	17/39/137/137	-
22	CLA	v	304	-	1/1/14/20	13/33/109/115	-
22	CLA	B	611	-	1/1/15/20	15/39/115/115	-
27	NEX	n	319	-	-	7/27/83/83	0/3/3/3
22	CLA	b	603	-	1/1/15/20	12/39/115/115	-
22	CLA	U	306	-	1/1/14/20	12/33/109/115	-
26	CHL	P	315	-	3/3/16/26	7/18/116/137	-
22	CLA	C	510	-	1/1/15/20	11/39/115/115	-
22	CLA	U	301	-	-	9/39/115/115	-
22	CLA	p	305	-	1/1/15/20	12/39/115/115	-
26	CHL	u	315	-	3/3/16/26	6/20/118/137	-
26	CHL	u	316	-	3/3/20/26	21/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	U	313	-	3/3/20/26	13/39/137/137	-
22	CLA	B	615	-	1/1/15/20	16/39/115/115	-
22	CLA	V	302	-	1/1/15/20	16/39/115/115	-
32	SQD	M	101	-	-	21/37/57/69	0/1/1/1
22	CLA	S	303	-	1/1/12/20	5/21/97/115	-
27	NEX	r	617	-	-	2/27/83/83	0/3/3/3
27	NEX	u	320	-	-	2/27/83/83	0/3/3/3
22	CLA	p	308	-	1/1/14/20	12/33/109/115	-
26	CHL	R	315	-	3/3/20/26	21/39/137/137	-
22	CLA	U	304	-	1/1/14/20	6/33/109/115	-
22	CLA	n	303	-	1/1/12/20	6/21/97/115	-
22	CLA	p	306	-	1/1/14/20	11/33/109/115	-
22	CLA	2	305	-	1/1/14/20	10/33/109/115	-
26	CHL	5	318	-	3/3/20/26	18/39/137/137	-
22	CLA	B	610	-	1/1/15/20	18/39/115/115	-
22	CLA	s	309	-	1/1/11/20	4/20/96/115	-
25	LHG	6	311	-	-	18/53/53/53	-
37	HEM	E	101	4	-	2/14/54/54	-
25	LHG	D	406	-	-	29/50/50/53	-
22	CLA	v	305	-	1/1/14/20	9/33/109/115	-
26	CHL	3	315	-	3/3/20/26	21/39/137/137	-
22	CLA	g	307	-	1/1/15/20	14/39/115/115	-
26	CHL	V	318	-	3/3/20/26	17/39/137/137	-
26	CHL	u	317	-	3/3/20/26	12/39/137/137	-
36	DGD	J	101	-	-	21/49/89/95	0/2/2/2
25	LHG	B	623	-	-	21/53/53/53	-
23	LUT	4	310	-	-	0/29/67/67	0/2/2/2
25	LHG	C	524	-	-	11/53/53/53	-
26	CHL	1	318	-	3/3/20/26	13/39/137/137	-
27	NEX	P	301	-	-	3/27/83/83	0/3/3/3
22	CLA	c	502	-	1/1/15/20	8/39/115/115	-
31	BCR	b	620	-	-	12/29/63/63	0/2/2/2
25	LHG	U	312	-	-	30/53/53/53	-
26	CHL	4	313	-	3/3/20/26	13/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	XAT	3	309	-	-	8/31/93/93	0/4/4/4
24	XAT	2	311	-	-	6/31/93/93	0/4/4/4
23	LUT	u	309	-	-	2/29/67/67	0/2/2/2
22	CLA	S	306	-	1/1/13/20	8/29/105/115	-
22	CLA	u	306	-	1/1/14/20	11/33/109/115	-
26	CHL	G	316	-	3/3/19/26	13/33/131/137	-
34	LMG	D	408	-	-	17/41/61/70	0/1/1/1
22	CLA	r	602	-	1/1/14/20	9/33/109/115	-
25	LHG	4	312	-	-	17/53/53/53	-
22	CLA	r	603	-	1/1/14/20	13/33/109/115	-
22	CLA	U	308	-	1/1/11/20	9/19/95/115	-
22	CLA	b	606	-	1/1/15/20	18/39/115/115	-
23	LUT	5	310	-	-	0/29/67/67	0/2/2/2
22	CLA	b	617	-	1/1/15/20	14/39/115/115	-
22	CLA	u	301	-	-	9/39/115/115	-
23	LUT	s	311	-	-	6/29/67/67	0/2/2/2
31	BCR	b	618	-	-	8/29/63/63	0/2/2/2
26	CHL	Q	315	-	3/3/20/26	20/39/137/137	-
26	CHL	Q	313	-	3/3/16/26	6/20/118/137	-
23	LUT	2	309	-	-	4/29/67/67	0/2/2/2
22	CLA	2	302	-	1/1/15/20	15/39/115/115	-
22	CLA	2	306	-	1/1/14/20	11/33/109/115	-
26	CHL	5	313	18	3/3/20/26	23/39/137/137	-
22	CLA	3	308	-	1/1/11/20	10/19/95/115	-
36	DGD	C	520	-	-	29/51/91/95	0/2/2/2
22	CLA	c	504	-	1/1/15/20	18/39/115/115	-
22	CLA	q	304	-	1/1/14/20	12/38/114/115	-
22	CLA	b	613	-	1/1/15/20	13/39/115/115	-
22	CLA	s	304	-	1/1/11/20	9/15/91/115	-
22	CLA	b	609	-	1/1/15/20	11/39/115/115	-
22	CLA	6	303	-	1/1/15/20	13/39/115/115	-
22	CLA	S	308	-	1/1/13/20	9/27/103/115	-
25	LHG	v	312	-	-	19/53/53/53	-
22	CLA	P	303	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PL9	d	404	-	-	9/53/73/73	0/1/1/1
26	CHL	U	316	-	3/3/20/26	11/39/137/137	-
31	BCR	D	404	-	-	13/29/63/63	0/2/2/2
22	CLA	A	404	-	1/1/15/20	11/39/115/115	-
26	CHL	v	318	-	3/3/20/26	21/39/137/137	-
26	CHL	N	315	-	3/3/16/26	9/20/118/137	-
23	LUT	1	310	-	-	0/29/67/67	0/2/2/2
32	SQD	L	102	-	-	21/49/69/69	0/1/1/1
31	BCR	C	518	-	-	11/29/63/63	0/2/2/2
22	CLA	b	616	-	1/1/15/20	9/39/115/115	-
22	CLA	3	301	-	1/1/15/20	13/39/115/115	-
23	LUT	V	309	-	-	2/29/67/67	0/2/2/2
30	PHO	A	407	-	-	11/37/103/103	0/5/6/6
26	CHL	1	313	-	3/3/20/26	10/39/137/137	-
32	SQD	C	501	-	-	26/45/65/69	0/1/1/1
26	CHL	q	313	-	3/3/16/26	7/20/118/137	-
25	LHG	a	415	-	-	26/47/47/53	-
26	CHL	S	314	-	3/3/16/26	5/15/113/137	-
26	CHL	v	313	-	3/3/20/26	18/39/137/137	-
22	CLA	N	304	-	1/1/15/20	16/39/115/115	-
26	CHL	U	317	-	3/3/20/26	18/39/137/137	-
22	CLA	Q	308	-	1/1/11/20	10/19/95/115	-
22	CLA	B	609	-	1/1/15/20	9/39/115/115	-
23	LUT	R	312	-	-	4/29/67/67	0/2/2/2

The worst 5 of 5851 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	409	BCR	C26-C25	15.98	1.61	1.34
31	a	409	BCR	C26-C25	15.98	1.61	1.34
31	b	619	BCR	C5-C6	15.96	1.61	1.34
31	B	619	BCR	C5-C6	15.94	1.61	1.34
31	x	202	BCR	C5-C6	15.92	1.61	1.34

The worst 5 of 5132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	311	XAT	O4-C5-C4	48.19	158.66	113.49
24	2	311	XAT	O4-C5-C4	47.98	158.46	113.49
24	n	311	XAT	O24-C25-C24	47.82	158.31	113.49
24	N	311	XAT	O24-C25-C24	47.82	158.31	113.49
24	4	311	XAT	O4-C5-C4	47.82	158.31	113.49

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 6770 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	r	601	CLA	C2B-C3B-CAB-CBB
22	r	601	CLA	C4B-C3B-CAB-CBB
22	r	604	CLA	C1A-C2A-CAA-CBA
22	r	604	CLA	CHA-CBD-CGD-O1D
22	r	604	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

459 monomers are involved in 949 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	614	CLA	4	0
22	5	308	CLA	1	0
26	V	313	CHL	7	0
26	N	317	CHL	5	0
25	s	312	LHG	3	0
31	z	101	BCR	2	0
22	6	307	CLA	2	0
22	V	304	CLA	2	0
26	G	311	CHL	4	0
22	4	302	CLA	5	0
22	n	302	CLA	6	0
23	p	311	LUT	4	0
26	v	317	CHL	1	0
26	g	311	CHL	6	0
22	b	612	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	q	310	LHG	2	0
22	b	608	CLA	3	0
22	4	308	CLA	1	0
22	U	305	CLA	2	0
26	R	316	CHL	1	0
22	1	308	CLA	2	0
25	c	523	LHG	3	0
23	v	309	LUT	3	0
26	P	318	CHL	3	0
22	b	602	CLA	4	0
26	6	314	CHL	2	0
22	v	302	CLA	6	0
22	v	307	CLA	2	0
31	k	101	BCR	2	0
22	P	309	CLA	2	0
22	B	608	CLA	1	0
23	S	311	LUT	5	0
24	U	311	XAT	5	0
27	s	317	NEX	4	0
22	5	304	CLA	2	0
22	4	306	CLA	5	0
22	C	514	CLA	2	0
26	6	301	CHL	5	0
36	B	601	DGD	6	0
23	U	310	LUT	3	0
22	N	307	CLA	3	0
22	C	506	CLA	3	0
36	c	519	DGD	1	0
26	4	316	CHL	2	0
22	P	302	CLA	3	0
22	R	308	CLA	1	0
22	S	301	CLA	2	0
22	d	402	CLA	2	0
22	g	302	CLA	1	0
22	B	606	CLA	4	0
25	d	406	LHG	7	0
22	1	305	CLA	1	0
22	G	302	CLA	3	0
31	x	202	BCR	3	0
23	u	310	LUT	4	0
22	R	302	CLA	1	0
22	b	607	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	C	516	BCR	2	0
26	p	314	CHL	3	0
26	u	318	CHL	6	0
25	5	312	LHG	1	0
22	a	405	CLA	3	0
26	n	317	CHL	1	0
22	3	304	CLA	3	0
26	g	314	CHL	2	0
26	2	317	CHL	1	0
26	S	315	CHL	2	0
22	B	613	CLA	3	0
35	a	414	BCT	1	0
22	V	305	CLA	1	0
22	u	305	CLA	4	0
22	b	610	CLA	2	0
22	D	403	CLA	3	0
23	r	611	LUT	4	0
36	b	601	DGD	7	0
23	n	309	LUT	3	0
22	r	607	CLA	1	0
24	G	309	XAT	3	0
22	n	306	CLA	1	0
25	2	312	LHG	3	0
22	B	614	CLA	4	0
22	r	610	CLA	2	0
22	c	506	CLA	1	0
25	p	313	LHG	2	0
26	s	314	CHL	1	0
22	C	509	CLA	1	0
37	e	101	HEM	1	0
22	n	307	CLA	1	0
23	s	310	LUT	6	0
22	G	301	CLA	2	0
22	s	302	CLA	1	0
22	C	508	CLA	2	0
26	V	316	CHL	4	0
22	v	306	CLA	1	0
31	C	517	BCR	1	0
22	6	308	CLA	1	0
22	b	604	CLA	5	0
34	C	521	LMG	3	0
22	R	307	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	v	303	CLA	1	0
24	r	612	XAT	4	0
22	S	305	CLA	2	0
27	v	319	NEX	2	0
22	P	306	CLA	1	0
22	2	307	CLA	4	0
36	c	517	DGD	4	0
32	m	101	SQD	1	0
31	B	619	BCR	4	0
26	5	317	CHL	3	0
22	p	309	CLA	2	0
25	3	310	LHG	3	0
22	C	513	CLA	1	0
22	r	606	CLA	4	0
26	s	315	CHL	1	0
22	B	604	CLA	4	0
26	r	615	CHL	2	0
36	c	518	DGD	3	0
26	p	317	CHL	4	0
26	4	317	CHL	5	0
22	c	513	CLA	3	0
24	R	313	XAT	3	0
26	n	313	CHL	3	0
36	a	416	DGD	2	0
22	r	601	CLA	1	0
26	6	316	CHL	2	0
26	1	317	CHL	2	0
31	t	101	BCR	6	0
22	R	311	CLA	2	0
22	q	301	CLA	1	0
26	N	316	CHL	2	0
31	B	618	BCR	6	0
26	q	315	CHL	3	0
31	K	101	BCR	2	0
22	a	406	CLA	2	0
22	U	302	CLA	2	0
24	5	311	XAT	3	0
26	3	312	CHL	1	0
23	1	309	LUT	2	0
22	C	511	CLA	3	0
26	3	313	CHL	2	0
22	r	604	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	q	303	CLA	2	0
22	V	301	CLA	3	0
22	2	301	CLA	4	0
26	P	319	CHL	9	0
32	A	412	SQD	3	0
24	4	311	XAT	1	0
22	c	505	CLA	2	0
26	G	312	CHL	1	0
26	3	316	CHL	1	0
26	p	315	CHL	1	0
22	R	310	CLA	2	0
24	1	311	XAT	2	0
34	a	412	LMG	1	0
25	D	407	LHG	7	0
26	G	315	CHL	2	0
22	c	507	CLA	2	0
22	R	304	CLA	4	0
22	u	302	CLA	2	0
34	c	520	LMG	2	0
22	X	202	CLA	1	0
22	R	305	CLA	2	0
34	b	621	LMG	4	0
22	c	509	CLA	3	0
23	v	310	LUT	4	0
22	4	301	CLA	4	0
22	c	511	CLA	3	0
24	6	310	XAT	4	0
30	d	401	PHO	1	0
22	r	609	CLA	3	0
32	a	410	SQD	3	0
26	n	318	CHL	6	0
22	3	307	CLA	2	0
22	C	503	CLA	1	0
22	5	303	CLA	1	0
36	A	414	DGD	2	0
26	u	313	CHL	1	0
22	U	307	CLA	1	0
24	u	311	XAT	3	0
22	3	302	CLA	3	0
26	g	312	CHL	1	0
22	Q	301	CLA	3	0
34	B	621	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	s	306	CLA	3	0
22	p	304	CLA	1	0
25	Q	310	LHG	4	0
22	6	302	CLA	3	0
24	N	311	XAT	2	0
22	p	303	CLA	3	0
22	1	303	CLA	1	0
26	u	314	CHL	1	0
26	q	311	CHL	7	0
25	N	312	LHG	4	0
23	N	309	LUT	5	0
25	P	313	LHG	1	0
22	N	306	CLA	1	0
22	g	303	CLA	1	0
23	U	309	LUT	1	0
31	c	515	BCR	1	0
22	v	301	CLA	1	0
22	2	304	CLA	3	0
26	G	314	CHL	4	0
22	s	307	CLA	2	0
26	4	314	CHL	1	0
24	V	311	XAT	4	0
26	Q	316	CHL	2	0
23	P	310	LUT	3	0
27	u	319	NEX	1	0
22	c	514	CLA	3	0
23	P	311	LUT	4	0
26	R	317	CHL	3	0
22	A	405	CLA	5	0
26	p	320	CHL	2	0
25	V	312	LHG	6	0
26	U	315	CHL	5	0
27	S	317	NEX	3	0
22	C	515	CLA	3	0
23	N	310	LUT	4	0
31	b	619	BCR	4	0
22	3	303	CLA	2	0
22	S	304	CLA	2	0
31	a	409	BCR	3	0
26	Q	314	CHL	1	0
26	N	313	CHL	5	0
34	b	624	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	5	314	CHL	1	0
22	Q	302	CLA	4	0
22	q	302	CLA	2	0
34	A	411	LMG	1	0
22	Q	307	CLA	3	0
25	c	521	LHG	4	0
22	B	607	CLA	2	0
31	T	101	BCR	5	0
22	c	510	CLA	2	0
27	V	319	NEX	3	0
34	w	201	LMG	2	0
34	C	502	LMG	1	0
22	u	307	CLA	2	0
22	C	504	CLA	2	0
22	c	508	CLA	1	0
27	p	301	NEX	4	0
22	Q	305	CLA	1	0
34	W	201	LMG	2	0
22	n	304	CLA	1	0
26	1	314	CHL	1	0
26	g	315	CHL	3	0
22	3	306	CLA	2	0
31	X	201	BCR	4	0
26	q	314	CHL	2	0
22	P	308	CLA	3	0
25	S	312	LHG	5	0
25	A	413	LHG	3	0
22	6	304	CLA	1	0
22	N	308	CLA	1	0
22	P	304	CLA	1	0
25	u	312	LHG	2	0
22	n	301	CLA	3	0
22	G	303	CLA	1	0
26	V	317	CHL	2	0
22	A	406	CLA	2	0
22	B	602	CLA	4	0
22	5	302	CLA	6	0
22	q	307	CLA	2	0
22	N	303	CLA	1	0
24	P	312	XAT	4	0
22	5	307	CLA	2	0
22	V	307	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	U	319	CHL	6	0
26	v	316	CHL	7	0
26	2	314	CHL	1	0
22	6	305	CLA	3	0
25	r	613	LHG	1	0
25	g	310	LHG	2	0
27	r	618	NEX	3	0
33	D	405	PL9	3	0
22	C	505	CLA	4	0
22	n	305	CLA	1	0
22	6	309	CLA	1	0
22	G	307	CLA	3	0
22	b	605	CLA	1	0
23	n	310	LUT	4	0
22	4	307	CLA	4	0
30	a	407	PHO	2	0
22	p	307	CLA	2	0
22	1	302	CLA	4	0
34	B	624	LMG	1	0
24	g	309	XAT	5	0
25	L	101	LHG	2	0
22	a	404	CLA	1	0
22	1	307	CLA	3	0
22	g	304	CLA	1	0
22	C	512	CLA	3	0
24	p	312	XAT	3	0
22	V	306	CLA	2	0
27	R	301	NEX	3	0
26	p	319	CHL	4	0
25	d	405	LHG	5	0
26	3	314	CHL	6	0
26	6	317	CHL	2	0
26	3	311	CHL	4	0
22	g	301	CLA	1	0
26	S	313	CHL	1	0
22	c	512	CLA	1	0
22	B	605	CLA	2	0
22	1	306	CLA	2	0
23	5	309	LUT	6	0
22	5	306	CLA	2	0
22	P	305	CLA	2	0
23	V	310	LUT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	5	301	CLA	4	0
22	P	307	CLA	2	0
22	Q	303	CLA	1	0
23	p	310	LUT	1	0
22	p	302	CLA	2	0
23	2	310	LUT	4	0
36	C	519	DGD	4	0
22	N	305	CLA	1	0
22	C	507	CLA	1	0
27	2	319	NEX	1	0
26	2	313	CHL	1	0
30	D	401	PHO	1	0
25	n	312	LHG	1	0
32	l	102	SQD	3	0
23	4	309	LUT	4	0
22	s	301	CLA	2	0
26	r	616	CHL	4	0
22	R	303	CLA	2	0
26	Q	311	CHL	2	0
22	b	615	CLA	1	0
26	6	312	CHL	2	0
22	1	301	CLA	3	0
26	5	316	CHL	3	0
22	B	603	CLA	3	0
31	A	409	BCR	4	0
24	q	309	XAT	1	0
26	6	313	CHL	1	0
22	q	308	CLA	3	0
26	r	614	CHL	2	0
22	q	306	CLA	1	0
22	c	503	CLA	1	0
26	U	314	CHL	2	0
24	n	311	XAT	1	0
31	B	620	BCR	1	0
23	S	310	LUT	4	0
22	2	303	CLA	1	0
22	S	302	CLA	1	0
26	2	318	CHL	6	0
22	a	408	CLA	1	0
22	S	307	CLA	1	0
22	V	303	CLA	2	0
22	V	308	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	n	308	CLA	2	0
25	C	522	LHG	3	0
22	2	308	CLA	1	0
27	N	318	NEX	2	0
26	n	316	CHL	6	0
22	A	408	CLA	1	0
35	D	402	BCT	1	0
26	2	316	CHL	6	0
22	N	302	CLA	5	0
26	1	316	CHL	3	0
24	v	311	XAT	3	0
32	a	413	SQD	3	0
27	5	319	NEX	2	0
25	l	101	LHG	1	0
34	c	501	LMG	1	0
22	N	301	CLA	3	0
26	P	317	CHL	5	0
22	s	305	CLA	4	0
22	5	305	CLA	2	0
26	6	315	CHL	7	0
22	v	304	CLA	3	0
27	n	319	NEX	2	0
22	b	603	CLA	6	0
22	U	306	CLA	4	0
26	P	315	CHL	1	0
22	C	510	CLA	4	0
22	U	301	CLA	2	0
22	p	305	CLA	2	0
26	u	316	CHL	3	0
26	U	313	CHL	1	0
22	B	615	CLA	1	0
22	V	302	CLA	3	0
32	M	101	SQD	1	0
27	r	617	NEX	4	0
27	u	320	NEX	2	0
22	p	308	CLA	1	0
26	R	315	CHL	1	0
22	U	304	CLA	1	0
22	n	303	CLA	1	0
22	p	306	CLA	1	0
22	2	305	CLA	3	0
26	5	318	CHL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	610	CLA	4	0
25	6	311	LHG	3	0
37	E	101	HEM	1	0
25	D	406	LHG	4	0
22	v	305	CLA	1	0
26	3	315	CHL	3	0
22	g	307	CLA	1	0
26	V	318	CHL	4	0
26	u	317	CHL	1	0
36	J	101	DGD	2	0
23	4	310	LUT	5	0
25	C	524	LHG	2	0
26	1	318	CHL	5	0
27	P	301	NEX	1	0
22	c	502	CLA	1	0
31	b	620	BCR	3	0
25	U	312	LHG	4	0
26	4	313	CHL	3	0
24	3	309	XAT	2	0
24	2	311	XAT	5	0
23	u	309	LUT	2	0
22	S	306	CLA	2	0
22	u	306	CLA	2	0
26	G	316	CHL	2	0
22	r	602	CLA	3	0
25	4	312	LHG	1	0
22	r	603	CLA	4	0
22	b	606	CLA	3	0
23	5	310	LUT	8	0
22	b	617	CLA	2	0
22	u	301	CLA	5	0
23	s	311	LUT	4	0
31	b	618	BCR	5	0
26	Q	315	CHL	4	0
23	2	309	LUT	4	0
22	2	302	CLA	5	0
22	2	306	CLA	2	0
26	5	313	CHL	2	0
36	C	520	DGD	3	0
22	c	504	CLA	4	0
22	b	613	CLA	3	0
22	s	304	CLA	2	0

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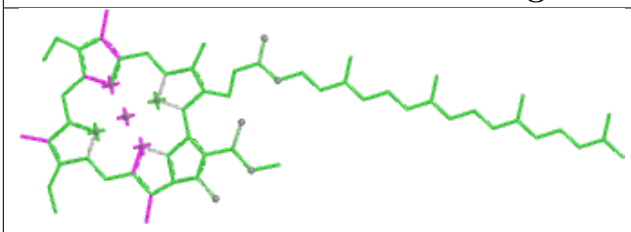
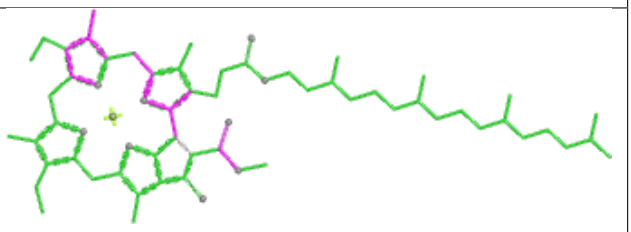
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	303	CLA	1	0
25	v	312	LHG	4	0
22	P	303	CLA	4	0
33	d	404	PL9	3	0
31	D	404	BCR	1	0
22	A	404	CLA	1	0
23	1	310	LUT	3	0
26	v	318	CHL	7	0
32	L	102	SQD	2	0
31	C	518	BCR	1	0
22	b	616	CLA	1	0
22	3	301	CLA	3	0
23	V	309	LUT	5	0
30	A	407	PHO	4	0
26	1	313	CHL	1	0
32	C	501	SQD	2	0
25	a	415	LHG	1	0
26	q	313	CHL	1	0
26	S	314	CHL	1	0
26	v	313	CHL	1	0
26	U	317	CHL	6	0
22	Q	308	CLA	2	0
22	B	609	CLA	1	0
23	R	312	LUT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

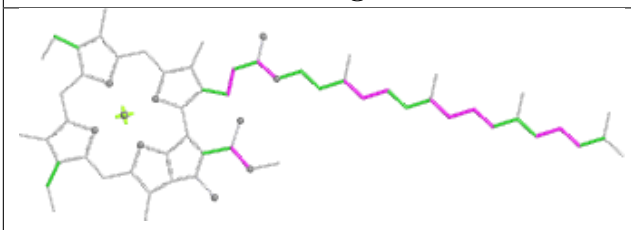
Ligand CLA b 614



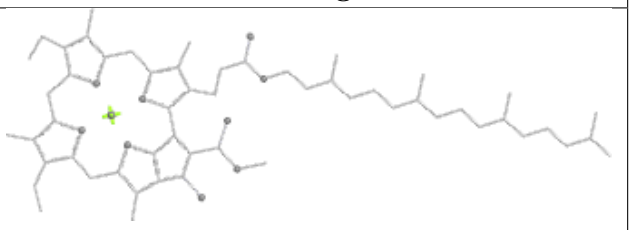
Bond lengths



Bond angles

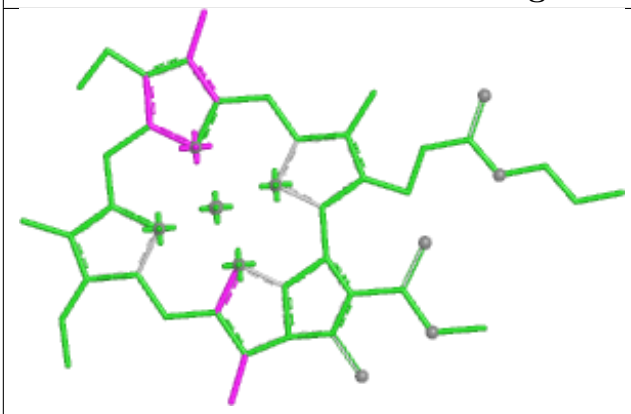


Torsions

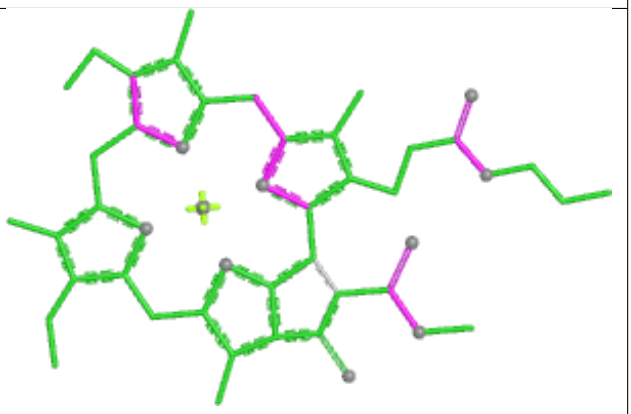


Rings

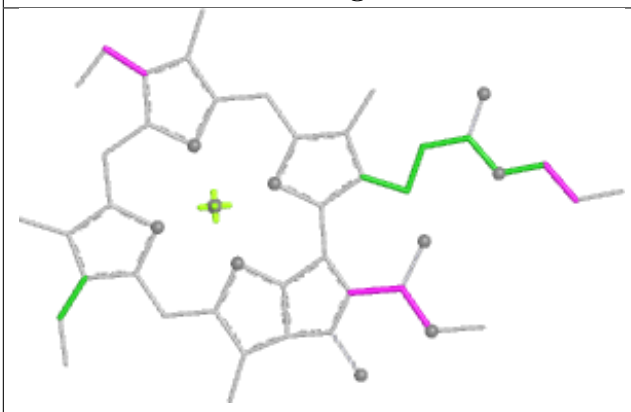
Ligand CLA 5 308



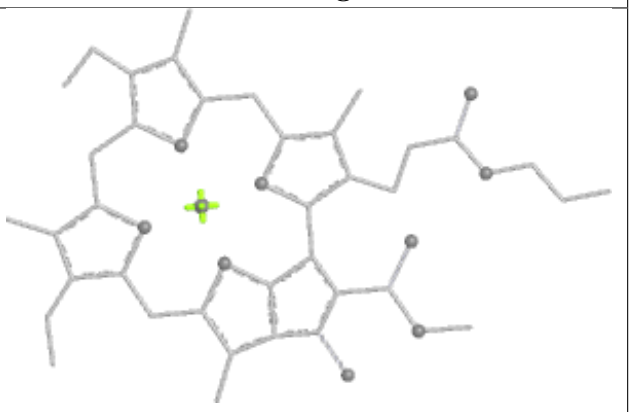
Bond lengths



Bond angles

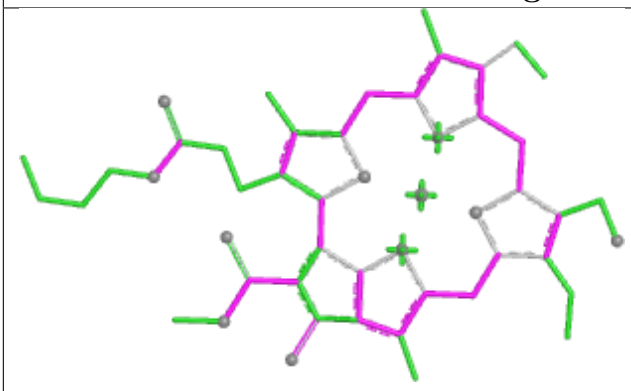


Torsions

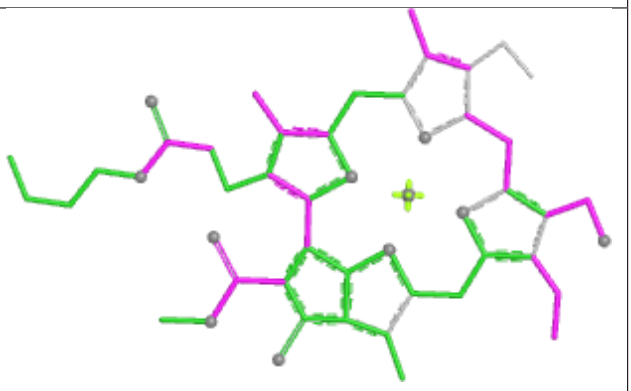


Rings

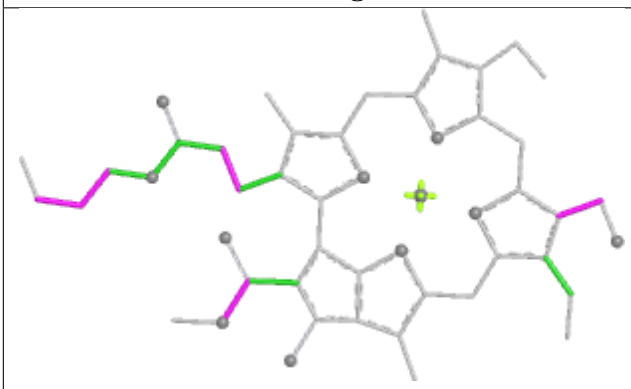
Ligand CHL V 315



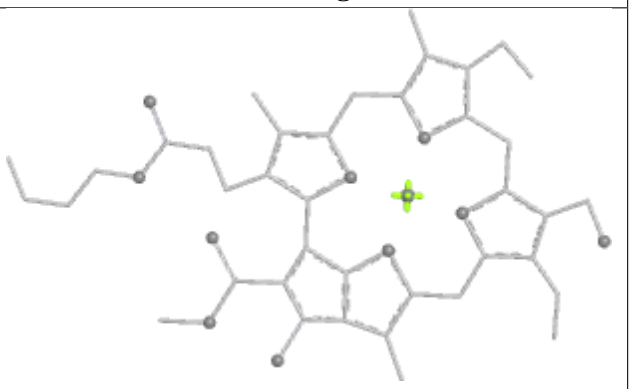
Bond lengths



Bond angles

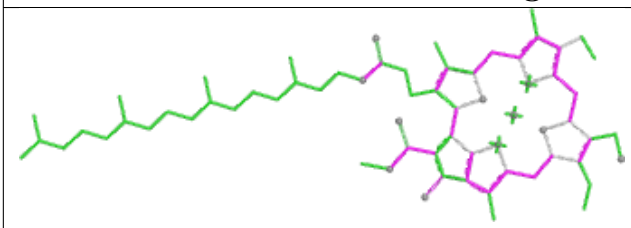


Torsions

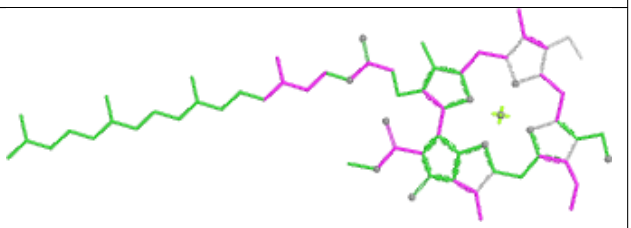


Rings

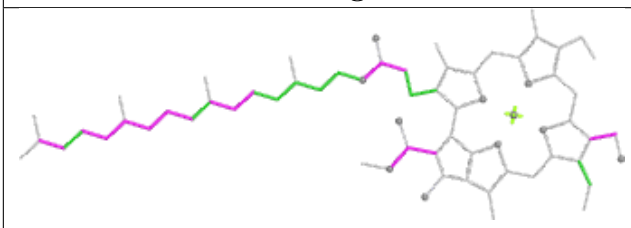
Ligand CHL V 313



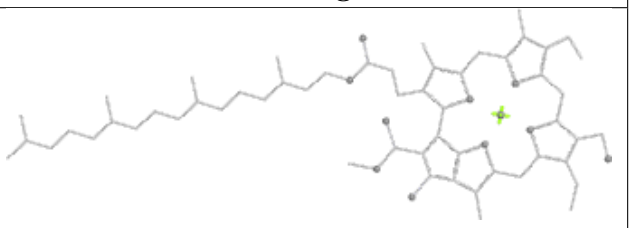
Bond lengths



Bond angles

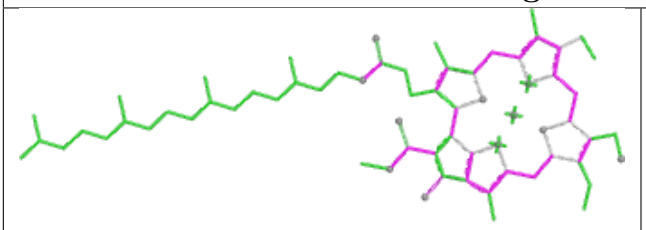


Torsions

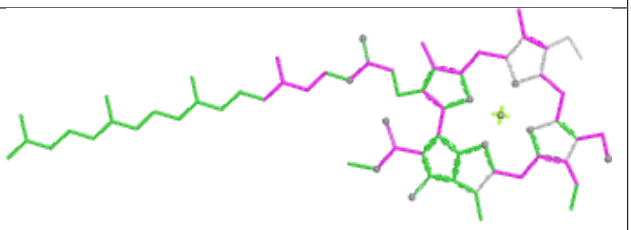


Rings

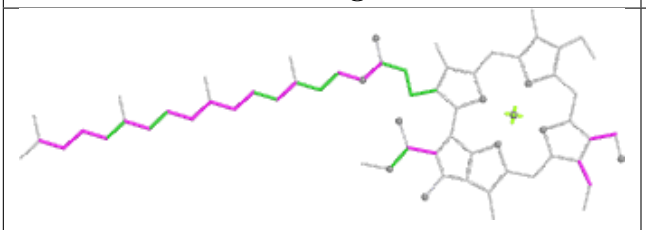
Ligand CHL N 317



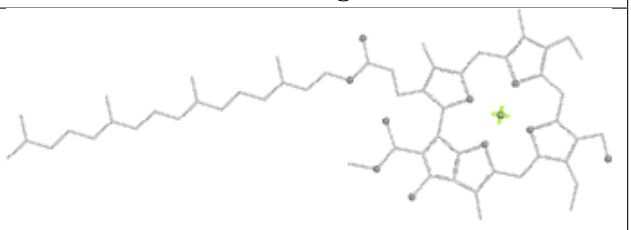
Bond lengths



Bond angles

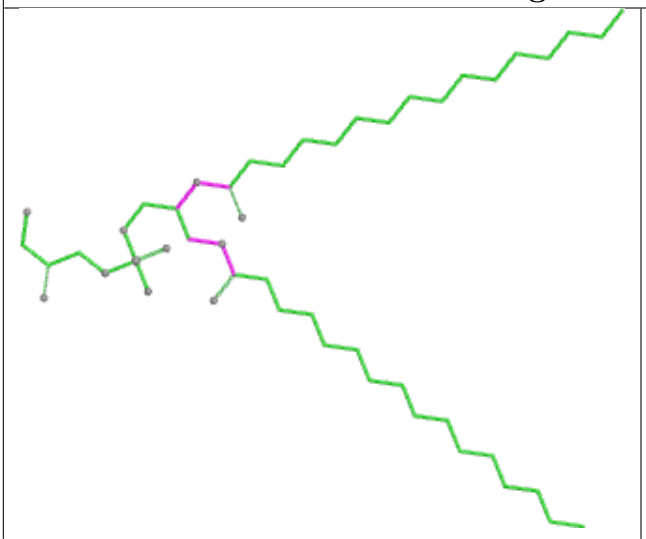


Torsions



Rings

Ligand LHG s 312



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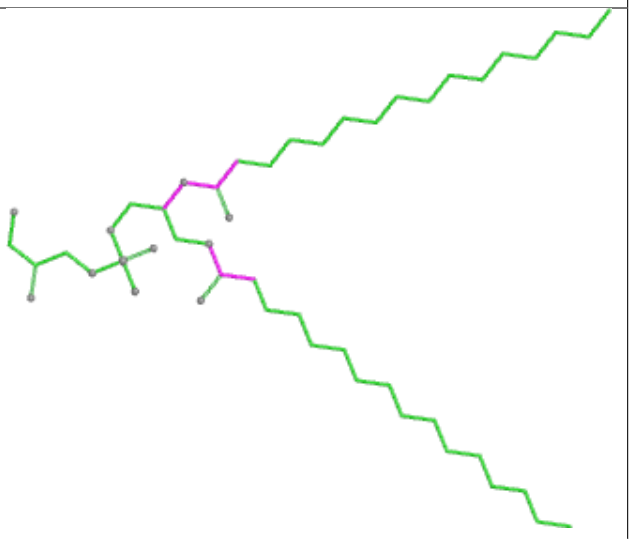

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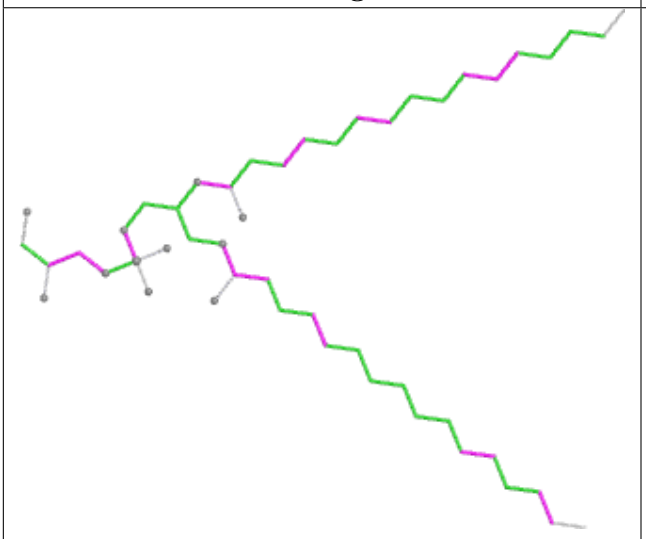

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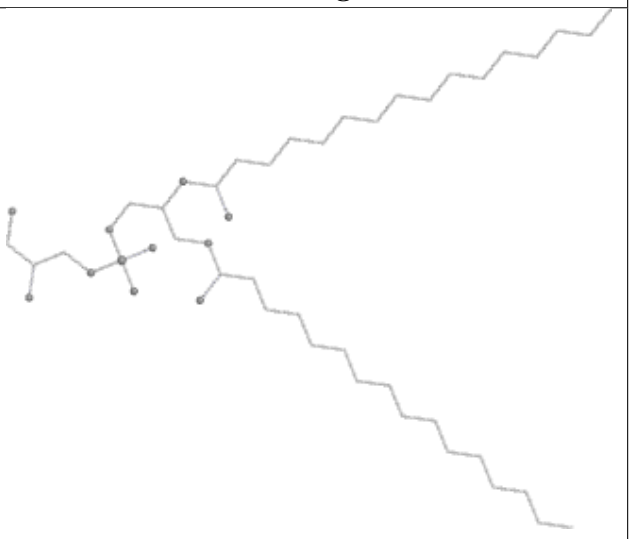
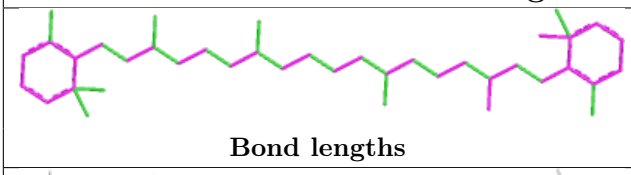


Rings

Ligand BCR z 101



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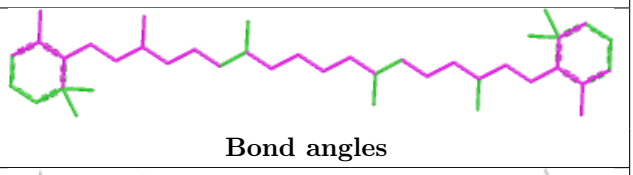

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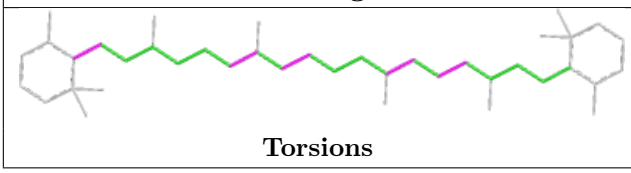

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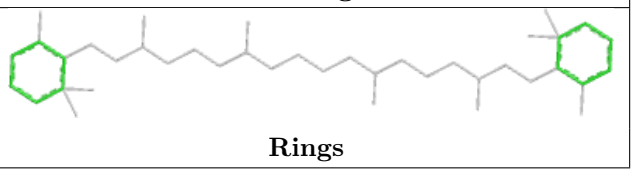
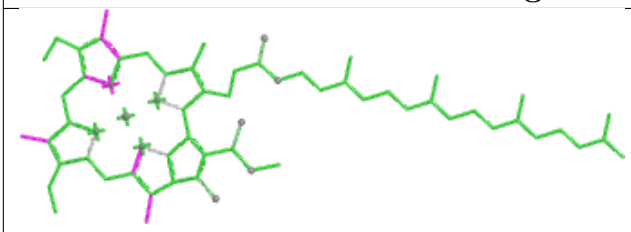


Rings

Ligand CLA B 616



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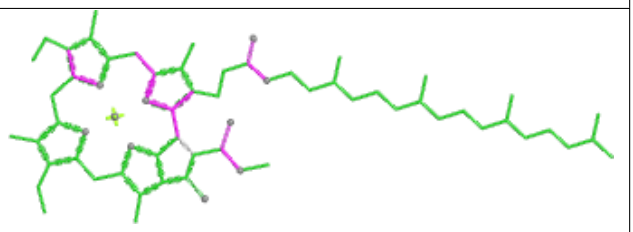

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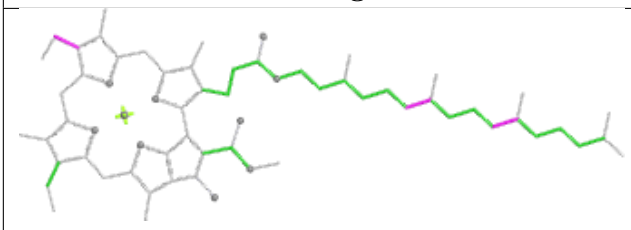

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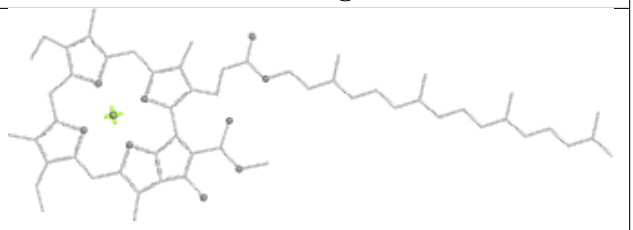
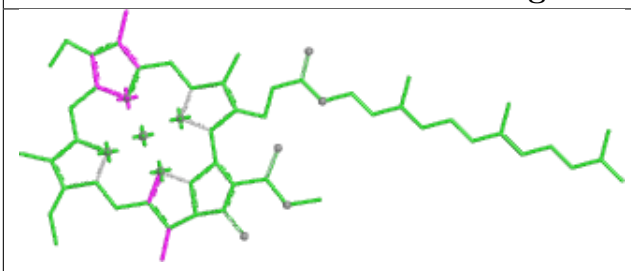


Rings

Ligand CLA 6 307



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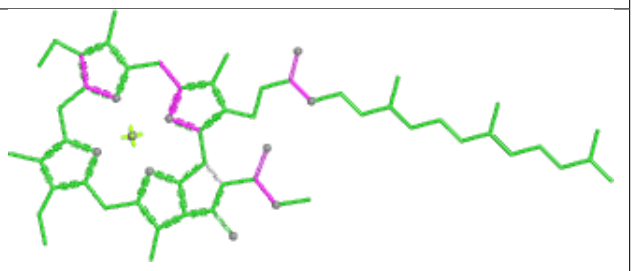

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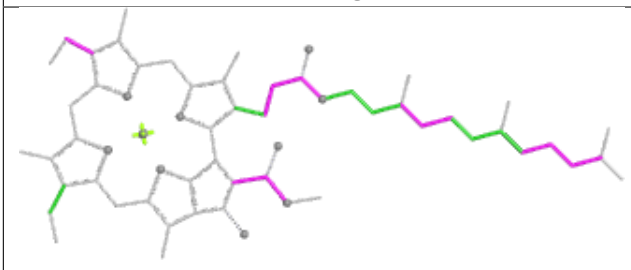

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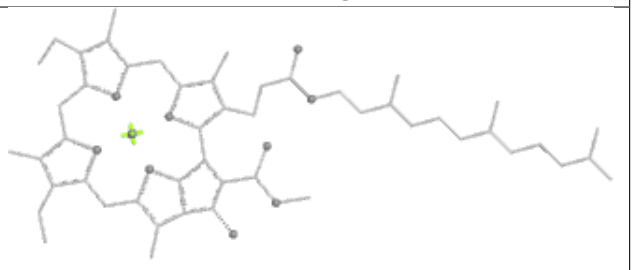
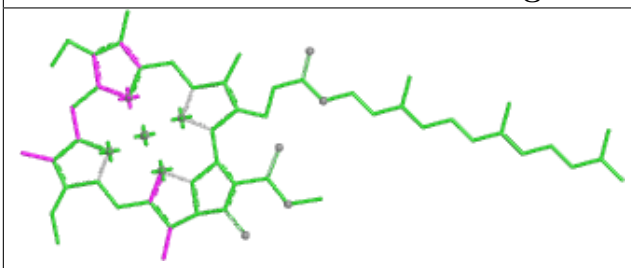


Rings

Ligand CLA V 304



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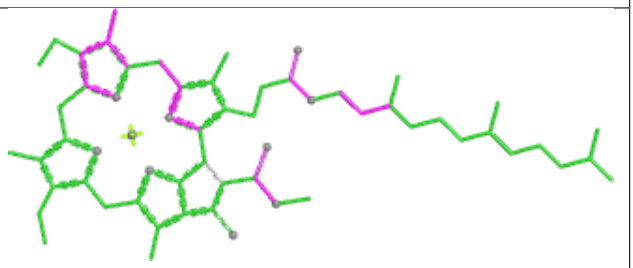
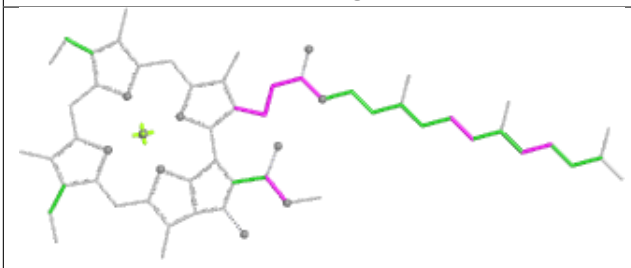


Bond angles



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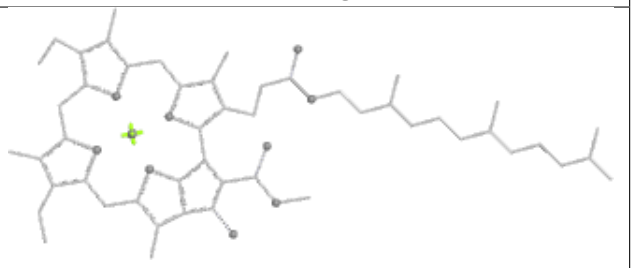
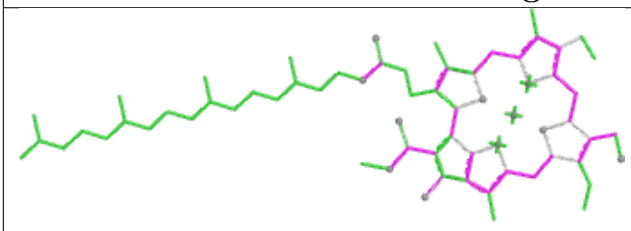


Rings

Ligand CHL G 311



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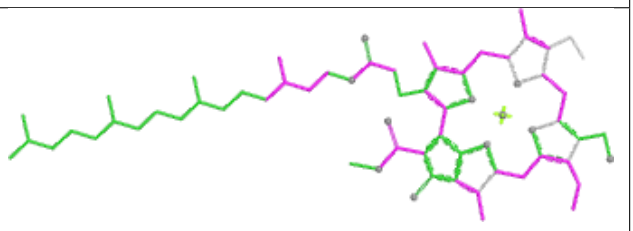

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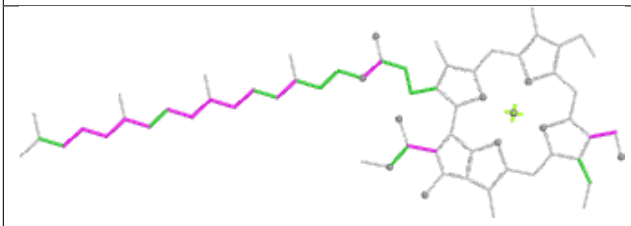

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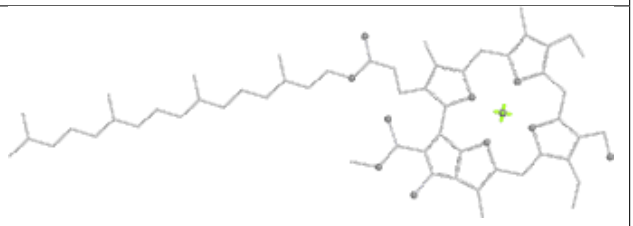
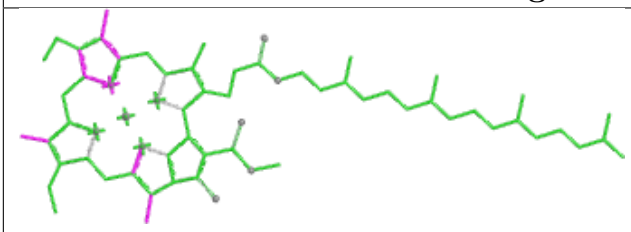


Rings

Ligand CLA 4 302



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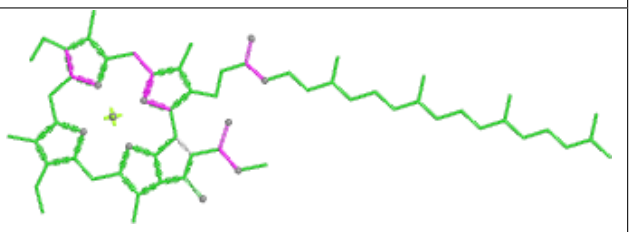

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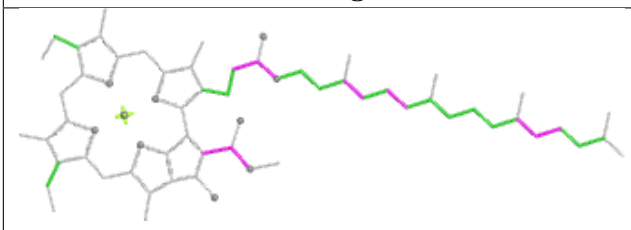

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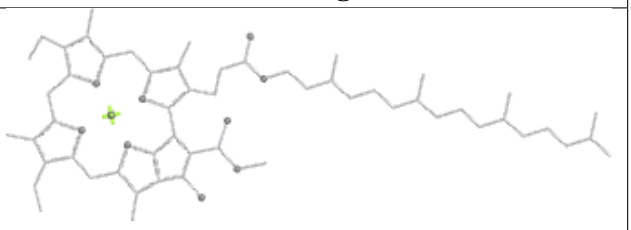
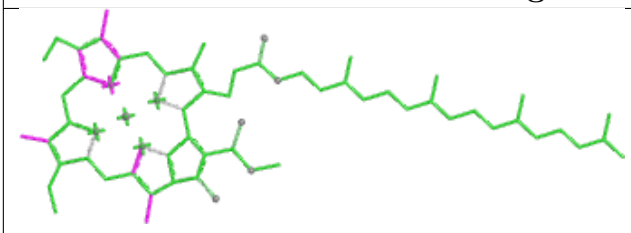


Rings

Ligand CLA n 302



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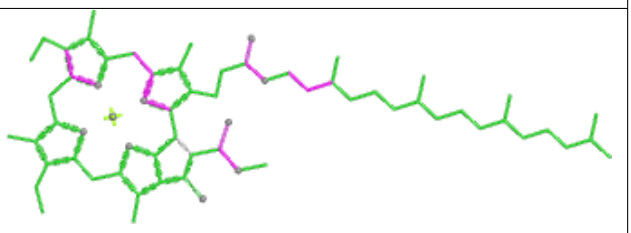

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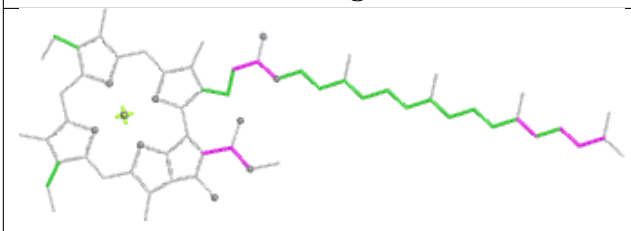

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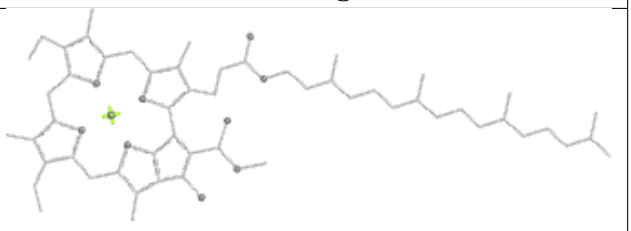
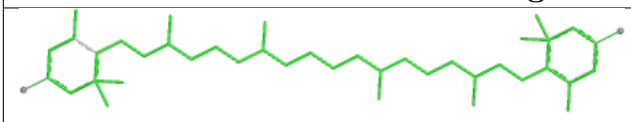


Rings

Ligand LUT p 311



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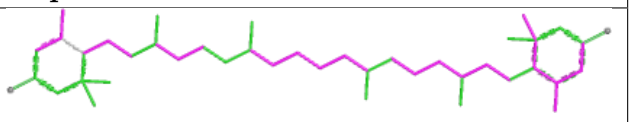
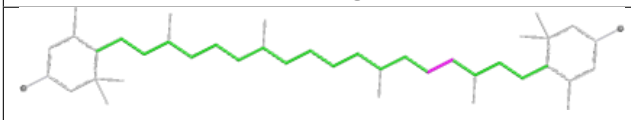


Bond angles



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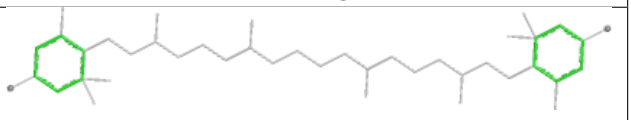
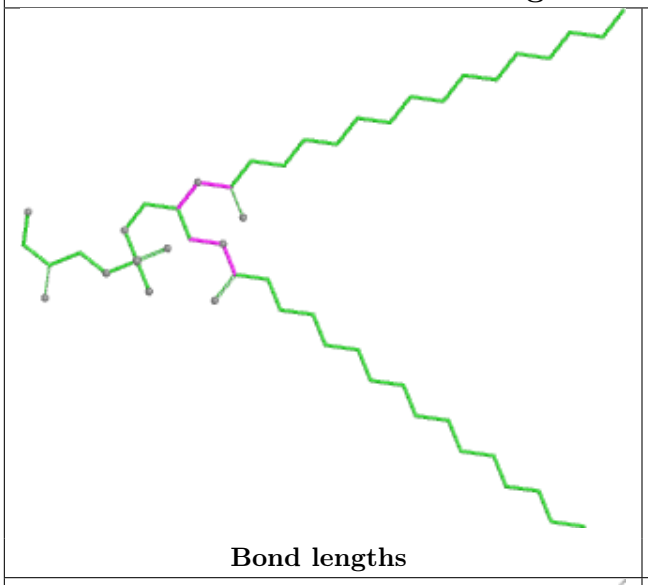


Rings

Ligand LHG b 623



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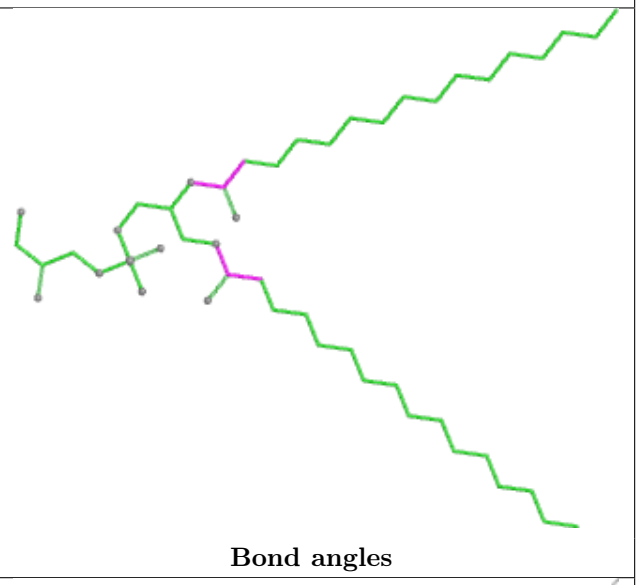
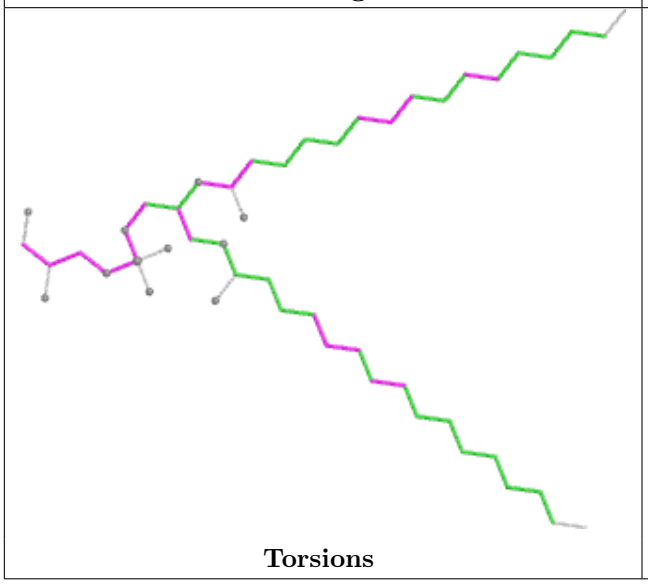


Bond angles



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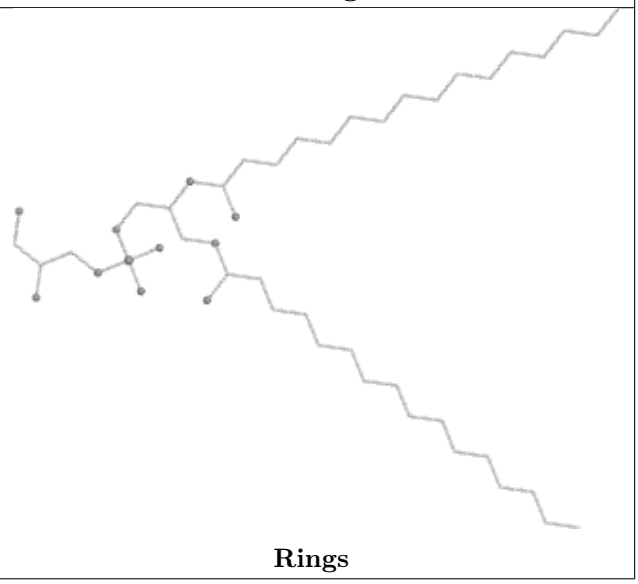
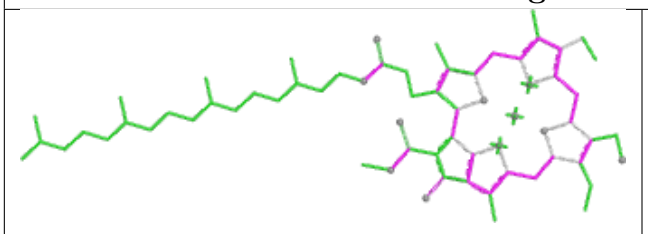


Rings

Ligand CHL v 317



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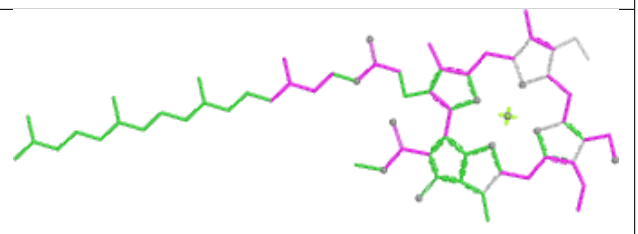
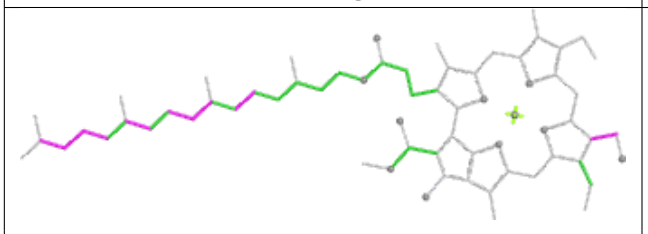
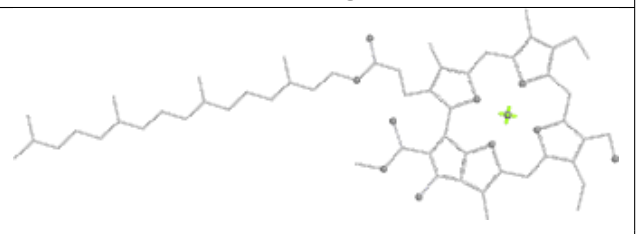


Bond angles

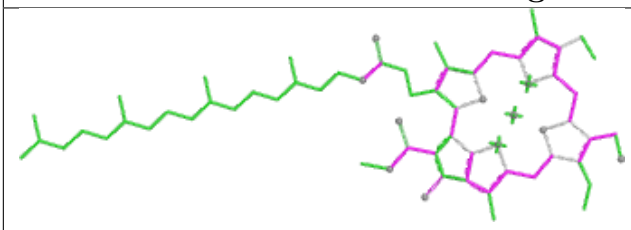


Torsions



Rings

Ligand CHL g 311



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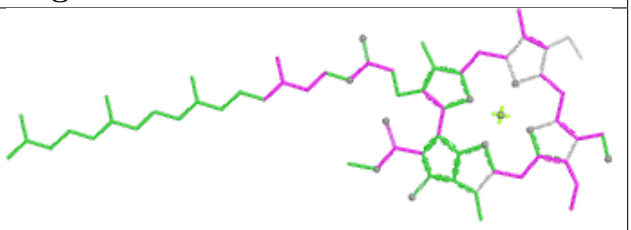
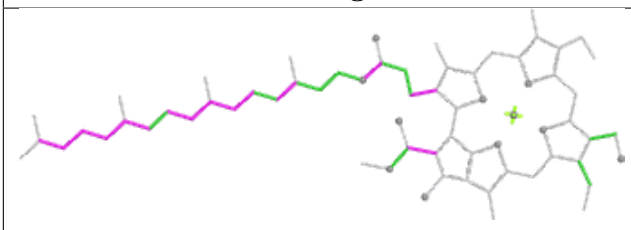
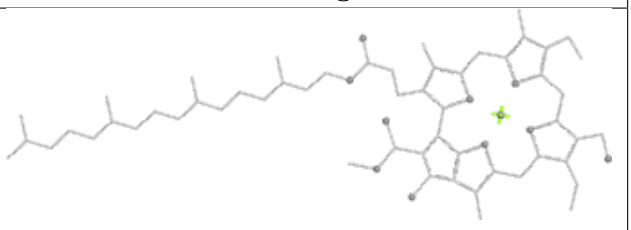


Bond angles

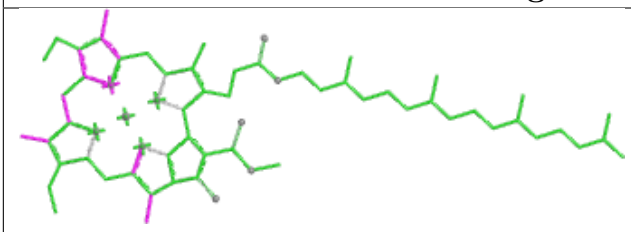


Torsions



Rings

Ligand CLA b 612



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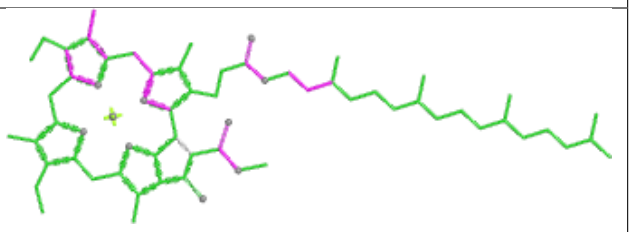
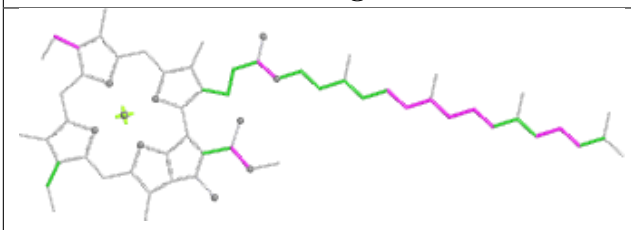
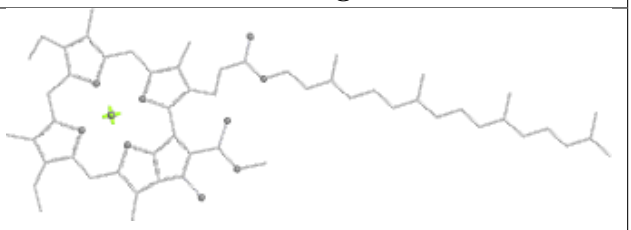


Bond angles

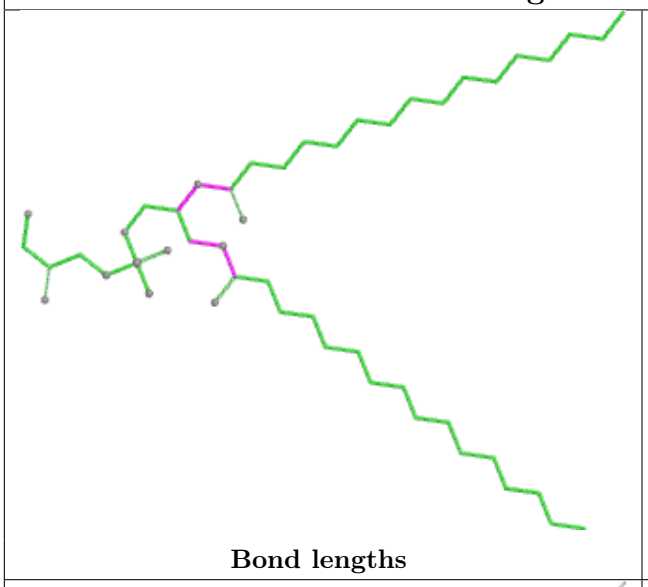


Torsions

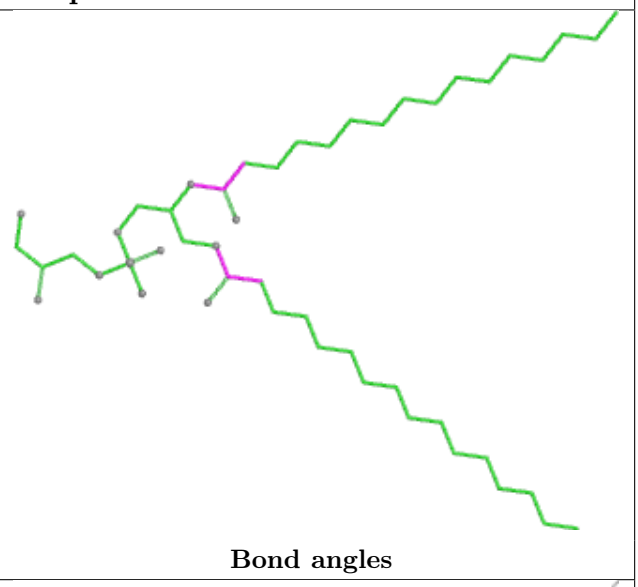


Rings

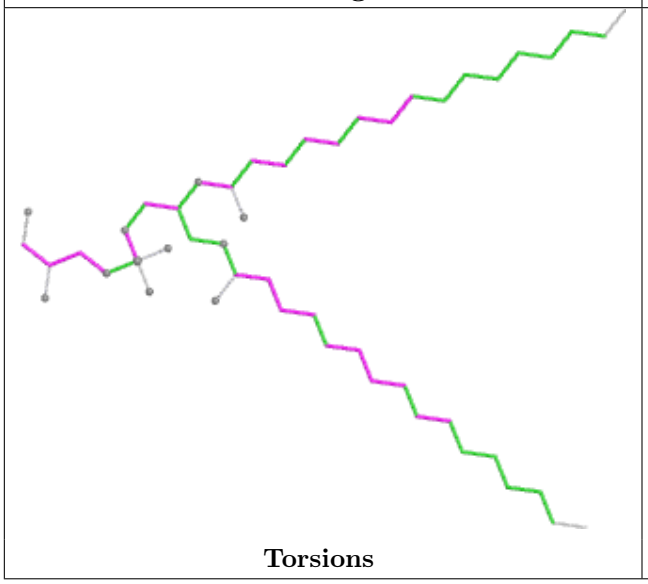
Ligand LHG q 310



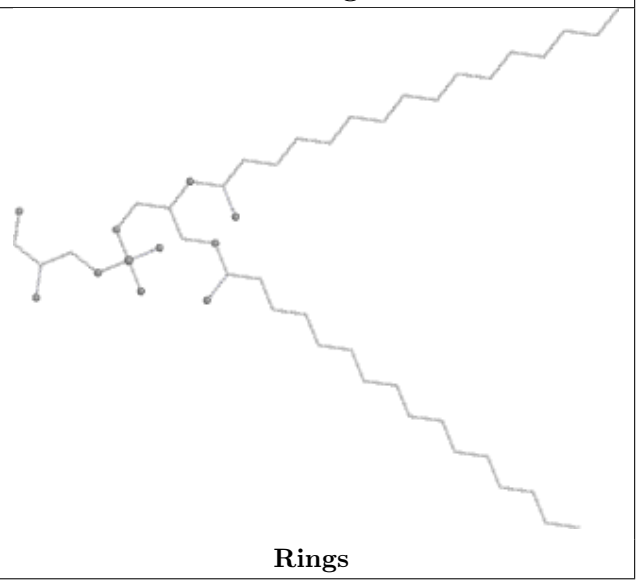
Bond lengths



Bond angles

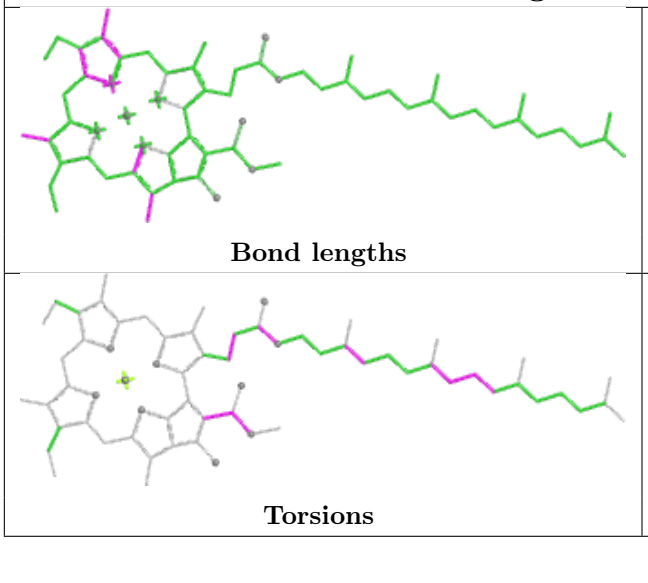


Torsions



Rings

Ligand CLA b 608



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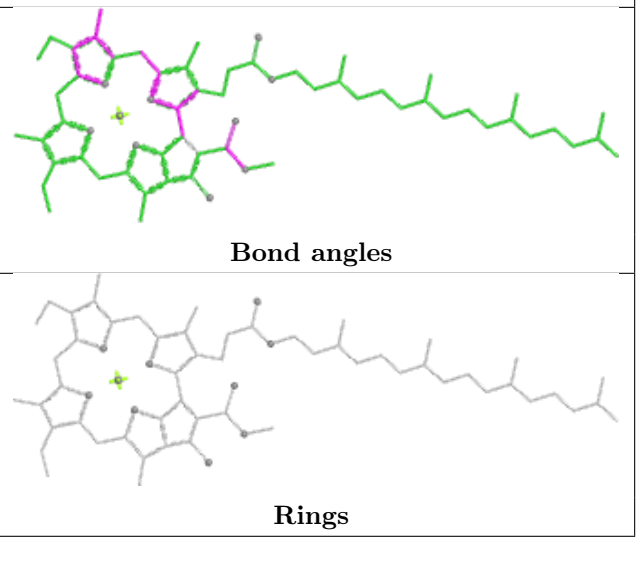
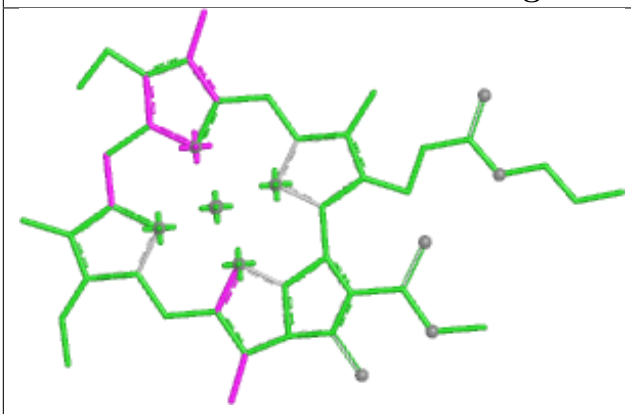


Bond angles

Torsions

Rings

Ligand CLA G 308



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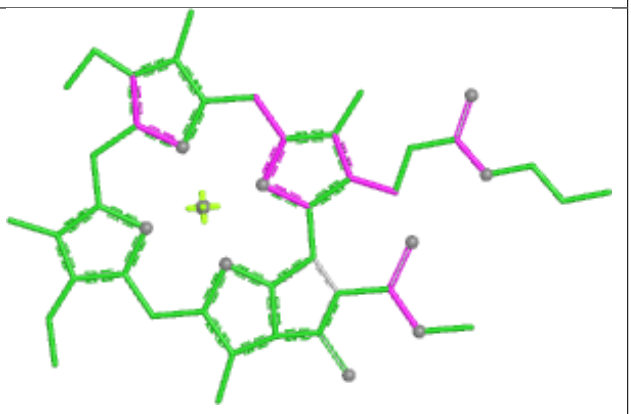

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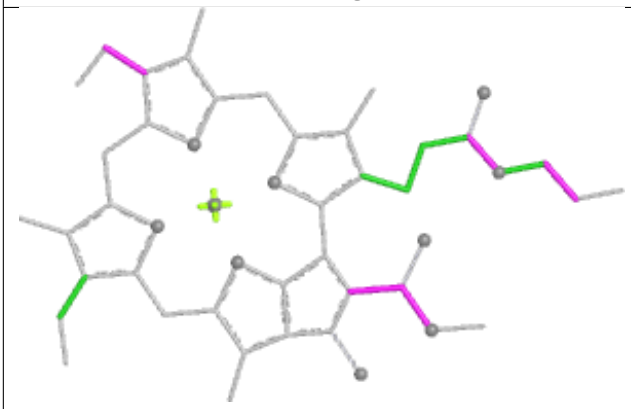

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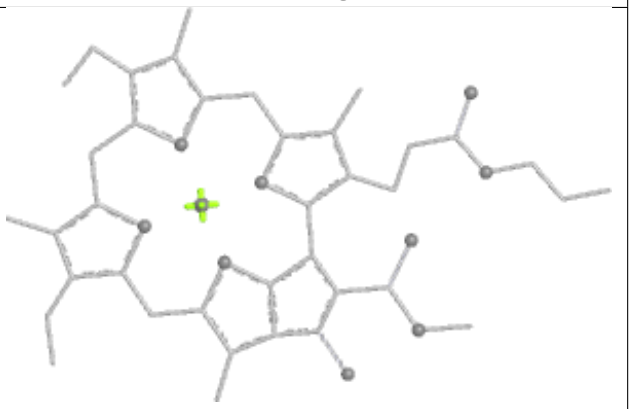
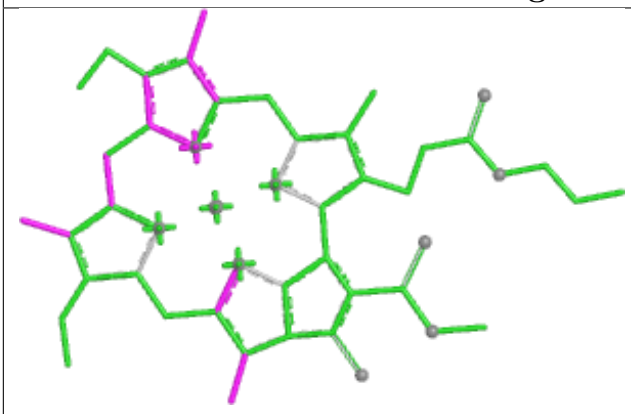


Rings

Ligand CLA 4 308



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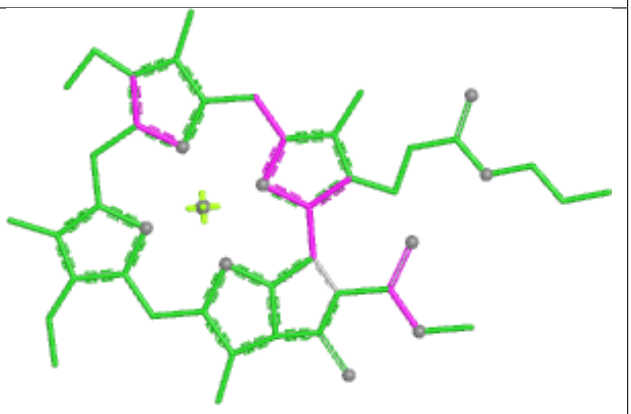

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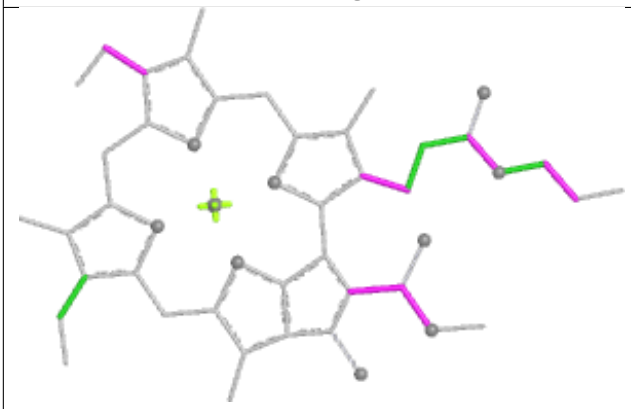

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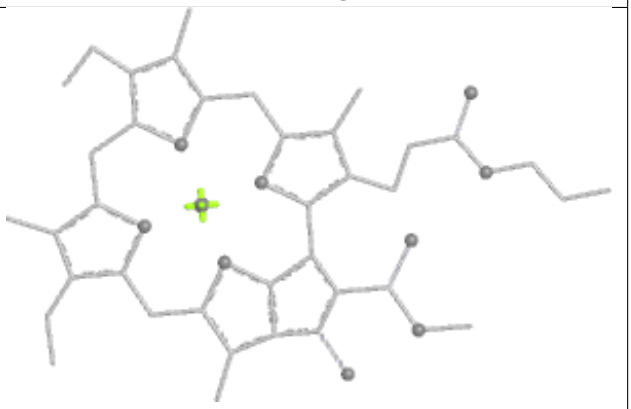
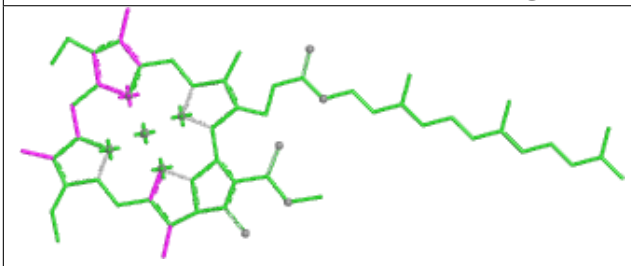


Rings

Ligand CLA U 305



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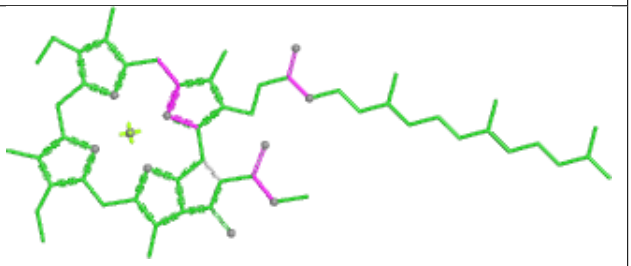
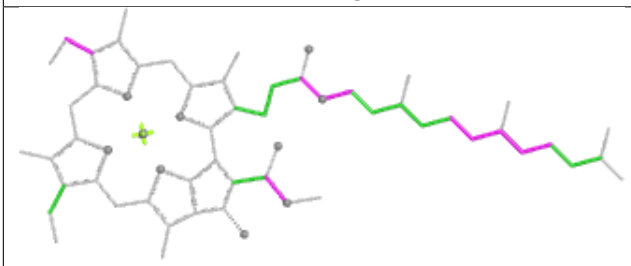


Bond angles



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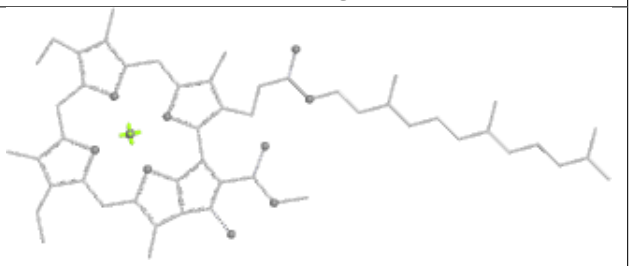
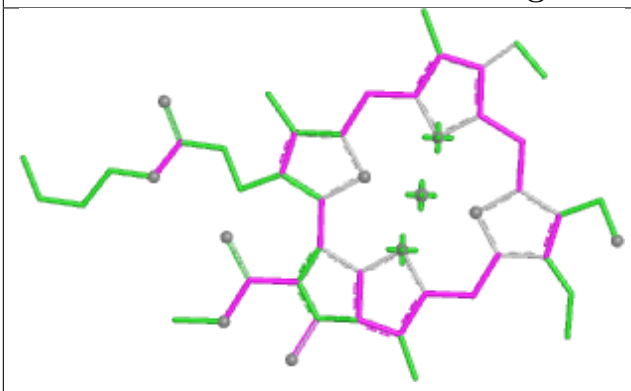


Rings

Ligand CHL v 315



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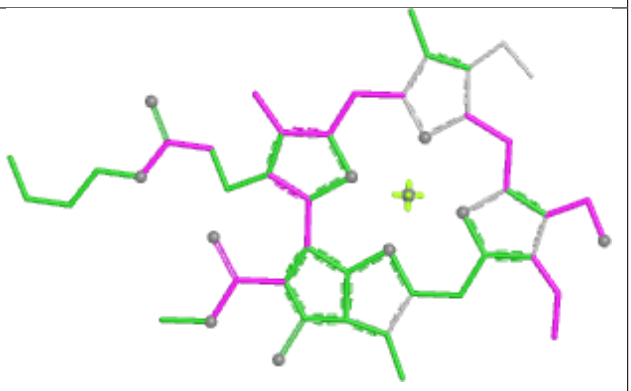

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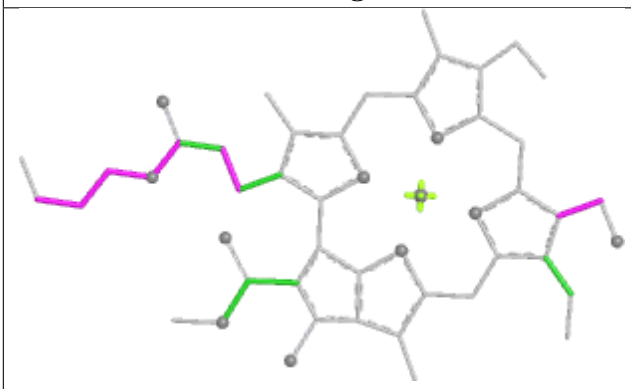

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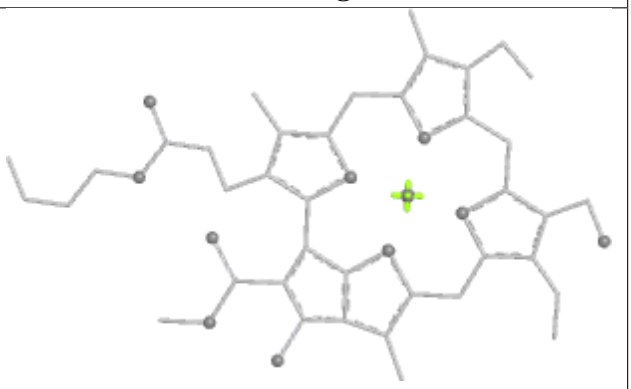
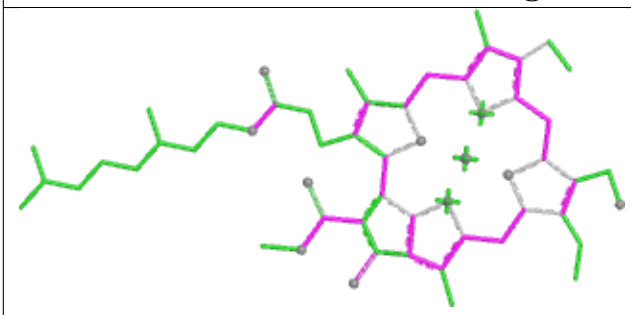


Rings

Ligand CHL R 316



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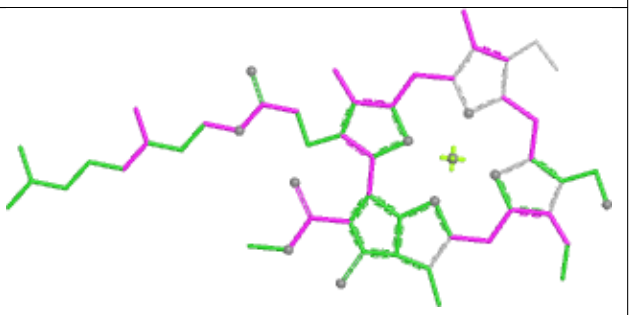
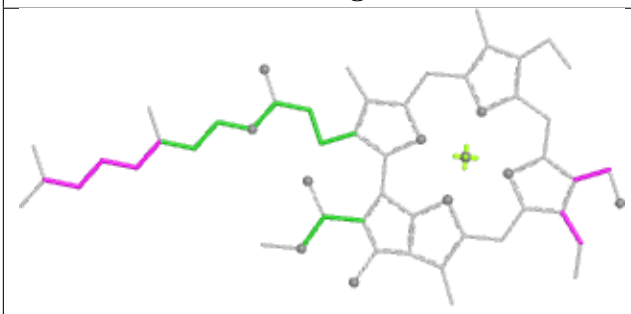


Bond angles



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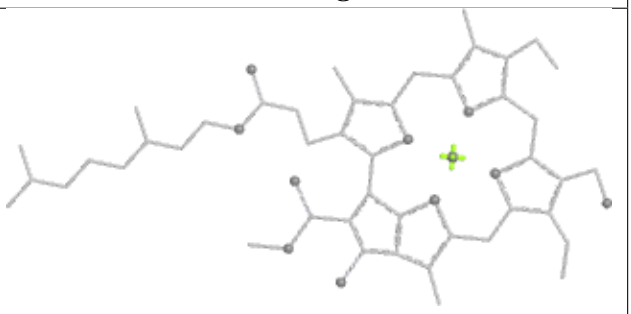
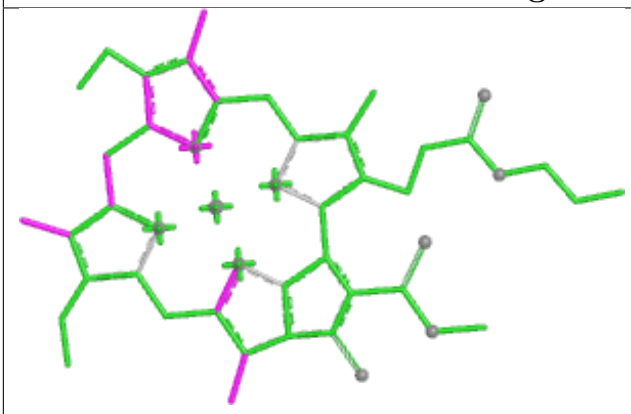


Rings

Ligand CLA 1 308



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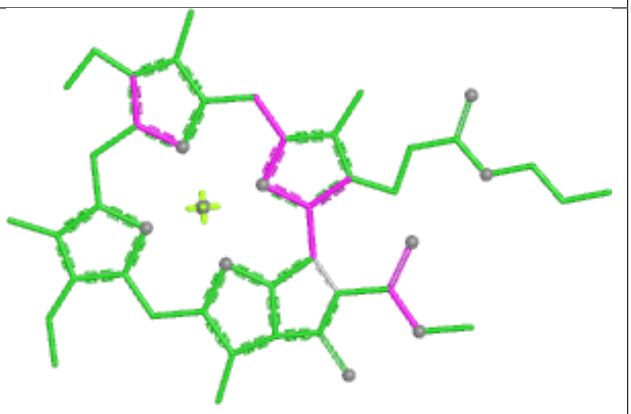
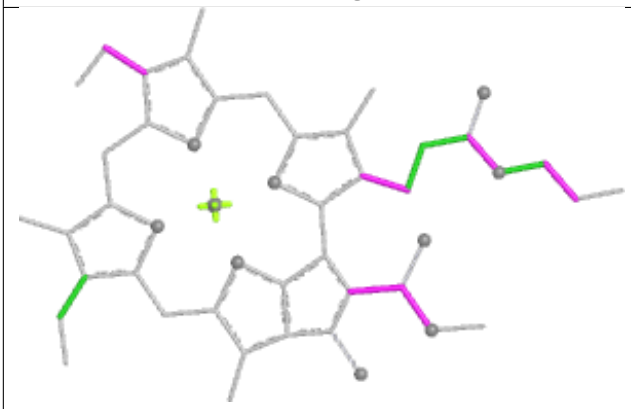
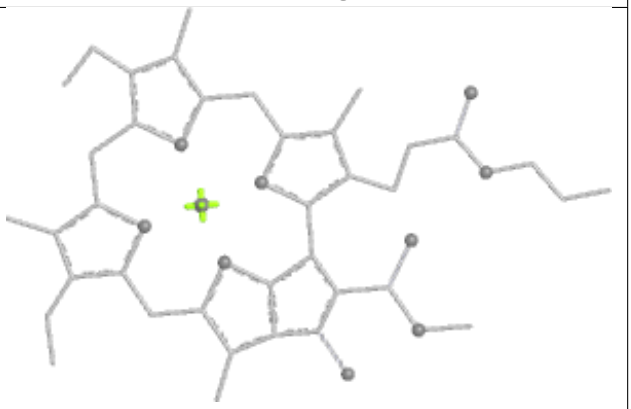


Bond angles

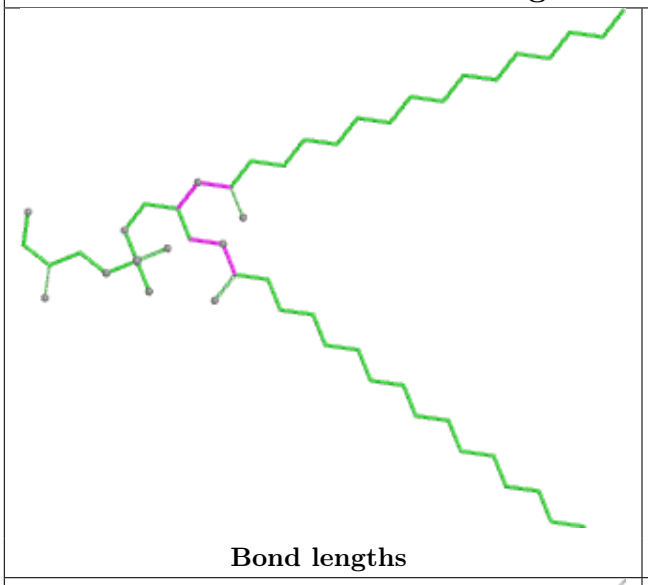


Torsions



Rings

Ligand LHG c 523



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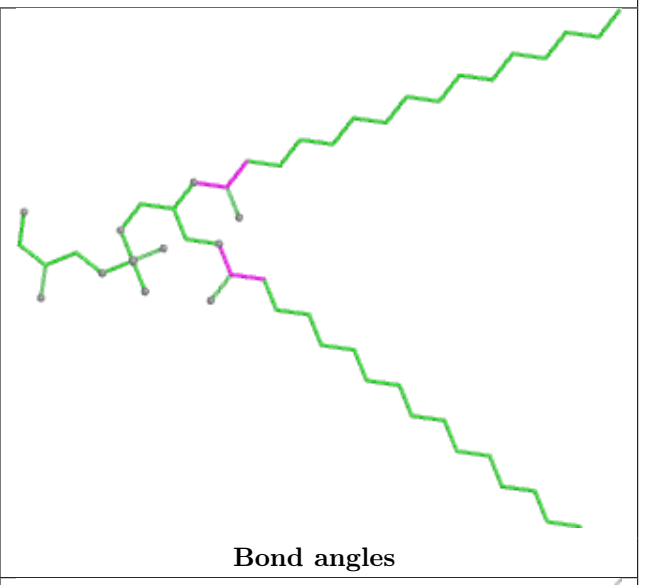
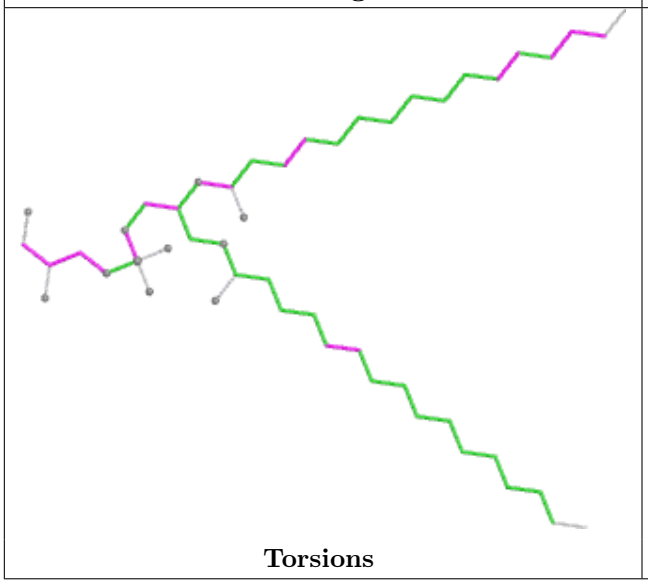


Bond angles



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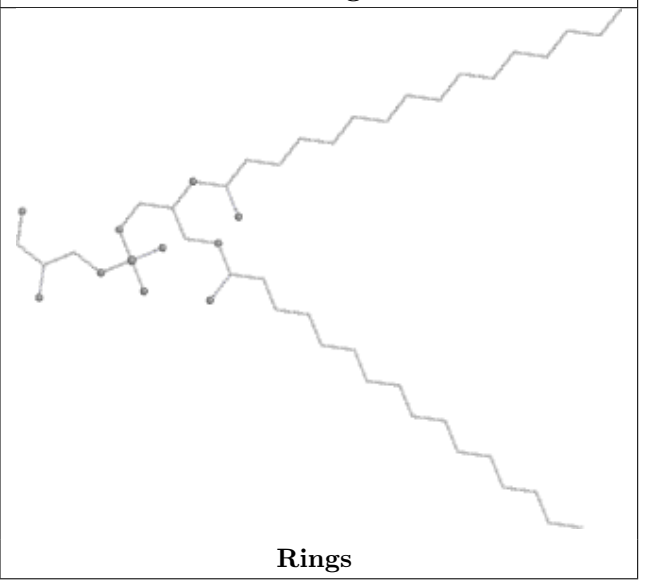
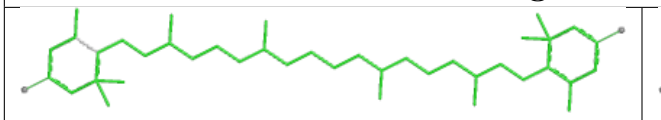


Rings

Ligand LUT v 309



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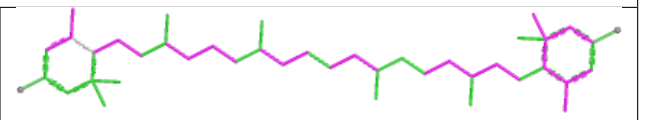

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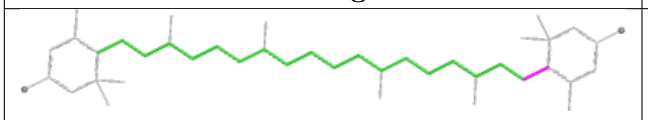

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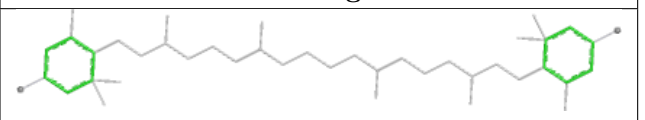
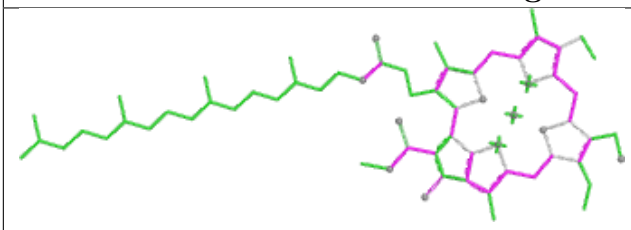


Rings

Ligand CHL P 318



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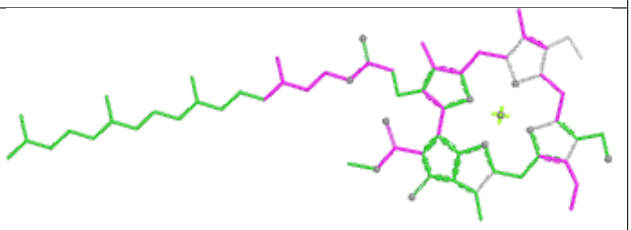

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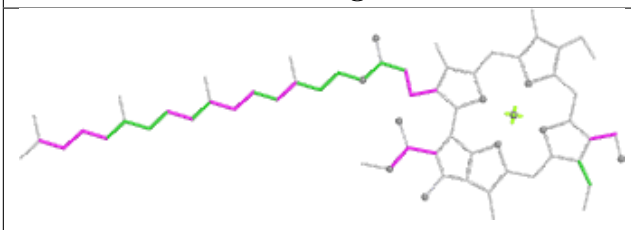

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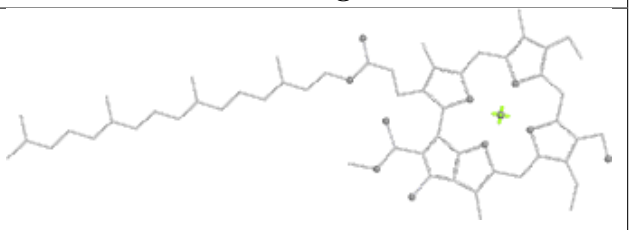
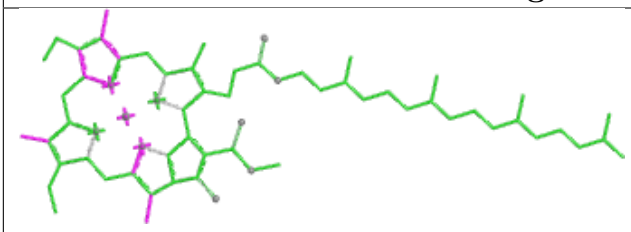


Rings

Ligand CLA b 602



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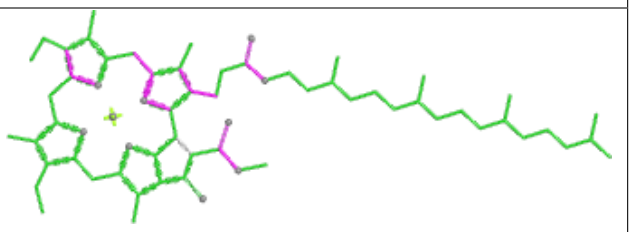
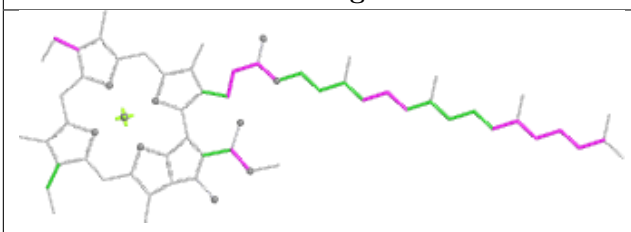


Bond angles



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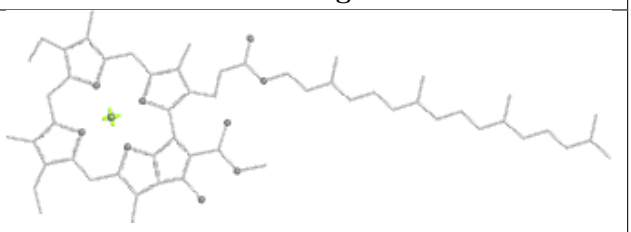
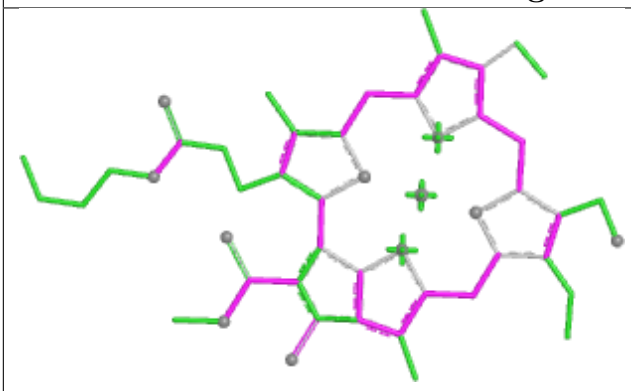


Rings

Ligand CHL 6 314



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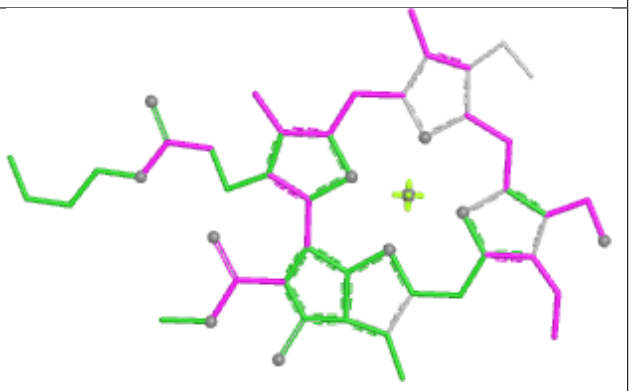
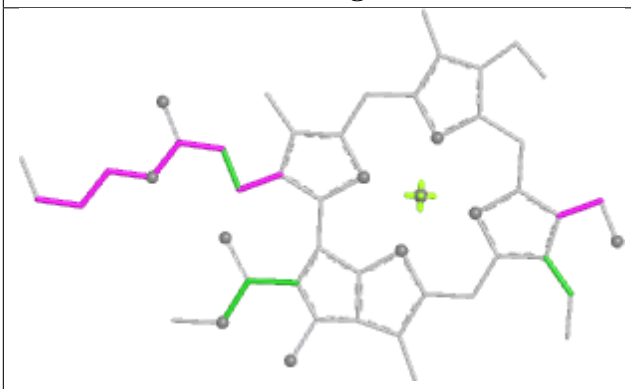


Bond angles



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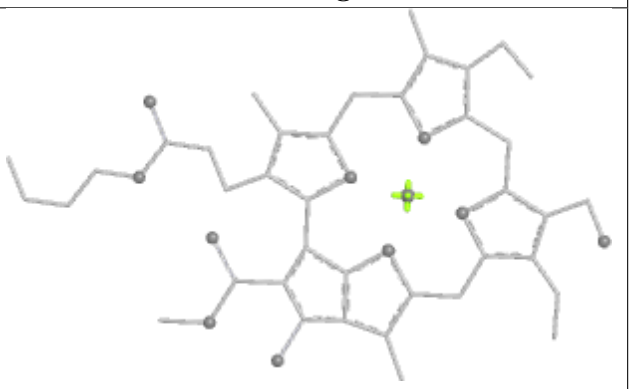
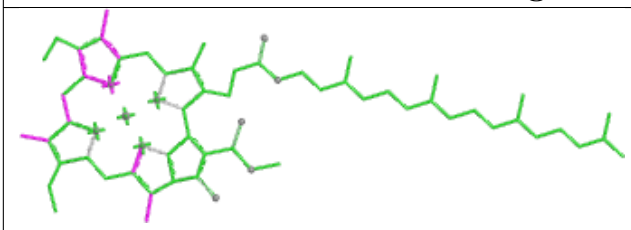


Rings

Ligand CLA v 302



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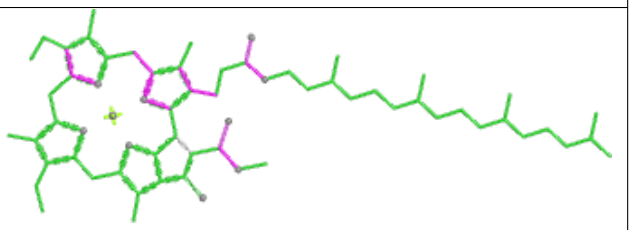
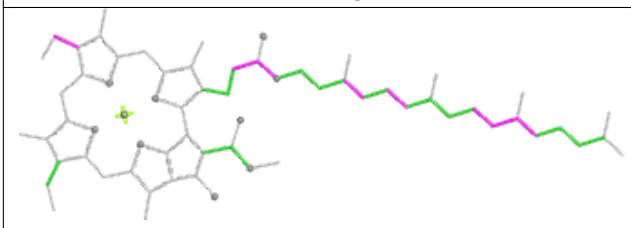


Bond angles



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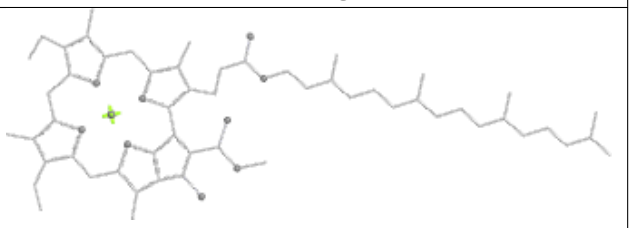
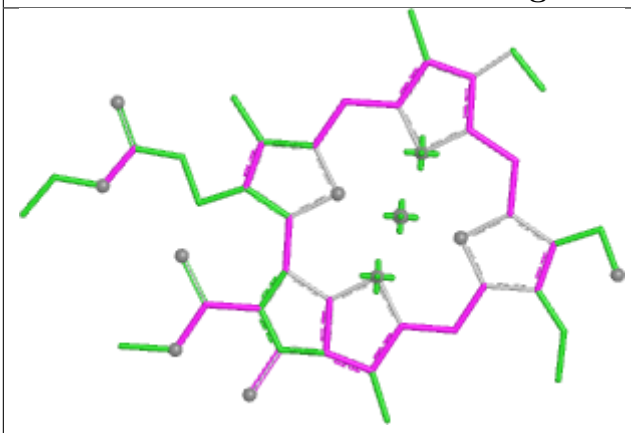
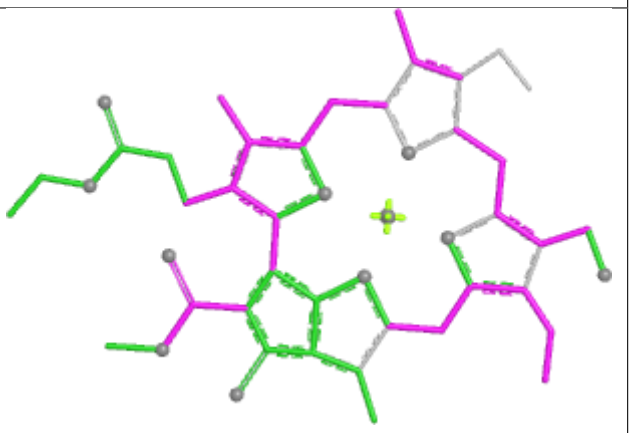


Rings

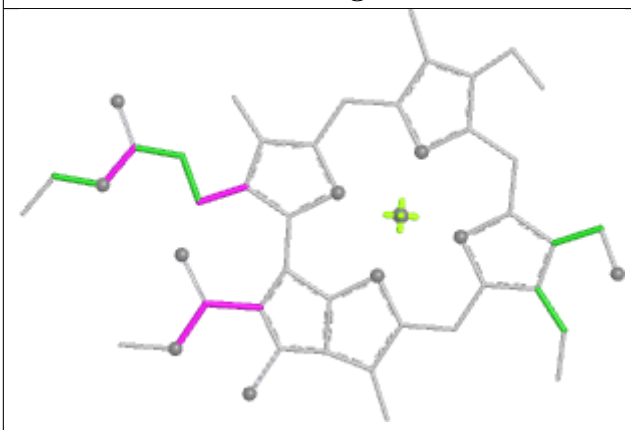
Ligand CHL r 619



Bond lengths



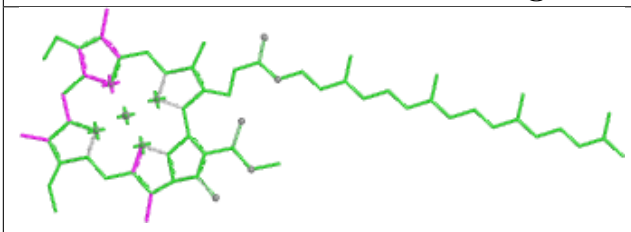
Bond angles



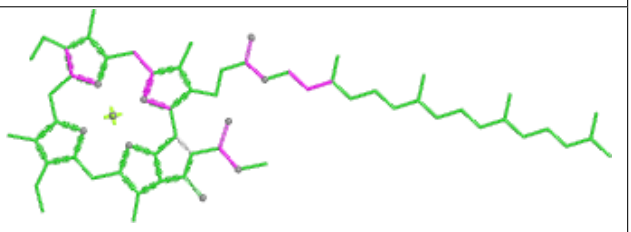
Torsions

Rings

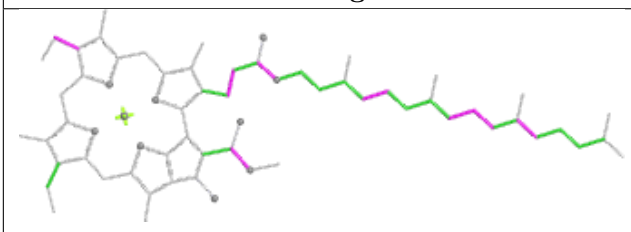
Ligand CLA v 307



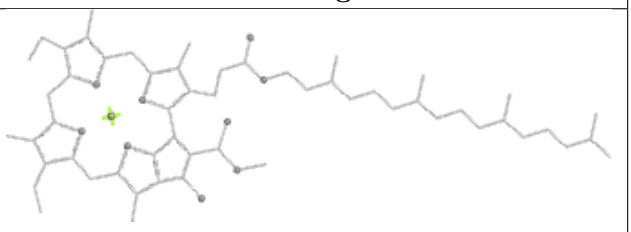
Bond lengths



Bond angles

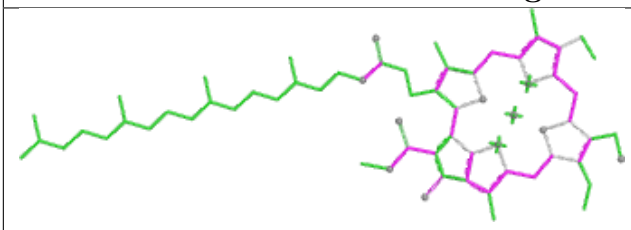


Torsions

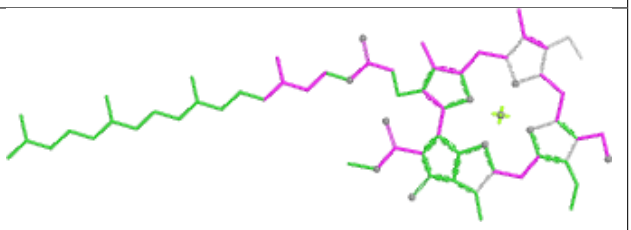


Rings

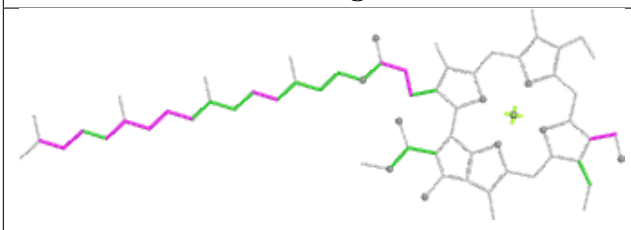
Ligand CHL P 314



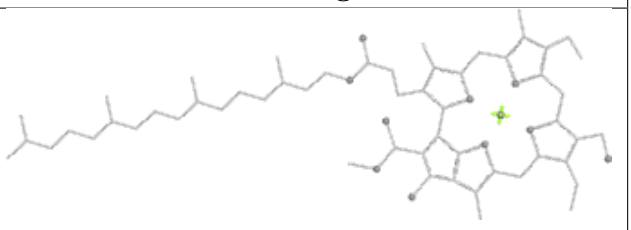
Bond lengths



Bond angles

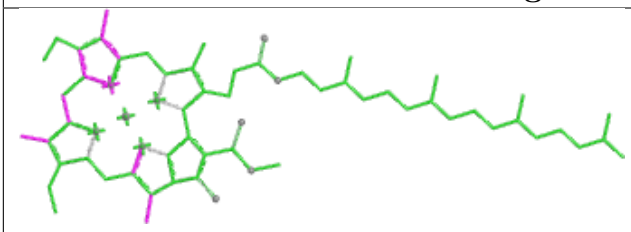


Torsions

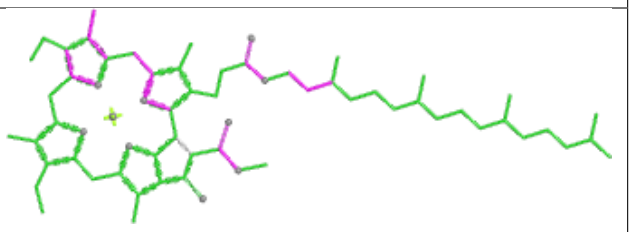


Rings

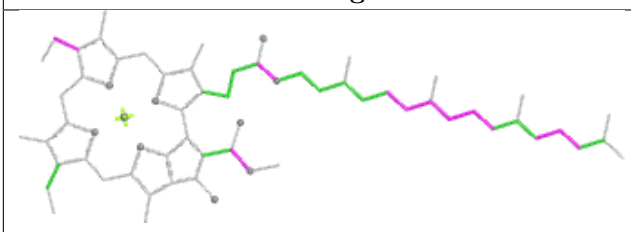
Ligand CLA B 612



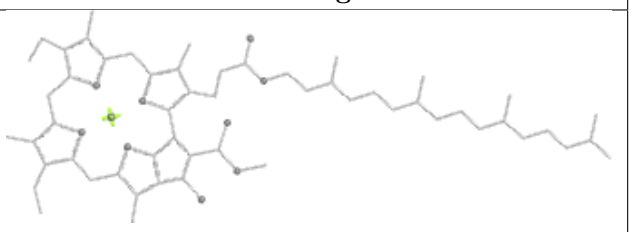
Bond lengths



Bond angles

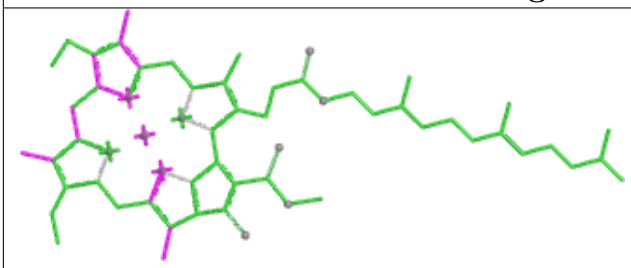


Torsions

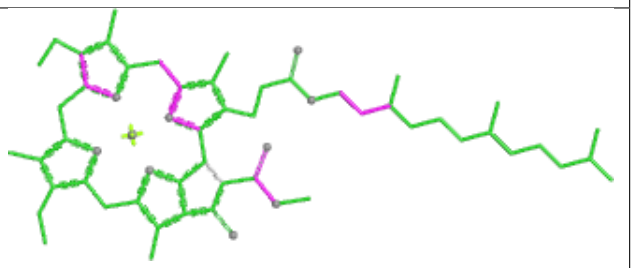


Rings

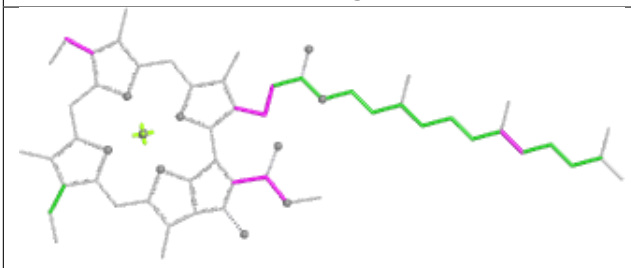
Ligand CLA 1 304



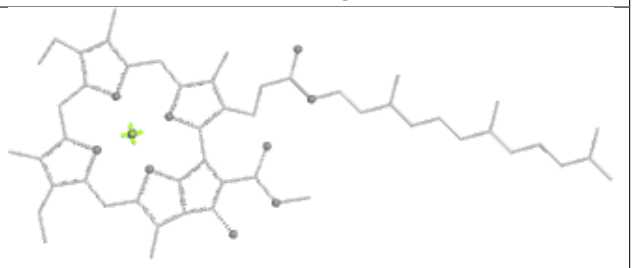
Bond lengths



Bond angles

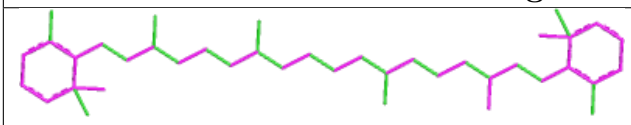


Torsions



Rings

Ligand BCR k 101



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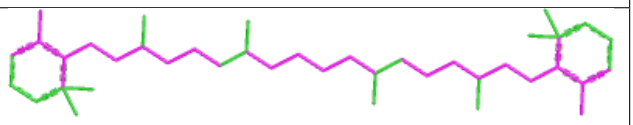
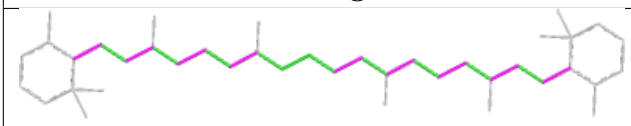
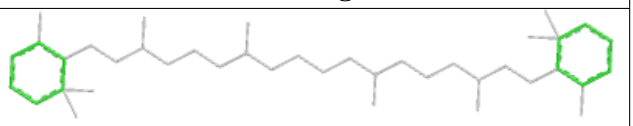


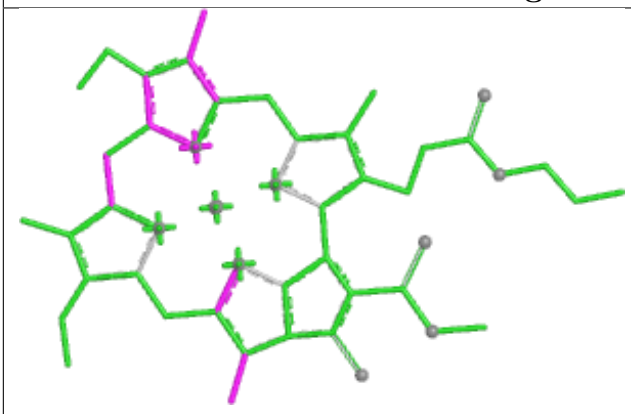
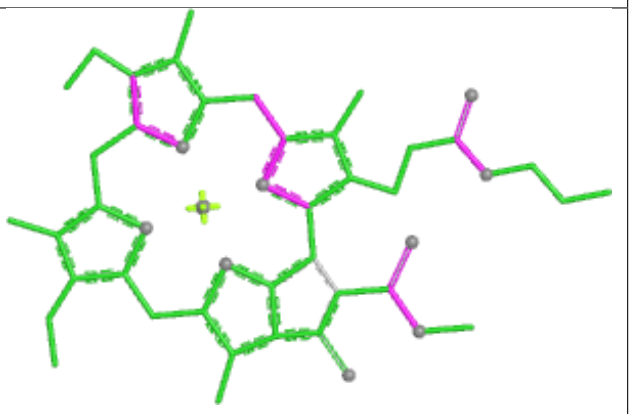
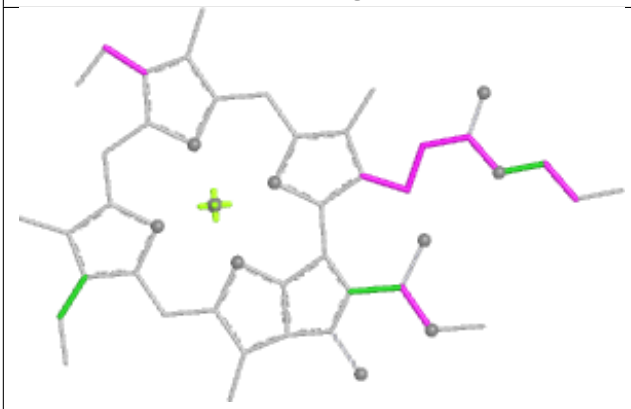
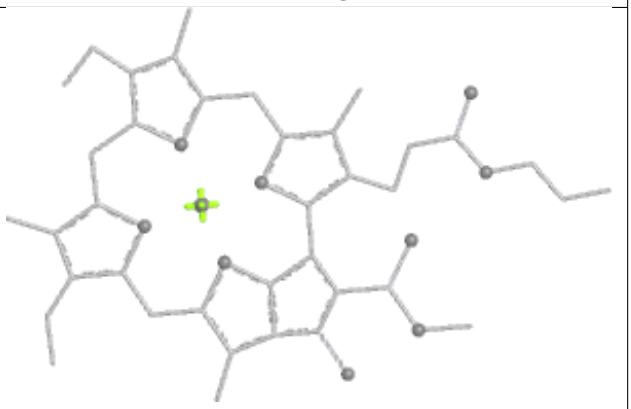
Bond angles

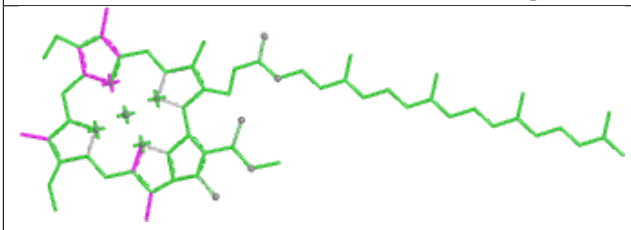
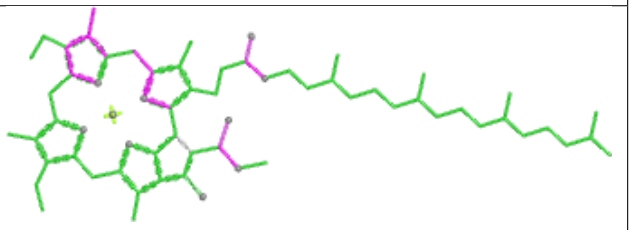
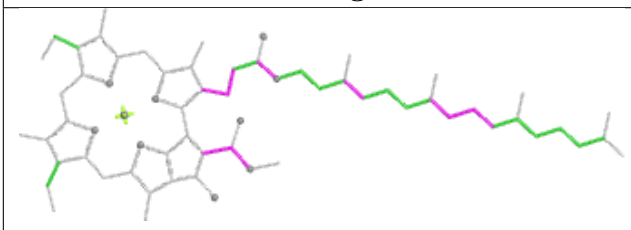
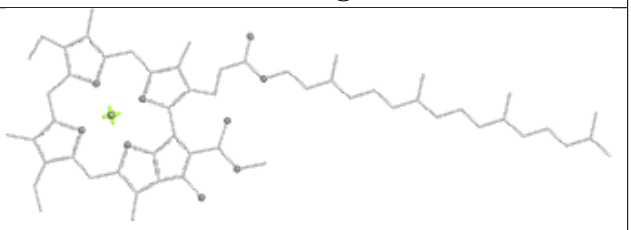


Torsions

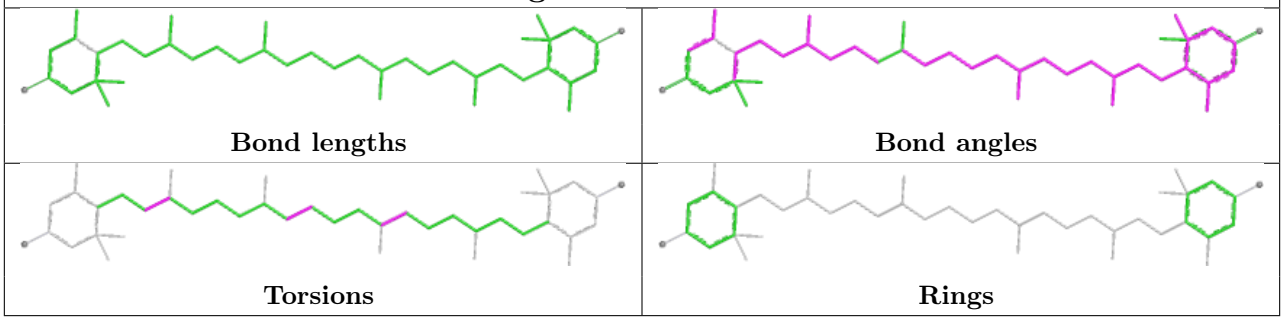


Rings

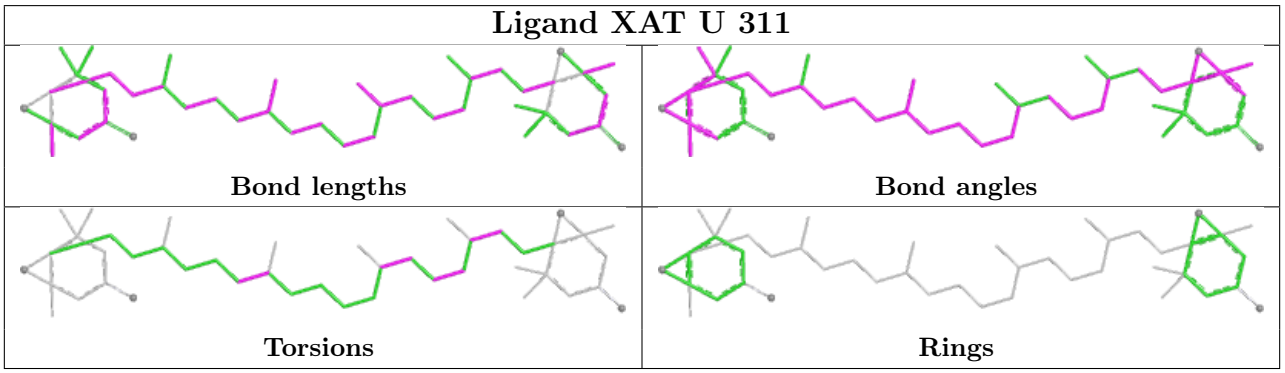
Ligand CLA P 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

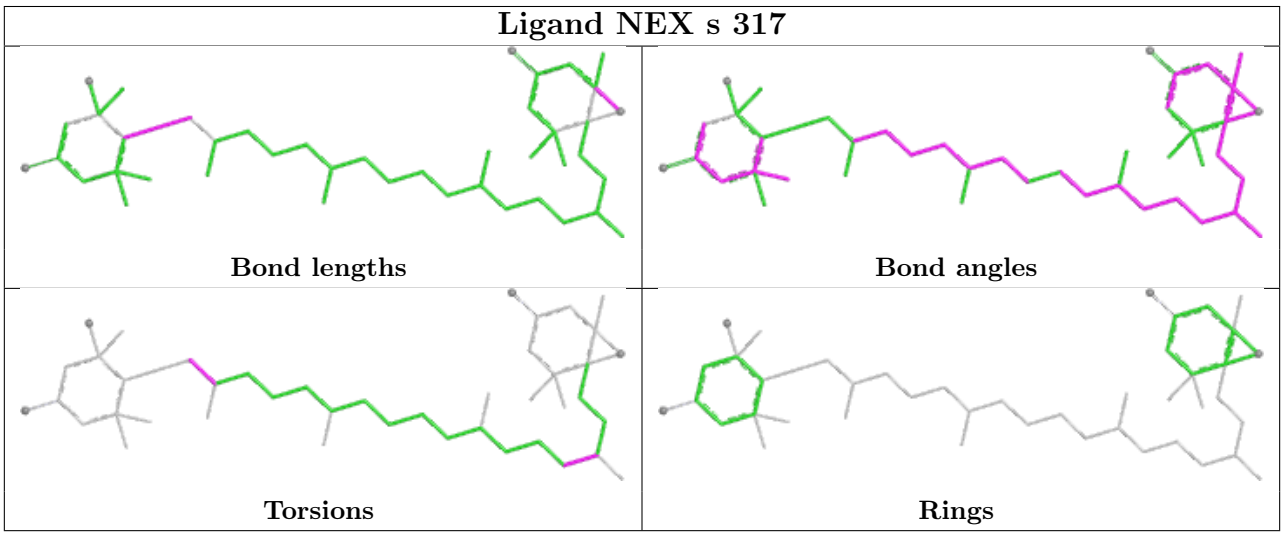
Ligand LUT S 311



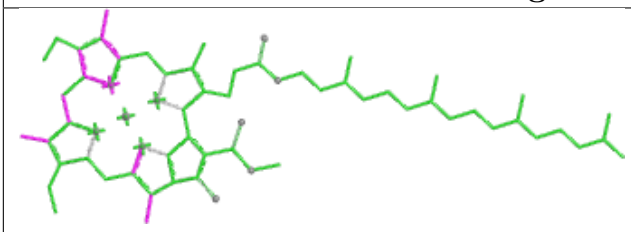
Ligand XAT U 311



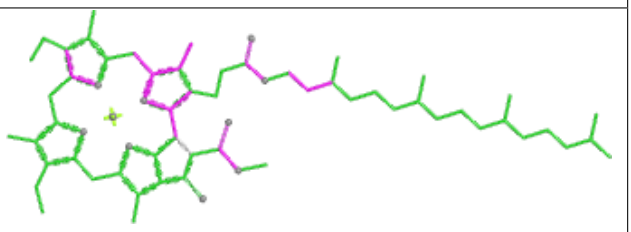
Ligand NEX s 317



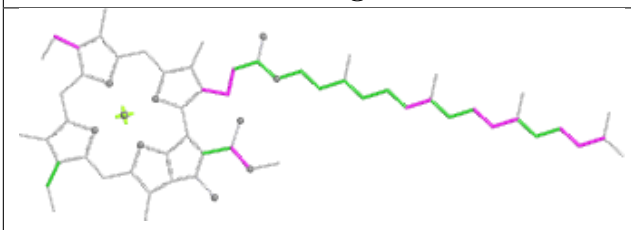
Ligand CLA 5 304



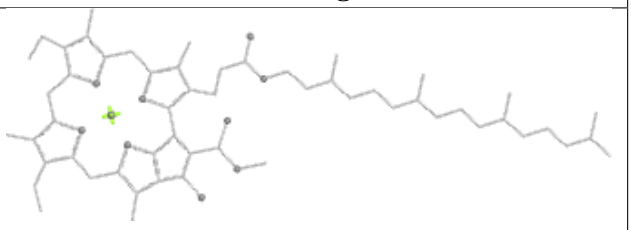
Bond lengths



Bond angles

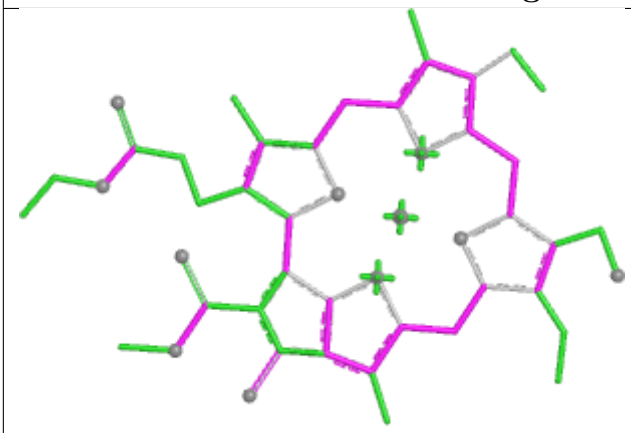


Torsions



Rings

Ligand CHL N 314



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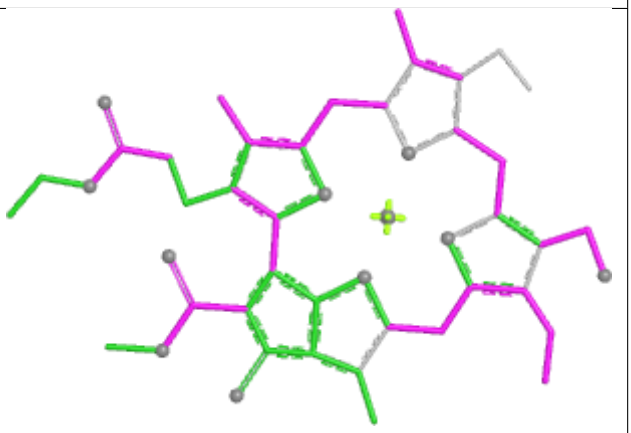
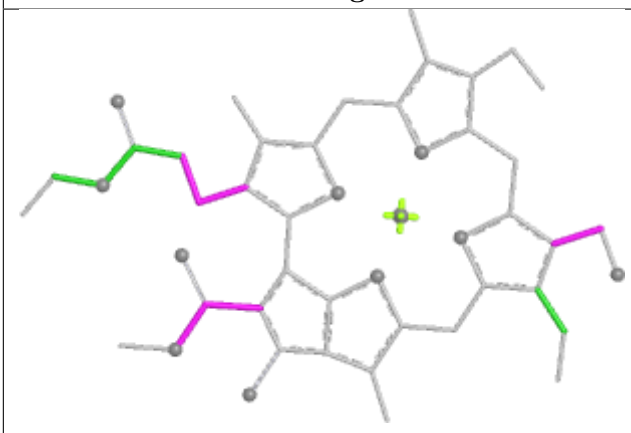
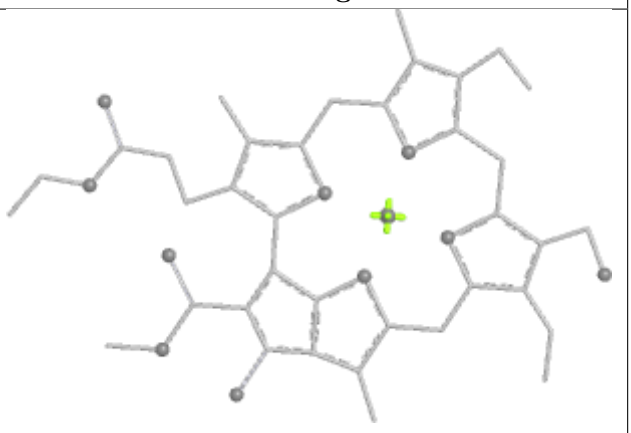


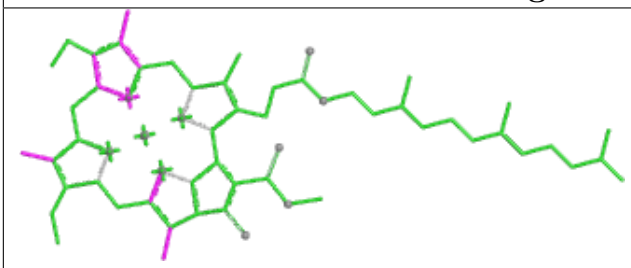
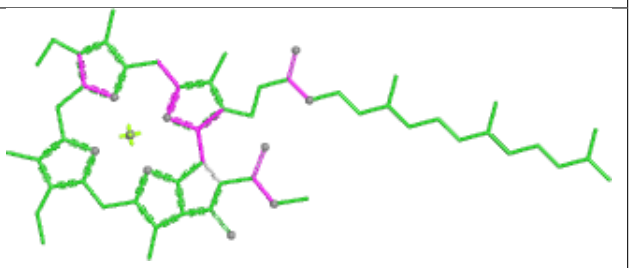
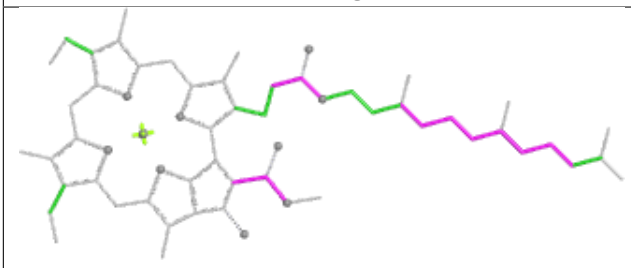
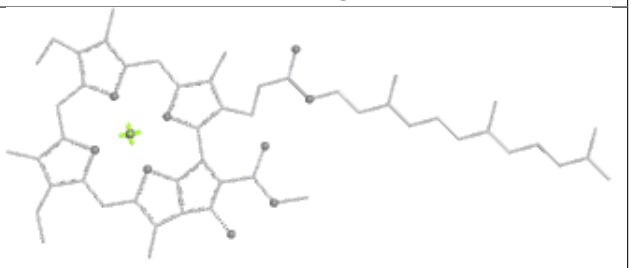
Bond angles

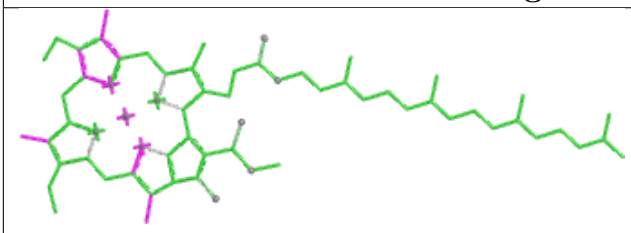
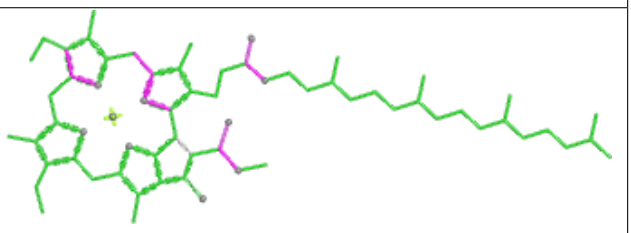
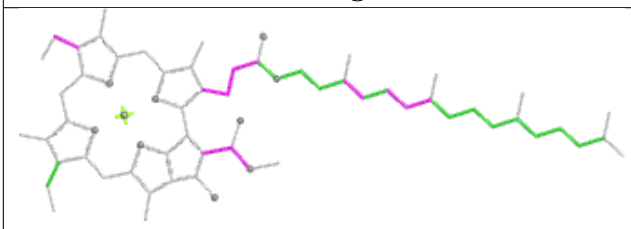
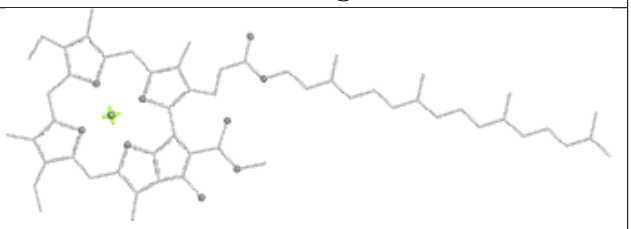


Torsions

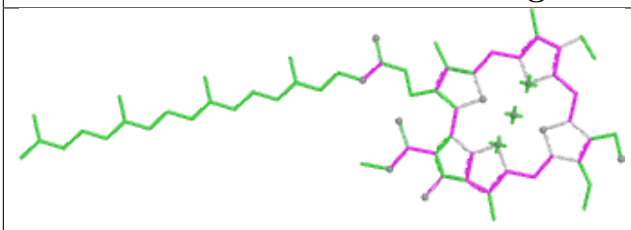


Rings

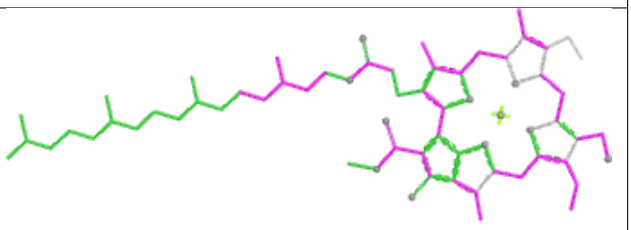
Ligand CLA 4 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

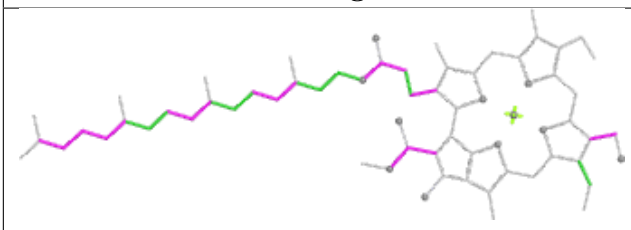
Ligand CHL 6 301



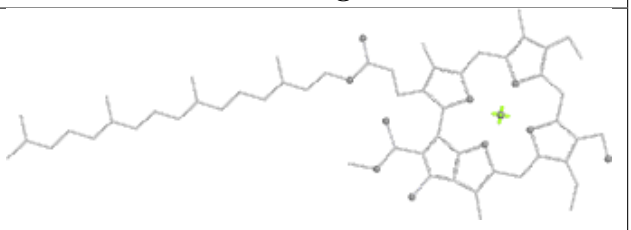
Bond lengths



Bond angles

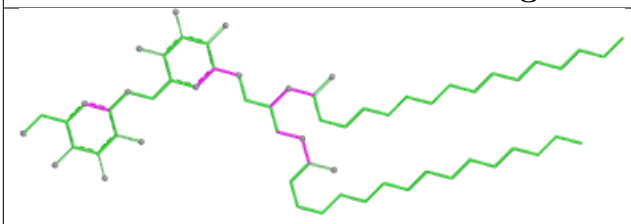


Torsions

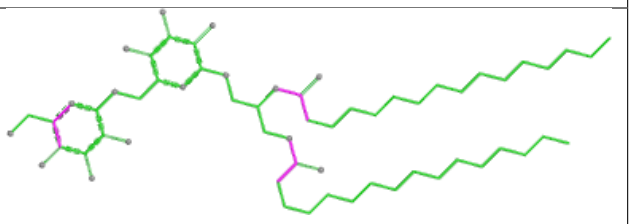


Rings

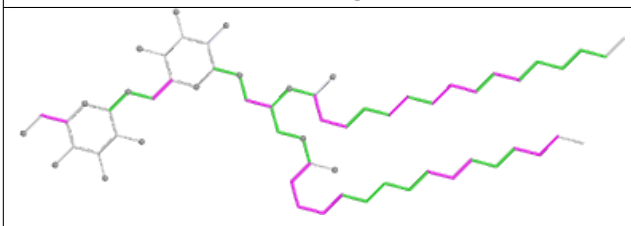
Ligand DGD B 601



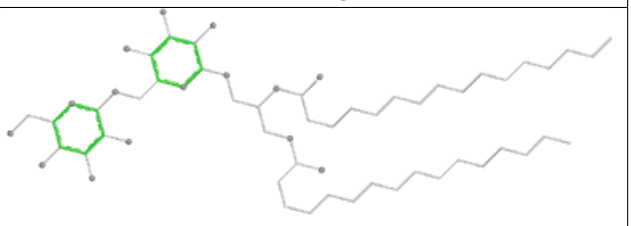
Bond lengths



Bond angles



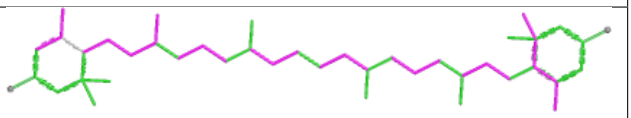
Torsions



Rings

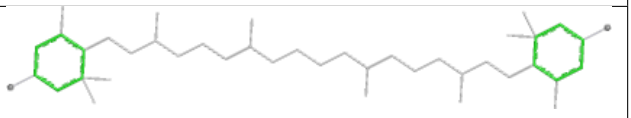
Ligand LUT U 310

Bond lengths



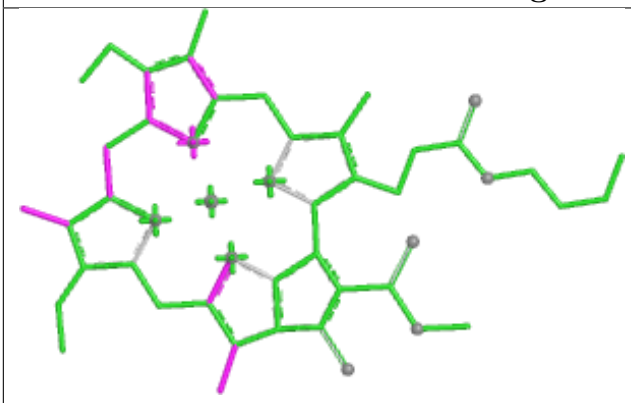
Bond angles

Torsions



Rings

Ligand CLA r 608



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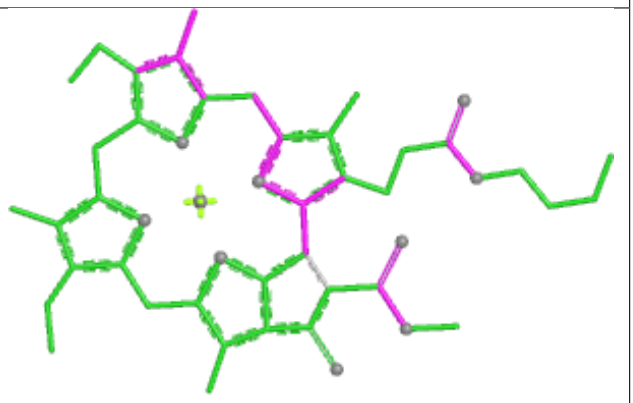
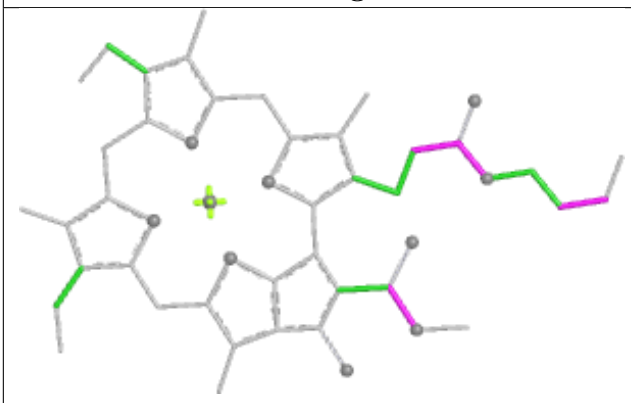


Bond angles



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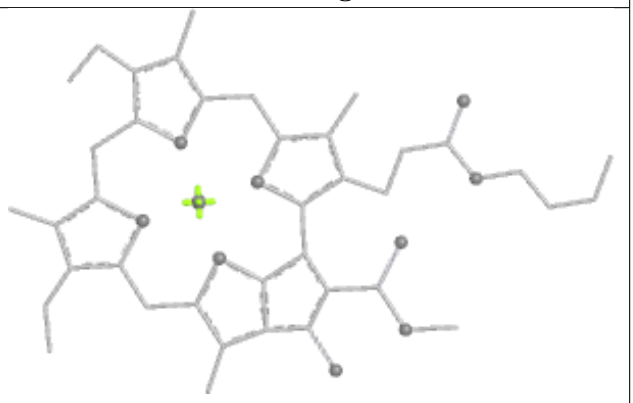
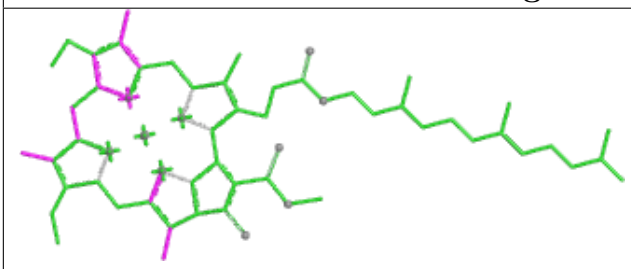


Rings

Ligand CLA N 307



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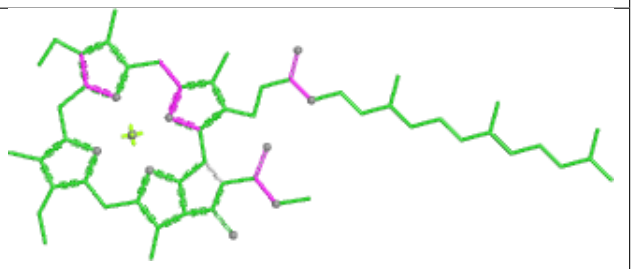
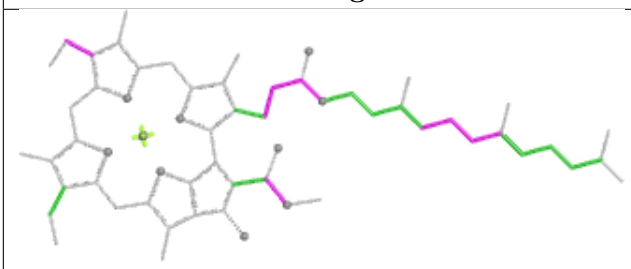


Bond angles



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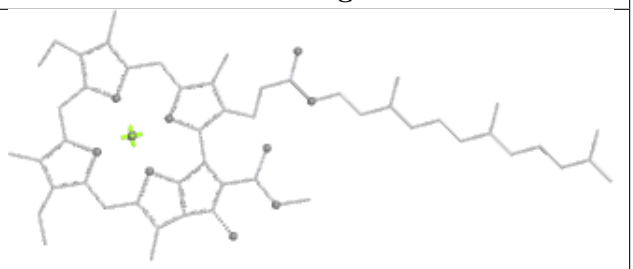
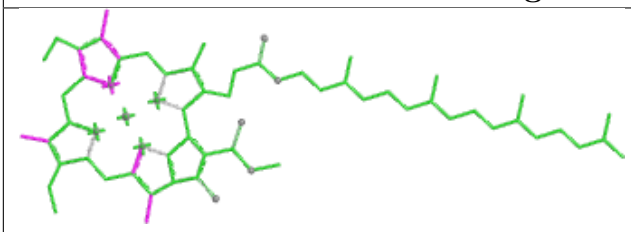


Rings

Ligand CLA C 506



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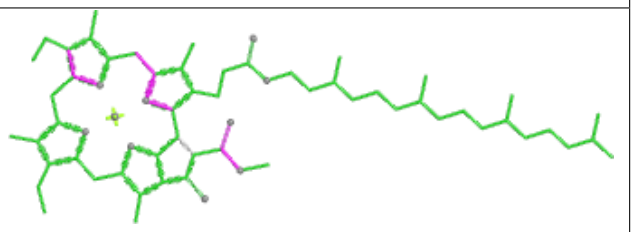
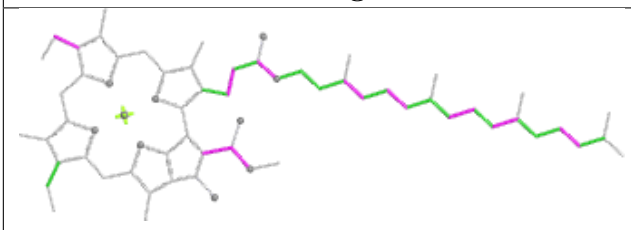


Bond angles



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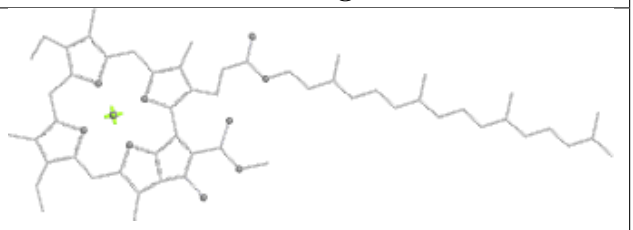
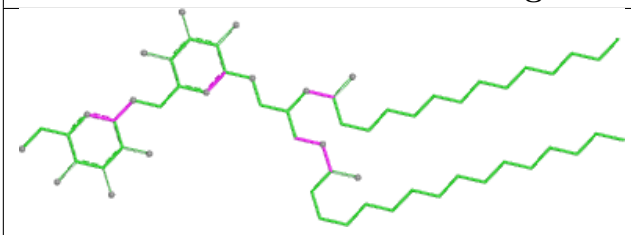


Rings

Ligand DGD c 519



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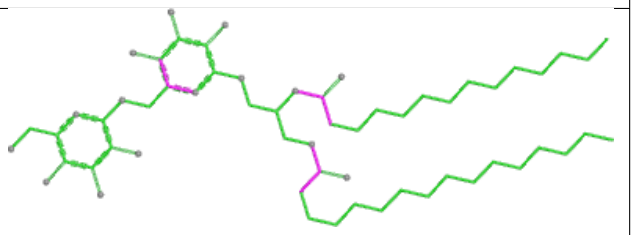
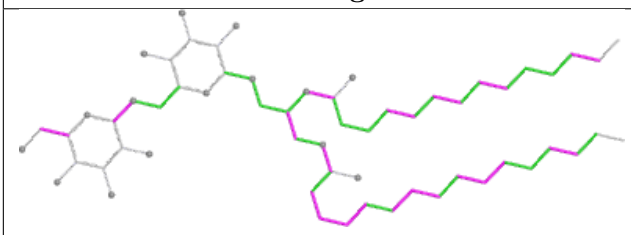


Bond angles



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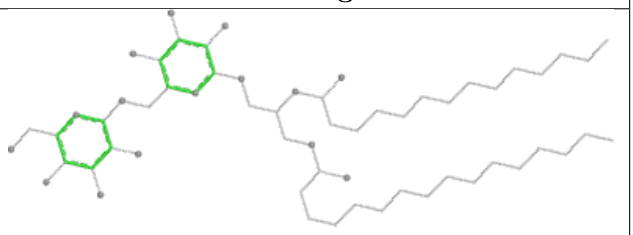
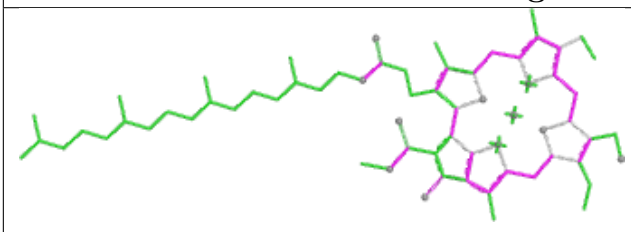


Rings

Ligand CHL 4 316



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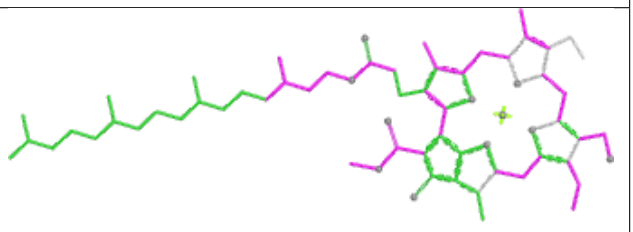
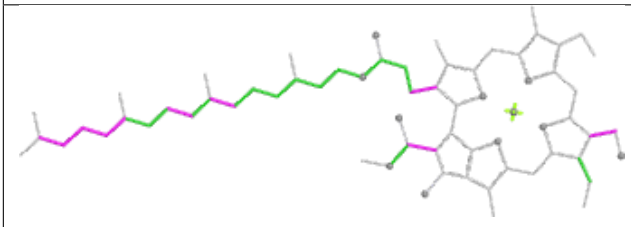


Bond angles



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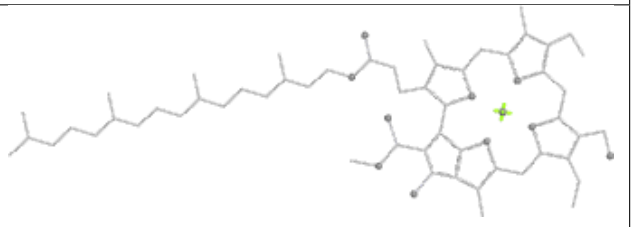
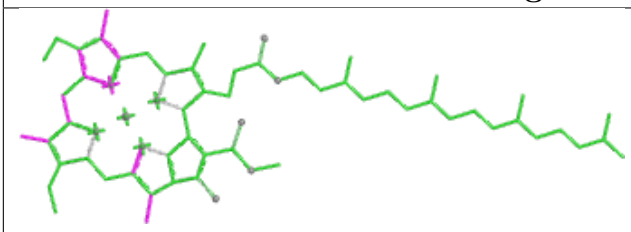


Rings

Ligand CLA P 302



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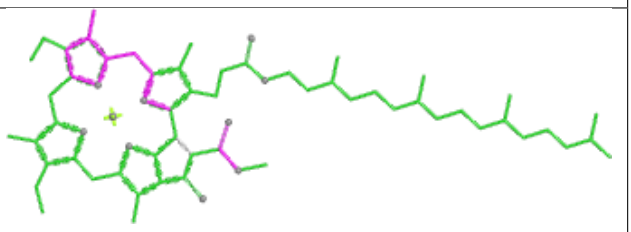
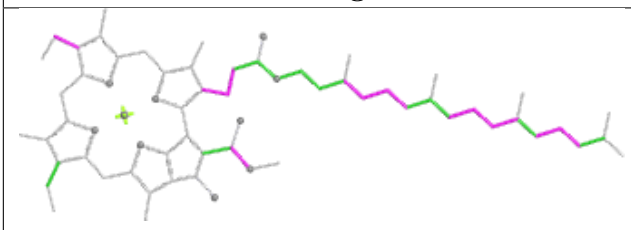


Bond angles



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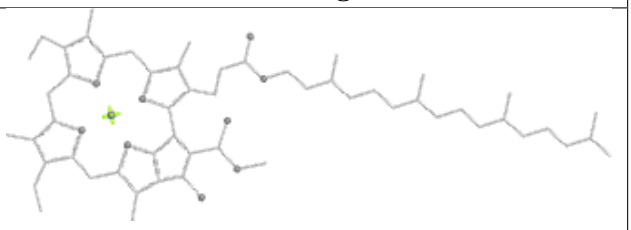
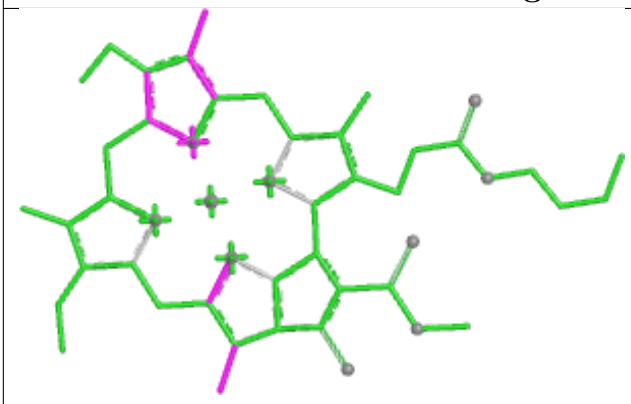


Rings

Ligand CLA R 308



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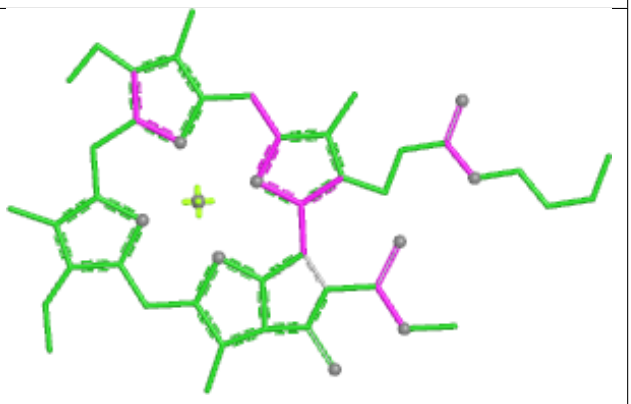

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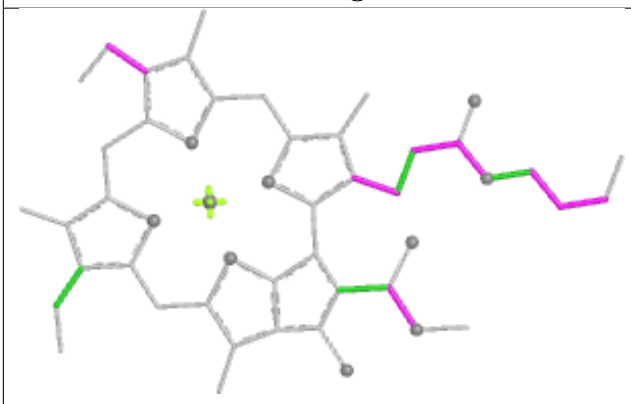

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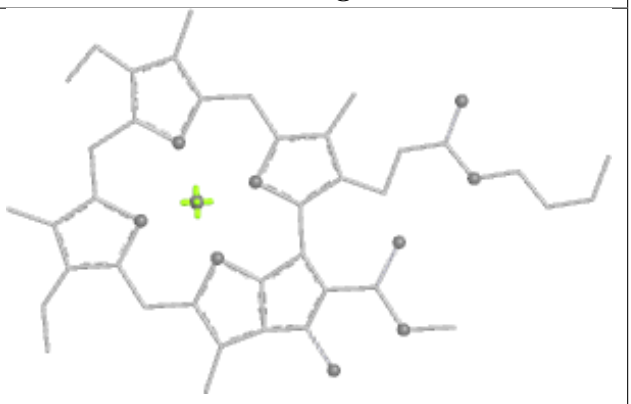
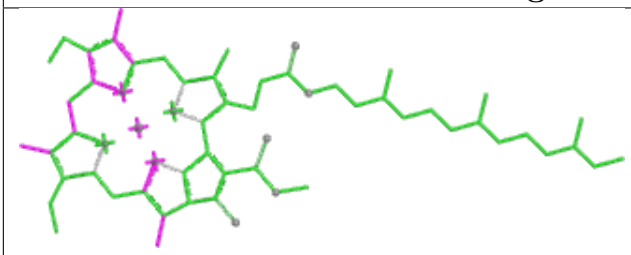


Rings

Ligand CLA S 301



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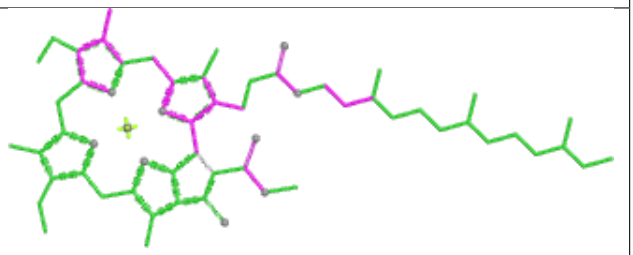
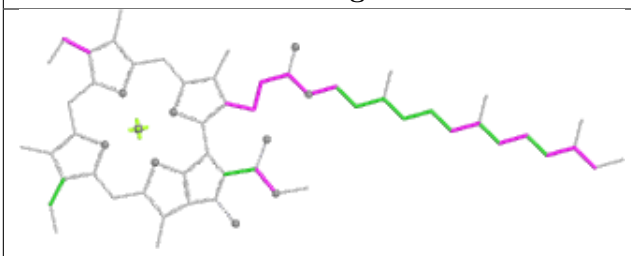


Bond angles



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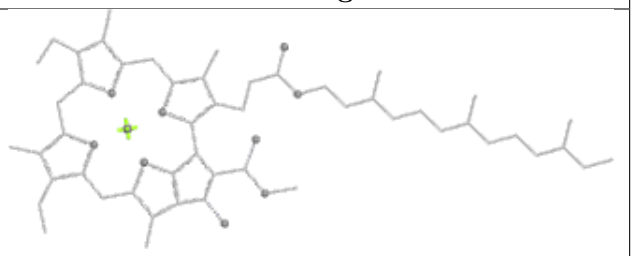
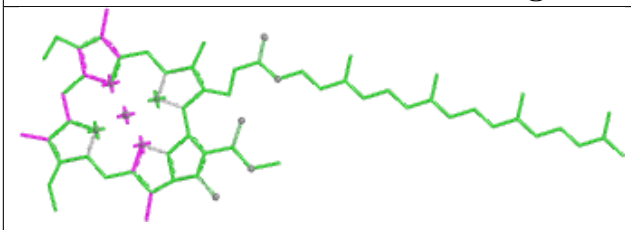


Rings

Ligand CLA d 402



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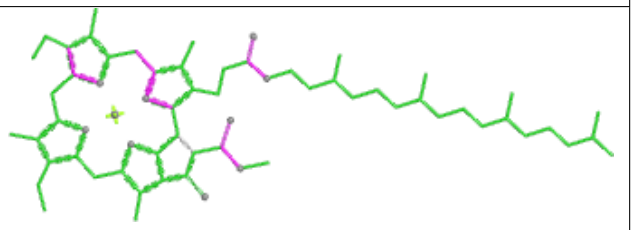

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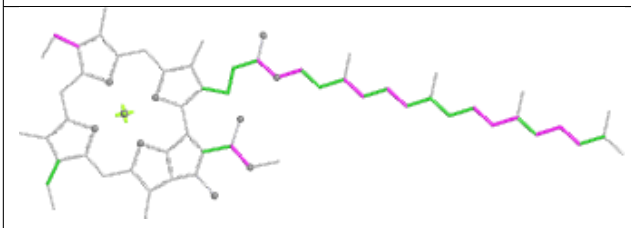

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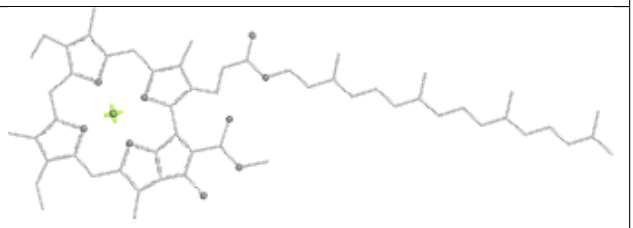
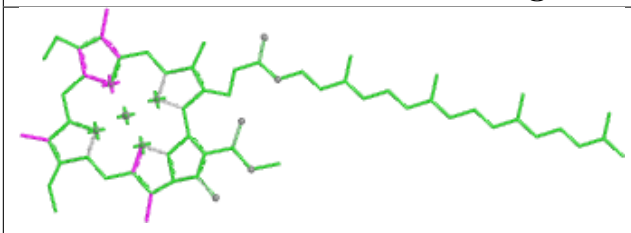


Rings

Ligand CLA g 302



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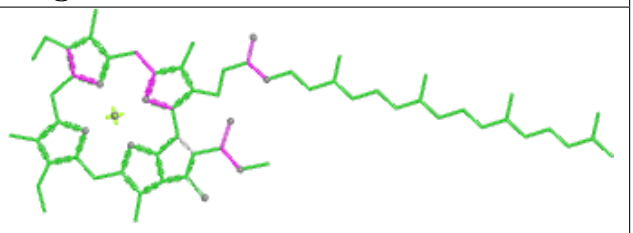

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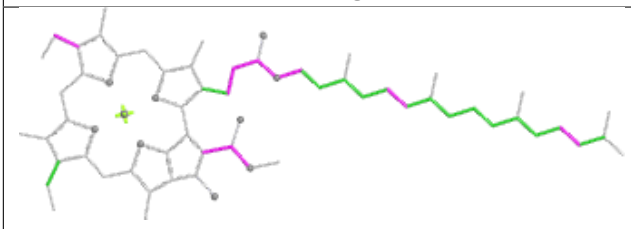

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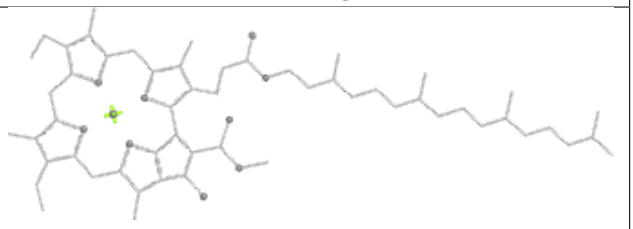
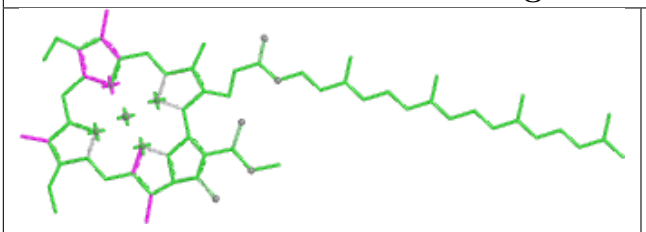


Rings

Ligand CLA B 606



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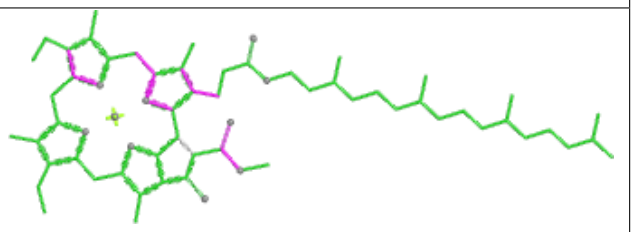
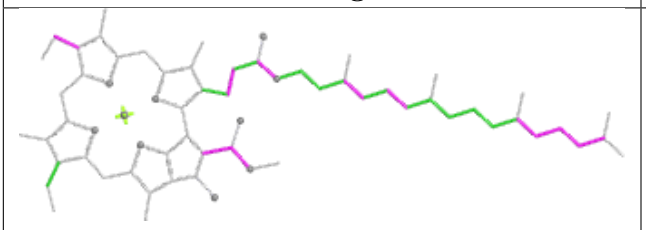


Bond angles



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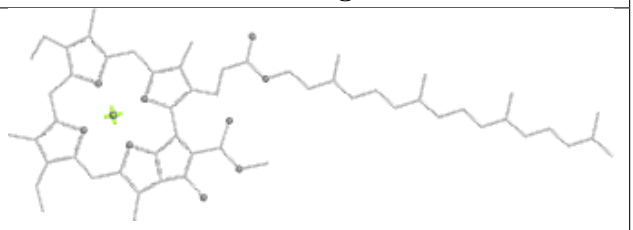
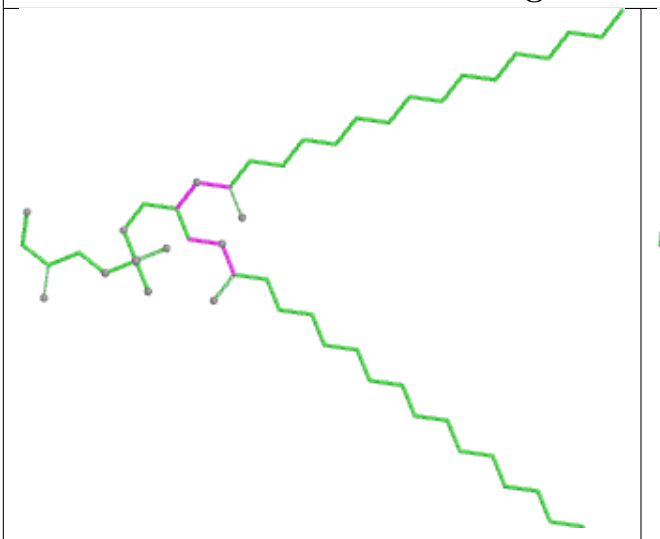


Rings

Ligand LHG d 406



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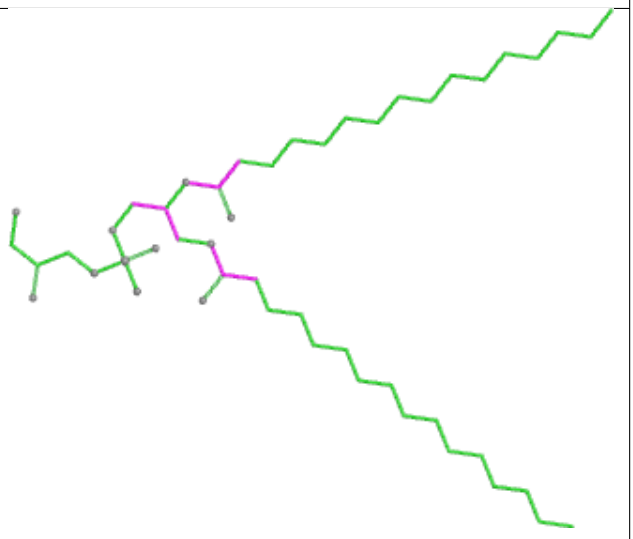
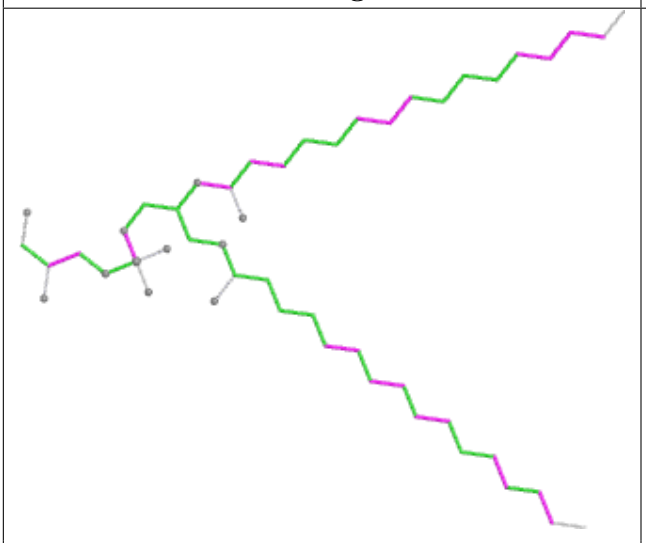


Bond angles



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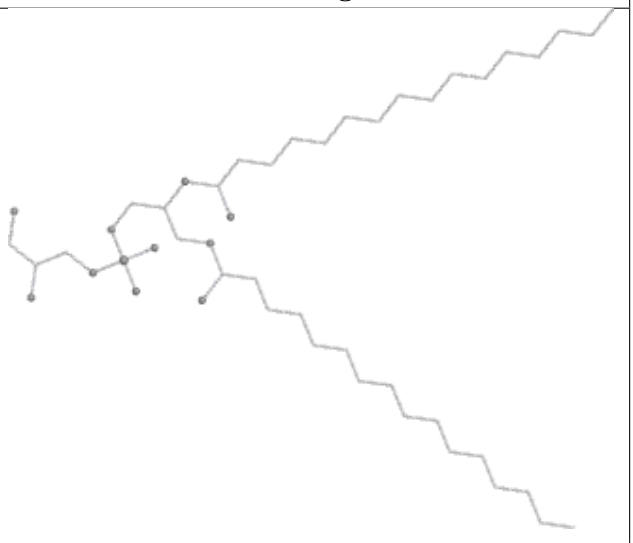
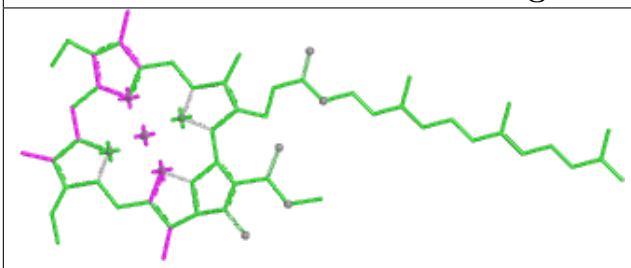
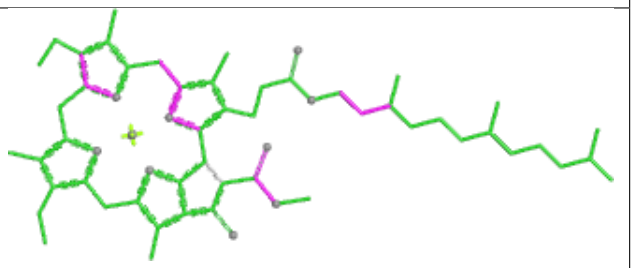
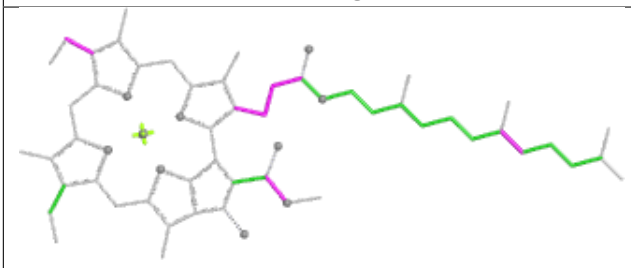
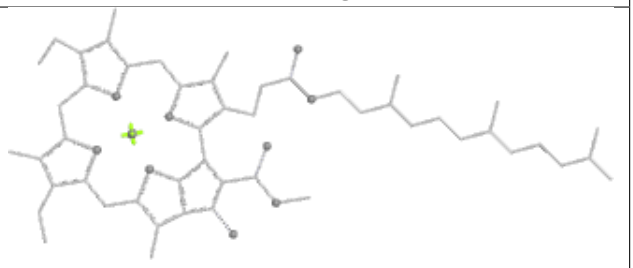
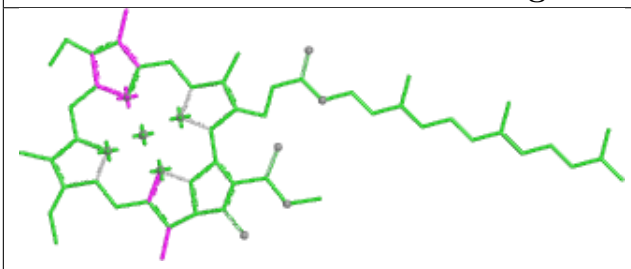
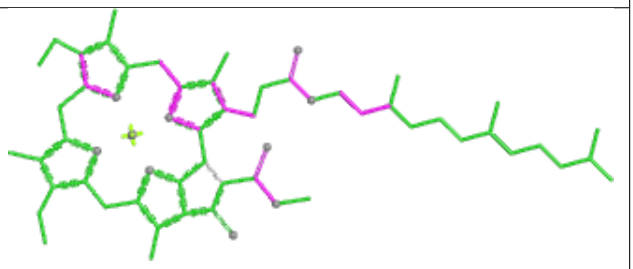
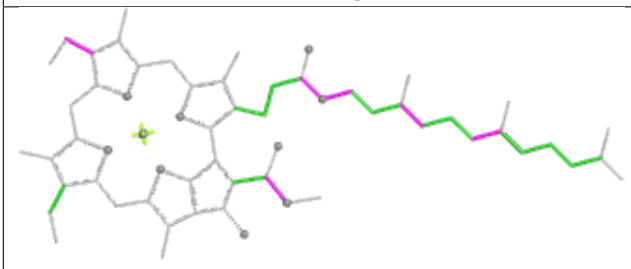
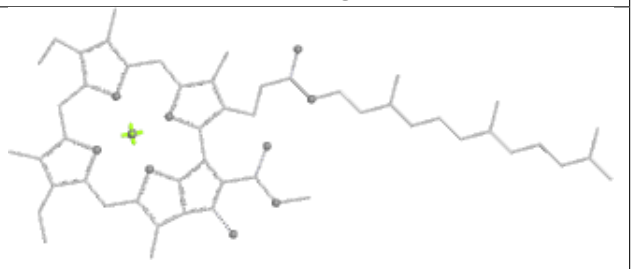
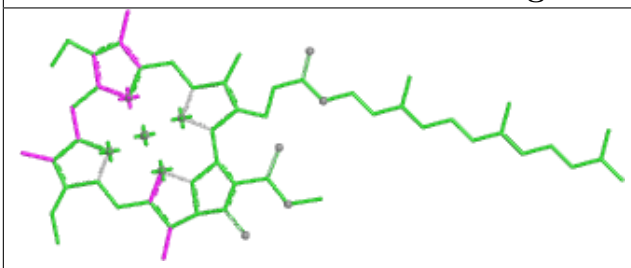


Rings

Ligand CLA 4 304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 1 305	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA u 304



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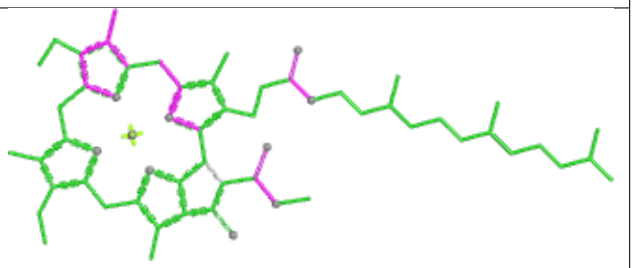

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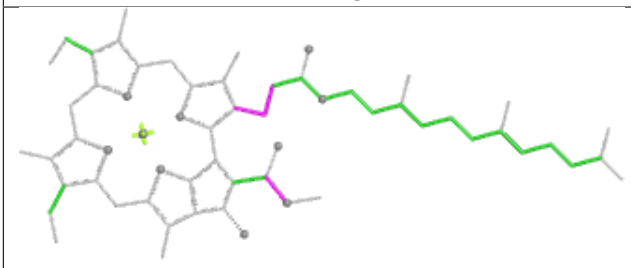

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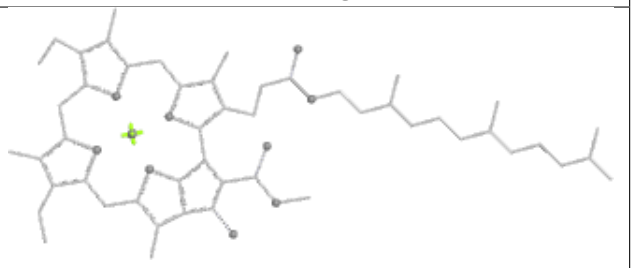
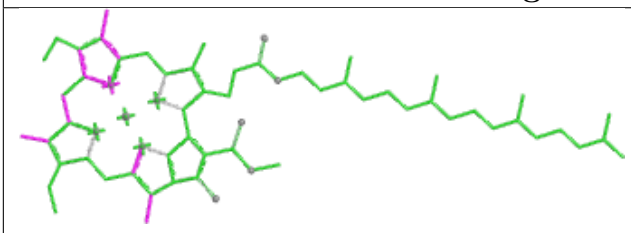


Rings

Ligand CLA G 302



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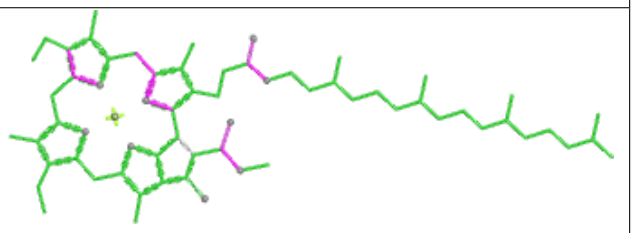

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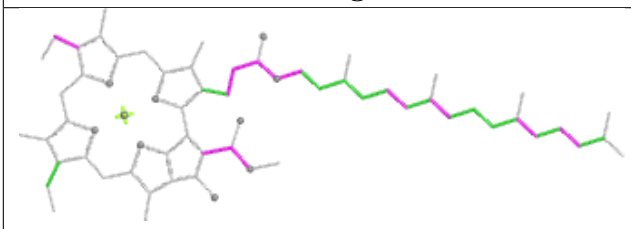

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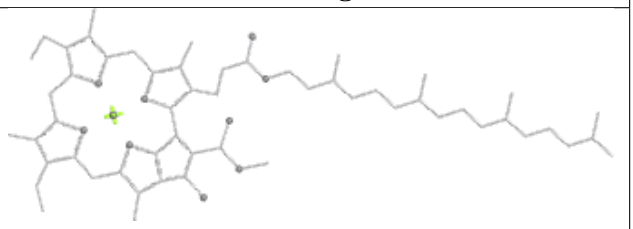
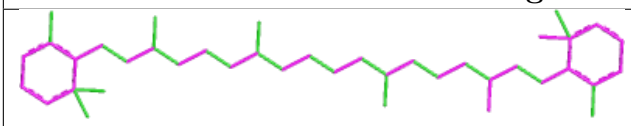


Rings

Ligand BCR x 202



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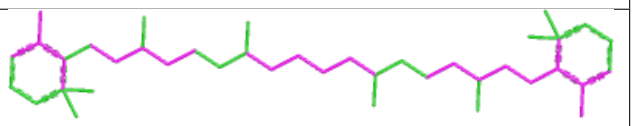

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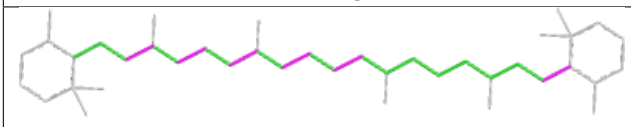

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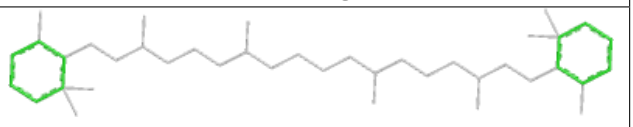
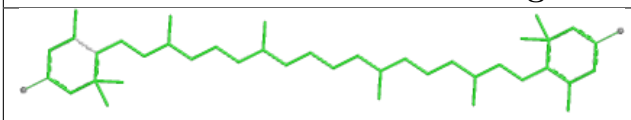


Rings

Ligand LUT u 310



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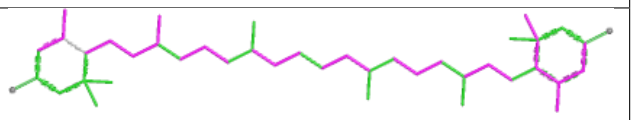

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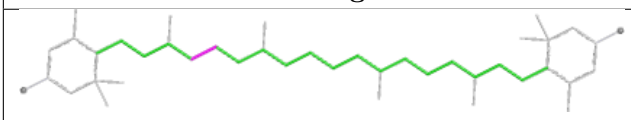

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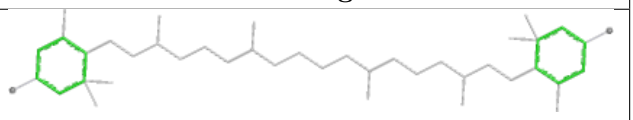
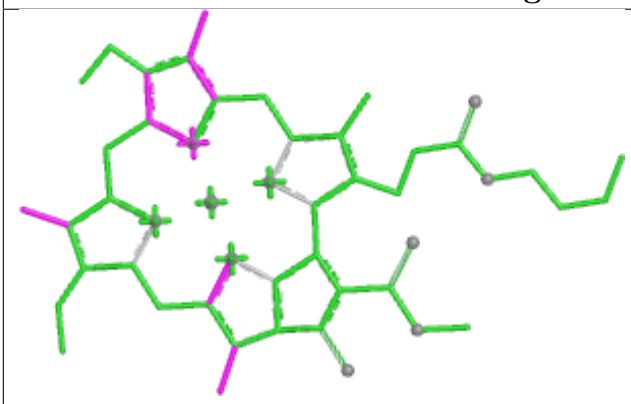


Rings

Ligand CLA R 302



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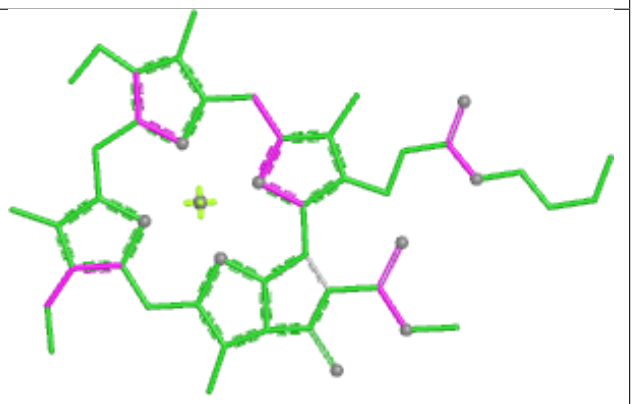

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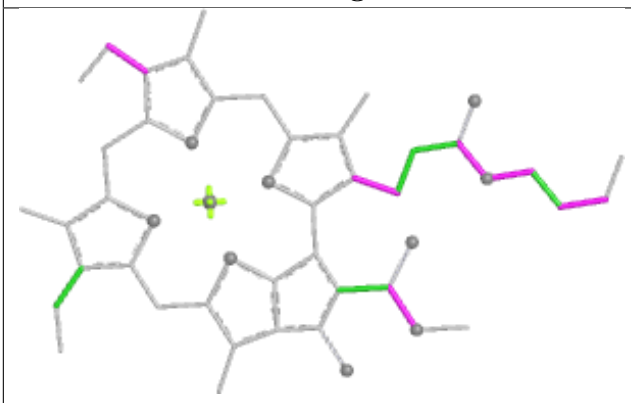

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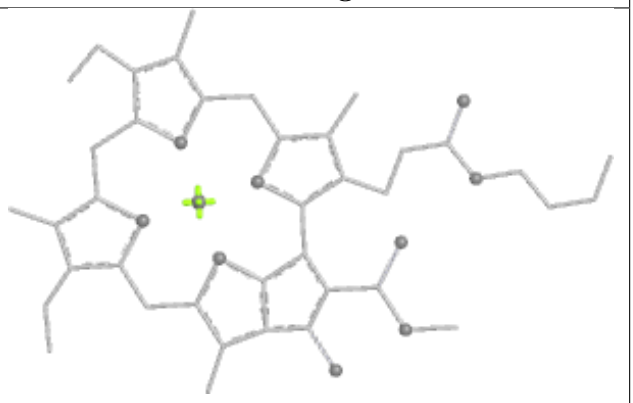
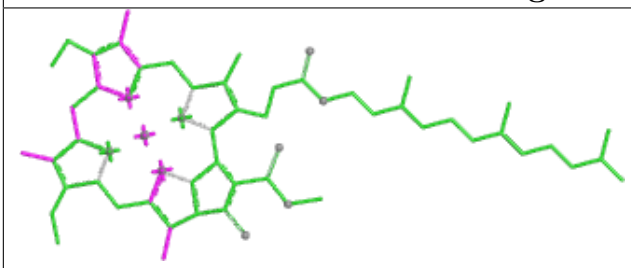


Rings

Ligand CLA 4 305



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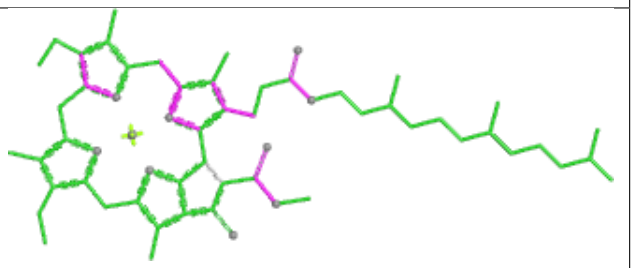

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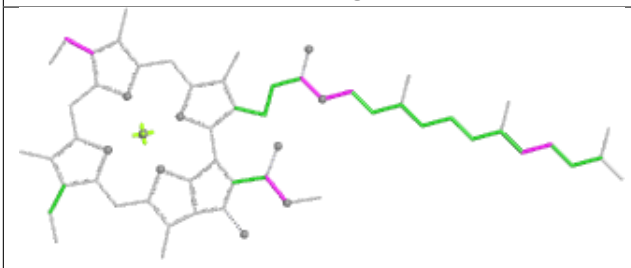

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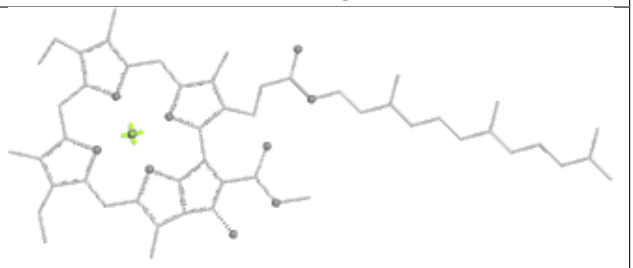
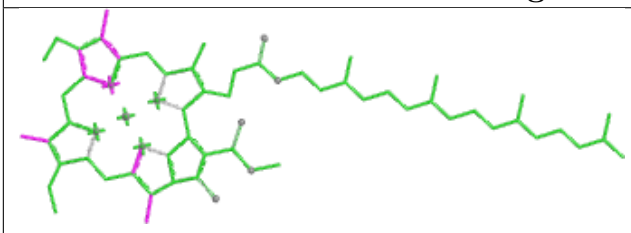


Rings

Ligand CLA b 607



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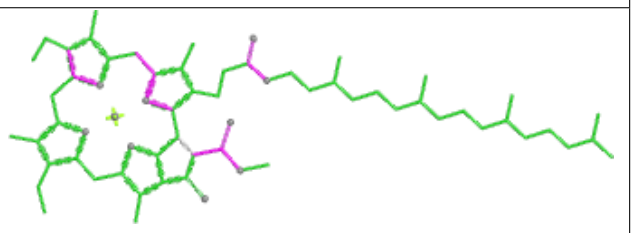

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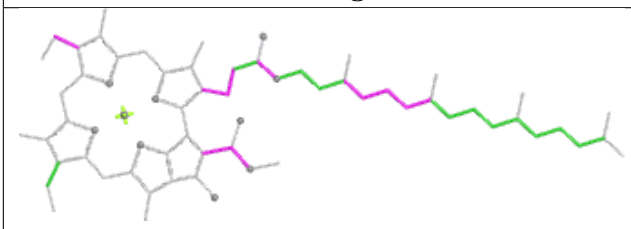

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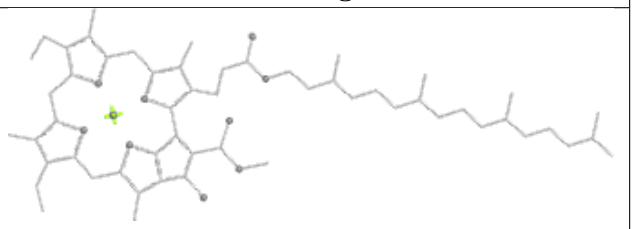
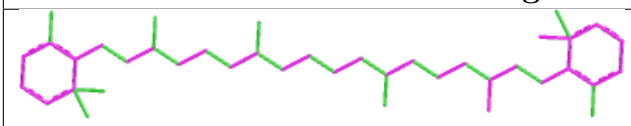


Rings

Ligand BCR C 516



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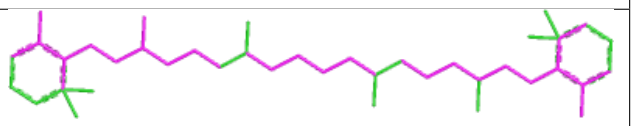

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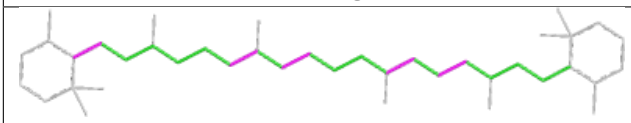

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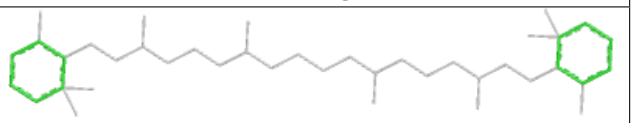
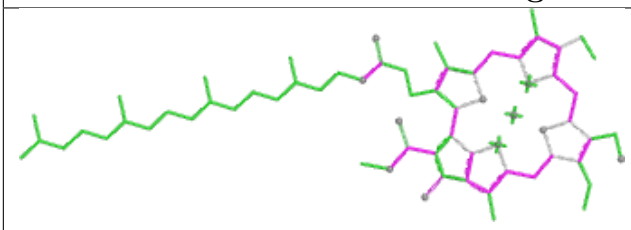


Rings

Ligand CHL p 314



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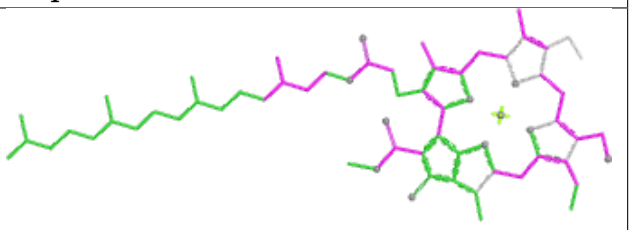

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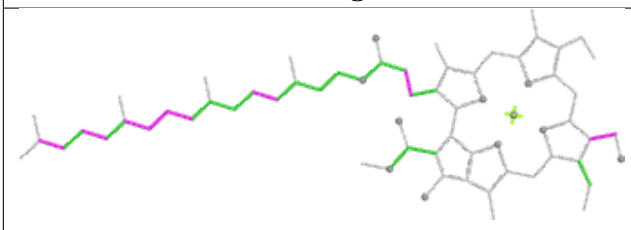

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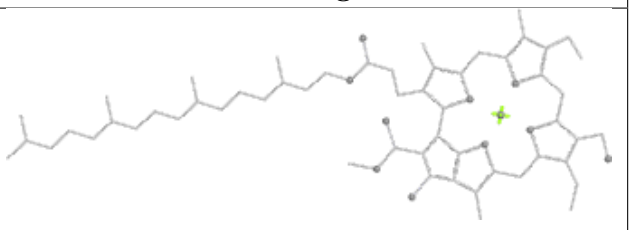
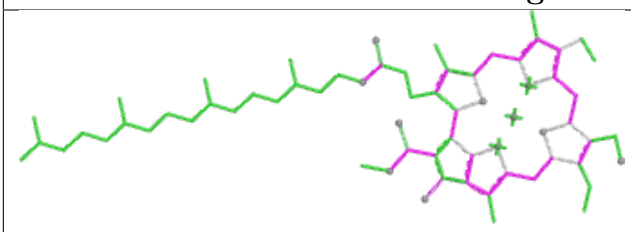


Rings

Ligand CHL u 318



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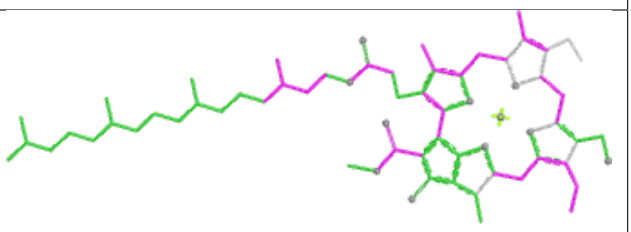

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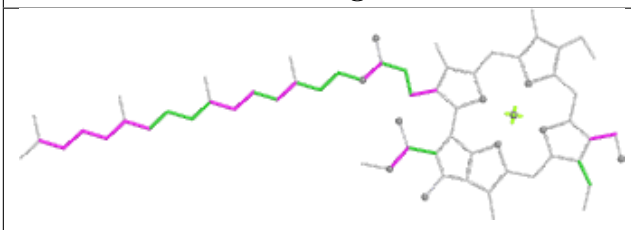

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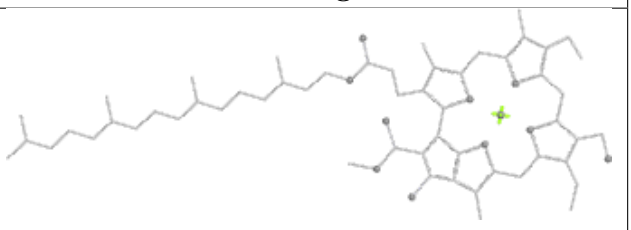
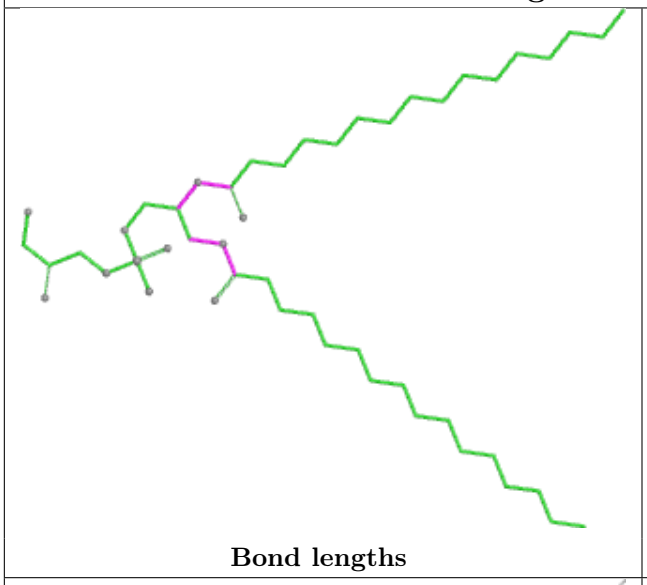


Rings

Ligand LHG 5 312



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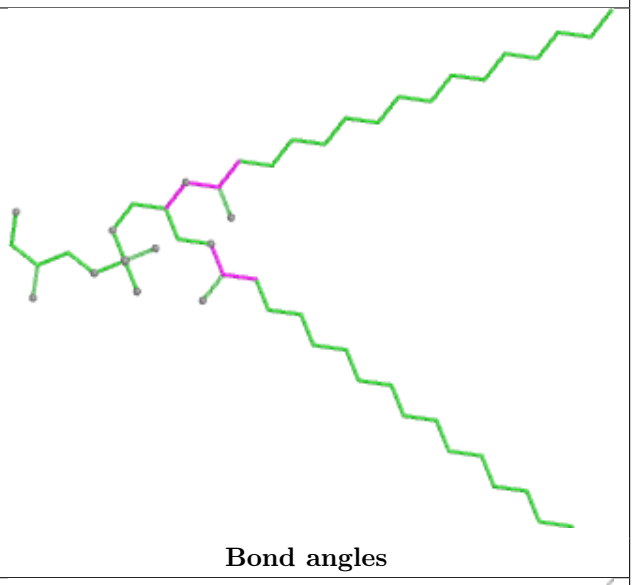

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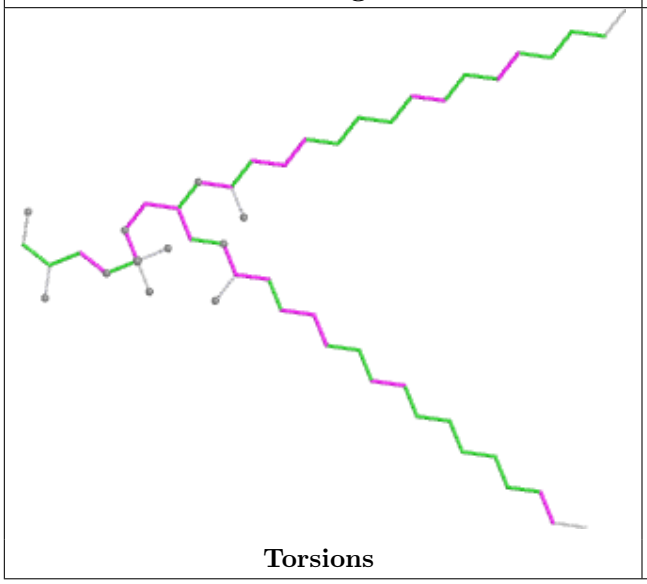

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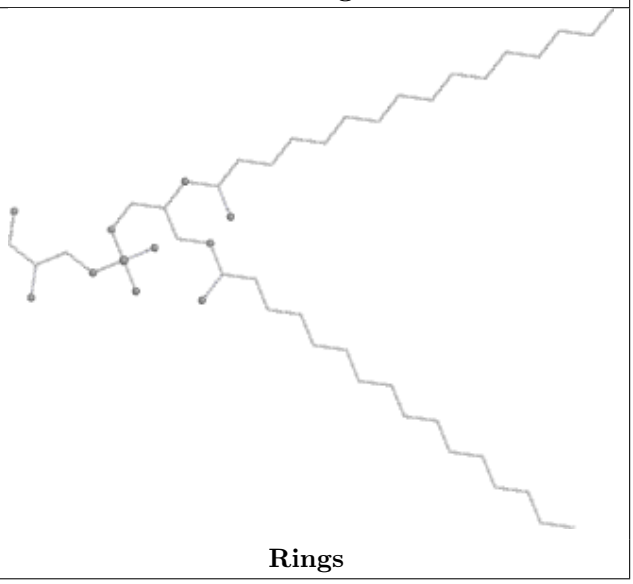
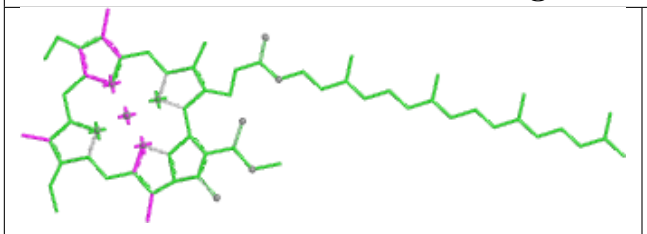


Rings

Ligand CLA a 405



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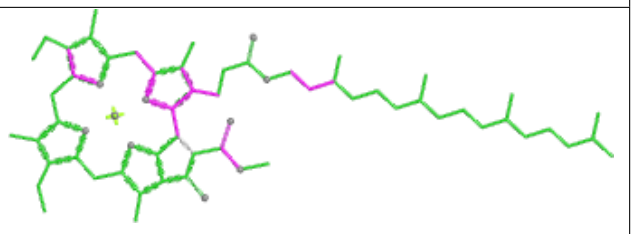

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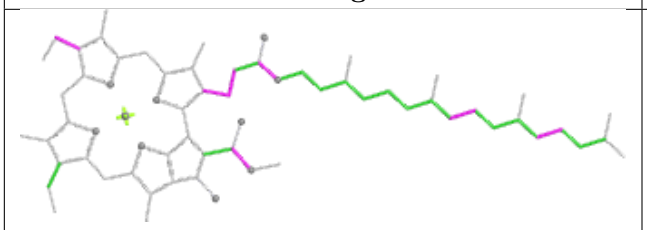

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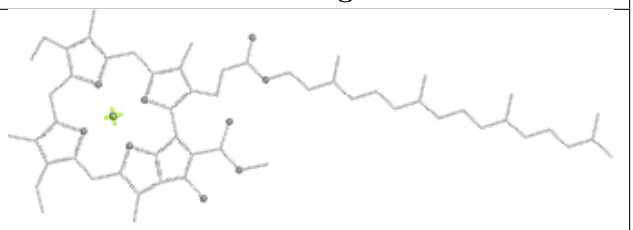
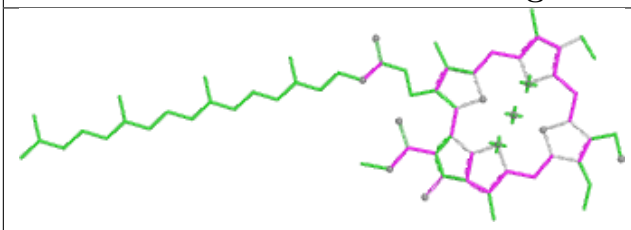


Rings

Ligand CHL n 317



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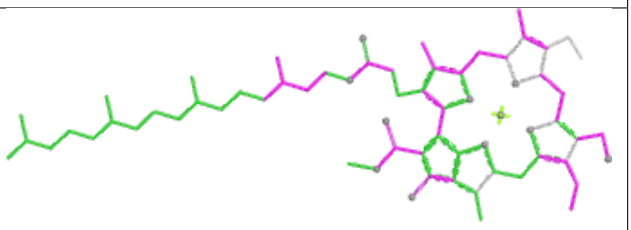
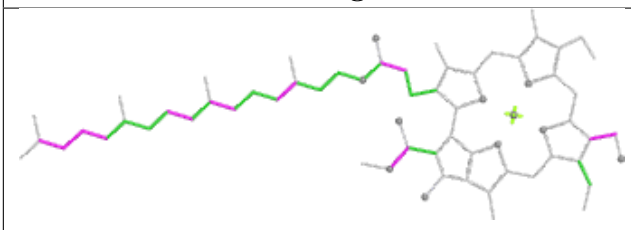


Bond angles



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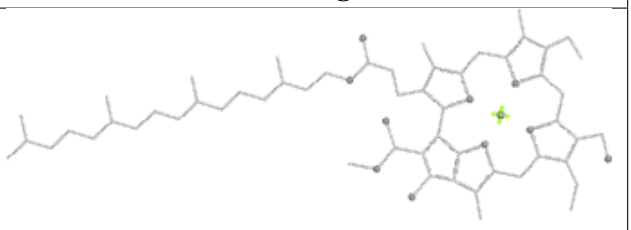
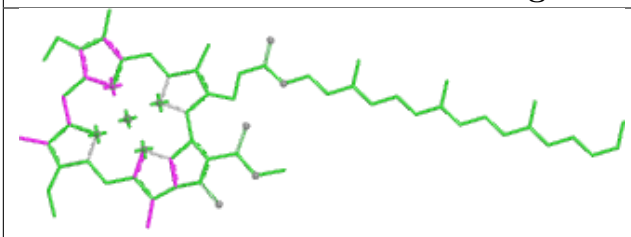


Rings

Ligand CLA 3 304



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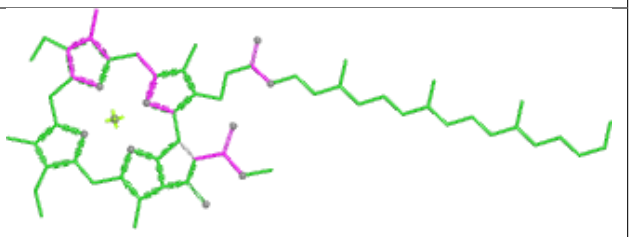

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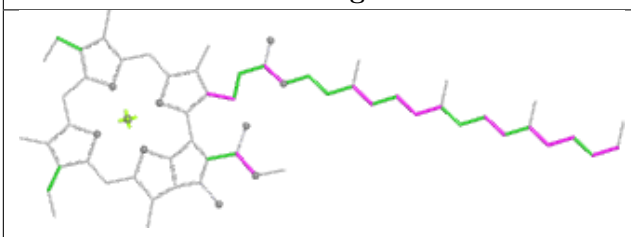
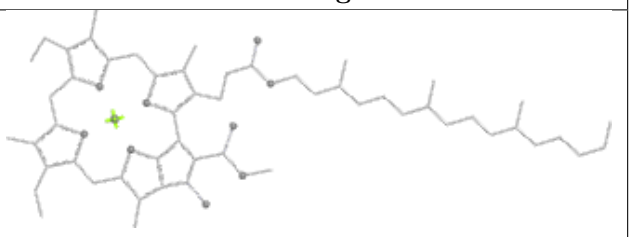
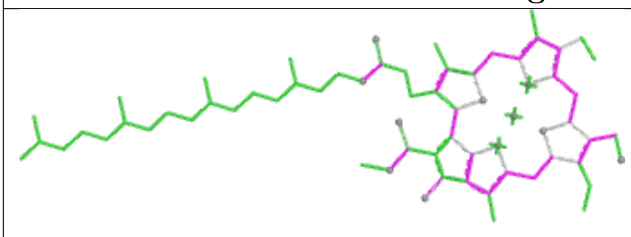


Torsions



Rings

Ligand CHL g 314



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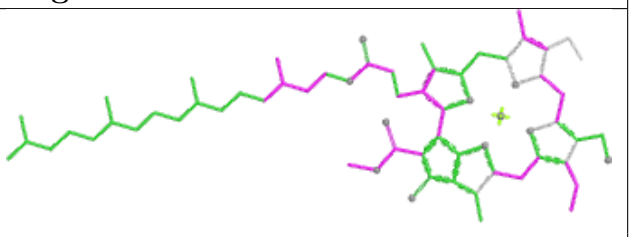

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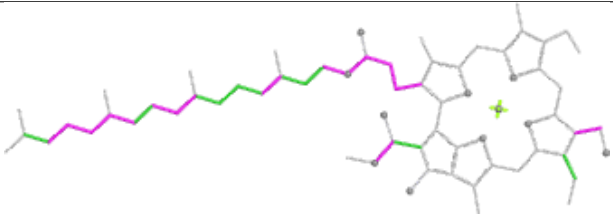

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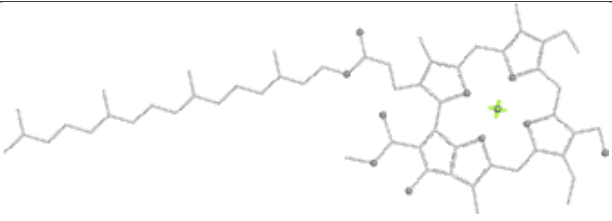
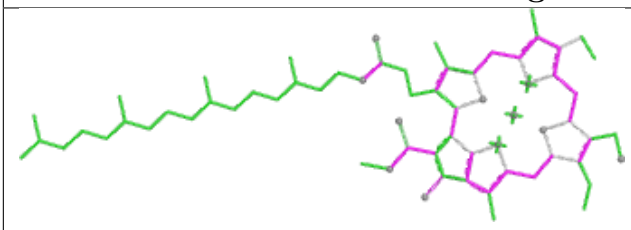


Rings

Ligand CHL 2 317



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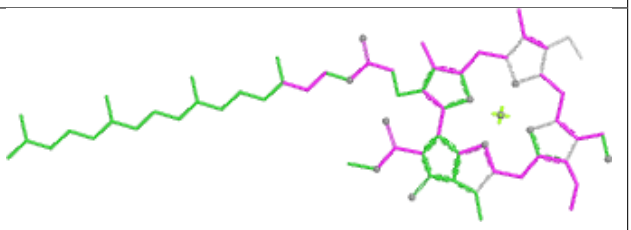

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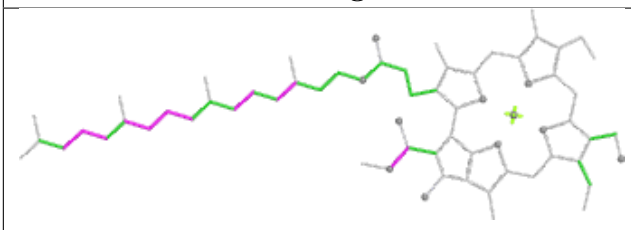

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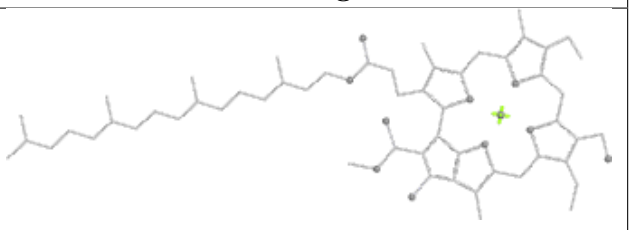
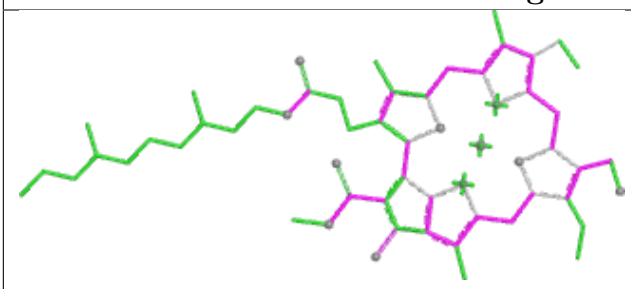


Rings

Ligand CHL S 315



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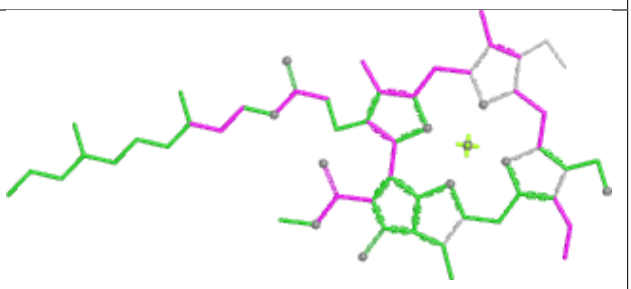

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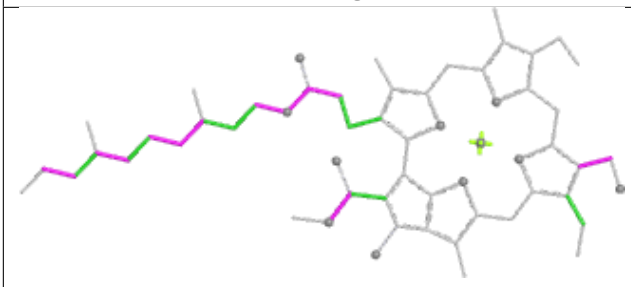

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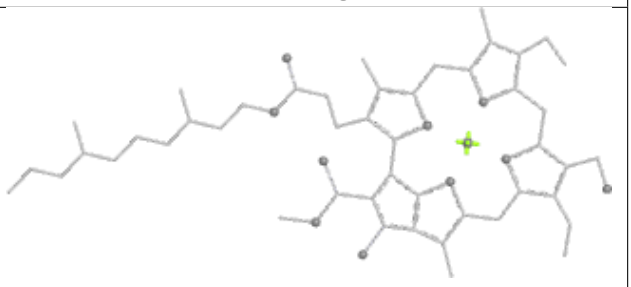
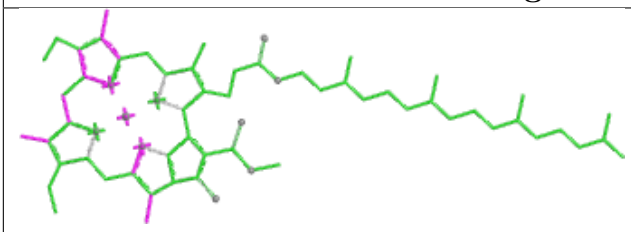


Rings

Ligand CLA B 613



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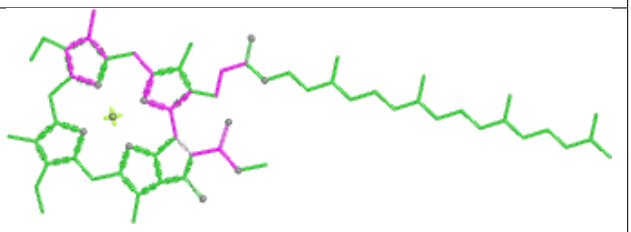

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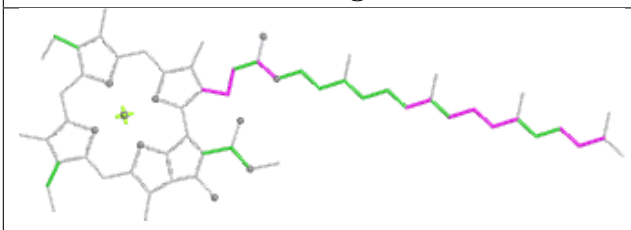

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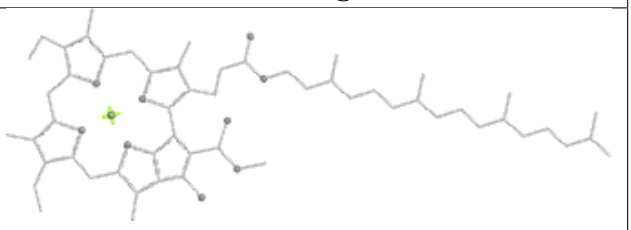
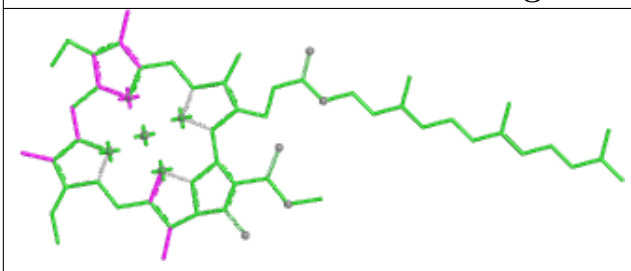


Rings

Ligand CLA V 305



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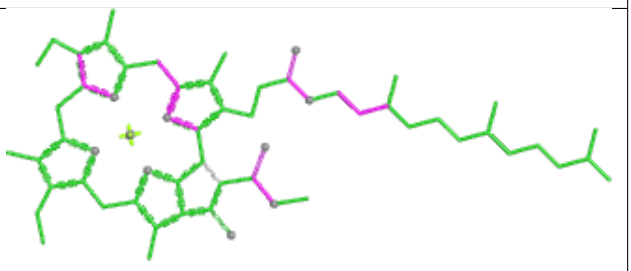
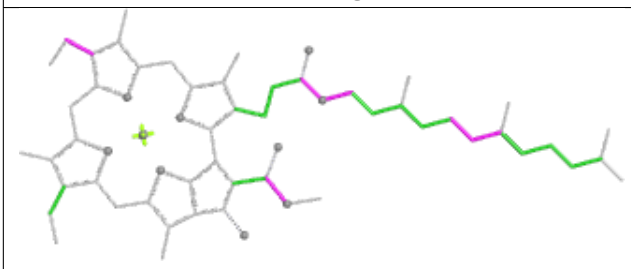


Bond angles



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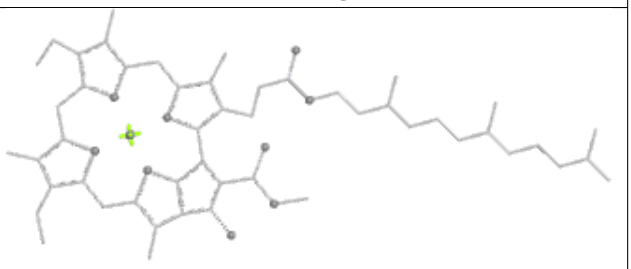
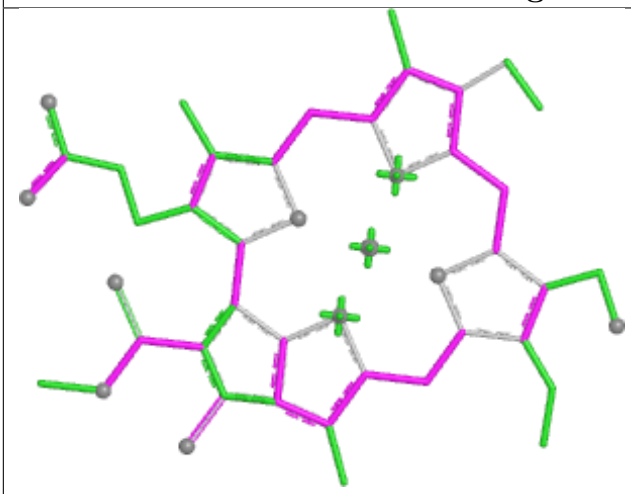


Rings

Ligand CHL S 316



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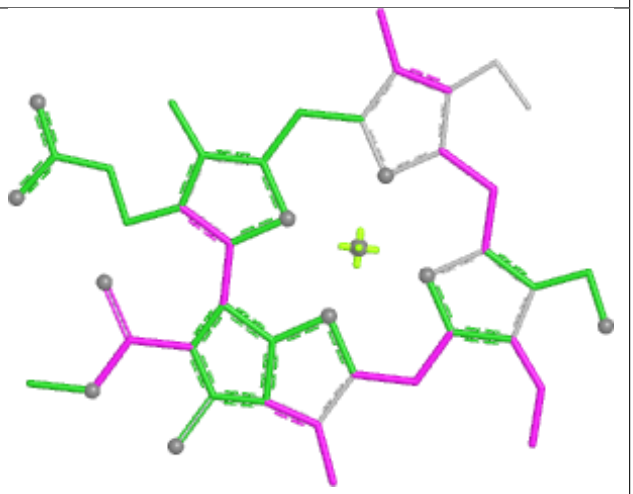

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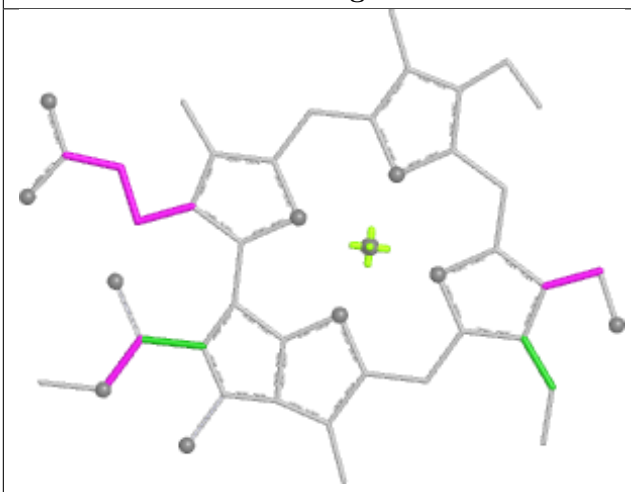

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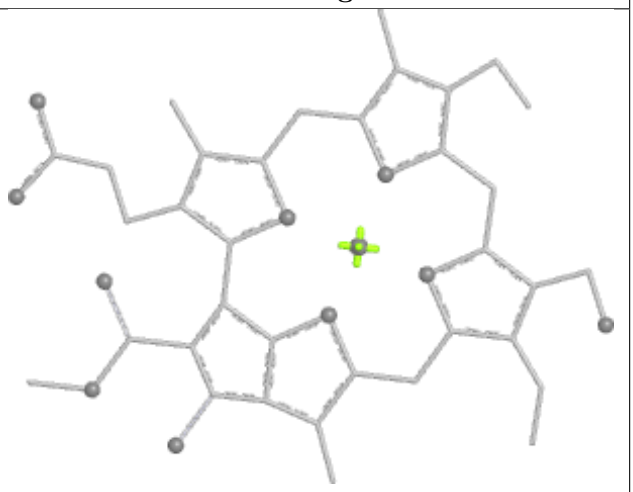
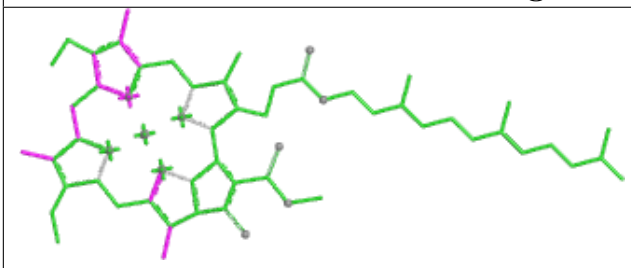


Rings

Ligand CLA u 305



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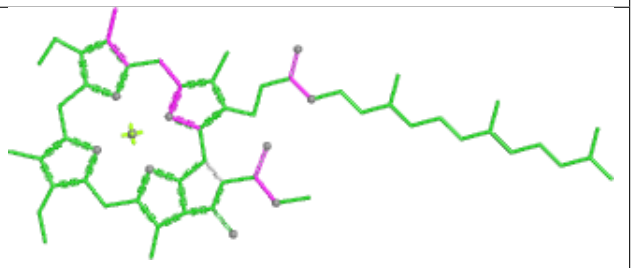

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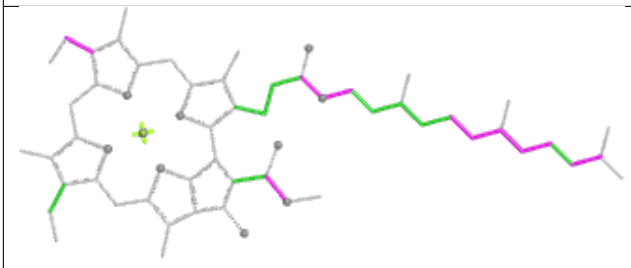

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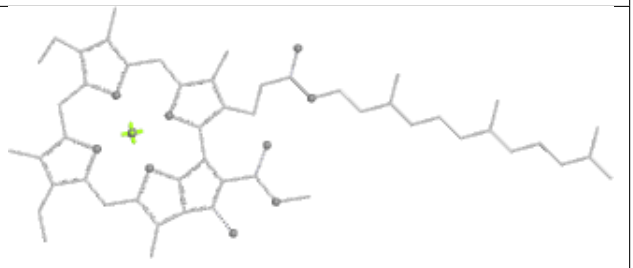
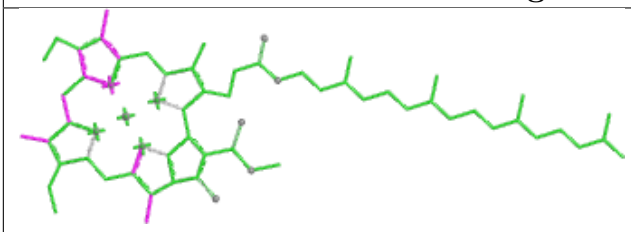


Rings

Ligand CLA b 610



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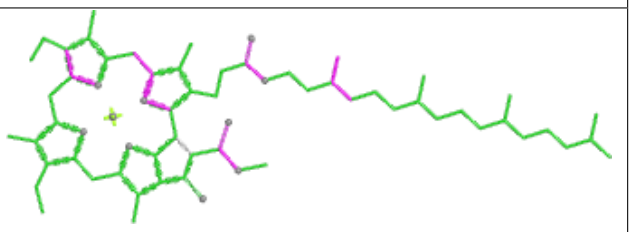

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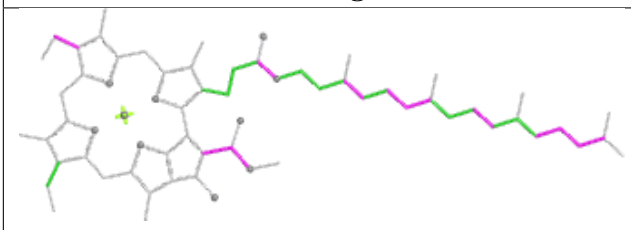

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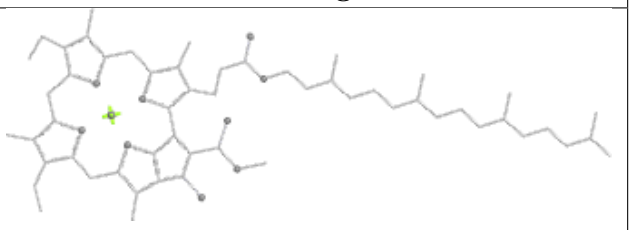
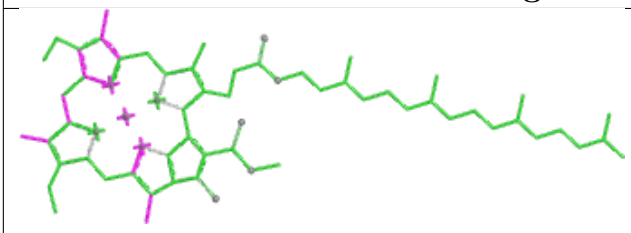


Rings

Ligand CLA D 403



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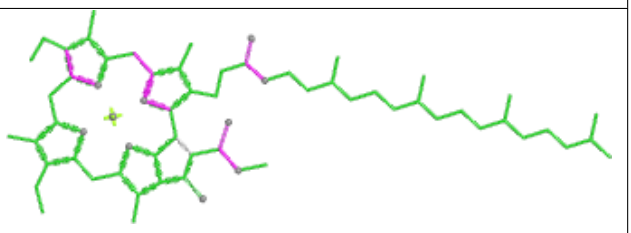

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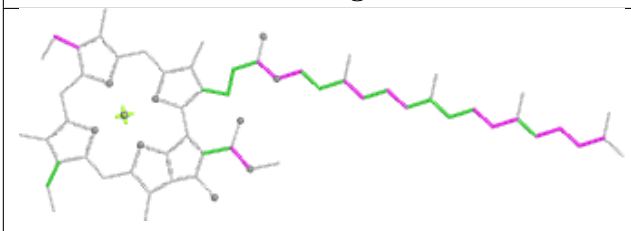

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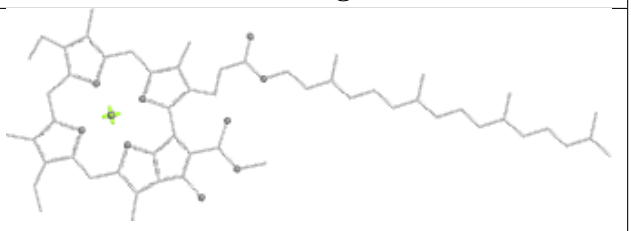
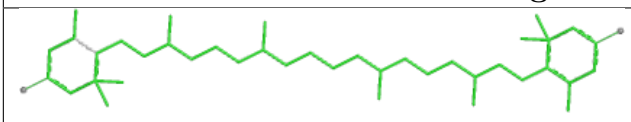


Rings

Ligand LUT r 611



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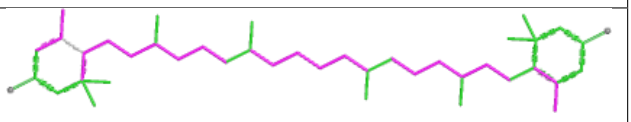

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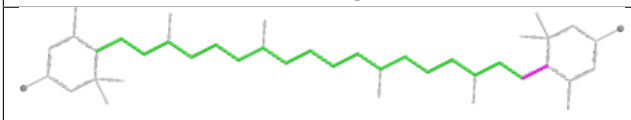

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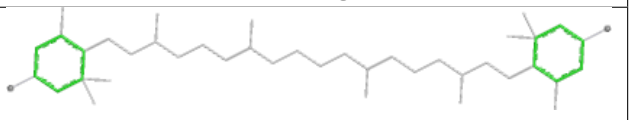
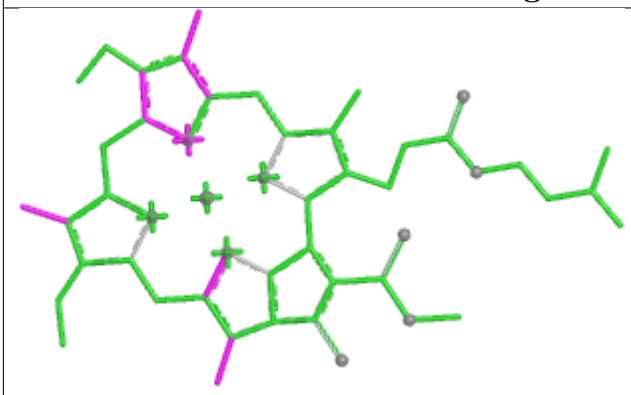


Rings

Ligand CLA U 303



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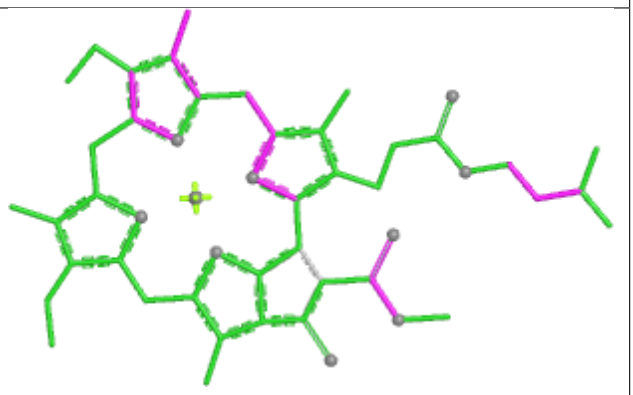
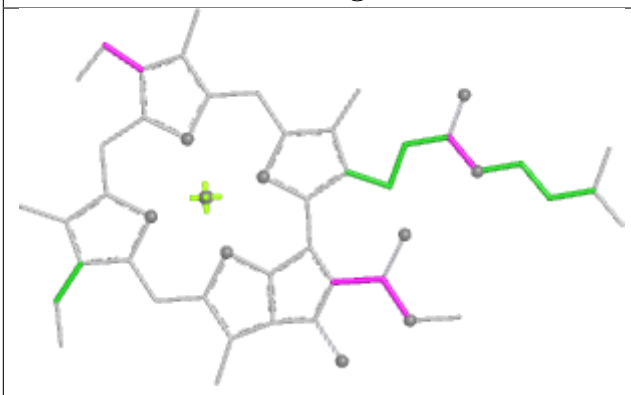


Bond angles



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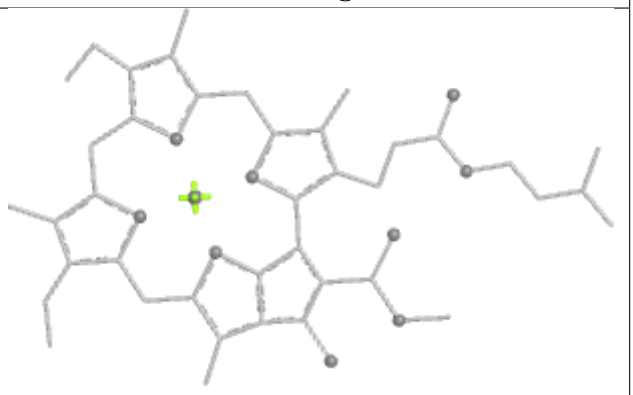
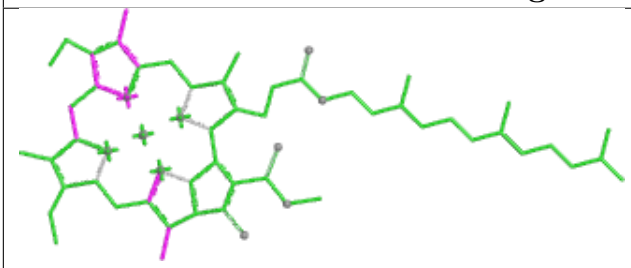


Rings

Ligand CLA 6 306



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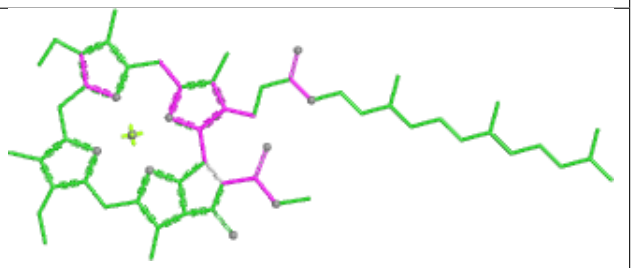
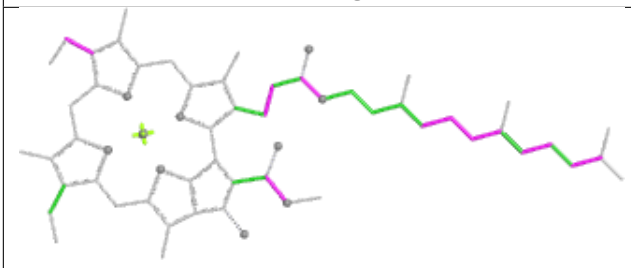


Bond angles



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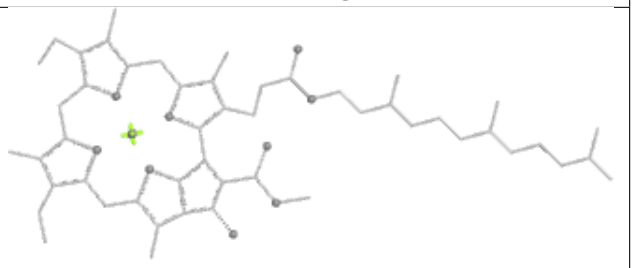
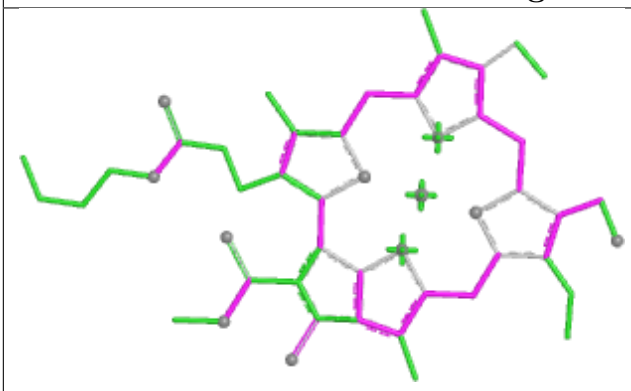


Rings

Ligand CHL g 313



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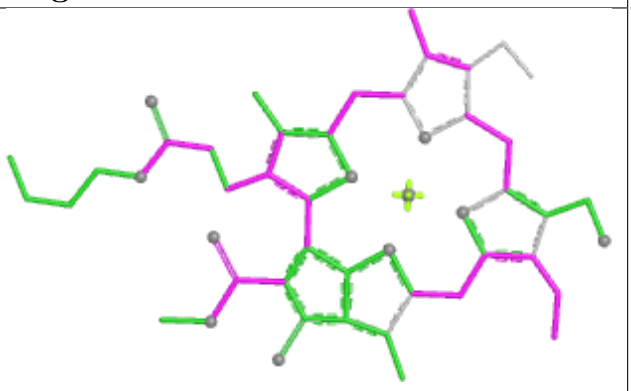
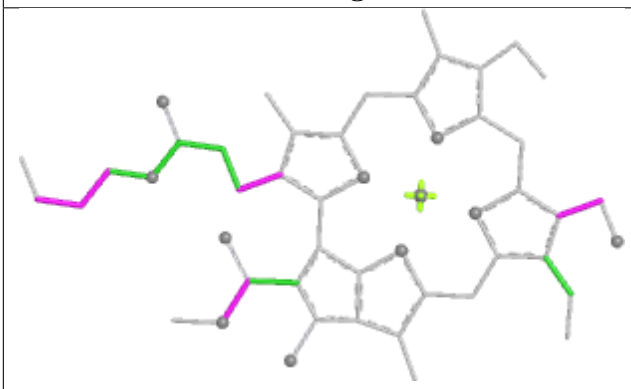
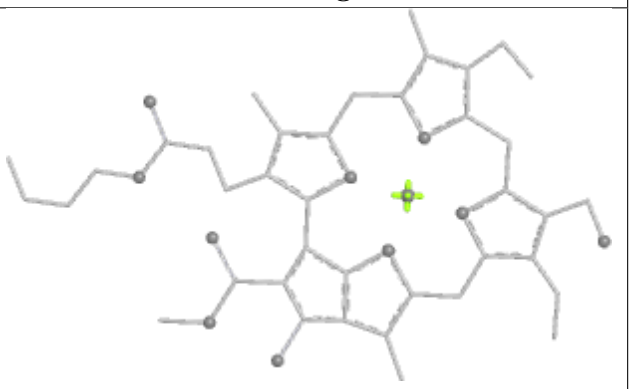


Bond angles

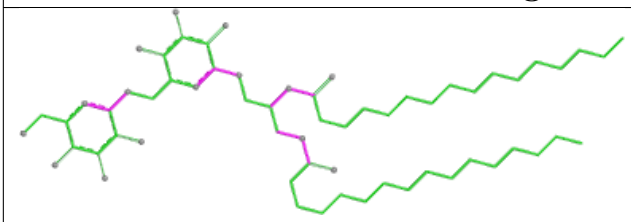


Torsions

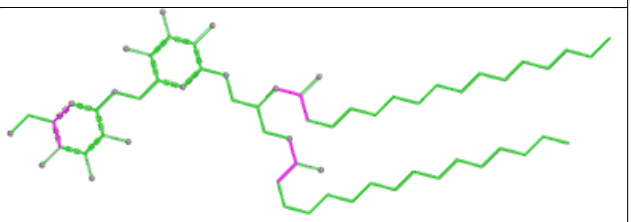


Rings

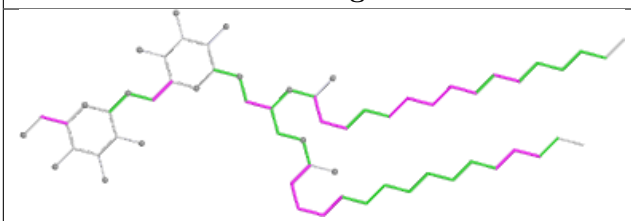
Ligand DGD b 601



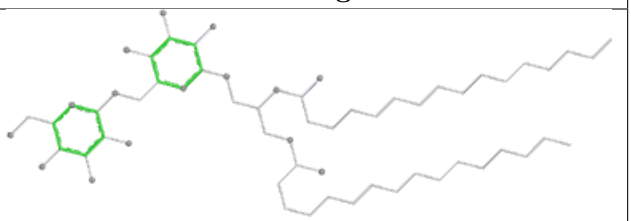
Bond lengths



Bond angles

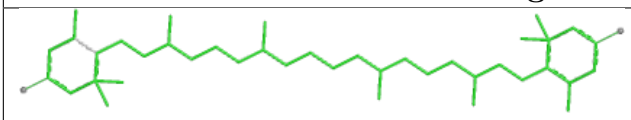


Torsions



Rings

Ligand LUT n 309



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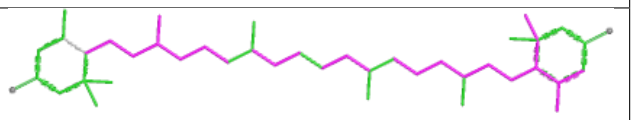

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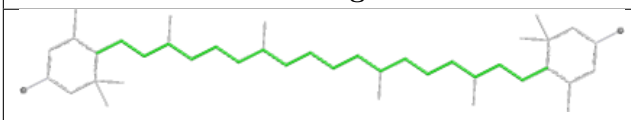
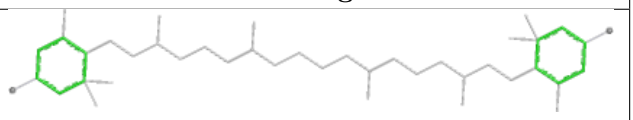
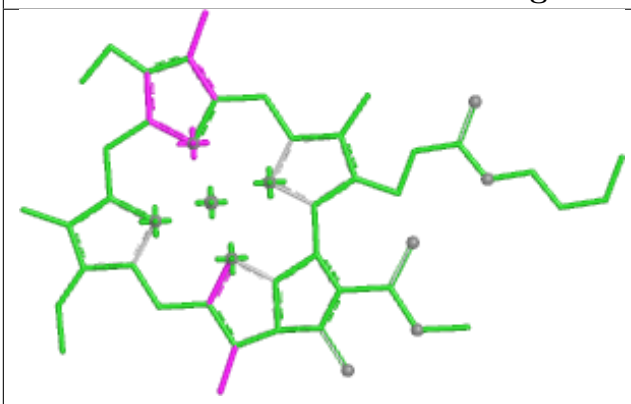


Torsions



Rings

Ligand CLA r 607



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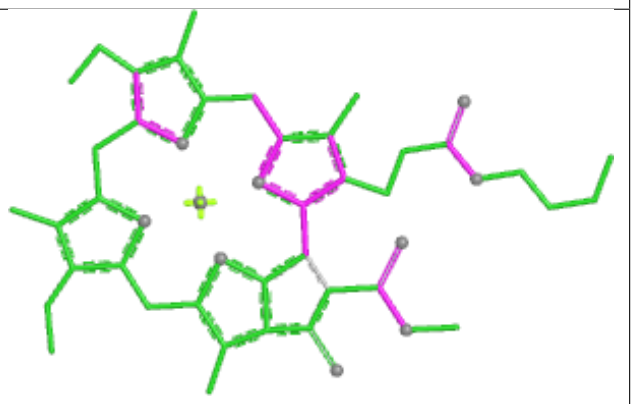
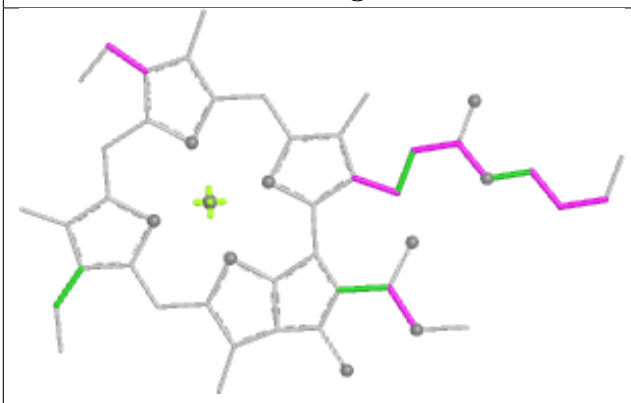


Bond angles



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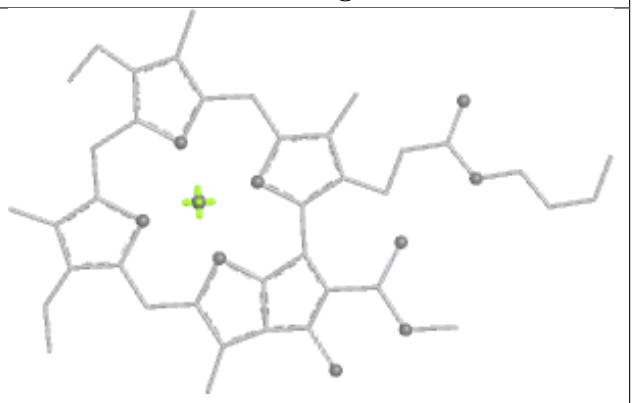
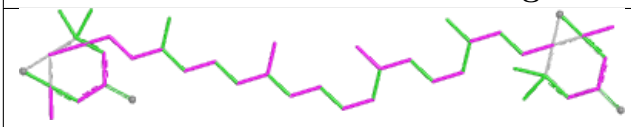


Rings

Ligand XAT G 309



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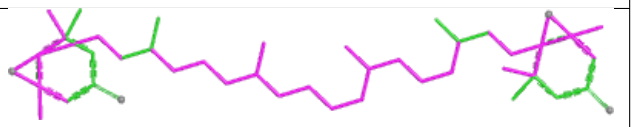
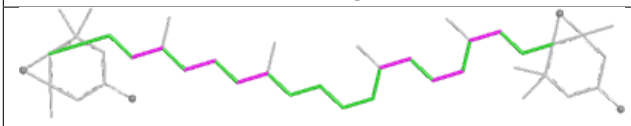
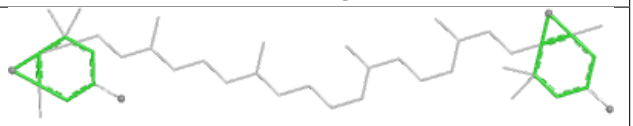


Bond angles

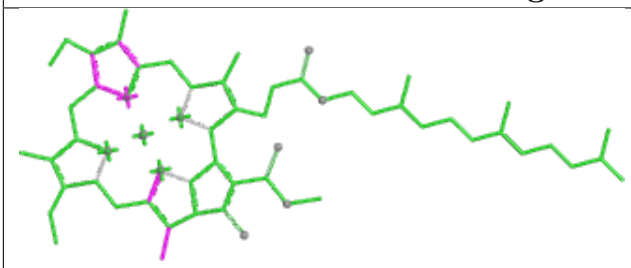


Torsions



Rings

Ligand CLA n 306



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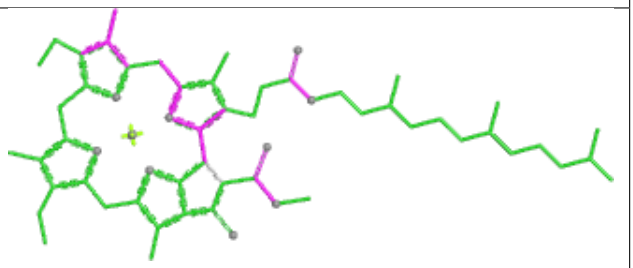
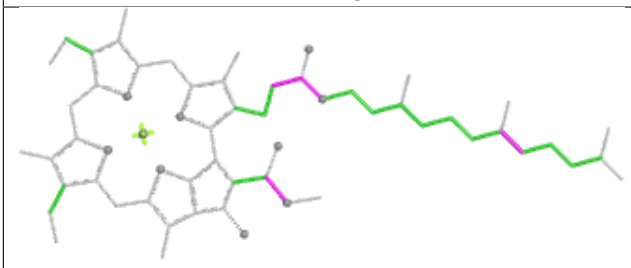


Bond angles



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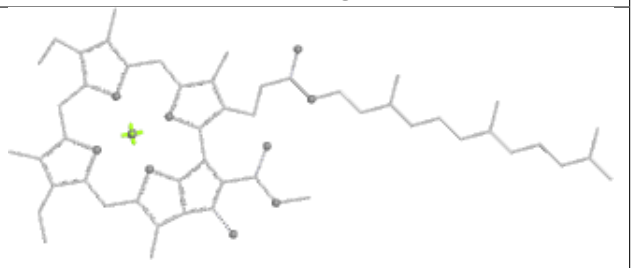
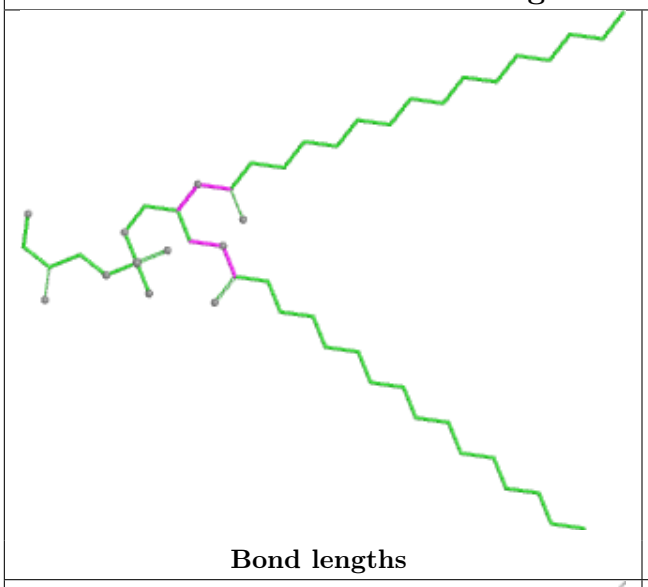


Rings

Ligand LHG 2 312



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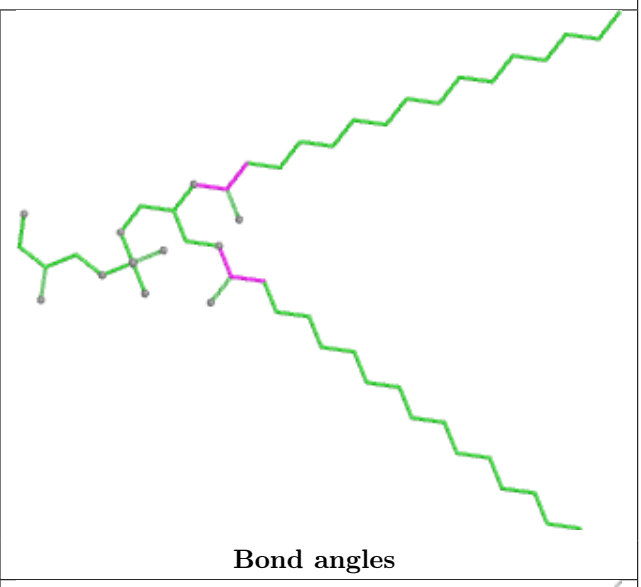
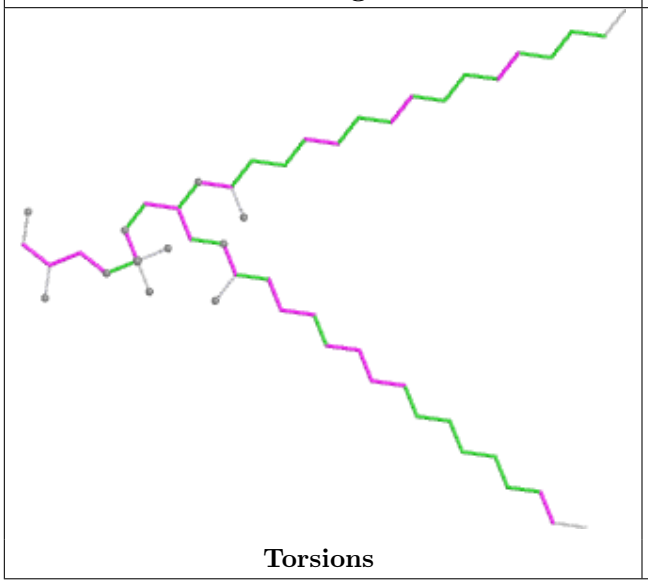


Bond angles



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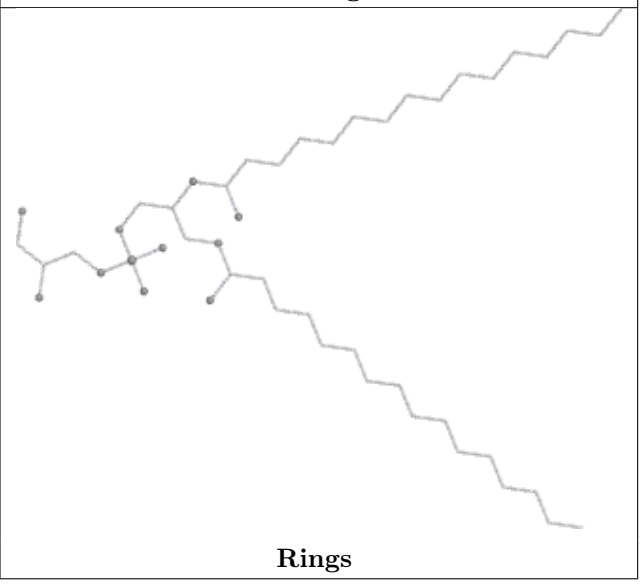
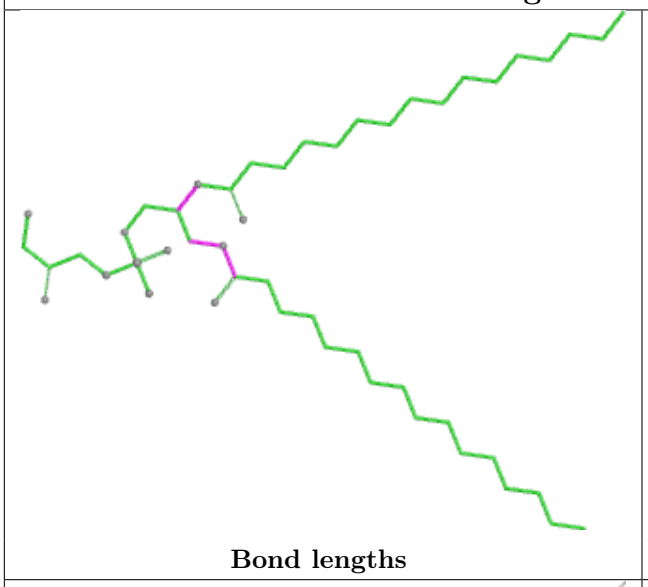


Rings

Ligand LHG C 523



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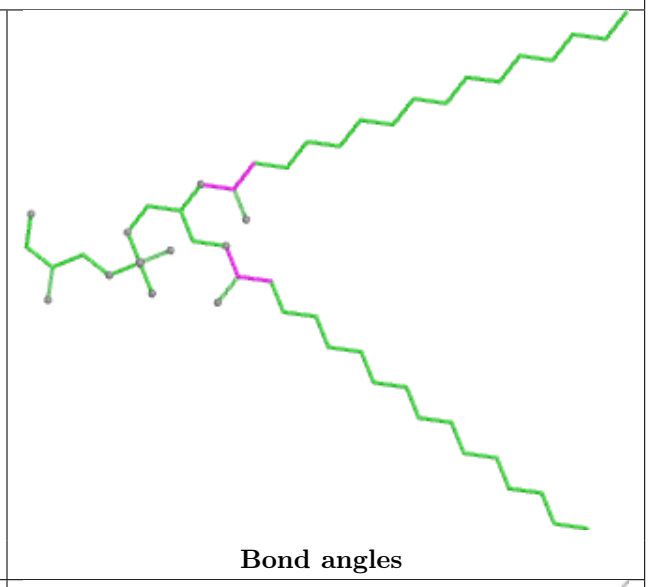
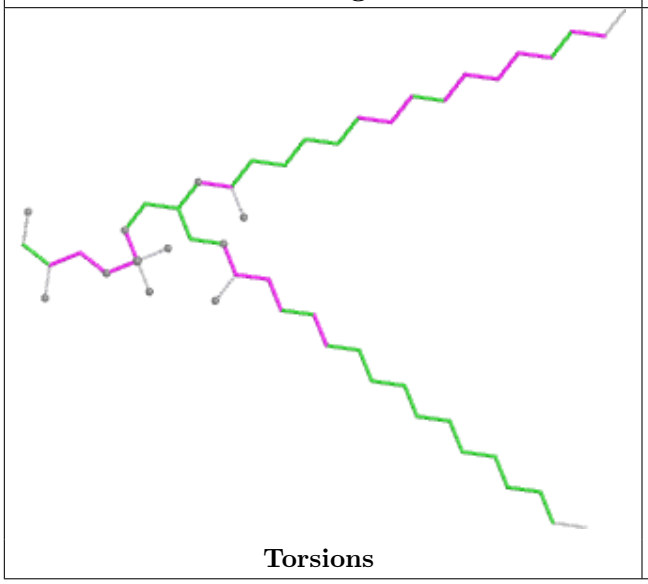


Bond angles



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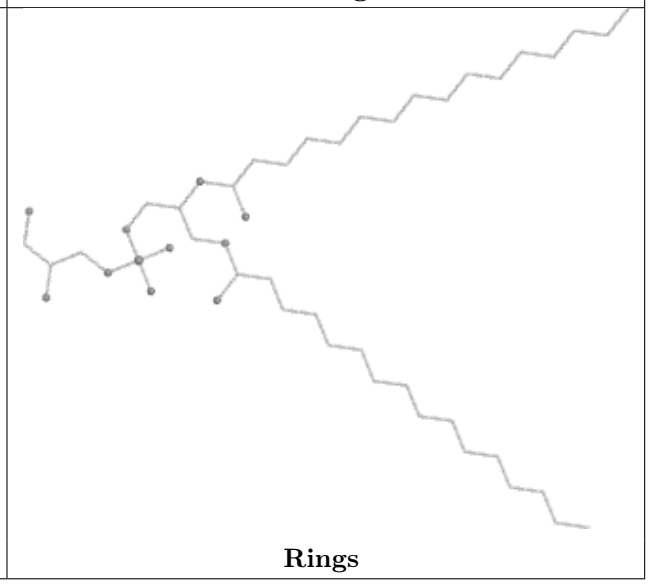
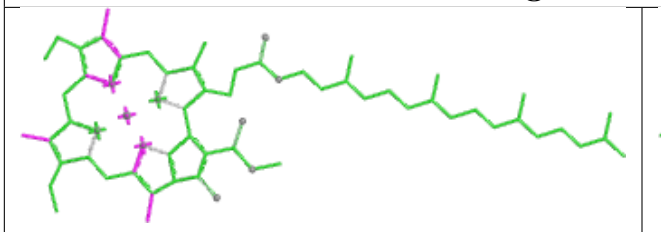


Rings

Ligand CLA B 614



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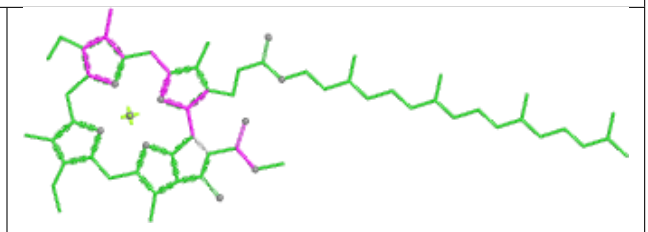
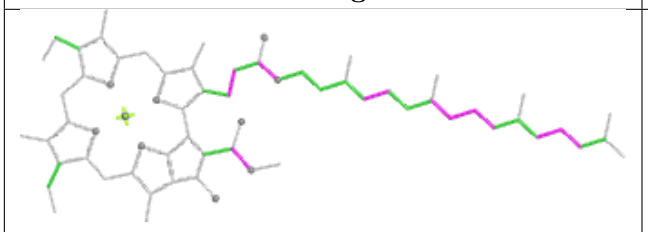


Bond angles



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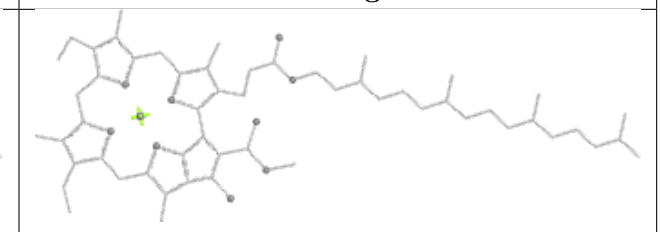
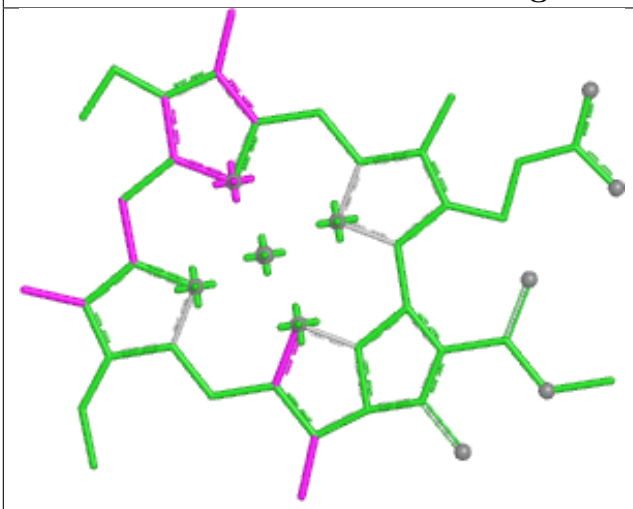


Rings

Ligand CLA r 610



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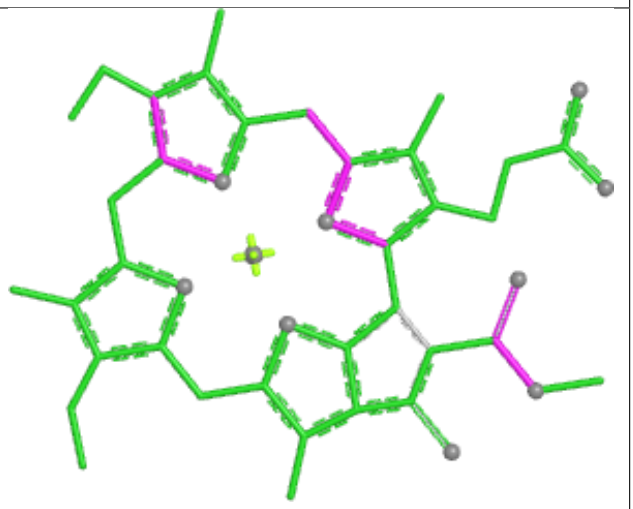
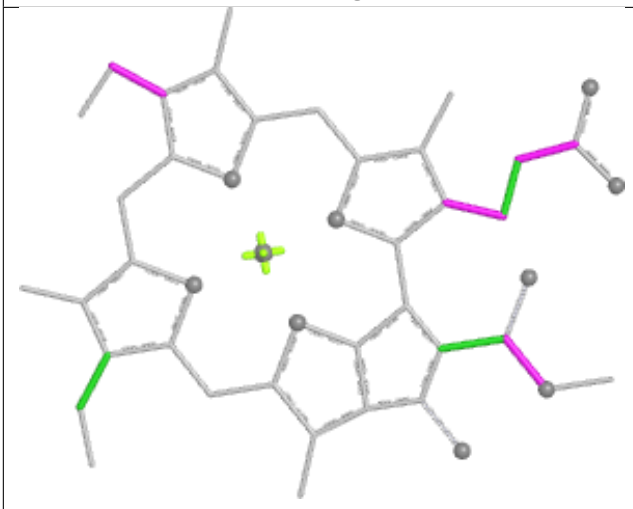


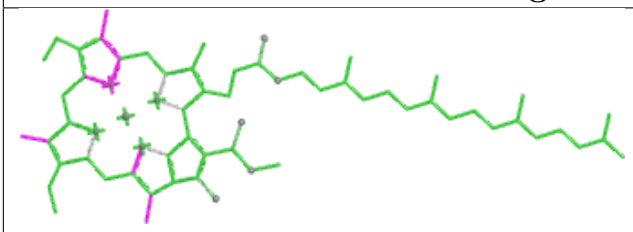
Bond angles



Torsions

Rings

Ligand CLA c 506



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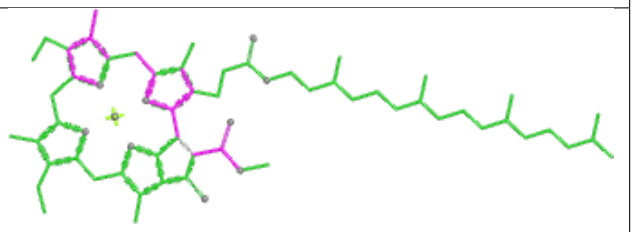

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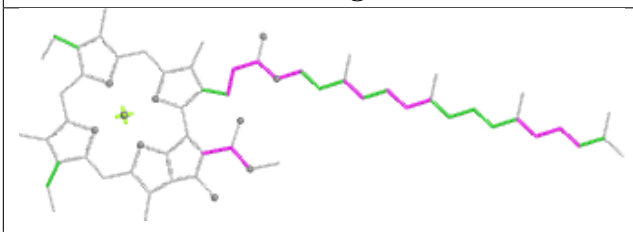

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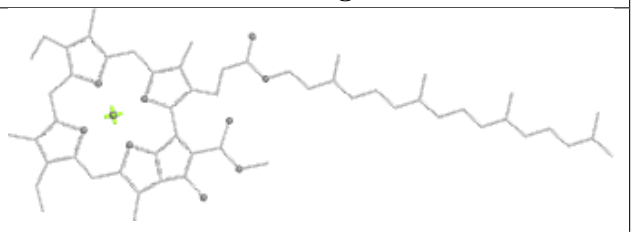
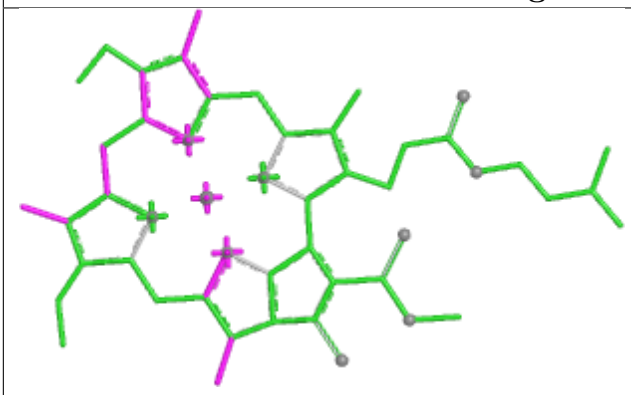


Rings

Ligand CLA 4 303



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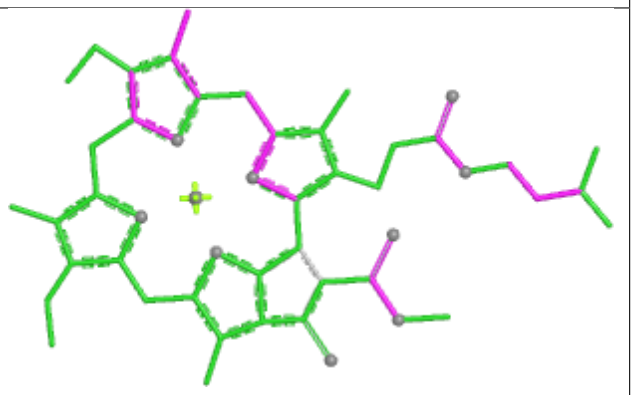
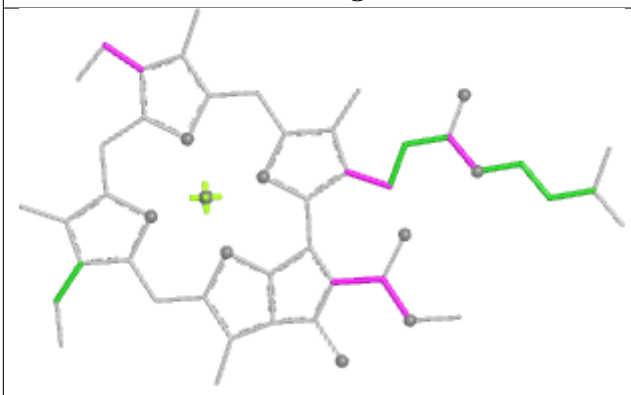


Bond angles



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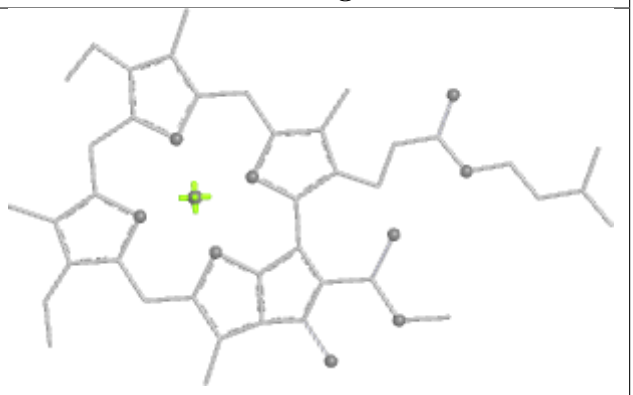
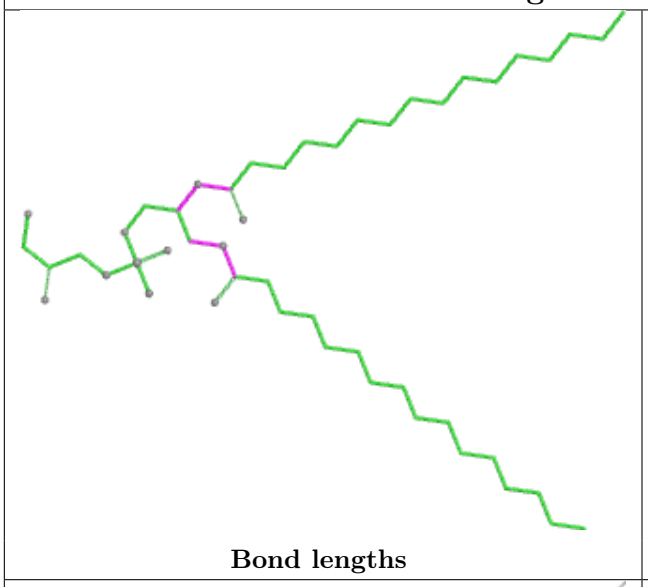


Rings

Ligand LHG p 313



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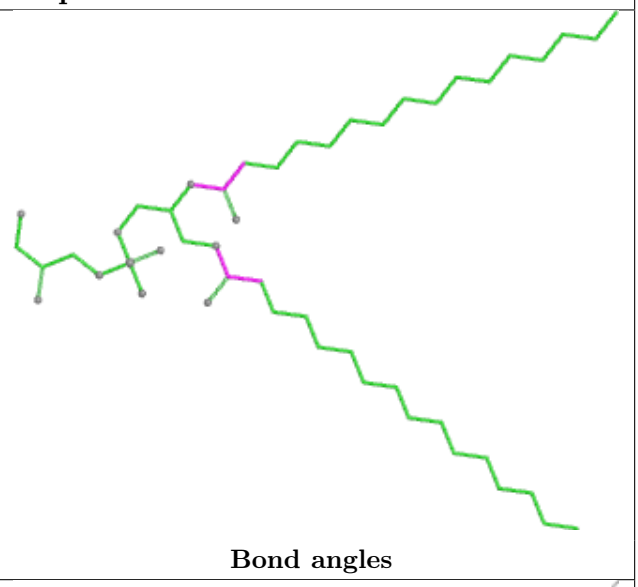
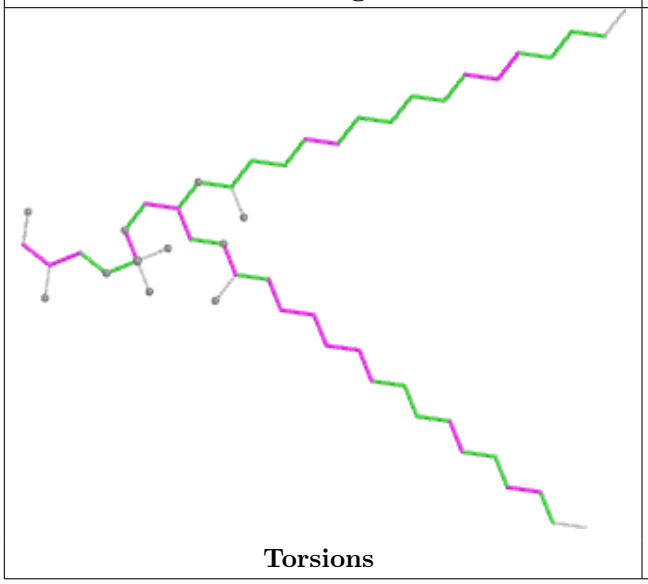


Bond angles



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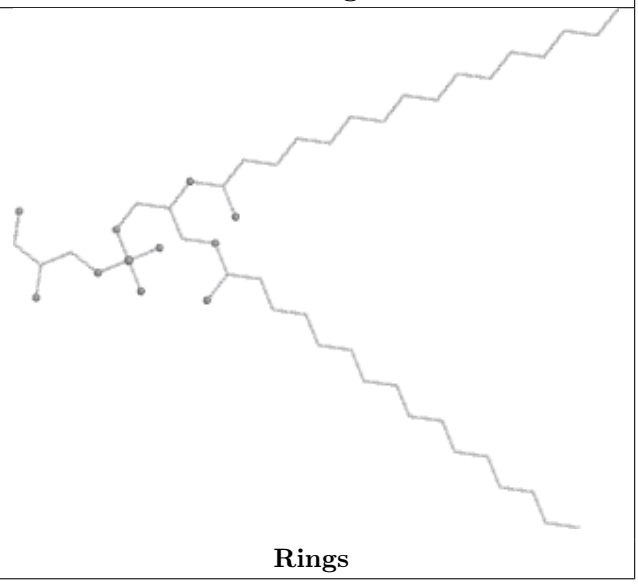
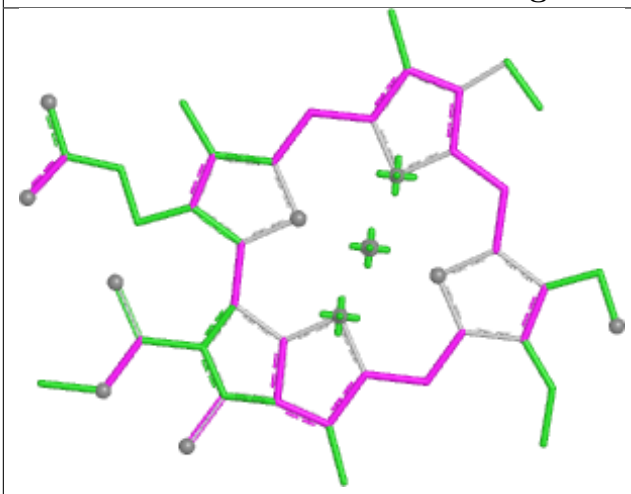


Rings

Ligand CHL s 314



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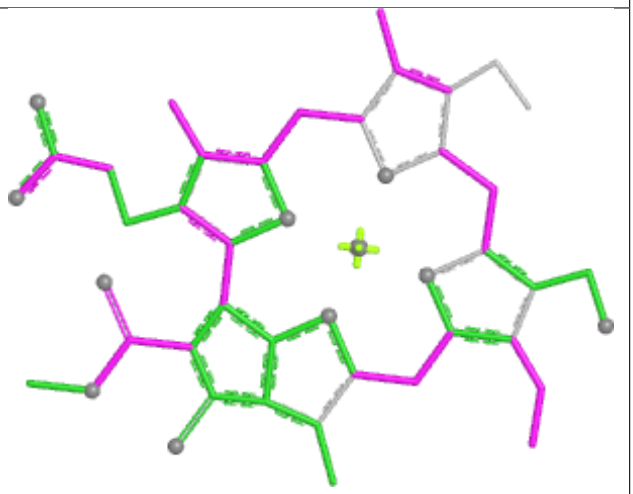
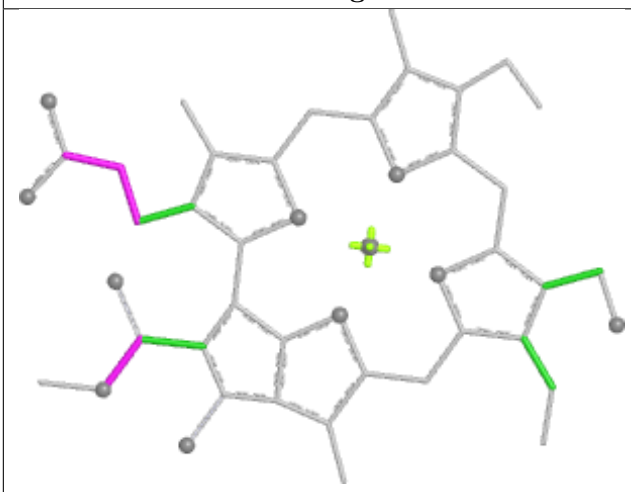


Bond angles



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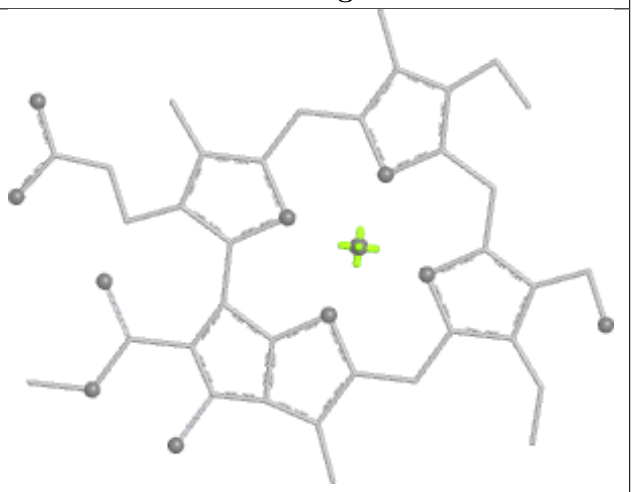
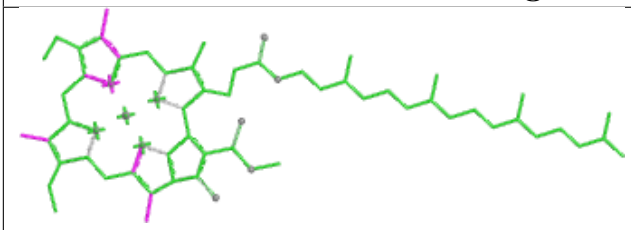


Rings

Ligand CLA C 509



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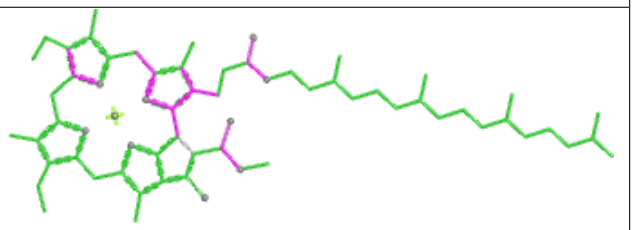
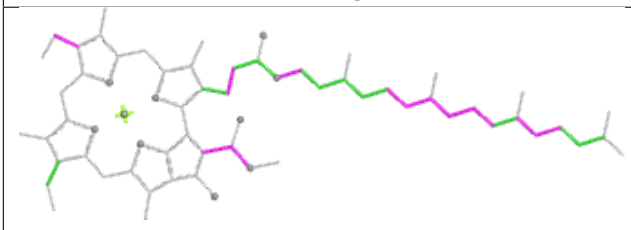


Bond angles



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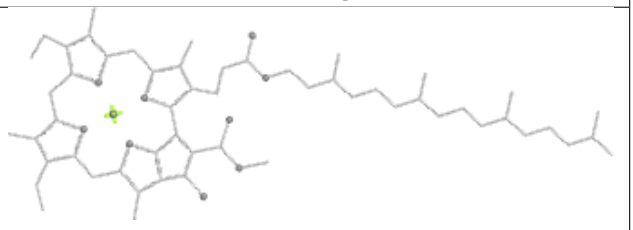
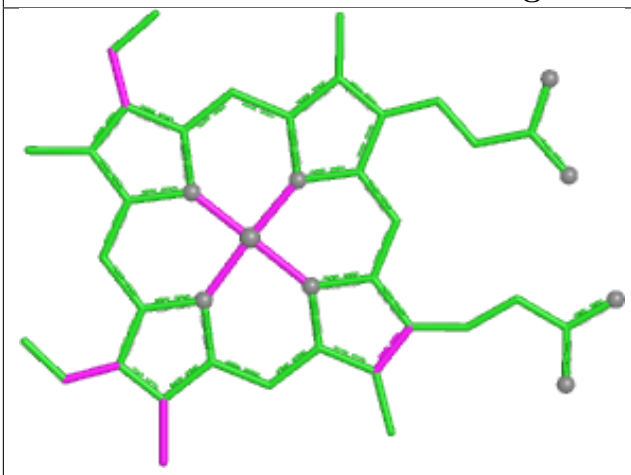


Rings

Ligand HEM e 101



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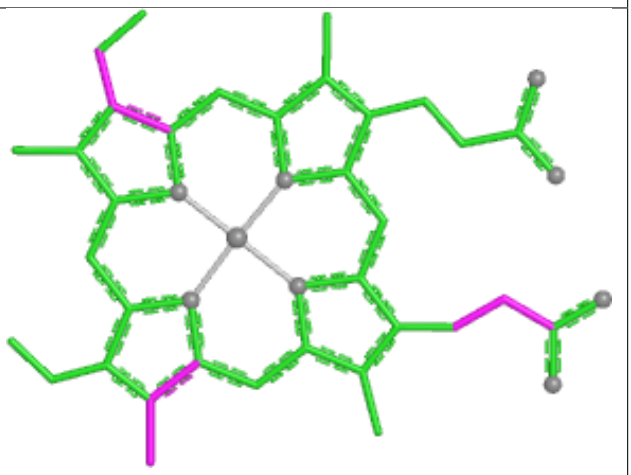
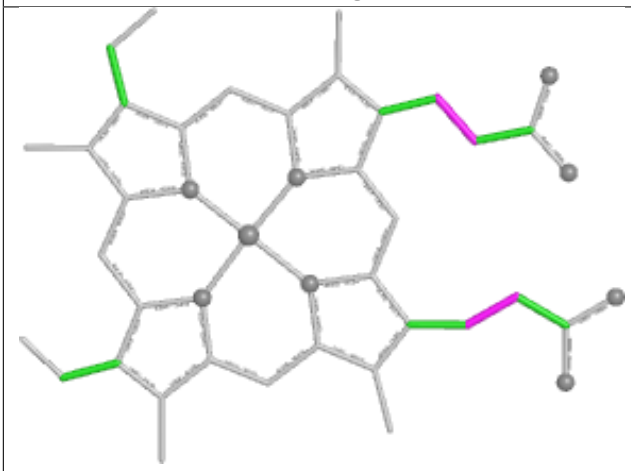
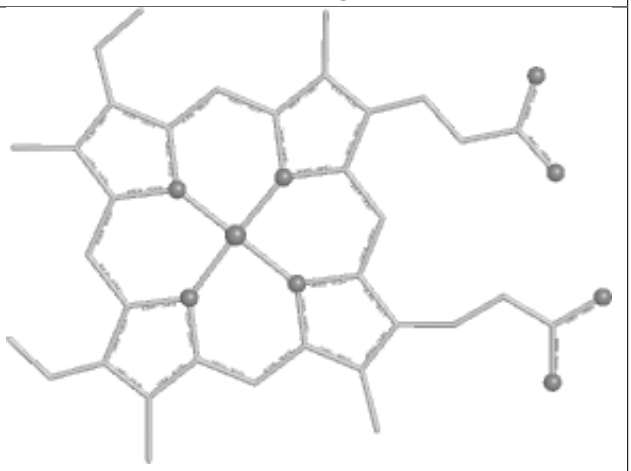


Bond angles

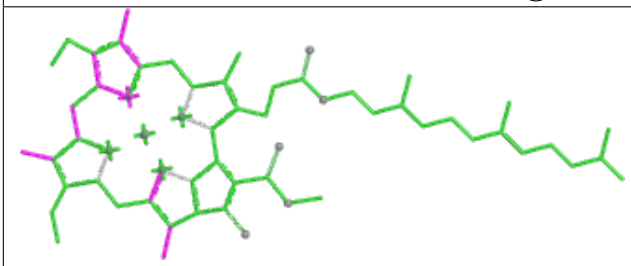


Torsions



Rings

Ligand CLA n 307



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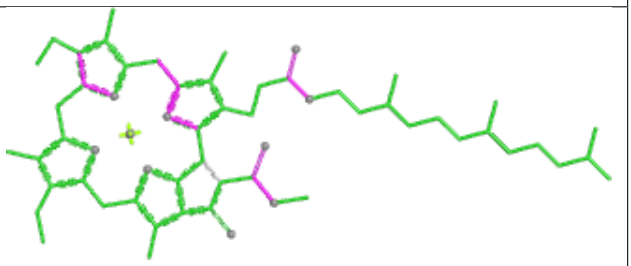

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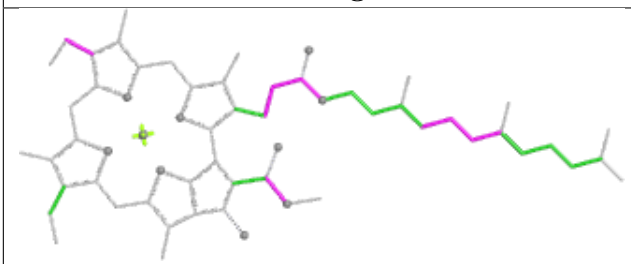

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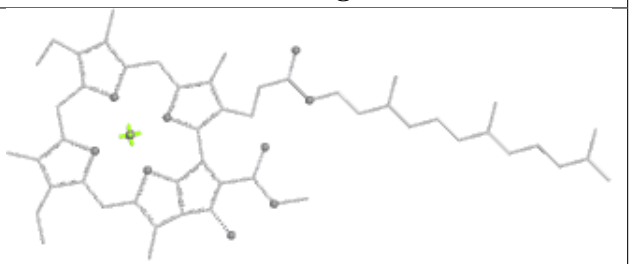
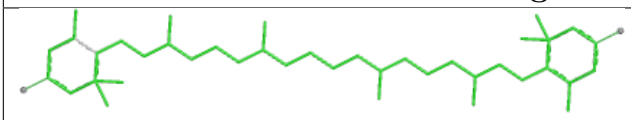


Rings

Ligand LUT s 310



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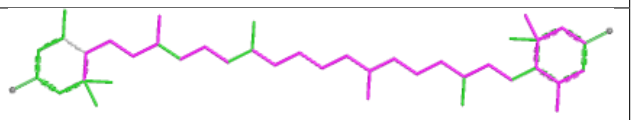
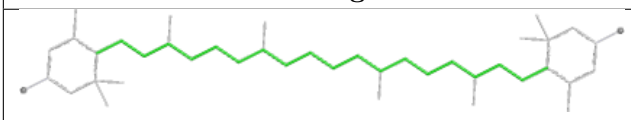
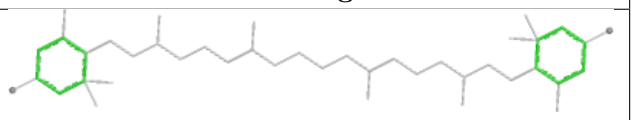


Bond angles

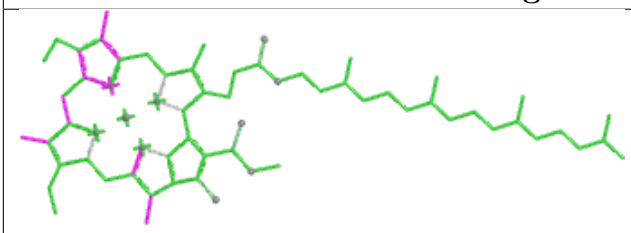


Torsions



Rings

Ligand CLA G 301



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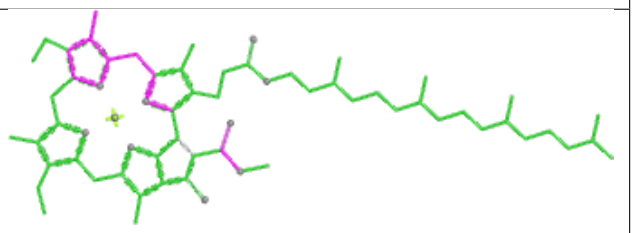
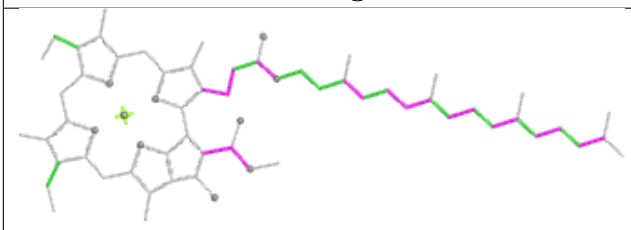


Bond angles



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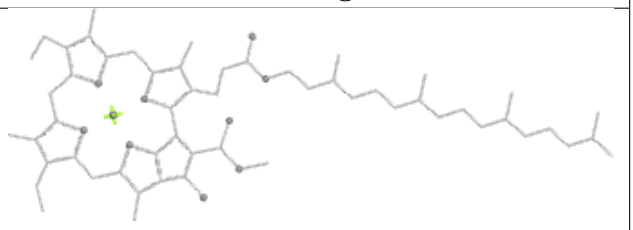
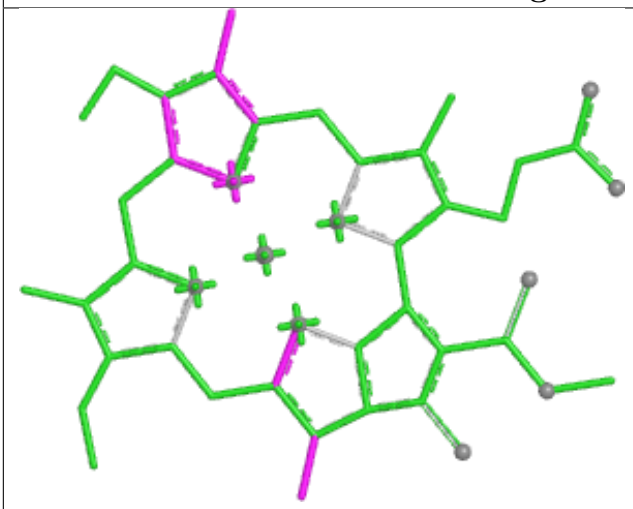


Rings

Ligand CLA s 302



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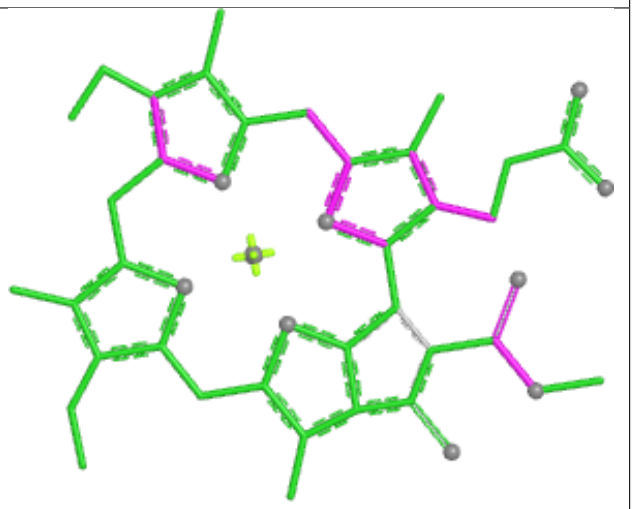
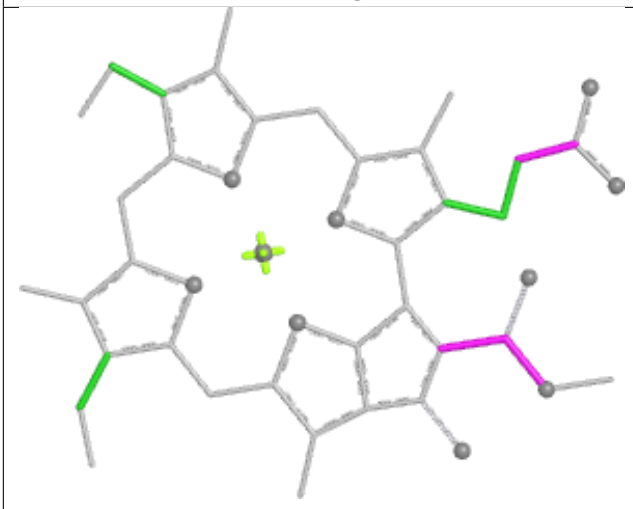


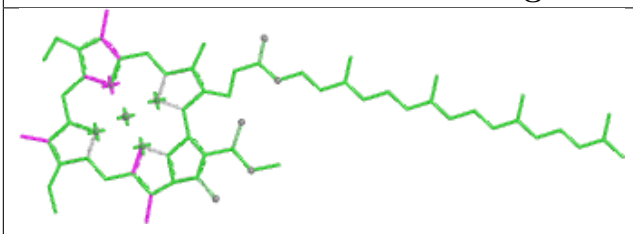
Bond angles



Torsions

Rings

Ligand CLA C 508



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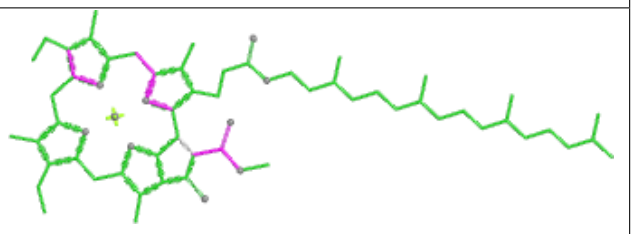

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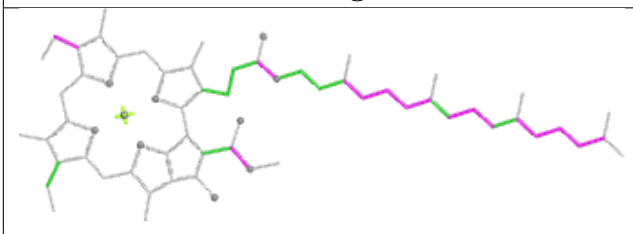

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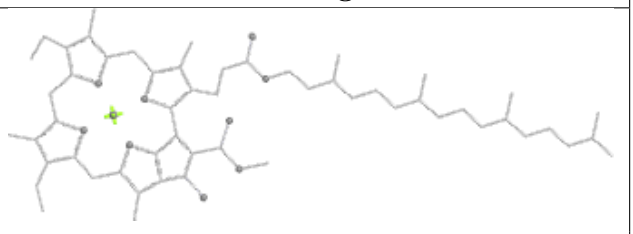
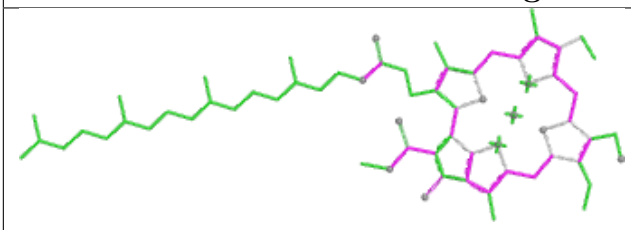


Rings

Ligand CHL V 316



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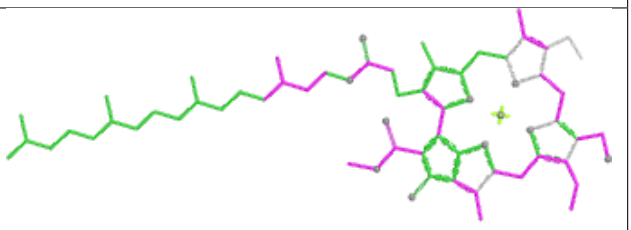
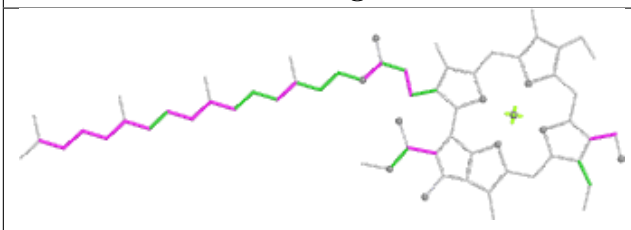


Bond angles



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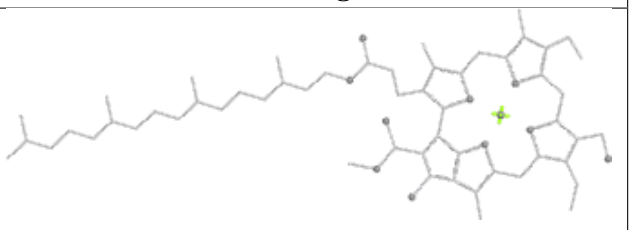
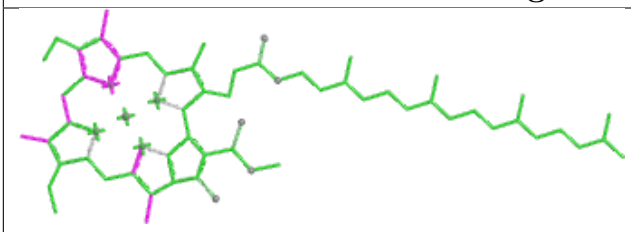


Rings

Ligand CLA x 201



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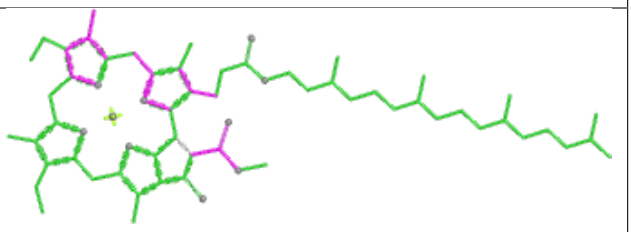
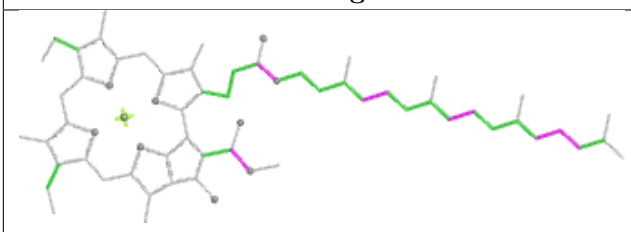


Bond angles



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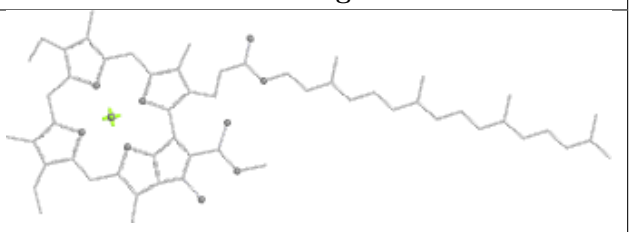
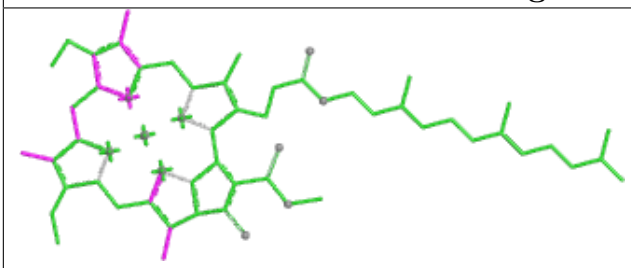


Rings

Ligand CLA 3 305



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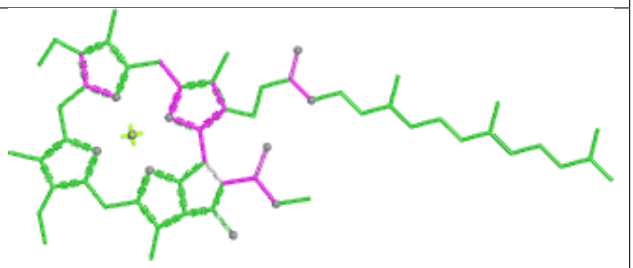
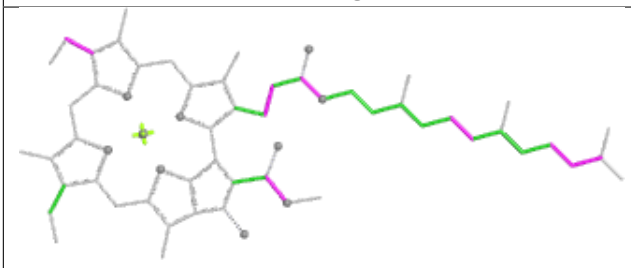


Bond angles



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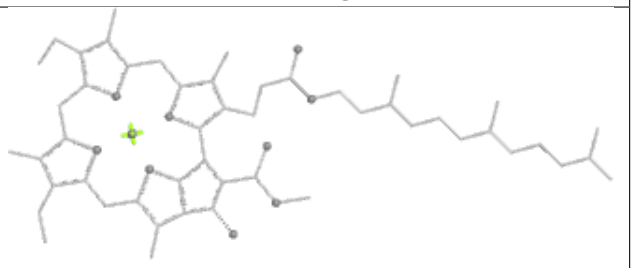
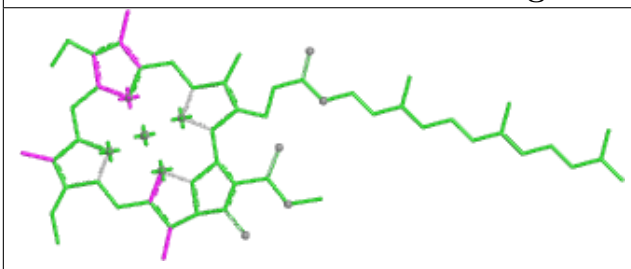


Rings

Ligand CLA v 306



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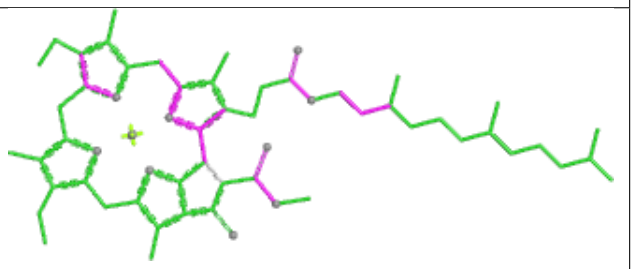

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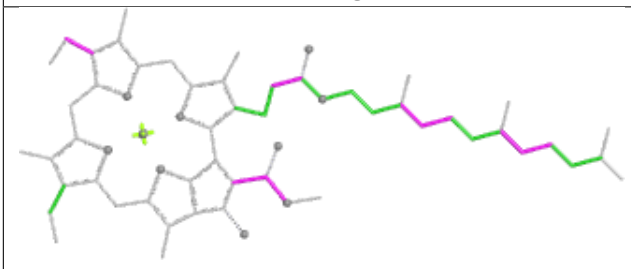

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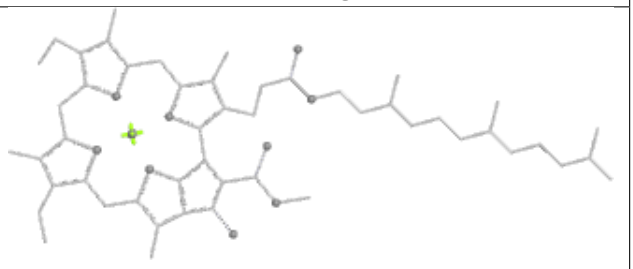
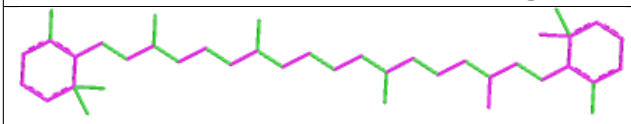


Rings

Ligand BCR C 517



Bond lengths

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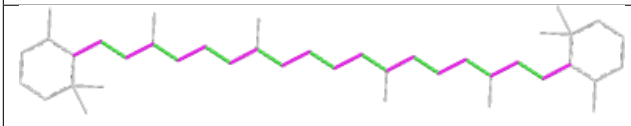

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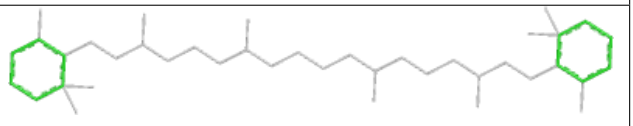
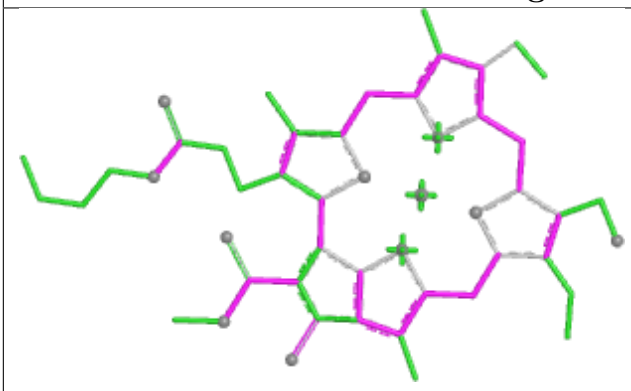


Rings

Ligand CHL 4 315



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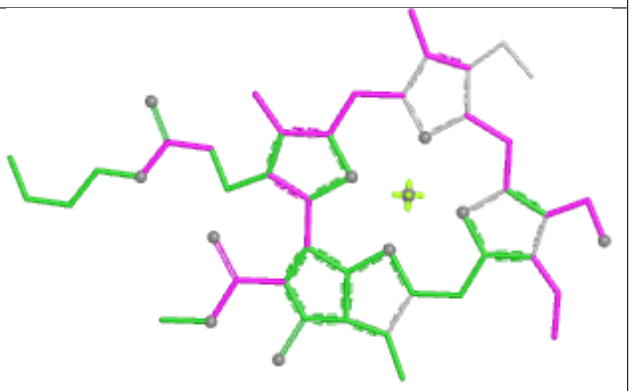
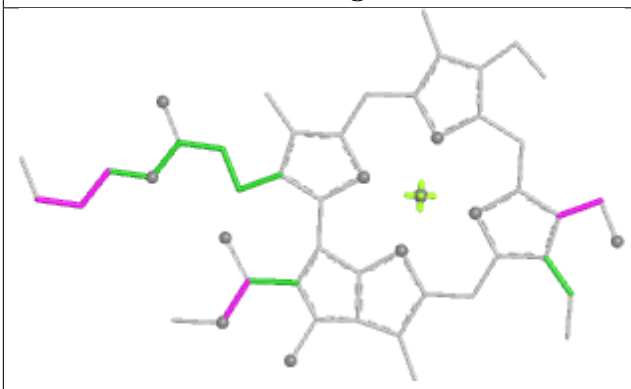


Bond angles



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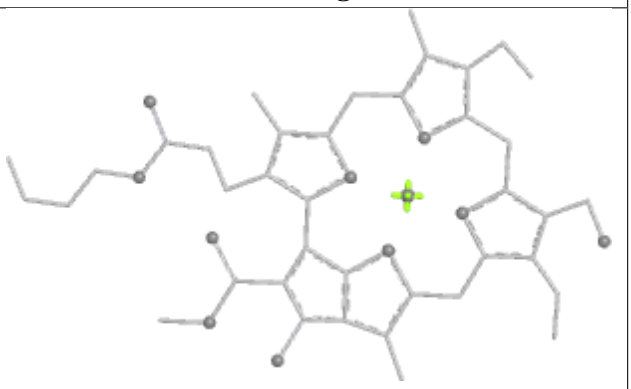
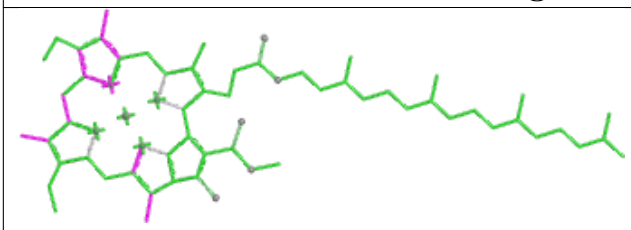


Rings

Ligand CLA 6 308



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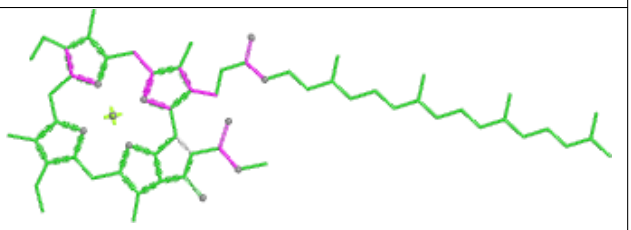
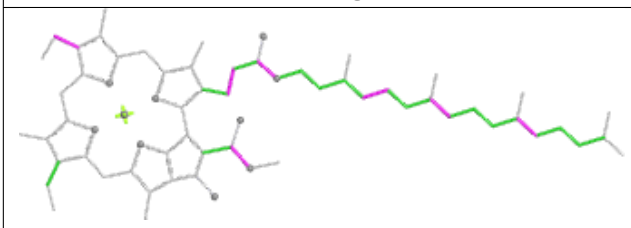


Bond angles



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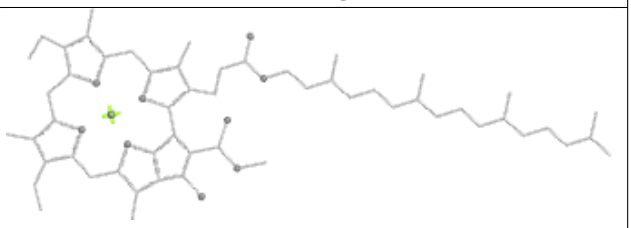
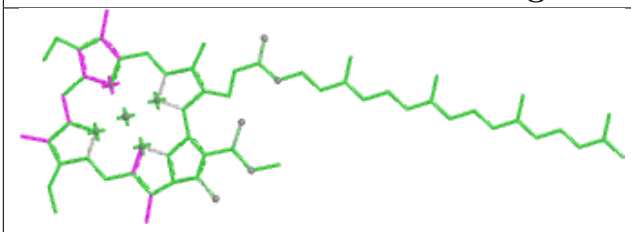


Rings

Ligand CLA b 604



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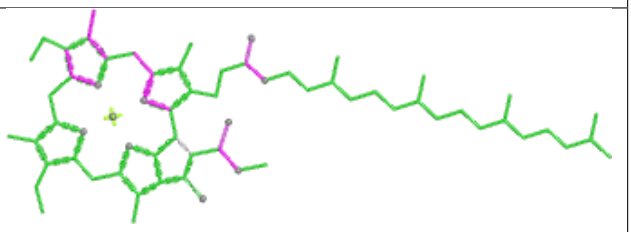
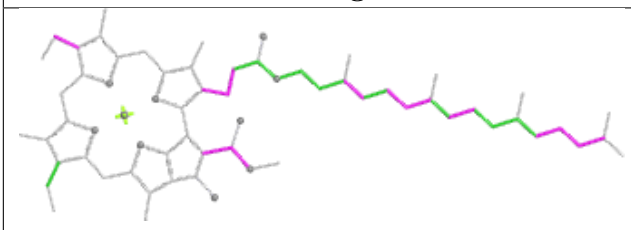


Bond angles



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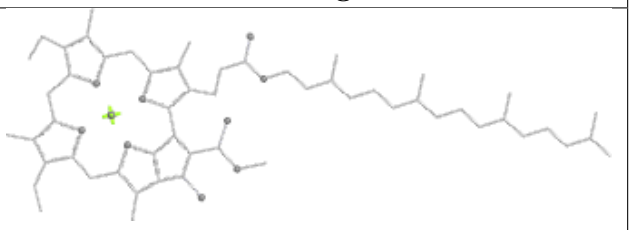
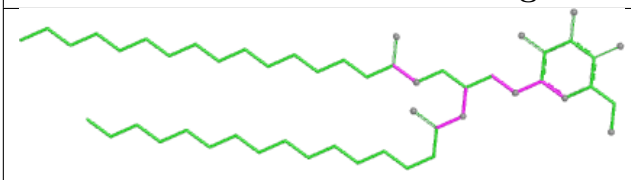


Rings

Ligand LMG C 521



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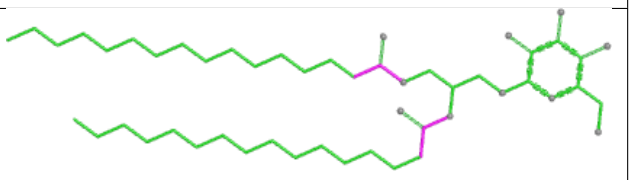
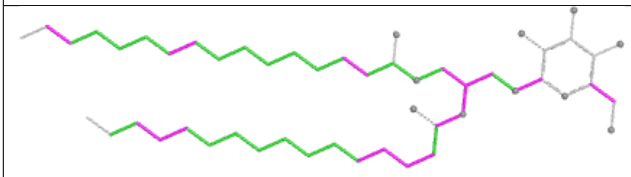
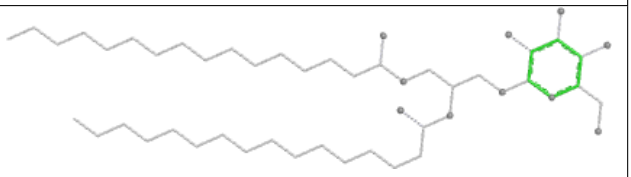


Bond angles

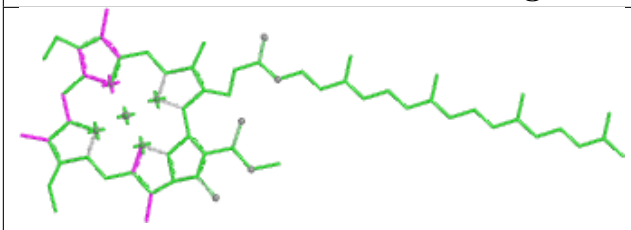


Torsions

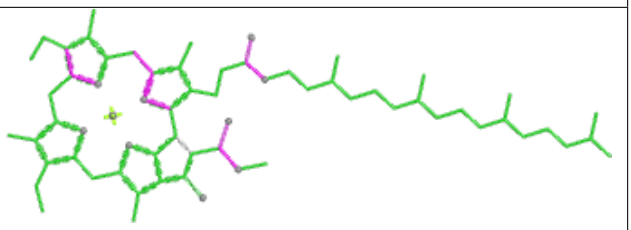


Rings

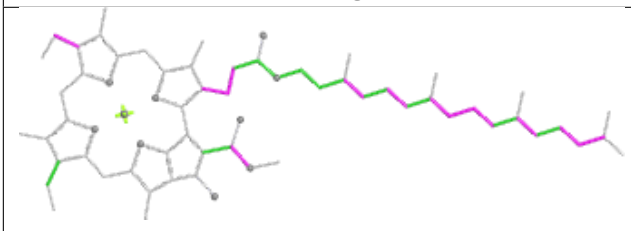
Ligand CLA R 307



Bond lengths



Bond angles



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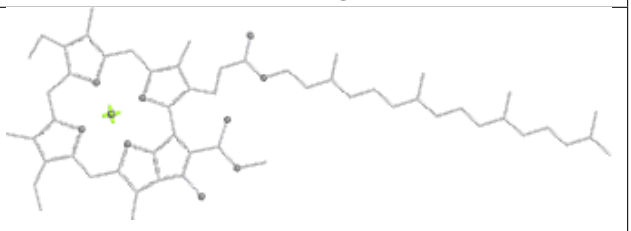
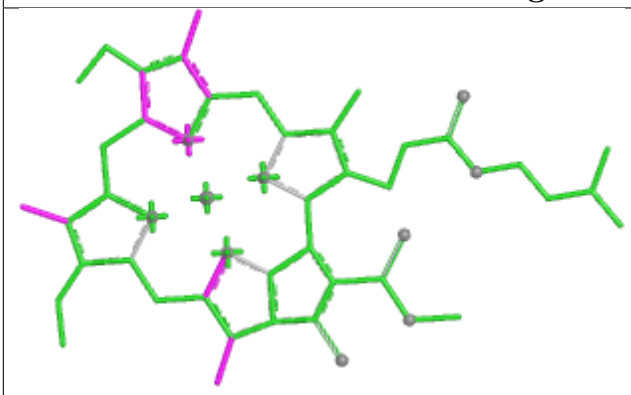


Rings

Ligand CLA v 303



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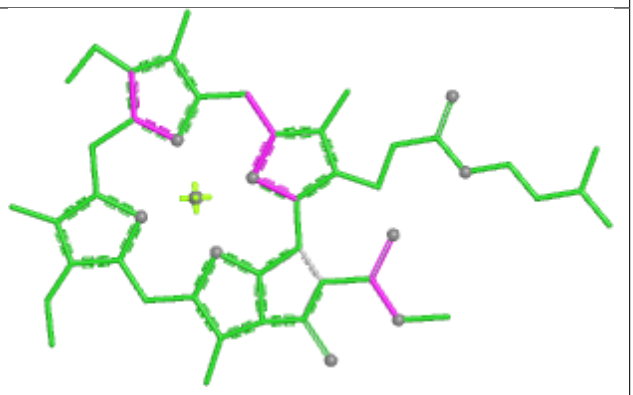
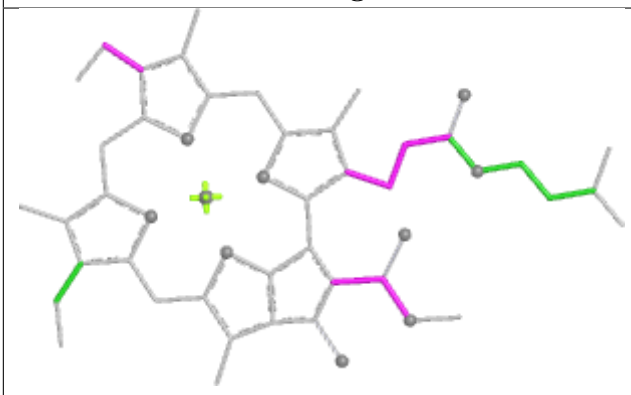


Bond angles



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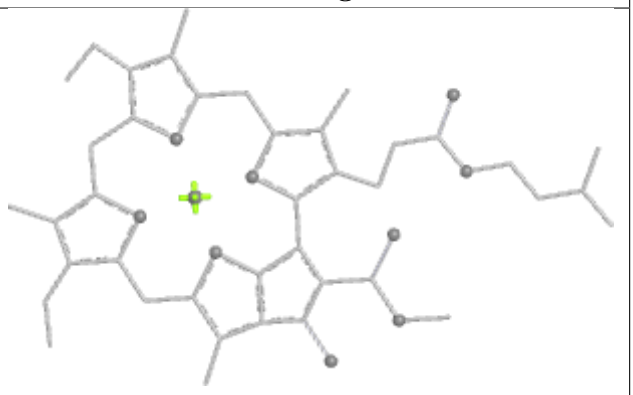
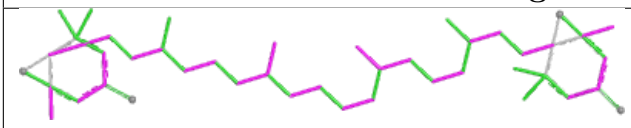


Rings

Ligand XAT r 612



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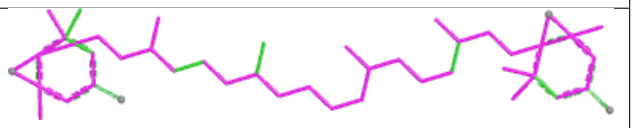
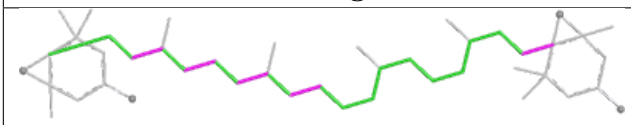


Bond angles



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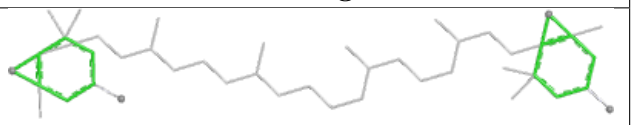
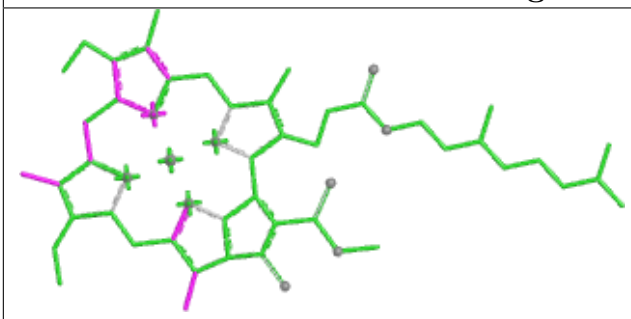


Rings

Ligand CLA S 305



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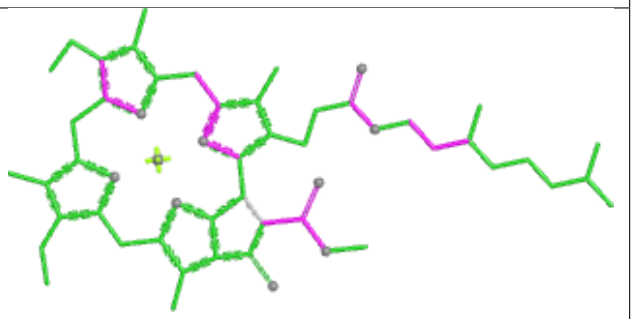
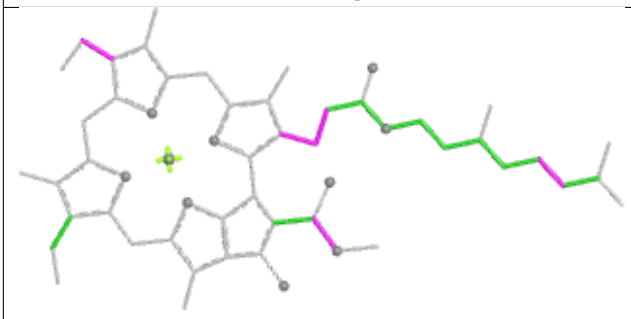


Bond angles



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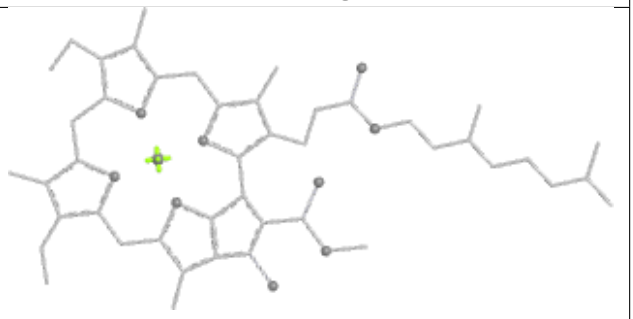
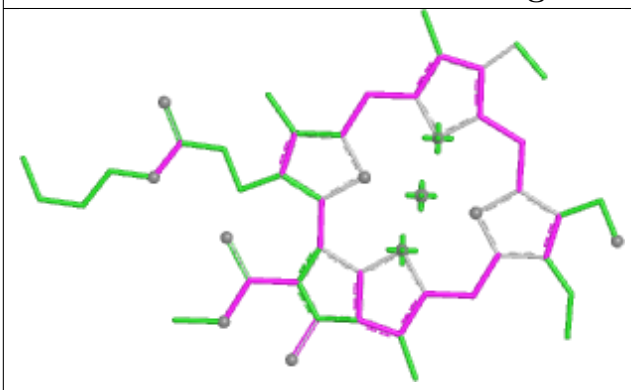


Rings

Ligand CHL 1 315



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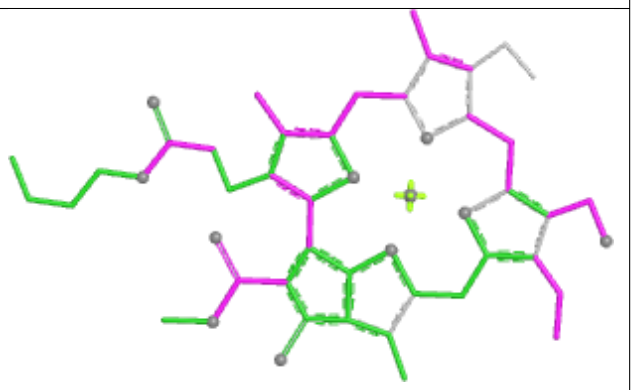
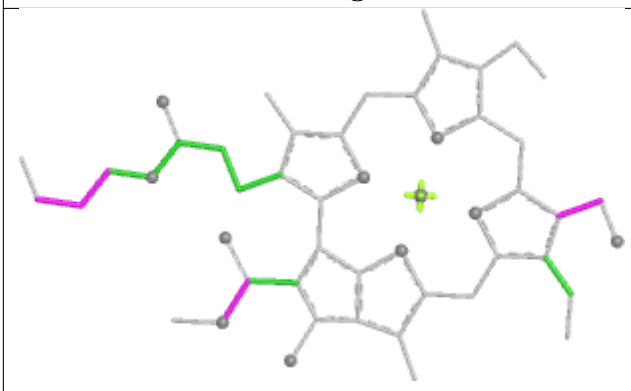


Bond angles



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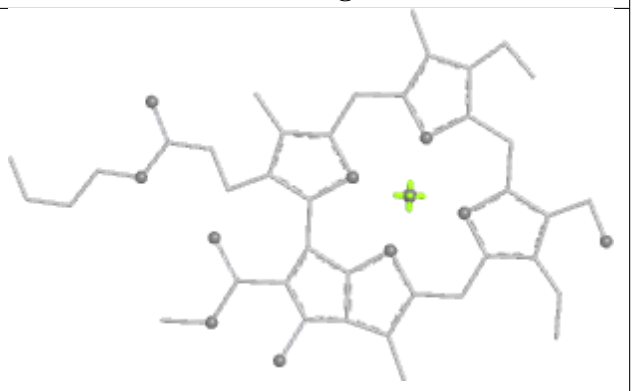
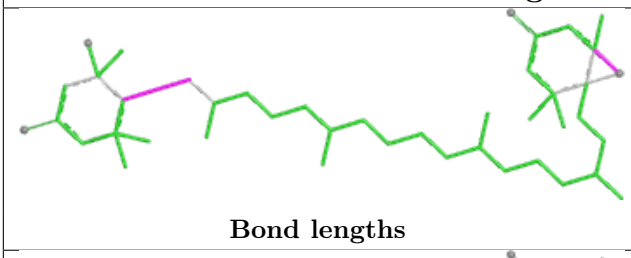


Rings

Ligand NEX v 319



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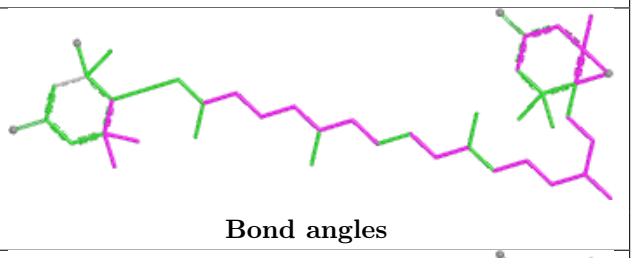
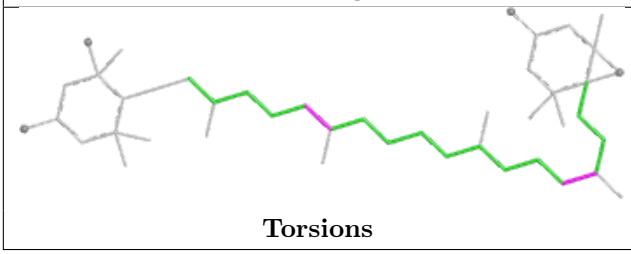


Bond angles



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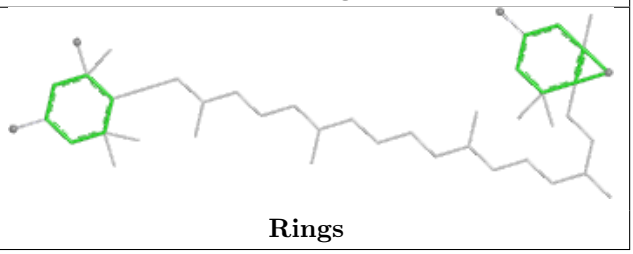
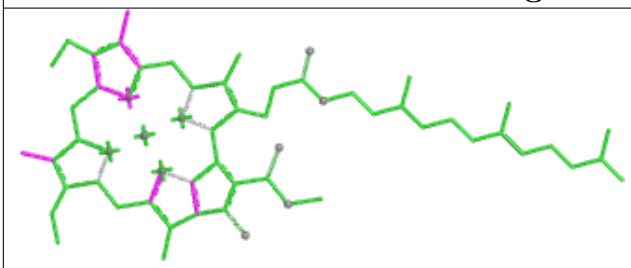


Rings

Ligand CLA P 306



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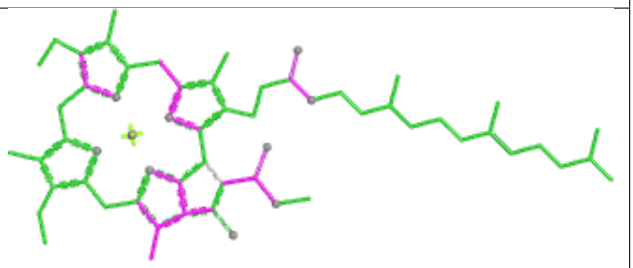

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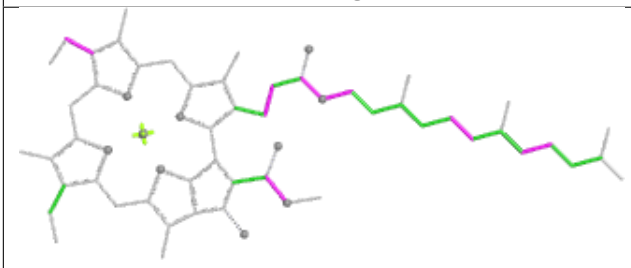

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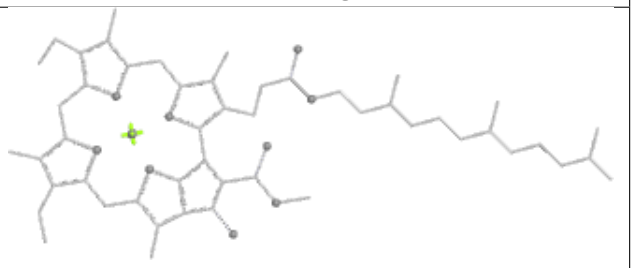
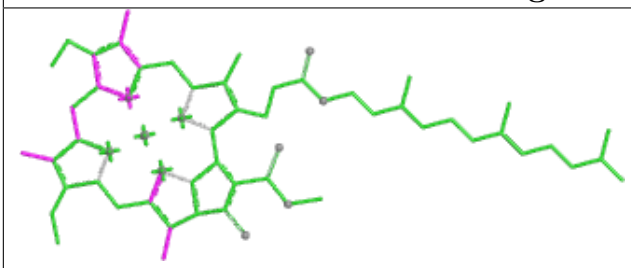


Rings

Ligand CLA 2 307



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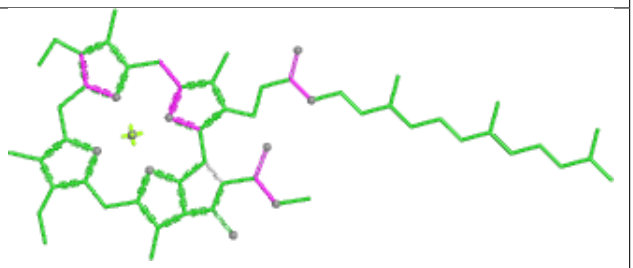
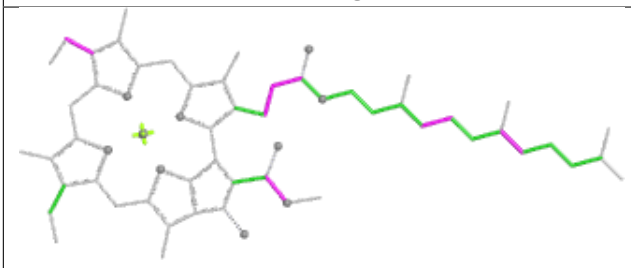


Bond angles



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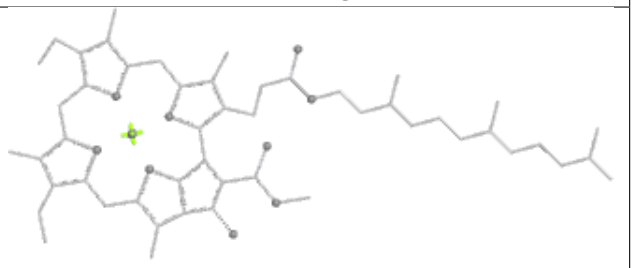
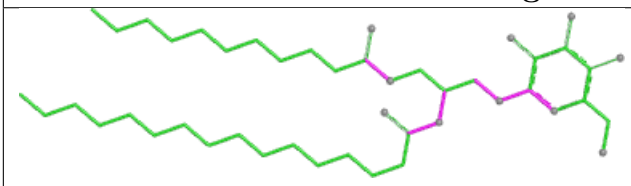


Rings

Ligand LMG d 407



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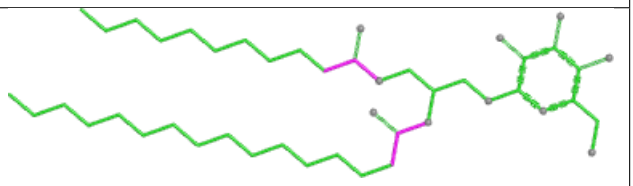
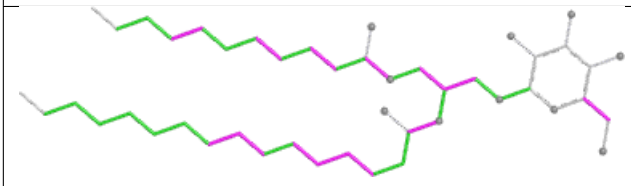


Bond angles



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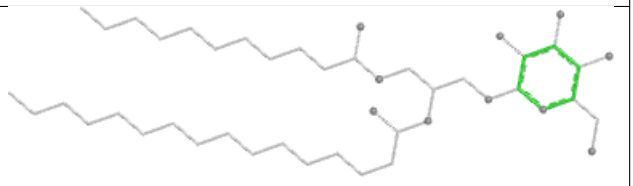
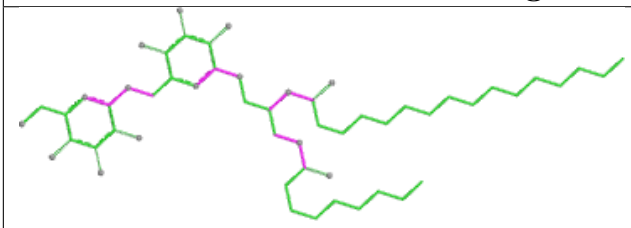


Rings

Ligand DGD c 517



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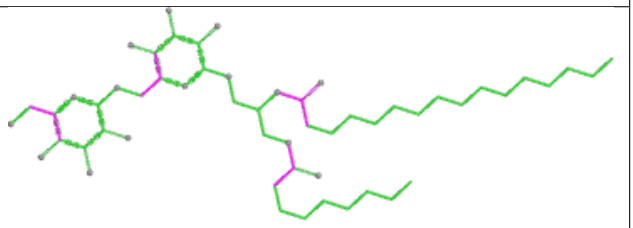
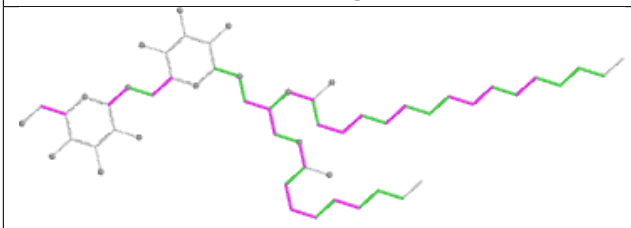


Bond angles



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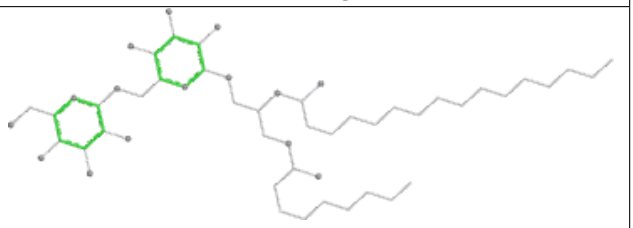
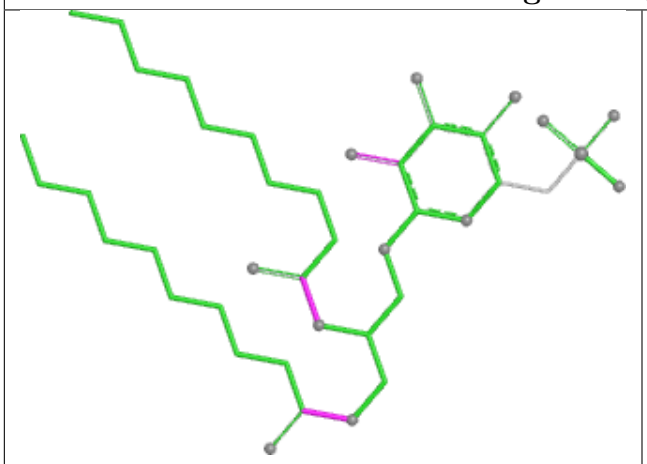


Rings

Ligand SQD m 101



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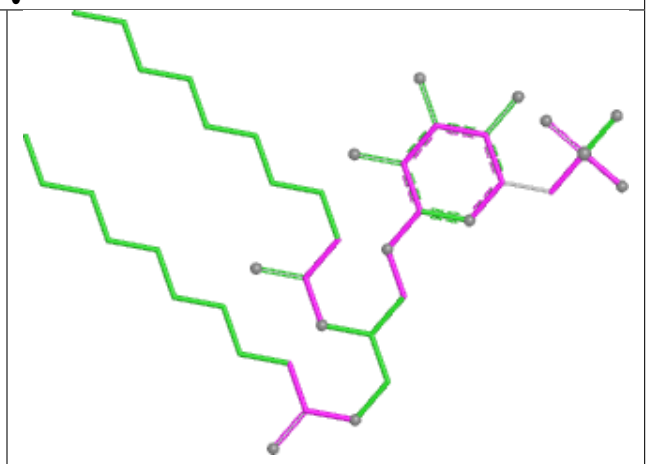
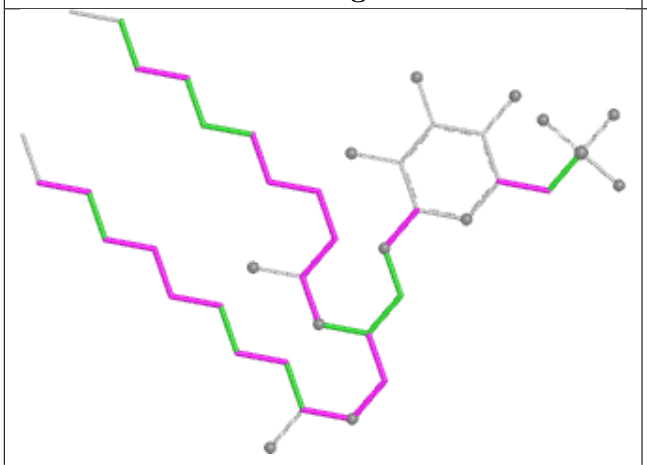


Bond angles



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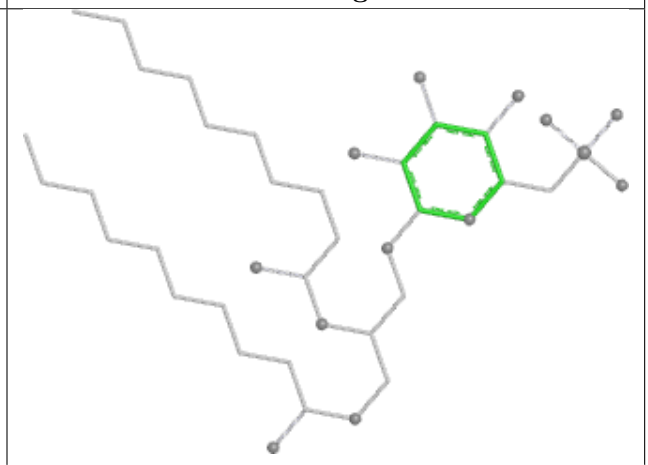
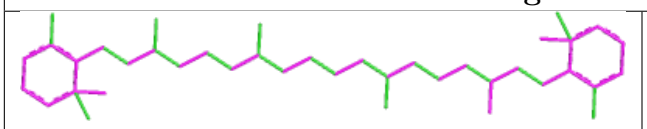


Rings

Ligand BCR B 619



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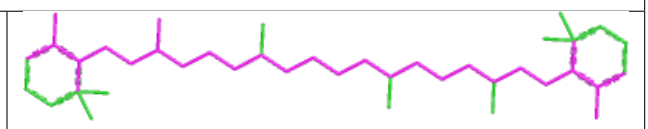
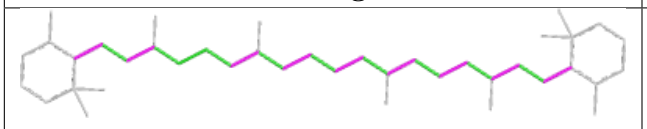


Bond angles



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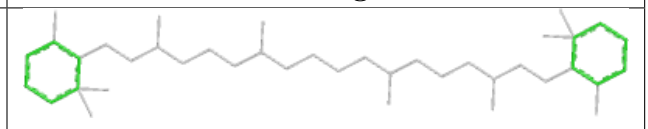
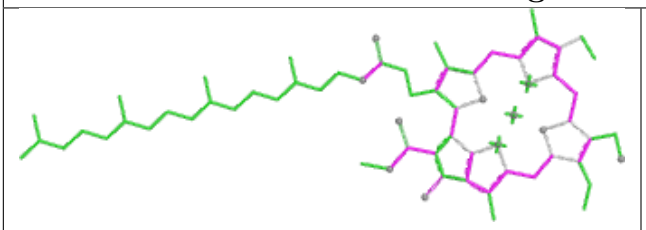


Rings

Ligand CHL 5 317



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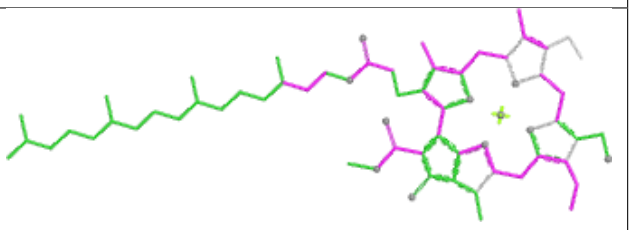
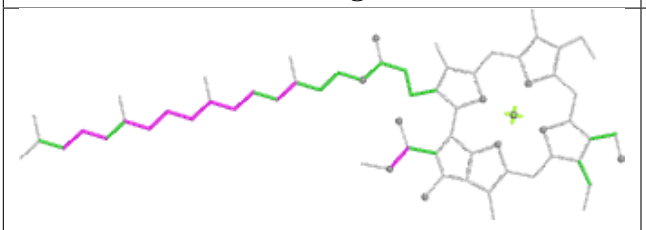
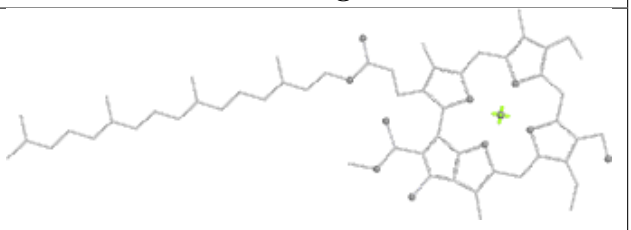


Bond angles

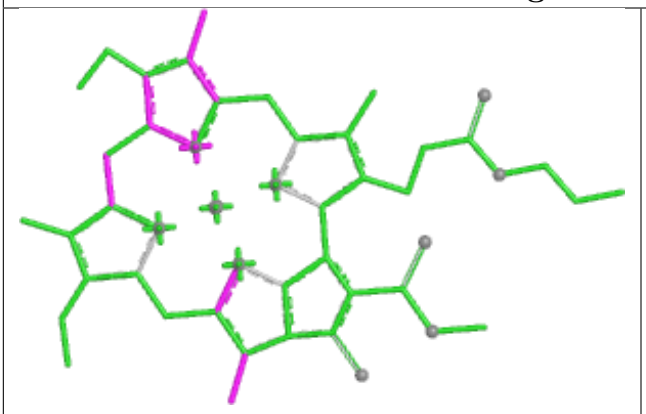


Torsions



Rings

Ligand CLA p 309



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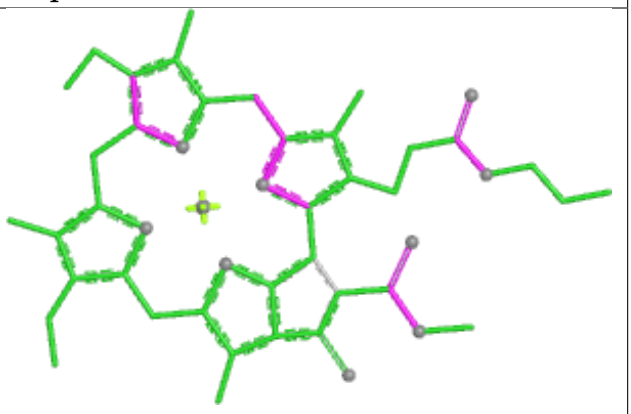
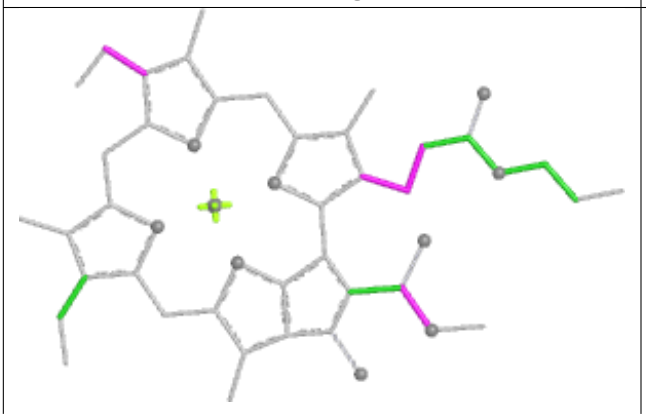
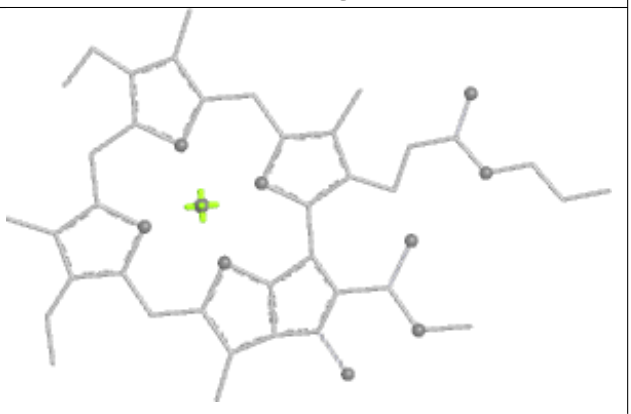


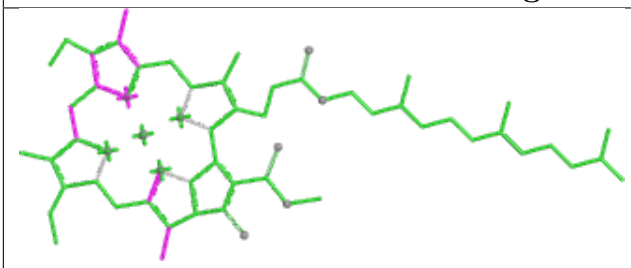
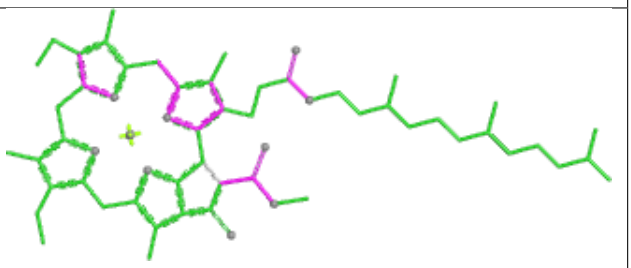
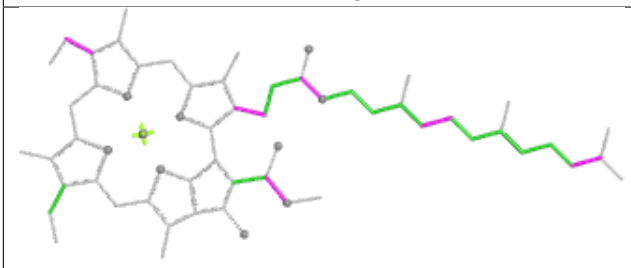
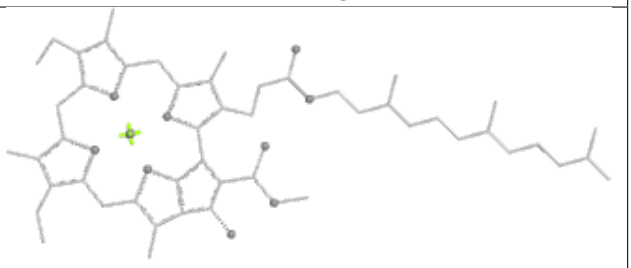
Bond angles

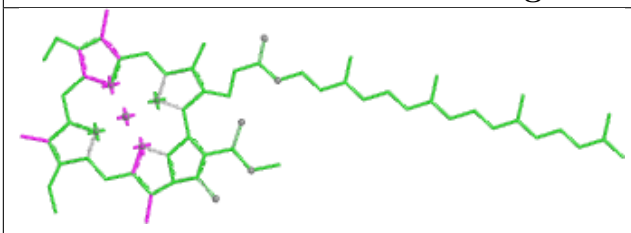
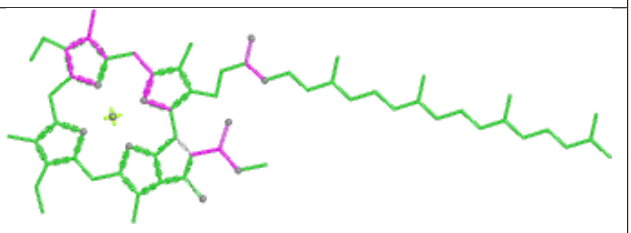
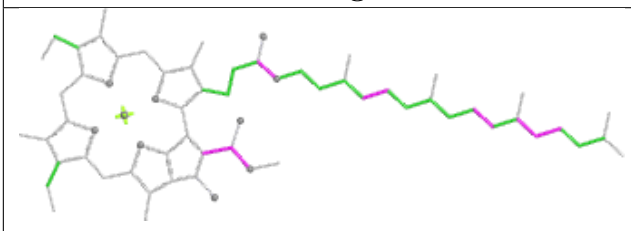
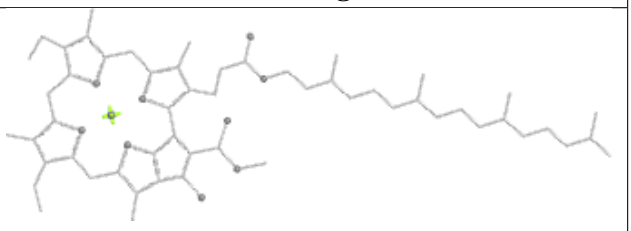


Torsions

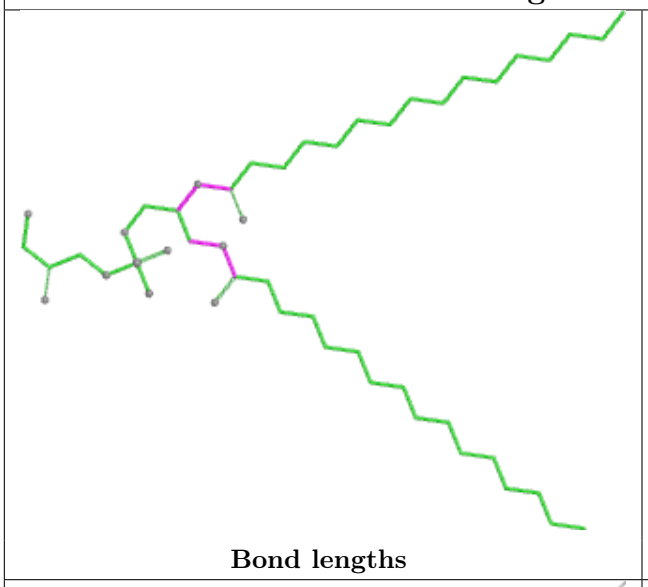


Rings

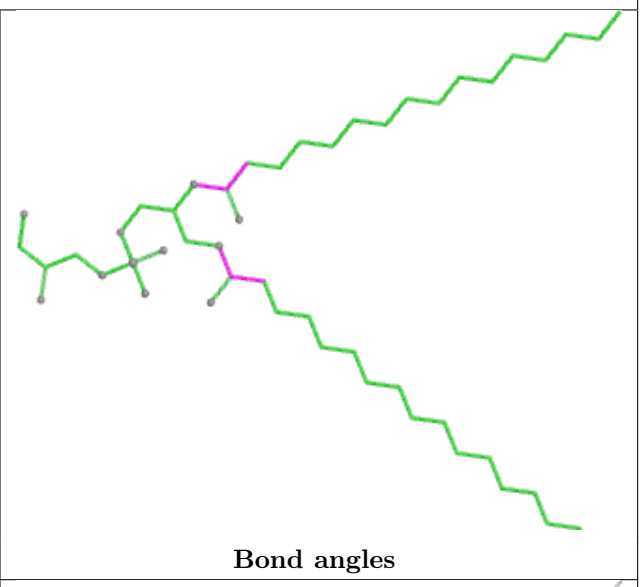
Ligand CLA G 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

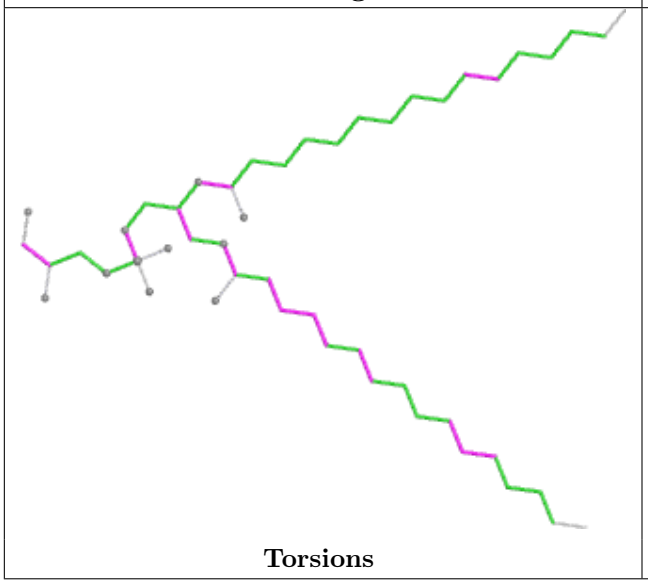
Ligand LHG 3 310



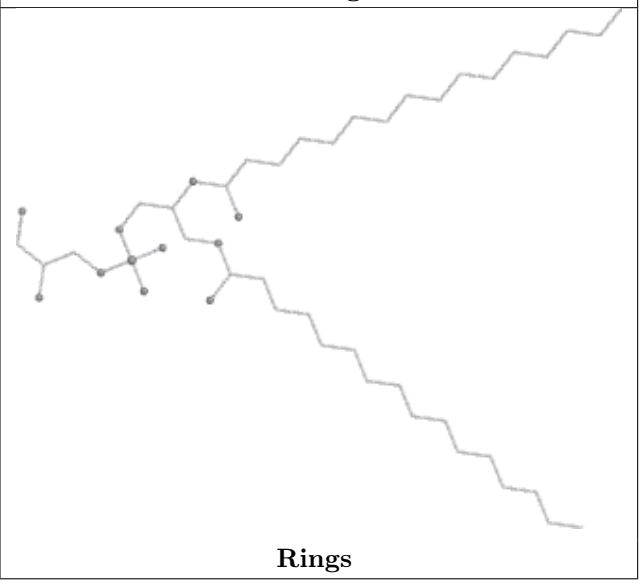
Bond lengths



Bond angles

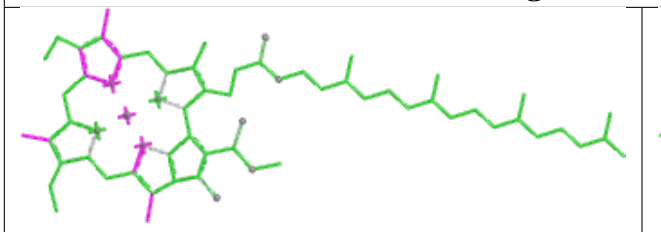


Torsions

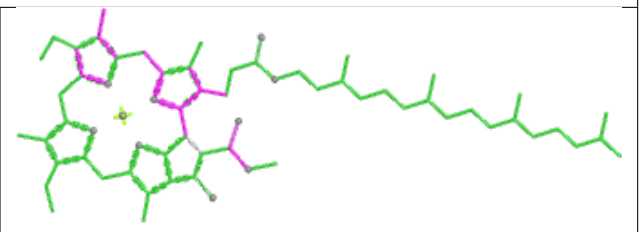


Rings

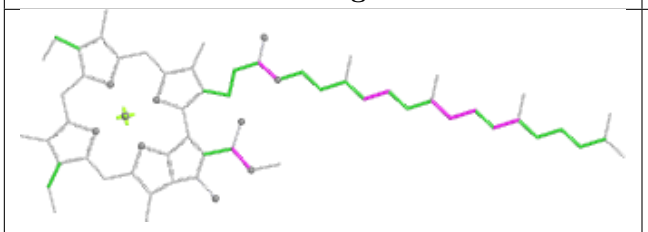
Ligand CLA C 513



Bond lengths



Bond angles



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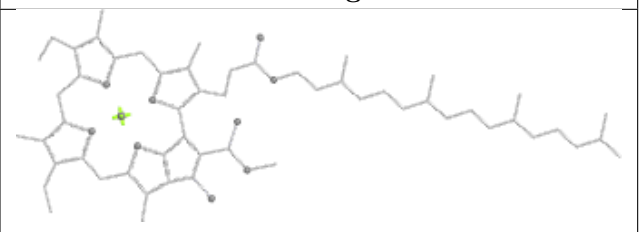
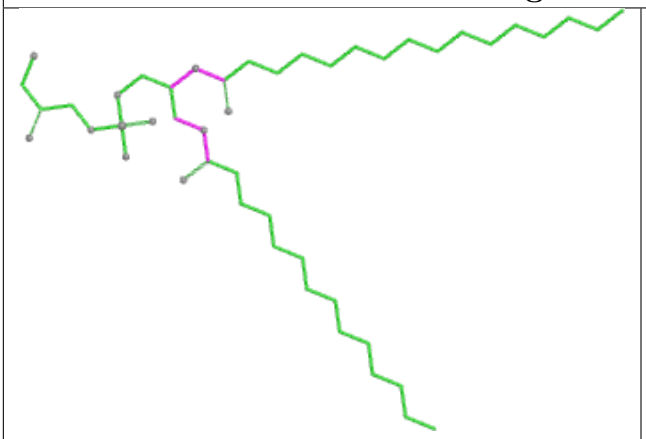


Rings

Ligand LHG b 622



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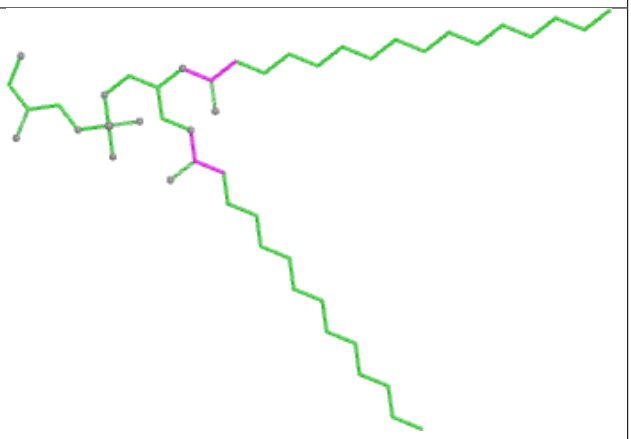
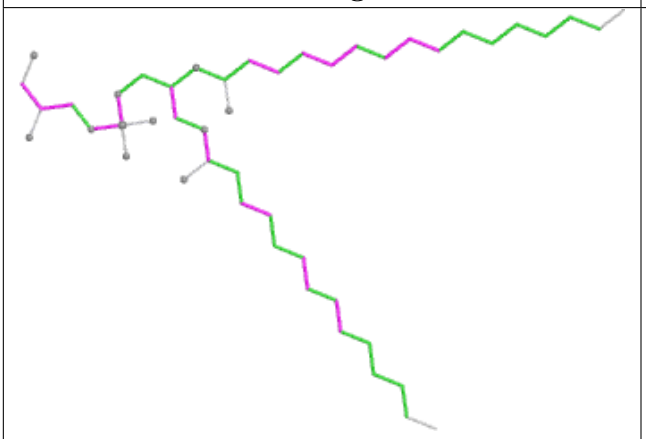


Bond angles



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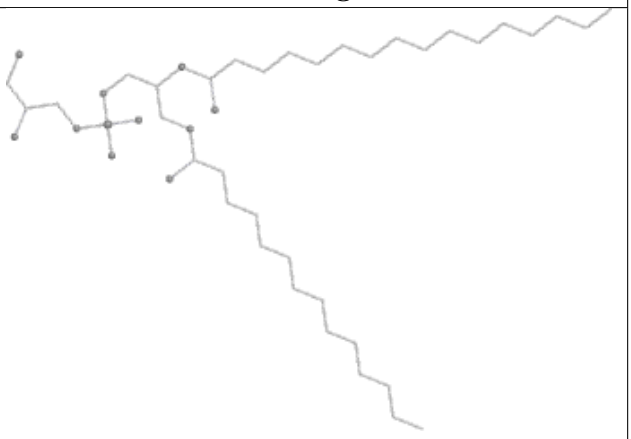
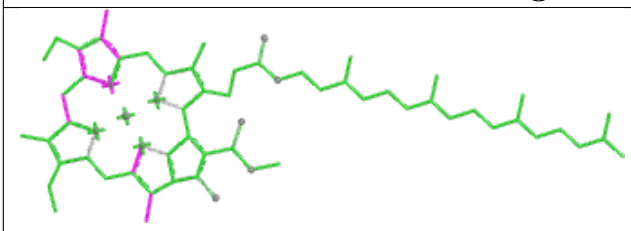
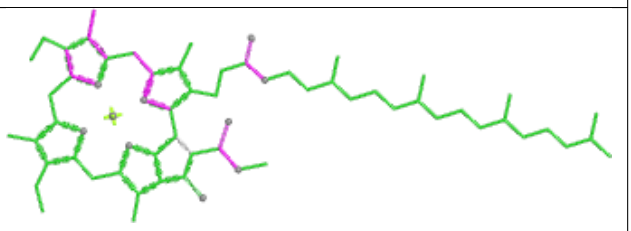


Rings

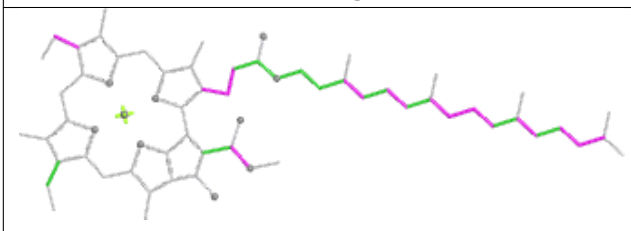
Ligand CLA r 606



Bond lengths



Bond angles



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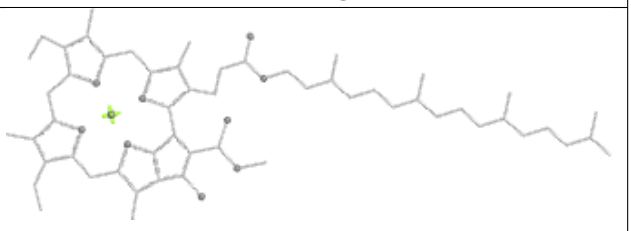
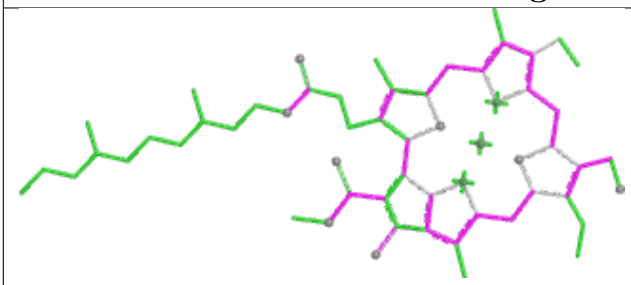


Rings

Ligand CHL s 315



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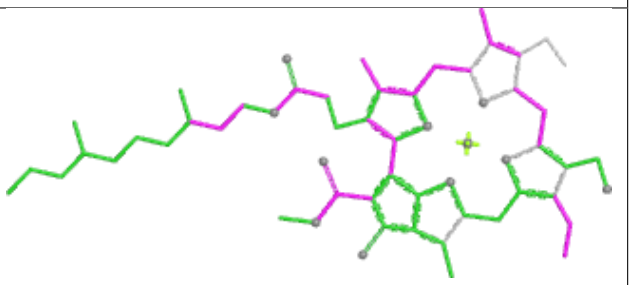
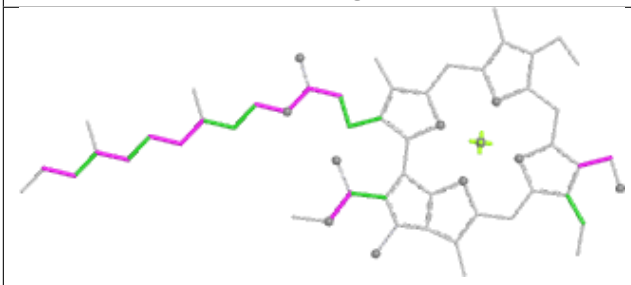


Bond angles



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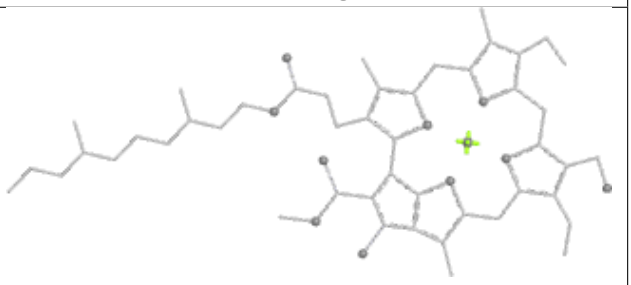
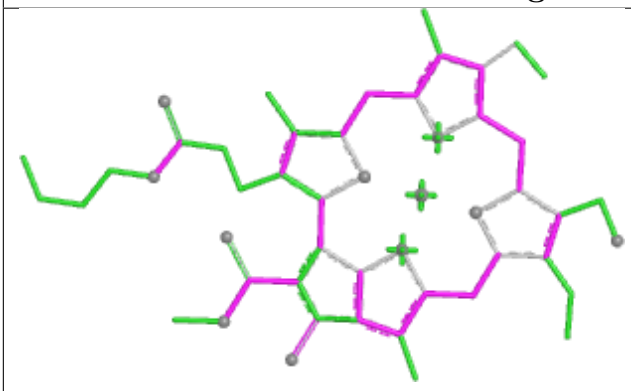


Rings

Ligand CHL 5 315



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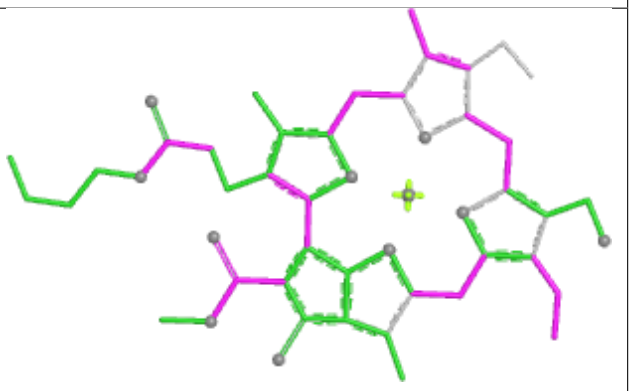
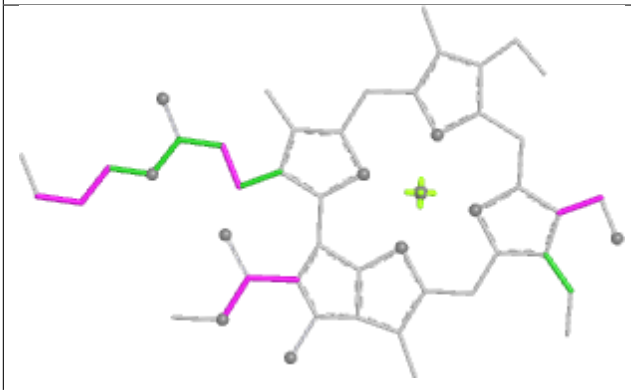


Bond angles



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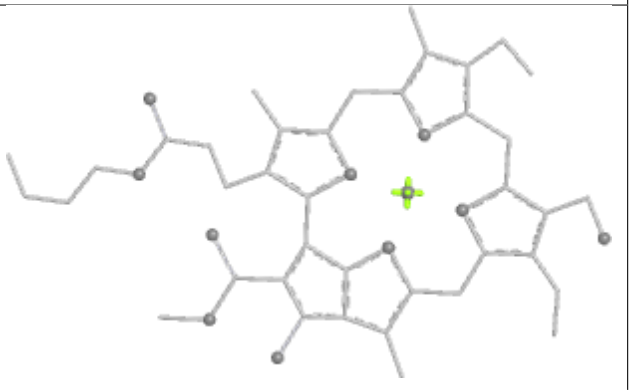
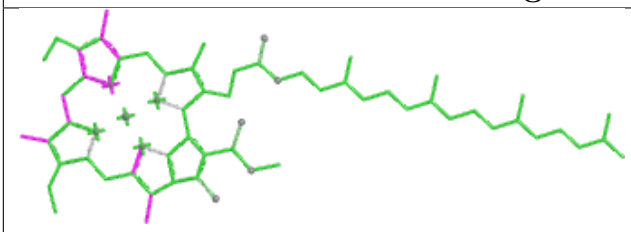
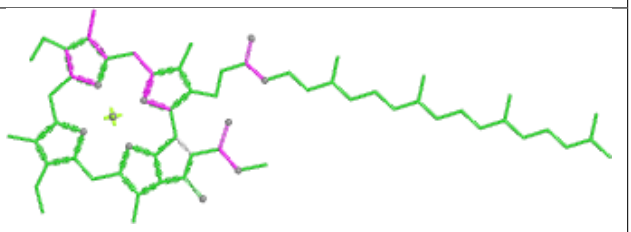
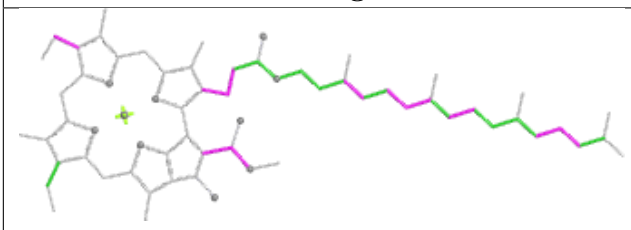
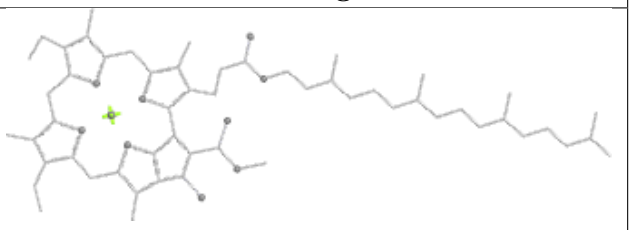
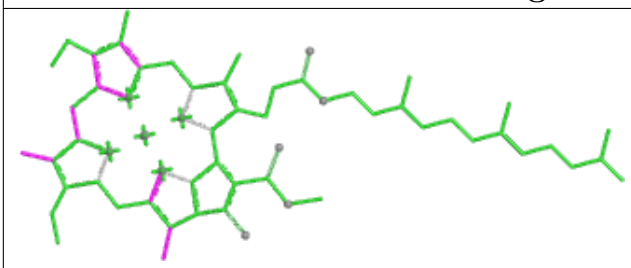
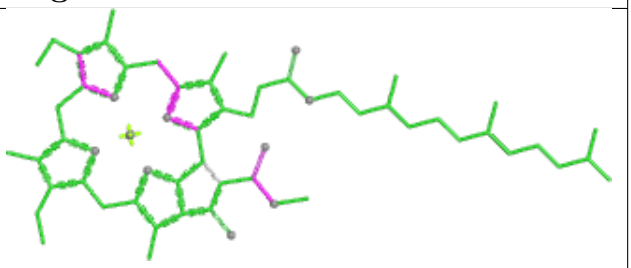
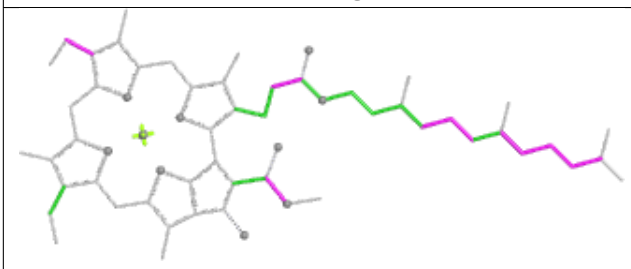
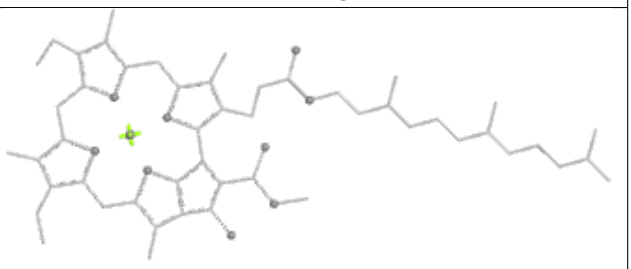
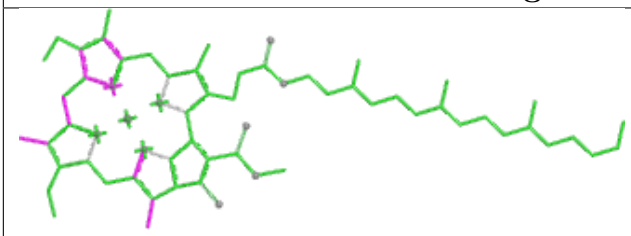


Rings

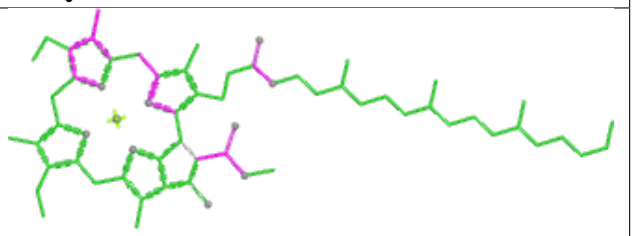
Ligand CLA B 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

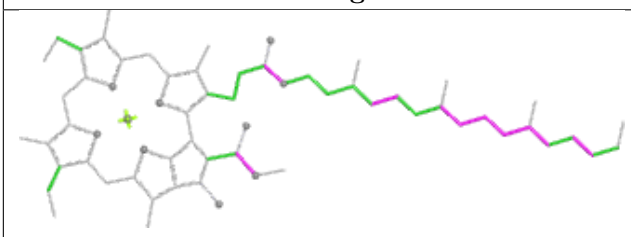
Ligand CLA Q 304



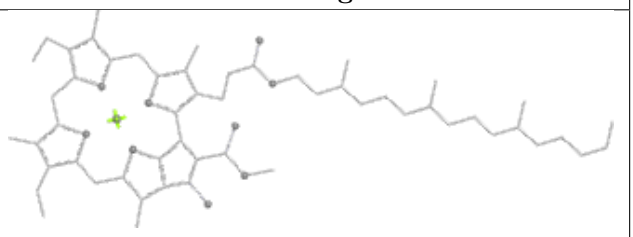
Bond lengths



Bond angles

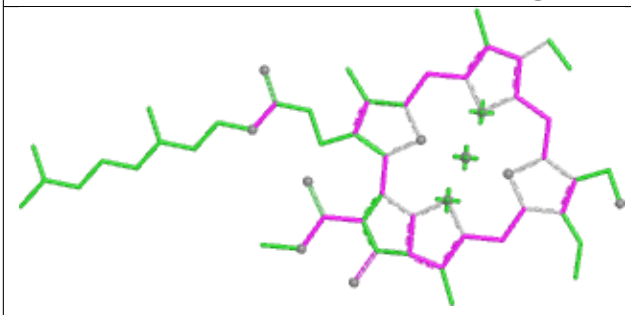


Torsions

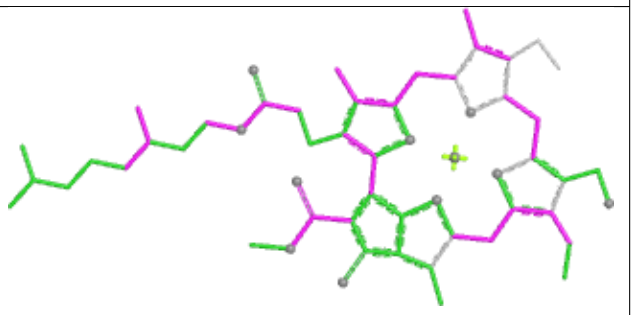


Rings

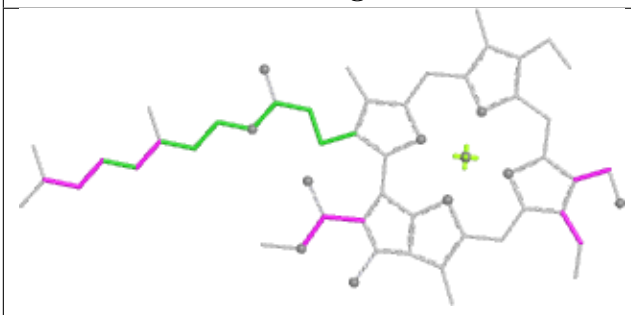
Ligand CHL r 615



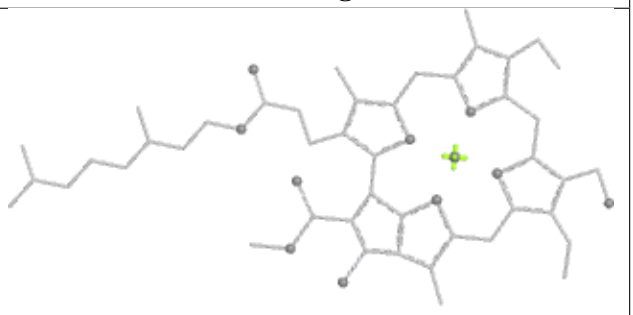
Bond lengths



Bond angles

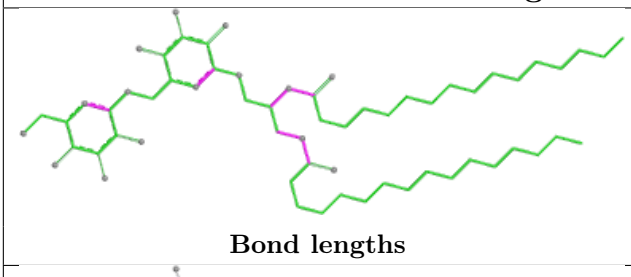


Torsions



Rings

Ligand DGD c 518



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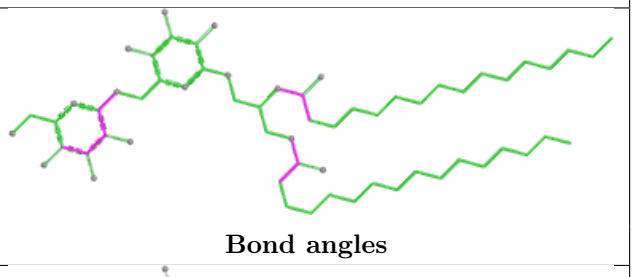
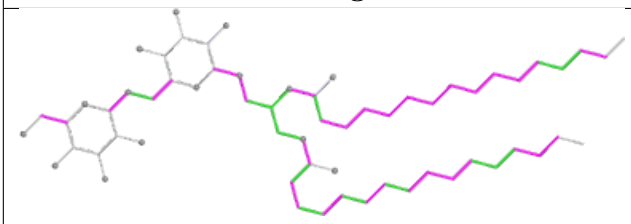
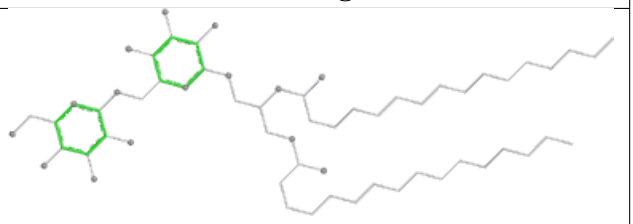


Bond angles

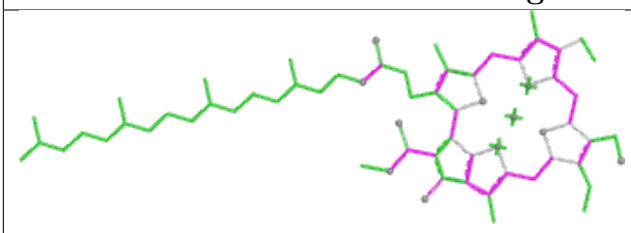


Torsions

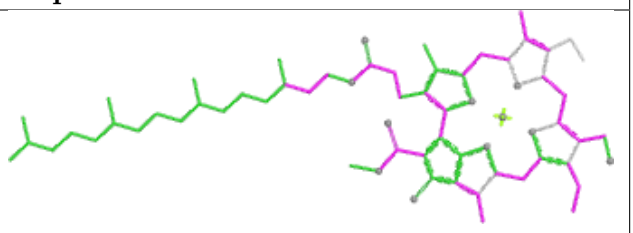


Rings

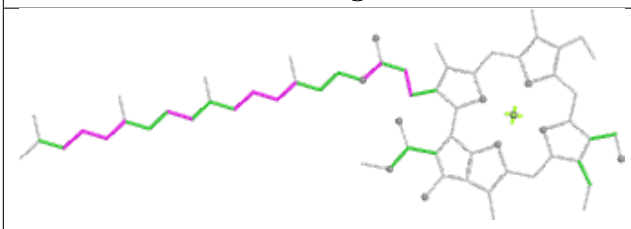
Ligand CHL p 317



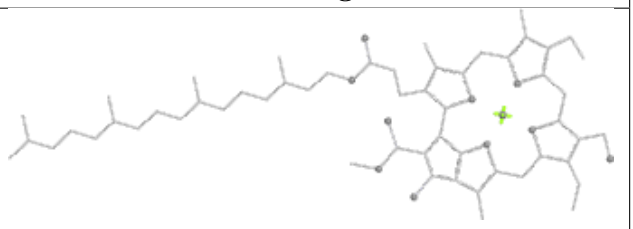
Bond lengths



Bond angles

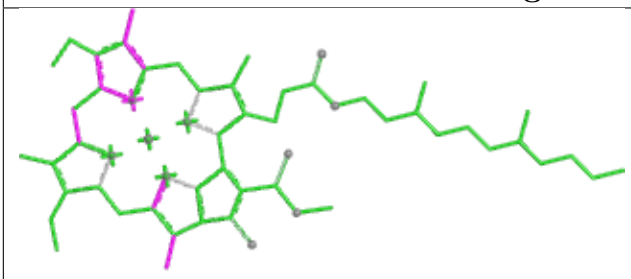


Torsions



Rings

Ligand CLA R 306



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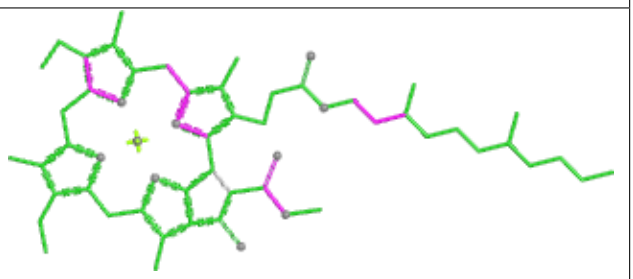

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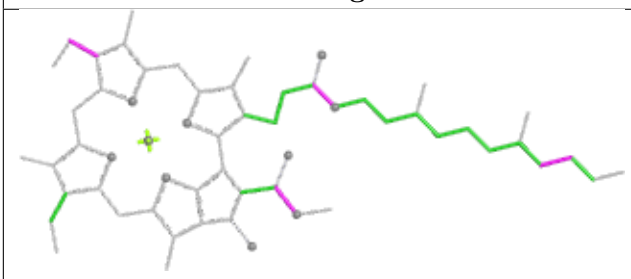

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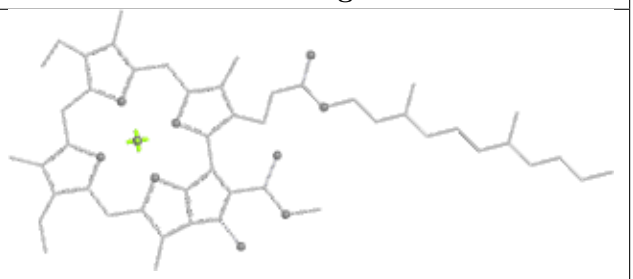
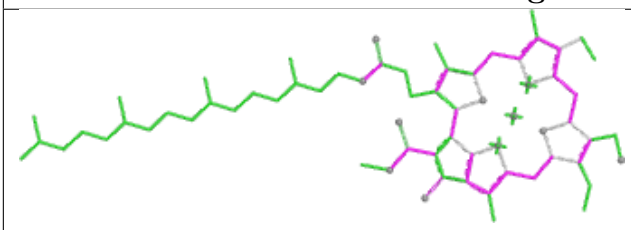


Rings

Ligand CHL 4 317



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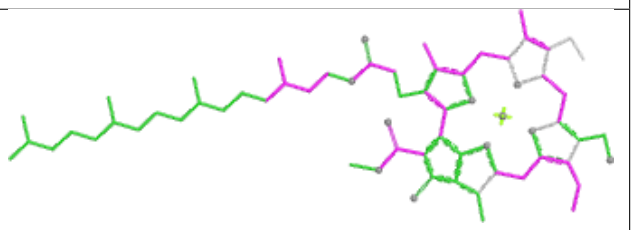
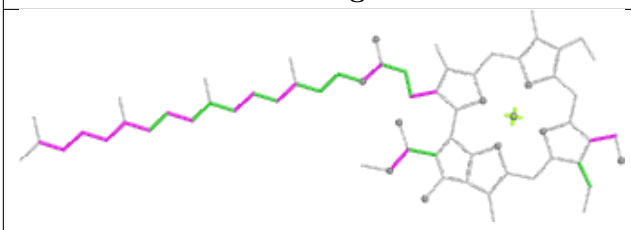


Bond angles



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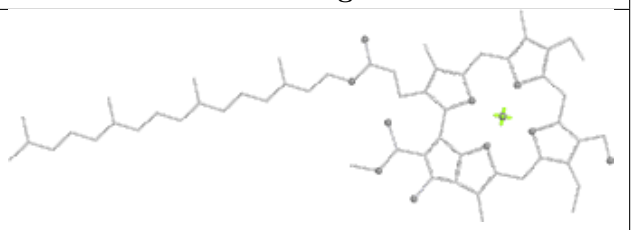
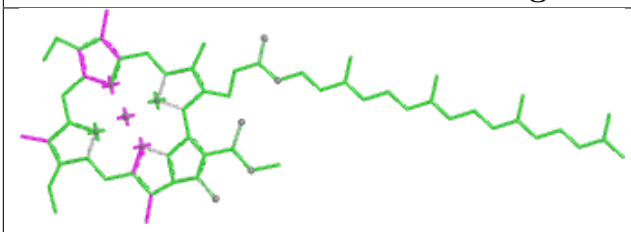


Rings

Ligand CLA c 513



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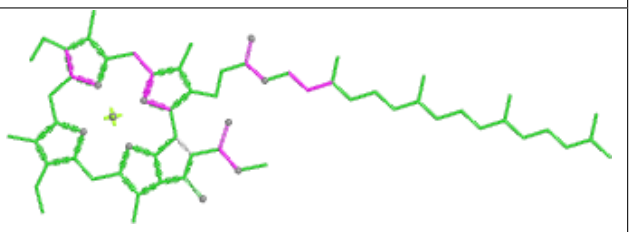
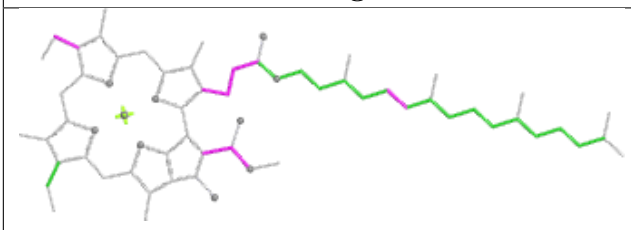


Bond angles



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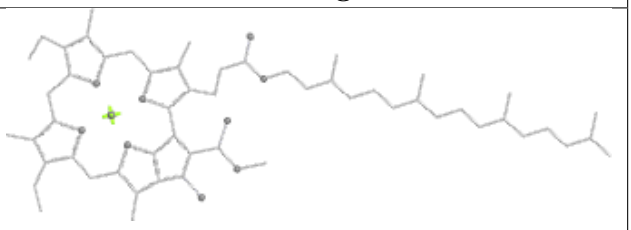
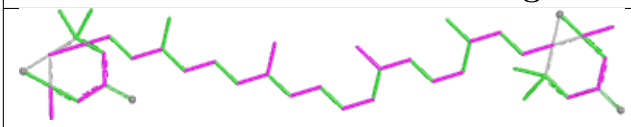


Rings

Ligand XAT R 313



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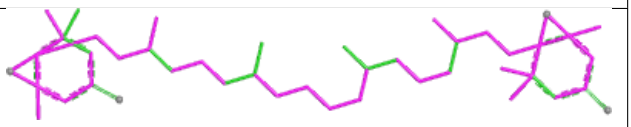
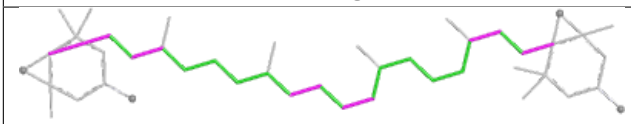


Bond angles



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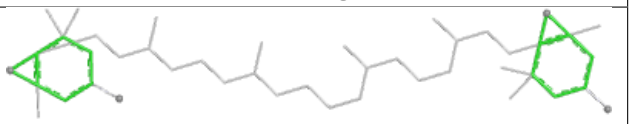
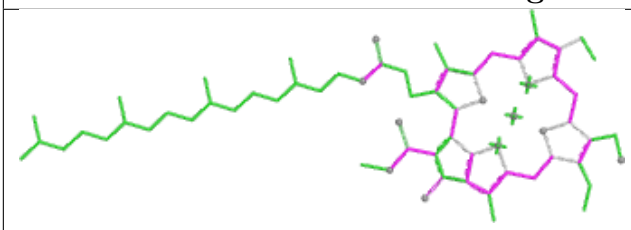


Rings

Ligand CHL n 313



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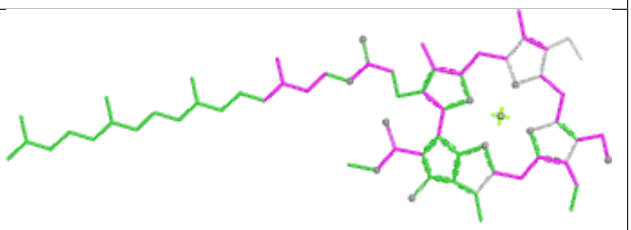
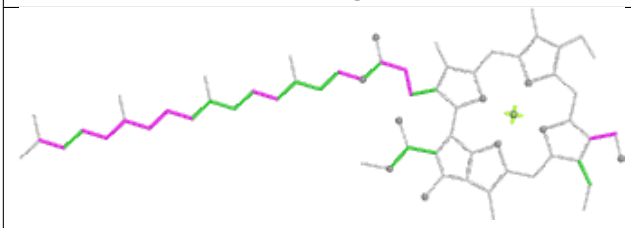


Bond angles



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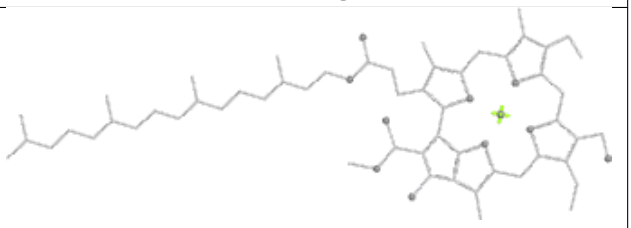
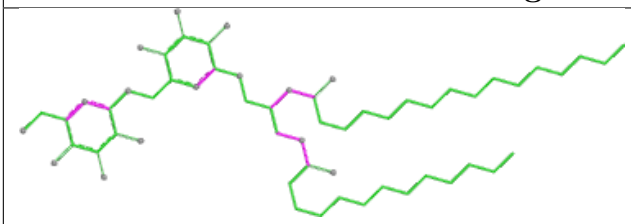


Rings

Ligand DGD a 416



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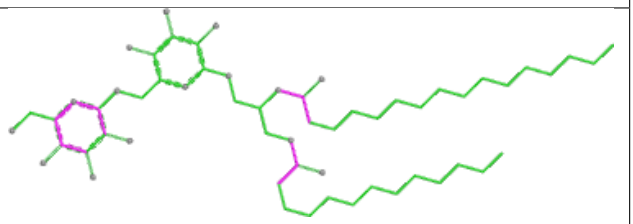
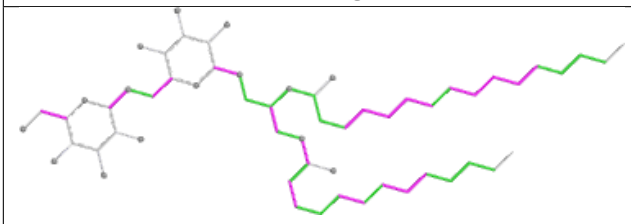


Bond angles



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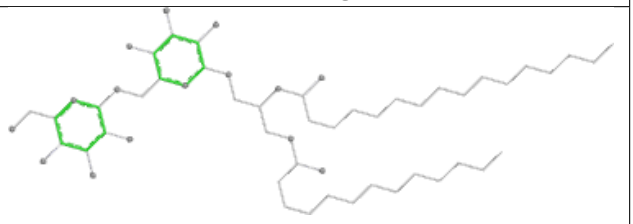
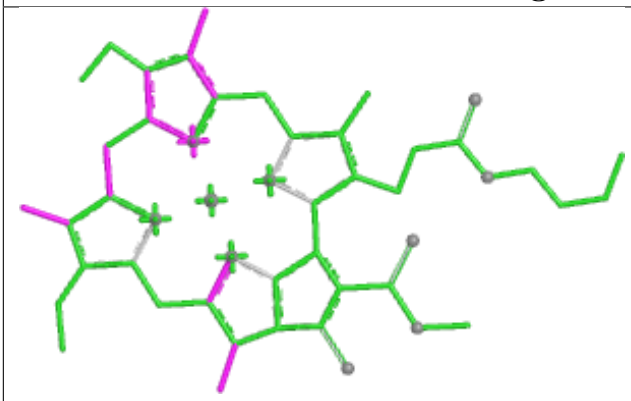


Rings

Ligand CLA r 601



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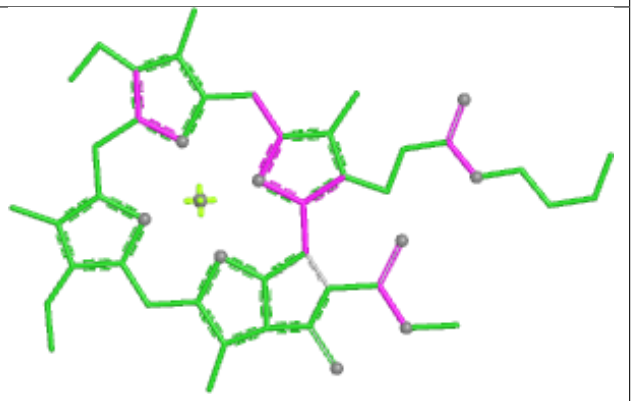
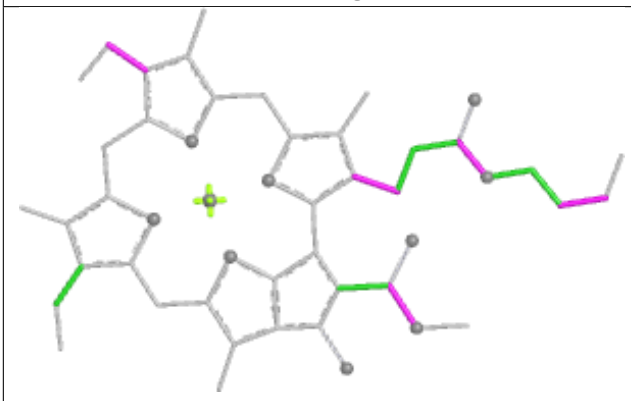


Bond angles



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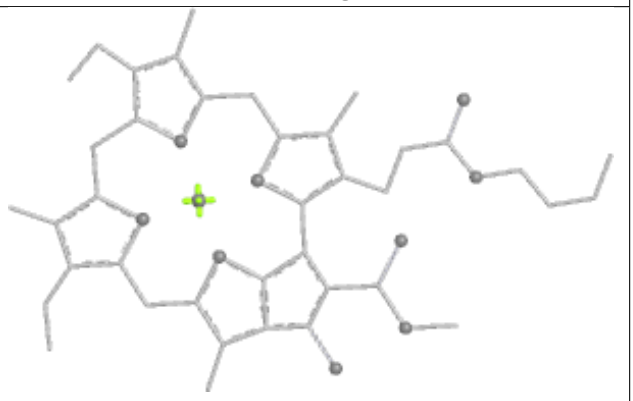
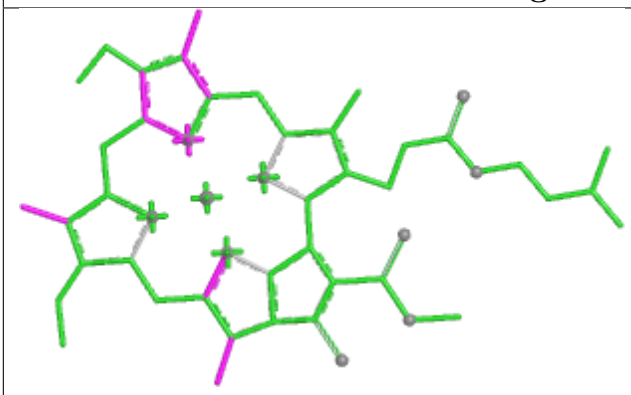


Rings

Ligand CLA s 303



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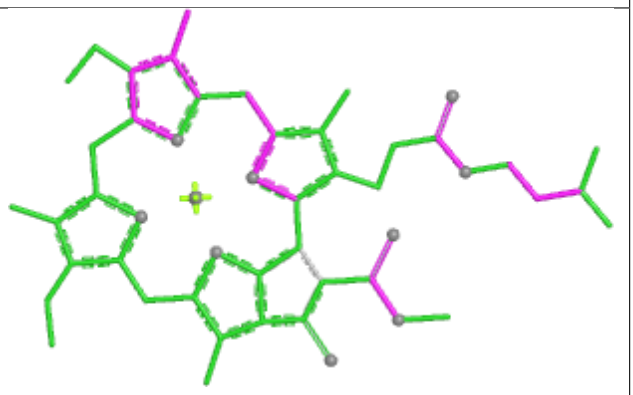
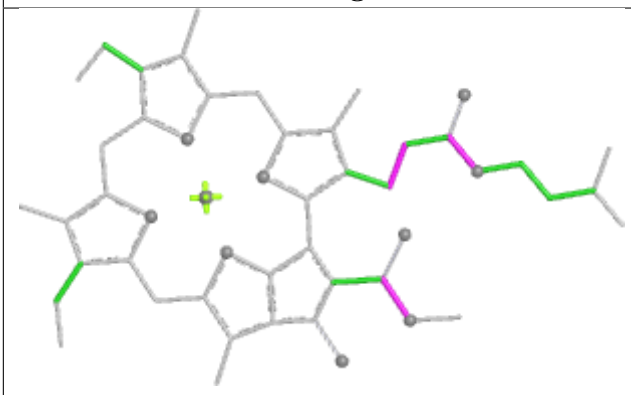
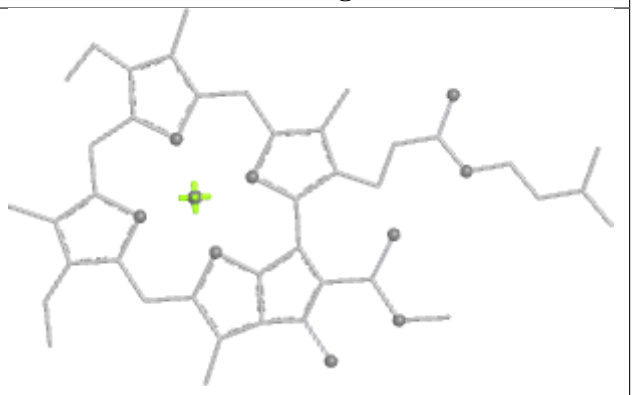


Bond angles

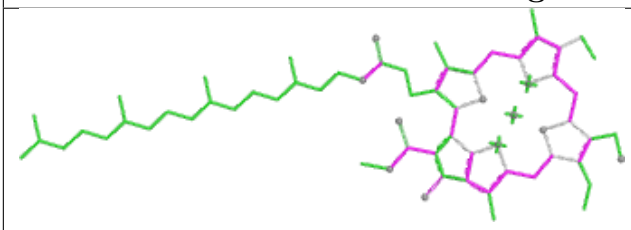


Torsions



Rings

Ligand CHL 6 316



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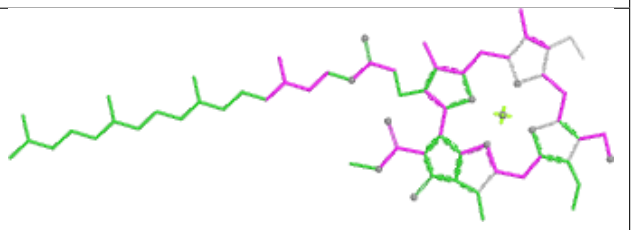
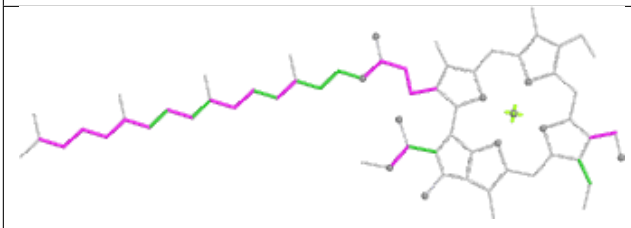


Bond angles



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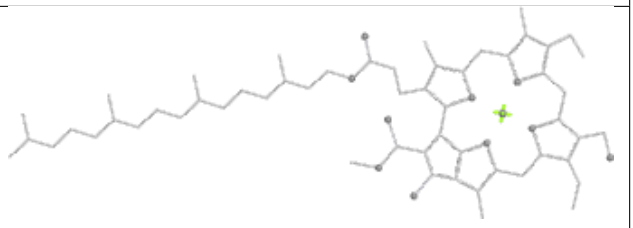
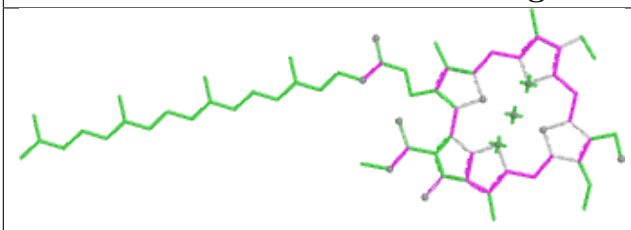


Rings

Ligand CHL 1 317



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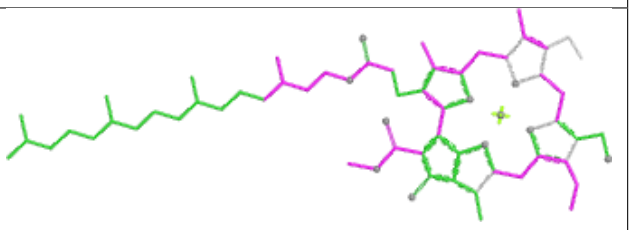
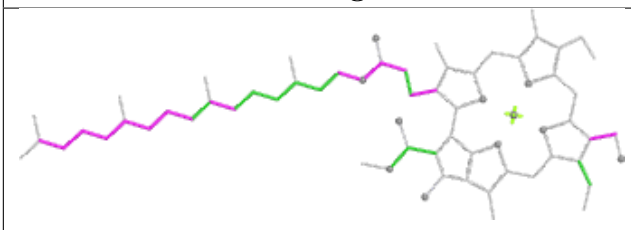


Bond angles



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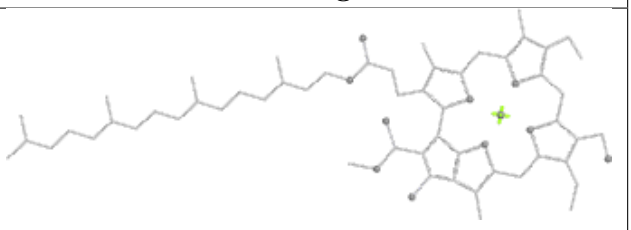
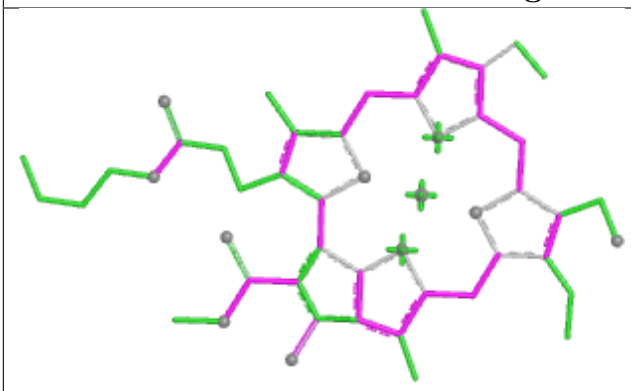


Rings

Ligand CHL P 316



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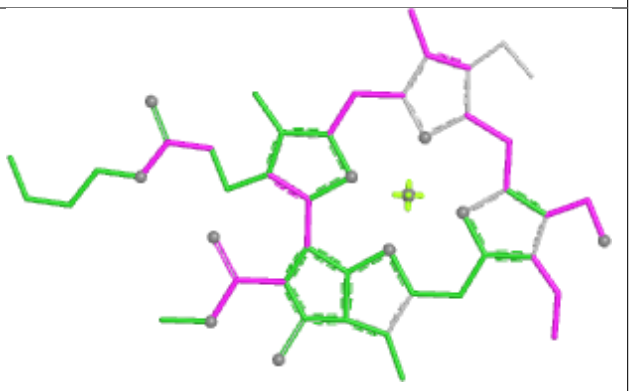
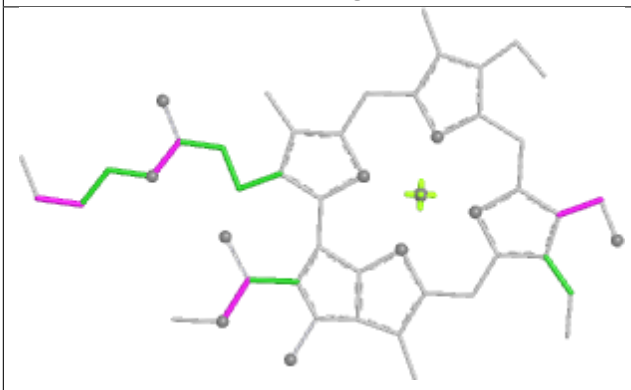


Bond angles



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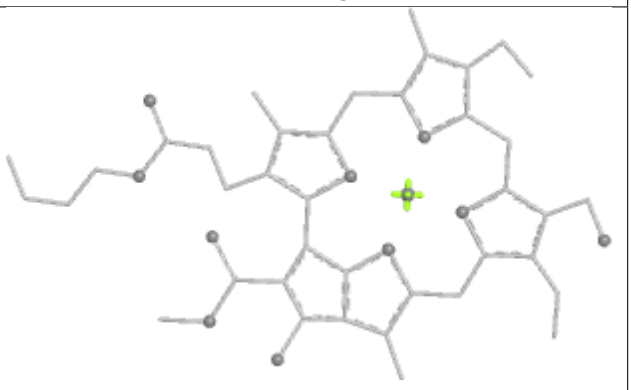
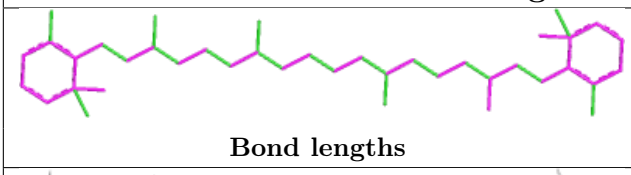
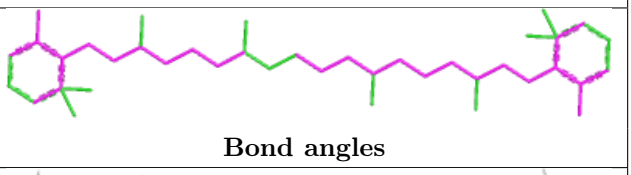


Rings

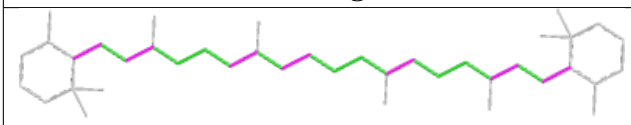
Ligand BCR t 101



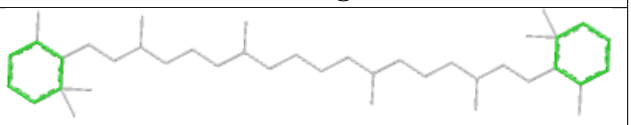
Bond lengths



Bond angles

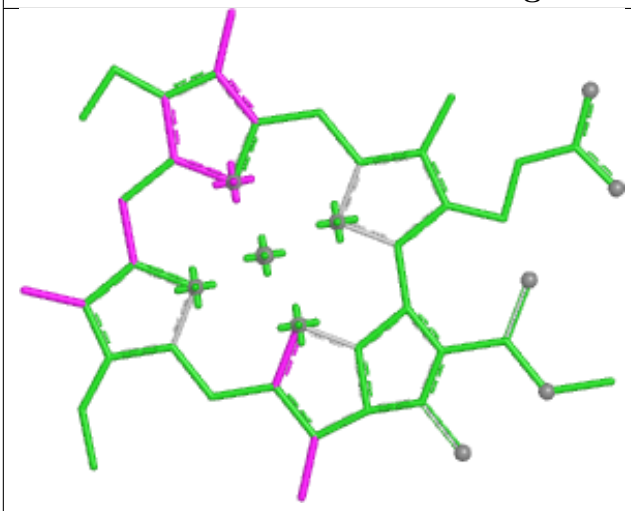


Torsions



Rings

Ligand CLA R 311



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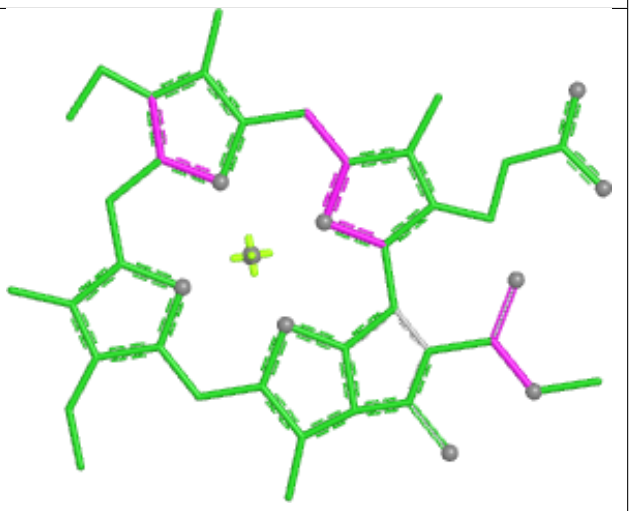
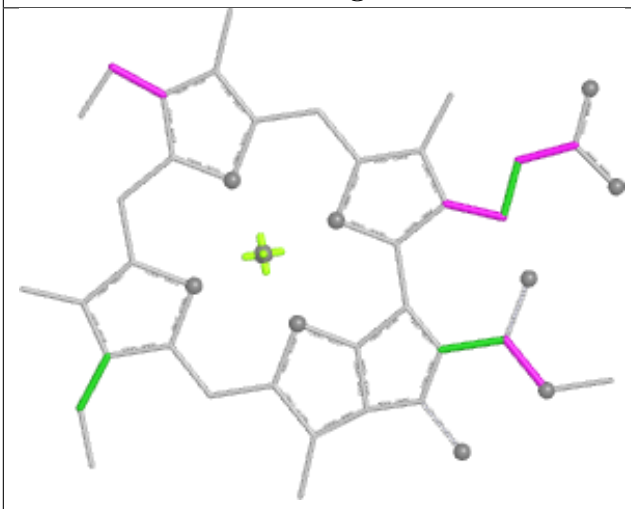


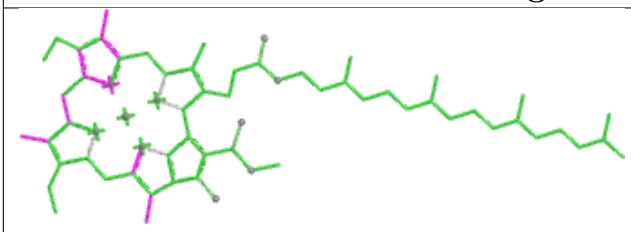
Bond angles



Torsions

Rings

Ligand CLA q 301



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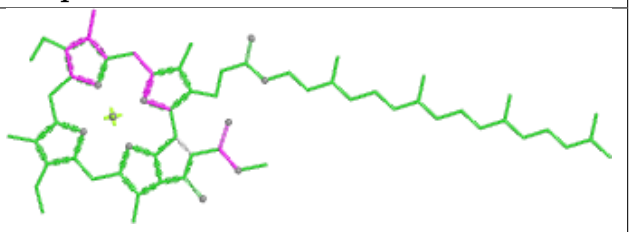
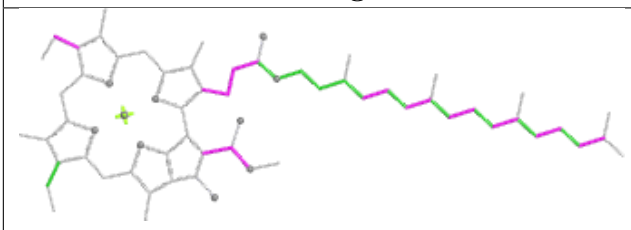
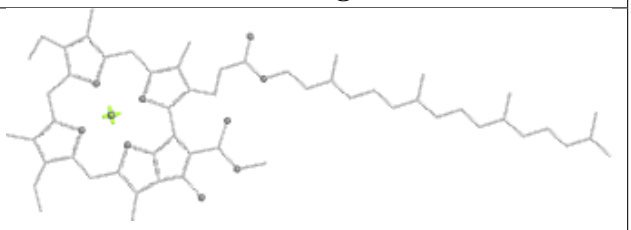


Bond angles

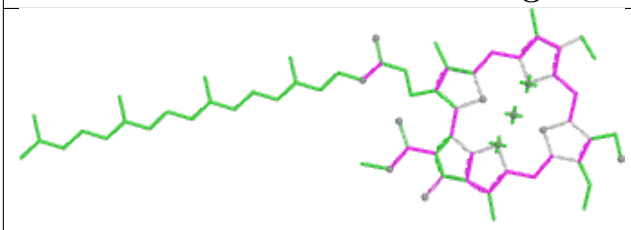


Torsions



Rings

Ligand CHL N 316



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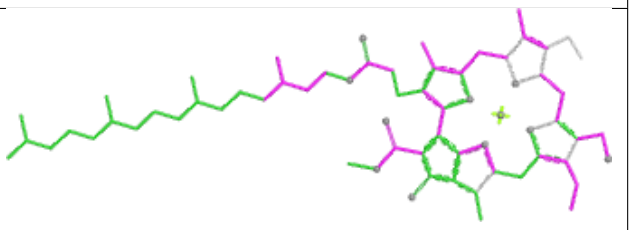

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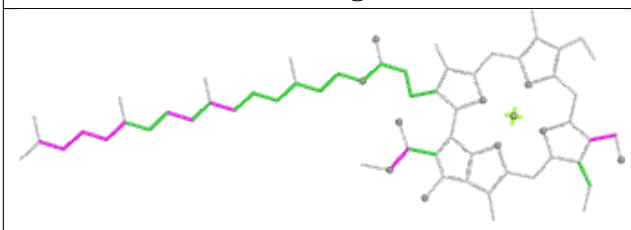

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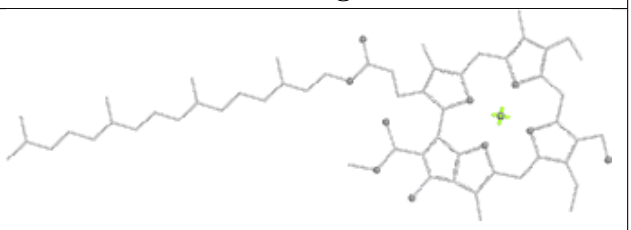
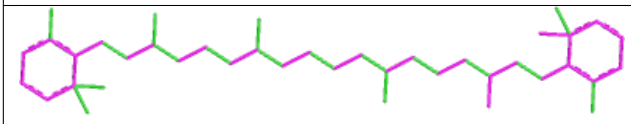


Rings

Ligand BCR B 618



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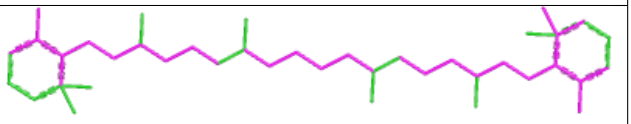

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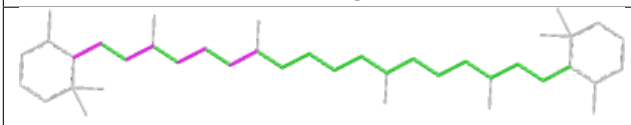
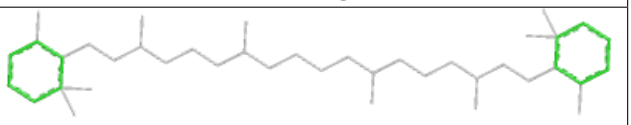
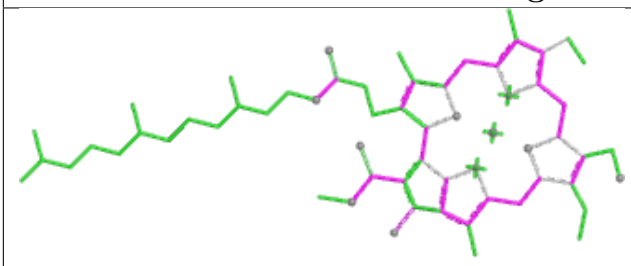
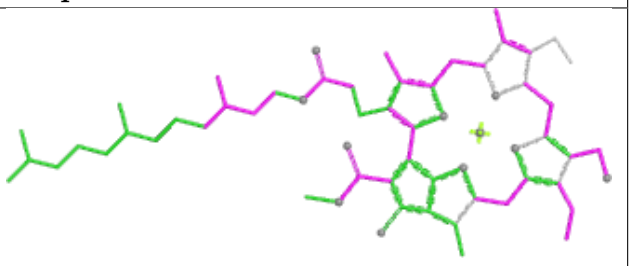
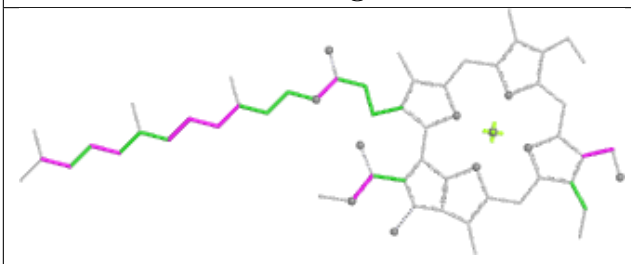
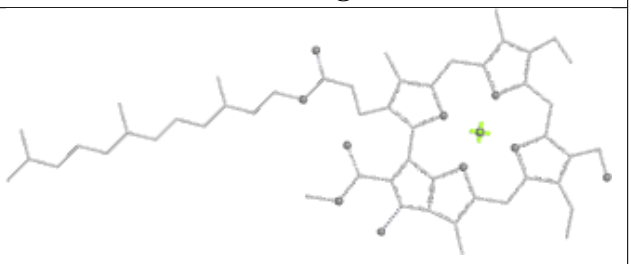


Torsions



Rings

Ligand CHL q 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

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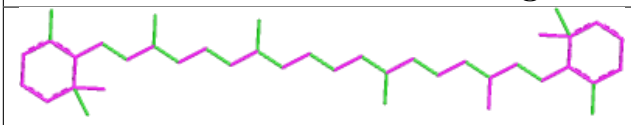
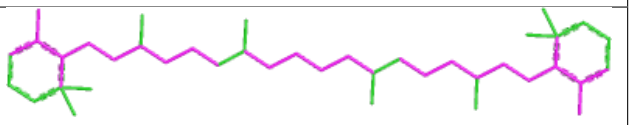
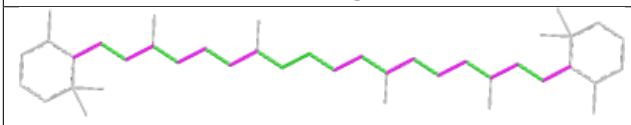
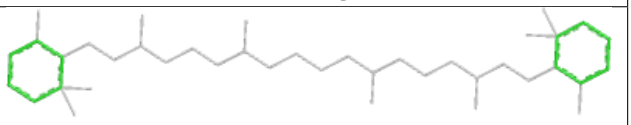
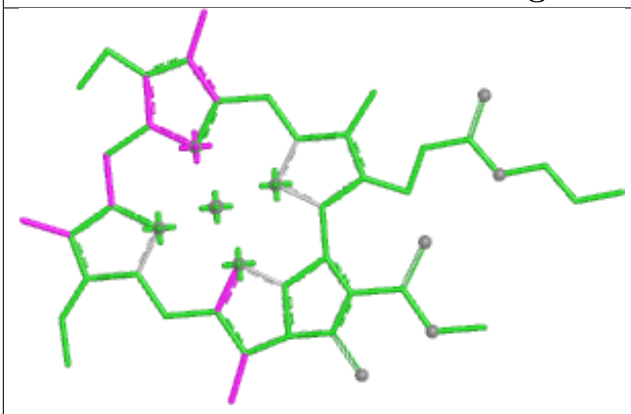
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 308



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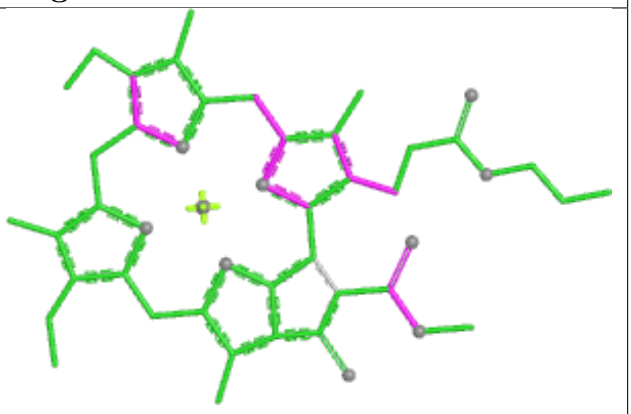
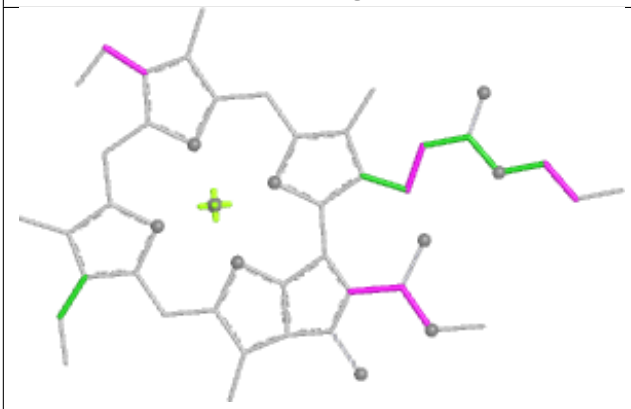


Bond angles



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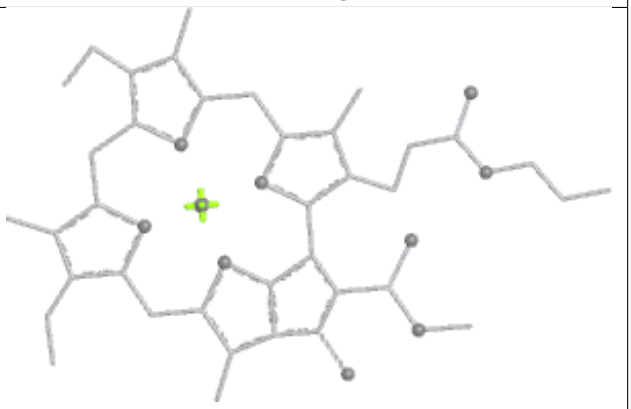
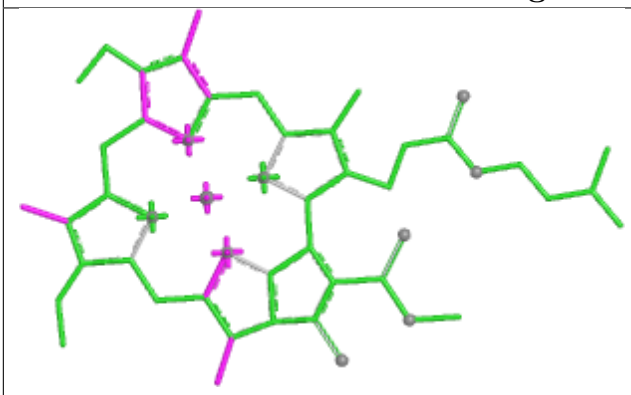


Rings

Ligand CLA a 406



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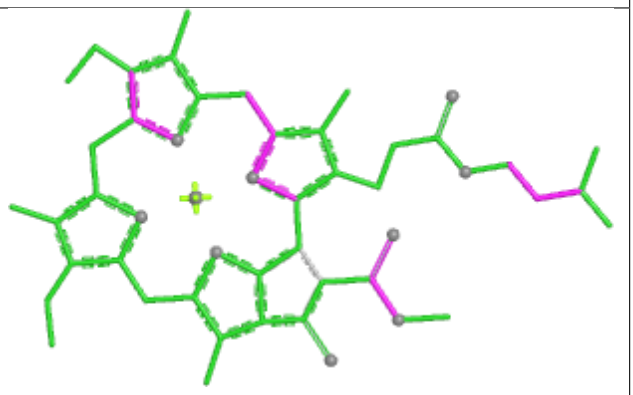
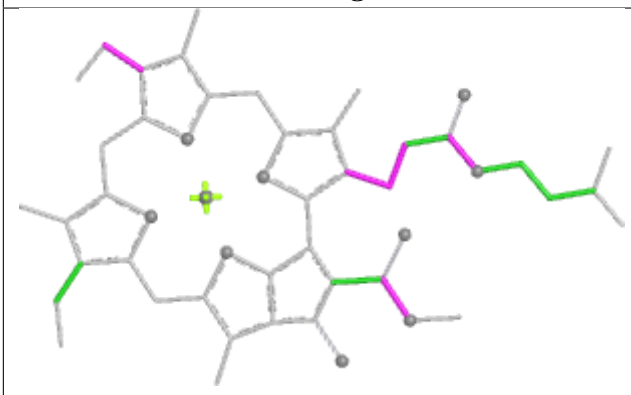


Bond angles



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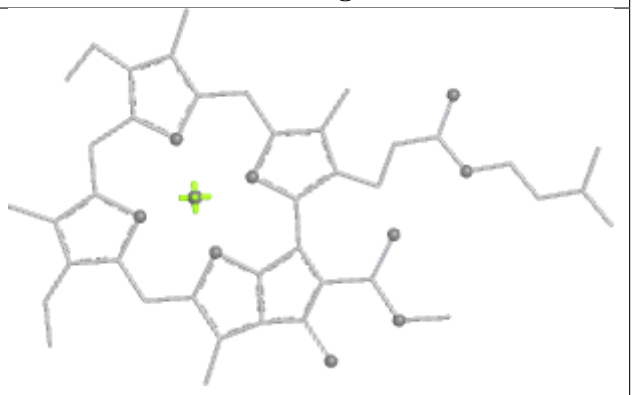
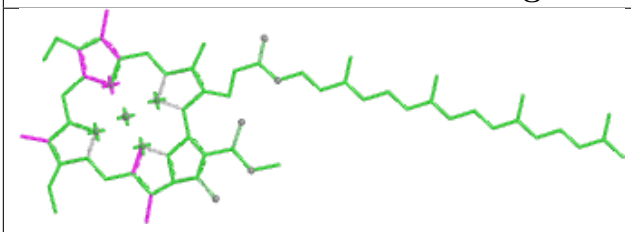


Rings

Ligand CLA U 302



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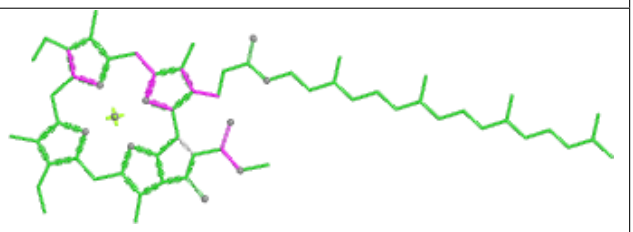

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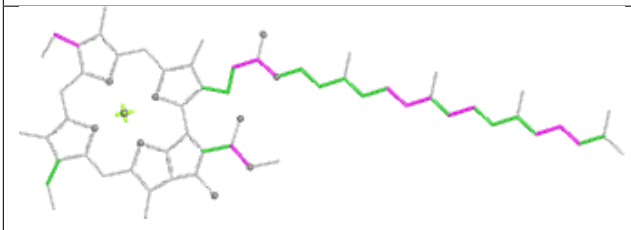

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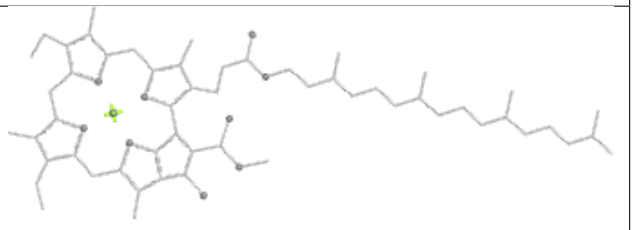
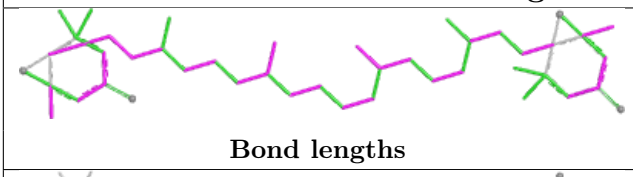


Rings

Ligand XAT 5 311



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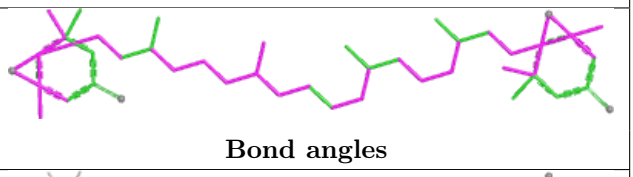

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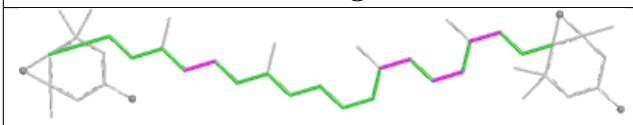

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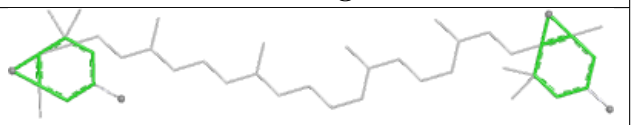
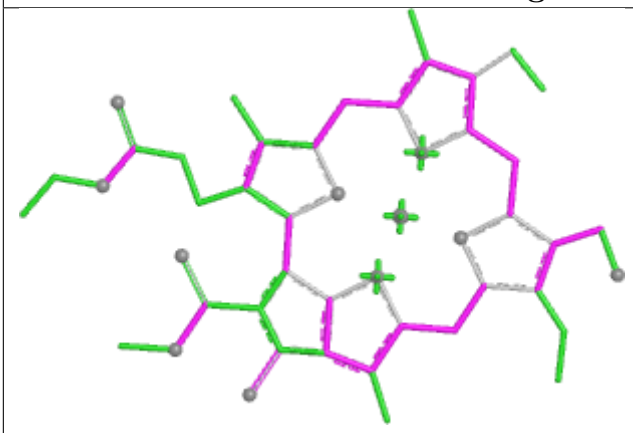


Rings

Ligand CHL 3 312



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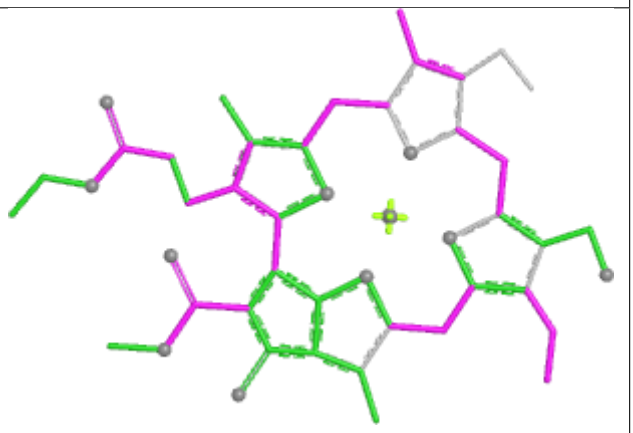
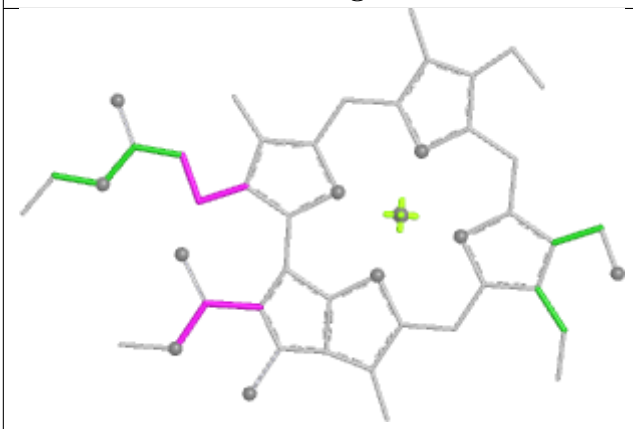


Bond angles



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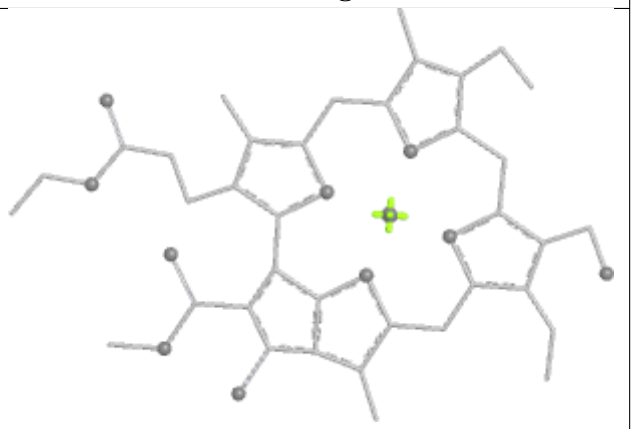
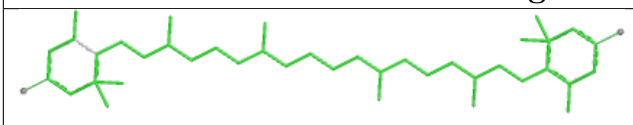


Rings

Ligand LUT 1 309



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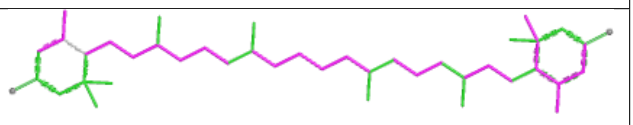

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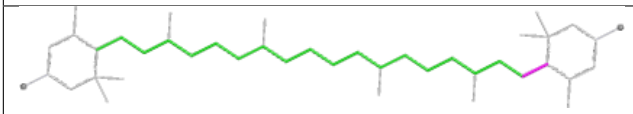

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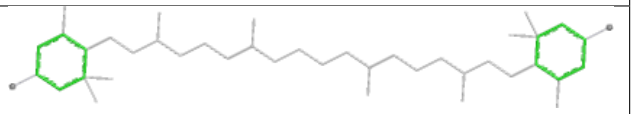
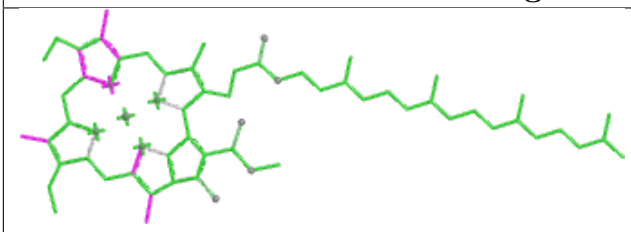


Rings

Ligand CLA C 511



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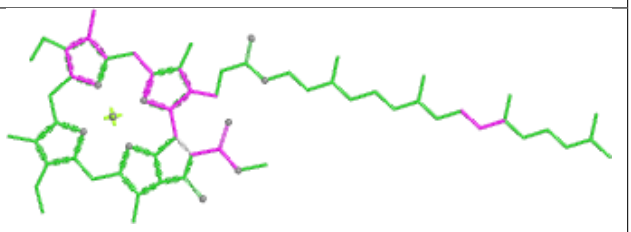
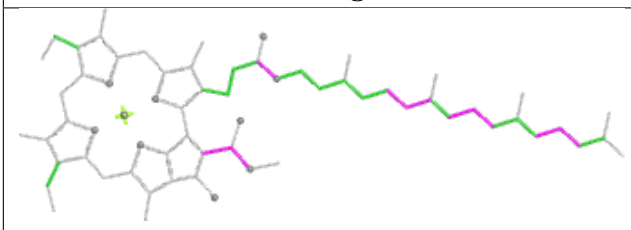


Bond angles



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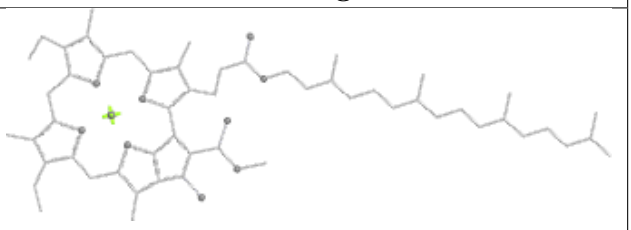
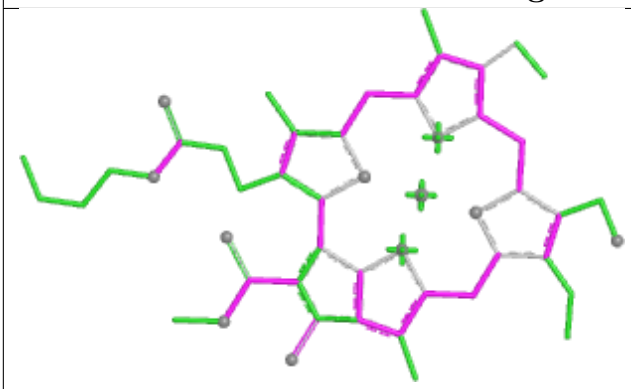


Rings

Ligand CHL 3 313



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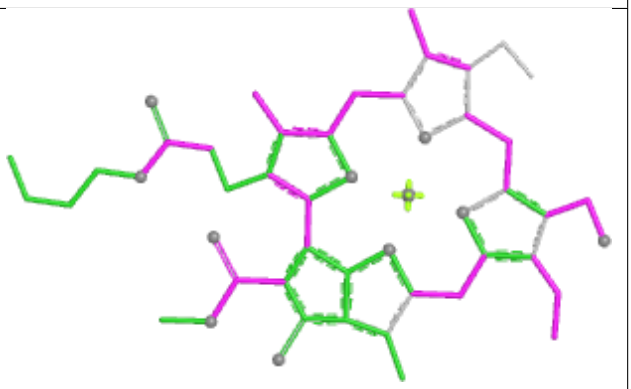
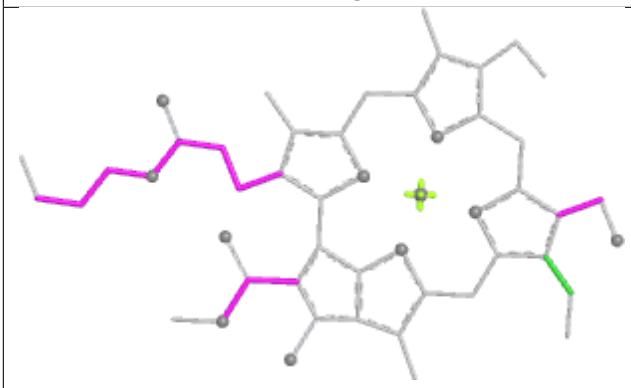
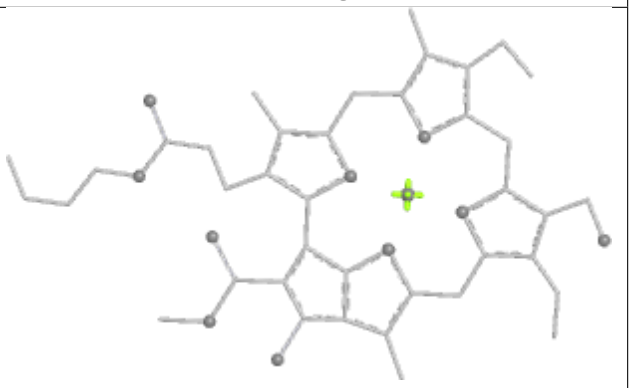


Bond angles

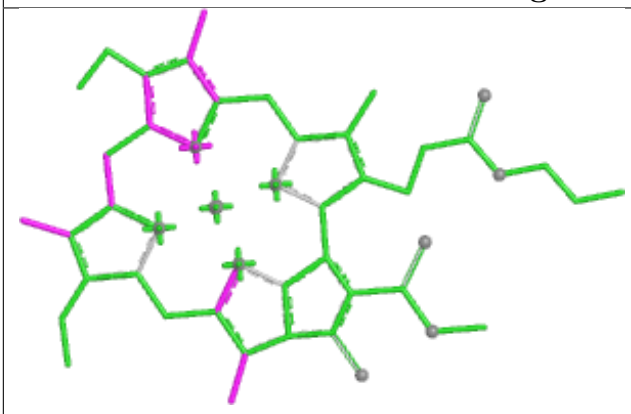


Torsions



Rings

Ligand CLA r 604



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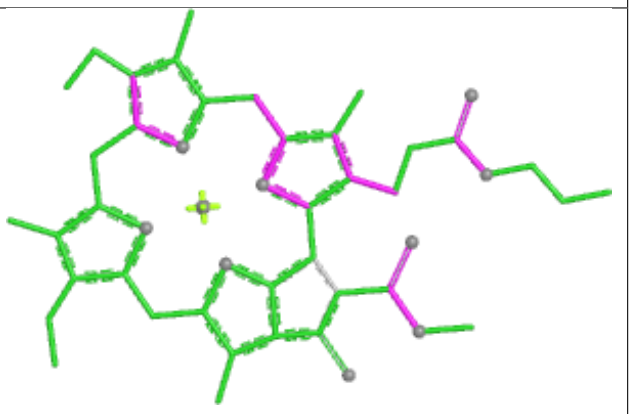
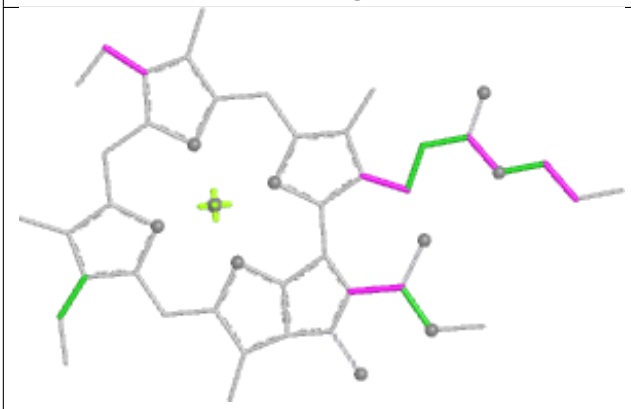
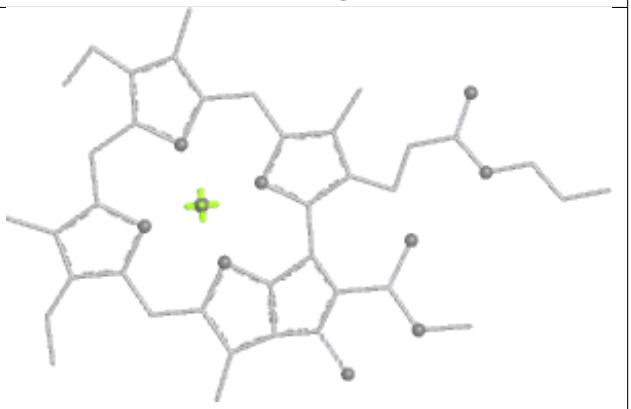


Bond angles

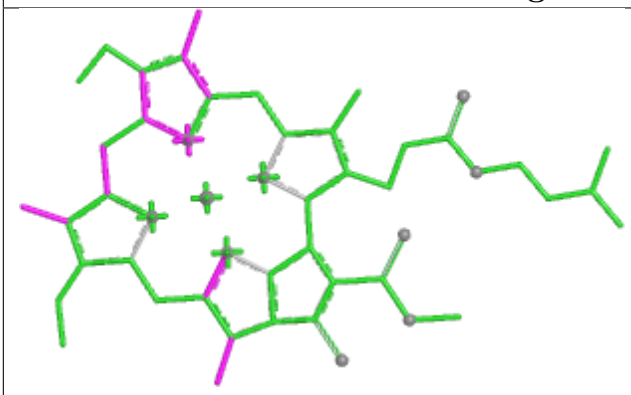


Torsions

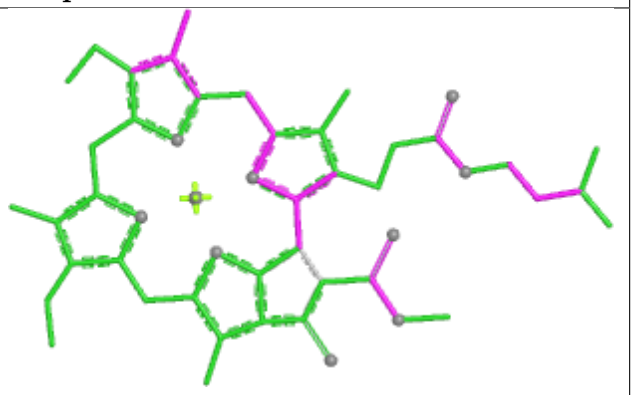


Rings

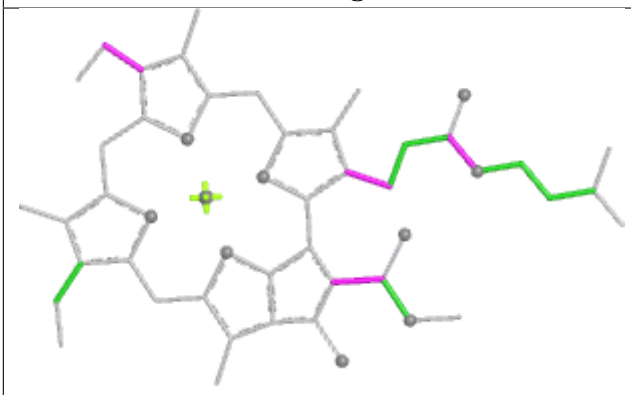
Ligand CLA q 303



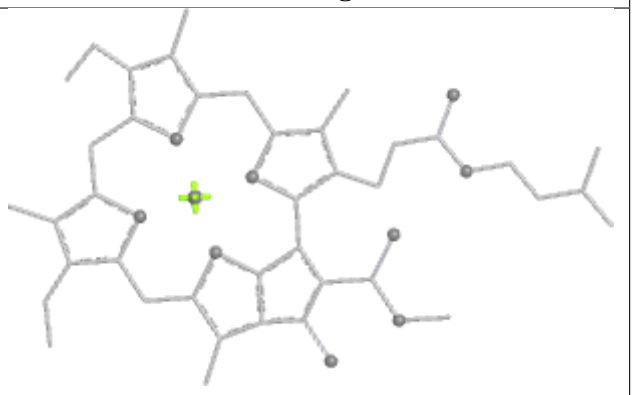
Bond lengths



Bond angles

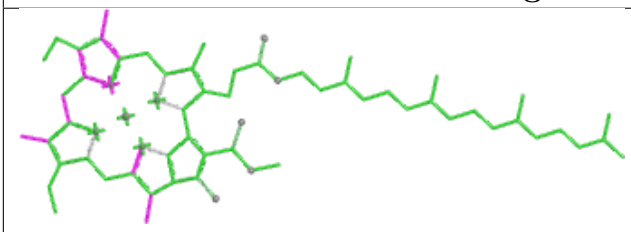


Torsions

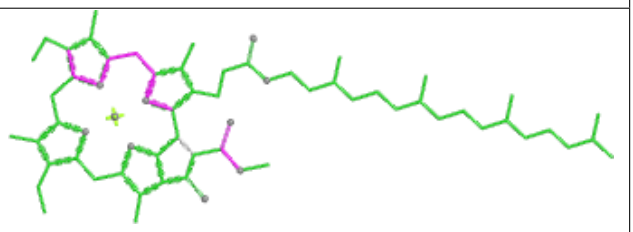


Rings

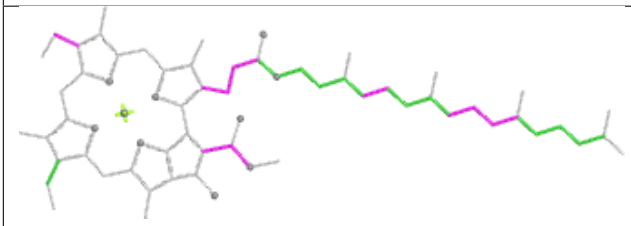
Ligand CLA V 301



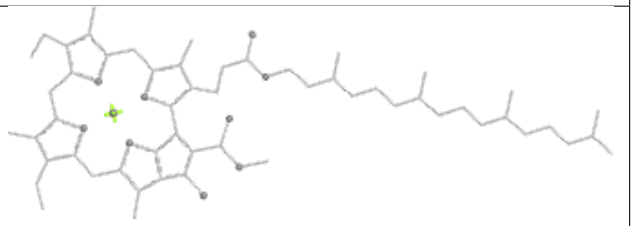
Bond lengths



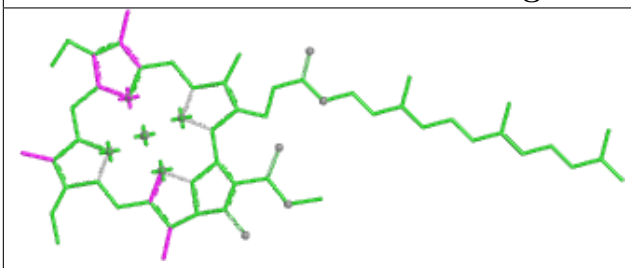
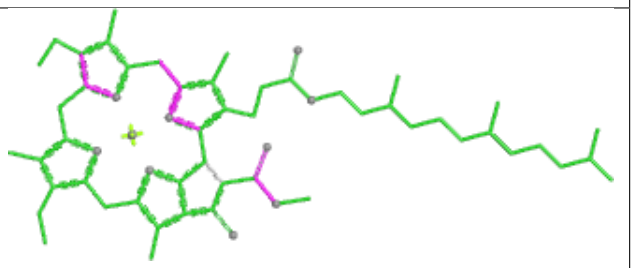
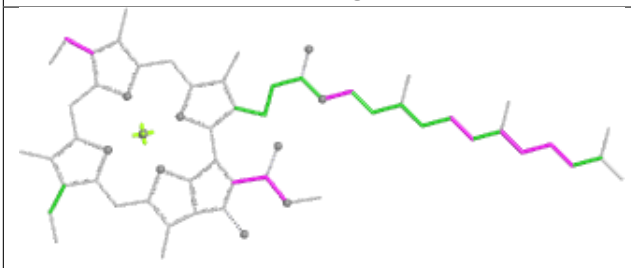
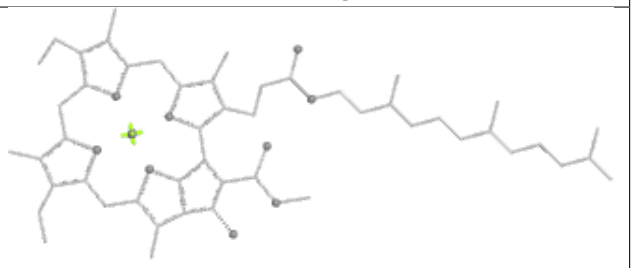
Bond angles

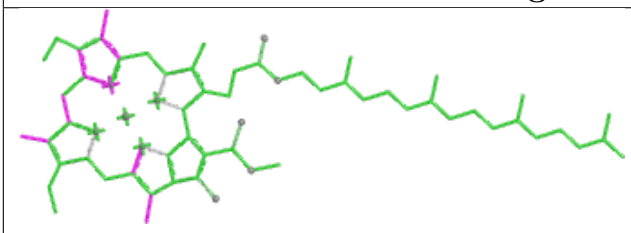
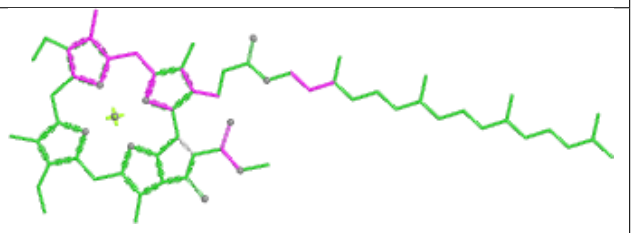
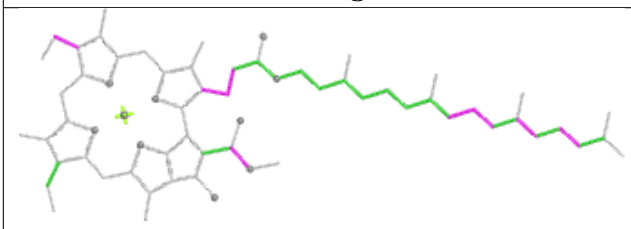
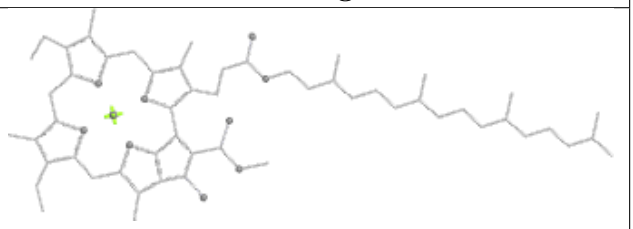


Torsions

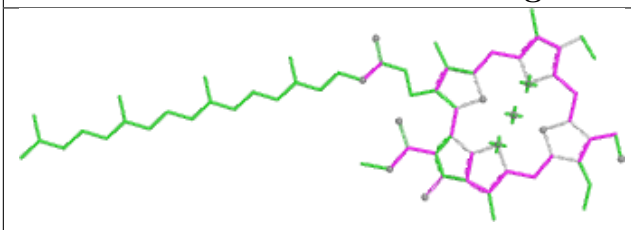


Rings

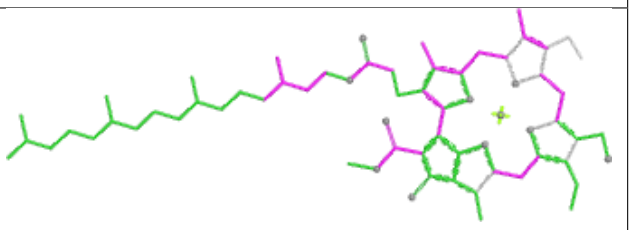
Ligand CLA G 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

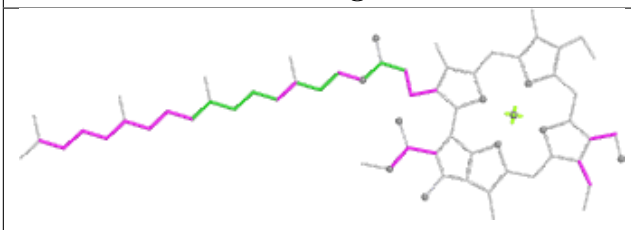
Ligand CHL P 319



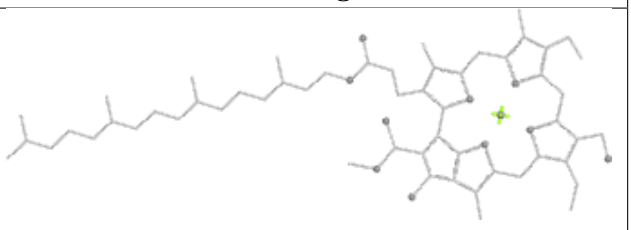
Bond lengths



Bond angles

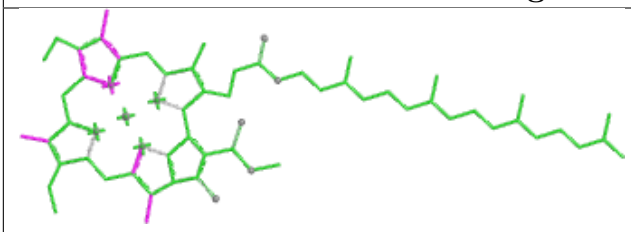


Torsions



Rings

Ligand CLA b 611



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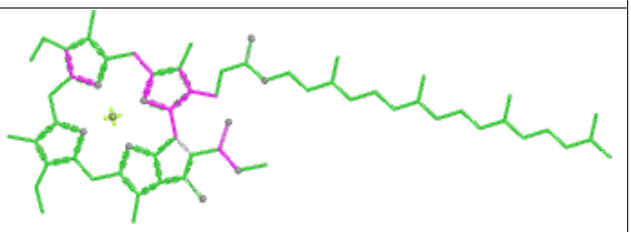
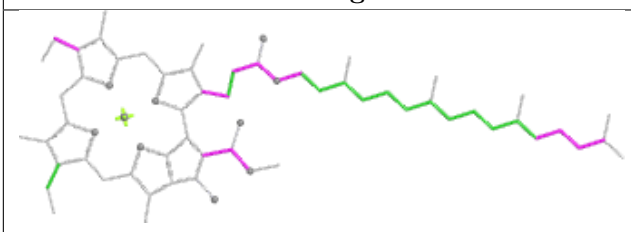
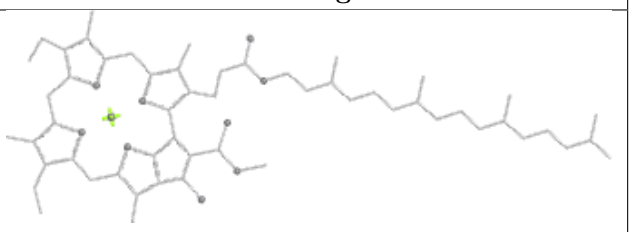


Bond angles

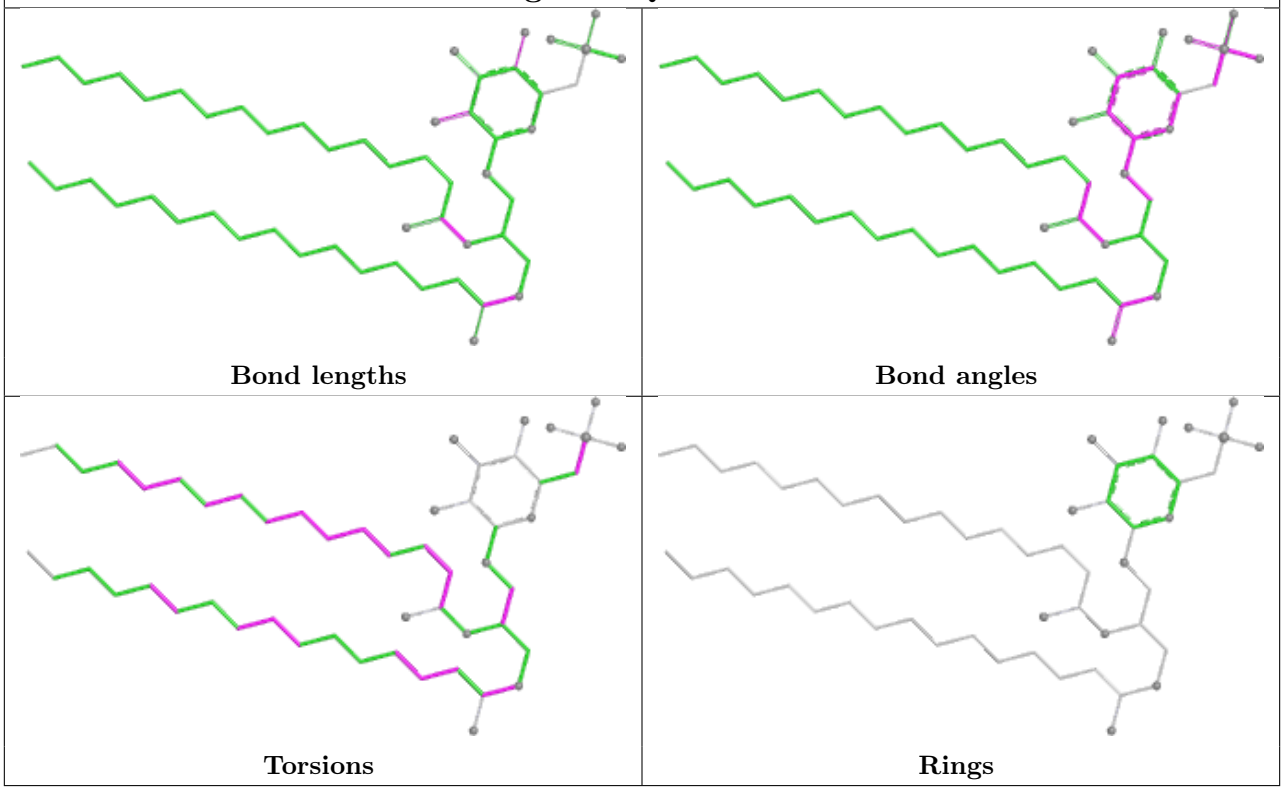


Torsions

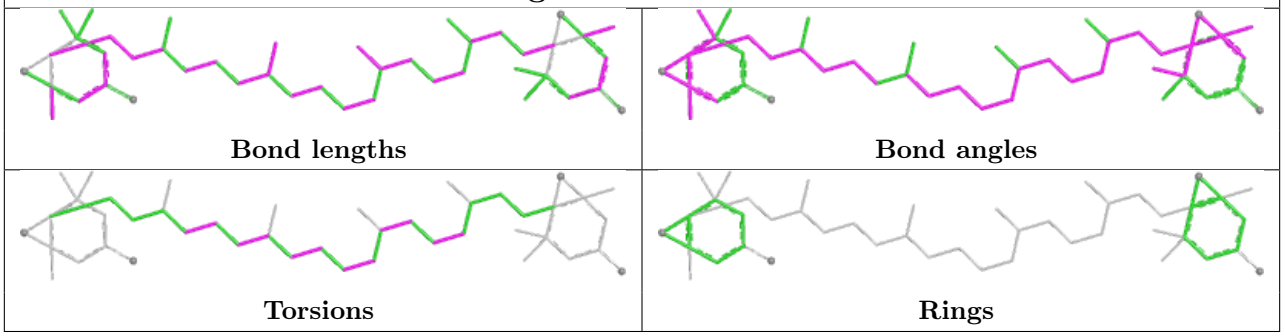


Rings

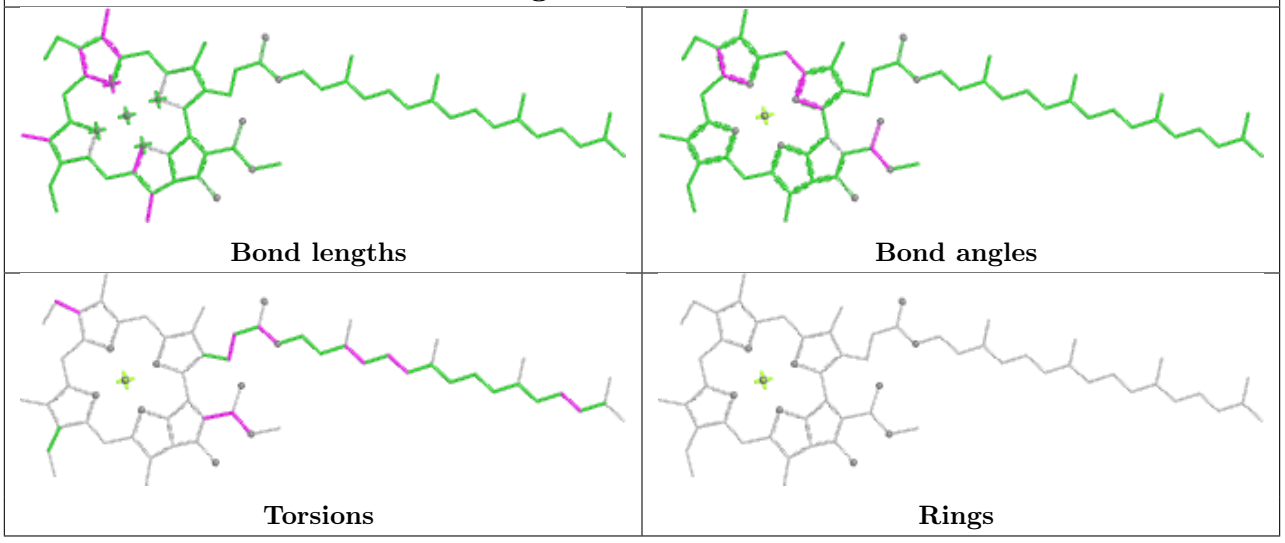
Ligand SQD A 412



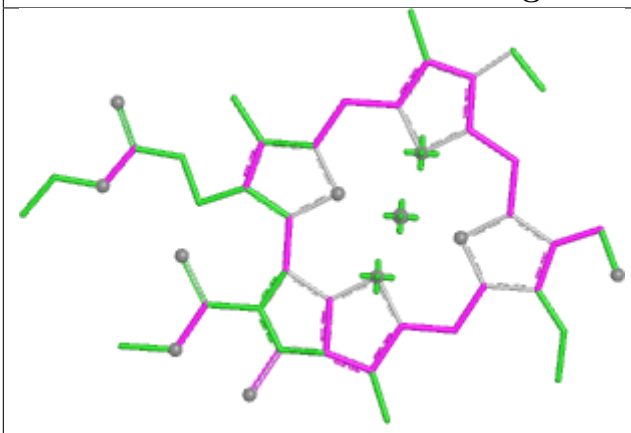
Ligand XAT 4 311



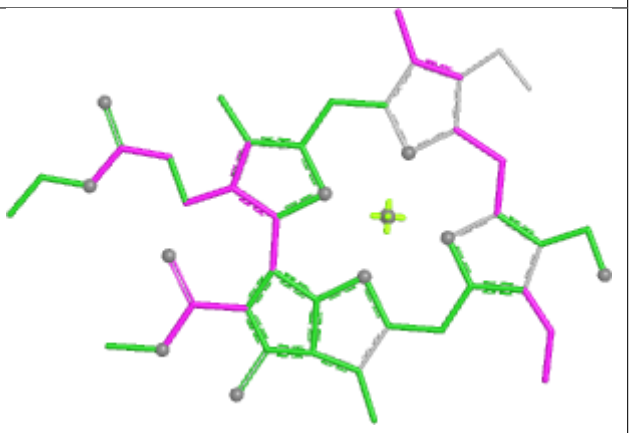
Ligand CLA c 505



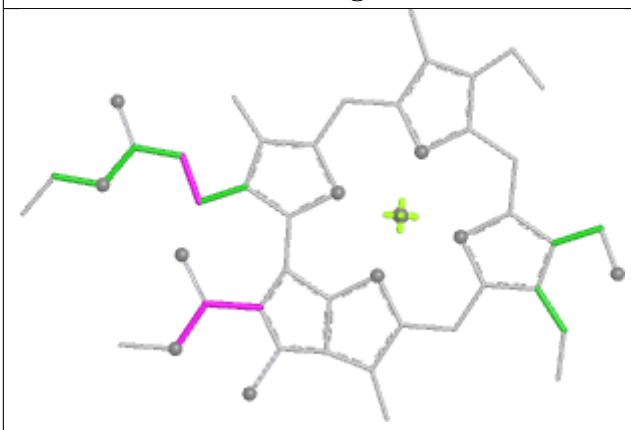
Ligand CHL G 312



Bond lengths



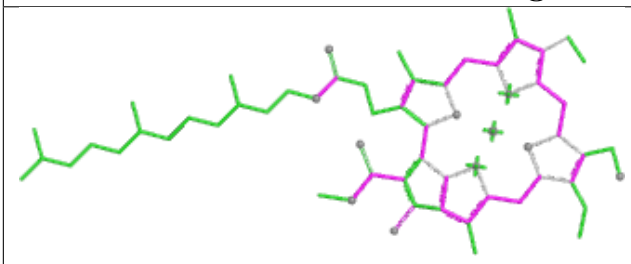
Bond angles



Torsions

Rings

Ligand CHL 3 316



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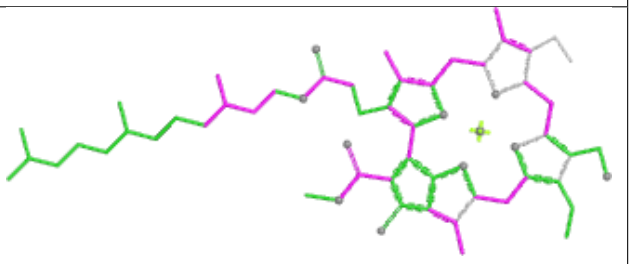

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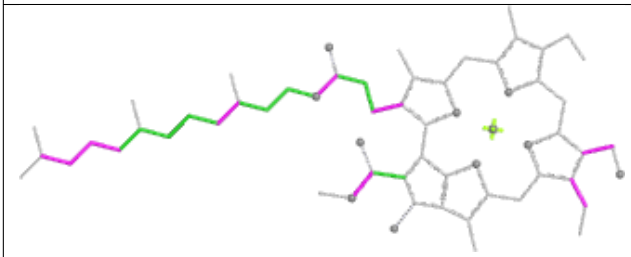
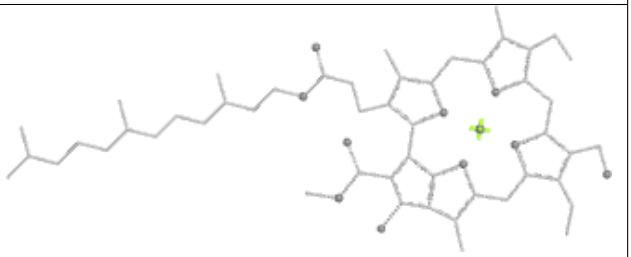
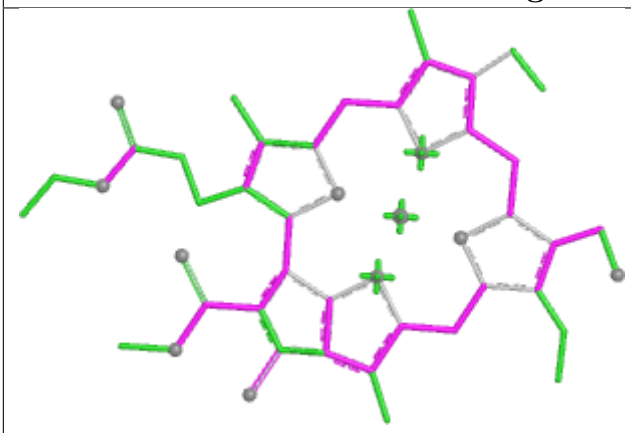


Torsions



Rings

Ligand CHL p 315



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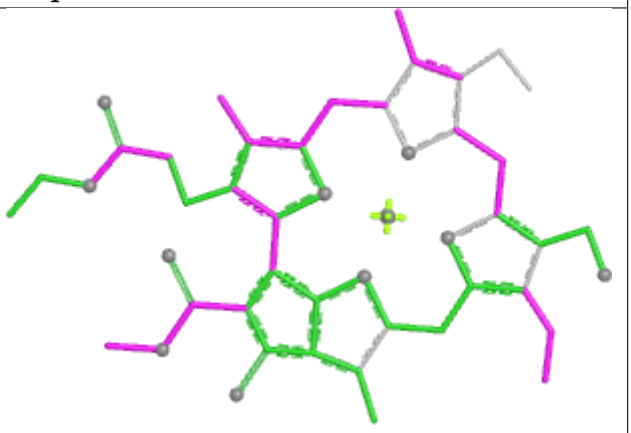
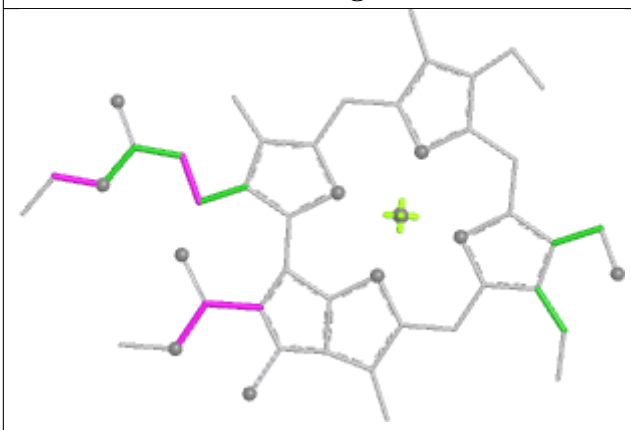


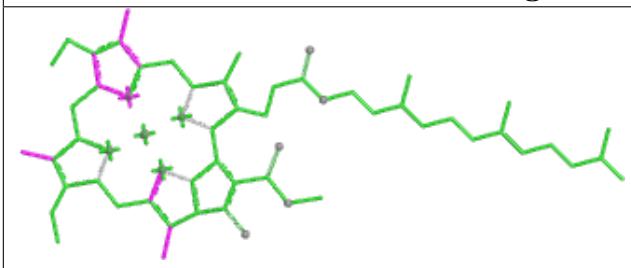
Bond angles



Torsions

Rings

Ligand CLA R 310



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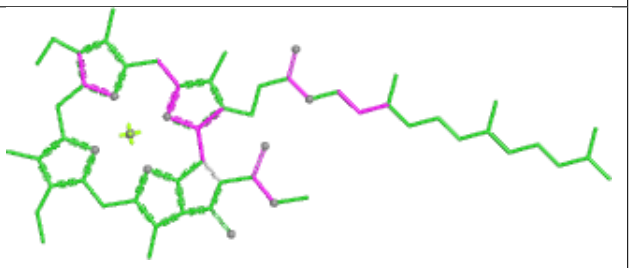
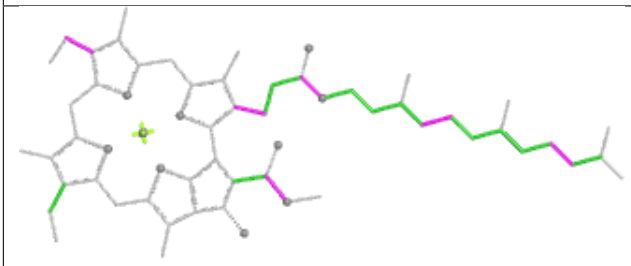
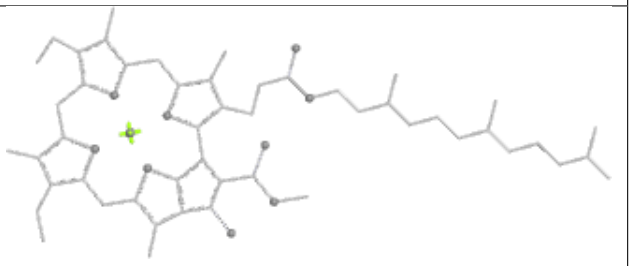


Bond angles

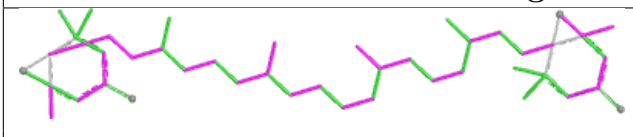


Torsions

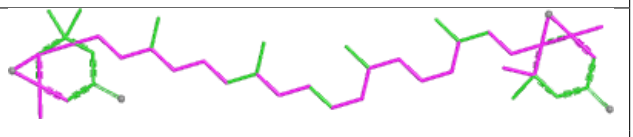


Rings

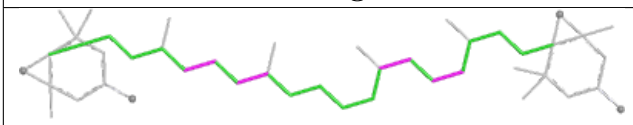
Ligand XAT 1 311



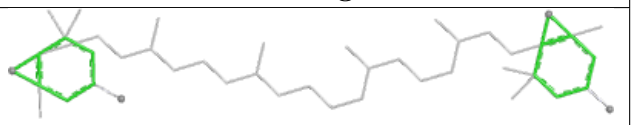
Bond lengths



Bond angles

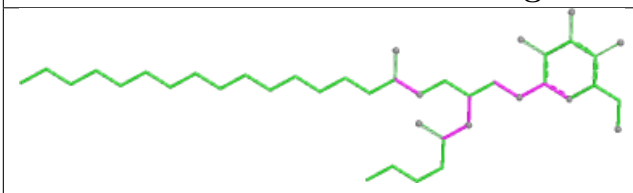


Torsions



Rings

Ligand LMG a 412



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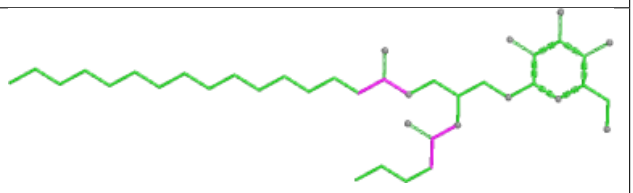
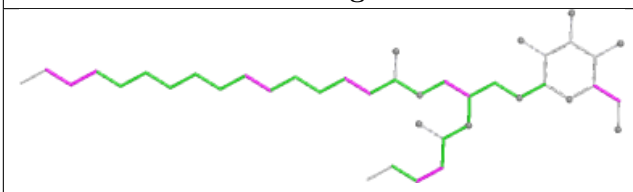


Bond angles



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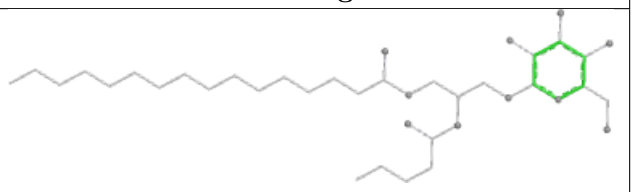
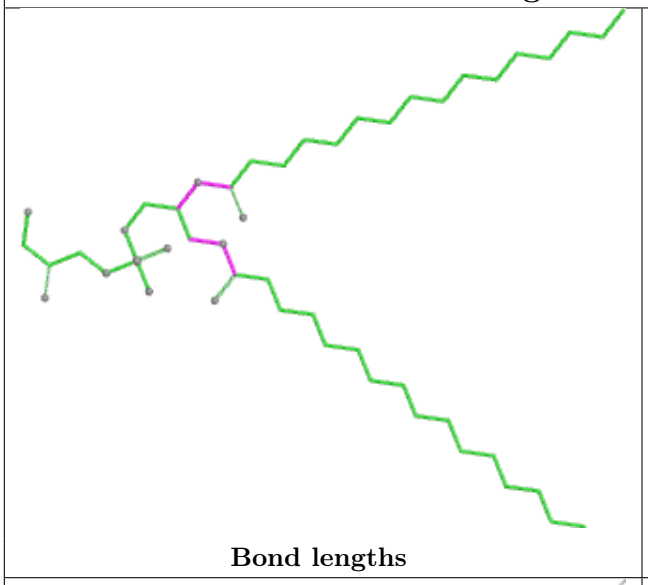
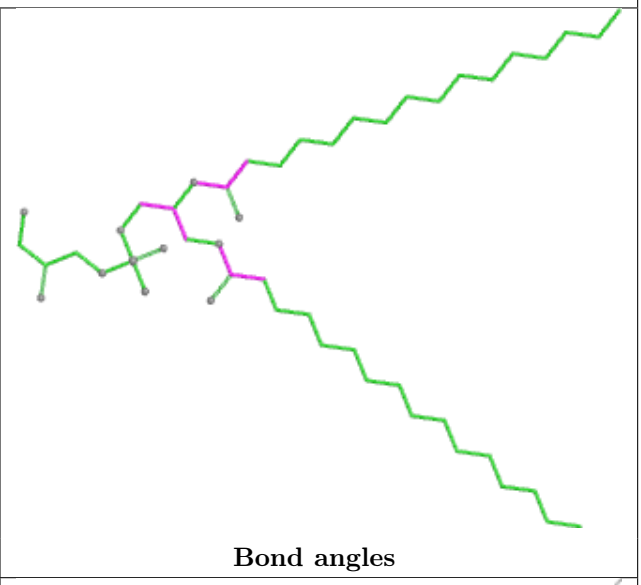


Rings

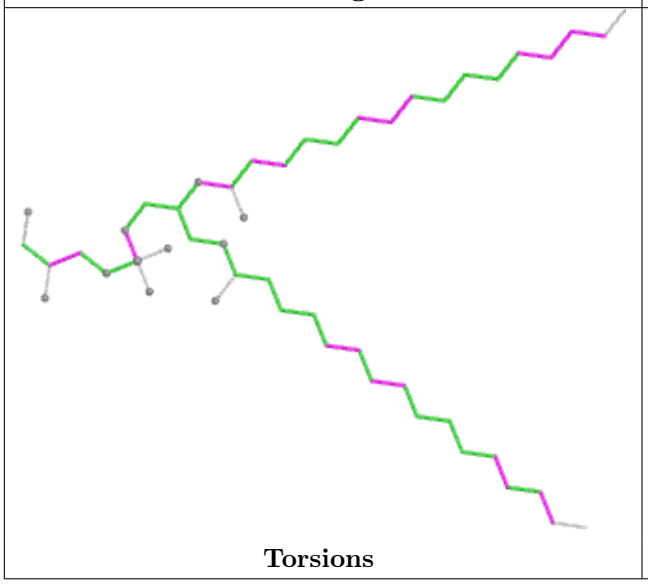
Ligand LHG D 407



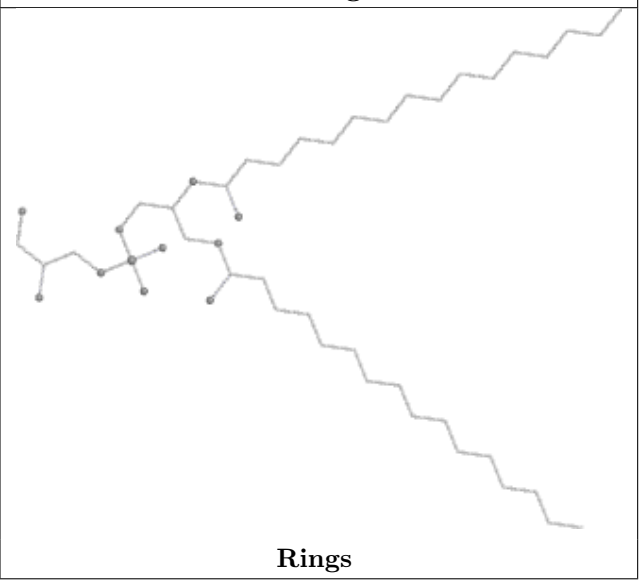
Bond lengths



Bond angles

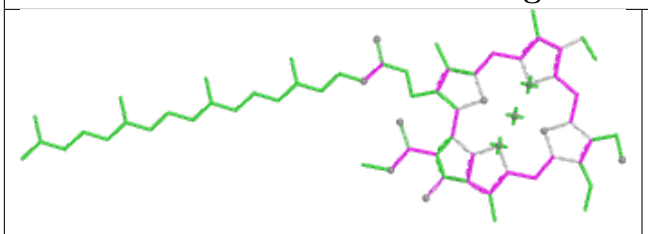


Torsions

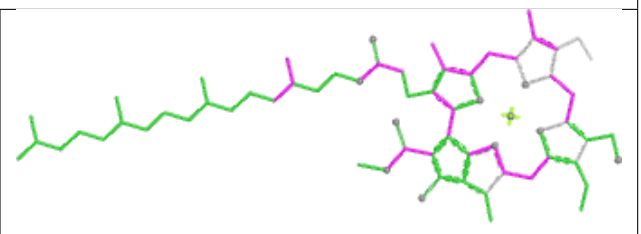


Rings

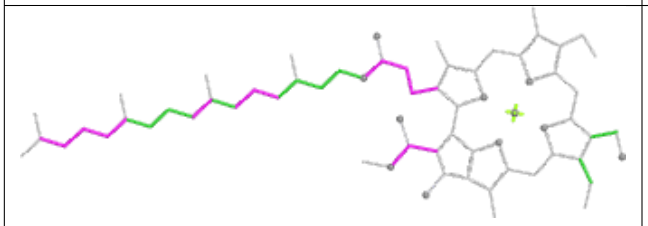
Ligand CHL G 315



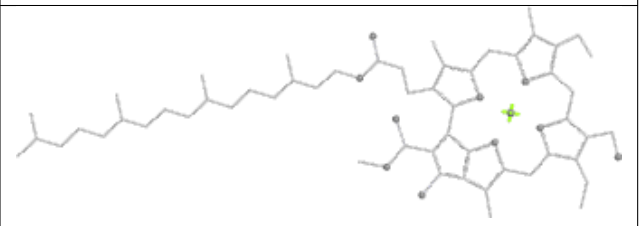
Bond lengths



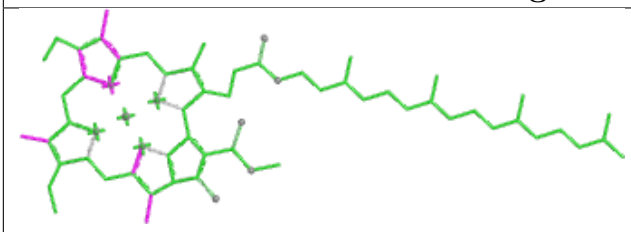
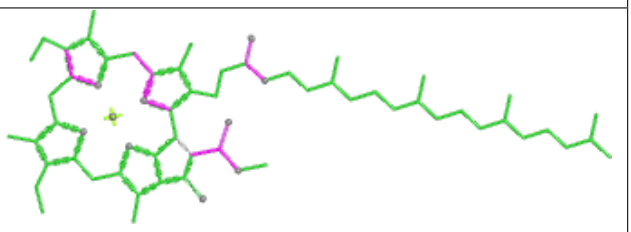
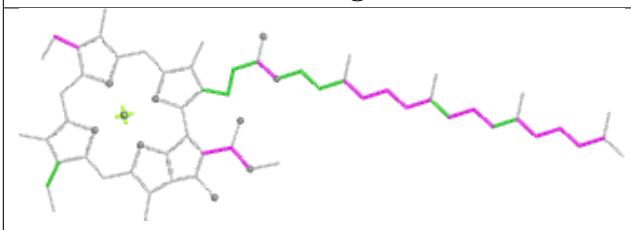
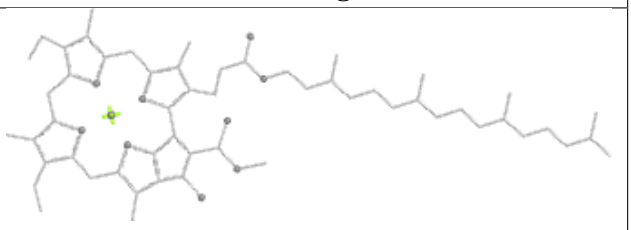
Bond angles

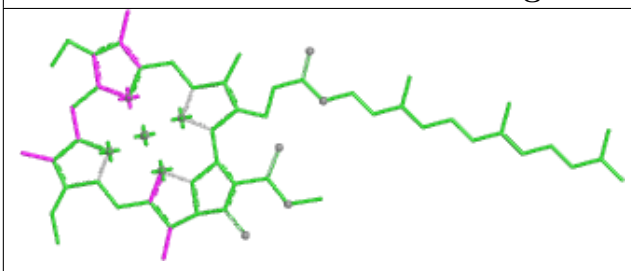
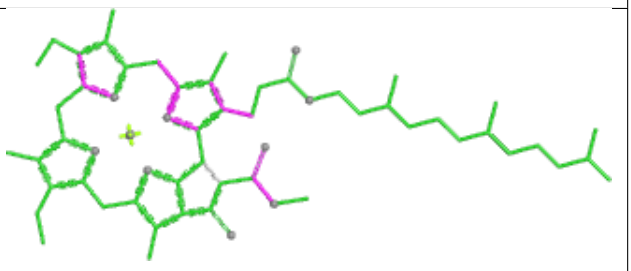
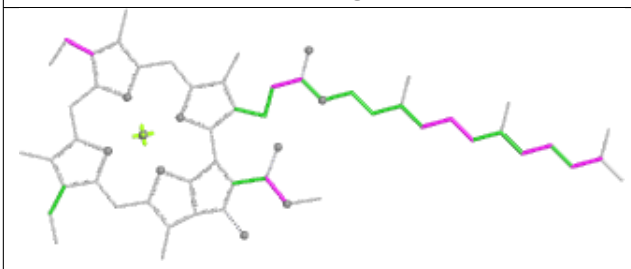
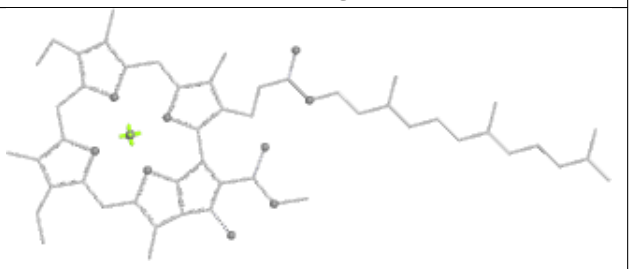


Torsions

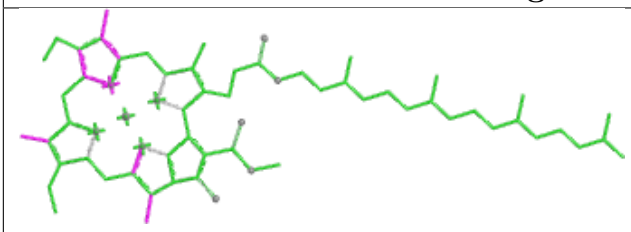


Rings

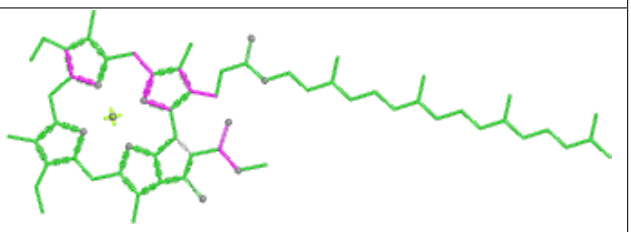
Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

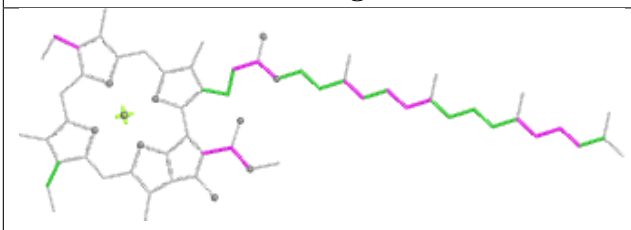
Ligand CLA u 302



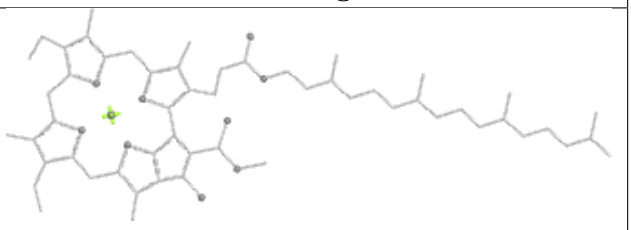
Bond lengths



Bond angles

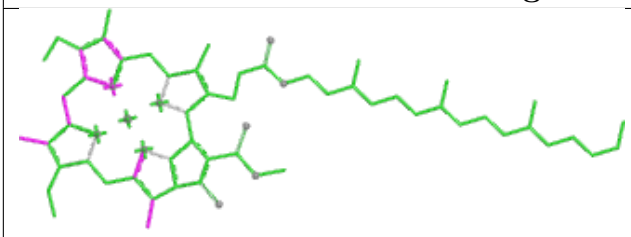


Torsions



Rings

Ligand CLA G 304



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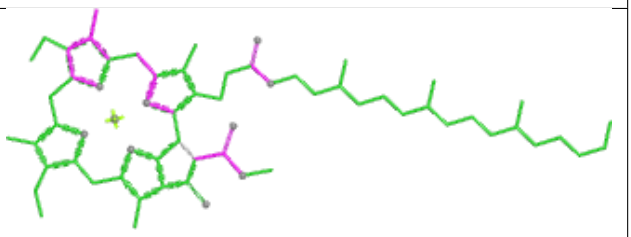
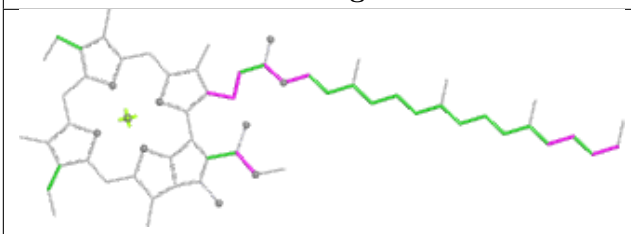
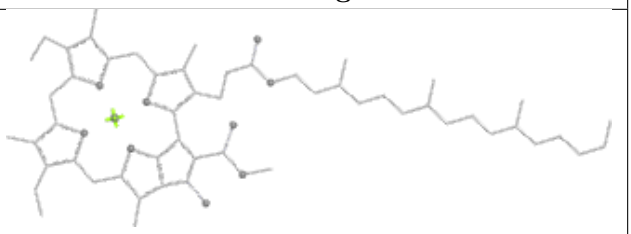


Bond angles

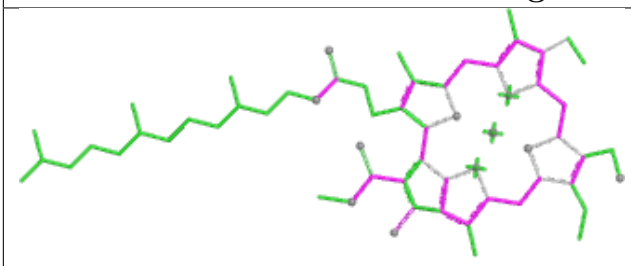


Torsions

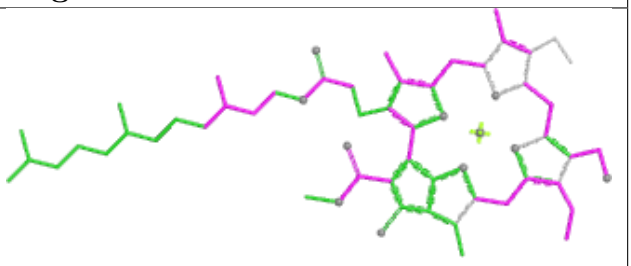


Rings

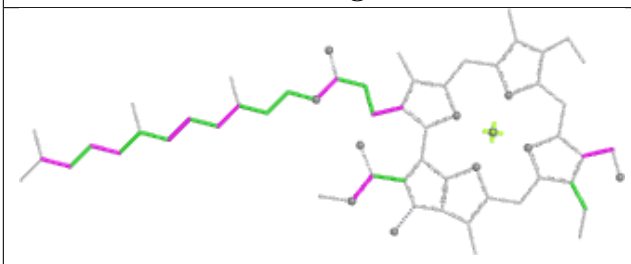
Ligand CHL g 316



Bond lengths



Bond angles



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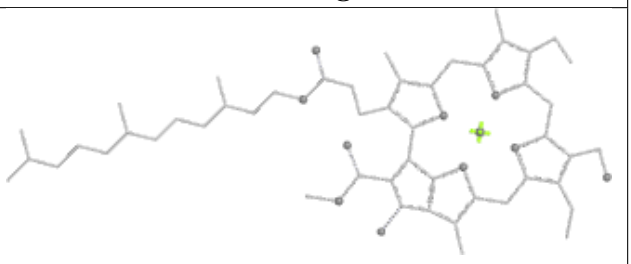
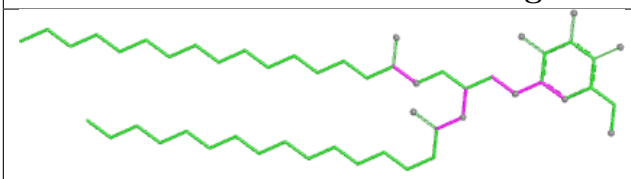


Rings

Ligand LMG c 520



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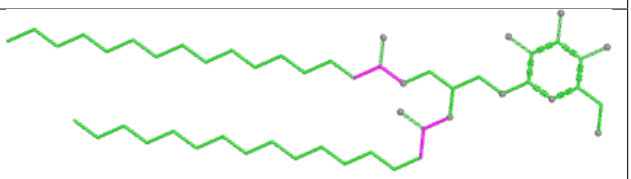
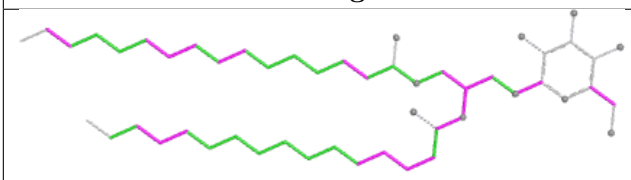


Bond angles



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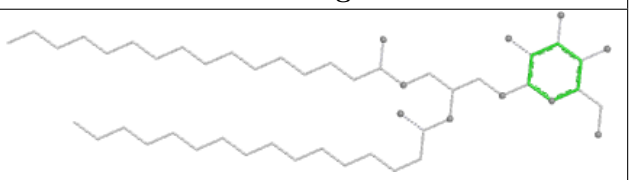
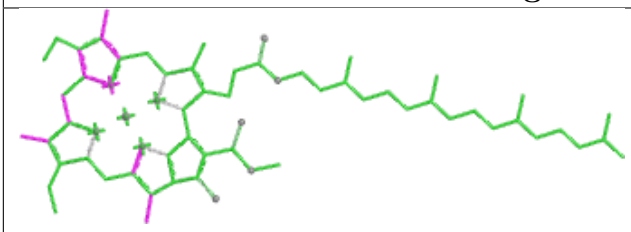


Rings

Ligand CLA X 202



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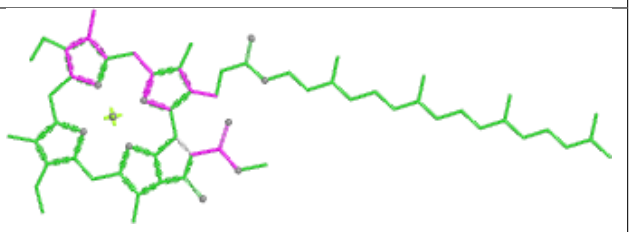
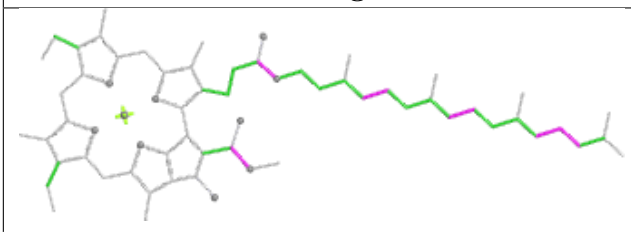


Bond angles



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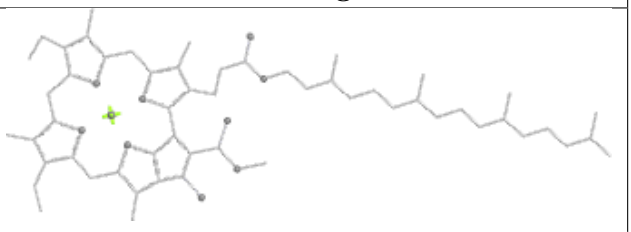
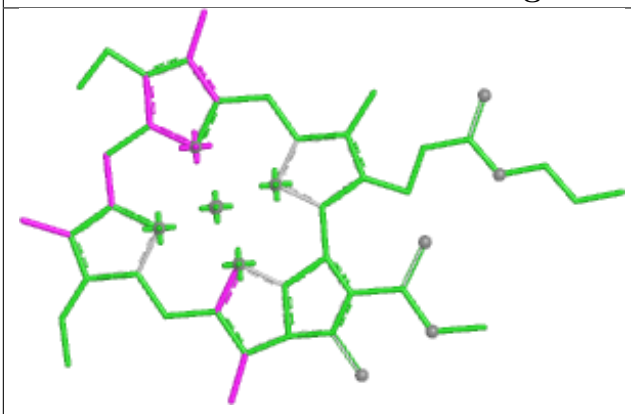
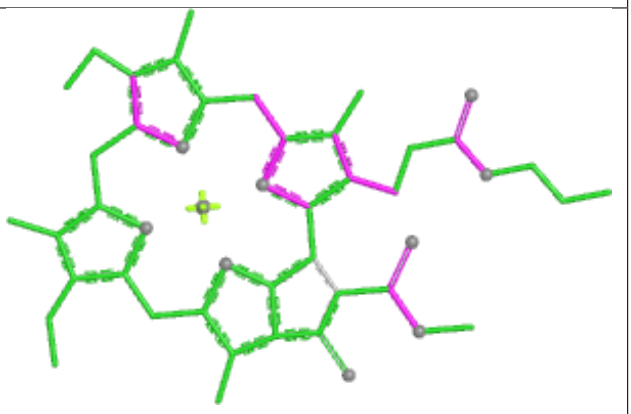


Rings

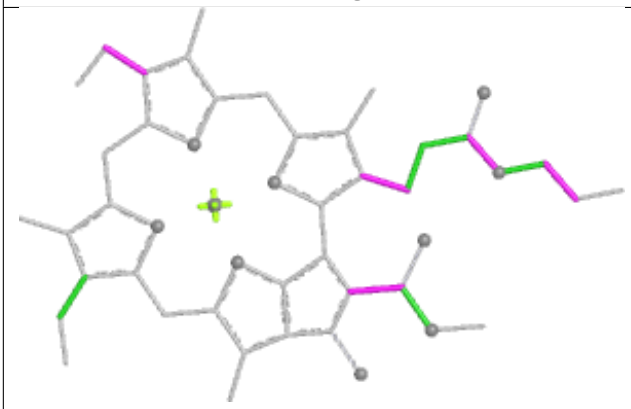
Ligand CLA R 305



Bond lengths



Bond angles



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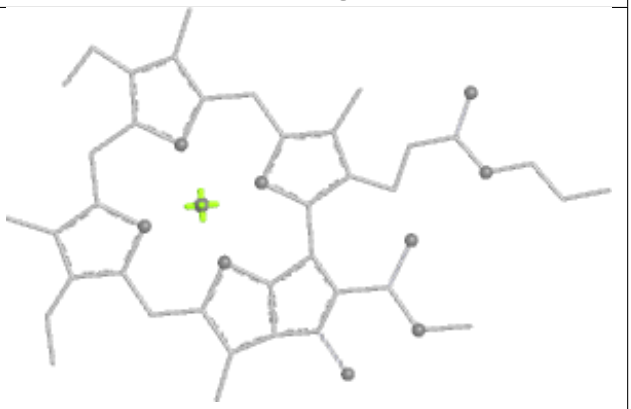
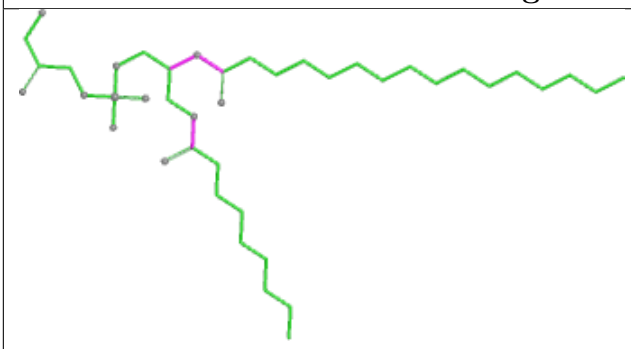
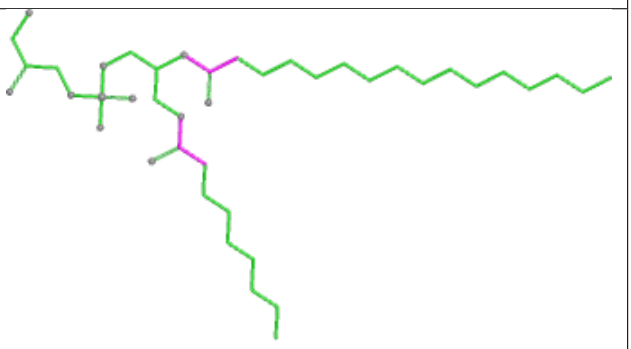


Rings

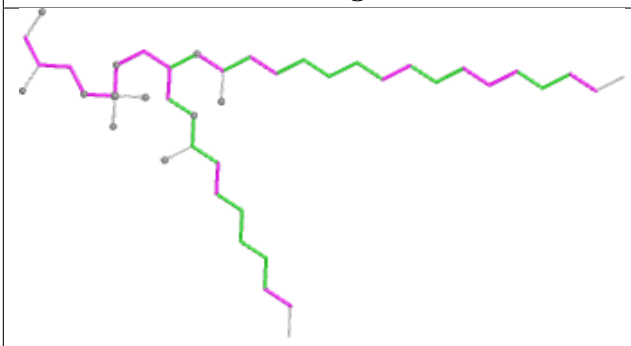
Ligand LHG R 314



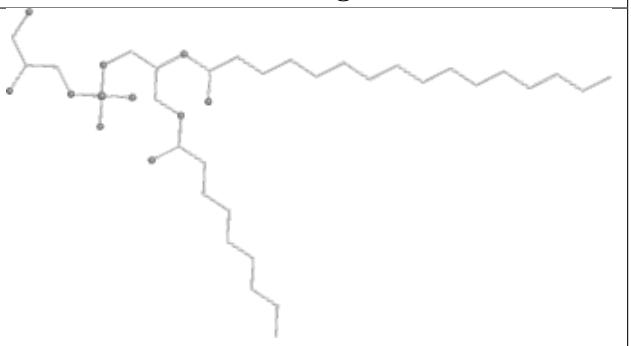
Bond lengths



Bond angles

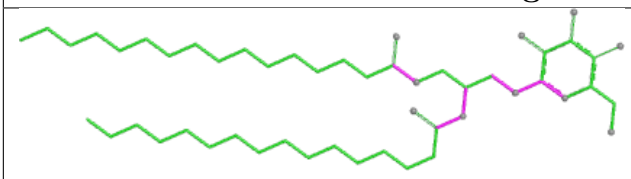


Torsions



Rings

Ligand LMG b 621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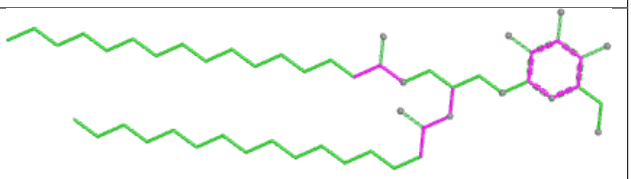
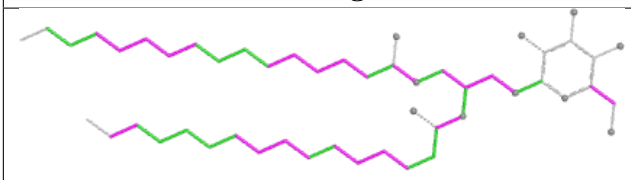

Bond angles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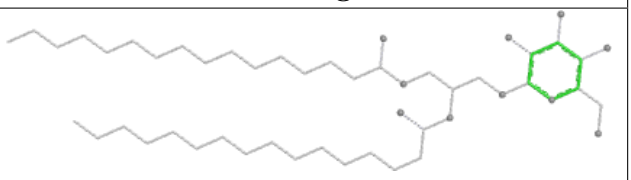
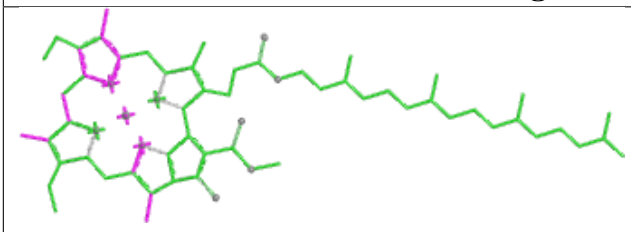

Rings

Ligand CLA c 509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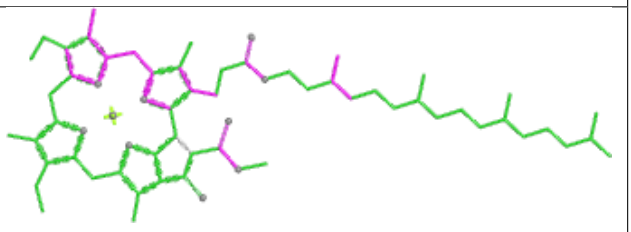
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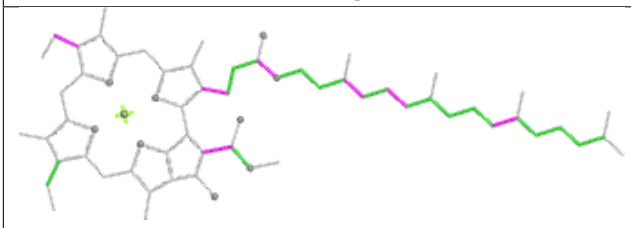
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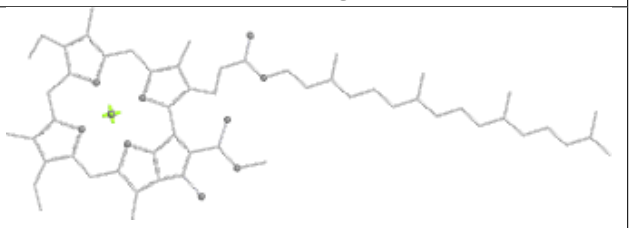
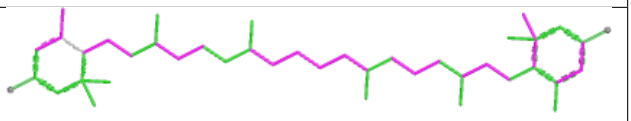
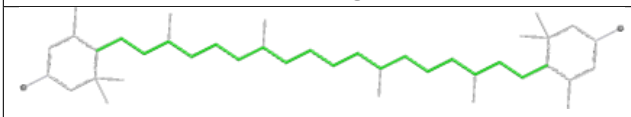

Rings

Ligand LUT v 310

Bond lengths


Bond angles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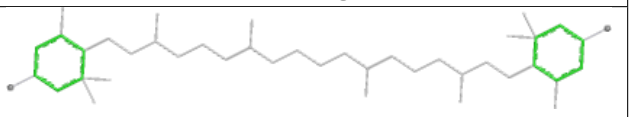
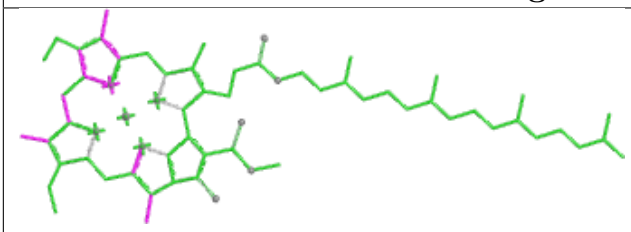

Rings

Ligand CLA 4 301



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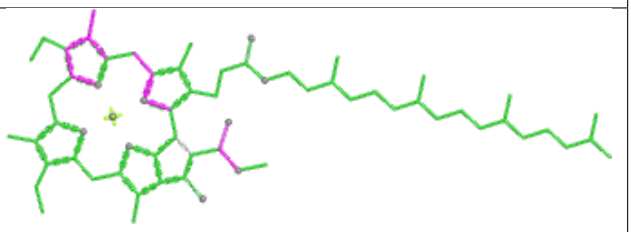
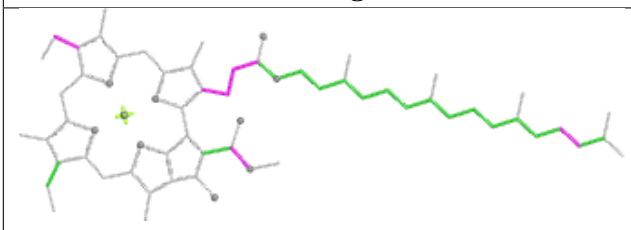
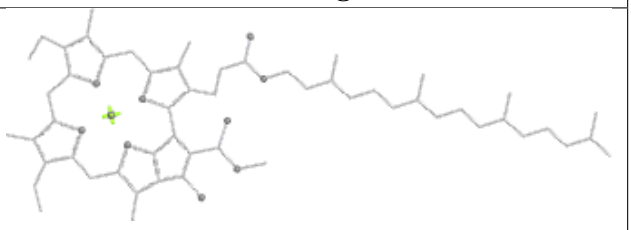


Bond angles

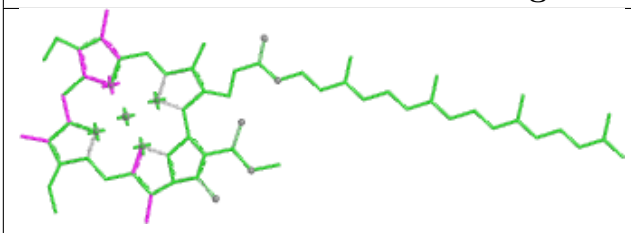


Torsions

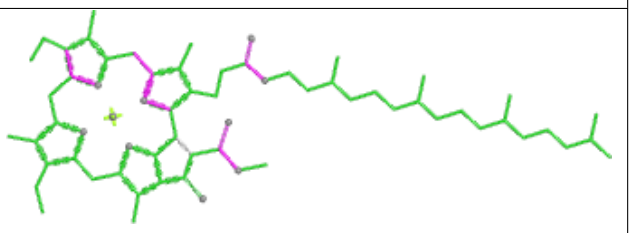


Rings

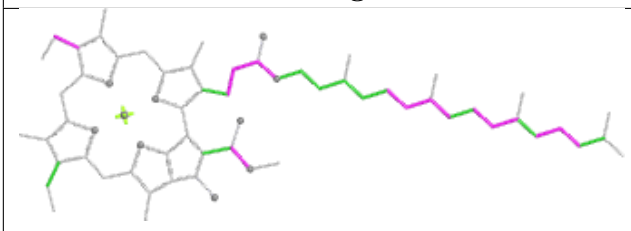
Ligand CLA c 511



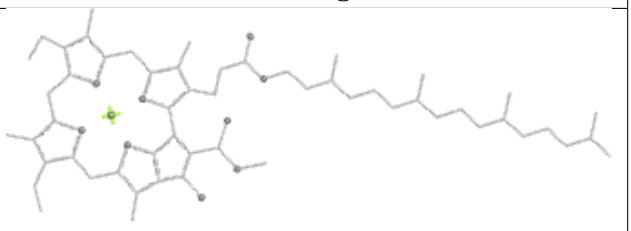
Bond lengths



Bond angles

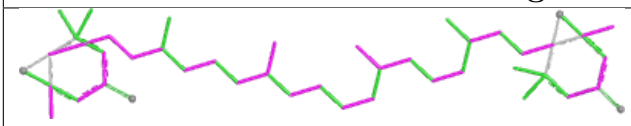


Torsions

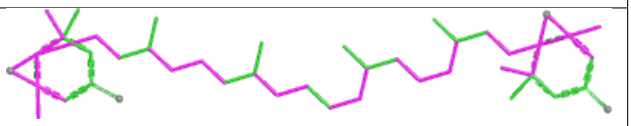


Rings

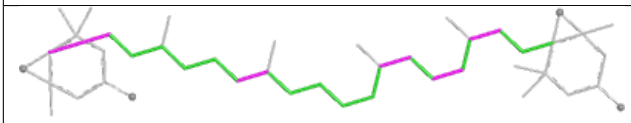
Ligand XAT 6 310



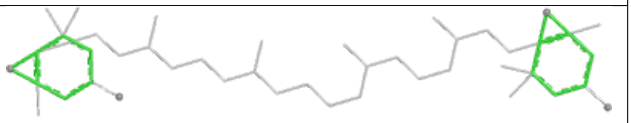
Bond lengths



Bond angles

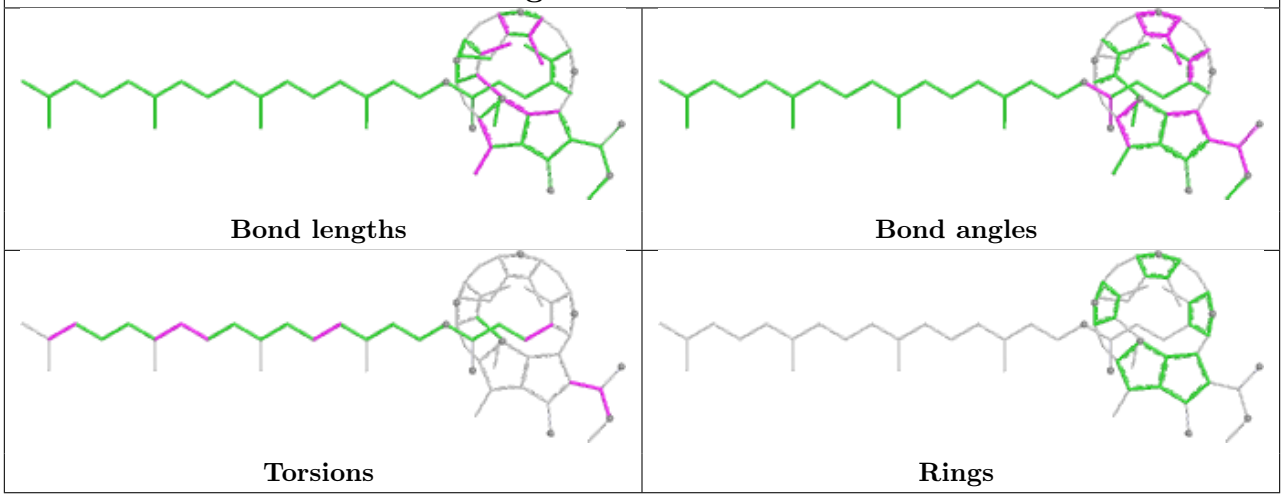


Torsions

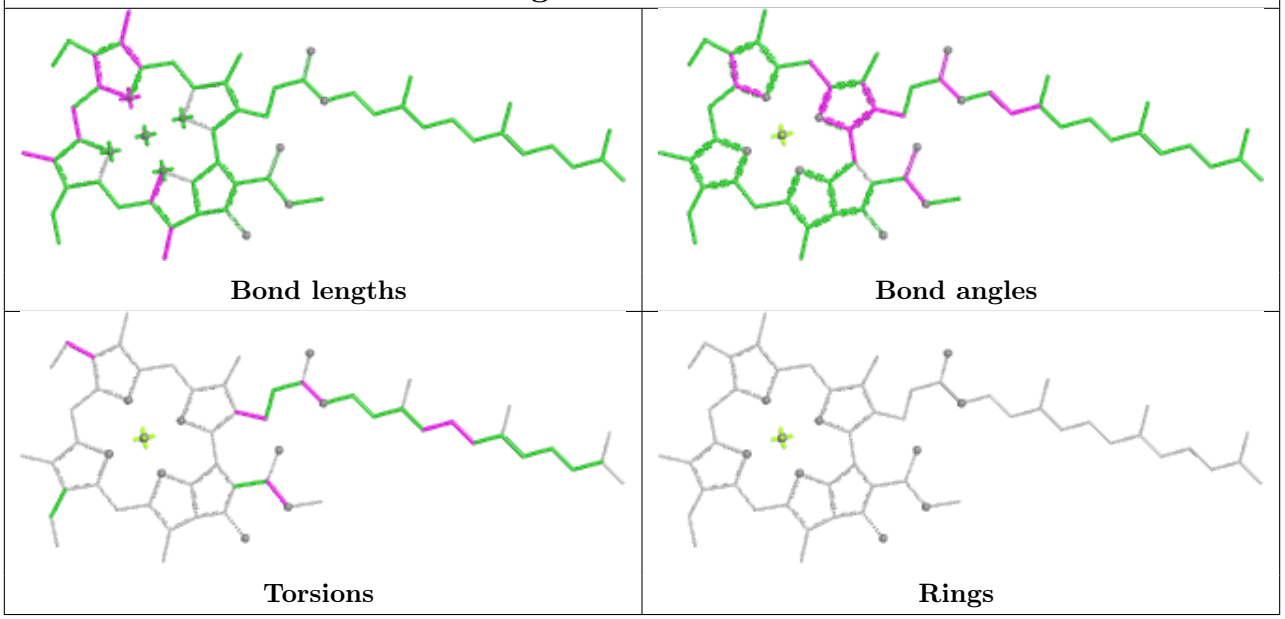


Rings

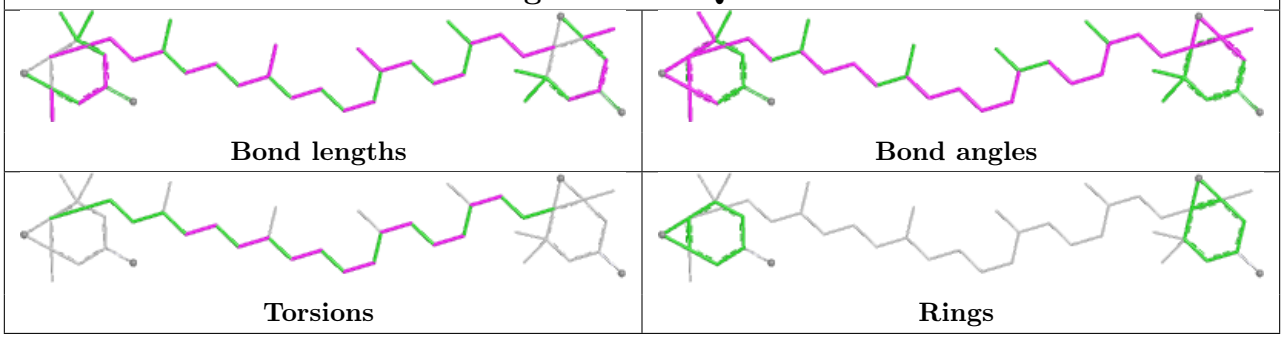
Ligand PHO d 401



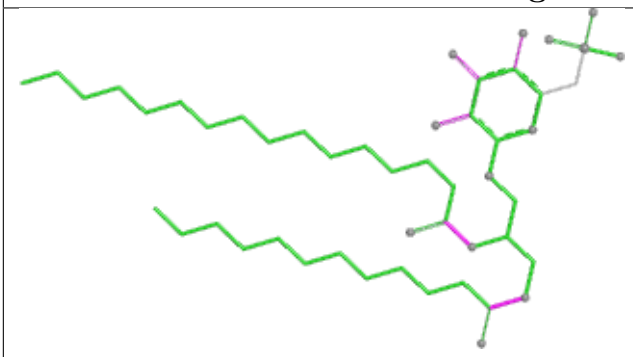
Ligand CLA r 609



Ligand XAT Q 309



Ligand SQD a 410



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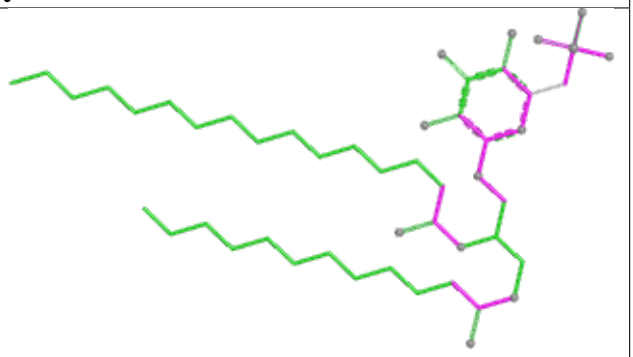
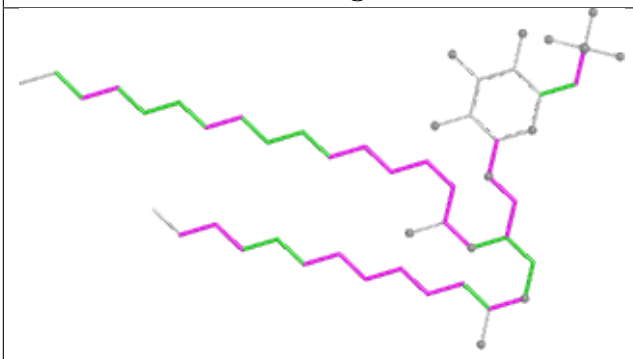


Bond angles



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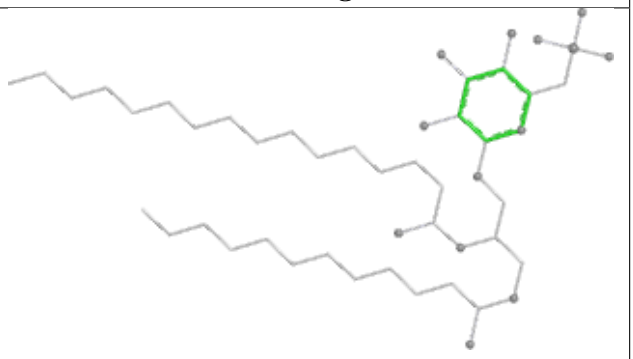
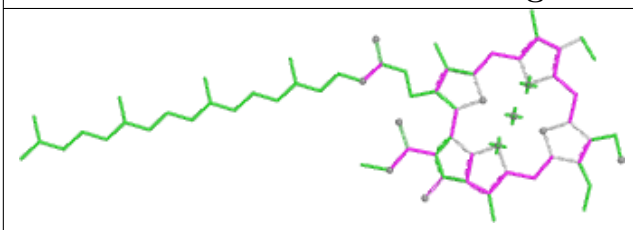


Rings

Ligand CHL n 318



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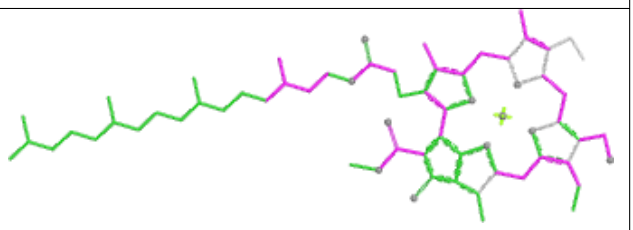
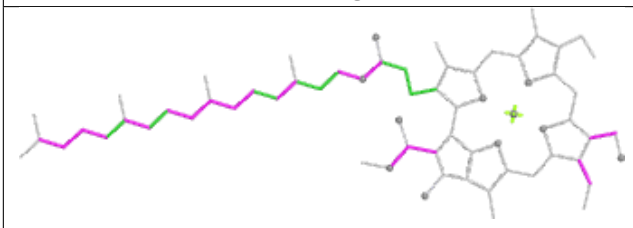


Bond angles



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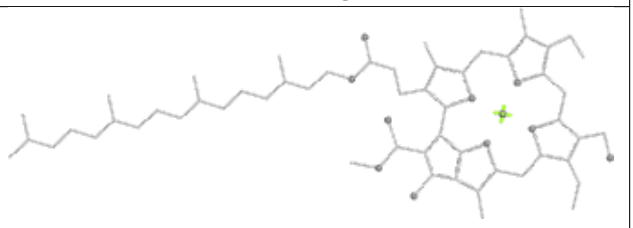
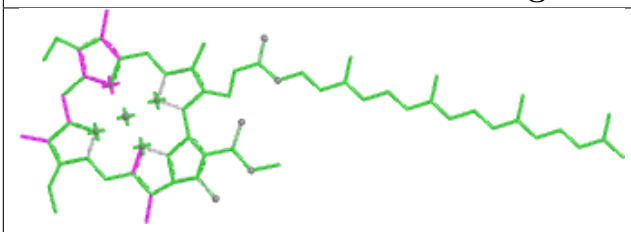


Rings

Ligand CLA 3 307



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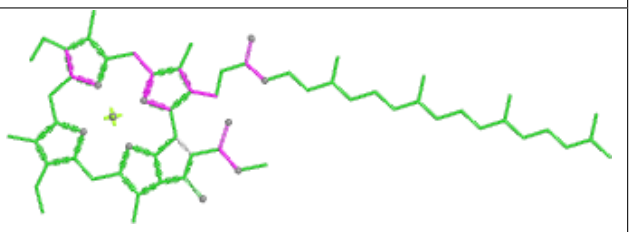

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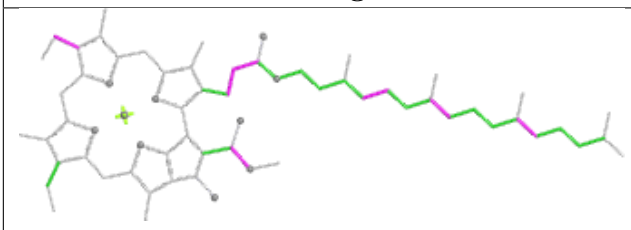

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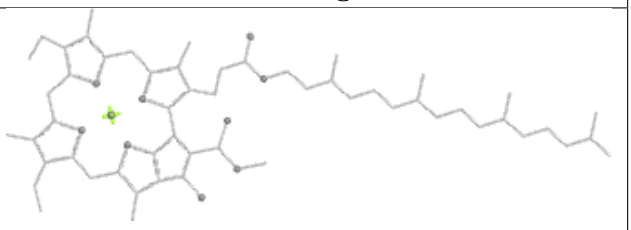
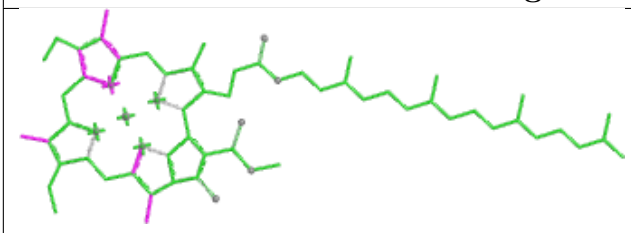


Rings

Ligand CLA C 503



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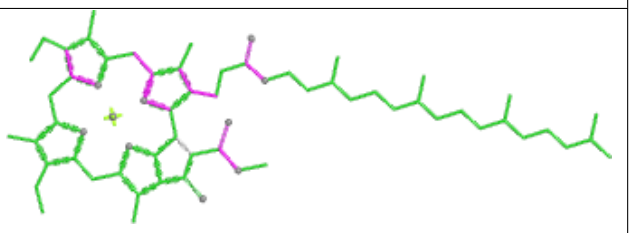
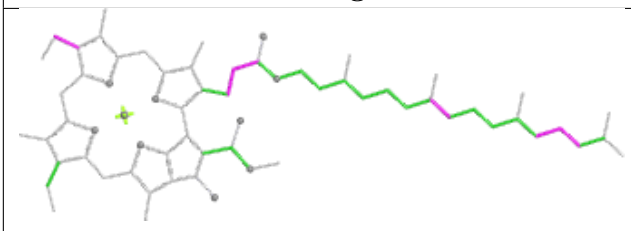


Bond angles



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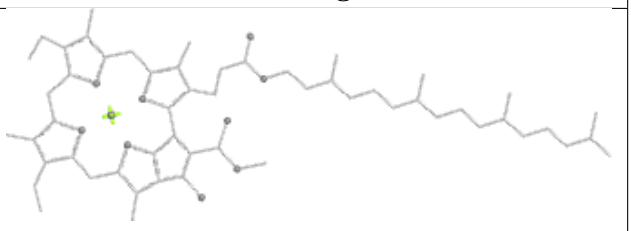
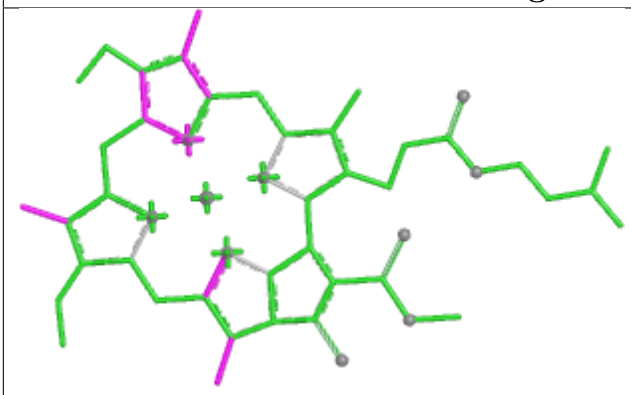


Rings

Ligand CLA 5 303



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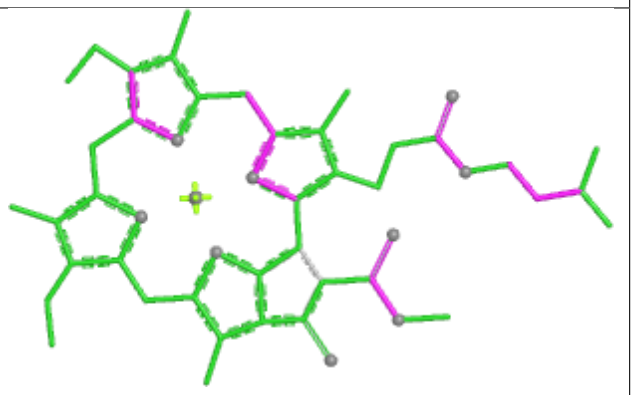
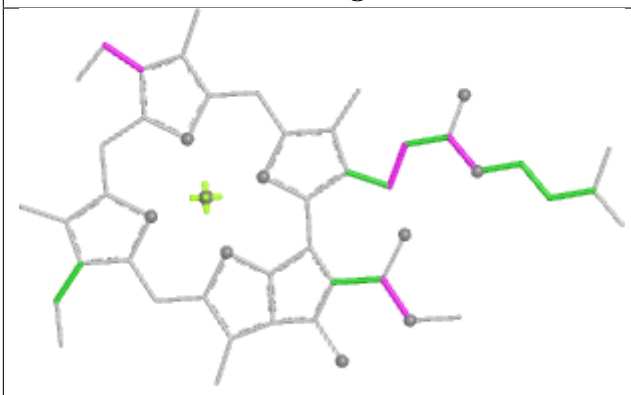


Bond angles



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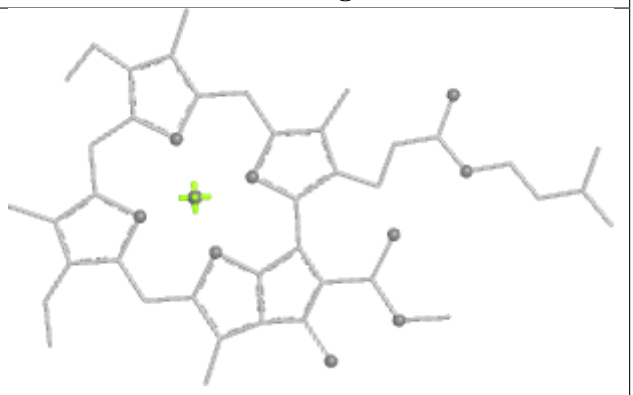
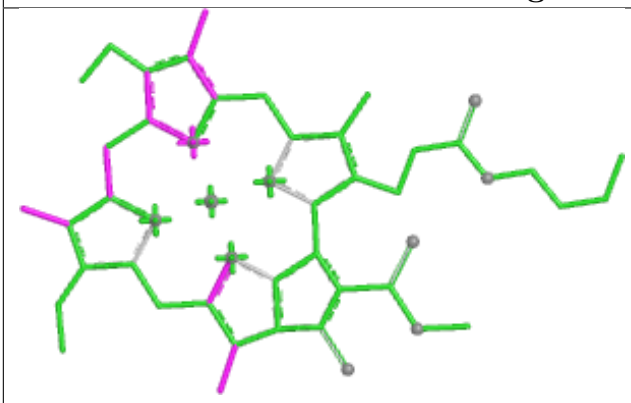


Rings

Ligand CLA S 309



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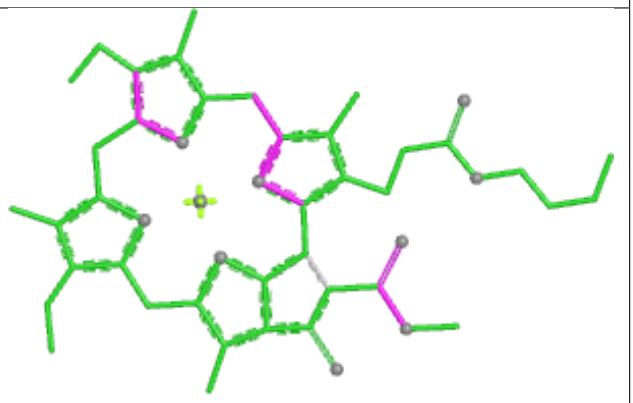
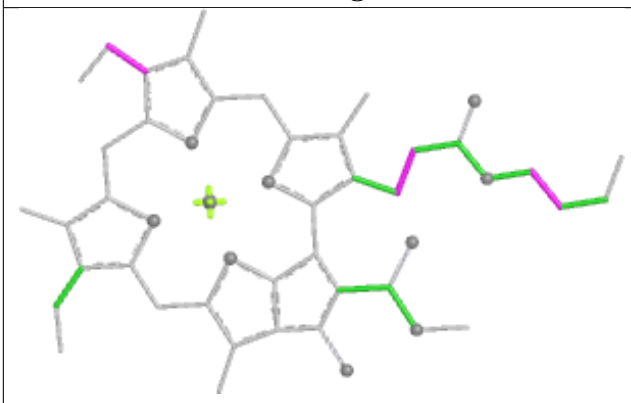


Bond angles



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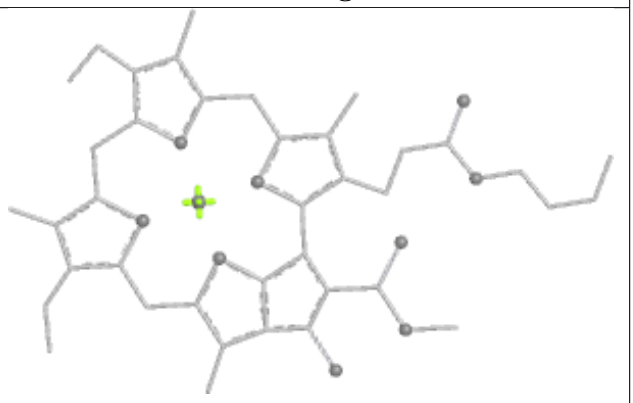
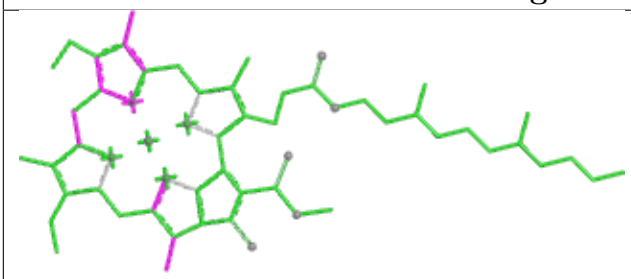


Rings

Ligand CLA r 605



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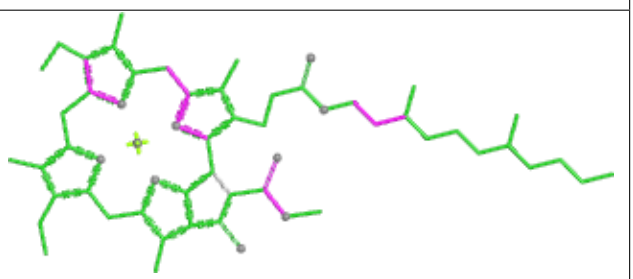
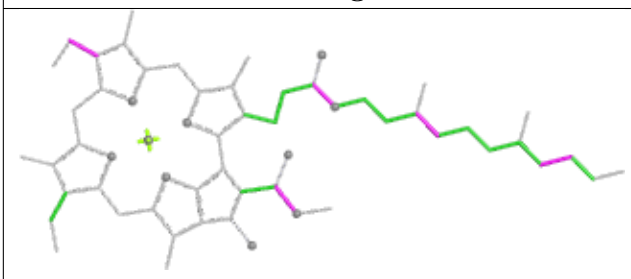


Bond angles



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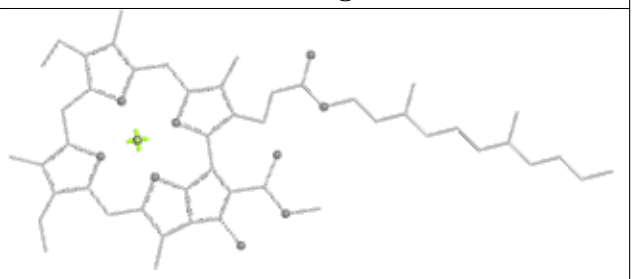
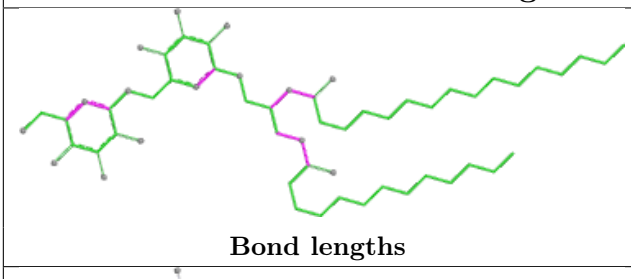


Rings

Ligand DGD A 414



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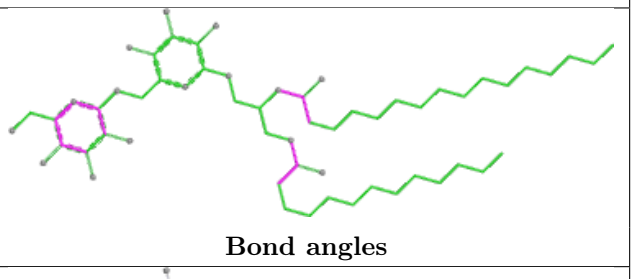
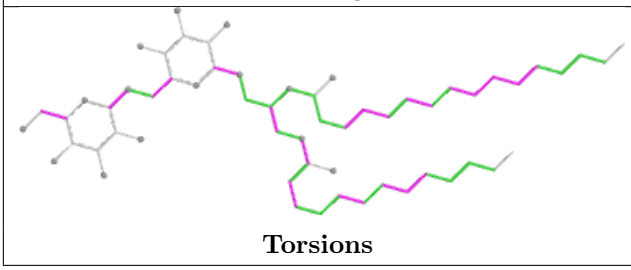


Bond angles



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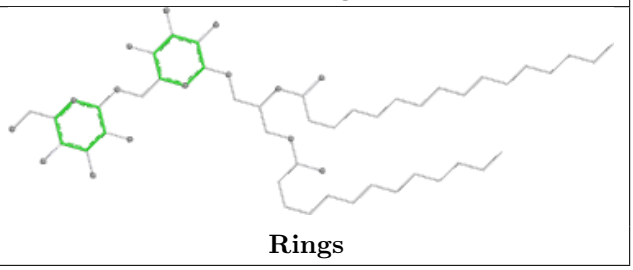
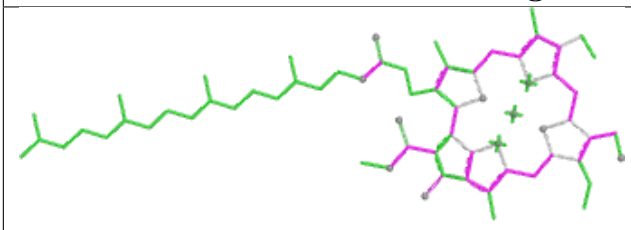


Rings

Ligand CHL u 313



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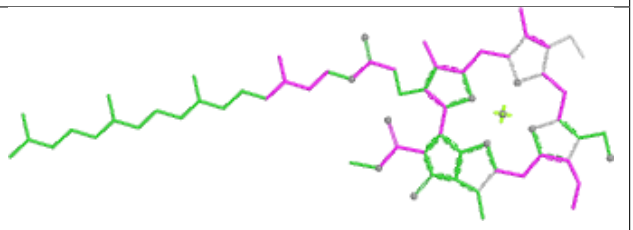
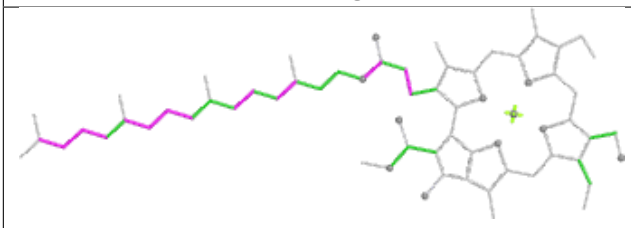


Bond angles



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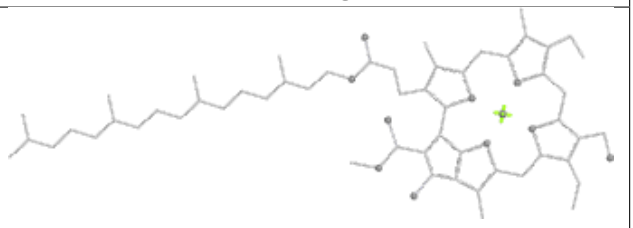
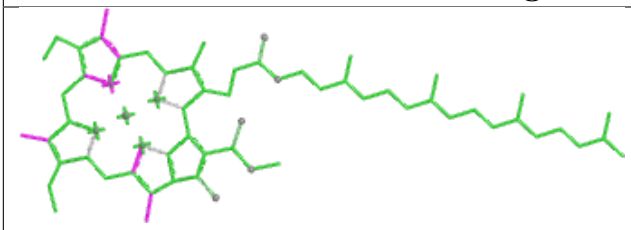


Rings

Ligand CLA U 307



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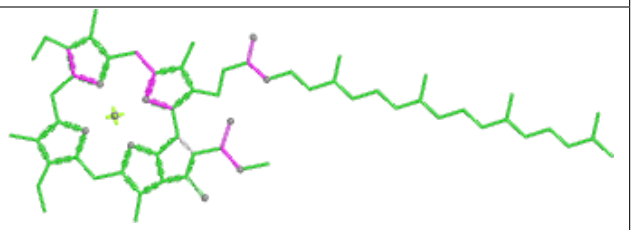
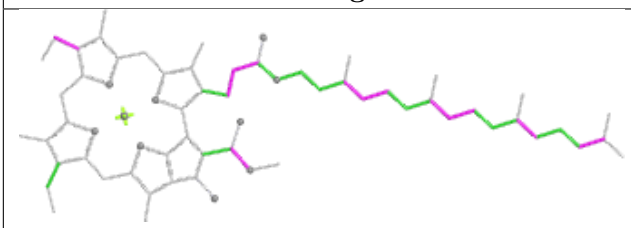


Bond angles



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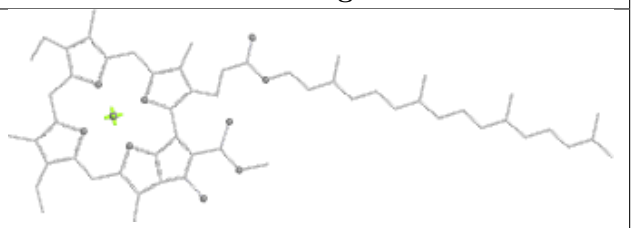
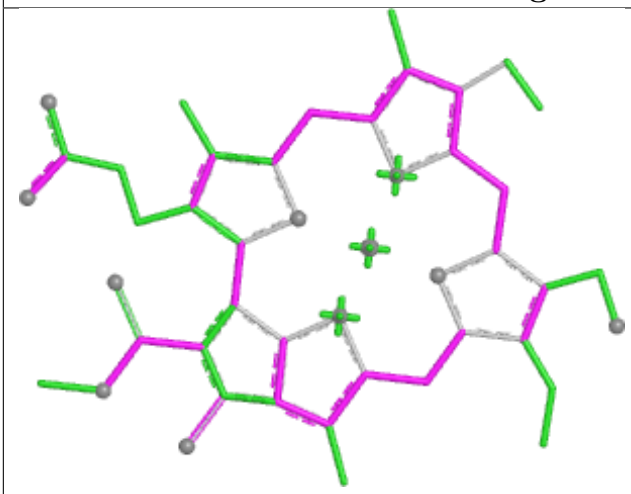


Rings

Ligand CHL s 316



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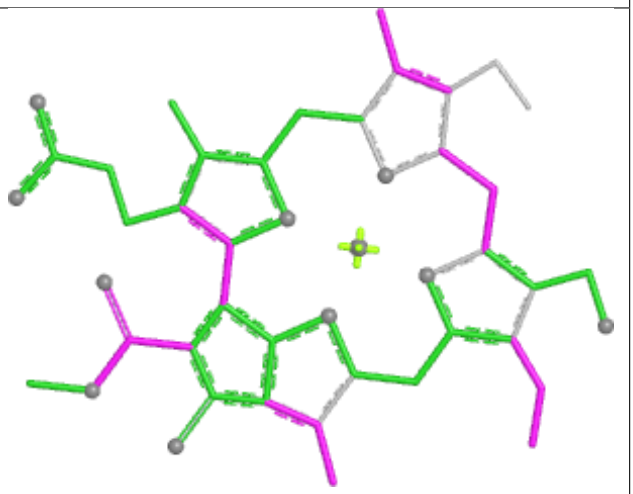
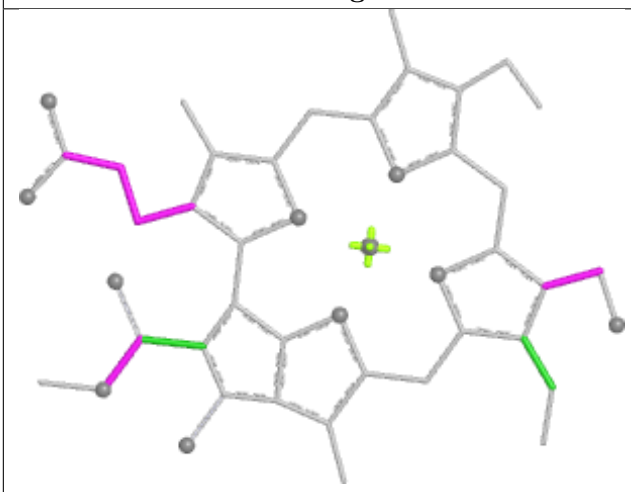


Bond angles



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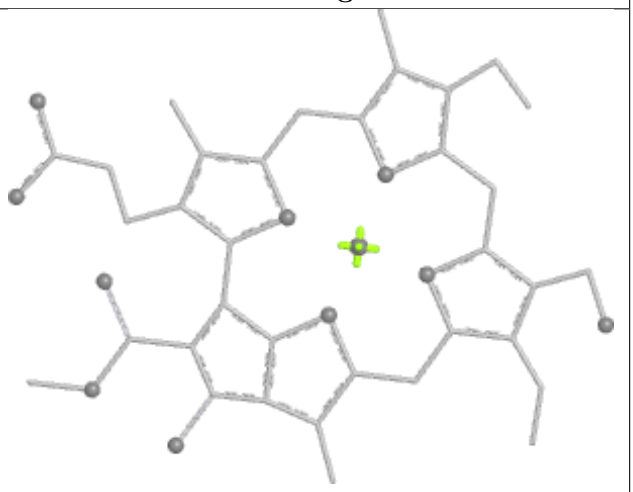
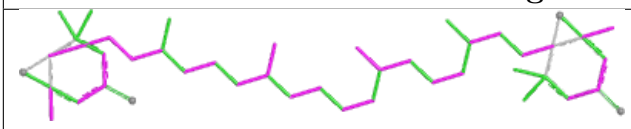


Rings

Ligand XAT u 311



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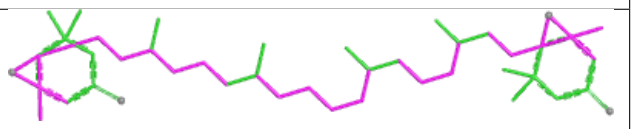
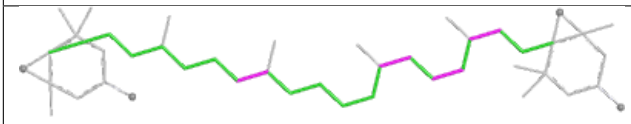


Bond angles



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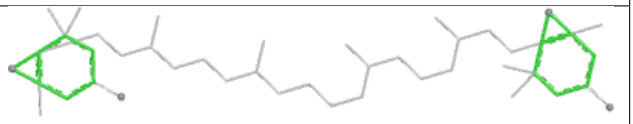
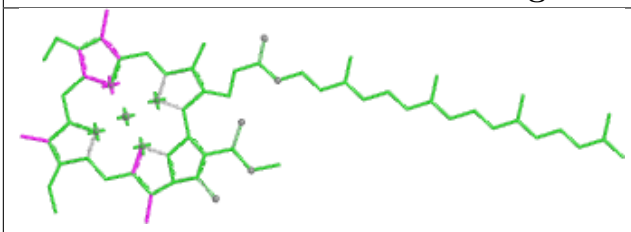


Rings

Ligand CLA 3 302



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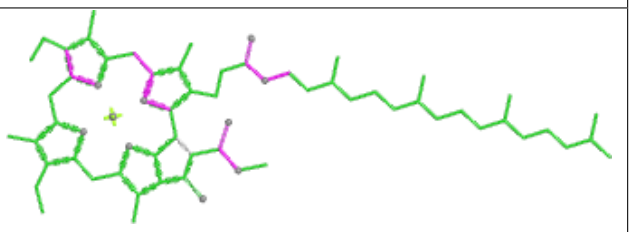
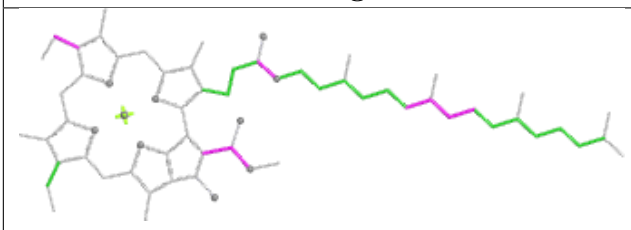
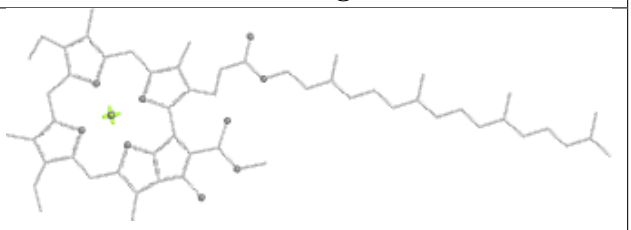


Bond angles

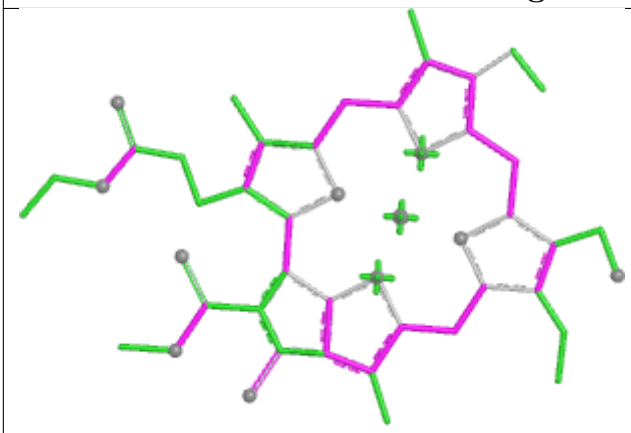


Torsions



Rings

Ligand CHL g 312



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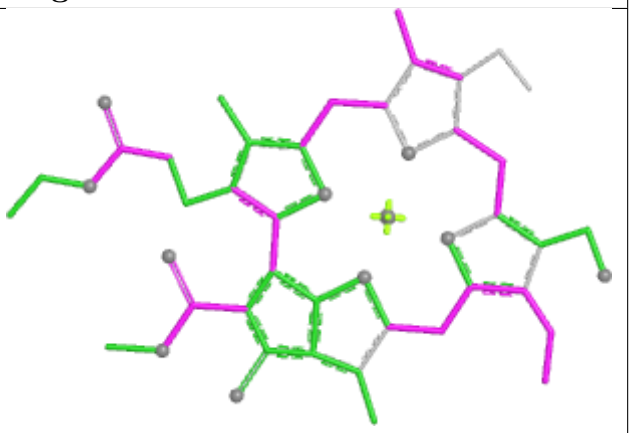

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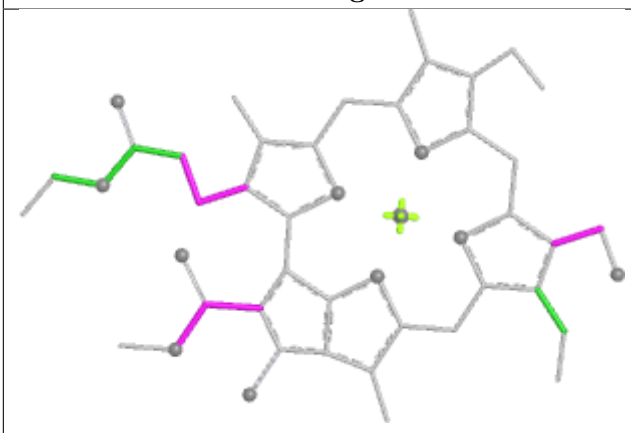

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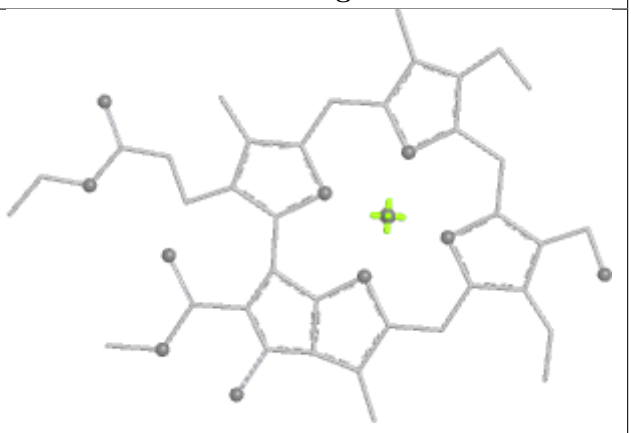
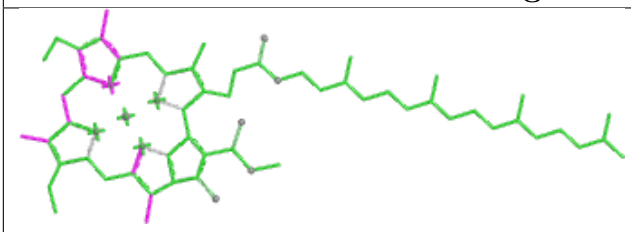


Rings

Ligand CLA Q 301



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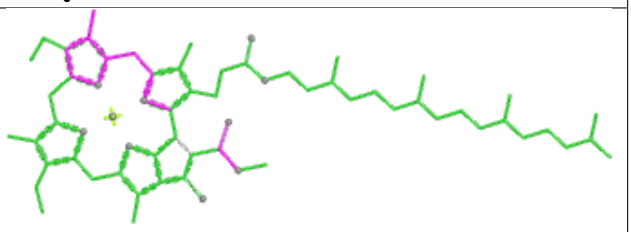

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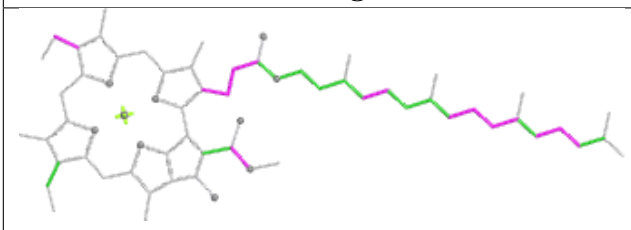

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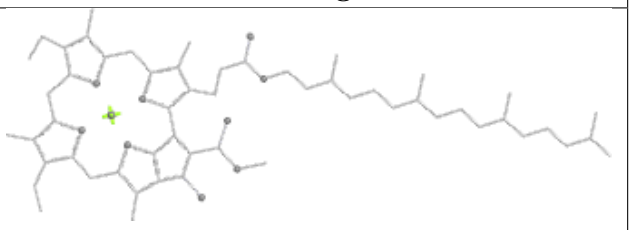
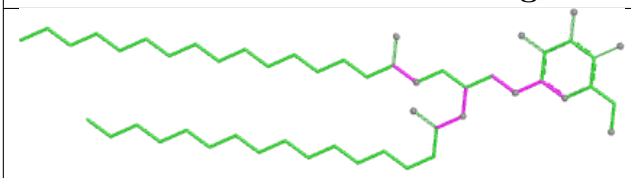


Rings

Ligand LMG B 621



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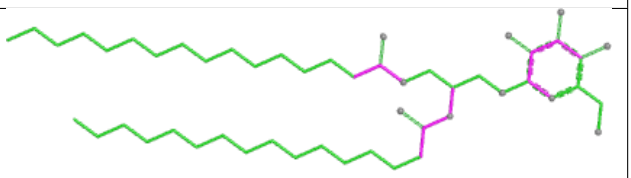
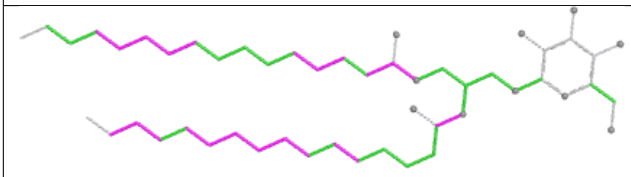


Bond angles



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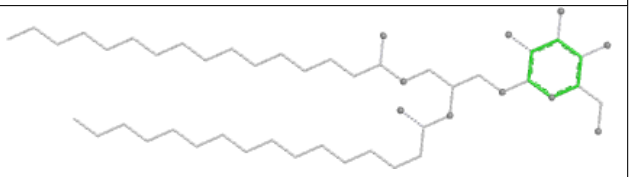
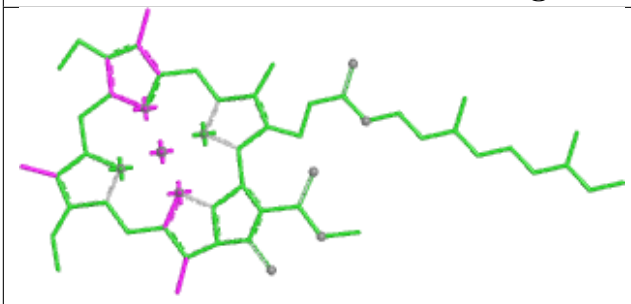


Rings

Ligand CLA s 306



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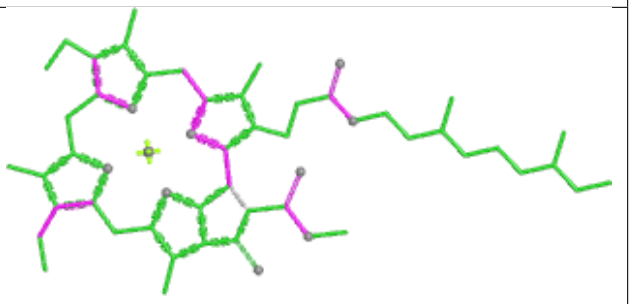
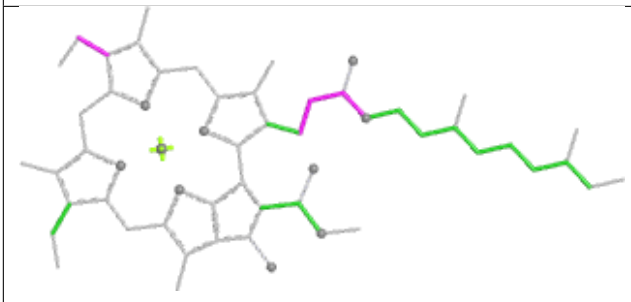


Bond angles



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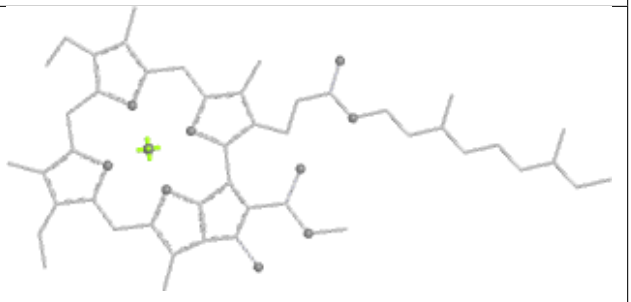
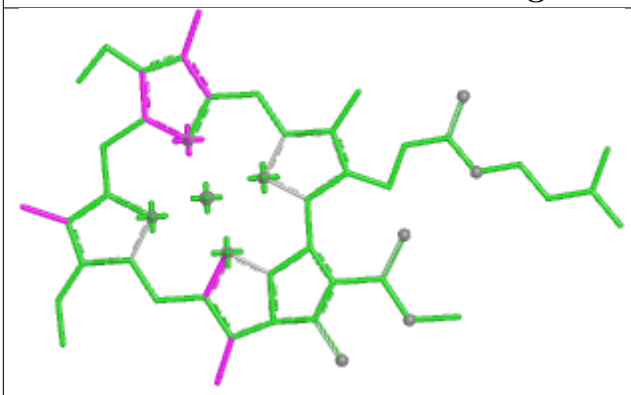


Rings

Ligand CLA p 304



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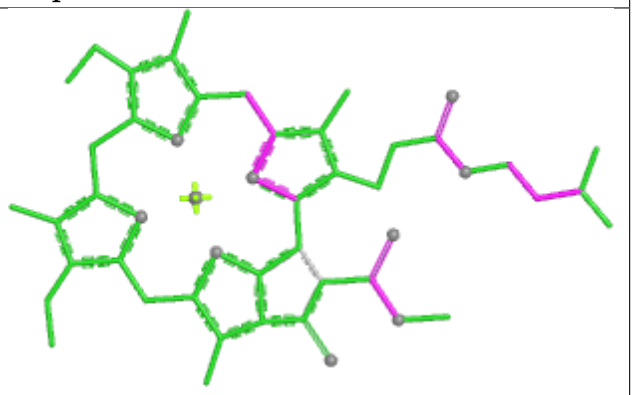
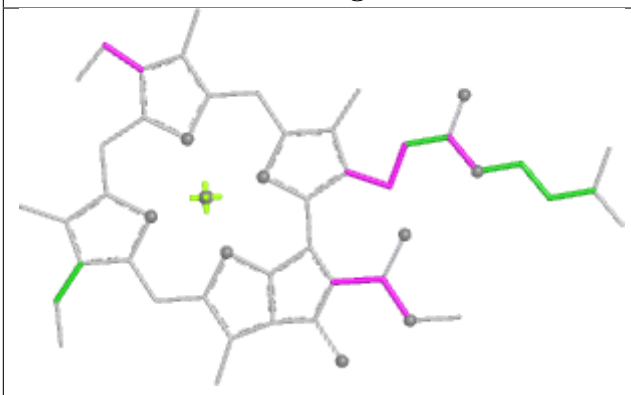


Bond angles



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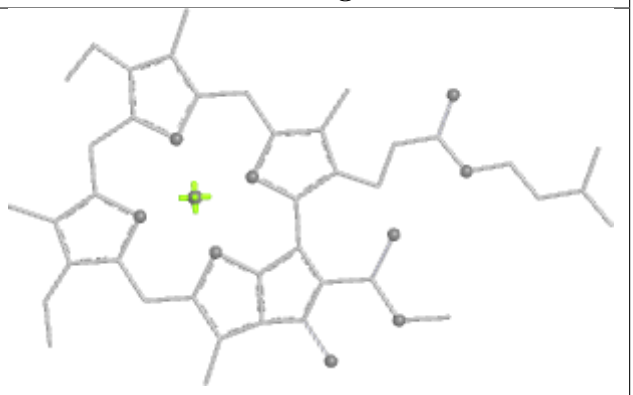
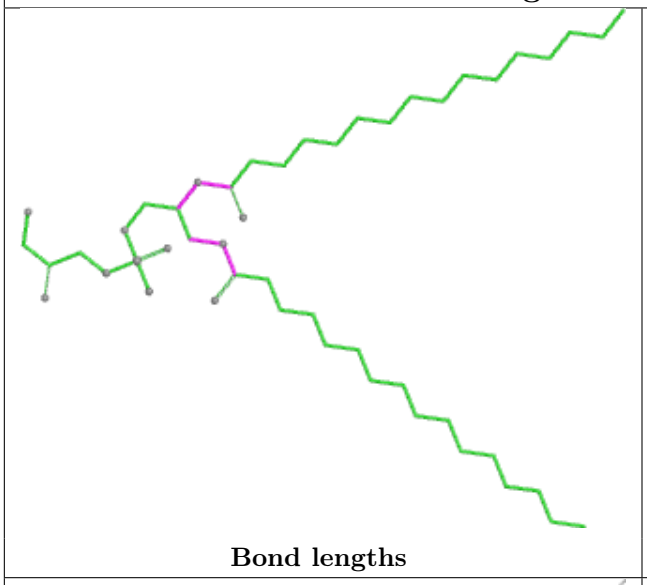


Rings

Ligand LHG Q 310



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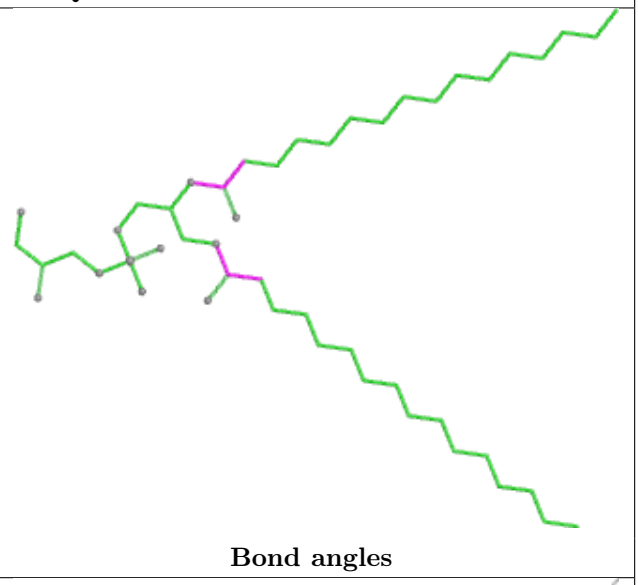
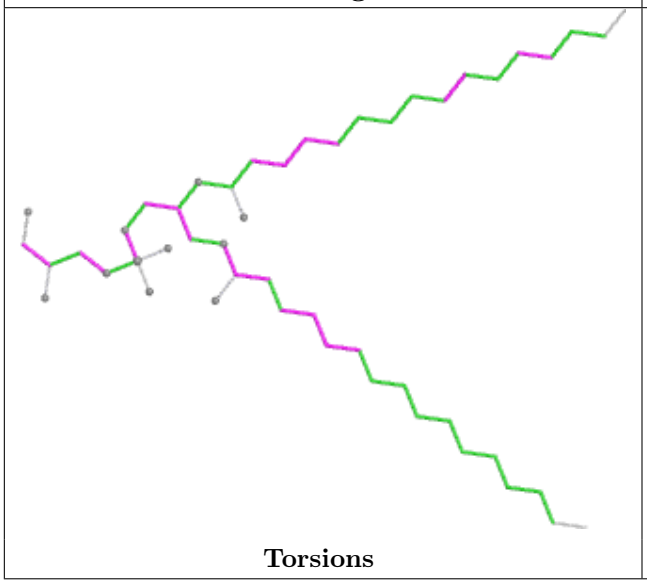


Bond angles



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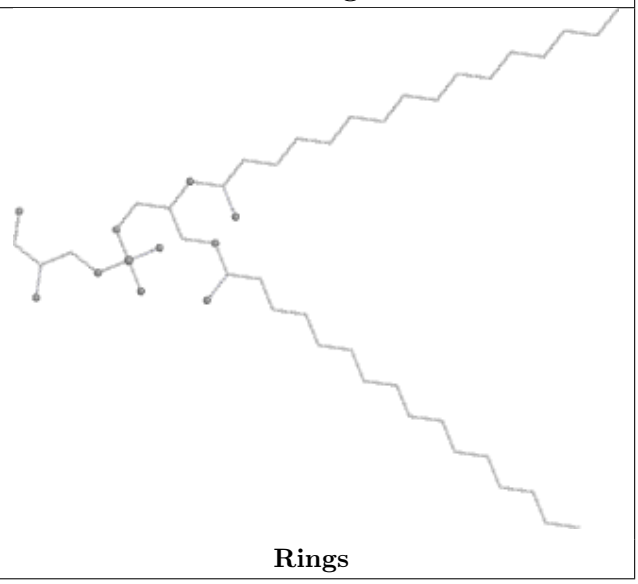
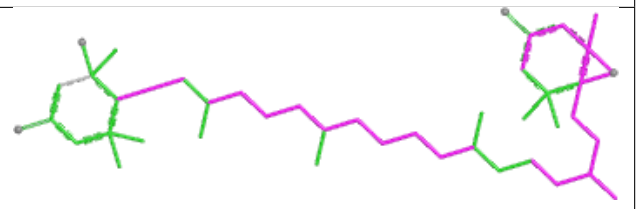


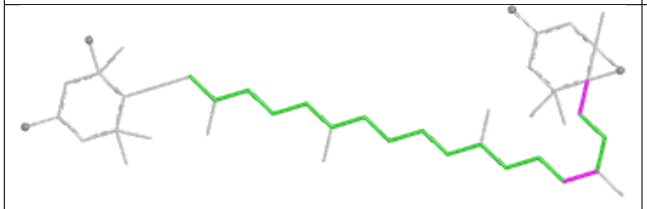
Rings

Ligand NEX U 318

Bond lengths



Bond angles



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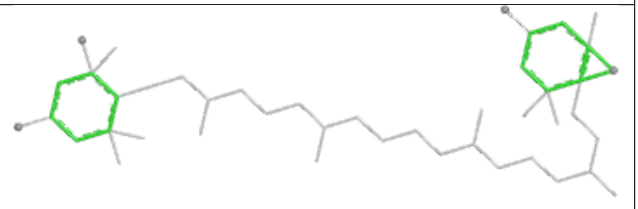
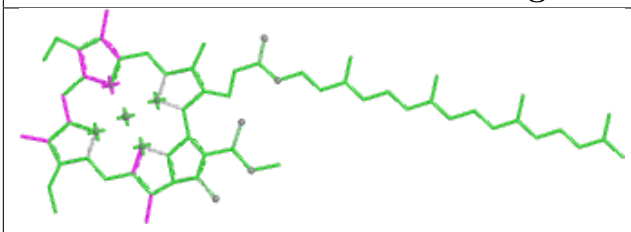


Rings

Ligand CLA 6 302



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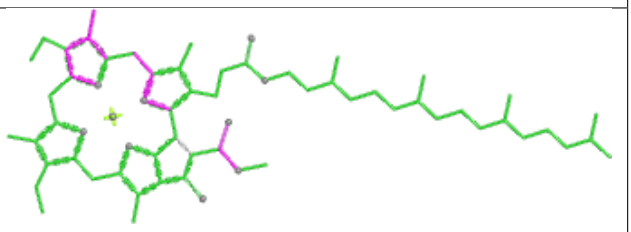
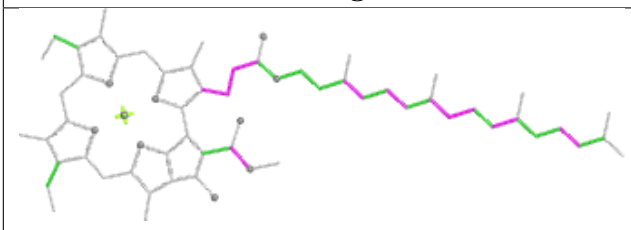


Bond angles



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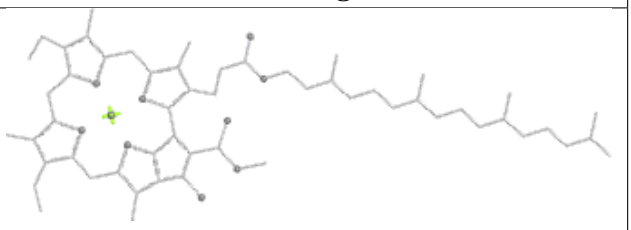
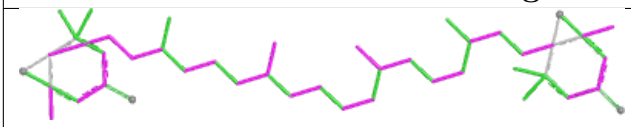


Rings

Ligand XAT N 311



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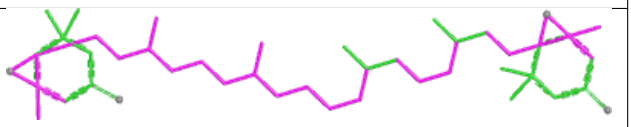
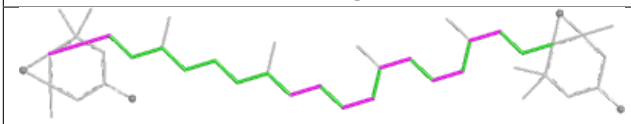


Bond angles



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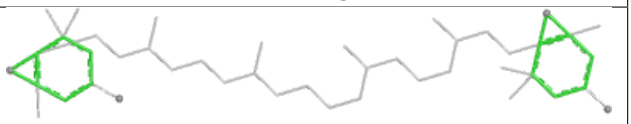
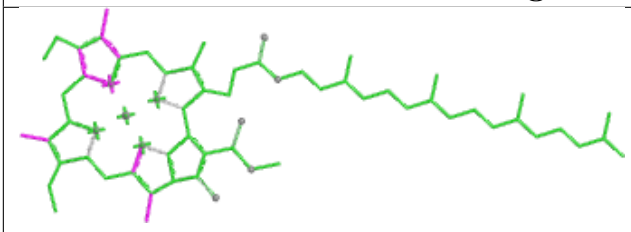


Rings

Ligand CLA p 303



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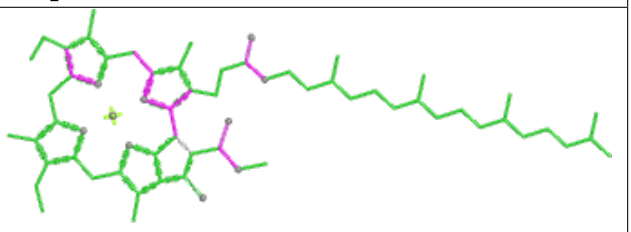
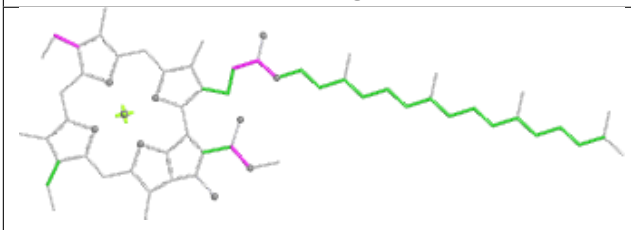


Bond angles



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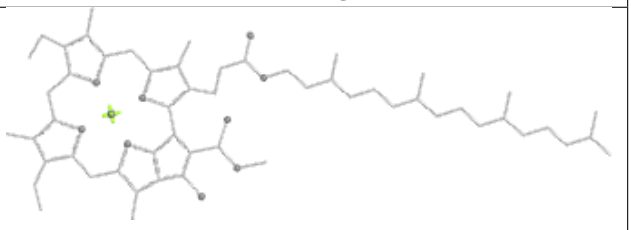
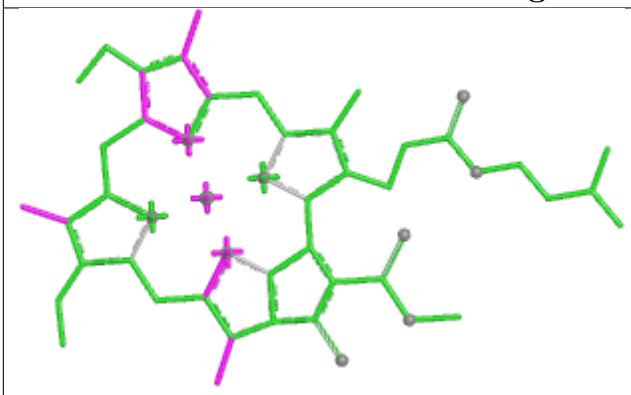


Rings

Ligand CLA 1 303



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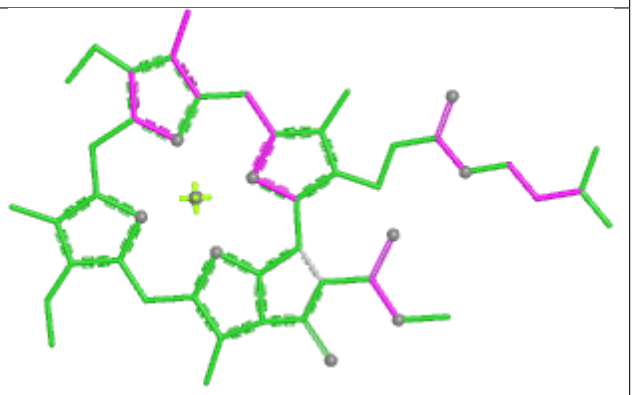
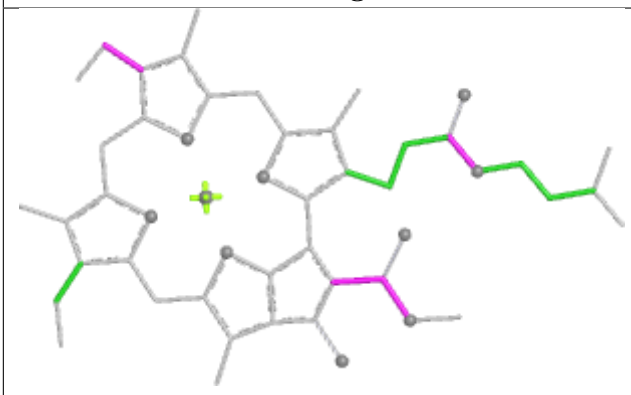


Bond angles



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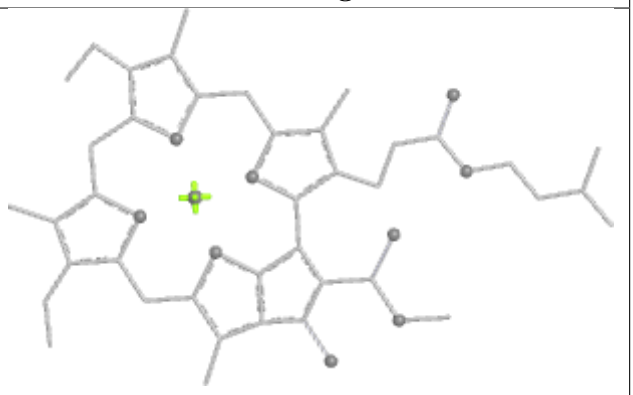
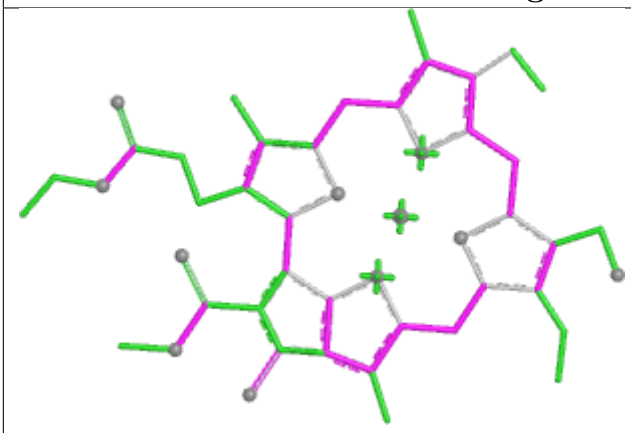


Rings

Ligand CHL u 314



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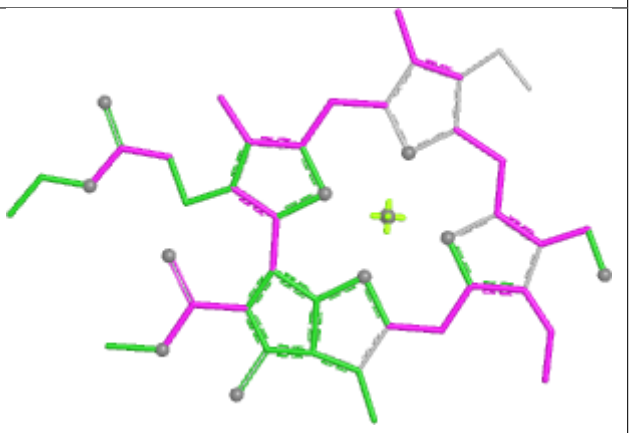
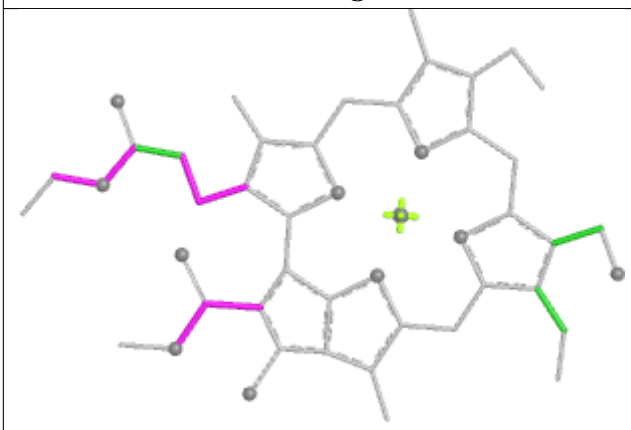


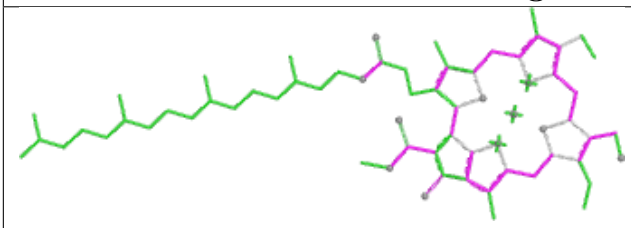
Bond angles



Torsions

Rings

Ligand CHL q 311



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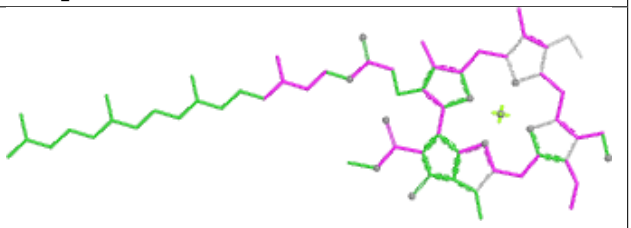
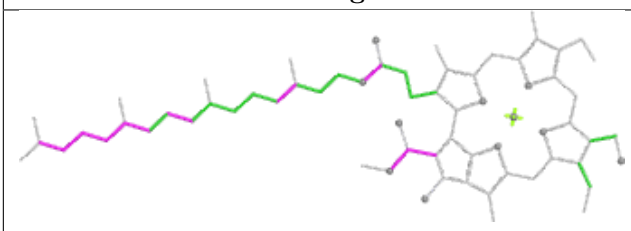
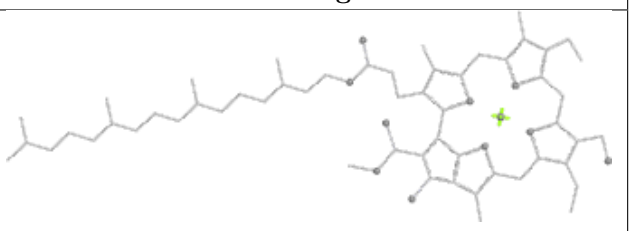


Bond angles

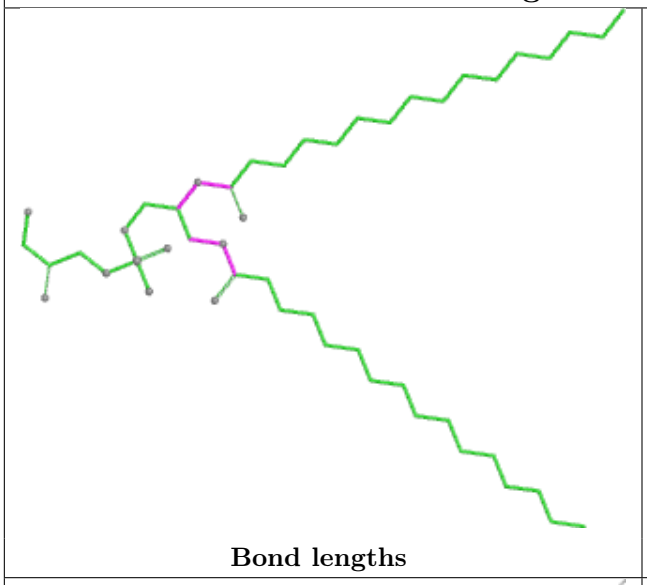


Torsions



Rings

Ligand LHG N 312



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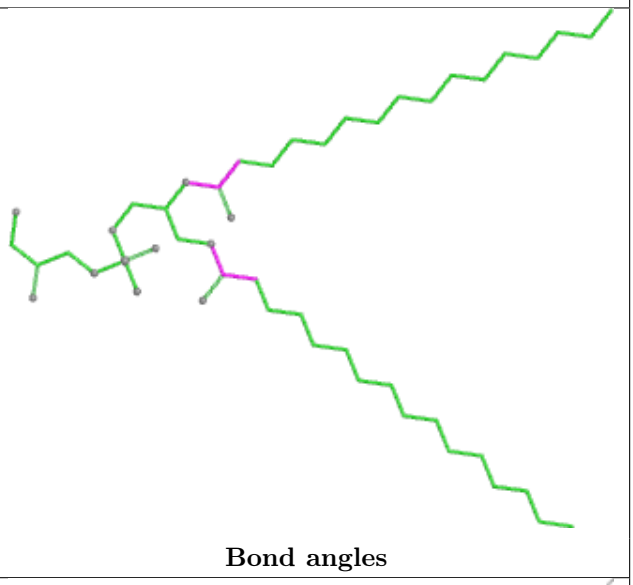
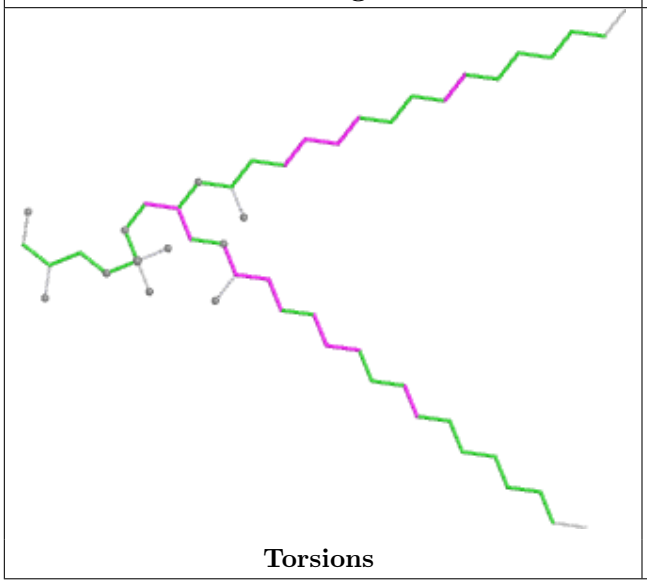


Bond angles



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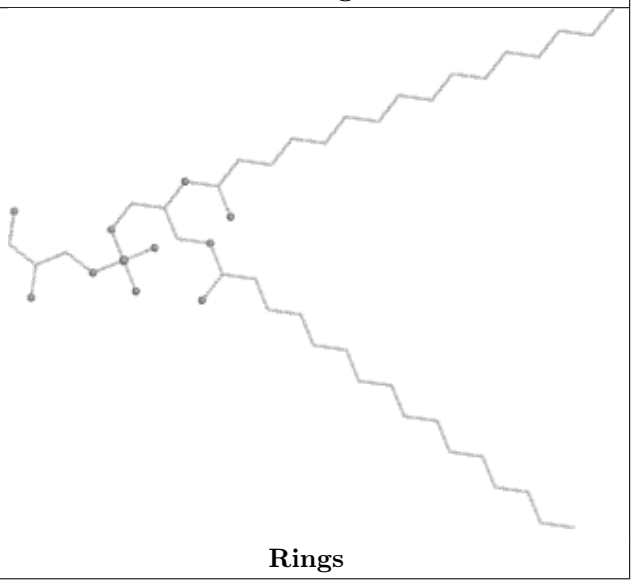
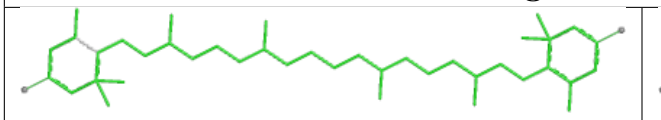
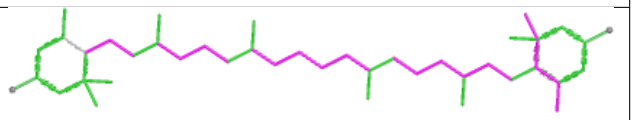


Rings

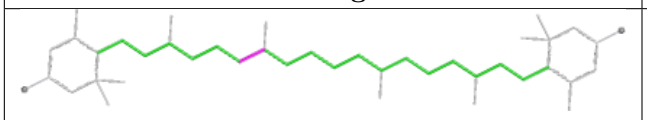
Ligand LUT N 309



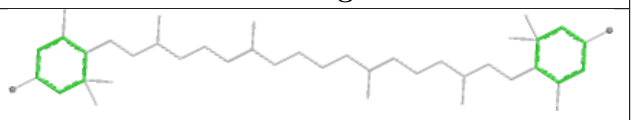
Bond lengths



Bond angles

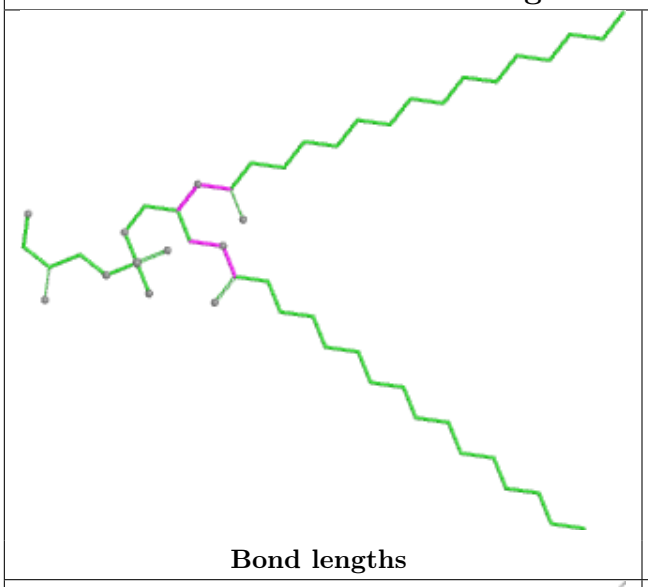


Torsions



Rings

Ligand LHG P 313



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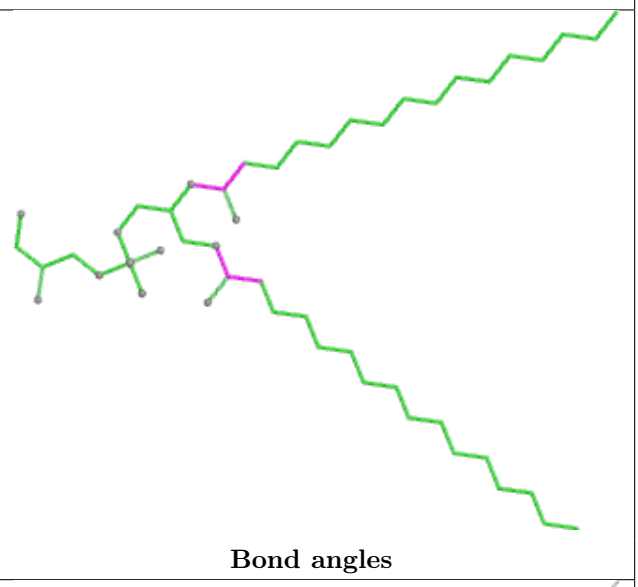
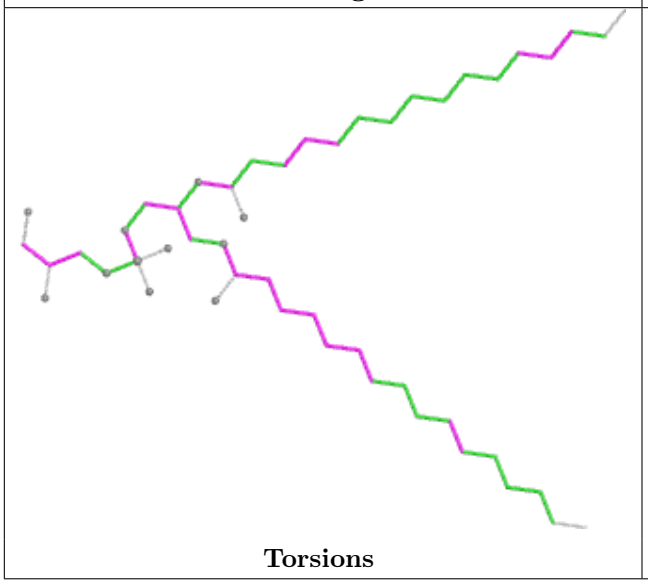
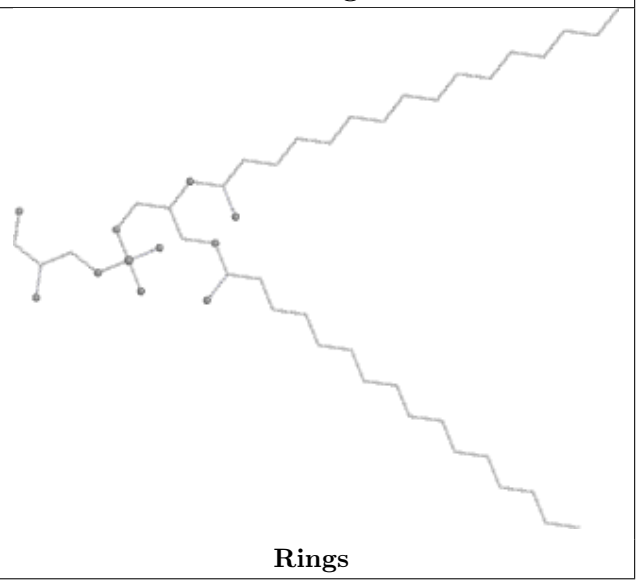


Bond angles

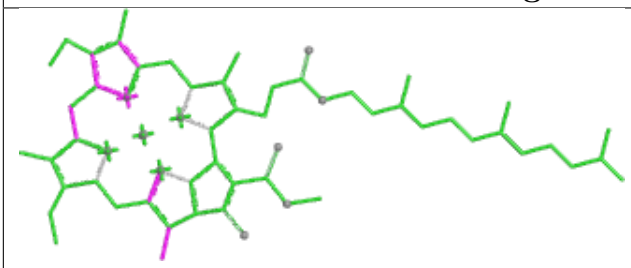


Torsions



Rings

Ligand CLA N 306



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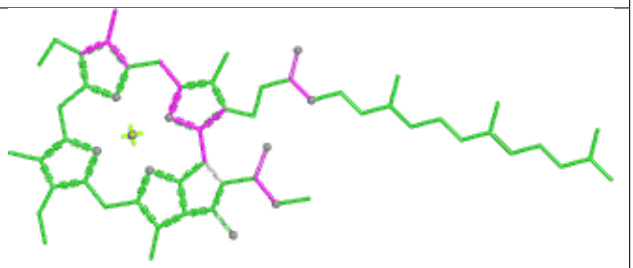
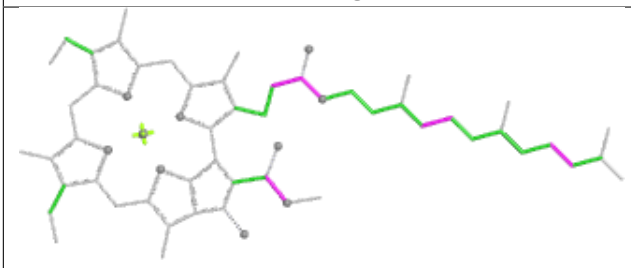


Bond angles



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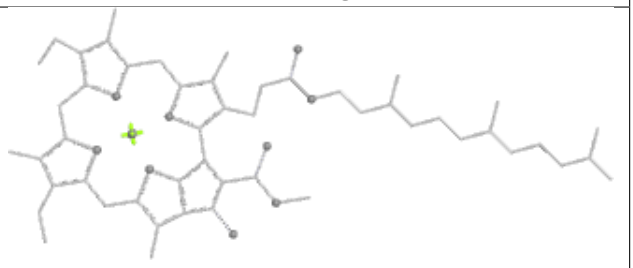
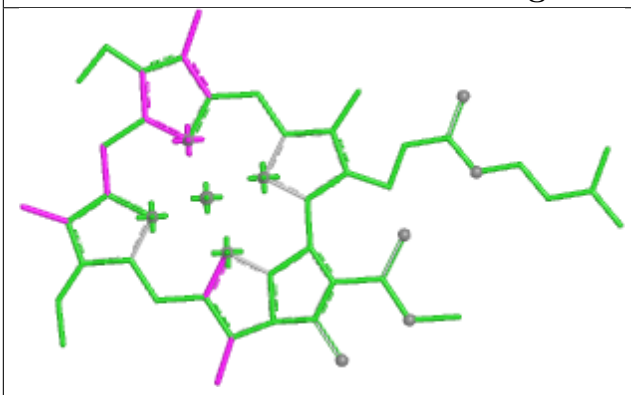


Rings

Ligand CLA g 303



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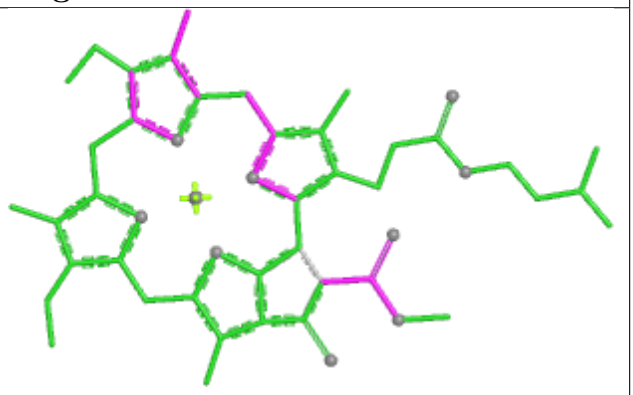
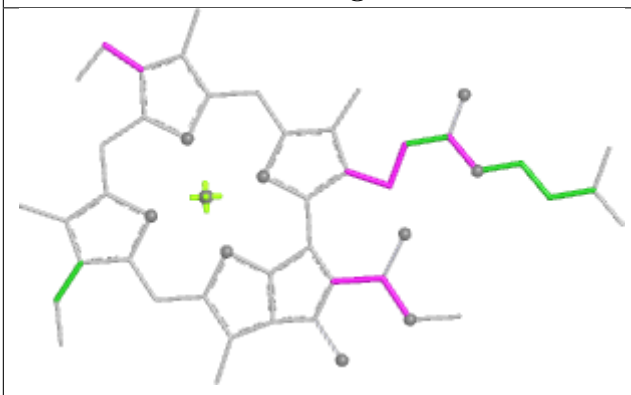


Bond angles



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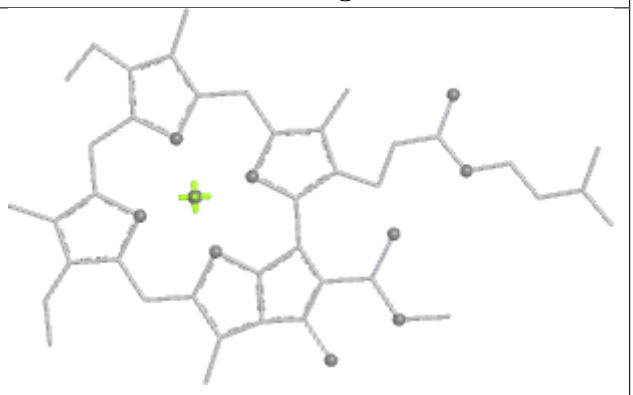
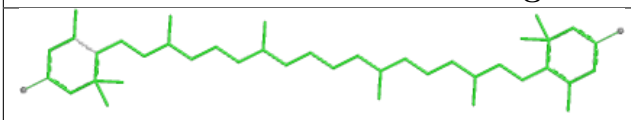


Rings

Ligand LUT U 309



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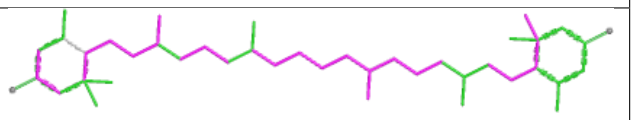
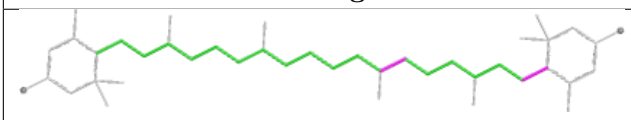


Bond angles



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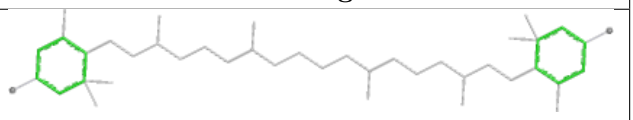
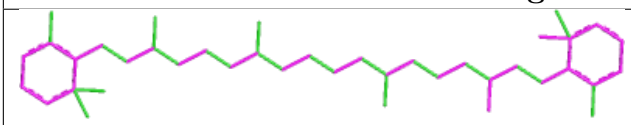


Rings

Ligand BCR c 515



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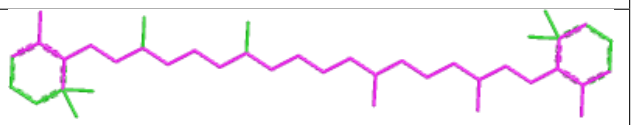
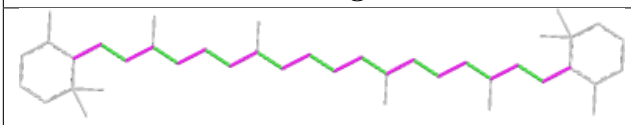
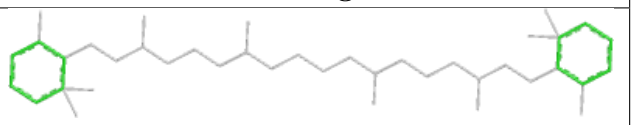


Bond angles

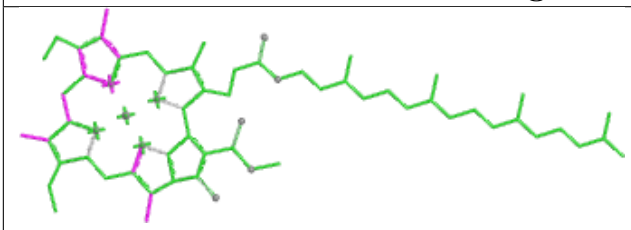


Torsions



Rings

Ligand CLA v 301



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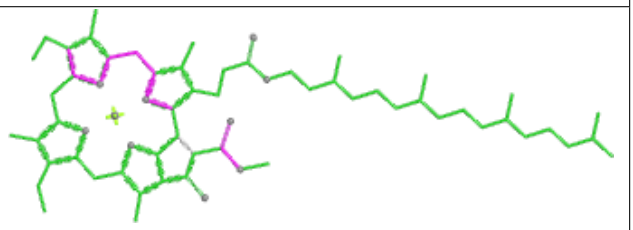
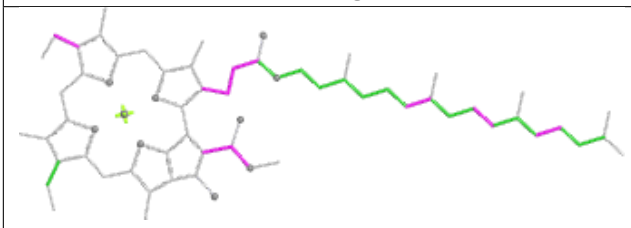


Bond angles



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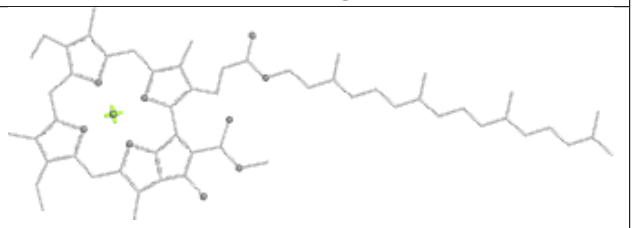
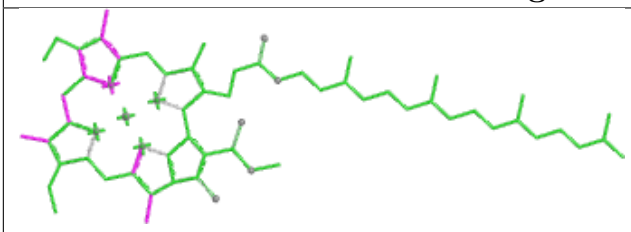


Rings

Ligand CLA 2 304



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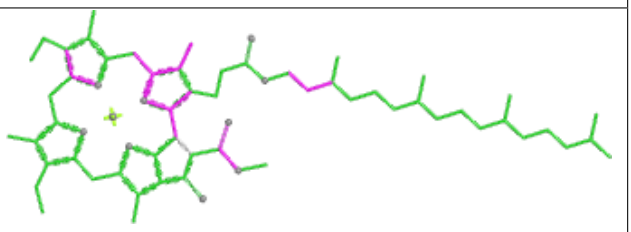
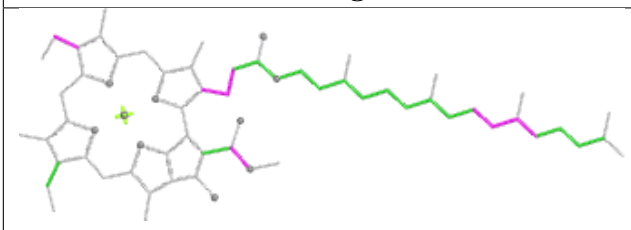


Bond angles



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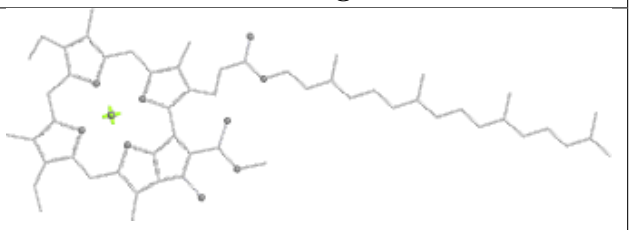
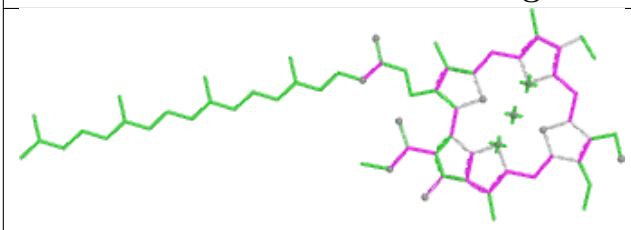


Rings

Ligand CHL G 314



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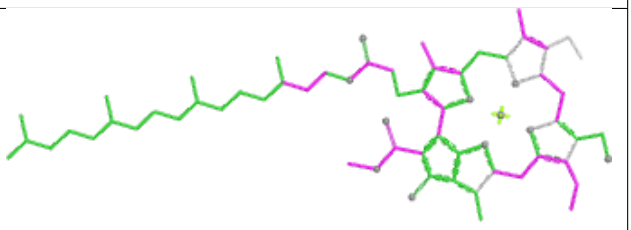
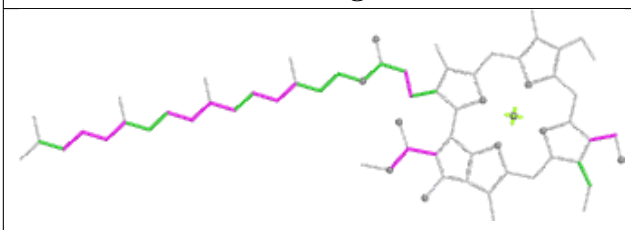
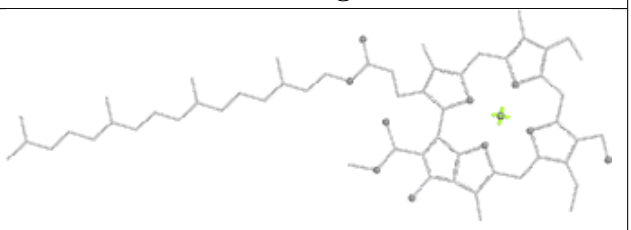


Bond angles

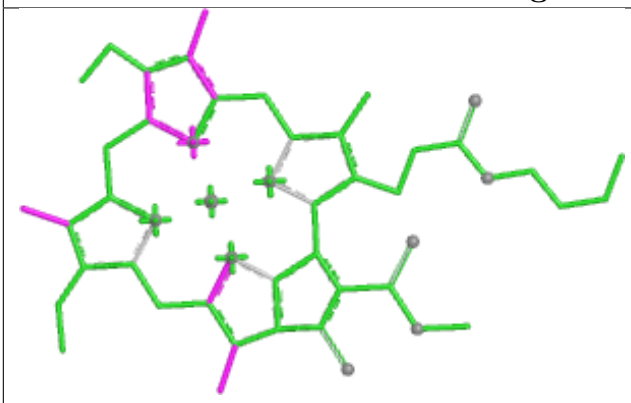


Torsions



Rings

Ligand CLA s 307



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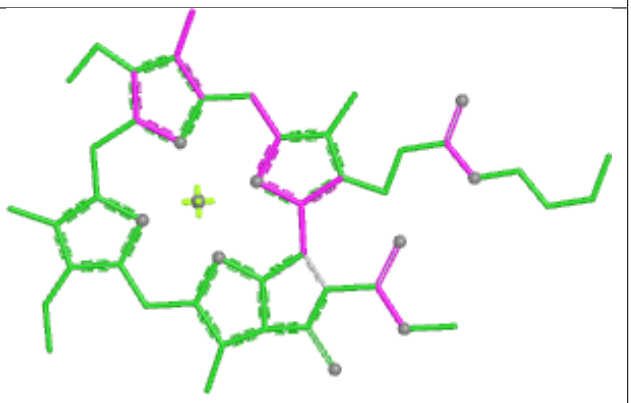
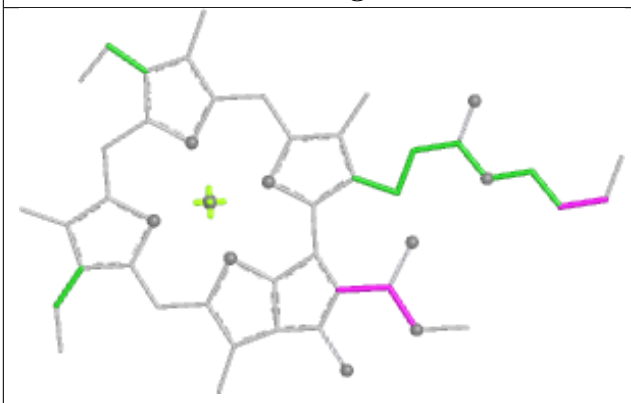


Bond angles



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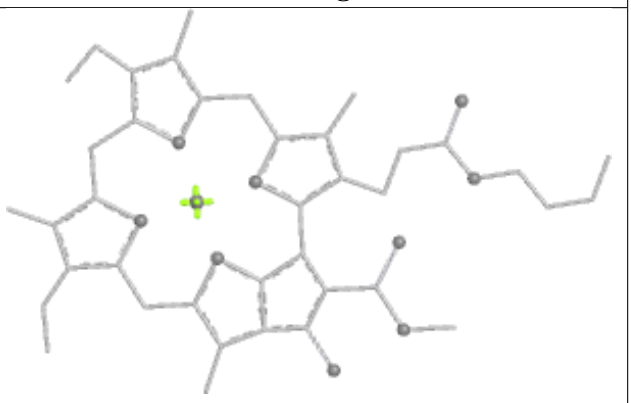
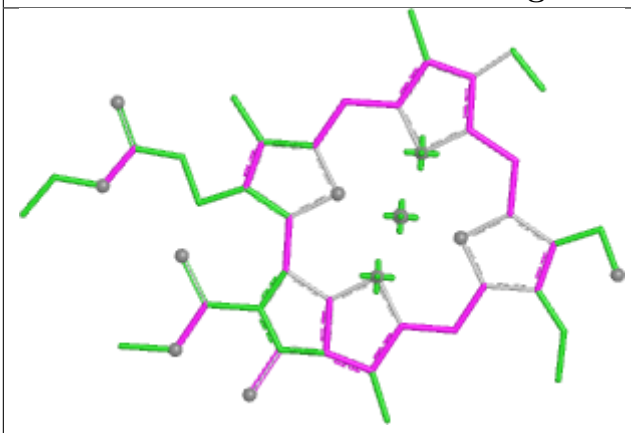


Rings

Ligand CHL 4 314



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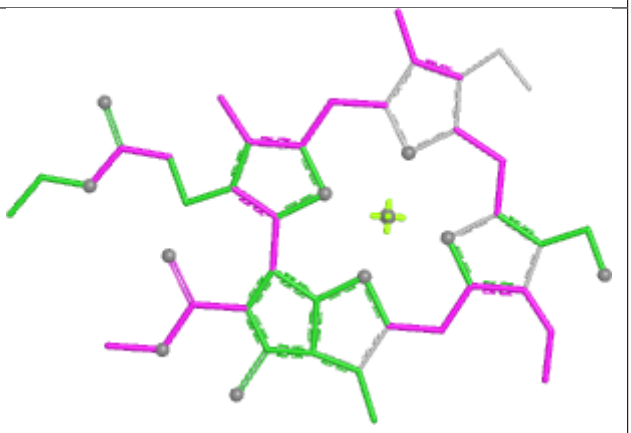
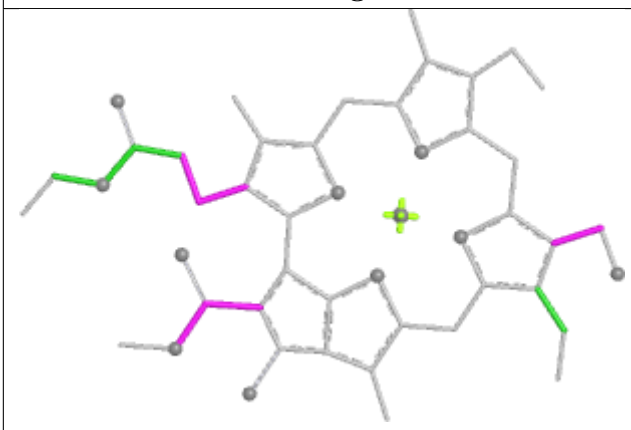


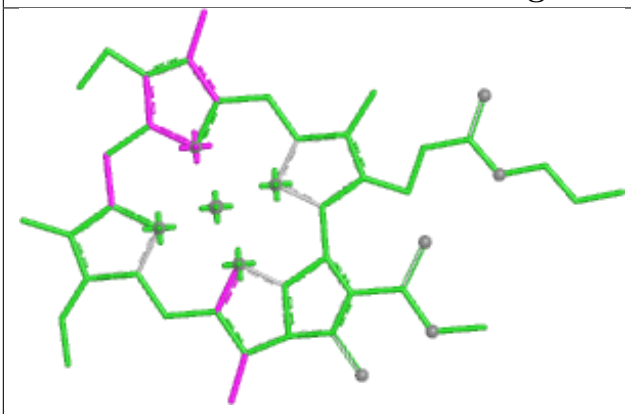
Bond angles



Torsions

Rings

Ligand CLA v 308



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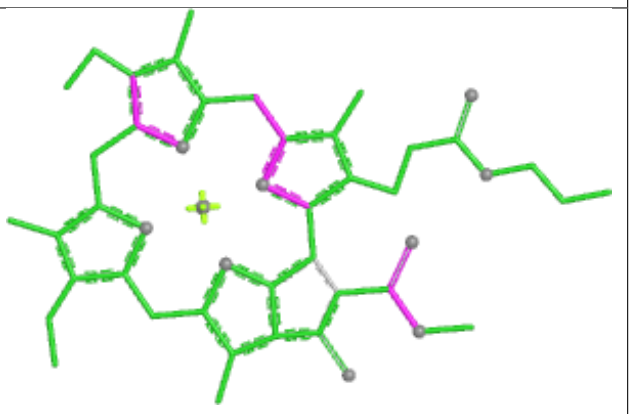
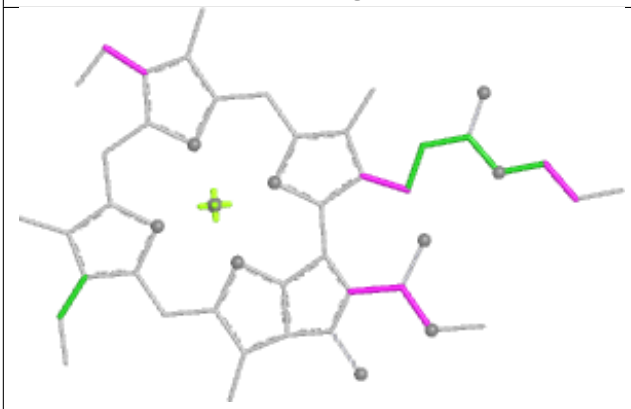
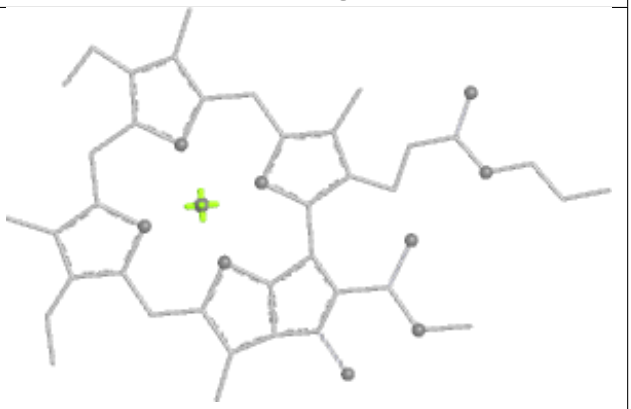


Bond angles

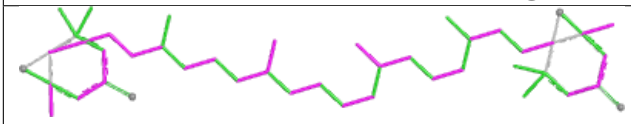


Torsions



Rings

Ligand XAT V 311



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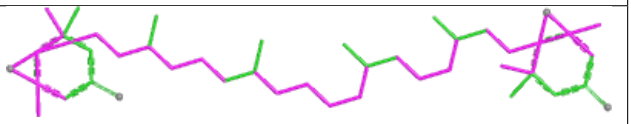
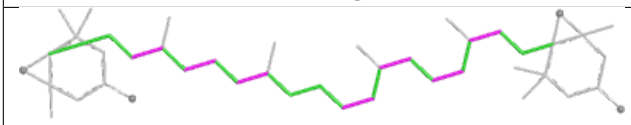
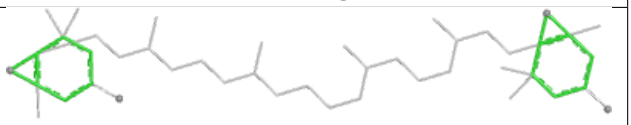


Bond angles

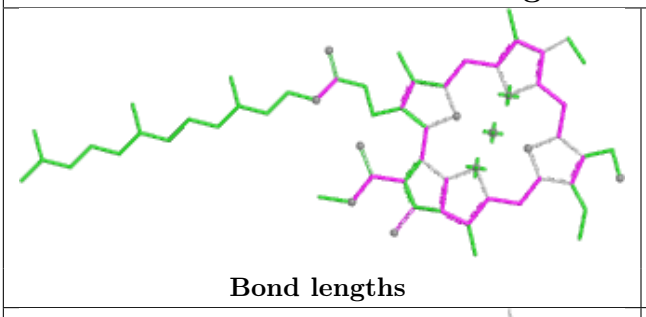


Torsions



Rings

Ligand CHL Q 316



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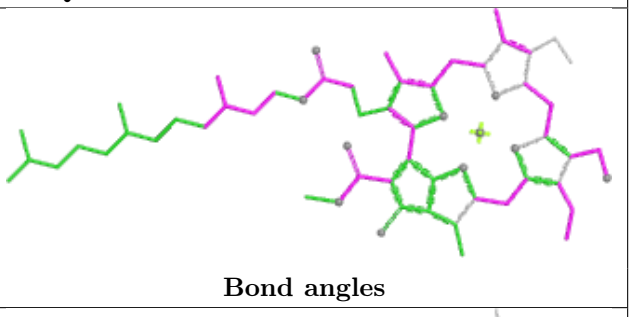
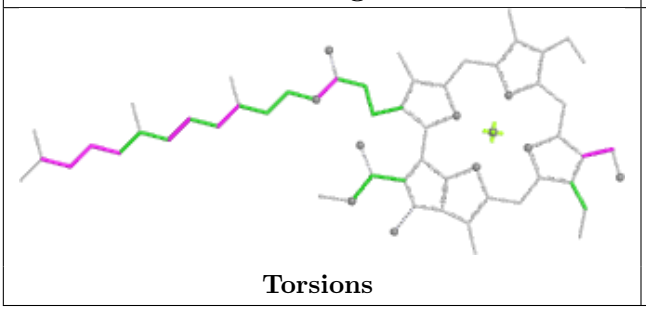
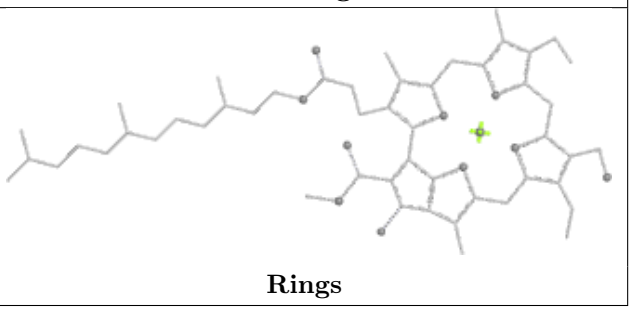


Bond angles



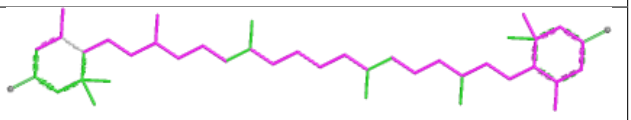
Torsions



Rings

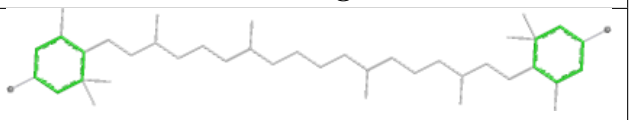
Ligand LUT P 310

Bond lengths



Bond angles

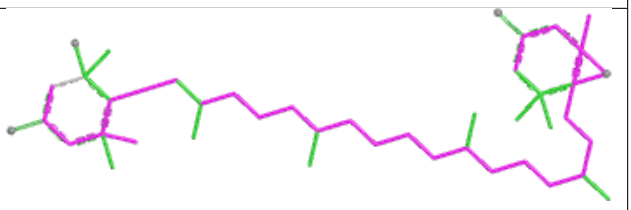
Torsions



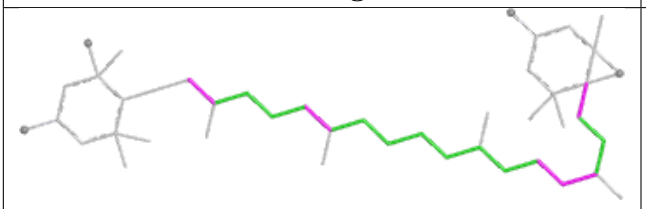
Rings

Ligand NEX u 319

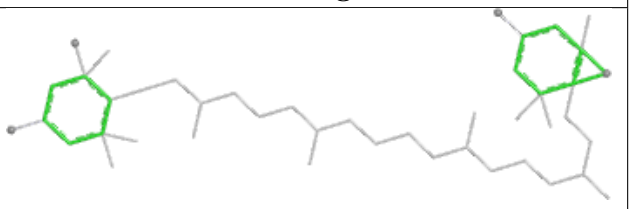
Bond lengths



Bond angles

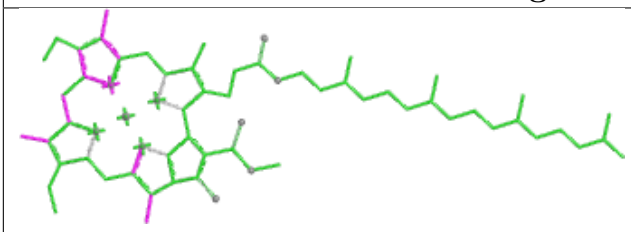


Torsions

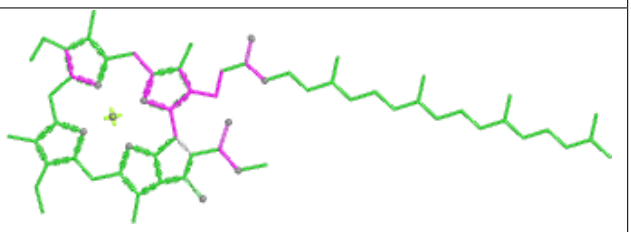


Rings

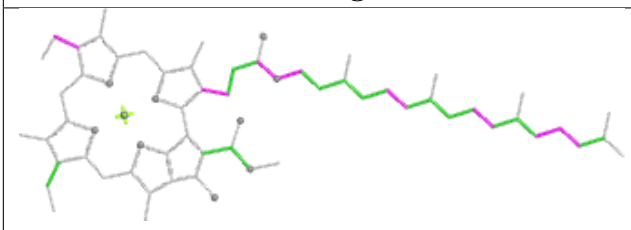
Ligand CLA c 514



Bond lengths



Bond angles



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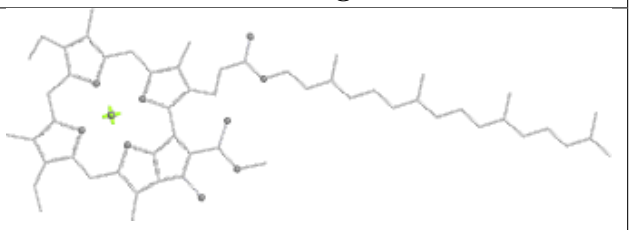

Rings

Ligand LUT P 311

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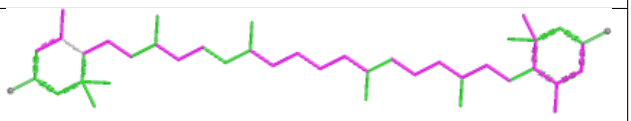
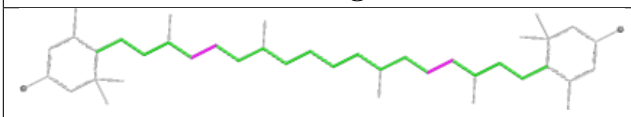


Bond angles



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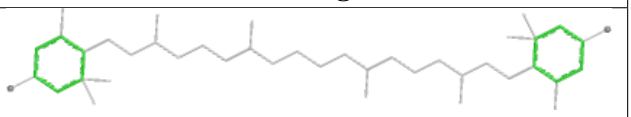
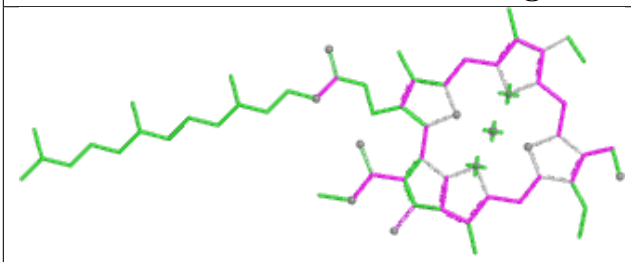


Rings

Ligand CHL R 317



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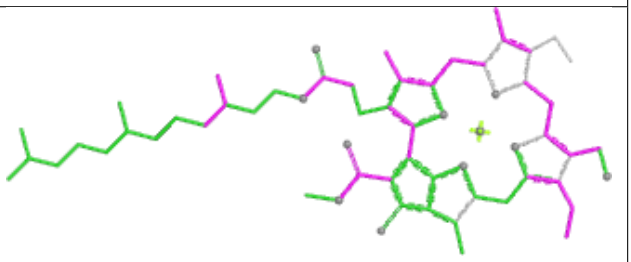
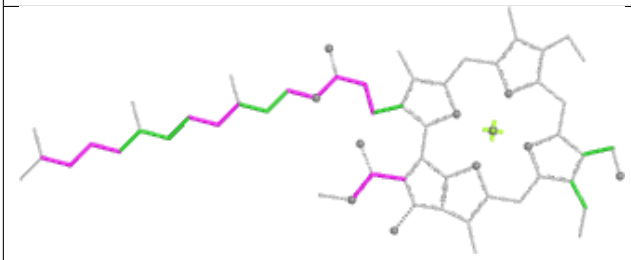


Bond angles



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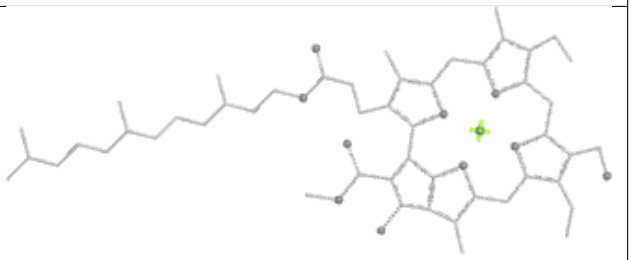
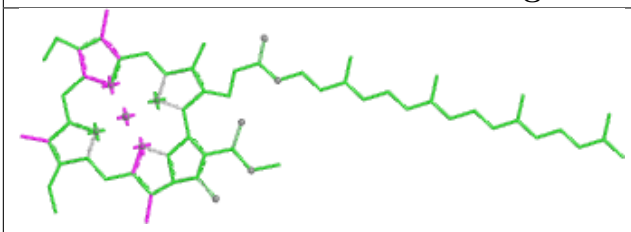


Rings

Ligand CLA A 405



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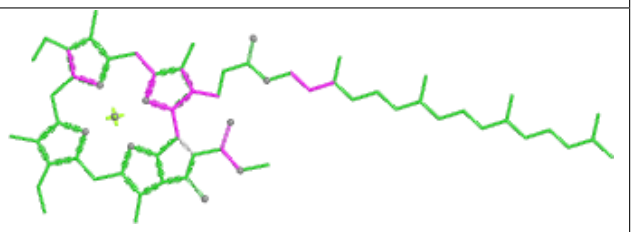
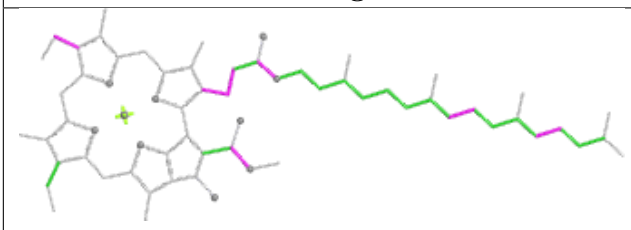


Bond angles



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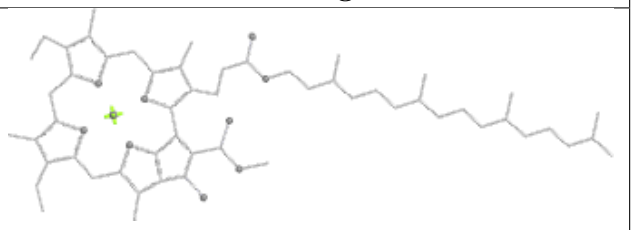
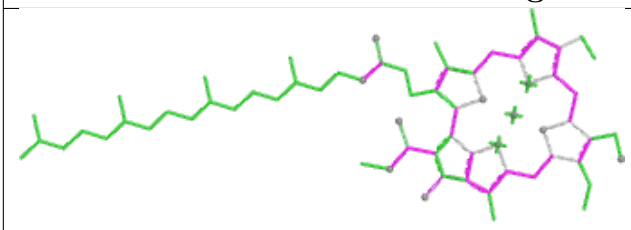


Rings

Ligand CHL p 320



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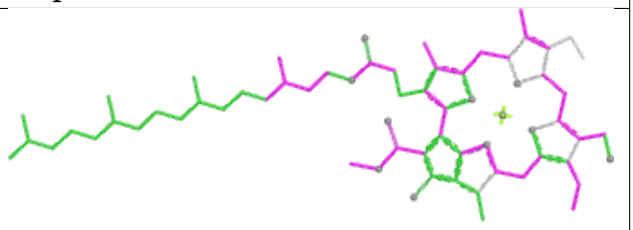
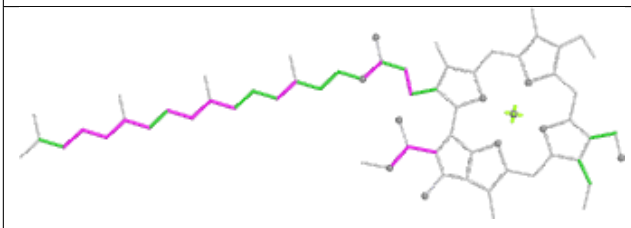


Bond angles



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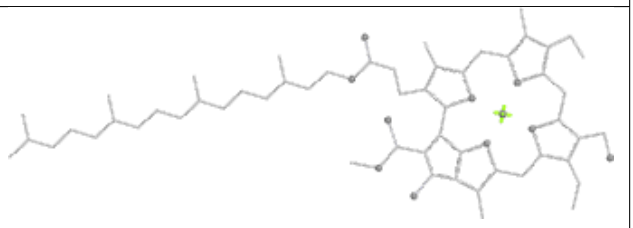
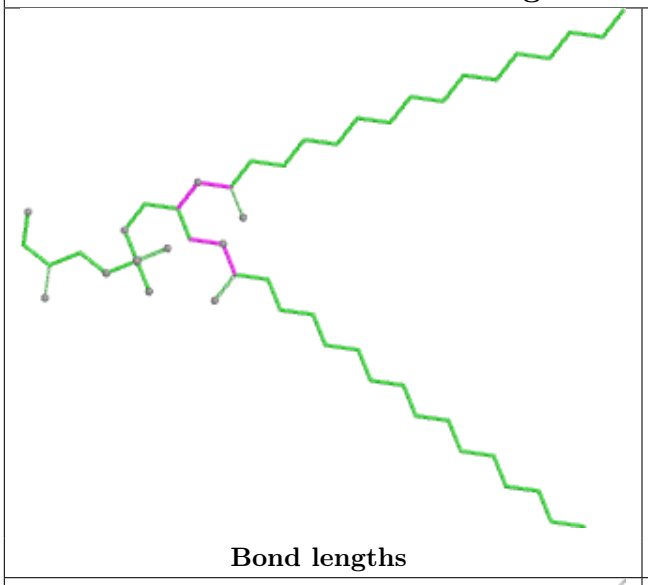


Rings

Ligand LHG V 312



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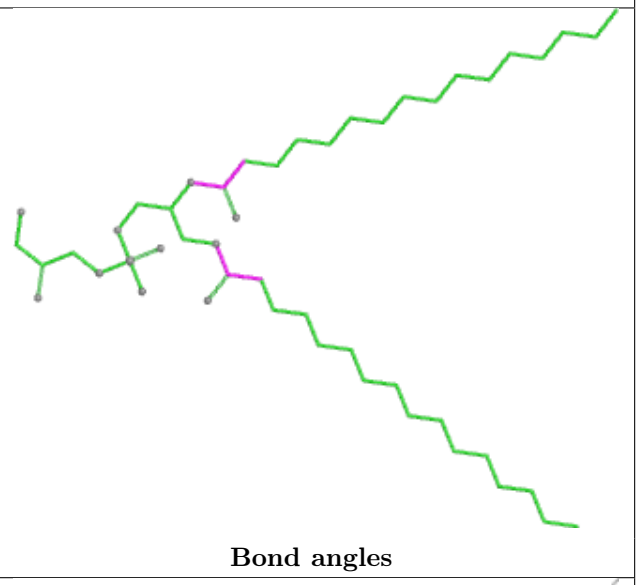
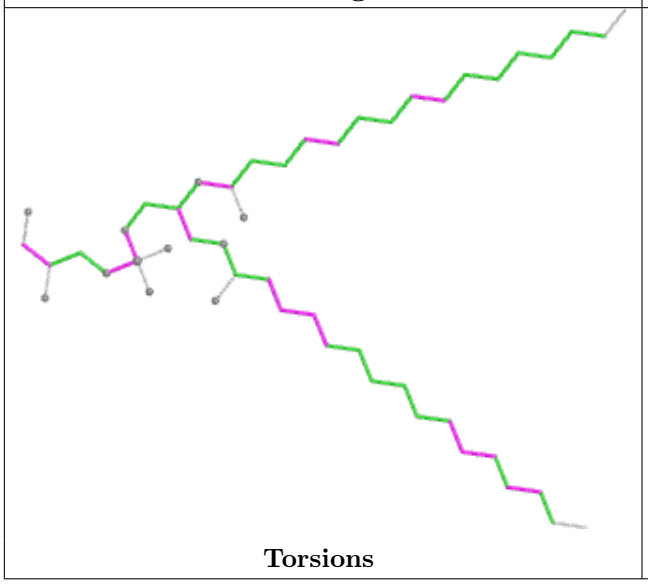


Bond angles



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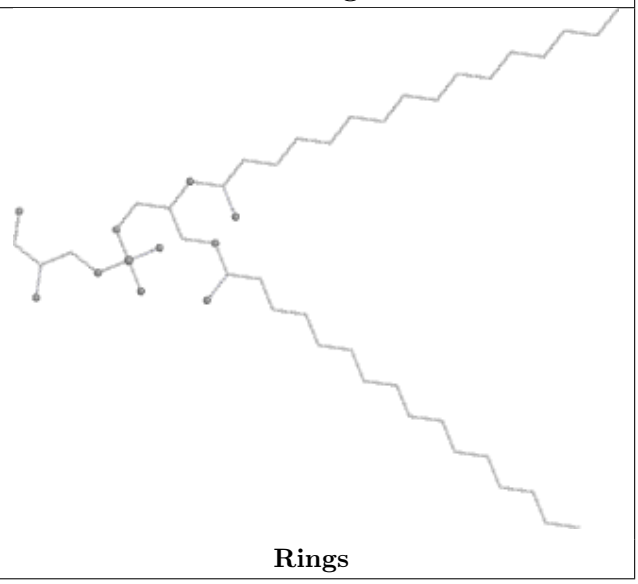
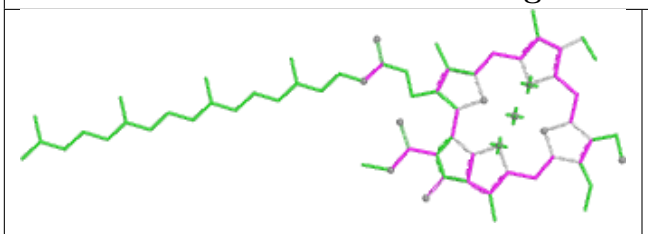


Rings

Ligand CHL U 315



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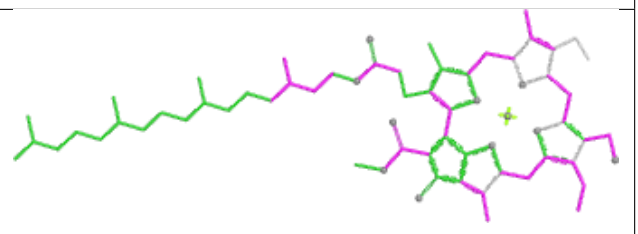
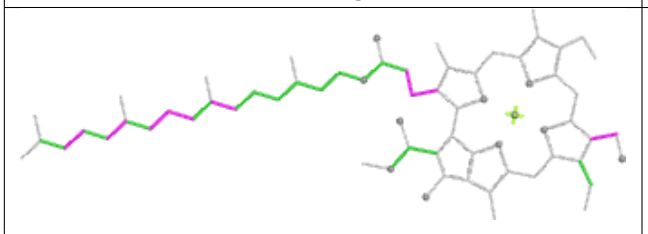


Bond angles



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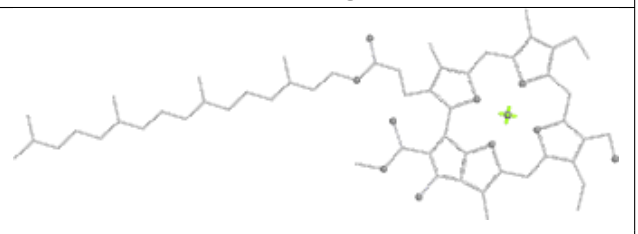
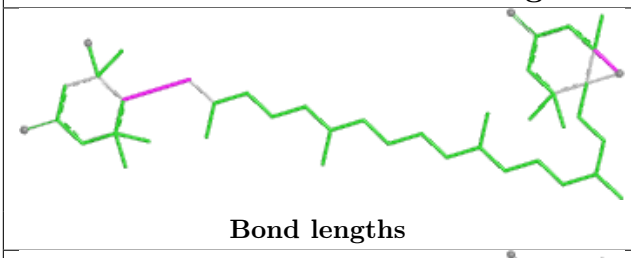


Rings

Ligand NEX S 317



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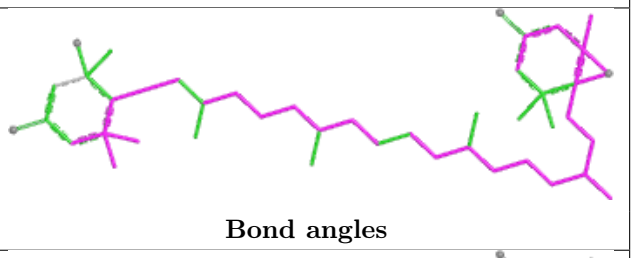
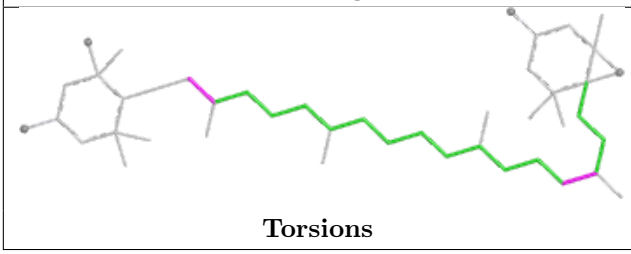


Bond angles



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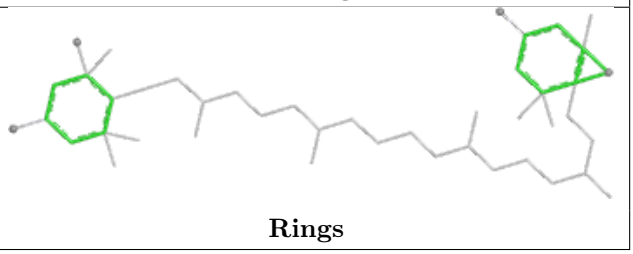
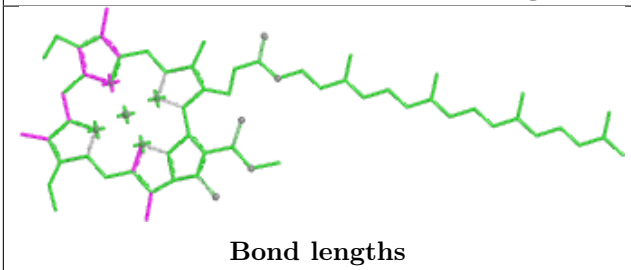


Rings

Ligand CLA C 515



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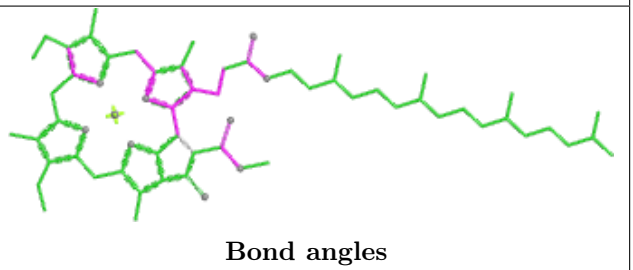
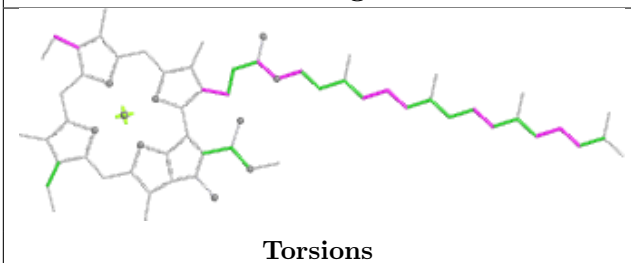


Bond angles



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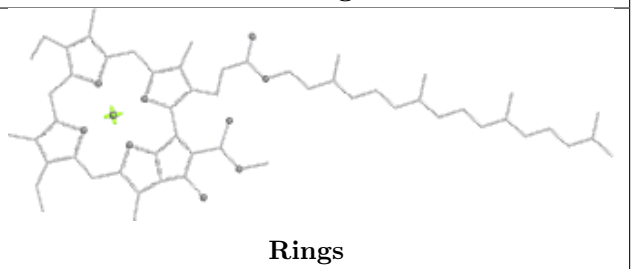
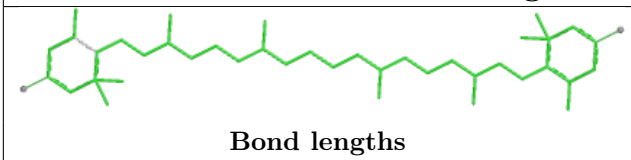


Rings

Ligand LUT N 310



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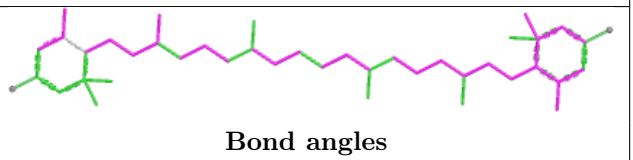
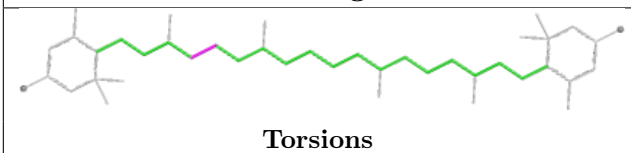


Bond angles



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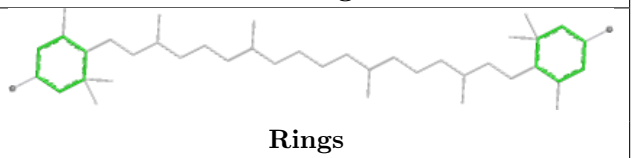
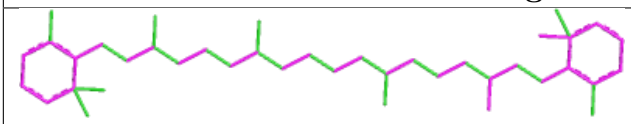


Rings

Ligand BCR b 619



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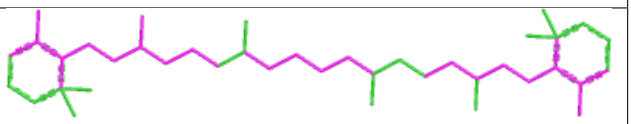
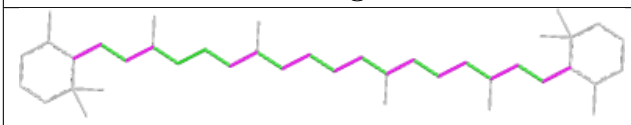


Bond angles



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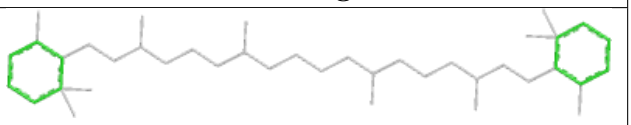
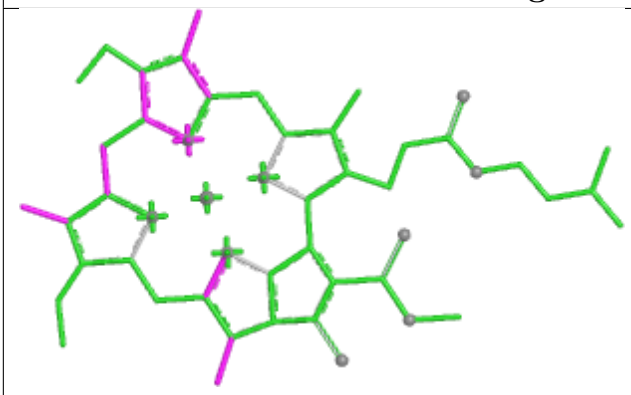
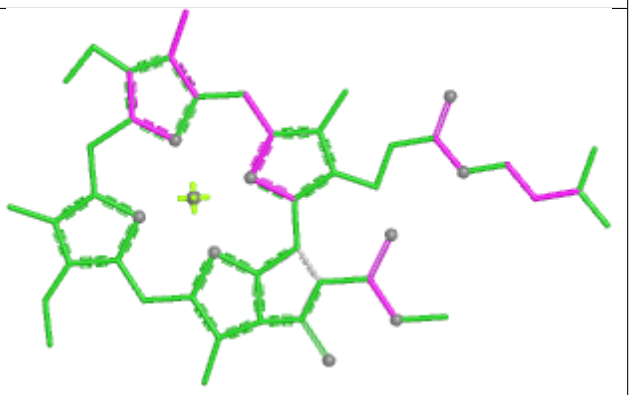


Rings

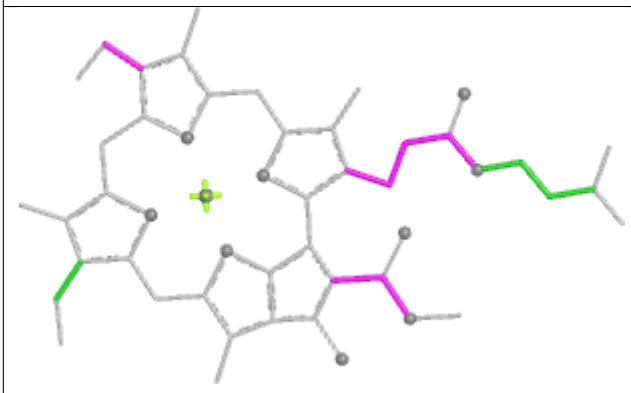
Ligand CLA 3 303



Bond lengths



Bond angles



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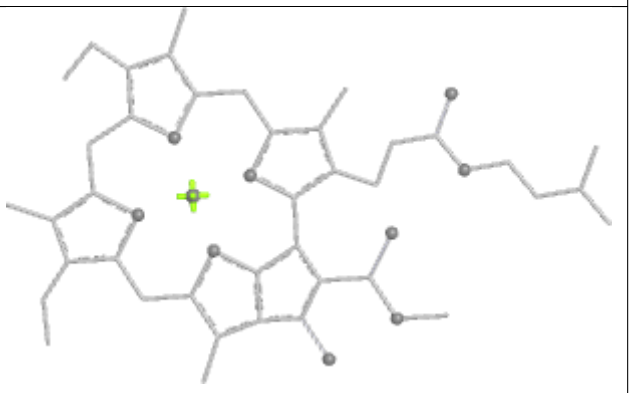
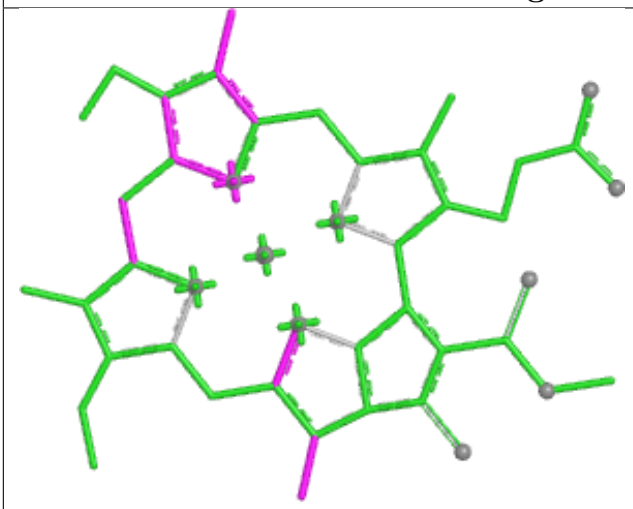


Rings

Ligand CLA S 304



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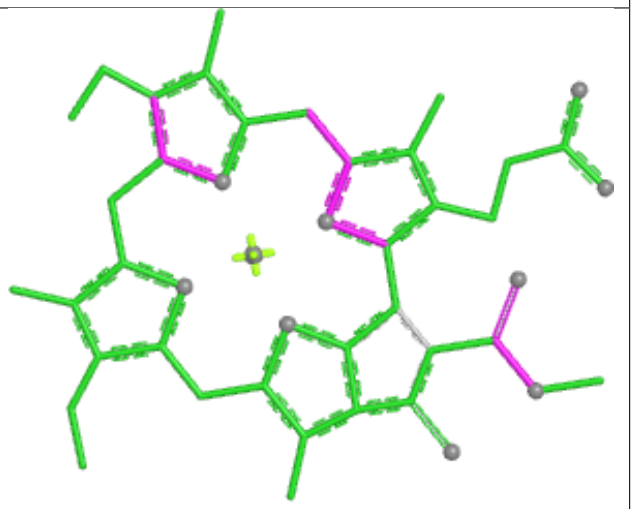
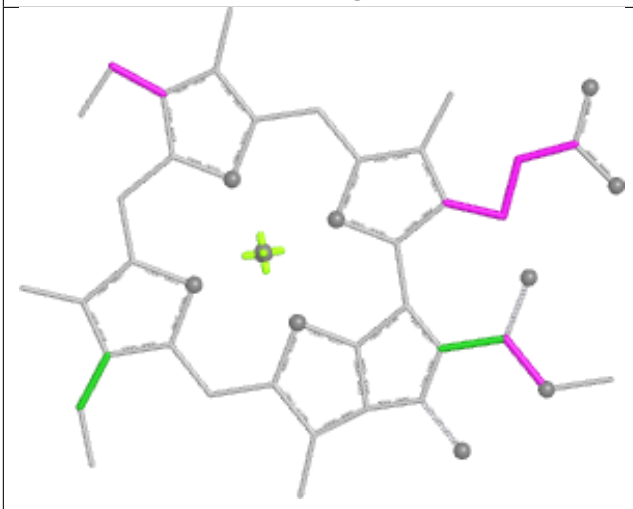


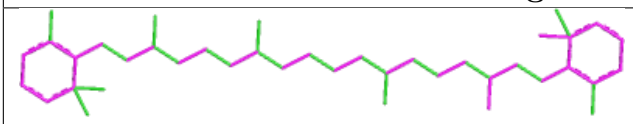
Bond angles



Torsions

Rings

Ligand BCR a 409



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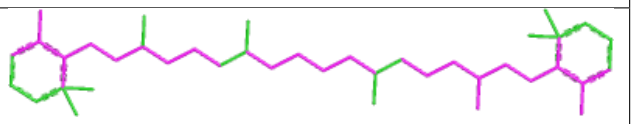
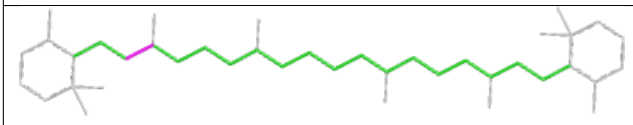
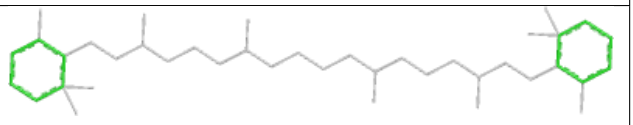


Bond angles

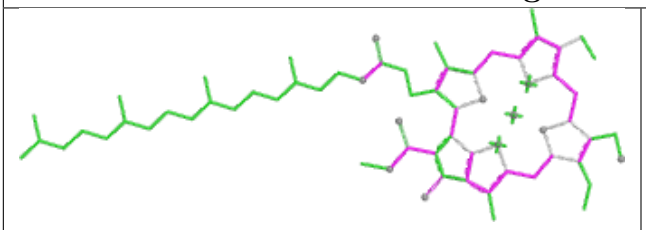


Torsions



Rings

Ligand CHL Q 314



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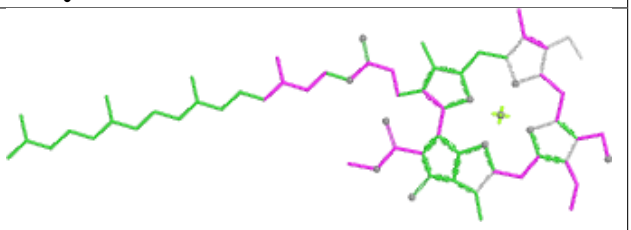

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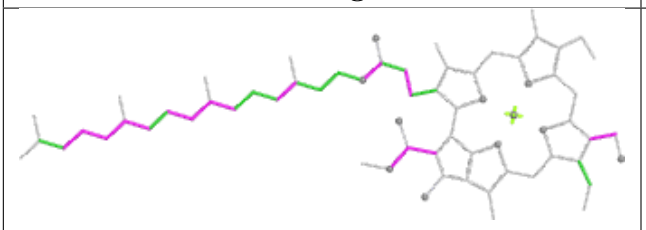

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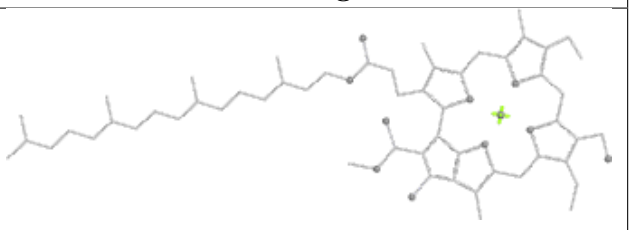
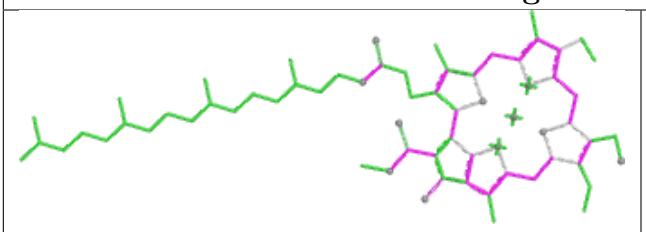


Rings

Ligand CHL N 313



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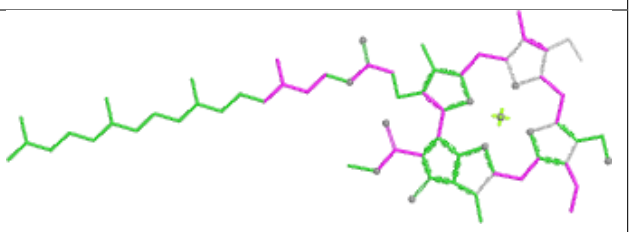

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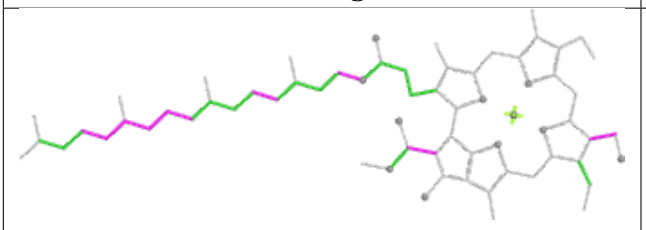

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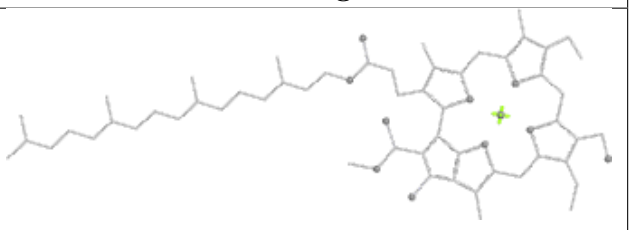
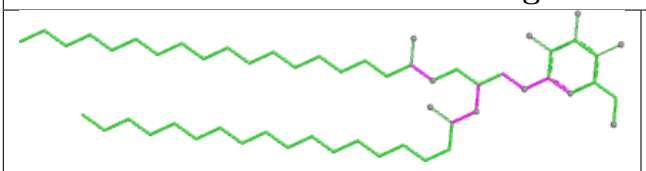


Rings

Ligand LMG b 624



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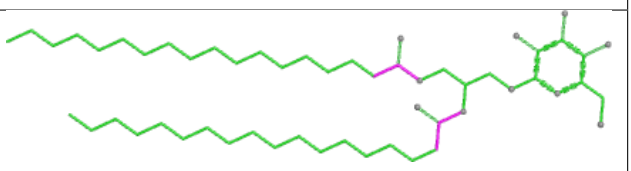

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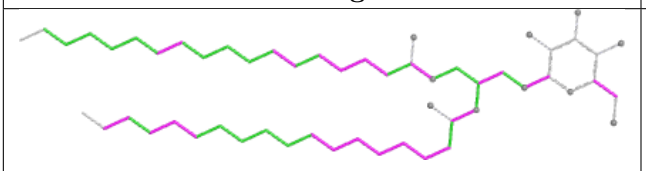

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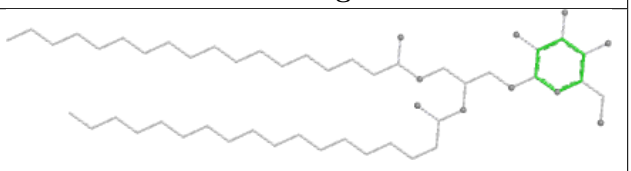
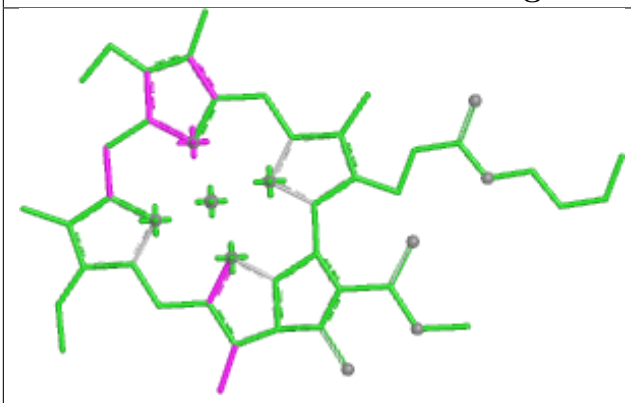


Rings

Ligand CLA R 309



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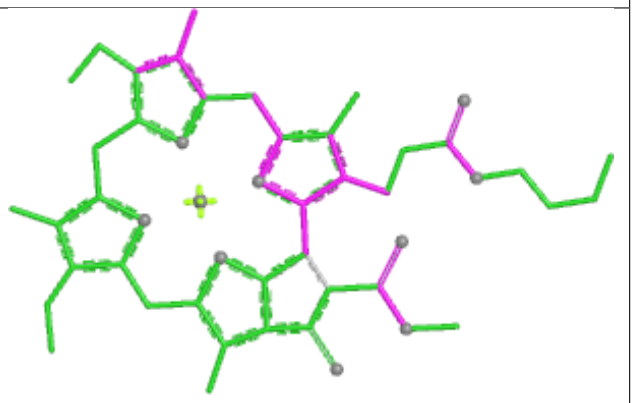

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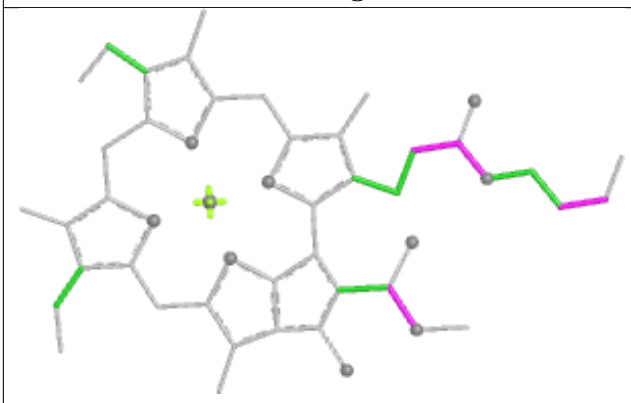

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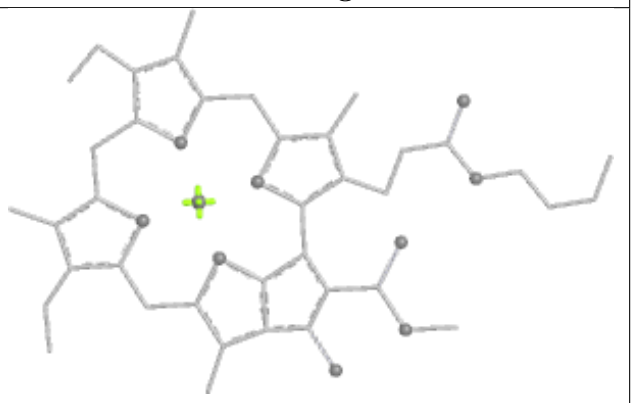
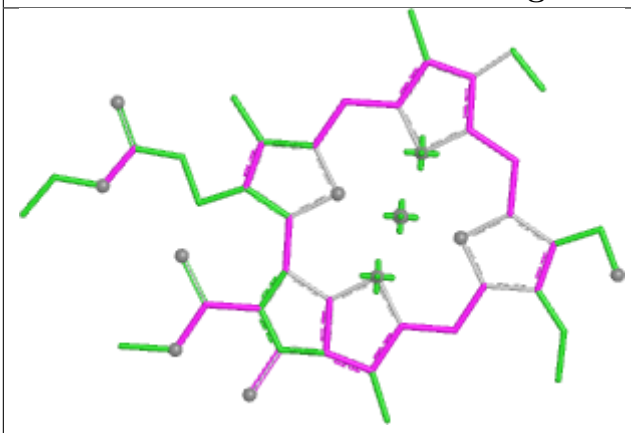


Rings

Ligand CHL 5 314



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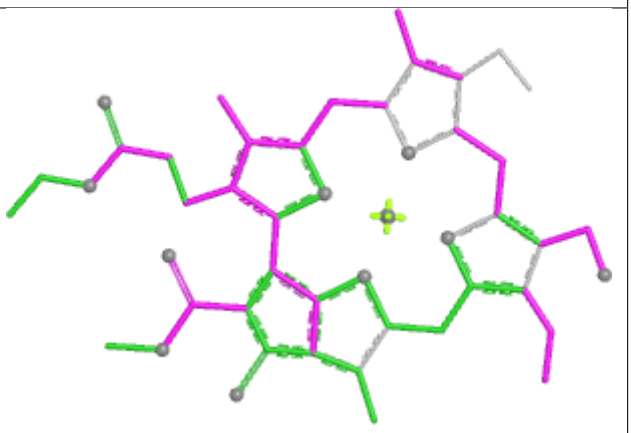

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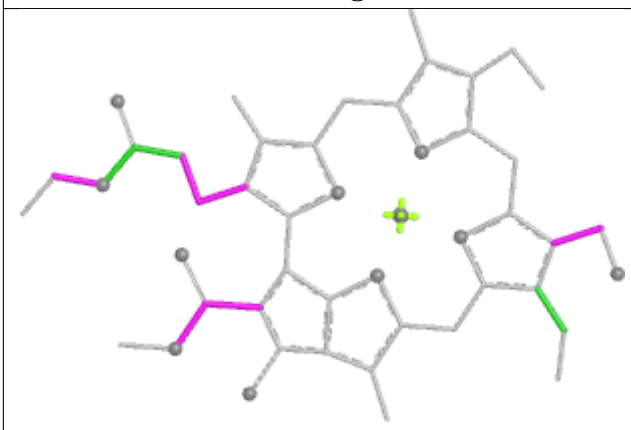
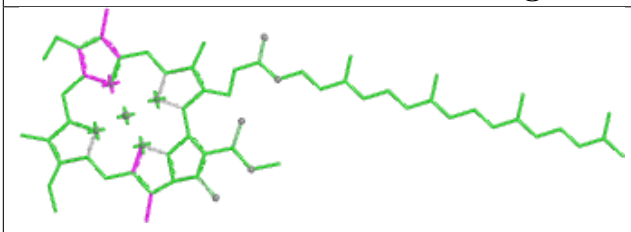


Torsions

Rings

Ligand CLA Q 302



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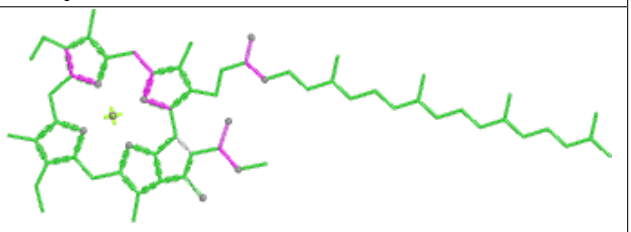
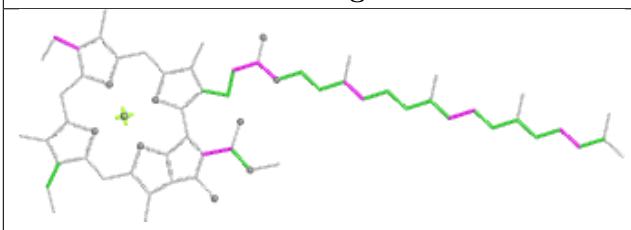


Bond angles



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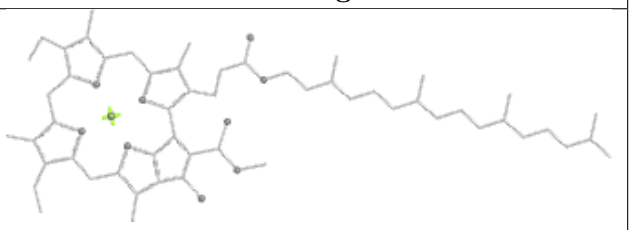
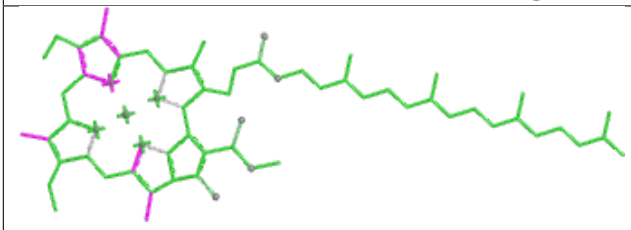


Rings

Ligand CLA q 302



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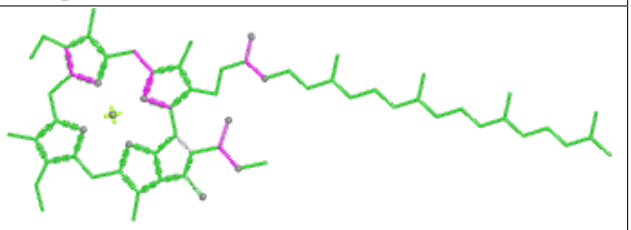

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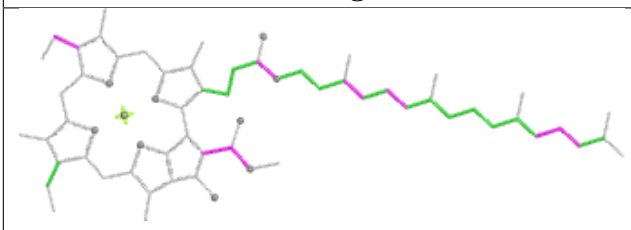

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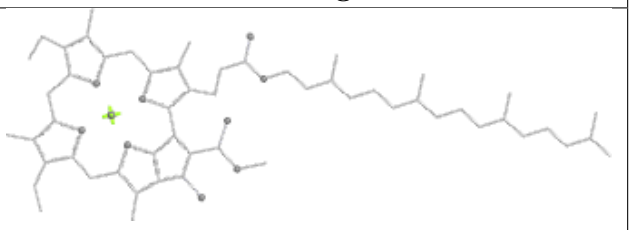
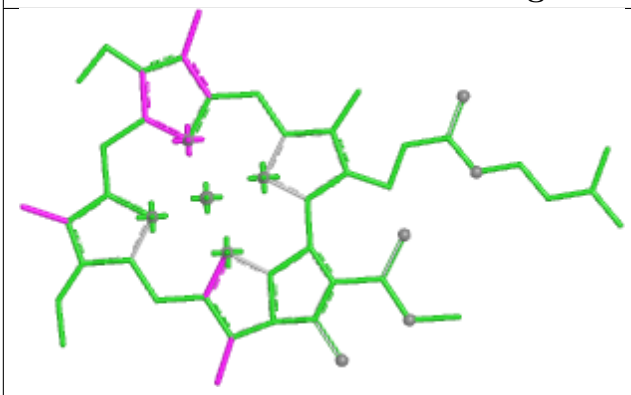


Rings

Ligand CLA u 303



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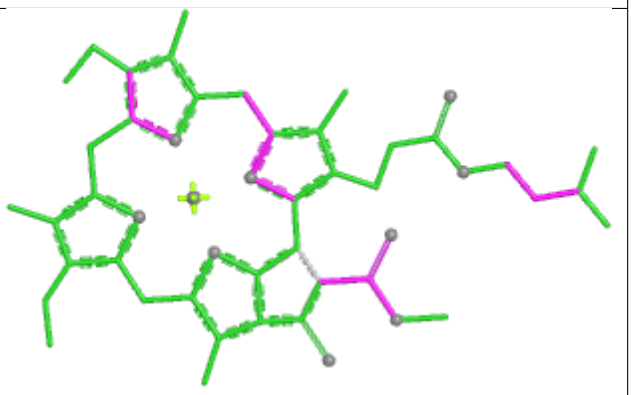
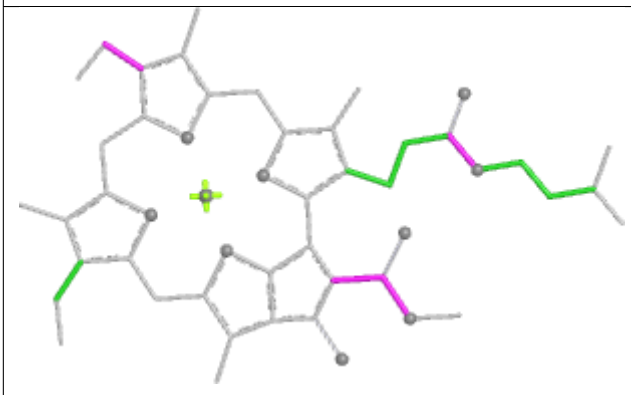


Bond angles



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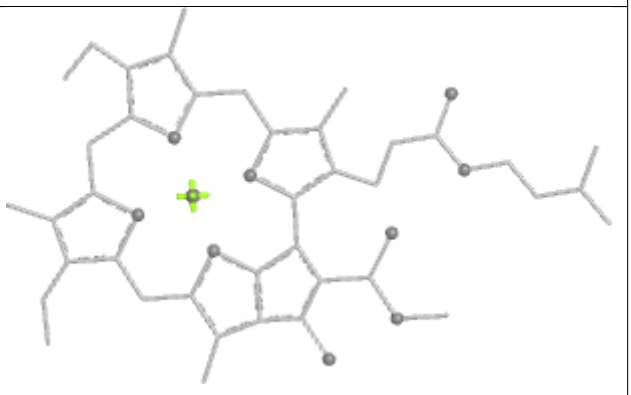
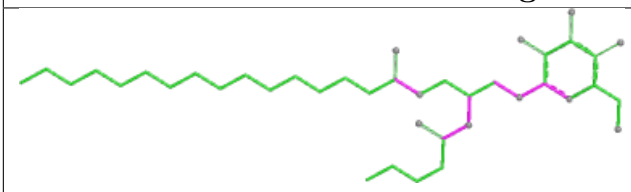


Rings

Ligand LMG A 411



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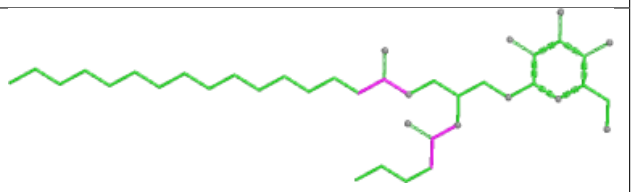
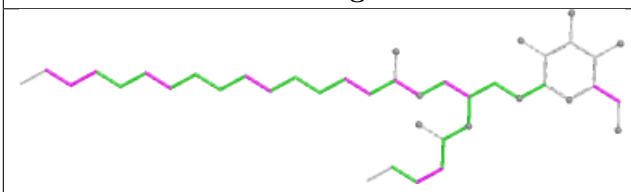


Bond angles



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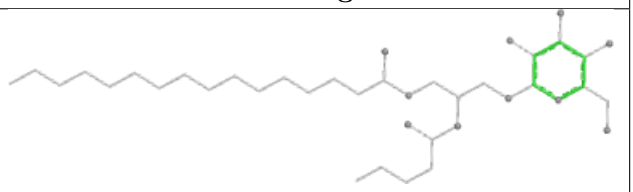
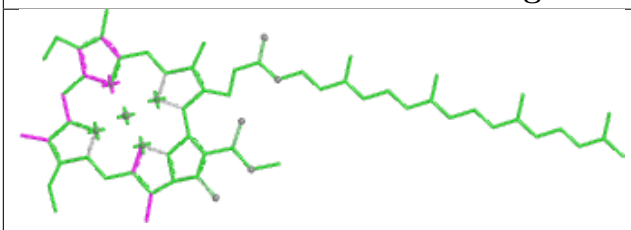


Rings

Ligand CLA Q 307



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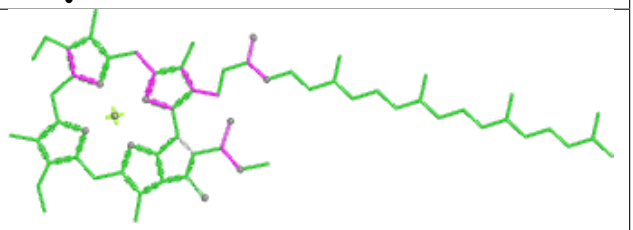

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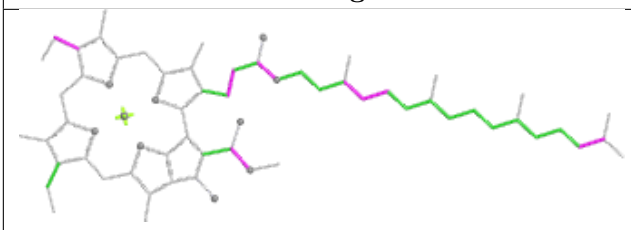

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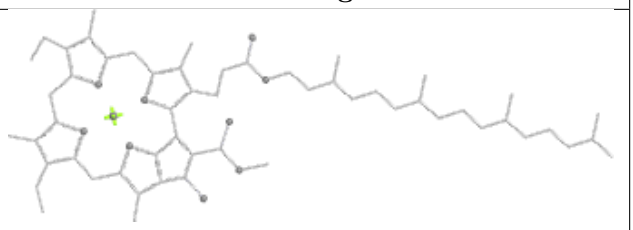
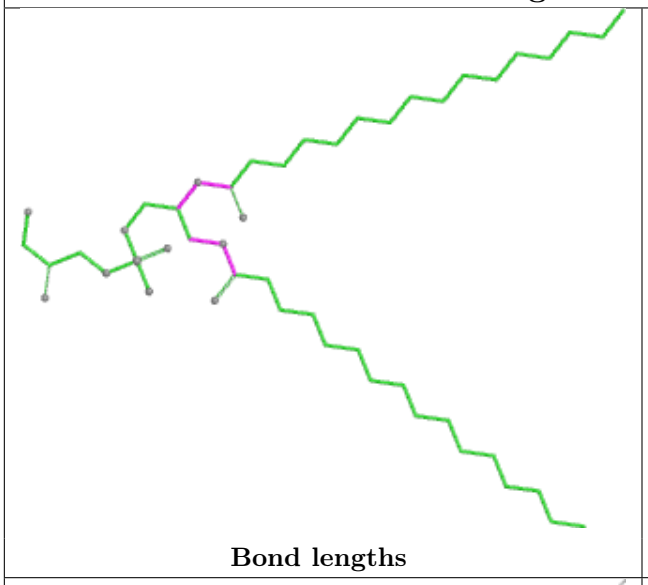


Rings

Ligand LHG c 521



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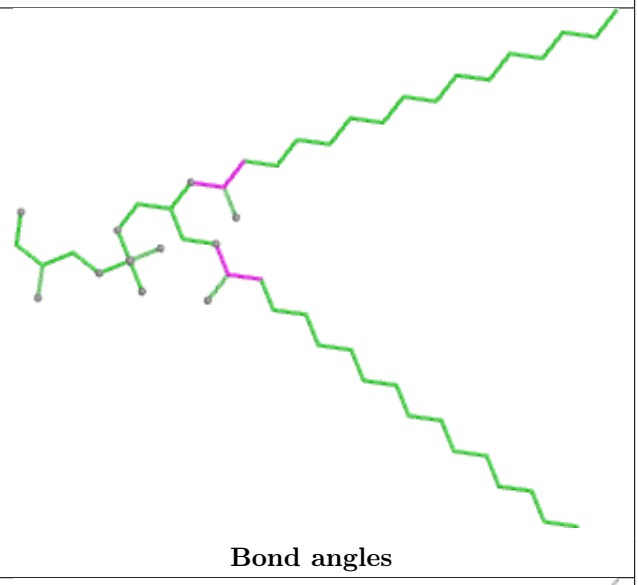
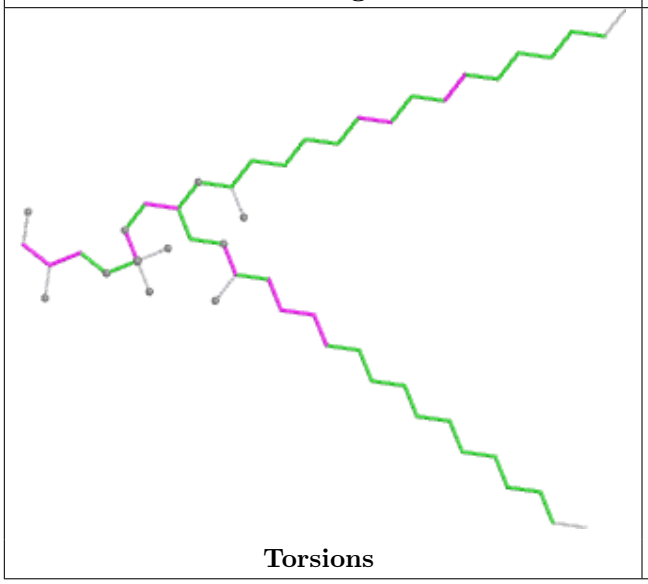


Bond angles



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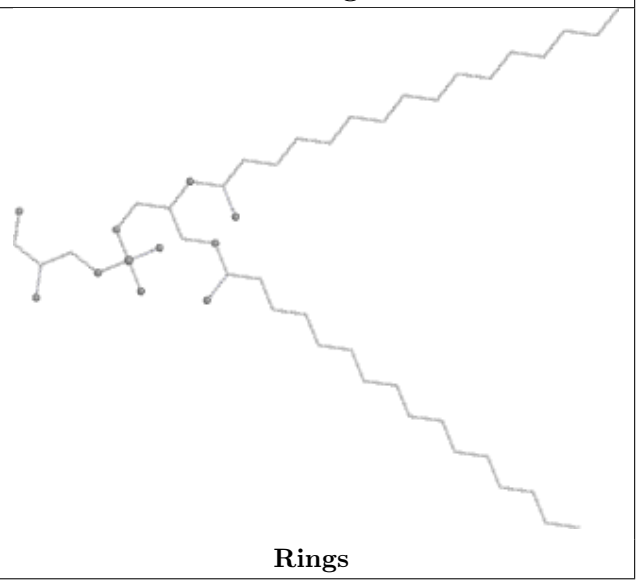
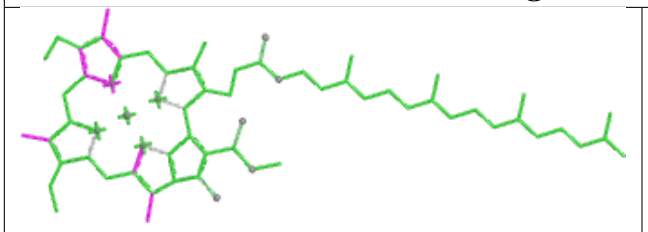


Rings

Ligand CLA B 607



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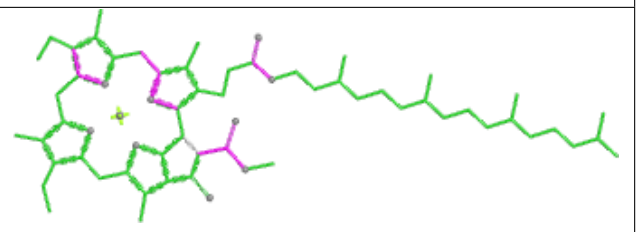
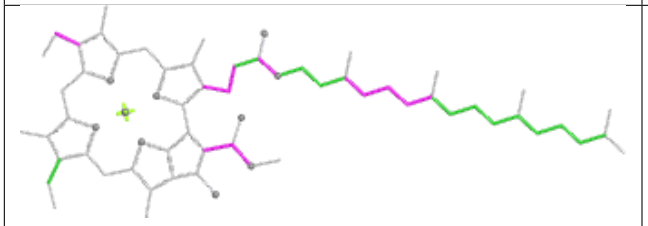


Bond angles



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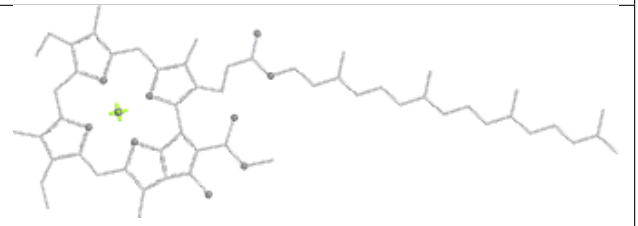
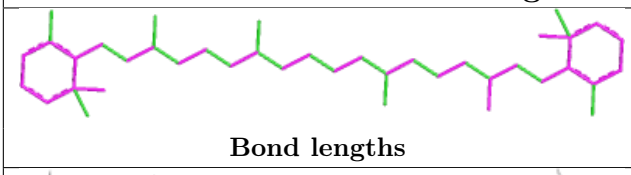


Rings

Ligand BCR T 101



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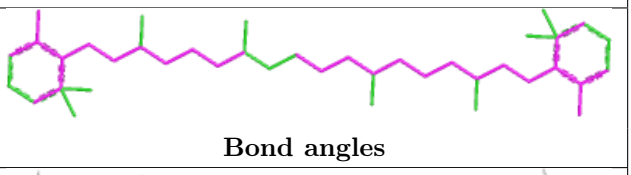
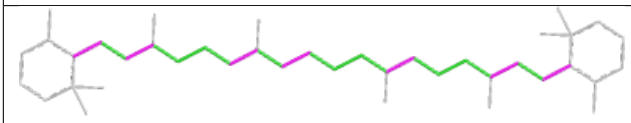
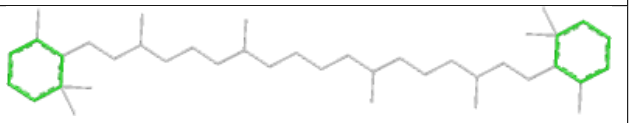


Bond angles

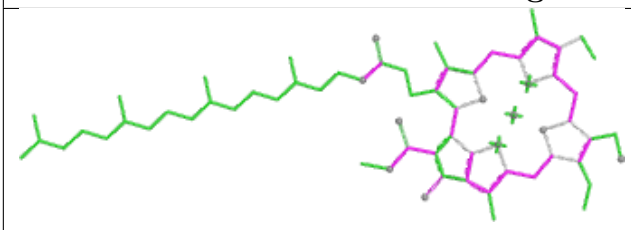


Torsions



Rings

Ligand CHL p 318



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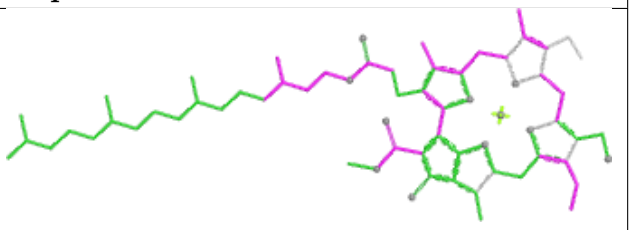
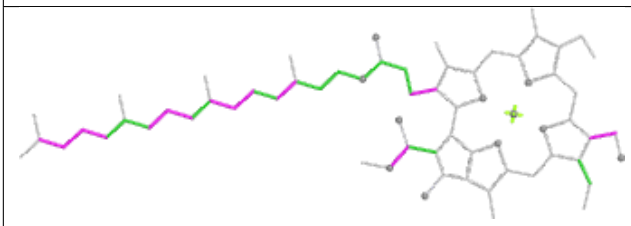
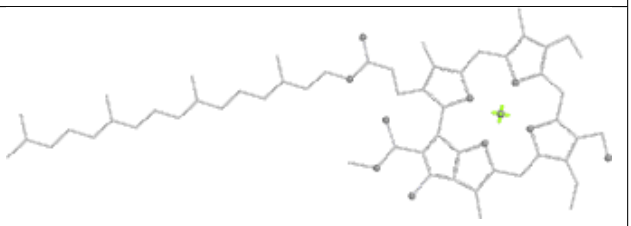


Bond angles

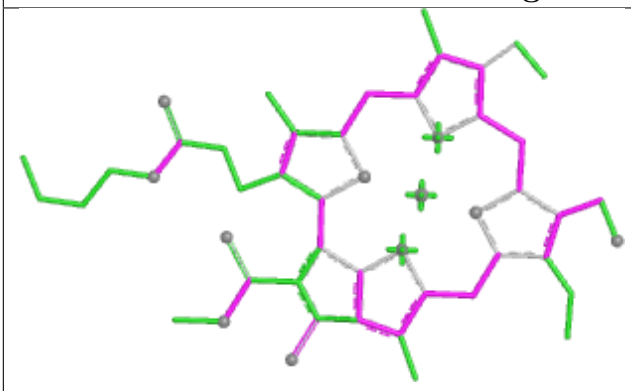


Torsions

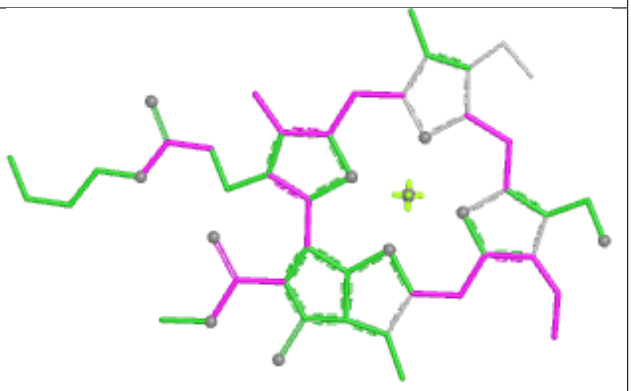


Rings

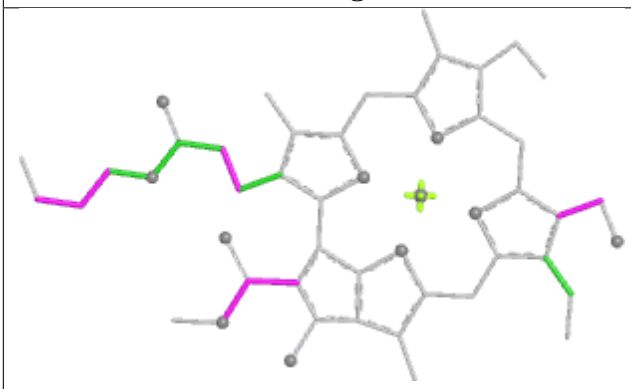
Ligand CHL G 313



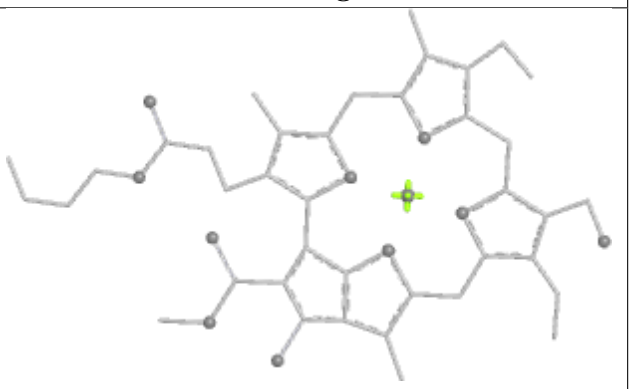
Bond lengths



Bond angles

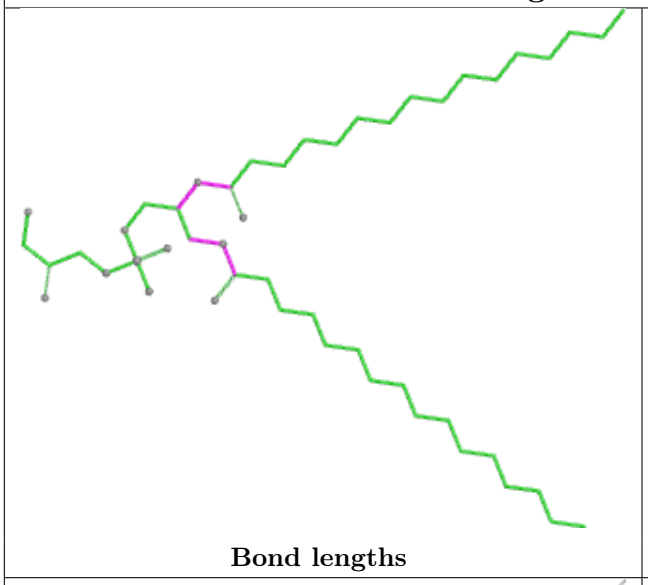


Torsions



Rings

Ligand LHG 1 312



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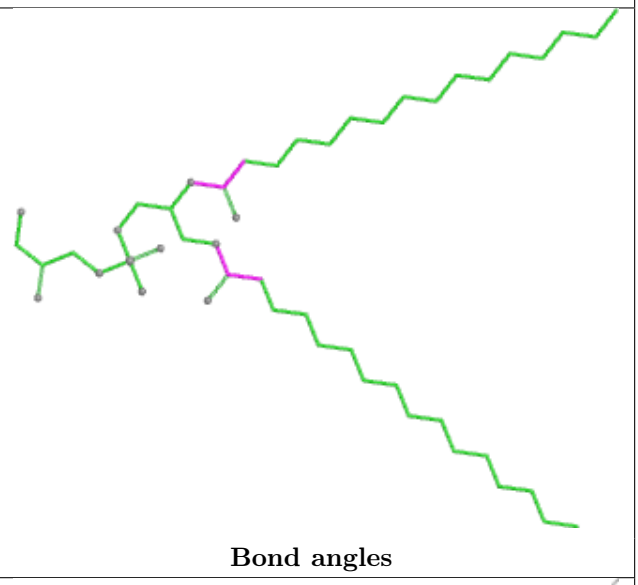

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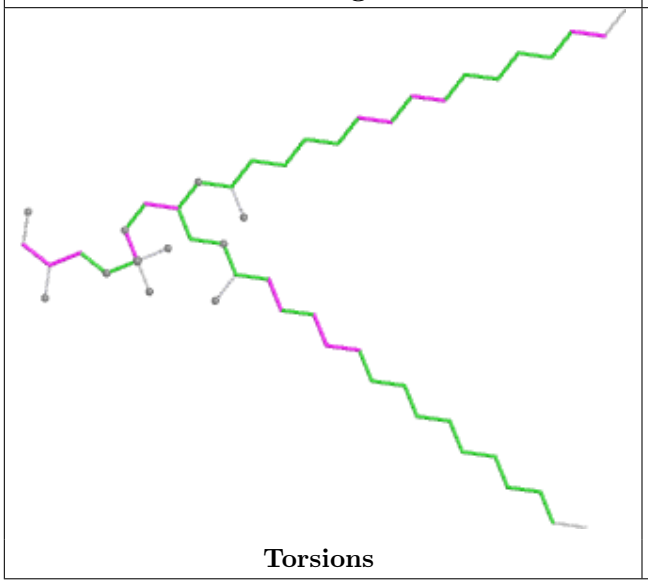

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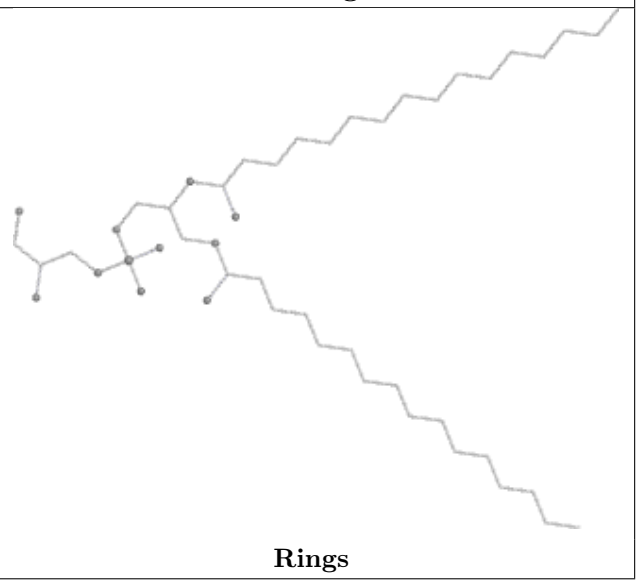
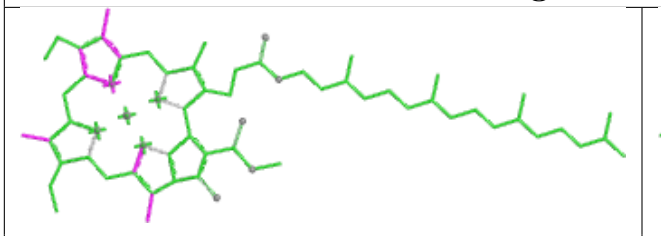


Rings

Ligand CLA c 510



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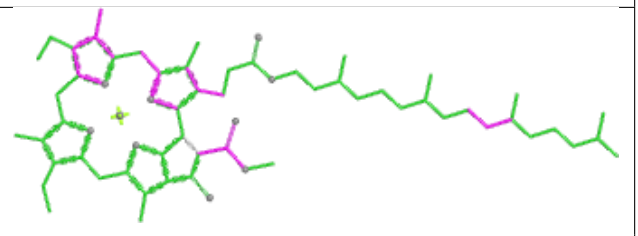

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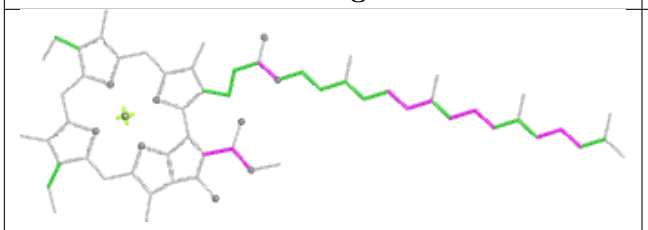

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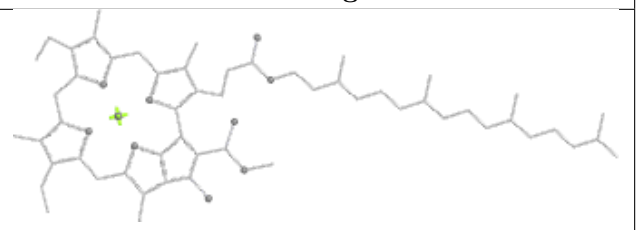
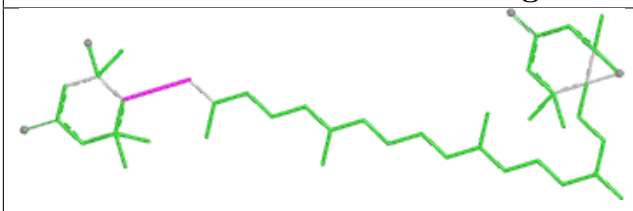


Rings

Ligand NEX V 319



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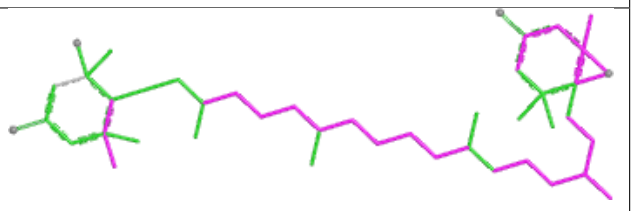
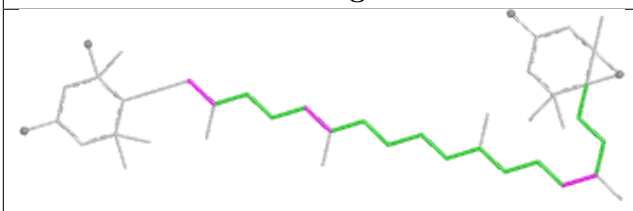


Bond angles



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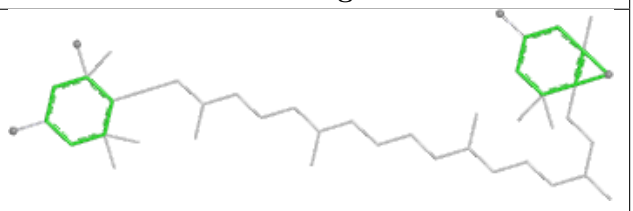
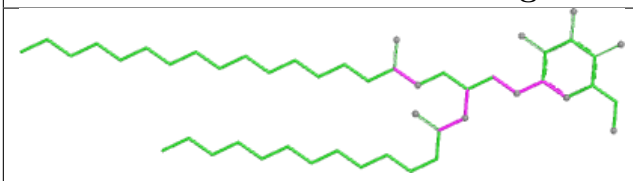


Rings

Ligand LMG w 201



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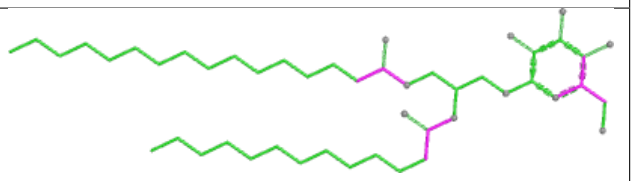
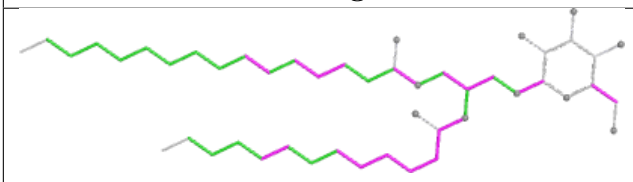


Bond angles



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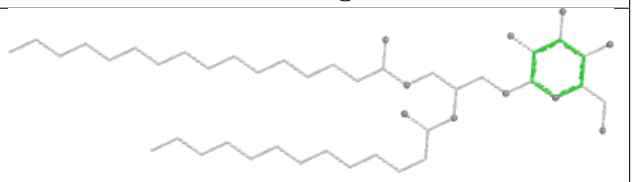
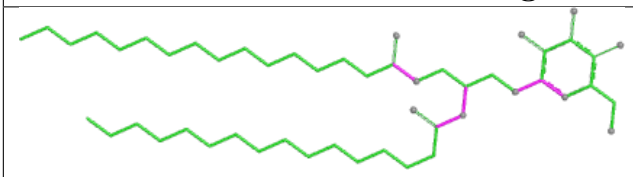


Rings

Ligand LMG C 502



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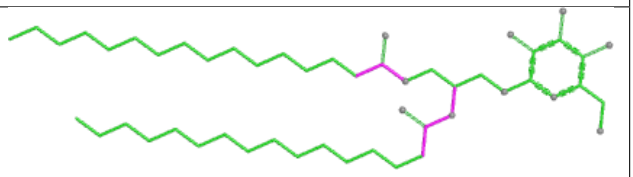
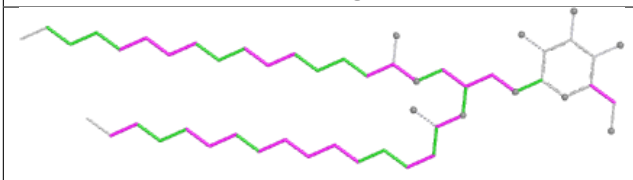


Bond angles



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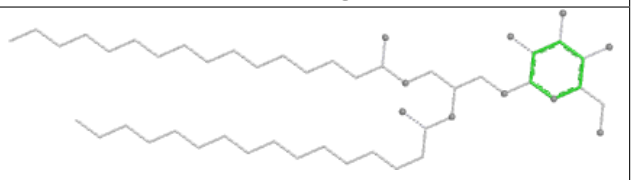
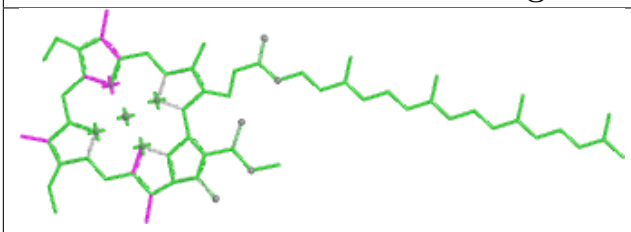


Rings

Ligand CLA u 307



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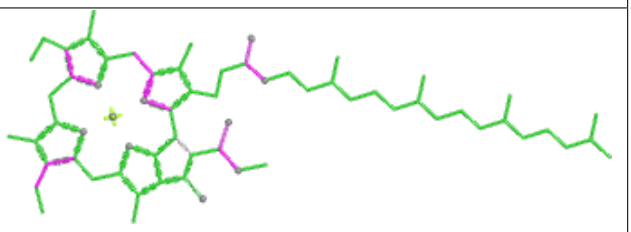
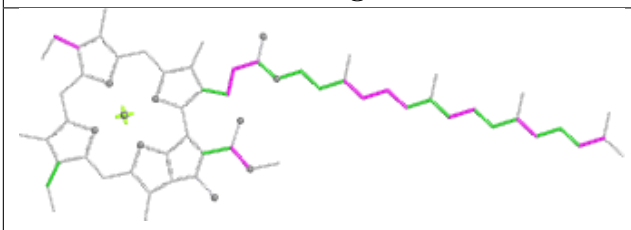


Bond angles



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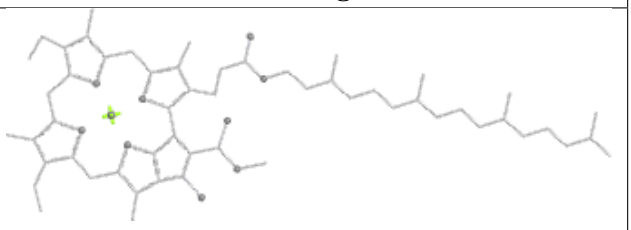
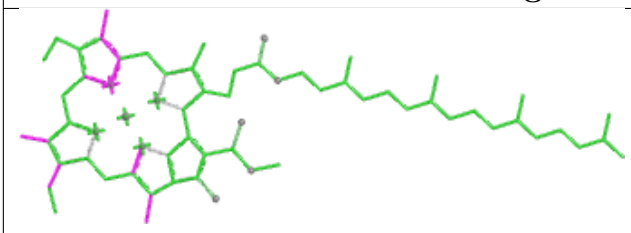


Rings

Ligand CLA C 504



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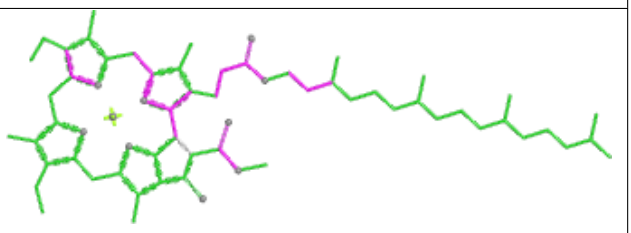
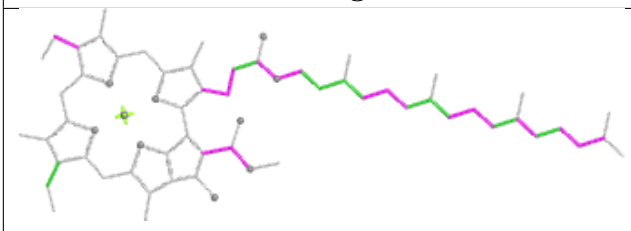
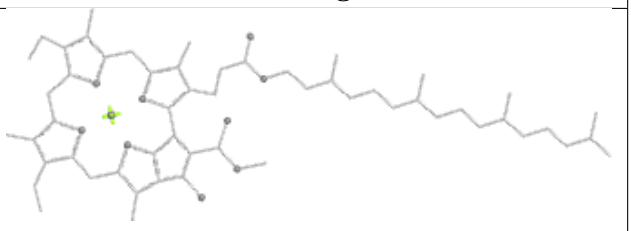


Bond angles

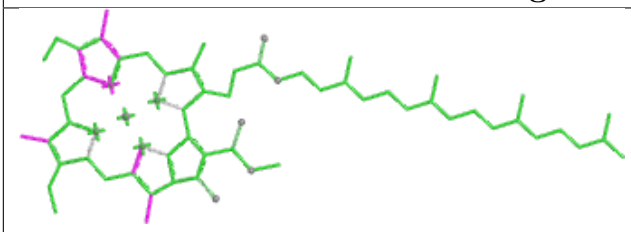


Torsions



Rings

Ligand CLA c 508



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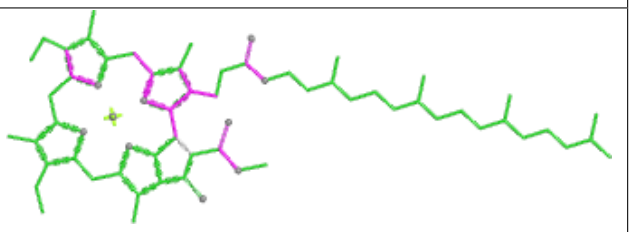
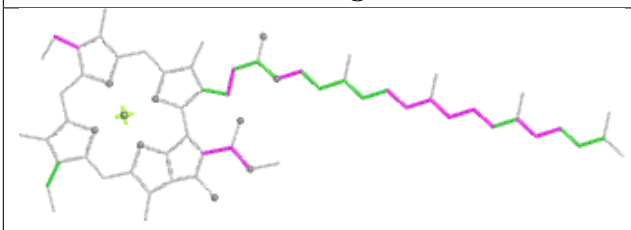


Bond angles



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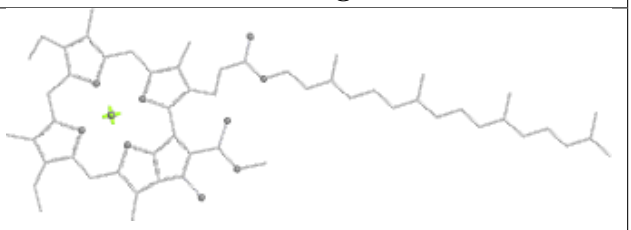
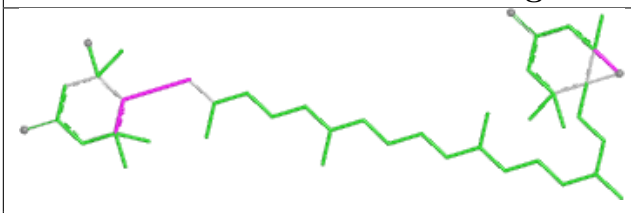


Rings

Ligand NEX p 301



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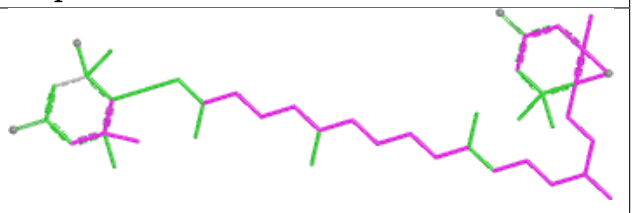
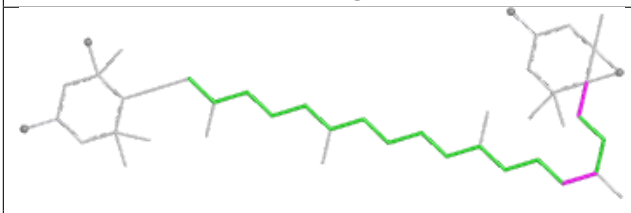


Bond angles



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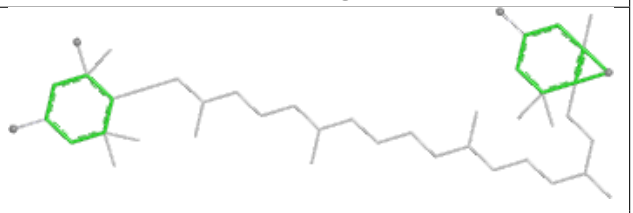
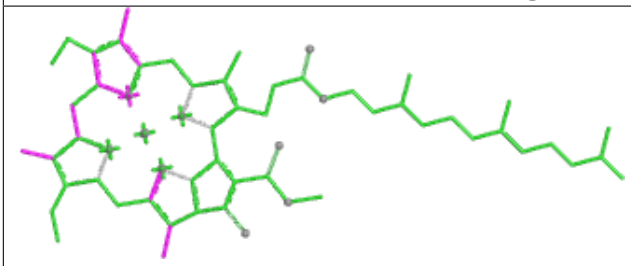


Rings

Ligand CLA Q 305



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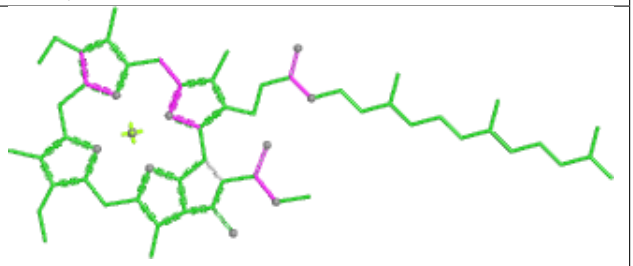
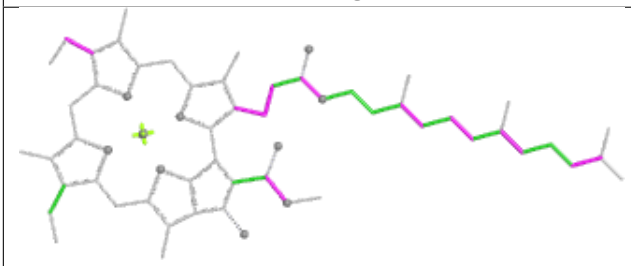


Bond angles



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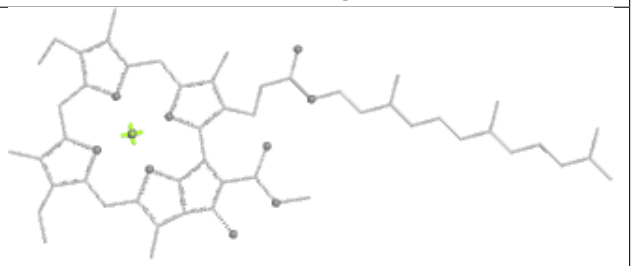
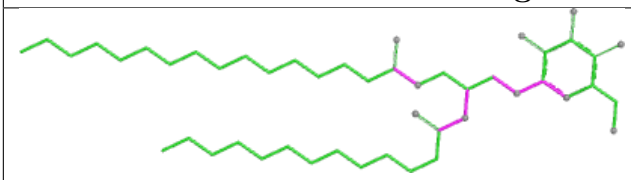


Rings

Ligand LMG W 201



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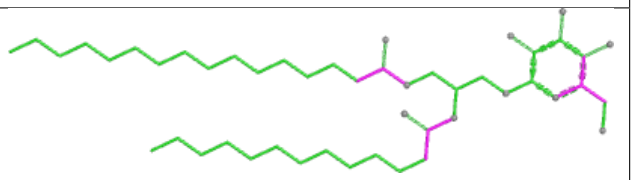
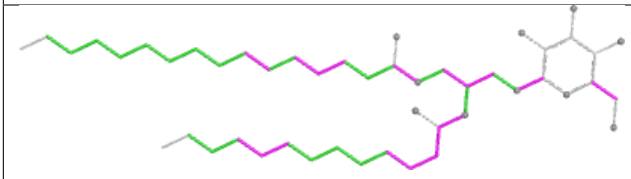


Bond angles



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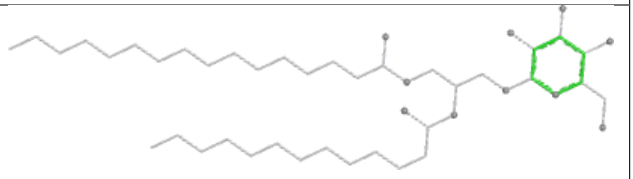
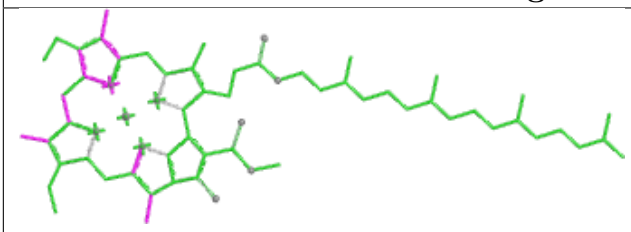


Rings

Ligand CLA n 304



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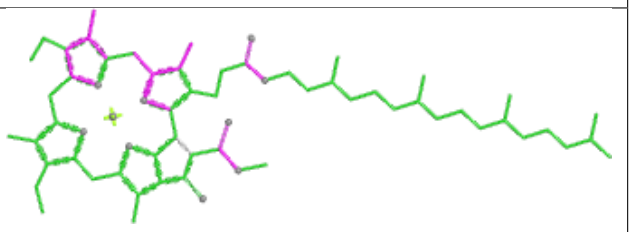
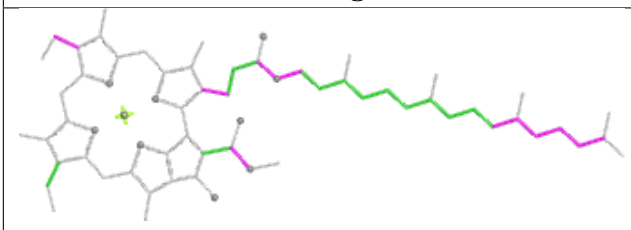
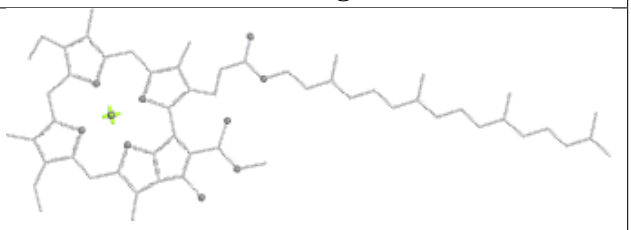


Bond angles

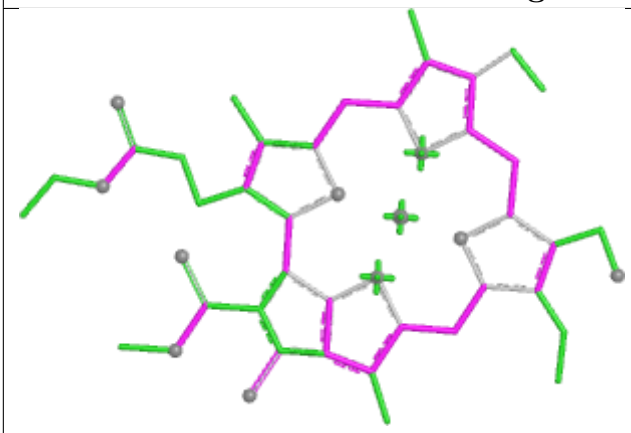


Torsions

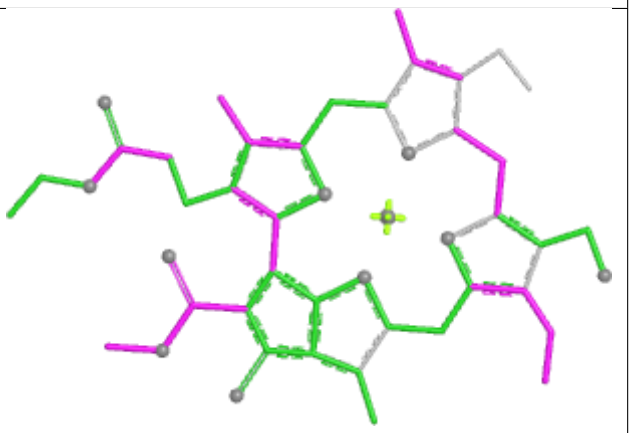


Rings

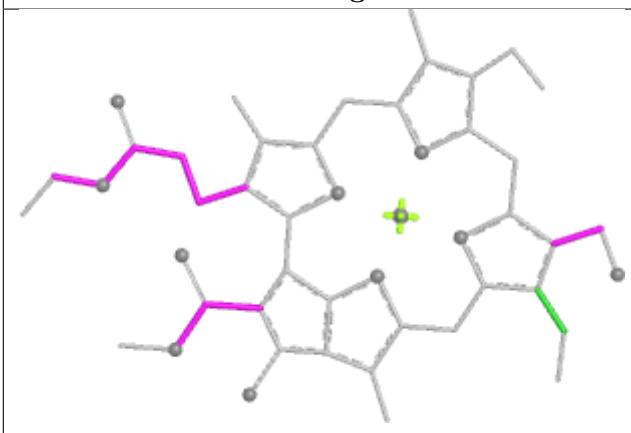
Ligand CHL 1 314



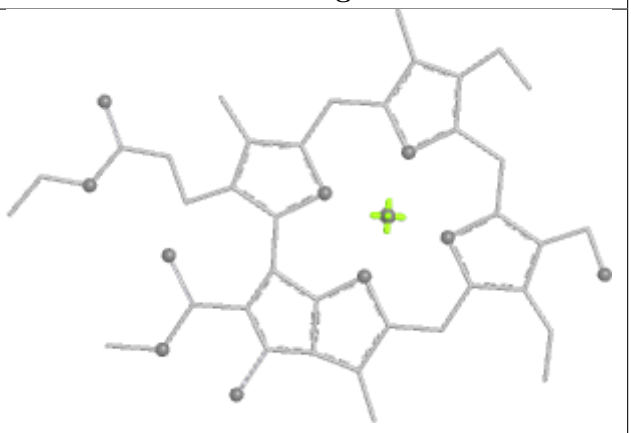
Bond lengths



Bond angles

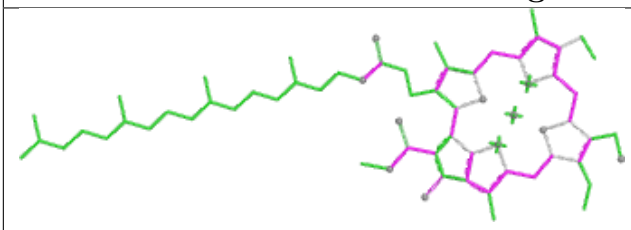


Torsions



Rings

Ligand CHL g 315



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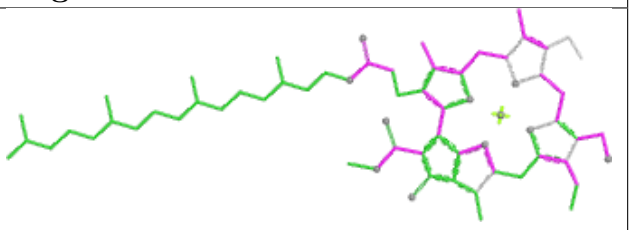

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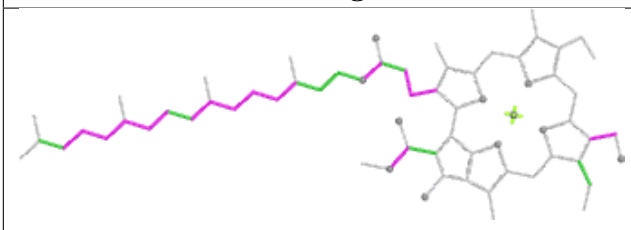

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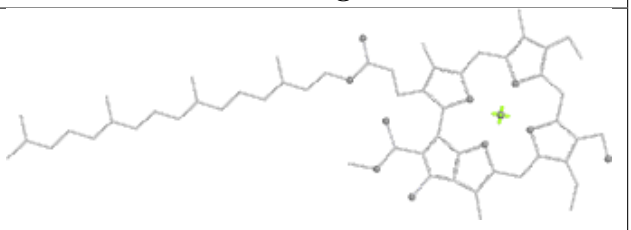
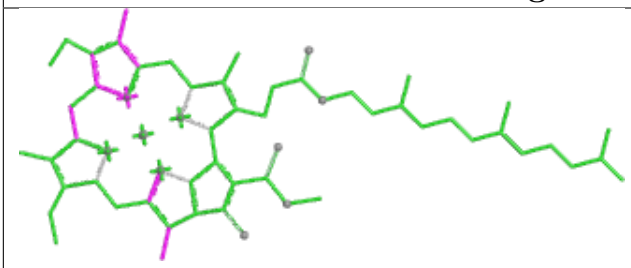


Rings

Ligand CLA 3 306



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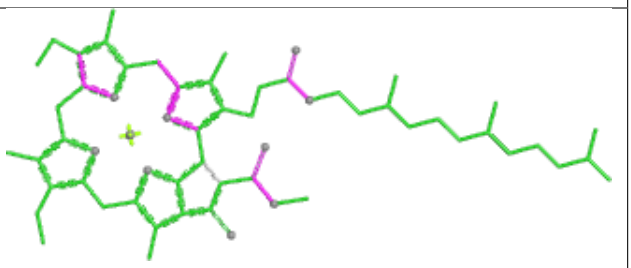

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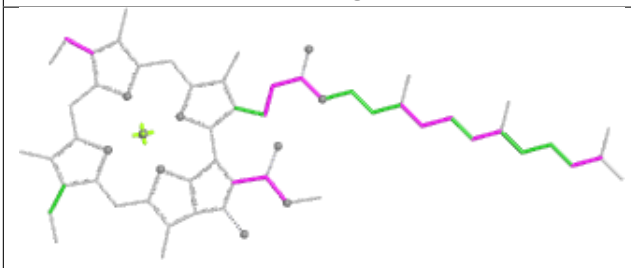

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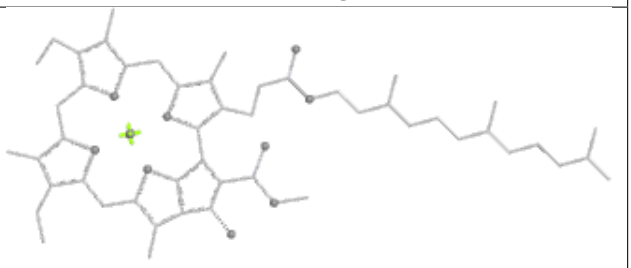
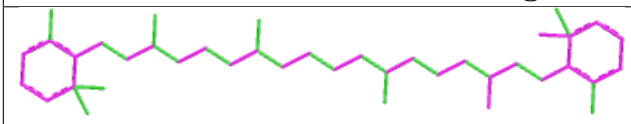


Rings

Ligand BCR X 201



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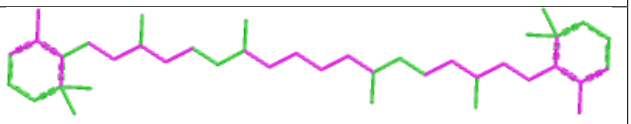
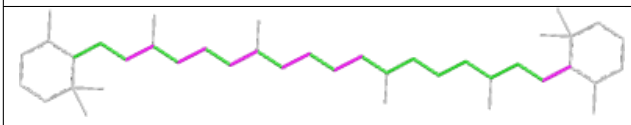


Bond angles



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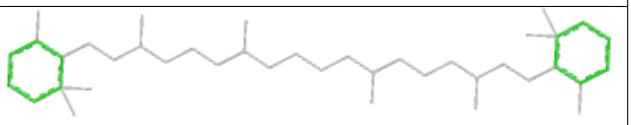
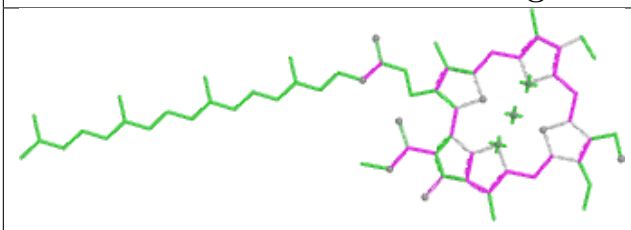


Rings

Ligand CHL q 314



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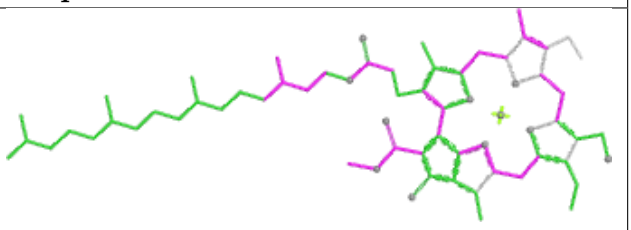
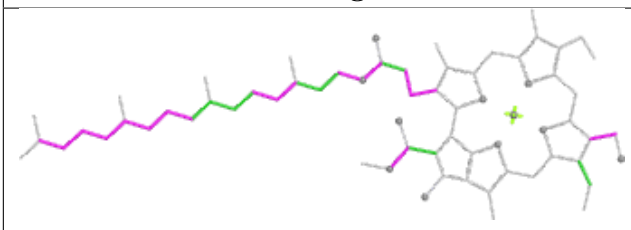


Bond angles



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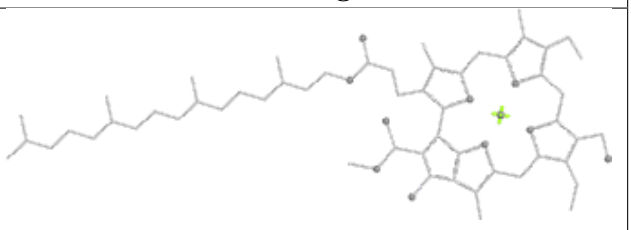
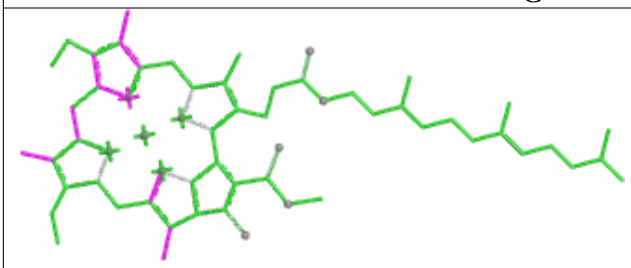


Rings

Ligand CLA P 308



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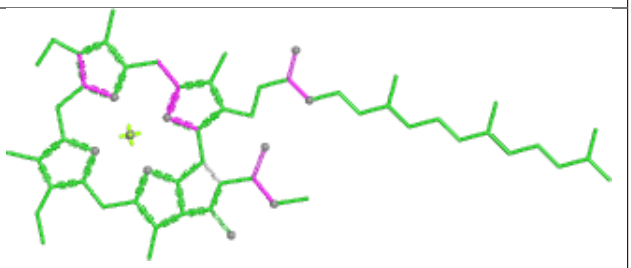
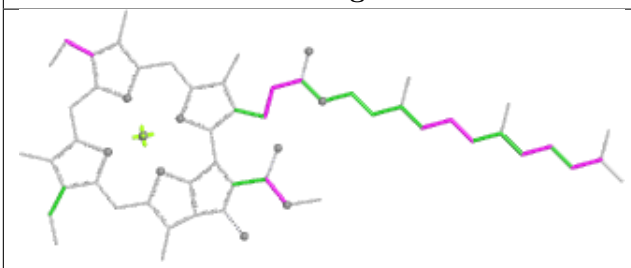


Bond angles



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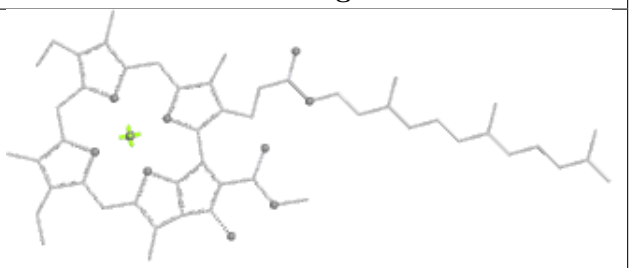
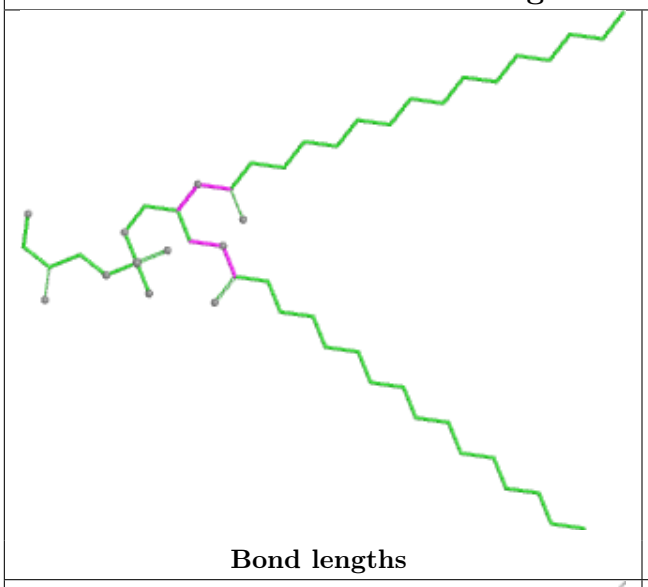


Rings

Ligand LHG S 312



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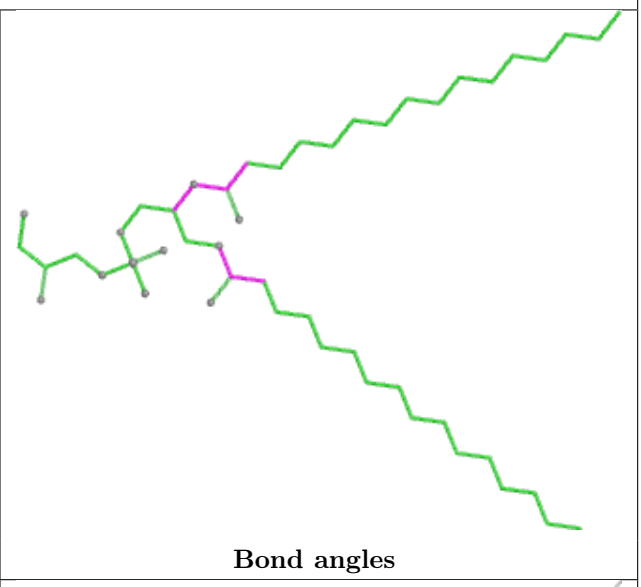
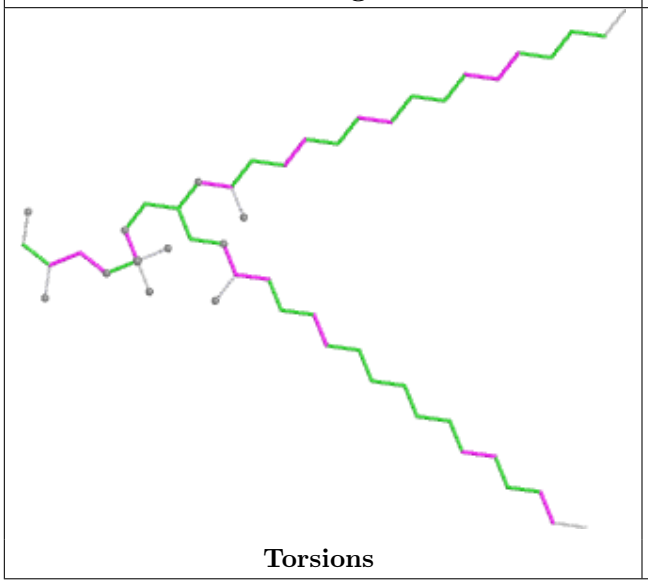


Bond angles



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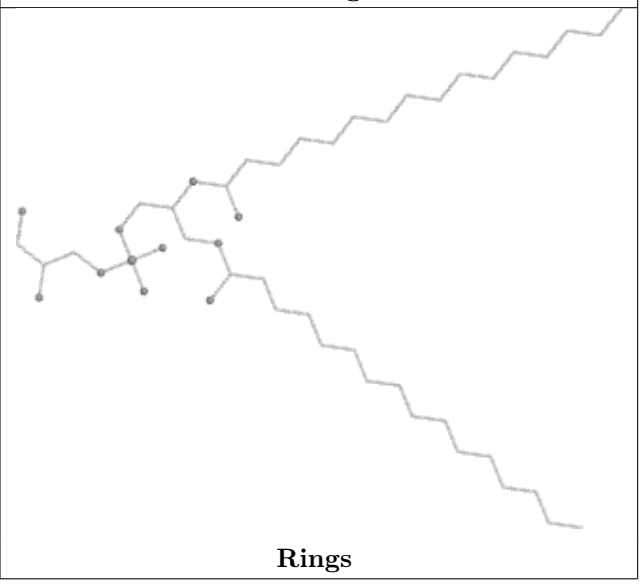
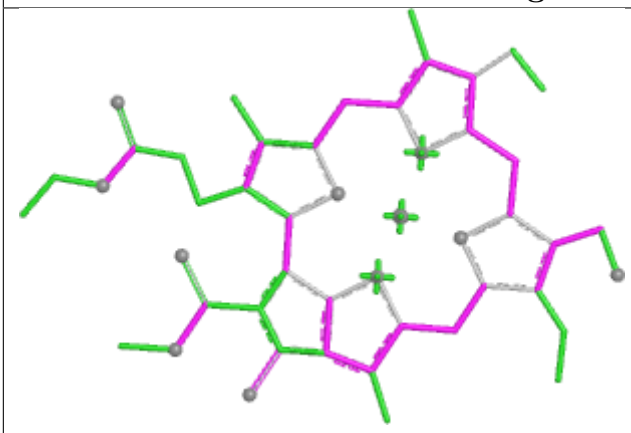


Rings

Ligand CHL v 314



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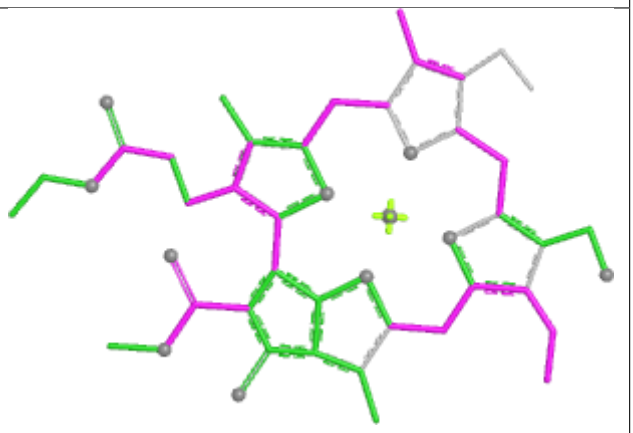
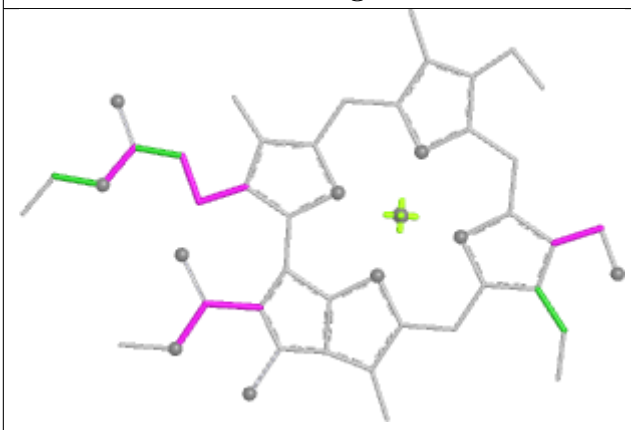


Bond angles



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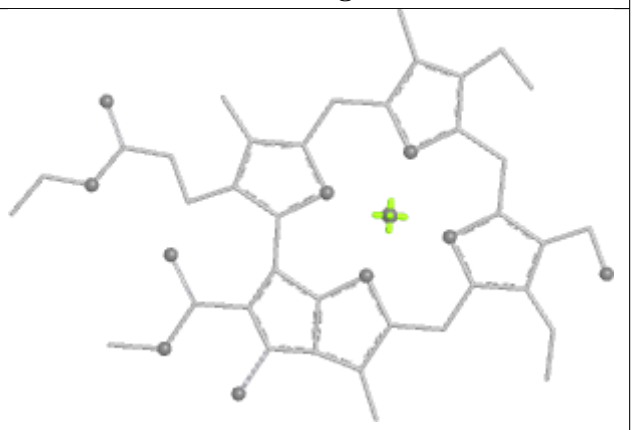
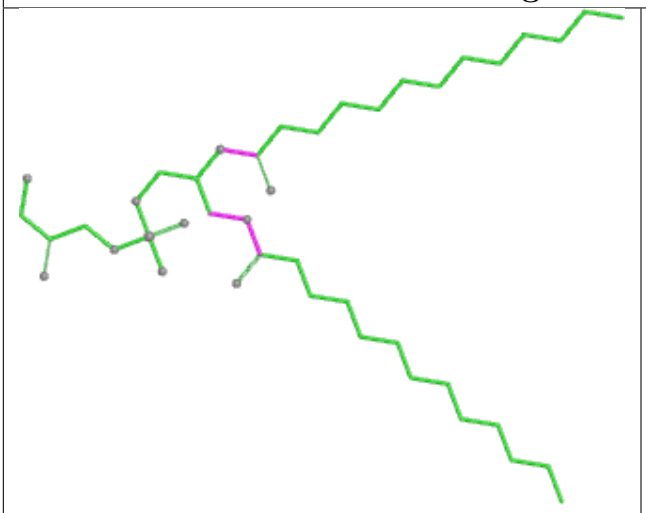


Rings

Ligand LHG A 413



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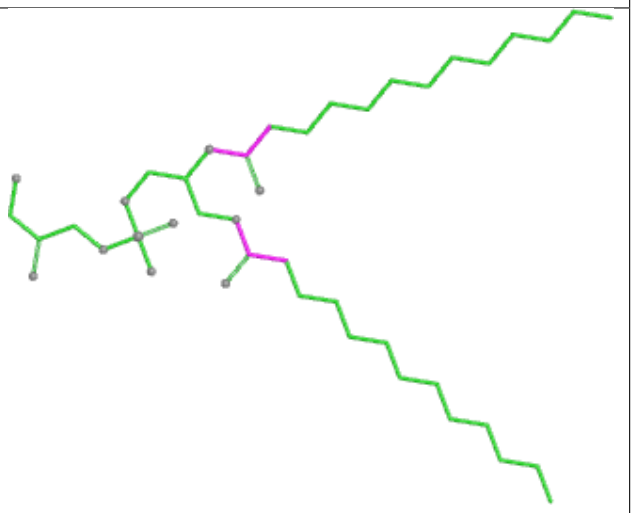
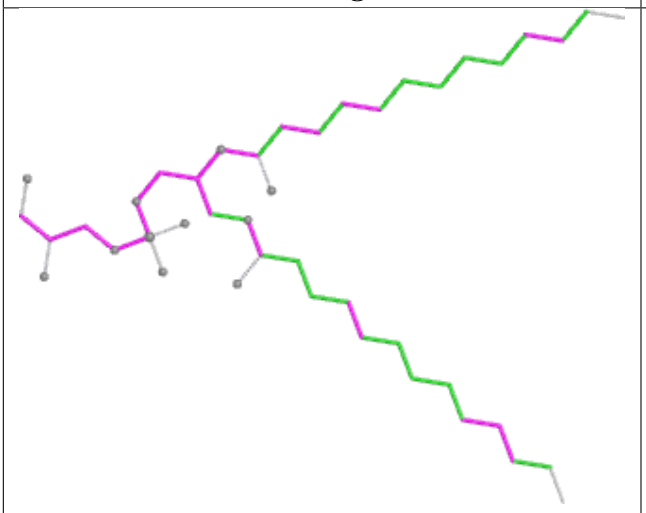


Bond angles



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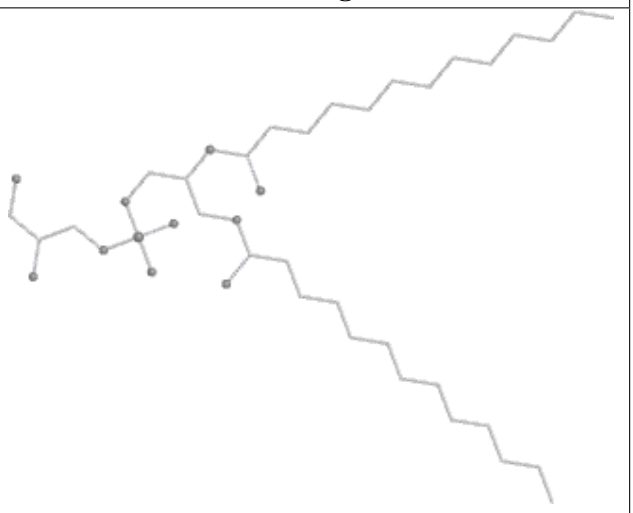
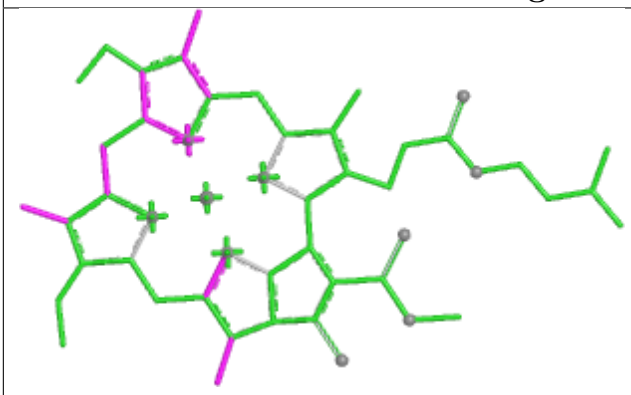


Rings

Ligand CLA 6 304



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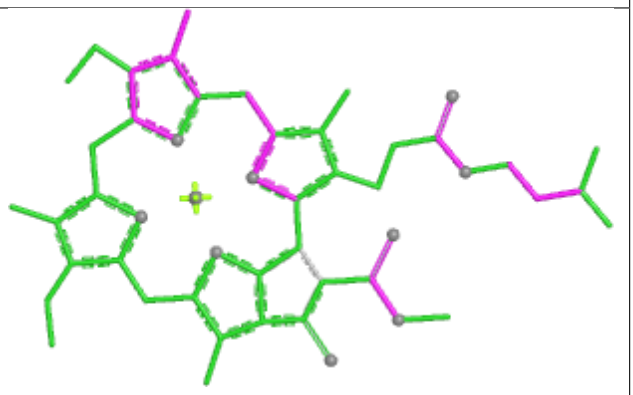
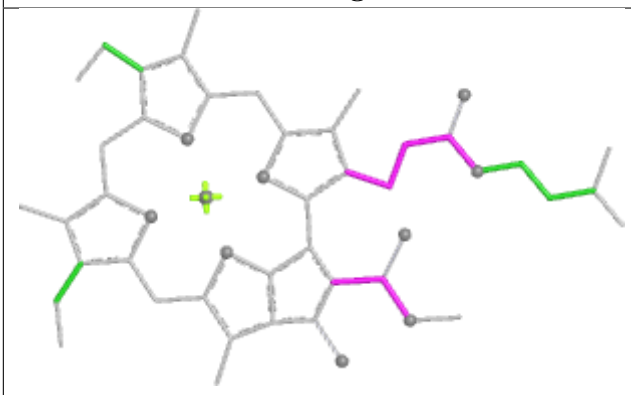


Bond angles



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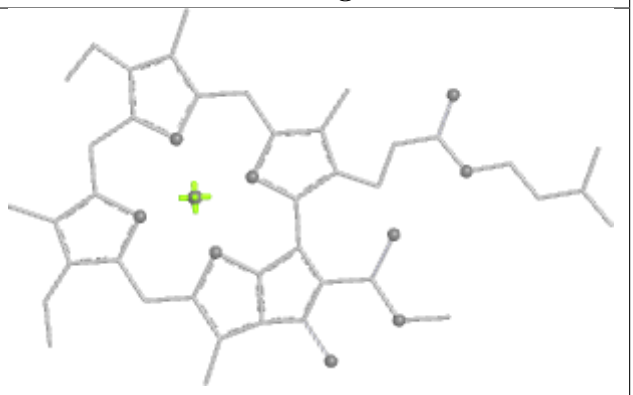
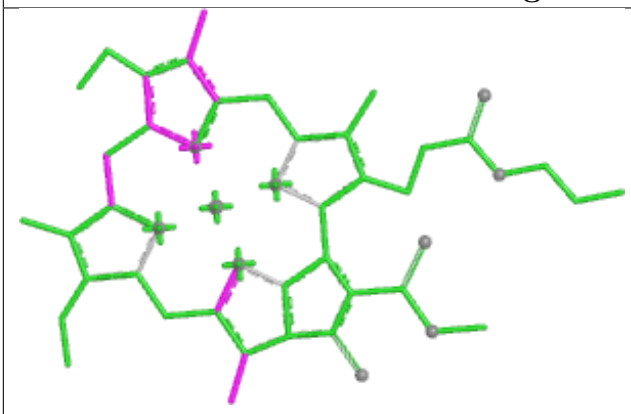


Rings

Ligand CLA N 308



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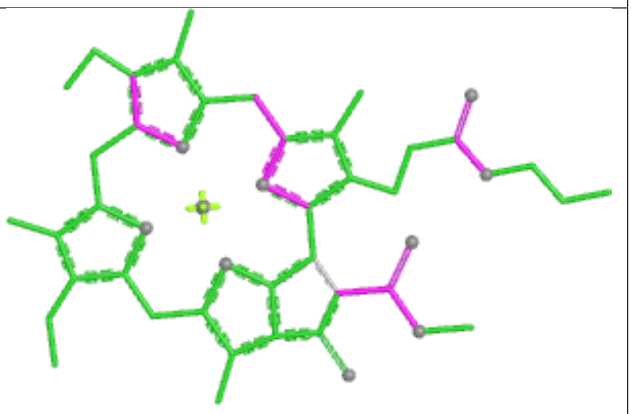
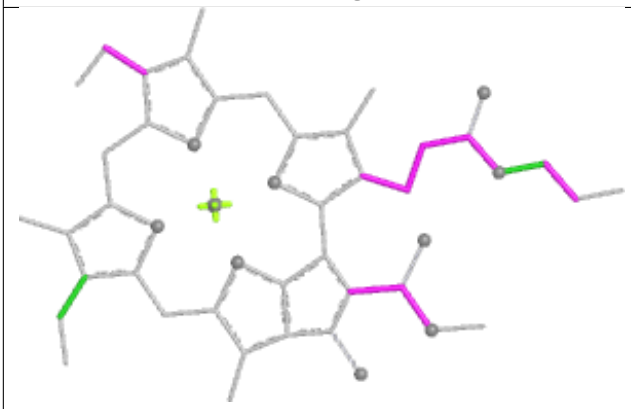


Bond angles



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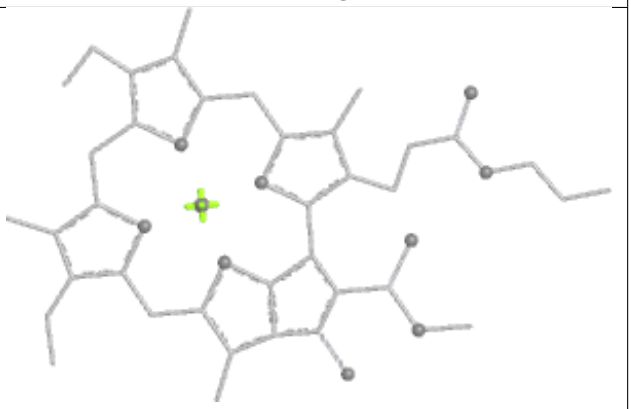
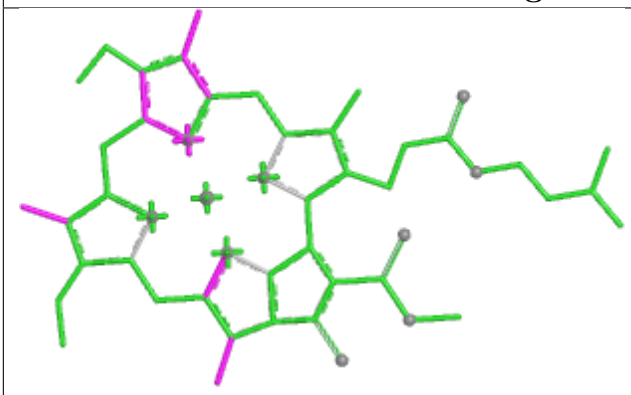


Rings

Ligand CLA P 304



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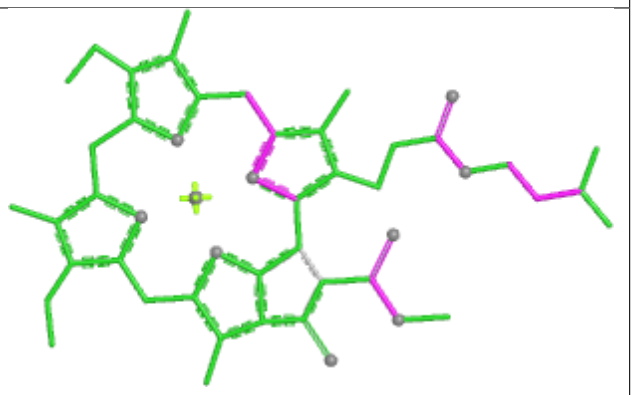
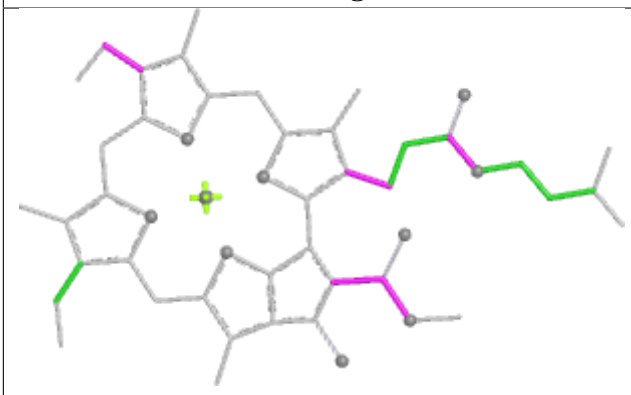


Bond angles



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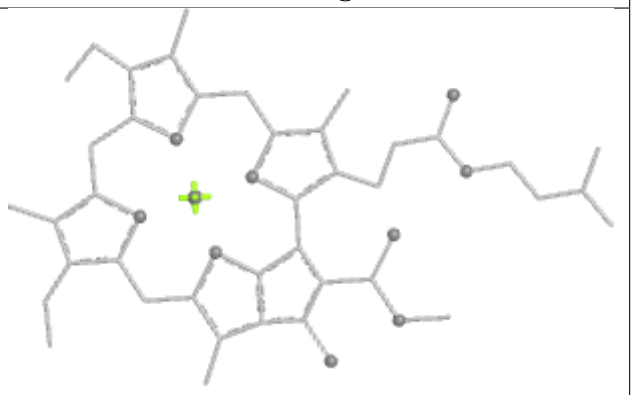
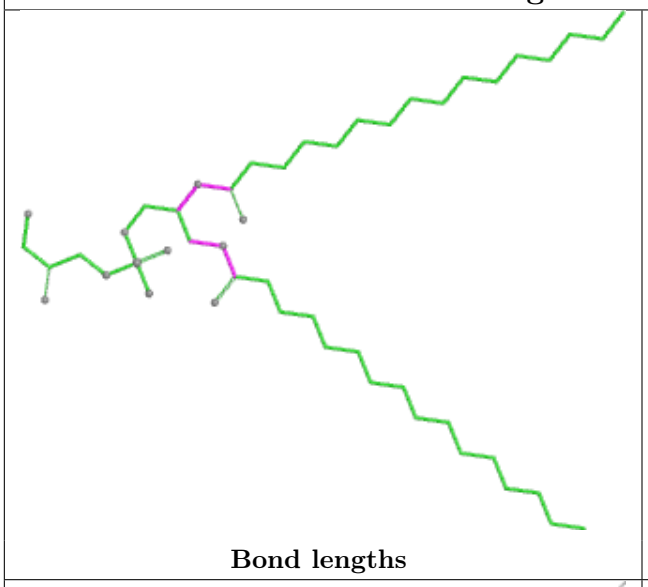


Rings

Ligand LHG u 312



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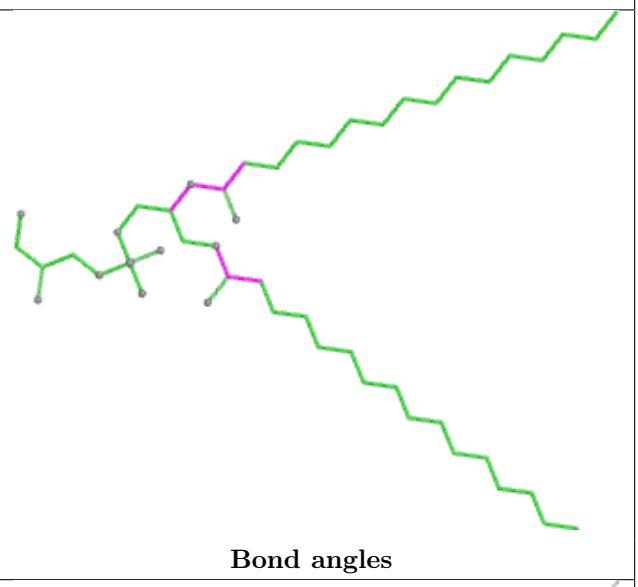
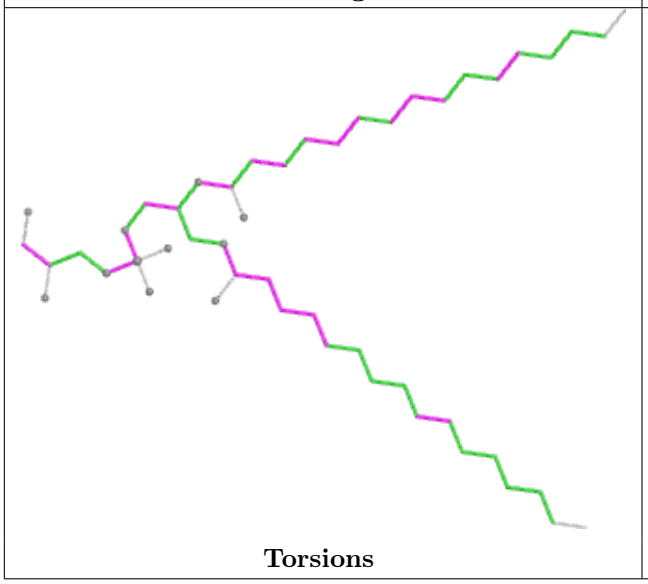
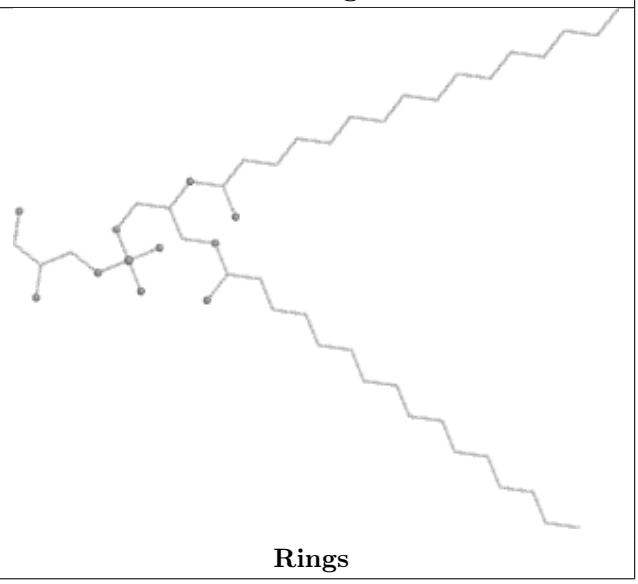


Bond angles

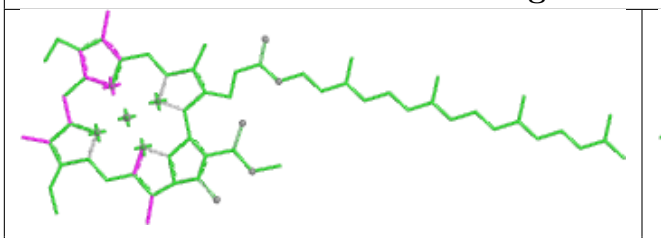


Torsions



Rings

Ligand CLA n 301



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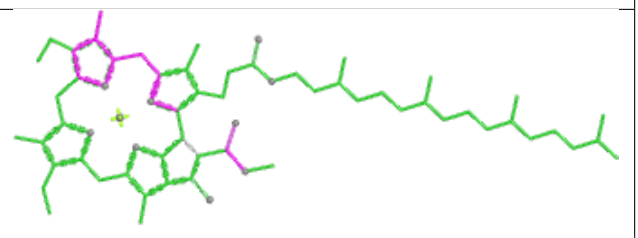
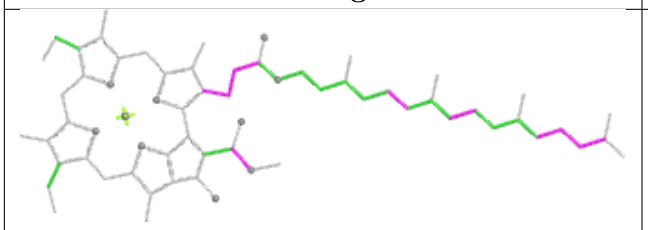
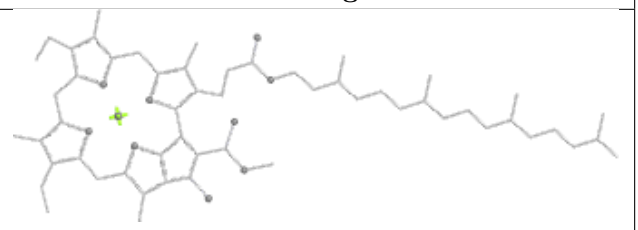


Bond angles

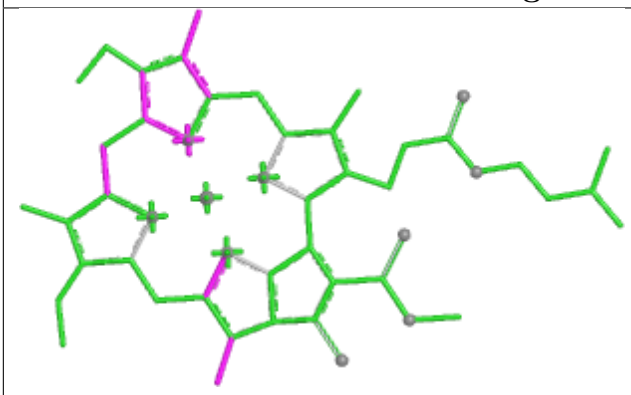


Torsions

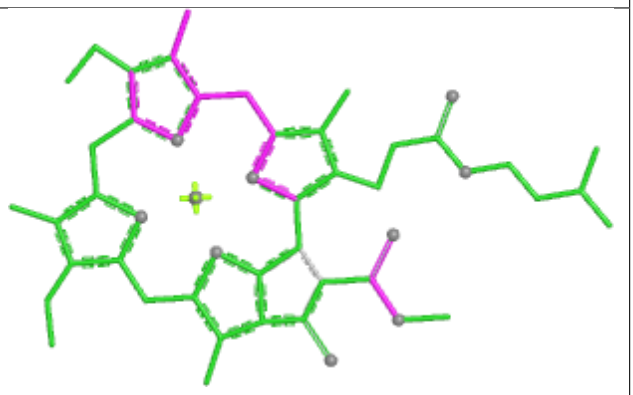


Rings

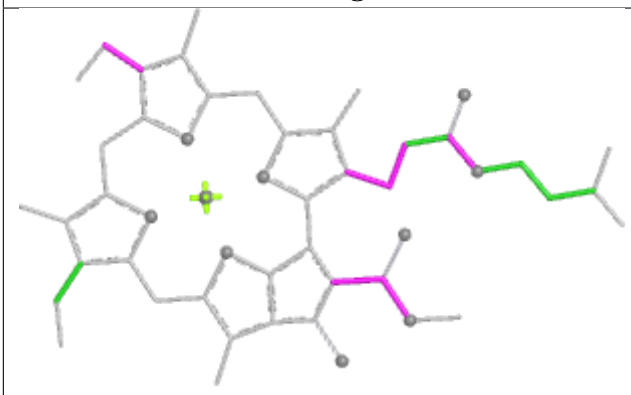
Ligand CLA G 303



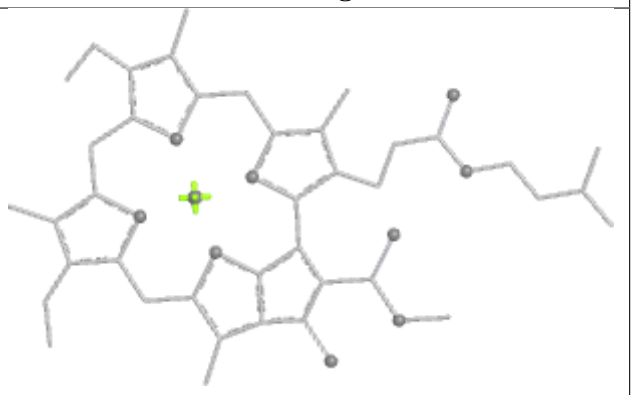
Bond lengths



Bond angles

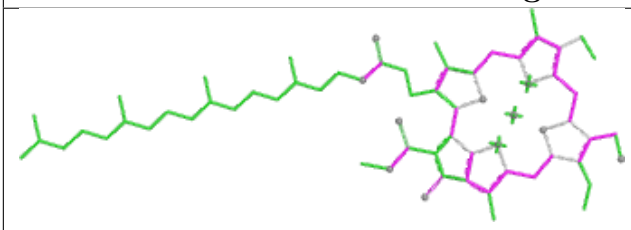


Torsions



Rings

Ligand CHL V 317



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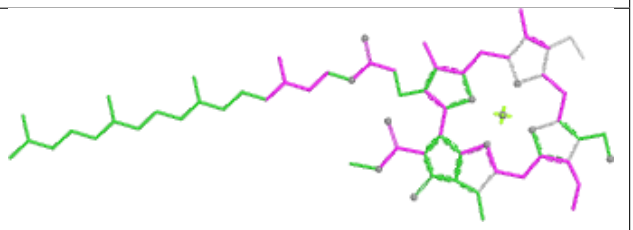
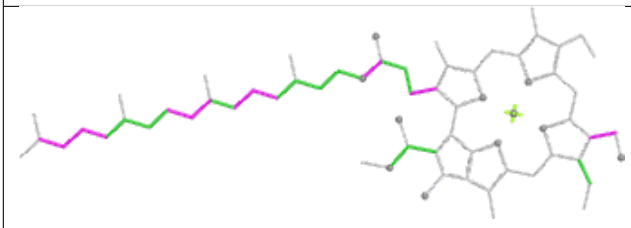
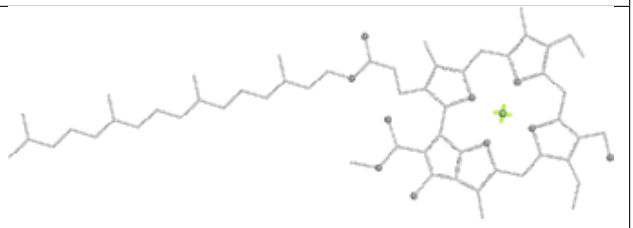


Bond angles

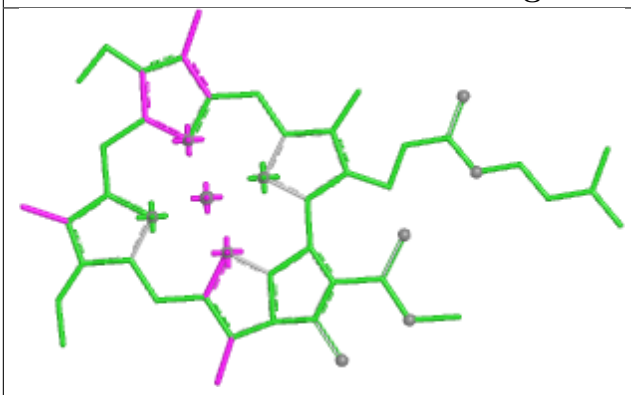


Torsions



Rings

Ligand CLA A 406



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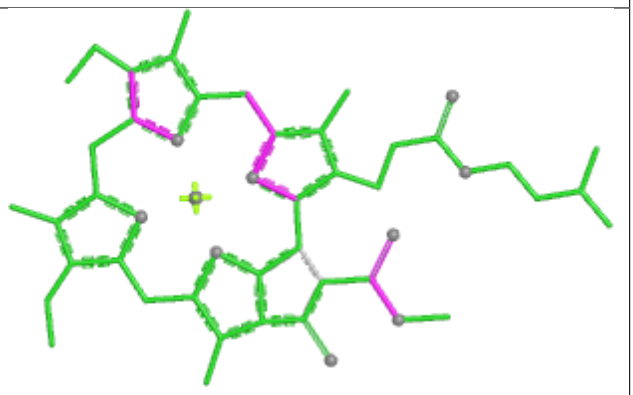

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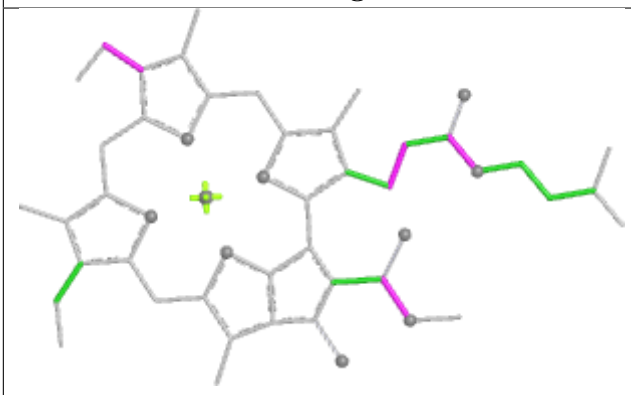

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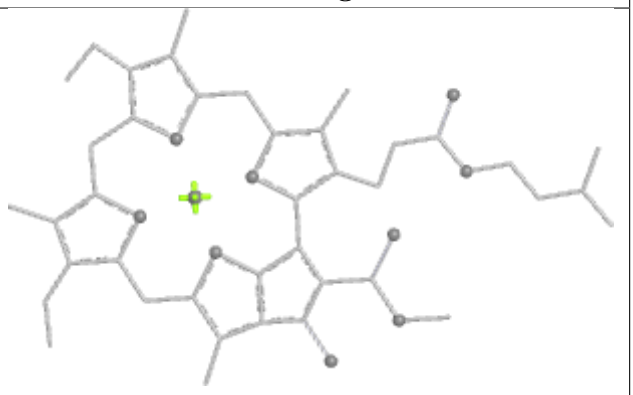
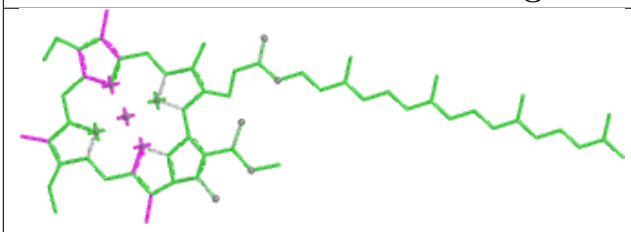


Rings

Ligand CLA B 602



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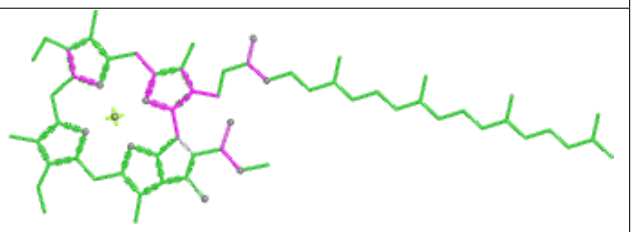

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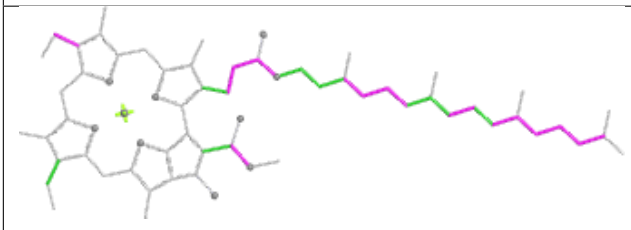

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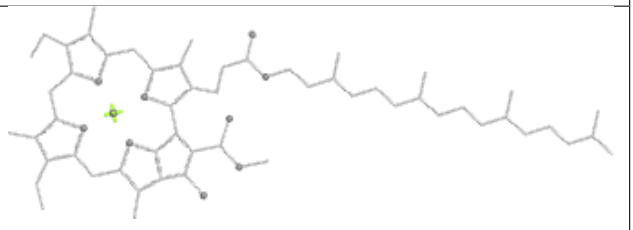
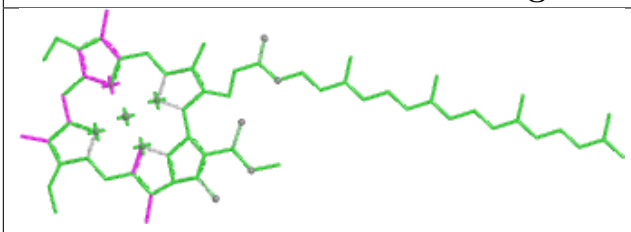


Rings

Ligand CLA 5 302



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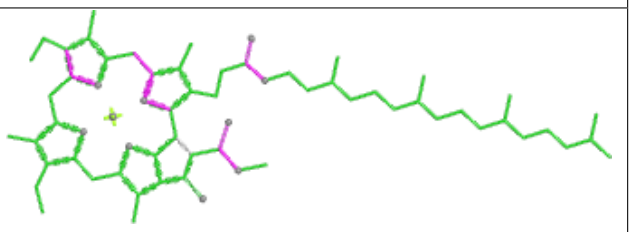
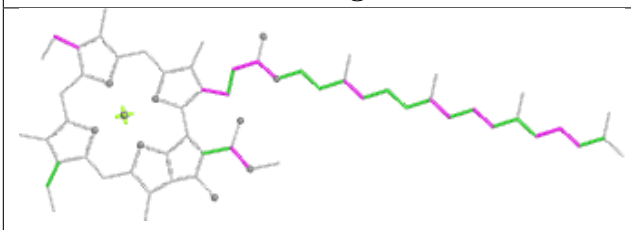


Bond angles



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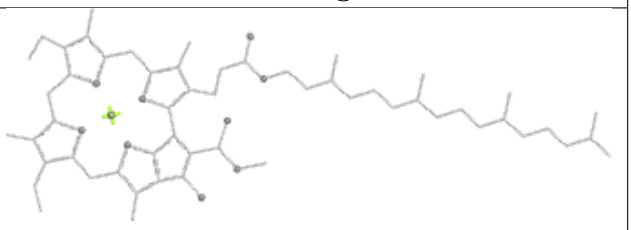
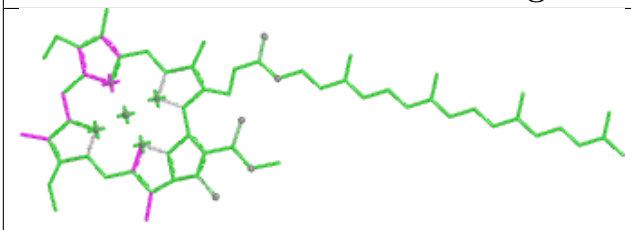


Rings

Ligand CLA q 307



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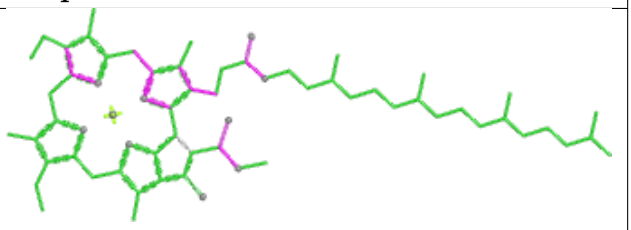

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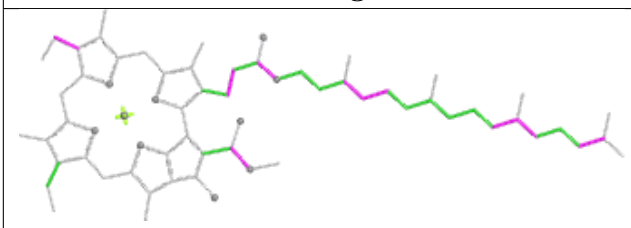

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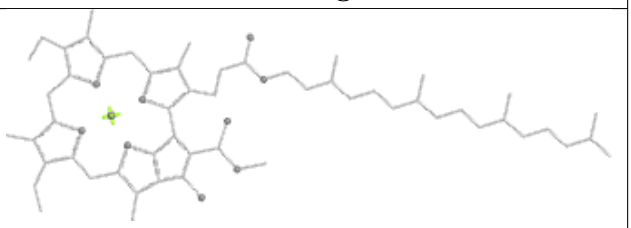
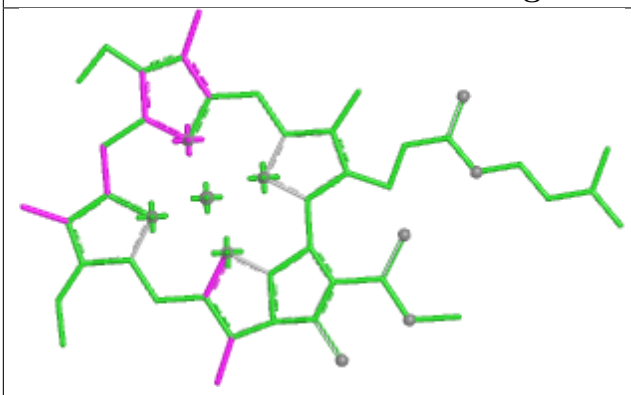


Rings

Ligand CLA N 303



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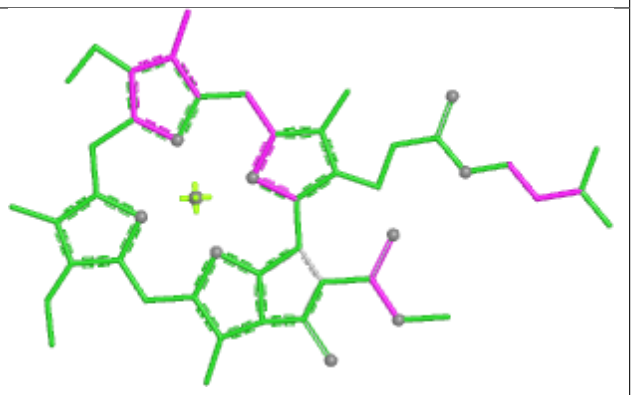
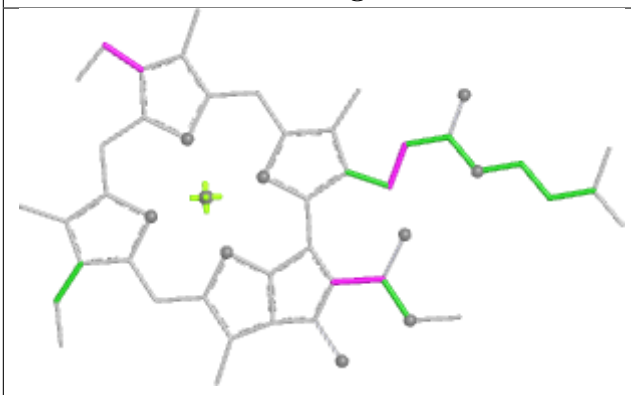


Bond angles



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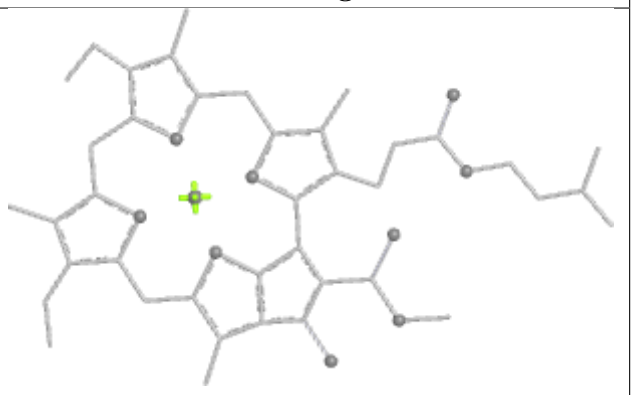
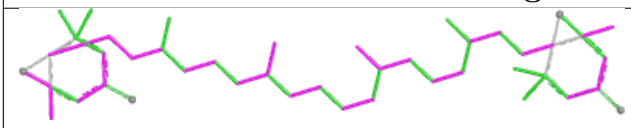


Rings

Ligand XAT P 312



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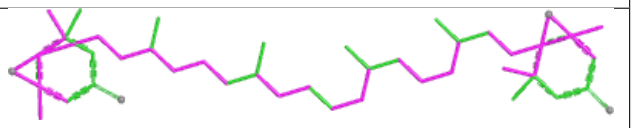
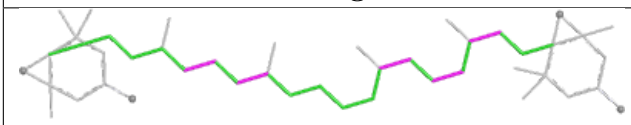


Bond angles



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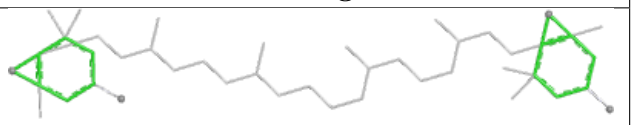
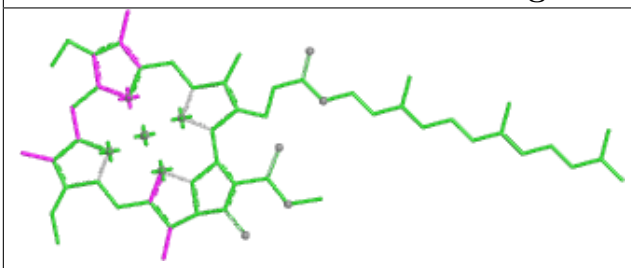
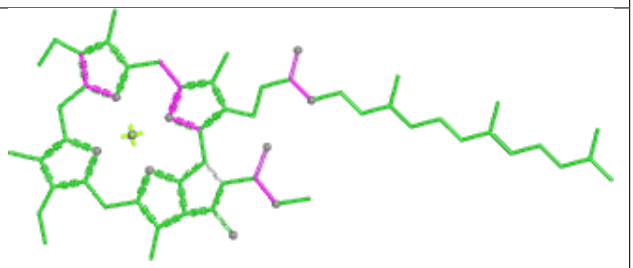
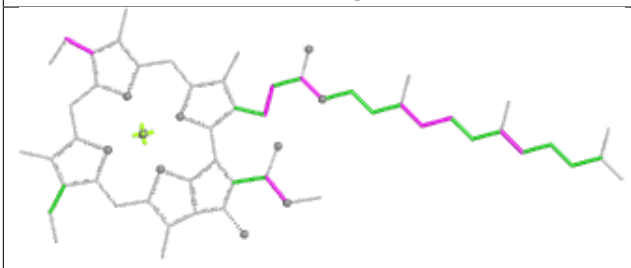
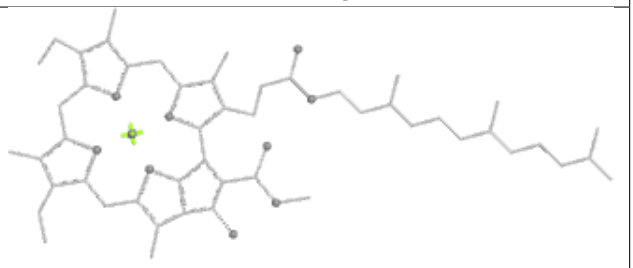
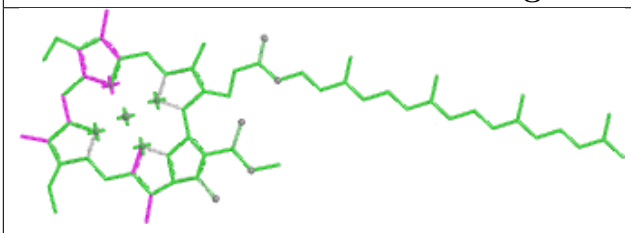
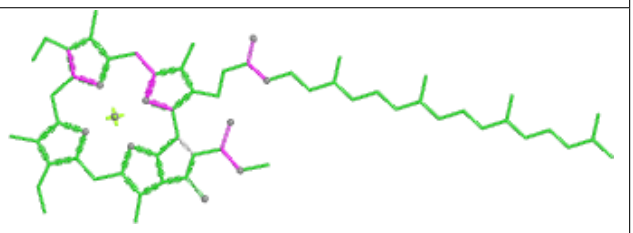
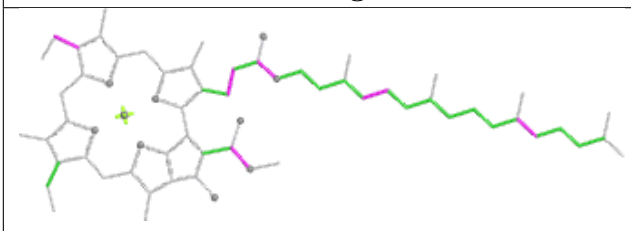
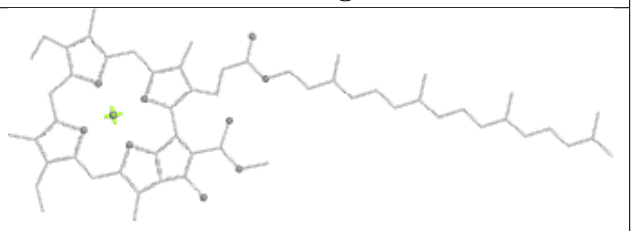
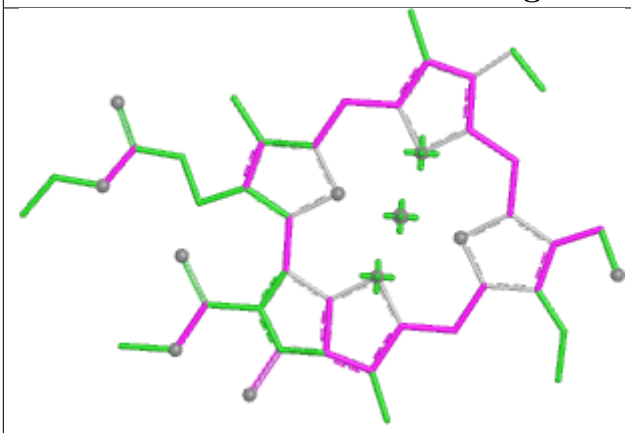


Rings

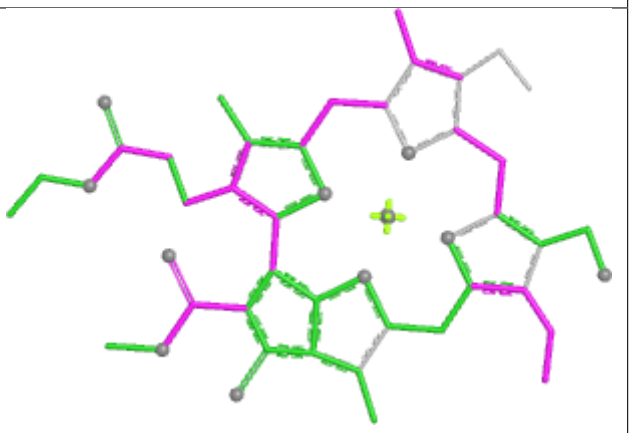
Ligand CLA 5 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA V 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

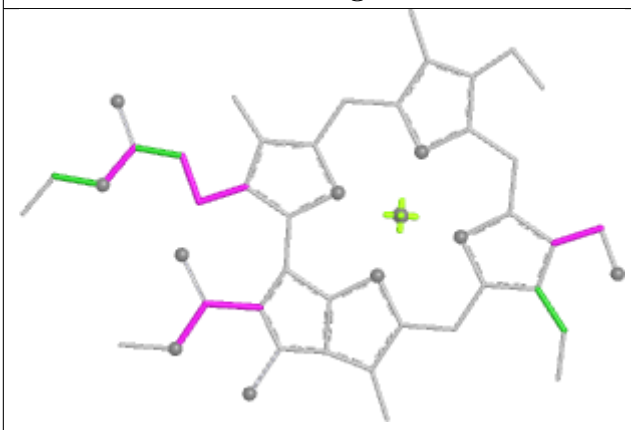
Ligand CHL V 314



Bond lengths



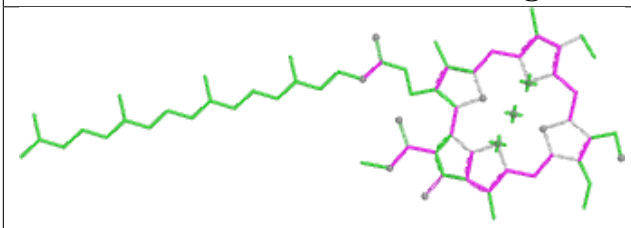
Bond angles



Torsions

Rings

Ligand CHL U 319



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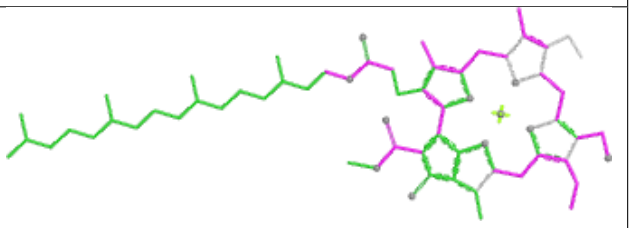
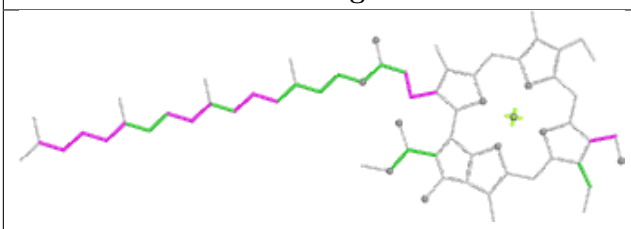
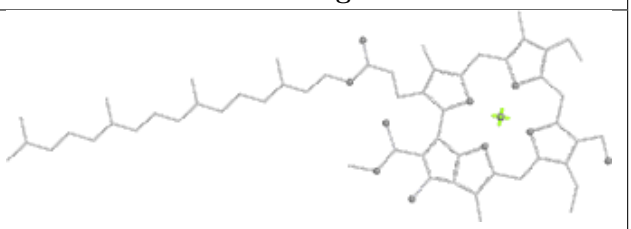


Bond angles

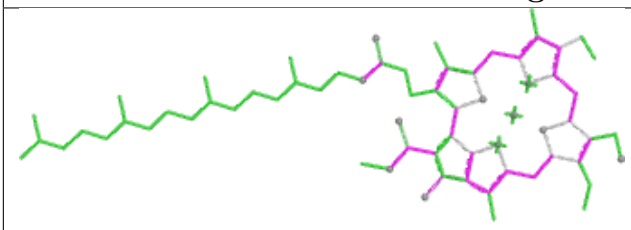


Torsions



Rings

Ligand CHL v 316



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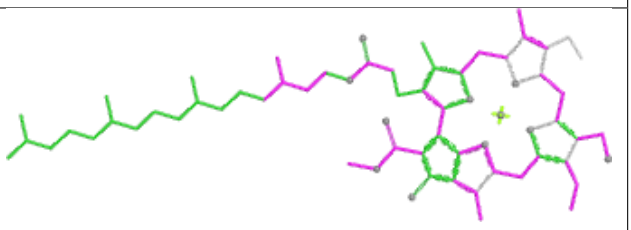
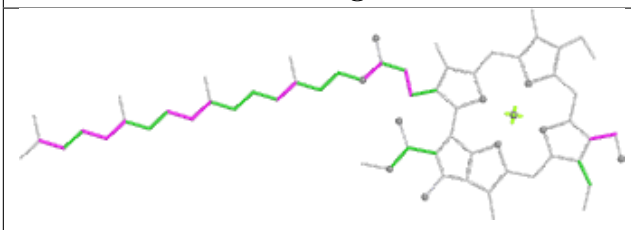


Bond angles



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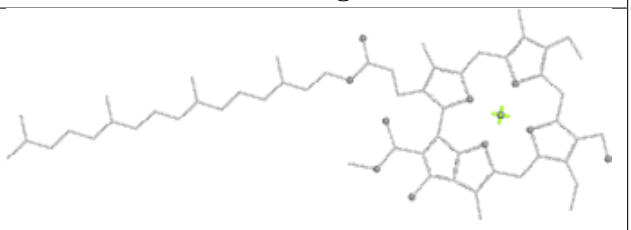
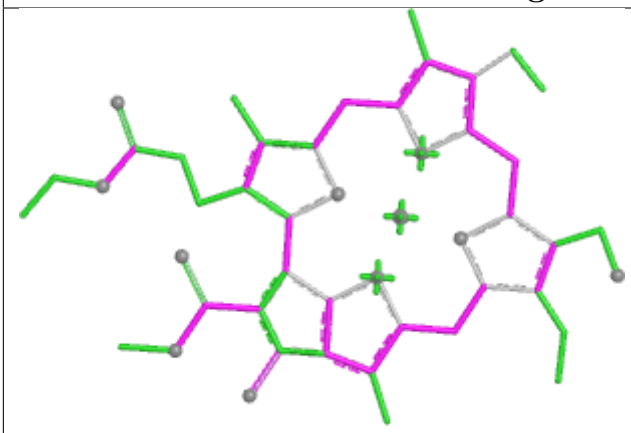


Rings

Ligand CHL 2 314



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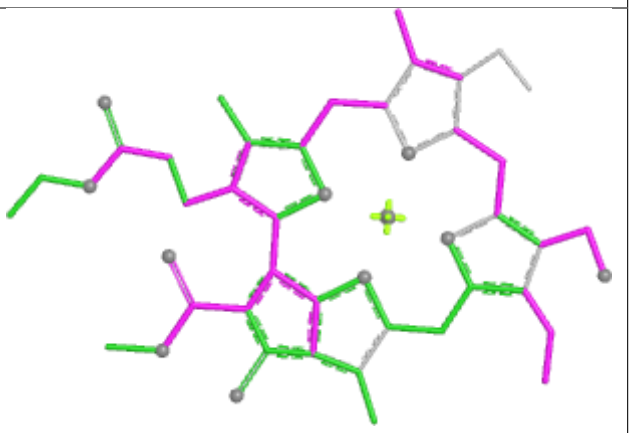
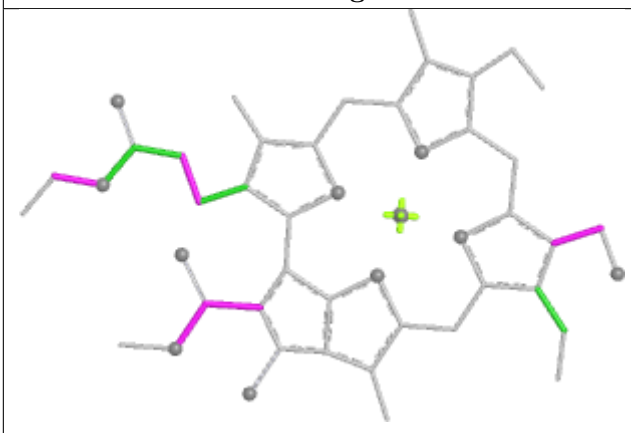


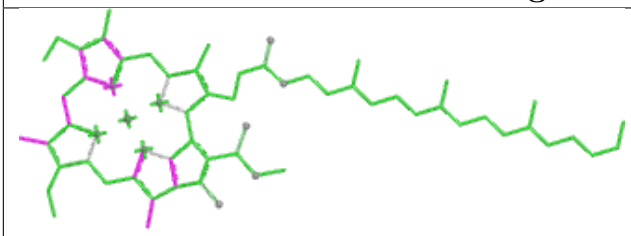
Bond angles



Torsions

Rings

Ligand CLA 6 305



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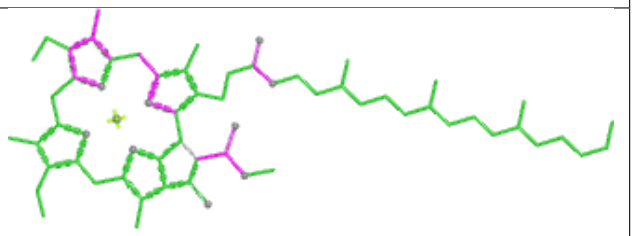
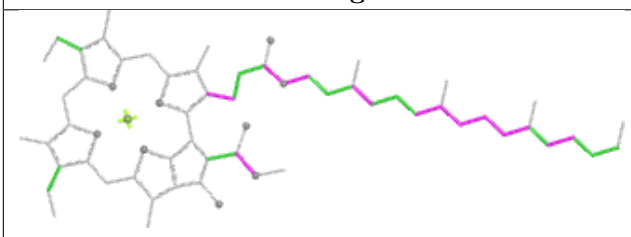
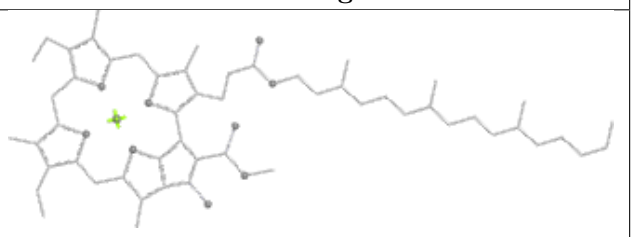


Bond angles

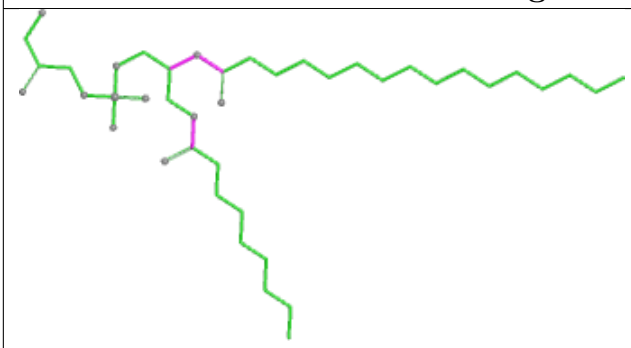


Torsions

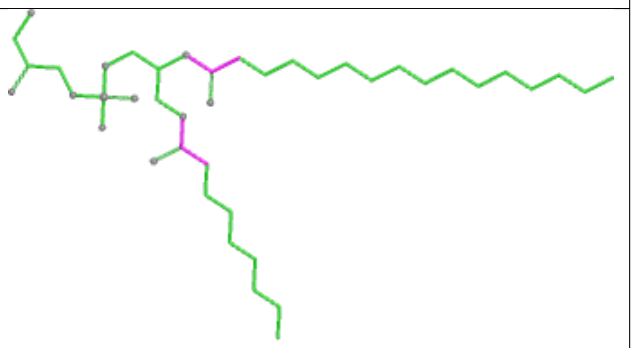


Rings

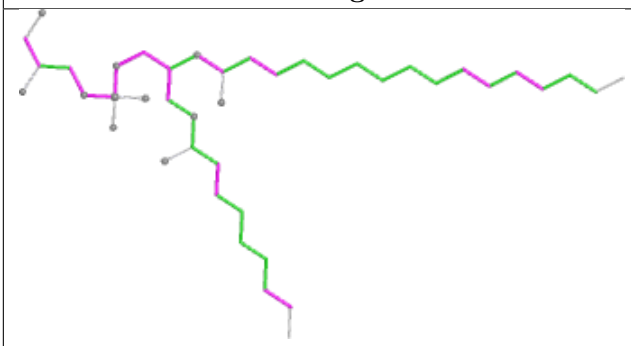
Ligand LHG r 613



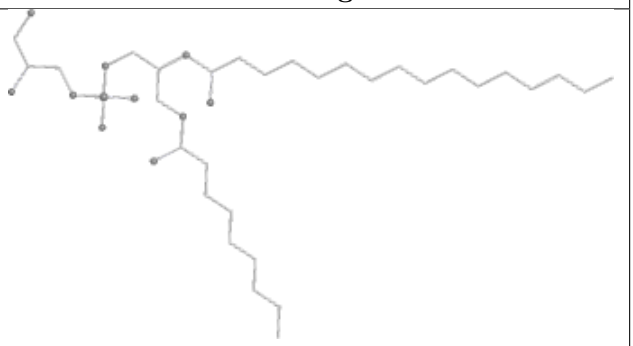
Bond lengths



Bond angles

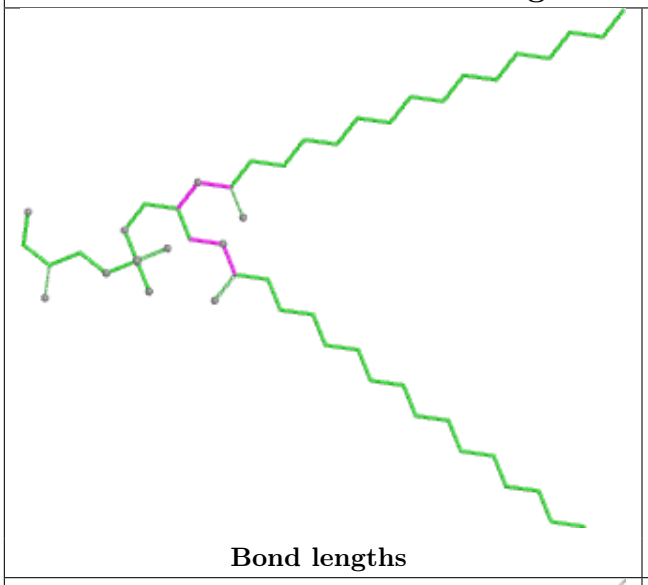


Torsions



Rings

Ligand LHG g 310



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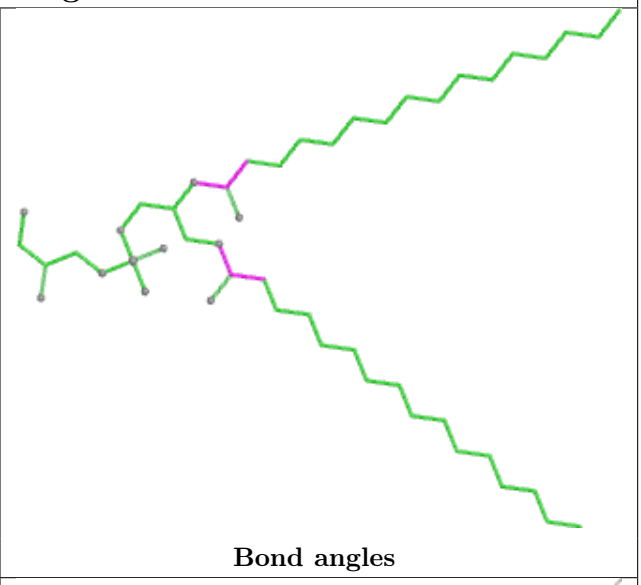

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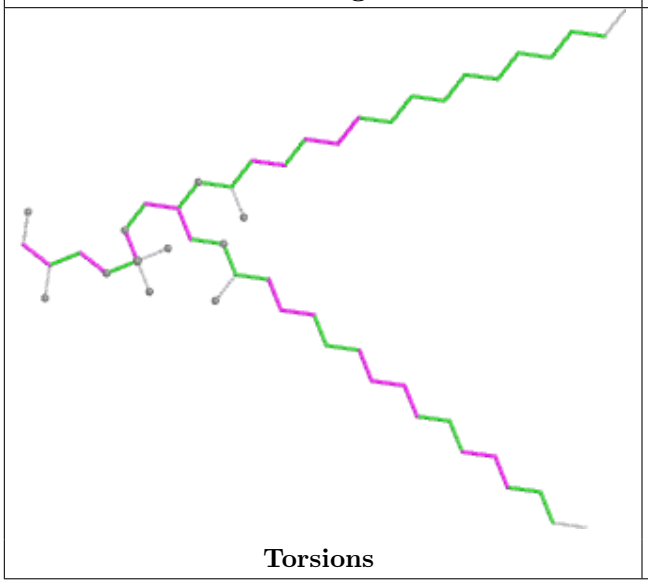

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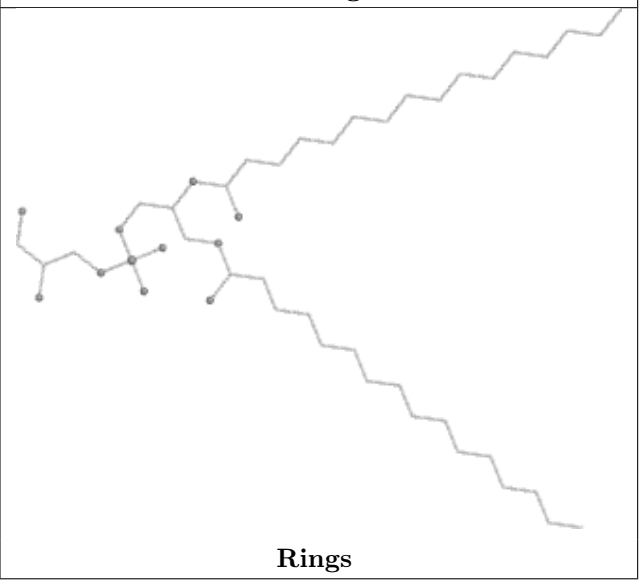

Rings

Ligand NEX r 618

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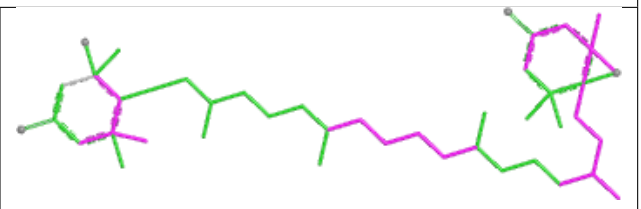

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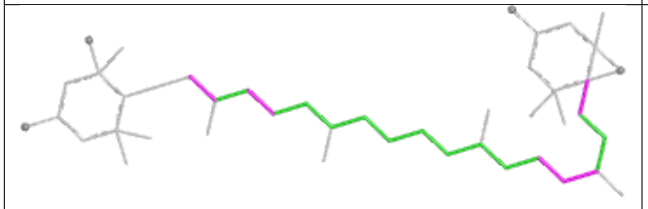

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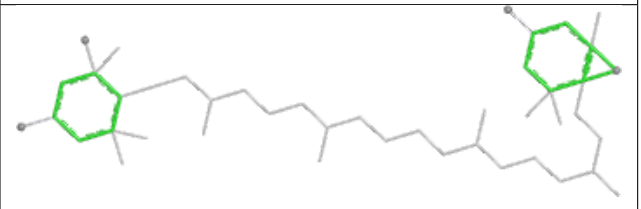
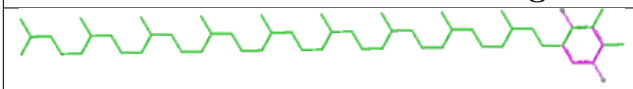


Rings

Ligand PL9 D 405



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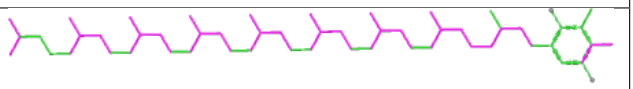

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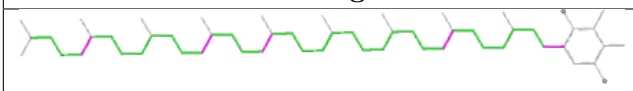

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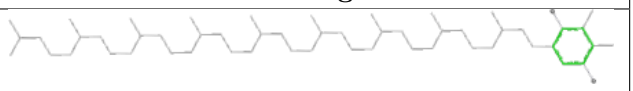
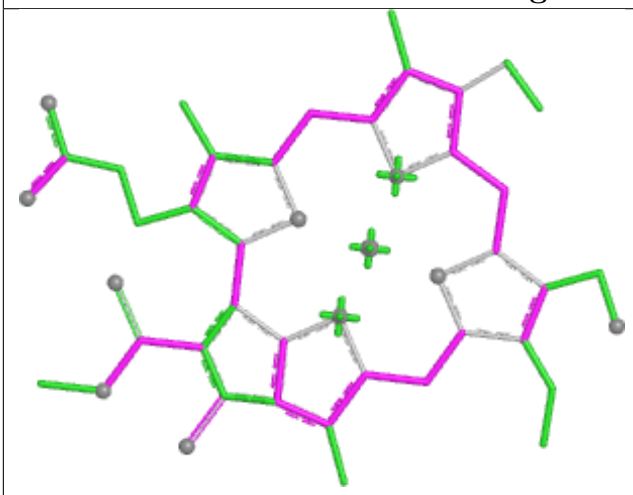


Rings

Ligand CHL s 313



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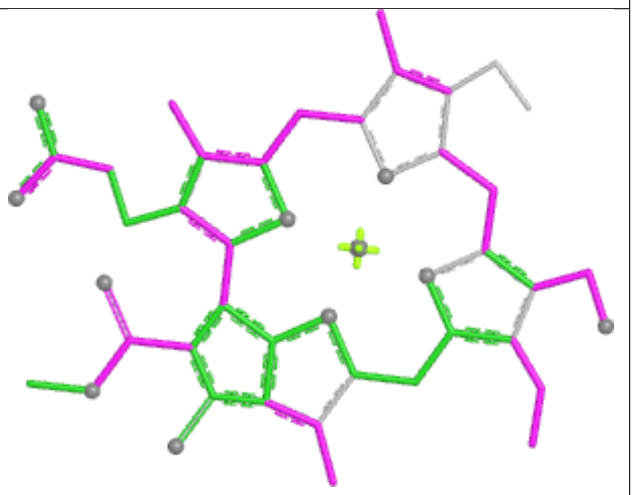

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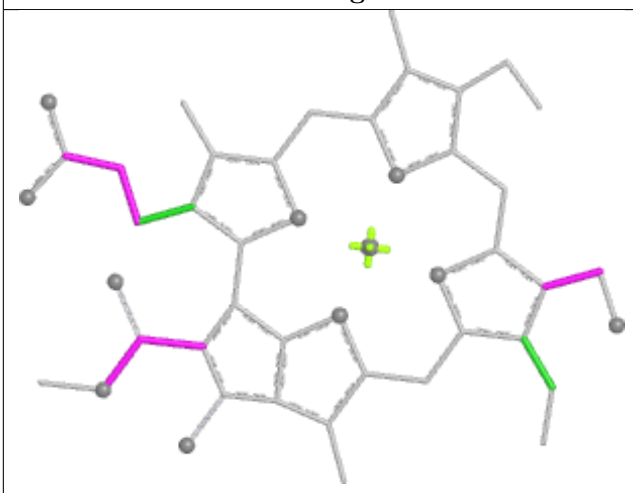

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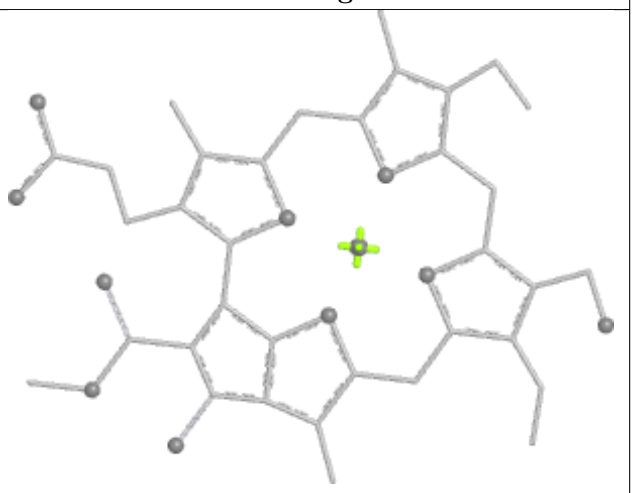
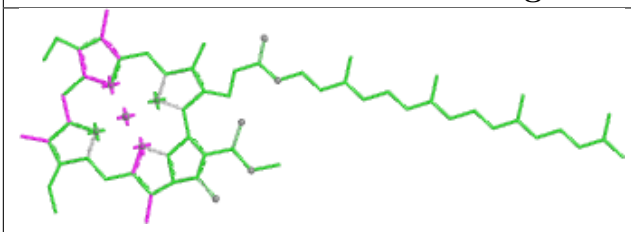


Rings

Ligand CLA C 505



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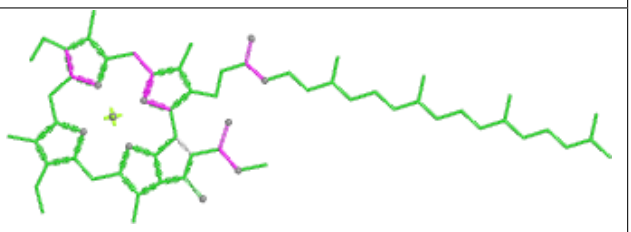
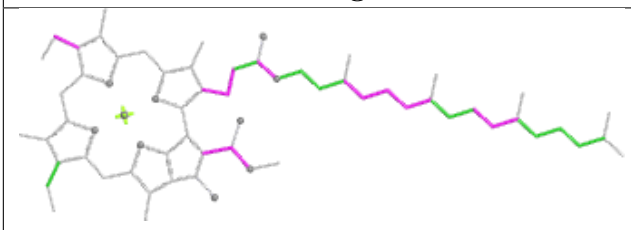


Bond angles



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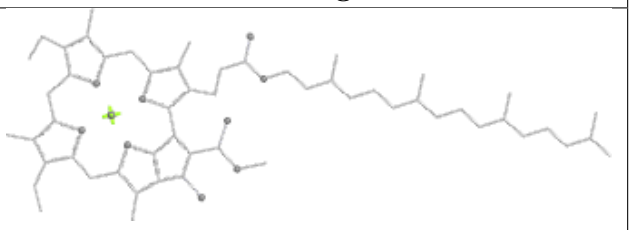
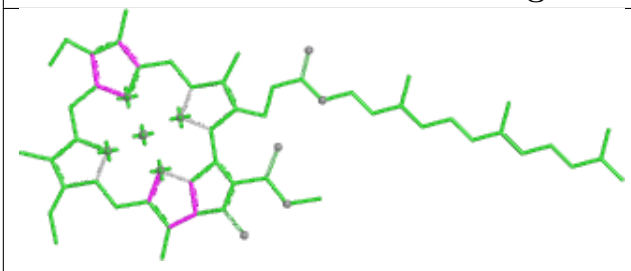


Rings

Ligand CLA n 305



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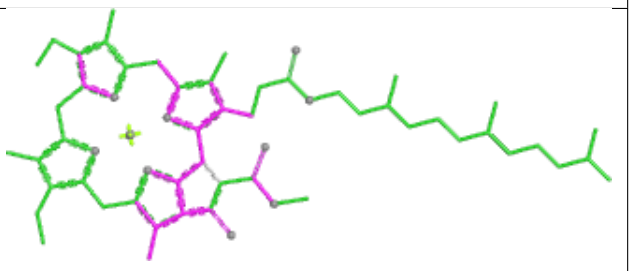

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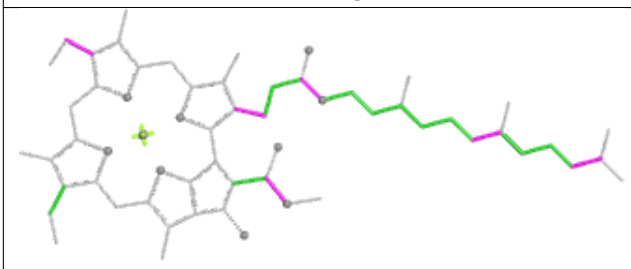

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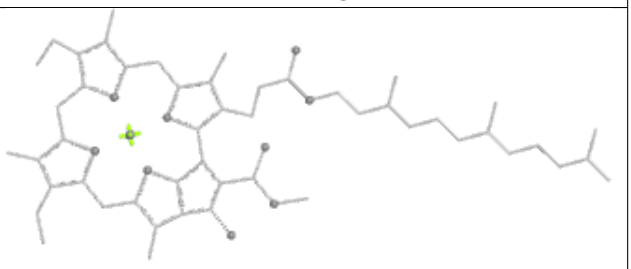
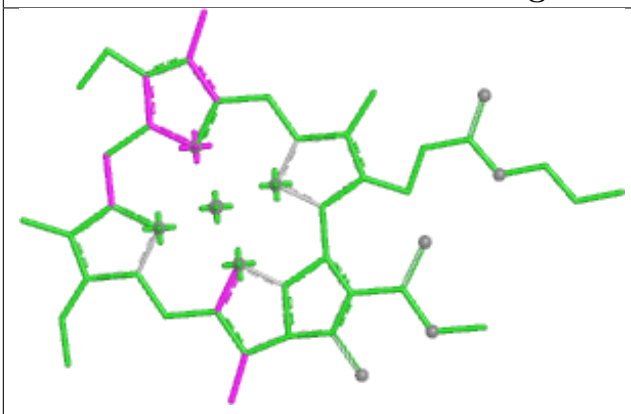


Rings

Ligand CLA 6 309



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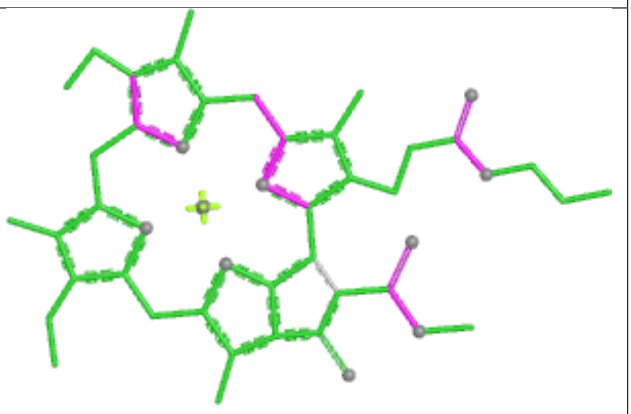

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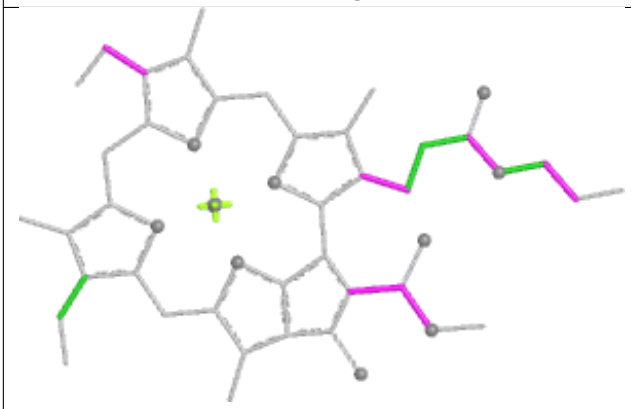

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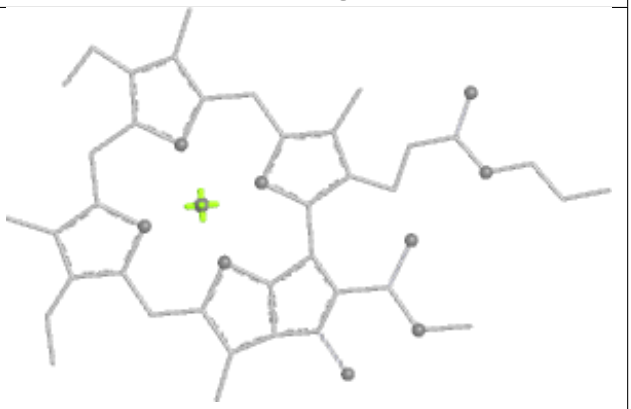
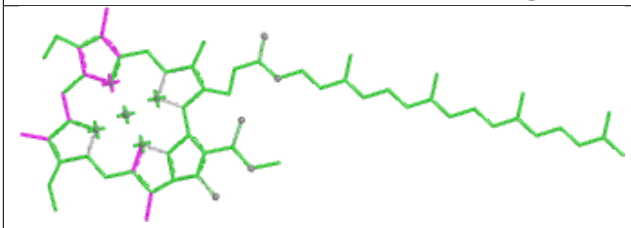


Rings

Ligand CLA G 307



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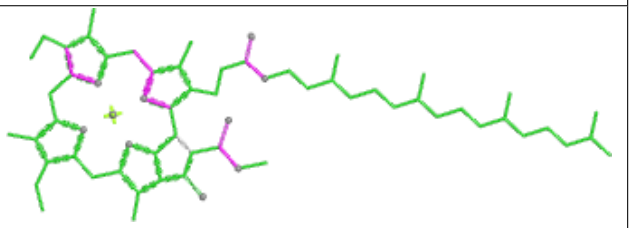
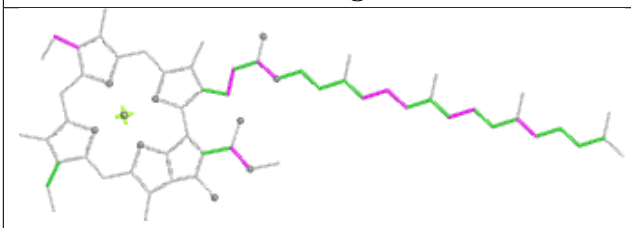


Bond angles



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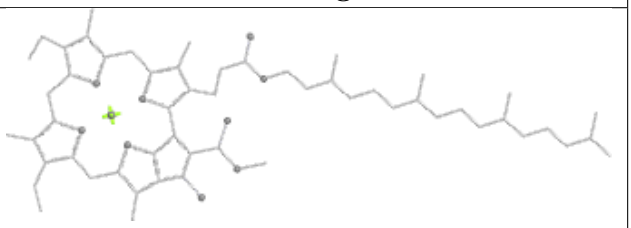
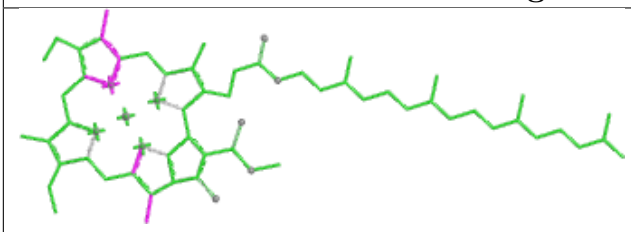


Rings

Ligand CLA b 605



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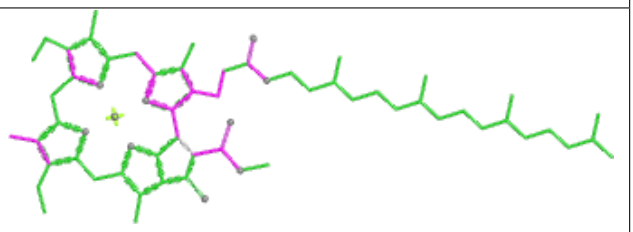

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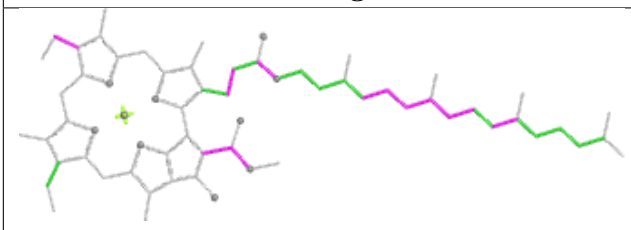

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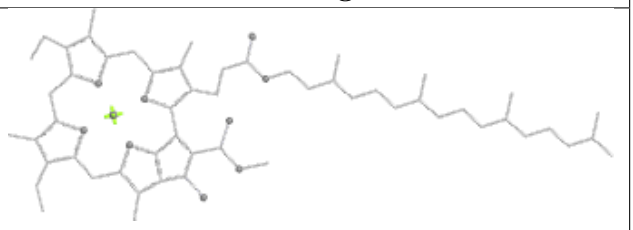
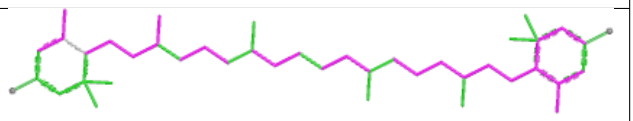


Rings

Ligand LUT n 310

Bond lengths



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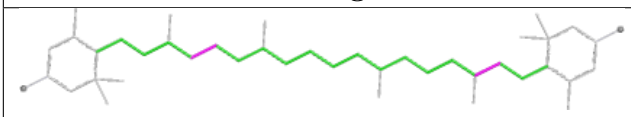

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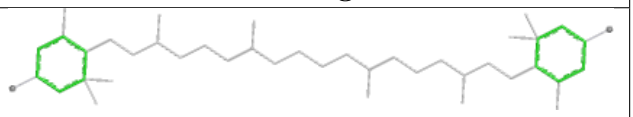
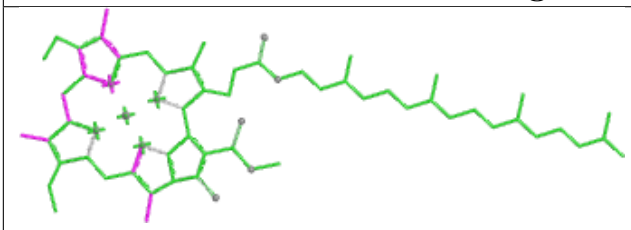


Rings

Ligand CLA 4 307



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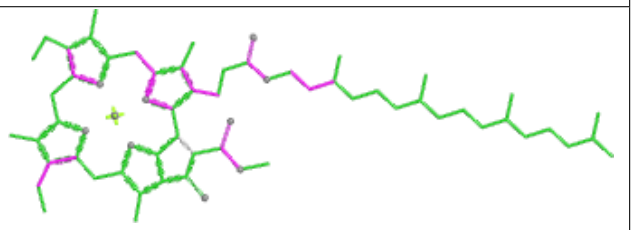
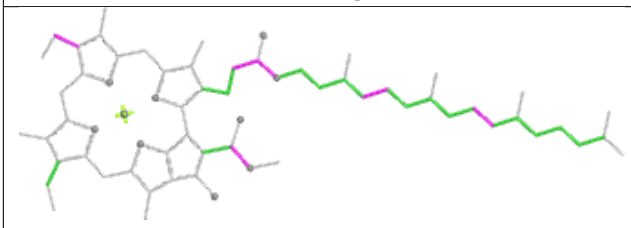


Bond angles



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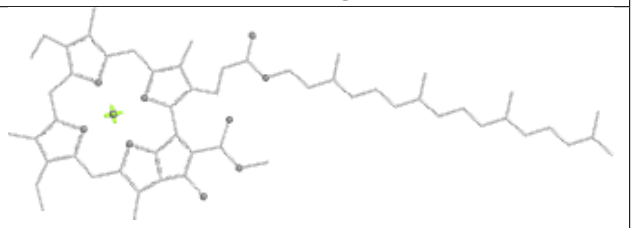
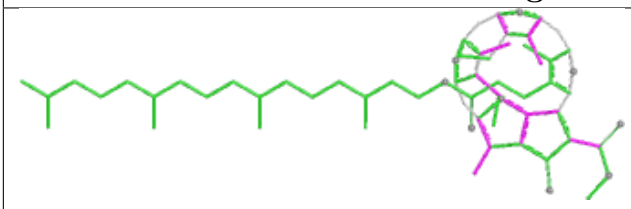


Rings

Ligand PHO a 407



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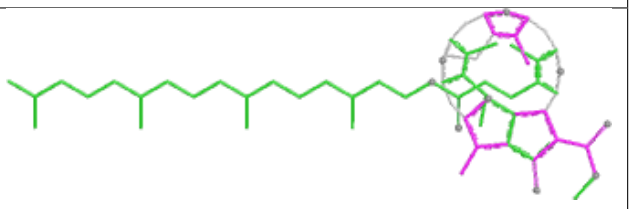
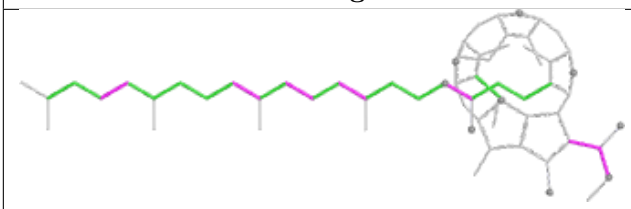
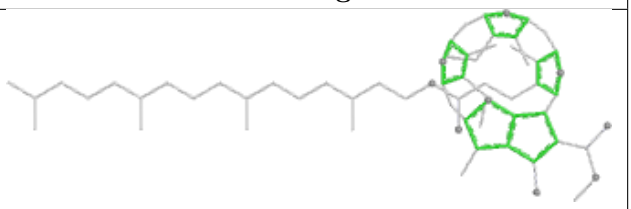


Bond angles

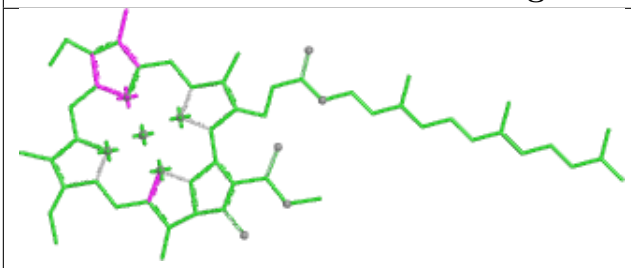


Torsions



Rings

Ligand CLA p 307



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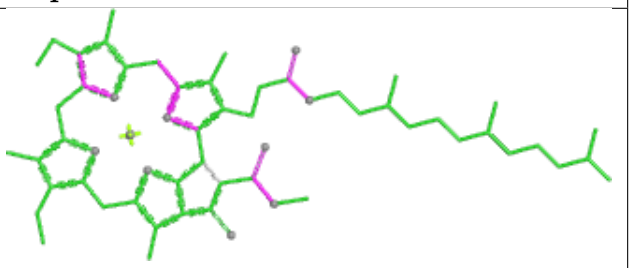
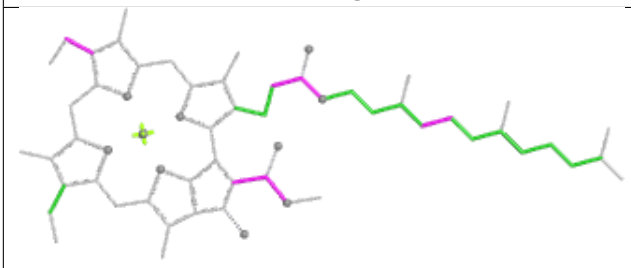


Bond angles



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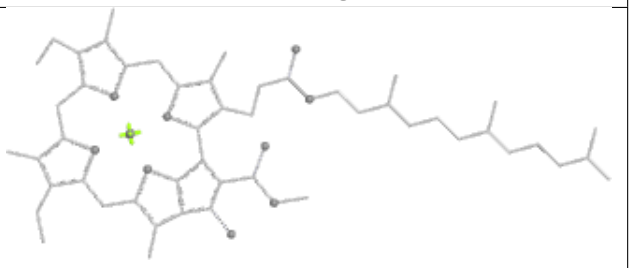
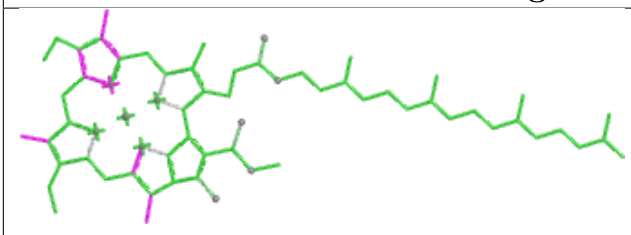
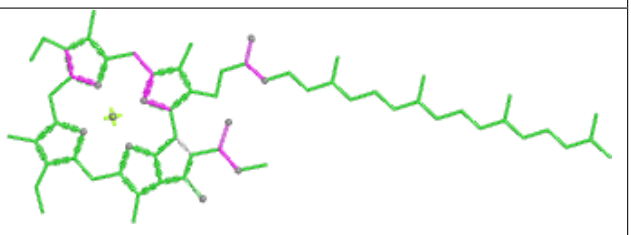


Rings

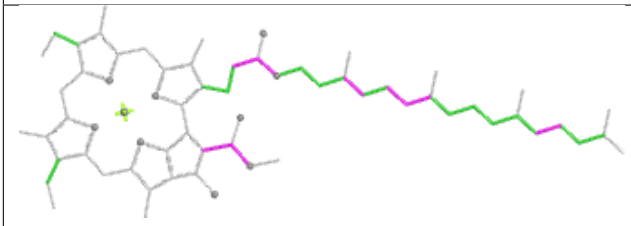
Ligand CLA 1 302



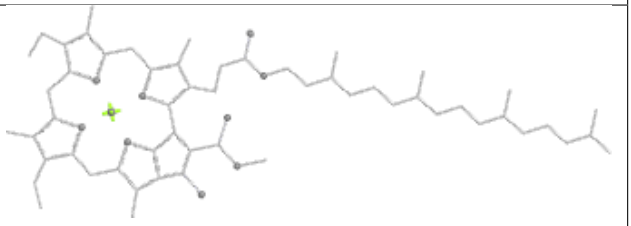
Bond lengths



Bond angles

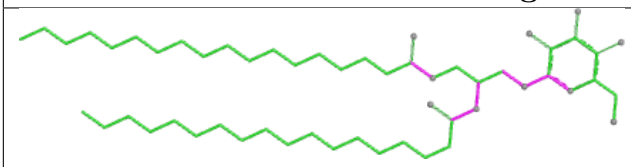


Torsions

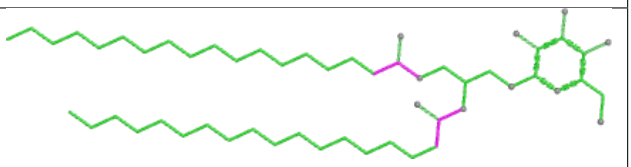


Rings

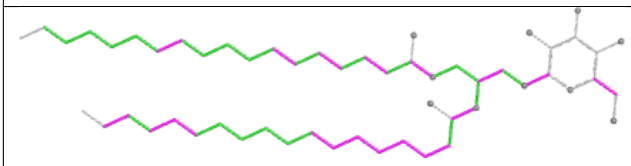
Ligand LMG B 624



Bond lengths



Bond angles



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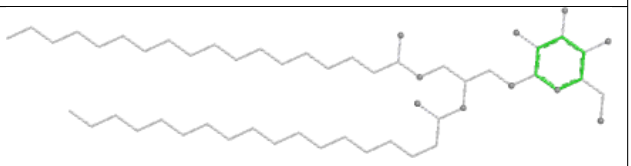
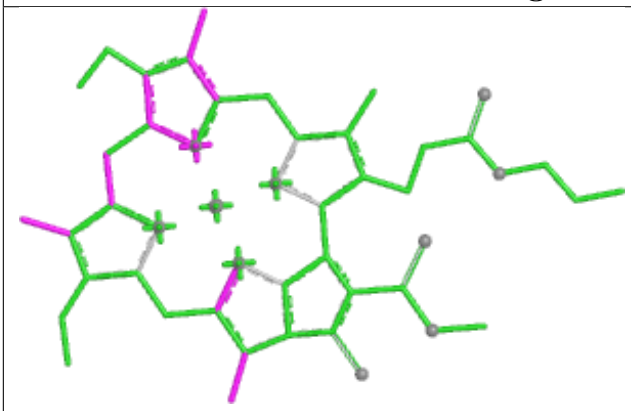


Rings

Ligand CLA u 308



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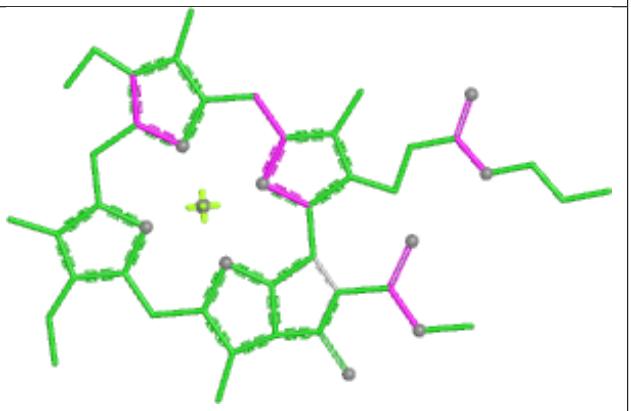

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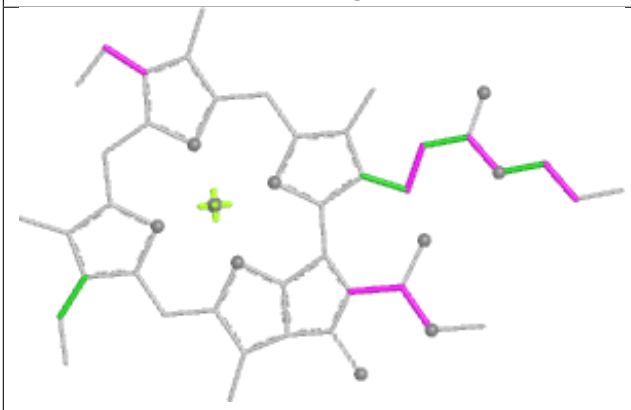

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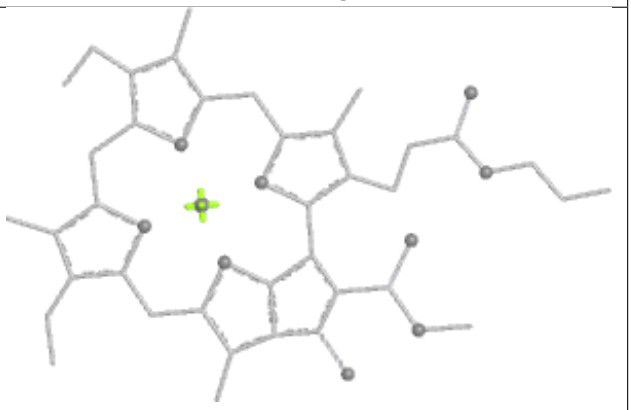
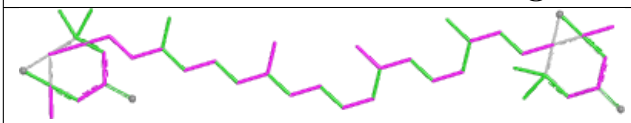


Rings

Ligand XAT g 309



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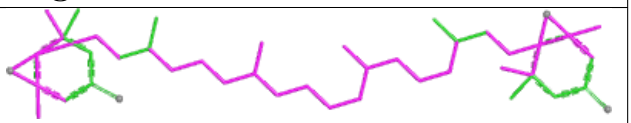

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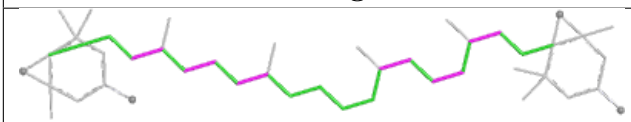

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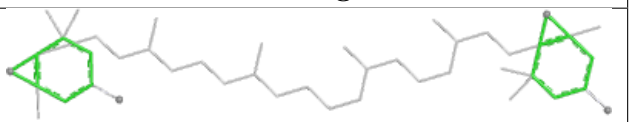
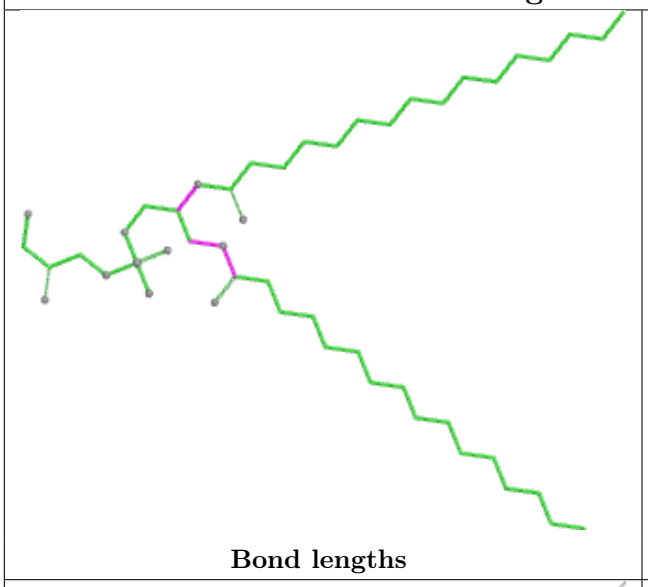


Rings

Ligand LHG L 101



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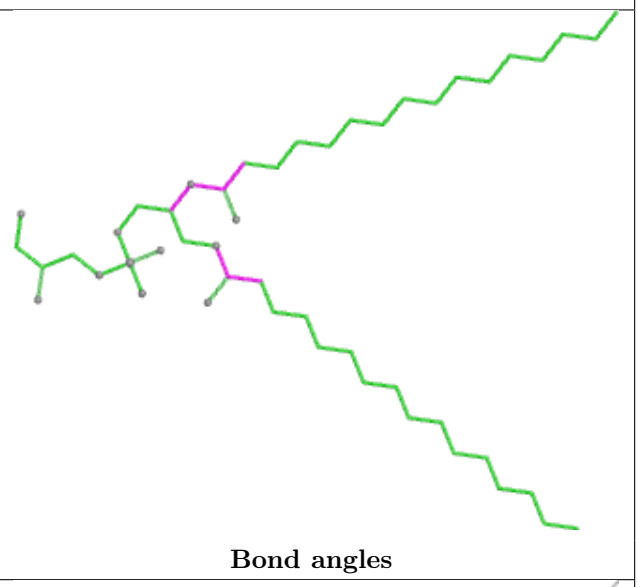
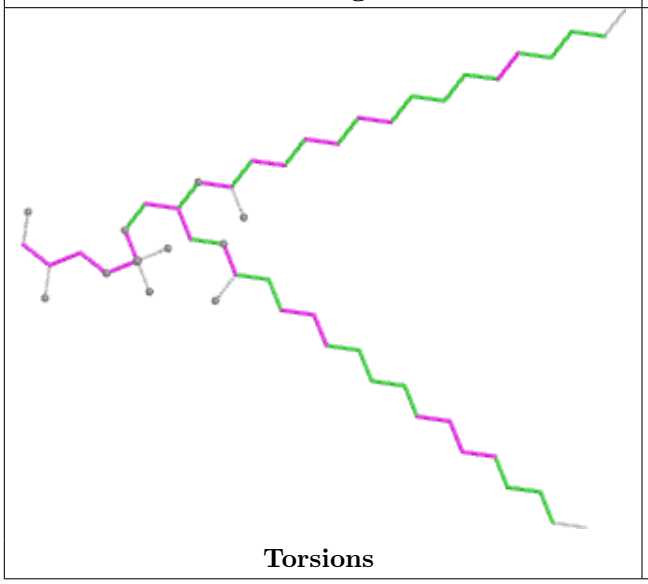


Bond angles



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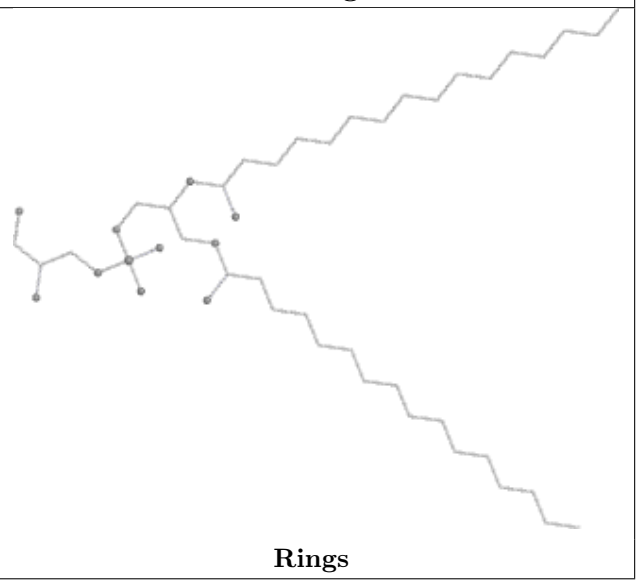
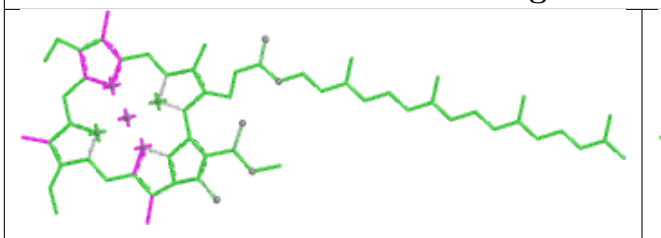


Rings

Ligand CLA a 404



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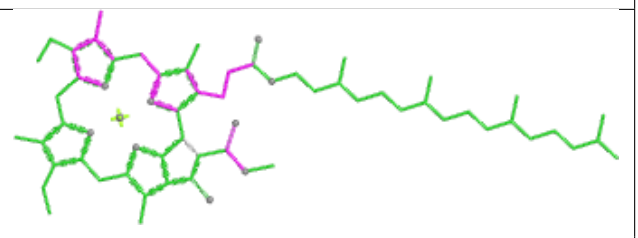
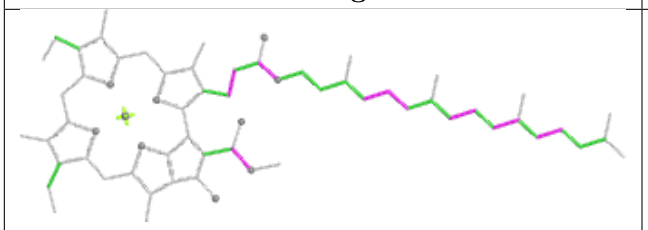


Bond angles



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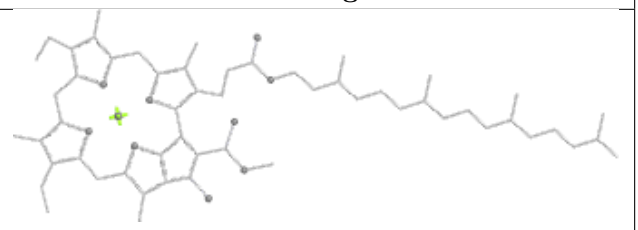
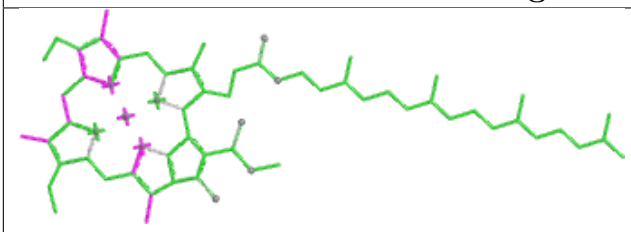


Rings

Ligand CLA 1 307



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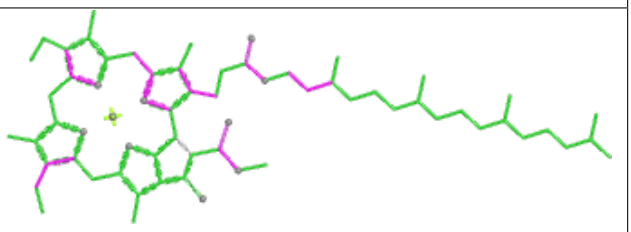
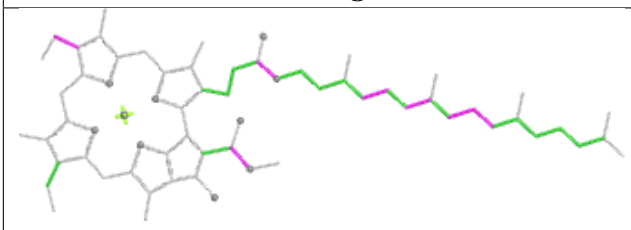


Bond angles



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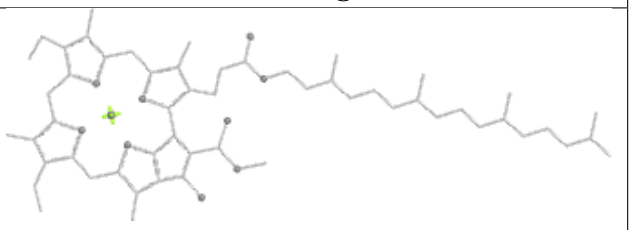
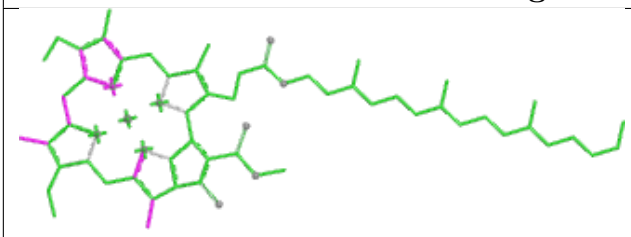


Rings

Ligand CLA g 304



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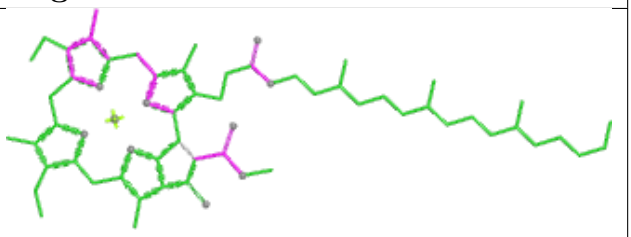
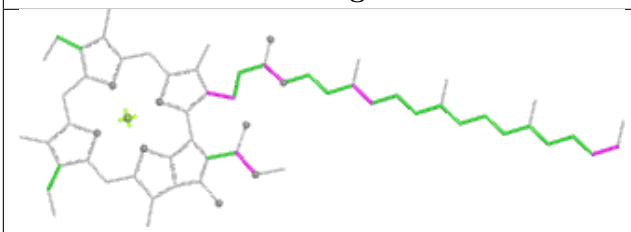


Bond angles



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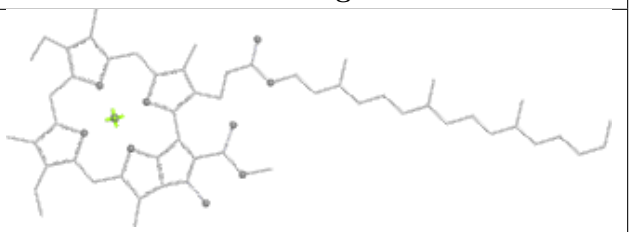
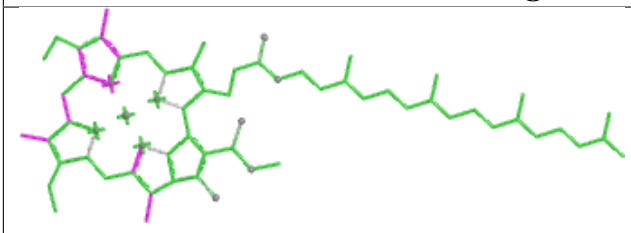


Rings

Ligand CLA C 512



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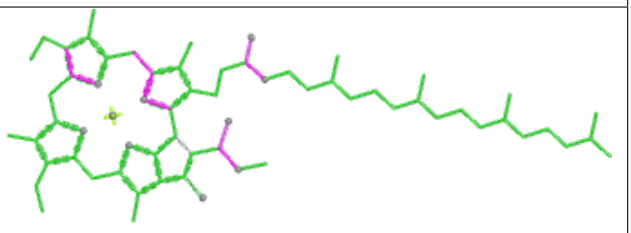
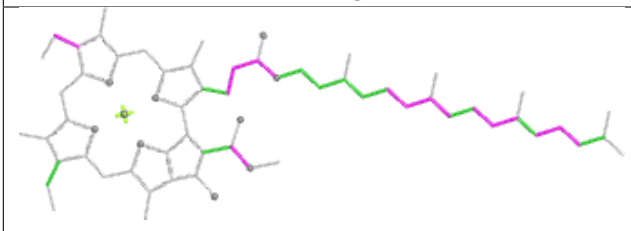


Bond angles



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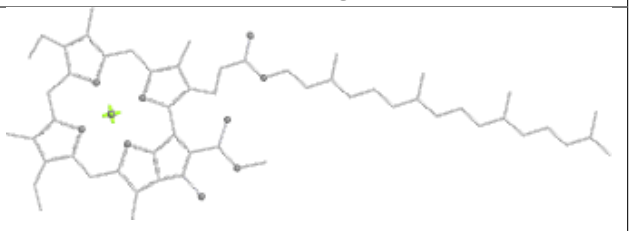
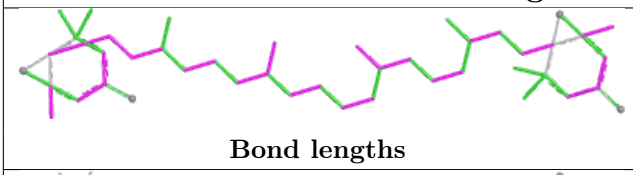


Rings

Ligand XAT p 312



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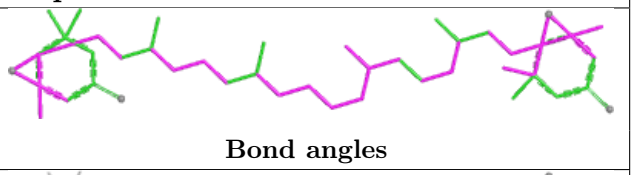
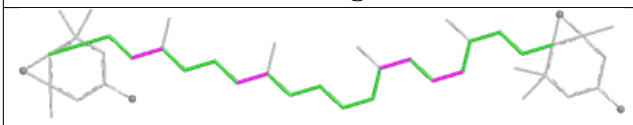


Bond angles



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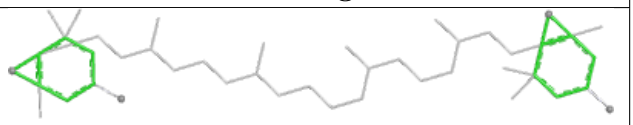
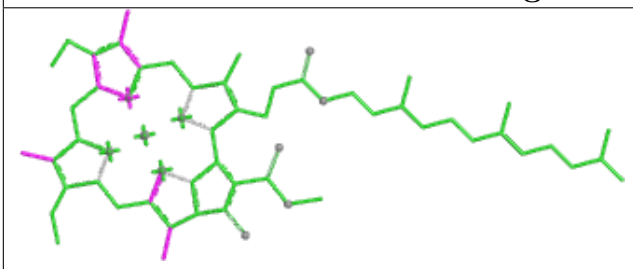


Rings

Ligand CLA V 306



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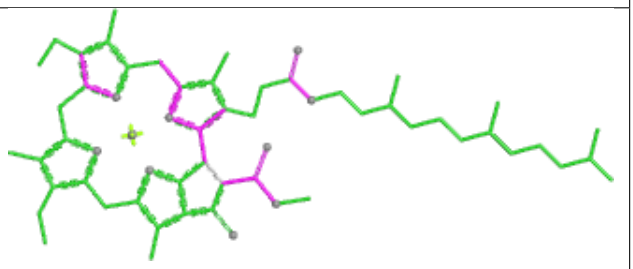
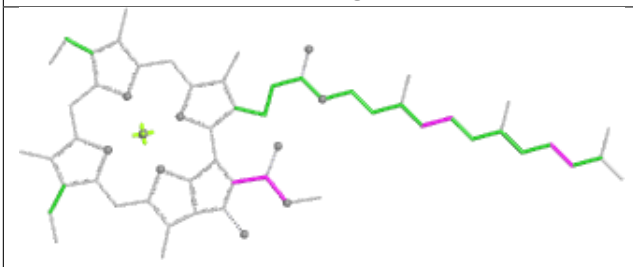


Bond angles



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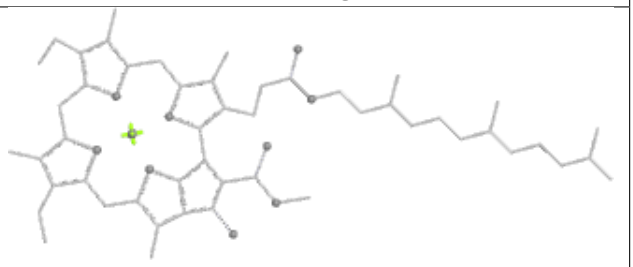
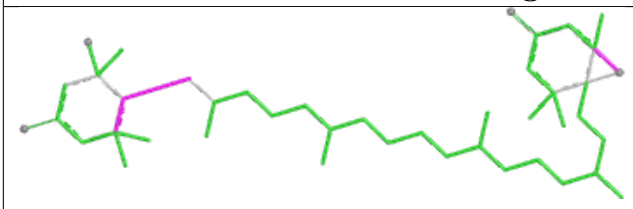


Rings

Ligand NEX R 301



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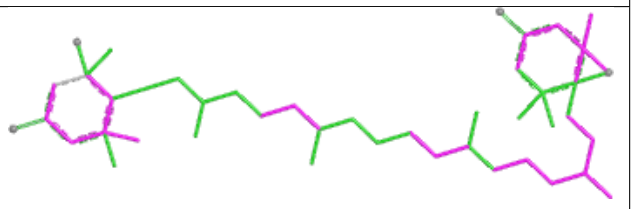
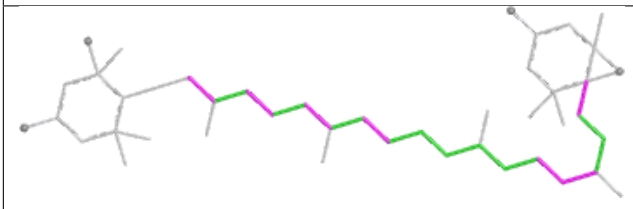


Bond angles



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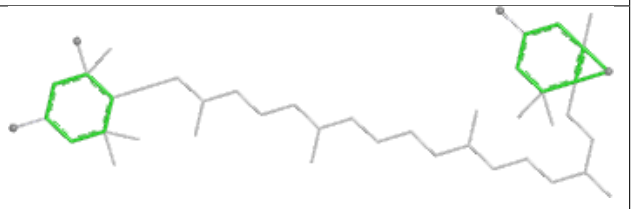
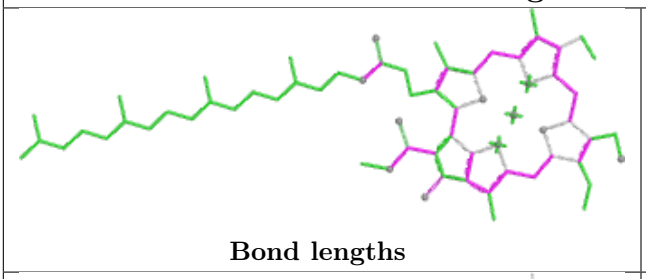


Rings

Ligand CHL p 319



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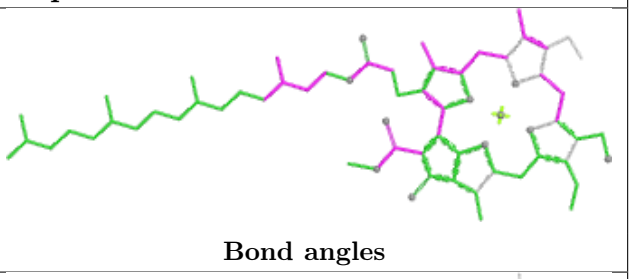
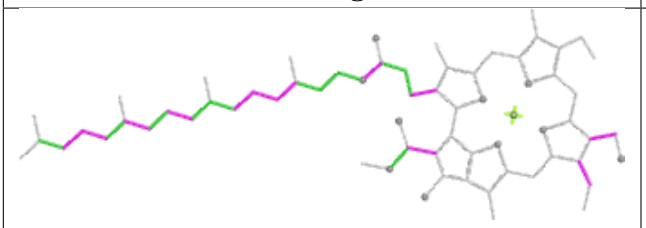


Bond angles



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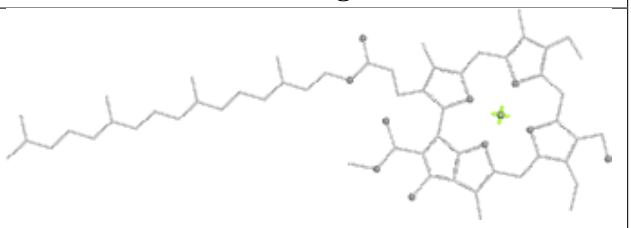
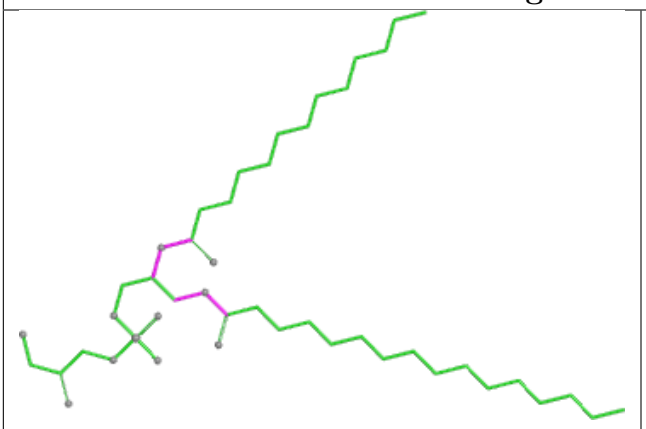


Rings

Ligand LHG d 405



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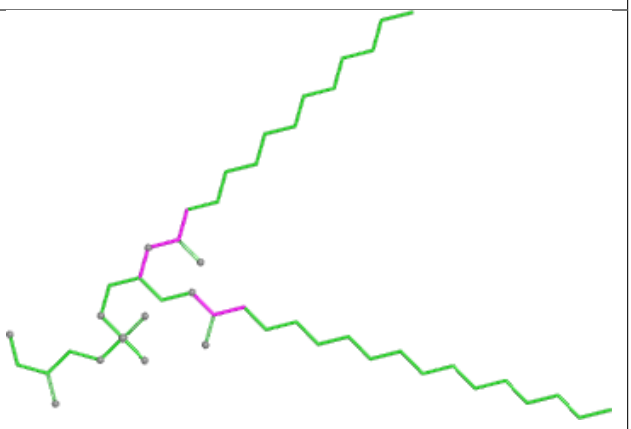
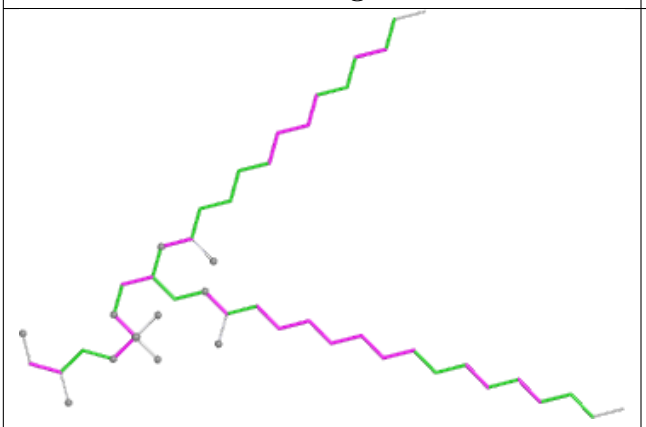


Bond angles



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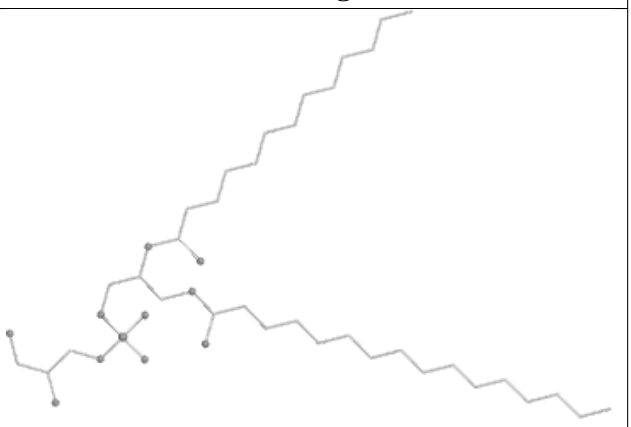
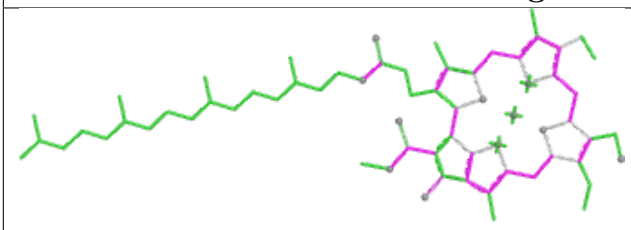


Rings

Ligand CHL 3 314



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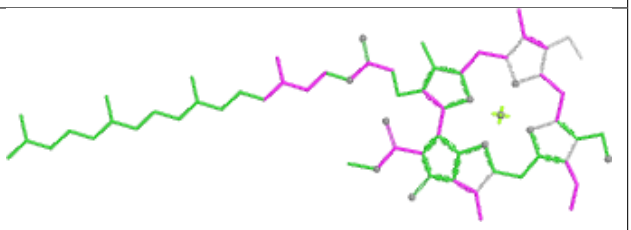
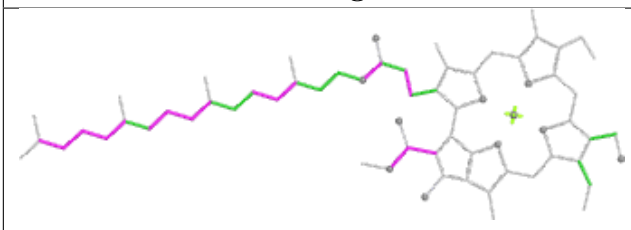
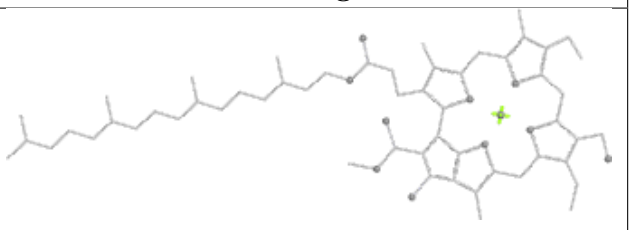


Bond angles

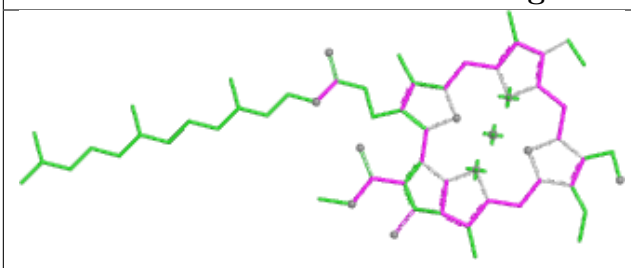


Torsions



Rings

Ligand CHL 6 317



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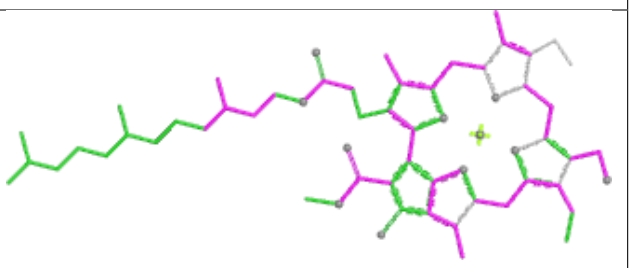

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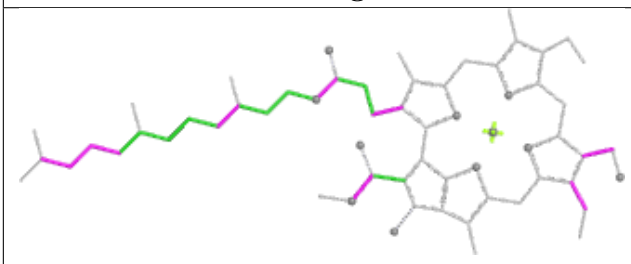

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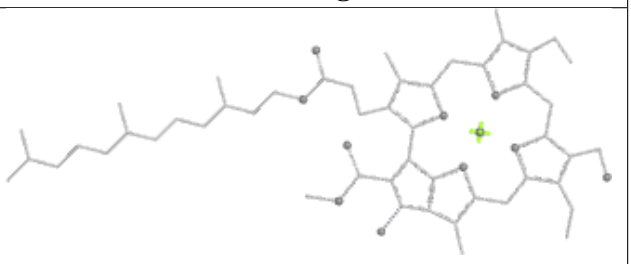
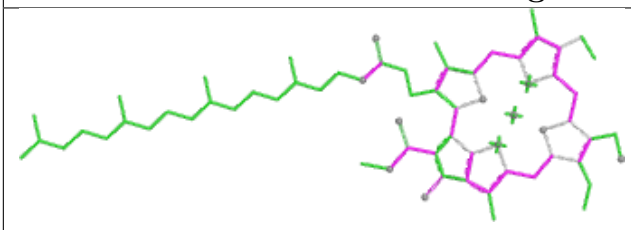


Rings

Ligand CHL 3 311



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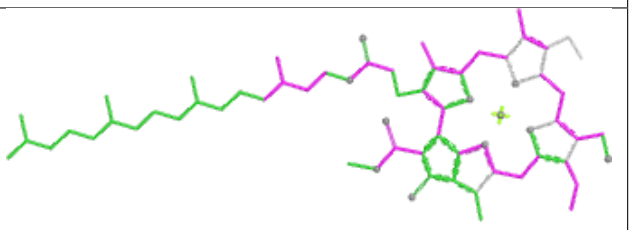

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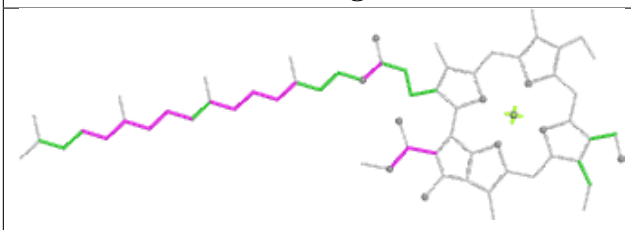

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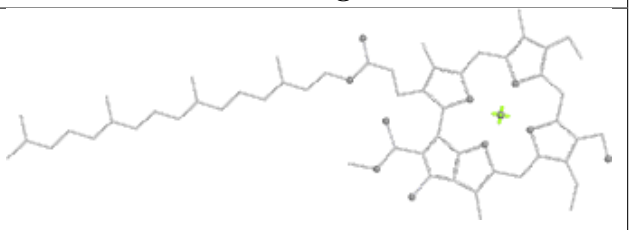
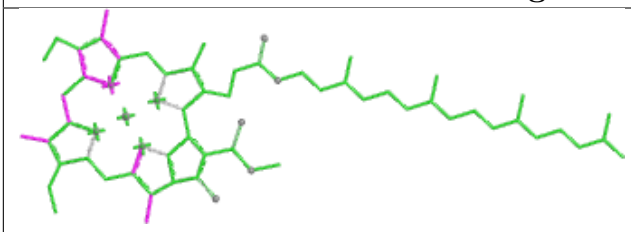


Rings

Ligand CLA g 301



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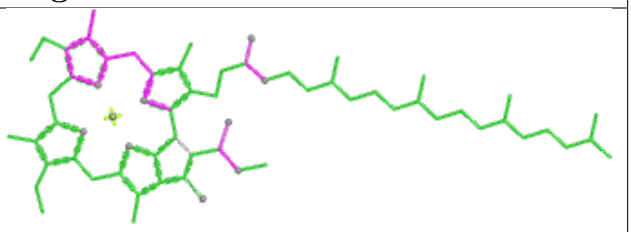
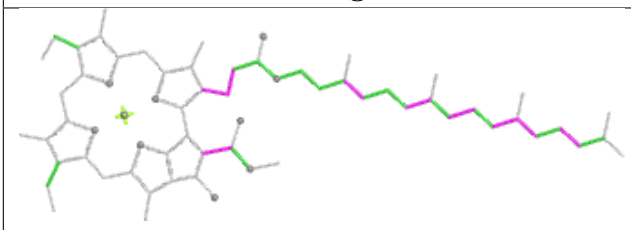


Bond angles



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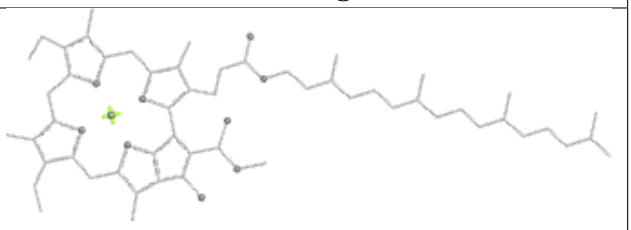
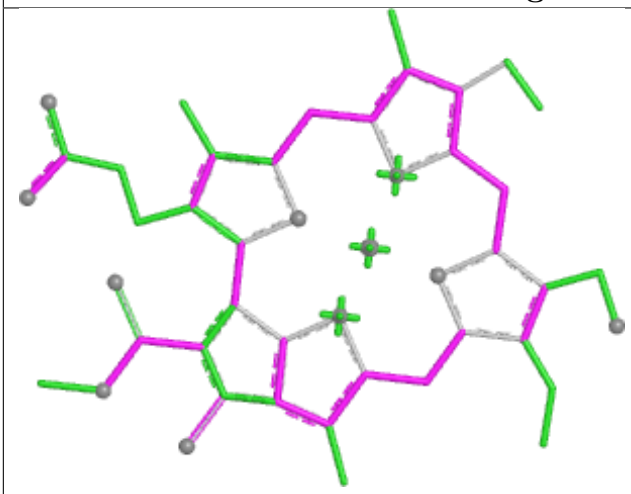


Rings

Ligand CHL S 313



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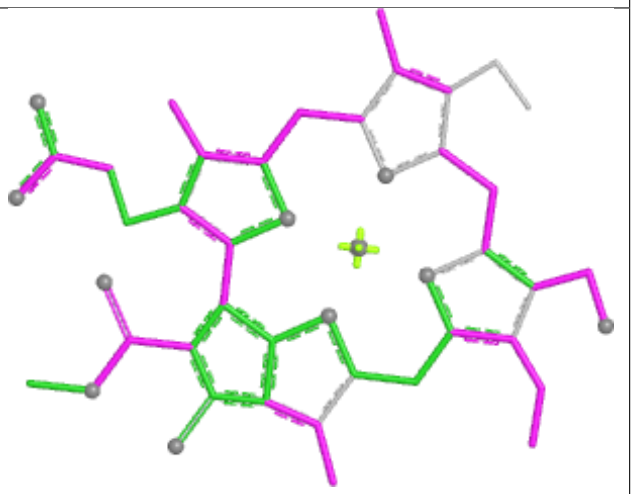

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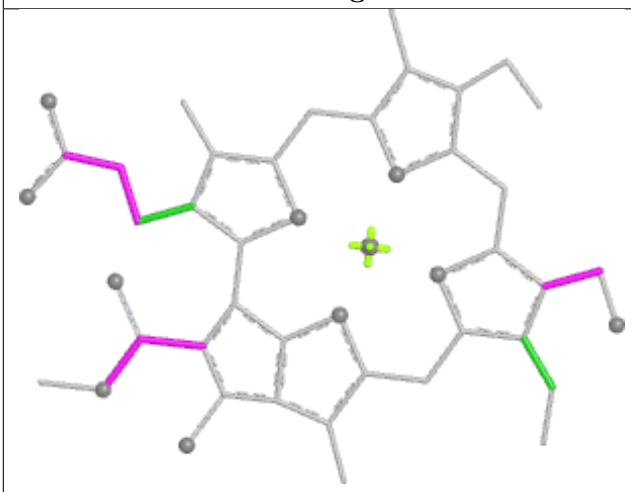

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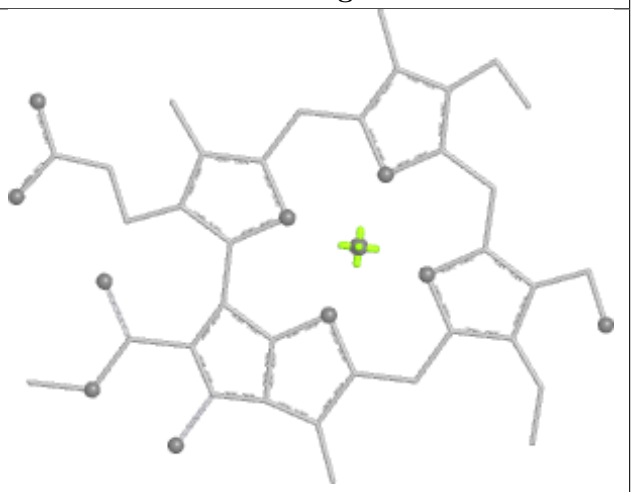
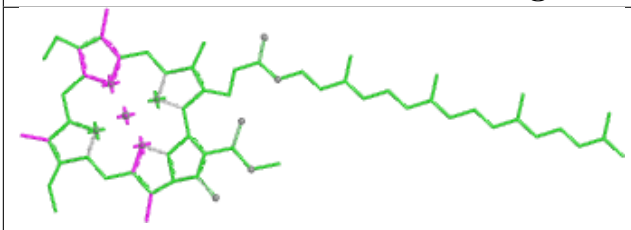


Rings

Ligand CLA c 512



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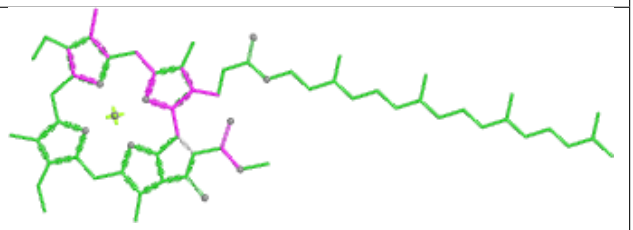
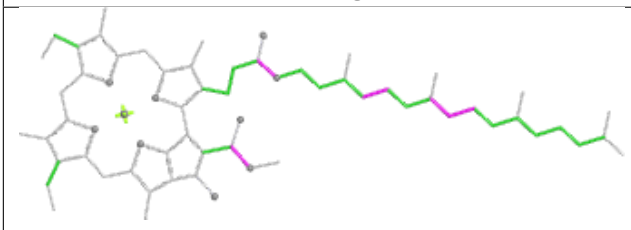


Bond angles



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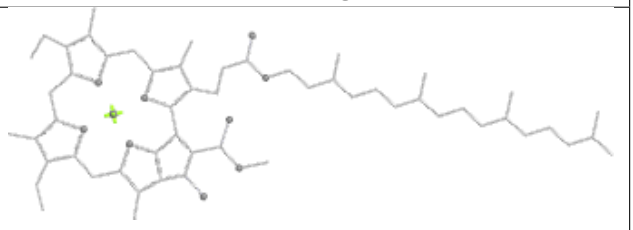
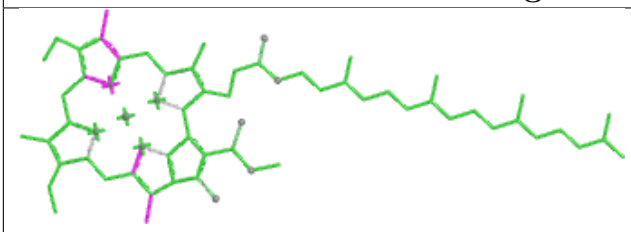


Rings

Ligand CLA B 605



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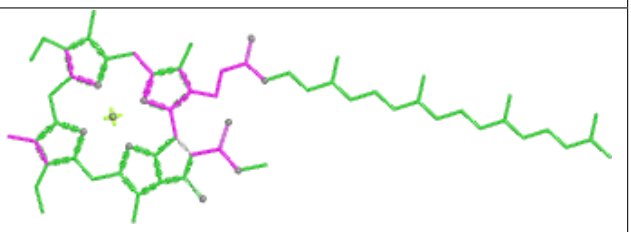

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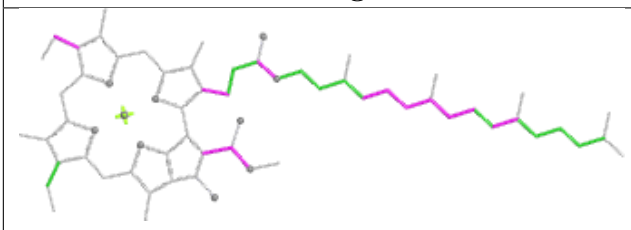

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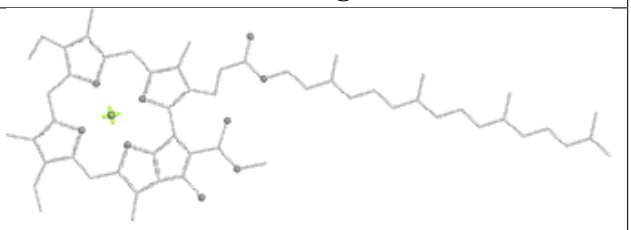
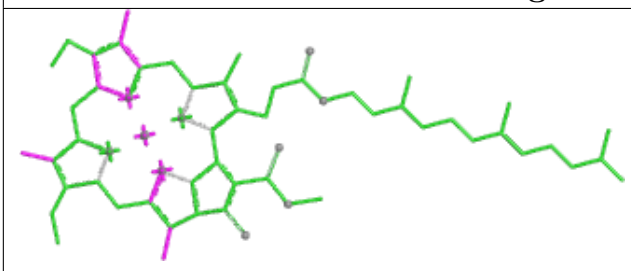


Rings

Ligand CLA 1 306



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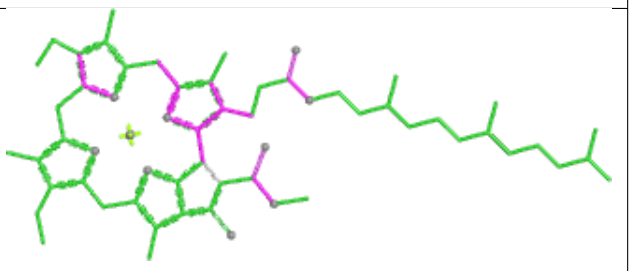

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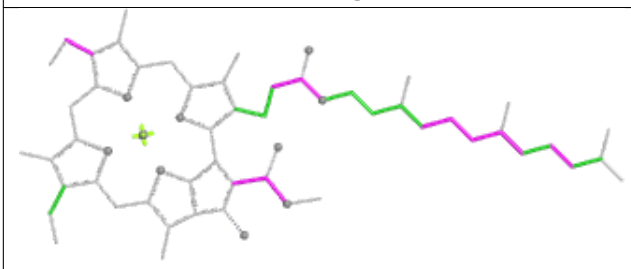

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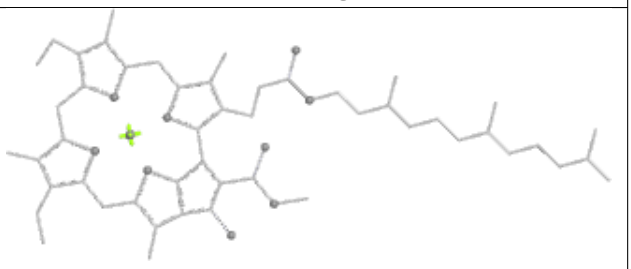

Rings

Ligand LUT 5 309

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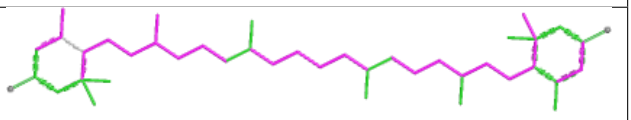
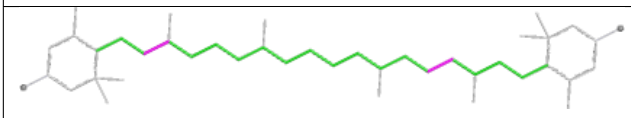


Bond angles



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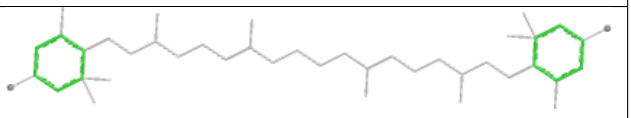
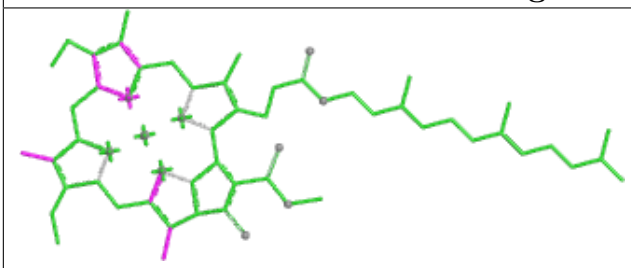


Rings

Ligand CLA 5 306



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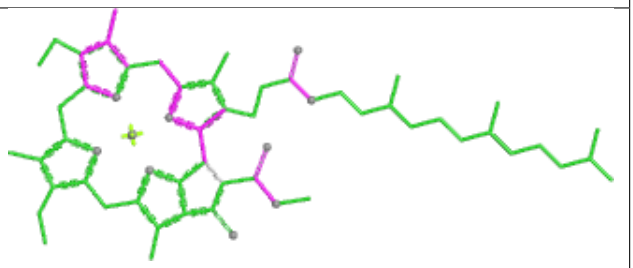

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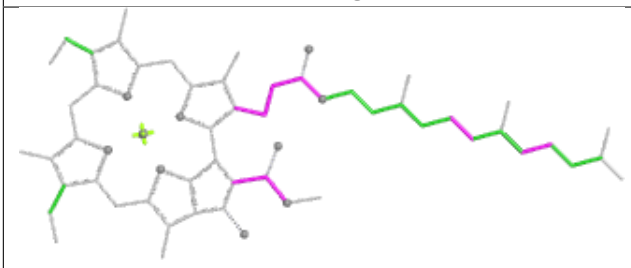

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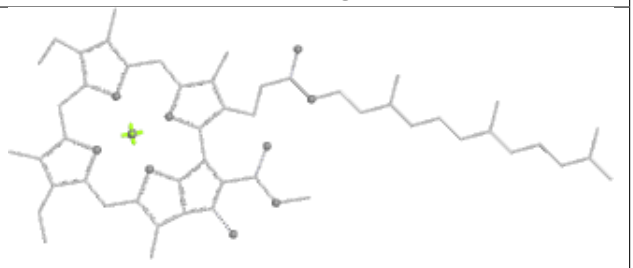
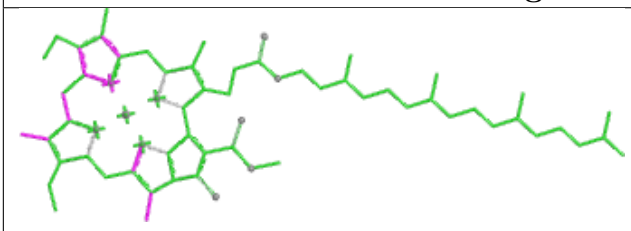


Rings

Ligand CLA P 305



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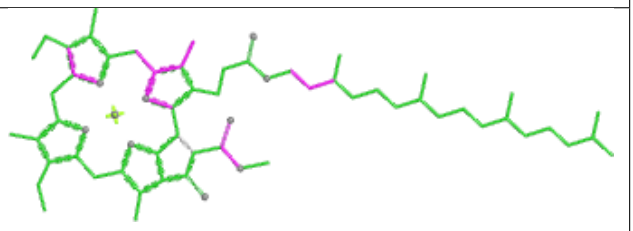

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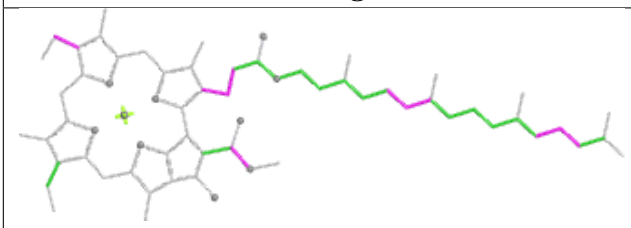

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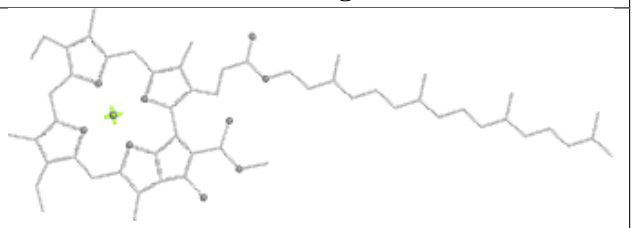
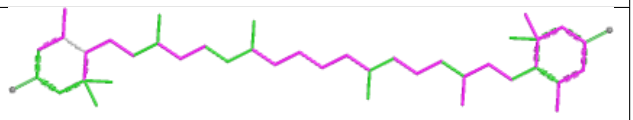


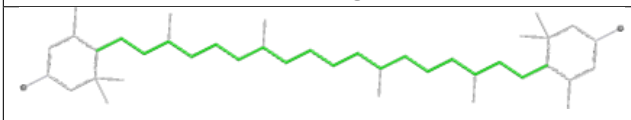
Rings

Ligand LUT V 310

Bond lengths



Bond angles



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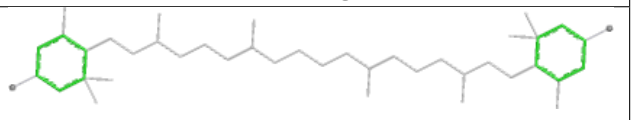
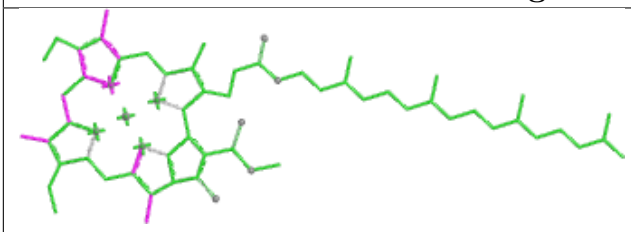


Rings

Ligand CLA 5 301



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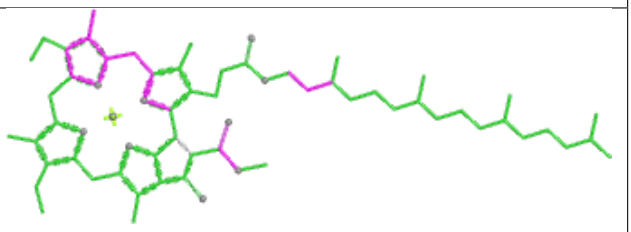

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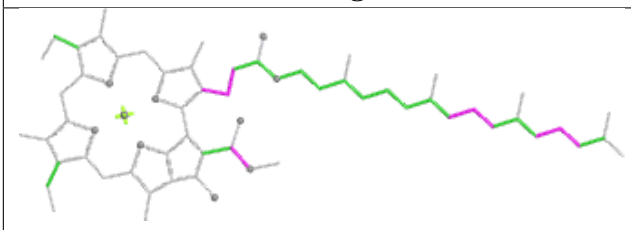

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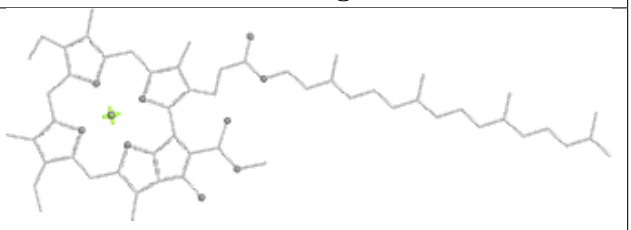
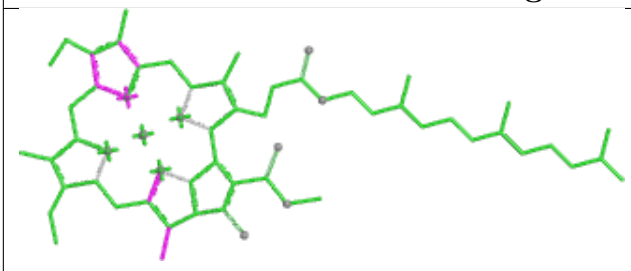


Rings

Ligand CLA P 307



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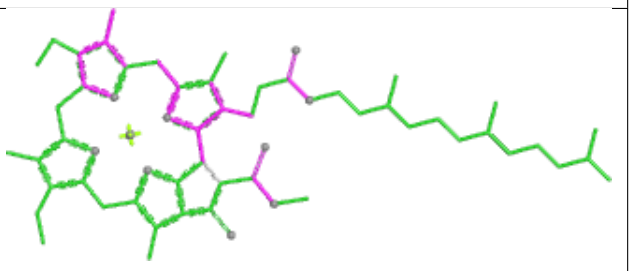
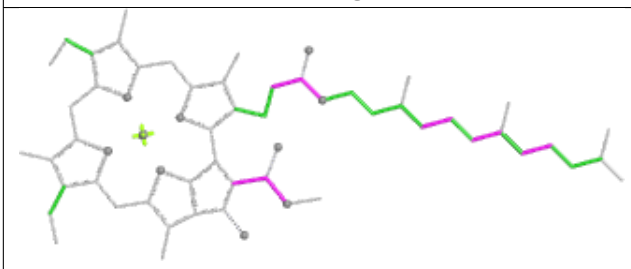


Bond angles



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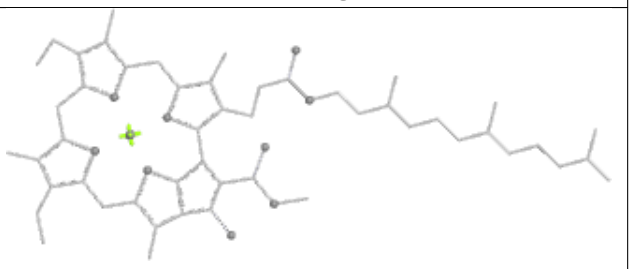
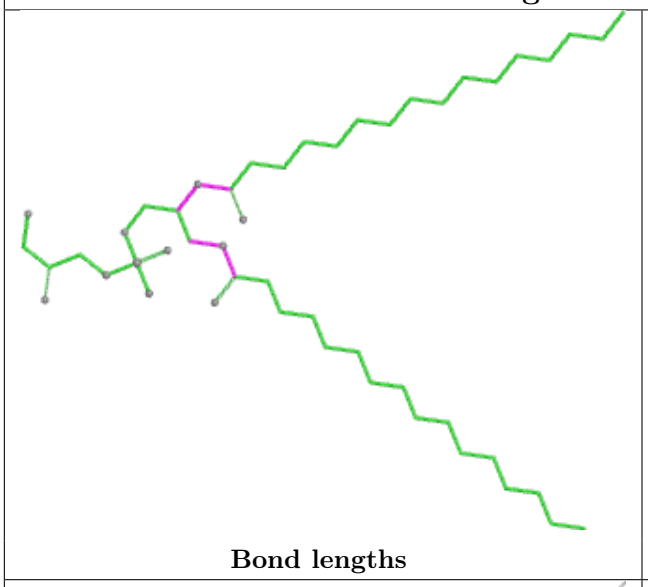


Rings

Ligand LHG G 310



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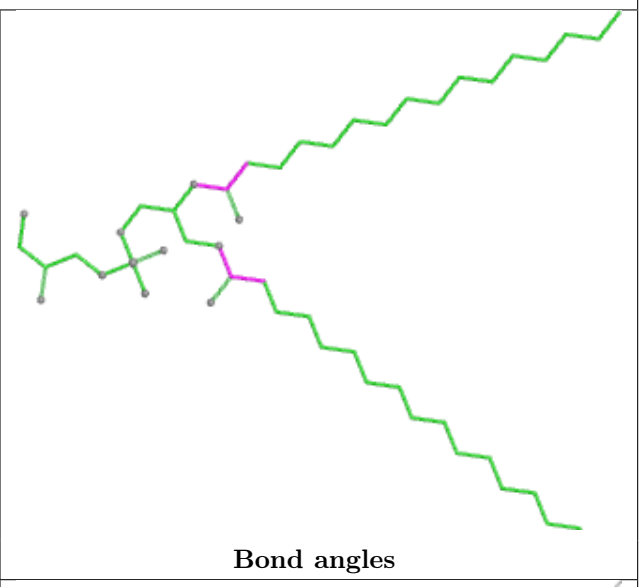
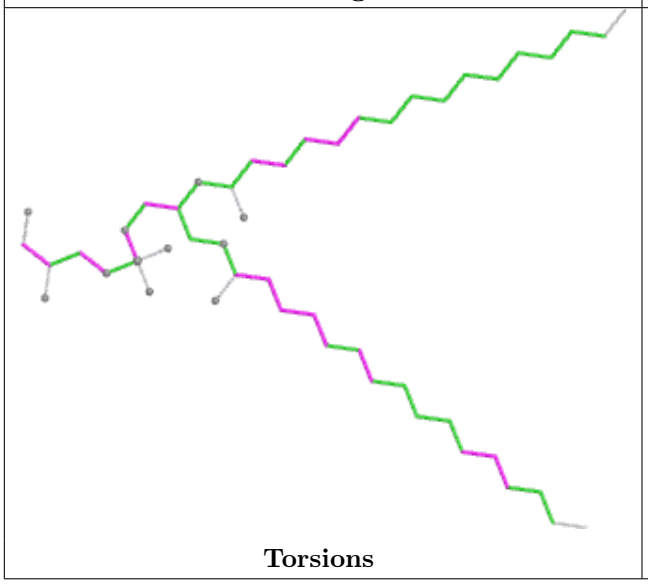
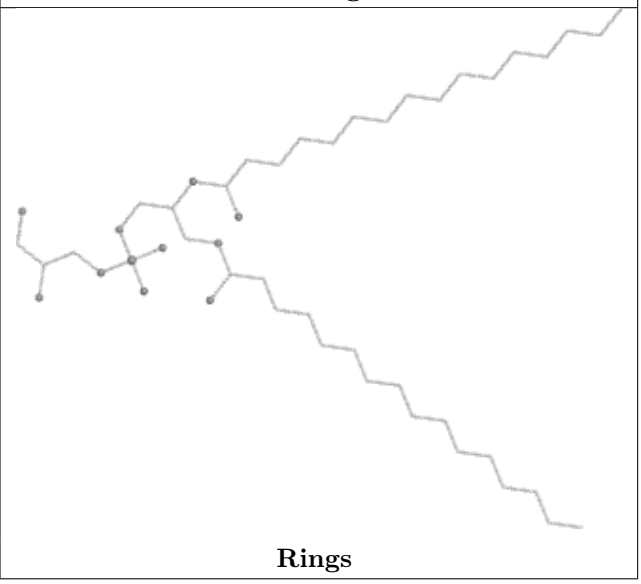


Bond angles

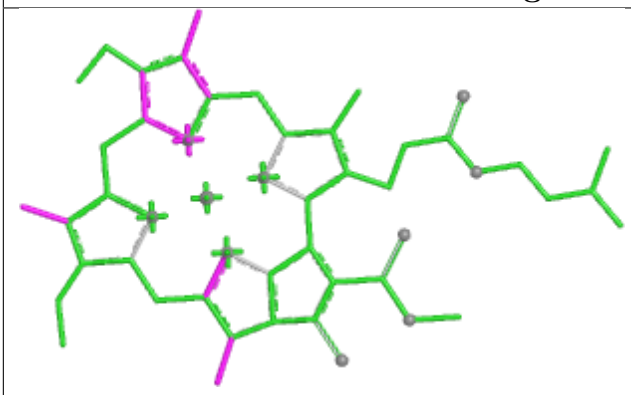


Torsions

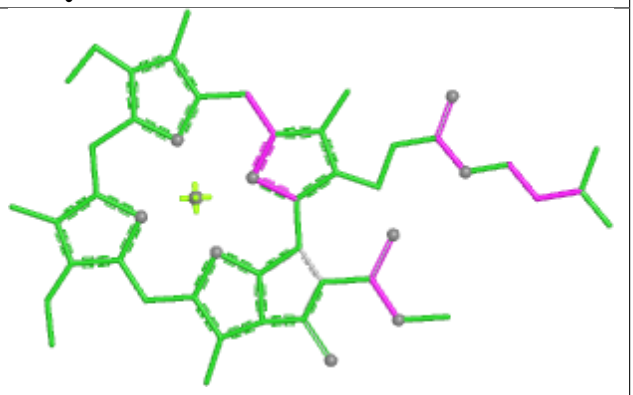


Rings

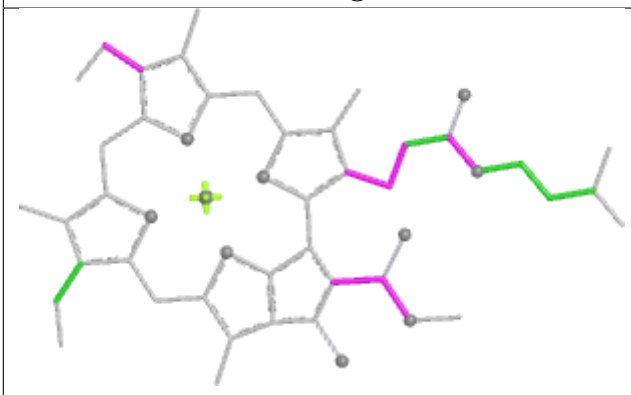
Ligand CLA Q 303



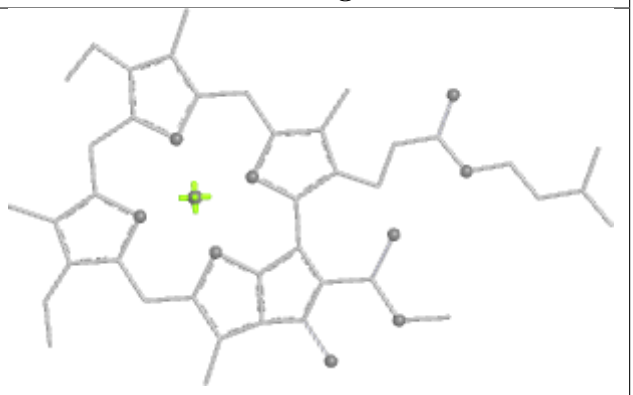
Bond lengths



Bond angles



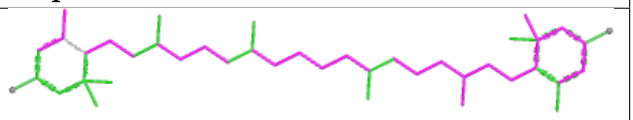
Torsions



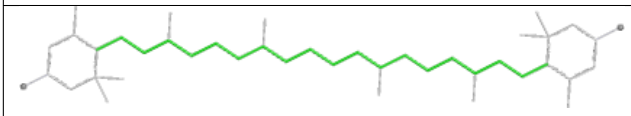
Rings

Ligand LUT p 310

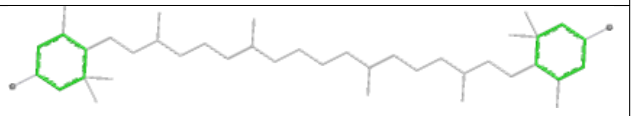
Bond lengths



Bond angles

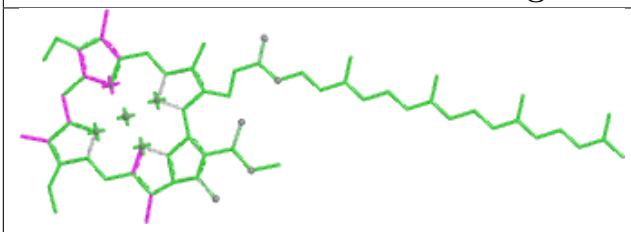


Torsions

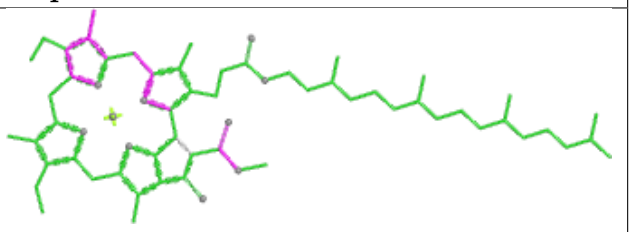


Rings

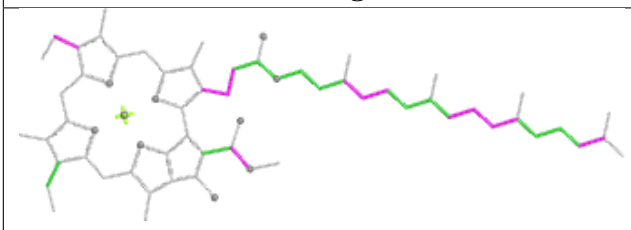
Ligand CLA p 302



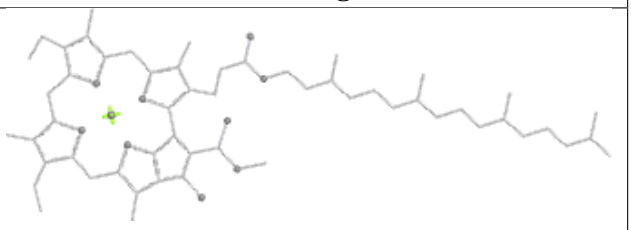
Bond lengths



Bond angles



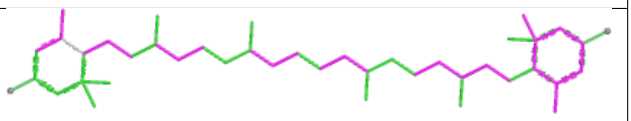
Torsions



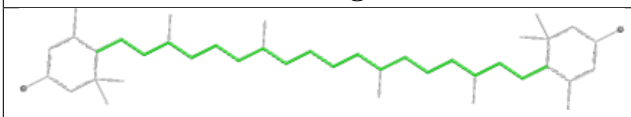
Rings

Ligand LUT 2 310

Bond lengths



Bond angles



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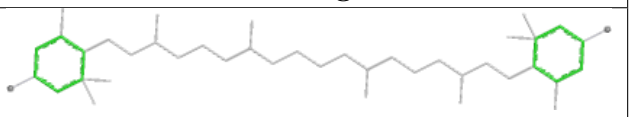
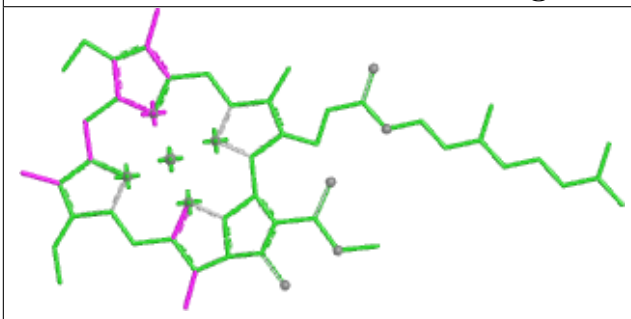
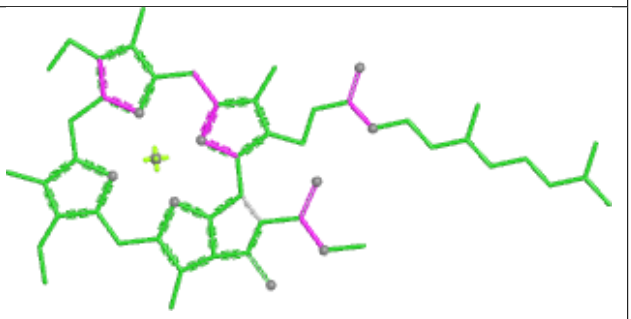


Rings

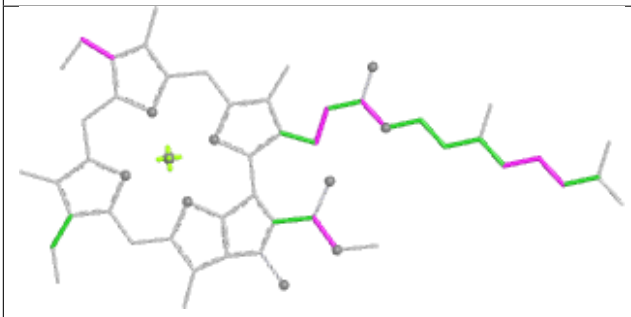
Ligand CLA s 308



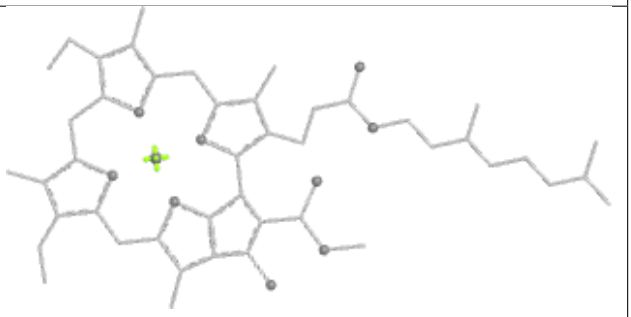
Bond lengths



Bond angles

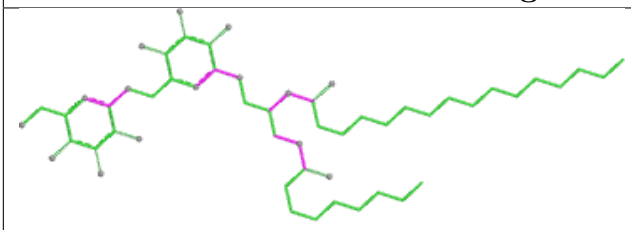


Torsions



Rings

Ligand DGD C 519



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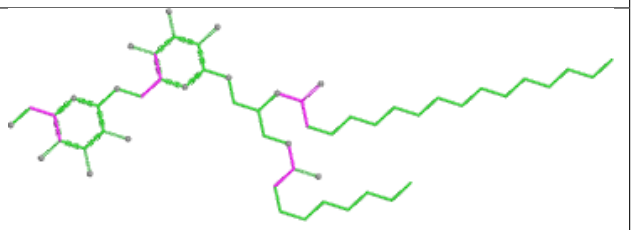
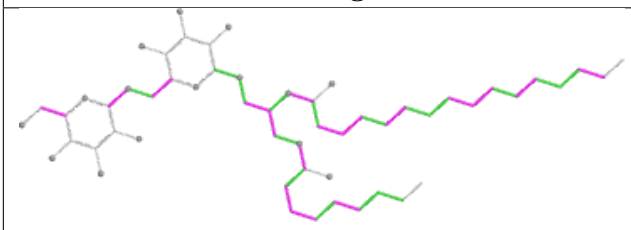


Bond angles



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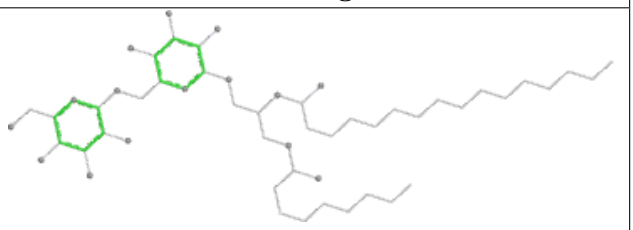
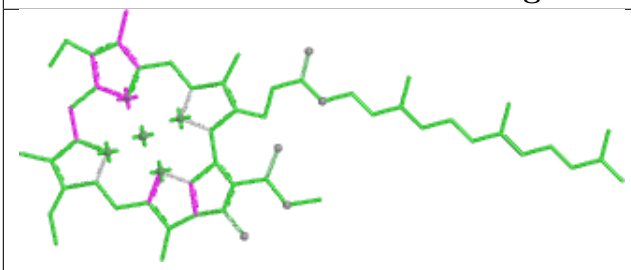


Rings

Ligand CLA N 305



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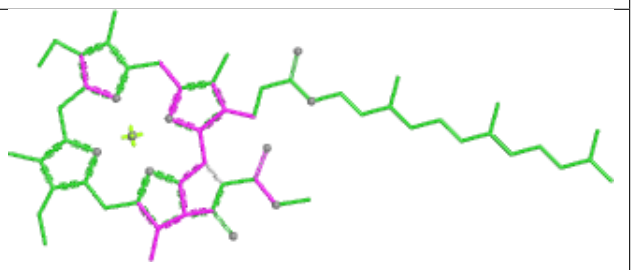
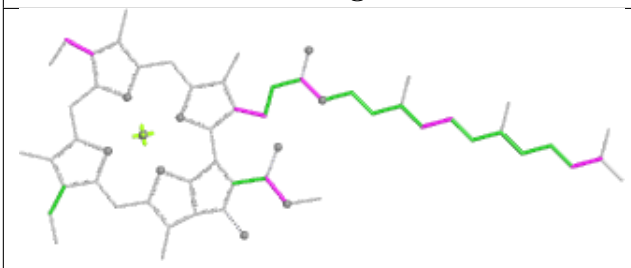


Bond angles



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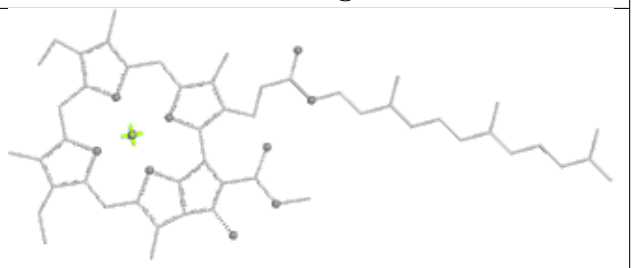
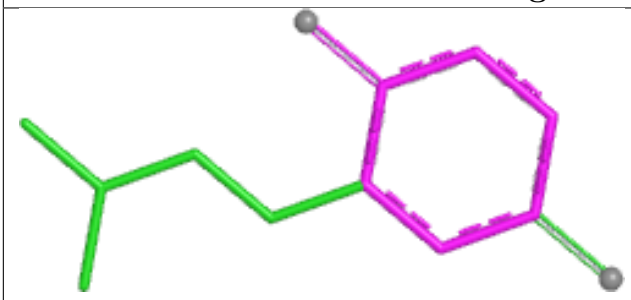


Rings

Ligand PL9 A 410



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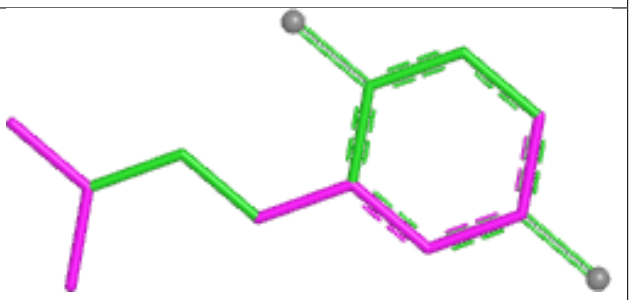
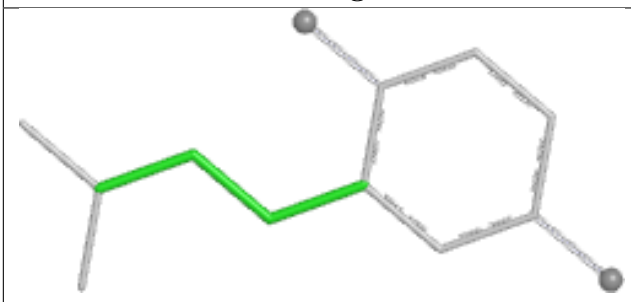


Bond angles



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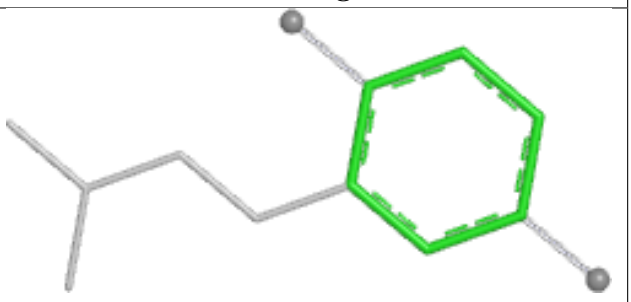
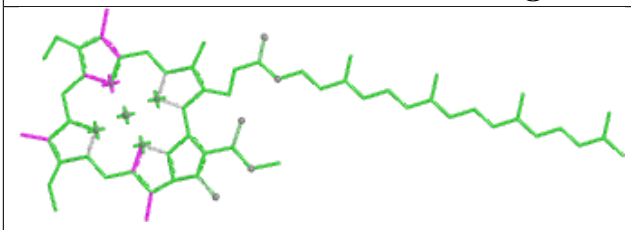


Rings

Ligand CLA C 507



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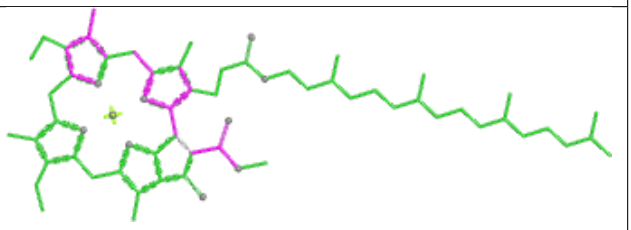
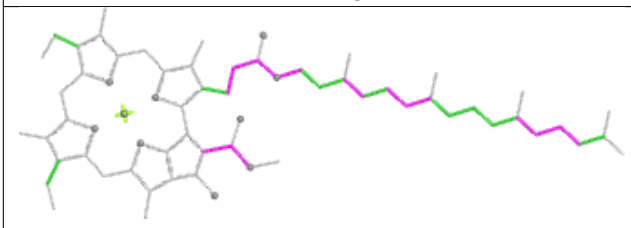
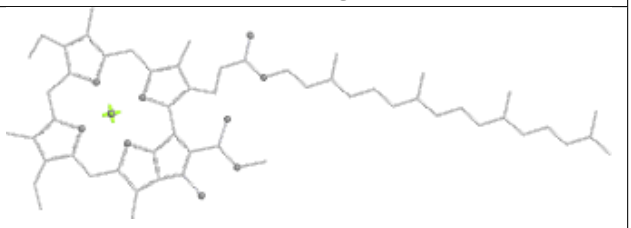


Bond angles

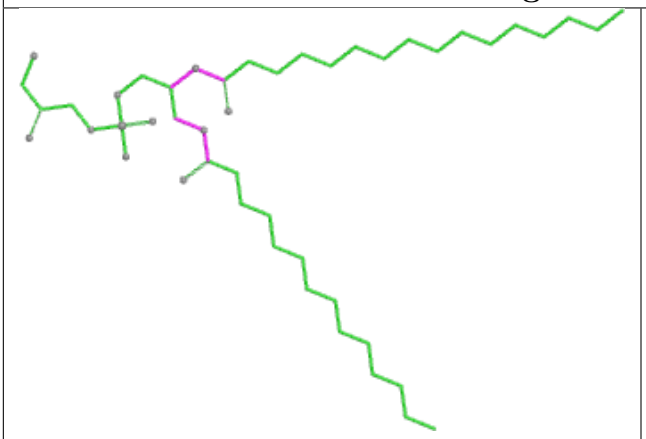


Torsions



Rings

Ligand LHG B 622



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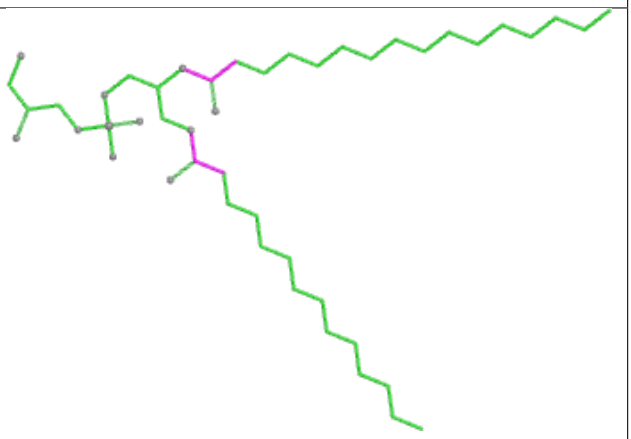
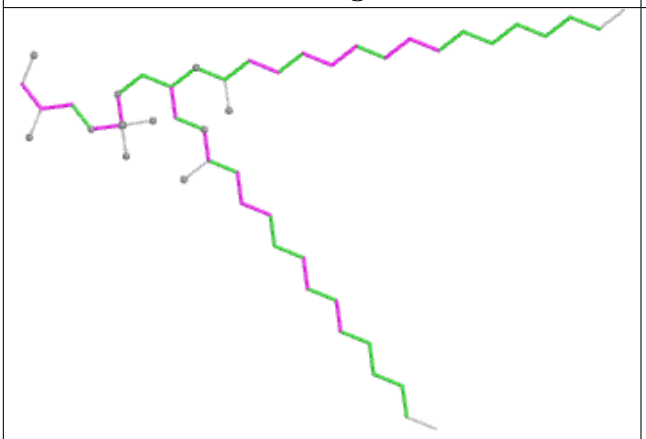
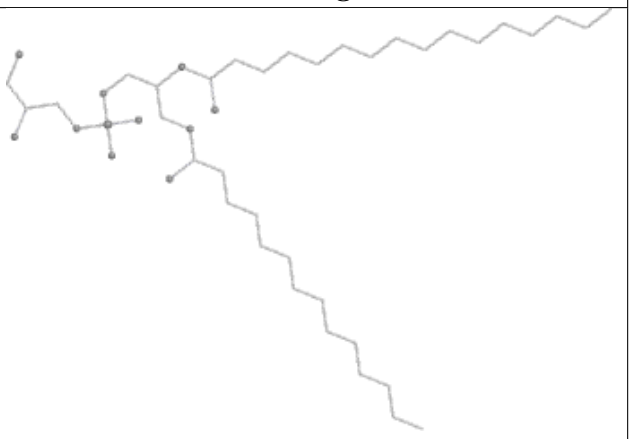


Bond angles

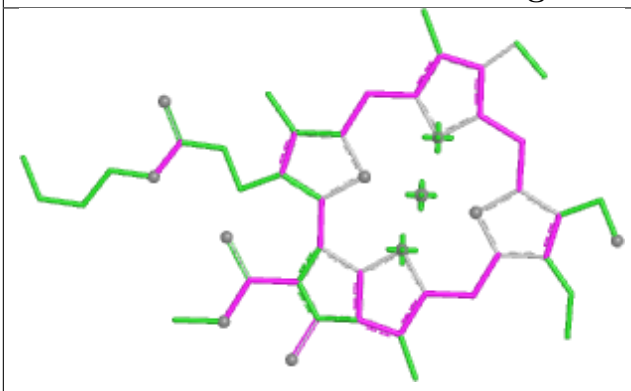


Torsions



Rings

Ligand CHL 2 315



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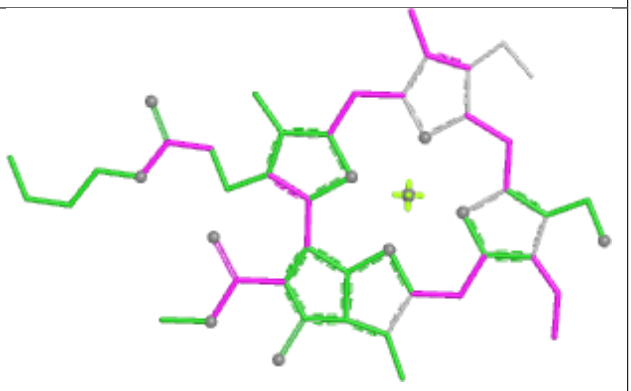
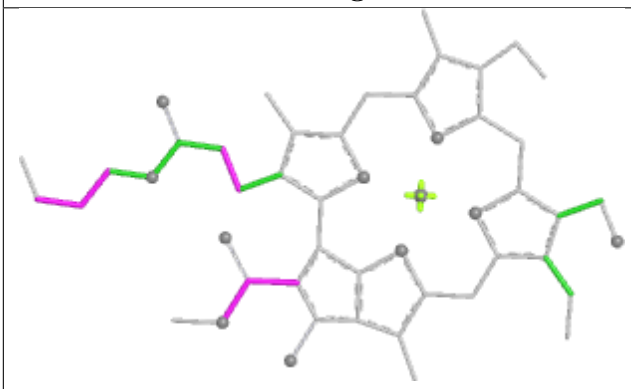


Bond angles



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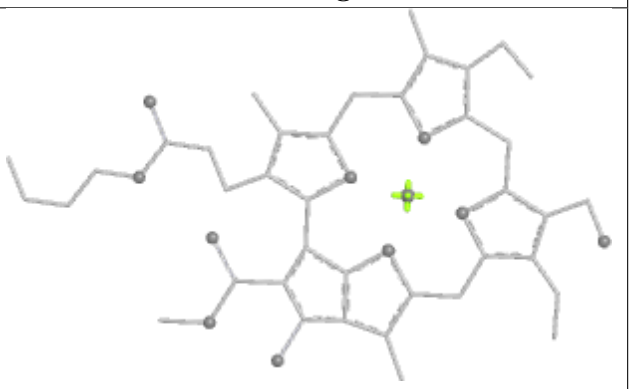
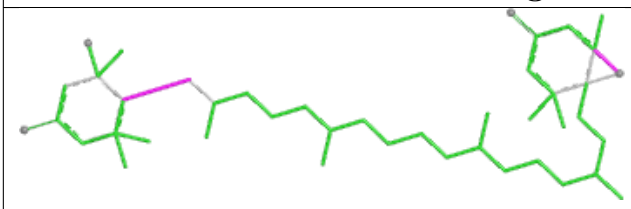


Rings

Ligand NEX 2 319



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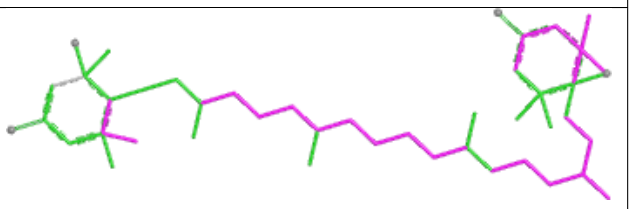
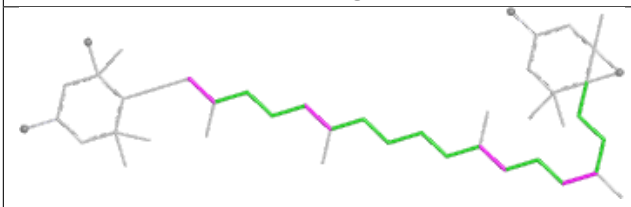
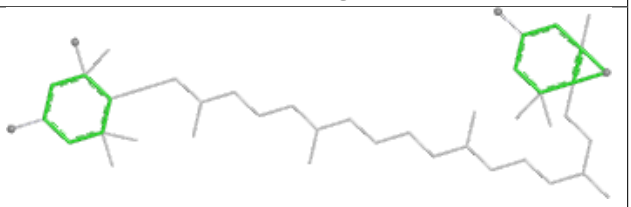


Bond angles

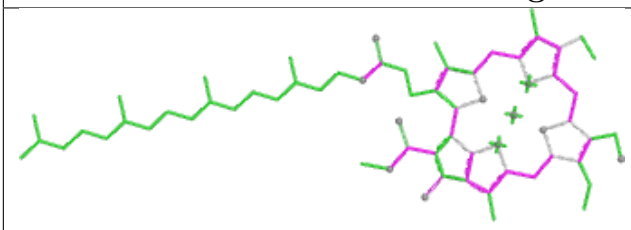


Torsions



Rings

Ligand CHL 2 313



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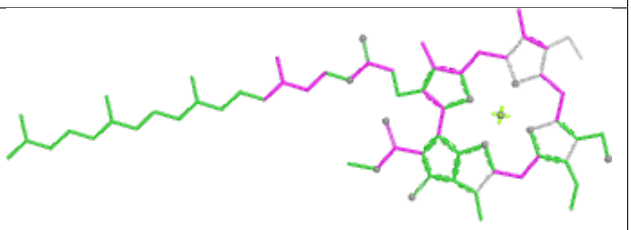
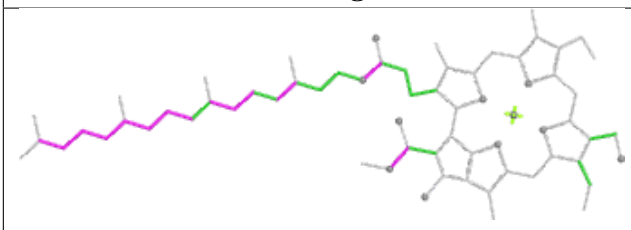
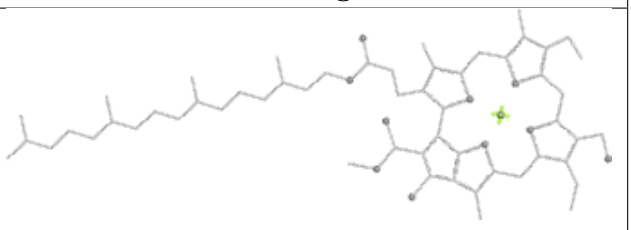


Bond angles

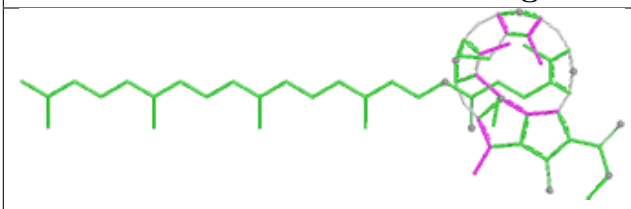


Torsions

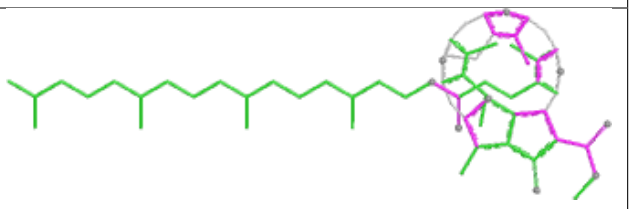


Rings

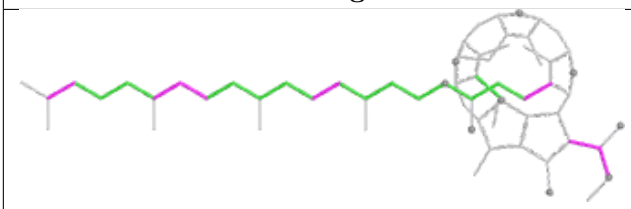
Ligand PHO D 401



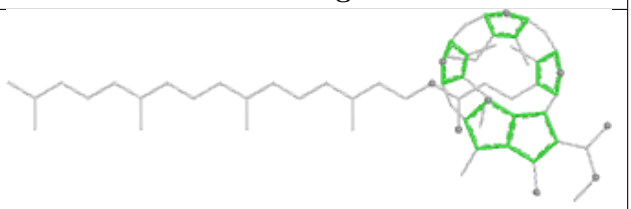
Bond lengths



Bond angles

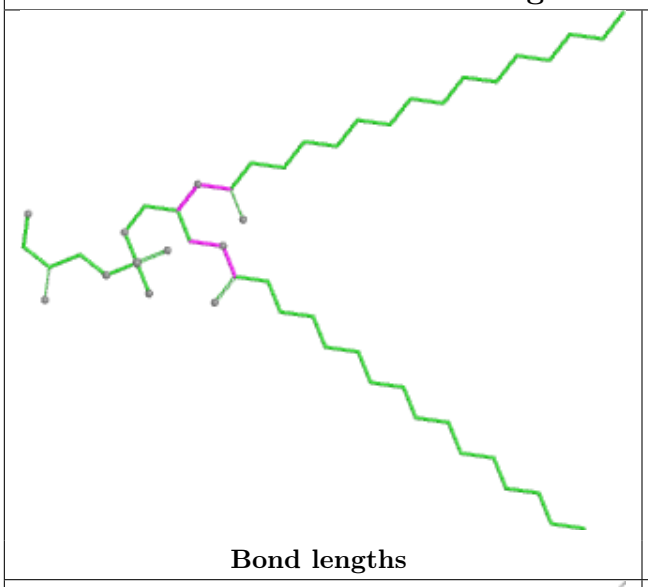


Torsions

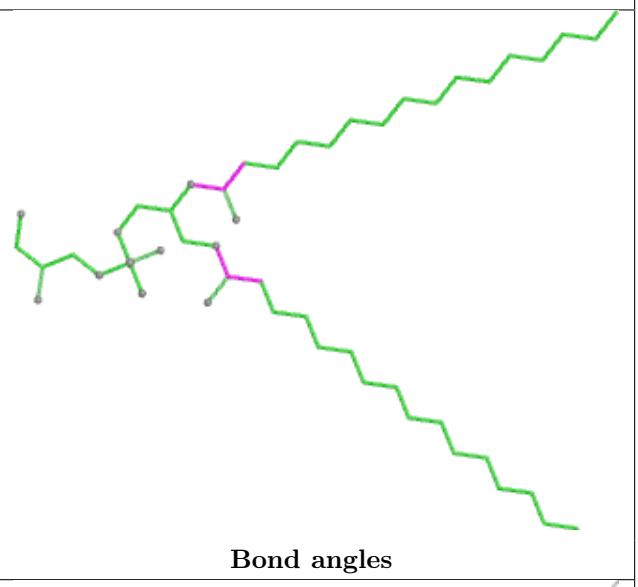


Rings

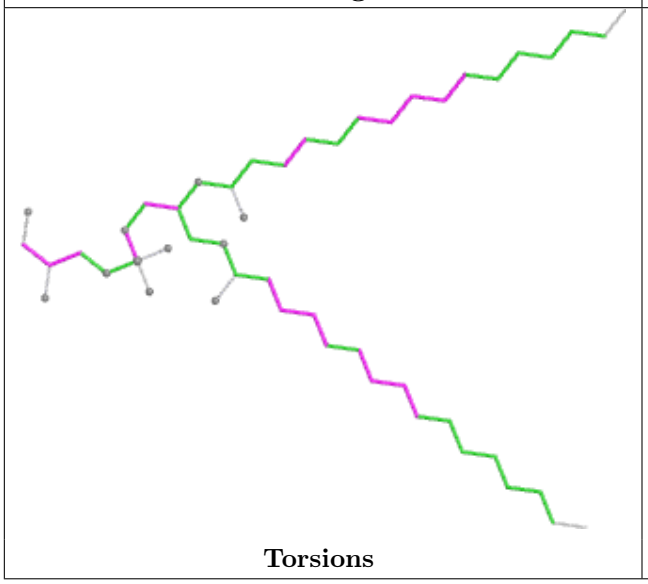
Ligand LHG n 312



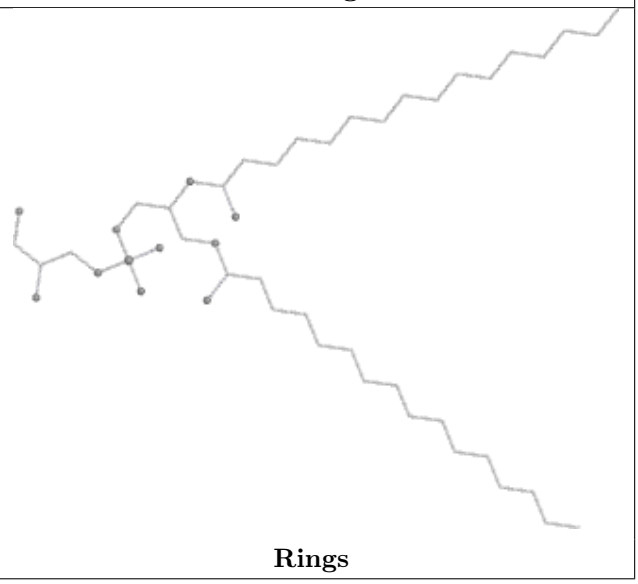
Bond lengths



Bond angles

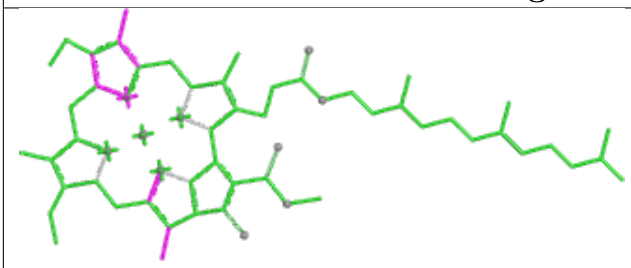


Torsions



Rings

Ligand CLA g 305



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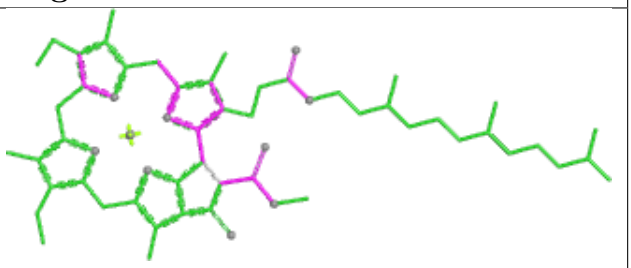

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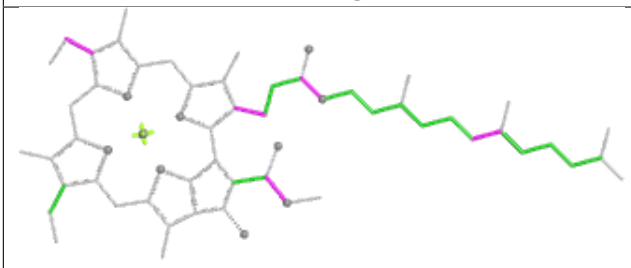

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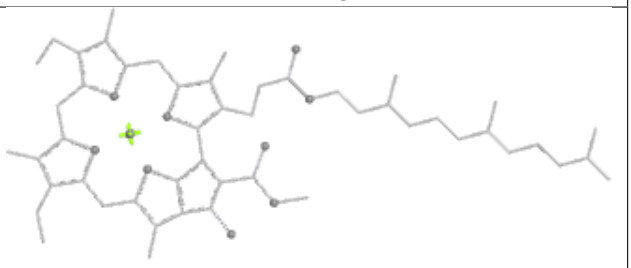
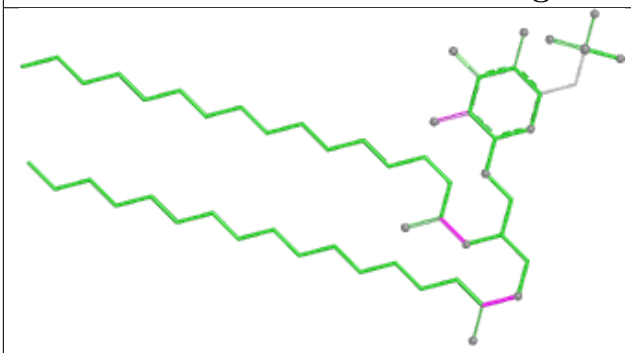


Rings

Ligand SQD l 102



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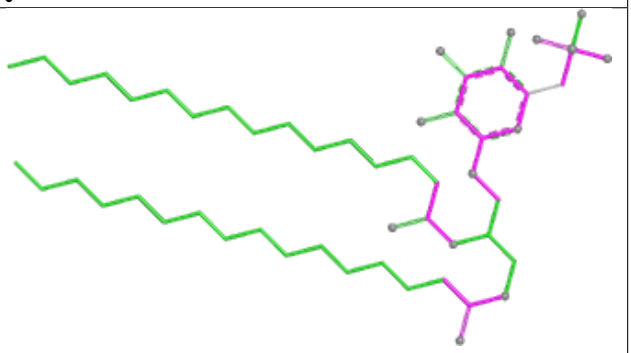

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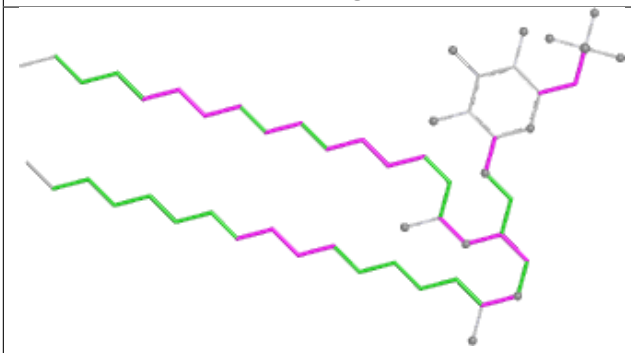

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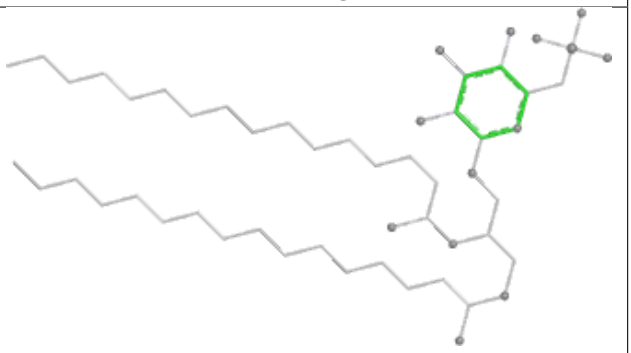
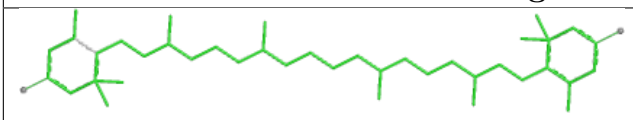


Rings

Ligand LUT 4 309



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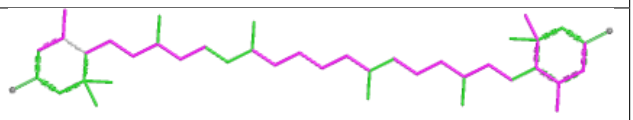

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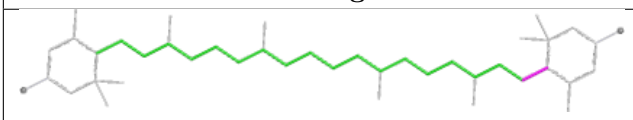

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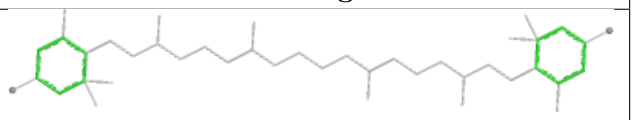
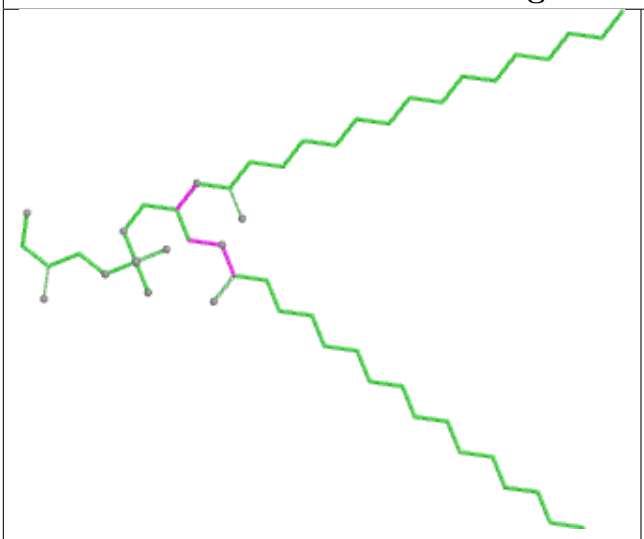


Rings

Ligand LHG c 522



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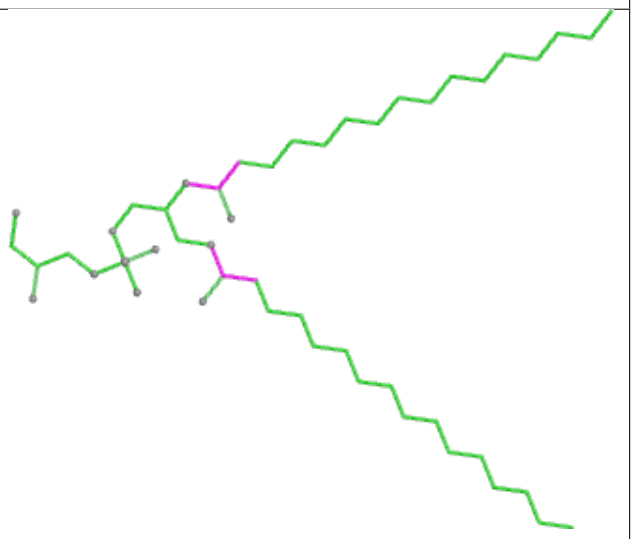

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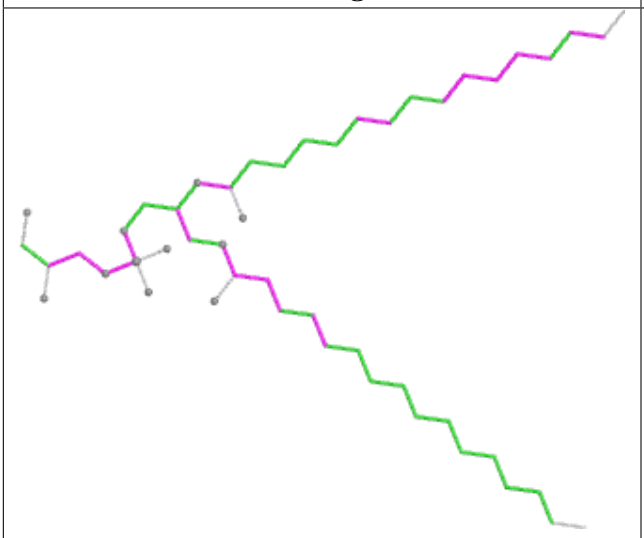

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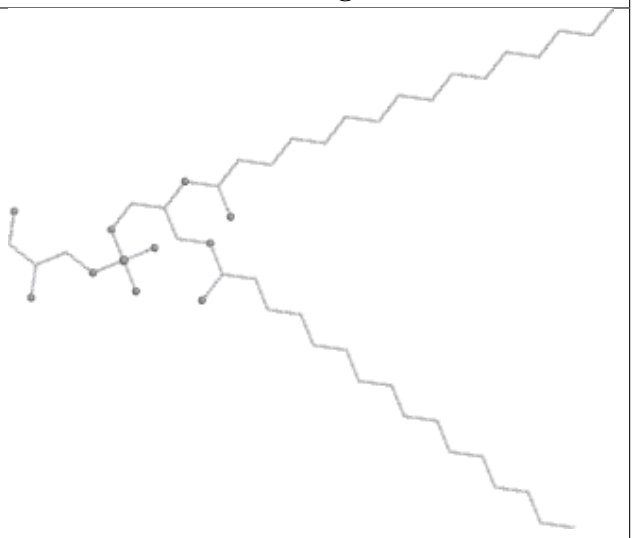
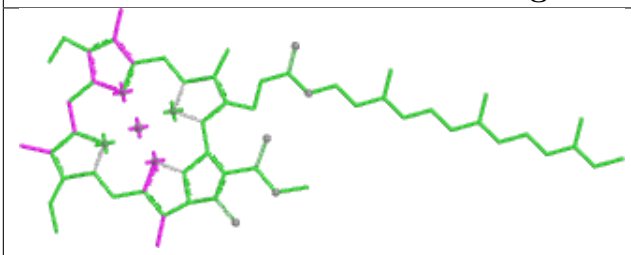


Rings

Ligand CLA s 301



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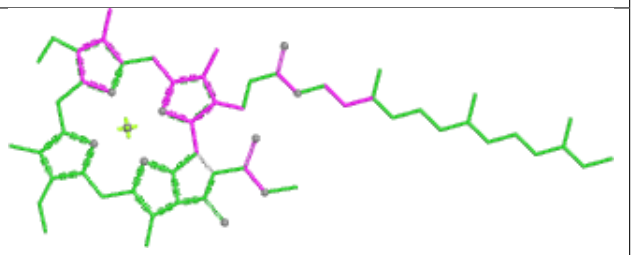

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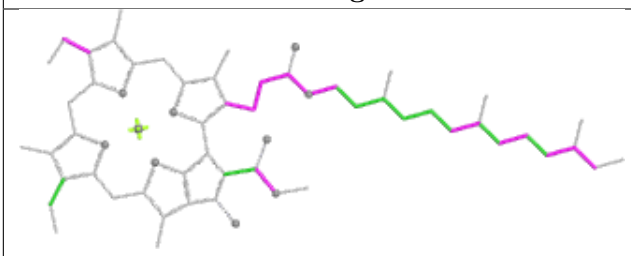

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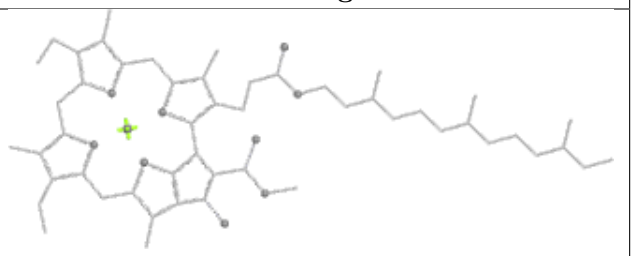
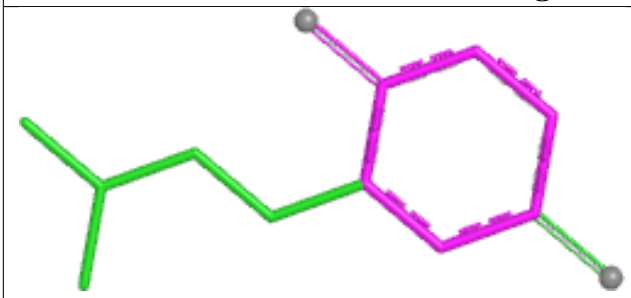


Rings

Ligand PL9 a 411



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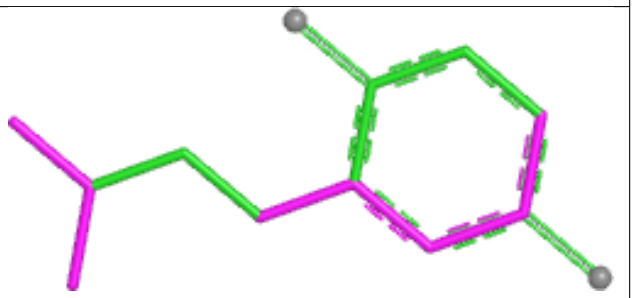

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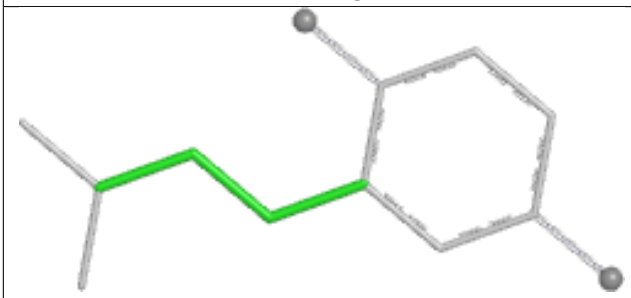

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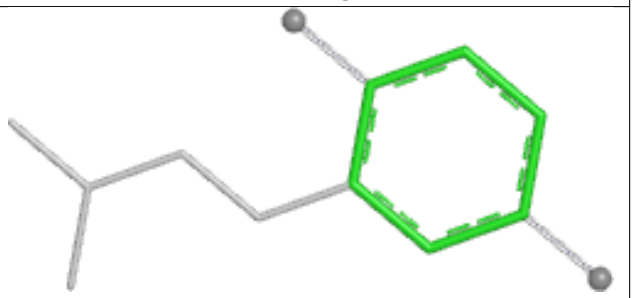
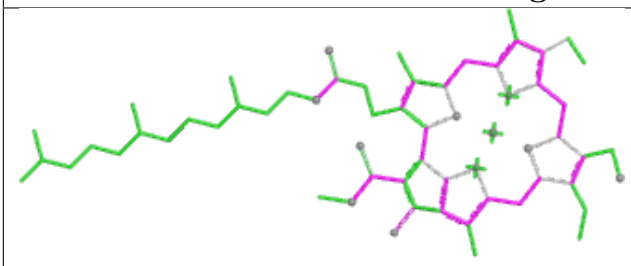
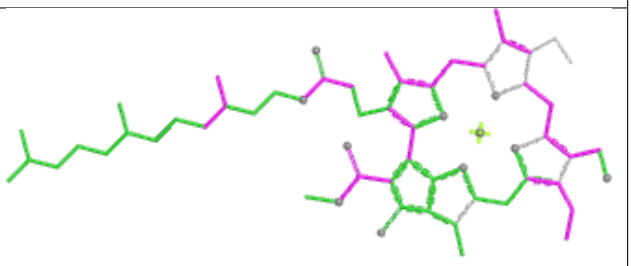
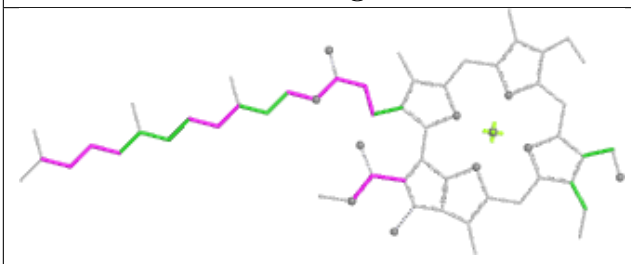
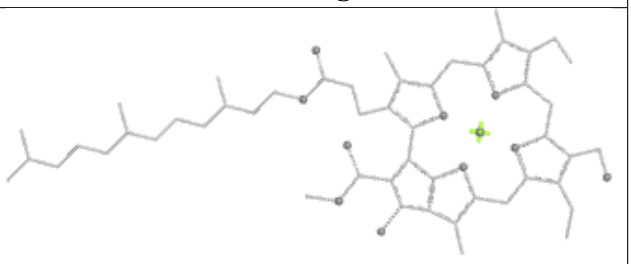
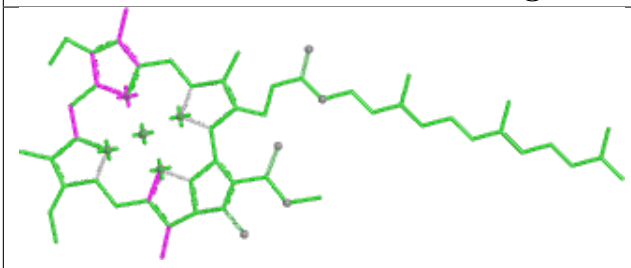
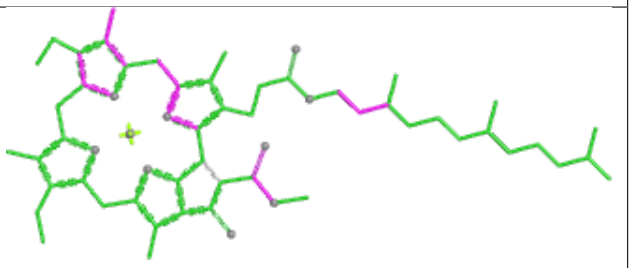
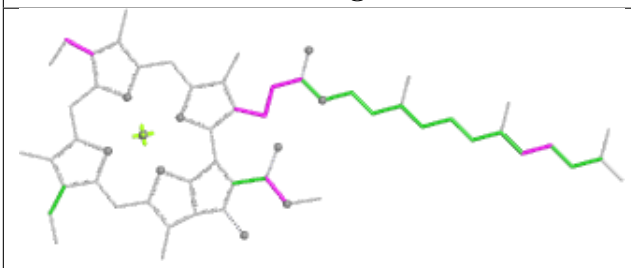
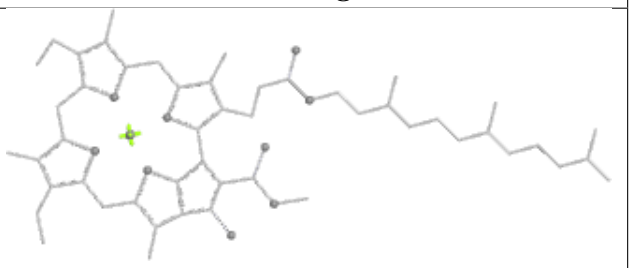
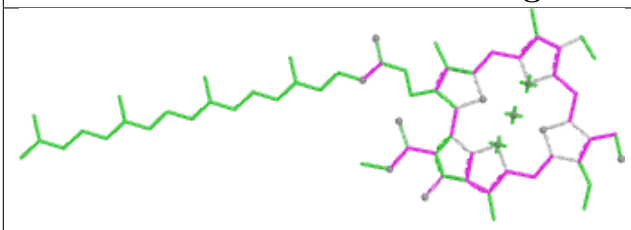


Rings

Ligand CHL r 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL Q 311



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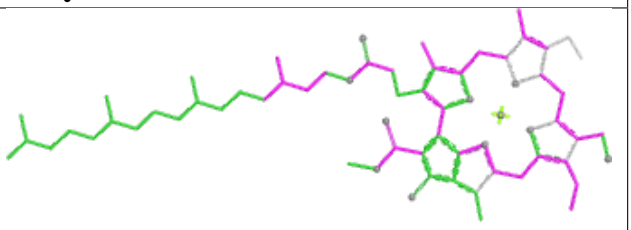
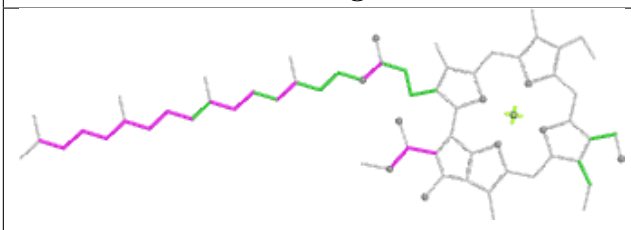


Bond angles



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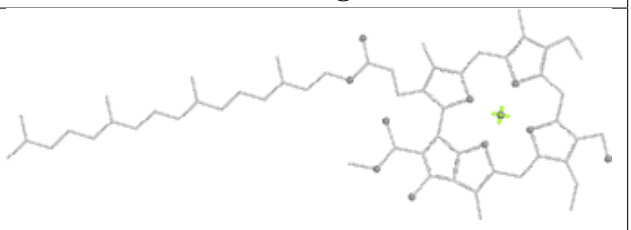
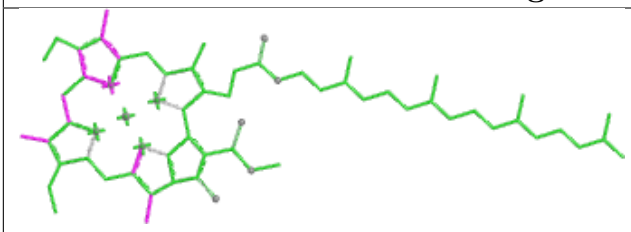


Rings

Ligand CLA b 615



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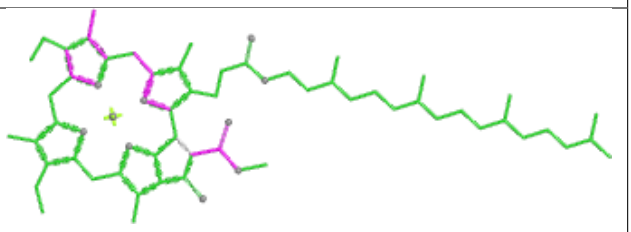

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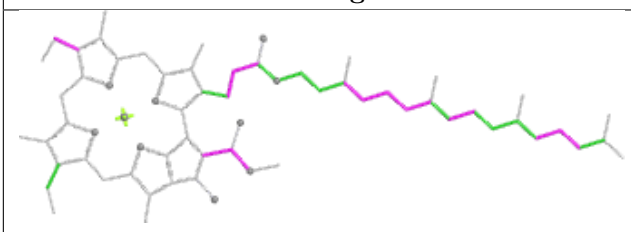

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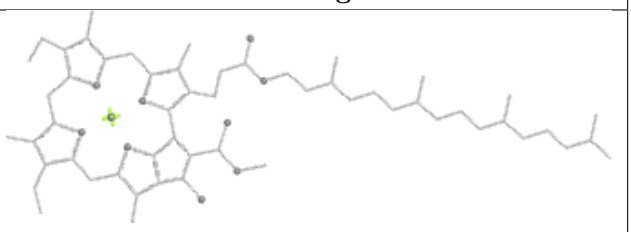
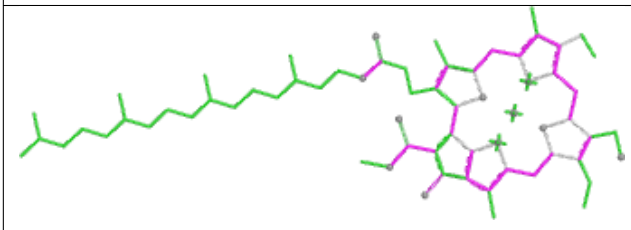


Rings

Ligand CHL 6 312



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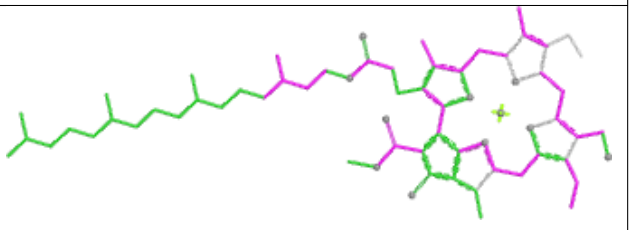
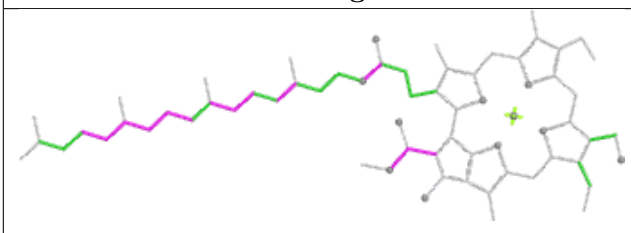
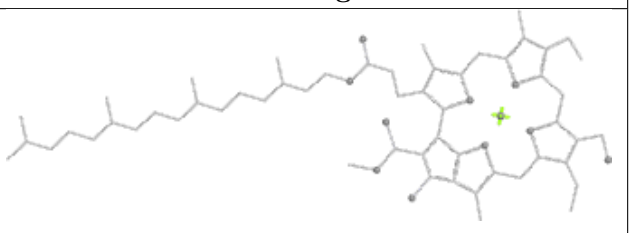


Bond angles

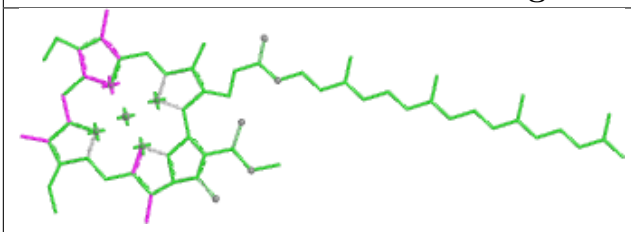


Torsions



Rings

Ligand CLA 1 301



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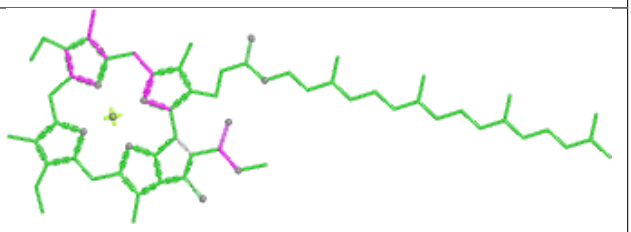
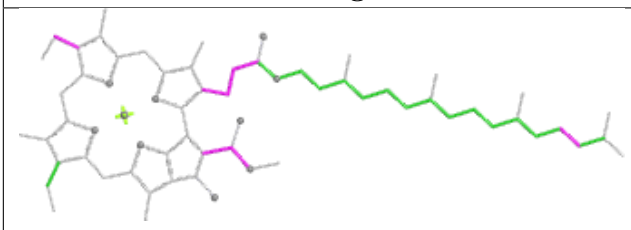


Bond angles



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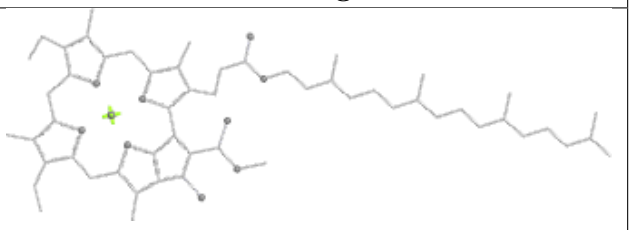
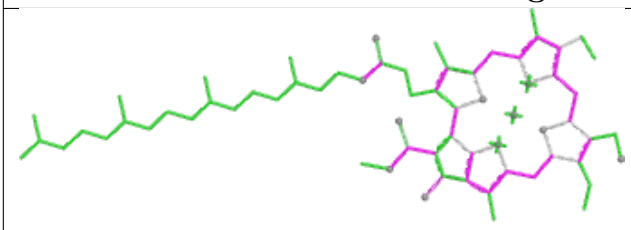


Rings

Ligand CHL 5 316



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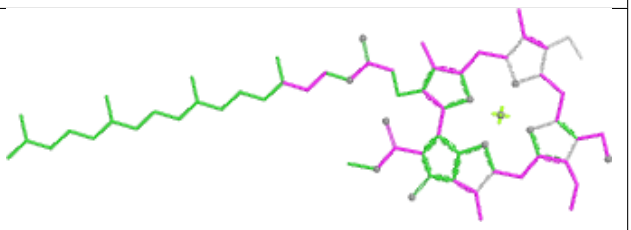
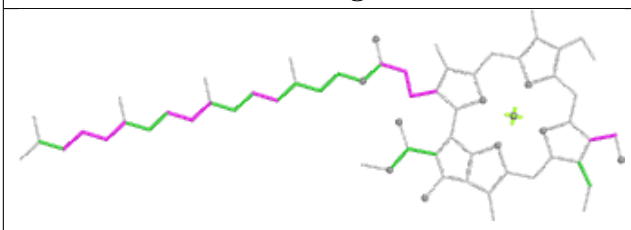
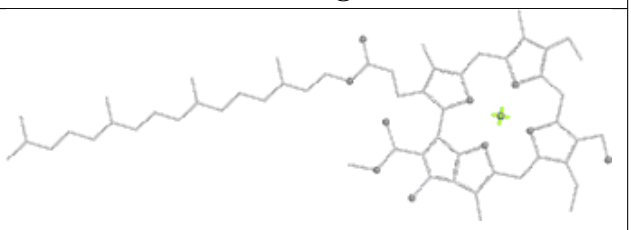


Bond angles

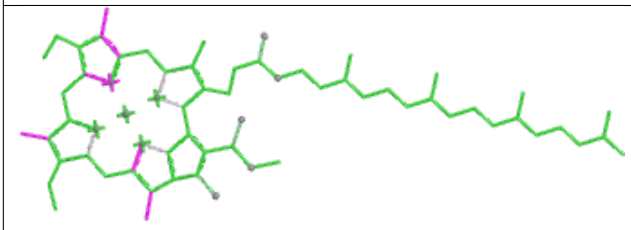


Torsions

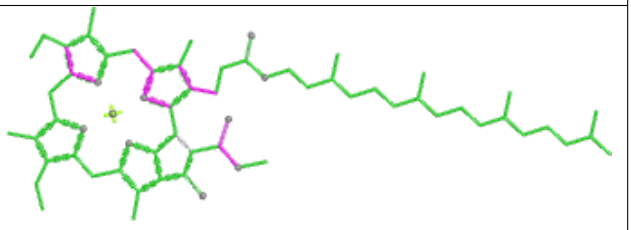


Rings

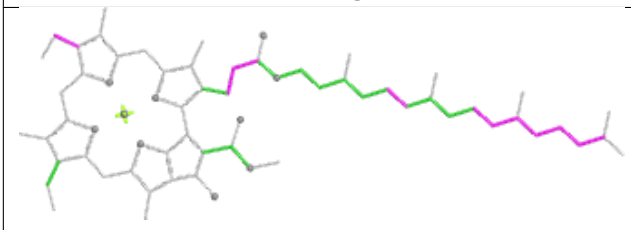
Ligand CLA B 603



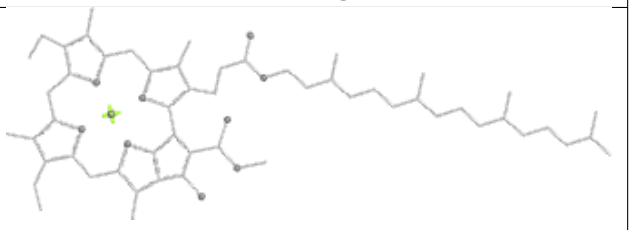
Bond lengths



Bond angles

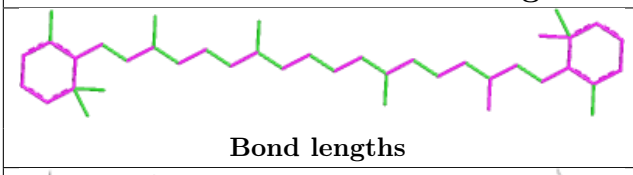


Torsions

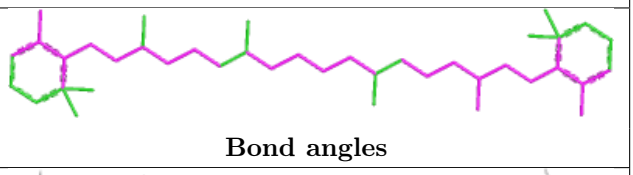


Rings

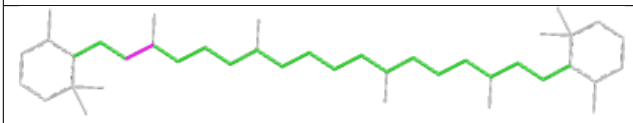
Ligand BCR A 409



Bond lengths



Bond angles



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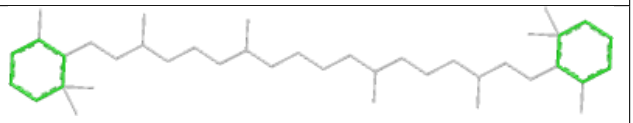
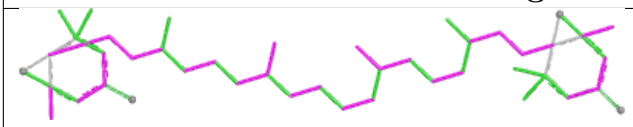
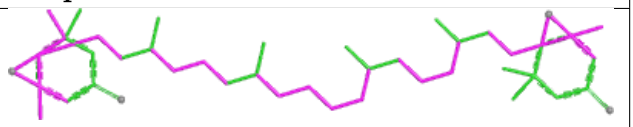


Rings

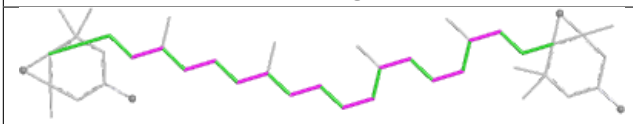
Ligand XAT q 309



Bond lengths



Bond angles



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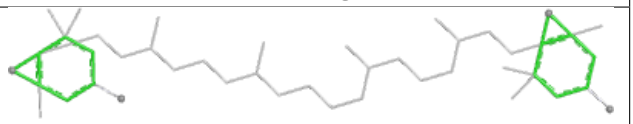
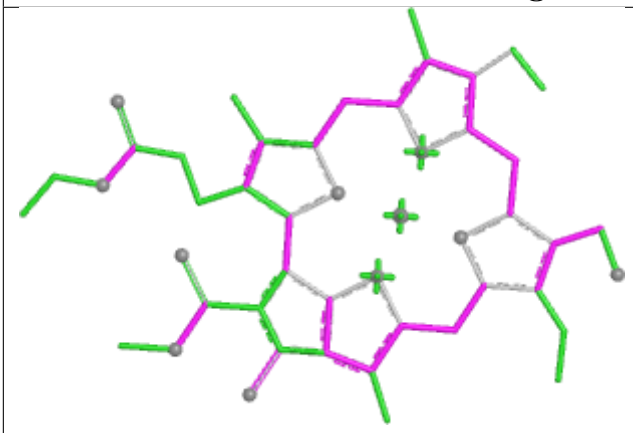


Rings

Ligand CHL 6 313



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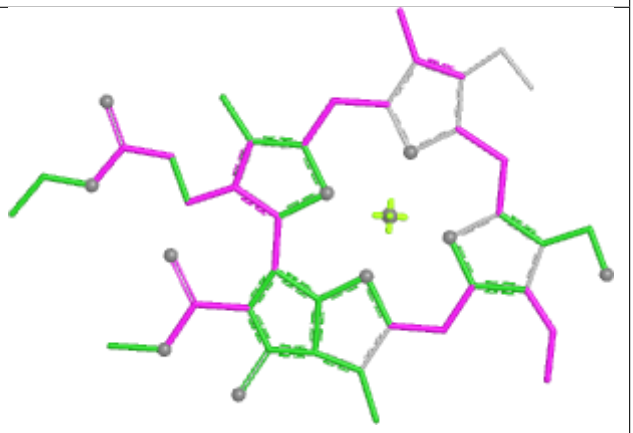
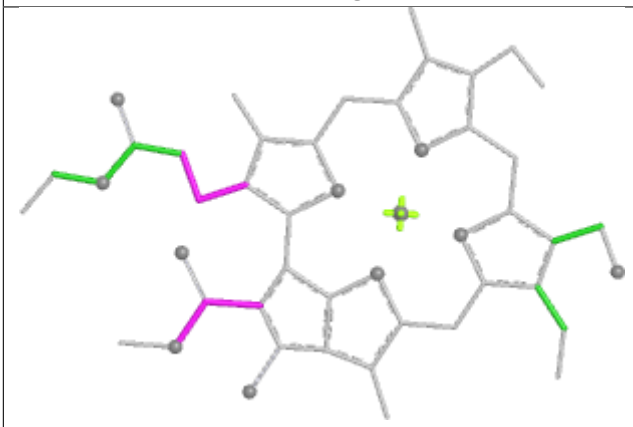


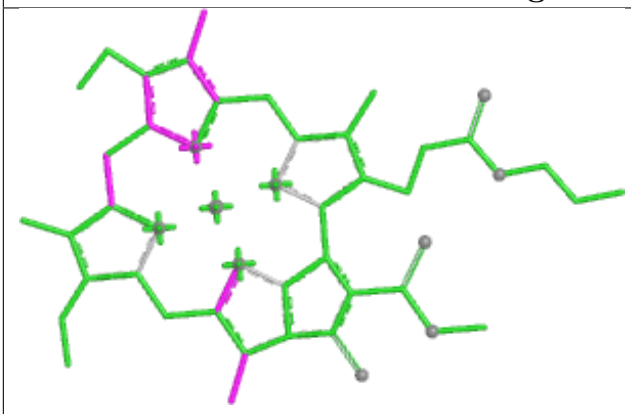
Bond angles



Torsions

Rings

Ligand CLA q 308



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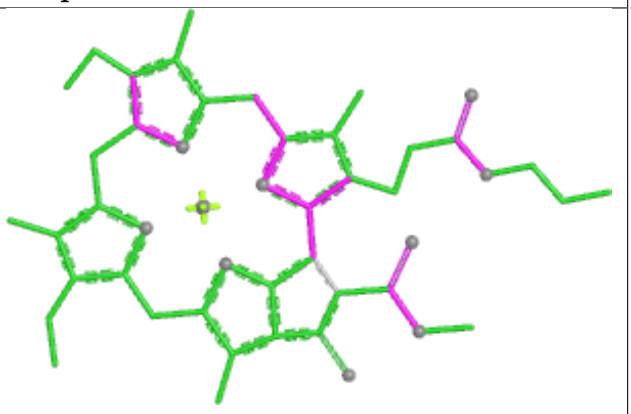
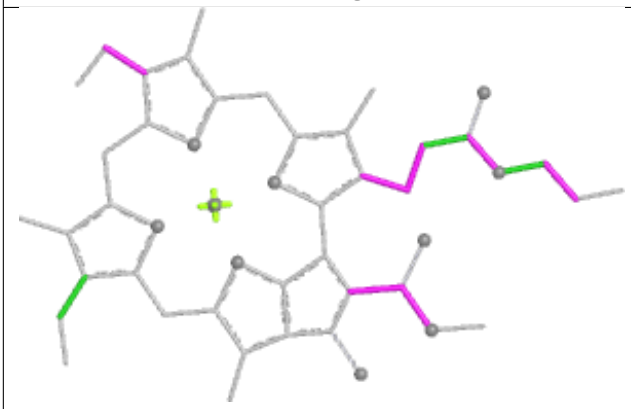
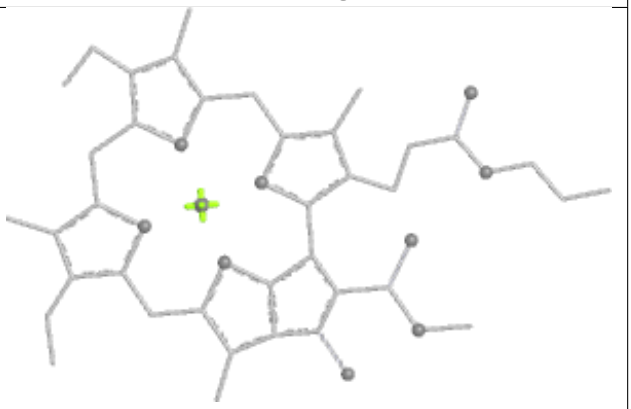


Bond angles

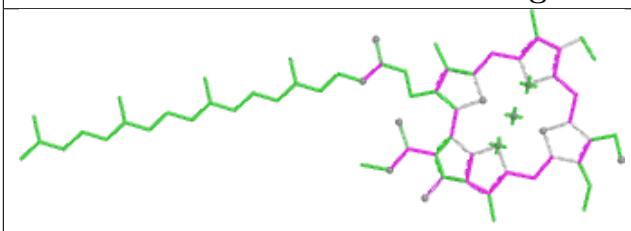


Torsions

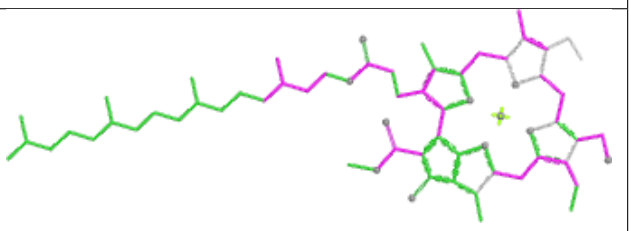


Rings

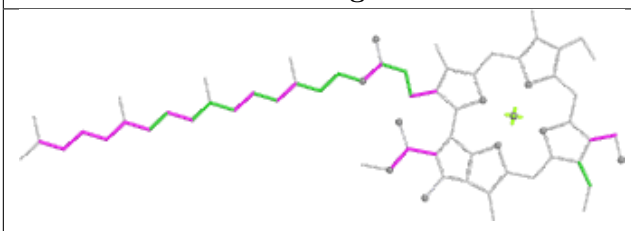
Ligand CHL r 614



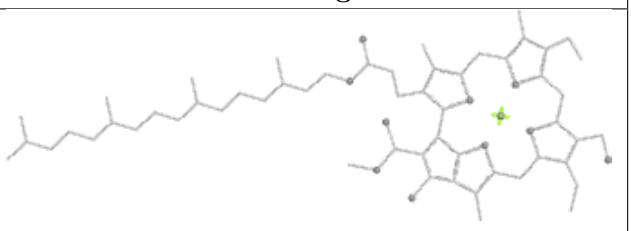
Bond lengths



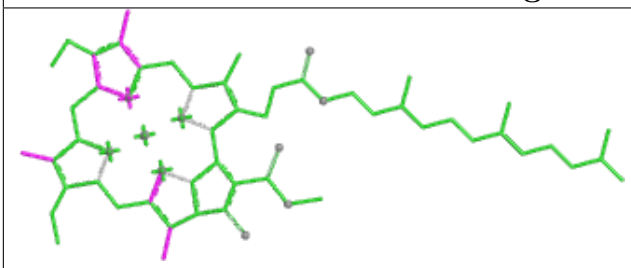
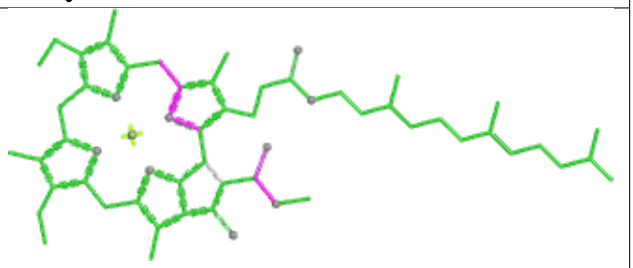
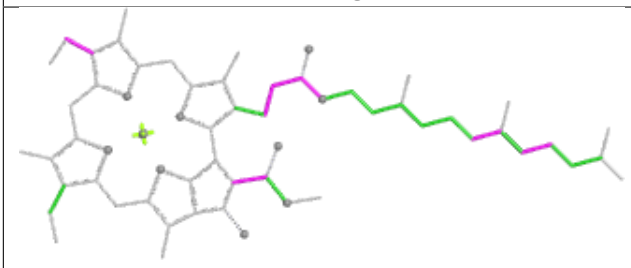
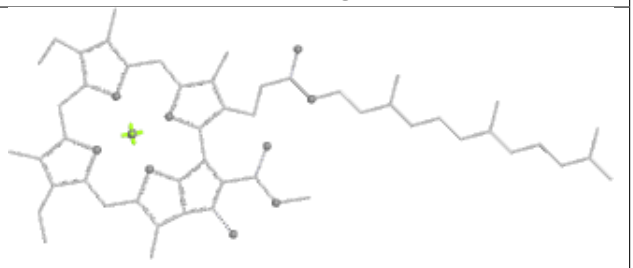
Bond angles

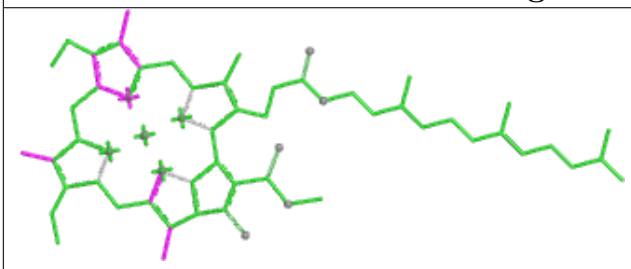
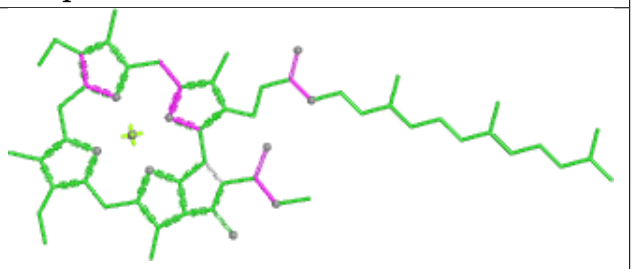
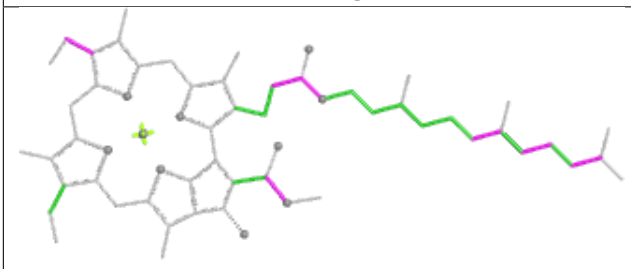
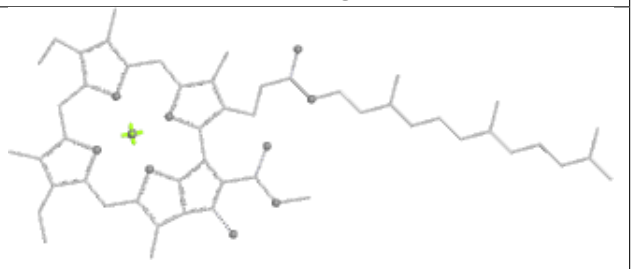


Torsions

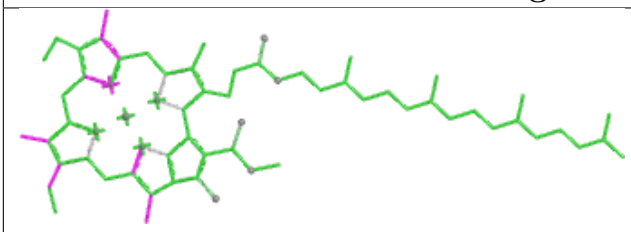


Rings

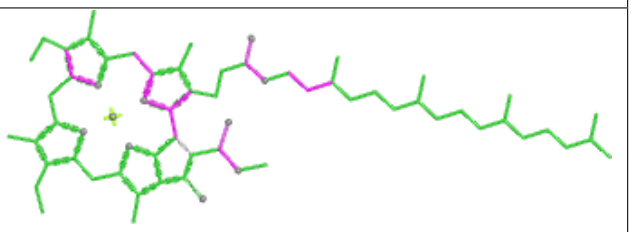
Ligand CLA Q 306	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA q 306	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

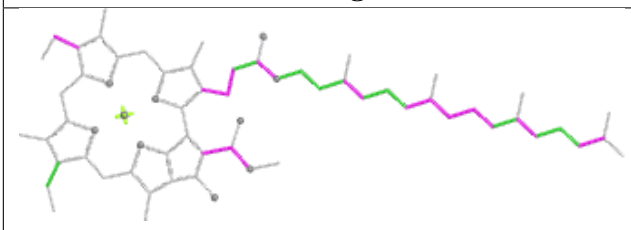
Ligand CLA c 503



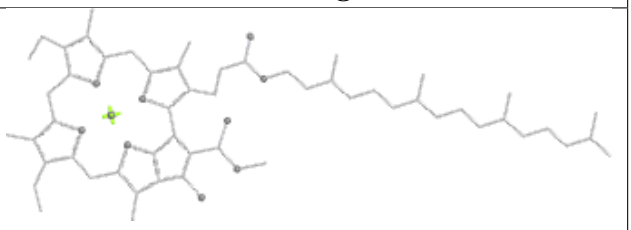
Bond lengths



Bond angles

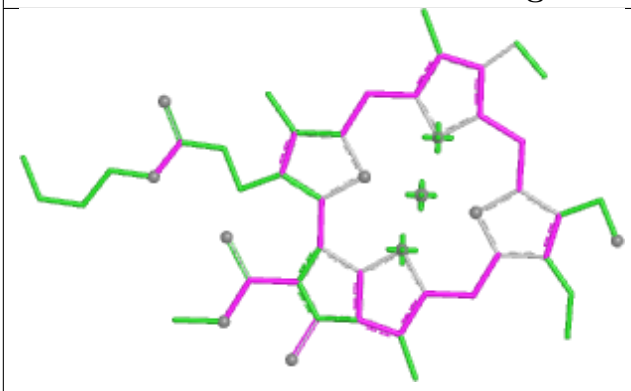


Torsions



Rings

Ligand CHL n 315



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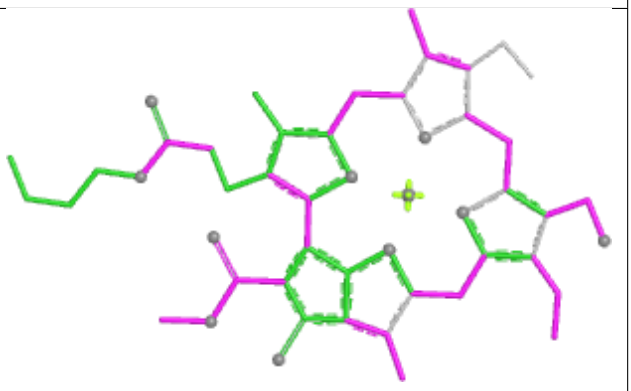
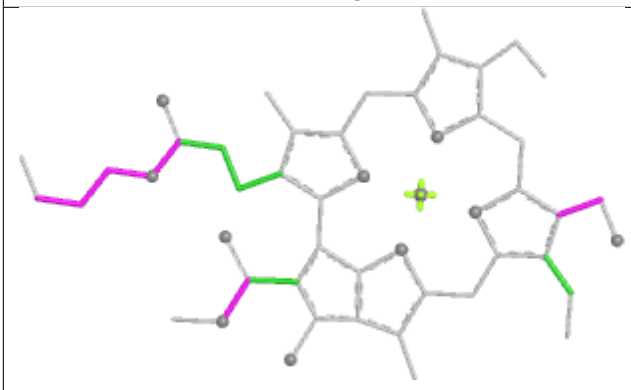


Bond angles



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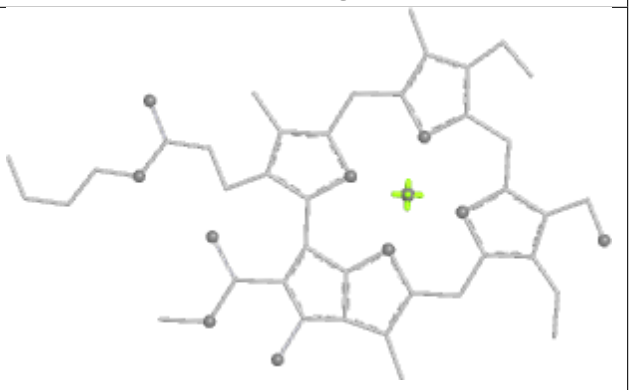
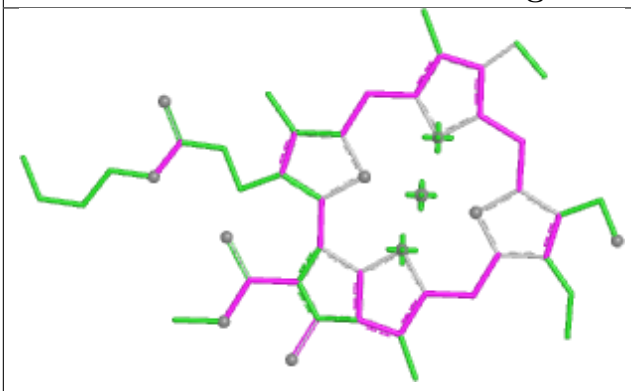


Rings

Ligand CHL p 316



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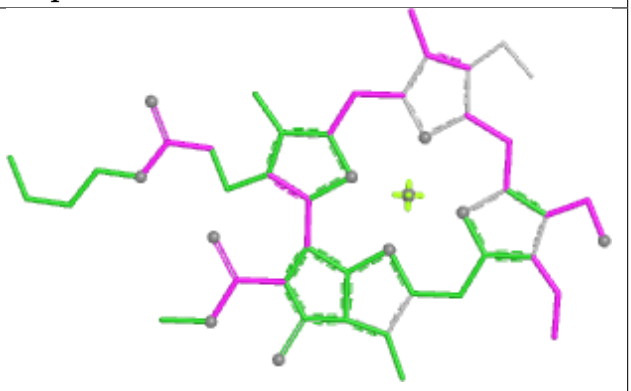
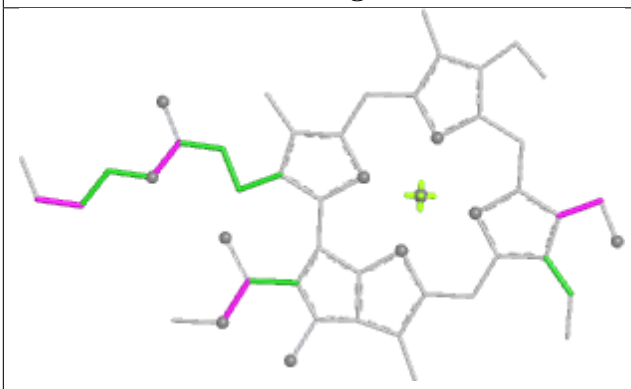
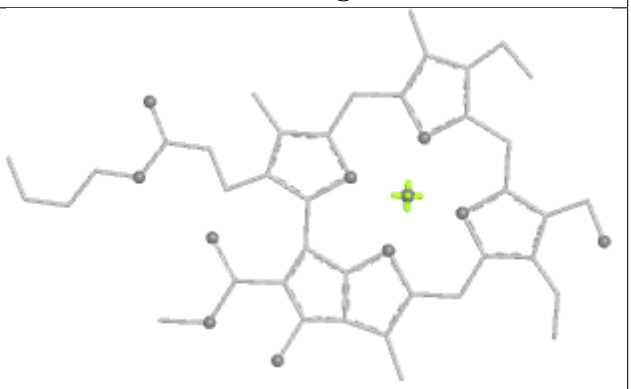


Bond angles

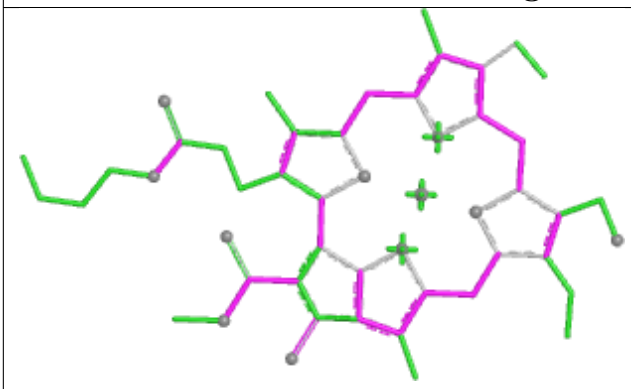


Torsions

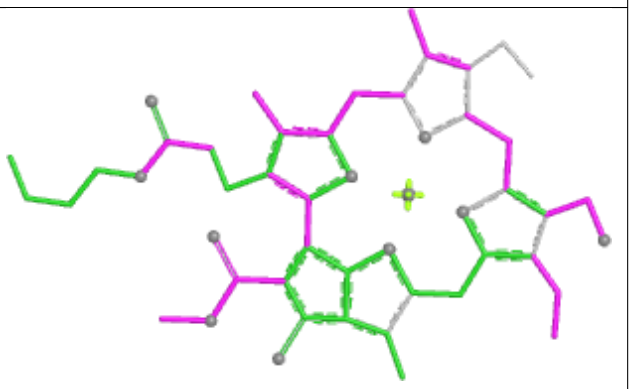


Rings

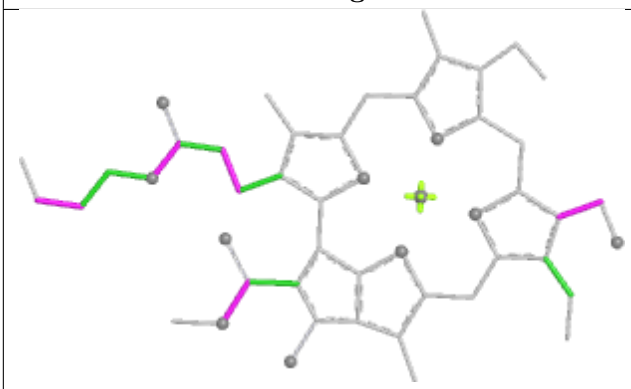
Ligand CHL U 314



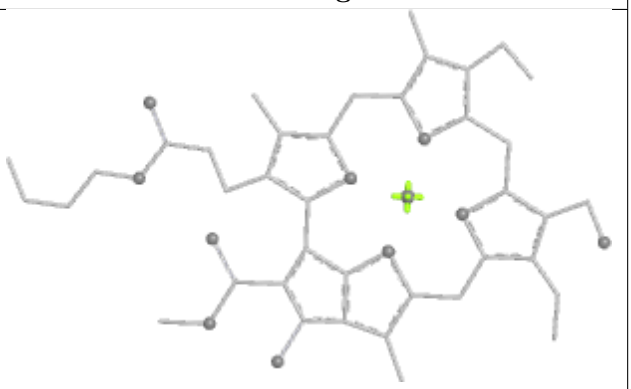
Bond lengths



Bond angles

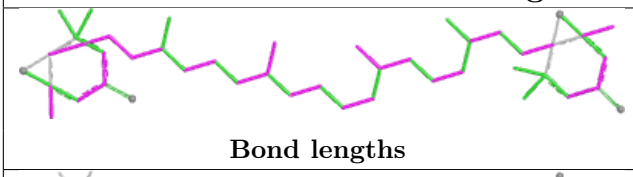


Torsions



Rings

Ligand XAT n 311



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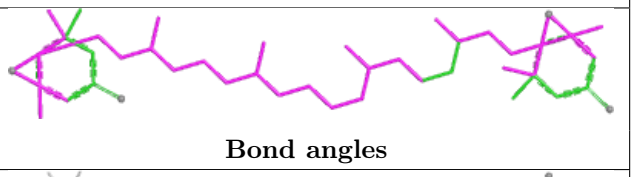
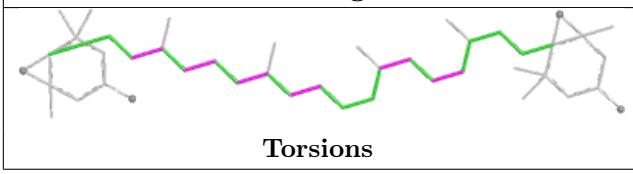
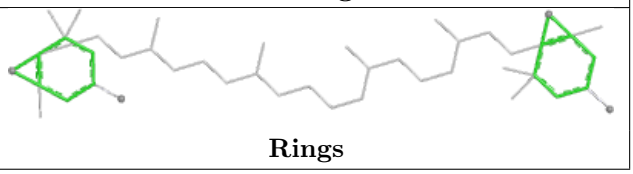


Bond angles

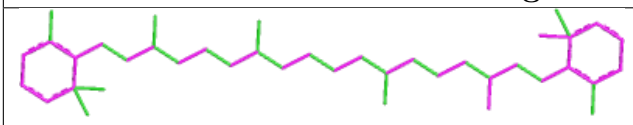


Torsions

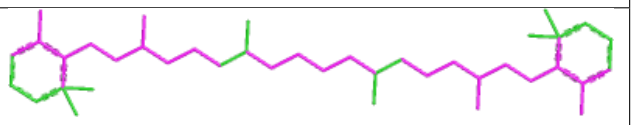


Rings

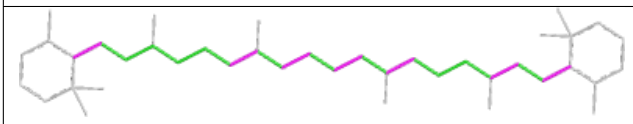
Ligand BCR B 620



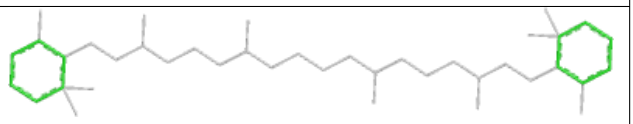
Bond lengths



Bond angles

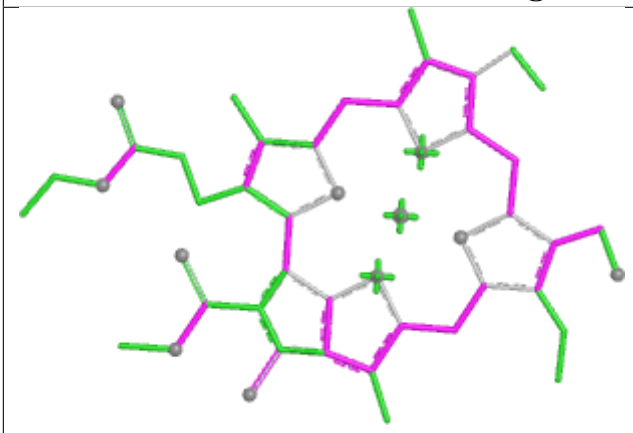


Torsions

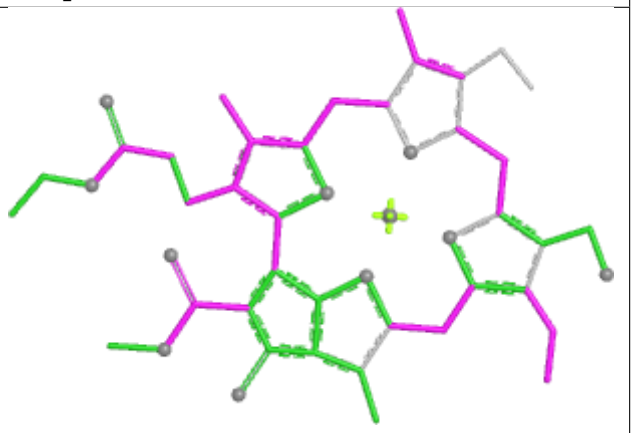


Rings

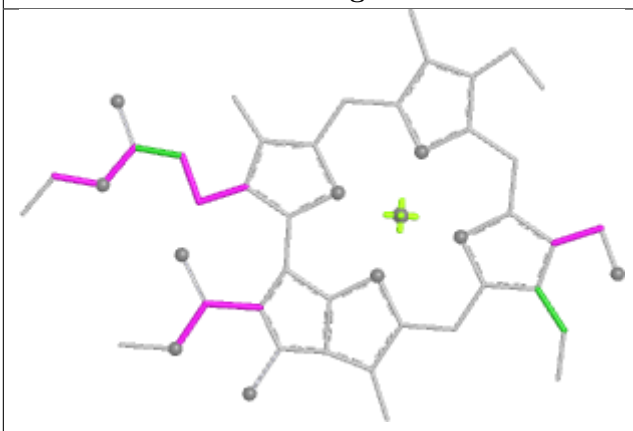
Ligand CHL q 312



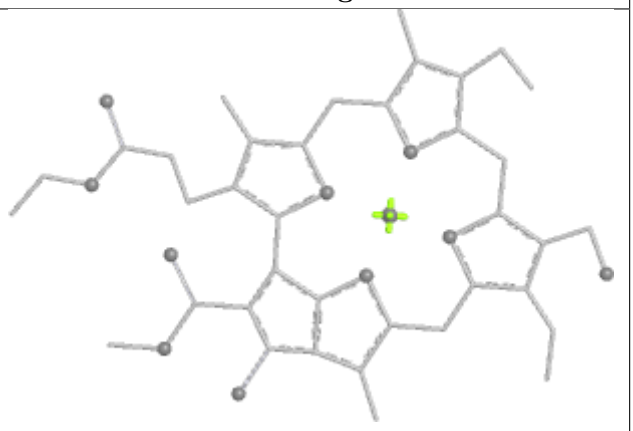
Bond lengths



Bond angles

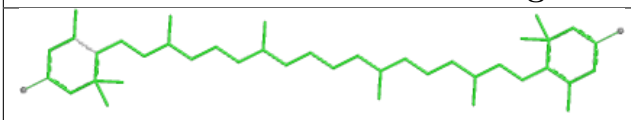


Torsions



Rings

Ligand LUT S 310



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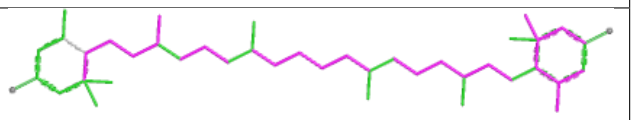
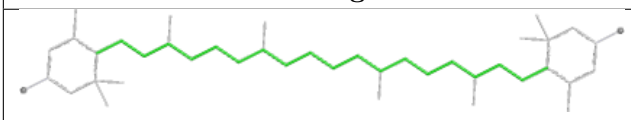
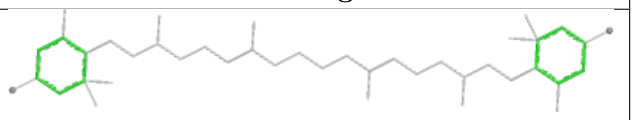


Bond angles

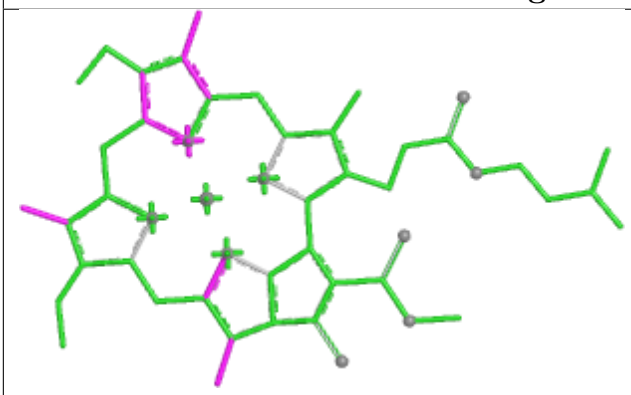


Torsions



Rings

Ligand CLA 2 303



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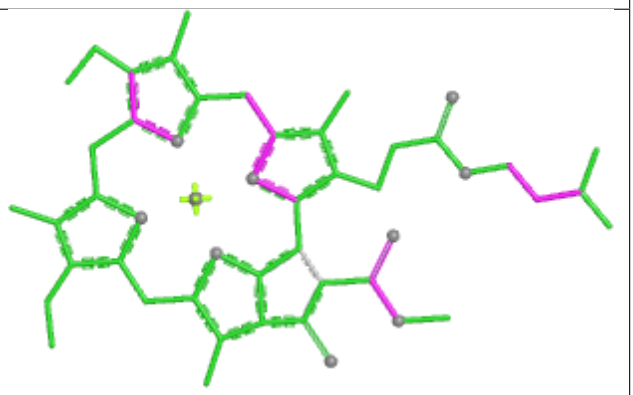
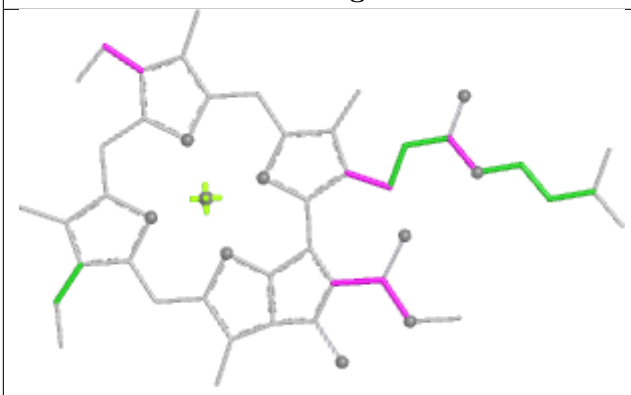


Bond angles



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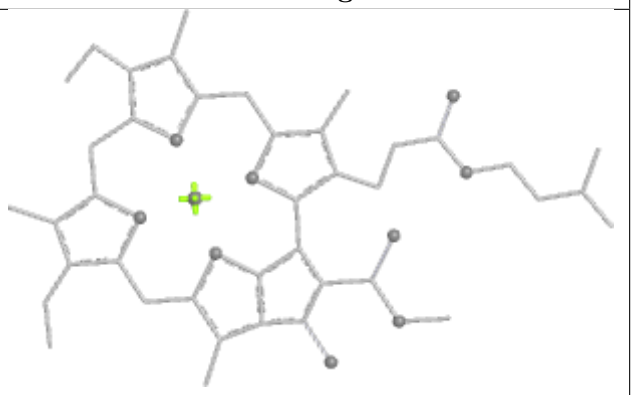
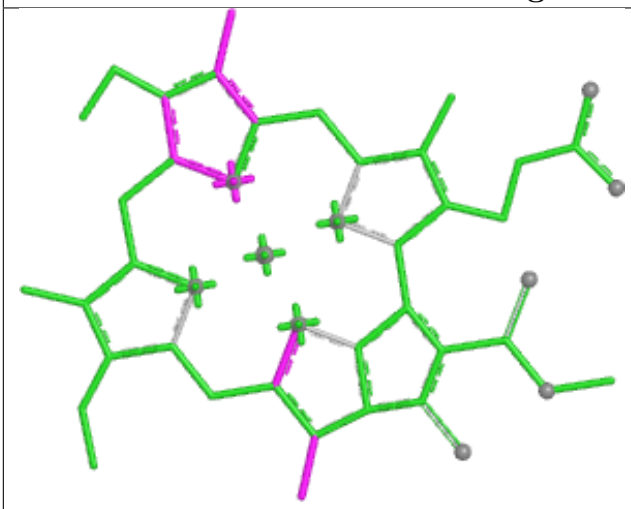


Rings

Ligand CLA S 302



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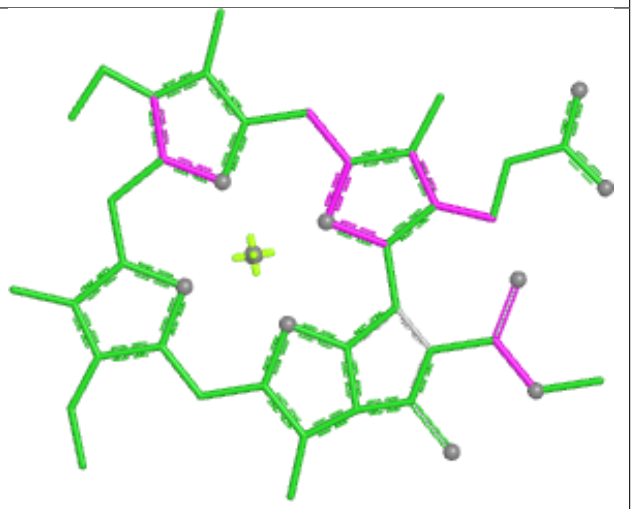
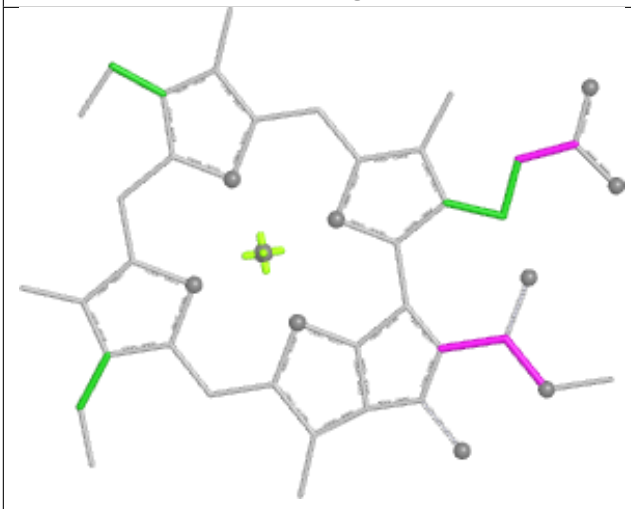


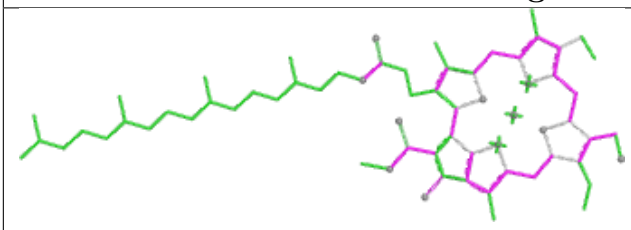
Bond angles



Torsions

Rings

Ligand CHL 2 318



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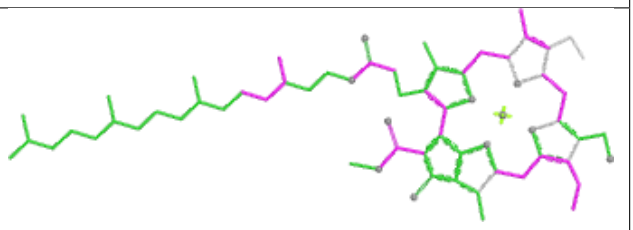
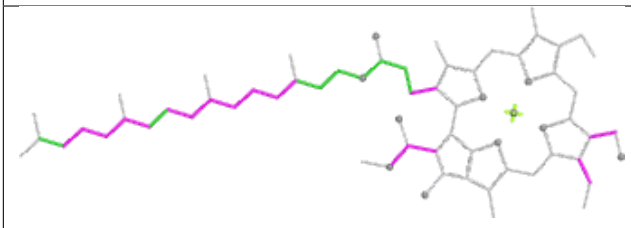


Bond angles



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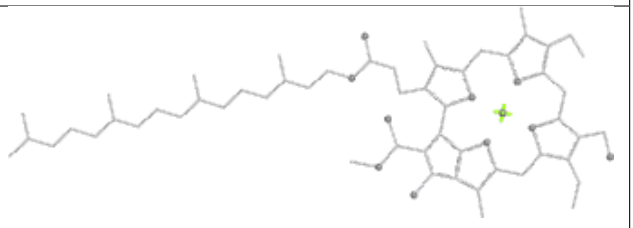
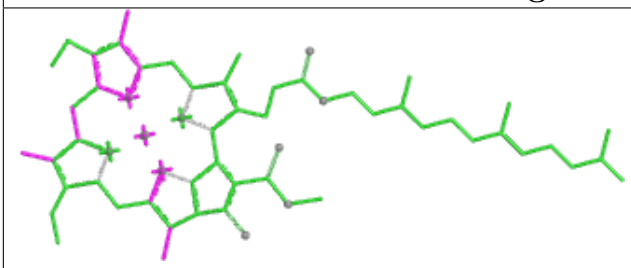


Rings

Ligand CLA a 408



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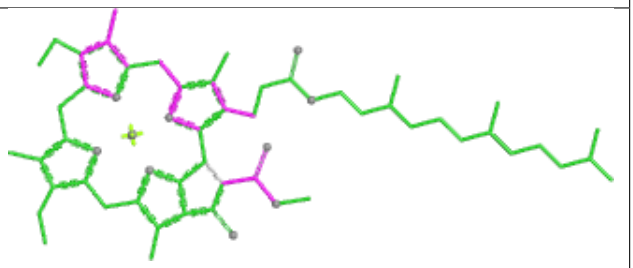
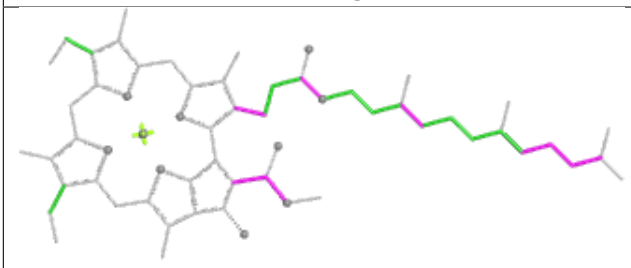


Bond angles



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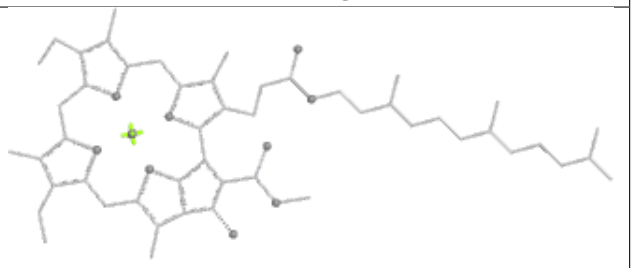
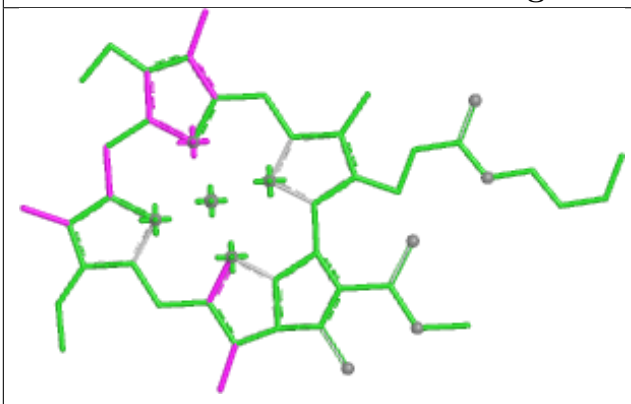


Rings

Ligand CLA S 307



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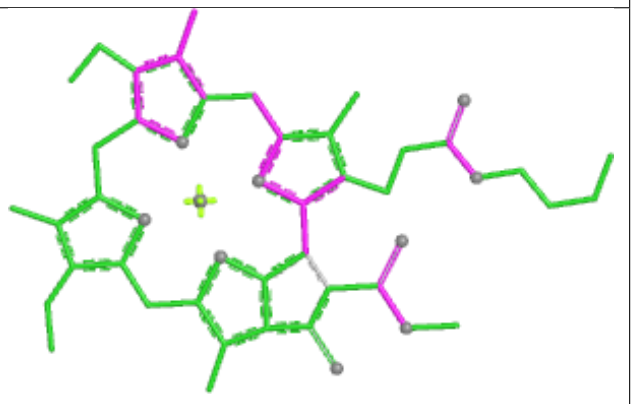
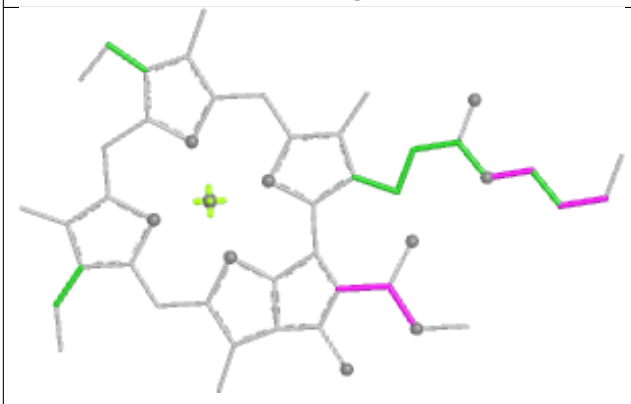


Bond angles



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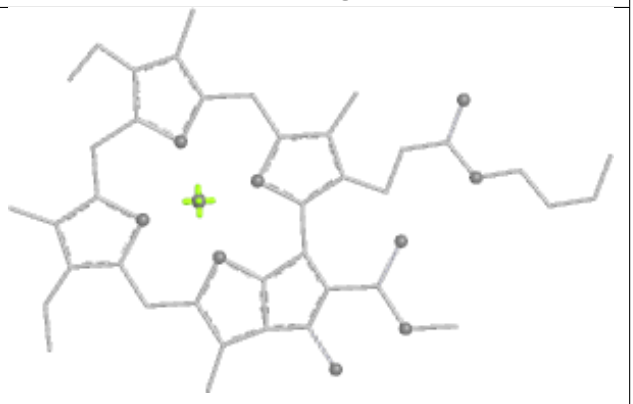
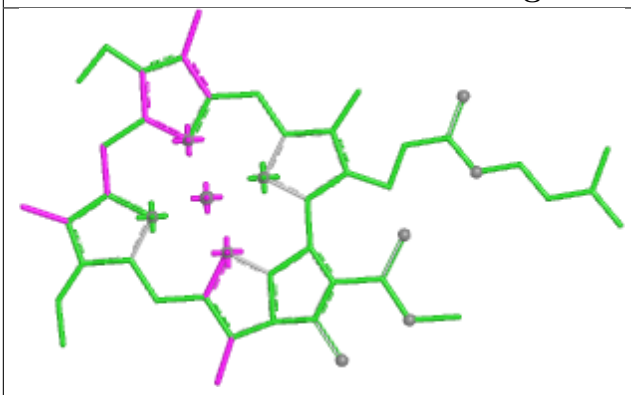


Rings

Ligand CLA V 303



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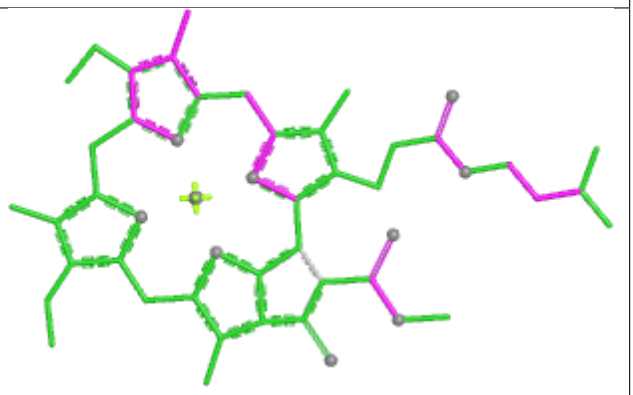
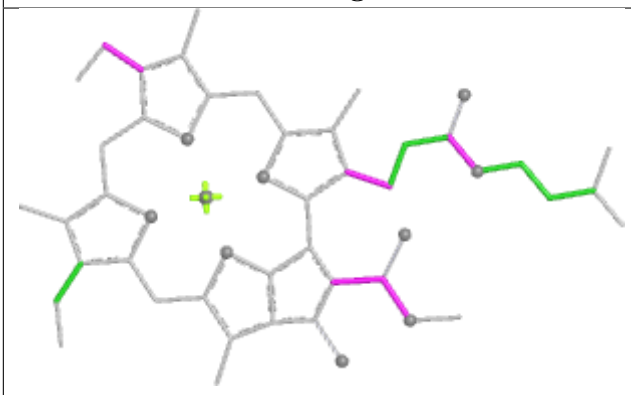


Bond angles



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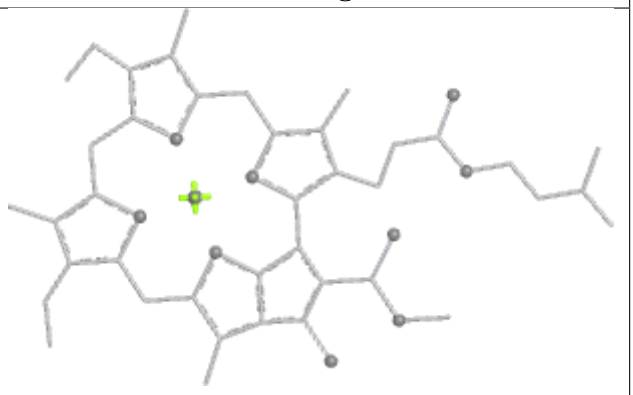
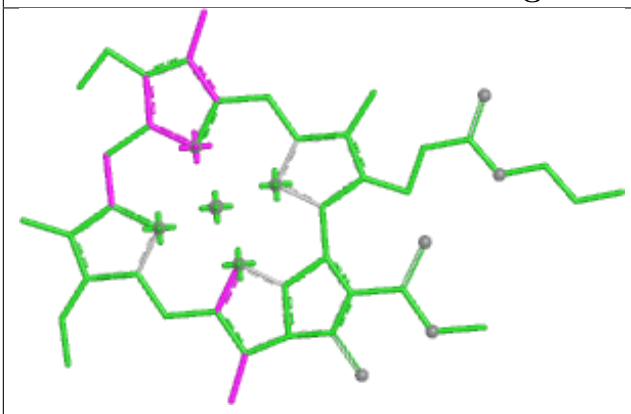


Rings

Ligand CLA V 308



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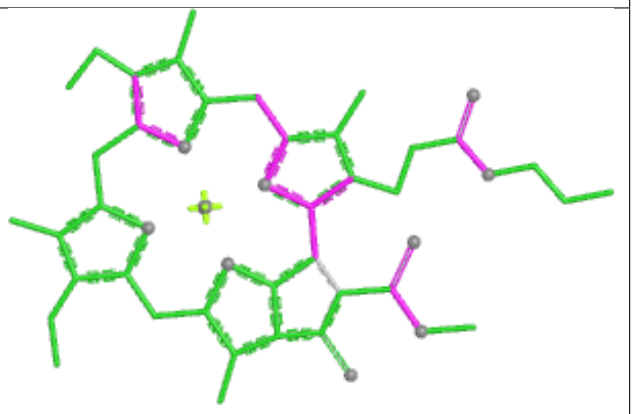
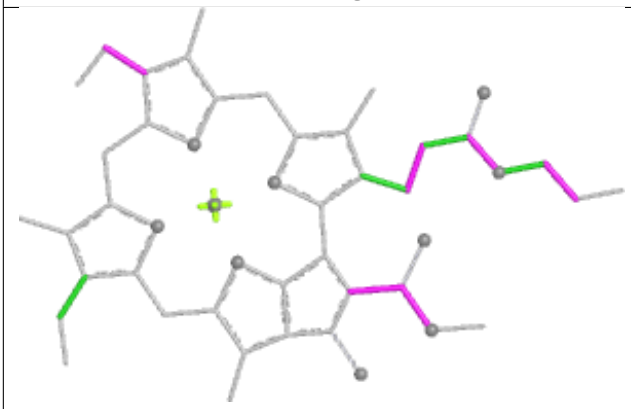


Bond angles



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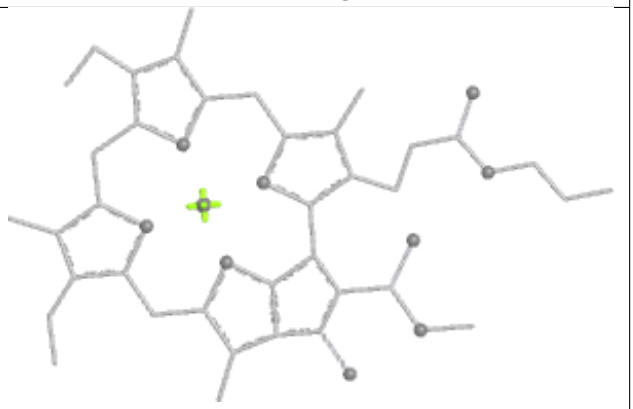
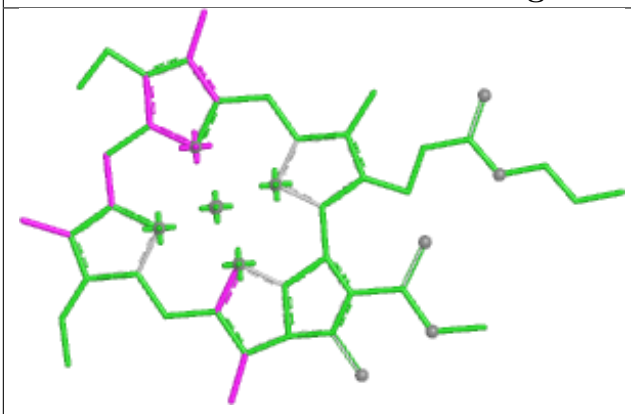


Rings

Ligand CLA n 308



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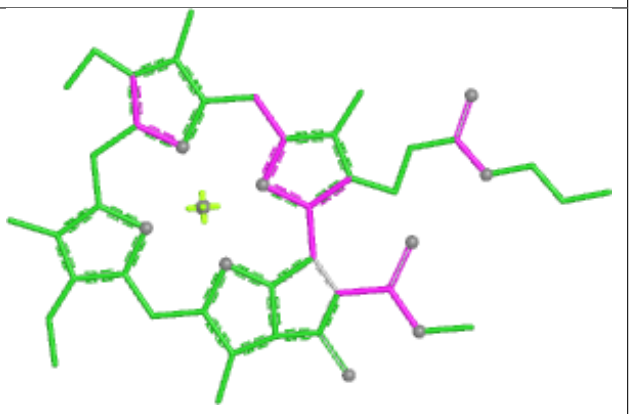
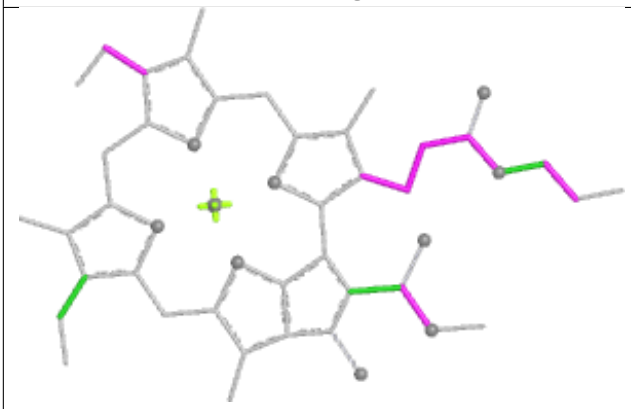


Bond angles



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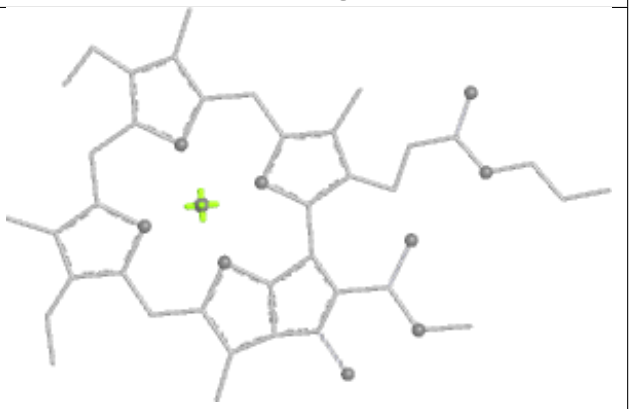
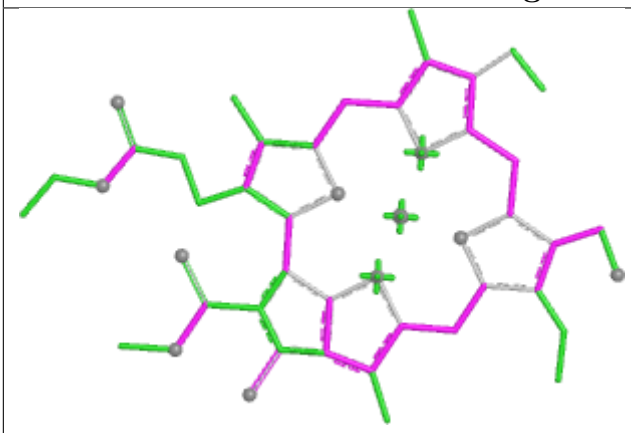


Rings

Ligand CHL Q 312



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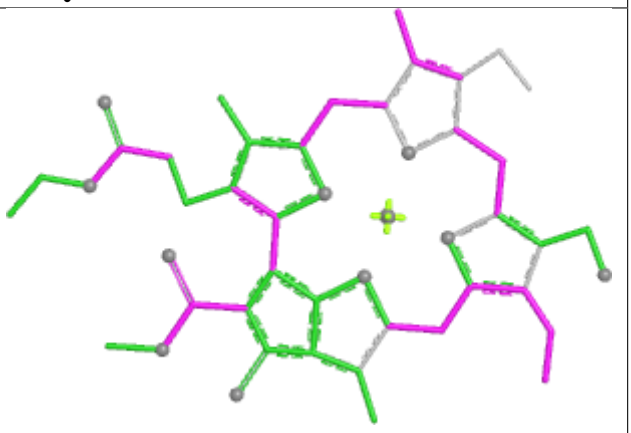
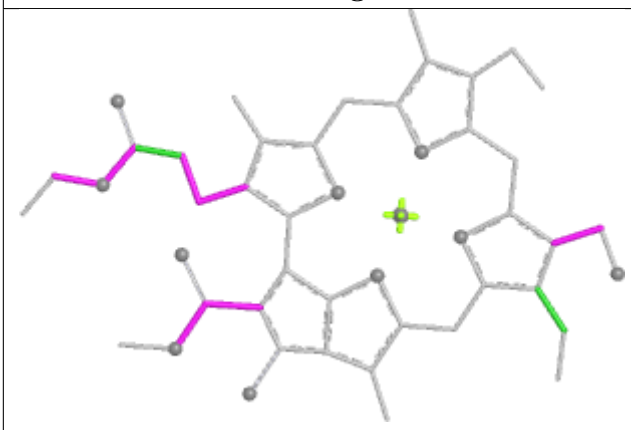


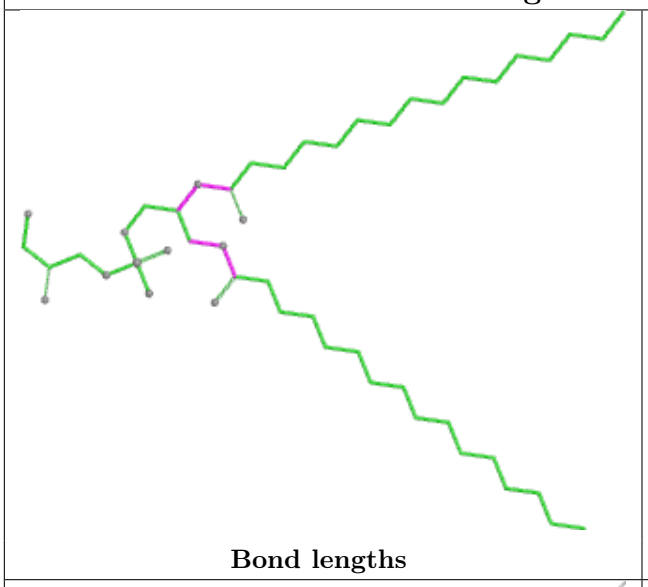
Bond angles



Torsions

Rings

Ligand LHG C 522



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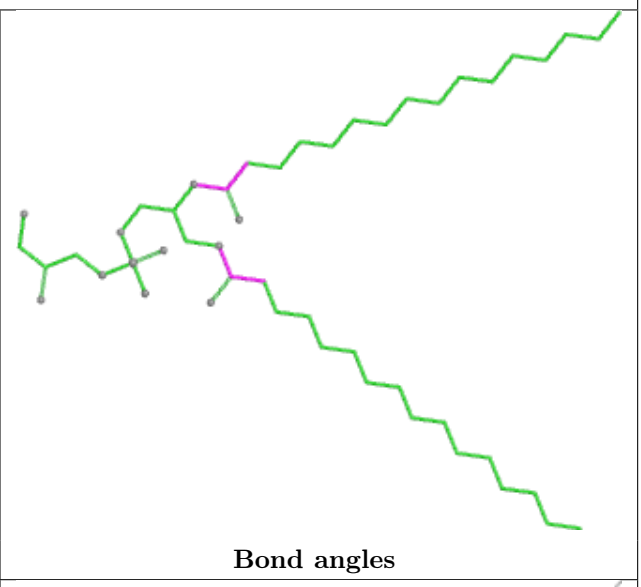
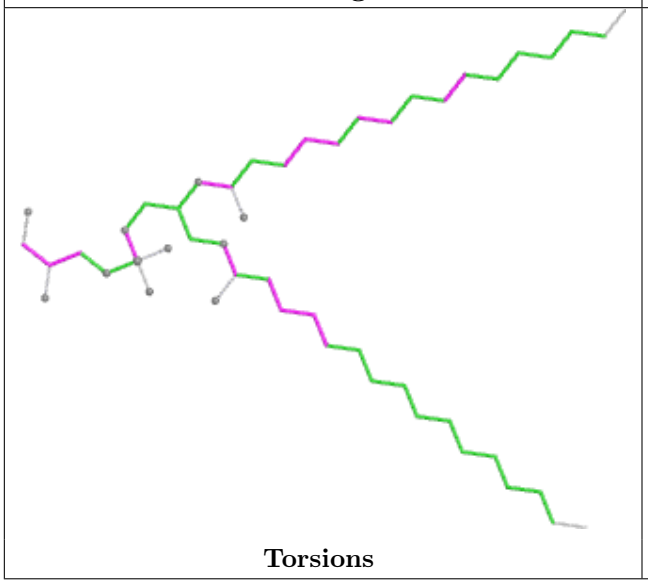


Bond angles



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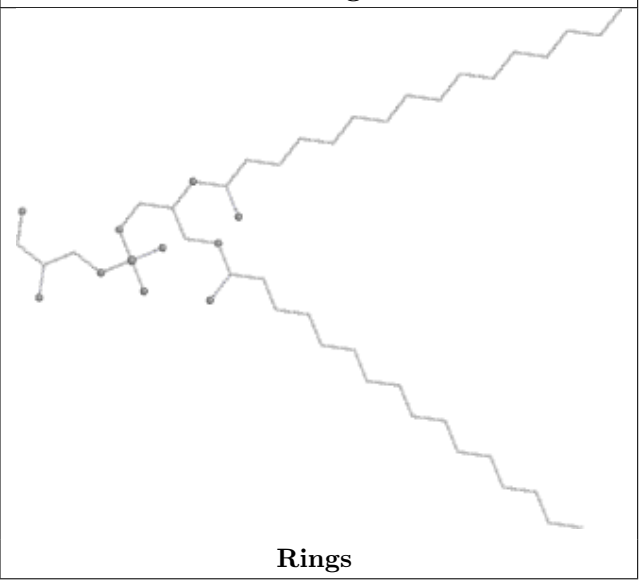
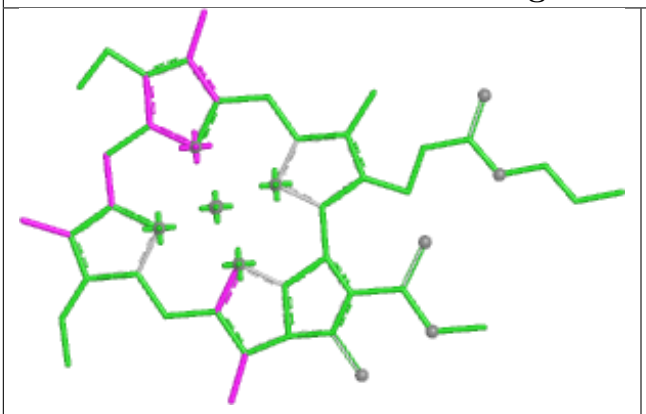


Rings

Ligand CLA 2 308



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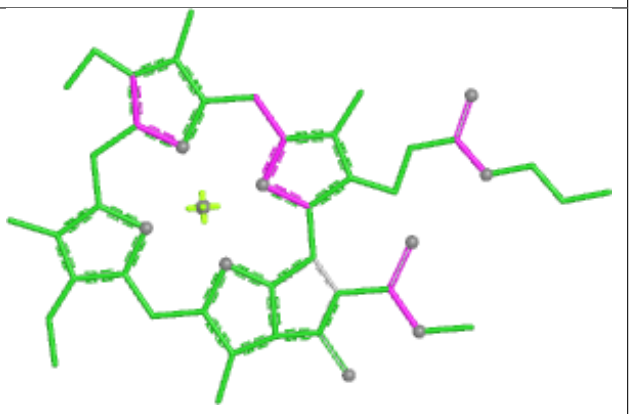
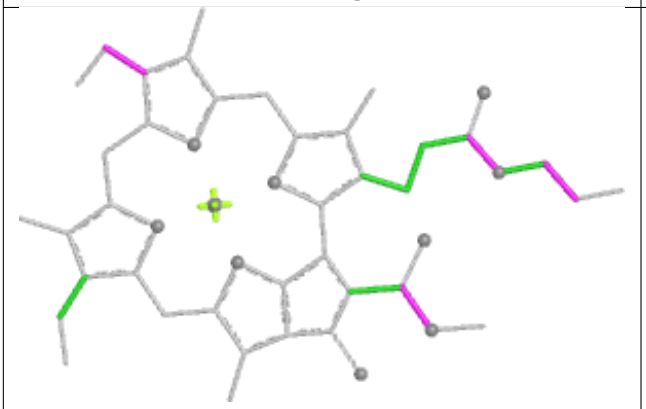


Bond angles



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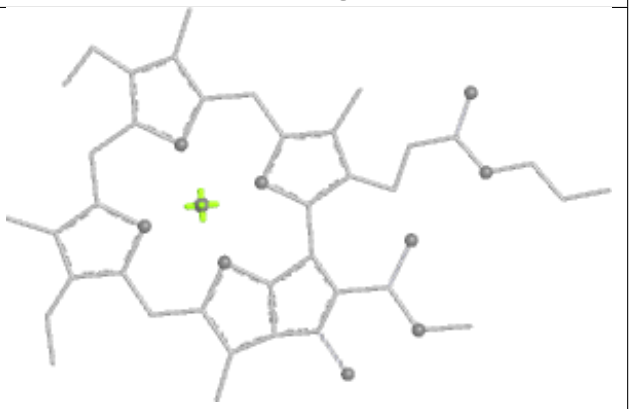
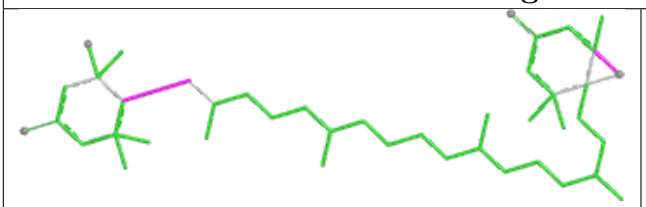
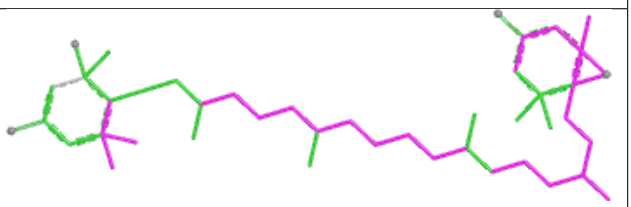


Rings

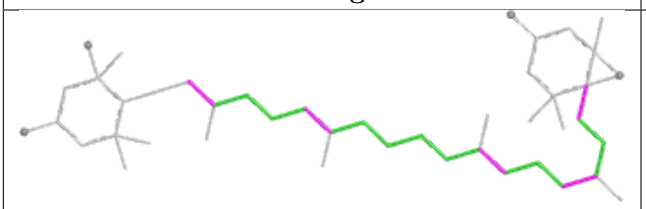
Ligand NEX N 318



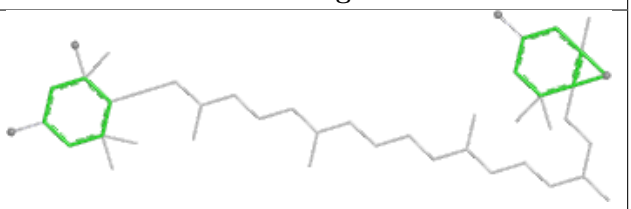
Bond lengths



Bond angles

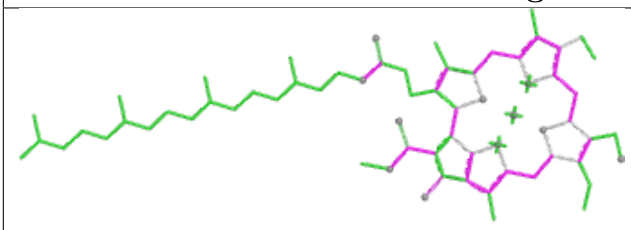


Torsions

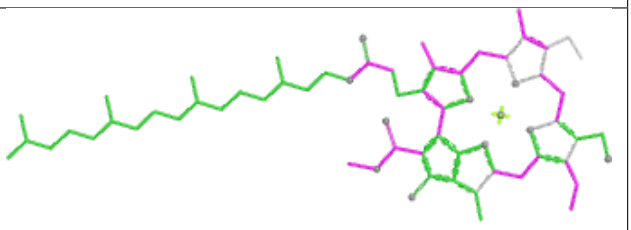


Rings

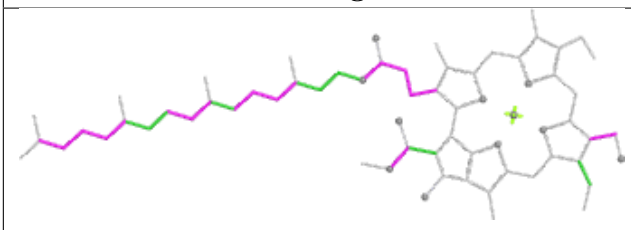
Ligand CHL n 316



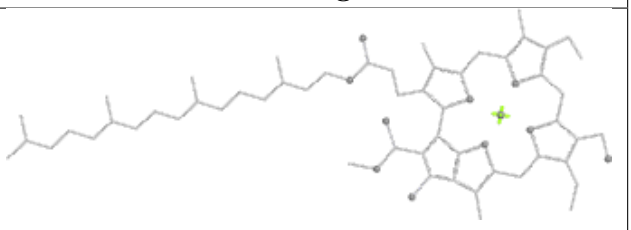
Bond lengths



Bond angles

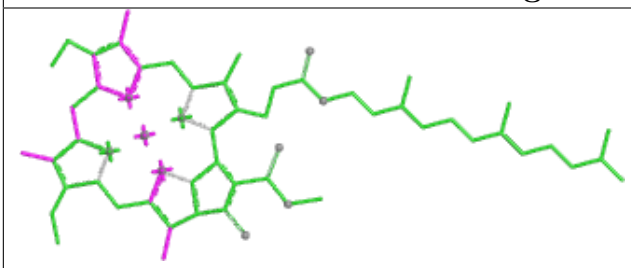


Torsions



Rings

Ligand CLA A 408



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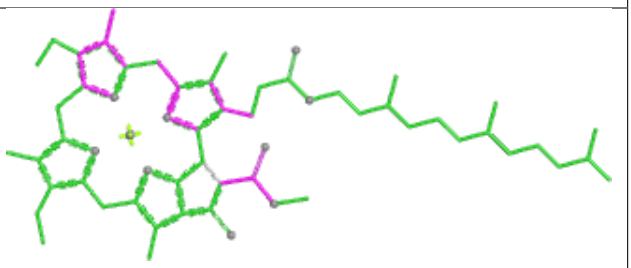

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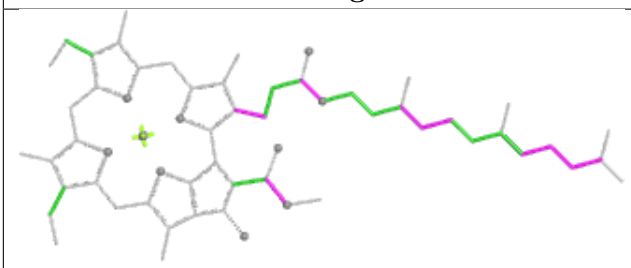

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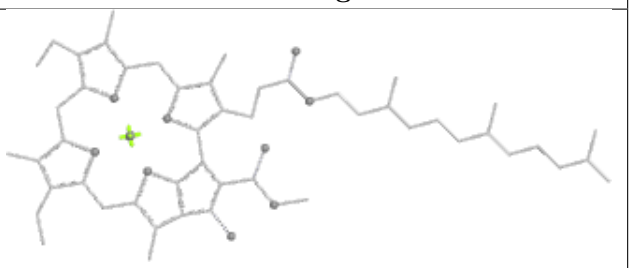
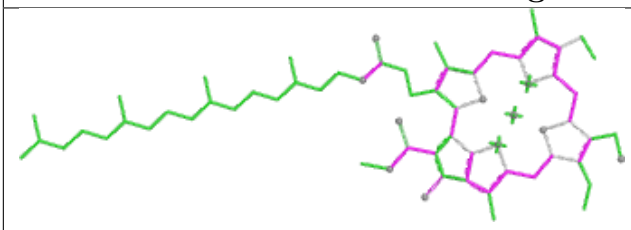


Rings

Ligand CHL 2 316



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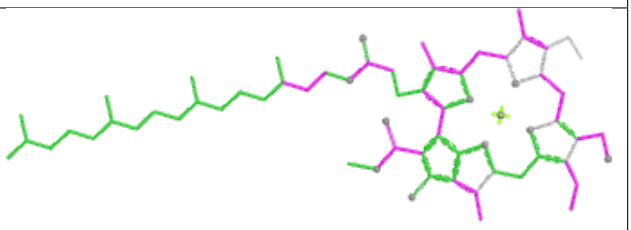

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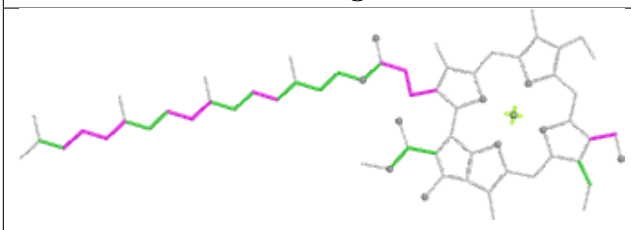

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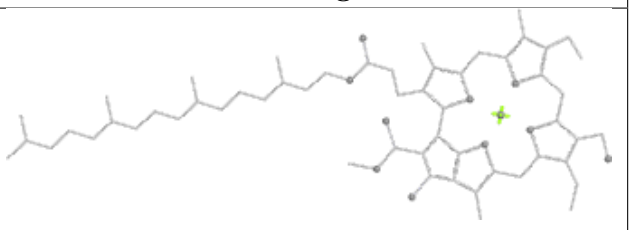
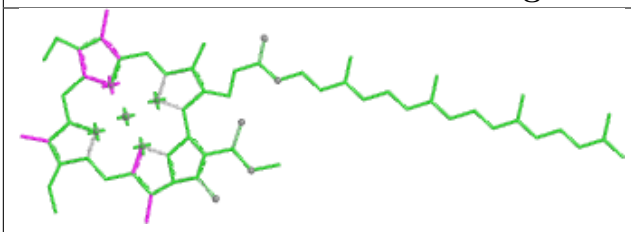


Rings

Ligand CLA N 302



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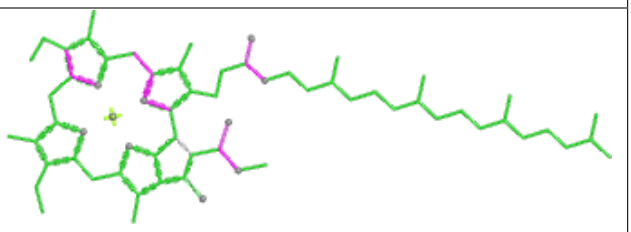
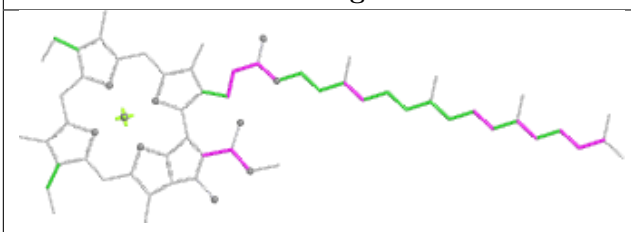


Bond angles



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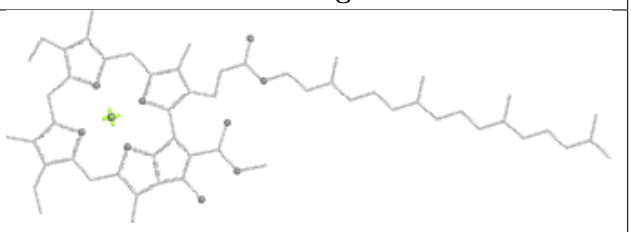
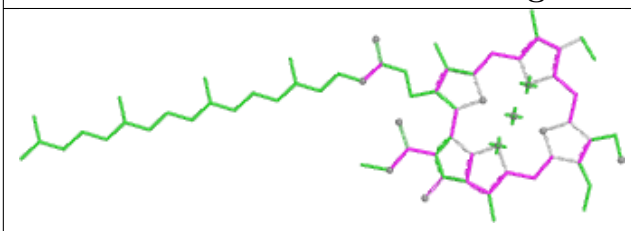


Rings

Ligand CHL 1 316



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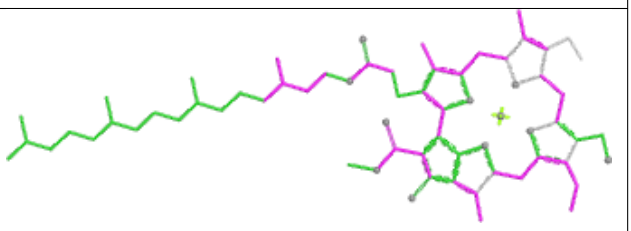

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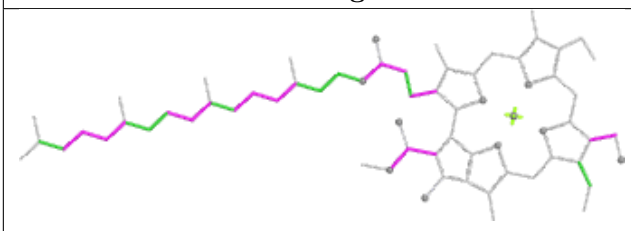

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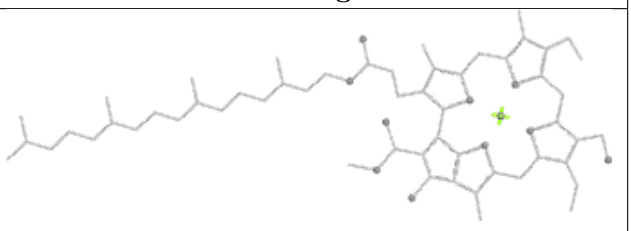
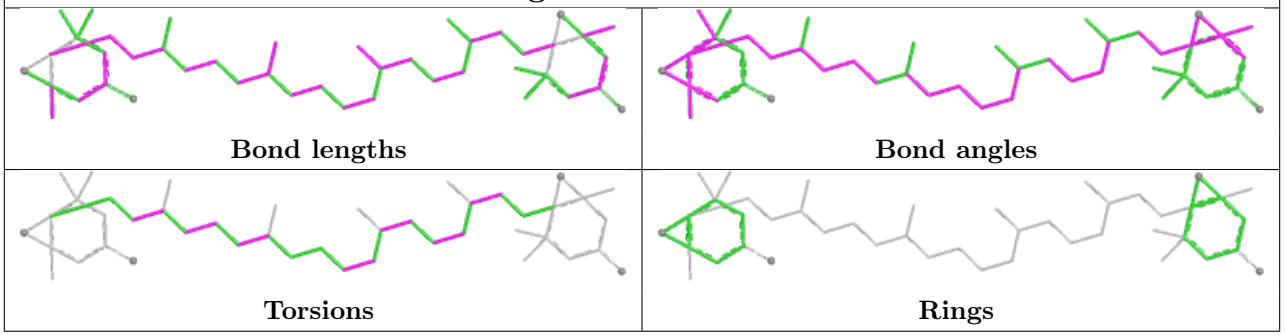
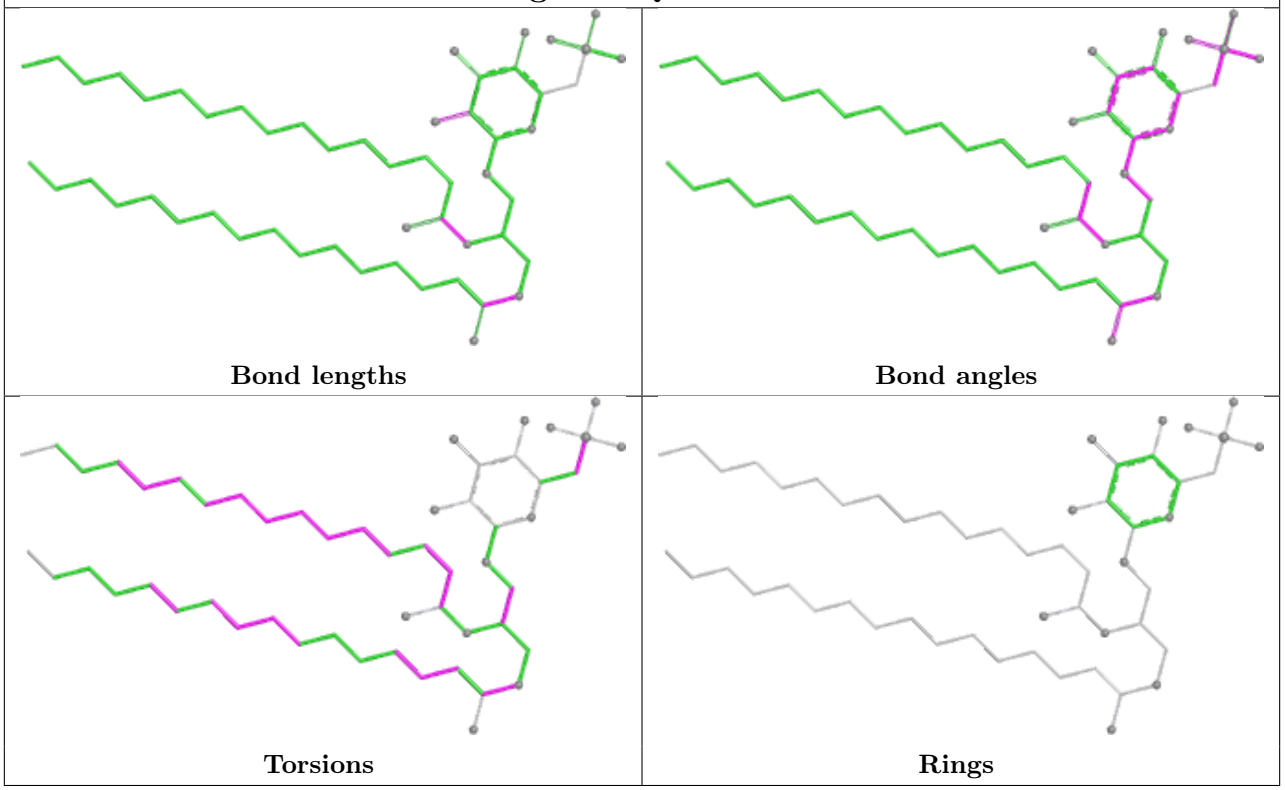


Rings

Ligand XAT v 311



Ligand SQD a 413



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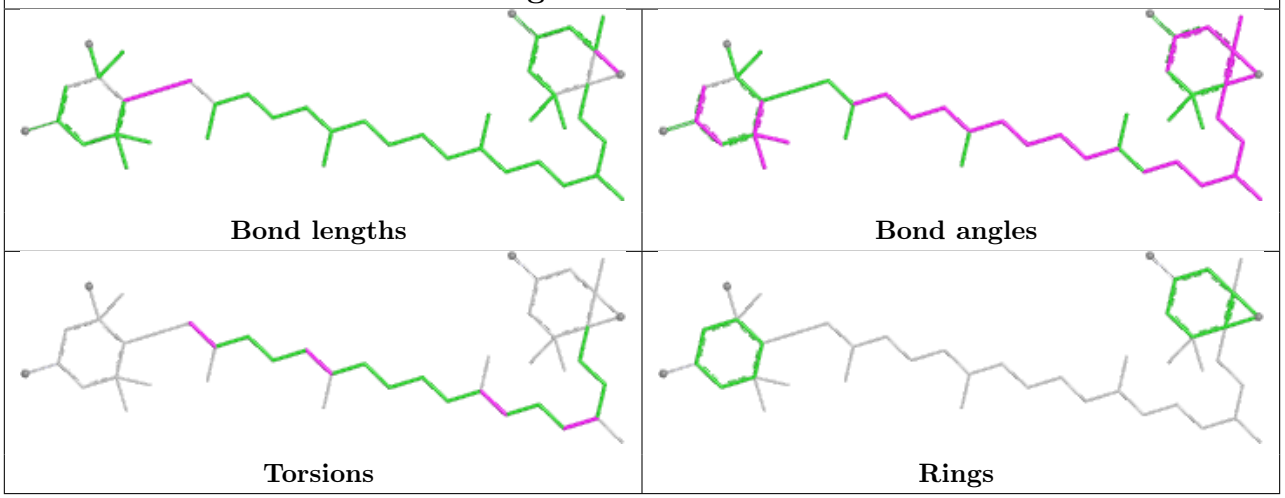
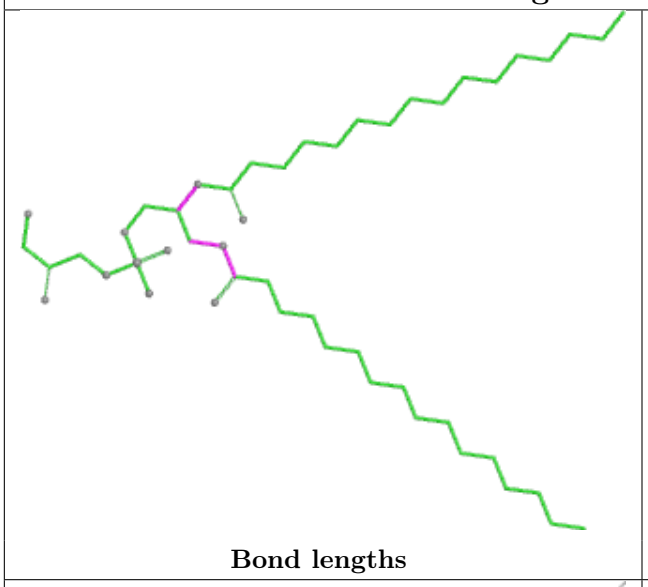
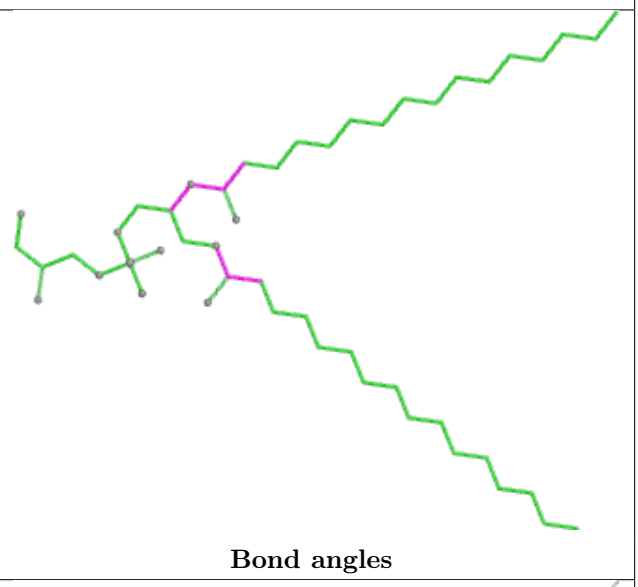


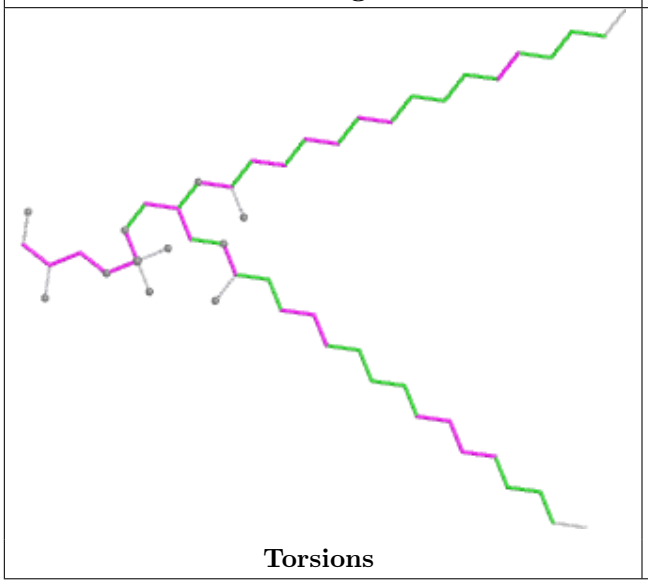
Ligand LHG l 101



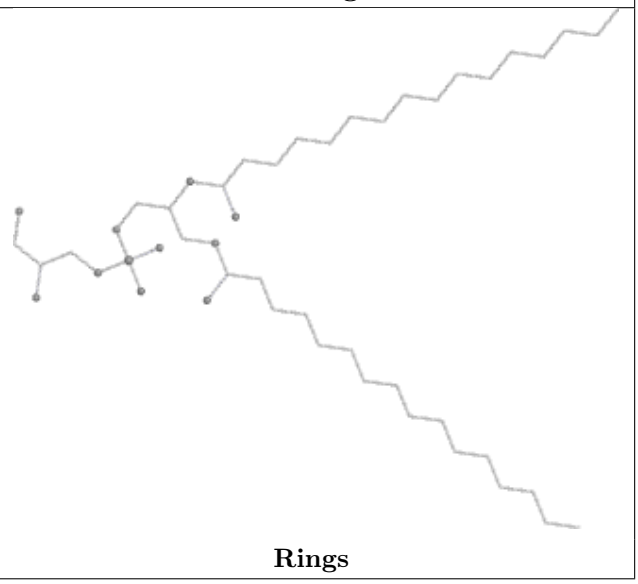
Bond lengths



Bond angles

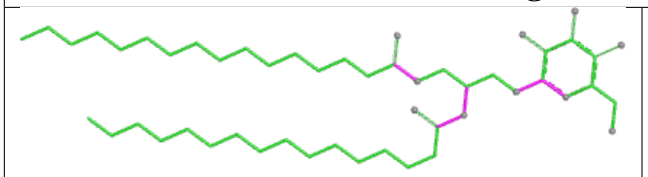


Torsions



Rings

Ligand LMG c 501



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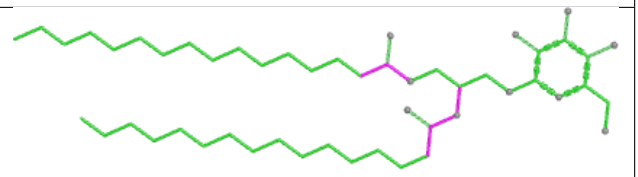
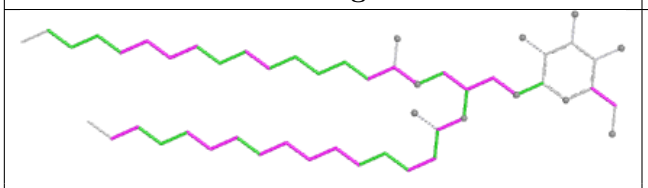


Bond angles



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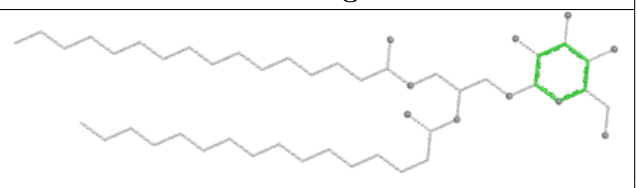
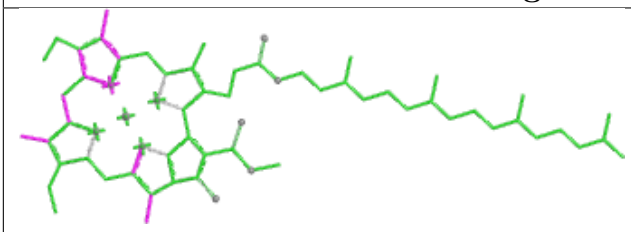


Rings

Ligand CLA N 301



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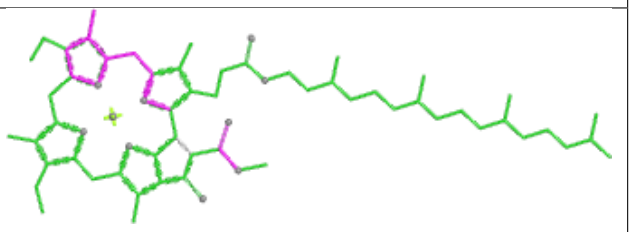
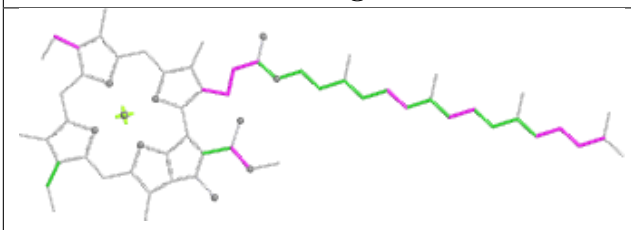


Bond angles



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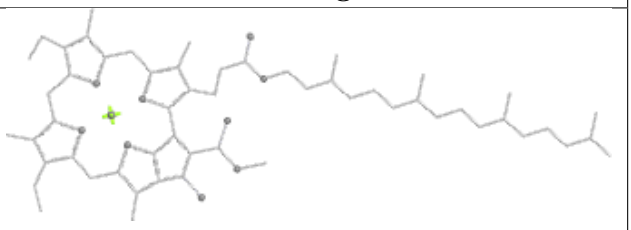
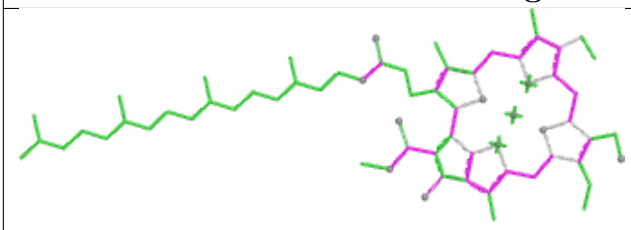


Rings

Ligand CHL P 317



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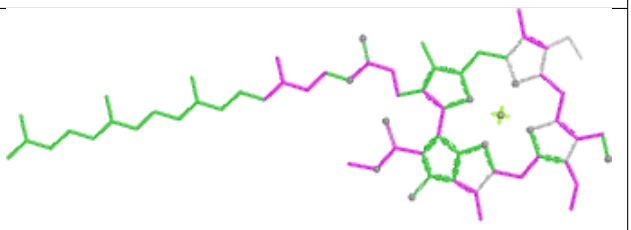
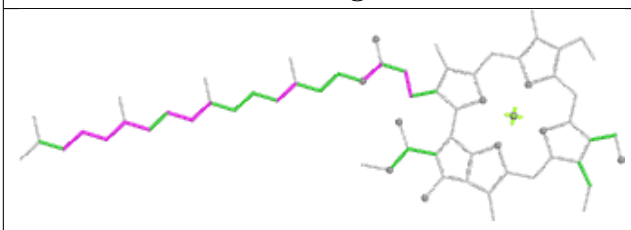
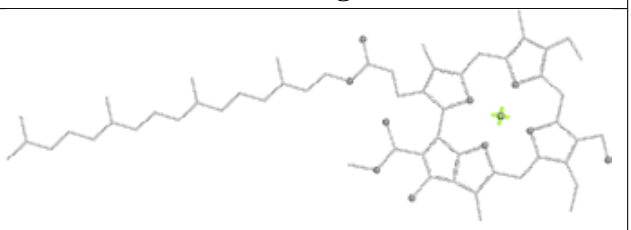


Bond angles

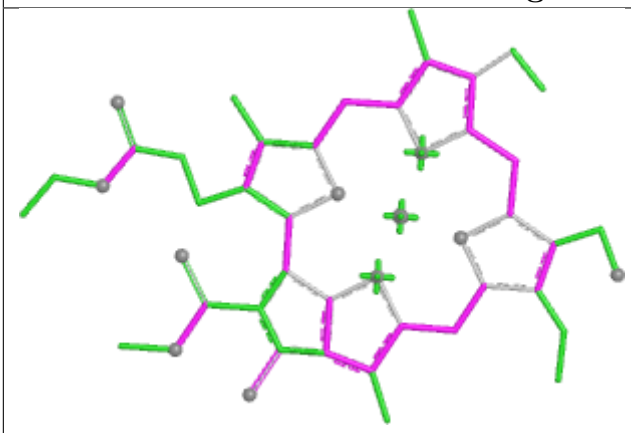


Torsions



Rings

Ligand CHL n 314



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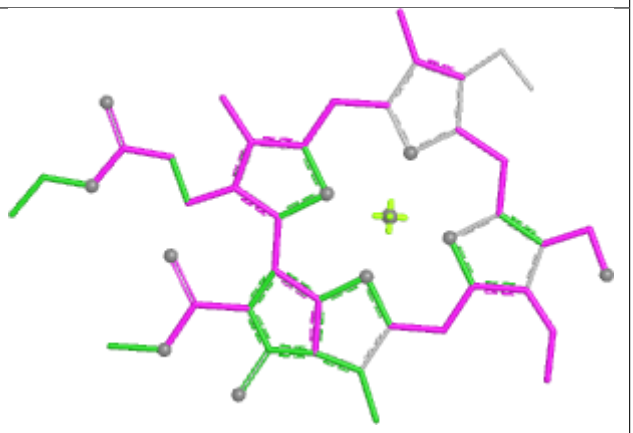
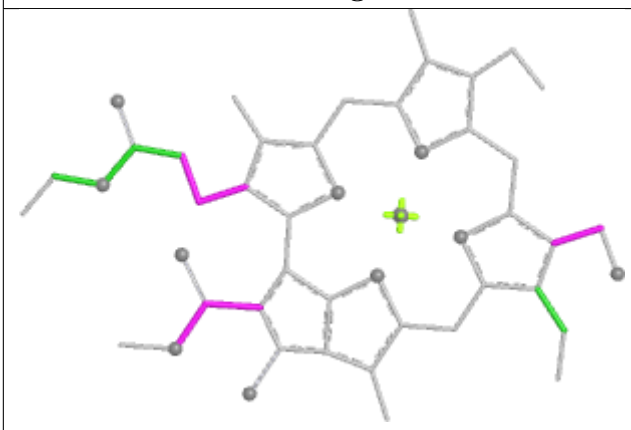


Bond angles



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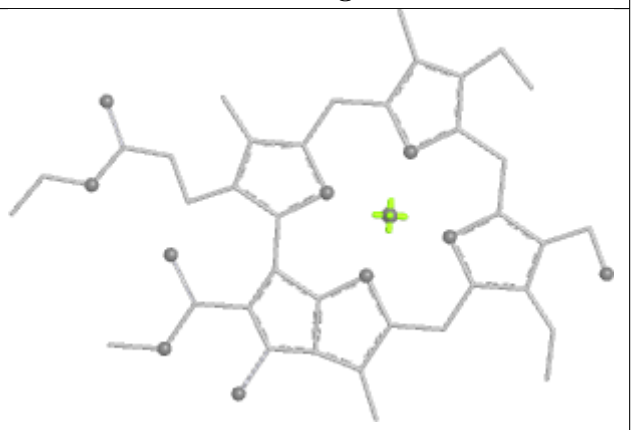
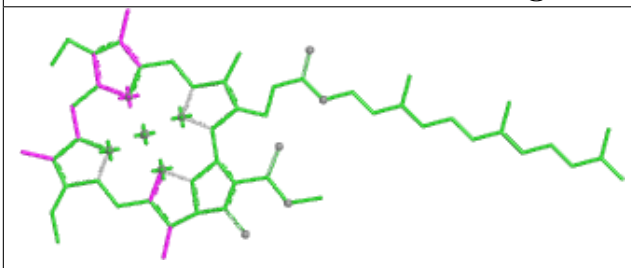


Rings

Ligand CLA q 305



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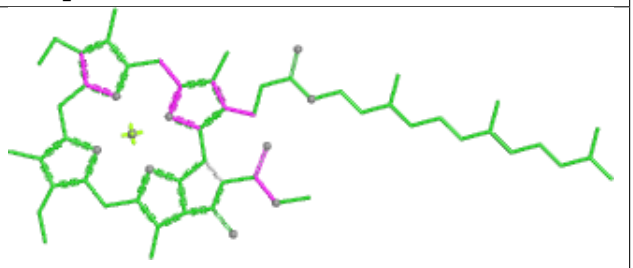

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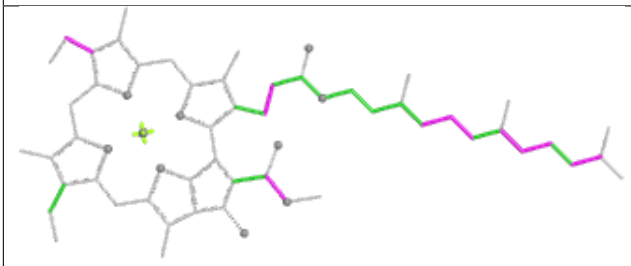

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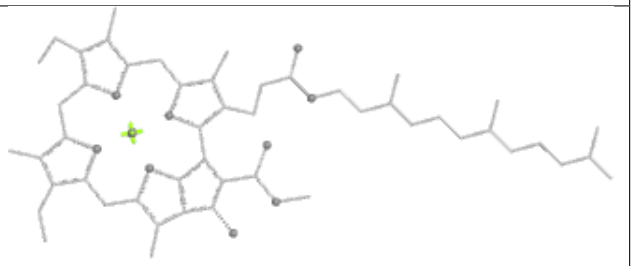
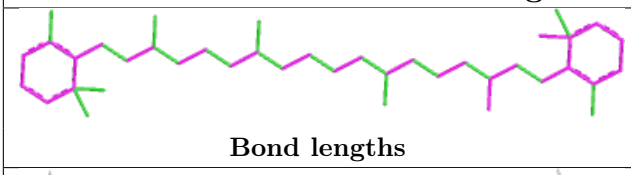


Rings

Ligand BCR d 403



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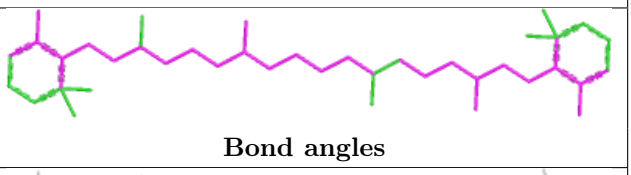
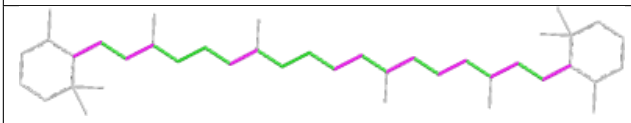


Bond angles



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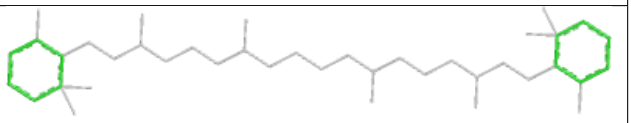
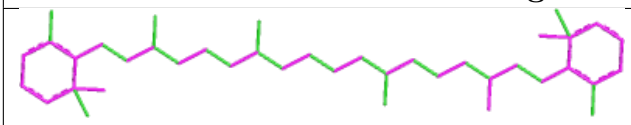


Rings

Ligand BCR c 516



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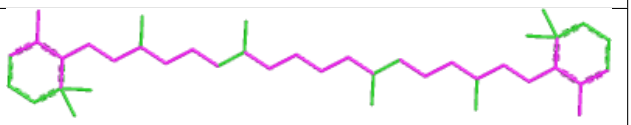
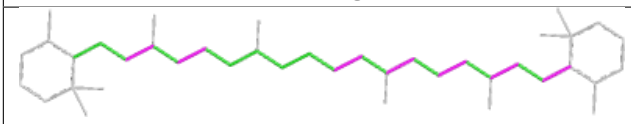


Bond angles



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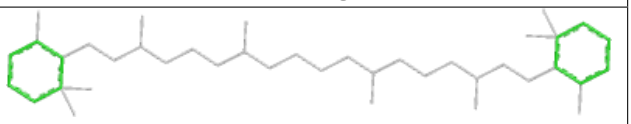
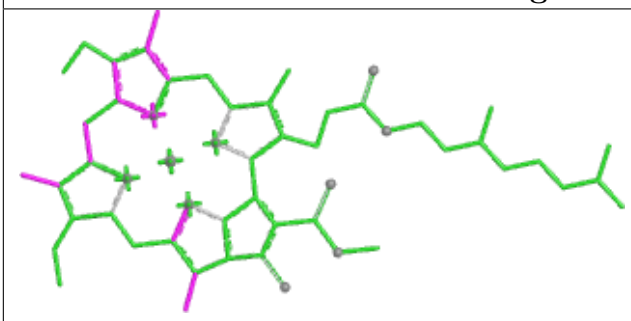


Rings

Ligand CLA s 305



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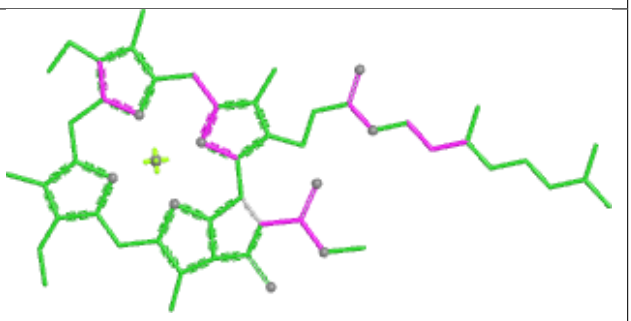
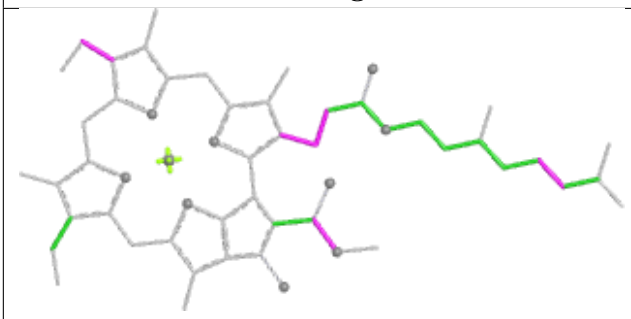
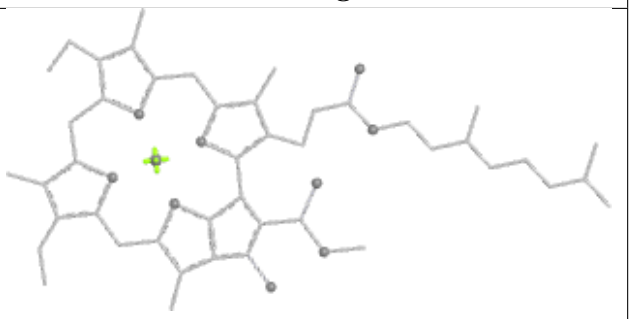


Bond angles

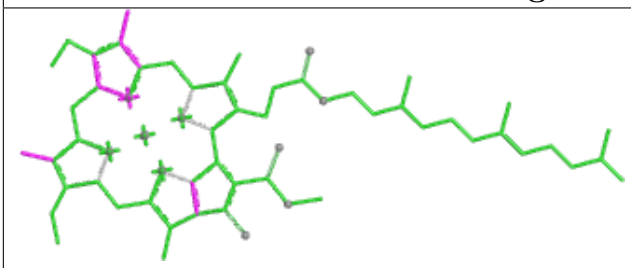


Torsions

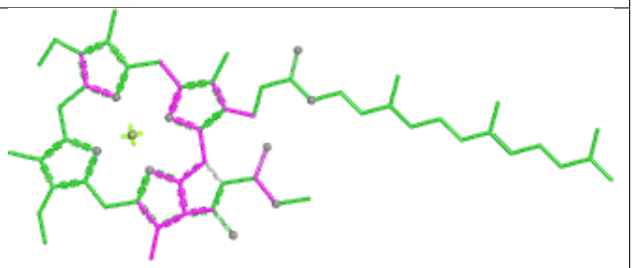


Rings

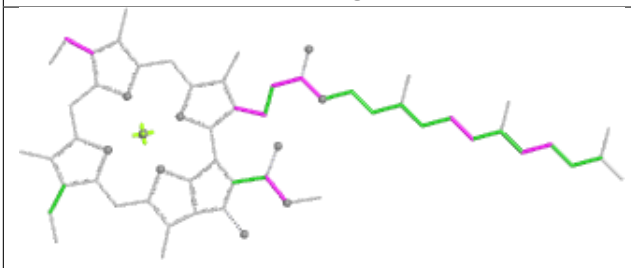
Ligand CLA 5 305



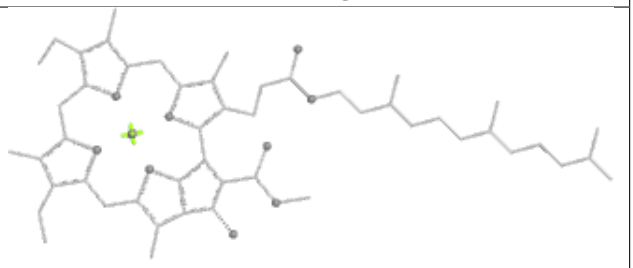
Bond lengths



Bond angles

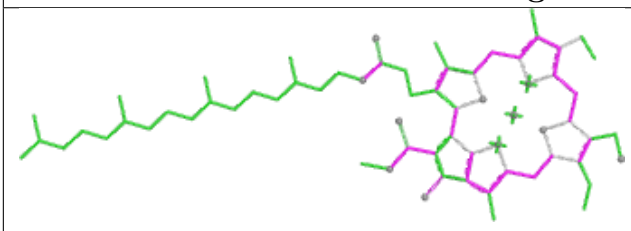


Torsions



Rings

Ligand CHL 6 315



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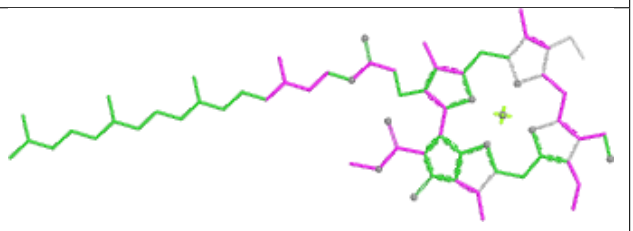

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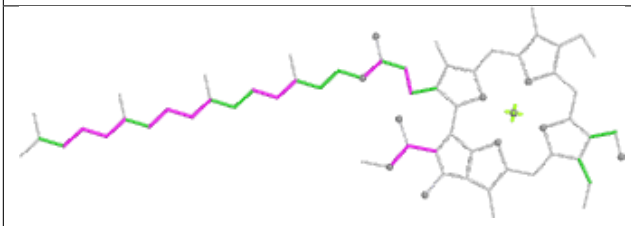
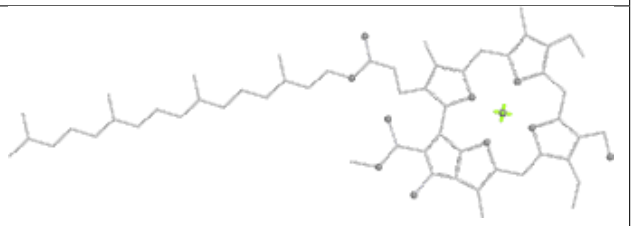
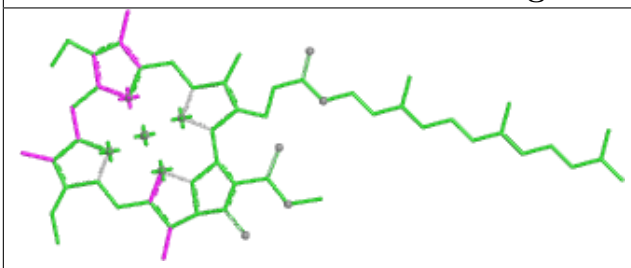


Torsions



Rings

Ligand CLA v 304



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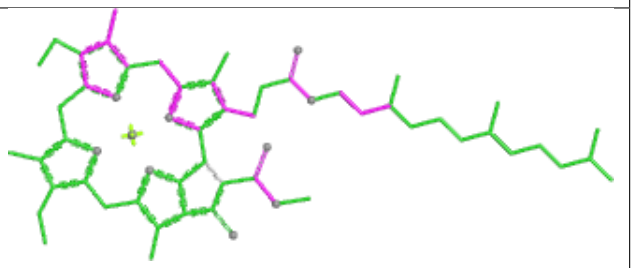

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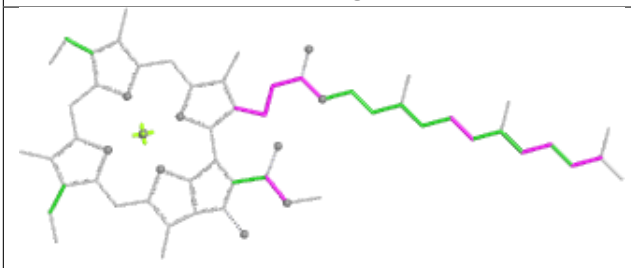

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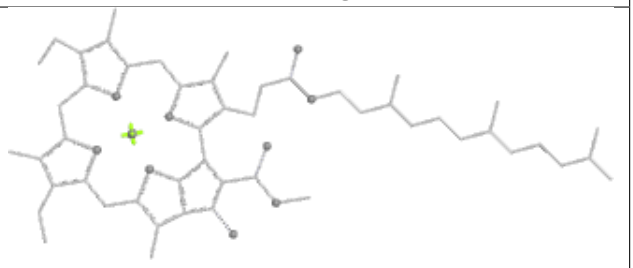
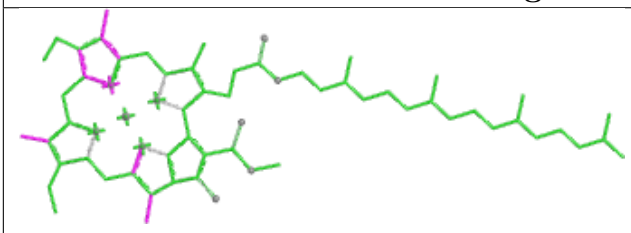
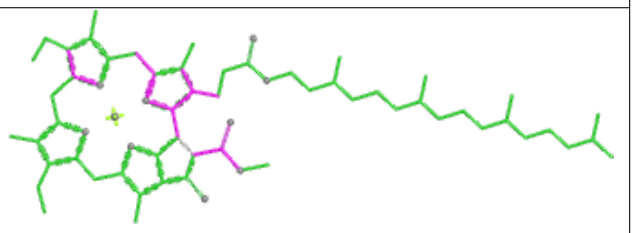


Rings

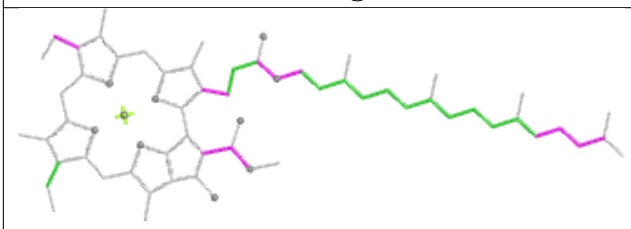
Ligand CLA B 611



Bond lengths



Bond angles



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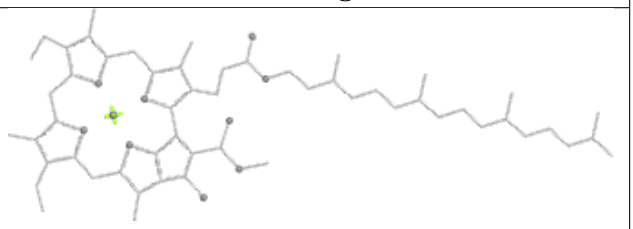
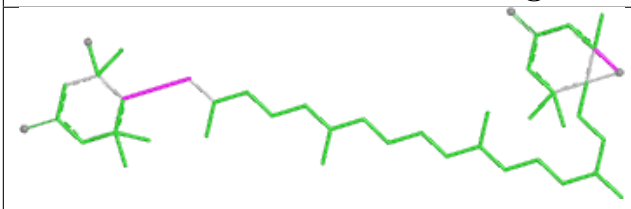


Rings

Ligand NEX n 319



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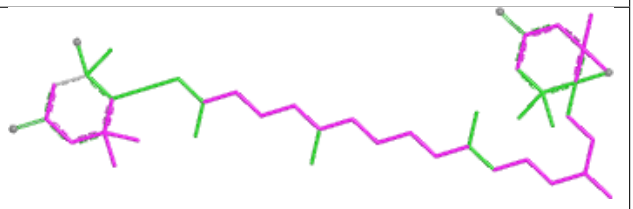
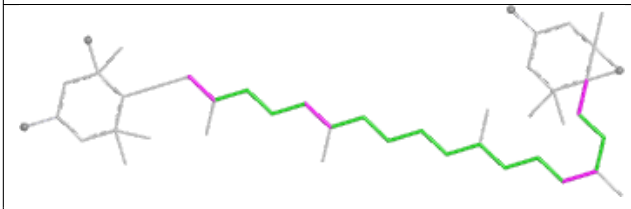


Bond angles



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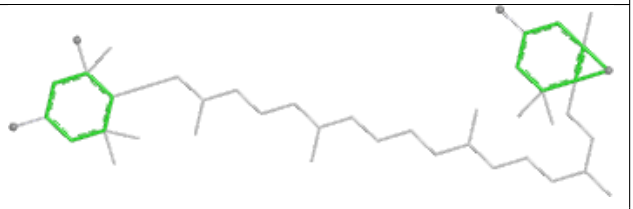
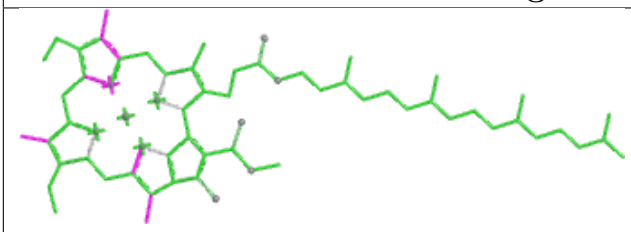
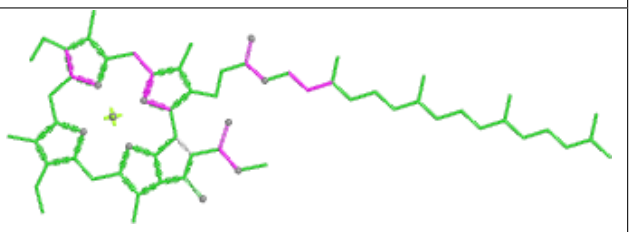
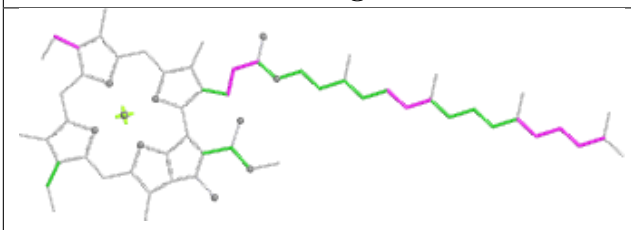
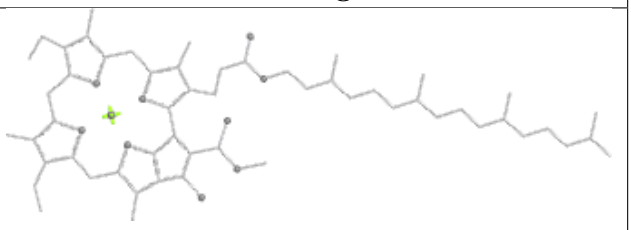
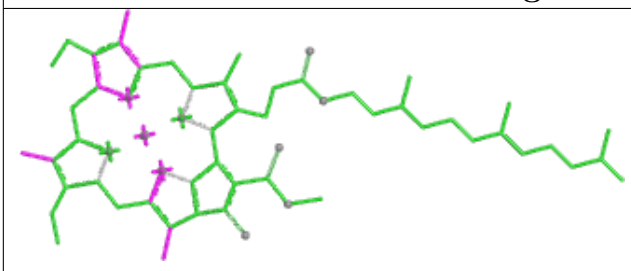
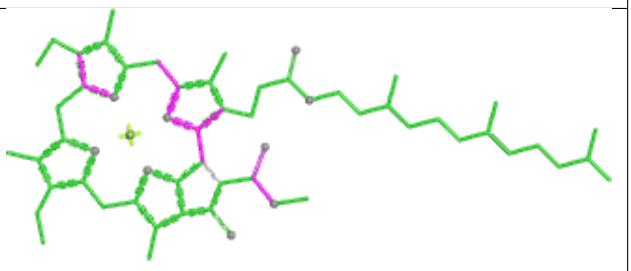
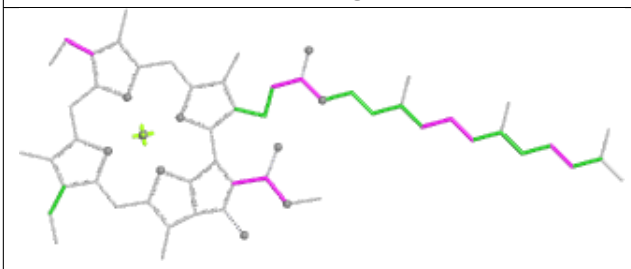
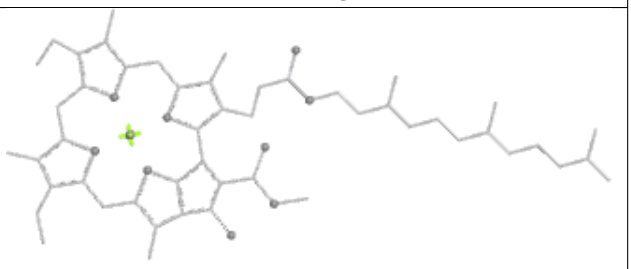
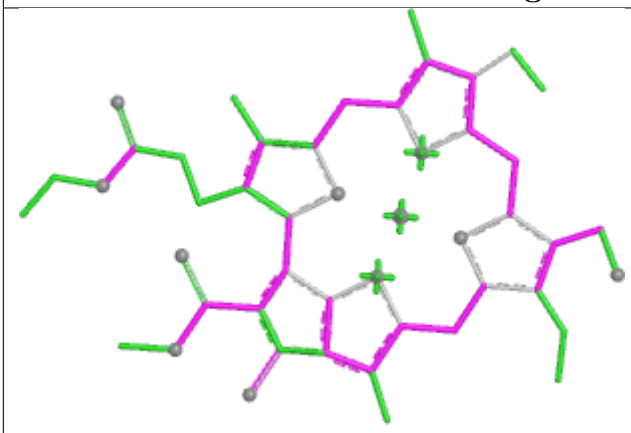


Rings

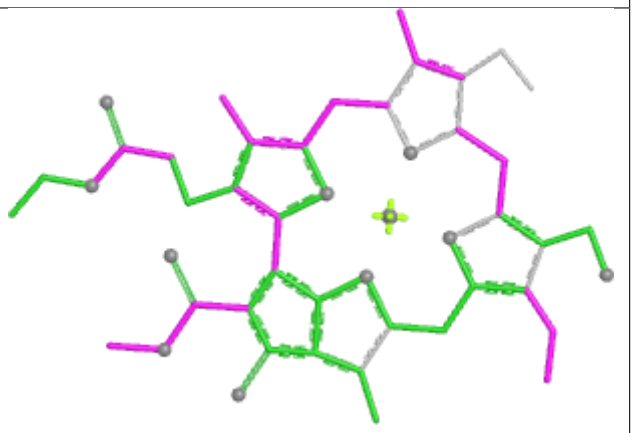
Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

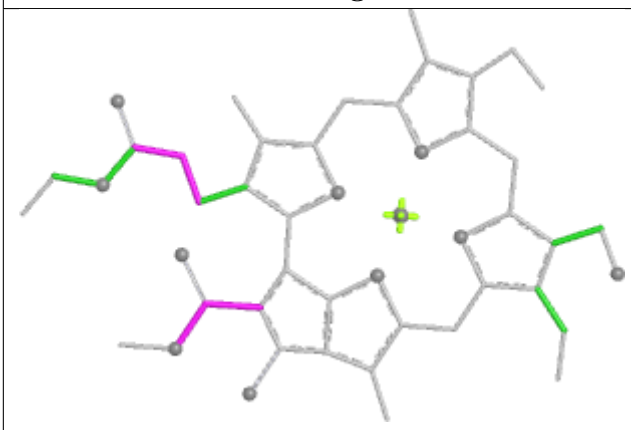
Ligand CHL P 315



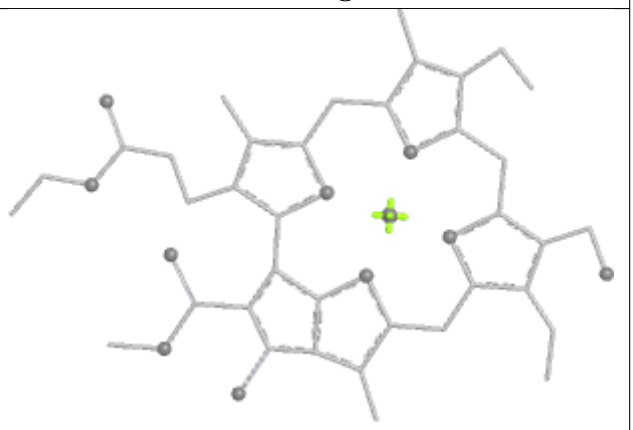
Bond lengths



Bond angles

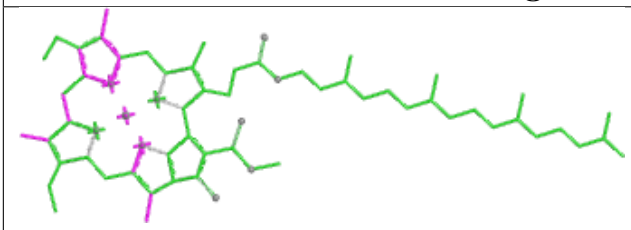


Torsions



Rings

Ligand CLA C 510



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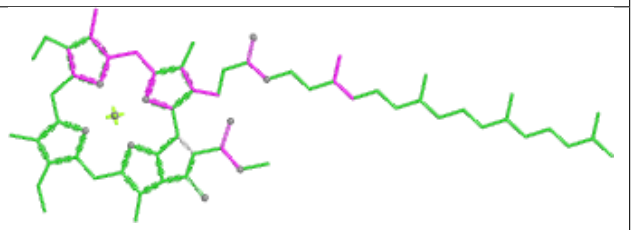
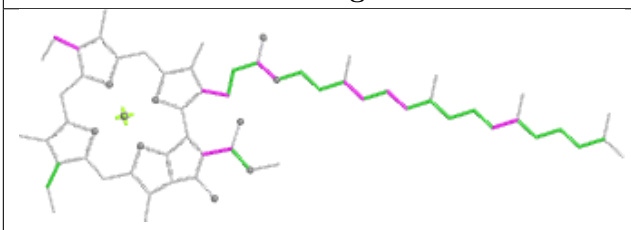
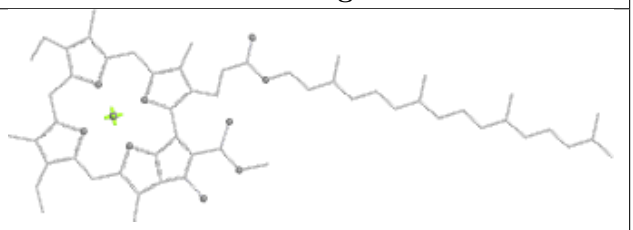


Bond angles

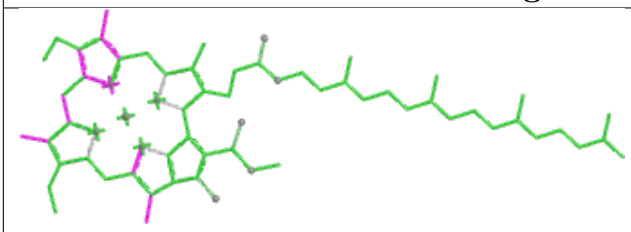


Torsions



Rings

Ligand CLA U 301



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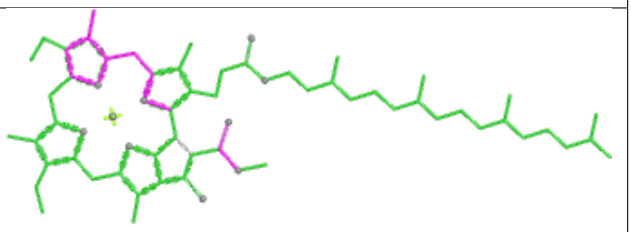

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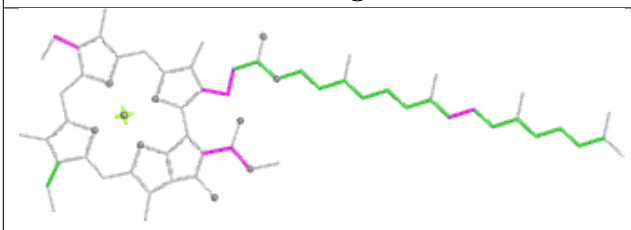

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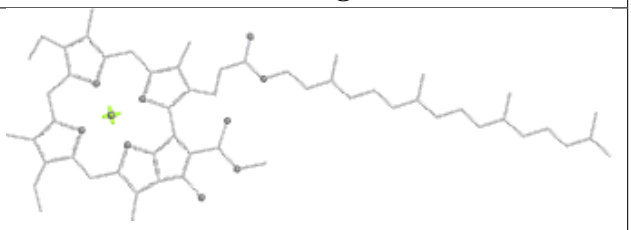
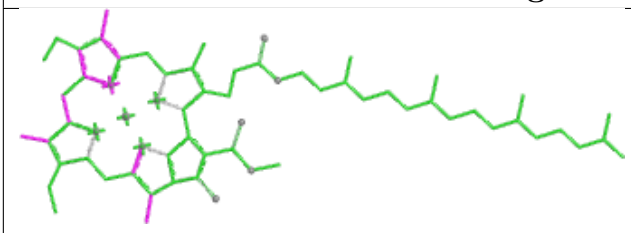


Rings

Ligand CLA p 305



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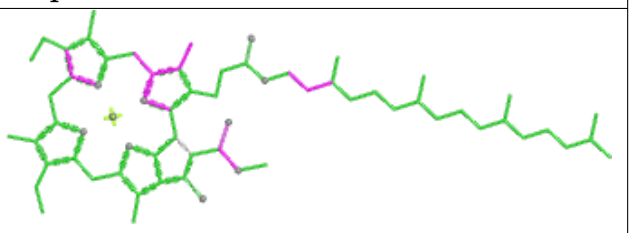
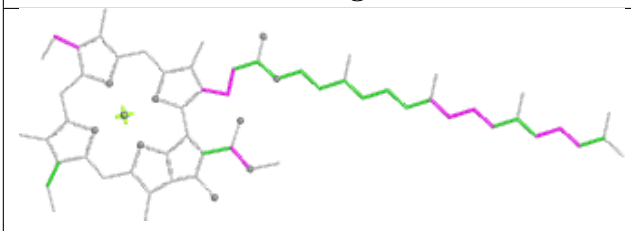


Bond angles



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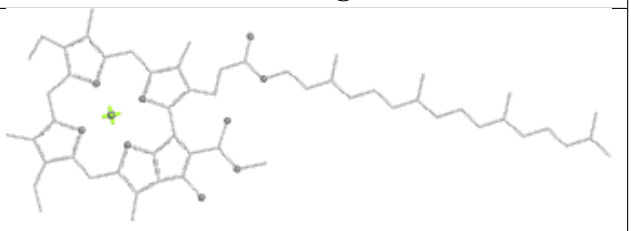
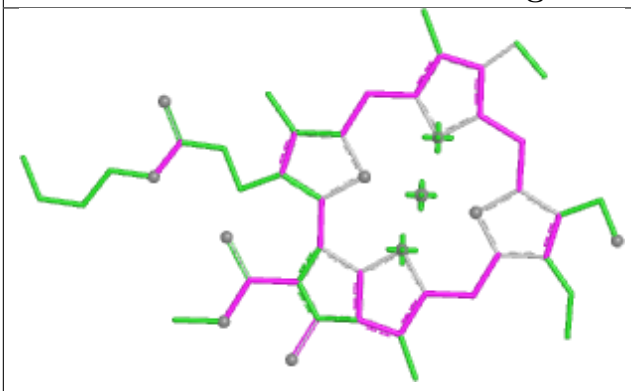


Rings

Ligand CHL u 315



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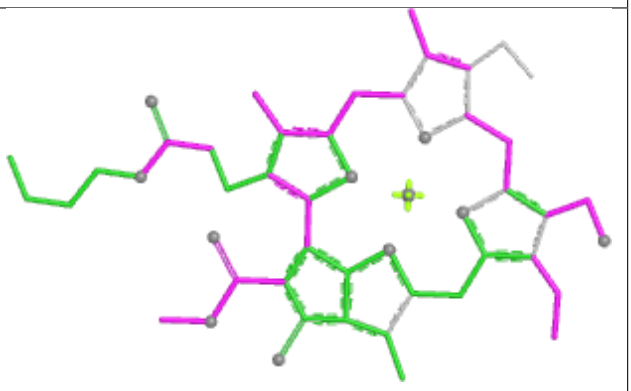
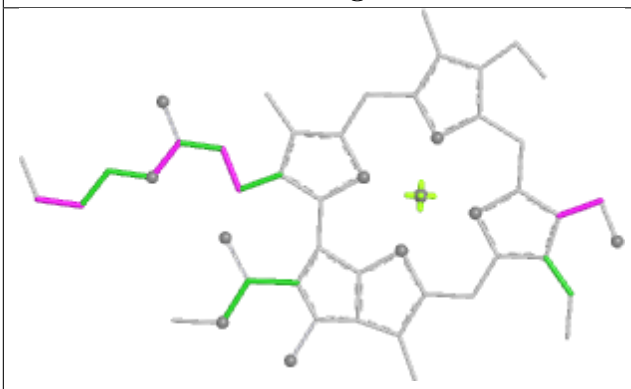
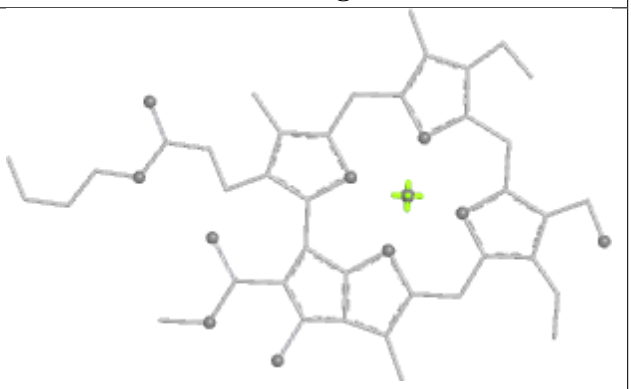


Bond angles

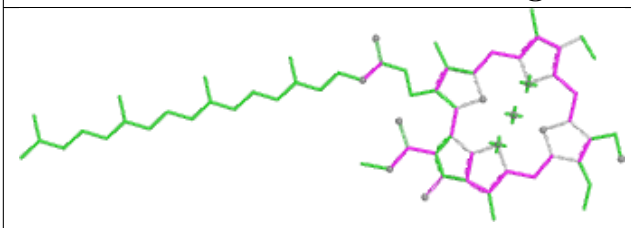


Torsions



Rings

Ligand CHL u 316



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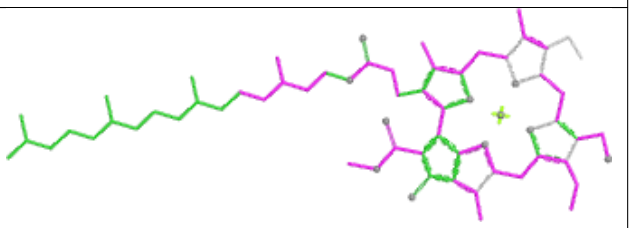
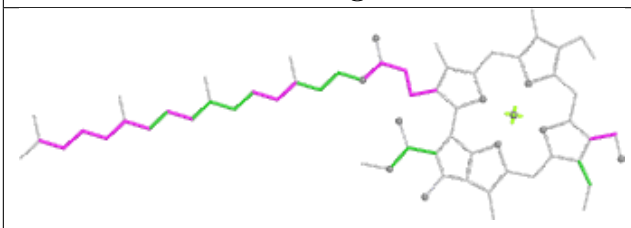
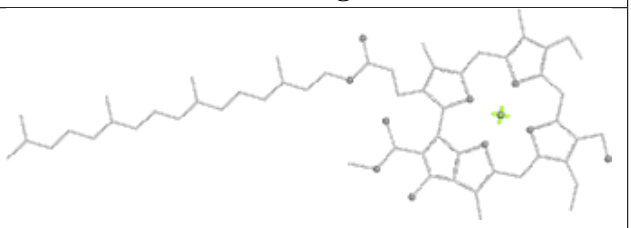


Bond angles

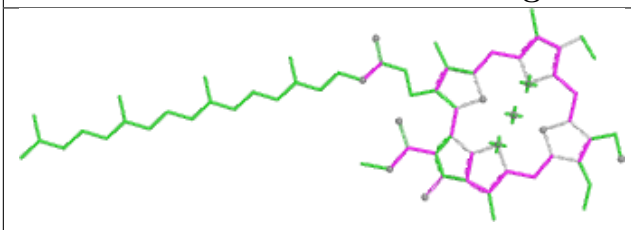


Torsions



Rings

Ligand CHL U 313



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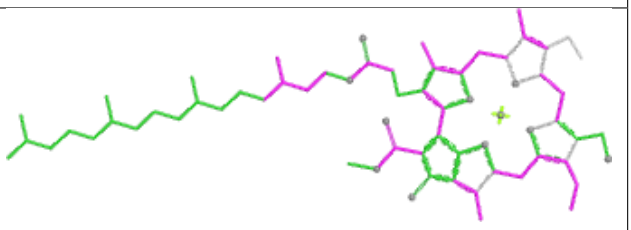
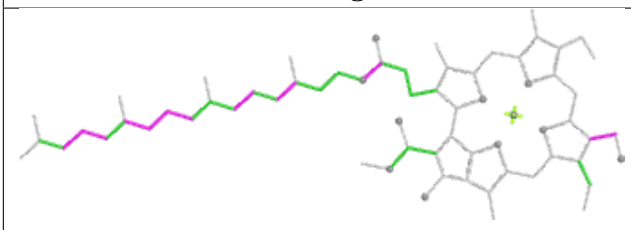
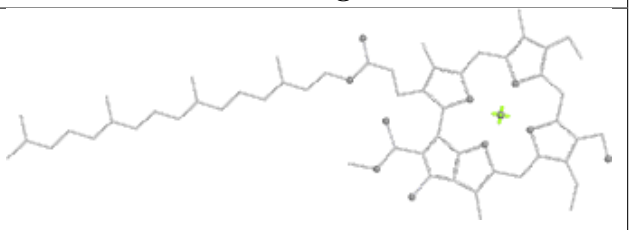


Bond angles

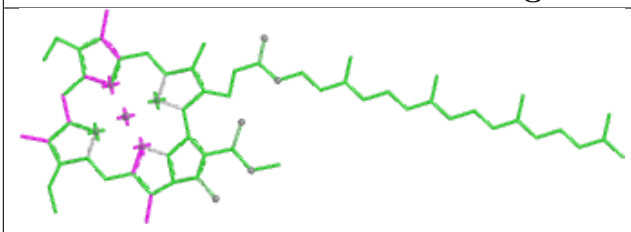


Torsions

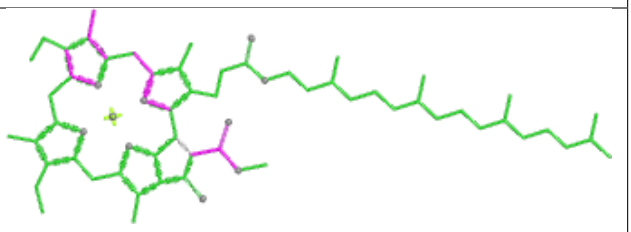


Rings

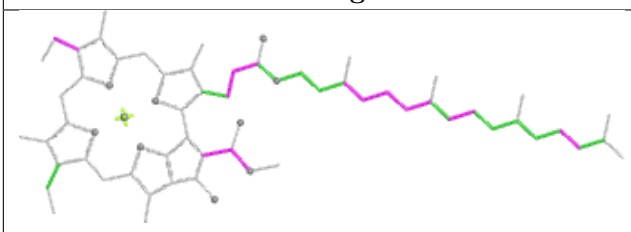
Ligand CLA B 615



Bond lengths



Bond angles



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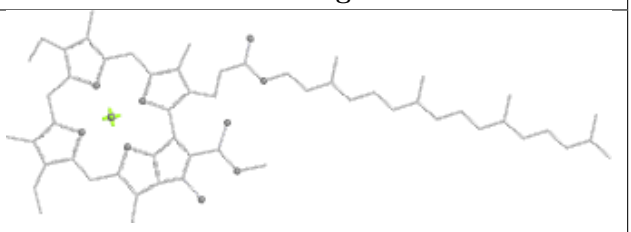
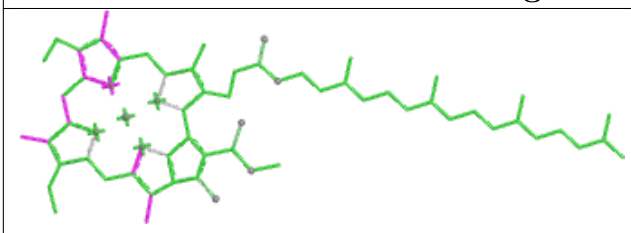


Rings

Ligand CLA V 302



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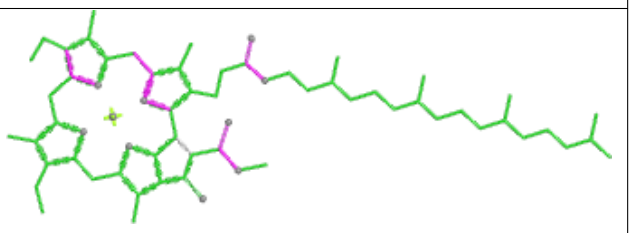
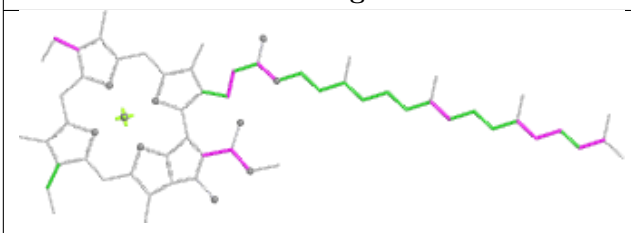


Bond angles



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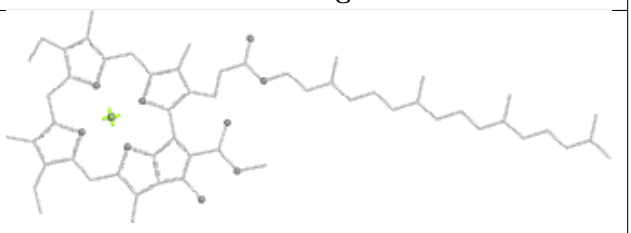
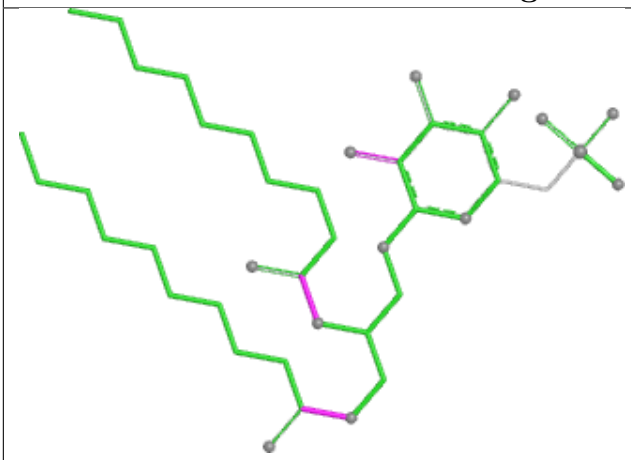


Rings

Ligand SQD M 101



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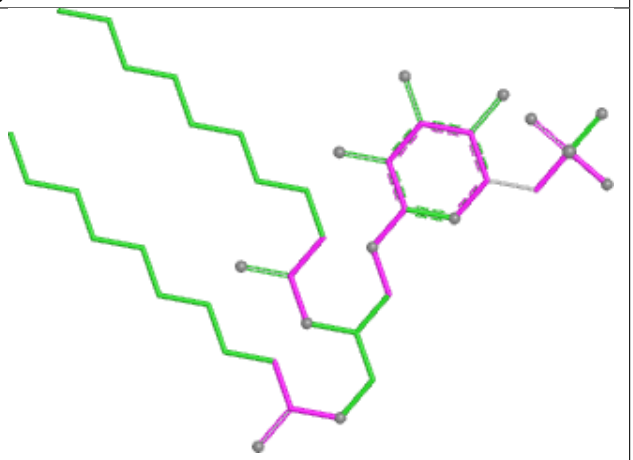

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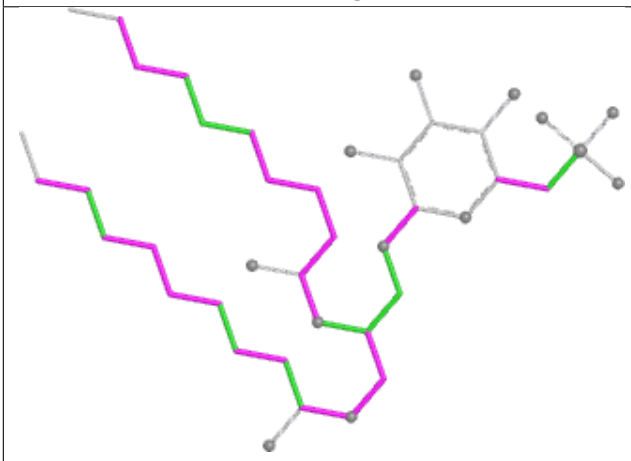

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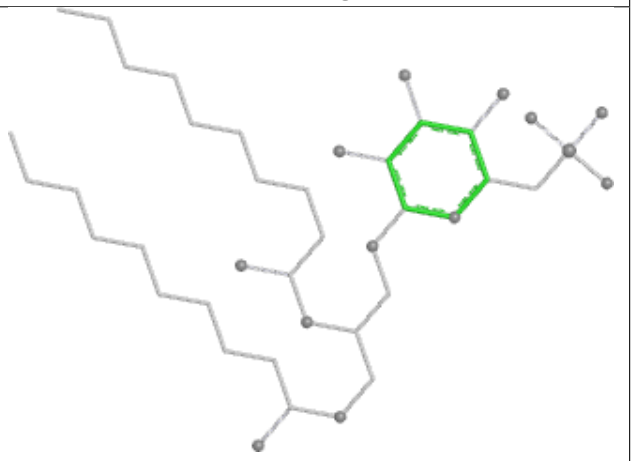
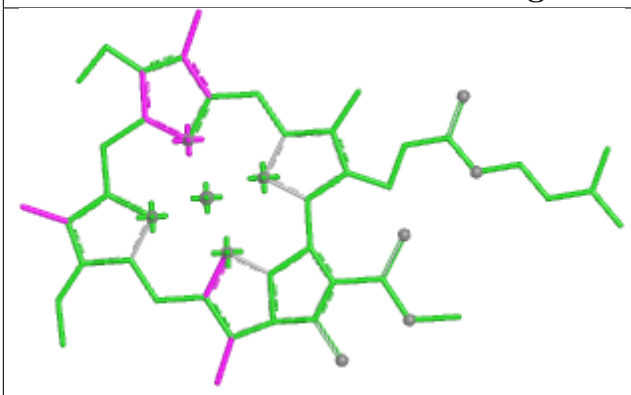


Rings

Ligand CLA S 303



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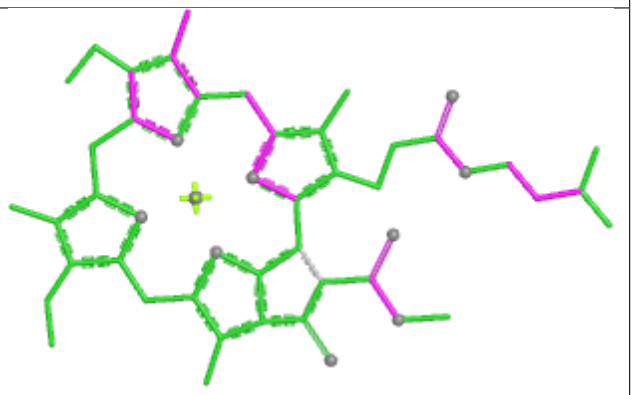
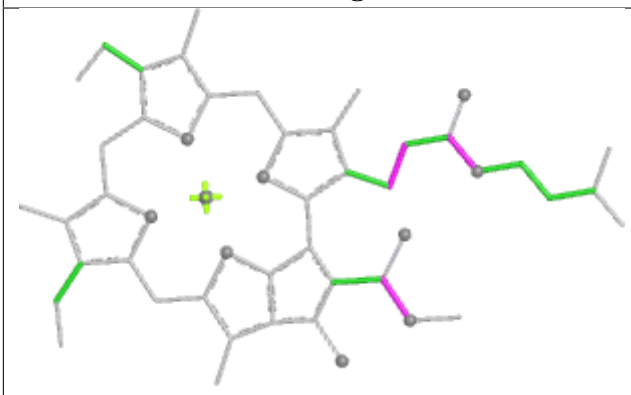


Bond angles



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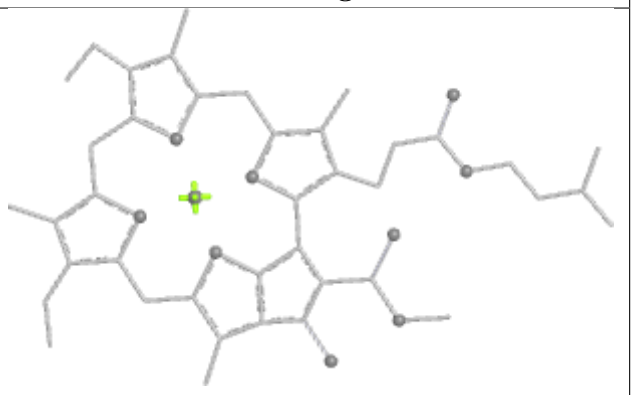
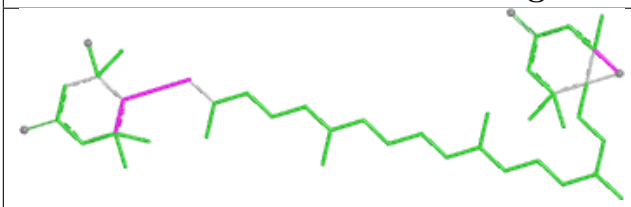
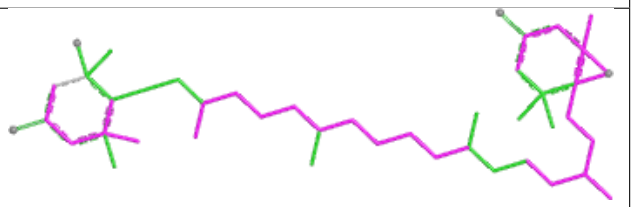


Rings

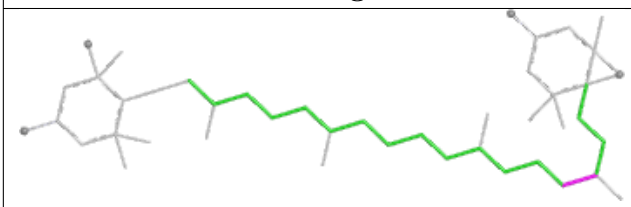
Ligand NEX r 617



Bond lengths



Bond angles



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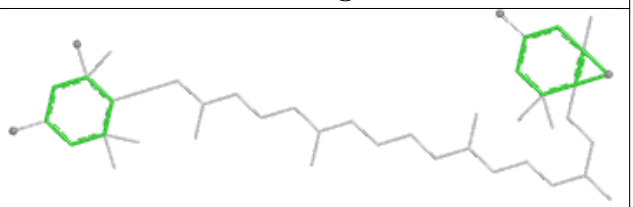
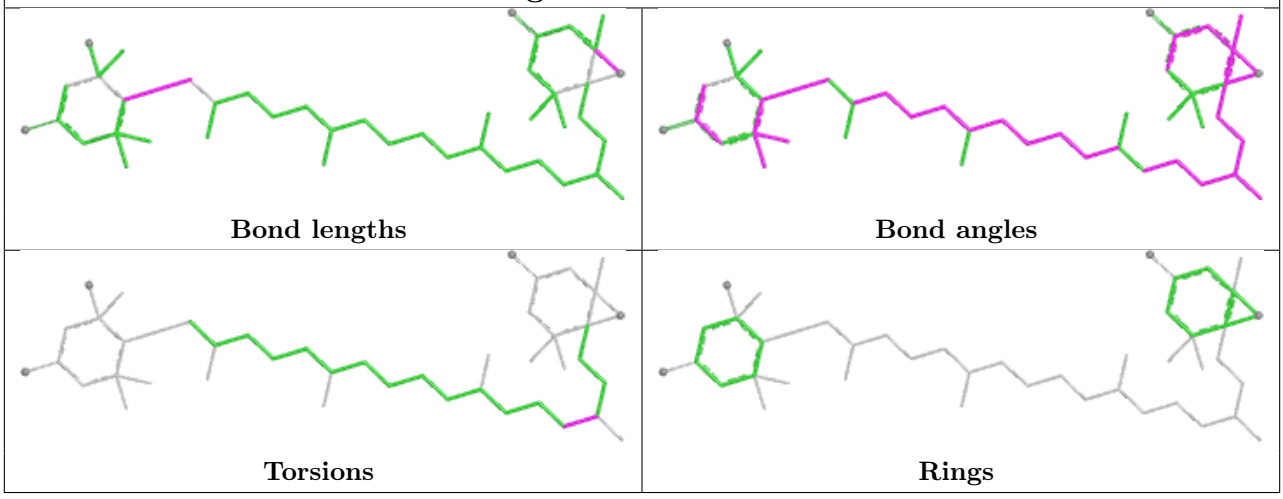
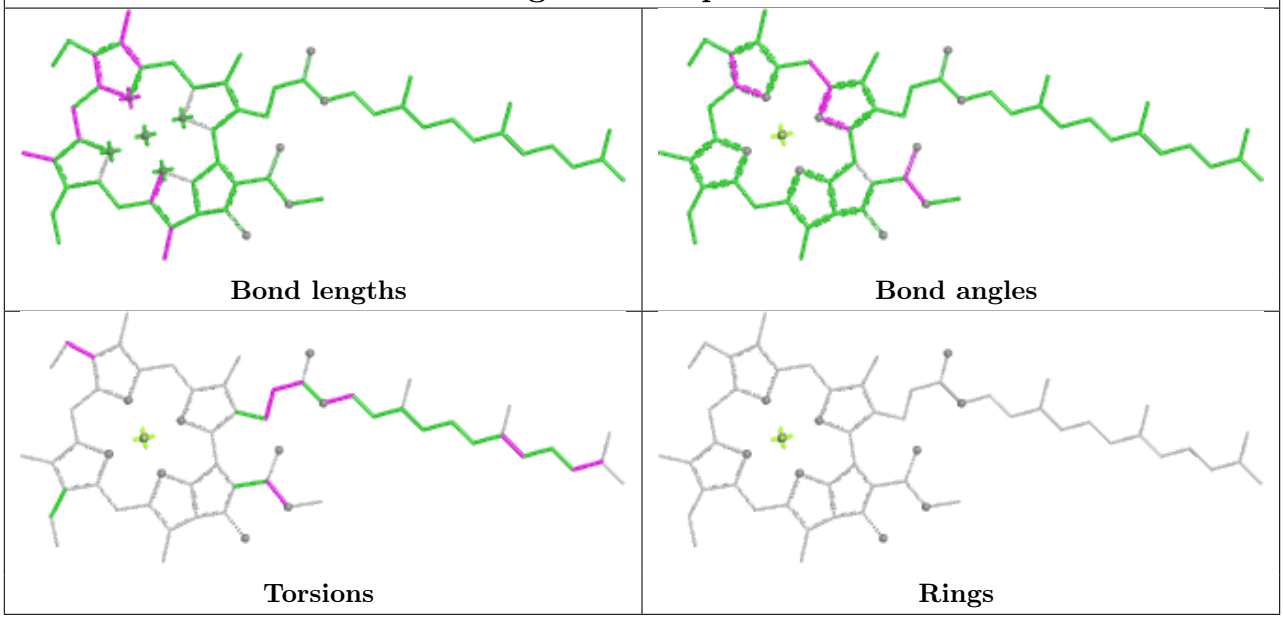


Rings

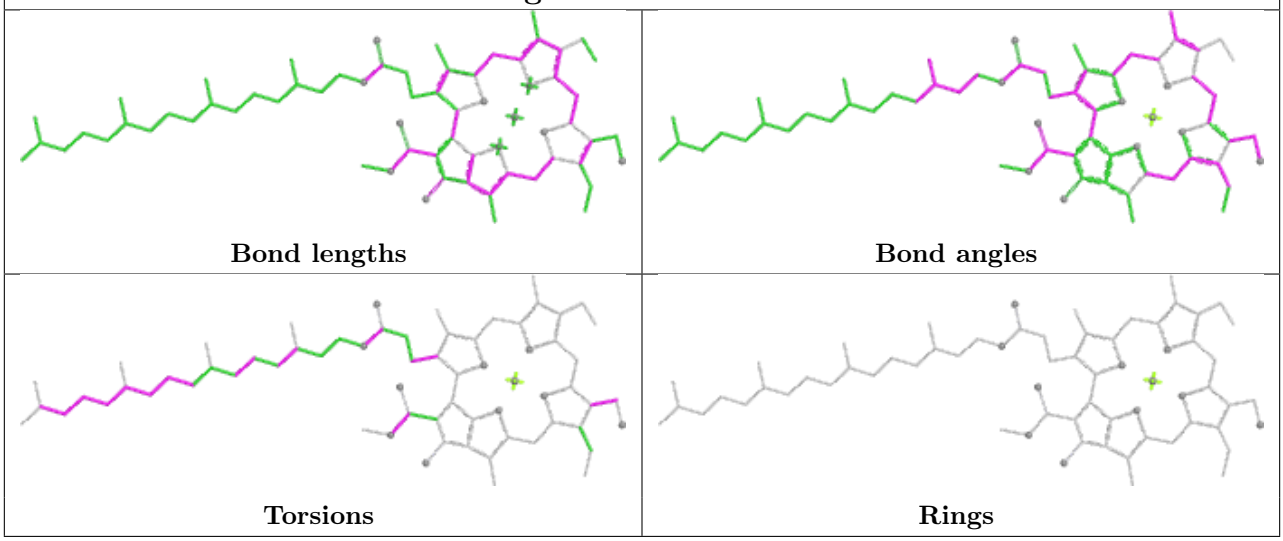
Ligand NEX u 320



Ligand CLA p 308



Ligand CHL R 315



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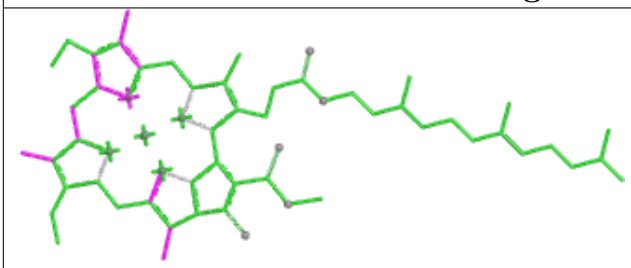
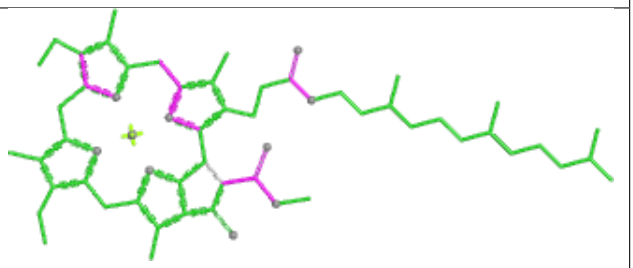
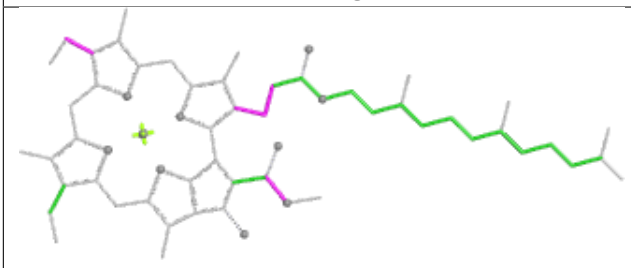


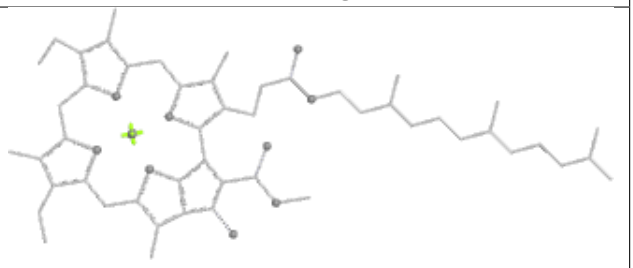
Bond lengths



Bond angles

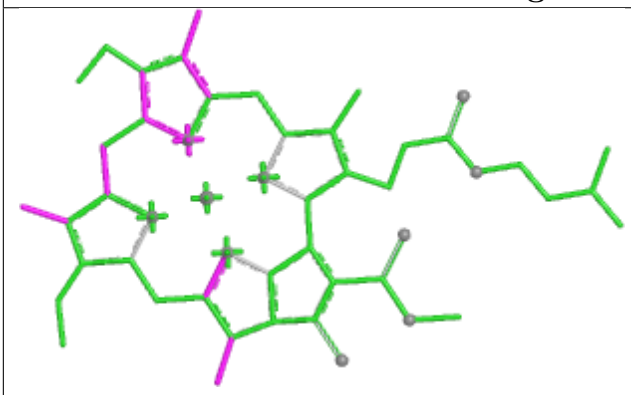


Torsions



Rings

Ligand CLA n 303



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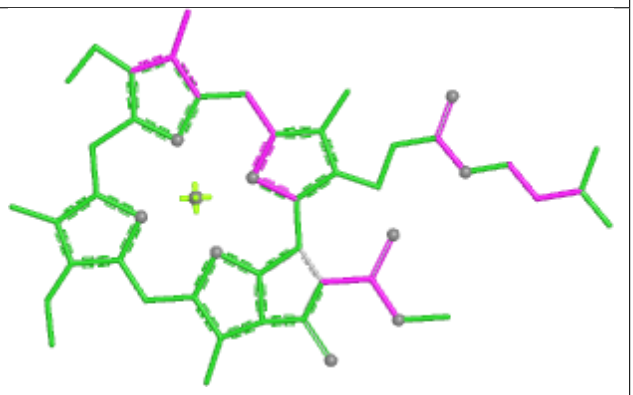

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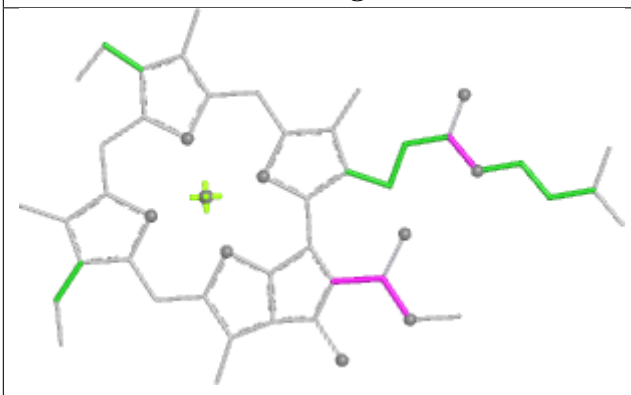

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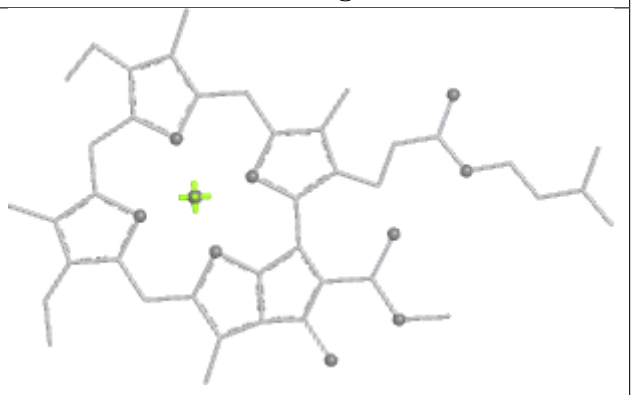
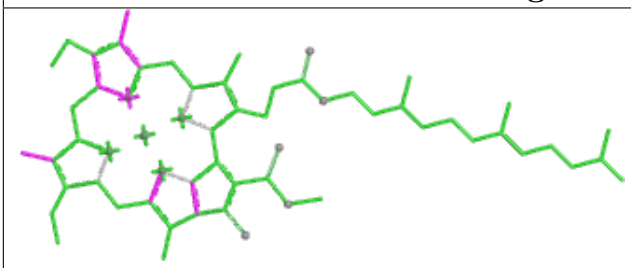
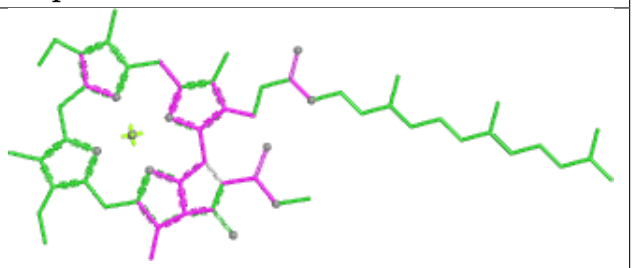


Rings

Ligand CLA p 306	
	
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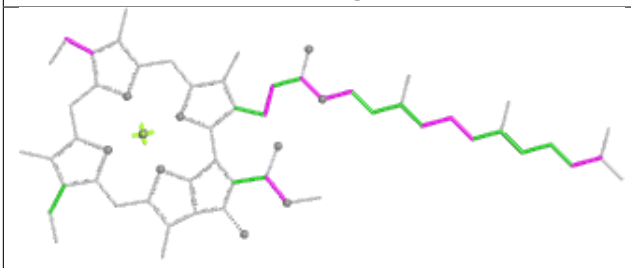
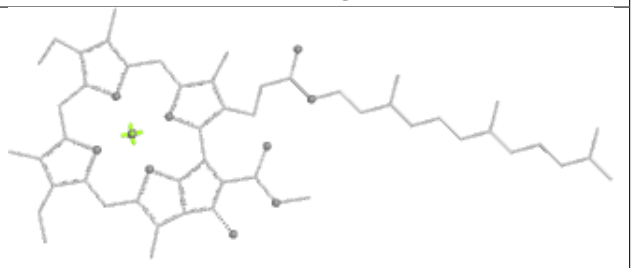
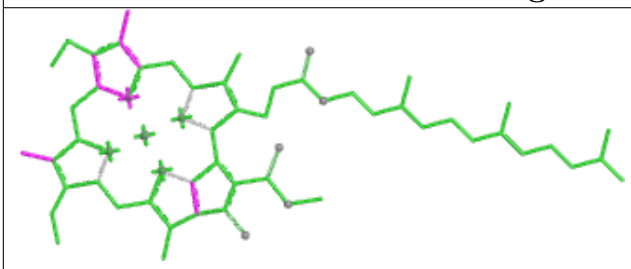
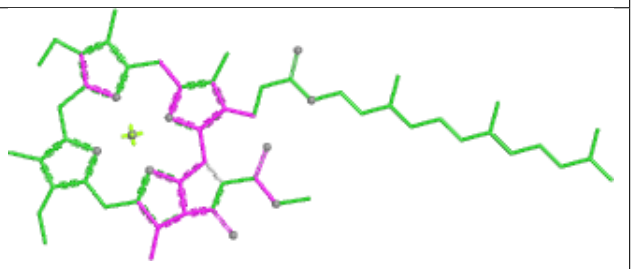
	
Torsions	**Rings**

Ligand CLA 2 305	
	
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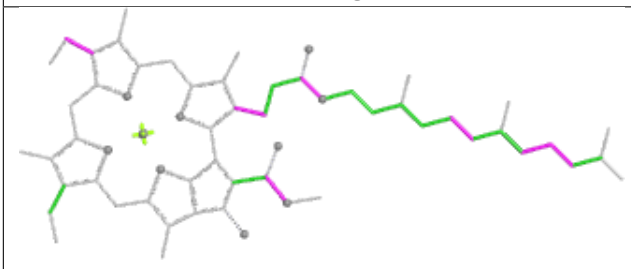
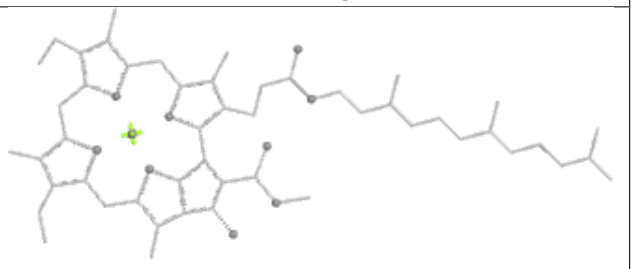
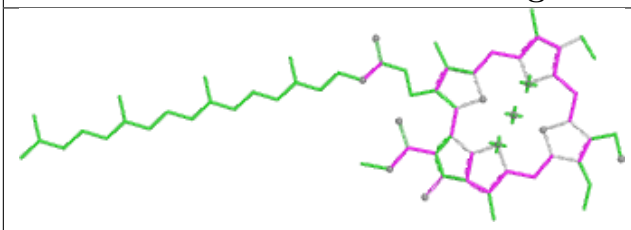
	
Torsions	**Rings**

Ligand CHL 5 318



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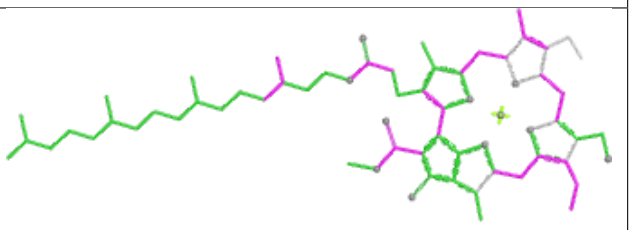
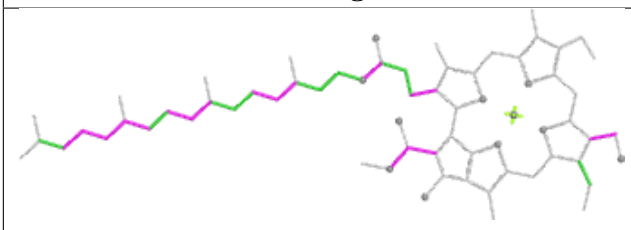
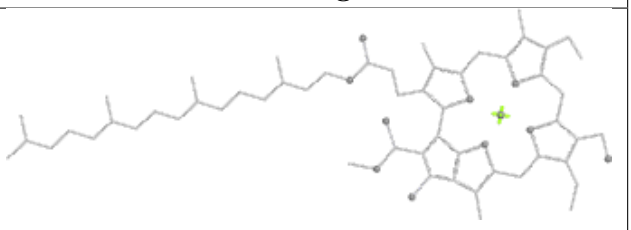


Bond angles

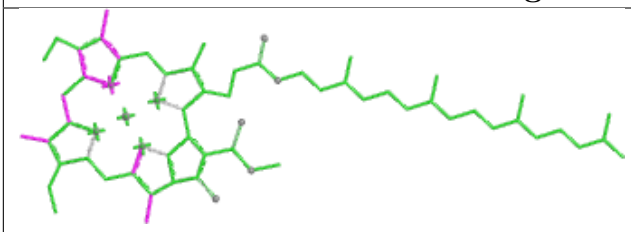


Torsions



Rings

Ligand CLA B 610



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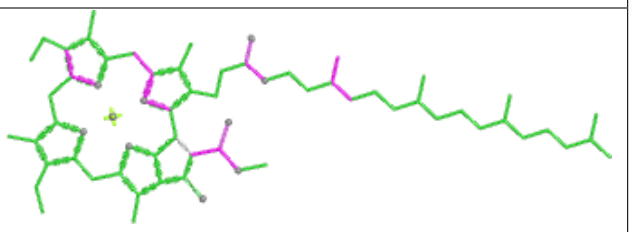
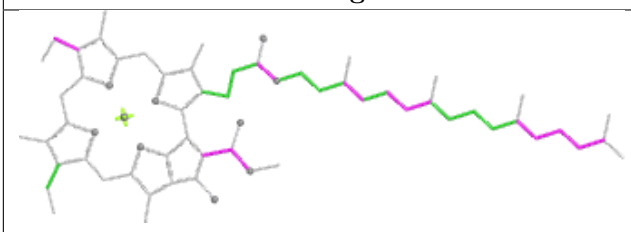


Bond angles



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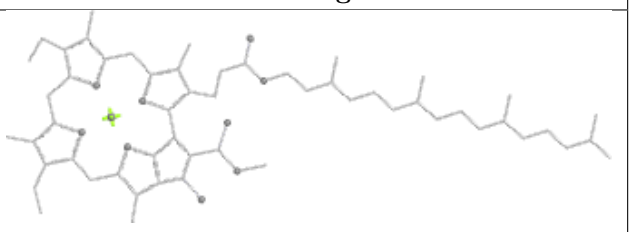
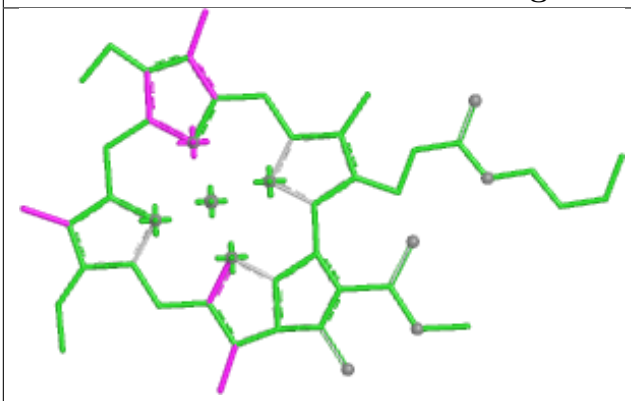


Rings

Ligand CLA s 309



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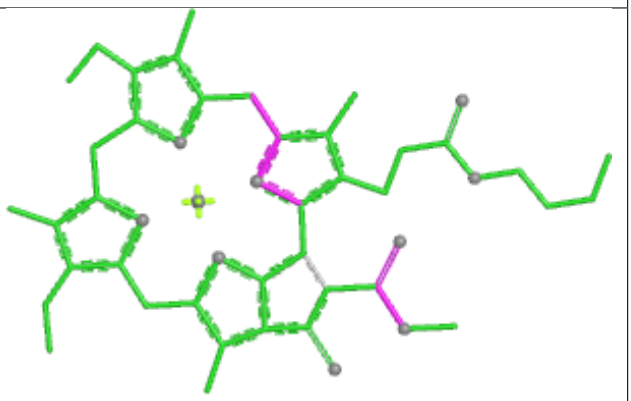
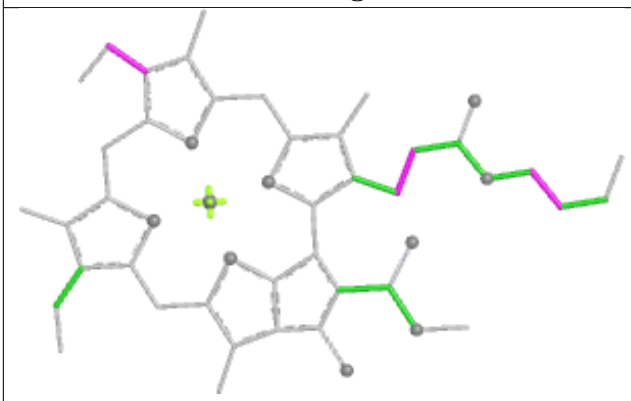
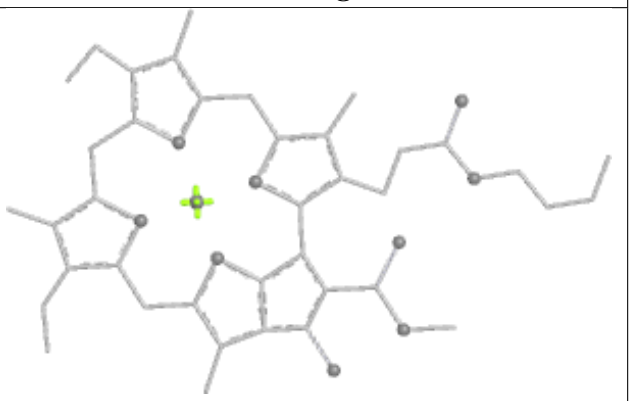


Bond angles

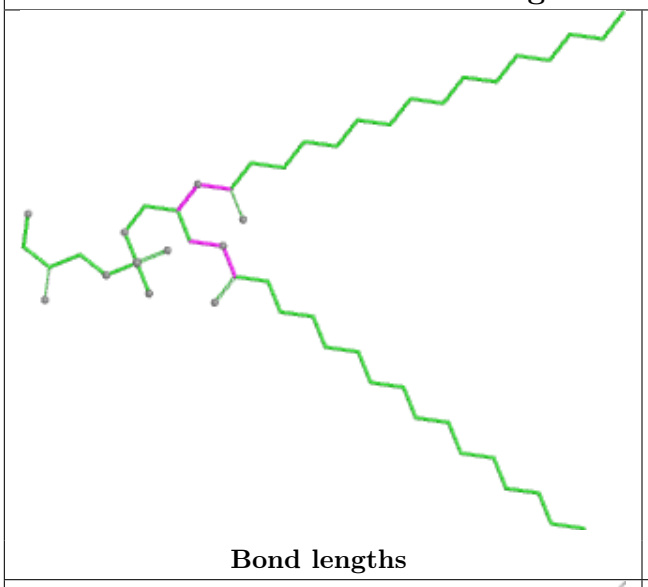


Torsions

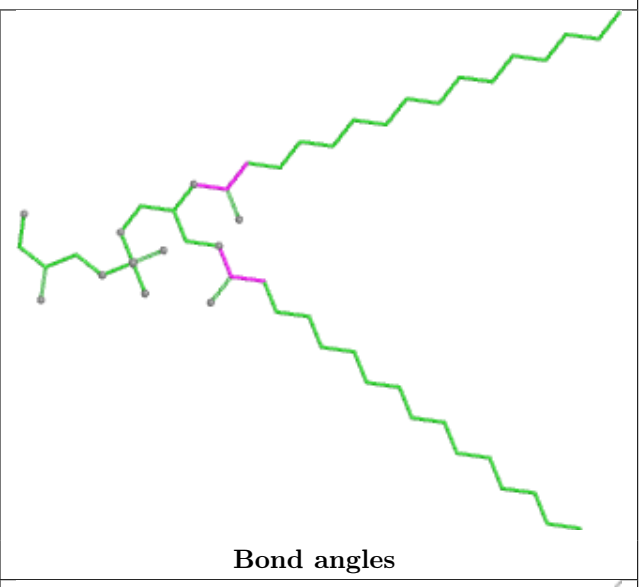


Rings

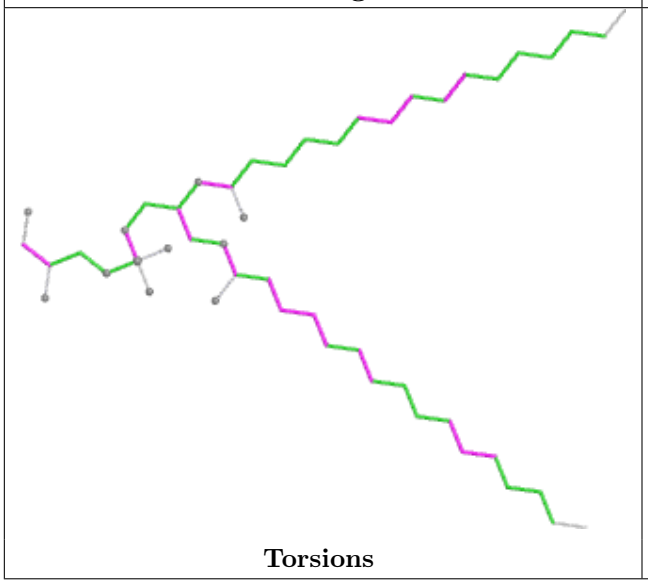
Ligand LHG 6 311



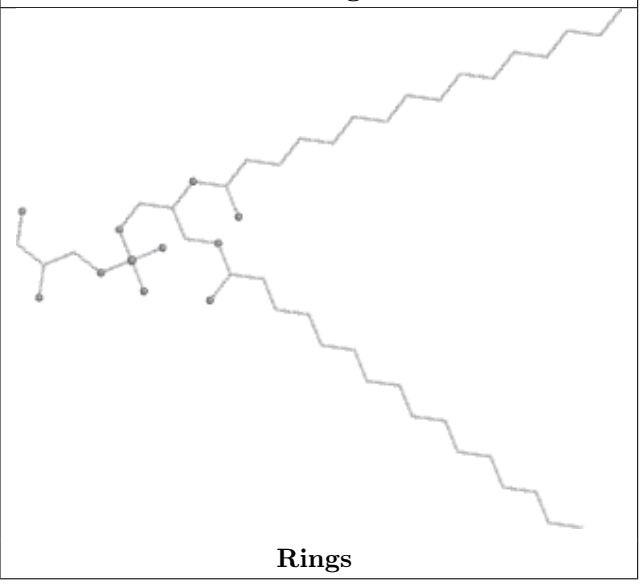
Bond lengths



Bond angles

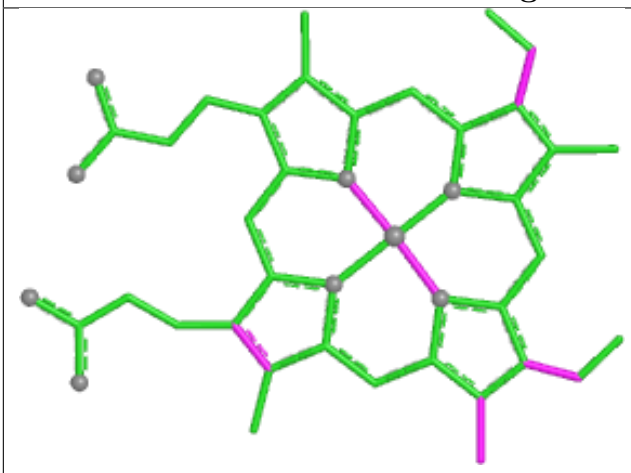


Torsions



Rings

Ligand HEM E 101



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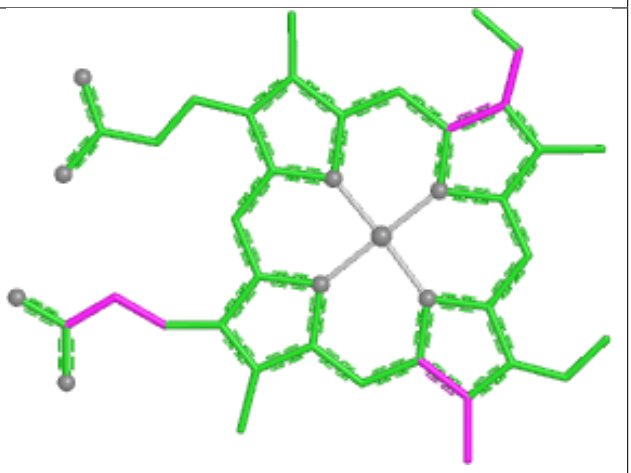

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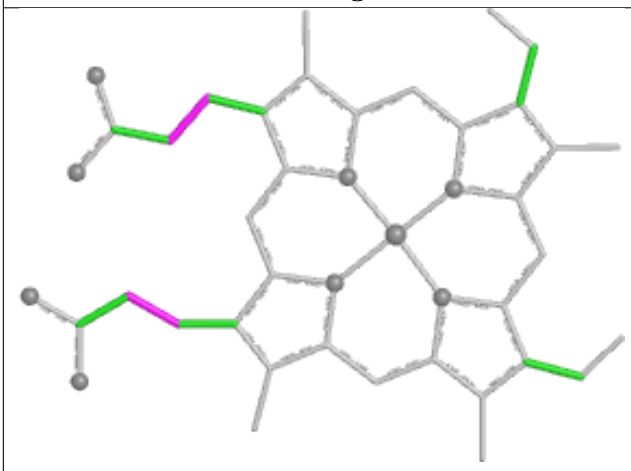
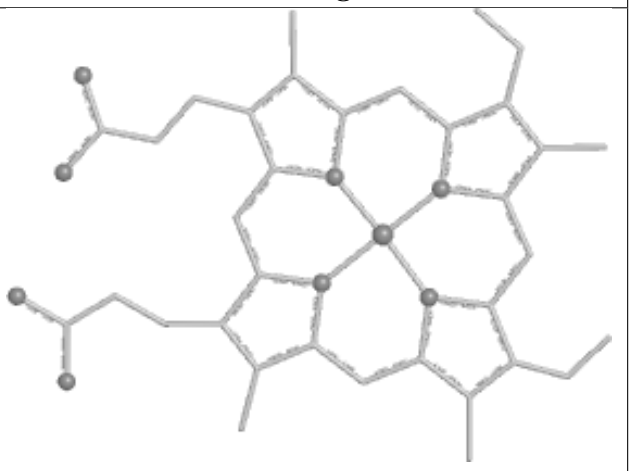
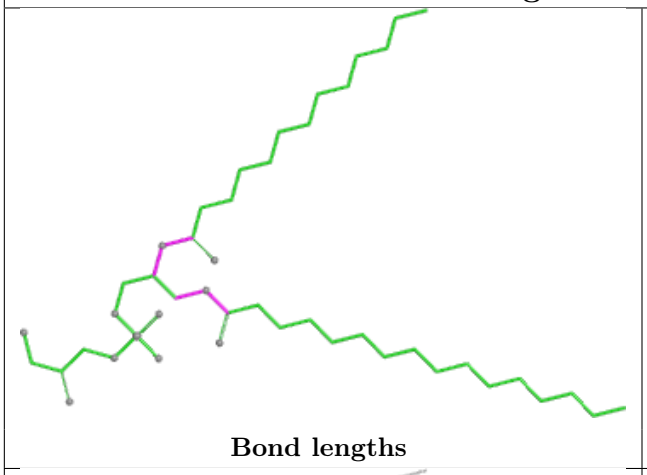


Torsions



Rings

Ligand LHG D 406



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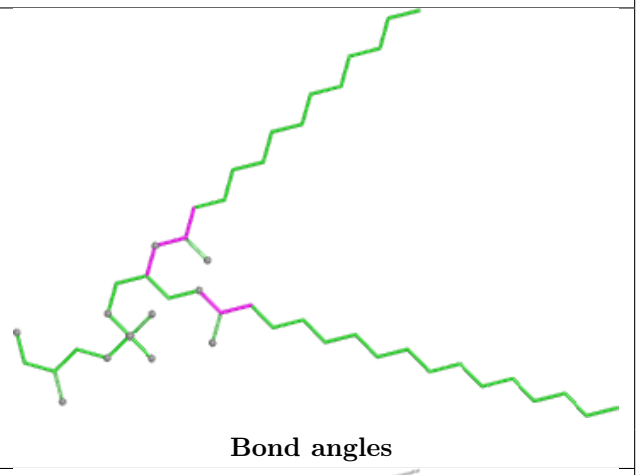

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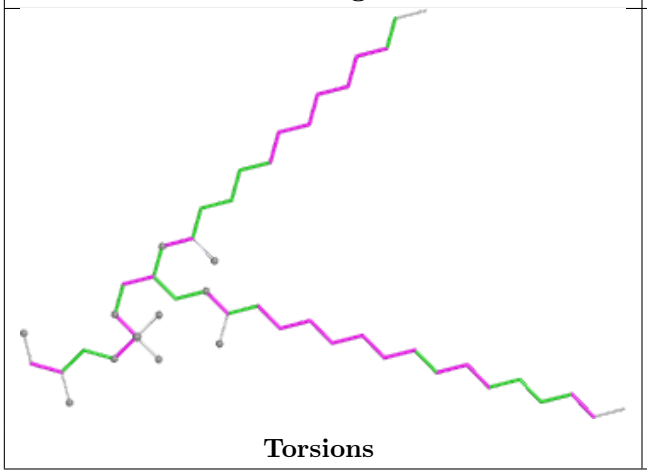

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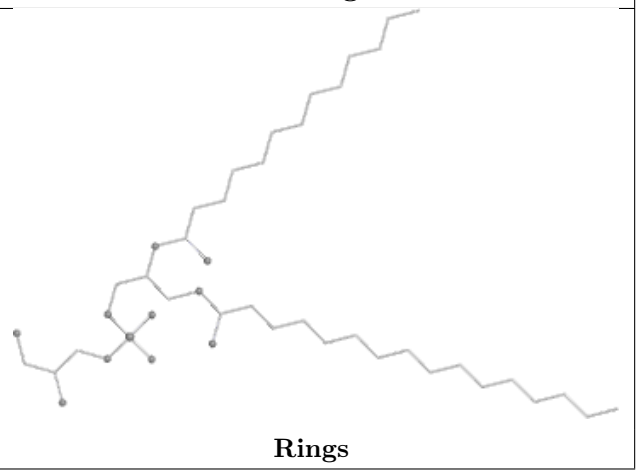
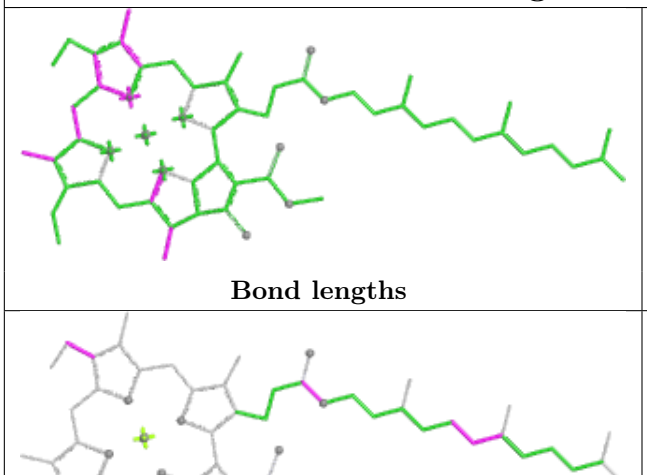


Rings

Ligand CLA v 305



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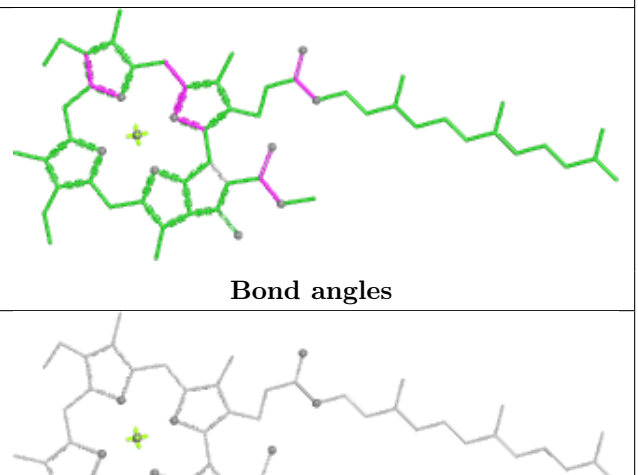

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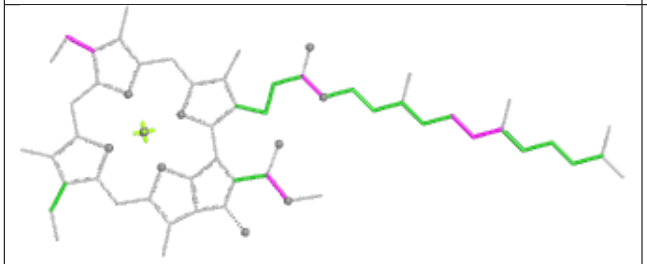

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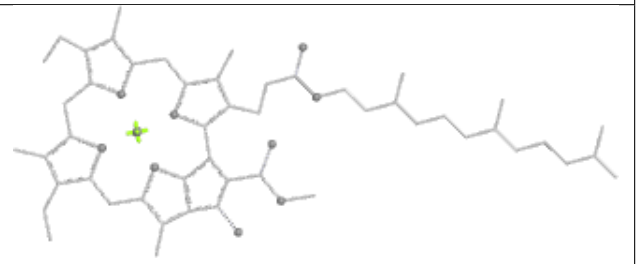
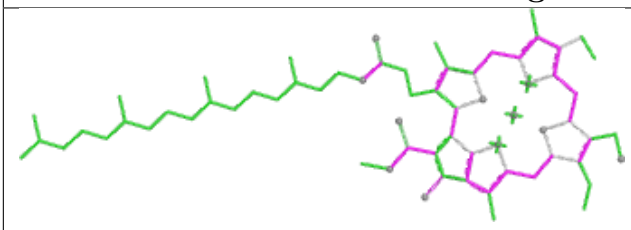


Rings

Ligand CHL 3 315



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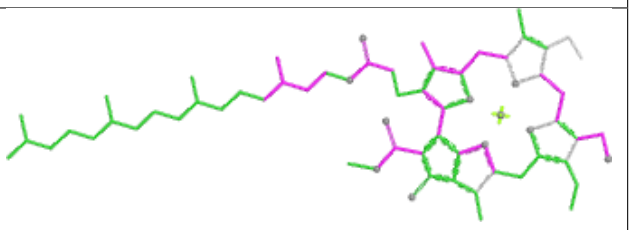

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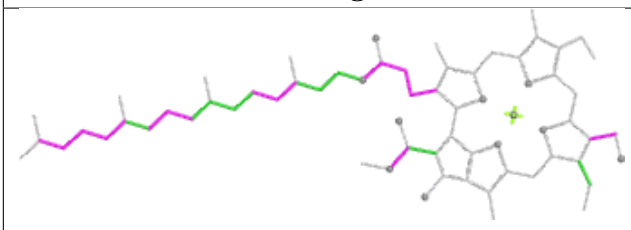

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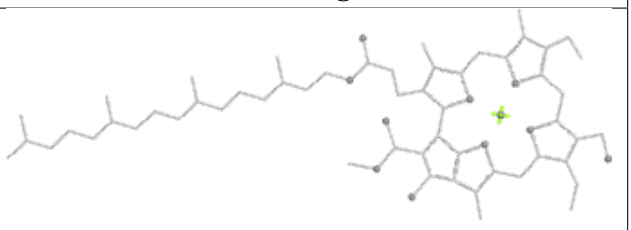
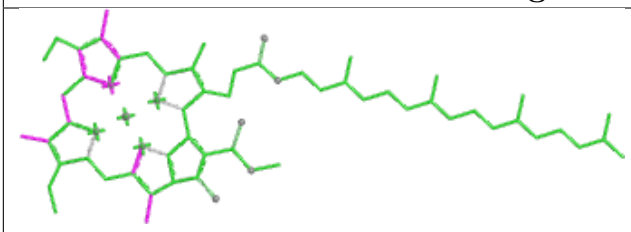


Rings

Ligand CLA g 307



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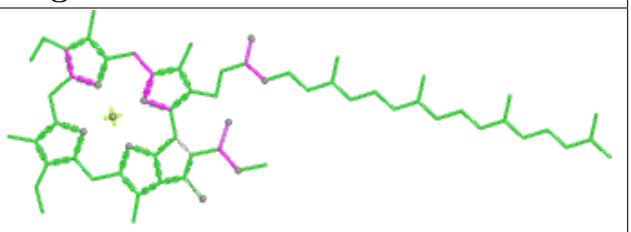

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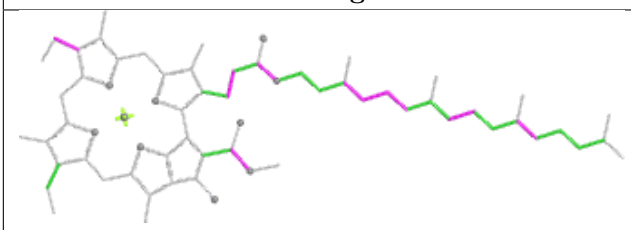

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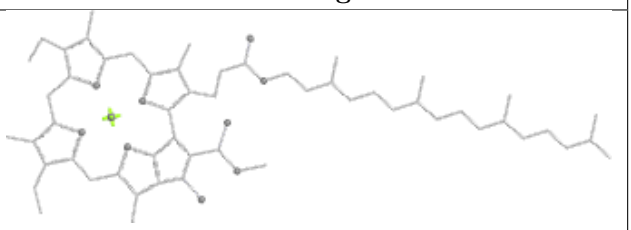
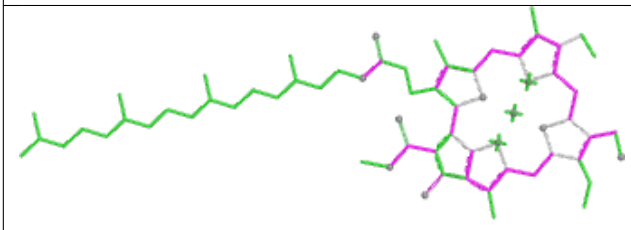


Rings

Ligand CHL V 318



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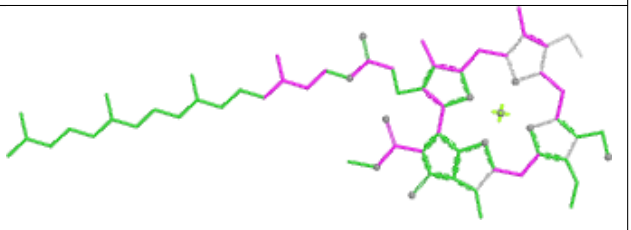

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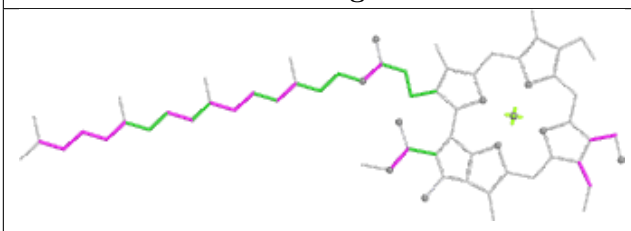

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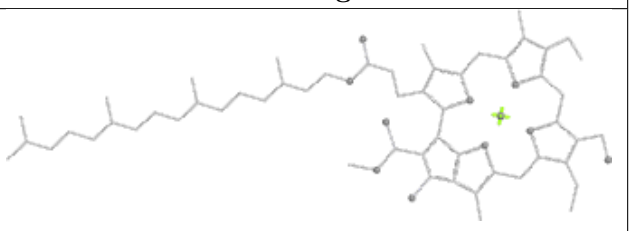
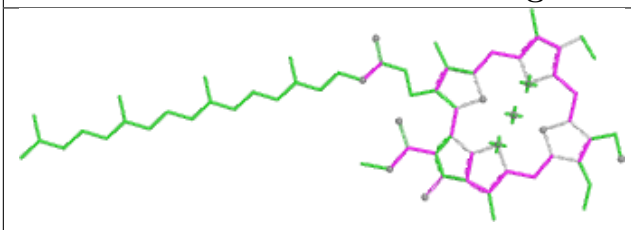


Rings

Ligand CHL u 317



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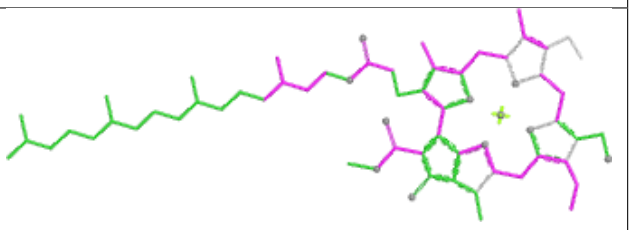

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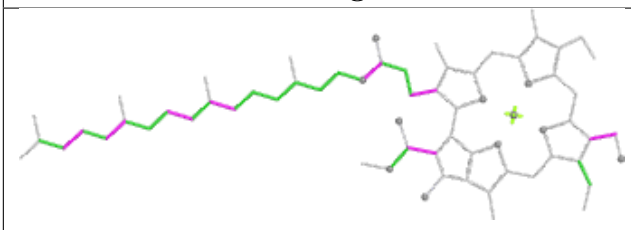

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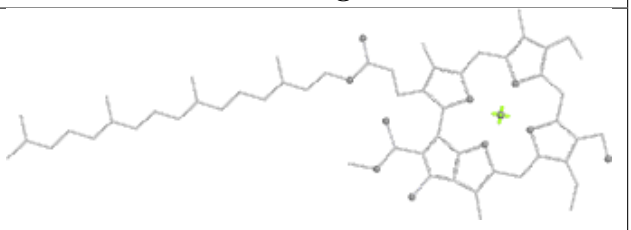
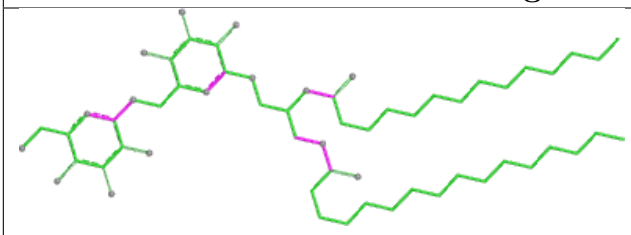


Rings

Ligand DGD J 101



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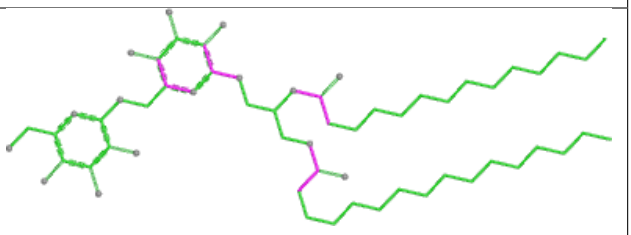

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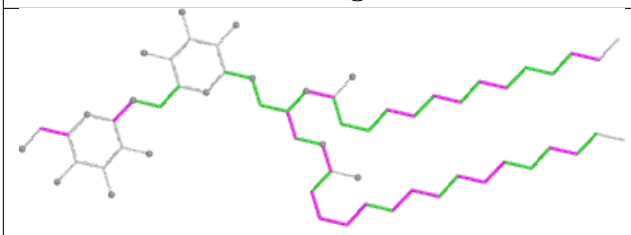

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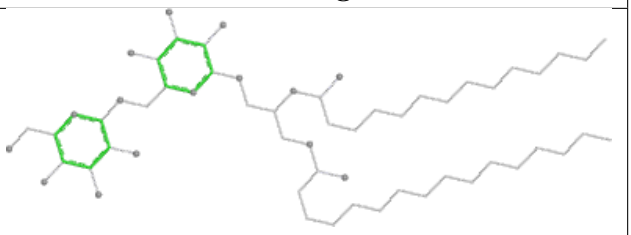
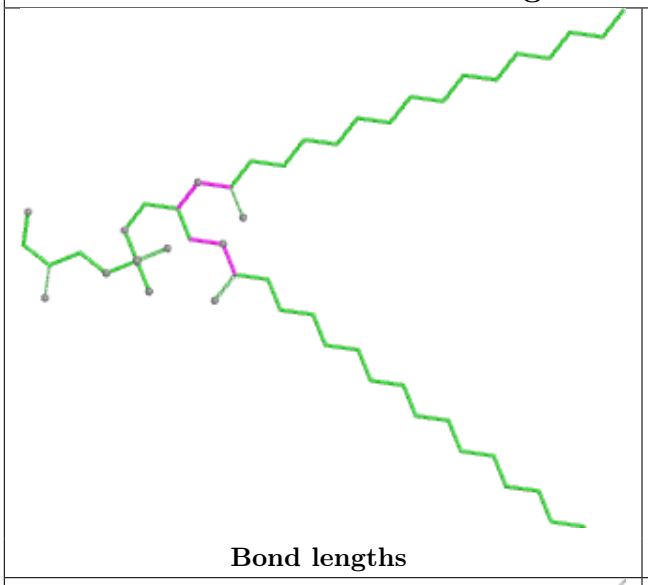


Rings

Ligand LHG B 623



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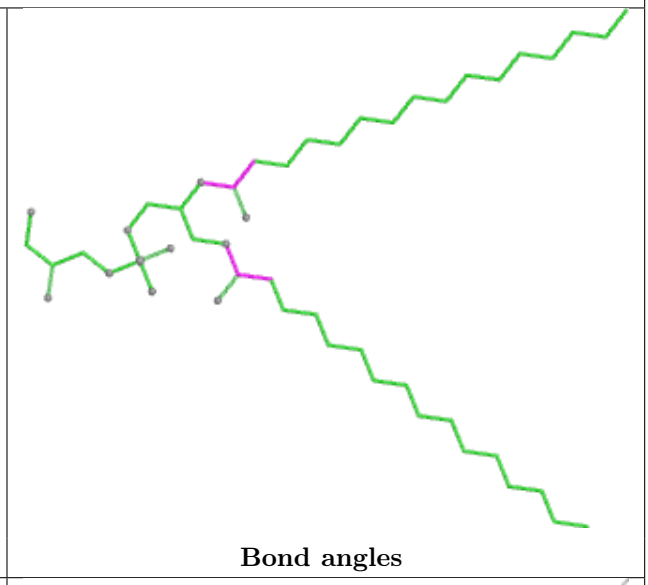

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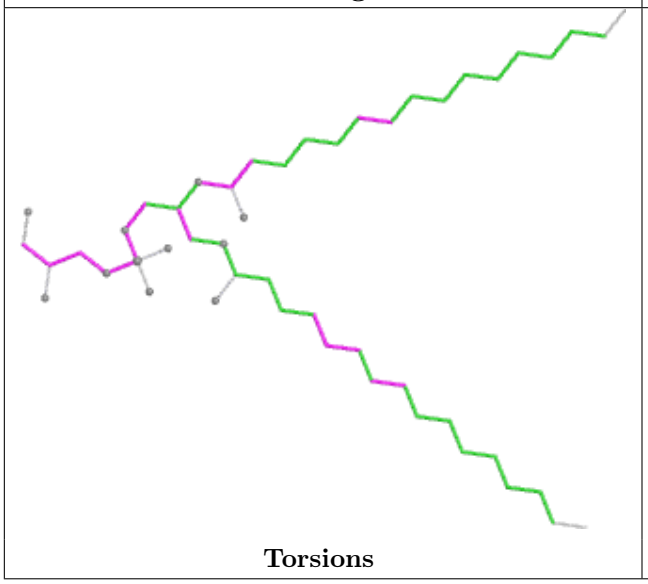

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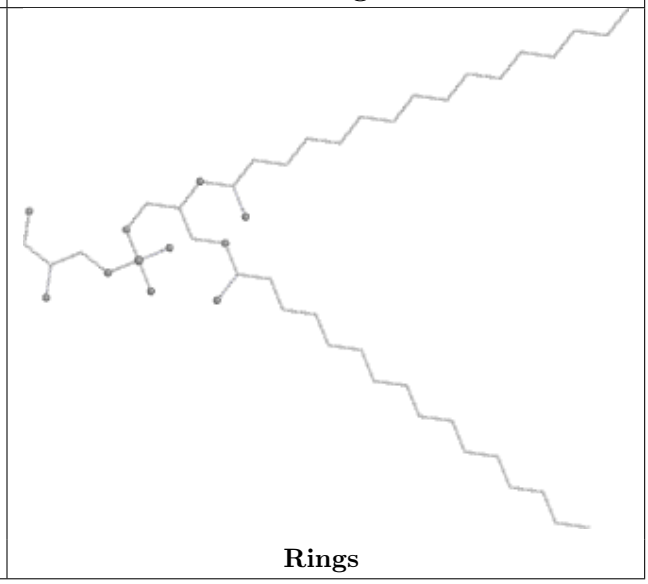
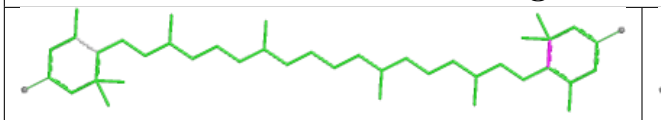


Rings

Ligand LUT 4 310



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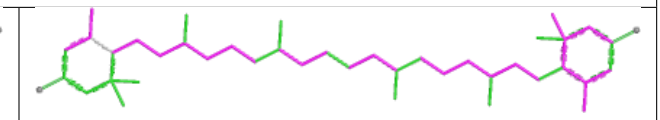

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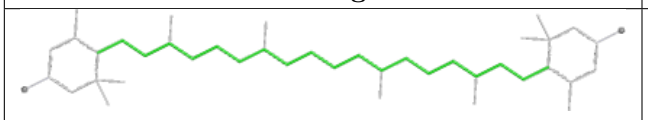

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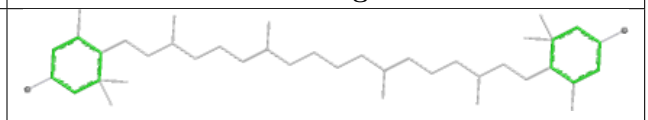
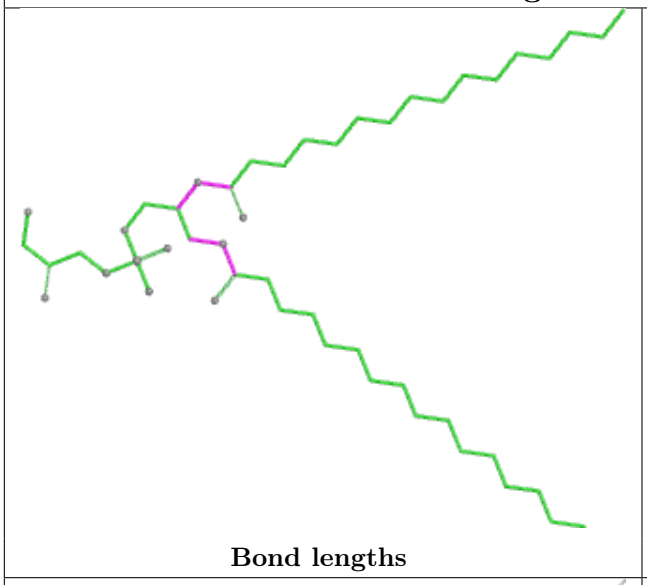


Rings

Ligand LHG C 524



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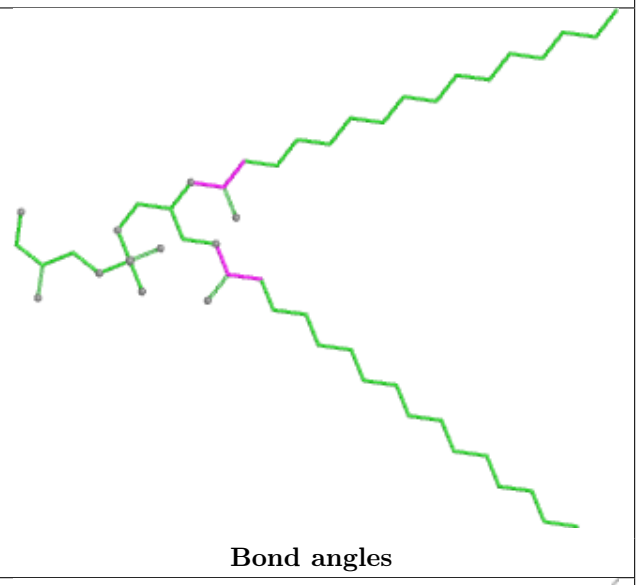
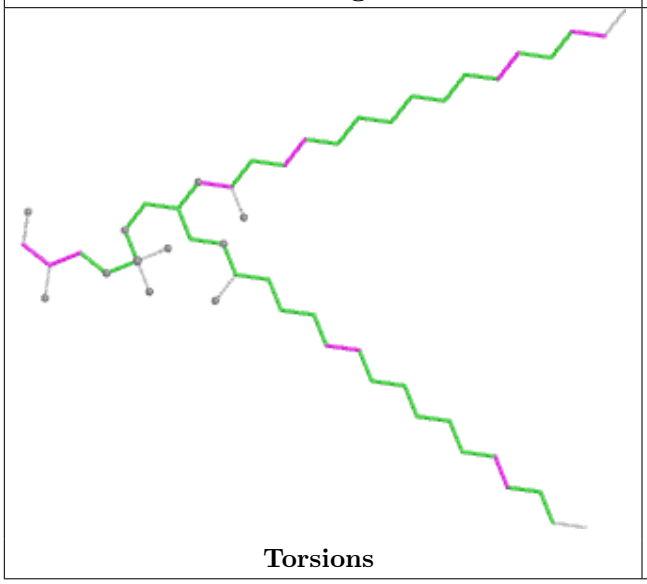


Bond angles



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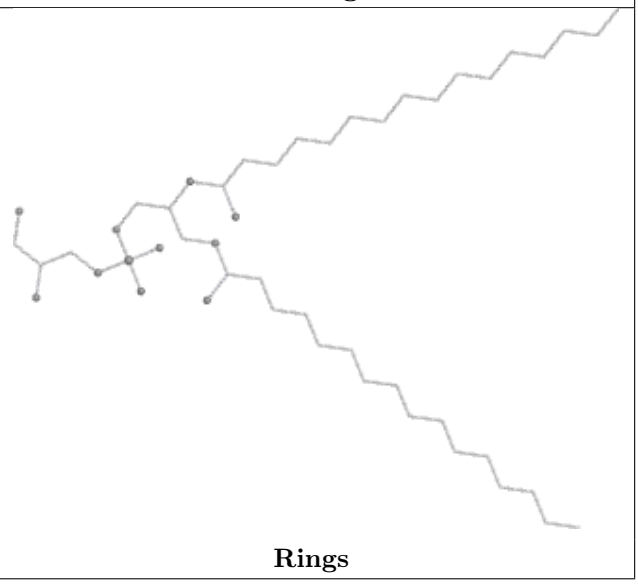
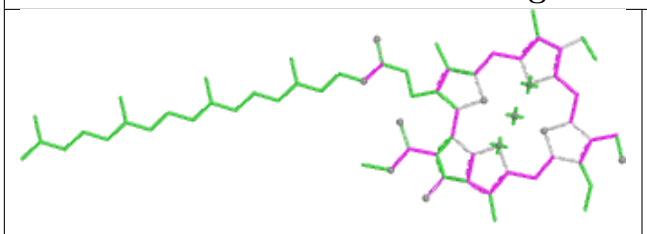


Rings

Ligand CHL 1 318



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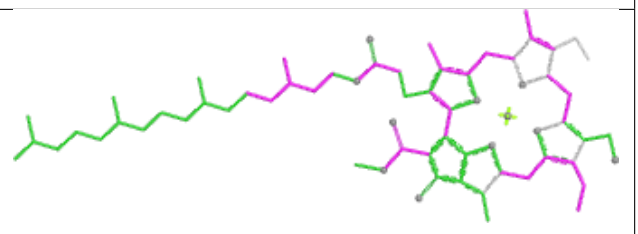
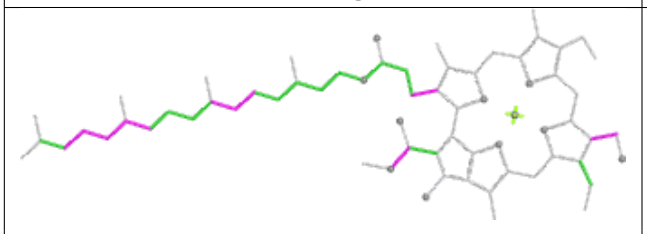


Bond angles



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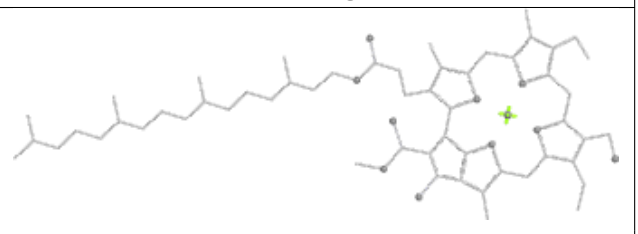
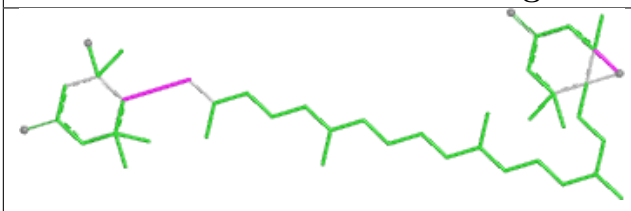


Rings

Ligand NEX P 301



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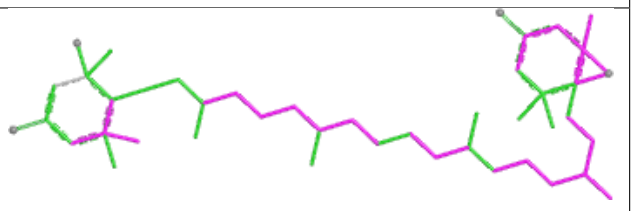
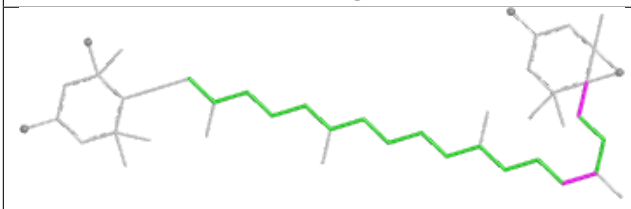


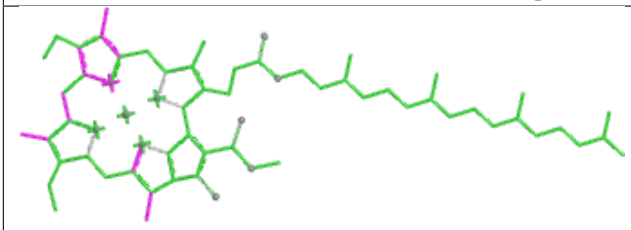
Bond angles



Torsions

Rings

Ligand CLA c 502



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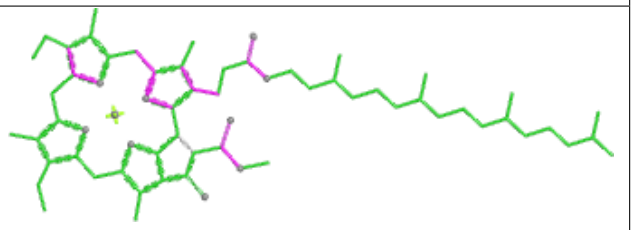
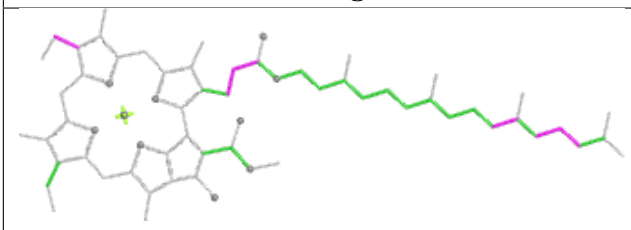
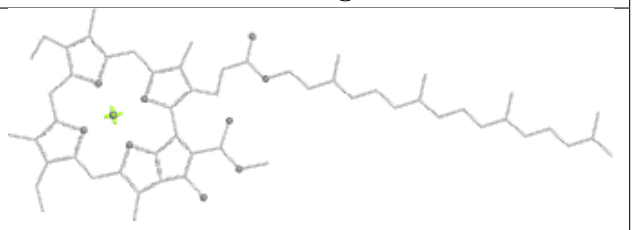


Bond angles

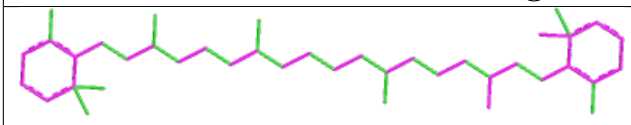


Torsions

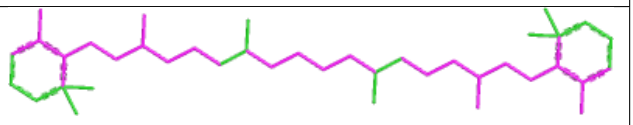


Rings

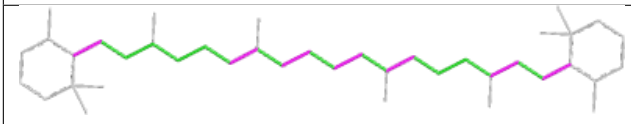
Ligand BCR b 620



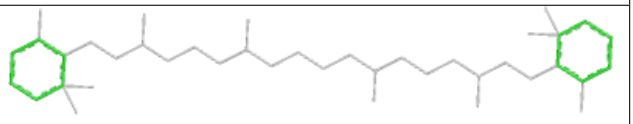
Bond lengths



Bond angles

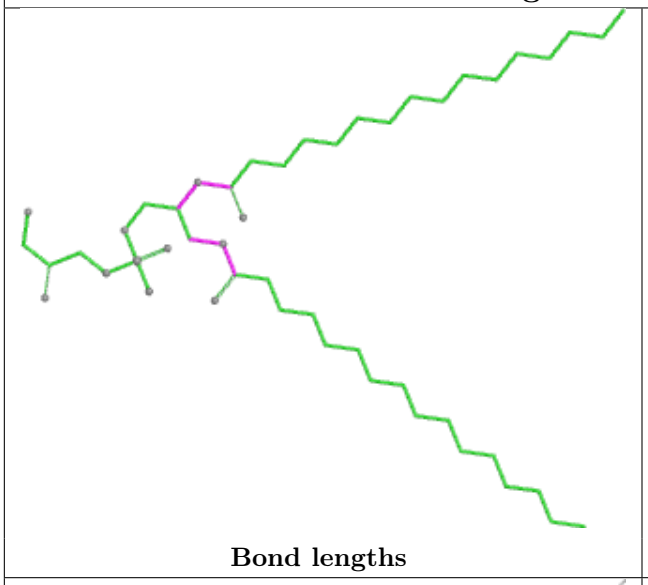


Torsions



Rings

Ligand LHG U 312



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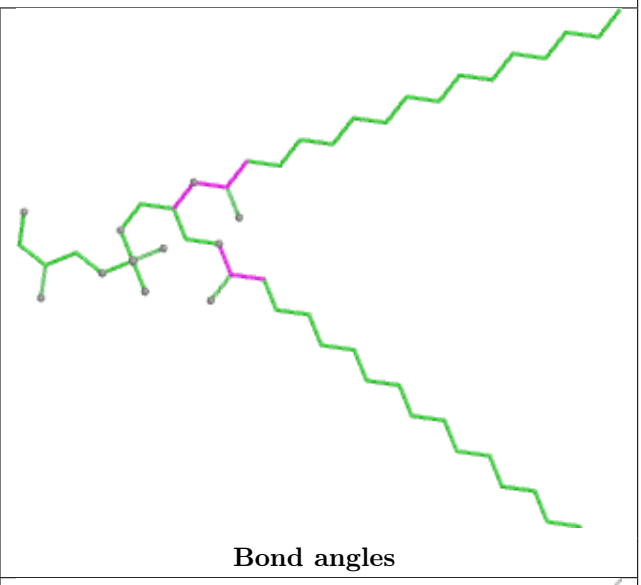
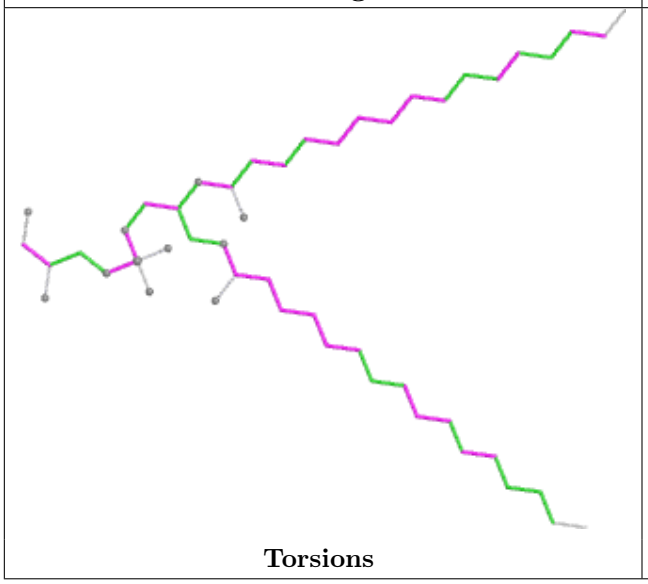
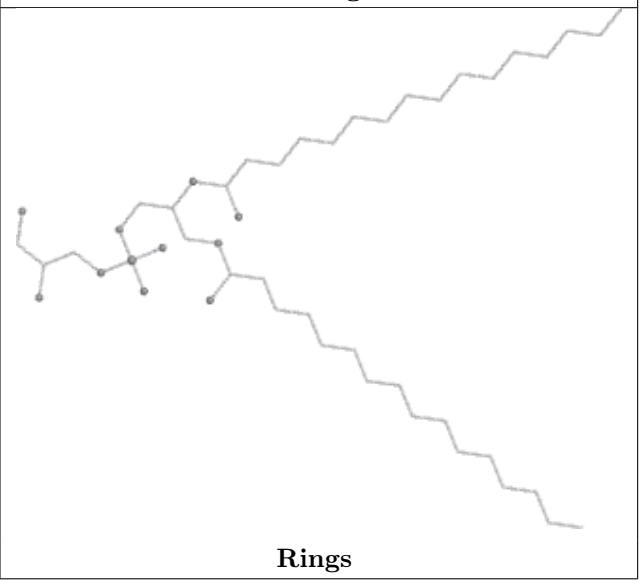


Bond angles

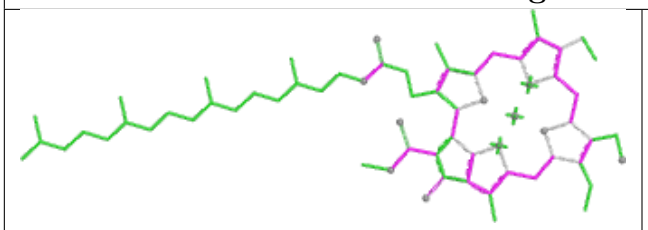


Torsions

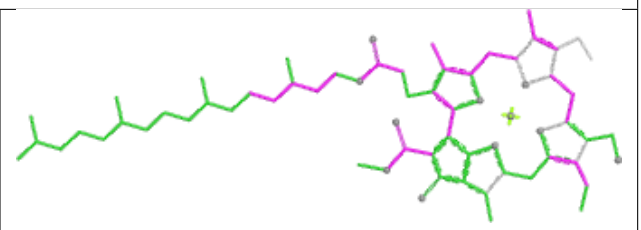


Rings

Ligand CHL 4 313



Bond lengths



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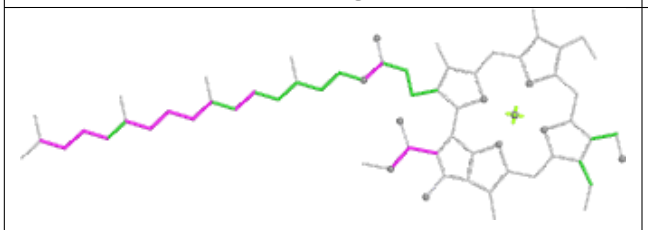
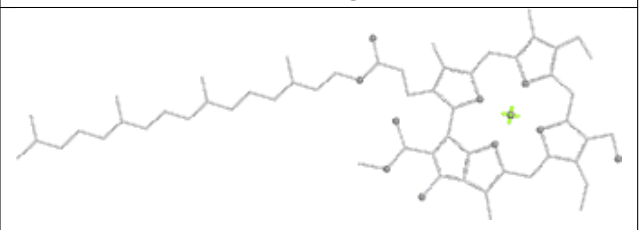
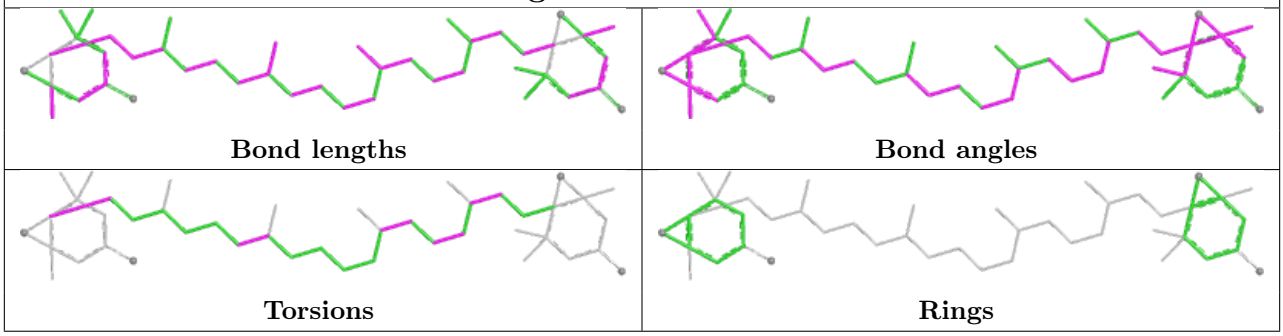


Torsions



Rings

Ligand XAT 3 309



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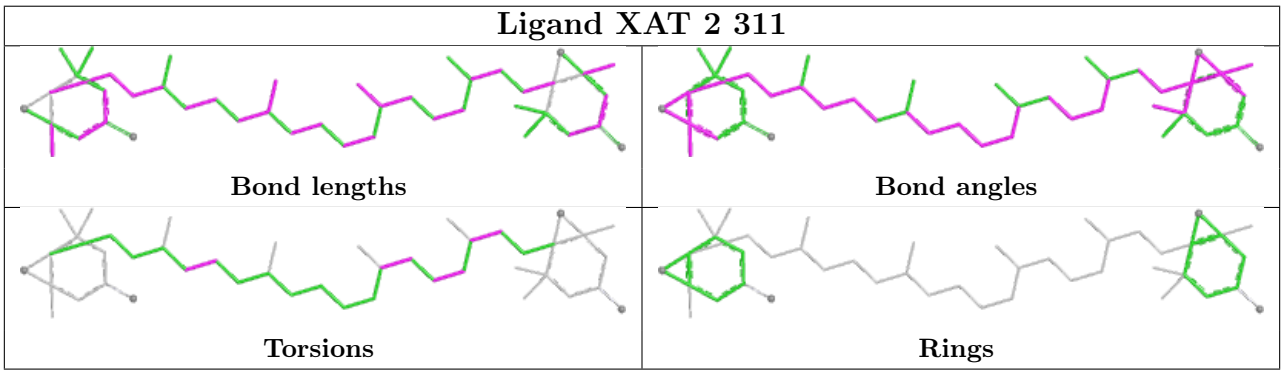
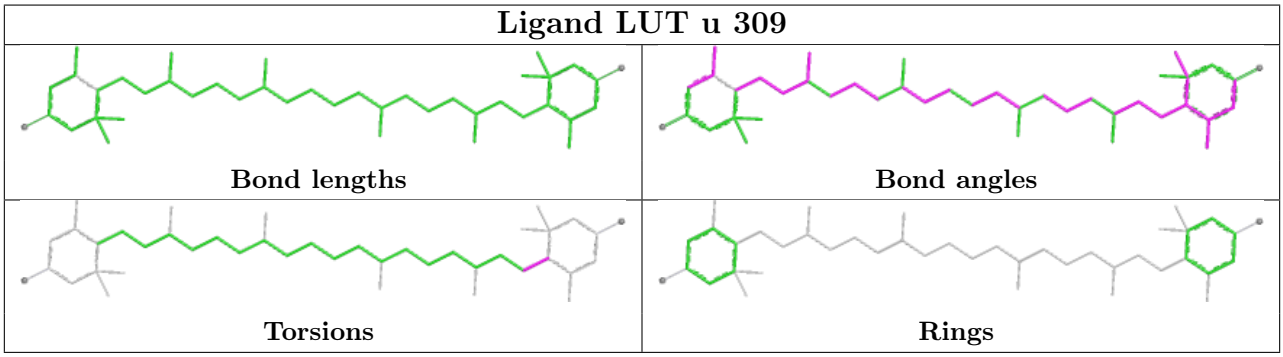
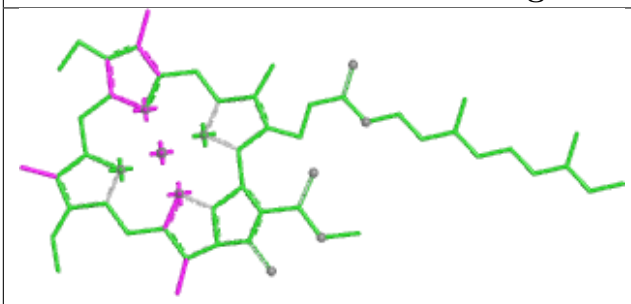
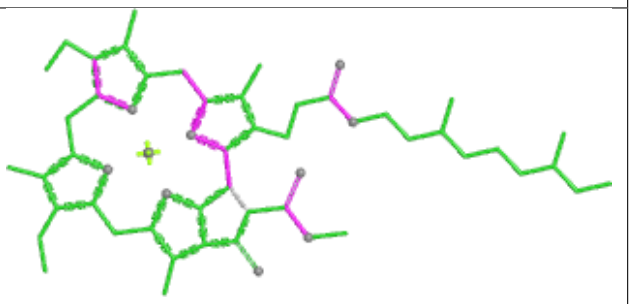
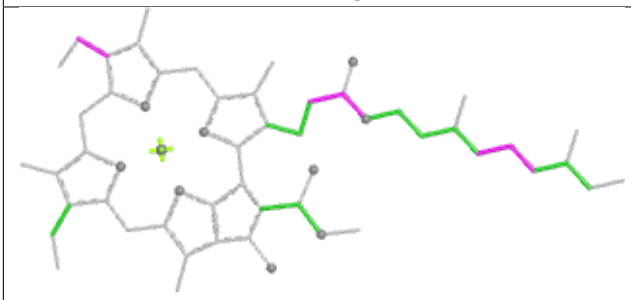
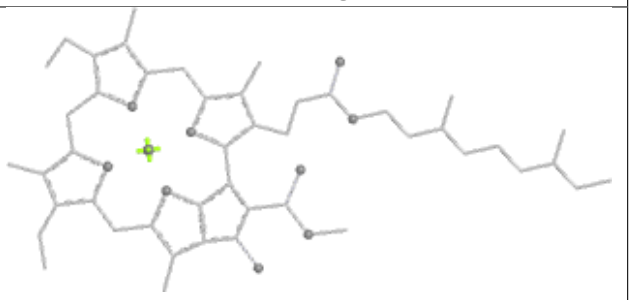
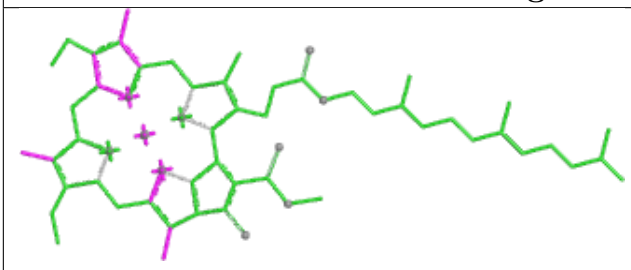
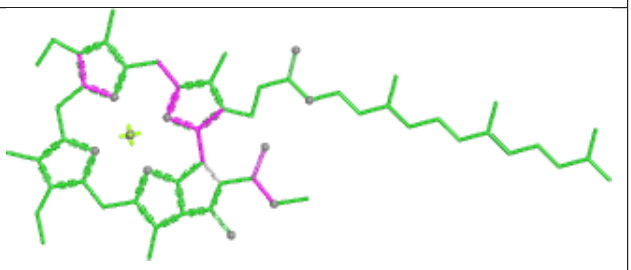
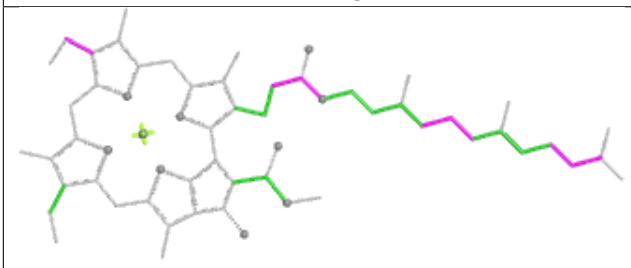
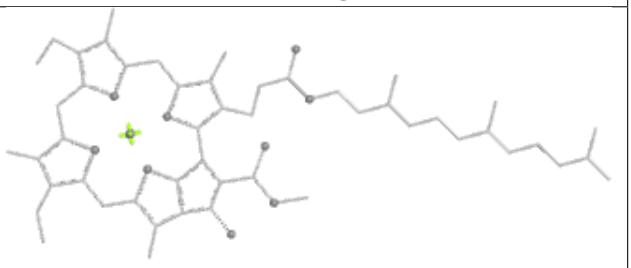


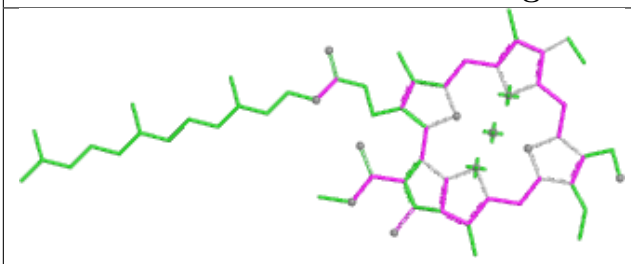
Ligand LUT u 309



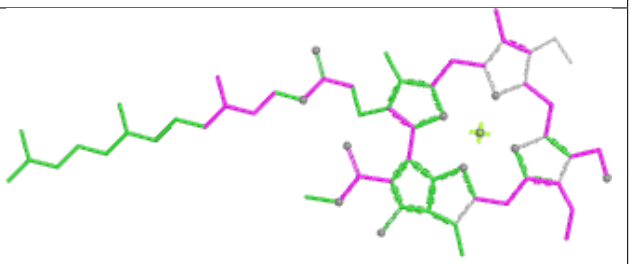
Ligand CLA S 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

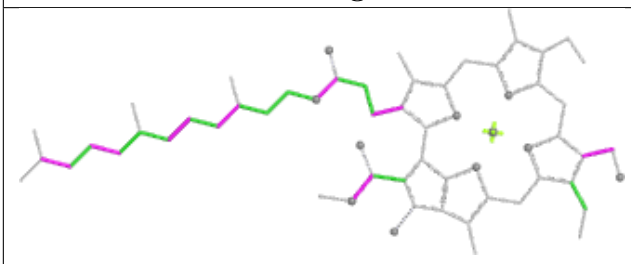
Ligand CHL G 316



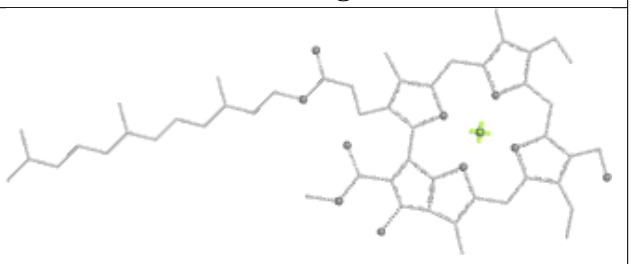
Bond lengths



Bond angles

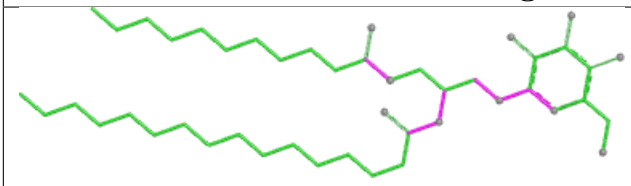


Torsions



Rings

Ligand LMG D 408



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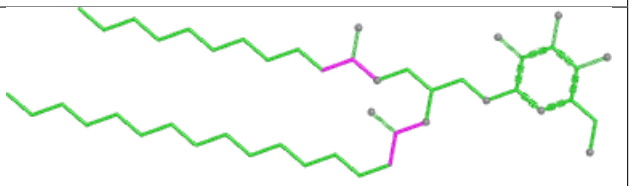
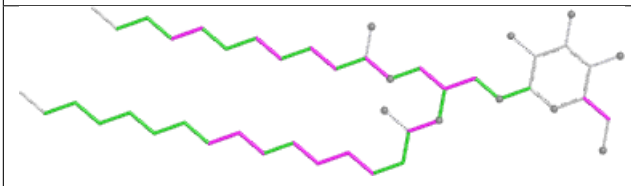


Bond angles



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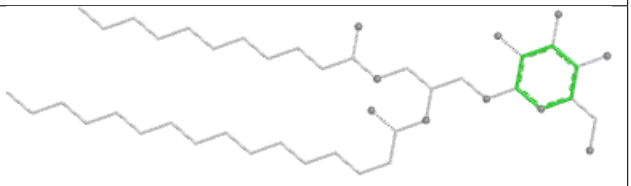
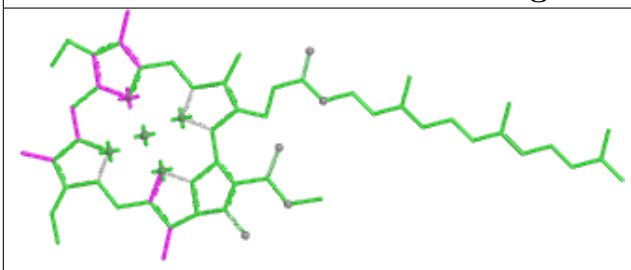
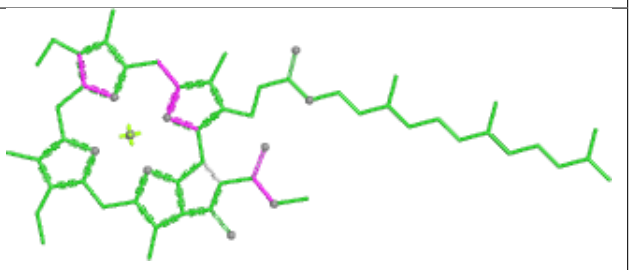


Rings

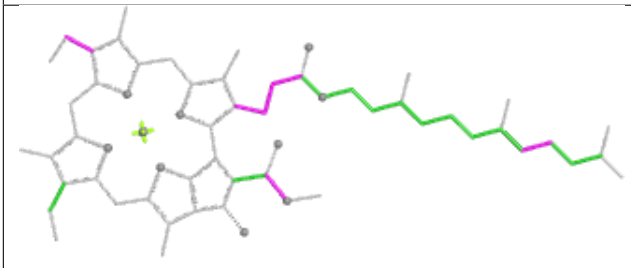
Ligand CLA r 602



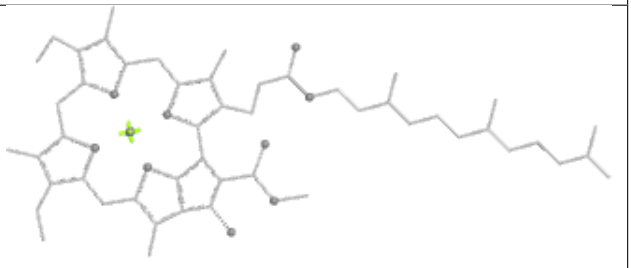
Bond lengths



Bond angles

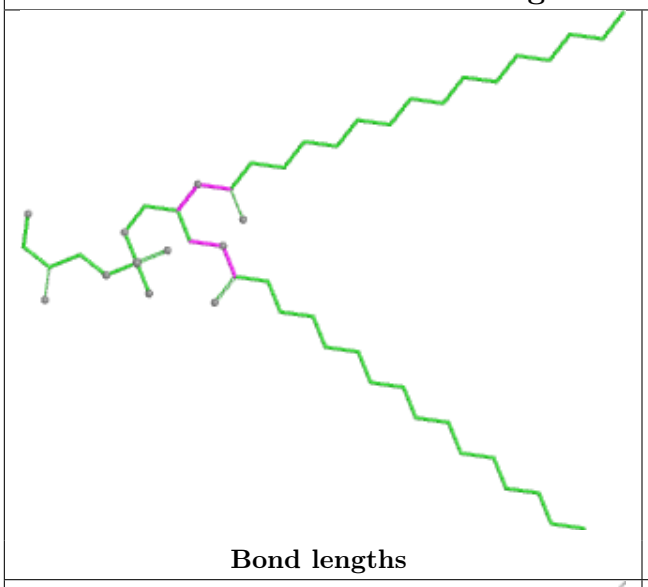


Torsions



Rings

Ligand LHG 4 312



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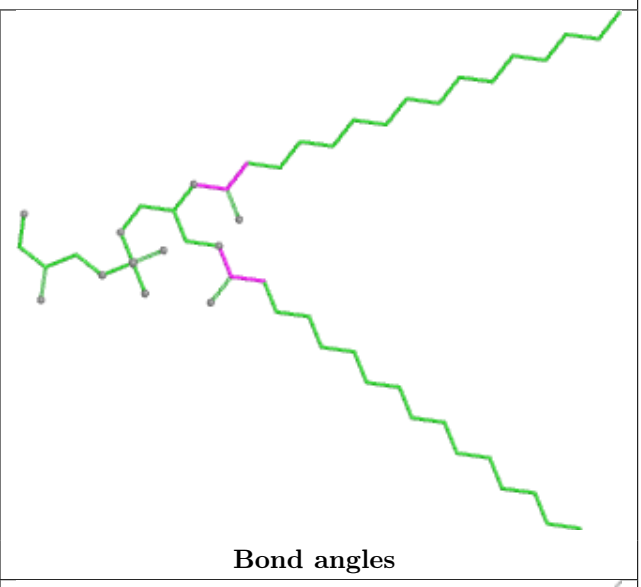
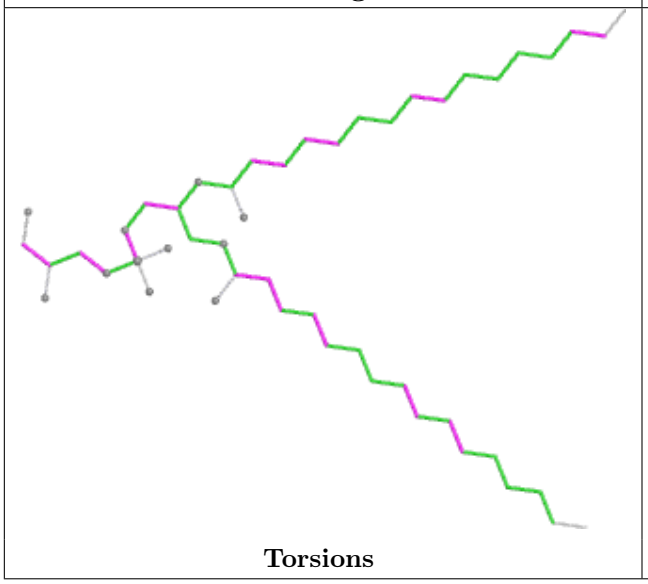


Bond angles



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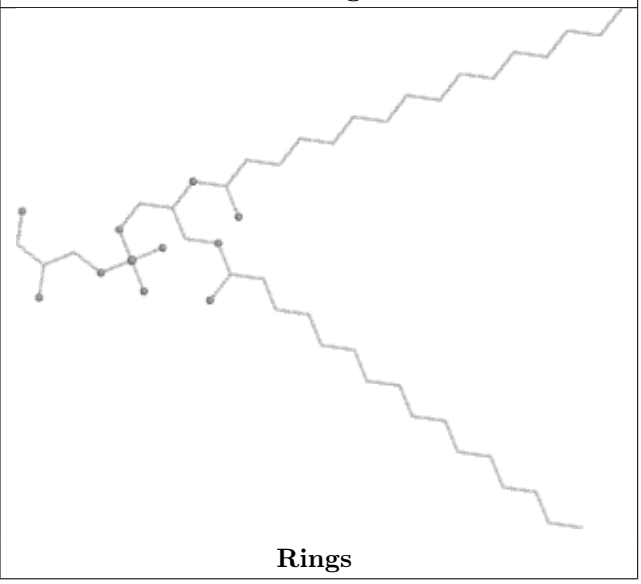
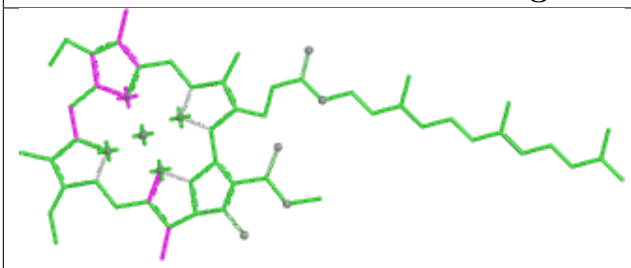


Rings

Ligand CLA r 603



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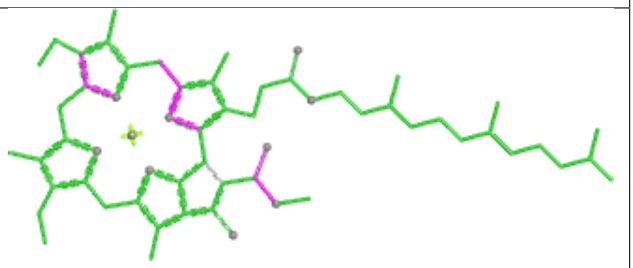
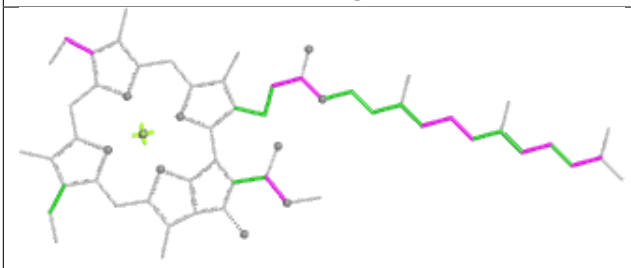


Bond angles



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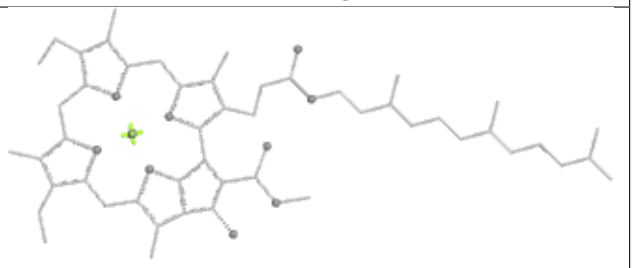
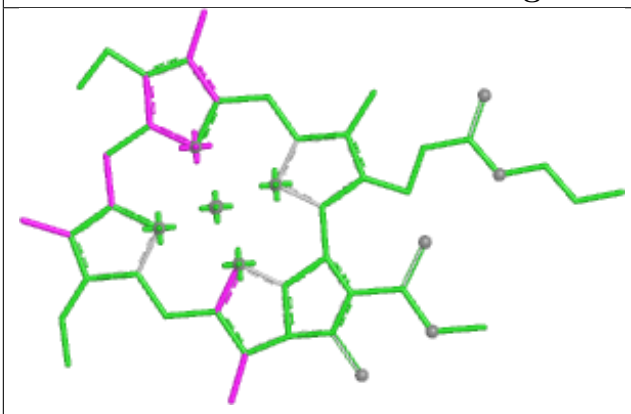


Rings

Ligand CLA U 308



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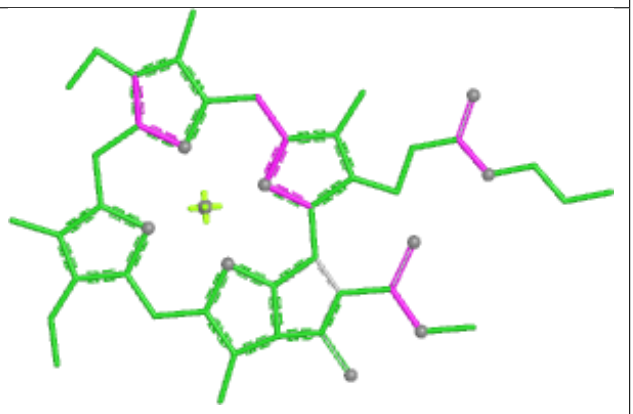
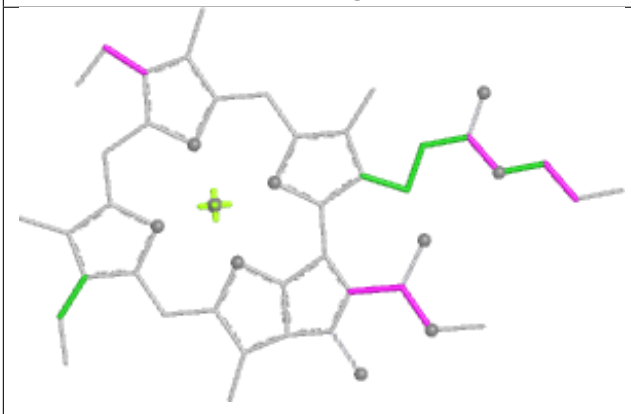
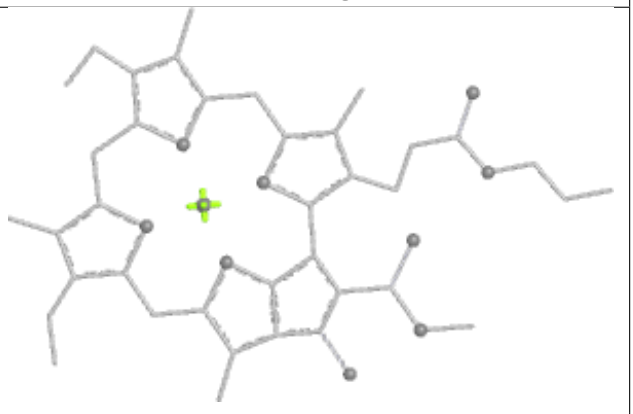


Bond angles

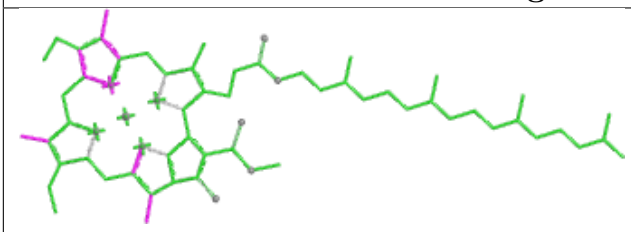


Torsions

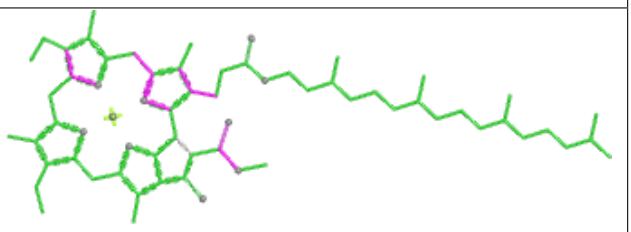


Rings

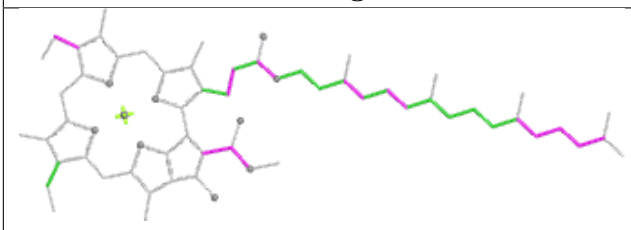
Ligand CLA b 606



Bond lengths



Bond angles



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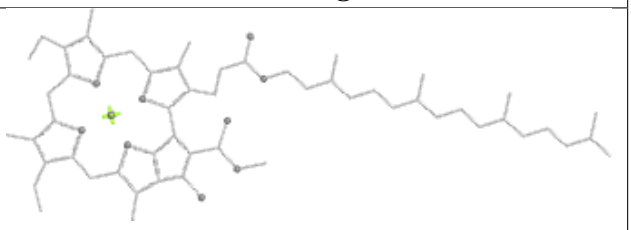
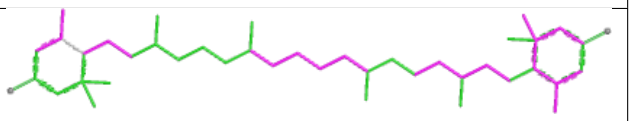


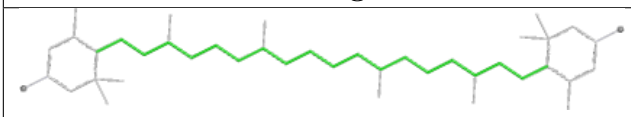
Rings

Ligand LUT 5 310

Bond lengths



Bond angles



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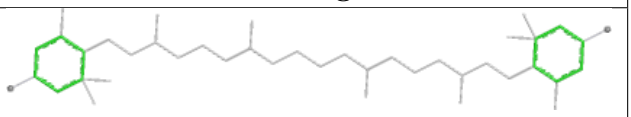
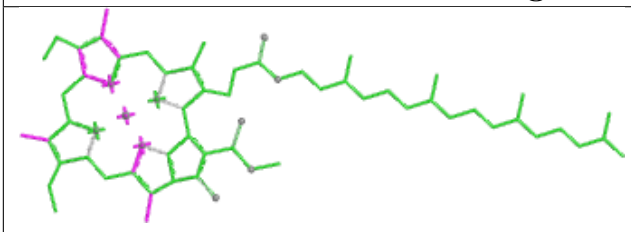
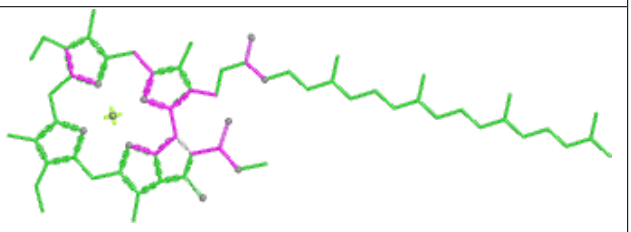


Rings

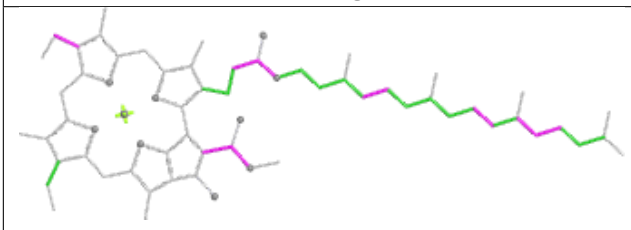
Ligand CLA b 617



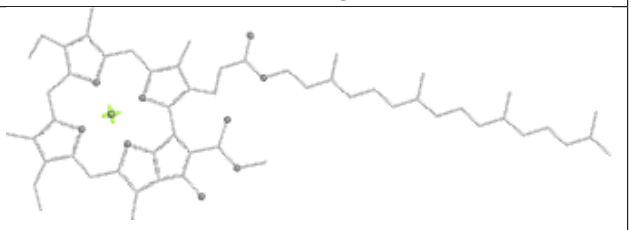
Bond lengths



Bond angles

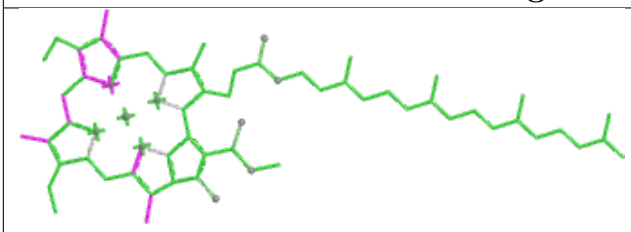


Torsions

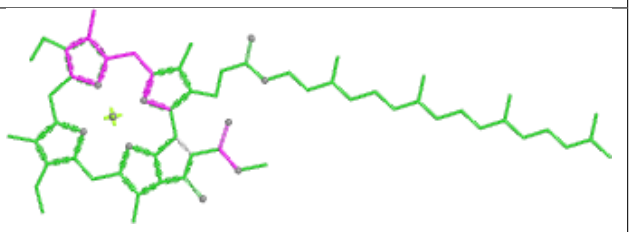


Rings

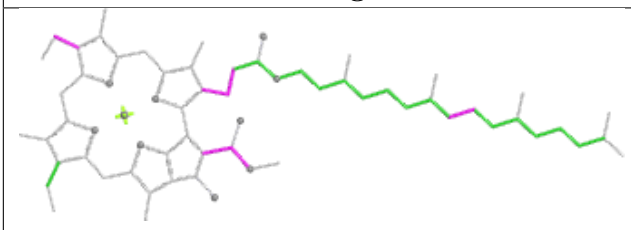
Ligand CLA u 301



Bond lengths



Bond angles



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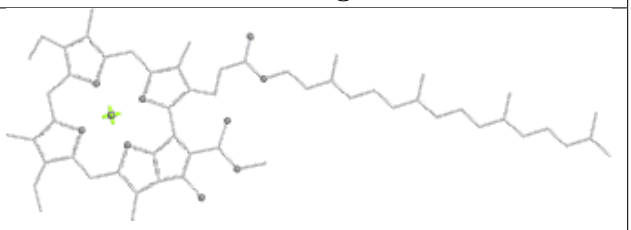
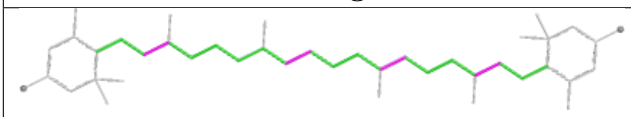


Rings

Ligand LUT s 311

Bond lengths

Bond angles



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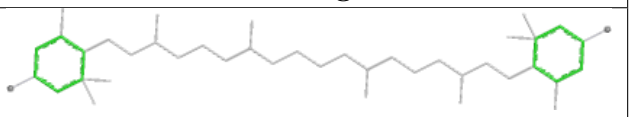
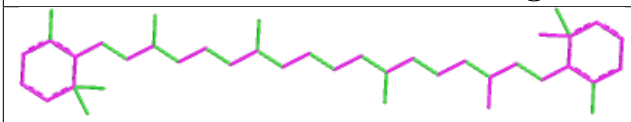
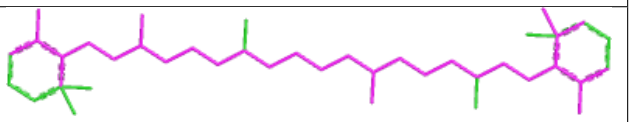


Rings

Ligand BCR b 618



Bond lengths



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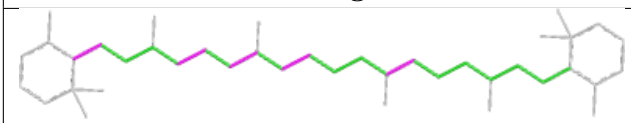

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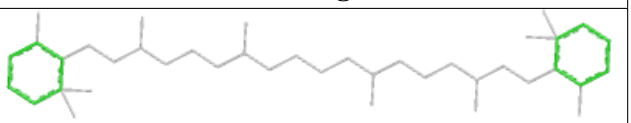
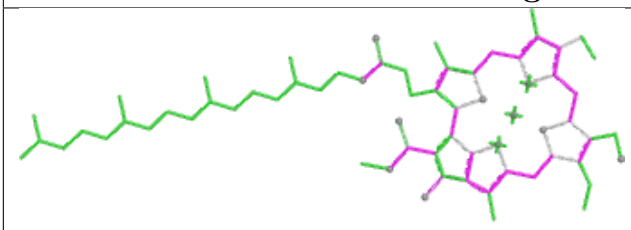


Rings

Ligand CHL Q 315



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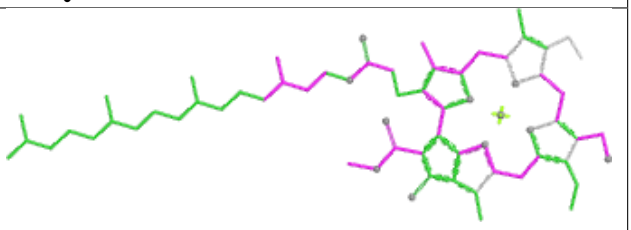
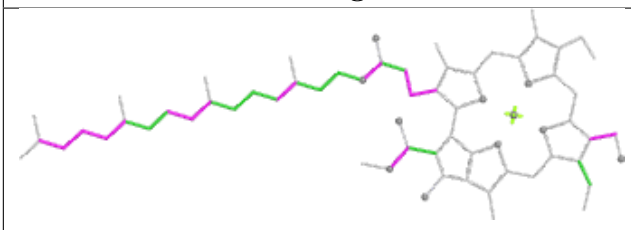


Bond angles



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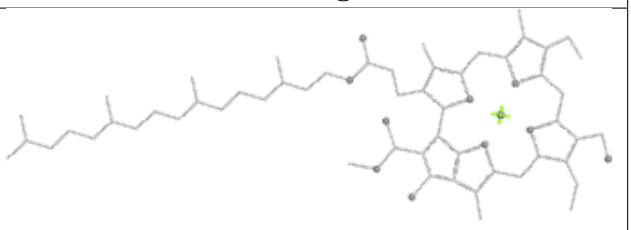
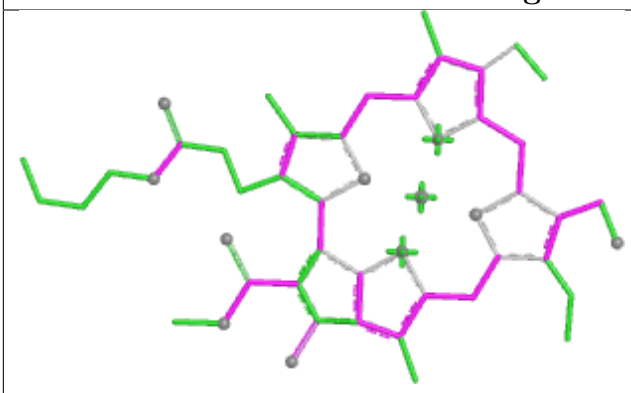


Rings

Ligand CHL Q 313



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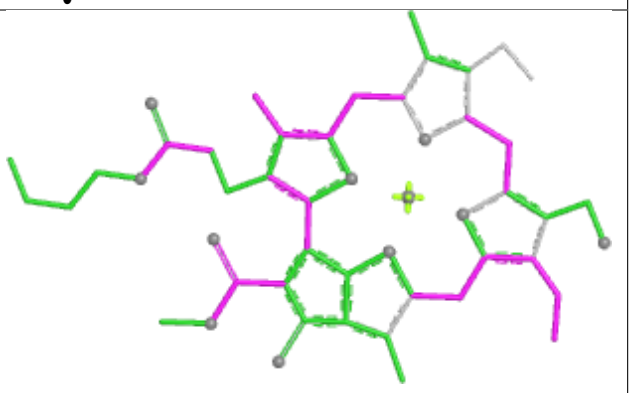
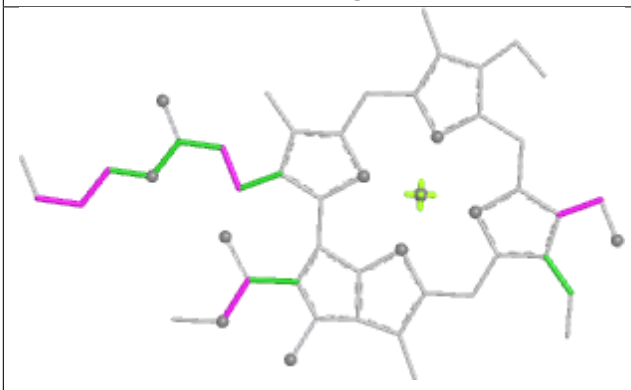


Bond angles



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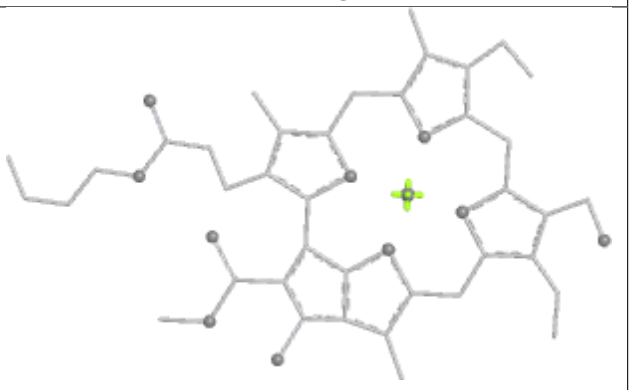
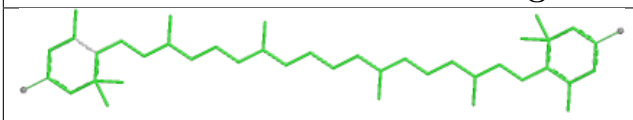


Rings

Ligand LUT 2 309



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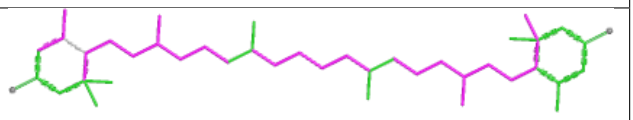
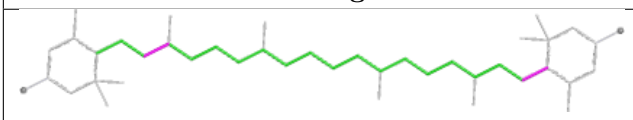


Bond angles



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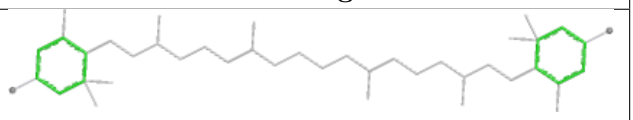
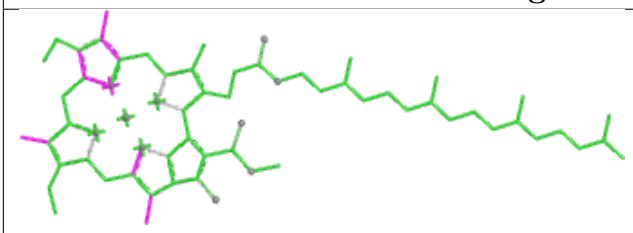


Rings

Ligand CLA 2 302



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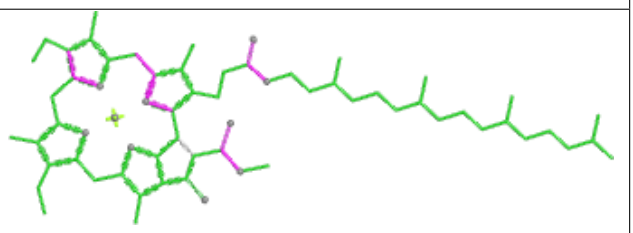

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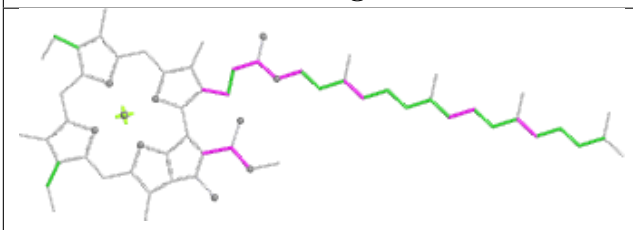

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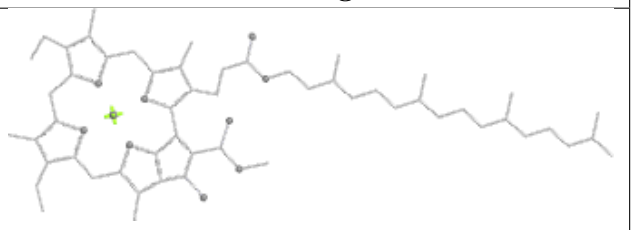
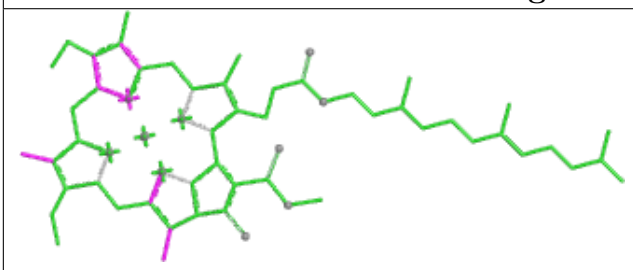


Rings

Ligand CLA 2 306



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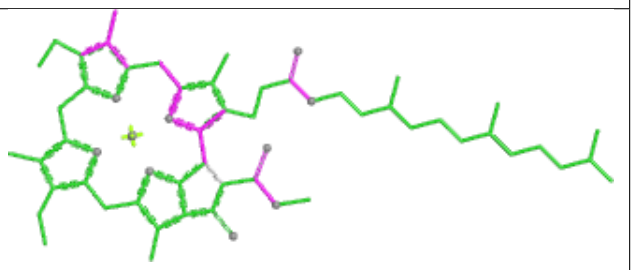

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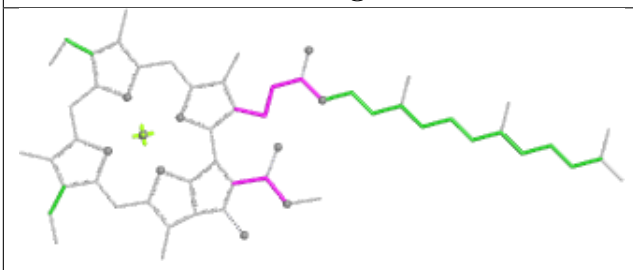

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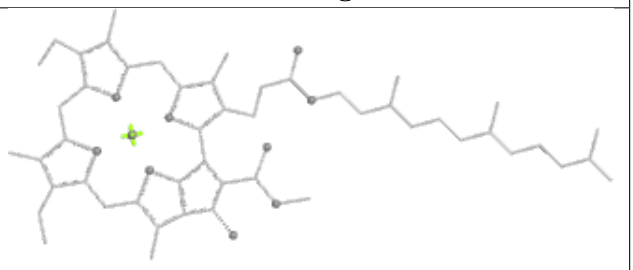
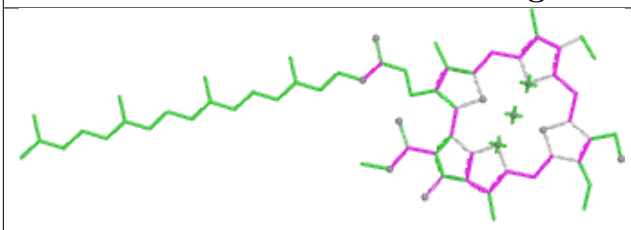


Rings

Ligand CHL 5 313



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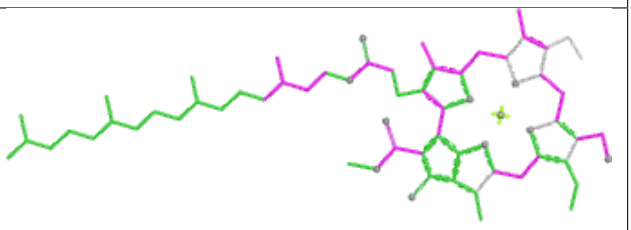

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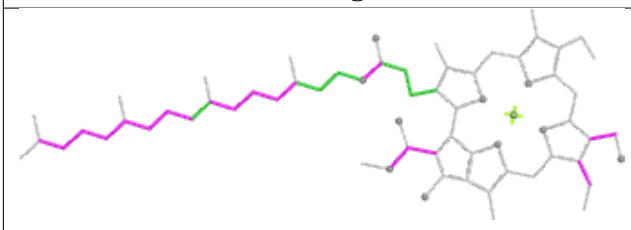

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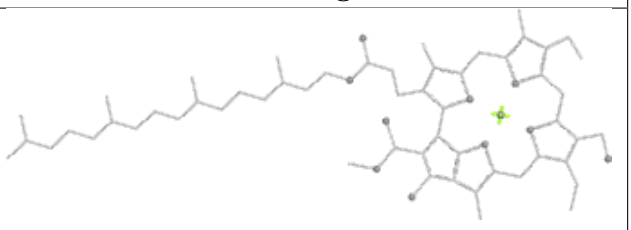
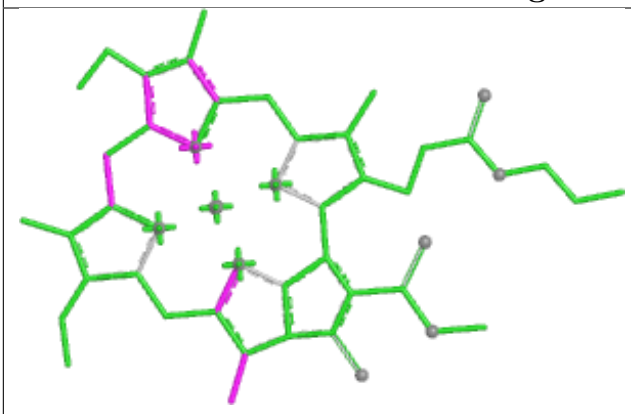


Rings

Ligand CLA 3 308



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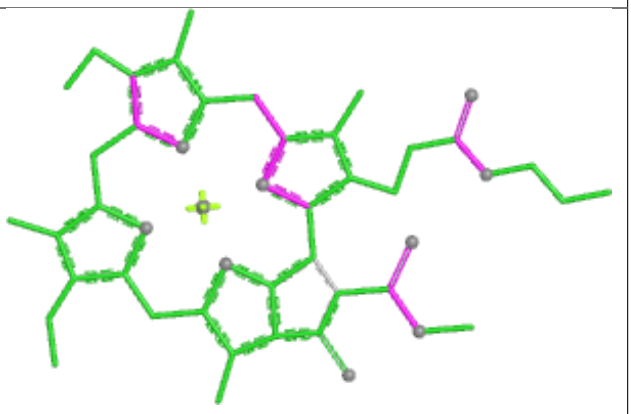
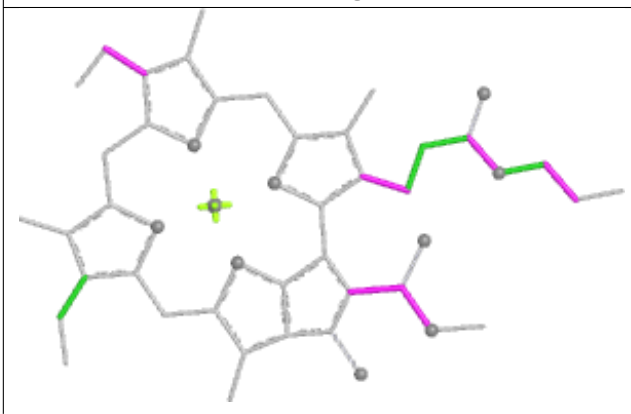


Bond angles



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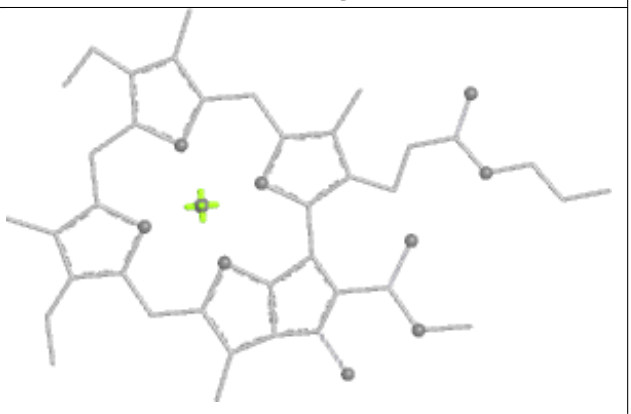
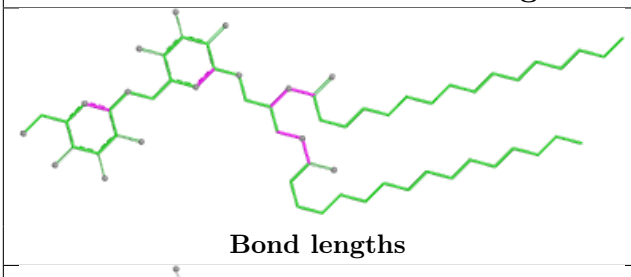


Rings

Ligand DGD C 520



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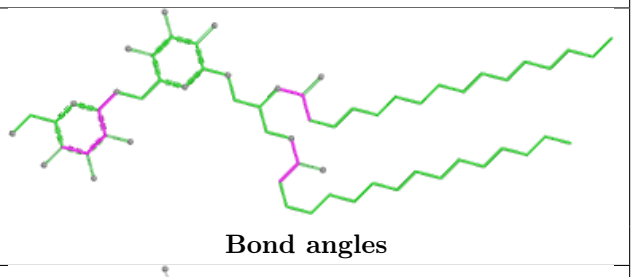
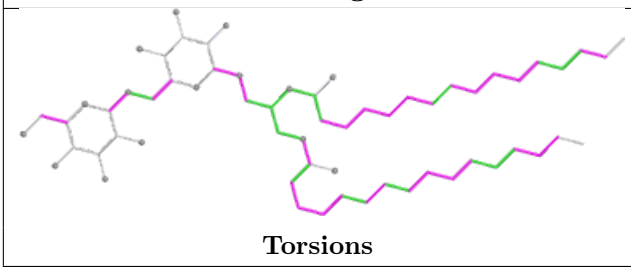


Bond angles



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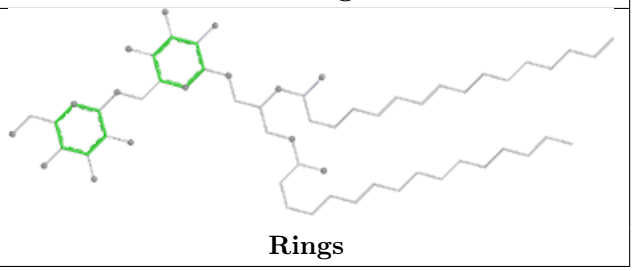
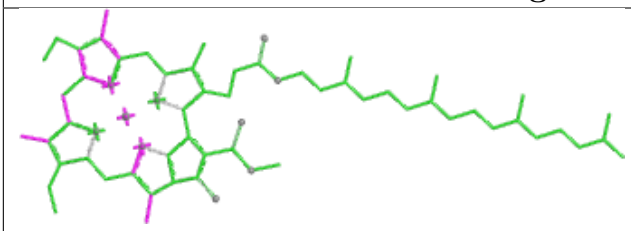


Rings

Ligand CLA c 504



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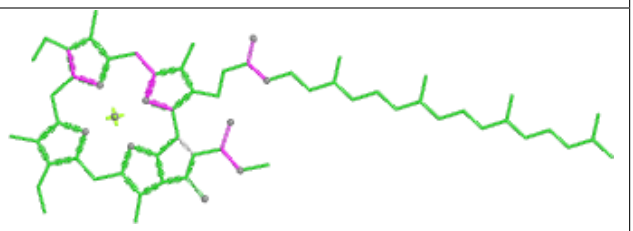
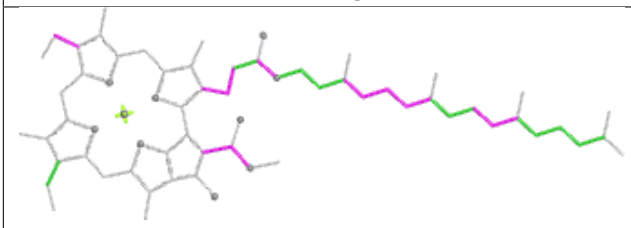
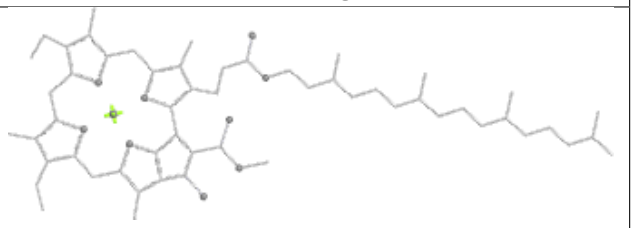


Bond angles

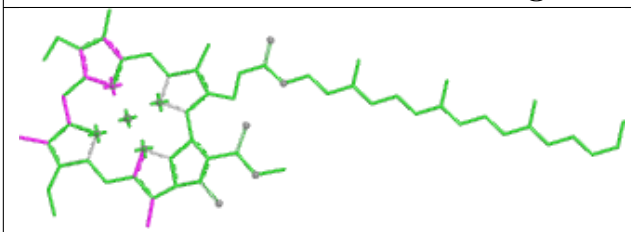


Torsions



Rings

Ligand CLA q 304



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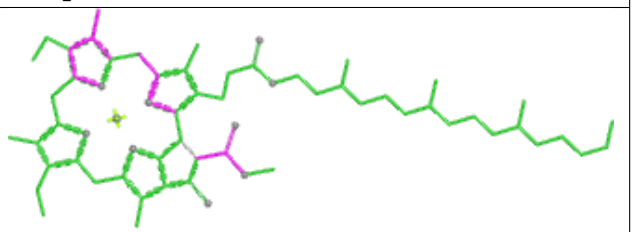
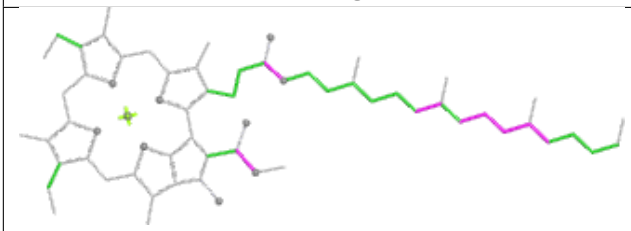
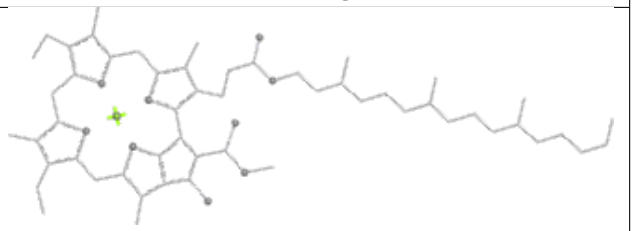


Bond angles

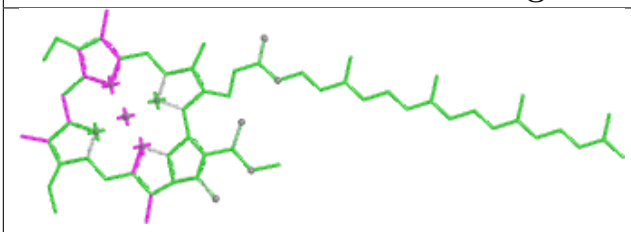


Torsions



Rings

Ligand CLA b 613



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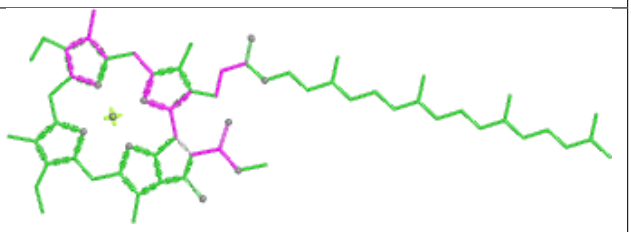
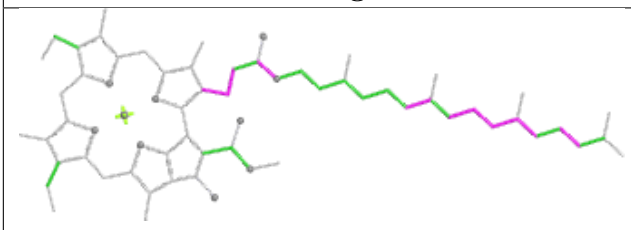
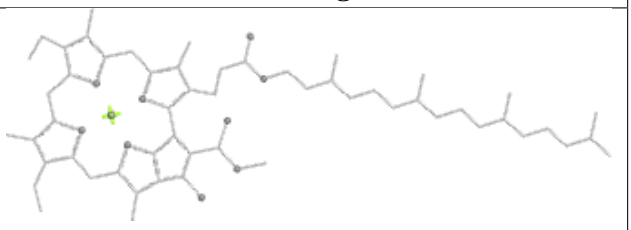


Bond angles

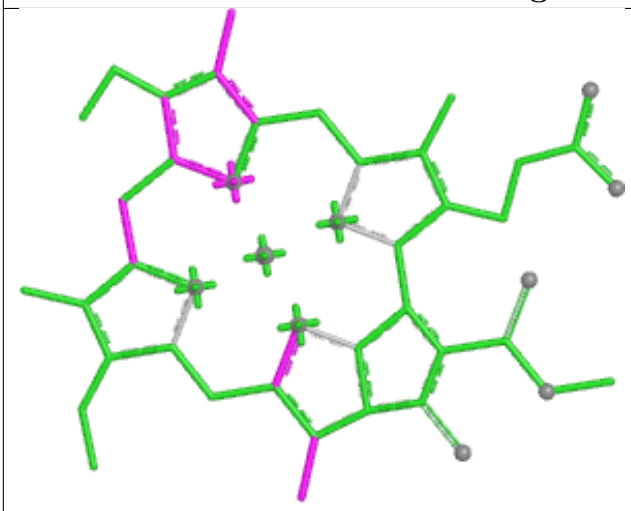


Torsions



Rings

Ligand CLA s 304



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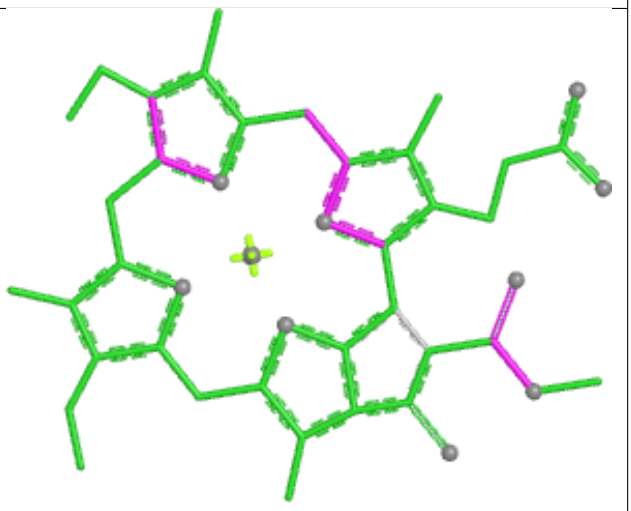
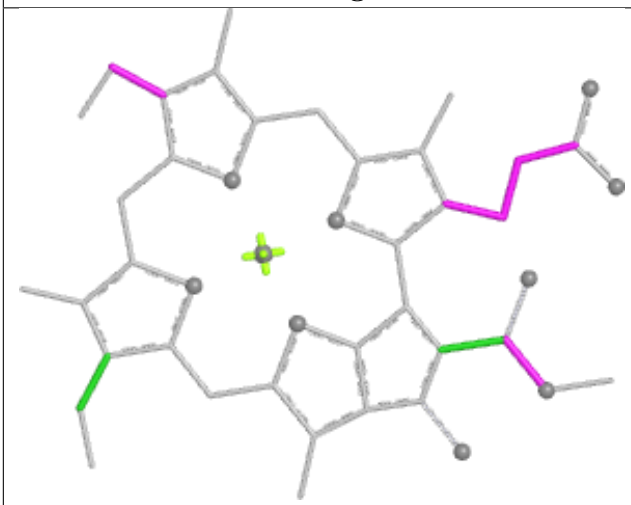


Bond angles



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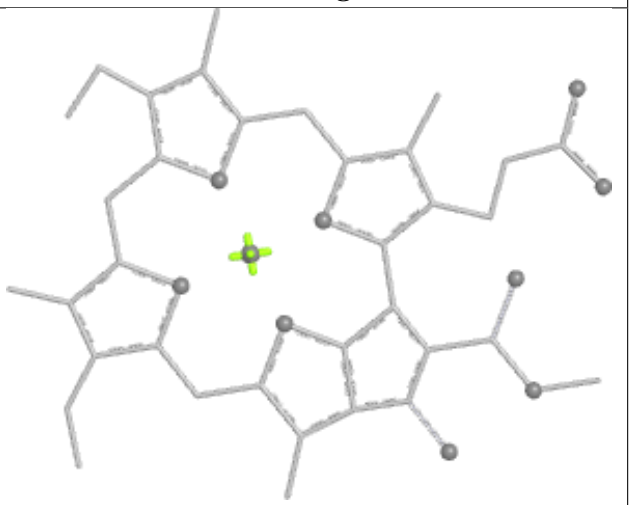
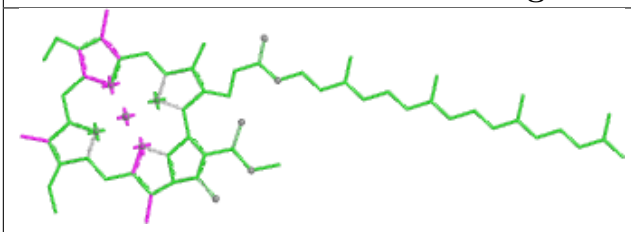


Rings

Ligand CLA b 609



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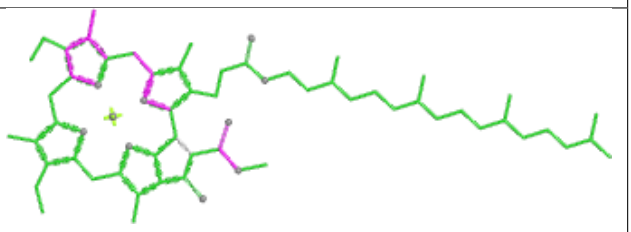

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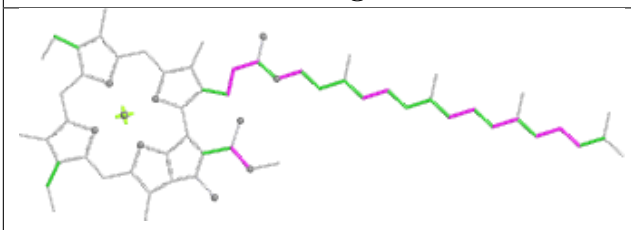

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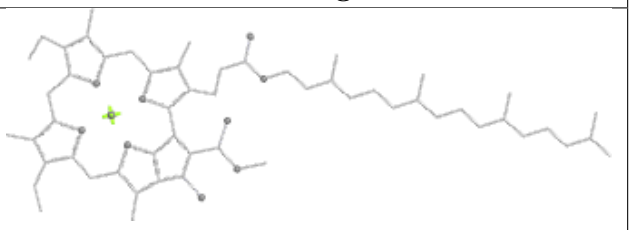
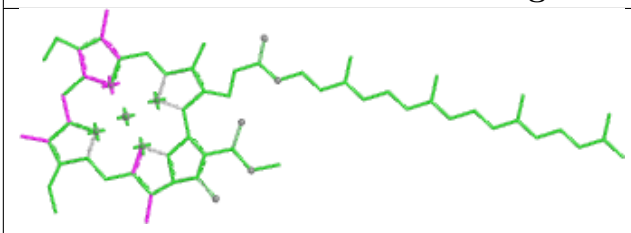


Rings

Ligand CLA 6 303



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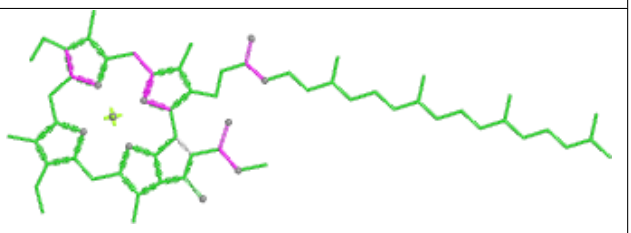

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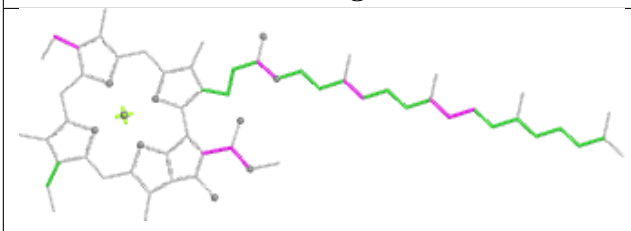

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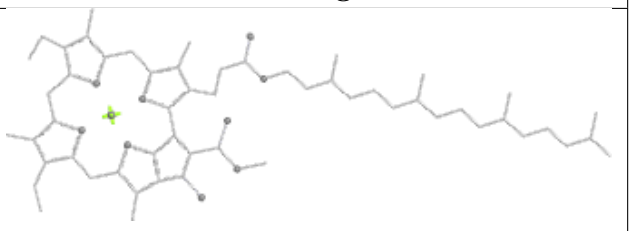
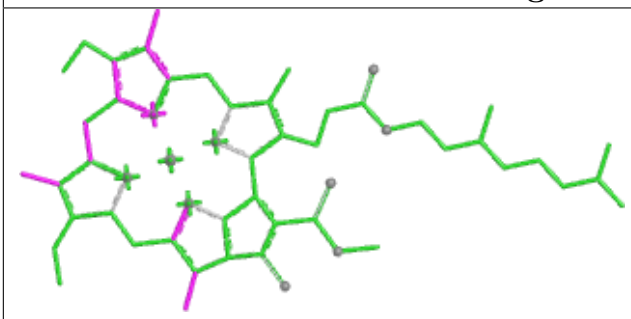


Rings

Ligand CLA S 308



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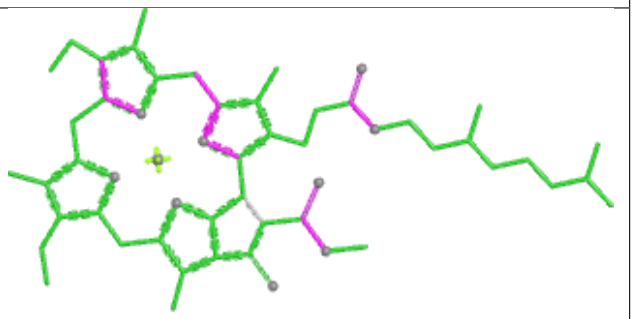
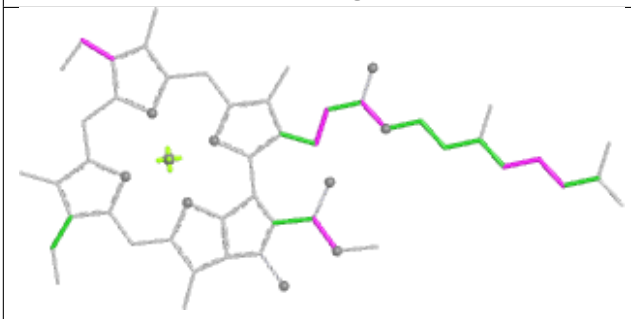


Bond angles



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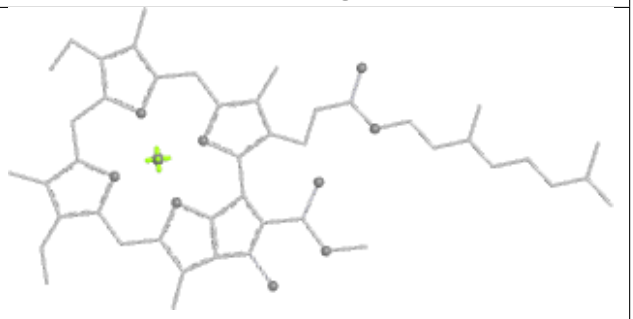
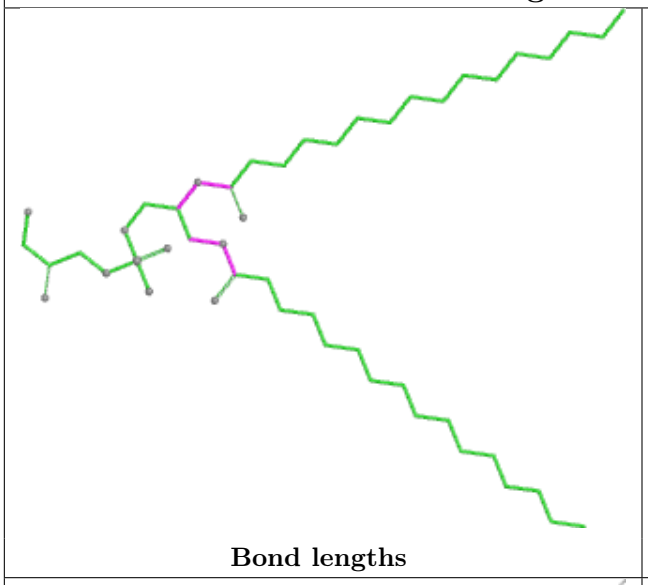


Rings

Ligand LHG v 312



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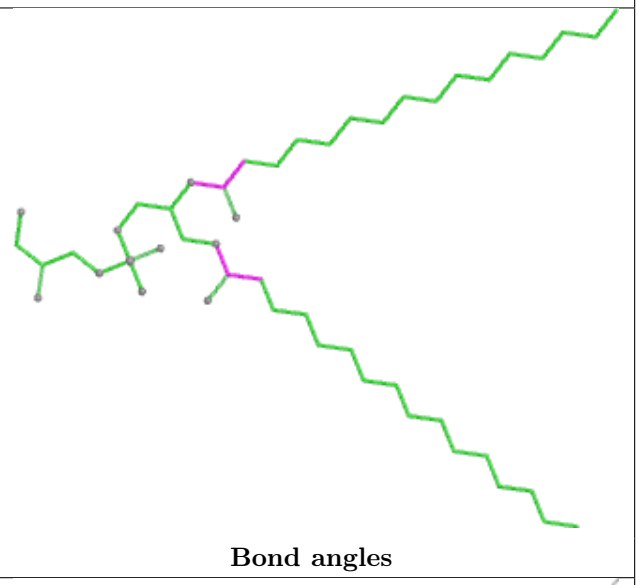

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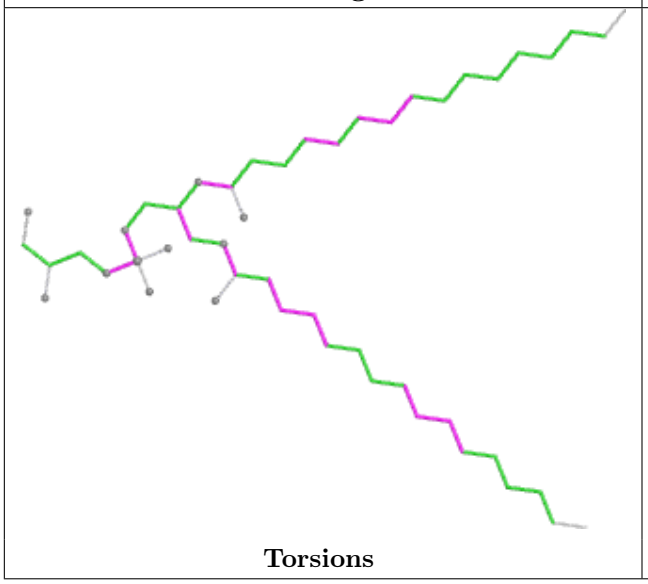

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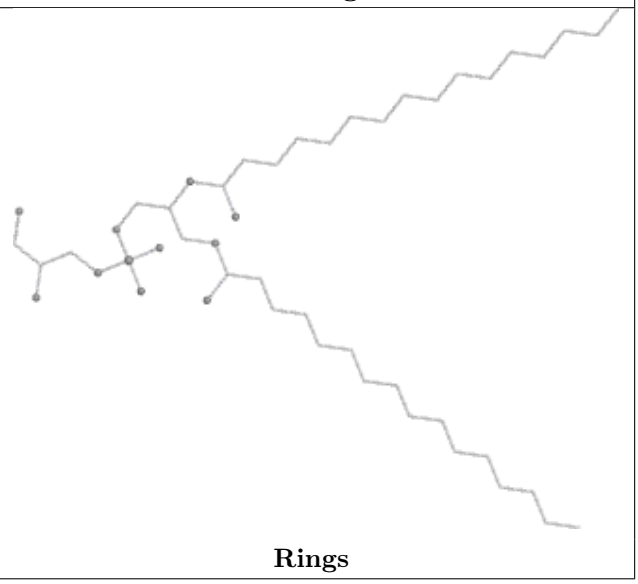
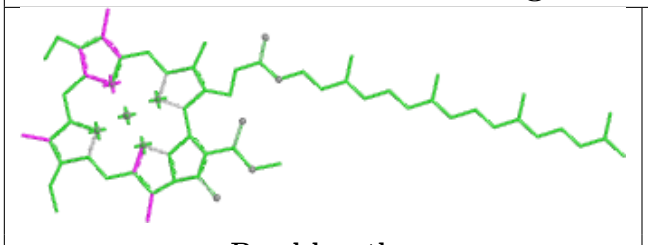


Rings

Ligand CLA P 303



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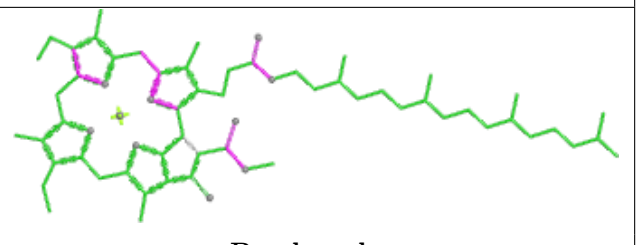
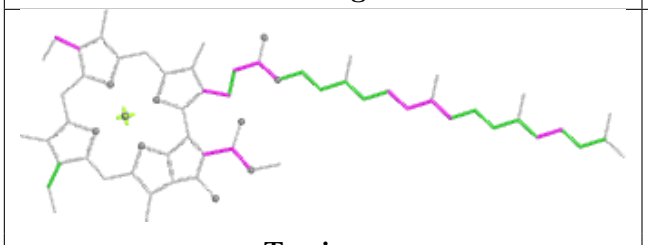


Bond angles



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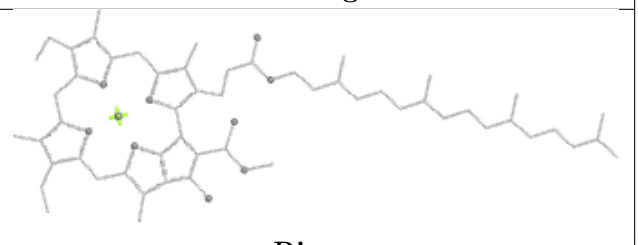
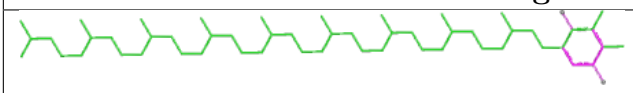


Rings

Ligand PL9 d 404



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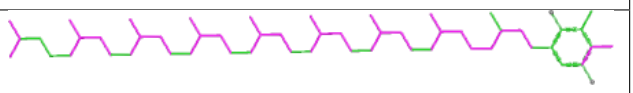

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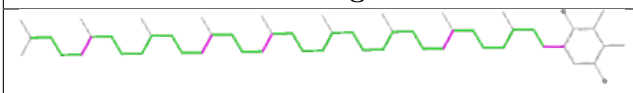

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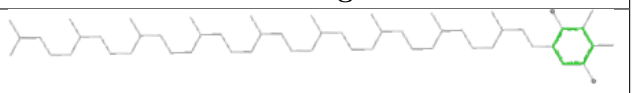
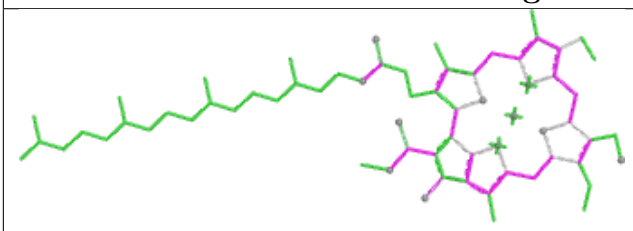


Rings

Ligand CHL U 316



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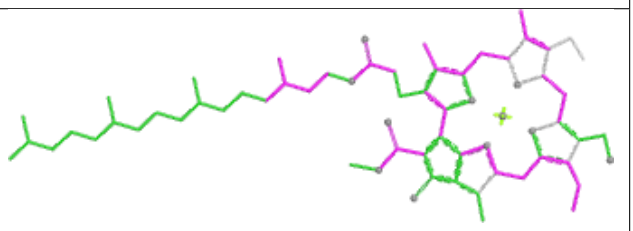

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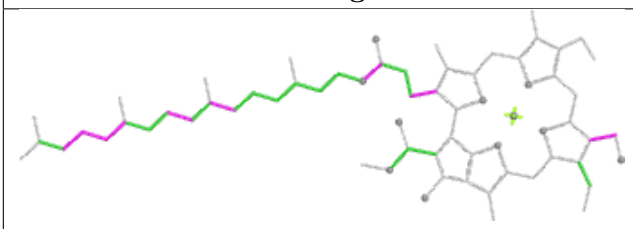

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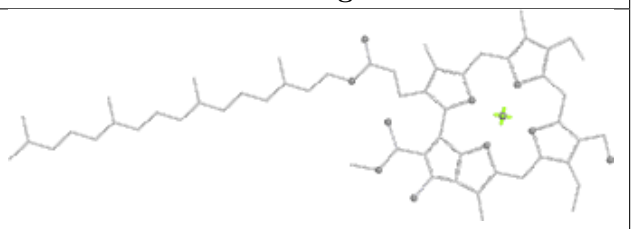
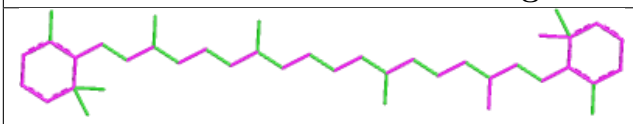


Rings

Ligand BCR D 404



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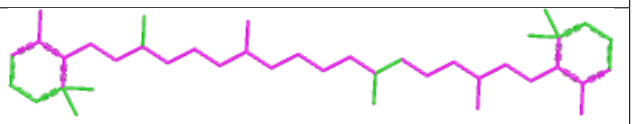

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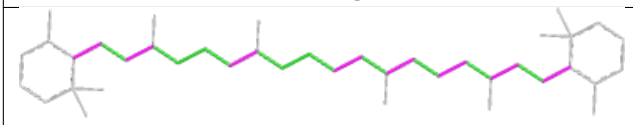

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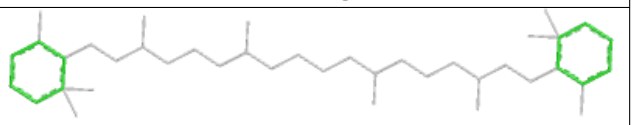
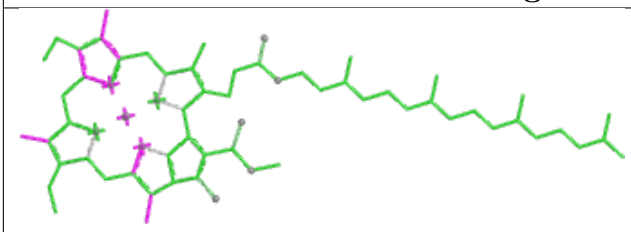


Rings

Ligand CLA A 404



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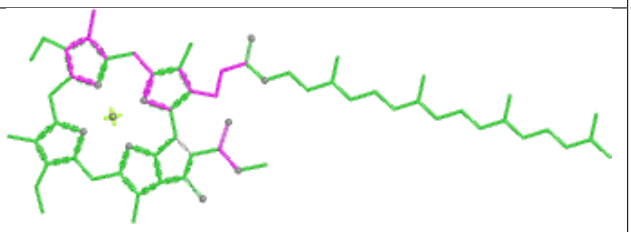
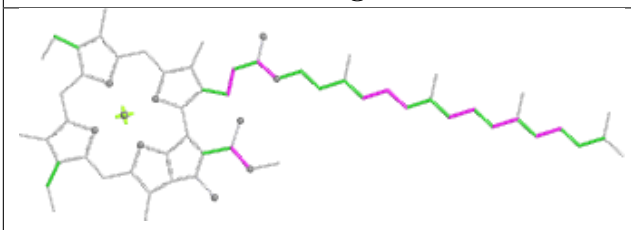


Bond angles



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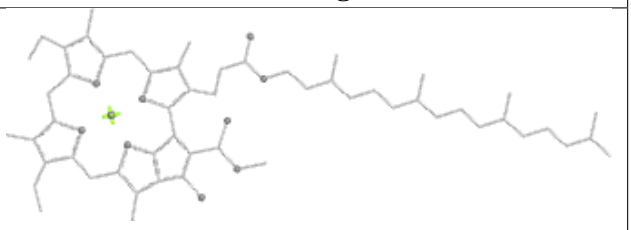
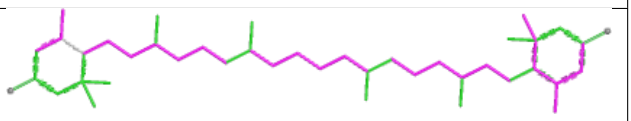


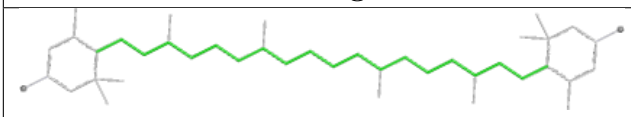
Rings

Ligand LUT 1 310

Bond lengths



Bond angles



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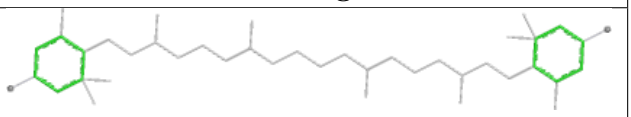
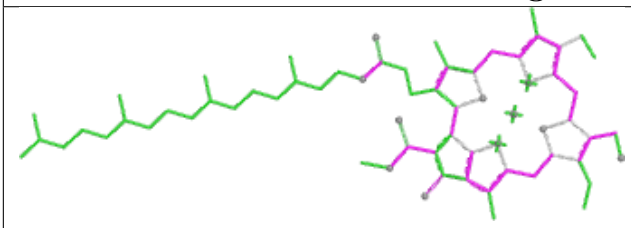


Rings

Ligand CHL v 318



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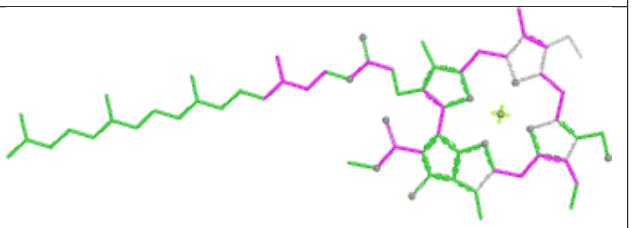
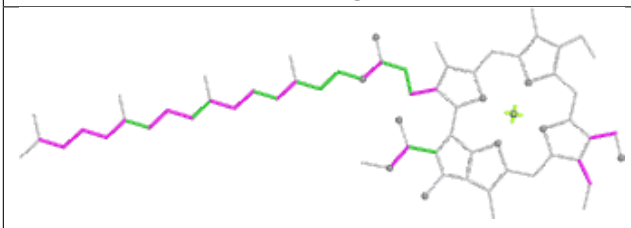


Bond angles



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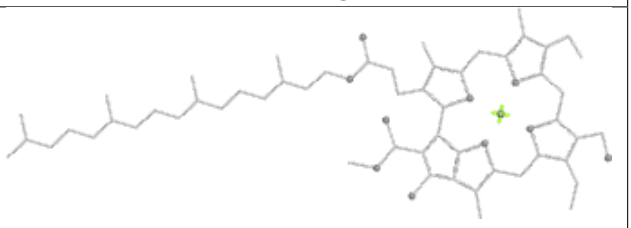
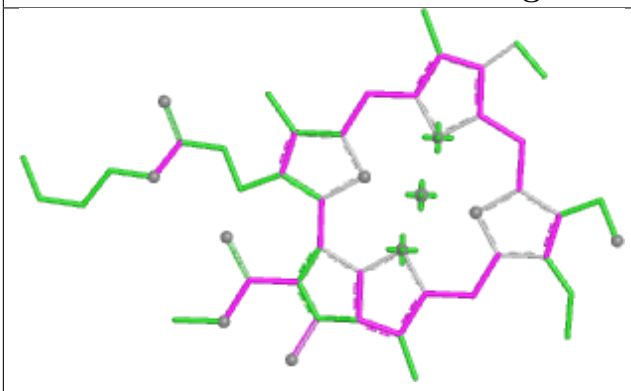


Rings

Ligand CHL N 315



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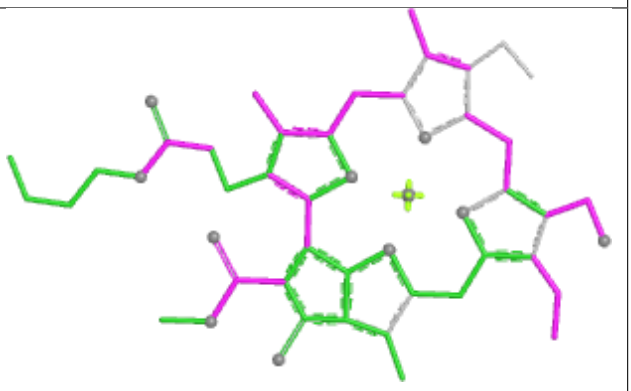
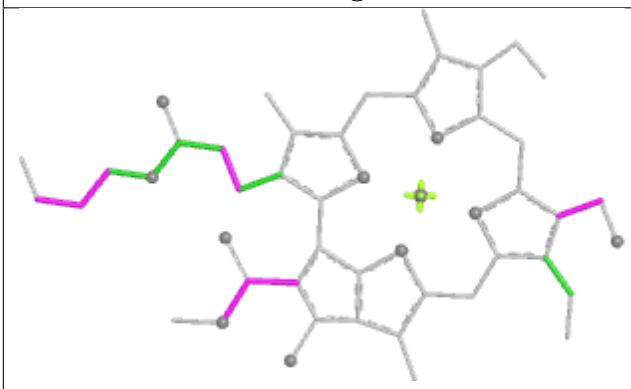


Bond angles



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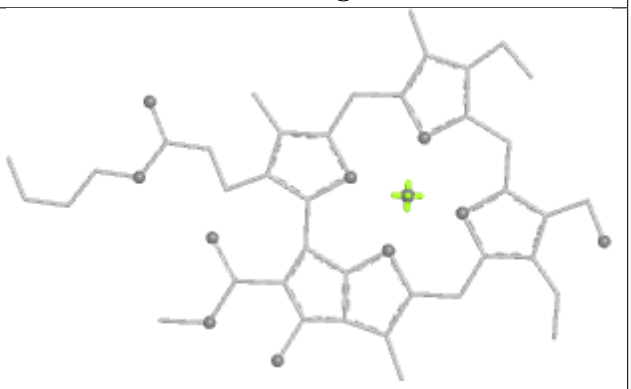
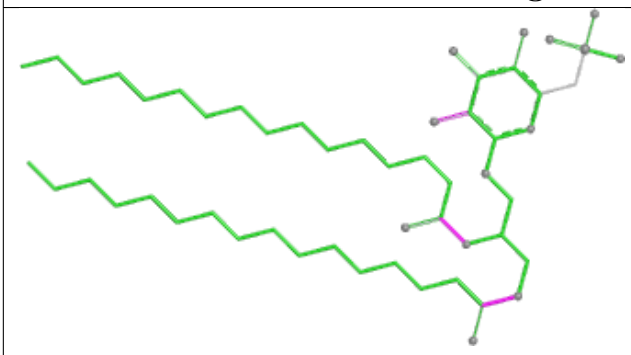


Rings

Ligand SQD L 102



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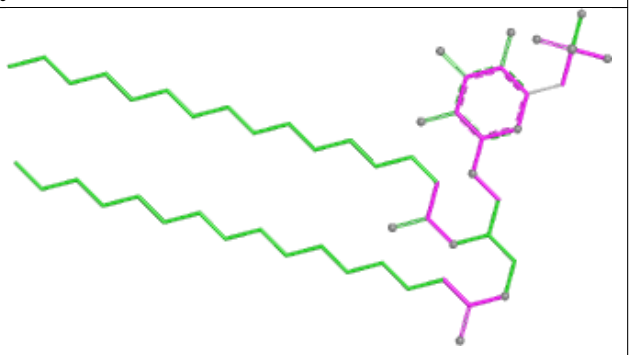
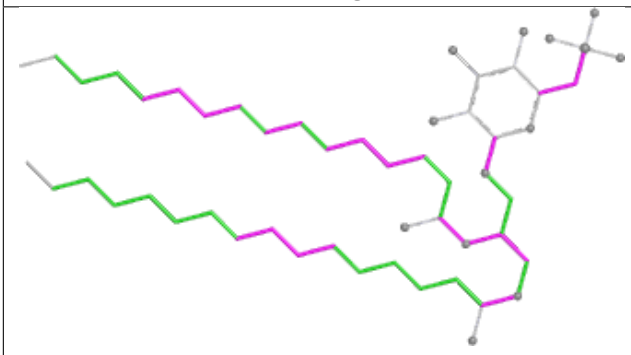


Bond angles



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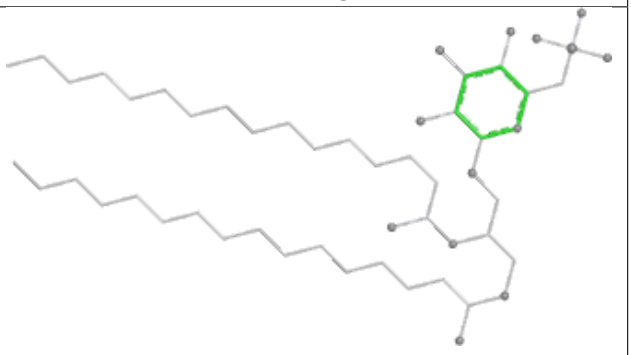
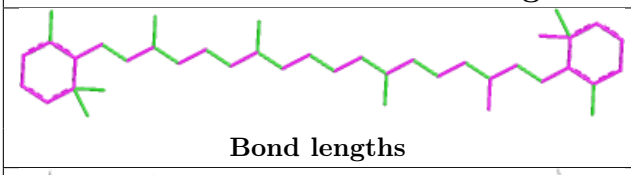


Rings

Ligand BCR C 518



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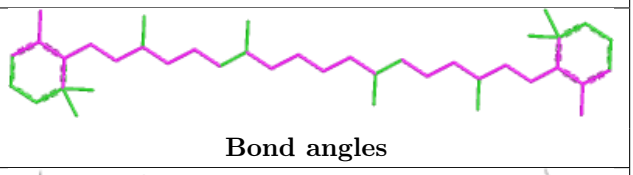
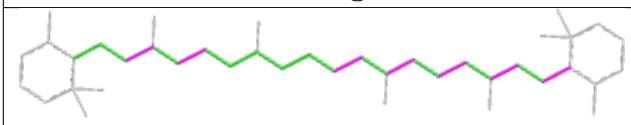
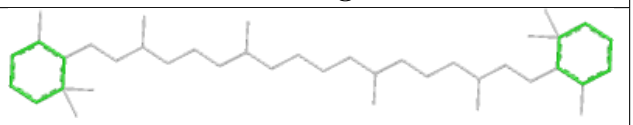


Bond angles

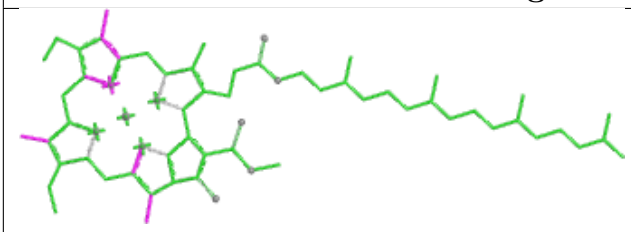


Torsions



Rings

Ligand CLA b 616



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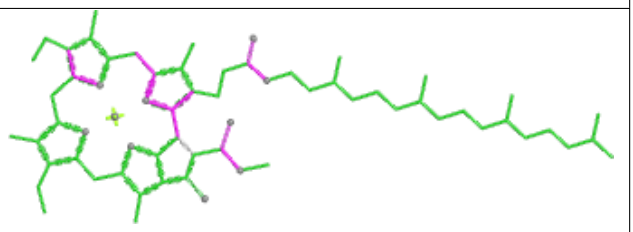

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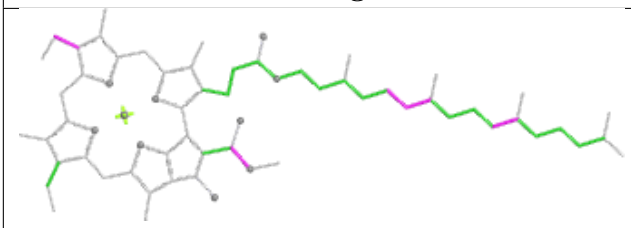

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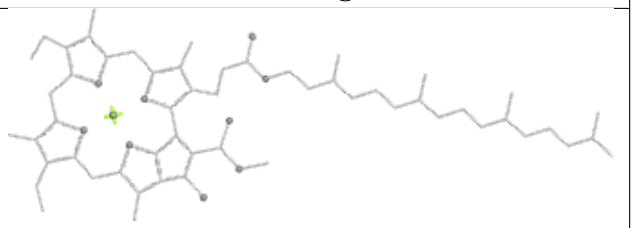
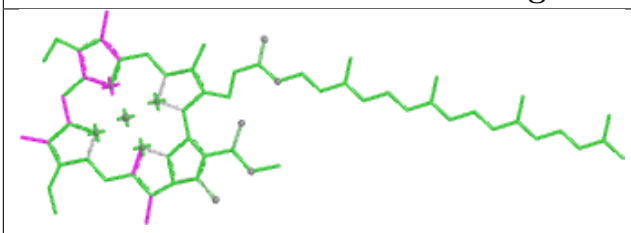


Rings

Ligand CLA 3 301



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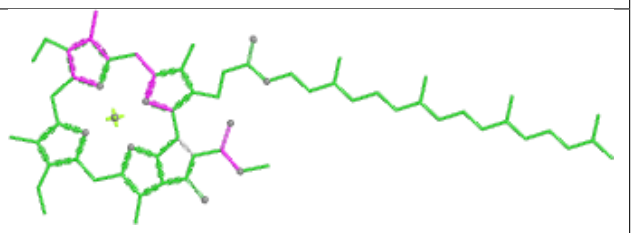

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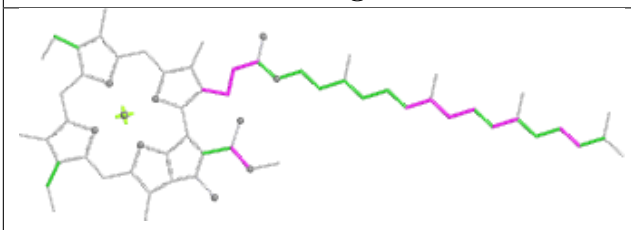

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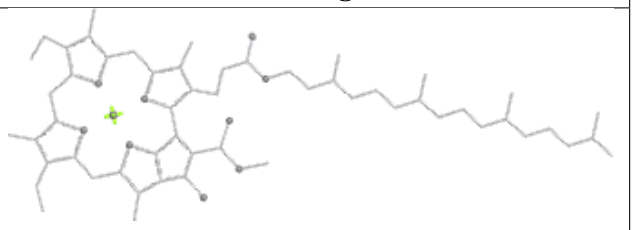
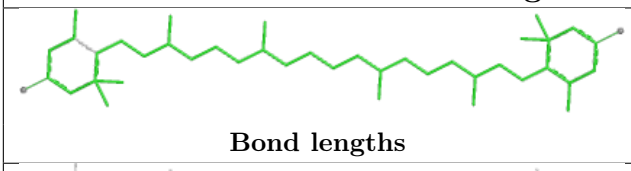


Rings

Ligand LUT V 309



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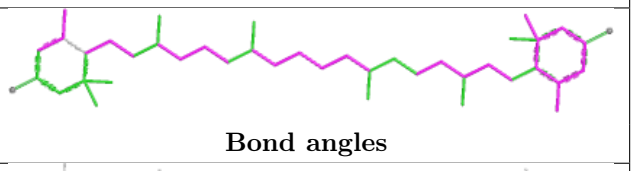
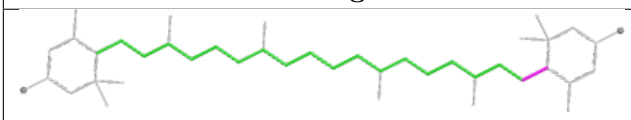


Bond angles



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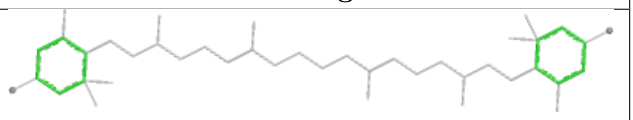
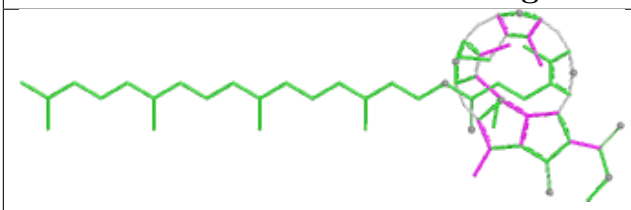


Rings

Ligand PHO A 407



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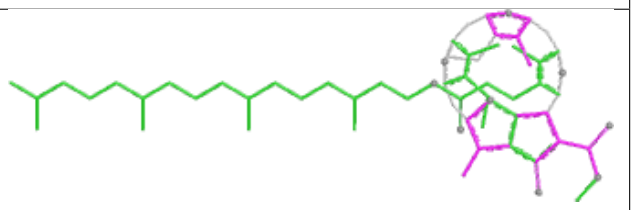
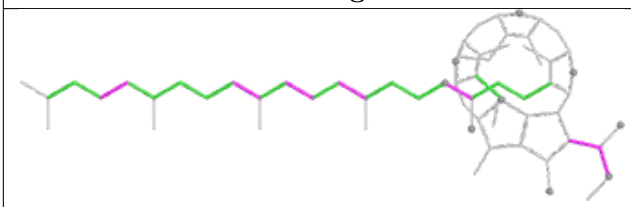


Bond angles



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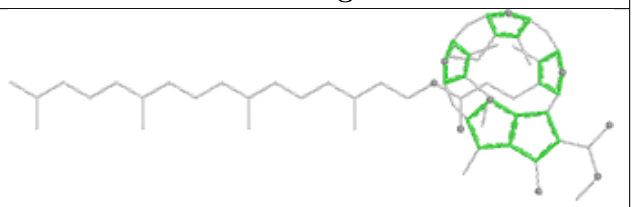
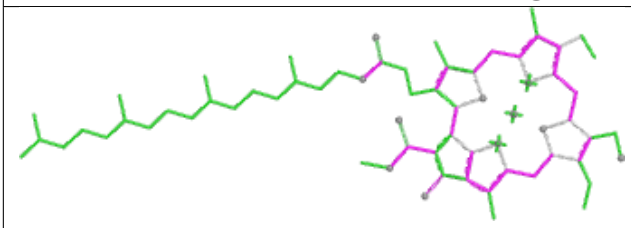


Rings

Ligand CHL 1 313



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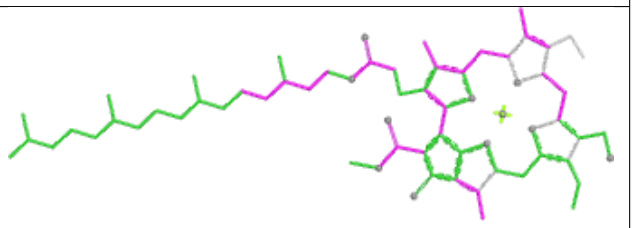
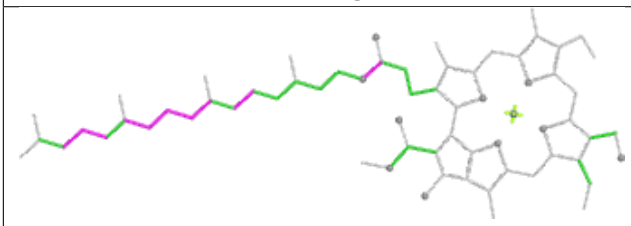


Bond angles



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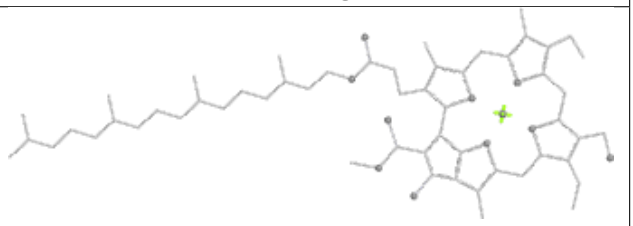
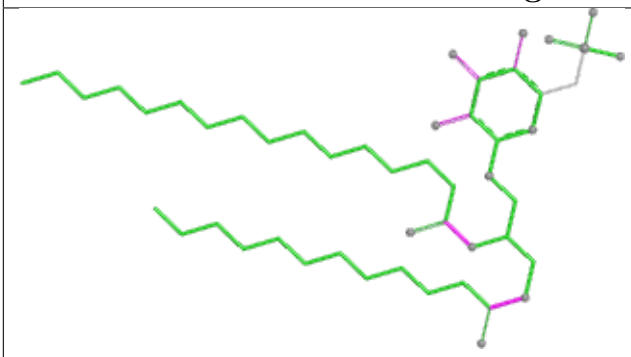


Rings

Ligand SQD C 501



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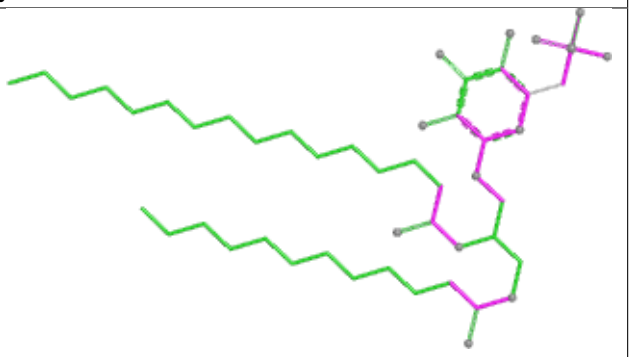

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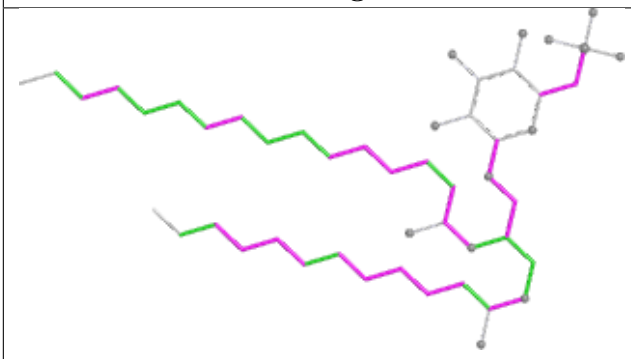

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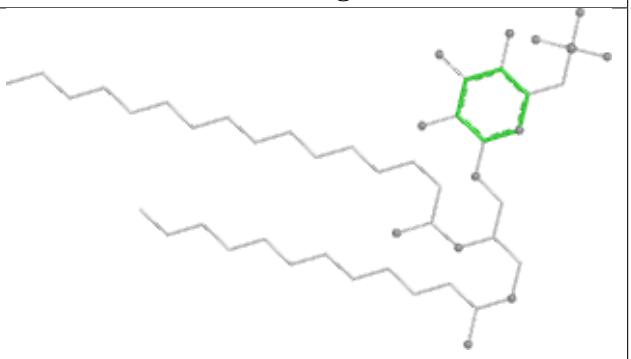
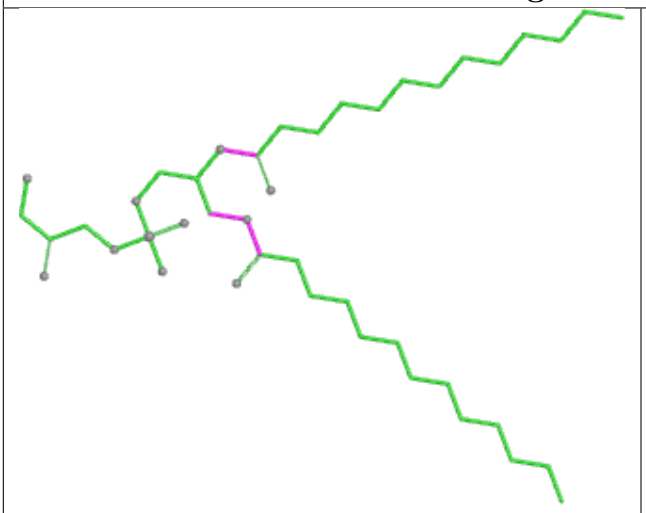


Rings

Ligand LHG a 415



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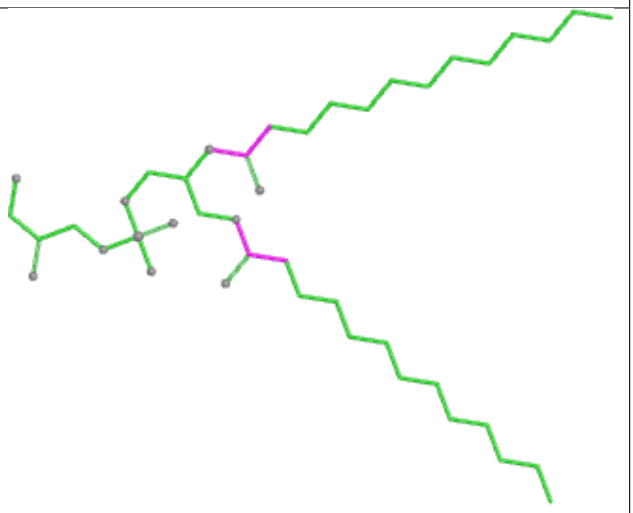

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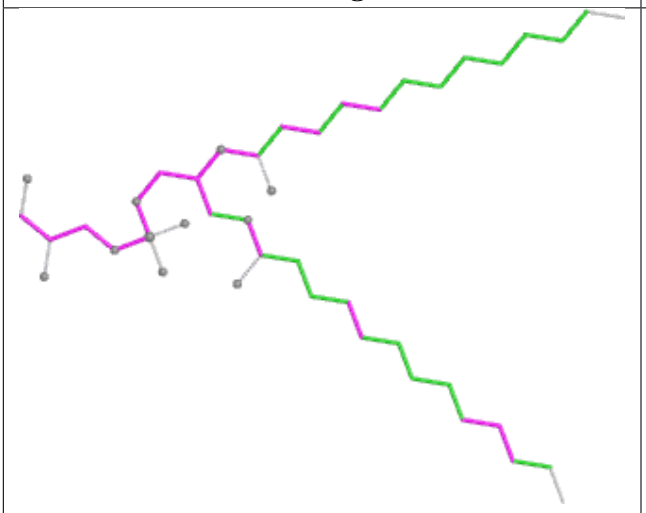

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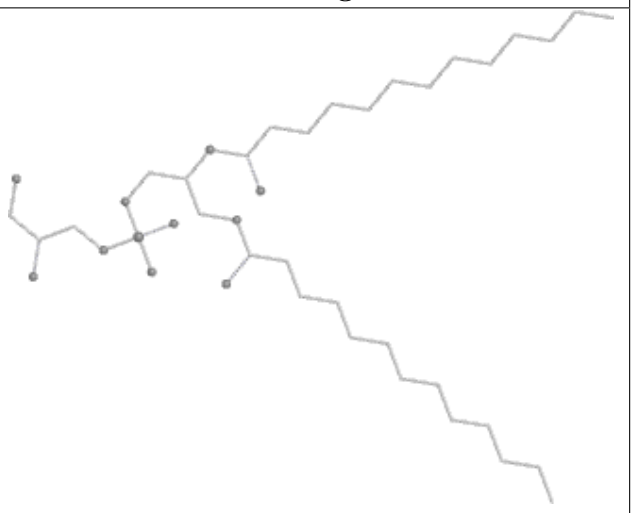
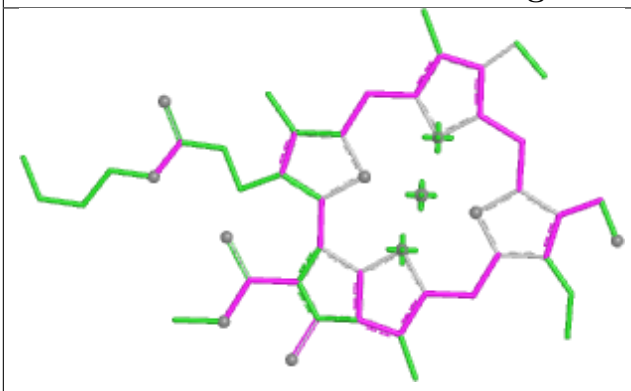


Rings

Ligand CHL q 313



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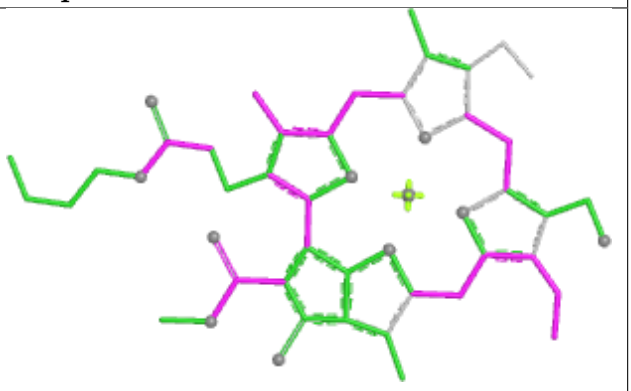

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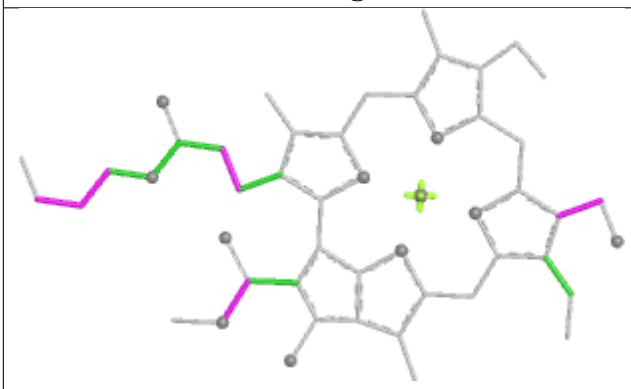

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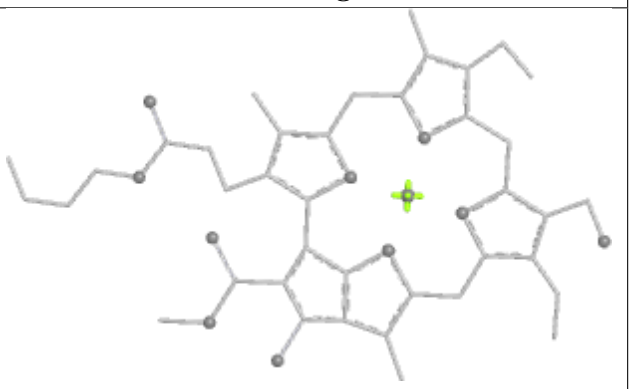
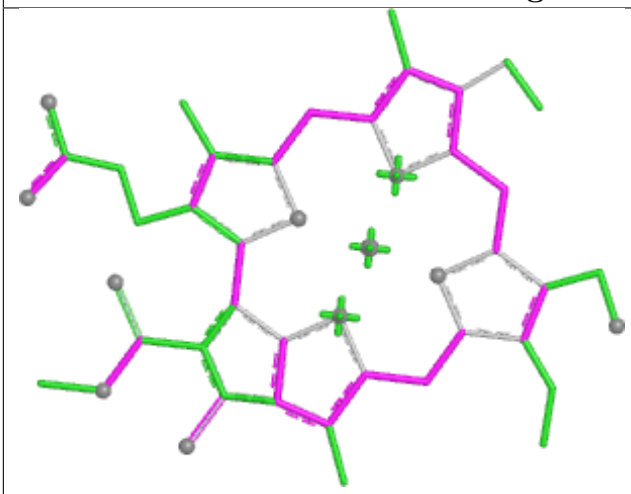


Rings

Ligand CHL S 314



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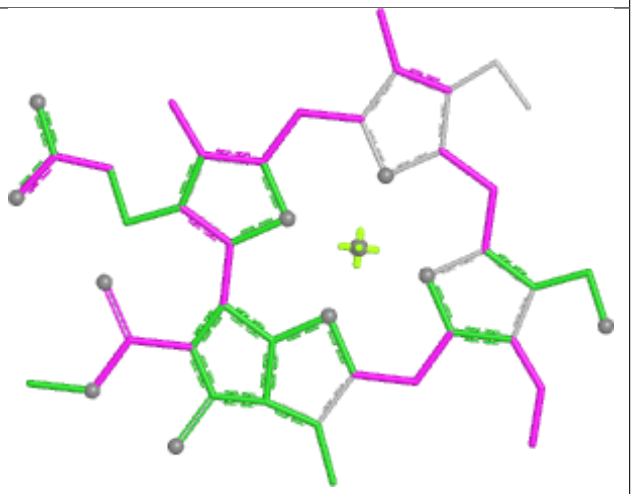
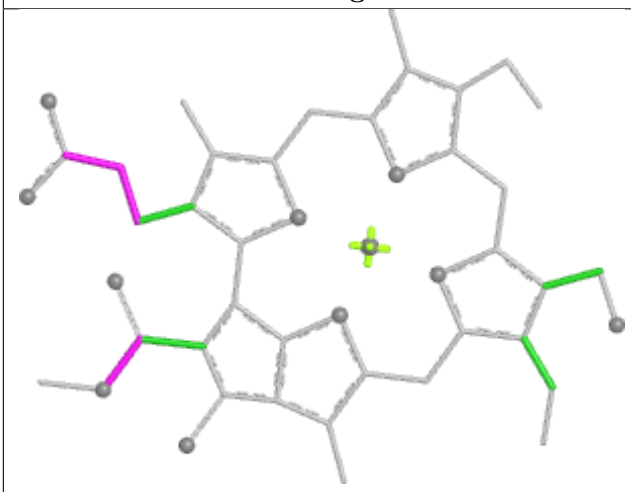


Bond angles



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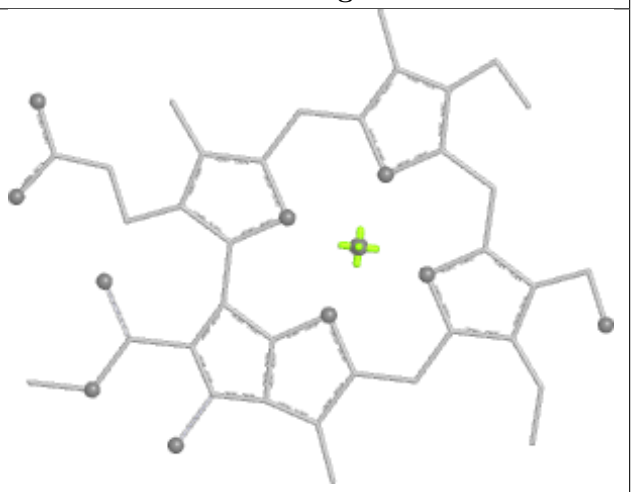
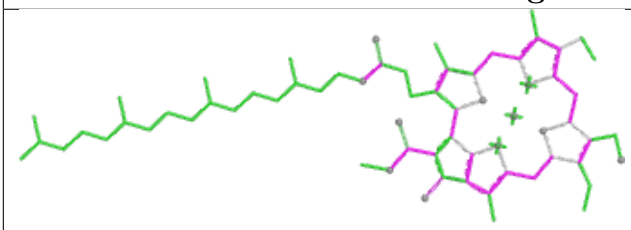


Rings

Ligand CHL v 313



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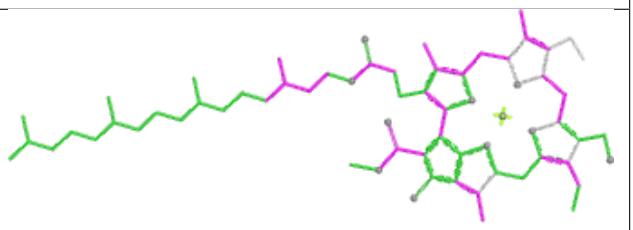
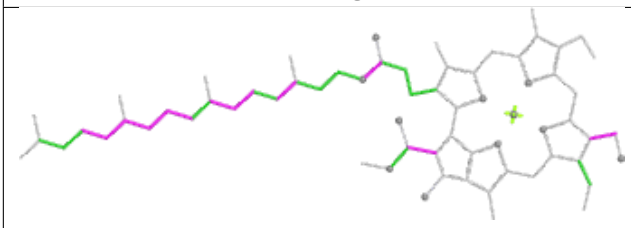


Bond angles



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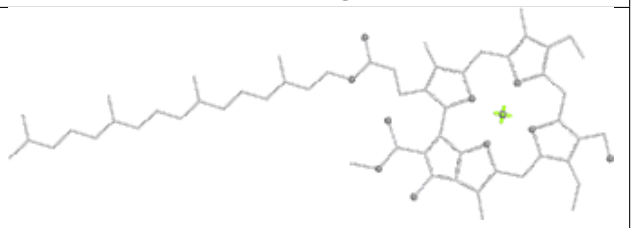
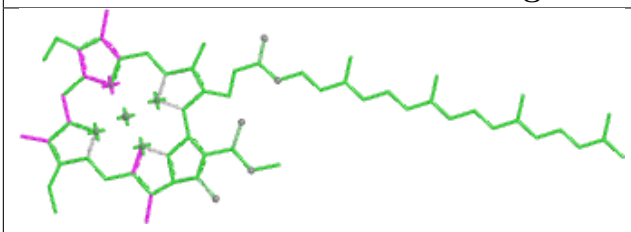


Rings

Ligand CLA N 304



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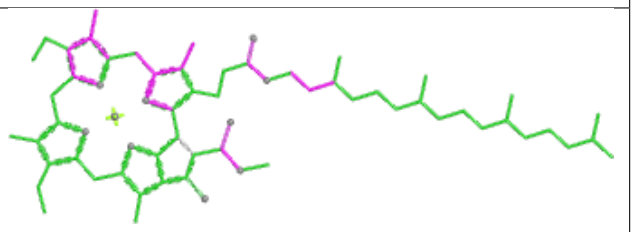
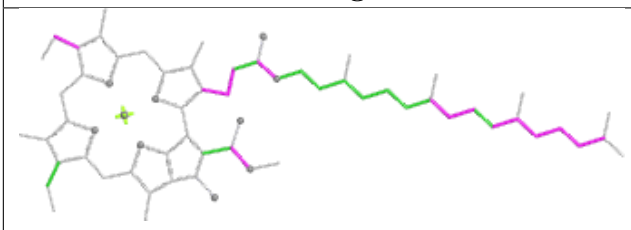
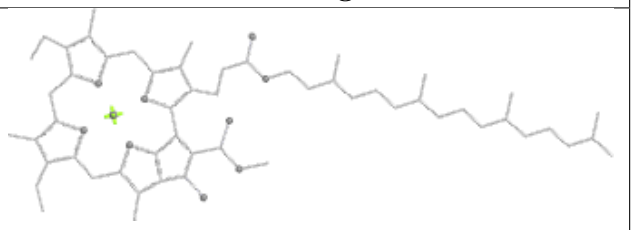


Bond angles

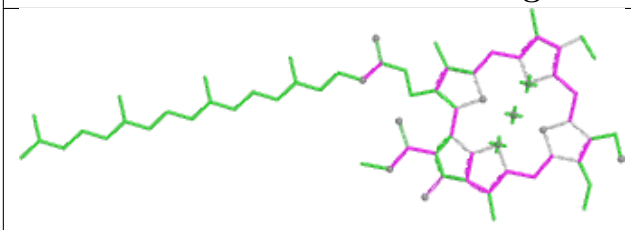


Torsions



Rings

Ligand CHL U 317



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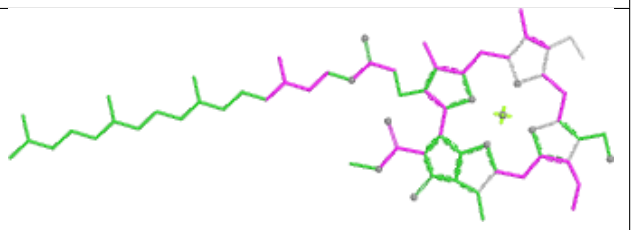
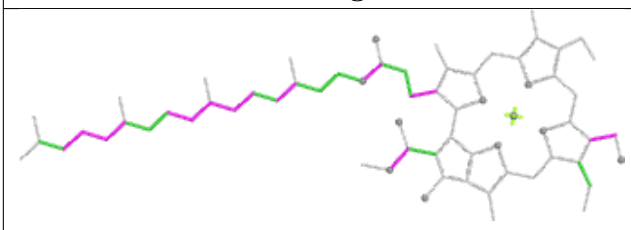
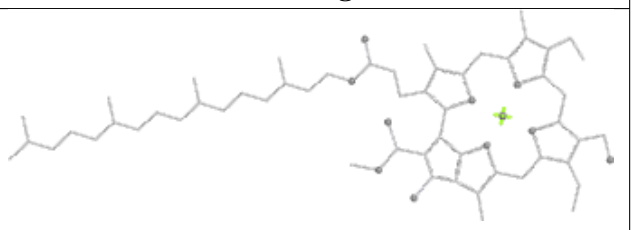


Bond angles

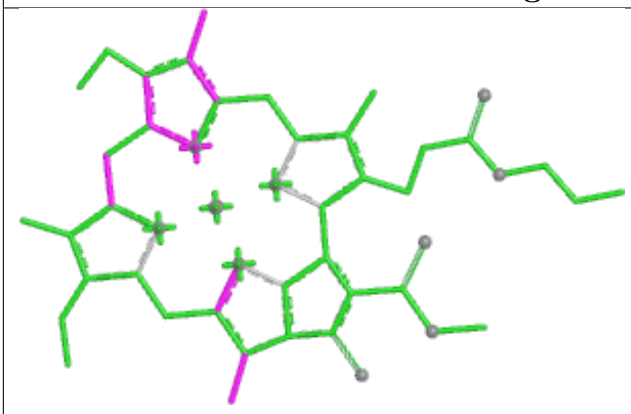


Torsions



Rings

Ligand CLA Q 308



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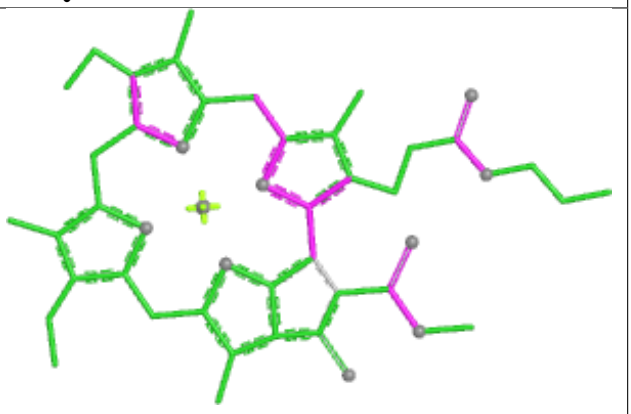
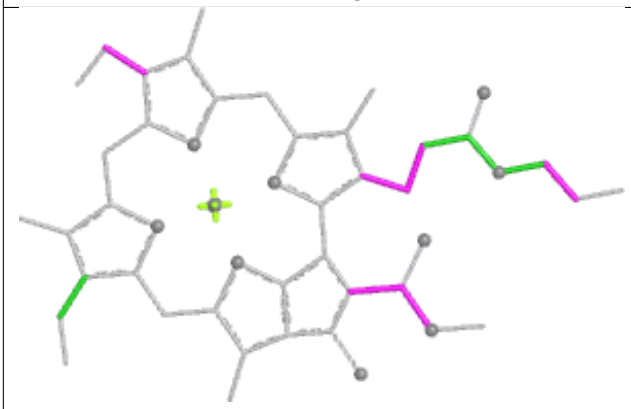
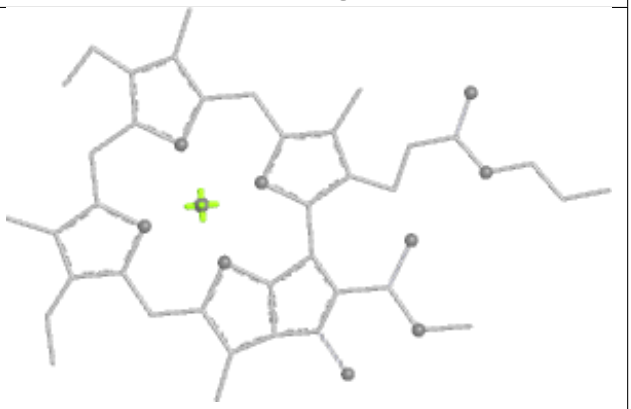


Bond angles

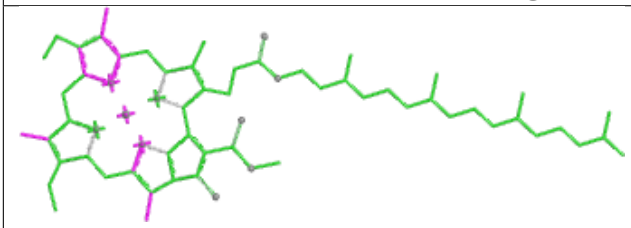


Torsions

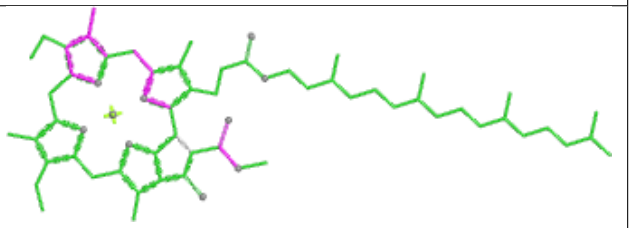


Rings

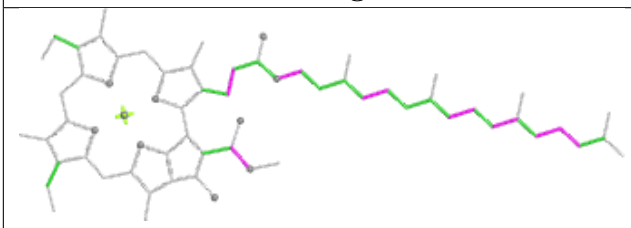
Ligand CLA B 609



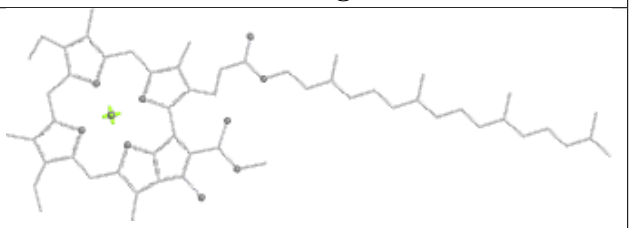
Bond lengths



Bond angles

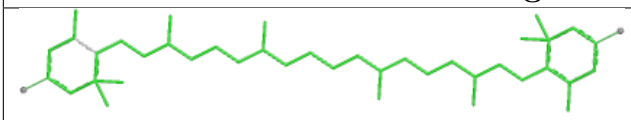


Torsions

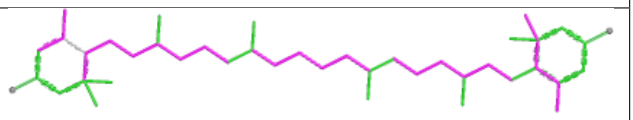


Rings

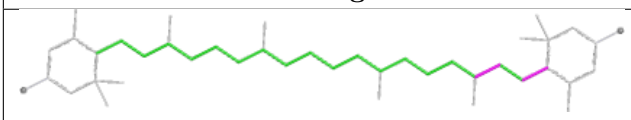
Ligand LUT R 312



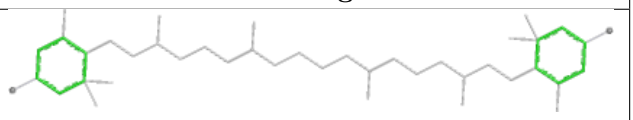
Bond lengths



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.

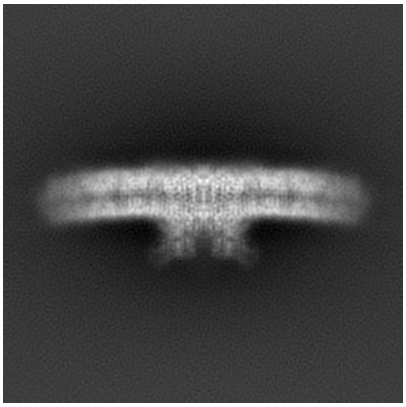
6 Map visualisation

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.

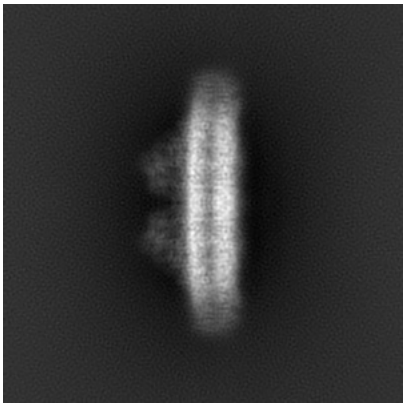
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

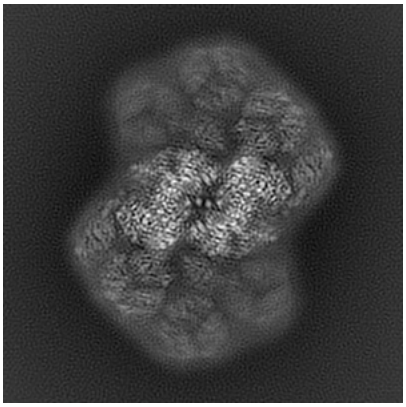
6.1.1 Primary map



X



Y

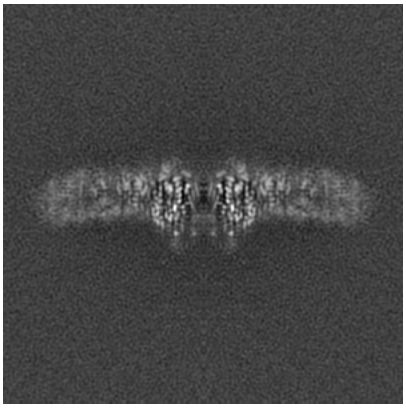


Z

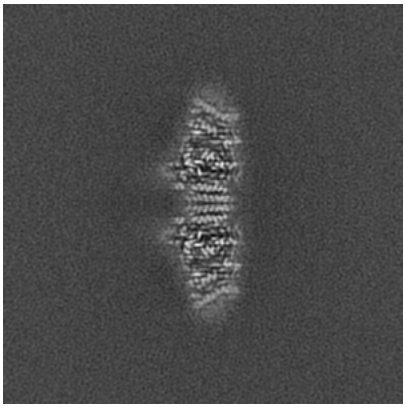
The images above show the map projected in three orthogonal directions.

6.2 Central slices

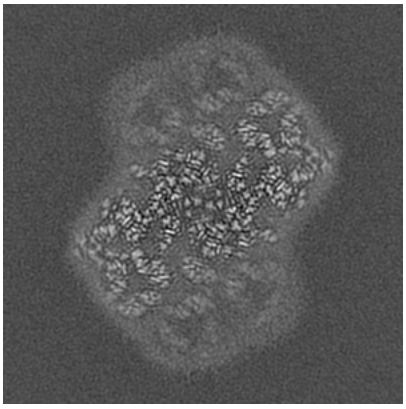
6.2.1 Primary map



X Index: 150



Y Index: 150

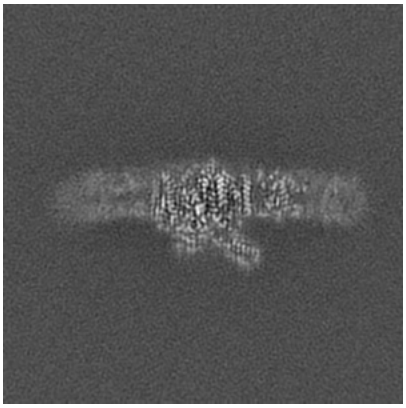


Z Index: 150

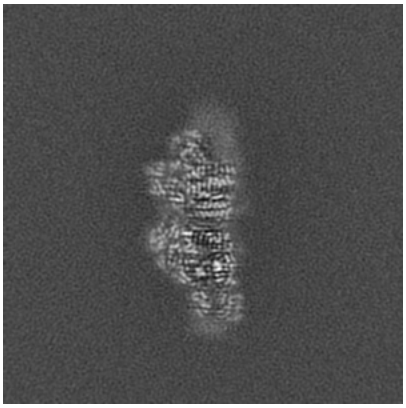
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

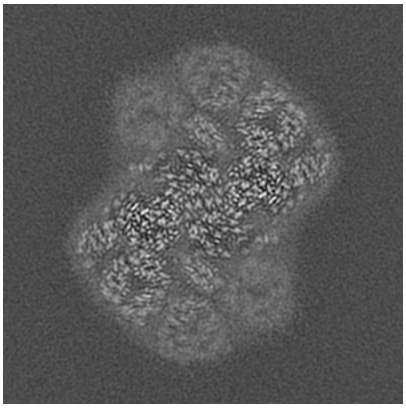
6.3.1 Primary map



X Index: 180



Y Index: 131

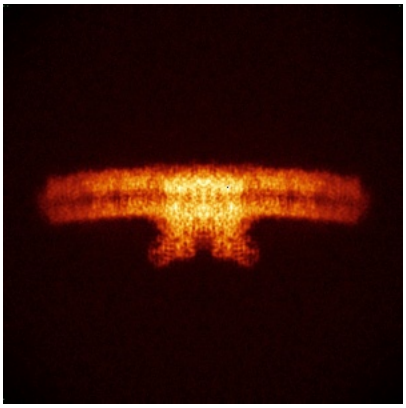


Z Index: 164

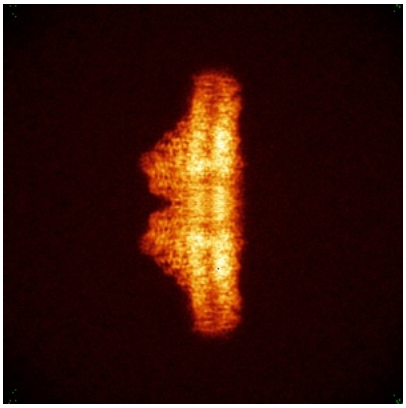
The images above show the largest variance slices of the map in three orthogonal directions.

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

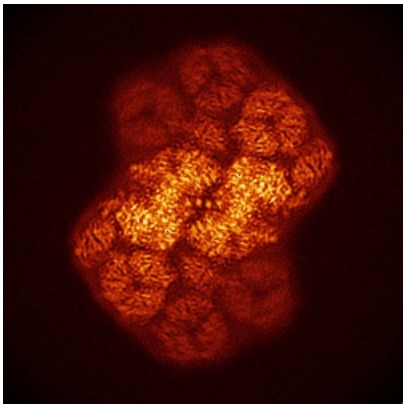
6.4.1 Primary map



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.

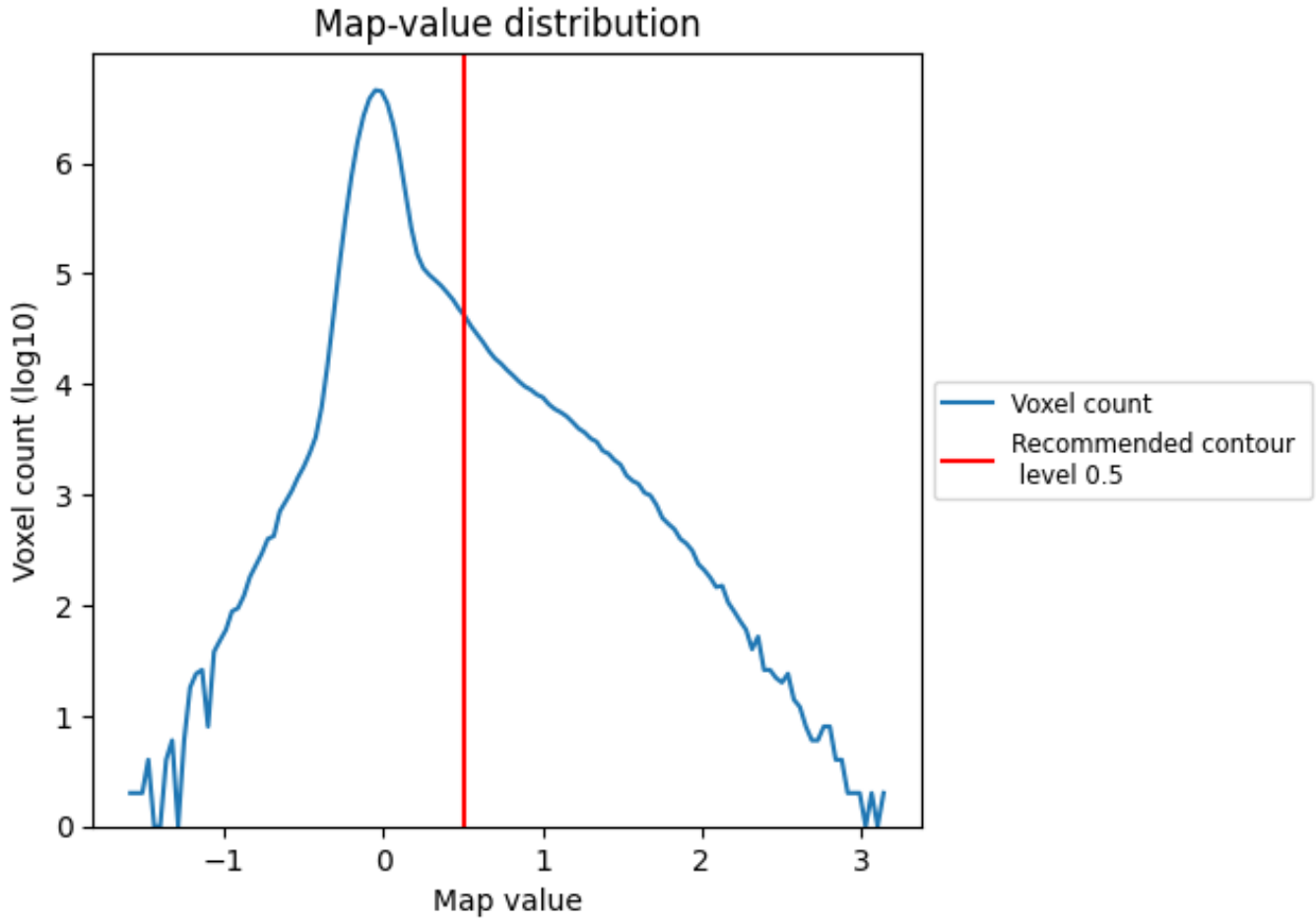
6.6 Mask visualisation (i)

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

7 Map analysis

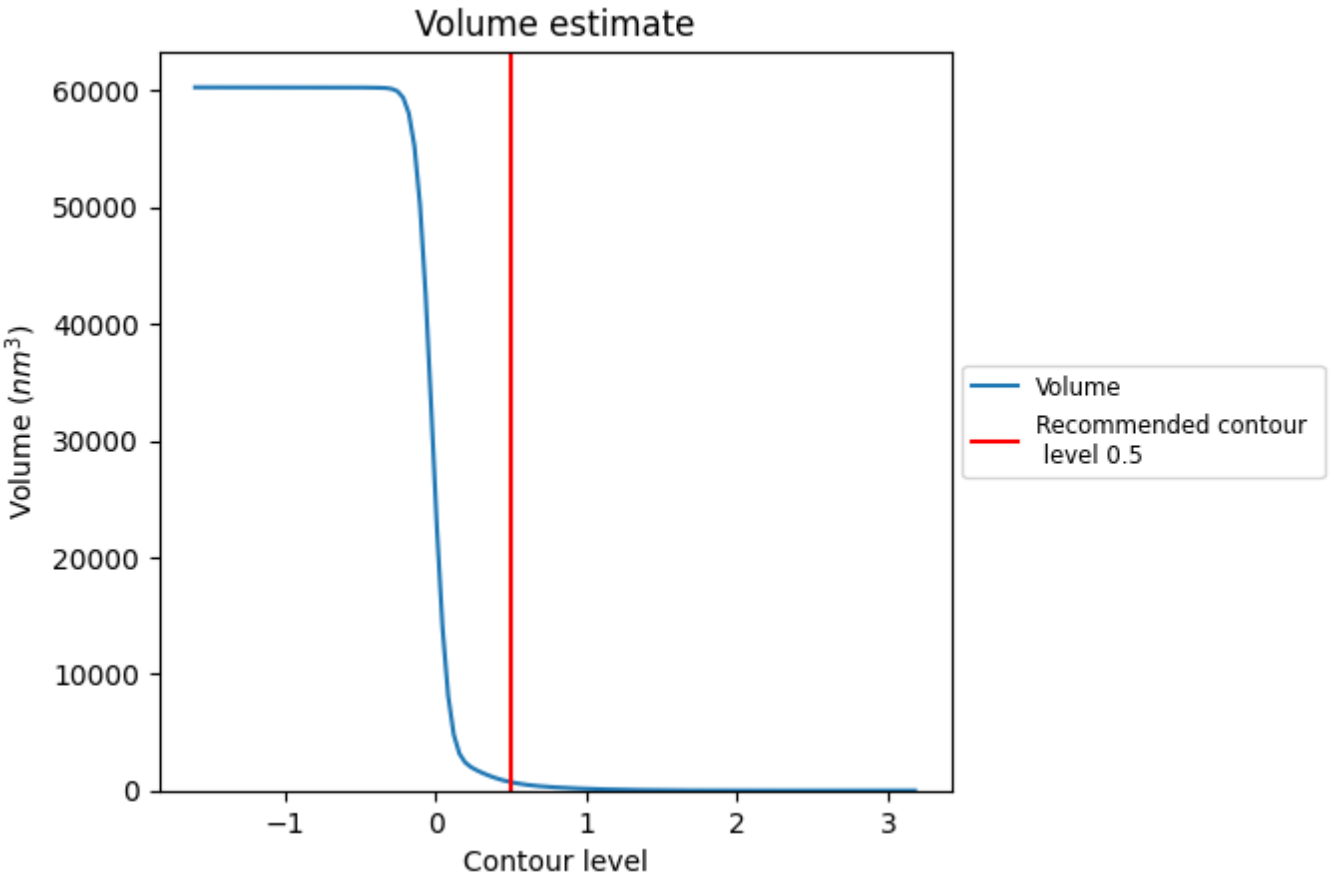
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

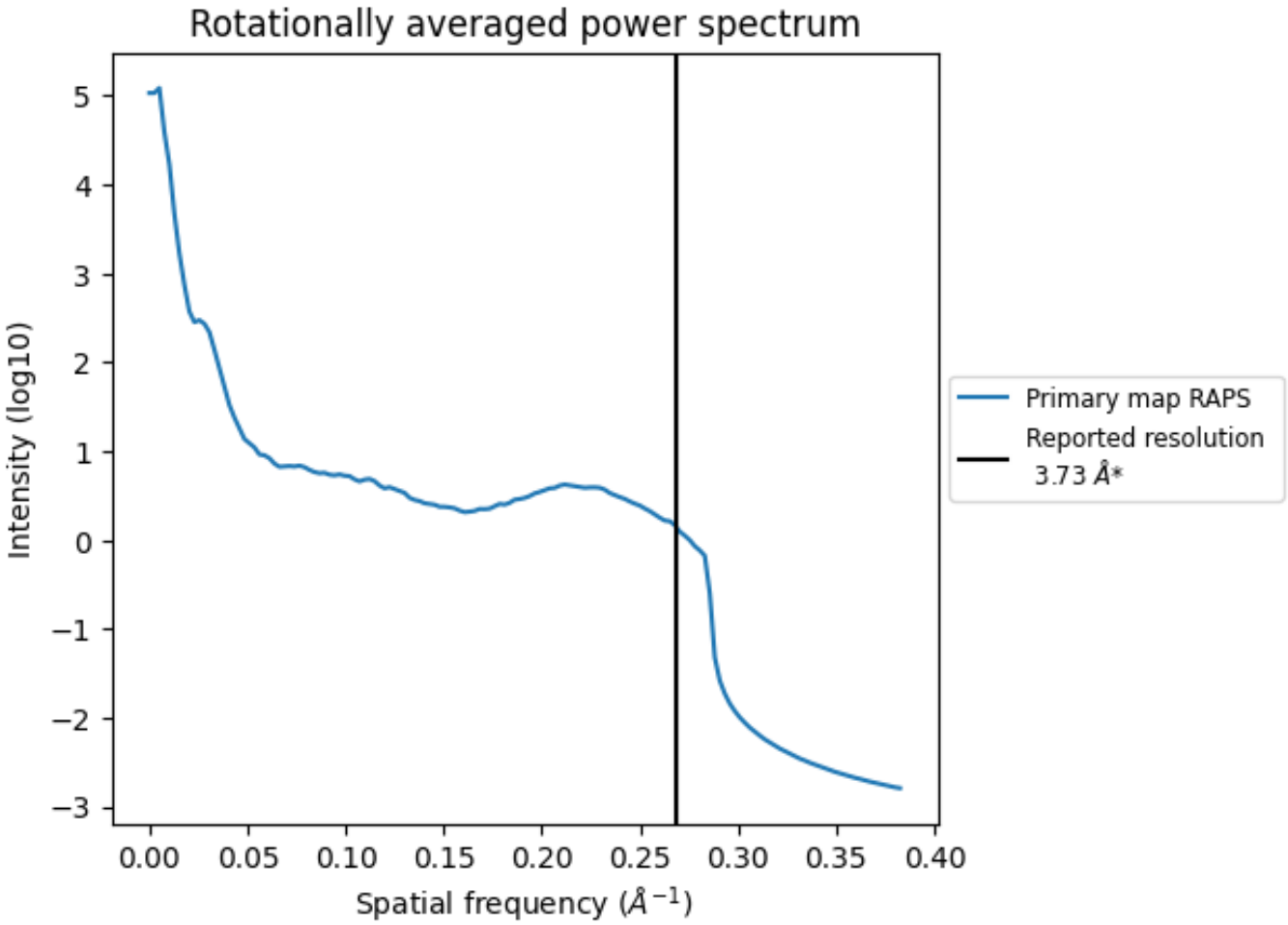
7.2 Volume estimate



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}

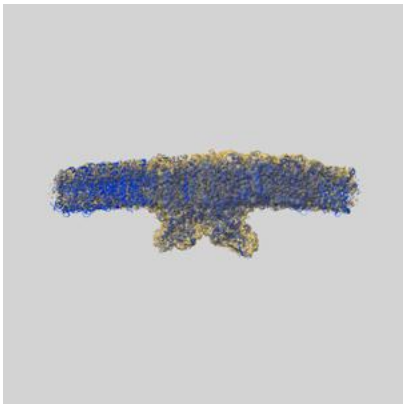
8 Fourier-Shell correlation

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

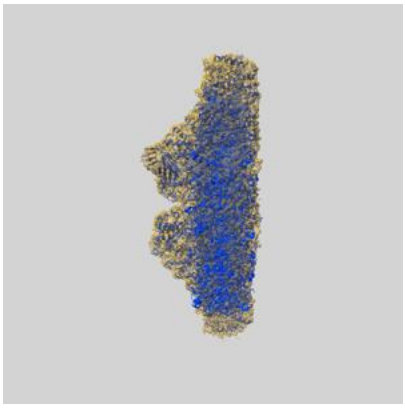
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9957 and PDB model 6KAF. Per-residue inclusion information can be found in section 3 on page 54.

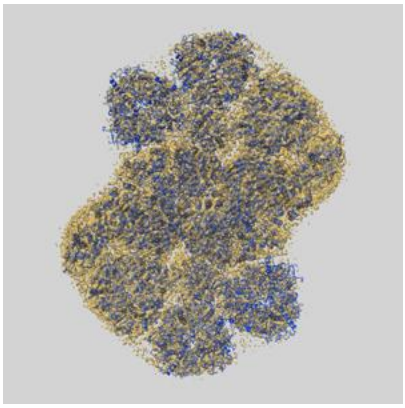
9.1 Map-model overlay



X



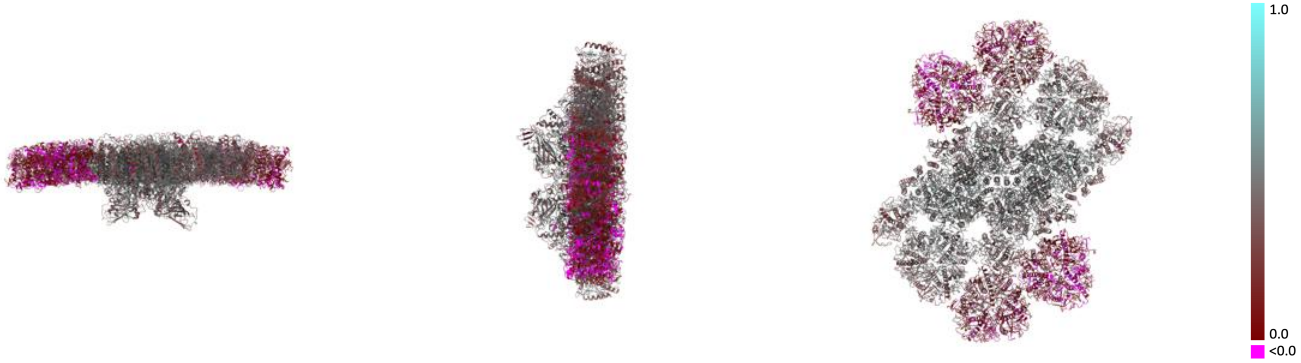
Y



Z

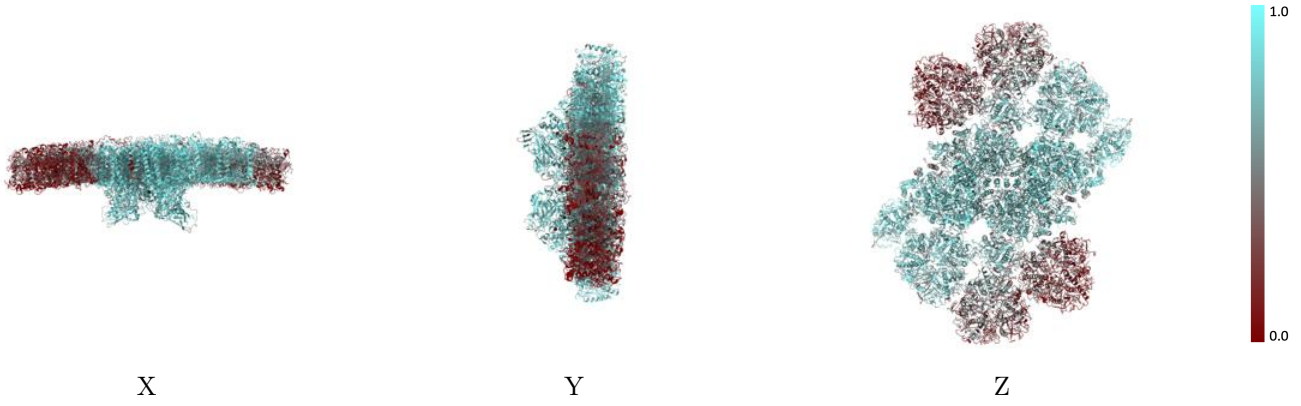
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



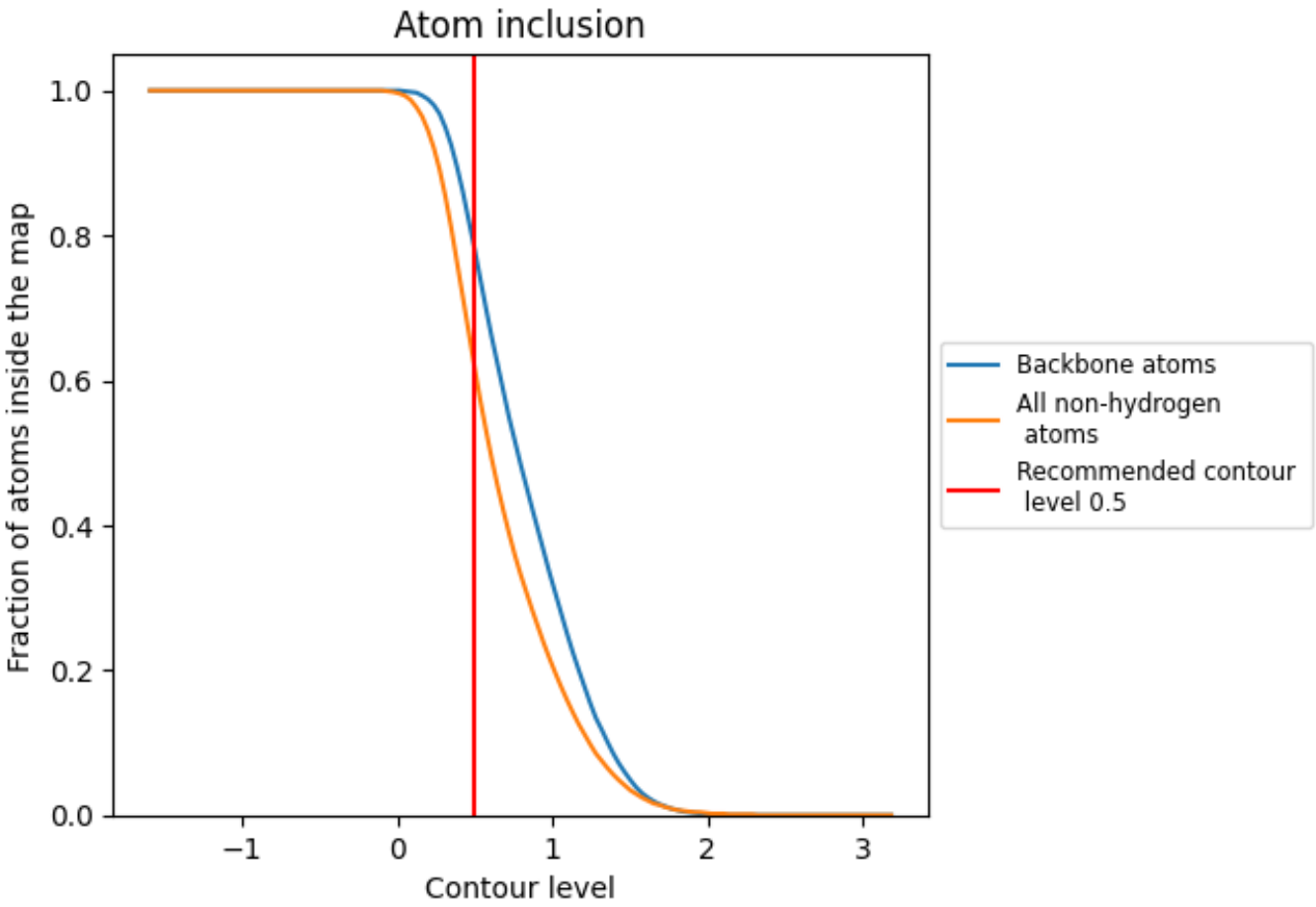
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

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

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