wwPDB EM Validation Summary Report

Jun 11, 2024 – 10:50 AM JST

PDB ID	:	8XR6
EMDB ID	:	EMD-38596
Title	:	Cryo-EM structure of cryptophyte photosystem II
Authors	:	Li, K.; Zhao, L.S.; Zhang, Y.Z.; Liu, L.N.
Deposited on	:	2024-01-06
Resolution	:	2.53 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:

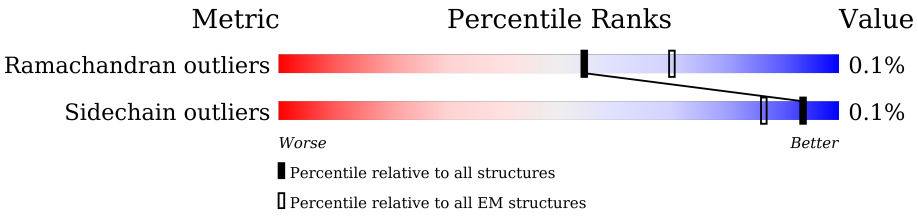
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.53 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	360	93% 7%
1	a	360	92% 7%
2	0	219	80% 19%
2	4	219	80% 19%
3	1	218	80% 20%
3	7	218	80% 20%
4	2	200	94% 6%
4	8	200	94% 6%
5	3	229	80% 19%

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Mol	Chain	Length	Quality of chain
5	9	229	81% 19%
6	5	216	78% 21%
6	g	216	79% 21%
7	6	234	81% 18%
7	p	234	82% 18%
8	B	509	99%
8	b	509	99%
9	C	473	95% 5%
9	c	473	95% 5%
10	D	351	97%
10	d	351	97%
11	E	84	89% 11%
11	e	84	89% 11%
12	F	42	69% 31%
12	f	42	69% 31%
13	H	67	97%
13	h	67	97%
14	I	38	92% 8%
14	i	38	92% 8%
15	J	39	87% 13%
15	j	39	87% 13%
16	K	45	82% 18%
16	k	45	82% 18%
17	L	38	97%
17	l	38	97%

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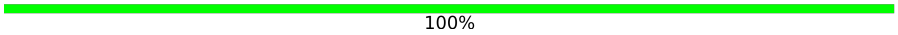
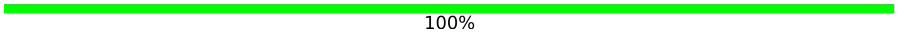
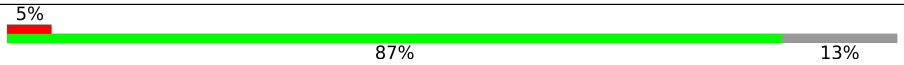
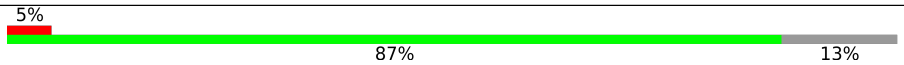
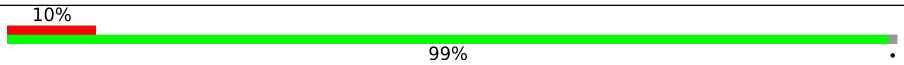
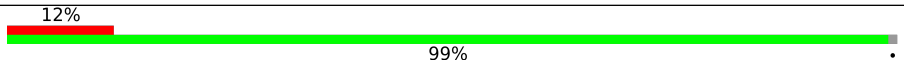
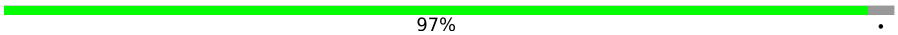
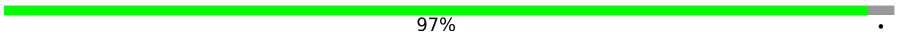
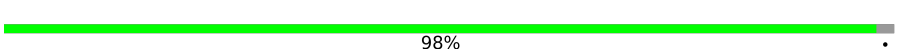
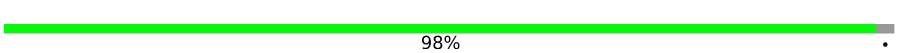
Mol	Chain	Length	Quality of chain
18	M	37	
18	m	37	
19	N	297	
19	n	297	
20	O	300	
20	o	300	
21	Q	144	
21	q	144	
22	T	32	
22	t	32	
23	U	121	
23	u	121	
24	V	163	
24	v	163	
25	W	130	
25	w	130	
26	X	39	
26	x	39	
27	Y	34	
27	y	34	
28	Z	62	
28	z	62	

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
33	CLA	0	301	X	-	-	-
33	CLA	0	302	X	-	-	-
33	CLA	0	303	X	-	-	-
33	CLA	0	304	X	-	-	-
33	CLA	0	306	X	-	-	-
33	CLA	0	307	X	-	-	-
33	CLA	0	308	X	-	-	-
33	CLA	0	309	X	-	-	-
33	CLA	0	310	X	-	-	-
33	CLA	0	311	X	-	-	-
33	CLA	1	301	X	-	-	-
33	CLA	1	302	X	-	-	-
33	CLA	1	303	X	-	-	-
33	CLA	1	304	X	-	-	-
33	CLA	1	305	X	-	-	-
33	CLA	1	306	X	-	-	-
33	CLA	1	307	X	-	-	-
33	CLA	1	308	X	-	-	-
33	CLA	1	309	X	-	-	-
33	CLA	2	301	X	-	-	-
33	CLA	2	302	X	-	-	-
33	CLA	2	303	X	-	-	-
33	CLA	2	304	X	-	-	-
33	CLA	2	305	X	-	-	-
33	CLA	2	306	X	-	-	-
33	CLA	2	307	X	-	-	-
33	CLA	2	308	X	-	-	-
33	CLA	2	310	X	-	-	-
33	CLA	3	303	X	-	-	-
33	CLA	3	304	X	-	-	-
33	CLA	3	305	X	-	-	-
33	CLA	3	306	X	-	-	-
33	CLA	3	307	X	-	-	-
33	CLA	3	308	X	-	-	-
33	CLA	3	309	X	-	-	-
33	CLA	3	310	X	-	-	-
33	CLA	3	312	X	-	-	-
33	CLA	3	313	X	-	-	-
33	CLA	3	314	X	-	-	-
33	CLA	3	315	X	-	-	-
33	CLA	4	301	X	-	-	-
33	CLA	4	302	X	-	-	-
33	CLA	4	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	4	304	X	-	-	-
33	CLA	4	306	X	-	-	-
33	CLA	4	307	X	-	-	-
33	CLA	4	308	X	-	-	-
33	CLA	4	309	X	-	-	-
33	CLA	4	310	X	-	-	-
33	CLA	5	301	X	-	-	-
33	CLA	5	302	X	-	-	-
33	CLA	5	303	X	-	-	-
33	CLA	5	304	X	-	-	-
33	CLA	5	305	X	-	-	-
33	CLA	5	306	X	-	-	-
33	CLA	5	307	X	-	-	-
33	CLA	5	308	X	-	-	-
33	CLA	5	310	X	-	-	-
33	CLA	5	311	X	-	-	-
33	CLA	5	317	X	-	-	-
33	CLA	6	302	X	-	-	-
33	CLA	6	303	X	-	-	-
33	CLA	6	304	X	-	-	-
33	CLA	6	305	X	-	-	-
33	CLA	6	306	X	-	-	-
33	CLA	6	307	X	-	-	-
33	CLA	6	308	X	-	-	-
33	CLA	6	309	X	-	-	-
33	CLA	6	310	X	-	-	-
33	CLA	6	312	X	-	-	-
33	CLA	6	313	X	-	-	-
33	CLA	6	319	X	-	-	-
33	CLA	7	301	X	-	-	-
33	CLA	7	302	X	-	-	-
33	CLA	7	303	X	-	-	-
33	CLA	7	304	X	-	-	-
33	CLA	7	305	X	-	-	-
33	CLA	7	306	X	-	-	-
33	CLA	7	307	X	-	-	-
33	CLA	7	308	X	-	-	-
33	CLA	7	309	X	-	-	-
33	CLA	8	301	X	-	-	-
33	CLA	8	302	X	-	-	-
33	CLA	8	303	X	-	-	-
33	CLA	8	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	8	305	X	-	-	-
33	CLA	8	306	X	-	-	-
33	CLA	8	307	X	-	-	-
33	CLA	8	308	X	-	-	-
33	CLA	8	310	X	-	-	-
33	CLA	9	303	X	-	-	-
33	CLA	9	304	X	-	-	-
33	CLA	9	305	X	-	-	-
33	CLA	9	306	X	-	-	-
33	CLA	9	307	X	-	-	-
33	CLA	9	308	X	-	-	-
33	CLA	9	309	X	-	-	-
33	CLA	9	310	X	-	-	-
33	CLA	9	312	X	-	-	-
33	CLA	9	313	X	-	-	-
33	CLA	9	314	X	-	-	-
33	CLA	9	315	X	-	-	-
33	CLA	A	405	X	-	-	-
33	CLA	A	406	X	-	-	-
33	CLA	A	408	X	-	-	-
33	CLA	A	412	X	-	-	-
33	CLA	B	602	X	-	-	-
33	CLA	B	603	X	-	-	-
33	CLA	B	604	X	-	-	-
33	CLA	B	605	X	-	-	-
33	CLA	B	606	X	-	-	-
33	CLA	B	607	X	-	-	-
33	CLA	B	608	X	-	-	-
33	CLA	B	609	X	-	-	-
33	CLA	B	610	X	-	-	-
33	CLA	B	611	X	-	-	-
33	CLA	B	612	X	-	-	-
33	CLA	B	613	X	-	-	-
33	CLA	B	614	X	-	-	-
33	CLA	B	615	X	-	-	-
33	CLA	B	616	X	-	-	-
33	CLA	B	617	X	-	-	-
33	CLA	B	618	X	-	-	-
33	CLA	C	502	X	-	-	-
33	CLA	C	503	X	-	-	-
33	CLA	C	504	X	-	-	-
33	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	C	506	X	-	-	-
33	CLA	C	507	X	-	-	-
33	CLA	C	508	X	-	-	-
33	CLA	C	509	X	-	-	-
33	CLA	C	510	X	-	-	-
33	CLA	C	511	X	-	-	-
33	CLA	C	512	X	-	-	-
33	CLA	C	513	X	-	-	-
33	CLA	C	514	X	-	-	-
33	CLA	D	404	X	-	-	-
33	CLA	D	405	X	-	-	-
33	CLA	N	301	X	-	-	-
33	CLA	N	302	X	-	-	-
33	CLA	N	303	X	-	-	-
33	CLA	N	304	X	-	-	-
33	CLA	N	305	X	-	-	-
33	CLA	N	306	X	-	-	-
33	CLA	N	307	X	-	-	-
33	CLA	a	405	X	-	-	-
33	CLA	a	406	X	-	-	-
33	CLA	a	408	X	-	-	-
33	CLA	a	412	X	-	-	-
33	CLA	b	602	X	-	-	-
33	CLA	b	603	X	-	-	-
33	CLA	b	604	X	-	-	-
33	CLA	b	605	X	-	-	-
33	CLA	b	606	X	-	-	-
33	CLA	b	607	X	-	-	-
33	CLA	b	608	X	-	-	-
33	CLA	b	609	X	-	-	-
33	CLA	b	610	X	-	-	-
33	CLA	b	611	X	-	-	-
33	CLA	b	612	X	-	-	-
33	CLA	b	613	X	-	-	-
33	CLA	b	614	X	-	-	-
33	CLA	b	615	X	-	-	-
33	CLA	b	616	X	-	-	-
33	CLA	b	617	X	-	-	-
33	CLA	b	618	X	-	-	-
33	CLA	c	502	X	-	-	-
33	CLA	c	503	X	-	-	-
33	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	c	505	X	-	-	-
33	CLA	c	506	X	-	-	-
33	CLA	c	507	X	-	-	-
33	CLA	c	508	X	-	-	-
33	CLA	c	509	X	-	-	-
33	CLA	c	510	X	-	-	-
33	CLA	c	511	X	-	-	-
33	CLA	c	512	X	-	-	-
33	CLA	c	513	X	-	-	-
33	CLA	c	514	X	-	-	-
33	CLA	d	404	X	-	-	-
33	CLA	d	405	X	-	-	-
33	CLA	g	301	X	-	-	-
33	CLA	g	302	X	-	-	-
33	CLA	g	303	X	-	-	-
33	CLA	g	304	X	-	-	-
33	CLA	g	305	X	-	-	-
33	CLA	g	306	X	-	-	-
33	CLA	g	307	X	-	-	-
33	CLA	g	308	X	-	-	-
33	CLA	g	310	X	-	-	-
33	CLA	g	311	X	-	-	-
33	CLA	g	317	X	-	-	-
33	CLA	n	301	X	-	-	-
33	CLA	n	302	X	-	-	-
33	CLA	n	303	X	-	-	-
33	CLA	n	304	X	-	-	-
33	CLA	n	305	X	-	-	-
33	CLA	n	306	X	-	-	-
33	CLA	p	302	X	-	-	-
33	CLA	p	303	X	-	-	-
33	CLA	p	304	X	-	-	-
33	CLA	p	305	X	-	-	-
33	CLA	p	306	X	-	-	-
33	CLA	p	307	X	-	-	-
33	CLA	p	308	X	-	-	-
33	CLA	p	309	X	-	-	-
33	CLA	p	310	X	-	-	-
33	CLA	p	312	X	-	-	-
33	CLA	p	313	X	-	-	-
33	CLA	p	319	X	-	-	-

2 Entry composition (i)

There are 45 unique types of molecules in this entry. The entry contains 82310 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	334	Total	C	N	O	S	0	0
			2617	1712	430	463	12		
1	A	334	Total	C	N	O	S	0	0
			2617	1712	430	463	12		

- Molecule 2 is a protein called ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	177	Total	C	N	O	S	0	0
			1365	882	229	245	9		
2	4	177	Total	C	N	O	S	0	0
			1365	882	229	245	9		

- Molecule 3 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	175	Total	C	N	O	S	0	0
			1360	886	223	243	8		
3	7	175	Total	C	N	O	S	0	0
			1360	886	223	243	8		

- Molecule 4 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	187	Total	C	N	O	S	0	0
			1469	955	243	266	5		
4	8	187	Total	C	N	O	S	0	0
			1469	955	243	266	5		

- Molecule 5 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	185	Total	C	N	O	S	0	0
			1400	904	240	247	9		
5	9	185	Total	C	N	O	S	0	0
			1400	904	240	247	9		

- Molecule 6 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	170	Total	C	N	O	S	0	0
			1339	885	218	233	3		
6	g	170	Total	C	N	O	S	0	0
			1339	885	218	233	3		

- Molecule 7 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	192	Total	C	N	O	S	0	0
			1455	933	254	260	8		
7	p	192	Total	C	N	O	S	0	0
			1455	933	254	260	8		

- Molecule 8 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	503	Total	C	N	O	S	0	0
			3953	2581	674	687	11		
8	b	503	Total	C	N	O	S	0	0
			3953	2581	674	687	11		

- Molecule 9 is a protein called PsbC_CP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	451	Total	C	N	O	S	0	0
			3503	2290	589	614	10		
9	c	451	Total	C	N	O	S	0	0
			3503	2290	589	614	10		

- Molecule 10 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		

- Molecule 11 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	E	75	Total	C	N	O	0	0
			616	402	102	112		
11	e	75	Total	C	N	O	0	0
			616	402	102	112		

- Molecule 12 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	29	Total	C	N	O	S	0	0
			235	159	40	35	1		
12	f	29	Total	C	N	O	S	0	0
			235	159	40	35	1		

- Molecule 13 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	65	Total	C	N	O	S	0	0
			515	344	81	88	2		
13	h	65	Total	C	N	O	S	0	0
			515	344	81	88	2		

- Molecule 14 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	35	Total	C	N	O	S	0	0
			287	191	46	49	1		
14	i	35	Total	C	N	O	S	0	0
			287	191	46	49	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	J	34	Total	C	N	O	0	0
			249	168	38	43		
15	j	34	Total	C	N	O	0	0
			249	168	38	43		

- Molecule 16 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	K	37	Total	C	N	O	0	0
			296	209	44	43		
16	k	37	Total	C	N	O	0	0
			296	209	44	43		

- Molecule 17 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	L	37	Total	C	N	O	0	0
			301	204	47	50		
17	l	37	Total	C	N	O	0	0
			301	204	47	50		

- Molecule 18 is a protein called PsbM.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	37	Total	C	N	O	S	0	0
			276	182	43	50	1		
18	m	37	Total	C	N	O	S	0	0
			276	182	43	50	1		

- Molecule 19 is a protein called Psb-gama_linker.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	190	Total	C	N	O	S	0	0
			1474	954	234	283	3		
19	n	190	Total	C	N	O	S	0	0
			1474	954	234	283	3		

- Molecule 20 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	262	Total	C	N	O	S	0	0
			1993	1253	326	408	6		
20	o	262	Total	C	N	O	S	0	0
			1993	1253	326	408	6		

- Molecule 21 is a protein called PsbQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	143	Total	C	N	O	S	0	0
			1102	698	190	211	3		
21	q	143	Total	C	N	O	S	0	0
			1102	698	190	211	3		

- Molecule 22 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	31	Total	C	N	O	S	0	0
			250	173	38	38	1		
22	t	31	Total	C	N	O	S	0	0
			250	173	38	38	1		

- Molecule 23 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	93	Total	C	N	O	S	0	0
			741	476	122	141	2		
23	u	93	Total	C	N	O	S	0	0
			741	476	122	141	2		

- Molecule 24 is a protein called Photosystem II cytochrome c550.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	137	Total	C	N	O	S	0	0
			1043	653	177	209	4		
24	v	137	Total	C	N	O	S	0	0
			1043	653	177	209	4		

- Molecule 25 is a protein called PsbW.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	49	Total	C	N	O	0	0
			391	251	61	79		
25	w	49	Total	C	N	O	0	0
			391	251	61	79		

- Molecule 26 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	39	Total	C	N	O	S	0	0
			291	192	47	51	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	x	39	Total	C	N	O	S	0	0
			291	192	47	51	1		

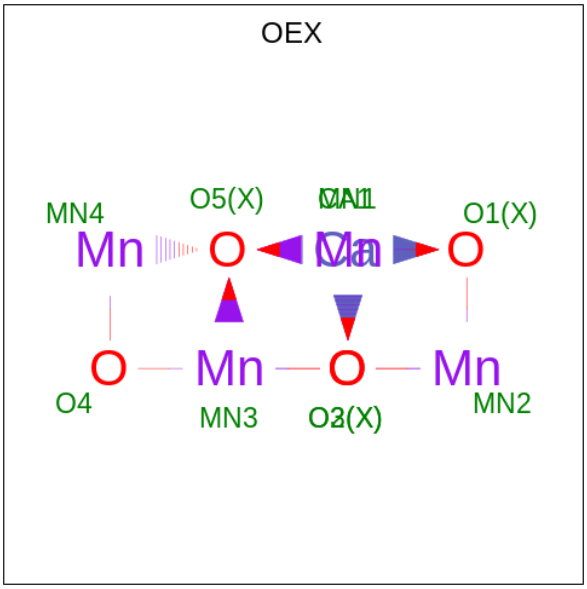
- Molecule 27 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	34	Total	C	N	O	S	0	0
			265	180	43	41	1		
27	y	34	Total	C	N	O	S	0	0
			265	180	43	41	1		

- Molecule 28 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		
28	z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).

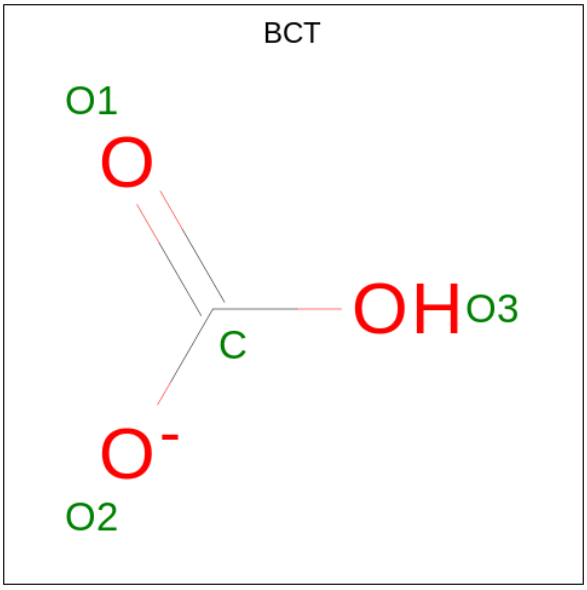


Mol	Chain	Residues	Atoms				AltConf
29	a	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 30 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

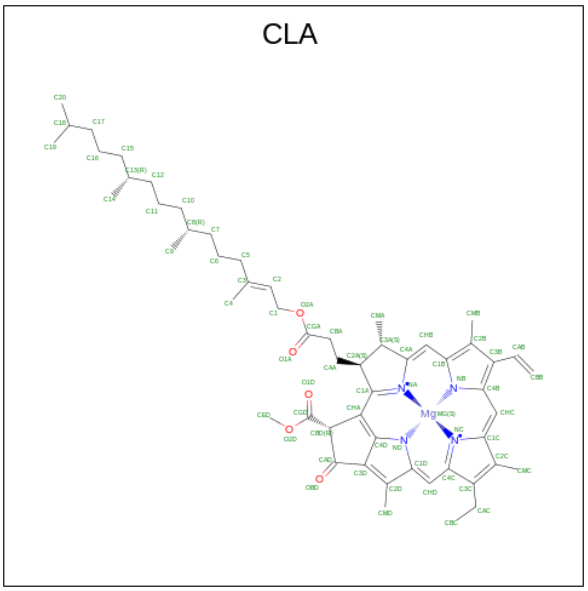


Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total C O 4 1 3	0
31	A	1	Total C O 4 1 3	0

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total Cl 1 1	0
32	A	1	Total Cl 1 1	0

- Molecule 33 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	0	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
33	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	9	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms	AltConf
33	B	1	Total C Mg N O 65 55 1 4 5	0
33	B	1	Total C Mg N O 65 55 1 4 5	0
33	B	1	Total C Mg N O 65 55 1 4 5	0
33	B	1	Total C Mg N O 65 55 1 4 5	0
33	B	1	Total C Mg N O 45 35 1 4 5	0
33	B	1	Total C Mg N O 65 55 1 4 5	0
33	B	1	Total C Mg N O 60 50 1 4 5	0
33	B	1	Total C Mg N O 40 32 1 4 3	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0
33	C	1	Total C Mg N O 56 46 1 4 5	0
33	C	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
33	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	b	1	Total 40	C 32	Mg 1	N 4	O 3	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 56	C 46	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	g	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
33	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	g	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	n	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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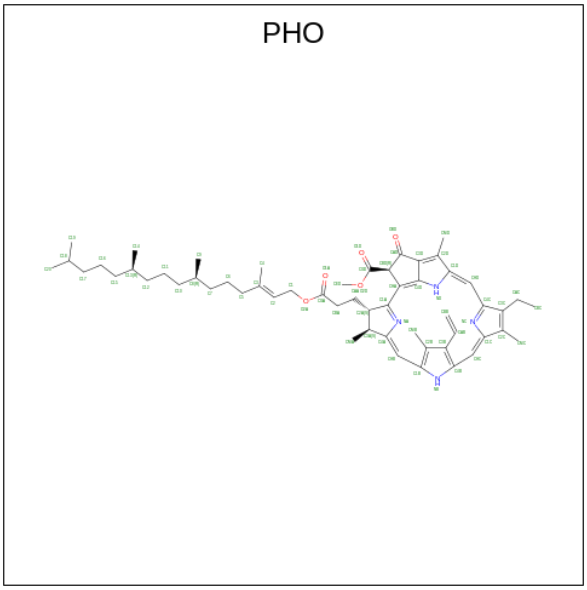
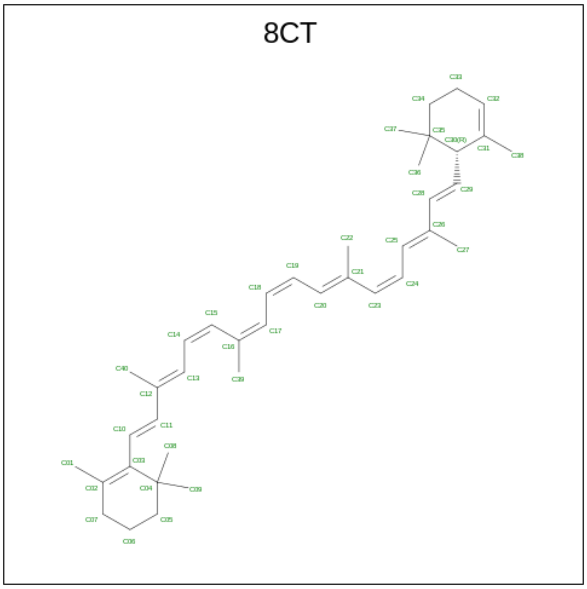
Mol	Chain	Residues	Atoms					AltConf
33	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 34 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 35 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
35	a	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	0	1	Total C 40 40	0
35	1	1	Total C 40 40	0
35	4	1	Total C 40 40	0
35	7	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	C	1	Total C 40 40	0
35	C	1	Total C 40 40	0
35	C	1	Total C 40 40	0

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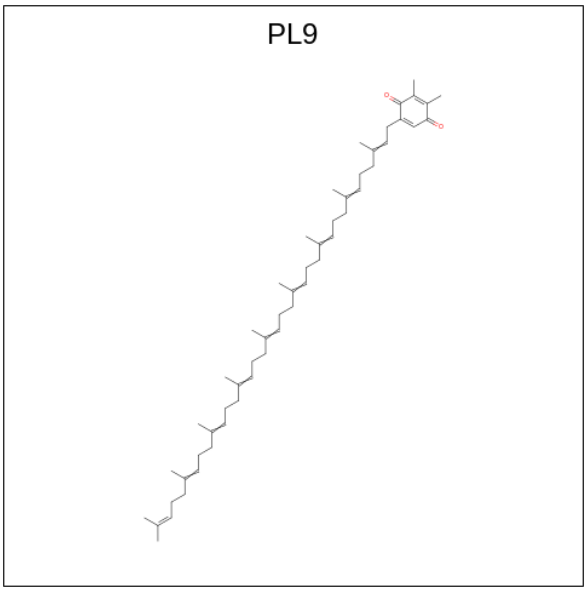
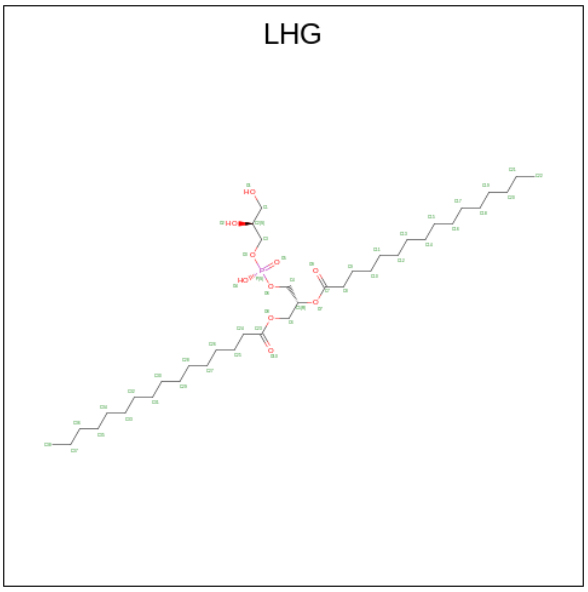
Mol	Chain	Residues	Atoms	AltConf
35	D	1	Total C 40 40	0
35	H	1	Total C 40 40	0
35	Y	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	c	1	Total C 40 40	0
35	c	1	Total C 40 40	0
35	c	1	Total C 40 40	0
35	d	1	Total C 40 40	0
35	h	1	Total C 40 40	0
35	y	1	Total C 40 40	0

- Molecule 36 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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms	AltConf
36	a	1	Total C O 30 28 2	0
36	A	1	Total C O 30 28 2	0
36	D	1	Total C O 55 53 2	0
36	d	1	Total C O 55 53 2	0

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
37	a	1	Total	C	O	P	0
			24	13	10	1	
37	A	1	Total	C	O	P	0
			24	13	10	1	
37	0	1	Total	C	O	P	0
			24	13	10	1	
37	1	1	Total	C	O	P	0
			49	38	10	1	
37	2	1	Total	C	O	P	0
			46	35	10	1	
37	3	1	Total	C	O	P	0
			41	30	10	1	
37	3	1	Total	C	O	P	0
			24	13	10	1	
37	3	1	Total	C	O	P	0
			41	30	10	1	
37	4	1	Total	C	O	P	0
			24	13	10	1	
37	5	1	Total	C	O	P	0
			22	12	9	1	
37	7	1	Total	C	O	P	0
			49	38	10	1	
37	8	1	Total	C	O	P	0
			46	35	10	1	
37	9	1	Total	C	O	P	0
			41	30	10	1	
37	9	1	Total	C	O	P	0
			24	13	10	1	
37	9	1	Total	C	O	P	0
			41	30	10	1	
37	B	1	Total	C	O	P	0
			49	38	10	1	
37	D	1	Total	C	O	P	0
			46	35	10	1	
37	D	1	Total	C	O	P	0
			47	36	10	1	
37	D	1	Total	C	O	P	0
			49	38	10	1	
37	b	1	Total	C	O	P	0
			49	38	10	1	
37	d	1	Total	C	O	P	0
			46	35	10	1	
37	d	1	Total	C	O	P	0
			47	36	10	1	

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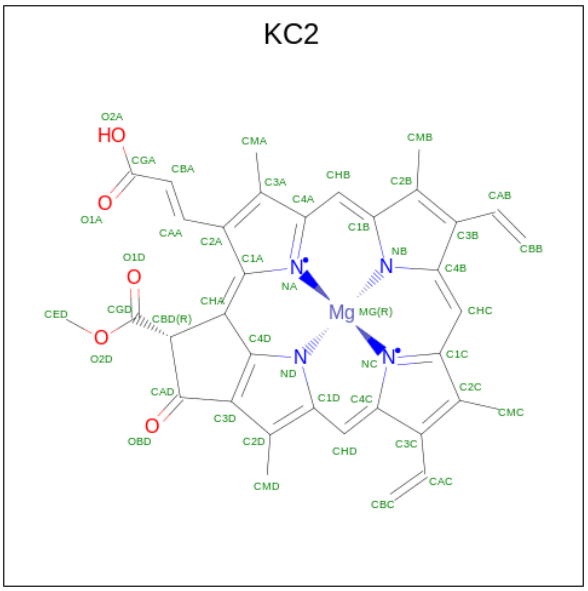
Mol	Chain	Residues	Atoms	AltConf
37	d	1	Total C O P 49 38 10 1	0
37	g	1	Total C O P 22 12 9 1	0

- Molecule 38 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
38	0	1	Total C Mg N O 45 35 1 4 5	0
38	1	1	Total C Mg N O 45 35 1 4 5	0
38	1	1	Total C Mg N O 45 35 1 4 5	0
38	2	1	Total C Mg N O 45 35 1 4 5	0
38	3	1	Total C Mg N O 45 35 1 4 5	0
38	4	1	Total C Mg N O 45 35 1 4 5	0
38	5	1	Total C Mg N O 45 35 1 4 5	0
38	6	1	Total C Mg N O 45 35 1 4 5	0
38	7	1	Total C Mg N O 45 35 1 4 5	0

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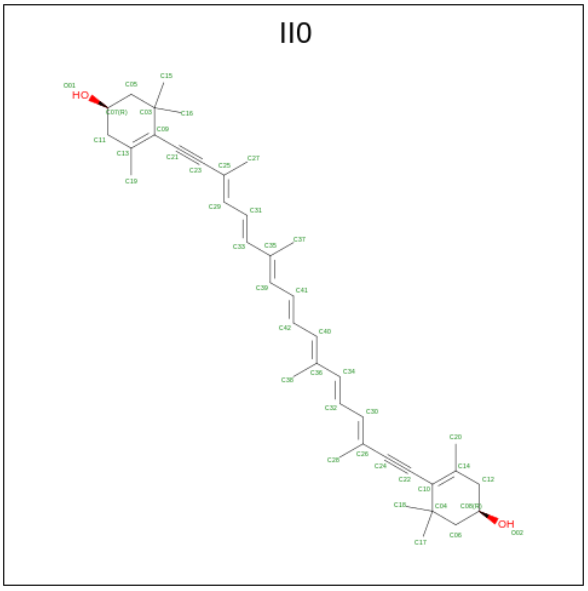
Mol	Chain	Residues	Atoms					AltConf
38	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 39 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (three-letter code: II0) (formula: $C_{40}H_{52}O_2$).



Mol	Chain	Residues	Atoms			AltConf
39	0	1	Total	C	O	0
			42	40	2	
39	0	1	Total	C	O	0
			42	40	2	
39	0	1	Total	C	O	0
			42	40	2	
39	0	1	Total	C	O	0
			42	40	2	
39	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
39	1	1	Total C O 42 40 2	0
39	1	1	Total C O 42 40 2	0
39	1	1	Total C O 42 40 2	0
39	2	1	Total C O 42 40 2	0
39	2	1	Total C O 42 40 2	0
39	2	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	4	1	Total C O 42 40 2	0
39	4	1	Total C O 42 40 2	0
39	4	1	Total C O 42 40 2	0
39	4	1	Total C O 42 40 2	0
39	5	1	Total C O 42 40 2	0
39	5	1	Total C O 42 40 2	0
39	5	1	Total C O 42 40 2	0
39	6	1	Total C O 42 40 2	0
39	6	1	Total C O 42 40 2	0
39	6	1	Total C O 42 40 2	0

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Mol	Chain	Residues	Atoms	AltConf
39	6	1	Total C O 42 40 2	0
39	6	1	Total C O 42 40 2	0
39	7	1	Total C O 42 40 2	0
39	7	1	Total C O 42 40 2	0
39	7	1	Total C O 42 40 2	0
39	7	1	Total C O 42 40 2	0
39	8	1	Total C O 42 40 2	0
39	8	1	Total C O 42 40 2	0
39	8	1	Total C O 42 40 2	0
39	9	1	Total C O 42 40 2	0
39	9	1	Total C O 42 40 2	0
39	9	1	Total C O 42 40 2	0
39	9	1	Total C O 42 40 2	0
39	9	1	Total C O 42 40 2	0
39	g	1	Total C O 42 40 2	0
39	g	1	Total C O 42 40 2	0
39	g	1	Total C O 42 40 2	0
39	p	1	Total C O 42 40 2	0
39	p	1	Total C O 42 40 2	0
39	p	1	Total C O 42 40 2	0
39	p	1	Total C O 42 40 2	0

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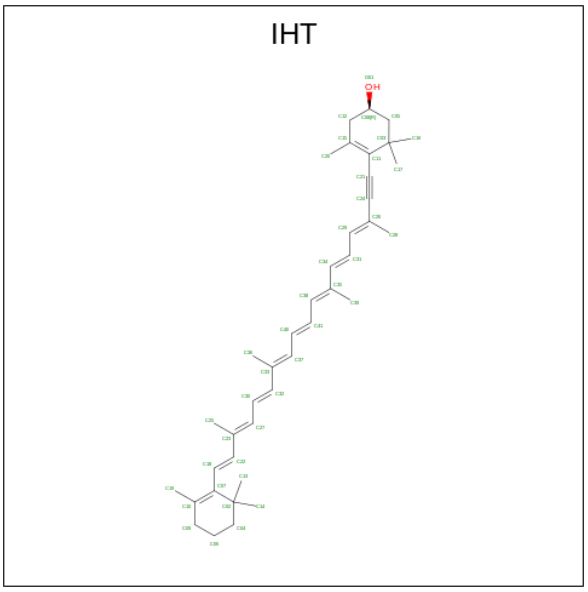
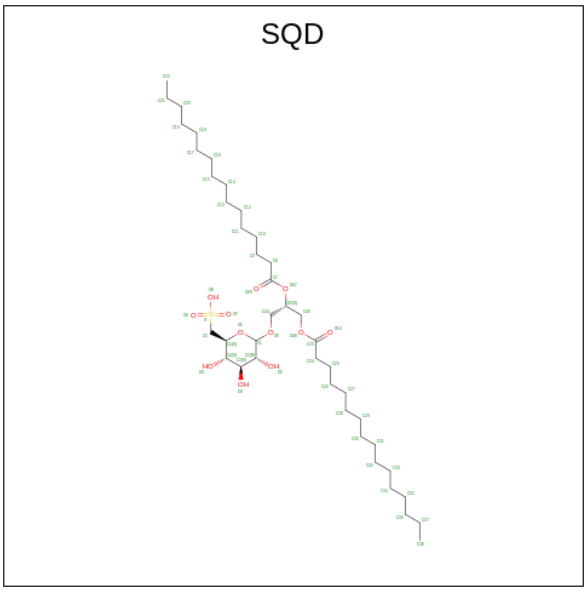
Mol	Chain	Residues	Atoms			AltConf
39	p	1	Total	C	O	0
			42	40	2	

- Molecule 40 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (three-letter code: IHT) (formula: $C_{40}H_{54}O$).



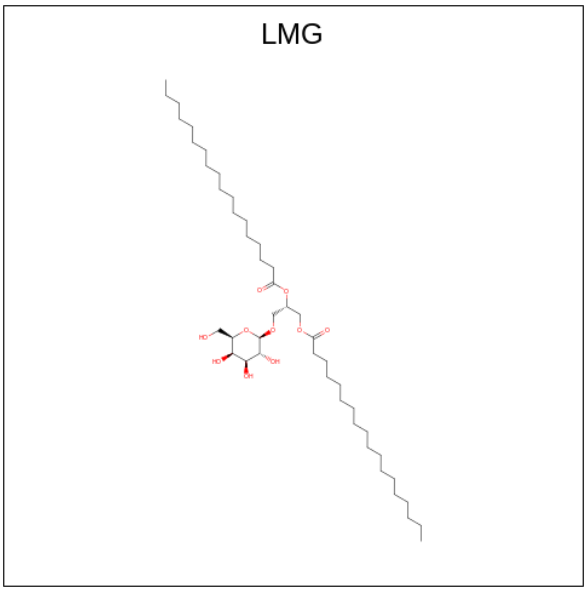
Mol	Chain	Residues	Atoms			AltConf
40	2	1	Total	C	O	0
			41	40	1	
40	3	1	Total	C	O	0
			41	40	1	
40	5	1	Total	C	O	0
			41	40	1	
40	6	1	Total	C	O	0
			41	40	1	
40	8	1	Total	C	O	0
			41	40	1	
40	9	1	Total	C	O	0
			41	40	1	
40	g	1	Total	C	O	0
			41	40	1	
40	p	1	Total	C	O	0
			41	40	1	

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



Mol	Chain	Residues	Atoms				AltConf
41	B	1	Total	C	O	S	0
			38	25	12	1	
41	C	1	Total	C	O	S	0
			42	29	12	1	
41	J	1	Total	C	O	S	0
			46	33	12	1	
41	L	1	Total	C	O	S	0
			54	41	12	1	
41	b	1	Total	C	O	S	0
			38	25	12	1	
41	c	1	Total	C	O	S	0
			42	29	12	1	
41	j	1	Total	C	O	S	0
			46	33	12	1	
41	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 42 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
42	B	1	Total C O 49 39 10	0
42	B	1	Total C O 43 33 10	0
42	C	1	Total C O 51 41 10	0
42	D	1	Total C O 46 36 10	0
42	D	1	Total C O 46 36 10	0
42	T	1	Total C O 43 33 10	0
42	W	1	Total C O 47 37 10	0
42	b	1	Total C O 49 39 10	0
42	b	1	Total C O 43 33 10	0
42	c	1	Total C O 51 41 10	0
42	d	1	Total C O 46 36 10	0
42	d	1	Total C O 46 36 10	0
42	l	1	Total C O 38 28 10	0
42	m	1	Total C O 38 28 10	0

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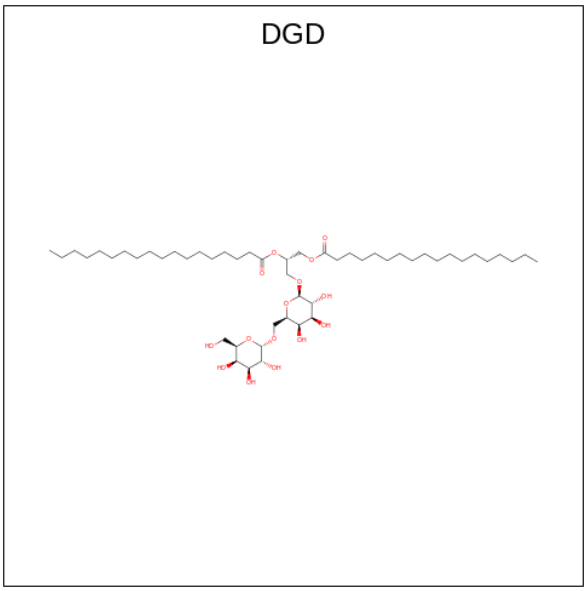
Mol	Chain	Residues	Atoms	AltConf
42	t	1	Total C O 43 33 10	0
42	w	1	Total C O 47 37 10	0

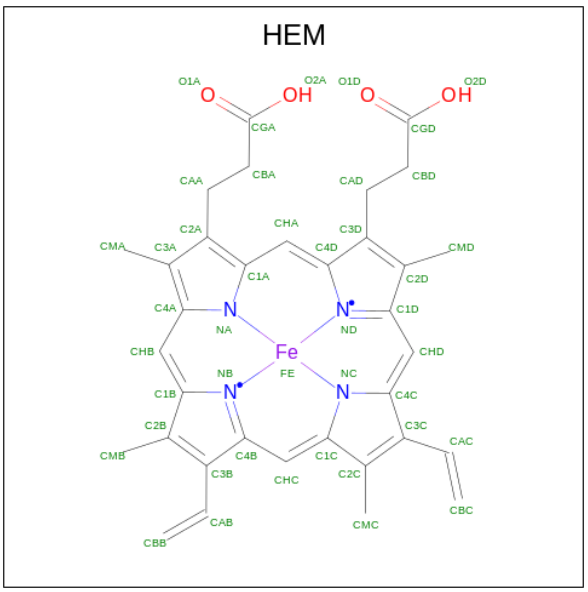
- Molecule 43 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	AltConf
43	C	1	Total C O 55 40 15	0
43	C	1	Total C O 62 47 15	0
43	C	1	Total C O 62 47 15	0
43	H	1	Total C O 60 45 15	0
43	c	1	Total C O 55 40 15	0
43	c	1	Total C O 62 47 15	0
43	c	1	Total C O 62 47 15	0
43	h	1	Total C O 60 45 15	0

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
44	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 45 is water.

Mol	Chain	Residues	Atoms		AltConf
45	a	24	Total	O	0
			24	24	
45	A	24	Total	O	0
			24	24	
45	B	3	Total	O	0
			3	3	
45	C	11	Total	O	0
			11	11	
45	O	1	Total	O	0
			1	1	
45	U	2	Total	O	0
			2	2	
45	W	1	Total	O	0
			1	1	

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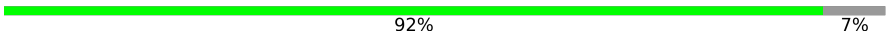
Mol	Chain	Residues	Atoms	AltConf
45	b	3	Total O 3 3	0
45	c	11	Total O 11 11	0
45	o	1	Total O 1 1	0
45	u	2	Total O 2 2	0
45	w	1	Total O 1 1	0

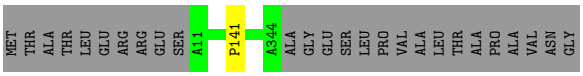
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

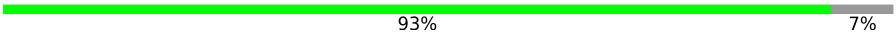
Chain a:





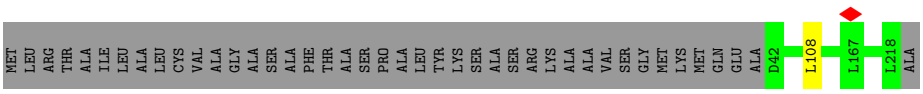
• Molecule 1: Photosystem II protein D1

Chain A:



• Molecule 2: ACPII-4

Chain 0:



• Molecule 2: ACPII-4

Chain 4:

• Molecule 3: ACPII-1

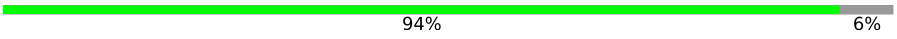
Chain 1:

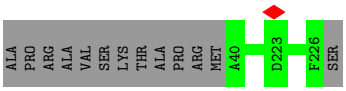
• Molecule 3: ACPII-1

Chain 7:

• Molecule 4: ACPII-2

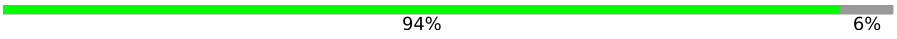
Chain 2:

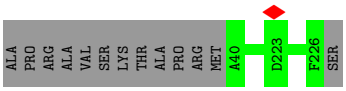




• Molecule 4: ACPII-2

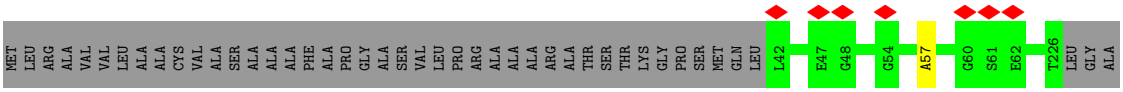
Chain 8:





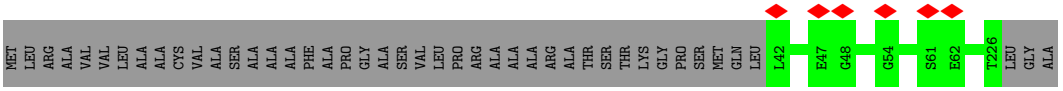
• Molecule 5: ACPII-3

Chain 3:



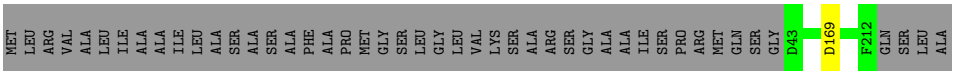
• Molecule 5: ACPII-3

Chain 9:



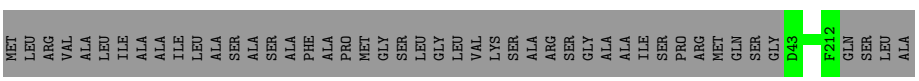
• Molecule 6: ACPII-5

Chain 5:



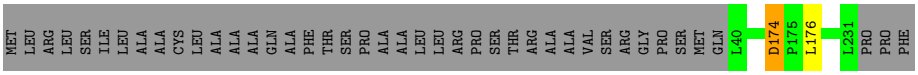
• Molecule 6: ACPII-5

Chain g:



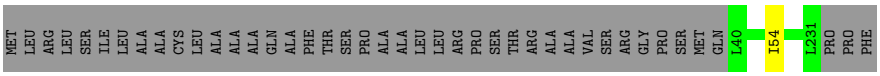
• Molecule 7: ACPII-6

Chain 6:



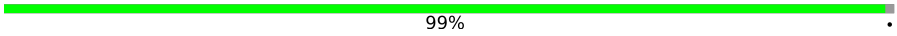
• Molecule 7: ACPII-6

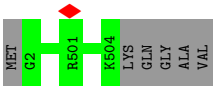
Chain p:



• Molecule 8: Photosystem II CP47 reaction center protein

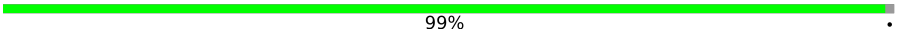
Chain B:

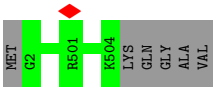




• Molecule 8: Photosystem II CP47 reaction center protein

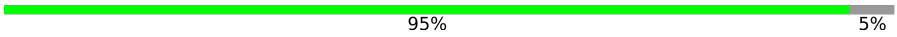
Chain b:

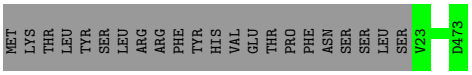




• Molecule 9: PsbC_CP43

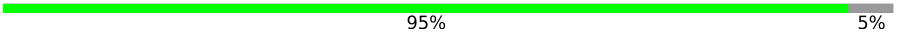
Chain C:

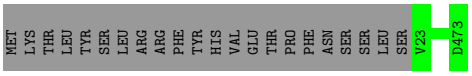




• Molecule 9: PsbC_CP43

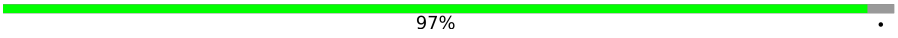
Chain c:





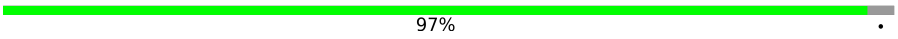
• Molecule 10: Photosystem II D2 protein

Chain D:



• Molecule 10: Photosystem II D2 protein

Chain d:



• Molecule 11: Cytochrome b559 subunit alpha

Chain E:

• Molecule 11: Cytochrome b559 subunit alpha

Chain e:

• Molecule 12: Cytochrome b559 subunit beta

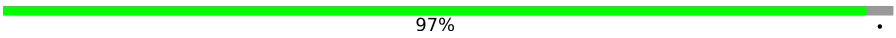
Chain F:

• Molecule 12: Cytochrome b559 subunit beta

Chain f:

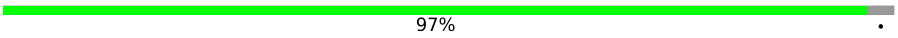
• Molecule 13: Photosystem II reaction center protein H

Chain H:



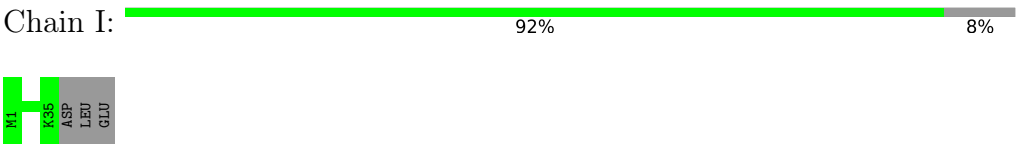
• Molecule 13: Photosystem II reaction center protein H

Chain h:



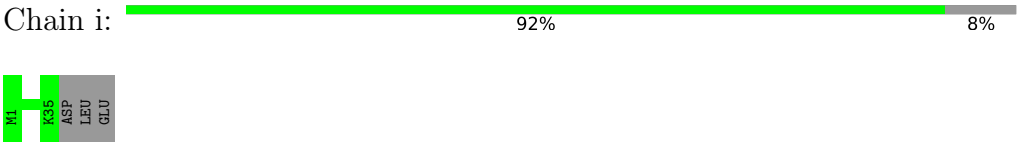
• Molecule 14: Photosystem II reaction center protein I

Chain I:



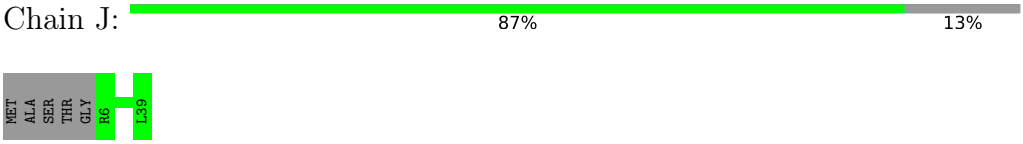
• Molecule 14: Photosystem II reaction center protein I

Chain i:



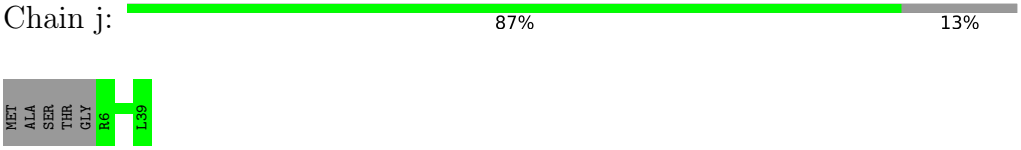
• Molecule 15: Photosystem II reaction center protein J

Chain J:



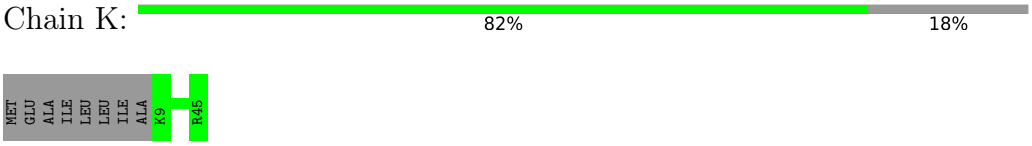
• Molecule 15: Photosystem II reaction center protein J

Chain j:



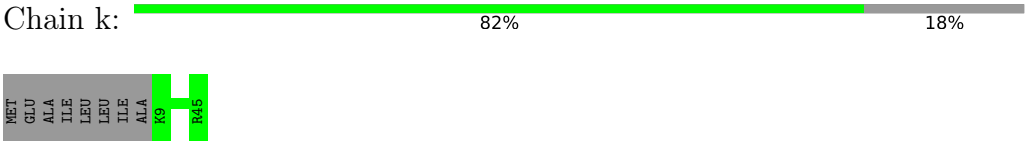
• Molecule 16: Photosystem II reaction center protein K

Chain K:



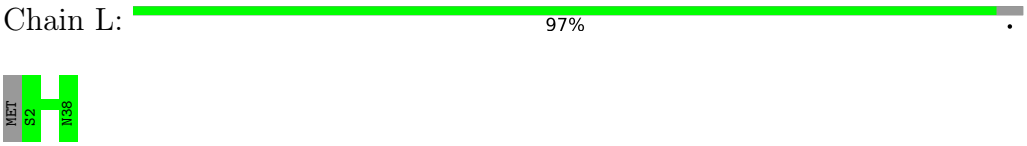
• Molecule 16: Photosystem II reaction center protein K

Chain k:



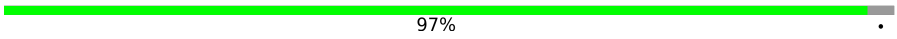
• Molecule 17: Photosystem II reaction center protein L

Chain L:



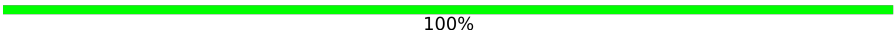
• Molecule 17: Photosystem II reaction center protein L

Chain l:



• Molecule 18: PsbM

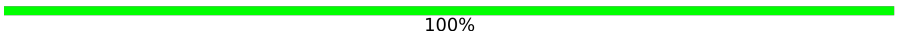
Chain M:



There are no outlier residues recorded for this chain.

• Molecule 18: PsbM

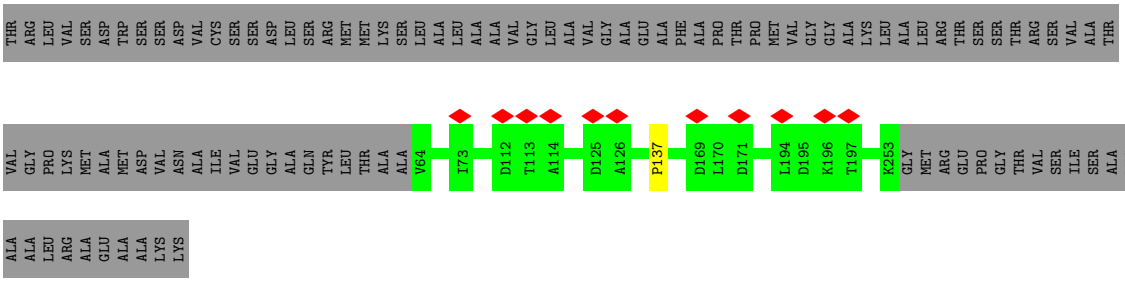
Chain m:



There are no outlier residues recorded for this chain.

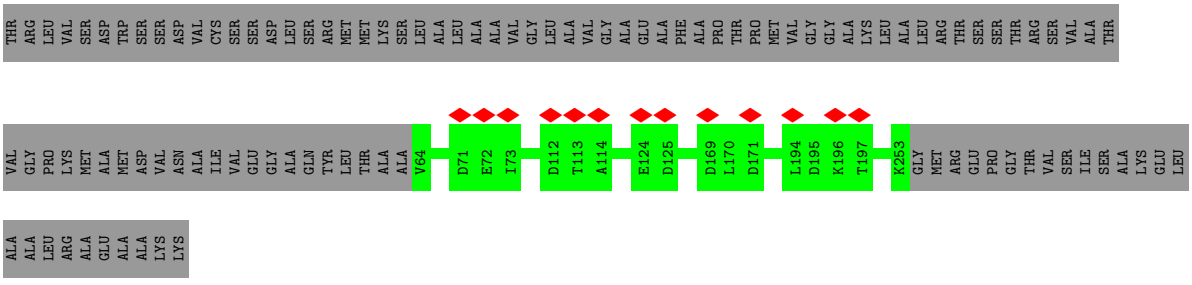
• Molecule 19: Psb-gama_linker

Chain N:



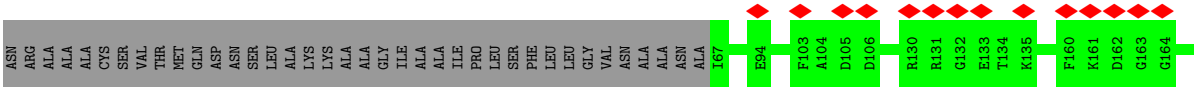
• Molecule 19: Psb-gama_linker

Chain n:



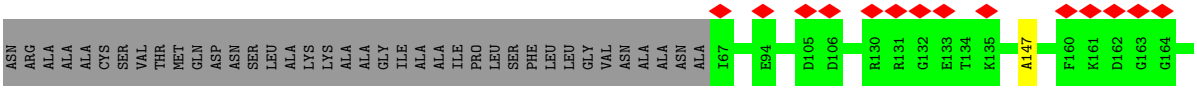
• Molecule 20: PsbO

Chain O:



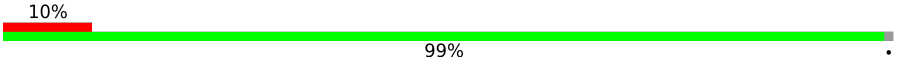
• Molecule 20: PsbO

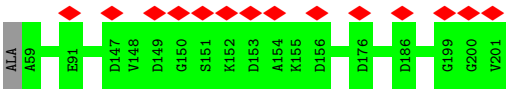
Chain o:



• Molecule 21: PsbQ

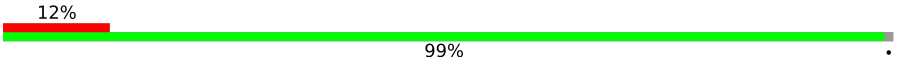
Chain Q:

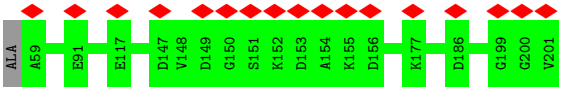




• Molecule 21: PsbQ

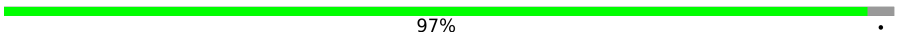
Chain q:





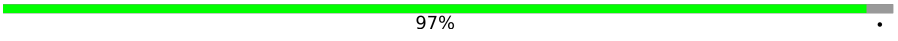
• Molecule 22: Photosystem II reaction center protein T

Chain T:



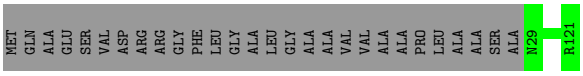
• Molecule 22: Photosystem II reaction center protein T

Chain t:



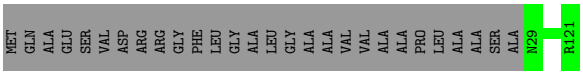
• Molecule 23: PsbU

Chain U:



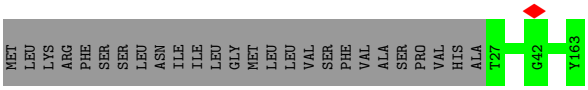
• Molecule 23: PsbU

Chain u:



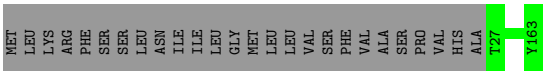
• Molecule 24: Photosystem II cytochrome c550

Chain V:



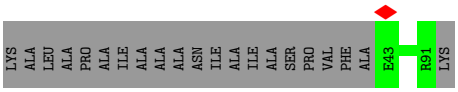
• Molecule 24: Photosystem II cytochrome c550

Chain v:



• Molecule 25: PsbW

Chain W:

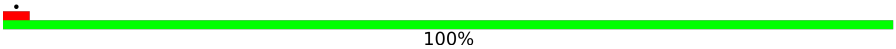


• Molecule 25: PsbW

Chain w:

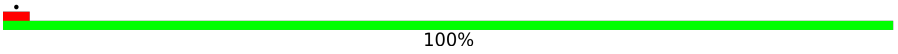
• Molecule 26: Photosystem II reaction center protein X

Chain X:



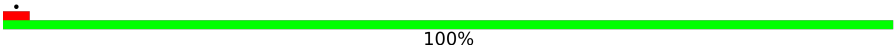
• Molecule 26: Photosystem II reaction center protein X

Chain x:



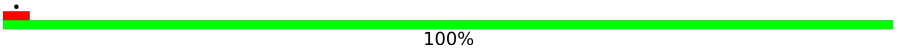
• Molecule 27: Photosystem II reaction center protein Psb30

Chain Y:



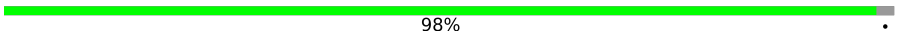
• Molecule 27: Photosystem II reaction center protein Psb30

Chain y:



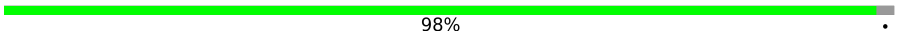
• Molecule 28: Photosystem II reaction center protein Z

Chain Z:



• Molecule 28: Photosystem II reaction center protein Z

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168683	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)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.868	Depositor
Minimum map value	0.000	Depositor
Average map value	0.088	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: CL, KC2, SQD, OEX, HEM, IHT, II0, FE2, PHO, BCT, CLA, PL9, DGD, LMG, LHG, 8CT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.31	0/2701	0.54	0/3687
1	a	0.30	0/2701	0.55	0/3687
2	0	0.52	0/1398	0.77	0/1888
2	4	0.52	0/1398	0.73	0/1888
3	1	0.32	0/1396	0.58	0/1892
3	7	0.32	0/1396	0.58	0/1892
4	2	0.32	0/1508	0.57	0/2044
4	8	0.32	0/1508	0.57	0/2044
5	3	0.31	0/1434	0.58	0/1943
5	9	0.32	0/1434	0.61	0/1943
6	5	0.46	0/1376	0.60	0/1862
6	g	0.45	0/1376	0.58	0/1862
7	6	0.68	0/1487	0.86	0/2014
7	p	0.69	0/1487	0.82	0/2014
8	B	0.29	0/4084	0.56	0/5558
8	b	0.29	0/4084	0.56	0/5558
9	C	0.30	0/3618	0.53	0/4937
9	c	0.29	0/3618	0.53	0/4937
10	D	0.28	0/2806	0.53	0/3823
10	d	0.28	0/2806	0.53	0/3823
11	E	0.32	0/634	0.64	0/865
11	e	0.32	0/634	0.64	0/865
12	F	0.29	0/242	0.59	0/328
12	f	0.29	0/242	0.59	0/328
13	H	0.31	0/527	0.58	0/717
13	h	0.30	0/527	0.59	0/717
14	I	0.28	0/294	0.54	0/397
14	i	0.28	0/294	0.54	0/397
15	J	0.34	0/255	0.56	0/348
15	j	0.34	0/255	0.56	0/348
16	K	0.33	0/307	0.54	0/421
16	k	0.34	0/307	0.55	0/421

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	L	0.30	0/311	0.54	0/424
17	l	0.30	0/311	0.54	0/424
18	M	0.34	0/280	0.52	0/381
18	m	0.32	0/280	0.50	0/381
19	N	0.33	0/1516	0.65	0/2070
19	n	0.33	0/1516	0.64	0/2070
20	O	0.30	0/2024	0.58	0/2722
20	o	0.30	0/2024	0.59	0/2722
21	Q	0.28	0/1121	0.54	0/1508
21	q	0.28	0/1121	0.54	0/1508
22	T	0.30	0/257	0.54	0/348
22	t	0.30	0/257	0.54	0/348
23	U	0.29	0/757	0.55	0/1031
23	u	0.29	0/757	0.54	0/1031
24	V	0.27	0/1063	0.55	0/1443
24	v	0.27	0/1063	0.54	0/1443
25	W	0.31	0/398	0.56	0/541
25	w	0.31	0/398	0.56	0/541
26	X	0.29	0/295	0.61	0/402
26	x	0.29	0/295	0.61	0/402
27	Y	0.32	0/270	0.66	0/367
27	y	0.32	0/270	0.66	0/367
28	Z	0.28	0/467	0.45	0/638
28	z	0.28	0/467	0.45	0/638
All	All	0.35	0/65652	0.59	0/89198

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/360 (92%)	322 (97%)	10 (3%)	0	100	100
1	a	332/360 (92%)	322 (97%)	9 (3%)	1 (0%)	41	59
2	0	175/219 (80%)	167 (95%)	8 (5%)	0	100	100
2	4	175/219 (80%)	165 (94%)	9 (5%)	1 (1%)	25	41
3	1	173/218 (79%)	171 (99%)	2 (1%)	0	100	100
3	7	173/218 (79%)	171 (99%)	2 (1%)	0	100	100
4	2	185/200 (92%)	180 (97%)	5 (3%)	0	100	100
4	8	185/200 (92%)	181 (98%)	4 (2%)	0	100	100
5	3	183/229 (80%)	173 (94%)	9 (5%)	1 (0%)	29	47
5	9	183/229 (80%)	173 (94%)	10 (6%)	0	100	100
6	5	168/216 (78%)	164 (98%)	4 (2%)	0	100	100
6	g	168/216 (78%)	163 (97%)	5 (3%)	0	100	100
7	6	190/234 (81%)	181 (95%)	8 (4%)	1 (0%)	29	47
7	p	190/234 (81%)	183 (96%)	7 (4%)	0	100	100
8	B	501/509 (98%)	490 (98%)	11 (2%)	0	100	100
8	b	501/509 (98%)	488 (97%)	13 (3%)	0	100	100
9	C	449/473 (95%)	439 (98%)	10 (2%)	0	100	100
9	c	449/473 (95%)	439 (98%)	10 (2%)	0	100	100
10	D	340/351 (97%)	330 (97%)	10 (3%)	0	100	100
10	d	340/351 (97%)	330 (97%)	10 (3%)	0	100	100
11	E	73/84 (87%)	73 (100%)	0	0	100	100
11	e	73/84 (87%)	73 (100%)	0	0	100	100
12	F	27/42 (64%)	27 (100%)	0	0	100	100
12	f	27/42 (64%)	27 (100%)	0	0	100	100
13	H	63/67 (94%)	61 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	h	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
14	I	33/38 (87%)	33 (100%)	0	0	100	100
14	i	33/38 (87%)	33 (100%)	0	0	100	100
15	J	32/39 (82%)	32 (100%)	0	0	100	100
15	j	32/39 (82%)	32 (100%)	0	0	100	100
16	K	35/45 (78%)	33 (94%)	2 (6%)	0	100	100
16	k	35/45 (78%)	33 (94%)	2 (6%)	0	100	100
17	L	35/38 (92%)	35 (100%)	0	0	100	100
17	l	35/38 (92%)	35 (100%)	0	0	100	100
18	M	35/37 (95%)	35 (100%)	0	0	100	100
18	m	35/37 (95%)	35 (100%)	0	0	100	100
19	N	188/297 (63%)	171 (91%)	16 (8%)	1 (0%)	29	47
19	n	188/297 (63%)	172 (92%)	16 (8%)	0	100	100
20	O	260/300 (87%)	256 (98%)	4 (2%)	0	100	100
20	o	260/300 (87%)	255 (98%)	4 (2%)	1 (0%)	34	53
21	Q	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
21	q	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
22	T	29/32 (91%)	29 (100%)	0	0	100	100
22	t	29/32 (91%)	29 (100%)	0	0	100	100
23	U	91/121 (75%)	87 (96%)	4 (4%)	0	100	100
23	u	91/121 (75%)	87 (96%)	4 (4%)	0	100	100
24	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
24	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
25	W	47/130 (36%)	47 (100%)	0	0	100	100
25	w	47/130 (36%)	47 (100%)	0	0	100	100
26	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
26	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
27	Y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
27	y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
28	Z	59/62 (95%)	59 (100%)	0	0	100	100
28	z	59/62 (95%)	59 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8096/9442 (86%)	7858 (97%)	232 (3%)	6 (0%)	54 71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	3	57	ALA
20	o	147	ALA
7	6	174	ASP
1	a	141	PRO
2	4	208	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/289 (93%)	270 (100%)	0	100 100
1	a	270/289 (93%)	270 (100%)	0	100 100
2	0	143/171 (84%)	142 (99%)	1 (1%)	84 93
2	4	143/171 (84%)	142 (99%)	1 (1%)	84 93
3	1	143/173 (83%)	143 (100%)	0	100 100
3	7	143/173 (83%)	143 (100%)	0	100 100
4	2	156/166 (94%)	156 (100%)	0	100 100
4	8	156/166 (94%)	156 (100%)	0	100 100
5	3	145/172 (84%)	145 (100%)	0	100 100
5	9	145/172 (84%)	145 (100%)	0	100 100
6	5	136/167 (81%)	135 (99%)	1 (1%)	84 93
6	g	136/167 (81%)	136 (100%)	0	100 100
7	6	147/178 (83%)	145 (99%)	2 (1%)	67 85
7	p	147/178 (83%)	146 (99%)	1 (1%)	84 93
8	B	400/404 (99%)	400 (100%)	0	100 100
8	b	400/404 (99%)	400 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	C	356/378 (94%)	356 (100%)	0	100	100
9	c	356/378 (94%)	356 (100%)	0	100	100
10	D	274/281 (98%)	274 (100%)	0	100	100
10	d	274/281 (98%)	274 (100%)	0	100	100
11	E	67/73 (92%)	67 (100%)	0	100	100
11	e	67/73 (92%)	67 (100%)	0	100	100
12	F	24/37 (65%)	24 (100%)	0	100	100
12	f	24/37 (65%)	24 (100%)	0	100	100
13	H	56/58 (97%)	56 (100%)	0	100	100
13	h	56/58 (97%)	56 (100%)	0	100	100
14	I	33/36 (92%)	33 (100%)	0	100	100
14	i	33/36 (92%)	33 (100%)	0	100	100
15	J	26/29 (90%)	26 (100%)	0	100	100
15	j	26/29 (90%)	26 (100%)	0	100	100
16	K	30/36 (83%)	30 (100%)	0	100	100
16	k	30/36 (83%)	30 (100%)	0	100	100
17	L	34/35 (97%)	34 (100%)	0	100	100
17	l	34/35 (97%)	34 (100%)	0	100	100
18	M	31/31 (100%)	31 (100%)	0	100	100
18	m	31/31 (100%)	31 (100%)	0	100	100
19	N	153/231 (66%)	153 (100%)	0	100	100
19	n	153/231 (66%)	153 (100%)	0	100	100
20	O	214/239 (90%)	214 (100%)	0	100	100
20	o	214/239 (90%)	214 (100%)	0	100	100
21	Q	113/113 (100%)	113 (100%)	0	100	100
21	q	113/113 (100%)	113 (100%)	0	100	100
22	T	26/27 (96%)	26 (100%)	0	100	100
22	t	26/27 (96%)	26 (100%)	0	100	100
23	U	80/96 (83%)	80 (100%)	0	100	100
23	u	80/96 (83%)	80 (100%)	0	100	100
24	V	118/141 (84%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	v	118/141 (84%)	118 (100%)	0	100	100
25	W	42/101 (42%)	42 (100%)	0	100	100
25	w	42/101 (42%)	42 (100%)	0	100	100
26	X	34/34 (100%)	34 (100%)	0	100	100
26	x	34/34 (100%)	34 (100%)	0	100	100
27	Y	29/29 (100%)	29 (100%)	0	100	100
27	y	29/29 (100%)	29 (100%)	0	100	100
28	Z	50/51 (98%)	50 (100%)	0	100	100
28	z	50/51 (98%)	50 (100%)	0	100	100
All	All	6660/7552 (88%)	6654 (100%)	6 (0%)	93	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	6	174	ASP
7	6	176	LEU
7	p	54	ILE
2	4	59	SER
2	0	108	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
7	6	189	GLN
7	p	189	GLN
20	O	295	GLN
24	v	148	GLN
20	o	295	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 380 ligands modelled in this entry, 4 are monoatomic - leaving 376 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	$\#\|Z\| > 2$
33	CLA	b	603	-	65,73,73	2.19	8 (12%)	76,113,113	1.44	6 (7%)
33	CLA	b	613	-	65,73,73	2.18	8 (12%)	76,113,113	1.38	4 (5%)
35	8CT	y	101	-	40,41,41	0.23	0	50,56,56	0.51	0
29	OEX	a	401	9,45,1	0,15,15	-	-	-		
33	CLA	n	303	-	41,49,73	2.88	9 (21%)	47,84,113	1.95	7 (14%)
42	LMG	b	622	-	49,49,55	0.77	0	57,57,63	1.21	5 (8%)
33	CLA	9	309	5	55,63,73	2.40	8 (14%)	64,101,113	1.66	8 (12%)
33	CLA	c	509	-	65,73,73	2.16	8 (12%)	76,113,113	1.33	4 (5%)
33	CLA	8	310	-	46,54,73	2.65	8 (17%)	53,90,113	1.76	6 (11%)
33	CLA	1	303	-	51,59,73	2.43	8 (15%)	59,96,113	1.54	4 (6%)
39	II0	9	319	-	39,43,43	0.22	0	50,60,60	0.68	3 (6%)
33	CLA	B	602	-	50,58,73	2.50	8 (16%)	58,95,113	1.56	7 (12%)
33	CLA	9	310	-	41,49,73	2.81	9 (21%)	47,84,113	1.78	4 (8%)
33	CLA	2	302	4	55,63,73	2.37	8 (14%)	64,101,113	1.81	10 (15%)
36	PL9	d	407	-	55,55,55	0.96	4 (7%)	68,69,69	1.45	11 (16%)
33	CLA	6	319	-	41,49,73	2.72	9 (21%)	47,84,113	1.90	9 (19%)
33	CLA	p	319	-	41,49,73	2.73	9 (21%)	47,84,113	1.90	9 (19%)
33	CLA	p	303	7	41,49,73	2.71	9 (21%)	47,84,113	1.97	7 (14%)
37	LHG	9	302	-	40,40,48	0.69	1 (2%)	43,46,54	1.17	3 (6%)
33	CLA	D	404	-	65,73,73	2.16	8 (12%)	76,113,113	1.49	6 (7%)
38	KC2	5	309	-	48,53,53	1.31	7 (14%)	54,89,89	1.07	4 (7%)
33	CLA	3	314	-	41,49,73	2.82	9 (21%)	47,84,113	1.90	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	A	405	-	65,73,73	2.16	8 (12%)	76,113,113	1.41	7 (9%)
33	CLA	7	301	3	45,53,73	2.60	8 (17%)	52,89,113	1.84	6 (11%)
35	8CT	D	406	-	40,41,41	0.21	0	50,56,56	0.69	1 (2%)
33	CLA	9	313	-	41,49,73	2.82	9 (21%)	47,84,113	1.71	5 (10%)
38	KC2	4	305	-	48,53,53	1.41	7 (14%)	54,89,89	1.12	6 (11%)
44	HEM	f	101	11	41,50,50	0.85	0	45,82,82	0.71	0
33	CLA	A	408	-	60,68,73	2.29	8 (13%)	70,107,113	1.47	5 (7%)
33	CLA	9	305	-	55,63,73	2.32	8 (14%)	64,101,113	1.50	4 (6%)
33	CLA	5	301	6	42,50,73	2.72	8 (19%)	48,85,113	1.75	7 (14%)
38	KC2	6	311	7	48,53,53	1.30	7 (14%)	54,89,89	1.12	6 (11%)
33	CLA	N	304	-	41,49,73	2.88	9 (21%)	47,84,113	1.94	7 (14%)
42	LMG	D	409	-	46,46,55	0.77	0	54,54,63	1.21	2 (3%)
33	CLA	0	306	2	55,63,73	2.32	8 (14%)	64,101,113	1.49	9 (14%)
34	PHO	A	407	-	51,69,69	0.62	1 (1%)	47,99,99	1.01	3 (6%)
42	LMG	b	624	-	43,43,55	0.80	1 (2%)	51,51,63	1.25	5 (9%)
37	LHG	D	402	-	46,46,48	0.69	0	49,52,54	1.14	3 (6%)
33	CLA	2	308	-	55,63,73	2.36	8 (14%)	64,101,113	1.43	5 (7%)
33	CLA	8	306	4	60,68,73	2.19	8 (13%)	70,107,113	1.54	7 (10%)
37	LHG	3	302	-	40,40,48	0.69	1 (2%)	43,46,54	1.17	3 (6%)
33	CLA	8	301	4	45,53,73	2.65	8 (17%)	52,89,113	1.74	6 (11%)
39	II0	1	313	-	39,43,43	0.24	0	50,60,60	0.58	0
37	LHG	0	317	33	23,23,48	0.90	0	26,29,54	1.23	1 (3%)
33	CLA	3	310	-	41,49,73	2.82	9 (21%)	47,84,113	1.78	4 (8%)
33	CLA	3	307	-	45,53,73	2.63	8 (17%)	52,89,113	1.80	6 (11%)
41	SQD	C	501	-	41,42,54	1.34	4 (9%)	50,53,65	1.26	5 (10%)
38	KC2	g	309	-	48,53,53	1.31	7 (14%)	54,89,89	1.07	4 (7%)
42	LMG	C	520	-	51,51,55	0.72	1 (1%)	59,59,63	1.35	7 (11%)
33	CLA	b	605	-	65,73,73	2.13	8 (12%)	76,113,113	1.33	5 (6%)
33	CLA	p	302	7	41,49,73	2.99	9 (21%)	47,84,113	1.99	8 (17%)
33	CLA	b	616	-	65,73,73	2.17	8 (12%)	76,113,113	1.32	7 (9%)
33	CLA	b	612	-	65,73,73	2.20	8 (12%)	76,113,113	1.44	5 (6%)
39	II0	4	314	-	39,43,43	0.37	0	50,60,60	0.54	1 (2%)
38	KC2	7	311	-	48,53,53	1.54	8 (16%)	54,89,89	1.09	5 (9%)
33	CLA	B	605	-	65,73,73	2.13	8 (12%)	76,113,113	1.33	5 (6%)
33	CLA	9	315	-	41,49,73	2.84	9 (21%)	47,84,113	1.70	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	3	305	-	55,63,73	2.31	8 (14%)	64,101,113	1.49	4 (6%)
35	8CT	c	517	-	40,41,41	0.17	0	50,56,56	0.38	0
39	II0	p	315	-	39,43,43	0.33	0	50,60,60	0.54	1 (2%)
33	CLA	C	503	-	65,73,73	2.10	8 (12%)	76,113,113	1.36	5 (6%)
33	CLA	d	405	-	65,73,73	2.20	8 (12%)	76,113,113	1.39	5 (6%)
33	CLA	b	607	-	65,73,73	2.19	8 (12%)	76,113,113	1.38	5 (6%)
33	CLA	b	610	-	65,73,73	2.13	8 (12%)	76,113,113	1.37	7 (9%)
33	CLA	p	307	-	43,51,73	2.61	8 (18%)	49,86,113	1.84	7 (14%)
44	HEM	V	201	-	41,50,50	0.88	0	45,82,82	0.77	1 (2%)
33	CLA	3	309	5	55,63,73	2.41	8 (14%)	64,101,113	1.67	8 (12%)
39	II0	0	316	-	39,43,43	0.25	0	50,60,60	0.29	0
33	CLA	C	507	-	65,73,73	2.19	8 (12%)	76,113,113	1.43	6 (7%)
36	PL9	D	407	-	55,55,55	0.95	3 (5%)	68,69,69	1.44	11 (16%)
39	II0	g	314	-	39,43,43	0.37	0	50,60,60	1.06	2 (4%)
35	8CT	1	312	-	40,41,41	0.21	0	50,56,56	0.42	0
39	II0	6	301	-	39,43,43	0.33	0	50,60,60	0.56	2 (4%)
33	CLA	B	610	-	65,73,73	2.14	8 (12%)	76,113,113	1.37	7 (9%)
39	II0	1	315	-	39,43,43	0.18	0	50,60,60	0.60	2 (4%)
35	8CT	B	619	-	40,41,41	0.21	0	50,56,56	0.42	0
33	CLA	7	305	3	60,68,73	2.27	8 (13%)	70,107,113	1.37	5 (7%)
33	CLA	6	303	7	41,49,73	2.71	9 (21%)	47,84,113	1.96	8 (17%)
43	DGD	H	101	-	61,61,67	0.88	1 (1%)	75,75,81	1.22	5 (6%)
35	8CT	b	620	-	40,41,41	0.23	0	50,56,56	0.51	0
33	CLA	N	305	-	55,63,73	2.46	8 (14%)	64,101,113	1.49	8 (12%)
42	LMG	w	101	-	47,47,55	0.74	0	55,55,63	1.24	2 (3%)
33	CLA	A	406	-	49,57,73	2.55	8 (16%)	55,93,113	1.69	6 (10%)
36	PL9	a	410	-	30,30,55	0.92	1 (3%)	38,39,69	1.33	6 (15%)
33	CLA	6	309	7	42,50,73	2.59	8 (19%)	48,85,113	1.89	9 (18%)
42	LMG	t	101	-	43,43,55	0.81	1 (2%)	51,51,63	1.40	9 (17%)
33	CLA	2	303	-	52,60,73	2.44	8 (15%)	60,97,113	1.83	8 (13%)
35	8CT	B	621	-	40,41,41	0.18	0	50,56,56	0.36	0
33	CLA	C	513	-	56,64,73	2.39	8 (14%)	65,102,113	1.52	6 (9%)
39	II0	2	311	-	39,43,43	0.24	0	50,60,60	0.53	1 (2%)
33	CLA	p	304	-	42,50,73	2.81	8 (19%)	48,85,113	1.74	6 (12%)
33	CLA	a	406	-	49,57,73	2.55	8 (16%)	55,93,113	1.69	6 (10%)
33	CLA	5	310	-	41,49,73	2.92	9 (21%)	47,84,113	1.90	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	c	512	-	65,73,73	2.16	8 (12%)	76,113,113	1.32	7 (9%)
33	CLA	0	309	-	47,55,73	2.49	8 (17%)	54,91,113	1.65	5 (9%)
42	LMG	W	101	-	47,47,55	0.74	0	55,55,63	1.24	2 (3%)
38	KC2	8	309	-	48,53,53	1.57	8 (16%)	54,89,89	1.12	5 (9%)
33	CLA	6	305	-	55,63,73	2.19	8 (14%)	64,101,113	1.47	7 (10%)
39	II0	9	317	-	39,43,43	0.23	0	50,60,60	0.63	1 (2%)
38	KC2	3	311	-	48,53,53	1.58	8 (16%)	54,89,89	1.02	6 (11%)
34	PHO	D	403	-	51,69,69	0.42	0	47,99,99	0.66	1 (2%)
33	CLA	0	310	-	39,48,73	2.68	8 (20%)	45,82,113	2.11	10 (22%)
33	CLA	1	306	-	60,68,73	2.22	8 (13%)	70,107,113	1.46	5 (7%)
33	CLA	0	301	2	41,49,73	2.85	9 (21%)	47,84,113	1.90	8 (17%)
33	CLA	B	607	-	65,73,73	2.18	8 (12%)	76,113,113	1.38	5 (6%)
37	LHG	8	315	-	45,45,48	0.62	0	48,51,54	1.21	4 (8%)
39	II0	3	301	-	39,43,43	0.22	0	50,60,60	0.52	0
33	CLA	2	310	-	46,54,73	2.65	8 (17%)	53,90,113	1.77	6 (11%)
37	LHG	b	623	-	48,48,48	0.64	1 (2%)	51,54,54	1.30	6 (11%)
39	II0	4	312	-	39,43,43	0.36	0	50,60,60	0.56	0
33	CLA	D	405	-	65,73,73	2.20	8 (12%)	76,113,113	1.40	4 (5%)
37	LHG	1	317	-	48,48,48	0.62	0	51,54,54	1.24	6 (11%)
39	II0	6	314	-	39,43,43	0.35	0	50,60,60	0.74	1 (2%)
42	LMG	l	102	-	38,38,55	0.96	1 (2%)	46,46,63	1.23	6 (13%)
39	II0	p	316	-	39,43,43	0.32	0	50,60,60	0.71	2 (4%)
33	CLA	6	302	7	41,49,73	2.99	9 (21%)	47,84,113	1.99	8 (17%)
33	CLA	9	303	5	55,63,73	2.36	8 (14%)	64,101,113	1.61	8 (12%)
37	LHG	D	401	-	45,45,48	0.66	1 (2%)	48,51,54	1.18	4 (8%)
33	CLA	6	307	-	43,51,73	2.62	8 (18%)	49,86,113	1.85	7 (14%)
33	CLA	n	305	-	55,63,73	2.38	8 (14%)	64,101,113	1.56	6 (9%)
33	CLA	3	303	5	55,63,73	2.35	8 (14%)	64,101,113	1.61	8 (12%)
31	BCT	a	403	30	2,3,3	1.26	0	2,3,3	4.17	2 (100%)
33	CLA	B	609	-	65,73,73	2.21	8 (12%)	76,113,113	1.44	7 (9%)
37	LHG	B	623	-	48,48,48	0.64	1 (2%)	51,54,54	1.30	6 (11%)
33	CLA	b	604	-	65,73,73	2.13	8 (12%)	76,113,113	1.40	4 (5%)
33	CLA	p	309	7	42,50,73	2.59	8 (19%)	48,85,113	1.90	9 (18%)
37	LHG	d	402	-	46,46,48	0.69	0	49,52,54	1.14	3 (6%)
33	CLA	0	302	2	51,59,73	2.36	8 (15%)	59,96,113	1.72	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	n	304	-	55,63,73	2.46	8 (14%)	64,101,113	1.48	8 (12%)
33	CLA	C	512	-	65,73,73	2.16	8 (12%)	76,113,113	1.32	7 (9%)
33	CLA	N	301	-	65,73,73	2.17	8 (12%)	76,113,113	1.45	5 (6%)
33	CLA	c	502	-	65,73,73	2.18	8 (12%)	76,113,113	1.35	6 (7%)
33	CLA	4	310	-	45,53,73	2.57	8 (17%)	52,89,113	1.91	8 (15%)
41	SQD	B	601	-	37,38,54	1.40	4 (10%)	46,49,65	1.09	5 (10%)
33	CLA	3	304	-	45,53,73	2.64	8 (17%)	52,89,113	1.67	5 (9%)
39	II0	3	319	-	39,43,43	0.22	0	50,60,60	0.68	2 (4%)
33	CLA	B	606	-	65,73,73	2.20	9 (13%)	76,113,113	1.46	7 (9%)
34	PHO	a	407	-	51,69,69	0.63	1 (1%)	47,99,99	1.01	3 (6%)
37	LHG	3	322	-	40,40,48	0.70	2 (5%)	43,46,54	1.23	4 (9%)
35	8CT	C	517	-	40,41,41	0.17	0	50,56,56	0.38	0
43	DGD	c	521	-	63,63,67	0.92	2 (3%)	77,77,81	1.33	8 (10%)
41	SQD	b	601	-	37,38,54	1.40	4 (10%)	46,49,65	1.09	5 (10%)
33	CLA	0	311	-	45,53,73	2.58	8 (17%)	52,89,113	1.91	9 (17%)
33	CLA	9	314	-	41,49,73	2.83	9 (21%)	47,84,113	1.91	6 (12%)
33	CLA	g	306	6	45,53,73	2.59	8 (17%)	52,89,113	1.69	5 (9%)
44	HEM	v	201	-	41,50,50	0.87	0	45,82,82	0.77	1 (2%)
43	DGD	h	101	-	61,61,67	0.88	1 (1%)	75,75,81	1.22	5 (6%)
33	CLA	g	308	-	41,49,73	2.91	9 (21%)	47,84,113	1.88	6 (12%)
33	CLA	8	303	-	52,60,73	2.45	8 (15%)	60,97,113	1.84	8 (13%)
33	CLA	4	302	2	51,59,73	2.37	8 (15%)	59,96,113	1.71	6 (10%)
33	CLA	3	313	-	41,49,73	2.82	9 (21%)	47,84,113	1.71	5 (10%)
33	CLA	1	307	-	65,73,73	2.23	8 (12%)	76,113,113	1.53	7 (9%)
37	LHG	a	411	-	23,23,48	0.86	1 (4%)	26,29,54	1.32	2 (7%)
33	CLA	6	304	-	42,50,73	2.81	8 (19%)	48,85,113	1.74	6 (12%)
33	CLA	p	310	-	41,49,73	2.78	9 (21%)	47,84,113	1.80	10 (21%)
33	CLA	4	309	-	39,48,73	2.69	8 (20%)	45,82,113	2.10	10 (22%)
33	CLA	5	307	-	55,63,73	2.26	8 (14%)	64,101,113	1.57	8 (12%)
33	CLA	4	306	2	55,63,73	2.32	8 (14%)	64,101,113	1.48	9 (14%)
33	CLA	5	311	-	45,53,73	2.71	8 (17%)	52,89,113	1.77	7 (13%)
33	CLA	C	508	-	65,73,73	2.15	8 (12%)	76,113,113	1.32	7 (9%)
39	II0	4	313	-	39,43,43	0.32	0	50,60,60	0.49	1 (2%)
40	IHT	8	314	-	40,42,42	0.19	0	53,58,58	0.55	1 (1%)
33	CLA	7	303	-	51,59,73	2.42	8 (15%)	59,96,113	1.54	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	p	305	-	55,63,73	2.20	8 (14%)	64,101,113	1.47	7 (10%)
42	LMG	T	101	-	43,43,55	0.81	1 (2%)	51,51,63	1.40	9 (17%)
41	SQD	J	101	-	45,46,54	1.26	4 (8%)	54,57,65	1.28	5 (9%)
33	CLA	B	617	-	60,68,73	2.28	8 (13%)	70,107,113	1.42	6 (8%)
33	CLA	C	509	-	65,73,73	2.16	8 (12%)	76,113,113	1.33	4 (5%)
33	CLA	n	302	-	65,73,73	2.18	8 (12%)	76,113,113	1.44	6 (7%)
33	CLA	8	302	4	55,63,73	2.36	8 (14%)	64,101,113	1.81	10 (15%)
35	8CT	c	515	-	40,41,41	0.45	1 (2%)	50,56,56	0.64	0
33	CLA	n	306	-	50,58,73	2.57	8 (16%)	58,95,113	1.65	8 (13%)
33	CLA	p	306	-	45,53,73	2.53	8 (17%)	52,89,113	1.71	9 (17%)
39	II0	3	316	-	39,43,43	0.28	0	50,60,60	0.63	1 (2%)
33	CLA	2	304	-	60,68,73	2.29	8 (13%)	70,107,113	1.50	5 (7%)
33	CLA	4	304	-	47,55,73	2.44	8 (17%)	54,91,113	1.72	7 (12%)
33	CLA	B	603	-	65,73,73	2.18	8 (12%)	76,113,113	1.44	6 (7%)
33	CLA	C	505	-	65,73,73	2.18	8 (12%)	76,113,113	1.43	6 (7%)
33	CLA	1	309	-	55,63,73	2.35	8 (14%)	64,101,113	1.45	5 (7%)
40	IHT	p	318	-	40,42,42	0.32	0	53,58,58	0.45	0
39	II0	8	313	-	39,43,43	0.20	0	50,60,60	0.55	0
33	CLA	g	303	-	55,63,73	2.42	8 (14%)	64,101,113	1.60	5 (7%)
33	CLA	4	308	-	47,55,73	2.49	8 (17%)	54,91,113	1.65	5 (9%)
39	II0	p	317	-	39,43,43	0.31	0	50,60,60	0.62	1 (2%)
33	CLA	5	302	6	55,63,73	2.39	8 (14%)	64,101,113	1.70	11 (17%)
33	CLA	C	502	-	65,73,73	2.18	8 (12%)	76,113,113	1.36	6 (7%)
39	II0	7	313	-	39,43,43	0.24	0	50,60,60	0.58	0
29	OEX	A	401	9,1	0,15,15	-	-	-		
40	IHT	2	314	-	40,42,42	0.19	0	53,58,58	0.55	1 (1%)
33	CLA	c	505	-	65,73,73	2.18	8 (12%)	76,113,113	1.43	6 (7%)
39	II0	4	315	-	39,43,43	0.25	0	50,60,60	0.29	0
33	CLA	0	307	2	55,63,73	2.33	8 (14%)	64,101,113	1.59	9 (14%)
39	II0	9	301	-	39,43,43	0.22	0	50,60,60	0.52	0
33	CLA	2	305	-	55,63,73	2.33	8 (14%)	64,101,113	1.55	6 (9%)
33	CLA	6	312	-	41,49,73	2.69	9 (21%)	47,84,113	1.79	8 (17%)
33	CLA	c	506	-	65,73,73	2.15	8 (12%)	76,113,113	1.38	6 (7%)
33	CLA	6	308	7	42,50,73	2.61	8 (19%)	48,85,113	1.88	9 (18%)
38	KC2	0	305	-	48,53,53	1.41	7 (14%)	54,89,89	1.12	5 (9%)
33	CLA	a	412	-	65,73,73	2.21	8 (12%)	76,113,113	1.57	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	8CT	A	409	-	40,41,41	0.20	0	50,56,56	0.38	0
33	CLA	1	302	3	64,72,73	2.18	8 (12%)	74,111,113	1.60	9 (12%)
33	CLA	c	510	-	65,73,73	2.17	8 (12%)	76,113,113	1.38	6 (7%)
38	KC2	2	309	-	48,53,53	1.56	8 (16%)	54,89,89	1.12	5 (9%)
37	LHG	A	411	-	23,23,48	0.86	1 (4%)	26,29,54	1.32	2 (7%)
37	LHG	g	316	-	21,21,48	0.78	0	23,26,54	1.26	2 (8%)
33	CLA	b	609	-	65,73,73	2.21	8 (12%)	76,113,113	1.43	7 (9%)
33	CLA	9	312	5	55,63,73	2.39	8 (14%)	64,101,113	1.52	6 (9%)
33	CLA	2	306	4	60,68,73	2.19	8 (13%)	70,107,113	1.53	7 (10%)
37	LHG	2	315	-	45,45,48	0.62	0	48,51,54	1.21	4 (8%)
33	CLA	2	301	4	45,53,73	2.63	8 (17%)	52,89,113	1.75	6 (11%)
43	DGD	C	519	-	63,63,67	0.91	2 (3%)	77,77,81	1.26	5 (6%)
33	CLA	8	308	-	55,63,73	2.35	8 (14%)	64,101,113	1.43	5 (7%)
35	8CT	7	312	-	40,41,41	0.20	0	50,56,56	0.42	0
33	CLA	5	303	-	55,63,73	2.43	9 (16%)	64,101,113	1.59	5 (7%)
39	II0	7	315	-	39,43,43	0.18	0	50,60,60	0.60	2 (4%)
33	CLA	B	611	-	65,73,73	2.20	8 (12%)	76,113,113	1.45	9 (11%)
33	CLA	g	311	-	45,53,73	2.71	8 (17%)	52,89,113	1.76	7 (13%)
33	CLA	6	306	-	45,53,73	2.54	8 (17%)	52,89,113	1.71	9 (17%)
33	CLA	1	308	-	51,59,73	2.48	8 (15%)	59,96,113	1.55	4 (6%)
33	CLA	C	504	-	65,73,73	2.18	8 (12%)	76,113,113	1.34	4 (5%)
37	LHG	7	317	-	48,48,48	0.62	0	51,54,54	1.25	6 (11%)
33	CLA	a	405	-	65,73,73	2.17	8 (12%)	76,113,113	1.42	7 (9%)
35	8CT	a	409	-	40,41,41	0.20	0	50,56,56	0.38	0
33	CLA	g	307	-	55,63,73	2.26	8 (14%)	64,101,113	1.57	8 (12%)
42	LMG	m	101	-	38,38,55	0.96	1 (2%)	46,46,63	1.23	6 (13%)
33	CLA	B	612	-	65,73,73	2.19	8 (12%)	76,113,113	1.44	6 (7%)
40	IHT	6	318	-	40,42,42	0.32	0	53,58,58	0.45	0
33	CLA	C	510	-	65,73,73	2.16	8 (12%)	76,113,113	1.38	6 (7%)
33	CLA	C	514	-	65,73,73	2.21	8 (12%)	76,113,113	1.31	5 (6%)
39	II0	6	317	-	39,43,43	0.31	0	50,60,60	0.62	1 (2%)
40	IHT	9	320	-	40,42,42	0.21	0	53,58,58	0.49	0
39	II0	3	317	-	39,43,43	0.23	0	50,60,60	0.63	1 (2%)
33	CLA	3	312	5	55,63,73	2.39	8 (14%)	64,101,113	1.52	6 (9%)
34	PHO	d	403	-	51,69,69	0.41	0	47,99,99	0.66	1 (2%)
41	SQD	j	101	-	45,46,54	1.26	4 (8%)	54,57,65	1.28	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	LMG	c	520	-	51,51,55	0.72	1 (1%)	59,59,63	1.35	7 (11%)
35	8CT	d	406	-	40,41,41	0.21	0	50,56,56	0.70	1 (2%)
33	CLA	g	317	-	39,48,73	2.92	8 (20%)	45,82,113	1.94	8 (17%)
35	8CT	C	515	-	40,41,41	0.45	1 (2%)	50,56,56	0.64	0
33	CLA	b	618	-	39,48,73	2.84	8 (20%)	45,82,113	2.01	9 (20%)
33	CLA	7	306	-	60,68,73	2.23	8 (13%)	70,107,113	1.47	5 (7%)
39	II0	g	313	-	39,43,43	0.33	0	50,60,60	0.92	2 (4%)
33	CLA	2	307	-	60,68,73	2.29	8 (13%)	70,107,113	1.43	4 (5%)
35	8CT	B	620	-	40,41,41	0.23	0	50,56,56	0.51	0
39	II0	5	313	-	39,43,43	0.32	0	50,60,60	0.92	2 (4%)
39	II0	8	312	-	39,43,43	0.20	0	50,60,60	0.87	3 (6%)
35	8CT	c	516	-	40,41,41	0.19	0	50,56,56	0.39	0
33	CLA	6	310	-	41,49,73	2.78	9 (21%)	47,84,113	1.81	10 (21%)
35	8CT	h	102	-	40,41,41	0.22	0	50,56,56	0.43	0
33	CLA	3	306	-	41,49,73	2.91	9 (21%)	47,84,113	1.97	6 (12%)
33	CLA	9	308	-	49,57,73	2.42	8 (16%)	55,93,113	1.64	7 (12%)
33	CLA	3	315	-	41,49,73	2.85	9 (21%)	47,84,113	1.69	6 (12%)
42	LMG	D	410	-	46,46,55	0.82	1 (2%)	54,54,63	1.32	6 (11%)
33	CLA	4	301	2	41,49,73	2.86	9 (21%)	47,84,113	1.91	8 (17%)
42	LMG	d	410	-	46,46,55	0.82	1 (2%)	54,54,63	1.32	6 (11%)
39	II0	1	316	-	39,43,43	0.23	0	50,60,60	0.58	0
37	LHG	D	408	-	48,48,48	0.66	1 (2%)	51,54,54	1.13	2 (3%)
41	SQD	L	101	-	53,54,54	1.20	4 (7%)	62,65,65	1.08	4 (6%)
43	DGD	C	518	-	56,56,67	0.88	1 (1%)	70,70,81	1.44	11 (15%)
33	CLA	c	511	-	65,73,73	2.15	8 (12%)	76,113,113	1.36	5 (6%)
38	KC2	9	311	-	48,53,53	1.58	8 (16%)	54,89,89	1.02	5 (9%)
33	CLA	b	608	-	65,73,73	2.16	8 (12%)	76,113,113	1.38	5 (6%)
43	DGD	c	519	-	63,63,67	0.91	2 (3%)	77,77,81	1.26	5 (6%)
33	CLA	5	304	-	45,53,73	2.59	8 (17%)	52,89,113	1.80	6 (11%)
33	CLA	b	615	-	45,53,73	2.68	8 (17%)	52,89,113	1.80	5 (9%)
39	II0	0	314	-	39,43,43	0.32	0	50,60,60	0.49	1 (2%)
41	SQD	l	101	-	53,54,54	1.20	4 (7%)	62,65,65	1.08	4 (6%)
33	CLA	B	614	-	65,73,73	2.18	8 (12%)	76,113,113	1.40	9 (11%)
33	CLA	1	305	3	60,68,73	2.28	8 (13%)	70,107,113	1.37	4 (5%)
33	CLA	B	618	-	39,48,73	2.86	8 (20%)	45,82,113	2.04	9 (20%)
35	8CT	H	102	-	40,41,41	0.22	0	50,56,56	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	HEM	F	101	12,11	41,50,50	1.34	5 (12%)	45,82,82	1.87	9 (20%)
33	CLA	0	304	-	47,55,73	2.45	8 (17%)	54,91,113	1.73	7 (12%)
33	CLA	9	304	-	45,53,73	2.64	8 (17%)	52,89,113	1.67	6 (11%)
39	II0	g	312	-	39,43,43	0.40	0	50,60,60	0.74	3 (6%)
33	CLA	B	615	-	45,53,73	2.68	8 (17%)	52,89,113	1.80	6 (11%)
40	IHT	g	315	-	40,42,42	0.22	0	53,58,58	0.41	0
33	CLA	A	412	-	65,73,73	2.21	8 (12%)	76,113,113	1.58	10 (13%)
33	CLA	c	514	-	65,73,73	2.21	8 (12%)	76,113,113	1.32	5 (6%)
35	8CT	b	621	-	40,41,41	0.18	0	50,56,56	0.36	0
33	CLA	1	301	3	45,53,73	2.60	8 (17%)	52,89,113	1.85	6 (11%)
33	CLA	7	304	-	55,63,73	2.35	8 (14%)	64,101,113	1.53	5 (7%)
33	CLA	C	511	-	65,73,73	2.15	8 (12%)	76,113,113	1.36	6 (7%)
37	LHG	9	321	-	23,23,48	0.86	1 (4%)	26,29,54	1.21	1 (3%)
38	KC2	1	310	-	48,53,53	1.59	8 (16%)	54,89,89	1.04	5 (9%)
43	DGD	c	518	-	56,56,67	0.88	1 (1%)	70,70,81	1.44	11 (15%)
33	CLA	7	308	-	51,59,73	2.47	8 (15%)	59,96,113	1.54	4 (6%)
33	CLA	g	310	-	41,49,73	2.92	9 (21%)	47,84,113	1.90	6 (12%)
39	II0	2	312	-	39,43,43	0.20	0	50,60,60	0.87	3 (6%)
33	CLA	c	504	-	65,73,73	2.17	8 (12%)	76,113,113	1.34	4 (5%)
33	CLA	g	301	6	42,50,73	2.72	8 (19%)	48,85,113	1.76	7 (14%)
33	CLA	N	303	37	47,55,73	2.50	8 (17%)	54,91,113	1.94	11 (20%)
33	CLA	d	404	-	65,73,73	2.15	8 (12%)	76,113,113	1.49	6 (7%)
33	CLA	8	305	-	55,63,73	2.33	8 (14%)	64,101,113	1.54	6 (9%)
35	8CT	b	619	-	40,41,41	0.21	0	50,56,56	0.42	0
39	II0	3	318	-	39,43,43	0.22	0	50,60,60	0.61	2 (4%)
33	CLA	6	313	-	41,49,73	2.51	9 (21%)	47,84,113	1.84	9 (19%)
33	CLA	7	302	3	64,72,73	2.17	8 (12%)	74,111,113	1.60	9 (12%)
35	8CT	4	311	-	40,41,41	0.32	0	50,56,56	0.35	0
37	LHG	d	408	-	48,48,48	0.65	1 (2%)	51,54,54	1.13	2 (3%)
39	II0	p	314	-	39,43,43	0.36	0	50,60,60	0.74	1 (2%)
33	CLA	g	305	-	39,48,73	2.71	8 (20%)	45,82,113	1.89	9 (20%)
37	LHG	5	316	-	21,21,48	0.78	0	23,26,54	1.26	2 (8%)
33	CLA	g	304	-	45,53,73	2.59	8 (17%)	52,89,113	1.78	6 (11%)
33	CLA	7	309	-	55,63,73	2.36	8 (14%)	64,101,113	1.44	5 (7%)
33	CLA	4	307	2	55,63,73	2.33	8 (14%)	64,101,113	1.59	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	II0	5	314	-	39,43,43	0.37	0	50,60,60	1.06	2 (4%)
33	CLA	n	301	-	65,73,73	2.17	8 (12%)	76,113,113	1.45	5 (6%)
33	CLA	5	305	-	39,48,73	2.72	8 (20%)	45,82,113	1.89	9 (20%)
33	CLA	5	317	-	39,48,73	2.92	8 (20%)	45,82,113	1.94	8 (17%)
33	CLA	8	307	-	60,68,73	2.30	8 (13%)	70,107,113	1.43	4 (5%)
33	CLA	C	506	-	65,73,73	2.16	8 (12%)	76,113,113	1.38	6 (7%)
33	CLA	b	606	-	65,73,73	2.20	9 (13%)	76,113,113	1.46	7 (9%)
37	LHG	3	321	-	23,23,48	0.86	0	26,29,54	1.21	1 (3%)
38	KC2	1	311	-	48,53,53	1.55	8 (16%)	54,89,89	1.09	5 (9%)
31	BCT	A	403	30	2,3,3	1.25	0	2,3,3	4.17	2 (100%)
35	8CT	Y	101	-	40,41,41	0.22	0	50,56,56	0.51	0
33	CLA	a	408	-	60,68,73	2.28	8 (13%)	70,107,113	1.46	5 (7%)
39	II0	8	311	-	39,43,43	0.24	0	50,60,60	0.53	1 (2%)
33	CLA	5	308	-	41,49,73	2.90	9 (21%)	47,84,113	1.88	6 (12%)
33	CLA	N	306	-	55,63,73	2.38	8 (14%)	64,101,113	1.56	6 (9%)
33	CLA	7	307	-	65,73,73	2.23	8 (12%)	76,113,113	1.53	7 (9%)
33	CLA	p	312	-	41,49,73	2.69	9 (21%)	47,84,113	1.80	8 (17%)
33	CLA	N	302	-	65,73,73	2.18	8 (12%)	76,113,113	1.44	6 (7%)
33	CLA	0	303	-	50,58,73	2.52	8 (16%)	58,95,113	1.66	6 (10%)
39	II0	p	301	-	39,43,43	0.33	0	50,60,60	0.55	2 (4%)
39	II0	1	314	-	39,43,43	0.26	0	50,60,60	0.51	1 (2%)
33	CLA	B	608	-	65,73,73	2.17	8 (12%)	76,113,113	1.37	4 (5%)
35	8CT	C	516	-	40,41,41	0.19	0	50,56,56	0.39	0
33	CLA	0	308	37	47,55,73	2.50	8 (17%)	54,91,113	1.94	11 (20%)
33	CLA	c	513	-	56,64,73	2.39	8 (14%)	65,102,113	1.52	6 (9%)
33	CLA	g	302	6	55,63,73	2.39	8 (14%)	64,101,113	1.70	11 (17%)
40	IHT	5	315	-	40,42,42	0.22	0	53,58,58	0.42	0
42	LMG	B	622	-	49,49,55	0.77	0	57,57,63	1.21	5 (8%)
33	CLA	c	503	-	65,73,73	2.09	8 (12%)	76,113,113	1.37	5 (6%)
43	DGD	C	521	-	63,63,67	0.92	2 (3%)	77,77,81	1.33	8 (10%)
36	PL9	A	410	-	30,30,55	0.92	1 (3%)	38,39,69	1.33	6 (15%)
42	LMG	B	624	-	43,43,55	0.81	1 (2%)	51,51,63	1.25	5 (9%)
39	II0	7	314	-	39,43,43	0.25	0	50,60,60	0.52	1 (2%)
33	CLA	9	306	5	41,49,73	2.91	9 (21%)	47,84,113	1.99	6 (12%)
41	SQD	c	501	-	41,42,54	1.34	4 (9%)	50,53,65	1.26	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	p	308	7	42,50,73	2.61	8 (19%)	48,85,113	1.88	9 (18%)
33	CLA	b	611	-	65,73,73	2.20	8 (12%)	76,113,113	1.45	9 (11%)
39	II0	9	318	-	39,43,43	0.22	0	50,60,60	0.61	2 (4%)
42	LMG	d	409	-	46,46,55	0.77	0	54,54,63	1.21	2 (3%)
33	CLA	8	304	-	60,68,73	2.29	8 (13%)	70,107,113	1.50	5 (7%)
33	CLA	1	304	-	55,63,73	2.36	8 (14%)	64,101,113	1.53	5 (7%)
33	CLA	b	617	-	60,68,73	2.28	8 (13%)	70,107,113	1.42	6 (8%)
33	CLA	B	604	-	65,73,73	2.12	8 (12%)	76,113,113	1.40	4 (5%)
33	CLA	9	307	-	45,53,73	2.64	8 (17%)	52,89,113	1.80	6 (11%)
33	CLA	3	308	-	49,57,73	2.42	8 (16%)	55,93,113	1.64	7 (12%)
33	CLA	N	307	-	50,58,73	2.57	8 (16%)	58,95,113	1.65	8 (13%)
33	CLA	5	306	6	45,53,73	2.58	8 (17%)	52,89,113	1.68	5 (9%)
33	CLA	b	614	-	65,73,73	2.18	8 (12%)	76,113,113	1.40	9 (11%)
39	II0	6	316	-	39,43,43	0.33	0	50,60,60	0.71	2 (4%)
33	CLA	B	613	-	65,73,73	2.17	8 (12%)	76,113,113	1.38	4 (5%)
33	CLA	c	507	-	65,73,73	2.18	8 (12%)	76,113,113	1.44	6 (7%)
33	CLA	4	303	-	50,58,73	2.52	8 (16%)	58,95,113	1.66	6 (10%)
33	CLA	b	602	-	50,58,73	2.50	8 (16%)	58,95,113	1.57	7 (12%)
37	LHG	d	401	-	45,45,48	0.67	1 (2%)	48,51,54	1.18	4 (8%)
39	II0	0	313	-	39,43,43	0.36	0	50,60,60	0.56	0
33	CLA	B	616	-	65,73,73	2.16	8 (12%)	76,113,113	1.31	7 (9%)
39	II0	6	315	-	39,43,43	0.33	0	50,60,60	0.54	1 (2%)
39	II0	9	316	-	39,43,43	0.28	0	50,60,60	0.63	1 (2%)
40	IHT	3	320	-	40,42,42	0.21	0	53,58,58	0.49	0
35	8CT	0	312	-	40,41,41	0.32	0	50,56,56	0.35	0
38	KC2	p	311	7	48,53,53	1.30	7 (14%)	54,89,89	1.12	6 (11%)
39	II0	2	313	-	39,43,43	0.20	0	50,60,60	0.55	0
39	II0	0	315	-	39,43,43	0.37	0	50,60,60	0.55	1 (2%)
39	II0	5	312	-	39,43,43	0.39	0	50,60,60	0.74	3 (6%)
39	II0	7	316	-	39,43,43	0.23	0	50,60,60	0.58	0
33	CLA	c	508	-	65,73,73	2.15	8 (12%)	76,113,113	1.32	7 (9%)
37	LHG	9	322	-	40,40,48	0.70	2 (5%)	43,46,54	1.23	4 (9%)
33	CLA	p	313	-	41,49,73	2.52	9 (21%)	47,84,113	1.84	9 (19%)
38	KC2	7	310	-	48,53,53	1.58	8 (16%)	54,89,89	1.03	5 (9%)
37	LHG	4	316	33	23,23,48	0.90	0	26,29,54	1.23	1 (3%)

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
33	CLA	b	603	-	1/1/15/20	4/37/115/115	-
33	CLA	b	613	-	1/1/15/20	8/37/115/115	-
35	8CT	y	101	-	-	8/29/63/63	0/2/2/2
33	CLA	n	303	-	1/1/10/20	1/8/86/115	-
42	LMG	b	622	-	-	21/44/64/70	0/1/1/1
33	CLA	9	309	5	1/1/13/20	6/25/103/115	-
33	CLA	c	509	-	1/1/15/20	4/37/115/115	-
33	CLA	8	310	-	1/1/11/20	2/15/93/115	-
33	CLA	1	303	-	1/1/12/20	3/21/99/115	-
39	II0	9	319	-	-	2/21/67/67	0/2/2/2
33	CLA	B	602	-	1/1/12/20	6/19/97/115	-
33	CLA	9	310	-	1/1/10/20	2/8/86/115	-
33	CLA	2	302	4	1/1/13/20	10/25/103/115	-
36	PL9	d	407	-	-	18/53/73/73	0/1/1/1
33	CLA	6	319	-	1/1/10/20	6/8/86/115	-
33	CLA	p	319	-	1/1/10/20	6/8/86/115	-
33	CLA	p	303	7	1/1/10/20	2/8/86/115	-
37	LHG	9	302	-	-	19/45/45/53	-
33	CLA	D	404	-	1/1/15/20	1/37/115/115	-
38	KC2	5	309	-	-	4/15/71/71	-
33	CLA	3	314	-	1/1/10/20	0/8/86/115	-
33	CLA	A	405	-	1/1/15/20	4/37/115/115	-
33	CLA	7	301	3	1/1/11/20	3/13/91/115	-
35	8CT	D	406	-	-	9/29/63/63	0/2/2/2
33	CLA	9	313	-	1/1/10/20	2/8/86/115	-
38	KC2	4	305	-	-	9/15/71/71	-
44	HEM	f	101	11	-	0/12/54/54	-
33	CLA	A	408	-	1/1/14/20	2/31/109/115	-
33	CLA	9	305	-	1/1/13/20	4/25/103/115	-
33	CLA	5	301	6	1/1/10/20	5/10/88/115	-
38	KC2	6	311	7	-	3/15/71/71	-
33	CLA	N	304	-	1/1/10/20	1/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	LMG	D	409	-	-	17/41/61/70	0/1/1/1
33	CLA	0	306	2	1/1/13/20	9/25/103/115	-
34	PHO	A	407	-	-	10/37/103/103	0/5/6/6
42	LMG	b	624	-	-	16/38/58/70	0/1/1/1
37	LHG	D	402	-	-	19/51/51/53	-
33	CLA	2	308	-	1/1/13/20	1/25/103/115	-
33	CLA	8	306	4	1/1/14/20	3/31/109/115	-
37	LHG	3	302	-	-	19/45/45/53	-
33	CLA	8	301	4	1/1/11/20	4/13/91/115	-
39	II0	1	313	-	-	1/21/67/67	0/2/2/2
37	LHG	0	317	33	-	7/27/27/53	-
33	CLA	3	310	-	1/1/10/20	2/8/86/115	-
33	CLA	3	307	-	1/1/11/20	7/13/91/115	-
41	SQD	C	501	-	-	9/37/57/69	0/1/1/1
38	KC2	g	309	-	-	4/15/71/71	-
42	LMG	C	520	-	-	28/46/66/70	0/1/1/1
33	CLA	b	605	-	1/1/15/20	14/37/115/115	-
33	CLA	p	302	7	1/1/10/20	0/8/86/115	-
33	CLA	b	616	-	1/1/15/20	5/37/115/115	-
33	CLA	b	612	-	1/1/15/20	3/37/115/115	-
39	II0	4	314	-	-	1/21/67/67	0/2/2/2
38	KC2	7	311	-	-	6/15/71/71	-
33	CLA	B	605	-	1/1/15/20	14/37/115/115	-
33	CLA	9	315	-	1/1/10/20	4/8/86/115	-
33	CLA	3	305	-	1/1/13/20	4/25/103/115	-
35	8CT	c	517	-	-	6/29/63/63	0/2/2/2
39	II0	p	315	-	-	2/21/67/67	0/2/2/2
33	CLA	C	503	-	1/1/15/20	8/37/115/115	-
33	CLA	d	405	-	1/1/15/20	9/37/115/115	-
33	CLA	b	607	-	1/1/15/20	9/37/115/115	-
33	CLA	b	610	-	1/1/15/20	8/37/115/115	-
33	CLA	p	307	-	1/1/10/20	1/11/89/115	-
44	HEM	V	201	-	-	3/12/54/54	-
33	CLA	3	309	5	1/1/13/20	6/25/103/115	-
39	II0	0	316	-	-	2/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	C	507	-	1/1/15/20	10/37/115/115	-
36	PL9	D	407	-	-	18/53/73/73	0/1/1/1
39	II0	g	314	-	-	0/21/67/67	0/2/2/2
35	8CT	1	312	-	-	5/29/63/63	0/2/2/2
39	II0	6	301	-	-	0/21/67/67	0/2/2/2
33	CLA	B	610	-	1/1/15/20	8/37/115/115	-
39	II0	1	315	-	-	2/21/67/67	0/2/2/2
35	8CT	B	619	-	-	3/29/63/63	0/2/2/2
33	CLA	7	305	3	1/1/14/20	7/31/109/115	-
33	CLA	6	303	7	1/1/10/20	2/8/86/115	-
43	DGD	H	101	-	-	13/49/89/95	0/2/2/2
35	8CT	b	620	-	-	10/29/63/63	0/2/2/2
33	CLA	N	305	-	1/1/13/20	5/25/103/115	-
42	LMG	w	101	-	-	26/42/62/70	0/1/1/1
33	CLA	A	406	-	1/1/11/20	6/18/96/115	-
36	PL9	a	410	-	-	5/23/43/73	0/1/1/1
33	CLA	6	309	7	1/1/10/20	2/10/88/115	-
42	LMG	t	101	-	-	15/38/58/70	0/1/1/1
33	CLA	2	303	-	1/1/12/20	13/22/100/115	-
35	8CT	B	621	-	-	8/29/63/63	0/2/2/2
33	CLA	C	513	-	1/1/13/20	6/27/105/115	-
39	II0	2	311	-	-	0/21/67/67	0/2/2/2
33	CLA	p	304	-	1/1/10/20	2/10/88/115	-
33	CLA	a	406	-	1/1/11/20	6/18/96/115	-
33	CLA	5	310	-	1/1/10/20	0/8/86/115	-
33	CLA	c	512	-	1/1/15/20	7/37/115/115	-
33	CLA	0	309	-	1/1/11/20	11/16/94/115	-
42	LMG	W	101	-	-	26/42/62/70	0/1/1/1
38	KC2	8	309	-	-	9/15/71/71	-
33	CLA	6	305	-	1/1/13/20	4/25/103/115	-
39	II0	9	317	-	-	0/21/67/67	0/2/2/2
38	KC2	3	311	-	-	7/15/71/71	-
34	PHO	D	403	-	-	6/37/103/103	0/5/6/6
33	CLA	0	310	-	1/1/9/20	8/8/82/115	-
33	CLA	1	306	-	1/1/14/20	6/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	0	301	2	1/1/10/20	3/8/86/115	-
33	CLA	B	607	-	1/1/15/20	9/37/115/115	-
37	LHG	8	315	-	-	35/50/50/53	-
39	II0	3	301	-	-	1/21/67/67	0/2/2/2
33	CLA	2	310	-	1/1/11/20	2/15/93/115	-
37	LHG	b	623	-	-	28/53/53/53	-
39	II0	4	312	-	-	2/21/67/67	0/2/2/2
33	CLA	D	405	-	1/1/15/20	9/37/115/115	-
37	LHG	1	317	-	-	21/53/53/53	-
39	II0	6	314	-	-	0/21/67/67	0/2/2/2
42	LMG	l	102	-	-	9/33/53/70	0/1/1/1
39	II0	p	316	-	-	0/21/67/67	0/2/2/2
33	CLA	6	302	7	1/1/10/20	0/8/86/115	-
33	CLA	9	303	5	1/1/13/20	6/25/103/115	-
37	LHG	D	401	-	-	25/50/50/53	-
33	CLA	6	307	-	1/1/10/20	1/11/89/115	-
33	CLA	n	305	-	1/1/13/20	2/25/103/115	-
33	CLA	3	303	5	1/1/13/20	6/25/103/115	-
33	CLA	B	609	-	1/1/15/20	2/37/115/115	-
37	LHG	B	623	-	-	28/53/53/53	-
33	CLA	b	604	-	1/1/15/20	3/37/115/115	-
33	CLA	p	309	7	1/1/10/20	2/10/88/115	-
37	LHG	d	402	-	-	19/51/51/53	-
33	CLA	0	302	2	1/1/12/20	3/21/99/115	-
33	CLA	n	304	-	1/1/13/20	5/25/103/115	-
33	CLA	C	512	-	1/1/15/20	7/37/115/115	-
33	CLA	N	301	-	1/1/15/20	12/37/115/115	-
33	CLA	c	502	-	1/1/15/20	3/37/115/115	-
33	CLA	4	310	-	1/1/11/20	5/13/91/115	-
41	SQD	B	601	-	-	11/33/53/69	0/1/1/1
33	CLA	3	304	-	1/1/11/20	0/13/91/115	-
39	II0	3	319	-	-	2/21/67/67	0/2/2/2
33	CLA	B	606	-	1/1/15/20	3/37/115/115	-
34	PHO	a	407	-	-	10/37/103/103	0/5/6/6
37	LHG	3	322	-	-	19/45/45/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	8CT	C	517	-	-	6/29/63/63	0/2/2/2
43	DGD	c	521	-	-	23/51/91/95	0/2/2/2
41	SQD	b	601	-	-	11/33/53/69	0/1/1/1
33	CLA	0	311	-	1/1/11/20	5/13/91/115	-
33	CLA	9	314	-	1/1/10/20	0/8/86/115	-
33	CLA	g	306	6	1/1/11/20	0/13/91/115	-
44	HEM	v	201	-	-	3/12/54/54	-
43	DGD	h	101	-	-	13/49/89/95	0/2/2/2
33	CLA	g	308	-	1/1/10/20	1/8/86/115	-
33	CLA	8	303	-	1/1/12/20	13/22/100/115	-
33	CLA	4	302	2	1/1/12/20	3/21/99/115	-
33	CLA	3	313	-	1/1/10/20	2/8/86/115	-
33	CLA	1	307	-	1/1/15/20	5/37/115/115	-
37	LHG	a	411	-	-	6/28/28/53	-
33	CLA	6	304	-	1/1/10/20	2/10/88/115	-
33	CLA	p	310	-	1/1/10/20	5/8/86/115	-
33	CLA	4	309	-	1/1/9/20	8/8/82/115	-
33	CLA	5	307	-	1/1/13/20	8/25/103/115	-
33	CLA	4	306	2	1/1/13/20	9/25/103/115	-
33	CLA	5	311	-	1/1/11/20	7/13/91/115	-
33	CLA	C	508	-	1/1/15/20	6/37/115/115	-
39	II0	4	313	-	-	2/21/67/67	0/2/2/2
40	IHT	8	314	-	-	0/25/65/65	0/2/2/2
33	CLA	7	303	-	1/1/12/20	3/21/99/115	-
33	CLA	p	305	-	1/1/13/20	4/25/103/115	-
42	LMG	T	101	-	-	15/38/58/70	0/1/1/1
41	SQD	J	101	-	-	20/41/61/69	0/1/1/1
33	CLA	B	617	-	1/1/14/20	3/31/109/115	-
33	CLA	C	509	-	1/1/15/20	4/37/115/115	-
33	CLA	n	302	-	1/1/15/20	6/37/115/115	-
33	CLA	8	302	4	1/1/13/20	10/25/103/115	-
35	8CT	c	515	-	-	8/29/63/63	0/2/2/2
33	CLA	n	306	-	1/1/12/20	4/19/97/115	-
33	CLA	p	306	-	1/1/11/20	6/13/91/115	-
39	II0	3	316	-	-	3/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	2	304	-	1/1/14/20	5/31/109/115	-
33	CLA	4	304	-	1/1/11/20	4/16/94/115	-
33	CLA	B	603	-	1/1/15/20	4/37/115/115	-
33	CLA	C	505	-	1/1/15/20	11/37/115/115	-
33	CLA	1	309	-	1/1/13/20	0/25/103/115	-
40	IHT	p	318	-	-	2/25/65/65	0/2/2/2
39	II0	8	313	-	-	5/21/67/67	0/2/2/2
33	CLA	g	303	-	1/1/13/20	3/25/103/115	-
33	CLA	4	308	-	1/1/11/20	11/16/94/115	-
39	II0	p	317	-	-	2/21/67/67	0/2/2/2
33	CLA	5	302	6	1/1/13/20	8/25/103/115	-
33	CLA	C	502	-	1/1/15/20	3/37/115/115	-
39	II0	7	313	-	-	1/21/67/67	0/2/2/2
40	IHT	2	314	-	-	0/25/65/65	0/2/2/2
33	CLA	c	505	-	1/1/15/20	11/37/115/115	-
39	II0	4	315	-	-	3/21/67/67	0/2/2/2
33	CLA	0	307	2	1/1/13/20	10/25/103/115	-
39	II0	9	301	-	-	1/21/67/67	0/2/2/2
33	CLA	2	305	-	1/1/13/20	5/25/103/115	-
33	CLA	6	312	-	1/1/10/20	2/8/86/115	-
33	CLA	c	506	-	1/1/15/20	7/37/115/115	-
33	CLA	6	308	7	1/1/10/20	5/10/88/115	-
38	KC2	0	305	-	-	9/15/71/71	-
33	CLA	a	412	-	1/1/15/20	8/37/115/115	-
35	8CT	A	409	-	-	3/29/63/63	0/2/2/2
33	CLA	1	302	3	1/1/14/20	7/36/114/115	-
33	CLA	c	510	-	1/1/15/20	3/37/115/115	-
38	KC2	2	309	-	-	9/15/71/71	-
37	LHG	A	411	-	-	6/28/28/53	-
37	LHG	g	316	-	-	10/24/24/53	-
33	CLA	b	609	-	1/1/15/20	2/37/115/115	-
33	CLA	9	312	5	1/1/13/20	2/25/103/115	-
33	CLA	2	306	4	1/1/14/20	3/31/109/115	-
37	LHG	2	315	-	-	35/50/50/53	-
33	CLA	2	301	4	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	DGD	C	519	-	-	23/51/91/95	0/2/2/2
33	CLA	8	308	-	1/1/13/20	1/25/103/115	-
35	8CT	7	312	-	-	5/29/63/63	0/2/2/2
33	CLA	5	303	-	1/1/13/20	3/25/103/115	-
39	II0	7	315	-	-	2/21/67/67	0/2/2/2
33	CLA	B	611	-	1/1/15/20	5/37/115/115	-
33	CLA	g	311	-	1/1/11/20	7/13/91/115	-
33	CLA	6	306	-	1/1/11/20	6/13/91/115	-
33	CLA	1	308	-	1/1/12/20	6/21/99/115	-
33	CLA	C	504	-	1/1/15/20	2/37/115/115	-
37	LHG	7	317	-	-	21/53/53/53	-
33	CLA	a	405	-	1/1/15/20	4/37/115/115	-
35	8CT	a	409	-	-	3/29/63/63	0/2/2/2
33	CLA	g	307	-	1/1/13/20	8/25/103/115	-
42	LMG	m	101	-	-	9/33/53/70	0/1/1/1
33	CLA	B	612	-	1/1/15/20	3/37/115/115	-
40	IHT	6	318	-	-	2/25/65/65	0/2/2/2
33	CLA	C	510	-	1/1/15/20	3/37/115/115	-
33	CLA	C	514	-	1/1/15/20	4/37/115/115	-
39	II0	6	317	-	-	2/21/67/67	0/2/2/2
40	IHT	9	320	-	-	7/25/65/65	0/2/2/2
39	II0	3	317	-	-	0/21/67/67	0/2/2/2
33	CLA	3	312	5	1/1/13/20	2/25/103/115	-
34	PHO	d	403	-	-	6/37/103/103	0/5/6/6
41	SQD	j	101	-	-	20/41/61/69	0/1/1/1
42	LMG	c	520	-	-	28/46/66/70	0/1/1/1
35	8CT	d	406	-	-	9/29/63/63	0/2/2/2
33	CLA	g	317	-	1/1/9/20	1/8/82/115	-
35	8CT	C	515	-	-	8/29/63/63	0/2/2/2
33	CLA	b	618	-	1/1/9/20	2/8/82/115	-
33	CLA	7	306	-	1/1/14/20	6/31/109/115	-
39	II0	g	313	-	-	1/21/67/67	0/2/2/2
33	CLA	2	307	-	1/1/14/20	5/31/109/115	-
35	8CT	B	620	-	-	10/29/63/63	0/2/2/2
39	II0	5	313	-	-	1/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	II0	8	312	-	-	1/21/67/67	0/2/2/2
35	8CT	c	516	-	-	5/29/63/63	0/2/2/2
33	CLA	6	310	-	1/1/10/20	5/8/86/115	-
35	8CT	h	102	-	-	7/29/63/63	0/2/2/2
33	CLA	3	306	-	1/1/10/20	1/8/86/115	-
33	CLA	9	308	-	1/1/11/20	2/18/96/115	-
33	CLA	3	315	-	1/1/10/20	4/8/86/115	-
42	LMG	D	410	-	-	17/41/61/70	0/1/1/1
33	CLA	4	301	2	1/1/10/20	3/8/86/115	-
42	LMG	d	410	-	-	17/41/61/70	0/1/1/1
39	II0	1	316	-	-	2/21/67/67	0/2/2/2
37	LHG	D	408	-	-	21/53/53/53	-
41	SQD	L	101	-	-	19/49/69/69	0/1/1/1
43	DGD	C	518	-	-	13/44/84/95	0/2/2/2
33	CLA	c	511	-	1/1/15/20	8/37/115/115	-
38	KC2	9	311	-	-	7/15/71/71	-
33	CLA	b	608	-	1/1/15/20	6/37/115/115	-
43	DGD	c	519	-	-	23/51/91/95	0/2/2/2
33	CLA	5	304	-	1/1/11/20	3/13/91/115	-
33	CLA	b	615	-	1/1/11/20	4/13/91/115	-
39	II0	0	314	-	-	2/21/67/67	0/2/2/2
41	SQD	l	101	-	-	18/49/69/69	0/1/1/1
33	CLA	B	614	-	1/1/15/20	8/37/115/115	-
33	CLA	1	305	3	1/1/14/20	7/31/109/115	-
33	CLA	B	618	-	1/1/9/20	2/8/82/115	-
35	8CT	H	102	-	-	7/29/63/63	0/2/2/2
44	HEM	F	101	12,11	-	6/12/54/54	-
33	CLA	0	304	-	1/1/11/20	4/16/94/115	-
33	CLA	9	304	-	1/1/11/20	0/13/91/115	-
39	II0	g	312	-	-	1/21/67/67	0/2/2/2
33	CLA	B	615	-	1/1/11/20	4/13/91/115	-
40	IHT	g	315	-	-	0/25/65/65	0/2/2/2
33	CLA	A	412	-	1/1/15/20	8/37/115/115	-
33	CLA	c	514	-	1/1/15/20	4/37/115/115	-
35	8CT	b	621	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	1	301	3	1/1/11/20	3/13/91/115	-
33	CLA	7	304	-	1/1/13/20	4/25/103/115	-
33	CLA	C	511	-	1/1/15/20	8/37/115/115	-
37	LHG	9	321	-	-	13/27/27/53	-
38	KC2	1	310	-	-	7/15/71/71	-
43	DGD	c	518	-	-	12/44/84/95	0/2/2/2
33	CLA	7	308	-	1/1/12/20	6/21/99/115	-
33	CLA	g	310	-	1/1/10/20	0/8/86/115	-
39	II0	2	312	-	-	1/21/67/67	0/2/2/2
33	CLA	c	504	-	1/1/15/20	2/37/115/115	-
33	CLA	g	301	6	1/1/10/20	5/10/88/115	-
33	CLA	N	303	37	1/1/11/20	11/16/94/115	-
33	CLA	d	404	-	1/1/15/20	1/37/115/115	-
33	CLA	8	305	-	1/1/13/20	5/25/103/115	-
35	8CT	b	619	-	-	3/29/63/63	0/2/2/2
39	II0	3	318	-	-	1/21/67/67	0/2/2/2
33	CLA	6	313	-	1/1/10/20	4/8/86/115	-
33	CLA	7	302	3	1/1/14/20	7/36/114/115	-
35	8CT	4	311	-	-	4/29/63/63	0/2/2/2
37	LHG	d	408	-	-	20/53/53/53	-
39	II0	p	314	-	-	0/21/67/67	0/2/2/2
33	CLA	g	305	-	1/1/9/20	2/8/82/115	-
37	LHG	5	316	-	-	10/24/24/53	-
33	CLA	g	304	-	1/1/11/20	3/13/91/115	-
33	CLA	7	309	-	1/1/13/20	0/25/103/115	-
33	CLA	4	307	2	1/1/13/20	10/25/103/115	-
39	II0	5	314	-	-	0/21/67/67	0/2/2/2
33	CLA	n	301	-	1/1/15/20	12/37/115/115	-
33	CLA	5	305	-	1/1/9/20	2/8/82/115	-
33	CLA	5	317	-	1/1/9/20	1/8/82/115	-
33	CLA	8	307	-	1/1/14/20	5/31/109/115	-
33	CLA	C	506	-	1/1/15/20	7/37/115/115	-
33	CLA	b	606	-	1/1/15/20	3/37/115/115	-
37	LHG	3	321	-	-	13/27/27/53	-
38	KC2	1	311	-	-	6/15/71/71	-
35	8CT	Y	101	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	a	408	-	1/1/14/20	2/31/109/115	-
39	II0	8	311	-	-	0/21/67/67	0/2/2/2
33	CLA	5	308	-	1/1/10/20	1/8/86/115	-
33	CLA	N	306	-	1/1/13/20	2/25/103/115	-
33	CLA	7	307	-	1/1/15/20	5/37/115/115	-
33	CLA	p	312	-	1/1/10/20	2/8/86/115	-
33	CLA	N	302	-	1/1/15/20	6/37/115/115	-
33	CLA	0	303	-	1/1/12/20	5/19/97/115	-
39	II0	p	301	-	-	0/21/67/67	0/2/2/2
39	II0	1	314	-	-	1/21/67/67	0/2/2/2
33	CLA	B	608	-	1/1/15/20	6/37/115/115	-
35	8CT	C	516	-	-	5/29/63/63	0/2/2/2
33	CLA	0	308	37	1/1/11/20	11/16/94/115	-
33	CLA	c	513	-	1/1/13/20	6/27/105/115	-
33	CLA	g	302	6	1/1/13/20	8/25/103/115	-
40	IHT	5	315	-	-	0/25/65/65	0/2/2/2
42	LMG	B	622	-	-	21/44/64/70	0/1/1/1
33	CLA	c	503	-	1/1/15/20	7/37/115/115	-
43	DGD	C	521	-	-	23/51/91/95	0/2/2/2
36	PL9	A	410	-	-	5/23/43/73	0/1/1/1
42	LMG	B	624	-	-	16/38/58/70	0/1/1/1
39	II0	7	314	-	-	1/21/67/67	0/2/2/2
33	CLA	9	306	5	1/1/10/20	1/8/86/115	-
41	SQD	c	501	-	-	9/37/57/69	0/1/1/1
33	CLA	p	308	7	1/1/10/20	5/10/88/115	-
33	CLA	b	611	-	1/1/15/20	5/37/115/115	-
39	II0	9	318	-	-	1/21/67/67	0/2/2/2
42	LMG	d	409	-	-	17/41/61/70	0/1/1/1
33	CLA	8	304	-	1/1/14/20	5/31/109/115	-
33	CLA	1	304	-	1/1/13/20	4/25/103/115	-
33	CLA	b	617	-	1/1/14/20	3/31/109/115	-
33	CLA	B	604	-	1/1/15/20	3/37/115/115	-
33	CLA	9	307	-	1/1/11/20	7/13/91/115	-
33	CLA	3	308	-	1/1/11/20	2/18/96/115	-
33	CLA	N	307	-	1/1/12/20	4/19/97/115	-
33	CLA	5	306	6	1/1/11/20	0/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	b	614	-	1/1/15/20	7/37/115/115	-
39	II0	6	316	-	-	0/21/67/67	0/2/2/2
33	CLA	B	613	-	1/1/15/20	8/37/115/115	-
33	CLA	c	507	-	1/1/15/20	10/37/115/115	-
33	CLA	4	303	-	1/1/12/20	5/19/97/115	-
33	CLA	b	602	-	1/1/12/20	6/19/97/115	-
37	LHG	d	401	-	-	25/50/50/53	-
39	II0	0	313	-	-	2/21/67/67	0/2/2/2
33	CLA	B	616	-	1/1/15/20	5/37/115/115	-
39	II0	6	315	-	-	2/21/67/67	0/2/2/2
39	II0	9	316	-	-	3/21/67/67	0/2/2/2
40	IHT	3	320	-	-	7/25/65/65	0/2/2/2
35	8CT	0	312	-	-	4/29/63/63	0/2/2/2
38	KC2	p	311	7	-	3/15/71/71	-
39	II0	2	313	-	-	5/21/67/67	0/2/2/2
39	II0	0	315	-	-	1/21/67/67	0/2/2/2
39	II0	5	312	-	-	2/21/67/67	0/2/2/2
39	II0	7	316	-	-	2/21/67/67	0/2/2/2
33	CLA	c	508	-	1/1/15/20	6/37/115/115	-
37	LHG	9	322	-	-	19/45/45/53	-
33	CLA	p	313	-	1/1/10/20	4/8/86/115	-
38	KC2	7	310	-	-	7/15/71/71	-
37	LHG	4	316	33	-	7/27/27/53	-

The worst 5 of 1906 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	p	302	CLA	C1B-NB	11.31	1.45	1.35
33	6	302	CLA	C1B-NB	11.28	1.45	1.35
33	g	308	CLA	C1B-NB	10.86	1.44	1.35
33	5	308	CLA	C1B-NB	10.86	1.44	1.35
33	5	310	CLA	C1B-NB	10.82	1.44	1.35

The worst 5 of 1835 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	p	302	CLA	C4A-NA-C1A	-8.29	102.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	302	CLA	C4A-NA-C1A	-8.28	102.98	106.71
33	2	302	CLA	C4A-NA-C1A	-8.27	102.99	106.71
33	0	310	CLA	C4A-NA-C1A	-8.25	103.00	106.71
33	8	302	CLA	C4A-NA-C1A	-8.23	103.01	106.71

5 of 210 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	a	405	CLA	ND
33	a	406	CLA	ND
33	a	408	CLA	ND
33	a	412	CLA	ND
33	A	405	CLA	ND

5 of 2423 torsion outliers are listed below:

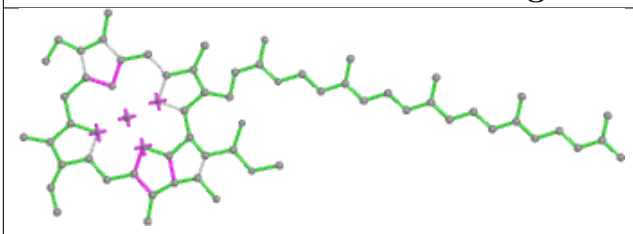
Mol	Chain	Res	Type	Atoms
33	a	412	CLA	C1A-C2A-CAA-CBA
33	a	412	CLA	C3A-C2A-CAA-CBA
33	A	412	CLA	C1A-C2A-CAA-CBA
33	A	412	CLA	C3A-C2A-CAA-CBA
33	0	306	CLA	C2-C3-C5-C6

There are no ring outliers.

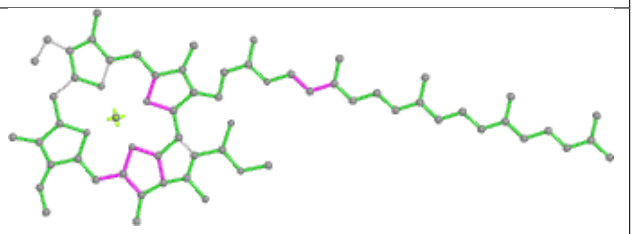
No monomer is involved in short contacts.

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

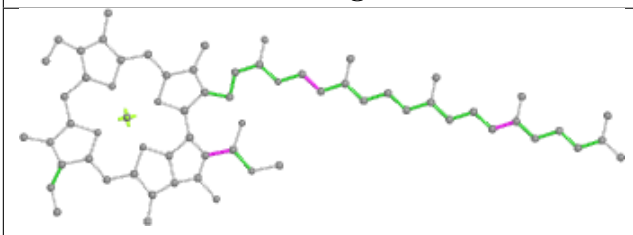
Ligand CLA b 603



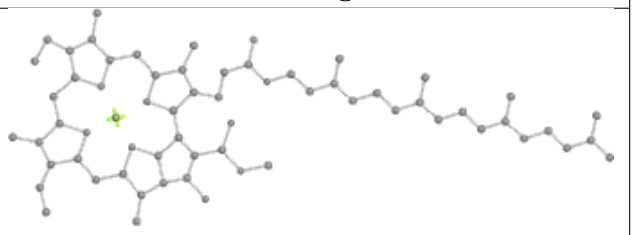
Bond lengths



Bond angles

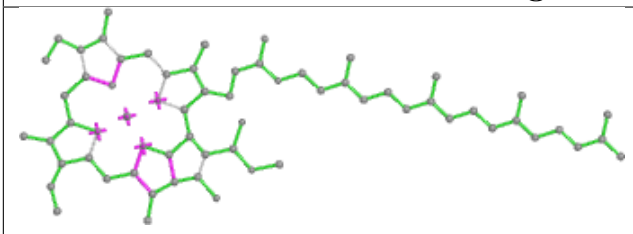


Torsions



Rings

Ligand CLA b 613



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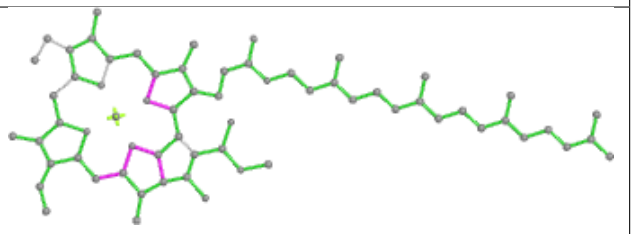

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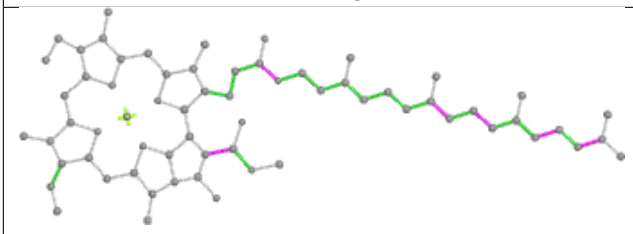

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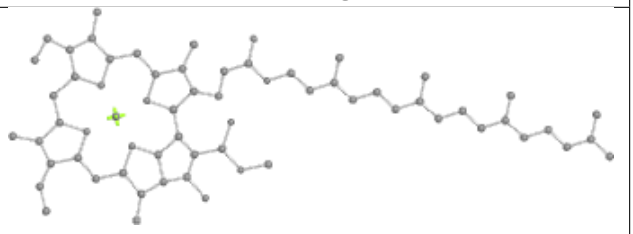
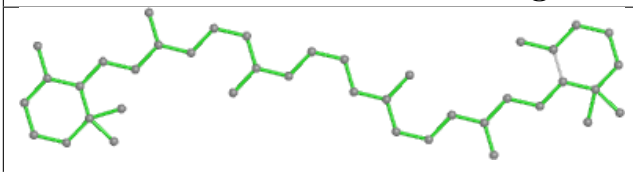


Rings

Ligand 8CT y 101



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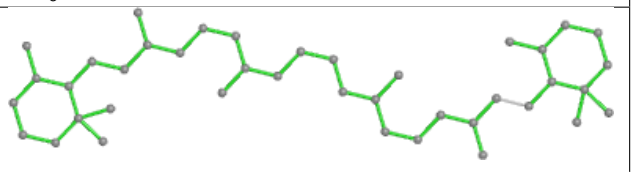
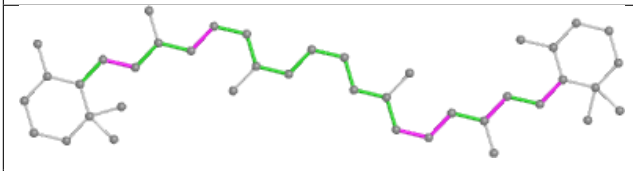


Bond angles



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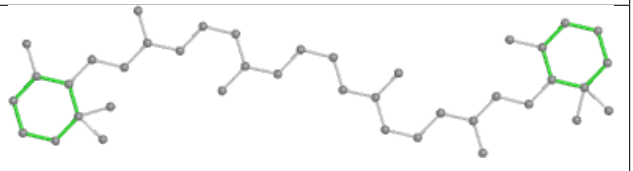
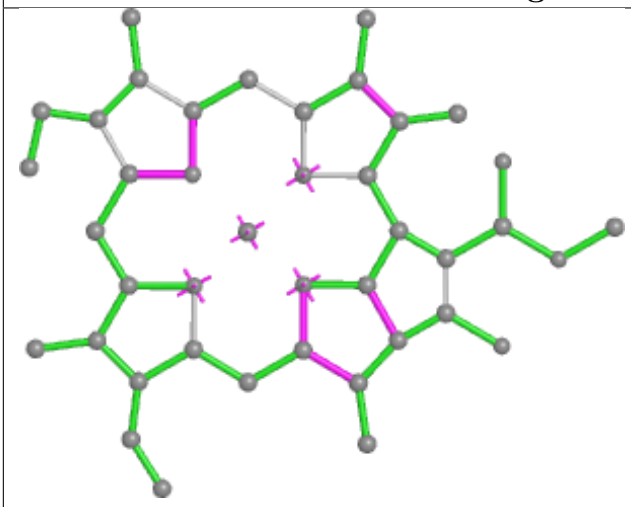


Rings

Ligand CLA n 303



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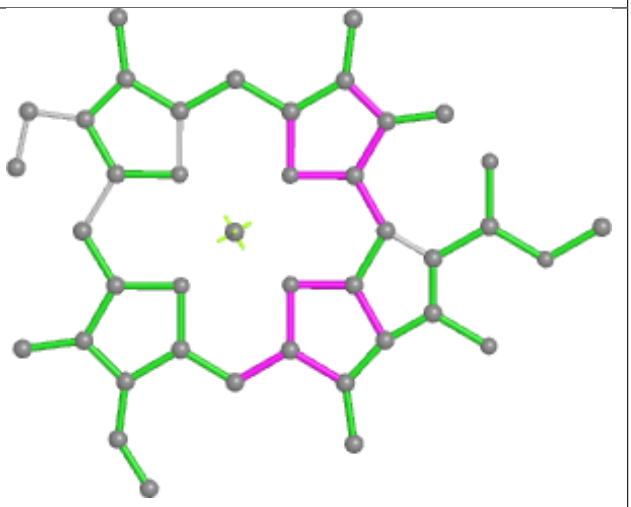
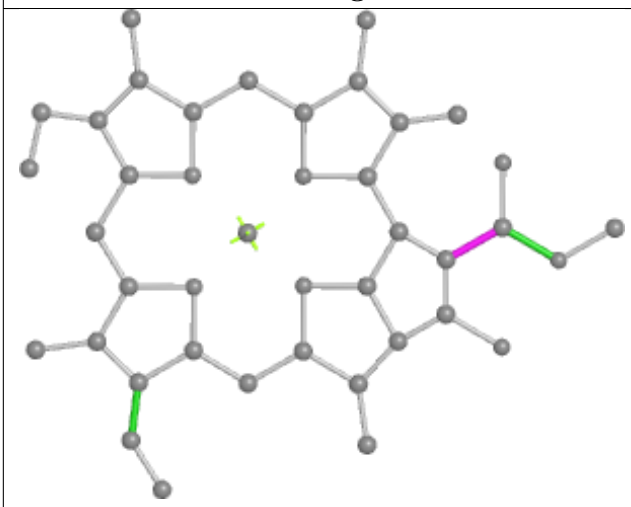
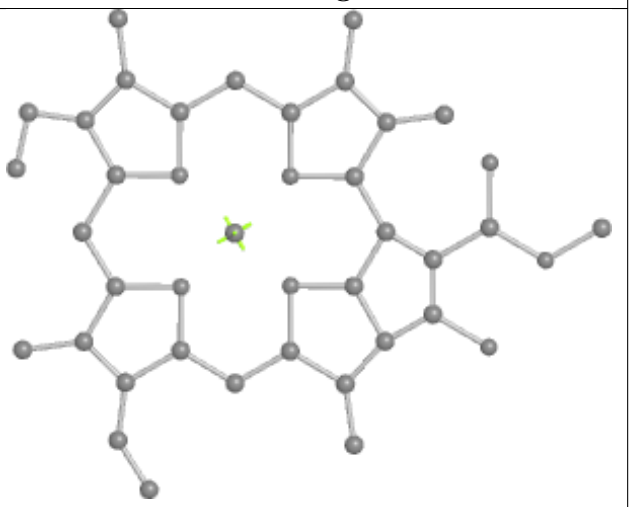


Bond angles

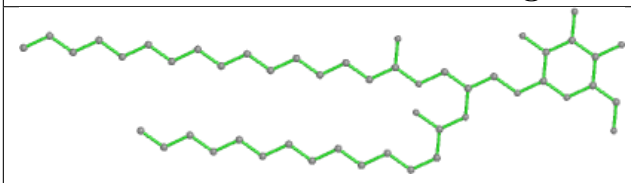


Torsions



Rings

Ligand LMG b 622



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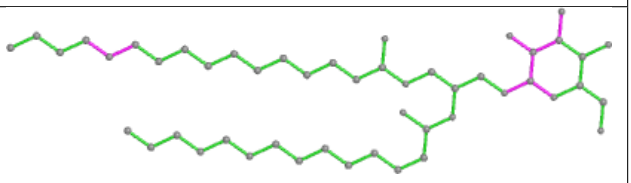
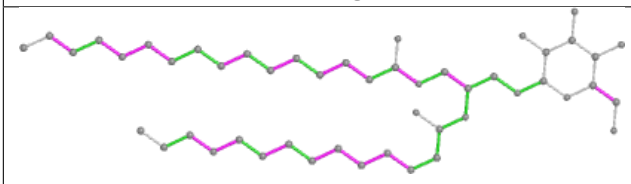


Bond angles



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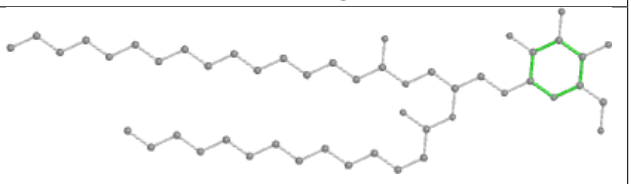
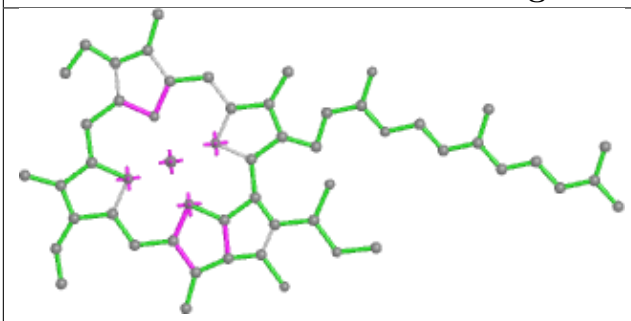
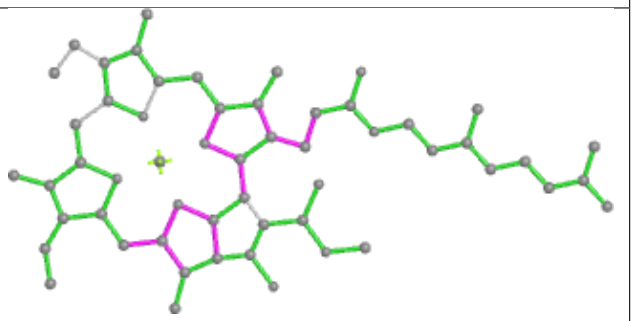
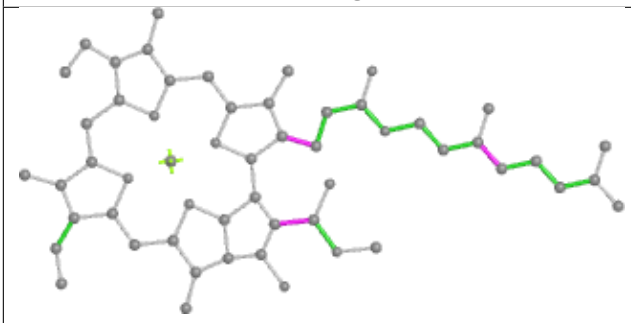
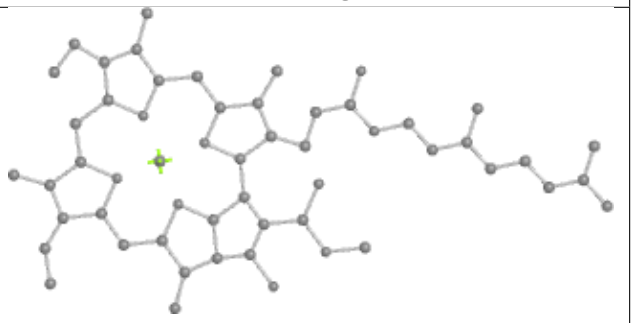


Rings

Ligand CLA 9 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

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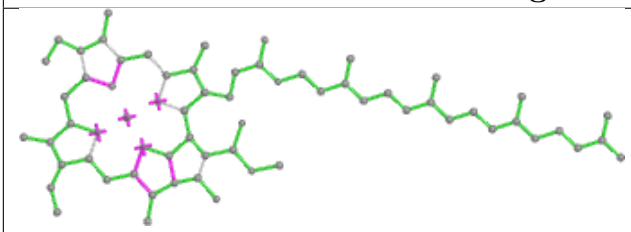
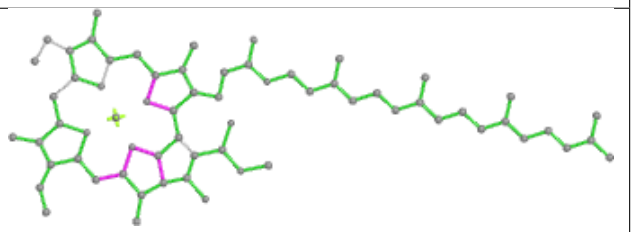
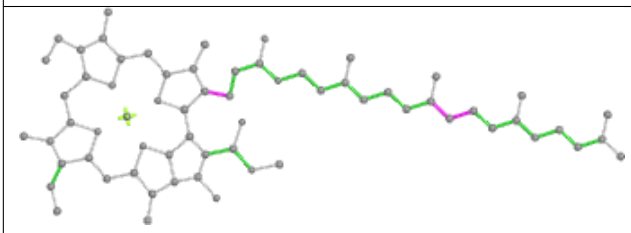
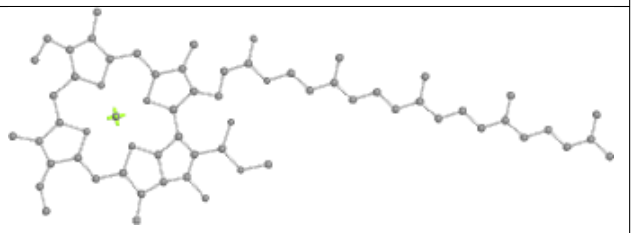
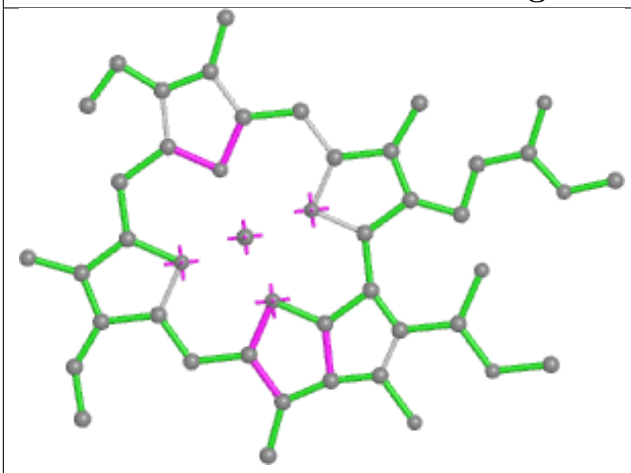
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 310



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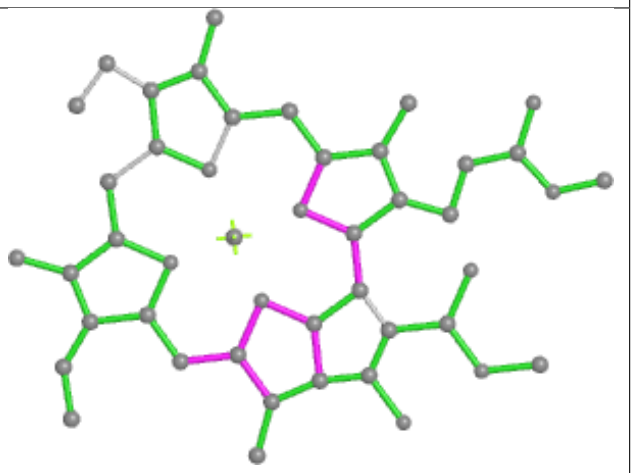
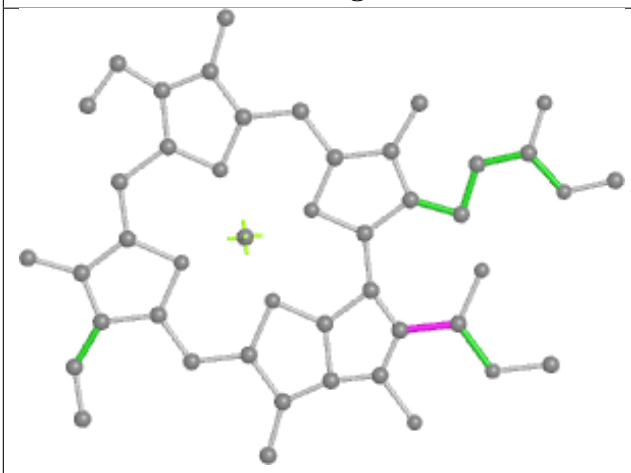


Bond angles



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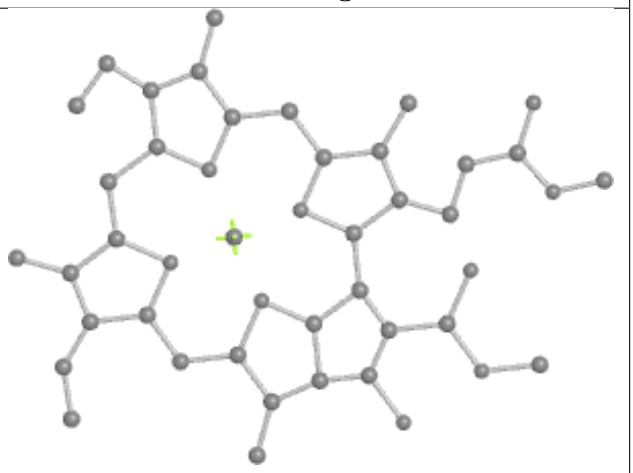
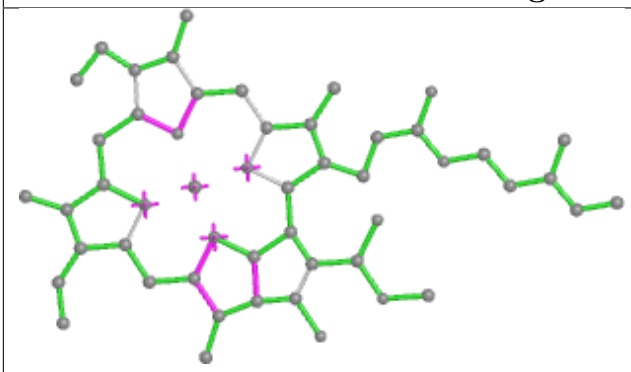


Rings

Ligand CLA 1 303



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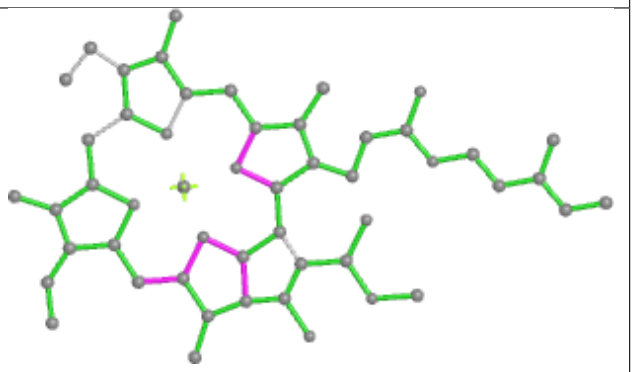

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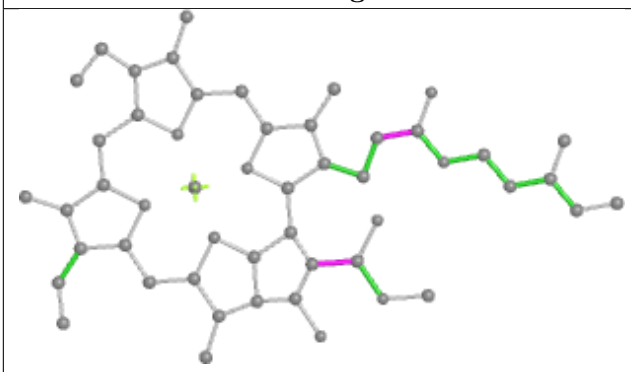

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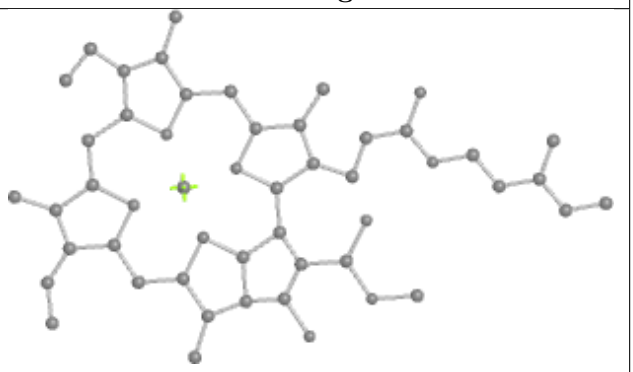
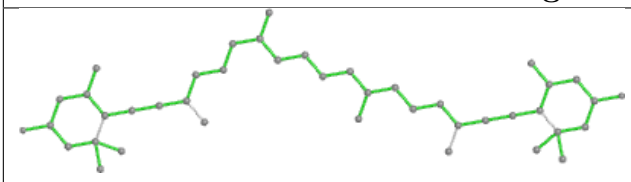


Rings

Ligand II0 9 319



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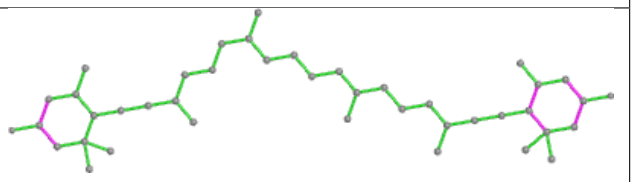
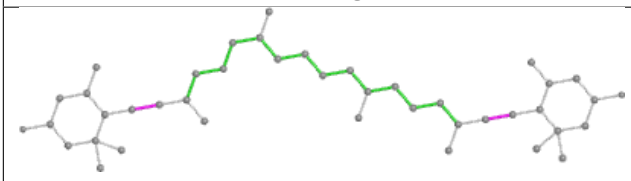


Bond angles



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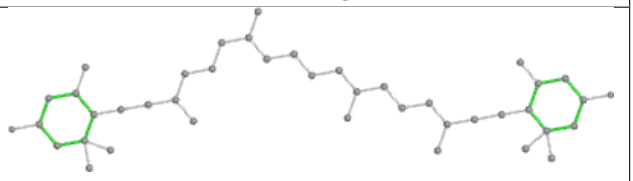
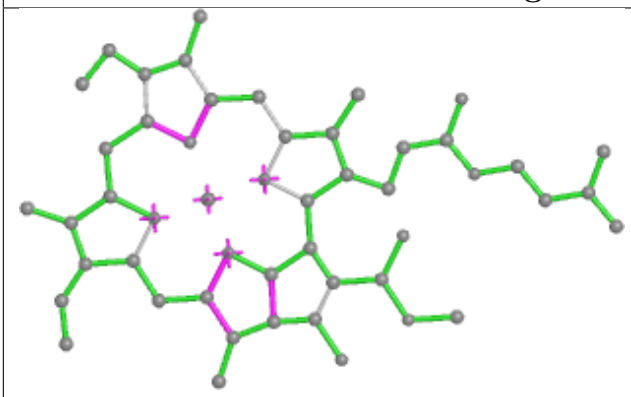


Rings

Ligand CLA B 602



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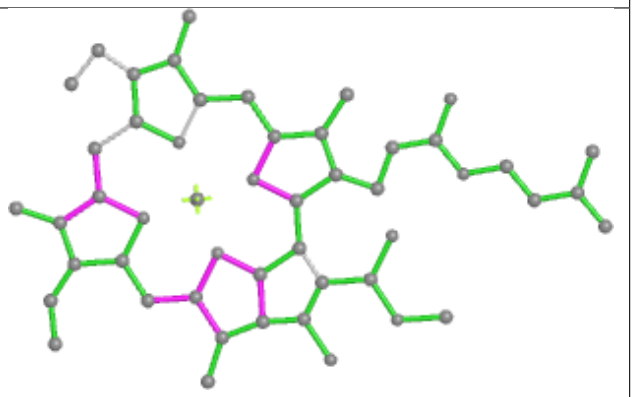
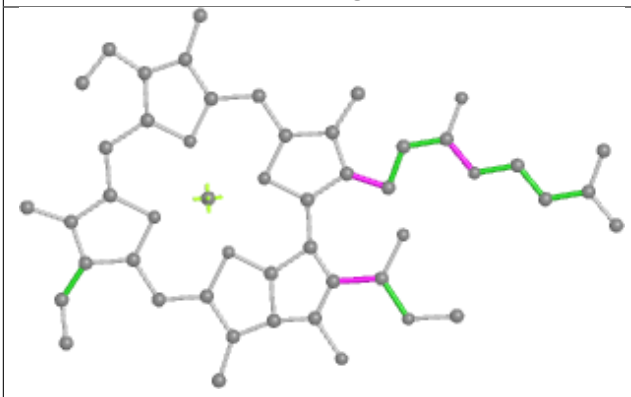


Bond angles



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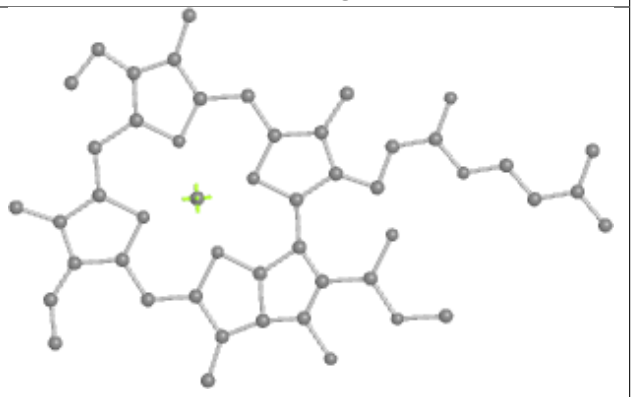
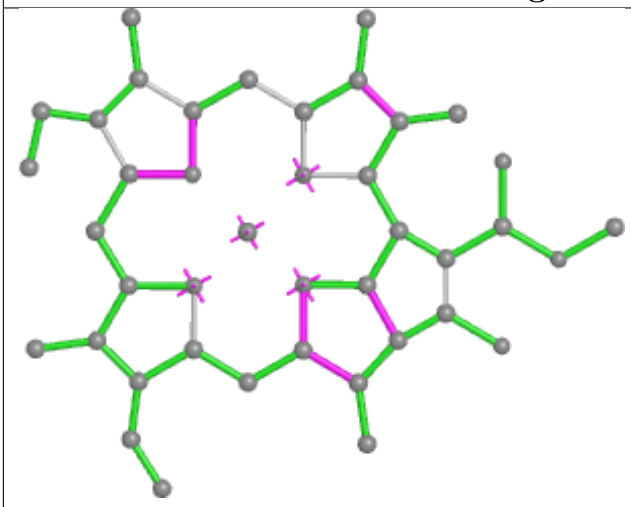


Rings

Ligand CLA 9 310



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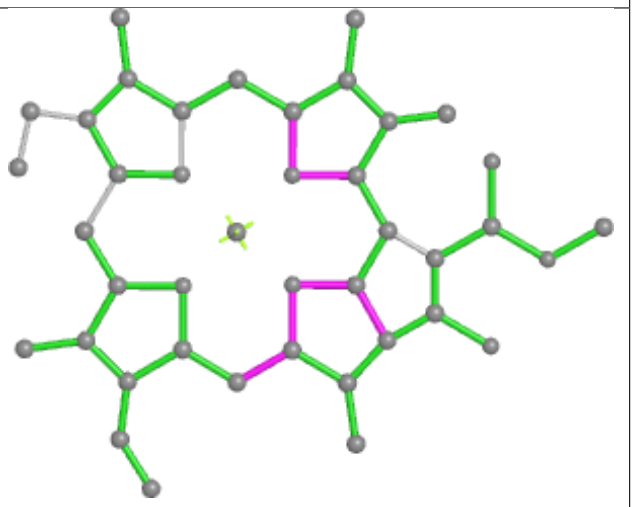
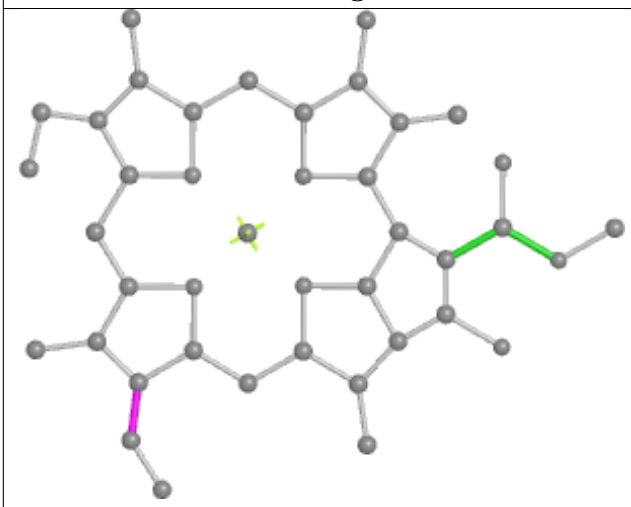


Bond angles



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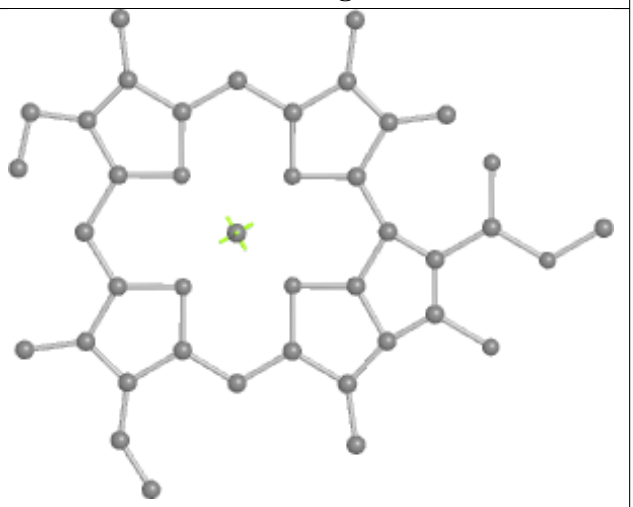
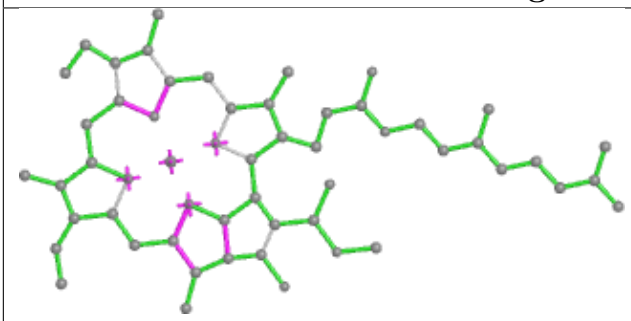
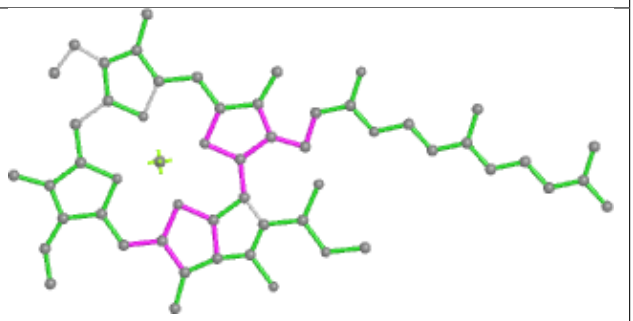


Rings

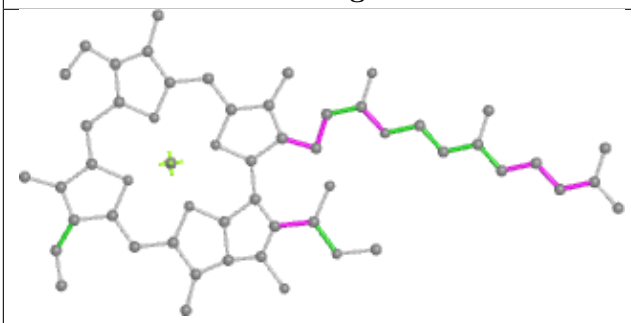
Ligand CLA 2 302



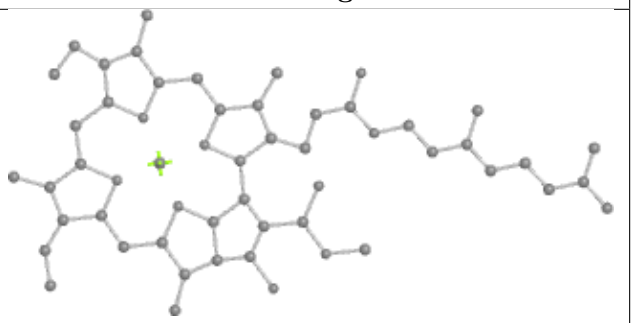
Bond lengths



Bond angles

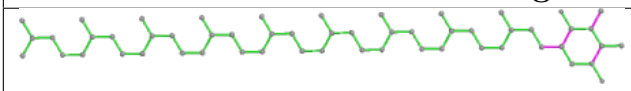


Torsions

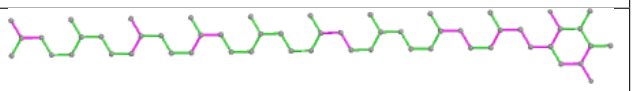


Rings

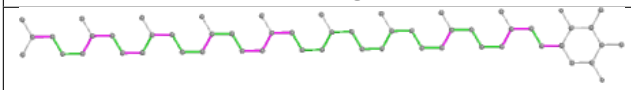
Ligand PL9 d 407



Bond lengths



Bond angles



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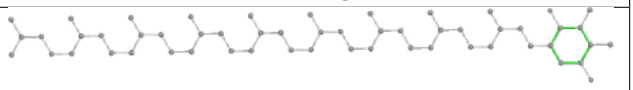
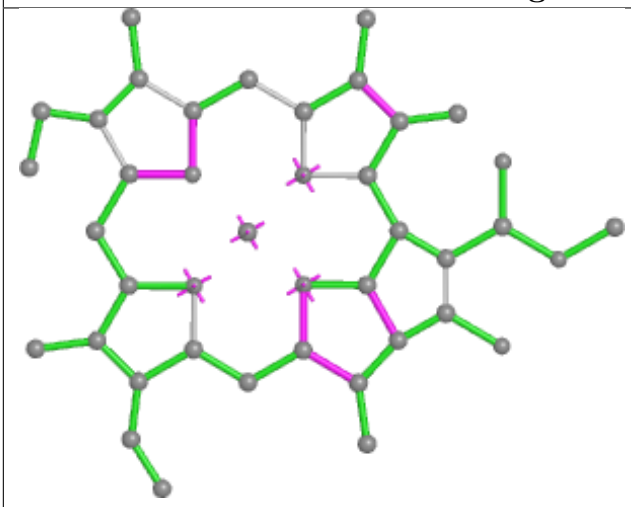
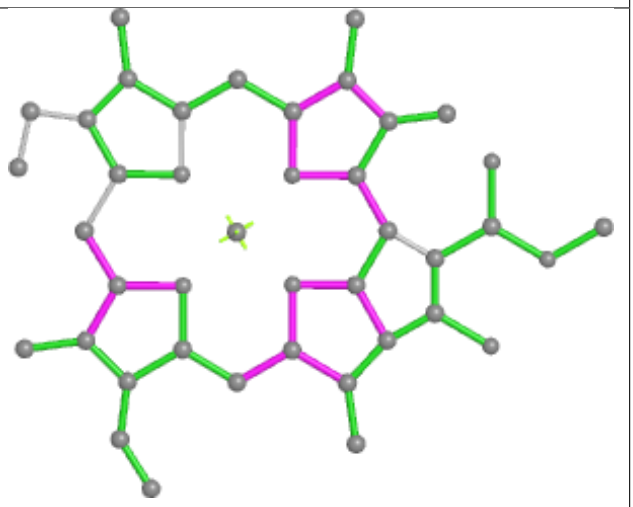


Rings

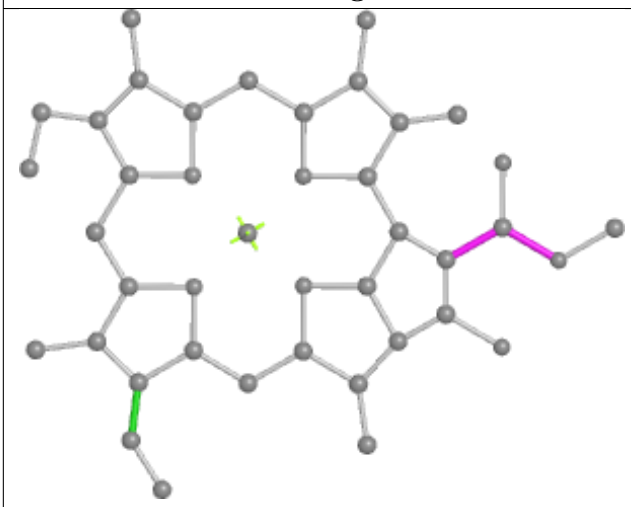
Ligand CLA 6 319



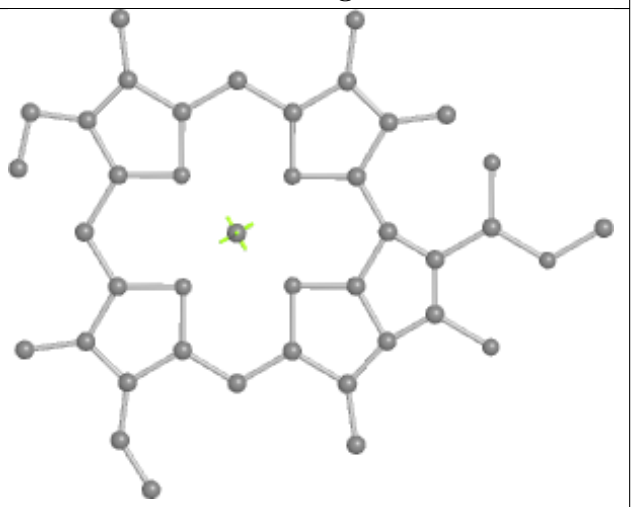
Bond lengths



Bond angles

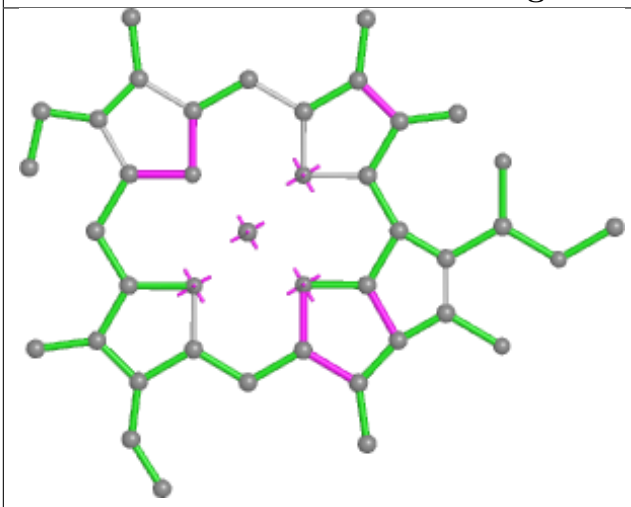


Torsions



Rings

Ligand CLA p 319



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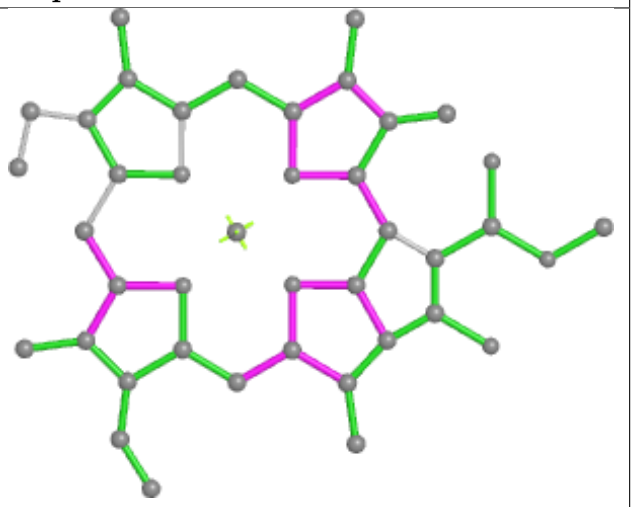
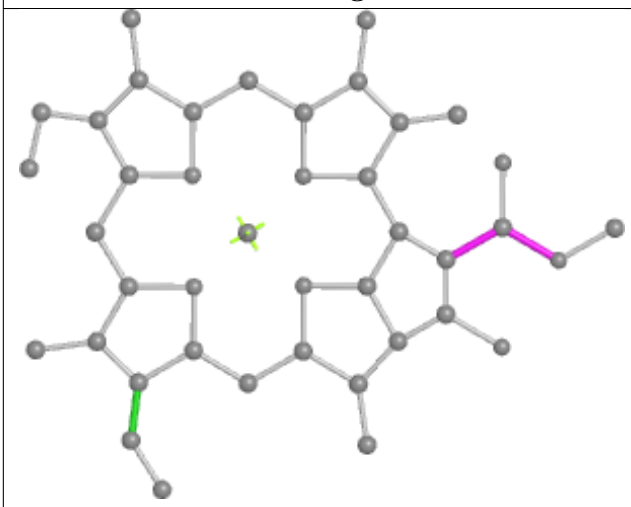
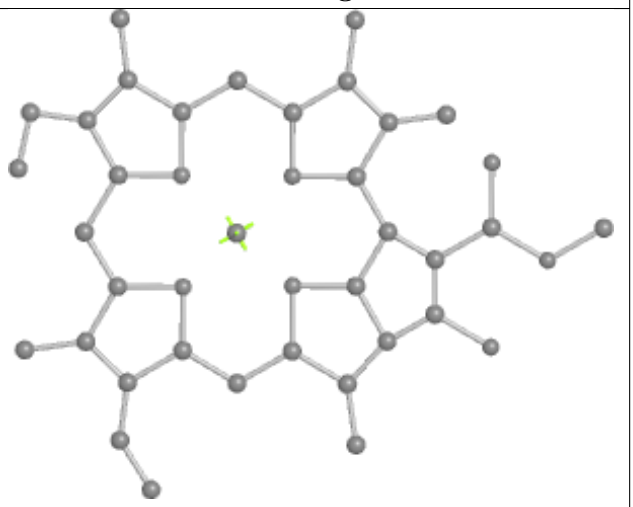


Bond angles

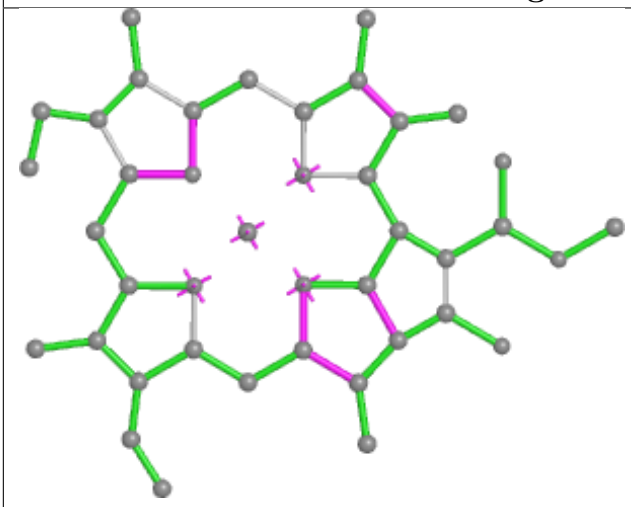


Torsions



Rings

Ligand CLA p 303



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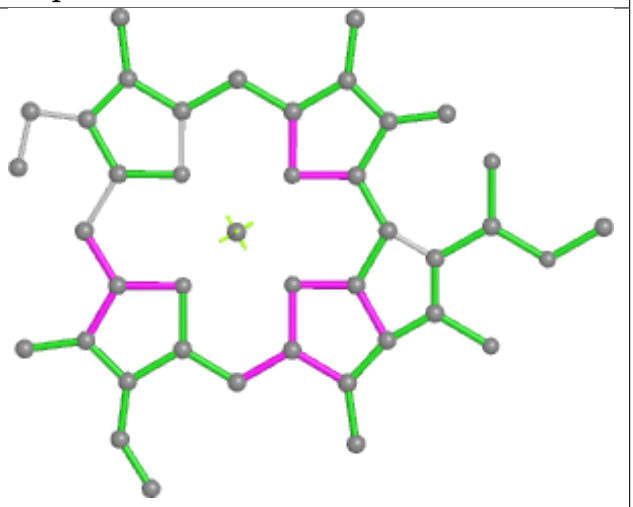

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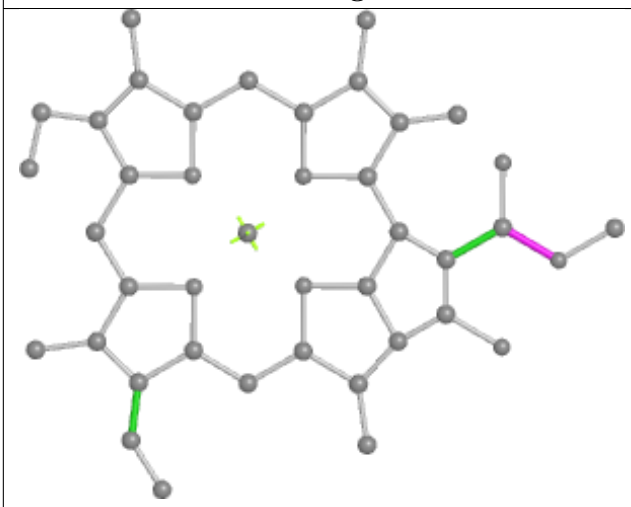

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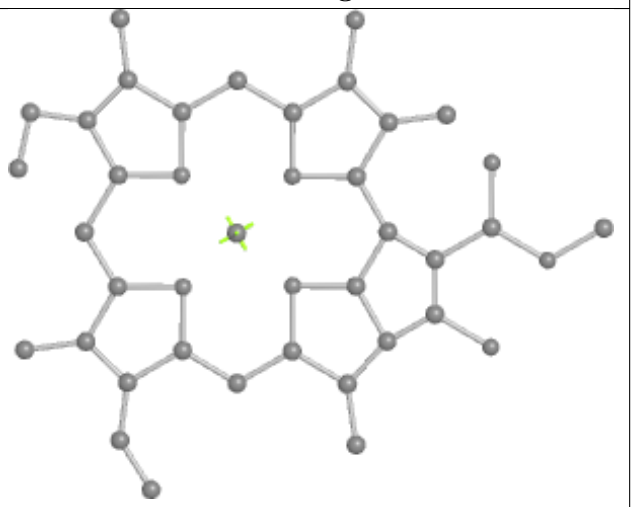
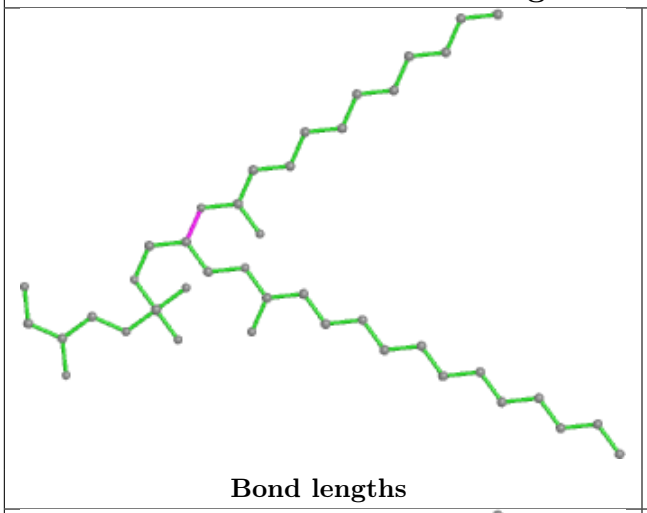


Rings

Ligand LHG 9 302



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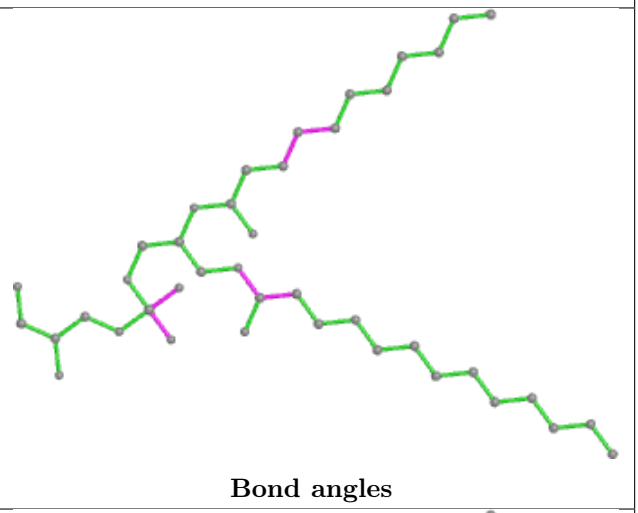
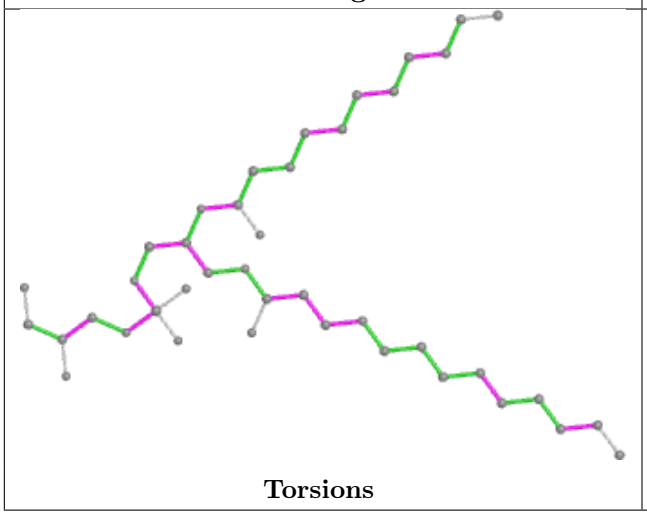
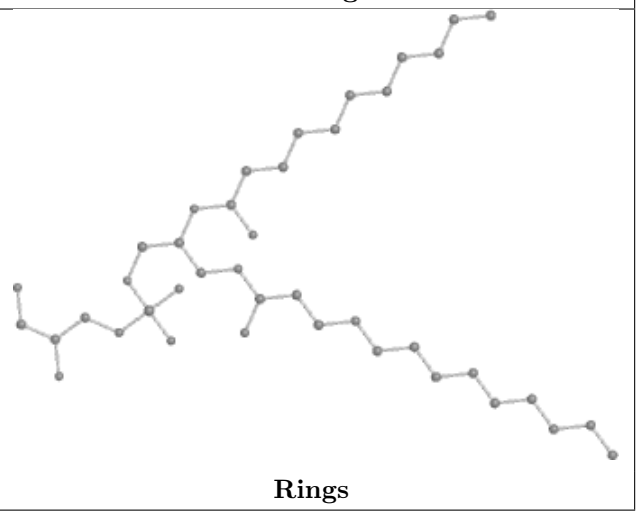


Bond angles

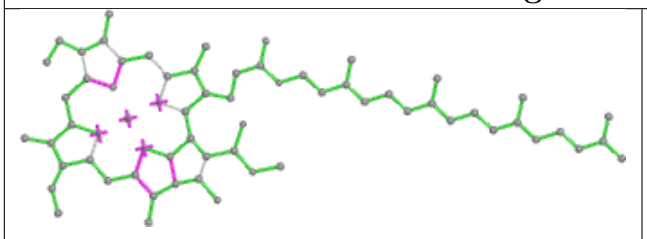


Torsions



Rings

Ligand CLA D 404



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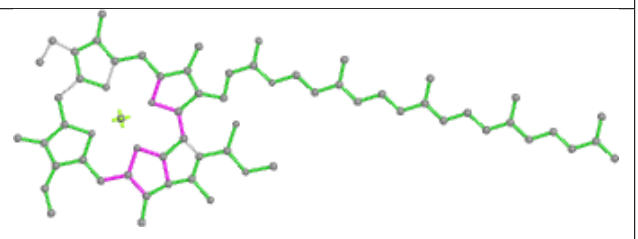
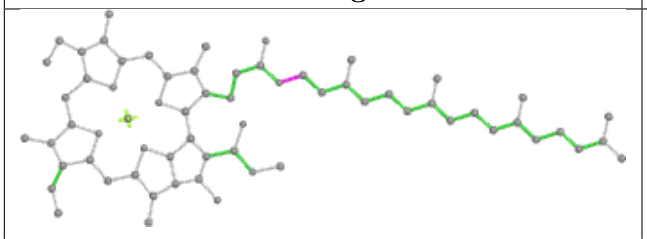


Bond angles



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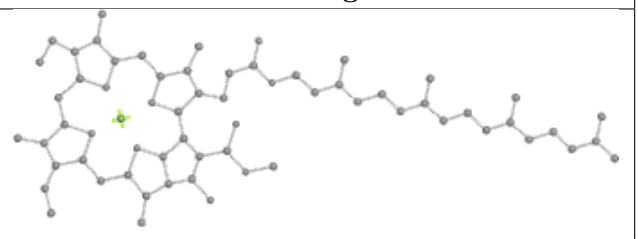
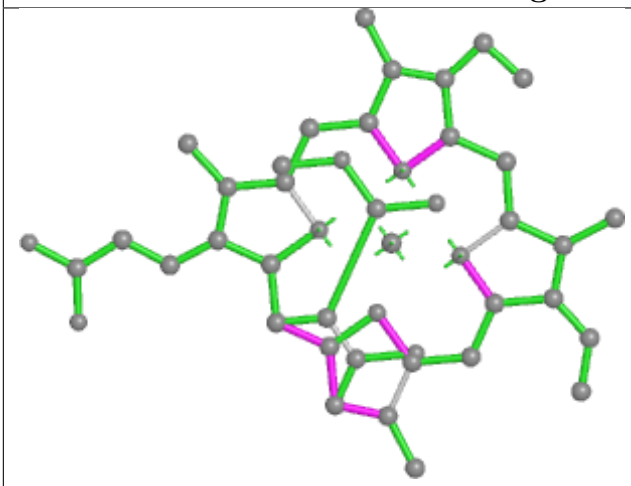


Rings

Ligand KC2 5 309



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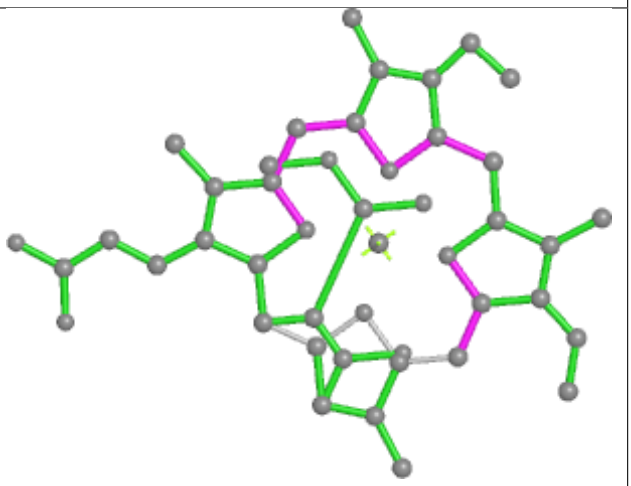
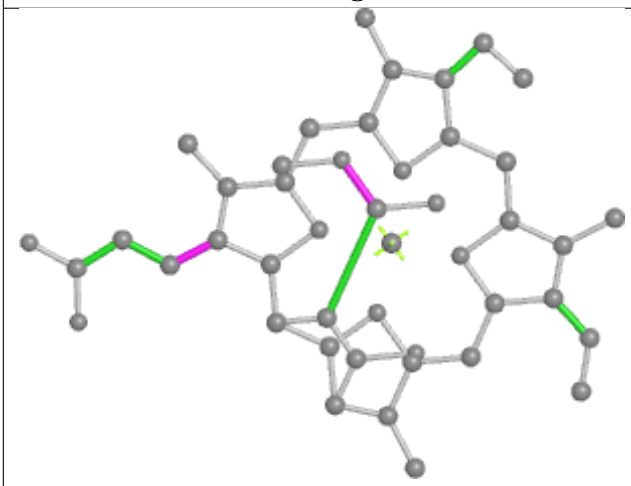
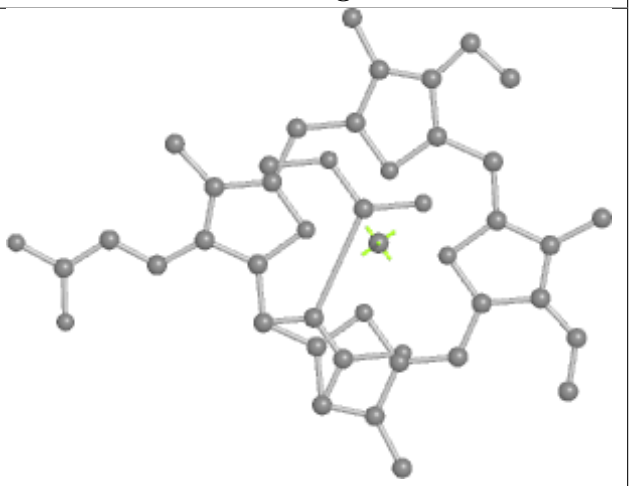


Bond angles

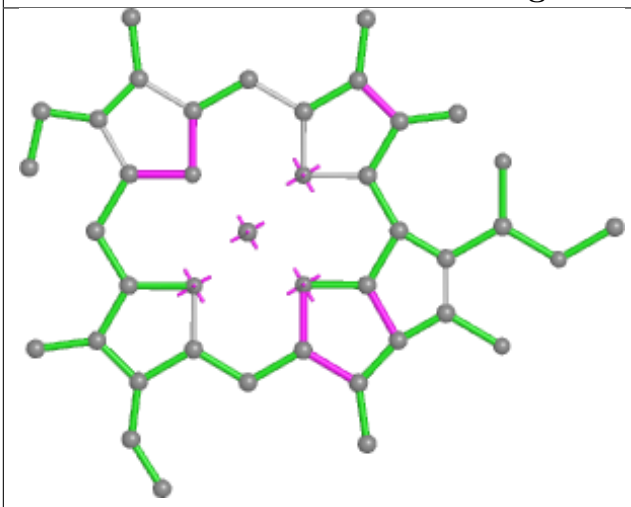


Torsions



Rings

Ligand CLA 3 314



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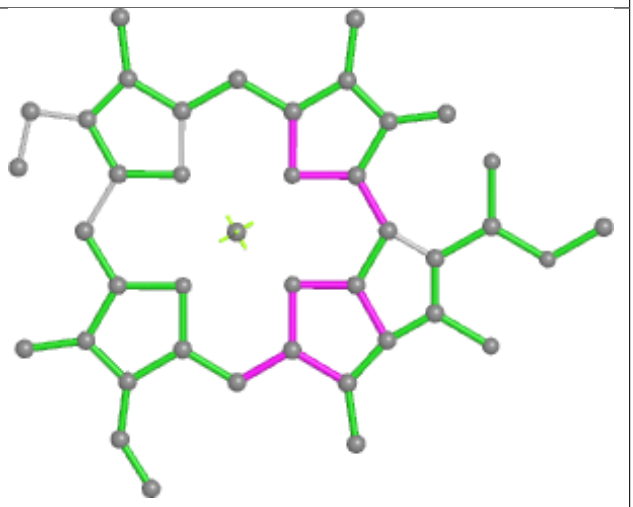
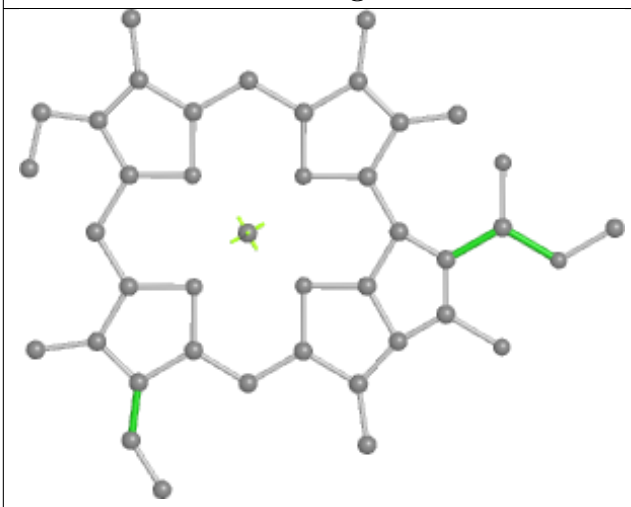


Bond angles



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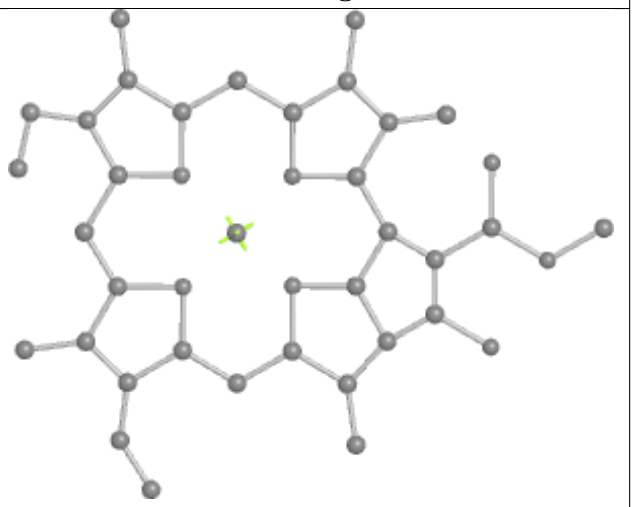
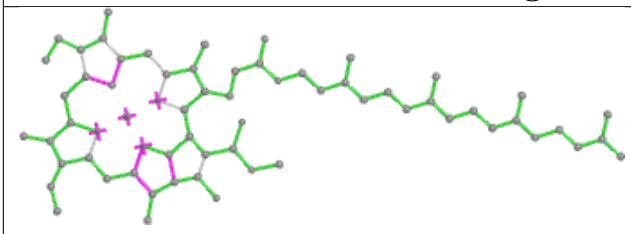


Rings

Ligand CLA A 405



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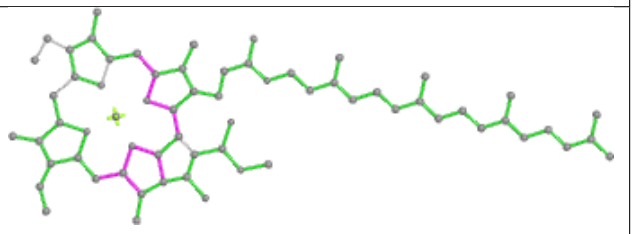

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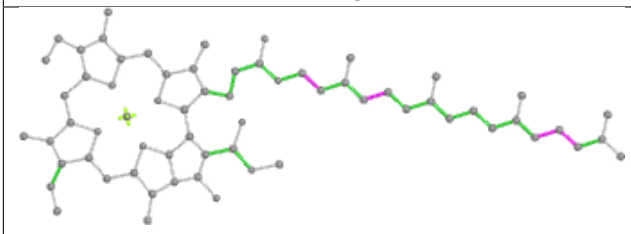

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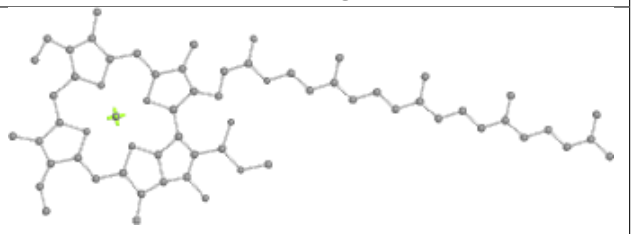
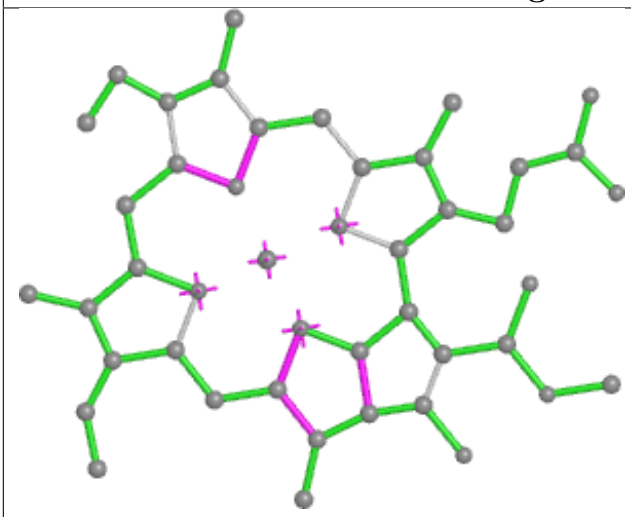


Rings

Ligand CLA 7 301



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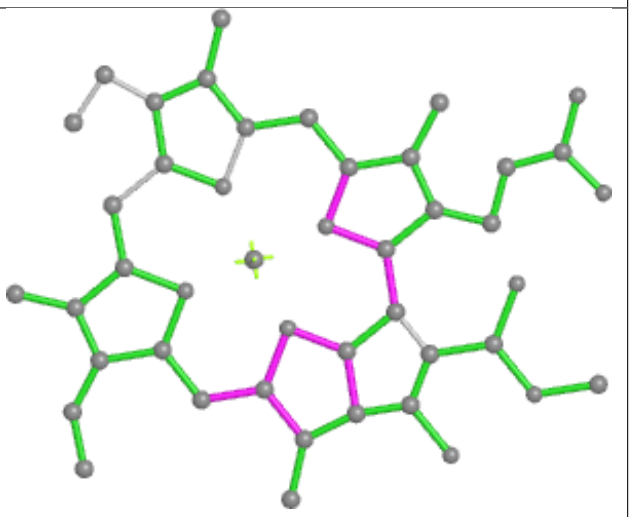
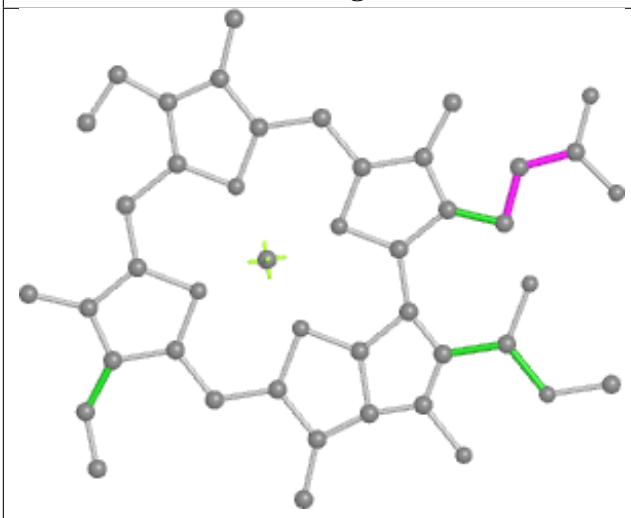


Bond angles



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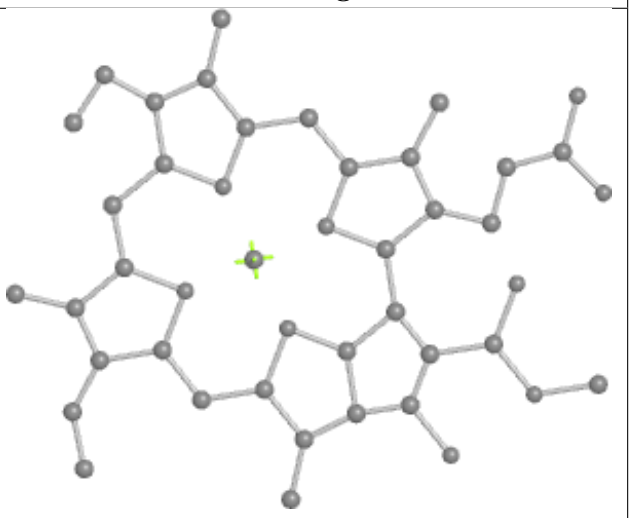
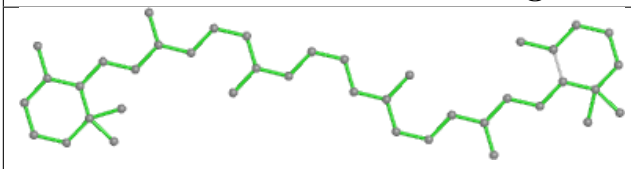
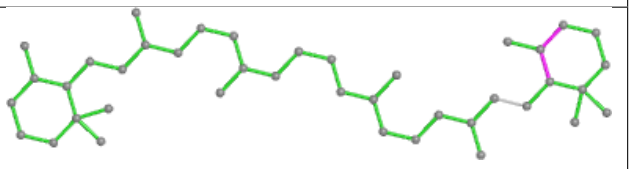


Rings

Ligand 8CT D 406



Bond lengths



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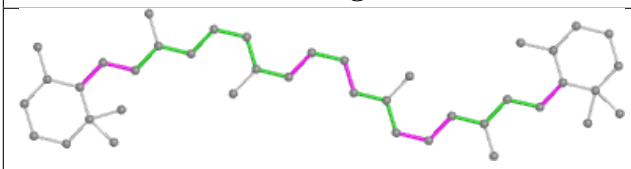
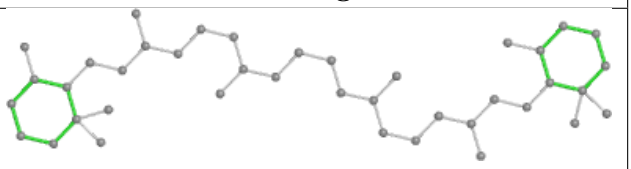
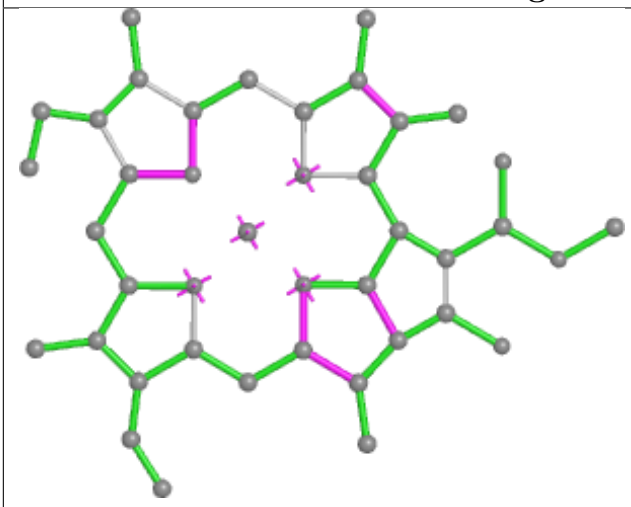


Torsions

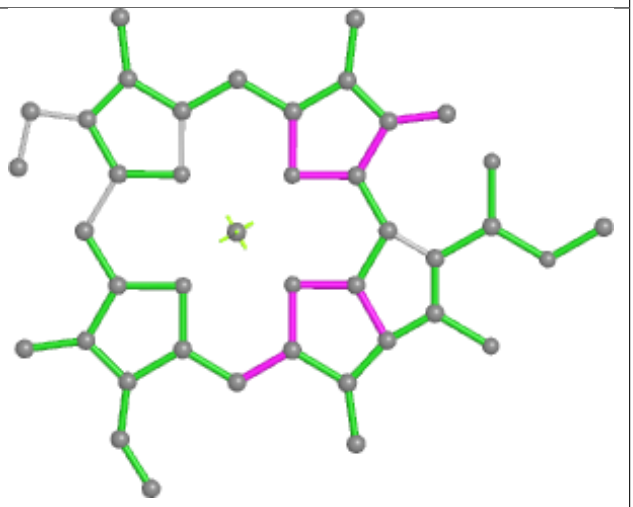


Rings

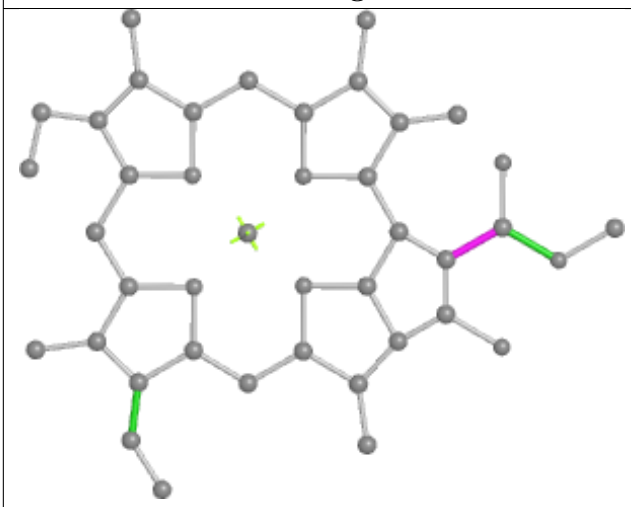
Ligand CLA 9 313



Bond lengths



Bond angles



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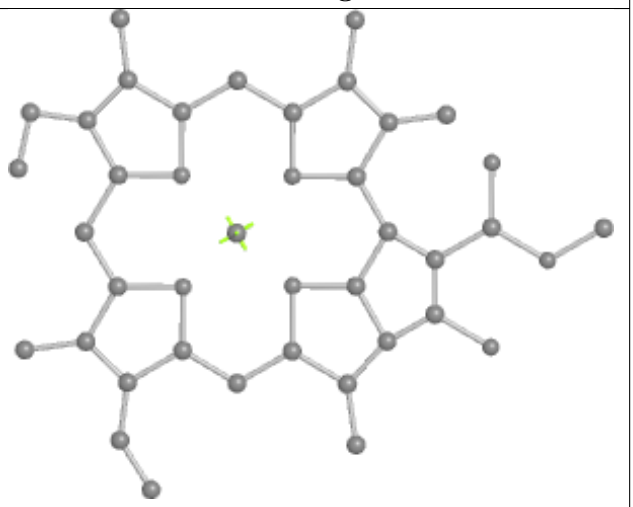
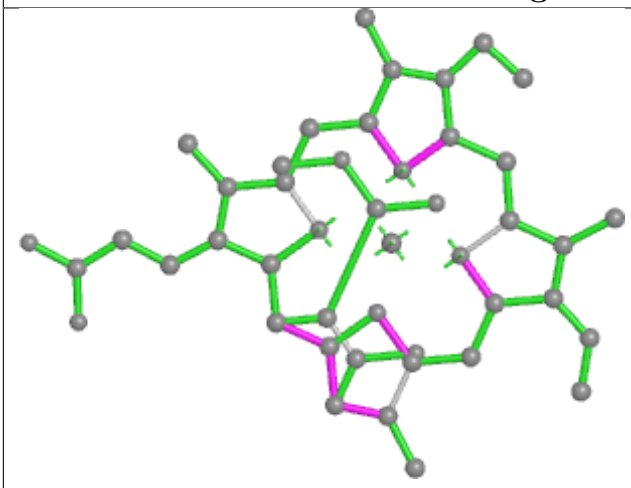


Rings

Ligand KC2 4 305



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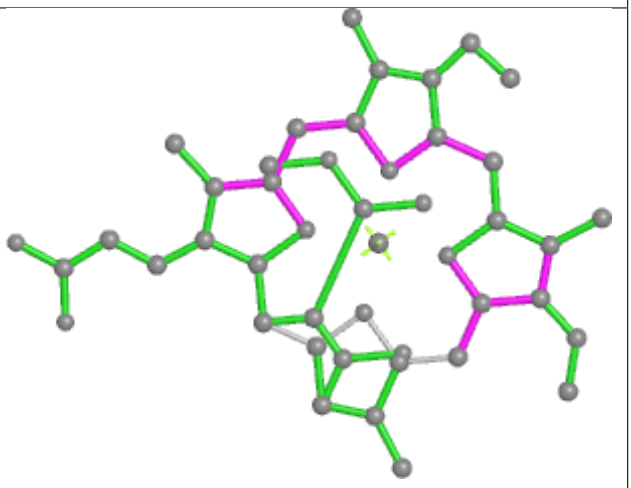

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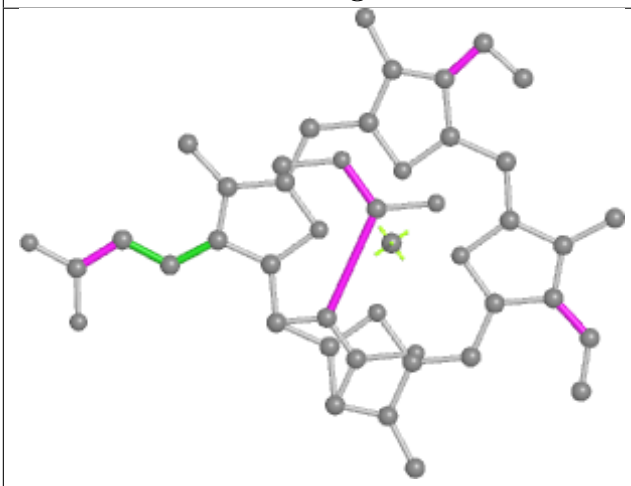

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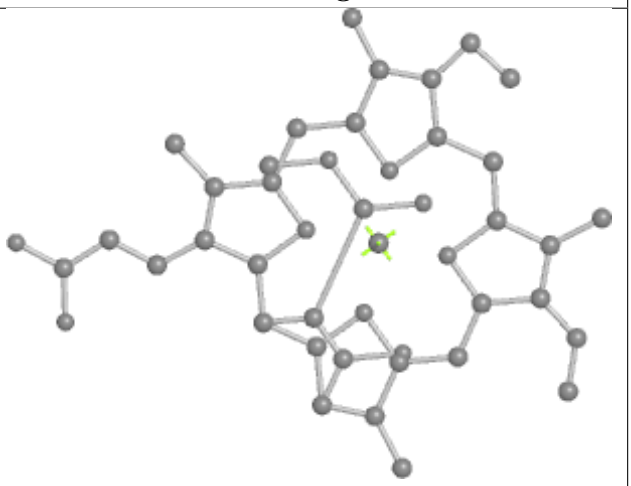
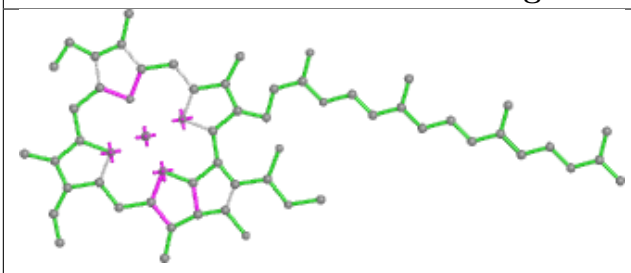


Rings

Ligand CLA A 408



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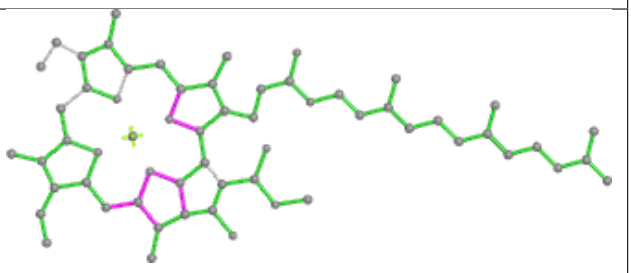
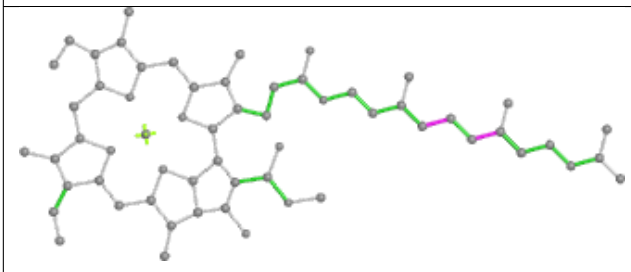


Bond angles



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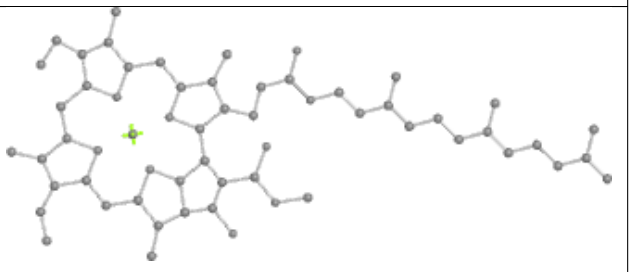
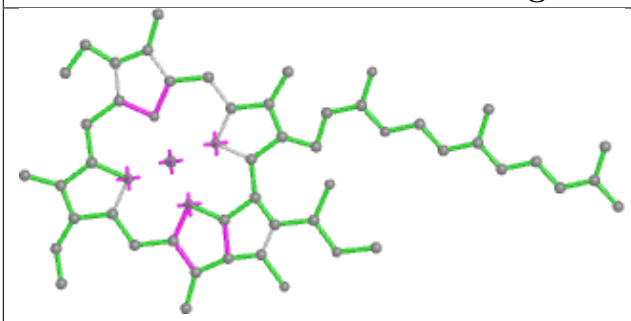
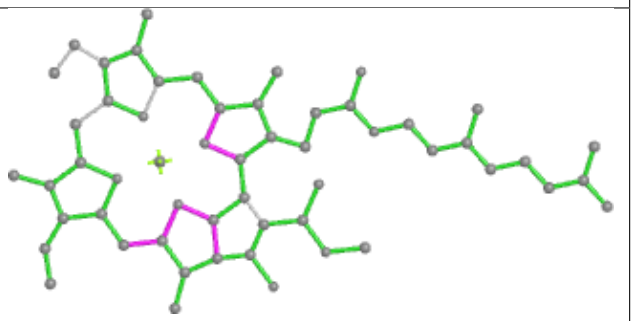


Rings

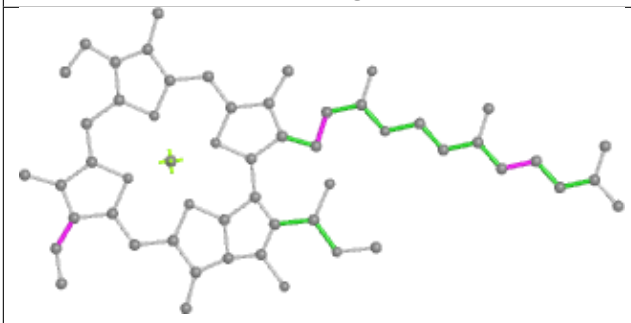
Ligand CLA 9 305



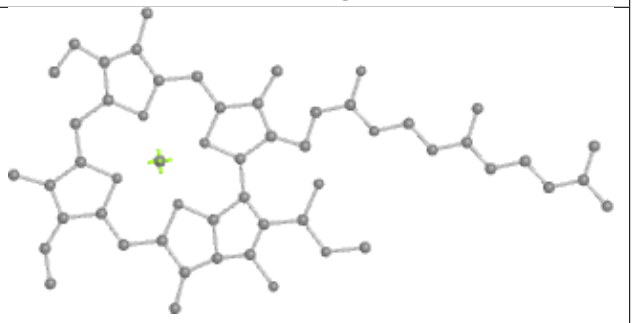
Bond lengths



Bond angles

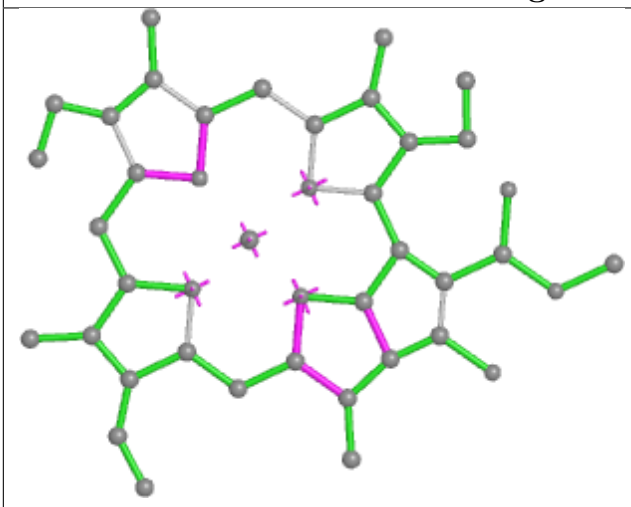


Torsions

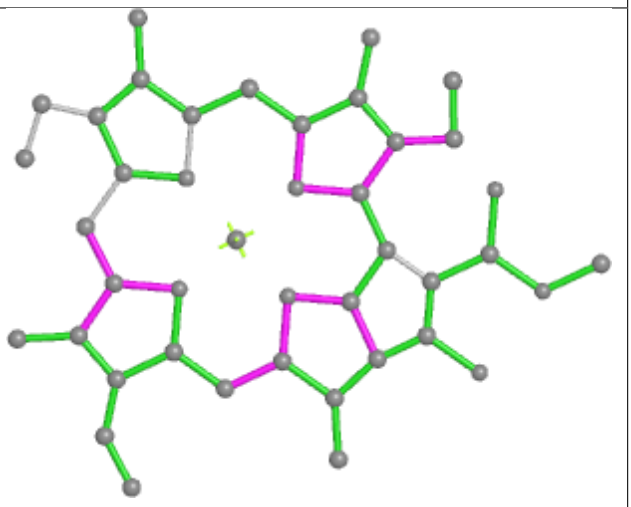


Rings

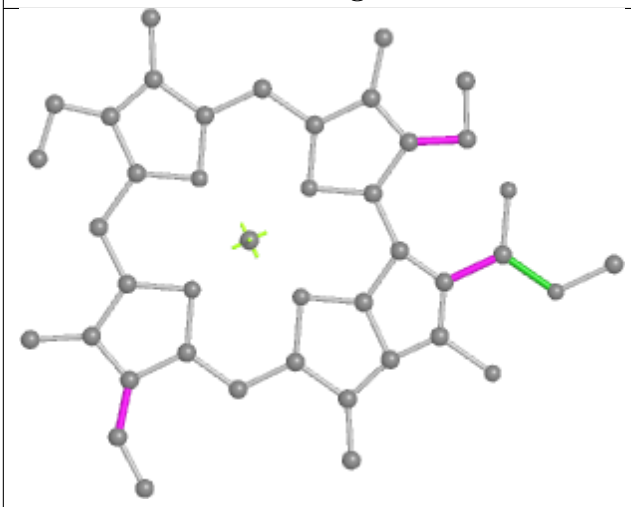
Ligand CLA 5 301



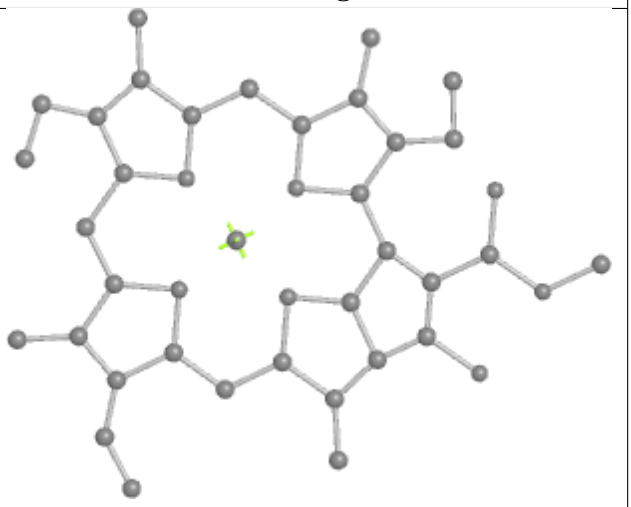
Bond lengths



Bond angles

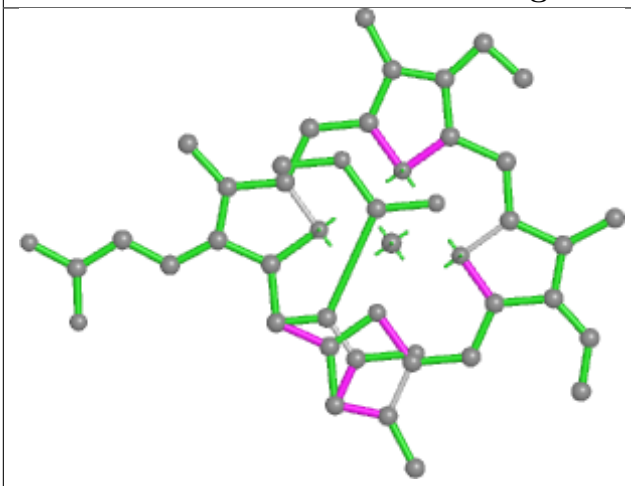


Torsions

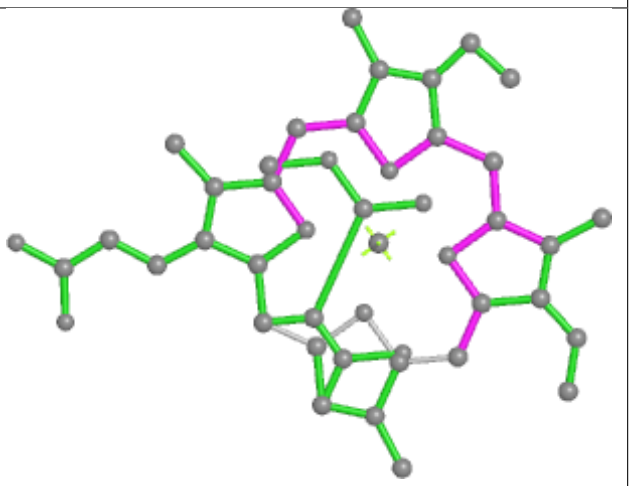


Rings

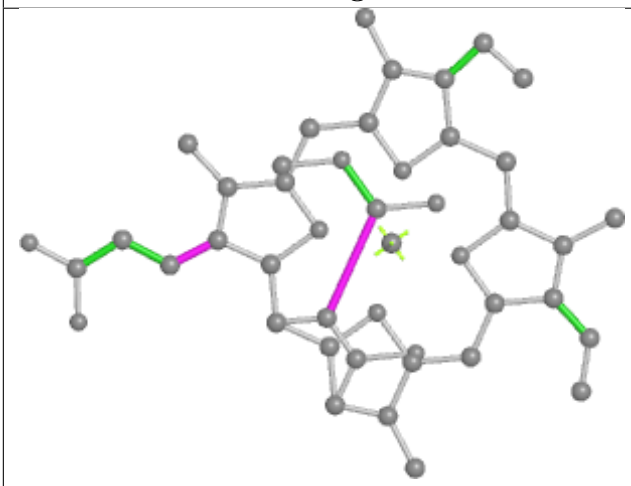
Ligand KC2 6 311



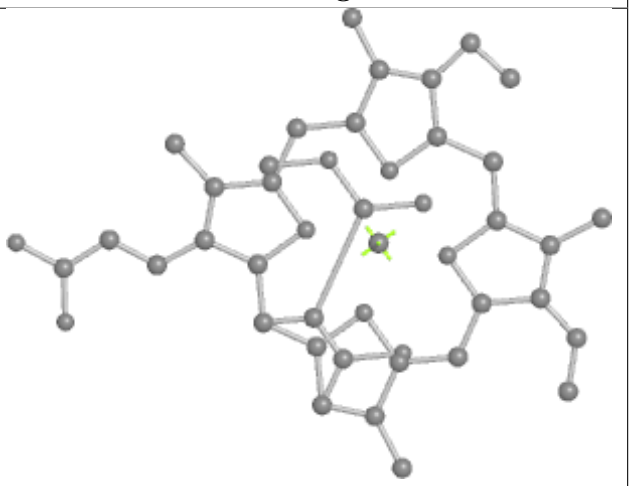
Bond lengths



Bond angles

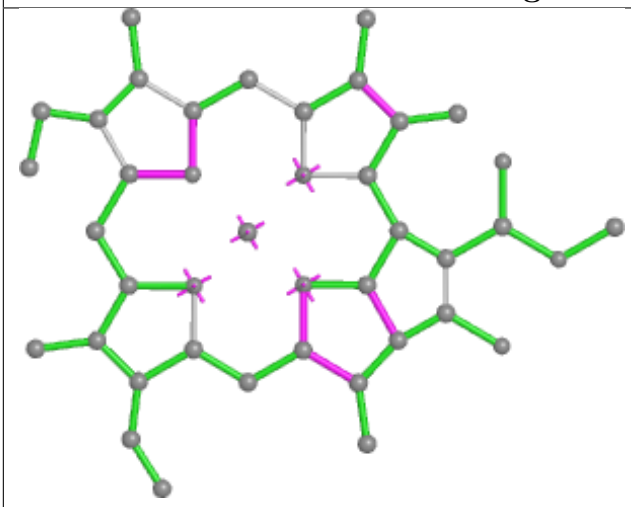


Torsions

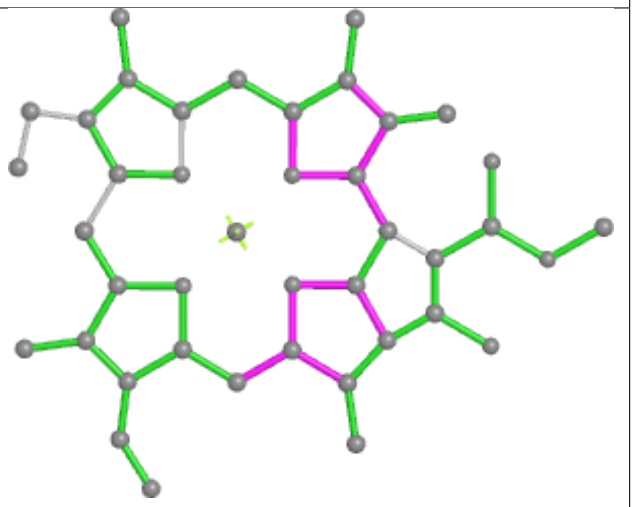


Rings

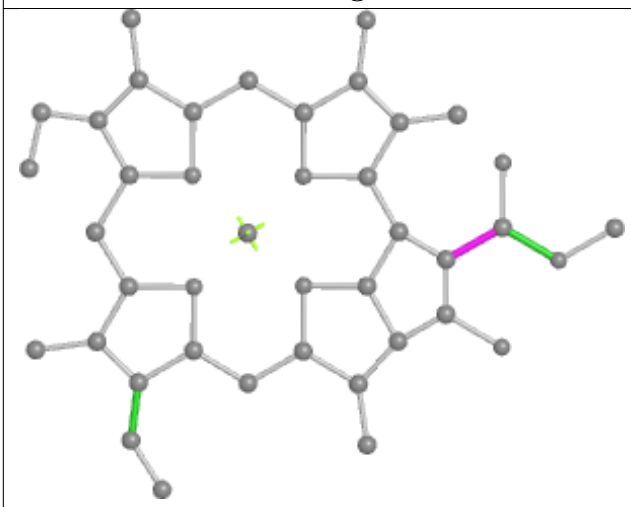
Ligand CLA N 304



Bond lengths



Bond angles



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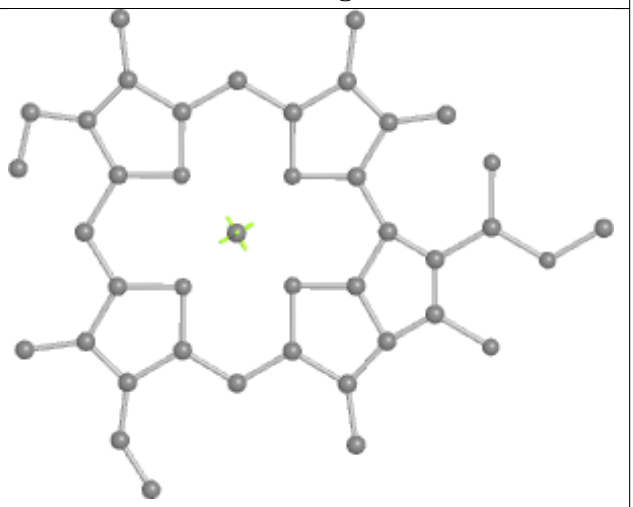
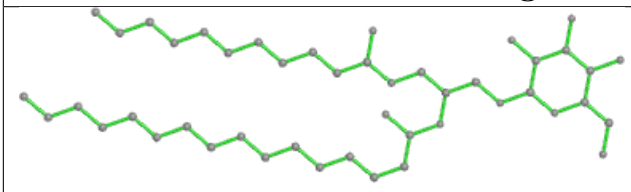


Rings

Ligand LMG D 409



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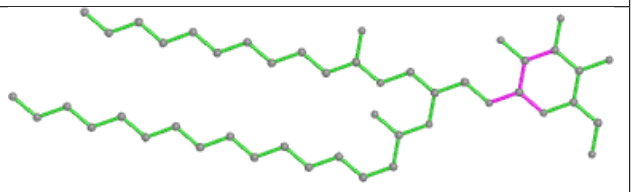
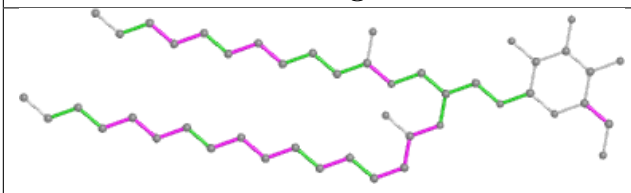
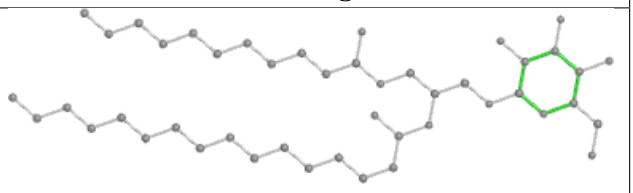


Bond angles

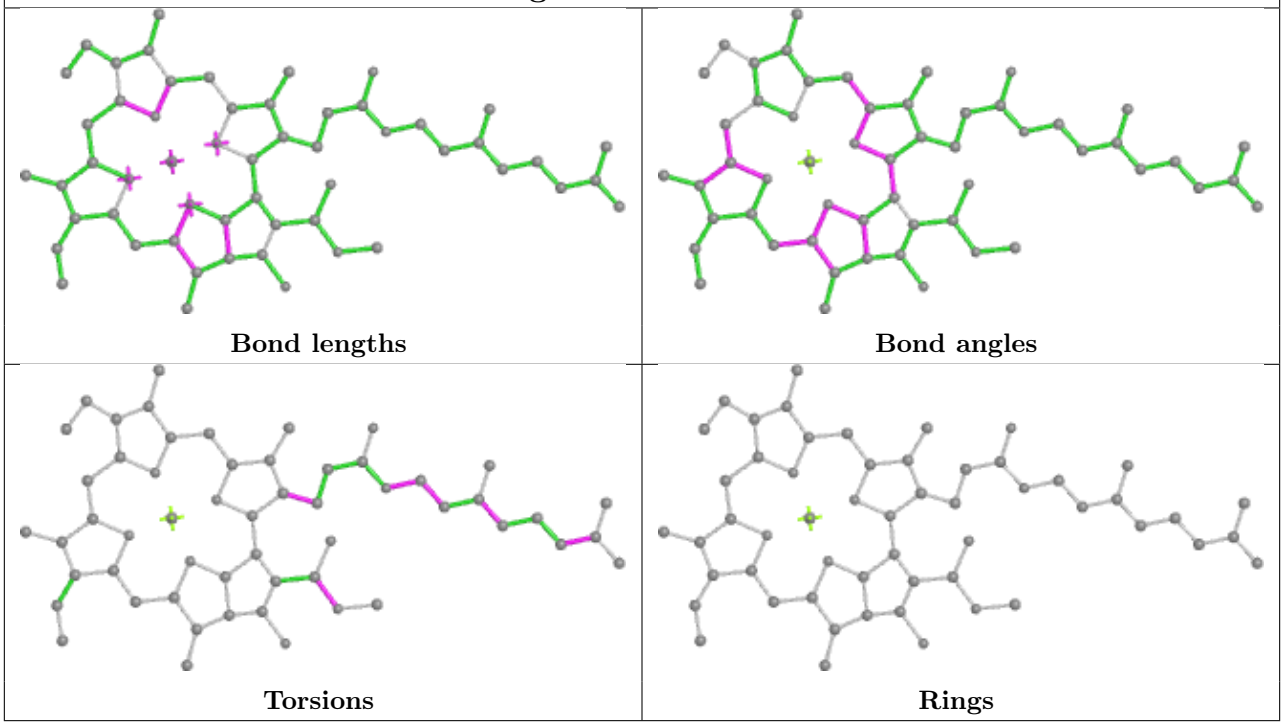


Torsions

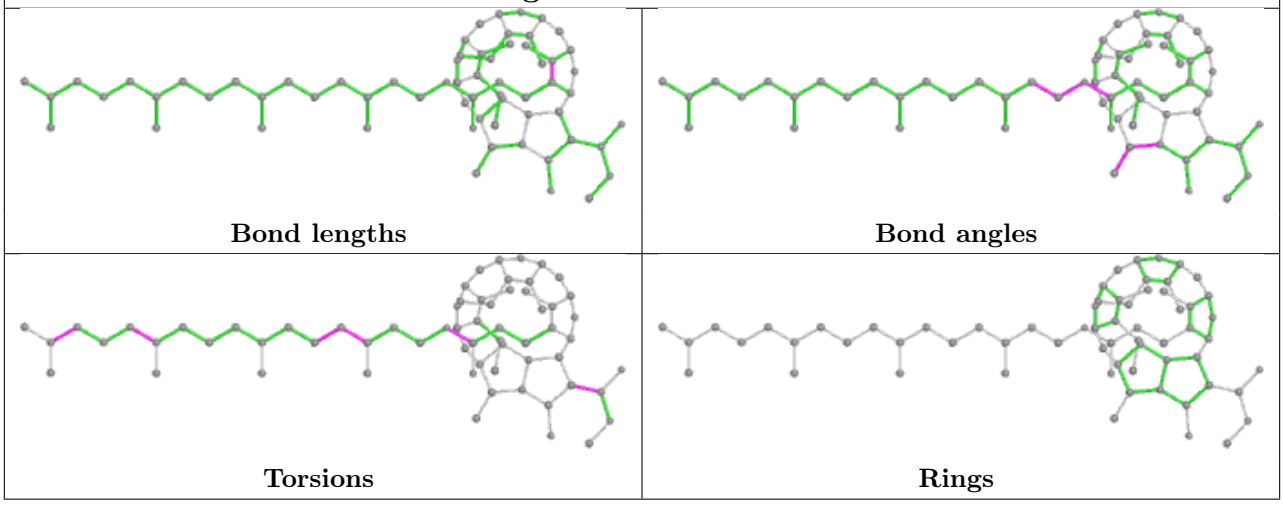


Rings

Ligand CLA 0 306



Ligand PHO A 407



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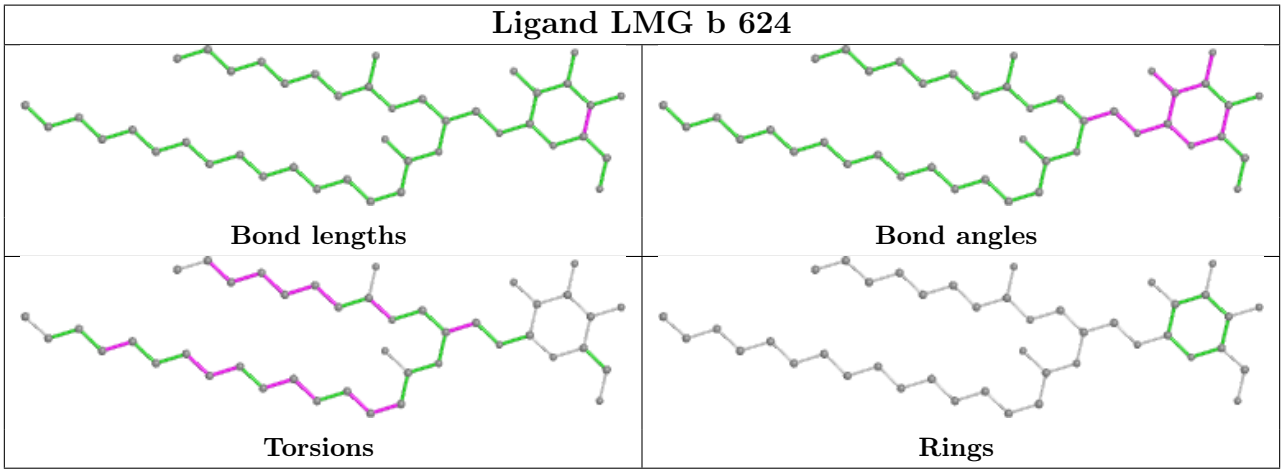
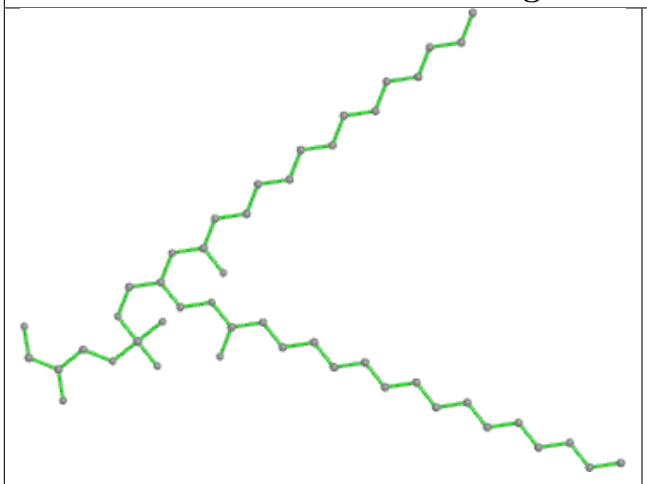
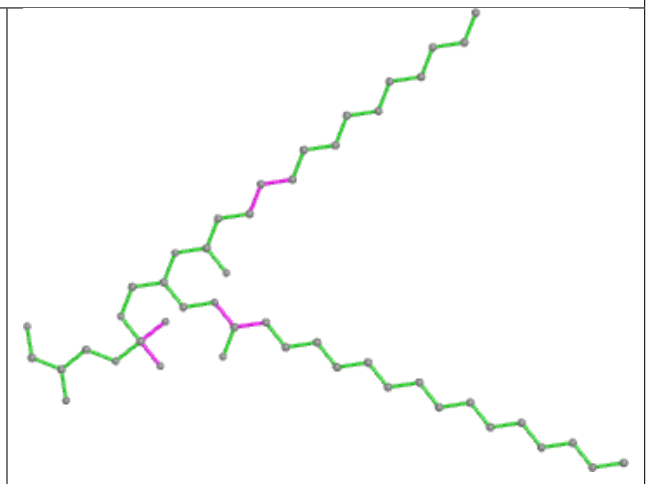


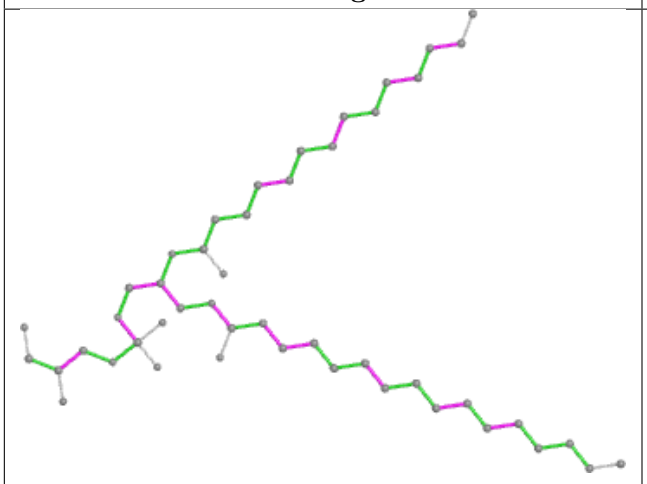
Ligand LHG D 402



Bond lengths



Bond angles



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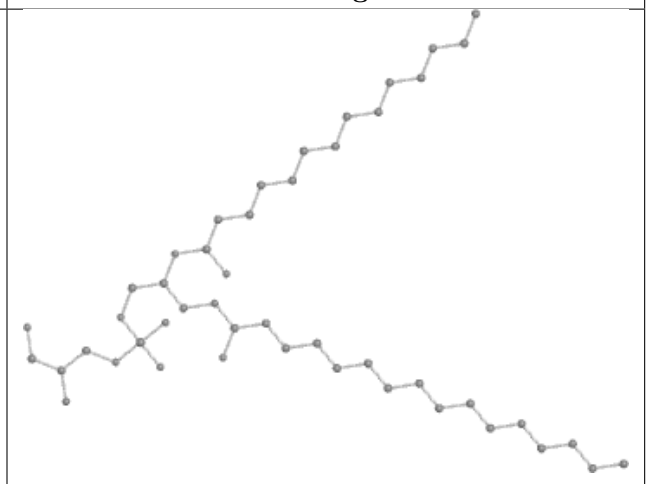
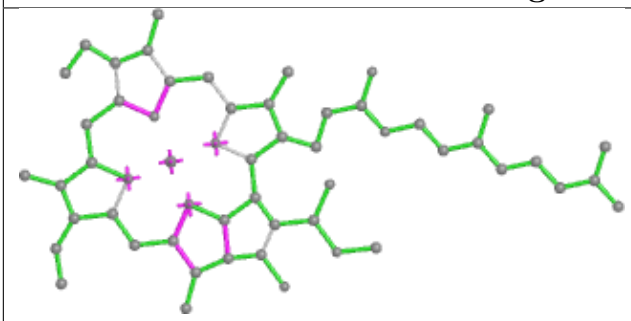


Rings

Ligand CLA 2 308



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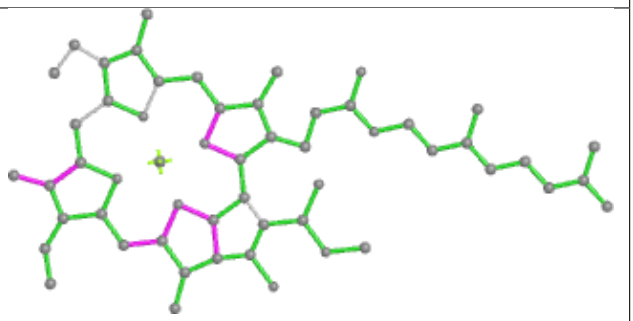
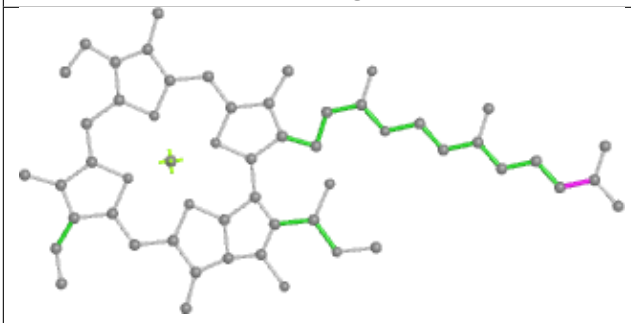


Bond angles



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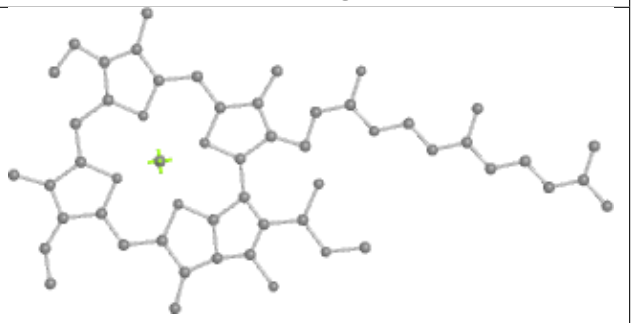
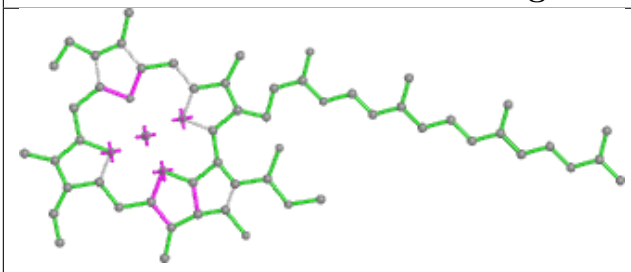
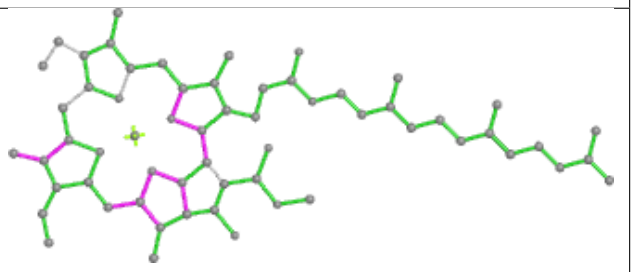


Rings

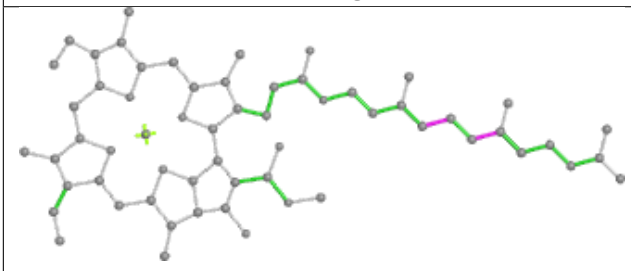
Ligand CLA 8 306



Bond lengths



Bond angles



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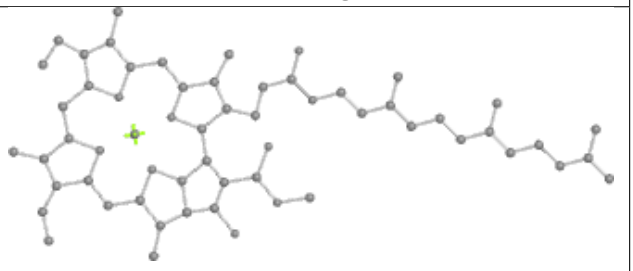
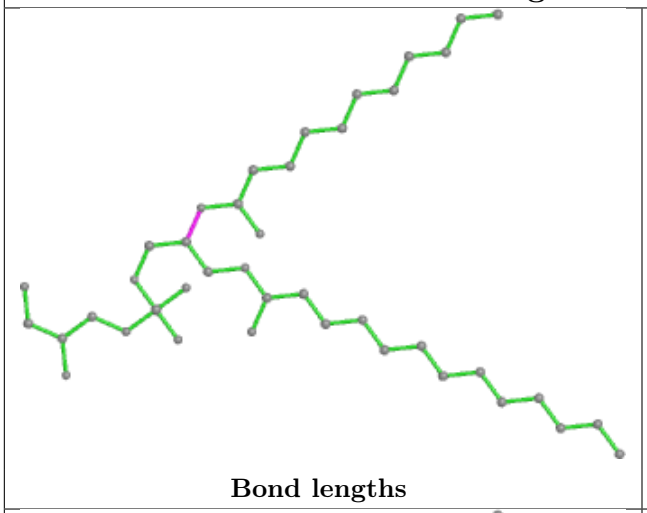


Rings

Ligand LHG 3 302



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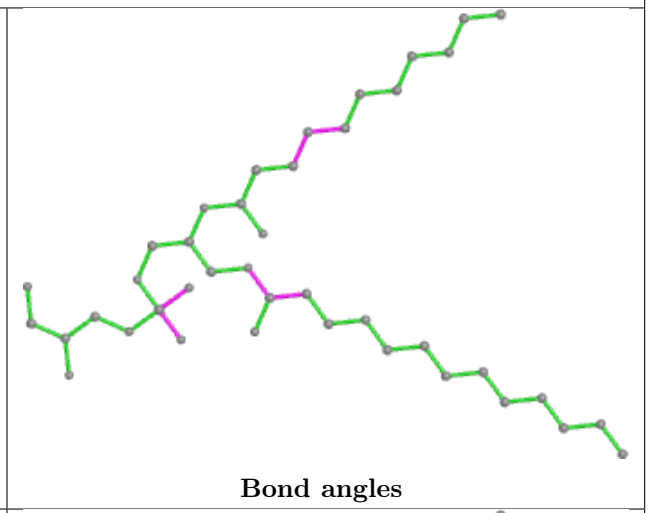
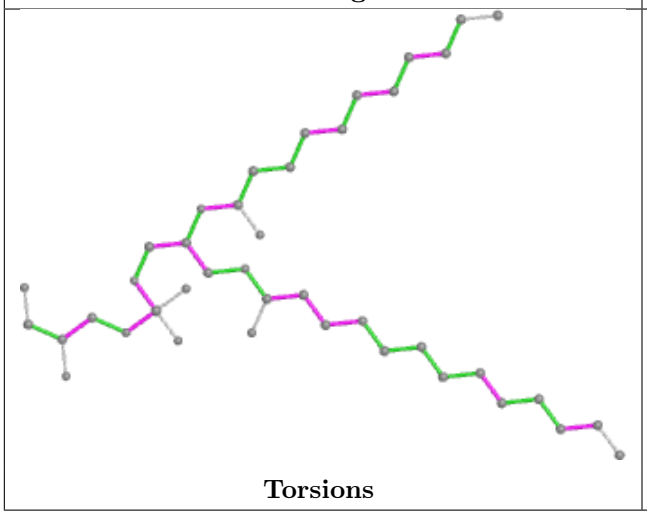


Bond angles



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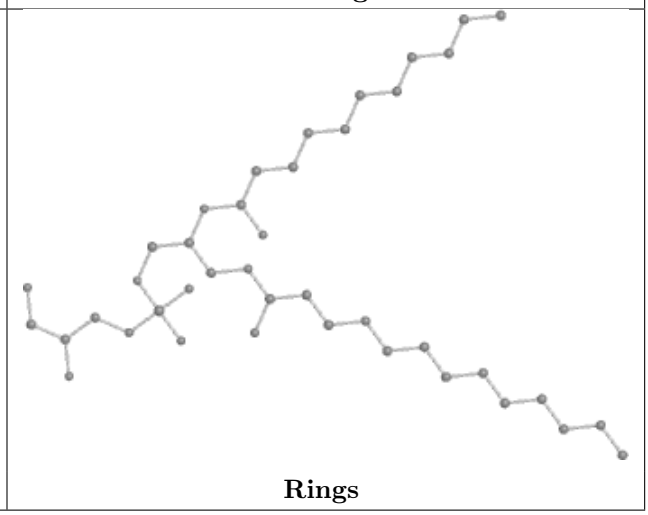
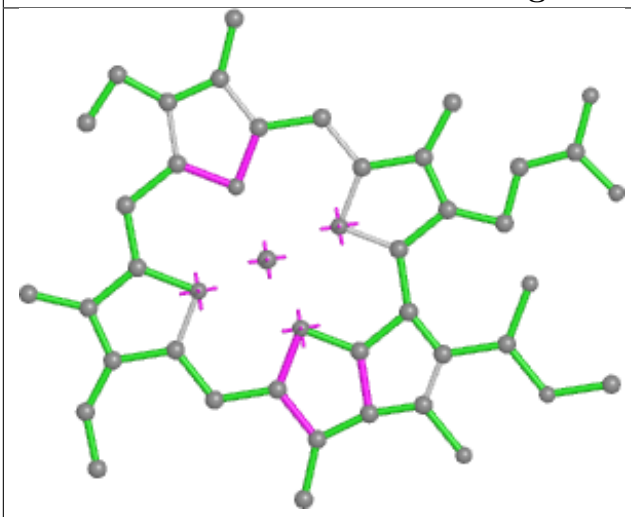


Rings

Ligand CLA 8 301



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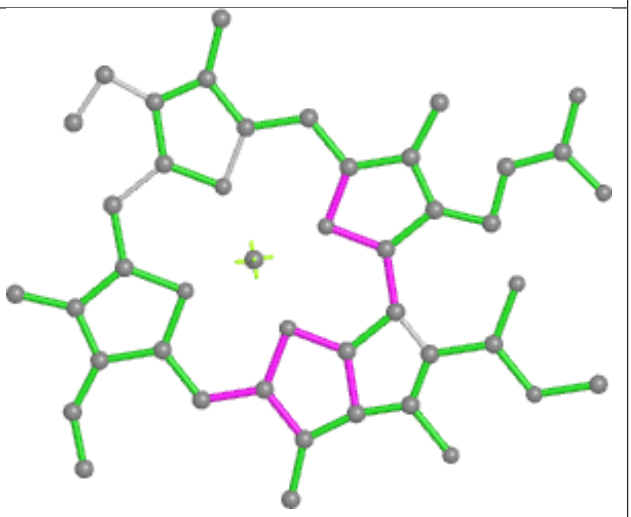
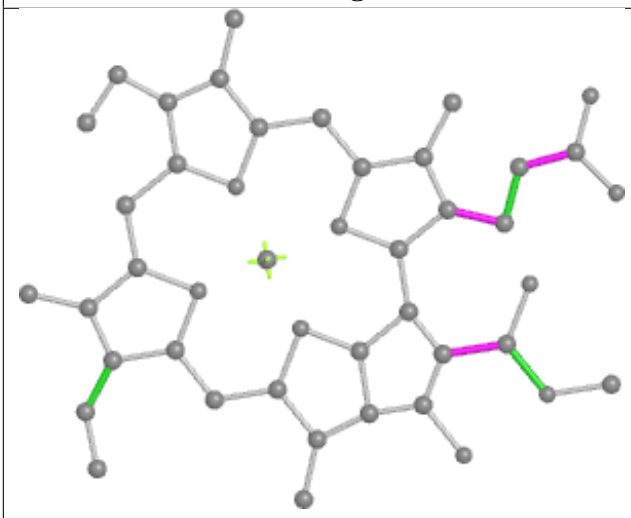
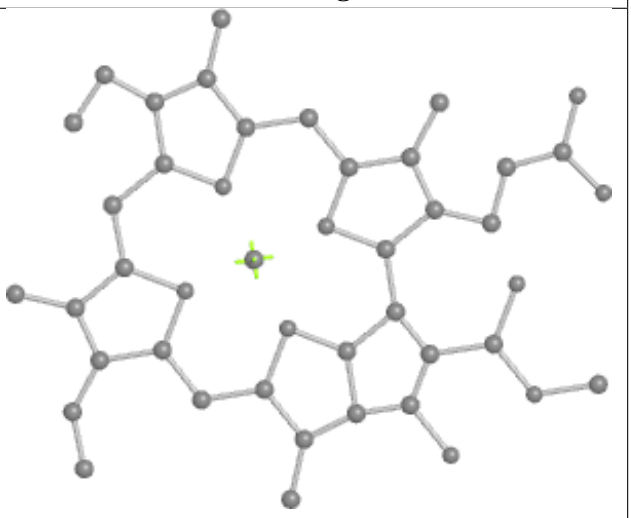


Bond angles

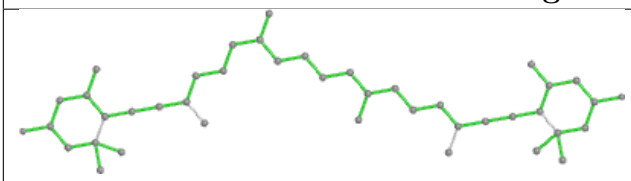


Torsions

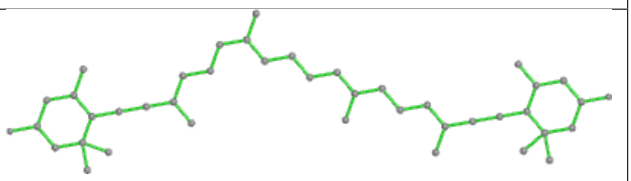


Rings

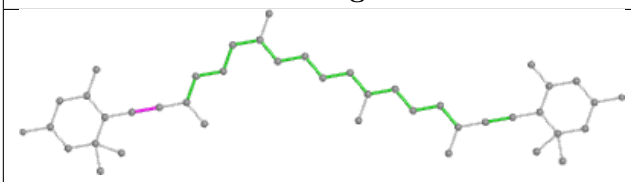
Ligand II0 1 313



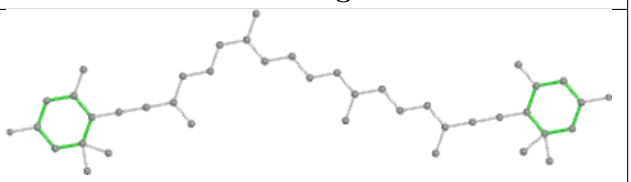
Bond lengths



Bond angles

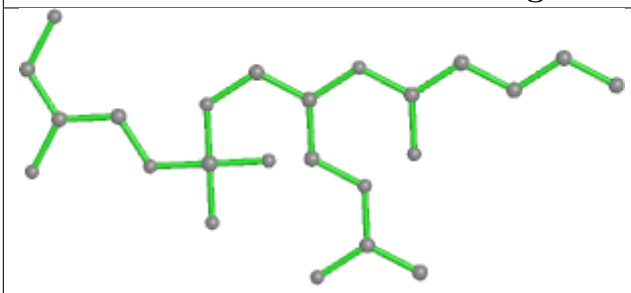


Torsions



Rings

Ligand LHG 0 317



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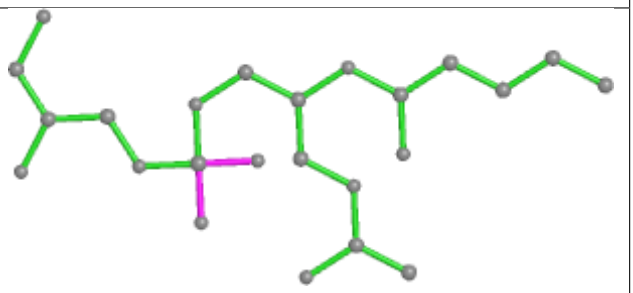
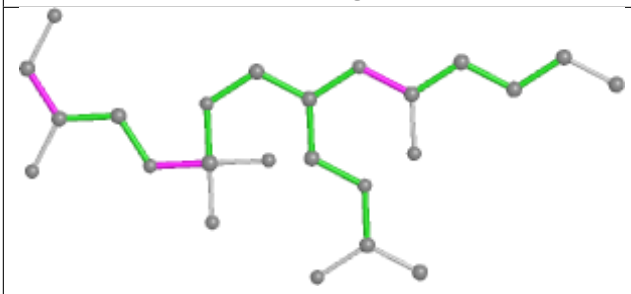
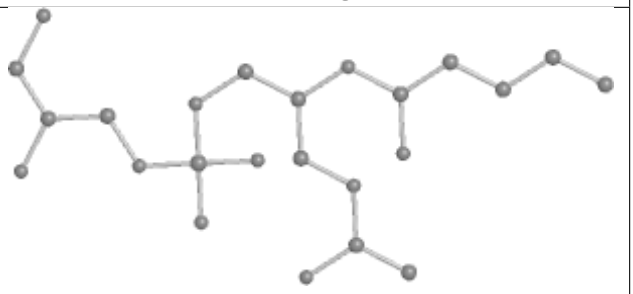


Bond angles

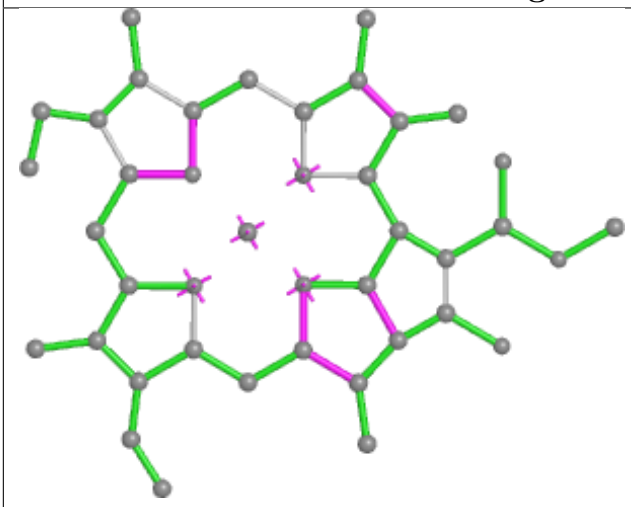


Torsions



Rings

Ligand CLA 3 310



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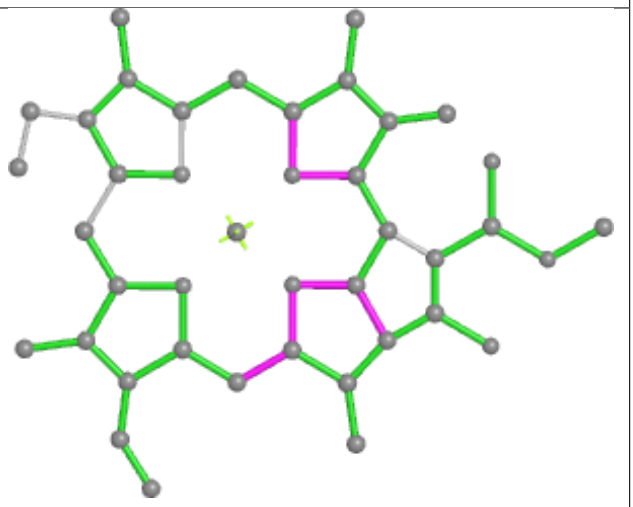
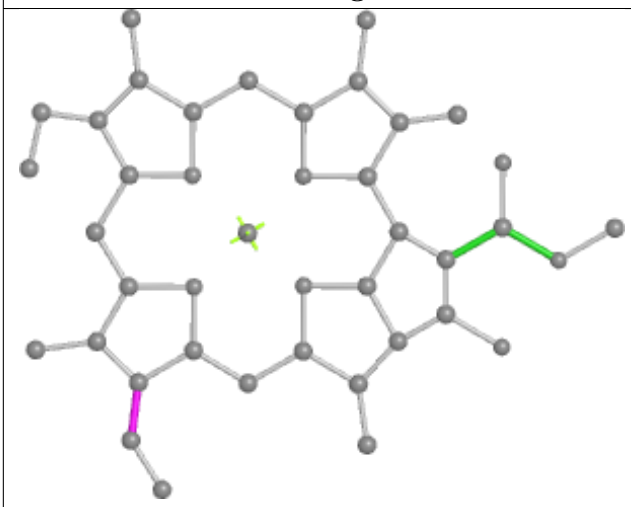


Bond angles



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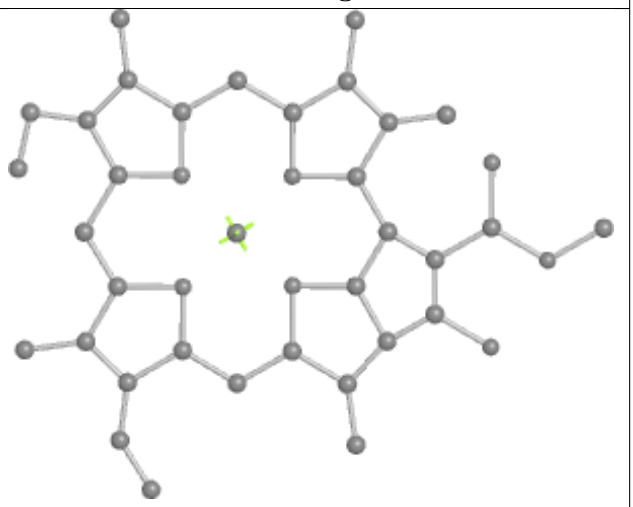
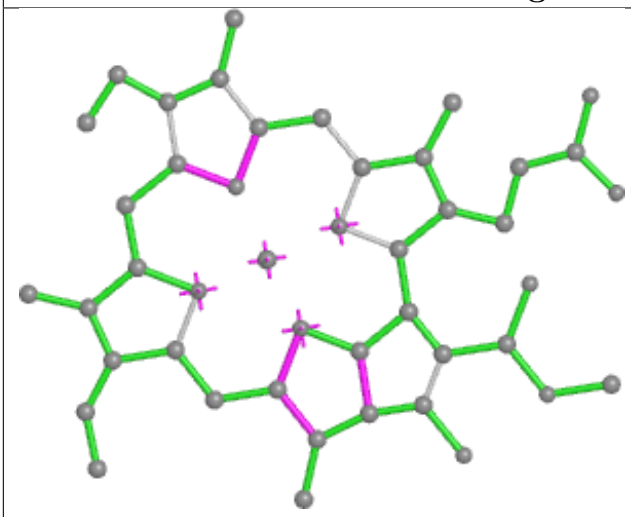


Rings

Ligand CLA 3 307



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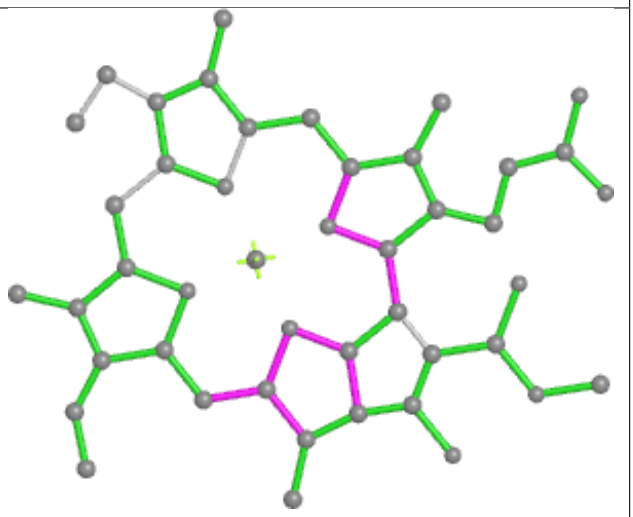
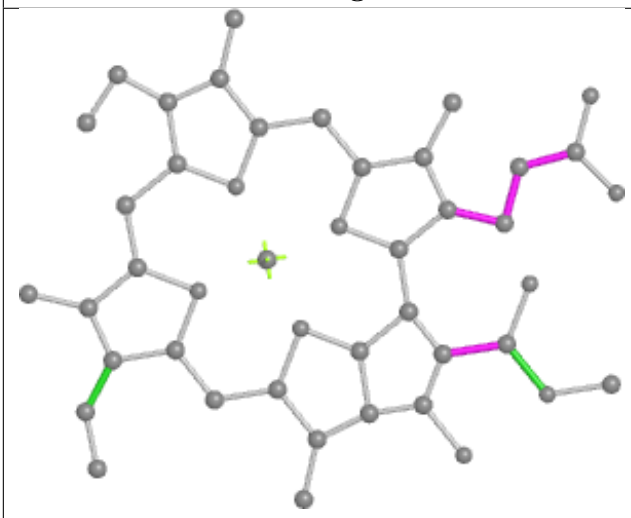


Bond angles



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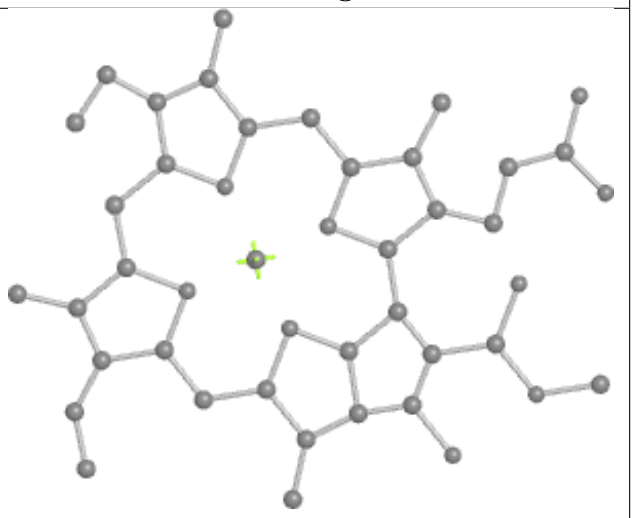
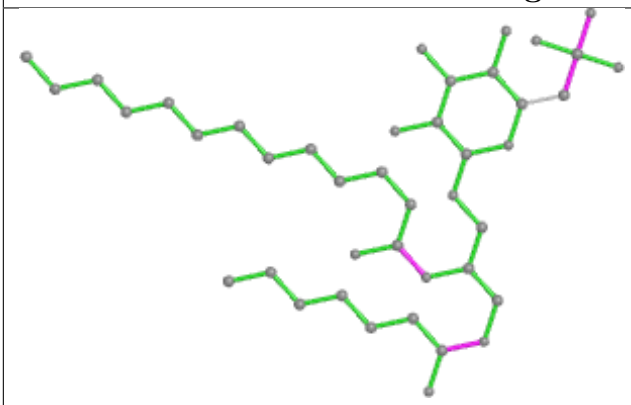
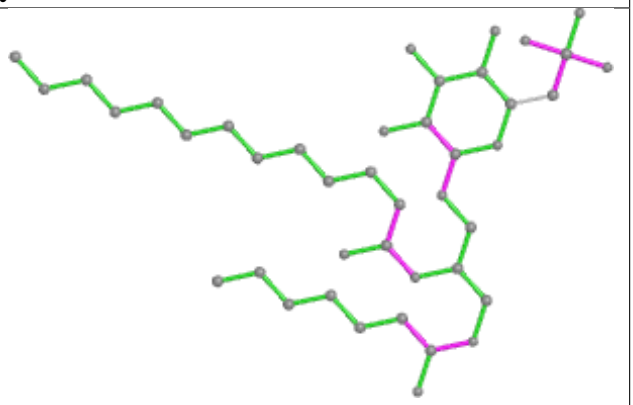


Rings

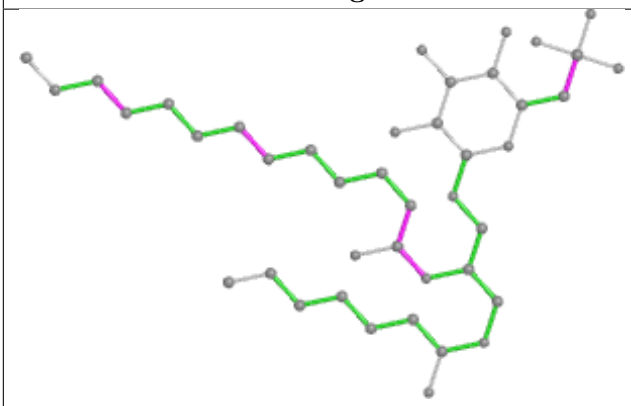
Ligand SQD C 501



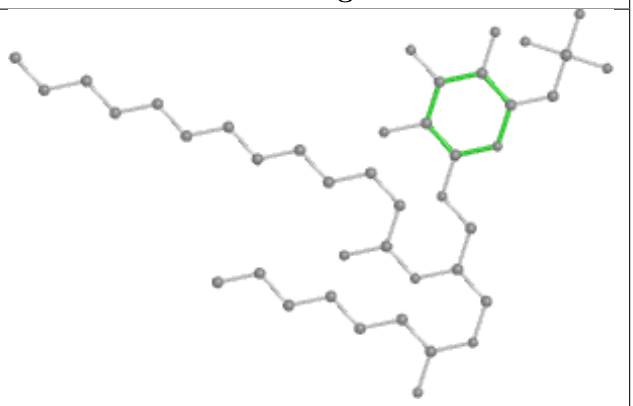
Bond lengths



Bond angles

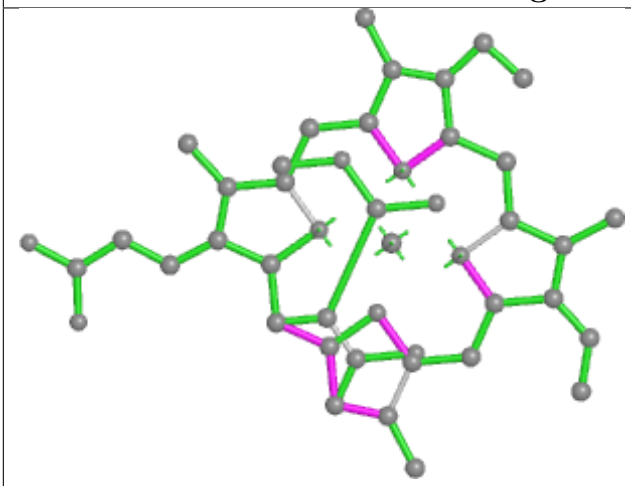


Torsions

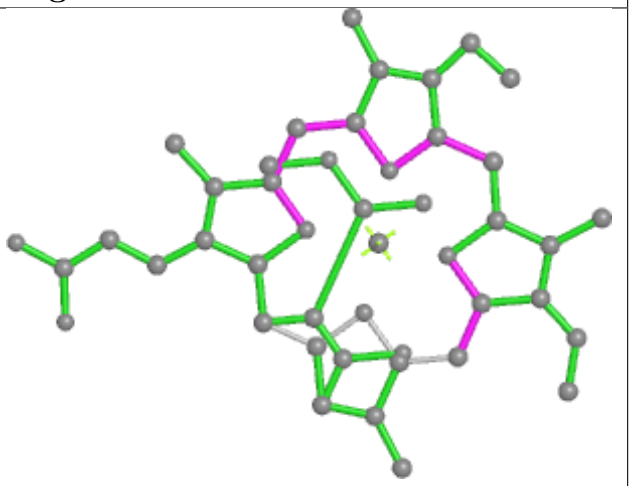


Rings

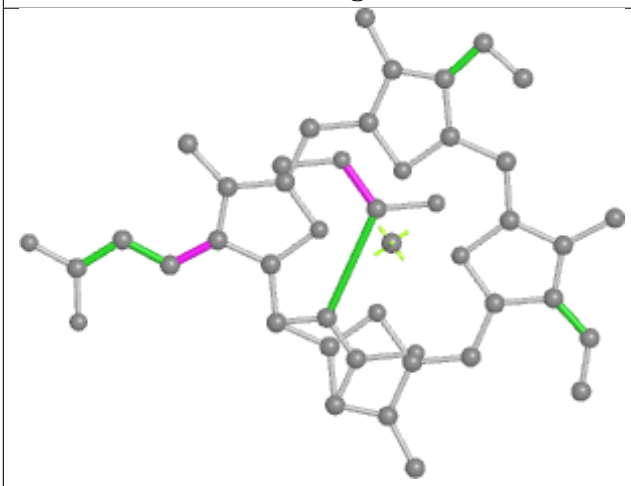
Ligand KC2 g 309



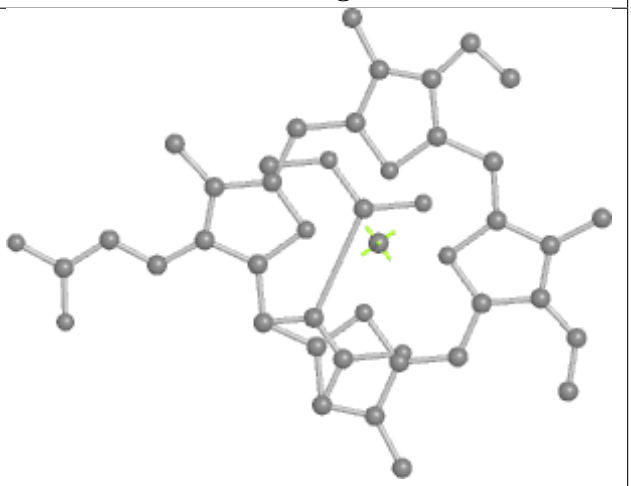
Bond lengths



Bond angles

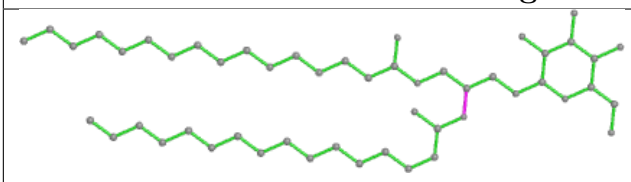


Torsions

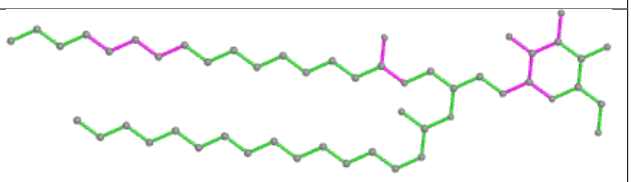


Rings

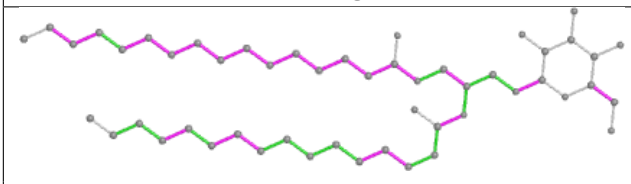
Ligand LMG C 520



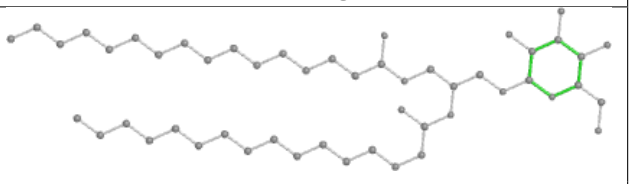
Bond lengths



Bond angles

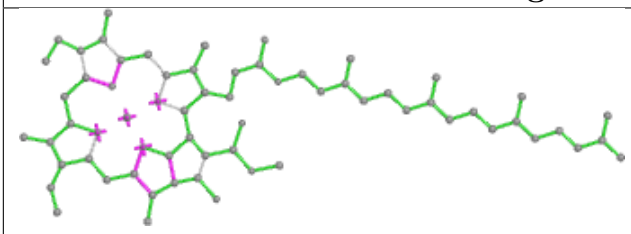


Torsions

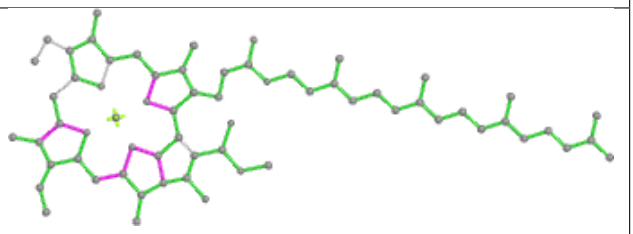


Rings

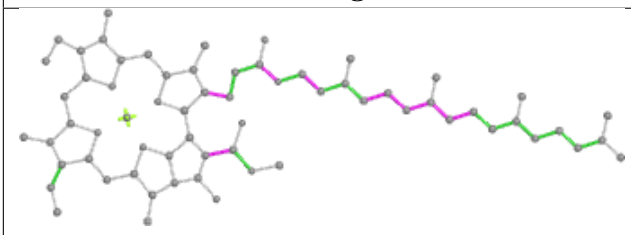
Ligand CLA b 605



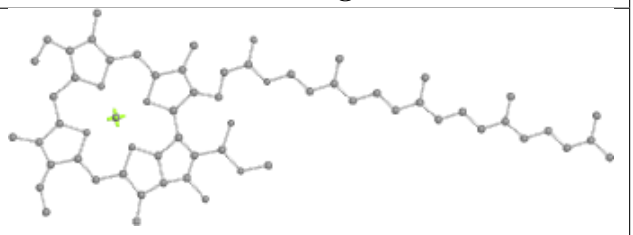
Bond lengths



Bond angles

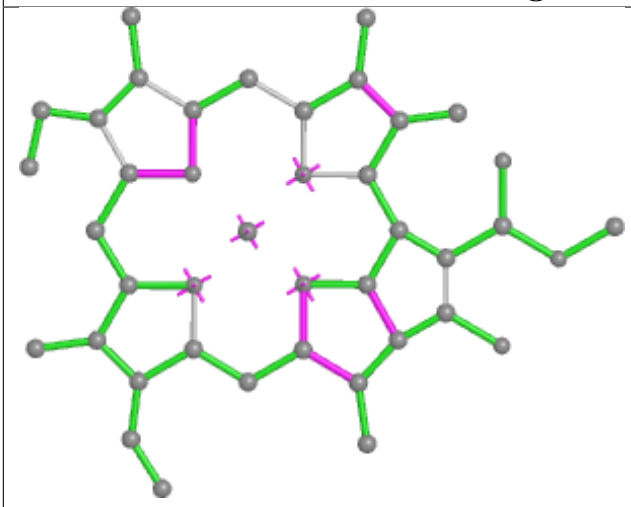


Torsions

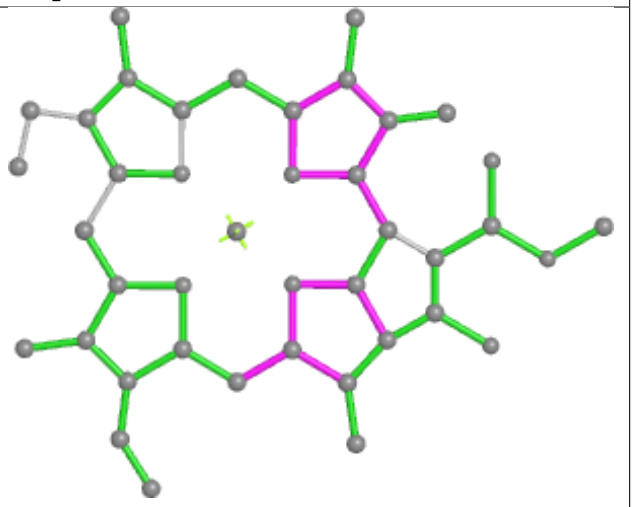


Rings

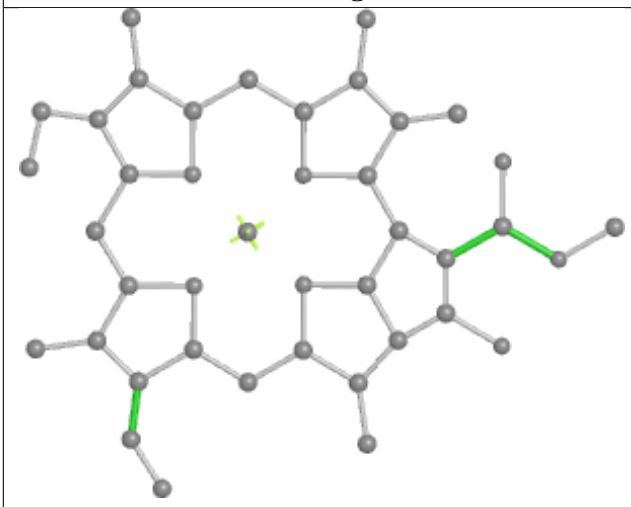
Ligand CLA p 302



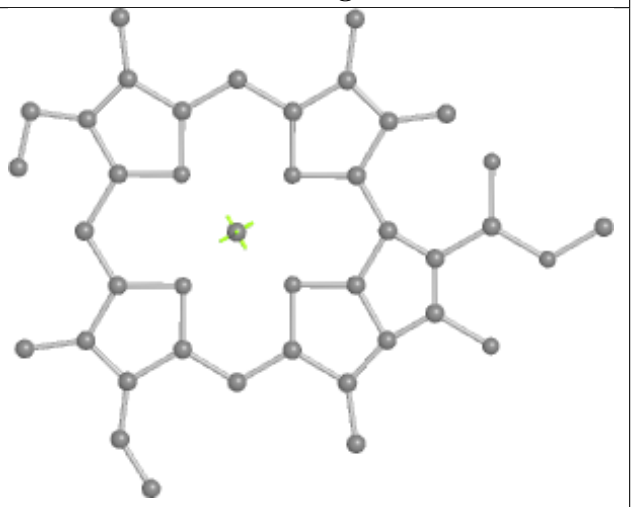
Bond lengths



Bond angles

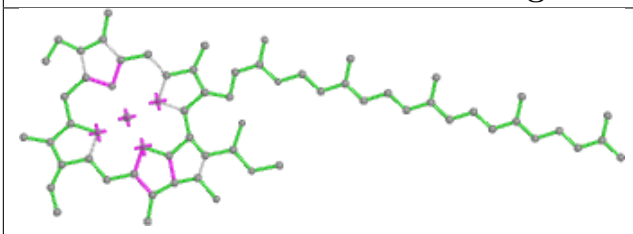


Torsions

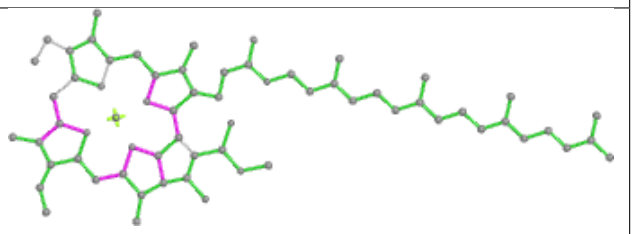


Rings

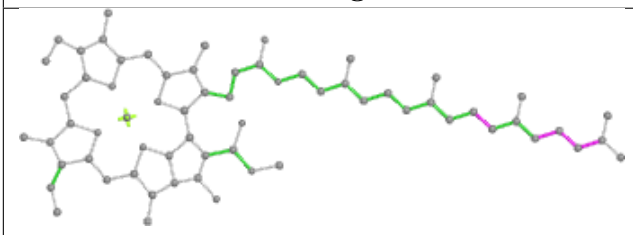
Ligand CLA b 616



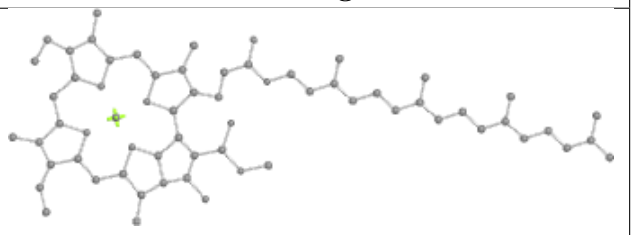
Bond lengths



Bond angles

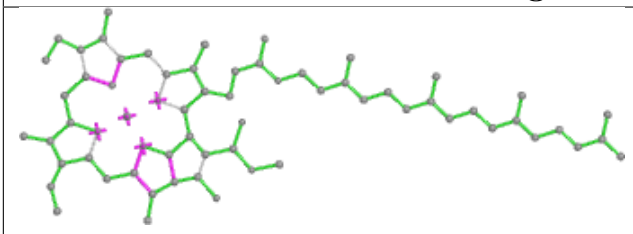


Torsions

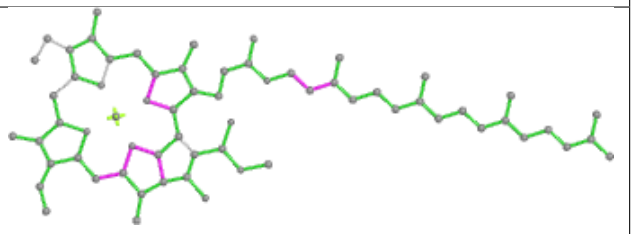


Rings

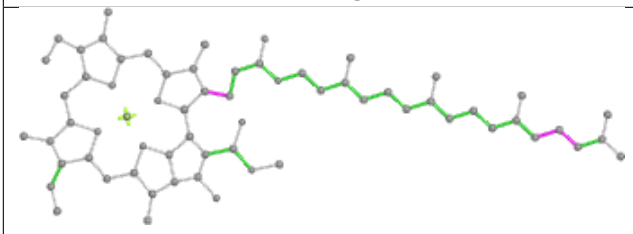
Ligand CLA b 612



Bond lengths



Bond angles



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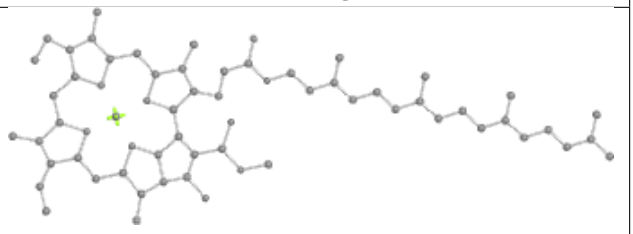
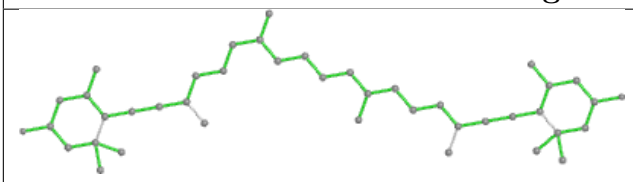
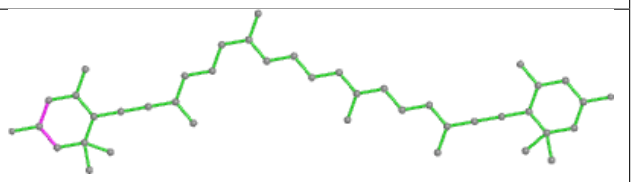


Rings

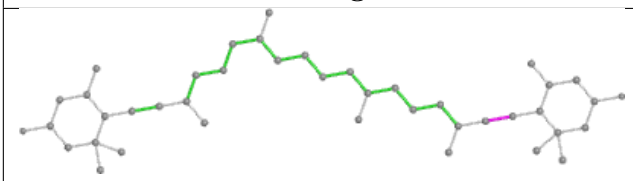
Ligand II0 4 314



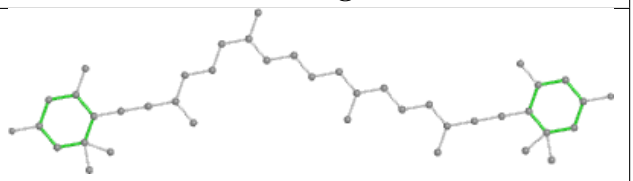
Bond lengths



Bond angles

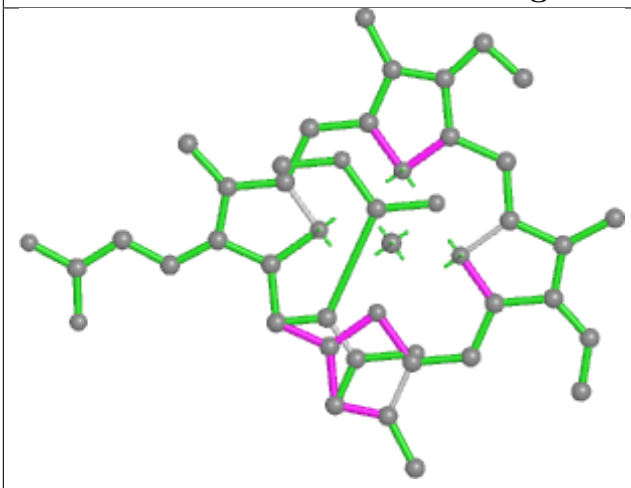


Torsions

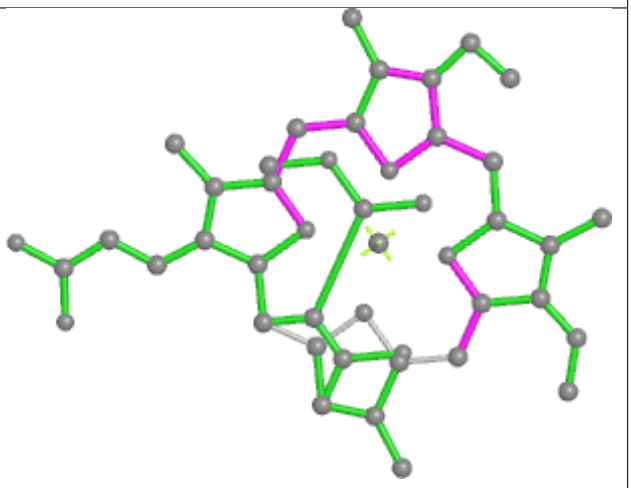


Rings

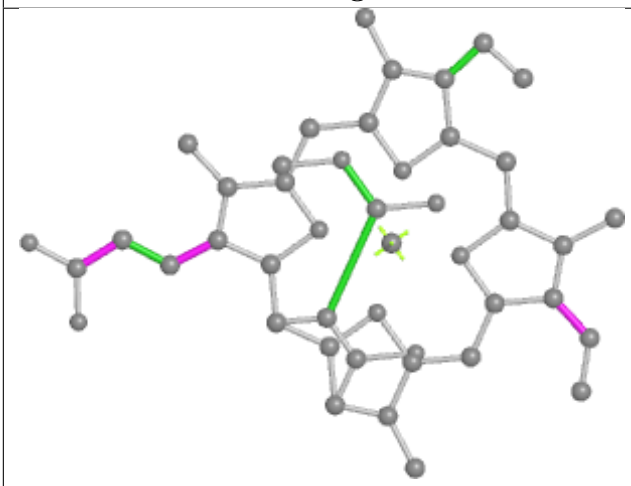
Ligand KC2 7 311



Bond lengths



Bond angles



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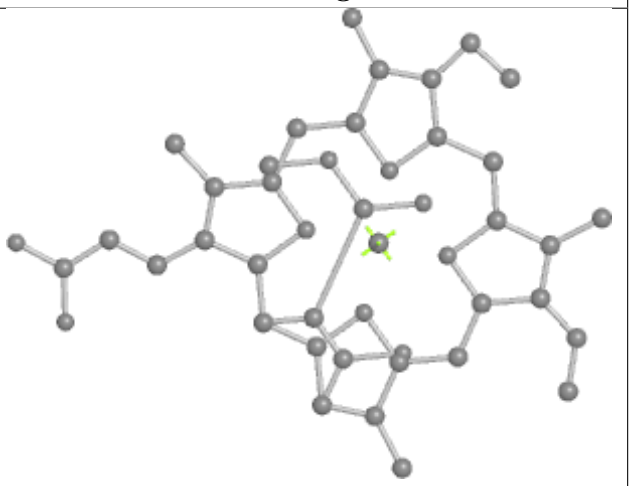
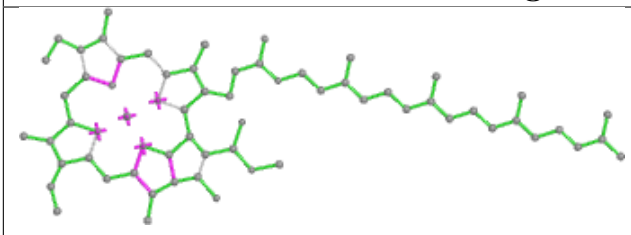
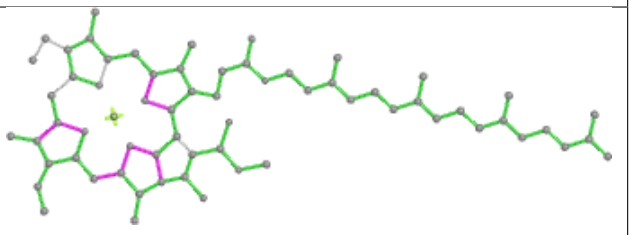


Rings

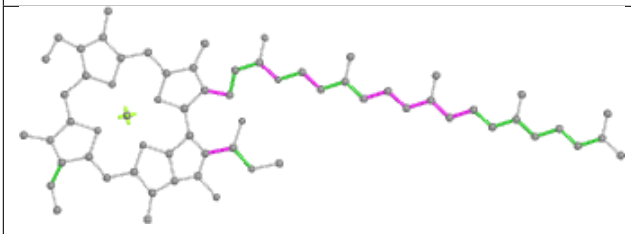
Ligand CLA B 605



Bond lengths



Bond angles



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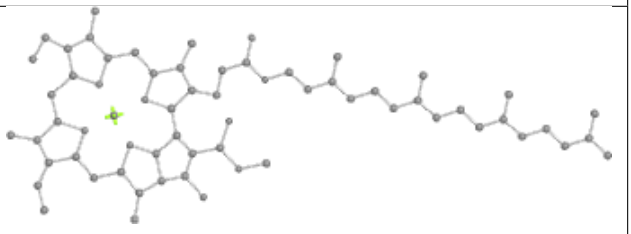
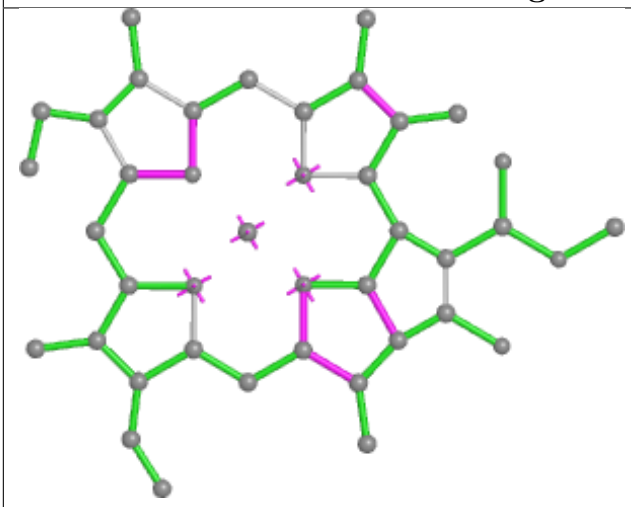
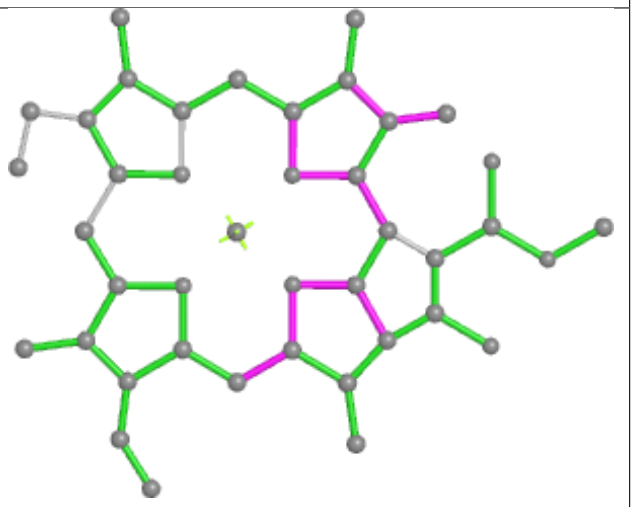


Rings

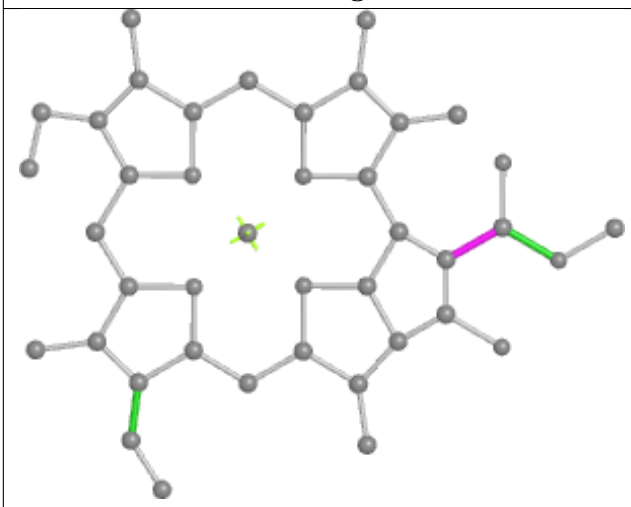
Ligand CLA 9 315



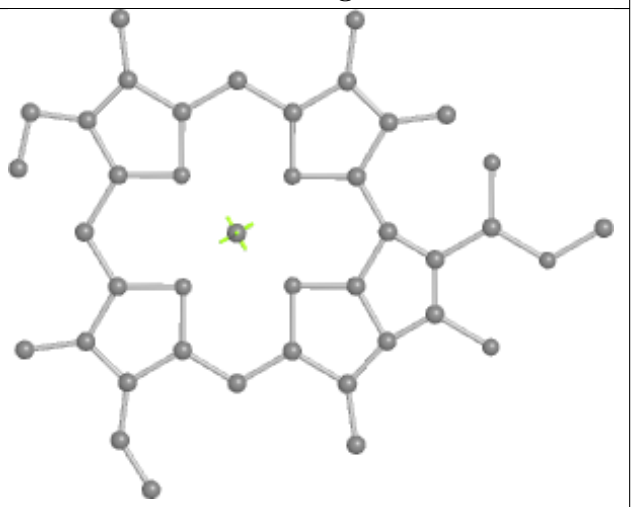
Bond lengths



Bond angles

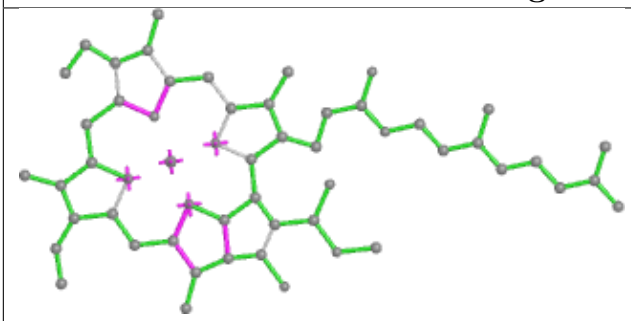


Torsions

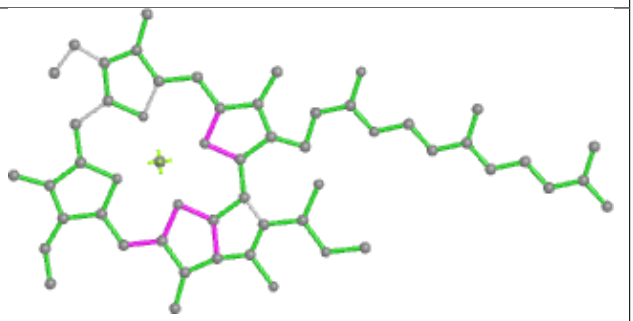


Rings

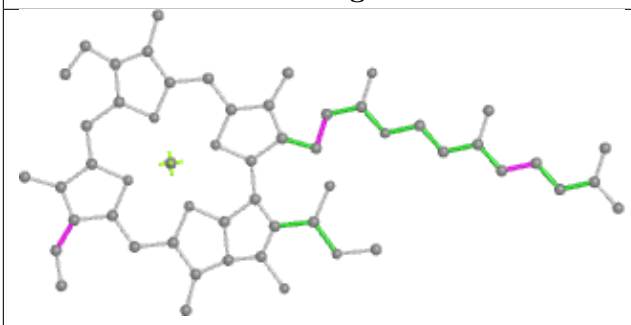
Ligand CLA 3 305



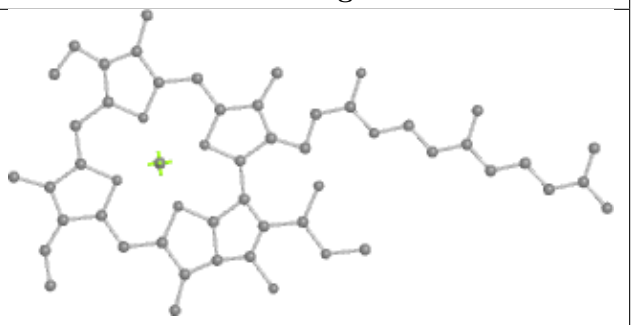
Bond lengths



Bond angles

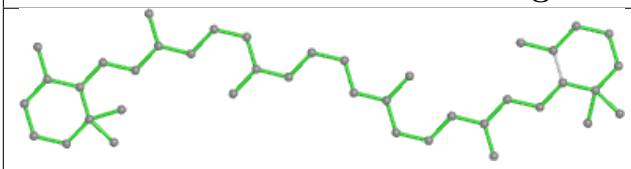


Torsions

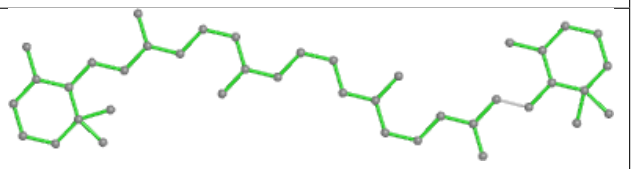


Rings

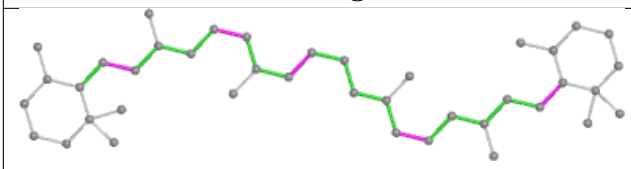
Ligand 8CT c 517



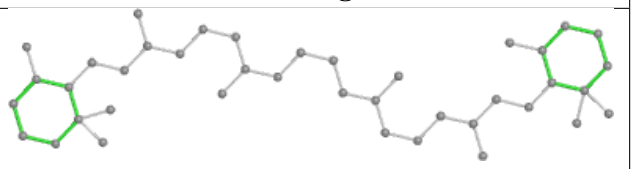
Bond lengths



Bond angles

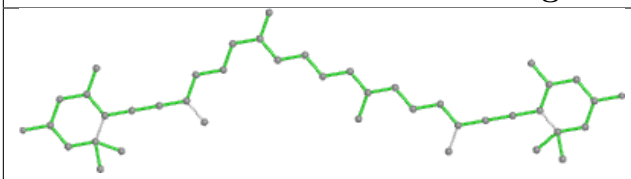


Torsions

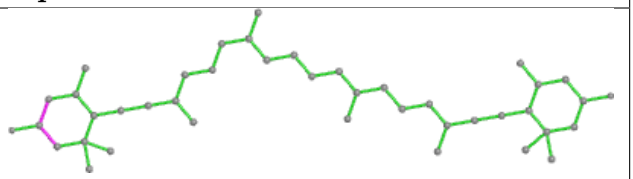


Rings

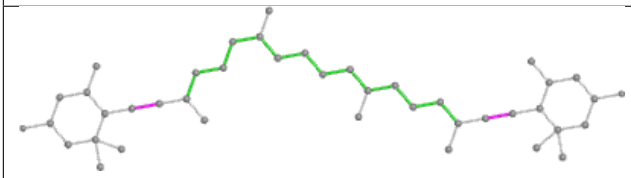
Ligand II0 p 315



Bond lengths



Bond angles



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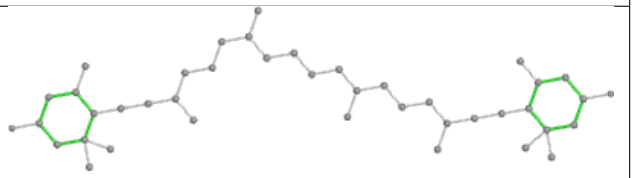
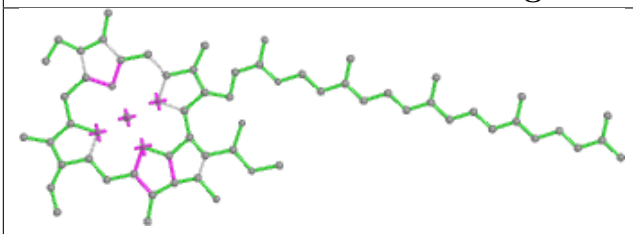
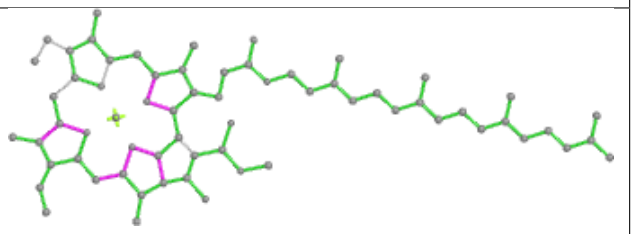


Rings

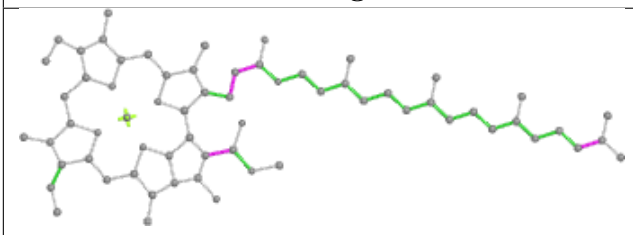
Ligand CLA C 503



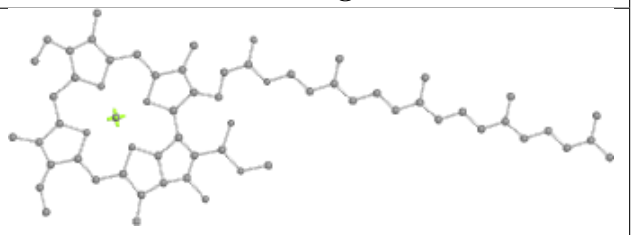
Bond lengths



Bond angles

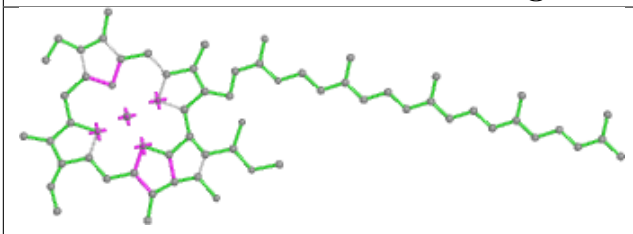


Torsions

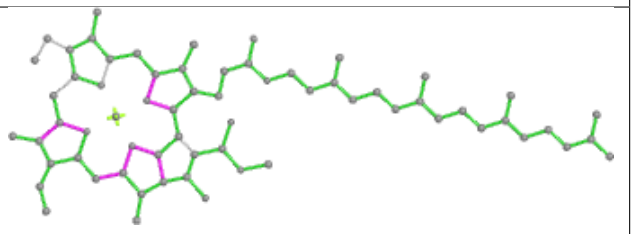


Rings

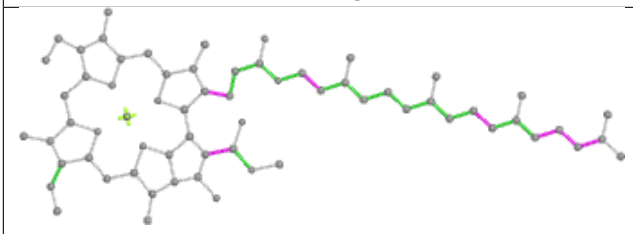
Ligand CLA d 405



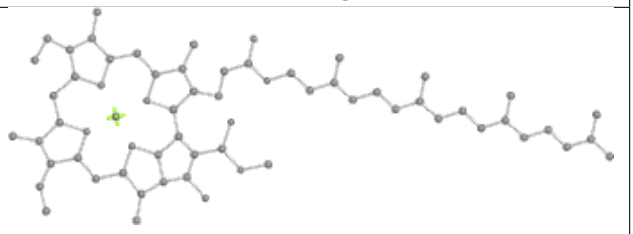
Bond lengths



Bond angles

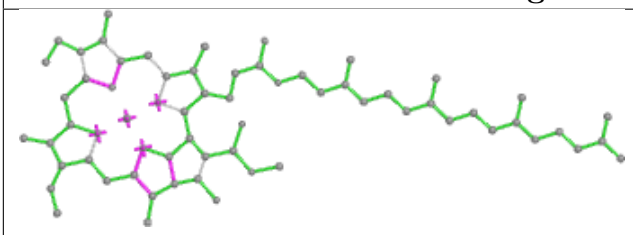


Torsions

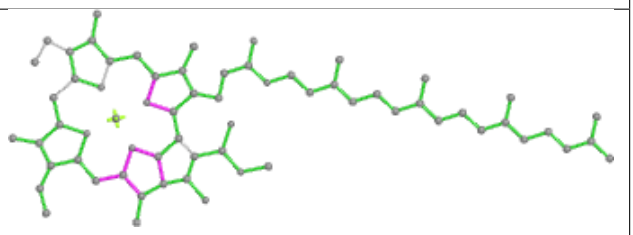


Rings

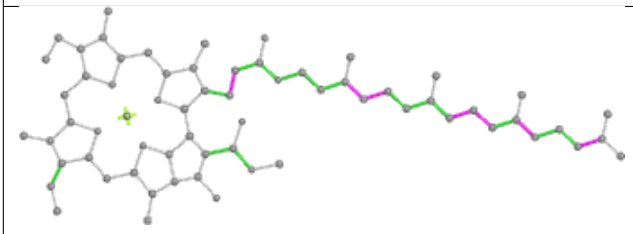
Ligand CLA b 607



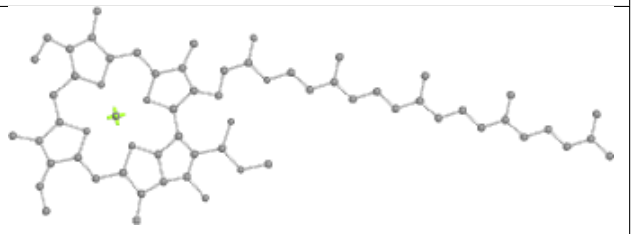
Bond lengths



Bond angles

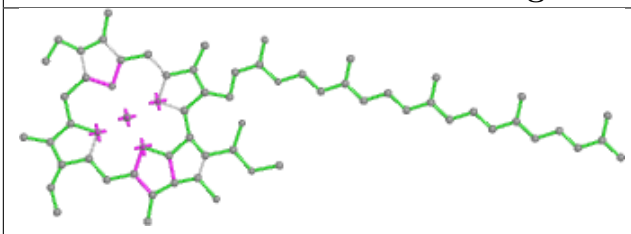


Torsions

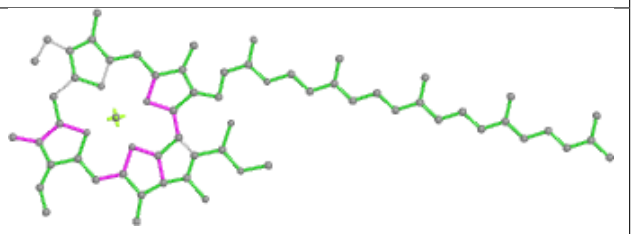


Rings

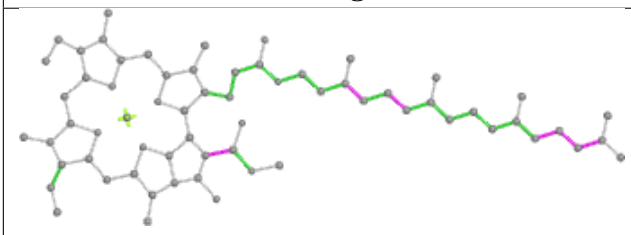
Ligand CLA b 610



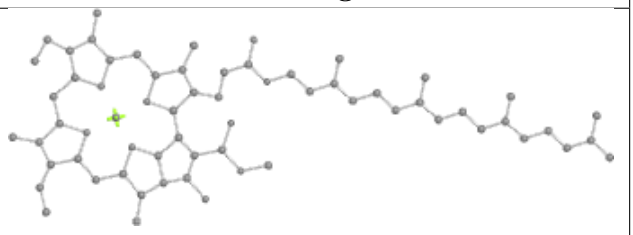
Bond lengths



Bond angles

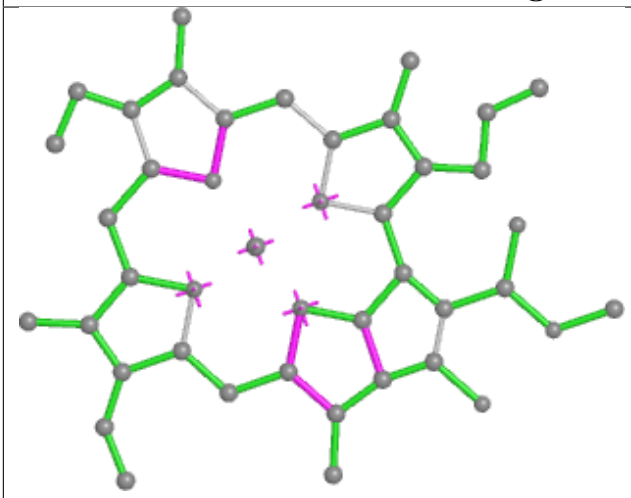


Torsions



Rings

Ligand CLA p 307



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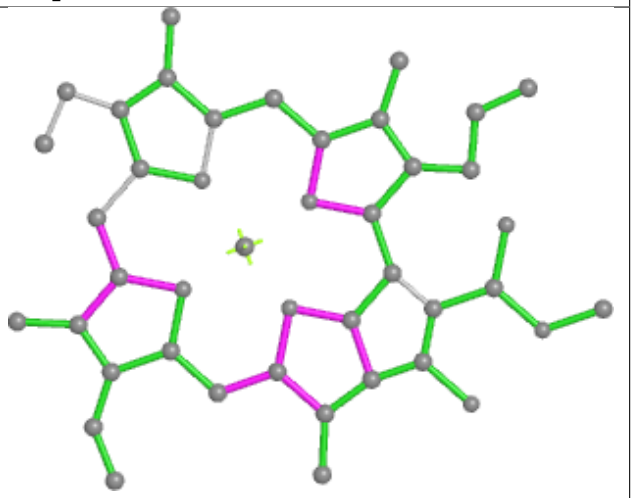

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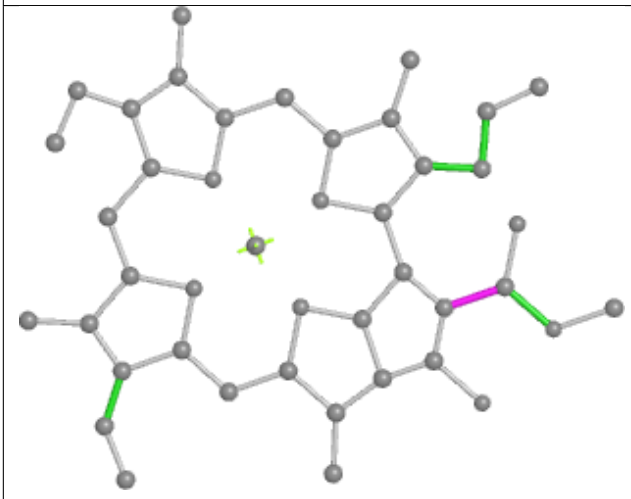

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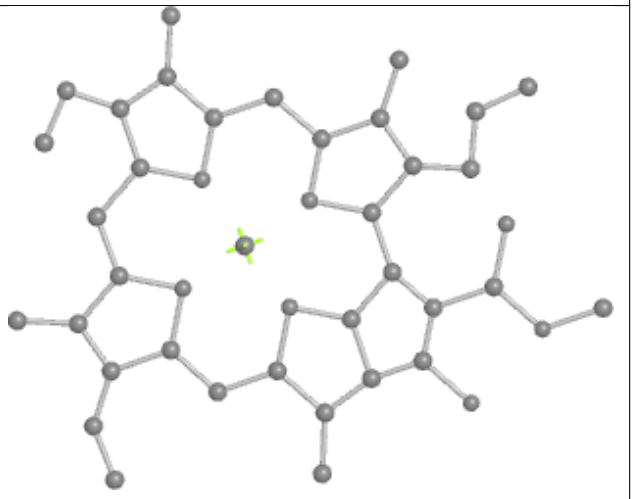
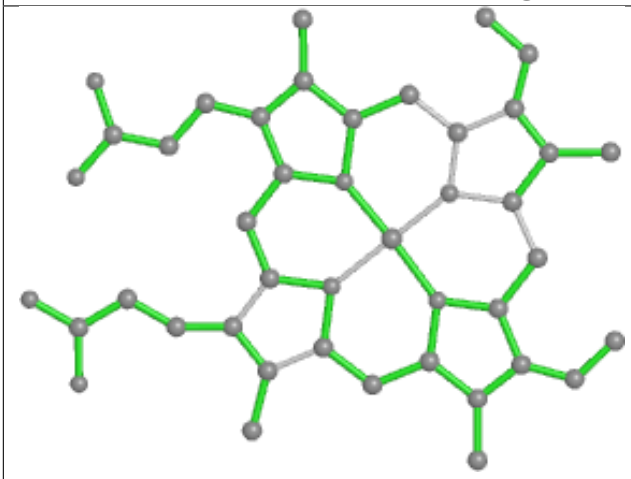


Rings

Ligand HEM V 201



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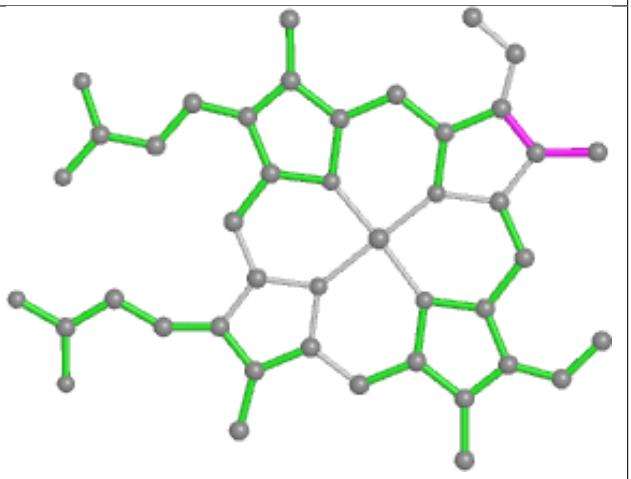

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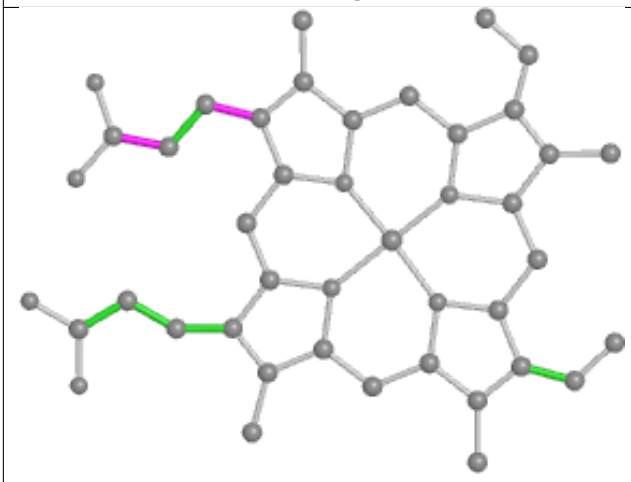

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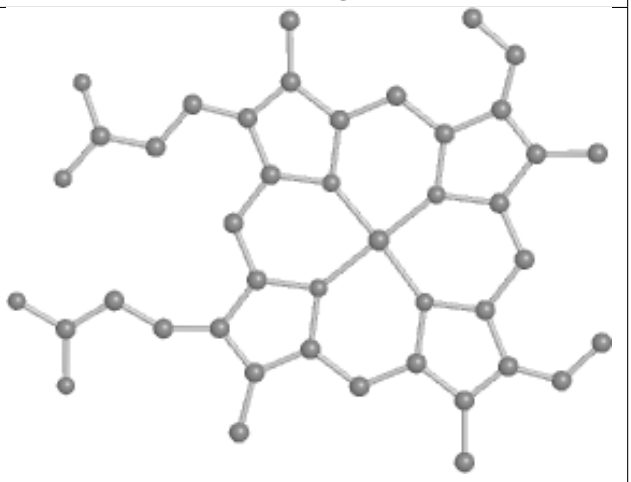
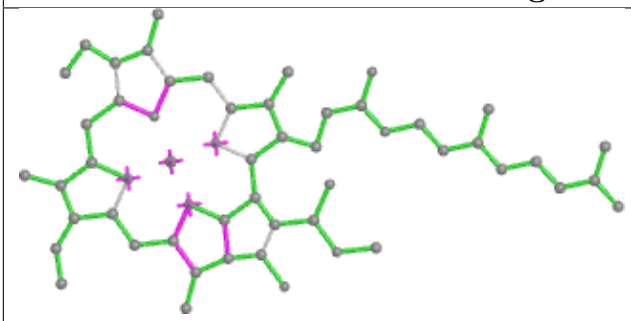


Rings

Ligand CLA 3 309



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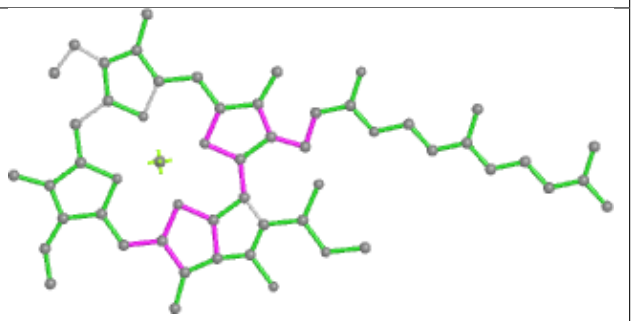
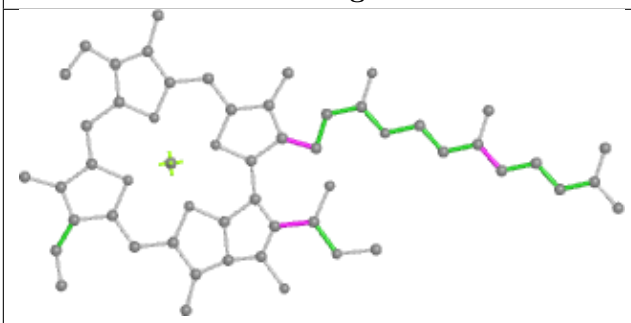


Bond angles



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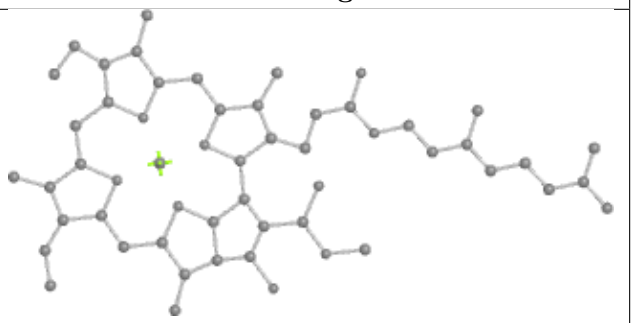
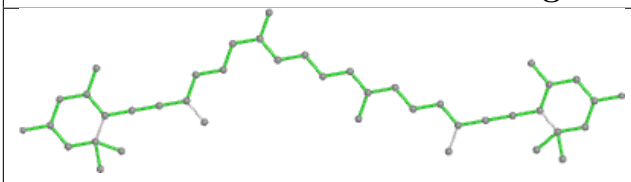


Rings

Ligand II0 0 316



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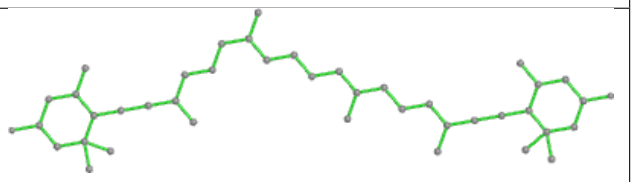

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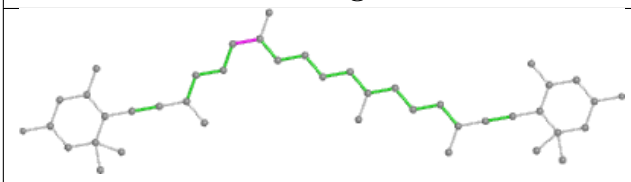

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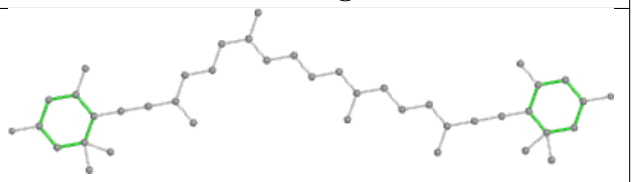
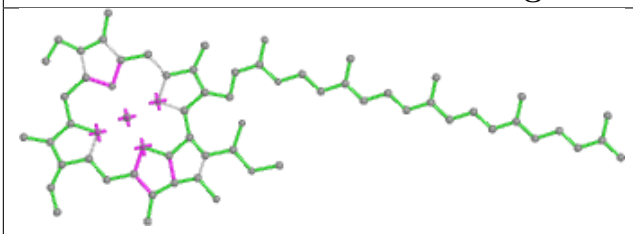


Rings

Ligand CLA C 507



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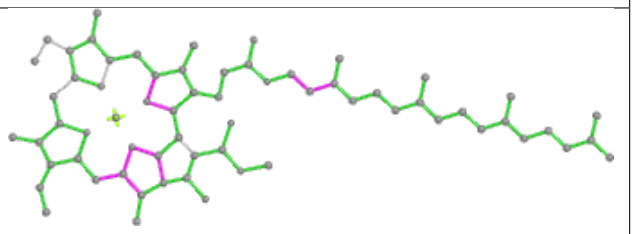

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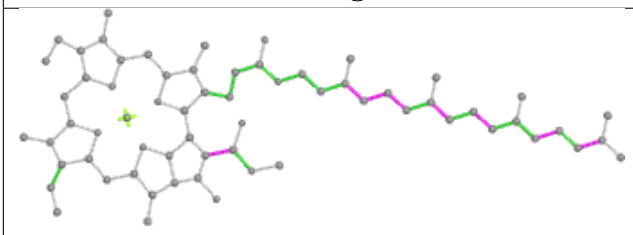

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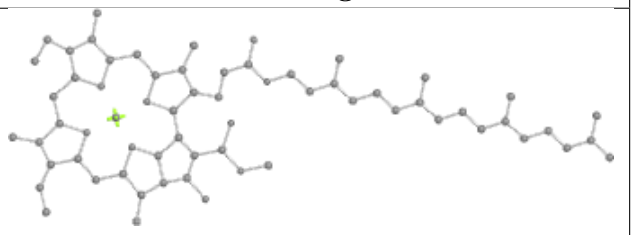
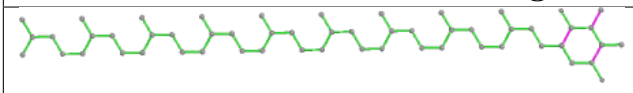


Rings

Ligand PL9 D 407



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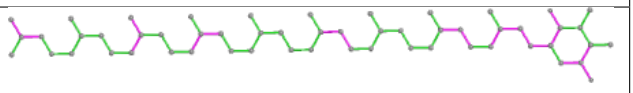
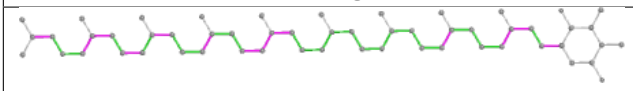


Bond angles



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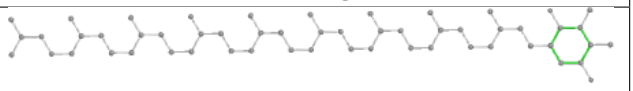
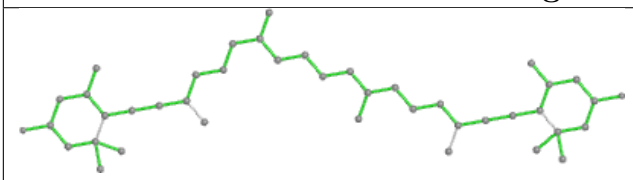


Rings

Ligand II0 g 314



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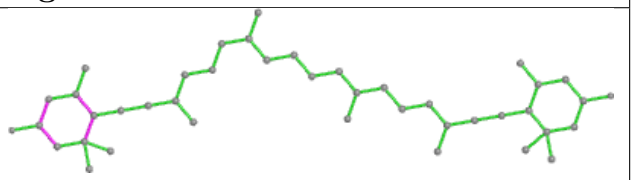

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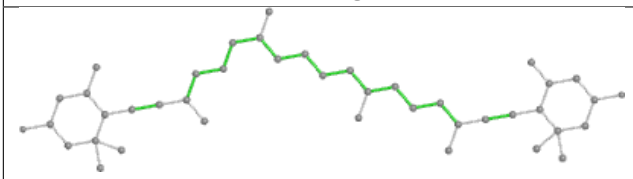

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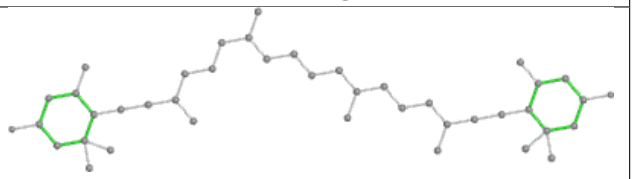
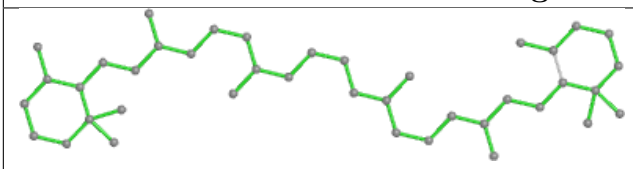


Rings

Ligand 8CT 1 312



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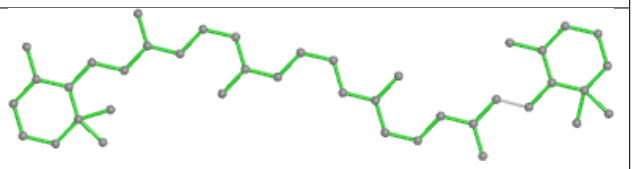

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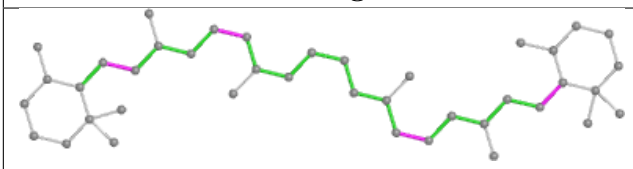

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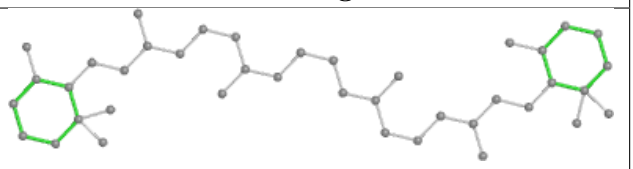
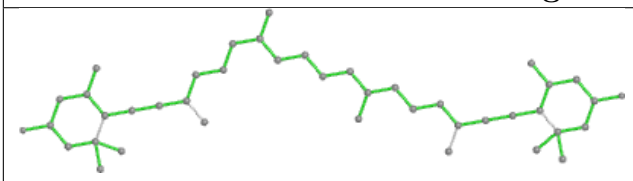


Rings

Ligand II0 6 301



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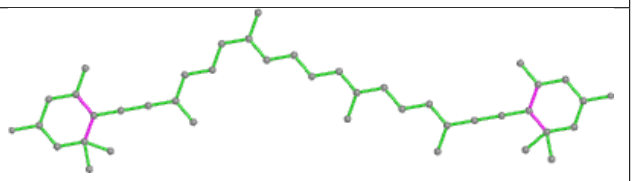

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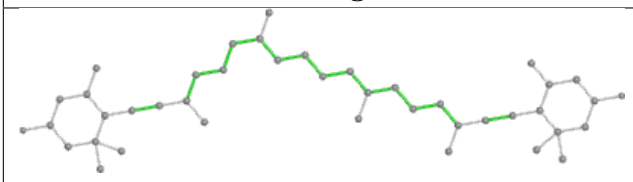

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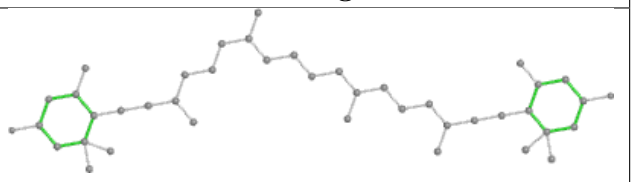
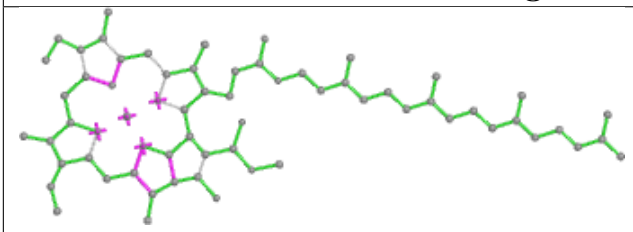


Rings

Ligand CLA B 610



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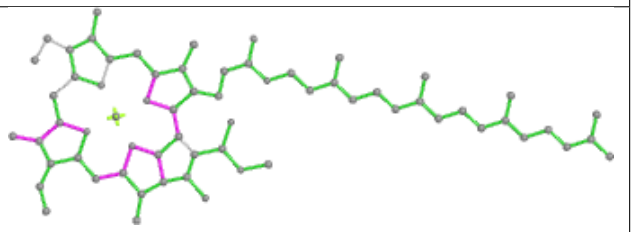

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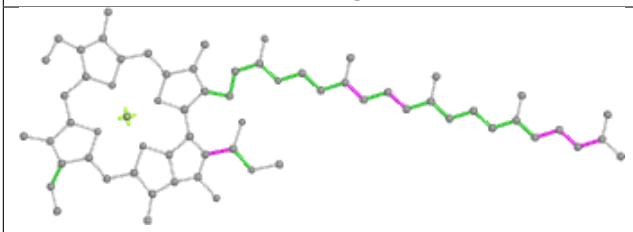

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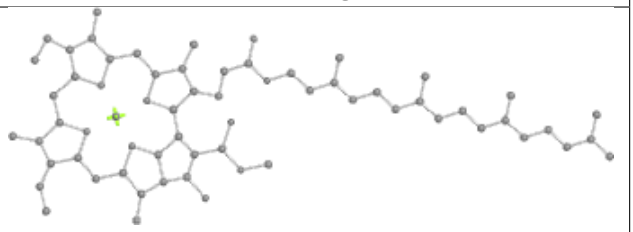
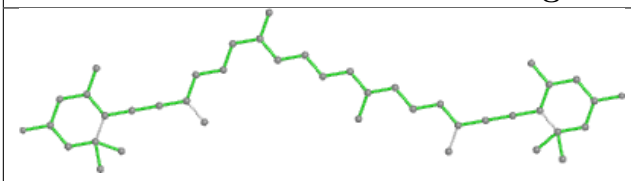


Rings

Ligand II0 1 315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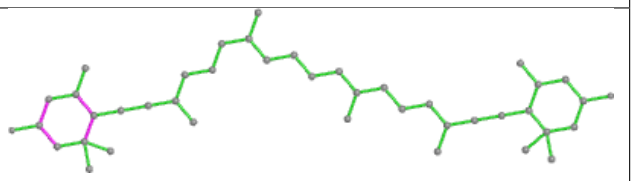
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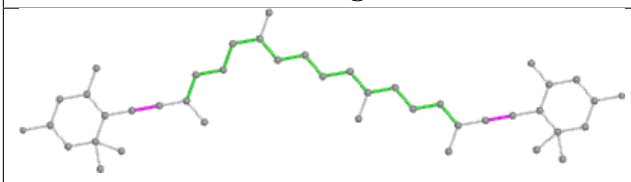
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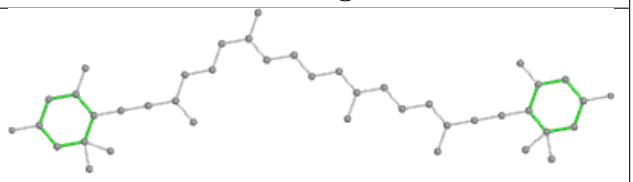
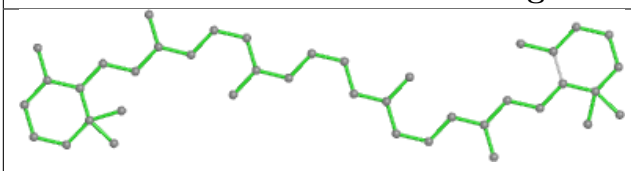

Rings

Ligand 8CT B 619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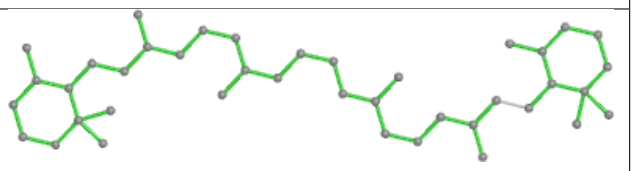
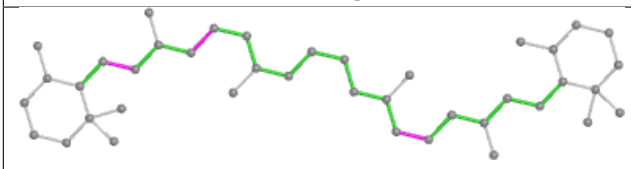

Bond angles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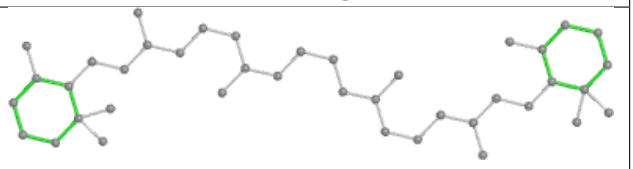
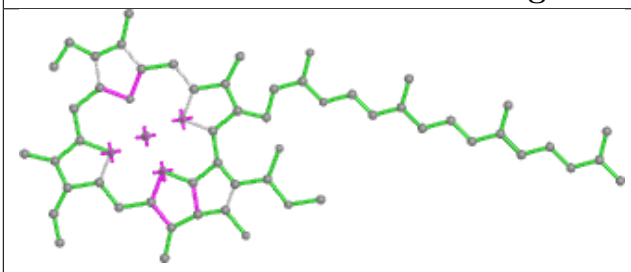
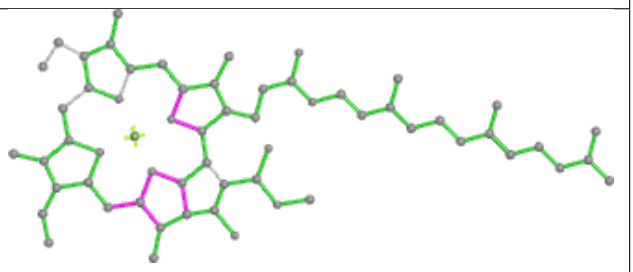
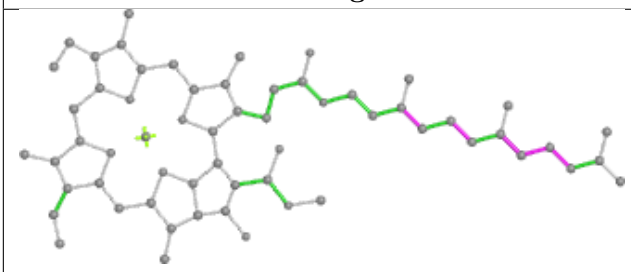
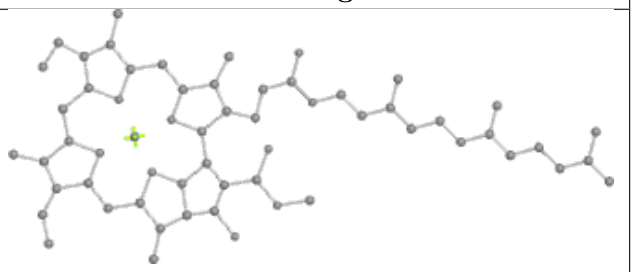

Rings

Ligand CLA 7 305

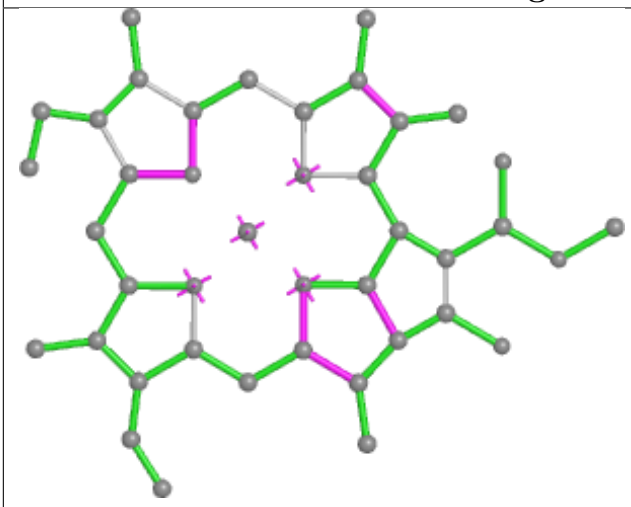

Bond lengths


Bond angles

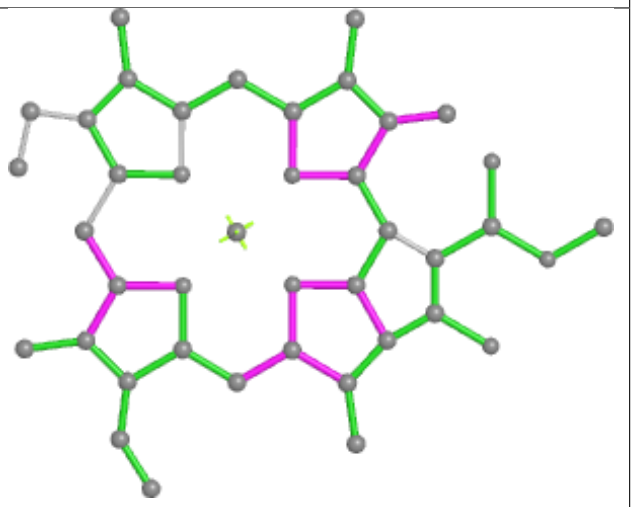

Torsions


Rings

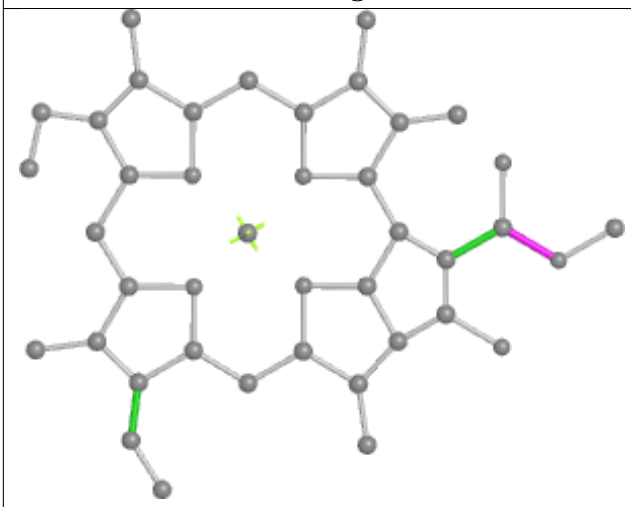
Ligand CLA 6 303



Bond lengths



Bond angles



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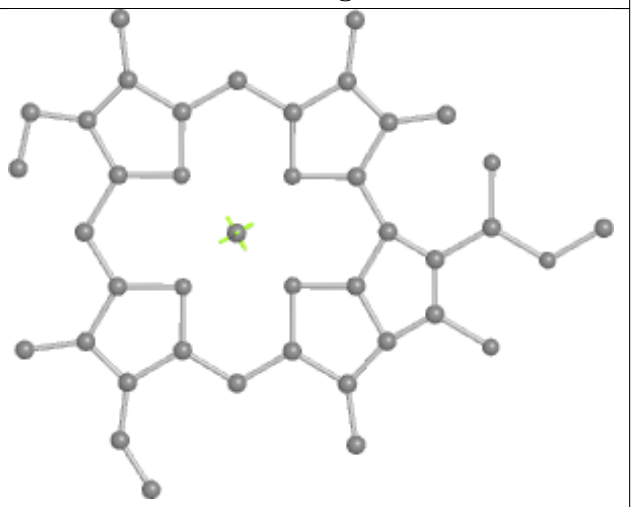
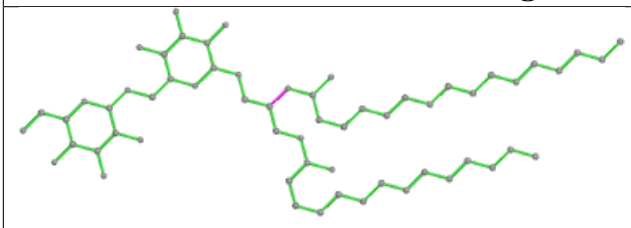
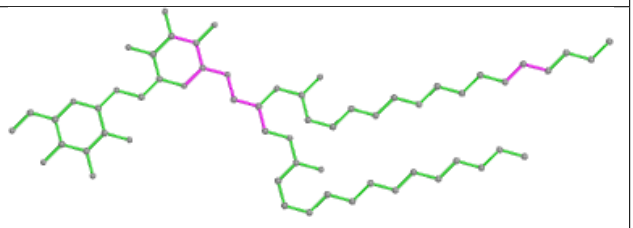


Rings

Ligand DGD H 101



Bond lengths



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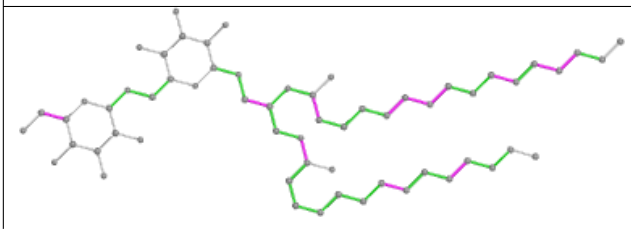
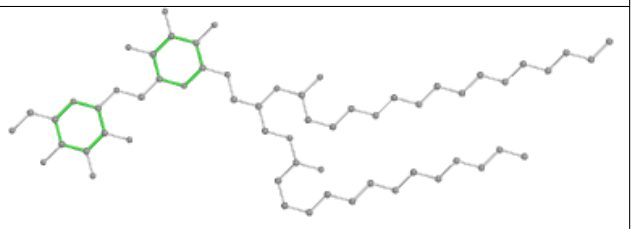
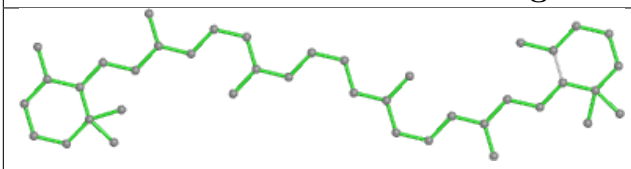


Torsions



Rings

Ligand 8CT b 620



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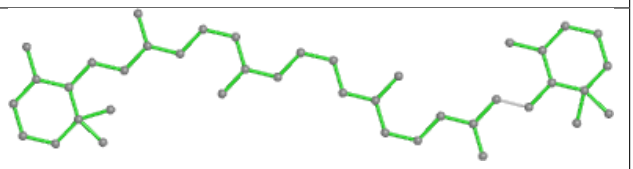

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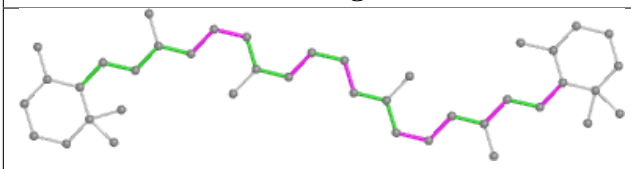

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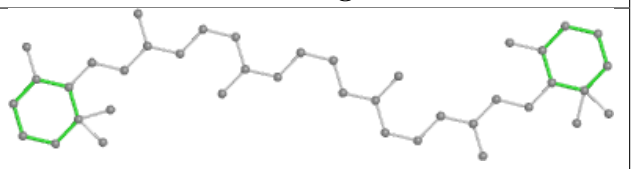
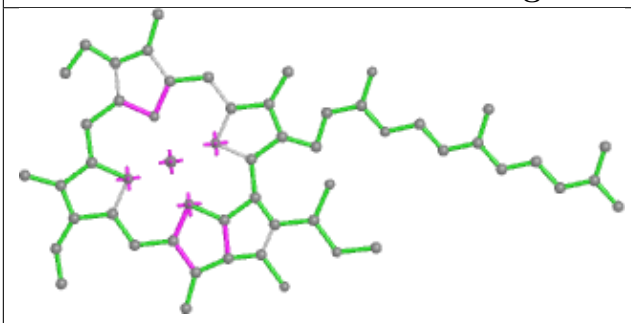


Rings

Ligand CLA N 305



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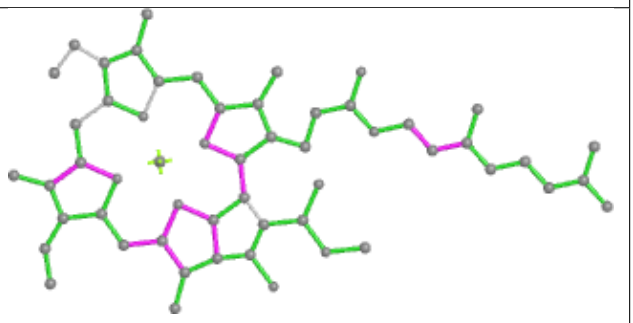

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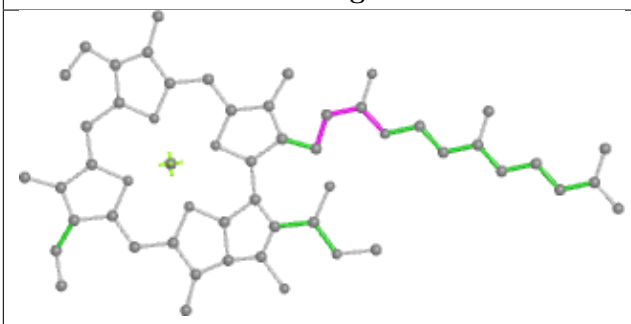

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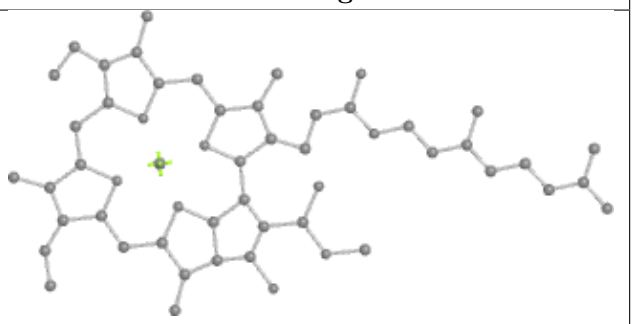
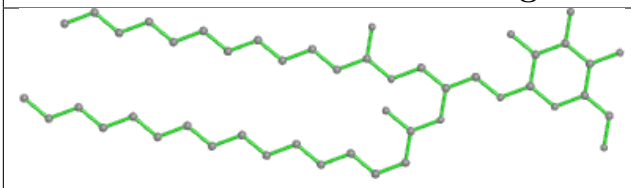


Rings

Ligand LMG w 101



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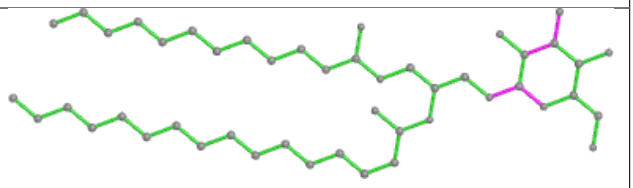

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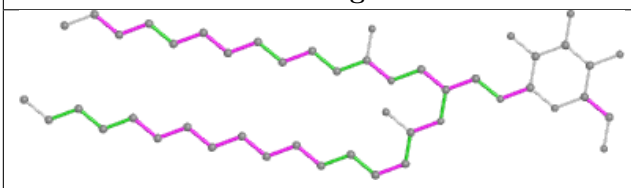

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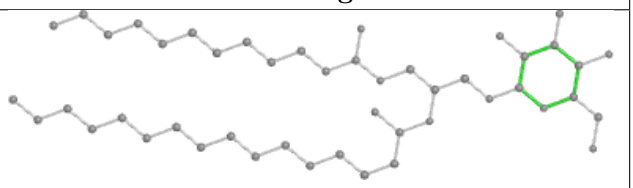
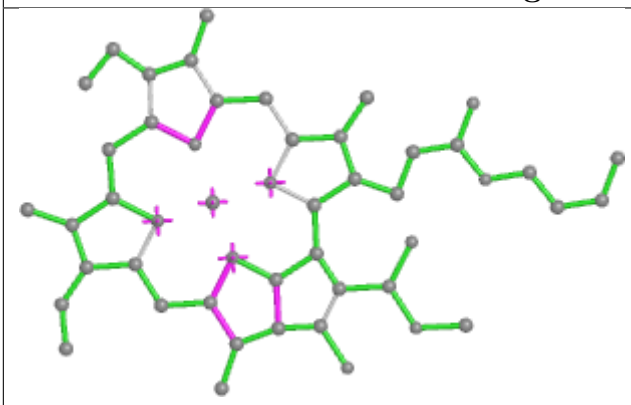


Rings

Ligand CLA A 406



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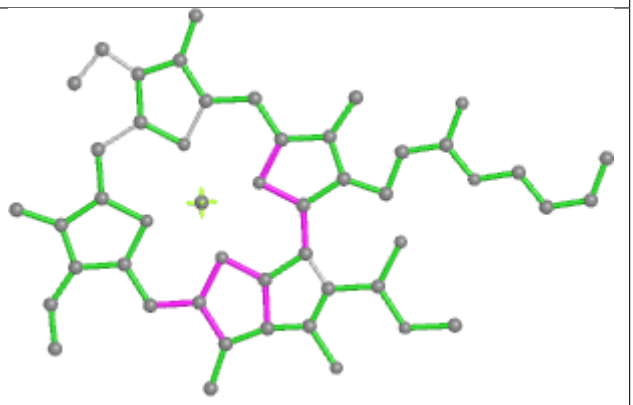

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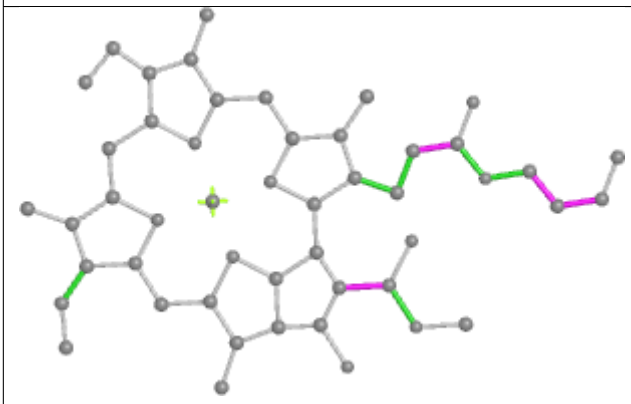

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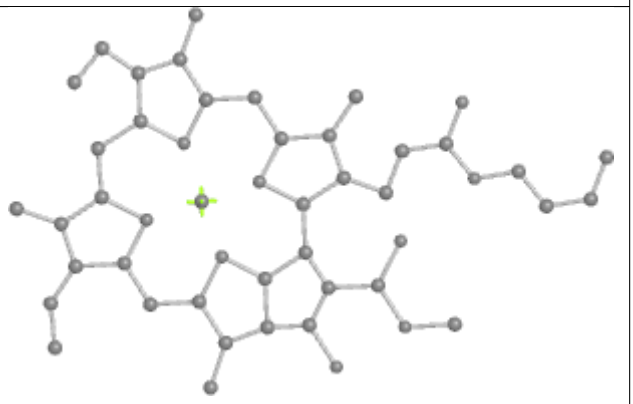
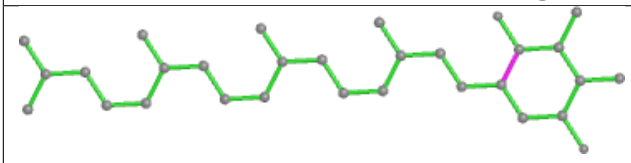


Rings

Ligand PL9 a 410



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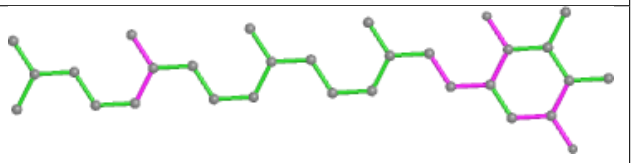

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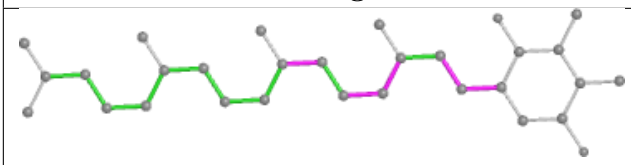

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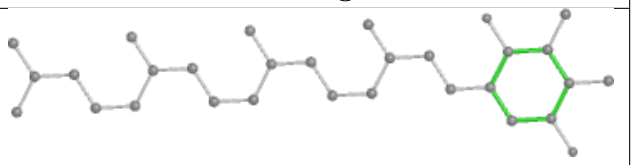
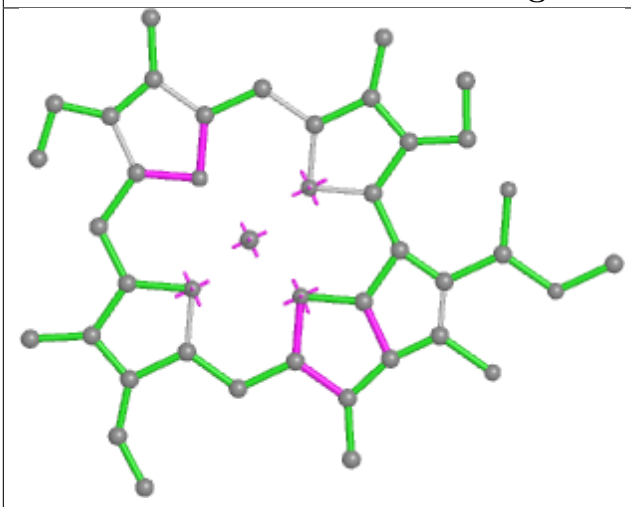


Rings

Ligand CLA 6 309



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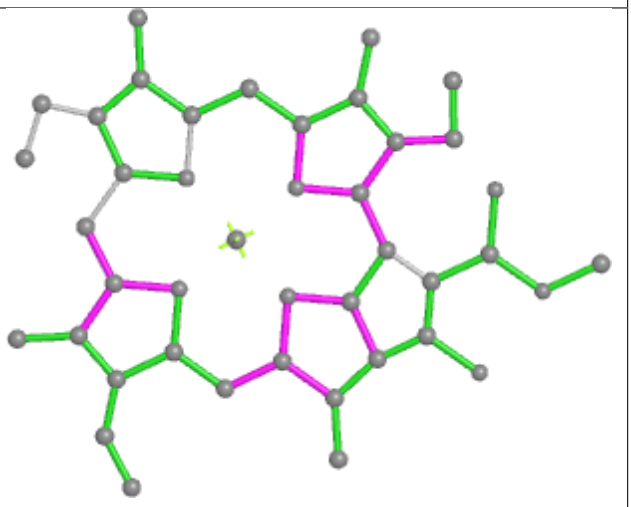

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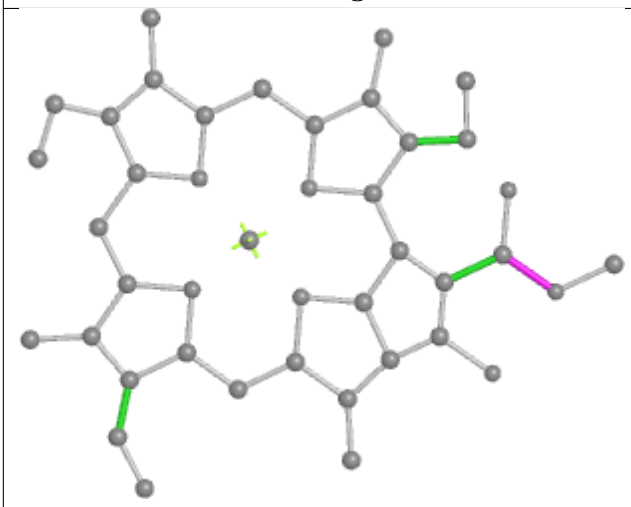

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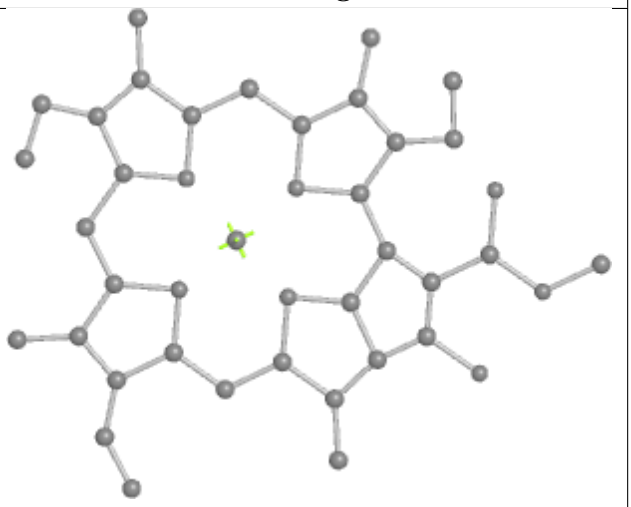
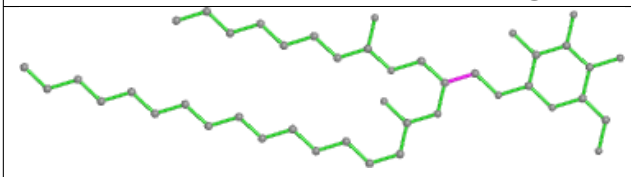


Rings

Ligand LMG t 101



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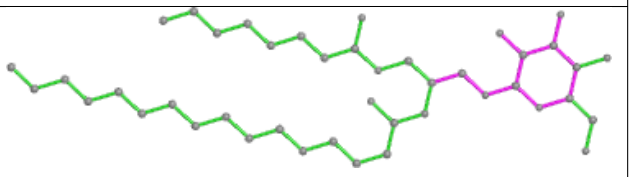

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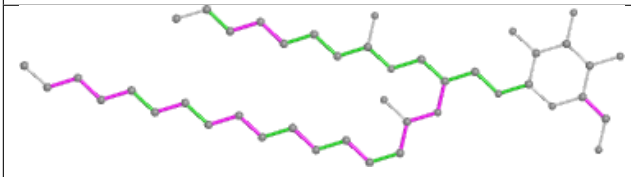

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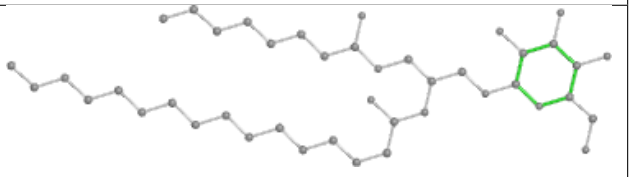
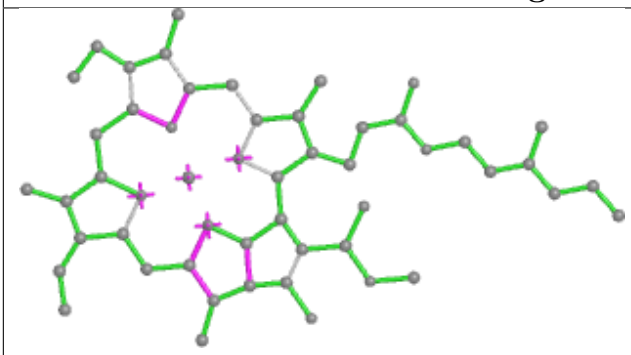
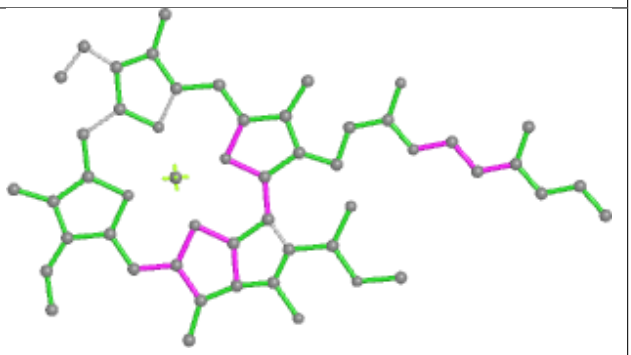
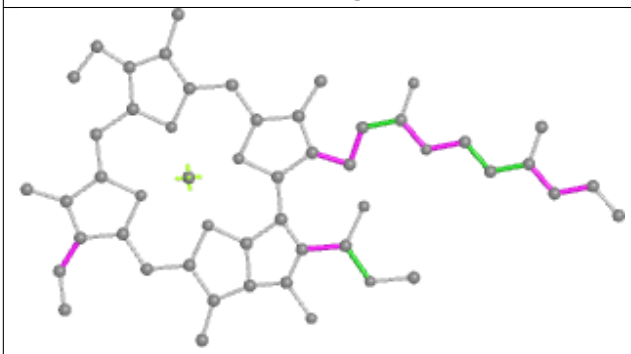
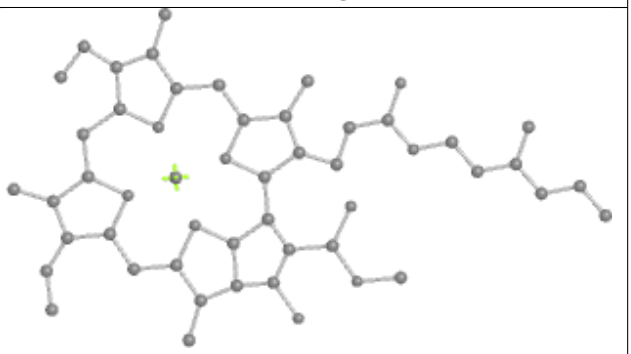


Rings

Ligand CLA 2 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

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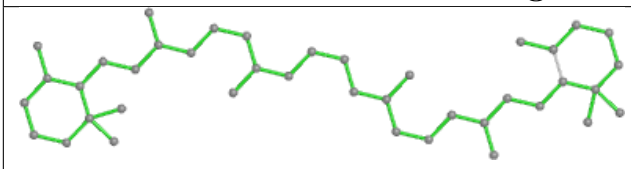
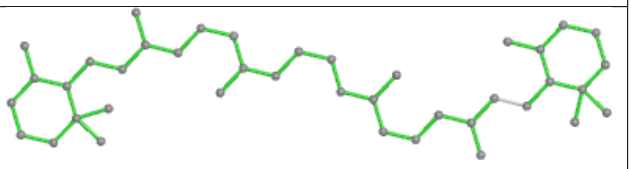
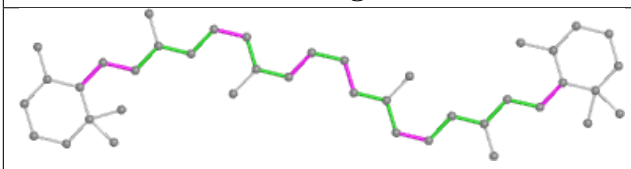
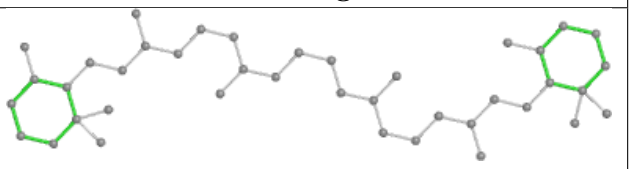
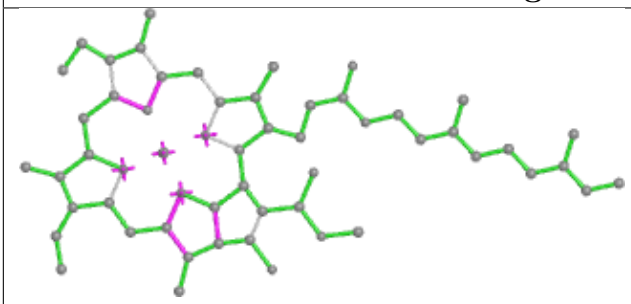
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 513



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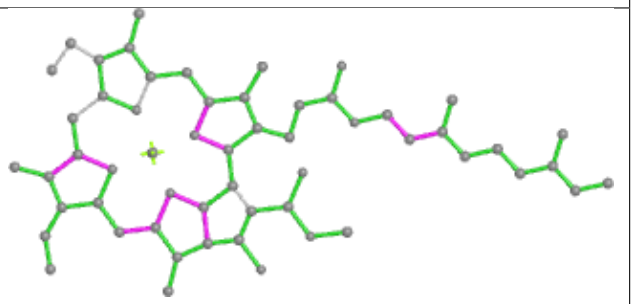

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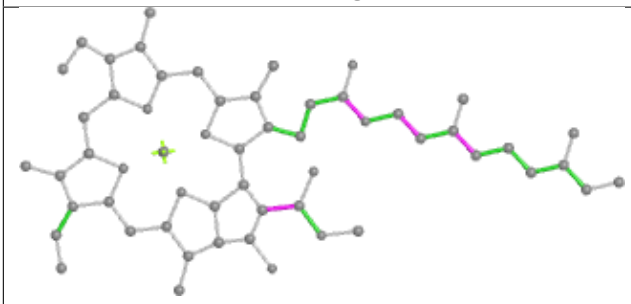

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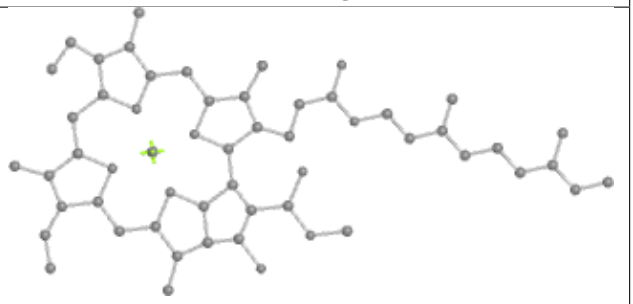
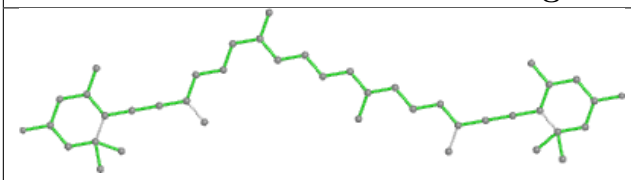


Rings

Ligand II0 2 311



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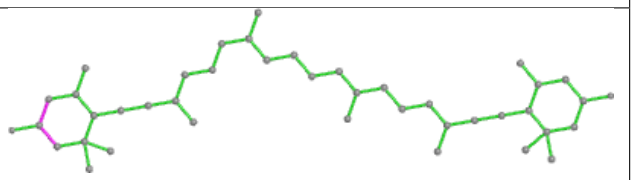
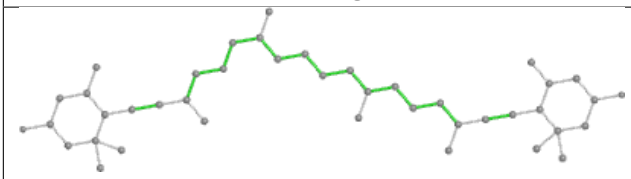


Bond angles



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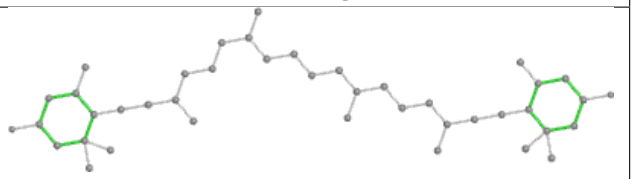
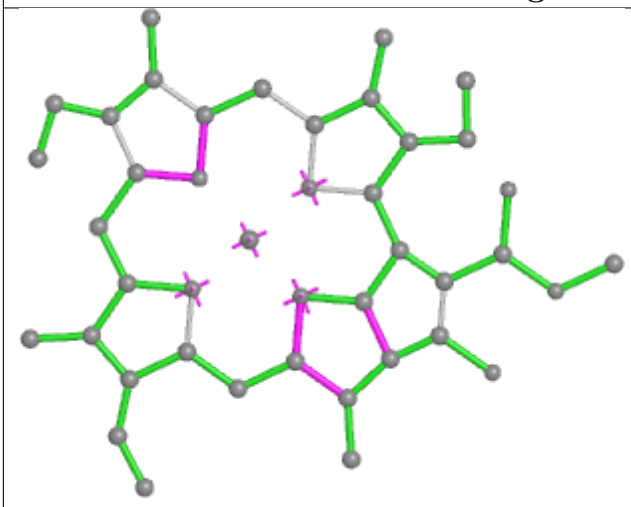


Rings

Ligand CLA p 304



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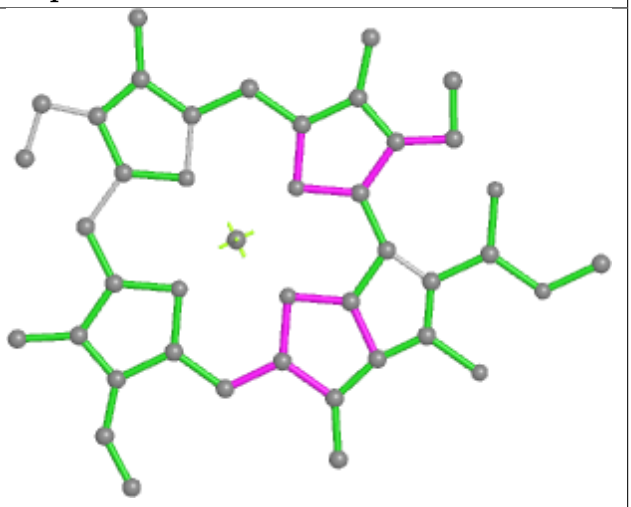
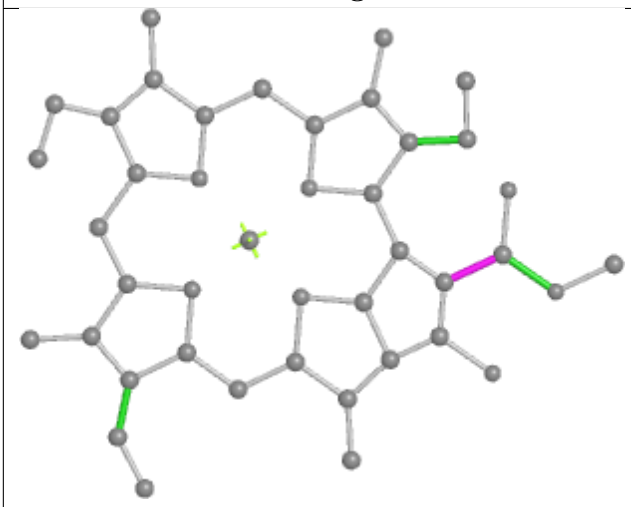


Bond angles



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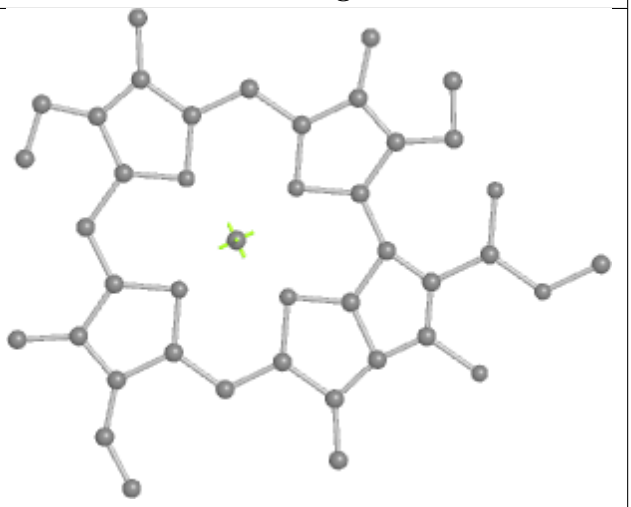
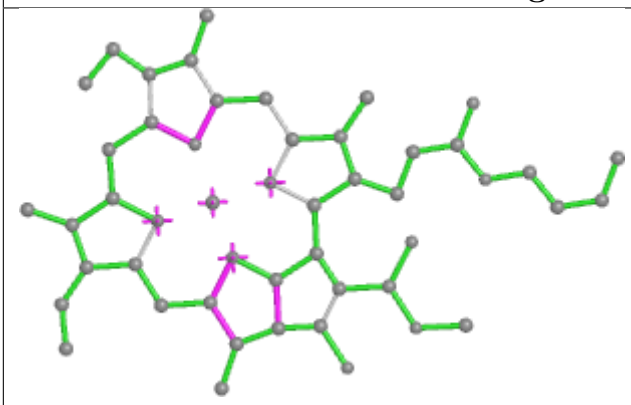


Rings

Ligand CLA a 406



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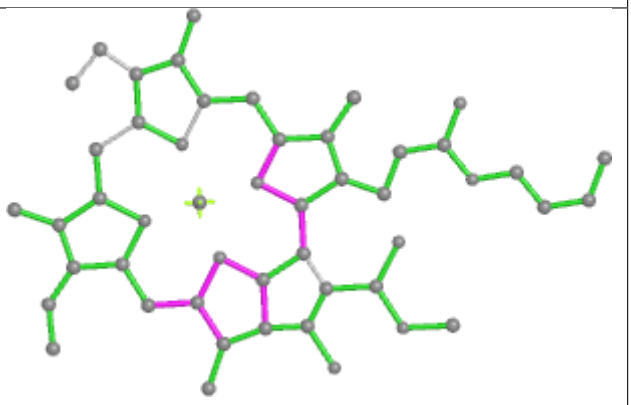
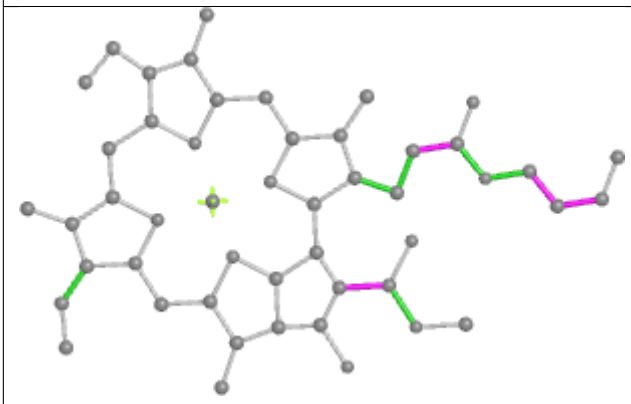
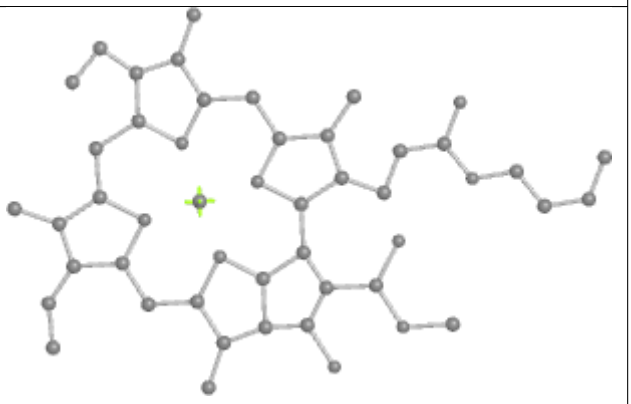


Bond angles

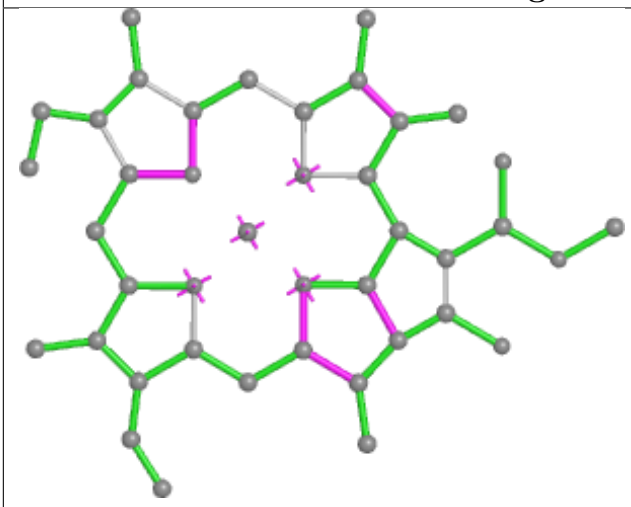


Torsions

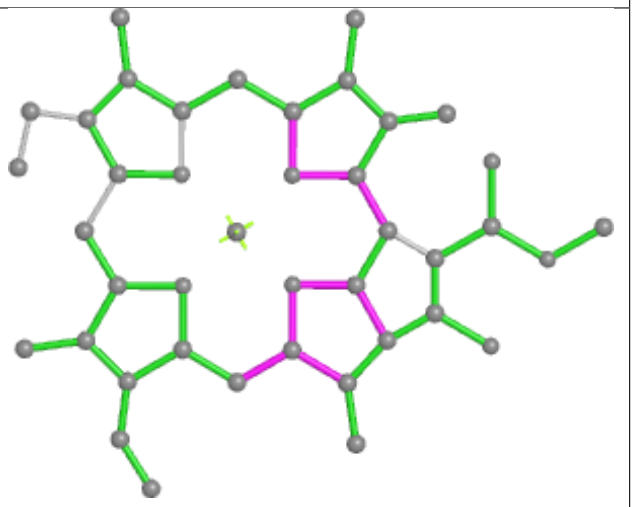


Rings

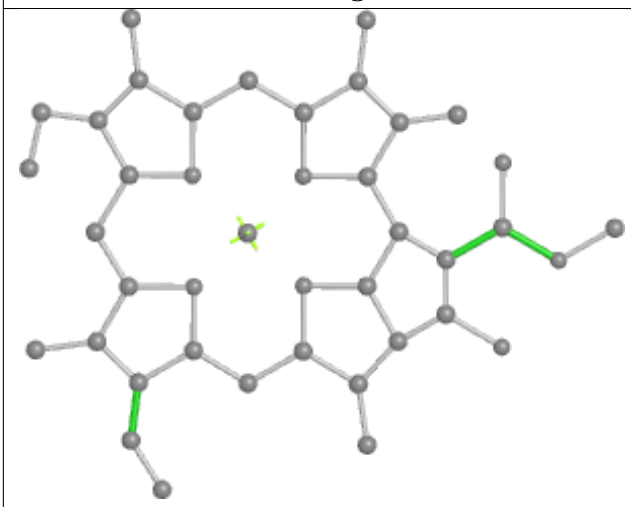
Ligand CLA 5 310



Bond lengths



Bond angles



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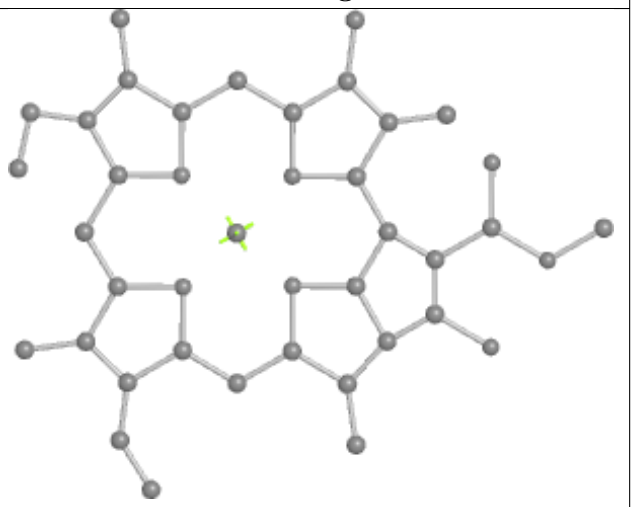
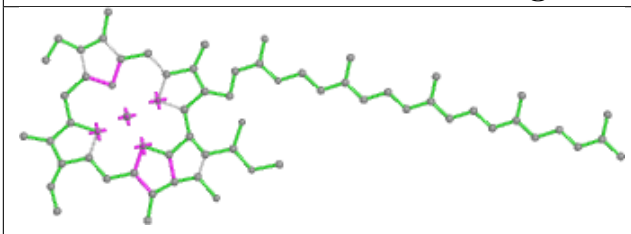
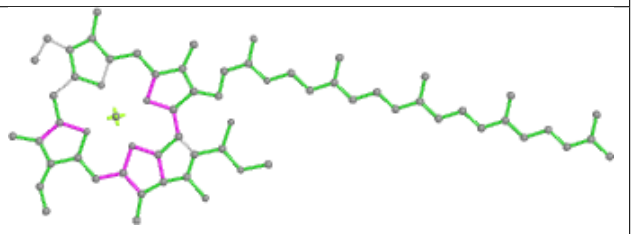


Rings

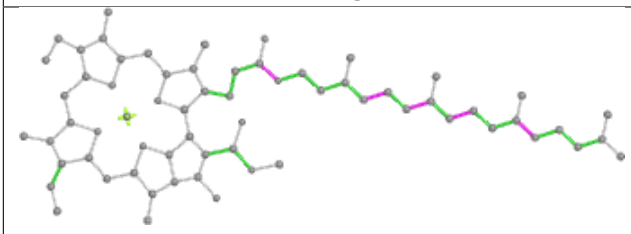
Ligand CLA c 512



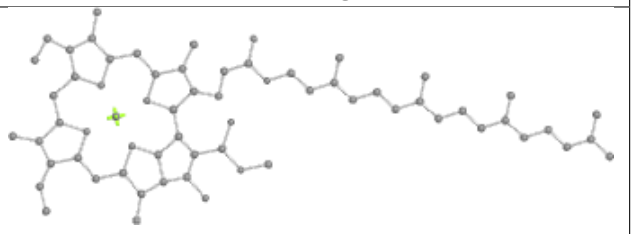
Bond lengths



Bond angles

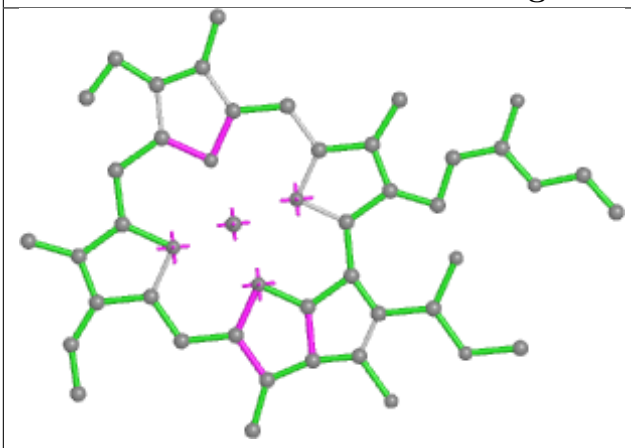


Torsions



Rings

Ligand CLA 0 309



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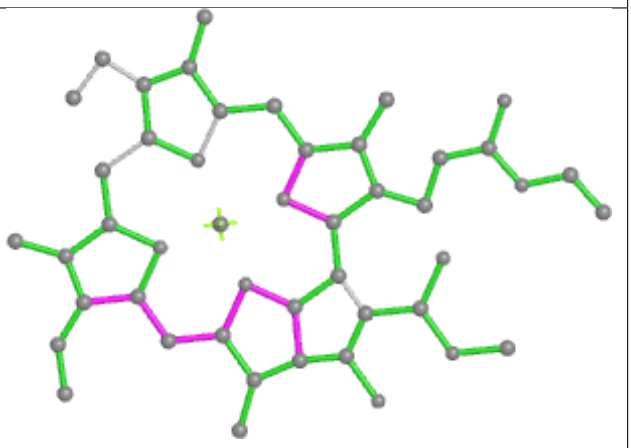

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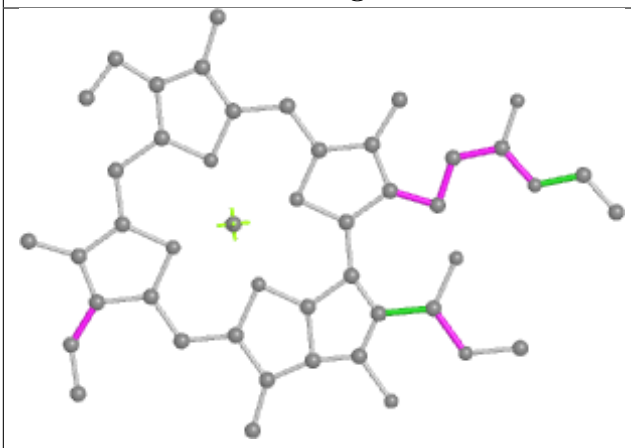

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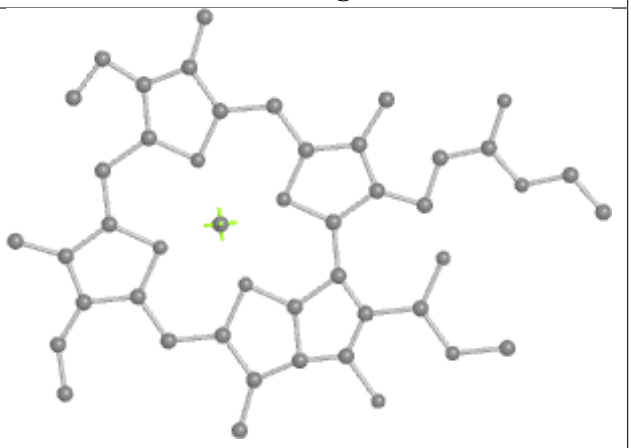
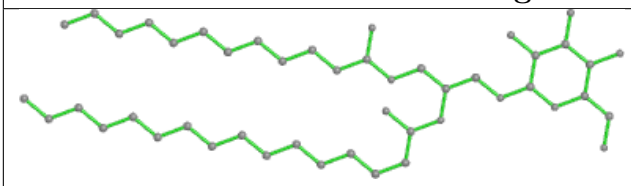


Rings

Ligand LMG W 101



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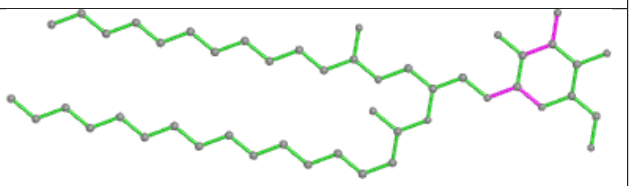

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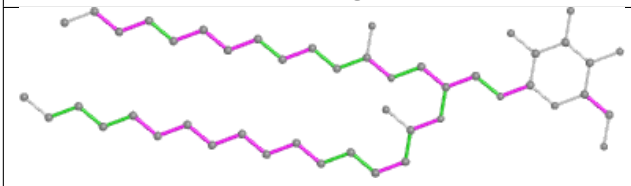

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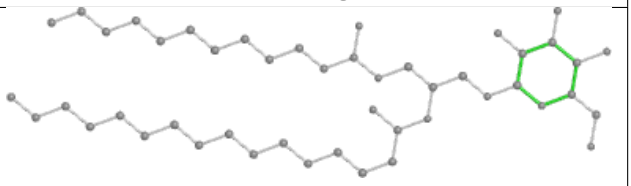
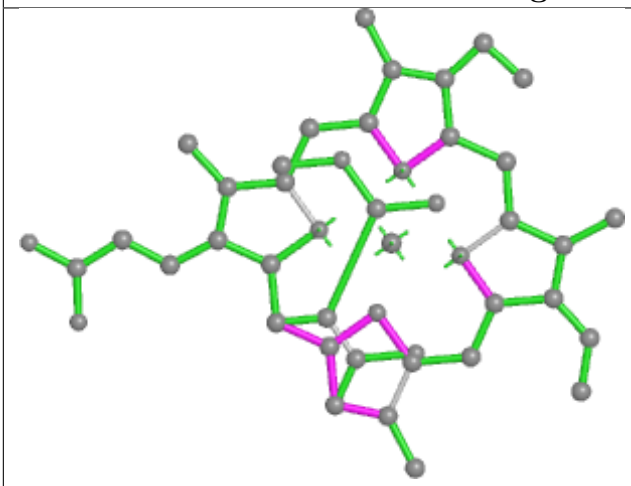


Rings

Ligand KC2 8 309



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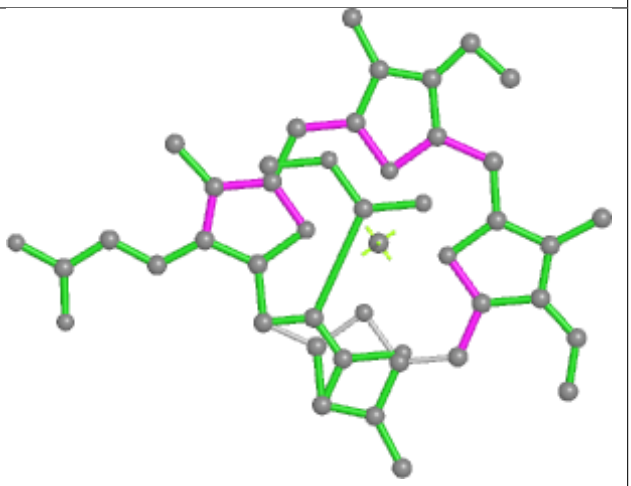

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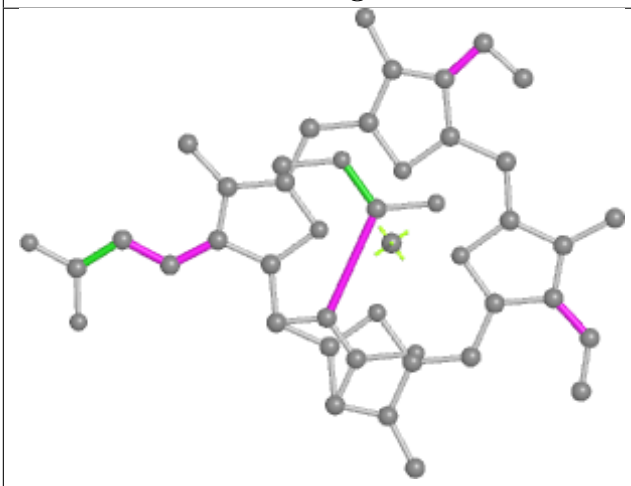

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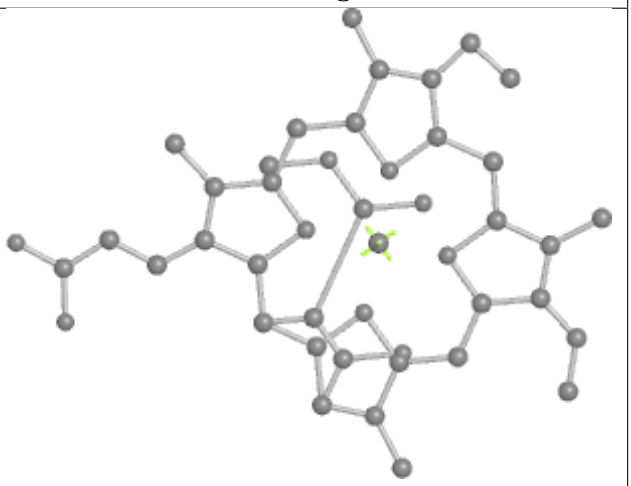
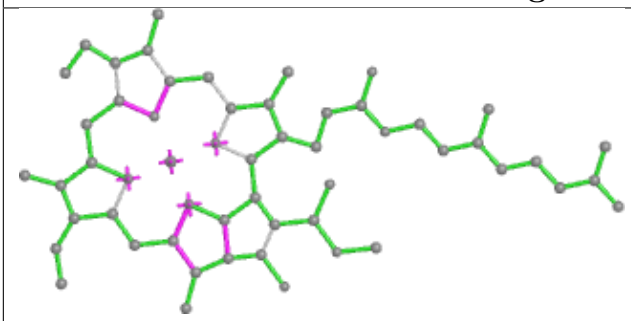


Rings

Ligand CLA 6 305



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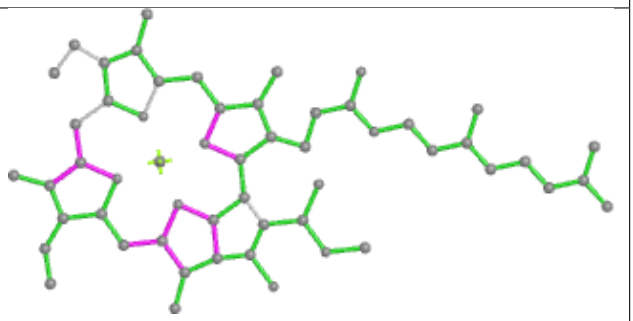

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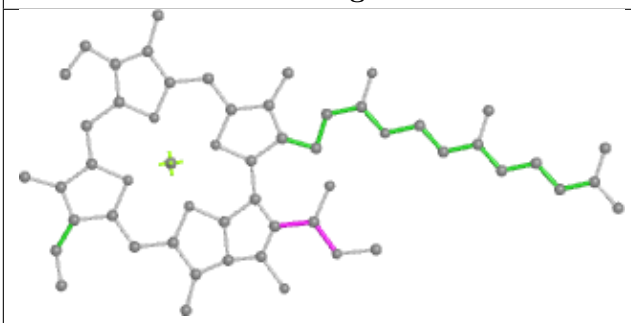

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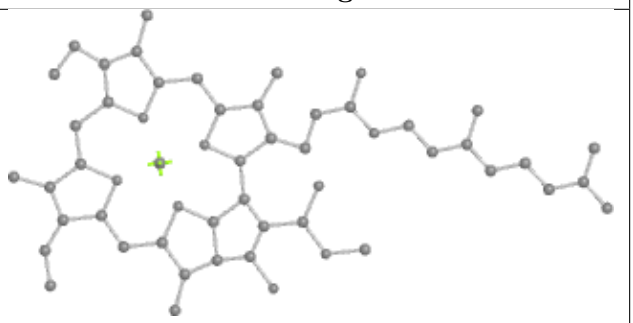
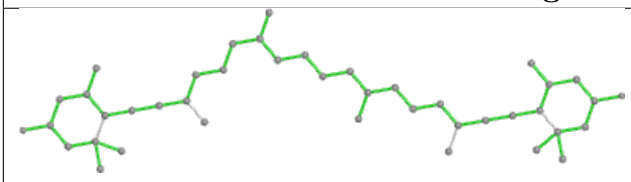


Rings

Ligand II0 9 317



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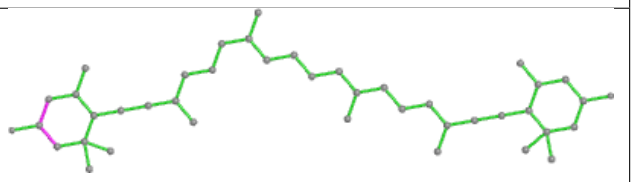

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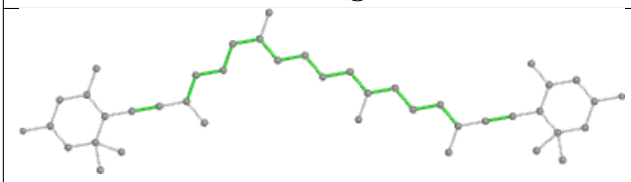

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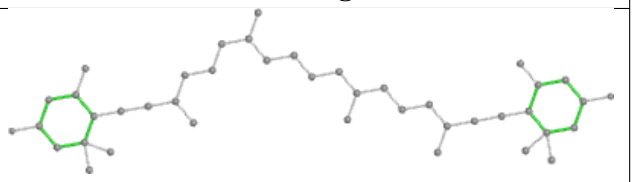
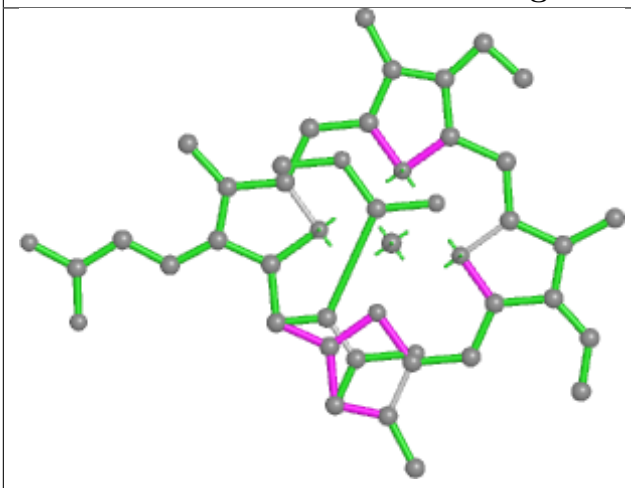


Rings

Ligand KC2 3 311



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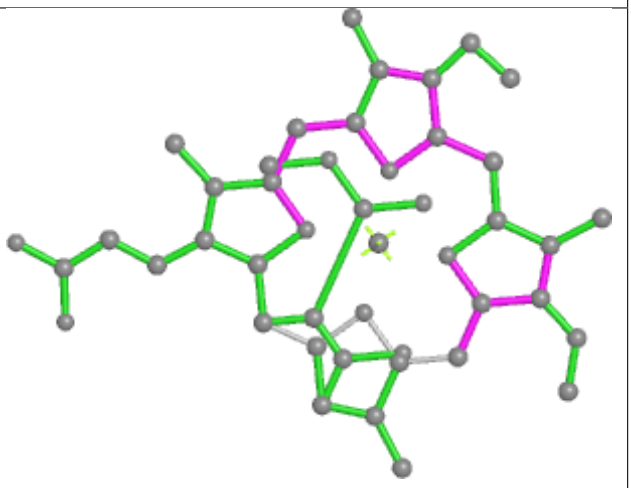

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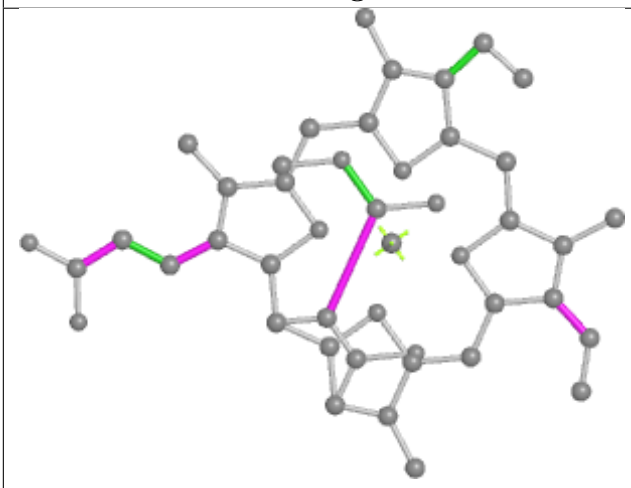

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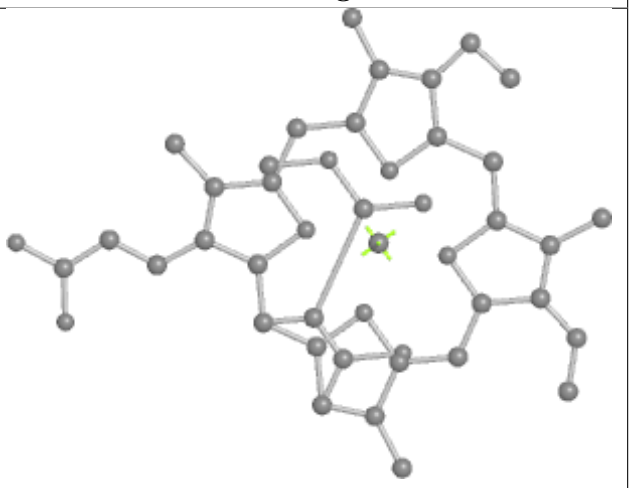
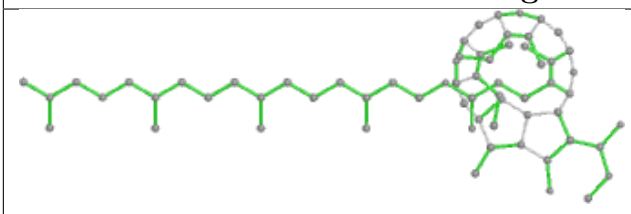


Rings

Ligand PHO D 403



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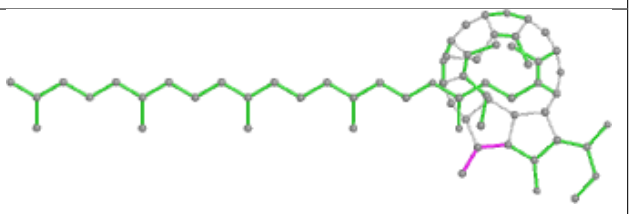

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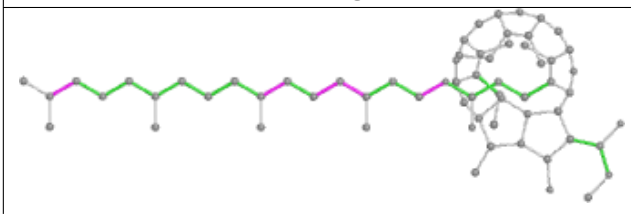

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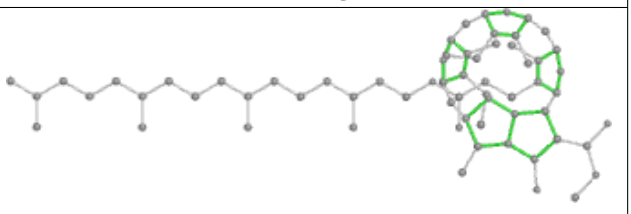
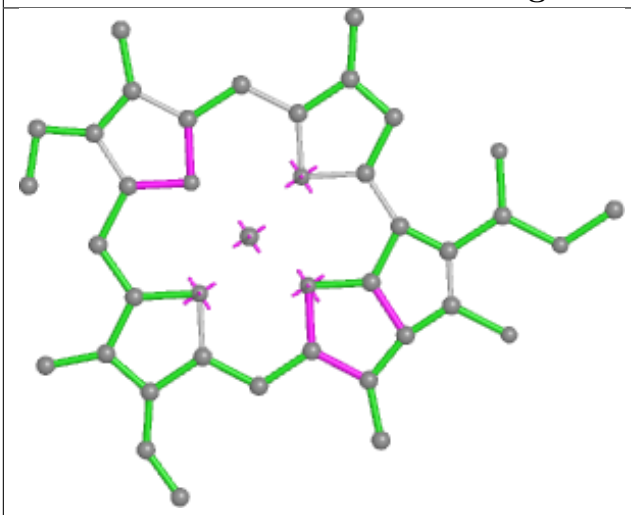


Rings

Ligand CLA 0 310



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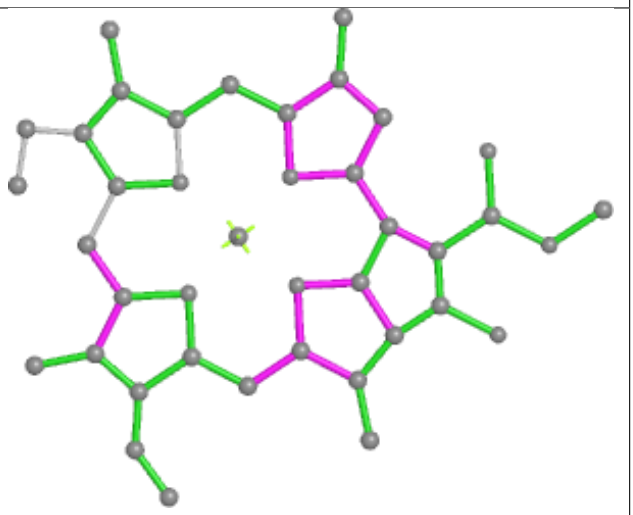

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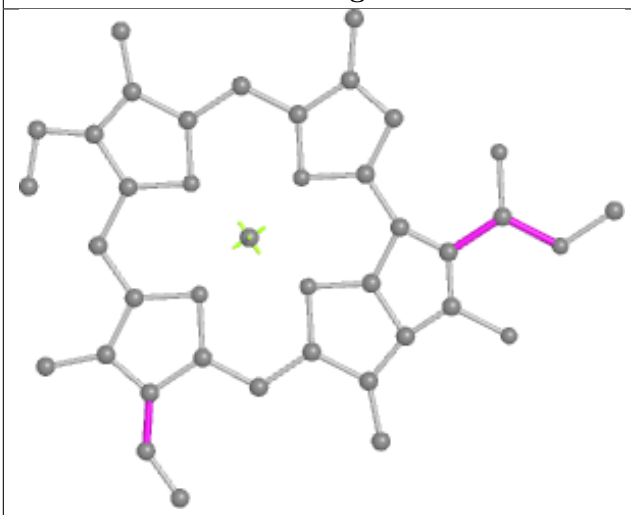

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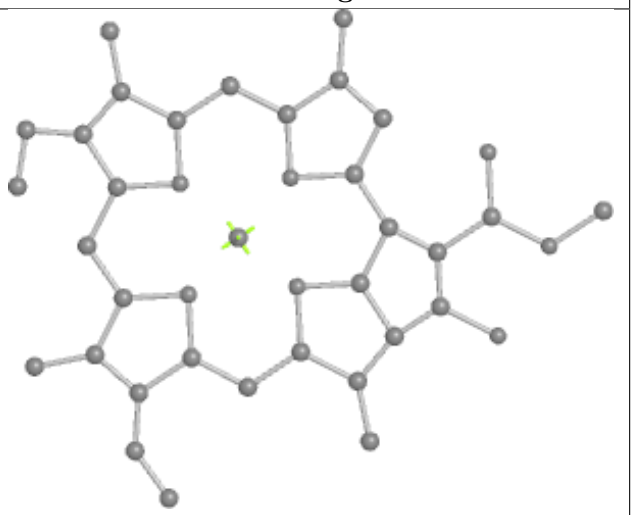
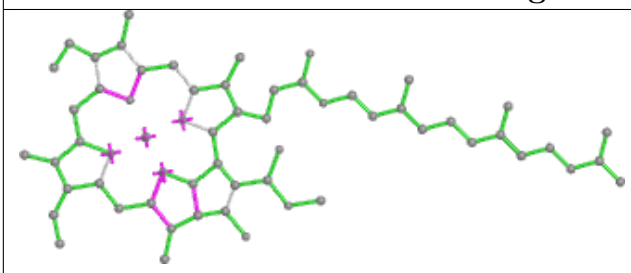


Rings

Ligand CLA 1 306



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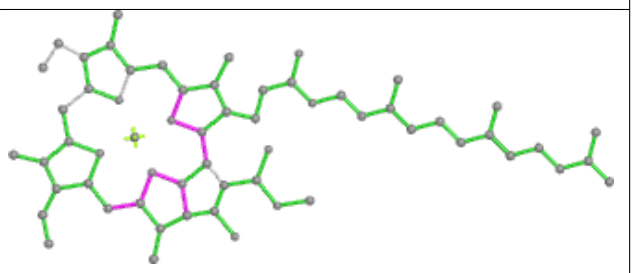

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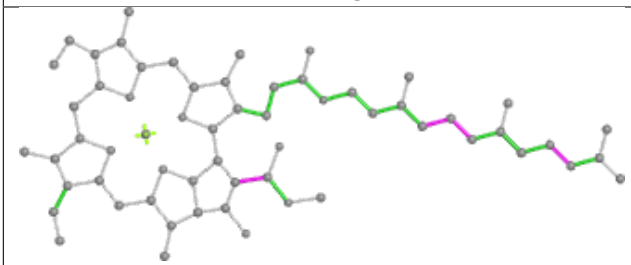

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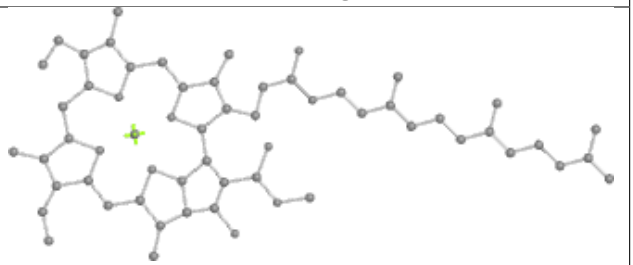
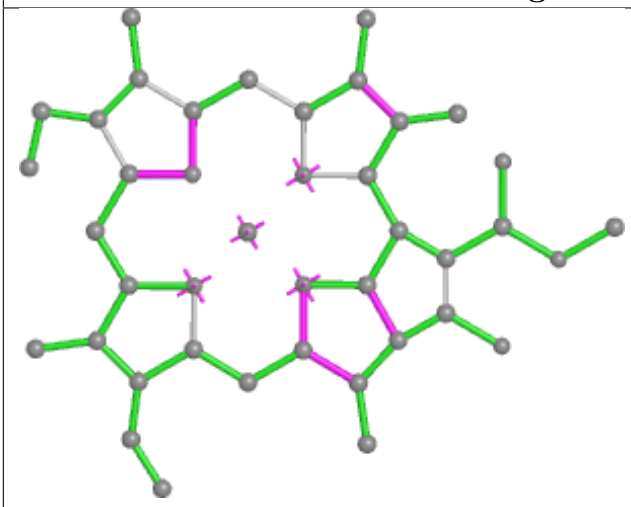


Rings

Ligand CLA 0 301



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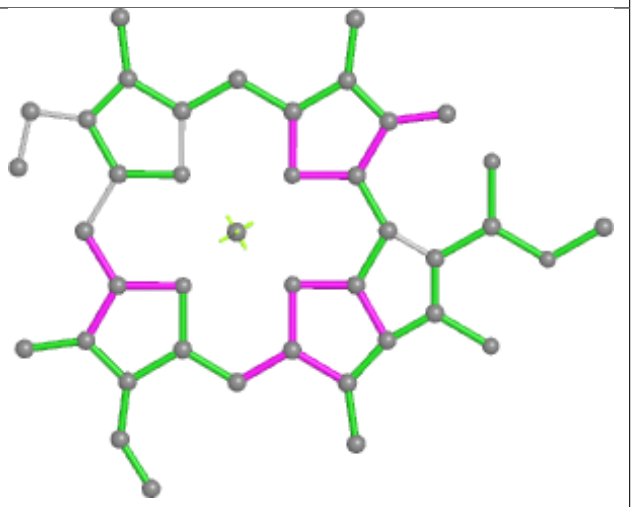

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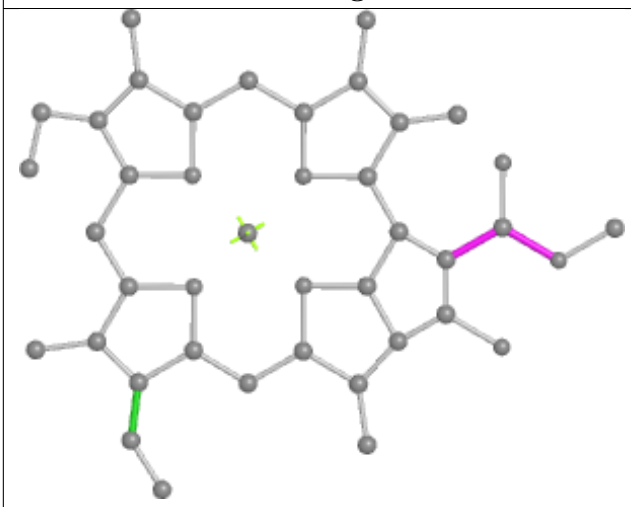

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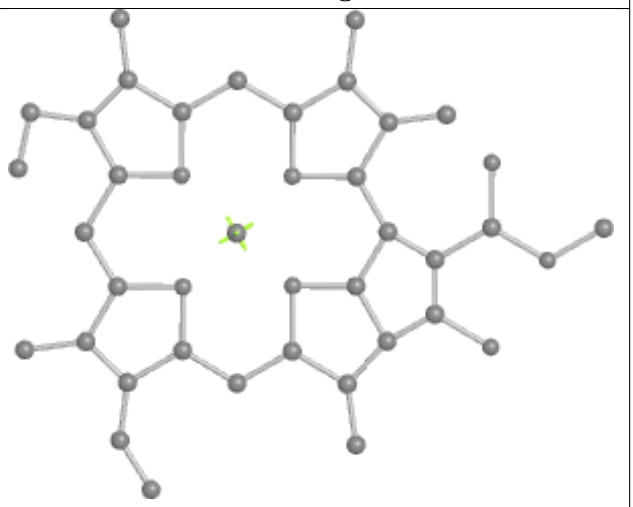
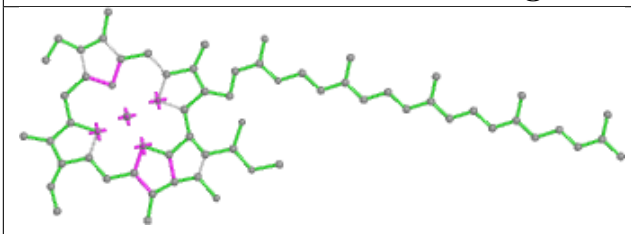


Rings

Ligand CLA B 607



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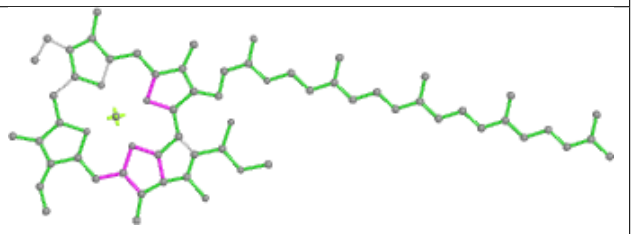
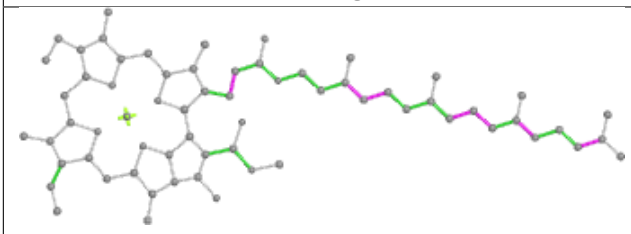


Bond angles



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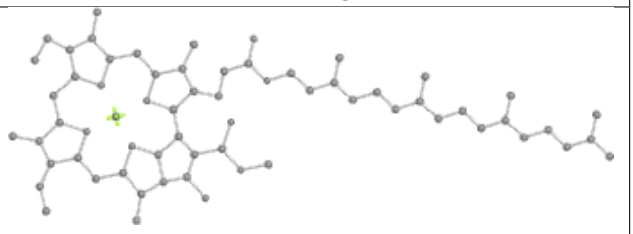
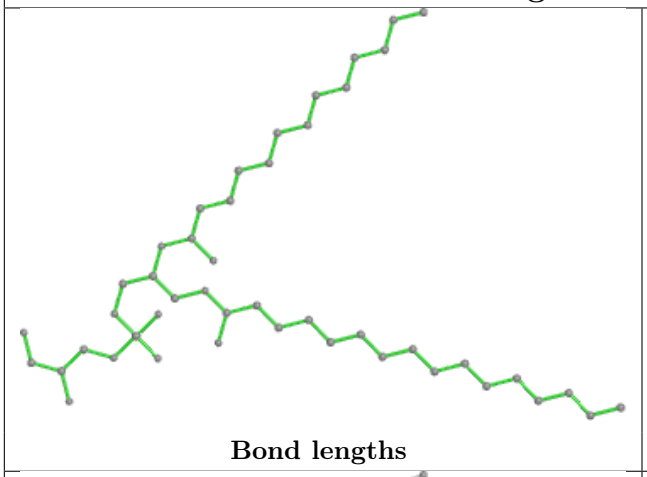


Rings

Ligand LHG 8 315



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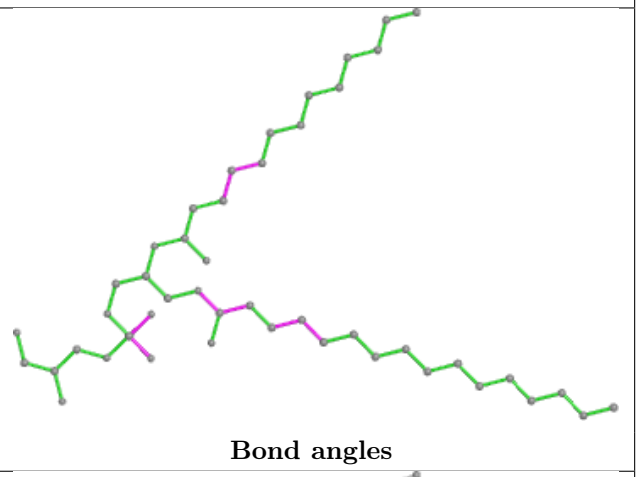
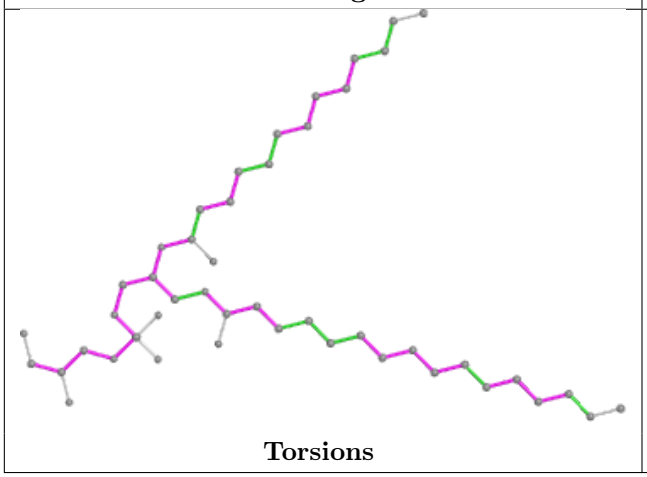
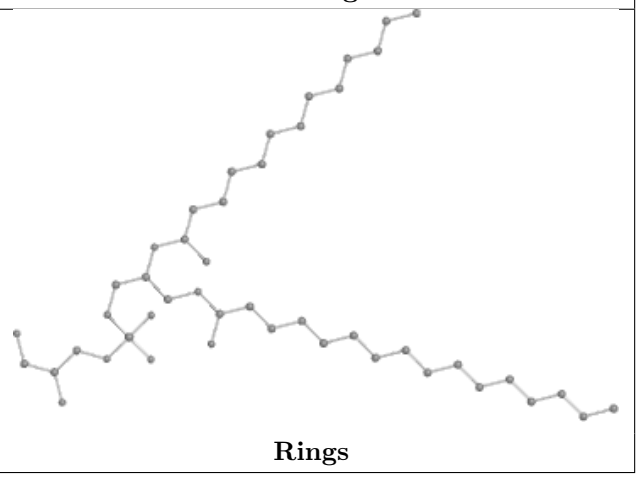


Bond angles

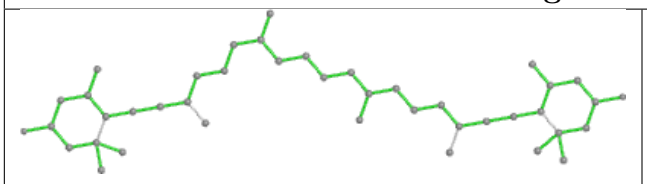


Torsions

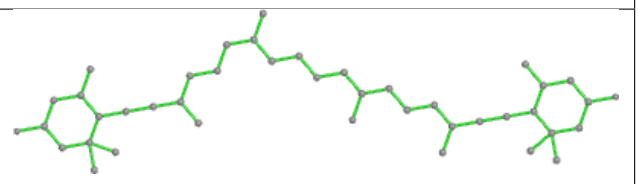


Rings

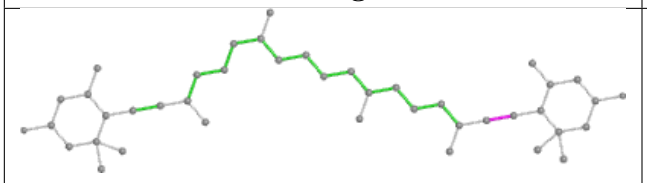
Ligand II0 3 301



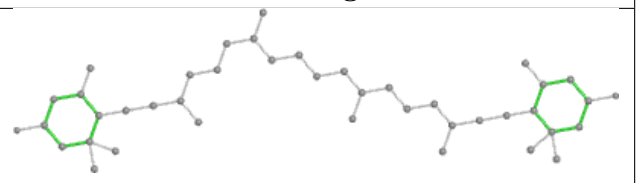
Bond lengths



Bond angles

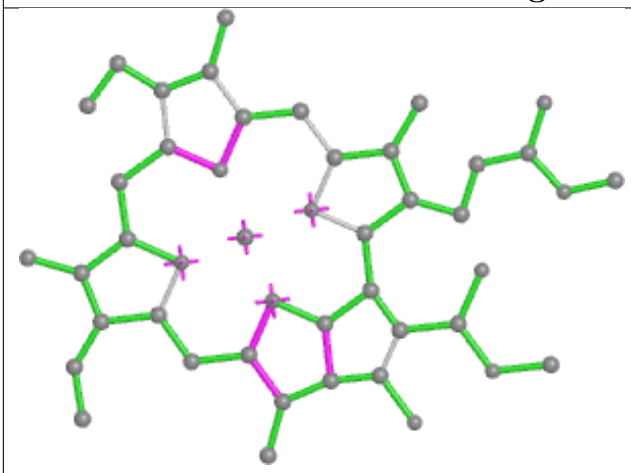


Torsions

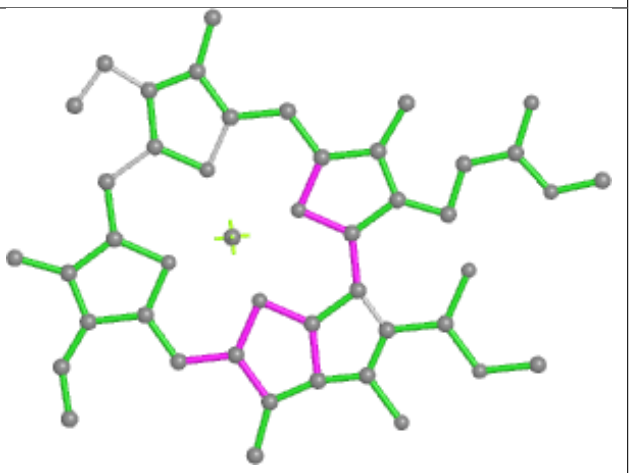


Rings

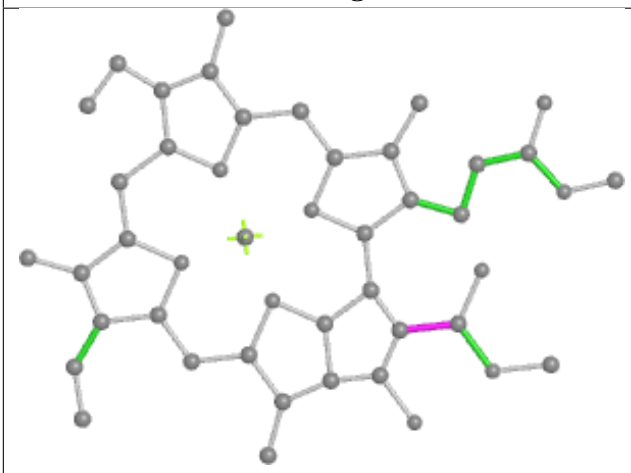
Ligand CLA 2 310



Bond lengths



Bond angles



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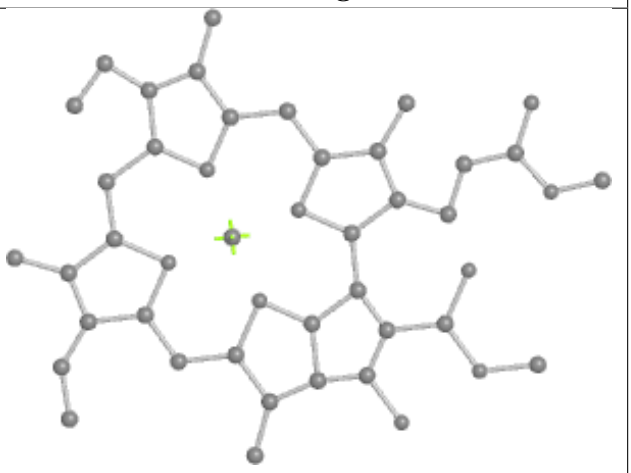
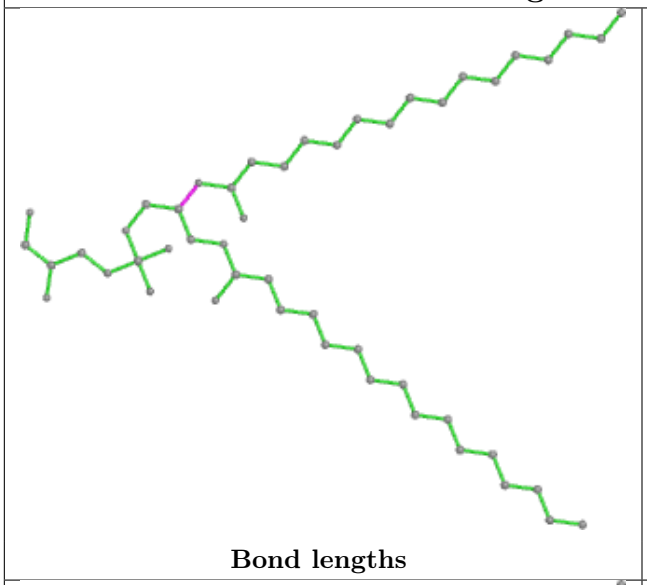
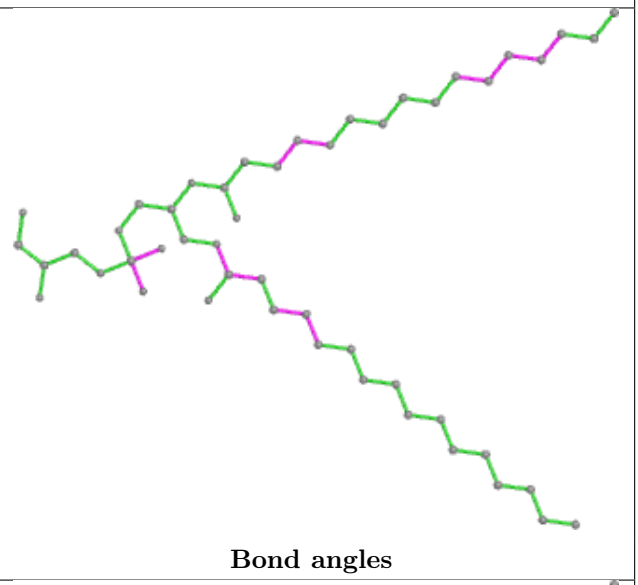


Rings

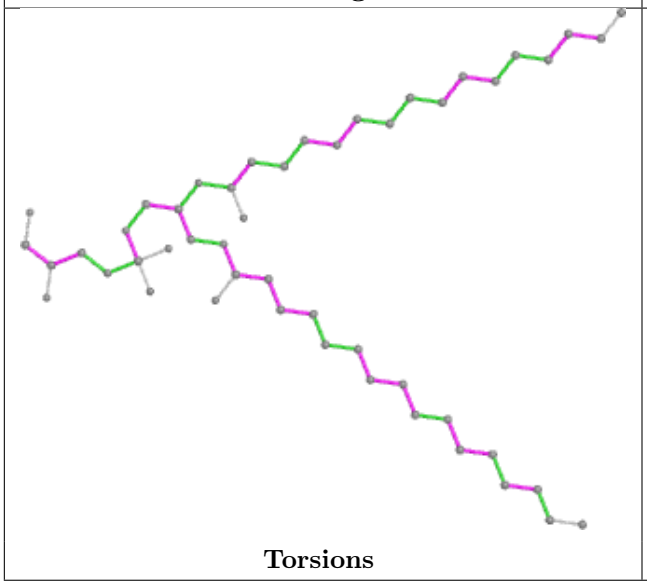
Ligand LHG b 623



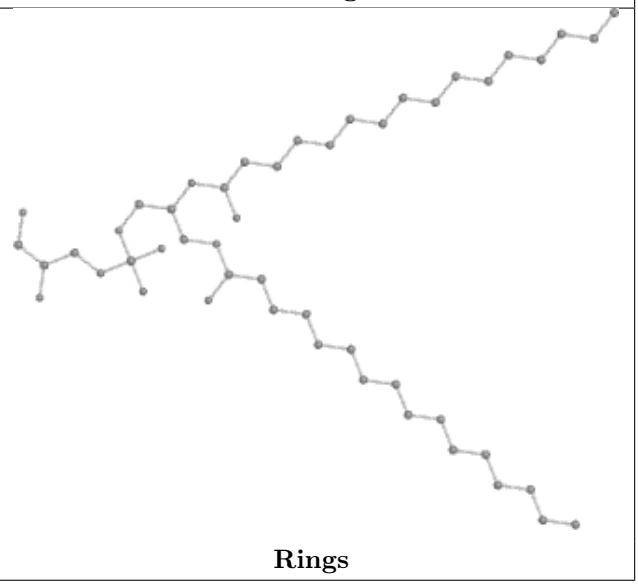
Bond lengths



Bond angles

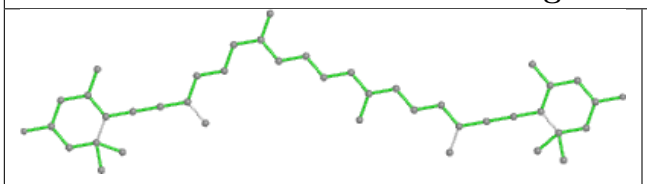


Torsions



Rings

Ligand II0 4 312



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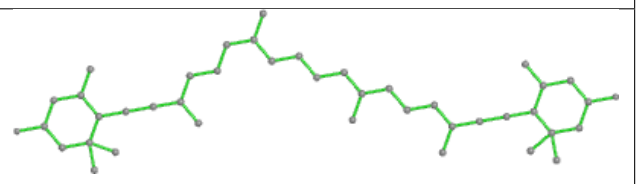

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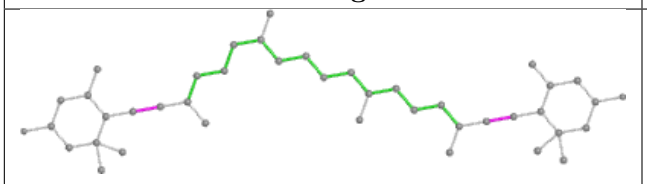

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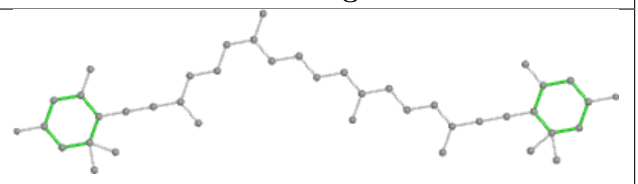
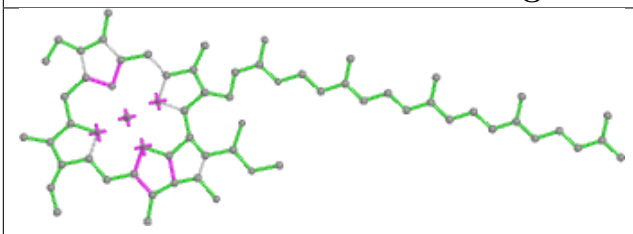


Rings

Ligand CLA D 405



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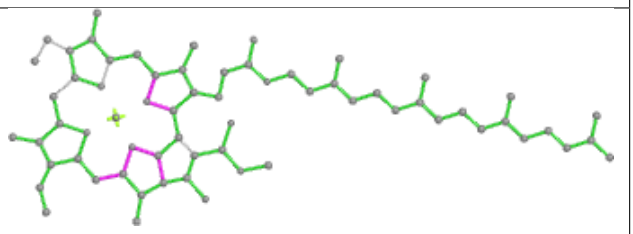

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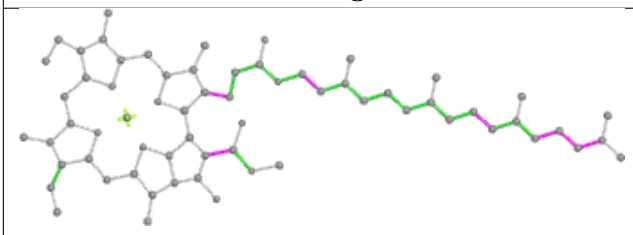

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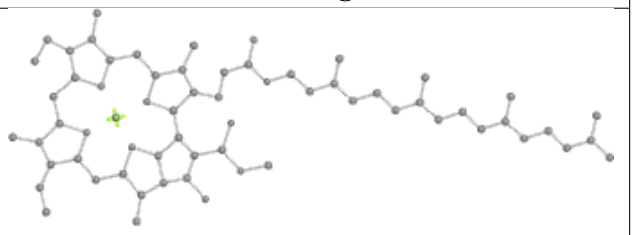
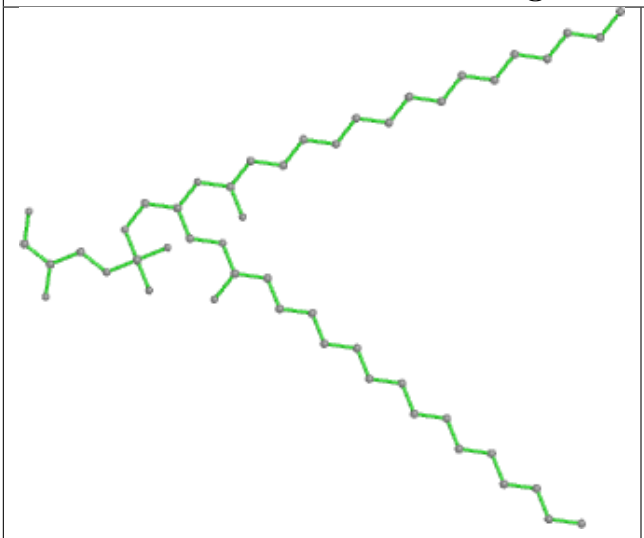


Rings

Ligand LHG 1 317



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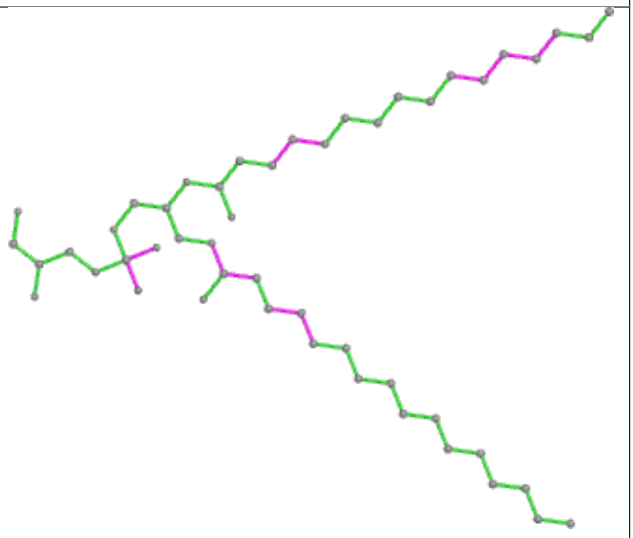
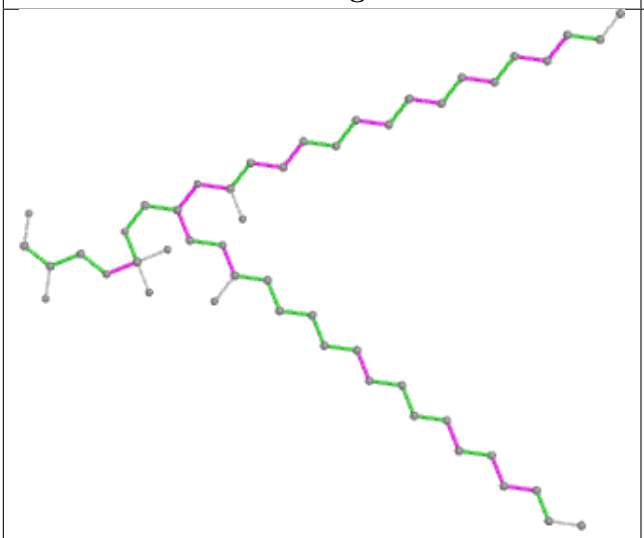


Bond angles



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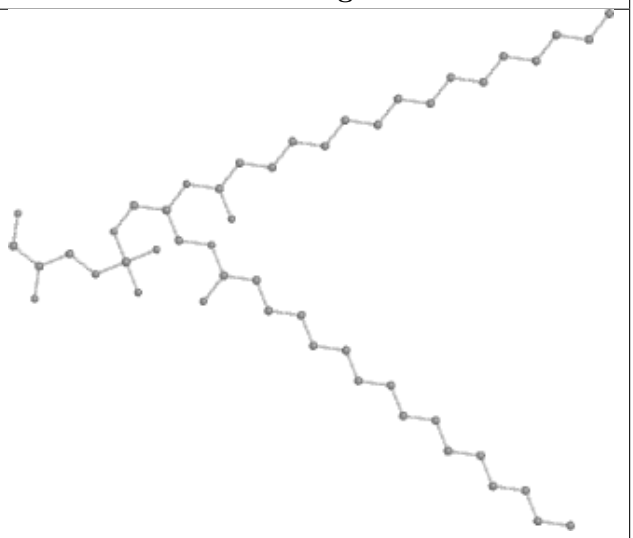
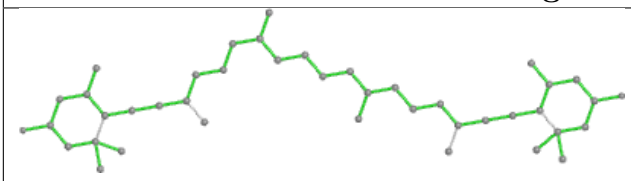


Rings

Ligand II0 6 314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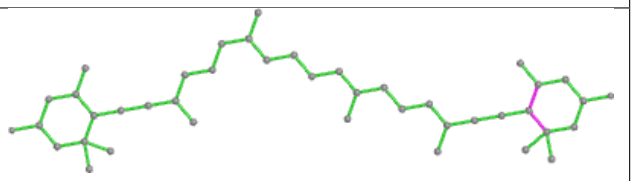
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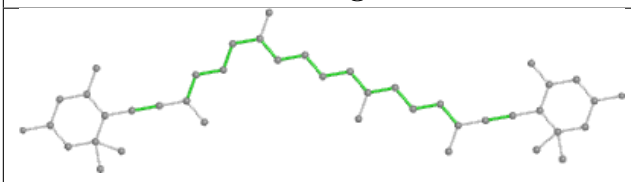
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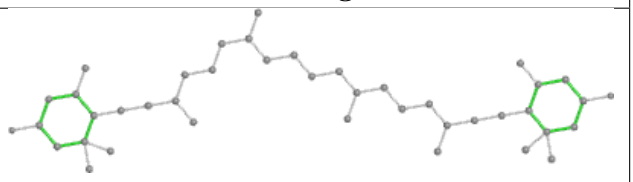
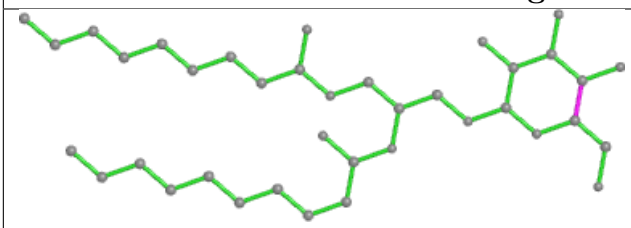

Rings

Ligand LMG l 102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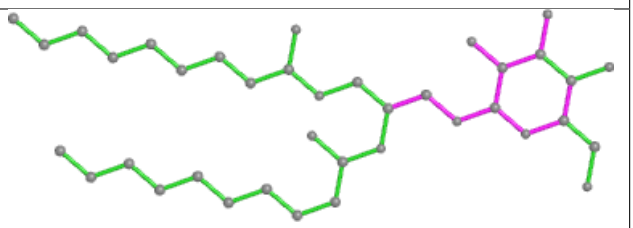
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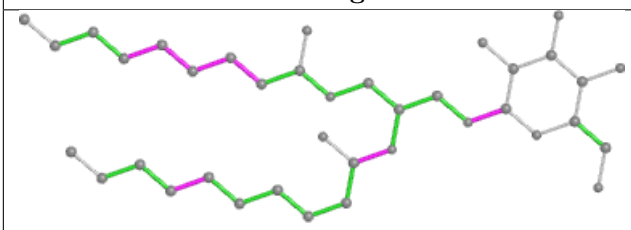
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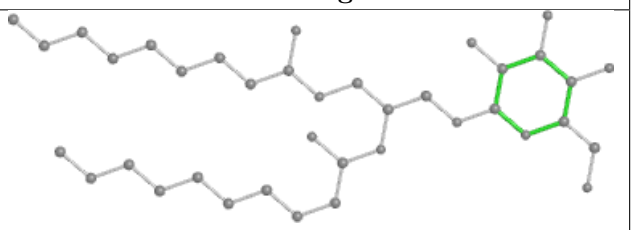
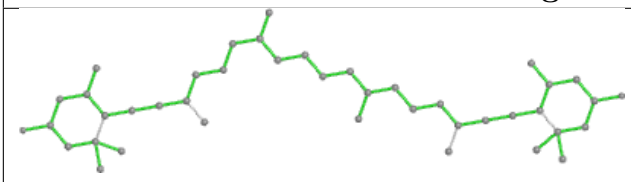

Rings

Ligand II0 p 316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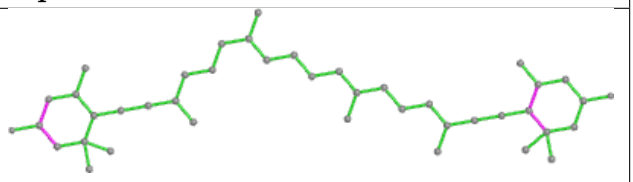
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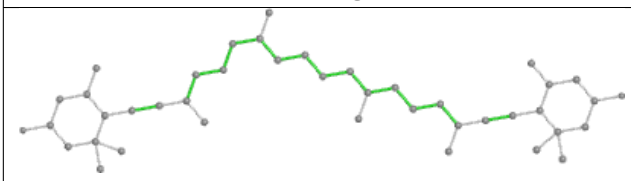
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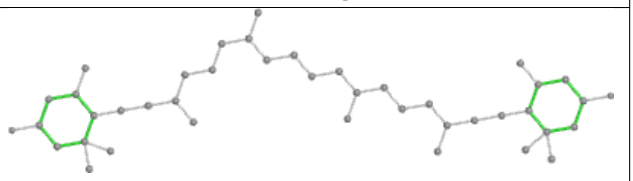
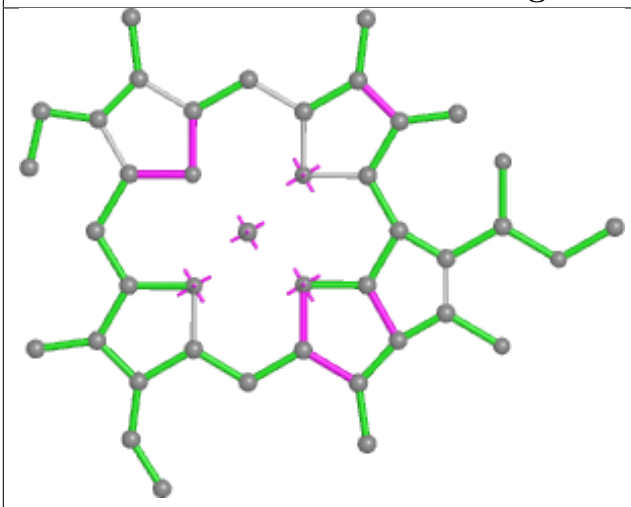

Rings

Ligand CLA 6 302



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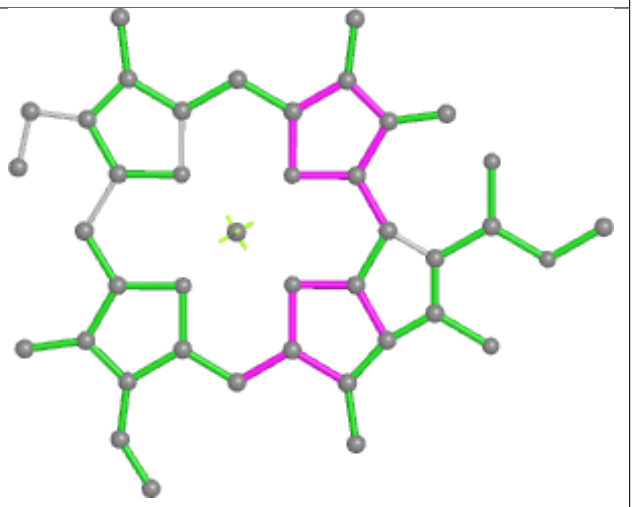
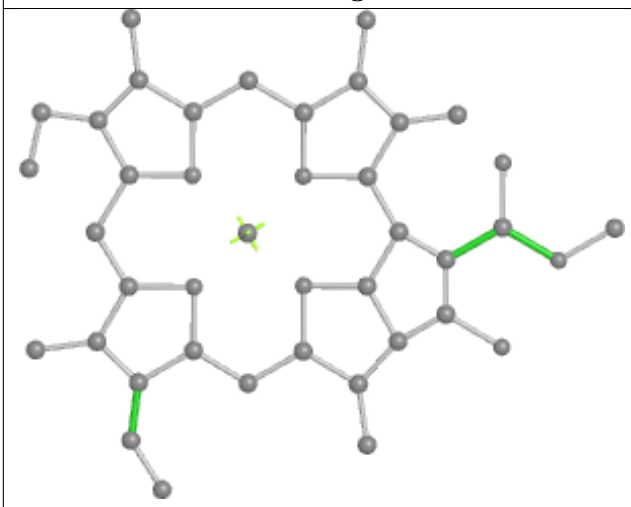


Bond angles



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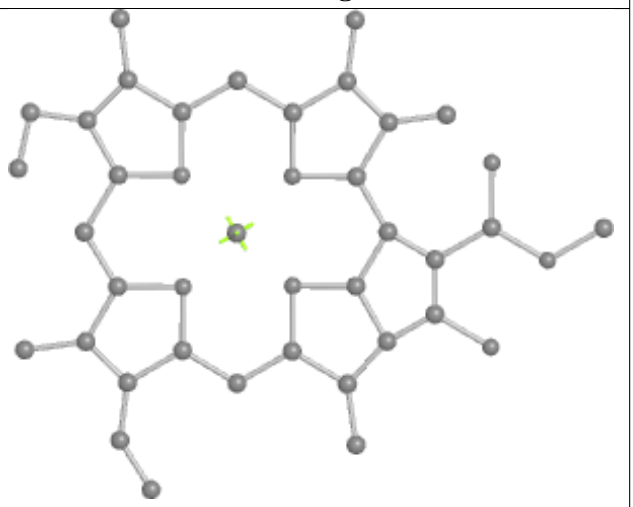
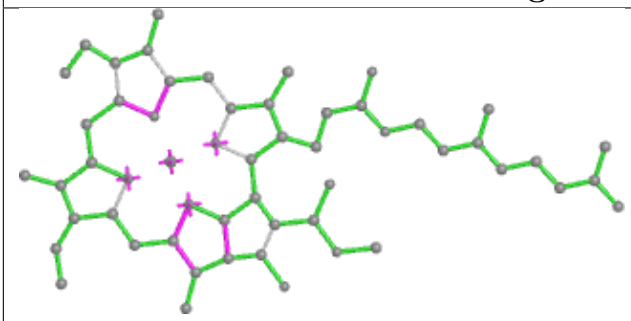


Rings

Ligand CLA 9 303



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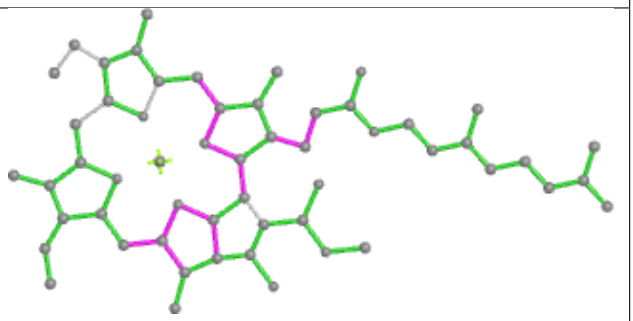
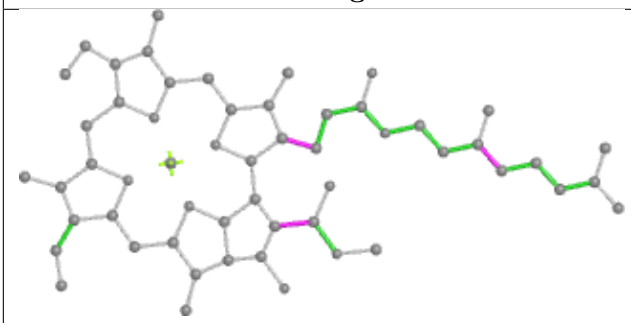


Bond angles



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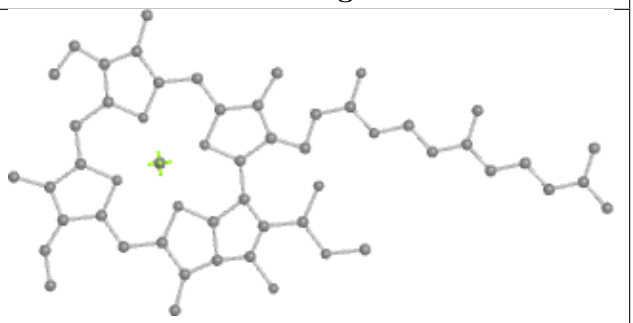
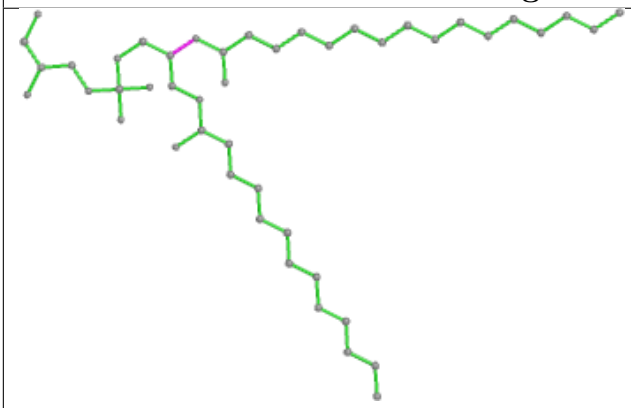


Rings

Ligand LHG D 401



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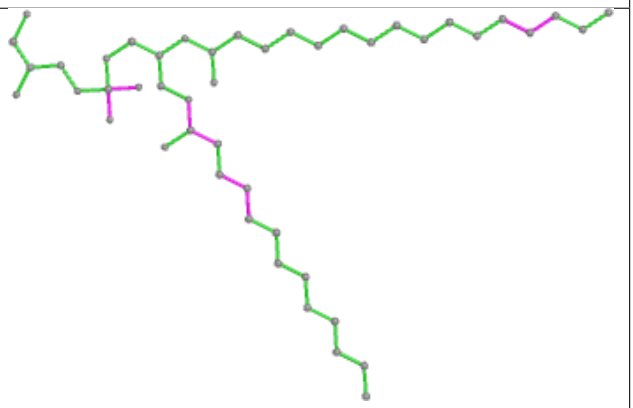
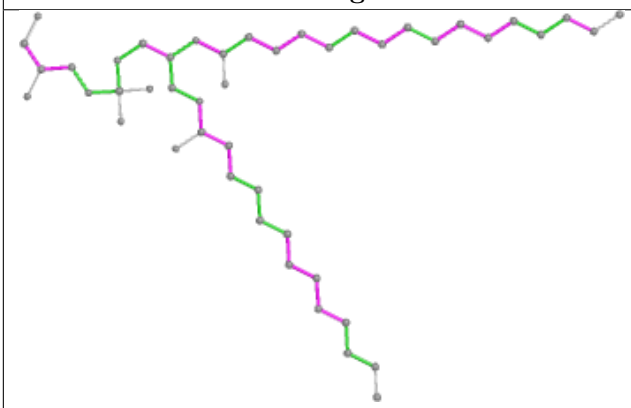


Bond angles



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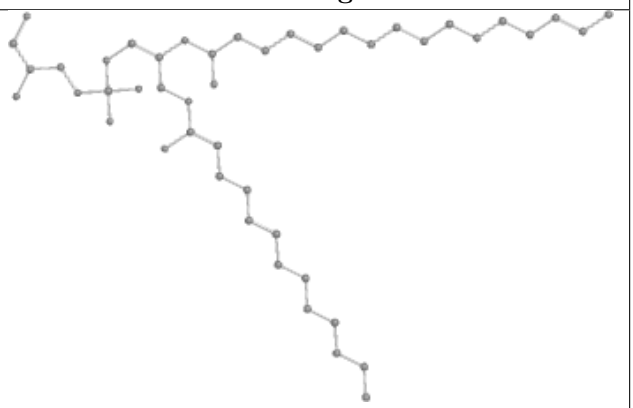
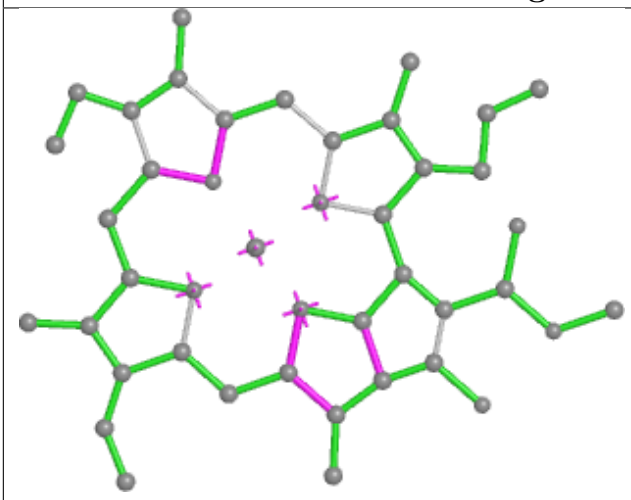


Rings

Ligand CLA 6 307



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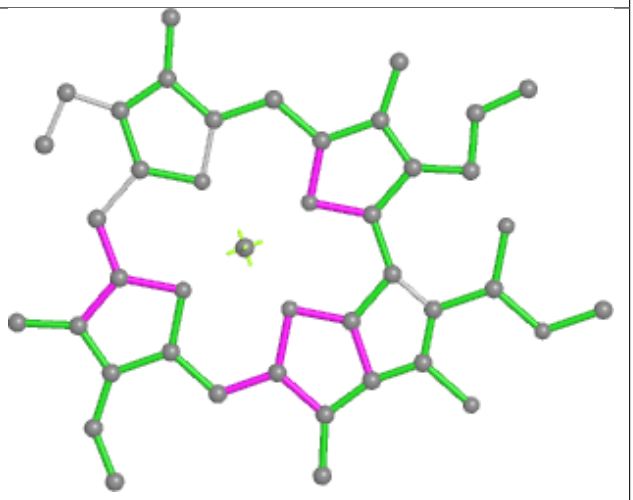
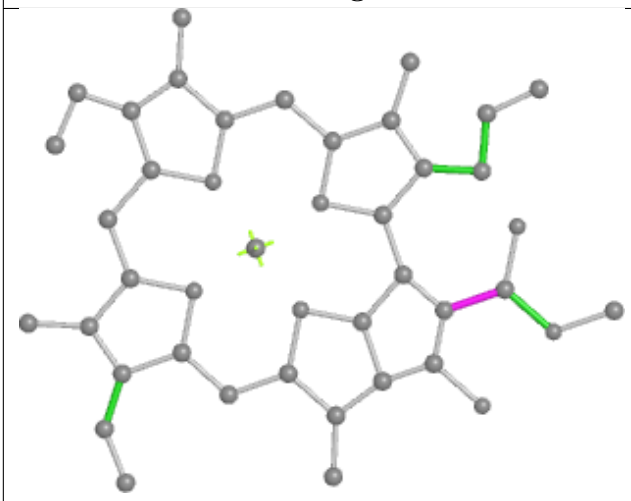


Bond angles



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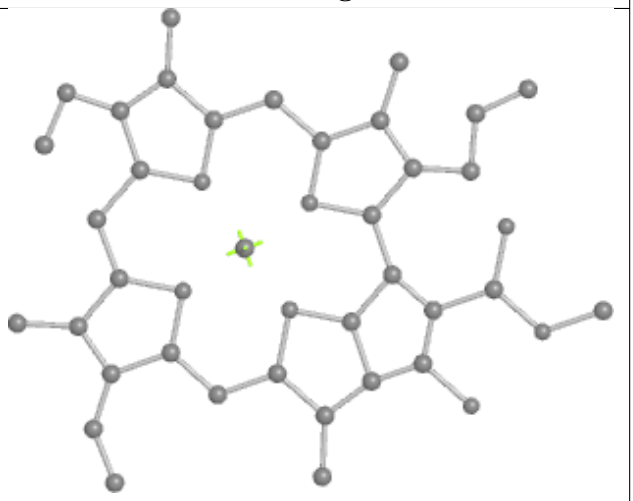
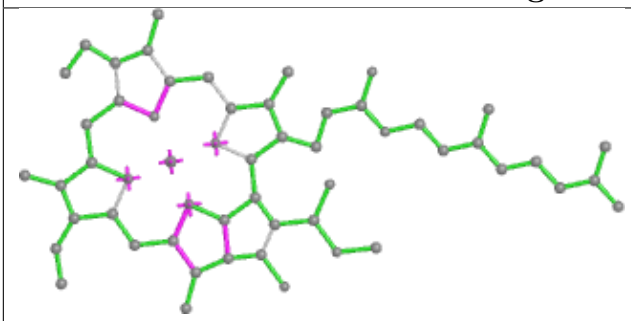


Rings

Ligand CLA n 305



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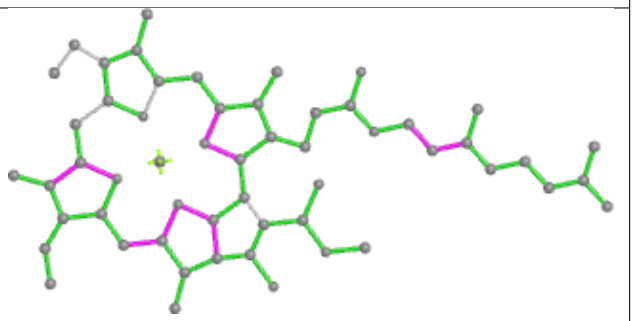
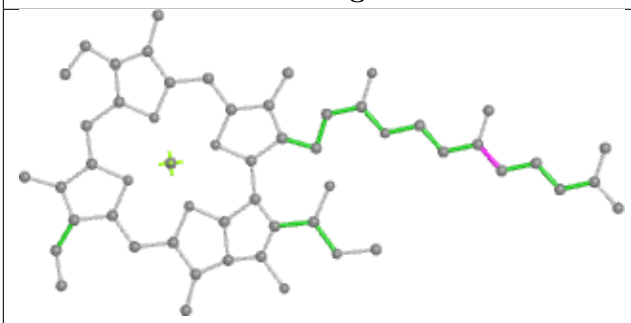


Bond angles



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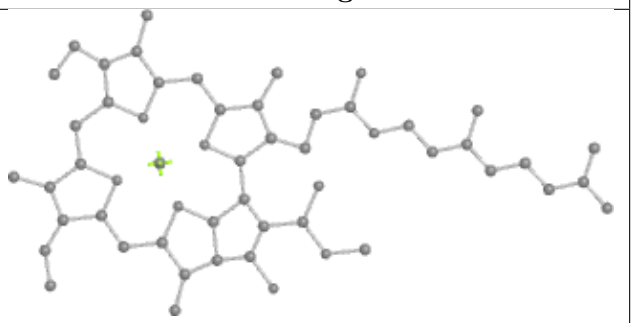
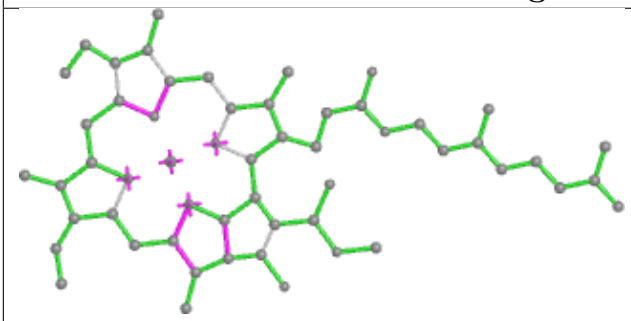
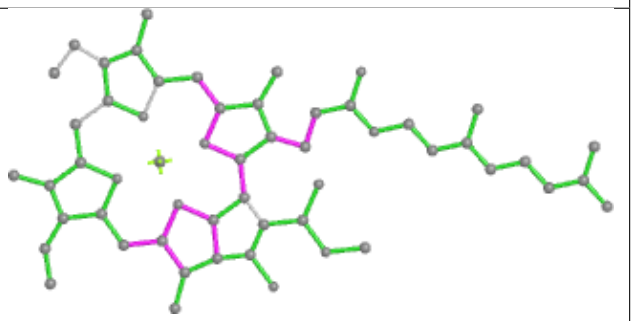


Rings

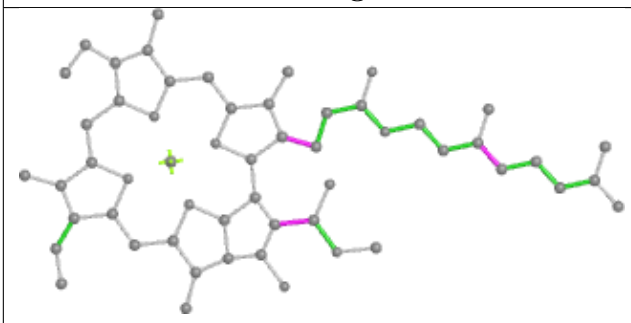
Ligand CLA 3 303



Bond lengths



Bond angles



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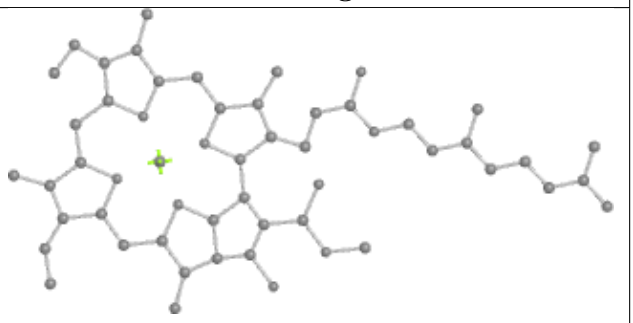
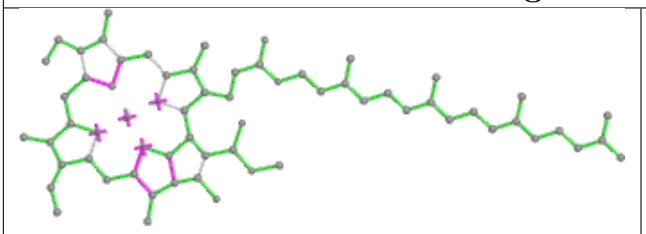
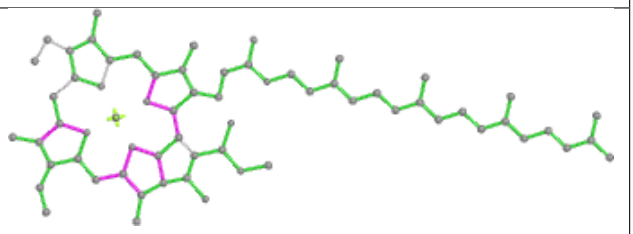


Rings

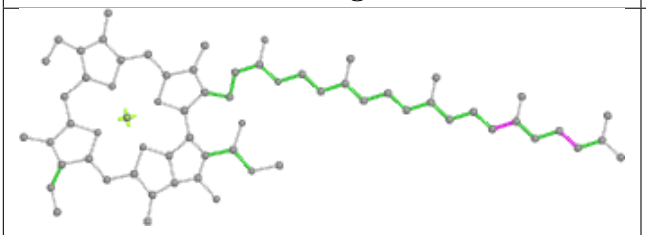
Ligand CLA B 609



Bond lengths



Bond angles



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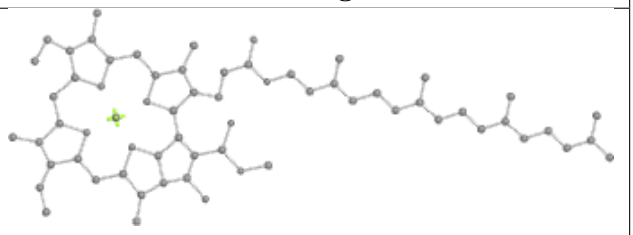
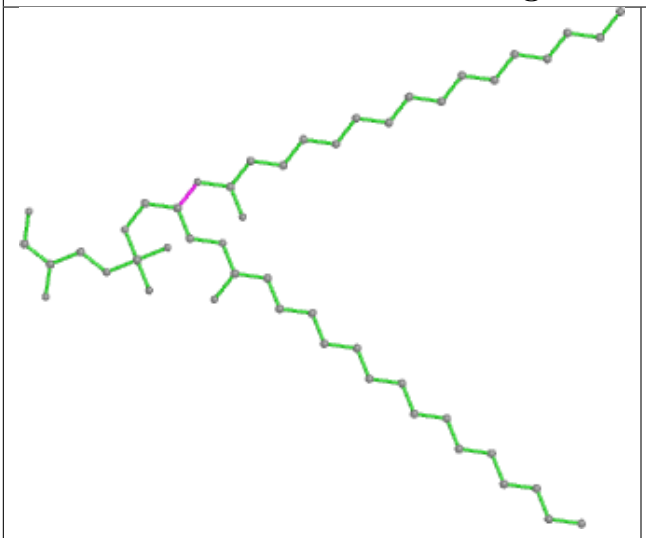


Rings

Ligand LHG B 623



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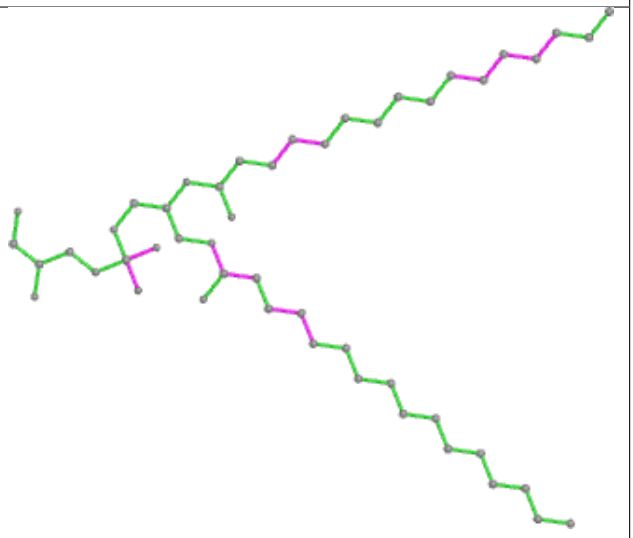
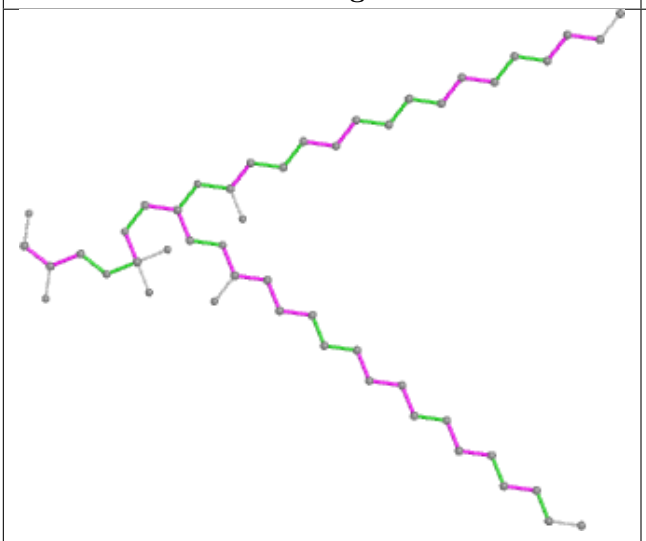


Bond angles



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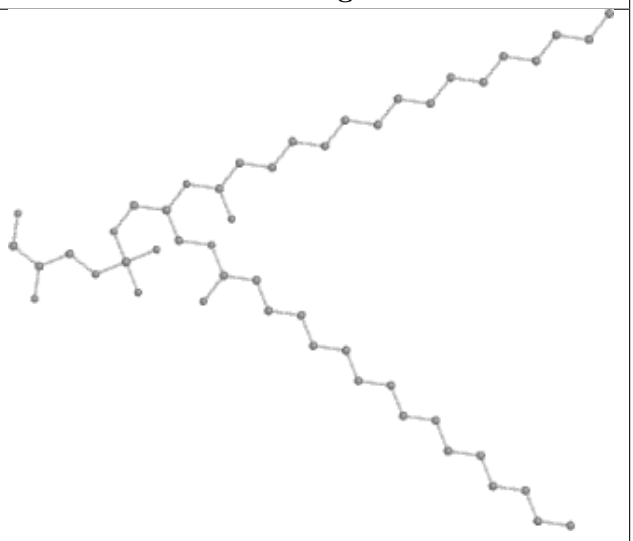
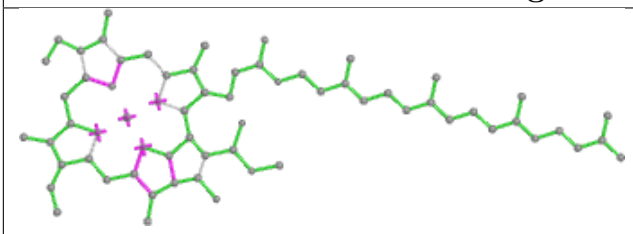
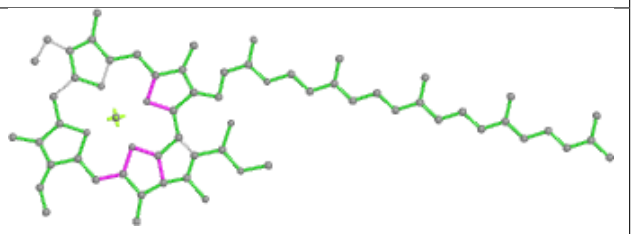


Rings

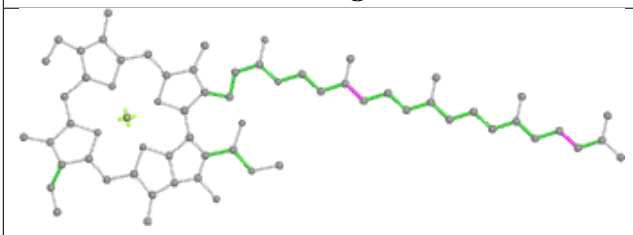
Ligand CLA b 604



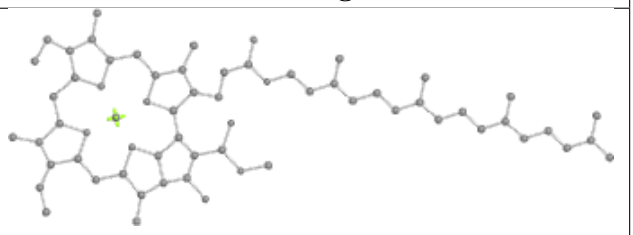
Bond lengths



Bond angles

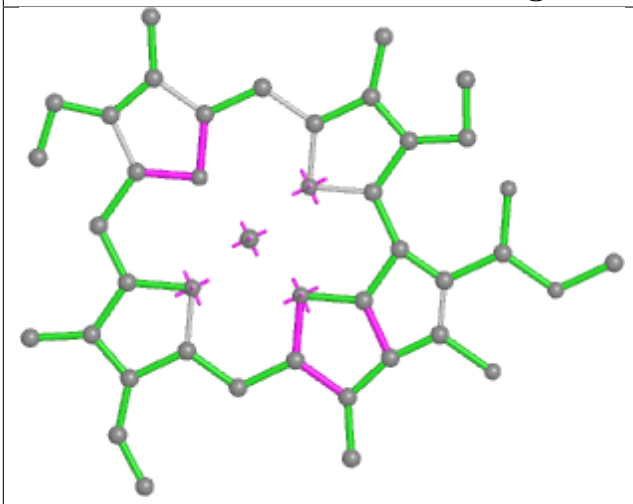


Torsions



Rings

Ligand CLA p 309



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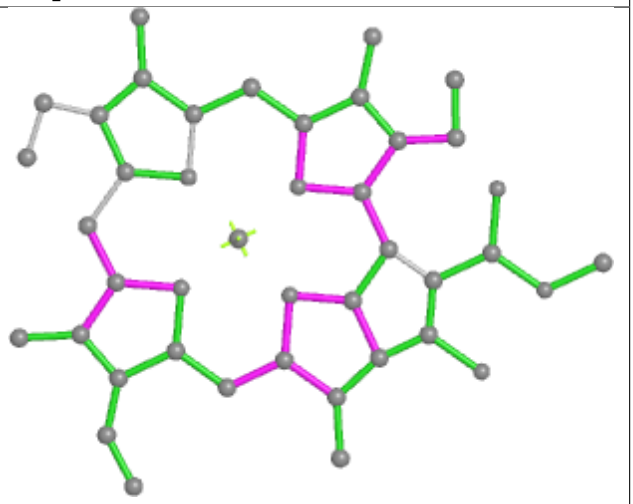

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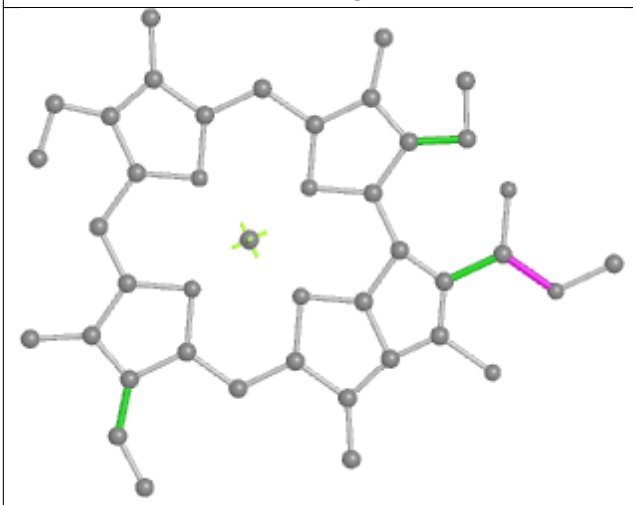

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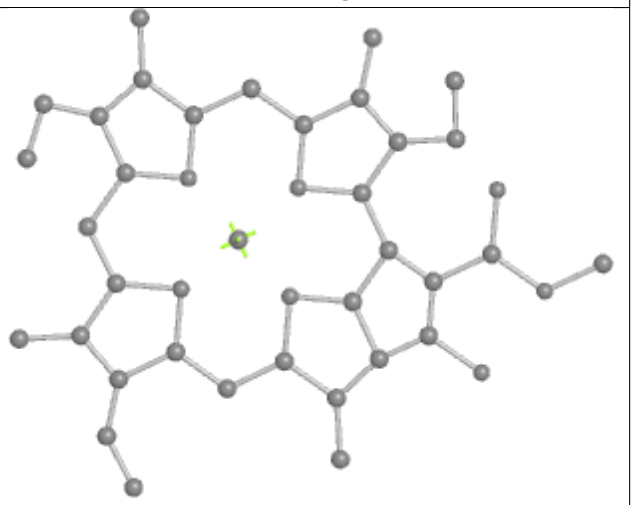
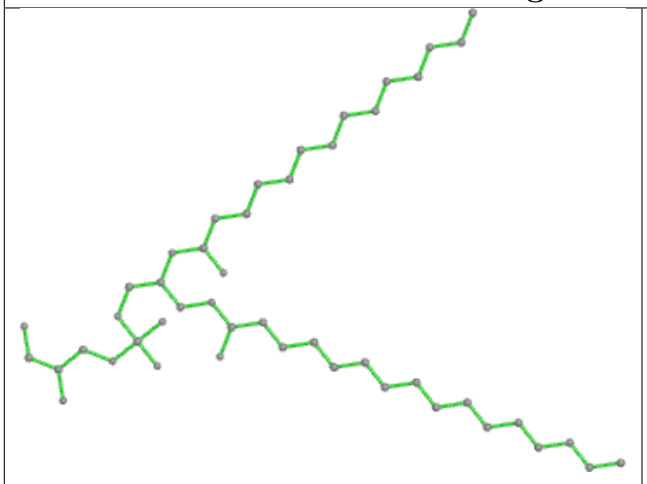


Rings

Ligand LHG d 402



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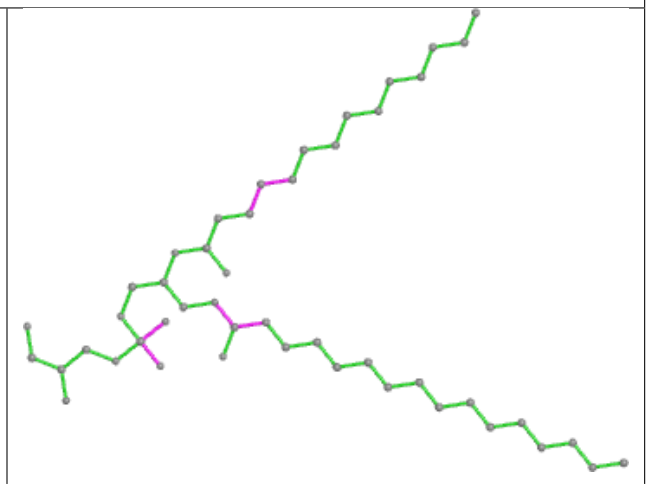
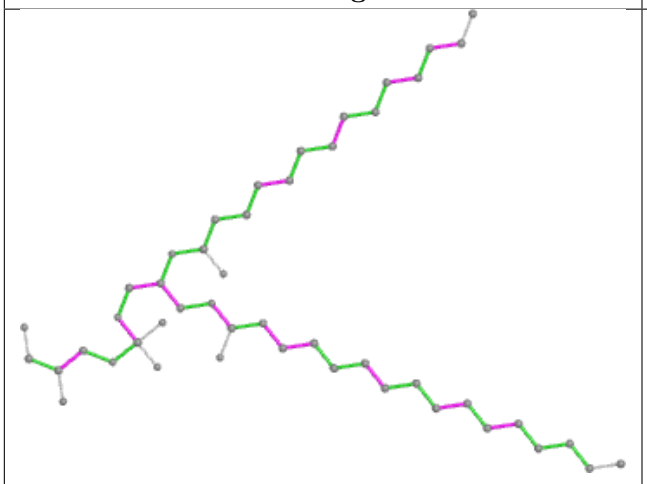


Bond angles



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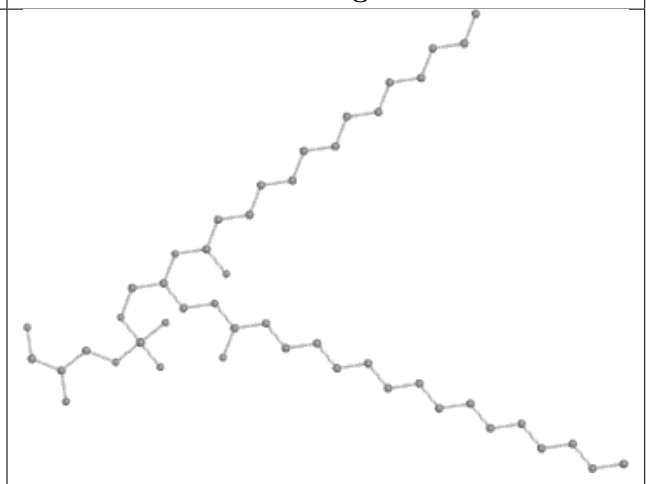
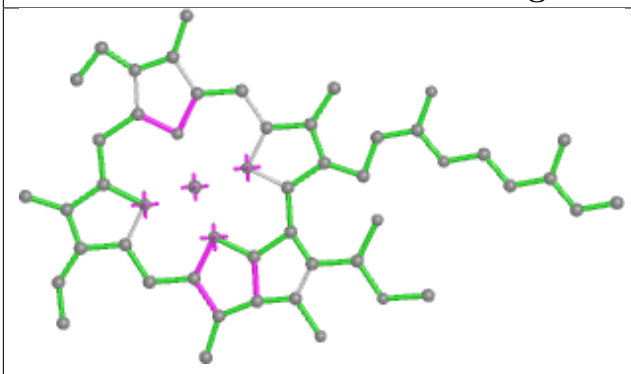


Rings

Ligand CLA 0 302



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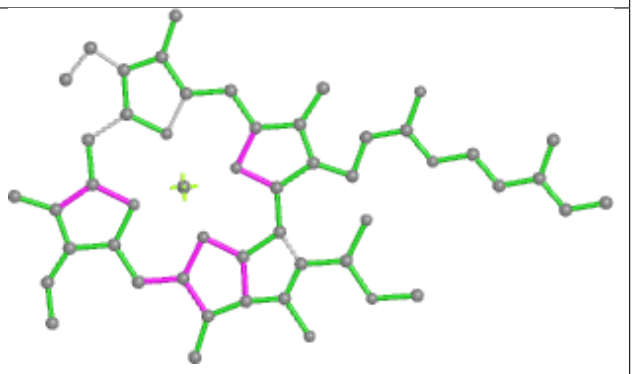
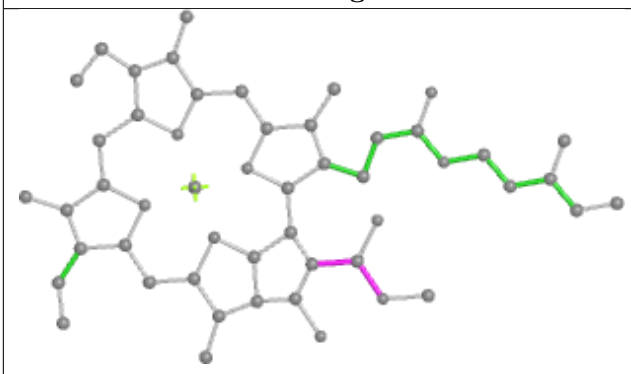


Bond angles



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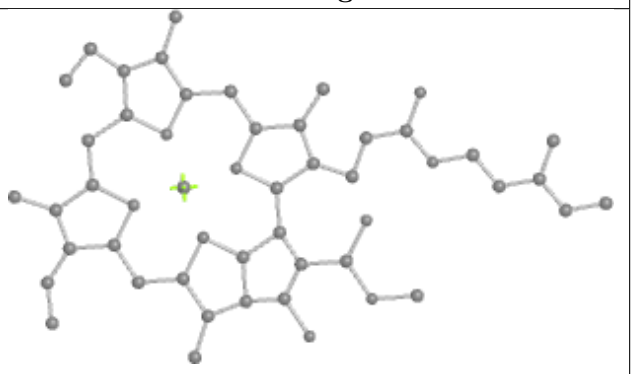
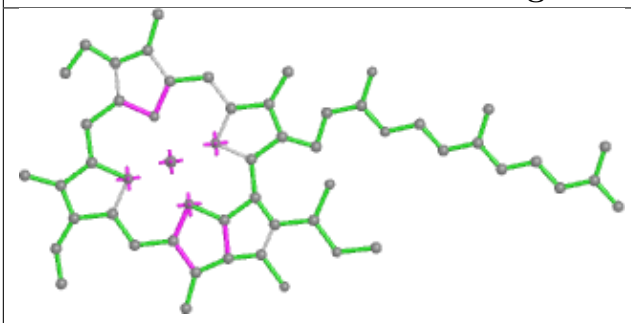


Rings

Ligand CLA n 304



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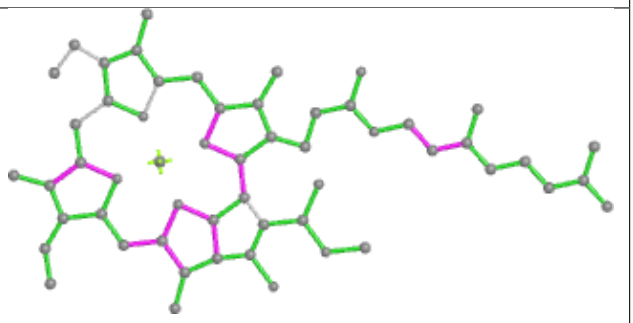
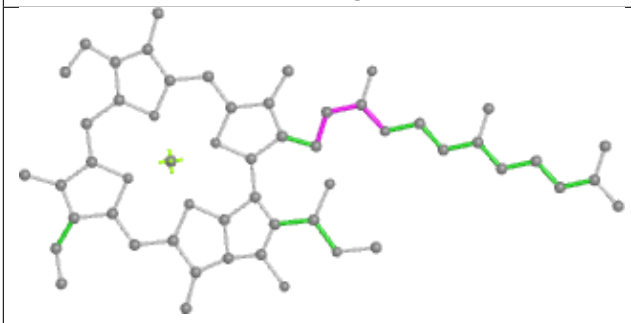


Bond angles



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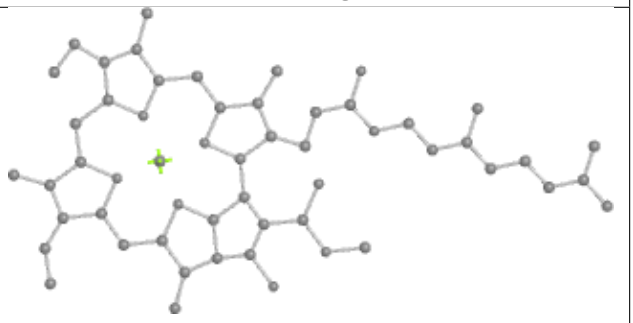
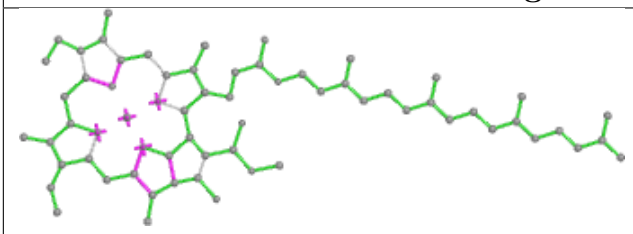


Rings

Ligand CLA C 512



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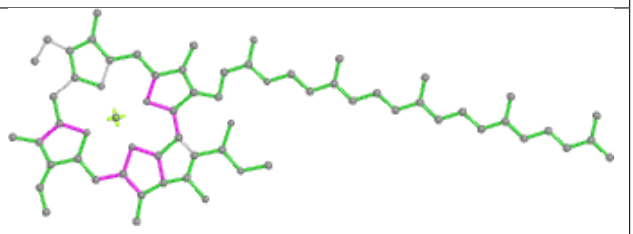

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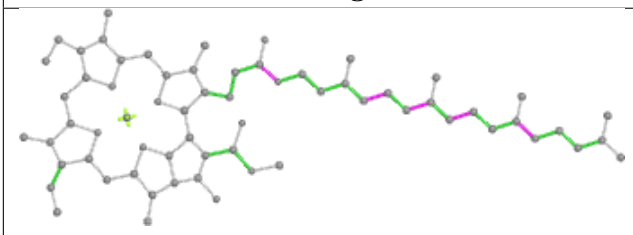

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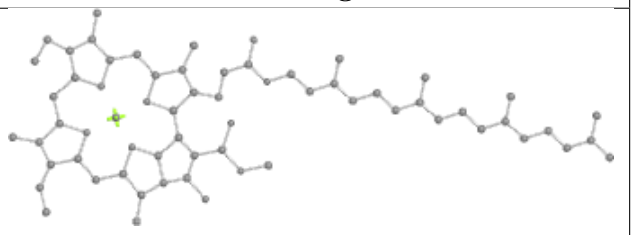
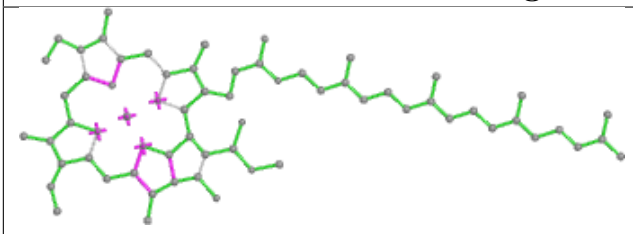


Rings

Ligand CLA N 301



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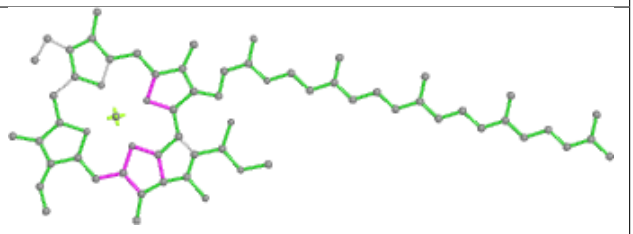
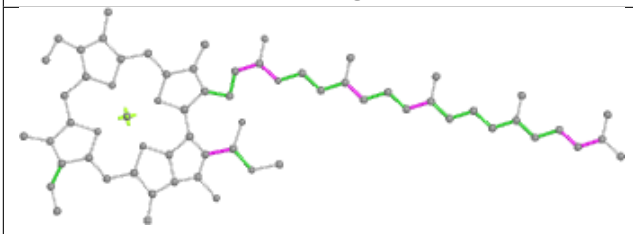


Bond angles



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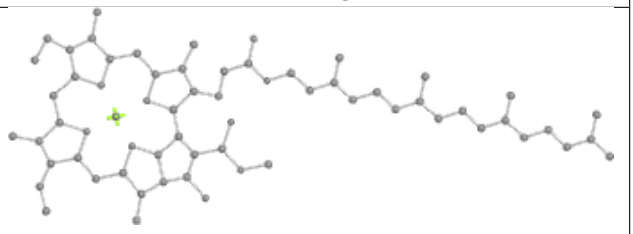
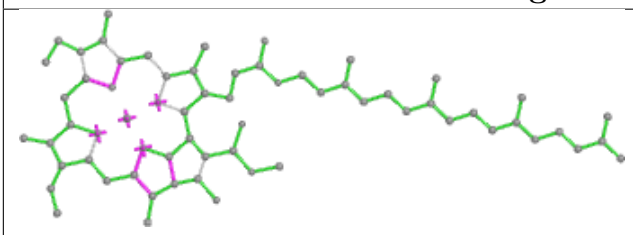


Rings

Ligand CLA c 502



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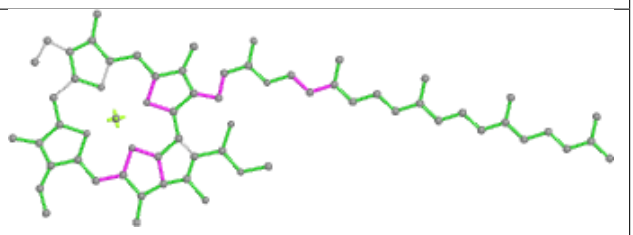

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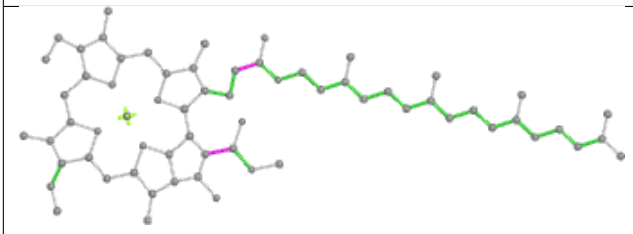

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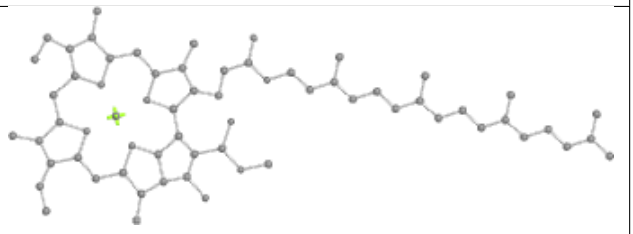
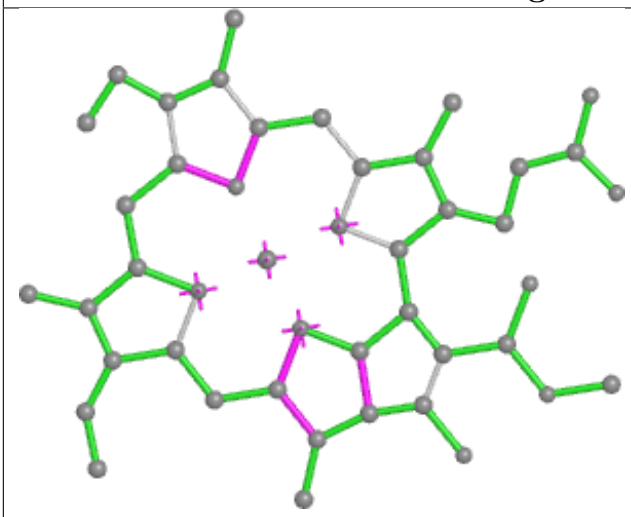


Rings

Ligand CLA 4 310



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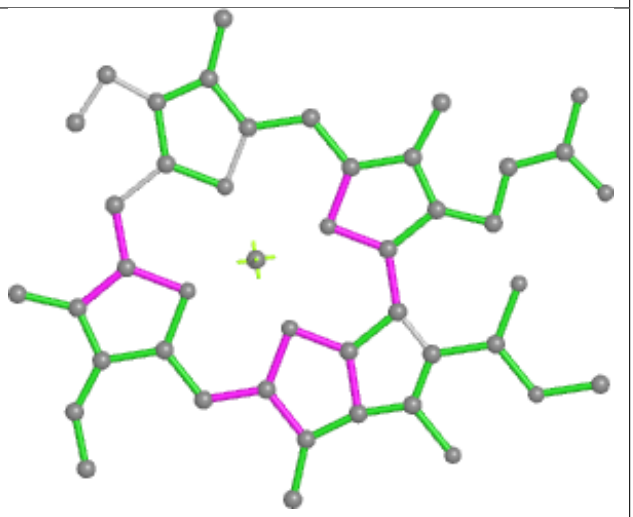
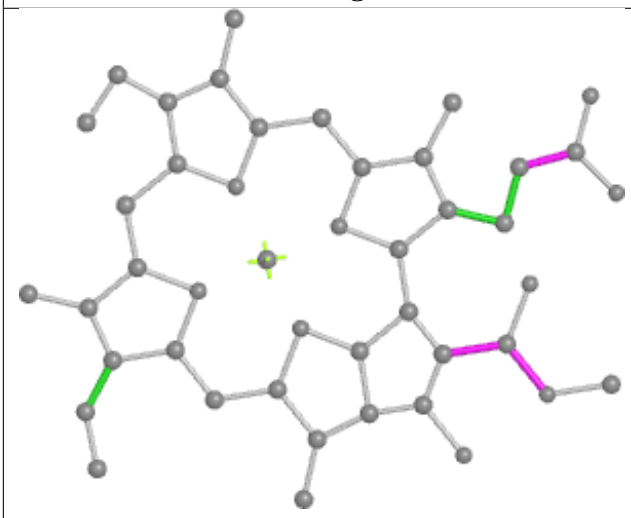
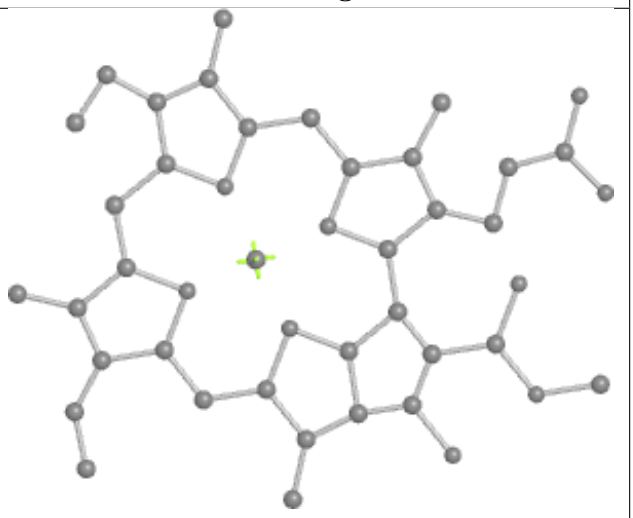


Bond angles

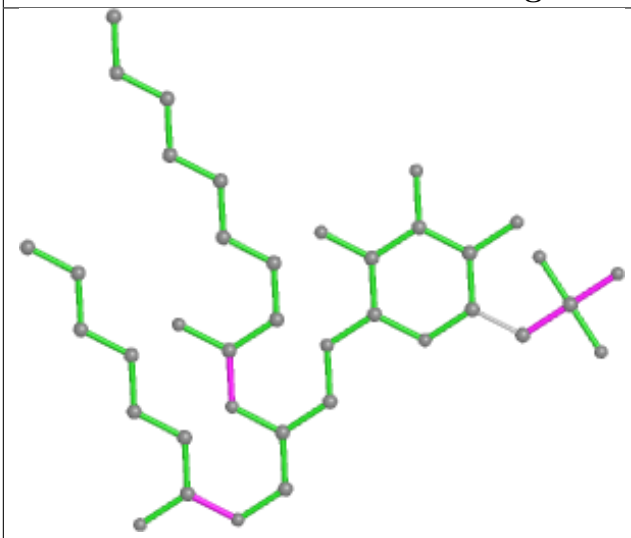


Torsions



Rings

Ligand SQD B 601



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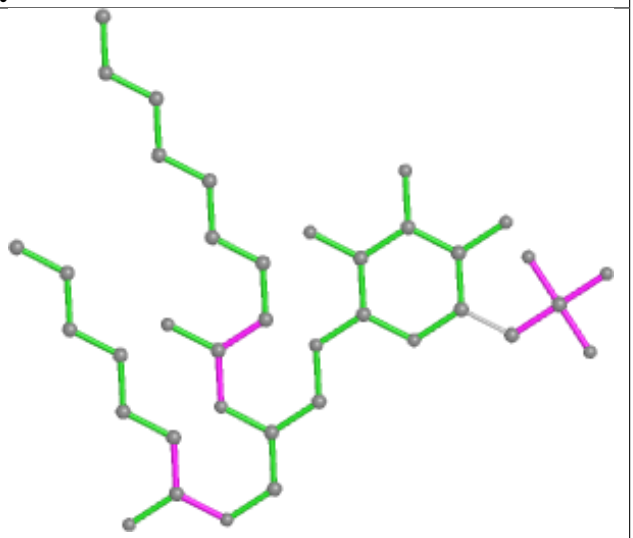
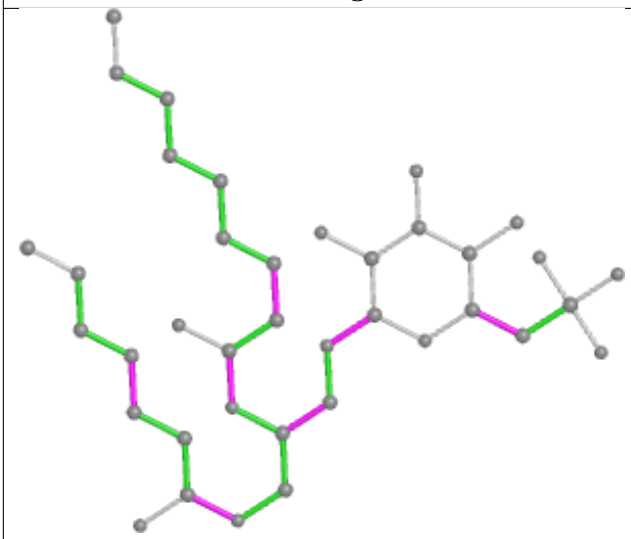
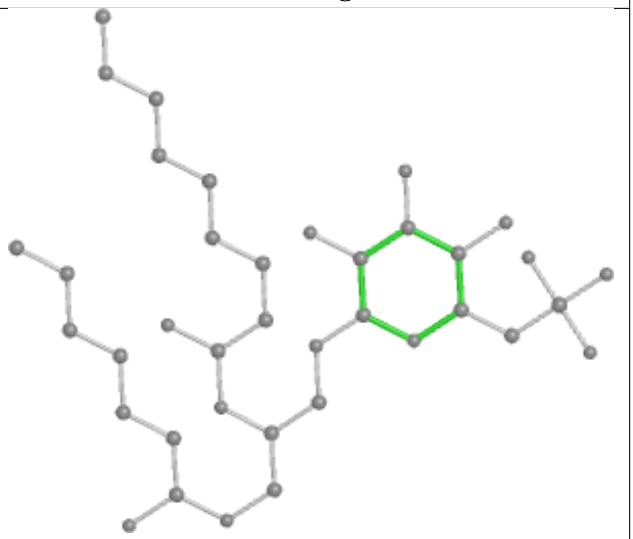


Bond angles

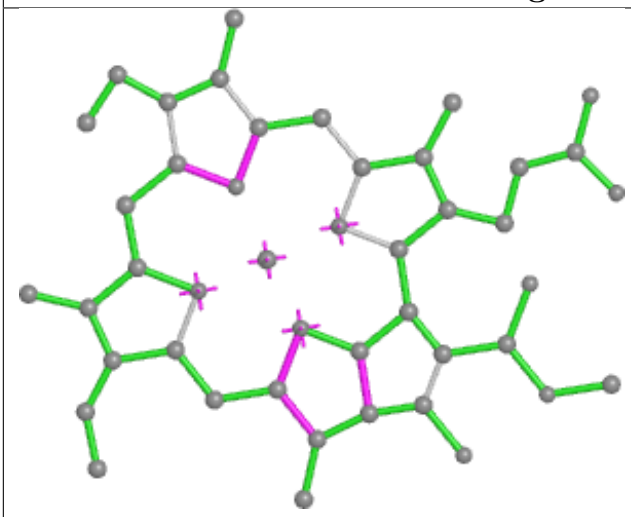


Torsions



Rings

Ligand CLA 3 304



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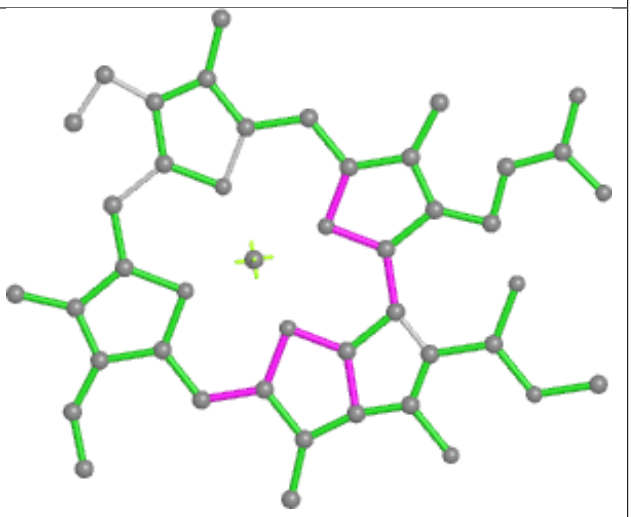
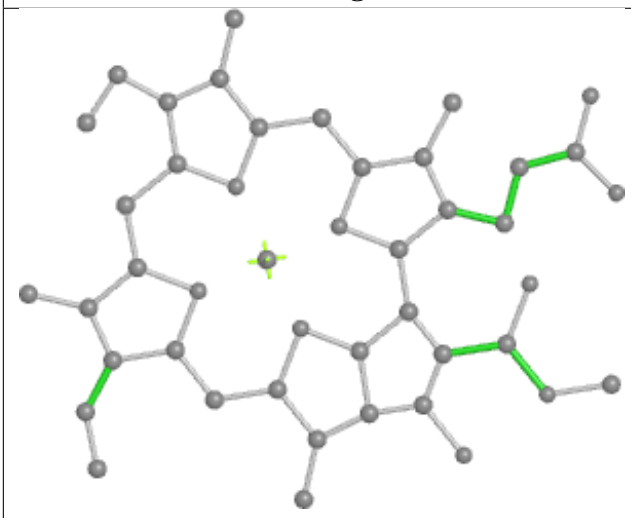


Bond angles



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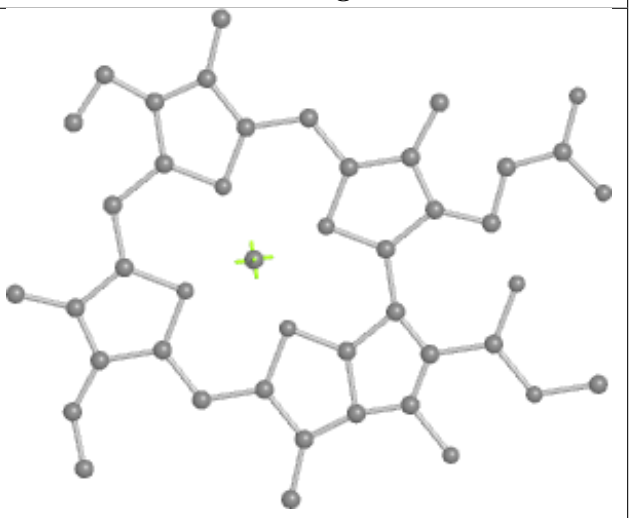
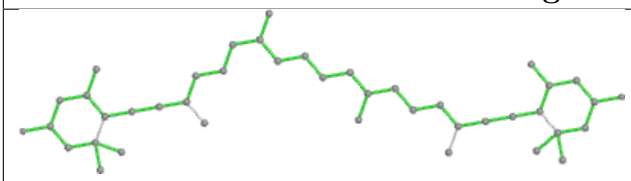


Rings

Ligand II0 3 319



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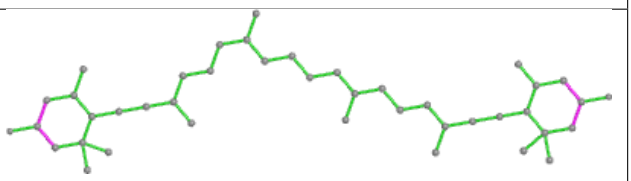
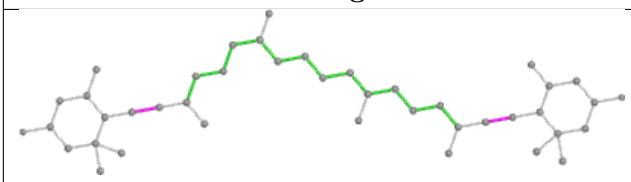


Bond angles



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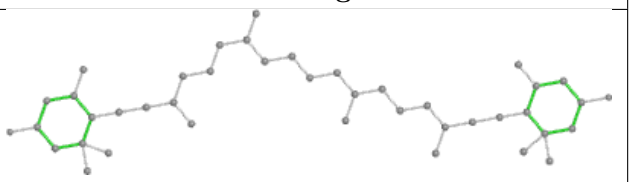
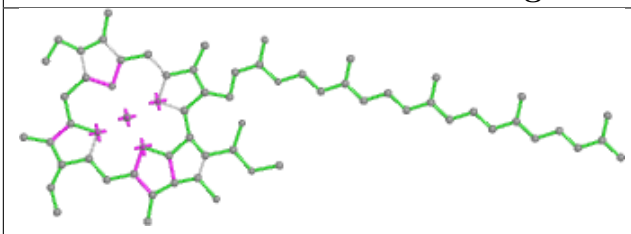
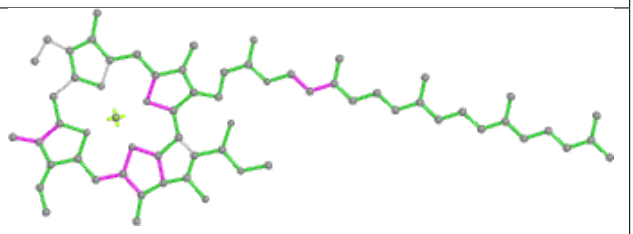


Rings

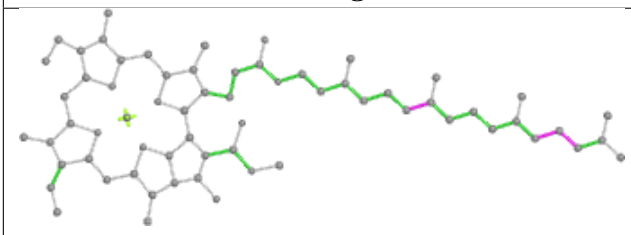
Ligand CLA B 606



Bond lengths



Bond angles



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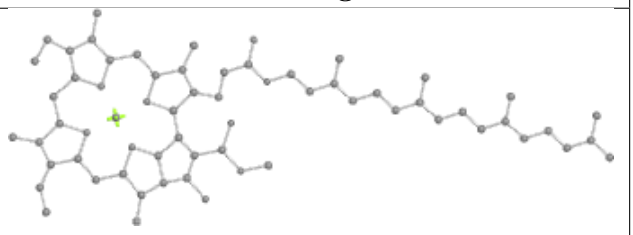
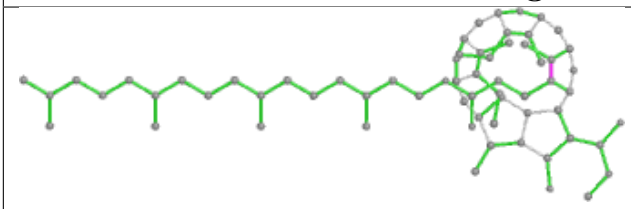
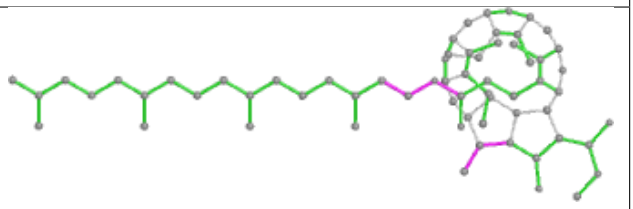


Rings

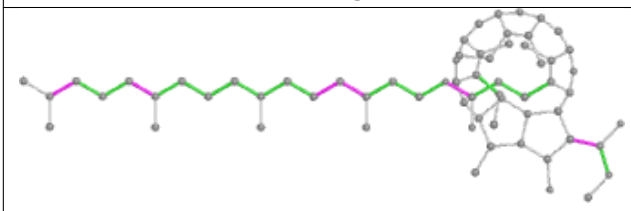
Ligand PHO a 407



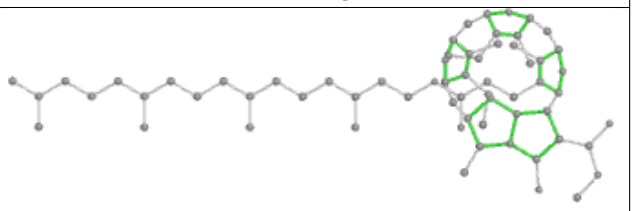
Bond lengths



Bond angles

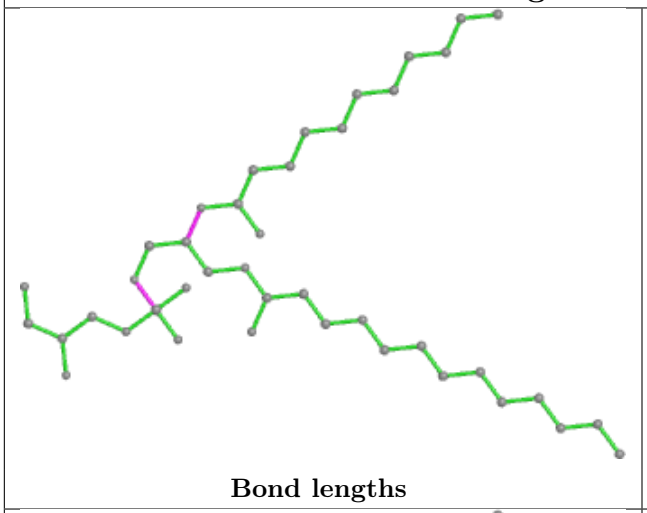


Torsions

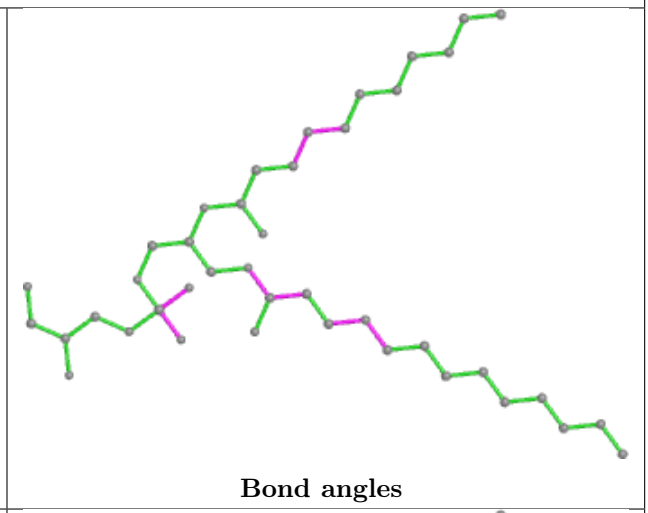


Rings

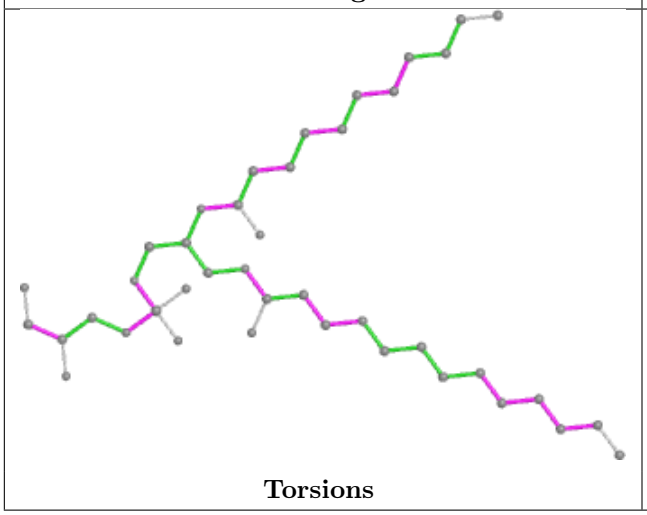
Ligand LHG 3 322



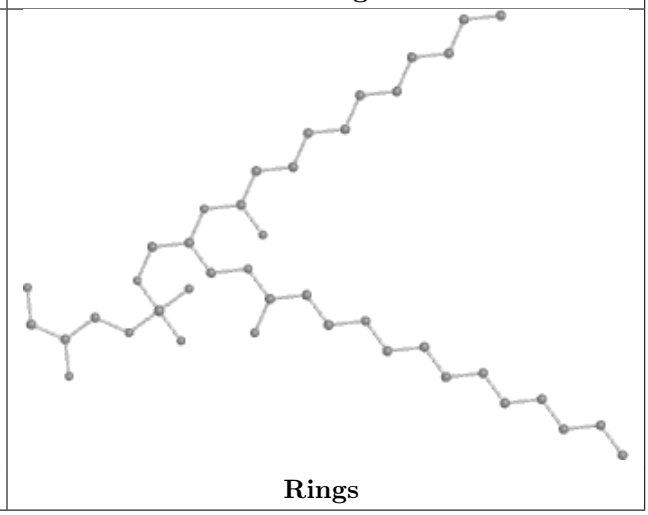
Bond lengths



Bond angles

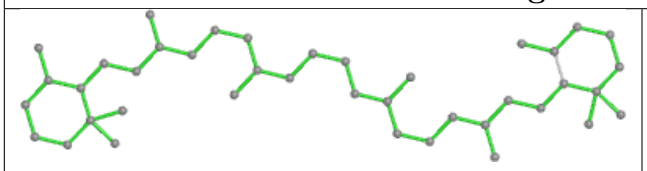


Torsions

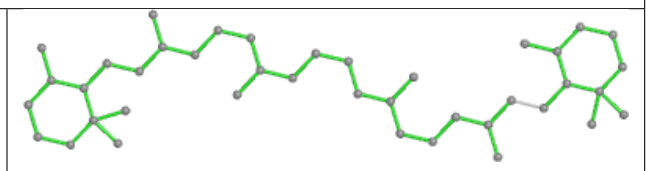


Rings

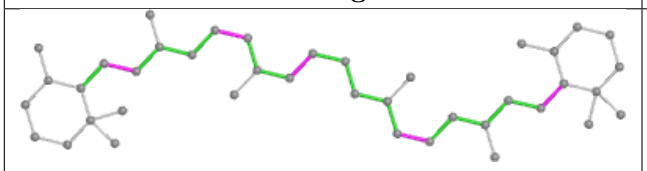
Ligand 8CT C 517



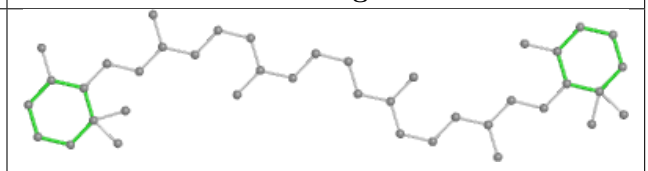
Bond lengths



Bond angles

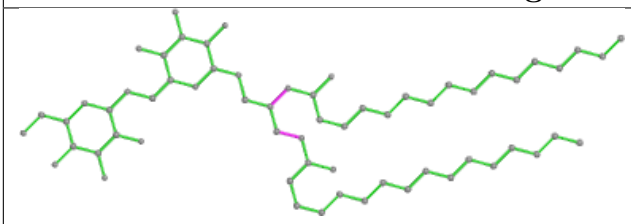


Torsions



Rings

Ligand DGD c 521



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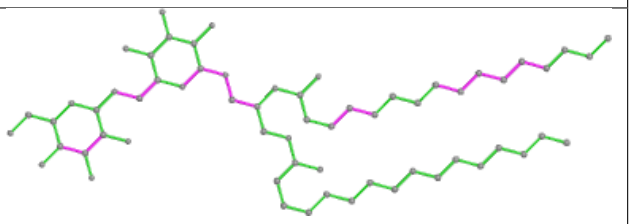

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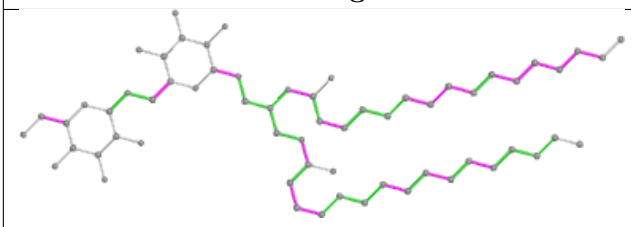

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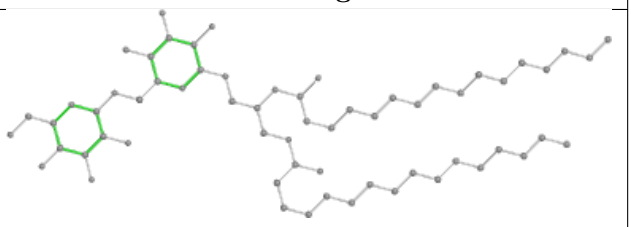
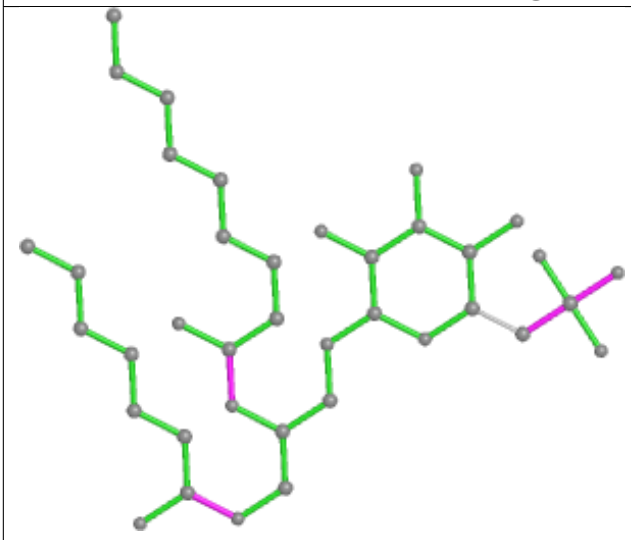


Rings

Ligand SQD b 601



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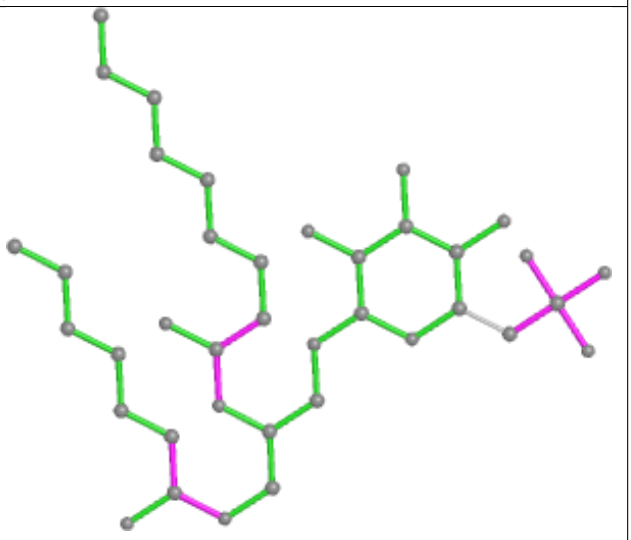

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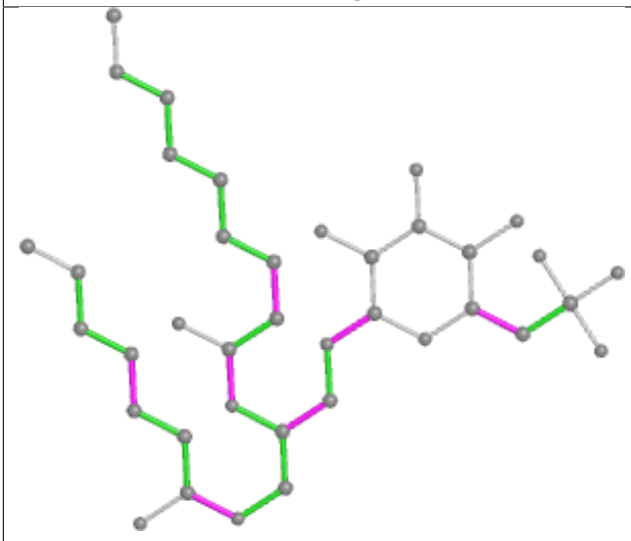

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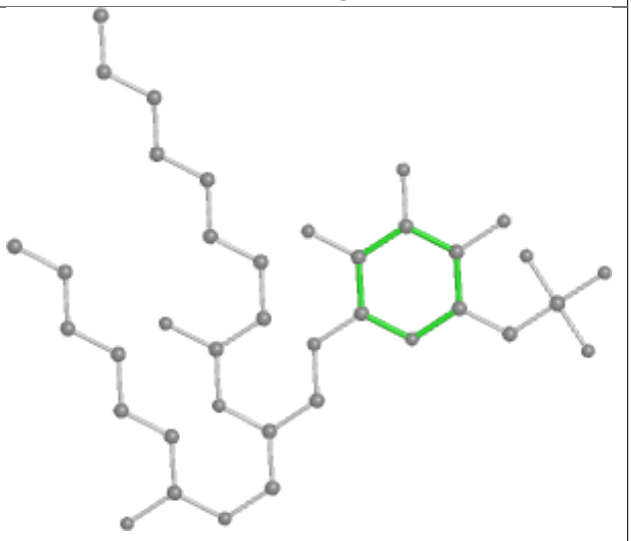
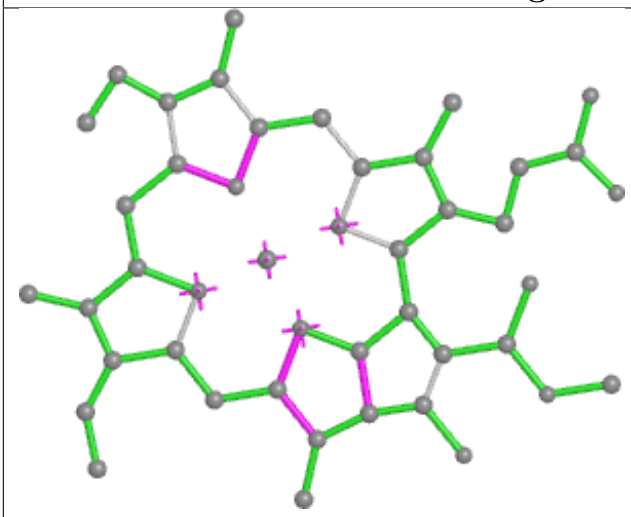


Rings

Ligand CLA 0 311



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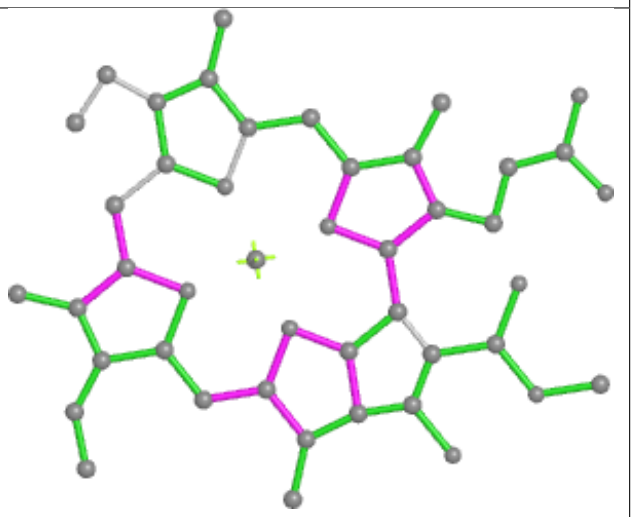
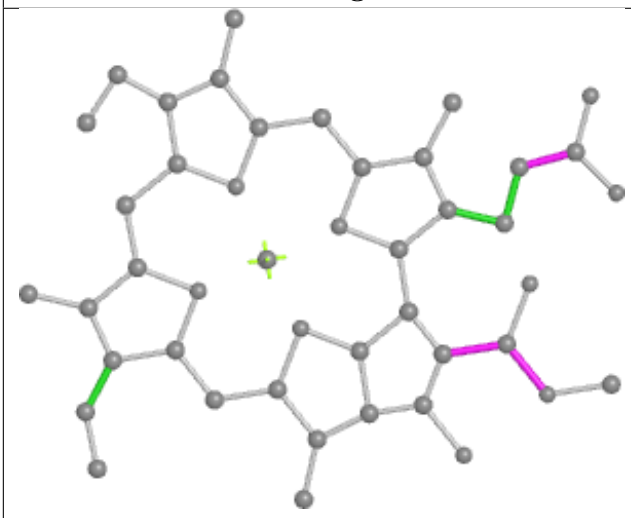


Bond angles



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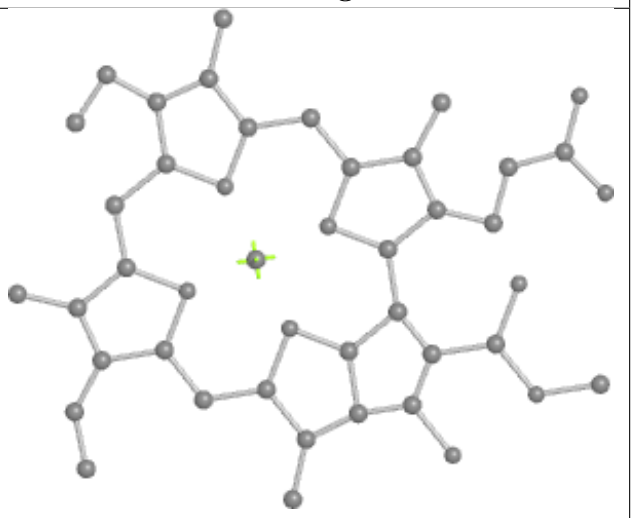
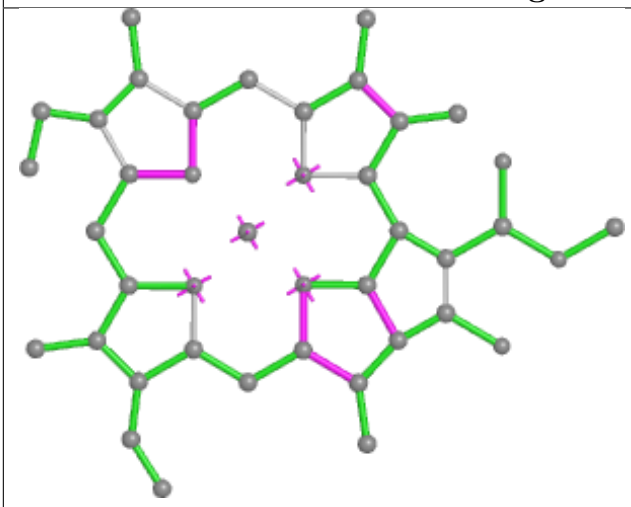


Rings

Ligand CLA 9 314



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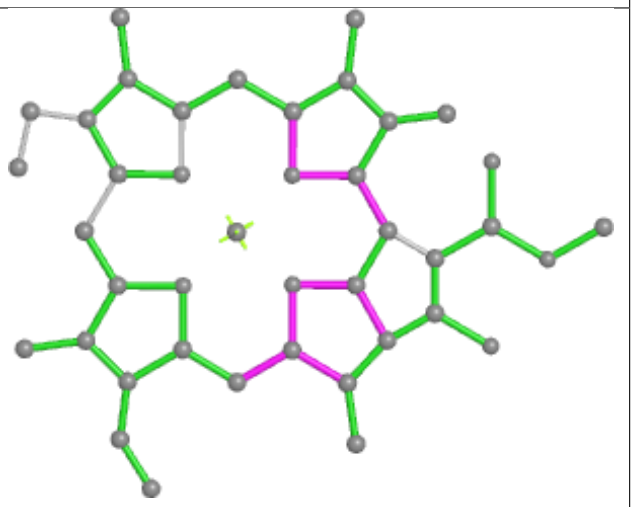

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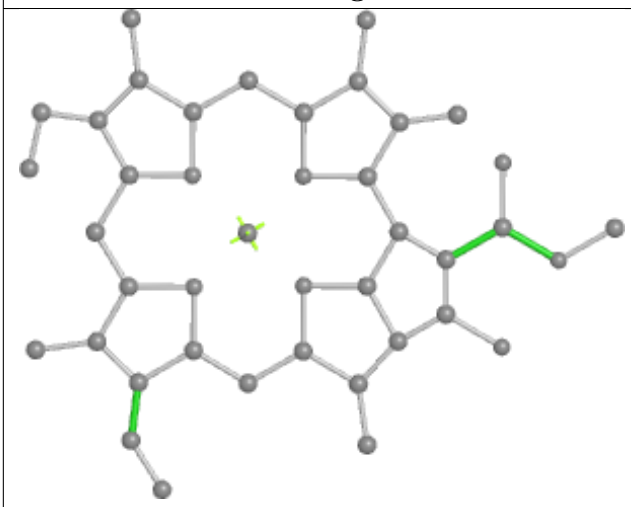

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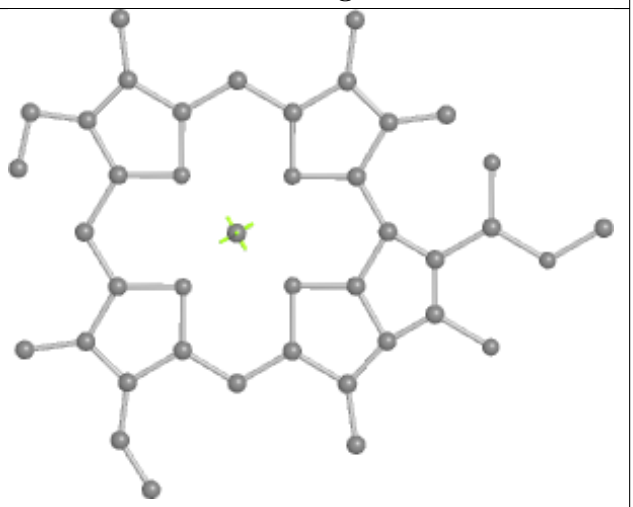
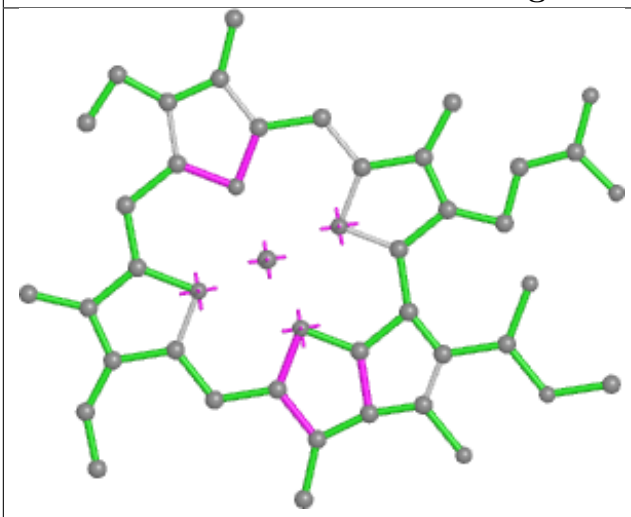


Rings

Ligand CLA g 306



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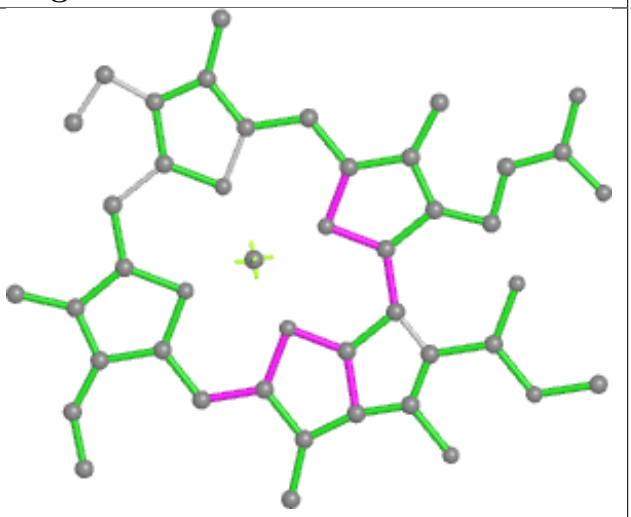

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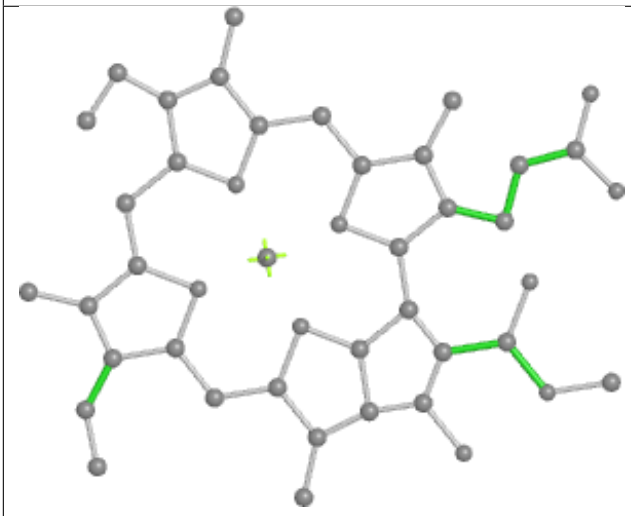

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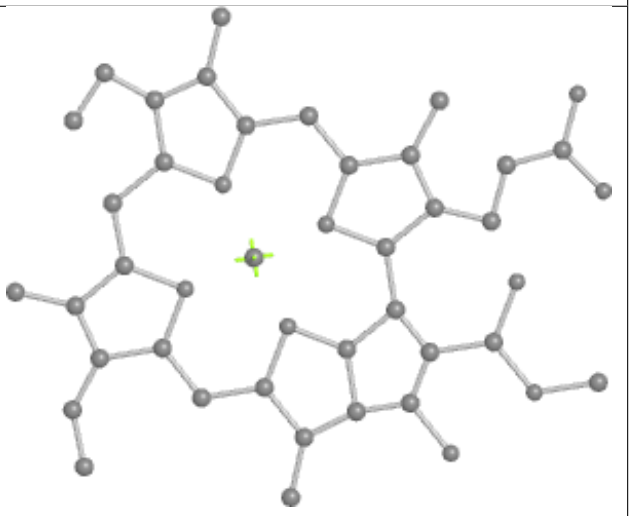
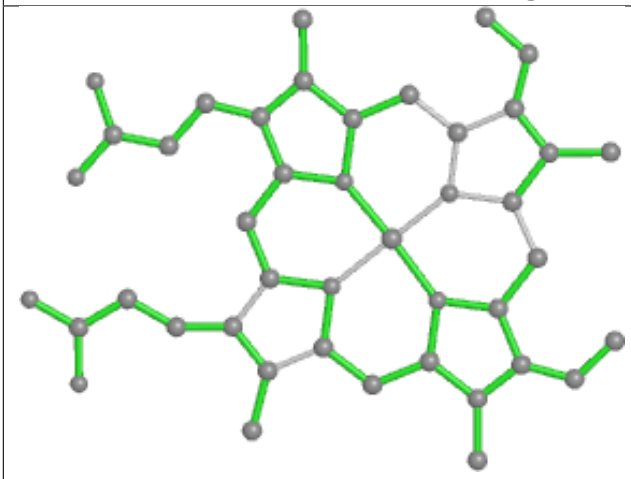


Rings

Ligand HEM v 201



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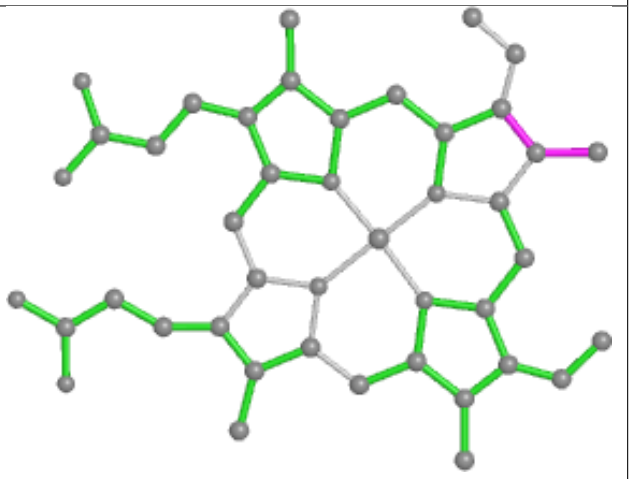
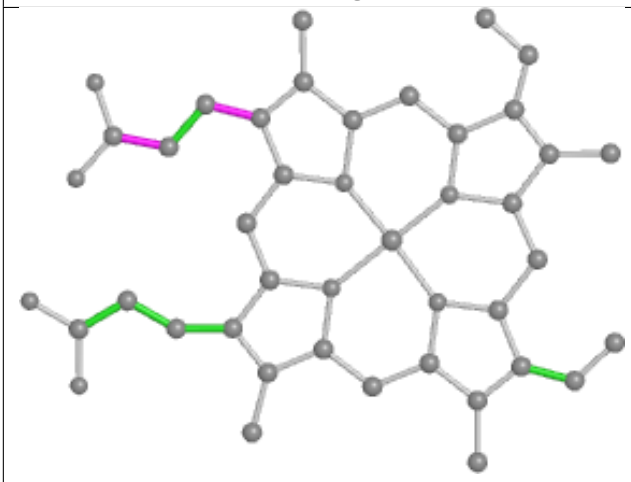


Bond angles



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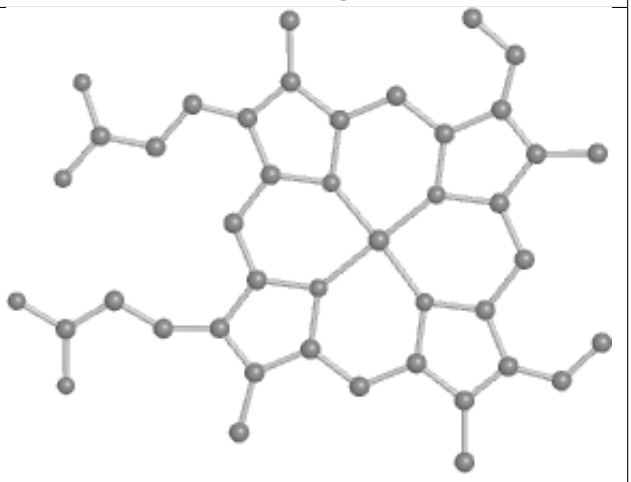
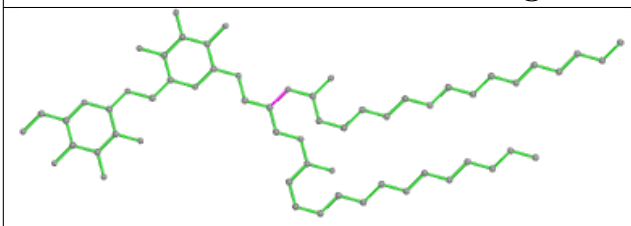


Rings

Ligand DGD h 101



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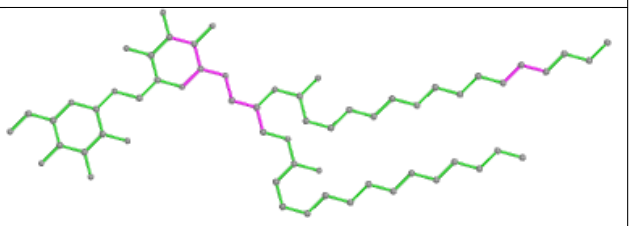

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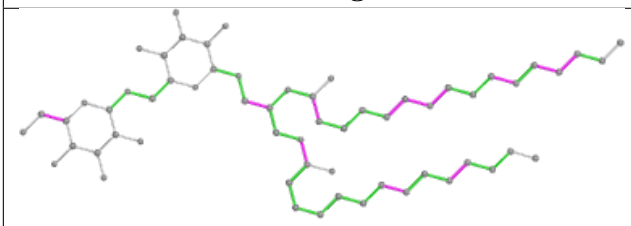

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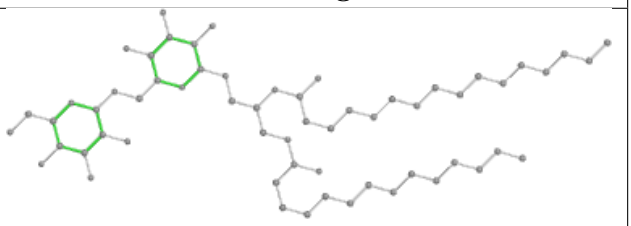
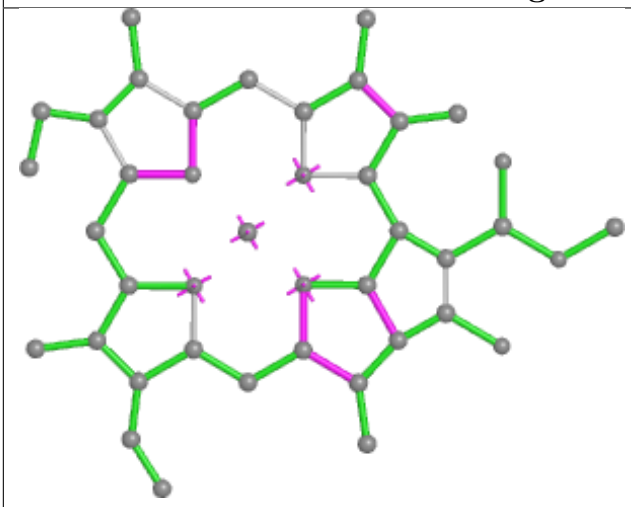


Rings

Ligand CLA g 308



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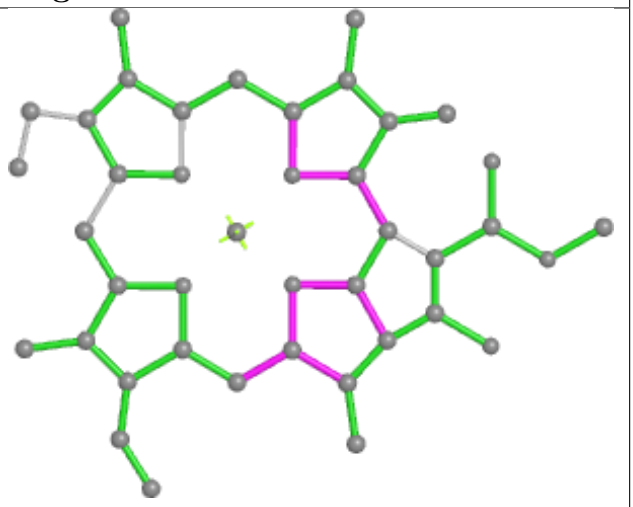
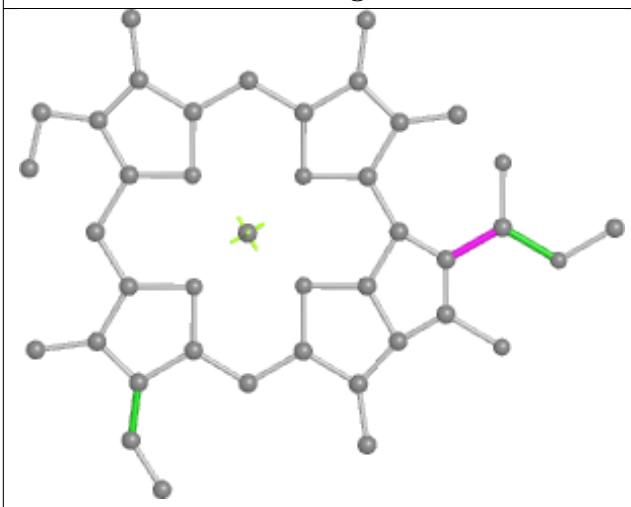


Bond angles



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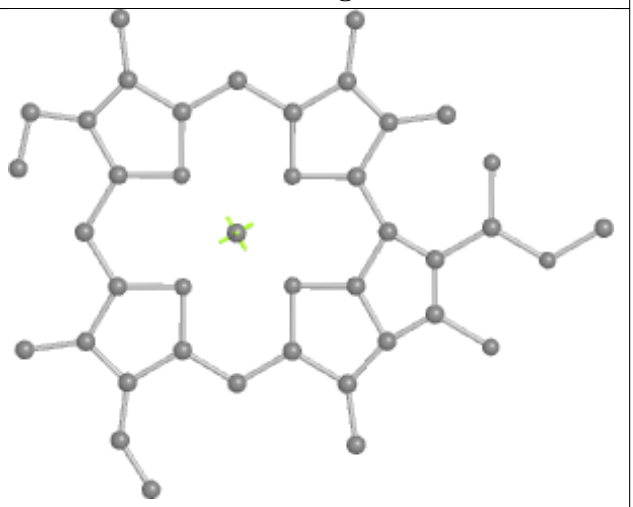
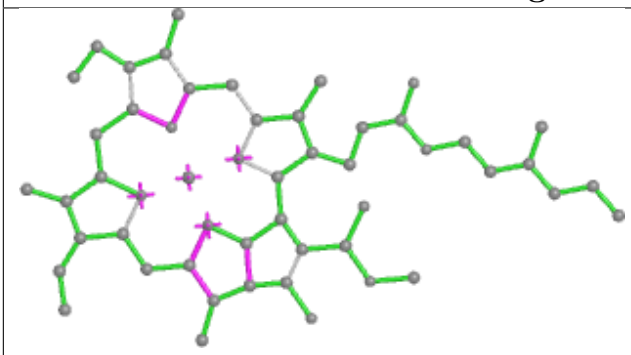


Rings

Ligand CLA 8 303



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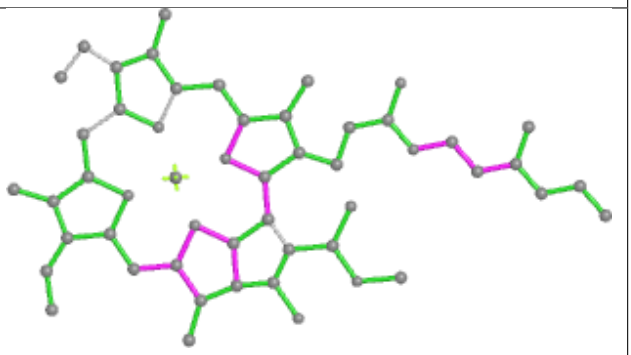

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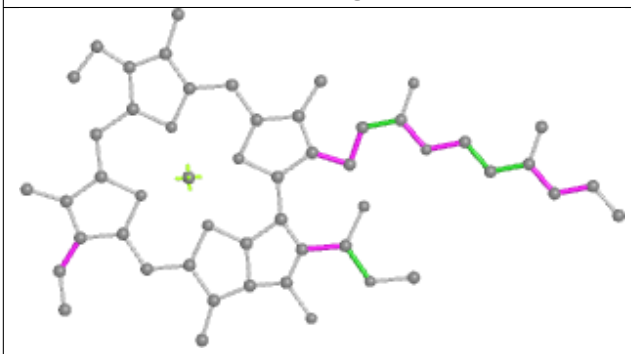

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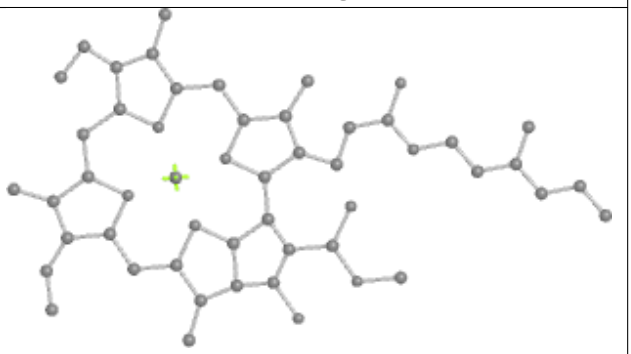
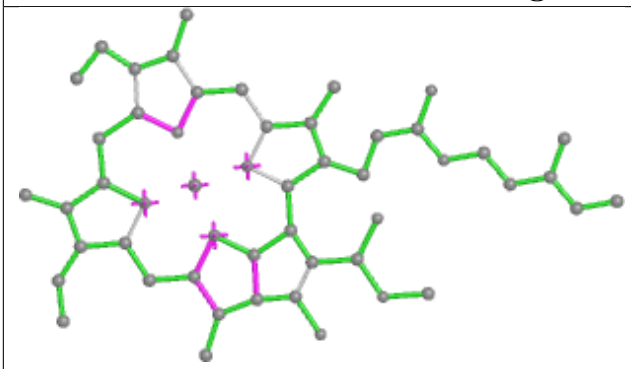


Rings

Ligand CLA 4 302



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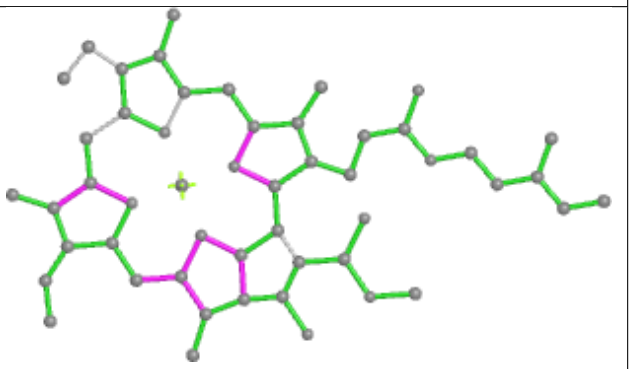
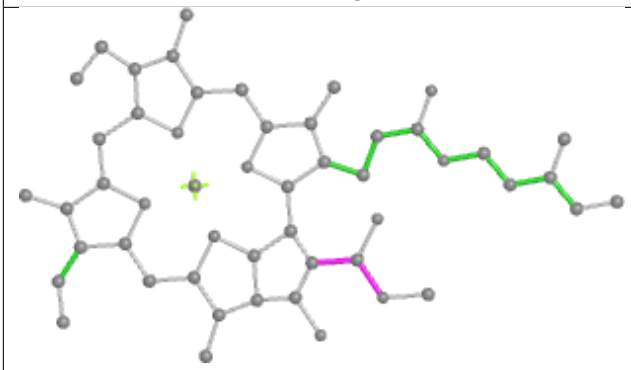


Bond angles



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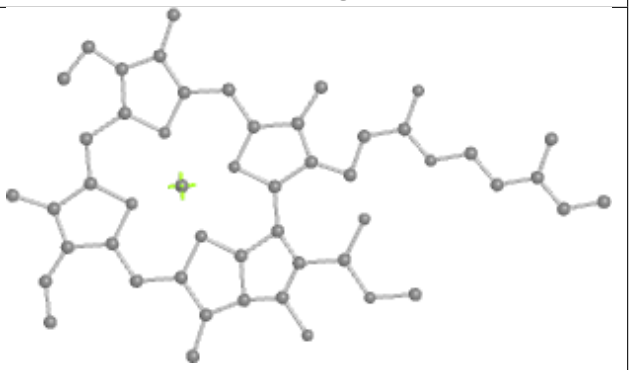
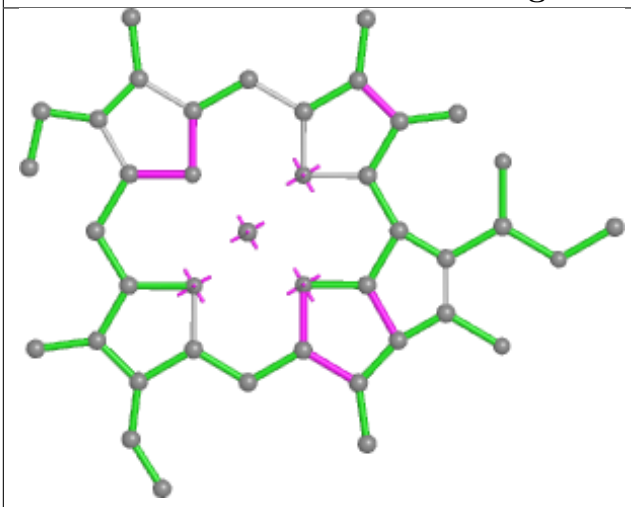


Rings

Ligand CLA 3 313



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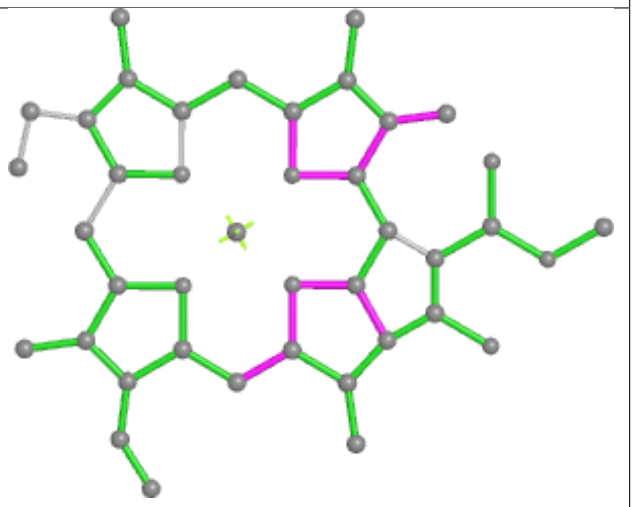
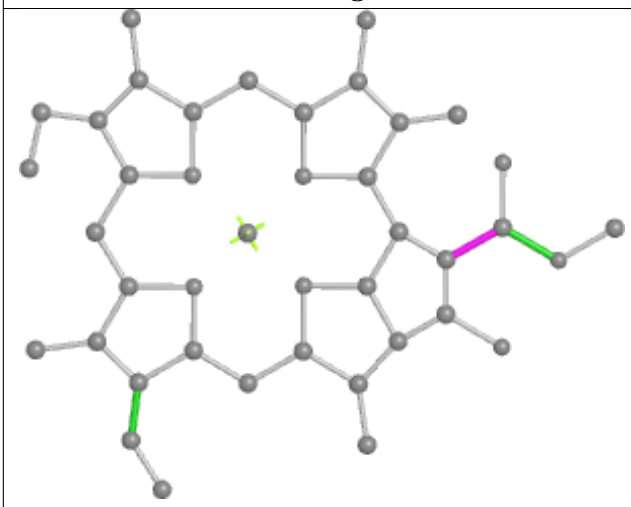


Bond angles



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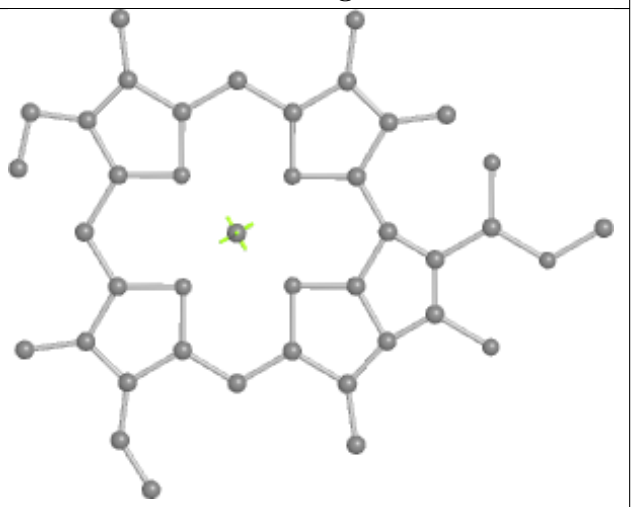
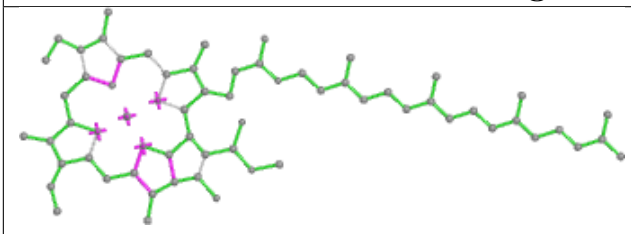


Rings

Ligand CLA 1 307



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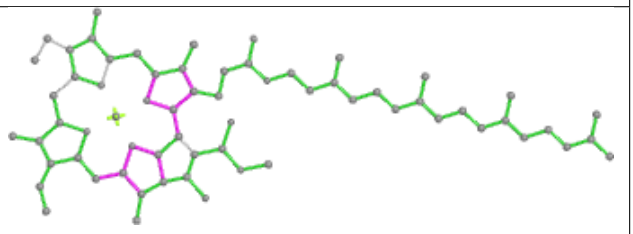

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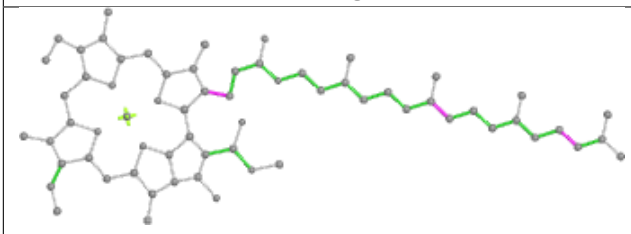

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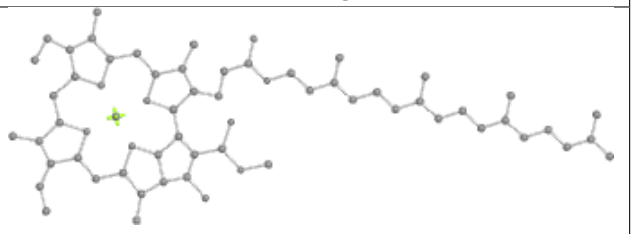
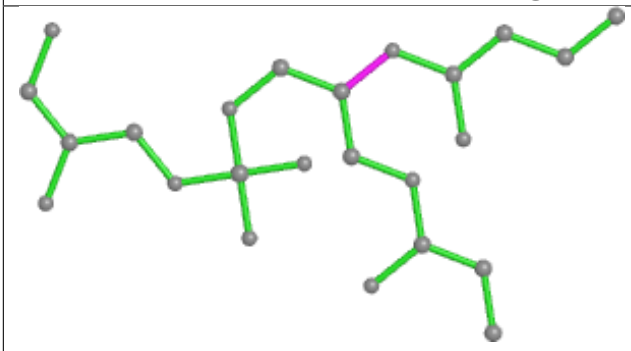


Rings

Ligand LHG a 411



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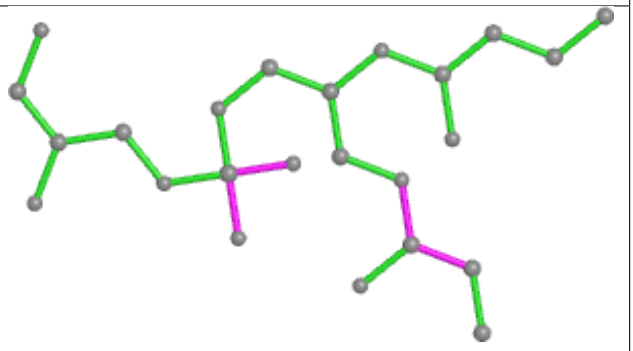
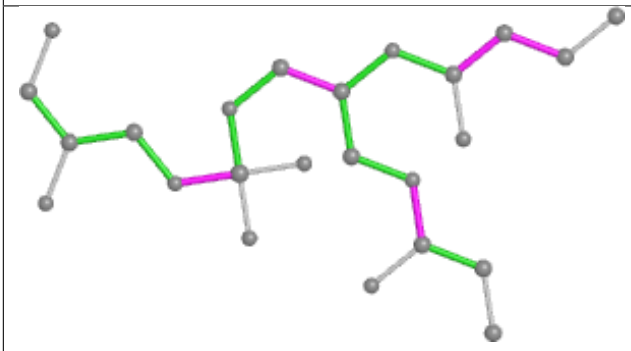


Bond angles



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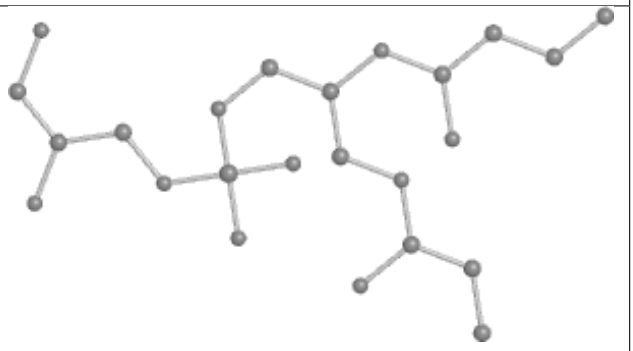
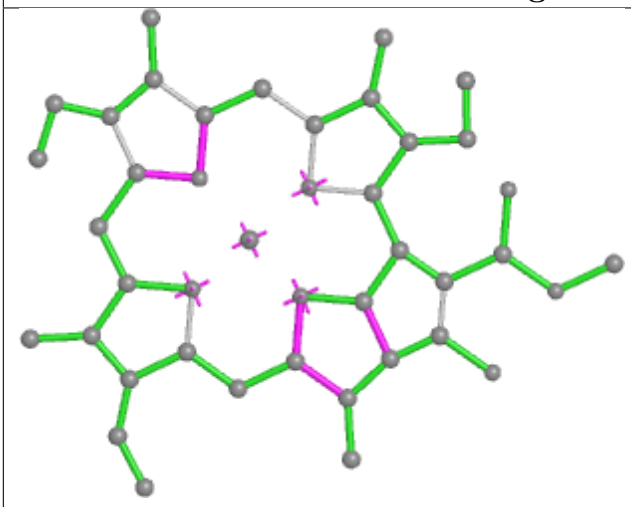


Rings

Ligand CLA 6 304



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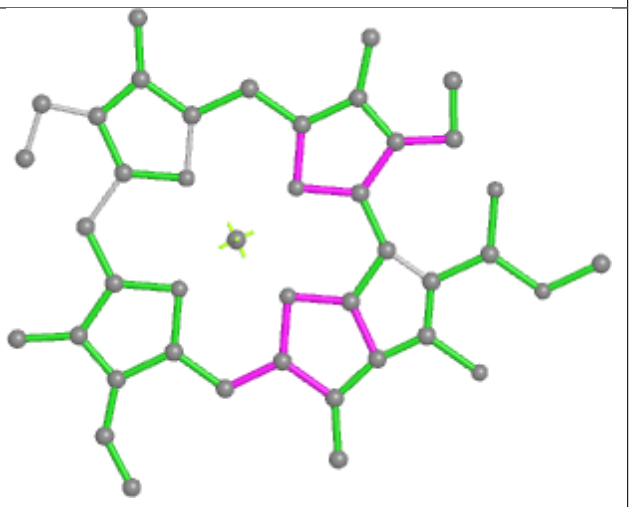
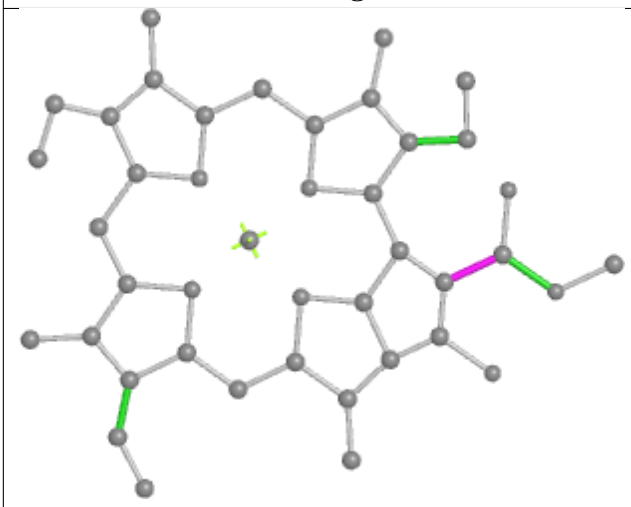


Bond angles



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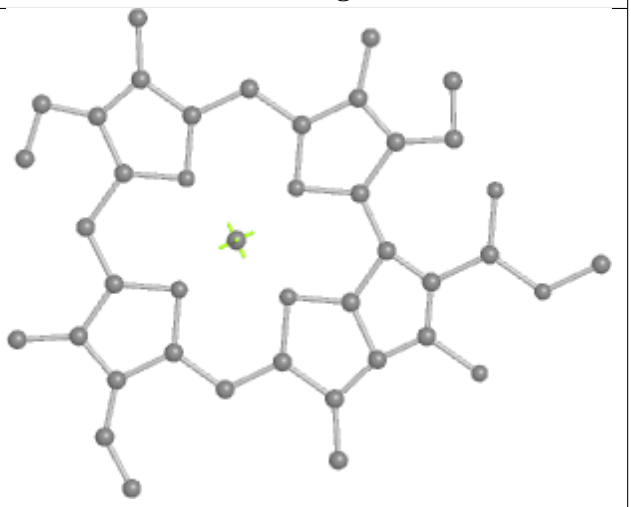
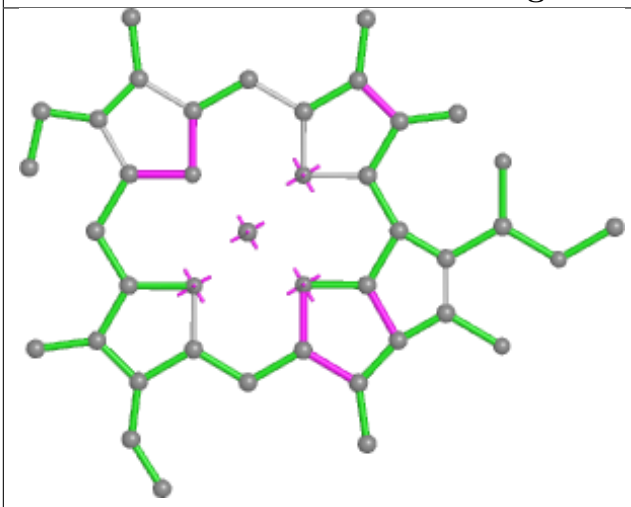
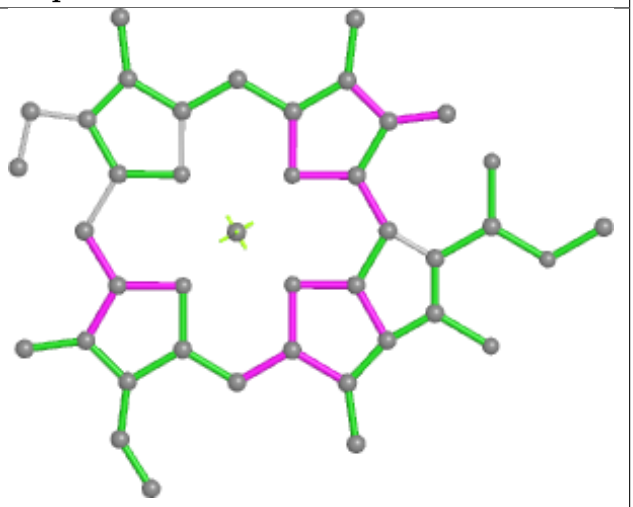


Rings

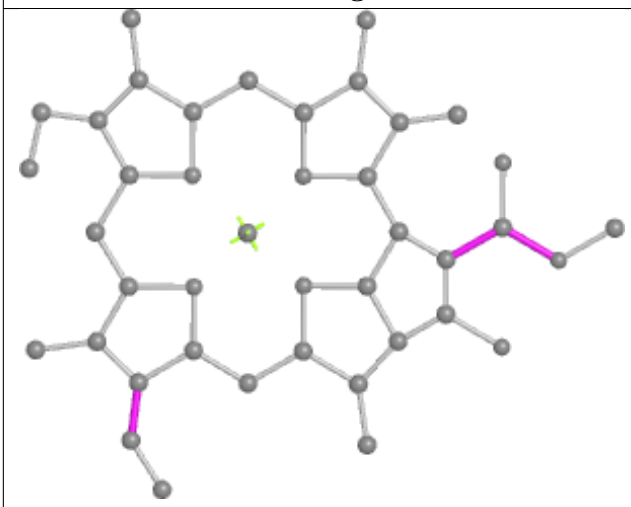
Ligand CLA p 310



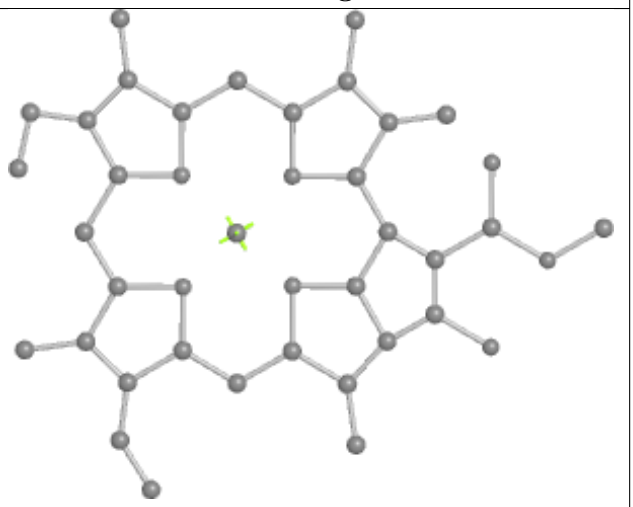
Bond lengths



Bond angles

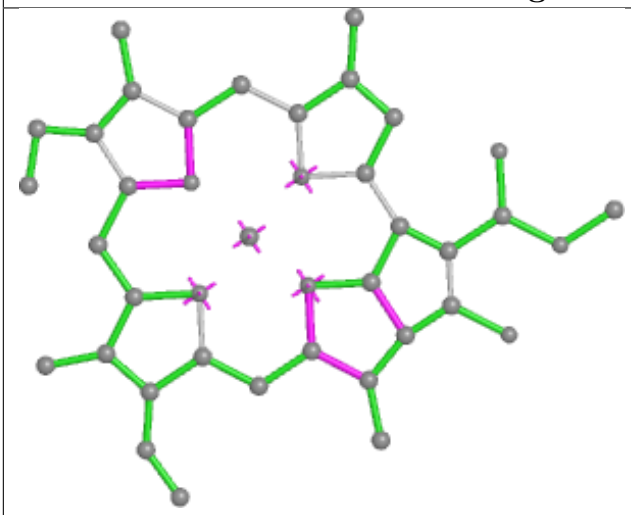


Torsions



Rings

Ligand CLA 4 309



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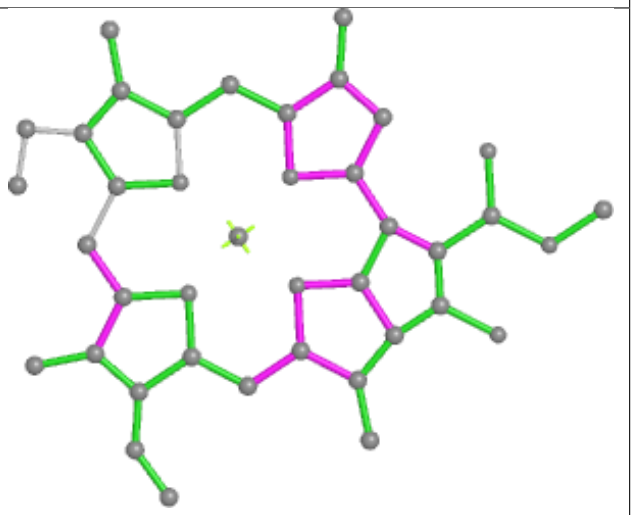
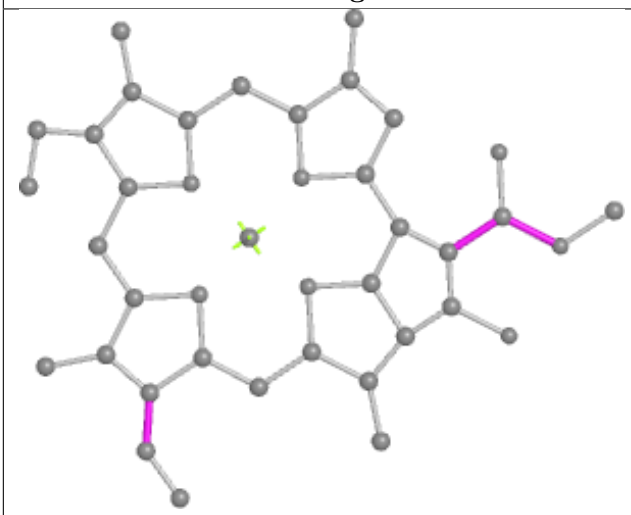


Bond angles



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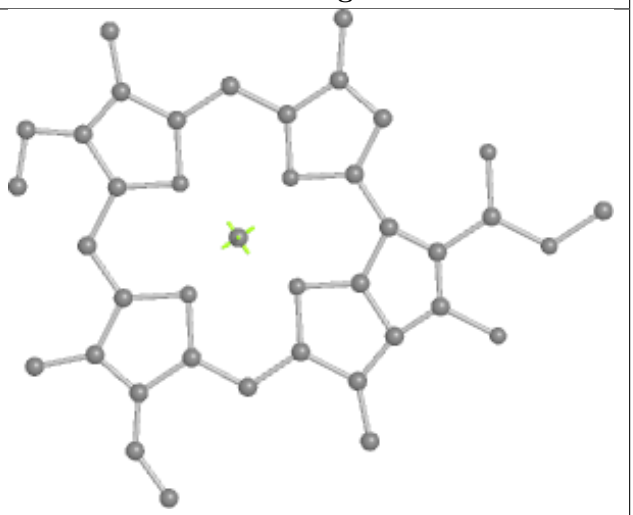
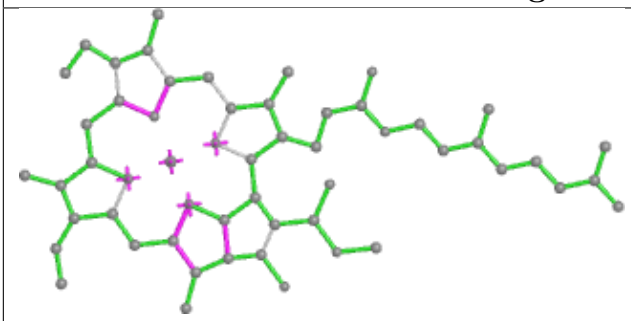


Rings

Ligand CLA 5 307



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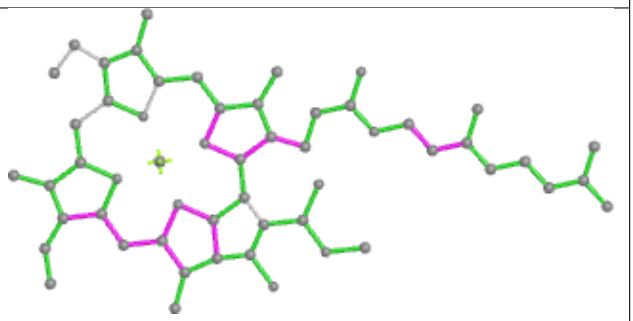

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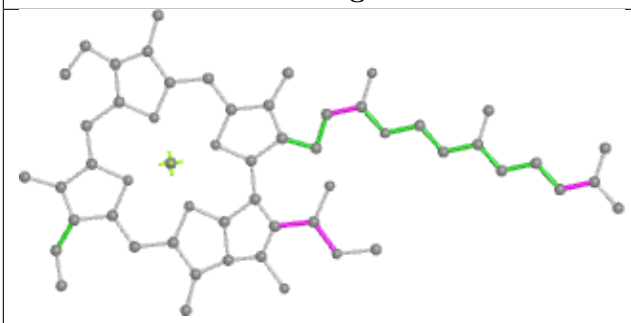

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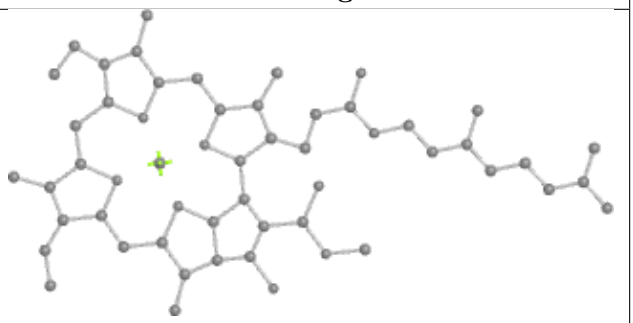
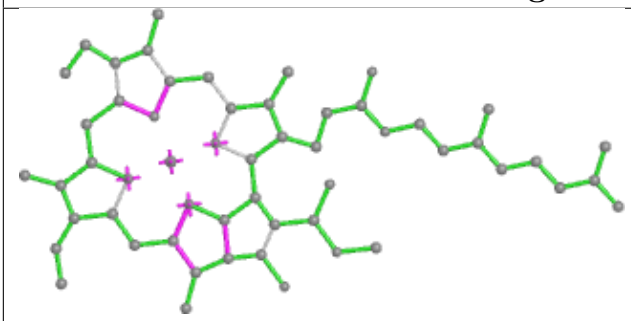


Rings

Ligand CLA 4 306



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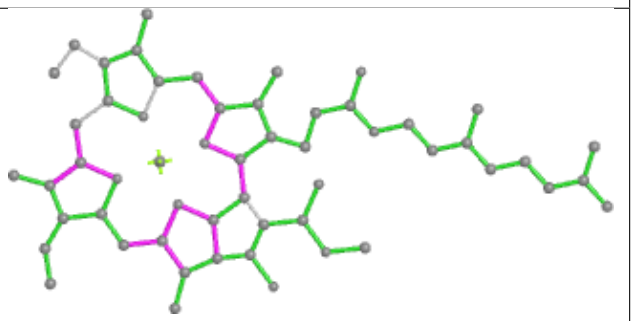
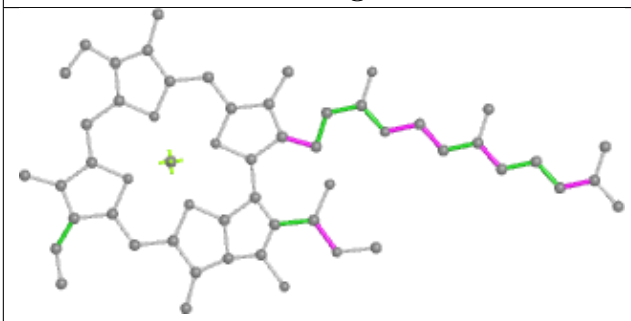


Bond angles



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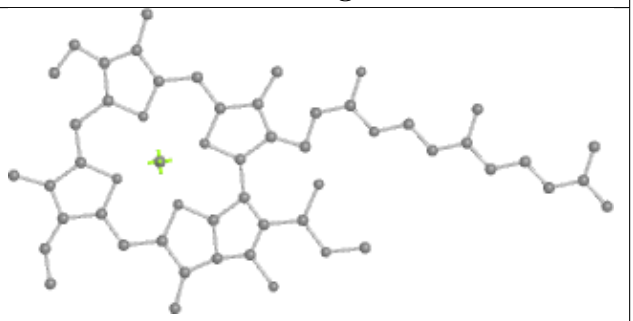
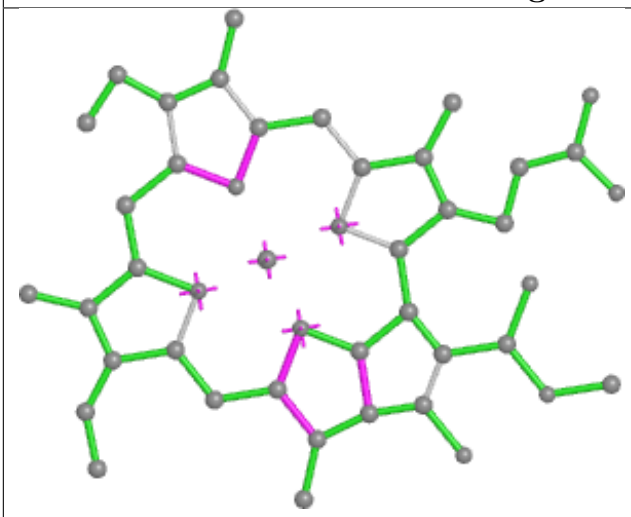


Rings

Ligand CLA 5 311



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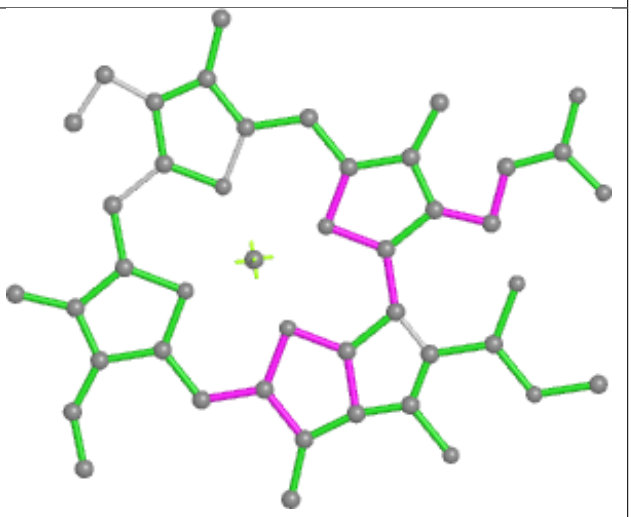
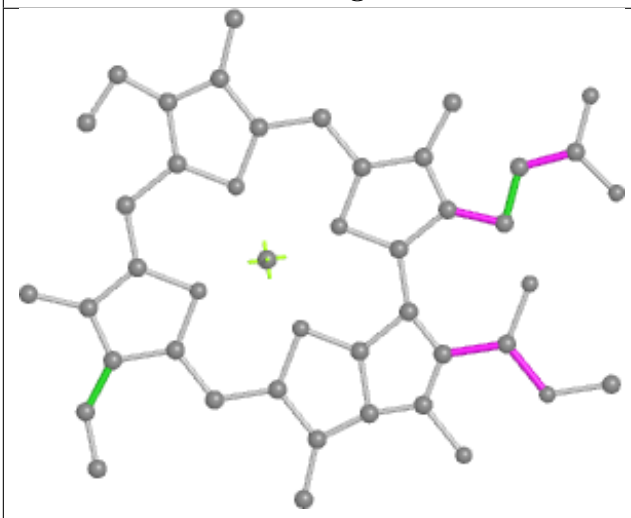


Bond angles



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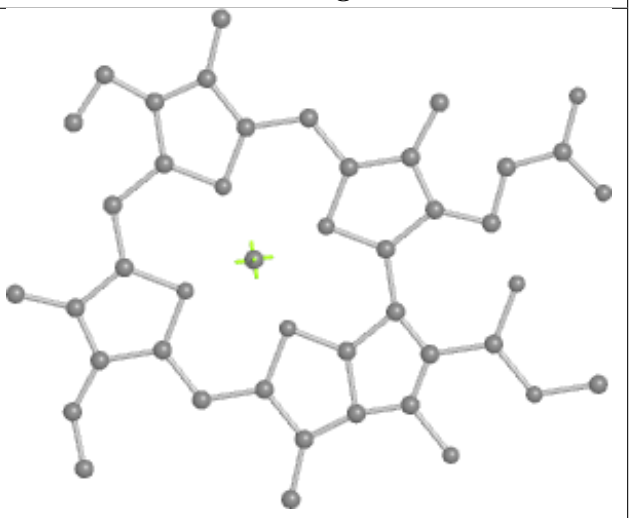
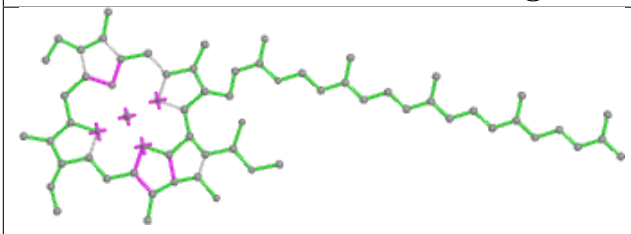


Rings

Ligand CLA C 508



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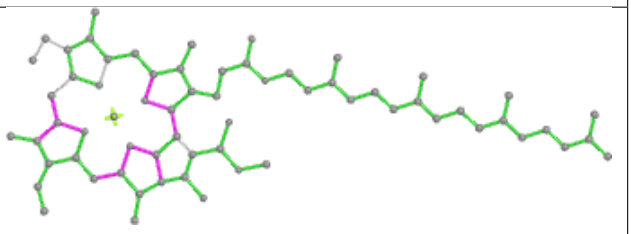
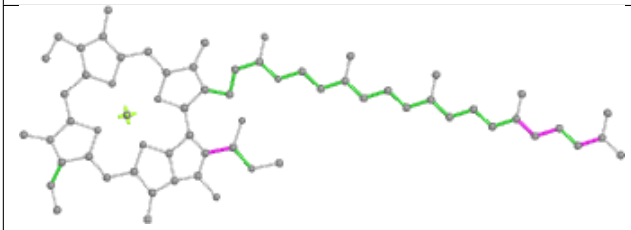


Bond angles



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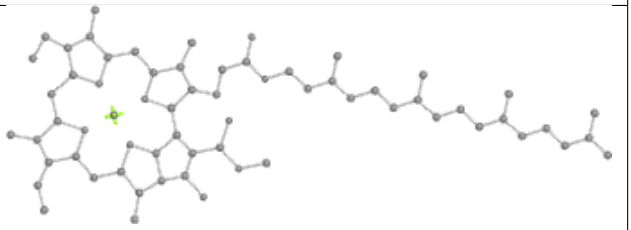
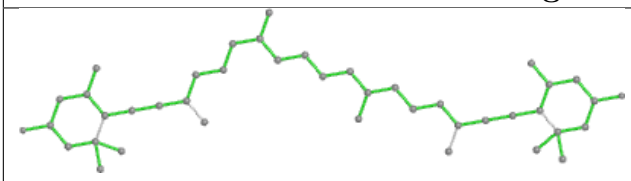


Rings

Ligand II0 4 313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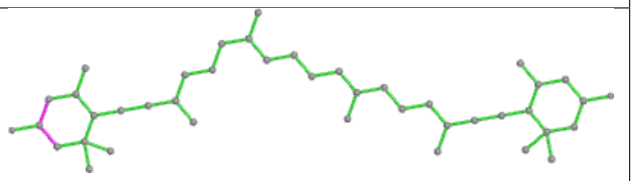
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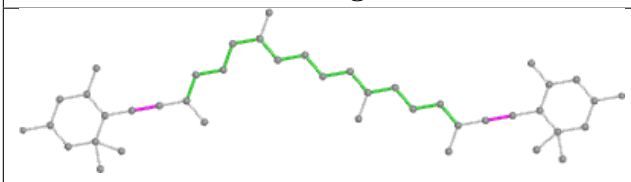
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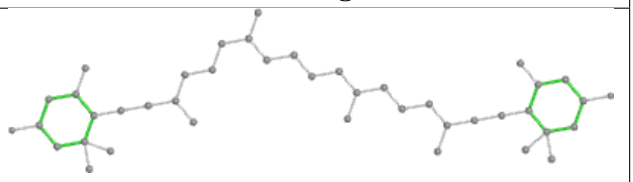
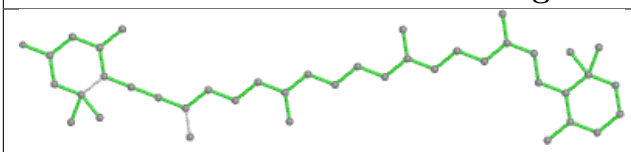

Rings

Ligand IHT 8 314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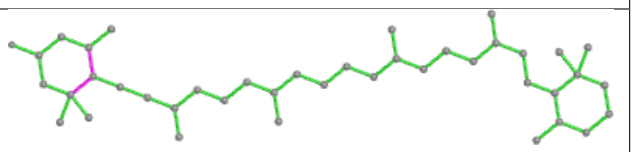
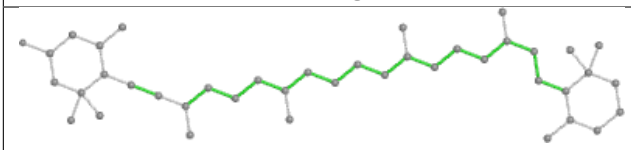
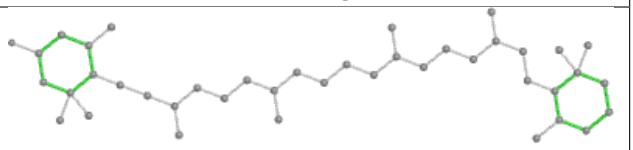
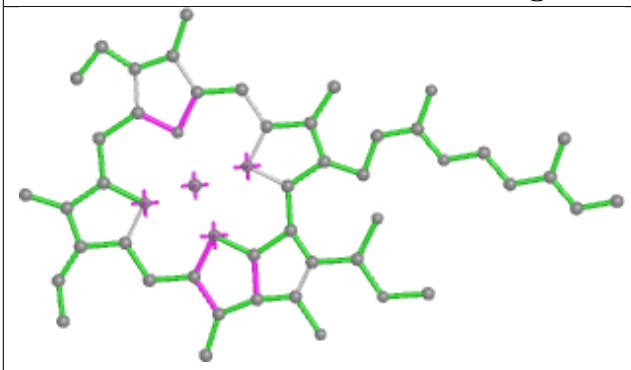

Bond angles


Torsions


Rings

Ligand CLA 7 303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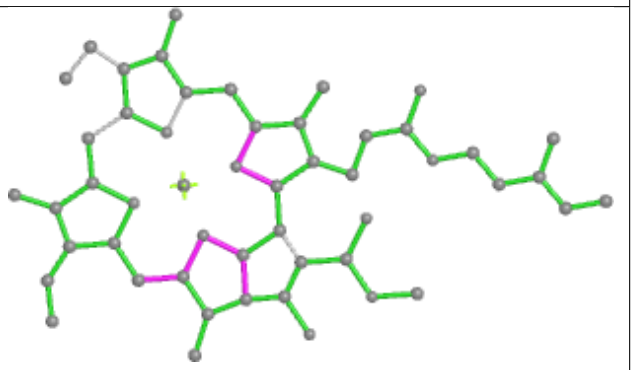
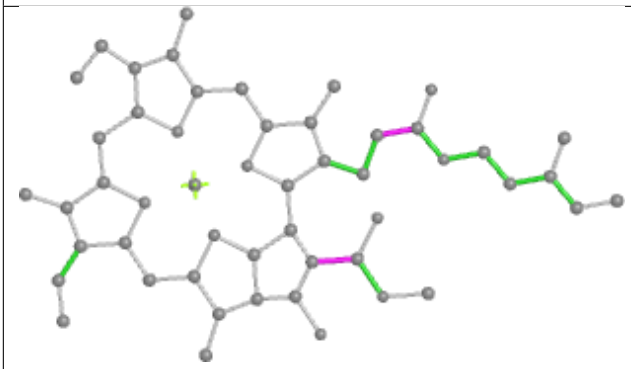

Bond angles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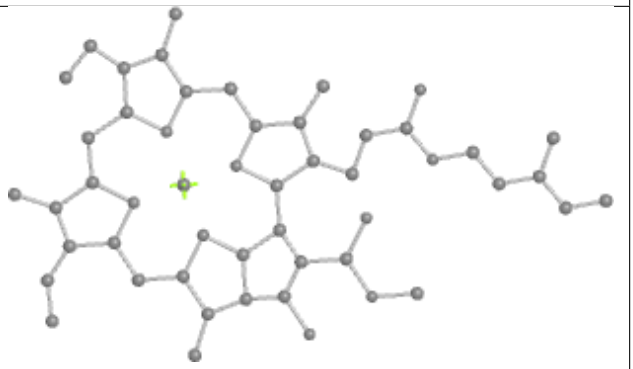
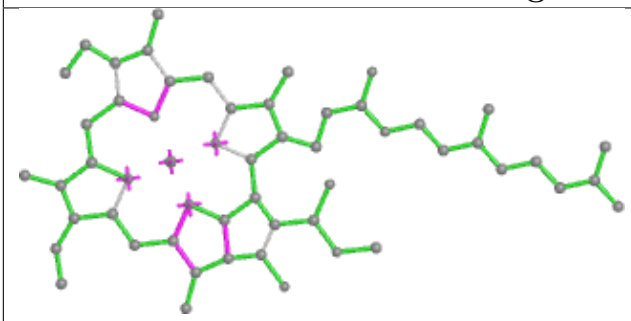
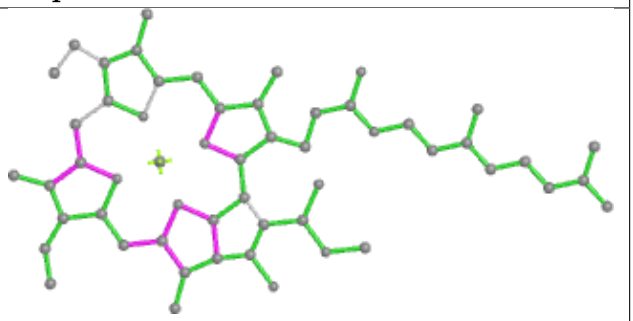

Rings

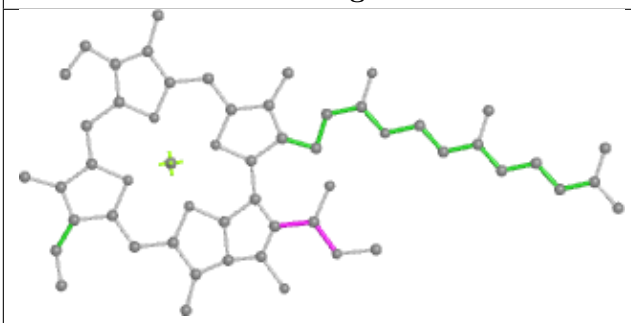
Ligand CLA p 305



Bond lengths



Bond angles



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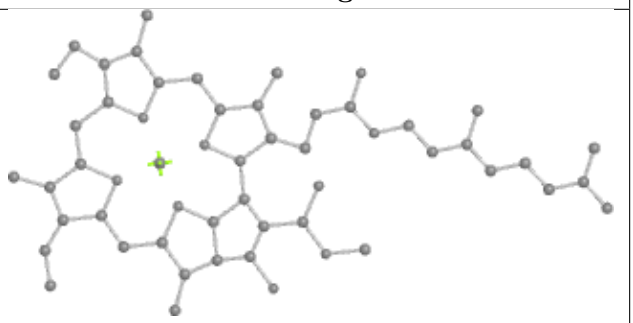
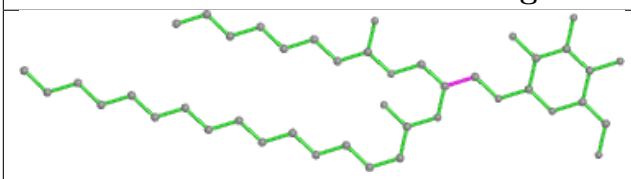


Rings

Ligand LMG T 101



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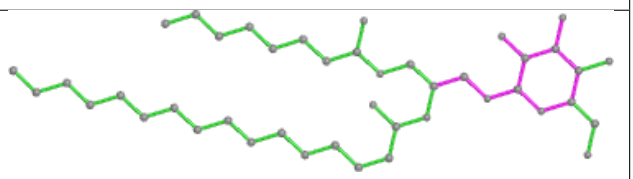
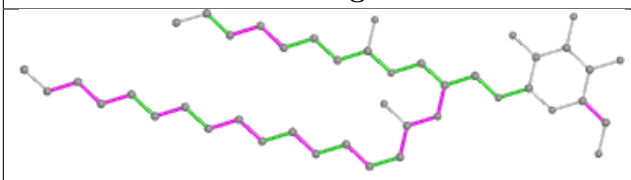
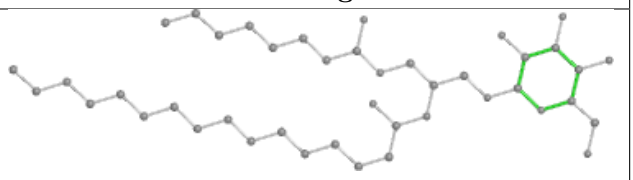


Bond angles

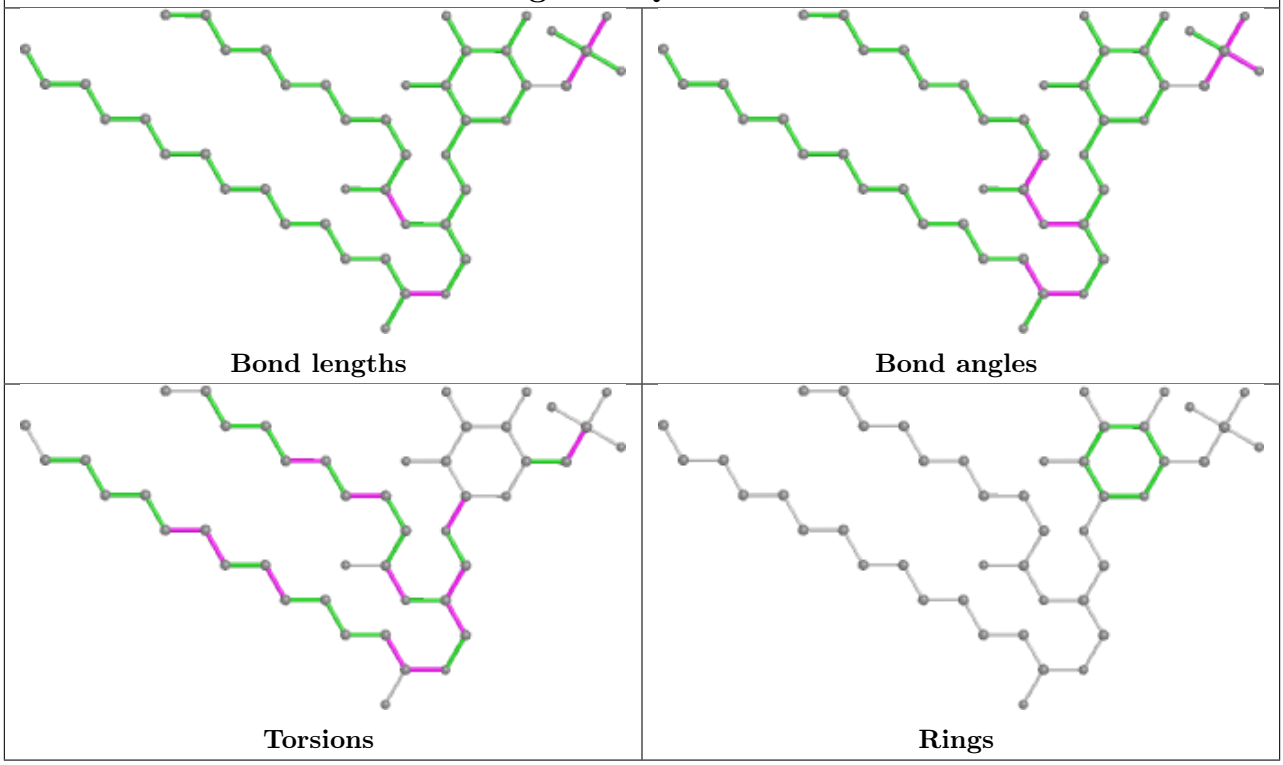


Torsions

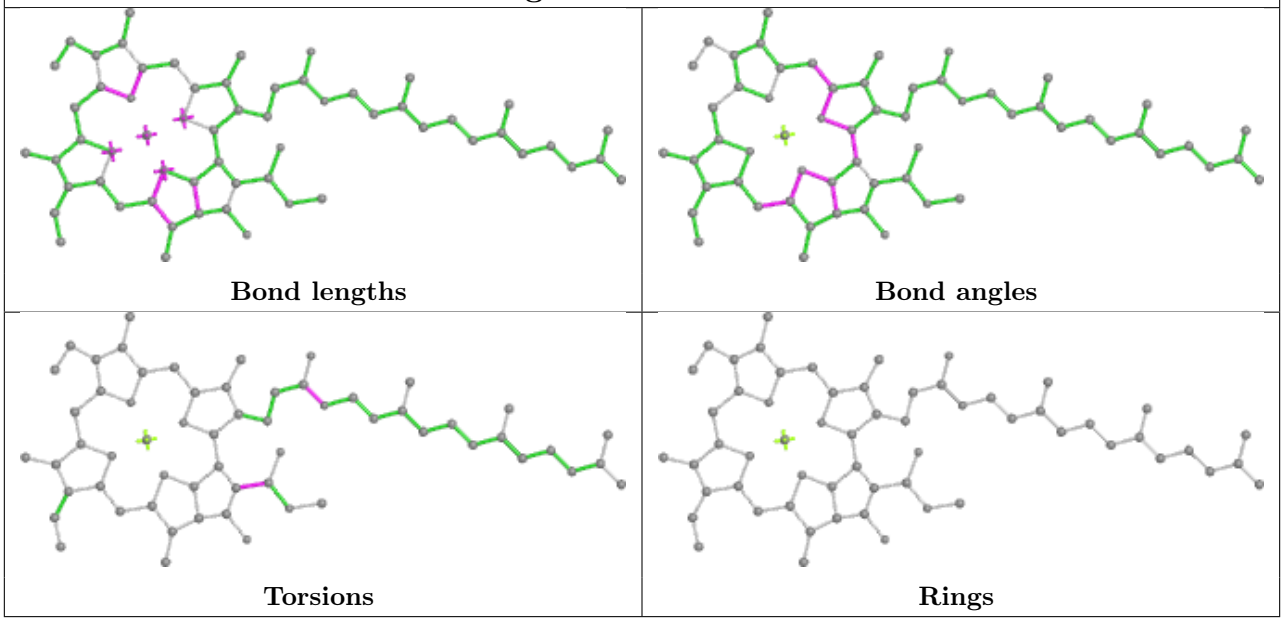


Rings

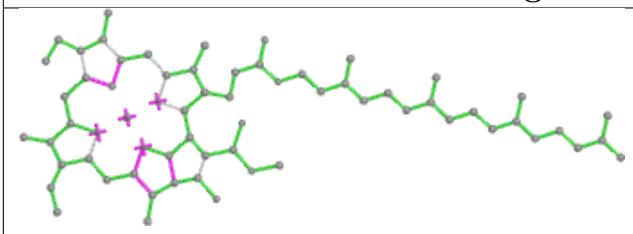
Ligand SQD J 101



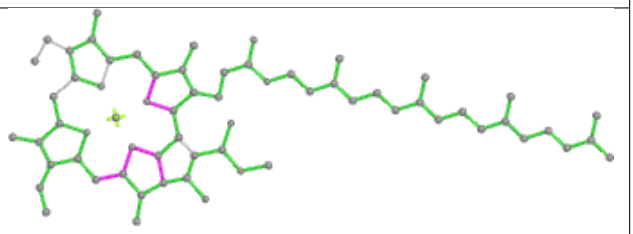
Ligand CLA B 617



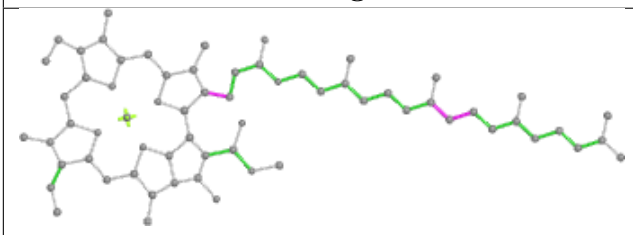
Ligand CLA C 509



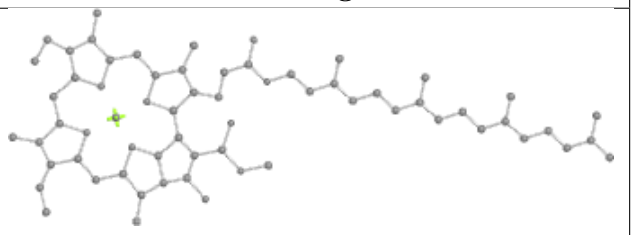
Bond lengths



Bond angles

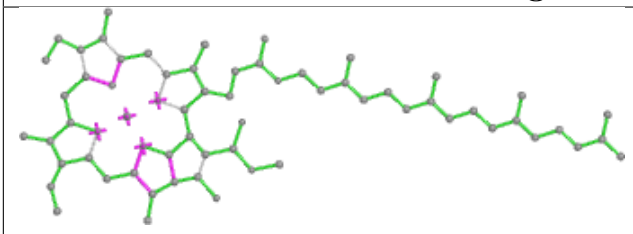


Torsions

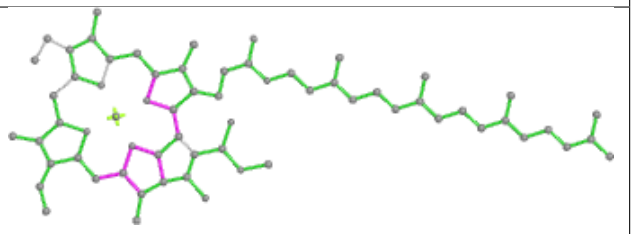


Rings

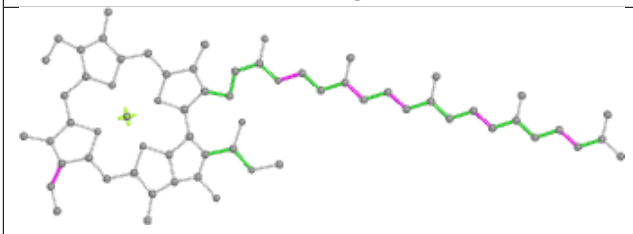
Ligand CLA n 302



Bond lengths



Bond angles



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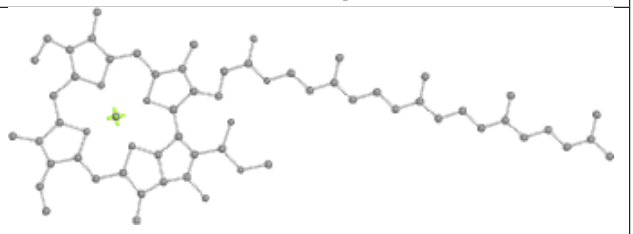
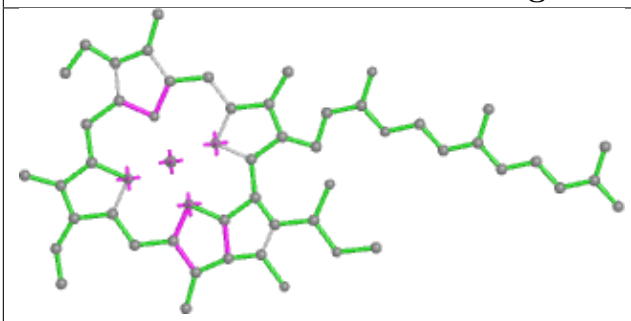
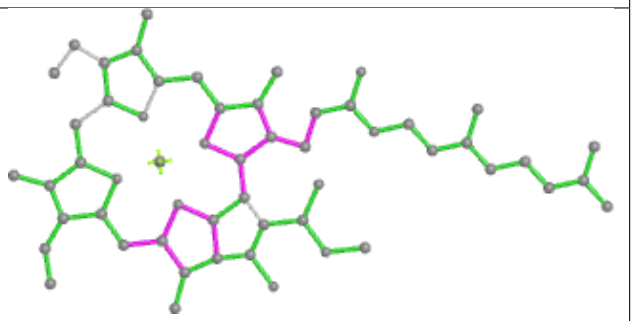


Rings

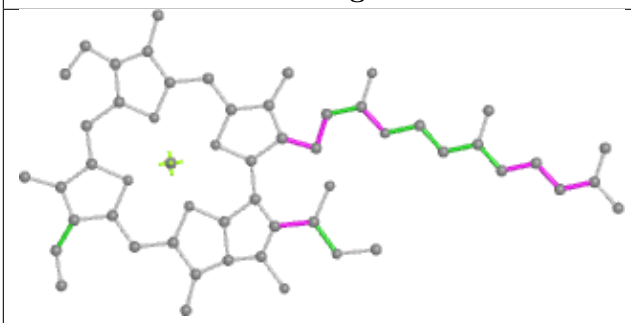
Ligand CLA 8 302



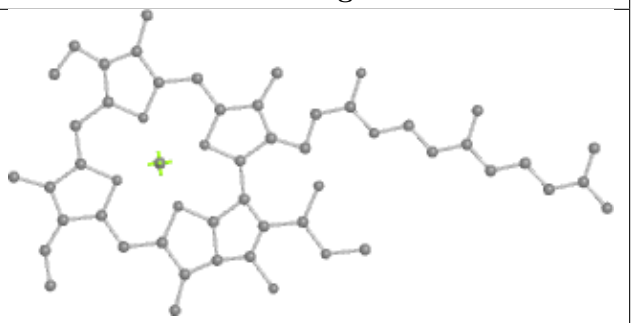
Bond lengths



Bond angles

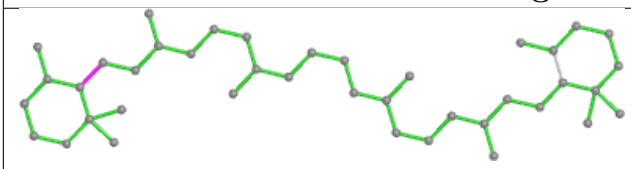


Torsions

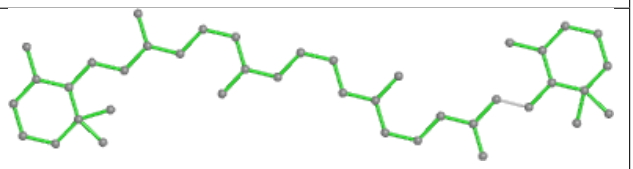


Rings

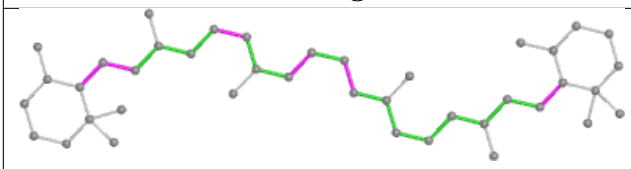
Ligand 8CT c 515



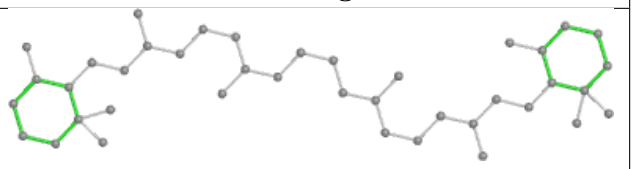
Bond lengths



Bond angles

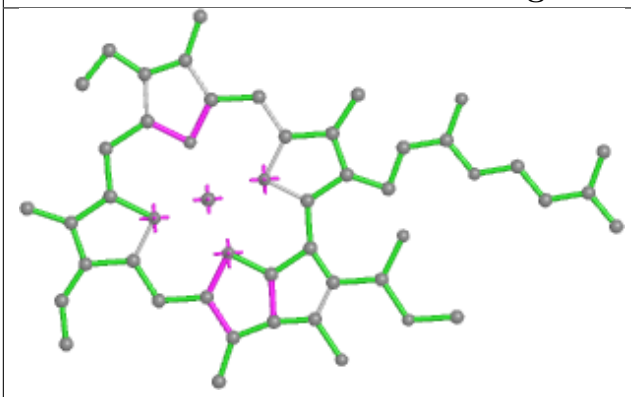


Torsions



Rings

Ligand CLA n 306



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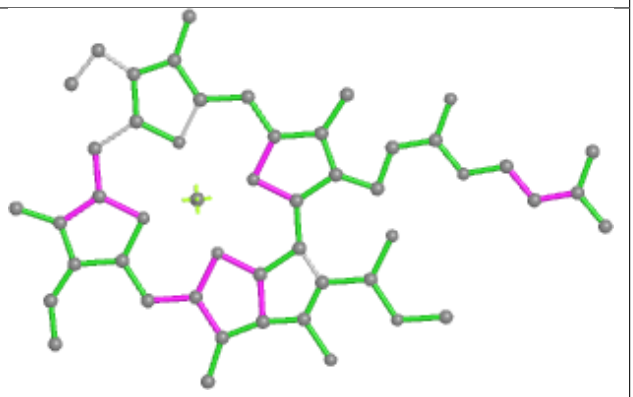
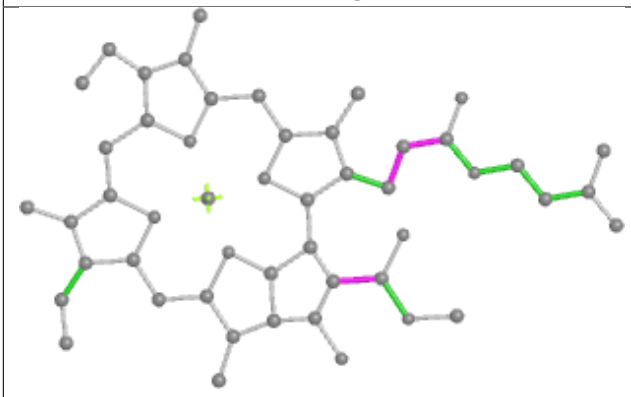


Bond angles



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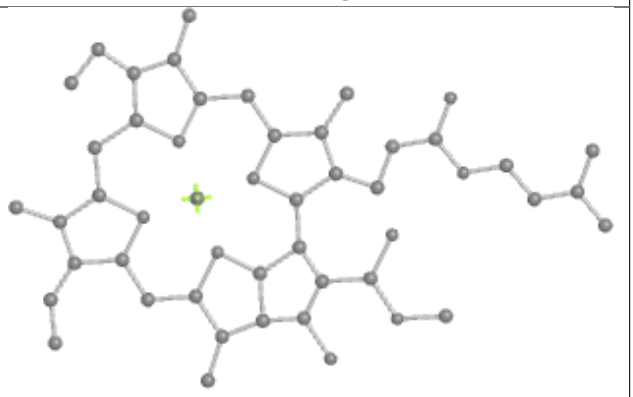
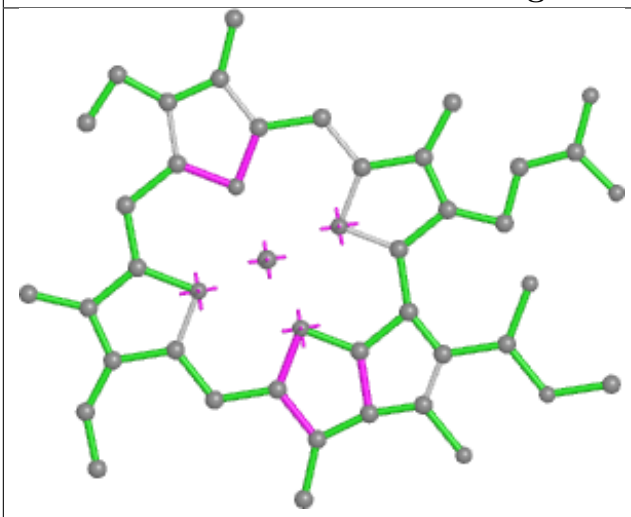


Rings

Ligand CLA p 306



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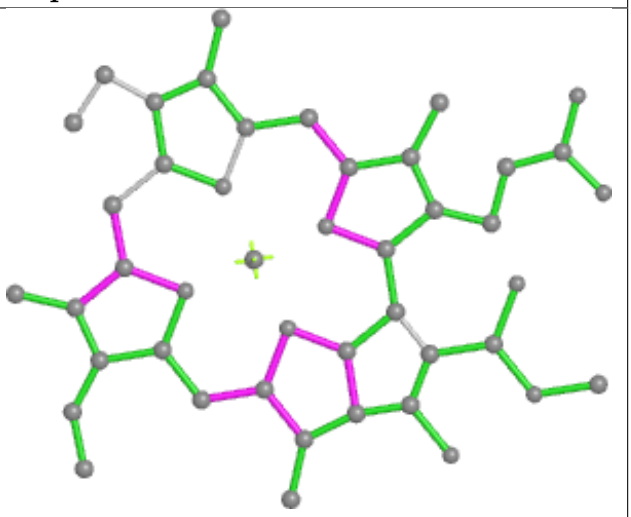

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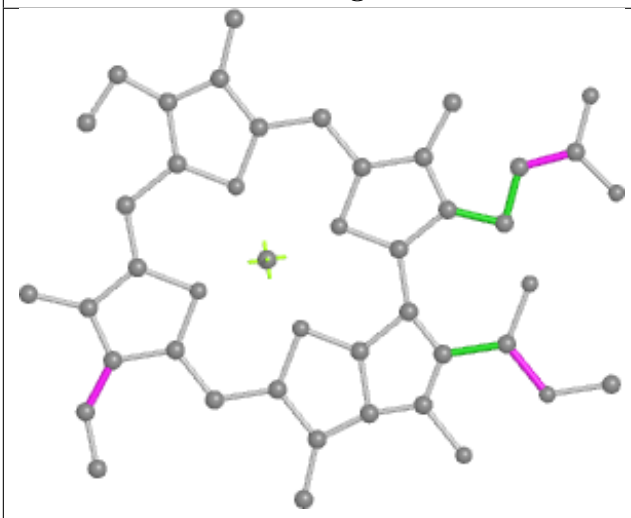
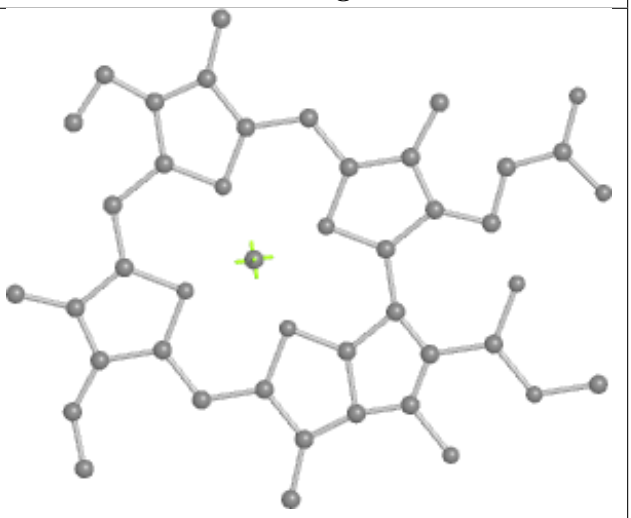
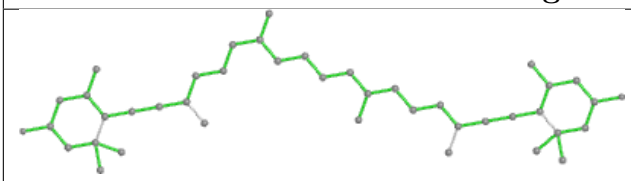


Torsions

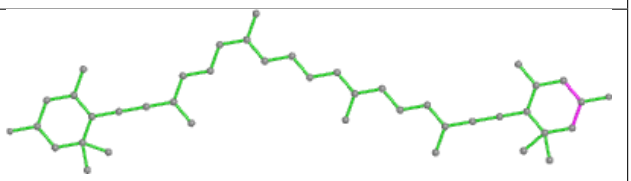


Rings

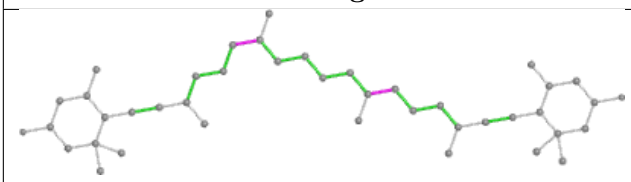
Ligand II0 3 316



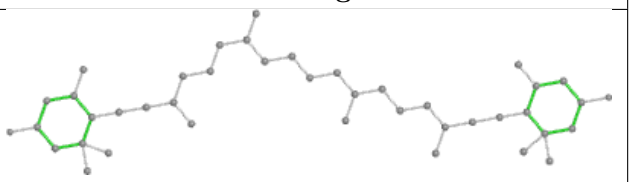
Bond lengths



Bond angles

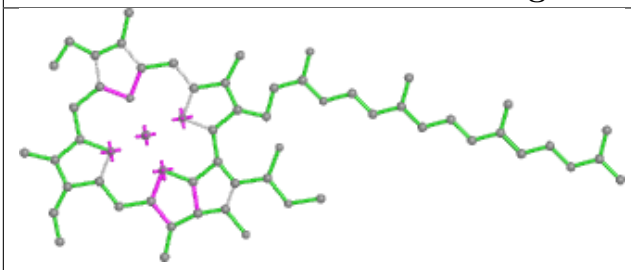


Torsions

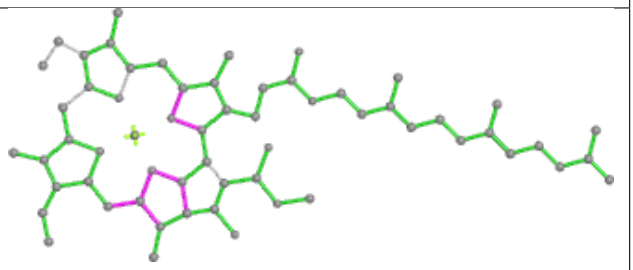


Rings

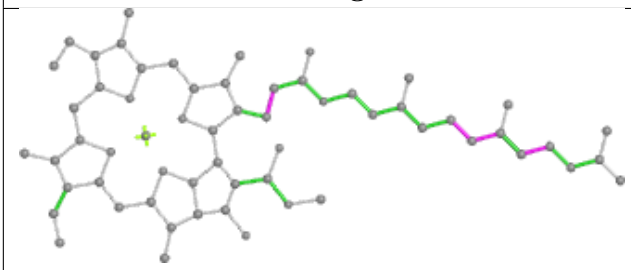
Ligand CLA 2 304



Bond lengths



Bond angles



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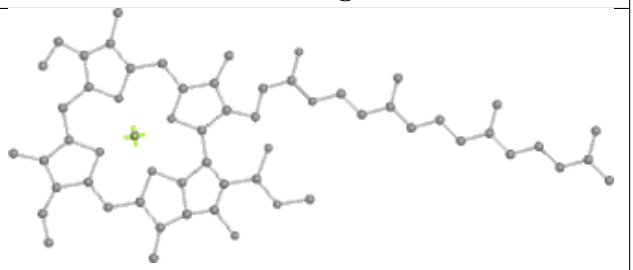
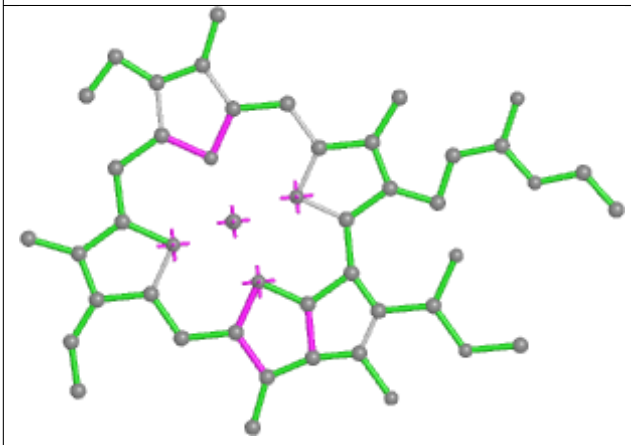


Rings

Ligand CLA 4 304



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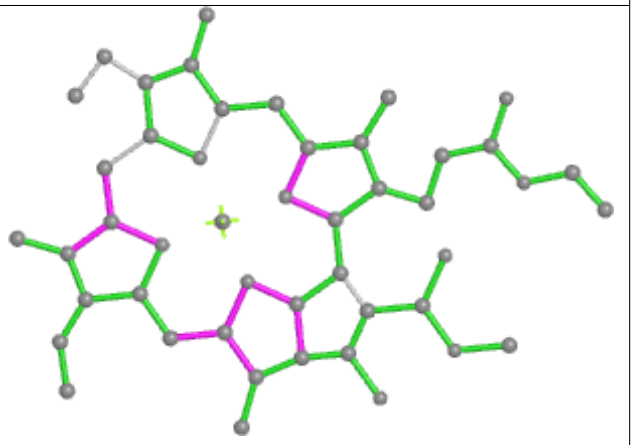
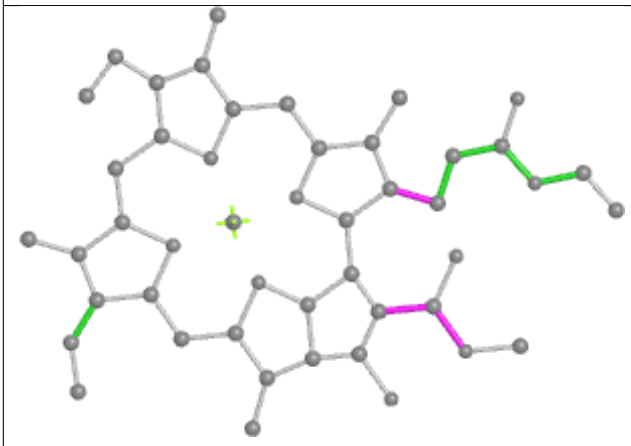
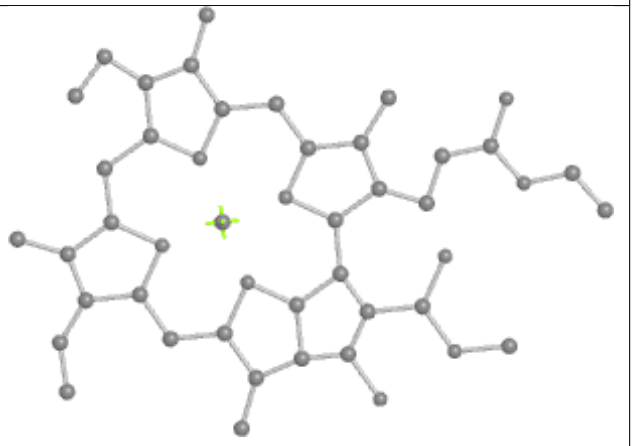


Bond angles

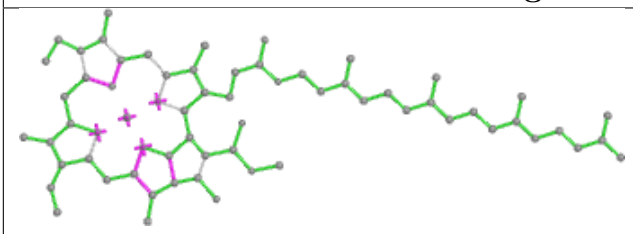


Torsions

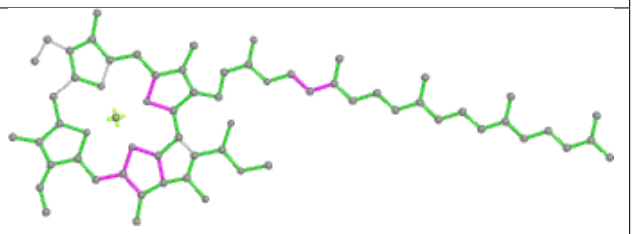


Rings

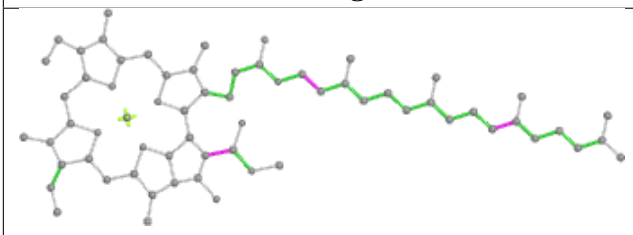
Ligand CLA B 603



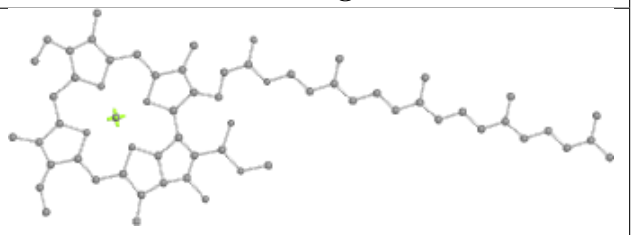
Bond lengths



Bond angles

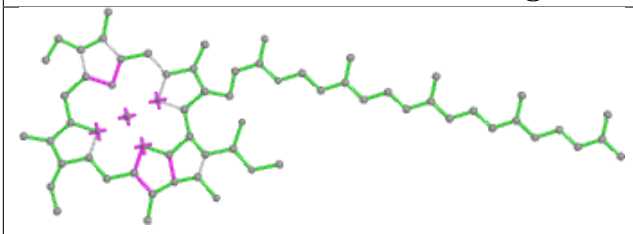


Torsions

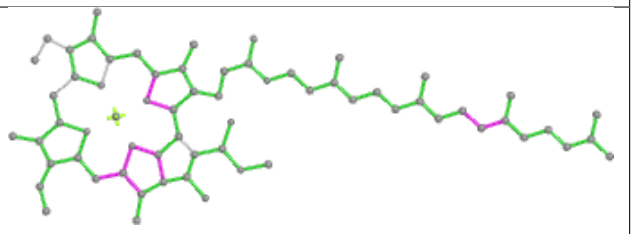


Rings

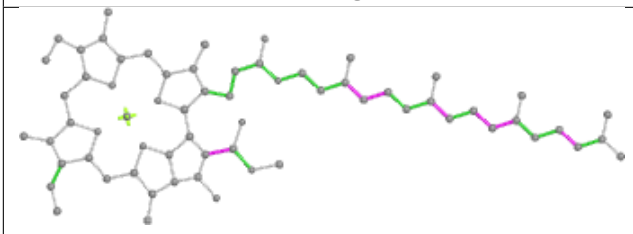
Ligand CLA C 505



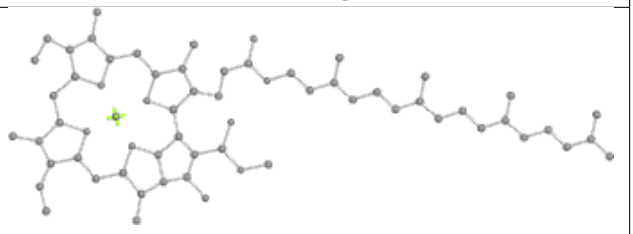
Bond lengths



Bond angles

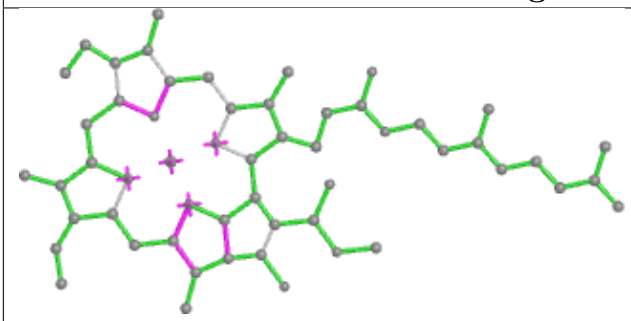


Torsions



Rings

Ligand CLA 1 309



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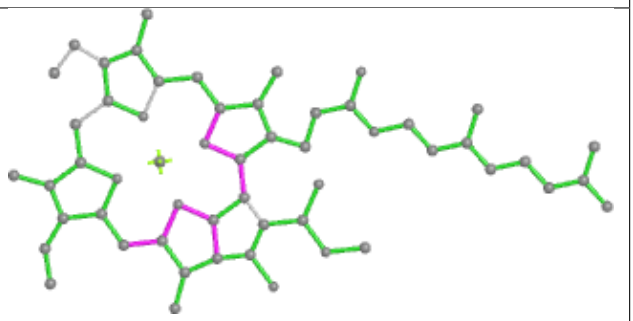
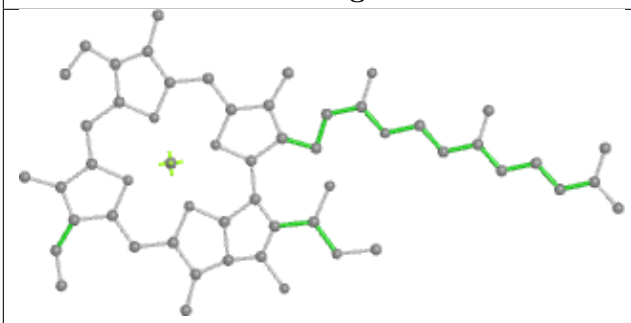


Bond angles



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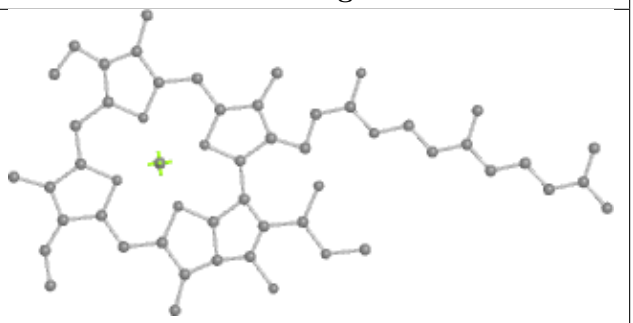
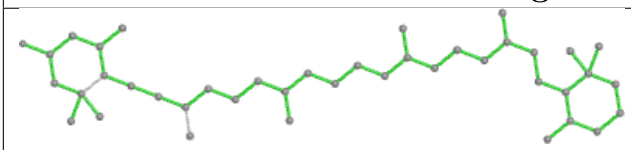
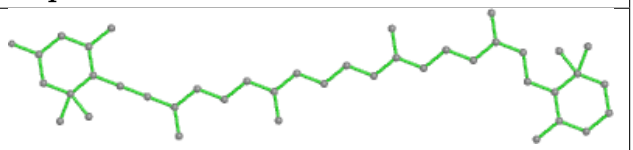


Rings

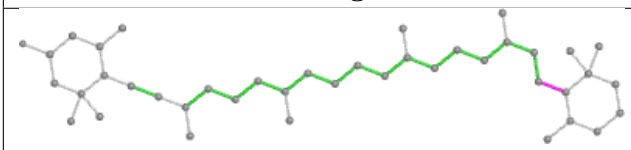
Ligand IHT p 318



Bond lengths



Bond angles



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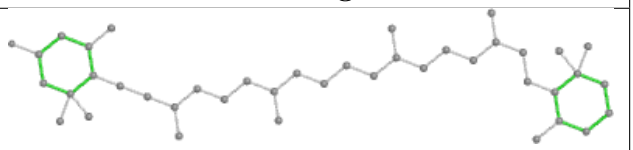
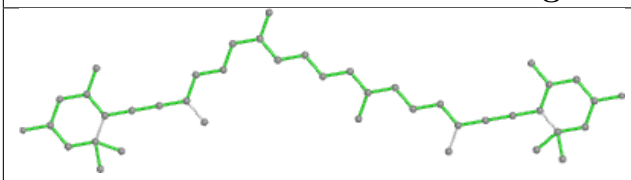


Rings

Ligand II0 8 313



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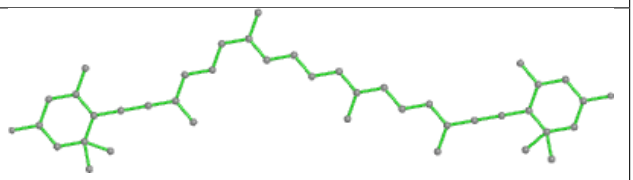
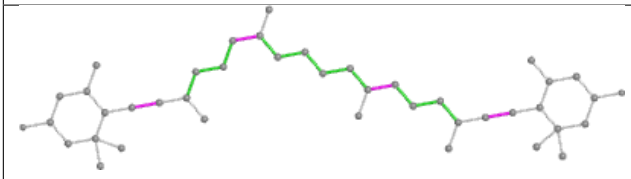


Bond angles



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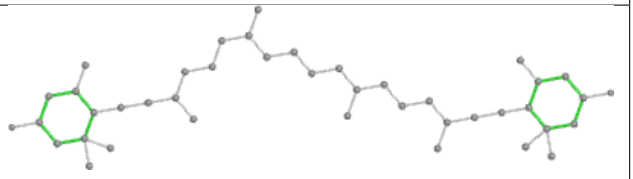
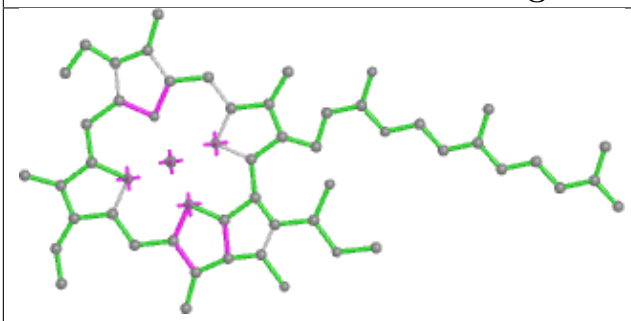


Rings

Ligand CLA g 303



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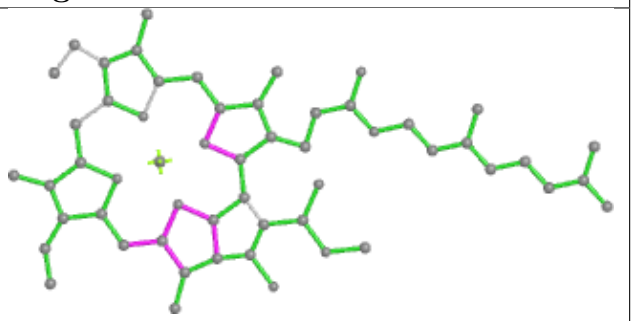
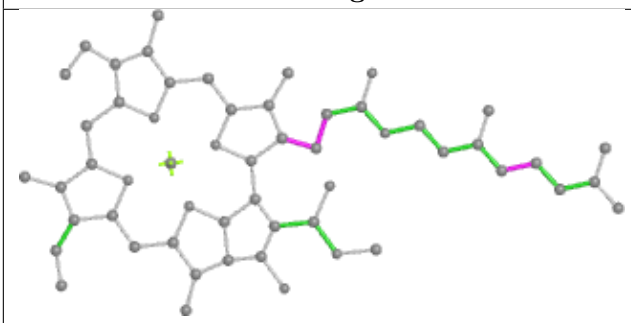


Bond angles



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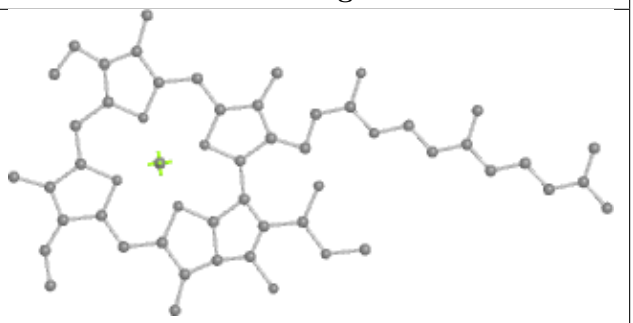
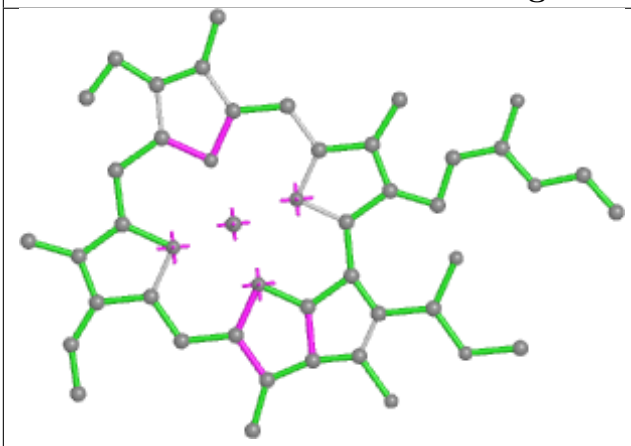


Rings

Ligand CLA 4 308



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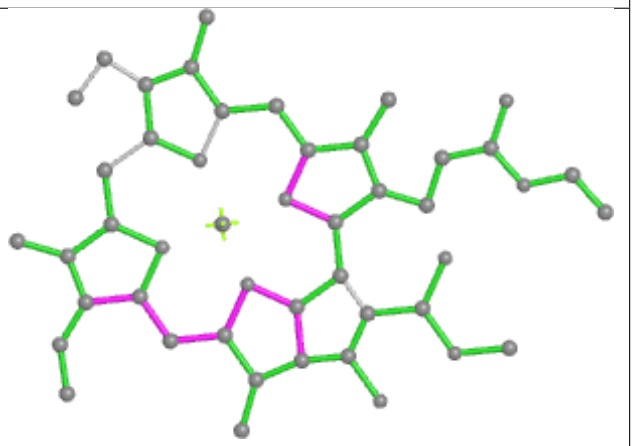

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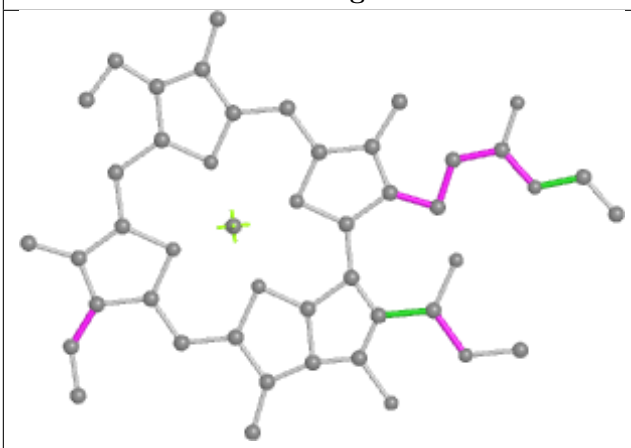

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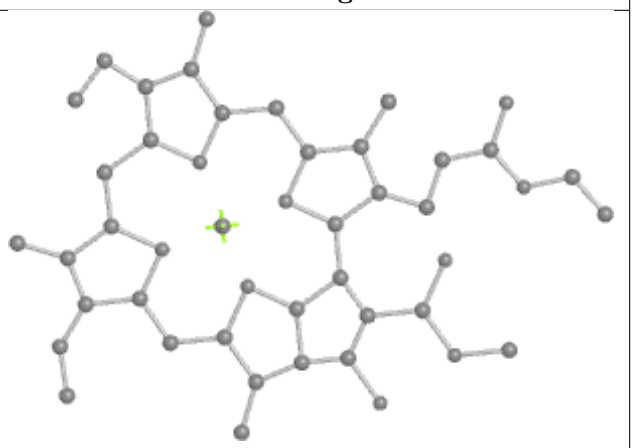
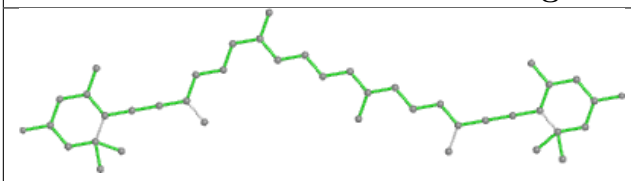
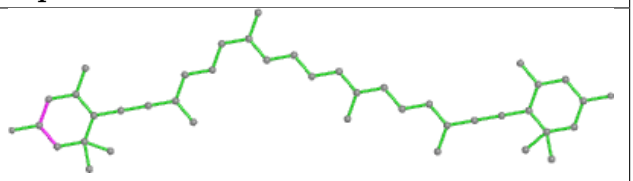
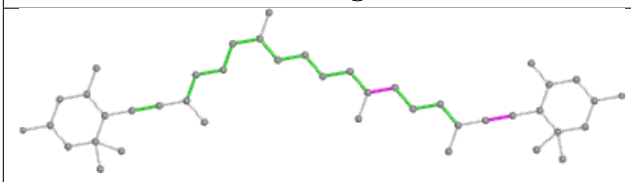
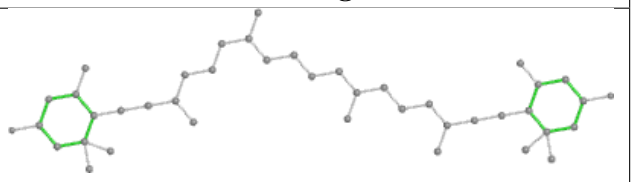
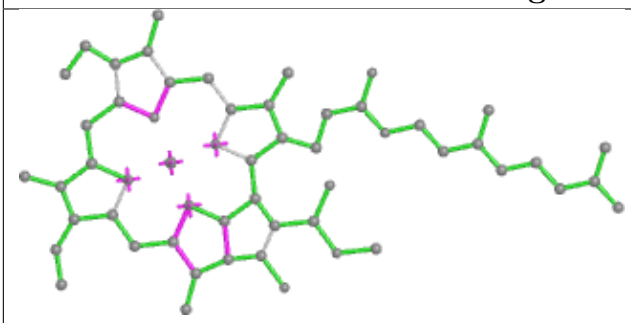
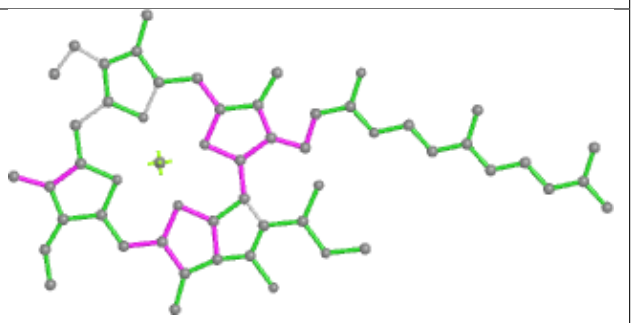
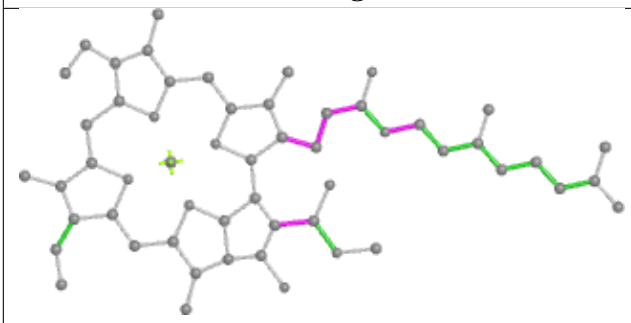
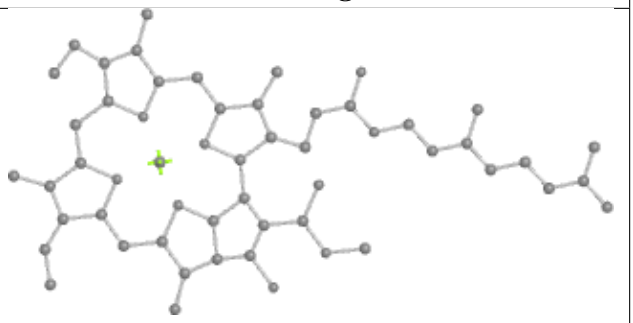
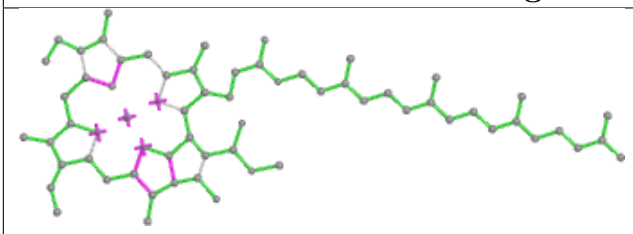


Rings

Ligand II0 p 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 502



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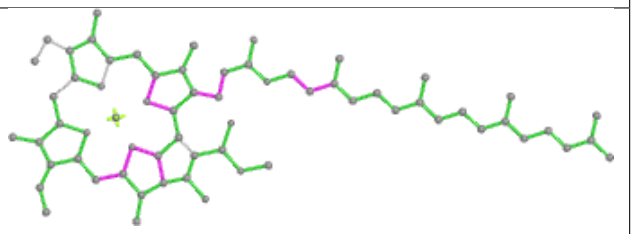
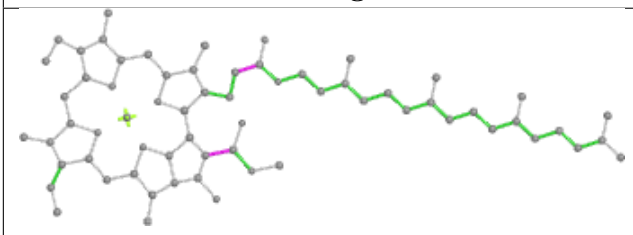


Bond angles



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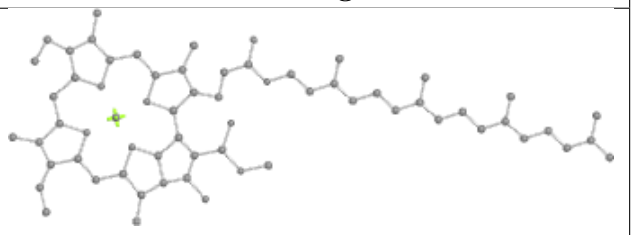

Rings

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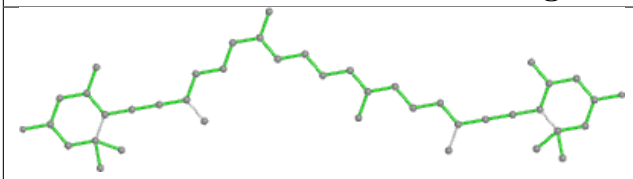

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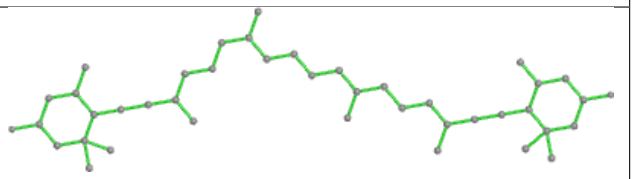

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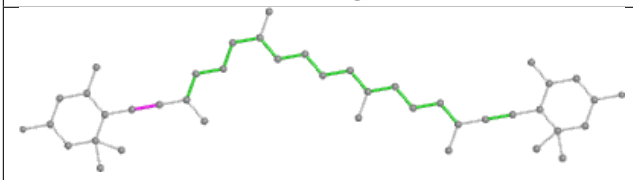

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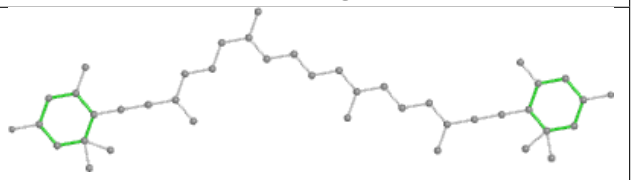

Rings

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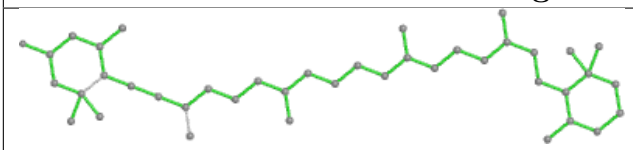

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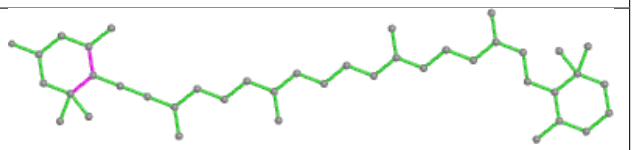

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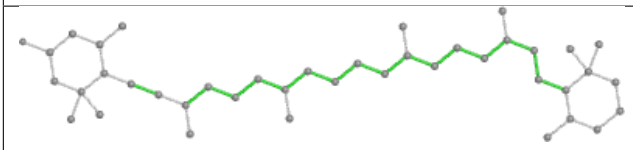

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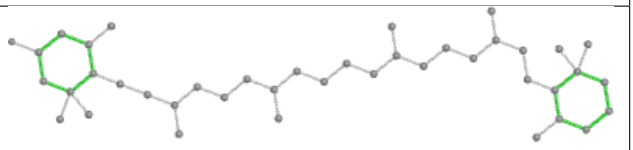
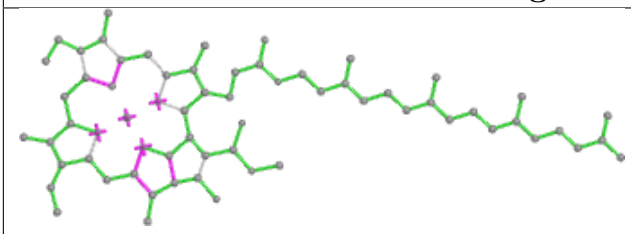


Rings

Ligand CLA c 505



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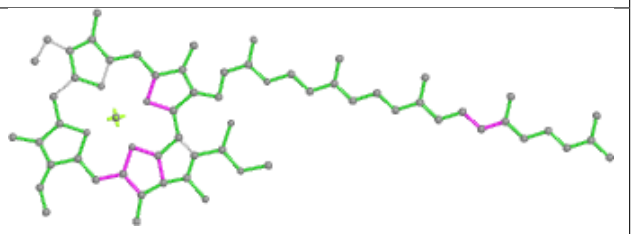

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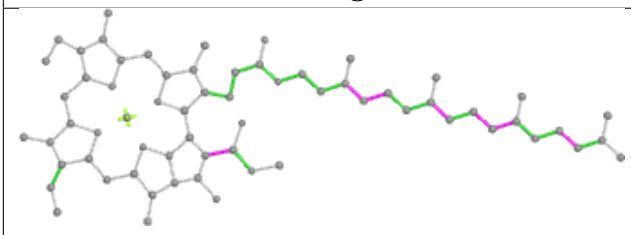

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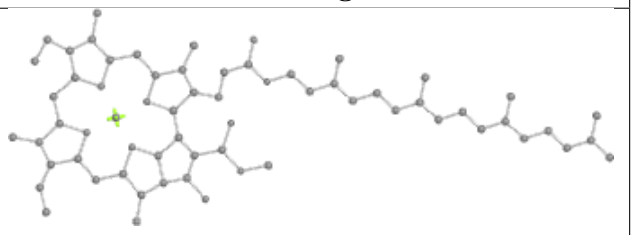
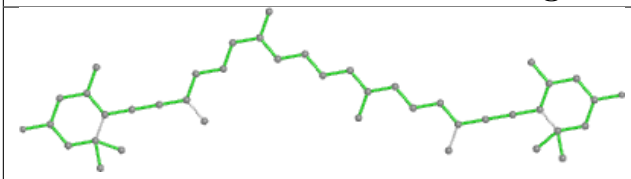


Rings

Ligand II0 4 315



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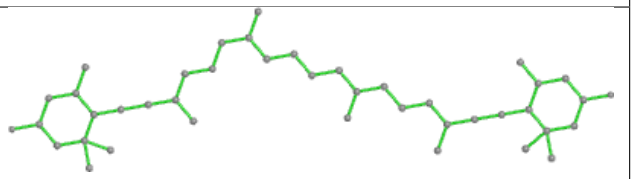

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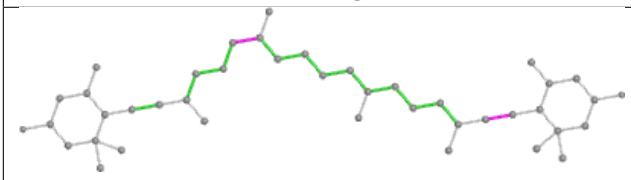

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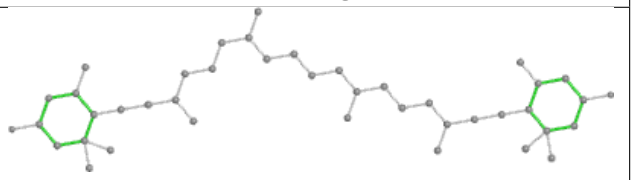

Rings

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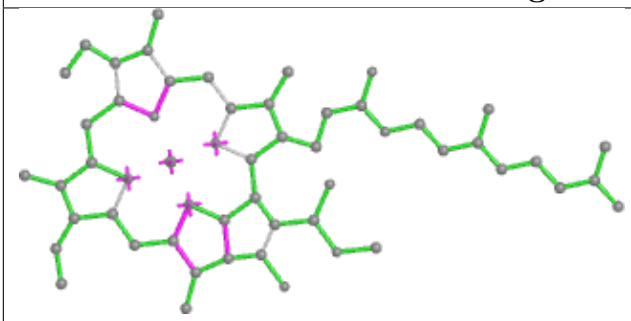

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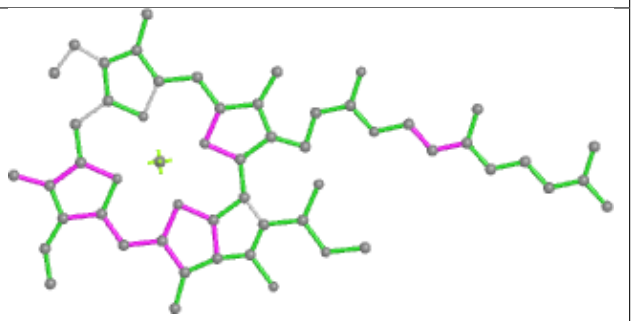

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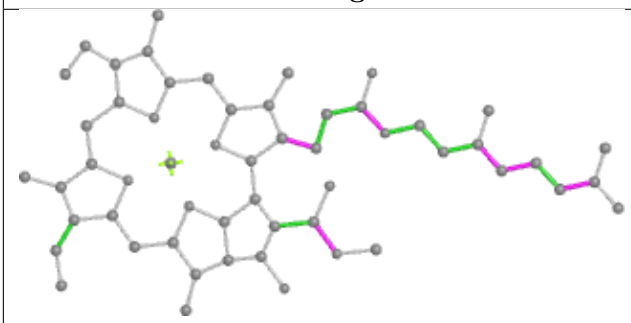

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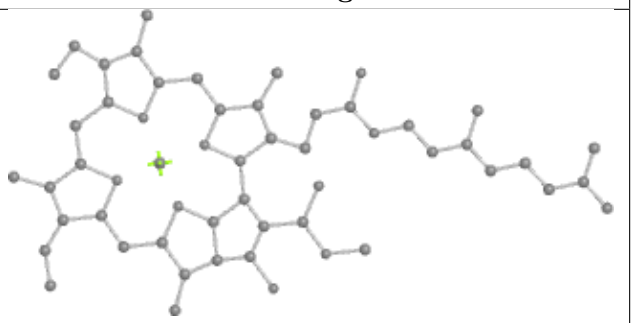

Rings

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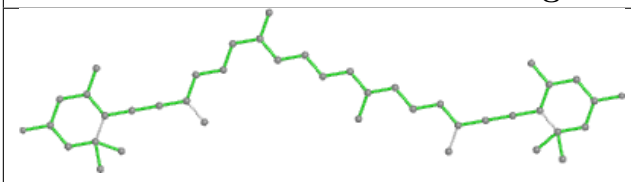

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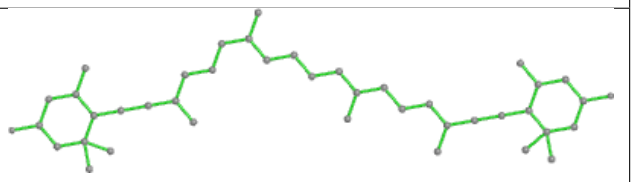

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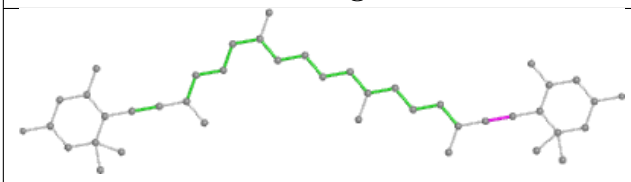

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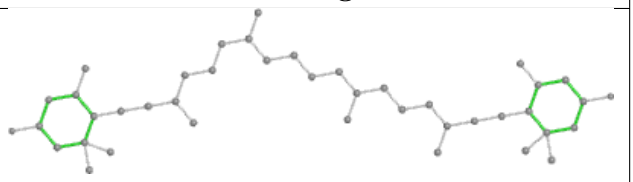
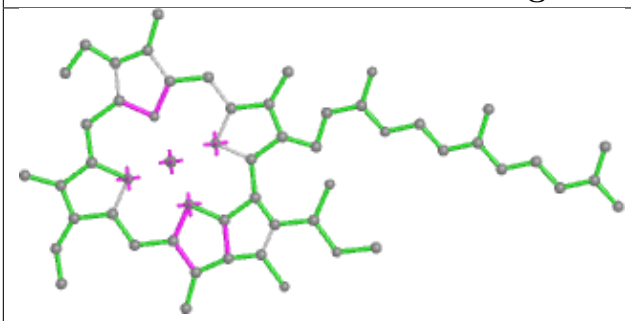


Rings

Ligand CLA 2 305



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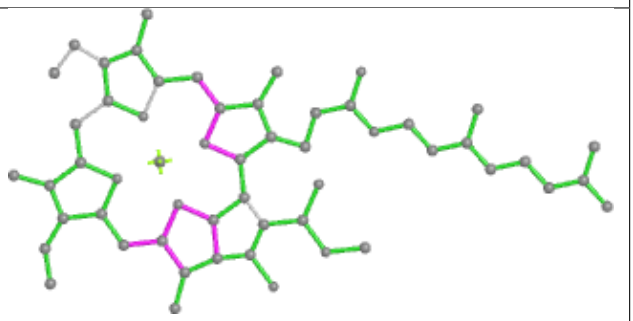

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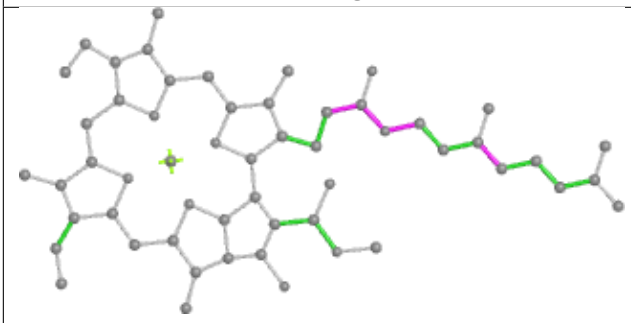

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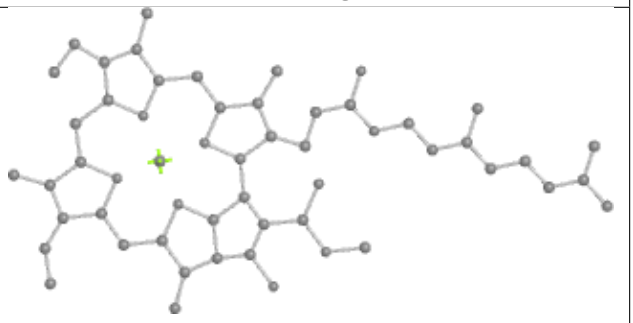
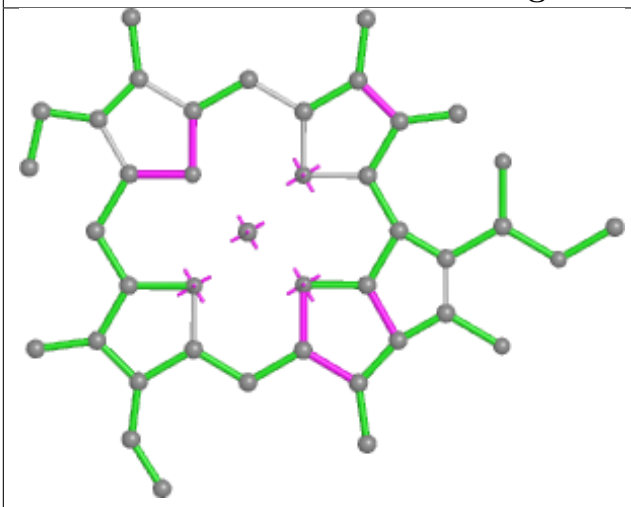


Rings

Ligand CLA 6 312



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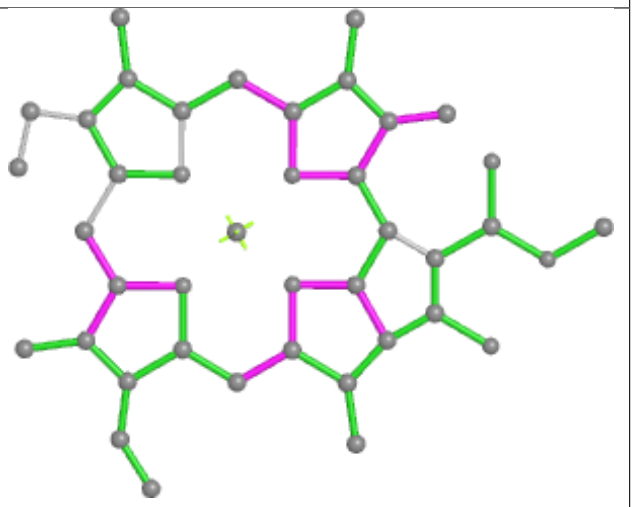
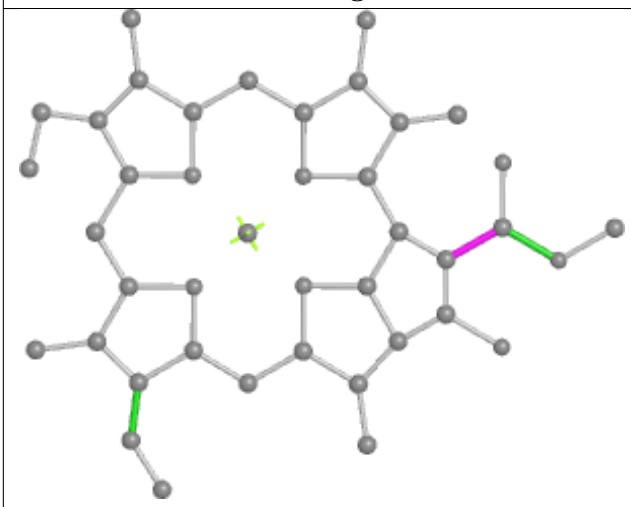


Bond angles



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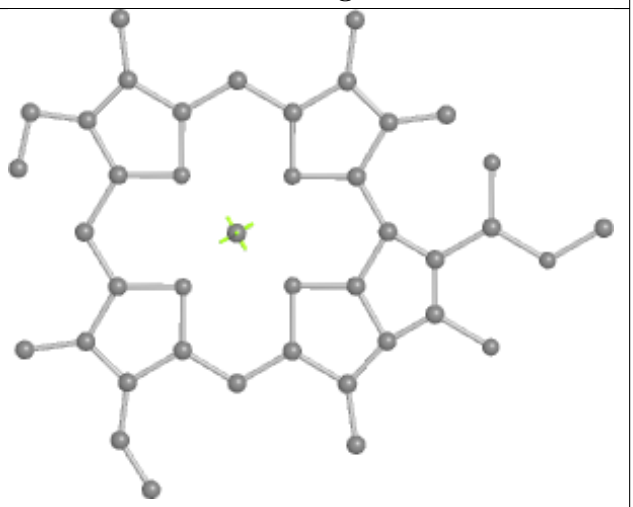
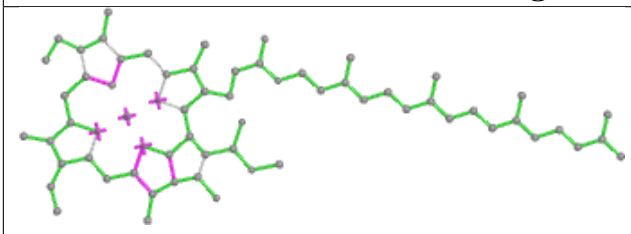


Rings

Ligand CLA c 506



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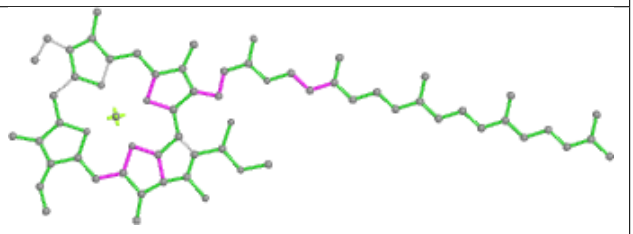
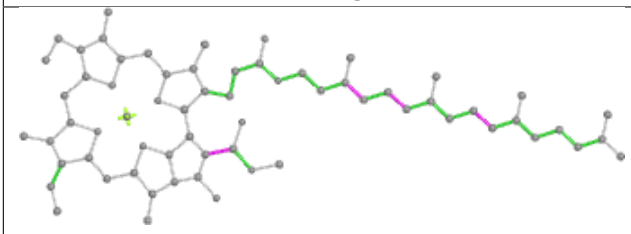


Bond angles



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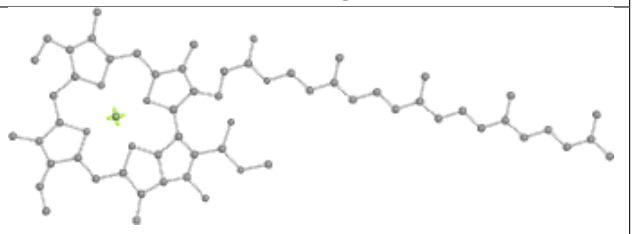
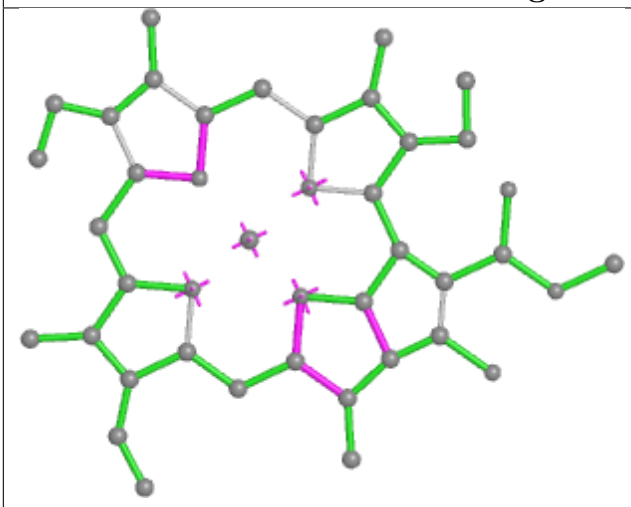


Rings

Ligand CLA 6 308



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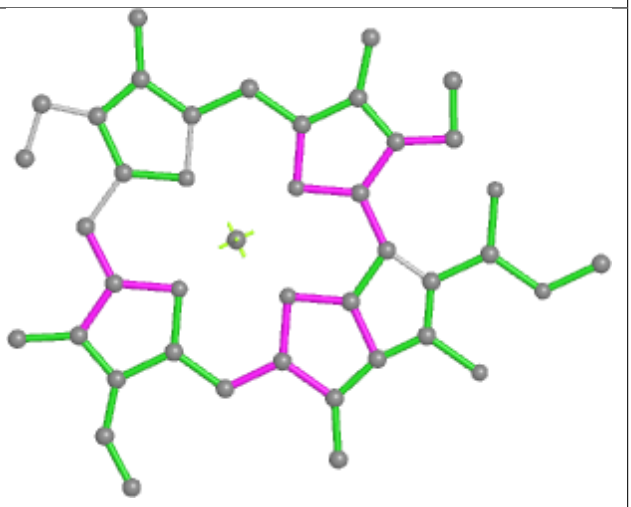

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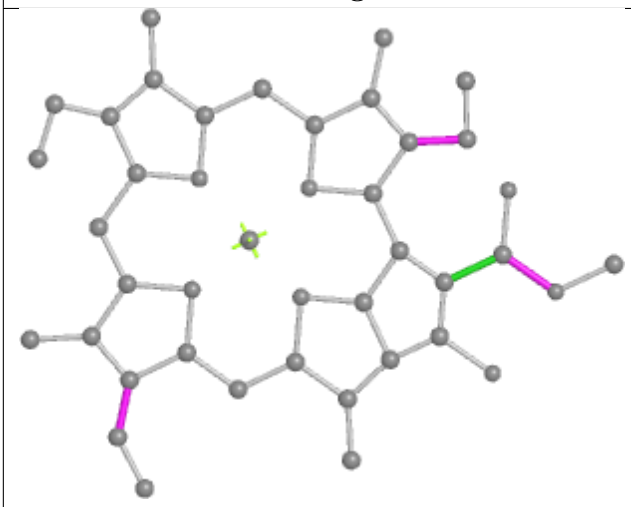

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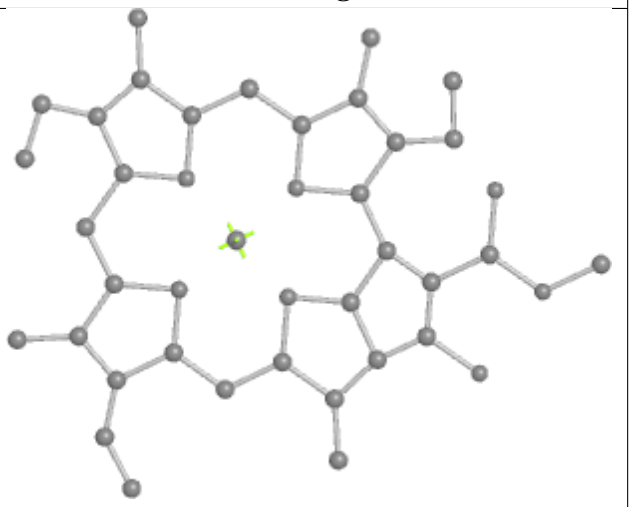
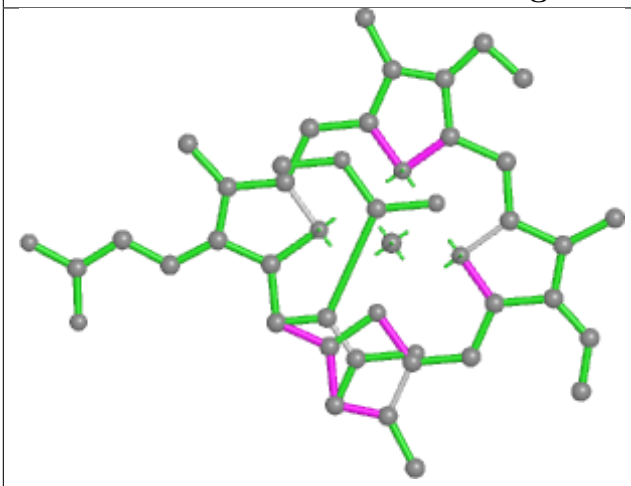


Rings

Ligand KC2 0 305



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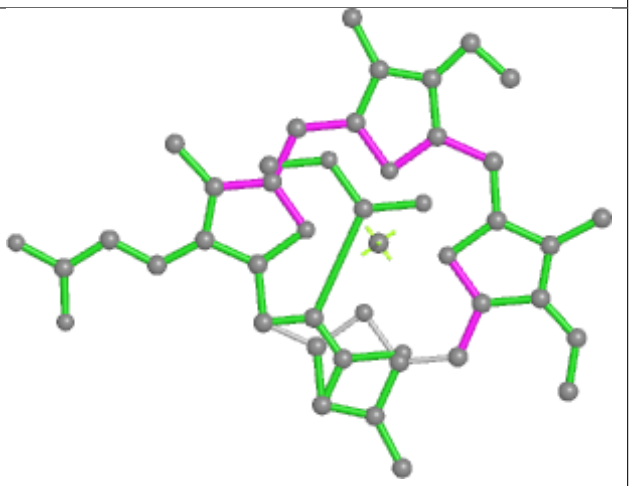

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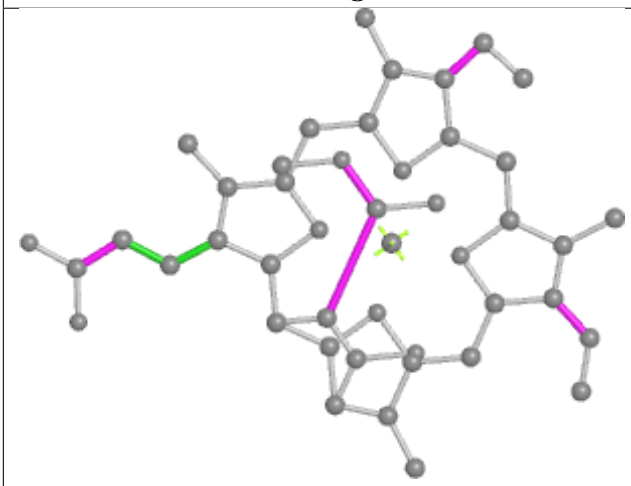

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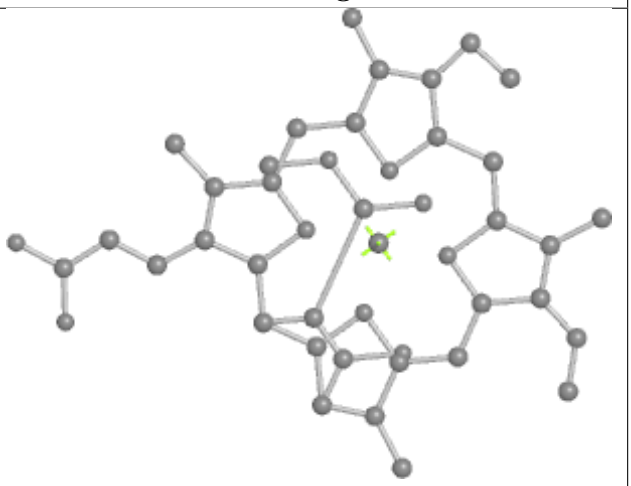
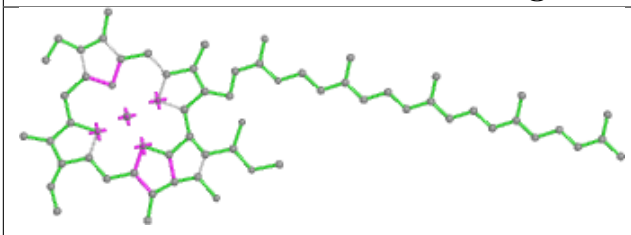


Rings

Ligand CLA a 412



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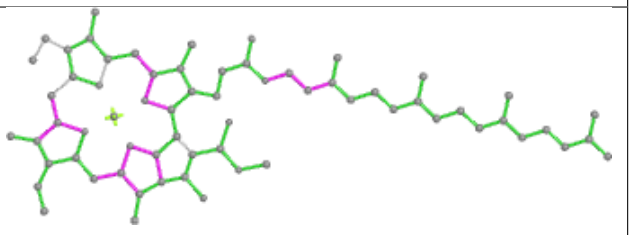

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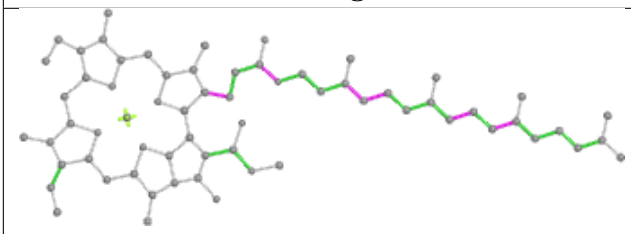

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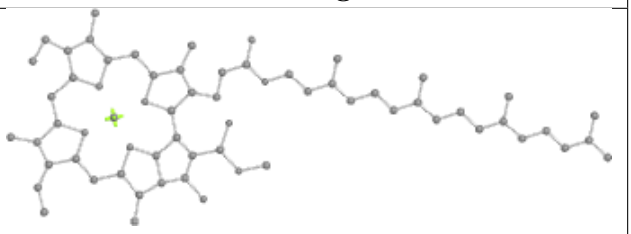
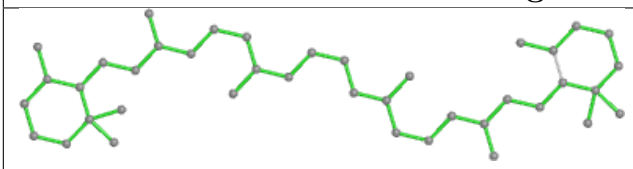


Rings

Ligand 8CT A 409



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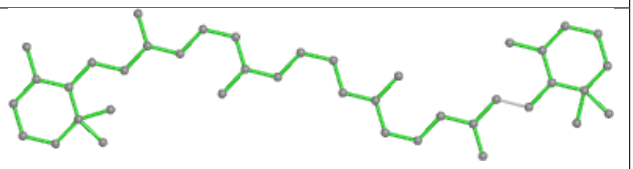

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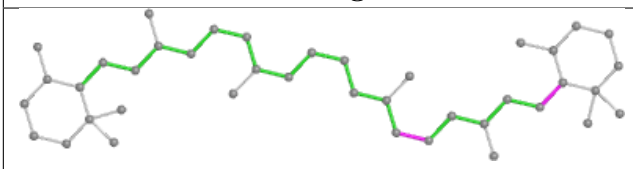

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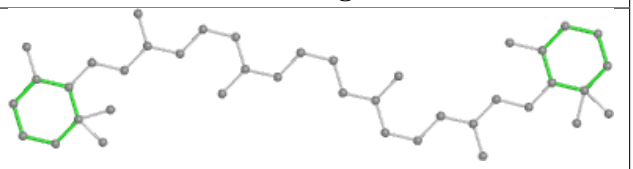
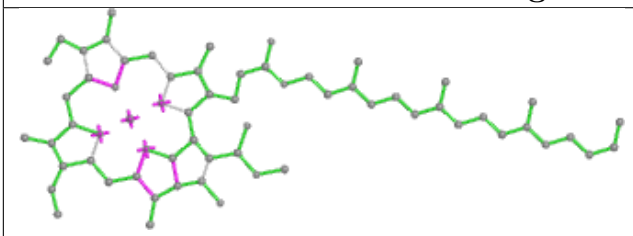


Rings

Ligand CLA 1 302



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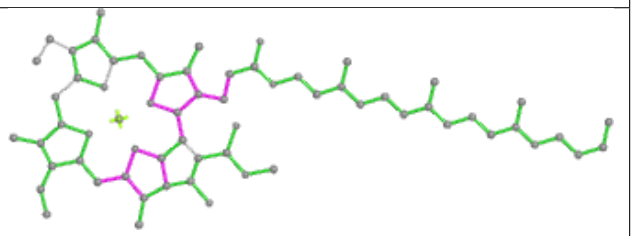
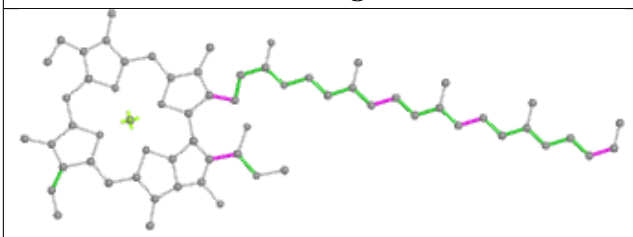
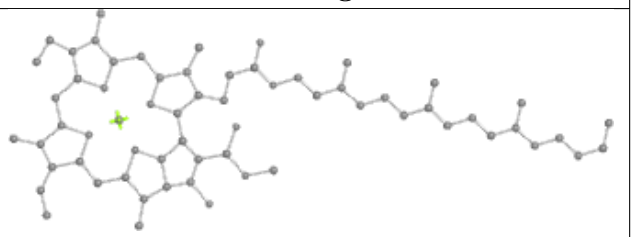


Bond angles

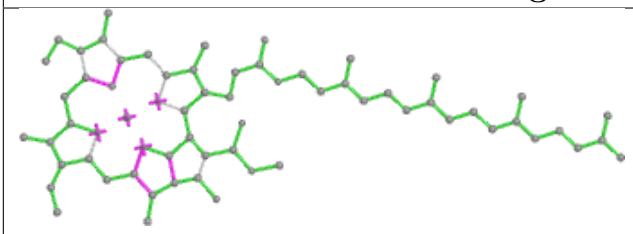


Torsions

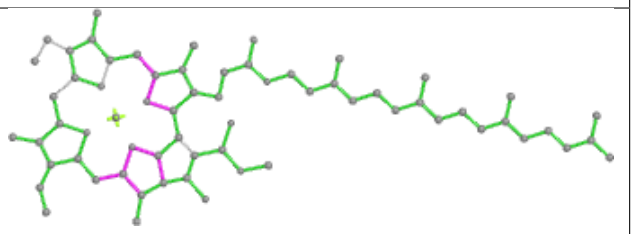


Rings

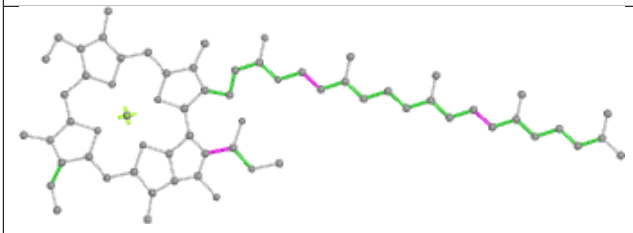
Ligand CLA c 510



Bond lengths



Bond angles



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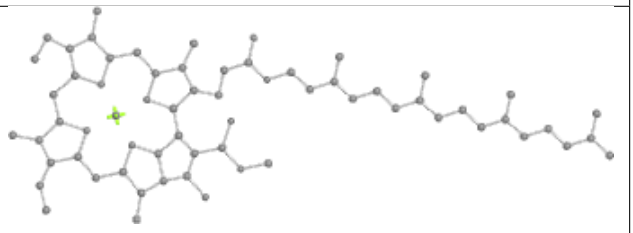
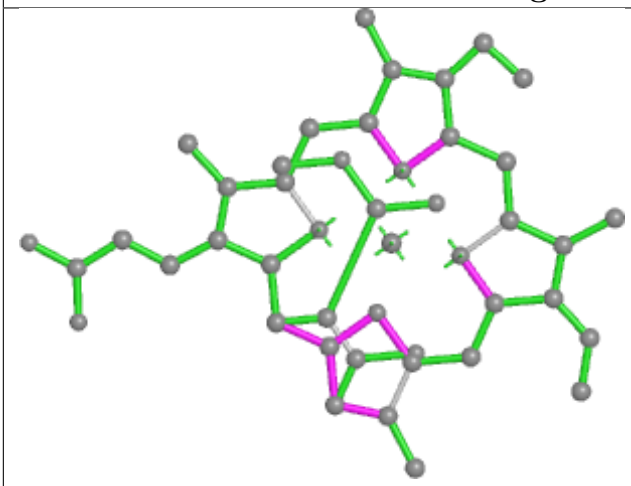


Rings

Ligand KC2 2 309



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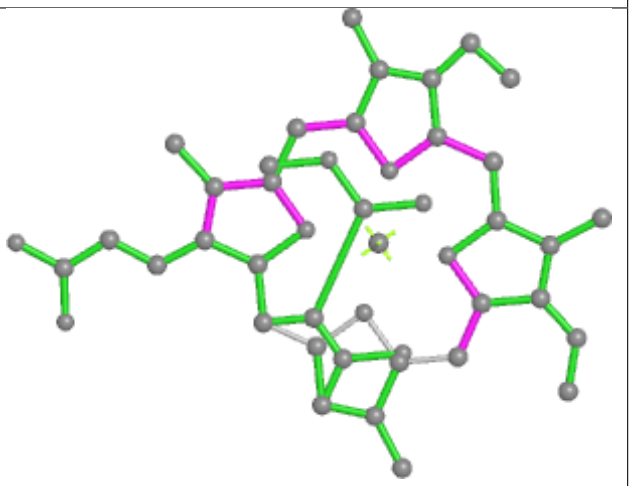
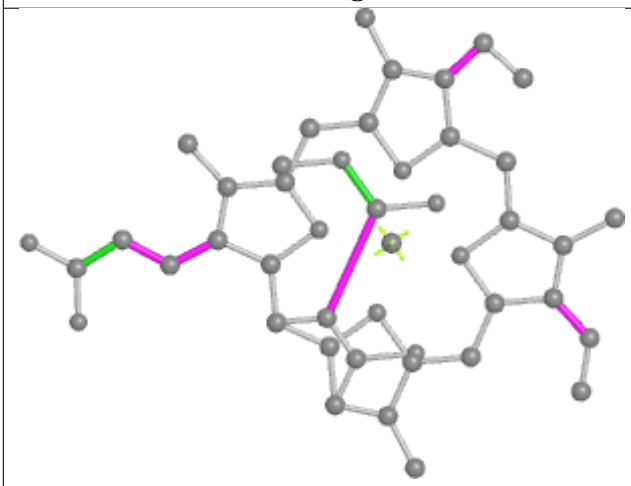


Bond angles



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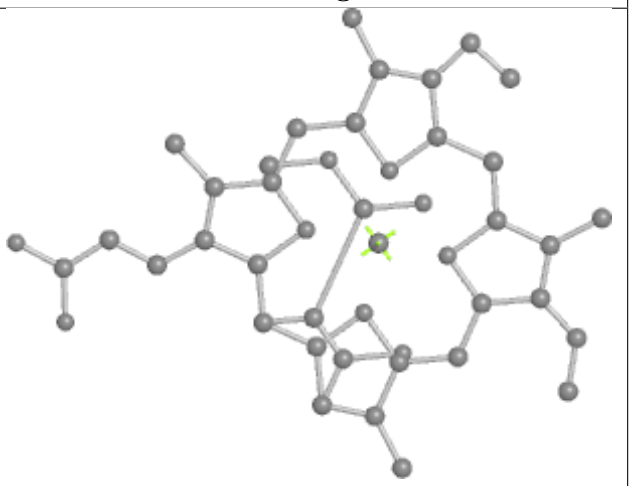
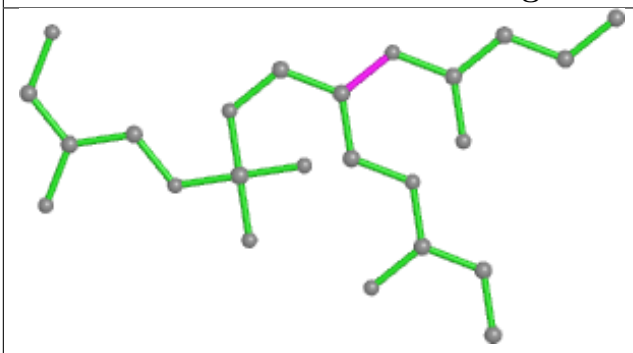


Rings

Ligand LHG A 411



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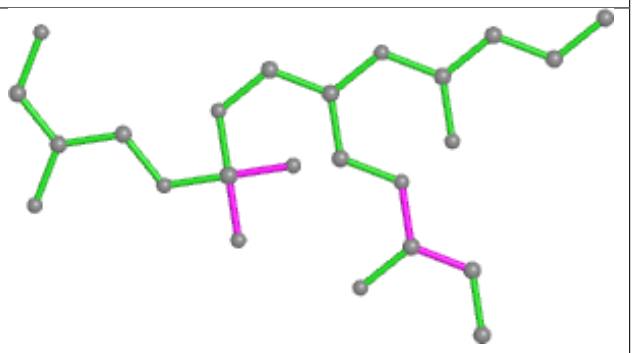
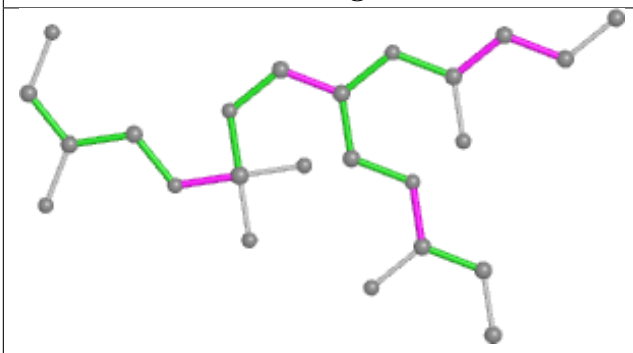


Bond angles



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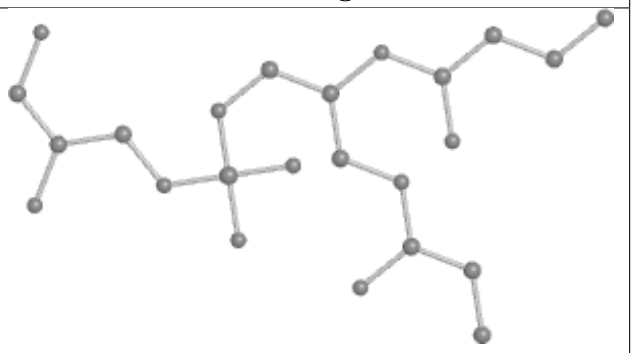
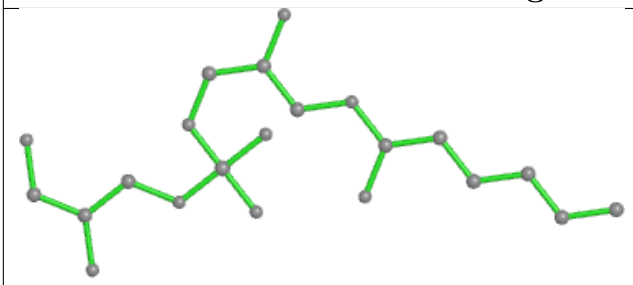


Rings

Ligand LHG g 316



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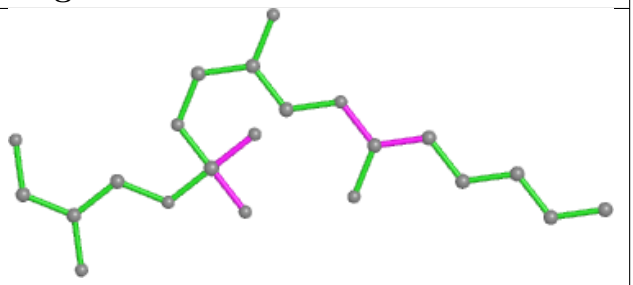
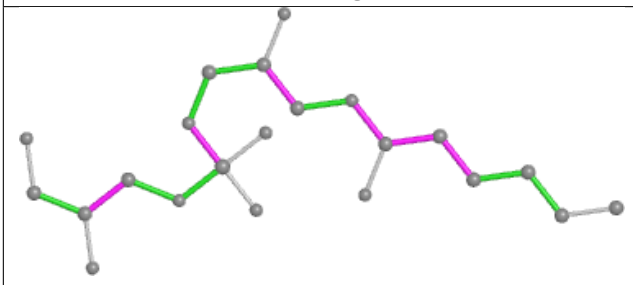


Bond angles



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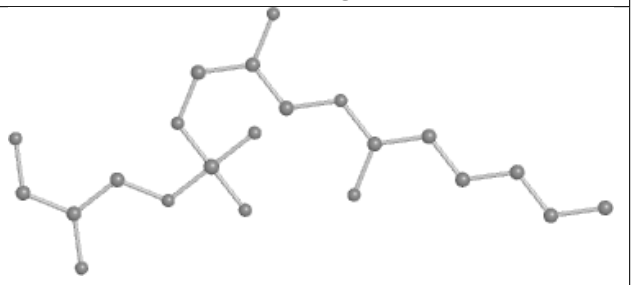
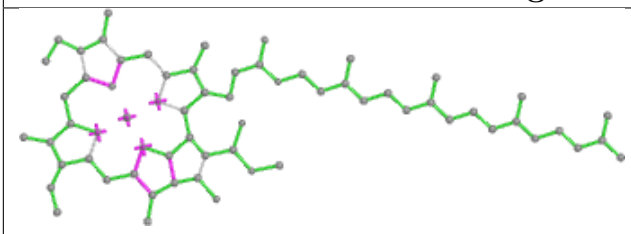


Rings

Ligand CLA b 609



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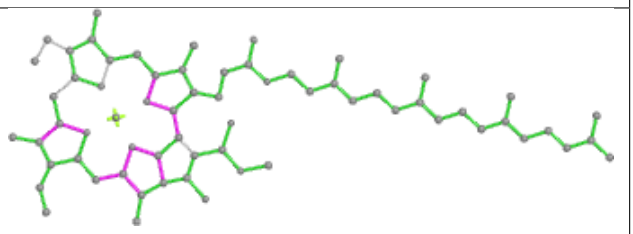

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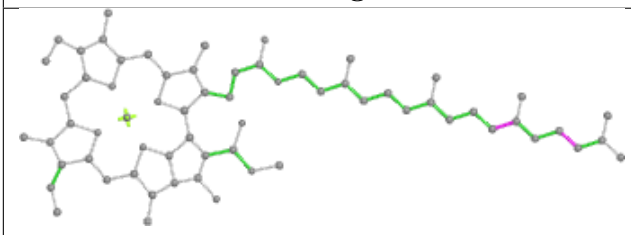

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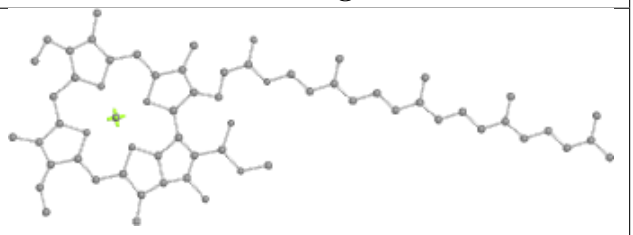
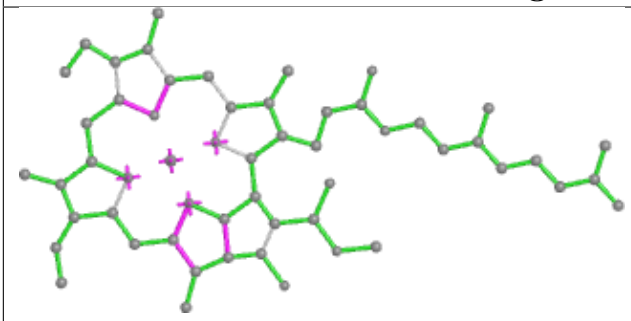


Rings

Ligand CLA 9 312



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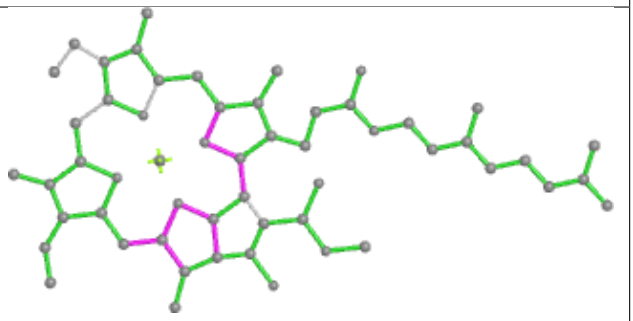
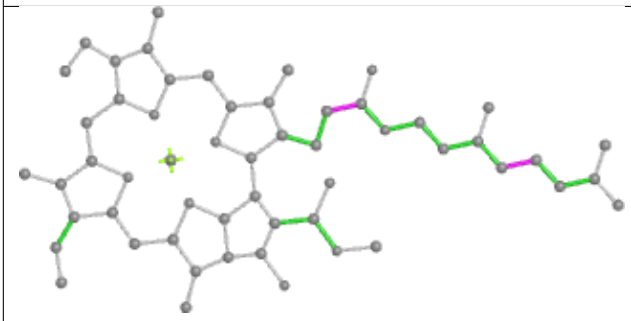


Bond angles



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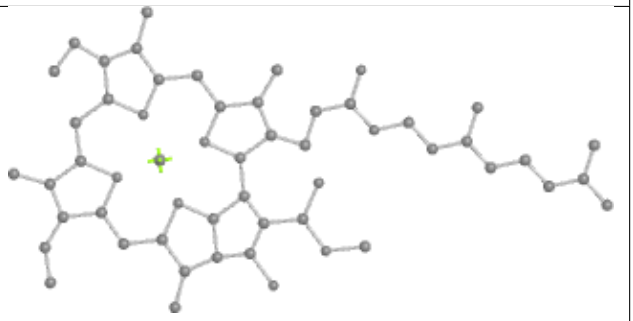
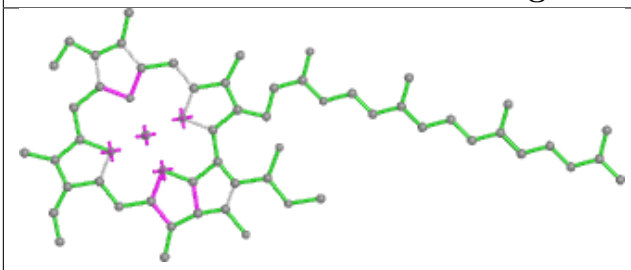


Rings

Ligand CLA 2 306



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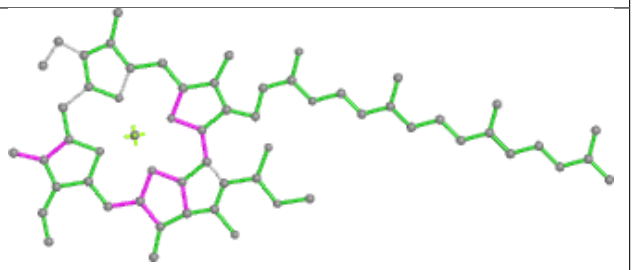

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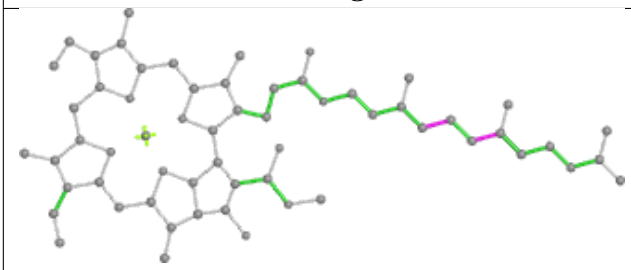

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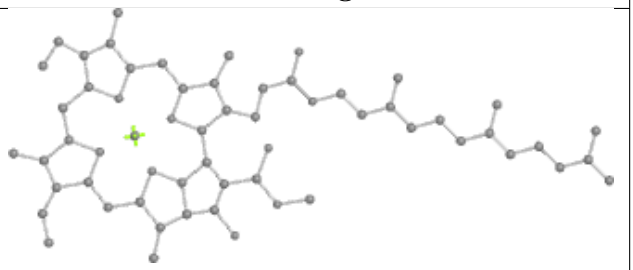
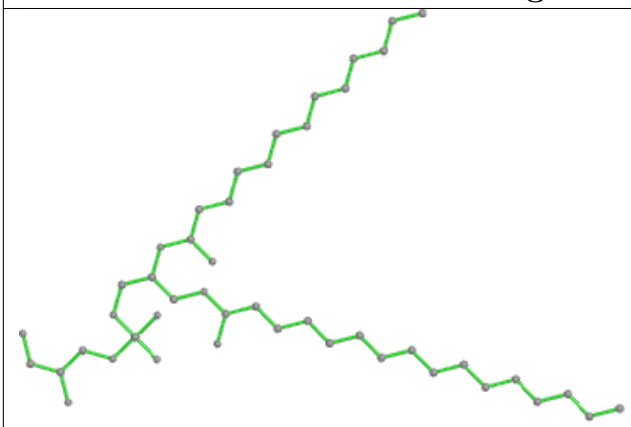


Rings

Ligand LHG 2 315



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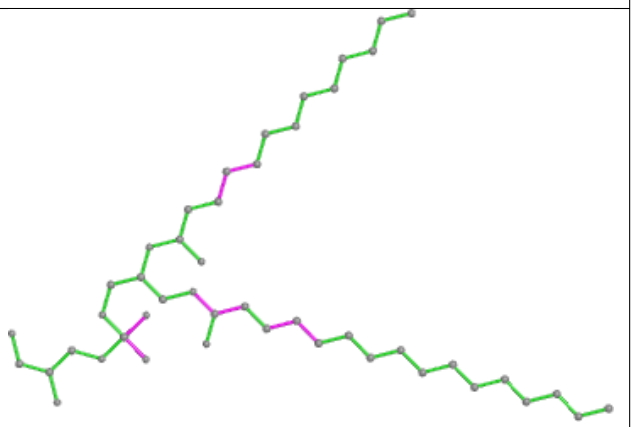
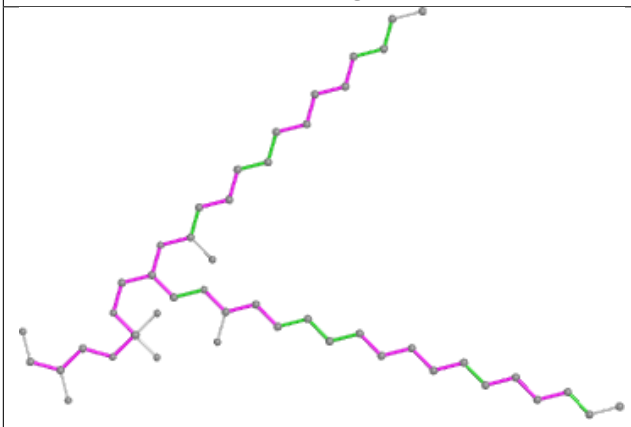


Bond angles



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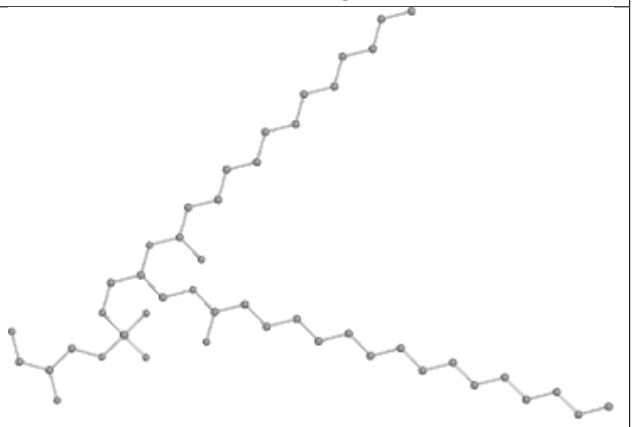
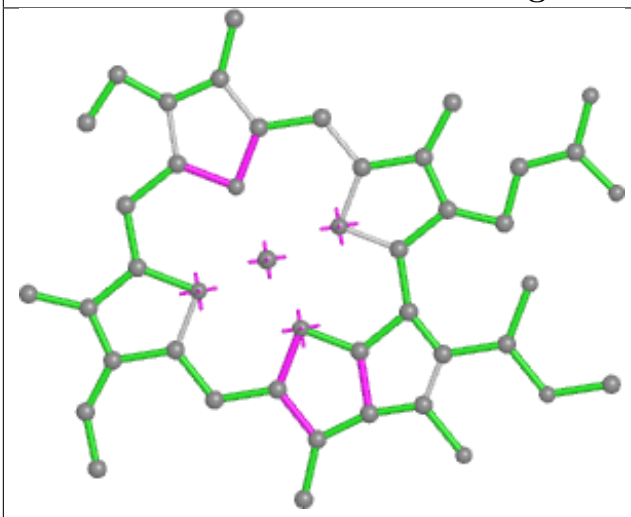
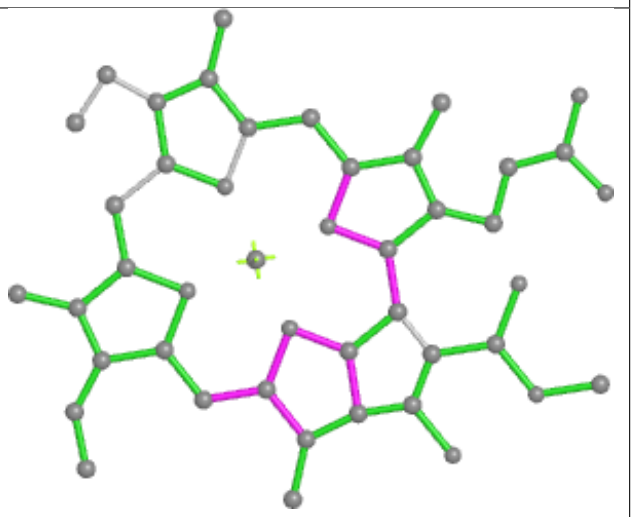


Rings

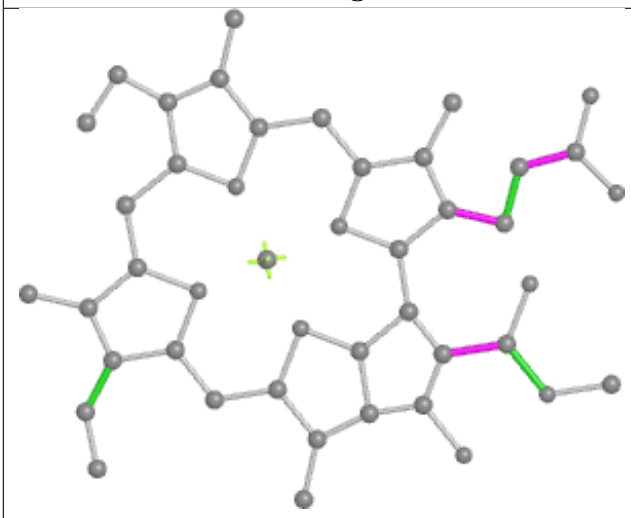
Ligand CLA 2 301



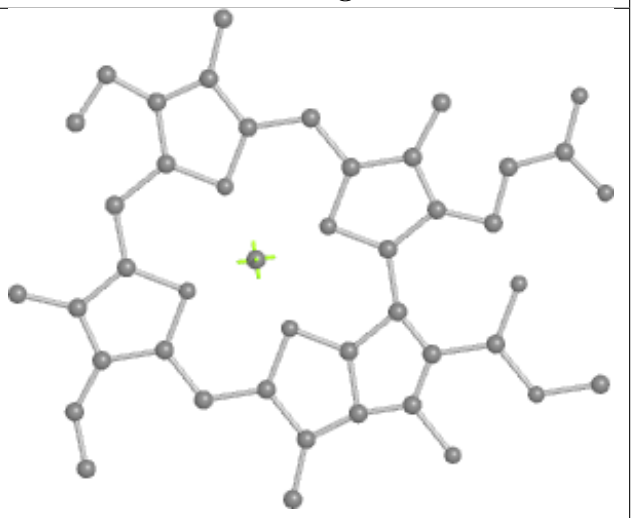
Bond lengths



Bond angles

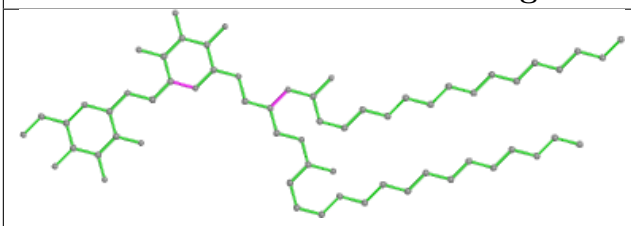


Torsions



Rings

Ligand DGD C 519



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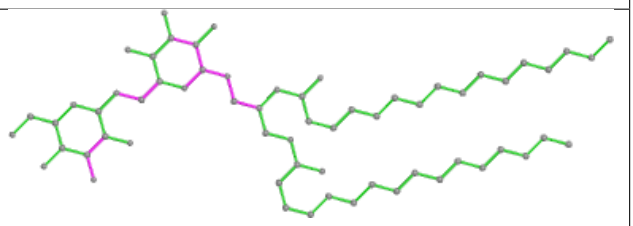
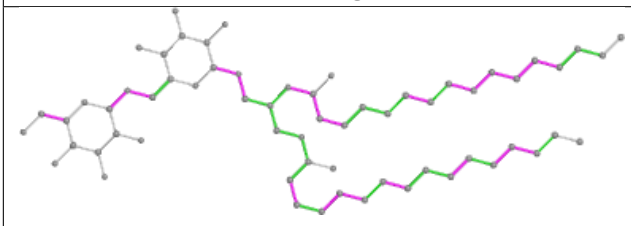


Bond angles



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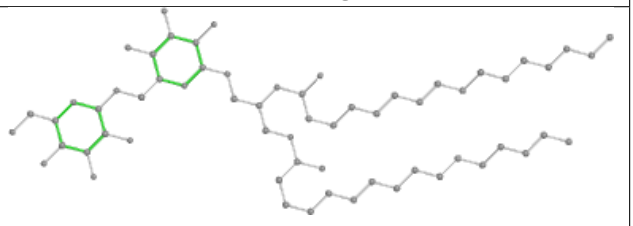
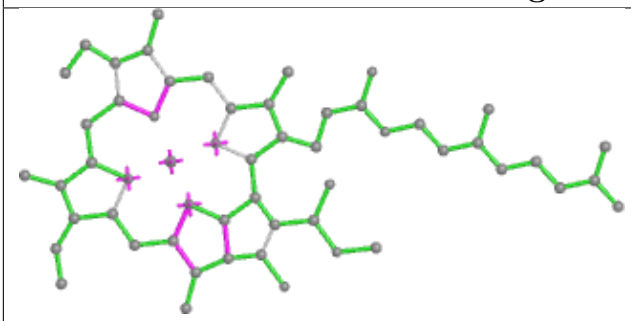


Rings

Ligand CLA 8 308



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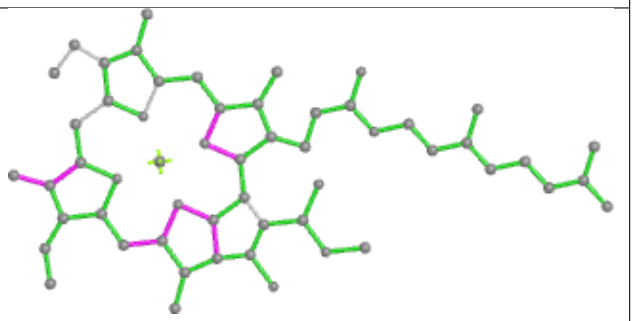

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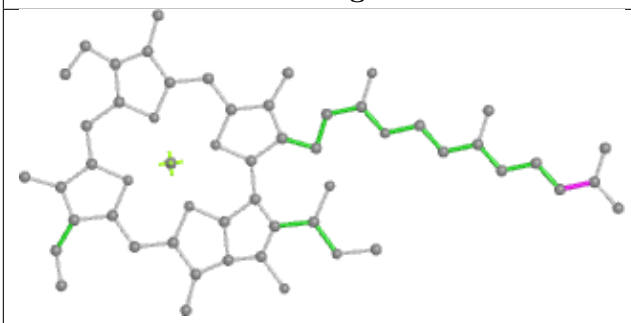

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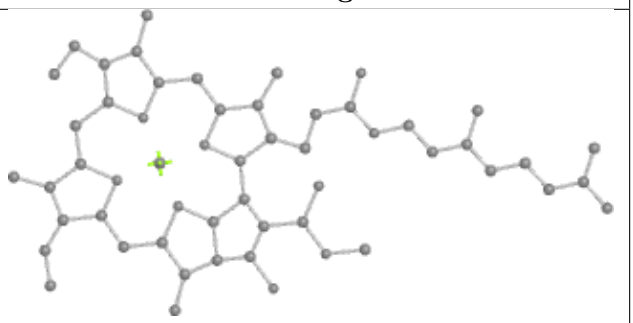
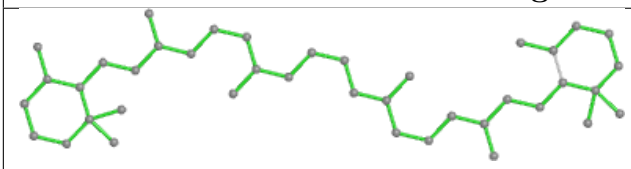


Rings

Ligand 8CT 7 312



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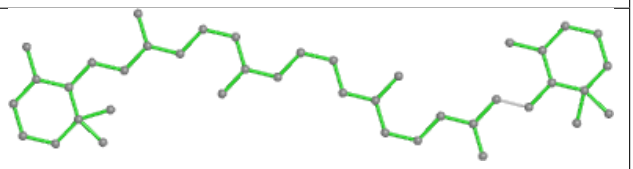
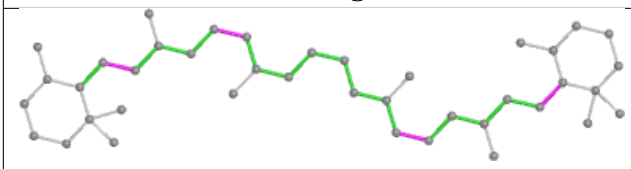


Bond angles



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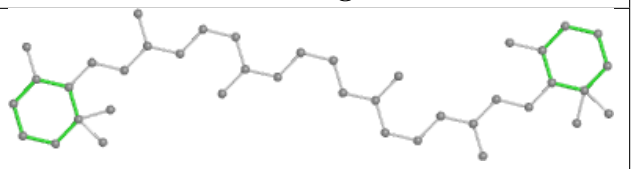
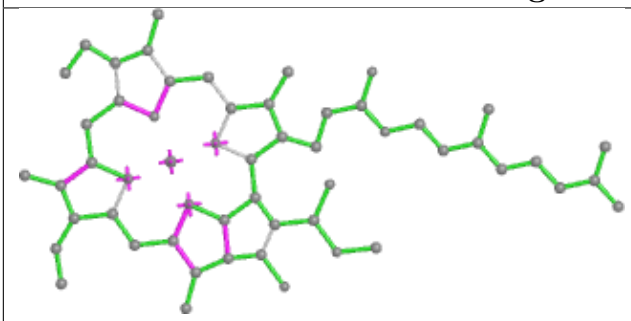


Rings

Ligand CLA 5 303



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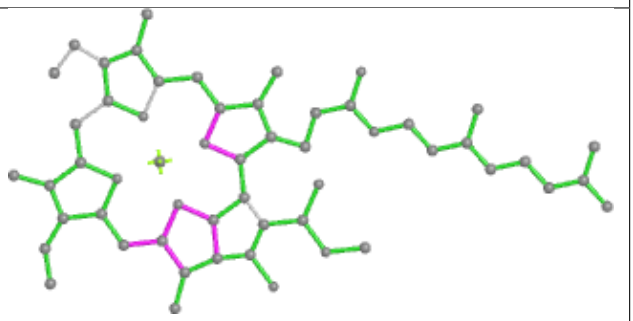
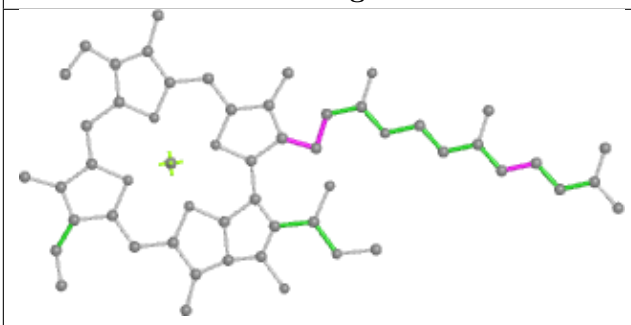


Bond angles



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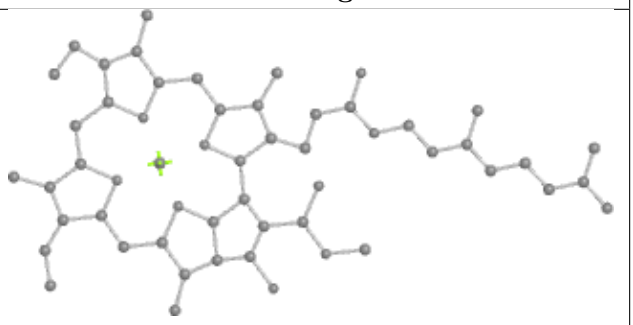
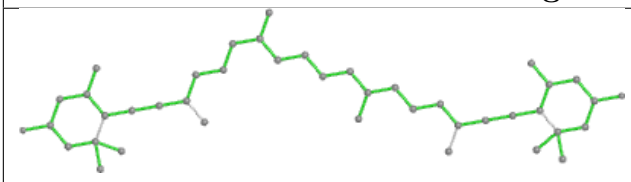
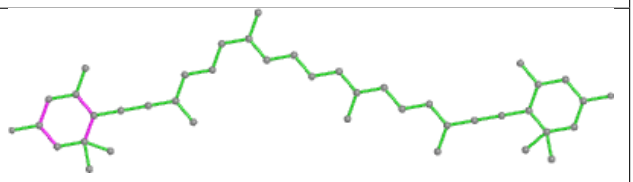


Rings

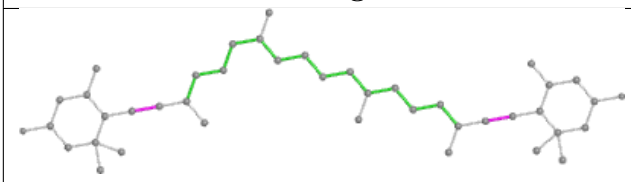
Ligand II0 7 315



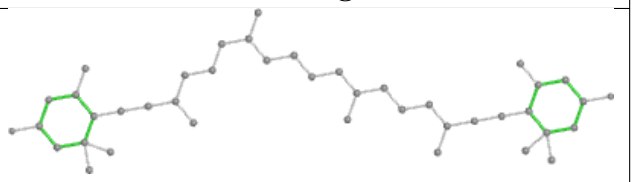
Bond lengths



Bond angles

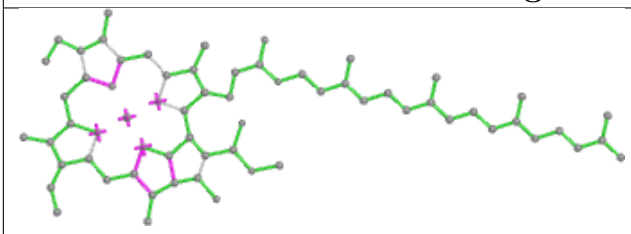


Torsions

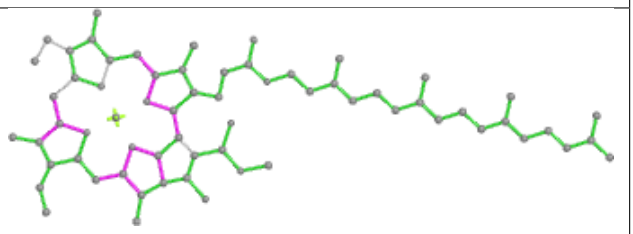


Rings

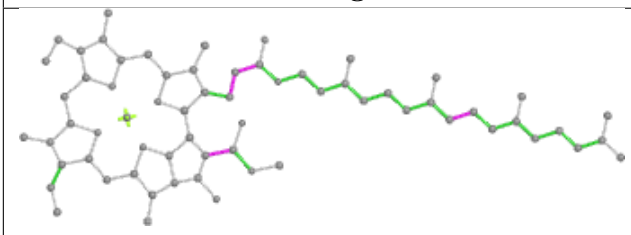
Ligand CLA B 611



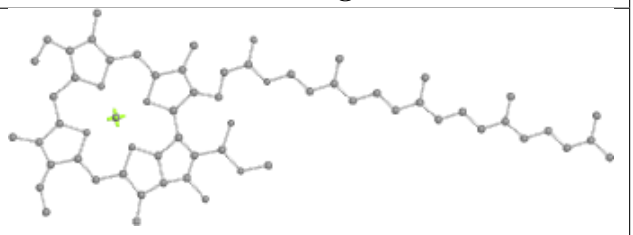
Bond lengths



Bond angles

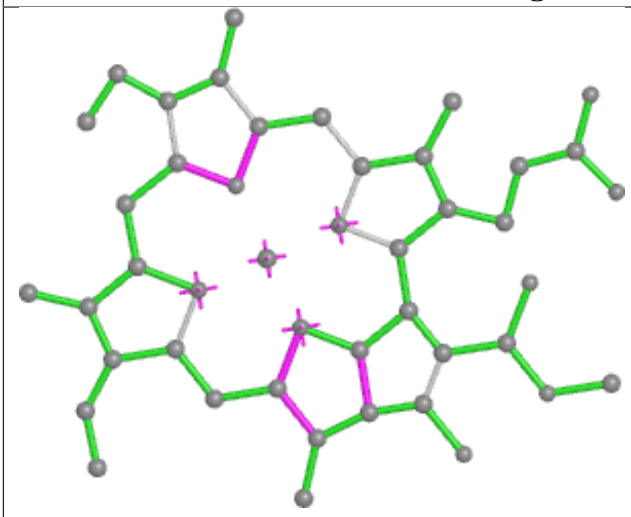


Torsions



Rings

Ligand CLA g 311



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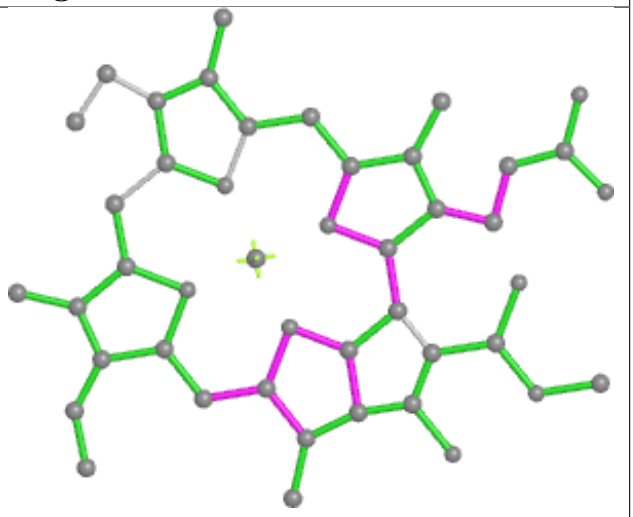
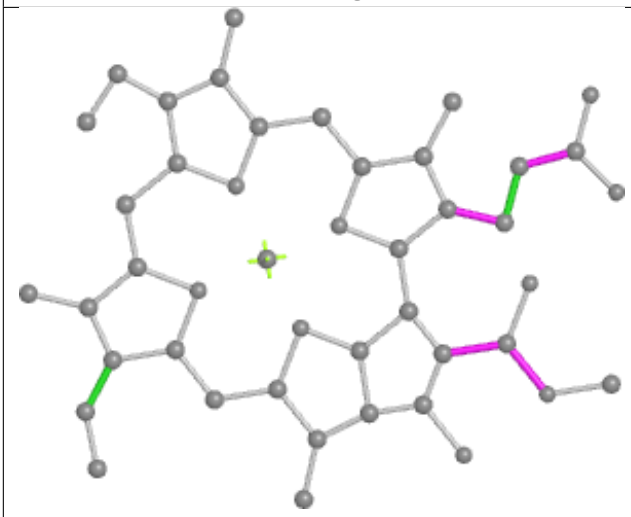


Bond angles



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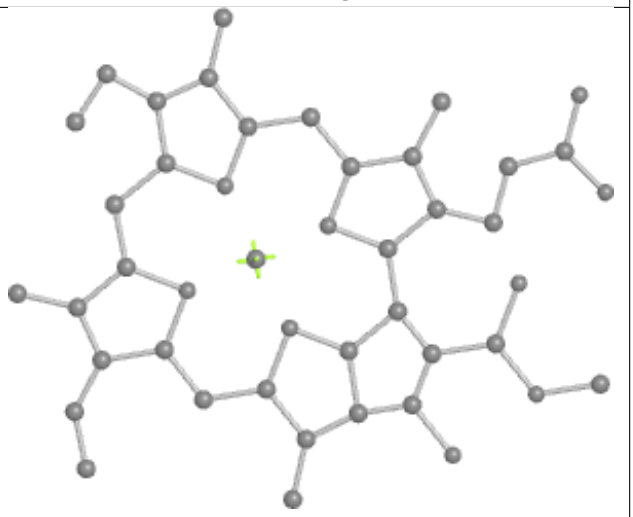
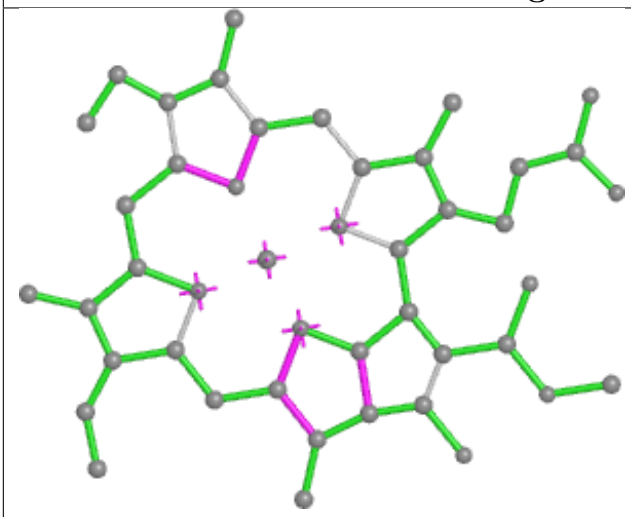
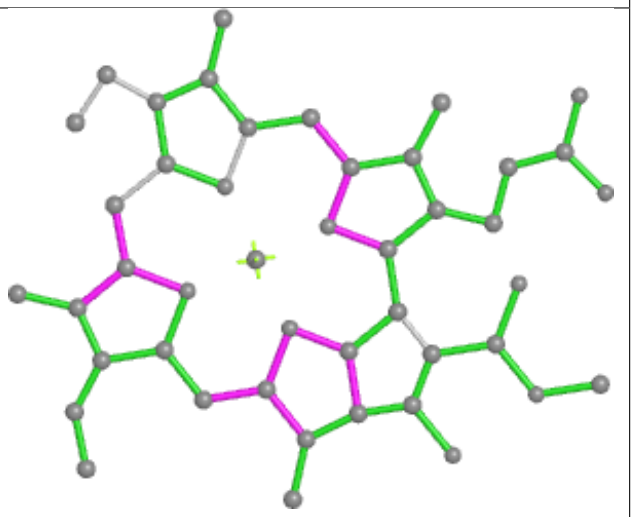


Rings

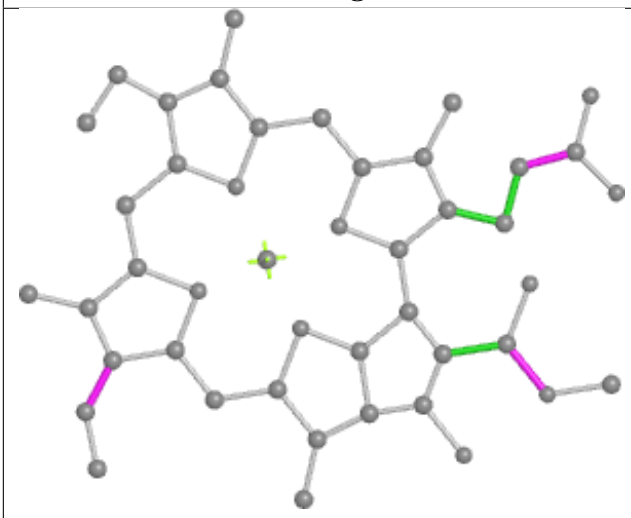
Ligand CLA 6 306



Bond lengths



Bond angles



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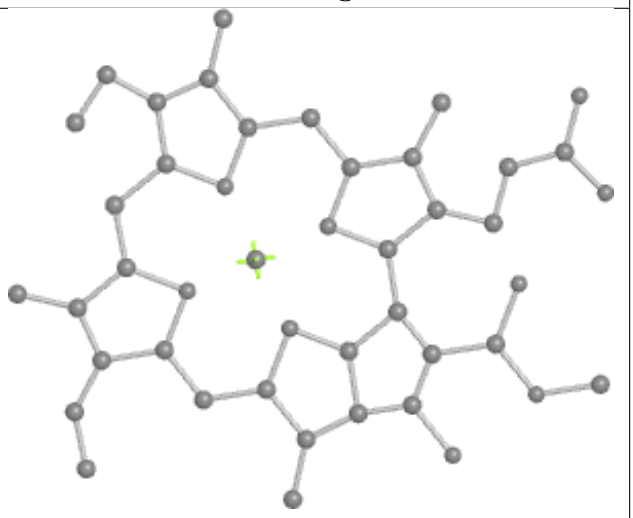
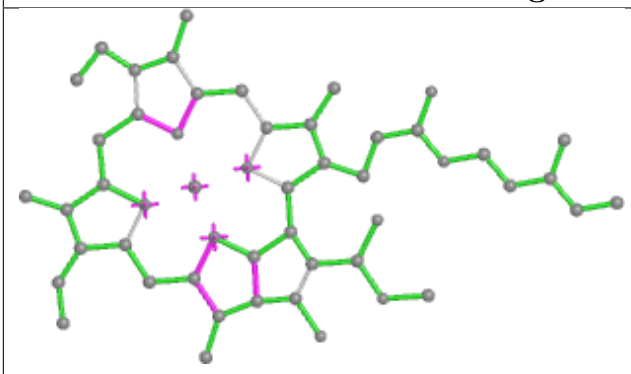
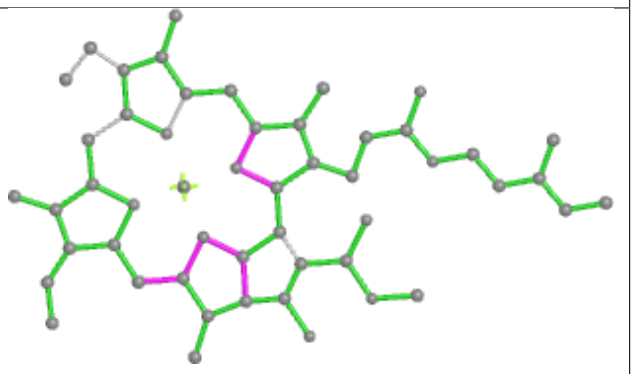


Rings

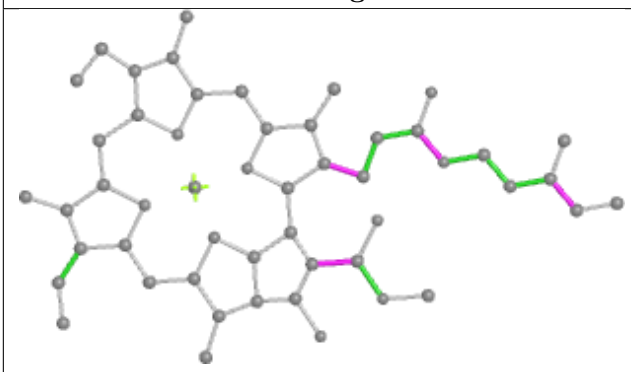
Ligand CLA 1 308



Bond lengths



Bond angles



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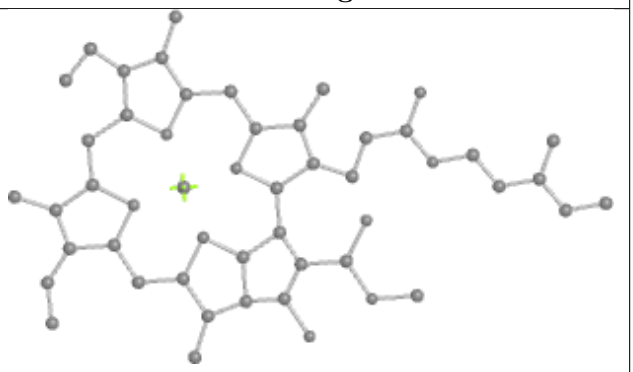
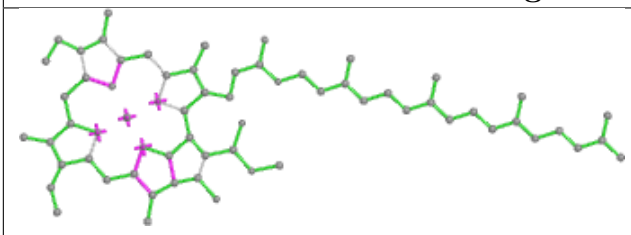
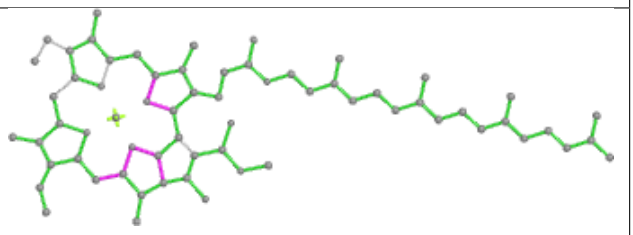


Rings

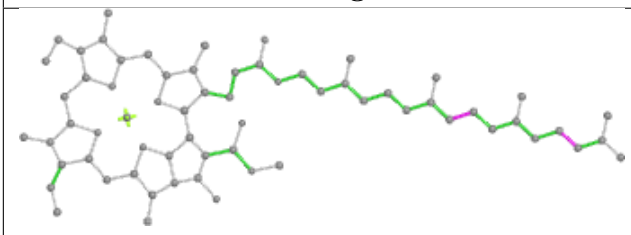
Ligand CLA C 504



Bond lengths



Bond angles



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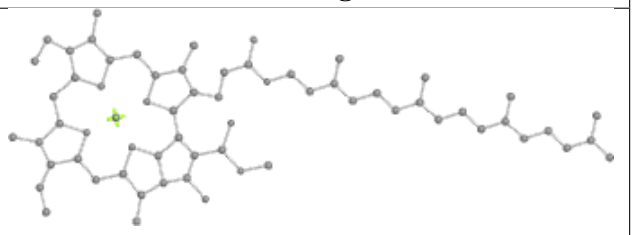
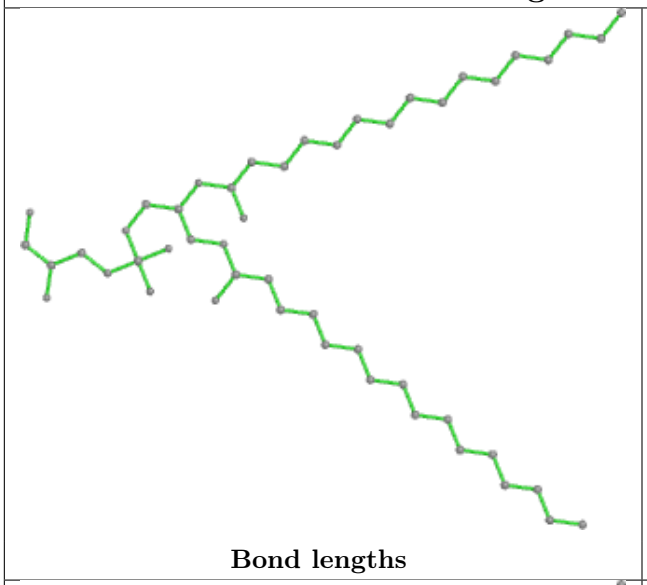


Rings

Ligand LHG 7 317



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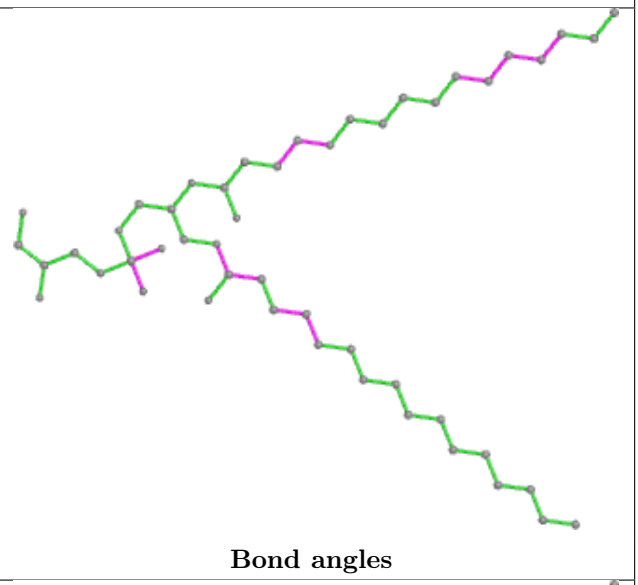

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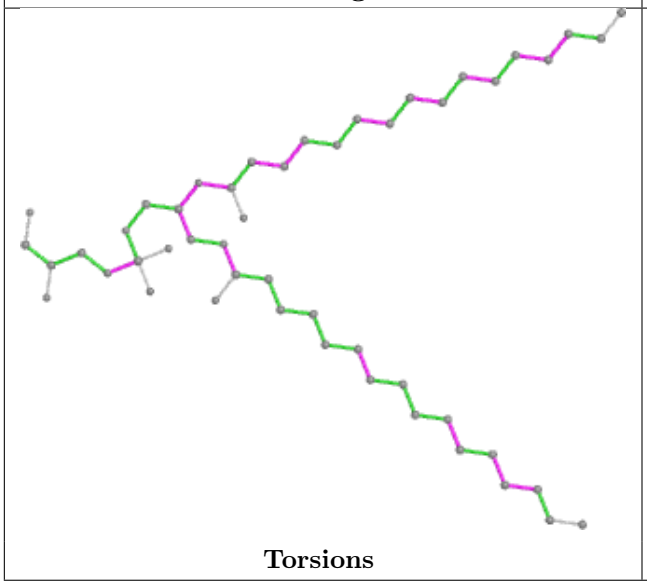

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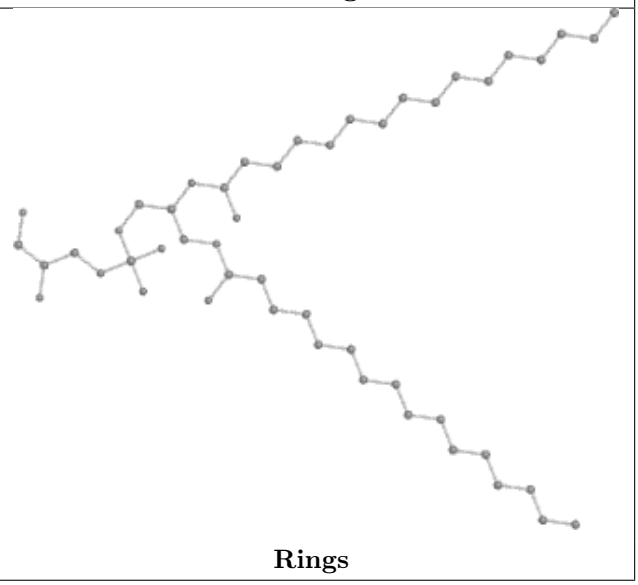
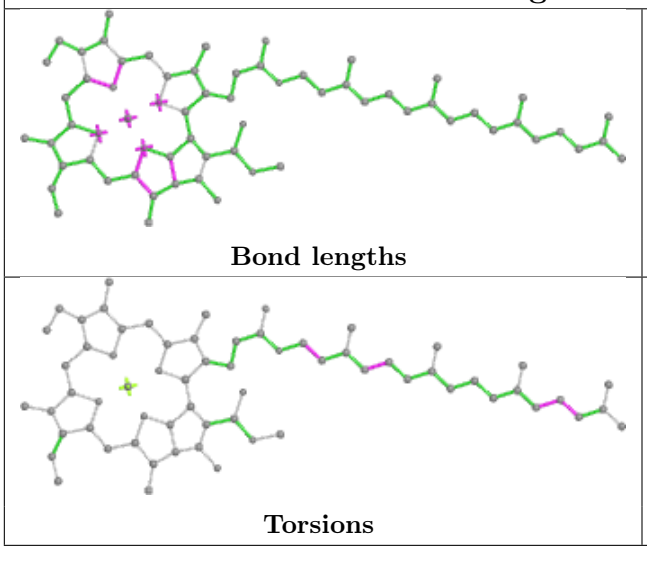
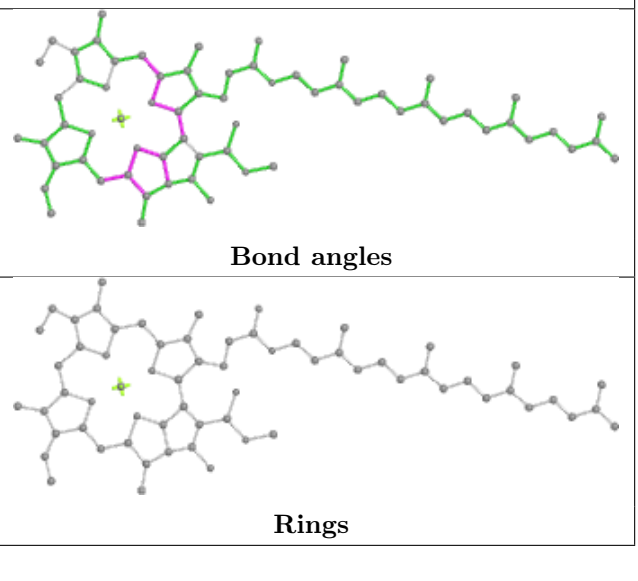


Rings

Ligand CLA a 405



Bond lengths

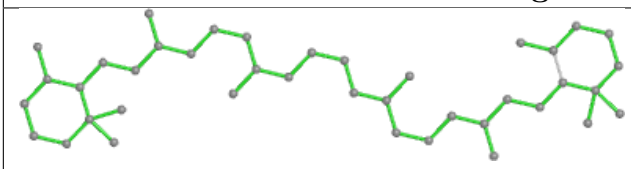


Bond angles

Torsions

Rings

Ligand 8CT a 409



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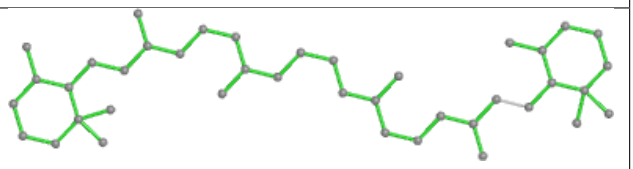
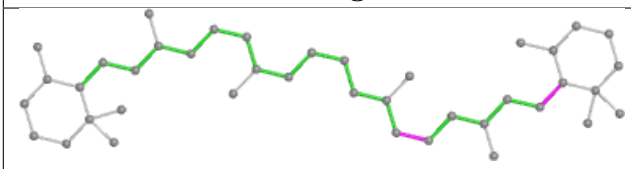


Bond angles



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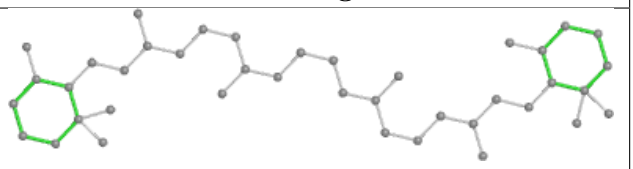
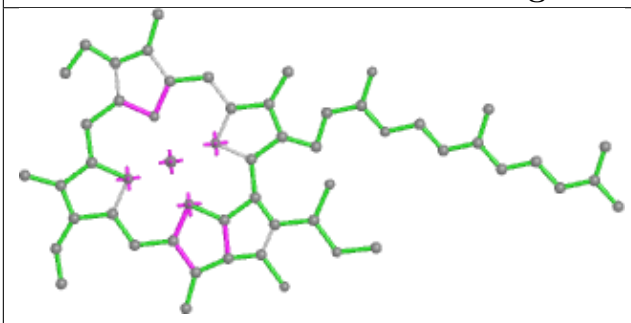


Rings

Ligand CLA g 307



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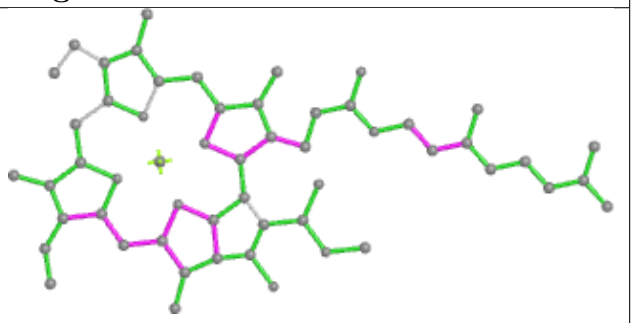
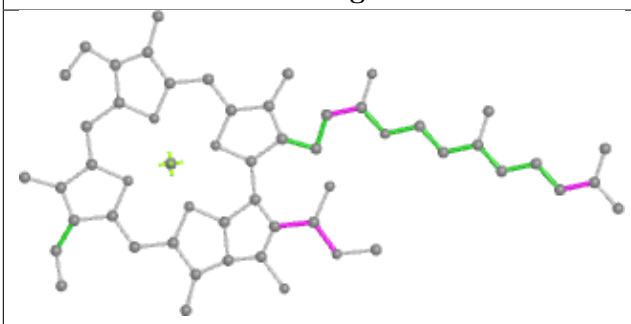
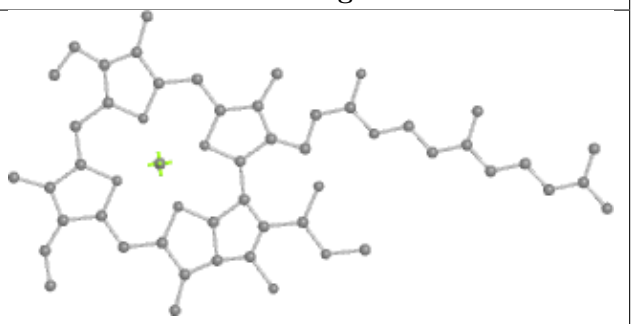


Bond angles

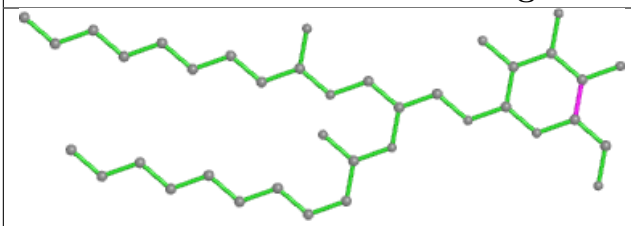


Torsions

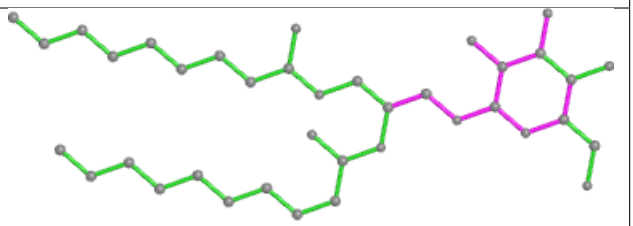


Rings

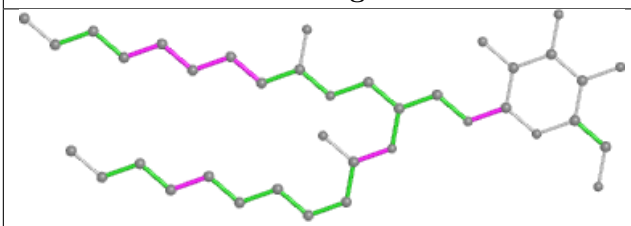
Ligand LMG m 101



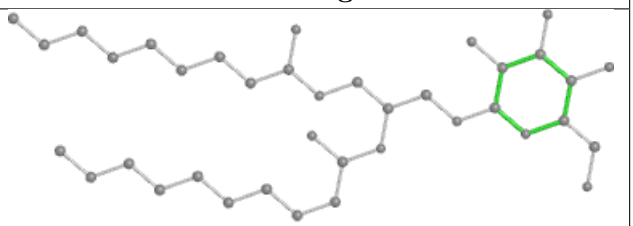
Bond lengths



Bond angles

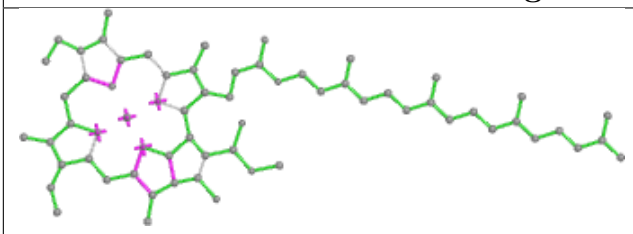


Torsions

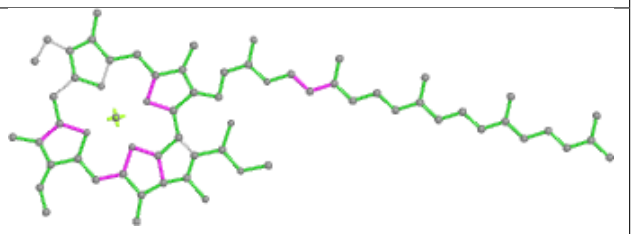


Rings

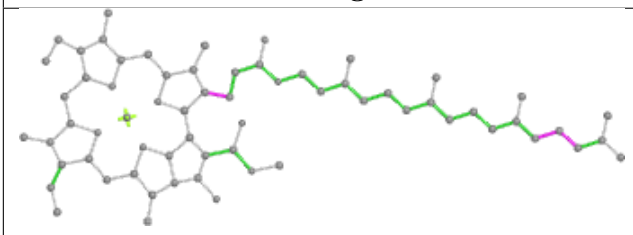
Ligand CLA B 612



Bond lengths



Bond angles



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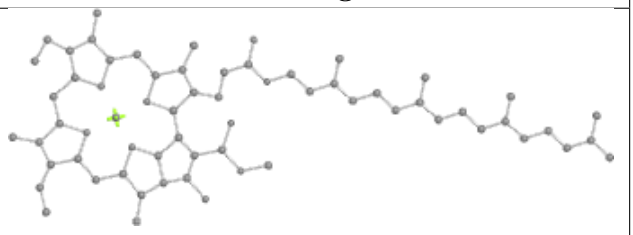
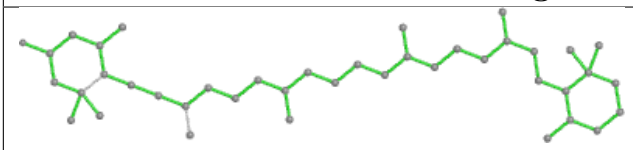


Rings

Ligand IHT 6 318



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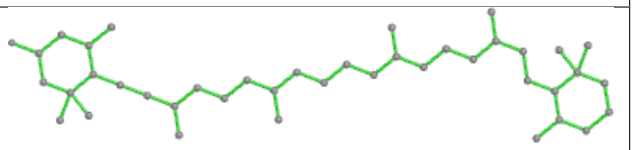
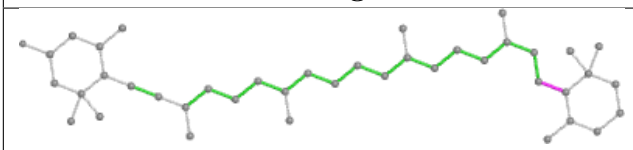


Bond angles



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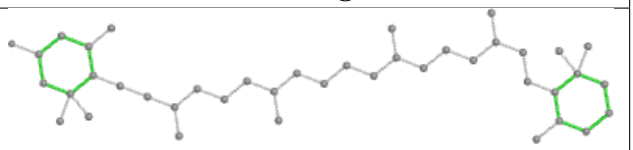
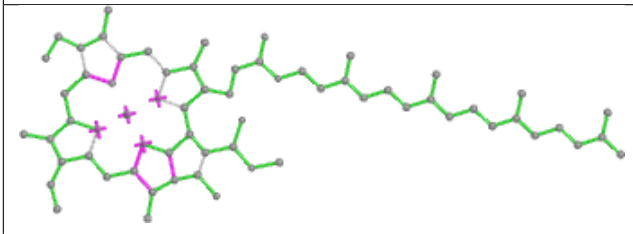


Rings

Ligand CLA C 510



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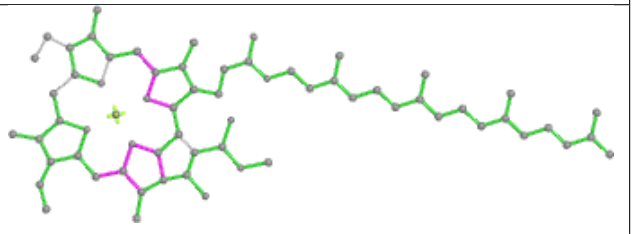
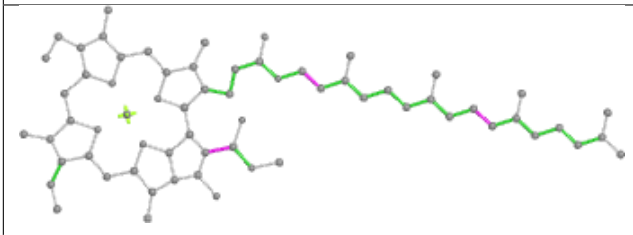


Bond angles



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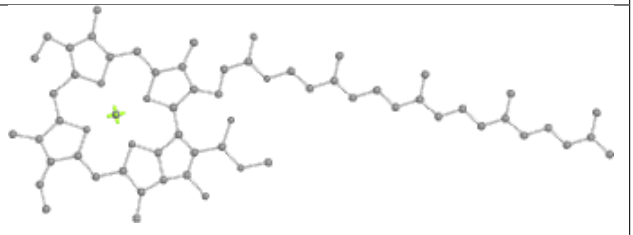
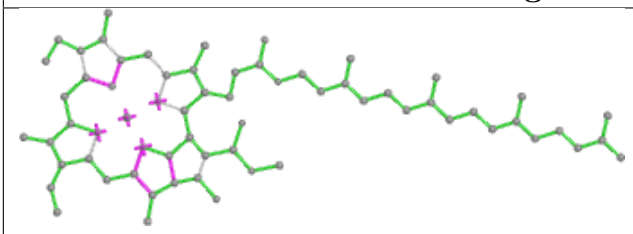
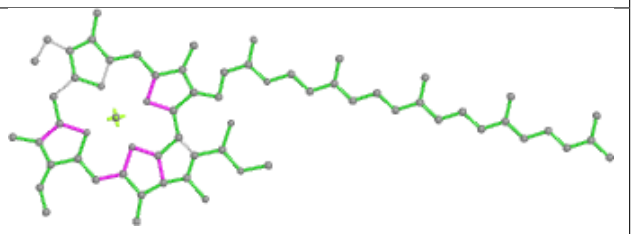


Rings

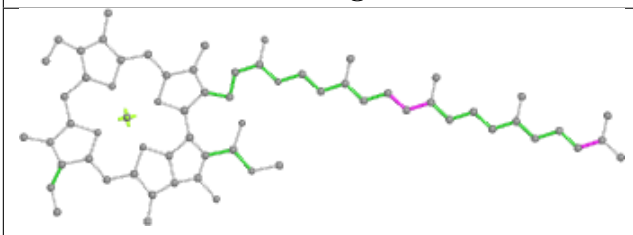
Ligand CLA C 514



Bond lengths



Bond angles



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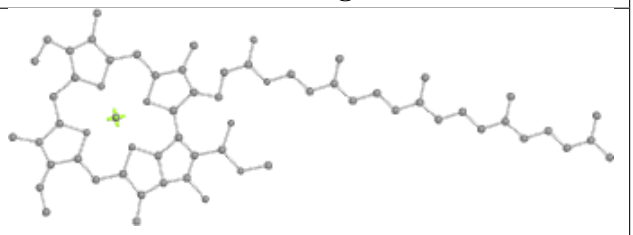
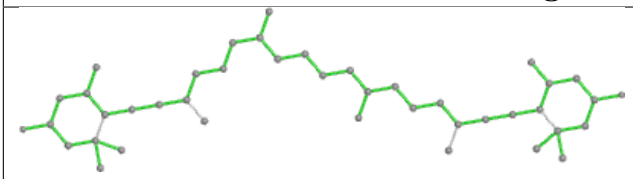
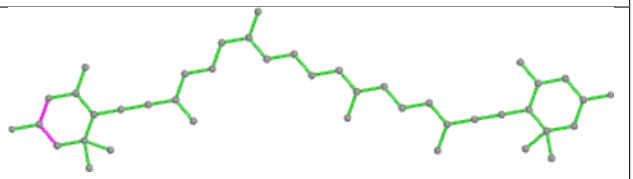


Rings

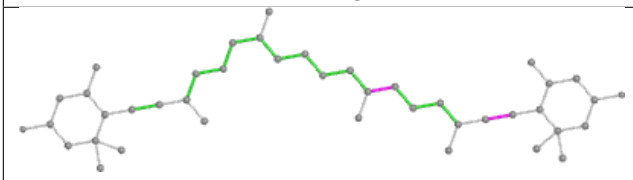
Ligand II0 6 317



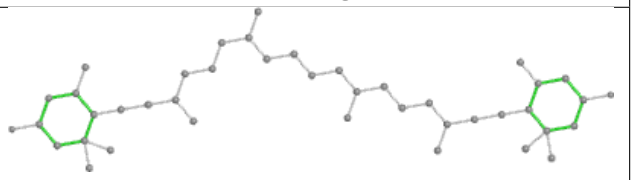
Bond lengths



Bond angles

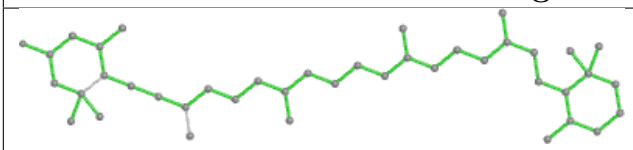


Torsions



Rings

Ligand IHT 9 320



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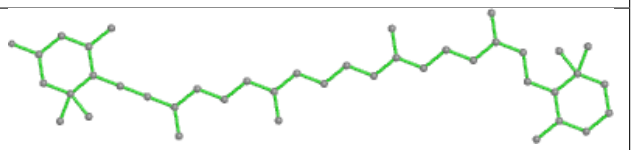
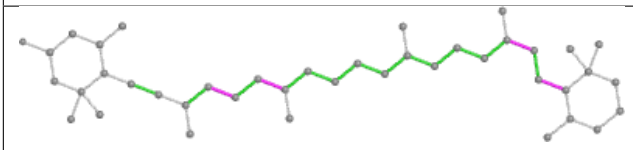
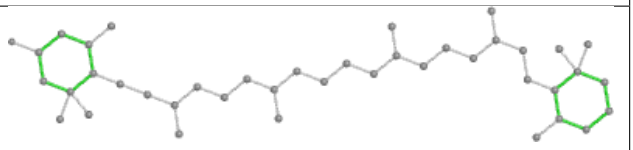


Bond angles

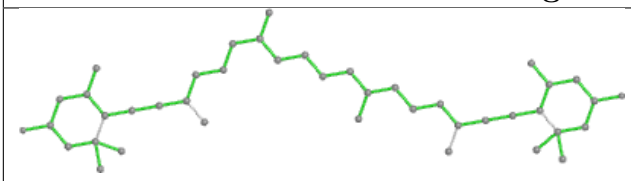


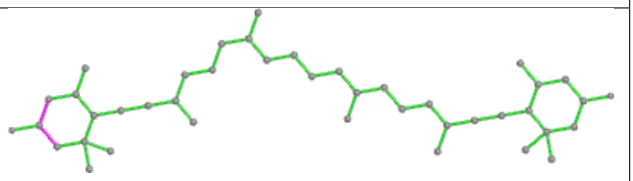
Torsions

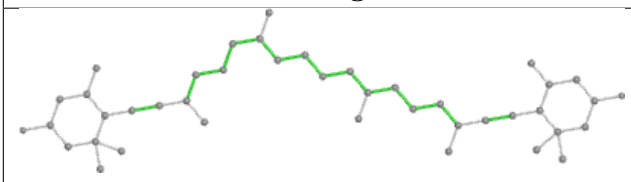


Rings

Ligand II0 3 317


Bond lengths


Bond angles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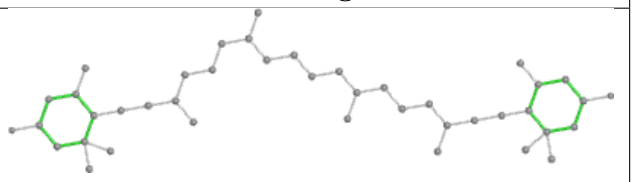
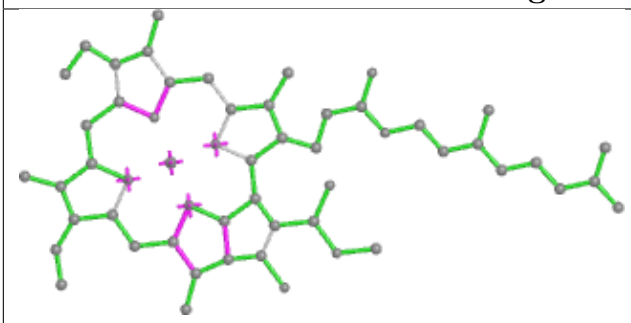
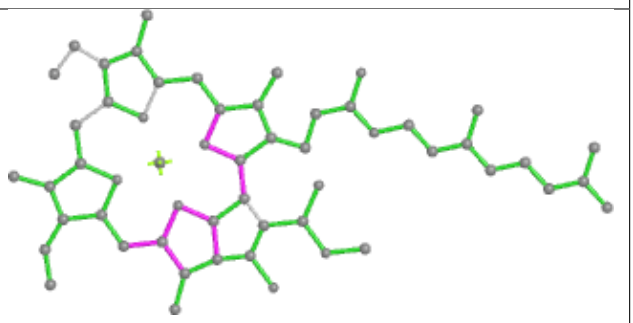
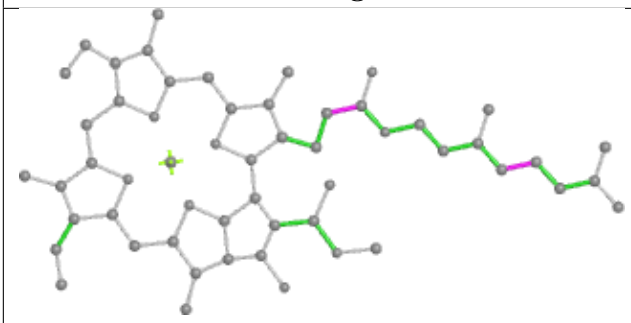

Rings

Ligand CLA 3 312


Bond lengths


Bond angles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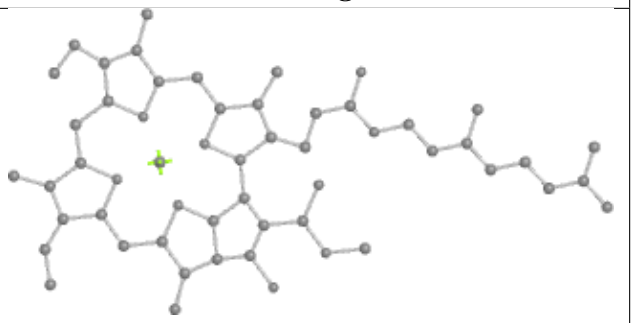
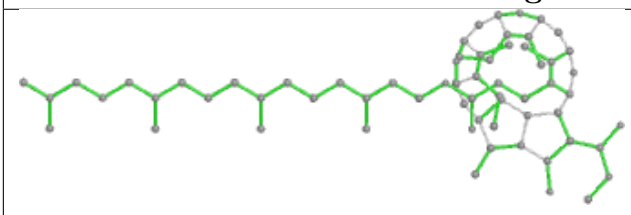

Rings

Ligand PHO d 403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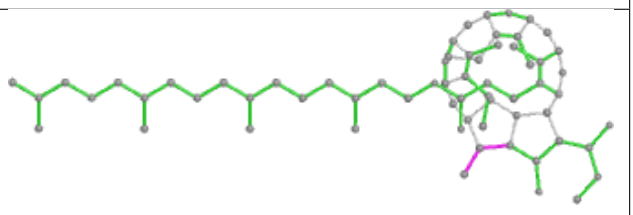
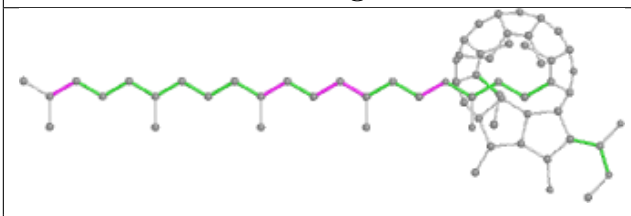

Bond angles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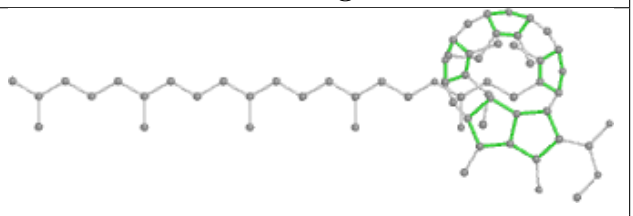
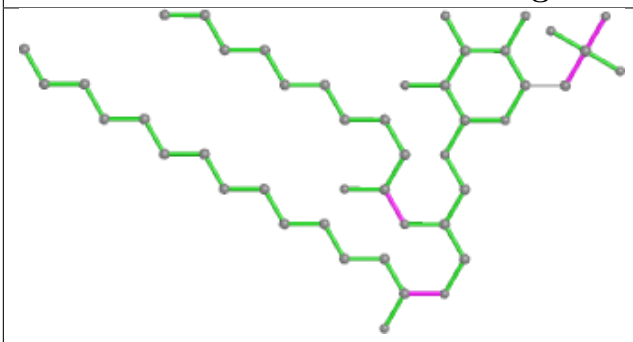
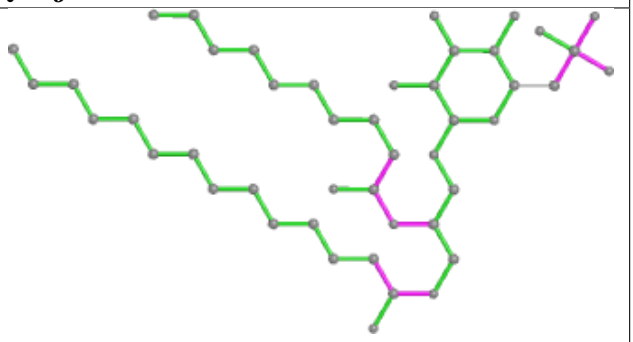

Rings

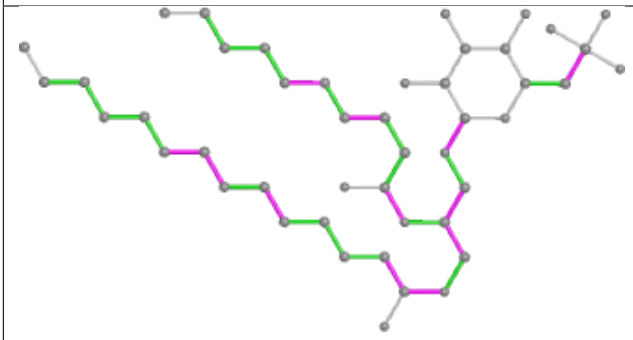
Ligand SQD j 101



Bond lengths



Bond angles



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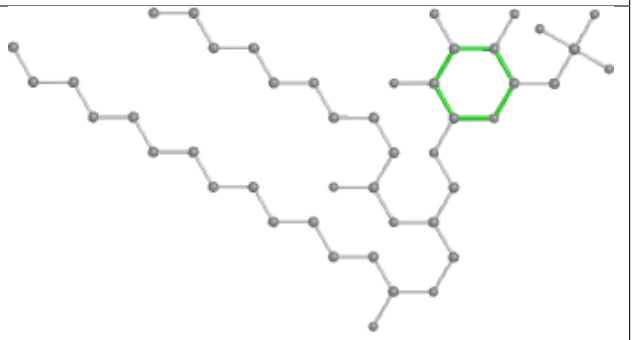
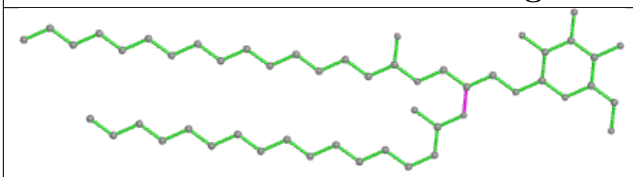


Rings

Ligand LMG c 520



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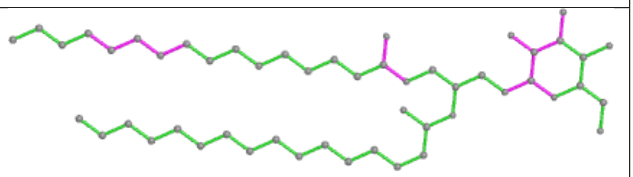
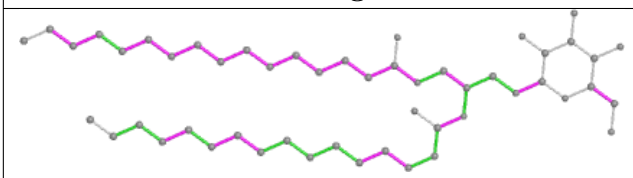


Bond angles



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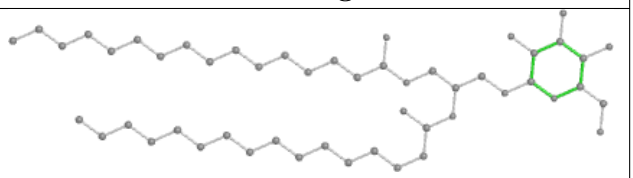
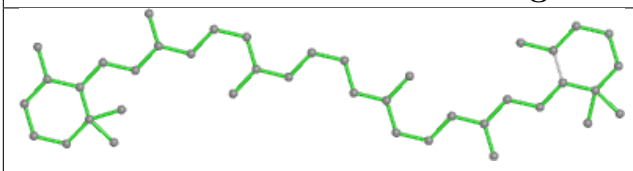


Rings

Ligand 8CT d 406



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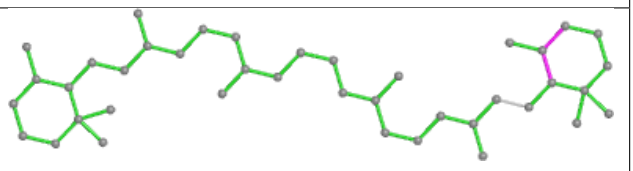
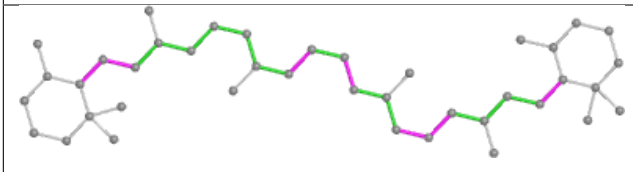


Bond angles



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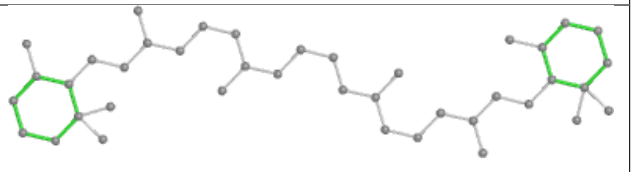
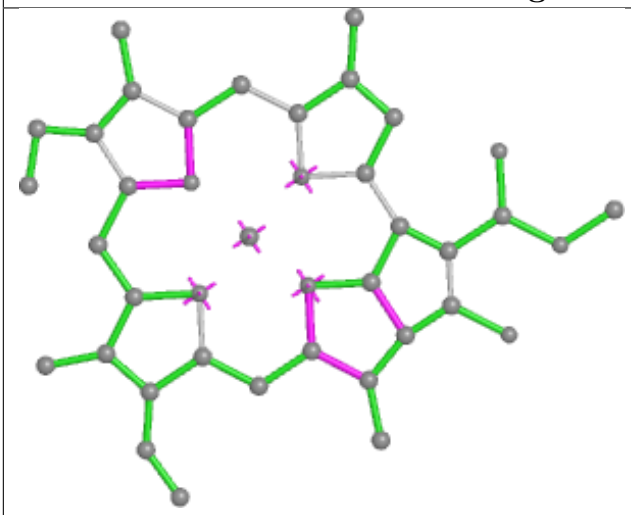


Rings

Ligand CLA g 317



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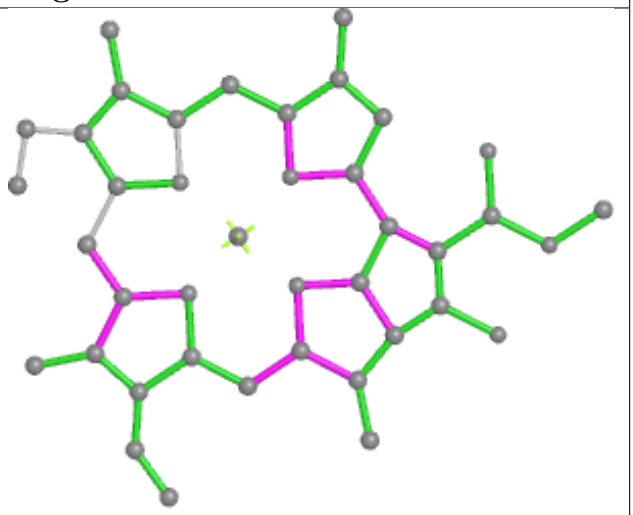
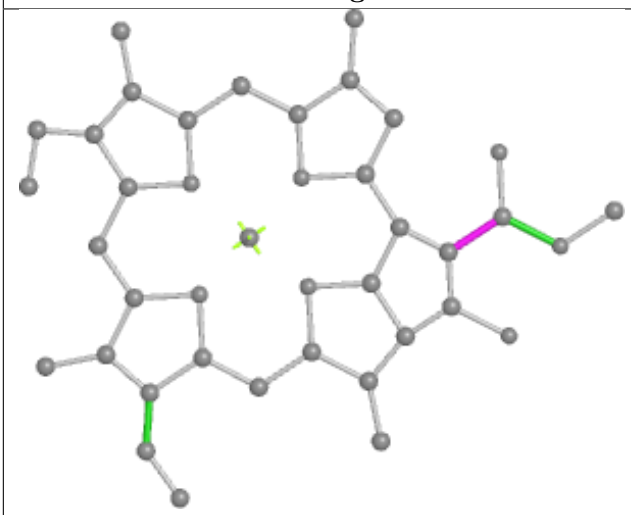


Bond angles



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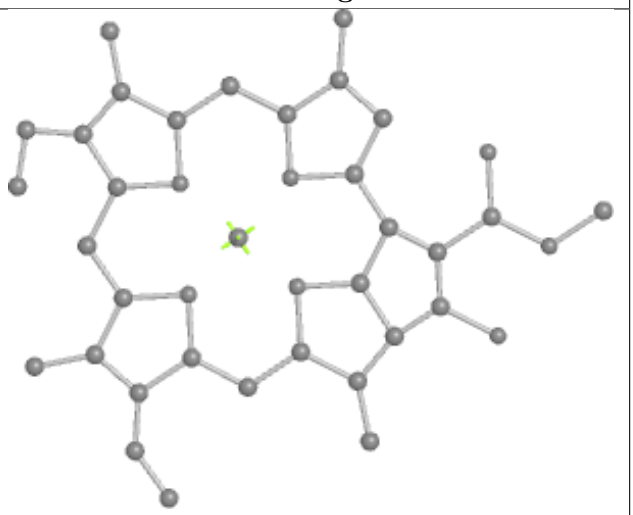
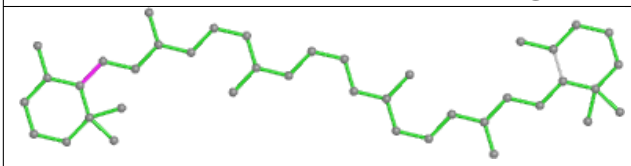


Rings

Ligand 8CT C 515



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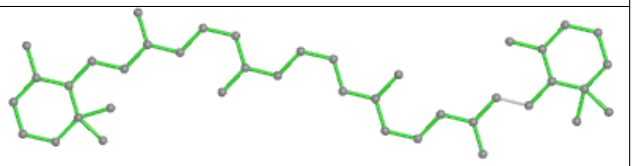
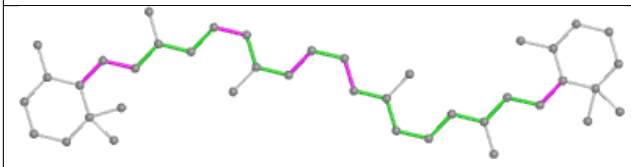


Bond angles



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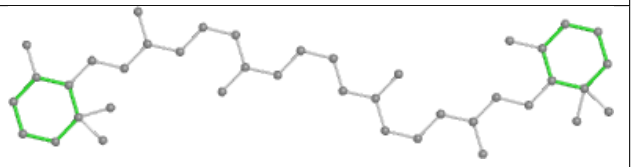
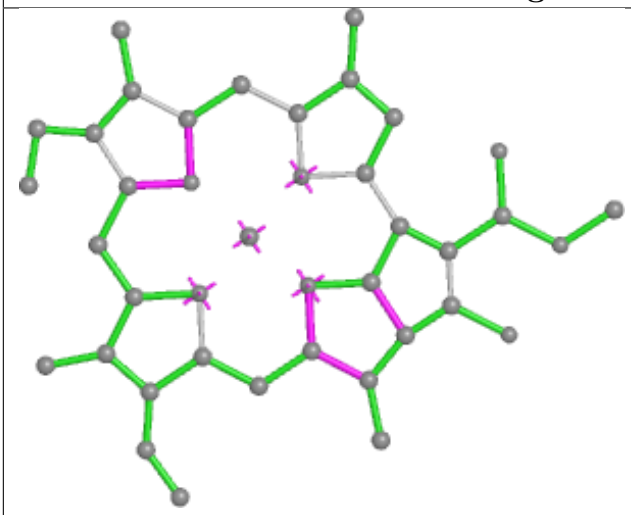
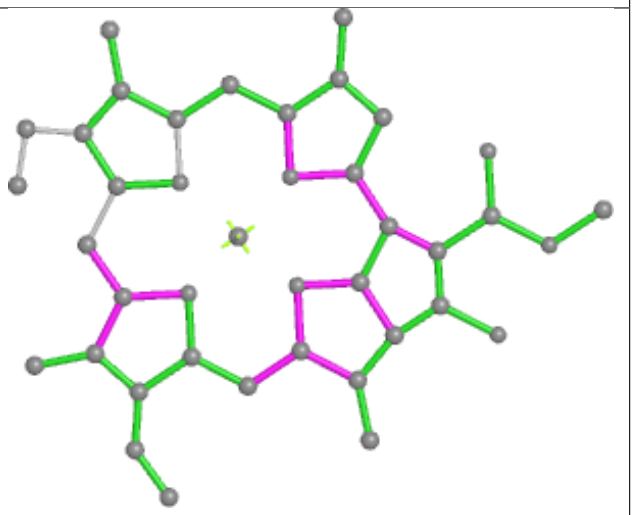


Rings

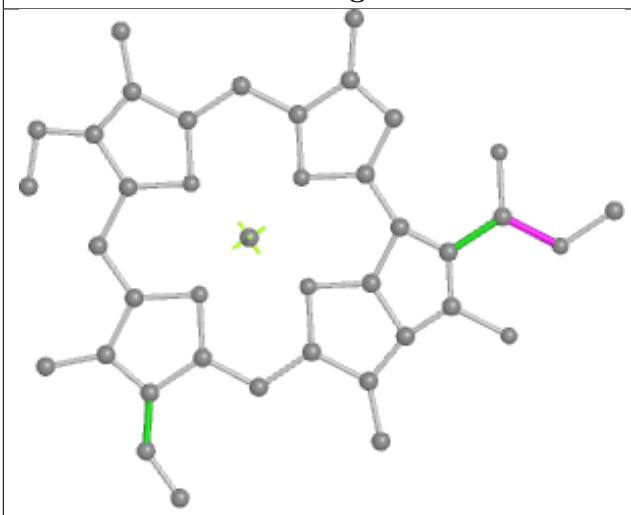
Ligand CLA b 618



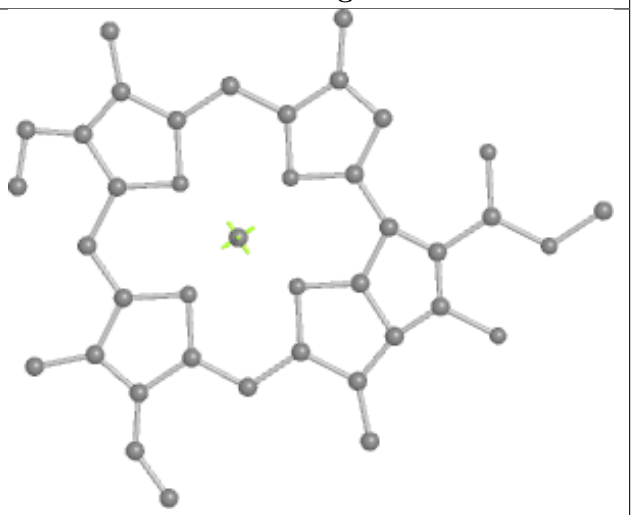
Bond lengths



Bond angles

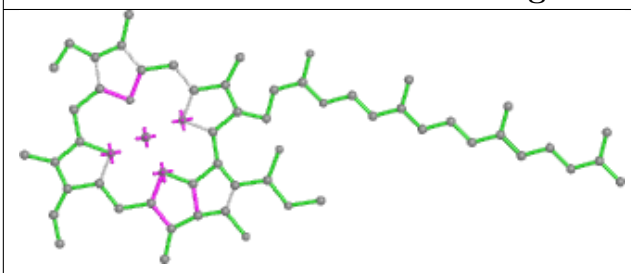


Torsions

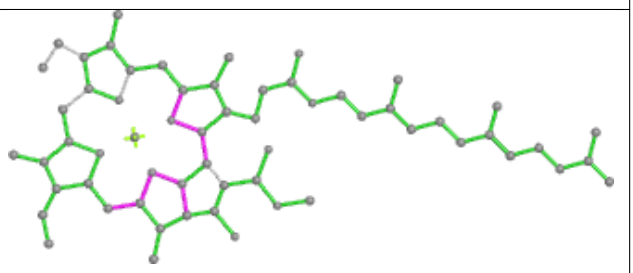


Rings

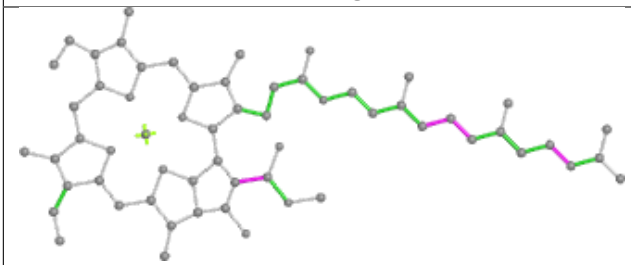
Ligand CLA 7 306



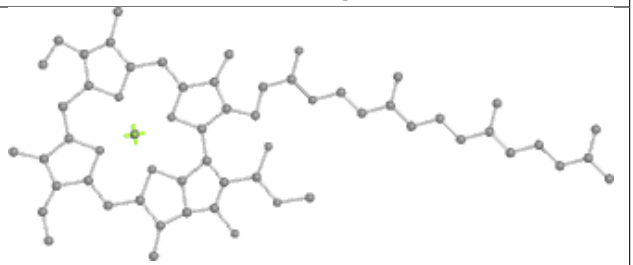
Bond lengths



Bond angles

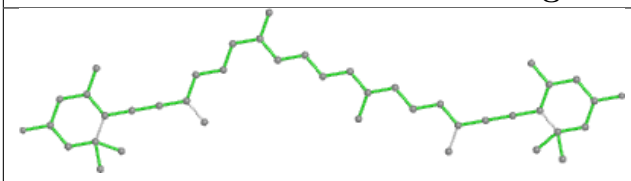


Torsions

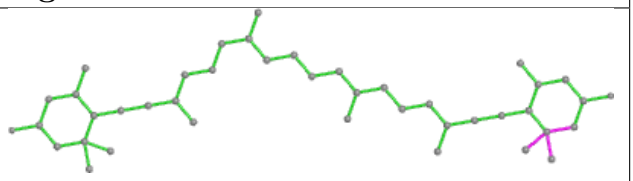


Rings

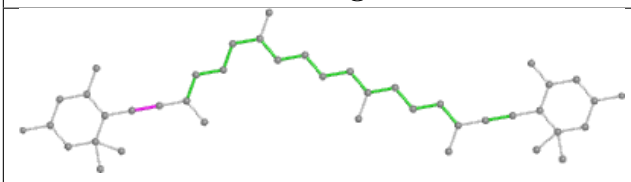
Ligand II0 g 313



Bond lengths



Bond angles



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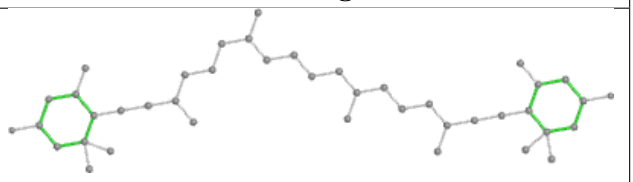
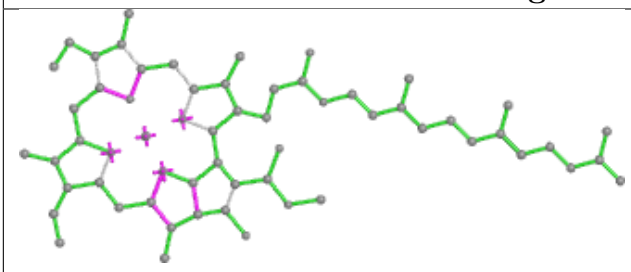


Rings

Ligand CLA 2 307



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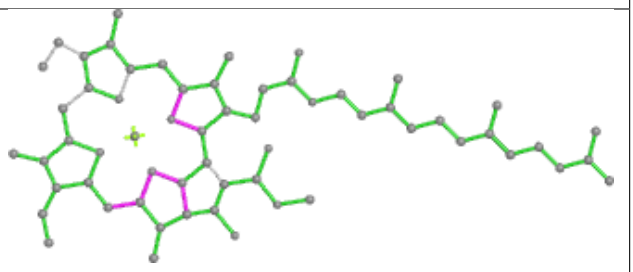
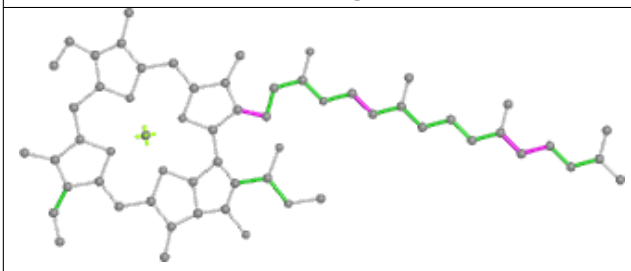
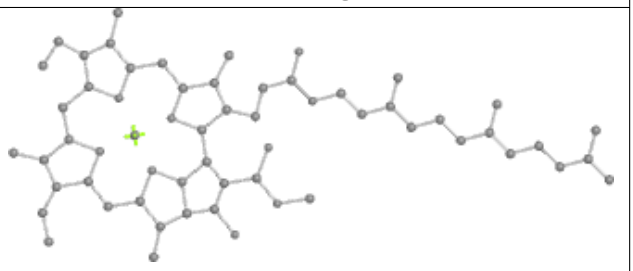


Bond angles

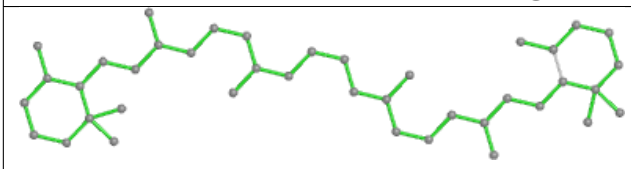


Torsions

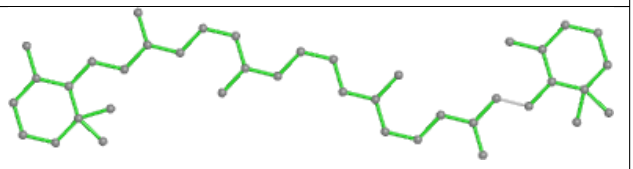


Rings

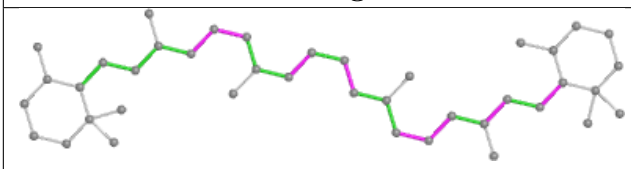
Ligand 8CT B 620



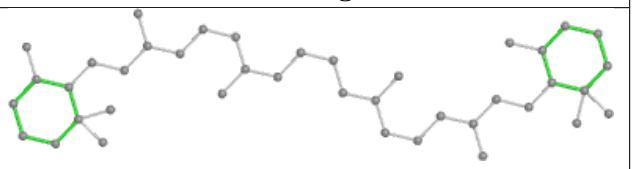
Bond lengths



Bond angles

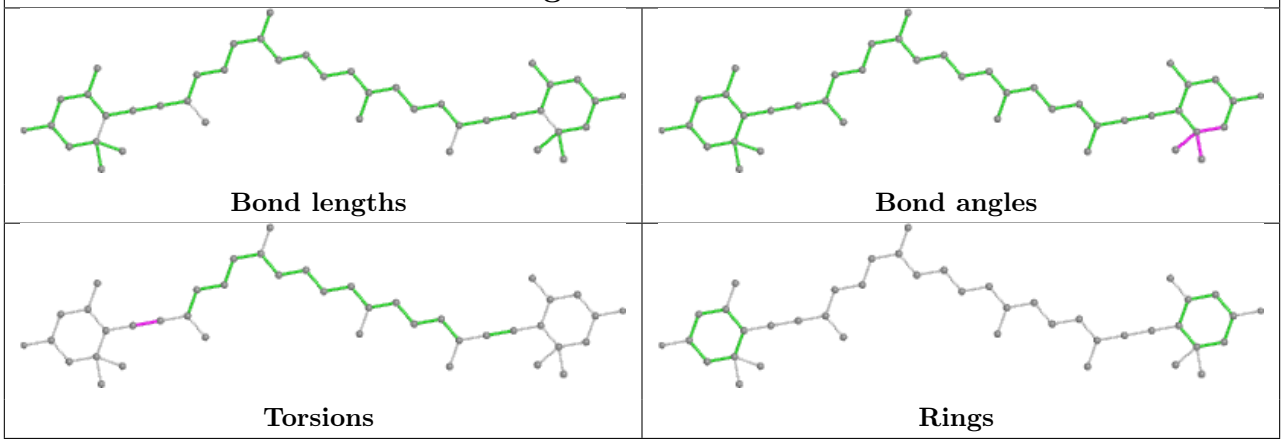


Torsions

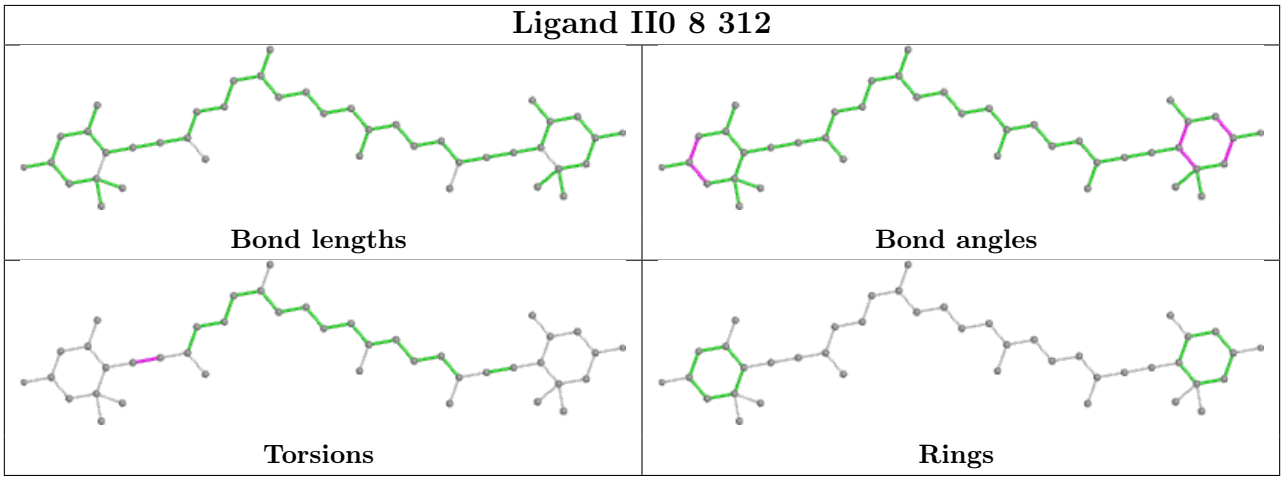


Rings

Ligand II0 5 313



Ligand II0 8 312



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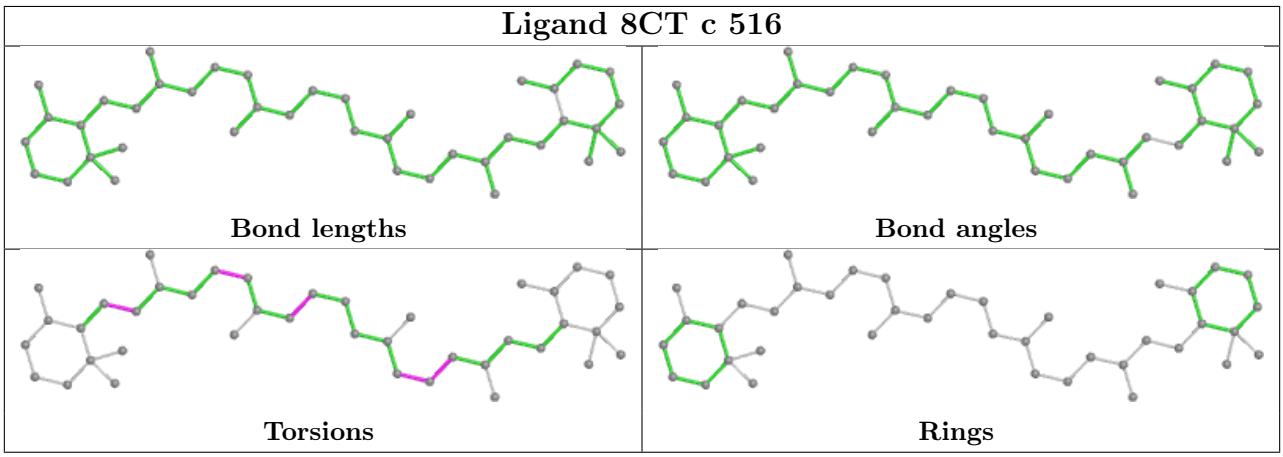
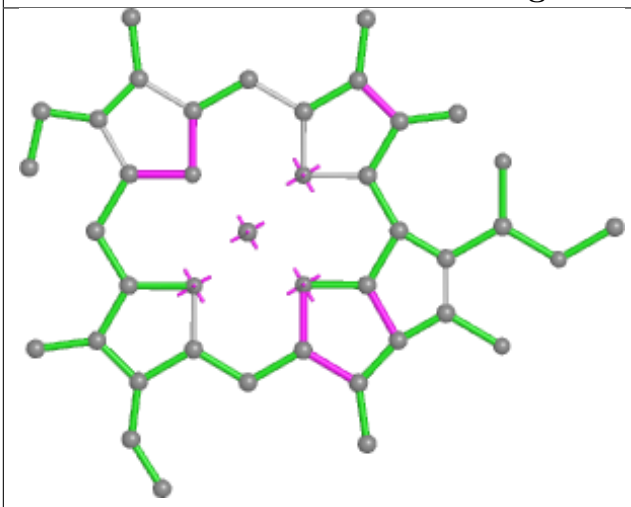
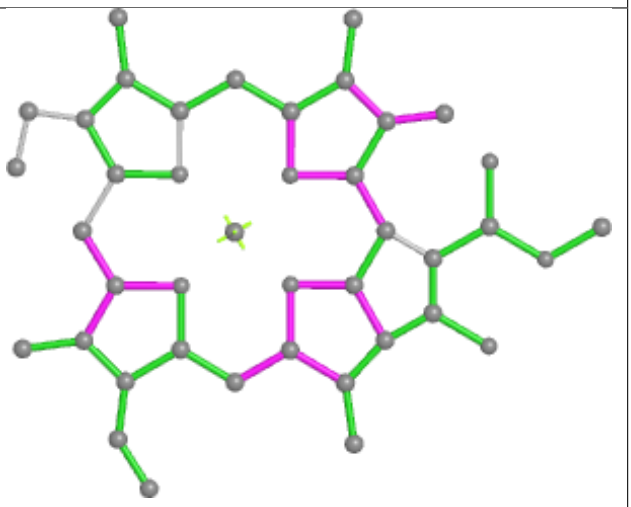


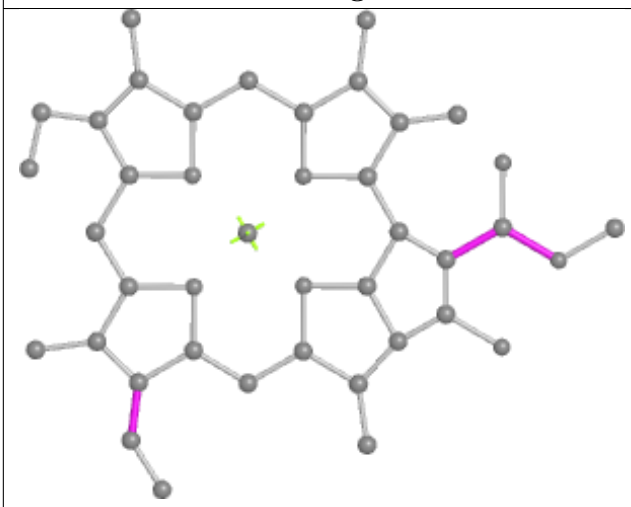
Ligand CLA 6 310



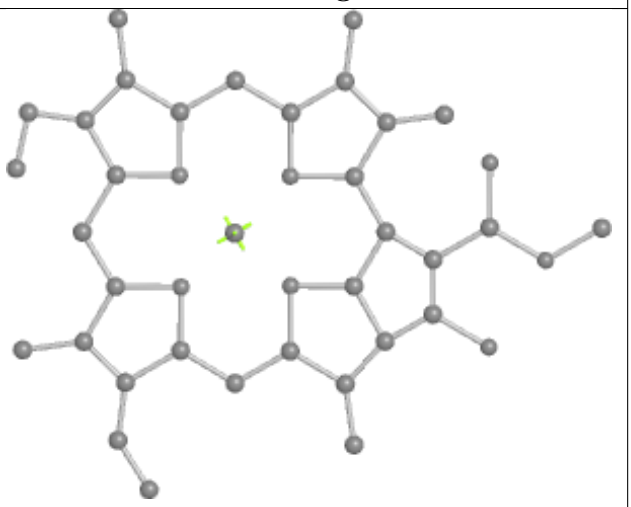
Bond lengths



Bond angles

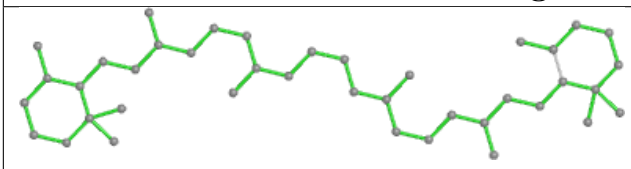


Torsions

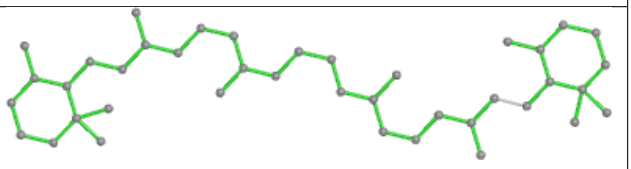


Rings

Ligand 8CT h 102



Bond lengths



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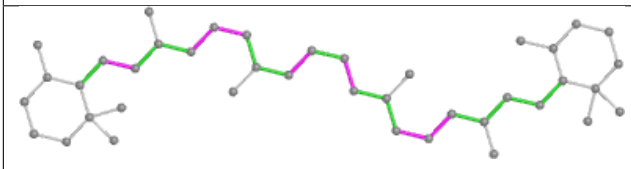

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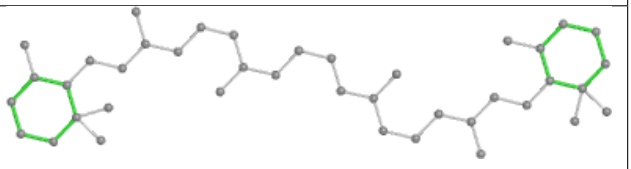
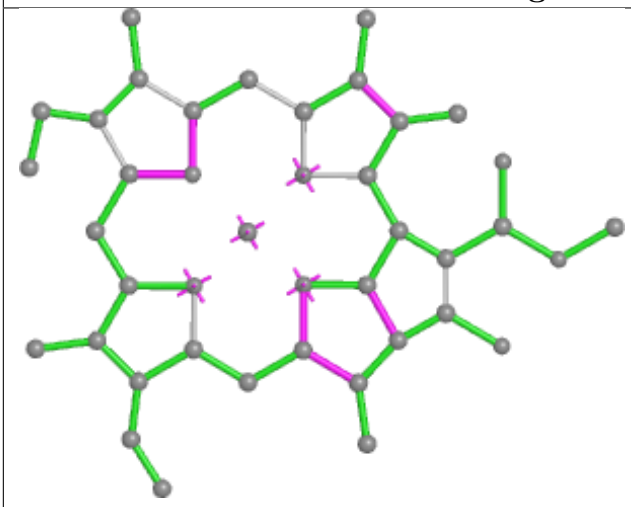


Rings

Ligand CLA 3 306



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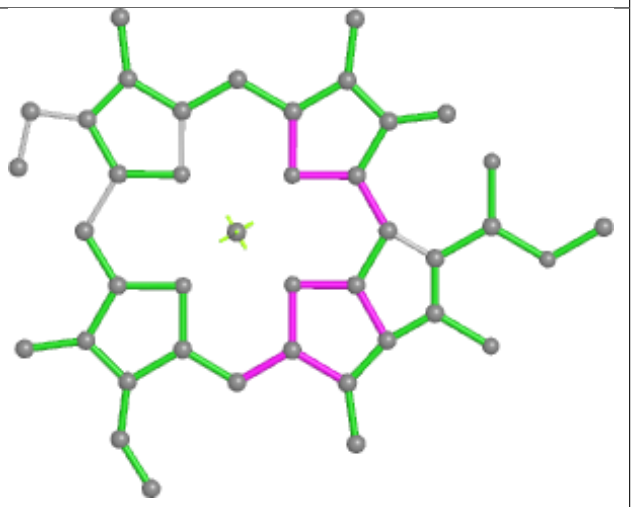
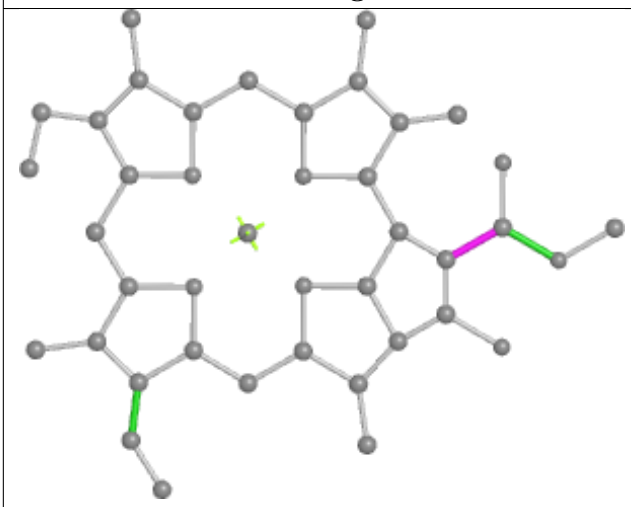


Bond angles



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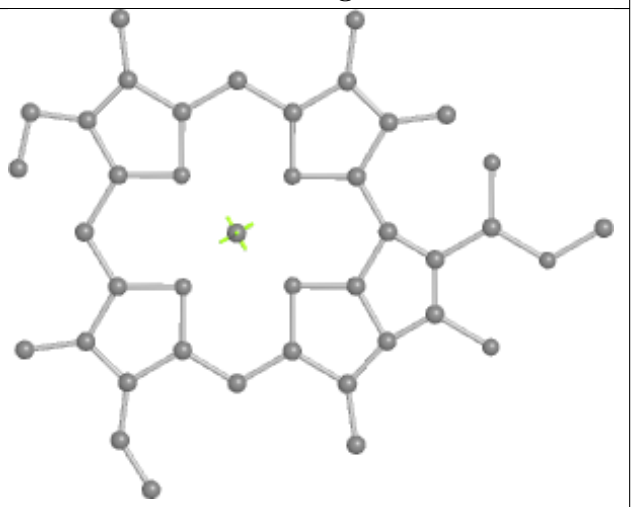
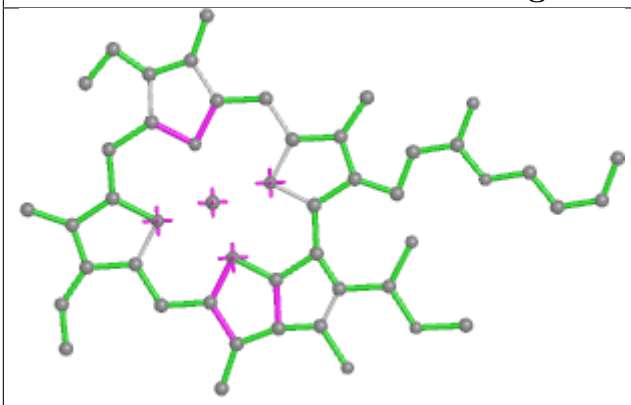


Rings

Ligand CLA 9 308



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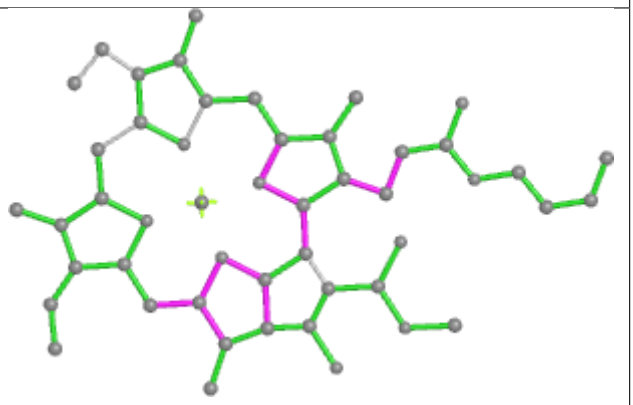
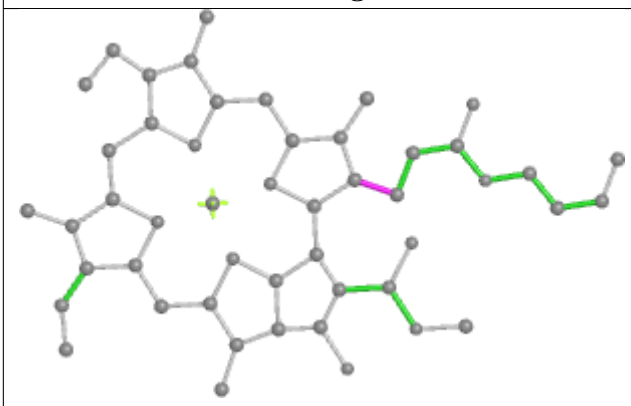


Bond angles



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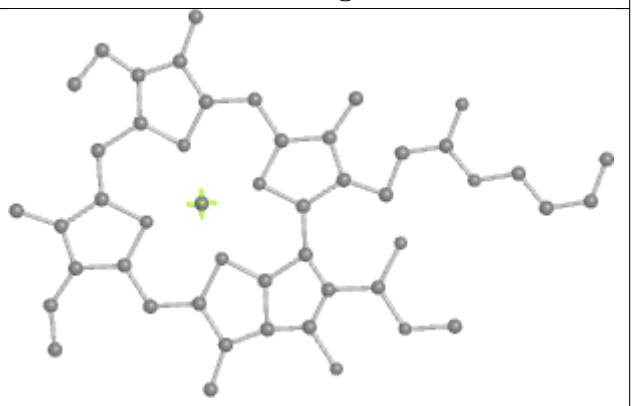
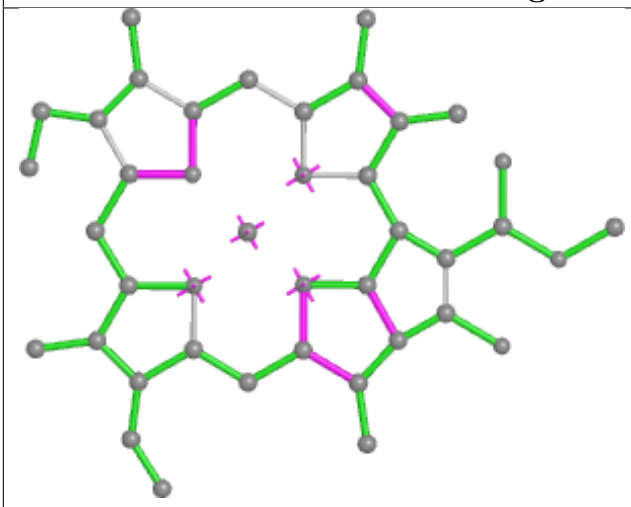


Rings

Ligand CLA 3 315



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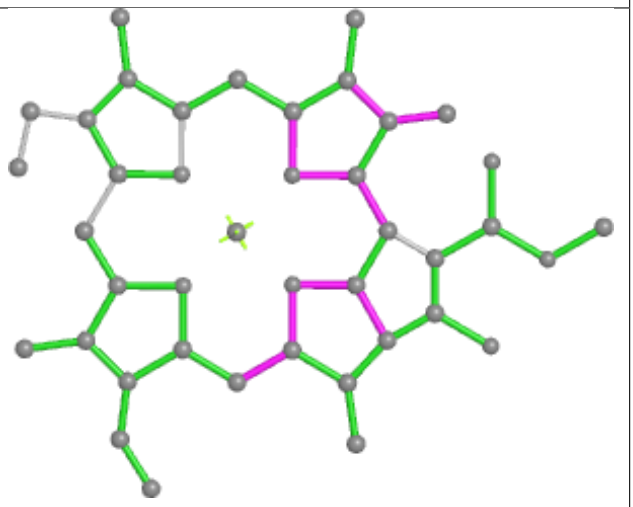
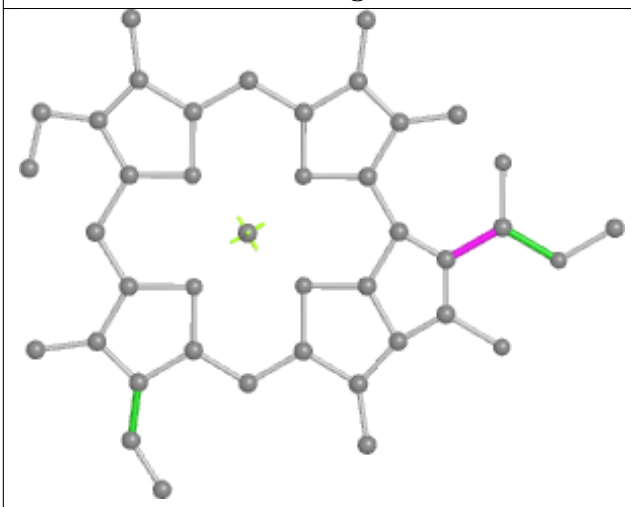


Bond angles



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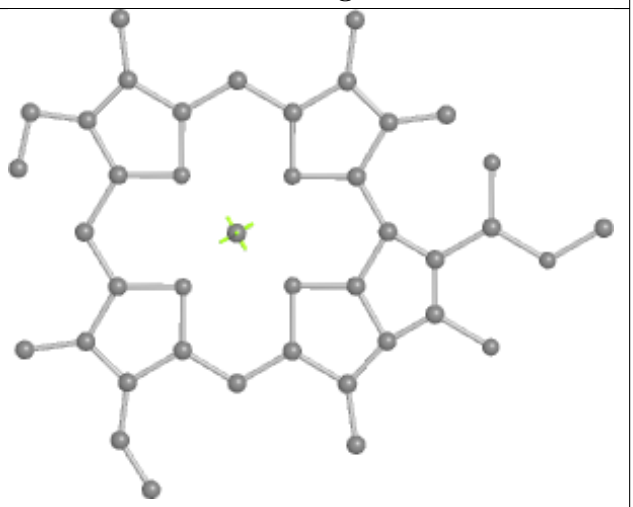
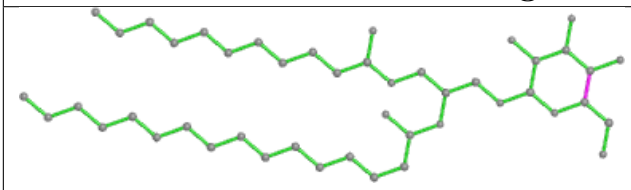


Rings

Ligand LMG D 410



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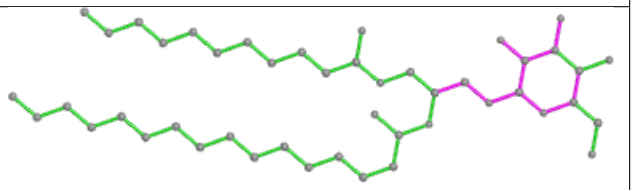

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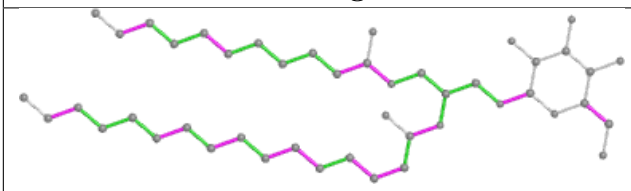

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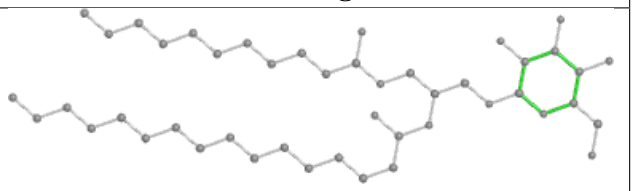
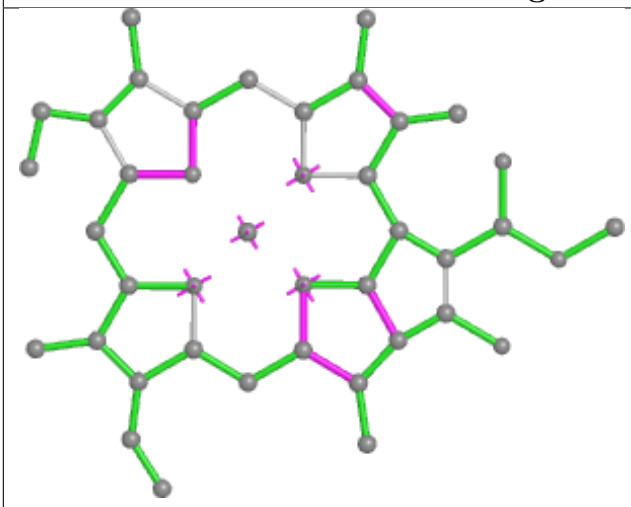
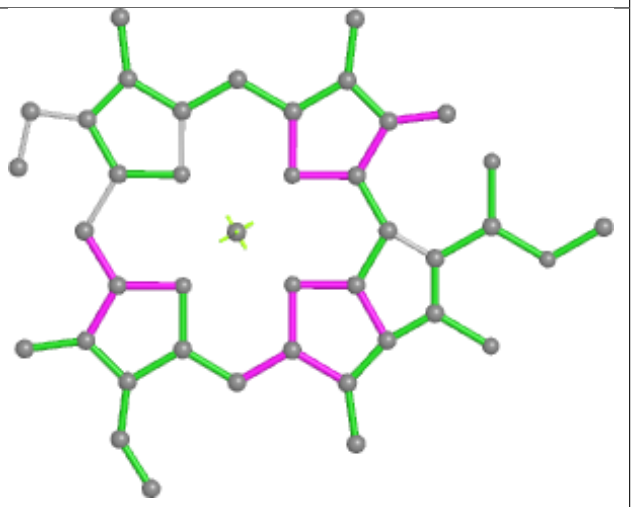


Rings

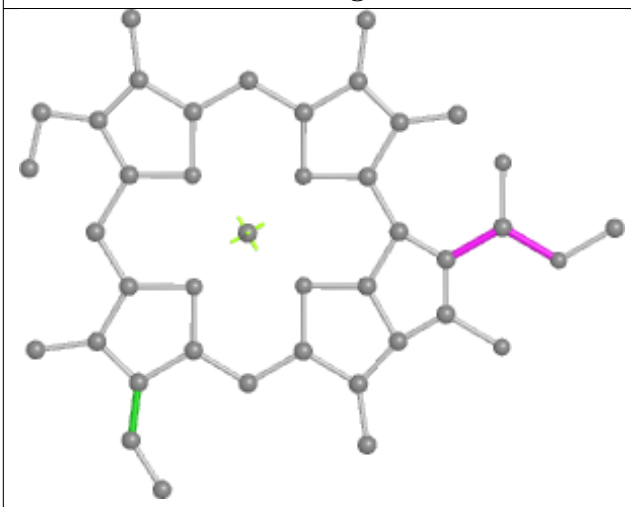
Ligand CLA 4 301



Bond lengths



Bond angles



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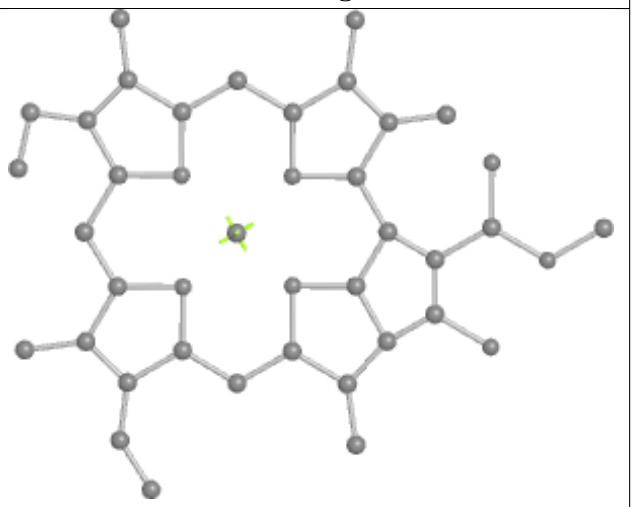
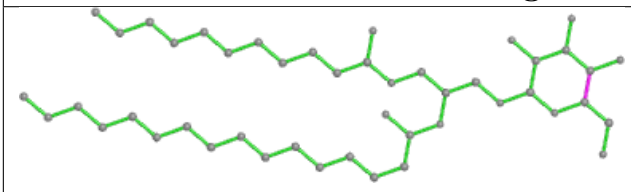


Rings

Ligand LMG d 410



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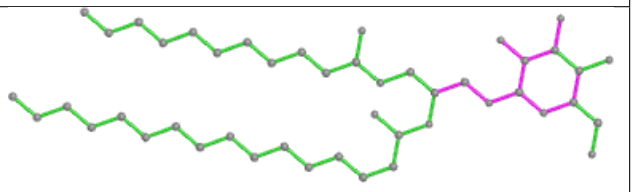

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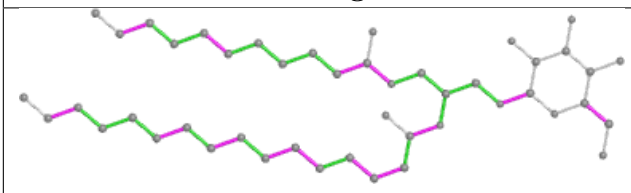

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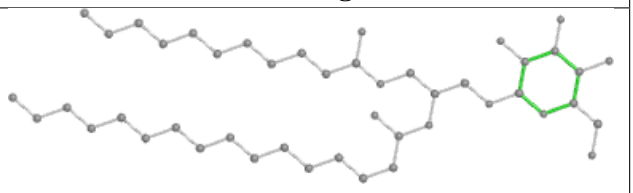
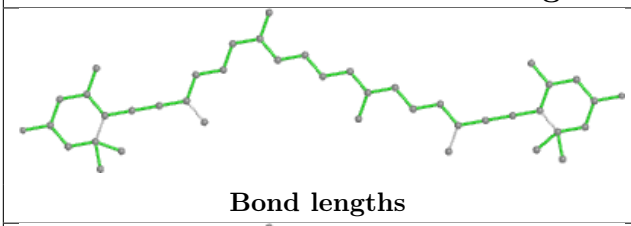


Rings

Ligand II0 1 316



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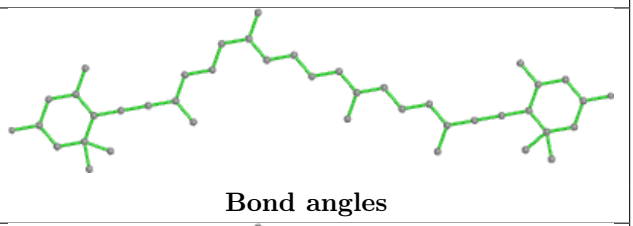

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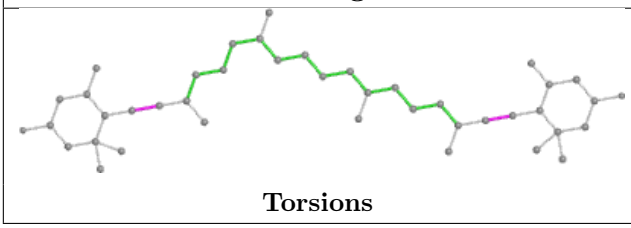

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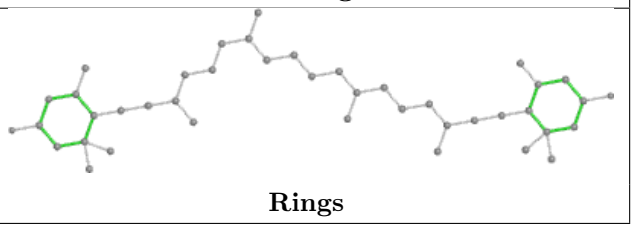
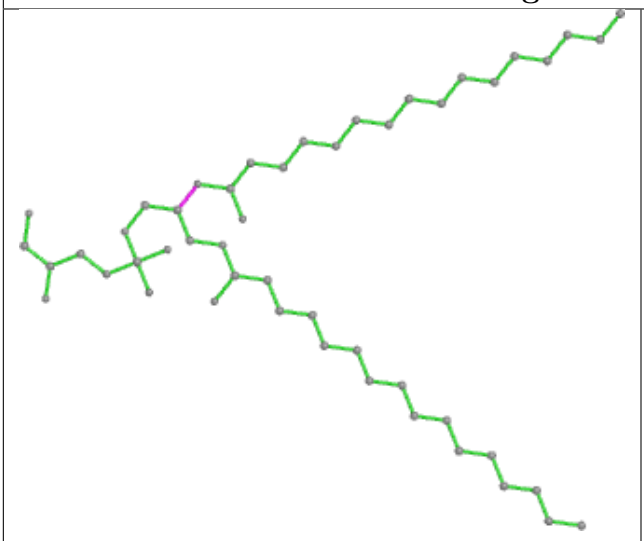
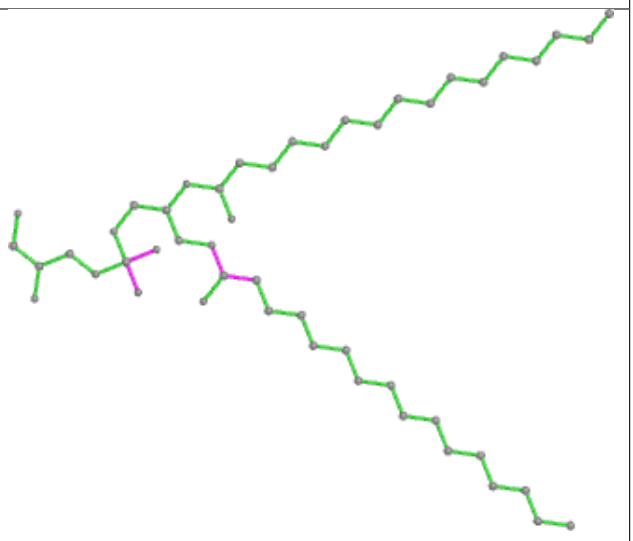


Rings

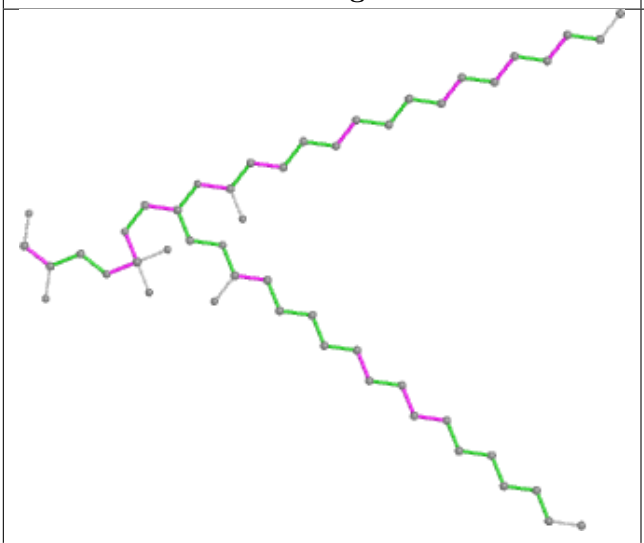
Ligand LHG D 408



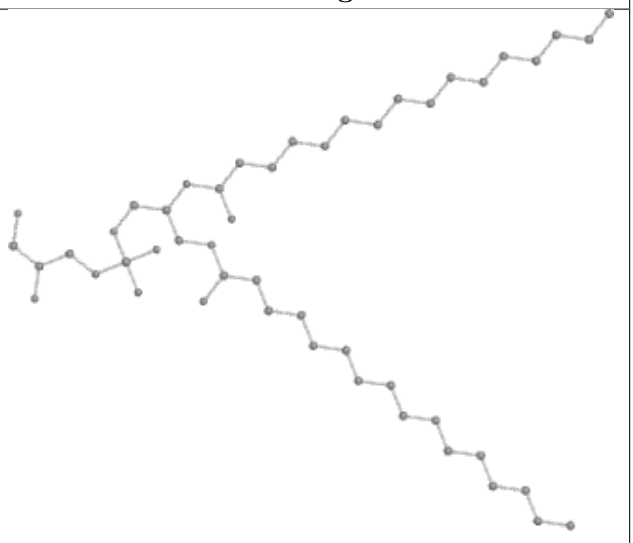
Bond lengths



Bond angles

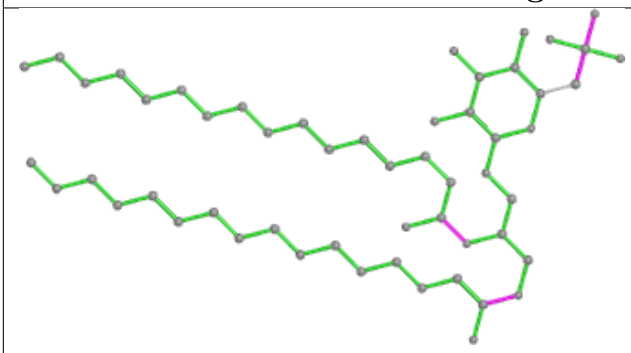


Torsions



Rings

Ligand SQD L 101



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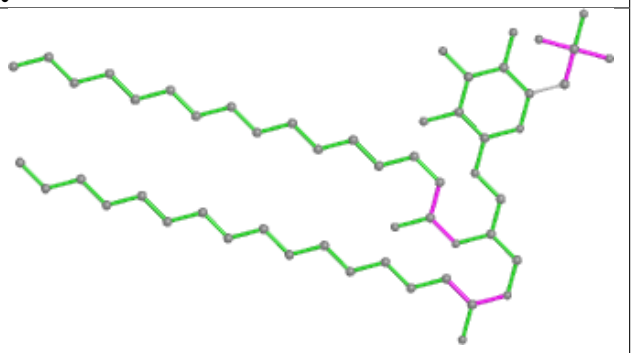
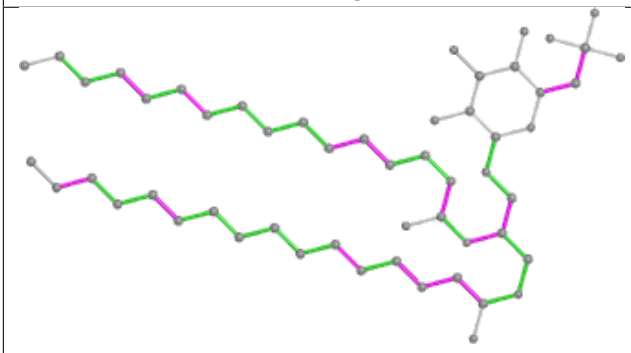


Bond angles



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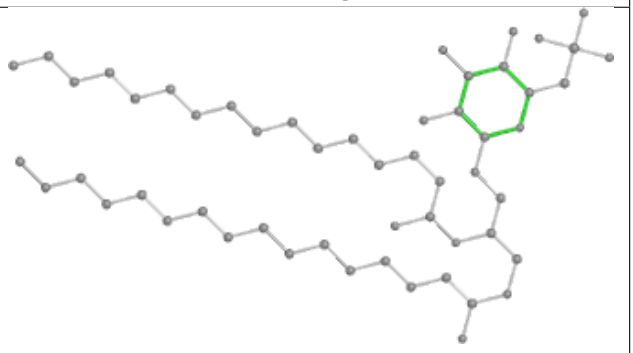
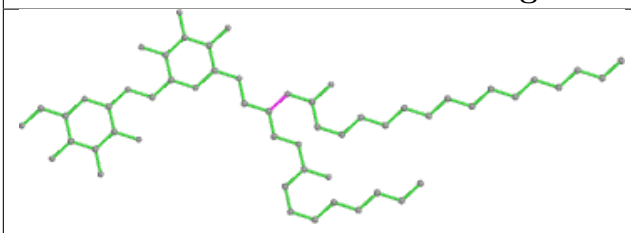


Rings

Ligand DGD C 518



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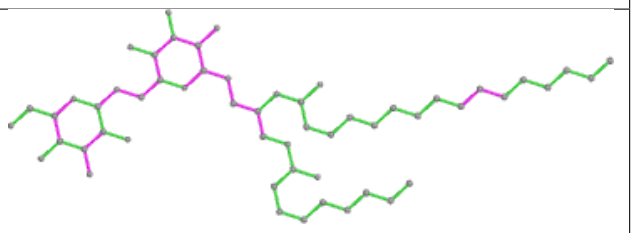
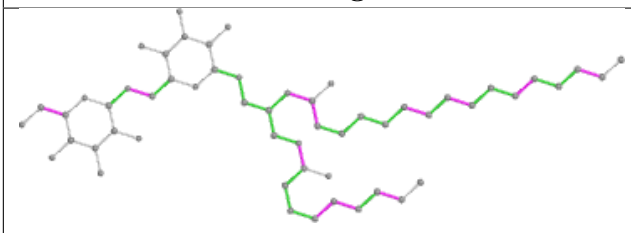


Bond angles



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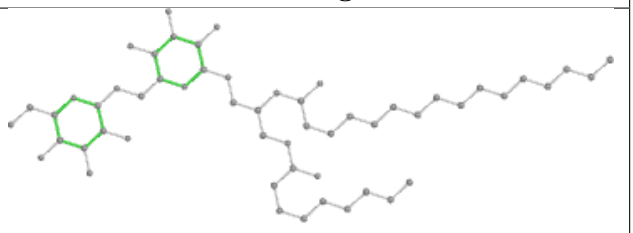
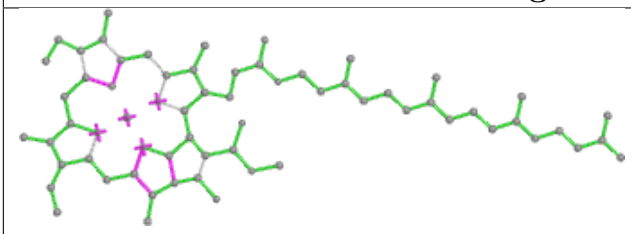


Rings

Ligand CLA c 511



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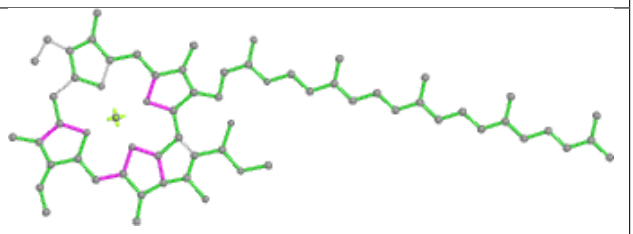
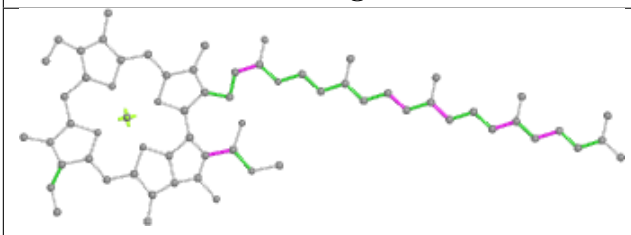


Bond angles



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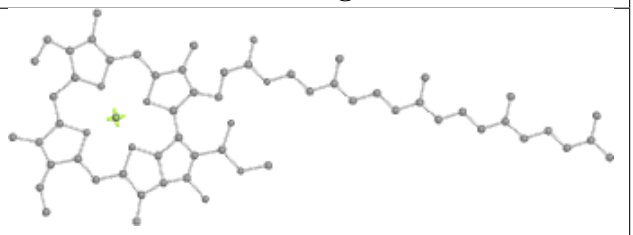
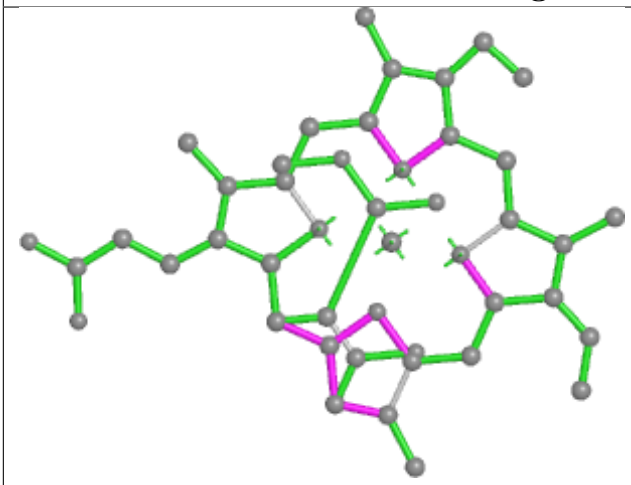
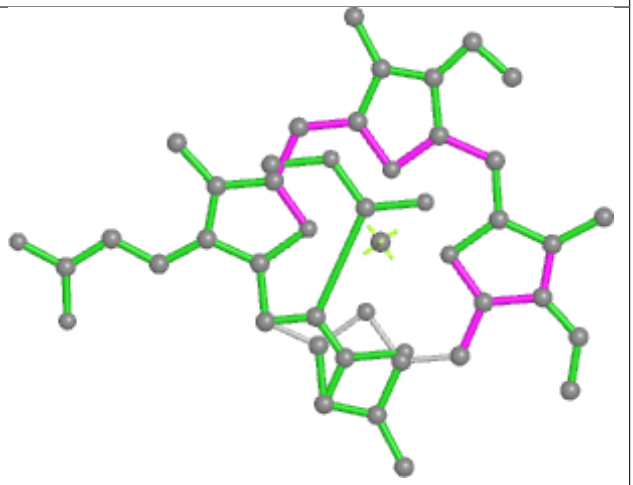


Rings

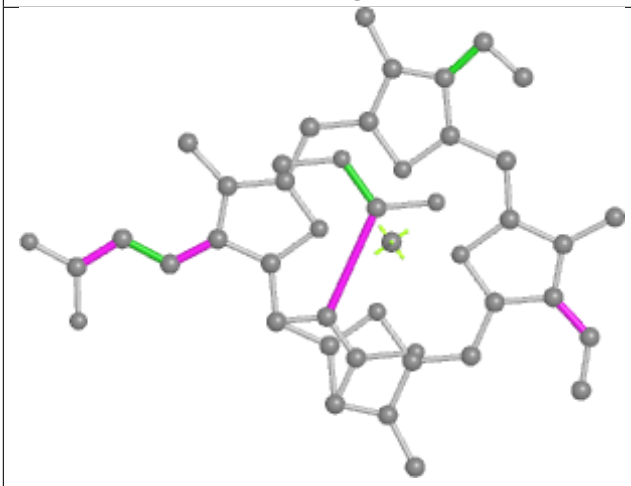
Ligand KC2 9 311



Bond lengths



Bond angles



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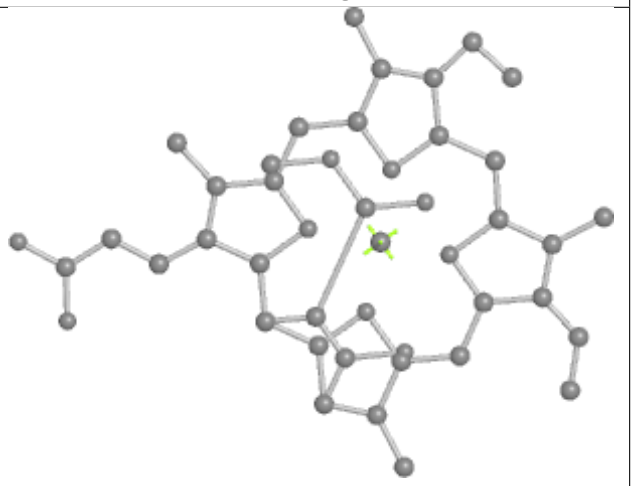
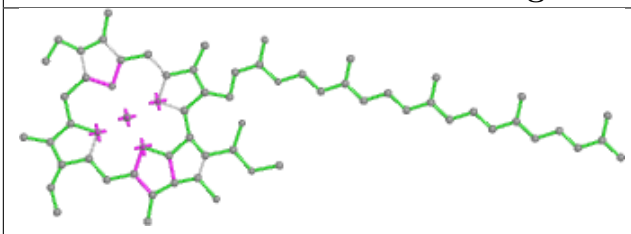
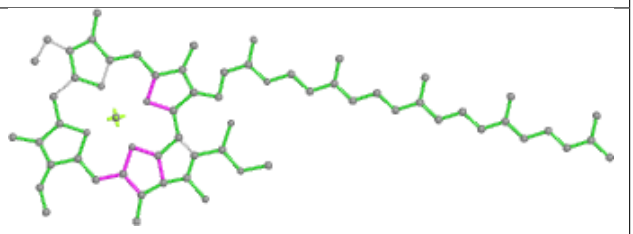


Rings

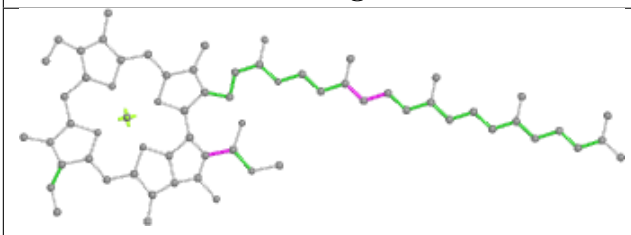
Ligand CLA b 608



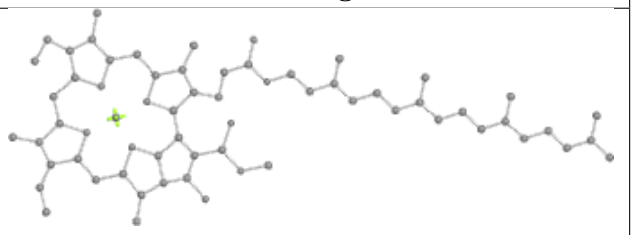
Bond lengths



Bond angles

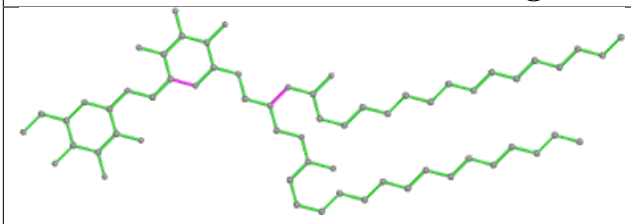


Torsions

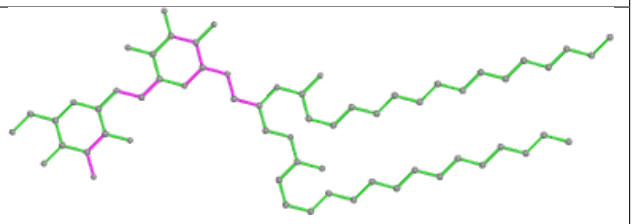


Rings

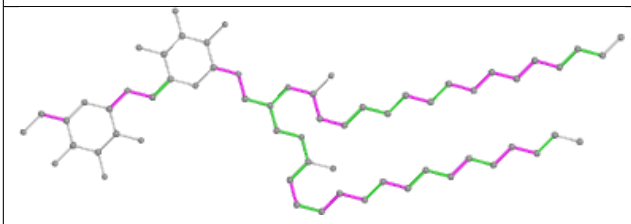
Ligand DGD c 519



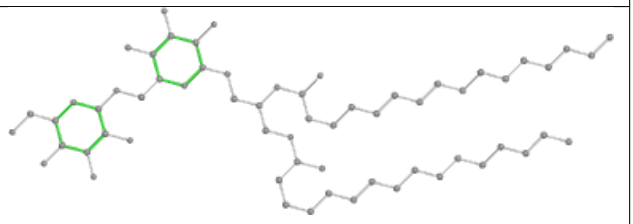
Bond lengths



Bond angles

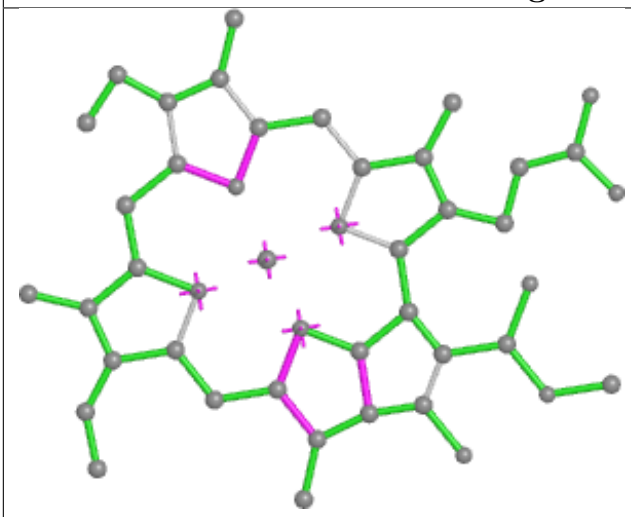


Torsions



Rings

Ligand CLA 5 304



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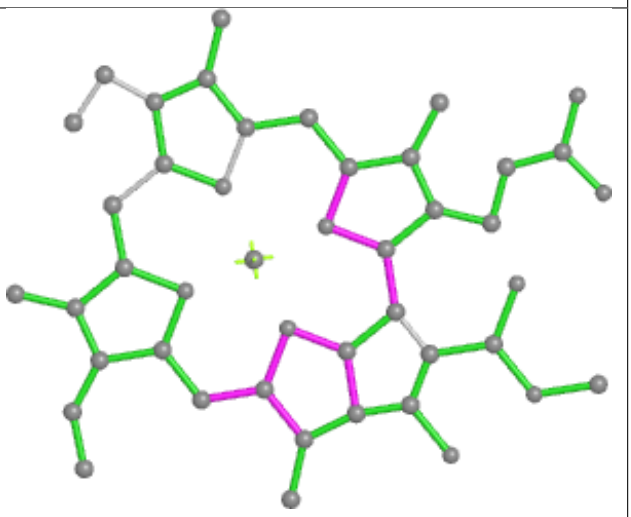
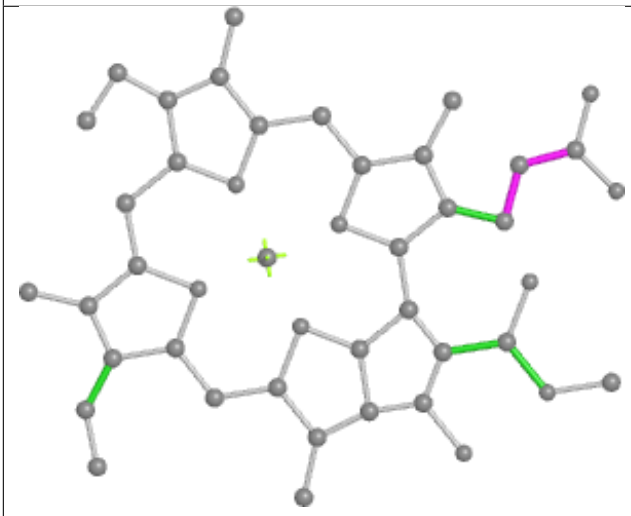


Bond angles



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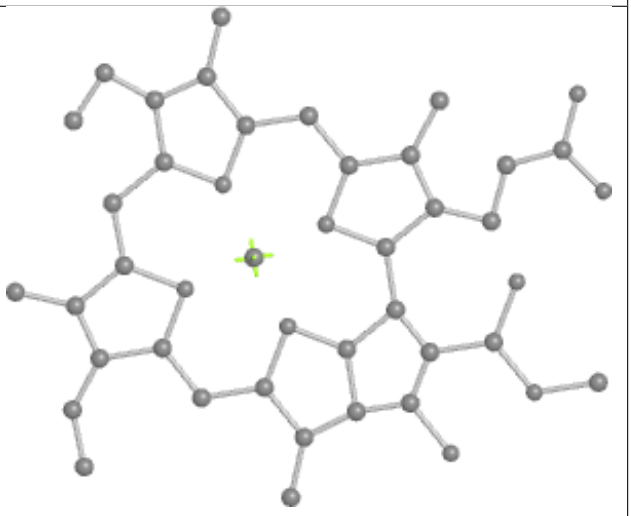
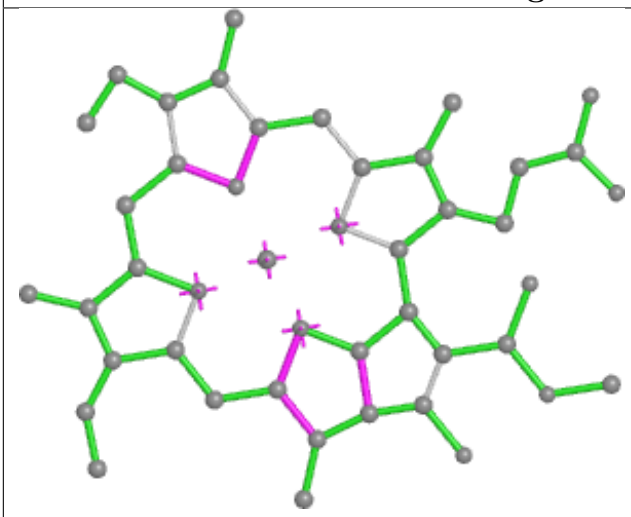


Rings

Ligand CLA b 615



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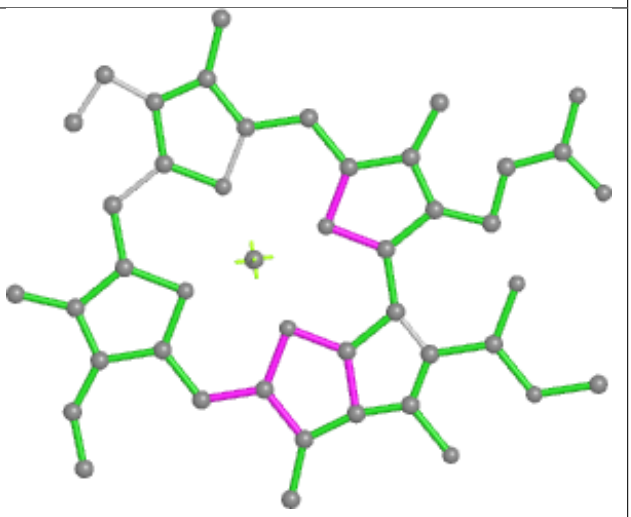
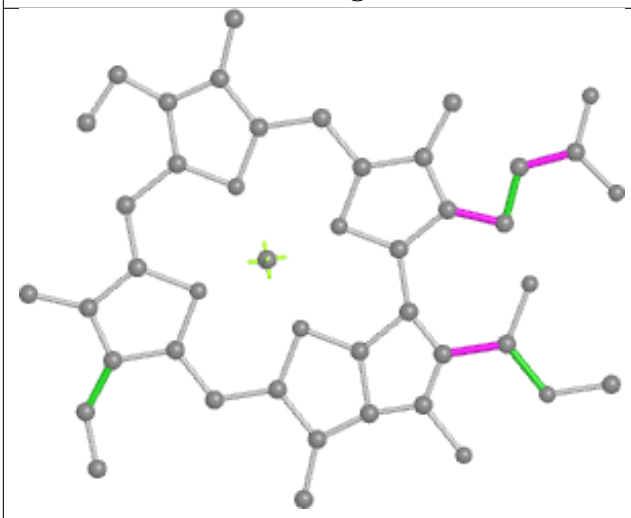


Bond angles



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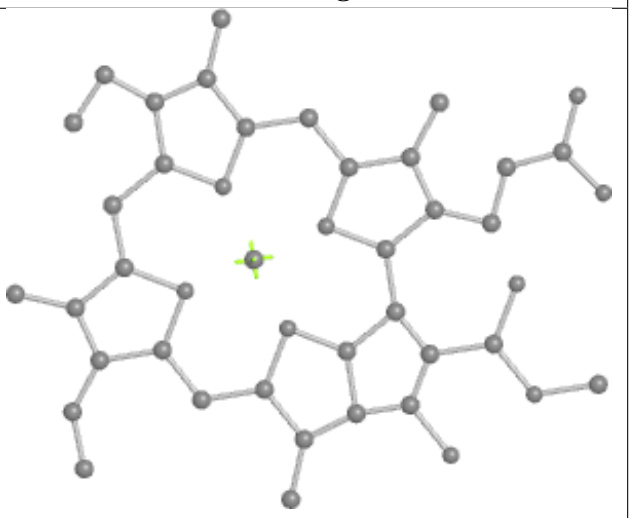
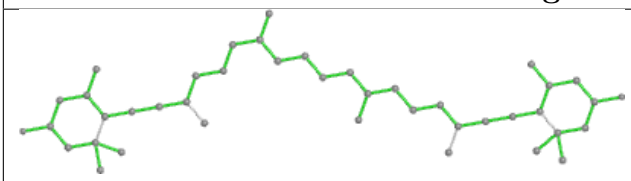


Rings

Ligand II0 0 314



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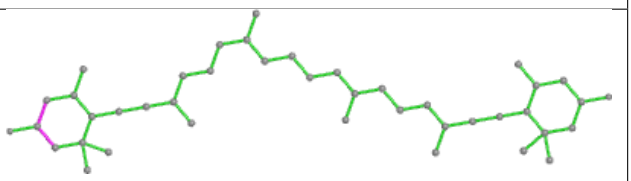
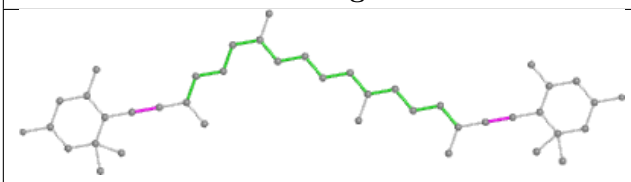
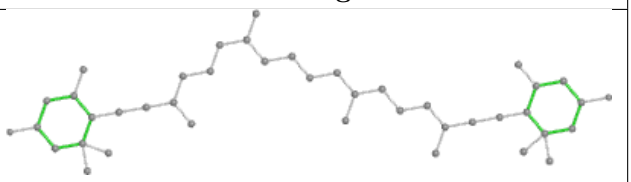


Bond angles

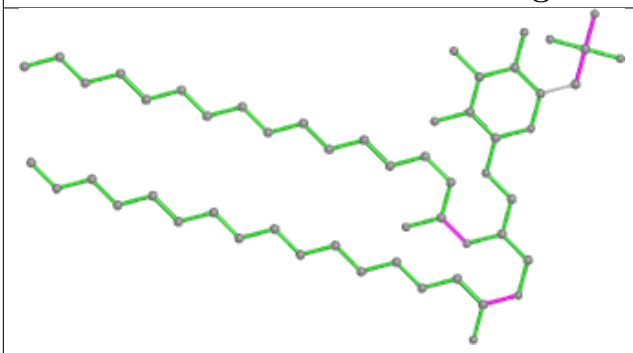


Torsions

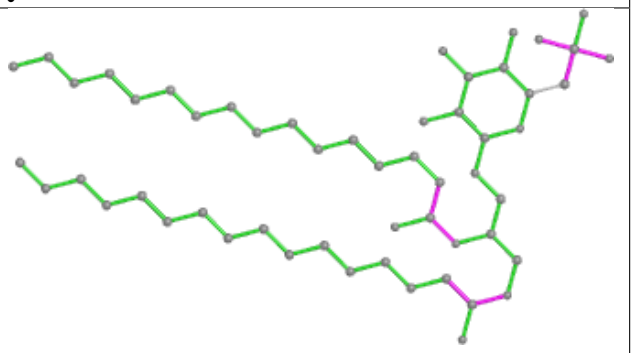


Rings

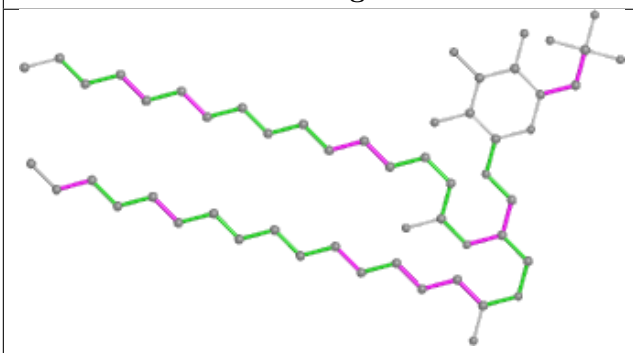
Ligand SQD l 101



Bond lengths



Bond angles



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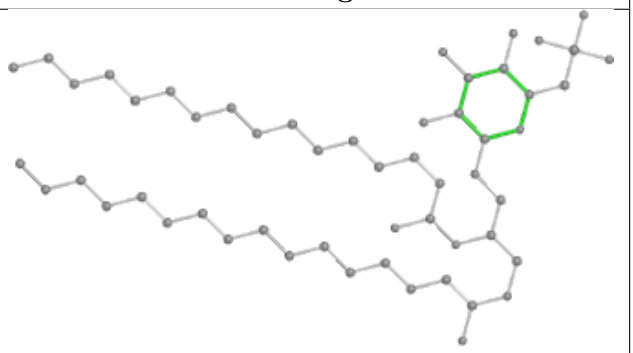
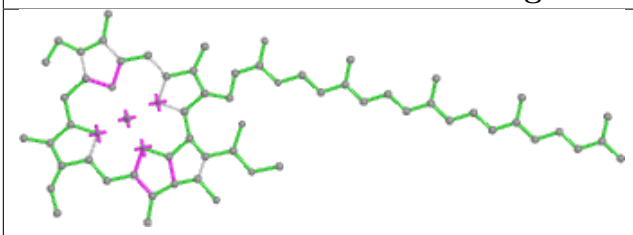


Rings

Ligand CLA B 614



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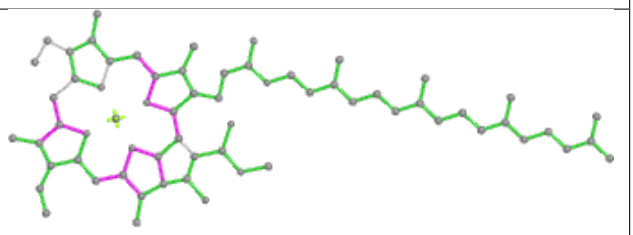

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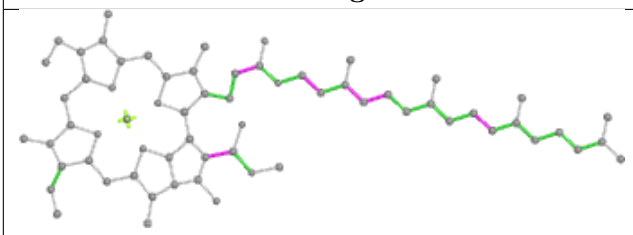

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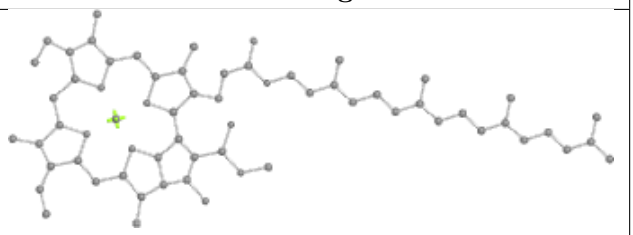
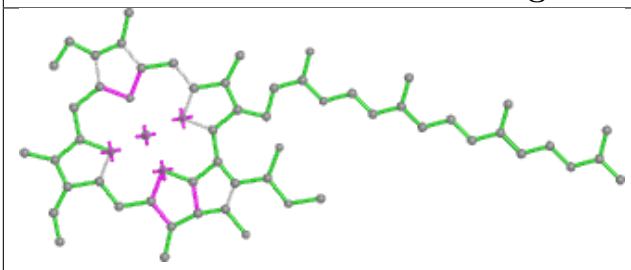


Rings

Ligand CLA 1 305



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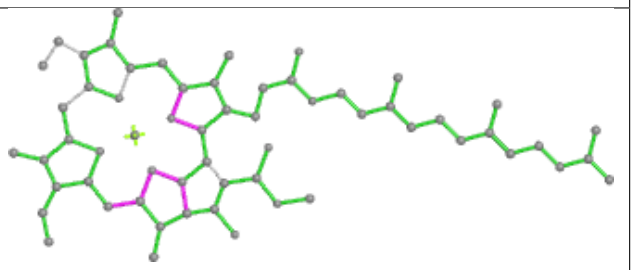
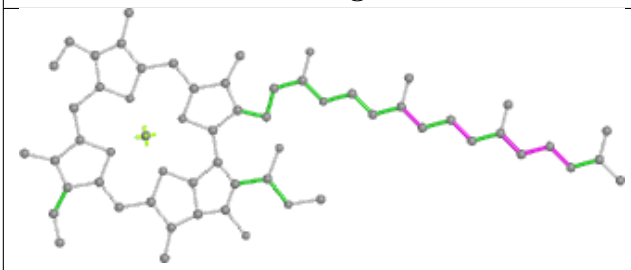


Bond angles



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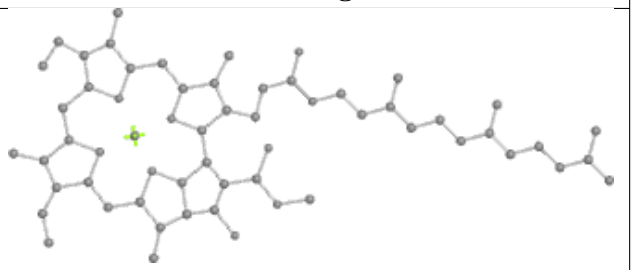
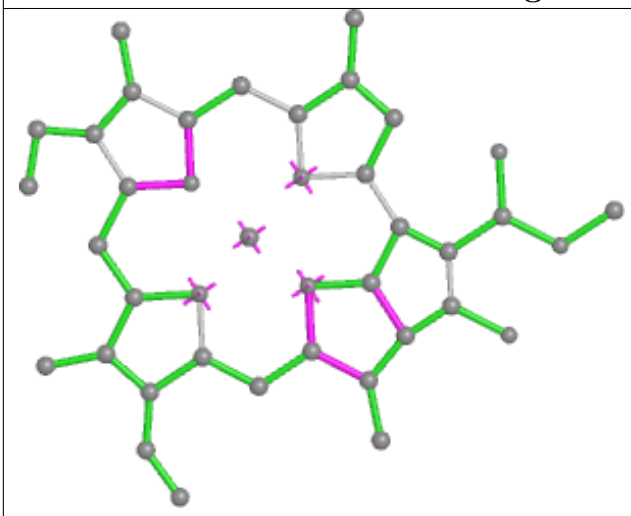
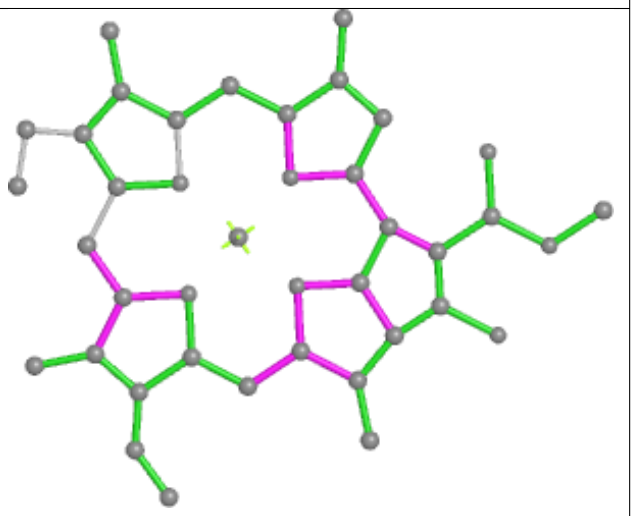


Rings

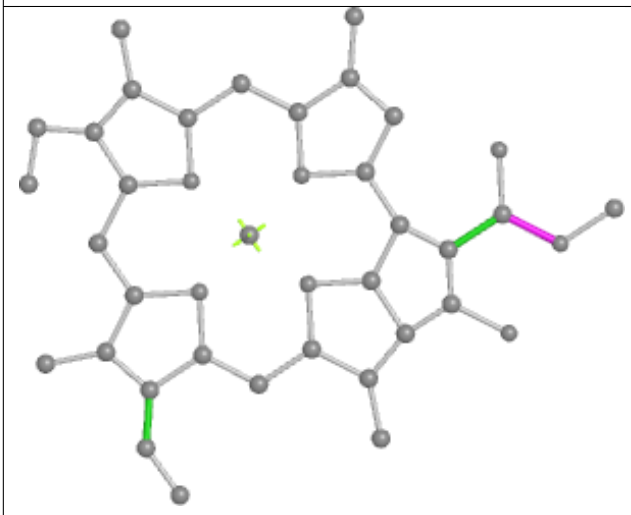
Ligand CLA B 618



Bond lengths



Bond angles



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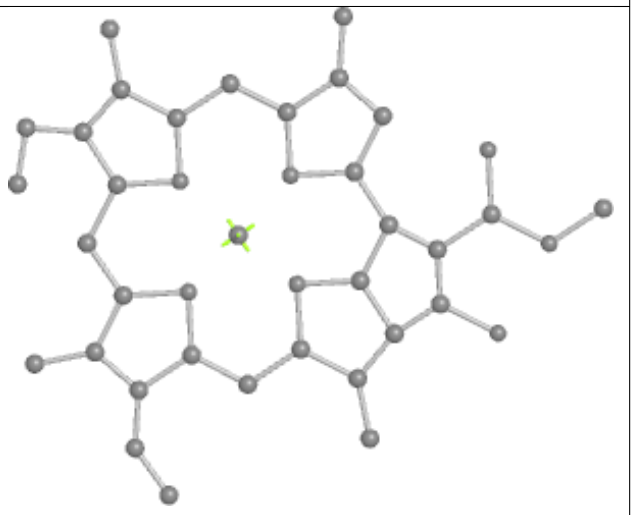
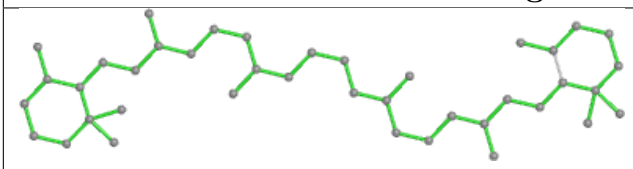


Rings

Ligand 8CT H 102



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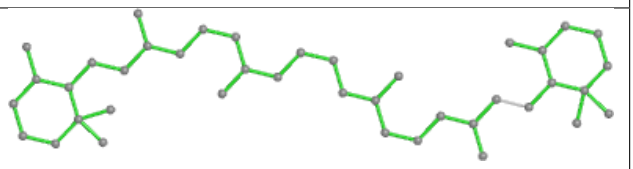
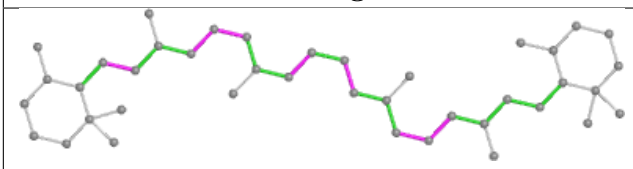
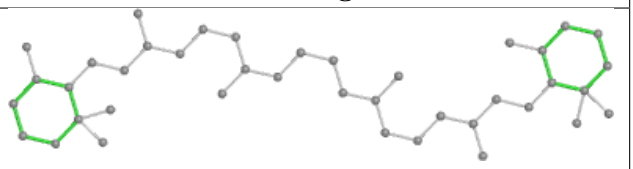


Bond angles

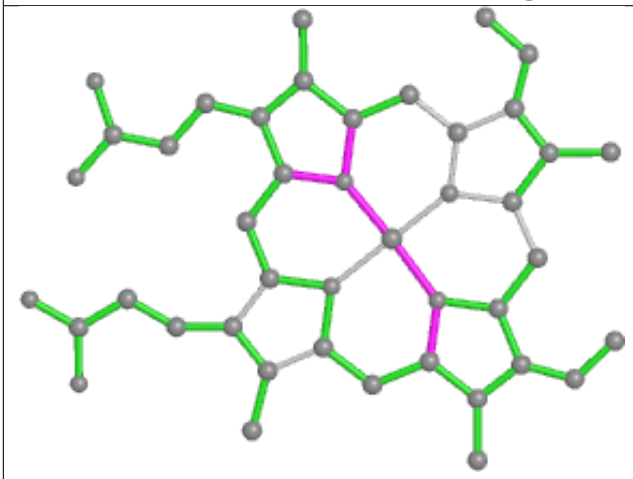


Torsions

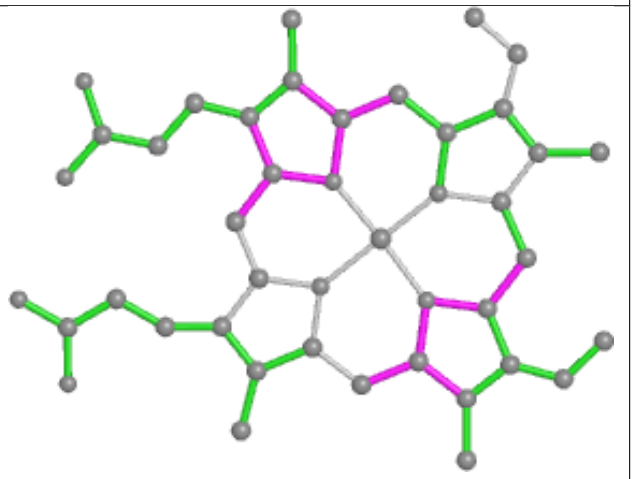


Rings

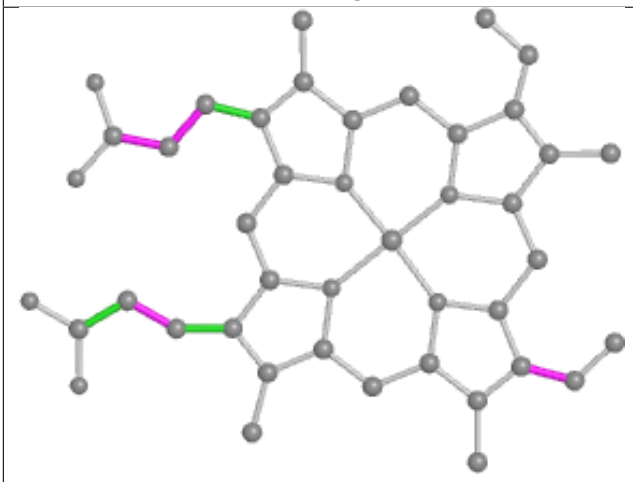
Ligand HEM F 101



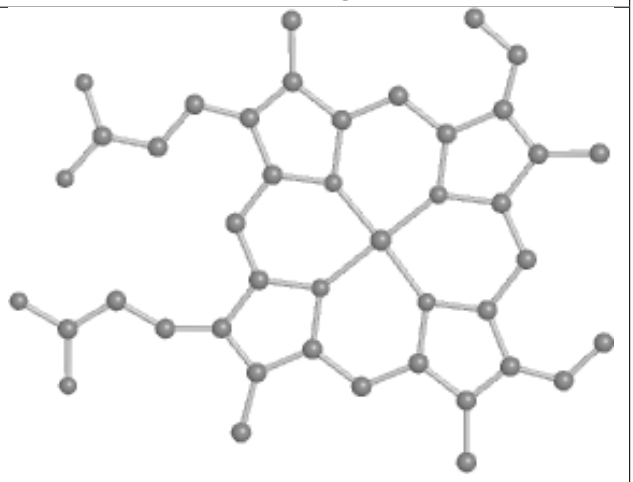
Bond lengths



Bond angles

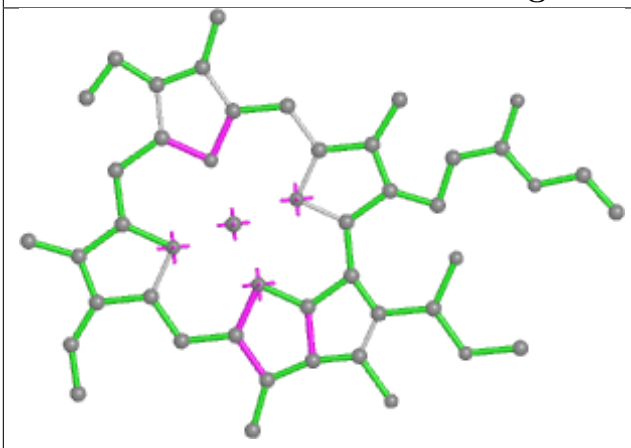


Torsions



Rings

Ligand CLA 0 304



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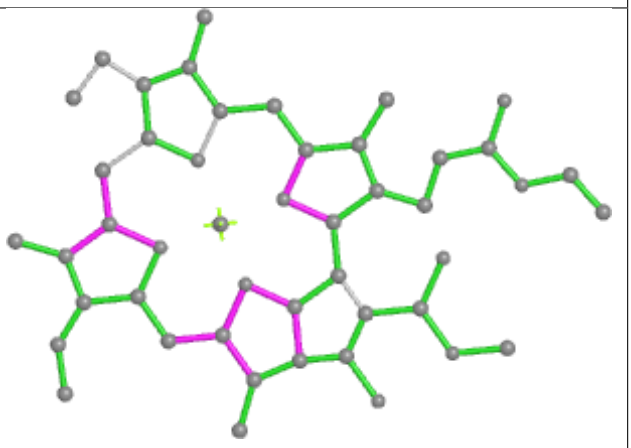
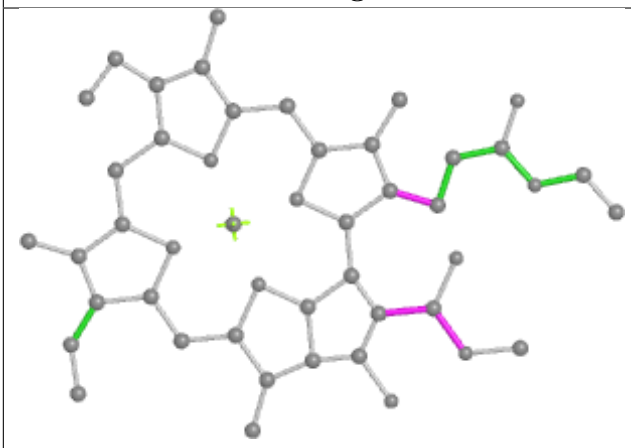


Bond angles



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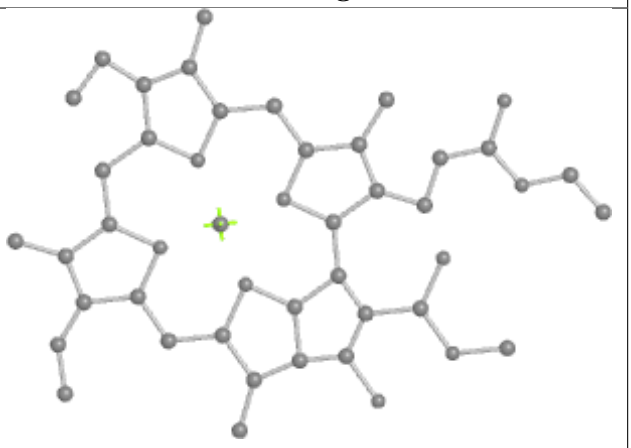
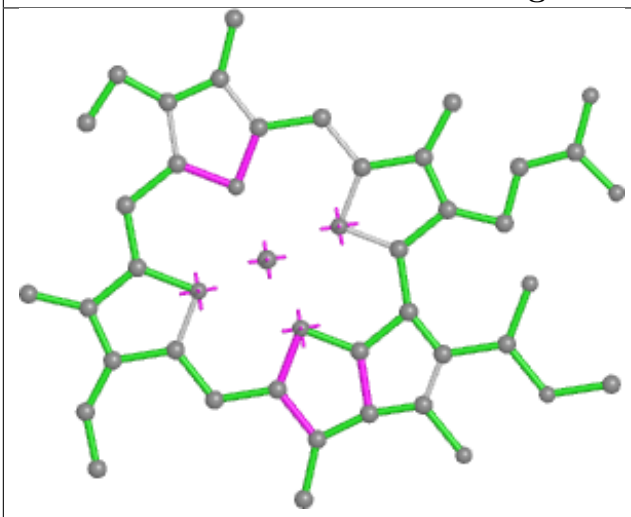


Rings

Ligand CLA 9 304



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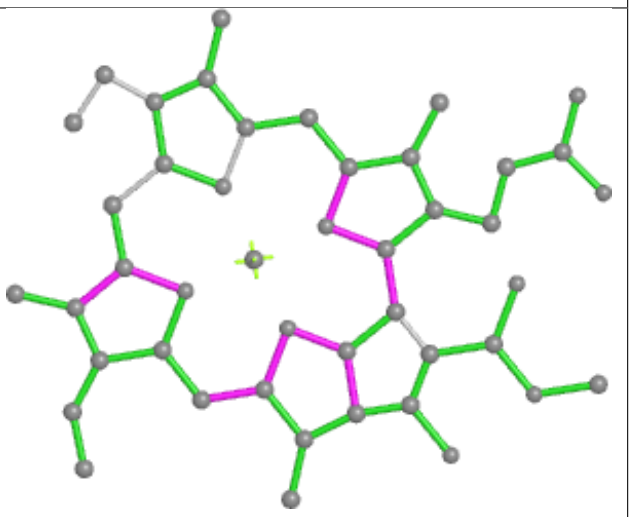
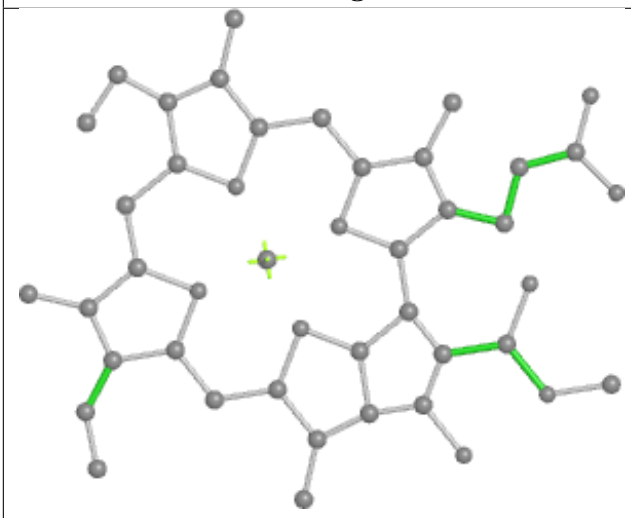


Bond angles



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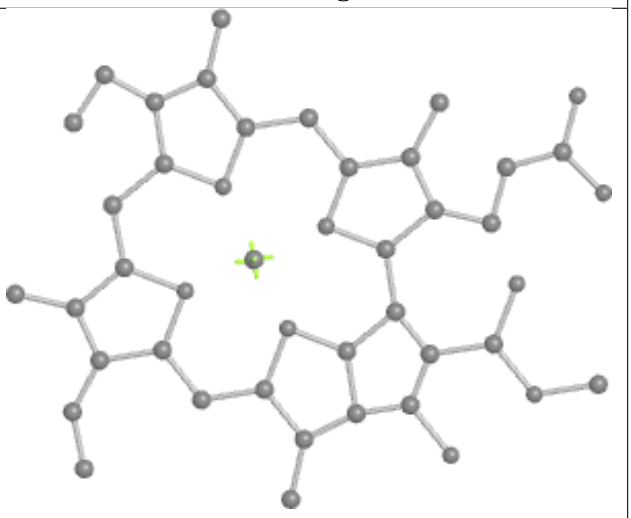
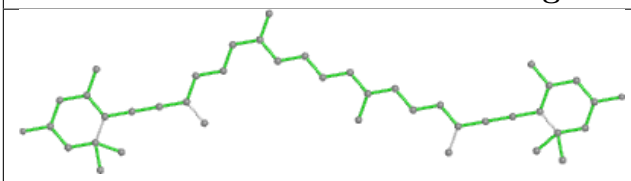


Rings

Ligand II0 g 312



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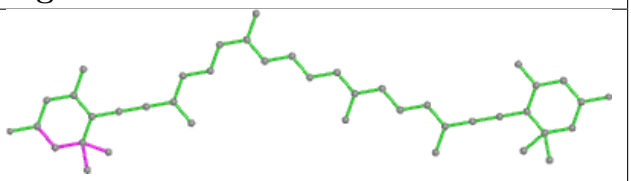
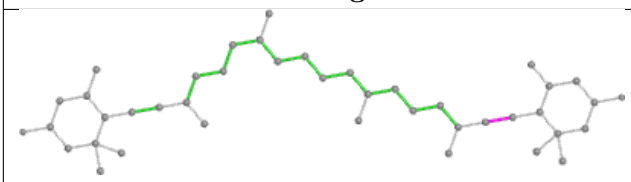


Bond angles



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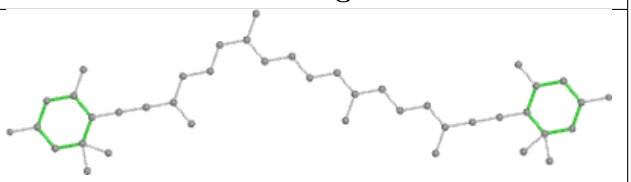
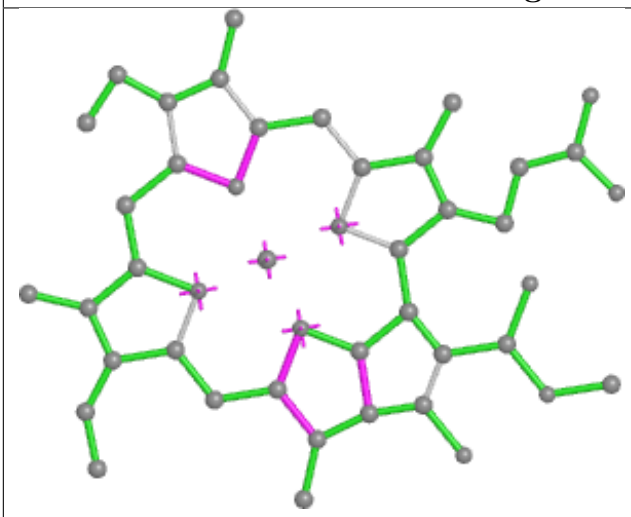


Rings

Ligand CLA B 615



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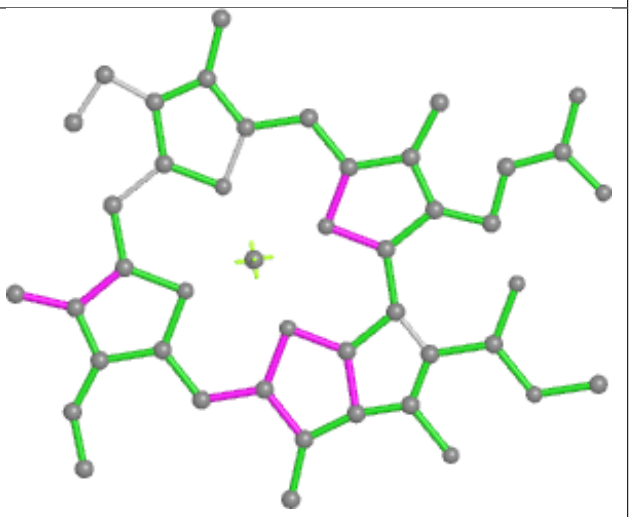
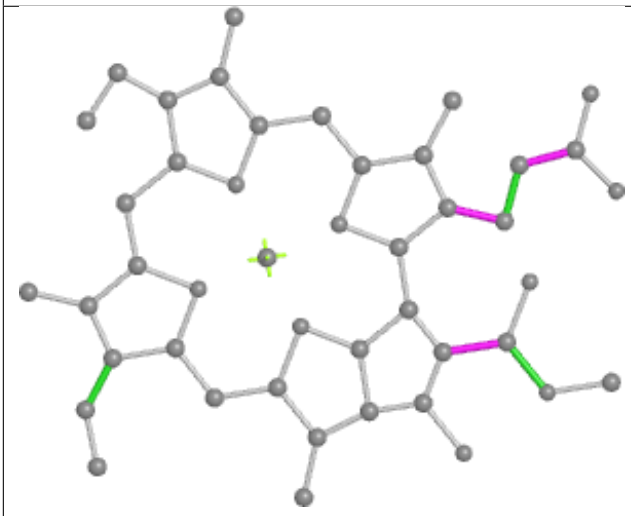
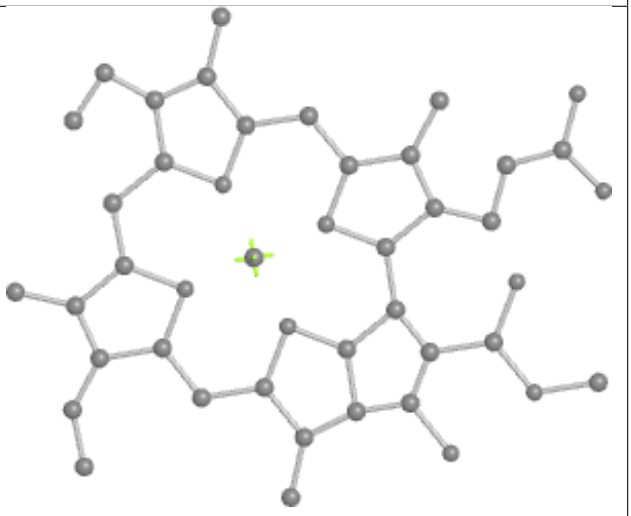


Bond angles

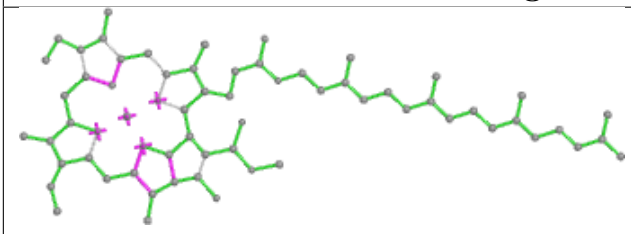


Torsions

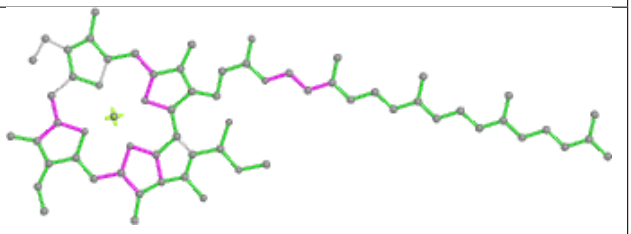


Rings

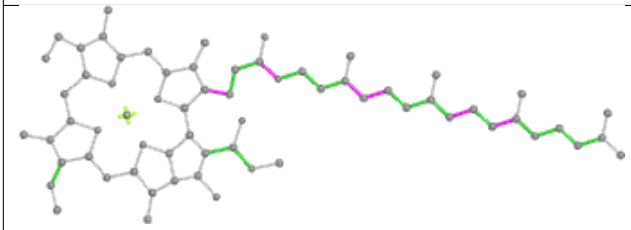
Ligand CLA A 412



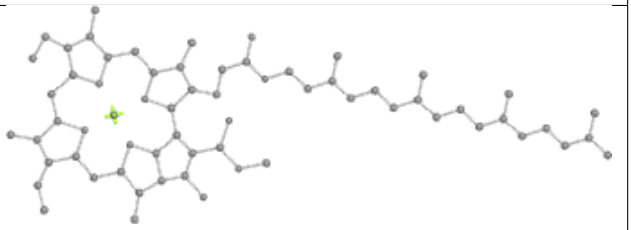
Bond lengths



Bond angles

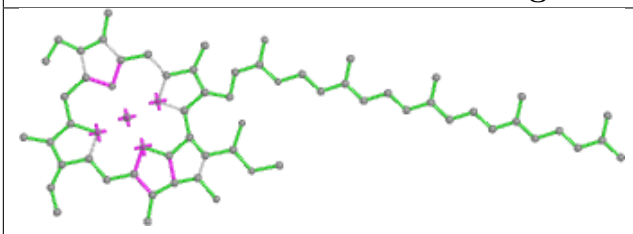


Torsions

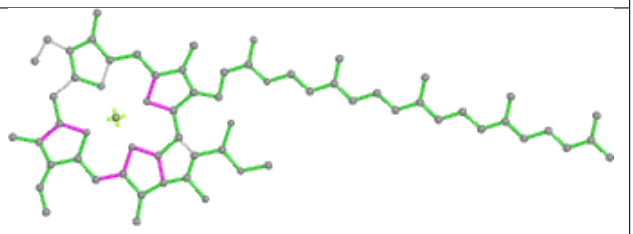


Rings

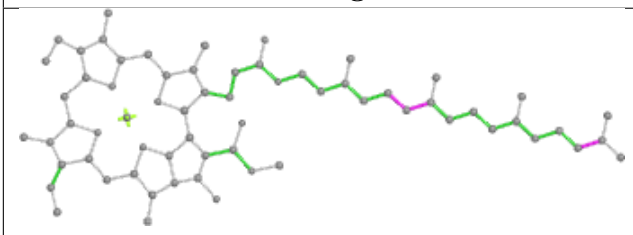
Ligand CLA c 514



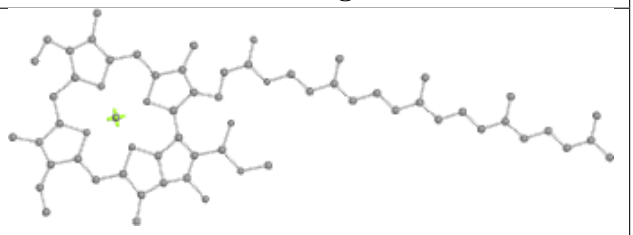
Bond lengths



Bond angles

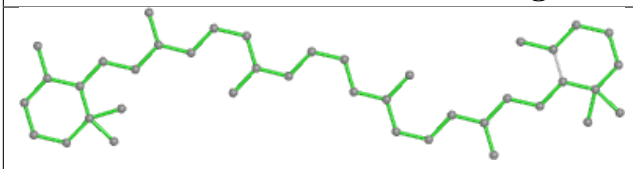


Torsions



Rings

Ligand 8CT b 621



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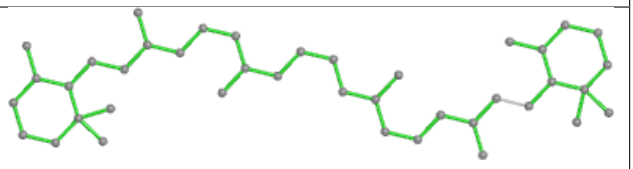

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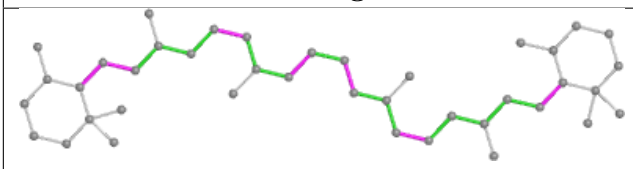

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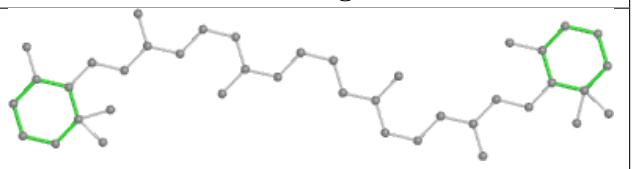
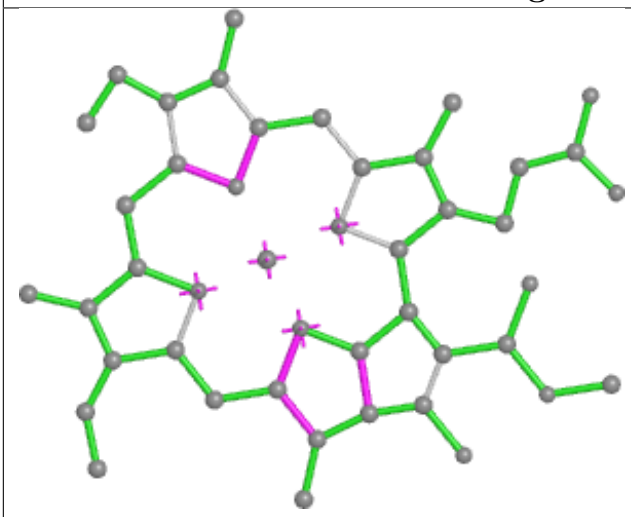


Rings

Ligand CLA 1 301



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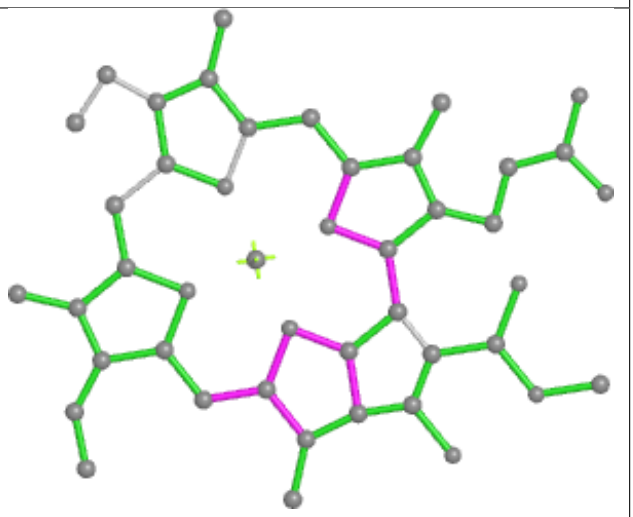
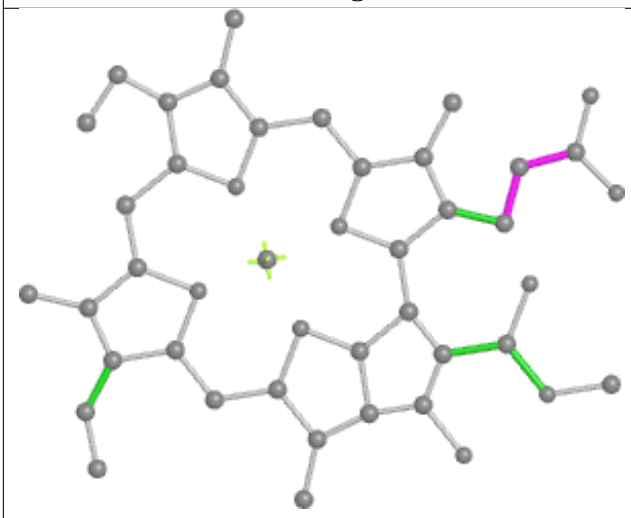


Bond angles



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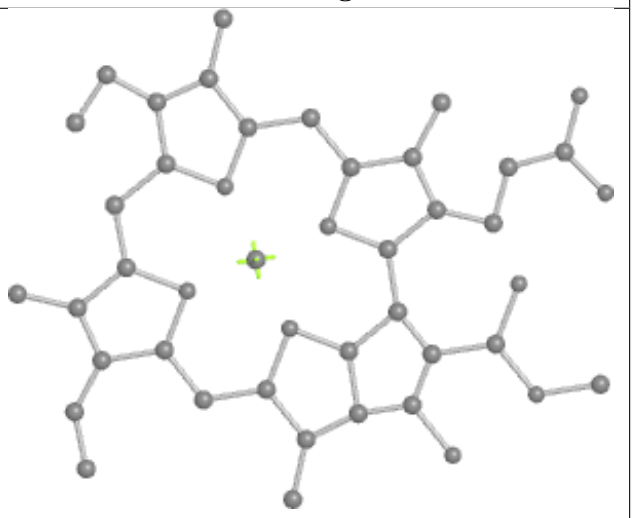
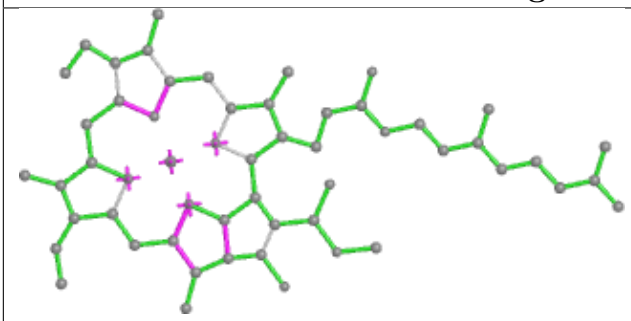


Rings

Ligand CLA 7 304



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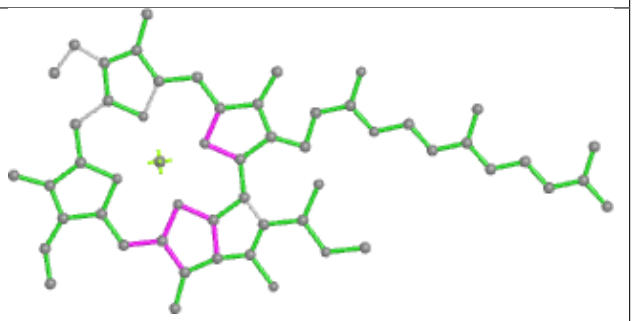
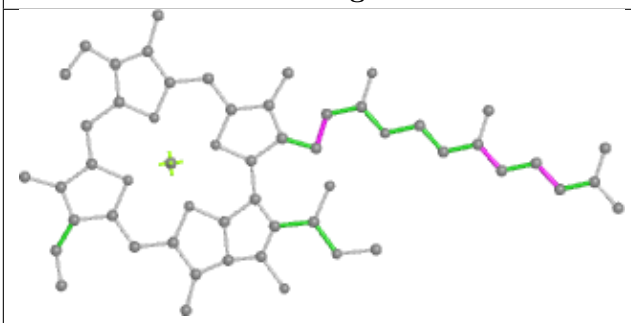


Bond angles



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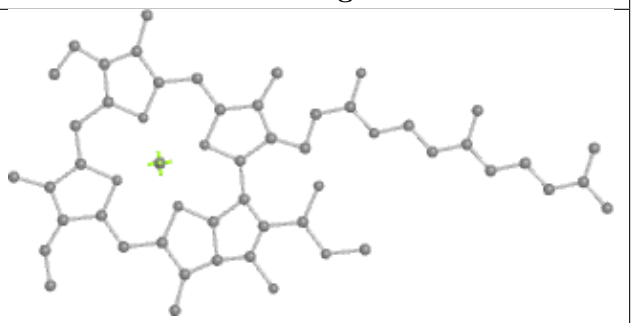
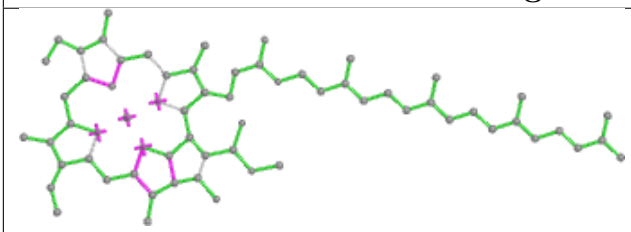


Rings

Ligand CLA C 511



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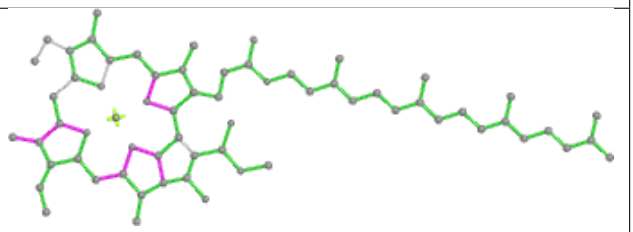
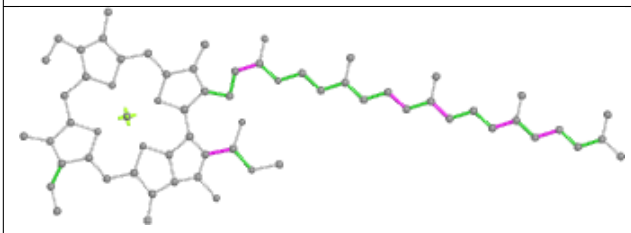


Bond angles



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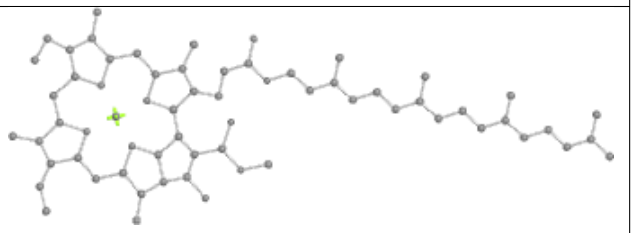
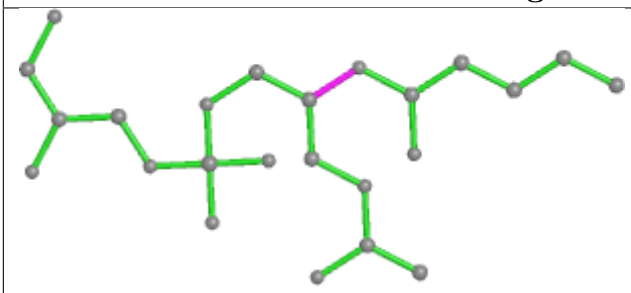


Rings

Ligand LHG 9 321



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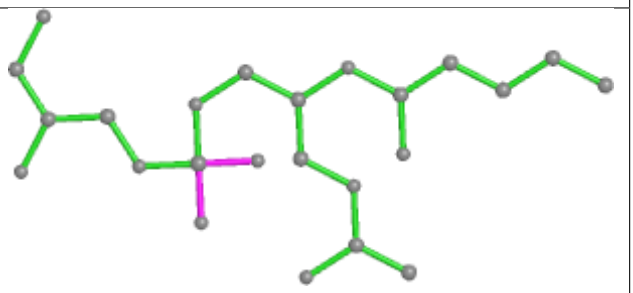
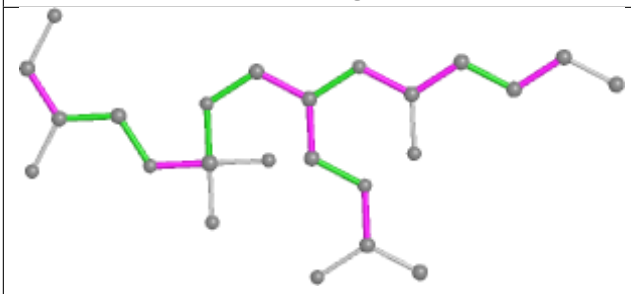


Bond angles



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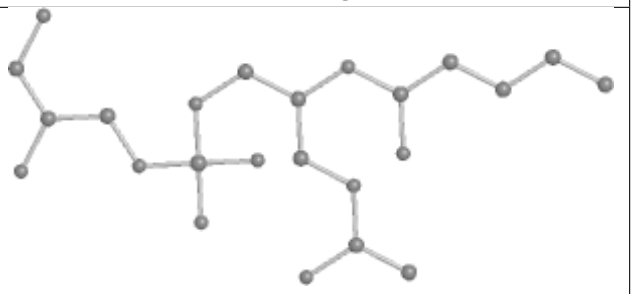
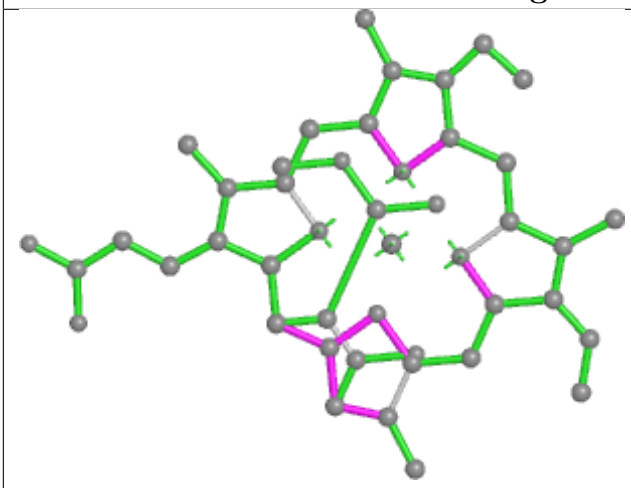
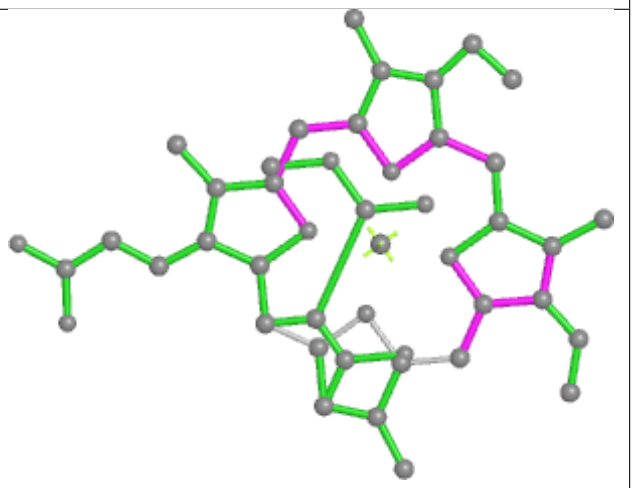


Rings

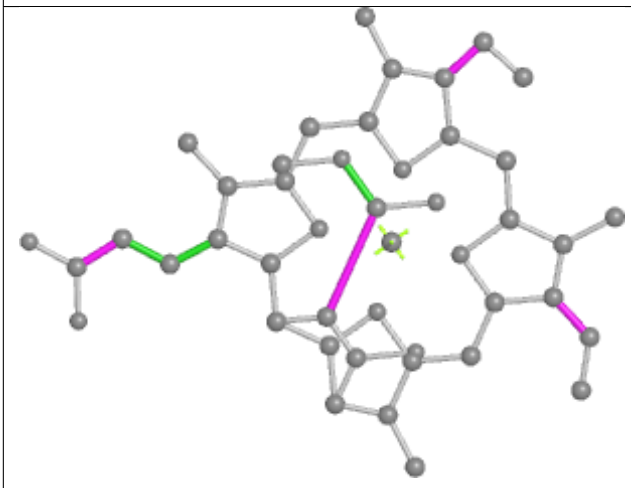
Ligand KC2 1 310



Bond lengths



Bond angles



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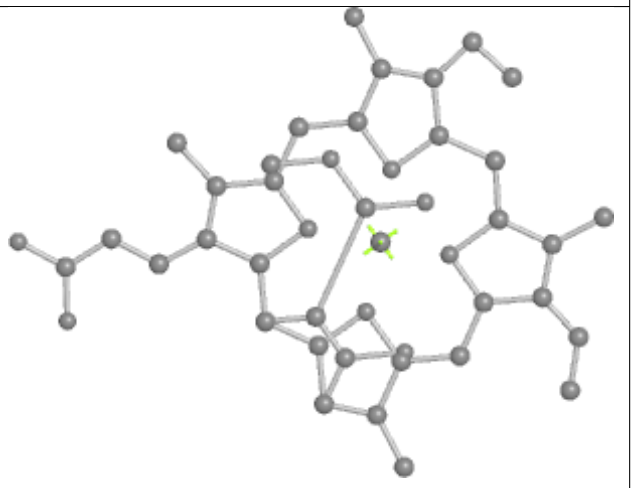
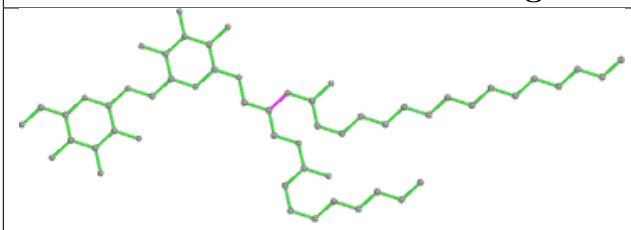


Rings

Ligand DGD c 518



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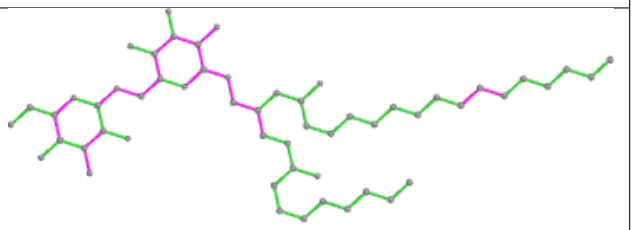
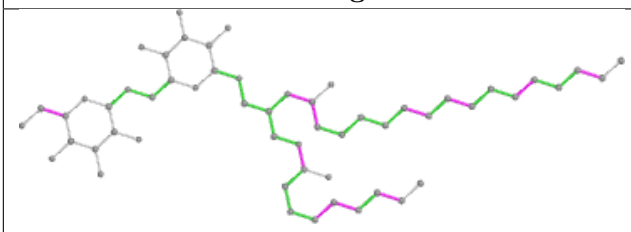


Bond angles



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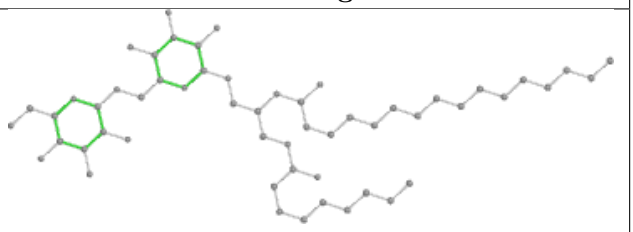
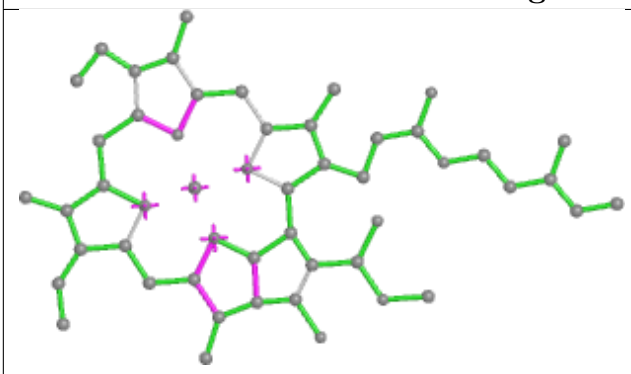


Rings

Ligand CLA 7 308



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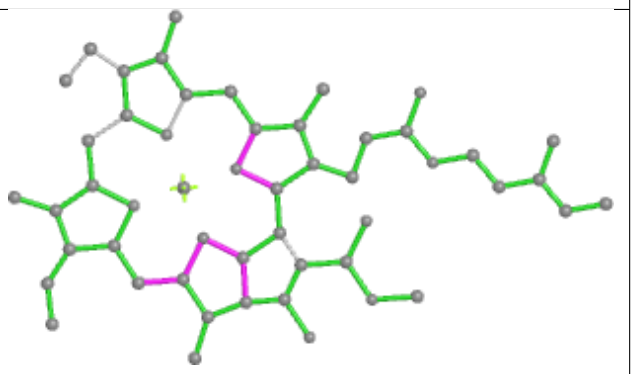
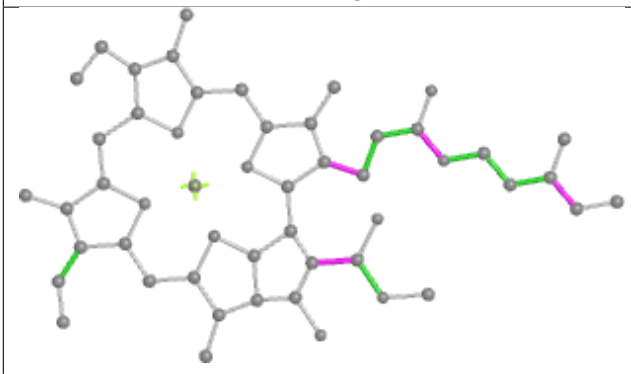


Bond angles



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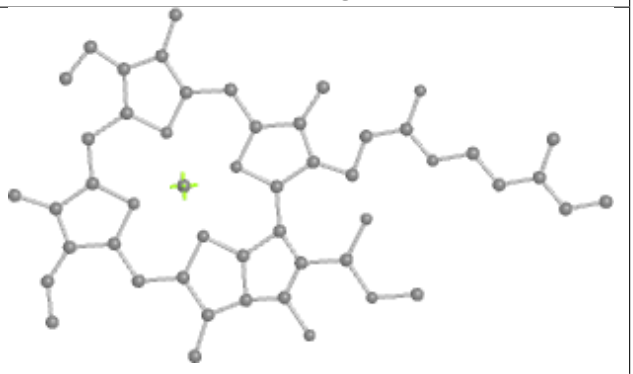
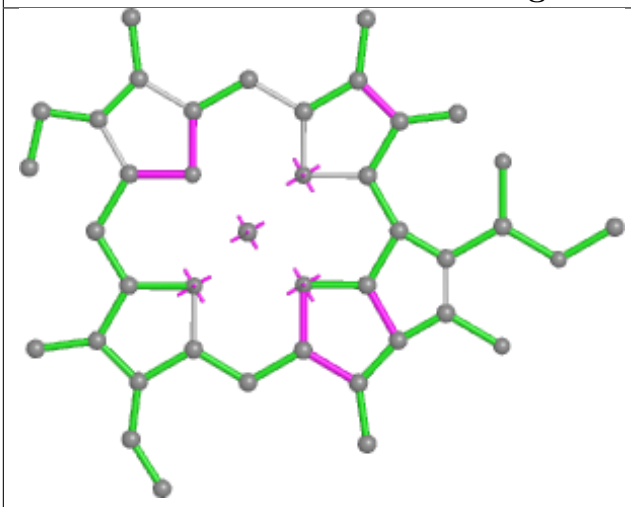


Rings

Ligand CLA g 310



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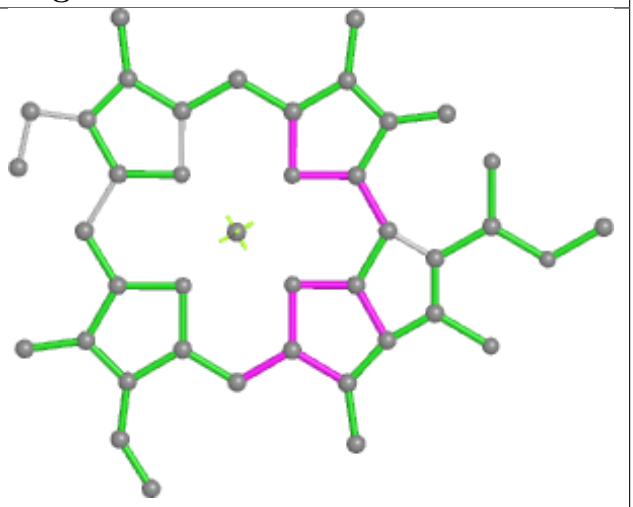
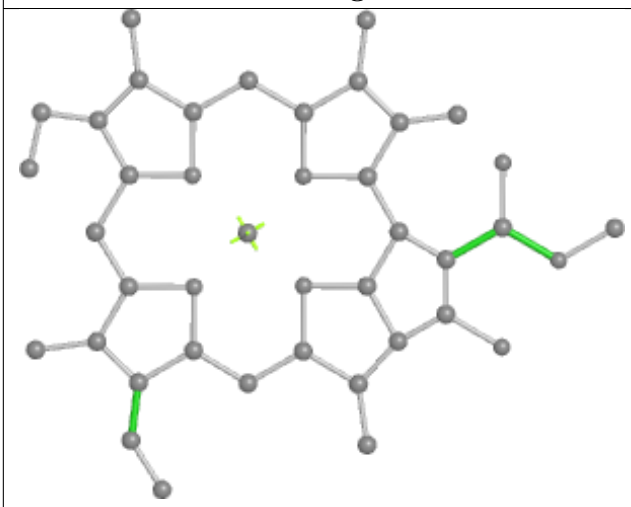
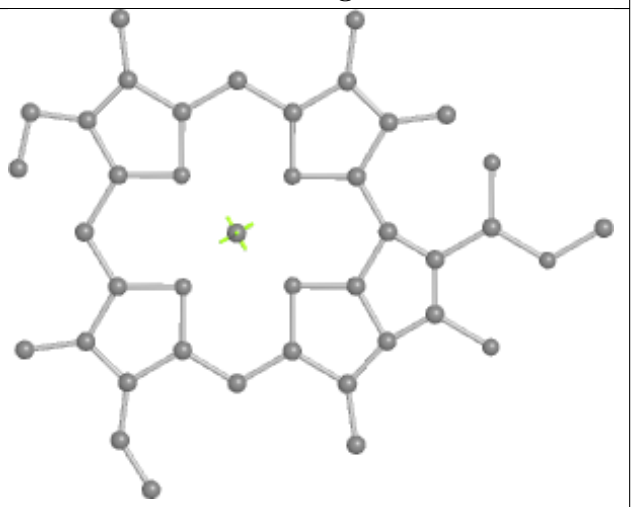


Bond angles

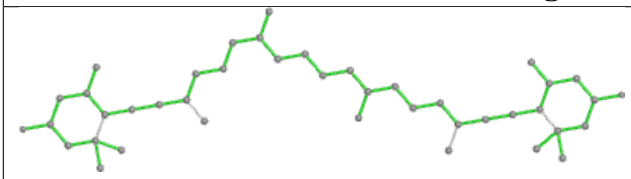


Torsions



Rings

Ligand II0 2 312



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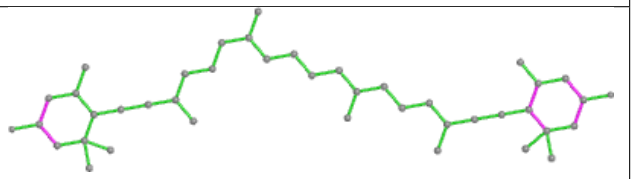
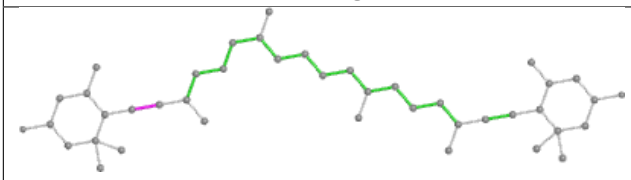
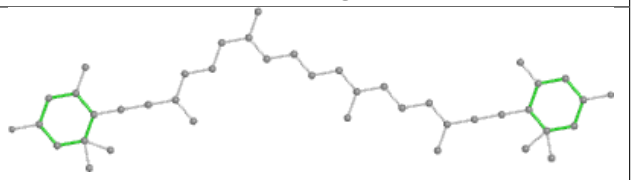


Bond angles

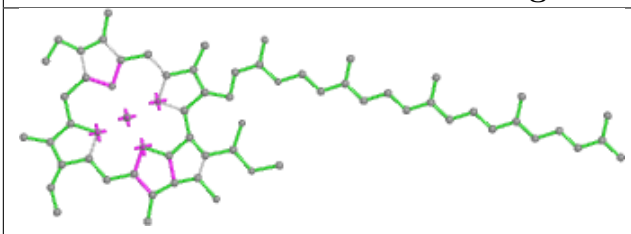


Torsions

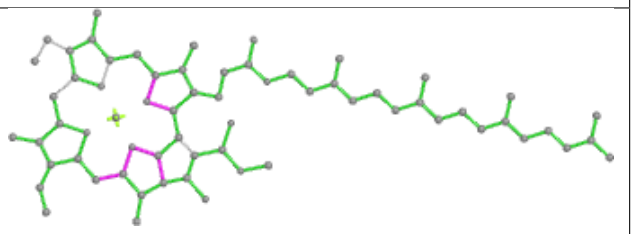


Rings

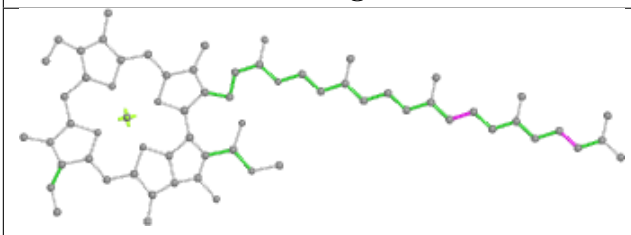
Ligand CLA c 504



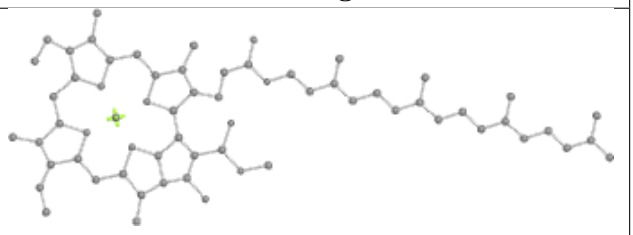
Bond lengths



Bond angles

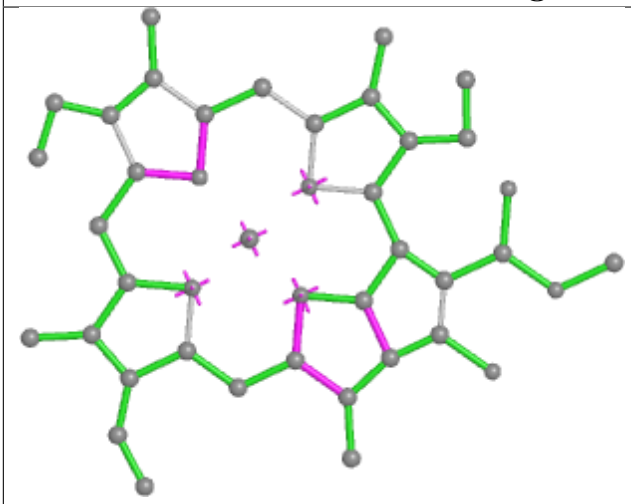


Torsions

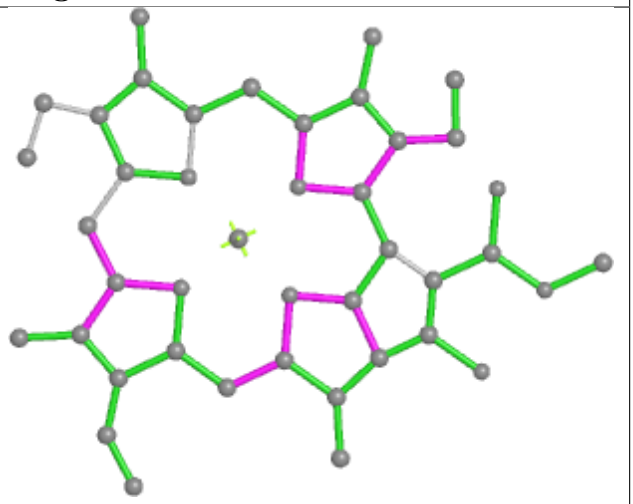


Rings

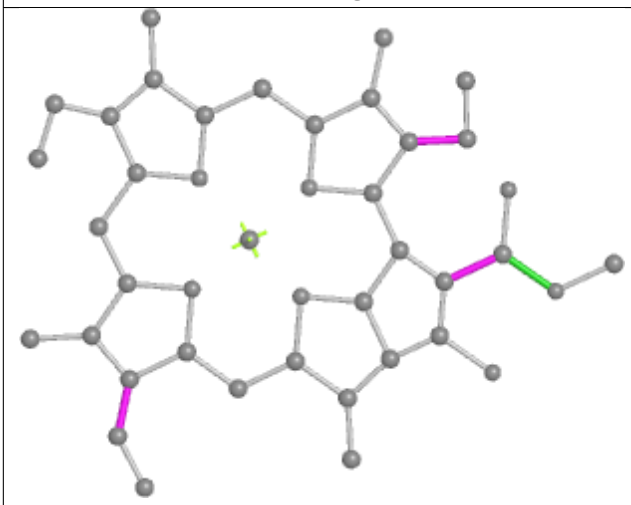
Ligand CLA g 301



Bond lengths



Bond angles



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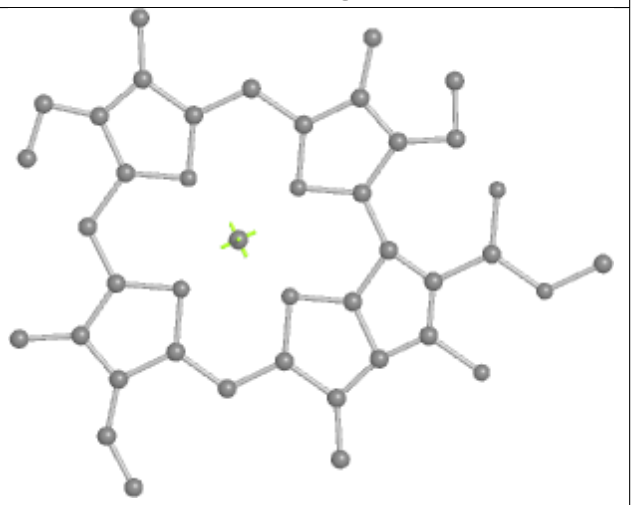
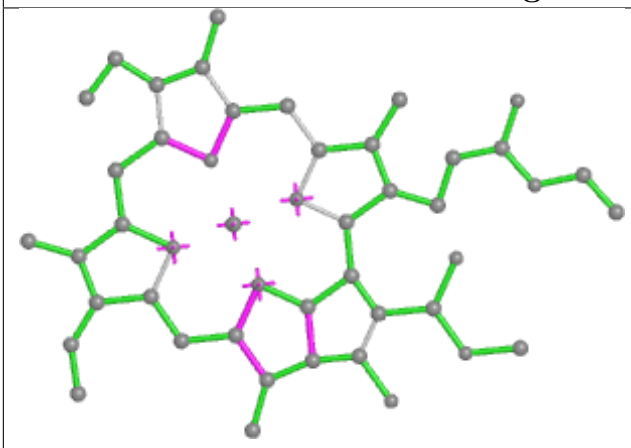
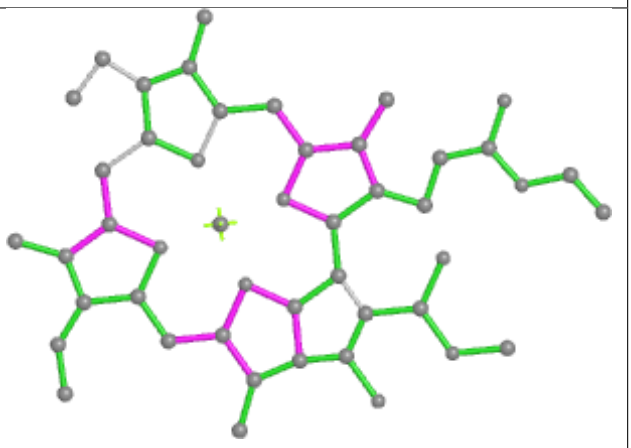


Rings

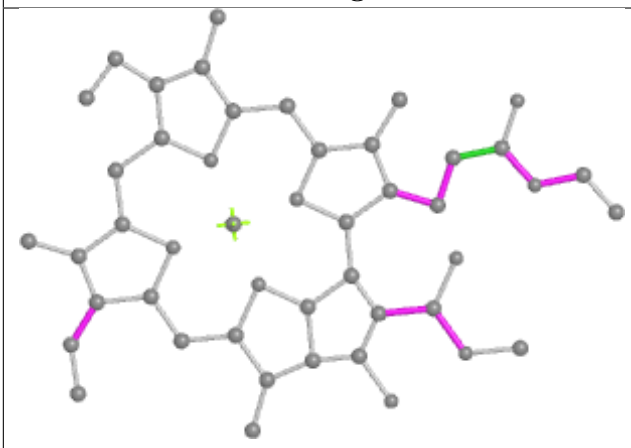
Ligand CLA N 303



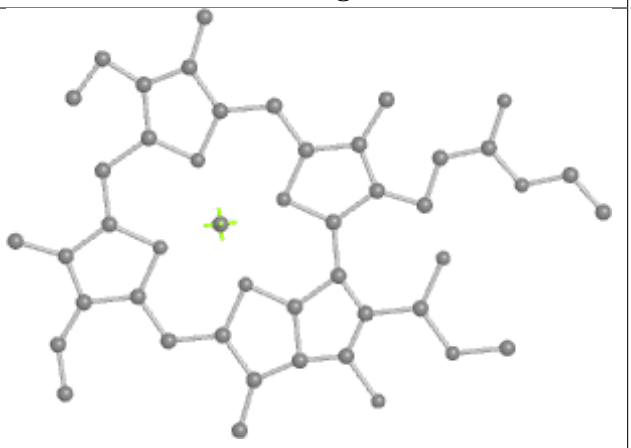
Bond lengths



Bond angles

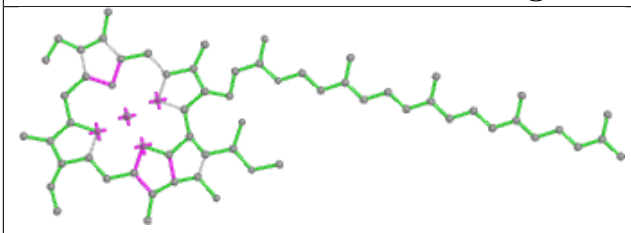


Torsions

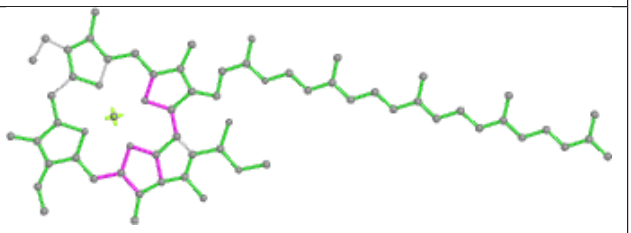


Rings

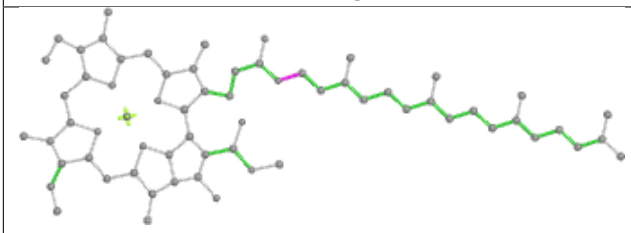
Ligand CLA d 404



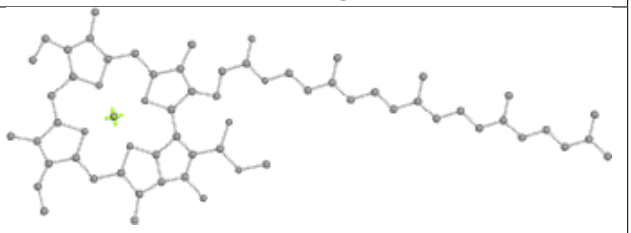
Bond lengths



Bond angles

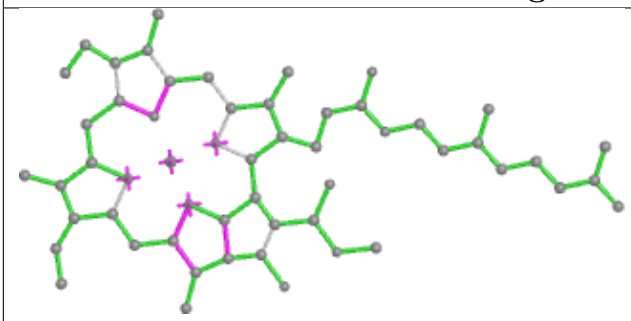


Torsions

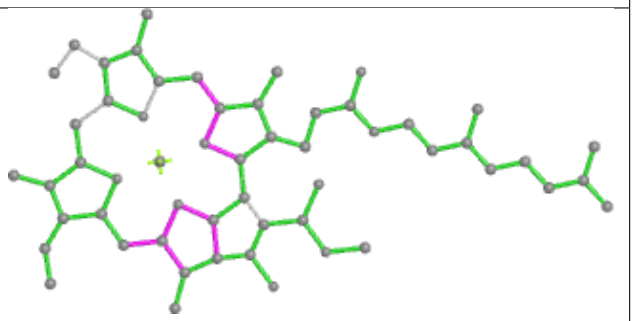


Rings

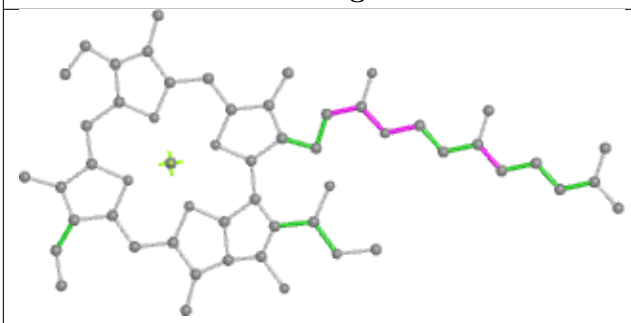
Ligand CLA 8 305



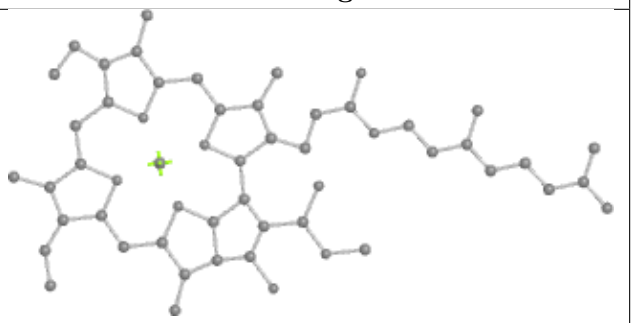
Bond lengths



Bond angles

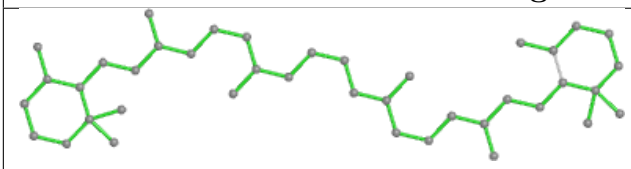


Torsions



Rings

Ligand 8CT b 619



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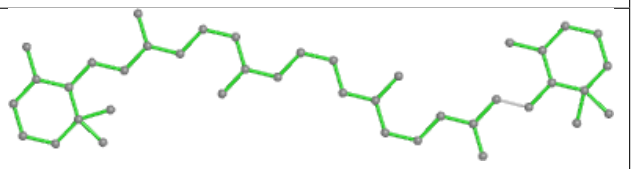

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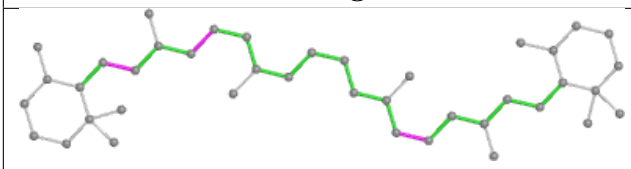

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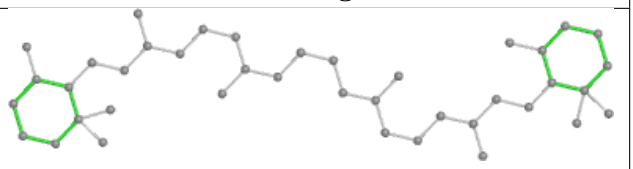
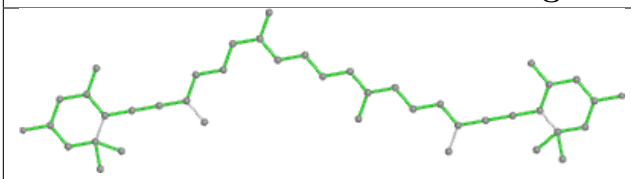


Rings

Ligand II0 3 318



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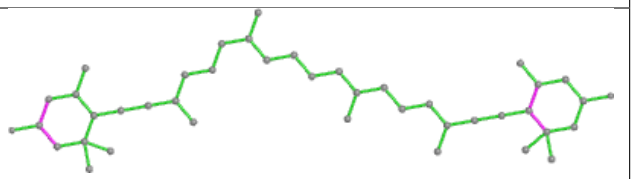
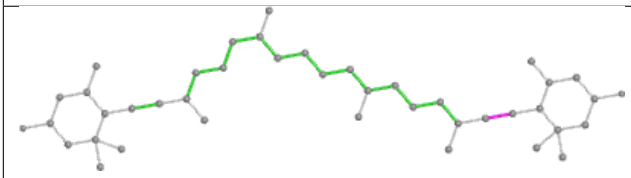


Bond angles



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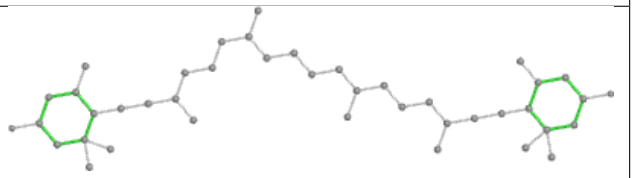
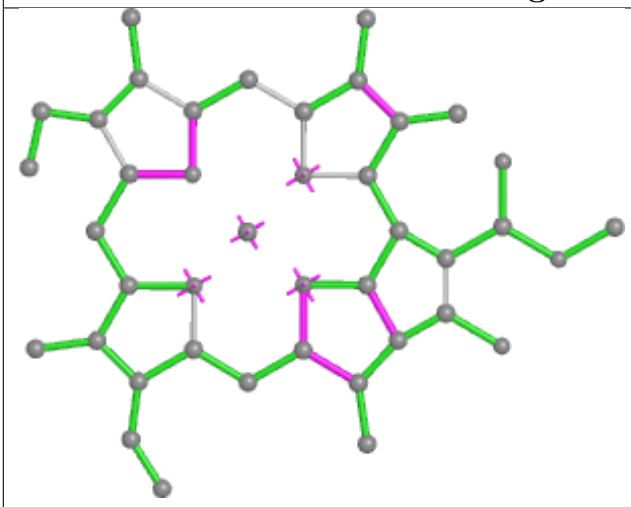


Rings

Ligand CLA 6 313



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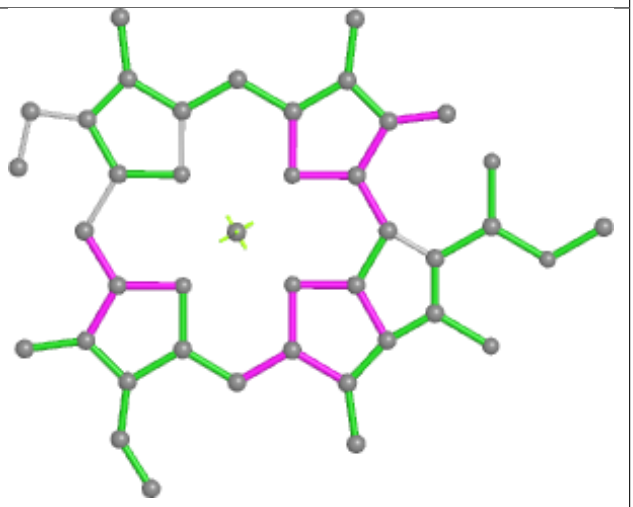
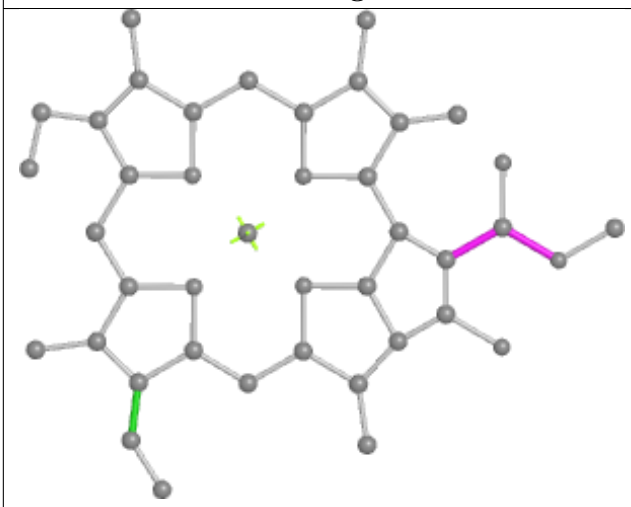


Bond angles



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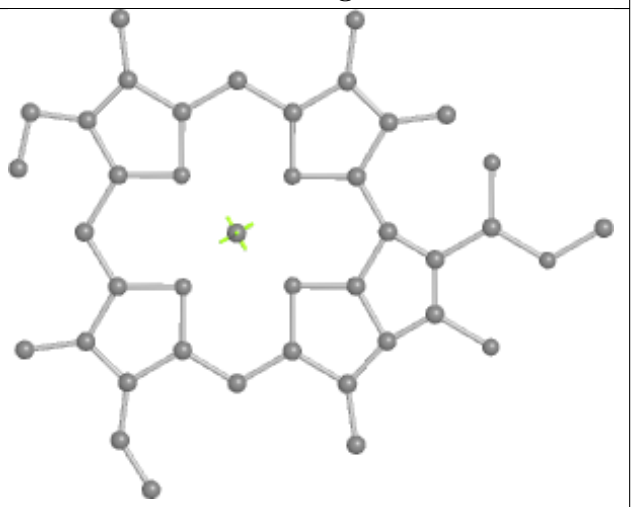
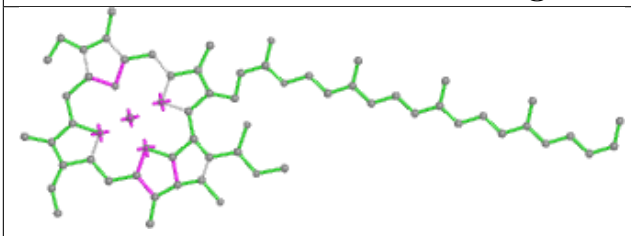


Rings

Ligand CLA 7 302



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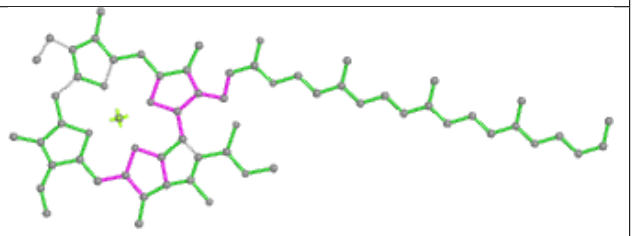

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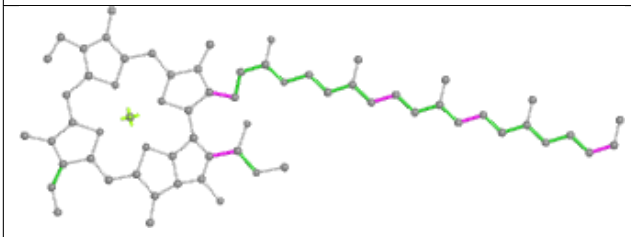

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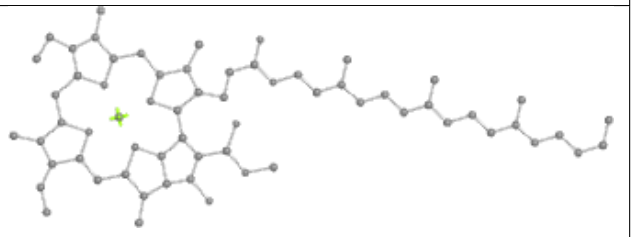
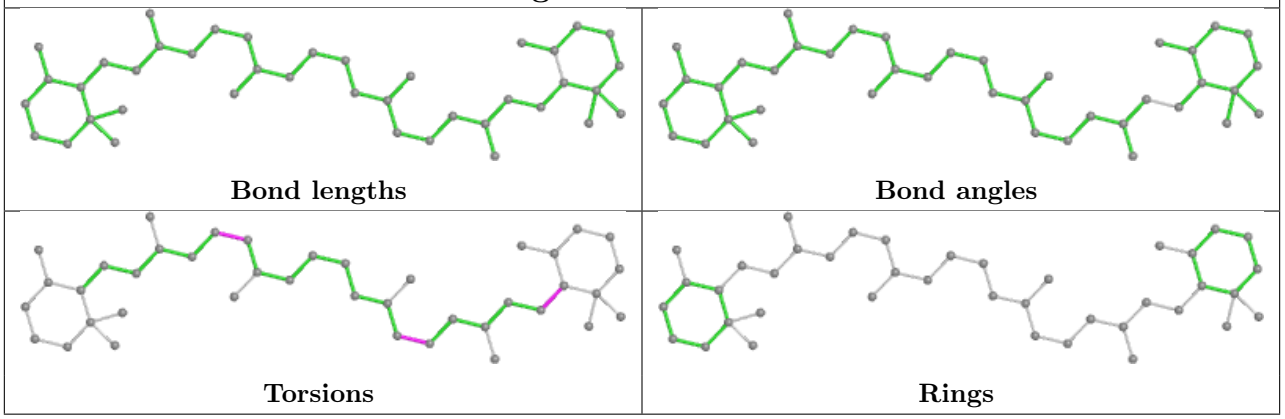
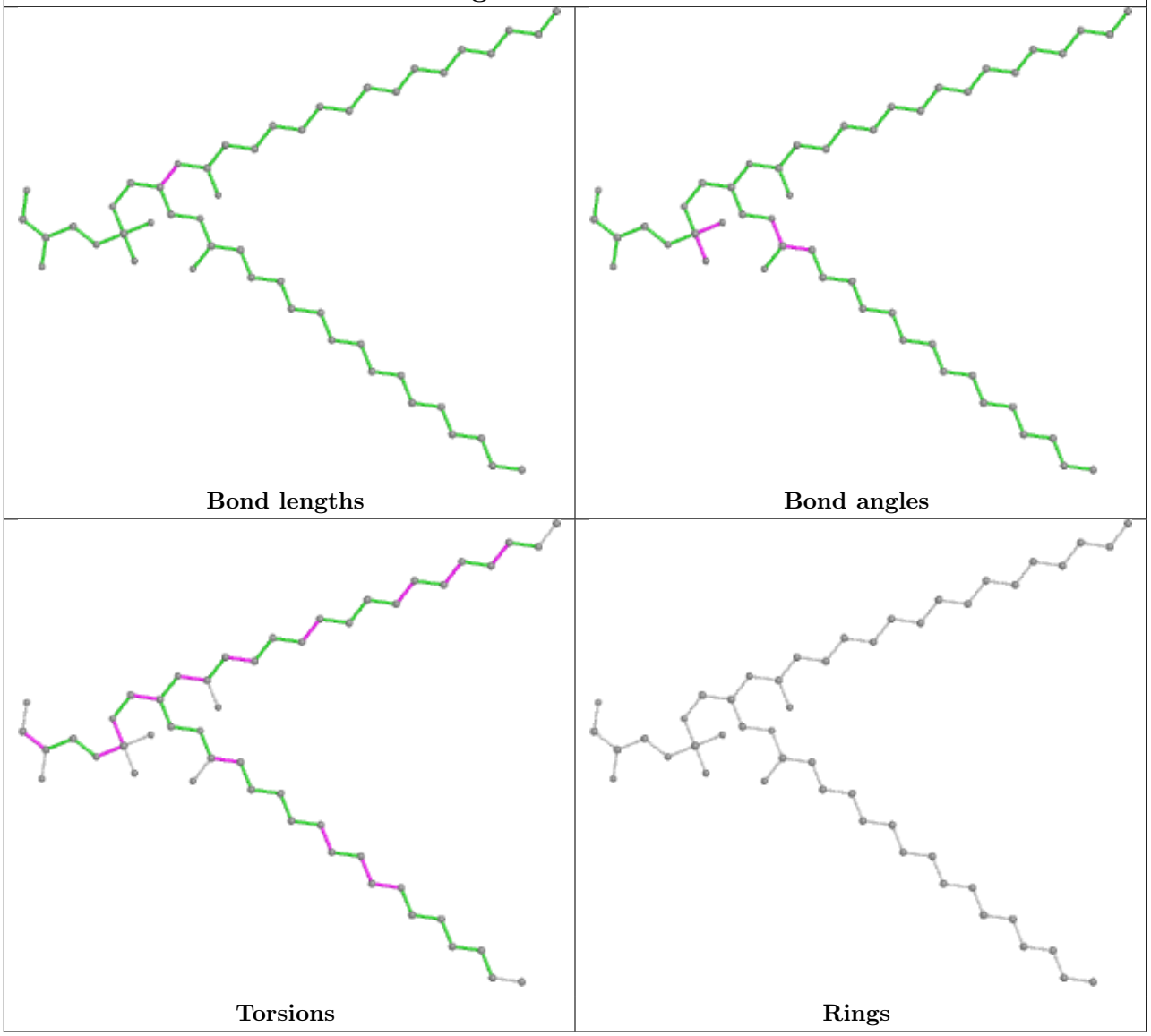


Rings

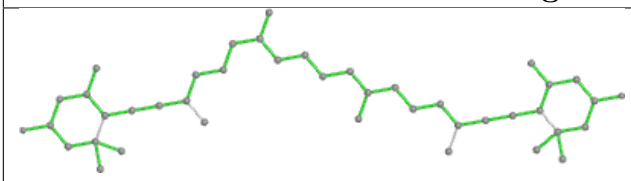
Ligand 8CT 4 311



Ligand LHG d 408



Ligand II0 p 314



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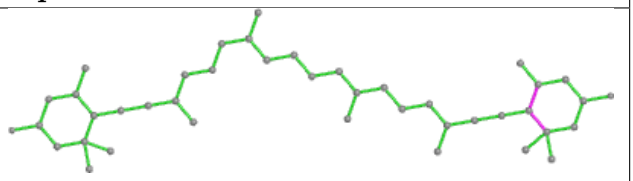

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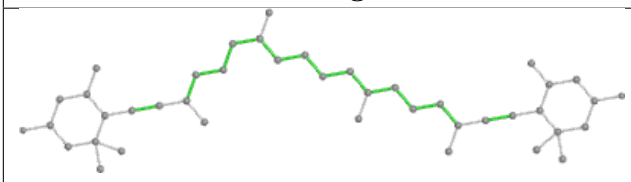

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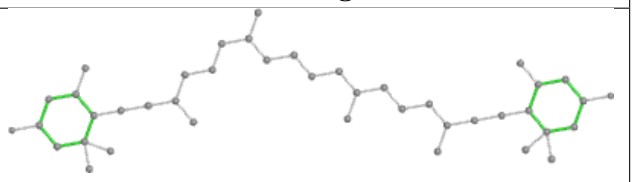
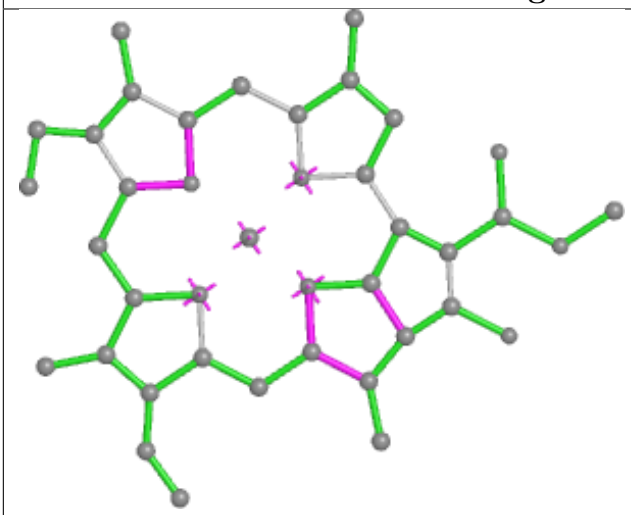


Rings

Ligand CLA g 305



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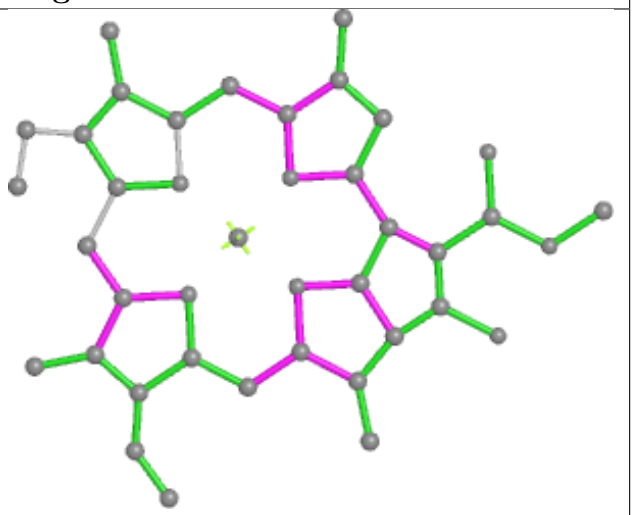

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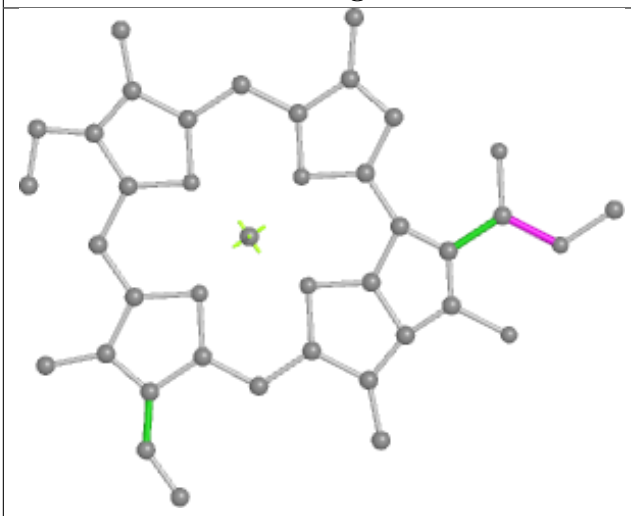

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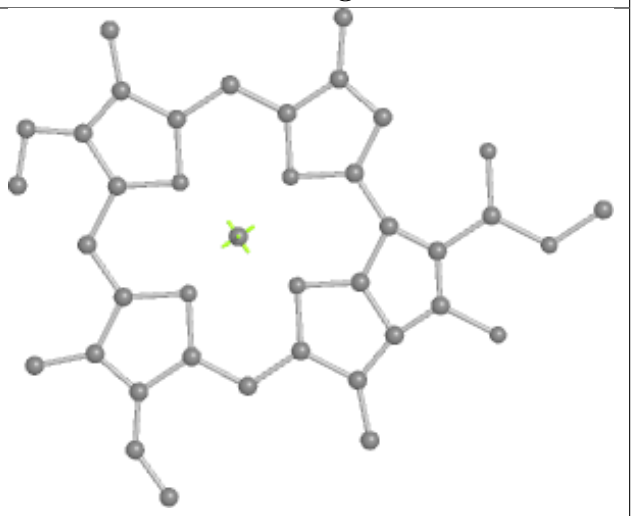

Rings

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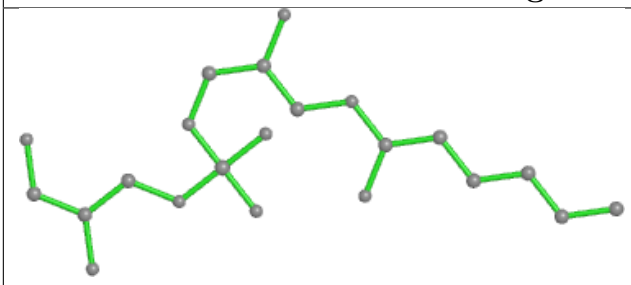

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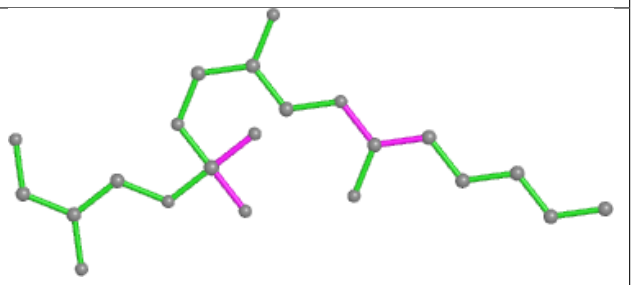

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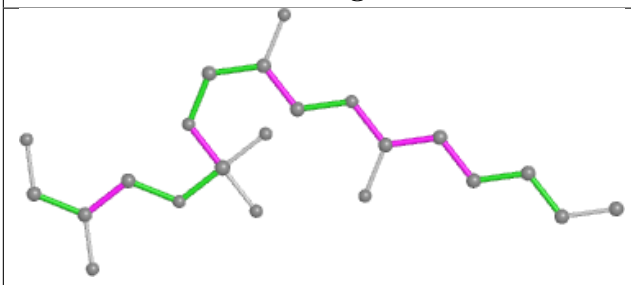

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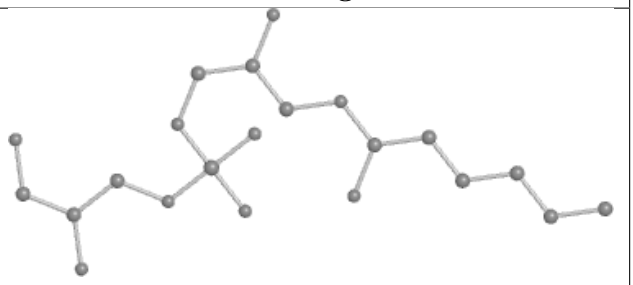
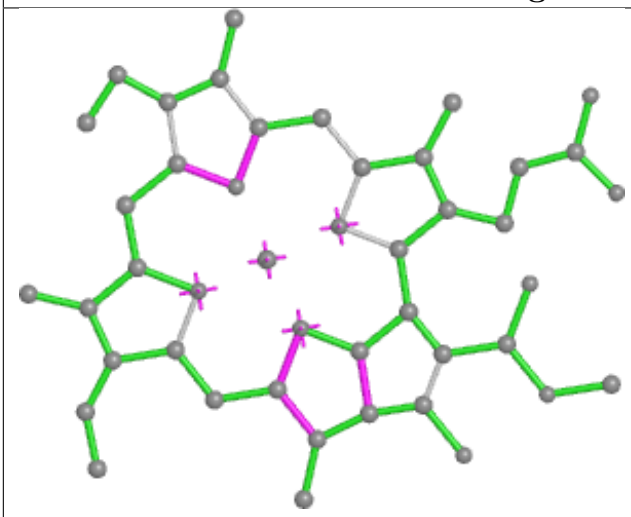


Rings

Ligand CLA g 304



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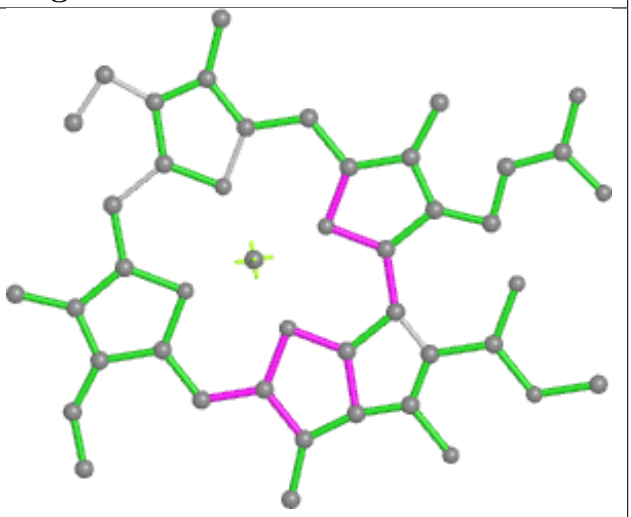

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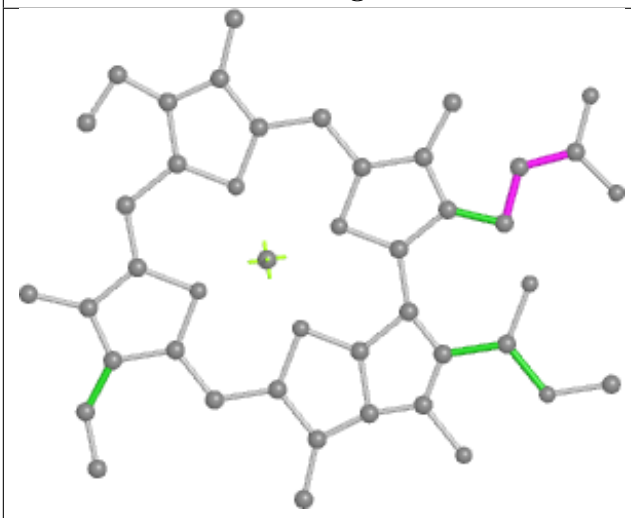

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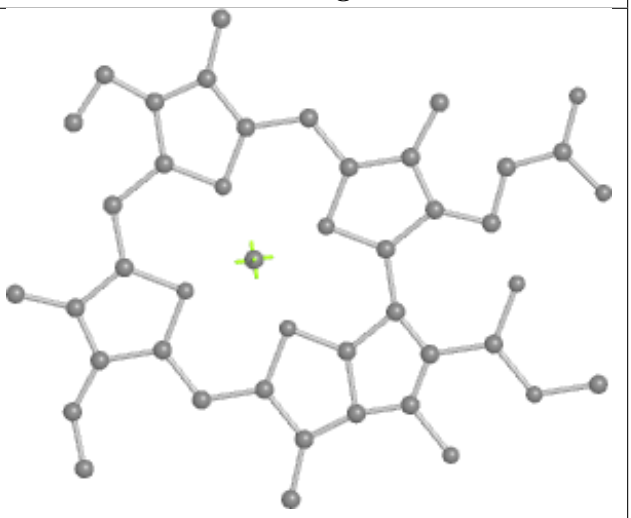
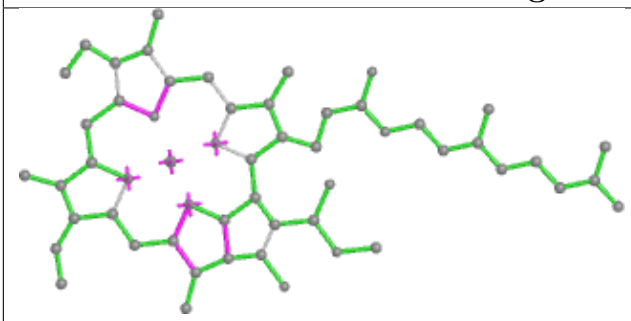


Rings

Ligand CLA 7 309



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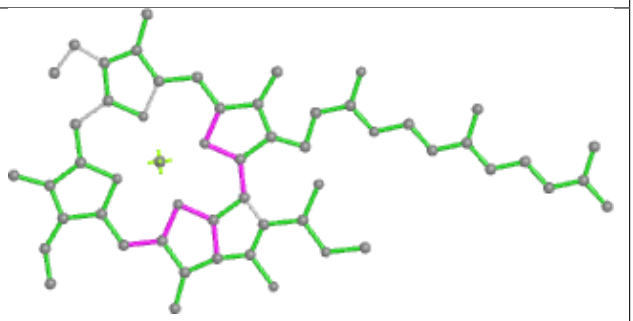
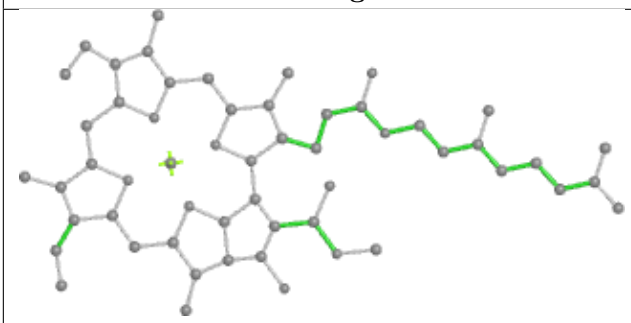


Bond angles



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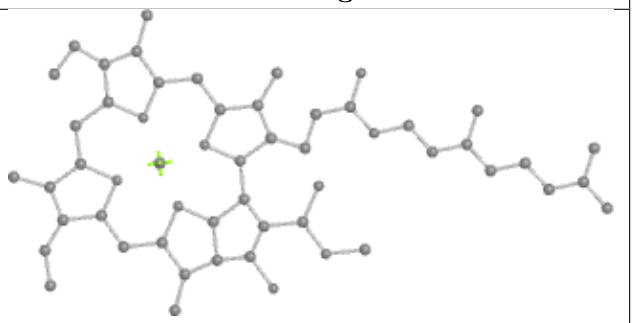
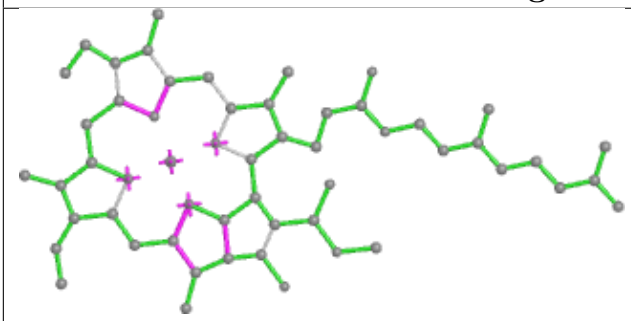


Rings

Ligand CLA 4 307



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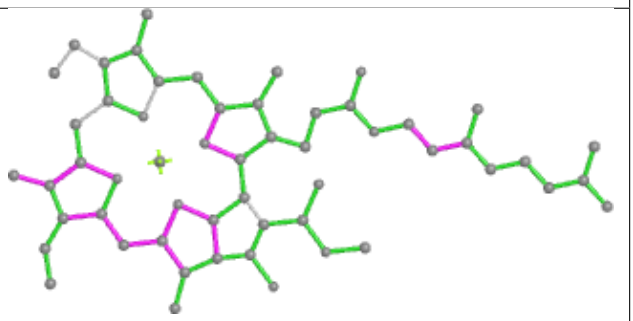
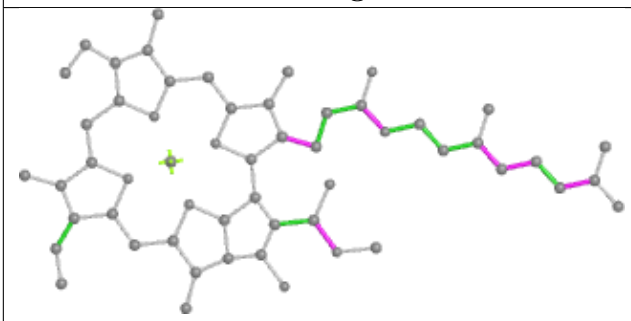


Bond angles



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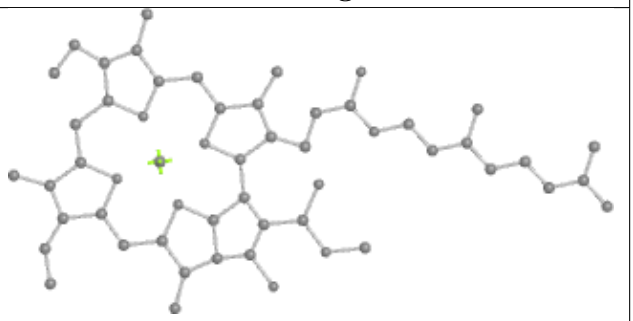
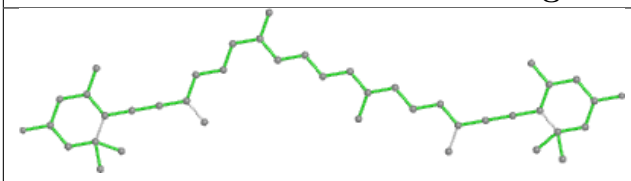


Rings

Ligand II0 5 314



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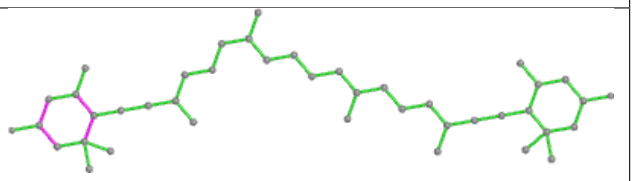
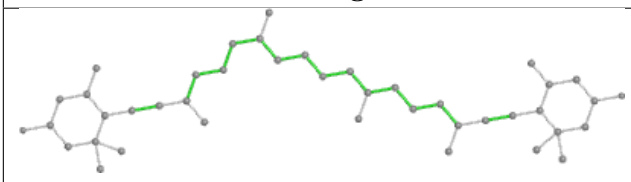


Bond angles



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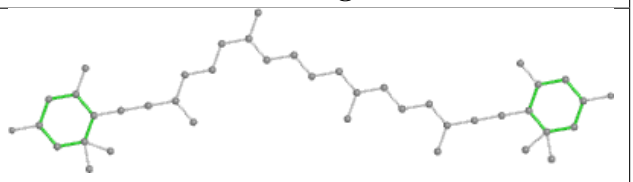
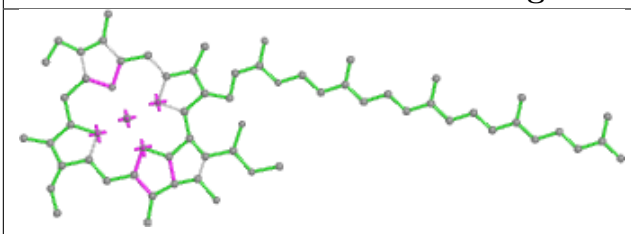
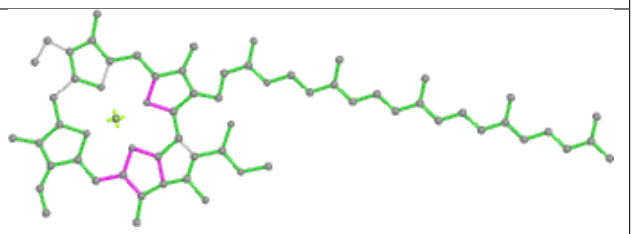


Rings

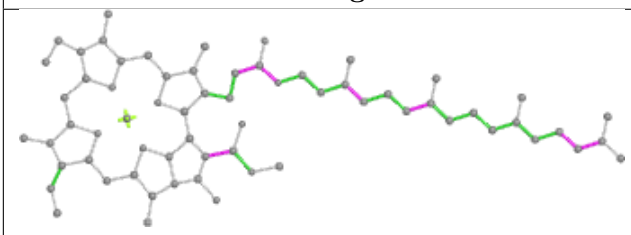
Ligand CLA n 301



Bond lengths



Bond angles



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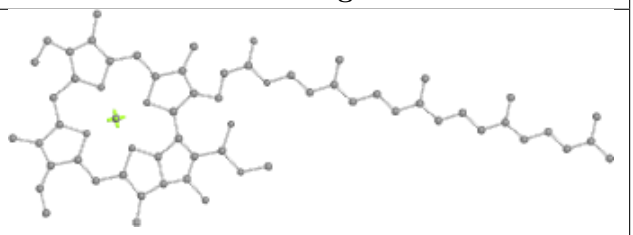
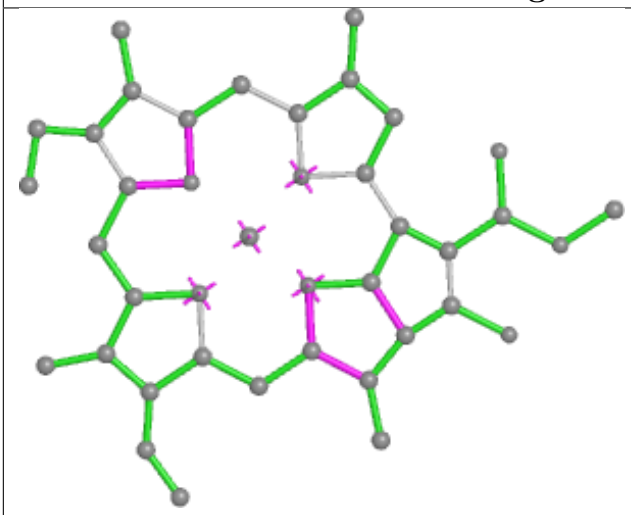


Rings

Ligand CLA 5 305



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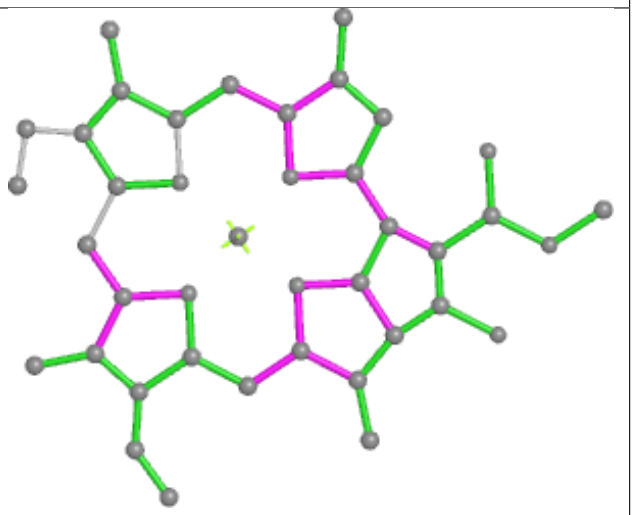
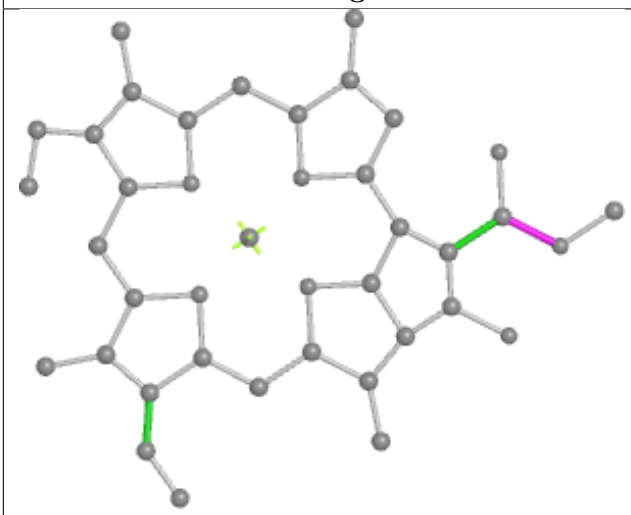


Bond angles



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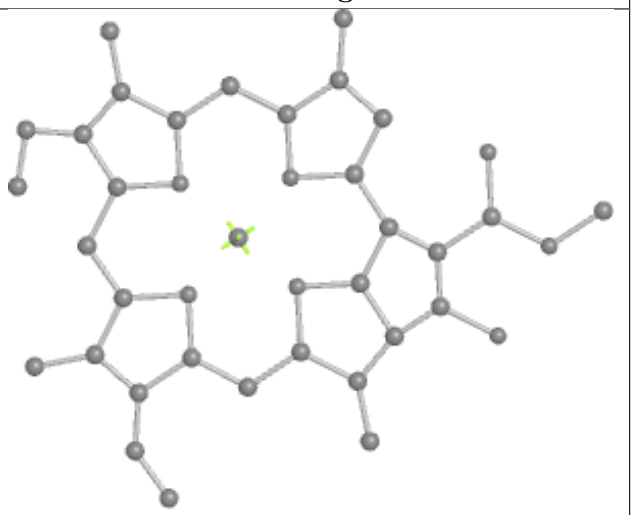
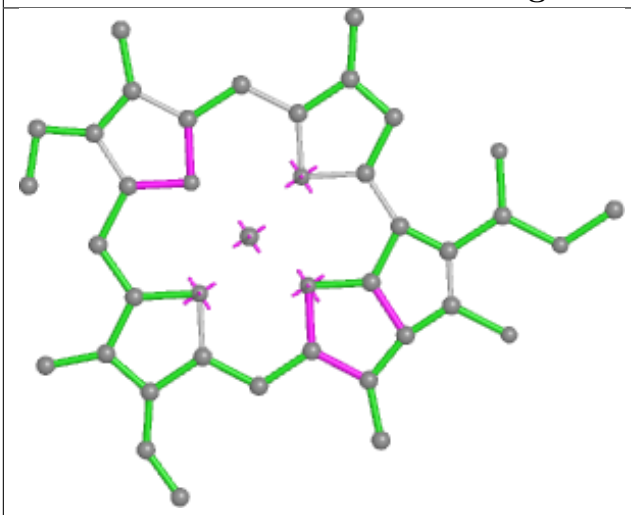
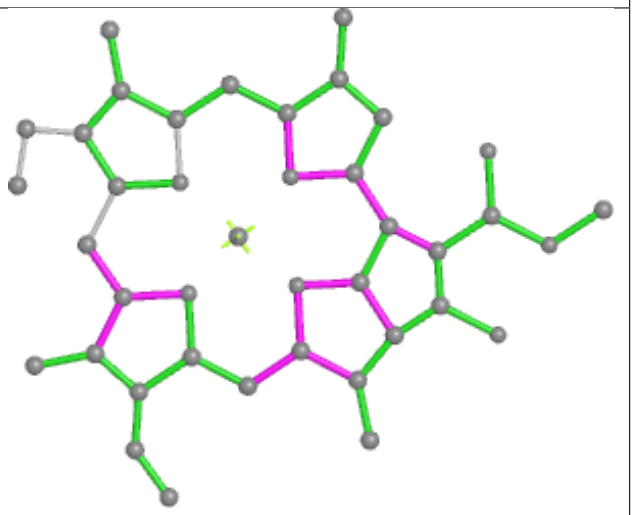


Rings

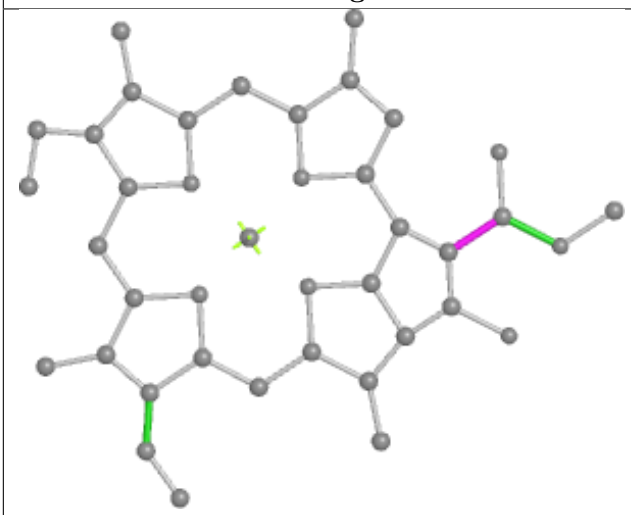
Ligand CLA 5 317



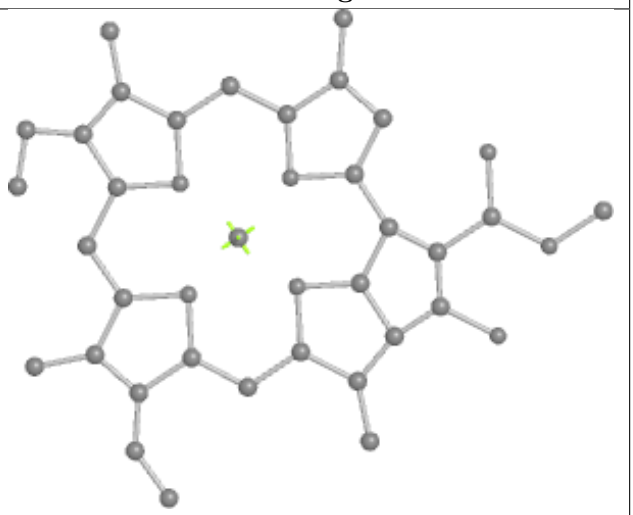
Bond lengths



Bond angles

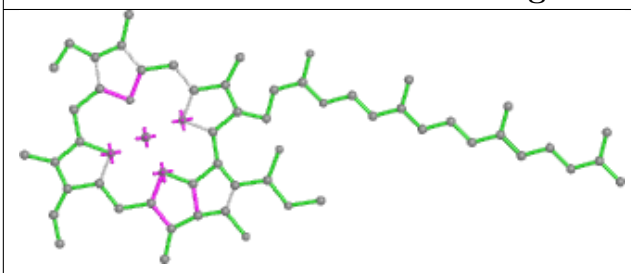


Torsions



Rings

Ligand CLA 8 307



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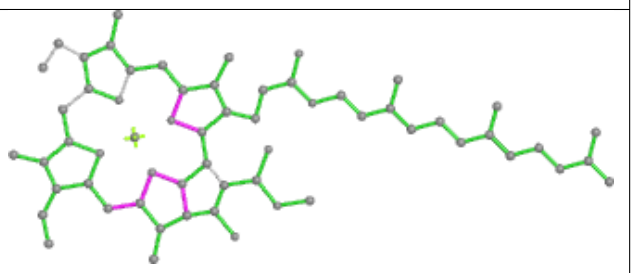

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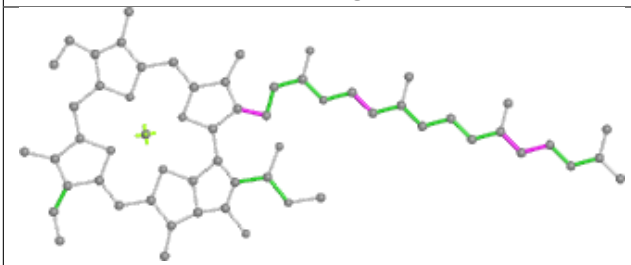

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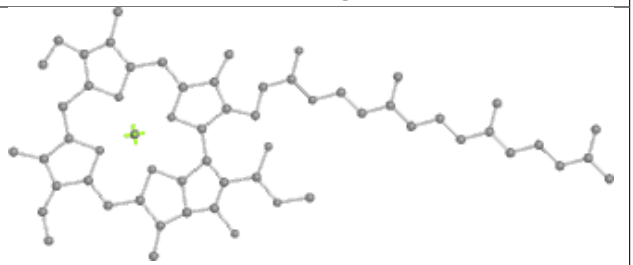
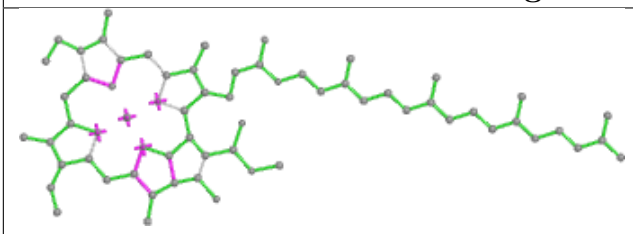


Rings

Ligand CLA C 506



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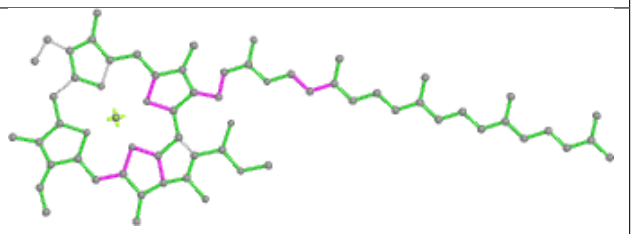
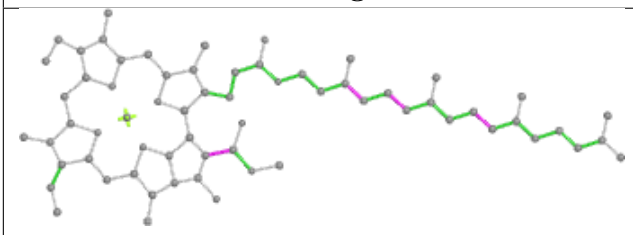


Bond angles



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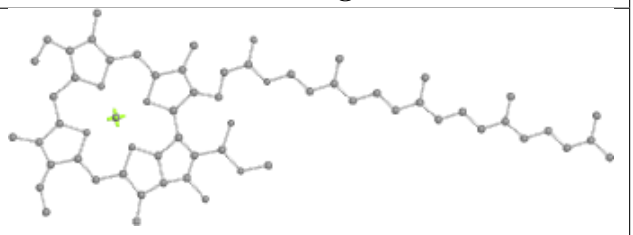
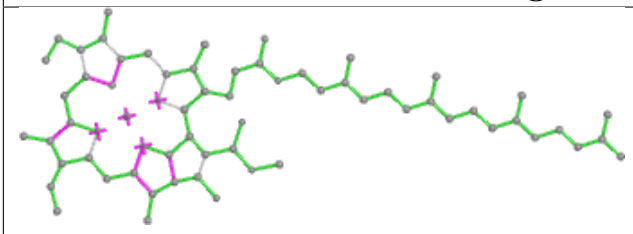
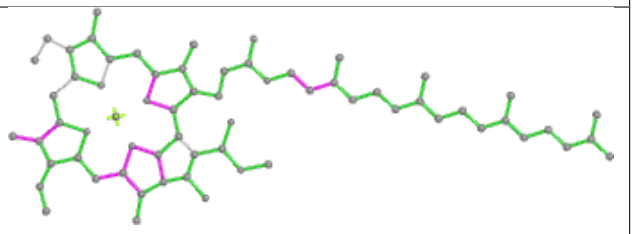


Rings

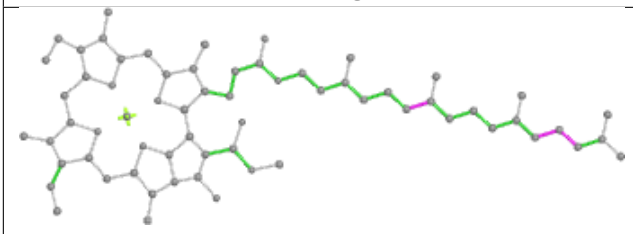
Ligand CLA b 606



Bond lengths



Bond angles



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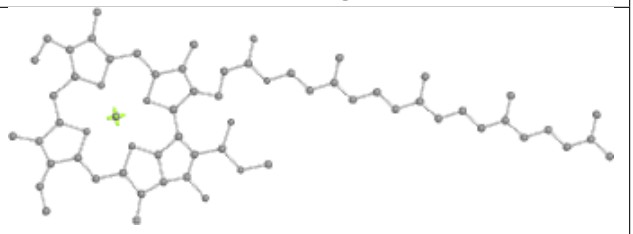
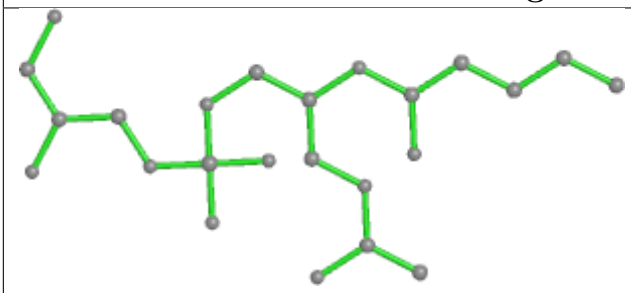
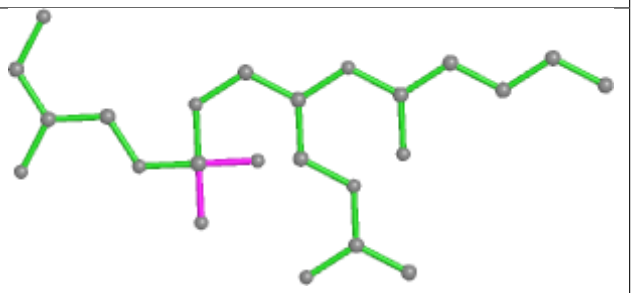


Rings

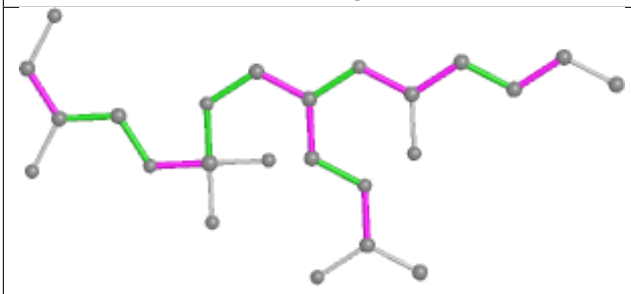
Ligand LHG 3 321



Bond lengths



Bond angles



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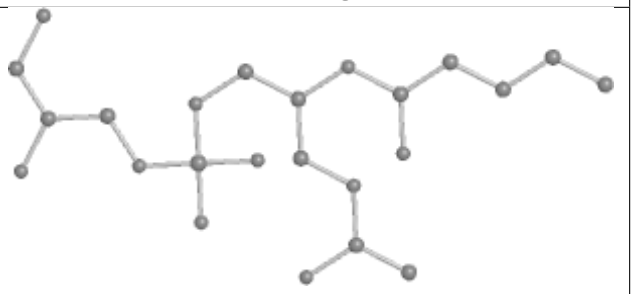
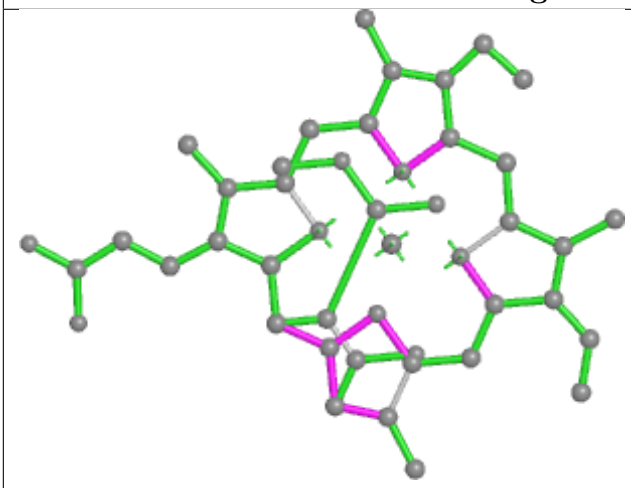


Rings

Ligand KC2 1 311



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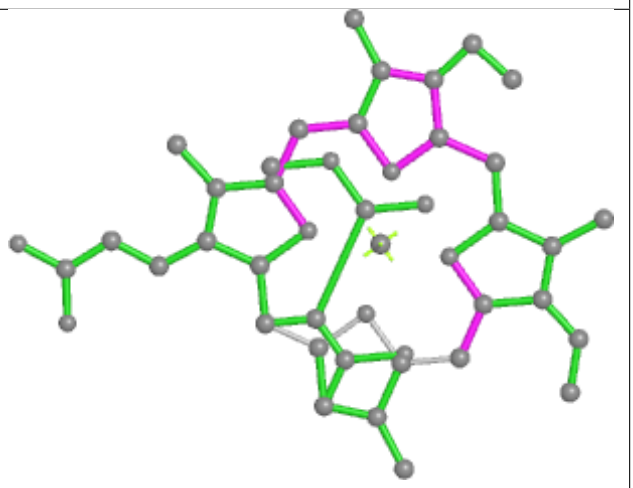
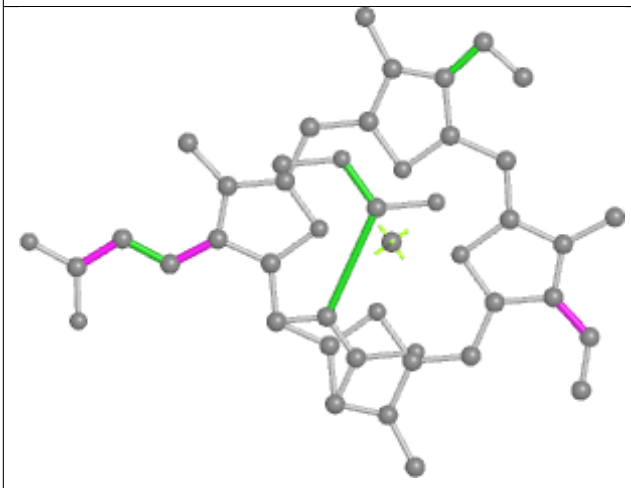


Bond angles



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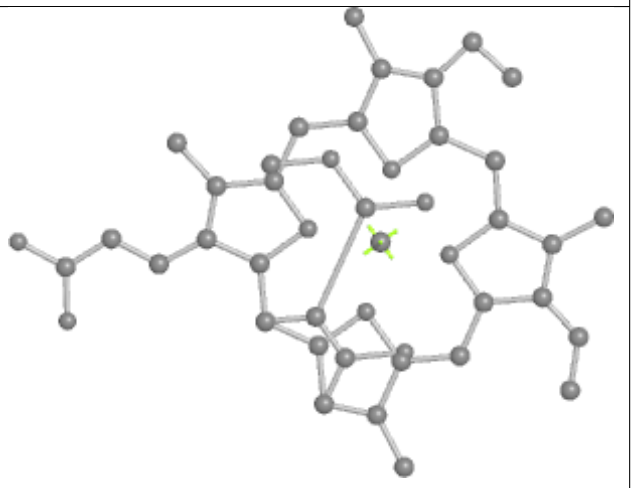
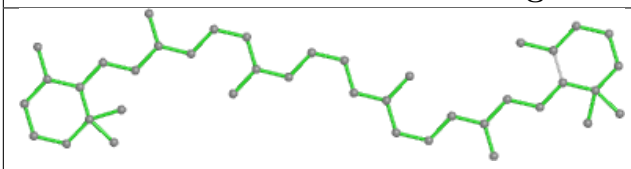


Rings

Ligand 8CT Y 101



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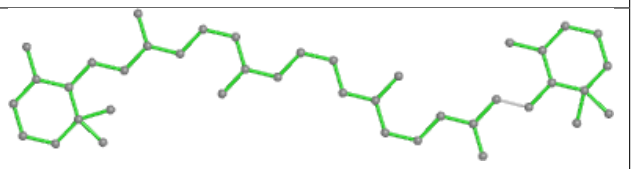
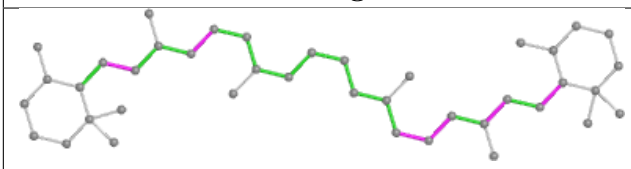


Bond angles



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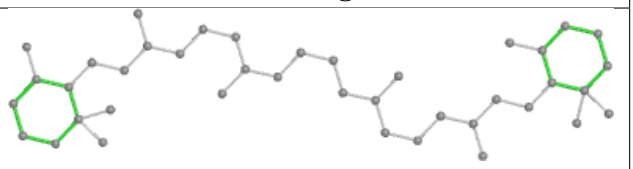
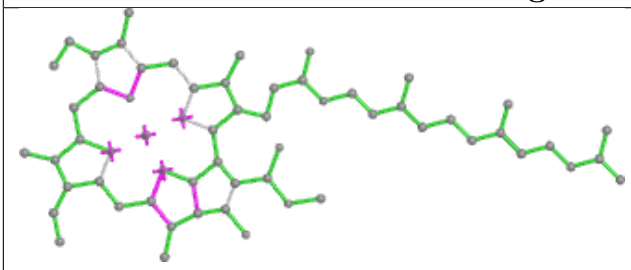


Rings

Ligand CLA a 408



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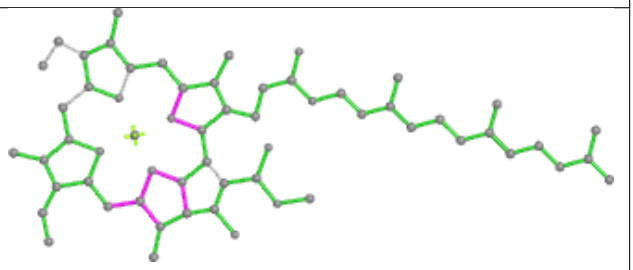
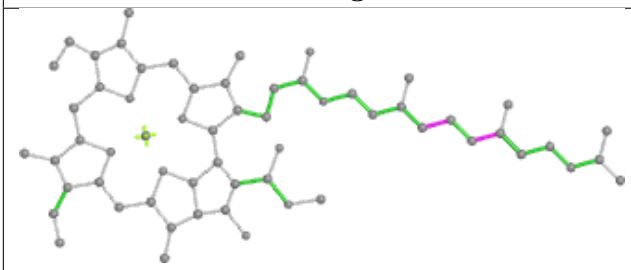


Bond angles



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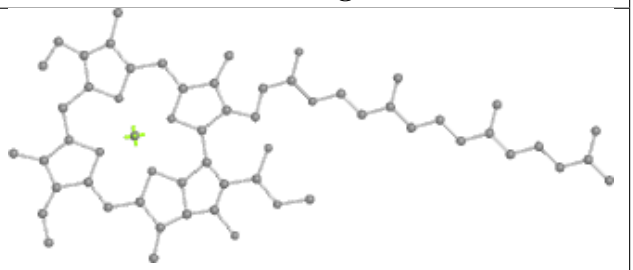
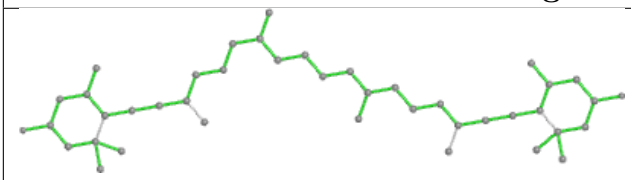


Rings

Ligand II0 8 311



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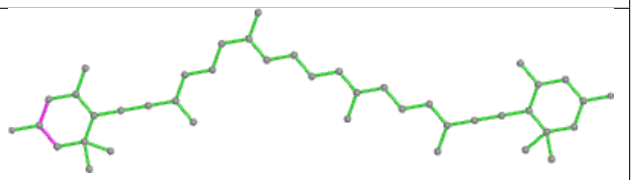
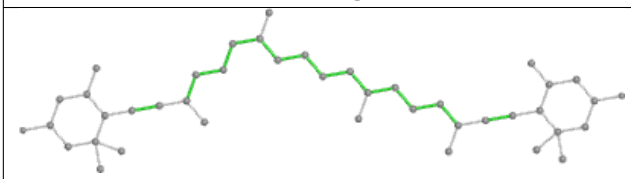


Bond angles



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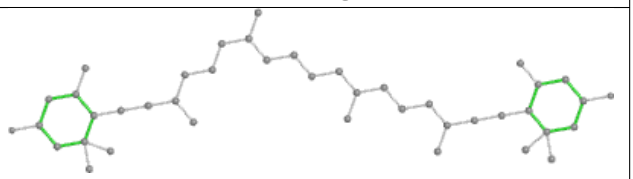
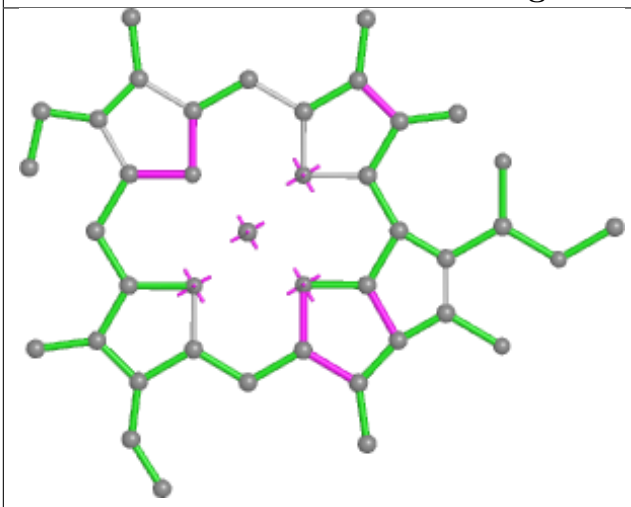


Rings

Ligand CLA 5 308



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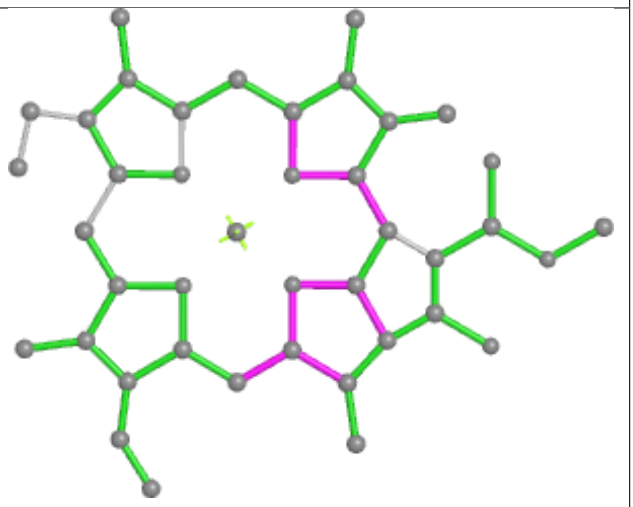
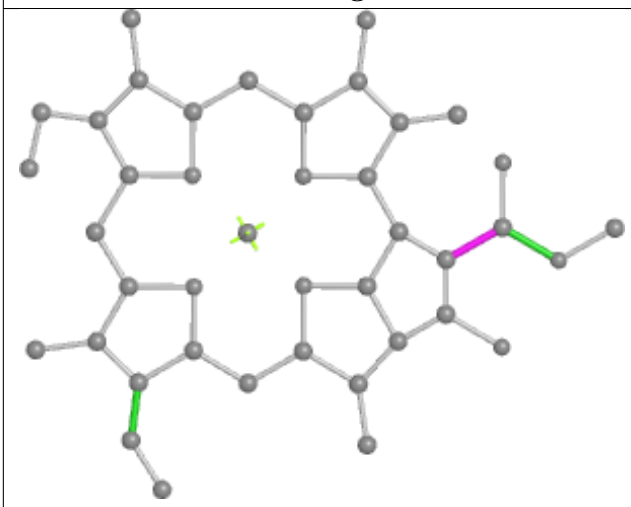
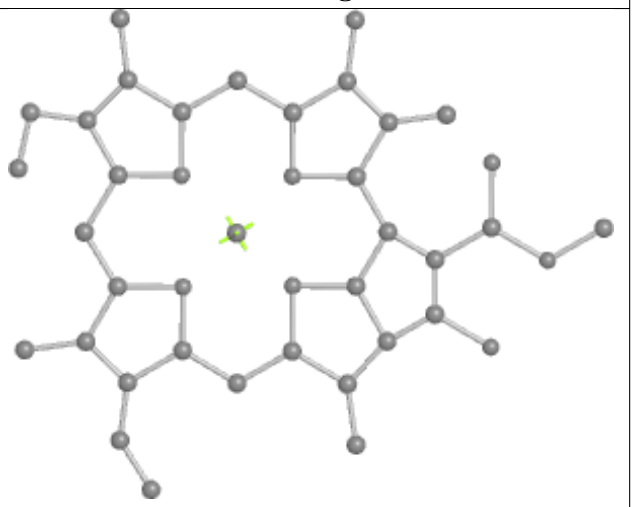


Bond angles

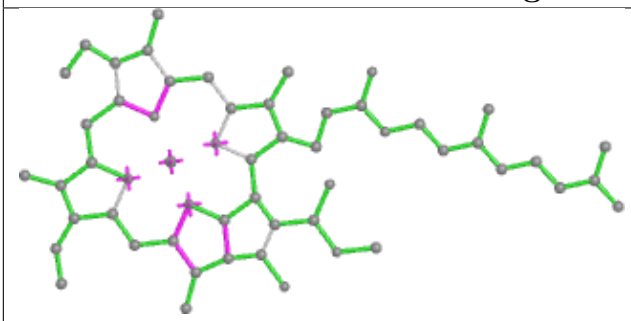


Torsions

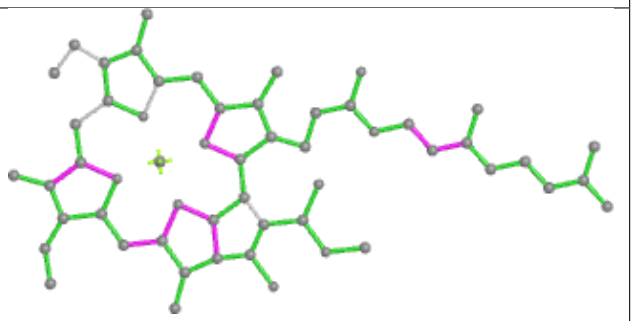


Rings

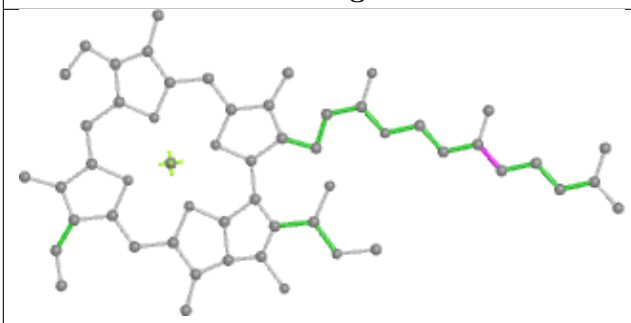
Ligand CLA N 306



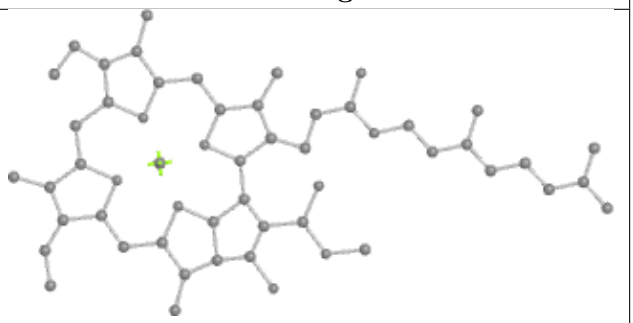
Bond lengths



Bond angles

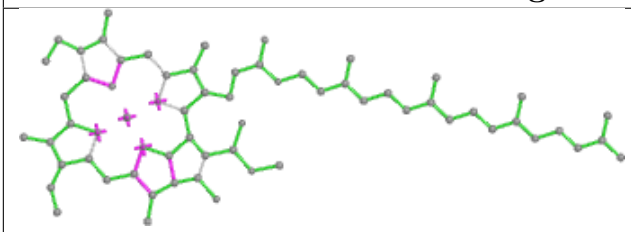


Torsions



Rings

Ligand CLA 7 307



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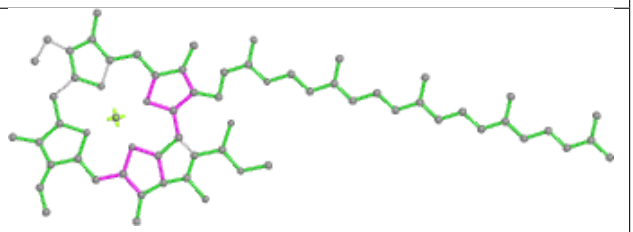
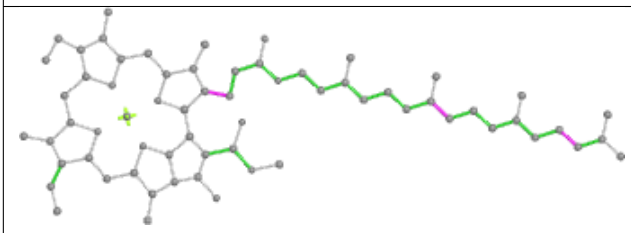


Bond angles



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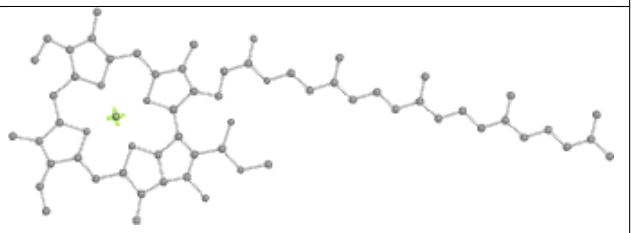
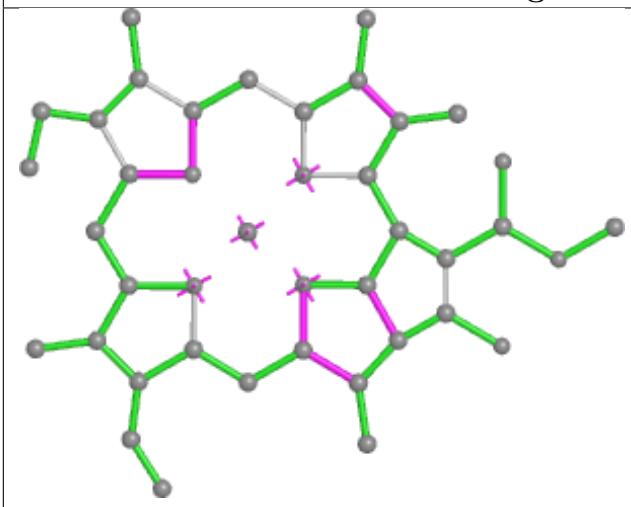


Rings

Ligand CLA p 312



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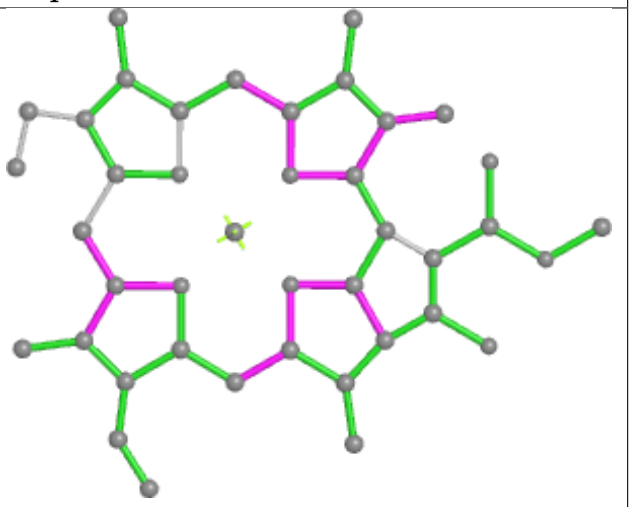
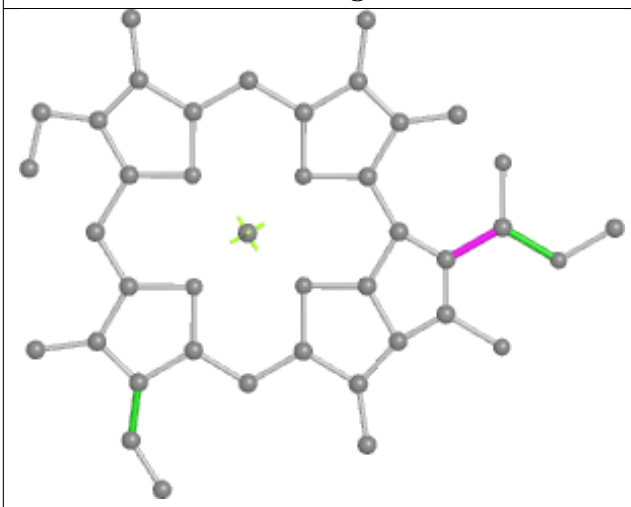


Bond angles



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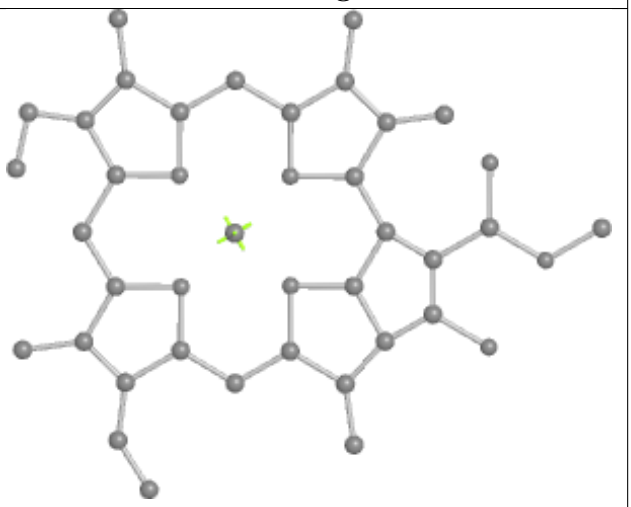
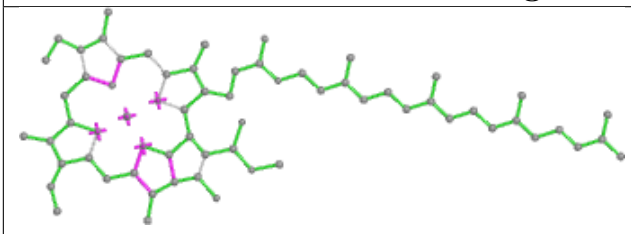
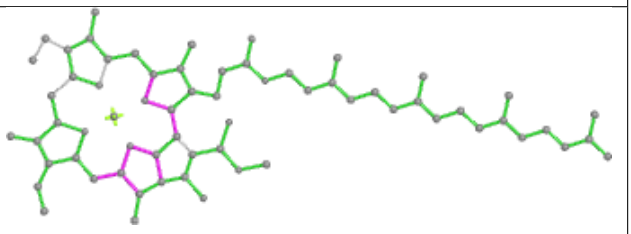


Rings

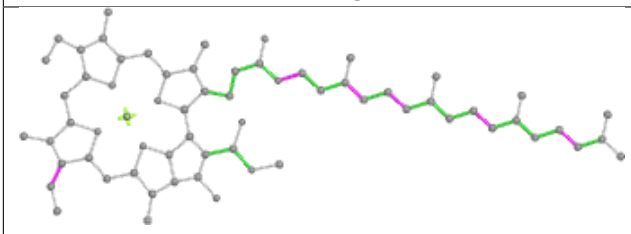
Ligand CLA N 302



Bond lengths



Bond angles



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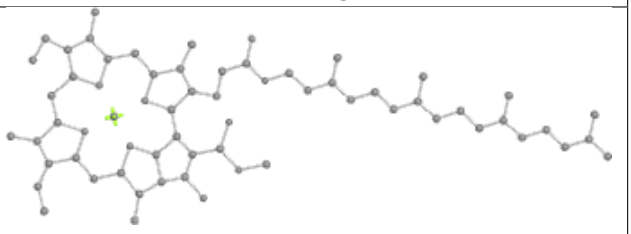
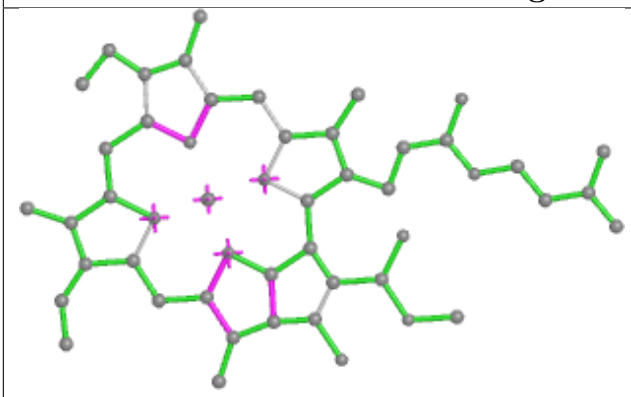
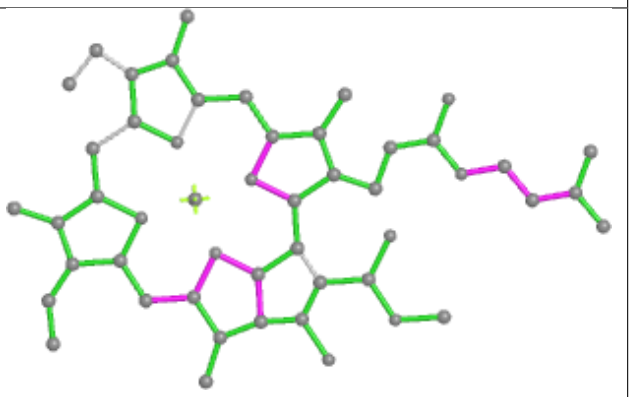
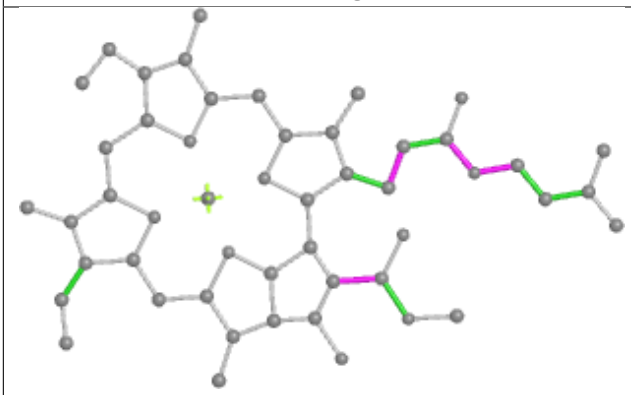
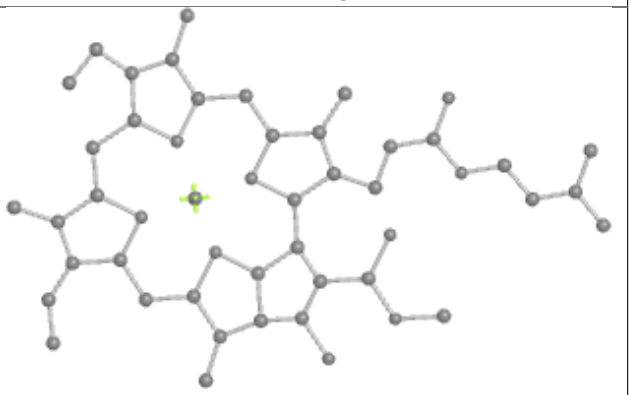
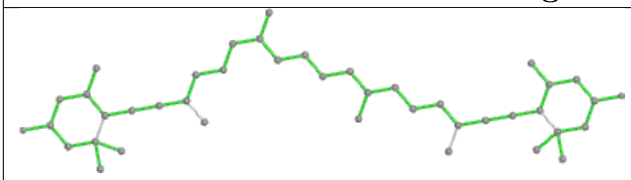
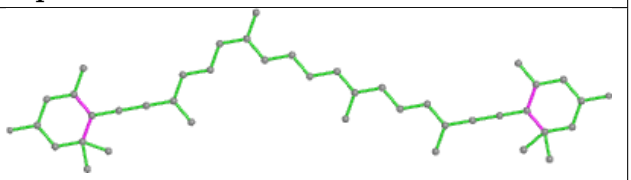
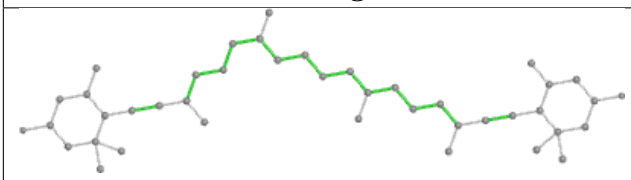
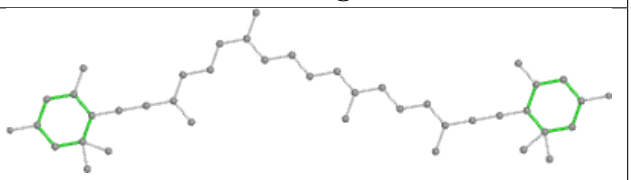
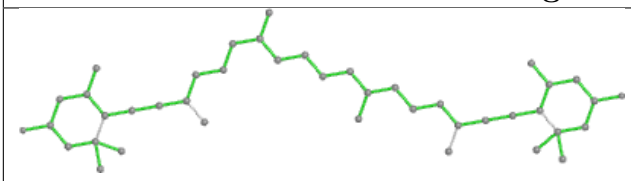


Rings

Ligand CLA 0 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 p 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 1 314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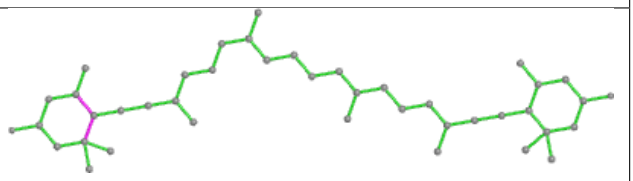
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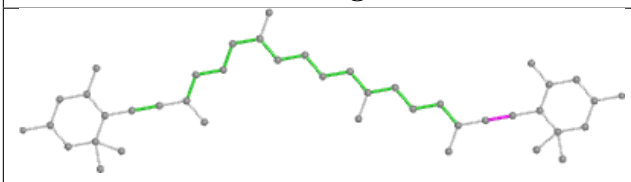
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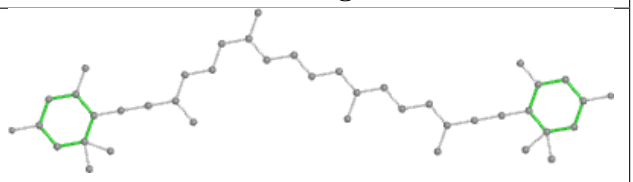
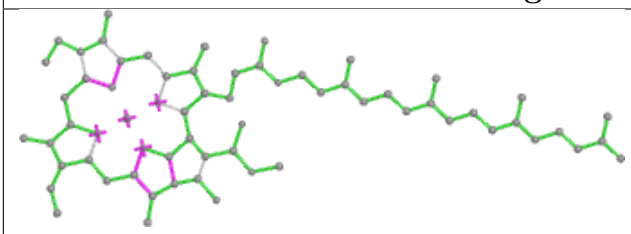

Rings

Ligand CLA B 608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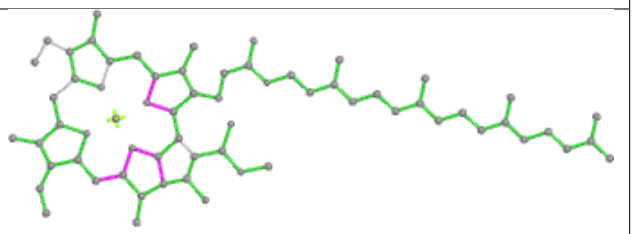
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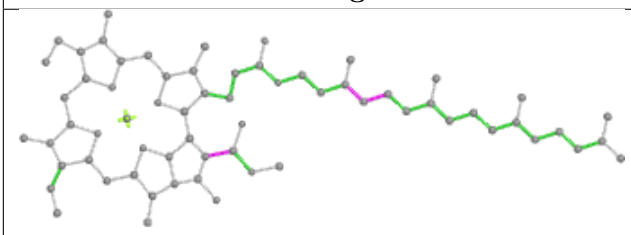
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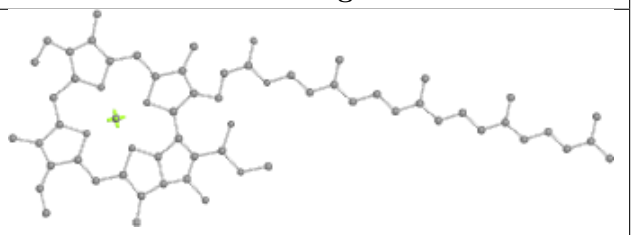
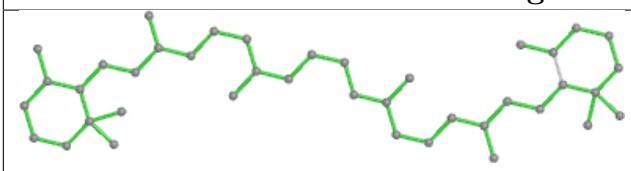

Rings

Ligand 8CT C 516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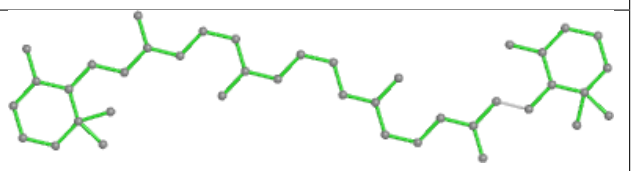
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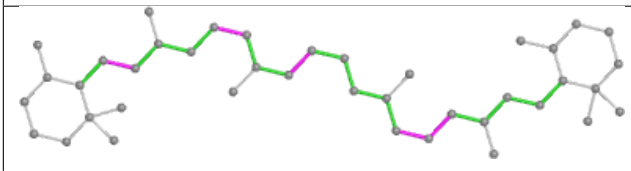
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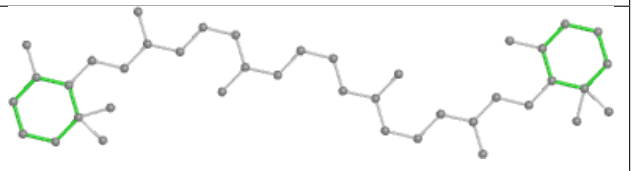
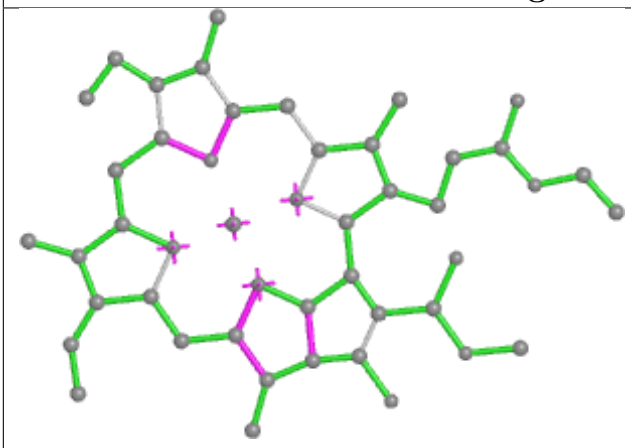

Rings

Ligand CLA 0 308



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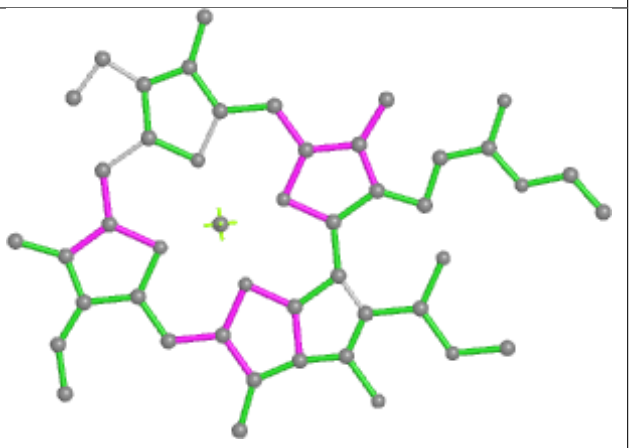

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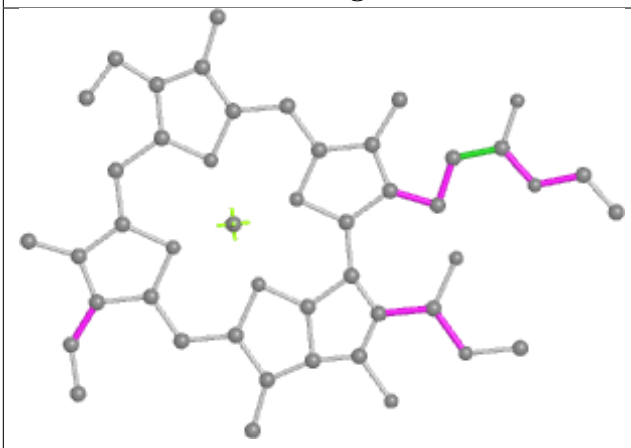

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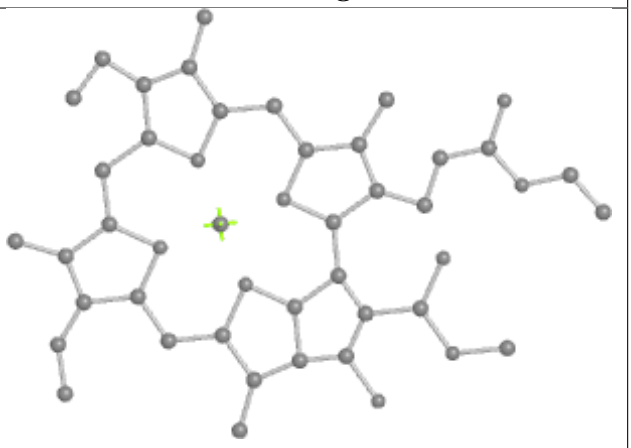
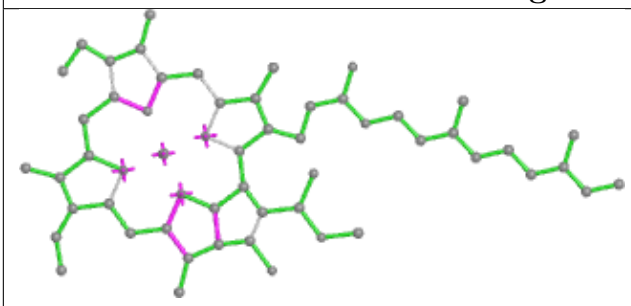


Rings

Ligand CLA c 513



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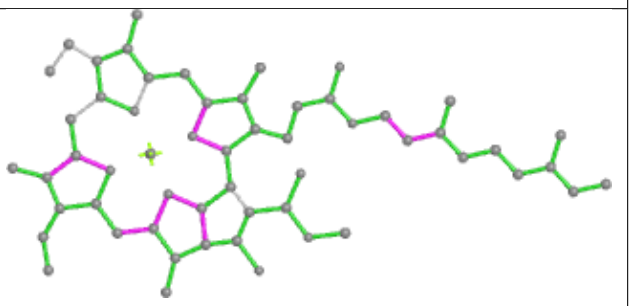
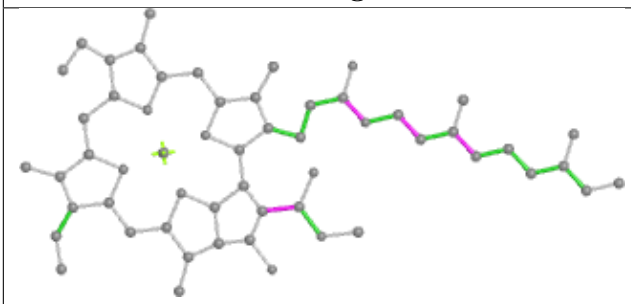


Bond angles



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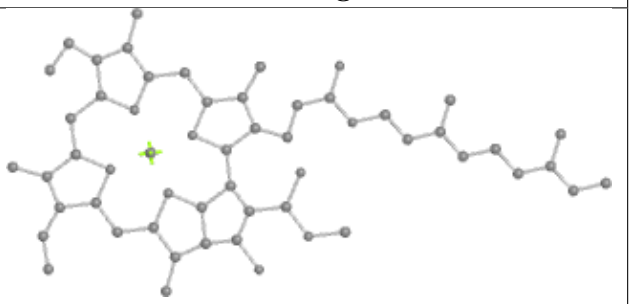
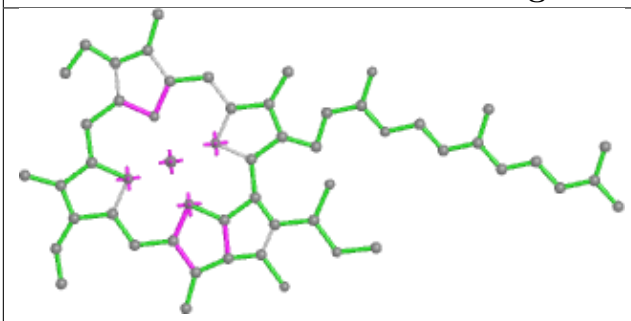


Rings

Ligand CLA g 302



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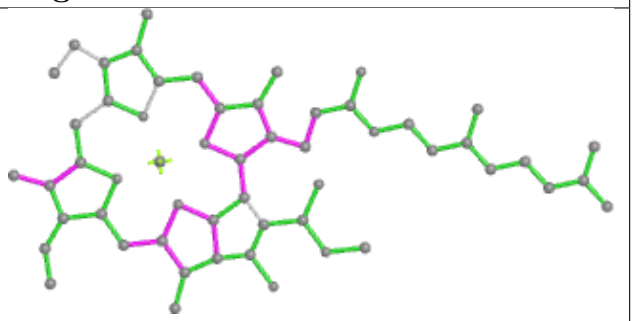

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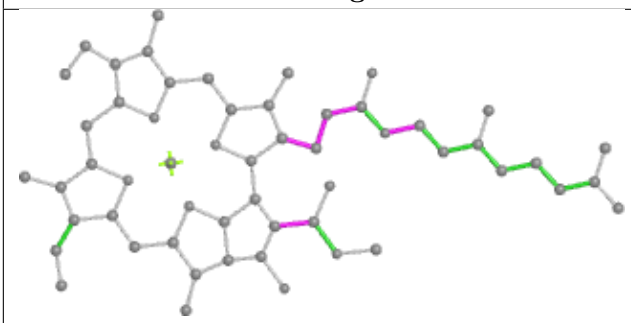

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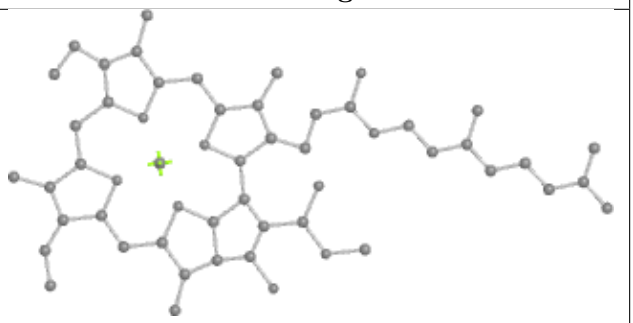
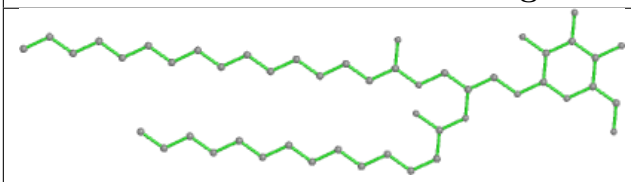
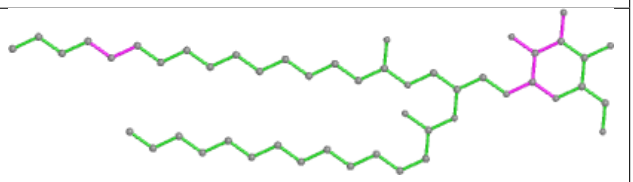


Rings

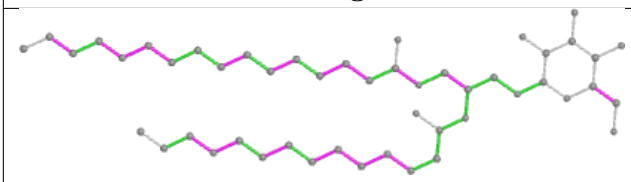
Ligand LMG B 622



Bond lengths



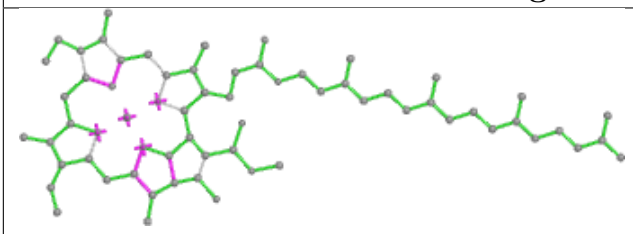
Bond angles



Torsions

Rings

Ligand CLA c 503



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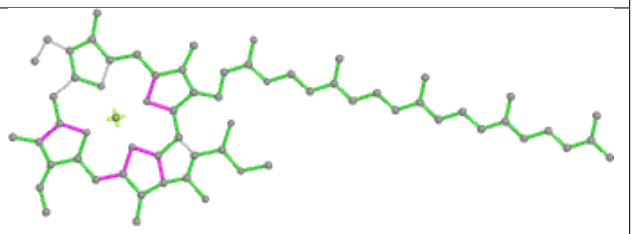
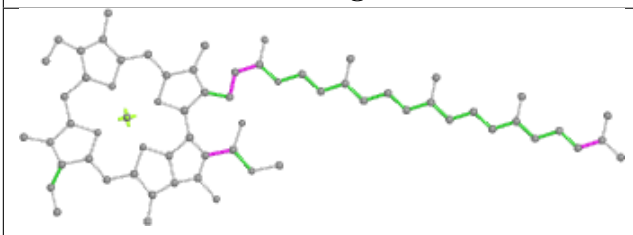


Bond angles



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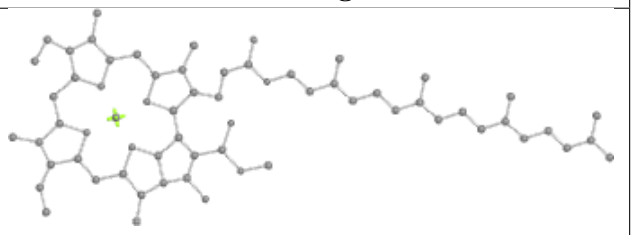
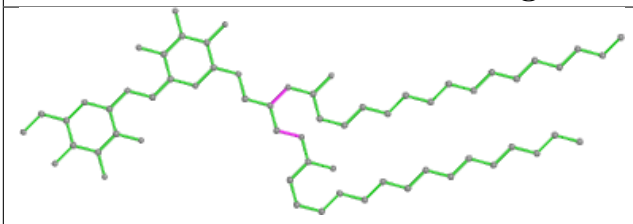
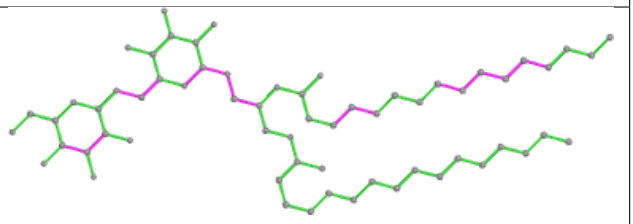


Rings

Ligand DGD C 521



Bond lengths



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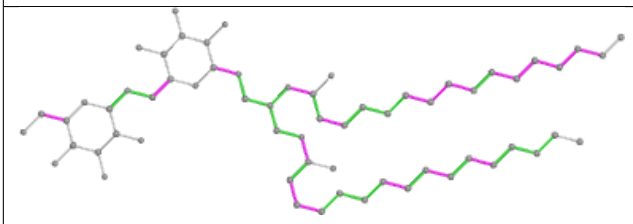

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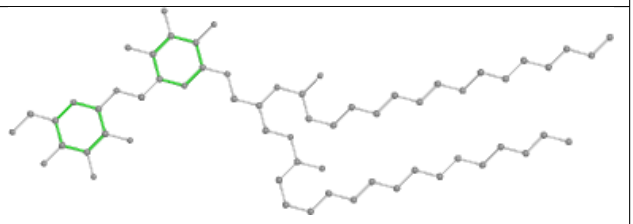
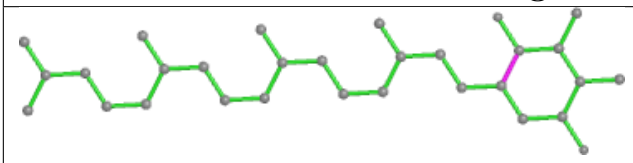


Rings

Ligand PL9 A 410



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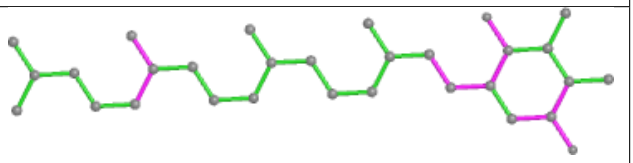
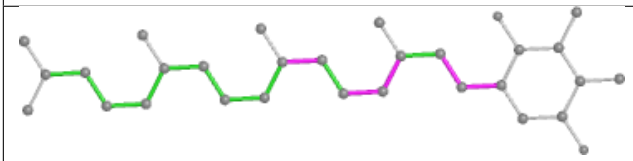


Bond angles



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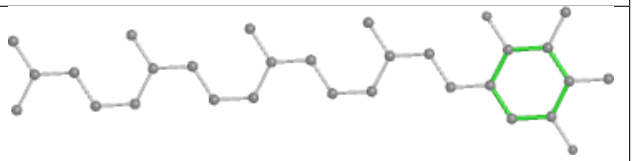
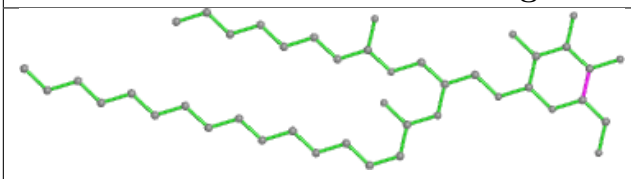
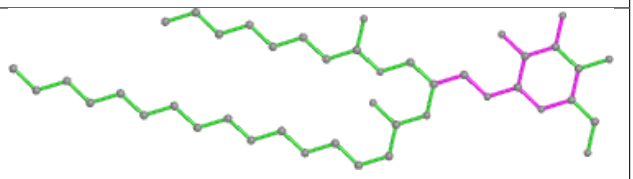


Rings

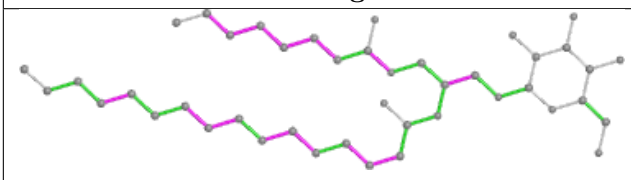
Ligand LMG B 624



Bond lengths



Bond angles



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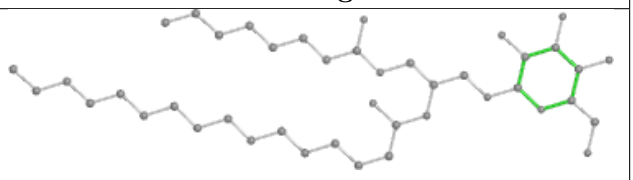
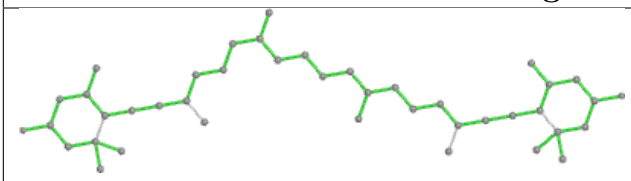


Rings

Ligand II0 7 314



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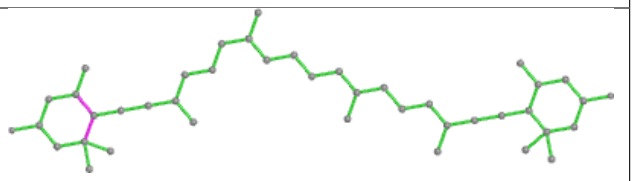
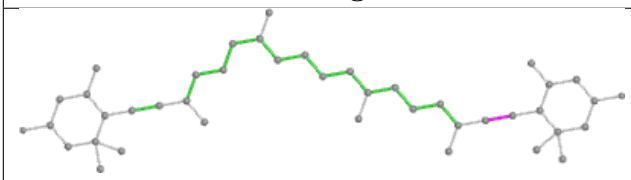


Bond angles



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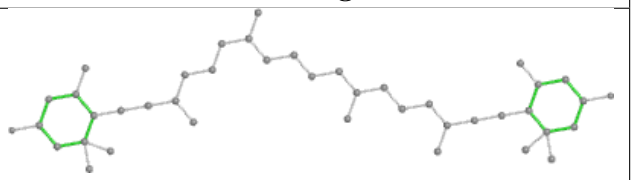
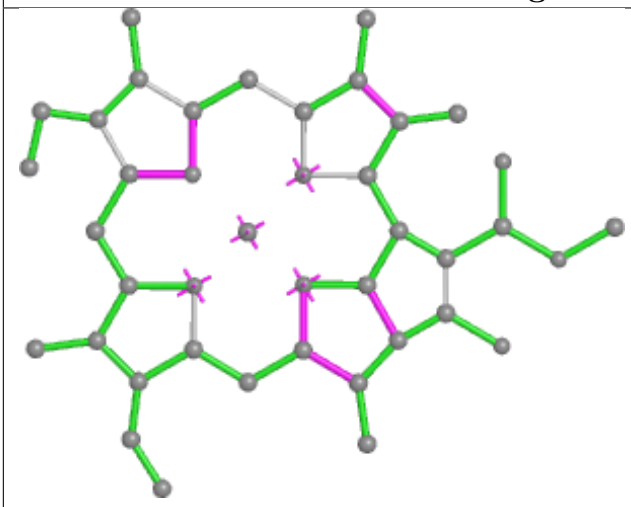


Rings

Ligand CLA 9 306



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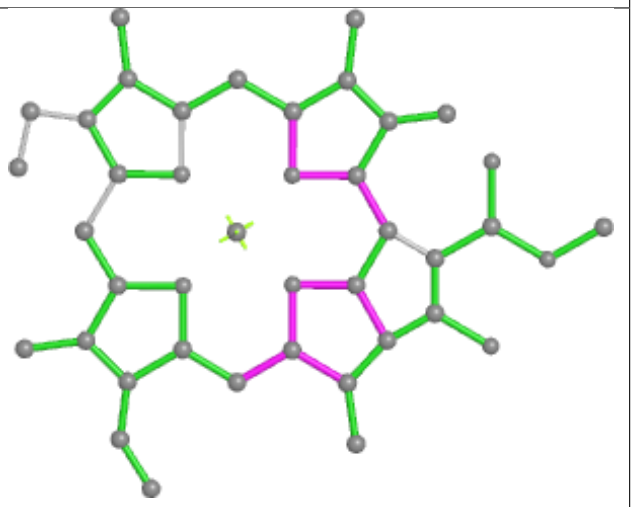
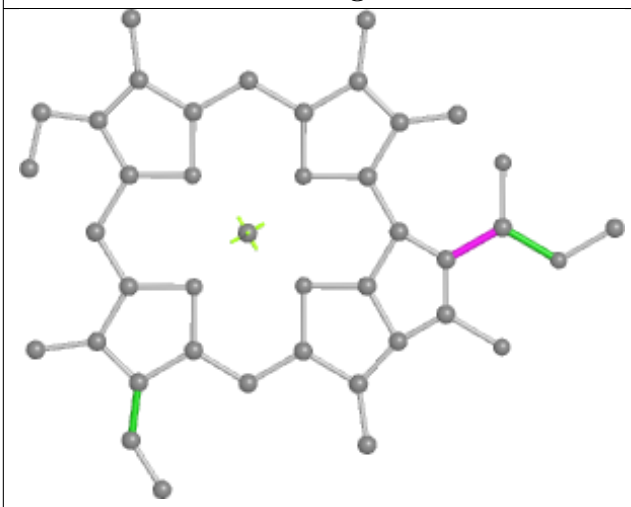


Bond angles



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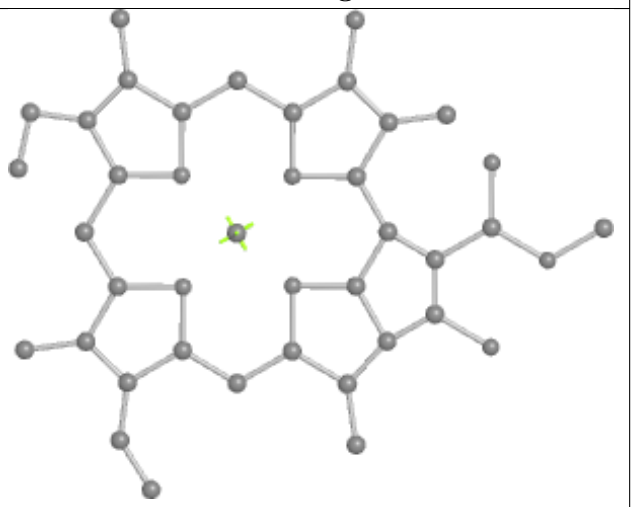
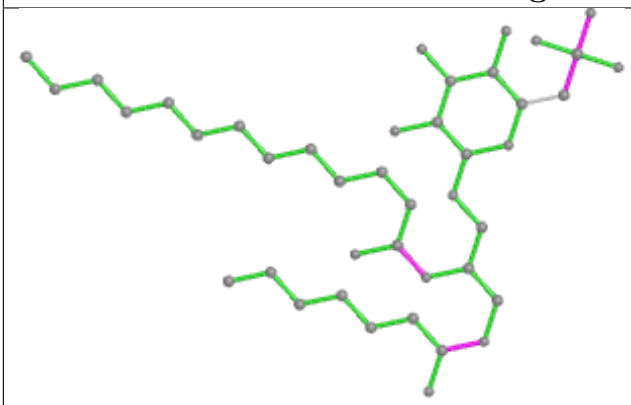
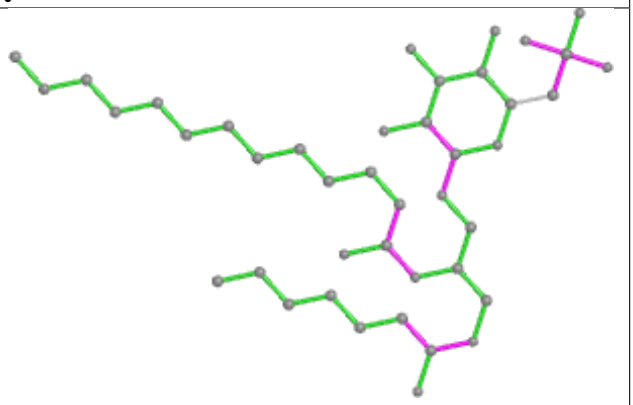


Rings

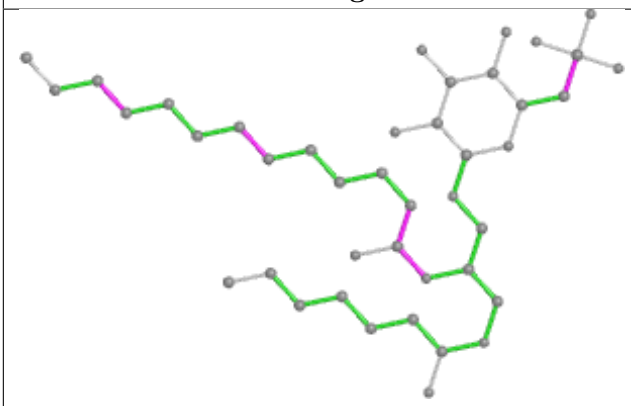
Ligand SQD c 501



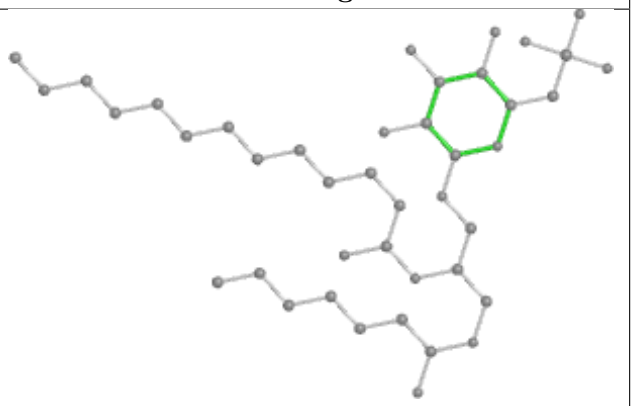
Bond lengths



Bond angles

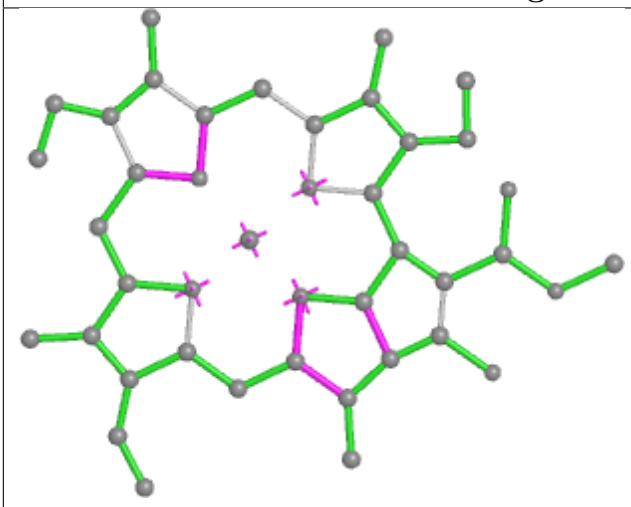


Torsions

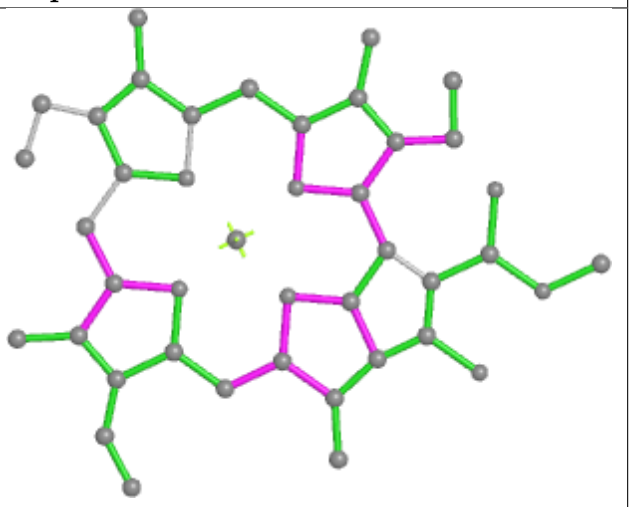


Rings

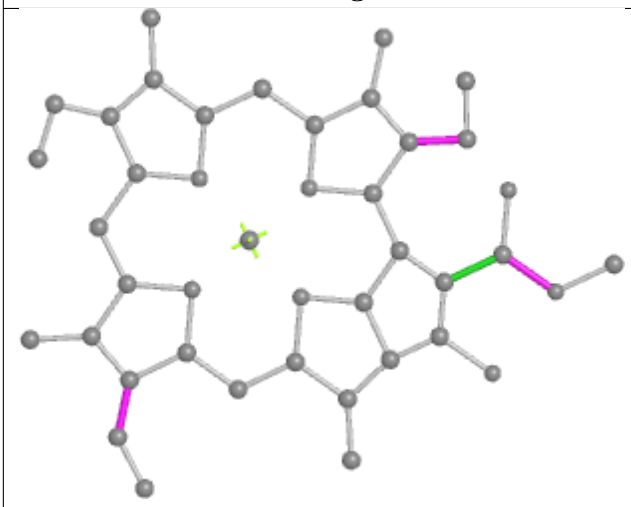
Ligand CLA p 308



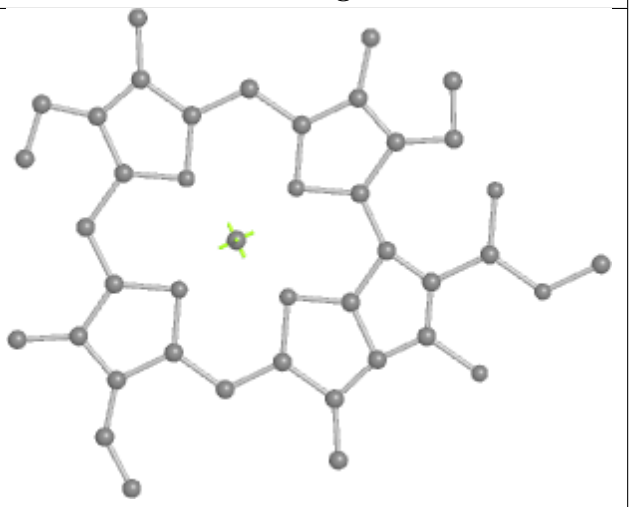
Bond lengths



Bond angles

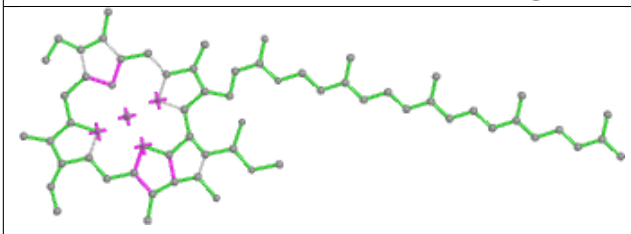


Torsions



Rings

Ligand CLA b 611



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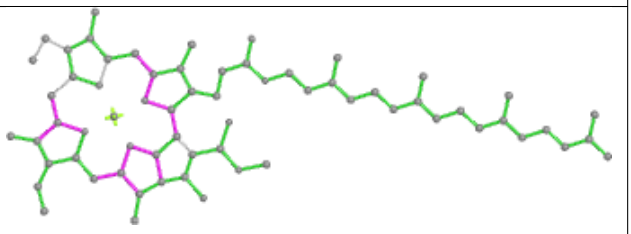
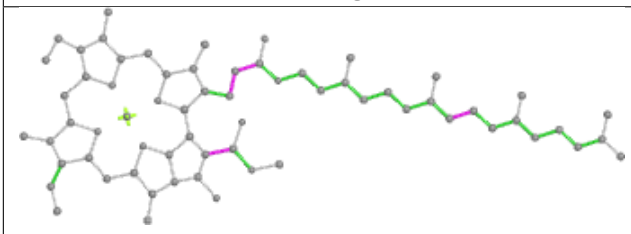
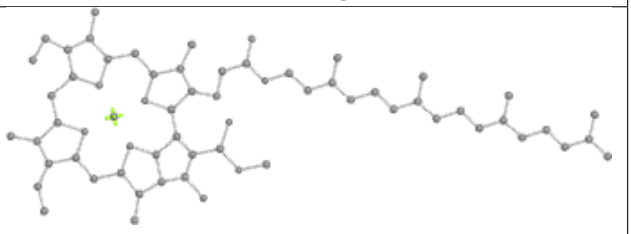


Bond angles

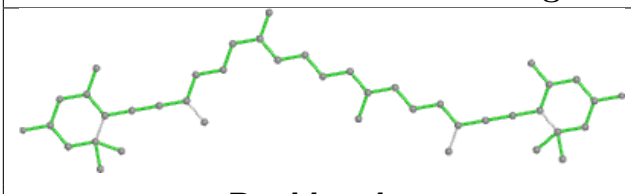


Torsions



Rings

Ligand II0 9 318



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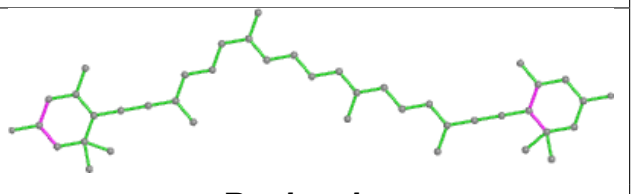
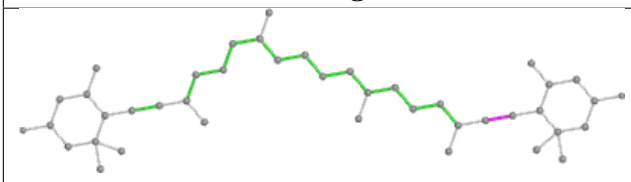
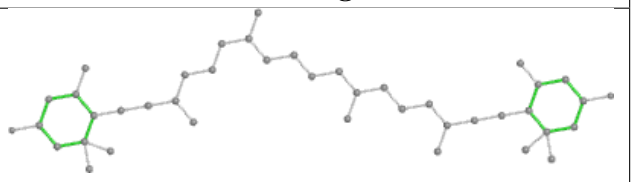


Bond angles

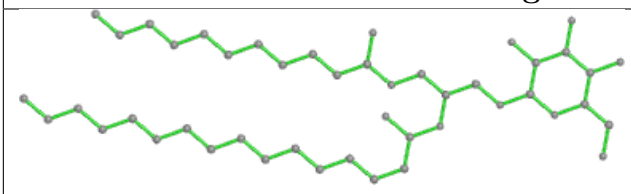


Torsions

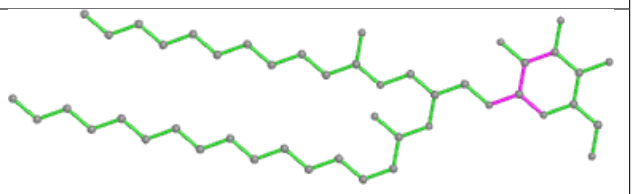


Rings

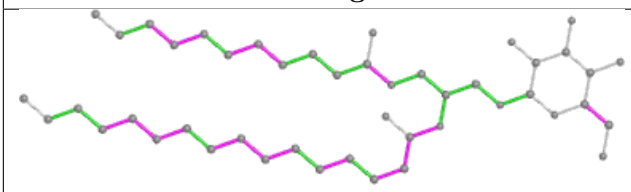
Ligand LMG d 409



Bond lengths



Bond angles



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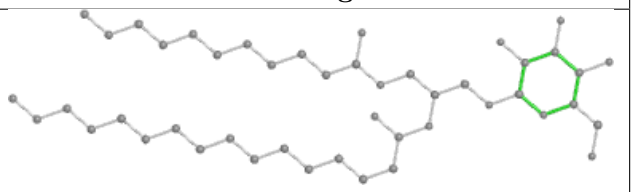
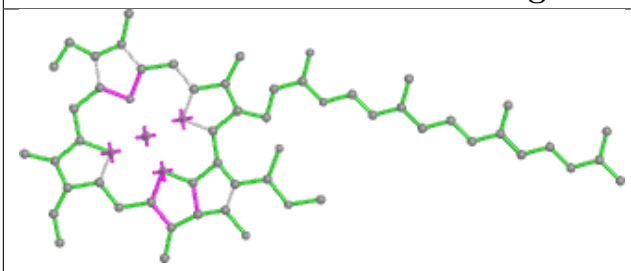


Rings

Ligand CLA 8 304



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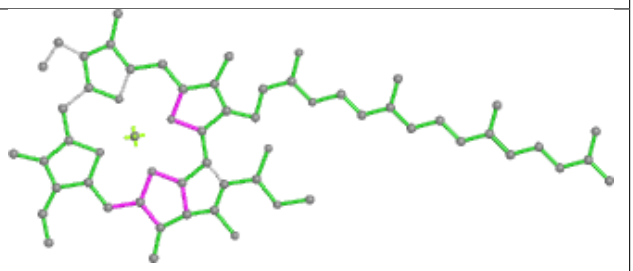
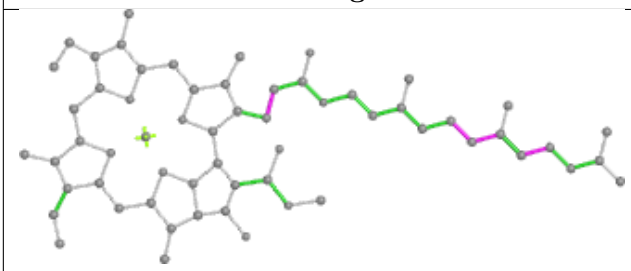


Bond angles



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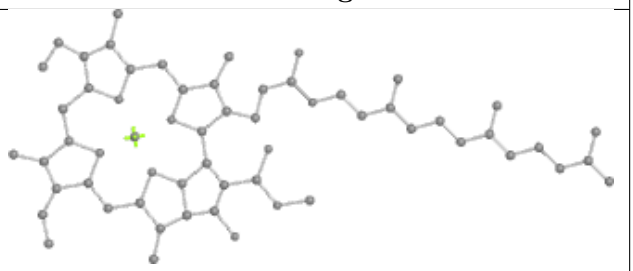
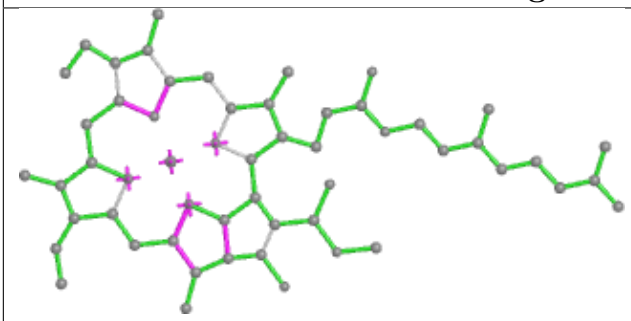


Rings

Ligand CLA 1 304



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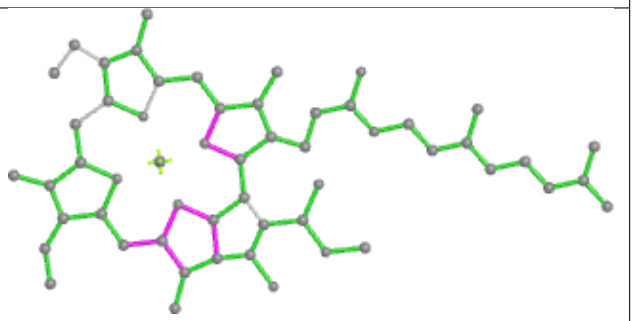
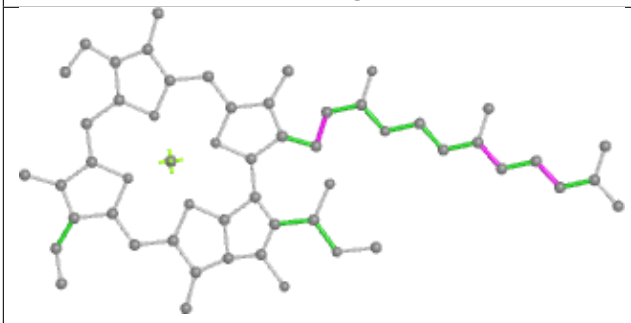


Bond angles



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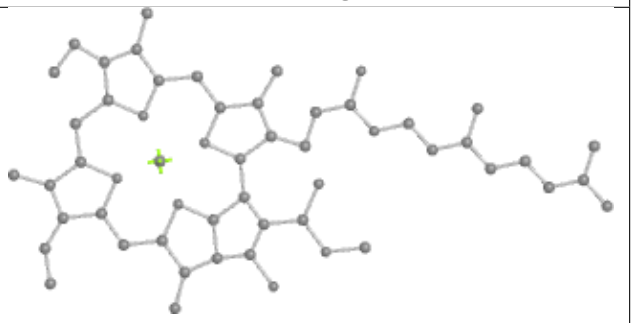
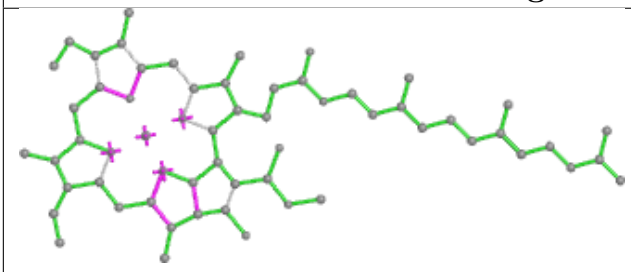


Rings

Ligand CLA b 617



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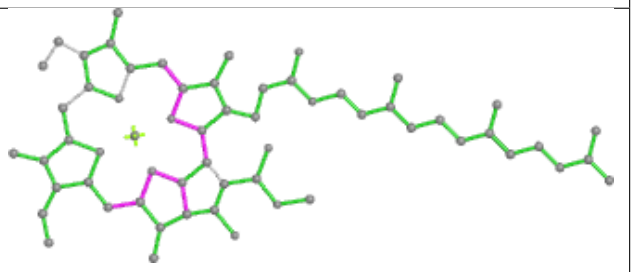
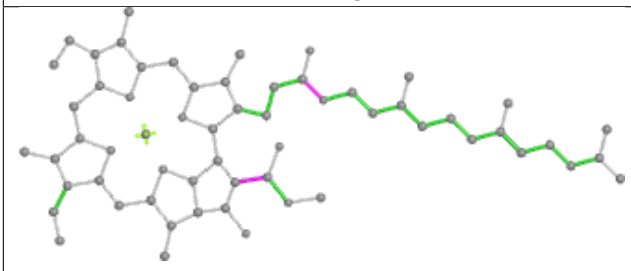


Bond angles



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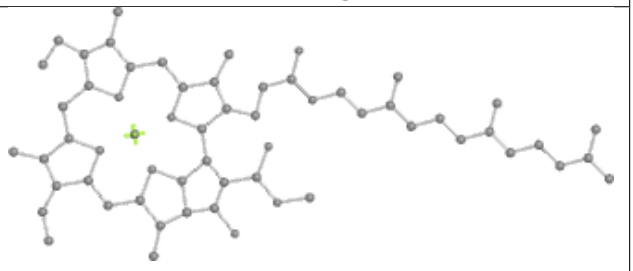
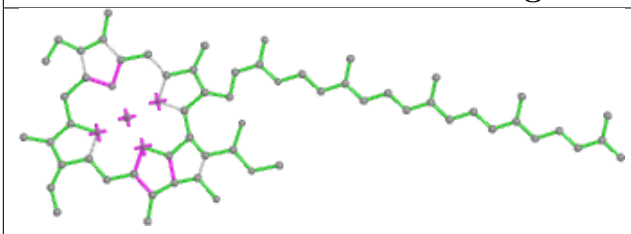
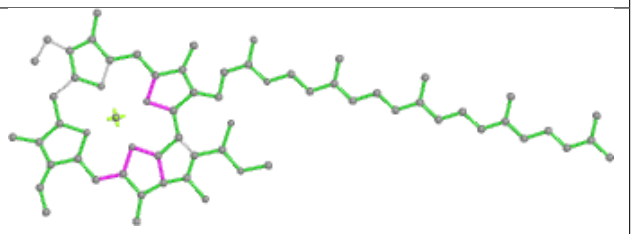


Rings

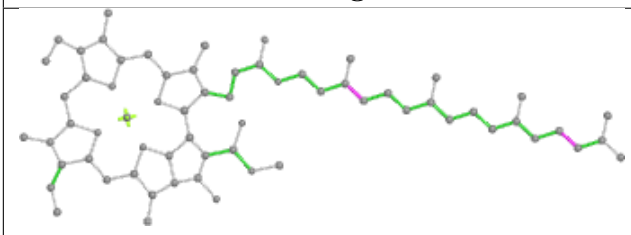
Ligand CLA B 604



Bond lengths



Bond angles



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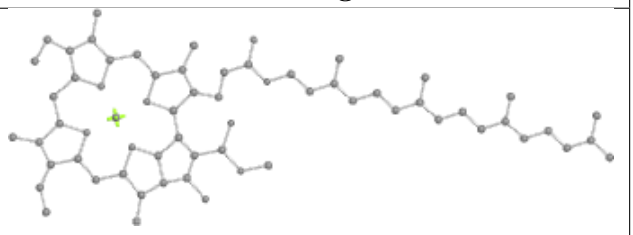
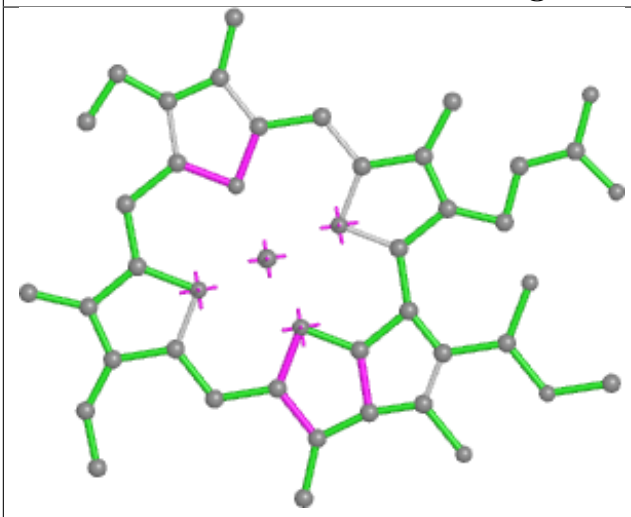


Rings

Ligand CLA 9 307



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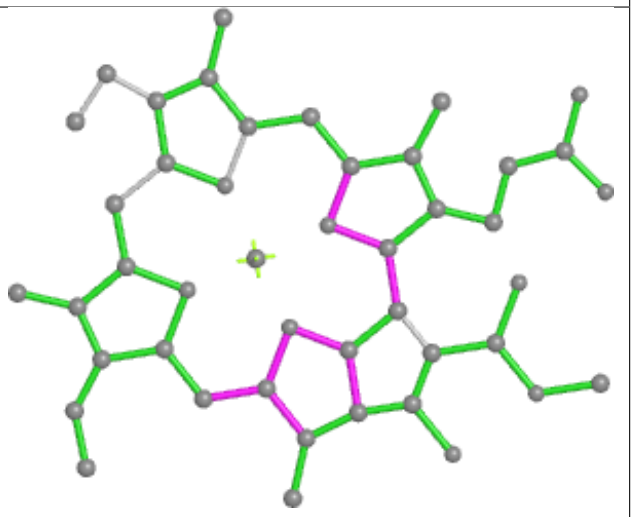
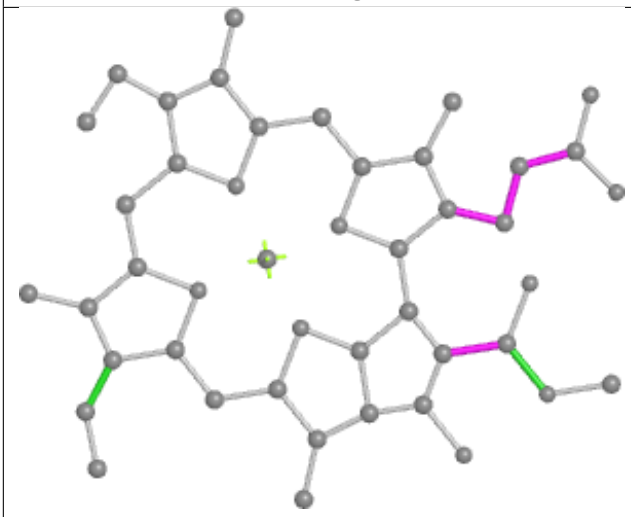


Bond angles



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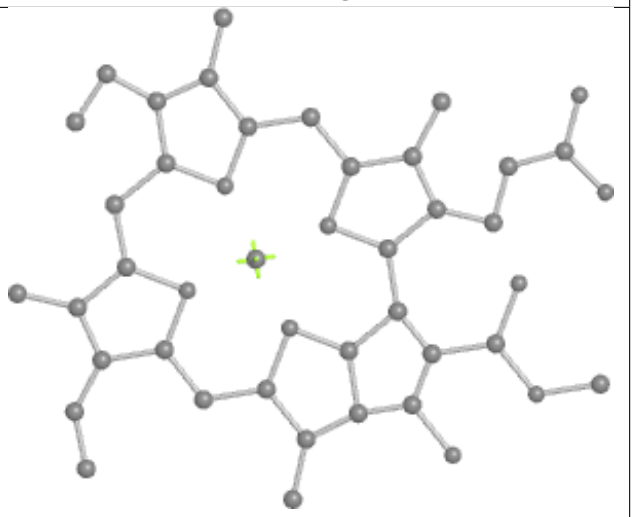
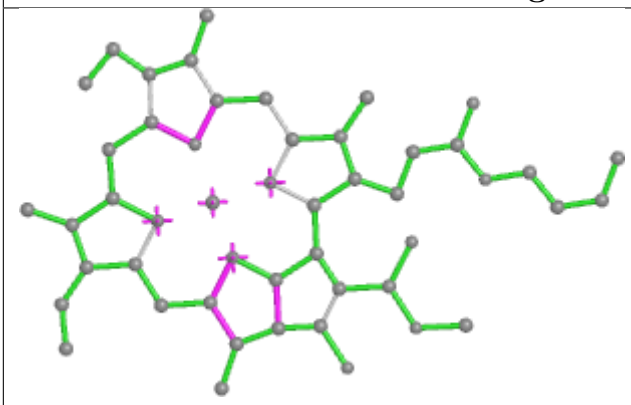


Rings

Ligand CLA 3 308



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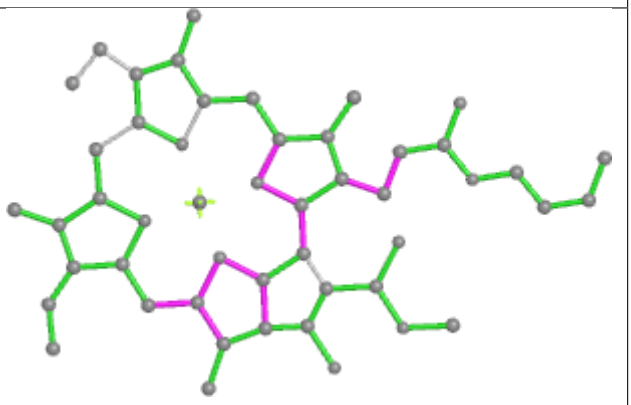
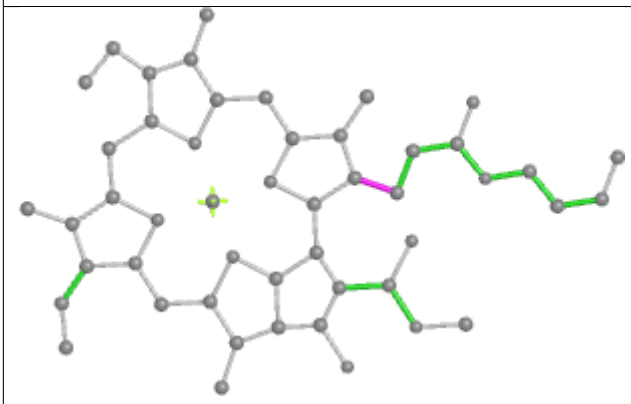


Bond angles



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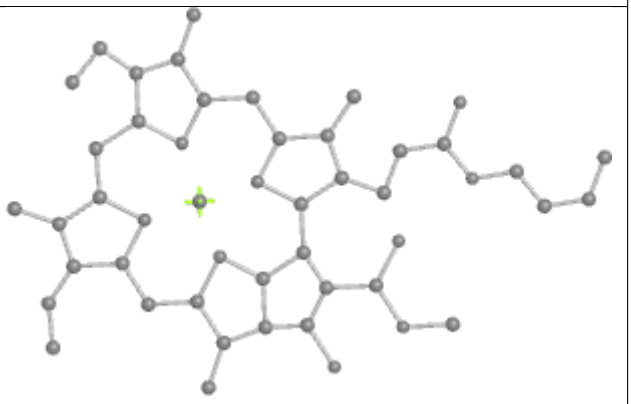
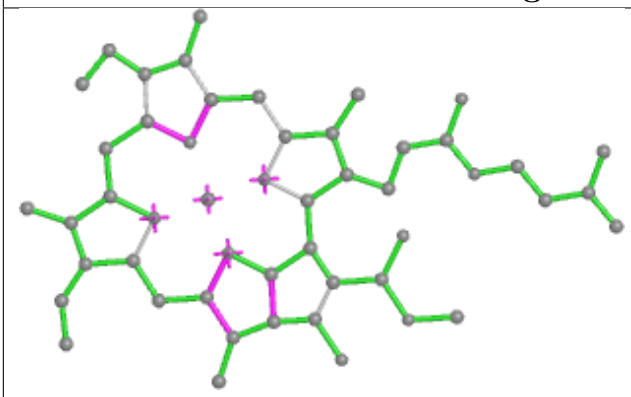


Rings

Ligand CLA N 307



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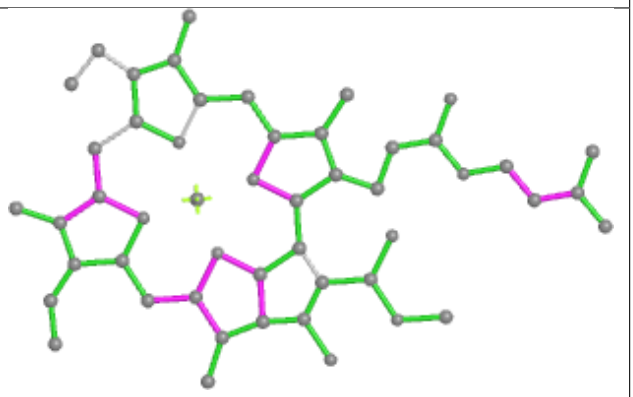

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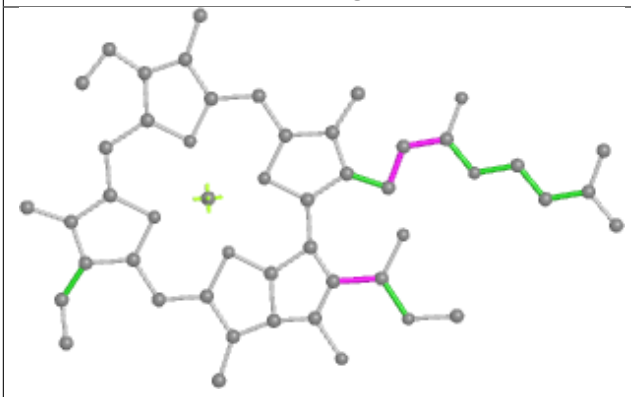

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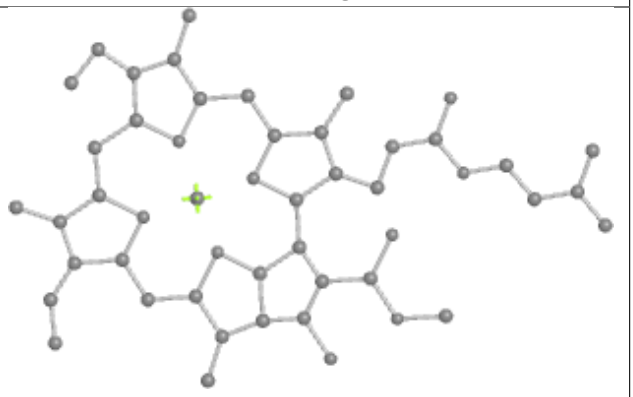
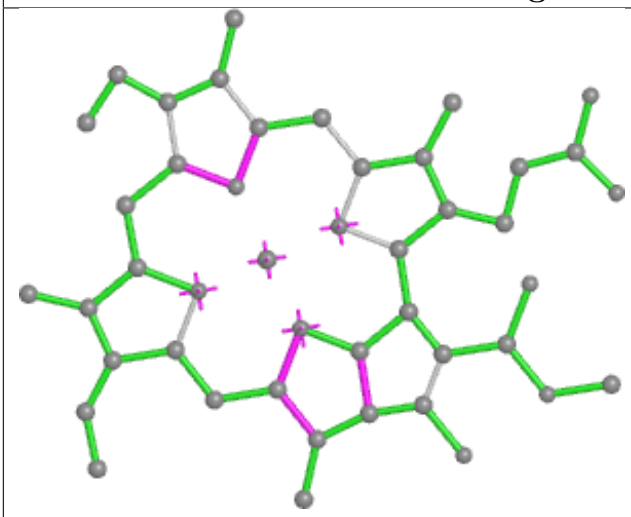


Rings

Ligand CLA 5 306



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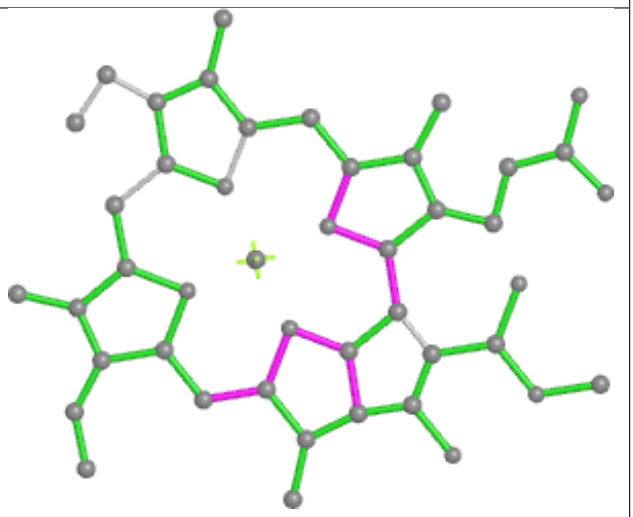
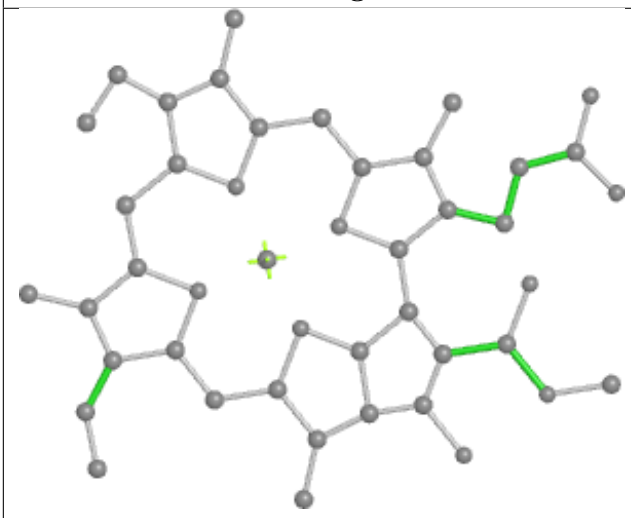
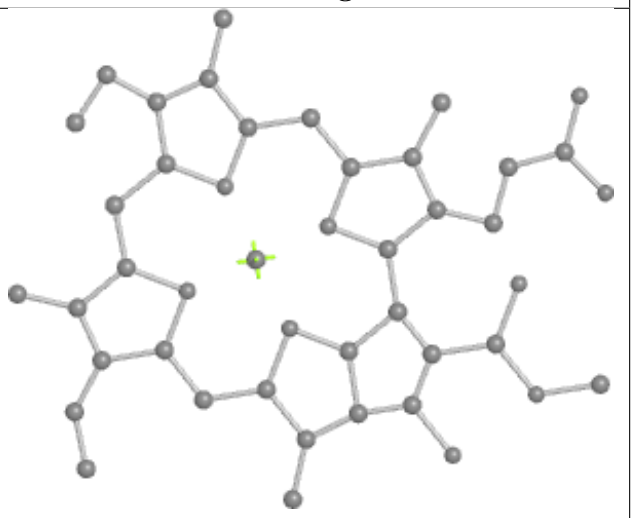


Bond angles

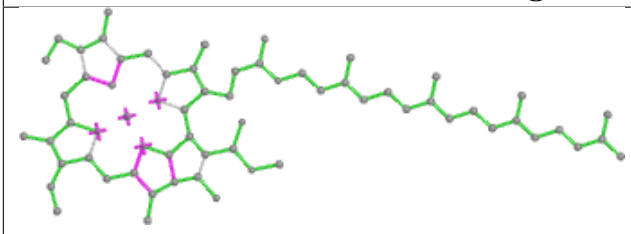


Torsions

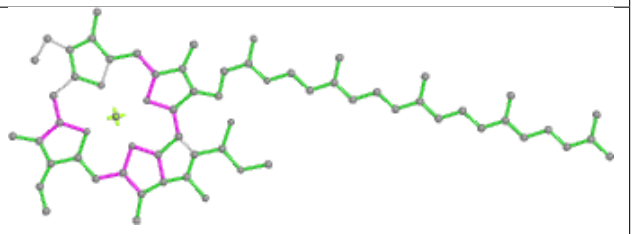


Rings

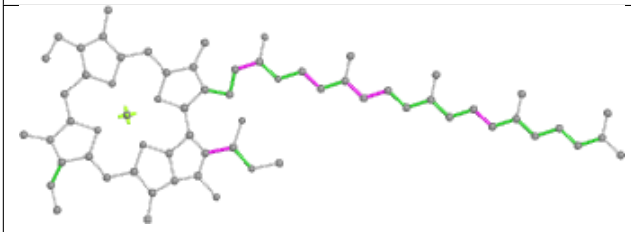
Ligand CLA b 614



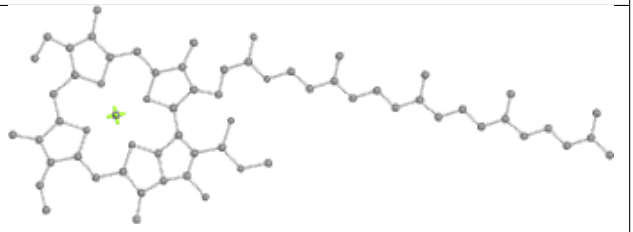
Bond lengths



Bond angles

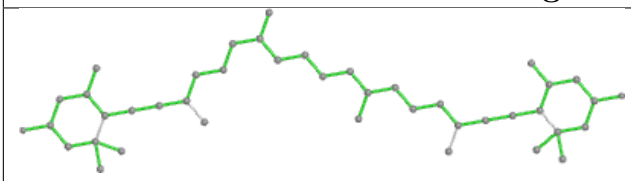


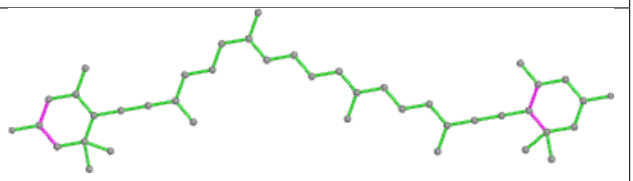
Torsions

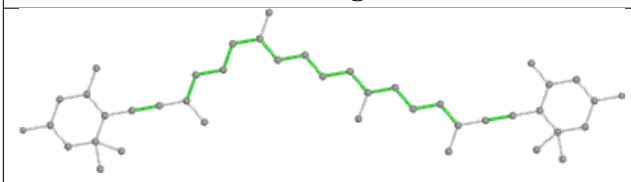


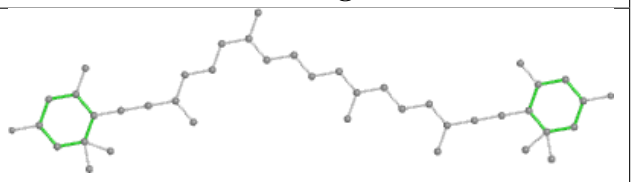
Rings

Ligand II0 6 316

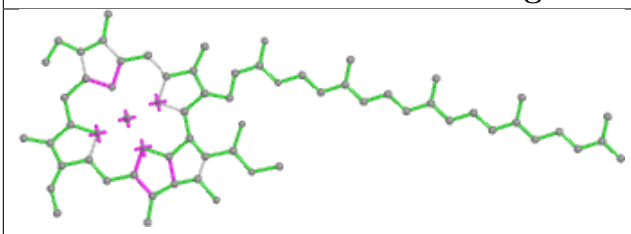

Bond lengths

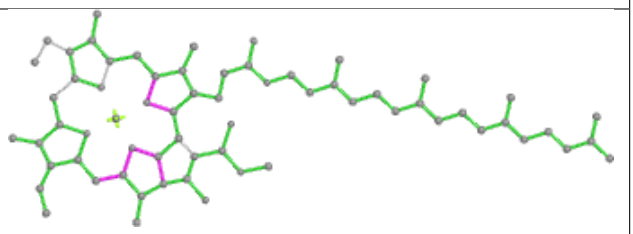

Bond angles

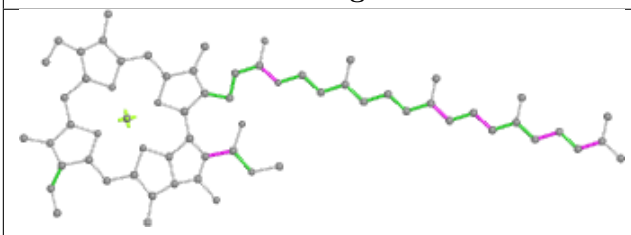

Torsions

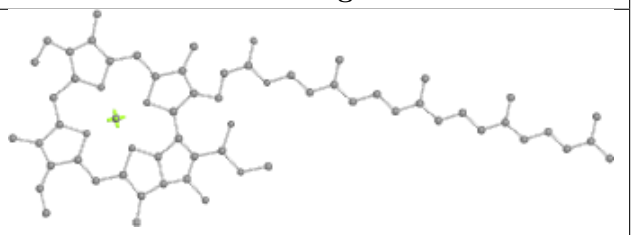

Rings

Ligand CLA B 613

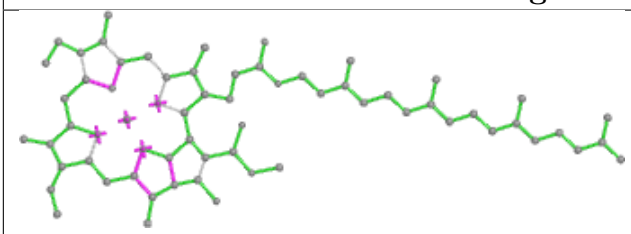

Bond lengths

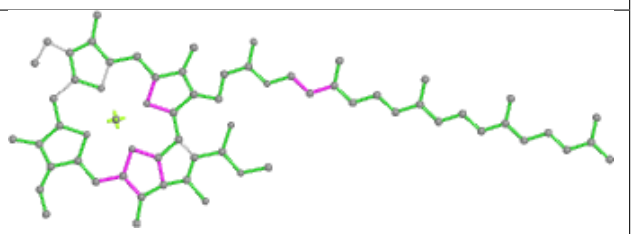

Bond angles

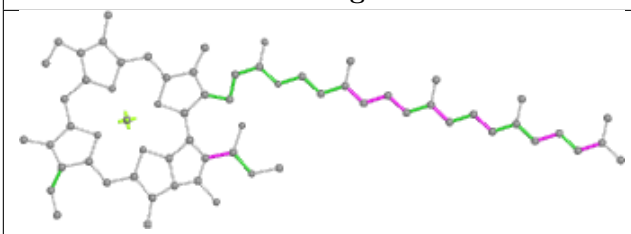

Torsions


Rings

Ligand CLA c 507


Bond lengths


Bond angles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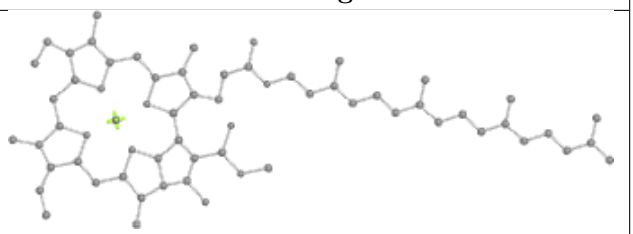
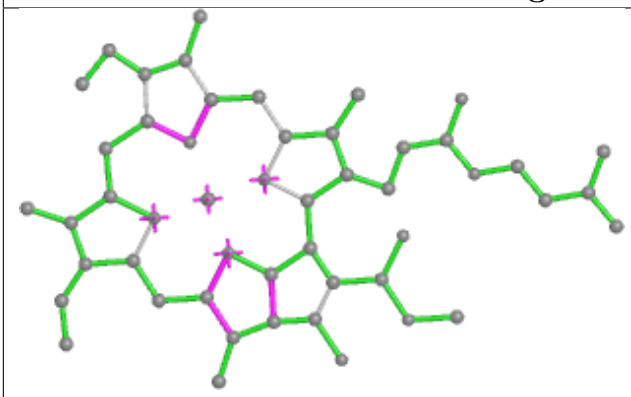
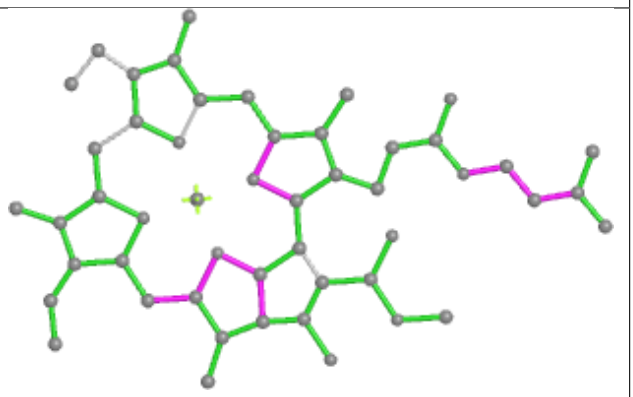

Rings

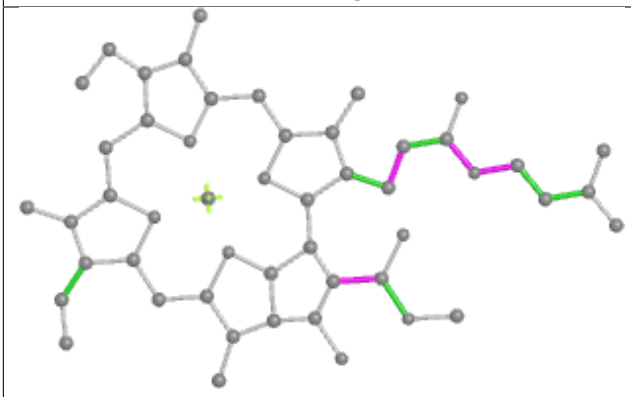
Ligand CLA 4 303



Bond lengths



Bond angles



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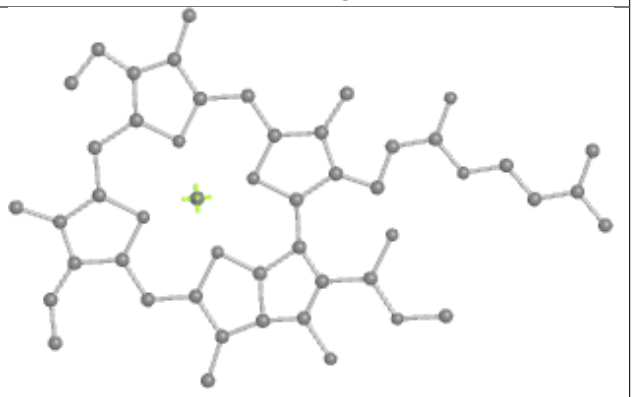
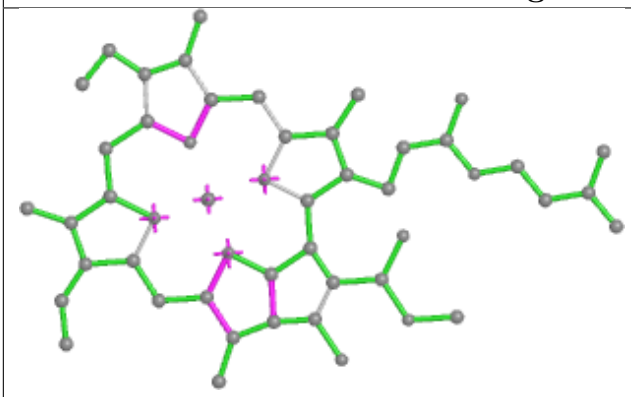


Rings

Ligand CLA b 602



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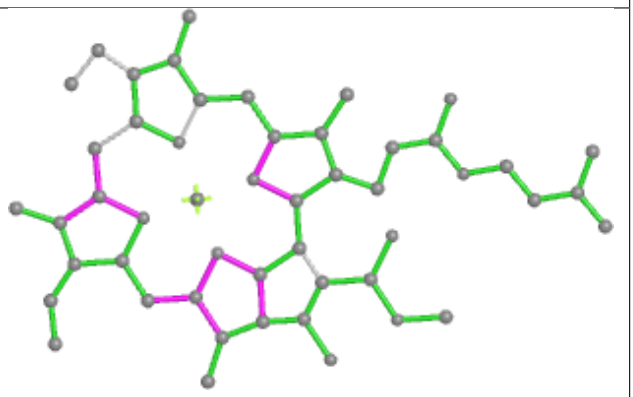
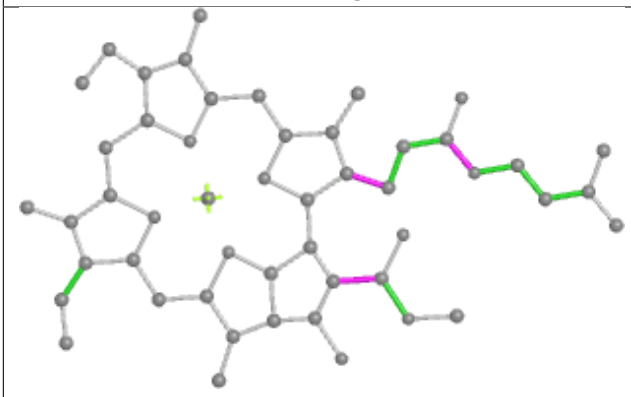


Bond angles



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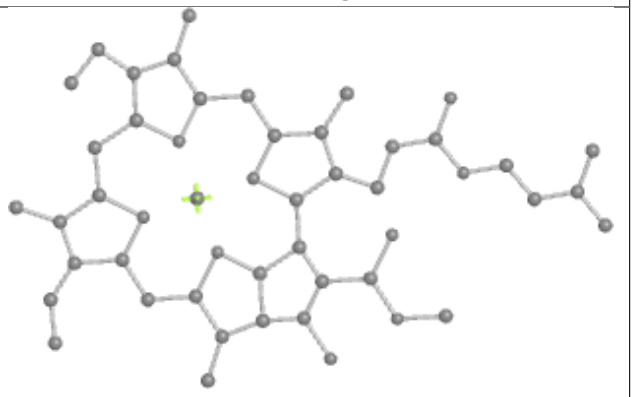
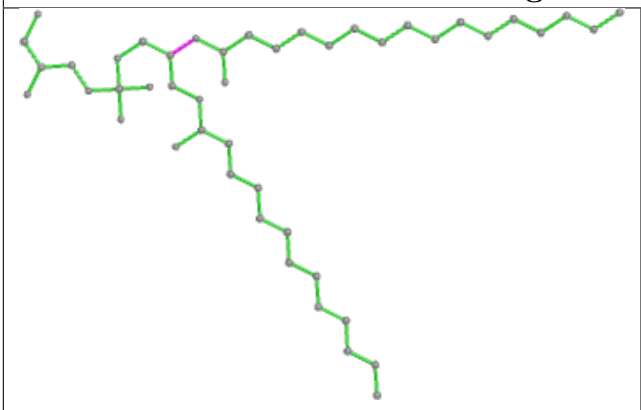


Rings

Ligand LHG d 401



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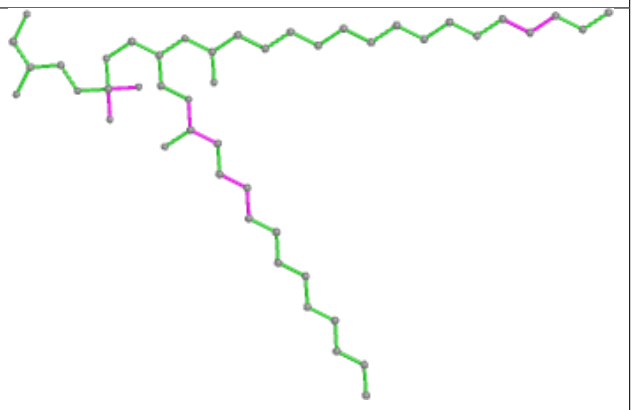
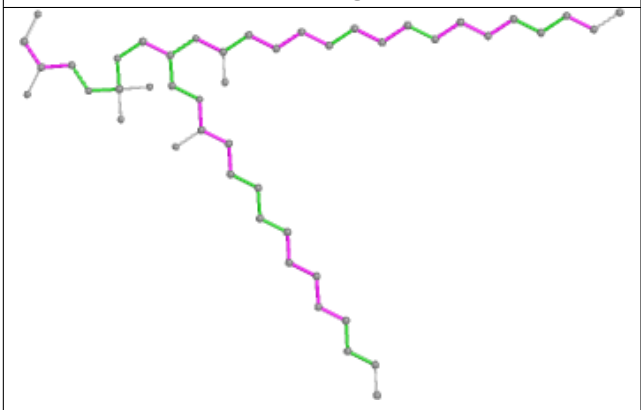


Bond angles



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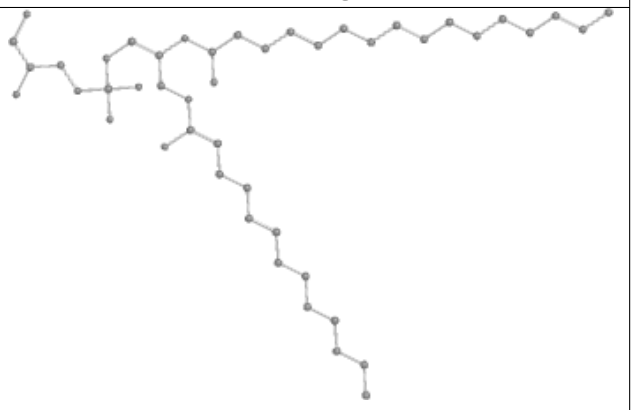
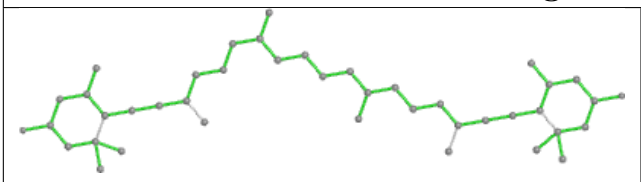


Rings

Ligand II0 0 313



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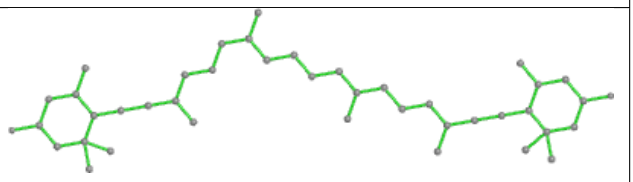

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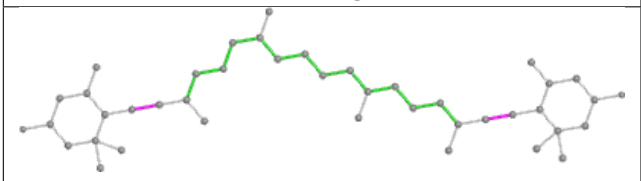

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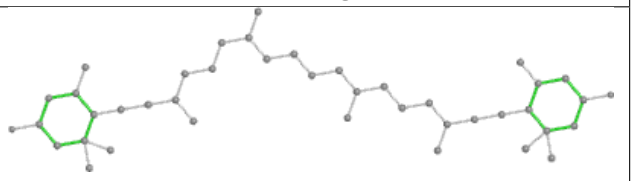
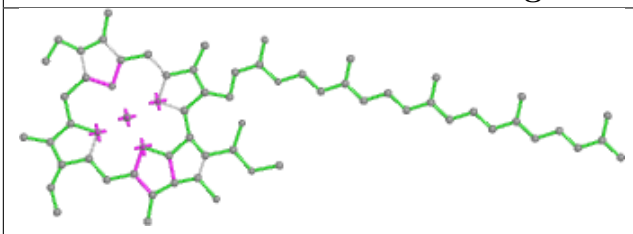
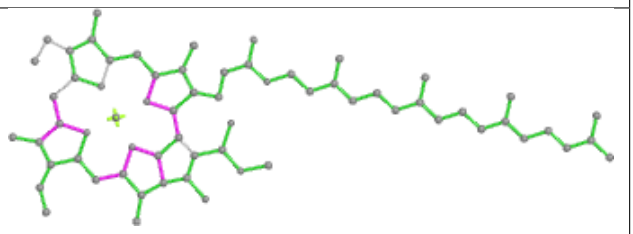


Rings

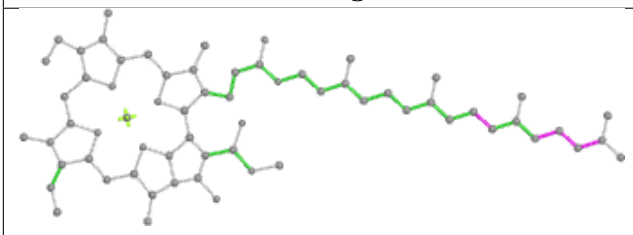
Ligand CLA B 616



Bond lengths



Bond angles



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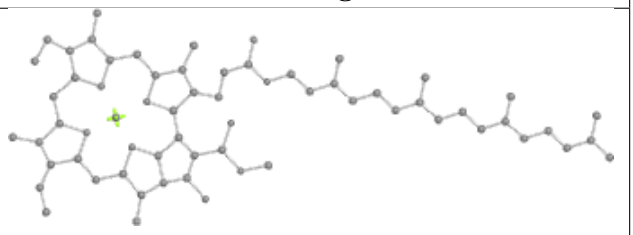
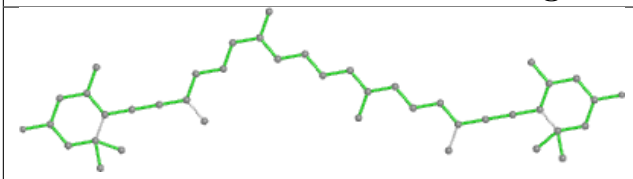
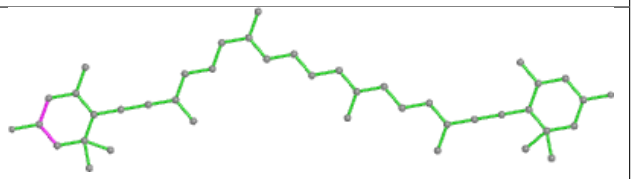


Rings

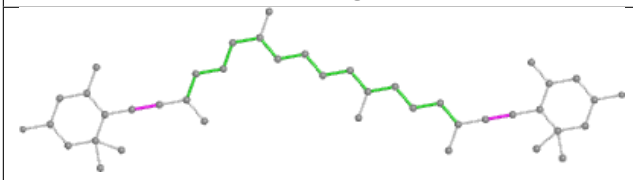
Ligand II0 6 315



Bond lengths



Bond angles



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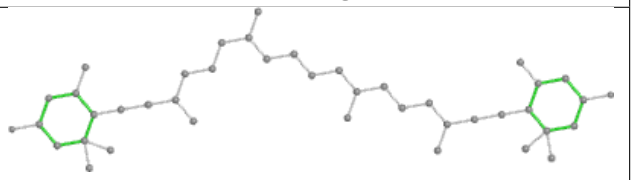
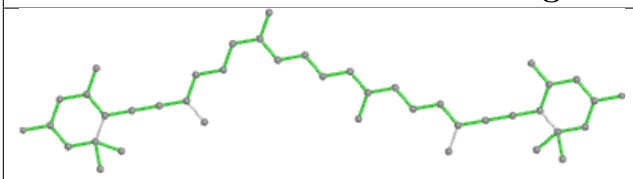


Rings

Ligand II0 9 316



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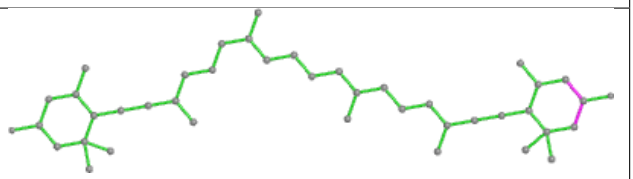
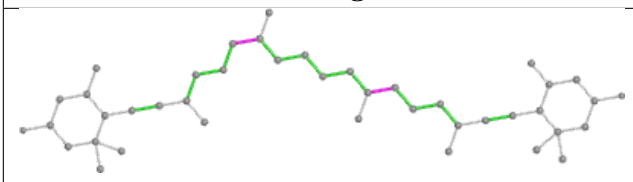


Bond angles



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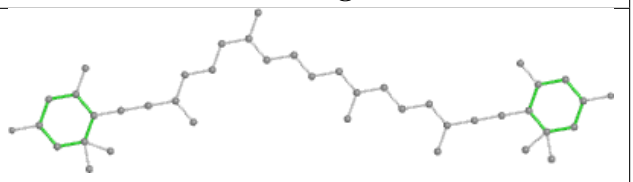
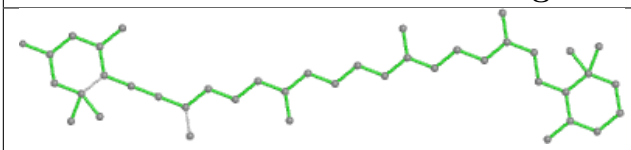
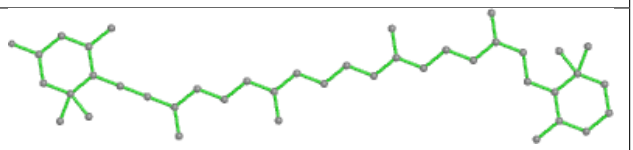
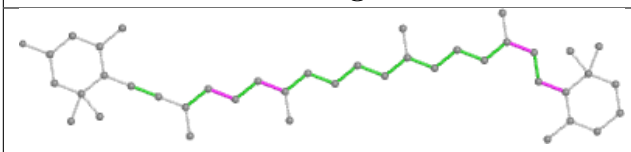
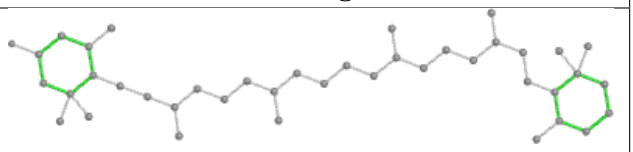
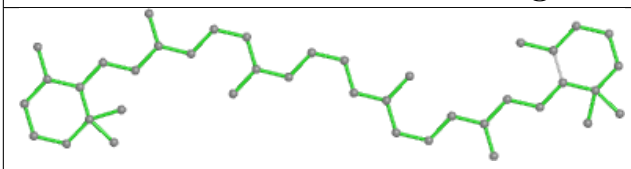
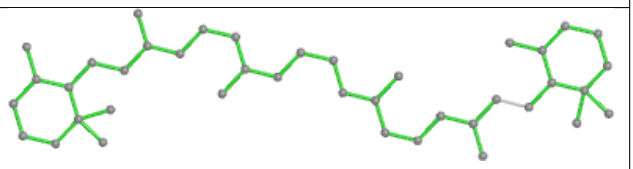
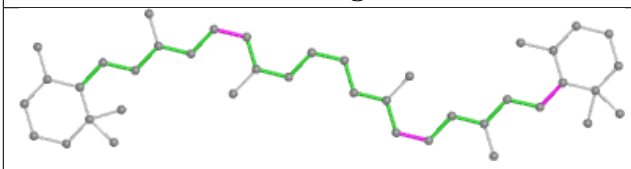
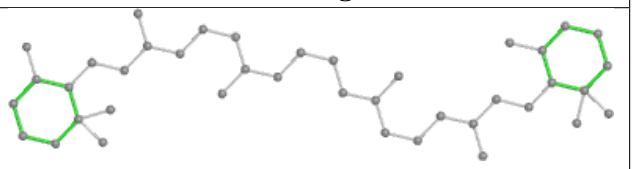
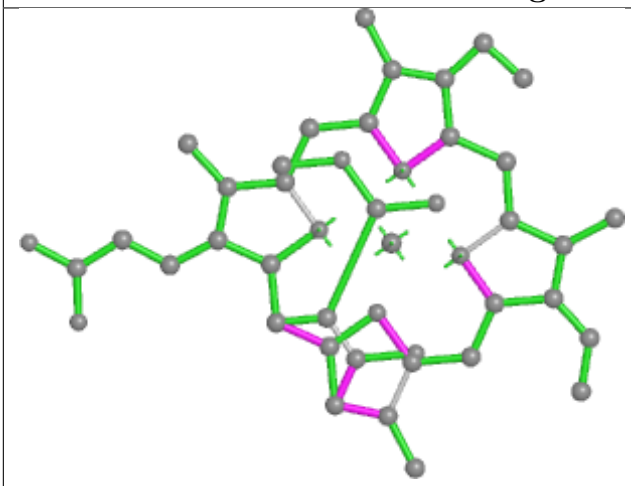


Rings

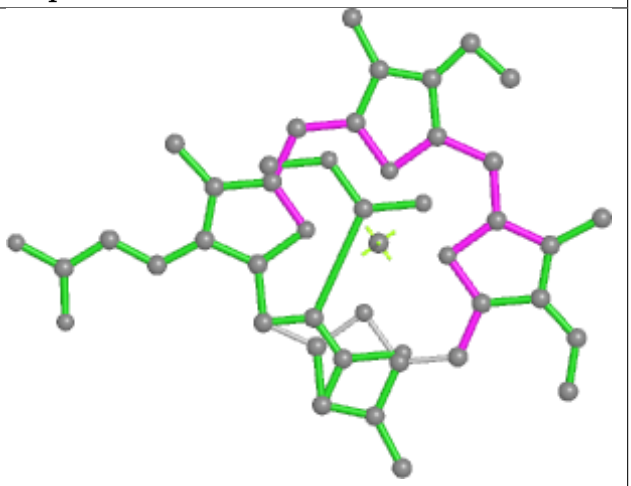
Ligand IHT 3 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT 0 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

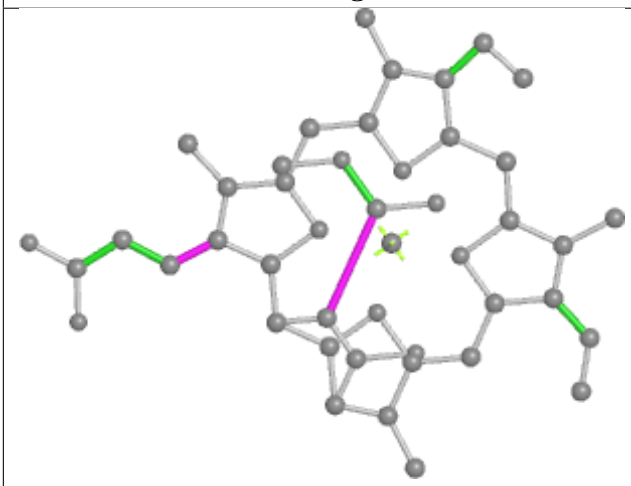
Ligand KC2 p 311



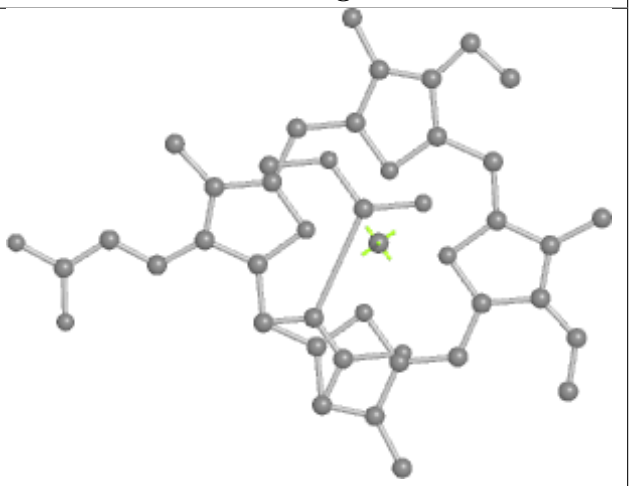
Bond lengths



Bond angles

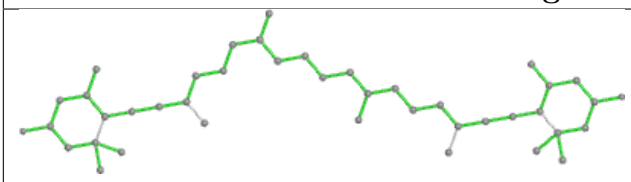


Torsions

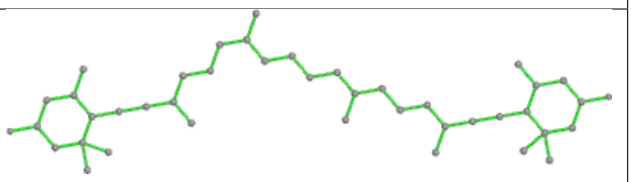


Rings

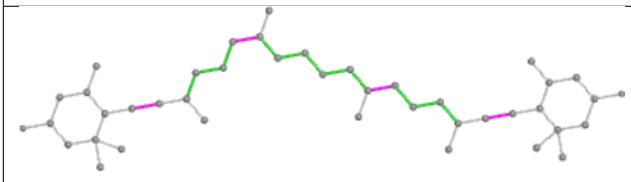
Ligand II0 2 313



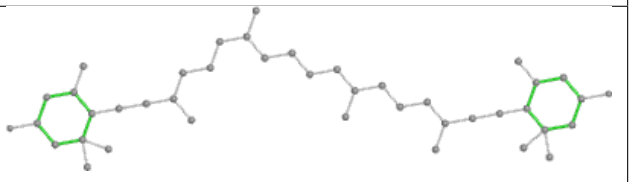
Bond lengths



Bond angles

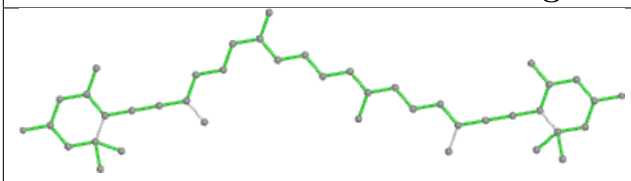


Torsions

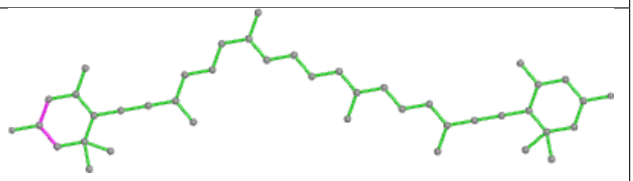


Rings

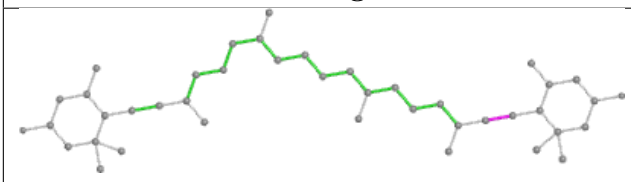
Ligand II0 0 315



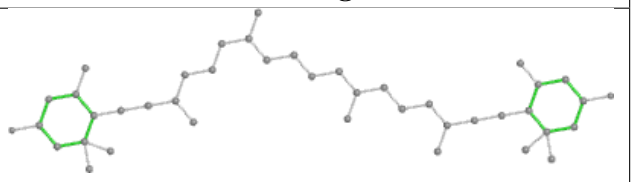
Bond lengths



Bond angles

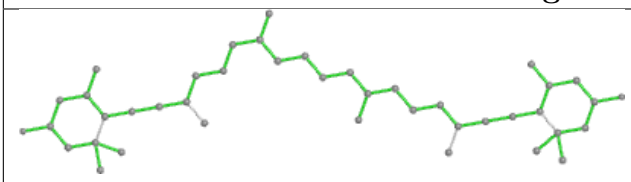


Torsions

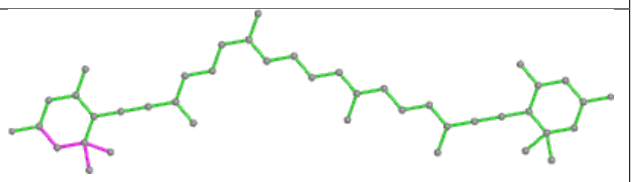


Rings

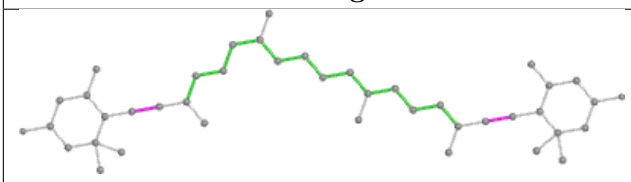
Ligand II0 5 312



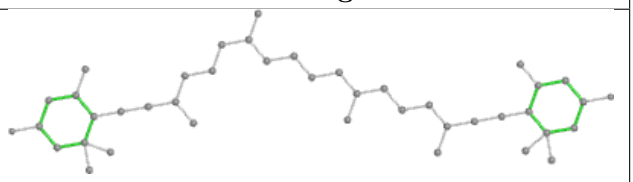
Bond lengths



Bond angles

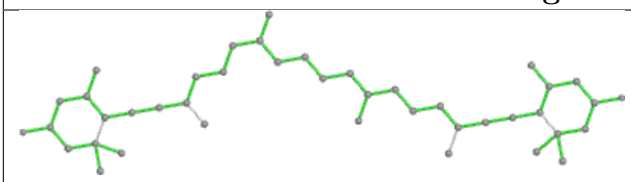


Torsions

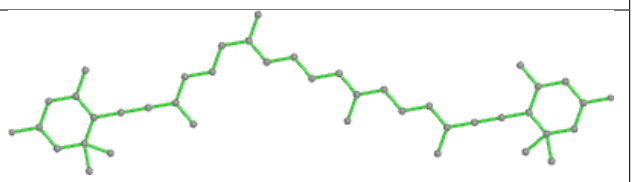


Rings

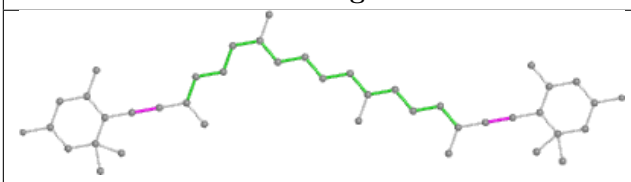
Ligand II0 7 316



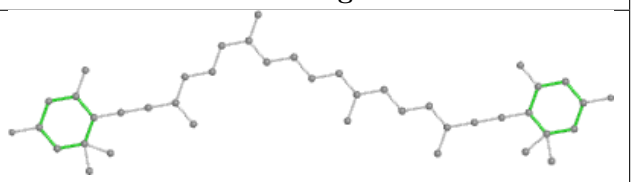
Bond lengths



Bond angles

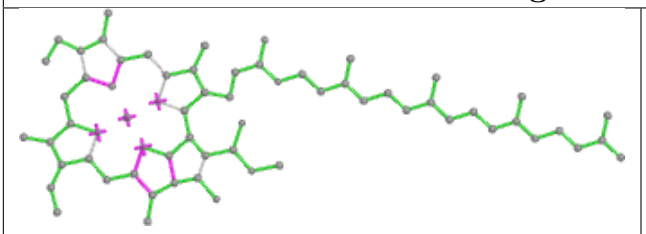


Torsions

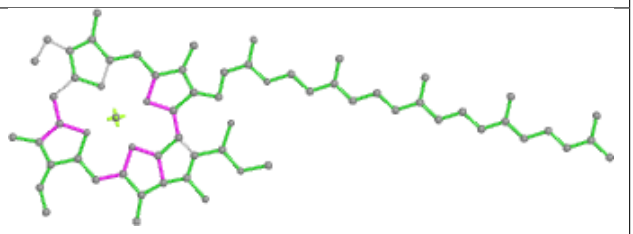


Rings

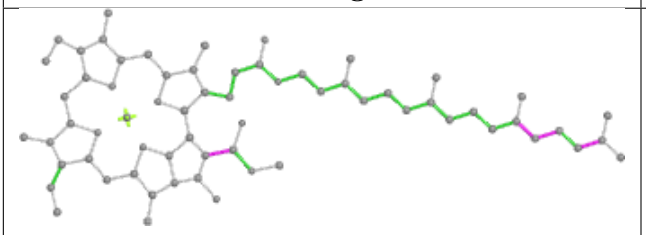
Ligand CLA c 508



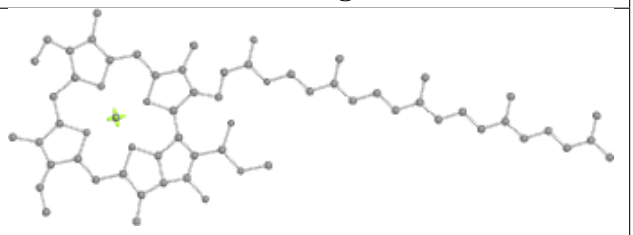
Bond lengths



Bond angles

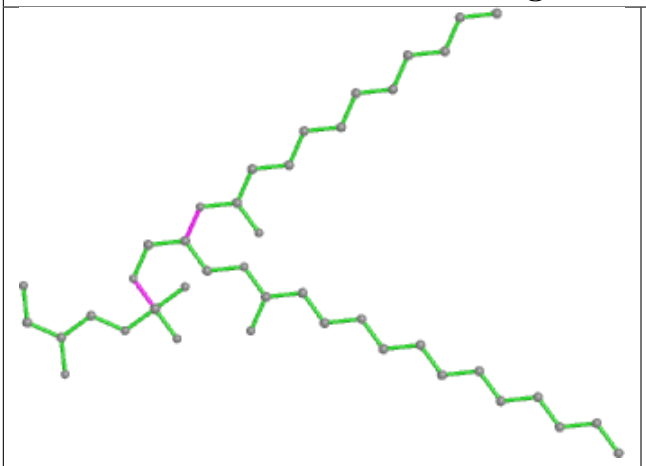


Torsions

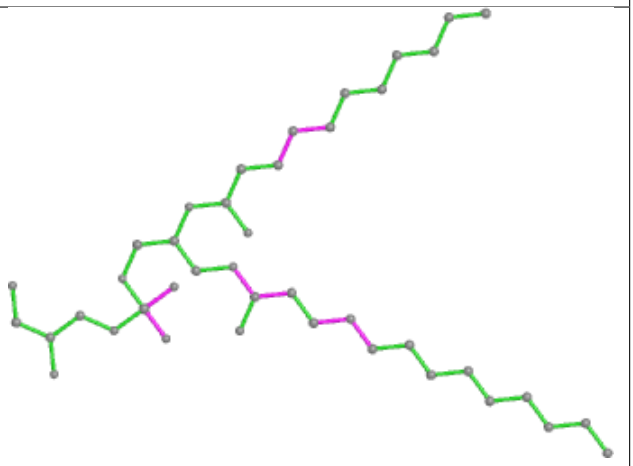


Rings

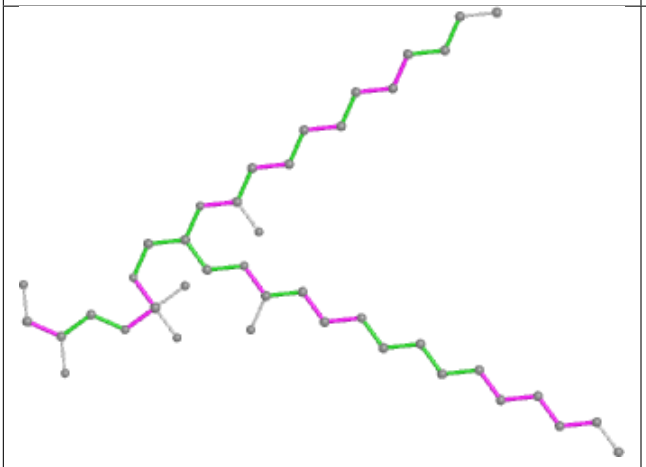
Ligand LHG 9 322



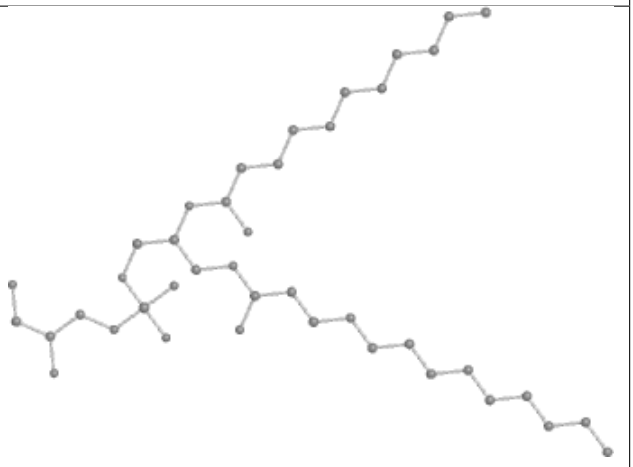
Bond lengths



Bond angles

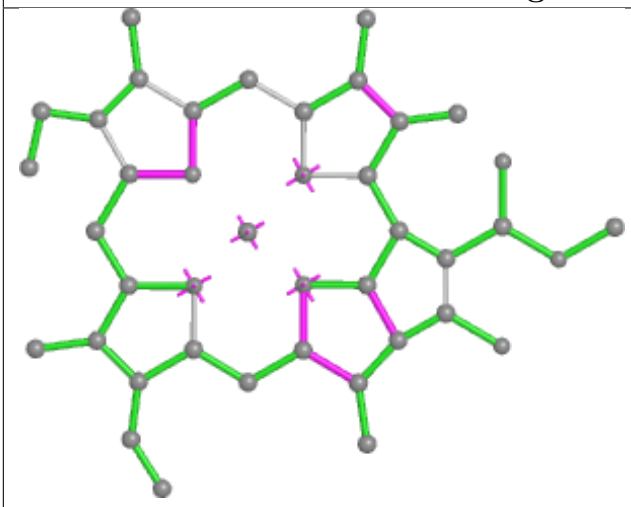


Torsions

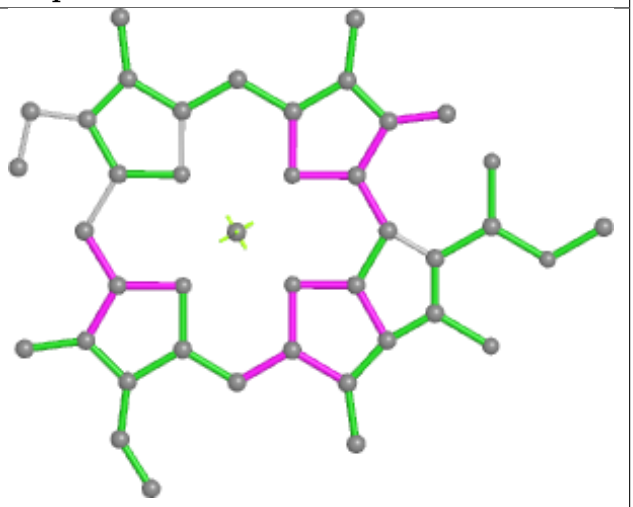


Rings

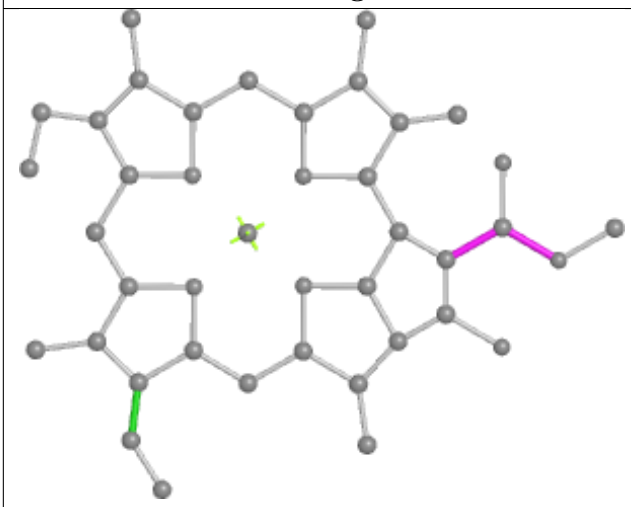
Ligand CLA p 313



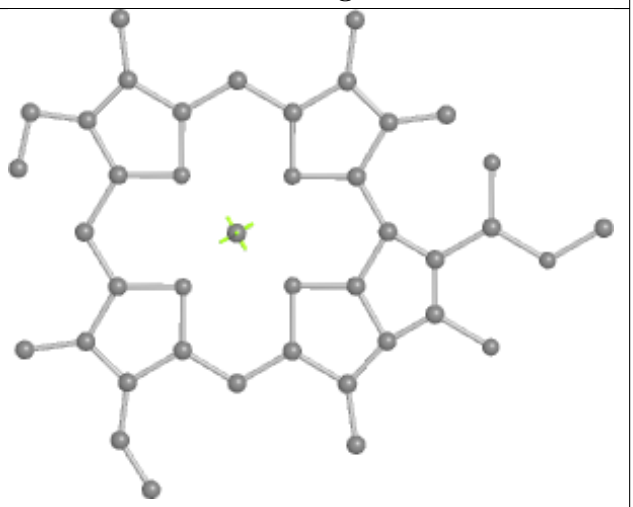
Bond lengths



Bond angles

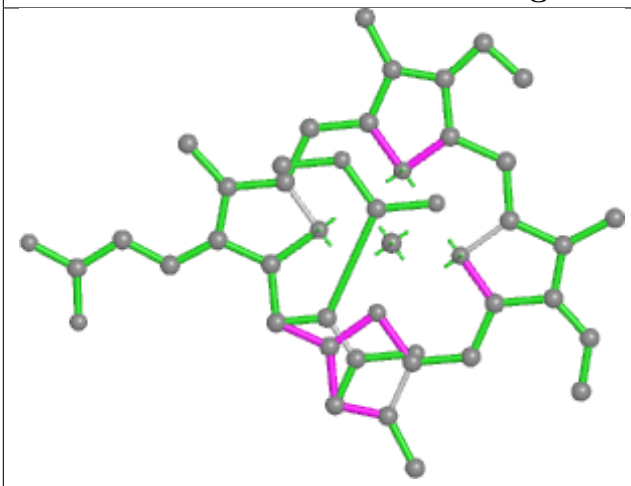


Torsions

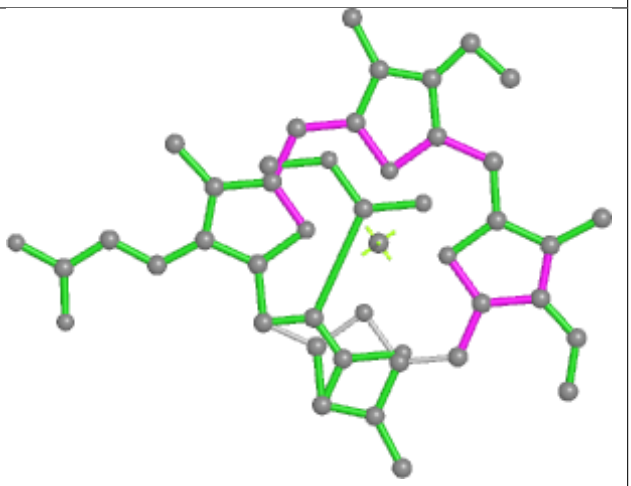


Rings

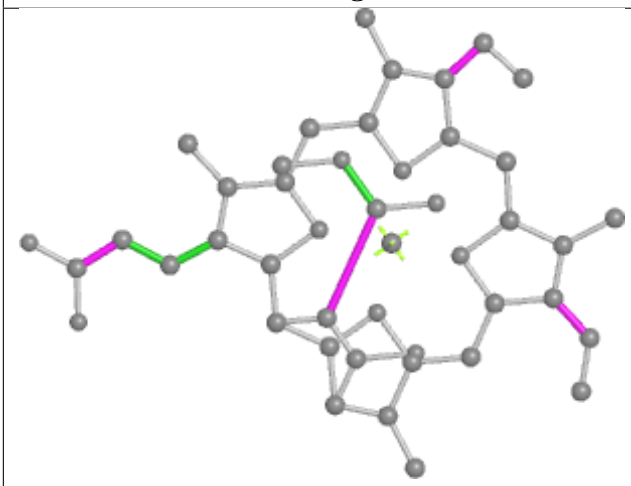
Ligand KC2 7 310



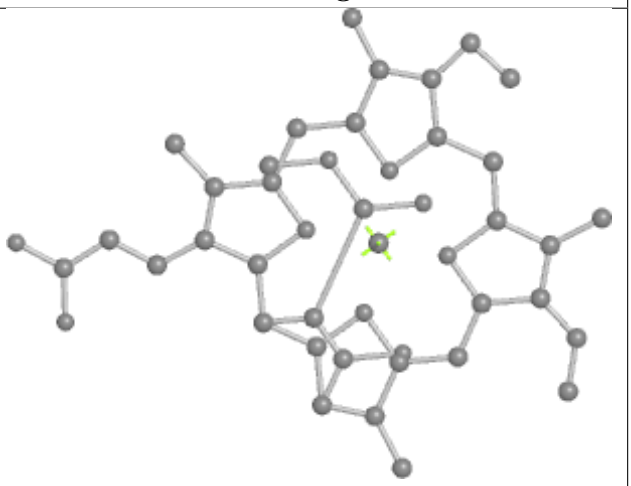
Bond lengths



Bond angles

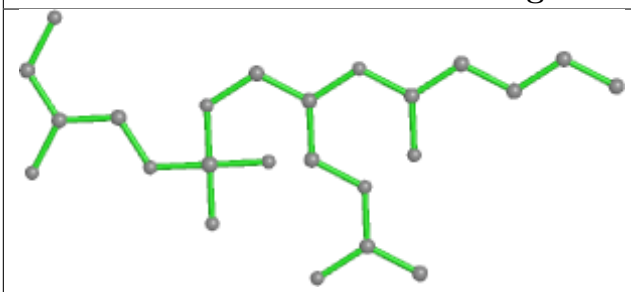


Torsions

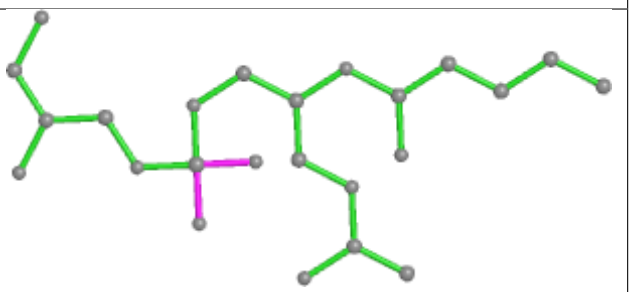


Rings

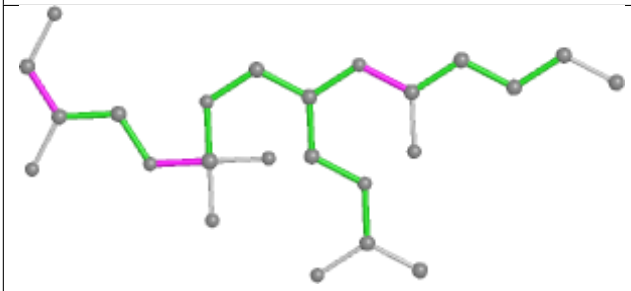
Ligand LHG 4 316



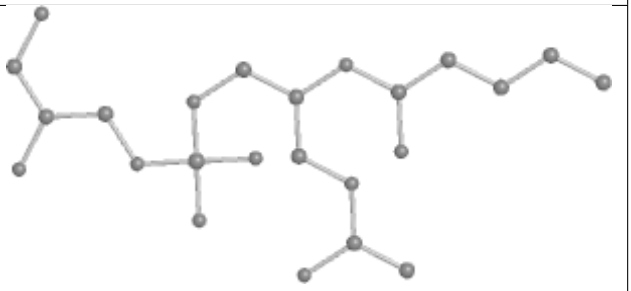
Bond lengths



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.

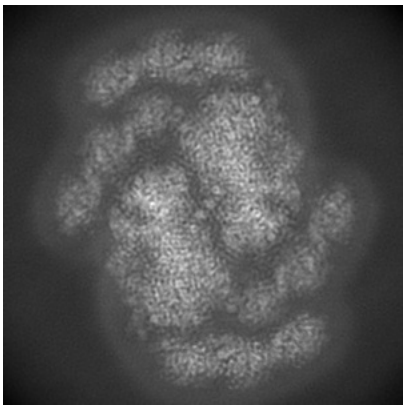
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38596. These allow visual inspection of the internal detail of the map and identification of artifacts.

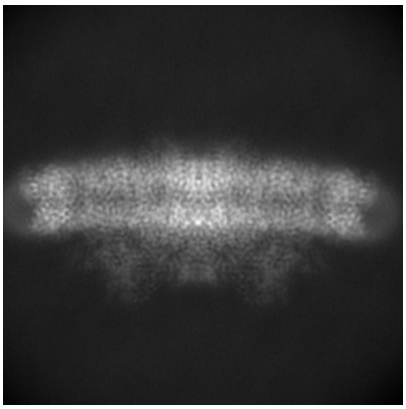
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

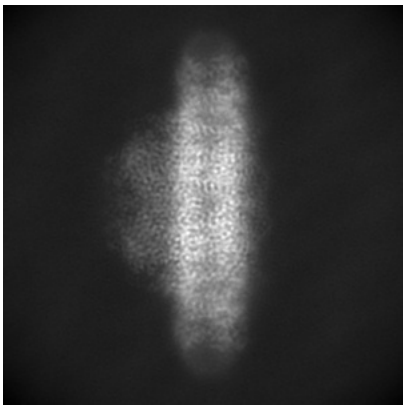
6.1.1 Primary map



X

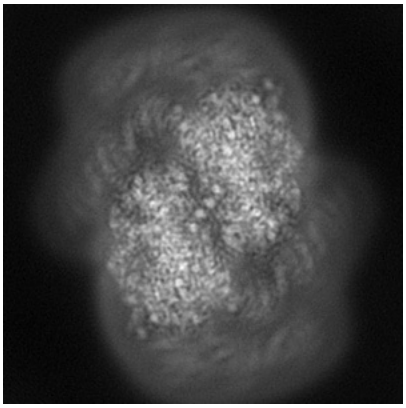


Y

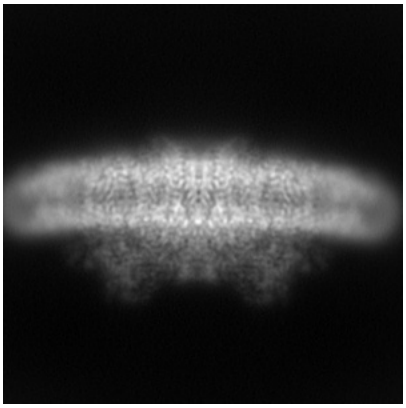


Z

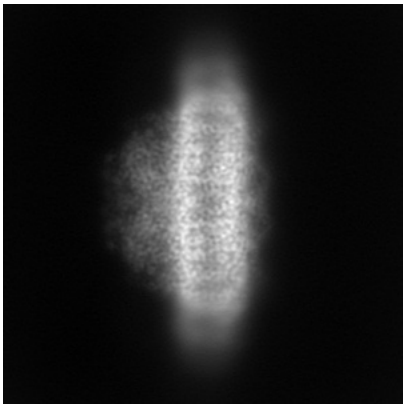
6.1.2 Raw map



X



Y

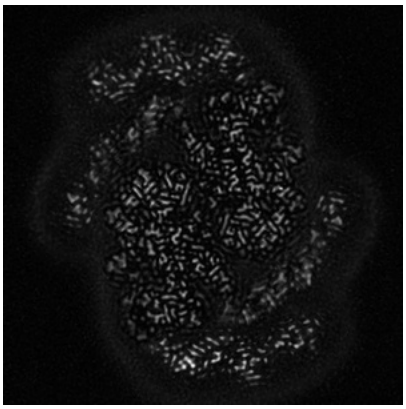


Z

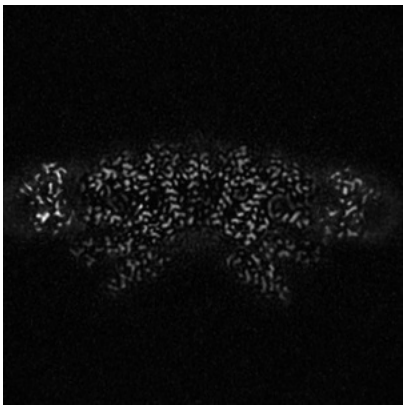
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

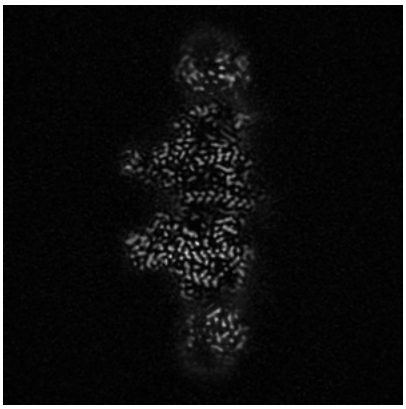
6.2.1 Primary map



X Index: 128

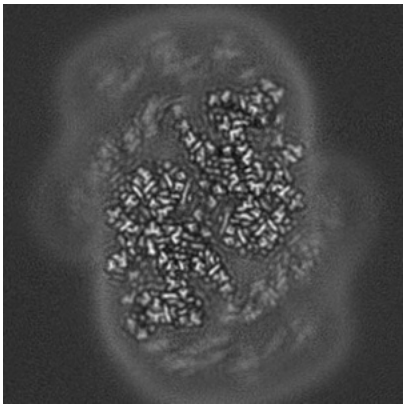


Y Index: 128

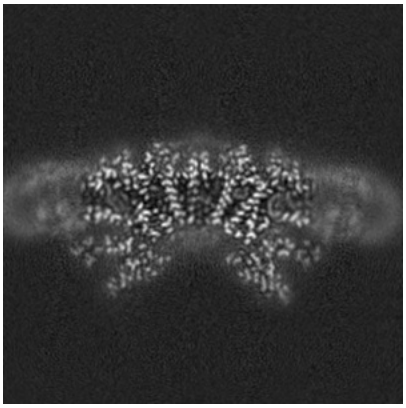


Z Index: 128

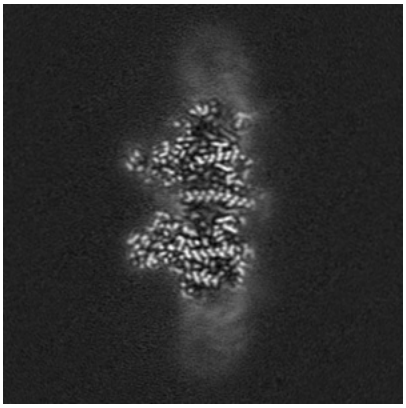
6.2.2 Raw map



X Index: 128



Y Index: 128

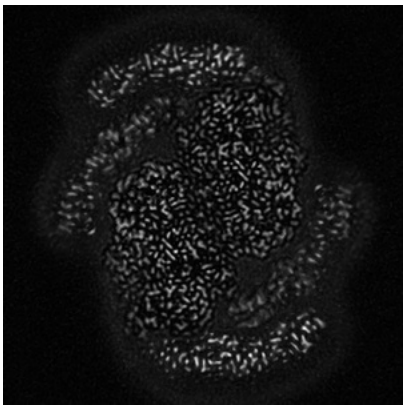


Z Index: 128

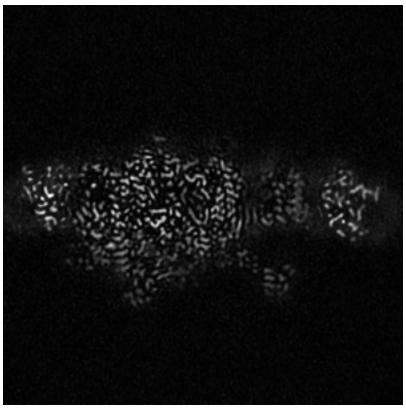
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

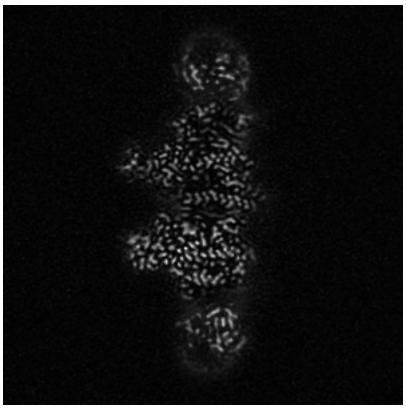
6.3.1 Primary map



X Index: 120

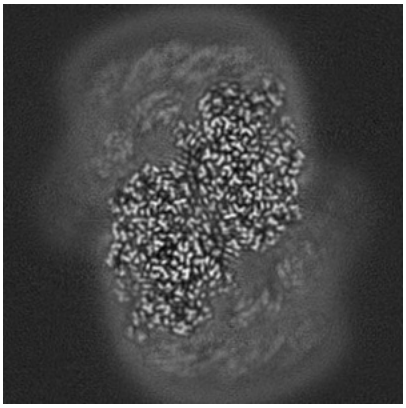


Y Index: 113

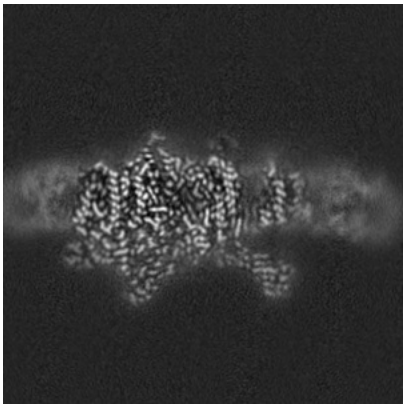


Z Index: 129

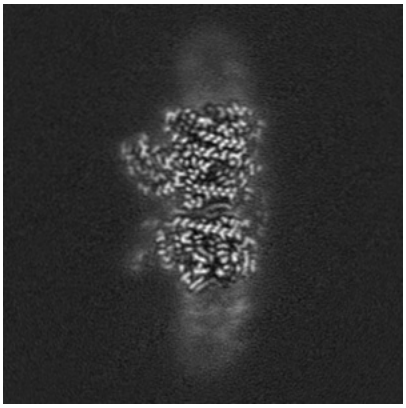
6.3.2 Raw map



X Index: 117



Y Index: 114

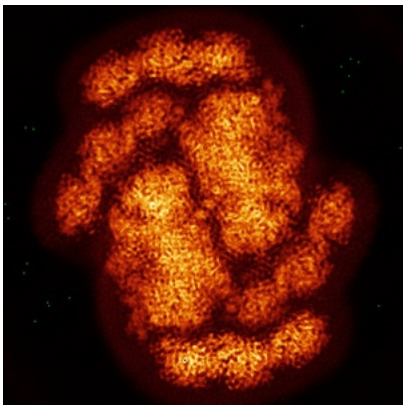


Z Index: 137

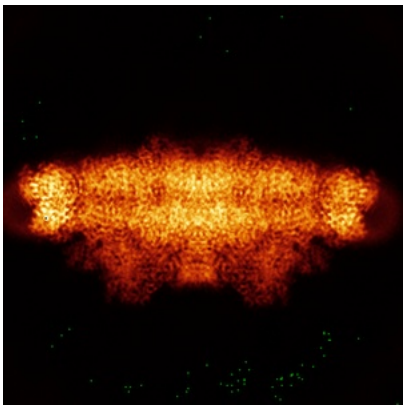
The images above show the largest variance slices of the map in three orthogonal directions.

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

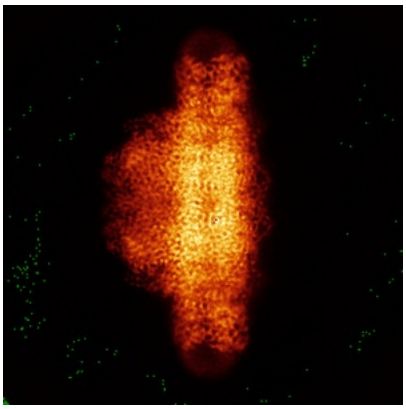
6.4.1 Primary map



X

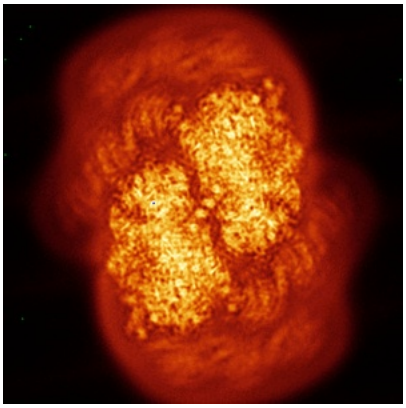


Y

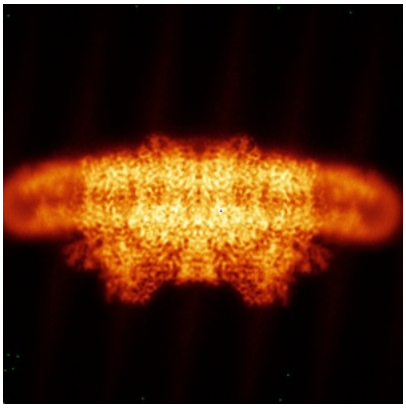


Z

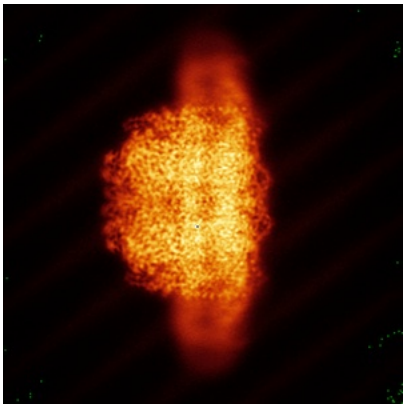
6.4.2 Raw map



X



Y

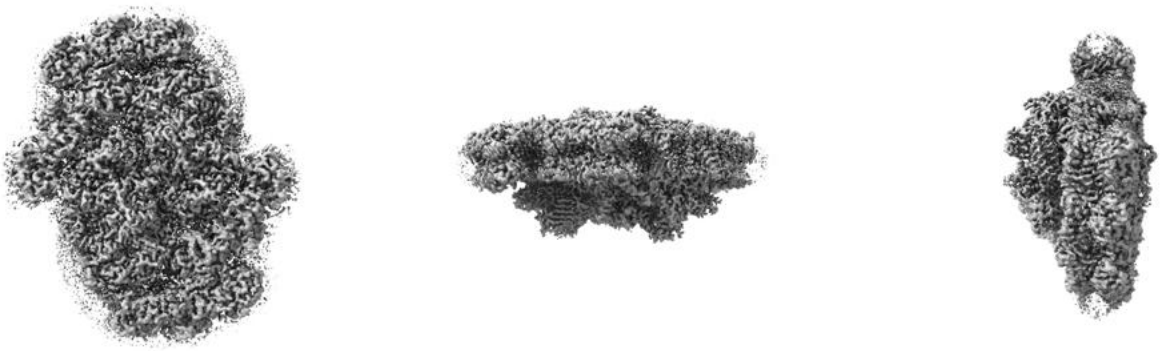


Z

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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

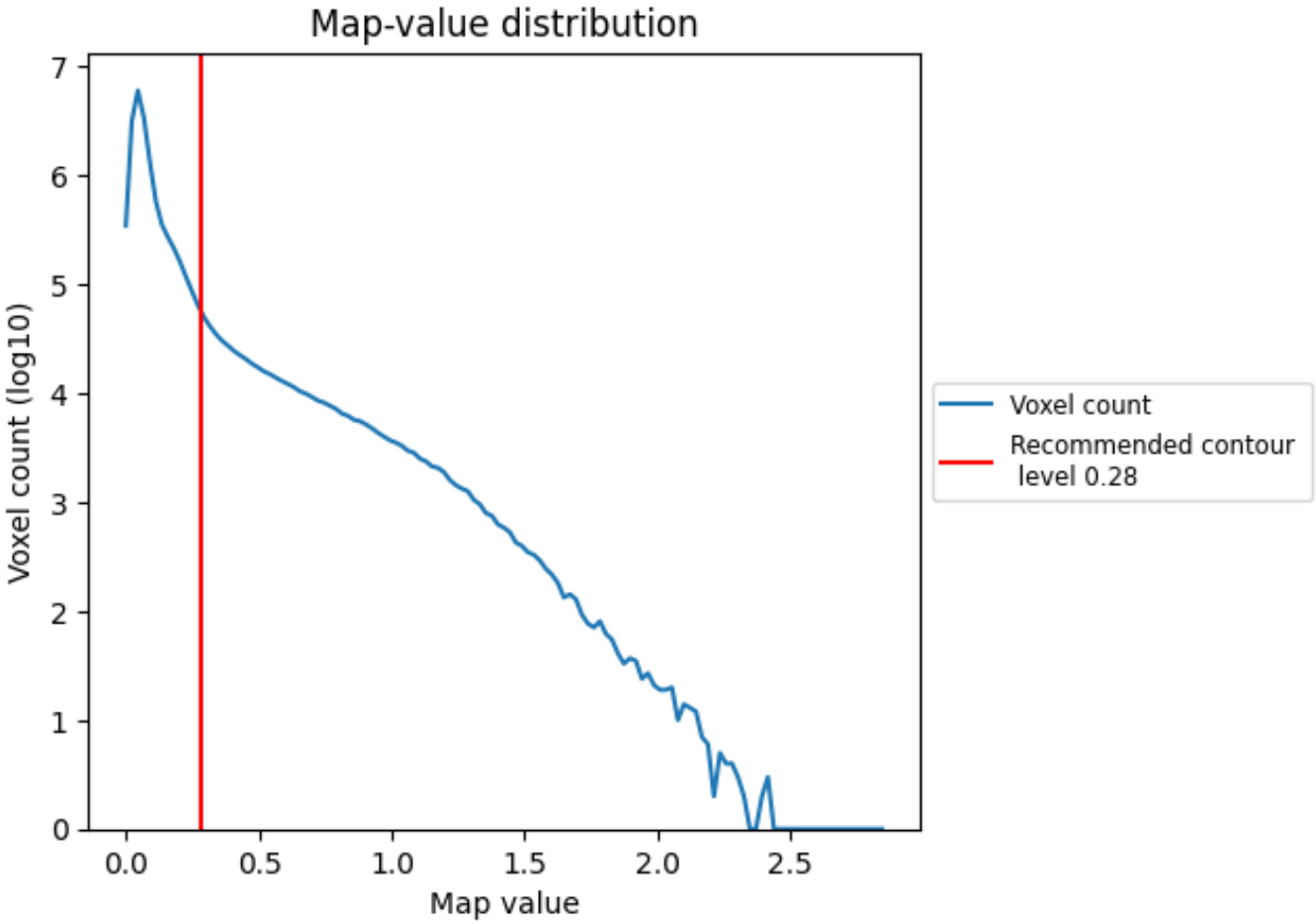
6.6 Mask visualisation (i)

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

7 Map analysis

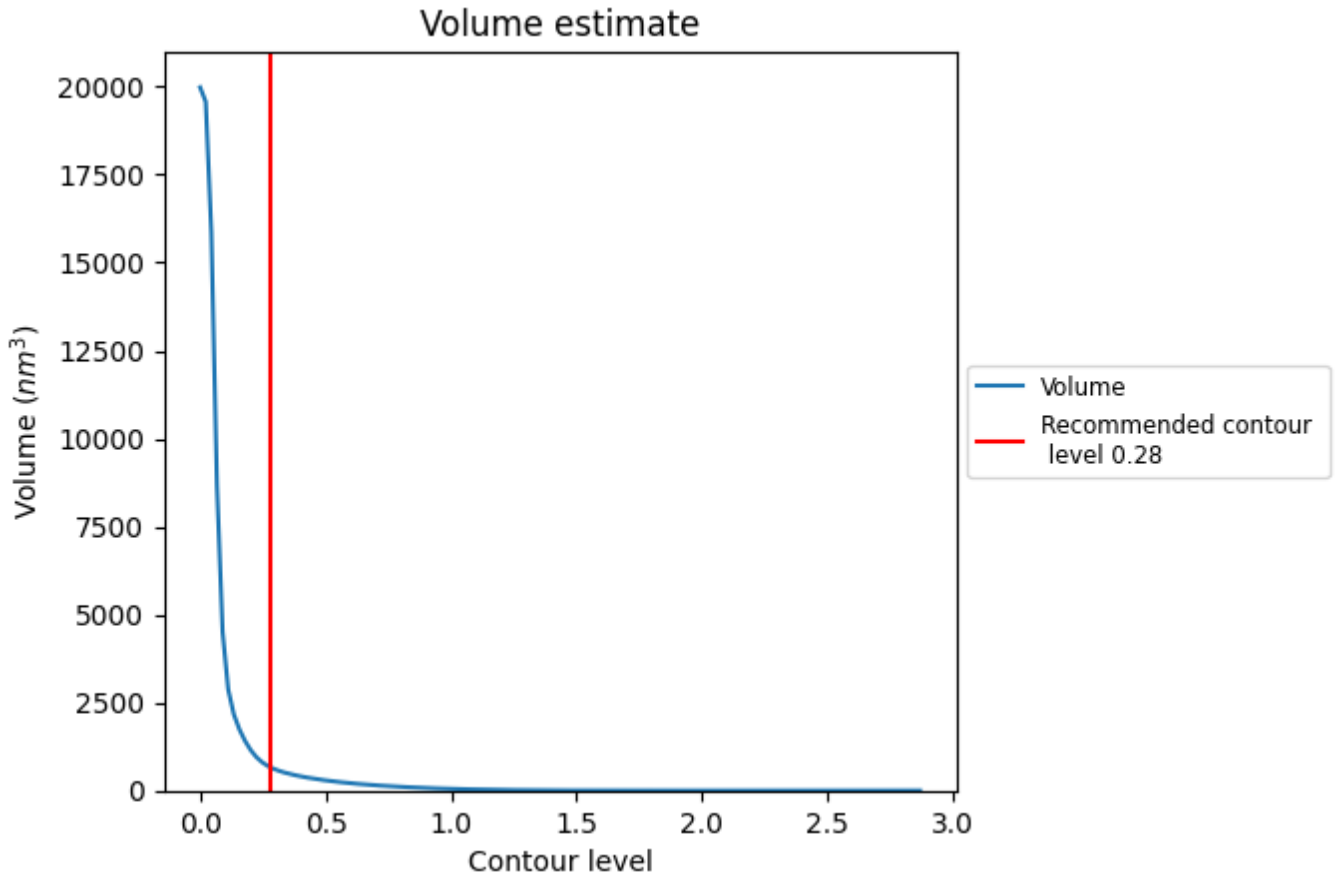
This section contains the results of statistical analysis of the map.

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.

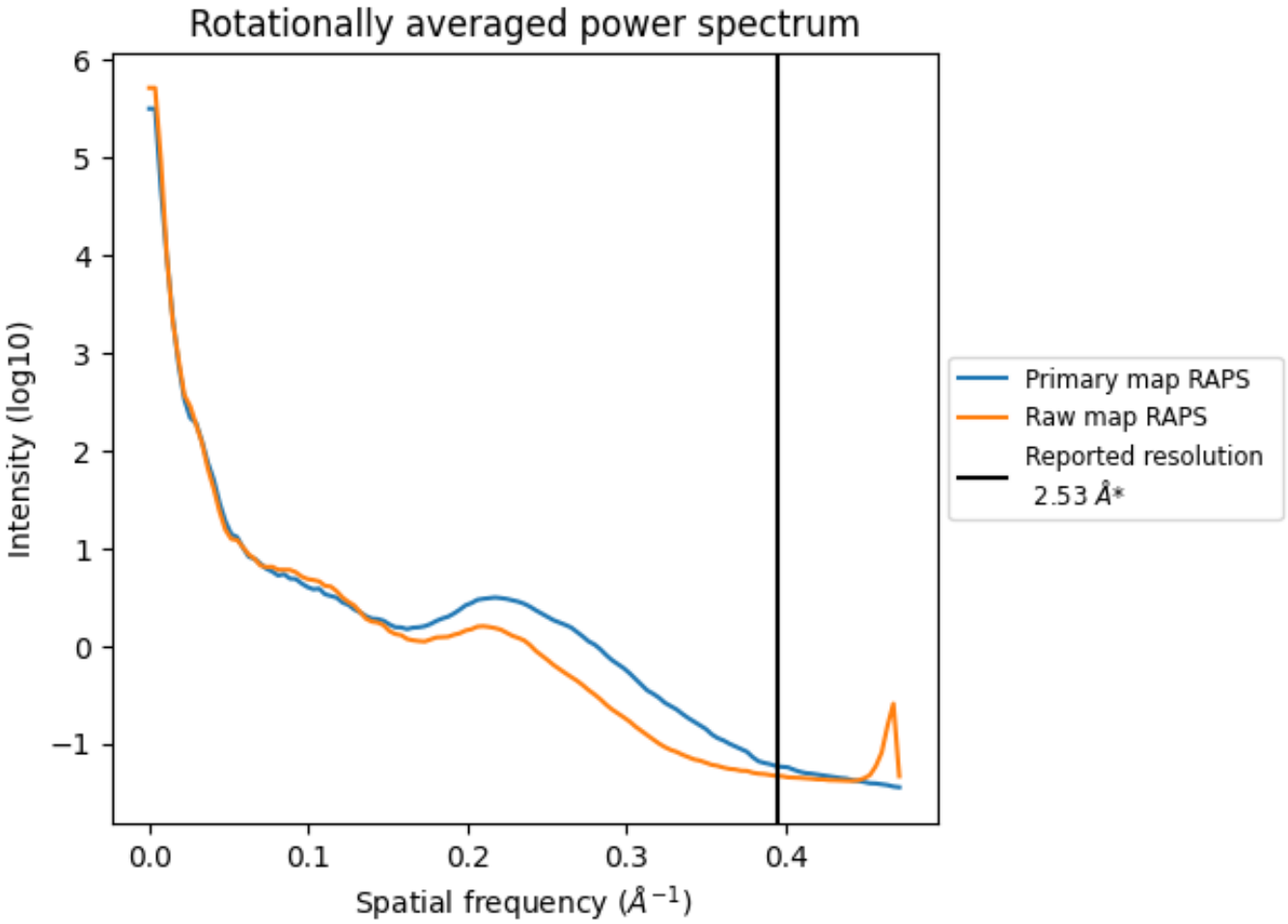
7.2 Volume estimate (i)



The volume at the recommended contour level is 663 nm^3; this corresponds to an approximate mass of 599 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)

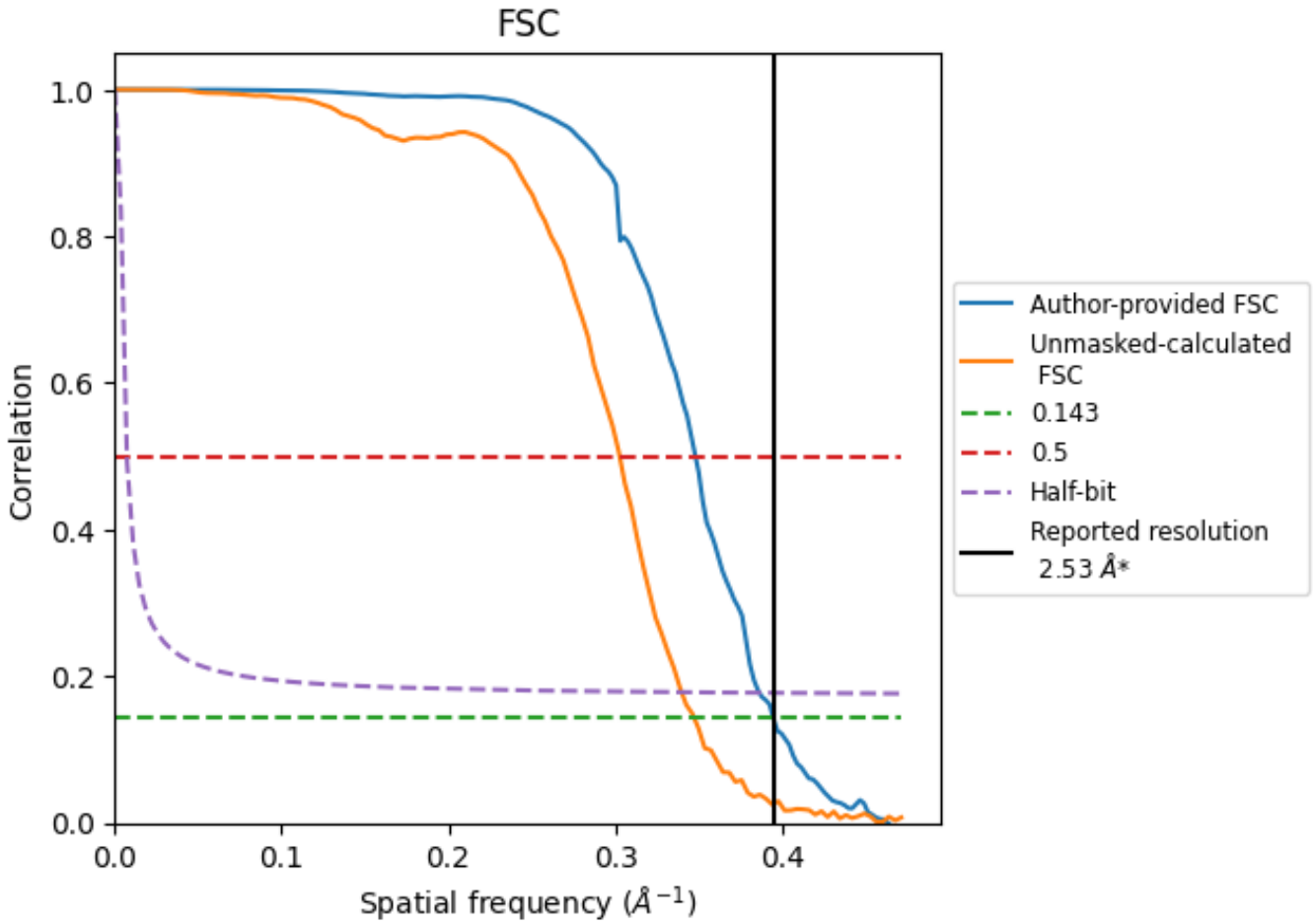


*Reported resolution corresponds to spatial frequency of 0.395 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.395 Å^{-1}

8.2 Resolution estimates (i)

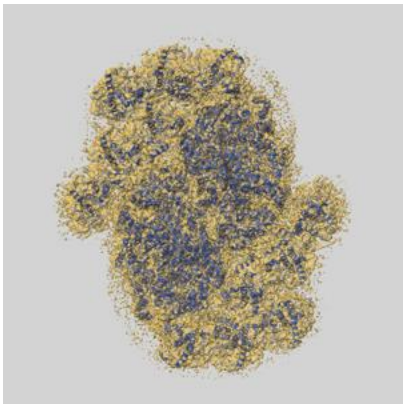
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.53	2.87	2.58
Unmasked-calculated*	2.88	3.30	2.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.88 differs from the reported value 2.53 by more than 10 %

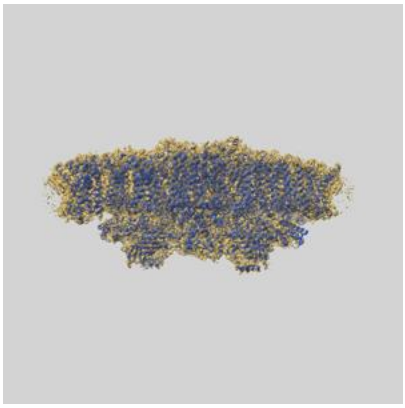
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38596 and PDB model 8XR6. Per-residue inclusion information can be found in section 3 on page 42.

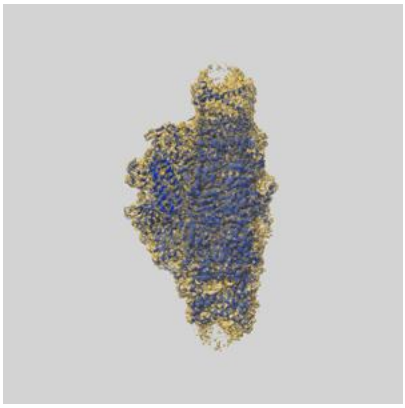
9.1 Map-model overlay



X



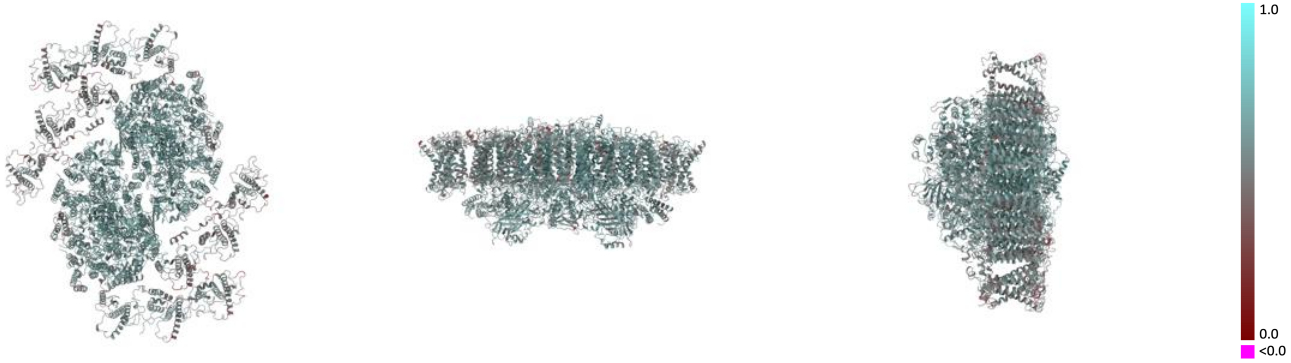
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

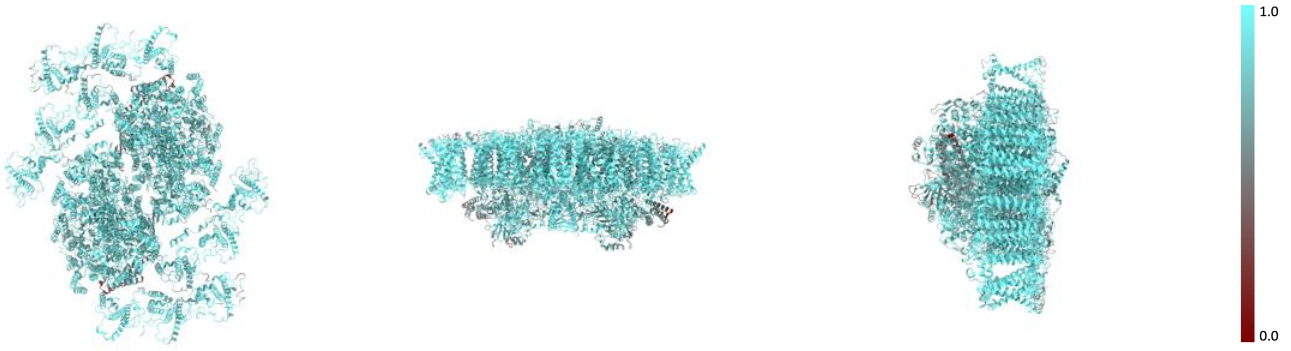
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

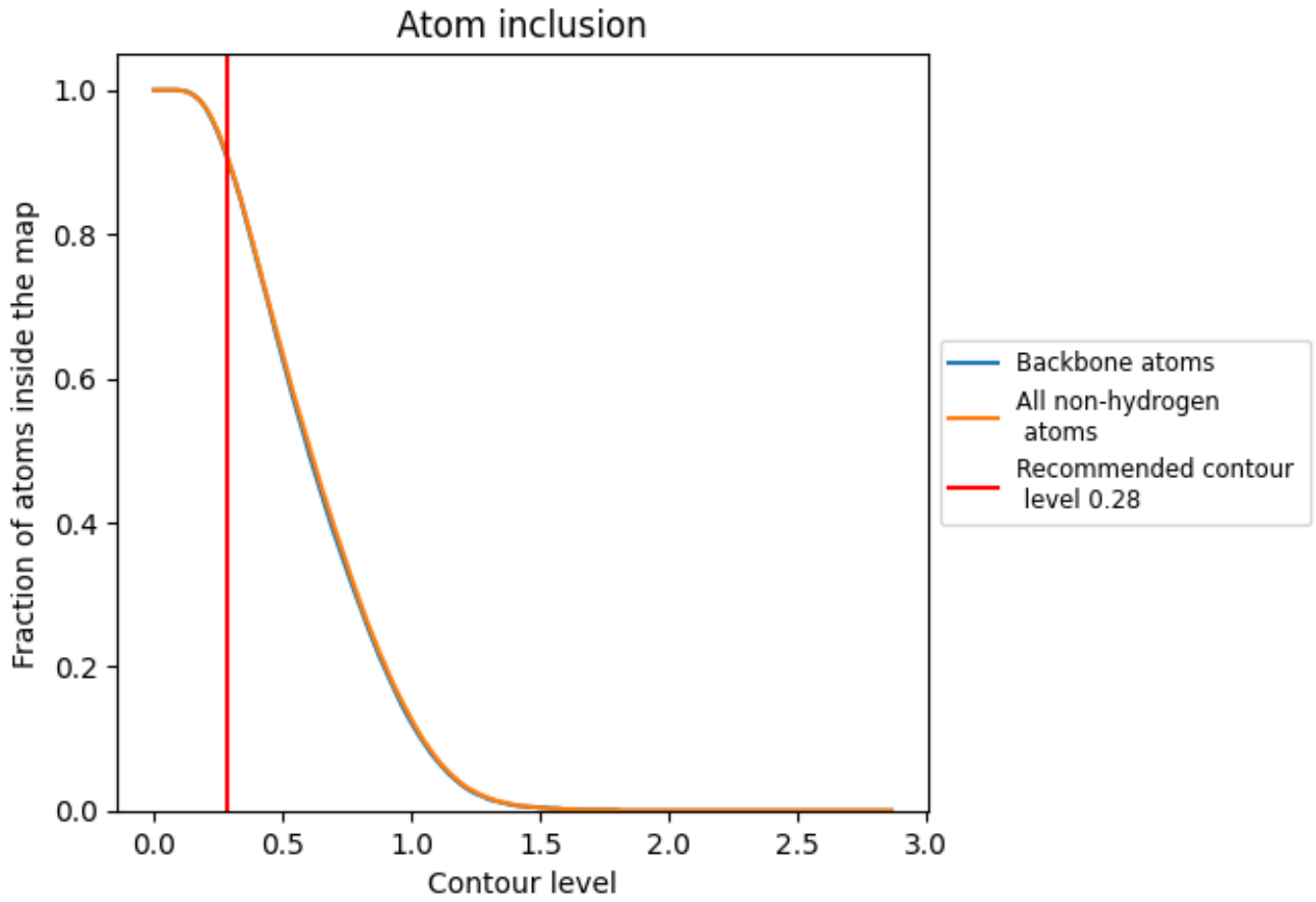
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.5740
0	0.9020	0.4810
1	0.9410	0.5430
2	0.9370	0.5470
3	0.9060	0.5260
4	0.9110	0.4900
5	0.9330	0.4860
6	0.8940	0.4950
7	0.9330	0.5320
8	0.9330	0.5380
9	0.8910	0.5130
A	0.9770	0.6470
B	0.9650	0.6220
C	0.9710	0.6230
D	0.9780	0.6400
E	0.8900	0.5270
F	0.8810	0.4910
H	0.9720	0.5900
I	0.9930	0.6410
J	0.8830	0.5920
K	0.9660	0.5930
L	0.9490	0.6280
M	0.9410	0.6170
N	0.8100	0.5080
O	0.7700	0.5860
Q	0.6440	0.5550
T	0.9410	0.6320
U	0.8080	0.5790
V	0.8390	0.5930
W	0.8880	0.5950
X	0.9130	0.5520
Y	0.8070	0.5410
Z	0.8440	0.5250
a	0.9790	0.6480
b	0.9610	0.6220

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Chain	Atom inclusion	Q-score
c	0.9660	0.6210
d	0.9780	0.6490
e	0.8830	0.5340
f	0.8920	0.5070
g	0.9380	0.4850
h	0.9670	0.5910
i	0.9930	0.6280
j	0.8860	0.5910
k	0.9660	0.5930
l	0.9540	0.6220
m	0.9290	0.6140
n	0.8110	0.5030
o	0.7570	0.5870
p	0.8960	0.4850
q	0.6280	0.5630
t	0.9440	0.6370
u	0.7990	0.5820
v	0.8430	0.5960
w	0.8980	0.6000
x	0.9230	0.5670
y	0.8240	0.5470
z	0.8440	0.5290