wwPDB EM Validation Summary Report (i)

Sep 14, 2026 – 04:56 PM JST

PDB ID	:	7YMM / pdb_00007ymm
EMDB ID	:	EMD-33933
Title	:	PSII-Pcb Tetramer of Acaryochloris Marina
Authors	:	Shen, L.L.; Gao, Y.Z.; Wang, W.D.; Zhang, X.; Shen, J.R.; Wang, P.Y.; Han, G.Y.
Deposited on	:	2022-07-28
Resolution	:	3.60 Å(reported)

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

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

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

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

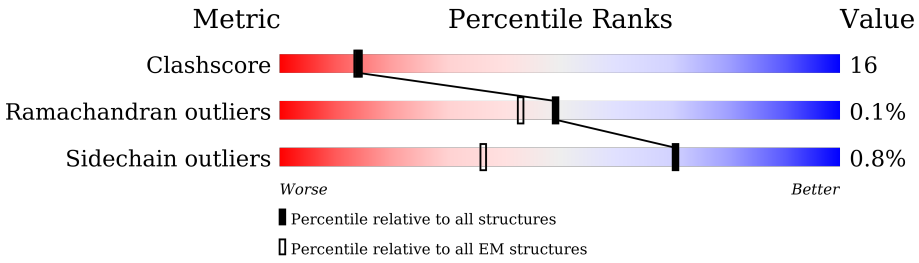
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

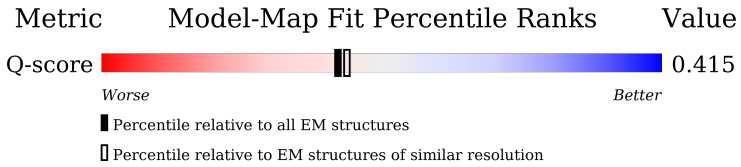
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	1A	360	21% 61% 18% 21%
1	2A	360	12% 60% 19% 21%
1	3A	360	12% 61% 18% 21%
1	4A	360	22% 59% 19% 21%

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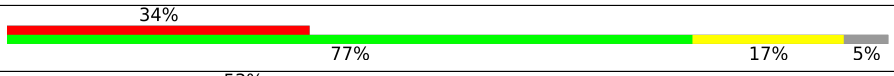
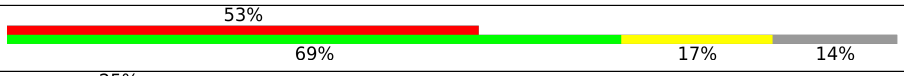
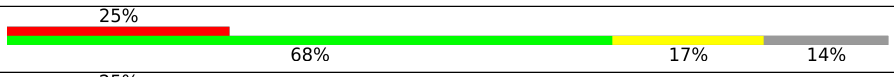
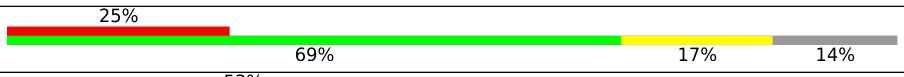
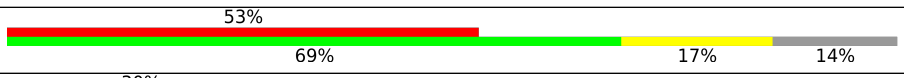
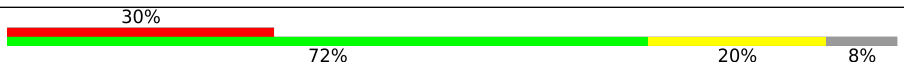
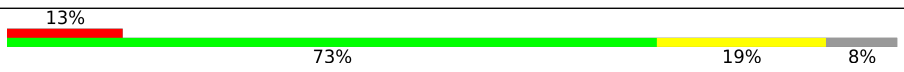
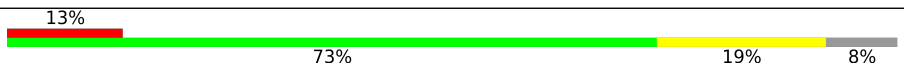
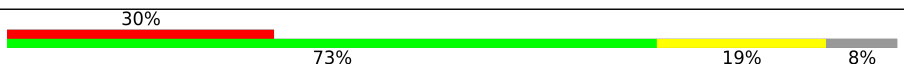
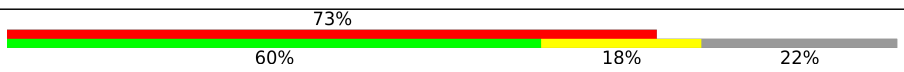
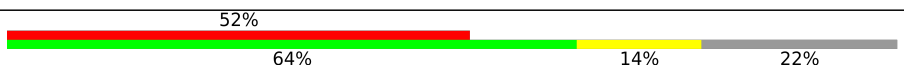
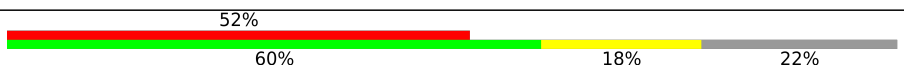
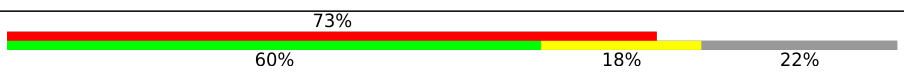
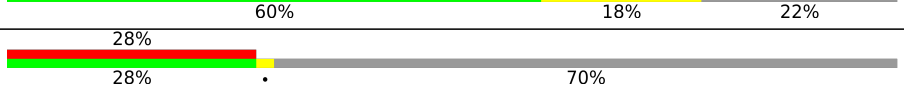
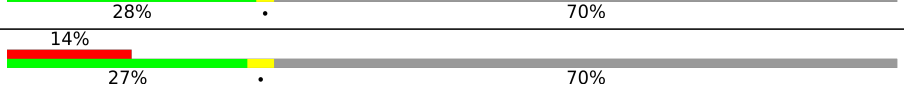
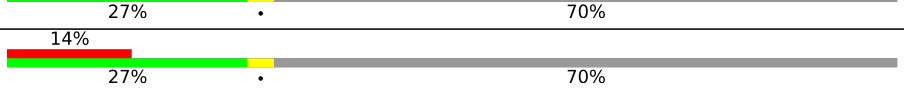
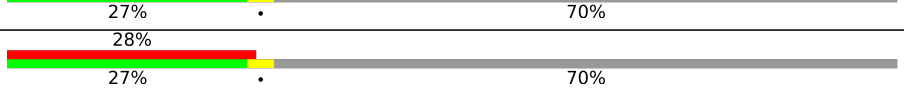
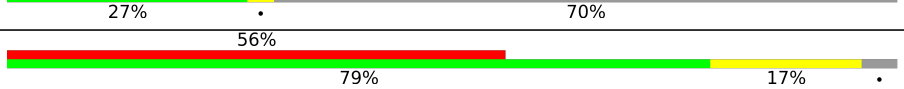
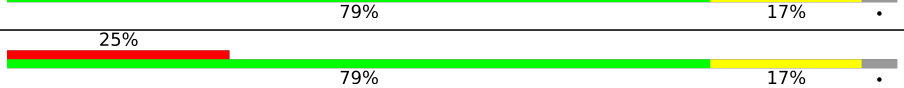
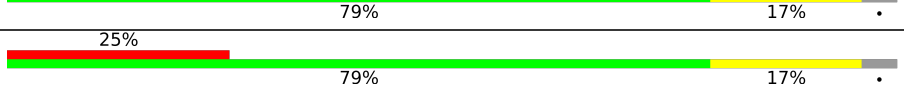
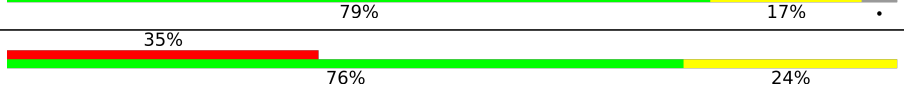
Mol	Chain	Length	Quality of chain
2	1B	506	
2	2B	506	
2	3B	506	
2	4B	506	
3	1C	490	
3	2C	490	
3	3C	490	
3	4C	490	
4	1D	351	
4	2D	351	
4	3D	351	
4	4D	351	
5	1E	83	
5	2E	83	
5	3E	83	
5	4E	83	
6	1F	99	
6	2F	99	
6	3F	99	
6	4F	99	
7	1H	71	
7	2H	71	
7	3H	71	
7	4H	71	
8	1I	34	

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Mol	Chain	Length	Quality of chain
8	2I	34	9% 79% 21%
8	3I	34	9% 82% 18%
8	4I	34	35% 79% 21%
9	1K	45	82% 49% 31% 18%
9	2K	45	60% 42% 38% 18%
9	3K	45	60% 42% 38% 18%
9	4K	45	82% 53% 27% 18%
10	1L	38	11% 84% 11% 5%
10	2L	38	11% 82% 13% 5%
10	3L	38	11% 87% 8% 5%
10	4L	38	11% 82% 13% 5%
11	1M	34	38% 76% 15% 9%
11	2M	34	26% 76% 15% 9%
11	3M	34	26% 76% 15% 9%
11	4M	34	38% 76% 15% 9%
12	1T	46	28% 57% 39%
12	2T	46	15% 54% 7% 39%
12	3T	46	15% 57% 39%
12	4T	46	28% 59% 39%
13	1X	40	82% 75% 12% 12%
13	2X	40	68% 75% 12% 12%
13	3X	40	68% 75% 12% 12%
13	4X	40	82% 75% 12% 12%
14	1Y	39	59% 54% 5% 41%
14	2Y	39	59% 46% 13% 41%

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Mol	Chain	Length	Quality of chain
14	3Y	39	59% 51% 8% 41%
14	4Y	39	59% 49% 10% 41%
15	1Z	62	95% 85% 10% 5%
15	2Z	62	85% 84% 11% 5%
15	3Z	62	85% 84% 11% 5%
15	4Z	62	95% 85% 10% 5%
16	12	352	57% 69% 30%
16	22	352	33% 70% 29%
16	32	352	32% 69% 30%
16	42	352	58% 69% 30%
17	1G	41	61% 93% 7%
17	2G	41	51% 93% 7%
17	3G	41	51% 93% 7%
17	4G	41	63% 93% 7%
18	11	356	83% 64% 28% 8%
18	21	356	43% 63% 29% 8%
18	31	356	43% 63% 29% 8%
18	41	356	83% 63% 29% 8%
19	13	349	42% 77% 21%
19	23	349	38% 76% 22%
19	33	349	38% 77% 21%
19	43	349	42% 76% 22%
20	14	353	71% 68% 25% 6%
20	24	353	36% 69% 25% 6%
20	34	353	37% 68% 25% 6%

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Mol	Chain	Length	Quality of chain
20	44	353	

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
21	CL7	11	402	X	-	-	-
21	CL7	11	403	X	-	-	-
21	CL7	11	404	X	-	-	-
21	CL7	11	405	X	-	-	-
21	CL7	11	406	X	-	-	-
21	CL7	11	407	X	-	-	-
21	CL7	11	408	X	-	-	-
21	CL7	11	409	X	-	-	-
21	CL7	11	410	X	-	-	-
21	CL7	11	411	X	-	-	-
21	CL7	11	412	X	-	-	-
21	CL7	11	413	X	-	-	-
21	CL7	11	414	X	-	-	-
21	CL7	11	415	X	-	-	-
21	CL7	11	416	X	-	-	-
21	CL7	11	417	X	-	-	-
21	CL7	11	418	X	-	-	-
21	CL7	11	419	X	-	-	-
21	CL7	11	420	X	-	-	-
21	CL7	12	501	X	-	-	-
21	CL7	12	502	X	-	-	-
21	CL7	12	503	X	-	-	-
21	CL7	12	504	X	-	-	-
21	CL7	12	505	X	-	-	-
21	CL7	12	506	X	-	-	-
21	CL7	12	507	X	-	-	-
21	CL7	12	508	X	-	-	-
21	CL7	12	509	X	-	-	-
21	CL7	12	510	X	-	-	-
21	CL7	12	511	X	-	-	-
21	CL7	12	512	X	-	-	-
21	CL7	12	513	X	-	-	-
21	CL7	12	514	X	-	-	-
21	CL7	12	515	X	-	-	-
21	CL7	12	516	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	12	517	X	-	-	-
21	CL7	12	518	X	-	-	-
21	CL7	13	501	X	-	-	-
21	CL7	13	502	X	-	-	-
21	CL7	13	503	X	-	-	-
21	CL7	13	504	X	-	-	-
21	CL7	13	505	X	-	-	-
21	CL7	13	506	X	-	-	-
21	CL7	13	507	X	-	-	-
21	CL7	13	508	X	-	-	-
21	CL7	13	509	X	-	-	-
21	CL7	13	510	X	-	-	-
21	CL7	13	511	X	-	-	-
21	CL7	13	512	X	-	-	-
21	CL7	13	513	X	-	-	-
21	CL7	13	514	X	-	-	-
21	CL7	13	515	X	-	-	-
21	CL7	13	516	X	-	-	-
21	CL7	13	517	X	-	-	-
21	CL7	13	518	X	-	-	-
21	CL7	14	404	X	-	-	-
21	CL7	14	405	X	-	-	-
21	CL7	14	406	X	-	-	-
21	CL7	14	407	X	-	-	-
21	CL7	14	408	X	-	-	-
21	CL7	14	409	X	-	-	-
21	CL7	14	410	X	-	-	-
21	CL7	14	411	X	-	-	-
21	CL7	14	412	X	-	-	-
21	CL7	14	413	X	-	-	-
21	CL7	14	414	X	-	-	-
21	CL7	14	415	X	-	-	-
21	CL7	14	416	X	-	-	-
21	CL7	14	417	X	-	-	-
21	CL7	1A	401	X	-	-	-
21	CL7	1A	403	X	-	-	-
21	CL7	1A	407	X	-	-	-
21	CL7	1B	601	X	-	-	-
21	CL7	1B	602	X	-	-	-
21	CL7	1B	603	X	-	-	-
21	CL7	1B	604	X	-	-	-
21	CL7	1B	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	1B	606	X	-	-	-
21	CL7	1B	607	X	-	-	-
21	CL7	1B	608	X	-	-	-
21	CL7	1B	609	X	-	-	-
21	CL7	1B	610	X	-	-	-
21	CL7	1B	611	X	-	-	-
21	CL7	1B	612	X	-	-	-
21	CL7	1B	613	X	-	-	-
21	CL7	1B	614	X	-	-	-
21	CL7	1B	615	X	-	-	-
21	CL7	1B	616	X	-	-	-
21	CL7	1B	622	X	-	-	-
21	CL7	1C	501	X	-	-	-
21	CL7	1C	502	X	-	-	-
21	CL7	1C	503	X	-	-	-
21	CL7	1C	504	X	-	-	-
21	CL7	1C	505	X	-	-	-
21	CL7	1C	506	X	-	-	-
21	CL7	1C	507	X	-	-	-
21	CL7	1C	508	X	-	-	-
21	CL7	1C	509	X	-	-	-
21	CL7	1C	510	X	-	-	-
21	CL7	1C	511	X	-	-	-
21	CL7	1C	512	X	-	-	-
21	CL7	1C	513	X	-	-	-
21	CL7	1C	517	X	-	-	-
21	CL7	1D	402	X	-	-	-
21	CL7	1D	404	X	-	-	-
21	CL7	1D	405	X	-	-	-
21	CL7	21	402	X	-	-	-
21	CL7	21	403	X	-	-	-
21	CL7	21	404	X	-	-	-
21	CL7	21	405	X	-	-	-
21	CL7	21	406	X	-	-	-
21	CL7	21	407	X	-	-	-
21	CL7	21	408	X	-	-	-
21	CL7	21	409	X	-	-	-
21	CL7	21	410	X	-	-	-
21	CL7	21	411	X	-	-	-
21	CL7	21	412	X	-	-	-
21	CL7	21	413	X	-	-	-
21	CL7	21	414	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	21	415	X	-	-	-
21	CL7	21	416	X	-	-	-
21	CL7	21	417	X	-	-	-
21	CL7	21	418	X	-	-	-
21	CL7	21	419	X	-	-	-
21	CL7	21	420	X	-	-	-
21	CL7	22	501	X	-	-	-
21	CL7	22	502	X	-	-	-
21	CL7	22	503	X	-	-	-
21	CL7	22	504	X	-	-	-
21	CL7	22	505	X	-	-	-
21	CL7	22	506	X	-	-	-
21	CL7	22	507	X	-	-	-
21	CL7	22	508	X	-	-	-
21	CL7	22	509	X	-	-	-
21	CL7	22	510	X	-	-	-
21	CL7	22	511	X	-	-	-
21	CL7	22	512	X	-	-	-
21	CL7	22	513	X	-	-	-
21	CL7	22	514	X	-	-	-
21	CL7	22	515	X	-	-	-
21	CL7	22	516	X	-	-	-
21	CL7	22	517	X	-	-	-
21	CL7	22	518	X	-	-	-
21	CL7	23	402	X	-	-	-
21	CL7	23	403	X	-	-	-
21	CL7	23	404	X	-	-	-
21	CL7	23	405	X	-	-	-
21	CL7	23	406	X	-	-	-
21	CL7	23	407	X	-	-	-
21	CL7	23	408	X	-	-	-
21	CL7	23	409	X	-	-	-
21	CL7	23	410	X	-	-	-
21	CL7	23	411	X	-	-	-
21	CL7	23	412	X	-	-	-
21	CL7	23	413	X	-	-	-
21	CL7	23	414	X	-	-	-
21	CL7	23	415	X	-	-	-
21	CL7	23	416	X	-	-	-
21	CL7	23	417	X	-	-	-
21	CL7	23	418	X	-	-	-
21	CL7	23	419	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	24	404	X	-	-	-
21	CL7	24	405	X	-	-	-
21	CL7	24	406	X	-	-	-
21	CL7	24	407	X	-	-	-
21	CL7	24	408	X	-	-	-
21	CL7	24	409	X	-	-	-
21	CL7	24	410	X	-	-	-
21	CL7	24	411	X	-	-	-
21	CL7	24	412	X	-	-	-
21	CL7	24	413	X	-	-	-
21	CL7	24	414	X	-	-	-
21	CL7	24	415	X	-	-	-
21	CL7	24	416	X	-	-	-
21	CL7	24	417	X	-	-	-
21	CL7	2A	401	X	-	-	-
21	CL7	2A	403	X	-	-	-
21	CL7	2A	407	X	-	-	-
21	CL7	2B	602	X	-	-	-
21	CL7	2B	603	X	-	-	-
21	CL7	2B	604	X	-	-	-
21	CL7	2B	605	X	-	-	-
21	CL7	2B	606	X	-	-	-
21	CL7	2B	607	X	-	-	-
21	CL7	2B	608	X	-	-	-
21	CL7	2B	609	X	-	-	-
21	CL7	2B	610	X	-	-	-
21	CL7	2B	611	X	-	-	-
21	CL7	2B	612	X	-	-	-
21	CL7	2B	613	X	-	-	-
21	CL7	2B	614	X	-	-	-
21	CL7	2B	615	X	-	-	-
21	CL7	2B	616	X	-	-	-
21	CL7	2B	617	X	-	-	-
21	CL7	2B	623	X	-	-	-
21	CL7	2C	501	X	-	-	-
21	CL7	2C	502	X	-	-	-
21	CL7	2C	503	X	-	-	-
21	CL7	2C	504	X	-	-	-
21	CL7	2C	505	X	-	-	-
21	CL7	2C	506	X	-	-	-
21	CL7	2C	507	X	-	-	-
21	CL7	2C	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	2C	509	X	-	-	-
21	CL7	2C	510	X	-	-	-
21	CL7	2C	511	X	-	-	-
21	CL7	2C	512	X	-	-	-
21	CL7	2C	513	X	-	-	-
21	CL7	2C	517	X	-	-	-
21	CL7	2D	402	X	-	-	-
21	CL7	2D	404	X	-	-	-
21	CL7	2D	405	X	-	-	-
21	CL7	31	402	X	-	-	-
21	CL7	31	403	X	-	-	-
21	CL7	31	404	X	-	-	-
21	CL7	31	405	X	-	-	-
21	CL7	31	406	X	-	-	-
21	CL7	31	407	X	-	-	-
21	CL7	31	408	X	-	-	-
21	CL7	31	409	X	-	-	-
21	CL7	31	410	X	-	-	-
21	CL7	31	411	X	-	-	-
21	CL7	31	412	X	-	-	-
21	CL7	31	413	X	-	-	-
21	CL7	31	414	X	-	-	-
21	CL7	31	415	X	-	-	-
21	CL7	31	416	X	-	-	-
21	CL7	31	417	X	-	-	-
21	CL7	31	418	X	-	-	-
21	CL7	31	419	X	-	-	-
21	CL7	31	420	X	-	-	-
21	CL7	32	501	X	-	-	-
21	CL7	32	502	X	-	-	-
21	CL7	32	503	X	-	-	-
21	CL7	32	504	X	-	-	-
21	CL7	32	505	X	-	-	-
21	CL7	32	506	X	-	-	-
21	CL7	32	507	X	-	-	-
21	CL7	32	508	X	-	-	-
21	CL7	32	509	X	-	-	-
21	CL7	32	510	X	-	-	-
21	CL7	32	511	X	-	-	-
21	CL7	32	512	X	-	-	-
21	CL7	32	513	X	-	-	-
21	CL7	32	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	32	515	X	-	-	-
21	CL7	32	516	X	-	-	-
21	CL7	32	517	X	-	-	-
21	CL7	32	518	X	-	-	-
21	CL7	33	501	X	-	-	-
21	CL7	33	502	X	-	-	-
21	CL7	33	503	X	-	-	-
21	CL7	33	504	X	-	-	-
21	CL7	33	505	X	-	-	-
21	CL7	33	506	X	-	-	-
21	CL7	33	507	X	-	-	-
21	CL7	33	508	X	-	-	-
21	CL7	33	509	X	-	-	-
21	CL7	33	510	X	-	-	-
21	CL7	33	511	X	-	-	-
21	CL7	33	512	X	-	-	-
21	CL7	33	513	X	-	-	-
21	CL7	33	514	X	-	-	-
21	CL7	33	515	X	-	-	-
21	CL7	33	516	X	-	-	-
21	CL7	33	517	X	-	-	-
21	CL7	33	518	X	-	-	-
21	CL7	34	404	X	-	-	-
21	CL7	34	405	X	-	-	-
21	CL7	34	406	X	-	-	-
21	CL7	34	407	X	-	-	-
21	CL7	34	408	X	-	-	-
21	CL7	34	409	X	-	-	-
21	CL7	34	410	X	-	-	-
21	CL7	34	411	X	-	-	-
21	CL7	34	412	X	-	-	-
21	CL7	34	413	X	-	-	-
21	CL7	34	414	X	-	-	-
21	CL7	34	415	X	-	-	-
21	CL7	34	416	X	-	-	-
21	CL7	34	417	X	-	-	-
21	CL7	3A	401	X	-	-	-
21	CL7	3A	403	X	-	-	-
21	CL7	3A	407	X	-	-	-
21	CL7	3B	601	X	-	-	-
21	CL7	3B	602	X	-	-	-
21	CL7	3B	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	3B	604	X	-	-	-
21	CL7	3B	605	X	-	-	-
21	CL7	3B	606	X	-	-	-
21	CL7	3B	607	X	-	-	-
21	CL7	3B	608	X	-	-	-
21	CL7	3B	609	X	-	-	-
21	CL7	3B	610	X	-	-	-
21	CL7	3B	611	X	-	-	-
21	CL7	3B	612	X	-	-	-
21	CL7	3B	613	X	-	-	-
21	CL7	3B	614	X	-	-	-
21	CL7	3B	615	X	-	-	-
21	CL7	3B	616	X	-	-	-
21	CL7	3B	622	X	-	-	-
21	CL7	3C	501	X	-	-	-
21	CL7	3C	502	X	-	-	-
21	CL7	3C	503	X	-	-	-
21	CL7	3C	504	X	-	-	-
21	CL7	3C	505	X	-	-	-
21	CL7	3C	506	X	-	-	-
21	CL7	3C	507	X	-	-	-
21	CL7	3C	508	X	-	-	-
21	CL7	3C	509	X	-	-	-
21	CL7	3C	510	X	-	-	-
21	CL7	3C	511	X	-	-	-
21	CL7	3C	512	X	-	-	-
21	CL7	3C	513	X	-	-	-
21	CL7	3C	517	X	-	-	-
21	CL7	3D	402	X	-	-	-
21	CL7	3D	404	X	-	-	-
21	CL7	3D	405	X	-	-	-
21	CL7	41	402	X	-	-	-
21	CL7	41	403	X	-	-	-
21	CL7	41	404	X	-	-	-
21	CL7	41	405	X	-	-	-
21	CL7	41	406	X	-	-	-
21	CL7	41	407	X	-	-	-
21	CL7	41	408	X	-	-	-
21	CL7	41	409	X	-	-	-
21	CL7	41	410	X	-	-	-
21	CL7	41	411	X	-	-	-
21	CL7	41	412	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	41	413	X	-	-	-
21	CL7	41	414	X	-	-	-
21	CL7	41	415	X	-	-	-
21	CL7	41	416	X	-	-	-
21	CL7	41	417	X	-	-	-
21	CL7	41	418	X	-	-	-
21	CL7	41	419	X	-	-	-
21	CL7	41	420	X	-	-	-
21	CL7	42	501	X	-	-	-
21	CL7	42	502	X	-	-	-
21	CL7	42	503	X	-	-	-
21	CL7	42	504	X	-	-	-
21	CL7	42	505	X	-	-	-
21	CL7	42	506	X	-	-	-
21	CL7	42	507	X	-	-	-
21	CL7	42	508	X	-	-	-
21	CL7	42	509	X	-	-	-
21	CL7	42	510	X	-	-	-
21	CL7	42	511	X	-	-	-
21	CL7	42	512	X	-	-	-
21	CL7	42	513	X	-	-	-
21	CL7	42	514	X	-	-	-
21	CL7	42	515	X	-	-	-
21	CL7	42	516	X	-	-	-
21	CL7	42	517	X	-	-	-
21	CL7	42	518	X	-	-	-
21	CL7	43	402	X	-	-	-
21	CL7	43	403	X	-	-	-
21	CL7	43	404	X	-	-	-
21	CL7	43	405	X	-	-	-
21	CL7	43	406	X	-	-	-
21	CL7	43	407	X	-	-	-
21	CL7	43	408	X	-	-	-
21	CL7	43	409	X	-	-	-
21	CL7	43	410	X	-	-	-
21	CL7	43	411	X	-	-	-
21	CL7	43	412	X	-	-	-
21	CL7	43	413	X	-	-	-
21	CL7	43	414	X	-	-	-
21	CL7	43	415	X	-	-	-
21	CL7	43	416	X	-	-	-
21	CL7	43	417	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	43	418	X	-	-	-
21	CL7	43	419	X	-	-	-
21	CL7	44	404	X	-	-	-
21	CL7	44	405	X	-	-	-
21	CL7	44	406	X	-	-	-
21	CL7	44	407	X	-	-	-
21	CL7	44	408	X	-	-	-
21	CL7	44	409	X	-	-	-
21	CL7	44	410	X	-	-	-
21	CL7	44	411	X	-	-	-
21	CL7	44	412	X	-	-	-
21	CL7	44	413	X	-	-	-
21	CL7	44	414	X	-	-	-
21	CL7	44	415	X	-	-	-
21	CL7	44	416	X	-	-	-
21	CL7	44	417	X	-	-	-
21	CL7	4A	401	X	-	-	-
21	CL7	4A	403	X	-	-	-
21	CL7	4A	407	X	-	-	-
21	CL7	4B	602	X	-	-	-
21	CL7	4B	603	X	-	-	-
21	CL7	4B	604	X	-	-	-
21	CL7	4B	605	X	-	-	-
21	CL7	4B	606	X	-	-	-
21	CL7	4B	607	X	-	-	-
21	CL7	4B	608	X	-	-	-
21	CL7	4B	609	X	-	-	-
21	CL7	4B	610	X	-	-	-
21	CL7	4B	611	X	-	-	-
21	CL7	4B	612	X	-	-	-
21	CL7	4B	613	X	-	-	-
21	CL7	4B	614	X	-	-	-
21	CL7	4B	615	X	-	-	-
21	CL7	4B	616	X	-	-	-
21	CL7	4B	617	X	-	-	-
21	CL7	4B	623	X	-	-	-
21	CL7	4C	501	X	-	-	-
21	CL7	4C	502	X	-	-	-
21	CL7	4C	503	X	-	-	-
21	CL7	4C	504	X	-	-	-
21	CL7	4C	505	X	-	-	-
21	CL7	4C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	4C	507	X	-	-	-
21	CL7	4C	508	X	-	-	-
21	CL7	4C	509	X	-	-	-
21	CL7	4C	510	X	-	-	-
21	CL7	4C	511	X	-	-	-
21	CL7	4C	512	X	-	-	-
21	CL7	4C	513	X	-	-	-
21	CL7	4C	517	X	-	-	-
21	CL7	4D	402	X	-	-	-
21	CL7	4D	404	X	-	-	-
21	CL7	4D	405	X	-	-	-
22	PHO	1D	408	X	-	-	-
22	PHO	2D	408	X	-	-	-
22	PHO	3D	408	X	-	-	-
22	PHO	4D	408	X	-	-	-
24	LMG	1A	405	X	-	-	-
24	LMG	2A	405	X	-	-	-
24	LMG	3A	405	X	-	-	-
24	LMG	4A	405	X	-	-	-
32	ZEX	11	422	-	-	X	-
32	ZEX	12	520	-	-	X	-
32	ZEX	13	522	-	-	X	-
32	ZEX	13	525	-	-	X	-
32	ZEX	14	403	-	-	X	-
32	ZEX	21	422	-	-	X	-
32	ZEX	22	520	-	-	X	-
32	ZEX	23	401	-	-	X	-
32	ZEX	23	423	-	-	X	-
32	ZEX	24	403	-	-	X	-
32	ZEX	31	422	-	-	X	-
32	ZEX	32	520	-	-	X	-
32	ZEX	33	522	-	-	X	-
32	ZEX	33	525	-	-	X	-
32	ZEX	34	403	-	-	X	-
32	ZEX	41	422	-	-	X	-
32	ZEX	42	520	-	-	X	-
32	ZEX	43	401	-	-	X	-
32	ZEX	43	423	-	-	X	-
32	ZEX	44	403	-	-	X	-

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 136856 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	2A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	3A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	4A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	2B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	3B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	4B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	2C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	3C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	4C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		

- Molecule 4 is a protein called Photosystem II D2 protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	2D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	3D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	4D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	2E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	3E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	4E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		

- Molecule 6 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	2F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	3F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	4F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		

- Molecule 7 is a protein called Photosystem II 10 kDa phosphoprotein PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		
7	2H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		
7	3H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	4H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		

- Molecule 8 is a protein called Photosystem II protein PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	2I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	3I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	4I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	2K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	3K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	4K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	1L	36	Total	C	N	O	0	0
			288	194	45	49		
10	2L	36	Total	C	N	O	0	0
			288	194	45	49		
10	3L	36	Total	C	N	O	0	0
			288	194	45	49		
10	4L	36	Total	C	N	O	0	0
			288	194	45	49		

- Molecule 11 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		
11	2M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		
11	3M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		
11	4M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		
12	2T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		
12	3T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		
12	4T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	1X	35	Total	C	N	O	0	0
			269	185	39	45		
13	2X	35	Total	C	N	O	0	0
			269	185	39	45		
13	3X	35	Total	C	N	O	0	0
			269	185	39	45		
13	4X	35	Total	C	N	O	0	0
			269	185	39	45		

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		
14	2Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		
14	3Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	4Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		
15	2Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		
15	3Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		
15	4Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		

- Molecule 16 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	12	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	22	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	32	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	42	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		

- Molecule 17 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1G	41	Total	C	N	O	0	0
			205	123	41	41		
17	2G	41	Total	C	N	O	0	0
			205	123	41	41		
17	3G	41	Total	C	N	O	0	0
			205	123	41	41		
17	4G	41	Total	C	N	O	0	0
			205	123	41	41		

- Molecule 18 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	11	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	21	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	31	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	41	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		

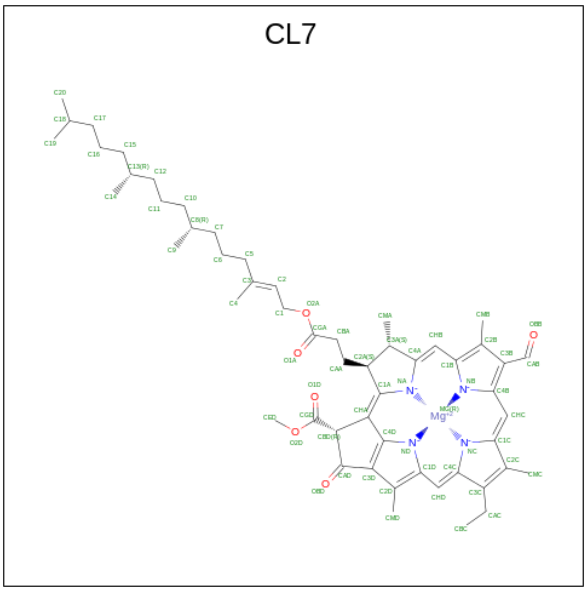
- Molecule 19 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	13	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	23	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	33	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	43	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		

- Molecule 20 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	14	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	24	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	34	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	44	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		

- Molecule 21 is CHLOROPHYLL D (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	1C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	1D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	1D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	11	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	11	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	11	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	11	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	11	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	11	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	13	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	14	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	14	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	14	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	2A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	2A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	2B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	2C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	2C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
21	2D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	2D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	2D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	21	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	21	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	21	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	21	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	21	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	21	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			58	47	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	23	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	24	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	24	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	24	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	3A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	3B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	3C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	3C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	3C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	3D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	3D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	3D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	31	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	31	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	31	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	31	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	31	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	33	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	33	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
21	34	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	34	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	4A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	4A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	4B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	4C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
21	4C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	4D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	4D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	4D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	41	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	41	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	41	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	41	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	41	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	43	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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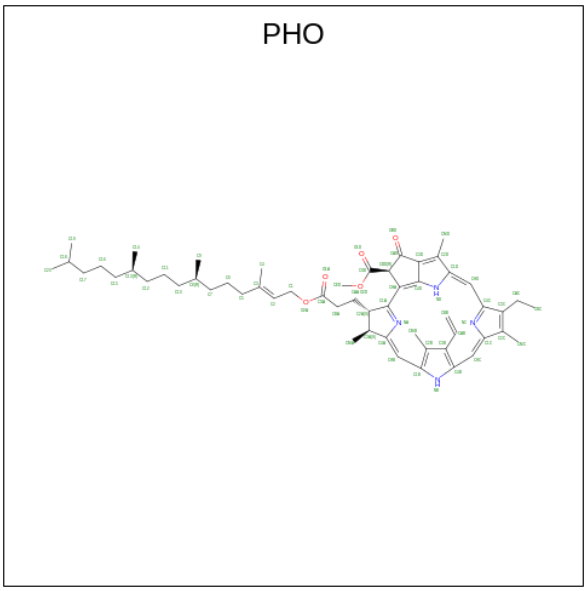
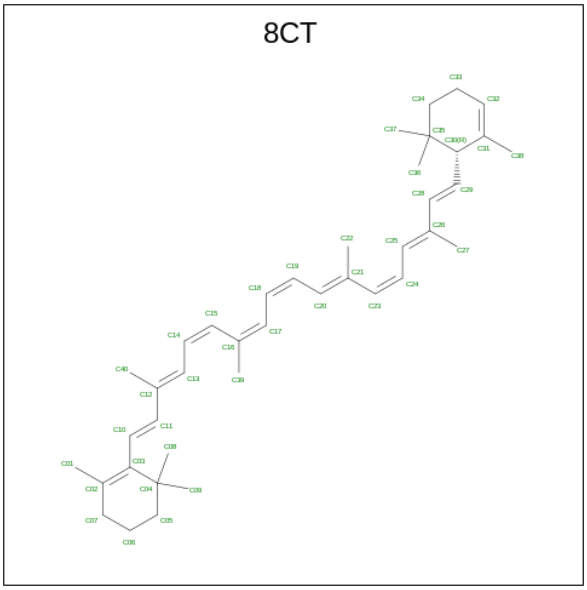
Mol	Chain	Residues	Atoms					AltConf
21	44	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	44	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 22 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
22	1A	1	Total C N O 64 55 4 5	0
22	1D	1	Total C N O 64 55 4 5	0
22	2A	1	Total C N O 64 55 4 5	0
22	2D	1	Total C N O 64 55 4 5	0
22	3A	1	Total C N O 64 55 4 5	0
22	3D	1	Total C N O 64 55 4 5	0
22	4A	1	Total C N O 64 55 4 5	0
22	4D	1	Total C N O 64 55 4 5	0

- Molecule 23 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
23	1A	1	Total C 40 40	0
23	1B	1	Total C 40 40	0
23	1B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
23	1B	1	Total C 40 40	0
23	1B	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1D	1	Total C 40 40	0
23	1K	1	Total C 40 40	0
23	14	1	Total C 40 40	0
23	2A	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2C	1	Total C 40 40	0
23	2C	1	Total C 40 40	0
23	2C	1	Total C 40 40	0
23	2D	1	Total C 40 40	0
23	2K	1	Total C 40 40	0
23	24	1	Total C 40 40	0
23	3A	1	Total C 40 40	0
23	3B	1	Total C 40 40	0

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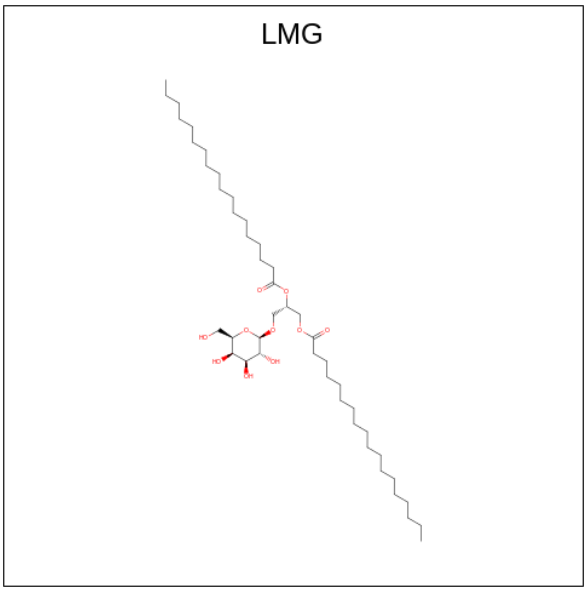
Mol	Chain	Residues	Atoms	AltConf
23	3B	1	Total C 40 40	0
23	3B	1	Total C 40 40	0
23	3B	1	Total C 40 40	0
23	3C	1	Total C 40 40	0
23	3C	1	Total C 40 40	0
23	3C	1	Total C 40 40	0
23	3D	1	Total C 40 40	0
23	3K	1	Total C 40 40	0
23	34	1	Total C 40 40	0
23	4A	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4C	1	Total C 40 40	0
23	4C	1	Total C 40 40	0
23	4C	1	Total C 40 40	0
23	4D	1	Total C 40 40	0
23	4K	1	Total C 40 40	0
23	44	1	Total C 40 40	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
24	1A	1	Total	C	O	0
			50	40	10	
24	1B	1	Total	C	O	0
			51	41	10	
24	1D	1	Total	C	O	0
			33	23	10	
24	11	1	Total	C	O	0
			51	41	10	
24	2A	1	Total	C	O	0
			50	40	10	
24	2B	1	Total	C	O	0
			51	41	10	
24	2D	1	Total	C	O	0
			33	23	10	
24	21	1	Total	C	O	0
			51	41	10	
24	3A	1	Total	C	O	0
			50	40	10	
24	3B	1	Total	C	O	0
			51	41	10	
24	3D	1	Total	C	O	0
			33	23	10	
24	31	1	Total	C	O	0
			51	41	10	
24	4A	1	Total	C	O	0
			50	40	10	
24	4B	1	Total	C	O	0
			51	41	10	

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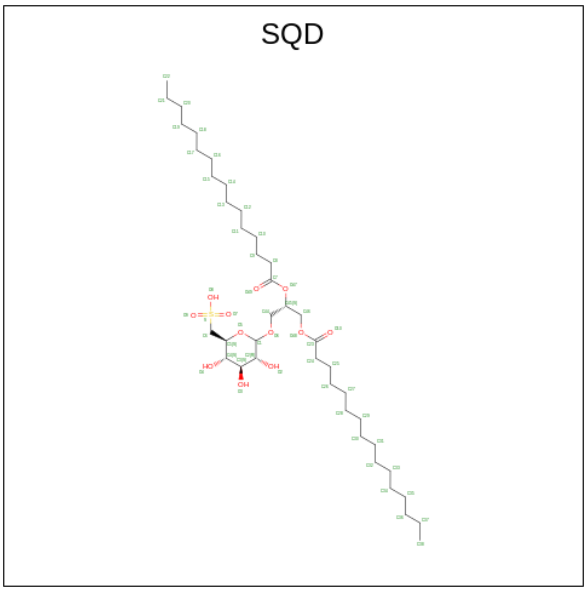
Mol	Chain	Residues	Atoms	AltConf
24	4D	1	Total C O 33 23 10	0
24	41	1	Total C O 51 41 10	0

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
25	1A	1	Total C O S 34 21 12 1	0
25	1B	1	Total C O S 54 41 12 1	0
25	12	1	Total C O S 50 37 12 1	0
25	12	1	Total C O S 41 28 12 1	0
25	11	1	Total C O S 32 19 12 1	0
25	13	1	Total C O S 46 33 12 1	0
25	13	1	Total C O S 50 37 12 1	0
25	2A	1	Total C O S 34 21 12 1	0

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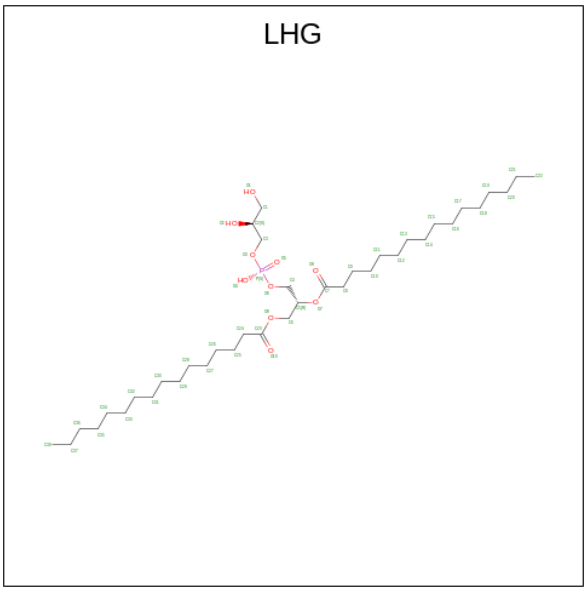
Mol	Chain	Residues	Atoms				AltConf
25	2B	1	Total	C	O	S	0
			54	41	12	1	
25	22	1	Total	C	O	S	0
			50	37	12	1	
25	22	1	Total	C	O	S	0
			41	28	12	1	
25	21	1	Total	C	O	S	0
			32	19	12	1	
25	23	1	Total	C	O	S	0
			46	33	12	1	
25	23	1	Total	C	O	S	0
			50	37	12	1	
25	3A	1	Total	C	O	S	0
			34	21	12	1	
25	3B	1	Total	C	O	S	0
			54	41	12	1	
25	32	1	Total	C	O	S	0
			50	37	12	1	
25	32	1	Total	C	O	S	0
			41	28	12	1	
25	31	1	Total	C	O	S	0
			32	19	12	1	
25	33	1	Total	C	O	S	0
			46	33	12	1	
25	33	1	Total	C	O	S	0
			50	37	12	1	
25	4A	1	Total	C	O	S	0
			34	21	12	1	
25	4B	1	Total	C	O	S	0
			54	41	12	1	
25	42	1	Total	C	O	S	0
			50	37	12	1	
25	42	1	Total	C	O	S	0
			41	28	12	1	
25	41	1	Total	C	O	S	0
			32	19	12	1	
25	43	1	Total	C	O	S	0
			46	33	12	1	
25	43	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
26	1A	1	Total	C	O	P	0
			46	35	10	1	
26	1B	1	Total	C	O	P	0
			45	34	10	1	
26	1B	1	Total	C	O	P	0
			49	38	10	1	
26	1D	1	Total	C	O	P	0
			49	38	10	1	
26	13	1	Total	C	O	P	0
			36	25	10	1	
26	14	1	Total	C	O	P	0
			49	38	10	1	
26	2A	1	Total	C	O	P	0
			46	35	10	1	
26	2B	1	Total	C	O	P	0
			45	34	10	1	
26	2B	1	Total	C	O	P	0
			49	38	10	1	
26	2D	1	Total	C	O	P	0
			49	38	10	1	
26	23	1	Total	C	O	P	0
			36	25	10	1	
26	24	1	Total	C	O	P	0
			49	38	10	1	
26	3A	1	Total	C	O	P	0
			46	35	10	1	
26	3B	1	Total	C	O	P	0
			45	34	10	1	

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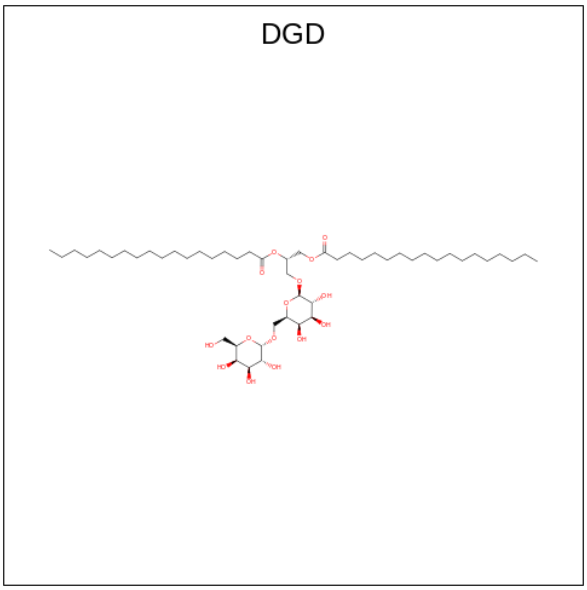
Mol	Chain	Residues	Atoms				AltConf
26	3B	1	Total	C	O	P	0
			49	38	10	1	
26	3D	1	Total	C	O	P	0
			49	38	10	1	
26	33	1	Total	C	O	P	0
			36	25	10	1	
26	34	1	Total	C	O	P	0
			49	38	10	1	
26	4A	1	Total	C	O	P	0
			46	35	10	1	
26	4B	1	Total	C	O	P	0
			45	34	10	1	
26	4B	1	Total	C	O	P	0
			49	38	10	1	
26	4D	1	Total	C	O	P	0
			49	38	10	1	
26	43	1	Total	C	O	P	0
			36	25	10	1	
26	44	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	1B	1	Total	C	O	0
			62	47	15	

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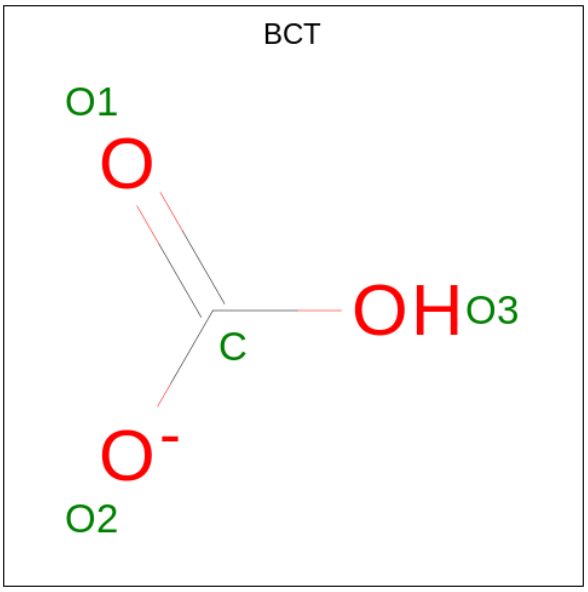
Mol	Chain	Residues	Atoms	AltConf
27	1C	1	Total C O 62 47 15	0
27	2B	1	Total C O 62 47 15	0
27	2C	1	Total C O 62 47 15	0
27	3B	1	Total C O 62 47 15	0
27	3C	1	Total C O 62 47 15	0
27	4B	1	Total C O 62 47 15	0
27	4C	1	Total C O 62 47 15	0

- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

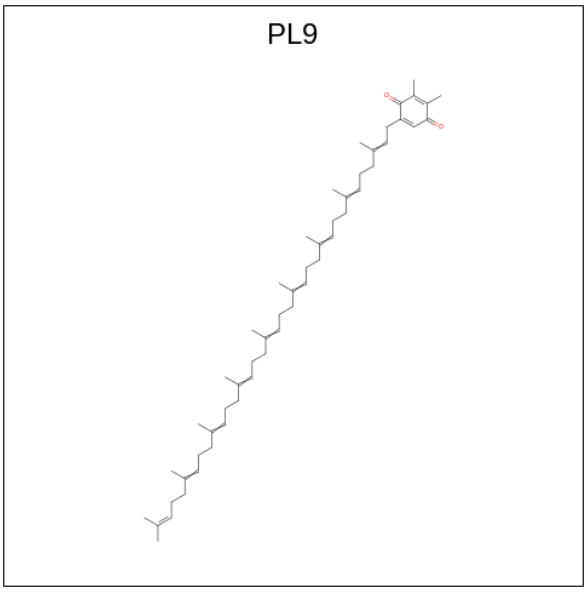
Mol	Chain	Residues	Atoms	AltConf
28	1D	1	Total Fe 1 1	0
28	2D	1	Total Fe 1 1	0
28	3D	1	Total Fe 1 1	0
28	4D	1	Total Fe 1 1	0

- Molecule 29 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



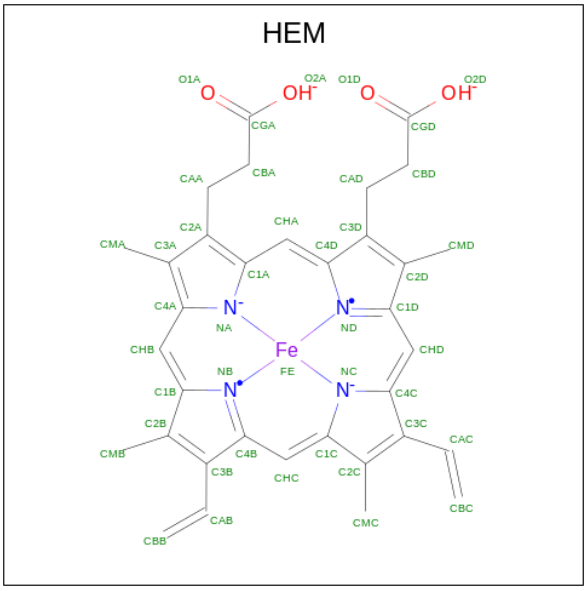
Mol	Chain	Residues	Atoms			AltConf
29	1D	1	Total	C	O	0
			4	1	3	
29	2D	1	Total	C	O	0
			4	1	3	
29	3D	1	Total	C	O	0
			4	1	3	
29	4D	1	Total	C	O	0
			4	1	3	

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



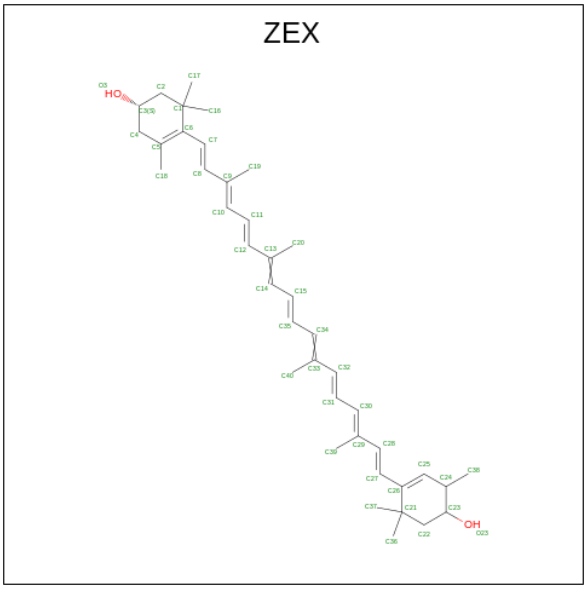
Mol	Chain	Residues	Atoms	AltConf
30	1D	1	Total C O 55 53 2	0
30	2D	1	Total C O 55 53 2	0
30	3D	1	Total C O 55 53 2	0
30	4D	1	Total C O 55 53 2	0

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	1F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	2F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	3F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	4F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 32 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
32	12	1	Total	C	O	0
			42	40	2	
32	12	1	Total	C	O	0
			42	40	2	
32	12	1	Total	C	O	0
			42	40	2	
32	12	1	Total	C	O	0
			42	40	2	
32	11	1	Total	C	O	0
			42	40	2	
32	11	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
32	13	1	Total C O 42 40 2	0
32	13	1	Total C O 42 40 2	0
32	13	1	Total C O 42 40 2	0
32	13	1	Total C O 42 40 2	0
32	14	1	Total C O 42 40 2	0
32	14	1	Total C O 42 40 2	0
32	14	1	Total C O 42 40 2	0
32	14	1	Total C O 42 40 2	0
32	22	1	Total C O 42 40 2	0
32	22	1	Total C O 42 40 2	0
32	22	1	Total C O 42 40 2	0
32	22	1	Total C O 42 40 2	0
32	21	1	Total C O 42 40 2	0
32	21	1	Total C O 42 40 2	0
32	23	1	Total C O 42 40 2	0
32	23	1	Total C O 42 40 2	0
32	23	1	Total C O 42 40 2	0
32	23	1	Total C O 42 40 2	0
32	24	1	Total C O 42 40 2	0
32	24	1	Total C O 42 40 2	0
32	24	1	Total C O 42 40 2	0

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Mol	Chain	Residues	Atoms	AltConf
32	24	1	Total C O 42 40 2	0
32	32	1	Total C O 42 40 2	0
32	32	1	Total C O 42 40 2	0
32	32	1	Total C O 42 40 2	0
32	32	1	Total C O 42 40 2	0
32	31	1	Total C O 42 40 2	0
32	31	1	Total C O 42 40 2	0
32	33	1	Total C O 42 40 2	0
32	33	1	Total C O 42 40 2	0
32	33	1	Total C O 42 40 2	0
32	33	1	Total C O 42 40 2	0
32	34	1	Total C O 42 40 2	0
32	34	1	Total C O 42 40 2	0
32	34	1	Total C O 42 40 2	0
32	34	1	Total C O 42 40 2	0
32	42	1	Total C O 42 40 2	0
32	42	1	Total C O 42 40 2	0
32	42	1	Total C O 42 40 2	0
32	42	1	Total C O 42 40 2	0
32	41	1	Total C O 42 40 2	0
32	41	1	Total C O 42 40 2	0

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Mol	Chain	Residues	Atoms			AltConf
32	43	1	Total	C	O	0
			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	

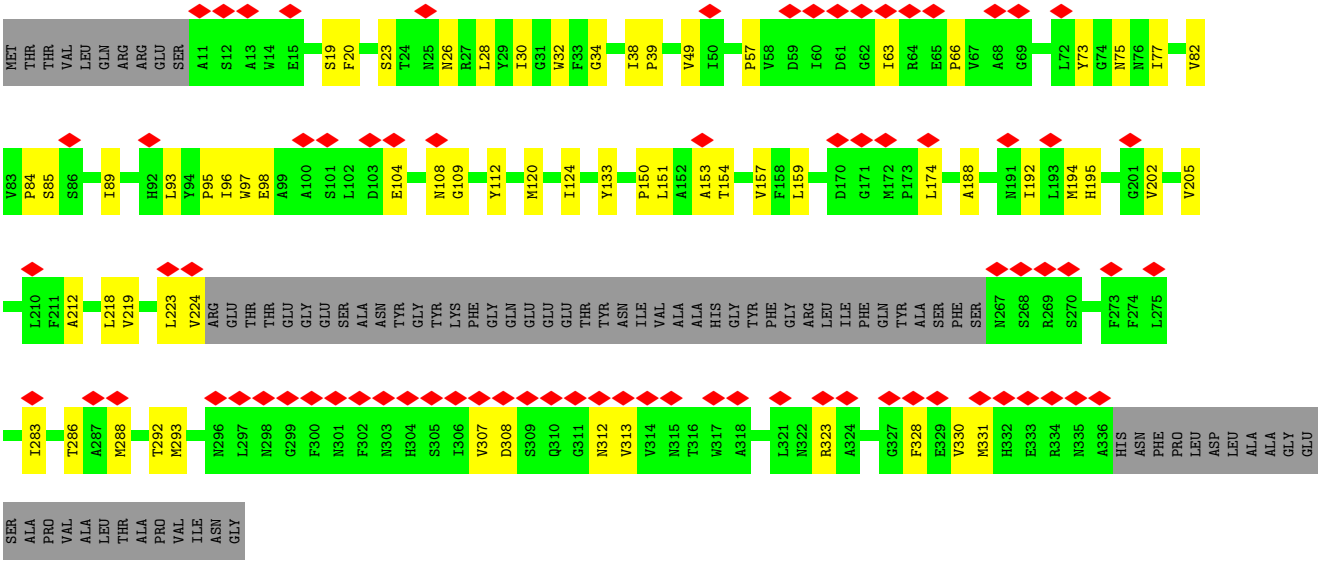
3 Residue-property plots (i)

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 2

Chain 1A:

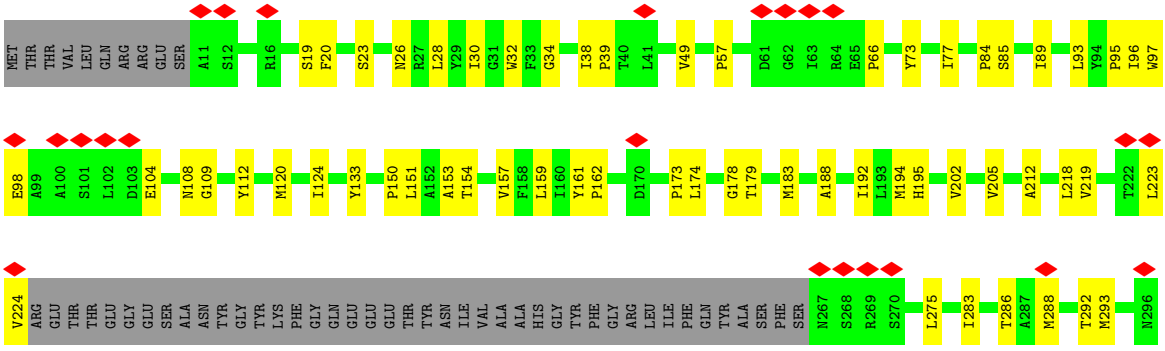


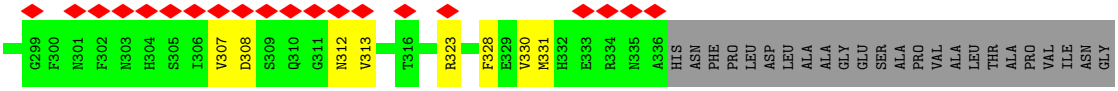


• Molecule 1: Photosystem II protein D1 2

Chain 2A:



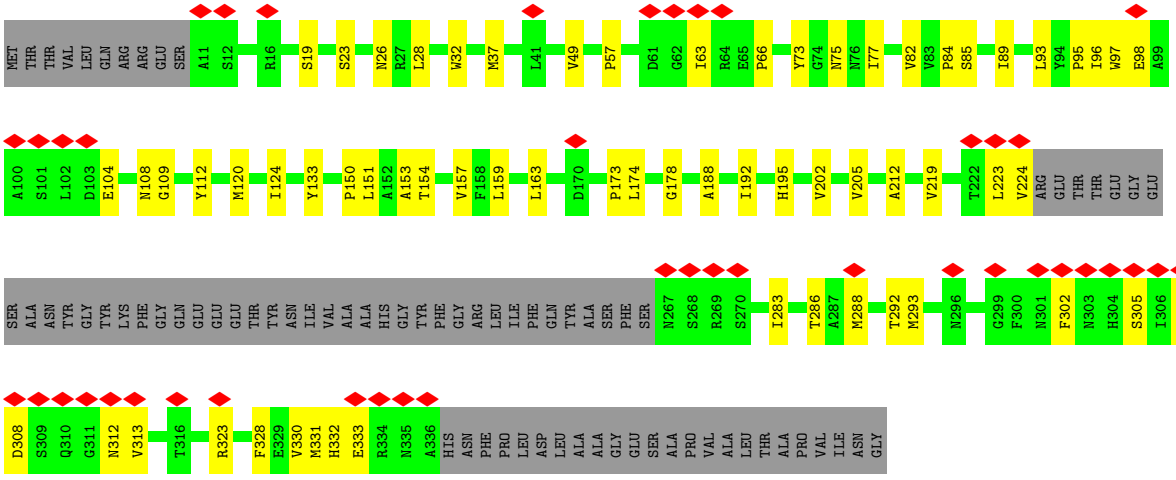




• Molecule 1: Photosystem II protein D1 2

Chain 3A:

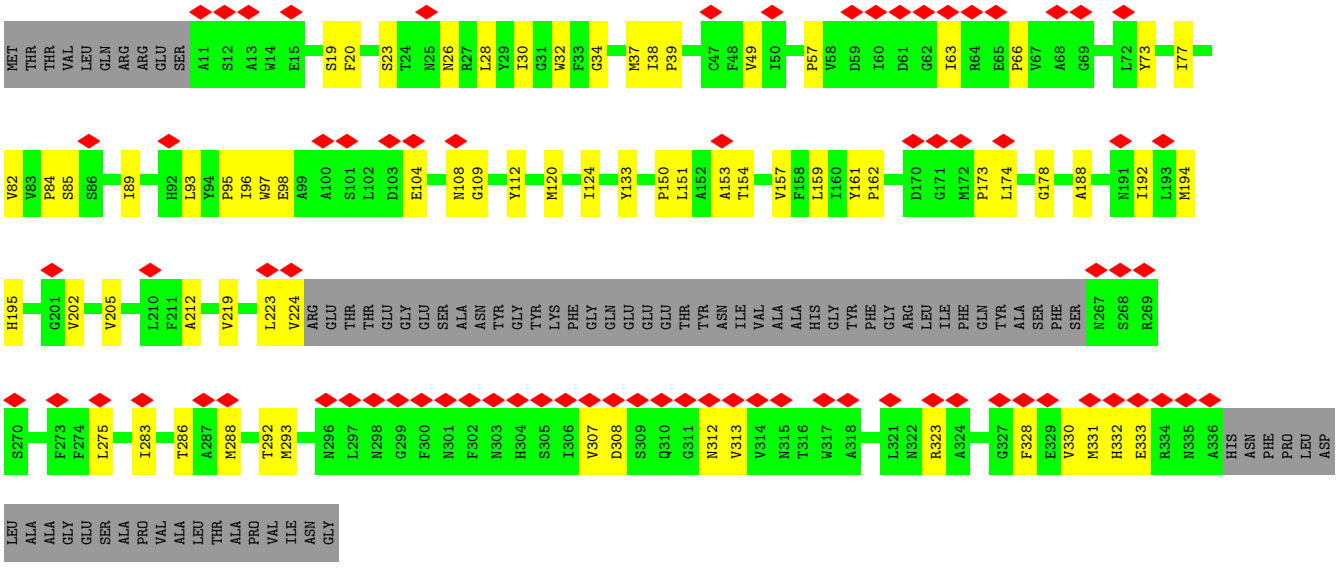




• Molecule 1: Photosystem II protein D1 2

Chain 4A:

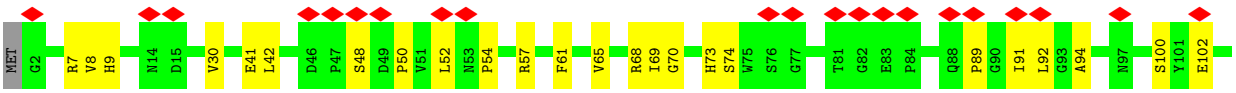


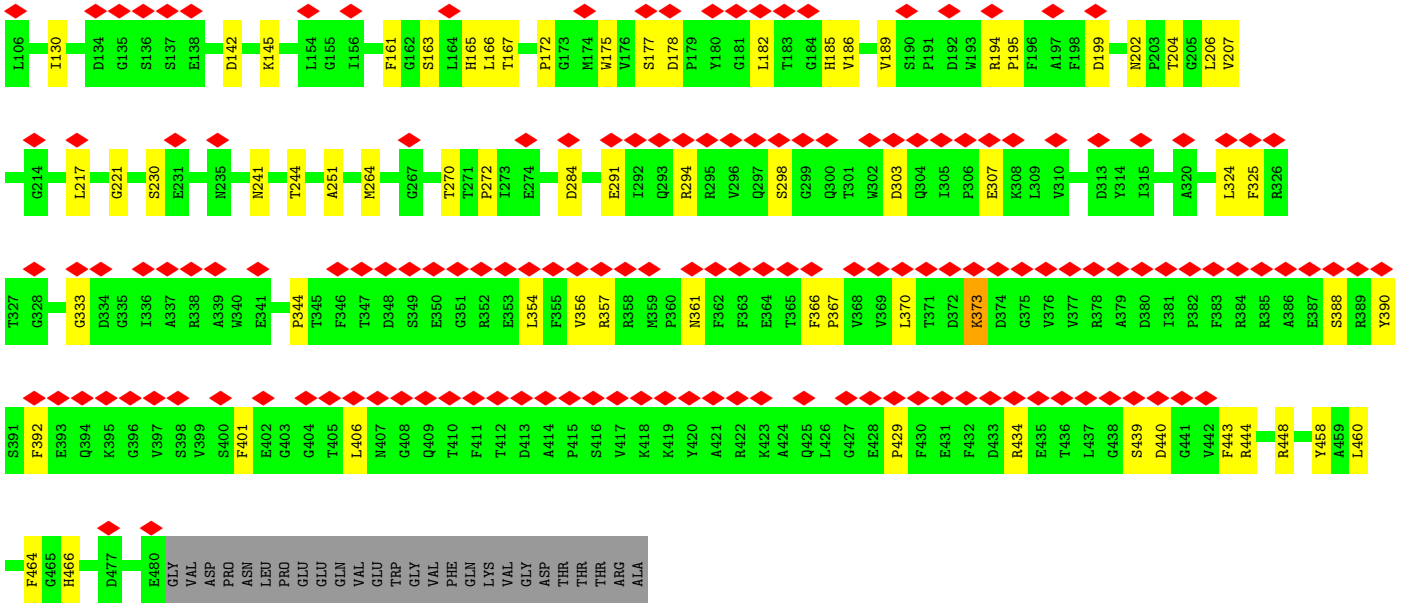


• Molecule 2: Photosystem II CP47 reaction center protein

Chain 1B:



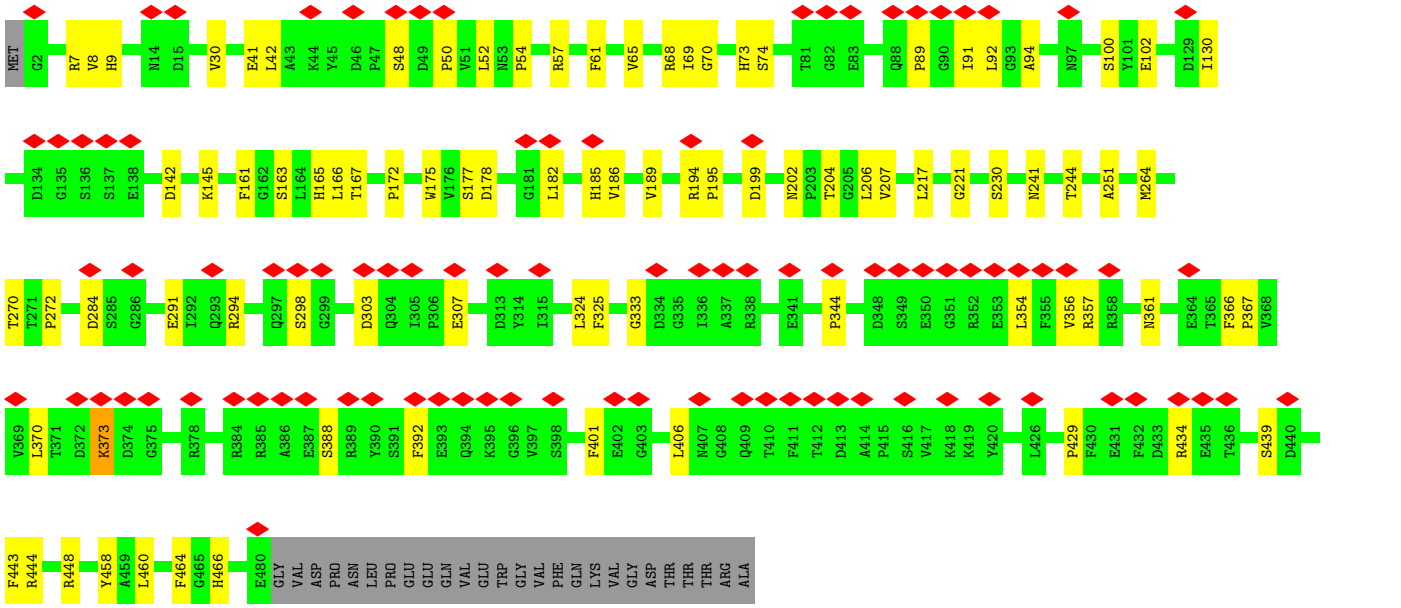




• Molecule 2: Photosystem II CP47 reaction center protein

Chain 2B:

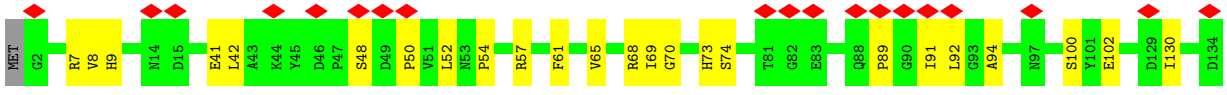


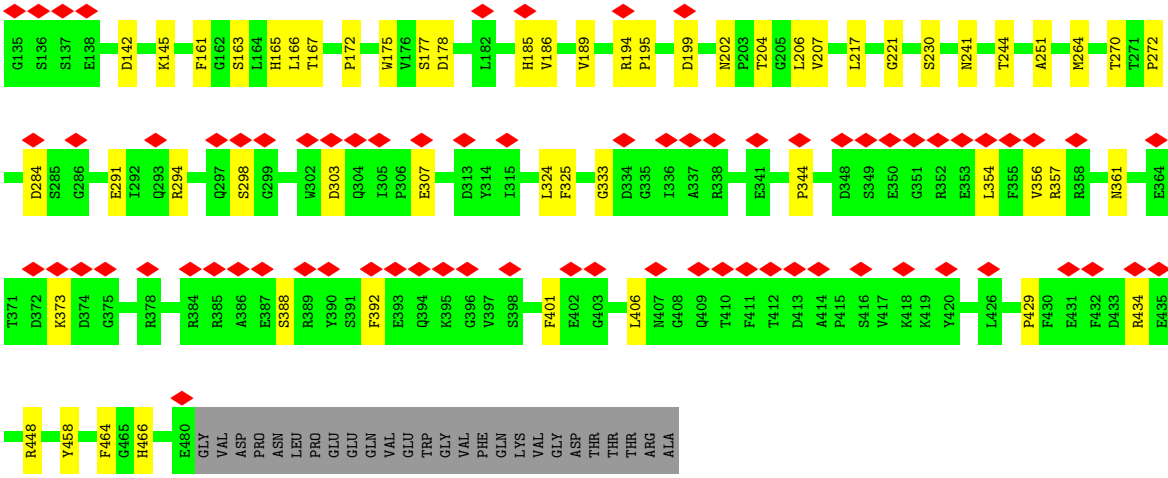


• Molecule 2: Photosystem II CP47 reaction center protein

Chain 3B:



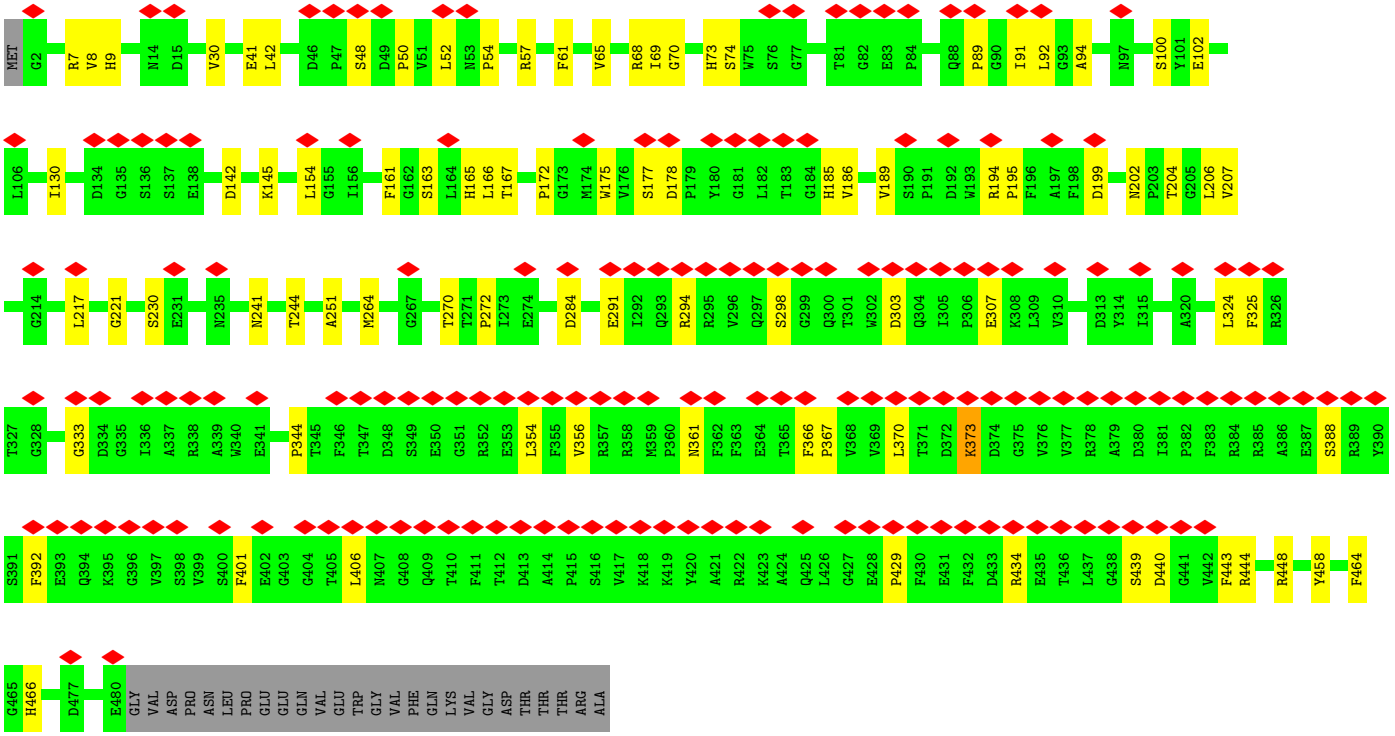




• Molecule 2: Photosystem II CP47 reaction center protein

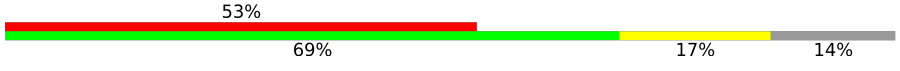
Chain 4B:

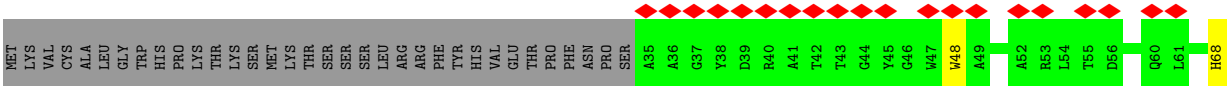


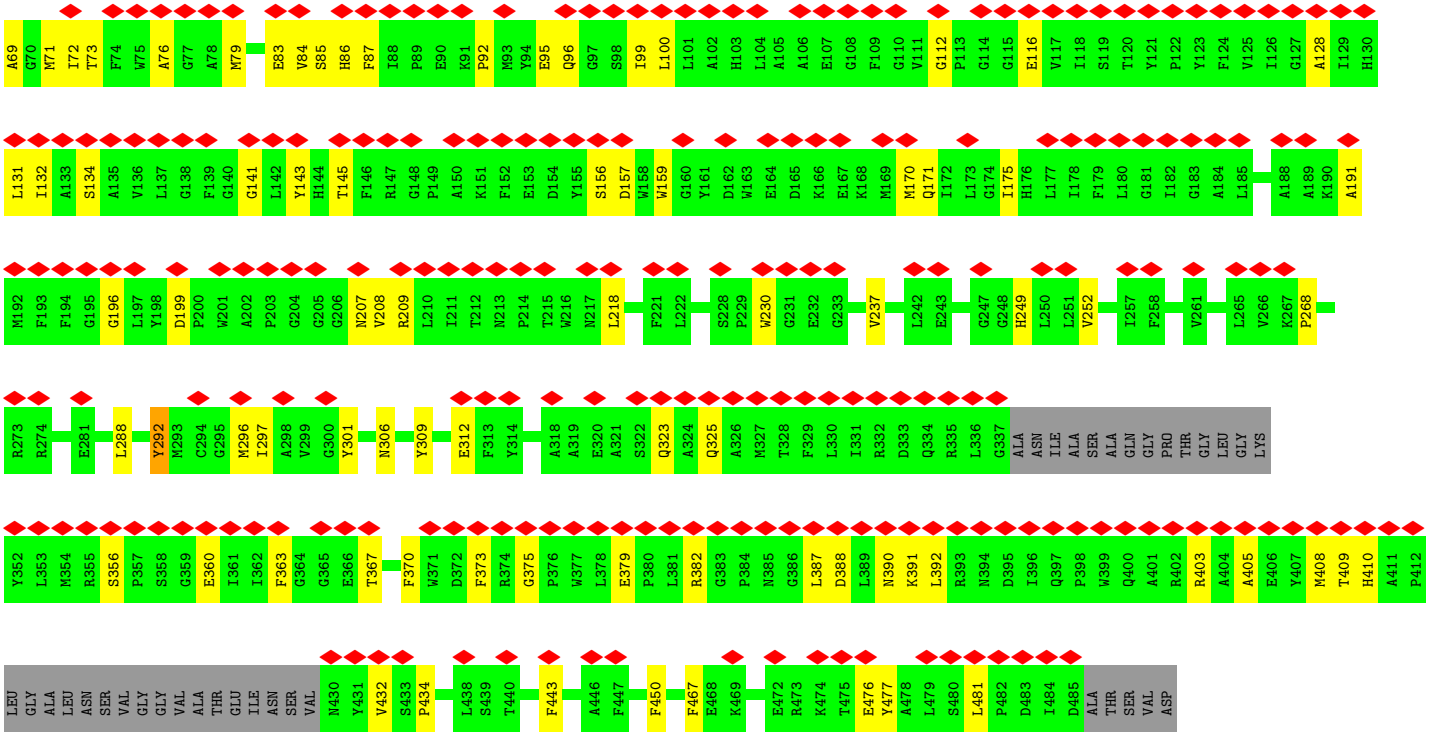


• Molecule 3: Photosystem II CP43 reaction center protein

Chain 1C:



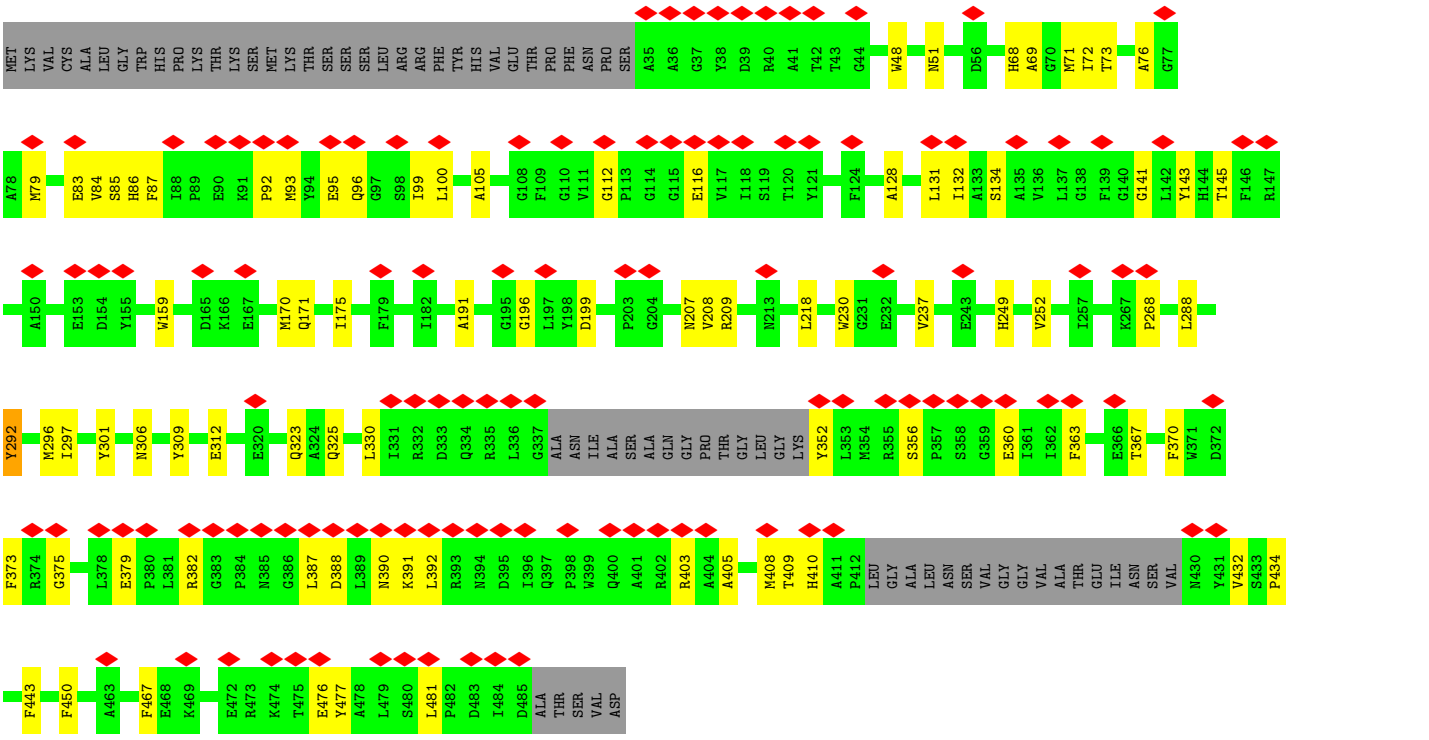




• Molecule 3: Photosystem II CP43 reaction center protein

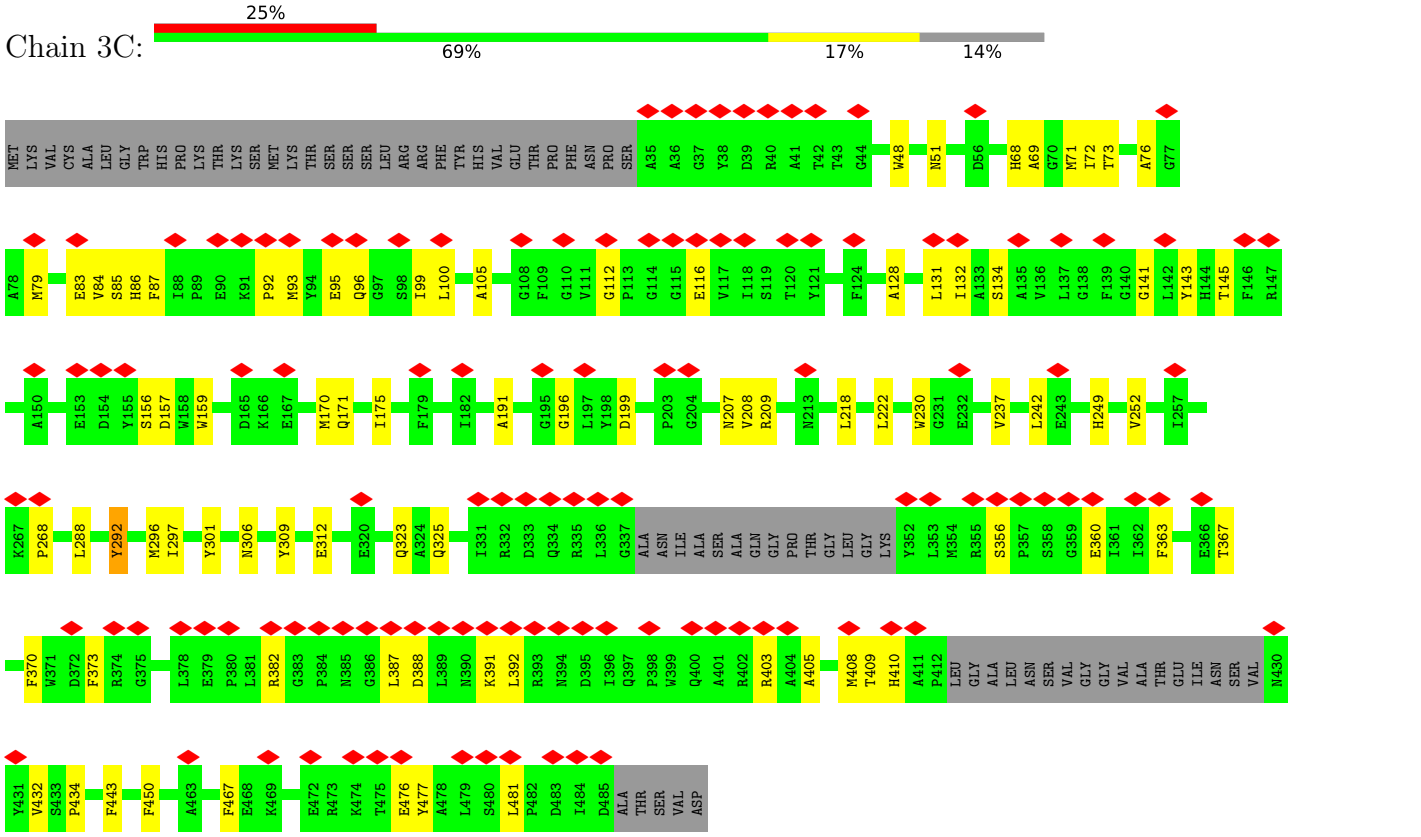
Chain 2C:





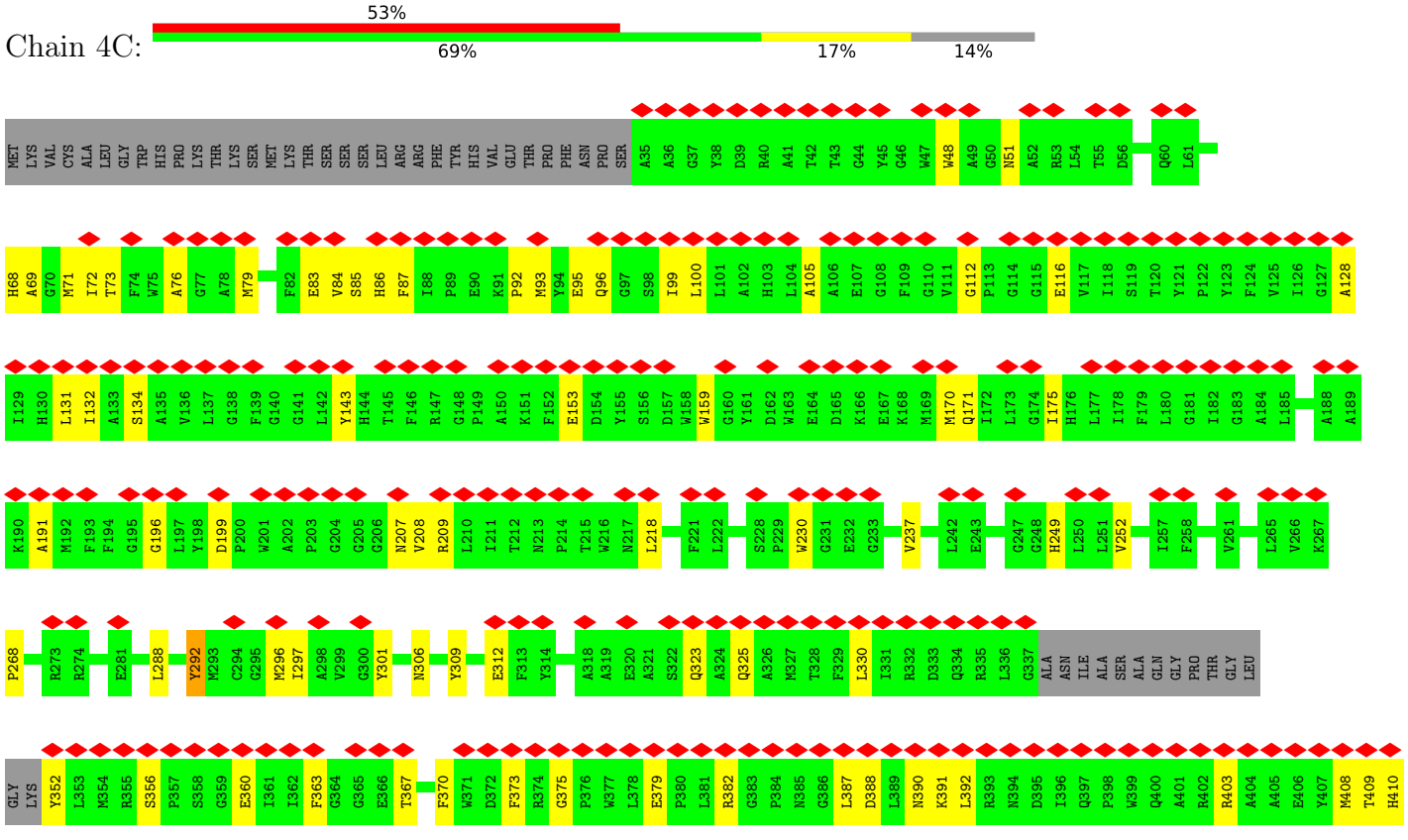
• Molecule 3: Photosystem II CP43 reaction center protein

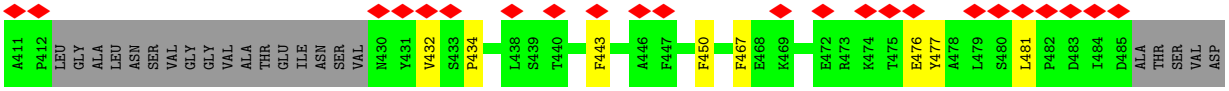
Chain 3C:



• Molecule 3: Photosystem II CP43 reaction center protein

Chain 4C:

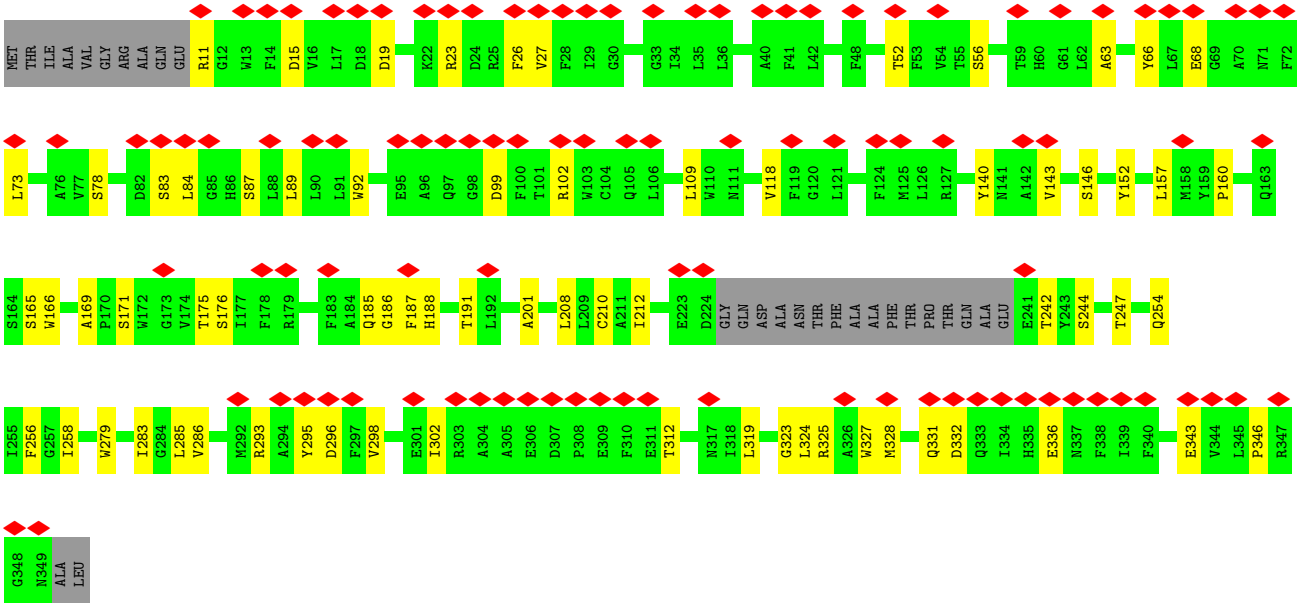




• Molecule 4: Photosystem II D2 protein 1

Chain 1D:

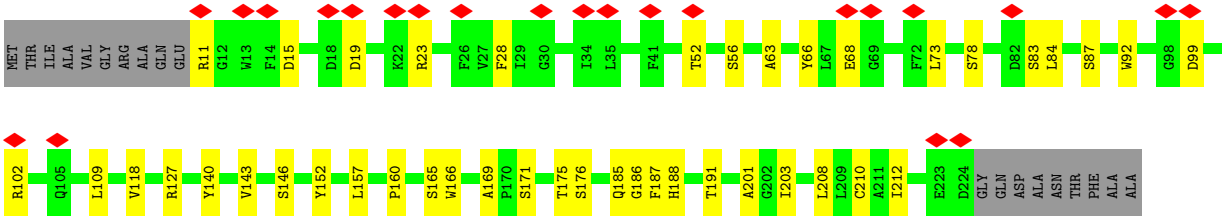




• Molecule 4: Photosystem II D2 protein 1

Chain 2D:

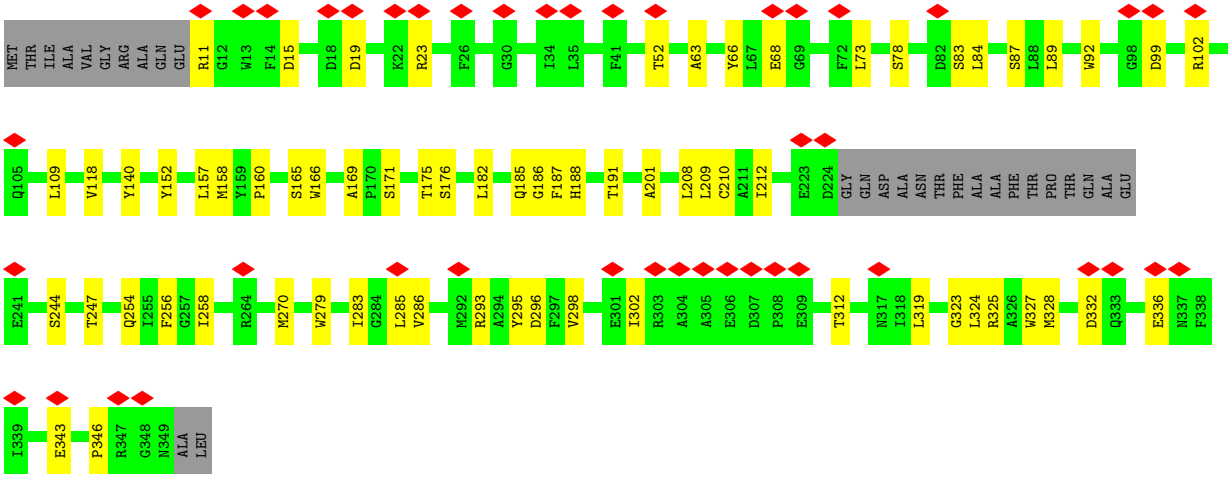




• Molecule 4: Photosystem II D2 protein 1

Chain 3D:





• Molecule 4: Photosystem II D2 protein 1

Chain 4D:

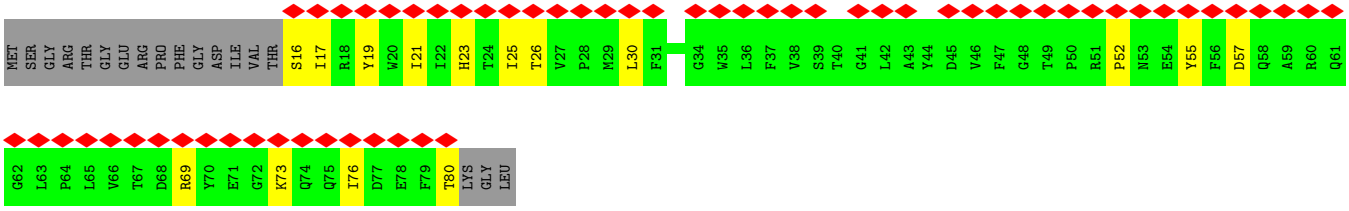




• Molecule 5: Cytochrome b559 subunit alpha

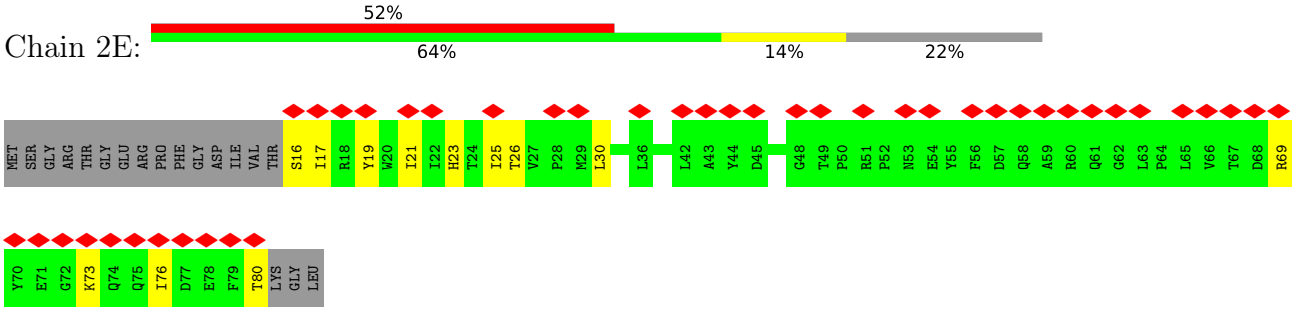
Chain 1E:





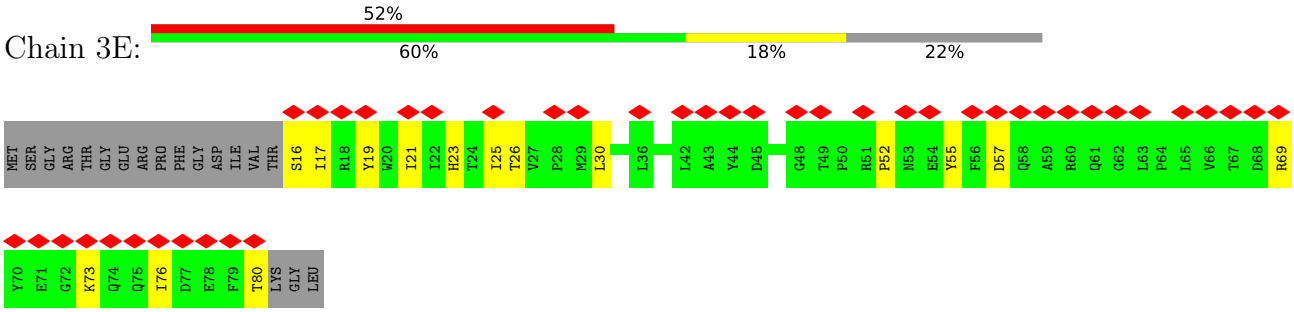
• Molecule 5: Cytochrome b559 subunit alpha

Chain 2E:



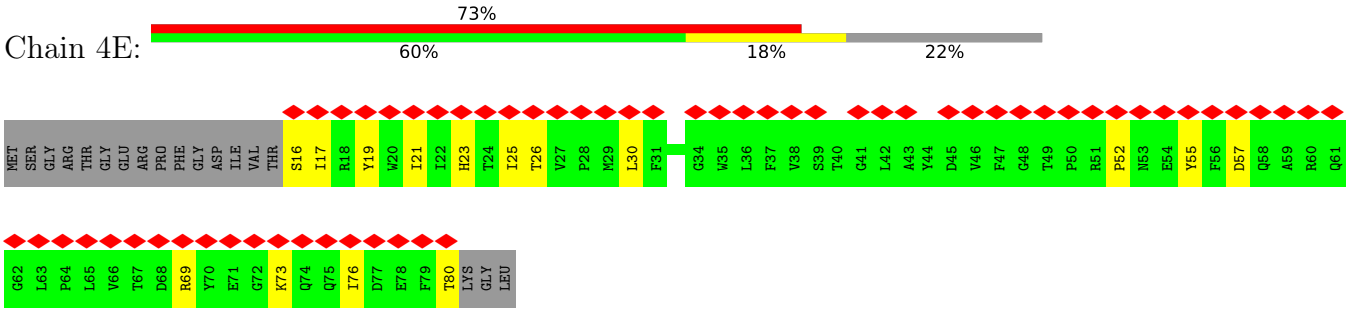
• Molecule 5: Cytochrome b559 subunit alpha

Chain 3E:



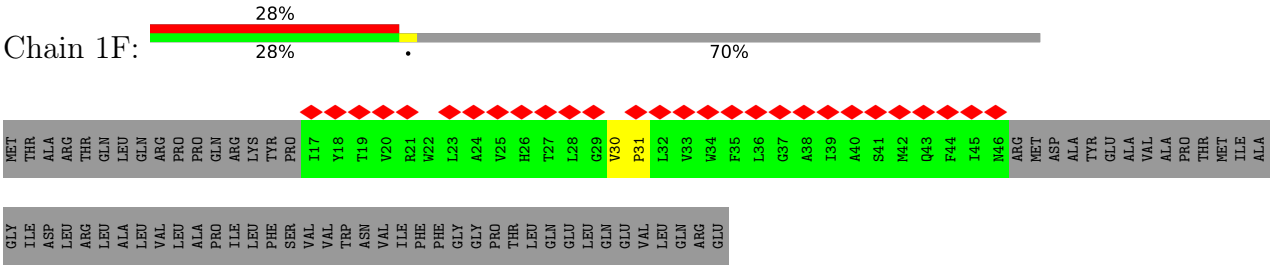
• Molecule 5: Cytochrome b559 subunit alpha

Chain 4E:



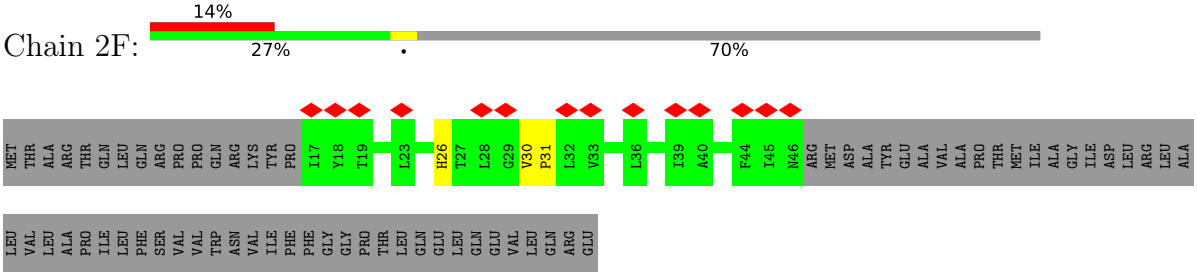
• Molecule 6: Photosystem II protein Y

Chain 1F:



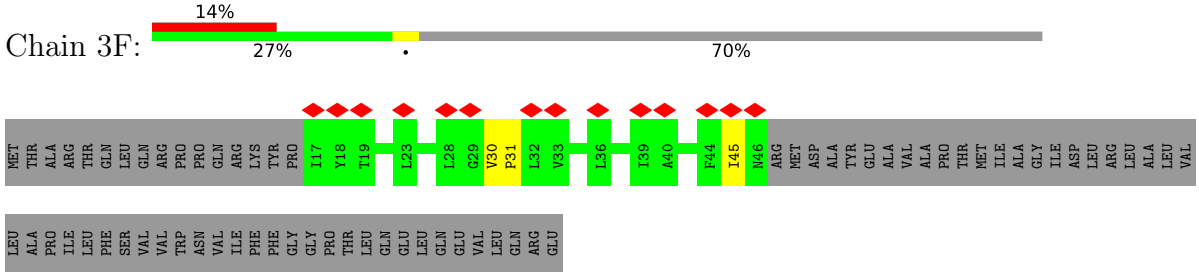
• Molecule 6: Photosystem II protein Y

Chain 2F:



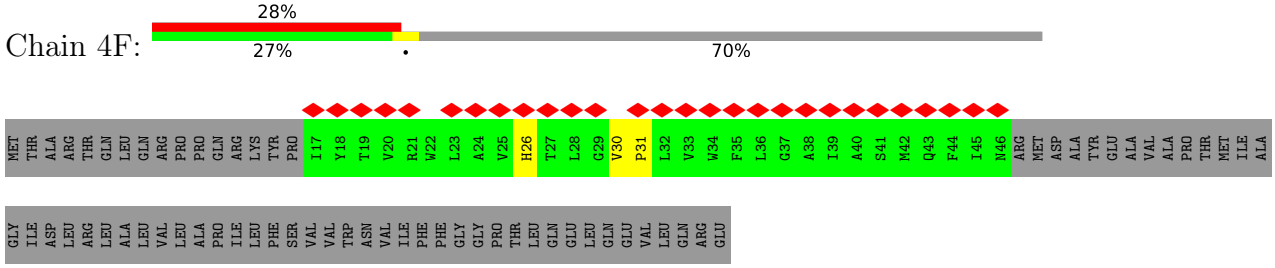
• Molecule 6: Photosystem II protein Y

Chain 3F:



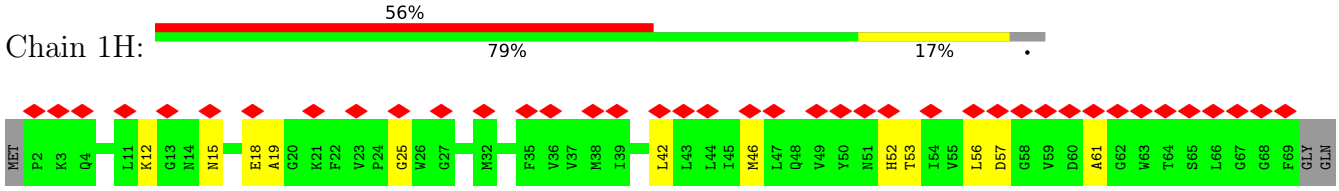
• Molecule 6: Photosystem II protein Y

Chain 4F:



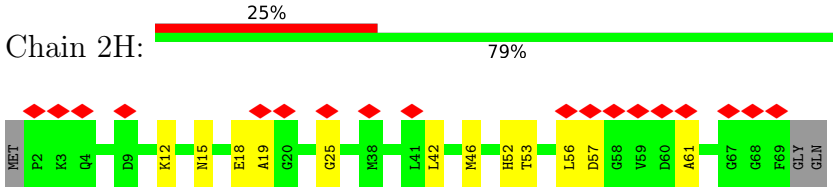
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

Chain 1H:



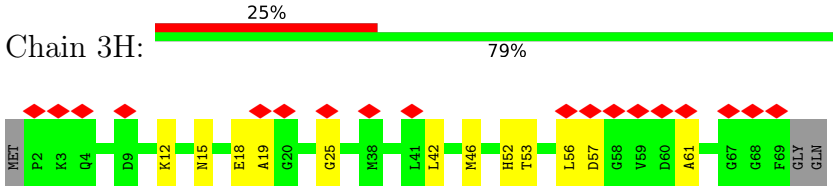
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

Chain 2H:



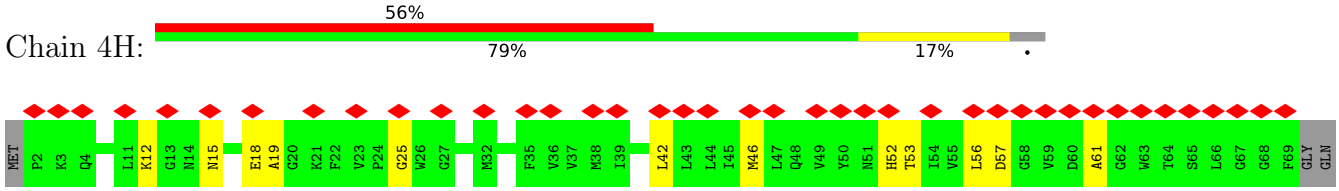
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

Chain 3H:



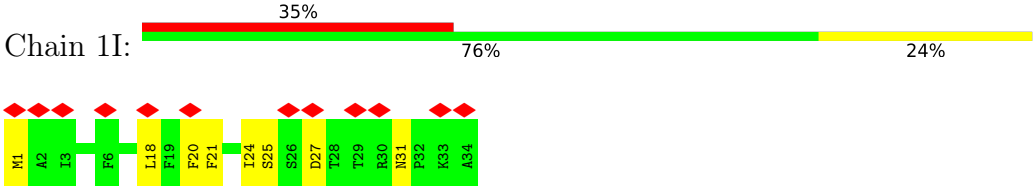
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

Chain 4H:



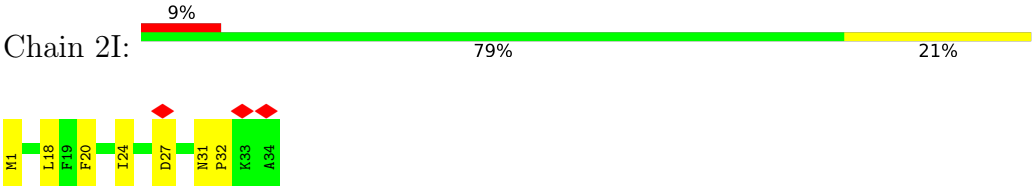
• Molecule 8: Photosystem II protein PsbI

Chain 1I:



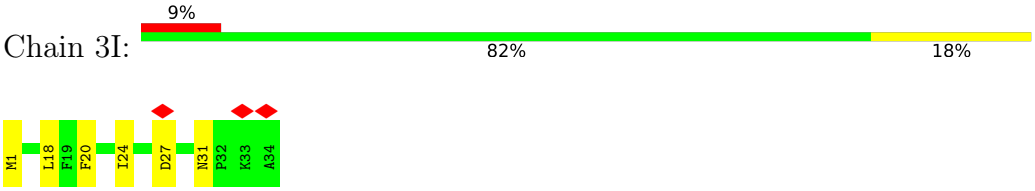
• Molecule 8: Photosystem II protein PsbI

Chain 2I:



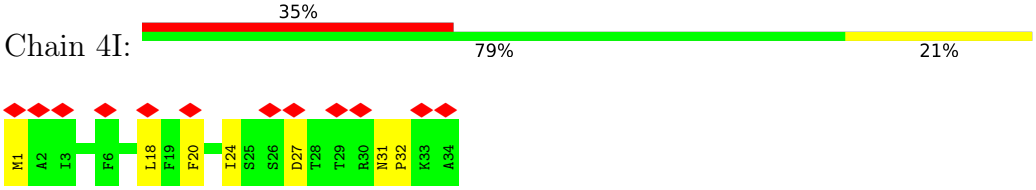
• Molecule 8: Photosystem II protein PsbI

Chain 3I:



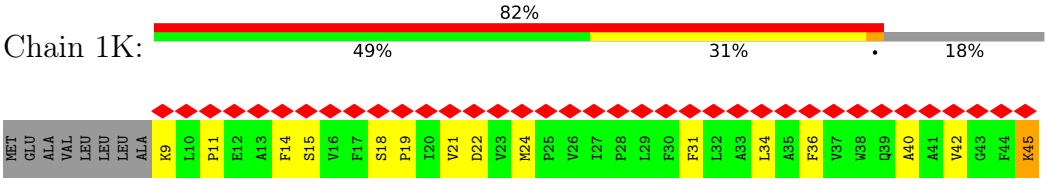
• Molecule 8: Photosystem II protein PsbI

Chain 4I:



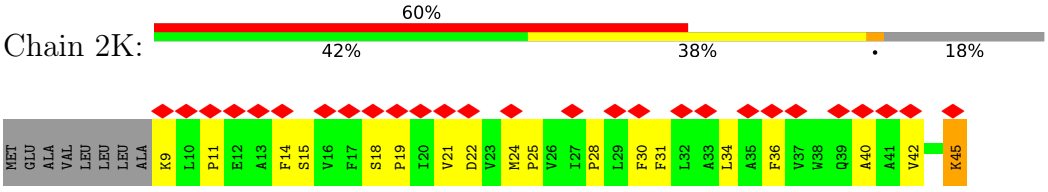
• Molecule 9: Photosystem II reaction center protein K

Chain 1K:



• Molecule 9: Photosystem II reaction center protein K

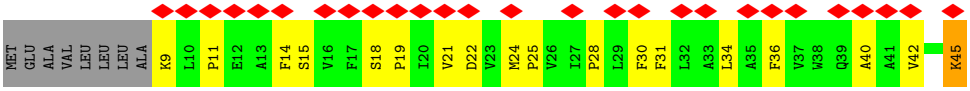
Chain 2K:



• Molecule 9: Photosystem II reaction center protein K

Chain 3K:

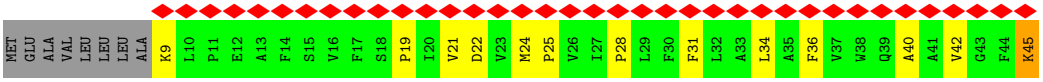




• Molecule 9: Photosystem II reaction center protein K

Chain 4K:





• Molecule 10: Photosystem II reaction center protein L

Chain 1L:

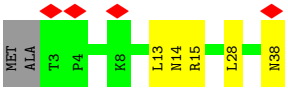




• Molecule 10: Photosystem II reaction center protein L

Chain 2L:

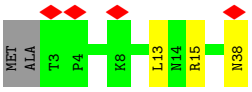




• Molecule 10: Photosystem II reaction center protein L

Chain 3L:

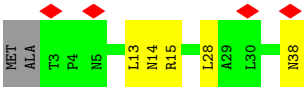




• Molecule 10: Photosystem II reaction center protein L

Chain 4L:





• Molecule 11: Photosystem II reaction center protein M

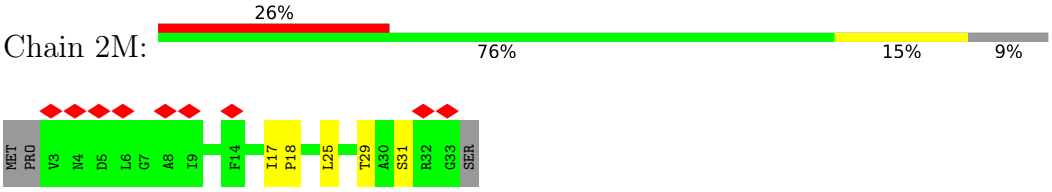
Chain 1M:





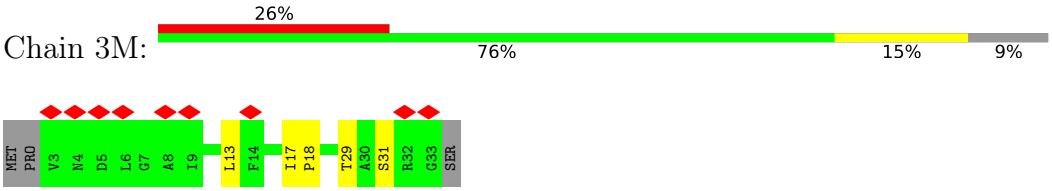
• Molecule 11: Photosystem II reaction center protein M

Chain 2M:



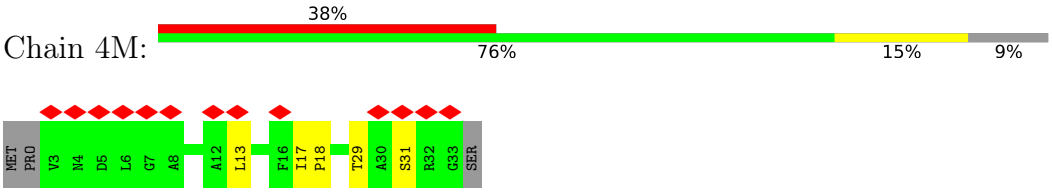
• Molecule 11: Photosystem II reaction center protein M

Chain 3M:



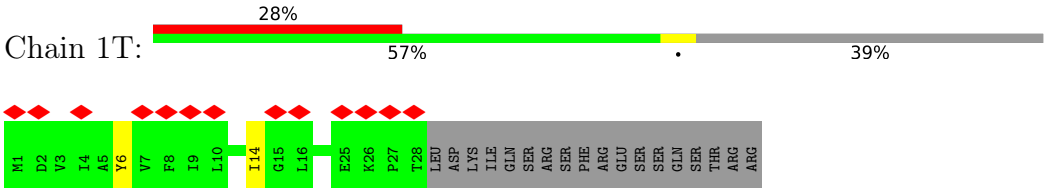
• Molecule 11: Photosystem II reaction center protein M

Chain 4M:



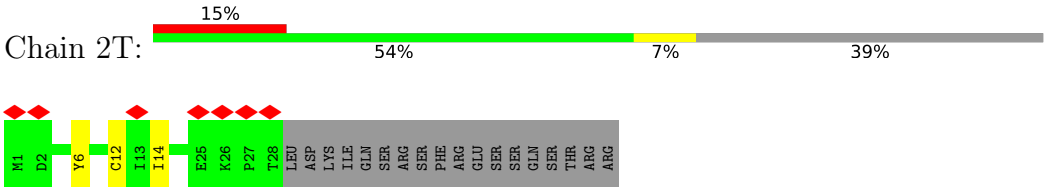
• Molecule 12: Photosystem II reaction center protein T

Chain 1T:



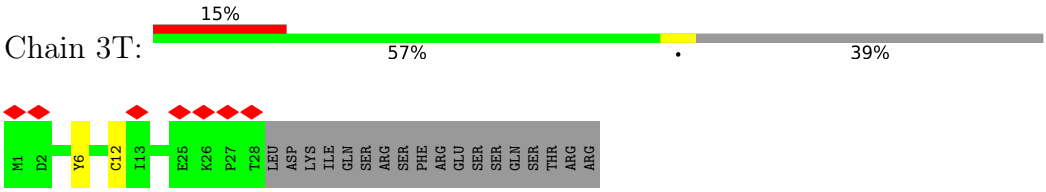
• Molecule 12: Photosystem II reaction center protein T

Chain 2T:



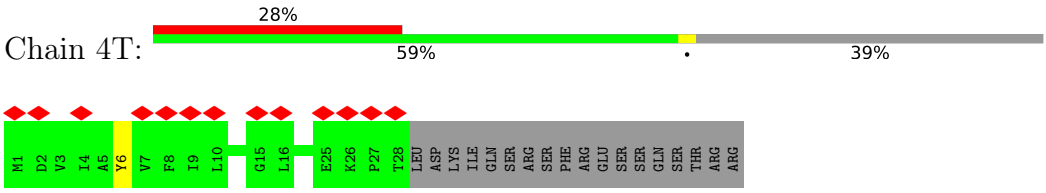
• Molecule 12: Photosystem II reaction center protein T

Chain 3T:



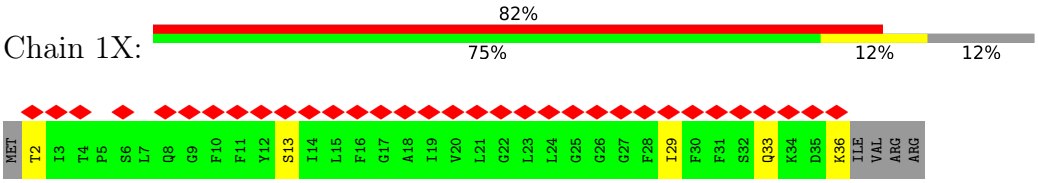
• Molecule 12: Photosystem II reaction center protein T

Chain 4T:



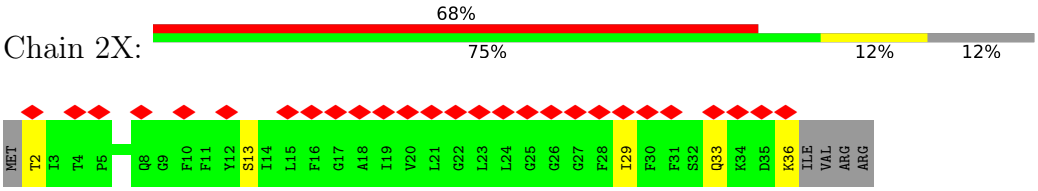
• Molecule 13: Photosystem II reaction center X protein

Chain 1X:



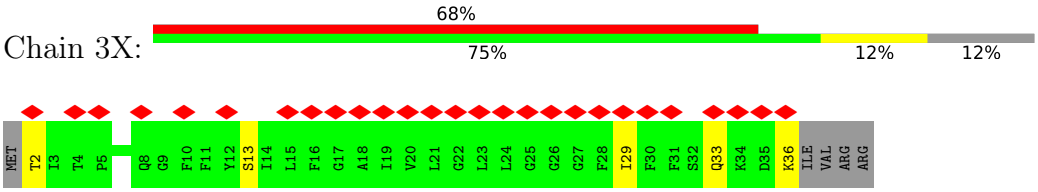
• Molecule 13: Photosystem II reaction center X protein

Chain 2X:



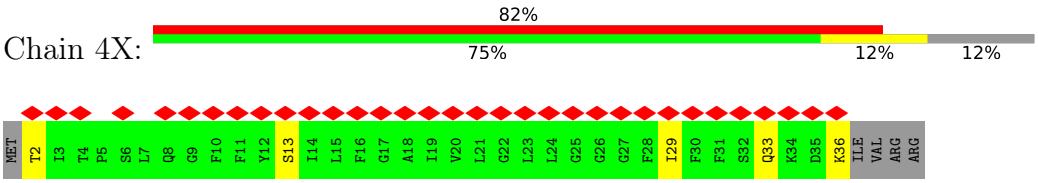
• Molecule 13: Photosystem II reaction center X protein

Chain 3X:



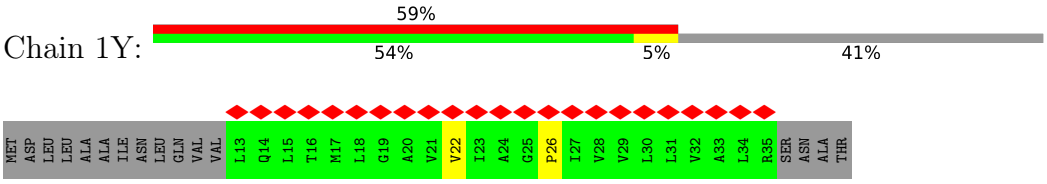
• Molecule 13: Photosystem II reaction center X protein

Chain 4X:



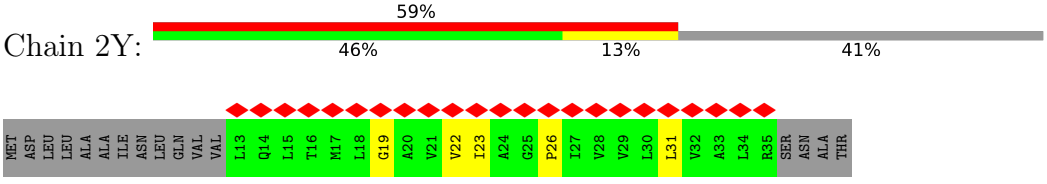
• Molecule 14: Photosystem II reaction center protein Ycf12

Chain 1Y:



• Molecule 14: Photosystem II reaction center protein Ycf12

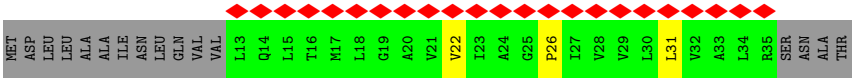
Chain 2Y:



• Molecule 14: Photosystem II reaction center protein Ycf12

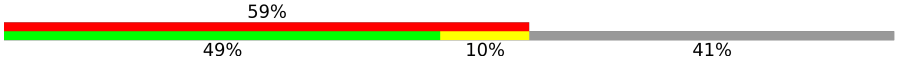
Chain 3Y:

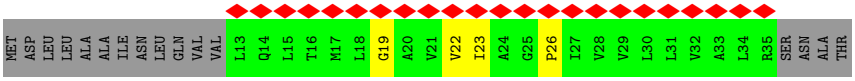




• Molecule 14: Photosystem II reaction center protein Ycf12

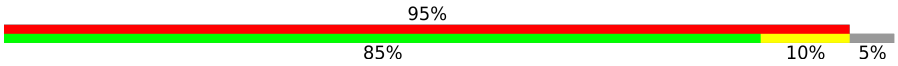
Chain 4Y:

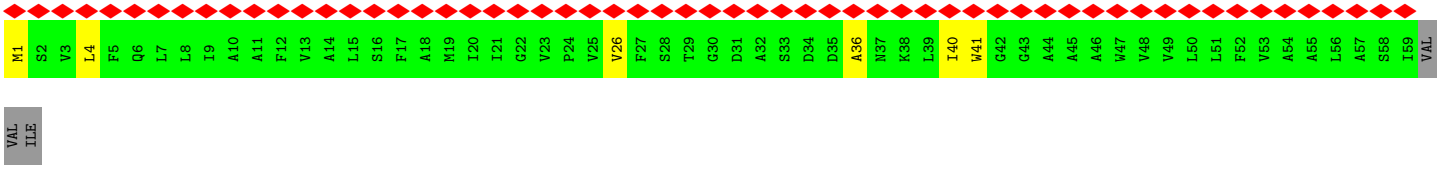




• Molecule 15: Photosystem II reaction center protein Z

Chain 1Z:

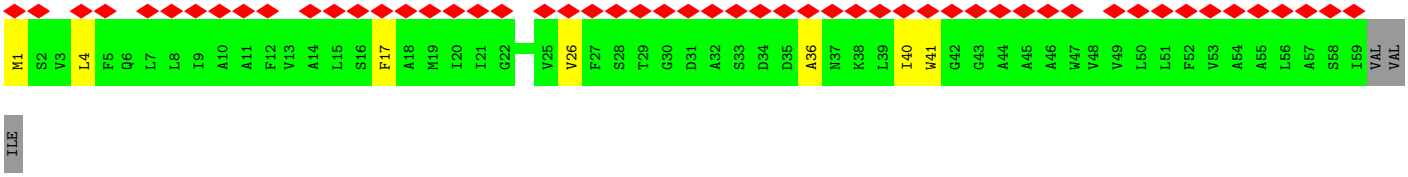




• Molecule 15: Photosystem II reaction center protein Z

Chain 2Z:

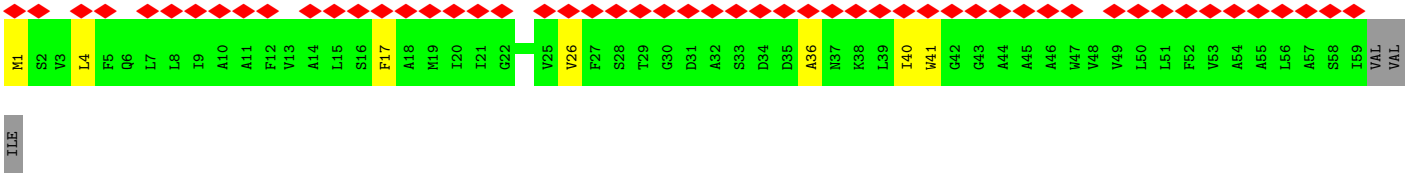




• Molecule 15: Photosystem II reaction center protein Z

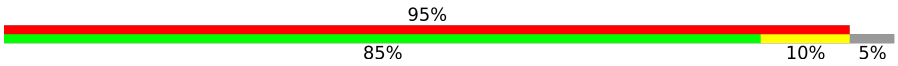
Chain 3Z:

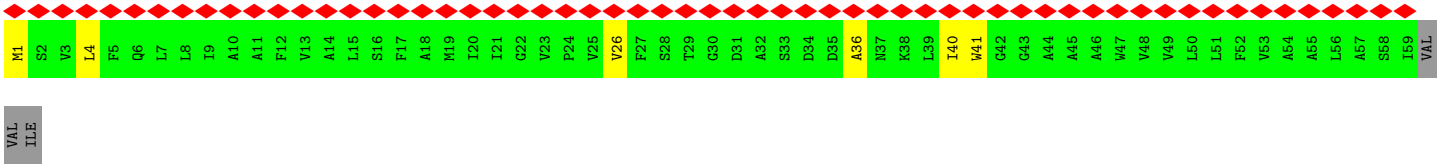




• Molecule 15: Photosystem II reaction center protein Z

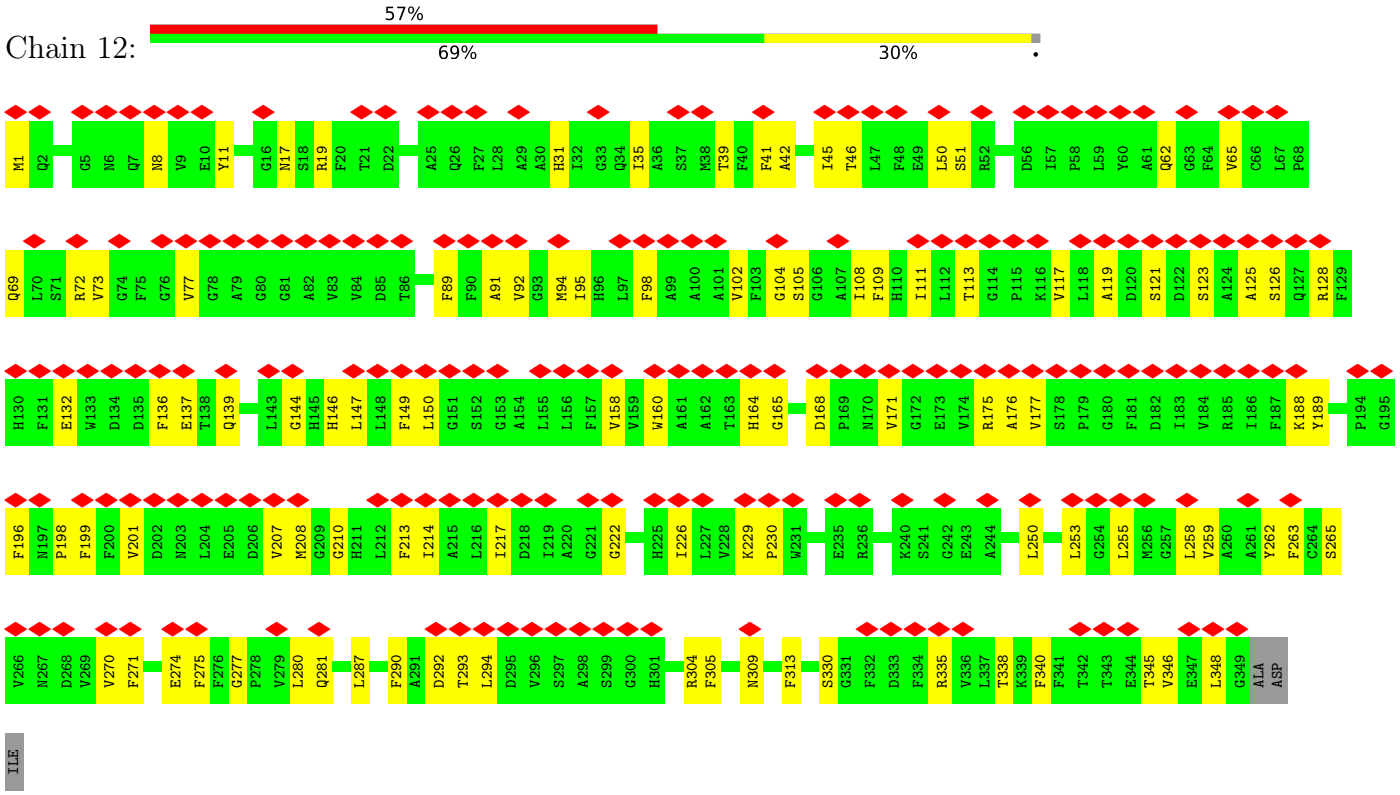
Chain 4Z:





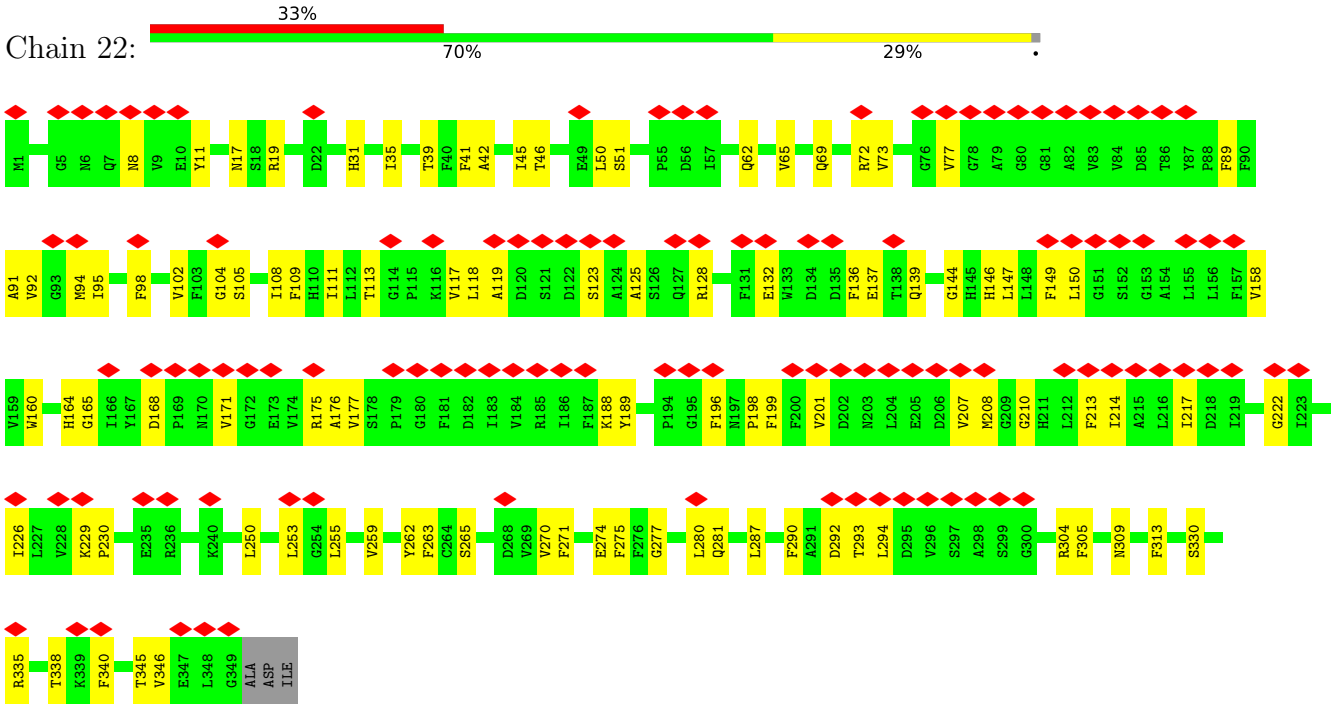
• Molecule 16: High light inducible protein

Chain 12:



• Molecule 16: High light inducible protein

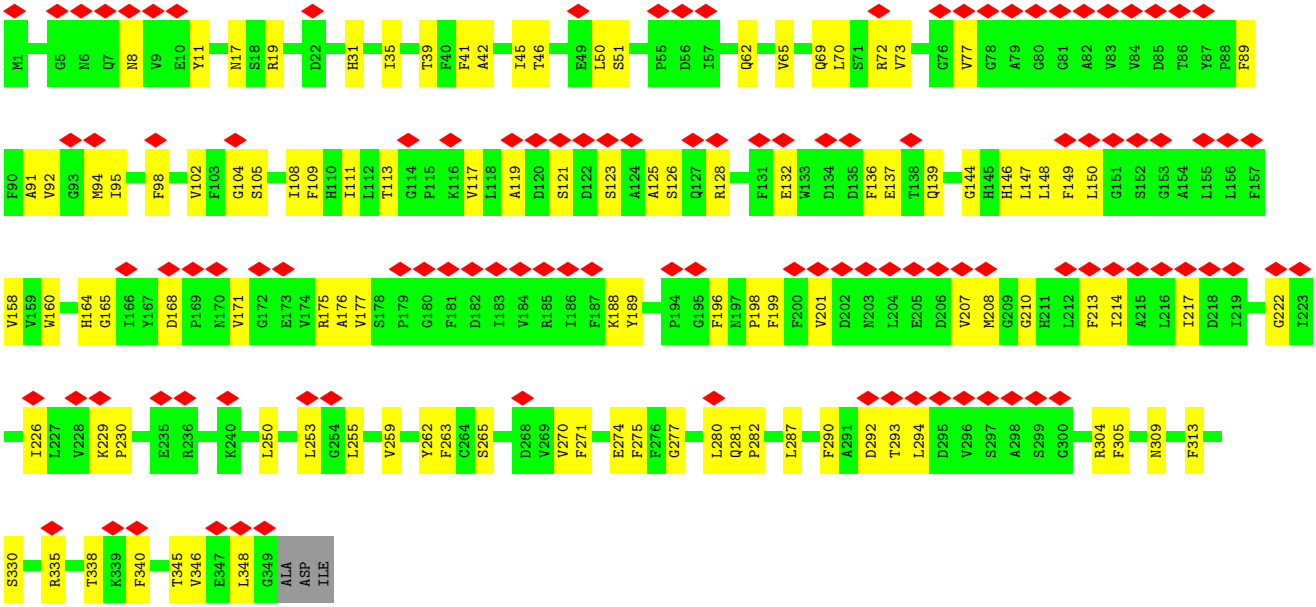
Chain 22:



• Molecule 16: High light inducible protein

Chain 32:

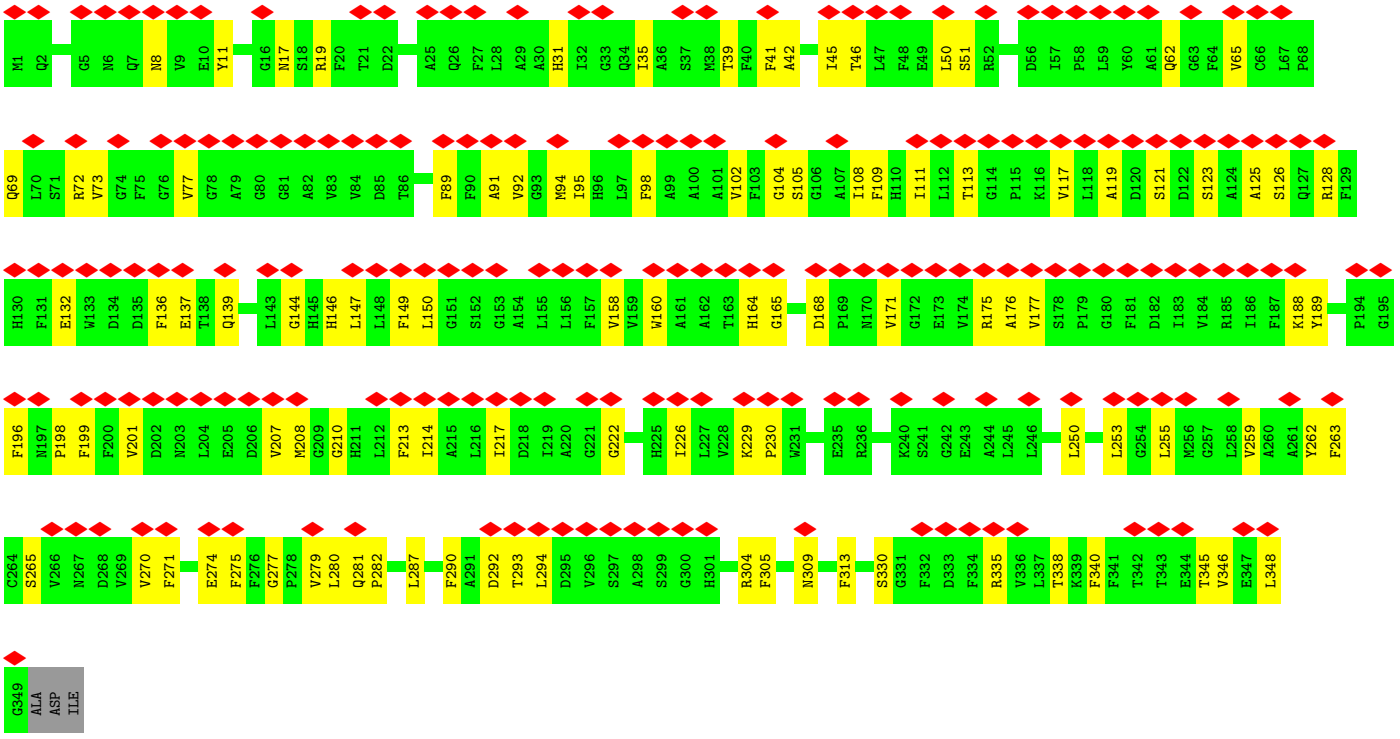




• Molecule 16: High light inducible protein

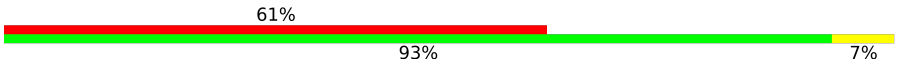
Chain 42:

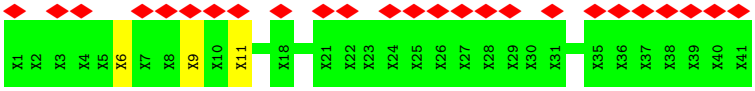




• Molecule 17: Unknown protein

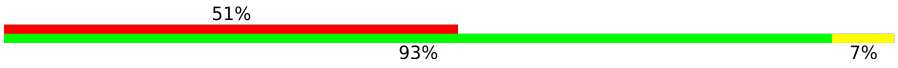
Chain 1G:

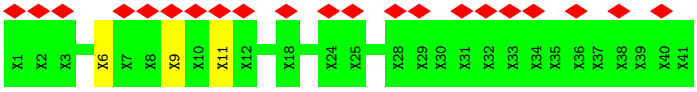




• Molecule 17: Unknown protein

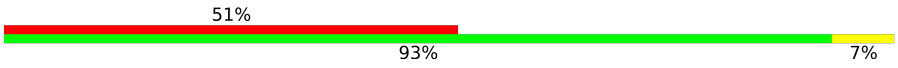
Chain 2G:

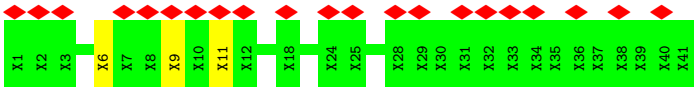




• Molecule 17: Unknown protein

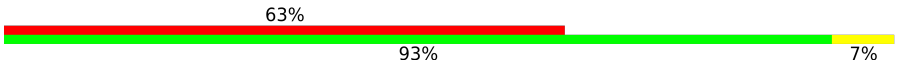
Chain 3G:

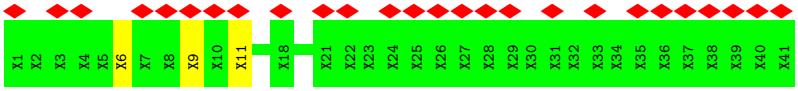




• Molecule 17: Unknown protein

Chain 4G:

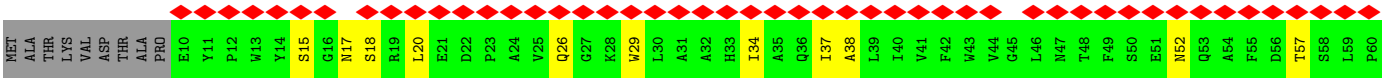


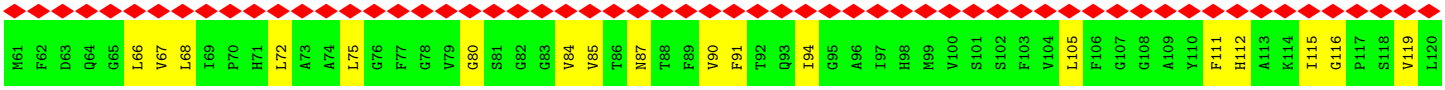


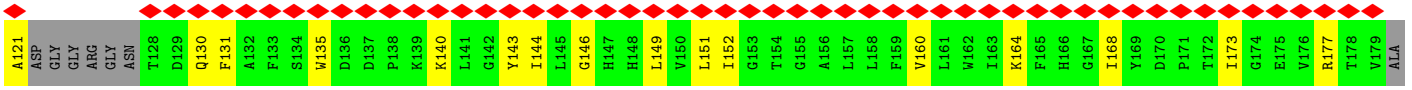
• Molecule 18: High light inducible protein

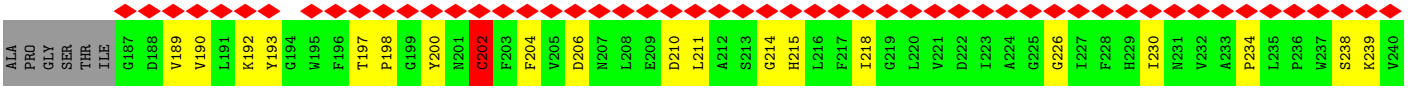
Chain 11:

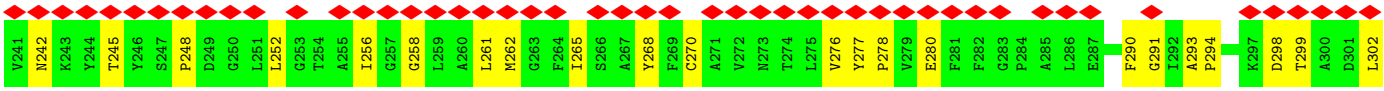


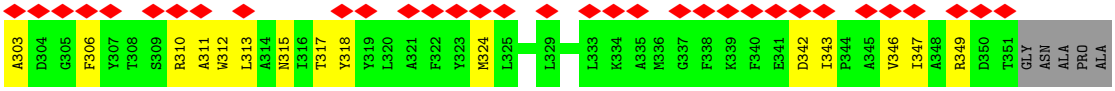








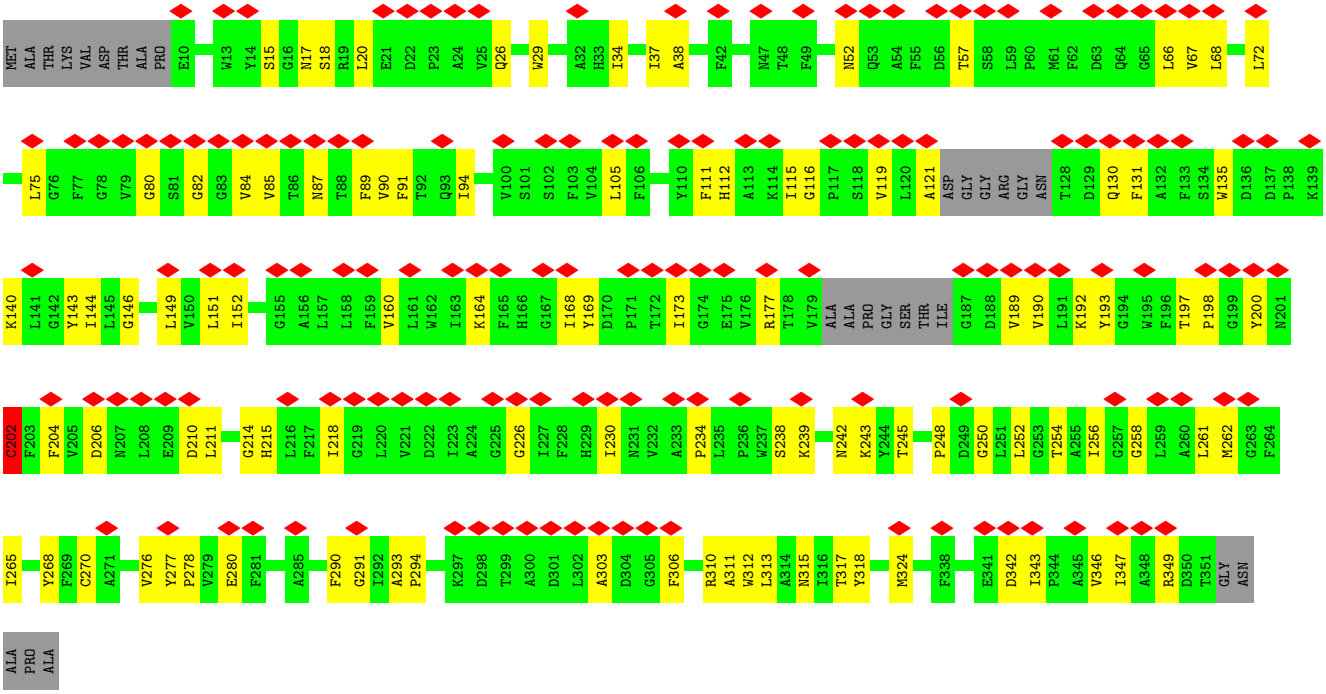




• Molecule 18: High light inducible protein

Chain 21:

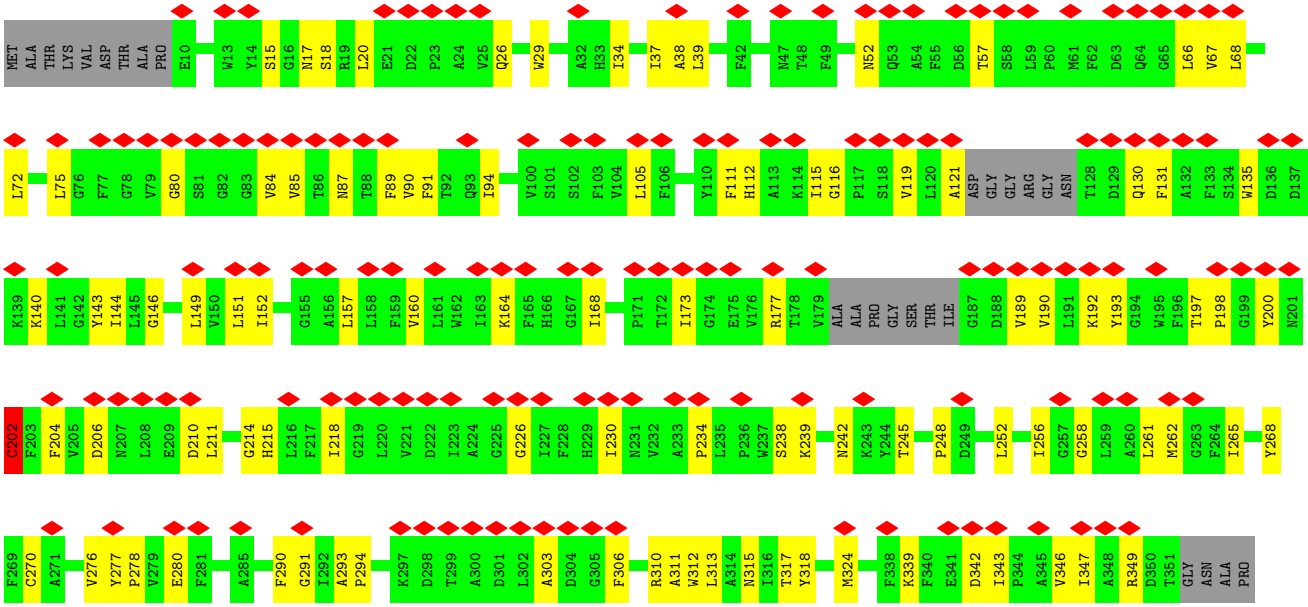




• Molecule 18: High light inducible protein

Chain 31:



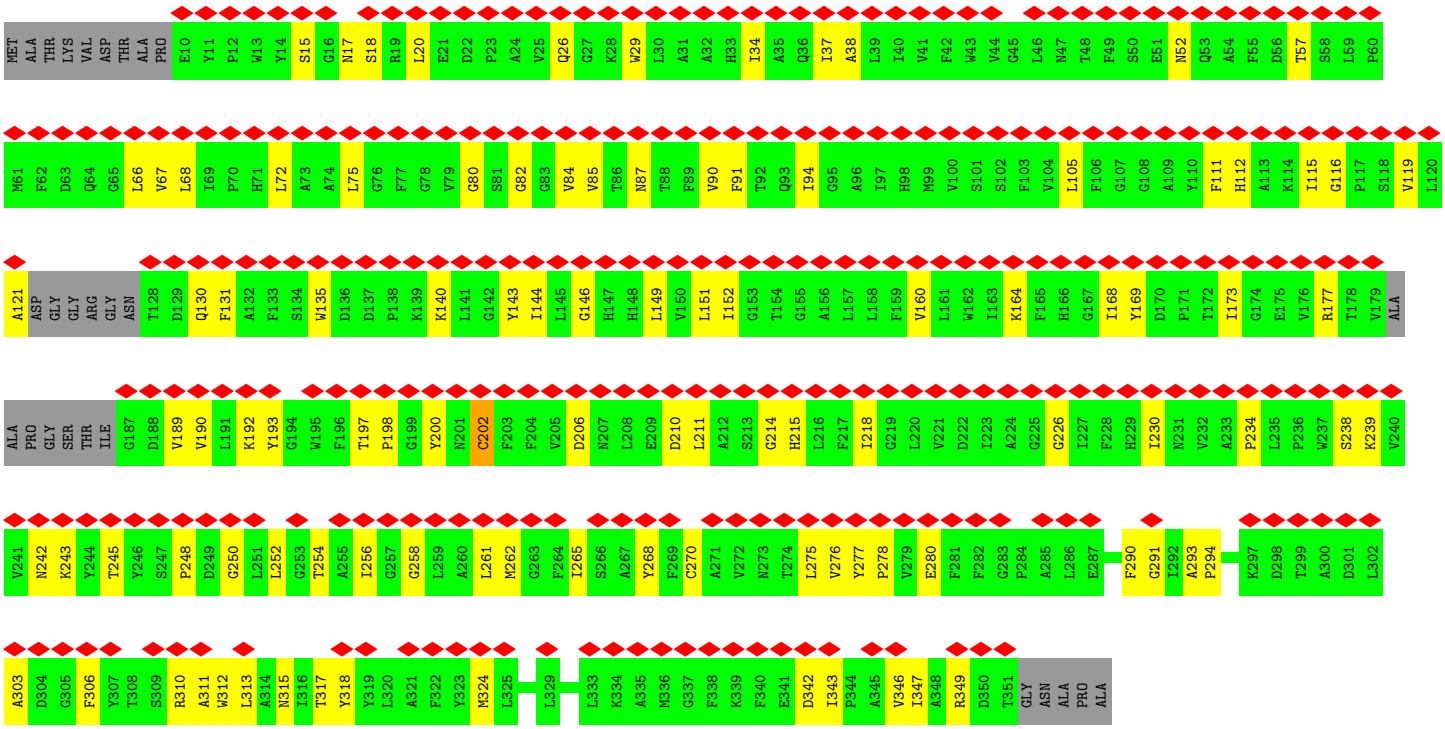


ALA

• Molecule 18: High light inducible protein

Chain 41:

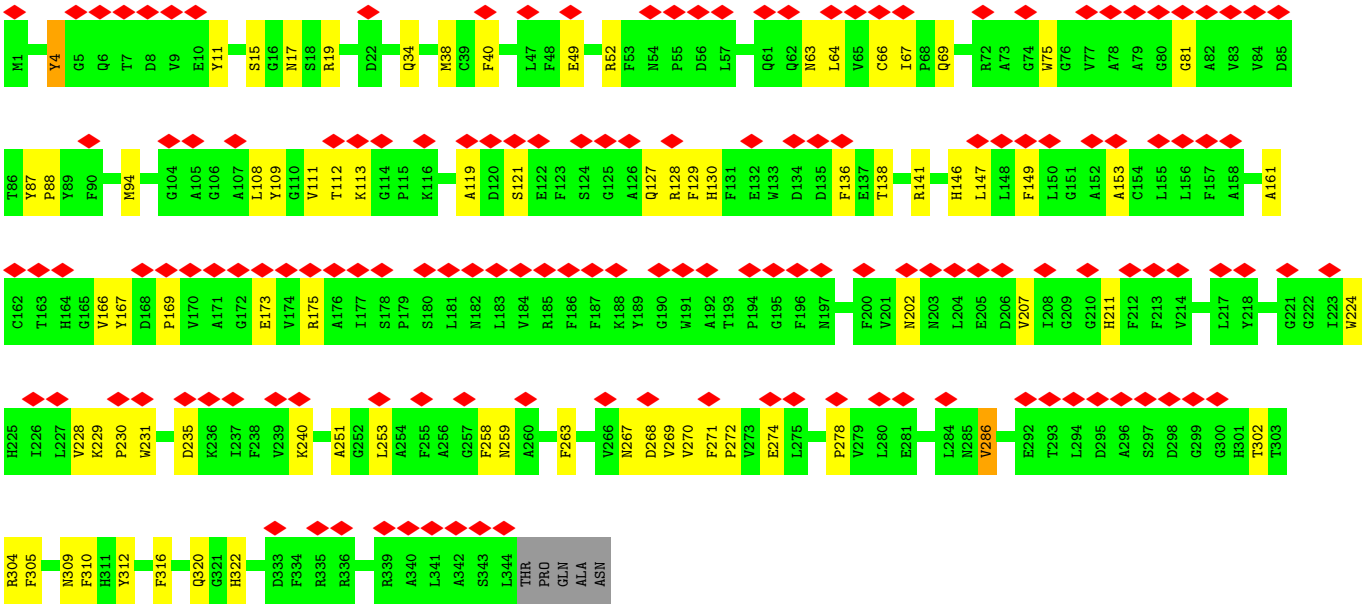




• Molecule 19: High light inducible protein

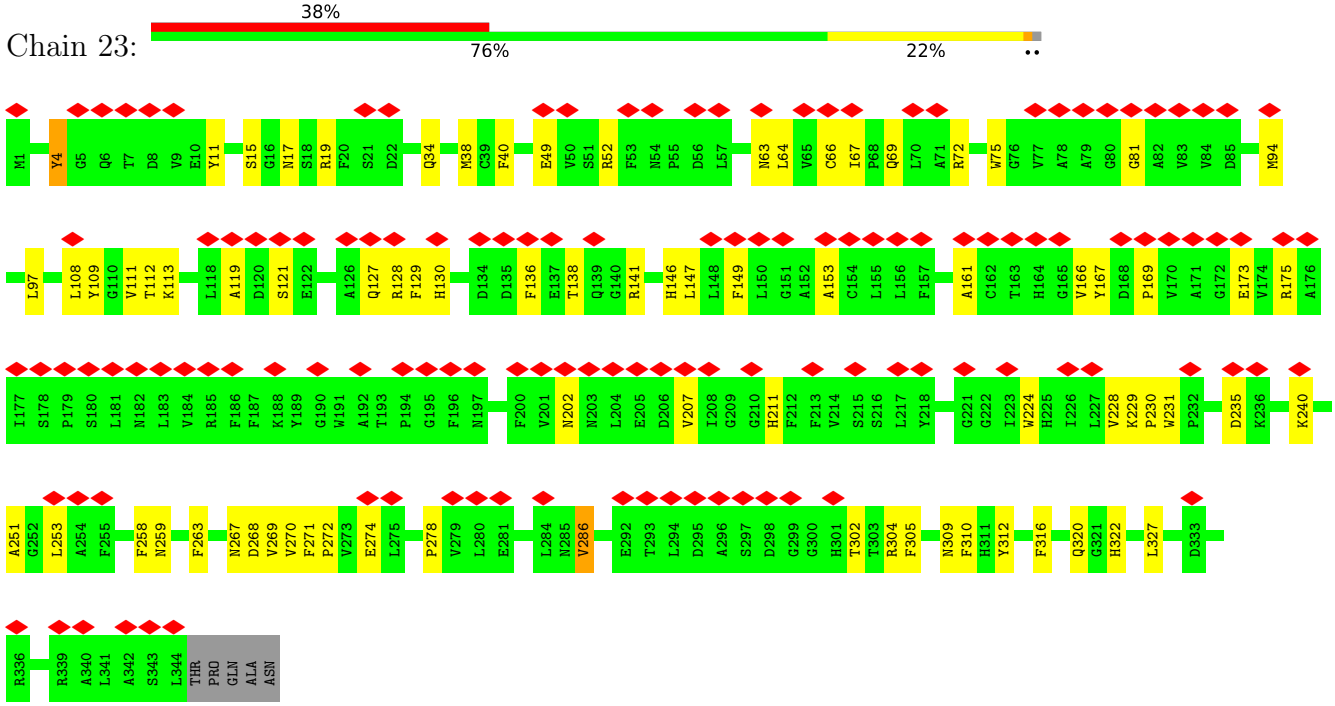
Chain 13:





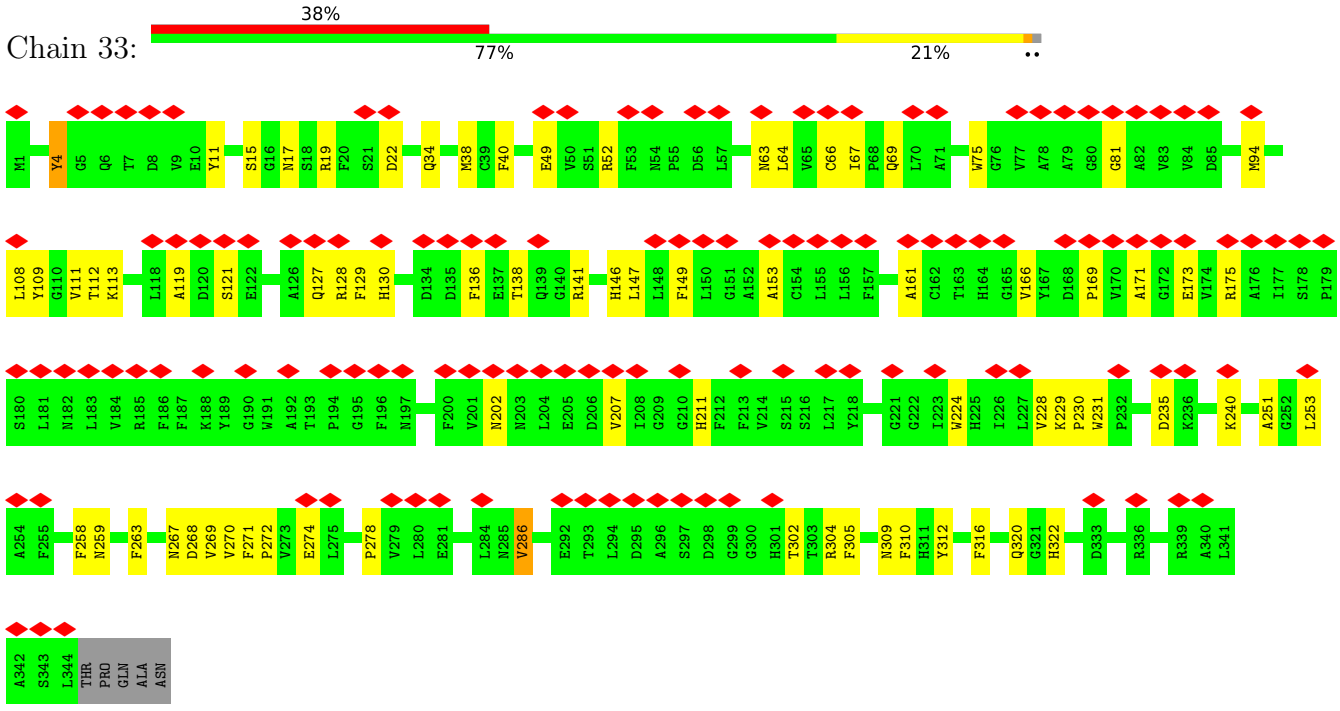
• Molecule 19: High light inducible protein

Chain 23:



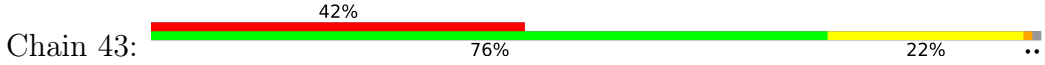
• Molecule 19: High light inducible protein

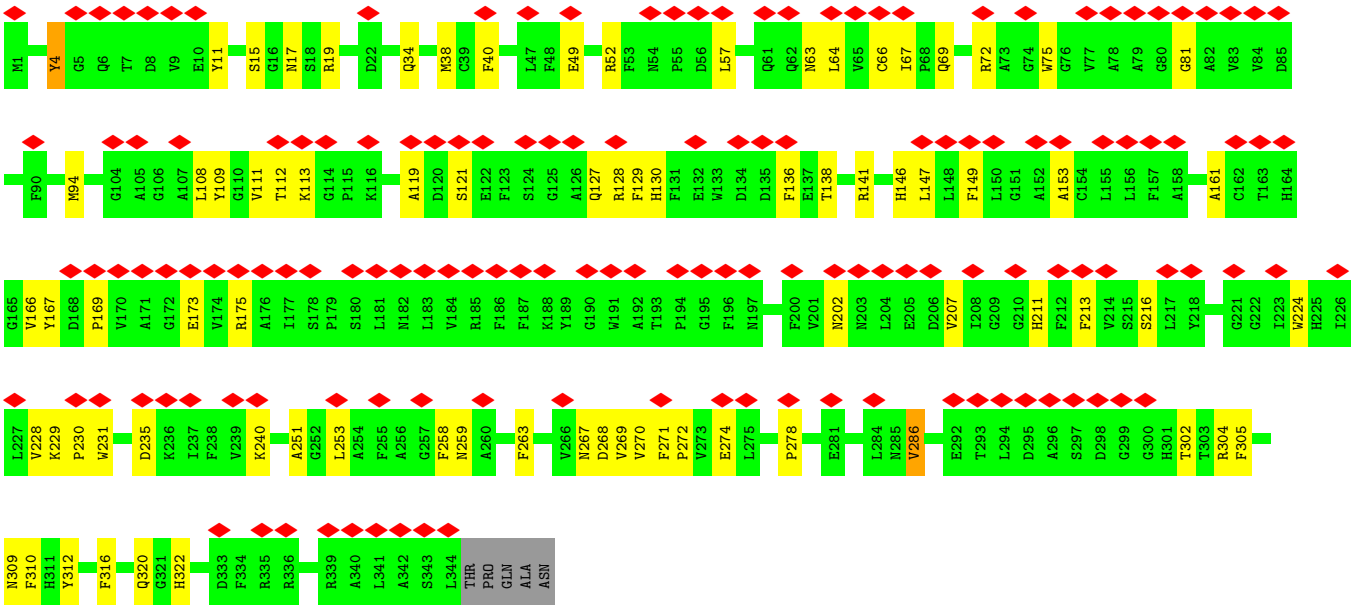
Chain 33:



• Molecule 19: High light inducible protein

Chain 43:

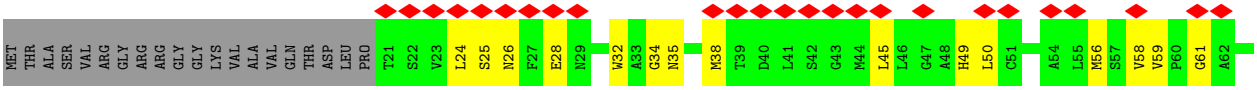


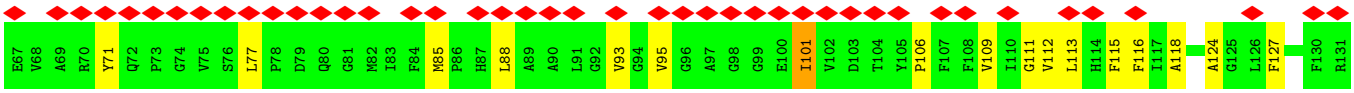


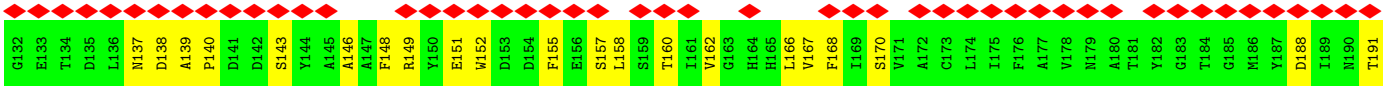
• Molecule 20: High light inducible protein

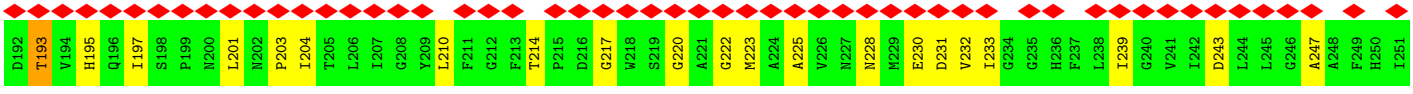
Chain 14:

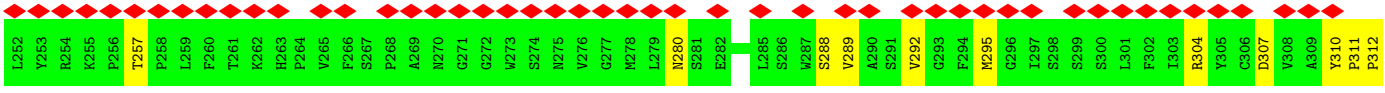


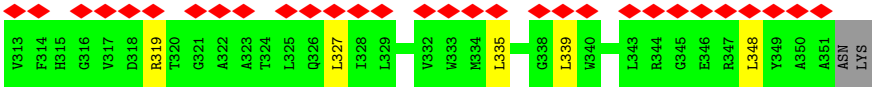








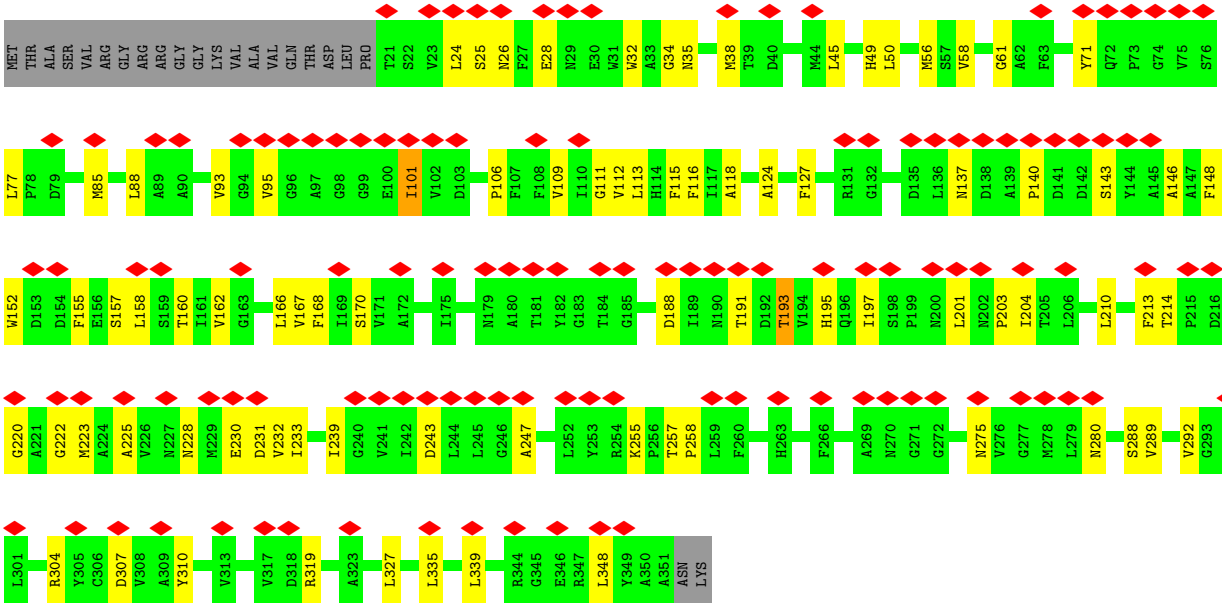




• Molecule 20: High light inducible protein

Chain 24:

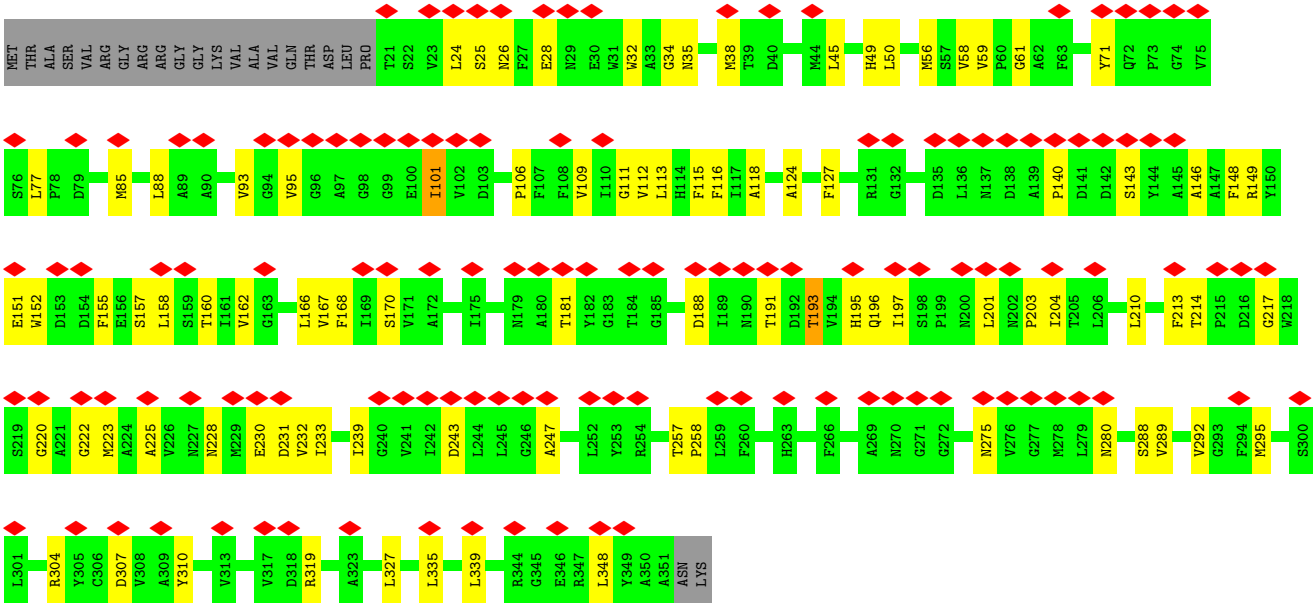




• Molecule 20: High light inducible protein

Chain 34:

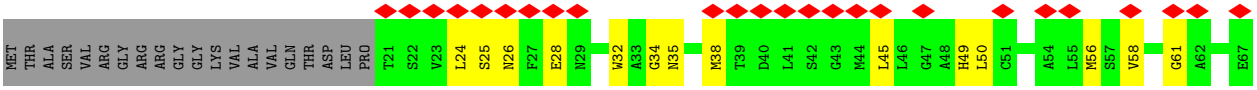


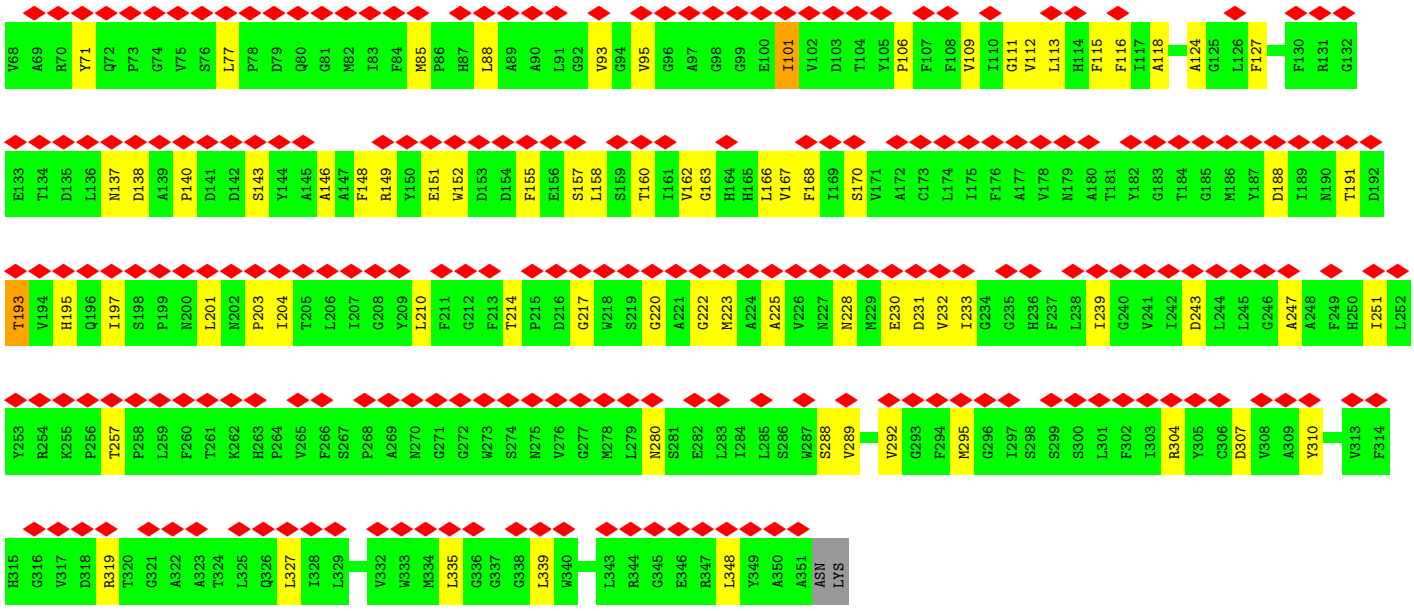


• Molecule 20: High light inducible protein

Chain 44:






V68 A69 R70 Y71 Q72 P73 G74 V75 S76 L77 P78 D79 Q80 G81 M82 I83 F84 M85 P86 H87 L88 A89 A90 L91 G92 V93 G94 V95 G96 A97 G98 G99 E100 I101 V102 D103 T104 Y105 P106 F107 F108 V109 I110 G111 V112 L113 H114 F115 F116 I117 A118 A124 G125 L126 F127 F130 R131 G132
E133 T134 D135 L136 N137 D138 A139 P140 D141 D142 S143 Y144 A145 A146 A147 F148 R149 Y150 E151 W152 D153 D154 F155 E156 S157 L158 S159 T160 I161 V162 G163 H164 H165 L166 V167 F168 I169 S170 V171 A172 C173 L174 I175 F176 A177 V178 N179 A180 T181 Y182 G183 T184 G185 M186 Y187 D188 I189 N190 T191 D192
T193 V194 H195 Q196 I197 S198 P199 N200 L201 N202 P203 I204 T205 L206 I207 G208 Y209 L210 F211 G212 F213 T214 P215 D216 G217 W218 S219 G220 A221 G222 M223 A224 A225 V226 N227 N228 M229 E230 D231 V232 I233 G234 G235 H236 F237 L238 I239 G240 V241 I242 D243 L244 L245 G246 A247 A248 F249 H250 I251 L252
Y253 R254 K255 P256 T257 P258 L259 F260 T261 K262 H263 P264 V265 P266 S267 P268 A269 N270 G271 G272 W273 S274 N275 V276 G277 M278 L279 N280 S281 E282 L283 I284 L285 S286 W287 S288 V289 V292 G293 P294 M295 G296 I297 S298 S299 S300 L301 F302 I303 R304 Y305 C306 D307 V308 A309 Y310 V313 F314
H315 G316 V317 D318 R319 T320 G321 A322 A323 T324 L325 Q326 L327 I328 L329 V332 W333 M334 L335 G336 G337 G338 L339 W340 L343 R344 G345 E346 R347 L348 Y349 A350 A351 ASN LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132346	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)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0171	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CL7, ZEX, LMG, SQD, PL9, 8CT, FE2, DGD, PHO, BCT, LHG

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	1A	0.39	0/2280	0.41	0/3112
1	2A	0.39	0/2280	0.41	0/3112
1	3A	0.39	0/2280	0.41	0/3112
1	4A	0.39	0/2280	0.41	0/3112
2	1B	0.37	0/3929	0.43	1/5360 (0.0%)
2	2B	0.37	0/3929	0.42	0/5360
2	3B	0.37	0/3929	0.42	0/5360
2	4B	0.37	0/3929	0.42	0/5360
3	1C	0.34	0/3431	0.41	0/4669
3	2C	0.34	0/3431	0.41	0/4669
3	3C	0.34	0/3431	0.41	0/4669
3	4C	0.34	0/3431	0.41	0/4669
4	1D	0.38	0/2672	0.40	0/3641
4	2D	0.38	0/2672	0.40	0/3641
4	3D	0.38	0/2672	0.40	0/3641
4	4D	0.38	0/2672	0.40	0/3641
5	1E	0.25	0/555	0.38	0/757
5	2E	0.25	0/555	0.38	0/757
5	3E	0.25	0/555	0.38	0/757
5	4E	0.25	0/555	0.38	0/757
6	1F	0.33	0/250	0.39	0/343
6	2F	0.33	0/250	0.39	0/343
6	3F	0.33	0/250	0.39	0/343
6	4F	0.33	0/250	0.39	0/343
7	1H	0.32	0/534	0.49	1/729 (0.1%)
7	2H	0.32	0/534	0.49	1/729 (0.1%)
7	3H	0.32	0/534	0.49	1/729 (0.1%)
7	4H	0.32	0/534	0.49	1/729 (0.1%)
8	1I	0.39	0/290	0.37	0/391
8	2I	0.39	0/290	0.37	0/391
8	3I	0.39	0/290	0.37	0/391
8	4I	0.39	0/290	0.37	0/391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
9	1K	0.26	0/303	0.39	0/413
9	2K	0.26	0/303	0.39	0/413
9	3K	0.26	0/303	0.39	0/413
9	4K	0.26	0/303	0.39	0/413
10	1L	0.37	0/295	0.38	0/401
10	2L	0.37	0/295	0.38	0/401
10	3L	0.37	0/295	0.38	0/401
10	4L	0.37	0/295	0.38	0/401
11	1M	0.33	0/236	0.44	0/322
11	2M	0.33	0/236	0.44	0/322
11	3M	0.33	0/236	0.44	0/322
11	4M	0.33	0/236	0.44	0/322
12	1T	0.31	0/238	0.35	0/321
12	2T	0.31	0/238	0.35	0/321
12	3T	0.31	0/238	0.35	0/321
12	4T	0.31	0/238	0.35	0/321
13	1X	0.25	0/276	0.29	0/370
13	2X	0.25	0/276	0.29	0/370
13	3X	0.25	0/276	0.29	0/370
13	4X	0.25	0/276	0.29	0/370
14	1Y	0.17	0/164	0.33	0/224
14	2Y	0.17	0/164	0.33	0/224
14	3Y	0.18	0/164	0.33	0/224
14	4Y	0.18	0/164	0.33	0/224
15	1Z	0.20	0/438	0.29	0/599
15	2Z	0.20	0/438	0.29	0/599
15	3Z	0.20	0/438	0.29	0/599
15	4Z	0.19	0/438	0.29	0/599
16	12	0.36	0/2830	0.42	0/3855
16	22	0.36	0/2830	0.42	0/3855
16	32	0.36	0/2830	0.42	0/3855
16	42	0.35	0/2830	0.42	0/3855
18	11	0.28	0/2652	0.41	0/3618
18	21	0.28	0/2652	0.41	0/3618
18	31	0.29	0/2652	0.41	0/3618
18	41	0.28	0/2652	0.41	0/3618
19	13	0.38	0/2814	0.46	1/3841 (0.0%)
19	23	0.38	0/2814	0.46	1/3841 (0.0%)
19	33	0.38	0/2814	0.46	1/3841 (0.0%)
19	43	0.38	0/2814	0.46	1/3841 (0.0%)
20	14	0.33	0/2590	0.43	0/3537
20	24	0.33	0/2590	0.43	0/3537
20	34	0.33	0/2590	0.43	0/3537

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
20	44	0.33	0/2590	0.43	0/3537
All	All	0.35	0/107108	0.42	9/146012 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2H	53	THR	N-CA-C	-7.26	101.88	111.24
7	1H	53	THR	N-CA-C	-7.24	101.90	111.24
7	4H	53	THR	N-CA-C	-7.24	101.90	111.24
7	3H	53	THR	N-CA-C	-7.21	101.93	111.24
19	23	286	VAL	N-CA-C	-6.79	102.78	112.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	2209	0	2142	61	0
1	2A	2209	0	2142	61	0
1	3A	2209	0	2142	59	0
1	4A	2209	0	2142	64	0
2	1B	3794	0	3626	66	0
2	2B	3794	0	3626	67	0
2	3B	3794	0	3626	63	0
2	4B	3794	0	3626	64	0
3	1C	3313	0	3162	58	0
3	2C	3313	0	3162	61	0
3	3C	3313	0	3162	59	0
3	4C	3313	0	3162	60	0
4	1D	2583	0	2493	61	0
4	2D	2583	0	2493	58	0
4	3D	2583	0	2493	61	0
4	4D	2583	0	2493	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1E	538	0	520	14	0
5	2E	538	0	520	18	0
5	3E	538	0	520	20	0
5	4E	538	0	520	14	0
6	1F	242	0	249	1	0
6	2F	242	0	249	2	0
6	3F	242	0	249	2	0
6	4F	242	0	249	2	0
7	1H	519	0	518	10	0
7	2H	519	0	518	10	0
7	3H	519	0	518	10	0
7	4H	519	0	518	10	0
8	1I	281	0	289	8	0
8	2I	281	0	289	8	0
8	3I	281	0	289	7	0
8	4I	281	0	289	8	0
9	1K	292	0	302	8	0
9	2K	292	0	302	10	0
9	3K	292	0	302	10	0
9	4K	292	0	302	7	0
10	1L	288	0	301	7	0
10	2L	288	0	301	8	0
10	3L	288	0	301	6	0
10	4L	288	0	301	8	0
11	1M	232	0	243	4	0
11	2M	232	0	243	4	0
11	3M	232	0	243	4	0
11	4M	232	0	243	4	0
12	1T	231	0	240	2	0
12	2T	231	0	240	3	0
12	3T	231	0	240	2	0
12	4T	231	0	240	1	0
13	1X	269	0	275	4	0
13	2X	269	0	275	4	0
13	3X	269	0	275	4	0
13	4X	269	0	275	5	0
14	1Y	164	0	197	1	0
14	2Y	164	0	197	4	0
14	3Y	164	0	197	3	0
14	4Y	164	0	197	2	0
15	1Z	429	0	450	3	0
15	2Z	429	0	450	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	3Z	429	0	450	7	0
15	4Z	429	0	450	3	0
16	12	2734	0	2611	108	0
16	22	2734	0	2611	101	0
16	32	2734	0	2611	108	0
16	42	2734	0	2611	106	0
17	1G	205	0	46	2	0
17	2G	205	0	46	2	0
17	3G	205	0	46	2	0
17	4G	205	0	46	2	0
18	11	2567	0	2508	97	0
18	21	2567	0	2508	106	0
18	31	2567	0	2508	107	0
18	41	2567	0	2508	100	0
19	13	2715	0	2580	77	0
19	23	2715	0	2580	79	0
19	33	2715	0	2580	79	0
19	43	2715	0	2580	78	0
20	14	2514	0	2436	79	0
20	24	2514	0	2436	91	0
20	34	2514	0	2436	90	0
20	44	2514	0	2436	78	0
21	11	972	0	822	78	0
21	12	1065	0	1050	104	0
21	13	1024	0	962	117	0
21	14	757	0	681	59	0
21	1A	185	0	187	30	0
21	1B	991	0	947	59	0
21	1C	799	0	763	40	0
21	1D	153	0	121	8	0
21	21	972	0	822	90	0
21	22	1065	0	1050	104	0
21	23	1024	0	962	118	0
21	24	757	0	681	57	0
21	2A	185	0	187	27	0
21	2B	991	0	947	60	0
21	2C	799	0	763	40	0
21	2D	153	0	121	9	0
21	31	972	0	821	88	0
21	32	1065	0	1050	103	0
21	33	1024	0	962	117	0
21	34	757	0	681	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	3A	185	0	187	29	0
21	3B	991	0	946	55	0
21	3C	799	0	763	39	0
21	3D	153	0	121	8	0
21	41	972	0	822	85	0
21	42	1065	0	1050	101	0
21	43	1024	0	962	124	0
21	44	757	0	681	58	0
21	4A	185	0	187	28	0
21	4B	991	0	947	56	0
21	4C	799	0	763	39	0
21	4D	153	0	121	9	0
22	1A	64	0	74	3	0
22	1D	64	0	74	4	0
22	2A	64	0	74	3	0
22	2D	64	0	74	3	0
22	3A	64	0	74	3	0
22	3D	64	0	74	4	0
22	4A	64	0	74	3	0
22	4D	64	0	74	3	0
23	14	40	0	0	0	0
23	1A	40	0	0	0	0
23	1B	160	0	0	0	0
23	1C	120	0	0	2	0
23	1D	40	0	0	0	0
23	1K	40	0	0	0	0
23	24	40	0	0	0	0
23	2A	40	0	0	0	0
23	2B	160	0	0	0	0
23	2C	120	0	0	2	0
23	2D	40	0	0	0	0
23	2K	40	0	0	0	0
23	34	40	0	0	0	0
23	3A	40	0	0	0	0
23	3B	160	0	0	0	0
23	3C	120	0	0	2	0
23	3D	40	0	0	0	0
23	3K	40	0	0	0	0
23	44	40	0	0	0	0
23	4A	40	0	0	0	0
23	4B	160	0	0	0	0
23	4C	120	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	4D	40	0	0	0	0
23	4K	40	0	0	0	0
24	11	51	0	72	2	0
24	1A	50	0	70	2	0
24	1B	51	0	72	5	0
24	1D	33	0	36	1	0
24	21	51	0	72	2	0
24	2A	50	0	70	2	0
24	2B	51	0	72	5	0
24	2D	33	0	36	1	0
24	31	51	0	72	3	0
24	3A	50	0	70	2	0
24	3B	51	0	72	6	0
24	3D	33	0	36	1	0
24	41	51	0	72	2	0
24	4A	50	0	70	2	0
24	4B	51	0	72	6	0
24	4D	33	0	36	1	0
25	11	32	0	28	1	0
25	12	91	0	113	2	0
25	13	96	0	123	6	0
25	1A	34	0	32	3	0
25	1B	54	0	78	3	0
25	21	32	0	28	1	0
25	22	91	0	113	2	0
25	23	96	0	123	6	0
25	2A	34	0	32	2	0
25	2B	54	0	78	2	0
25	31	32	0	28	1	0
25	32	91	0	113	1	0
25	33	96	0	123	5	0
25	3A	34	0	32	1	0
25	3B	54	0	78	2	0
25	41	32	0	28	1	0
25	42	91	0	113	2	0
25	43	96	0	123	5	0
25	4A	34	0	32	2	0
25	4B	54	0	78	3	0
26	13	36	0	42	1	0
26	14	49	0	74	2	0
26	1A	46	0	65	0	0
26	1B	94	0	137	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	1D	49	0	74	3	0
26	23	36	0	42	1	0
26	24	49	0	74	2	0
26	2A	46	0	65	0	0
26	2B	94	0	137	8	0
26	2D	49	0	74	4	0
26	33	36	0	42	1	0
26	34	49	0	74	2	0
26	3A	46	0	65	0	0
26	3B	94	0	137	7	0
26	3D	49	0	74	3	0
26	43	36	0	42	1	0
26	44	49	0	74	2	0
26	4A	46	0	65	0	0
26	4B	94	0	137	8	0
26	4D	49	0	74	3	0
27	1B	62	0	82	2	0
27	1C	62	0	82	5	0
27	2B	62	0	82	2	0
27	2C	62	0	82	4	0
27	3B	62	0	82	2	0
27	3C	62	0	82	5	0
27	4B	62	0	82	2	0
27	4C	62	0	82	4	0
28	1D	1	0	0	0	0
28	2D	1	0	0	0	0
28	3D	1	0	0	0	0
28	4D	1	0	0	0	0
29	1D	4	0	0	0	0
29	2D	4	0	0	0	0
29	3D	4	0	0	0	0
29	4D	4	0	0	0	0
30	1D	55	0	80	7	0
30	2D	55	0	80	7	0
30	3D	55	0	80	7	0
30	4D	55	0	80	7	0
31	1F	43	0	30	3	0
31	2F	43	0	30	4	0
31	3F	43	0	30	3	0
31	4F	43	0	30	4	0
32	11	84	0	112	34	0
32	12	168	0	224	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	13	168	0	224	77	0
32	14	168	0	224	49	0
32	21	84	0	112	36	0
32	22	168	0	224	66	0
32	23	168	0	224	77	0
32	24	168	0	224	51	0
32	31	84	0	112	37	0
32	32	168	0	224	67	0
32	33	168	0	224	77	0
32	34	168	0	224	48	0
32	41	84	0	112	38	0
32	42	168	0	224	70	0
32	43	168	0	224	79	0
32	44	168	0	224	51	0
All	All	136856	0	131770	4187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 4187 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:41:315:ASN:HB3	32:41:421:ZEX:C36	1.32	1.58
18:11:315:ASN:CB	32:11:421:ZEX:C36	1.81	1.58
18:41:315:ASN:CB	32:41:421:ZEX:C36	1.81	1.57
18:21:315:ASN:CB	32:21:421:ZEX:C36	1.81	1.57
18:31:315:ASN:CB	32:31:421:ZEX:C36	1.81	1.57

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	2A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	3A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	4A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
2	1B	477/506 (94%)	451 (94%)	26 (6%)	0	100	100
2	2B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
2	3B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
2	4B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
3	1C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	2C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	3C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	4C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
4	1D	319/351 (91%)	309 (97%)	10 (3%)	0	100	100
4	2D	319/351 (91%)	310 (97%)	9 (3%)	0	100	100
4	3D	319/351 (91%)	309 (97%)	10 (3%)	0	100	100
4	4D	319/351 (91%)	310 (97%)	9 (3%)	0	100	100
5	1E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	2E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	3E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	4E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
6	1F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	2F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	3F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	4F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
7	1H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	2H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	3H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	4H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
8	1I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	2I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	3I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	4I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	1K	35/45 (78%)	35 (100%)	0	0	100	100
9	2K	35/45 (78%)	35 (100%)	0	0	100	100
9	3K	35/45 (78%)	35 (100%)	0	0	100	100
9	4K	35/45 (78%)	35 (100%)	0	0	100	100
10	1L	34/38 (90%)	34 (100%)	0	0	100	100
10	2L	34/38 (90%)	34 (100%)	0	0	100	100
10	3L	34/38 (90%)	34 (100%)	0	0	100	100
10	4L	34/38 (90%)	34 (100%)	0	0	100	100
11	1M	29/34 (85%)	29 (100%)	0	0	100	100
11	2M	29/34 (85%)	29 (100%)	0	0	100	100
11	3M	29/34 (85%)	29 (100%)	0	0	100	100
11	4M	29/34 (85%)	29 (100%)	0	0	100	100
12	1T	26/46 (56%)	26 (100%)	0	0	100	100
12	2T	26/46 (56%)	26 (100%)	0	0	100	100
12	3T	26/46 (56%)	26 (100%)	0	0	100	100
12	4T	26/46 (56%)	26 (100%)	0	0	100	100
13	1X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	2X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	3X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	4X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
14	1Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	2Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	3Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	4Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
15	1Z	57/62 (92%)	57 (100%)	0	0	100	100
15	2Z	57/62 (92%)	57 (100%)	0	0	100	100
15	3Z	57/62 (92%)	57 (100%)	0	0	100	100
15	4Z	57/62 (92%)	57 (100%)	0	0	100	100
16	12	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
16	22	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
16	32	347/352 (99%)	325 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	42	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
18	11	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36	65
18	21	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36	65
18	31	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36	65
18	41	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36	65
19	13	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36	65
19	23	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36	65
19	33	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36	65
19	43	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36	65
20	14	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
20	24	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
20	34	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
20	44	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
All	All	13020/14832 (88%)	12413 (95%)	599 (5%)	8 (0%)	49	79

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	13	4	TYR
19	23	4	TYR
19	33	4	TYR
19	43	4	TYR
18	11	202	CYS

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	1A	232/292 (80%)	232 (100%)	0	100	100
1	2A	232/292 (80%)	232 (100%)	0	100	100
1	3A	232/292 (80%)	232 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4A	232/292 (80%)	232 (100%)	0	100	100
2	1B	395/418 (94%)	392 (99%)	3 (1%)	73	77
2	2B	395/418 (94%)	392 (99%)	3 (1%)	73	77
2	3B	395/418 (94%)	392 (99%)	3 (1%)	73	77
2	4B	395/418 (94%)	392 (99%)	3 (1%)	73	77
3	1C	322/378 (85%)	319 (99%)	3 (1%)	70	76
3	2C	322/378 (85%)	319 (99%)	3 (1%)	70	76
3	3C	322/378 (85%)	319 (99%)	3 (1%)	70	76
3	4C	322/378 (85%)	319 (99%)	3 (1%)	70	76
4	1D	265/284 (93%)	264 (100%)	1 (0%)	84	81
4	2D	265/284 (93%)	264 (100%)	1 (0%)	84	81
4	3D	265/284 (93%)	264 (100%)	1 (0%)	84	81
4	4D	265/284 (93%)	264 (100%)	1 (0%)	84	81
5	1E	57/71 (80%)	57 (100%)	0	100	100
5	2E	57/71 (80%)	57 (100%)	0	100	100
5	3E	57/71 (80%)	57 (100%)	0	100	100
5	4E	57/71 (80%)	57 (100%)	0	100	100
6	1F	25/84 (30%)	25 (100%)	0	100	100
6	2F	25/84 (30%)	25 (100%)	0	100	100
6	3F	25/84 (30%)	25 (100%)	0	100	100
6	4F	25/84 (30%)	25 (100%)	0	100	100
7	1H	55/57 (96%)	55 (100%)	0	100	100
7	2H	55/57 (96%)	55 (100%)	0	100	100
7	3H	55/57 (96%)	55 (100%)	0	100	100
7	4H	55/57 (96%)	55 (100%)	0	100	100
8	1I	30/30 (100%)	30 (100%)	0	100	100
8	2I	30/30 (100%)	30 (100%)	0	100	100
8	3I	30/30 (100%)	30 (100%)	0	100	100
8	4I	30/30 (100%)	30 (100%)	0	100	100
9	1K	31/37 (84%)	30 (97%)	1 (3%)	34	58
9	2K	31/37 (84%)	30 (97%)	1 (3%)	34	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	3K	31/37 (84%)	30 (97%)	1 (3%)	34 58
9	4K	31/37 (84%)	30 (97%)	1 (3%)	34 58
10	1L	33/34 (97%)	33 (100%)	0	100 100
10	2L	33/34 (97%)	33 (100%)	0	100 100
10	3L	33/34 (97%)	33 (100%)	0	100 100
10	4L	33/34 (97%)	33 (100%)	0	100 100
11	1M	24/27 (89%)	24 (100%)	0	100 100
11	2M	24/27 (89%)	24 (100%)	0	100 100
11	3M	24/27 (89%)	24 (100%)	0	100 100
11	4M	24/27 (89%)	24 (100%)	0	100 100
12	1T	24/42 (57%)	24 (100%)	0	100 100
12	2T	24/42 (57%)	24 (100%)	0	100 100
12	3T	24/42 (57%)	24 (100%)	0	100 100
12	4T	24/42 (57%)	24 (100%)	0	100 100
13	1X	28/33 (85%)	28 (100%)	0	100 100
13	2X	28/33 (85%)	28 (100%)	0	100 100
13	3X	28/33 (85%)	28 (100%)	0	100 100
13	4X	28/33 (85%)	28 (100%)	0	100 100
14	1Y	18/31 (58%)	18 (100%)	0	100 100
14	2Y	18/31 (58%)	18 (100%)	0	100 100
14	3Y	18/31 (58%)	18 (100%)	0	100 100
14	4Y	18/31 (58%)	18 (100%)	0	100 100
15	1Z	43/46 (94%)	43 (100%)	0	100 100
15	2Z	43/46 (94%)	43 (100%)	0	100 100
15	3Z	43/46 (94%)	43 (100%)	0	100 100
15	4Z	43/46 (94%)	43 (100%)	0	100 100
16	12	276/278 (99%)	272 (99%)	4 (1%)	59 71
16	22	276/278 (99%)	272 (99%)	4 (1%)	59 71
16	32	276/278 (99%)	272 (99%)	4 (1%)	59 71
16	42	276/278 (99%)	272 (99%)	4 (1%)	59 71
18	11	262/278 (94%)	259 (99%)	3 (1%)	65 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	21	262/278 (94%)	259 (99%)	3 (1%)	65	74
18	31	262/278 (94%)	259 (99%)	3 (1%)	65	74
18	41	262/278 (94%)	259 (99%)	3 (1%)	65	74
19	13	269/273 (98%)	266 (99%)	3 (1%)	65	74
19	23	269/273 (98%)	266 (99%)	3 (1%)	65	74
19	33	269/273 (98%)	266 (99%)	3 (1%)	65	74
19	43	269/273 (98%)	266 (99%)	3 (1%)	65	74
20	14	260/277 (94%)	256 (98%)	4 (2%)	57	70
20	24	260/277 (94%)	256 (98%)	4 (2%)	57	70
20	34	260/277 (94%)	256 (98%)	4 (2%)	57	70
20	44	260/277 (94%)	256 (98%)	4 (2%)	57	70
All	All	10596/11880 (89%)	10508 (99%)	88 (1%)	70	77

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	31	143	TYR
3	4C	432	VAL
19	33	4	TYR
20	34	204	ILE
16	42	263	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
2	3B	394	GLN
20	34	275	ASN
4	3D	196	HIS
18	31	331	HIS
1	4A	303	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 624 ligands modelled in this entry, 4 are monoatomic - leaving 620 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	$\#\|Z\| > 2$
21	CL7	33	502	19	64,66,73	1.77	15 (23%)	71,104,113	2.40	22 (30%)
21	CL7	31	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.78	18 (32%)
21	CL7	2C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
21	CL7	3C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.83	18 (35%)
25	SQD	32	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	22	507	-	71,73,73	1.71	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	23	404	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
21	CL7	23	415	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	3C	503	3	71,73,73	1.68	16 (22%)	80,113,113	2.40	21 (26%)
21	CL7	4B	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	19 (23%)
21	CL7	3B	616	2	51,53,73	1.97	19 (37%)	56,89,113	2.70	18 (32%)
21	CL7	1B	608	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	20 (25%)
21	CL7	33	513	-	51,53,73	1.97	16 (31%)	56,89,113	2.72	18 (32%)
32	ZEX	22	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	44	409	-	66,68,73	1.76	18 (27%)	74,107,113	2.67	24 (32%)
23	8CT	3C	514	-	40,41,41	4.65	21 (52%)	50,56,56	2.40	23 (46%)
25	SQD	42	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	21	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.49	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	31	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.40	21 (26%)
21	CL7	23	409	19	71,73,73	1.70	18 (25%)	80,113,113	2.31	21 (26%)
21	CL7	11	409	18	51,53,73	1.96	16 (31%)	56,89,113	2.72	20 (35%)
21	CL7	2B	610	2	71,73,73	1.69	17 (23%)	80,113,113	2.33	20 (25%)
21	CL7	14	406	20	71,73,73	1.70	16 (22%)	80,113,113	2.35	21 (26%)
21	CL7	3C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.37	23 (28%)
21	CL7	31	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.46	24 (30%)
21	CL7	4D	405	4	51,53,73	1.96	18 (35%)	56,89,113	2.77	22 (39%)
21	CL7	13	507	-	71,73,73	1.68	15 (21%)	80,113,113	2.40	23 (28%)
21	CL7	43	410	19	71,73,73	1.69	16 (22%)	80,113,113	2.34	22 (27%)
32	ZEX	14	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.43	25 (45%)
26	LHG	2B	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	2B	604	2	71,73,73	1.69	18 (25%)	80,113,113	2.37	21 (26%)
21	CL7	31	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.97	20 (39%)
21	CL7	34	414	20	59,61,73	1.84	18 (30%)	65,98,113	2.65	21 (32%)
21	CL7	21	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.50	23 (28%)
23	8CT	2C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	32	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.38	22 (27%)
27	DGD	1C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
30	PL9	4D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	34	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
21	CL7	14	405	-	71,73,73	1.70	16 (22%)	80,113,113	2.45	25 (31%)
21	CL7	2B	608	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	20 (27%)
21	CL7	32	517	16	71,73,73	1.68	15 (21%)	80,113,113	2.36	21 (26%)
21	CL7	2B	617	2	51,53,73	1.97	18 (35%)	56,89,113	2.70	18 (32%)
24	LMG	1B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	41	412	18	51,53,73	1.95	16 (31%)	56,89,113	2.77	20 (35%)
32	ZEX	13	525	-	42,43,43	1.18	5 (11%)	55,60,60	2.44	18 (32%)
21	CL7	43	409	19	71,73,73	1.70	18 (25%)	80,113,113	2.31	22 (27%)
32	ZEX	12	520	-	42,43,43	0.97	3 (7%)	55,60,60	2.19	17 (30%)
32	ZEX	34	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	18 (32%)
32	ZEX	44	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
32	ZEX	34	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
24	LMG	1A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	1D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	22	501	16	71,73,73	1.68	17 (23%)	80,113,113	2.42	21 (26%)
21	CL7	1B	616	2	51,53,73	1.97	18 (35%)	56,89,113	2.69	18 (32%)
21	CL7	12	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.64	19 (33%)
32	ZEX	12	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
26	LHG	14	401	-	48,48,48	0.29	0	51,54,54	0.34	0
21	CL7	2B	602	-	47,49,73	1.94	12 (25%)	51,84,113	2.87	18 (35%)
21	CL7	24	411	20	71,73,73	1.68	15 (21%)	80,113,113	2.41	23 (28%)
21	CL7	2C	506	3	66,68,73	1.76	17 (25%)	74,107,113	2.50	23 (31%)
24	LMG	4B	622	-	51,51,55	0.24	0	59,59,63	0.33	0
26	LHG	4B	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	4C	502	3	66,68,73	1.76	16 (24%)	74,107,113	2.45	19 (25%)
21	CL7	4C	517	3	47,49,73	1.93	13 (27%)	51,84,113	2.88	19 (37%)
21	CL7	43	407	19	51,53,73	1.97	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	1C	504	-	61,63,73	1.85	17 (27%)	68,101,113	2.55	19 (27%)
24	LMG	3D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
26	LHG	3A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	23	418	19	56,58,73	1.89	16 (28%)	62,95,113	2.65	20 (32%)
21	CL7	44	417	20	48,50,73	1.93	14 (29%)	51,85,113	2.94	18 (35%)
25	SQD	3B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
22	PHO	4D	408	-	58,69,69	0.80	3 (5%)	56,99,99	1.27	5 (8%)
21	CL7	12	512	16	71,73,73	1.69	14 (19%)	80,113,113	2.43	21 (26%)
21	CL7	1B	615	2	56,58,73	1.89	17 (30%)	62,95,113	2.68	21 (33%)
21	CL7	14	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
21	CL7	34	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.69	21 (37%)
21	CL7	41	410	-	71,73,73	1.70	17 (23%)	80,113,113	2.34	23 (28%)
32	ZEX	12	522	-	42,43,43	1.04	4 (9%)	55,60,60	2.47	17 (30%)
21	CL7	42	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.39	22 (27%)
21	CL7	24	408	20	51,53,73	1.97	16 (31%)	56,89,113	2.69	21 (37%)
21	CL7	42	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.31	20 (25%)
23	8CT	3C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
26	LHG	23	425	-	35,35,48	0.35	0	38,41,54	0.47	0
21	CL7	2B	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.33	23 (28%)
21	CL7	42	518	16	71,73,73	1.68	13 (18%)	80,113,113	2.32	23 (28%)
21	CL7	34	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.43	21 (28%)
21	CL7	42	516	16	71,73,73	1.70	16 (22%)	80,113,113	2.39	23 (28%)
24	LMG	3A	405	-	50,50,55	0.24	0	58,58,63	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	3A	401	1	71,73,73	1.74	14 (19%)	80,113,113	2.47	25 (31%)
21	CL7	33	518	19	51,53,73	1.98	13 (25%)	56,89,113	2.74	20 (35%)
21	CL7	44	415	-	51,53,73	1.96	20 (39%)	56,89,113	2.88	21 (37%)
25	SQD	43	422	-	45,46,54	0.42	0	54,57,65	0.48	0
23	8CT	2K	101	-	40,41,41	4.75	25 (62%)	50,56,56	2.65	15 (30%)
21	CL7	12	518	16	71,73,73	1.69	13 (18%)	80,113,113	2.33	23 (28%)
21	CL7	3C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.47	23 (28%)
21	CL7	13	512	19	61,63,73	1.84	19 (31%)	68,101,113	2.58	23 (33%)
23	8CT	44	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
32	ZEX	22	520	-	42,43,43	0.99	3 (7%)	55,60,60	2.18	17 (30%)
32	ZEX	32	520	-	42,43,43	0.97	3 (7%)	55,60,60	2.18	17 (30%)
32	ZEX	21	421	-	42,43,43	0.92	2 (4%)	55,60,60	2.23	20 (36%)
21	CL7	3C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
21	CL7	31	413	-	47,49,73	1.94	12 (25%)	51,84,113	2.97	22 (43%)
21	CL7	31	405	-	51,53,73	1.97	18 (35%)	56,89,113	2.70	19 (33%)
21	CL7	44	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.70	20 (35%)
32	ZEX	23	423	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	18 (32%)
21	CL7	2C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.84	18 (35%)
21	CL7	2C	504	-	61,63,73	1.85	17 (27%)	68,101,113	2.54	19 (27%)
21	CL7	3B	604	2	71,73,73	1.68	18 (25%)	80,113,113	2.32	23 (28%)
21	CL7	43	417	19	61,63,73	1.81	18 (29%)	68,101,113	2.56	25 (36%)
21	CL7	32	516	16	71,73,73	1.70	17 (23%)	80,113,113	2.39	23 (28%)
21	CL7	2B	615	2	66,68,73	1.79	18 (27%)	74,107,113	2.49	25 (33%)
21	CL7	13	501	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	24 (30%)
21	CL7	32	512	16	71,73,73	1.69	14 (19%)	80,113,113	2.42	21 (26%)
26	LHG	44	401	-	48,48,48	0.28	0	51,54,54	0.34	0
32	ZEX	43	401	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
32	ZEX	32	522	-	42,43,43	1.05	4 (9%)	55,60,60	2.47	17 (30%)
25	SQD	41	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	4C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.46	23 (28%)
23	8CT	2B	619	-	40,41,41	4.70	20 (50%)	50,56,56	2.67	20 (40%)
32	ZEX	23	420	-	42,43,43	1.02	4 (9%)	55,60,60	2.58	17 (30%)
21	CL7	2B	616	2	56,58,73	1.89	18 (32%)	62,95,113	2.69	21 (33%)
21	CL7	42	511	16	66,68,73	1.78	18 (27%)	74,107,113	2.40	21 (28%)
21	CL7	2D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	23	413	19	61,63,73	1.83	18 (29%)	68,101,113	2.58	22 (32%)
21	CL7	33	504	-	71,73,73	1.69	17 (23%)	80,113,113	2.41	21 (26%)
21	CL7	2C	513	3	51,53,73	1.95	14 (27%)	56,89,113	2.91	19 (33%)
22	PHO	3D	408	-	58,69,69	0.80	4 (6%)	56,99,99	1.27	5 (8%)
21	CL7	32	513	16	51,53,73	1.96	15 (29%)	56,89,113	2.84	21 (37%)
21	CL7	43	415	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
24	LMG	3B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	1C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
21	CL7	33	503	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
23	8CT	1C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
32	ZEX	41	422	-	42,43,43	0.95	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	1C	510	3	71,73,73	1.69	14 (19%)	80,113,113	2.38	21 (26%)
21	CL7	43	406	19	71,73,73	1.70	17 (23%)	80,113,113	2.39	21 (26%)
21	CL7	3C	513	3	51,53,73	1.94	14 (27%)	56,89,113	2.90	19 (33%)
21	CL7	3B	606	2	61,63,73	1.81	16 (26%)	68,101,113	2.63	21 (30%)
32	ZEX	32	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	21	410	-	71,73,73	1.69	16 (22%)	80,113,113	2.33	22 (27%)
25	SQD	4A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	23	416	-	47,49,73	1.93	12 (25%)	51,84,113	2.93	21 (41%)
21	CL7	3A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.60	23 (33%)
21	CL7	11	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.77	18 (32%)
21	CL7	31	409	18	51,53,73	1.95	16 (31%)	56,89,113	2.72	20 (35%)
21	CL7	3C	509	3	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
32	ZEX	12	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	2C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.46	22 (27%)
21	CL7	3D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)
23	8CT	4C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	13	517	19	56,58,73	1.89	16 (28%)	62,95,113	2.65	20 (32%)
23	8CT	1D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
24	LMG	21	401	-	51,51,55	0.22	0	59,59,63	0.42	1 (1%)
21	CL7	41	413	-	47,49,73	1.94	12 (25%)	51,84,113	2.98	22 (43%)
32	ZEX	43	420	-	42,43,43	1.01	4 (9%)	55,60,60	2.58	17 (30%)
21	CL7	43	413	19	61,63,73	1.84	19 (31%)	68,101,113	2.58	23 (33%)
26	LHG	3D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	1B	611	2	71,73,73	1.69	17 (23%)	80,113,113	2.34	20 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	11	416	-	47,49,73	1.95	13 (27%)	51,84,113	2.88	19 (37%)
21	CL7	1B	605	2	71,73,73	1.67	17 (23%)	80,113,113	2.40	20 (25%)
32	ZEX	23	421	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	32	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	19 (33%)
21	CL7	23	402	19	71,73,73	1.69	17 (23%)	80,113,113	2.39	23 (28%)
23	8CT	3B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.91	18 (36%)
21	CL7	14	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.68	25 (33%)
21	CL7	2C	502	3	66,68,73	1.77	17 (25%)	74,107,113	2.45	19 (25%)
26	LHG	1B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	32	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.36	22 (27%)
21	CL7	42	507	-	71,73,73	1.72	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	2A	401	1	71,73,73	1.73	13 (18%)	80,113,113	2.46	25 (31%)
23	8CT	1C	514	-	40,41,41	4.63	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	41	416	-	47,49,73	1.95	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	3B	602	2	66,68,73	1.78	17 (25%)	74,107,113	2.50	22 (29%)
21	CL7	41	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.98	19 (37%)
32	ZEX	42	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
32	ZEX	24	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
21	CL7	13	506	19	51,53,73	1.97	18 (35%)	56,89,113	2.75	19 (33%)
21	CL7	33	516	19	61,63,73	1.81	17 (27%)	68,101,113	2.55	25 (36%)
21	CL7	4B	608	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	21 (28%)
21	CL7	13	509	19	71,73,73	1.68	16 (22%)	80,113,113	2.33	22 (27%)
21	CL7	3C	502	3	66,68,73	1.77	17 (25%)	74,107,113	2.45	19 (25%)
21	CL7	44	412	20	71,73,73	1.69	16 (22%)	80,113,113	2.37	24 (30%)
21	CL7	1C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
21	CL7	22	513	16	51,53,73	1.97	14 (27%)	56,89,113	2.84	21 (37%)
23	8CT	2C	514	-	40,41,41	4.65	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	32	504	-	51,53,73	1.99	17 (33%)	56,89,113	2.77	19 (33%)
21	CL7	14	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.70	19 (33%)
21	CL7	4A	403	1	61,63,73	1.87	19 (31%)	68,101,113	2.61	23 (33%)
22	PHO	2D	408	-	58,69,69	0.80	4 (6%)	56,99,99	1.28	4 (7%)
21	CL7	1C	503	3	71,73,73	1.68	15 (21%)	80,113,113	2.40	21 (26%)
21	CL7	3C	517	3	47,49,73	1.93	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	4B	602	-	47,49,73	1.94	13 (27%)	51,84,113	2.87	18 (35%)
23	8CT	4B	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	23	411	-	71,73,73	1.69	17 (23%)	80,113,113	2.37	24 (30%)
30	PL9	1D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	21	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.45	23 (28%)
23	8CT	2D	406	-	40,41,41	4.63	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	43	402	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	23 (28%)
25	SQD	21	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	42	512	16	71,73,73	1.69	14 (19%)	80,113,113	2.43	21 (26%)
27	DGD	2C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
32	ZEX	33	525	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
32	ZEX	44	420	-	42,43,43	1.01	3 (7%)	55,60,60	2.20	18 (32%)
21	CL7	33	509	19	71,73,73	1.68	15 (21%)	80,113,113	2.33	22 (27%)
21	CL7	11	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.98	20 (39%)
23	8CT	1C	518	-	40,41,41	4.65	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	34	415	-	51,53,73	1.96	19 (37%)	56,89,113	2.87	20 (35%)
21	CL7	2B	623	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
21	CL7	31	420	18	51,53,73	1.95	13 (25%)	56,89,113	2.80	21 (37%)
21	CL7	21	403	-	66,68,73	1.75	17 (25%)	74,107,113	2.51	22 (29%)
21	CL7	21	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.57	20 (29%)
21	CL7	3C	510	3	71,73,73	1.69	16 (22%)	80,113,113	2.38	21 (26%)
32	ZEX	34	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
23	8CT	34	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	4D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.48	22 (30%)
21	CL7	34	405	-	71,73,73	1.70	16 (22%)	80,113,113	2.45	25 (31%)
21	CL7	23	408	-	71,73,73	1.68	15 (21%)	80,113,113	2.39	23 (28%)
21	CL7	43	412	19	71,73,73	1.68	18 (25%)	80,113,113	2.54	24 (30%)
21	CL7	42	501	16	71,73,73	1.67	16 (22%)	80,113,113	2.42	21 (26%)
23	8CT	3C	515	-	40,41,41	4.64	20 (50%)	50,56,56	3.06	22 (44%)
21	CL7	24	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
21	CL7	2B	606	2	71,73,73	1.67	18 (25%)	80,113,113	2.39	20 (25%)
21	CL7	14	416	20	47,49,73	1.96	14 (29%)	51,84,113	2.85	18 (35%)
21	CL7	31	415	-	47,49,73	1.94	11 (23%)	51,84,113	2.97	19 (37%)
21	CL7	22	502	16	71,73,73	1.69	17 (23%)	80,113,113	2.35	23 (28%)
21	CL7	2B	607	2	61,63,73	1.81	16 (26%)	68,101,113	2.63	21 (30%)
23	8CT	3D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	44	406	20	71,73,73	1.70	15 (21%)	80,113,113	2.36	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	33	508	19	71,73,73	1.71	18 (25%)	80,113,113	2.31	21 (26%)
21	CL7	3C	504	-	61,63,73	1.85	17 (27%)	68,101,113	2.54	19 (27%)
21	CL7	2B	612	2	71,73,73	1.70	18 (25%)	80,113,113	2.35	21 (26%)
21	CL7	4B	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.32	22 (27%)
32	ZEX	24	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	3B	607	-	66,68,73	1.76	17 (25%)	74,107,113	2.47	21 (28%)
21	CL7	33	515	-	47,49,73	1.94	12 (25%)	51,84,113	2.94	21 (41%)
21	CL7	34	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.85	18 (35%)
21	CL7	42	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.72	19 (33%)
21	CL7	4C	506	3	66,68,73	1.77	17 (25%)	74,107,113	2.50	23 (31%)
21	CL7	32	507	-	71,73,73	1.71	17 (23%)	80,113,113	2.43	21 (26%)
22	PHO	1D	408	-	58,69,69	0.80	4 (6%)	56,99,99	1.26	4 (7%)
32	ZEX	14	403	-	42,43,43	1.02	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	4C	510	3	71,73,73	1.69	14 (19%)	80,113,113	2.38	20 (25%)
21	CL7	42	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	13	510	-	71,73,73	1.69	17 (23%)	80,113,113	2.37	24 (30%)
21	CL7	44	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.44	21 (28%)
24	LMG	1D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
21	CL7	4B	606	2	71,73,73	1.68	18 (25%)	80,113,113	2.39	20 (25%)
21	CL7	13	513	-	51,53,73	1.98	17 (33%)	56,89,113	2.72	18 (32%)
21	CL7	2C	517	3	47,49,73	1.92	13 (27%)	51,84,113	2.88	19 (37%)
21	CL7	41	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	2A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.61	23 (33%)
21	CL7	24	414	20	59,61,73	1.85	18 (30%)	65,98,113	2.67	21 (32%)
21	CL7	14	415	-	51,53,73	1.97	20 (39%)	56,89,113	2.89	22 (39%)
32	ZEX	34	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
22	PHO	1A	402	-	58,69,69	0.83	3 (5%)	56,99,99	1.07	4 (7%)
23	8CT	4B	601	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	3B	612	2	71,73,73	1.68	18 (25%)	80,113,113	2.39	23 (28%)
23	8CT	14	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.77	21 (42%)
21	CL7	12	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.36	21 (26%)
21	CL7	22	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.48	25 (31%)
21	CL7	33	514	-	51,53,73	1.99	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	22	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.37	22 (27%)
21	CL7	1B	606	2	61,63,73	1.81	16 (26%)	68,101,113	2.63	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	4C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.84	18 (35%)
23	8CT	2B	601	-	40,41,41	4.71	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	42	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.35	21 (26%)
21	CL7	12	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.73	19 (33%)
21	CL7	32	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.38	22 (27%)
25	SQD	33	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
32	ZEX	33	519	-	42,43,43	1.01	3 (7%)	55,60,60	2.58	17 (30%)
23	8CT	1K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.66	16 (32%)
21	CL7	32	518	16	71,73,73	1.68	13 (18%)	80,113,113	2.33	22 (27%)
21	CL7	4B	616	2	56,58,73	1.90	17 (30%)	62,95,113	2.71	20 (32%)
21	CL7	13	505	19	71,73,73	1.69	17 (23%)	80,113,113	2.39	21 (26%)
21	CL7	4C	509	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	41	407	18	47,49,73	1.94	14 (29%)	51,84,113	2.86	21 (41%)
29	BCT	3D	403	28	2,3,3	1.00	0	2,3,3	1.66	1 (50%)
32	ZEX	24	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
26	LHG	34	401	-	48,48,48	0.28	0	51,54,54	0.34	0
32	ZEX	13	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	31	416	-	47,49,73	1.96	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	3D	405	4	51,53,73	1.95	18 (35%)	56,89,113	2.77	22 (39%)
21	CL7	3B	609	2	71,73,73	1.70	17 (23%)	80,113,113	2.33	20 (25%)
21	CL7	3B	613	2	61,63,73	1.83	19 (31%)	68,101,113	2.48	19 (27%)
21	CL7	41	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.77	18 (32%)
32	ZEX	43	421	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	34	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.68	24 (32%)
29	BCT	2D	403	28	2,3,3	0.99	0	2,3,3	1.67	1 (50%)
21	CL7	32	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.64	19 (33%)
21	CL7	33	501	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	23 (28%)
21	CL7	13	511	19	71,73,73	1.68	17 (23%)	80,113,113	2.55	24 (30%)
21	CL7	1C	513	3	51,53,73	1.94	14 (27%)	56,89,113	2.90	19 (33%)
21	CL7	24	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.86	18 (35%)
32	ZEX	44	418	-	42,43,43	0.85	1 (2%)	55,60,60	2.33	16 (29%)
23	8CT	2C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	4C	504	-	61,63,73	1.85	16 (26%)	68,101,113	2.54	19 (27%)
21	CL7	31	410	-	71,73,73	1.71	17 (23%)	80,113,113	2.34	23 (28%)
21	CL7	4A	401	1	71,73,73	1.73	13 (18%)	80,113,113	2.47	25 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	8CT	3K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.66	16 (32%)
24	LMG	11	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
23	8CT	24	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	41	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.39	21 (26%)
21	CL7	14	414	20	59,61,73	1.84	17 (28%)	65,98,113	2.66	21 (32%)
21	CL7	41	415	-	47,49,73	1.95	11 (23%)	51,84,113	2.97	19 (37%)
21	CL7	2B	613	2	71,73,73	1.68	18 (25%)	80,113,113	2.38	23 (28%)
23	8CT	4C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	13	516	19	61,63,73	1.81	17 (27%)	68,101,113	2.56	25 (36%)
21	CL7	1A	407	-	71,73,73	1.68	17 (23%)	80,113,113	2.44	21 (26%)
21	CL7	31	412	18	51,53,73	1.96	16 (31%)	56,89,113	2.76	20 (35%)
21	CL7	44	411	20	71,73,73	1.68	15 (21%)	80,113,113	2.41	23 (28%)
21	CL7	43	403	19	64,66,73	1.78	17 (26%)	71,104,113	2.41	22 (30%)
25	SQD	43	424	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	13	508	19	71,73,73	1.70	18 (25%)	80,113,113	2.32	21 (26%)
27	DGD	4C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
27	DGD	3B	624	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
24	LMG	2D	410	-	33,33,55	0.28	0	41,41,63	0.33	0
21	CL7	11	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.56	20 (29%)
21	CL7	3C	512	3	47,49,73	1.92	12 (25%)	51,84,113	2.98	20 (39%)
21	CL7	13	503	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
25	SQD	2B	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.53	1 (1%)
21	CL7	22	516	16	71,73,73	1.70	17 (23%)	80,113,113	2.39	23 (28%)
21	CL7	33	506	19	51,53,73	1.97	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	24	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.71	20 (35%)
21	CL7	1B	603	2	71,73,73	1.69	18 (25%)	80,113,113	2.36	21 (26%)
21	CL7	12	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	20 (35%)
21	CL7	44	407	-	47,49,73	1.95	13 (27%)	51,84,113	2.82	20 (39%)
21	CL7	1C	502	3	66,68,73	1.77	18 (27%)	74,107,113	2.45	19 (25%)
21	CL7	41	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.81	22 (39%)
21	CL7	43	408	-	71,73,73	1.68	15 (21%)	80,113,113	2.40	22 (27%)
21	CL7	22	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	21 (37%)
32	ZEX	33	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	23	419	19	51,53,73	1.97	14 (27%)	56,89,113	2.74	20 (35%)
21	CL7	22	503	-	71,73,73	1.68	18 (25%)	80,113,113	2.51	25 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	1B	610	-	71,73,73	1.68	17 (23%)	80,113,113	2.46	22 (27%)
21	CL7	43	414	-	51,53,73	1.98	18 (35%)	56,89,113	2.74	18 (32%)
21	CL7	32	503	-	71,73,73	1.68	17 (23%)	80,113,113	2.50	25 (31%)
21	CL7	4B	612	2	71,73,73	1.70	18 (25%)	80,113,113	2.36	20 (25%)
21	CL7	34	406	20	71,73,73	1.70	17 (23%)	80,113,113	2.35	21 (26%)
21	CL7	4B	617	2	51,53,73	1.97	18 (35%)	56,89,113	2.69	18 (32%)
32	ZEX	42	520	-	42,43,43	0.98	3 (7%)	55,60,60	2.18	17 (30%)
25	SQD	22	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
25	SQD	32	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	42	513	16	51,53,73	1.97	14 (27%)	56,89,113	2.84	21 (37%)
21	CL7	43	411	-	71,73,73	1.69	16 (22%)	80,113,113	2.37	24 (30%)
21	CL7	11	407	18	47,49,73	1.95	15 (31%)	51,84,113	2.86	20 (39%)
21	CL7	24	405	-	71,73,73	1.70	16 (22%)	80,113,113	2.46	26 (32%)
23	8CT	4D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.98	19 (38%)
21	CL7	2B	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	20 (25%)
21	CL7	24	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.67	25 (33%)
21	CL7	23	405	-	71,73,73	1.69	17 (23%)	80,113,113	2.40	21 (26%)
21	CL7	4B	623	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
26	LHG	4A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
32	ZEX	42	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
23	8CT	4C	514	-	40,41,41	4.64	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	31	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	34	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.70	19 (33%)
21	CL7	3B	608	2	71,73,73	1.69	19 (26%)	80,113,113	2.30	20 (25%)
21	CL7	1B	612	2	71,73,73	1.68	18 (25%)	80,113,113	2.37	23 (28%)
29	BCT	4D	403	28	2,3,3	0.99	0	2,3,3	1.66	1 (50%)
21	CL7	24	407	-	47,49,73	1.94	13 (27%)	51,84,113	2.81	20 (39%)
26	LHG	24	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	13	502	19	64,66,73	1.77	15 (23%)	71,104,113	2.40	22 (30%)
21	CL7	4C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
32	ZEX	11	421	-	42,43,43	0.93	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	11	403	-	66,68,73	1.76	16 (24%)	74,107,113	2.51	22 (29%)
21	CL7	11	415	-	47,49,73	1.95	11 (23%)	51,84,113	2.97	20 (39%)
21	CL7	2B	614	2	61,63,73	1.84	19 (31%)	68,101,113	2.48	18 (26%)
26	LHG	13	524	-	35,35,48	0.34	0	38,41,54	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	BCT	1D	403	28	2,3,3	1.00	0	2,3,3	1.66	1 (50%)
21	CL7	21	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.80	22 (39%)
21	CL7	4C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.37	26 (32%)
21	CL7	11	405	-	51,53,73	1.97	17 (33%)	56,89,113	2.72	19 (33%)
21	CL7	4B	607	2	61,63,73	1.81	16 (26%)	68,101,113	2.64	22 (32%)
22	PHO	3A	402	-	58,69,69	0.84	3 (5%)	56,99,99	1.07	4 (7%)
27	DGD	2B	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	21	419	-	51,53,73	1.97	15 (29%)	56,89,113	2.78	18 (32%)
21	CL7	21	413	-	47,49,73	1.94	13 (27%)	51,84,113	2.97	22 (43%)
32	ZEX	31	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.22	20 (36%)
21	CL7	33	517	19	56,58,73	1.88	15 (26%)	62,95,113	2.65	20 (32%)
21	CL7	41	405	-	51,53,73	1.97	17 (33%)	56,89,113	2.71	19 (33%)
32	ZEX	32	519	-	42,43,43	1.06	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	3B	614	2	66,68,73	1.78	18 (27%)	74,107,113	2.49	24 (32%)
21	CL7	11	412	18	51,53,73	1.96	16 (31%)	56,89,113	2.77	20 (35%)
23	8CT	2B	620	-	40,41,41	4.58	21 (52%)	50,56,56	2.91	18 (36%)
21	CL7	4C	512	3	47,49,73	1.92	14 (29%)	51,84,113	2.98	20 (39%)
21	CL7	3B	610	-	71,73,73	1.69	17 (23%)	80,113,113	2.46	21 (26%)
21	CL7	3D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
32	ZEX	23	401	-	42,43,43	1.18	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	12	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.38	22 (27%)
23	8CT	3A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
24	LMG	4D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
21	CL7	21	416	-	47,49,73	1.95	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	12	513	16	51,53,73	1.96	15 (29%)	56,89,113	2.83	21 (37%)
21	CL7	13	515	-	47,49,73	1.94	12 (25%)	51,84,113	2.92	21 (41%)
32	ZEX	31	422	-	42,43,43	0.96	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	11	413	-	47,49,73	1.94	13 (27%)	51,84,113	2.98	22 (43%)
21	CL7	3B	615	2	56,58,73	1.89	18 (32%)	62,95,113	2.70	21 (33%)
21	CL7	1D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
23	8CT	3B	626	-	40,41,41	4.70	24 (60%)	50,56,56	3.24	21 (42%)
21	CL7	23	412	19	71,73,73	1.69	18 (25%)	80,113,113	2.55	24 (30%)
21	CL7	34	417	20	48,50,73	1.93	13 (27%)	51,85,113	2.95	18 (35%)
21	CL7	14	407	-	47,49,73	1.95	13 (27%)	51,84,113	2.81	20 (39%)
21	CL7	42	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.65	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	8CT	4B	619	-	40,41,41	4.69	21 (52%)	50,56,56	2.67	20 (40%)
24	LMG	2A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	4D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.61	20 (32%)
31	HEM	1F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.82	15 (22%)
32	ZEX	43	423	-	42,43,43	1.01	4 (9%)	55,60,60	2.39	17 (30%)
21	CL7	3B	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.40	21 (26%)
25	SQD	33	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	32	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.73	19 (33%)
32	ZEX	21	422	-	42,43,43	0.95	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	12	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.38	22 (27%)
21	CL7	21	405	-	51,53,73	1.97	18 (35%)	56,89,113	2.71	18 (32%)
21	CL7	2B	611	-	71,73,73	1.68	16 (22%)	80,113,113	2.46	22 (27%)
21	CL7	14	417	20	48,50,73	1.93	13 (27%)	51,85,113	2.94	19 (37%)
21	CL7	33	505	19	71,73,73	1.69	16 (22%)	80,113,113	2.39	21 (26%)
21	CL7	22	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.32	20 (25%)
21	CL7	31	403	-	66,68,73	1.76	16 (24%)	74,107,113	2.51	22 (29%)
23	8CT	4A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
32	ZEX	42	522	-	42,43,43	1.04	5 (11%)	55,60,60	2.47	15 (27%)
21	CL7	12	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.48	26 (32%)
21	CL7	34	412	20	71,73,73	1.69	16 (22%)	80,113,113	2.36	23 (28%)
32	ZEX	44	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
23	8CT	4K	101	-	40,41,41	4.76	25 (62%)	50,56,56	2.66	16 (32%)
32	ZEX	14	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	1C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.83	18 (35%)
21	CL7	1C	506	3	66,68,73	1.77	17 (25%)	74,107,113	2.51	23 (31%)
21	CL7	1B	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.32	20 (25%)
21	CL7	24	415	-	51,53,73	1.96	20 (39%)	56,89,113	2.87	21 (37%)
23	8CT	1B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
21	CL7	31	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.51	23 (28%)
21	CL7	43	418	19	56,58,73	1.88	16 (28%)	62,95,113	2.65	20 (32%)
21	CL7	12	501	16	71,73,73	1.68	16 (22%)	80,113,113	2.41	21 (26%)
21	CL7	21	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	44	414	20	59,61,73	1.84	18 (30%)	65,98,113	2.66	21 (32%)
32	ZEX	33	520	-	42,43,43	0.92	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	3B	611	2	71,73,73	1.70	18 (25%)	80,113,113	2.34	20 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	21	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.98	19 (37%)
25	SQD	23	422	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	21	404	-	71,73,73	1.71	14 (19%)	80,113,113	2.39	21 (26%)
21	CL7	31	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.71	18 (32%)
21	CL7	1B	622	2	51,53,73	1.97	15 (29%)	56,89,113	2.78	17 (30%)
27	DGD	3C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	22	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.63	19 (33%)
21	CL7	1B	601	-	47,49,73	1.94	13 (27%)	51,84,113	2.86	18 (35%)
21	CL7	21	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.72	18 (32%)
21	CL7	33	512	19	61,63,73	1.83	19 (31%)	68,101,113	2.59	23 (33%)
21	CL7	14	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.70	21 (37%)
21	CL7	21	409	18	51,53,73	1.95	16 (31%)	56,89,113	2.72	20 (35%)
22	PHO	4A	402	-	58,69,69	0.83	3 (5%)	56,99,99	1.08	4 (7%)
26	LHG	1D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
25	SQD	3A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	23	407	19	51,53,73	1.96	17 (33%)	56,89,113	2.75	19 (33%)
21	CL7	1D	405	4	51,53,73	1.96	18 (35%)	56,89,113	2.77	22 (39%)
21	CL7	21	407	18	47,49,73	1.94	14 (29%)	51,84,113	2.87	20 (39%)
26	LHG	3B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	12	516	16	71,73,73	1.70	17 (23%)	80,113,113	2.39	24 (30%)
21	CL7	4C	503	3	71,73,73	1.68	15 (21%)	80,113,113	2.39	21 (26%)
24	LMG	31	401	-	51,51,55	0.22	0	59,59,63	0.42	1 (1%)
21	CL7	32	501	16	71,73,73	1.68	16 (22%)	80,113,113	2.42	21 (26%)
21	CL7	41	409	18	51,53,73	1.96	16 (31%)	56,89,113	2.72	20 (35%)
32	ZEX	22	524	-	42,43,43	1.03	3 (7%)	55,60,60	2.51	17 (30%)
31	HEM	2F	101	-	50,50,50	1.61	9 (18%)	66,82,82	1.81	15 (22%)
21	CL7	34	411	20	71,73,73	1.68	16 (22%)	80,113,113	2.41	23 (28%)
21	CL7	44	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.33	21 (26%)
21	CL7	32	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.47	25 (31%)
25	SQD	23	424	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
25	SQD	12	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	22	512	16	71,73,73	1.68	14 (19%)	80,113,113	2.43	21 (26%)
21	CL7	22	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.72	19 (33%)
24	LMG	41	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
21	CL7	42	503	-	71,73,73	1.69	18 (25%)	80,113,113	2.50	24 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	23	403	19	64,66,73	1.77	16 (25%)	71,104,113	2.41	22 (30%)
21	CL7	3B	603	2	71,73,73	1.69	18 (25%)	80,113,113	2.35	21 (26%)
21	CL7	1C	517	3	47,49,73	1.93	13 (27%)	51,84,113	2.89	19 (37%)
21	CL7	4B	610	2	71,73,73	1.69	17 (23%)	80,113,113	2.32	20 (25%)
21	CL7	31	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.56	20 (29%)
25	SQD	22	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	31	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.50	20 (27%)
32	ZEX	13	520	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	4C	513	3	51,53,73	1.95	14 (27%)	56,89,113	2.91	19 (33%)
26	LHG	2B	624	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	13	504	-	71,73,73	1.69	17 (23%)	80,113,113	2.41	21 (26%)
21	CL7	1B	602	2	66,68,73	1.77	17 (25%)	74,107,113	2.51	21 (28%)
21	CL7	11	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.39	21 (26%)
21	CL7	13	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	14	412	20	71,73,73	1.69	15 (21%)	80,113,113	2.38	25 (31%)
21	CL7	2C	503	3	71,73,73	1.68	16 (22%)	80,113,113	2.40	21 (26%)
27	DGD	4B	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
23	8CT	1B	618	-	40,41,41	4.69	20 (50%)	50,56,56	2.67	20 (40%)
21	CL7	24	413	20	66,68,73	1.77	17 (25%)	74,107,113	2.44	21 (28%)
21	CL7	33	510	-	71,73,73	1.69	17 (23%)	80,113,113	2.37	24 (30%)
21	CL7	34	407	-	47,49,73	1.94	13 (27%)	51,84,113	2.81	20 (39%)
21	CL7	3B	622	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
25	SQD	13	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
25	SQD	1B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.53	1 (1%)
25	SQD	1A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
26	LHG	1B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	23	406	19	71,73,73	1.69	17 (23%)	80,113,113	2.38	21 (26%)
26	LHG	2A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	24	417	20	48,50,73	1.94	13 (27%)	51,85,113	2.94	18 (35%)
32	ZEX	24	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	14	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.44	21 (28%)
21	CL7	42	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	20 (35%)
23	8CT	4B	620	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
21	CL7	22	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.37	22 (27%)
21	CL7	1C	509	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	14	411	20	71,73,73	1.67	15 (21%)	80,113,113	2.41	23 (28%)
21	CL7	41	403	-	66,68,73	1.75	16 (24%)	74,107,113	2.51	22 (29%)
32	ZEX	41	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	43	404	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
21	CL7	11	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.43	20 (26%)
21	CL7	4B	603	2	66,68,73	1.78	17 (25%)	74,107,113	2.51	22 (29%)
25	SQD	42	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	3A	407	-	71,73,73	1.68	17 (23%)	80,113,113	2.45	21 (26%)
21	CL7	22	518	16	71,73,73	1.68	14 (19%)	80,113,113	2.33	23 (28%)
27	DGD	1B	624	-	63,63,67	0.83	2 (3%)	77,77,81	1.00	3 (3%)
26	LHG	1A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	44	410	20	51,53,73	1.99	17 (33%)	56,89,113	2.71	19 (33%)
23	8CT	1B	626	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
31	HEM	3F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.81	15 (22%)
25	SQD	12	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	41	408	-	71,73,73	1.66	15 (21%)	80,113,113	2.51	23 (28%)
21	CL7	42	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.35	23 (28%)
21	CL7	23	414	-	51,53,73	1.98	17 (33%)	56,89,113	2.73	18 (32%)
21	CL7	1A	401	1	71,73,73	1.74	13 (18%)	80,113,113	2.46	25 (31%)
21	CL7	1C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.47	23 (28%)
21	CL7	24	412	20	71,73,73	1.69	17 (23%)	80,113,113	2.38	25 (31%)
21	CL7	4B	614	2	61,63,73	1.83	19 (31%)	68,101,113	2.47	18 (26%)
32	ZEX	22	522	-	42,43,43	1.04	3 (7%)	55,60,60	2.47	17 (30%)
31	HEM	4F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.82	15 (22%)
23	8CT	3B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.76	19 (38%)
21	CL7	4C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.36	22 (27%)
21	CL7	12	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.35	22 (27%)
21	CL7	3C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.36	22 (27%)
21	CL7	2D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
21	CL7	13	518	19	51,53,73	1.97	14 (27%)	56,89,113	2.75	20 (35%)
21	CL7	2D	405	4	51,53,73	1.95	17 (33%)	56,89,113	2.77	22 (39%)
21	CL7	11	410	-	71,73,73	1.70	17 (23%)	80,113,113	2.33	23 (28%)
25	SQD	2A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	21	415	-	47,49,73	1.94	11 (23%)	51,84,113	2.96	19 (37%)
21	CL7	22	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.36	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	12	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.31	20 (25%)
21	CL7	4B	604	2	71,73,73	1.69	18 (25%)	80,113,113	2.36	21 (26%)
30	PL9	3D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
26	LHG	2D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	12	511	16	66,68,73	1.78	16 (24%)	74,107,113	2.40	21 (28%)
21	CL7	1B	614	2	66,68,73	1.78	18 (27%)	74,107,113	2.49	25 (33%)
23	8CT	2A	404	-	40,41,41	4.63	20 (50%)	50,56,56	2.97	20 (40%)
21	CL7	4B	611	-	71,73,73	1.69	17 (23%)	80,113,113	2.46	22 (27%)
21	CL7	41	418	18	71,73,73	1.67	15 (21%)	80,113,113	2.46	23 (28%)
24	LMG	2B	622	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	1B	607	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	20 (27%)
21	CL7	3B	601	-	47,49,73	1.94	13 (27%)	51,84,113	2.86	18 (35%)
21	CL7	4A	407	-	71,73,73	1.67	17 (23%)	80,113,113	2.44	21 (26%)
26	LHG	43	425	-	35,35,48	0.34	0	38,41,54	0.47	0
21	CL7	41	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.49	19 (25%)
25	SQD	4B	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
21	CL7	12	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.78	19 (33%)
21	CL7	23	417	19	61,63,73	1.81	17 (27%)	68,101,113	2.56	25 (36%)
21	CL7	2C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
21	CL7	31	407	18	47,49,73	1.94	14 (29%)	51,84,113	2.87	19 (37%)
21	CL7	44	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.85	18 (35%)
21	CL7	2C	510	3	71,73,73	1.69	15 (21%)	80,113,113	2.38	21 (26%)
21	CL7	22	511	16	66,68,73	1.78	16 (24%)	74,107,113	2.40	21 (28%)
21	CL7	1B	604	2	71,73,73	1.67	18 (25%)	80,113,113	2.32	23 (28%)
21	CL7	1C	512	3	47,49,73	1.93	13 (27%)	51,84,113	2.99	20 (39%)
21	CL7	3C	506	3	66,68,73	1.77	17 (25%)	74,107,113	2.51	23 (31%)
21	CL7	11	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.46	22 (27%)
30	PL9	2D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	12	503	-	71,73,73	1.69	17 (23%)	80,113,113	2.51	25 (31%)
21	CL7	11	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.50	19 (25%)
25	SQD	11	423	-	31,32,54	0.49	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	33	511	19	71,73,73	1.69	18 (25%)	80,113,113	2.55	24 (30%)
21	CL7	44	405	-	71,73,73	1.69	16 (22%)	80,113,113	2.45	26 (32%)
21	CL7	11	411	-	51,53,73	1.98	16 (31%)	56,89,113	2.71	18 (32%)
21	CL7	2B	603	2	66,68,73	1.78	17 (25%)	74,107,113	2.51	22 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	43	419	19	51,53,73	1.98	14 (27%)	56,89,113	2.74	20 (35%)
21	CL7	43	405	-	71,73,73	1.69	17 (23%)	80,113,113	2.40	21 (26%)
21	CL7	42	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.47	25 (31%)
21	CL7	42	510	16	71,73,73	1.68	18 (25%)	80,113,113	2.37	22 (27%)
23	8CT	2B	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
26	LHG	4D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	24	406	20	71,73,73	1.70	16 (22%)	80,113,113	2.35	21 (26%)
21	CL7	2C	509	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	1C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.35	22 (27%)
21	CL7	32	509	-	71,73,73	1.68	18 (25%)	80,113,113	2.31	20 (25%)
21	CL7	4B	613	2	71,73,73	1.68	18 (25%)	80,113,113	2.38	23 (28%)
21	CL7	2C	512	3	47,49,73	1.92	13 (27%)	51,84,113	2.97	20 (39%)
25	SQD	31	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
32	ZEX	11	422	-	42,43,43	0.96	2 (4%)	55,60,60	2.23	18 (32%)
23	8CT	1B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	1A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.62	23 (33%)
21	CL7	41	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.71	18 (32%)
21	CL7	33	507	-	71,73,73	1.68	15 (21%)	80,113,113	2.39	23 (28%)
26	LHG	4B	624	-	44,44,48	0.31	0	47,50,54	0.39	0
21	CL7	4B	615	2	66,68,73	1.78	18 (27%)	74,107,113	2.49	25 (33%)
21	CL7	41	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.57	20 (29%)
22	PHO	2A	402	-	58,69,69	0.83	3 (5%)	56,99,99	1.08	4 (7%)
24	LMG	4A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	22	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.77	19 (33%)
26	LHG	3B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	11	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.50	23 (28%)
25	SQD	13	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
23	8CT	1A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
23	8CT	3B	618	-	40,41,41	4.69	21 (52%)	50,56,56	2.66	20 (40%)
21	CL7	32	511	16	66,68,73	1.78	17 (25%)	74,107,113	2.40	21 (28%)
21	CL7	43	416	-	47,49,73	1.93	12 (25%)	51,84,113	2.93	21 (41%)
21	CL7	11	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.80	22 (39%)
26	LHG	33	524	-	35,35,48	0.34	0	38,41,54	0.47	0
32	ZEX	13	519	-	42,43,43	1.02	3 (7%)	55,60,60	2.58	17 (30%)
21	CL7	2A	407	-	71,73,73	1.68	17 (23%)	80,113,113	2.44	21 (26%)
21	CL7	23	410	19	71,73,73	1.68	16 (22%)	80,113,113	2.33	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	ZEX	14	420	-	42,43,43	1.01	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	12	507	-	71,73,73	1.72	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	2C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.35	21 (26%)
21	CL7	1B	613	2	61,63,73	1.83	19 (31%)	68,101,113	2.48	19 (27%)
21	CL7	21	412	18	51,53,73	1.95	16 (31%)	56,89,113	2.76	20 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	33	502	19	2/2/13/20	12/31/107/115	-
21	CL7	31	419	-	2/2/11/20	9/15/91/115	-
21	CL7	2C	508	3	2/2/15/20	17/39/115/115	-
21	CL7	3C	511	3	2/2/10/20	5/12/88/115	-
25	SQD	32	521	-	-	7/45/65/69	0/1/1/1
21	CL7	22	507	-	2/2/15/20	20/39/115/115	-
21	CL7	23	404	-	2/2/15/20	20/39/115/115	-
21	CL7	23	415	-	2/2/11/20	5/15/91/115	-
21	CL7	3C	503	3	2/2/15/20	19/39/115/115	-
21	CL7	4B	609	2	2/2/15/20	15/39/115/115	-
21	CL7	3B	616	2	2/2/11/20	4/15/91/115	-
21	CL7	1B	608	2	2/2/15/20	15/39/115/115	-
21	CL7	33	513	-	2/2/11/20	9/15/91/115	-
32	ZEX	22	519	-	-	11/29/67/67	0/2/2/2
21	CL7	44	409	-	2/2/14/20	17/33/109/115	-
23	8CT	3C	514	-	-	14/29/63/63	0/2/2/2
25	SQD	42	521	-	-	7/45/65/69	0/1/1/1
21	CL7	21	402	18	2/2/14/20	16/33/109/115	-
21	CL7	31	404	-	2/2/15/20	15/39/115/115	-
21	CL7	23	409	19	2/2/15/20	16/39/115/115	-
21	CL7	11	409	18	2/2/11/20	6/15/91/115	-
21	CL7	2B	610	2	2/2/15/20	14/39/115/115	-
21	CL7	14	406	20	2/2/15/20	24/39/115/115	-
21	CL7	3C	505	3	2/2/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	31	418	18	2/2/15/20	22/39/115/115	-
21	CL7	4D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	13	507	-	2/2/15/20	15/39/115/115	-
21	CL7	43	410	19	2/2/15/20	17/39/115/115	-
32	ZEX	14	419	-	-	9/29/67/67	0/2/2/2
26	LHG	2B	626	-	-	6/53/53/53	-
21	CL7	2B	604	2	2/2/15/20	12/39/115/115	-
21	CL7	31	414	18	2/2/10/20	3/10/86/115	-
21	CL7	34	414	20	2/2/12/20	8/25/101/115	-
21	CL7	21	408	-	2/2/15/20	16/39/115/115	-
23	8CT	2C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	32	510	16	2/2/15/20	20/39/115/115	-
27	DGD	1C	516	-	-	9/51/91/95	0/2/2/2
30	PL9	4D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	34	404	20	2/2/15/20	14/39/115/115	-
21	CL7	14	405	-	2/2/15/20	18/39/115/115	-
21	CL7	2B	608	-	2/2/14/20	11/33/109/115	-
21	CL7	32	517	16	2/2/15/20	21/39/115/115	-
21	CL7	2B	617	2	2/2/11/20	4/15/91/115	-
24	LMG	1B	621	-	-	7/46/66/70	0/1/1/1
21	CL7	41	412	18	2/2/11/20	10/15/91/115	-
32	ZEX	13	525	-	-	7/29/67/67	0/2/2/2
21	CL7	43	409	19	2/2/15/20	16/39/115/115	-
32	ZEX	12	520	-	-	6/29/67/67	0/2/2/2
32	ZEX	34	420	-	-	12/29/67/67	0/2/2/2
32	ZEX	44	403	-	-	10/29/67/67	0/2/2/2
32	ZEX	34	418	-	-	9/29/67/67	0/2/2/2
24	LMG	1A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	1D	402	-	2/2/12/20	9/21/97/115	-
21	CL7	22	501	16	2/2/15/20	17/39/115/115	-
21	CL7	1B	616	2	2/2/11/20	4/15/91/115	-
21	CL7	12	508	16	2/2/11/20	5/15/91/115	-
32	ZEX	12	524	-	-	11/29/67/67	0/2/2/2
26	LHG	14	401	-	-	8/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2B	602	-	2/2/10/20	4/10/86/115	-
21	CL7	24	411	20	2/2/15/20	14/39/115/115	-
21	CL7	2C	506	3	2/2/14/20	15/33/109/115	-
24	LMG	4B	622	-	-	7/46/66/70	0/1/1/1
26	LHG	4B	626	-	-	6/53/53/53	-
21	CL7	4C	502	3	2/2/14/20	12/33/109/115	-
21	CL7	4C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	43	407	19	2/2/11/20	13/15/91/115	-
21	CL7	1C	504	-	2/2/13/20	13/27/103/115	-
24	LMG	3D	410	-	-	5/28/48/70	0/1/1/1
26	LHG	3A	408	-	-	5/50/50/53	-
21	CL7	23	418	19	2/2/12/20	9/21/97/115	-
21	CL7	44	417	20	2/2/10/20	6/12/88/115	-
25	SQD	3B	620	-	-	5/49/69/69	0/1/1/1
22	PHO	4D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	12	512	16	2/2/15/20	18/39/115/115	-
21	CL7	1B	615	2	2/2/12/20	8/21/97/115	-
21	CL7	14	404	20	2/2/15/20	15/39/115/115	-
21	CL7	34	408	20	2/2/11/20	4/15/91/115	-
21	CL7	41	410	-	2/2/15/20	17/39/115/115	-
32	ZEX	12	522	-	-	6/29/67/67	0/2/2/2
21	CL7	42	506	16	2/2/15/20	14/39/115/115	-
21	CL7	24	408	20	2/2/11/20	4/15/91/115	-
21	CL7	42	509	-	2/2/15/20	16/39/115/115	-
23	8CT	3C	518	-	-	8/29/63/63	0/2/2/2
26	LHG	23	425	-	-	3/40/40/53	-
21	CL7	2B	605	2	2/2/15/20	17/39/115/115	-
21	CL7	42	518	16	2/2/15/20	12/39/115/115	-
21	CL7	34	413	20	2/2/14/20	7/33/109/115	-
21	CL7	42	516	16	2/2/15/20	16/39/115/115	-
24	LMG	3A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	3A	401	1	2/2/15/20	18/39/115/115	-
21	CL7	33	518	19	2/2/11/20	7/15/91/115	-
21	CL7	44	415	-	2/2/11/20	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SQD	43	422	-	-	3/41/61/69	0/1/1/1
23	8CT	2K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	12	518	16	2/2/15/20	12/39/115/115	-
21	CL7	3C	507	-	2/2/15/20	17/39/115/115	-
21	CL7	13	512	19	2/2/13/20	12/27/103/115	-
23	8CT	44	402	-	-	4/29/63/63	0/2/2/2
32	ZEX	22	520	-	-	6/29/67/67	0/2/2/2
32	ZEX	32	520	-	-	6/29/67/67	0/2/2/2
32	ZEX	21	421	-	-	14/29/67/67	0/2/2/2
21	CL7	3C	508	3	2/2/15/20	17/39/115/115	-
21	CL7	31	413	-	2/2/10/20	2/10/86/115	-
21	CL7	31	405	-	2/2/11/20	10/15/91/115	-
21	CL7	44	408	20	2/2/11/20	4/15/91/115	-
32	ZEX	23	423	-	-	5/29/67/67	0/2/2/2
21	CL7	2C	511	3	2/2/10/20	5/12/88/115	-
21	CL7	2C	504	-	2/2/13/20	13/27/103/115	-
21	CL7	3B	604	2	2/2/15/20	17/39/115/115	-
21	CL7	43	417	19	2/2/13/20	16/27/103/115	-
21	CL7	32	516	16	2/2/15/20	16/39/115/115	-
21	CL7	2B	615	2	2/2/14/20	14/33/109/115	-
21	CL7	13	501	19	2/2/15/20	21/39/115/115	-
21	CL7	32	512	16	2/2/15/20	18/39/115/115	-
26	LHG	44	401	-	-	8/53/53/53	-
32	ZEX	43	401	-	-	7/29/67/67	0/2/2/2
32	ZEX	32	522	-	-	6/29/67/67	0/2/2/2
25	SQD	41	423	-	-	3/27/47/69	0/1/1/1
21	CL7	4C	507	-	2/2/15/20	17/39/115/115	-
23	8CT	2B	619	-	-	10/29/63/63	0/2/2/2
32	ZEX	23	420	-	-	10/29/67/67	0/2/2/2
21	CL7	2B	616	2	2/2/12/20	8/21/97/115	-
21	CL7	42	511	16	2/2/14/20	16/33/109/115	-
21	CL7	2D	402	-	2/2/12/20	9/21/97/115	-
21	CL7	23	413	19	2/2/13/20	12/27/103/115	-
21	CL7	33	504	-	2/2/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2C	513	3	2/2/11/20	8/15/91/115	-
22	PHO	3D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	32	513	16	2/2/11/20	8/15/91/115	-
21	CL7	43	415	-	2/2/11/20	5/15/91/115	-
24	LMG	3B	621	-	-	7/46/66/70	0/1/1/1
21	CL7	1C	505	3	2/2/15/20	16/39/115/115	-
21	CL7	33	503	-	2/2/15/20	20/39/115/115	-
23	8CT	1C	515	-	-	10/29/63/63	0/2/2/2
32	ZEX	41	422	-	-	6/29/67/67	0/2/2/2
21	CL7	1C	510	3	2/2/15/20	22/39/115/115	-
21	CL7	43	406	19	2/2/15/20	14/39/115/115	-
21	CL7	3C	513	3	2/2/11/20	8/15/91/115	-
21	CL7	3B	606	2	2/2/13/20	5/27/103/115	-
32	ZEX	32	524	-	-	11/29/67/67	0/2/2/2
21	CL7	21	410	-	2/2/15/20	17/39/115/115	-
25	SQD	4A	406	-	-	3/29/49/69	0/1/1/1
21	CL7	23	416	-	2/2/10/20	0/10/86/115	-
21	CL7	3A	403	1	2/2/13/20	9/27/103/115	-
21	CL7	11	419	-	2/2/11/20	9/15/91/115	-
21	CL7	31	409	18	2/2/11/20	6/15/91/115	-
21	CL7	3C	509	3	2/2/15/20	20/39/115/115	-
32	ZEX	12	519	-	-	11/29/67/67	0/2/2/2
21	CL7	2C	507	-	2/2/15/20	17/39/115/115	-
21	CL7	3D	402	-	2/2/12/20	9/21/97/115	-
23	8CT	4C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	13	517	19	2/2/12/20	9/21/97/115	-
23	8CT	1D	406	-	-	10/29/63/63	0/2/2/2
24	LMG	21	401	-	-	5/46/66/70	0/1/1/1
21	CL7	41	413	-	2/2/10/20	2/10/86/115	-
32	ZEX	43	420	-	-	10/29/67/67	0/2/2/2
21	CL7	43	413	19	2/2/13/20	12/27/103/115	-
26	LHG	3D	409	-	-	7/53/53/53	-
21	CL7	1B	611	2	2/2/15/20	17/39/115/115	-
21	CL7	11	416	-	2/2/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	1B	605	2	2/2/15/20	18/39/115/115	-
32	ZEX	23	421	-	-	10/29/67/67	0/2/2/2
21	CL7	32	515	-	2/2/11/20	8/15/91/115	-
21	CL7	23	402	19	2/2/15/20	21/39/115/115	-
23	8CT	3B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	14	409	-	2/2/14/20	17/33/109/115	-
21	CL7	2C	502	3	2/2/14/20	12/33/109/115	-
26	LHG	1B	623	-	-	3/49/49/53	-
21	CL7	32	502	16	2/2/15/20	17/39/115/115	-
21	CL7	42	507	-	2/2/15/20	20/39/115/115	-
21	CL7	2A	401	1	2/2/15/20	18/39/115/115	-
23	8CT	1C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	41	416	-	2/2/10/20	4/10/86/115	-
21	CL7	3B	602	2	2/2/14/20	9/33/109/115	-
21	CL7	41	414	18	2/2/10/20	3/10/86/115	-
32	ZEX	42	519	-	-	11/29/67/67	0/2/2/2
32	ZEX	24	419	-	-	9/29/67/67	0/2/2/2
21	CL7	13	506	19	2/2/11/20	13/15/91/115	-
21	CL7	33	516	19	2/2/13/20	16/27/103/115	-
21	CL7	4B	608	-	2/2/14/20	11/33/109/115	-
21	CL7	13	509	19	2/2/15/20	17/39/115/115	-
21	CL7	3C	502	3	2/2/14/20	12/33/109/115	-
21	CL7	44	412	20	2/2/15/20	17/39/115/115	-
21	CL7	1C	508	3	2/2/15/20	17/39/115/115	-
21	CL7	22	513	16	2/2/11/20	8/15/91/115	-
23	8CT	2C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	32	504	-	2/2/11/20	6/15/91/115	-
21	CL7	14	410	20	2/2/11/20	9/15/91/115	-
21	CL7	4A	403	1	2/2/13/20	9/27/103/115	-
22	PHO	2D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	1C	503	3	2/2/15/20	19/39/115/115	-
21	CL7	3C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	4B	602	-	2/2/10/20	4/10/86/115	-
23	8CT	4B	618	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	23	411	-	2/2/15/20	15/39/115/115	-
30	PL9	1D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	21	418	18	2/2/15/20	22/39/115/115	-
23	8CT	2D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	43	402	19	2/2/15/20	21/39/115/115	-
25	SQD	21	423	-	-	3/27/47/69	0/1/1/1
21	CL7	42	512	16	2/2/15/20	18/39/115/115	-
27	DGD	2C	516	-	-	9/51/91/95	0/2/2/2
32	ZEX	33	525	-	-	7/29/67/67	0/2/2/2
32	ZEX	44	420	-	-	12/29/67/67	0/2/2/2
21	CL7	33	509	19	2/2/15/20	17/39/115/115	-
21	CL7	11	414	18	2/2/10/20	3/10/86/115	-
23	8CT	1C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	34	415	-	2/2/11/20	11/15/91/115	-
21	CL7	2B	623	2	2/2/11/20	8/15/91/115	-
21	CL7	31	420	18	2/2/11/20	6/15/91/115	-
21	CL7	21	403	-	2/2/14/20	11/33/109/115	-
21	CL7	21	417	18	2/2/13/20	9/27/103/115	-
21	CL7	3C	510	3	2/2/15/20	22/39/115/115	-
32	ZEX	34	403	-	-	10/29/67/67	0/2/2/2
23	8CT	34	402	-	-	4/29/63/63	0/2/2/2
21	CL7	4D	404	4	2/2/13/20	13/31/107/115	-
21	CL7	34	405	-	2/2/15/20	18/39/115/115	-
21	CL7	23	408	-	2/2/15/20	15/39/115/115	-
21	CL7	43	412	19	2/2/15/20	19/39/115/115	-
21	CL7	42	501	16	2/2/15/20	17/39/115/115	-
23	8CT	3C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	24	404	20	2/2/15/20	15/39/115/115	-
21	CL7	2B	606	2	2/2/15/20	18/39/115/115	-
21	CL7	14	416	20	2/2/10/20	7/10/86/115	-
21	CL7	31	415	-	2/2/10/20	7/10/86/115	-
21	CL7	22	502	16	2/2/15/20	17/39/115/115	-
21	CL7	2B	607	2	2/2/13/20	5/27/103/115	-
23	8CT	3D	406	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	44	406	20	2/2/15/20	24/39/115/115	-
21	CL7	33	508	19	2/2/15/20	16/39/115/115	-
21	CL7	3C	504	-	2/2/13/20	13/27/103/115	-
21	CL7	2B	612	2	2/2/15/20	17/39/115/115	-
21	CL7	4B	605	2	2/2/15/20	17/39/115/115	-
32	ZEX	24	418	-	-	9/29/67/67	0/2/2/2
21	CL7	3B	607	-	2/2/14/20	11/33/109/115	-
21	CL7	33	515	-	2/2/10/20	0/10/86/115	-
21	CL7	34	416	20	2/2/10/20	7/10/86/115	-
21	CL7	42	514	-	2/2/11/20	9/15/91/115	-
21	CL7	4C	506	3	2/2/14/20	15/33/109/115	-
21	CL7	32	507	-	2/2/15/20	20/39/115/115	-
22	PHO	1D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
32	ZEX	14	403	-	-	10/29/67/67	0/2/2/2
21	CL7	4C	510	3	2/2/15/20	22/39/115/115	-
21	CL7	42	504	-	2/2/11/20	6/15/91/115	-
21	CL7	13	510	-	2/2/15/20	15/39/115/115	-
21	CL7	44	413	20	2/2/14/20	7/33/109/115	-
24	LMG	1D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	4B	606	2	2/2/15/20	18/39/115/115	-
21	CL7	13	513	-	2/2/11/20	9/15/91/115	-
21	CL7	2C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	41	406	18	2/2/14/20	13/36/112/115	-
21	CL7	2A	403	1	2/2/13/20	9/27/103/115	-
21	CL7	24	414	20	2/2/12/20	8/25/101/115	-
21	CL7	14	415	-	2/2/11/20	11/15/91/115	-
32	ZEX	34	419	-	-	9/29/67/67	0/2/2/2
22	PHO	1A	402	-	-	3/37/103/103	0/5/6/6
23	8CT	4B	601	-	-	10/29/63/63	0/2/2/2
21	CL7	3B	612	2	2/2/15/20	17/39/115/115	-
23	8CT	14	402	-	-	4/29/63/63	0/2/2/2
21	CL7	12	517	16	2/2/15/20	21/39/115/115	-
21	CL7	22	505	16	2/2/15/20	18/39/115/115	-
21	CL7	33	514	-	2/2/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	22	510	16	2/2/15/20	20/39/115/115	-
21	CL7	1B	606	2	2/2/13/20	5/27/103/115	-
21	CL7	4C	511	3	2/2/10/20	5/12/88/115	-
23	8CT	2B	601	-	-	10/29/63/63	0/2/2/2
21	CL7	42	517	16	2/2/15/20	21/39/115/115	-
21	CL7	12	514	-	2/2/11/20	9/15/91/115	-
21	CL7	32	506	16	2/2/15/20	14/39/115/115	-
25	SQD	33	521	-	-	3/41/61/69	0/1/1/1
32	ZEX	33	519	-	-	10/29/67/67	0/2/2/2
23	8CT	1K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	32	518	16	2/2/15/20	12/39/115/115	-
21	CL7	4B	616	2	2/2/12/20	8/21/97/115	-
21	CL7	13	505	19	2/2/15/20	14/39/115/115	-
21	CL7	4C	509	3	2/2/15/20	20/39/115/115	-
21	CL7	41	407	18	2/2/10/20	4/10/86/115	-
32	ZEX	24	420	-	-	12/29/67/67	0/2/2/2
26	LHG	34	401	-	-	8/53/53/53	-
32	ZEX	13	522	-	-	5/29/67/67	0/2/2/2
21	CL7	31	416	-	2/2/10/20	4/10/86/115	-
21	CL7	3D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	3B	609	2	2/2/15/20	14/39/115/115	-
21	CL7	3B	613	2	2/2/13/20	5/27/103/115	-
21	CL7	41	419	-	2/2/11/20	9/15/91/115	-
32	ZEX	43	421	-	-	10/29/67/67	0/2/2/2
21	CL7	34	409	-	2/2/14/20	17/33/109/115	-
21	CL7	32	508	16	2/2/11/20	5/15/91/115	-
21	CL7	33	501	19	2/2/15/20	21/39/115/115	-
21	CL7	13	511	19	2/2/15/20	19/39/115/115	-
21	CL7	1C	513	3	2/2/11/20	8/15/91/115	-
21	CL7	24	416	20	2/2/10/20	7/10/86/115	-
32	ZEX	44	418	-	-	9/29/67/67	0/2/2/2
23	8CT	2C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	4C	504	-	2/2/13/20	13/27/103/115	-
21	CL7	31	410	-	2/2/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	4A	401	1	2/2/15/20	18/39/115/115	-
23	8CT	3K	101	-	-	10/29/63/63	0/2/2/2
24	LMG	11	401	-	-	5/46/66/70	0/1/1/1
23	8CT	24	402	-	-	4/29/63/63	0/2/2/2
21	CL7	41	404	-	2/2/15/20	15/39/115/115	-
21	CL7	14	414	20	2/2/12/20	8/25/101/115	-
21	CL7	41	415	-	2/2/10/20	7/10/86/115	-
21	CL7	2B	613	2	2/2/15/20	17/39/115/115	-
23	8CT	4C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	13	516	19	2/2/13/20	16/27/103/115	-
21	CL7	1A	407	-	2/2/15/20	16/39/115/115	-
21	CL7	31	412	18	2/2/11/20	10/15/91/115	-
21	CL7	44	411	20	2/2/15/20	14/39/115/115	-
21	CL7	43	403	19	2/2/13/20	12/31/107/115	-
25	SQD	43	424	-	-	7/45/65/69	0/1/1/1
21	CL7	13	508	19	2/2/15/20	16/39/115/115	-
27	DGD	4C	516	-	-	9/51/91/95	0/2/2/2
27	DGD	3B	624	-	-	7/51/91/95	0/2/2/2
24	LMG	2D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	11	417	18	2/2/13/20	9/27/103/115	-
21	CL7	3C	512	3	2/2/10/20	4/10/86/115	-
21	CL7	13	503	-	2/2/15/20	20/39/115/115	-
25	SQD	2B	621	-	-	5/49/69/69	0/1/1/1
21	CL7	22	516	16	2/2/15/20	16/39/115/115	-
21	CL7	33	506	19	2/2/11/20	13/15/91/115	-
21	CL7	24	410	20	2/2/11/20	9/15/91/115	-
21	CL7	1B	603	2	2/2/15/20	12/39/115/115	-
21	CL7	12	515	-	2/2/11/20	8/15/91/115	-
21	CL7	44	407	-	2/2/10/20	3/10/86/115	-
21	CL7	1C	502	3	2/2/14/20	12/33/109/115	-
21	CL7	41	420	18	2/2/11/20	6/15/91/115	-
21	CL7	43	408	-	2/2/15/20	15/39/115/115	-
21	CL7	22	515	-	2/2/11/20	8/15/91/115	-
32	ZEX	33	522	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	23	419	19	2/2/11/20	7/15/91/115	-
21	CL7	22	503	-	2/2/15/20	17/39/115/115	-
21	CL7	1B	610	-	2/2/15/20	11/39/115/115	-
21	CL7	43	414	-	2/2/11/20	9/15/91/115	-
21	CL7	32	503	-	2/2/15/20	17/39/115/115	-
21	CL7	4B	612	2	2/2/15/20	17/39/115/115	-
21	CL7	34	406	20	2/2/15/20	24/39/115/115	-
21	CL7	4B	617	2	2/2/11/20	4/15/91/115	-
32	ZEX	42	520	-	-	6/29/67/67	0/2/2/2
25	SQD	22	523	-	-	0/36/56/69	0/1/1/1
25	SQD	32	523	-	-	0/36/56/69	0/1/1/1
21	CL7	42	513	16	2/2/11/20	8/15/91/115	-
21	CL7	43	411	-	2/2/15/20	16/39/115/115	-
21	CL7	11	407	18	2/2/10/20	4/10/86/115	-
21	CL7	24	405	-	2/2/15/20	18/39/115/115	-
23	8CT	4D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	2B	609	2	2/2/15/20	15/39/115/115	-
21	CL7	24	409	-	2/2/14/20	17/33/109/115	-
21	CL7	23	405	-	2/2/15/20	16/39/115/115	-
21	CL7	4B	623	2	2/2/11/20	8/15/91/115	-
26	LHG	4A	408	-	-	5/50/50/53	-
32	ZEX	42	524	-	-	11/29/67/67	0/2/2/2
23	8CT	4C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	31	406	18	2/2/14/20	13/36/112/115	-
21	CL7	34	410	20	2/2/11/20	9/15/91/115	-
21	CL7	3B	608	2	2/2/15/20	15/39/115/115	-
21	CL7	1B	612	2	2/2/15/20	17/39/115/115	-
21	CL7	24	407	-	2/2/10/20	3/10/86/115	-
26	LHG	24	401	-	-	8/53/53/53	-
21	CL7	13	502	19	2/2/13/20	12/31/107/115	-
21	CL7	4C	505	3	2/2/15/20	16/39/115/115	-
32	ZEX	11	421	-	-	14/29/67/67	0/2/2/2
21	CL7	11	403	-	2/2/14/20	11/33/109/115	-
21	CL7	11	415	-	2/2/10/20	7/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2B	614	2	2/2/13/20	5/27/103/115	-
26	LHG	13	524	-	-	3/40/40/53	-
21	CL7	21	420	18	2/2/11/20	6/15/91/115	-
21	CL7	4C	508	3	2/2/15/20	17/39/115/115	-
21	CL7	11	405	-	2/2/11/20	10/15/91/115	-
21	CL7	4B	607	2	2/2/13/20	5/27/103/115	-
22	PHO	3A	402	-	-	3/37/103/103	0/5/6/6
27	DGD	2B	625	-	-	7/51/91/95	0/2/2/2
21	CL7	21	419	-	2/2/11/20	9/15/91/115	-
21	CL7	21	413	-	2/2/10/20	2/10/86/115	-
32	ZEX	31	421	-	-	14/29/67/67	0/2/2/2
21	CL7	33	517	19	2/2/12/20	9/21/97/115	-
21	CL7	41	405	-	2/2/11/20	10/15/91/115	-
32	ZEX	32	519	-	-	11/29/67/67	0/2/2/2
21	CL7	3B	614	2	2/2/14/20	14/33/109/115	-
21	CL7	11	412	18	2/2/11/20	10/15/91/115	-
23	8CT	2B	620	-	-	4/29/63/63	0/2/2/2
21	CL7	4C	512	3	2/2/10/20	4/10/86/115	-
21	CL7	3B	610	-	2/2/15/20	11/39/115/115	-
21	CL7	3D	404	4	2/2/13/20	13/31/107/115	-
32	ZEX	23	401	-	-	7/29/67/67	0/2/2/2
21	CL7	12	510	16	2/2/15/20	20/39/115/115	-
23	8CT	3A	404	-	-	5/29/63/63	0/2/2/2
24	LMG	4D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	21	416	-	2/2/10/20	4/10/86/115	-
21	CL7	12	513	16	2/2/11/20	8/15/91/115	-
21	CL7	13	515	-	2/2/10/20	0/10/86/115	-
32	ZEX	31	422	-	-	6/29/67/67	0/2/2/2
21	CL7	11	413	-	2/2/10/20	2/10/86/115	-
21	CL7	3B	615	2	2/2/12/20	8/21/97/115	-
21	CL7	1D	404	4	2/2/13/20	13/31/107/115	-
23	8CT	3B	626	-	-	10/29/63/63	0/2/2/2
21	CL7	23	412	19	2/2/15/20	19/39/115/115	-
21	CL7	34	417	20	2/2/10/20	6/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	14	407	-	2/2/10/20	3/10/86/115	-
21	CL7	42	508	16	2/2/11/20	5/15/91/115	-
23	8CT	4B	619	-	-	10/29/63/63	0/2/2/2
24	LMG	2A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	4D	402	-	2/2/12/20	9/21/97/115	-
31	HEM	1F	101	-	-	8/14/54/54	-
32	ZEX	43	423	-	-	5/29/67/67	0/2/2/2
21	CL7	3B	605	2	2/2/15/20	18/39/115/115	-
25	SQD	33	523	-	-	7/45/65/69	0/1/1/1
21	CL7	32	514	-	2/2/11/20	9/15/91/115	-
32	ZEX	21	422	-	-	6/29/67/67	0/2/2/2
21	CL7	12	506	16	2/2/15/20	14/39/115/115	-
21	CL7	21	405	-	2/2/11/20	10/15/91/115	-
21	CL7	2B	611	-	2/2/15/20	11/39/115/115	-
21	CL7	14	417	20	2/2/10/20	6/12/88/115	-
21	CL7	33	505	19	2/2/15/20	14/39/115/115	-
21	CL7	22	509	-	2/2/15/20	16/39/115/115	-
21	CL7	31	403	-	2/2/14/20	11/33/109/115	-
23	8CT	4A	404	-	-	5/29/63/63	0/2/2/2
32	ZEX	42	522	-	-	6/29/67/67	0/2/2/2
21	CL7	12	505	16	2/2/15/20	18/39/115/115	-
21	CL7	34	412	20	2/2/15/20	17/39/115/115	-
32	ZEX	44	419	-	-	9/29/67/67	0/2/2/2
23	8CT	4K	101	-	-	10/29/63/63	0/2/2/2
32	ZEX	14	418	-	-	9/29/67/67	0/2/2/2
21	CL7	1C	511	3	2/2/10/20	5/12/88/115	-
21	CL7	1C	506	3	2/2/14/20	15/33/109/115	-
21	CL7	1B	609	2	2/2/15/20	14/39/115/115	-
21	CL7	24	415	-	2/2/11/20	11/15/91/115	-
23	8CT	1B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	31	408	-	2/2/15/20	16/39/115/115	-
21	CL7	43	418	19	2/2/12/20	9/21/97/115	-
21	CL7	12	501	16	2/2/15/20	17/39/115/115	-
21	CL7	21	406	18	2/2/14/20	13/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	44	414	20	2/2/12/20	8/25/101/115	-
32	ZEX	33	520	-	-	10/29/67/67	0/2/2/2
21	CL7	3B	611	2	2/2/15/20	17/39/115/115	-
21	CL7	21	414	18	2/2/10/20	3/10/86/115	-
25	SQD	23	422	-	-	3/41/61/69	0/1/1/1
21	CL7	21	404	-	2/2/15/20	15/39/115/115	-
21	CL7	31	411	-	2/2/11/20	7/15/91/115	-
21	CL7	1B	622	2	2/2/11/20	8/15/91/115	-
27	DGD	3C	516	-	-	9/51/91/95	0/2/2/2
21	CL7	22	508	16	2/2/11/20	5/15/91/115	-
21	CL7	1B	601	-	2/2/10/20	4/10/86/115	-
21	CL7	21	411	-	2/2/11/20	7/15/91/115	-
21	CL7	33	512	19	2/2/13/20	12/27/103/115	-
21	CL7	14	408	20	2/2/11/20	4/15/91/115	-
21	CL7	21	409	18	2/2/11/20	6/15/91/115	-
22	PHO	4A	402	-	-	3/37/103/103	0/5/6/6
26	LHG	1D	409	-	-	7/53/53/53	-
25	SQD	3A	406	-	-	3/29/49/69	0/1/1/1
21	CL7	23	407	19	2/2/11/20	13/15/91/115	-
21	CL7	1D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	21	407	18	2/2/10/20	4/10/86/115	-
26	LHG	3B	623	-	-	3/49/49/53	-
21	CL7	12	516	16	2/2/15/20	16/39/115/115	-
21	CL7	4C	503	3	2/2/15/20	19/39/115/115	-
24	LMG	31	401	-	-	5/46/66/70	0/1/1/1
21	CL7	32	501	16	2/2/15/20	17/39/115/115	-
21	CL7	41	409	18	2/2/11/20	6/15/91/115	-
32	ZEX	22	524	-	-	11/29/67/67	0/2/2/2
31	HEM	2F	101	-	-	8/14/54/54	-
21	CL7	34	411	20	2/2/15/20	14/39/115/115	-
21	CL7	44	404	20	2/2/15/20	14/39/115/115	-
21	CL7	32	505	16	2/2/15/20	18/39/115/115	-
25	SQD	23	424	-	-	7/45/65/69	0/1/1/1
25	SQD	12	521	-	-	7/45/65/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	22	512	16	2/2/15/20	18/39/115/115	-
21	CL7	22	514	-	2/2/11/20	9/15/91/115	-
24	LMG	41	401	-	-	5/46/66/70	0/1/1/1
21	CL7	42	503	-	2/2/15/20	17/39/115/115	-
21	CL7	23	403	19	2/2/13/20	12/31/107/115	-
21	CL7	3B	603	2	2/2/15/20	12/39/115/115	-
21	CL7	1C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	4B	610	2	2/2/15/20	14/39/115/115	-
21	CL7	31	417	18	2/2/13/20	9/27/103/115	-
25	SQD	22	521	-	-	7/45/65/69	0/1/1/1
21	CL7	31	402	18	2/2/14/20	16/33/109/115	-
32	ZEX	13	520	-	-	10/29/67/67	0/2/2/2
21	CL7	4C	513	3	2/2/11/20	8/15/91/115	-
26	LHG	2B	624	-	-	3/49/49/53	-
21	CL7	13	504	-	2/2/15/20	16/39/115/115	-
21	CL7	1B	602	2	2/2/14/20	9/33/109/115	-
21	CL7	11	404	-	2/2/15/20	15/39/115/115	-
21	CL7	13	514	-	2/2/11/20	5/15/91/115	-
21	CL7	14	412	20	2/2/15/20	17/39/115/115	-
21	CL7	2C	503	3	2/2/15/20	19/39/115/115	-
27	DGD	4B	625	-	-	7/51/91/95	0/2/2/2
23	8CT	1B	618	-	-	10/29/63/63	0/2/2/2
21	CL7	24	413	20	2/2/14/20	7/33/109/115	-
21	CL7	33	510	-	2/2/15/20	15/39/115/115	-
21	CL7	34	407	-	2/2/10/20	3/10/86/115	-
21	CL7	3B	622	2	2/2/11/20	8/15/91/115	-
25	SQD	13	521	-	-	3/41/61/69	0/1/1/1
25	SQD	1B	620	-	-	5/49/69/69	0/1/1/1
25	SQD	1A	406	-	-	3/29/49/69	0/1/1/1
26	LHG	1B	625	-	-	6/53/53/53	-
21	CL7	23	406	19	2/2/15/20	14/39/115/115	-
26	LHG	2A	408	-	-	5/50/50/53	-
21	CL7	24	417	20	2/2/10/20	6/12/88/115	-
32	ZEX	24	403	-	-	10/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	14	413	20	2/2/14/20	7/33/109/115	-
21	CL7	42	515	-	2/2/11/20	8/15/91/115	-
23	8CT	4B	620	-	-	4/29/63/63	0/2/2/2
21	CL7	22	506	16	2/2/15/20	14/39/115/115	-
21	CL7	1C	509	3	2/2/15/20	20/39/115/115	-
21	CL7	14	411	20	2/2/15/20	14/39/115/115	-
21	CL7	41	403	-	2/2/14/20	11/33/109/115	-
32	ZEX	41	421	-	-	14/29/67/67	0/2/2/2
21	CL7	43	404	-	2/2/15/20	20/39/115/115	-
21	CL7	11	406	18	2/2/14/20	13/36/112/115	-
21	CL7	4B	603	2	2/2/14/20	9/33/109/115	-
25	SQD	42	523	-	-	0/36/56/69	0/1/1/1
21	CL7	3A	407	-	2/2/15/20	16/39/115/115	-
21	CL7	22	518	16	2/2/15/20	12/39/115/115	-
27	DGD	1B	624	-	-	7/51/91/95	0/2/2/2
26	LHG	1A	408	-	-	5/50/50/53	-
21	CL7	44	410	20	2/2/11/20	9/15/91/115	-
23	8CT	1B	626	-	-	10/29/63/63	0/2/2/2
31	HEM	3F	101	-	-	8/14/54/54	-
25	SQD	12	523	-	-	0/36/56/69	0/1/1/1
21	CL7	41	408	-	2/2/15/20	16/39/115/115	-
21	CL7	42	502	16	2/2/15/20	17/39/115/115	-
21	CL7	23	414	-	2/2/11/20	9/15/91/115	-
21	CL7	1A	401	1	2/2/15/20	18/39/115/115	-
21	CL7	1C	507	-	2/2/15/20	17/39/115/115	-
21	CL7	24	412	20	2/2/15/20	17/39/115/115	-
21	CL7	4B	614	2	2/2/13/20	5/27/103/115	-
32	ZEX	22	522	-	-	6/29/67/67	0/2/2/2
31	HEM	4F	101	-	-	8/14/54/54	-
23	8CT	3B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	4C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	12	502	16	2/2/15/20	17/39/115/115	-
21	CL7	3C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	2D	404	4	2/2/13/20	13/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	13	518	19	2/2/11/20	7/15/91/115	-
21	CL7	2D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	11	410	-	2/2/15/20	17/39/115/115	-
25	SQD	2A	406	-	-	3/29/49/69	0/1/1/1
21	CL7	21	415	-	2/2/10/20	7/10/86/115	-
21	CL7	22	517	16	2/2/15/20	21/39/115/115	-
21	CL7	12	509	-	2/2/15/20	16/39/115/115	-
21	CL7	4B	604	2	2/2/15/20	12/39/115/115	-
30	PL9	3D	407	-	-	9/53/73/73	0/1/1/1
26	LHG	2D	409	-	-	7/53/53/53	-
21	CL7	12	511	16	2/2/14/20	16/33/109/115	-
21	CL7	1B	614	2	2/2/14/20	14/33/109/115	-
23	8CT	2A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	4B	611	-	2/2/15/20	11/39/115/115	-
21	CL7	41	418	18	2/2/15/20	22/39/115/115	-
24	LMG	2B	622	-	-	7/46/66/70	0/1/1/1
21	CL7	1B	607	-	2/2/14/20	11/33/109/115	-
21	CL7	3B	601	-	2/2/10/20	4/10/86/115	-
21	CL7	4A	407	-	2/2/15/20	16/39/115/115	-
26	LHG	43	425	-	-	3/40/40/53	-
21	CL7	41	402	18	2/2/14/20	16/33/109/115	-
25	SQD	4B	621	-	-	5/49/69/69	0/1/1/1
21	CL7	12	504	-	2/2/11/20	6/15/91/115	-
21	CL7	23	417	19	2/2/13/20	16/27/103/115	-
21	CL7	2C	505	3	2/2/15/20	16/39/115/115	-
21	CL7	31	407	18	2/2/10/20	4/10/86/115	-
21	CL7	44	416	20	2/2/10/20	7/10/86/115	-
21	CL7	2C	510	3	2/2/15/20	22/39/115/115	-
21	CL7	22	511	16	2/2/14/20	16/33/109/115	-
21	CL7	1B	604	2	2/2/15/20	17/39/115/115	-
21	CL7	1C	512	3	2/2/10/20	4/10/86/115	-
21	CL7	3C	506	3	2/2/14/20	15/33/109/115	-
21	CL7	11	418	18	2/2/15/20	22/39/115/115	-
30	PL9	2D	407	-	-	9/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	12	503	-	2/2/15/20	17/39/115/115	-
21	CL7	11	402	18	2/2/14/20	16/33/109/115	-
25	SQD	11	423	-	-	3/27/47/69	0/1/1/1
21	CL7	33	511	19	2/2/15/20	19/39/115/115	-
21	CL7	44	405	-	2/2/15/20	18/39/115/115	-
21	CL7	11	411	-	2/2/11/20	7/15/91/115	-
21	CL7	2B	603	2	2/2/14/20	9/33/109/115	-
21	CL7	43	419	19	2/2/11/20	7/15/91/115	-
21	CL7	43	405	-	2/2/15/20	16/39/115/115	-
21	CL7	42	505	16	2/2/15/20	18/39/115/115	-
21	CL7	42	510	16	2/2/15/20	20/39/115/115	-
23	8CT	2B	618	-	-	7/29/63/63	0/2/2/2
26	LHG	4D	409	-	-	7/53/53/53	-
21	CL7	24	406	20	2/2/15/20	24/39/115/115	-
21	CL7	2C	509	3	2/2/15/20	20/39/115/115	-
21	CL7	1C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	32	509	-	2/2/15/20	16/39/115/115	-
21	CL7	4B	613	2	2/2/15/20	17/39/115/115	-
21	CL7	2C	512	3	2/2/10/20	4/10/86/115	-
25	SQD	31	423	-	-	3/27/47/69	0/1/1/1
32	ZEX	11	422	-	-	6/29/67/67	0/2/2/2
23	8CT	1B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	1A	403	1	2/2/13/20	9/27/103/115	-
21	CL7	41	411	-	2/2/11/20	7/15/91/115	-
21	CL7	33	507	-	2/2/15/20	15/39/115/115	-
26	LHG	4B	624	-	-	3/49/49/53	-
21	CL7	4B	615	2	2/2/14/20	14/33/109/115	-
21	CL7	41	417	18	2/2/13/20	9/27/103/115	-
22	PHO	2A	402	-	-	3/37/103/103	0/5/6/6
24	LMG	4A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	22	504	-	2/2/11/20	6/15/91/115	-
26	LHG	3B	625	-	-	6/53/53/53	-
21	CL7	11	408	-	2/2/15/20	16/39/115/115	-
25	SQD	13	523	-	-	7/45/65/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	8CT	1A	404	-	-	5/29/63/63	0/2/2/2
23	8CT	3B	618	-	-	10/29/63/63	0/2/2/2
21	CL7	32	511	16	2/2/14/20	16/33/109/115	-
21	CL7	43	416	-	2/2/10/20	0/10/86/115	-
21	CL7	11	420	18	2/2/11/20	6/15/91/115	-
26	LHG	33	524	-	-	3/40/40/53	-
32	ZEX	13	519	-	-	10/29/67/67	0/2/2/2
21	CL7	2A	407	-	2/2/15/20	16/39/115/115	-
21	CL7	23	410	19	2/2/15/20	17/39/115/115	-
32	ZEX	14	420	-	-	12/29/67/67	0/2/2/2
21	CL7	12	507	-	2/2/15/20	20/39/115/115	-
21	CL7	2C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	1B	613	2	2/2/13/20	5/27/103/115	-
21	CL7	21	412	18	2/2/11/20	10/15/91/115	-

The worst 5 of 8119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2B	601	8CT	C02-C03	14.85	1.60	1.34
23	1B	626	8CT	C02-C03	14.83	1.60	1.34
23	4B	619	8CT	C02-C03	14.82	1.60	1.34
23	4B	601	8CT	C02-C03	14.80	1.60	1.34
23	3B	626	8CT	C02-C03	14.80	1.60	1.34

The worst 5 of 11011 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1A	403	CL7	C3C-C4C-NC	10.55	117.82	110.18
21	2A	403	CL7	C3C-C4C-NC	10.52	117.81	110.18
21	3A	403	CL7	C3C-C4C-NC	10.51	117.80	110.18
21	4A	403	CL7	C3C-C4C-NC	10.50	117.78	110.18
21	33	505	CL7	C3C-C4C-NC	10.30	117.64	110.18

5 of 860 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1A	401	CL7	NA
21	1A	401	CL7	NC
21	1A	403	CL7	NA

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Mol	Chain	Res	Type	Atom
21	1A	403	CL7	NC
21	1A	407	CL7	NA

5 of 6574 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1A	401	CL7	C2B-C3B-CAB-OBB
21	1A	401	CL7	C4B-C3B-CAB-OBB
21	1A	403	CL7	O1A-CGA-O2A-C1
21	1A	403	CL7	CBA-CGA-O2A-C1
21	1A	403	CL7	C1A-C2A-CAA-CBA

There are no ring outliers.

540 monomers are involved in 2632 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	33	502	CL7	7	0
21	2C	508	CL7	4	0
21	3C	511	CL7	1	0
25	32	521	SQD	1	0
21	22	507	CL7	5	0
21	23	404	CL7	11	0
21	23	415	CL7	2	0
21	3C	503	CL7	8	0
21	4B	609	CL7	4	0
21	1B	608	CL7	4	0
21	33	513	CL7	12	0
32	22	519	ZEX	3	0
21	44	409	CL7	2	0
25	42	521	SQD	2	0
21	21	402	CL7	10	0
21	31	404	CL7	8	0
21	23	409	CL7	14	0
21	11	409	CL7	3	0
21	2B	610	CL7	4	0
21	14	406	CL7	13	0
21	3C	505	CL7	5	0
21	31	418	CL7	7	0
21	4D	405	CL7	2	0
21	13	507	CL7	10	0
21	43	410	CL7	8	0
32	14	419	ZEX	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	2B	626	LHG	2	0
21	2B	604	CL7	9	0
21	31	414	CL7	8	0
21	34	414	CL7	4	0
21	21	408	CL7	7	0
23	2C	518	8CT	1	0
21	32	510	CL7	6	0
27	1C	516	DGD	5	0
30	4D	407	PL9	7	0
21	34	404	CL7	5	0
21	14	405	CL7	7	0
21	2B	608	CL7	7	0
21	32	517	CL7	10	0
24	1B	621	LMG	5	0
21	41	412	CL7	2	0
32	13	525	ZEX	24	0
21	43	409	CL7	14	0
32	12	520	ZEX	33	0
32	34	420	ZEX	10	0
32	44	403	ZEX	21	0
32	34	418	ZEX	9	0
24	1A	405	LMG	2	0
21	22	501	CL7	7	0
21	12	508	CL7	4	0
32	12	524	ZEX	16	0
26	14	401	LHG	2	0
21	24	411	CL7	7	0
21	2C	506	CL7	3	0
24	4B	622	LMG	6	0
26	4B	626	LHG	2	0
21	4C	502	CL7	3	0
21	43	407	CL7	5	0
21	1C	504	CL7	3	0
24	3D	410	LMG	1	0
21	23	418	CL7	2	0
21	44	417	CL7	4	0
25	3B	620	SQD	2	0
22	4D	408	PHO	3	0
21	12	512	CL7	8	0
21	1B	615	CL7	4	0
21	14	404	CL7	6	0
21	34	408	CL7	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	41	410	CL7	6	0
32	12	522	ZEX	18	0
21	42	506	CL7	2	0
21	24	408	CL7	4	0
21	42	509	CL7	7	0
23	3C	518	8CT	1	0
26	23	425	LHG	1	0
21	2B	605	CL7	7	0
21	42	518	CL7	10	0
21	34	413	CL7	4	0
21	42	516	CL7	6	0
24	3A	405	LMG	2	0
21	3A	401	CL7	19	0
21	33	518	CL7	3	0
21	44	415	CL7	4	0
25	43	422	SQD	3	0
21	12	518	CL7	11	0
21	3C	507	CL7	4	0
21	13	512	CL7	6	0
32	22	520	ZEX	29	0
32	32	520	ZEX	30	0
32	21	421	ZEX	15	0
21	3C	508	CL7	3	0
21	31	413	CL7	6	0
21	31	405	CL7	5	0
21	44	408	CL7	4	0
32	23	423	ZEX	26	0
21	2C	511	CL7	1	0
21	2C	504	CL7	3	0
21	3B	604	CL7	10	0
21	43	417	CL7	6	0
21	32	516	CL7	5	0
21	2B	615	CL7	2	0
21	13	501	CL7	8	0
21	32	512	CL7	7	0
26	44	401	LHG	2	0
32	43	401	ZEX	24	0
32	32	522	ZEX	17	0
25	41	423	SQD	1	0
21	4C	507	CL7	3	0
32	23	420	ZEX	17	0
21	2B	616	CL7	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	42	511	CL7	7	0
21	23	413	CL7	7	0
21	33	504	CL7	9	0
21	2C	513	CL7	3	0
22	3D	408	PHO	4	0
21	32	513	CL7	6	0
21	43	415	CL7	2	0
24	3B	621	LMG	6	0
21	1C	505	CL7	6	0
21	33	503	CL7	10	0
23	1C	515	8CT	1	0
32	41	422	ZEX	23	0
21	1C	510	CL7	4	0
21	43	406	CL7	18	0
21	3C	513	CL7	3	0
21	3B	606	CL7	5	0
32	32	524	ZEX	16	0
21	21	410	CL7	7	0
25	4A	406	SQD	2	0
21	23	416	CL7	2	0
21	3A	403	CL7	2	0
21	31	409	CL7	3	0
21	3C	509	CL7	4	0
32	12	519	ZEX	3	0
21	2C	507	CL7	5	0
23	4C	518	8CT	1	0
21	13	517	CL7	2	0
24	21	401	LMG	2	0
21	41	413	CL7	6	0
32	43	420	ZEX	17	0
21	43	413	CL7	8	0
26	3D	409	LHG	3	0
21	1B	611	CL7	4	0
21	11	416	CL7	1	0
21	1B	605	CL7	7	0
32	23	421	ZEX	10	0
21	32	515	CL7	2	0
21	23	402	CL7	10	0
21	14	409	CL7	2	0
21	2C	502	CL7	4	0
26	1B	623	LHG	6	0
21	32	502	CL7	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	42	507	CL7	5	0
21	2A	401	CL7	17	0
21	41	416	CL7	1	0
21	3B	602	CL7	4	0
21	41	414	CL7	2	0
32	42	519	ZEX	3	0
32	24	419	ZEX	7	0
21	13	506	CL7	5	0
21	33	516	CL7	5	0
21	4B	608	CL7	8	0
21	13	509	CL7	9	0
21	3C	502	CL7	3	0
21	44	412	CL7	2	0
21	1C	508	CL7	3	0
21	22	513	CL7	6	0
21	32	504	CL7	3	0
21	14	410	CL7	2	0
21	4A	403	CL7	2	0
22	2D	408	PHO	3	0
21	1C	503	CL7	7	0
21	23	411	CL7	4	0
30	1D	407	PL9	7	0
21	21	418	CL7	7	0
21	43	402	CL7	9	0
25	21	423	SQD	1	0
21	42	512	CL7	7	0
27	2C	516	DGD	4	0
32	33	525	ZEX	24	0
32	44	420	ZEX	12	0
21	33	509	CL7	8	0
21	11	414	CL7	2	0
23	1C	518	8CT	1	0
21	34	415	CL7	4	0
21	31	420	CL7	6	0
21	21	403	CL7	5	0
21	21	417	CL7	5	0
21	3C	510	CL7	4	0
32	34	403	ZEX	21	0
21	4D	404	CL7	7	0
21	34	405	CL7	7	0
21	23	408	CL7	9	0
21	43	412	CL7	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	42	501	CL7	6	0
23	3C	515	8CT	1	0
21	24	404	CL7	6	0
21	2B	606	CL7	7	0
21	22	502	CL7	7	0
21	2B	607	CL7	6	0
21	44	406	CL7	12	0
21	33	508	CL7	14	0
21	3C	504	CL7	3	0
21	2B	612	CL7	4	0
21	4B	605	CL7	8	0
32	24	418	ZEX	10	0
21	3B	607	CL7	8	0
21	33	515	CL7	2	0
21	42	514	CL7	2	0
21	4C	506	CL7	4	0
21	32	507	CL7	5	0
22	1D	408	PHO	4	0
32	14	403	ZEX	22	0
21	4C	510	CL7	3	0
21	42	504	CL7	3	0
21	13	510	CL7	6	0
21	44	413	CL7	4	0
24	1D	410	LMG	1	0
21	4B	606	CL7	6	0
21	13	513	CL7	12	0
21	41	406	CL7	14	0
21	2A	403	CL7	2	0
21	24	414	CL7	3	0
21	14	415	CL7	4	0
32	34	419	ZEX	8	0
22	1A	402	PHO	3	0
21	3B	612	CL7	3	0
21	12	517	CL7	8	0
21	22	505	CL7	17	0
21	33	514	CL7	2	0
21	22	510	CL7	6	0
21	1B	606	CL7	5	0
21	4C	511	CL7	1	0
21	42	517	CL7	10	0
21	12	514	CL7	2	0
21	32	506	CL7	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	33	521	SQD	4	0
32	33	519	ZEX	17	0
21	32	518	CL7	10	0
21	4B	616	CL7	4	0
21	13	505	CL7	17	0
21	4C	509	CL7	3	0
21	41	407	CL7	3	0
32	24	420	ZEX	12	0
26	34	401	LHG	2	0
32	13	522	ZEX	26	0
21	31	416	CL7	1	0
21	3D	405	CL7	2	0
21	3B	609	CL7	4	0
21	3B	613	CL7	2	0
32	43	421	ZEX	11	0
21	34	409	CL7	2	0
21	32	508	CL7	3	0
21	33	501	CL7	8	0
21	13	511	CL7	5	0
21	1C	513	CL7	3	0
32	44	418	ZEX	9	0
23	2C	515	8CT	1	0
21	4C	504	CL7	3	0
21	31	410	CL7	7	0
21	4A	401	CL7	18	0
24	11	401	LMG	2	0
21	41	404	CL7	8	0
21	14	414	CL7	4	0
21	2B	613	CL7	5	0
23	4C	515	8CT	1	0
21	13	516	CL7	5	0
21	1A	407	CL7	16	0
21	31	412	CL7	2	0
21	44	411	CL7	8	0
21	43	403	CL7	8	0
25	43	424	SQD	2	0
21	13	508	CL7	15	0
27	4C	516	DGD	4	0
27	3B	624	DGD	2	0
24	2D	410	LMG	1	0
21	11	417	CL7	3	0
21	3C	512	CL7	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	13	503	CL7	10	0
25	2B	621	SQD	2	0
21	22	516	CL7	6	0
21	33	506	CL7	5	0
21	24	410	CL7	2	0
21	1B	603	CL7	7	0
21	12	515	CL7	3	0
21	44	407	CL7	6	0
21	1C	502	CL7	4	0
21	41	420	CL7	6	0
21	43	408	CL7	10	0
21	22	515	CL7	3	0
32	33	522	ZEX	25	0
21	23	419	CL7	3	0
21	22	503	CL7	5	0
21	1B	610	CL7	3	0
21	43	414	CL7	13	0
21	32	503	CL7	9	0
21	4B	612	CL7	4	0
21	34	406	CL7	13	0
32	42	520	ZEX	31	0
21	42	513	CL7	6	0
21	43	411	CL7	6	0
21	11	407	CL7	3	0
21	24	405	CL7	6	0
21	2B	609	CL7	4	0
21	24	409	CL7	2	0
21	23	405	CL7	8	0
32	42	524	ZEX	17	0
21	31	406	CL7	13	0
21	34	410	CL7	2	0
21	3B	608	CL7	4	0
21	1B	612	CL7	3	0
21	24	407	CL7	6	0
26	24	401	LHG	2	0
21	13	502	CL7	7	0
21	4C	505	CL7	6	0
32	11	421	ZEX	13	0
21	11	403	CL7	4	0
21	2B	614	CL7	2	0
26	13	524	LHG	1	0
21	21	420	CL7	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	4C	508	CL7	5	0
21	11	405	CL7	4	0
21	4B	607	CL7	4	0
22	3A	402	PHO	3	0
27	2B	625	DGD	2	0
21	21	413	CL7	6	0
32	31	421	ZEX	15	0
21	33	517	CL7	2	0
21	41	405	CL7	4	0
32	32	519	ZEX	4	0
21	3B	614	CL7	2	0
21	11	412	CL7	2	0
21	4C	512	CL7	1	0
21	3B	610	CL7	1	0
21	3D	404	CL7	6	0
32	23	401	ZEX	24	0
21	12	510	CL7	6	0
24	4D	410	LMG	1	0
21	21	416	CL7	1	0
21	12	513	CL7	6	0
21	13	515	CL7	2	0
32	31	422	ZEX	22	0
21	11	413	CL7	6	0
21	3B	615	CL7	4	0
21	1D	404	CL7	6	0
21	23	412	CL7	5	0
21	34	417	CL7	4	0
21	14	407	CL7	6	0
21	42	508	CL7	3	0
24	2A	405	LMG	2	0
31	1F	101	HEM	3	0
32	43	423	ZEX	27	0
21	3B	605	CL7	6	0
25	33	523	SQD	1	0
21	32	514	CL7	2	0
32	21	422	ZEX	21	0
21	12	506	CL7	2	0
21	21	405	CL7	4	0
21	2B	611	CL7	3	0
21	14	417	CL7	4	0
21	33	505	CL7	18	0
21	22	509	CL7	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	31	403	CL7	5	0
32	42	522	ZEX	19	0
21	12	505	CL7	15	0
21	34	412	CL7	4	0
32	44	419	ZEX	9	0
32	14	418	ZEX	9	0
21	1C	511	CL7	1	0
21	1C	506	CL7	5	0
21	1B	609	CL7	4	0
21	24	415	CL7	4	0
21	31	408	CL7	7	0
21	43	418	CL7	2	0
21	12	501	CL7	5	0
21	21	406	CL7	13	0
21	44	414	CL7	4	0
32	33	520	ZEX	11	0
21	3B	611	CL7	5	0
21	21	414	CL7	8	0
25	23	422	SQD	4	0
21	21	404	CL7	8	0
21	31	411	CL7	2	0
27	3C	516	DGD	5	0
21	22	508	CL7	3	0
21	21	411	CL7	2	0
21	33	512	CL7	7	0
21	14	408	CL7	4	0
21	21	409	CL7	4	0
22	4A	402	PHO	3	0
26	1D	409	LHG	3	0
25	3A	406	SQD	1	0
21	23	407	CL7	5	0
21	1D	405	CL7	2	0
21	21	407	CL7	3	0
26	3B	623	LHG	6	0
21	12	516	CL7	5	0
21	4C	503	CL7	8	0
24	31	401	LMG	3	0
21	32	501	CL7	6	0
21	41	409	CL7	4	0
32	22	524	ZEX	16	0
31	2F	101	HEM	4	0
21	34	411	CL7	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	44	404	CL7	6	0
21	32	505	CL7	15	0
25	23	424	SQD	2	0
25	12	521	SQD	2	0
21	22	512	CL7	8	0
21	22	514	CL7	2	0
24	41	401	LMG	2	0
21	42	503	CL7	7	0
21	23	403	CL7	7	0
21	3B	603	CL7	6	0
21	4B	610	CL7	4	0
21	31	417	CL7	3	0
25	22	521	SQD	2	0
21	31	402	CL7	10	0
32	13	520	ZEX	11	0
21	4C	513	CL7	3	0
26	2B	624	LHG	6	0
21	13	504	CL7	8	0
21	1B	602	CL7	5	0
21	11	404	CL7	7	0
21	13	514	CL7	2	0
21	14	412	CL7	3	0
21	2C	503	CL7	7	0
27	4B	625	DGD	2	0
21	24	413	CL7	5	0
21	33	510	CL7	5	0
21	34	407	CL7	6	0
25	13	521	SQD	4	0
25	1B	620	SQD	3	0
25	1A	406	SQD	3	0
26	1B	625	LHG	1	0
21	23	406	CL7	17	0
21	24	417	CL7	4	0
32	24	403	ZEX	22	0
21	14	413	CL7	5	0
21	42	515	CL7	2	0
21	22	506	CL7	3	0
21	1C	509	CL7	3	0
21	14	411	CL7	7	0
21	41	403	CL7	5	0
32	41	421	ZEX	15	0
21	43	404	CL7	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	11	406	CL7	12	0
21	4B	603	CL7	3	0
21	3A	407	CL7	15	0
21	22	518	CL7	11	0
27	1B	624	DGD	2	0
21	44	410	CL7	2	0
31	3F	101	HEM	3	0
21	41	408	CL7	8	0
21	42	502	CL7	7	0
21	23	414	CL7	12	0
21	1A	401	CL7	18	0
21	1C	507	CL7	5	0
21	24	412	CL7	3	0
21	4B	614	CL7	2	0
32	22	522	ZEX	18	0
31	4F	101	HEM	4	0
21	4C	501	CL7	4	0
21	12	502	CL7	7	0
21	3C	501	CL7	4	0
21	2D	404	CL7	7	0
21	13	518	CL7	3	0
21	2D	405	CL7	2	0
21	11	410	CL7	8	0
25	2A	406	SQD	2	0
21	22	517	CL7	9	0
21	12	509	CL7	5	0
21	4B	604	CL7	8	0
30	3D	407	PL9	7	0
26	2D	409	LHG	4	0
21	12	511	CL7	8	0
21	1B	614	CL7	2	0
21	4B	611	CL7	1	0
21	41	418	CL7	6	0
24	2B	622	LMG	5	0
21	1B	607	CL7	8	0
21	4A	407	CL7	14	0
26	43	425	LHG	1	0
21	41	402	CL7	10	0
25	4B	621	SQD	3	0
21	12	504	CL7	3	0
21	23	417	CL7	5	0
21	2C	505	CL7	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	31	407	CL7	3	0
21	2C	510	CL7	4	0
21	22	511	CL7	8	0
21	1B	604	CL7	9	0
21	1C	512	CL7	1	0
21	3C	506	CL7	4	0
21	11	418	CL7	6	0
30	2D	407	PL9	7	0
21	12	503	CL7	9	0
21	11	402	CL7	10	0
25	11	423	SQD	1	0
21	33	511	CL7	6	0
21	44	405	CL7	8	0
21	11	411	CL7	2	0
21	2B	603	CL7	4	0
21	43	419	CL7	3	0
21	43	405	CL7	9	0
21	42	505	CL7	14	0
21	42	510	CL7	7	0
26	4D	409	LHG	3	0
21	24	406	CL7	13	0
21	2C	509	CL7	2	0
21	1C	501	CL7	3	0
21	32	509	CL7	5	0
21	4B	613	CL7	6	0
21	2C	512	CL7	1	0
25	31	423	SQD	1	0
32	11	422	ZEX	21	0
21	1A	403	CL7	2	0
21	41	411	CL7	2	0
21	33	507	CL7	10	0
26	4B	624	LHG	6	0
21	4B	615	CL7	2	0
21	41	417	CL7	6	0
22	2A	402	PHO	3	0
24	4A	405	LMG	2	0
21	22	504	CL7	3	0
26	3B	625	LHG	1	0
21	11	408	CL7	7	0
25	13	523	SQD	2	0
21	32	511	CL7	9	0
21	43	416	CL7	2	0

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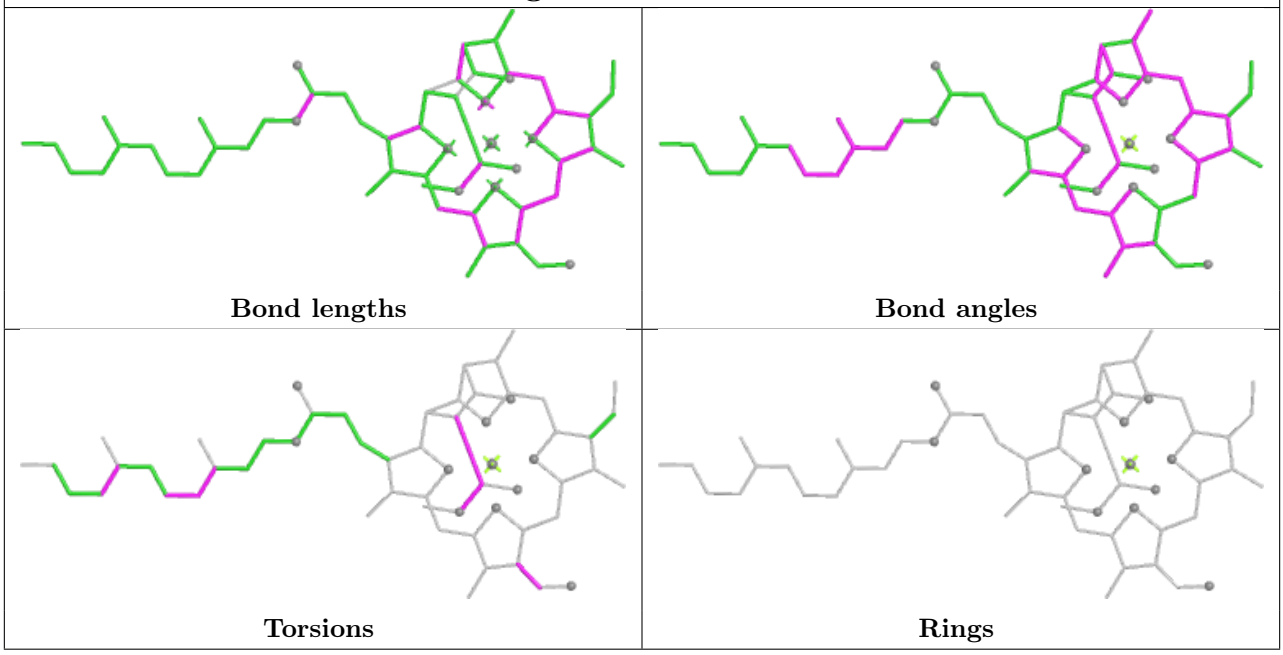
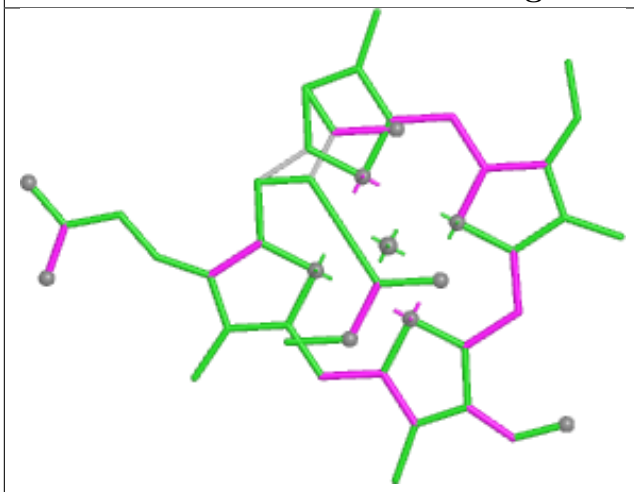
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	11	420	CL7	6	0
26	33	524	LHG	1	0
32	13	519	ZEX	16	0
21	2A	407	CL7	14	0
21	23	410	CL7	10	0
32	14	420	ZEX	10	0
21	12	507	CL7	6	0
21	2C	501	CL7	5	0
21	1B	613	CL7	2	0
21	21	412	CL7	2	0

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

Ligand CL7 33 502



Ligand CL7 31 419



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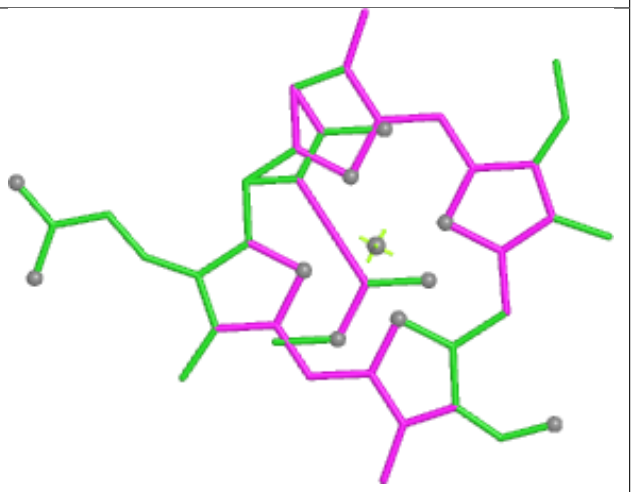
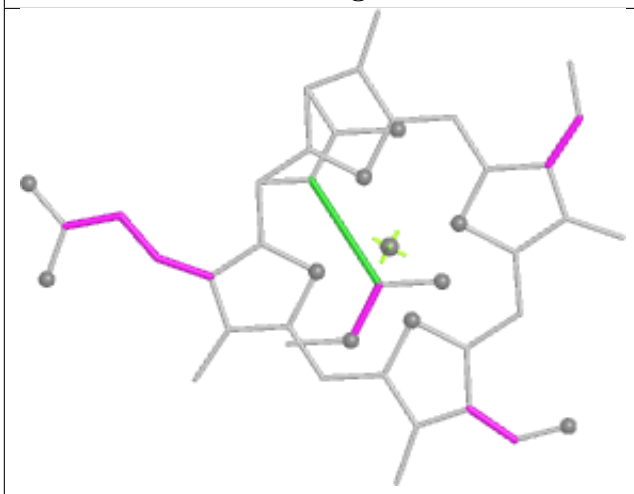


Bond angles

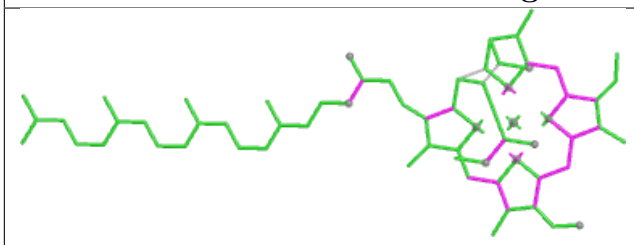


Torsions

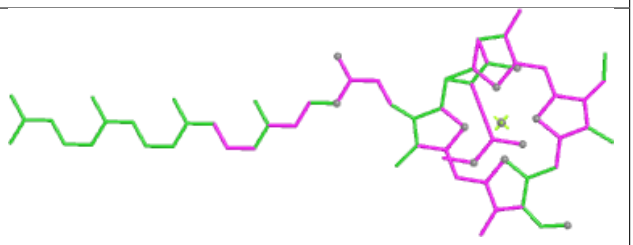


Rings

Ligand CL7 2C 508



Bond lengths



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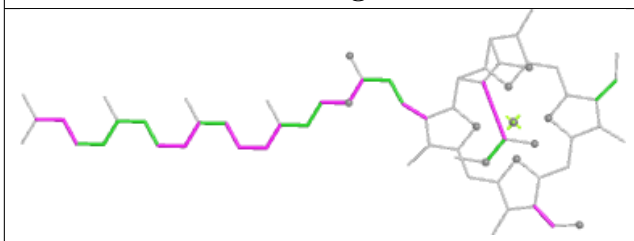
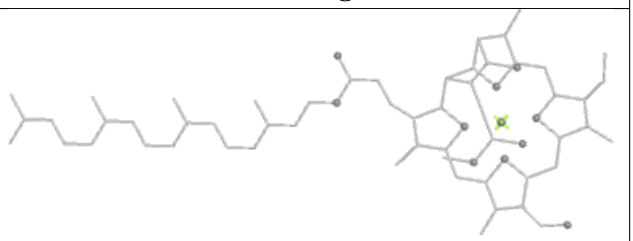
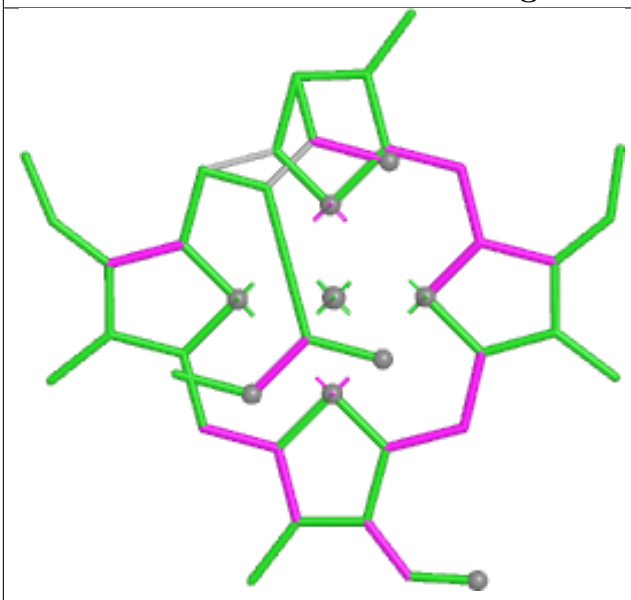


Torsions



Rings

Ligand CL7 3C 511



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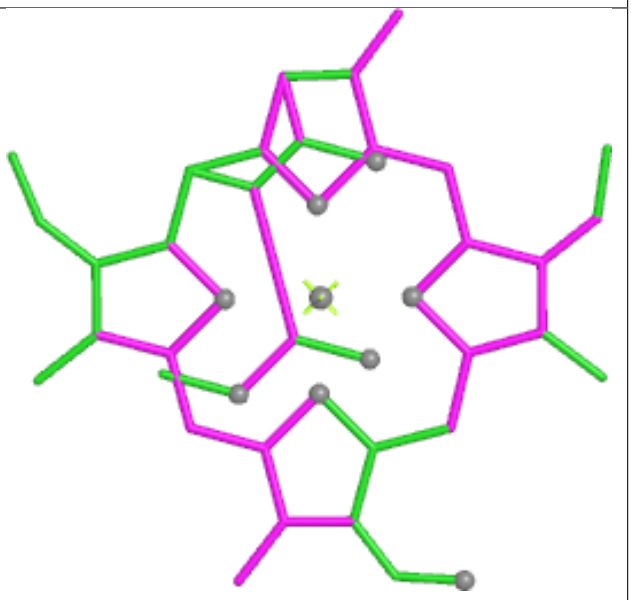

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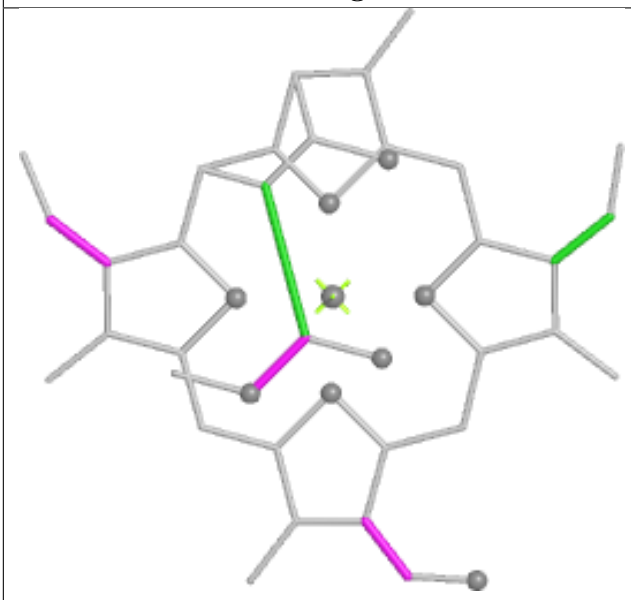
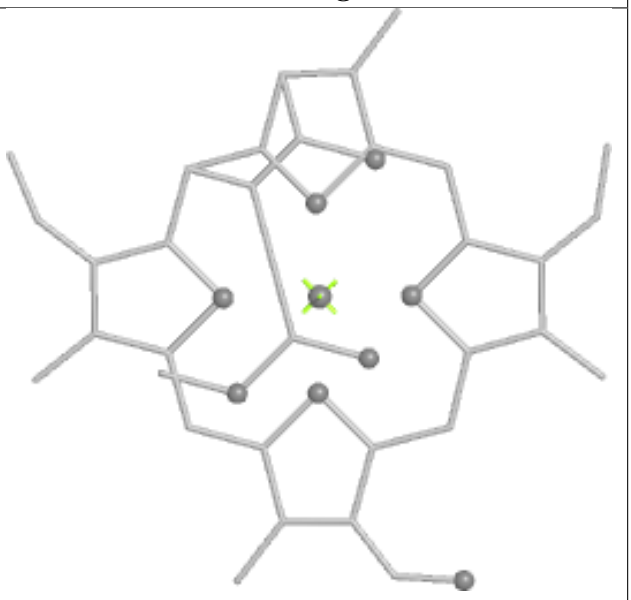
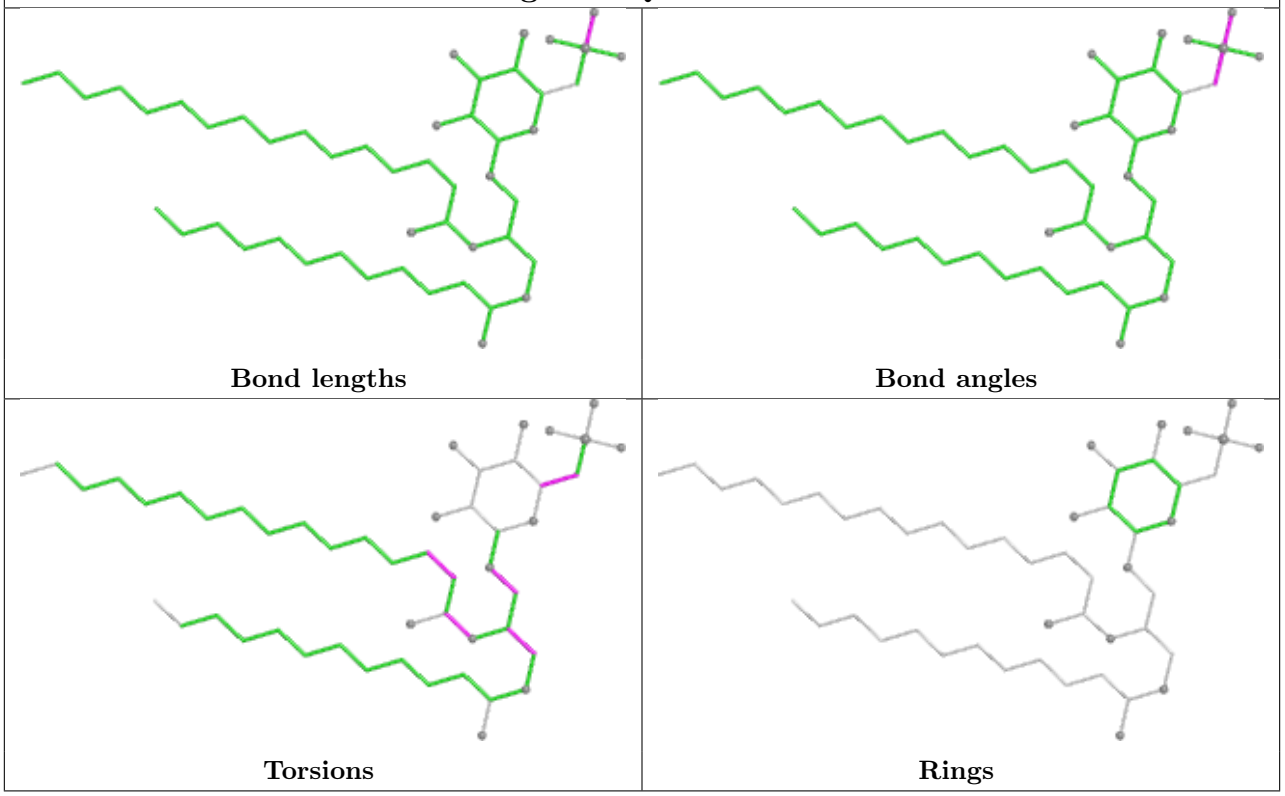


Torsions



Rings

Ligand SQD 32 521



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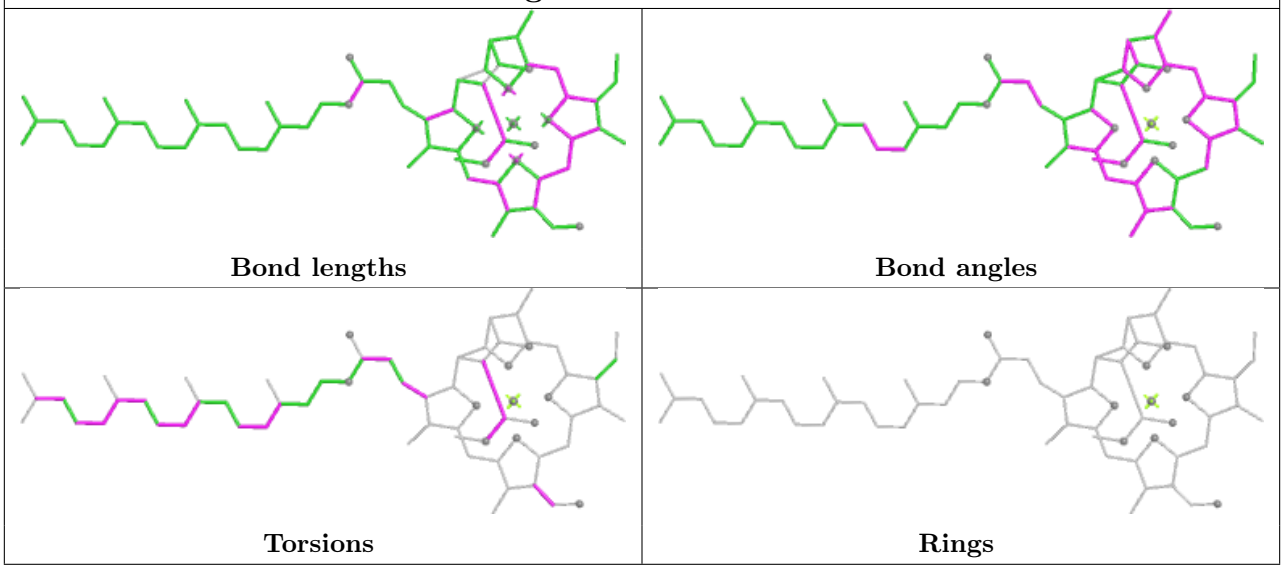

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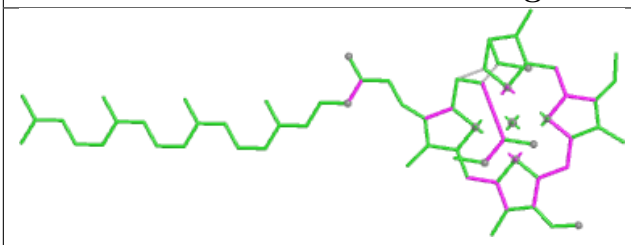

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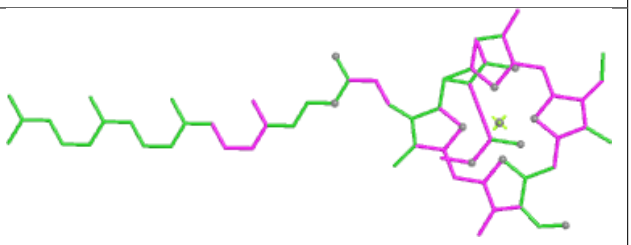

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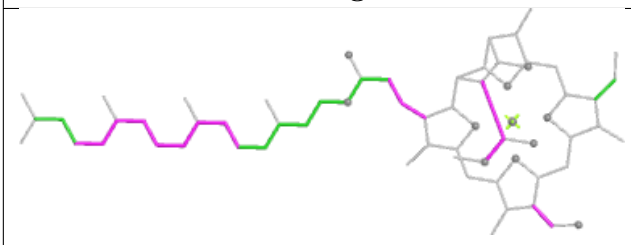

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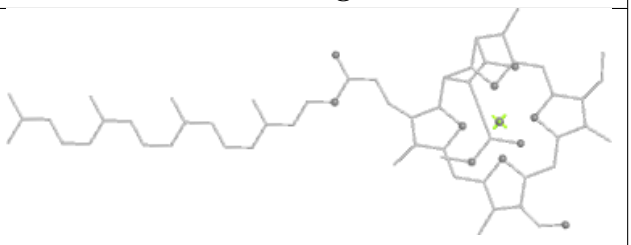

Rings

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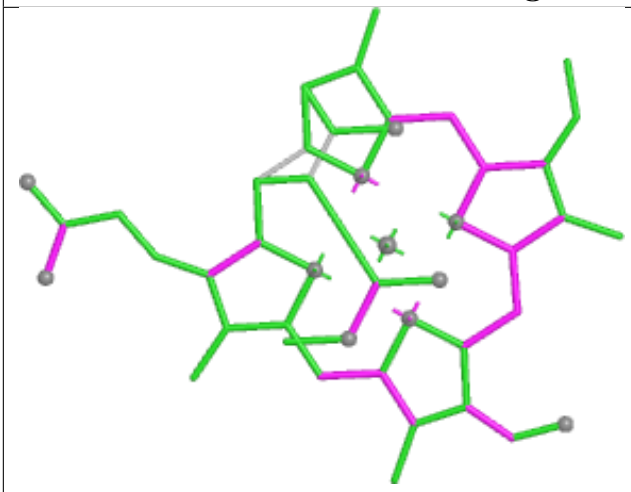

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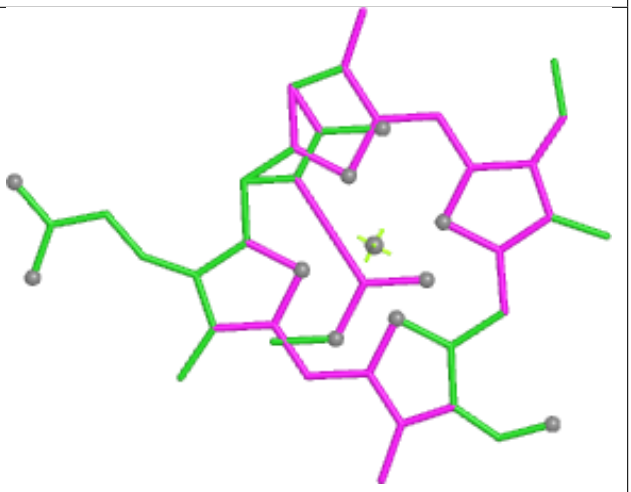

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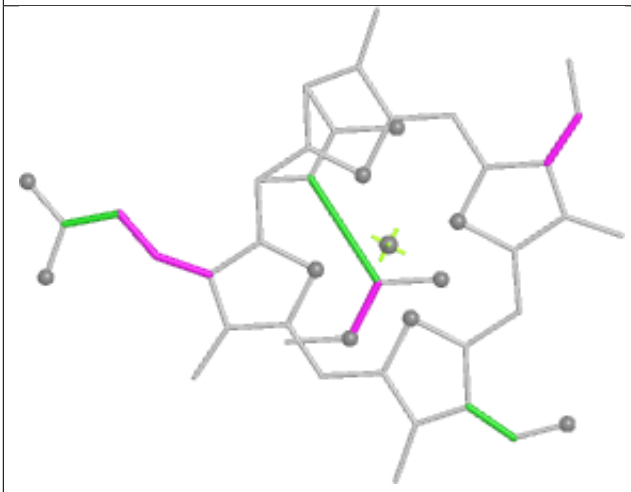
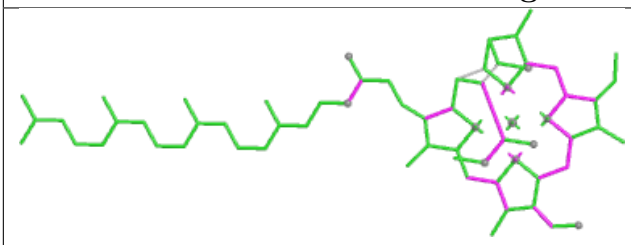


Torsions



Rings

Ligand CL7 3C 503



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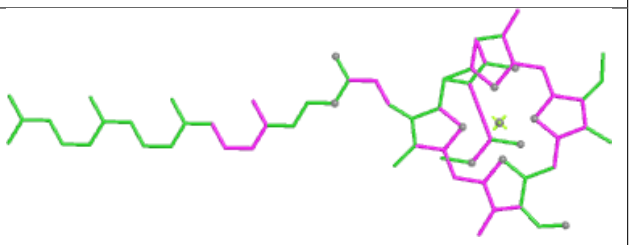

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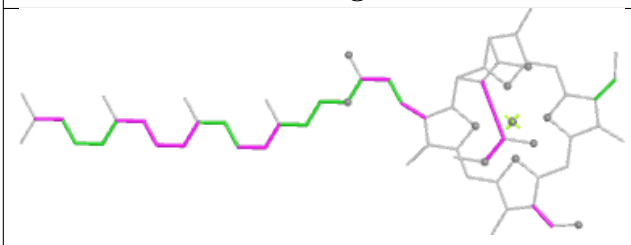

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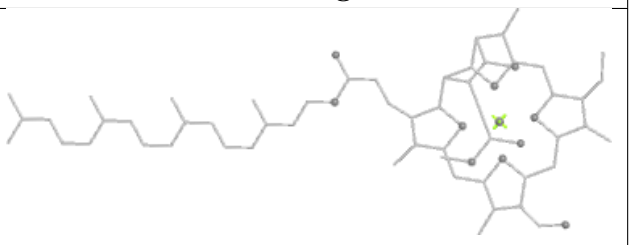
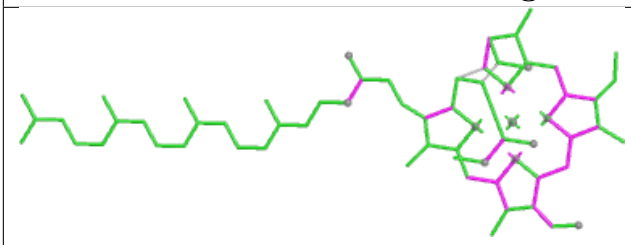


Rings

Ligand CL7 4B 609



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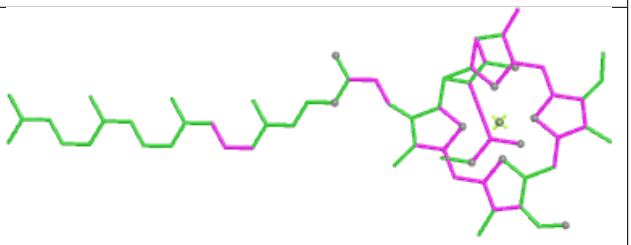

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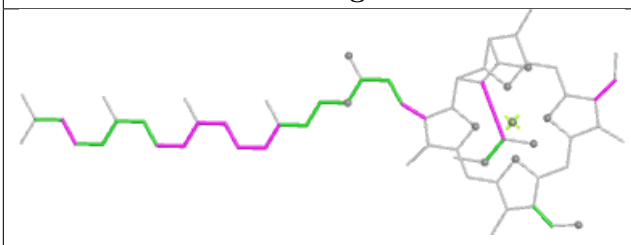

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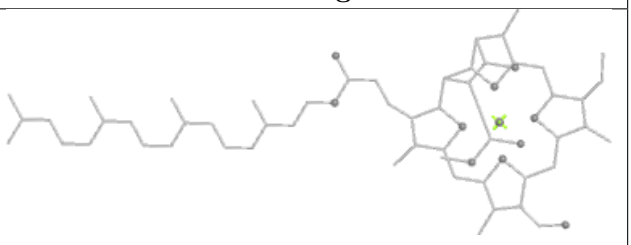
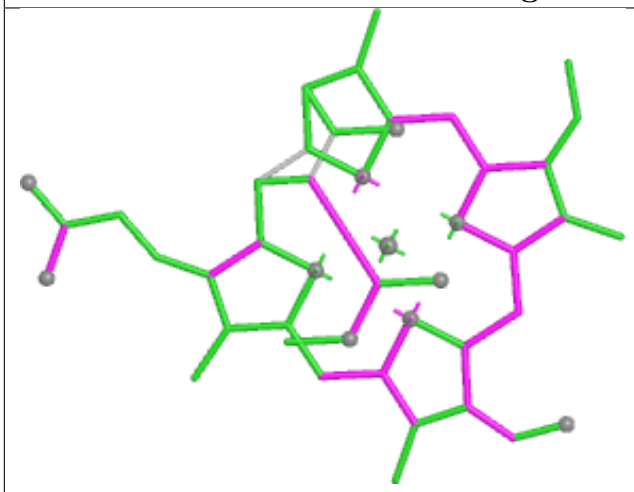


Rings

Ligand CL7 3B 616



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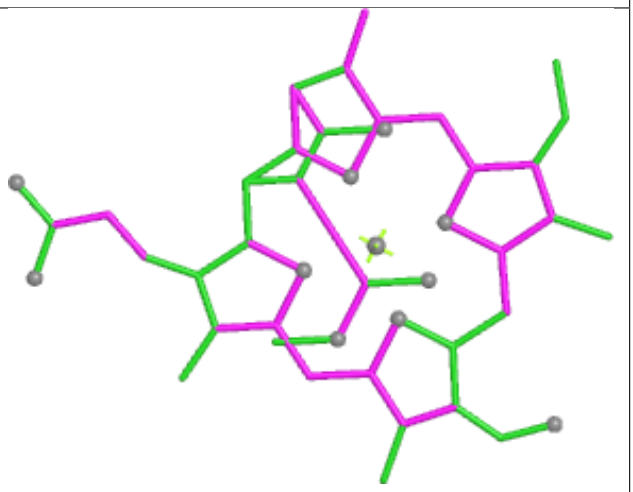

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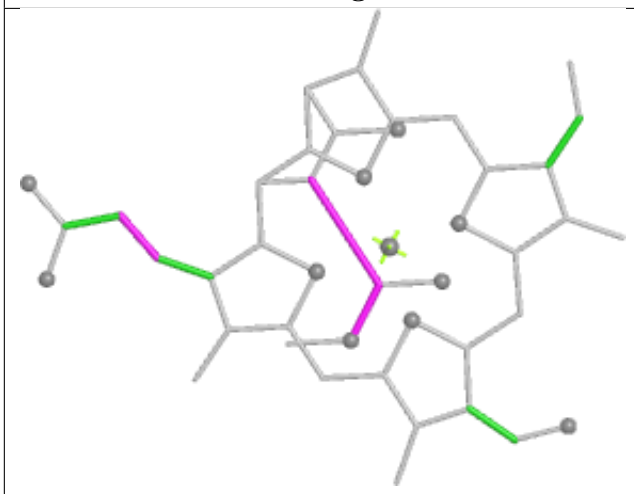
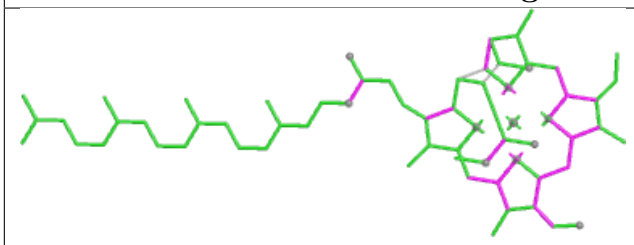


Torsions



Rings

Ligand CL7 1B 608



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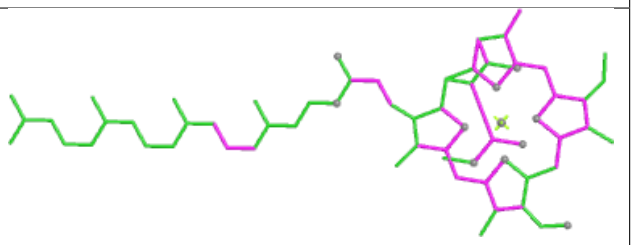

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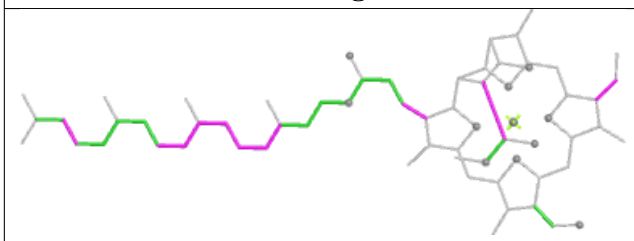

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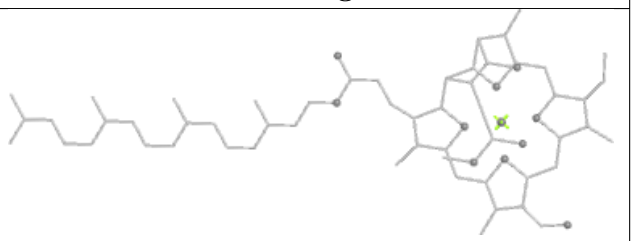
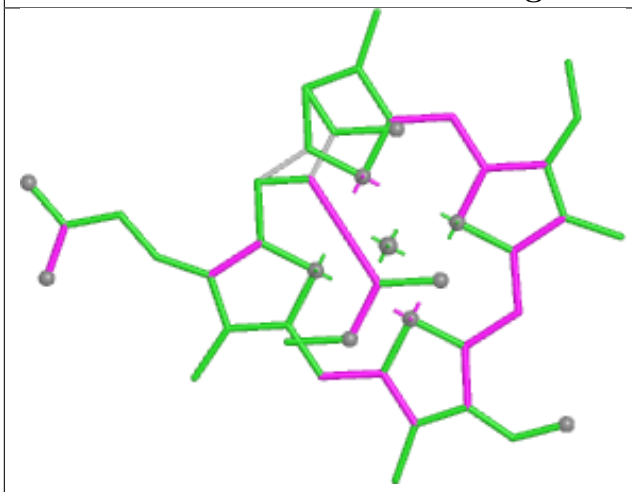


Rings

Ligand CL7 33 513



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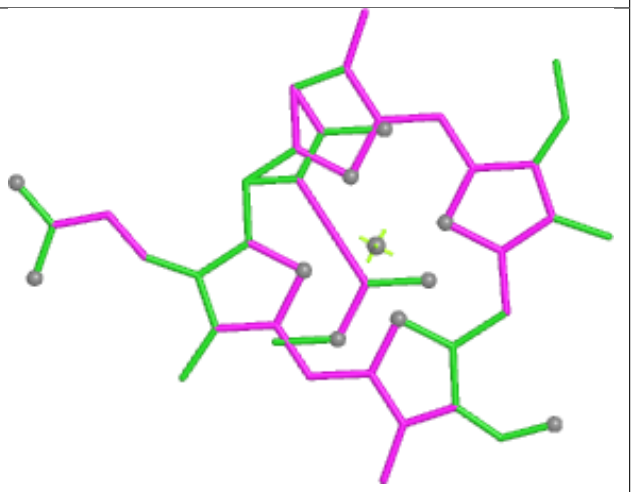

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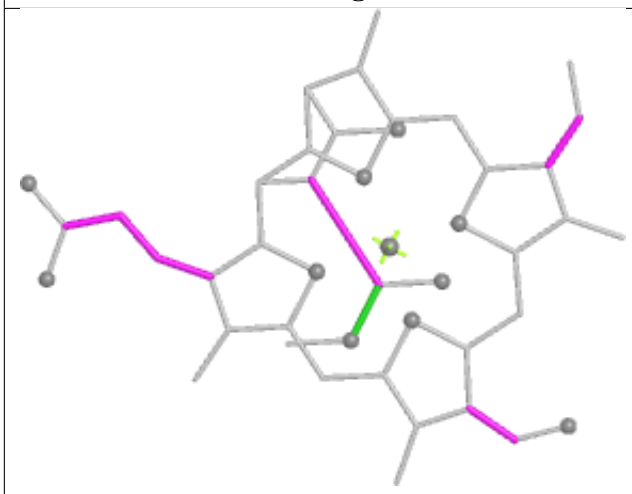
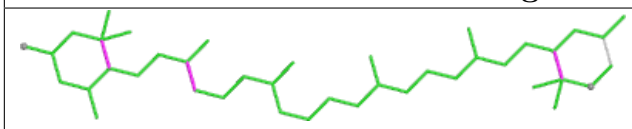


Torsions



Rings

Ligand ZEX 22 519



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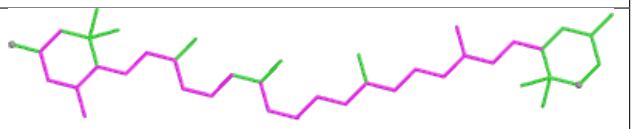

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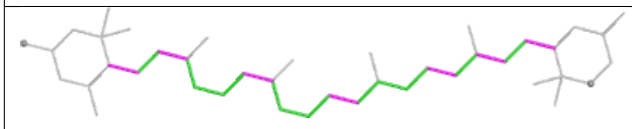

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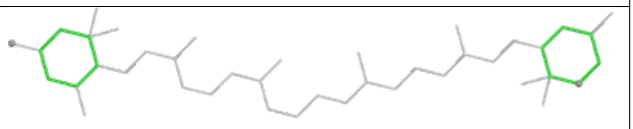
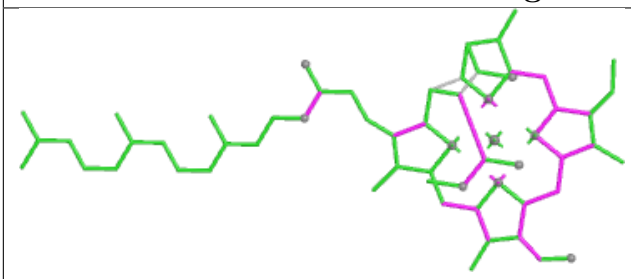


Rings

Ligand CL7 44 409



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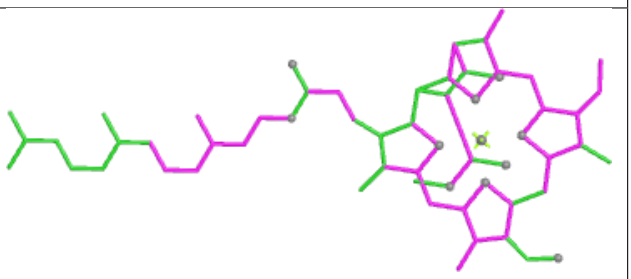

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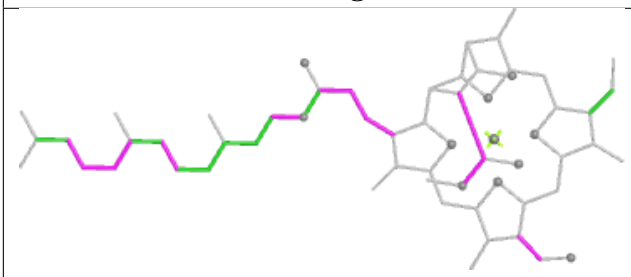
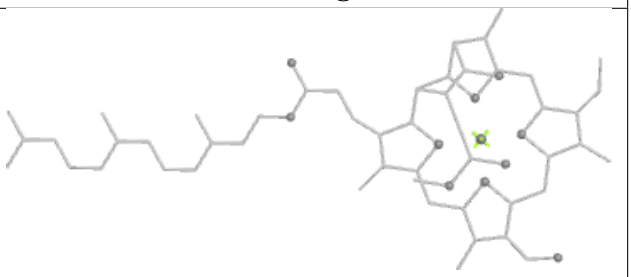
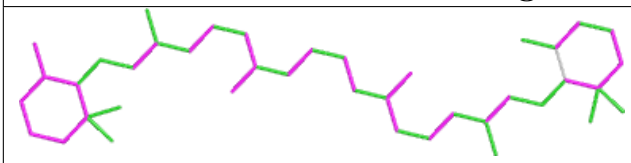


Torsions



Rings

Ligand 8CT 3C 514



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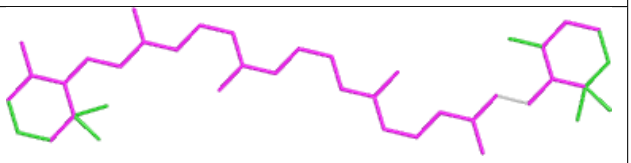
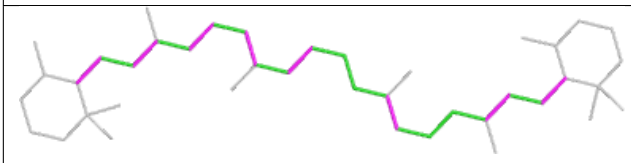
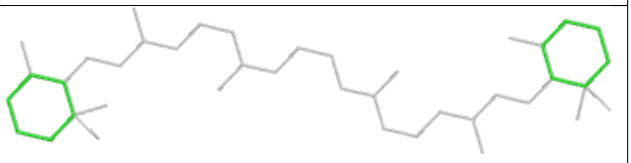


Bond angles

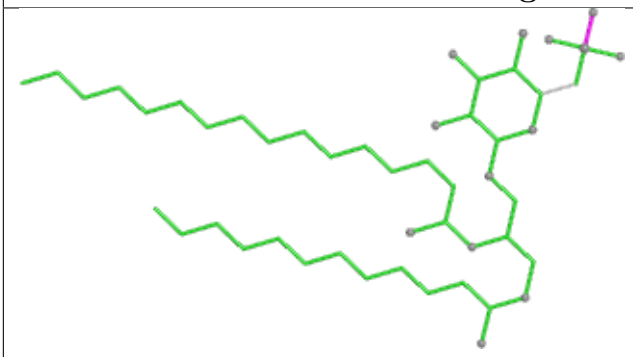


Torsions



Rings

Ligand SQD 42 521



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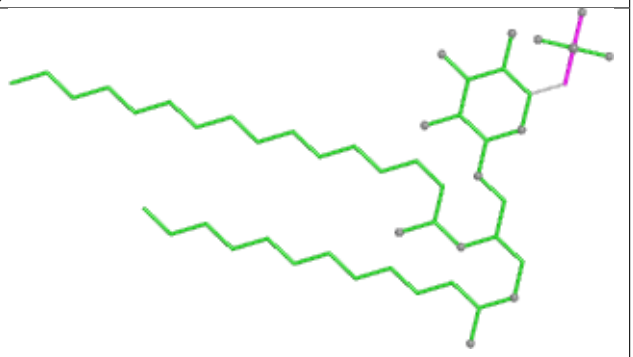
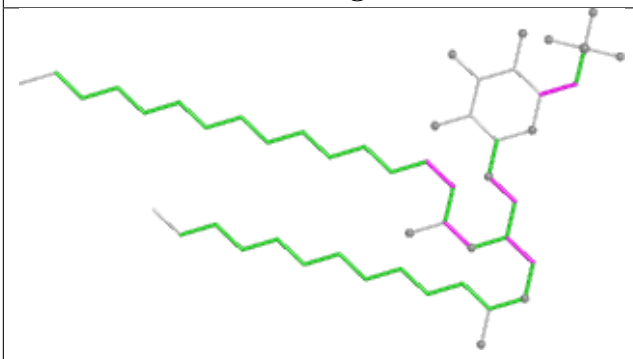


Bond angles



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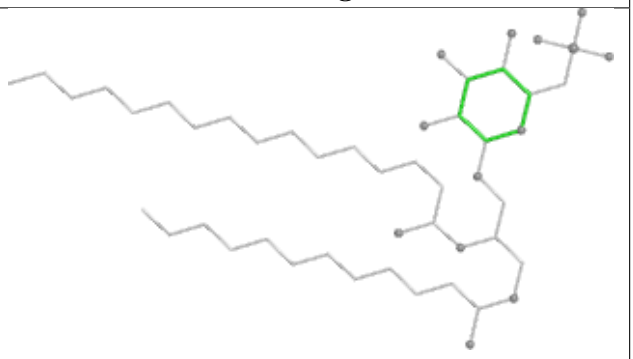
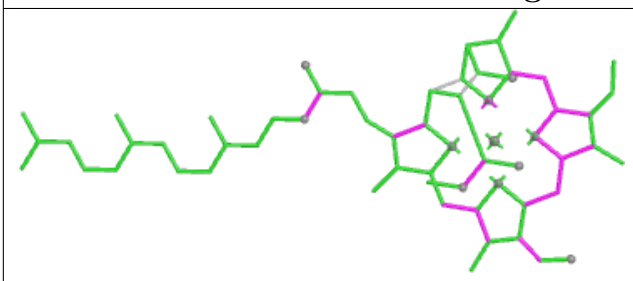


Rings

Ligand CL7 21 402



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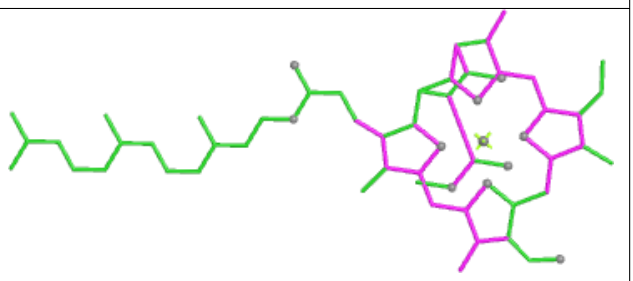

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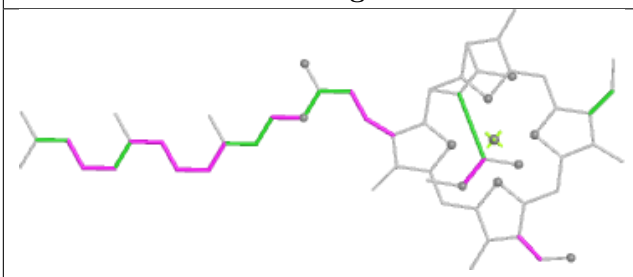

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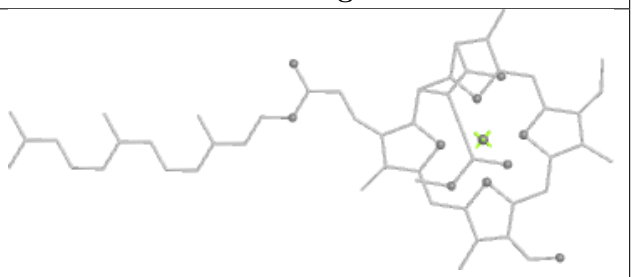

Rings

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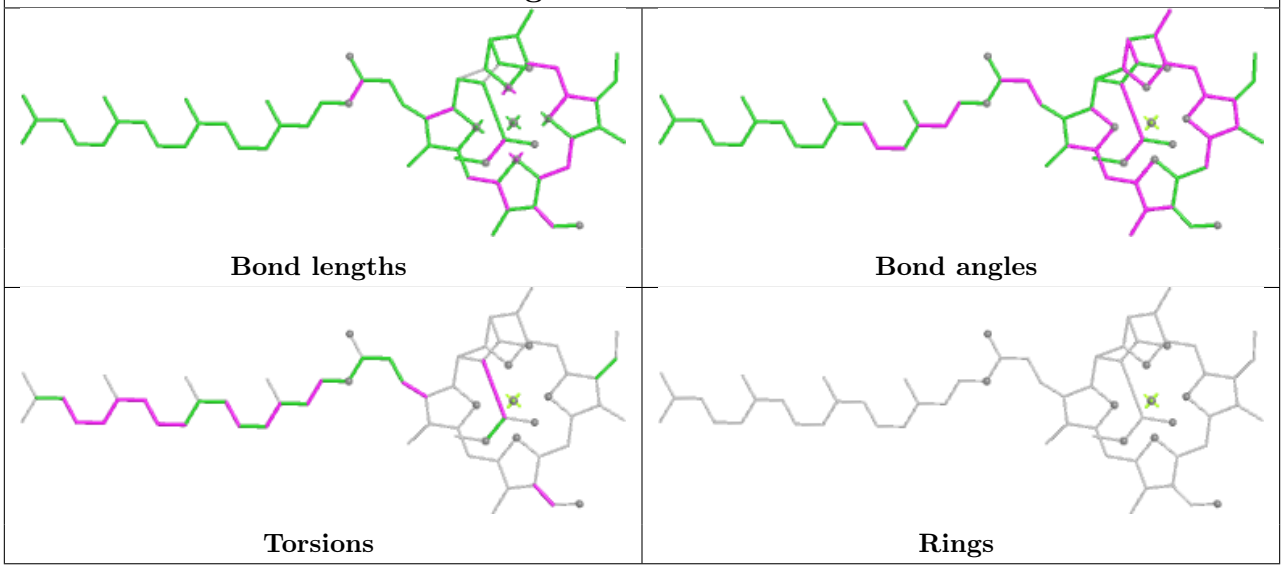

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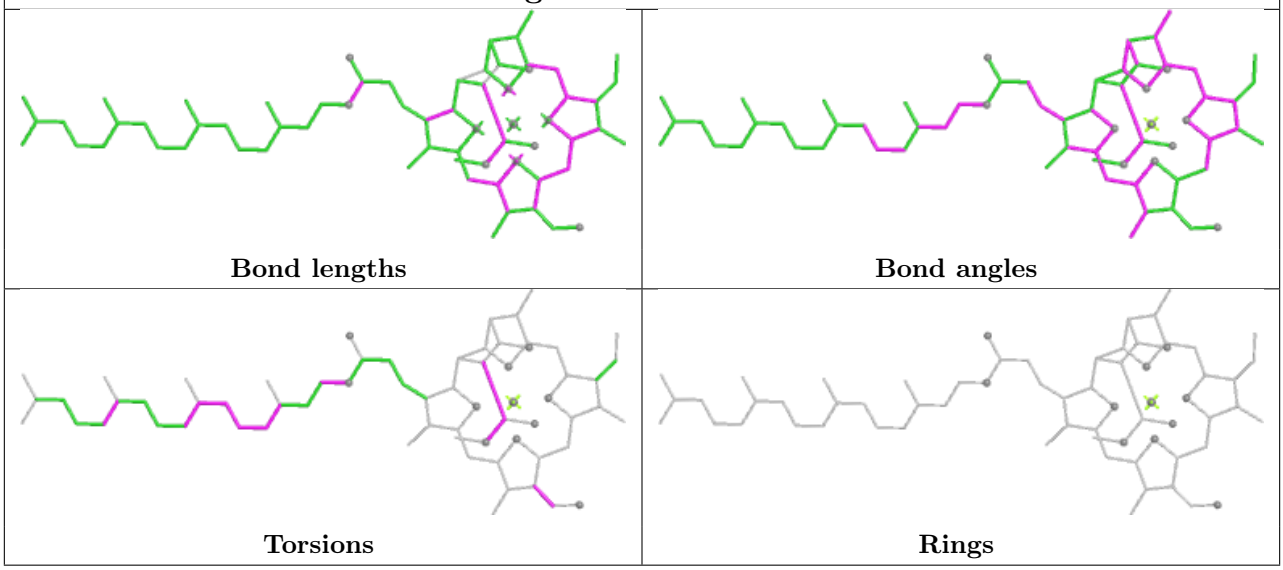

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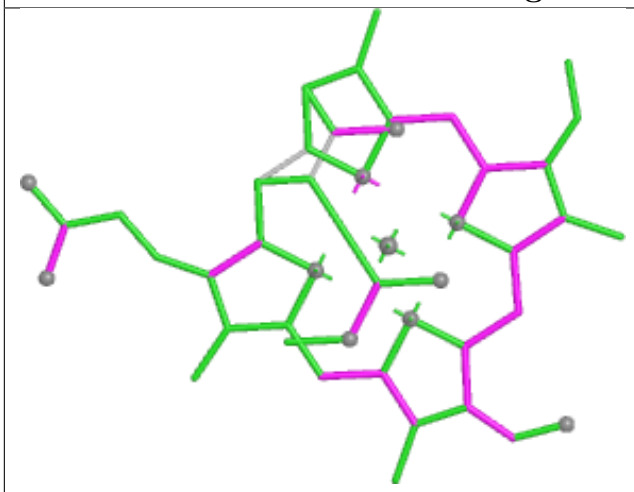

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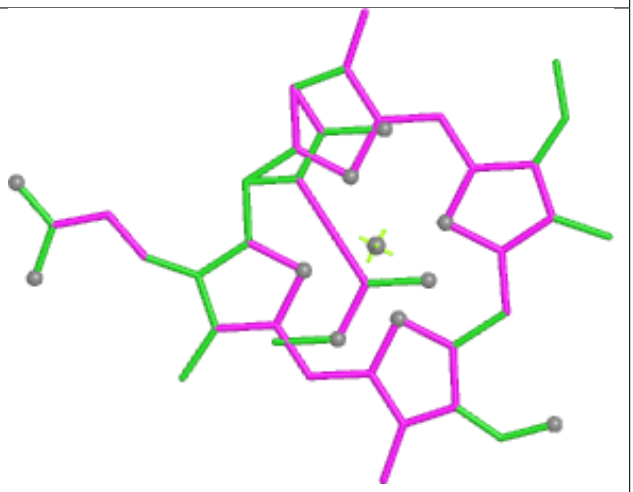

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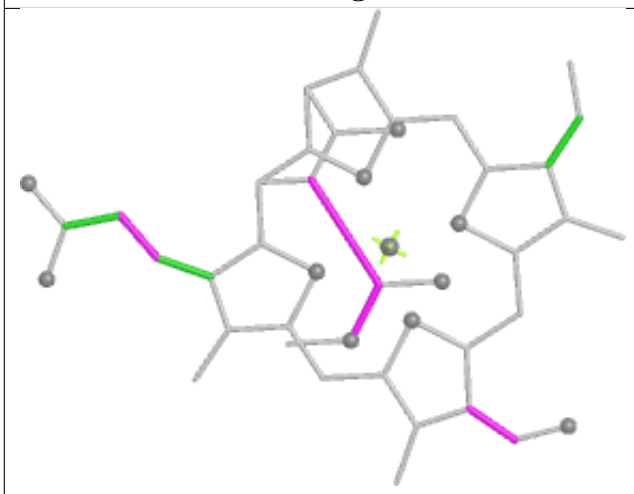

Torsions



Rings

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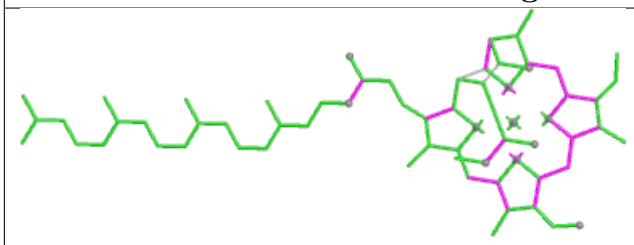

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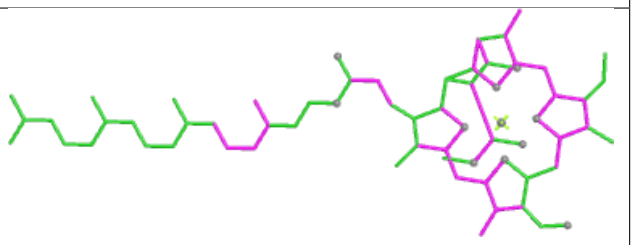

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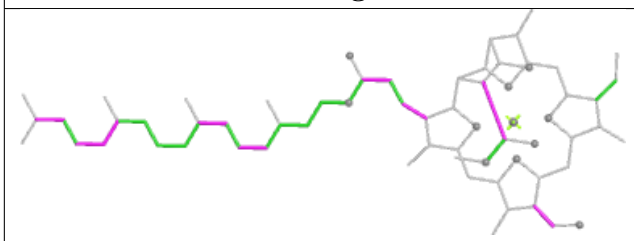

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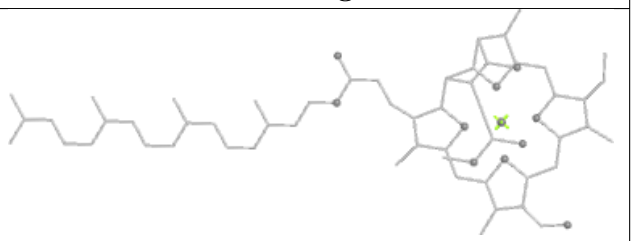

Rings

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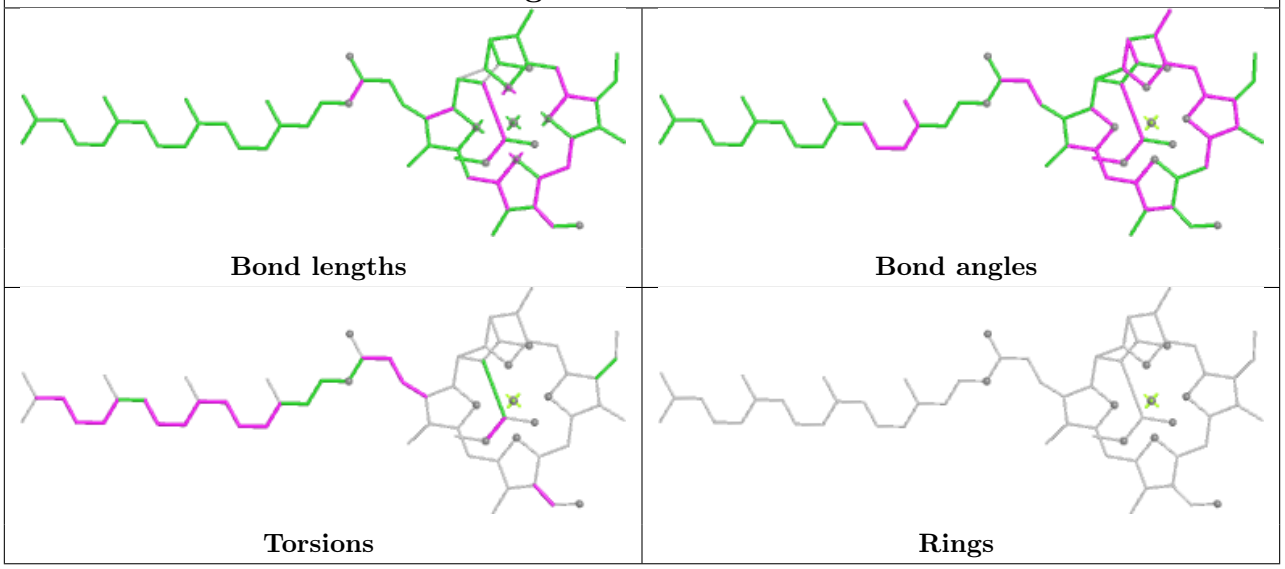

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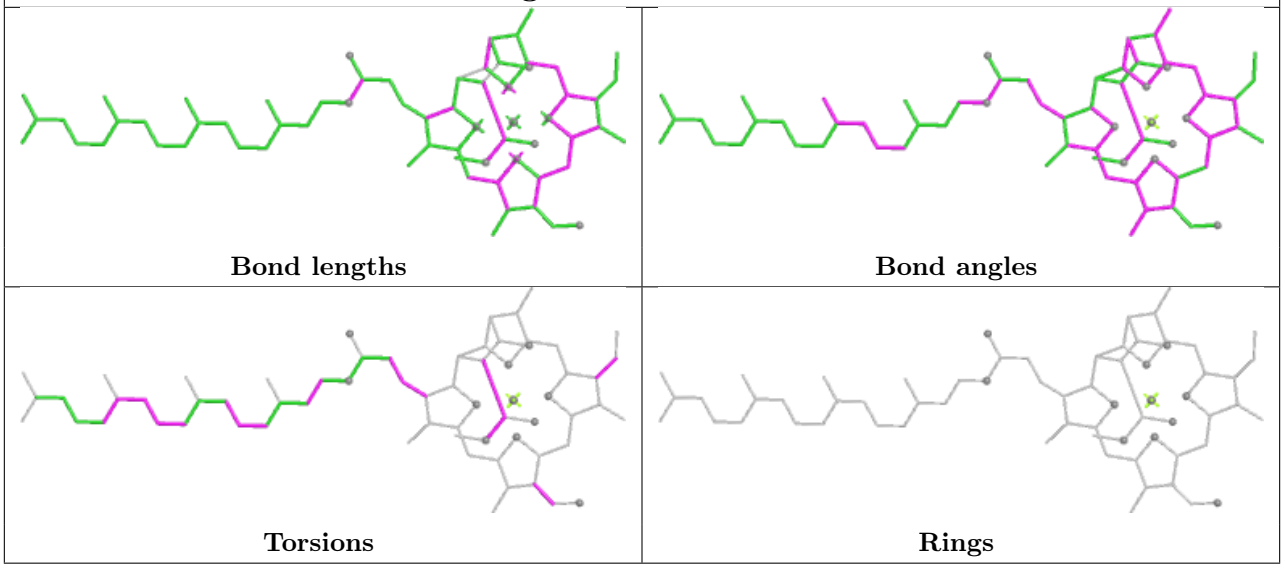

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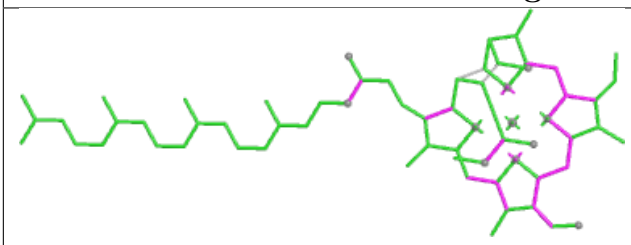

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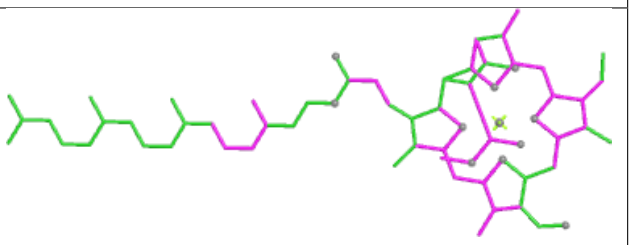

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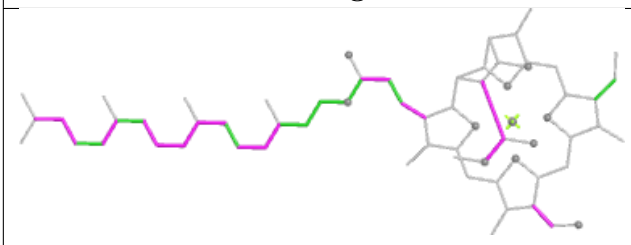

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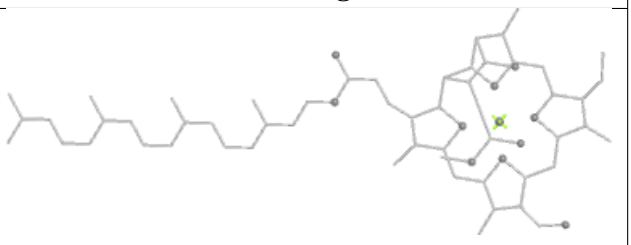

Rings

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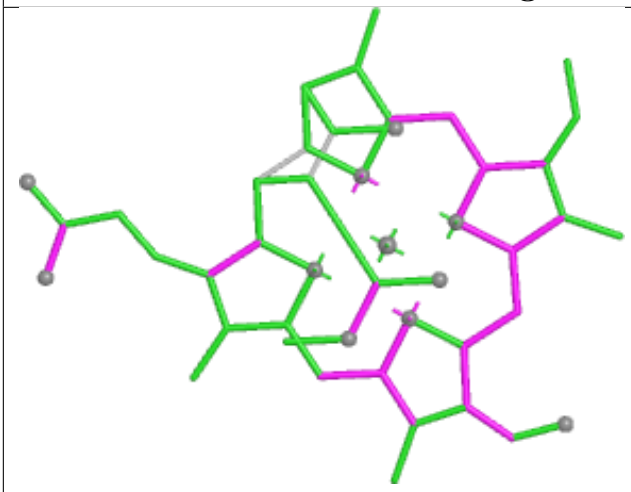

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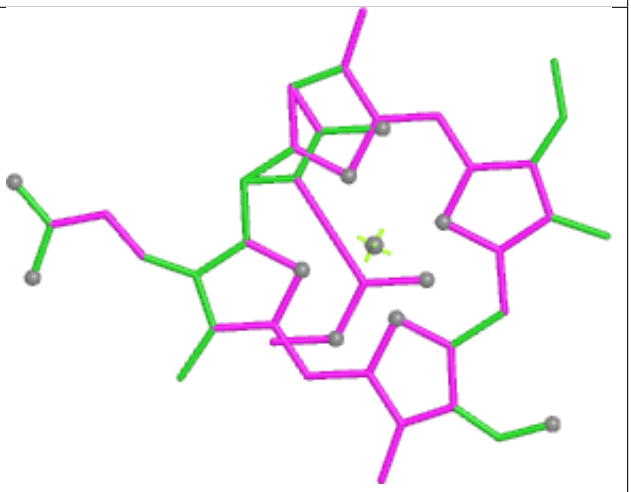

Bond angles



Torsions



Rings

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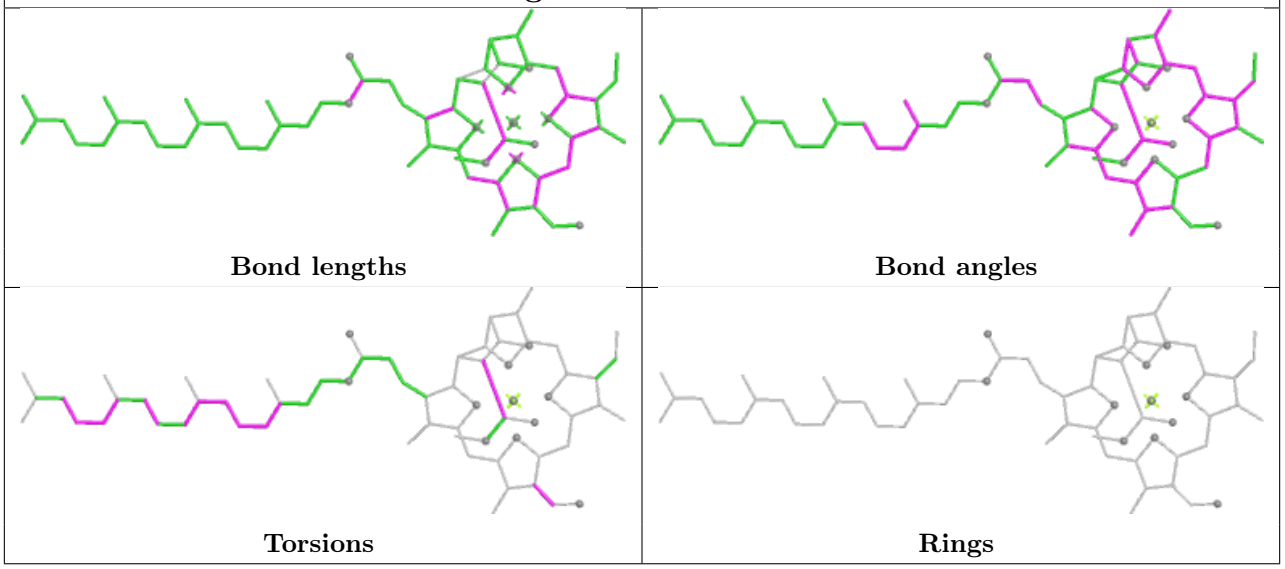

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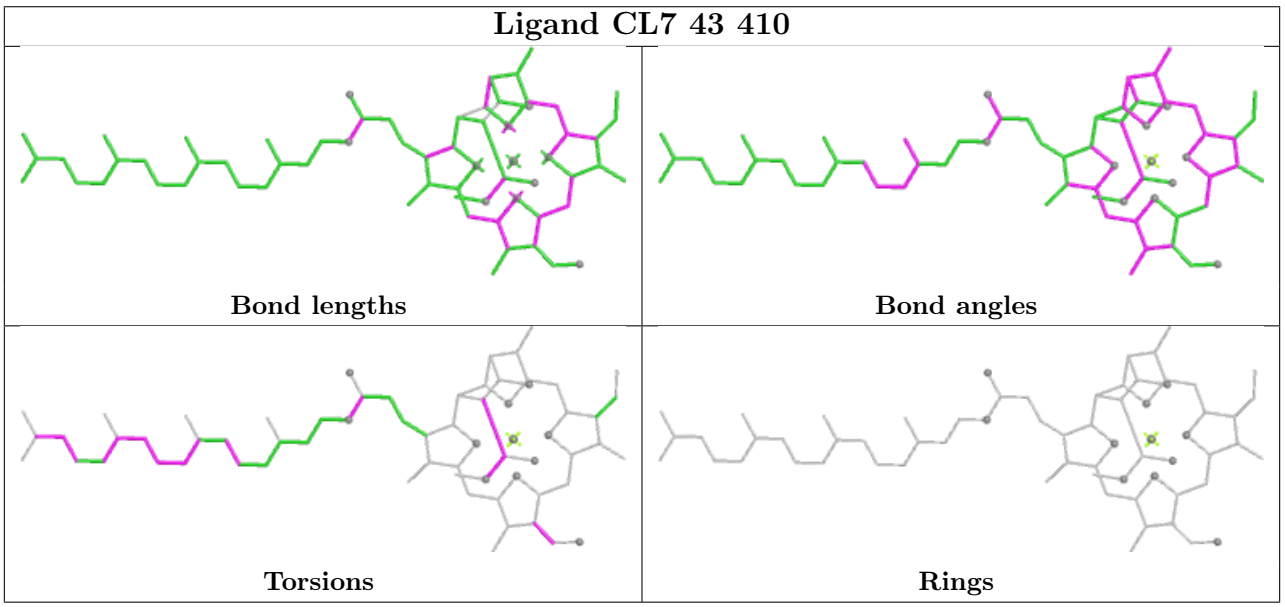

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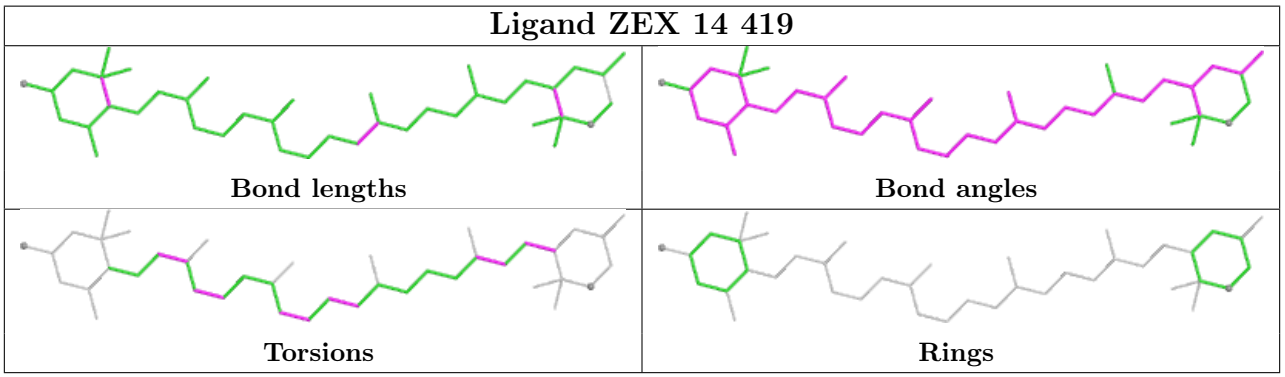

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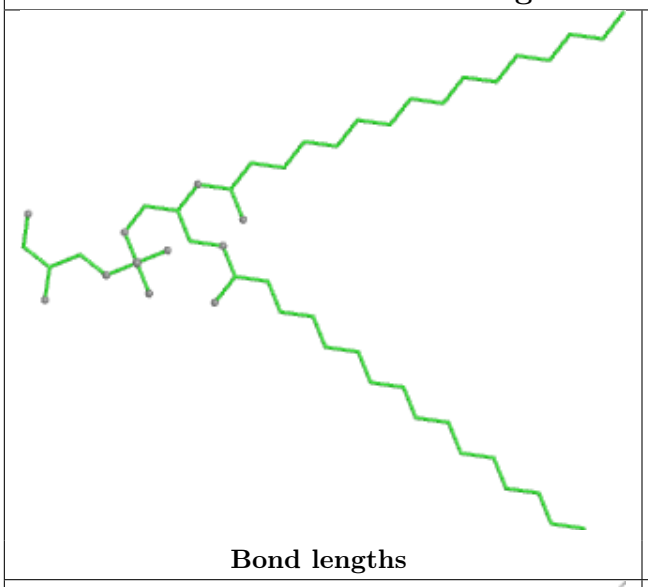

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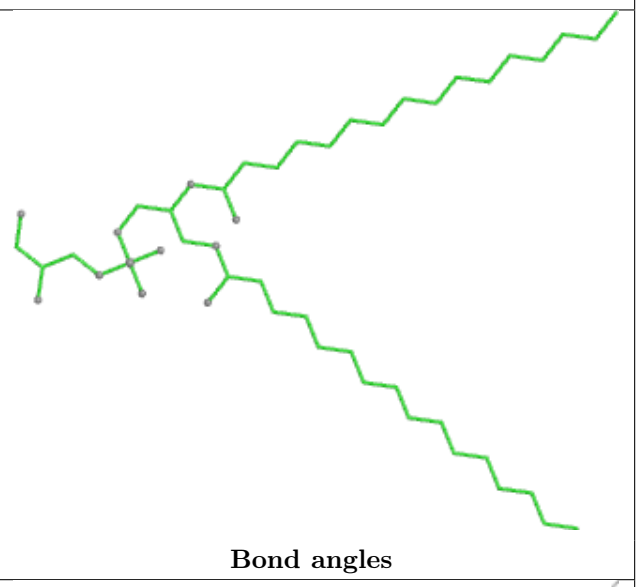

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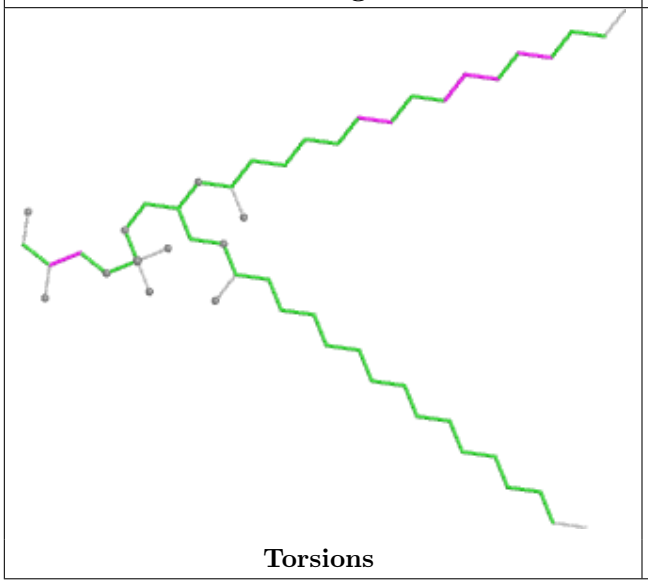

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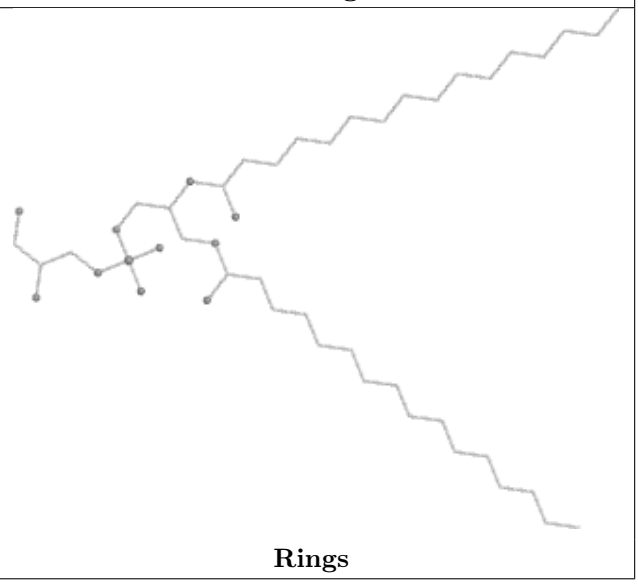

Rings

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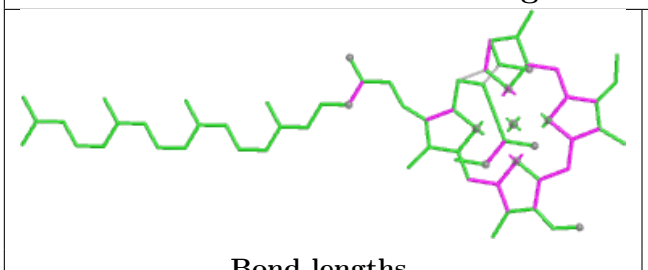

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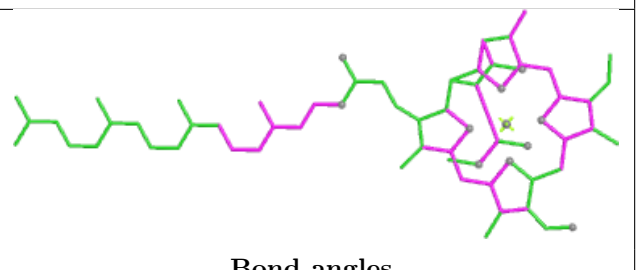

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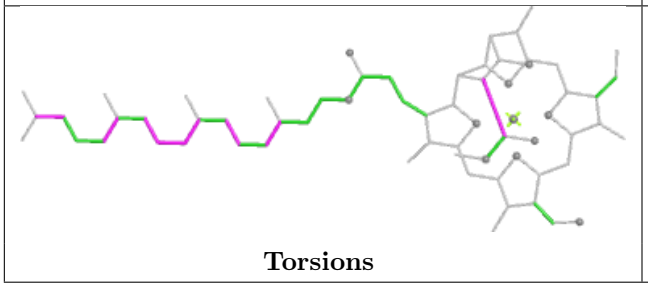

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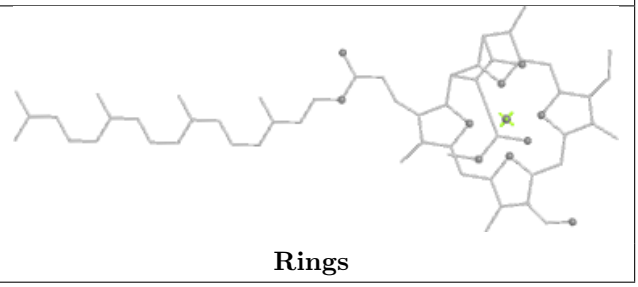

Rings

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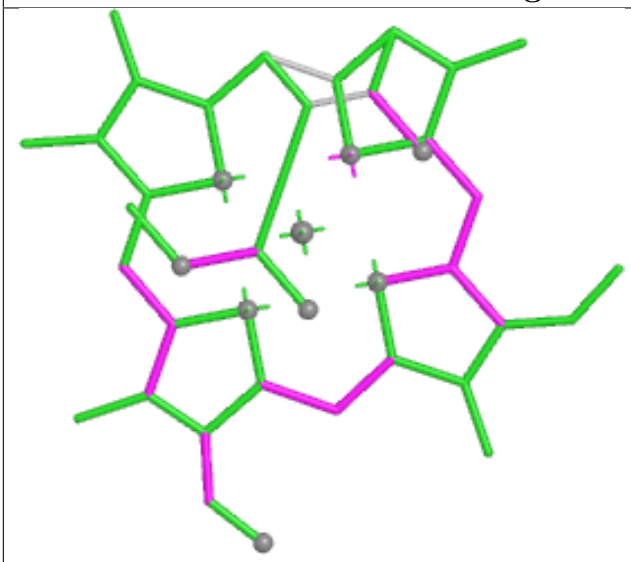

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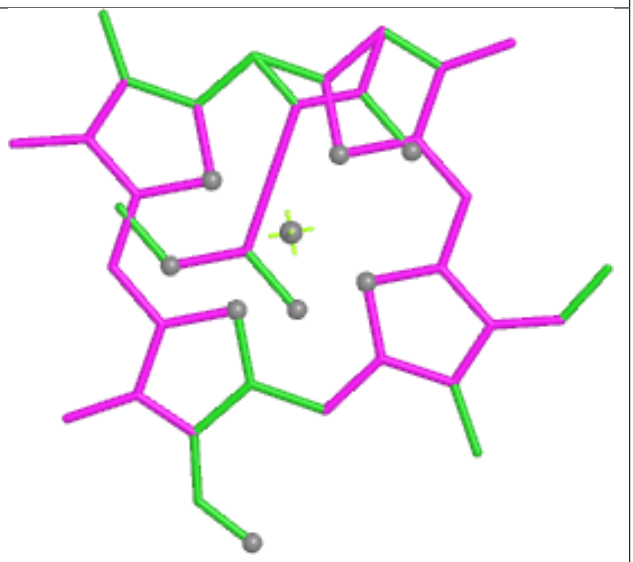

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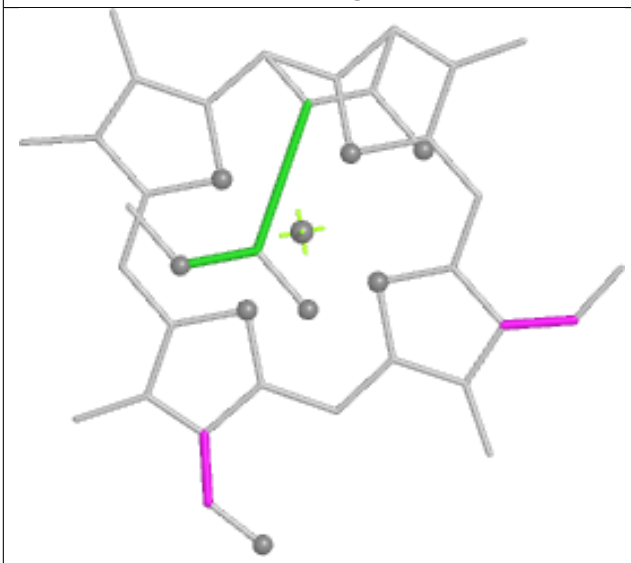

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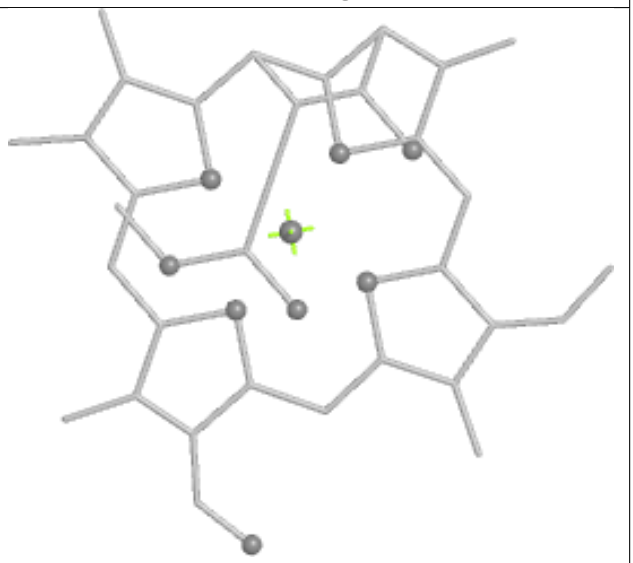

Rings

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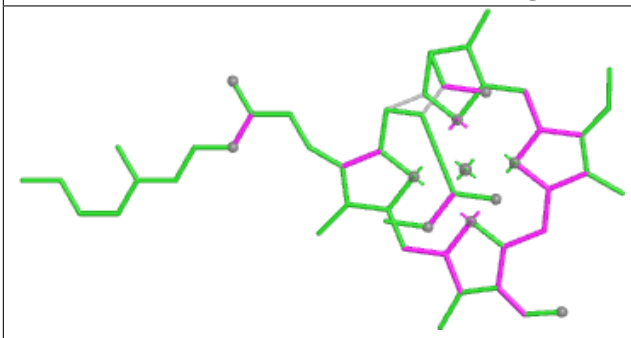

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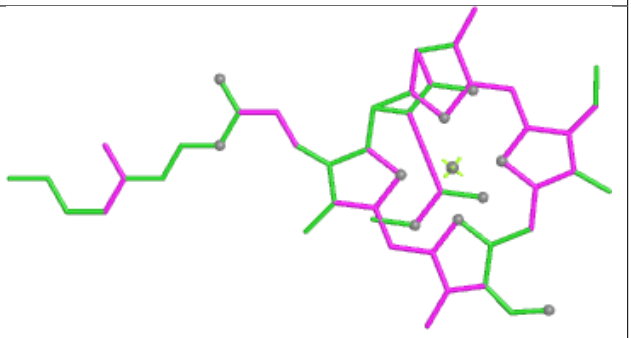

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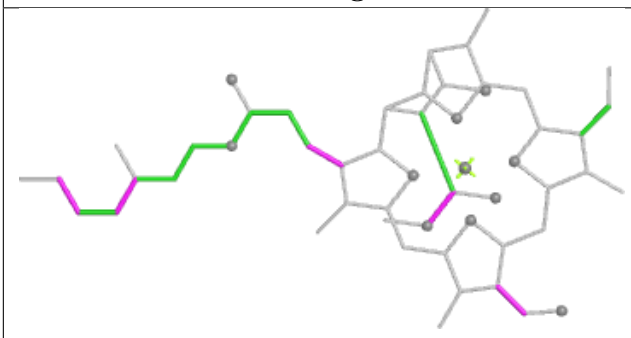

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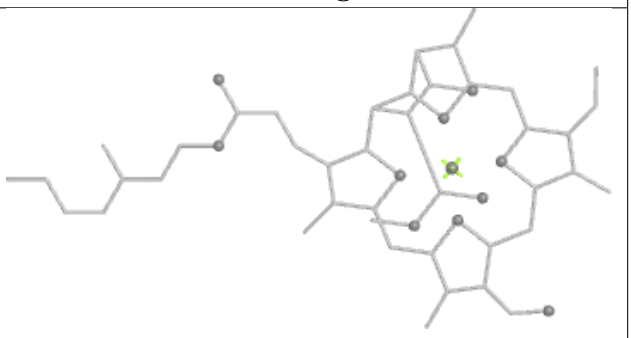

Rings

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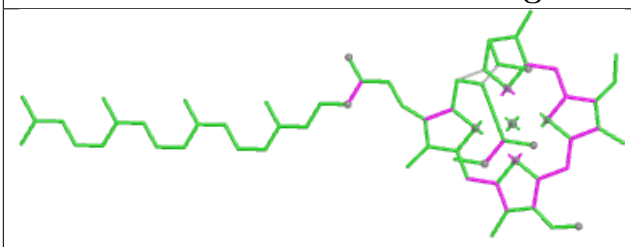

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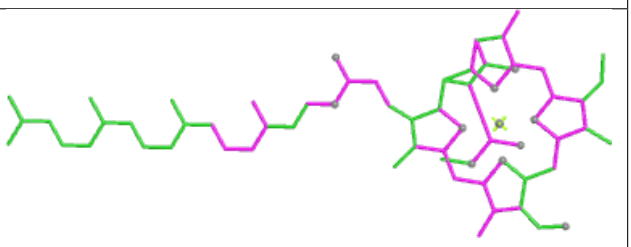

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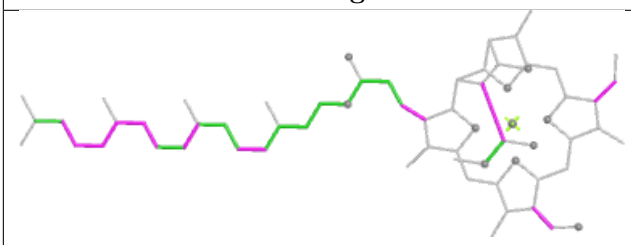

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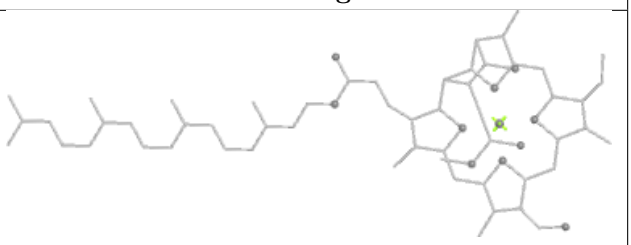
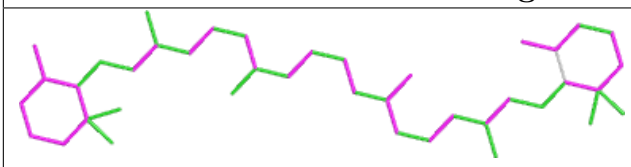


Rings

Ligand 8CT 2C 518



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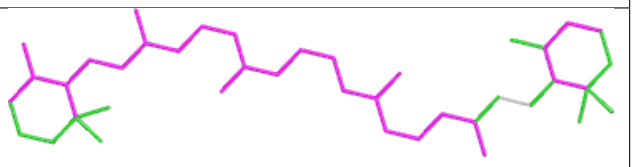
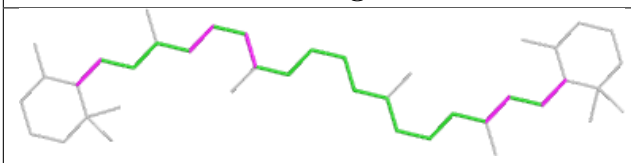


Bond angles



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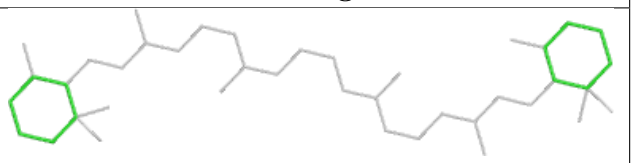

Rings

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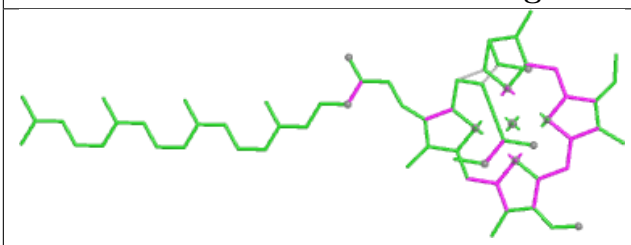

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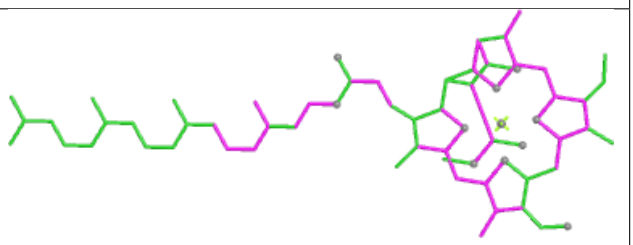
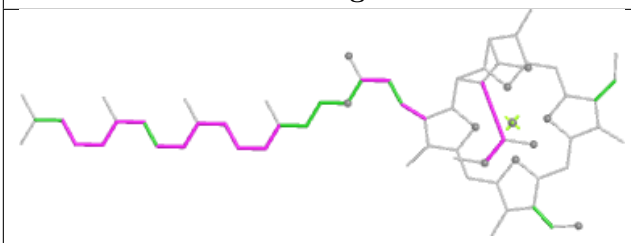


Bond angles



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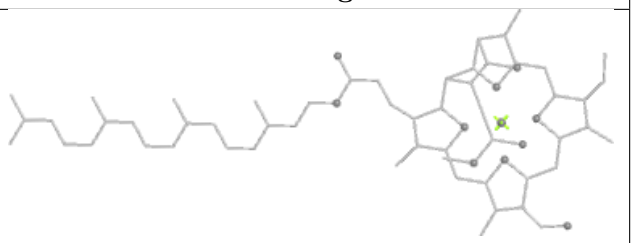

Rings

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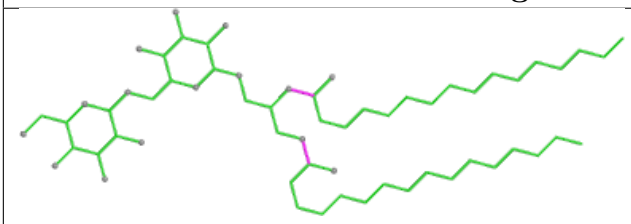
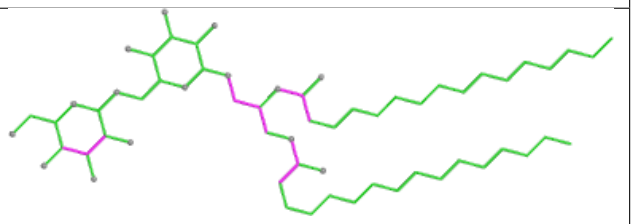
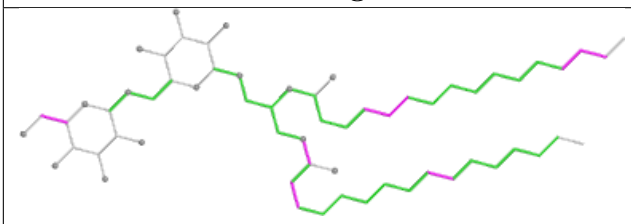


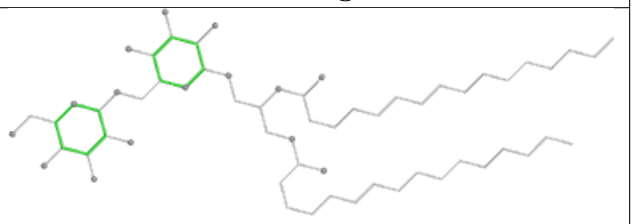
Bond lengths



Bond angles



Torsions



Rings

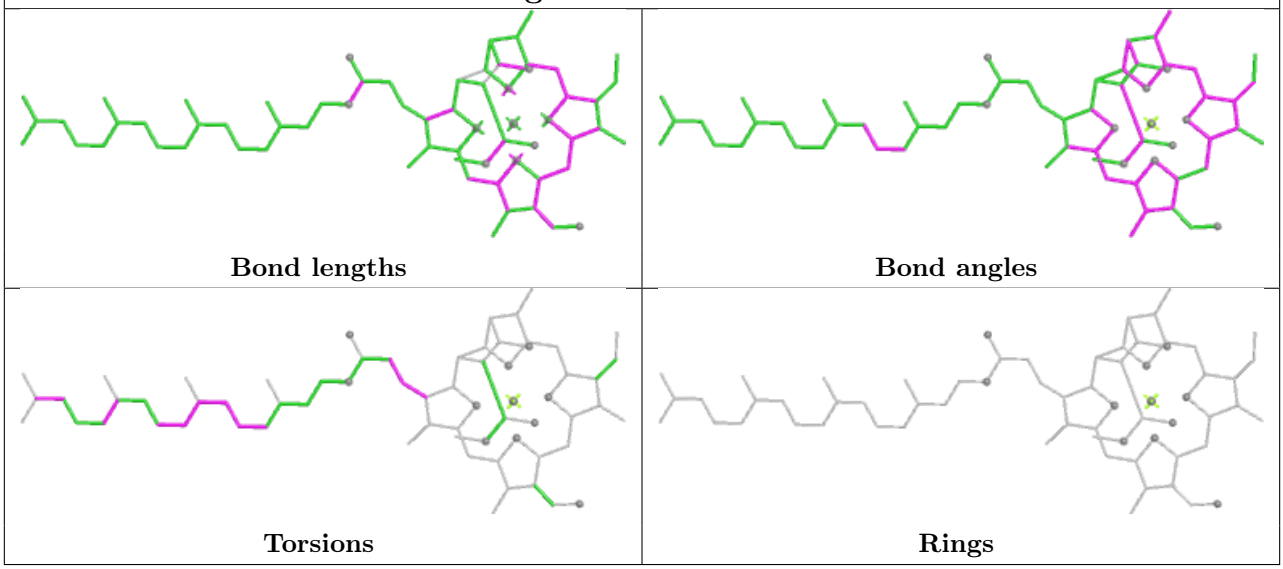
Ligand PL9 4D 407



Bond lengths | Bond angles

Torsions | Rings

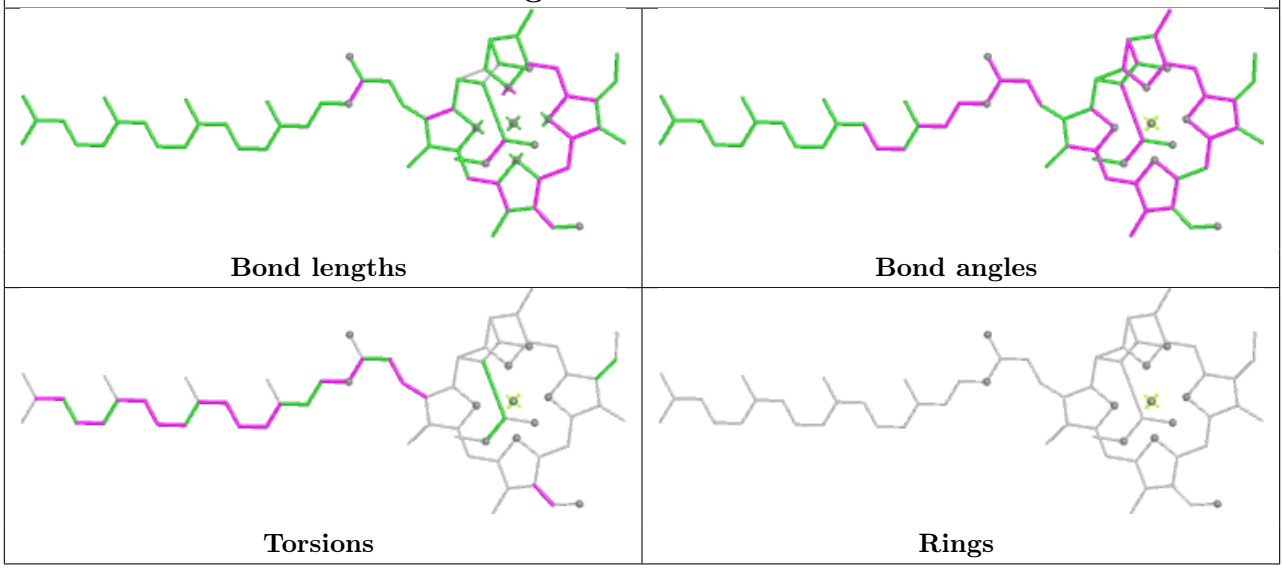
Ligand CL7 34 404



Bond lengths | Bond angles

Torsions | Rings

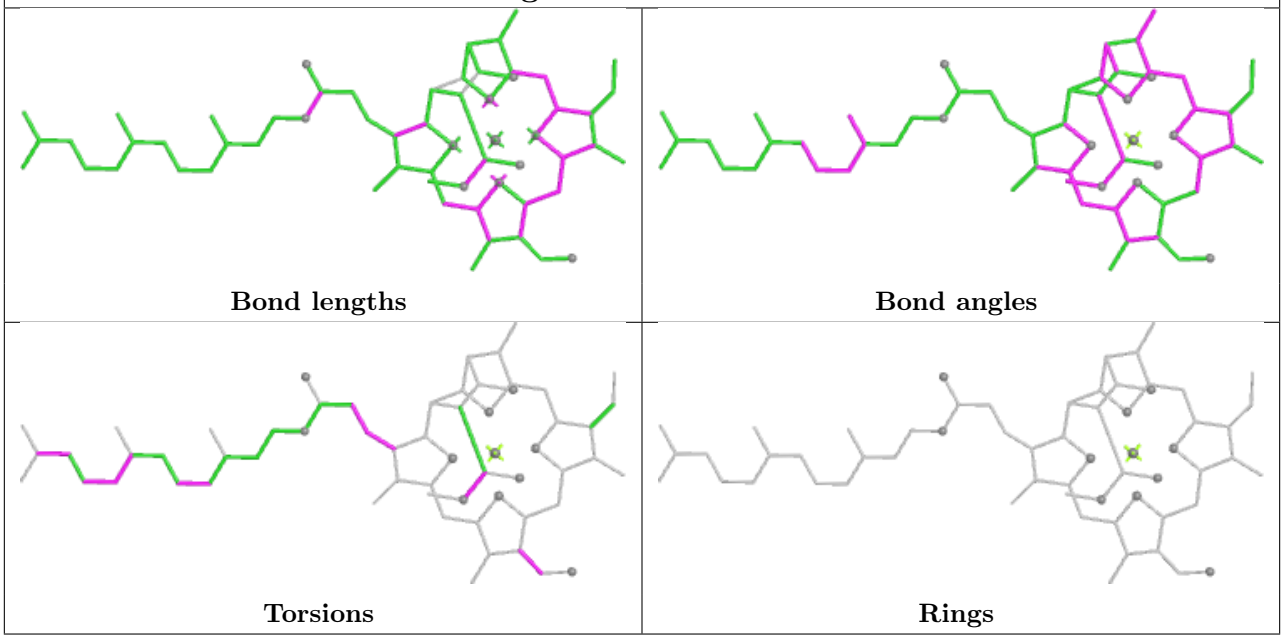
Ligand CL7 14 405



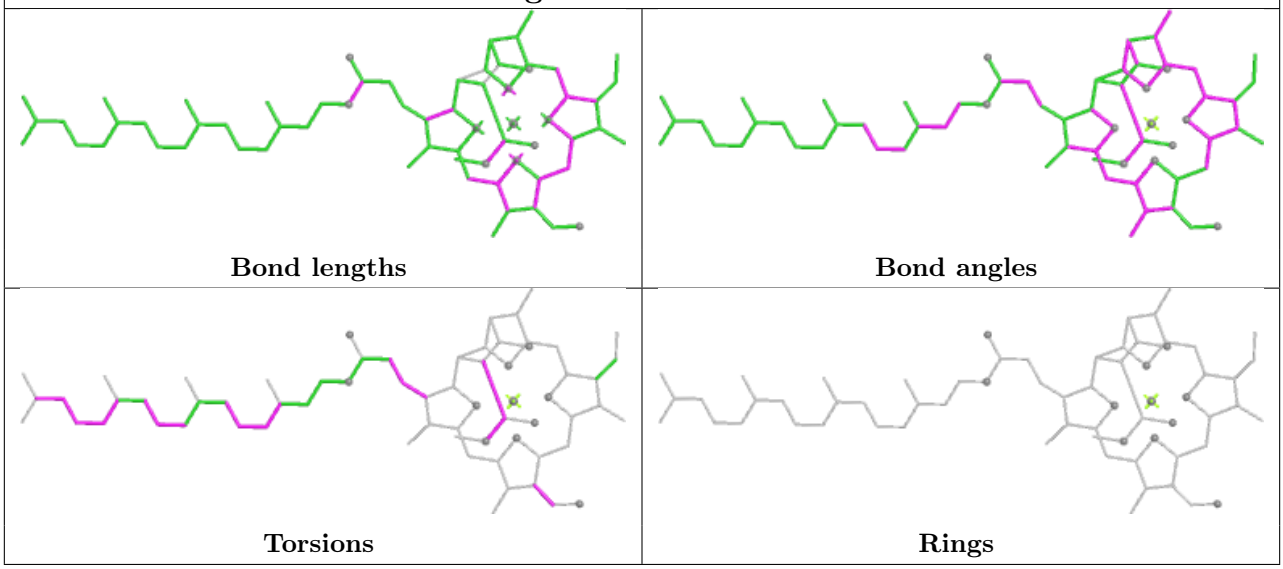
Bond lengths | Bond angles

Torsions | Rings

Ligand CL7 2B 608



Ligand CL7 32 517



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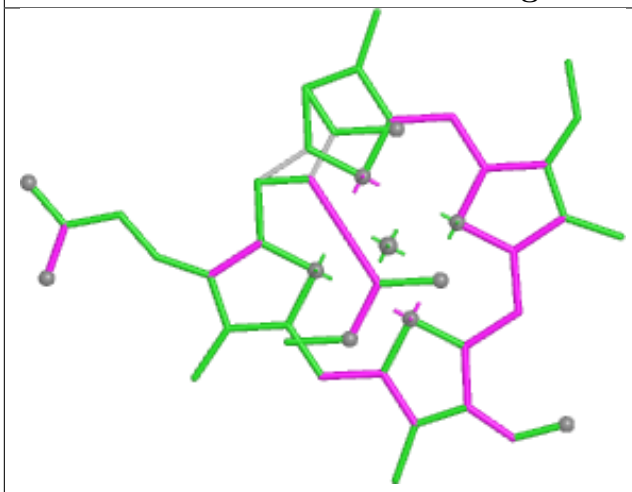
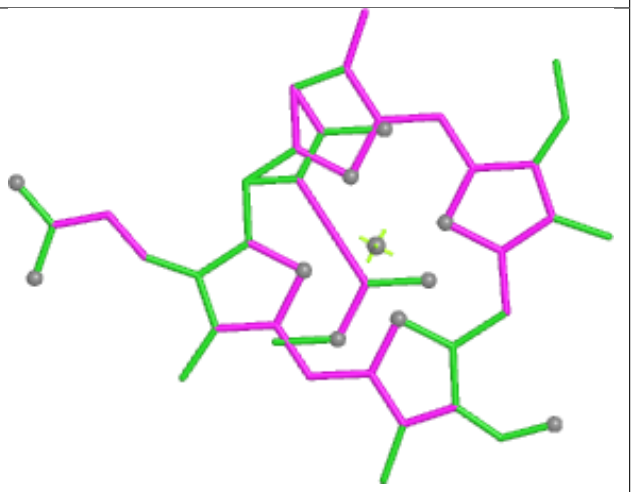
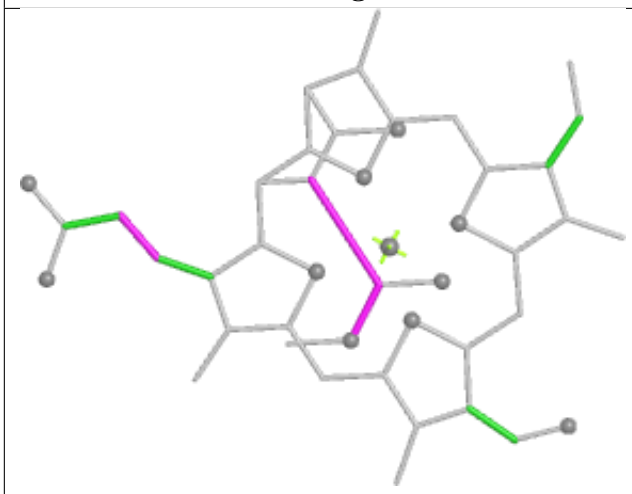


Bond lengths



Bond angles

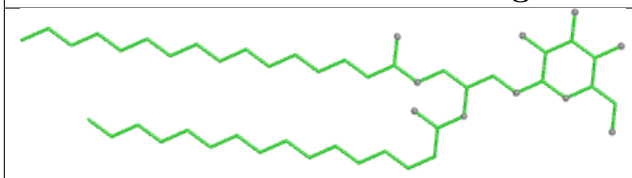


Torsions

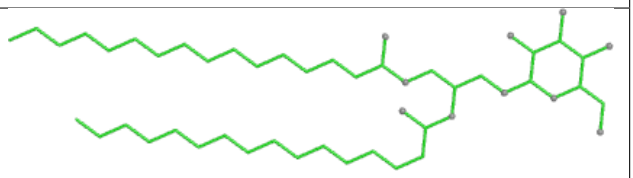


Rings

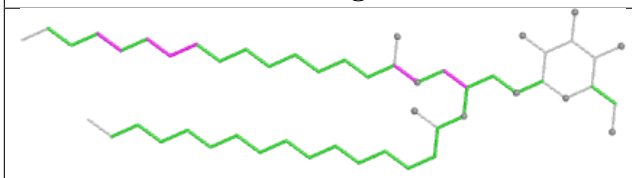
Ligand LMG 1B 621



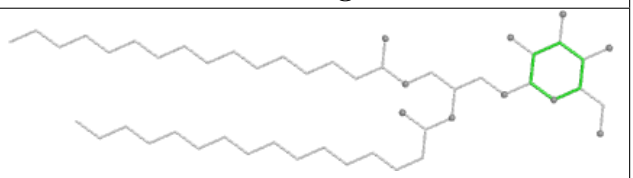
Bond lengths



Bond angles

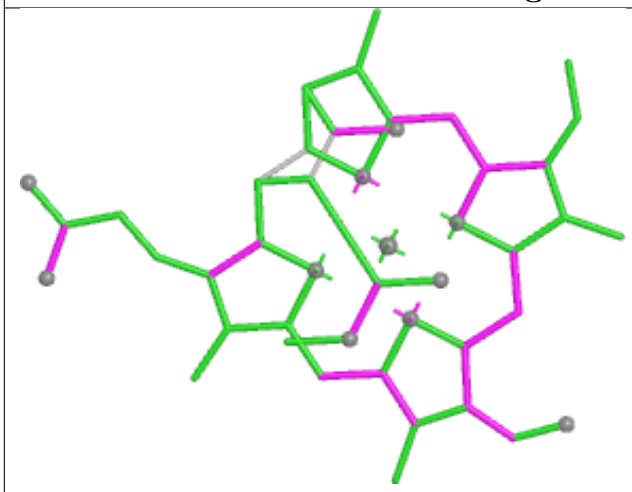


Torsions



Rings

Ligand CL7 41 412



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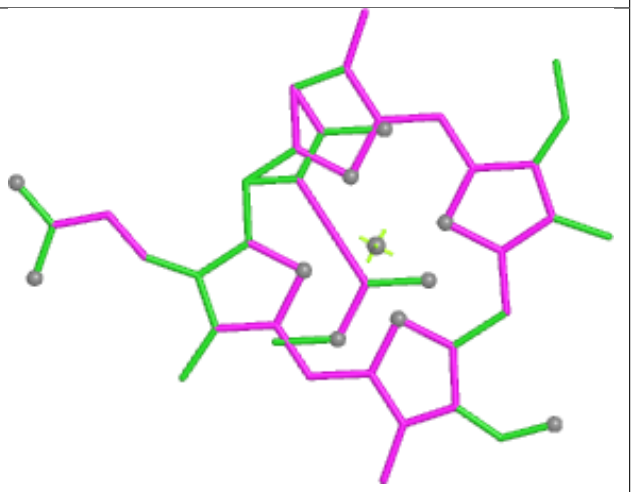
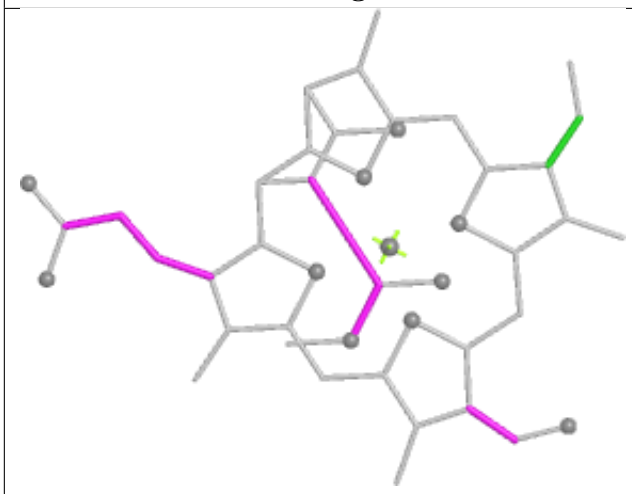


Bond angles

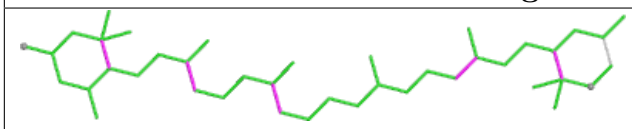


Torsions



Rings

Ligand ZEX 13 525



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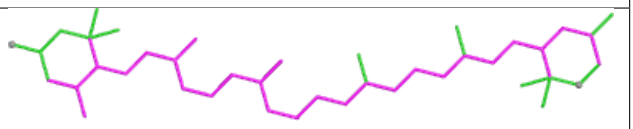
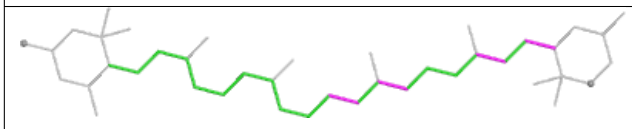
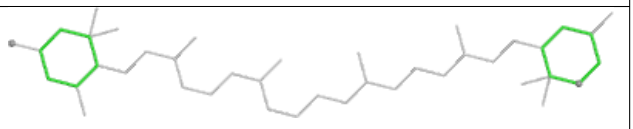


Bond angles

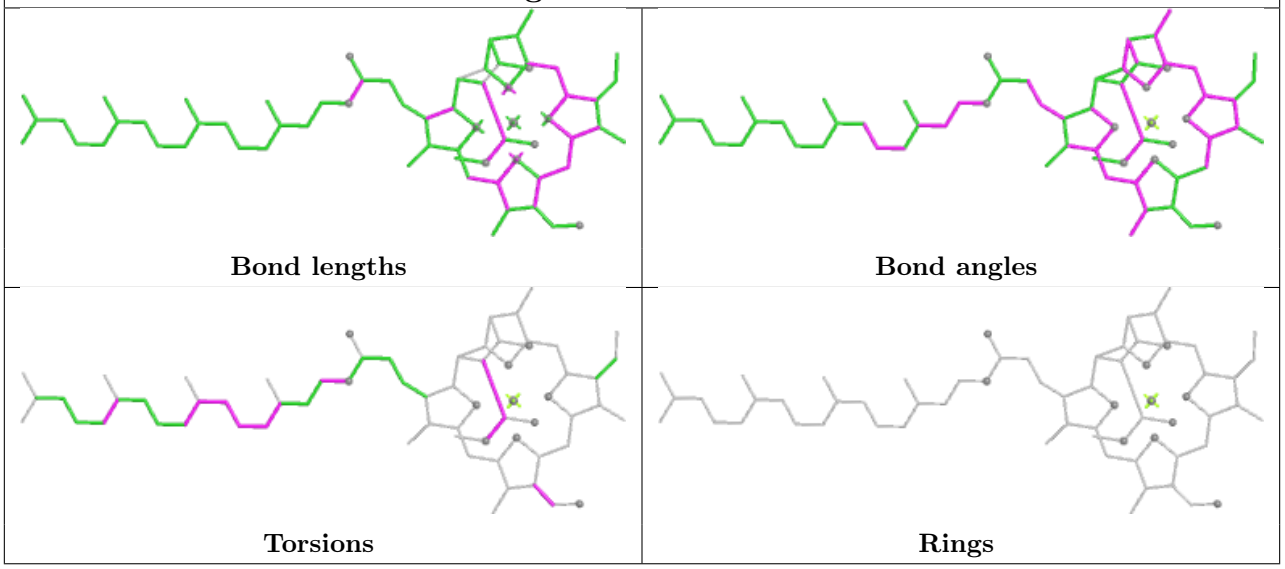


Torsions

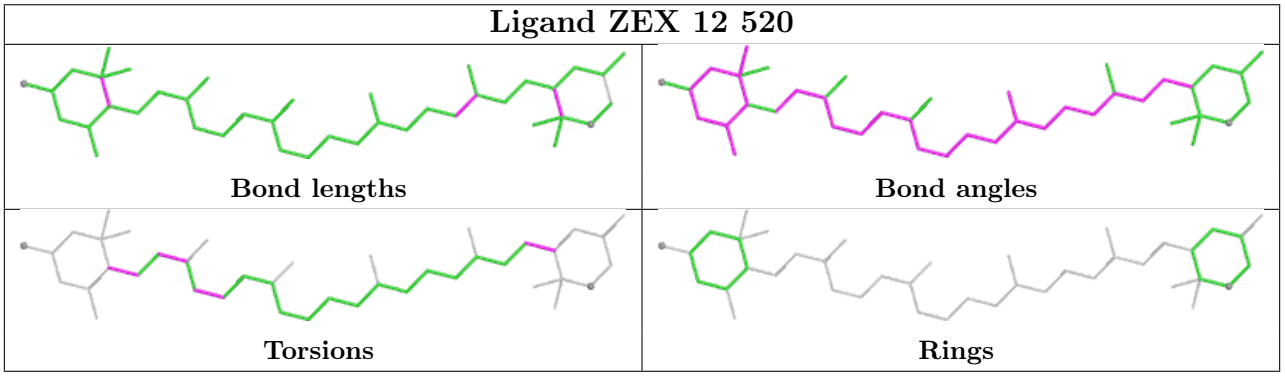


Rings

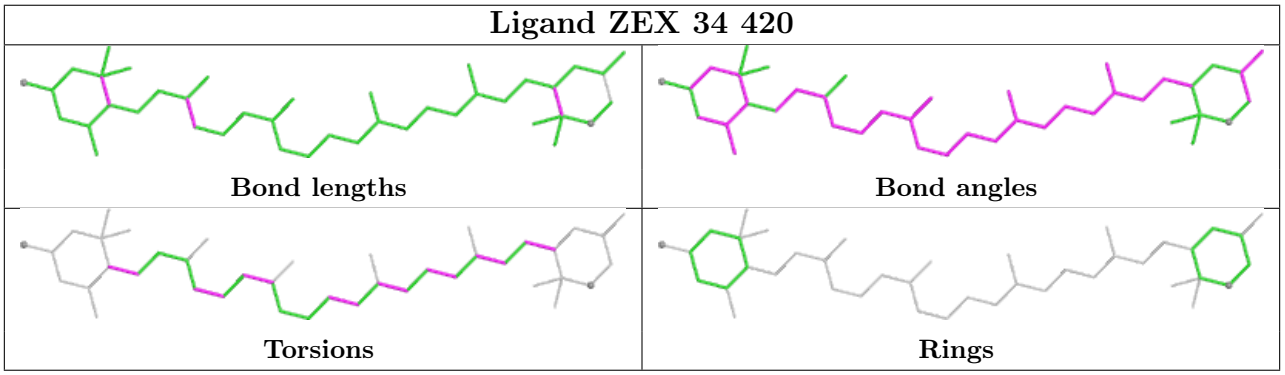
Ligand CL7 43 409



Ligand ZEX 12 520



Ligand ZEX 34 420



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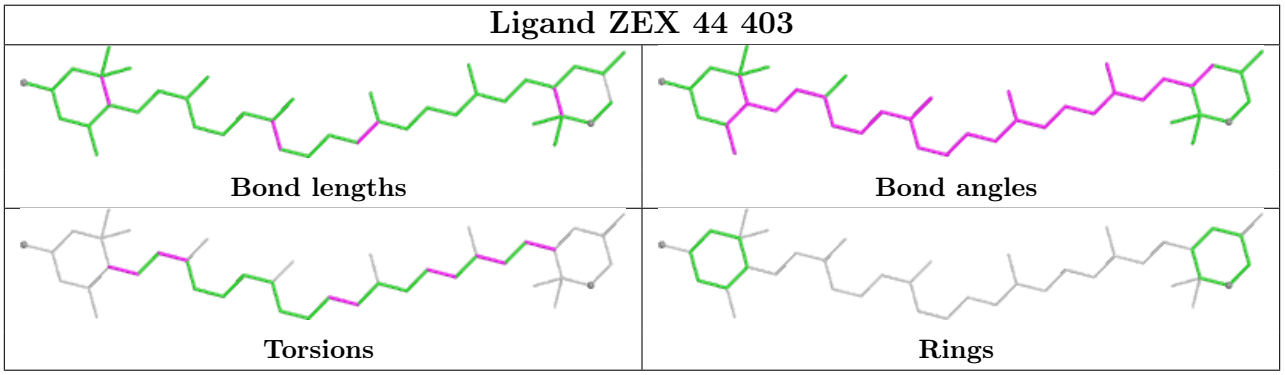

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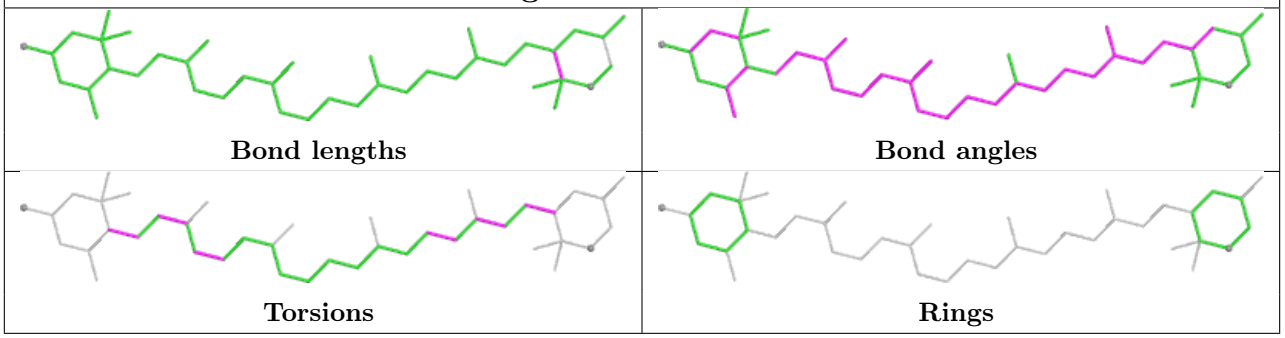

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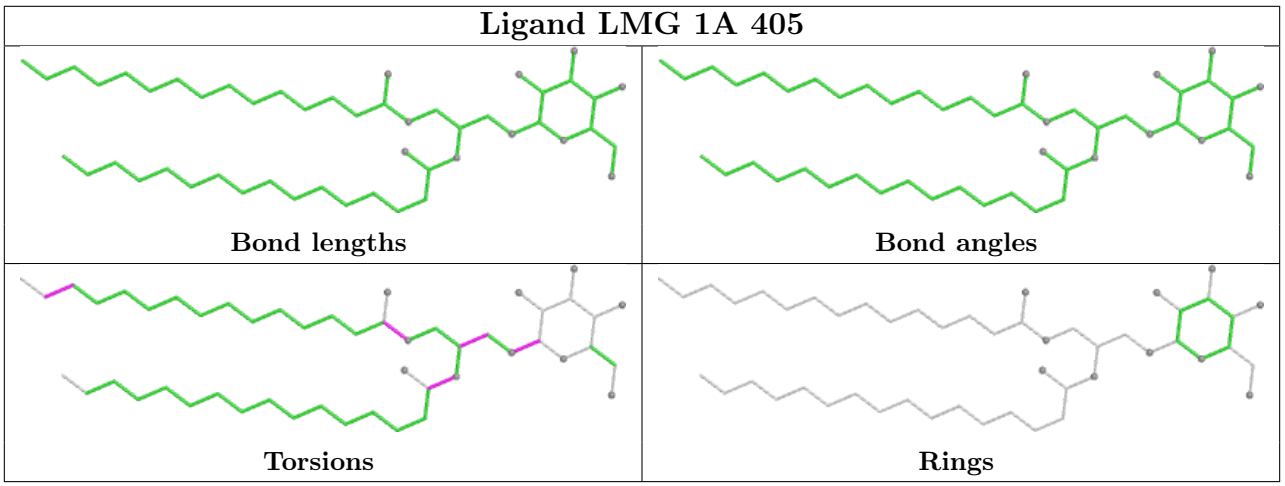

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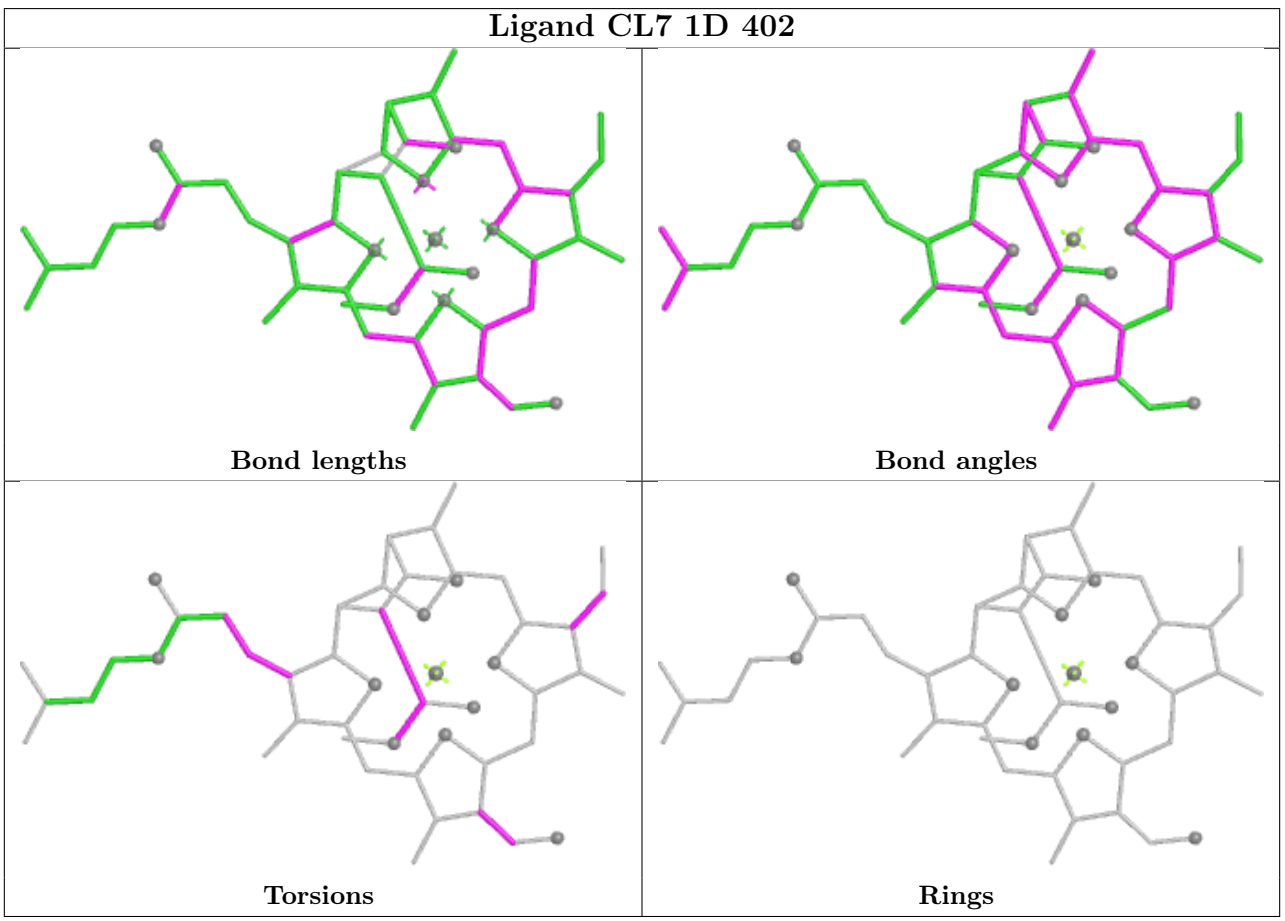

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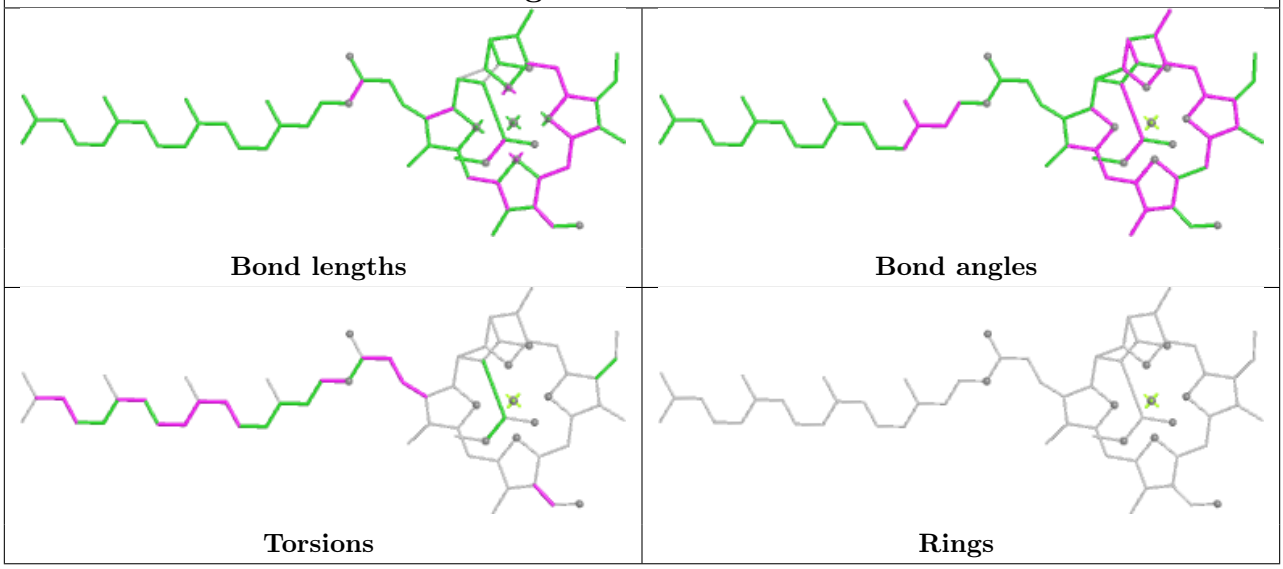

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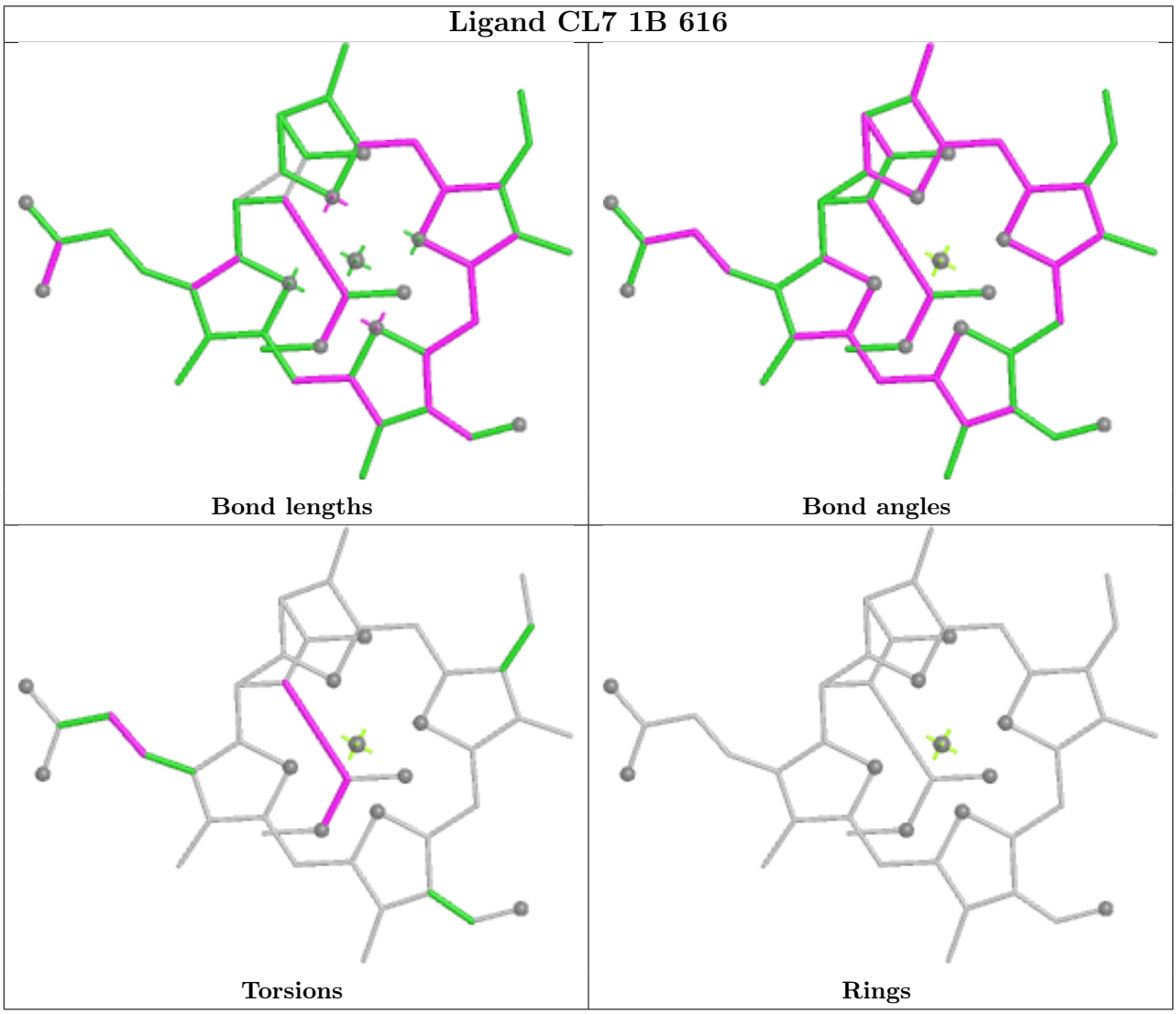
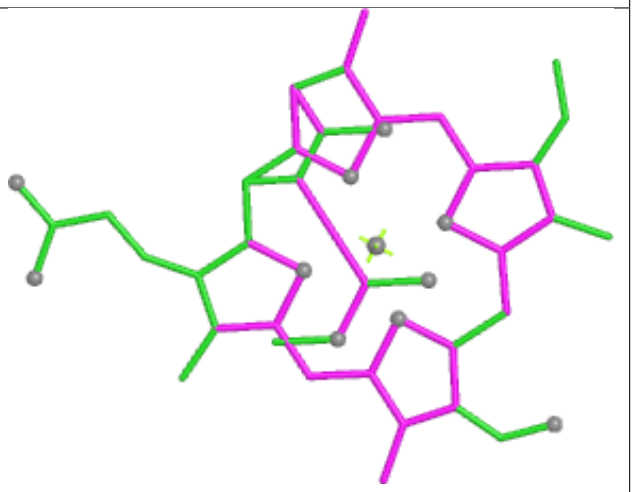


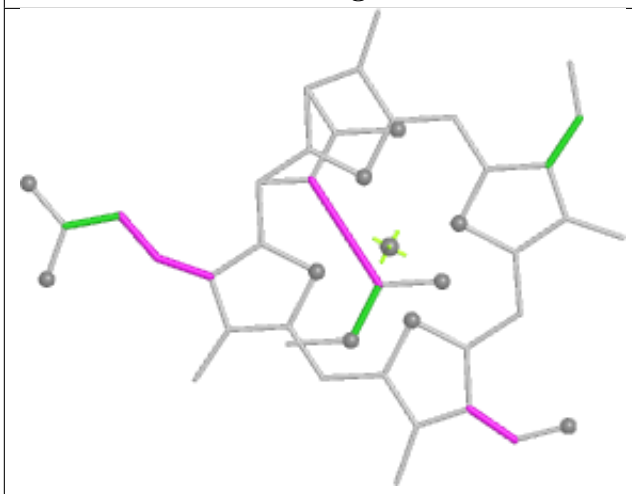
Ligand CL7 12 508



Bond lengths



Bond angles

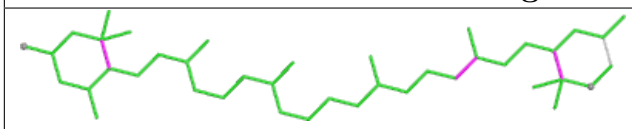


Torsions



Rings

Ligand ZEX 12 524



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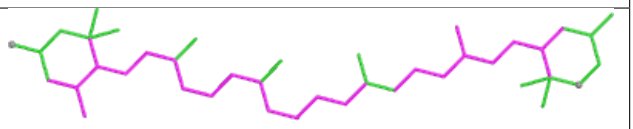
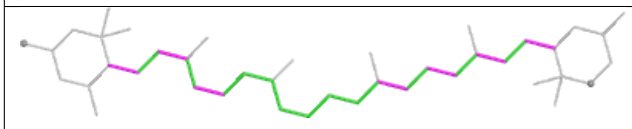
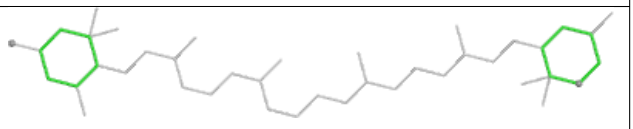


Bond angles

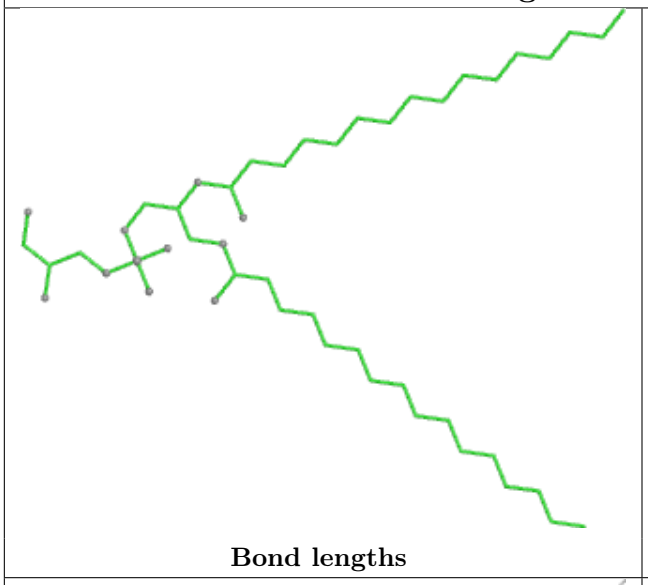


Torsions



Rings

Ligand LHG 14 401



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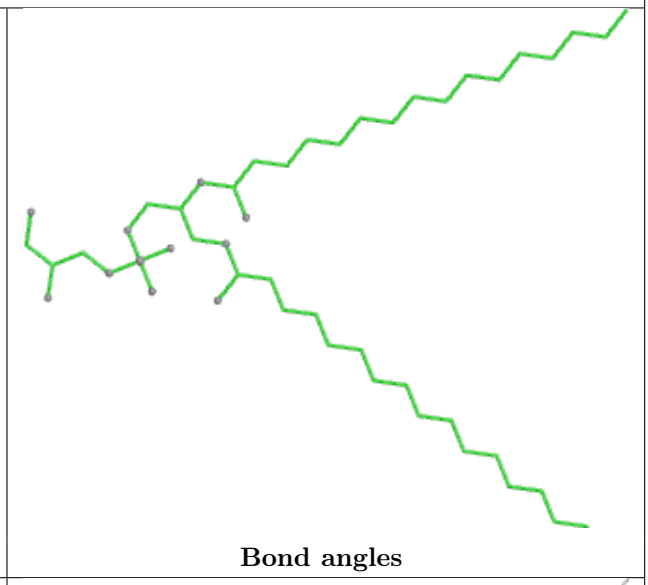
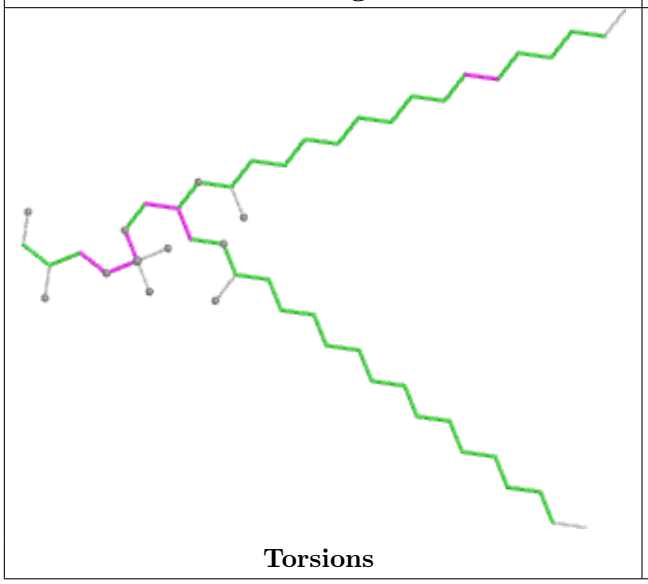


Bond angles



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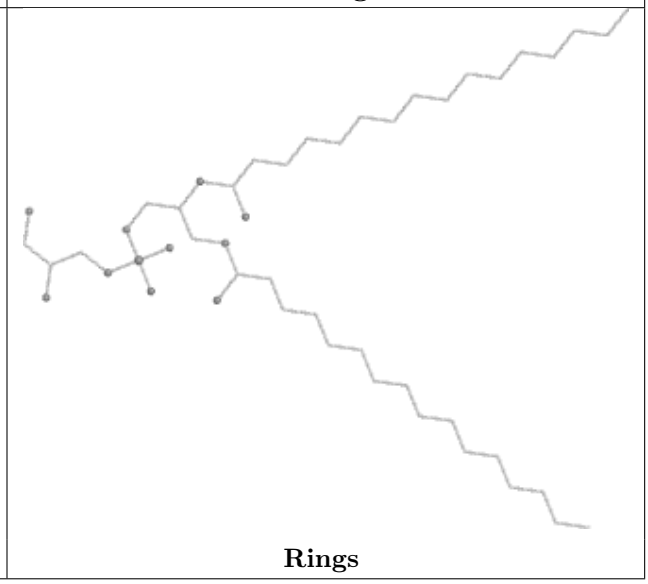
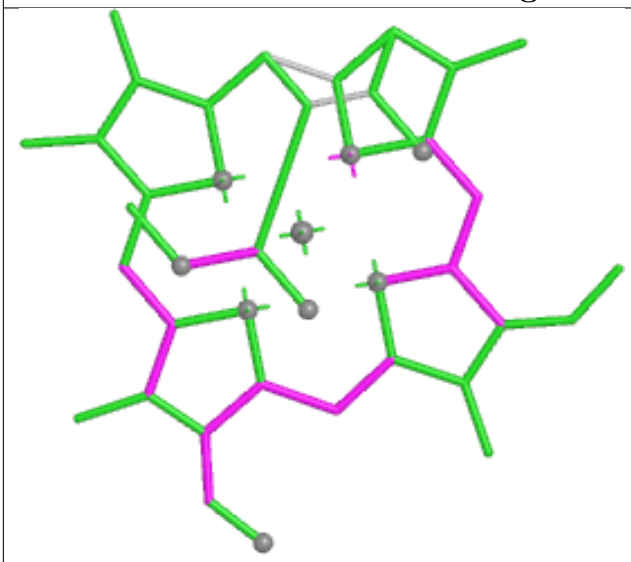


Rings

Ligand CL7 2B 602



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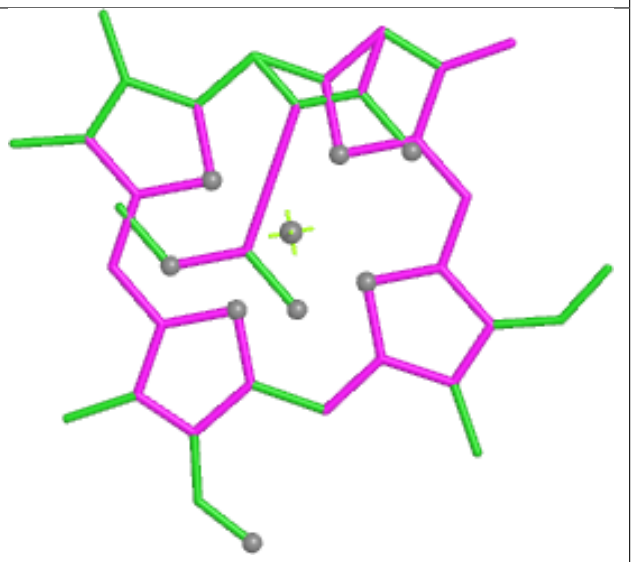
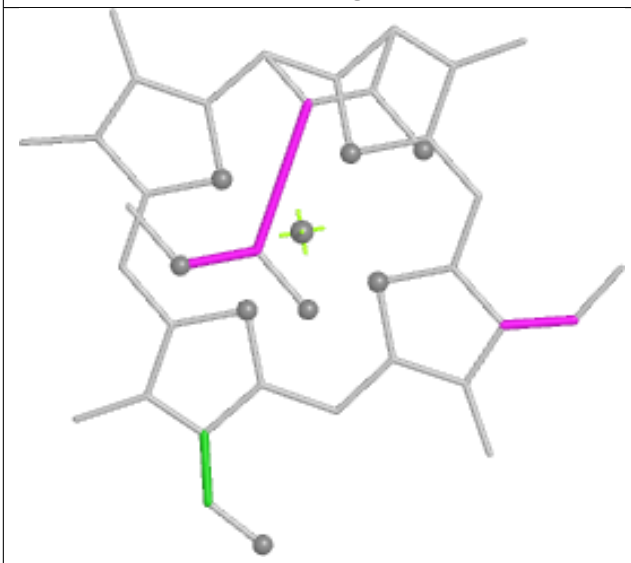


Bond angles



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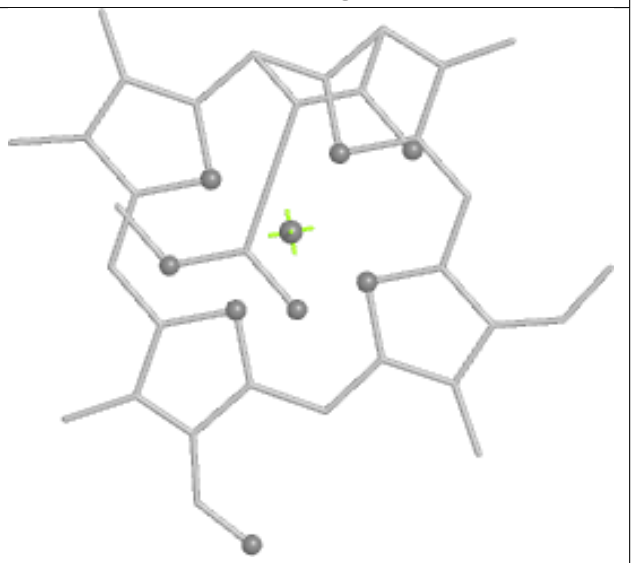
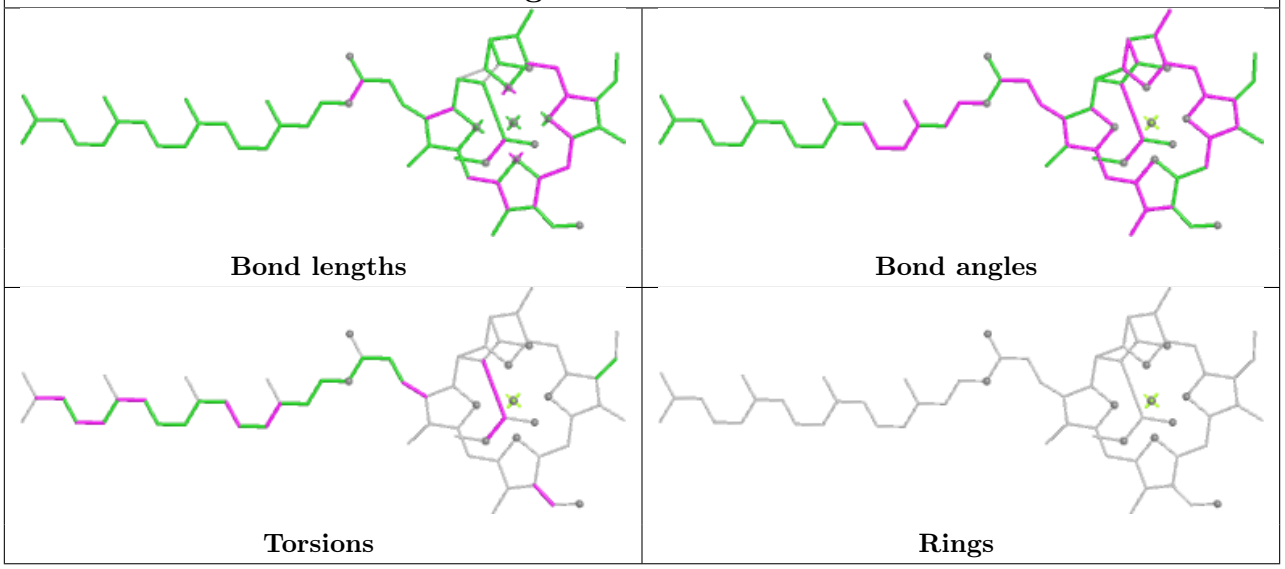
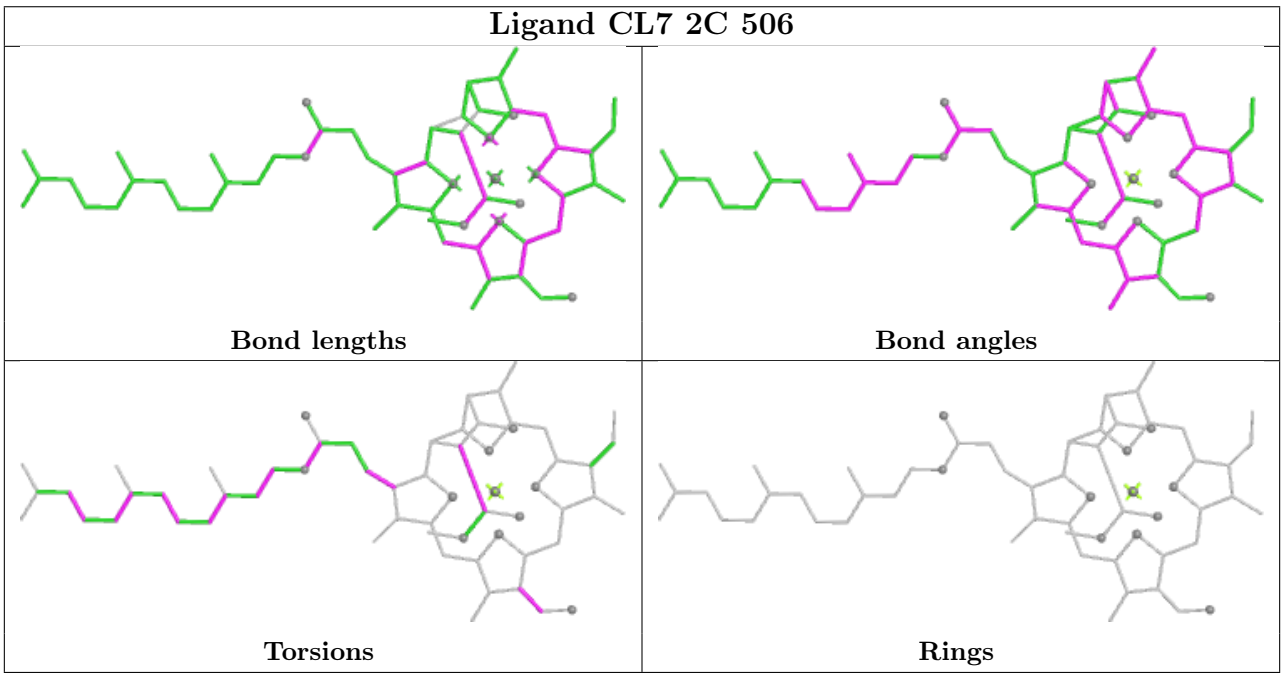


Rings

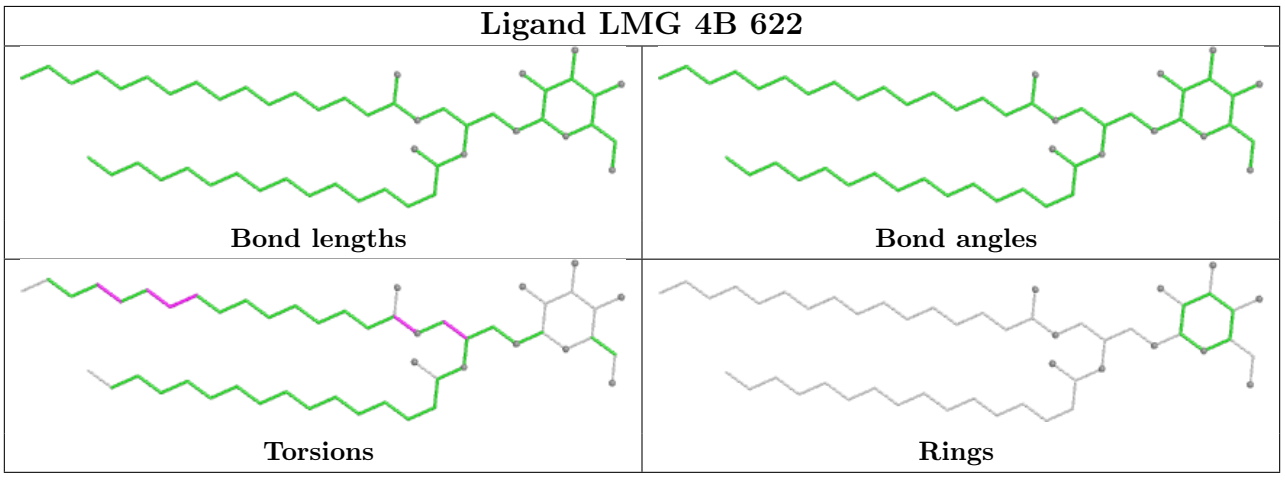
Ligand CL7 24 411



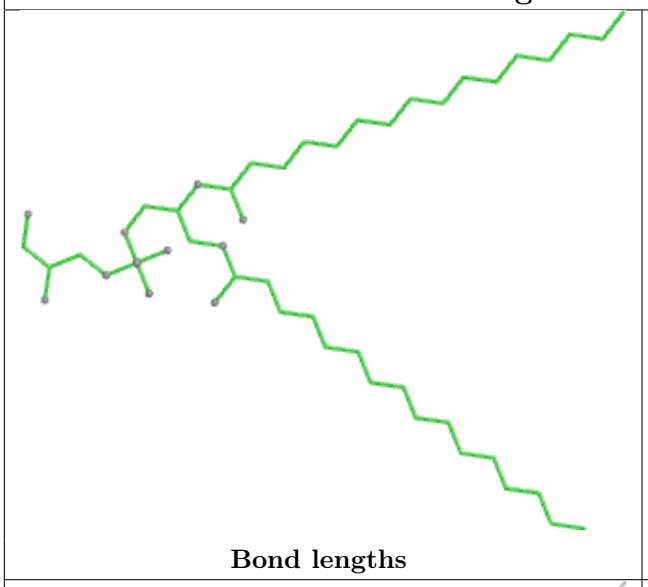
Ligand CL7 2C 506



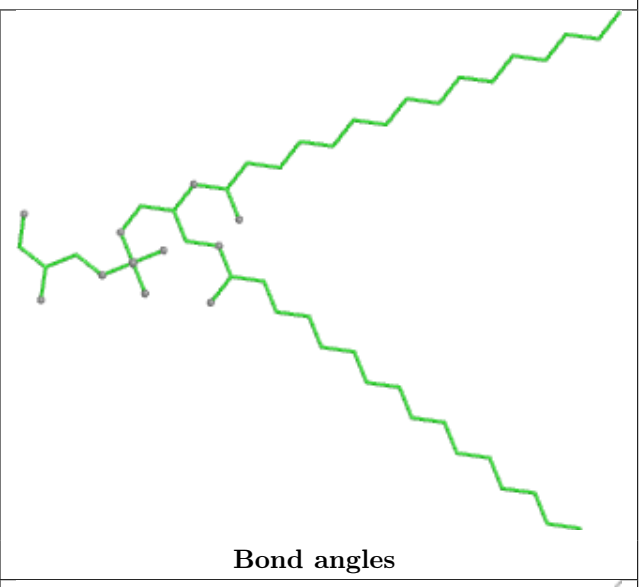
Ligand LMG 4B 622



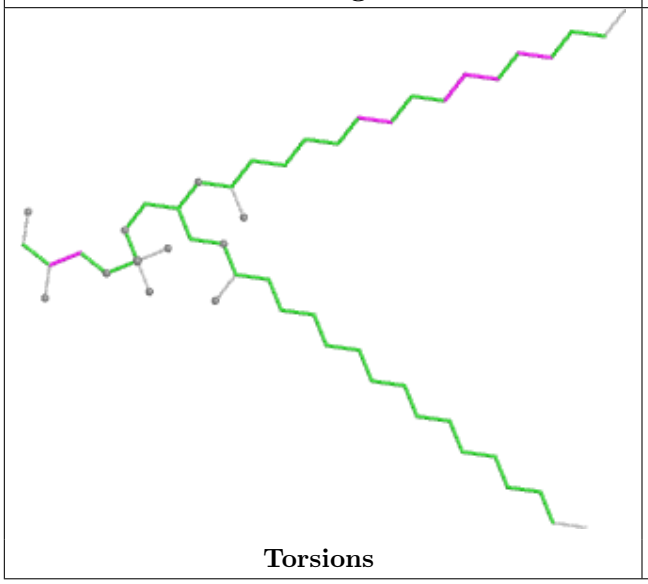
Ligand LHG 4B 626



Bond lengths



Bond angles



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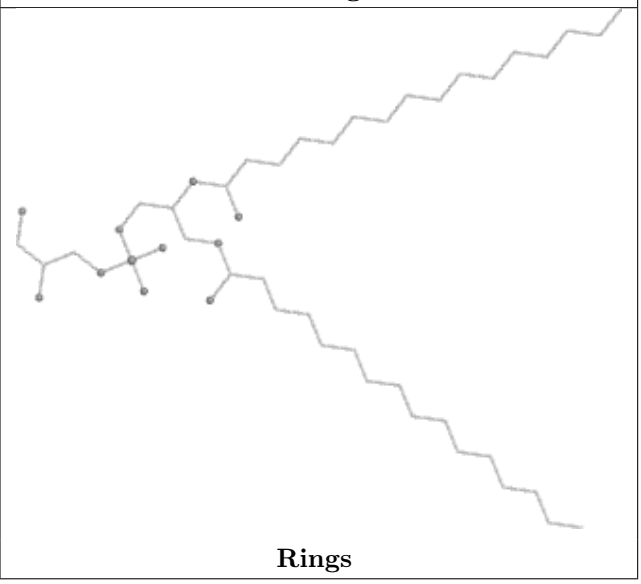
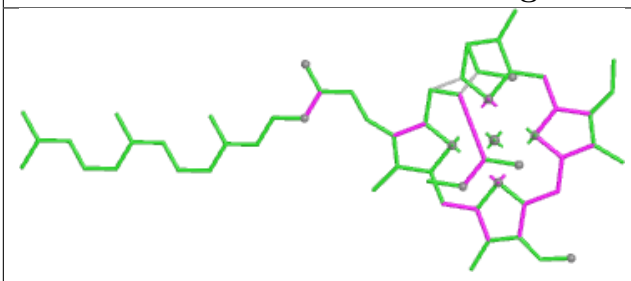


Rings

Ligand CL7 4C 502



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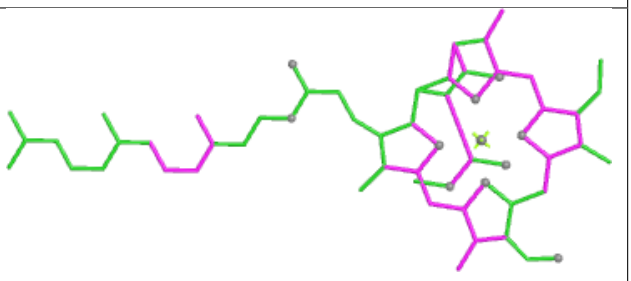
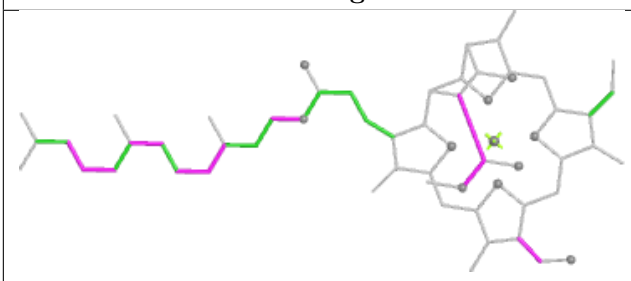
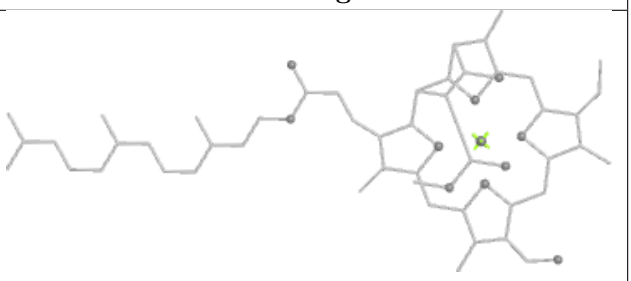


Bond angles

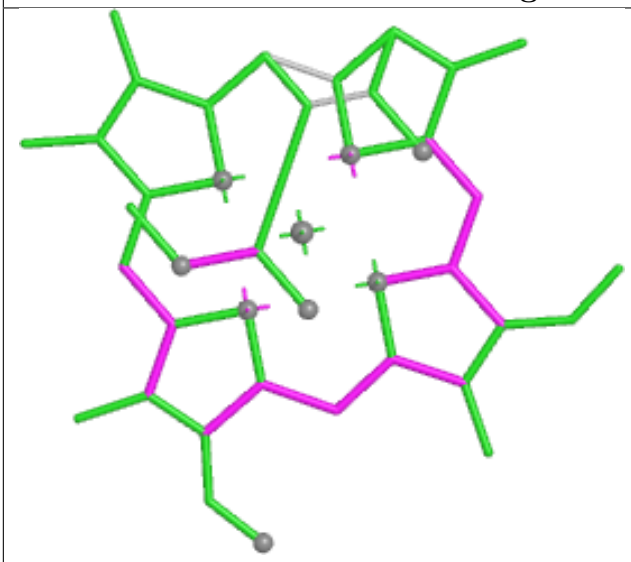


Torsions



Rings

Ligand CL7 4C 517



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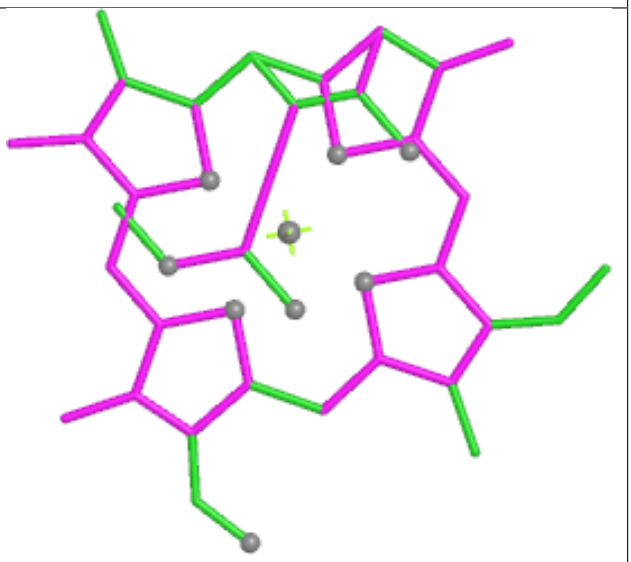
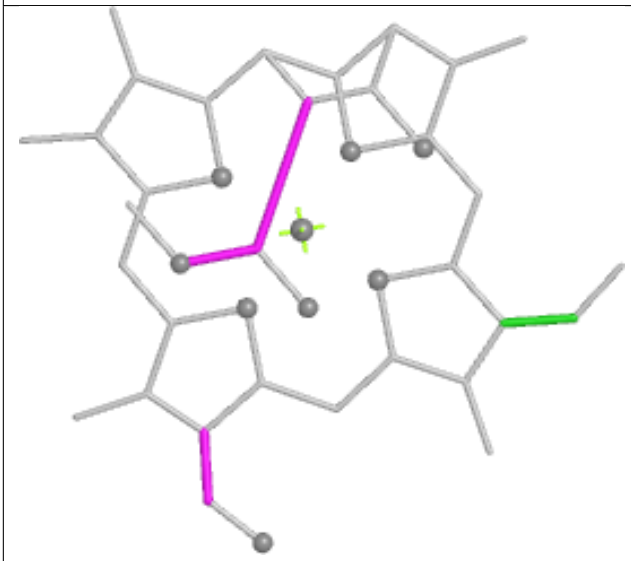
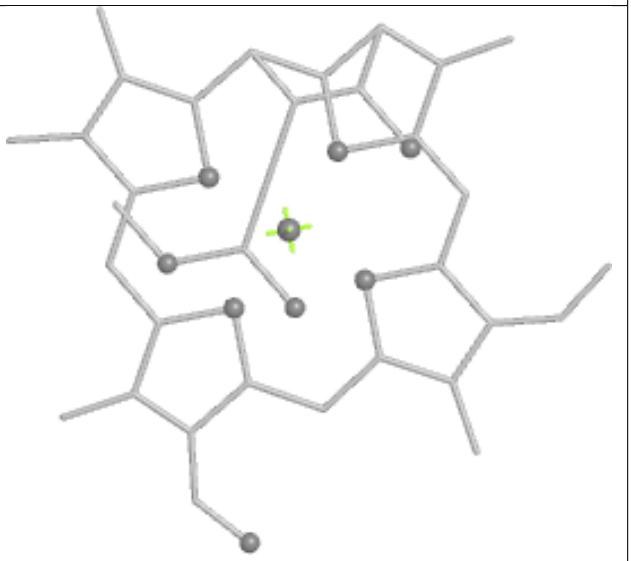


Bond angles

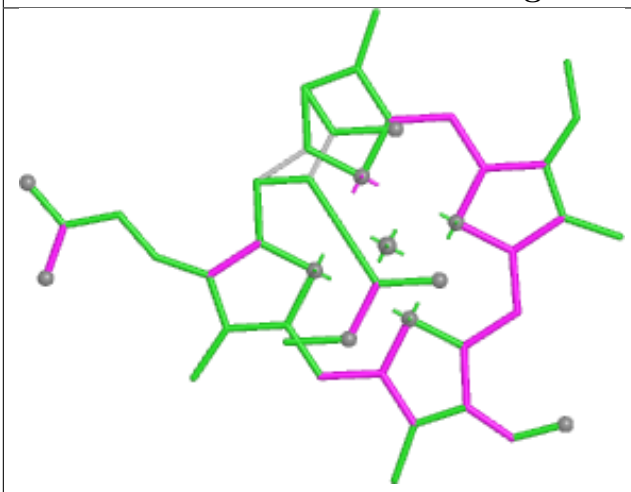


Torsions



Rings

Ligand CL7 43 407



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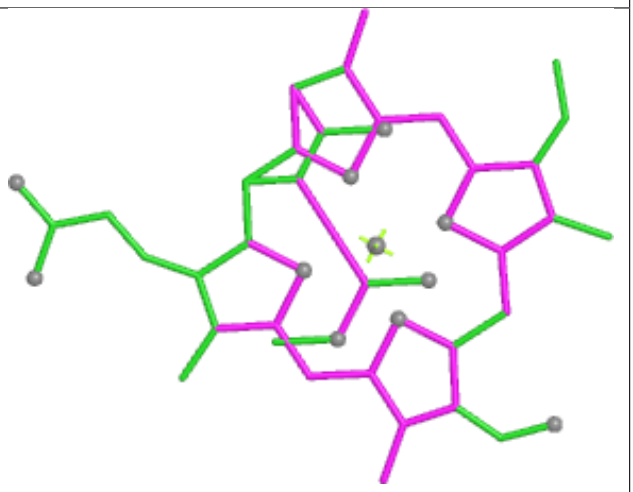

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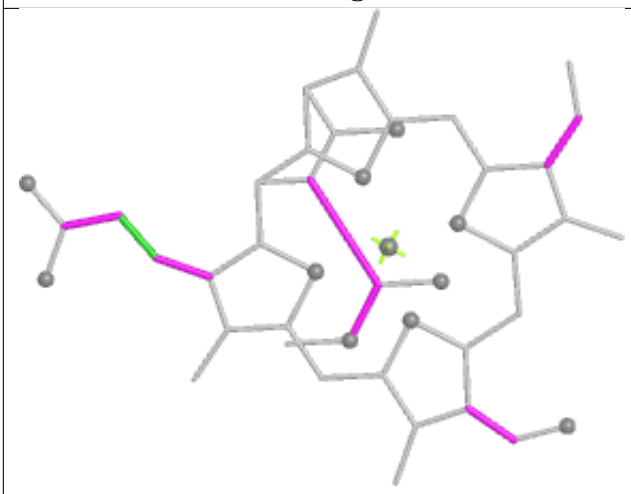

Torsions



Rings

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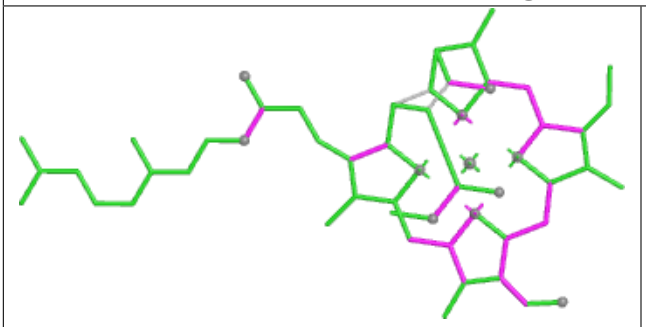

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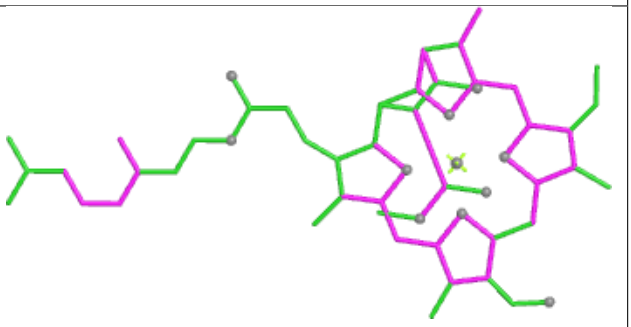

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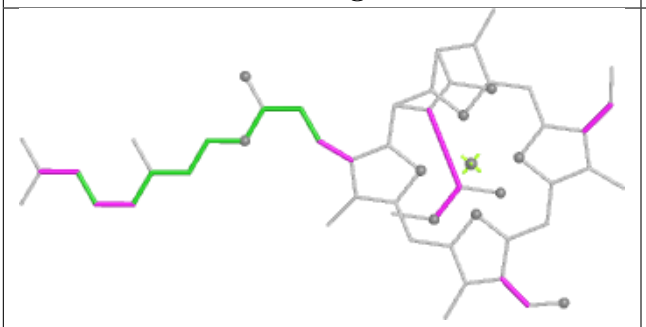

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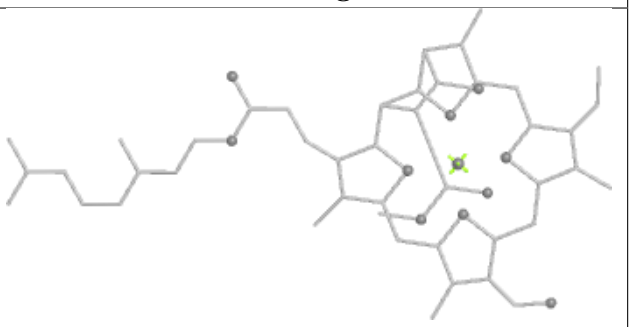
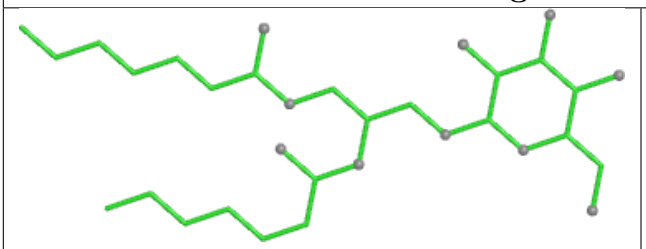


Rings

Ligand LMG 3D 410



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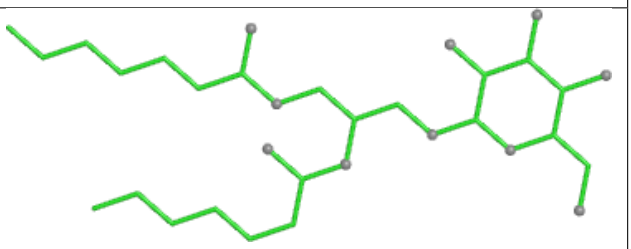

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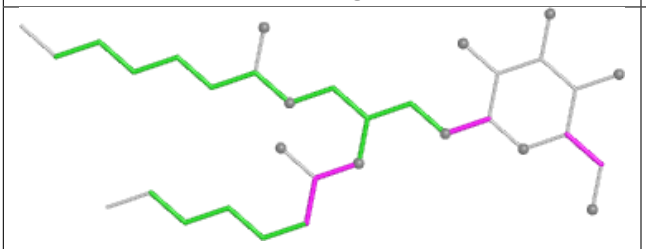

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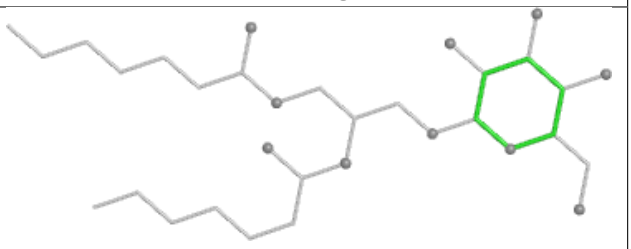
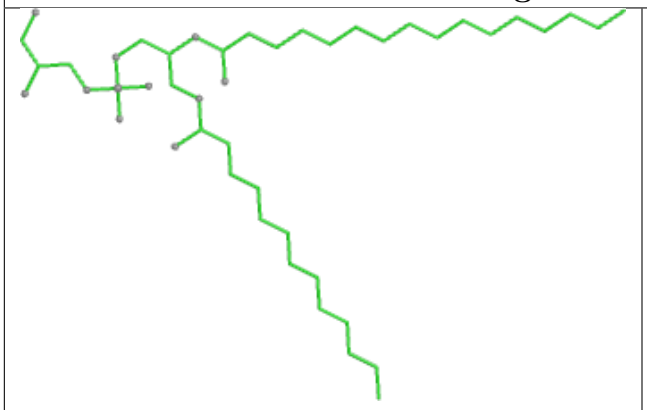


Rings

Ligand LHG 3A 408



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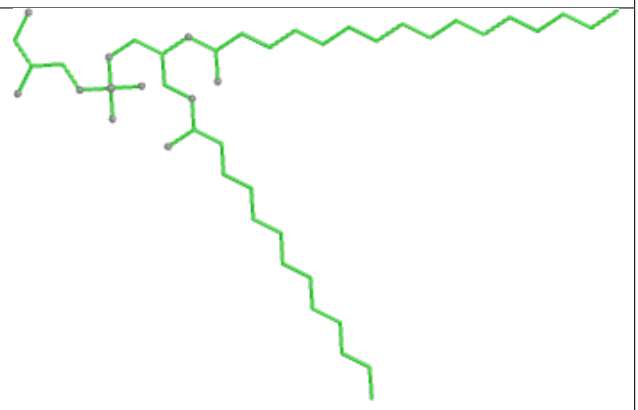

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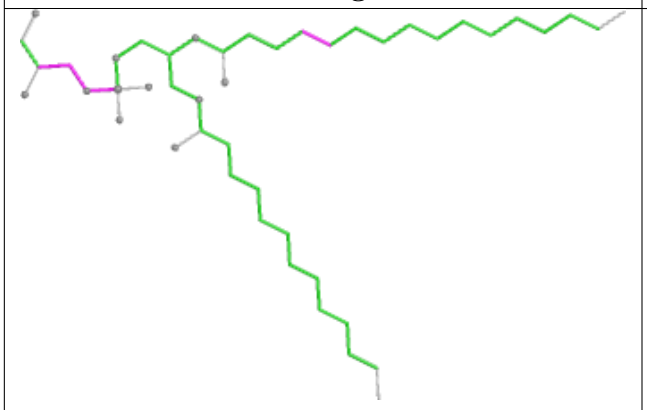

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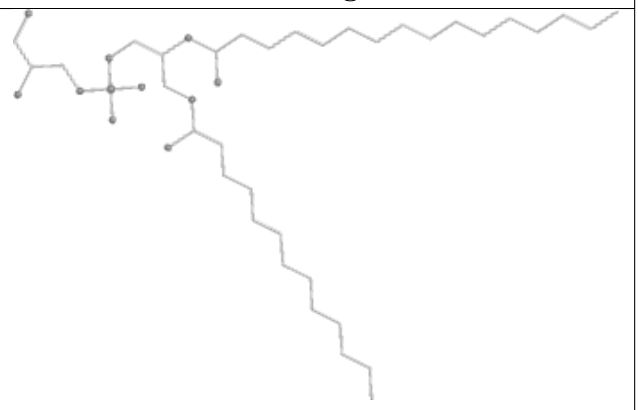
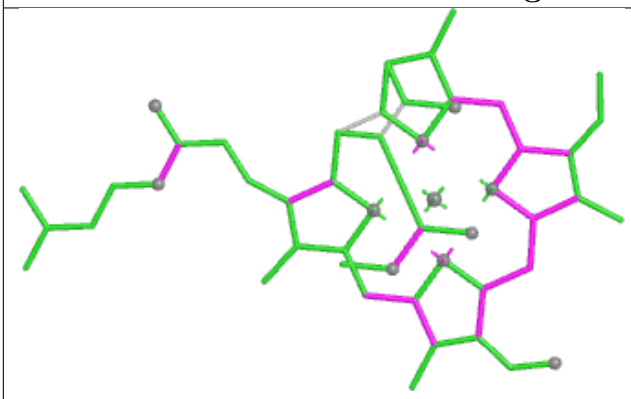


Rings

Ligand CL7 23 418



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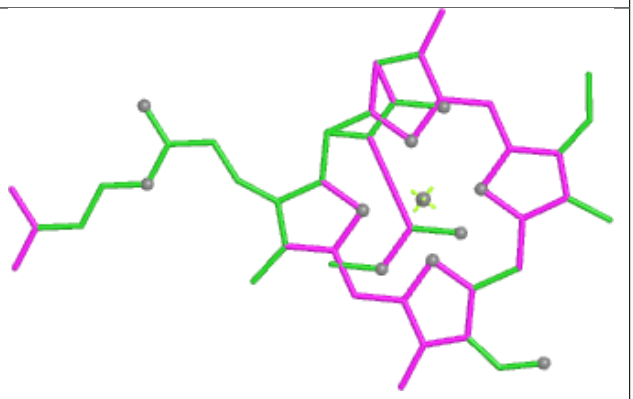

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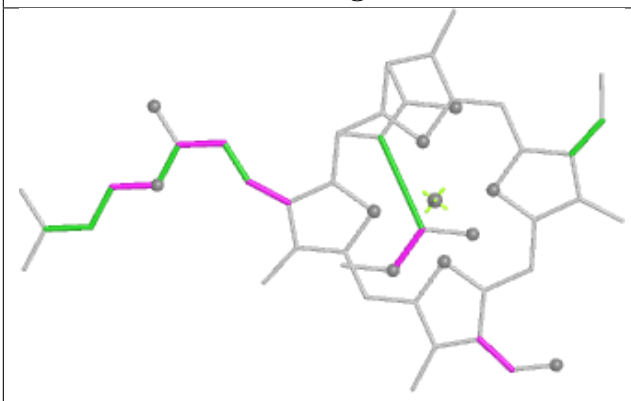

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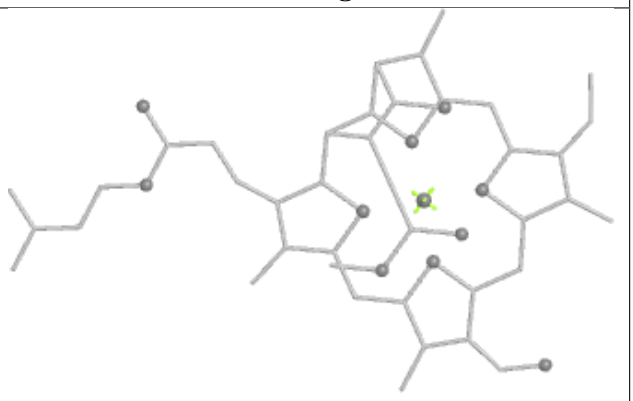

Rings

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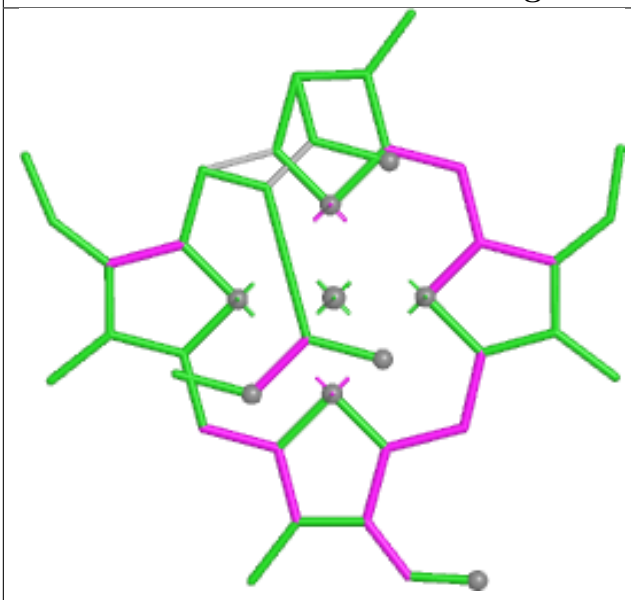

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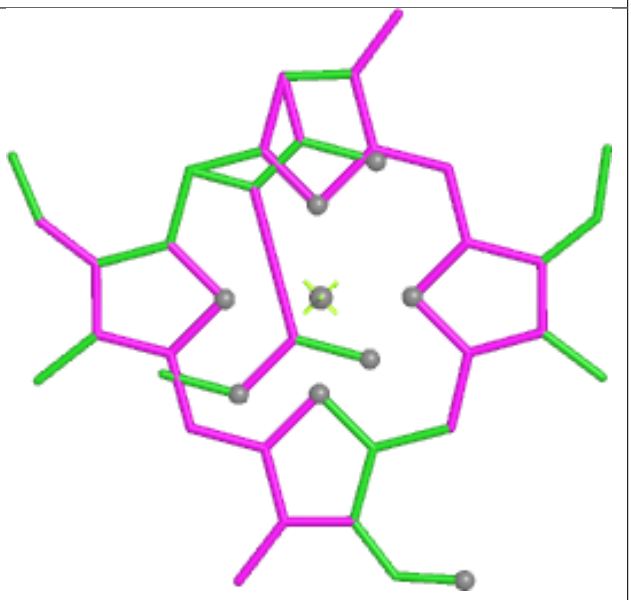

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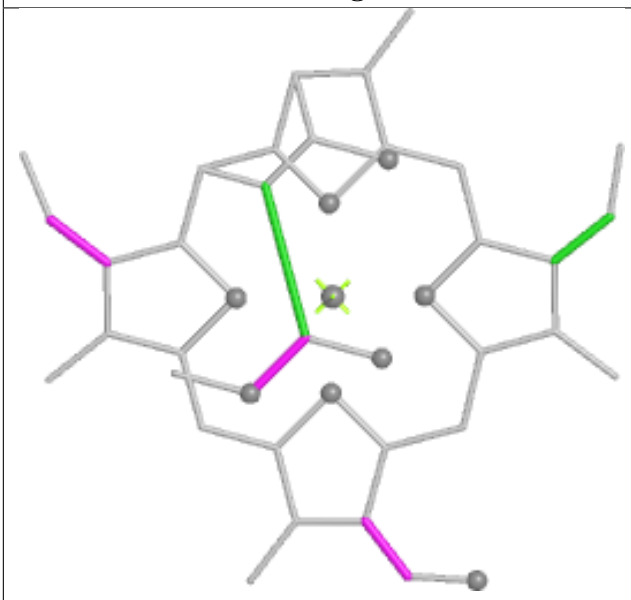

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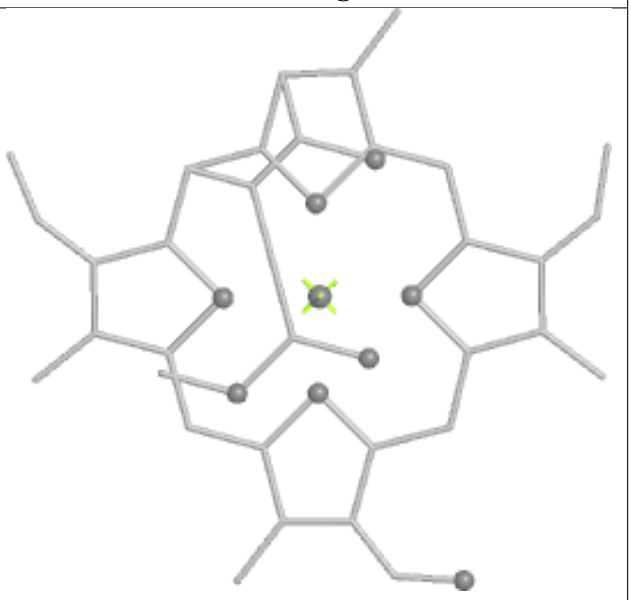
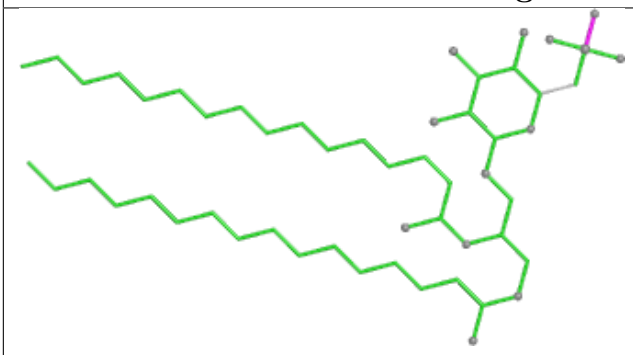


Rings

Ligand SQD 3B 620



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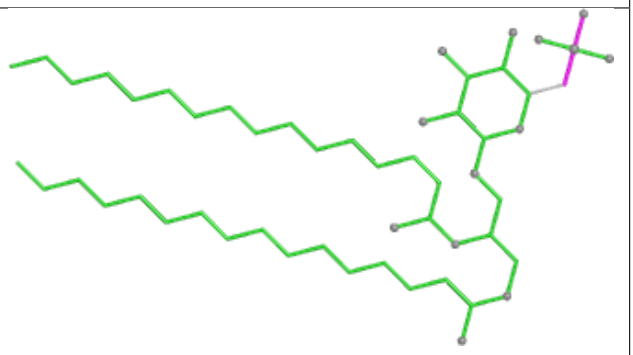

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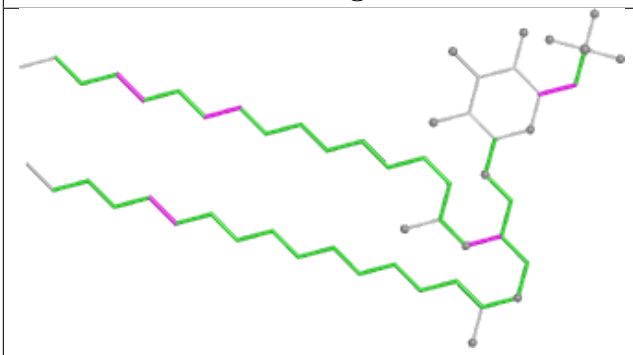

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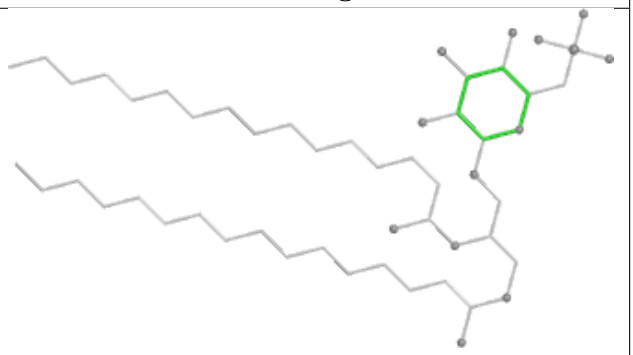
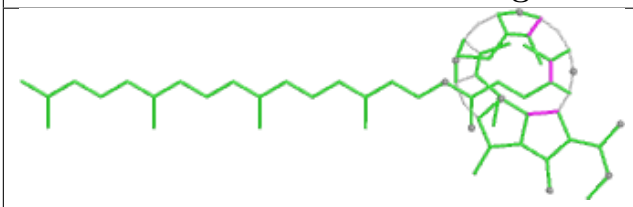


Rings

Ligand PHO 4D 408



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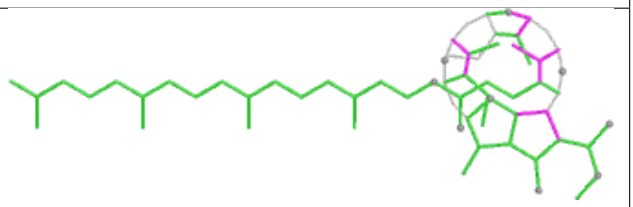

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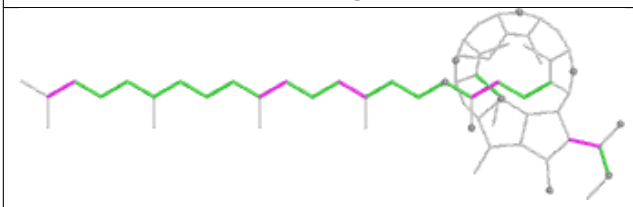

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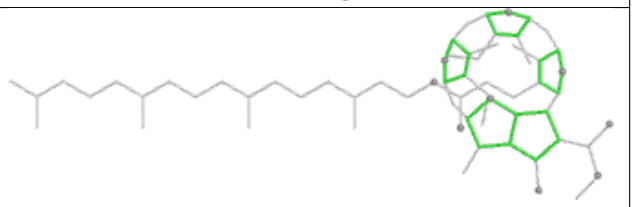
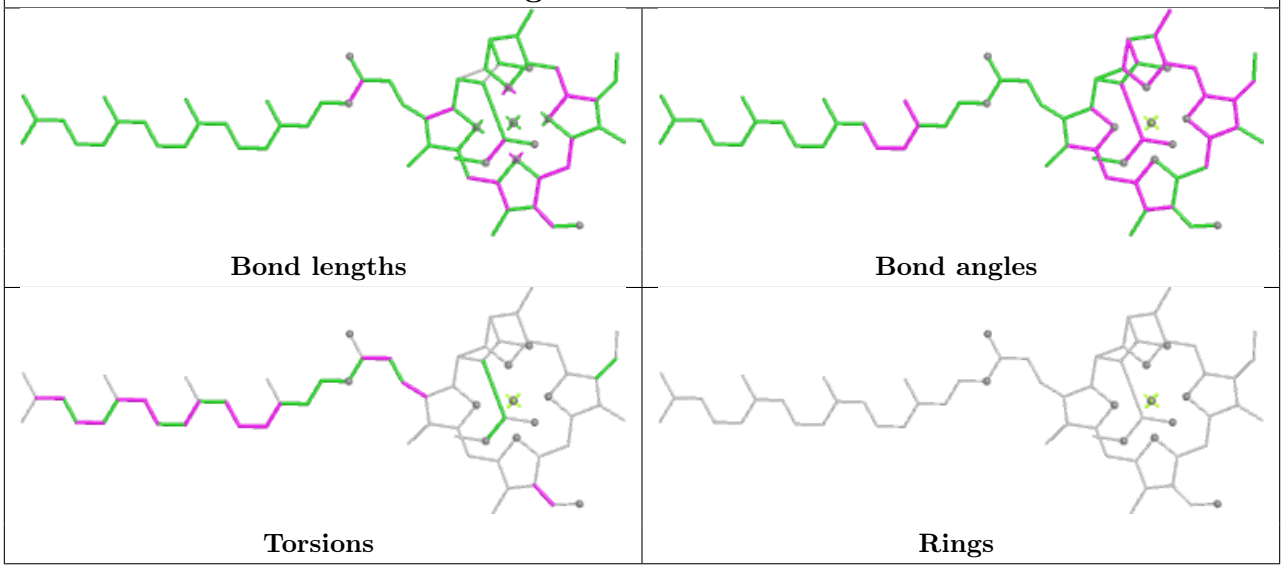


Rings

Ligand CL7 12 512



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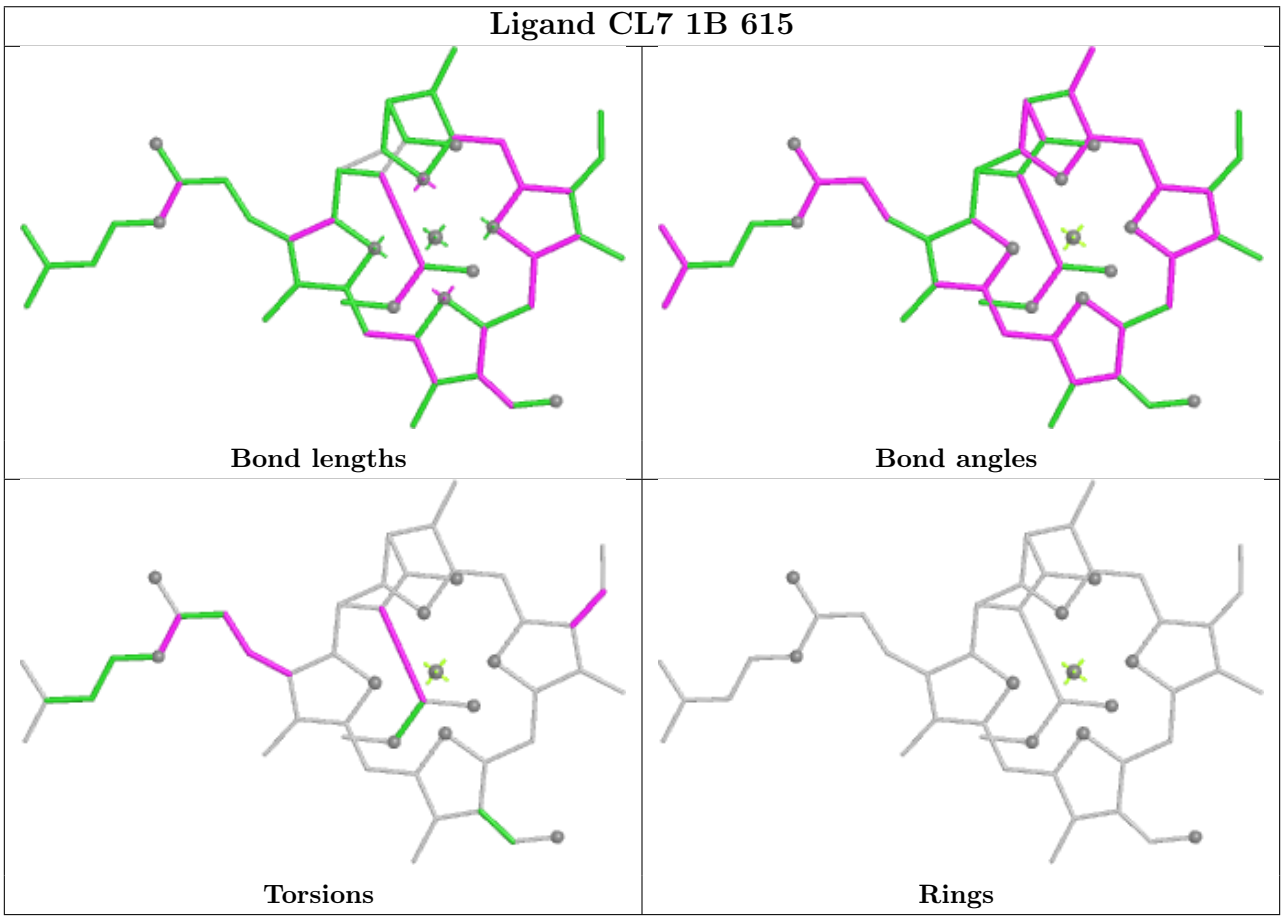

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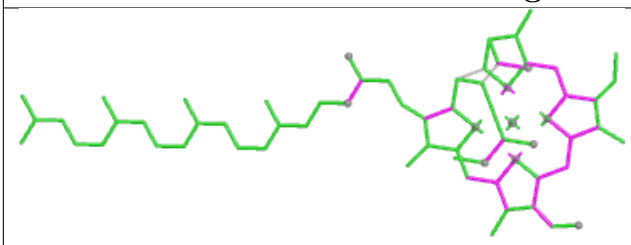

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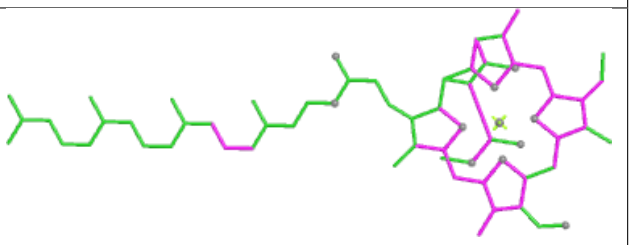
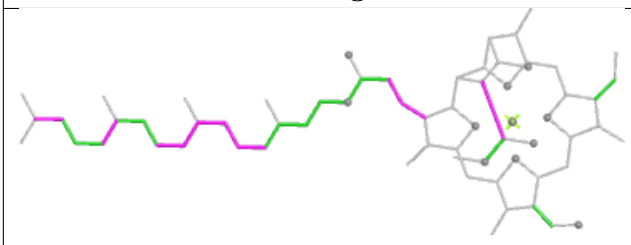


Bond angles



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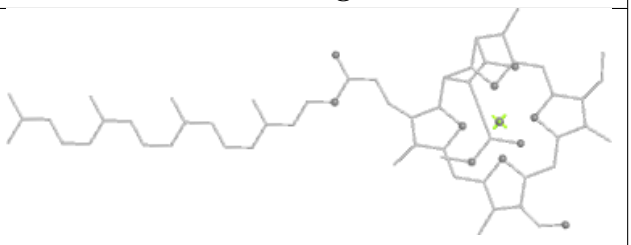
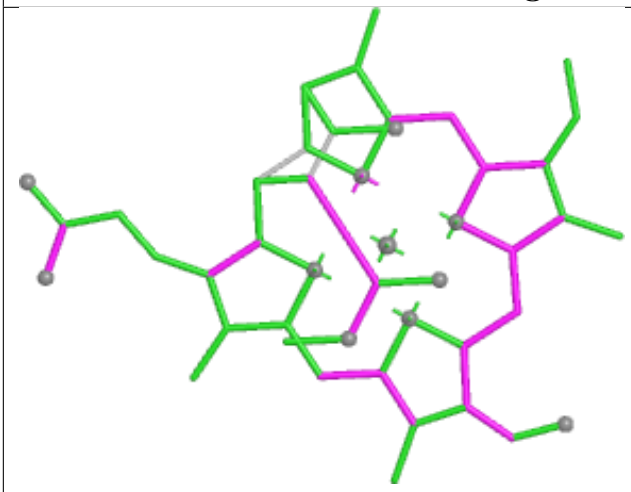


Rings

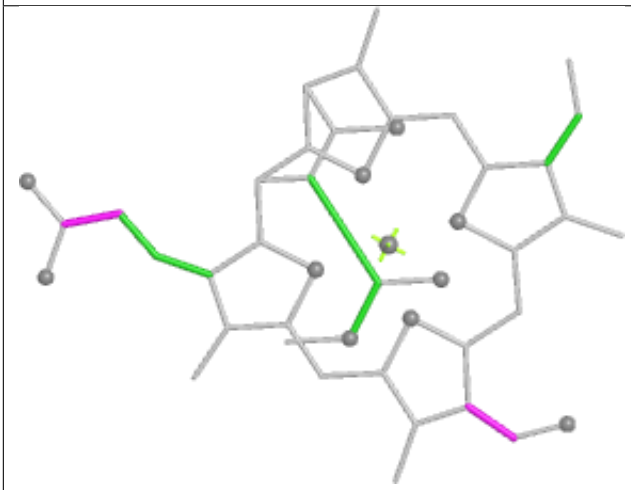
Ligand CL7 34 408



Bond lengths



Bond angles

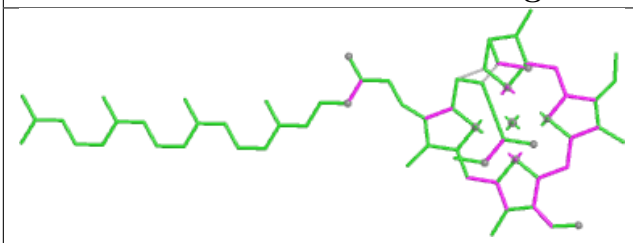


Torsions



Rings

Ligand CL7 41 410



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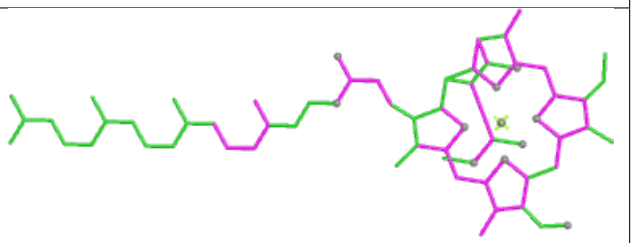

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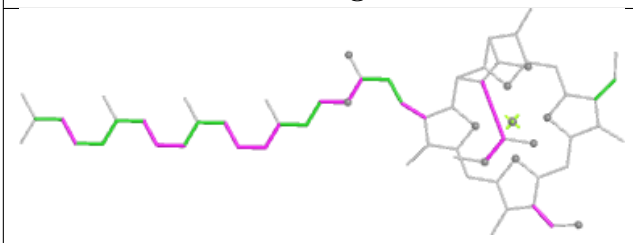

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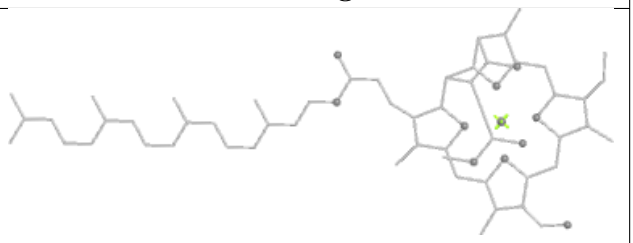
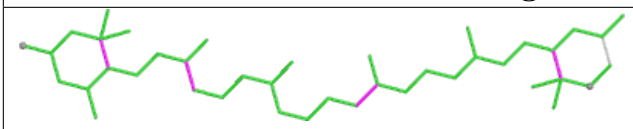


Rings

Ligand ZEX 12 522



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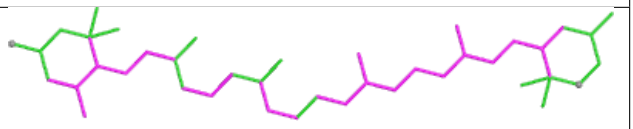

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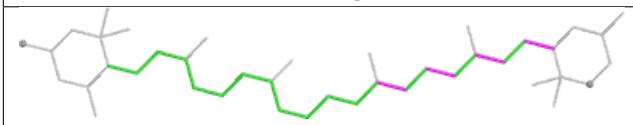

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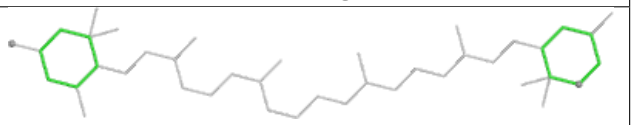
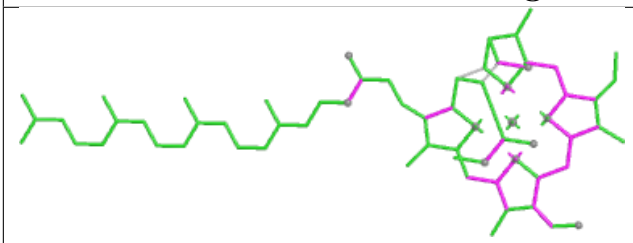


Rings

Ligand CL7 42 506



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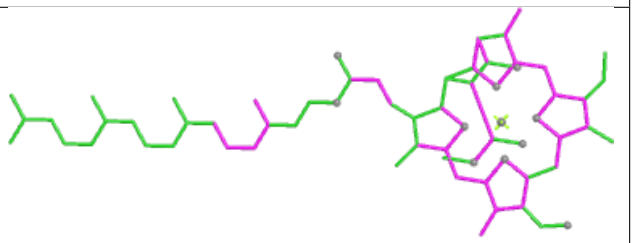
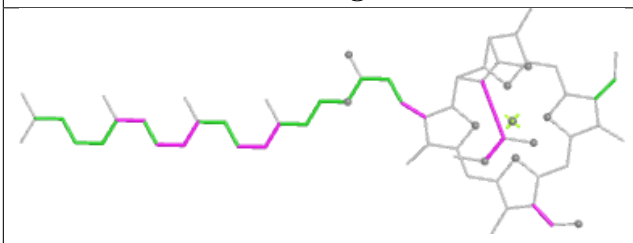


Bond angles



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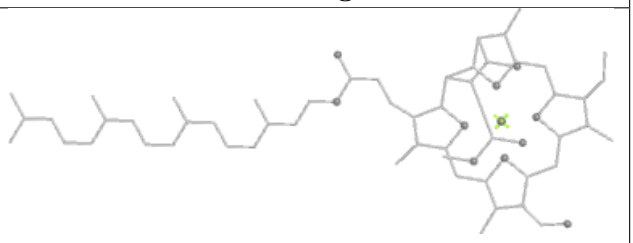
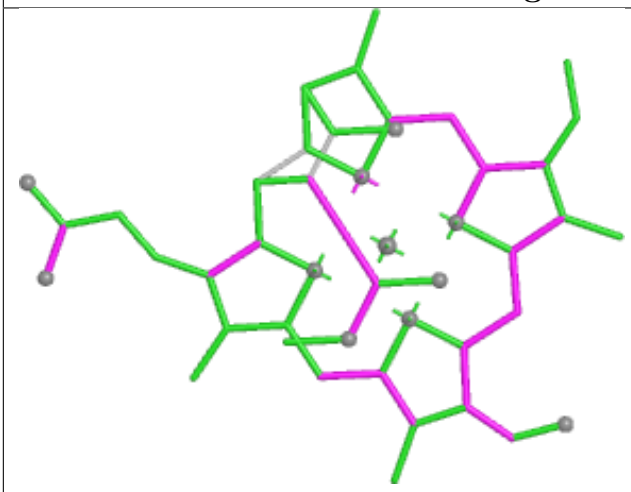


Rings

Ligand CL7 24 408



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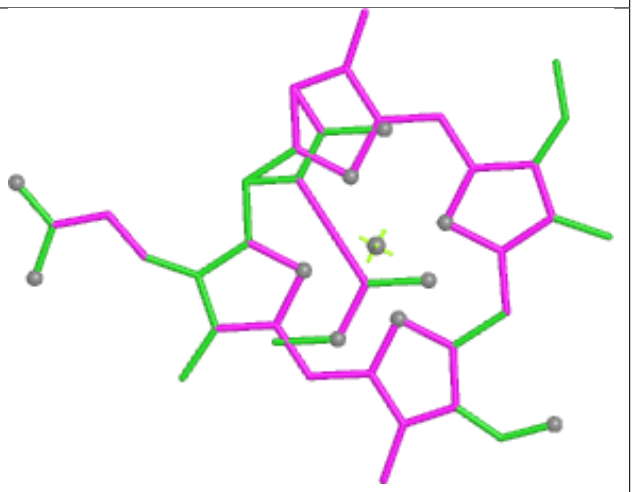
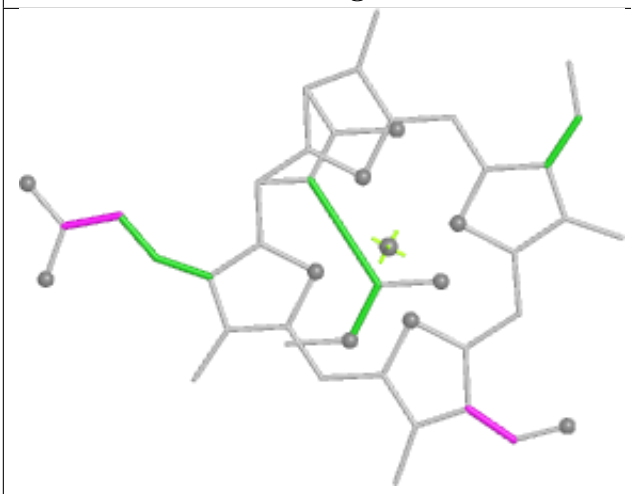


Bond angles

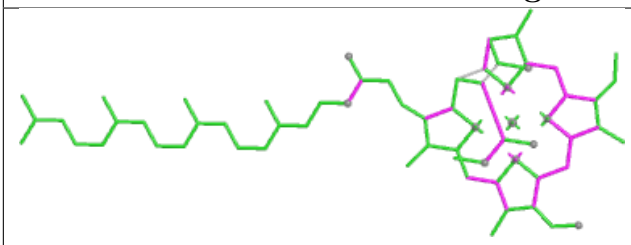


Torsions



Rings

Ligand CL7 42 509



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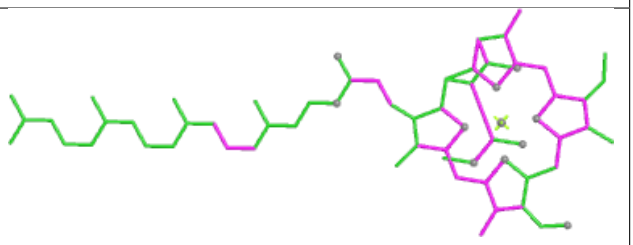
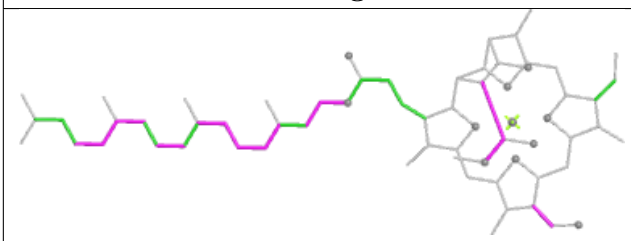
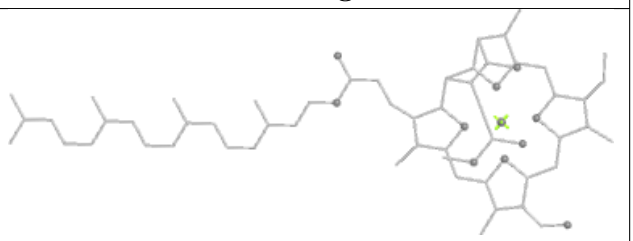


Bond angles

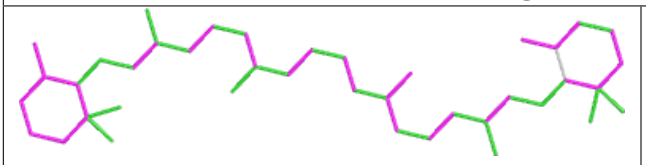


Torsions



Rings

Ligand 8CT 3C 518



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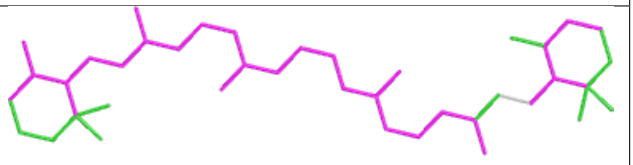
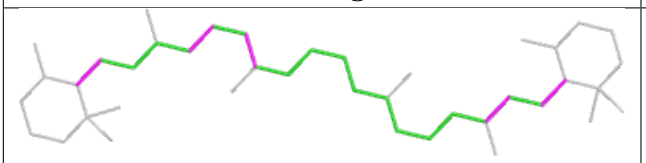


Bond angles



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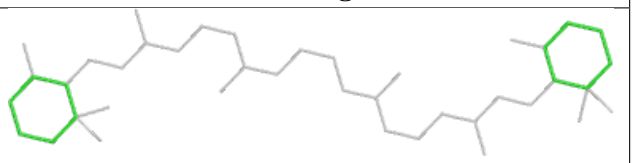
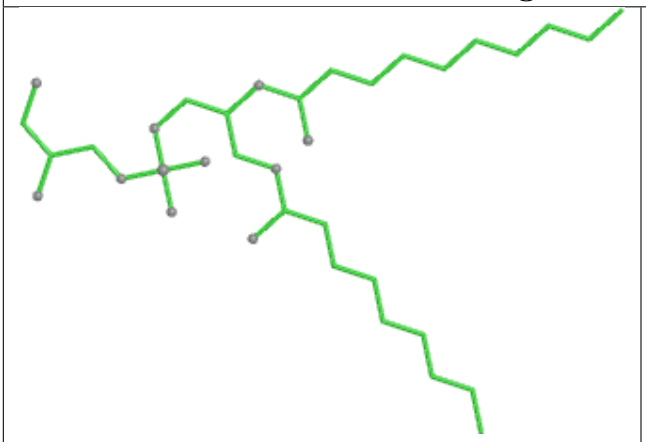


Rings

Ligand LHG 23 425



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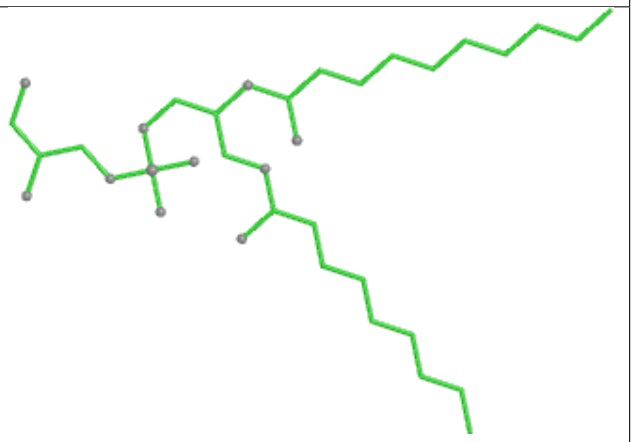
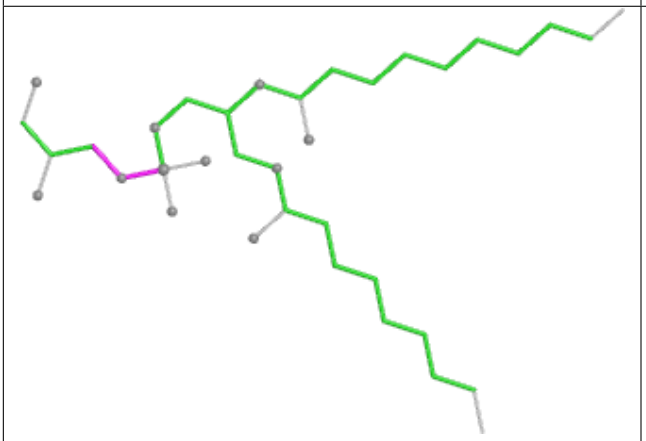


Bond angles



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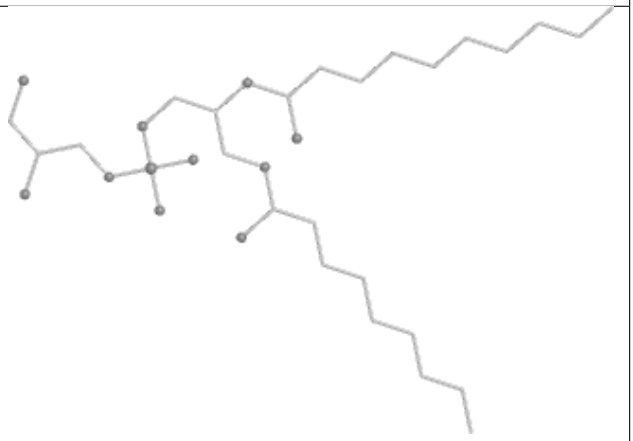
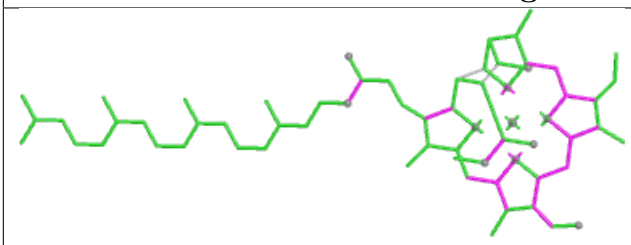


Rings

Ligand CL7 2B 605



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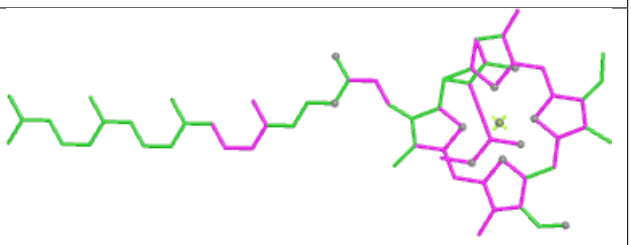

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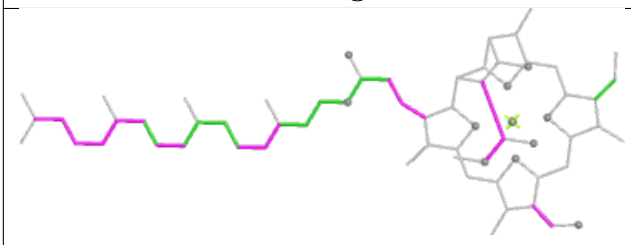

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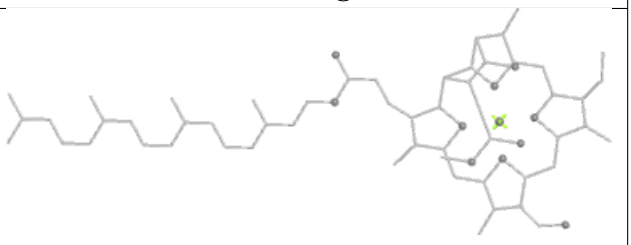
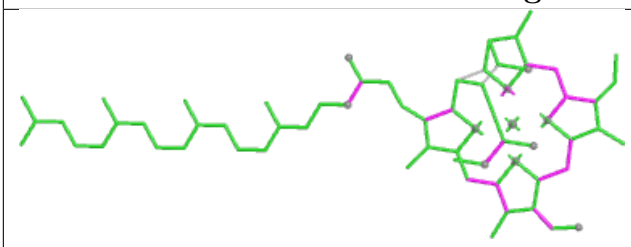


Rings

Ligand CL7 42 518



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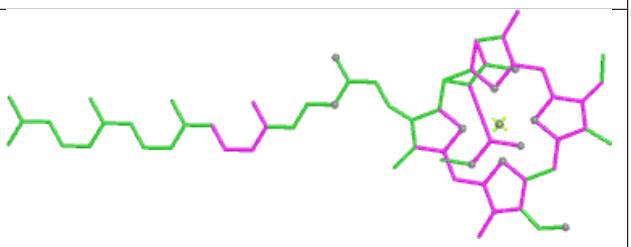
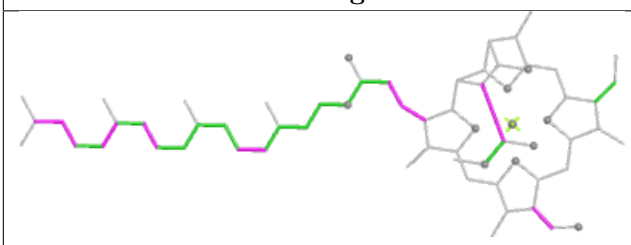


Bond angles



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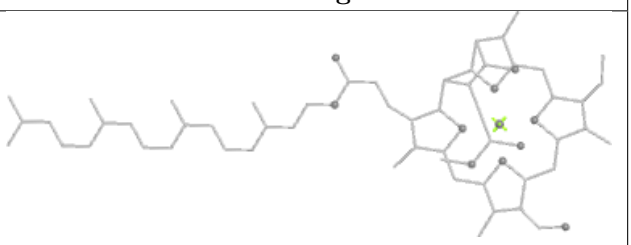
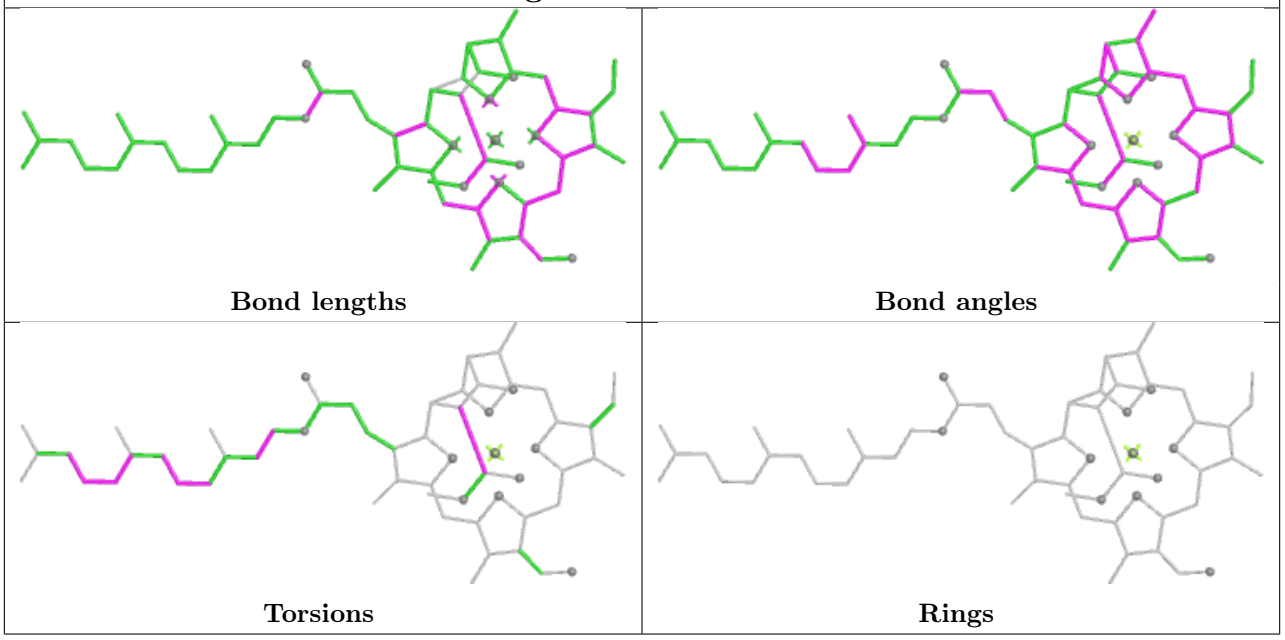


Rings

Ligand CL7 34 413



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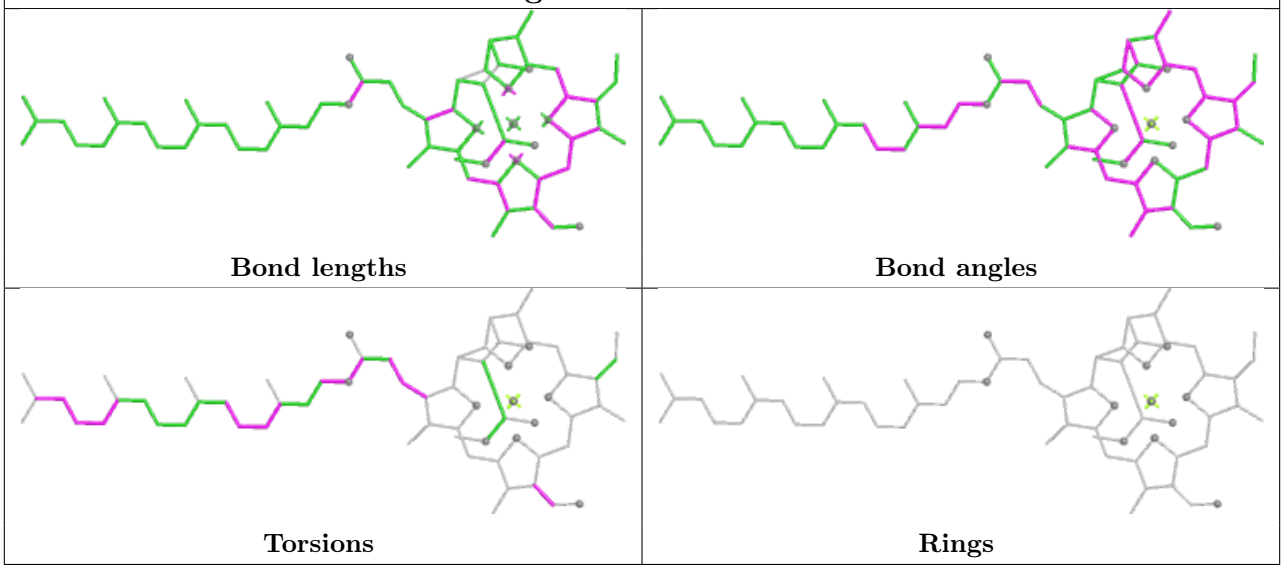

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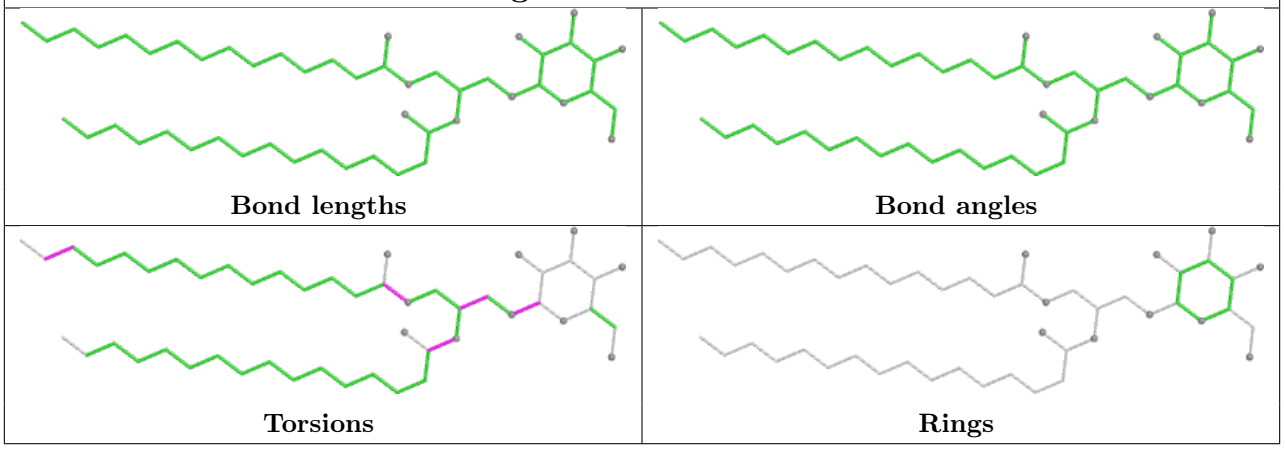

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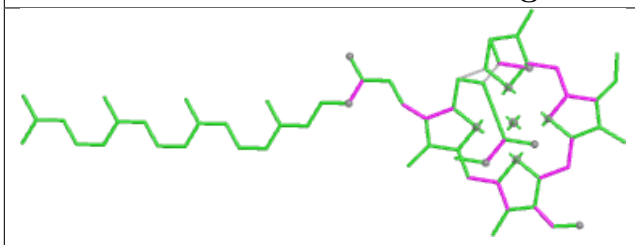

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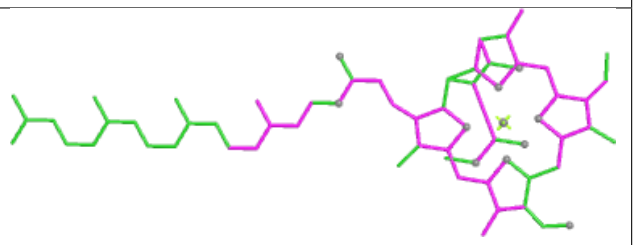
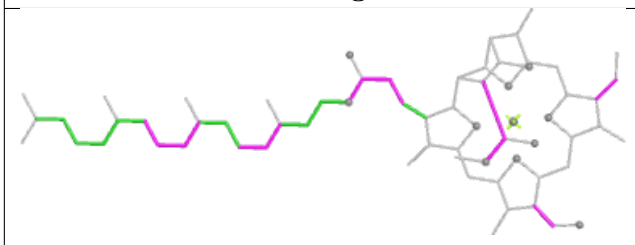


Bond angles



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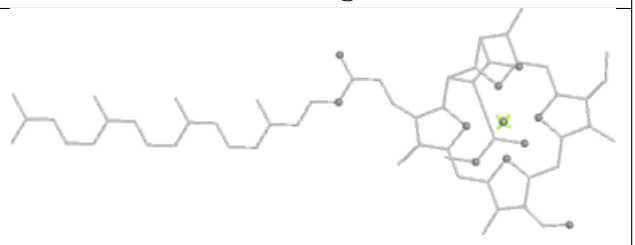
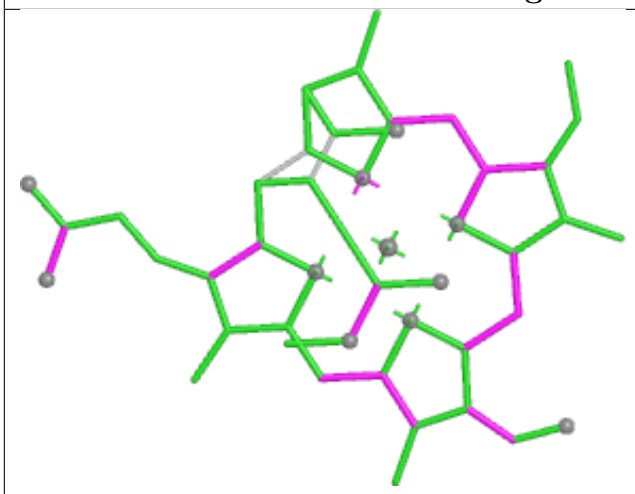


Rings

Ligand CL7 33 518



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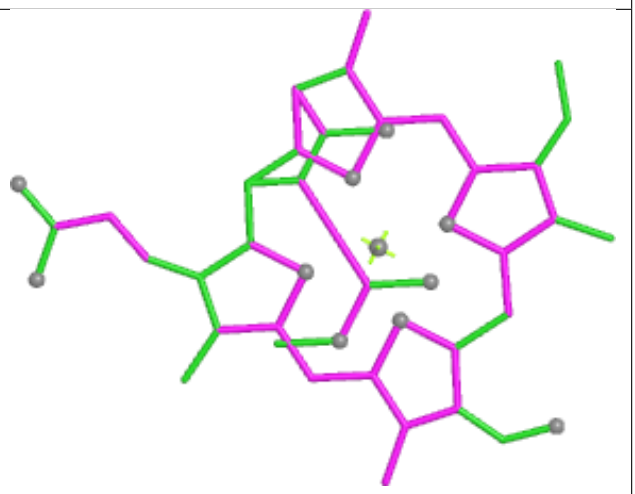
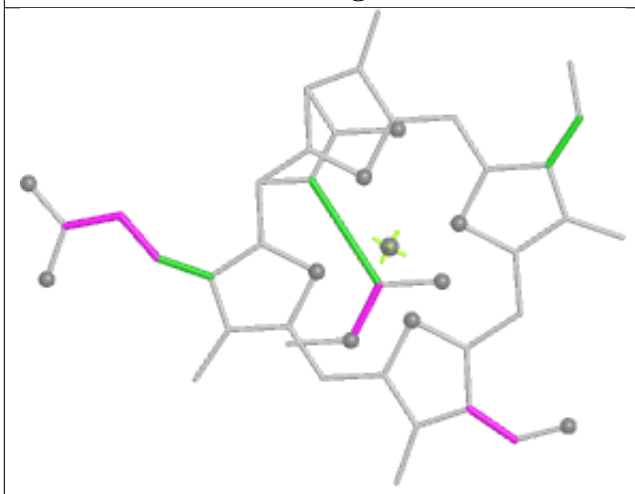


Bond angles

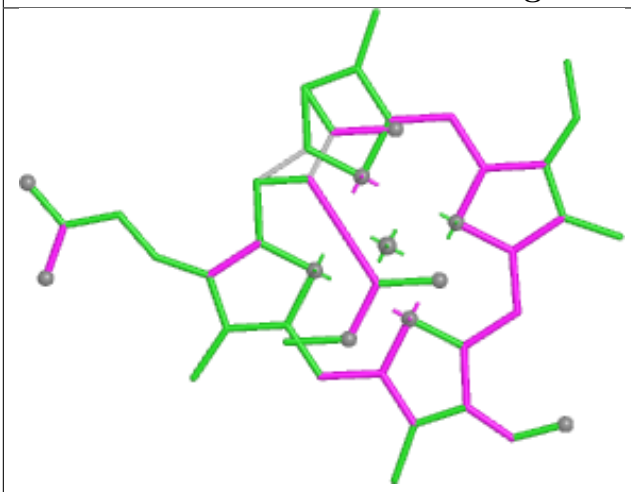


Torsions



Rings

Ligand CL7 44 415



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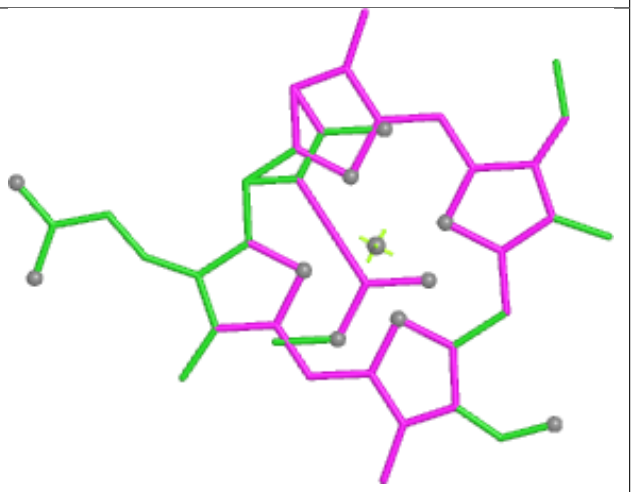
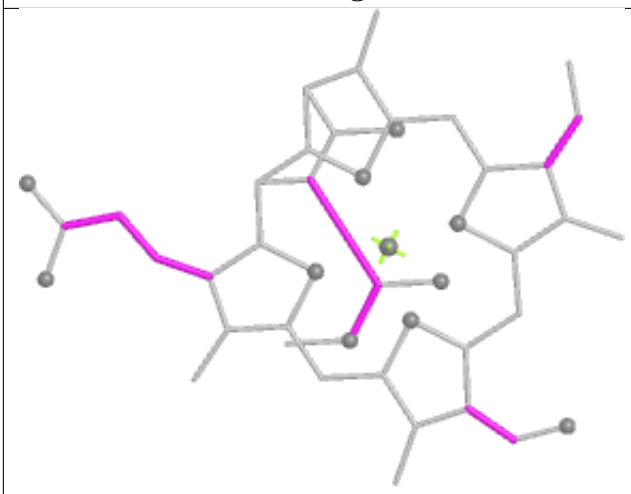


Bond angles



Torsions



Rings

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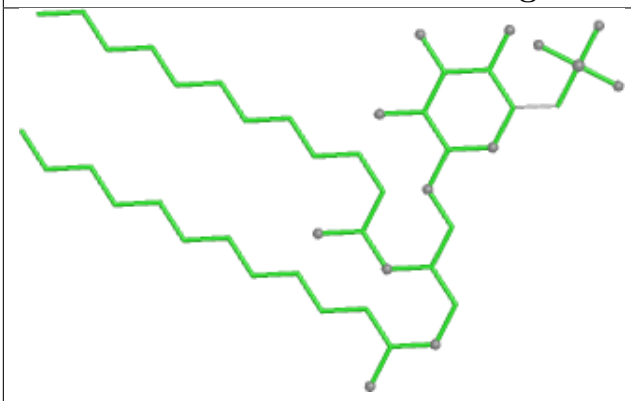

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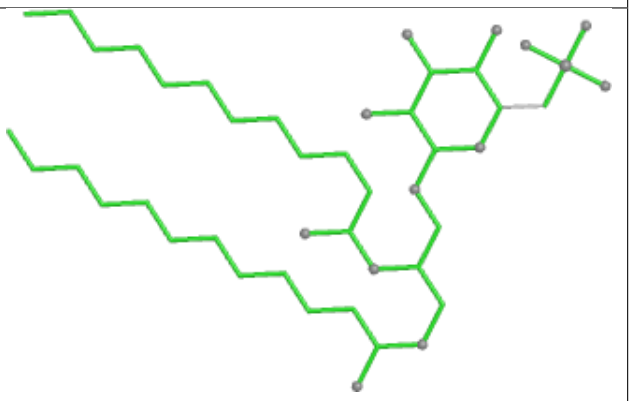
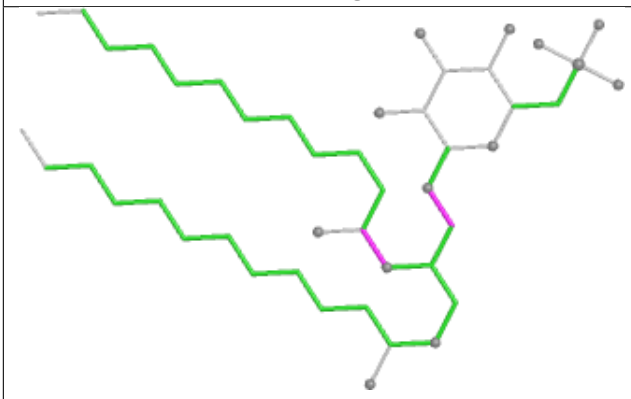


Bond angles



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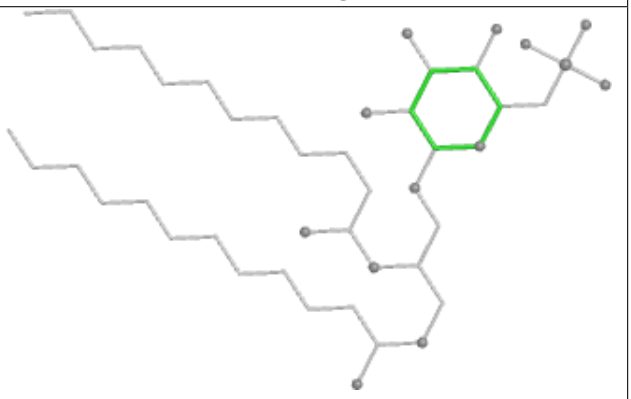
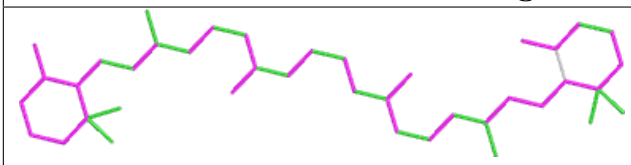


Rings

Ligand 8CT 2K 101



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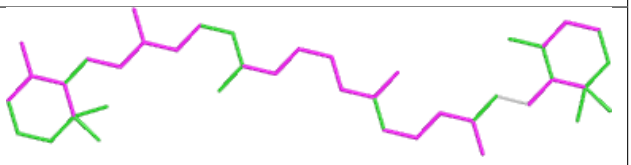
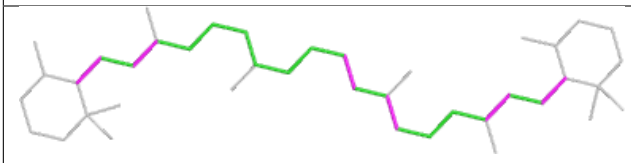


Bond angles



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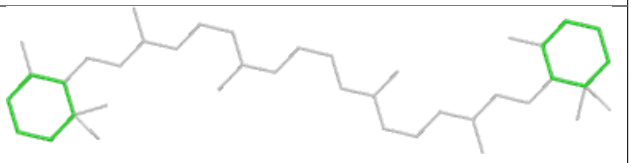
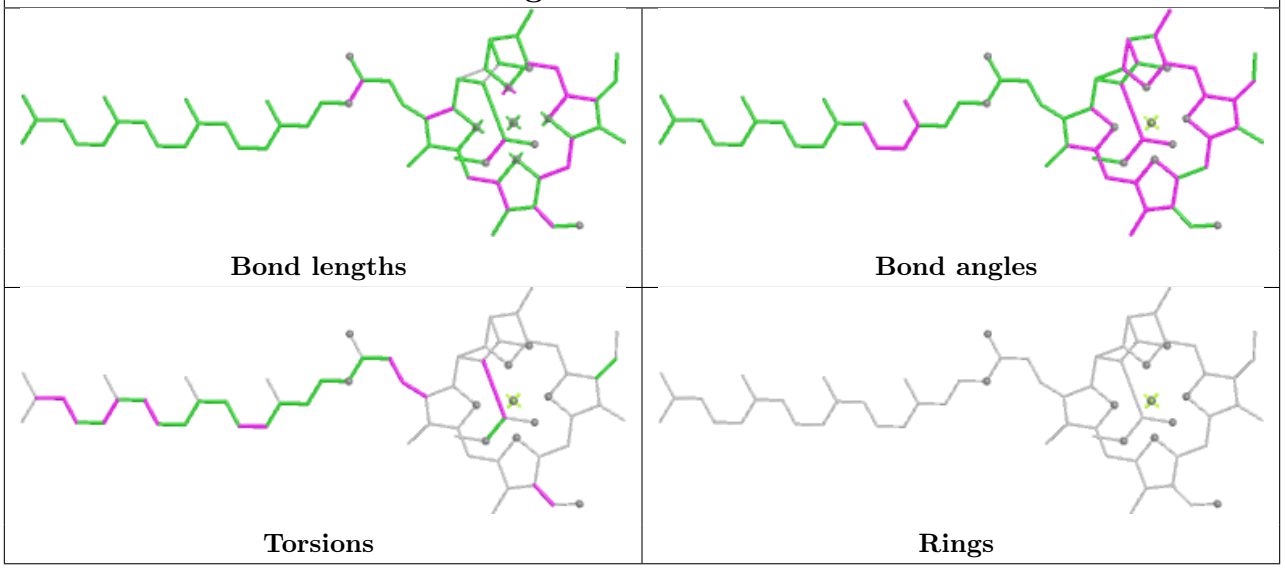


Rings

Ligand CL7 12 518



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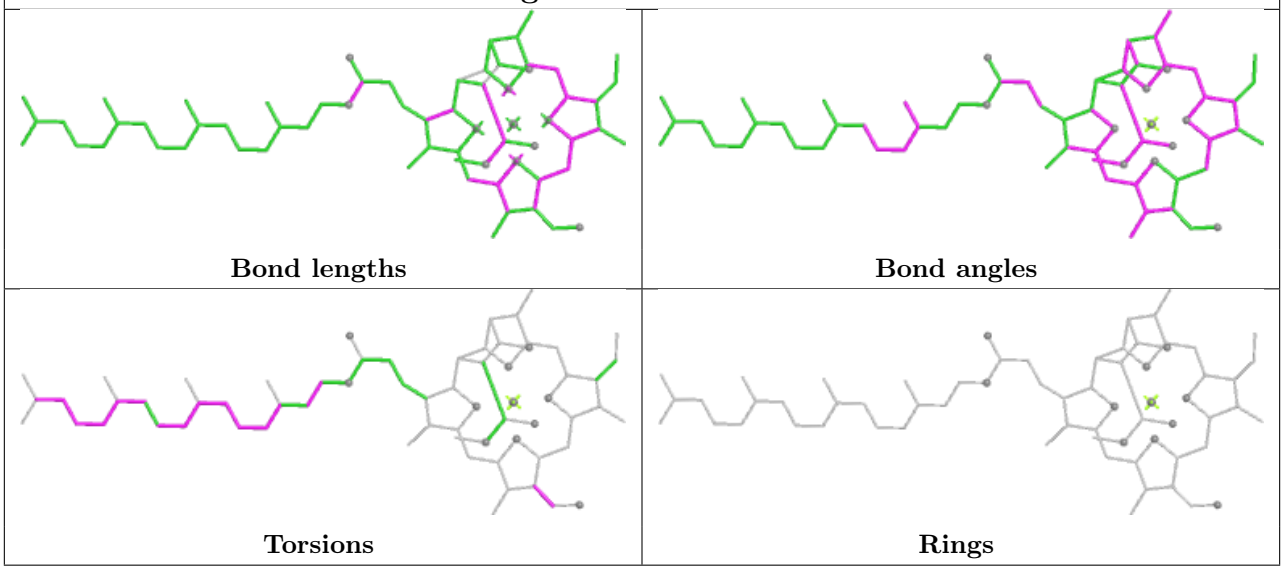

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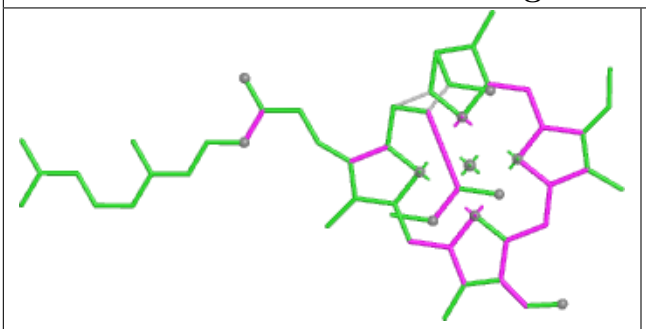

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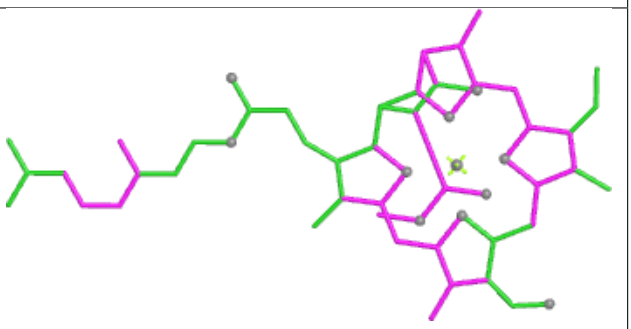
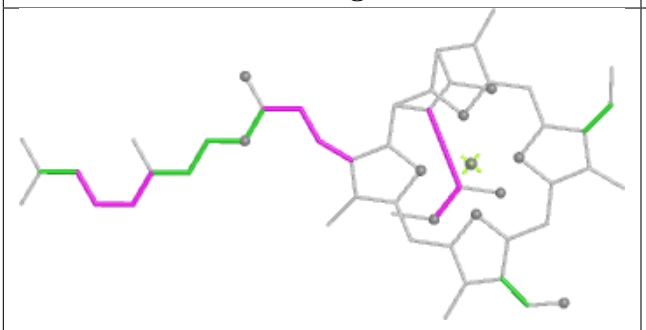


Bond angles



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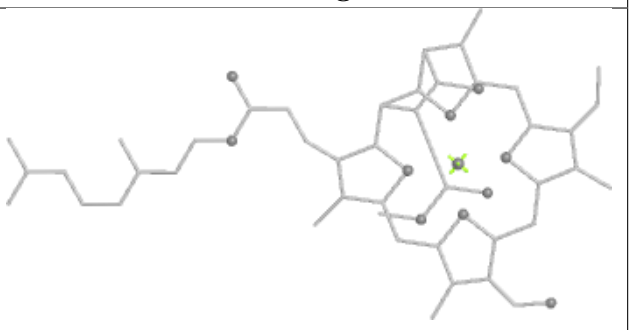
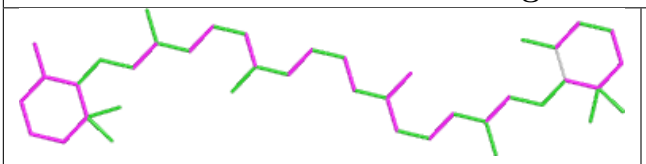


Rings

Ligand 8CT 44 402



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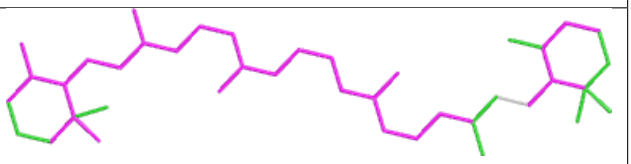
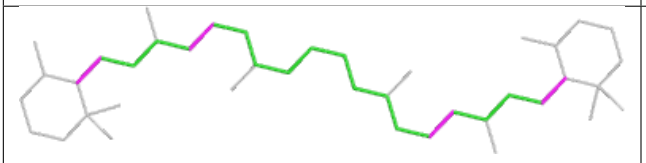


Bond angles



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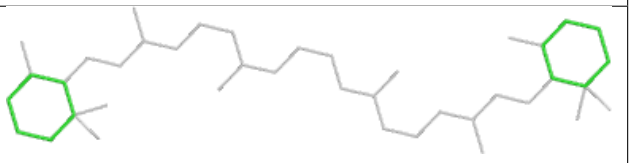
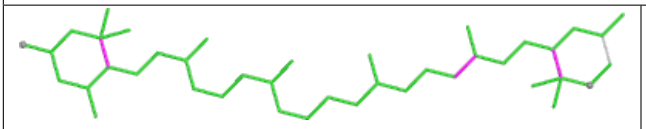


Rings

Ligand ZEX 22 520



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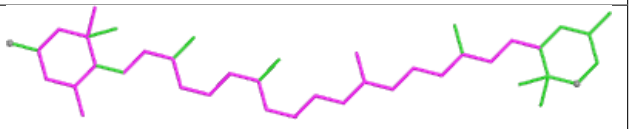
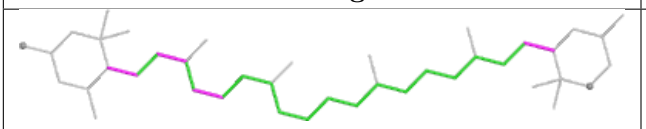


Bond angles



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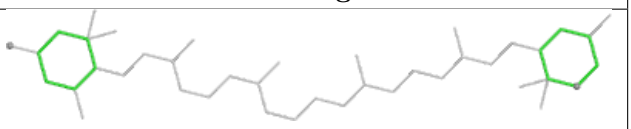

Rings

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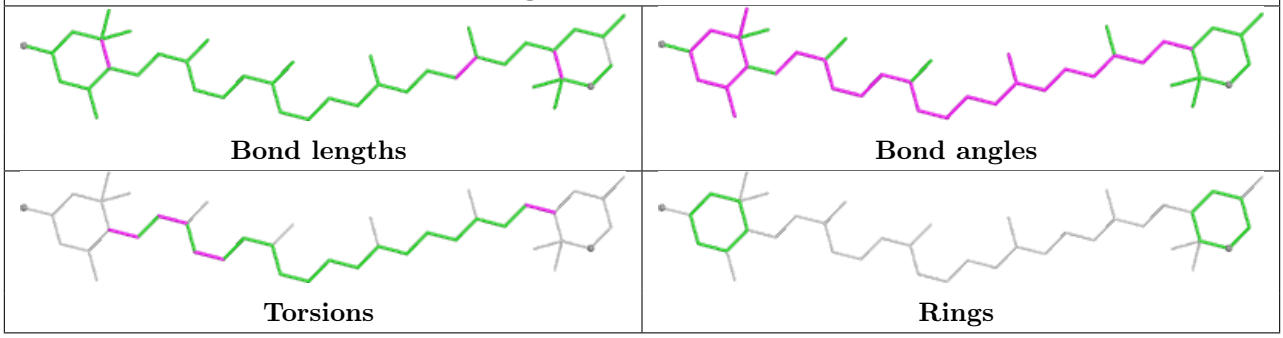

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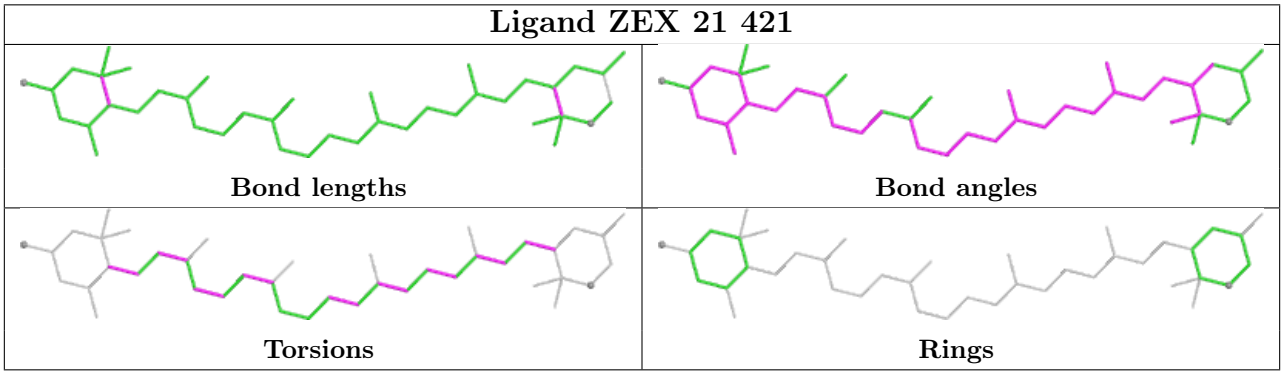
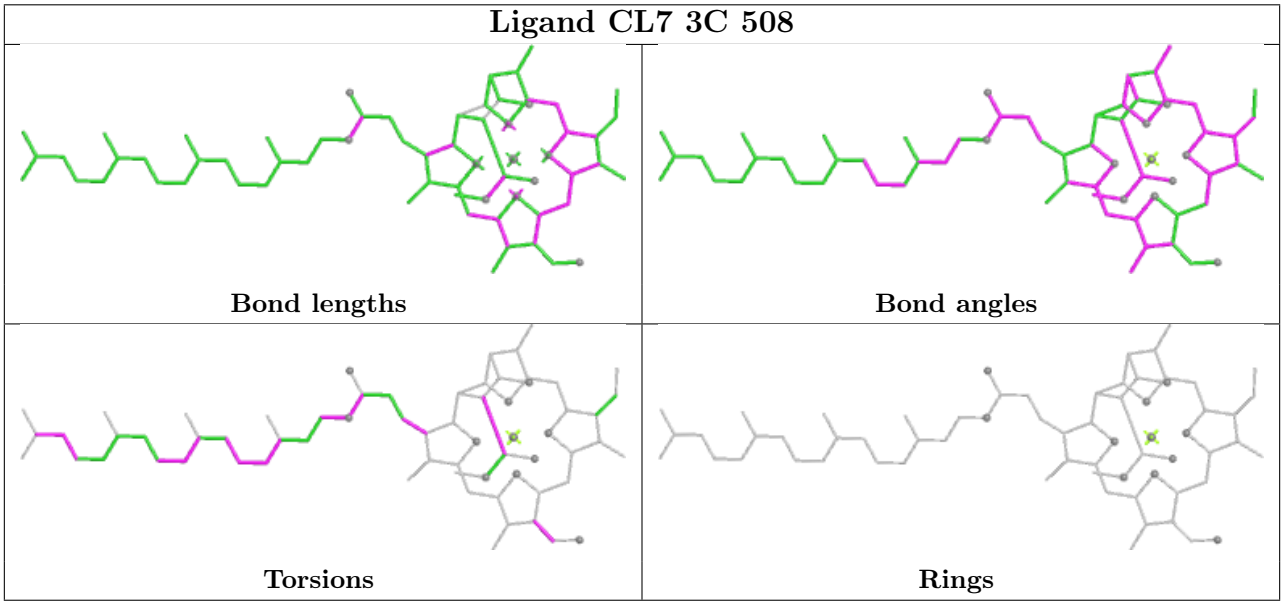


Ligand CL7 3C 508



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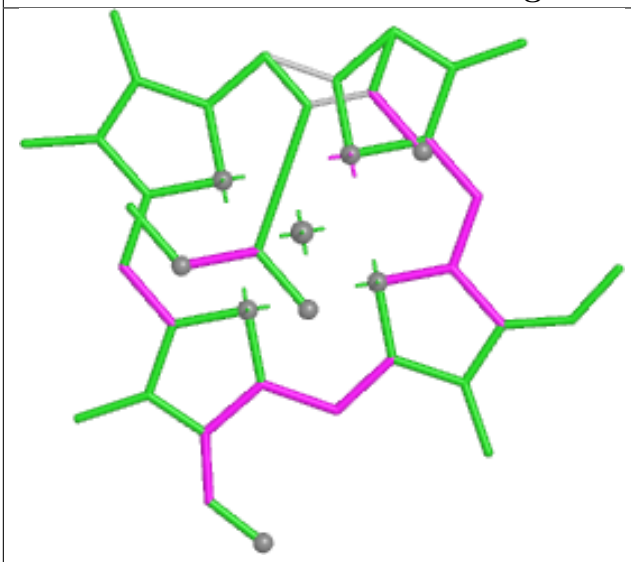

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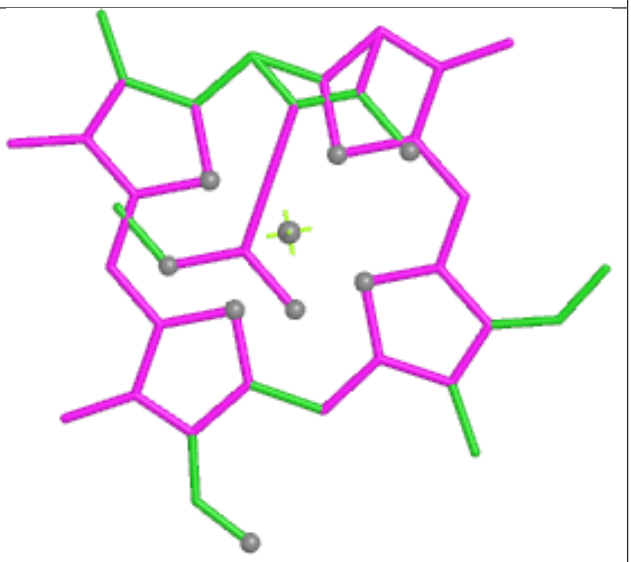
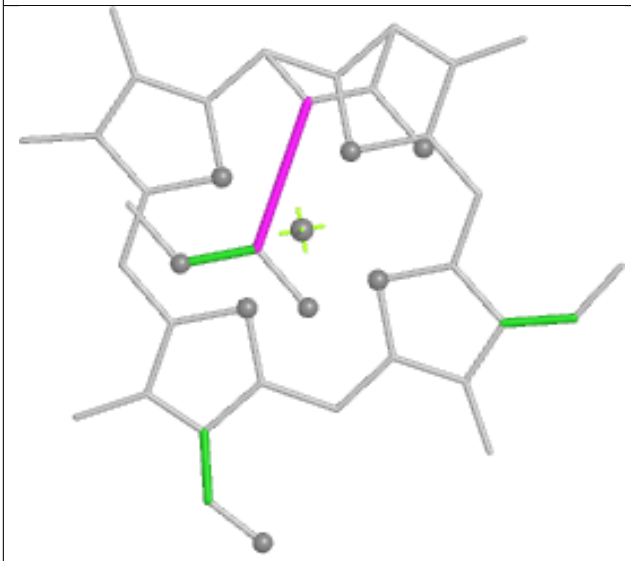
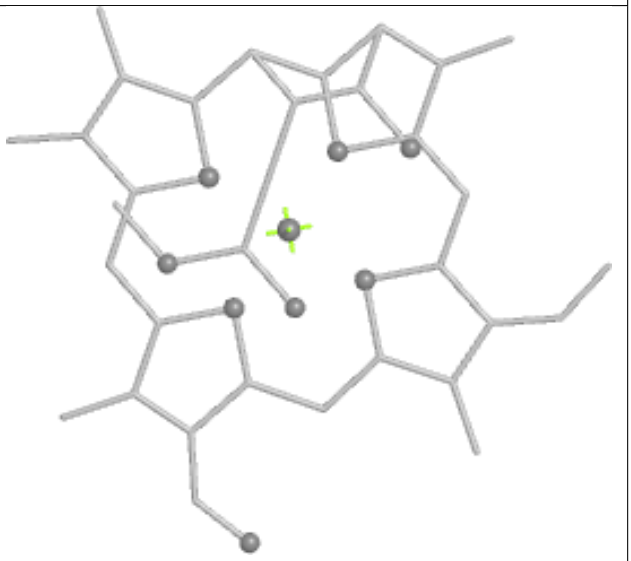


Bond angles

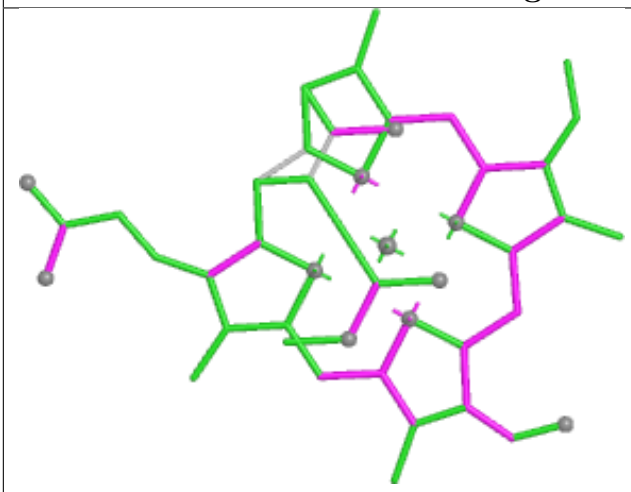


Torsions

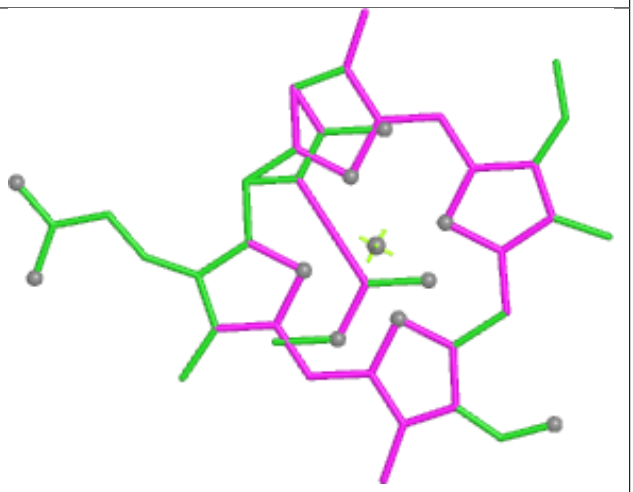


Rings

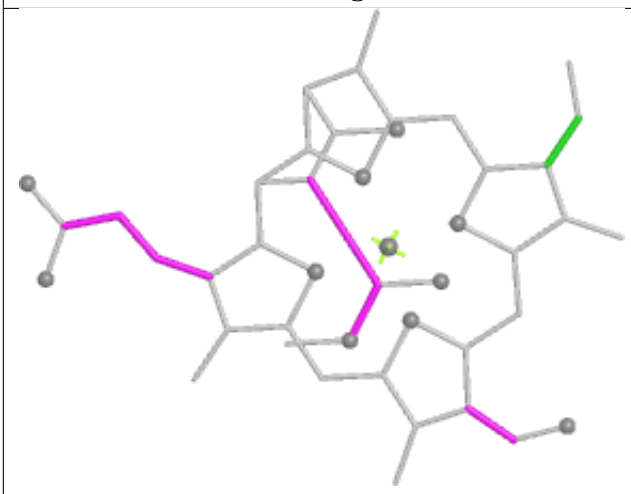
Ligand CL7 31 405



Bond lengths



Bond angles

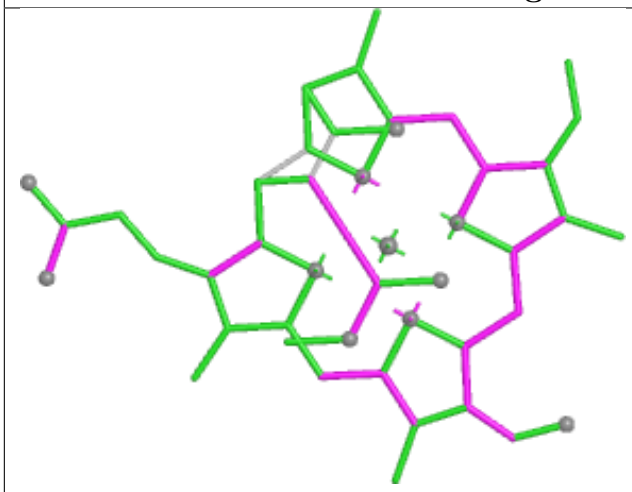


Torsions



Rings

Ligand CL7 44 408



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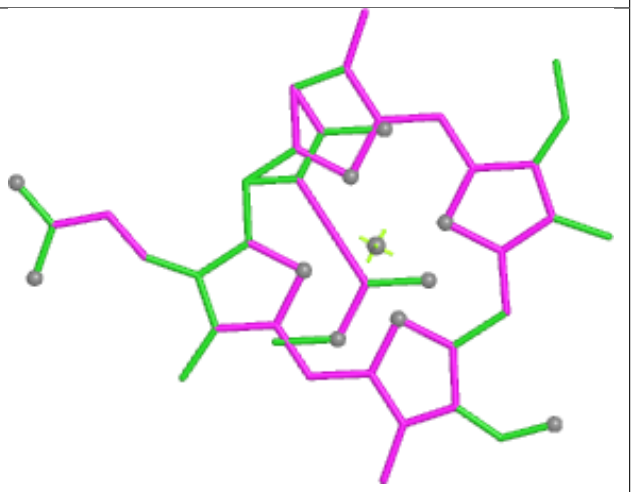

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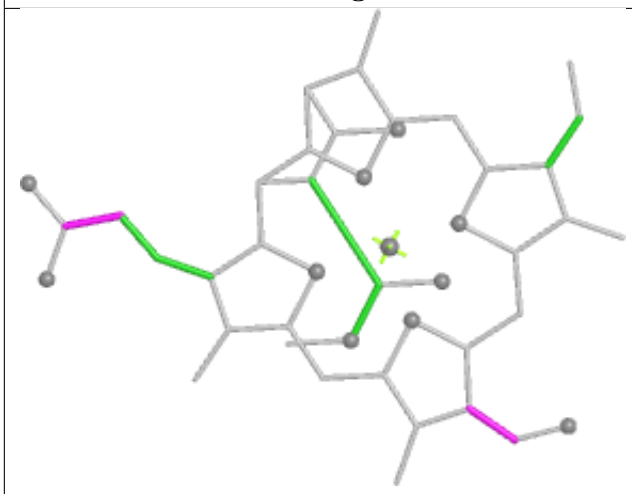
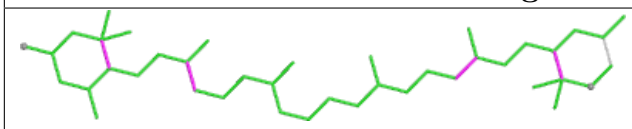


Torsions



Rings

Ligand ZEX 23 423



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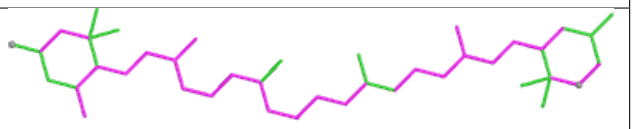
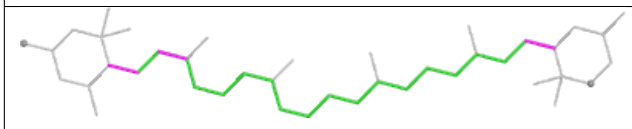


Bond angles



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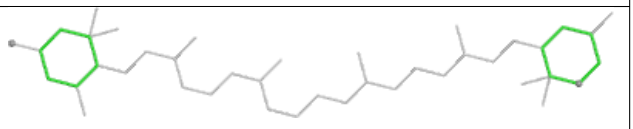
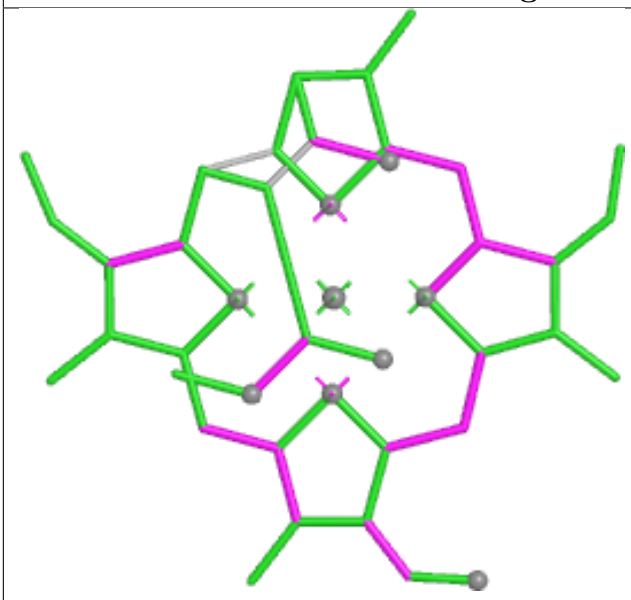


Rings

Ligand CL7 2C 511



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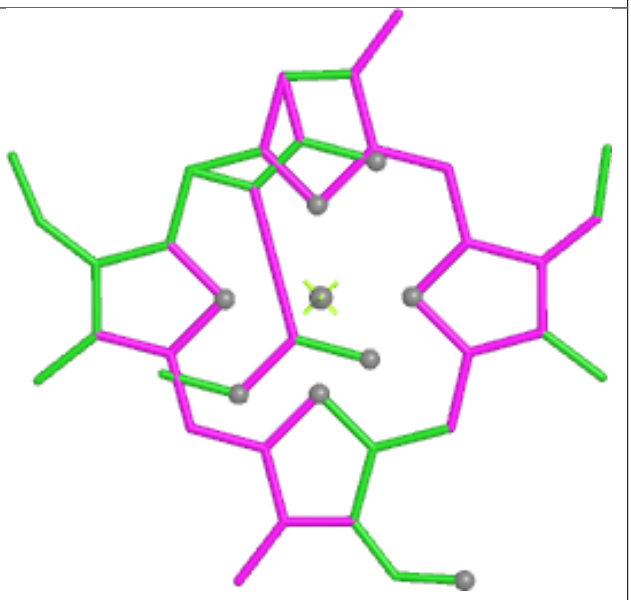
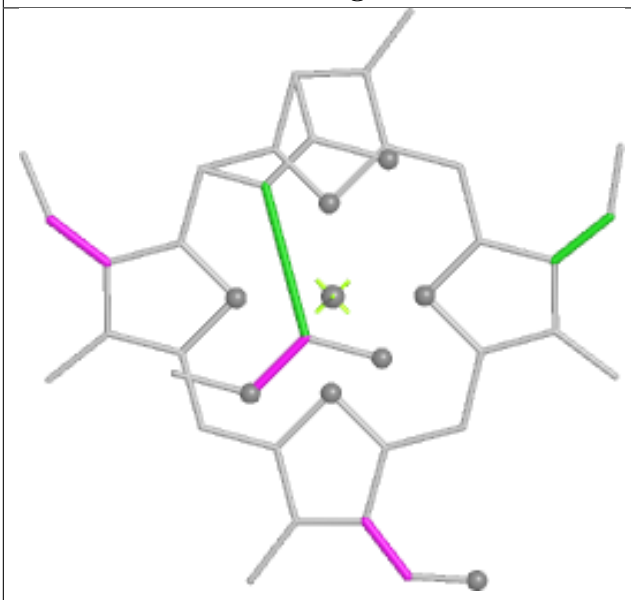


Bond angles



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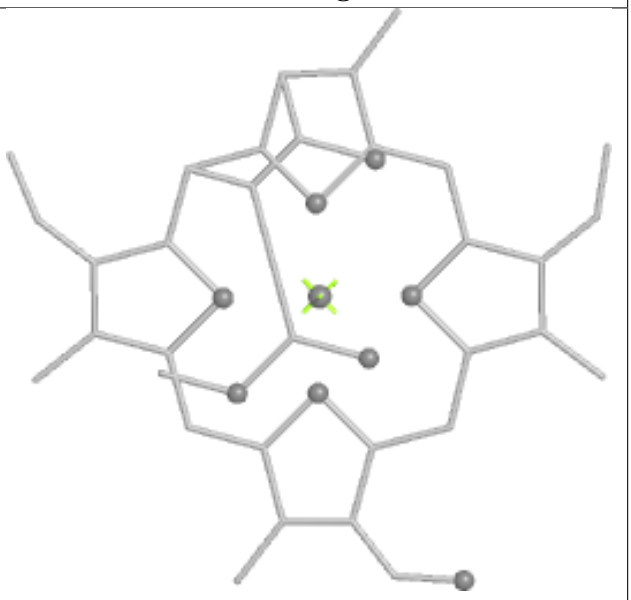
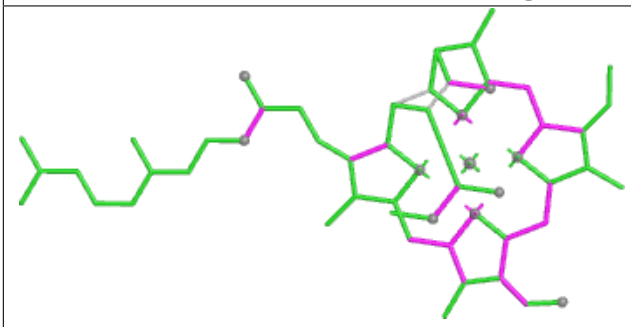


Rings

Ligand CL7 2C 504



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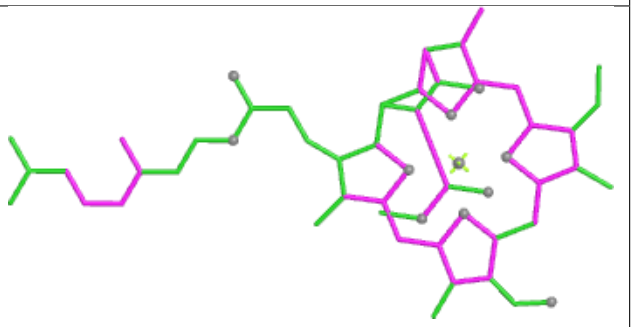
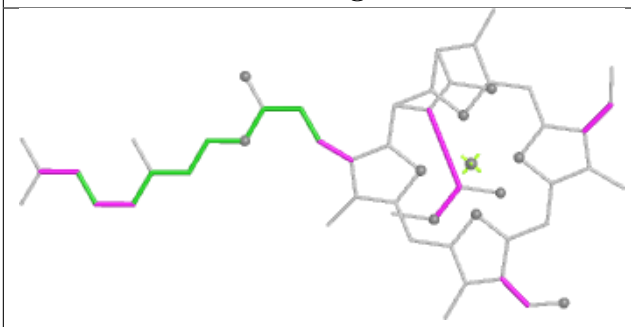


Bond angles



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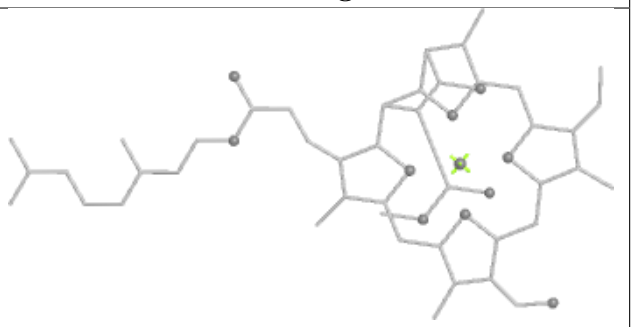
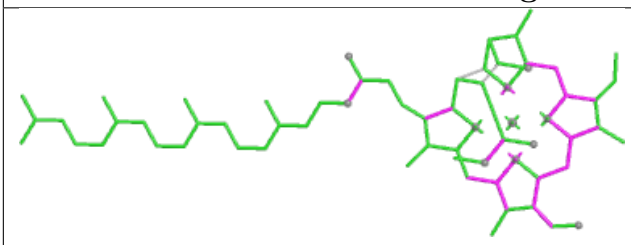


Rings

Ligand CL7 3B 604



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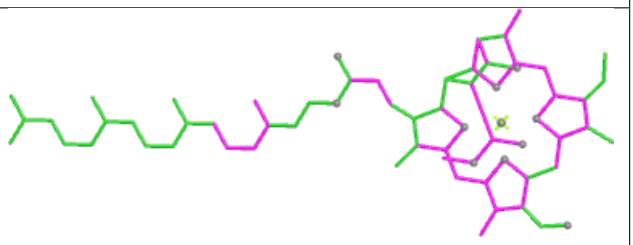
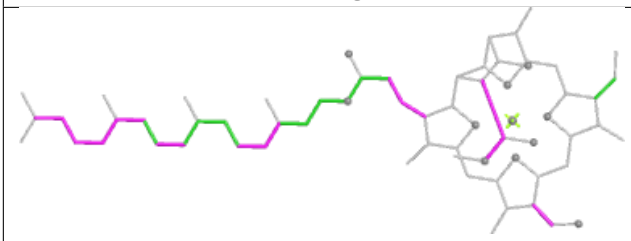


Bond angles



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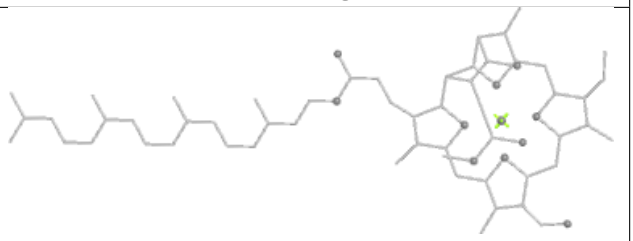
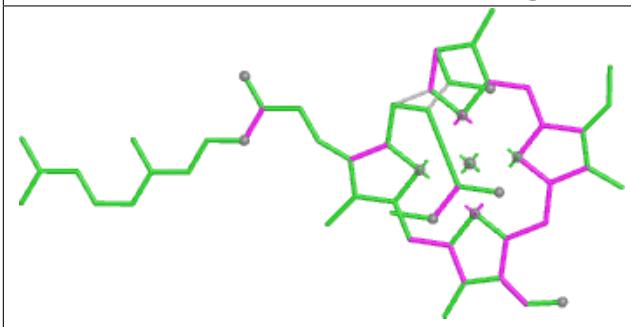


Rings

Ligand CL7 43 417



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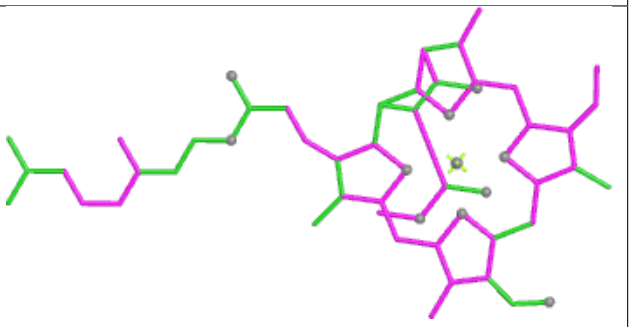
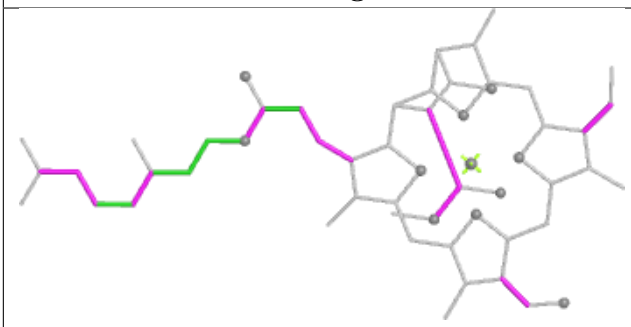


Bond angles



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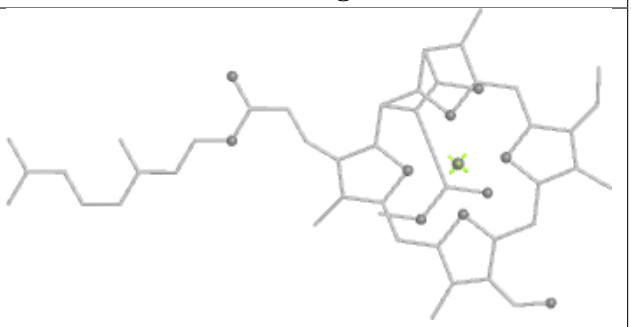
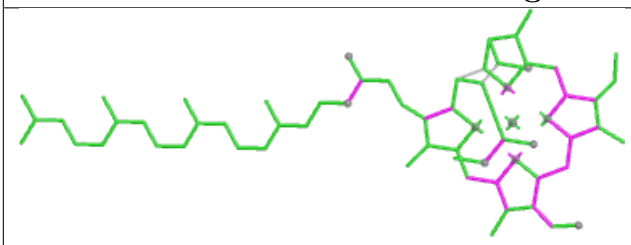


Rings

Ligand CL7 32 516



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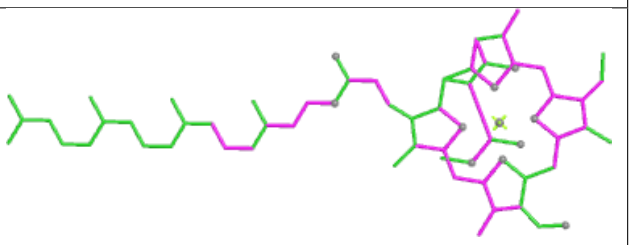
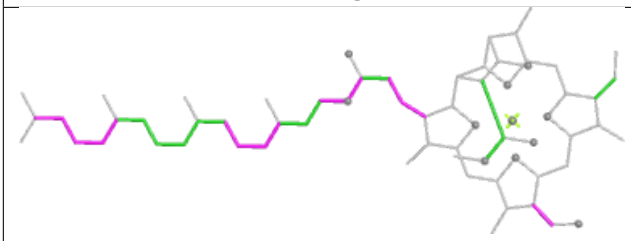


Bond angles



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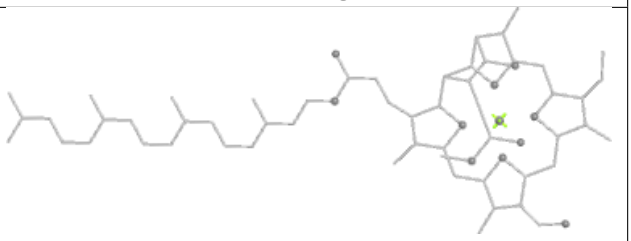
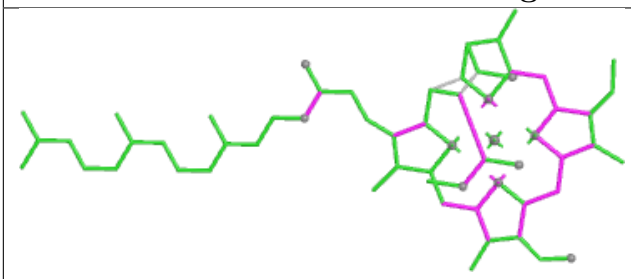


Rings

Ligand CL7 2B 615



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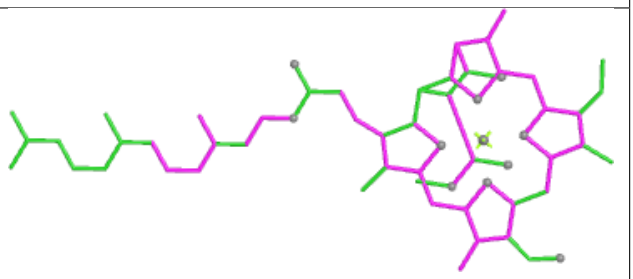
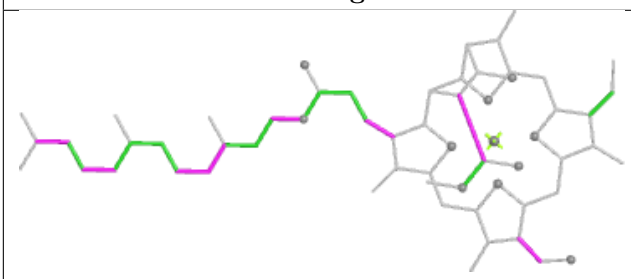


Bond angles



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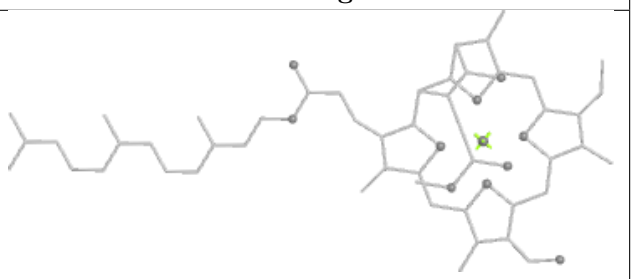
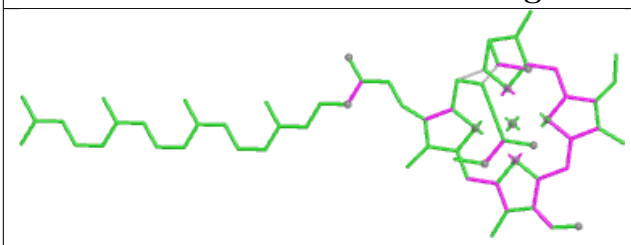


Rings

Ligand CL7 13 501



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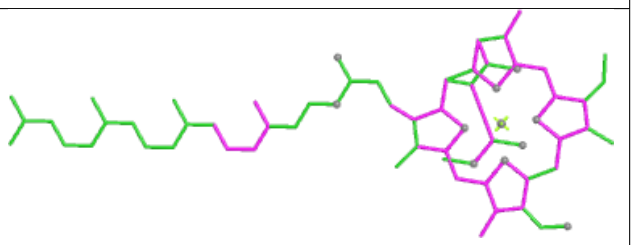
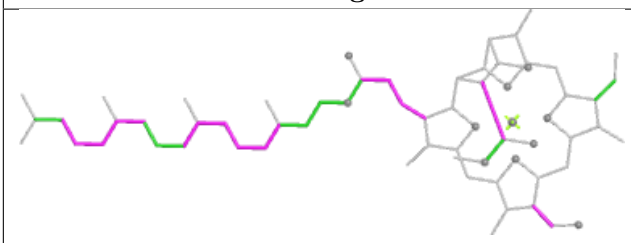


Bond angles



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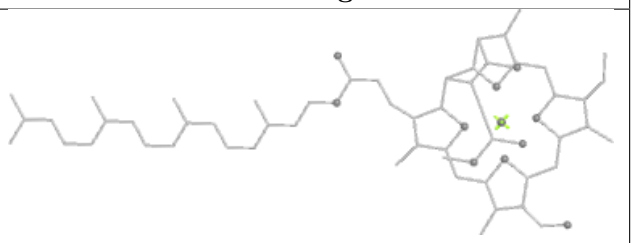
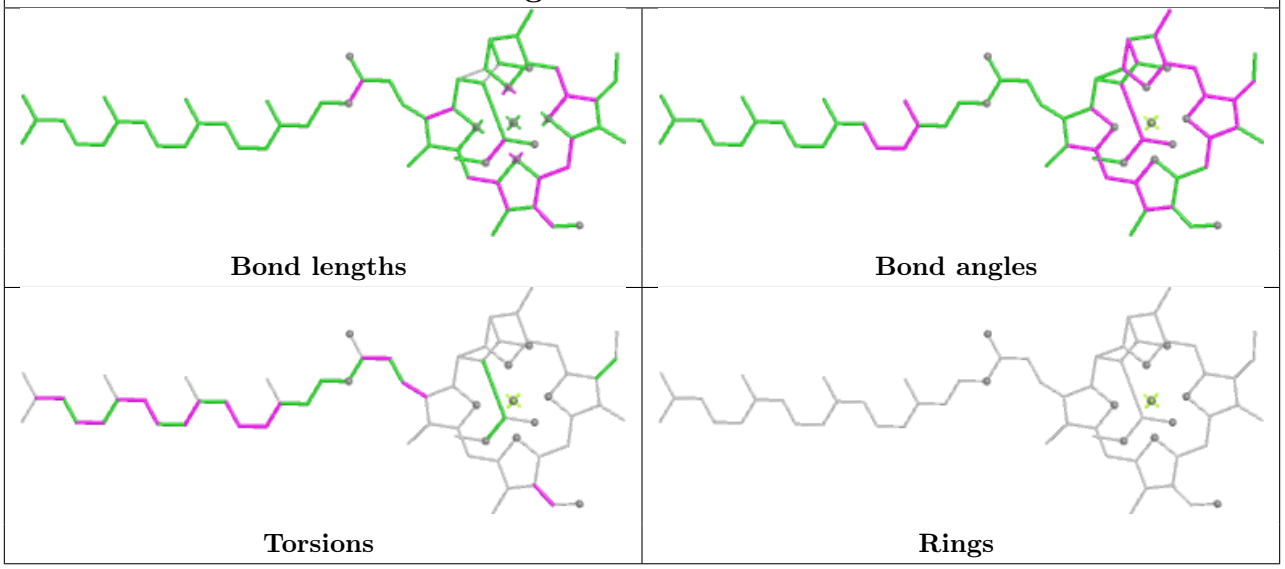
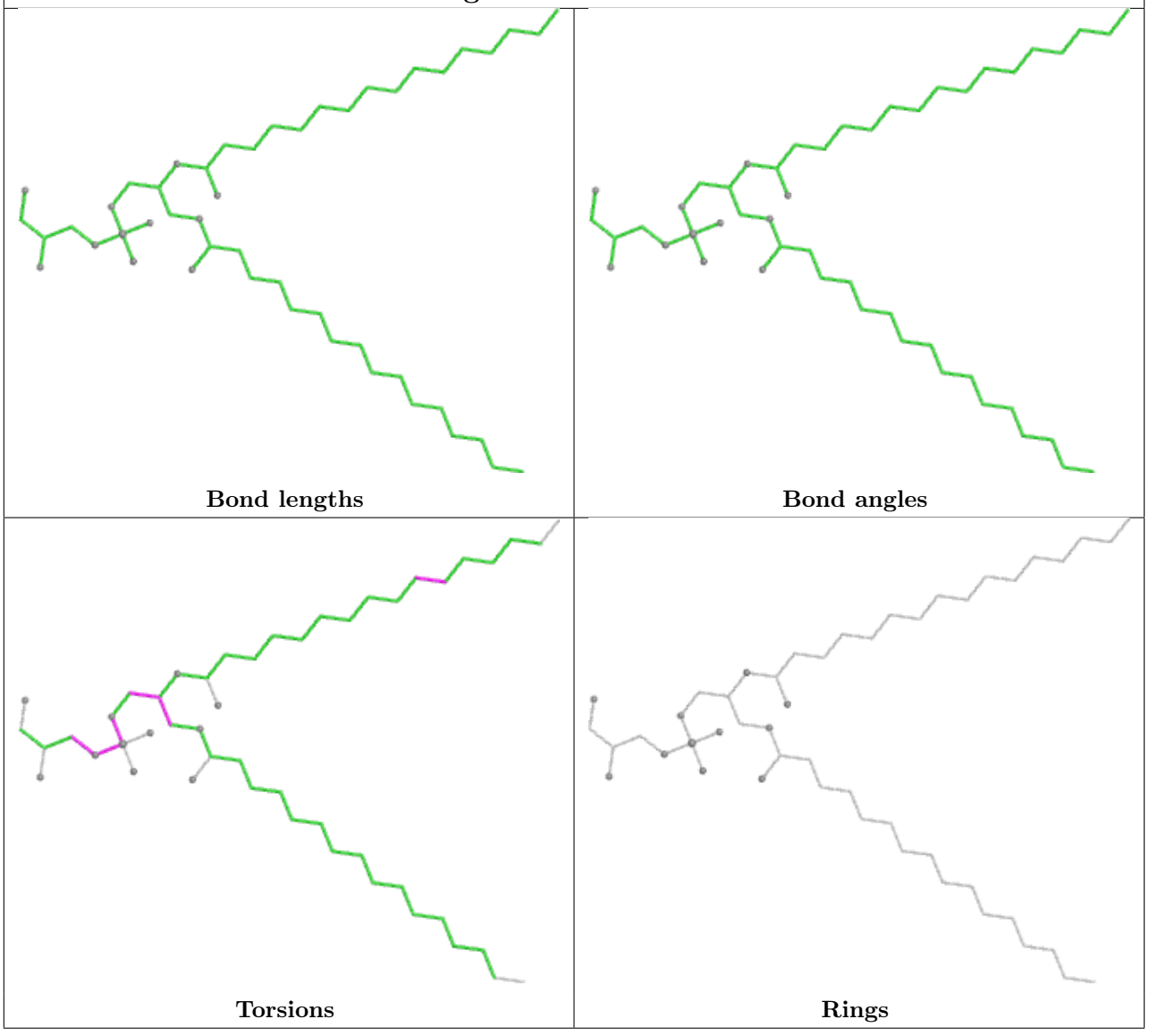


Rings

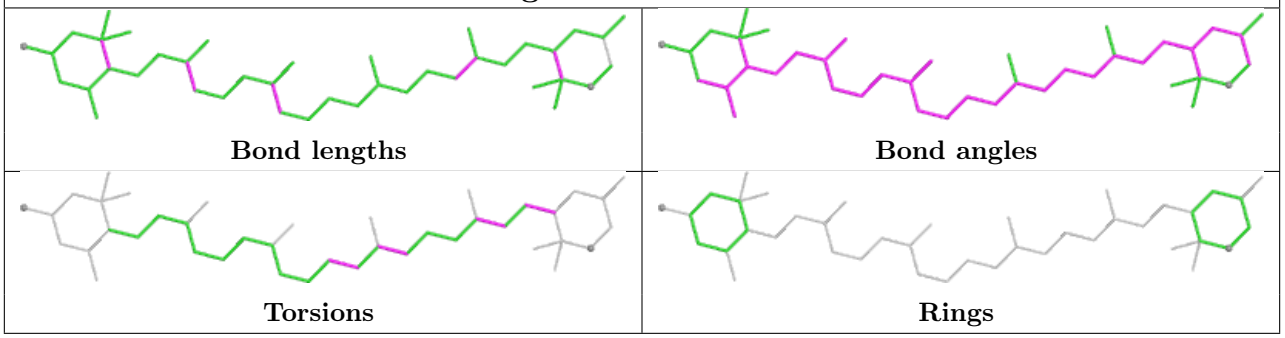
Ligand CL7 32 512



Ligand LHG 44 401



Ligand ZEX 43 401



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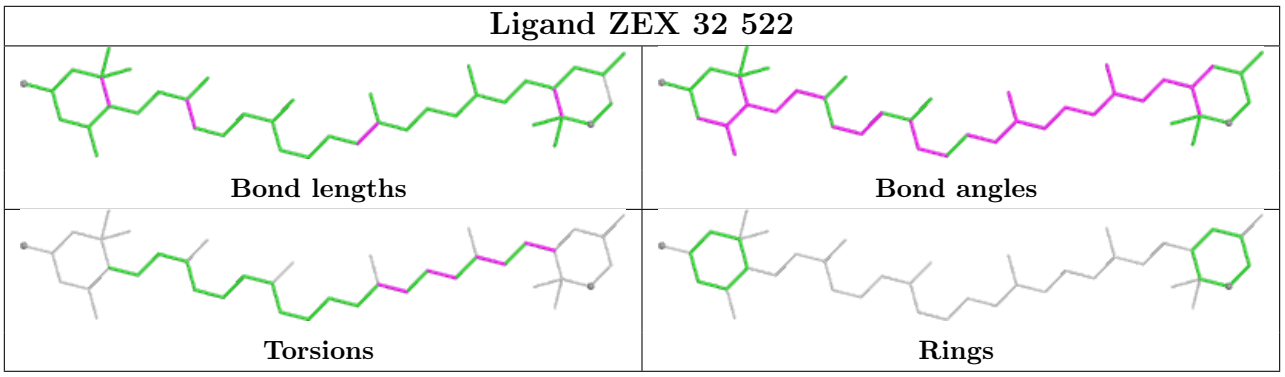

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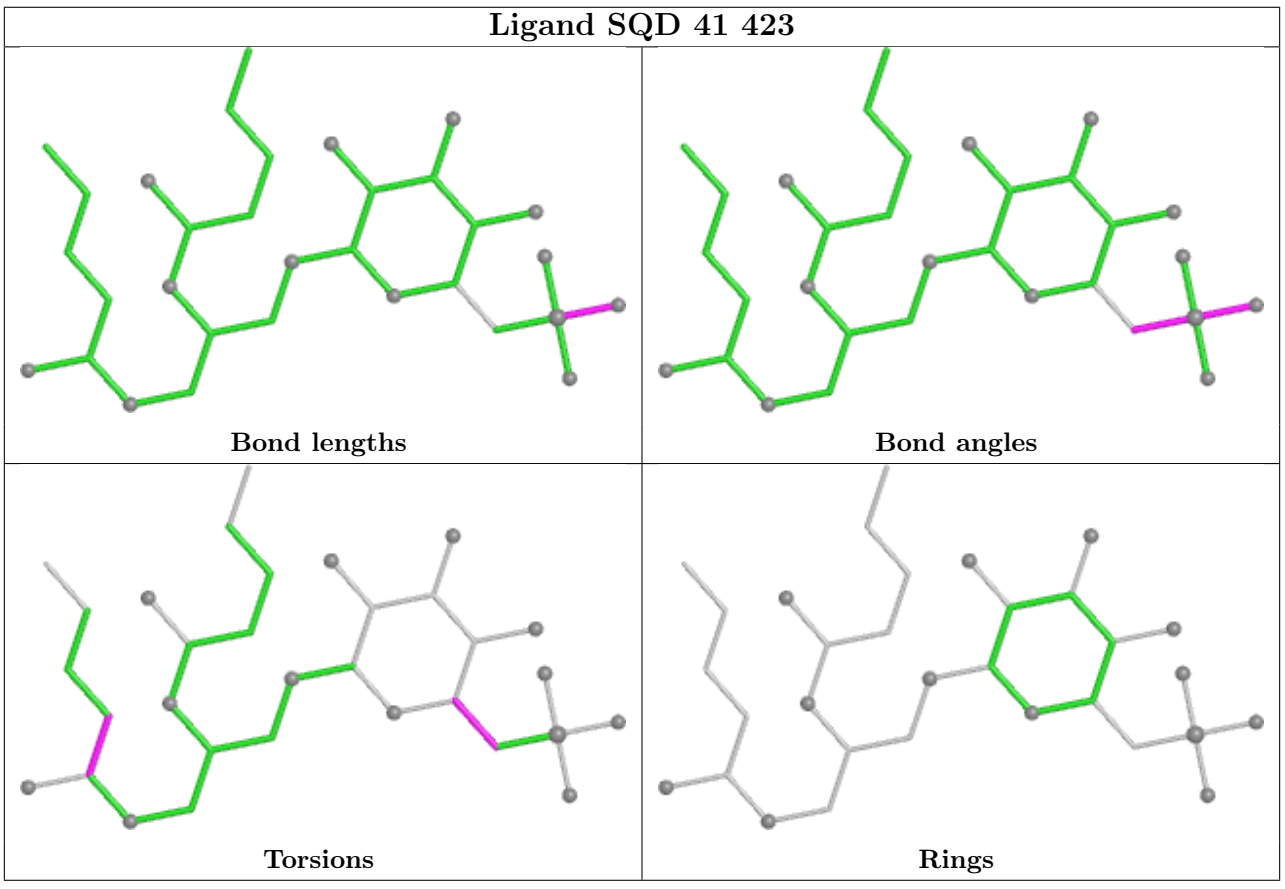

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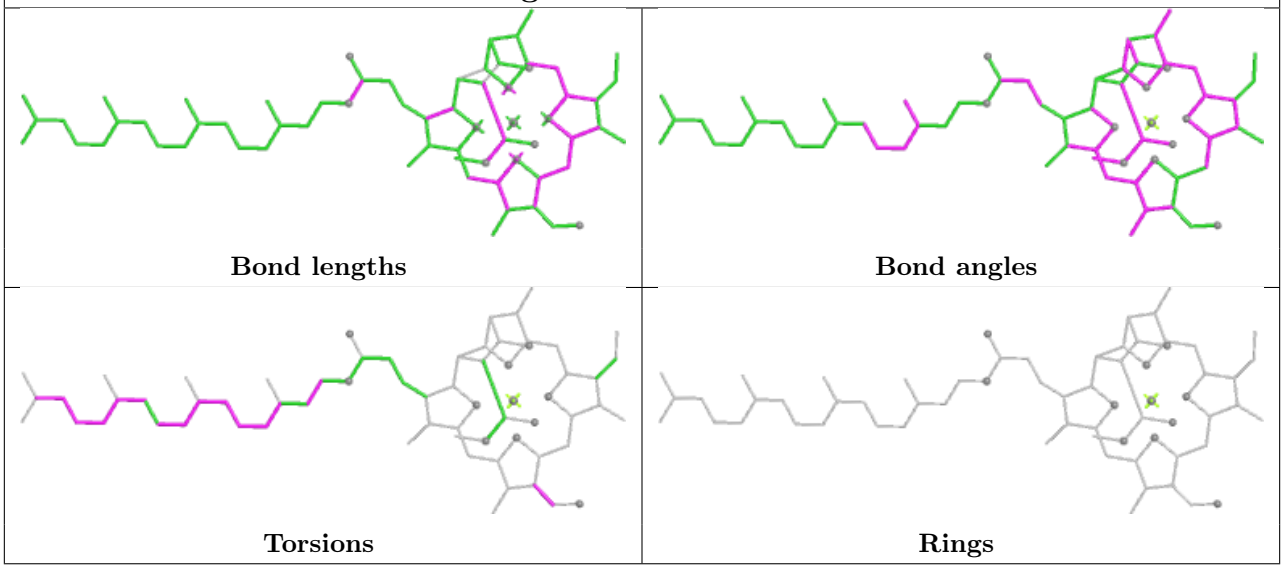
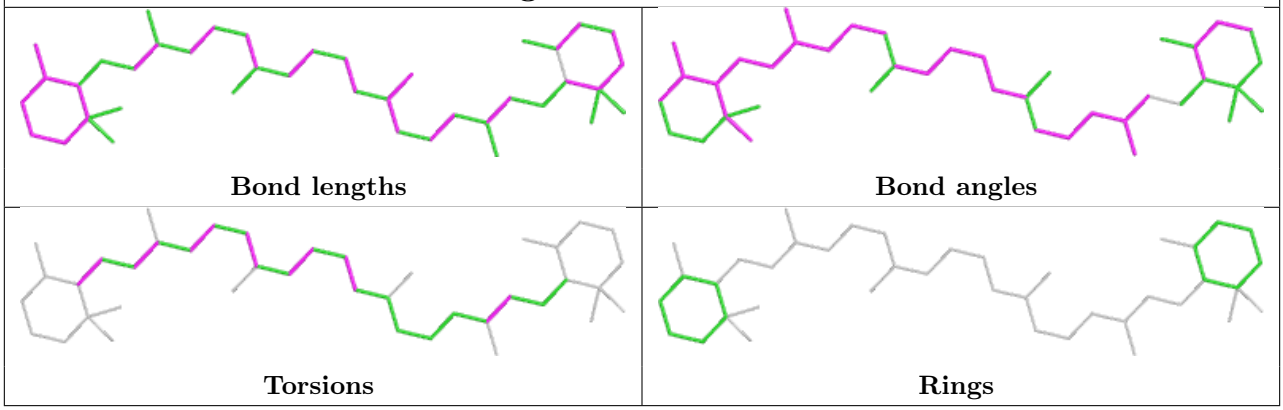
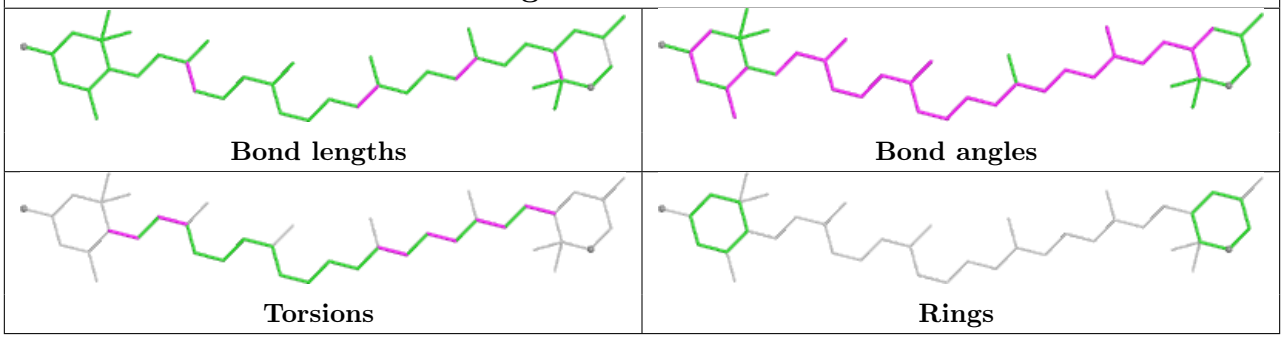


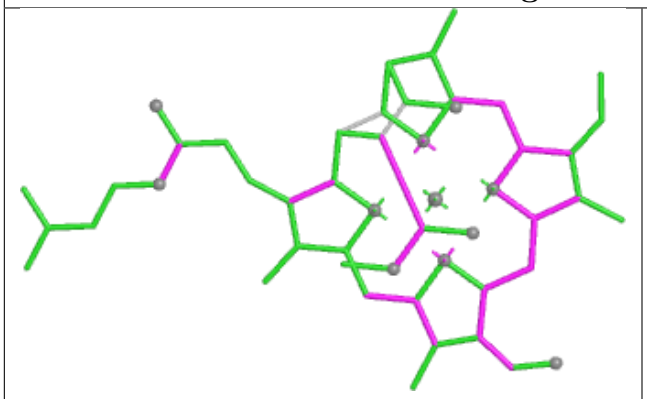
Ligand 8CT 2B 619



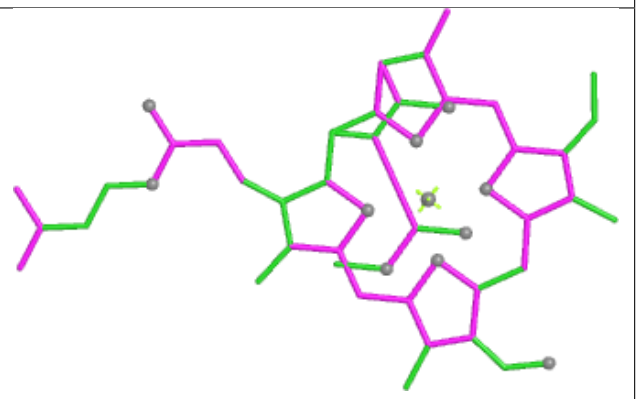
Ligand ZEX 23 420



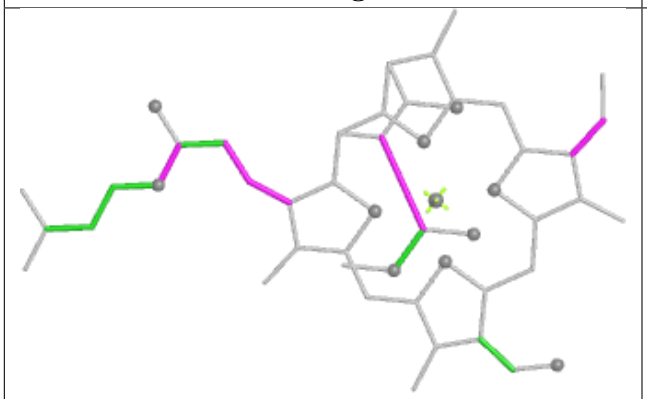
Ligand CL7 2B 616



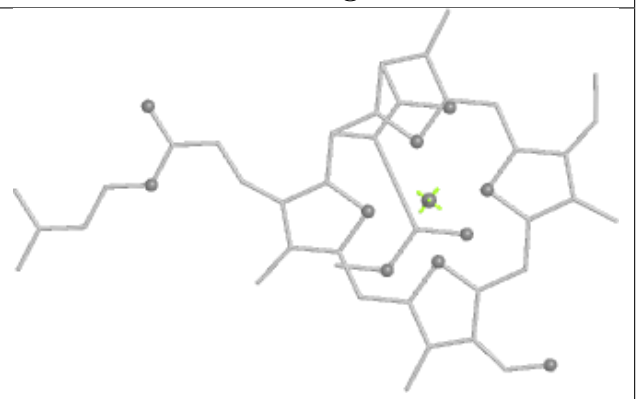
Bond lengths



Bond angles

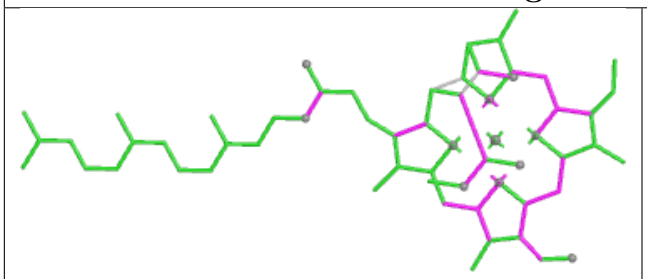


Torsions



Rings

Ligand CL7 42 511



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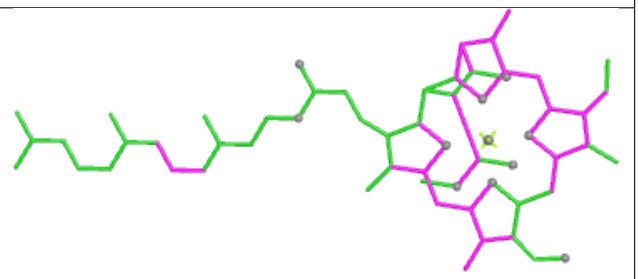
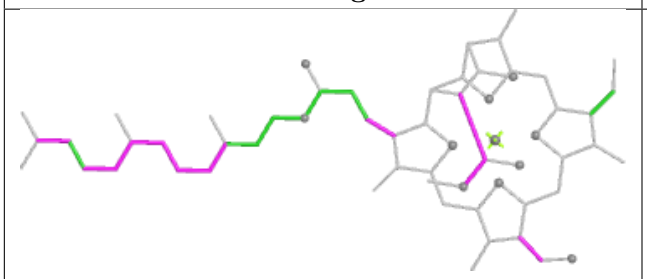


Bond angles



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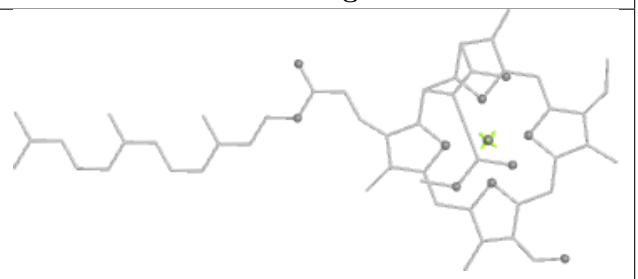
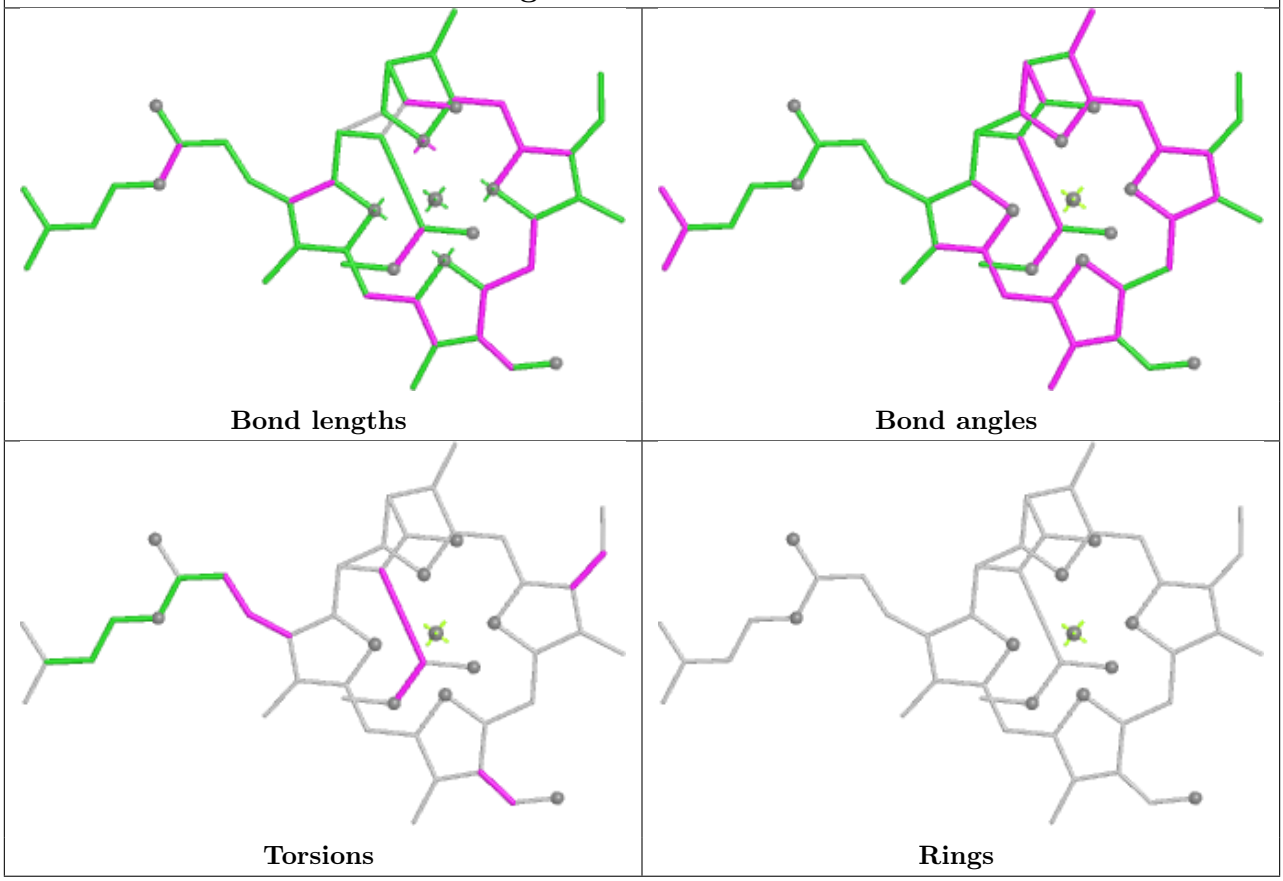


Rings

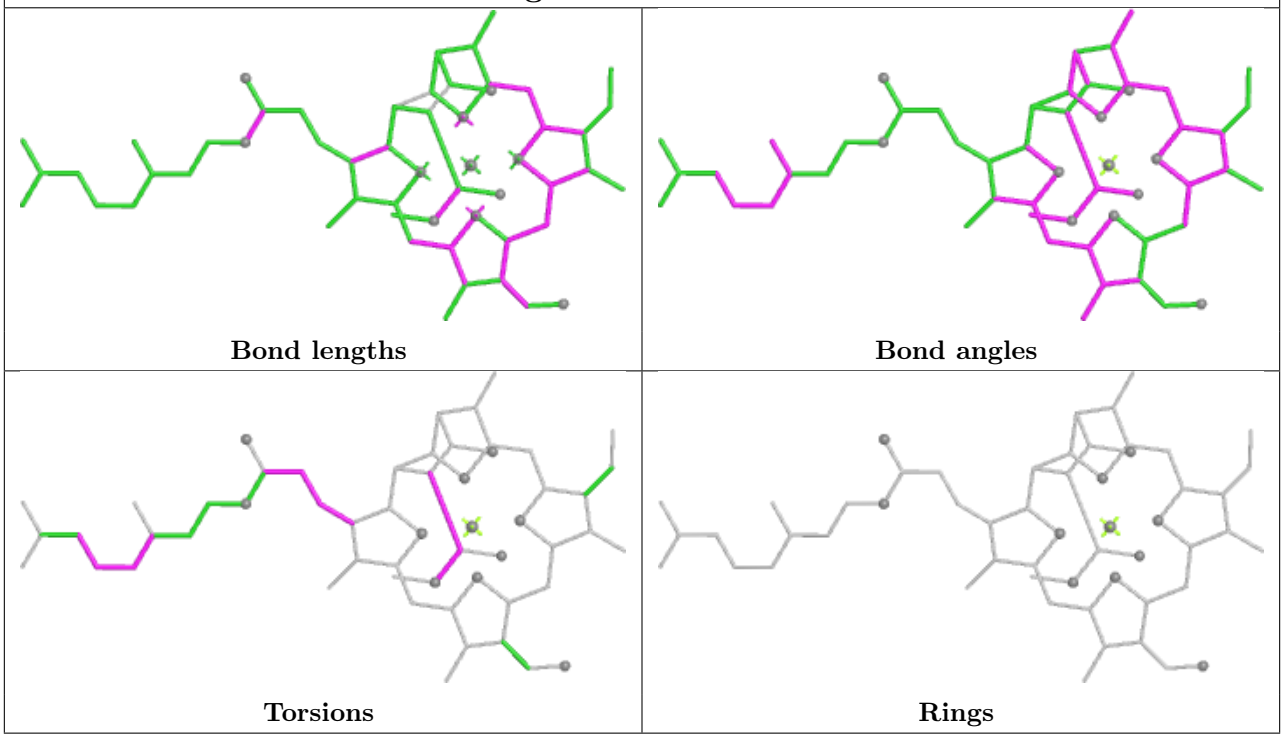
Ligand CL7 2D 402



Bond lengths | Bond angles

Torsions | Rings

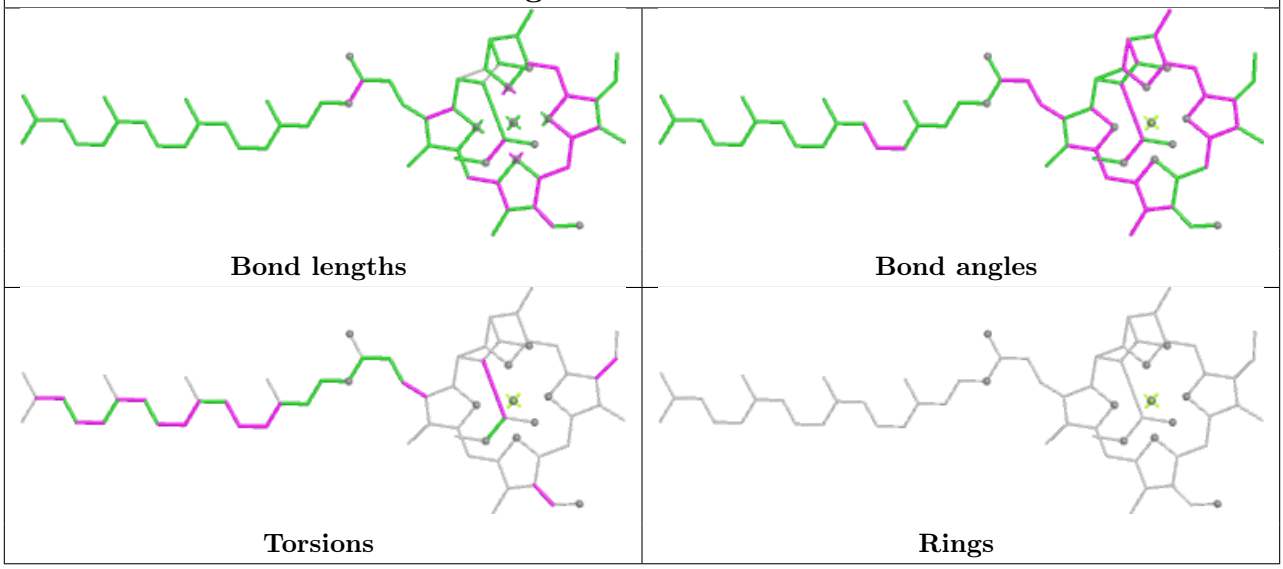
Ligand CL7 23 413



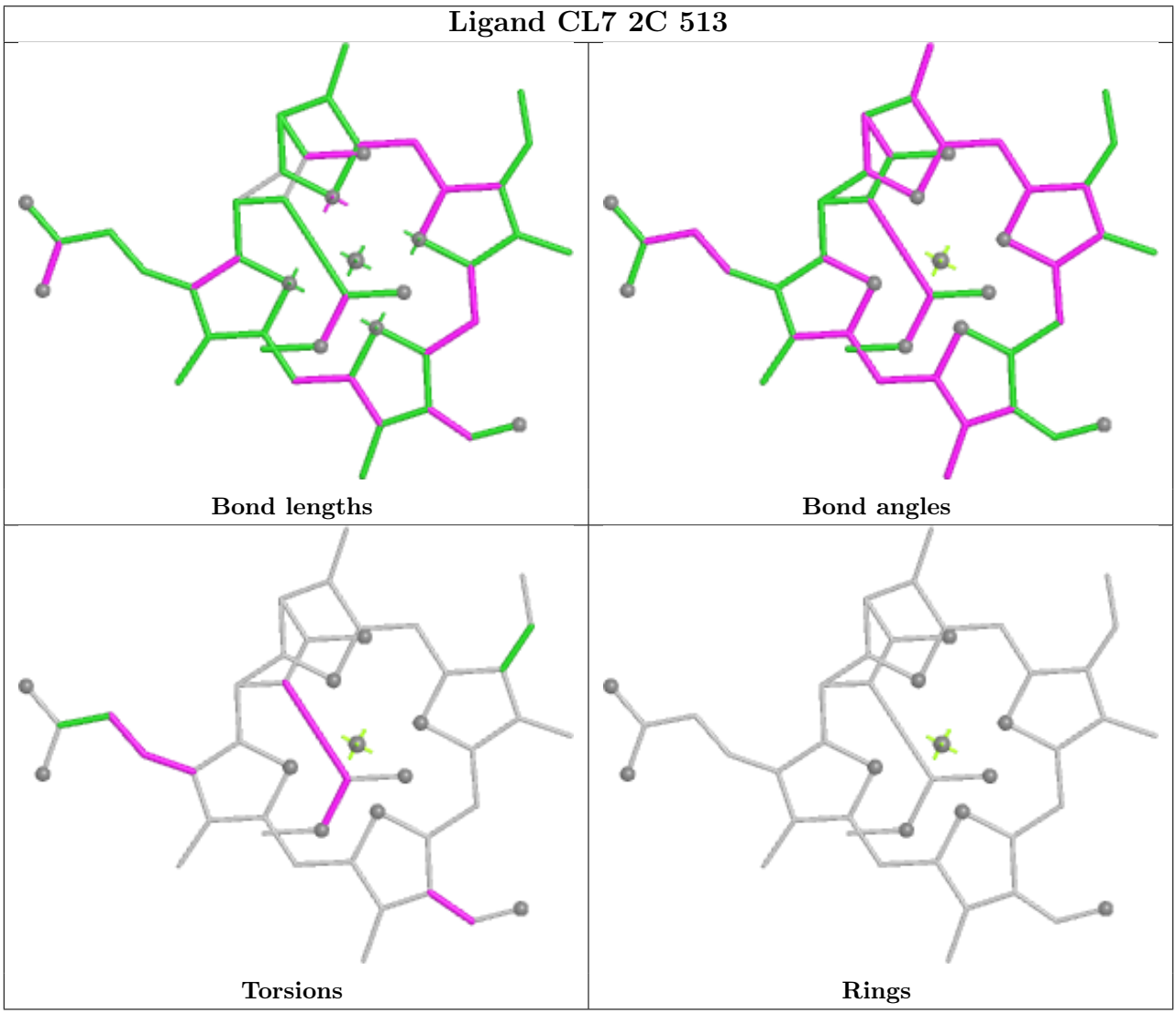
Bond lengths | Bond angles

Torsions | Rings

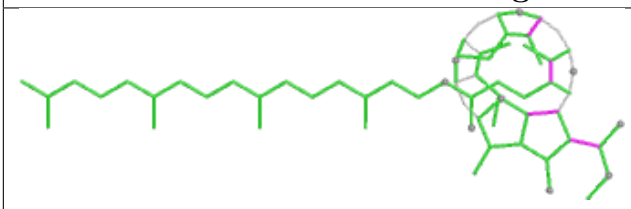
Ligand CL7 33 504



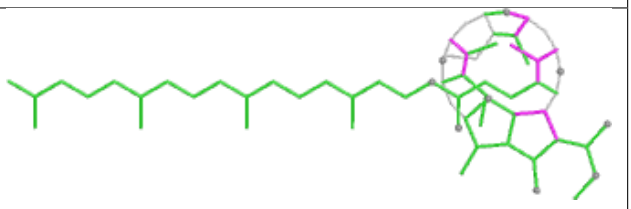
Ligand CL7 2C 513



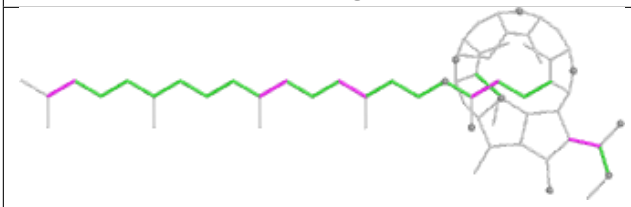
Ligand PHO 3D 408



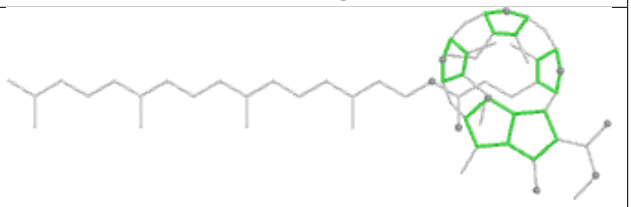
Bond lengths



Bond angles

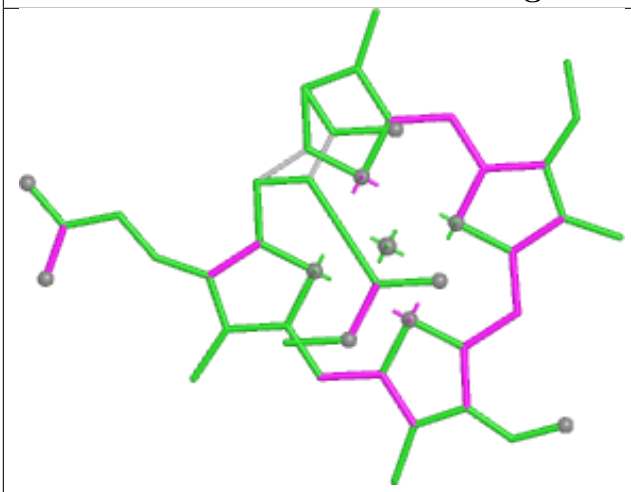


Torsions



Rings

Ligand CL7 32 513



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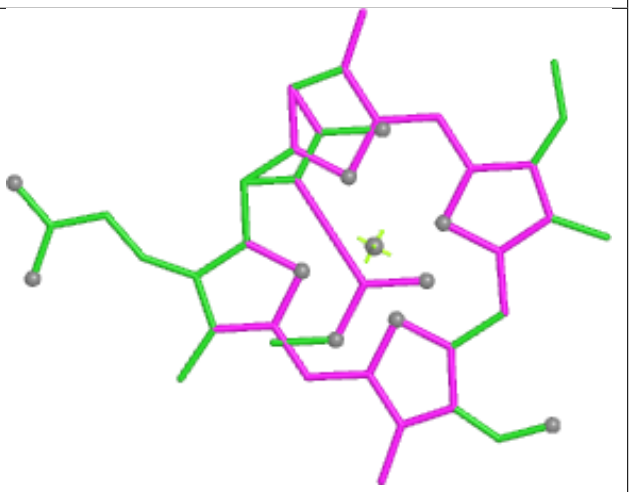
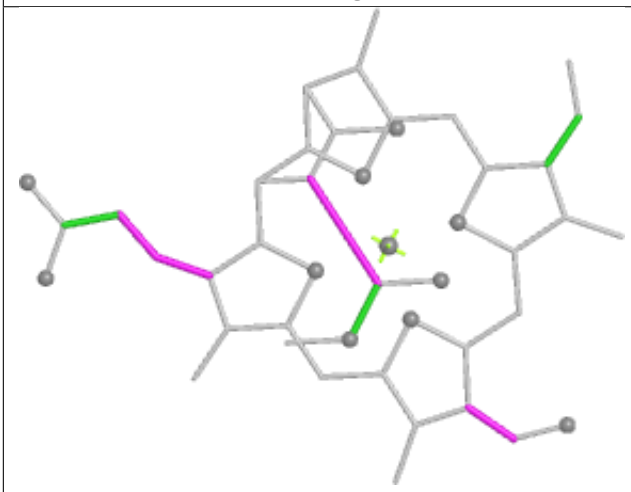


Bond angles



Torsions

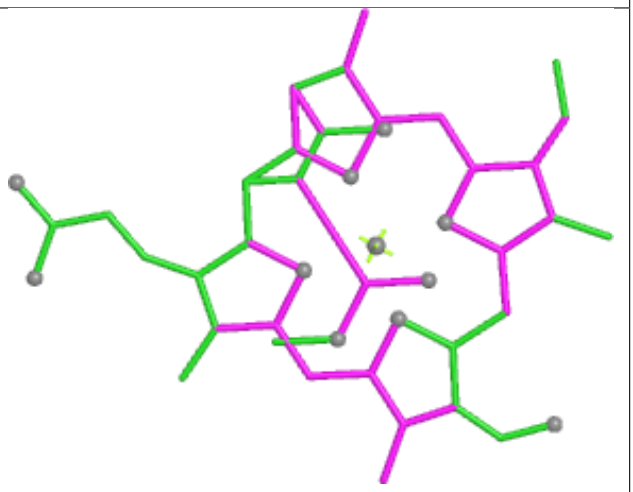


Rings

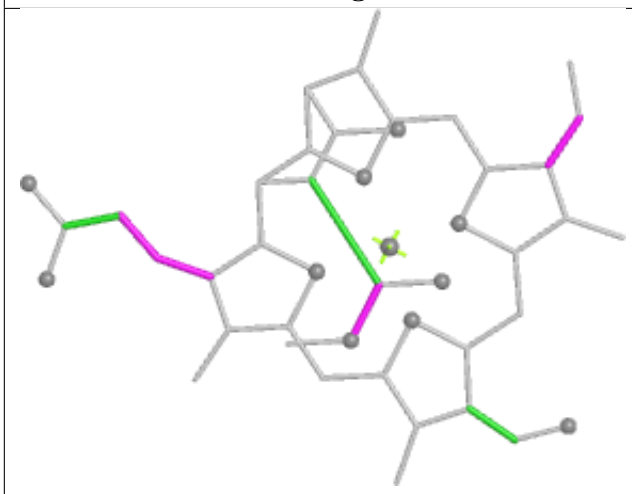
Ligand CL7 43 415



Bond lengths



Bond angles

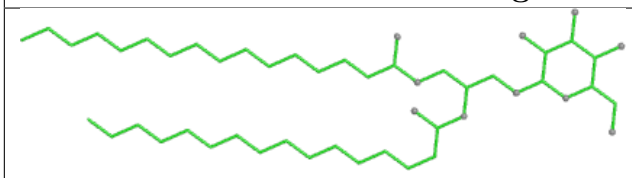


Torsions



Rings

Ligand LMG 3B 621



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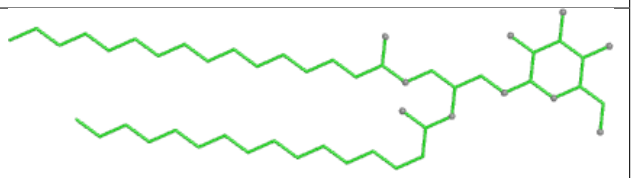
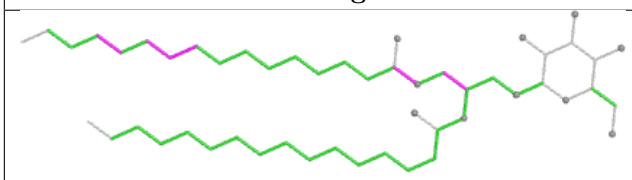


Bond angles



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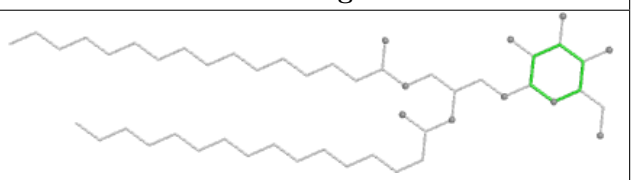
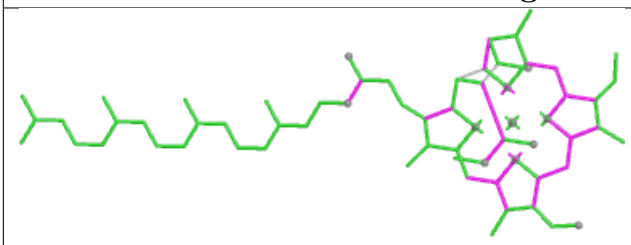
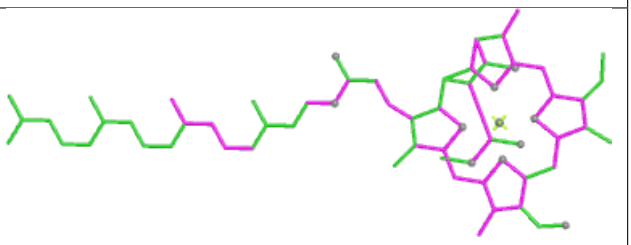


Rings

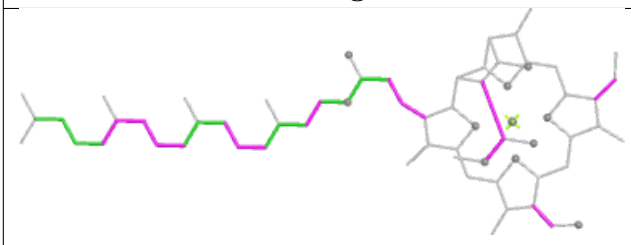
Ligand CL7 1C 505



Bond lengths



Bond angles



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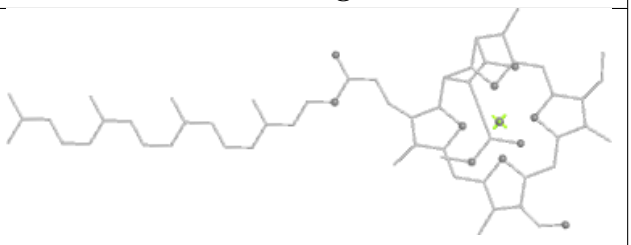
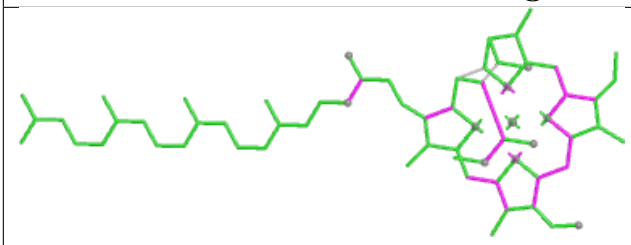


Rings

Ligand CL7 33 503



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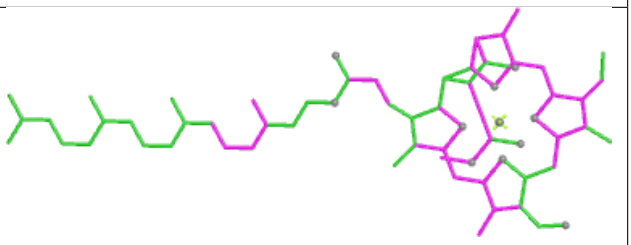

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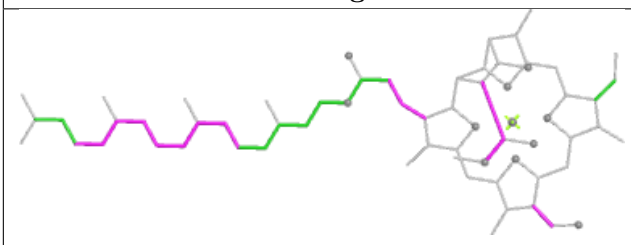

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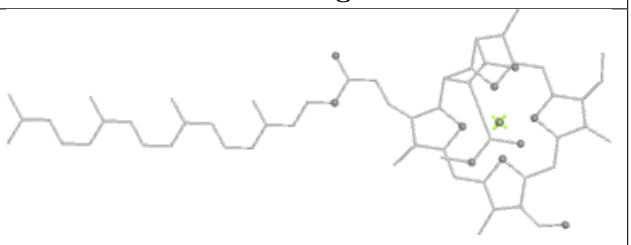
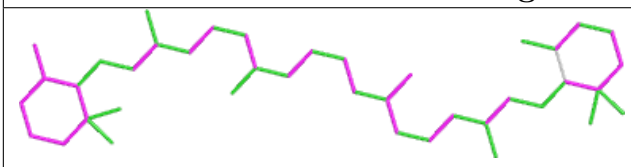


Rings

Ligand 8CT 1C 515



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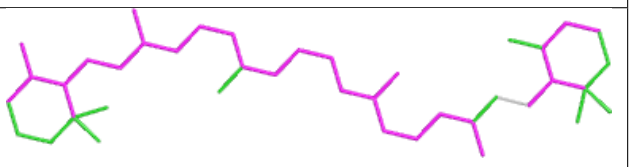
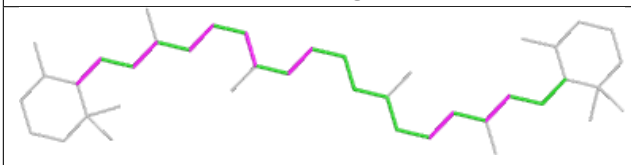


Bond angles



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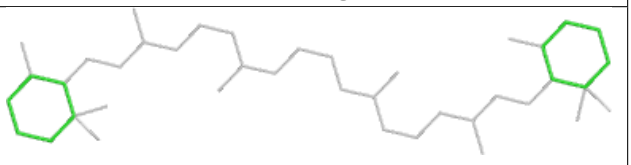
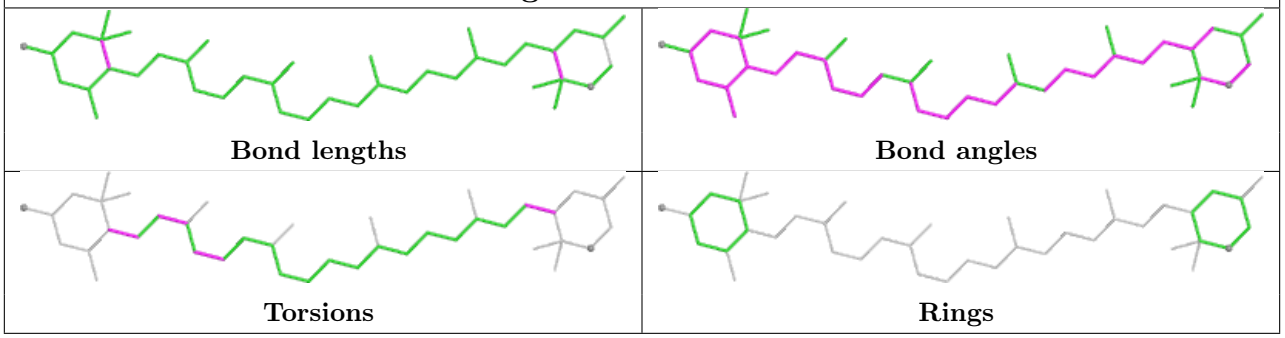
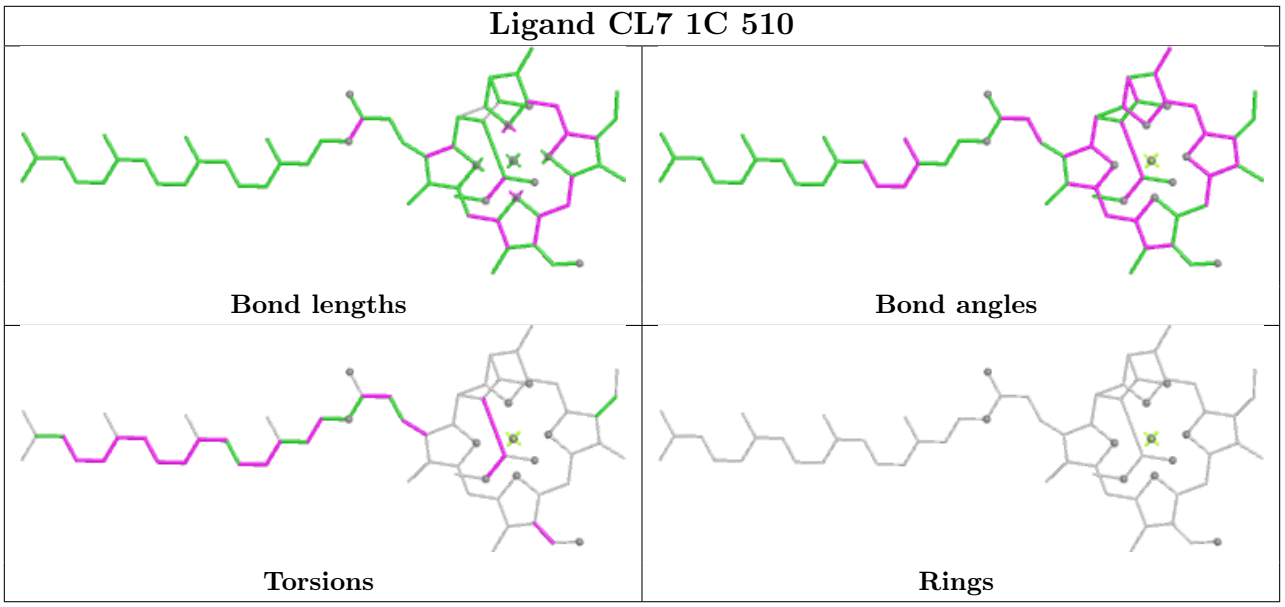


Rings

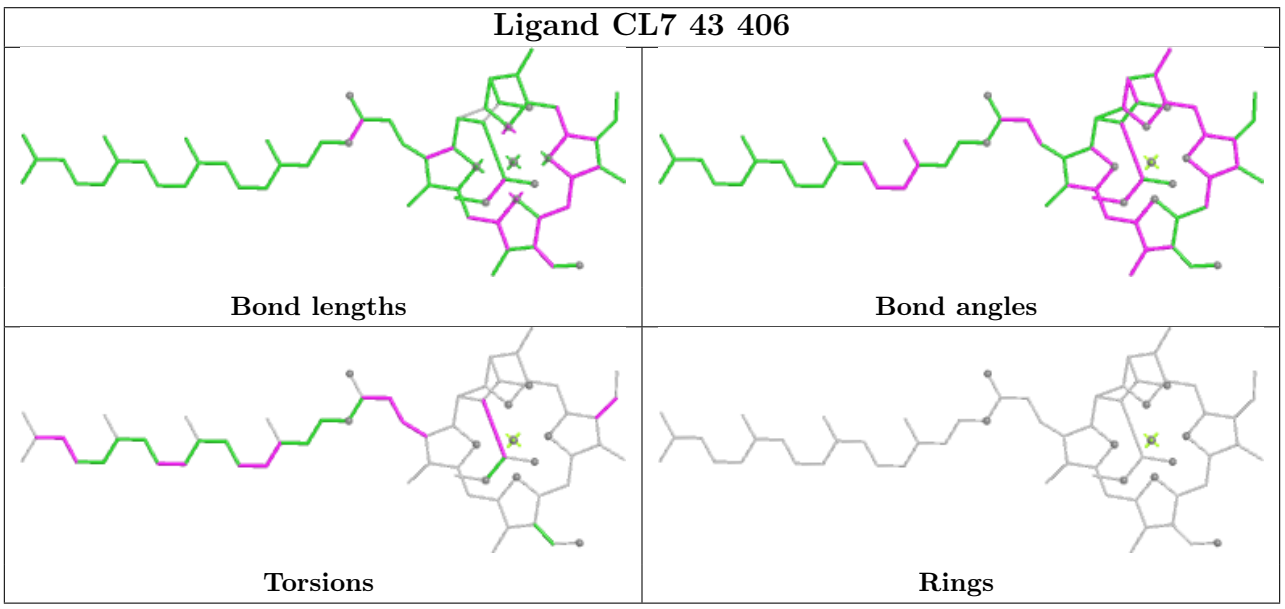
Ligand ZEX 41 422



Ligand CL7 1C 510



Ligand CL7 43 406



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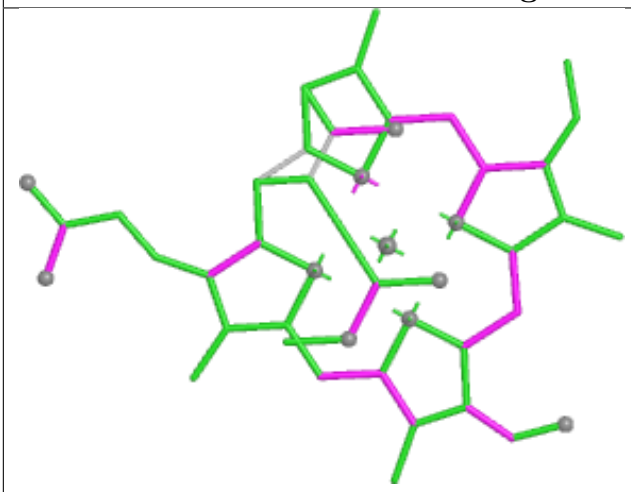

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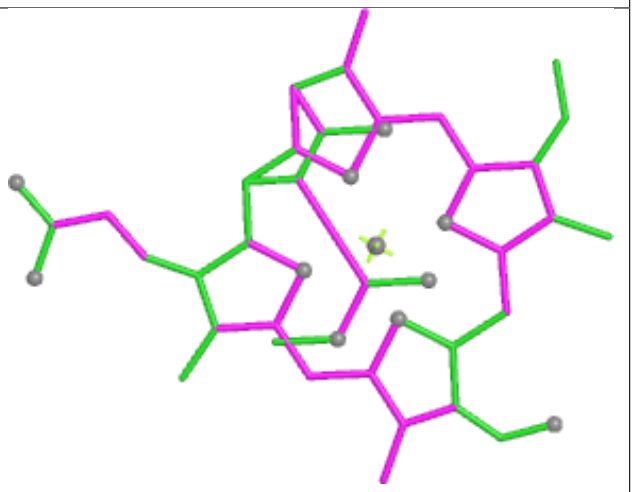
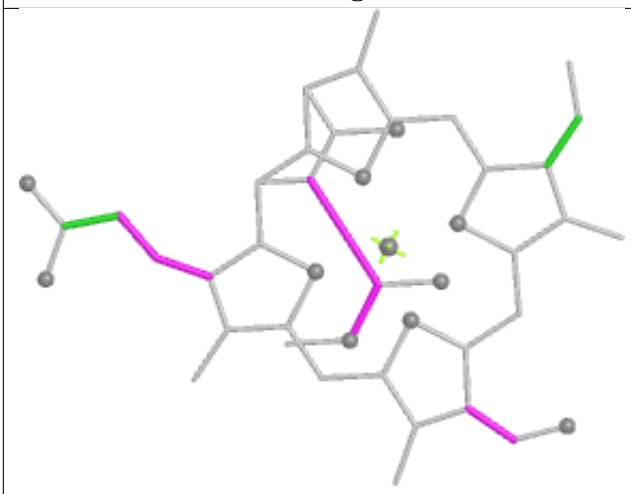


Bond angles

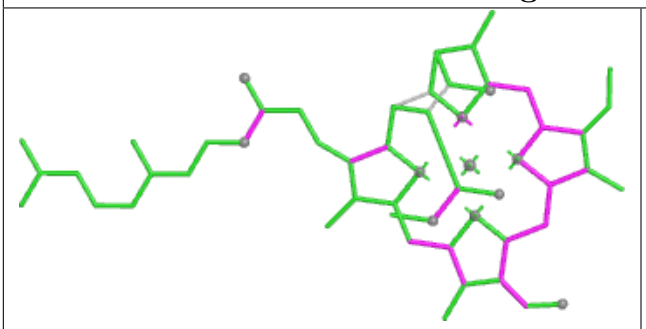


Torsions



Rings

Ligand CL7 3B 606



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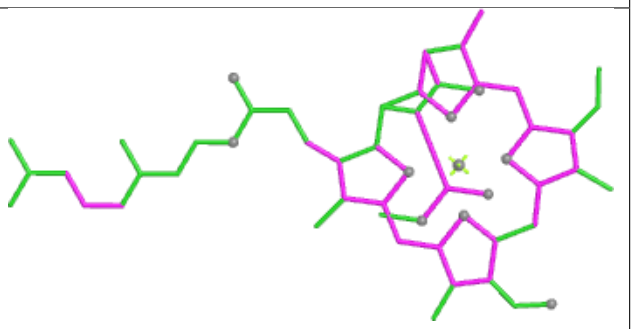
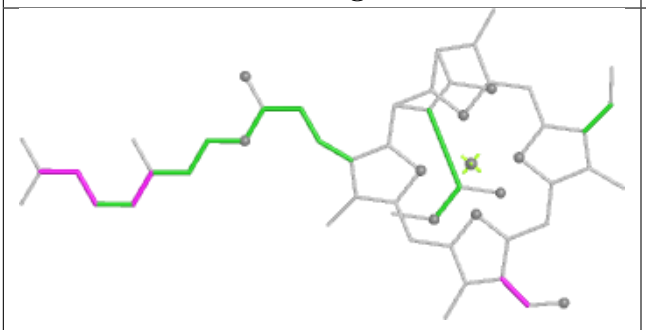


Bond angles



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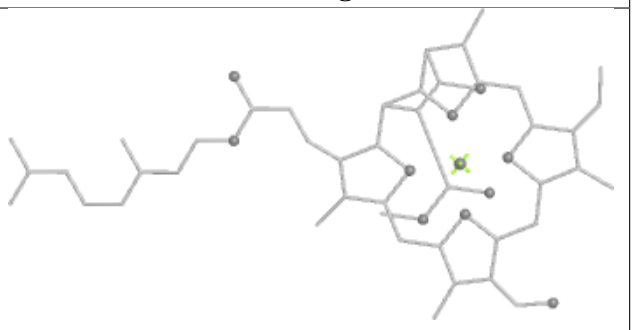
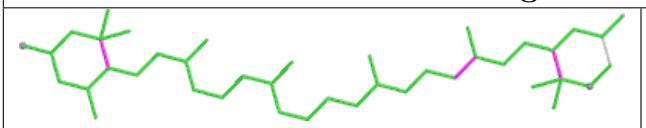


Rings

Ligand ZEX 32 524



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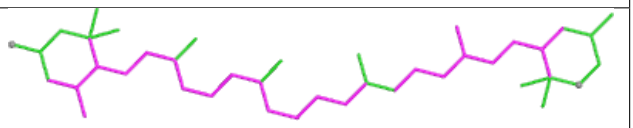
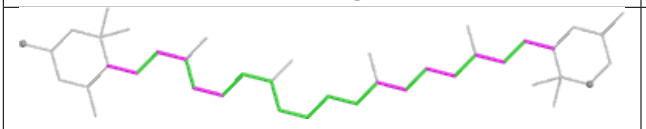


Bond angles



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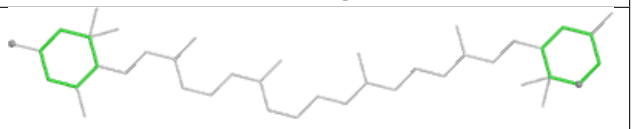
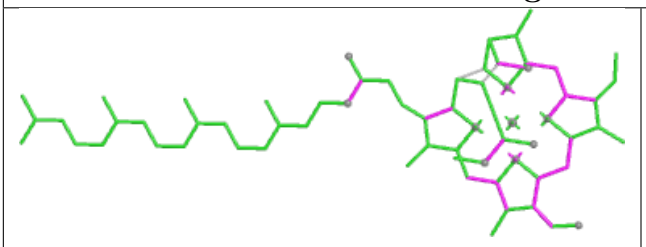


Rings

Ligand CL7 21 410



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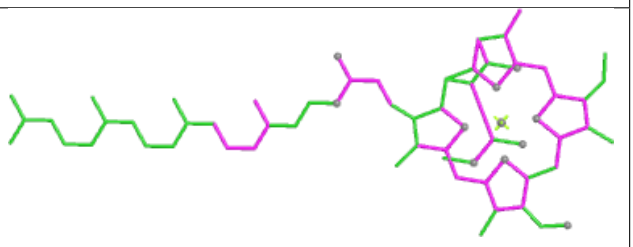
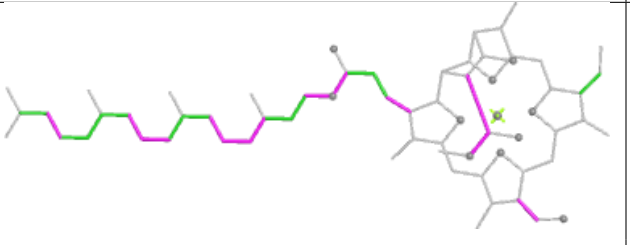


Bond angles



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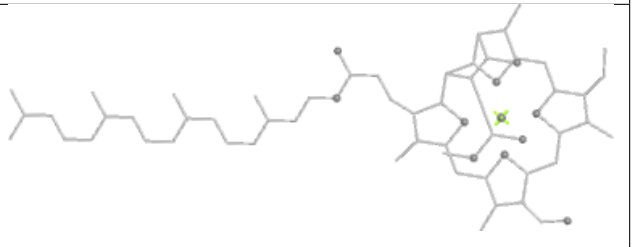
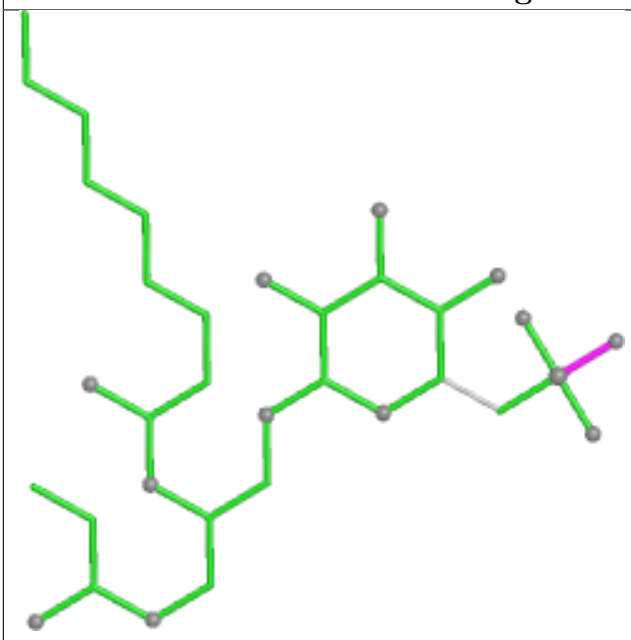


Rings

Ligand SQD 4A 406



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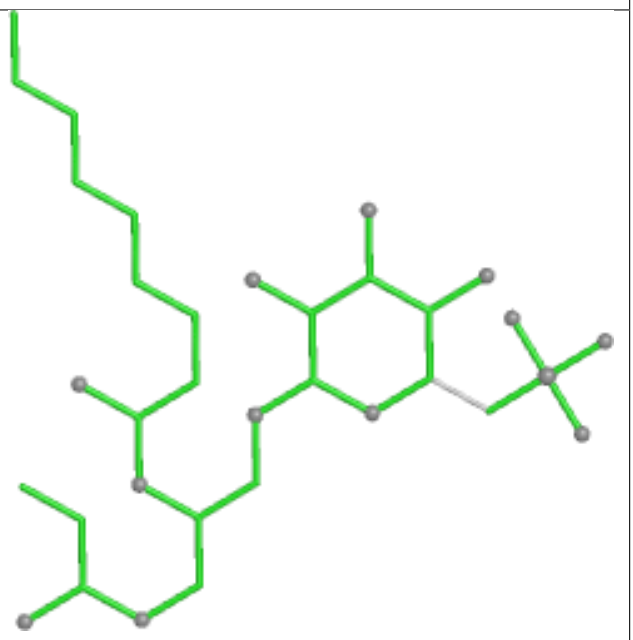
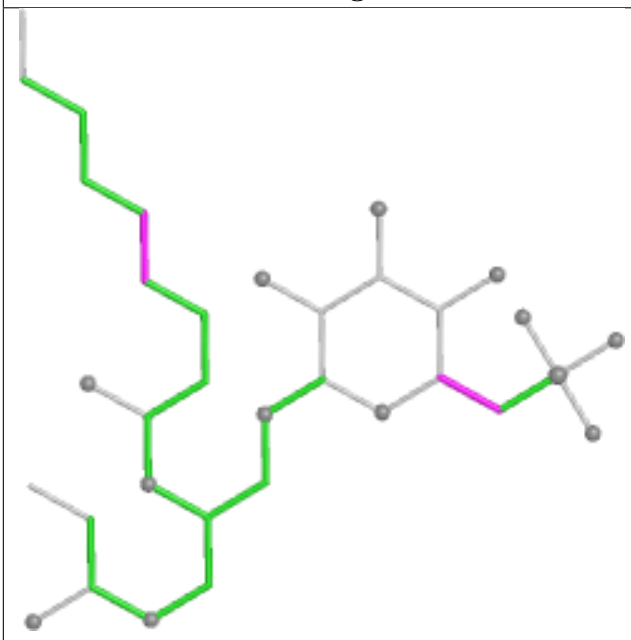


Bond angles



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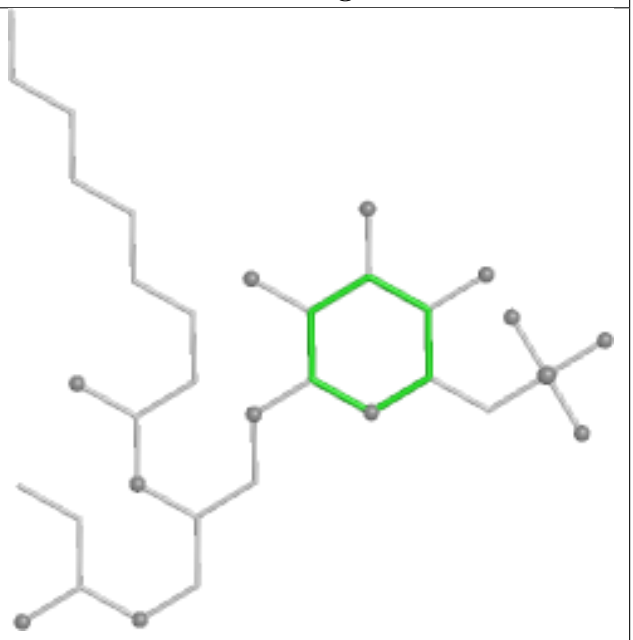
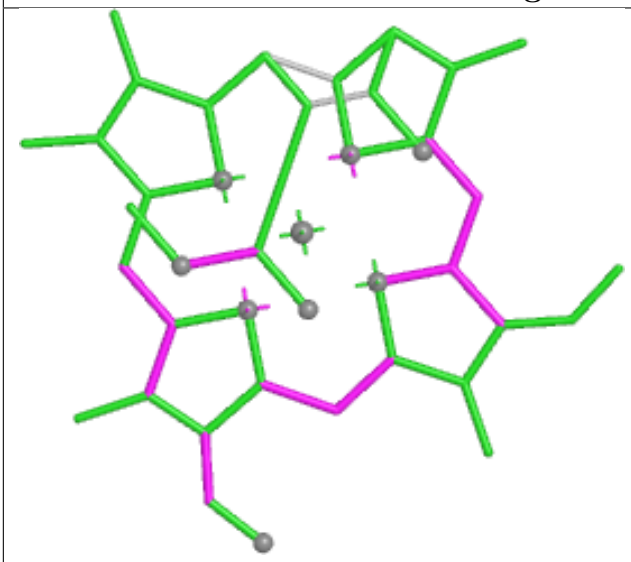


Rings

Ligand CL7 23 416



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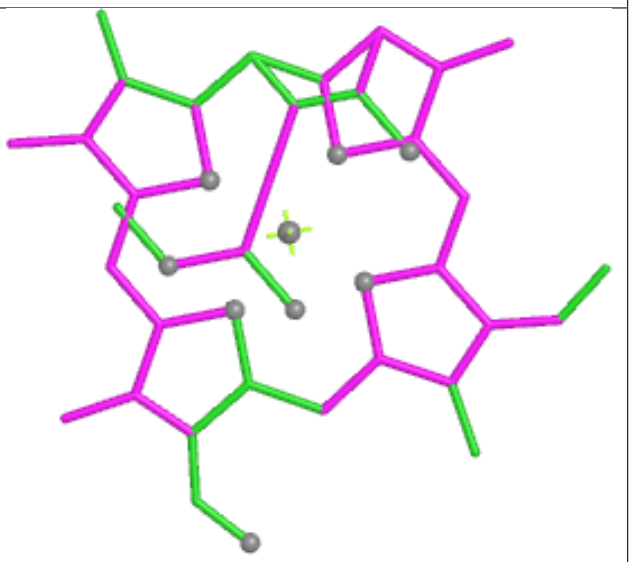
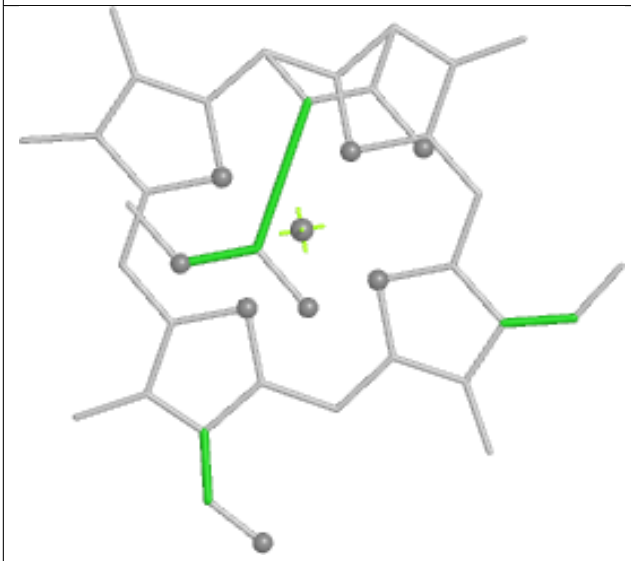


Bond angles



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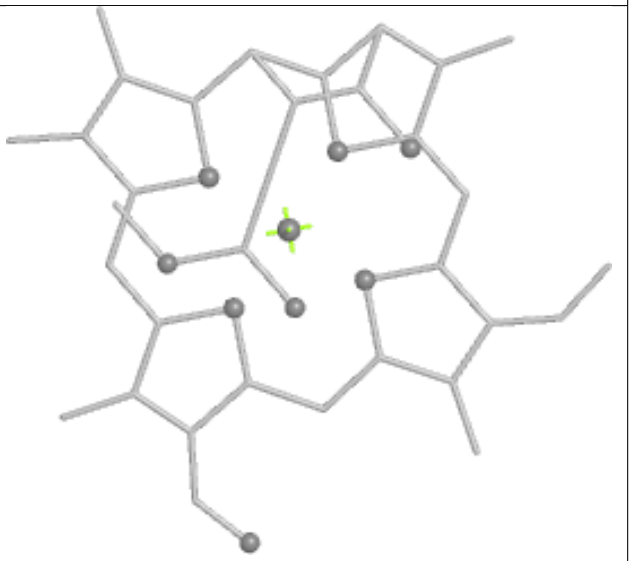
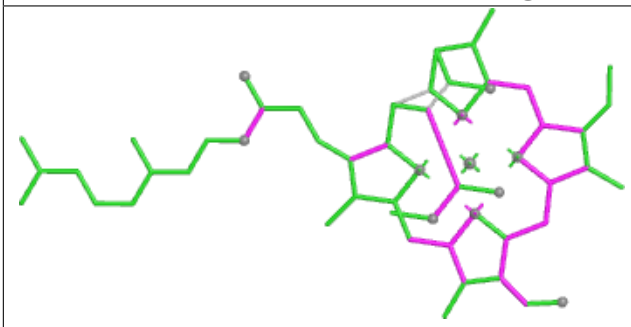


Rings

Ligand CL7 3A 403



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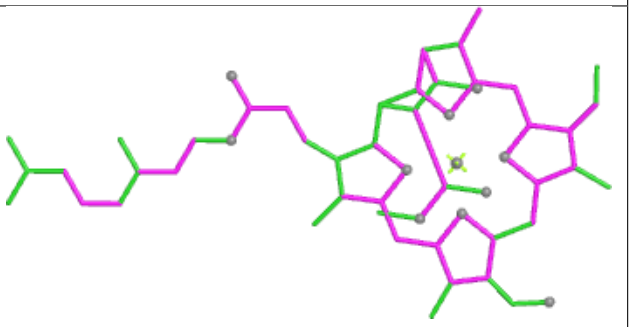
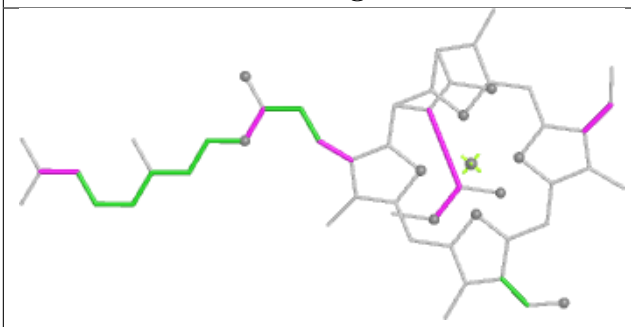


Bond angles



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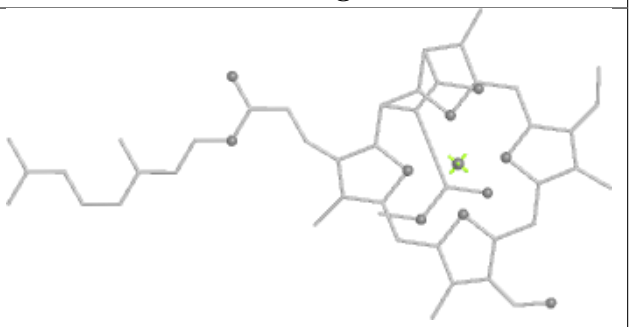

Rings

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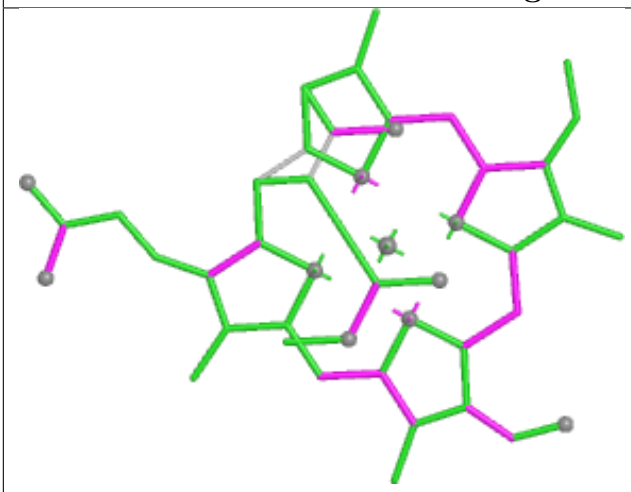

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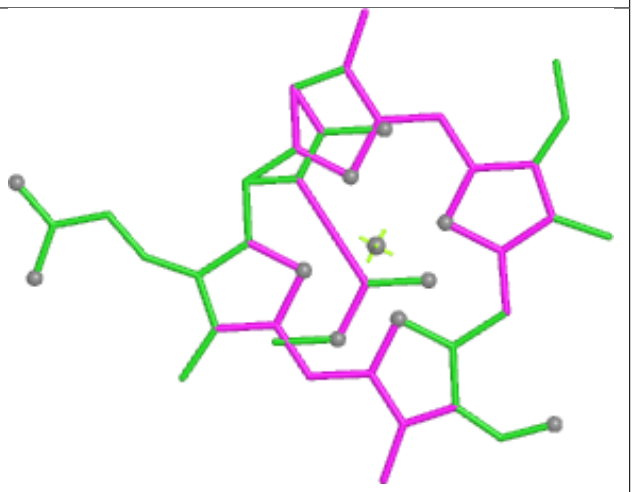
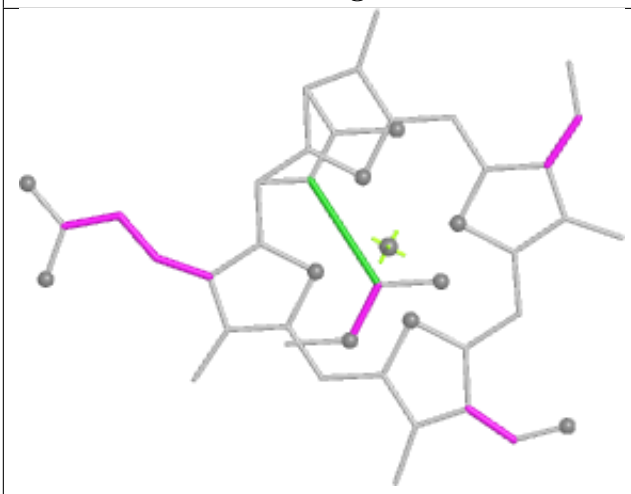


Bond angles

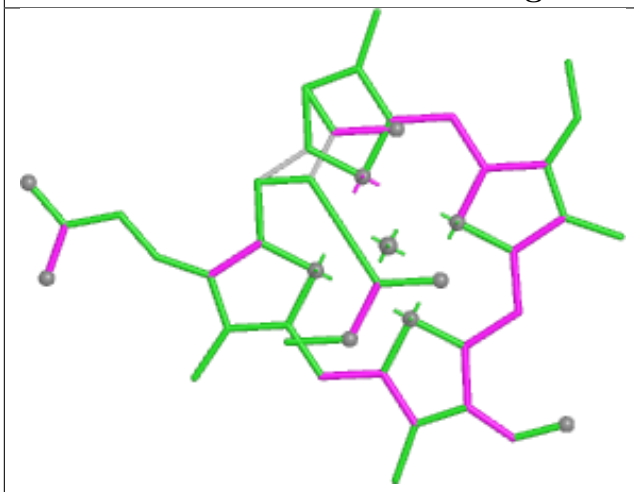


Torsions

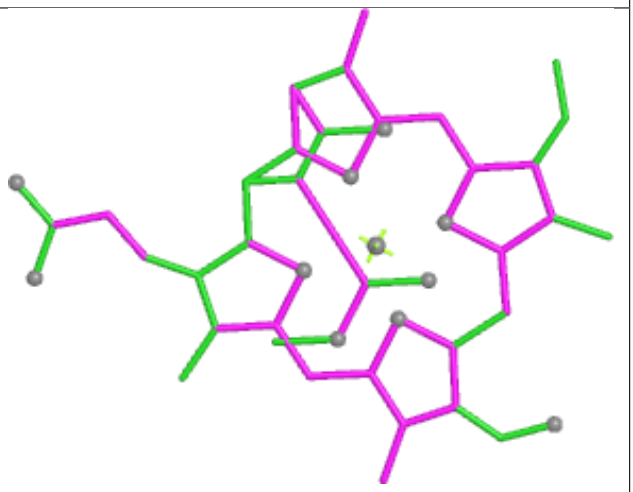


Rings

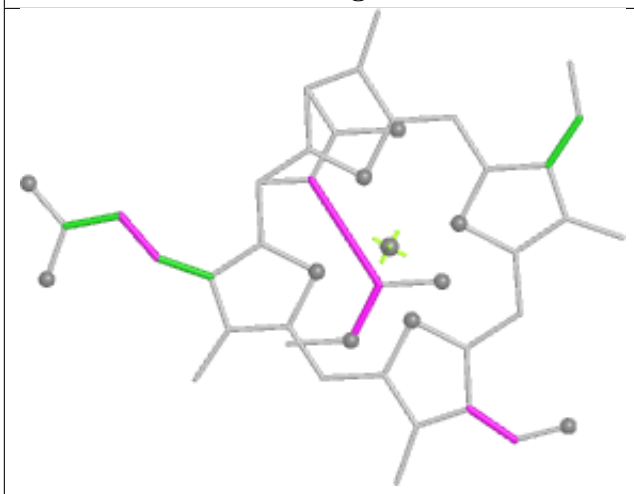
Ligand CL7 31 409



Bond lengths



Bond angles

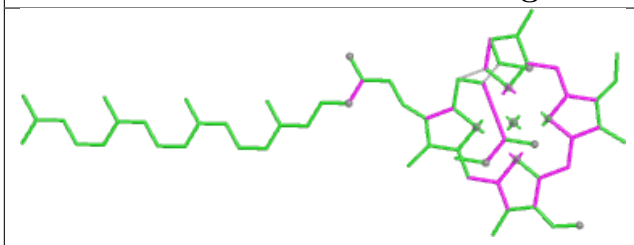


Torsions



Rings

Ligand CL7 3C 509



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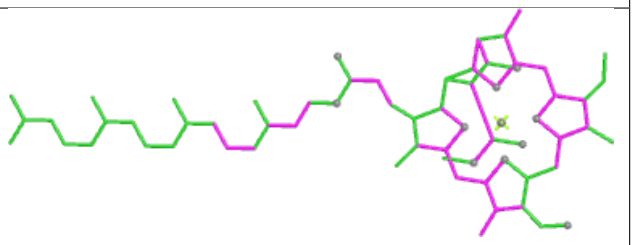
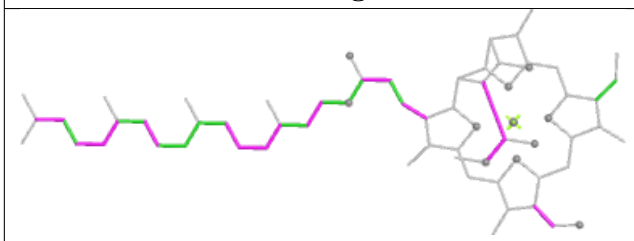


Bond angles



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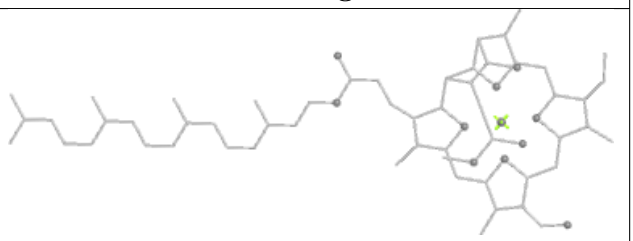
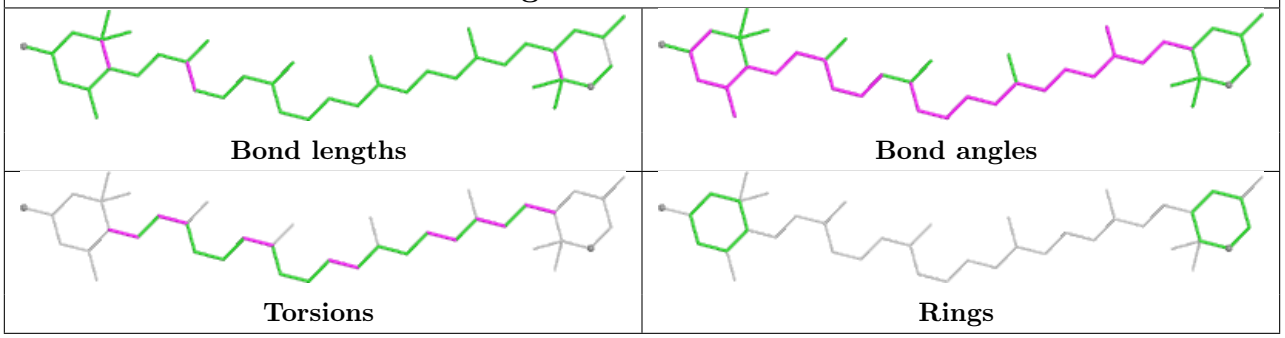
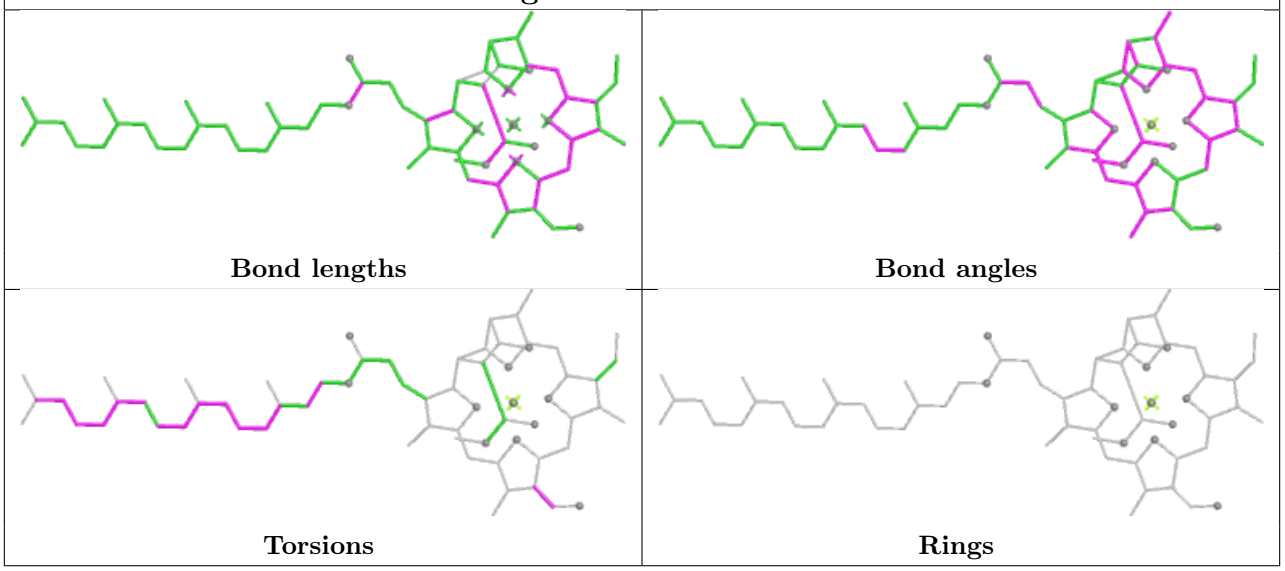


Rings

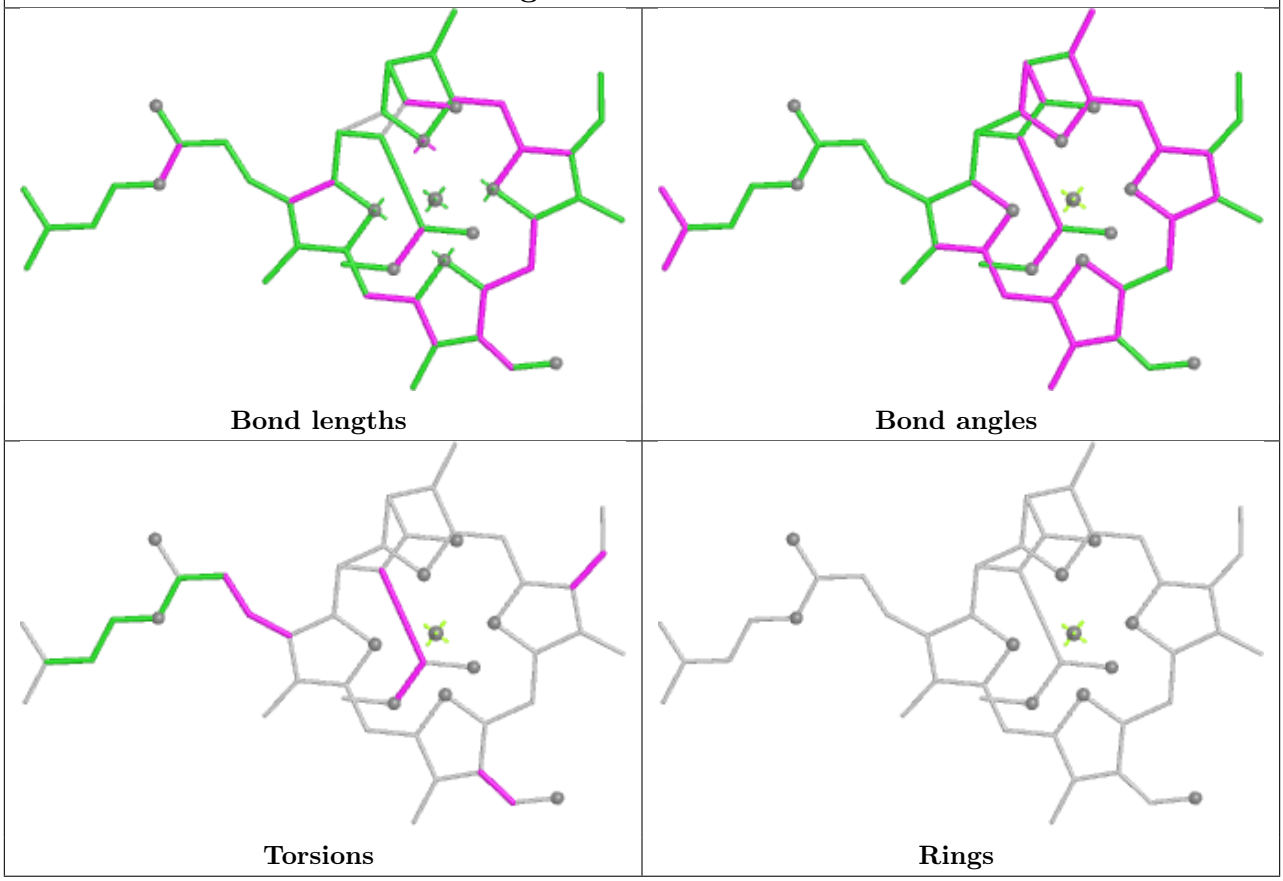
Ligand ZEX 12 519



Ligand CL7 2C 507



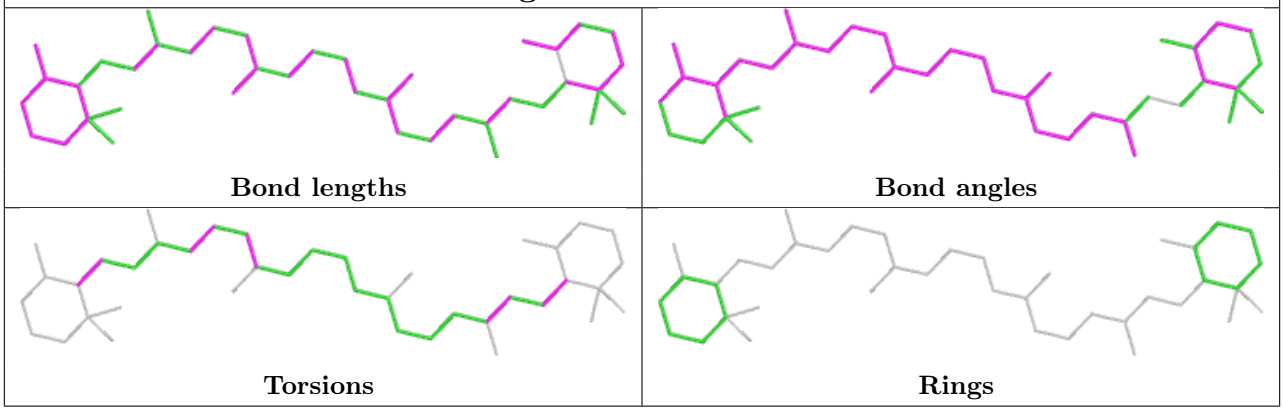
Ligand CL7 3D 402



Bond lengths | Bond angles

Torsions | Rings

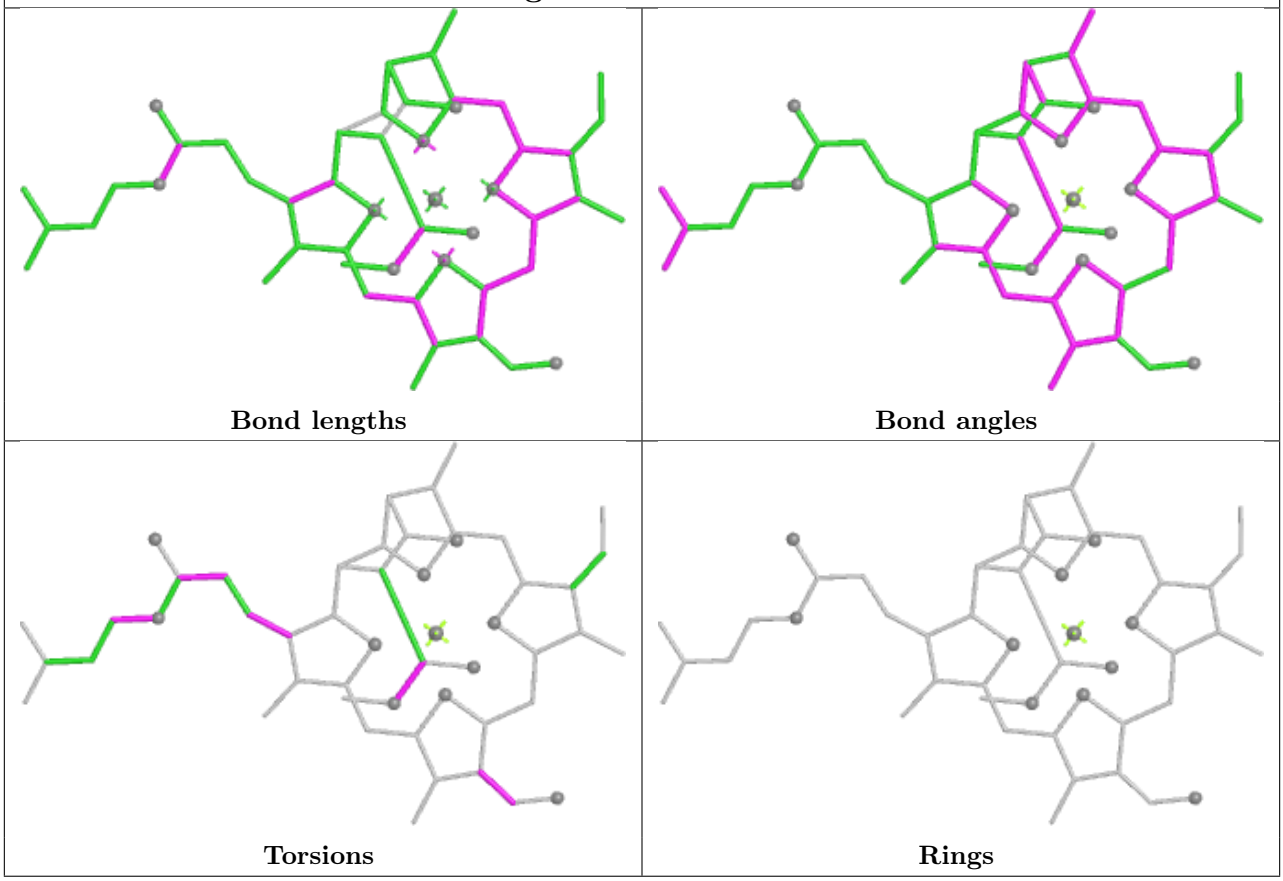
Ligand 8CT 4C 518



Bond lengths | Bond angles

Torsions | Rings

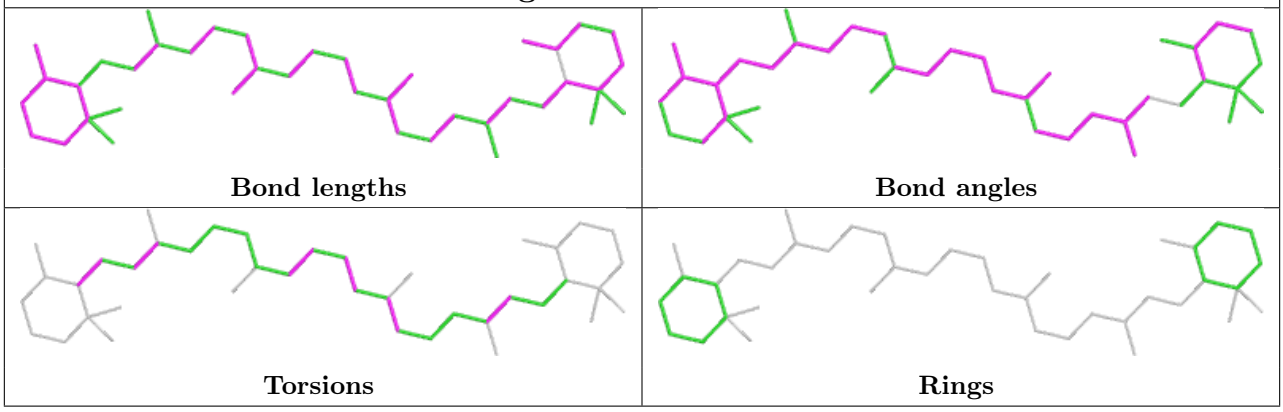
Ligand CL7 13 517



Bond lengths | Bond angles

Torsions | Rings

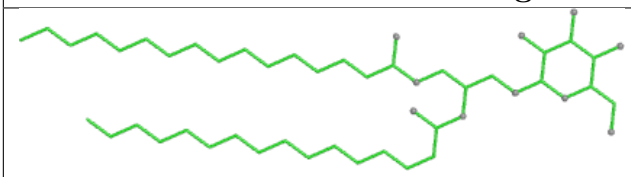
Ligand 8CT 1D 406



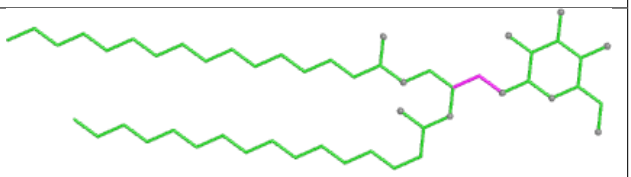
Bond lengths | Bond angles

Torsions | Rings

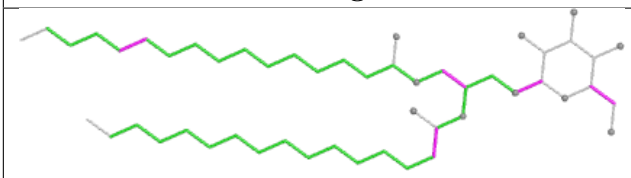
Ligand LMG 21 401



Bond lengths



Bond angles



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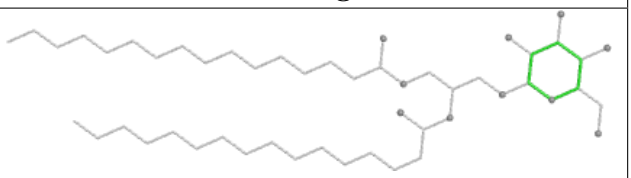
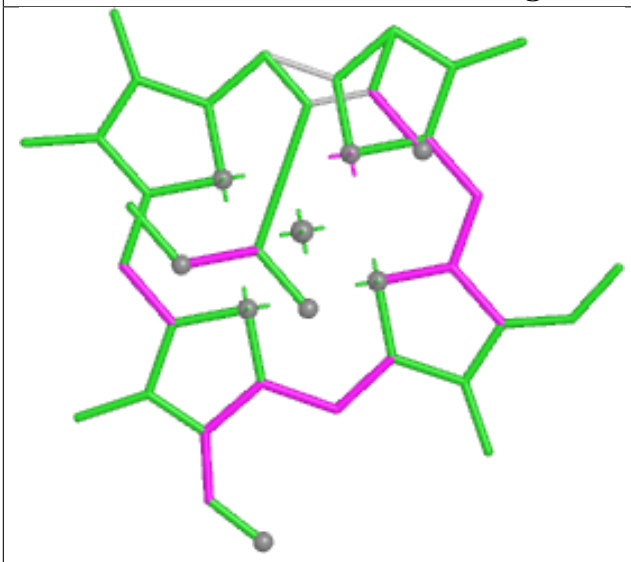
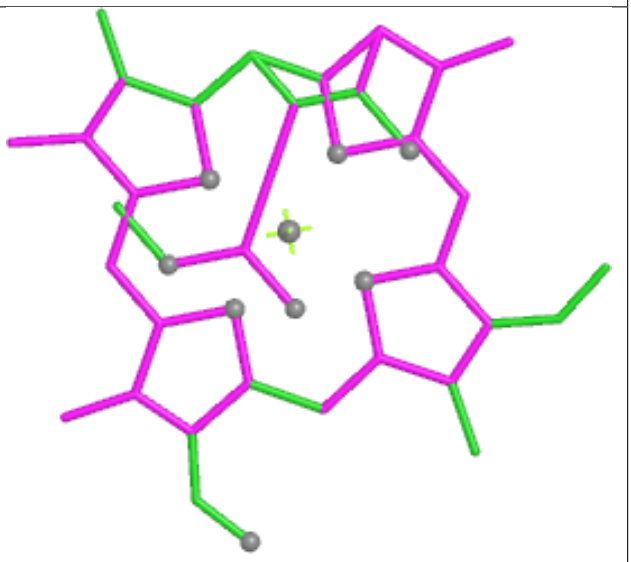


Rings

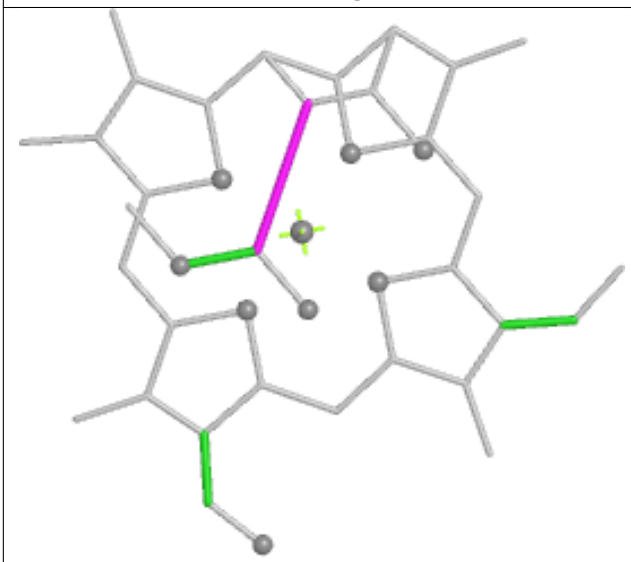
Ligand CL7 41 413



Bond lengths



Bond angles



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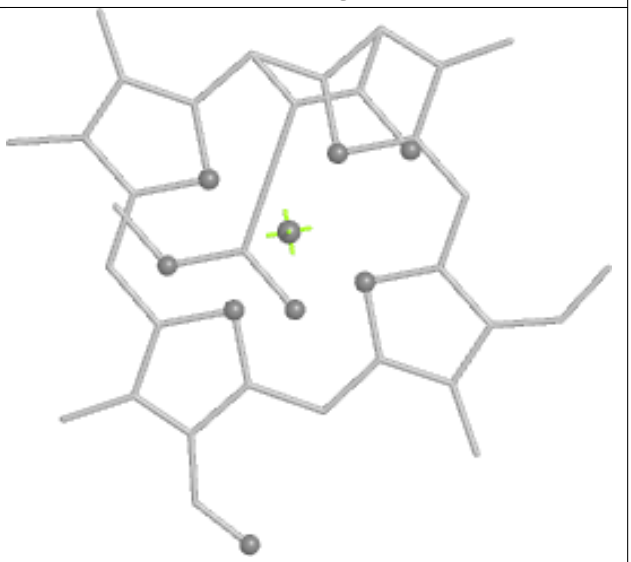
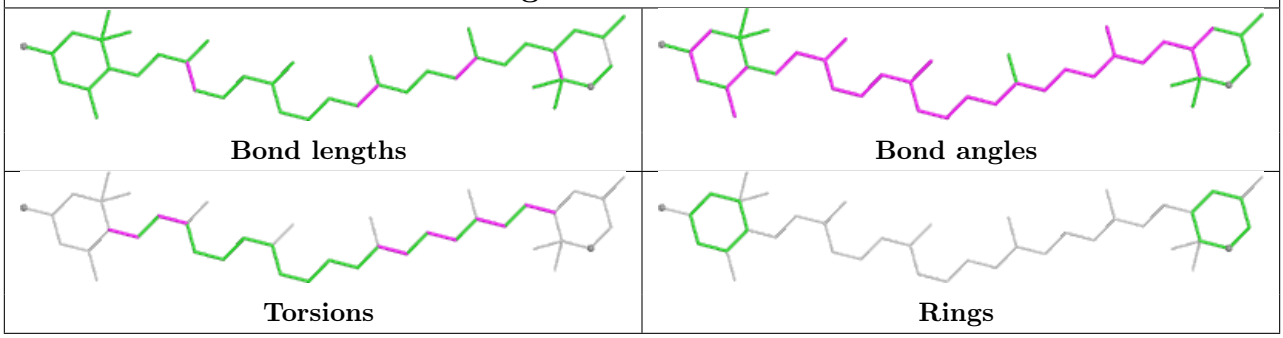


Rings

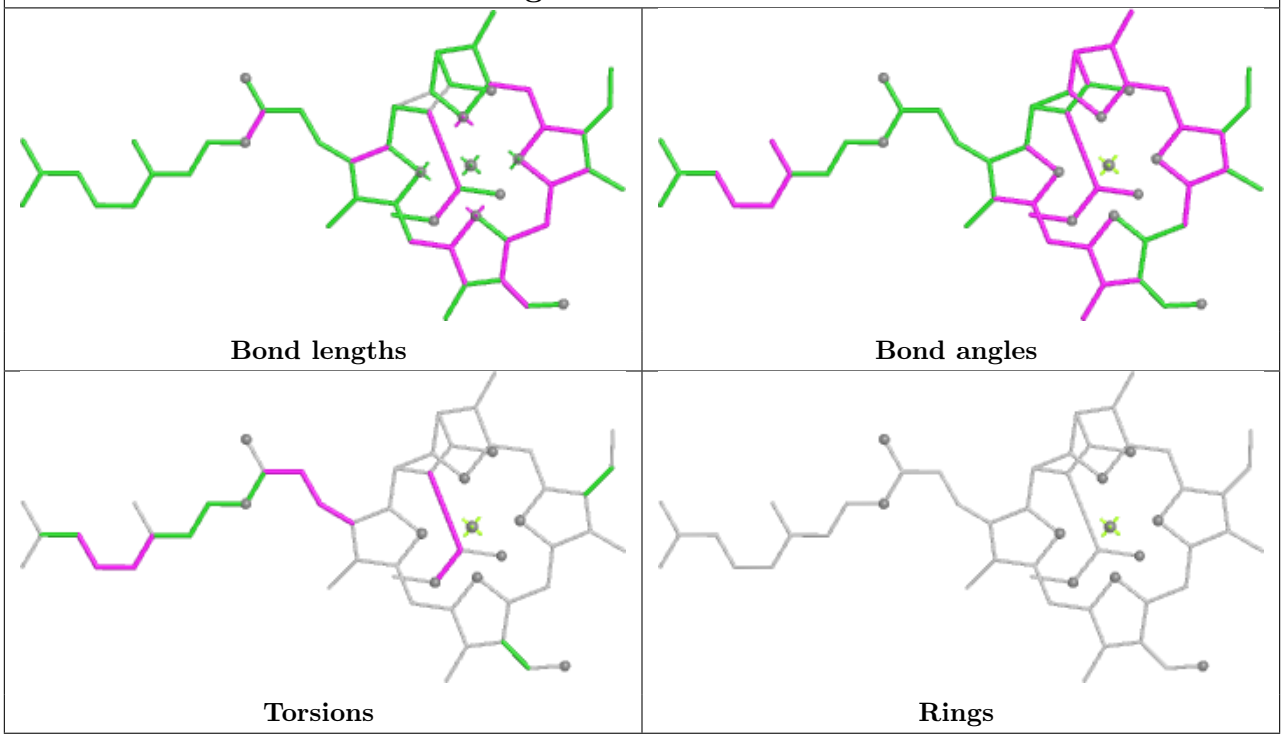
Ligand ZEX 43 420



Bond lengths | Bond angles

Torsions | Rings

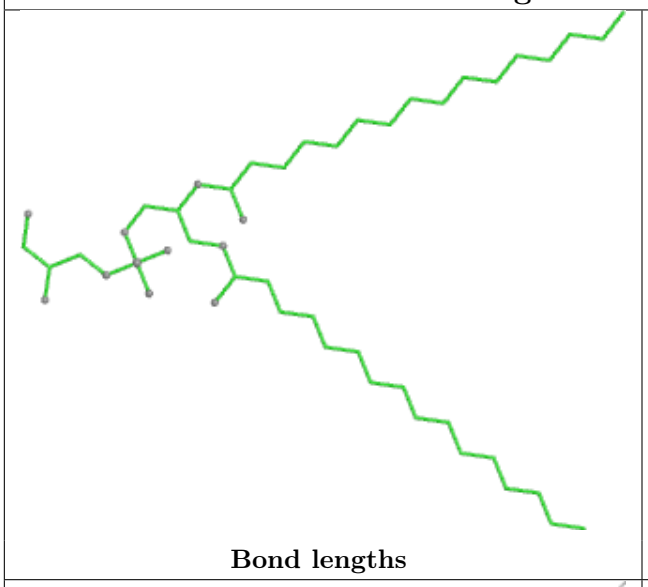
Ligand CL7 43 413



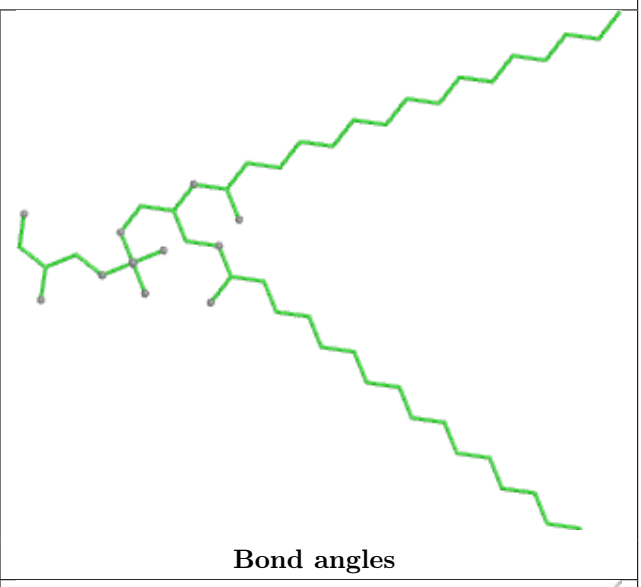
Bond lengths | Bond angles

Torsions | Rings

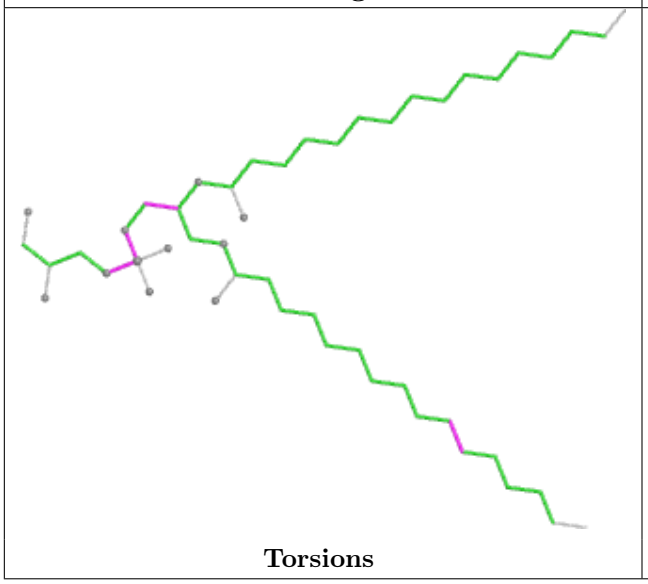
Ligand LHG 3D 409



Bond lengths



Bond angles



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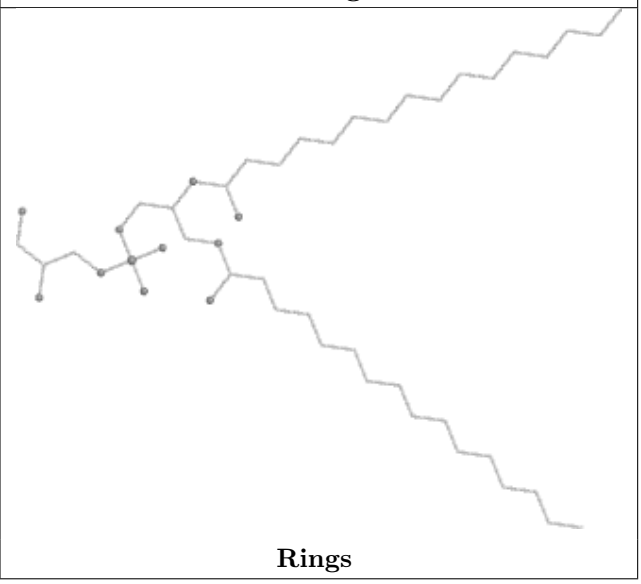
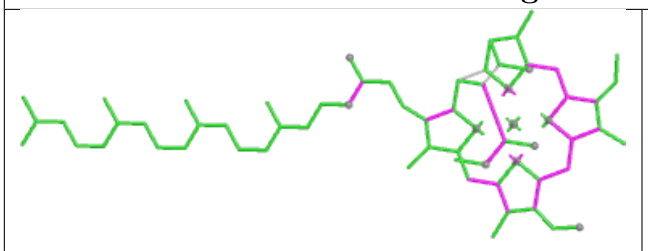
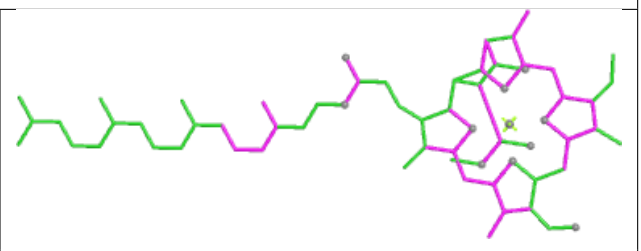


Rings

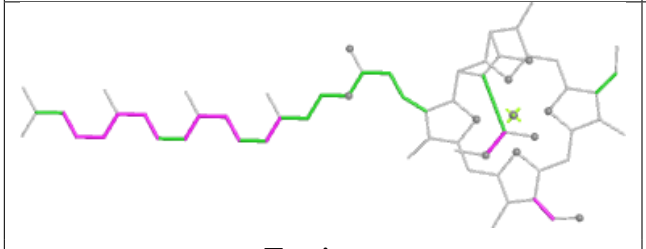
Ligand CL7 1B 611



Bond lengths



Bond angles



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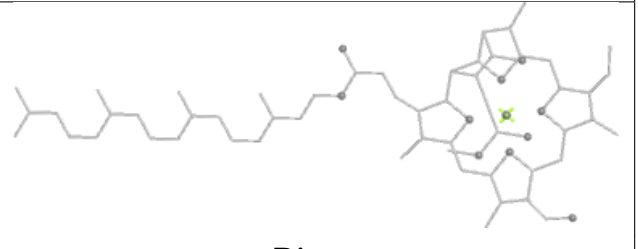
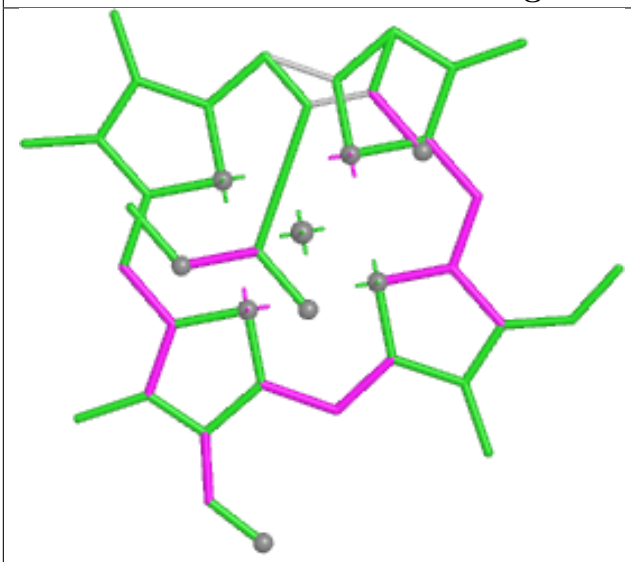


Rings

Ligand CL7 11 416



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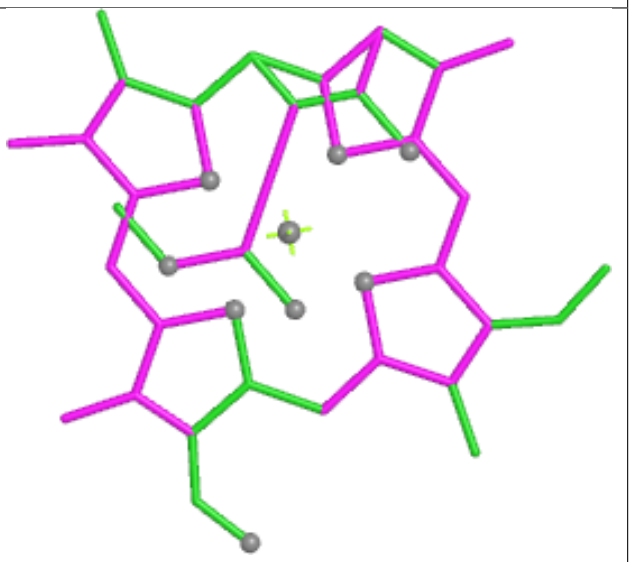
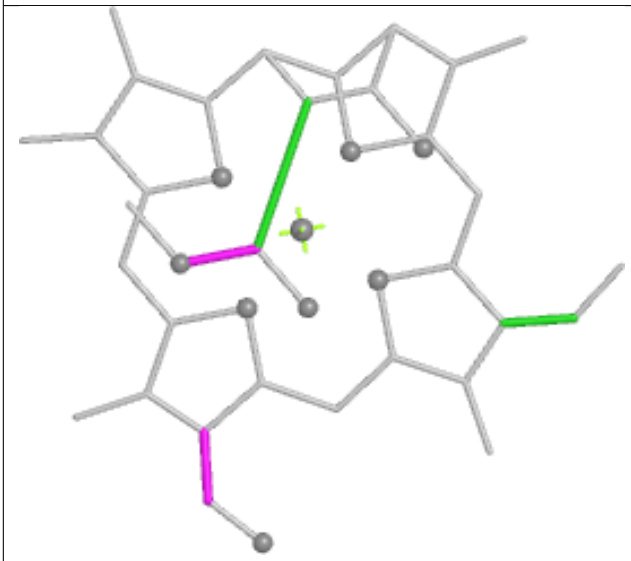


Bond angles



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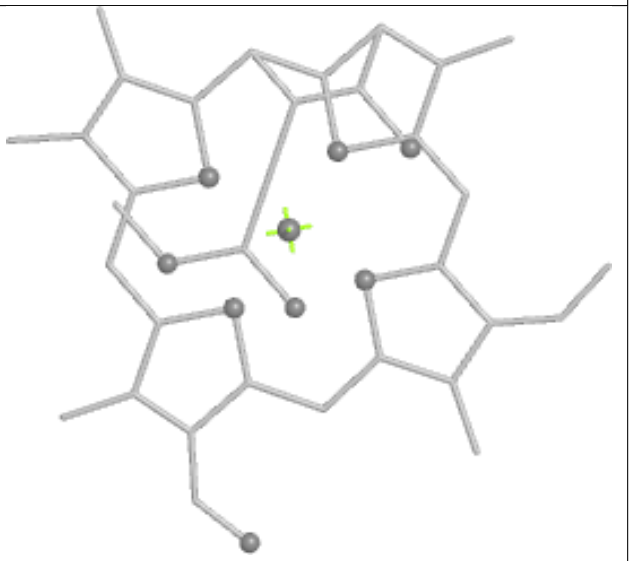
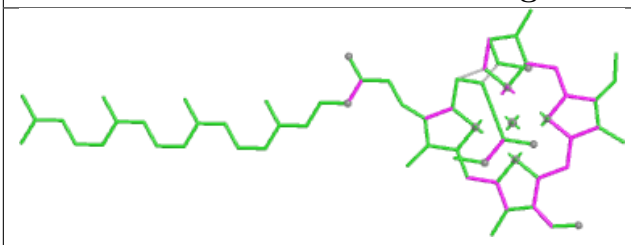


Rings

Ligand CL7 1B 605



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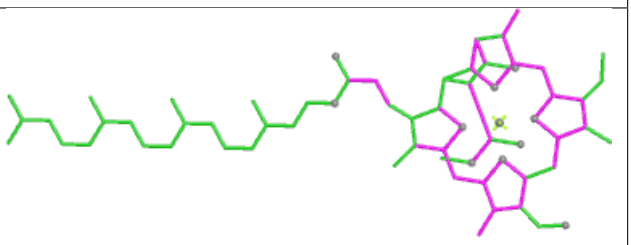
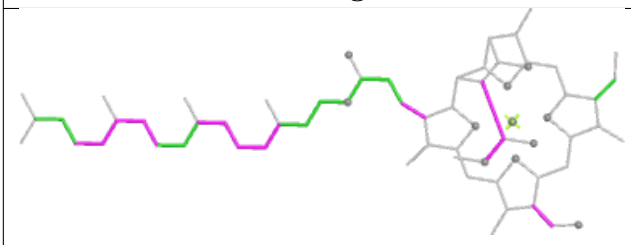


Bond angles



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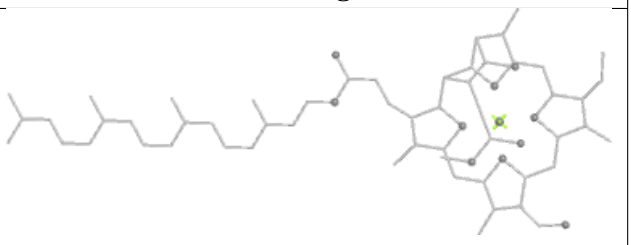
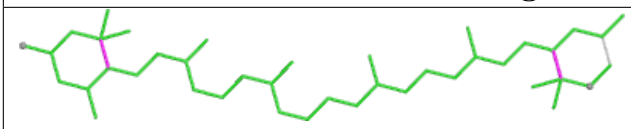


Rings

Ligand ZEX 23 421



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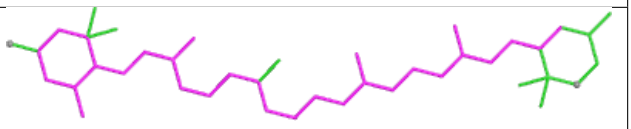
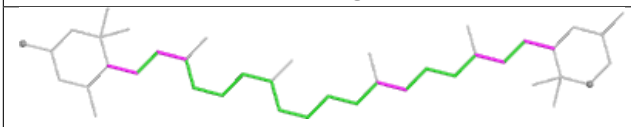


Bond angles



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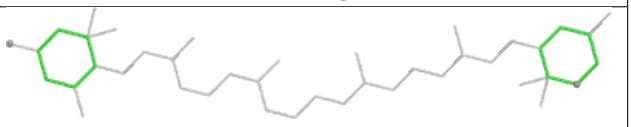
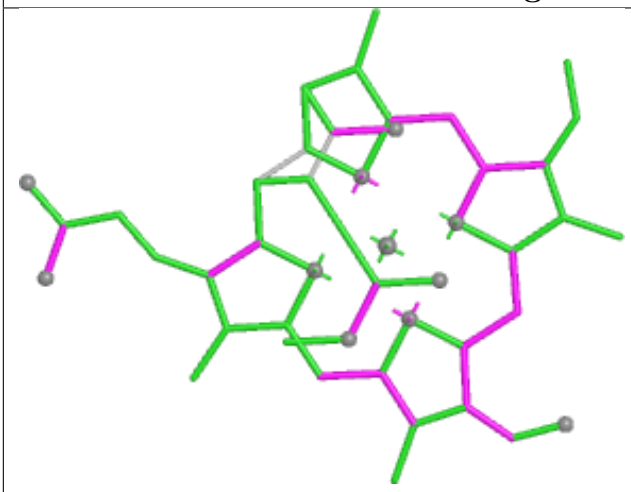


Rings

Ligand CL7 32 515



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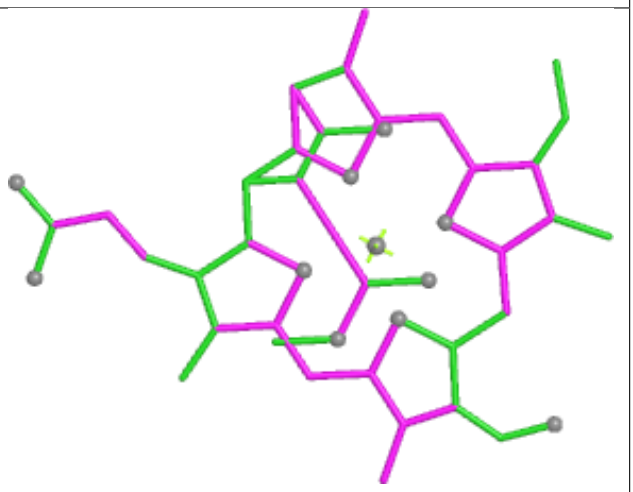
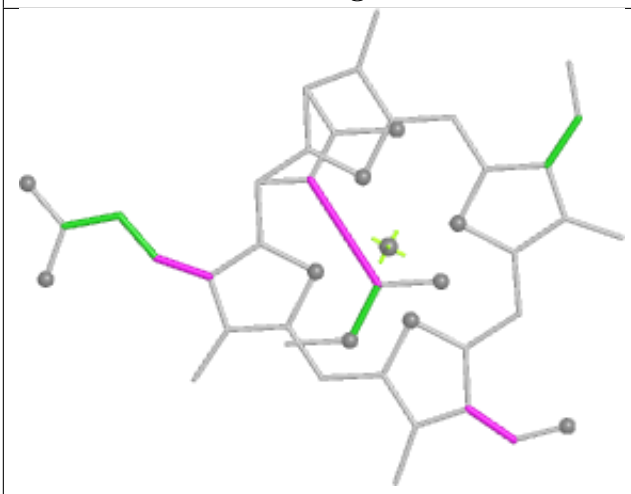


Bond angles

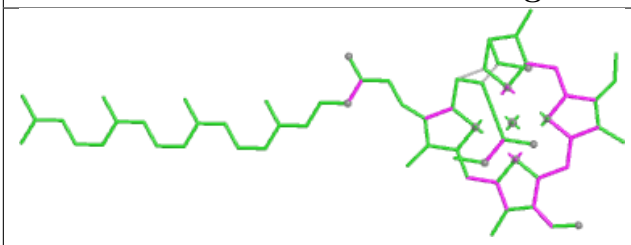


Torsions

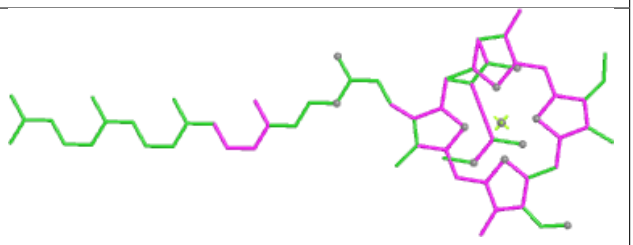


Rings

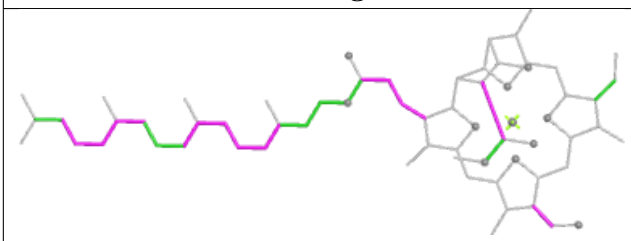
Ligand CL7 23 402



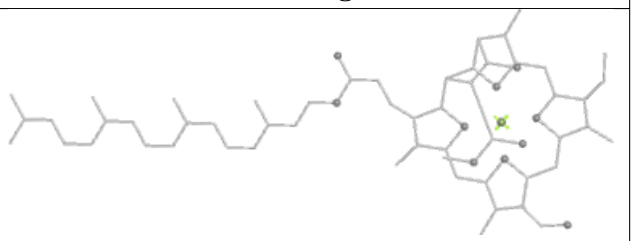
Bond lengths



Bond angles

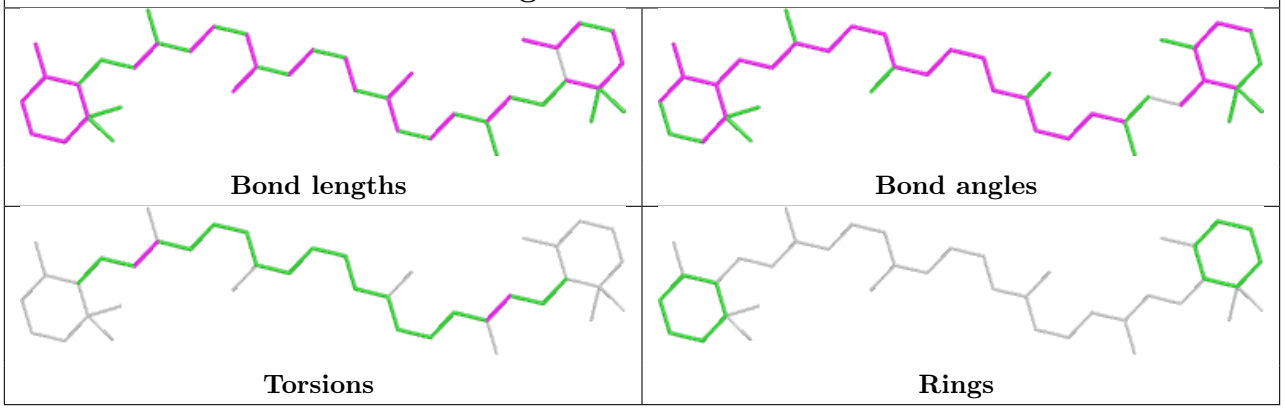


Torsions

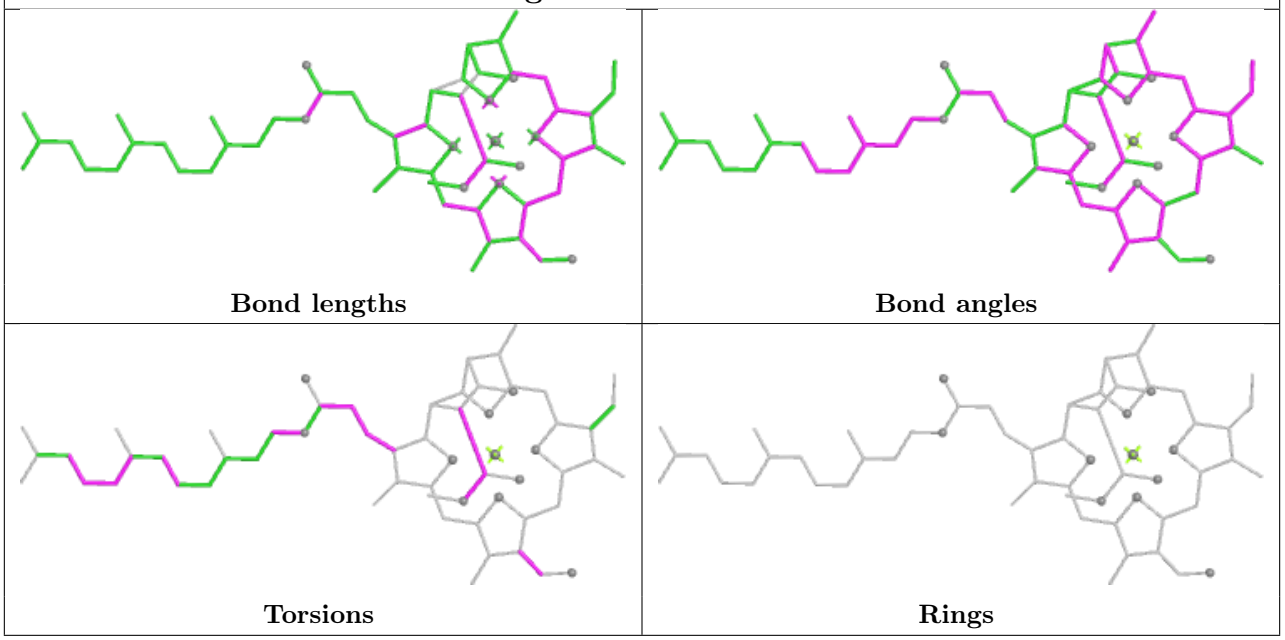


Rings

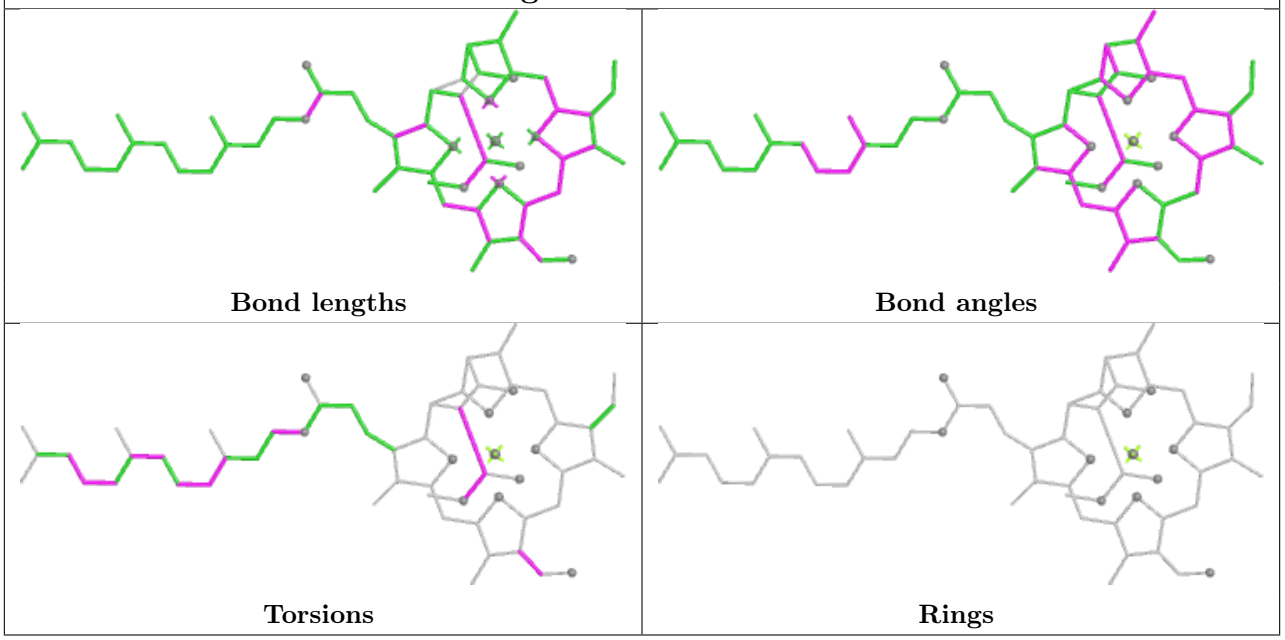
Ligand 8CT 3B 619



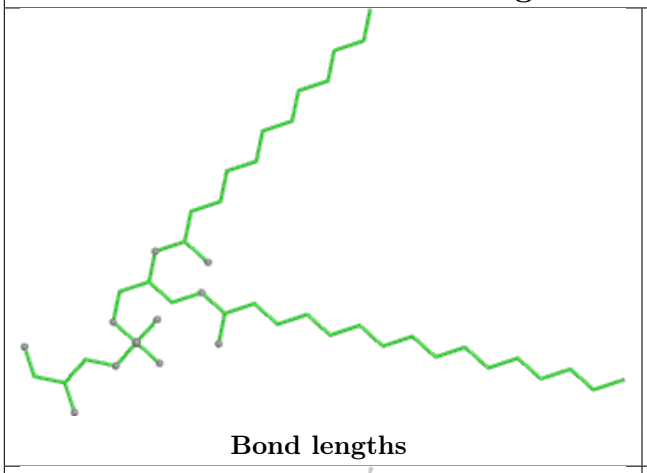
Ligand CL7 14 409



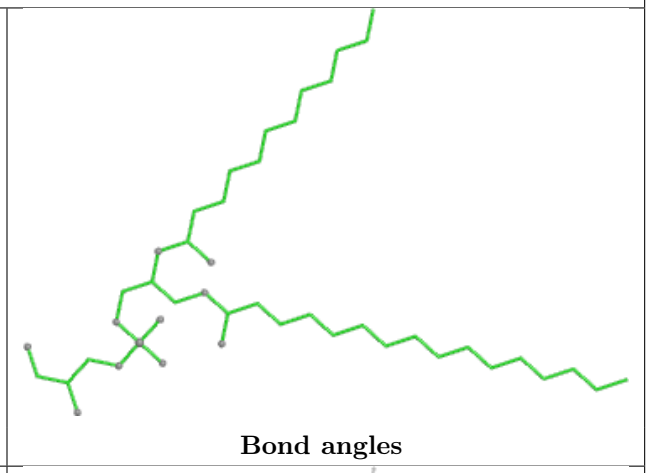
Ligand CL7 2C 502



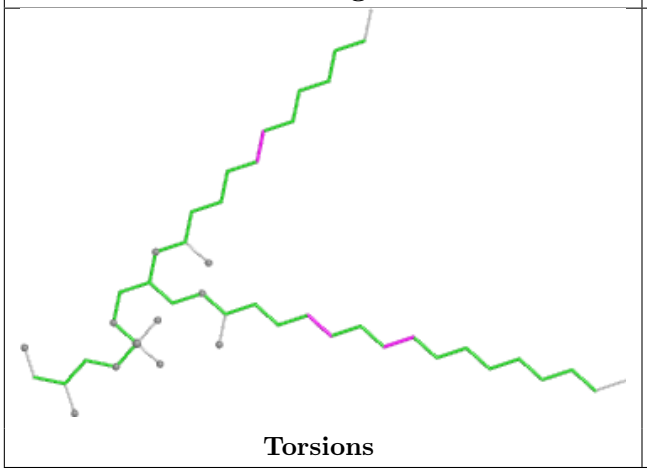
Ligand LHG 1B 623



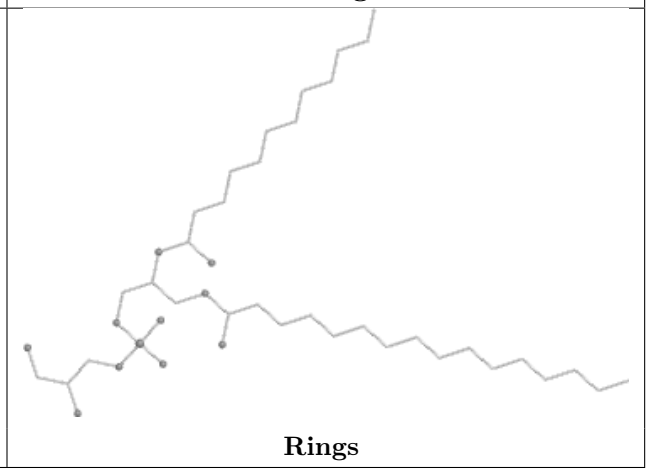
Bond lengths



Bond angles

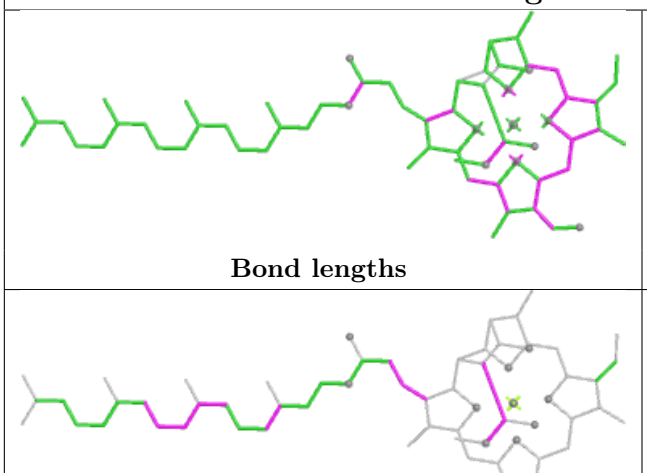


Torsions

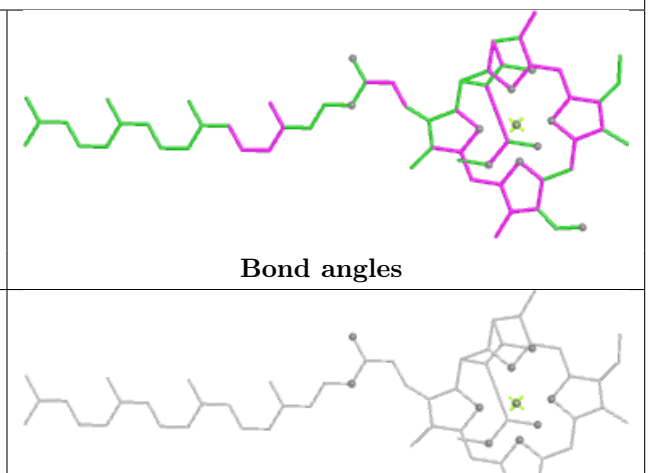


Rings

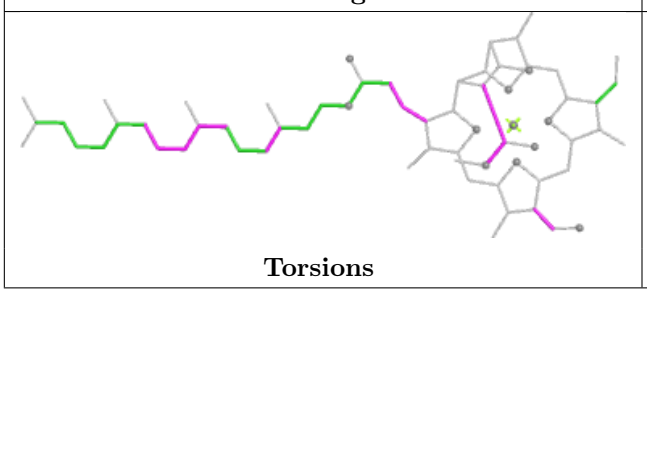
Ligand CL7 32 502



Bond lengths



Bond angles



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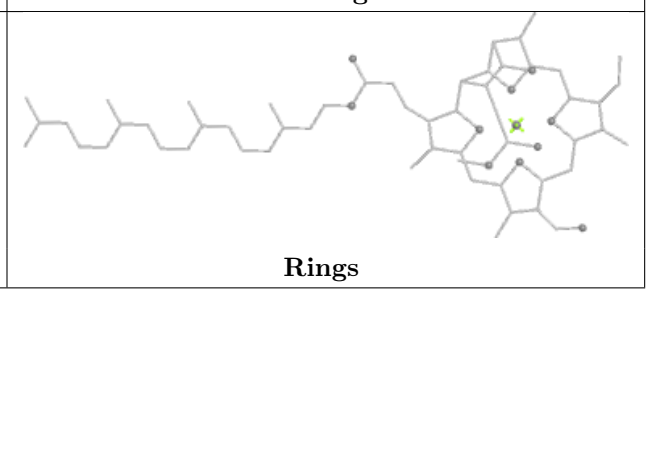
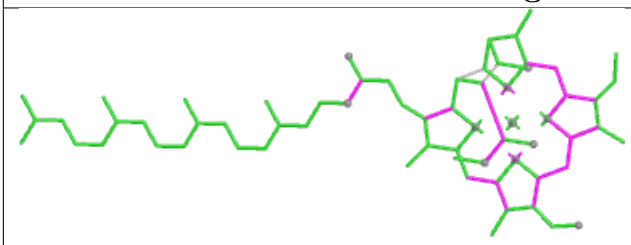


Rings

Ligand CL7 42 507



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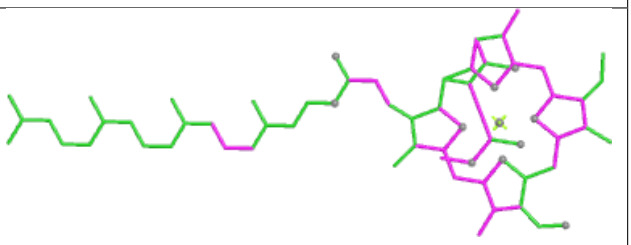

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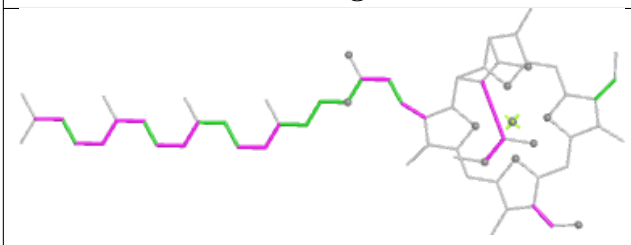

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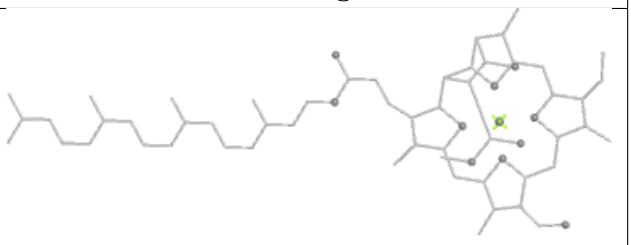
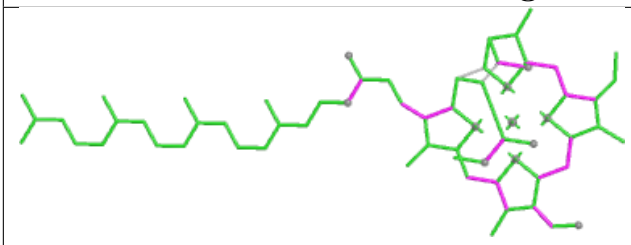


Rings

Ligand CL7 2A 401



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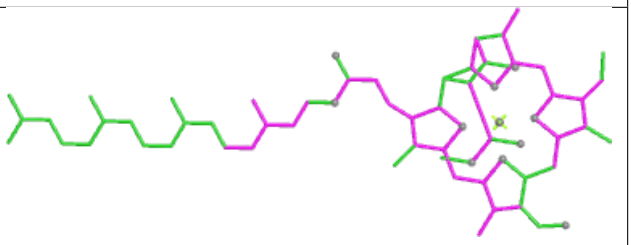
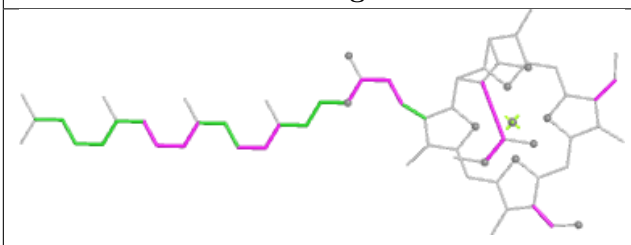


Bond angles



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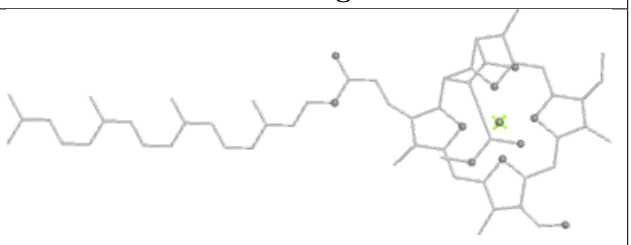
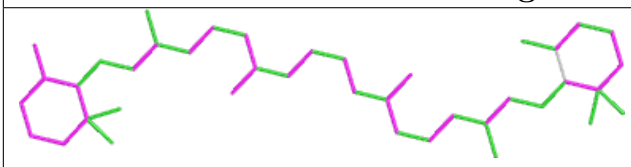


Rings

Ligand 8CT 1C 514



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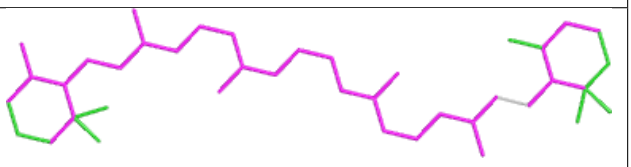

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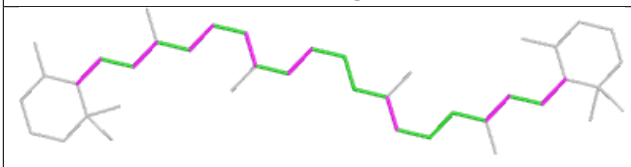

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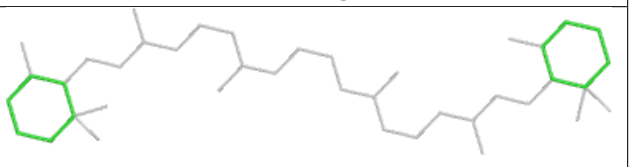
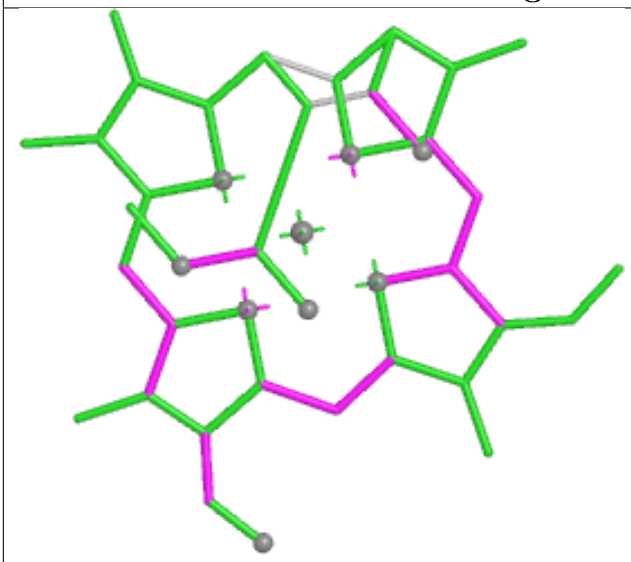


Rings

Ligand CL7 41 416



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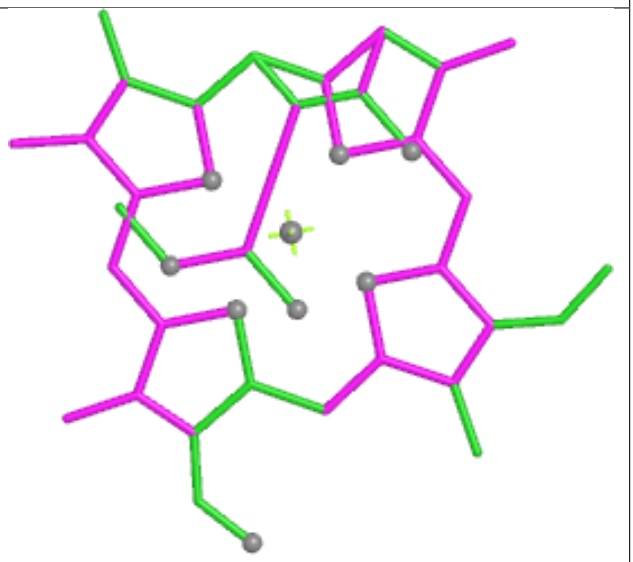
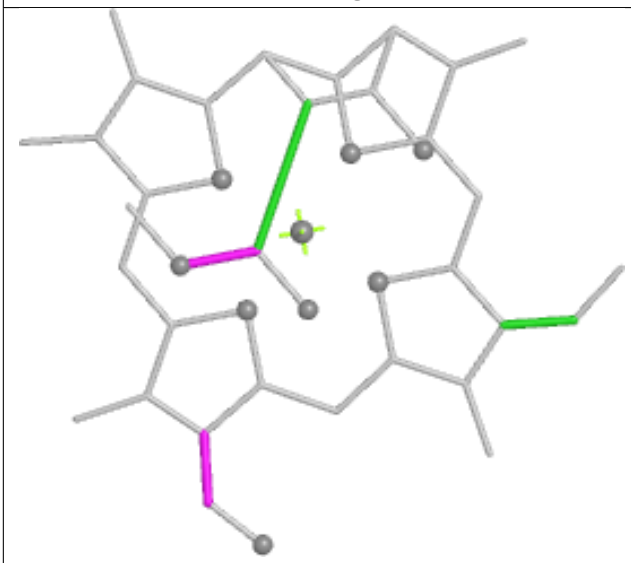


Bond angles



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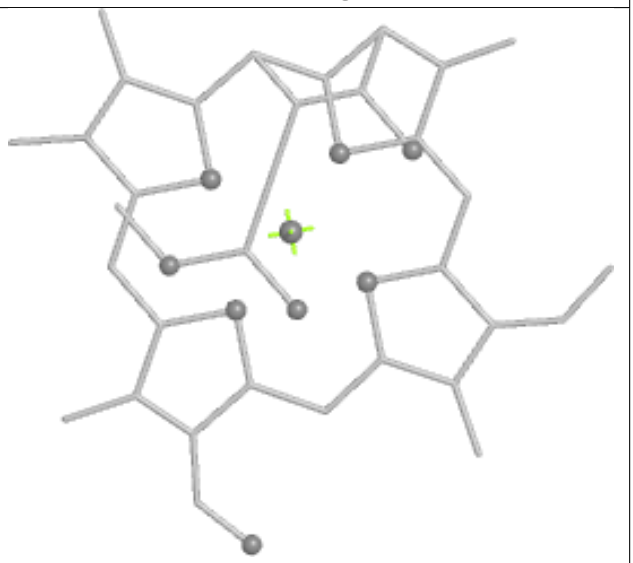
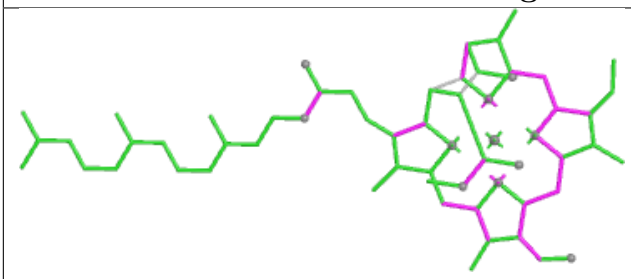


Rings

Ligand CL7 3B 602



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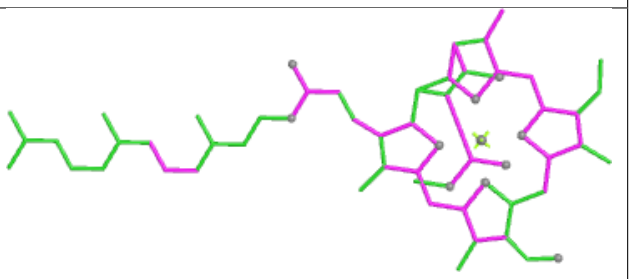
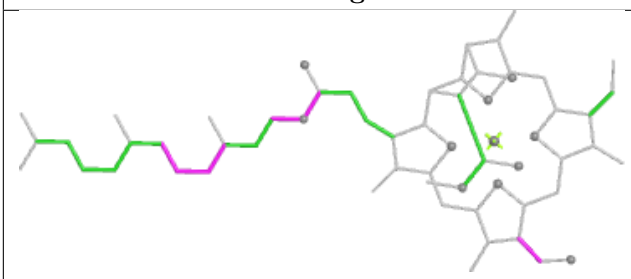


Bond angles



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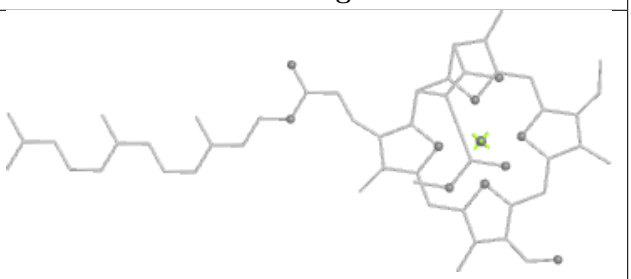
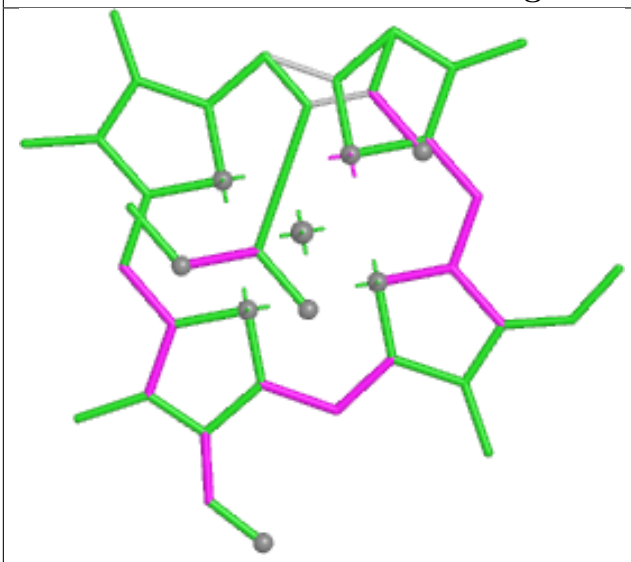


Rings

Ligand CL7 41 414



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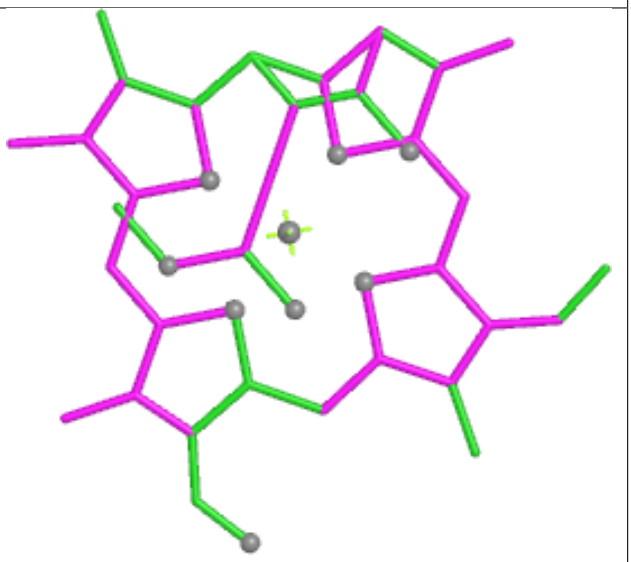

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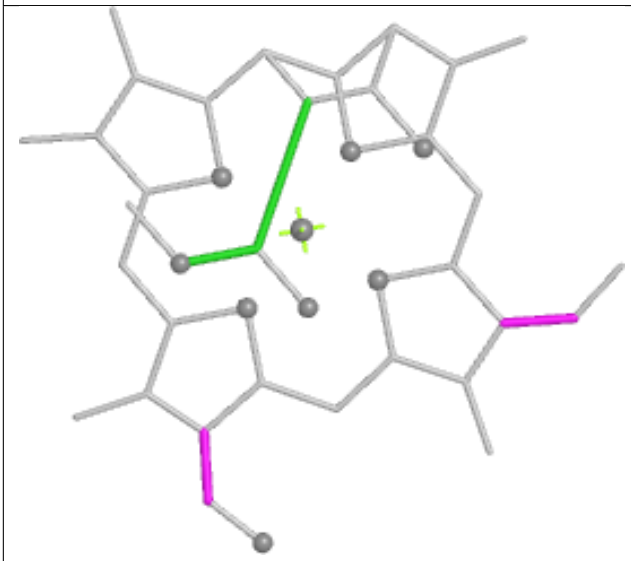

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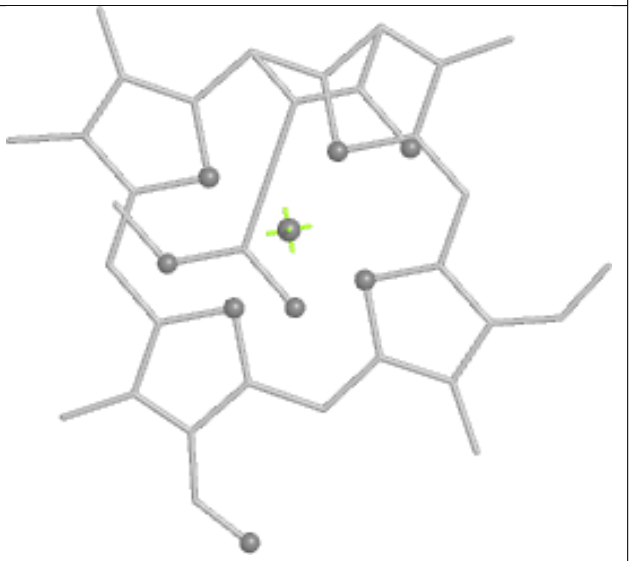
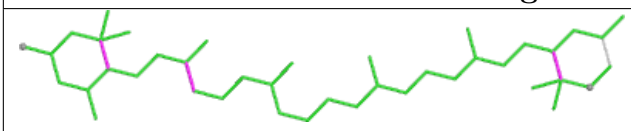


Rings

Ligand ZEX 42 519



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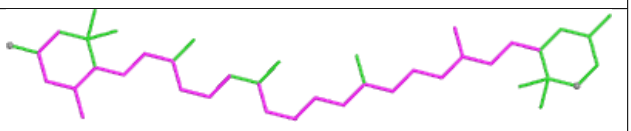

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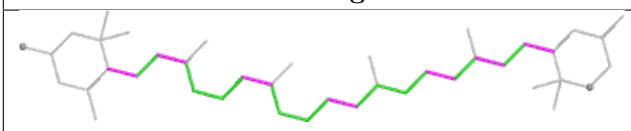

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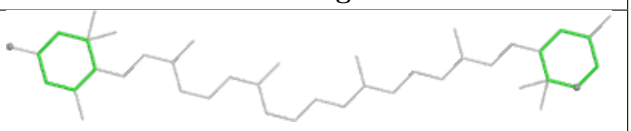
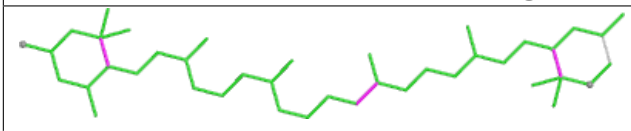


Rings

Ligand ZEX 24 419



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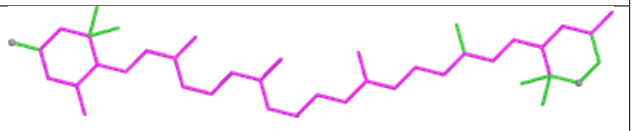

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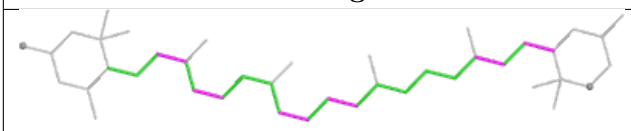

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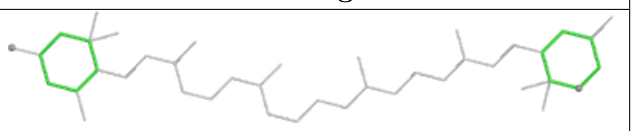
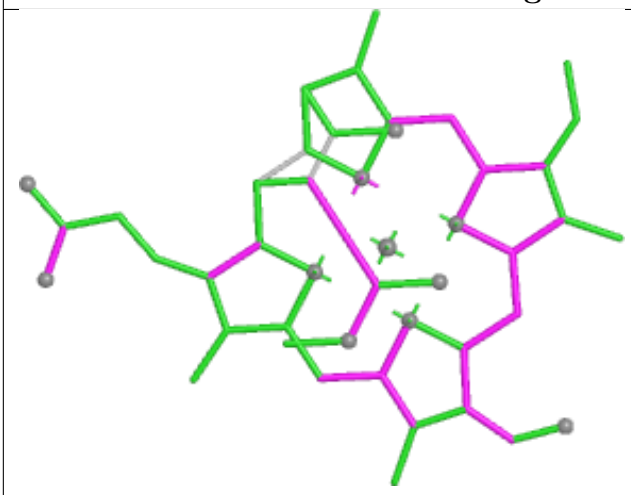


Rings

Ligand CL7 13 506



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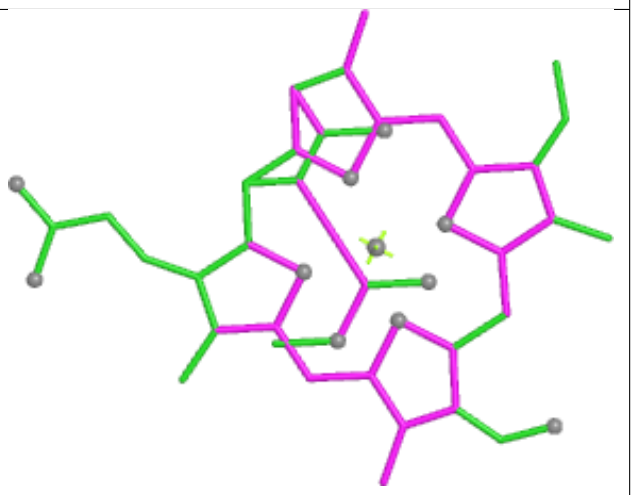

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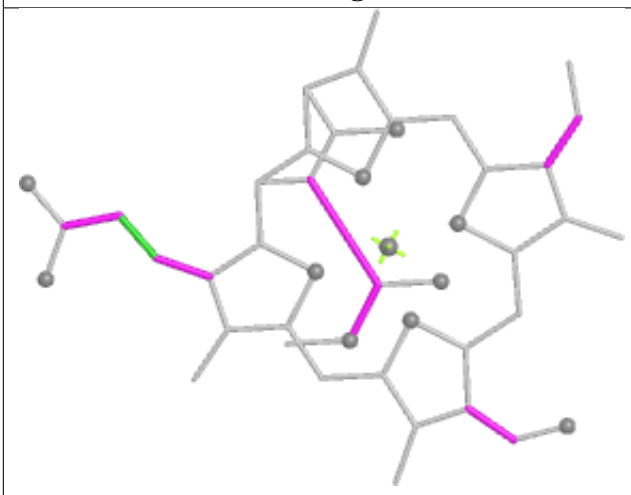
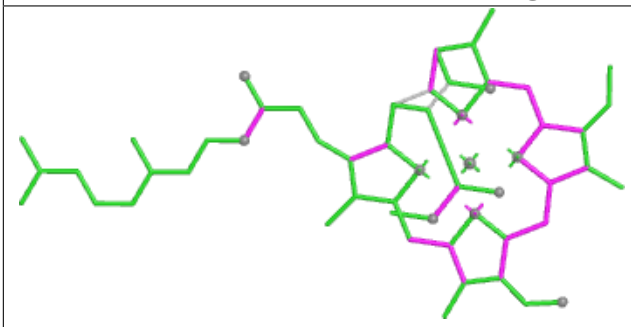


Torsions



Rings

Ligand CL7 33 516



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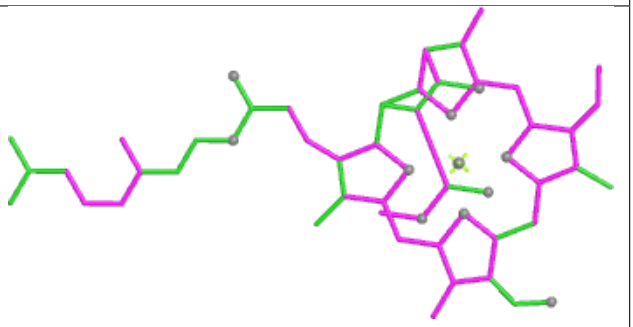
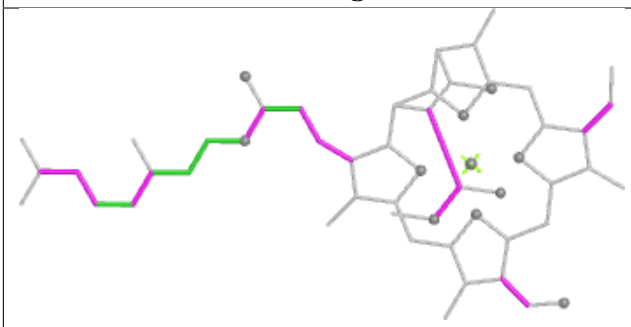


Bond angles



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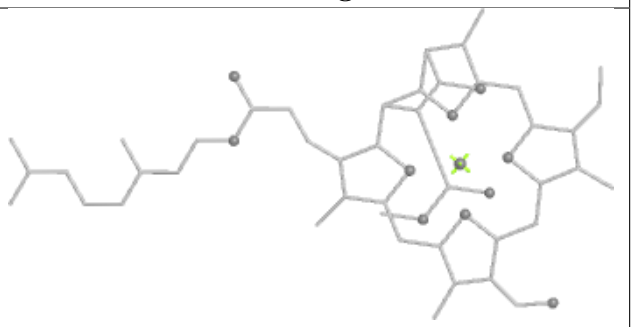
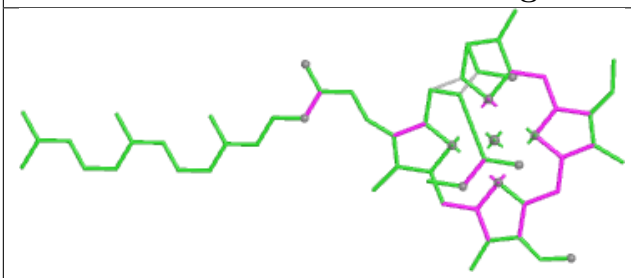


Rings

Ligand CL7 4B 608



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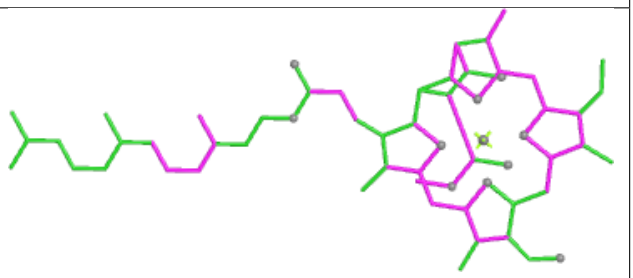

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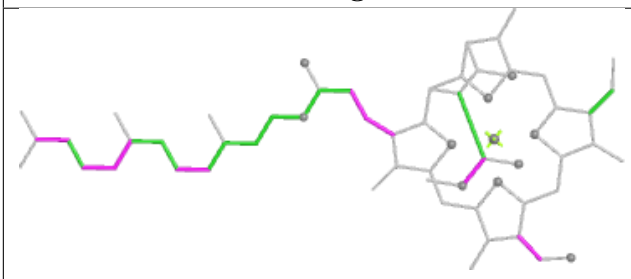

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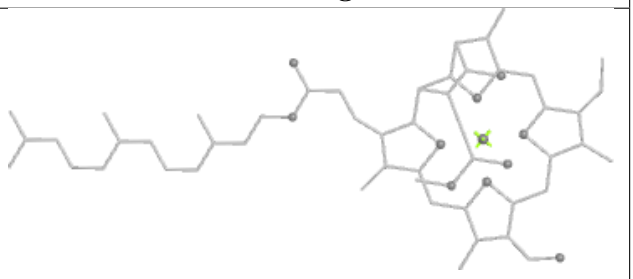
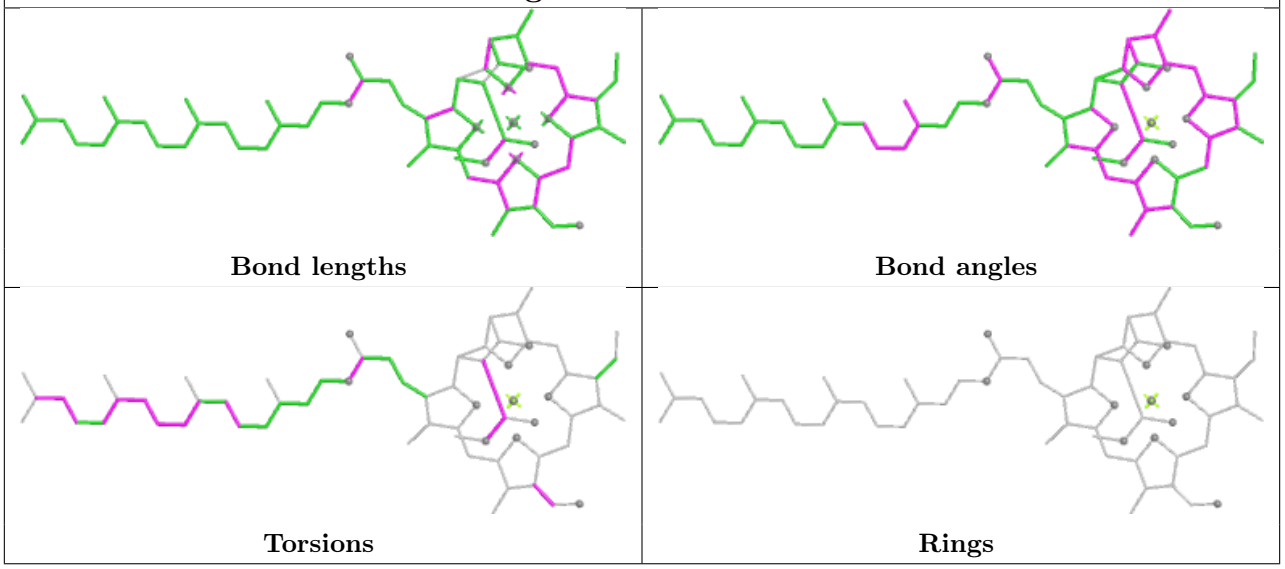
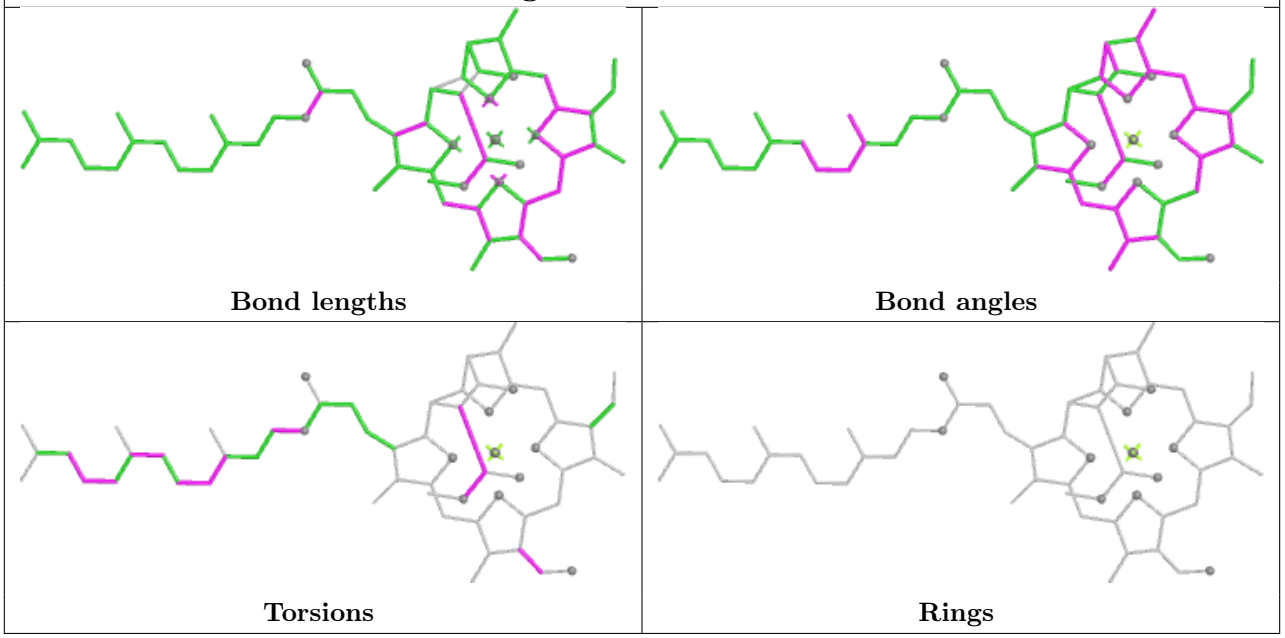


Rings

Ligand CL7 13 509



Ligand CL7 3C 502



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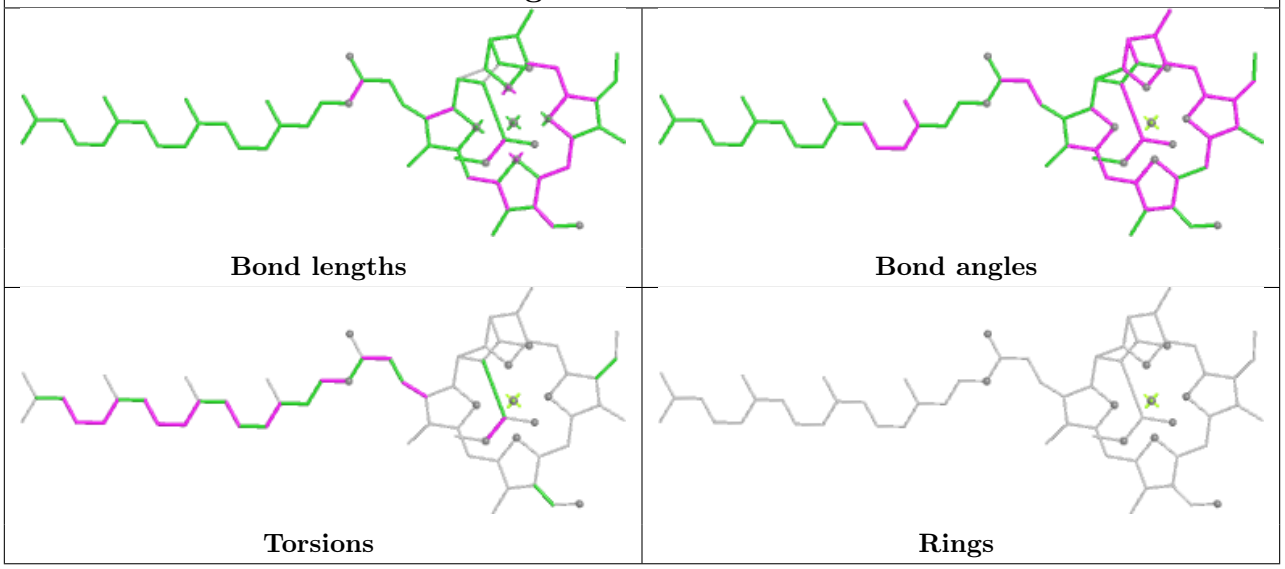

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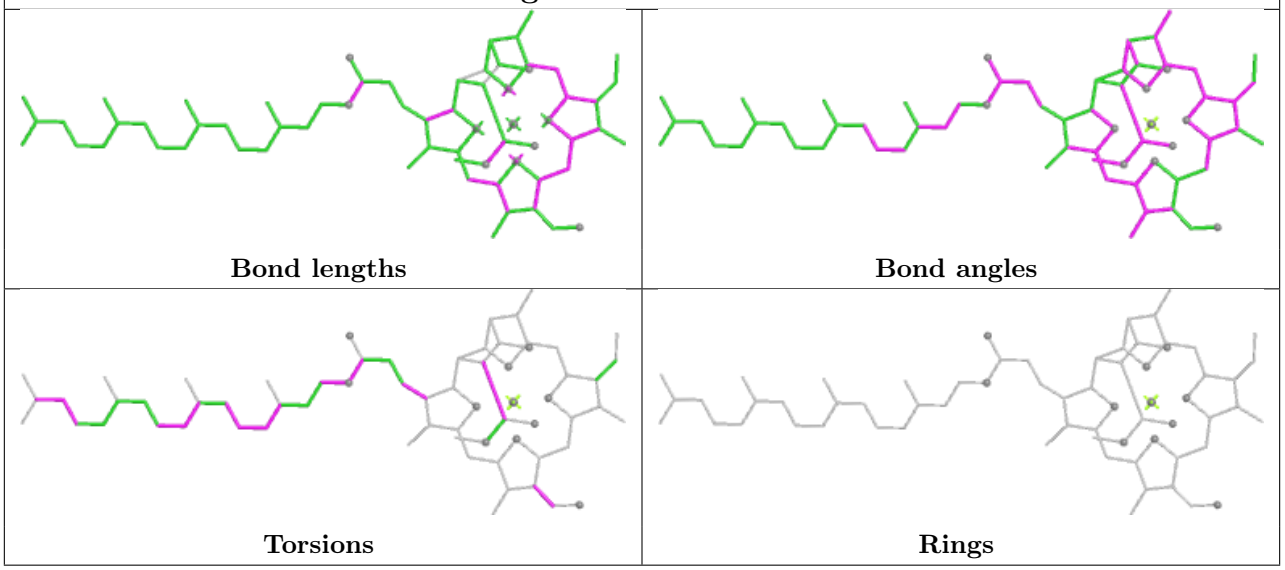

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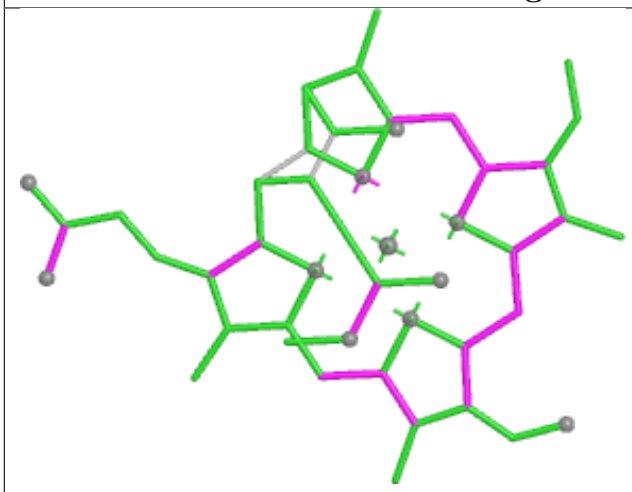
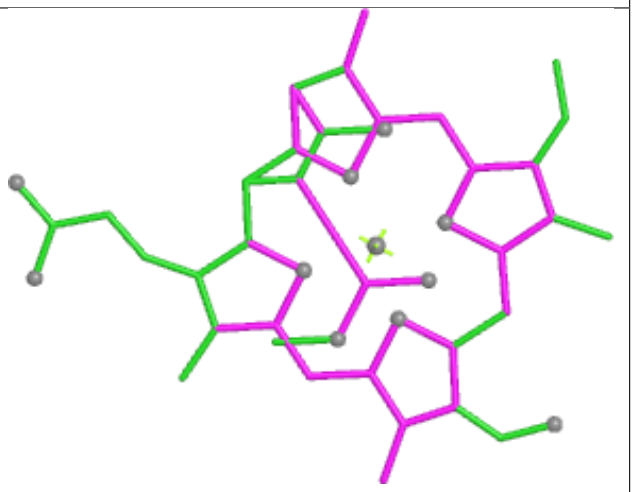
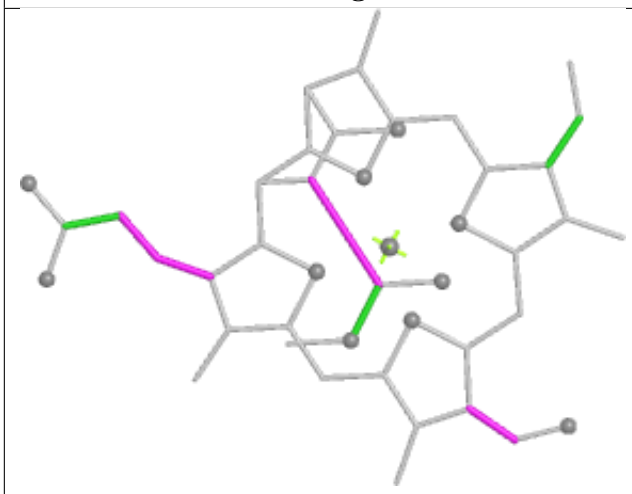


Bond lengths



Bond angles

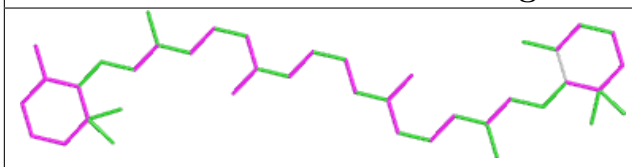


Torsions



Rings

Ligand 8CT 2C 514



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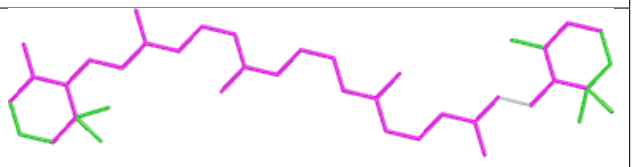
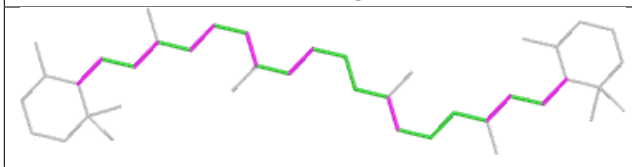
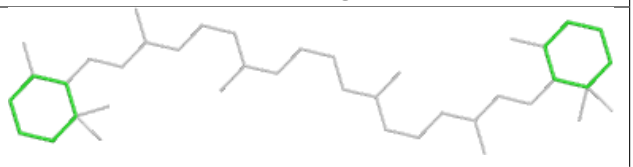


Bond angles

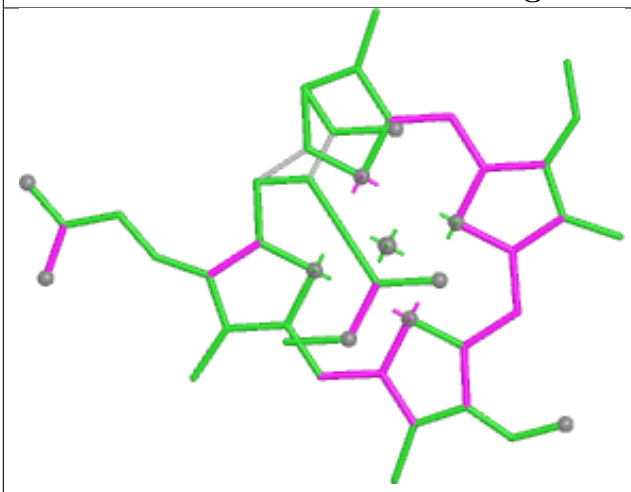


Torsions



Rings

Ligand CL7 32 504



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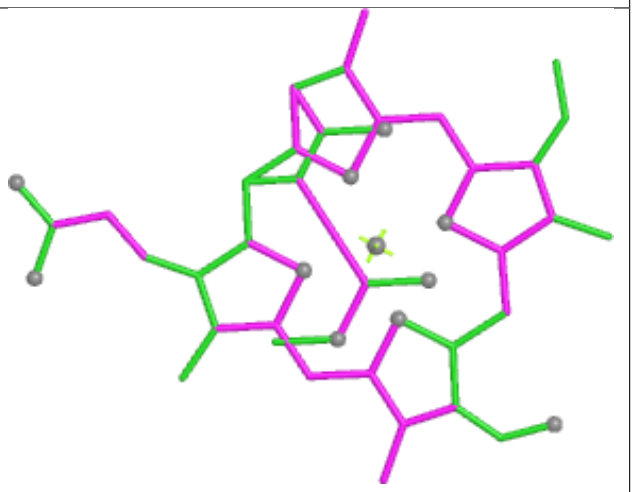
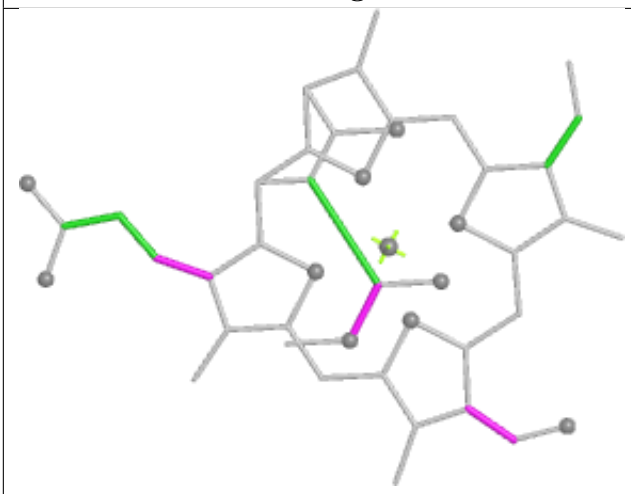


Bond angles

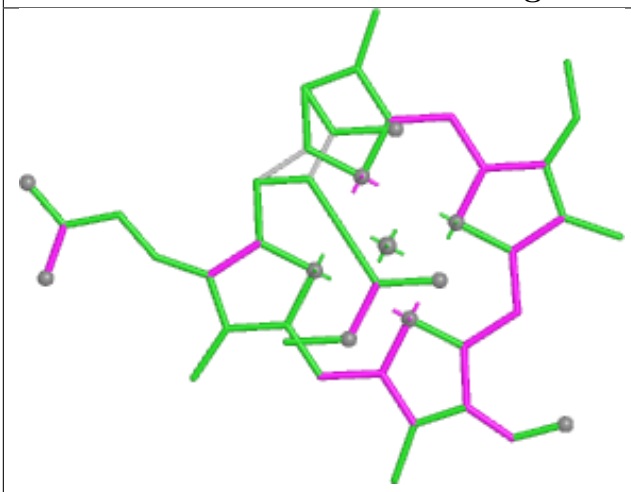


Torsions



Rings

Ligand CL7 14 410



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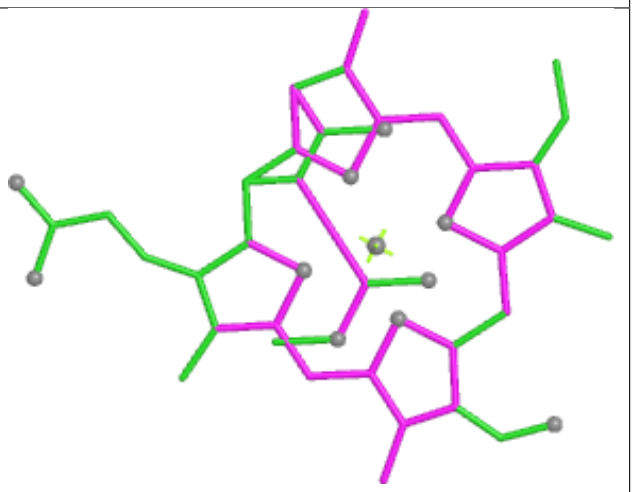

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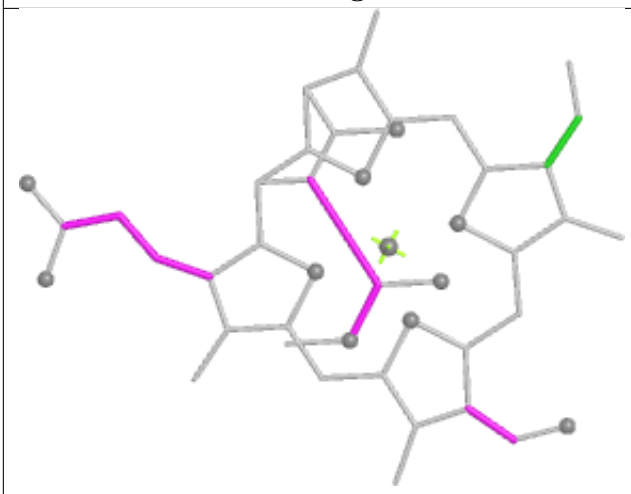
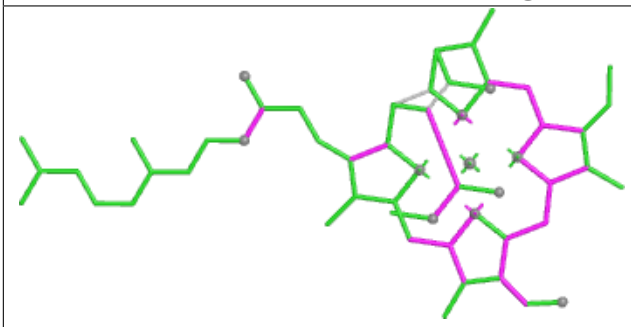


Torsions



Rings

Ligand CL7 4A 403



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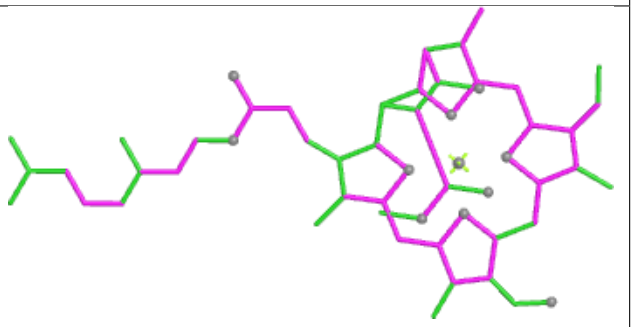

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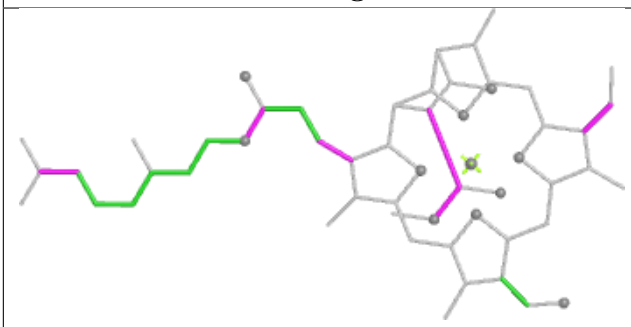

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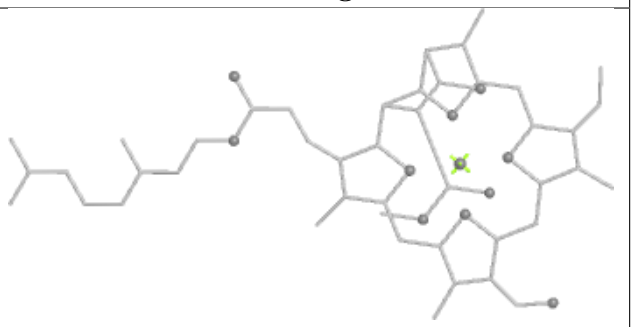
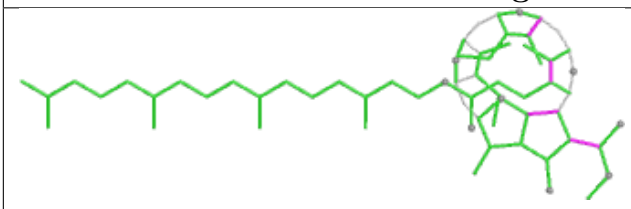


Rings

Ligand PHO 2D 408



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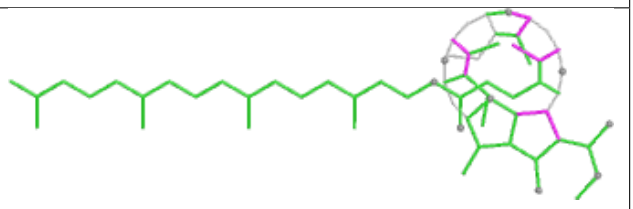

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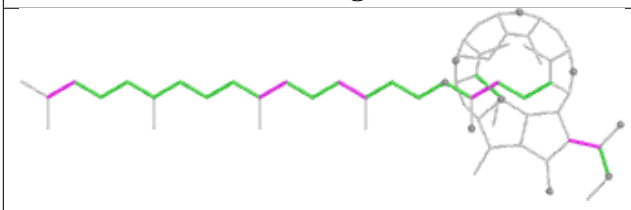

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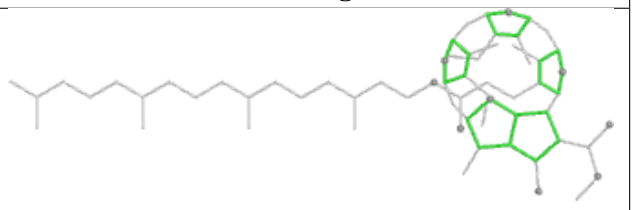
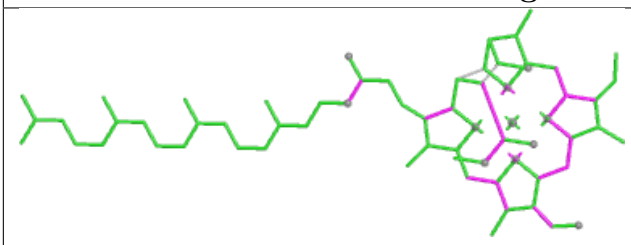


Rings

Ligand CL7 1C 503



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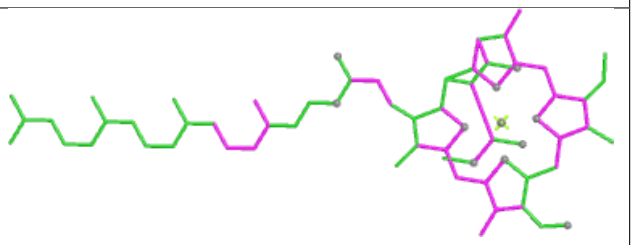

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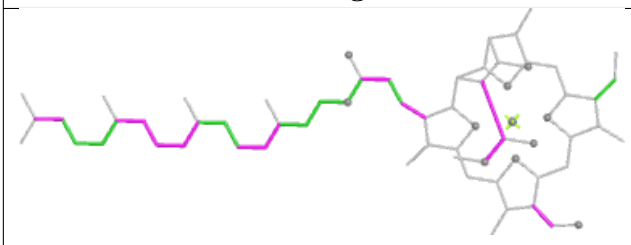

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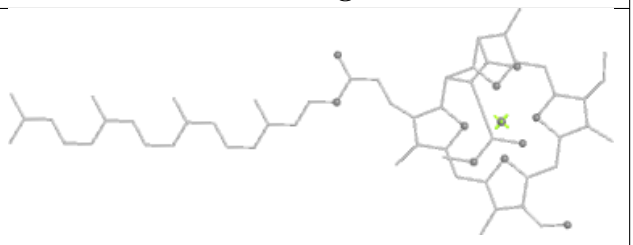
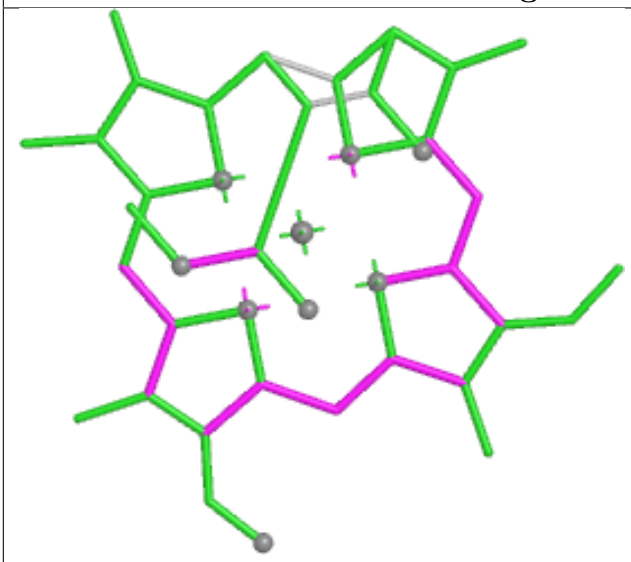


Rings

Ligand CL7 3C 517



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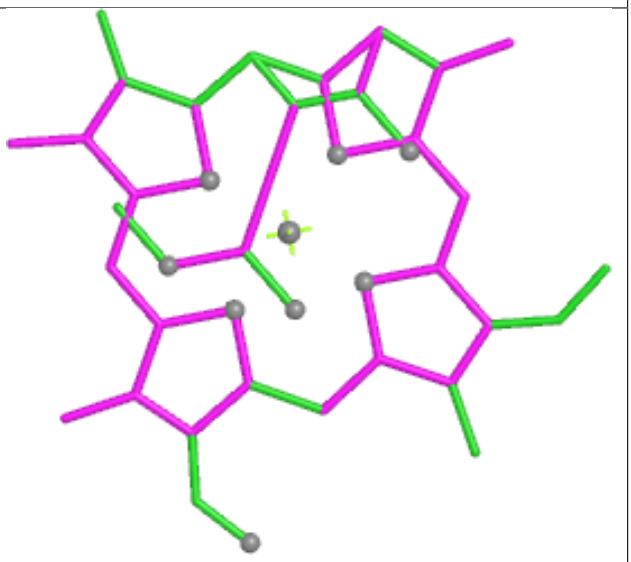

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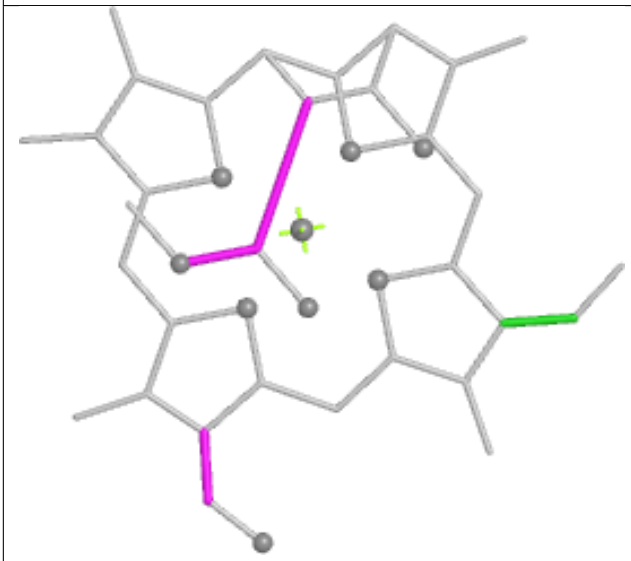

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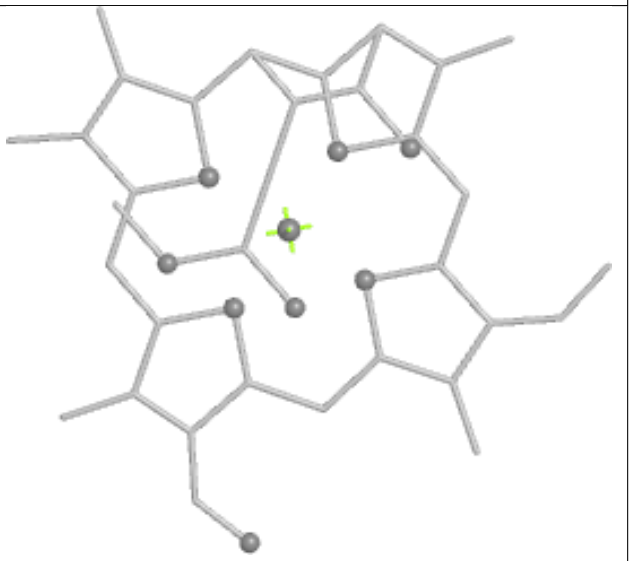
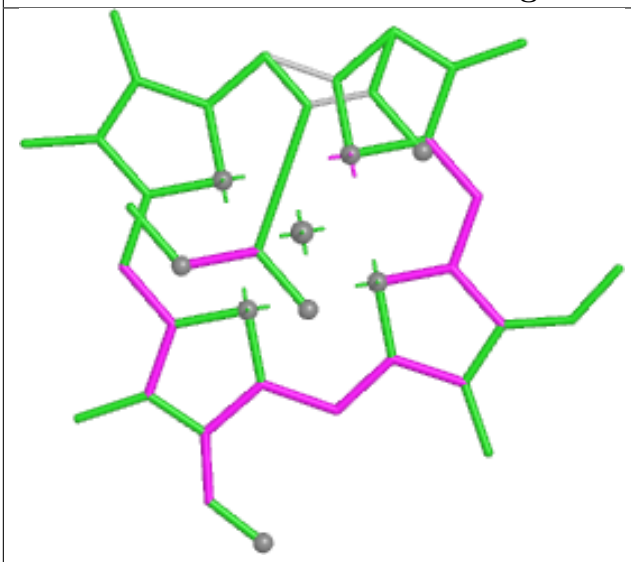


Rings

Ligand CL7 4B 602



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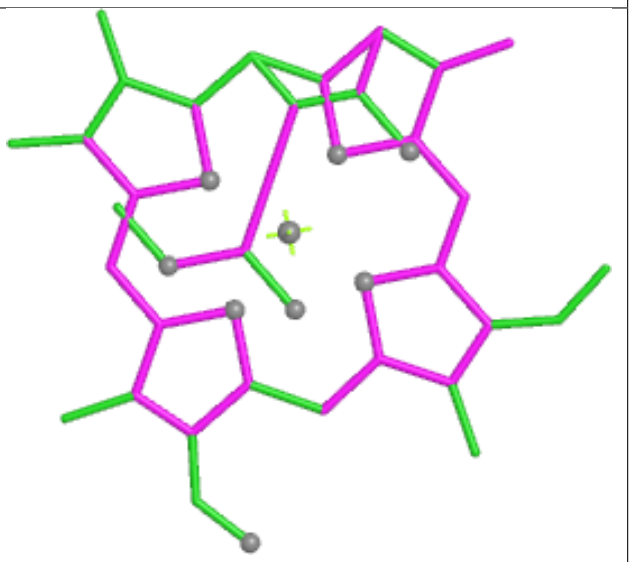
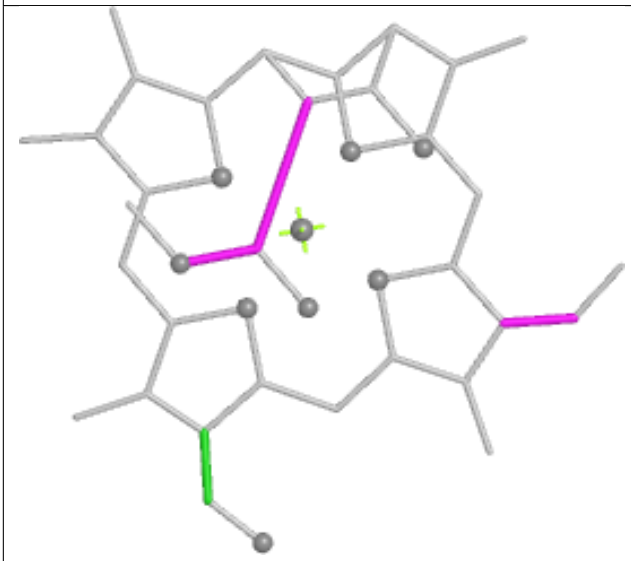


Bond angles



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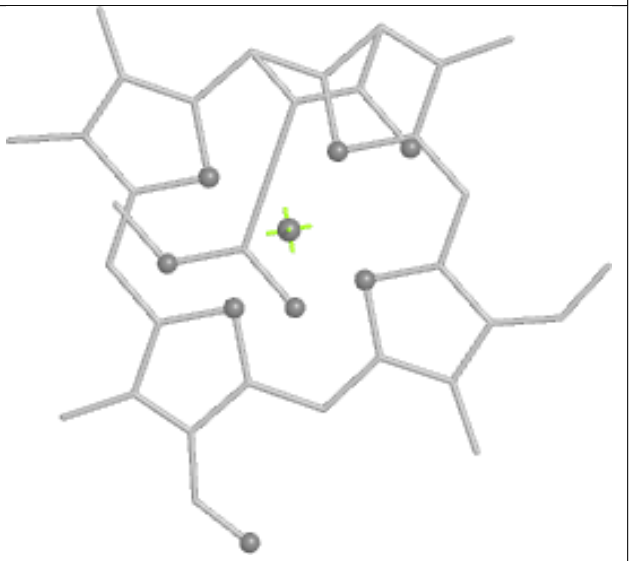
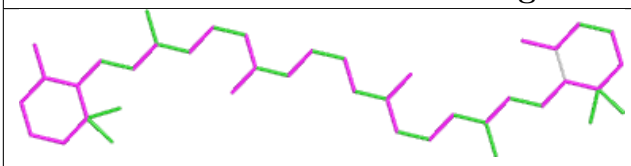


Rings

Ligand 8CT 4B 618



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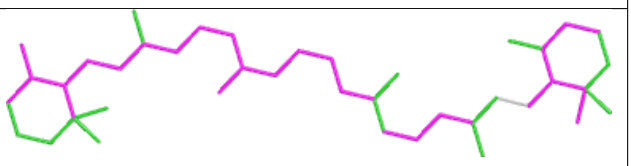

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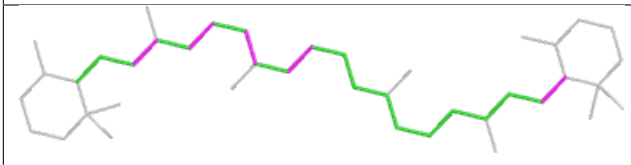

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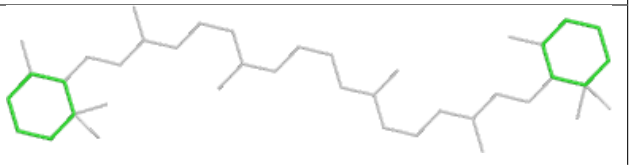
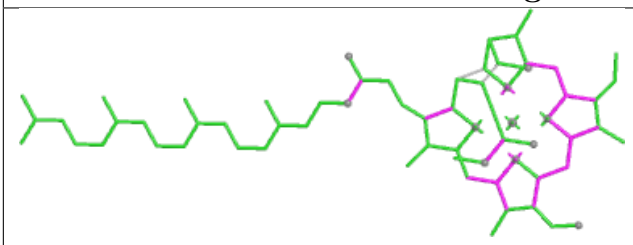


Rings

Ligand CL7 23 411



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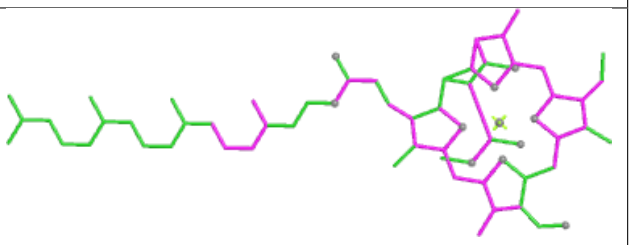
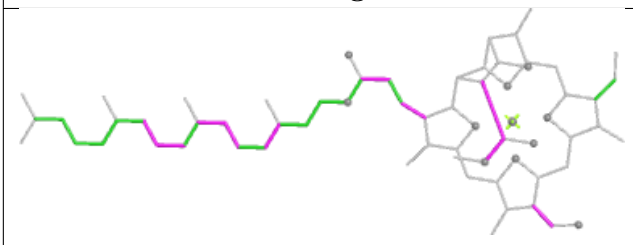


Bond angles



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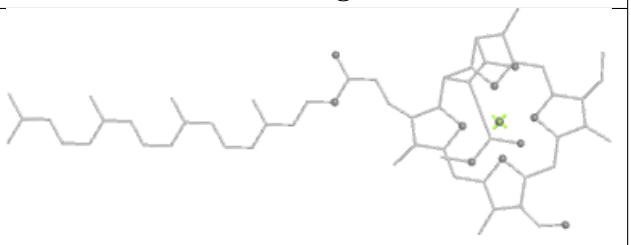


Rings

Ligand PL9 1D 407



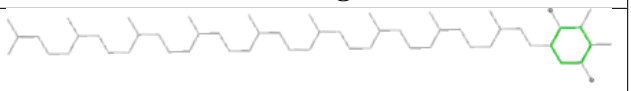
Bond lengths



Bond angles

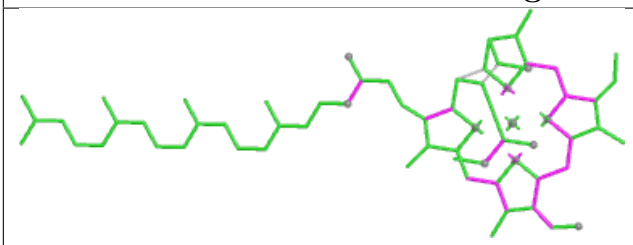


Torsions



Rings

Ligand CL7 21 418



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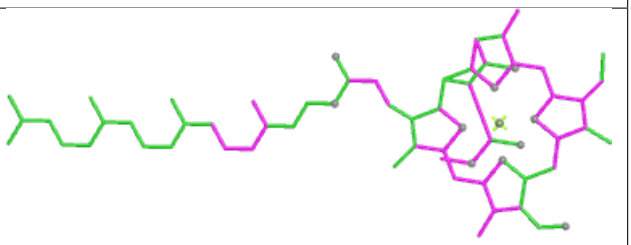
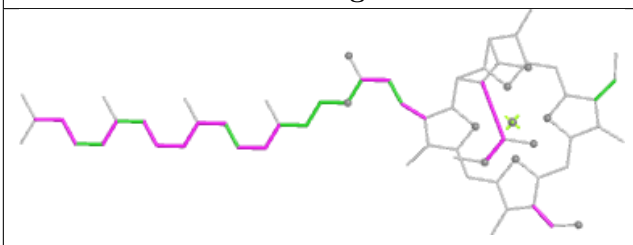


Bond angles



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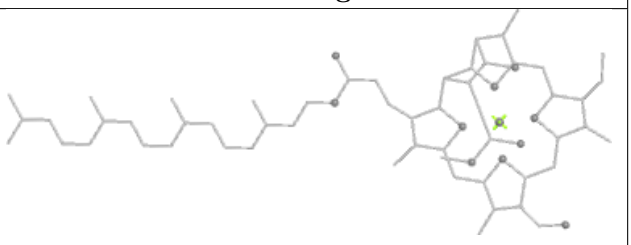
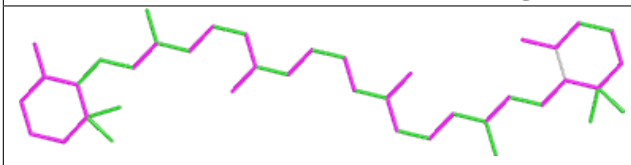


Rings

Ligand 8CT 2D 406



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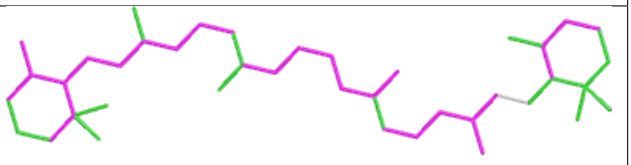
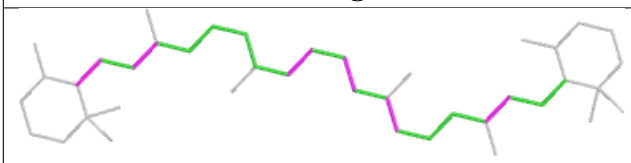


Bond angles



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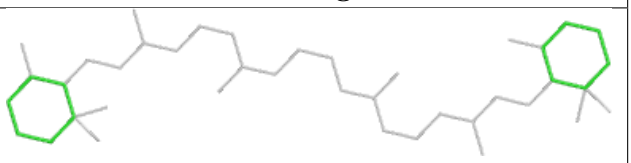
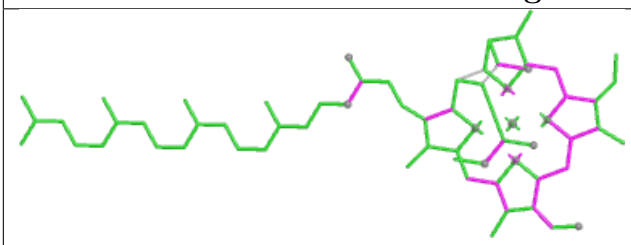


Rings

Ligand CL7 43 402



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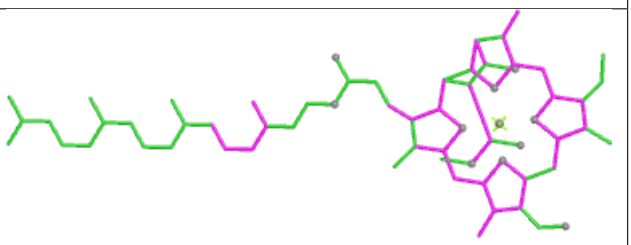
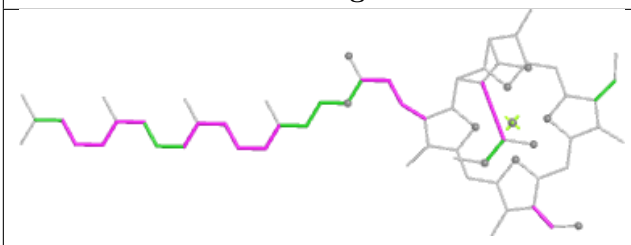


Bond angles



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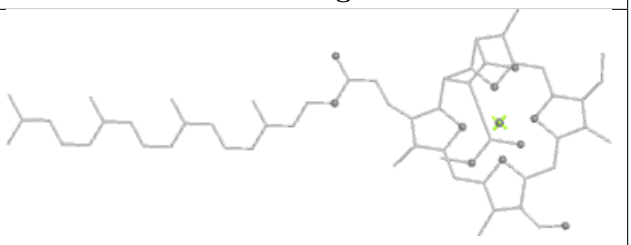
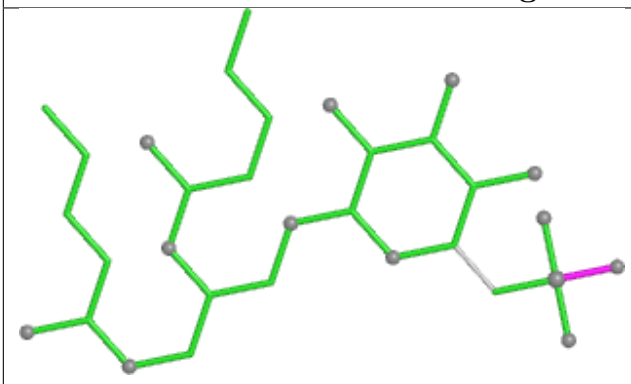


Rings

Ligand SQD 21 423



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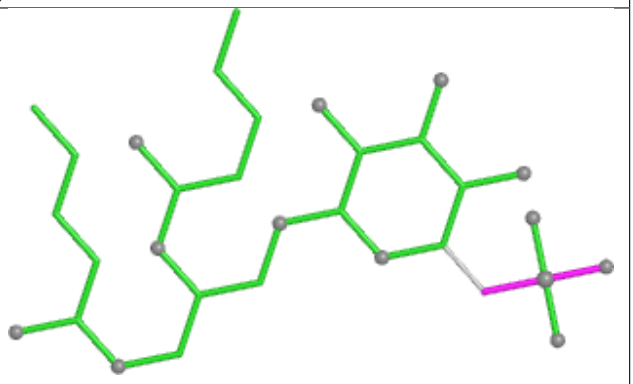
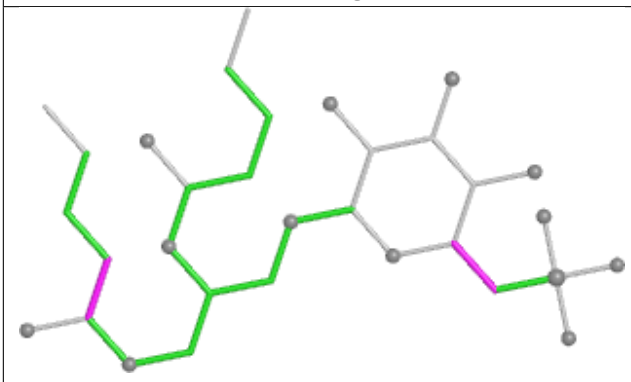


Bond angles



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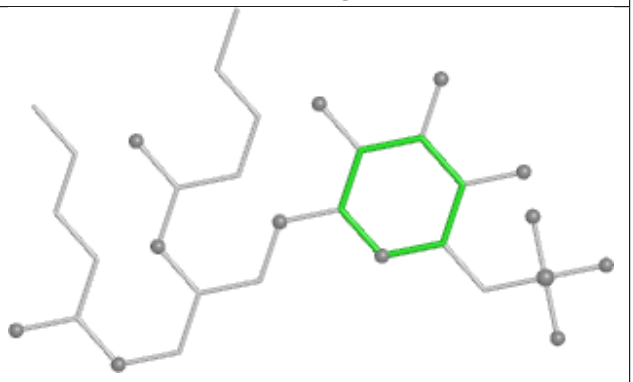
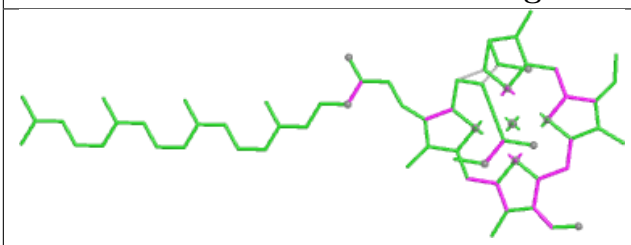


Rings

Ligand CL7 42 512



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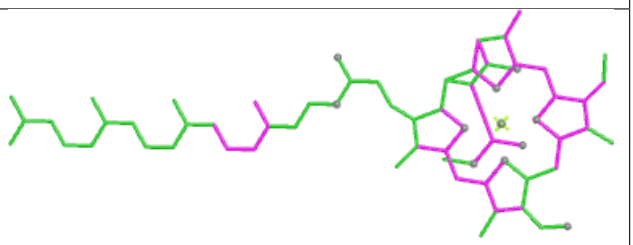
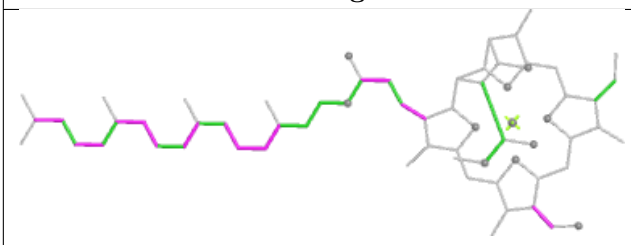


Bond angles



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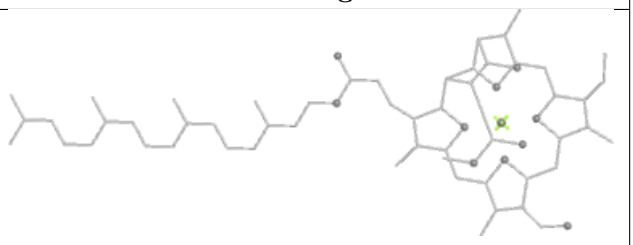
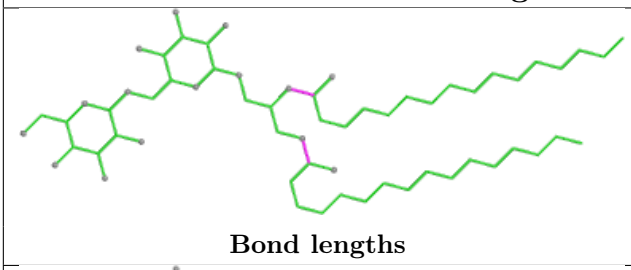


Rings

Ligand DGD 2C 516



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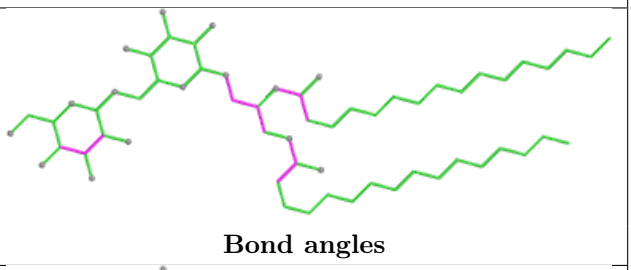
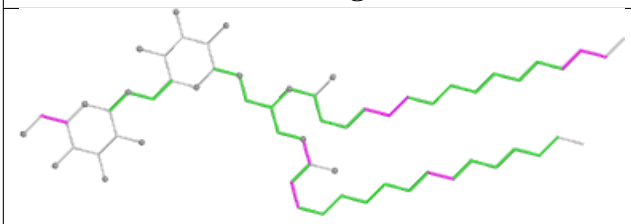
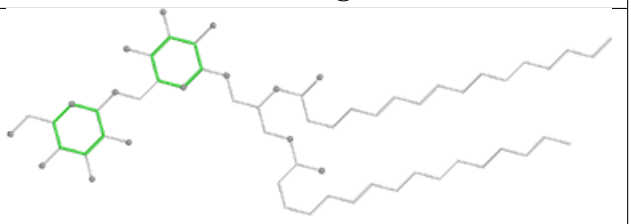


Bond angles

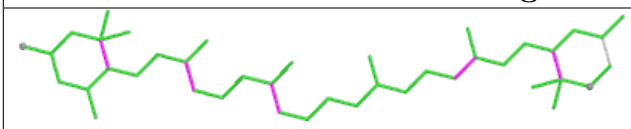


Torsions

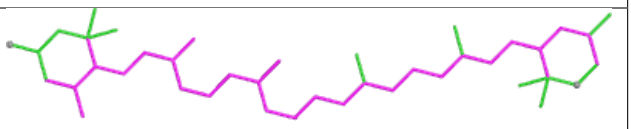


Rings

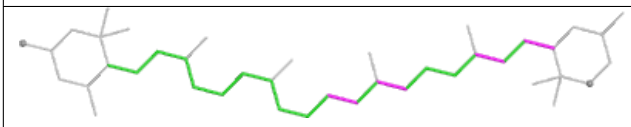
Ligand ZEX 33 525



Bond lengths



Bond angles



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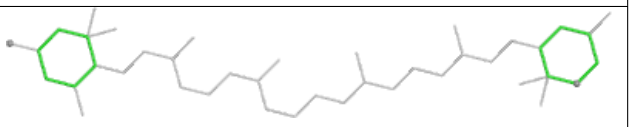
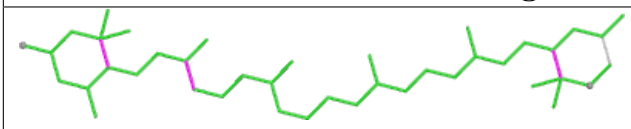


Rings

Ligand ZEX 44 420



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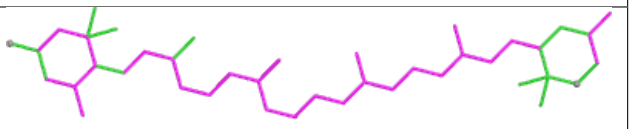
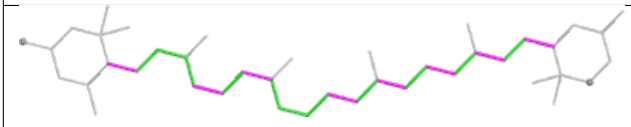


Bond angles



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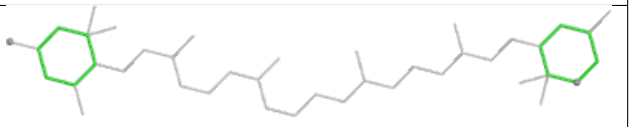
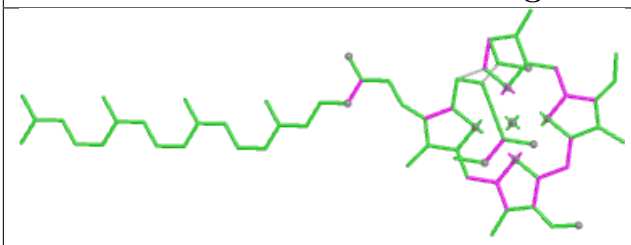


Rings

Ligand CL7 33 509



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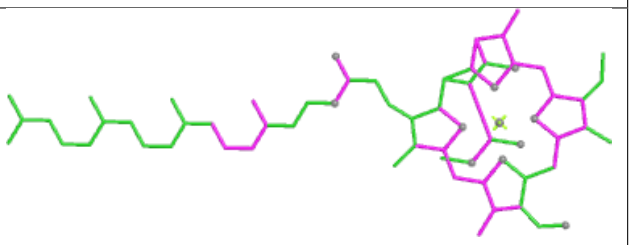
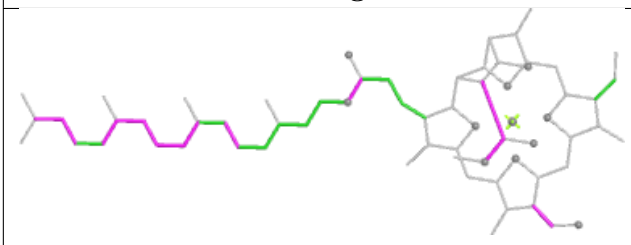


Bond angles



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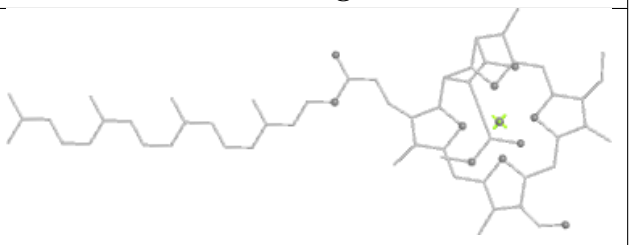
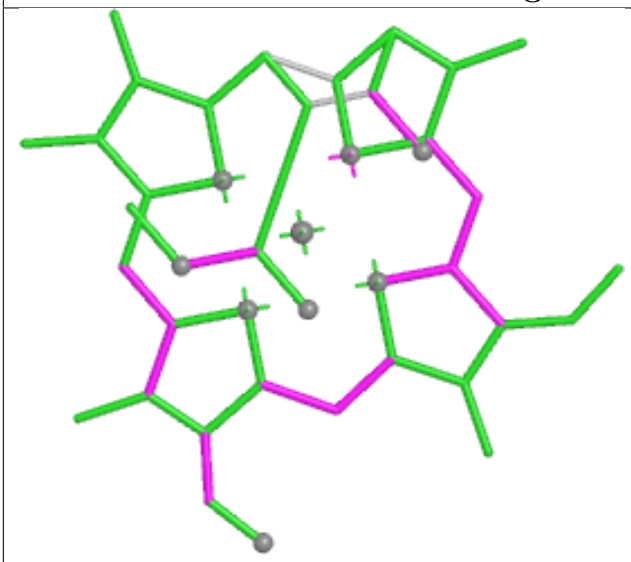


Rings

Ligand CL7 11 414



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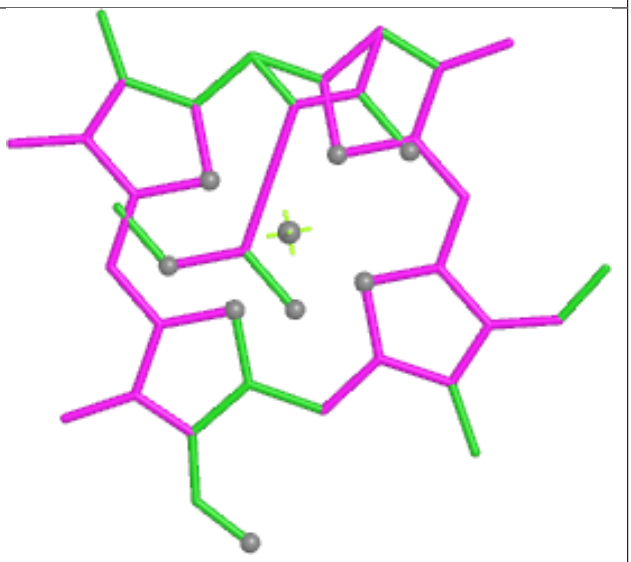
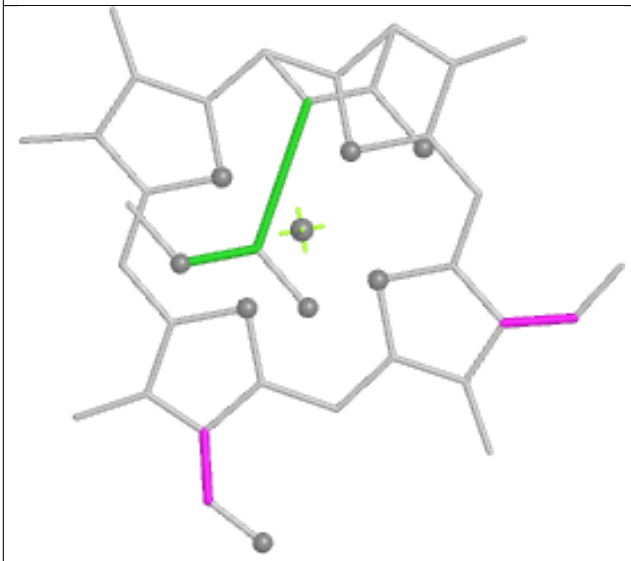


Bond angles



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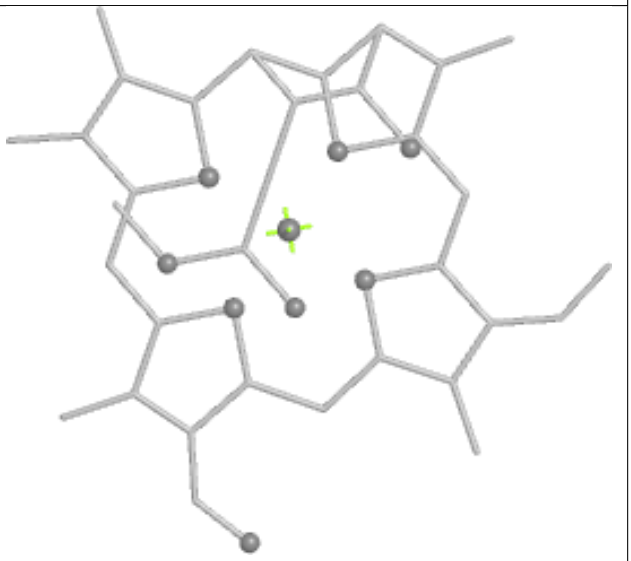
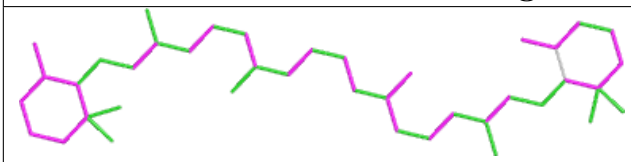


Rings

Ligand 8CT 1C 518



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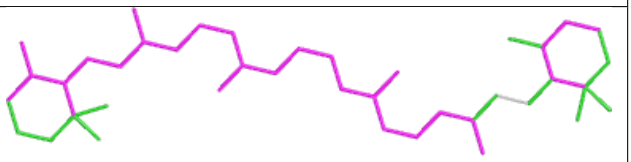
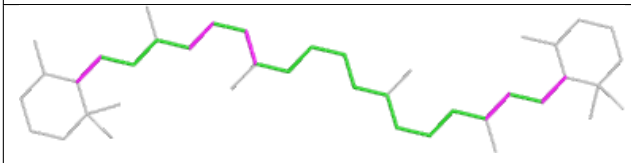


Bond angles



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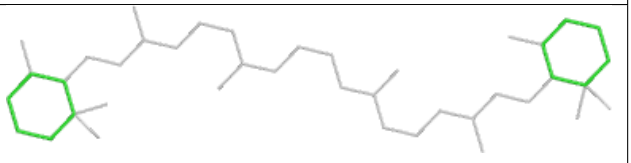
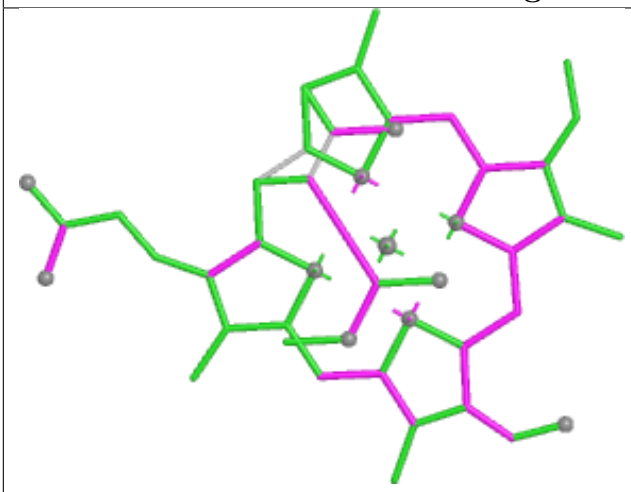


Rings

Ligand CL7 34 415



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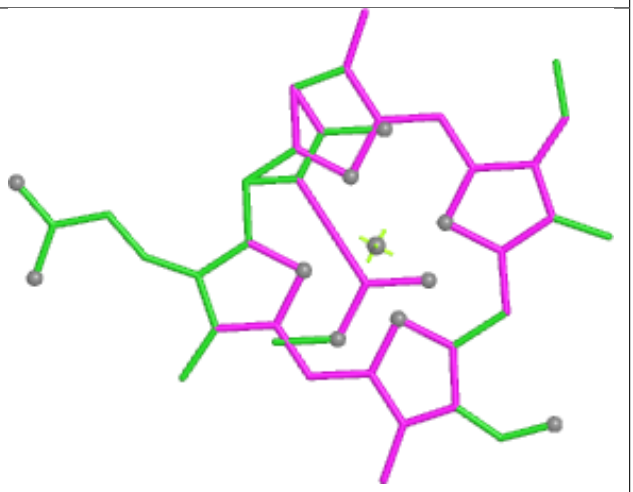
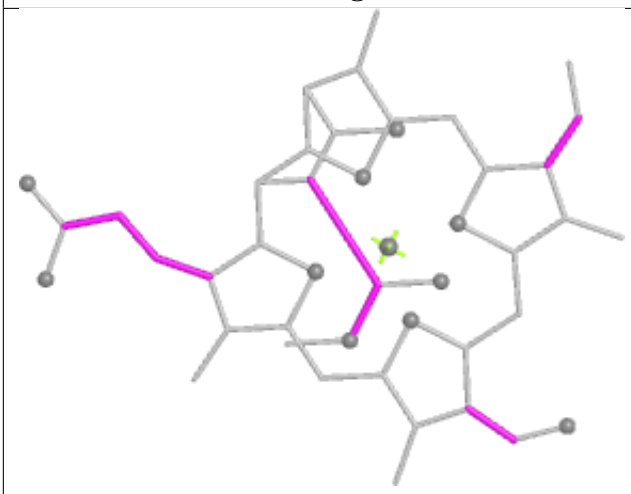


Bond angles

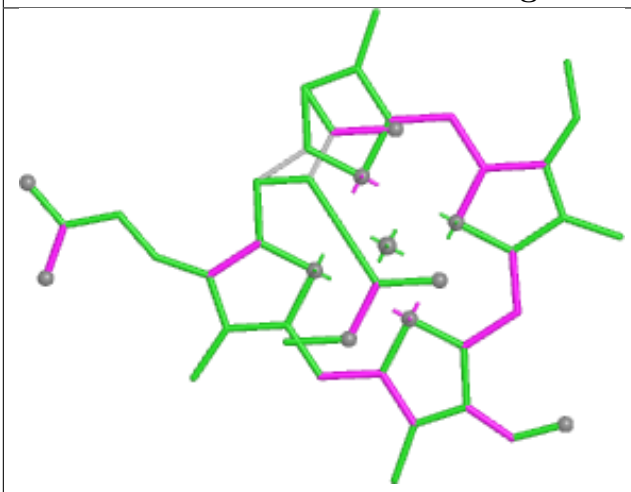


Torsions



Rings

Ligand CL7 2B 623



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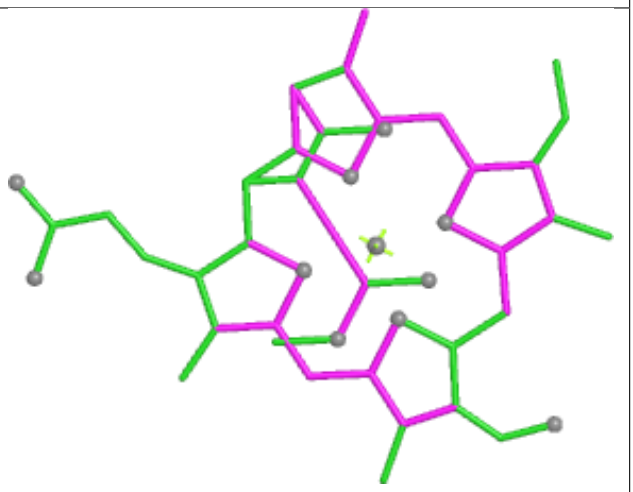
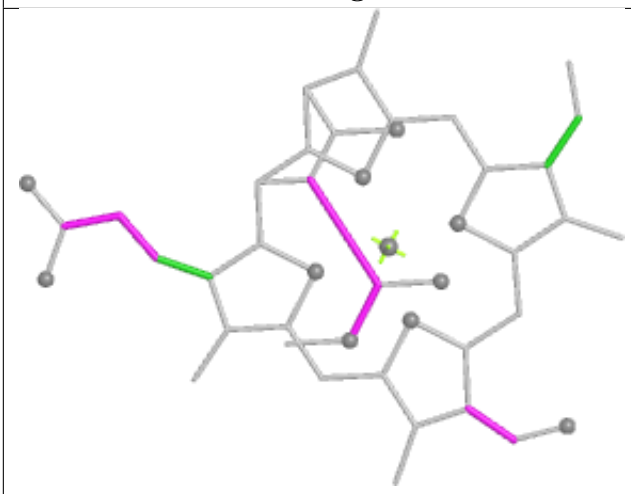


Bond angles



Torsions

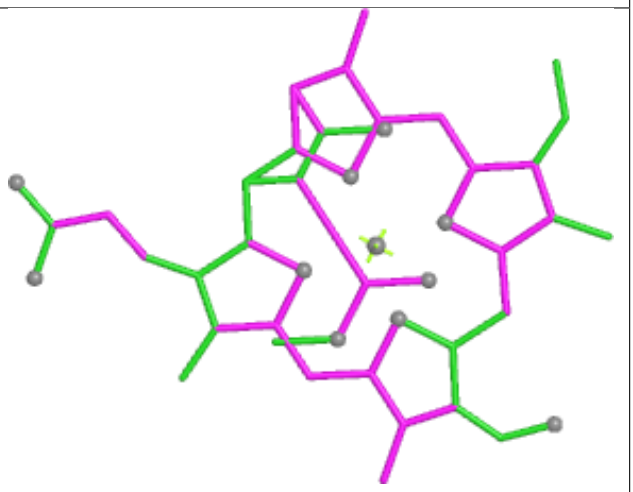


Rings

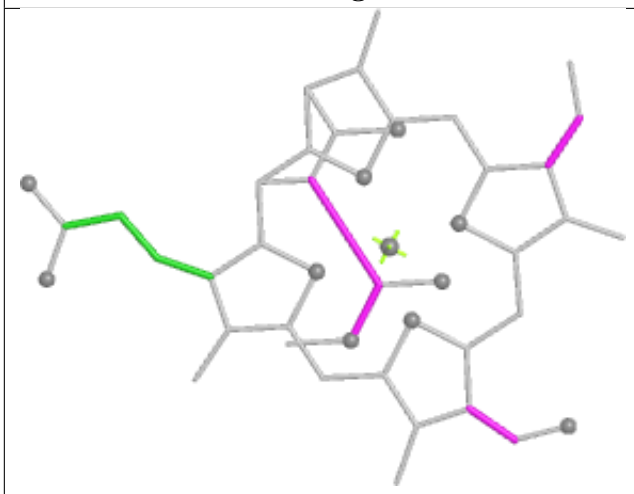
Ligand CL7 31 420



Bond lengths



Bond angles

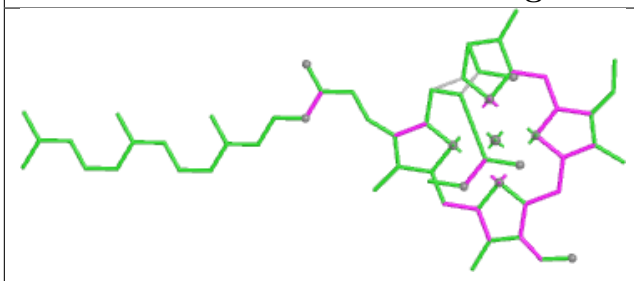


Torsions



Rings

Ligand CL7 21 403



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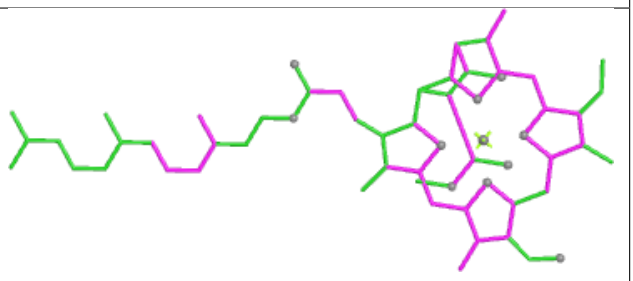
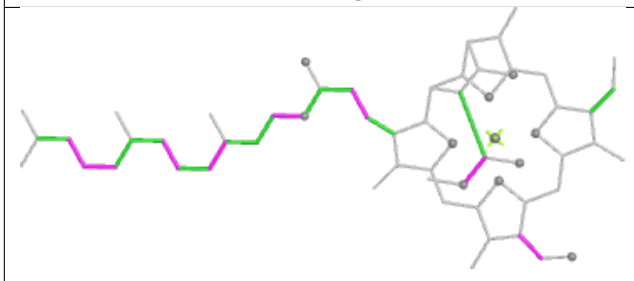


Bond angles



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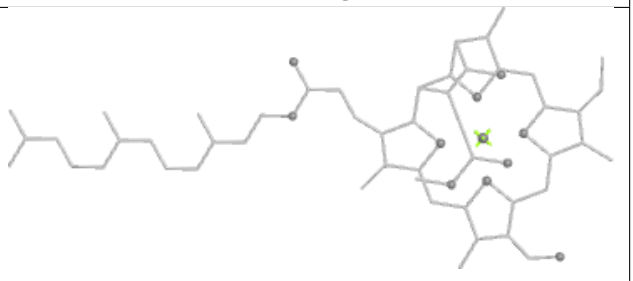
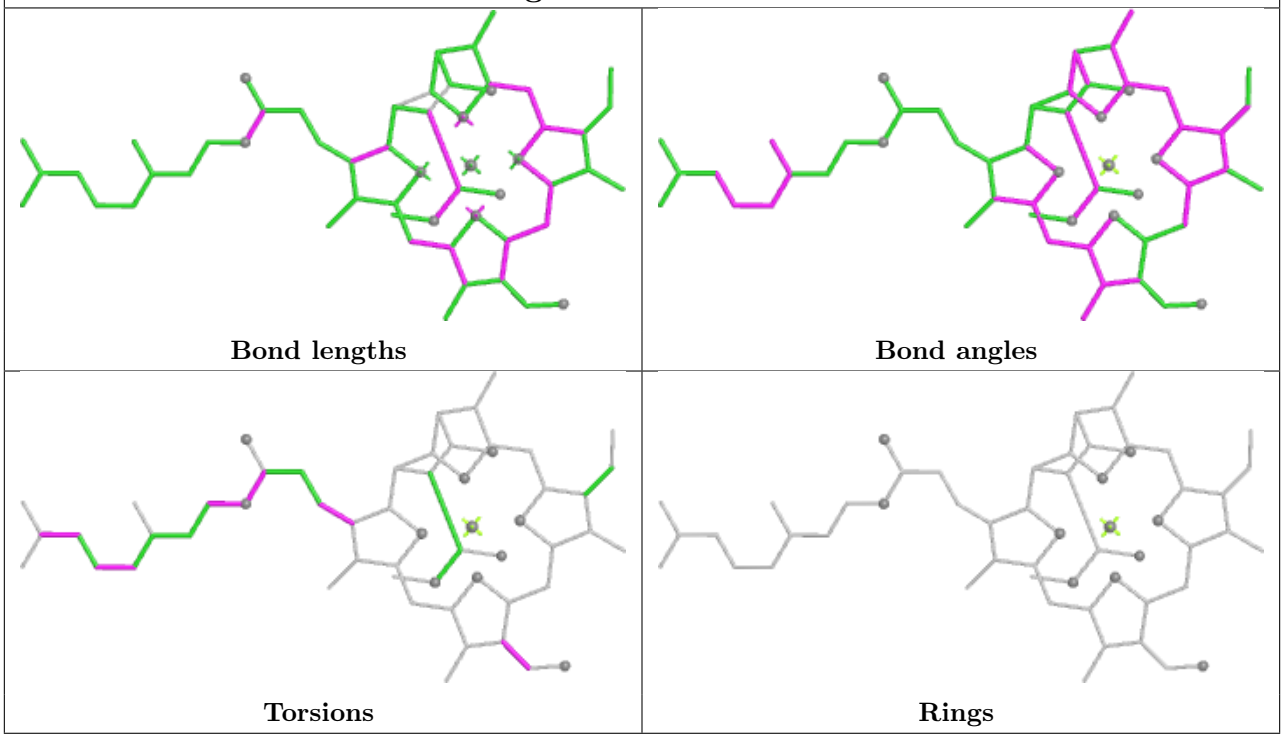
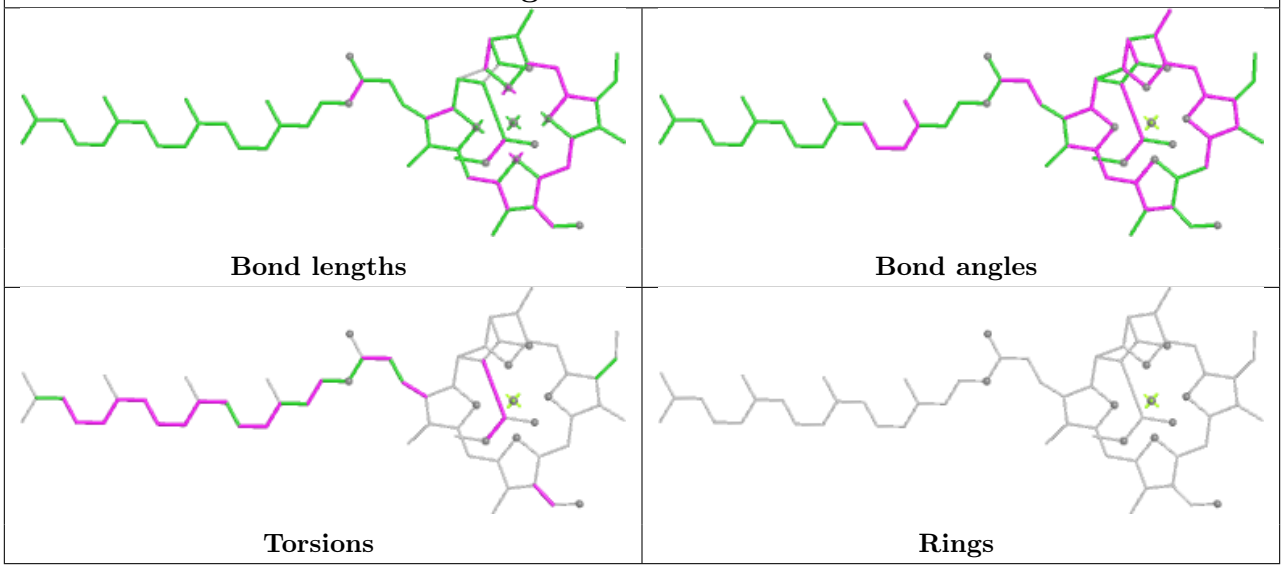


Rings

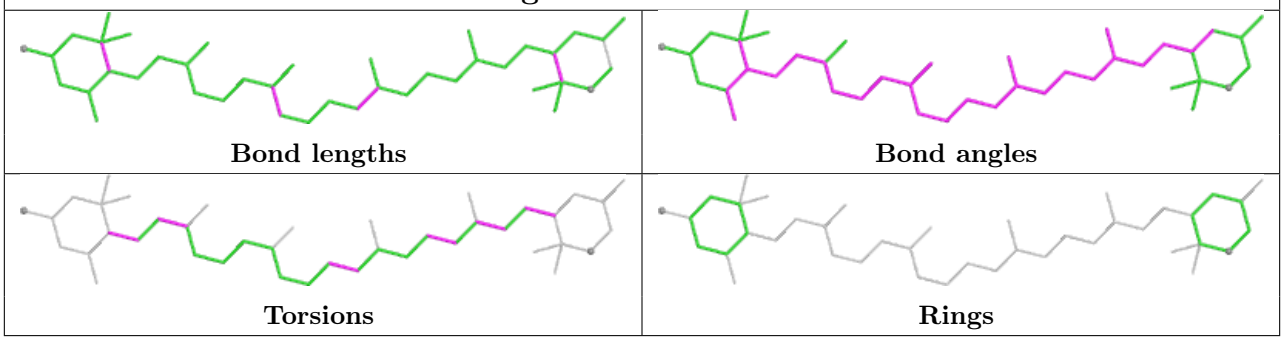
Ligand CL7 21 417



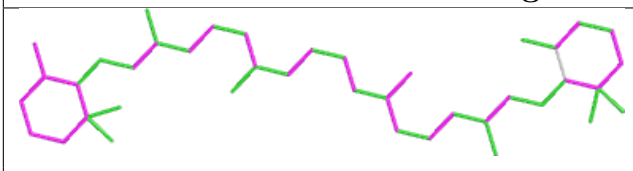
Ligand CL7 3C 510



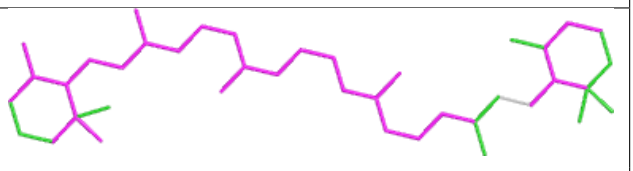
Ligand ZEX 34 403



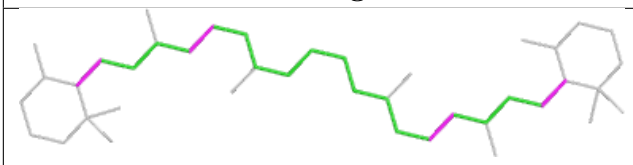
Ligand 8CT 34 402



Bond lengths



Bond angles



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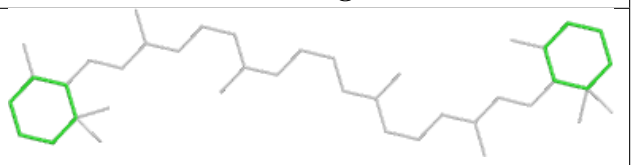
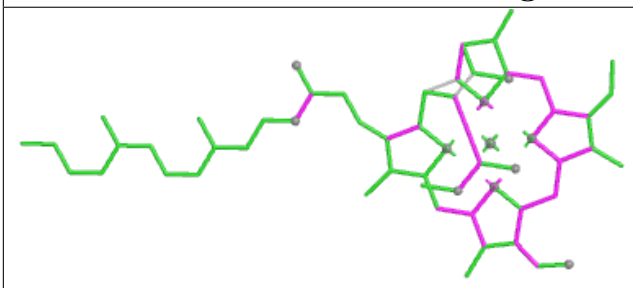


Rings

Ligand CL7 4D 404



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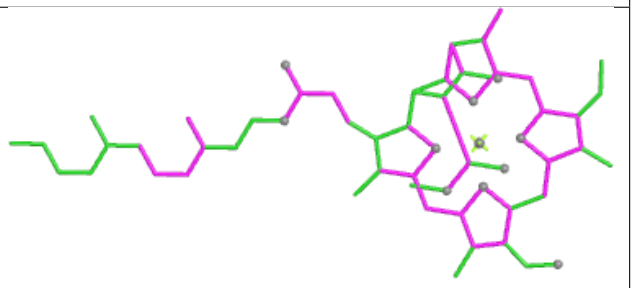
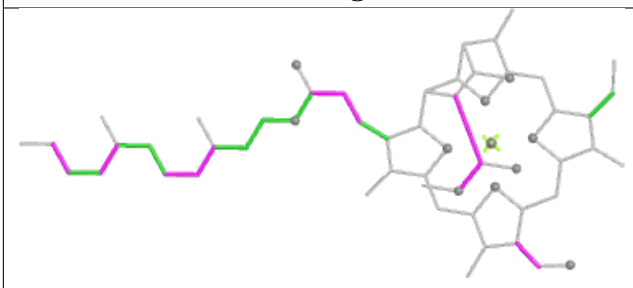


Bond angles



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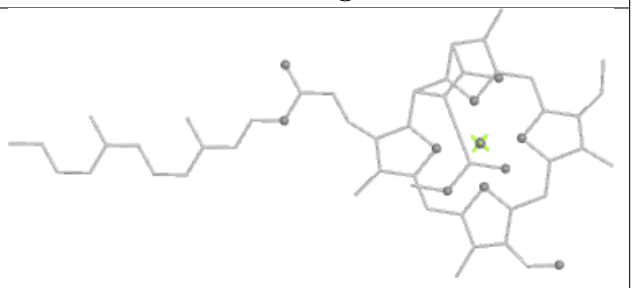
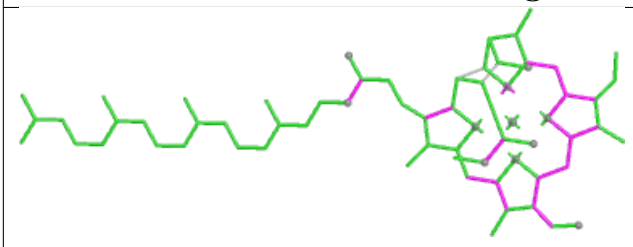


Rings

Ligand CL7 34 405



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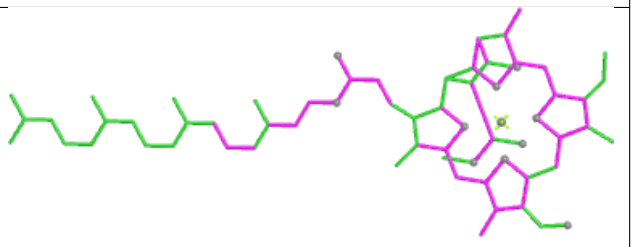
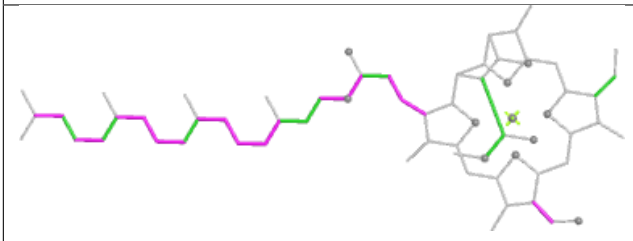


Bond angles



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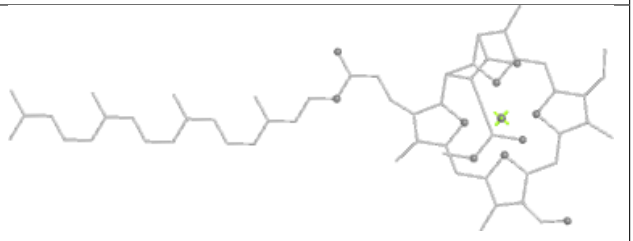
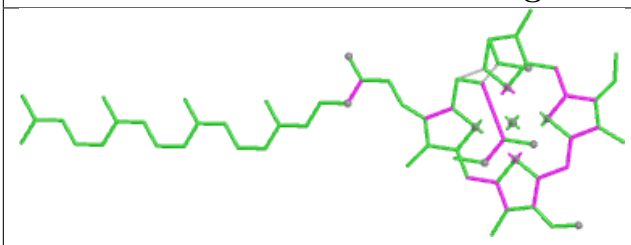


Rings

Ligand CL7 23 408



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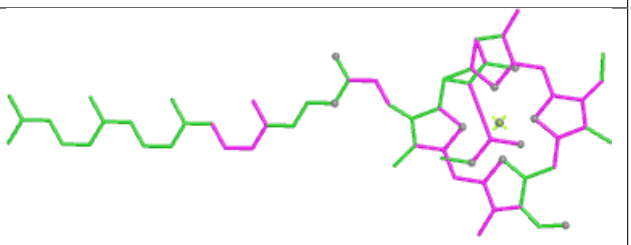

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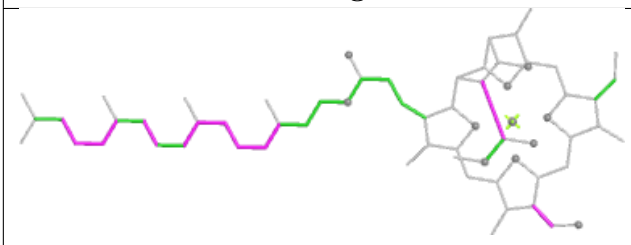

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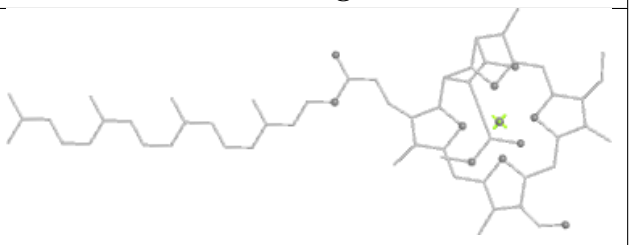
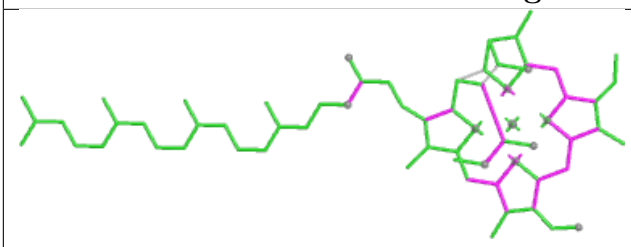


Rings

Ligand CL7 43 412



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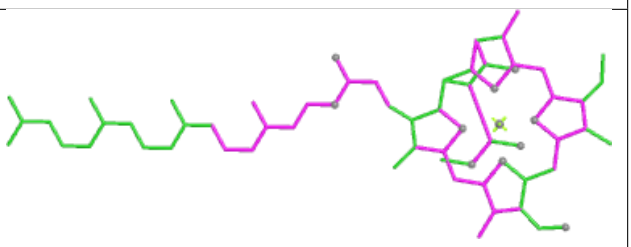
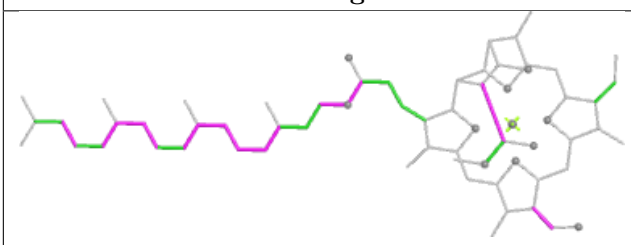


Bond angles



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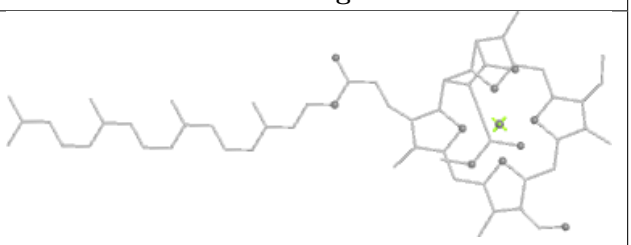
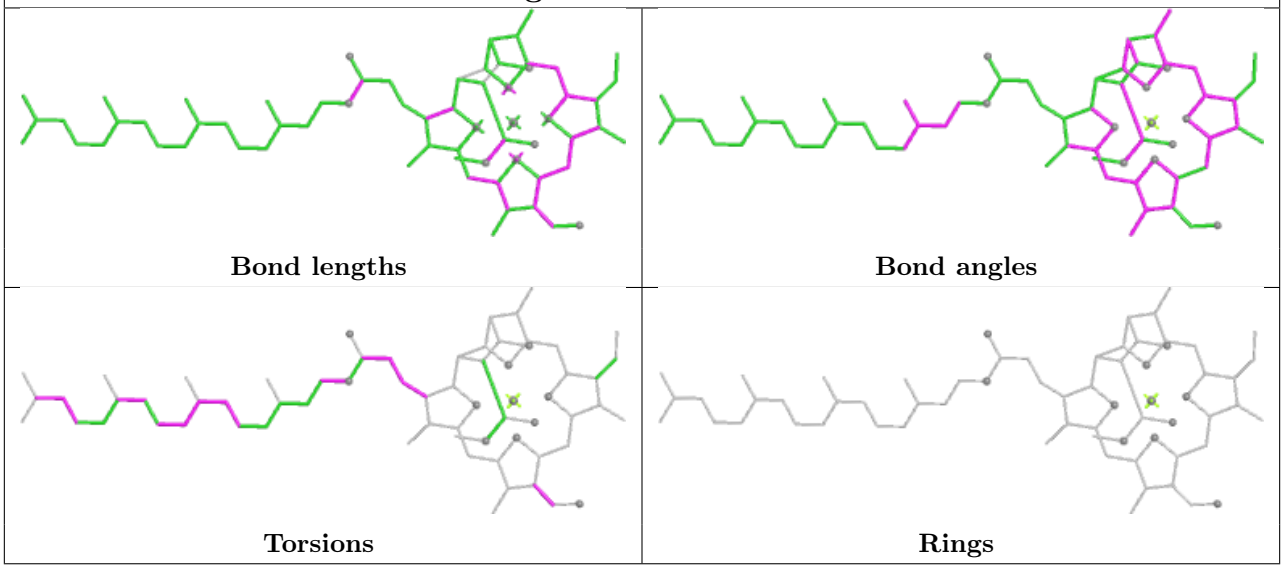
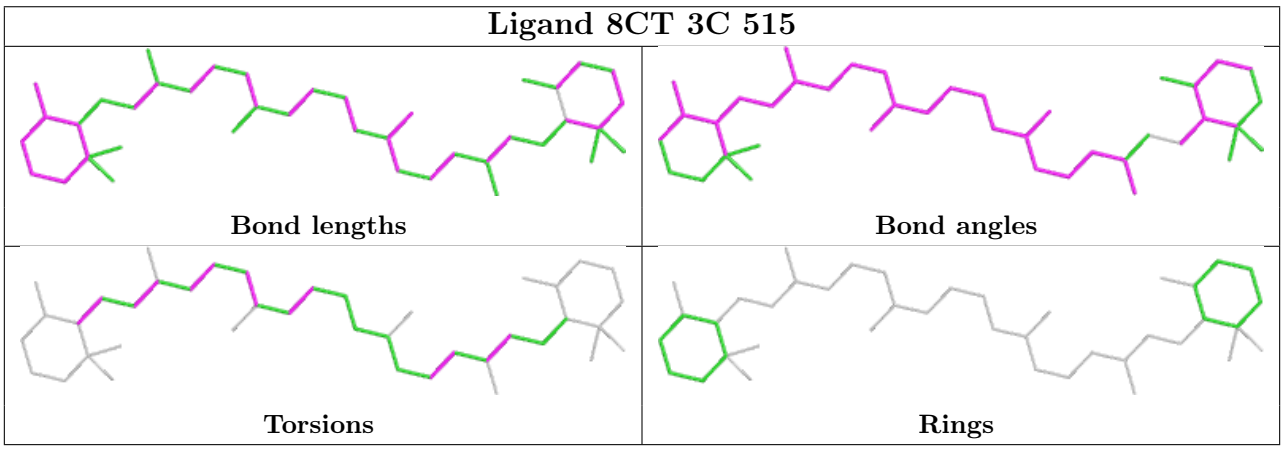


Rings

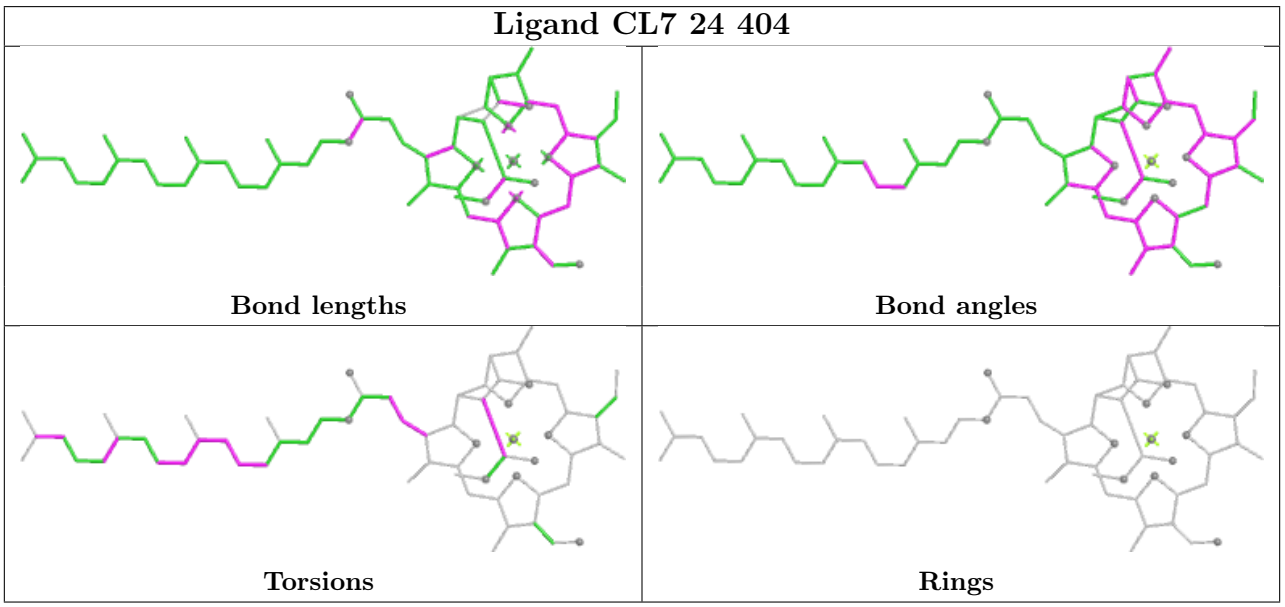
Ligand CL7 42 501



Ligand 8CT 3C 515



Ligand CL7 24 404



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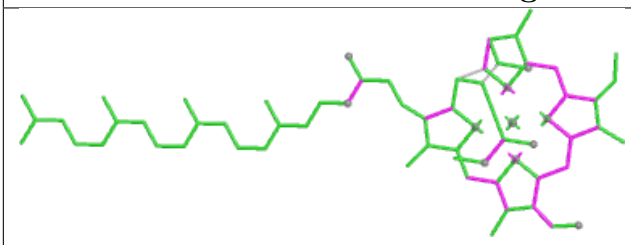
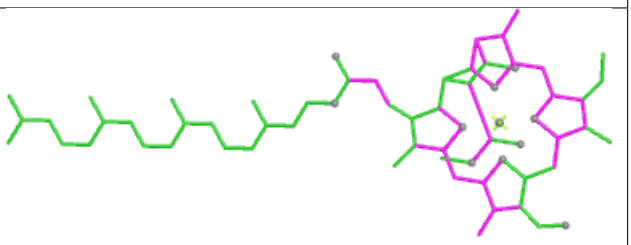
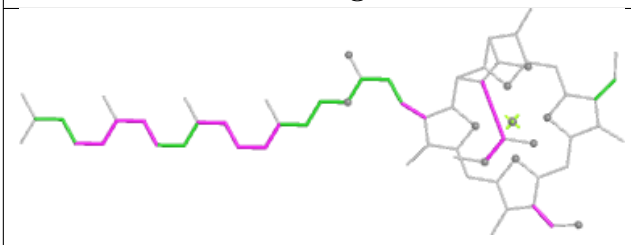


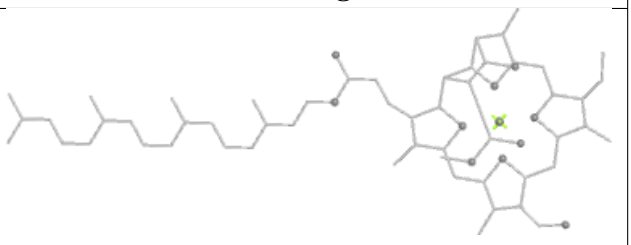
Bond lengths



Bond angles

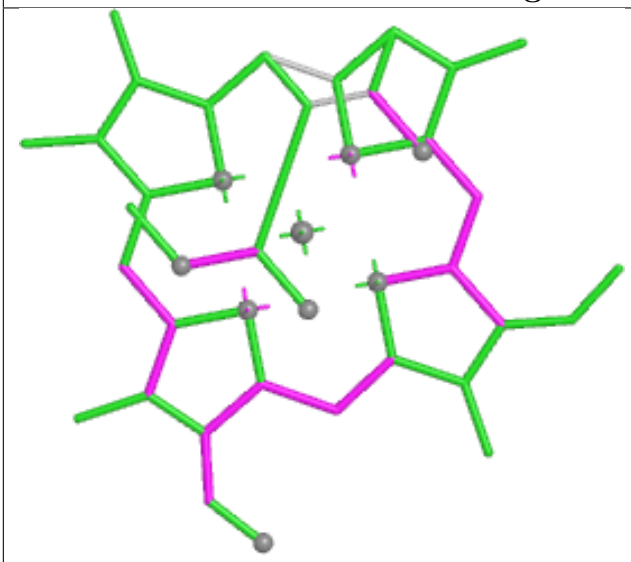


Torsions



Rings

Ligand CL7 14 416



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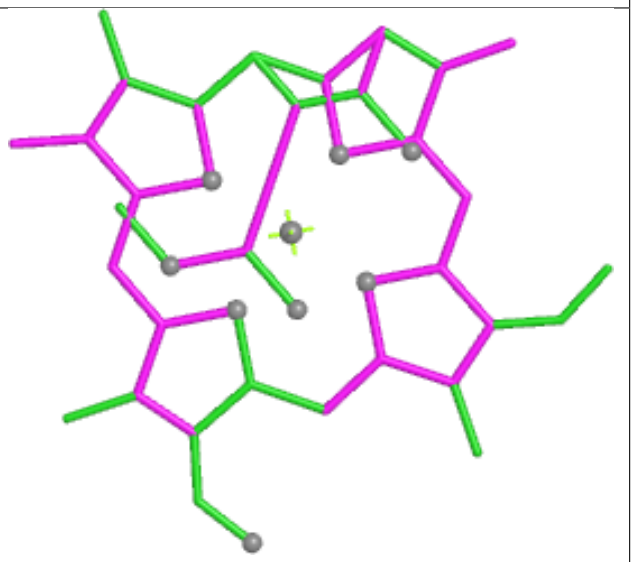

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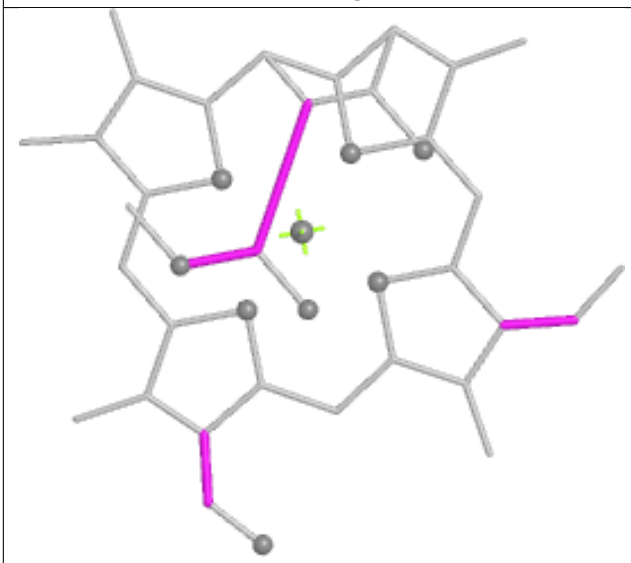

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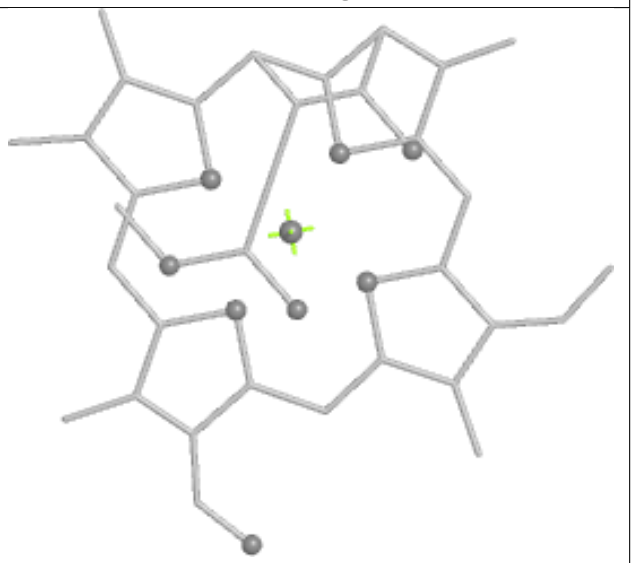

Rings

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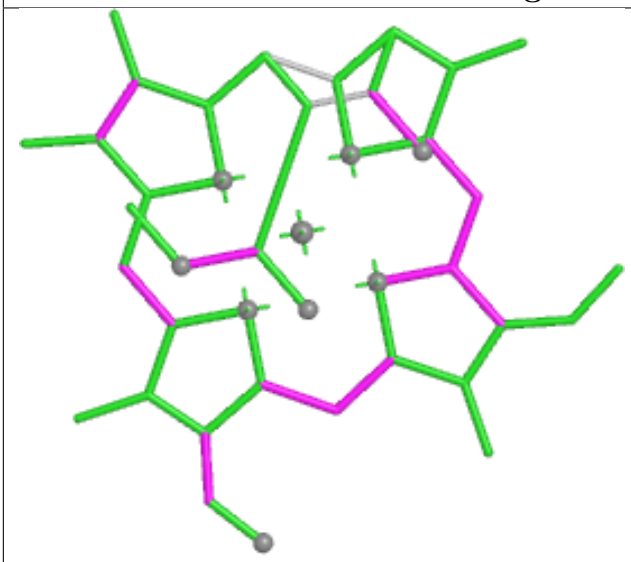

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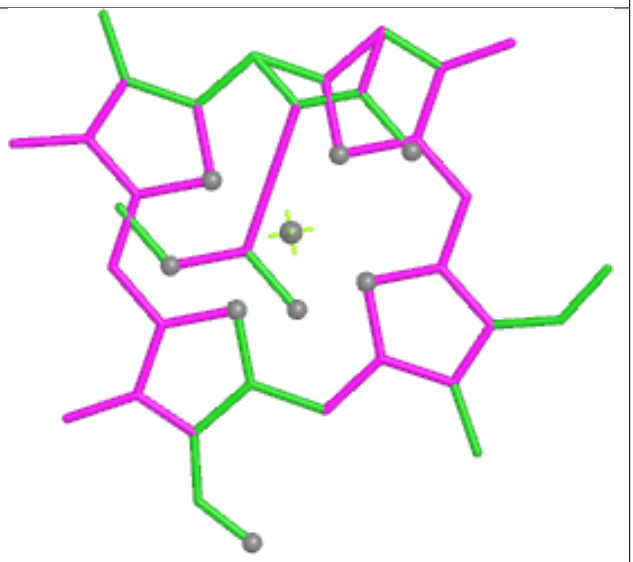

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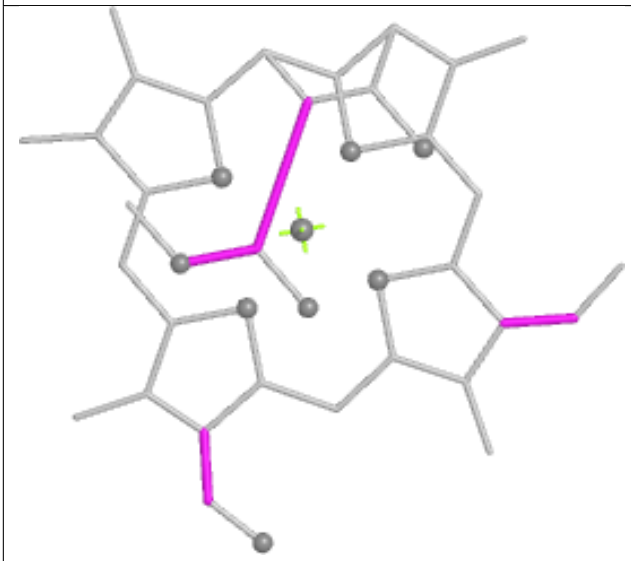

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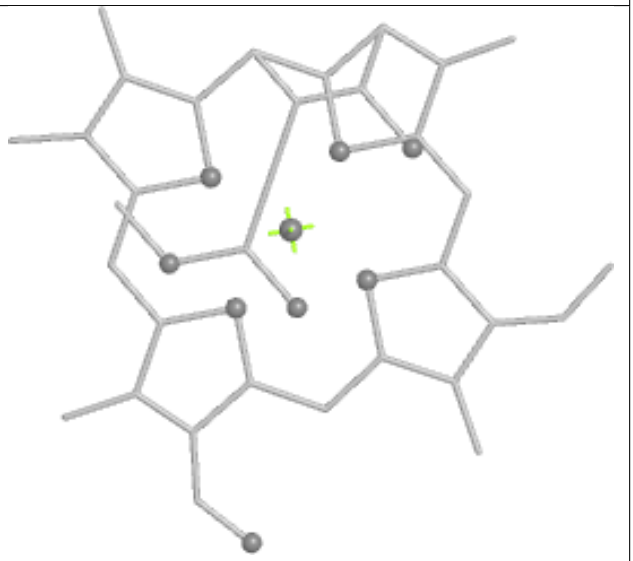

Rings

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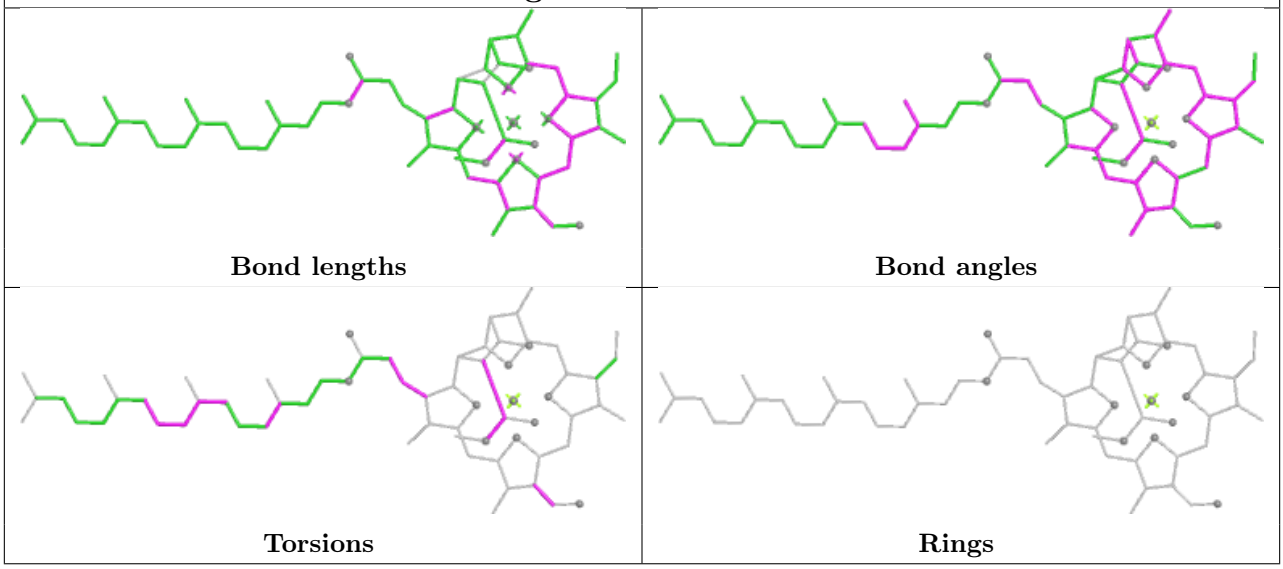

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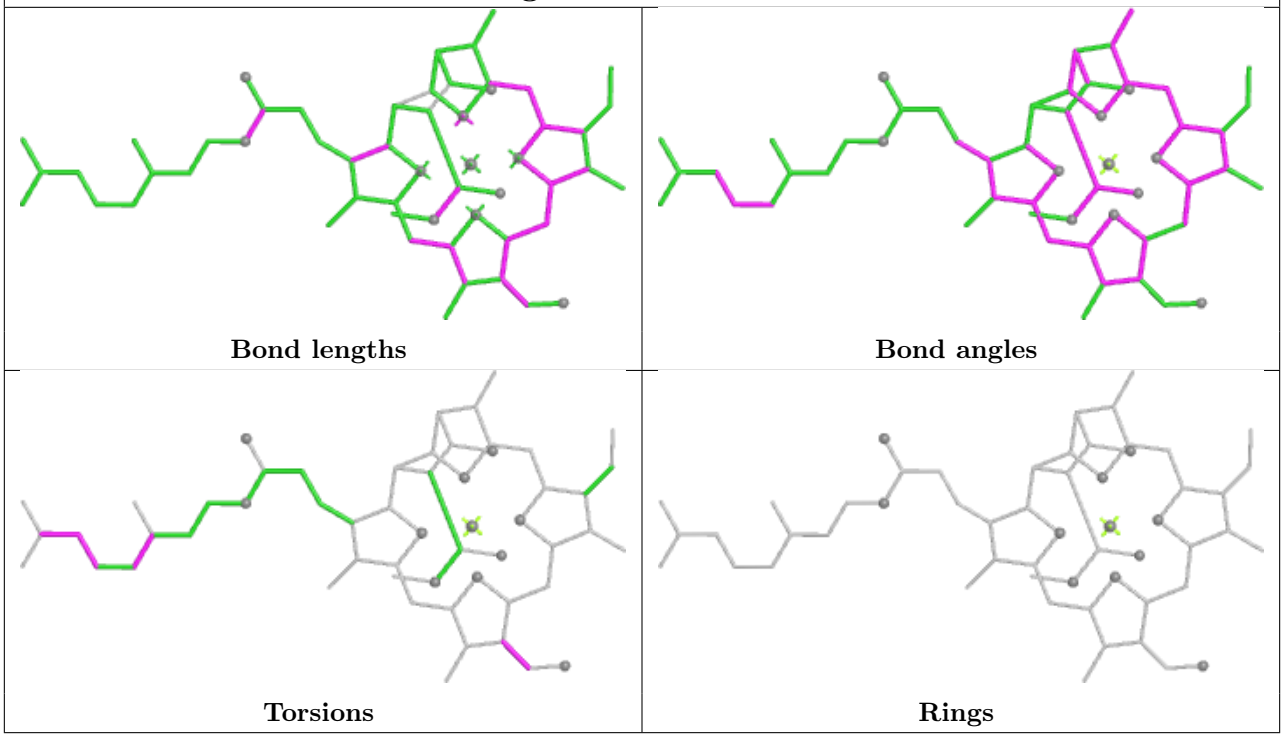
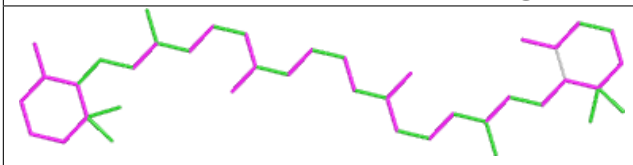


Ligand 8CT 3D 406



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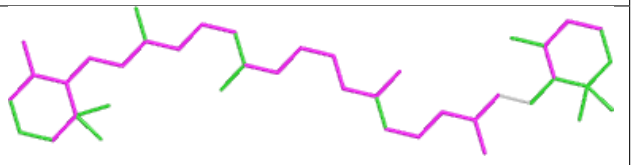
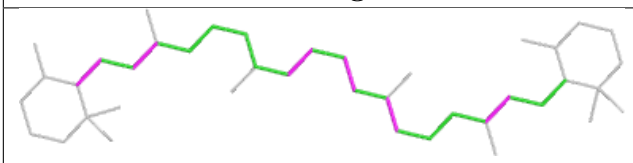


Bond angles



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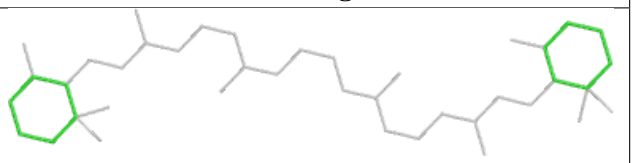

Rings

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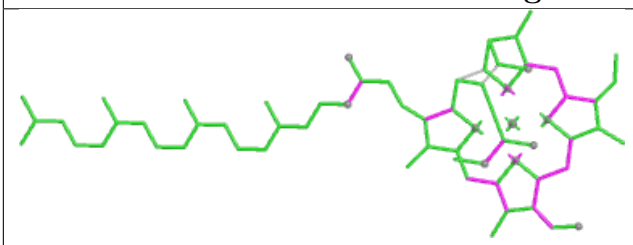

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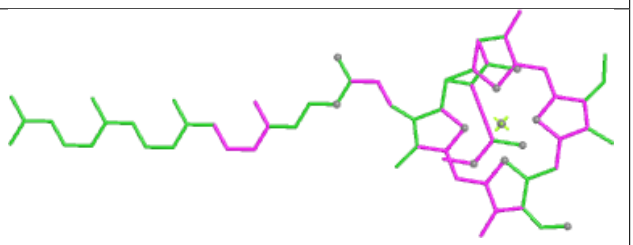

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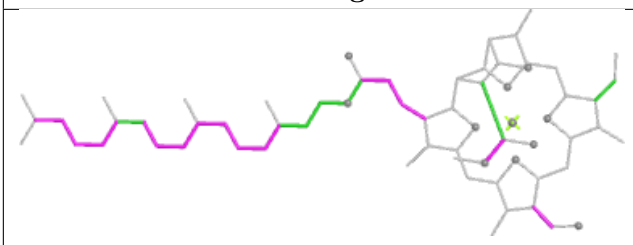

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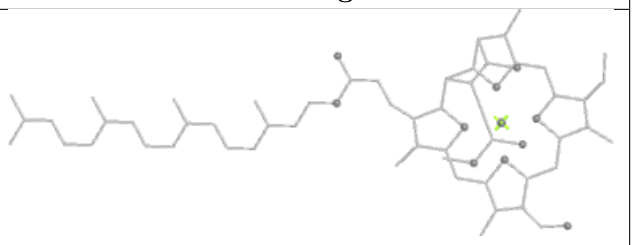
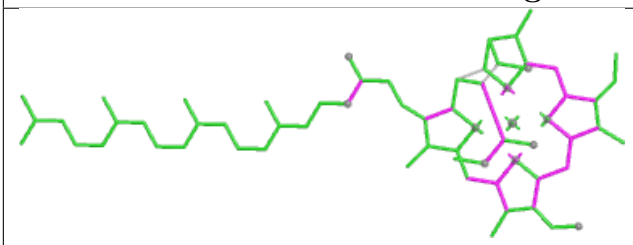


Rings

Ligand CL7 33 508



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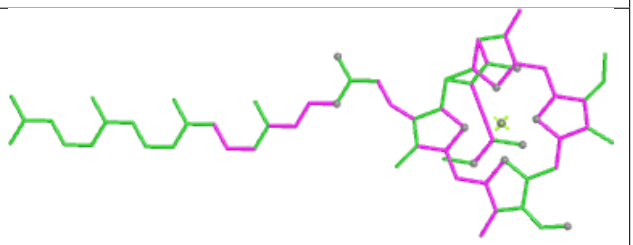

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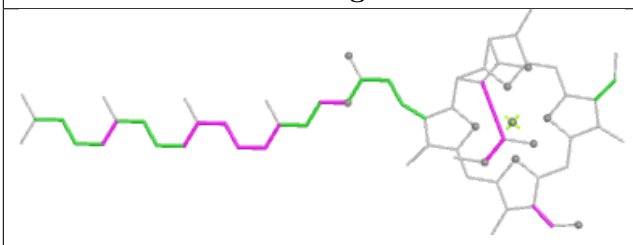

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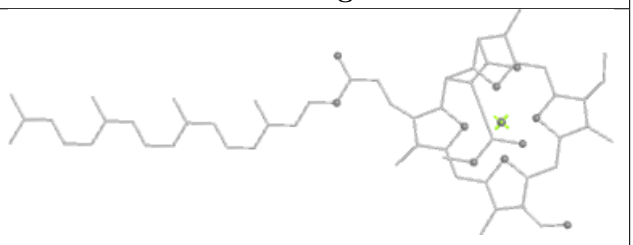
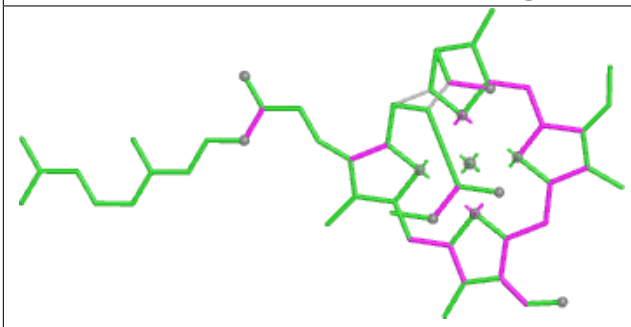


Rings

Ligand CL7 3C 504



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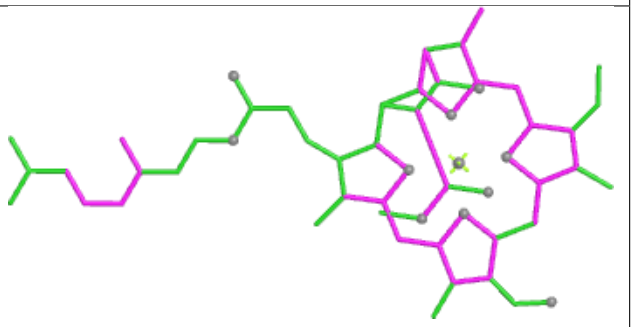
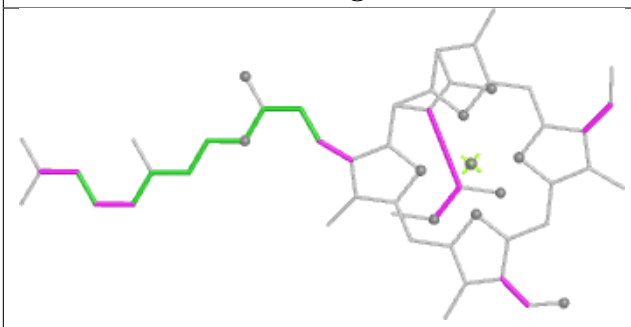


Bond angles



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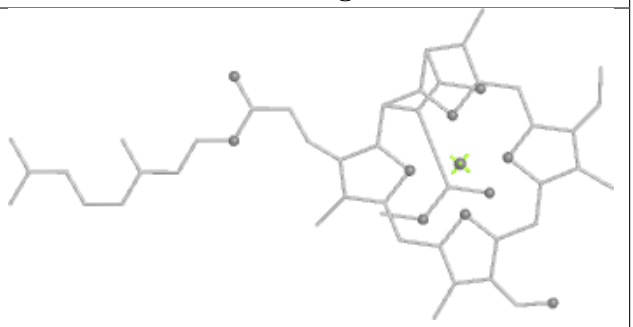
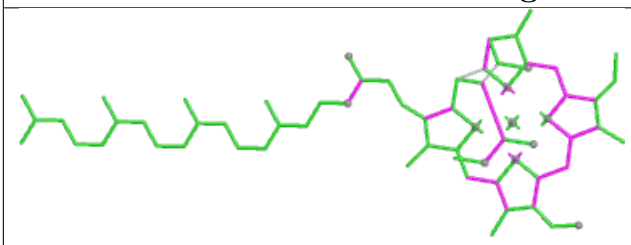


Rings

Ligand CL7 2B 612



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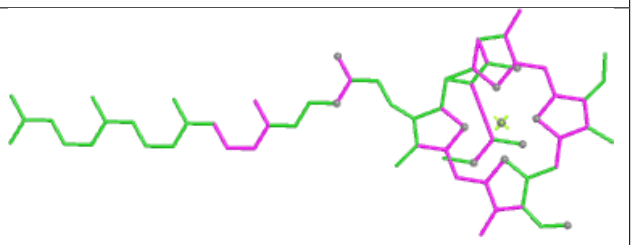

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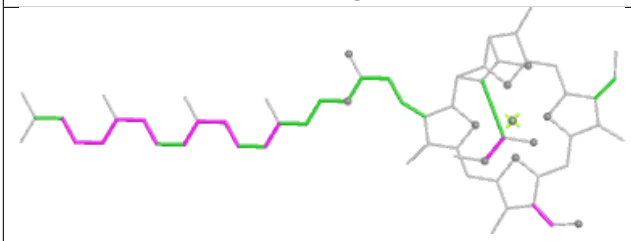

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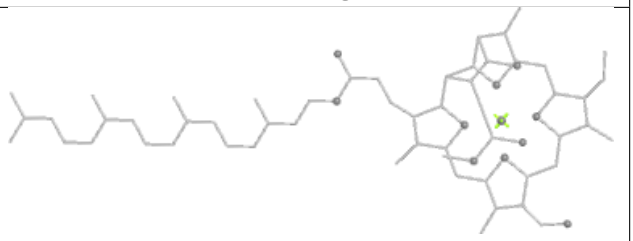
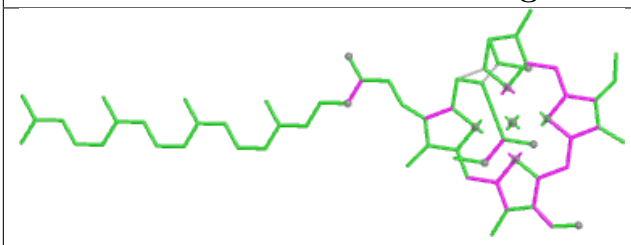


Rings

Ligand CL7 4B 605



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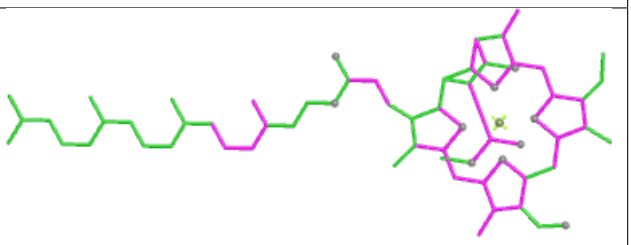
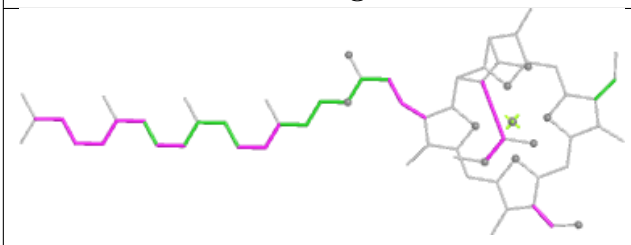


Bond angles



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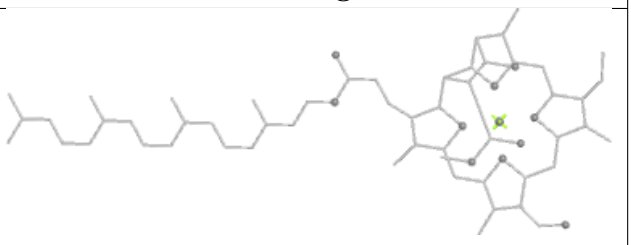
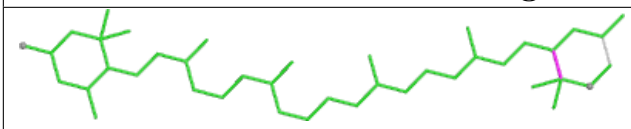


Rings

Ligand ZEX 24 418



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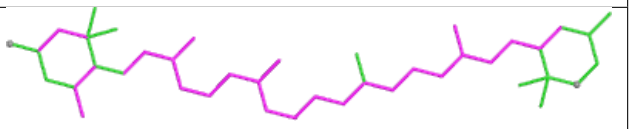
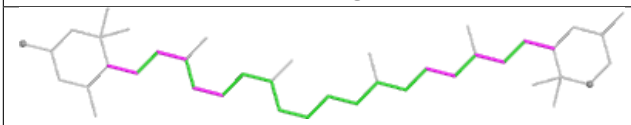


Bond angles



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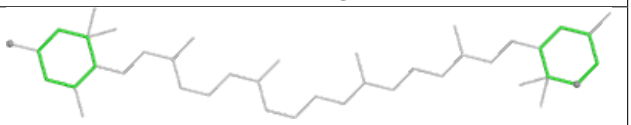
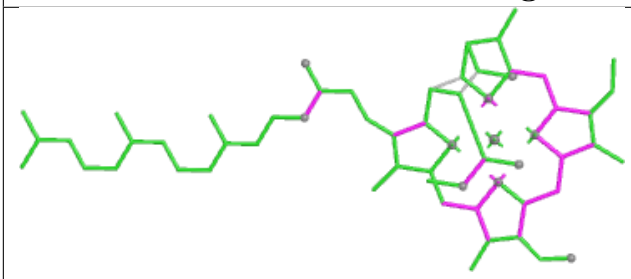


Rings

Ligand CL7 3B 607



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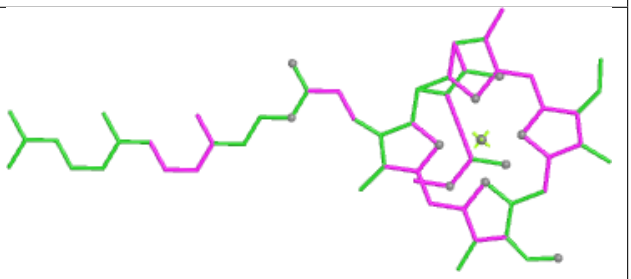

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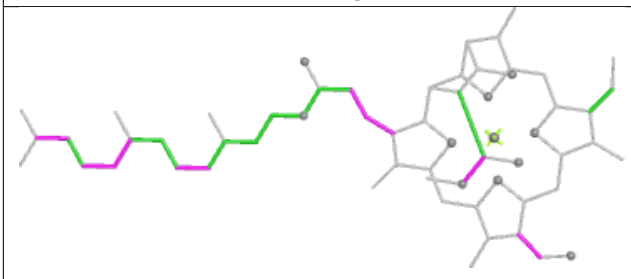

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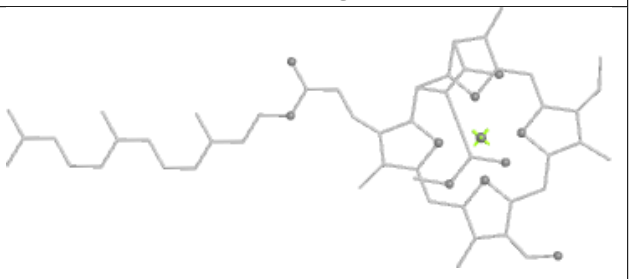
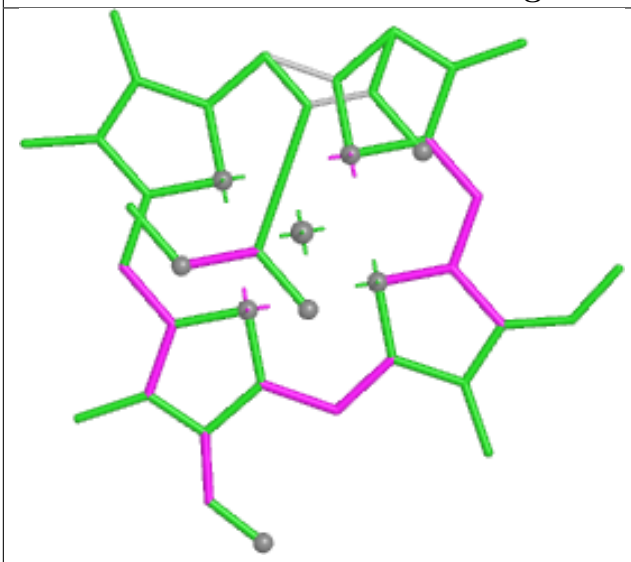


Rings

Ligand CL7 33 515



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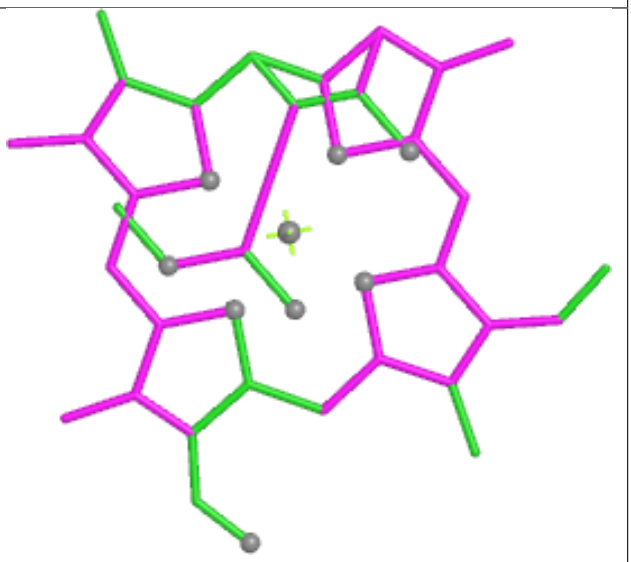
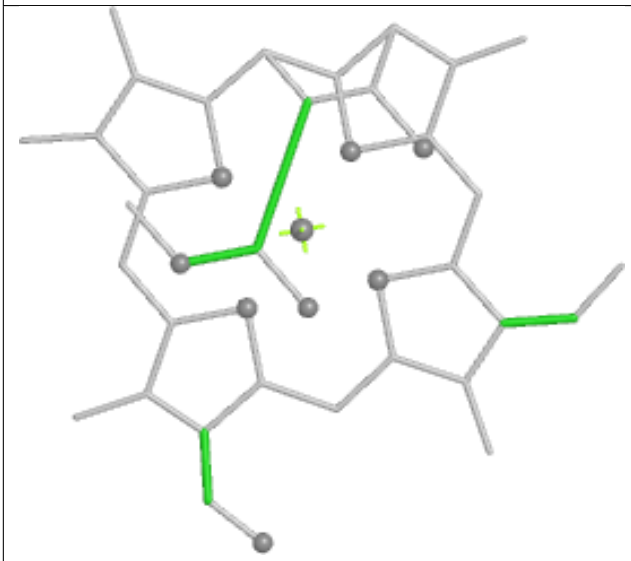


Bond angles



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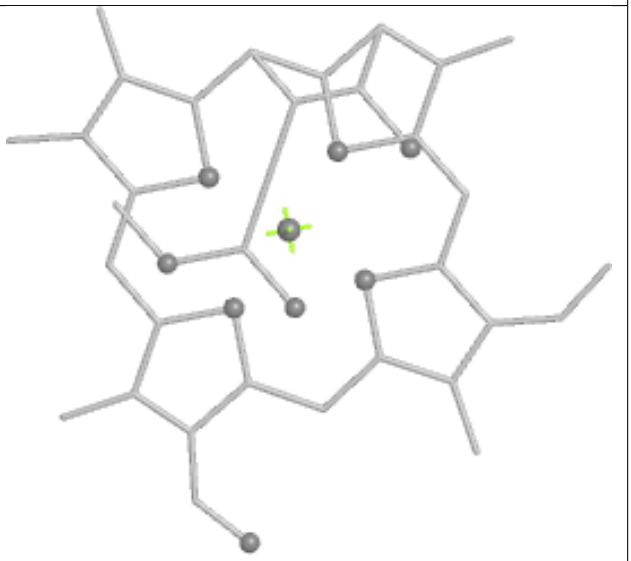

Rings

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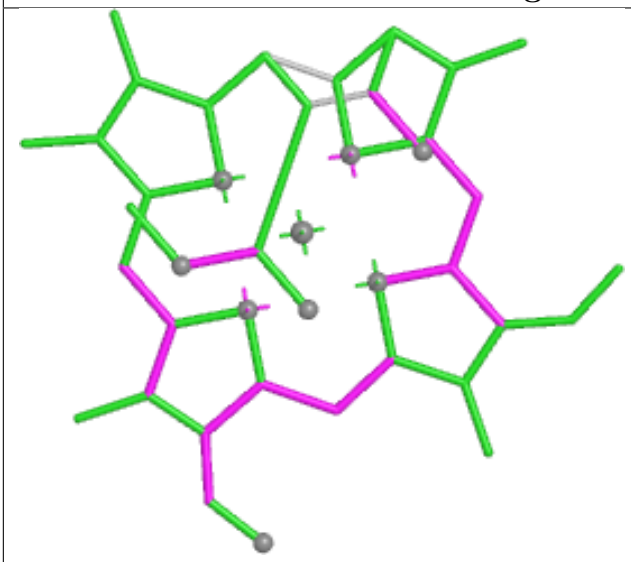

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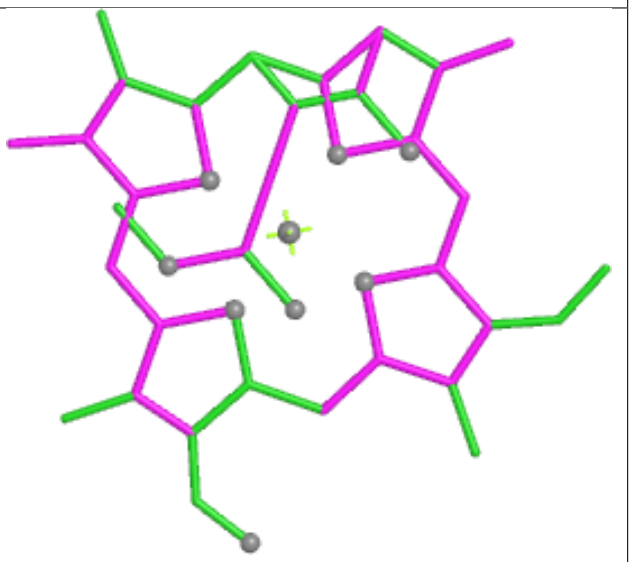
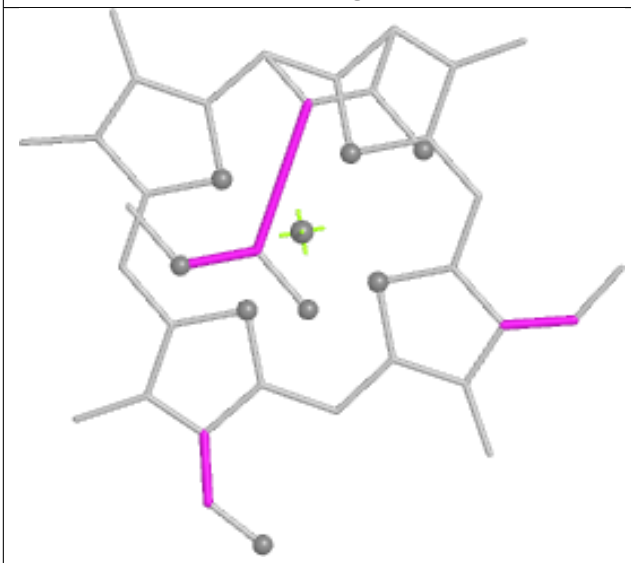


Bond angles



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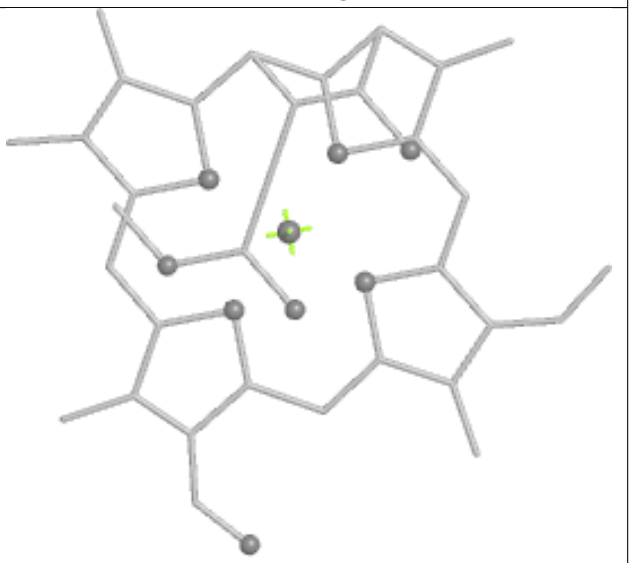
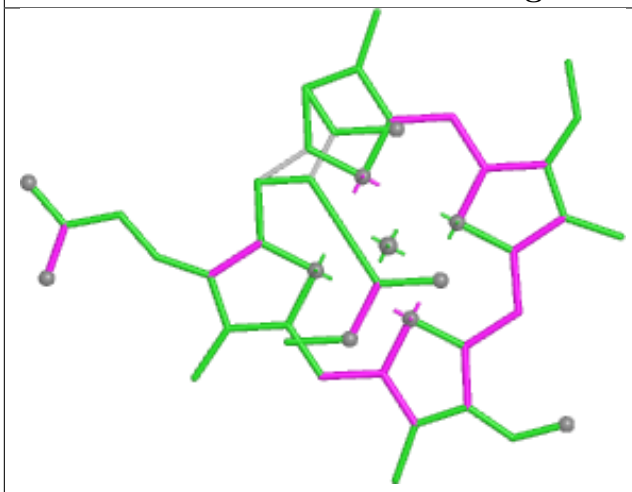


Rings

Ligand CL7 42 514



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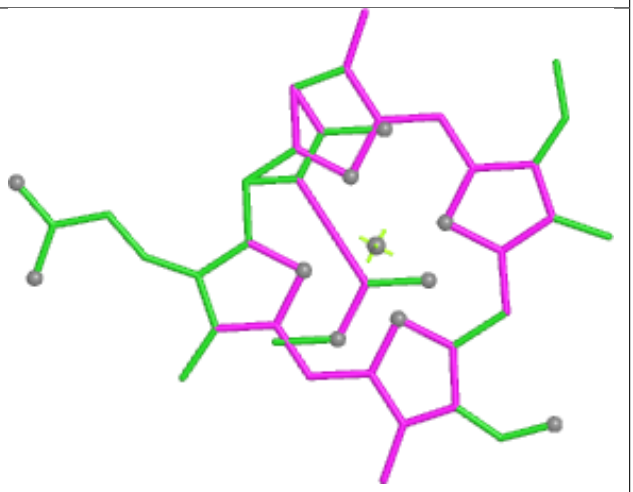
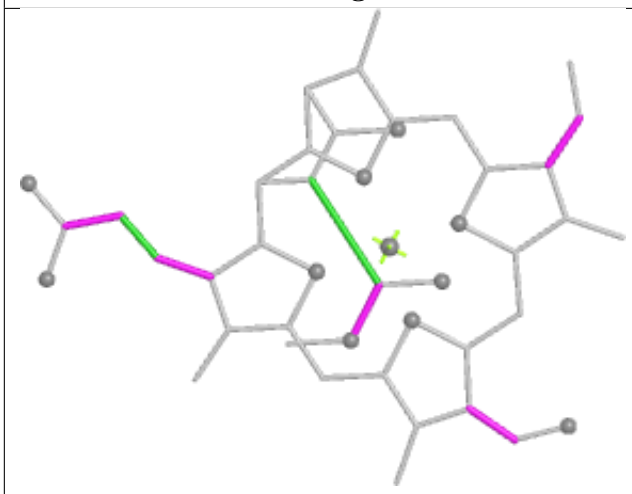


Bond angles

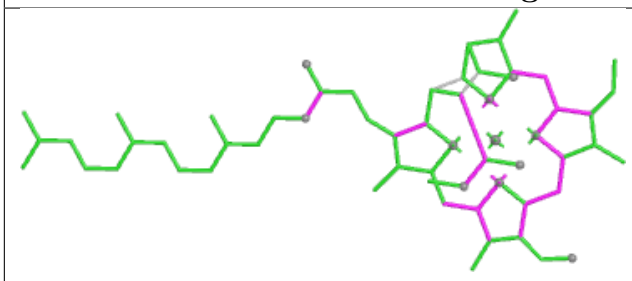


Torsions



Rings

Ligand CL7 4C 506



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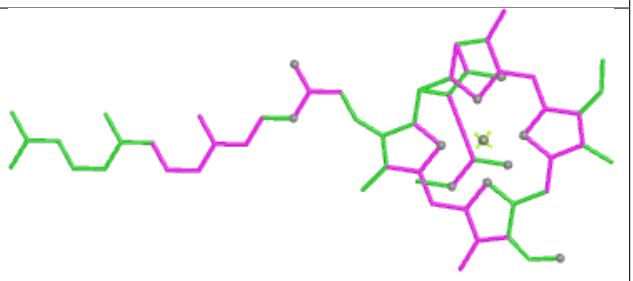

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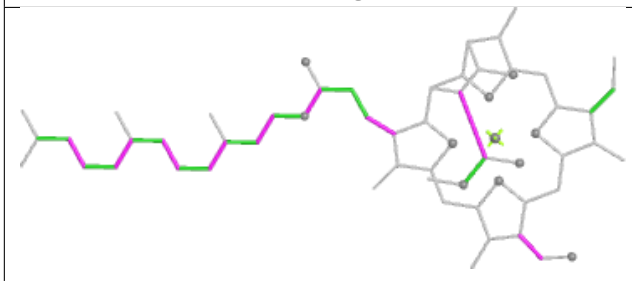
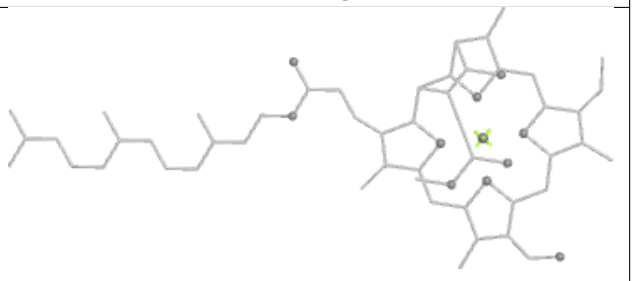
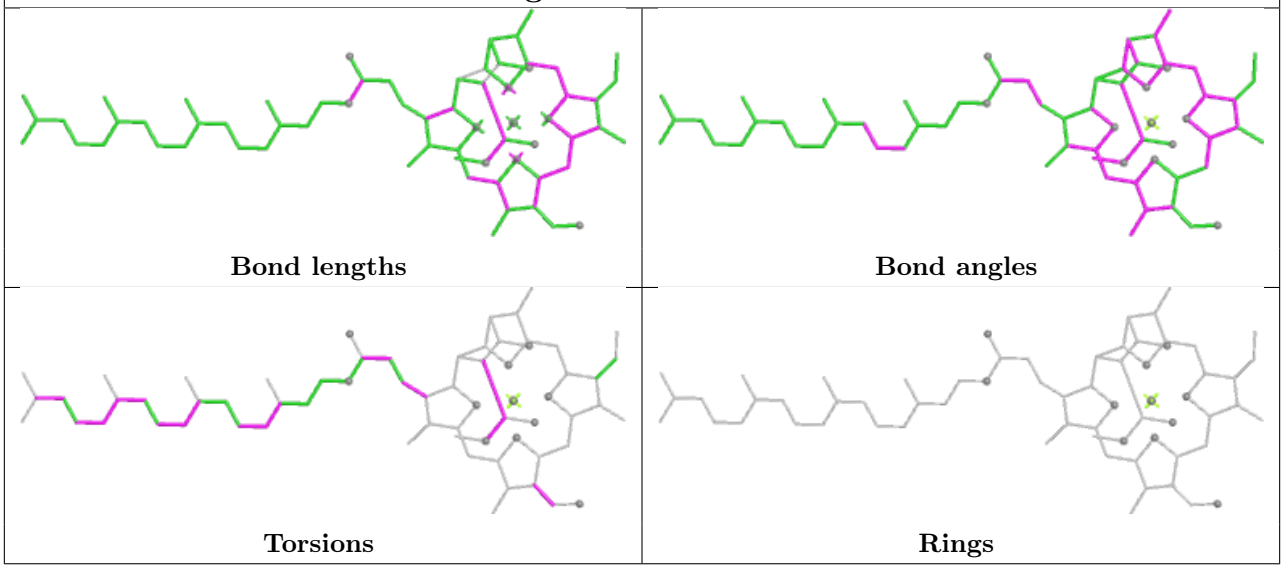


Torsions

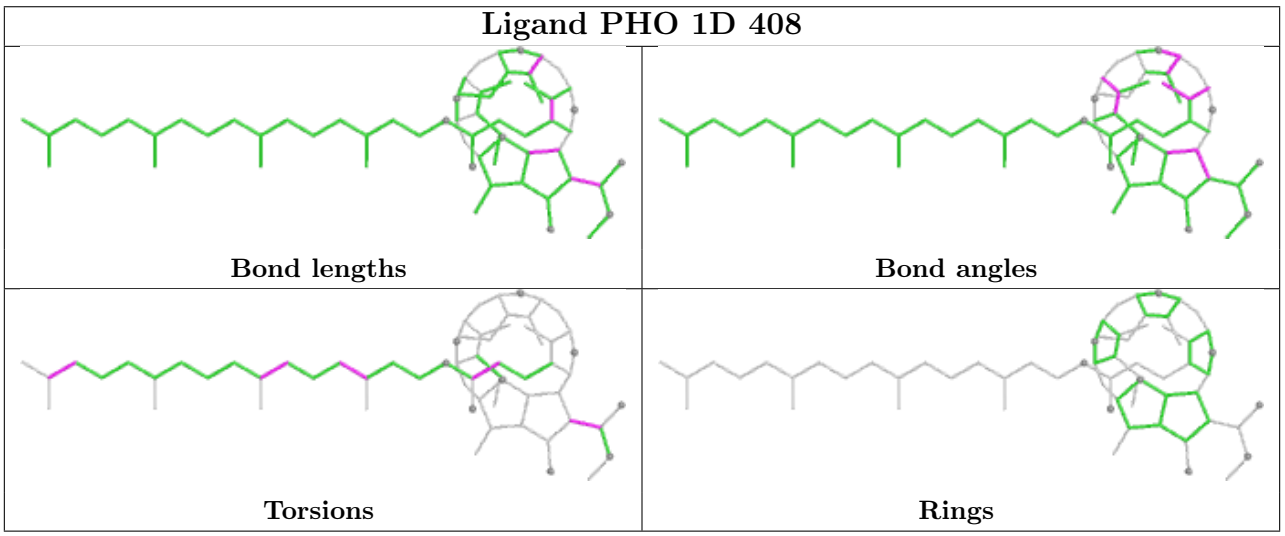


Rings

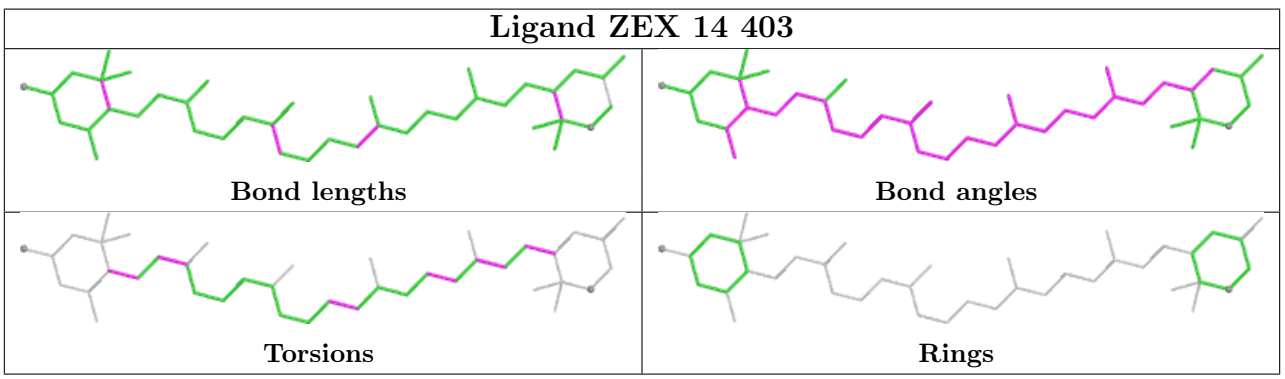
Ligand CL7 32 507



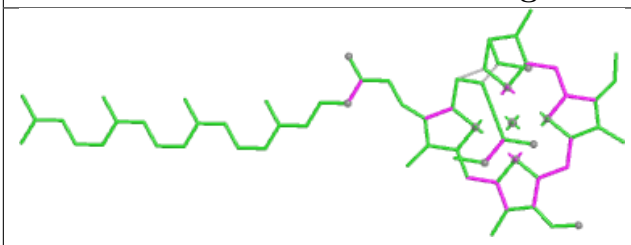
Ligand PHO 1D 408



Ligand ZEX 14 403



Ligand CL7 4C 510



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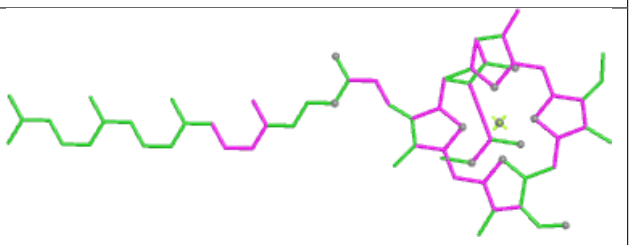
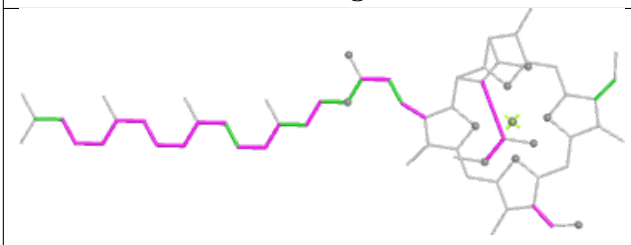


Bond angles



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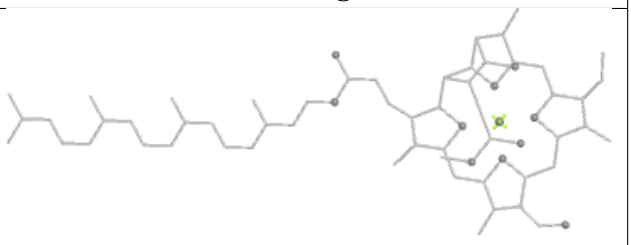
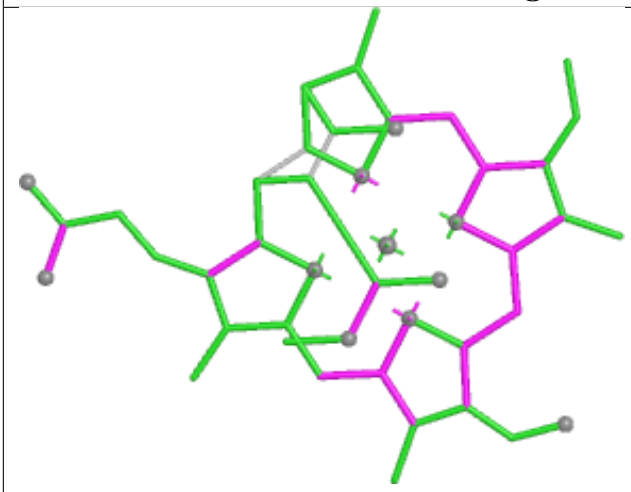


Rings

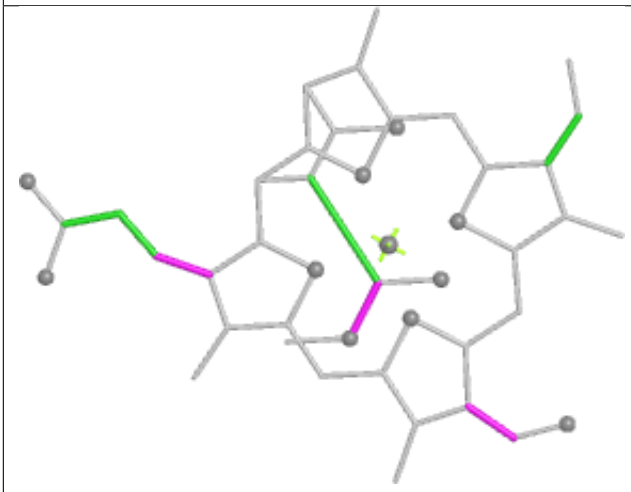
Ligand CL7 42 504



Bond lengths



Bond angles

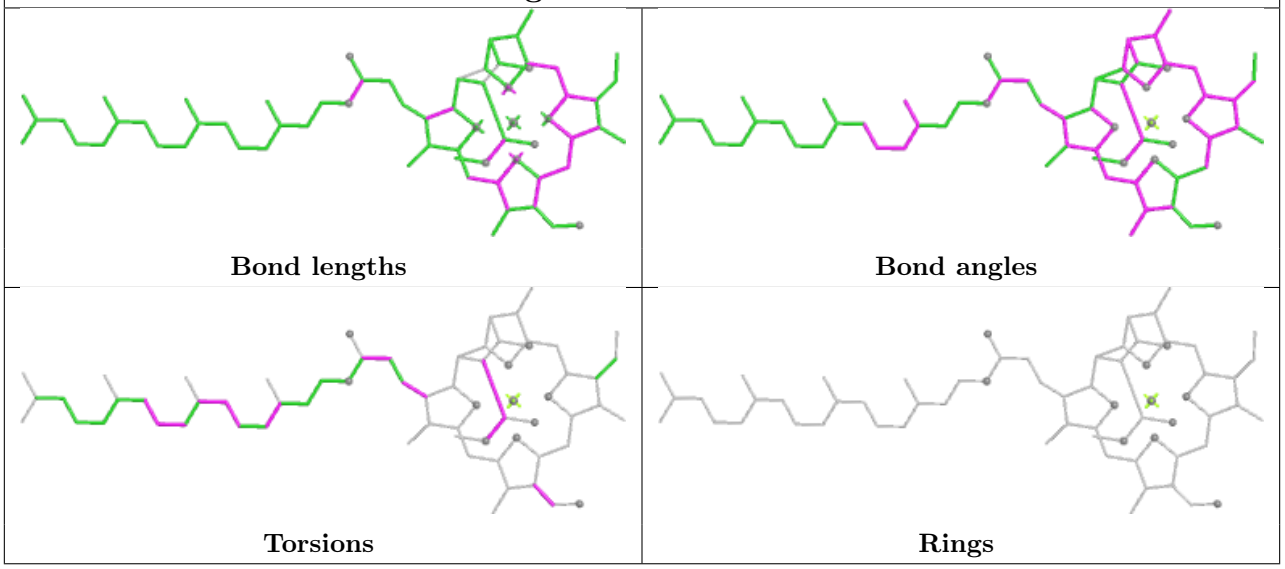


Torsions



Rings

Ligand CL7 13 510



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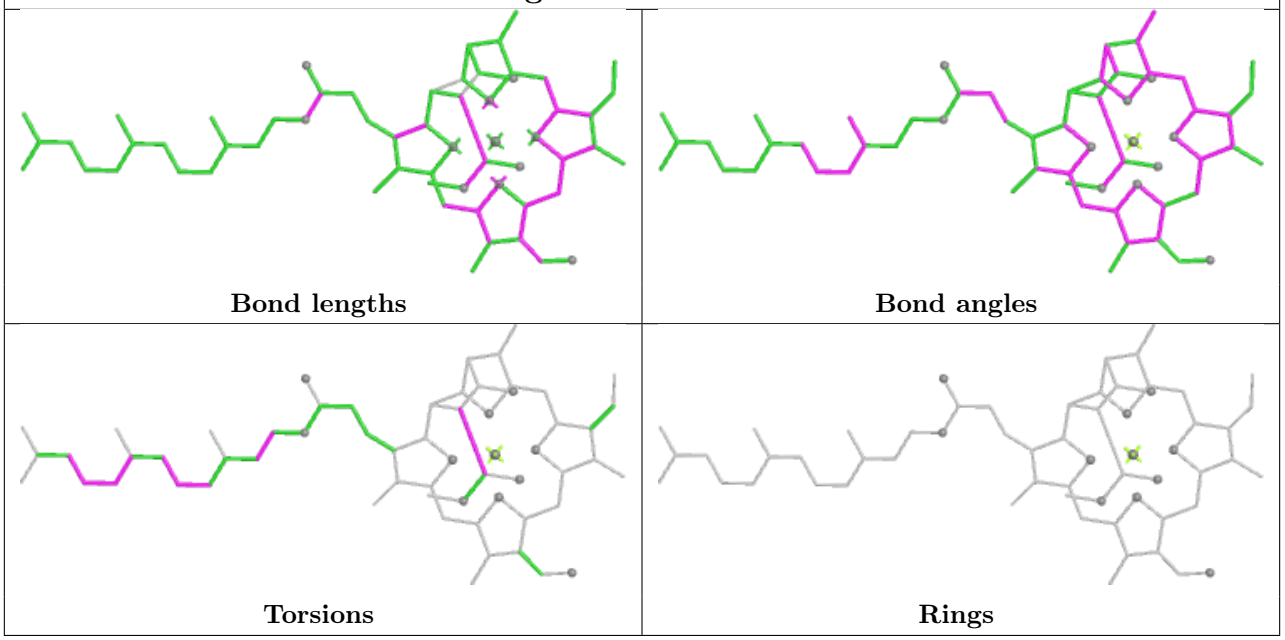
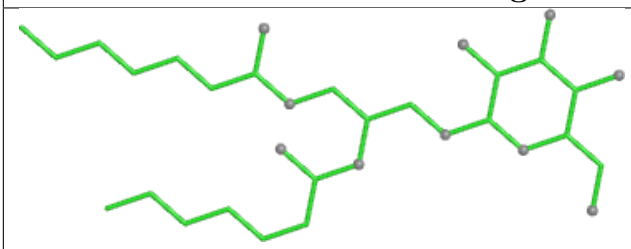


Ligand LMG 1D 410



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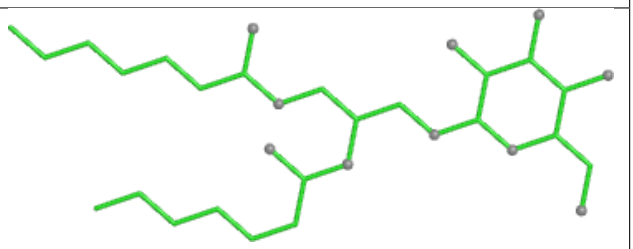
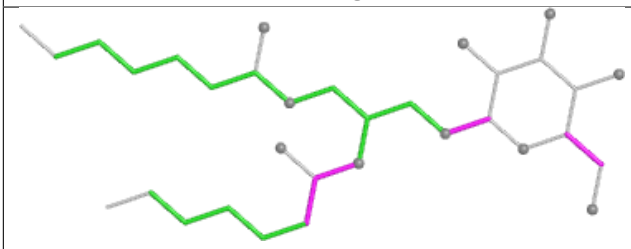


Bond angles



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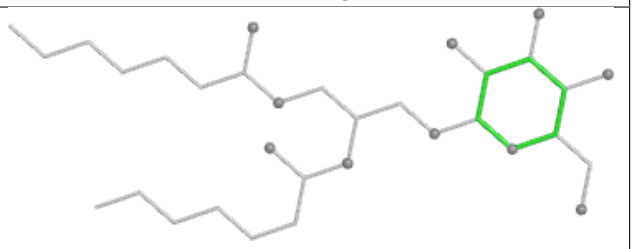
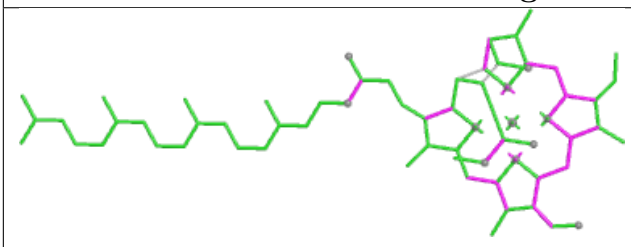


Rings

Ligand CL7 4B 606



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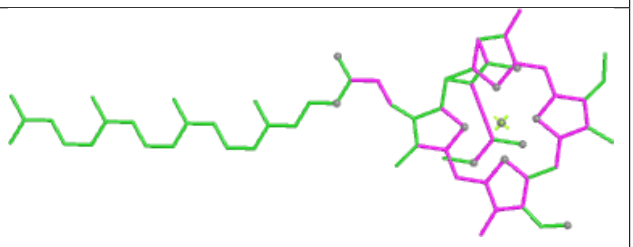
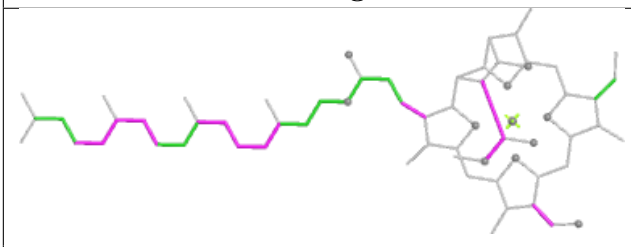


Bond angles



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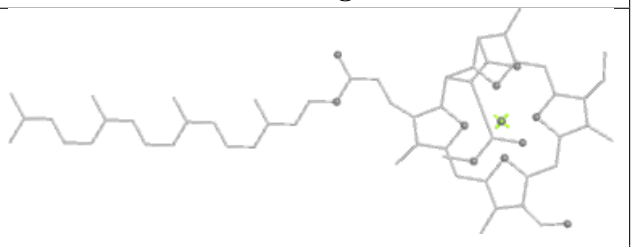
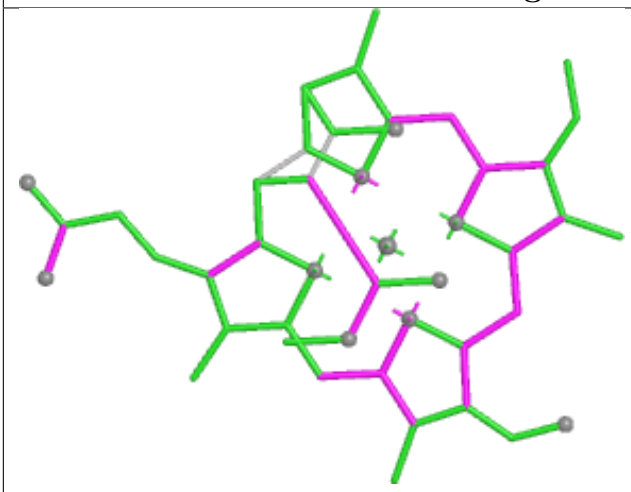


Rings

Ligand CL7 13 513



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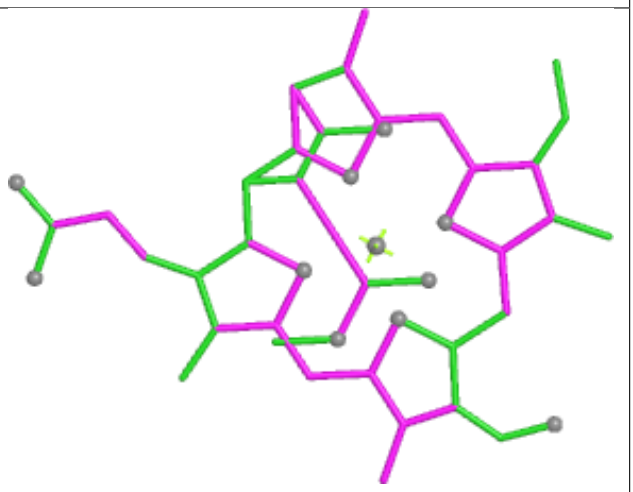

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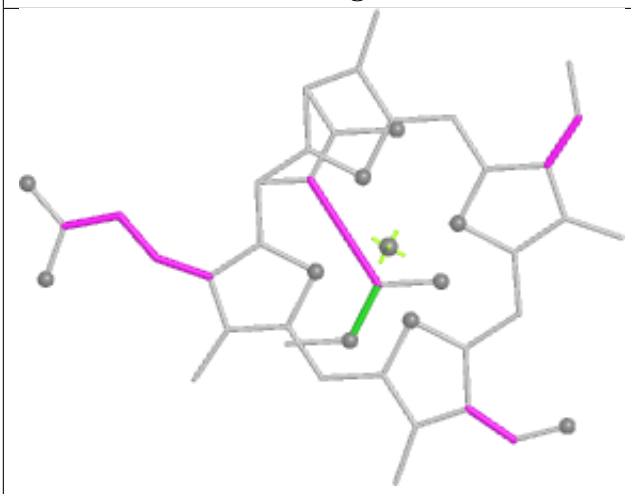
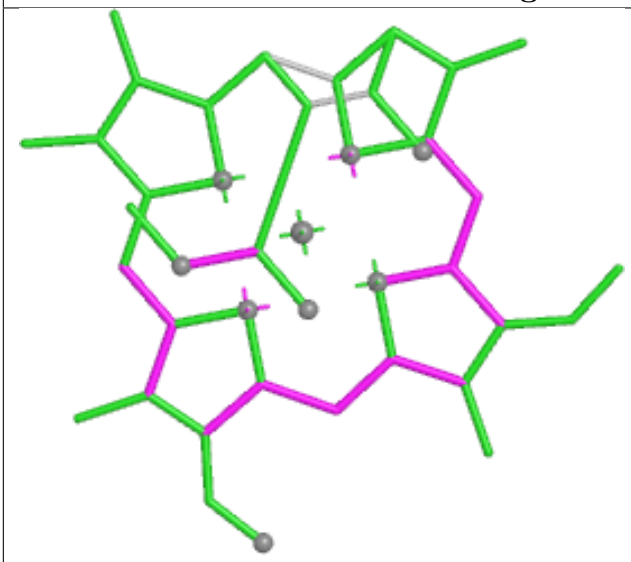


Torsions



Rings

Ligand CL7 2C 517



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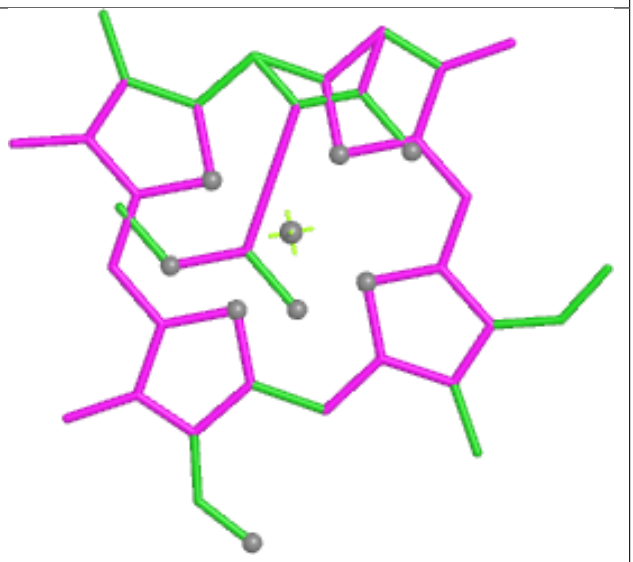

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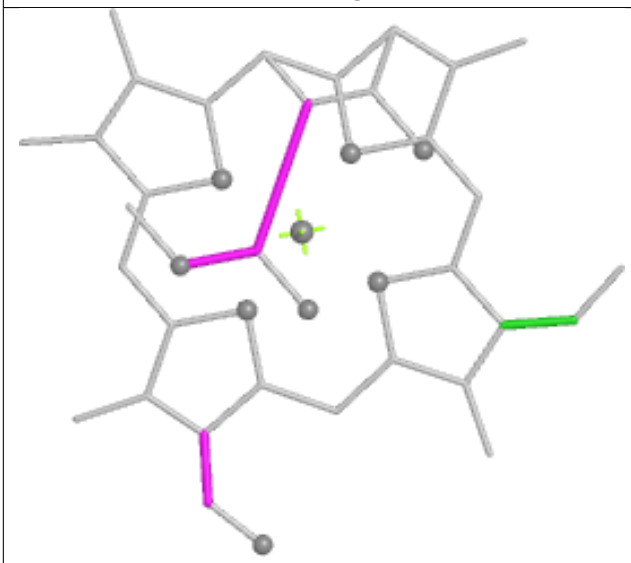

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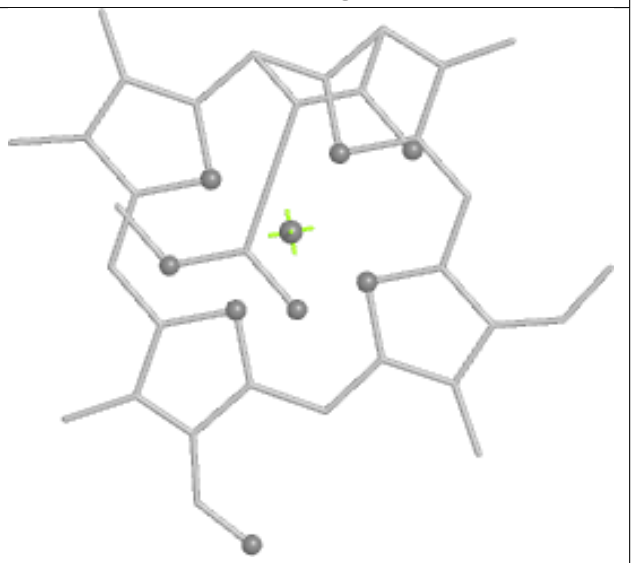
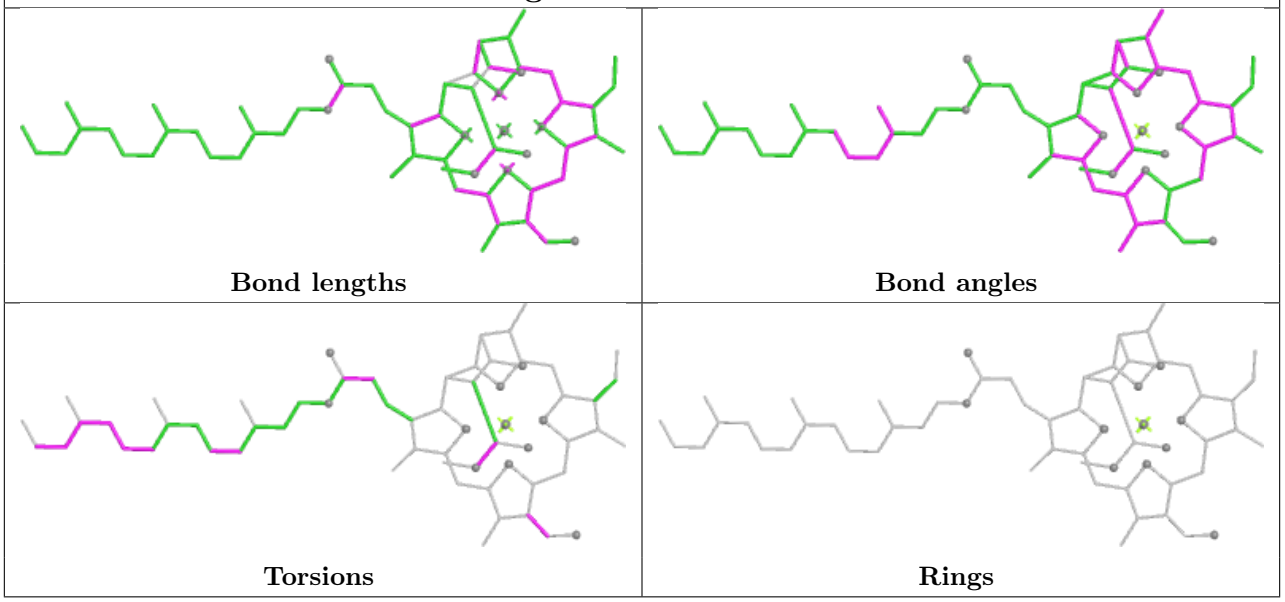


Rings

Ligand CL7 41 406



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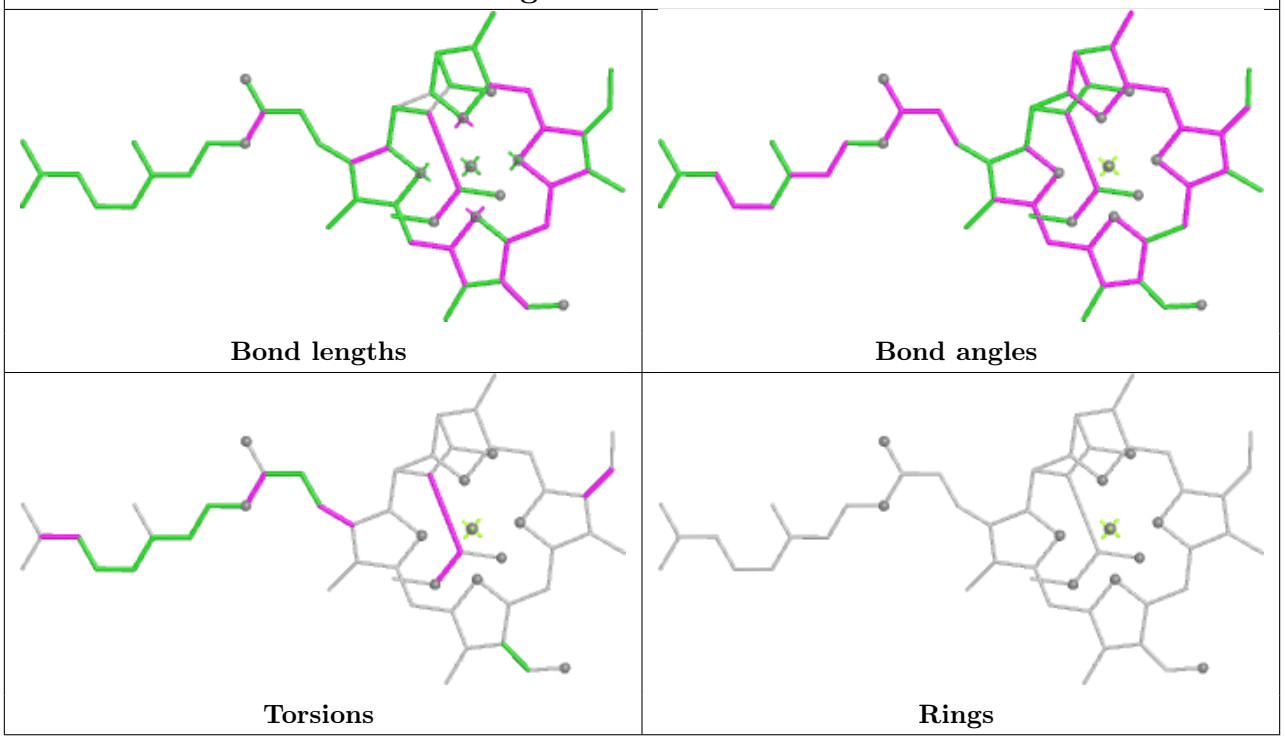

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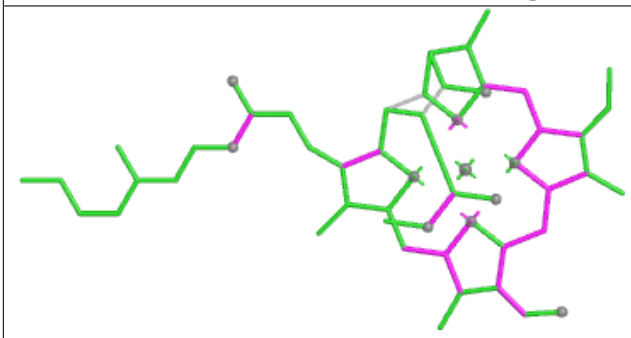

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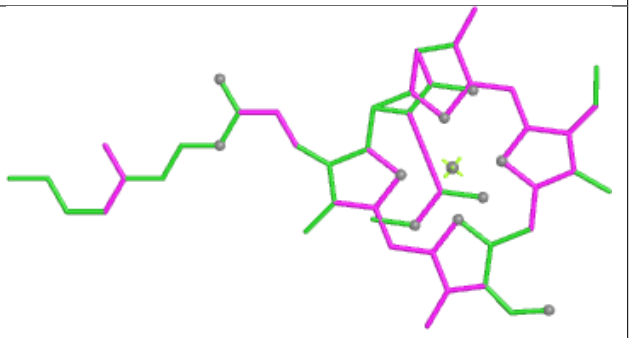
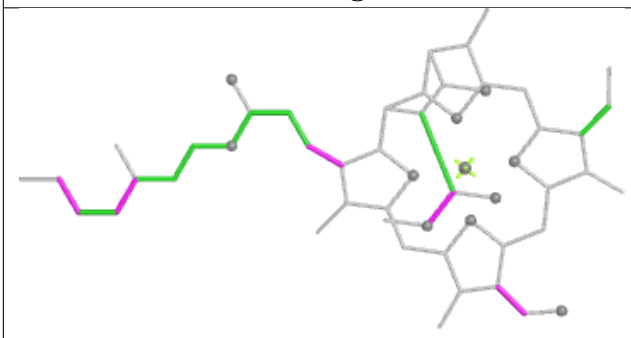


Bond angles



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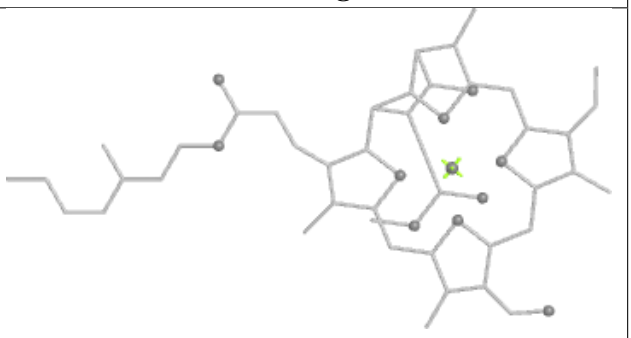

Rings

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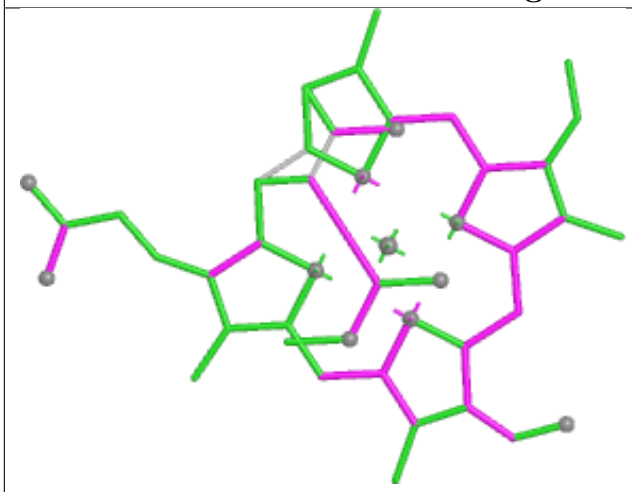

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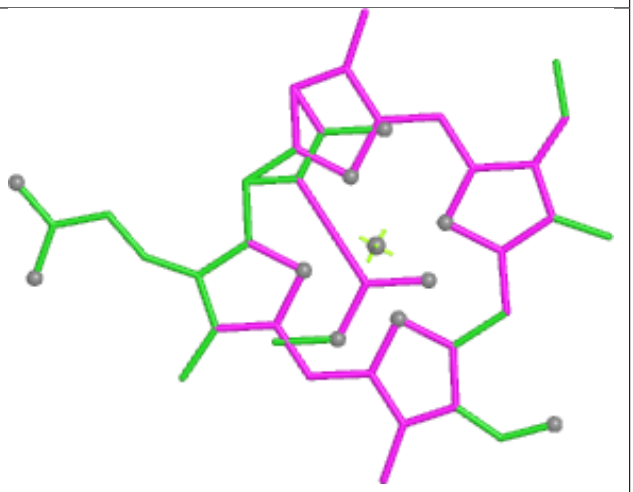

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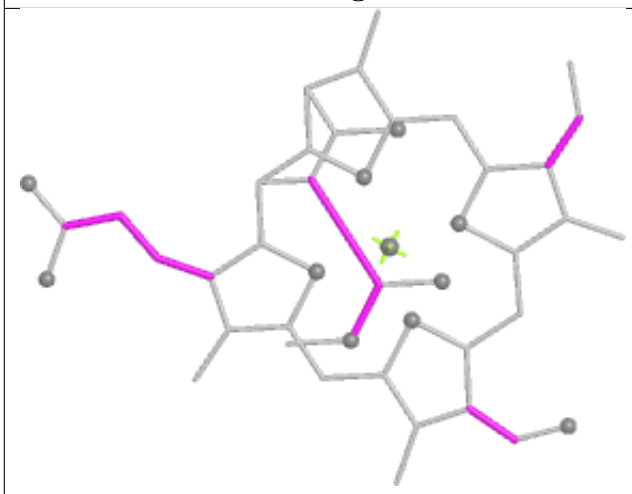
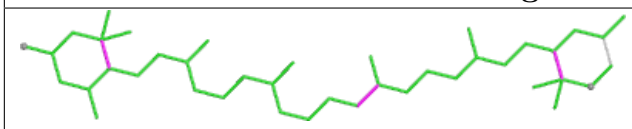


Torsions



Rings

Ligand ZEX 34 419



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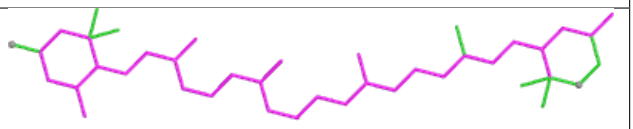

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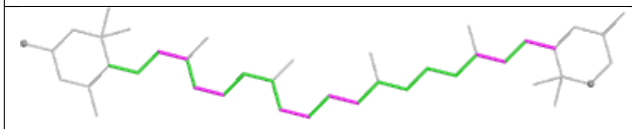

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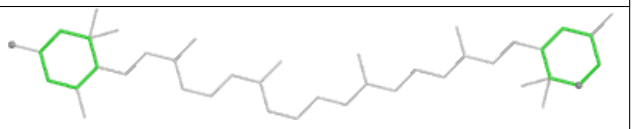
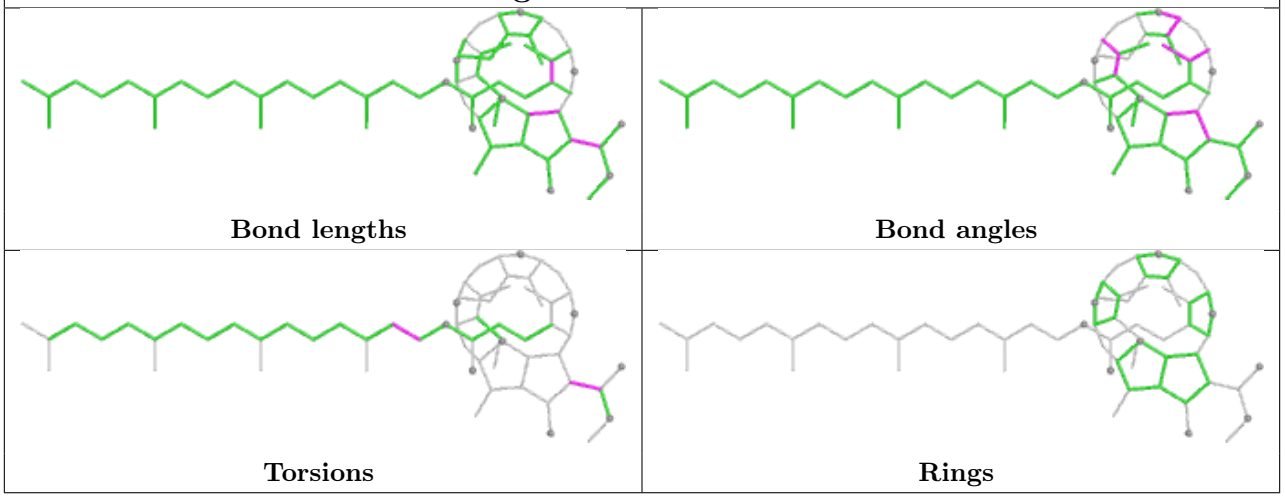
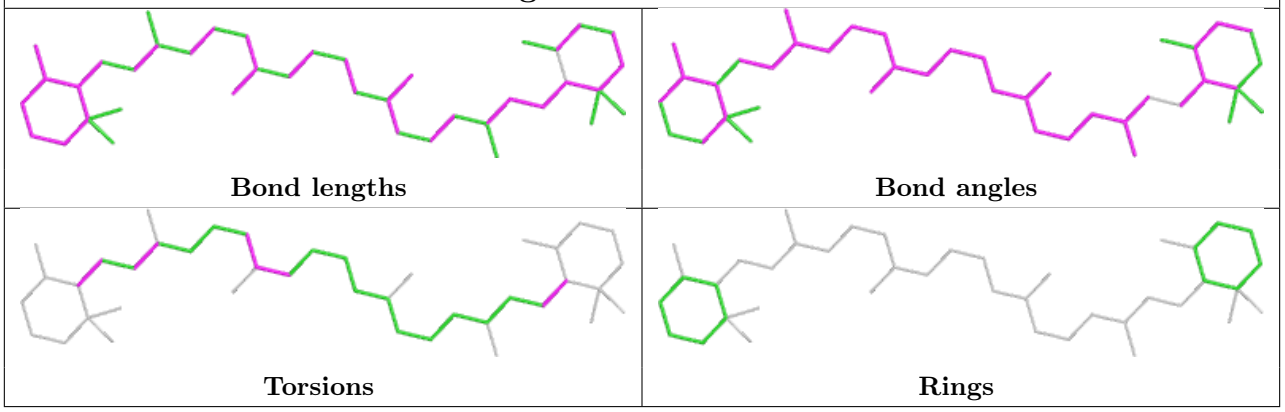


Rings

Ligand PHO 1A 402



Ligand 8CT 4B 601



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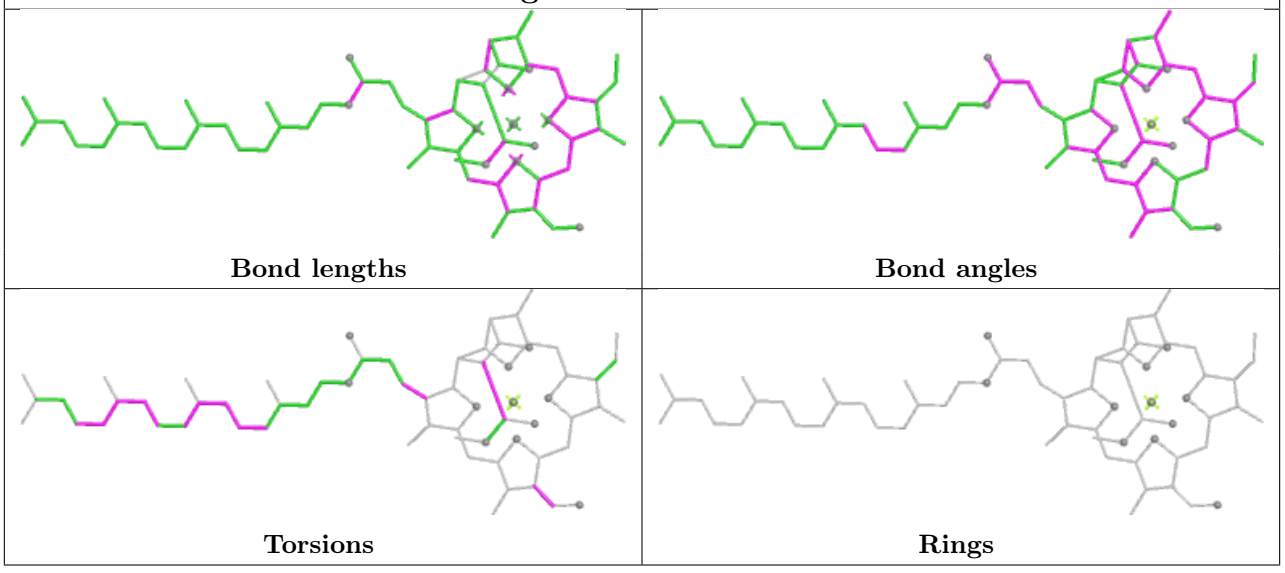

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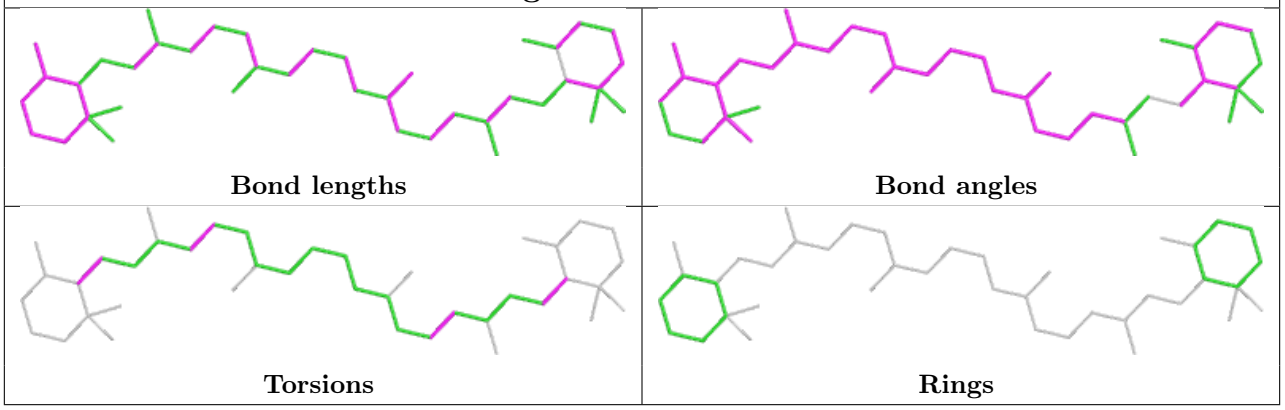

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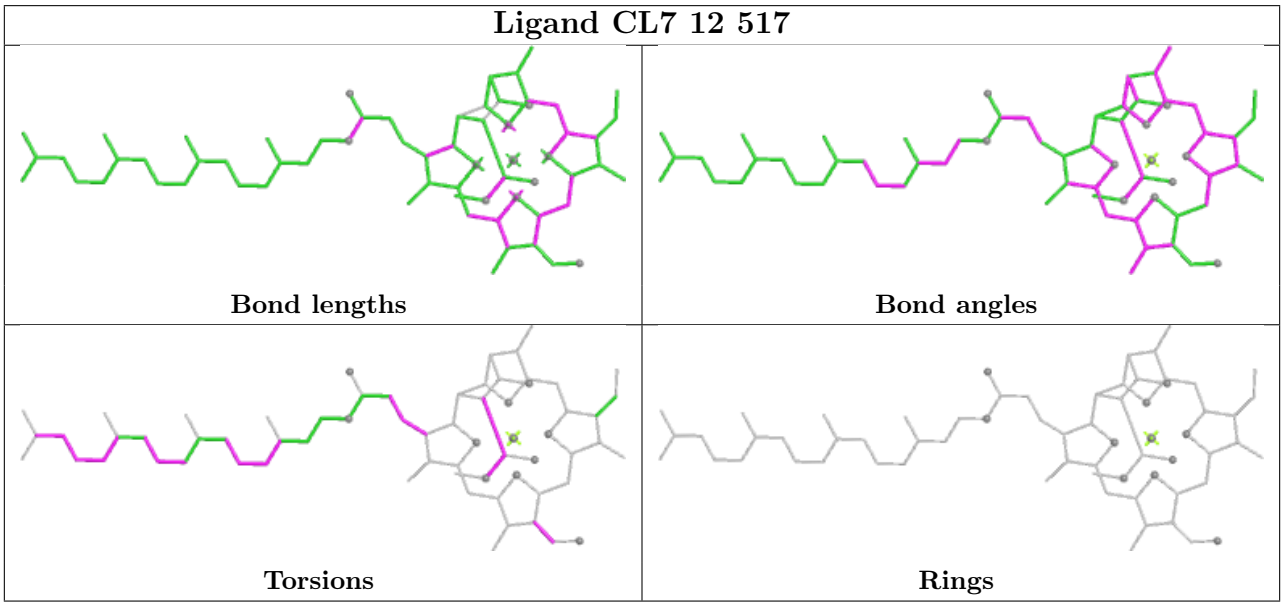

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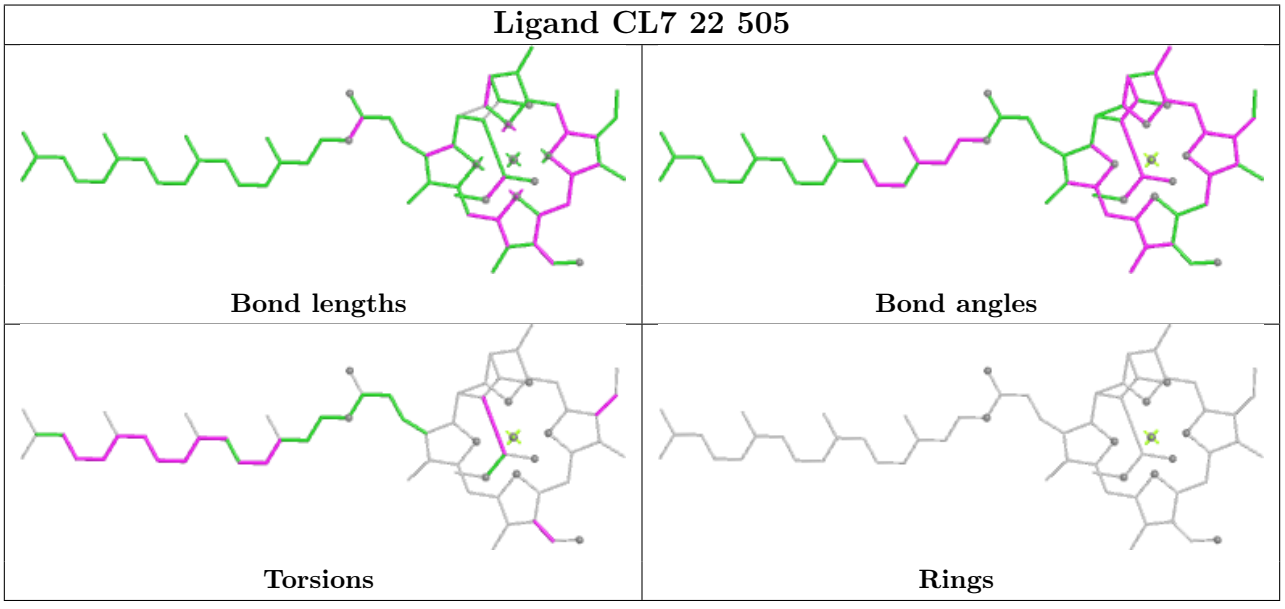
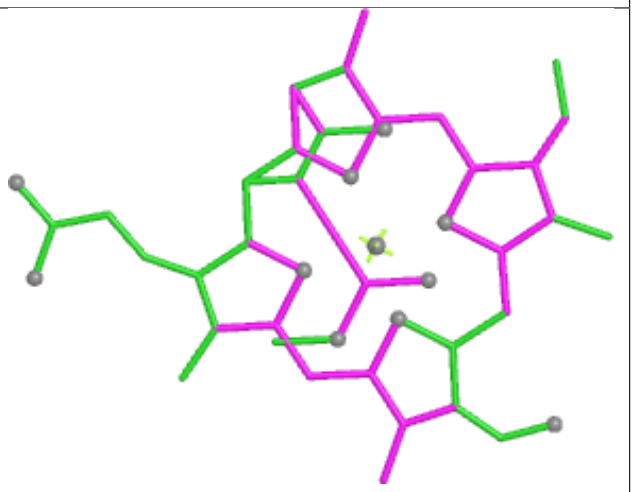


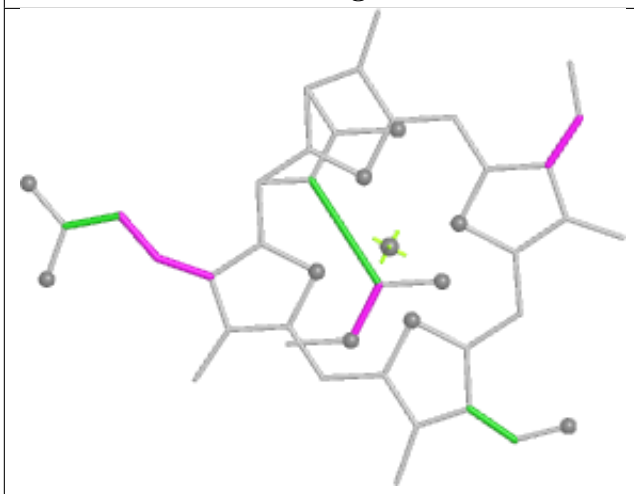
Ligand CL7 33 514



Bond lengths



Bond angles

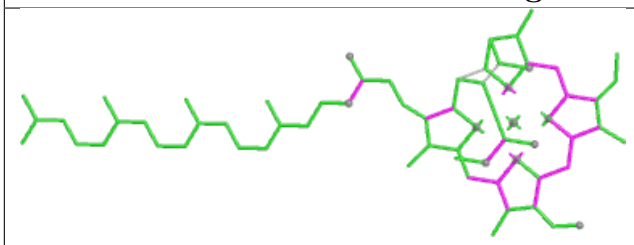


Torsions



Rings

Ligand CL7 22 510



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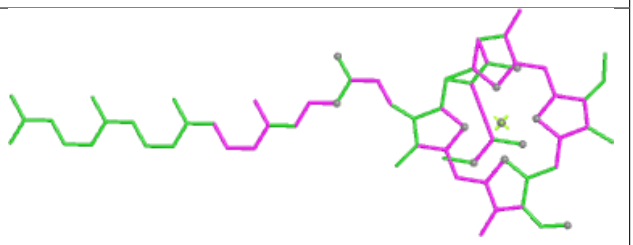
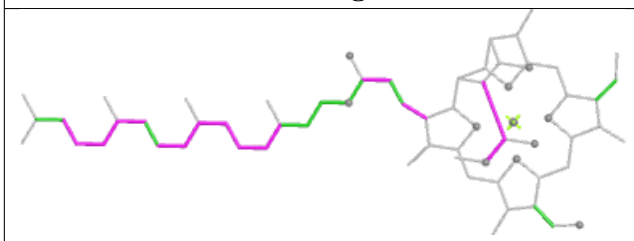
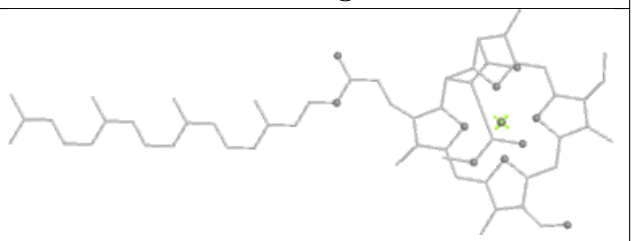


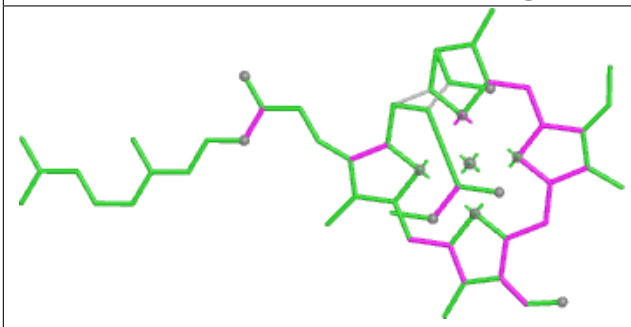
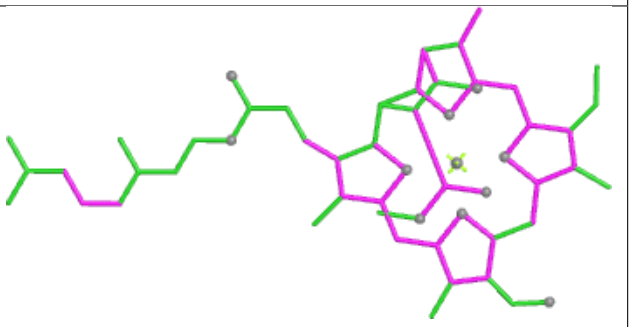
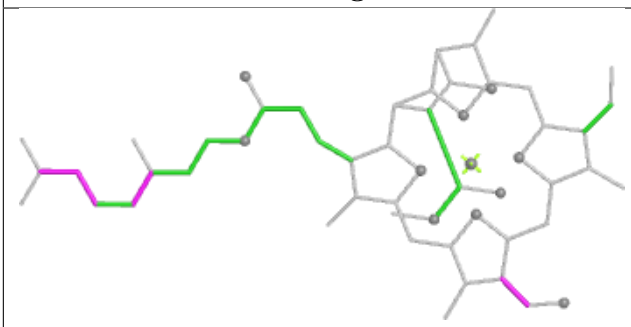
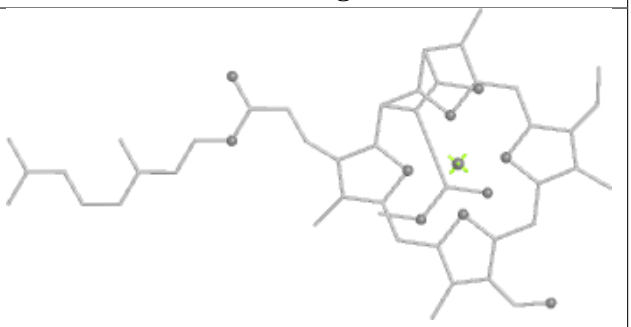
Bond angles



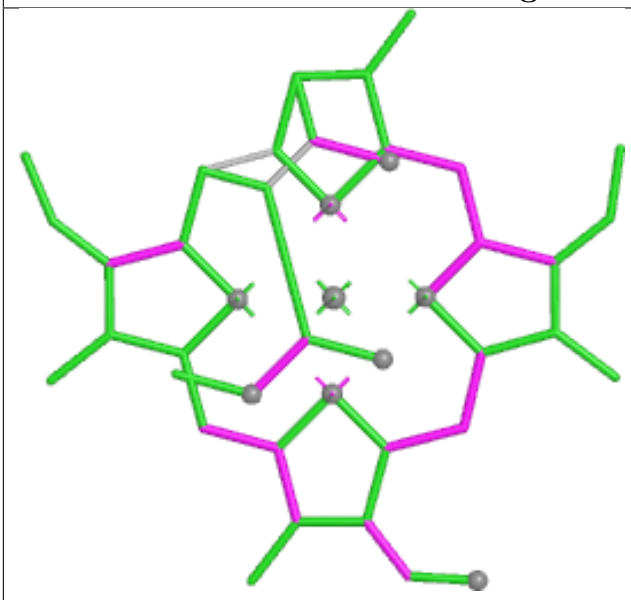
Torsions



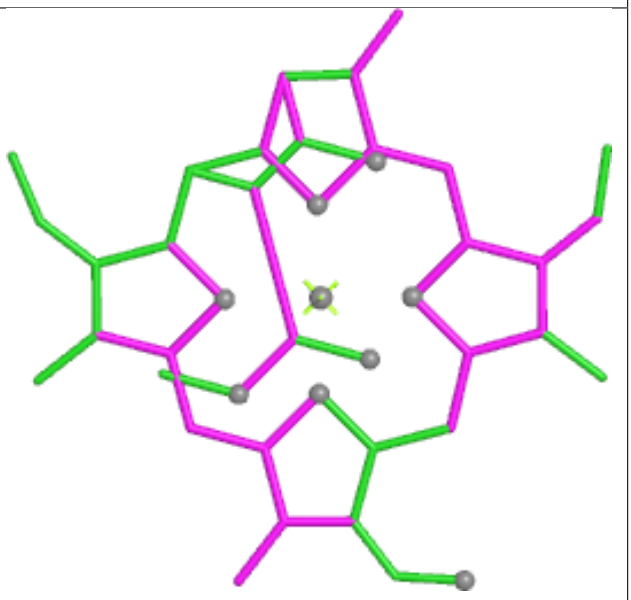
Rings

Ligand CL7 1B 606	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

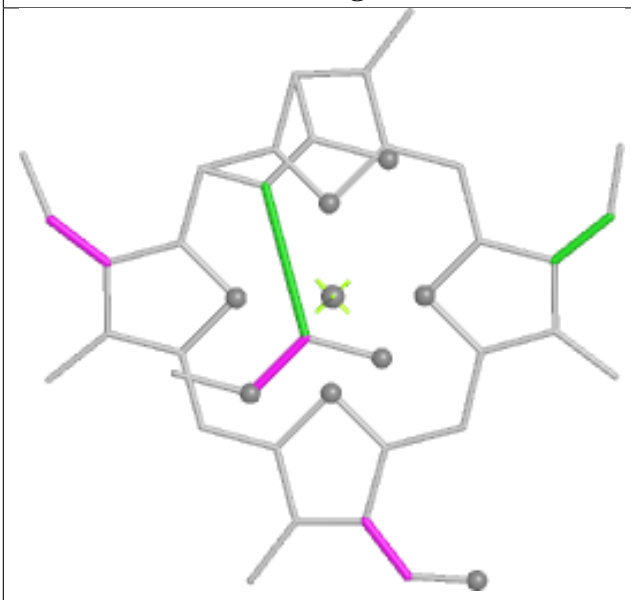
Ligand CL7 4C 511



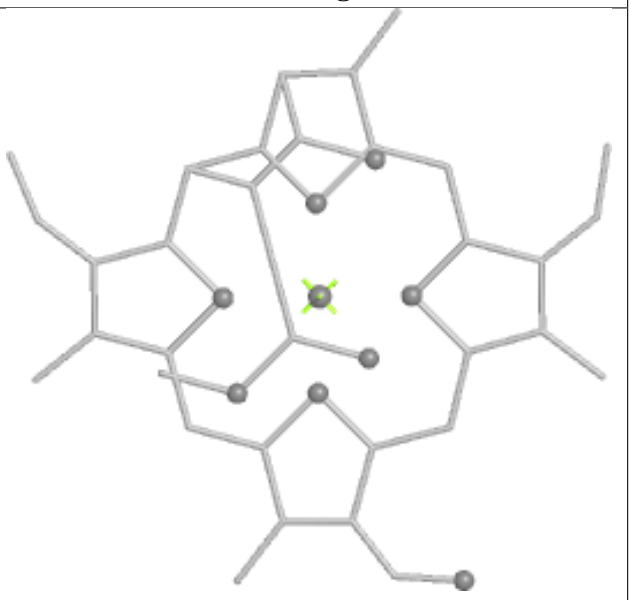
Bond lengths



Bond angles

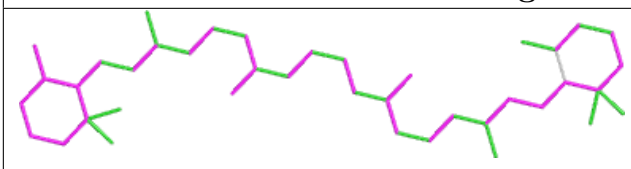


Torsions



Rings

Ligand 8CT 2B 601



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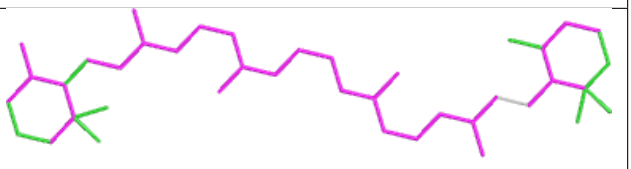
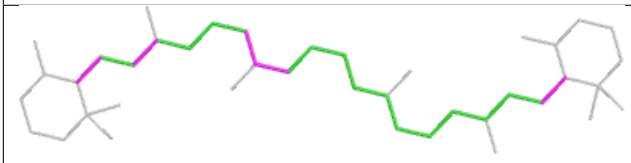


Bond angles



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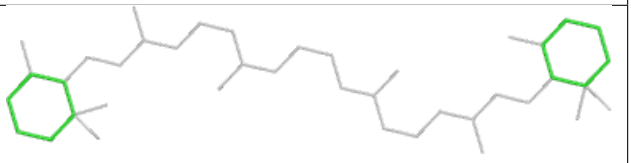
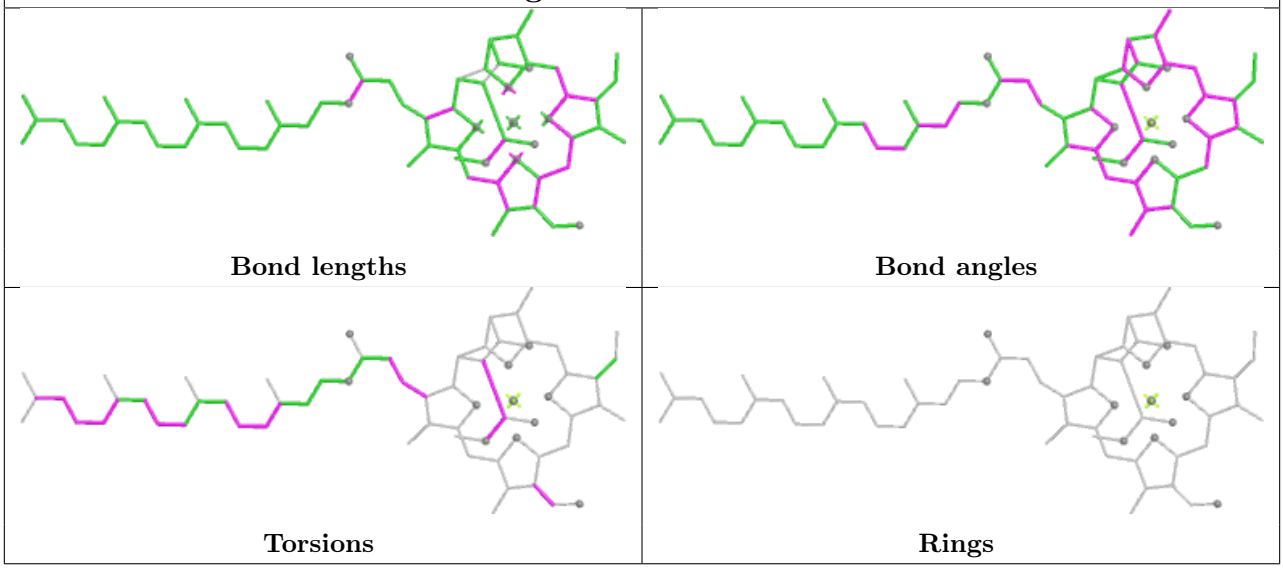
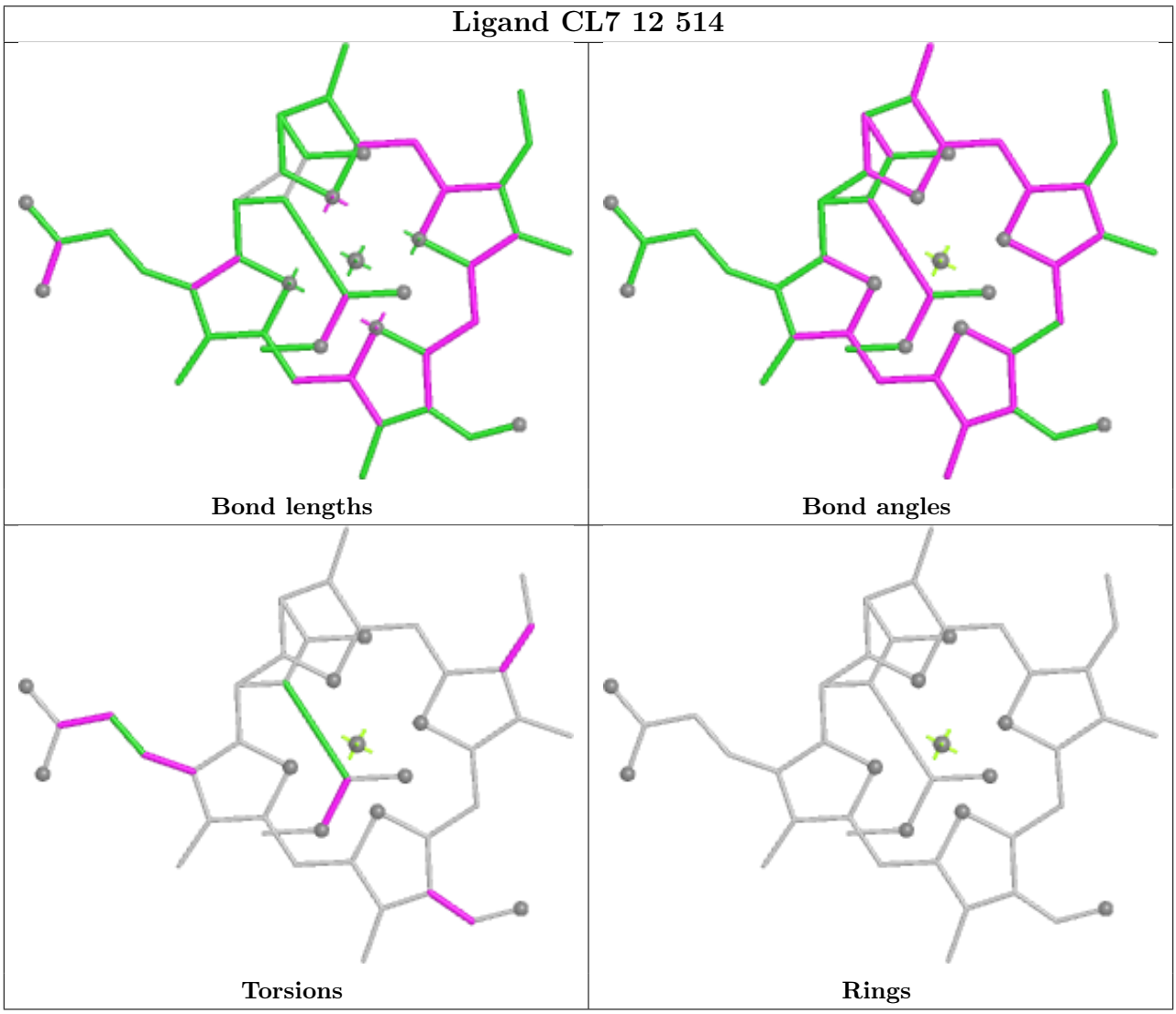


Rings

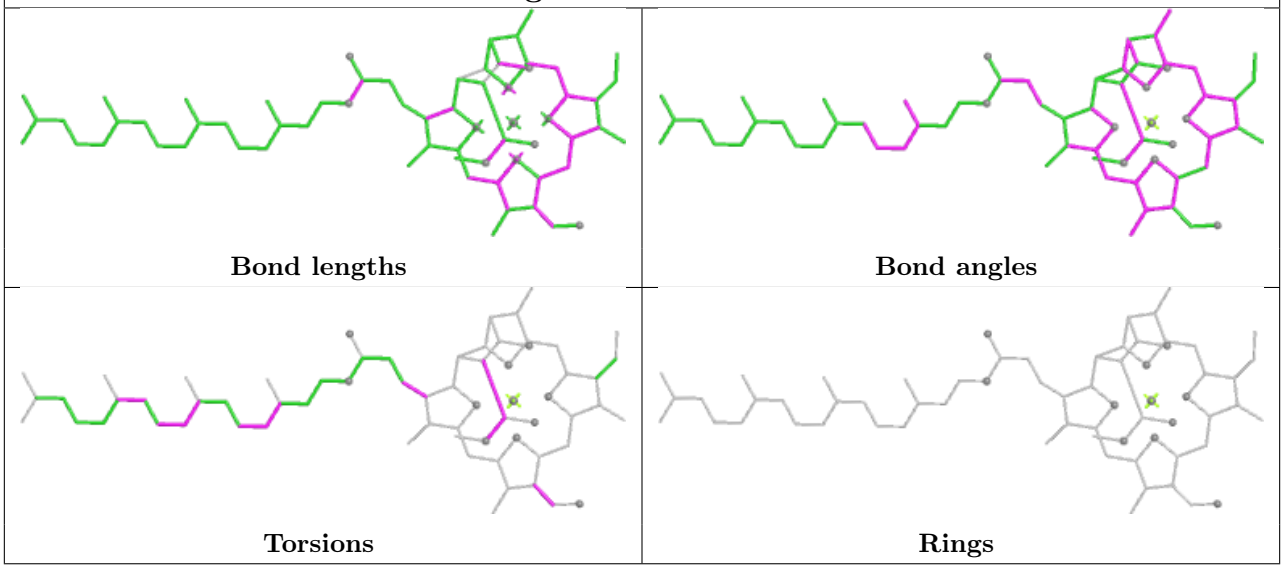
Ligand CL7 42 517



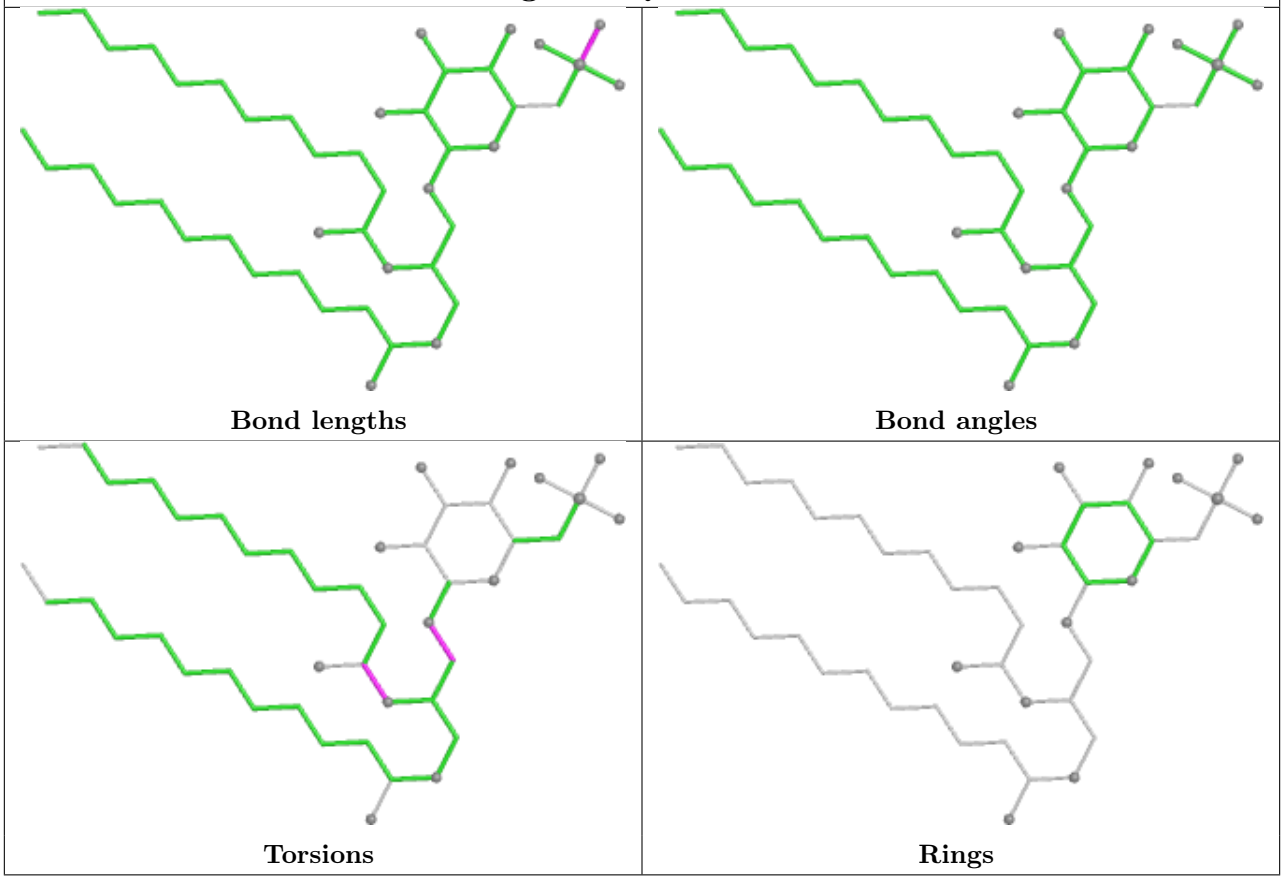
Ligand CL7 12 514



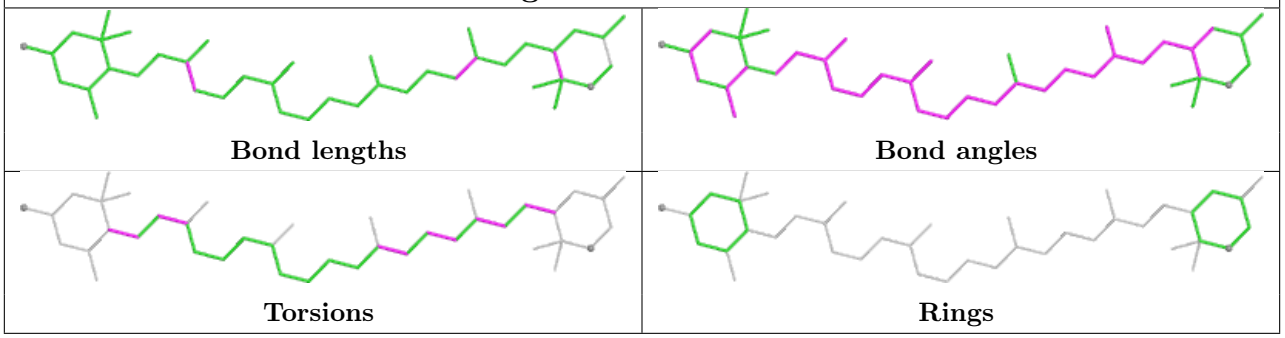
Ligand CL7 32 506



Ligand SQD 33 521



Ligand ZEX 33 519



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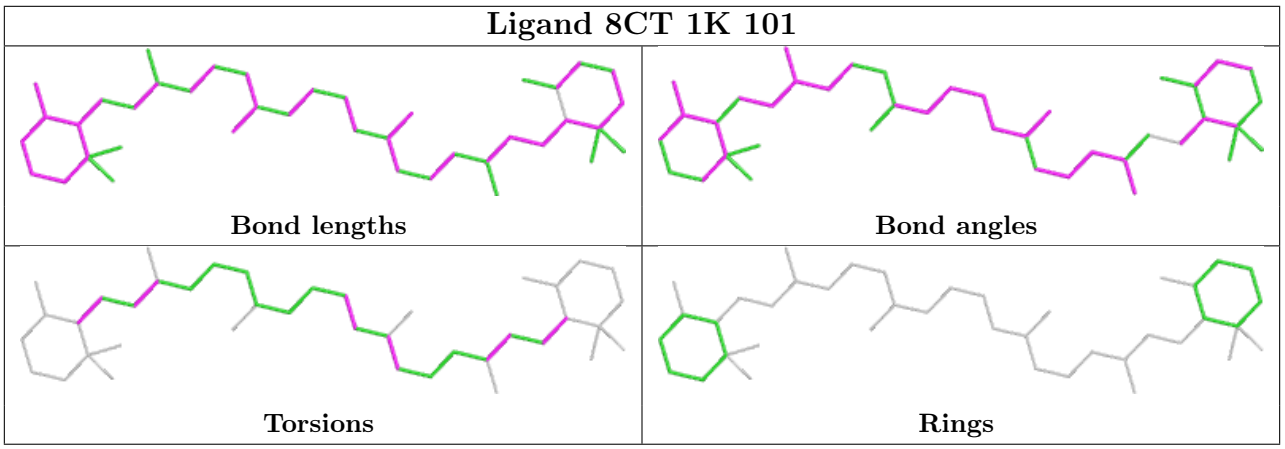

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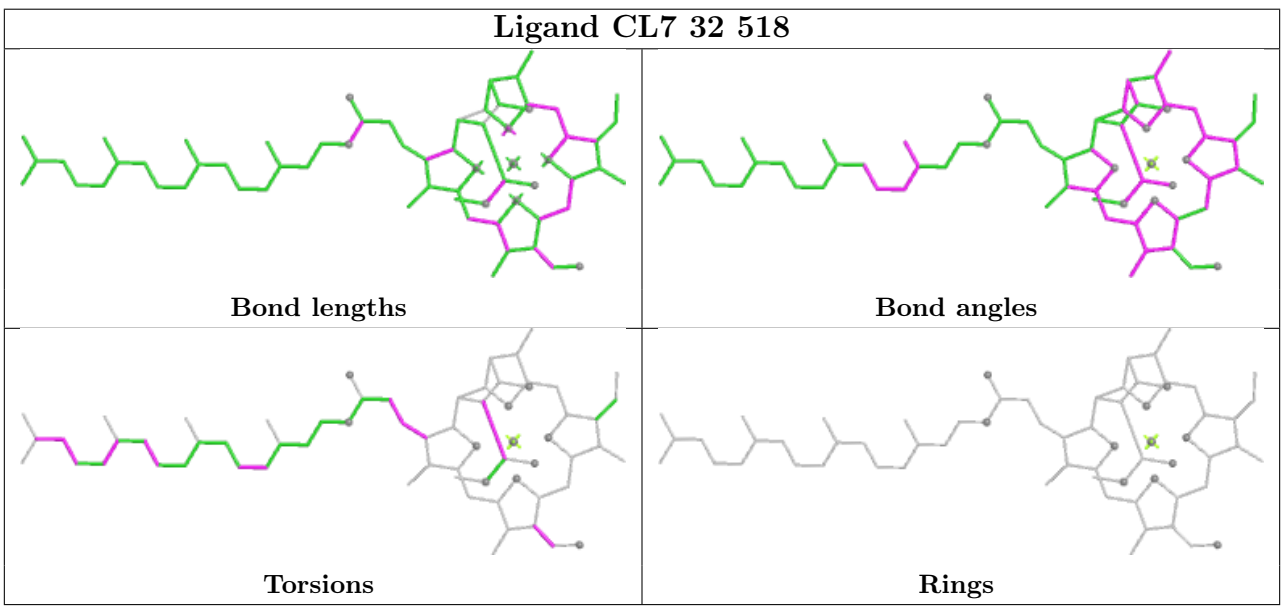
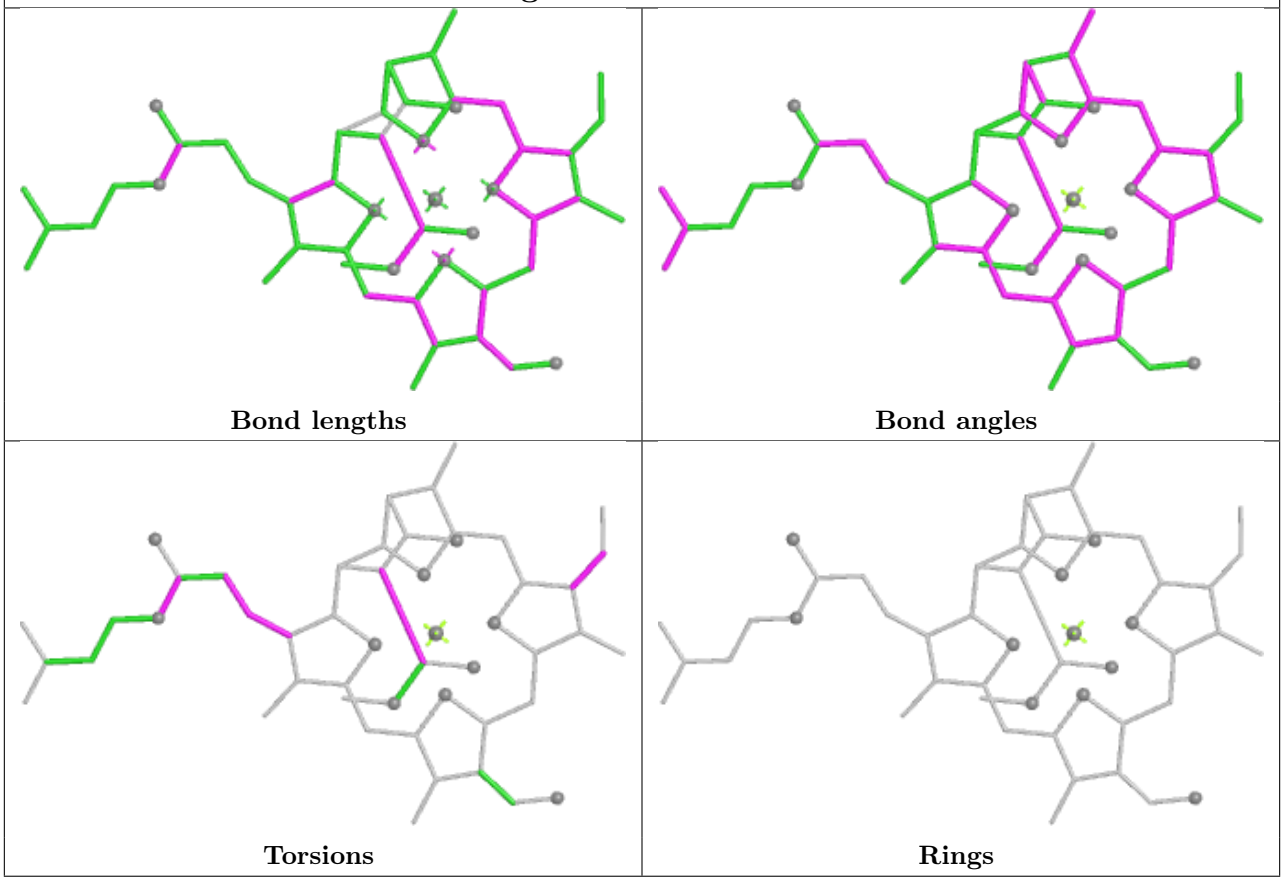


Ligand CL7 4B 616



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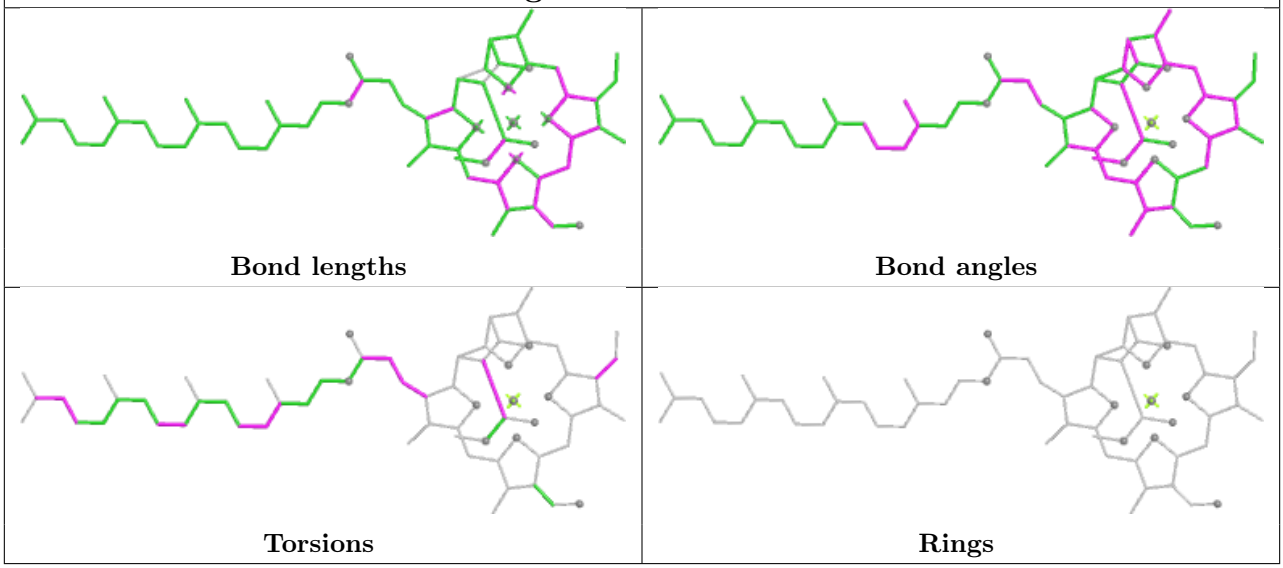

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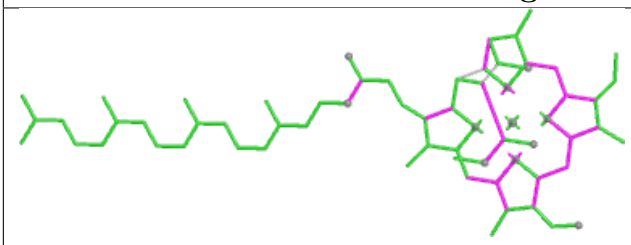
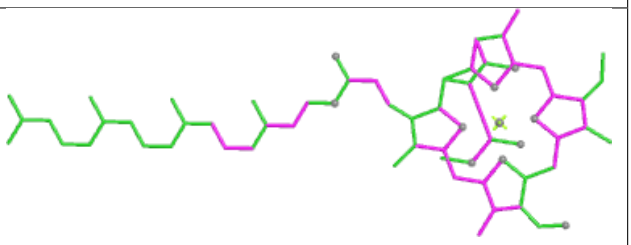
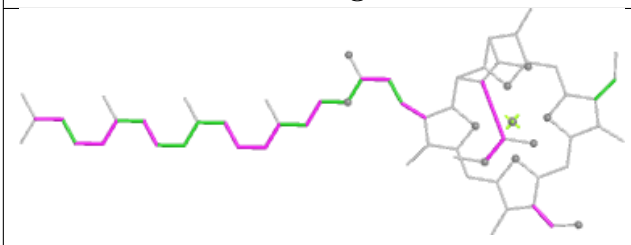


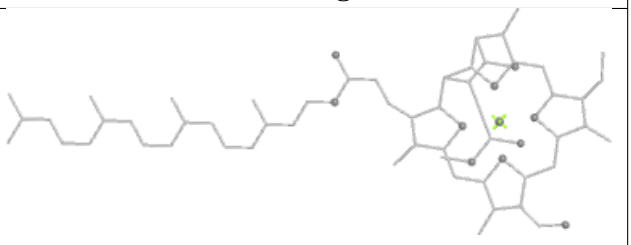
Bond lengths



Bond angles

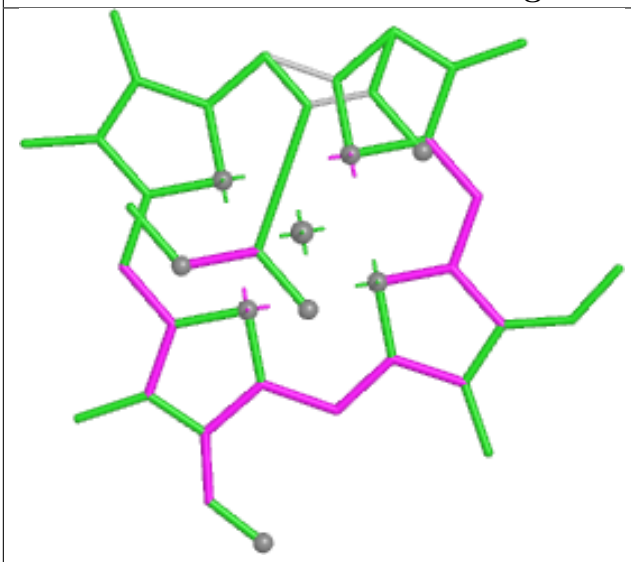


Torsions



Rings

Ligand CL7 41 407



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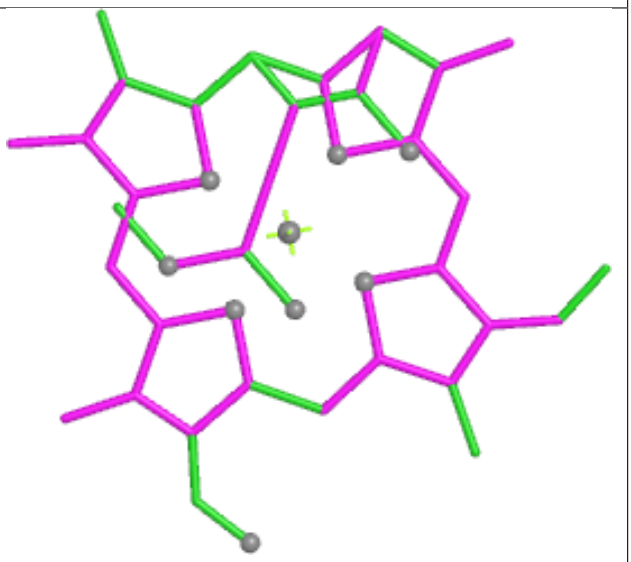
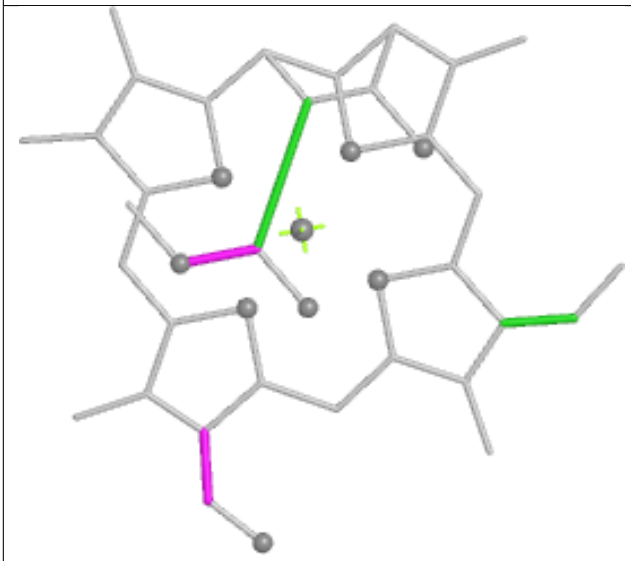


Bond angles



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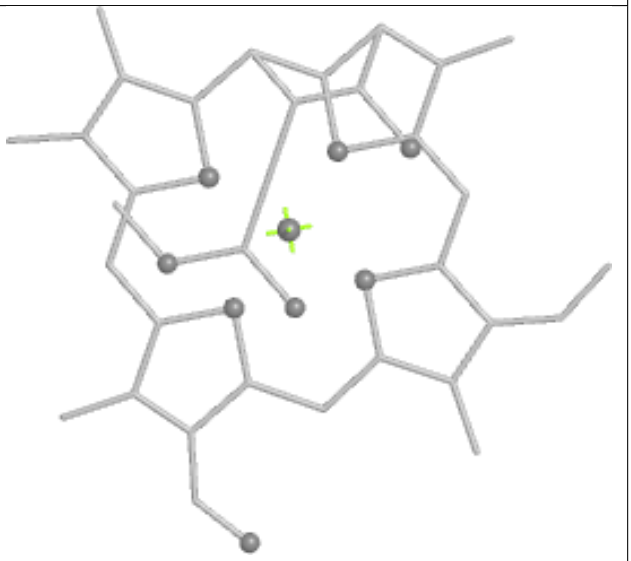
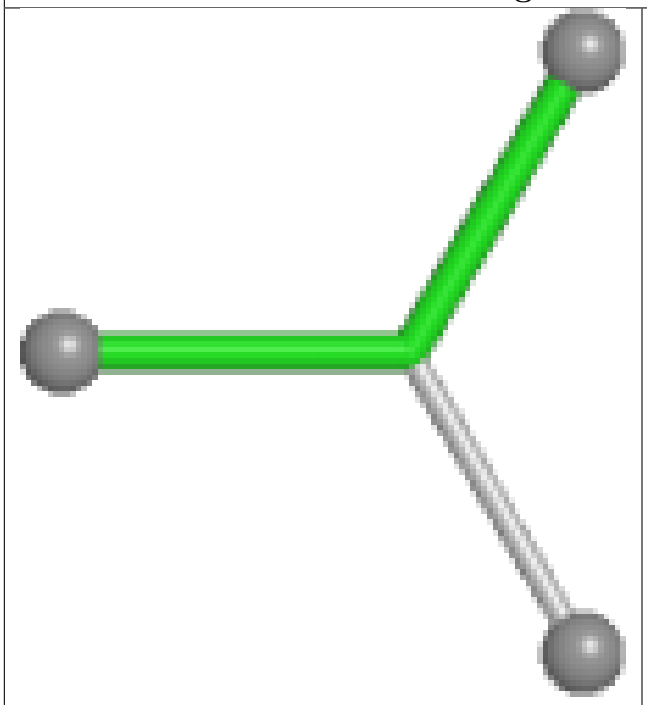


Rings

Ligand BCT 3D 403



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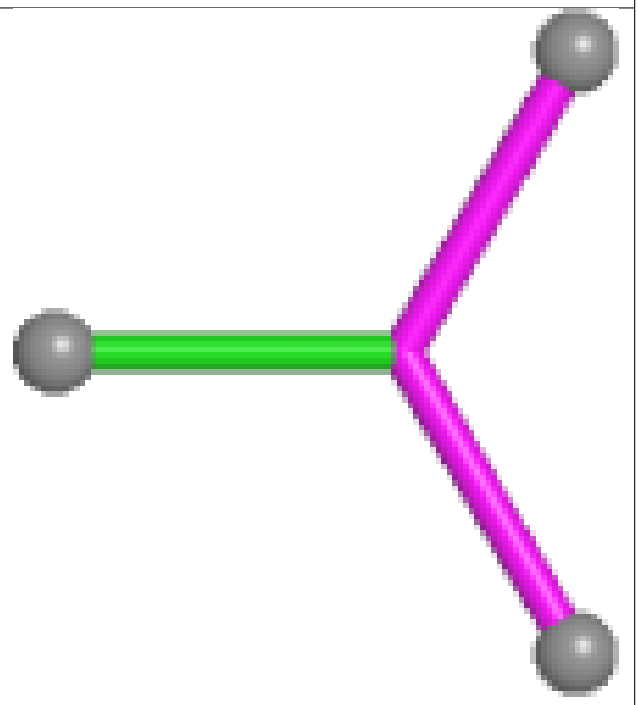
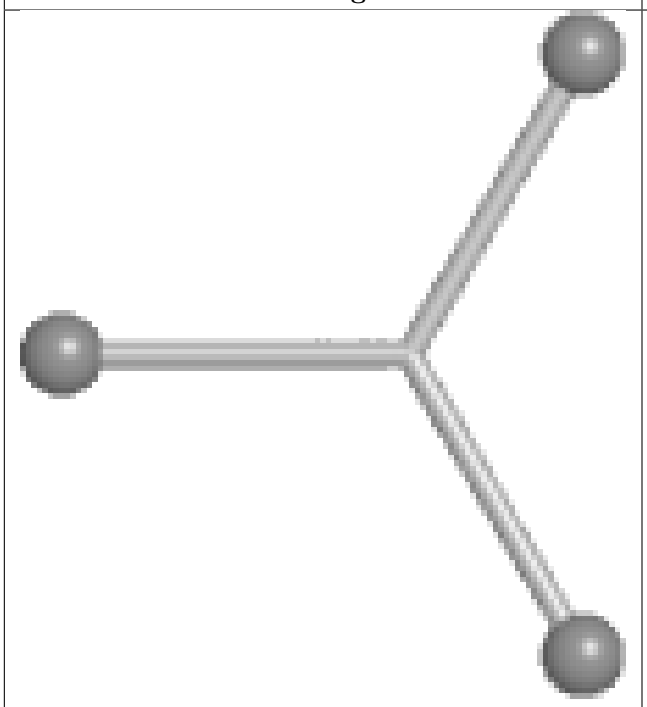


Bond angles



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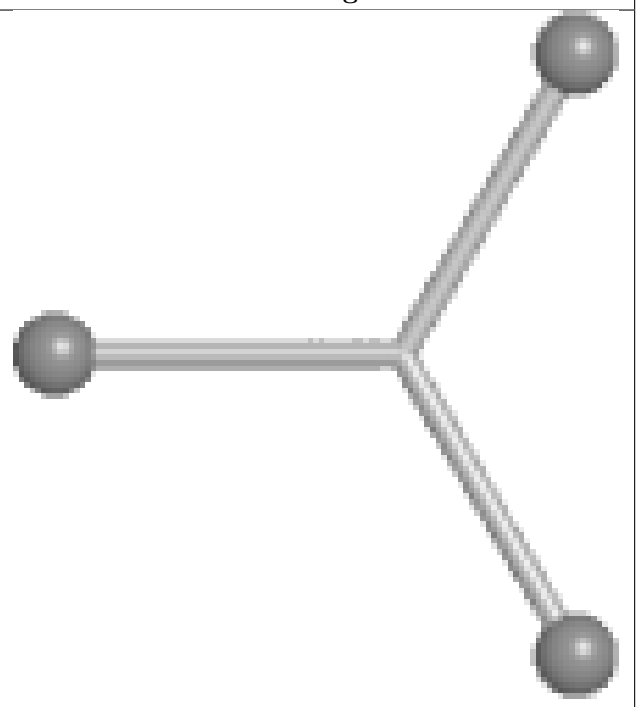
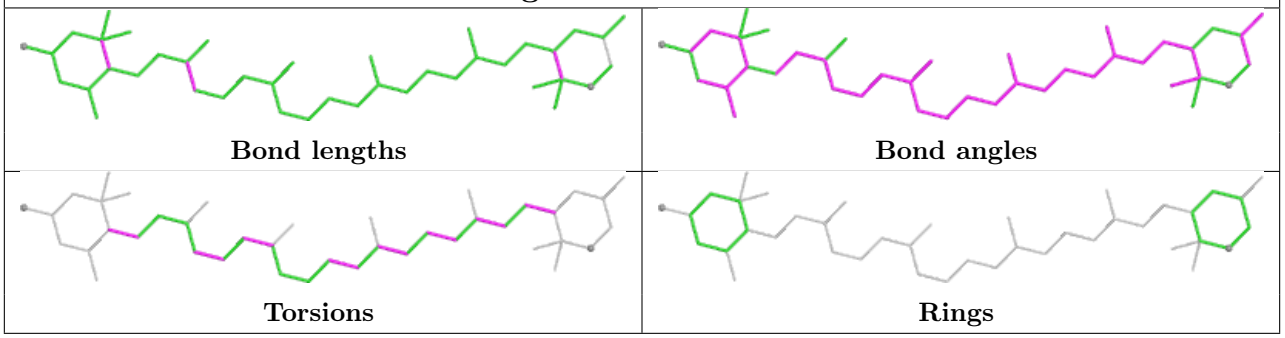
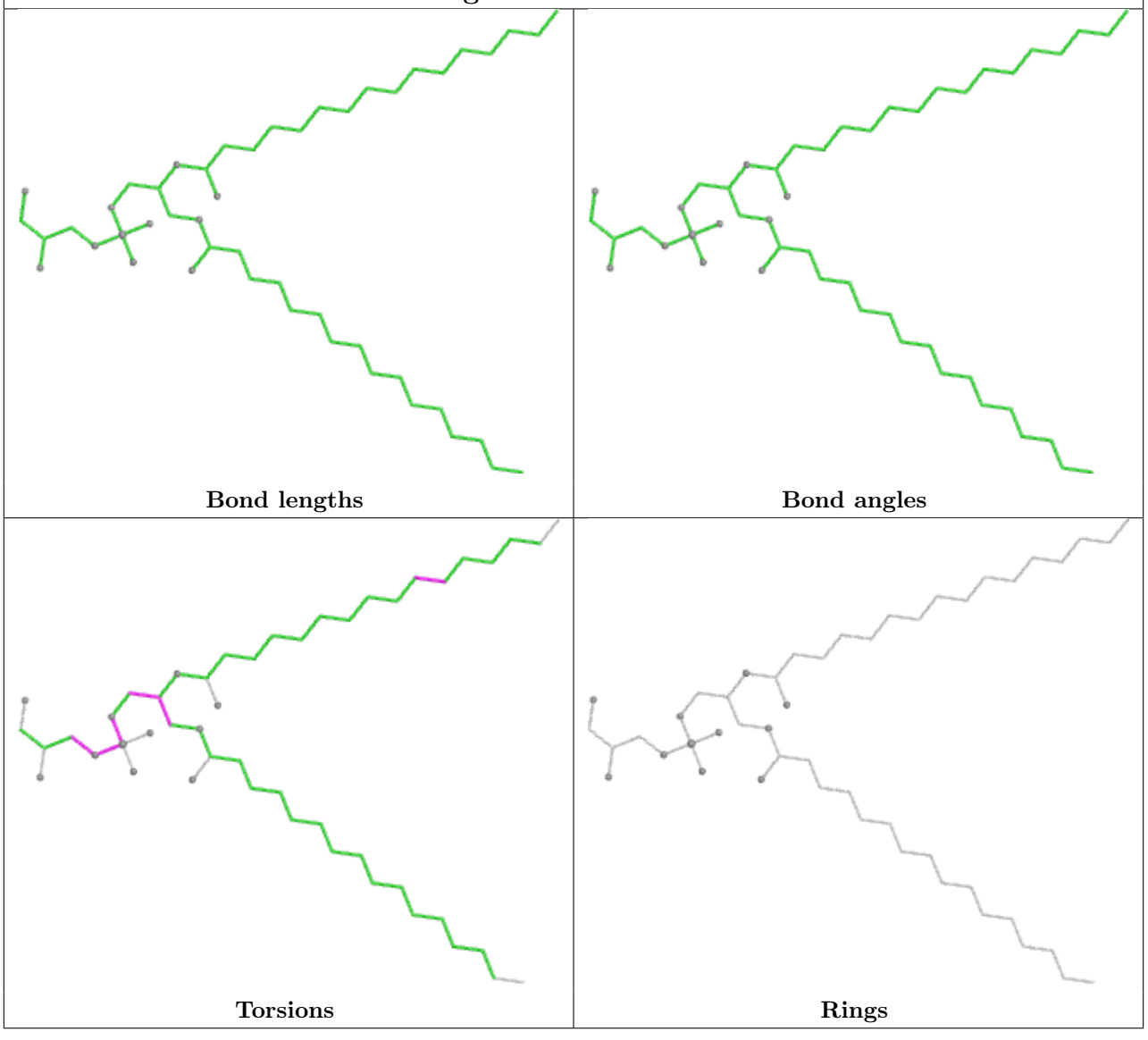


Rings

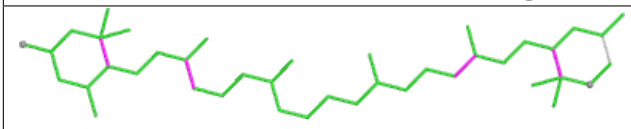
Ligand ZEX 24 420



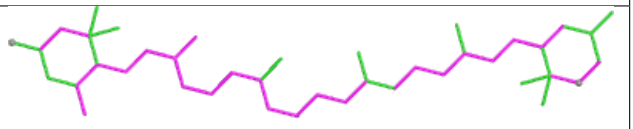
Ligand LHG 34 401



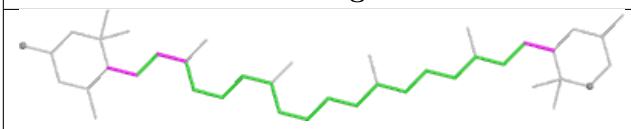
Ligand ZEX 13 522



Bond lengths



Bond angles



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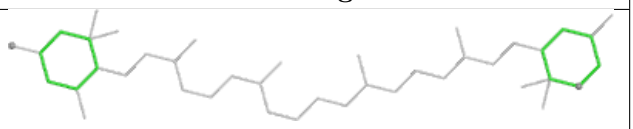
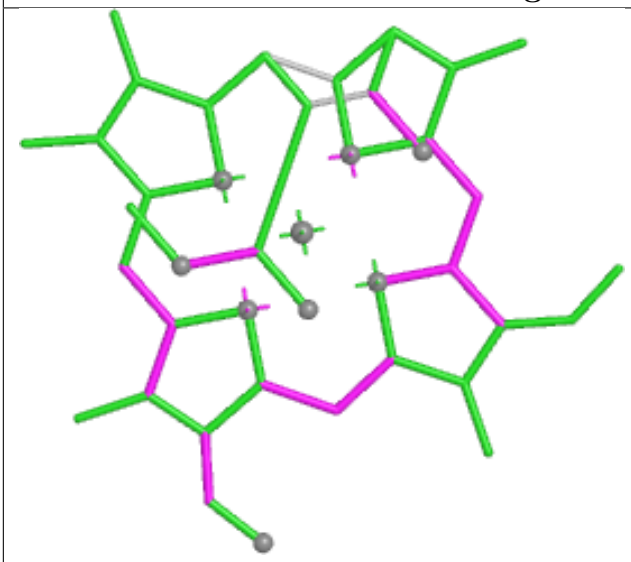


Rings

Ligand CL7 31 416



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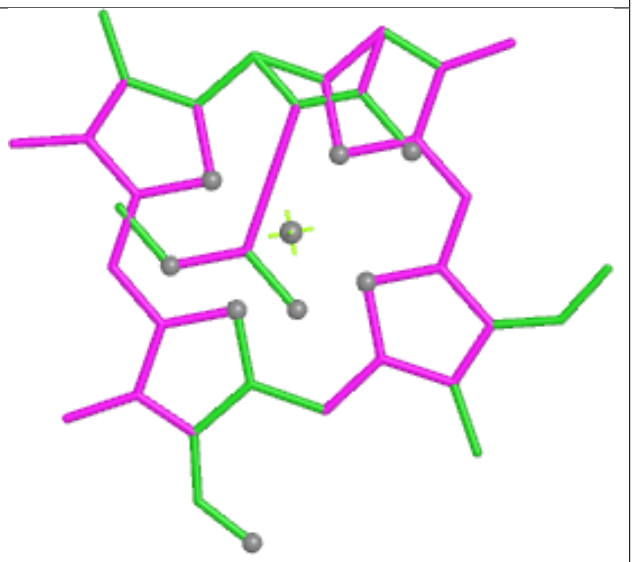

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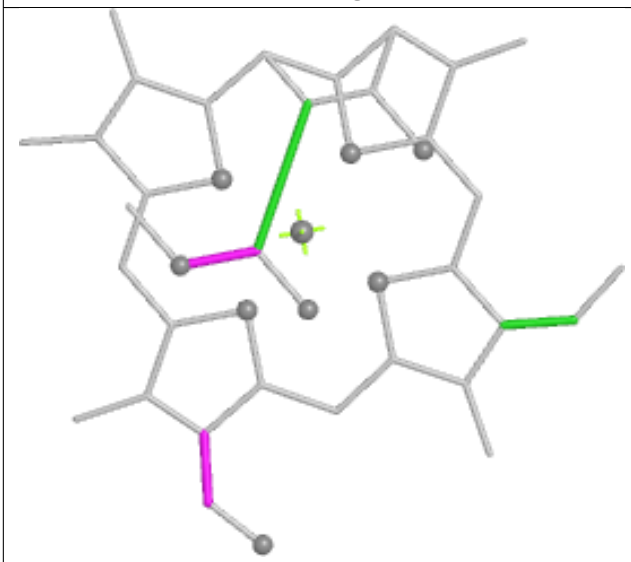

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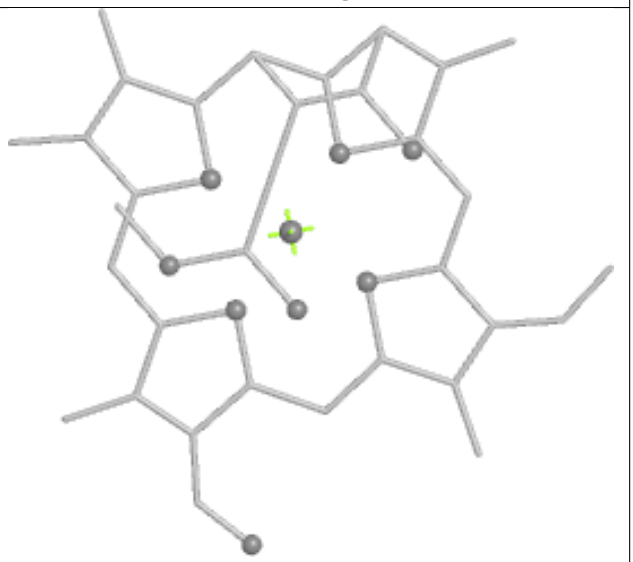
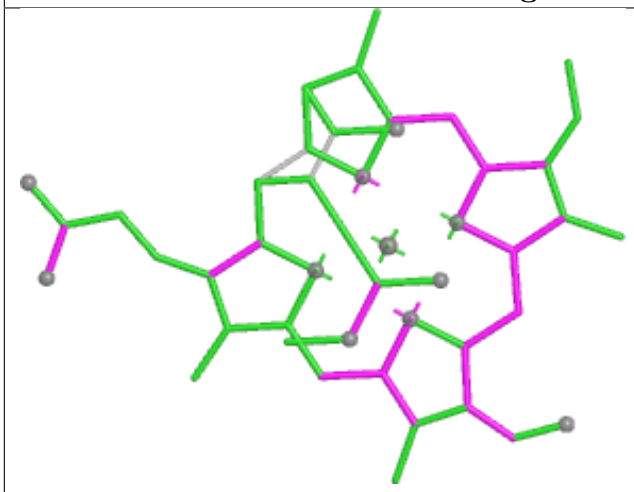


Rings

Ligand CL7 3D 405



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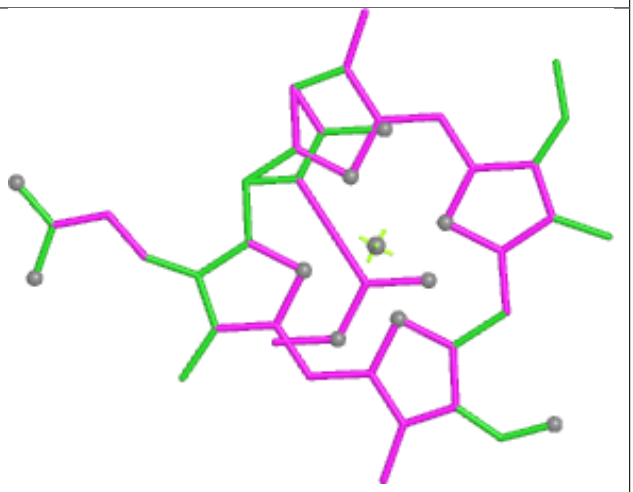
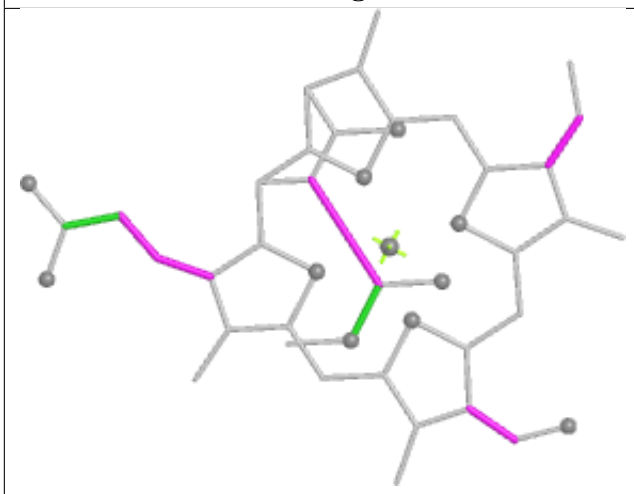


Bond angles

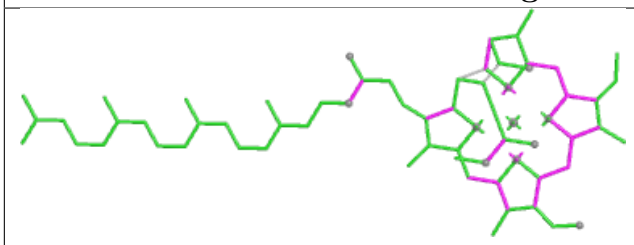


Torsions



Rings

Ligand CL7 3B 609



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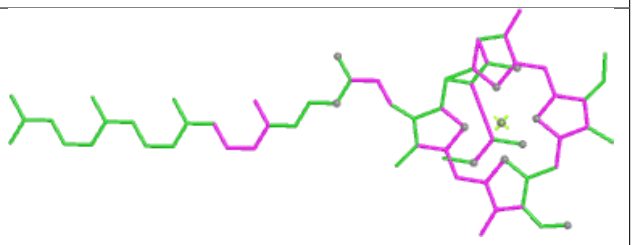
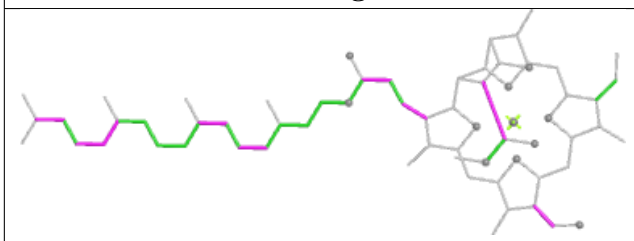


Bond angles



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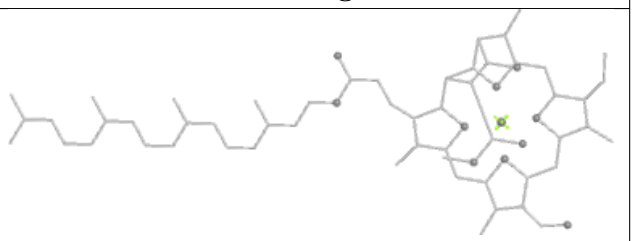

Rings

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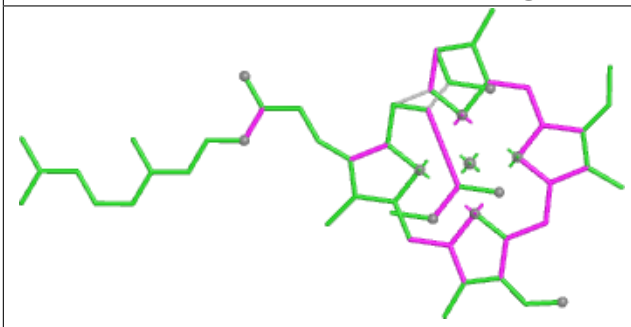

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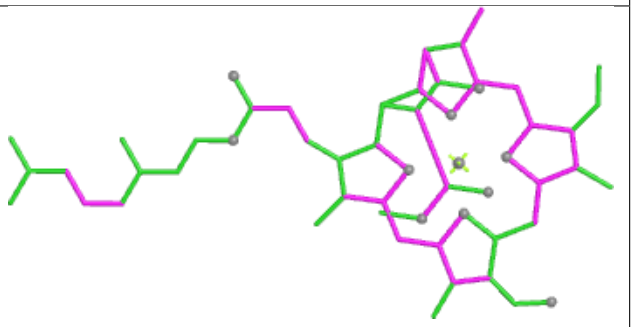
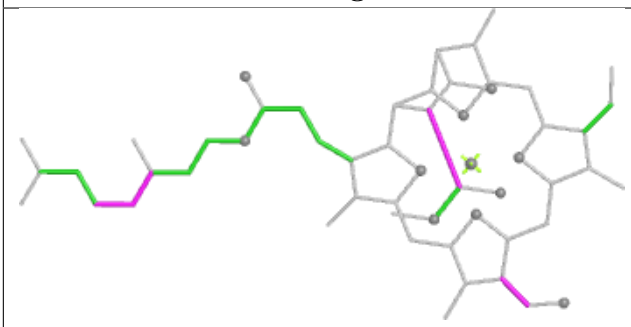


Bond angles



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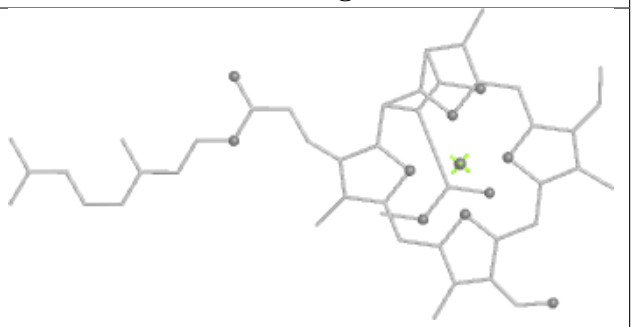
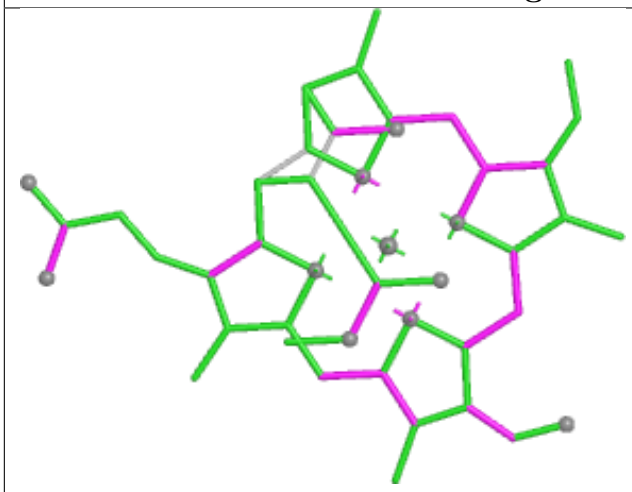
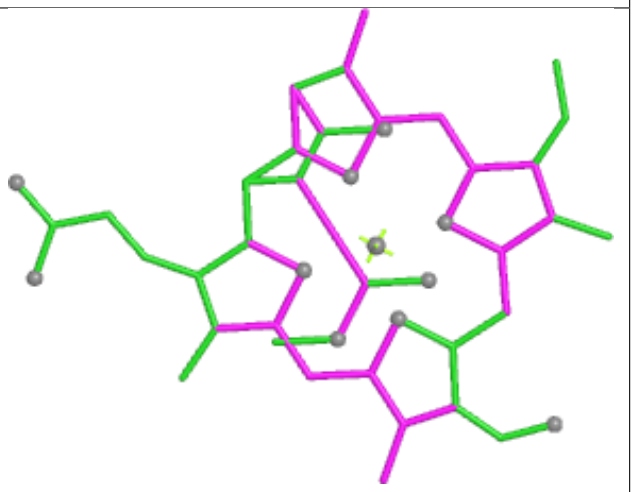


Rings

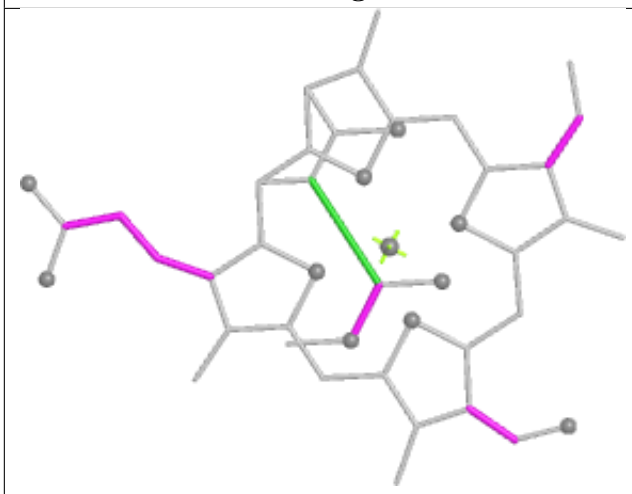
Ligand CL7 41 419



Bond lengths



Bond angles

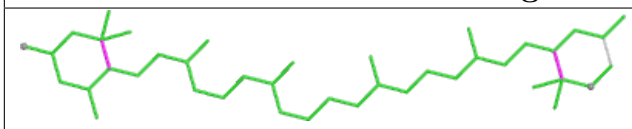


Torsions

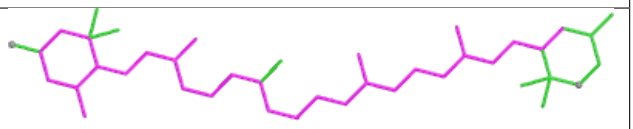


Rings

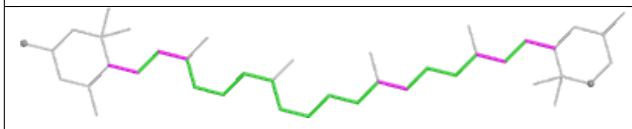
Ligand ZEX 43 421



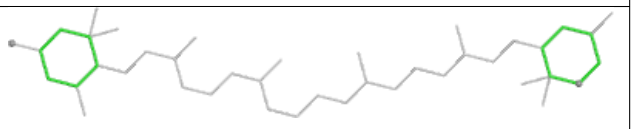
Bond lengths



Bond angles

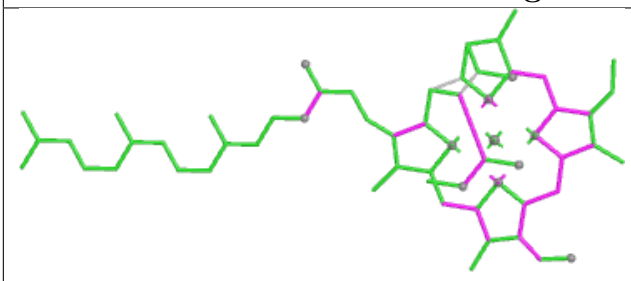


Torsions



Rings

Ligand CL7 34 409



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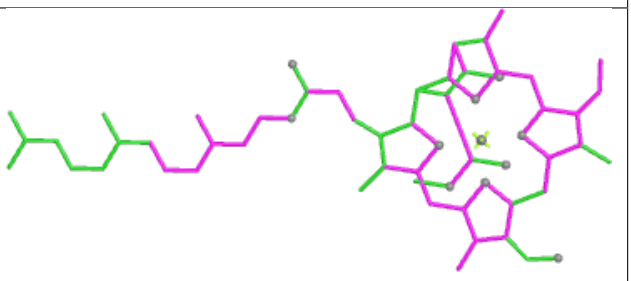

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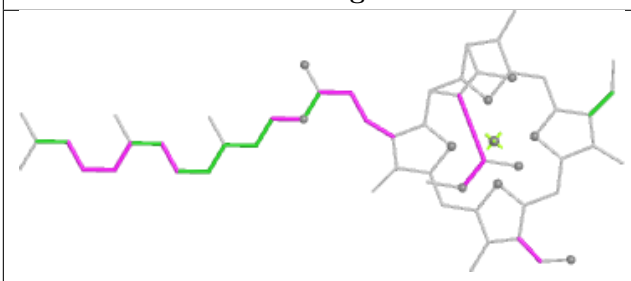

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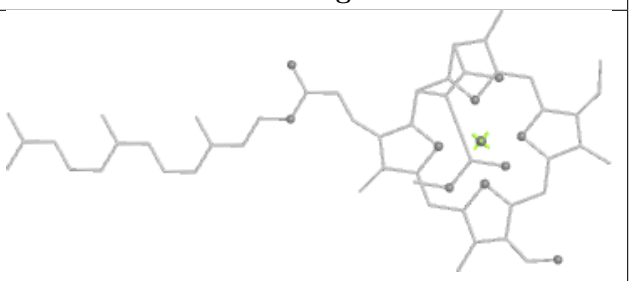

Rings

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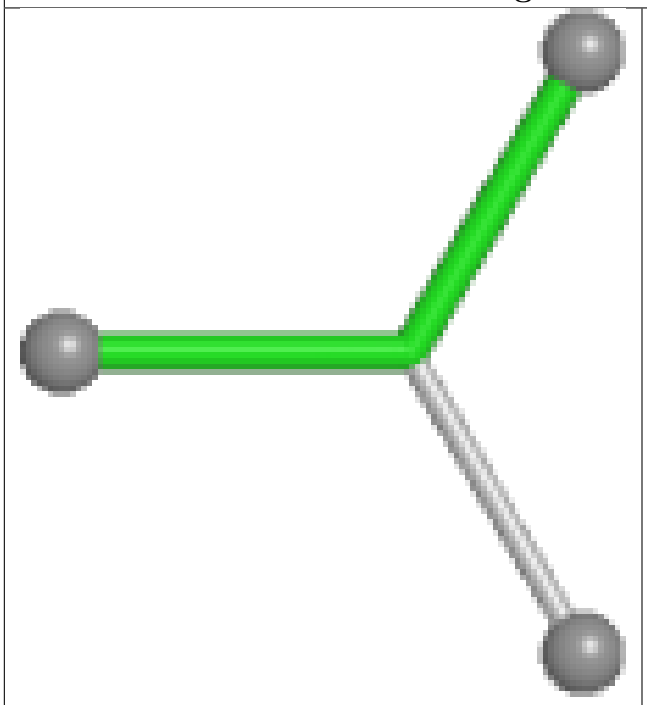

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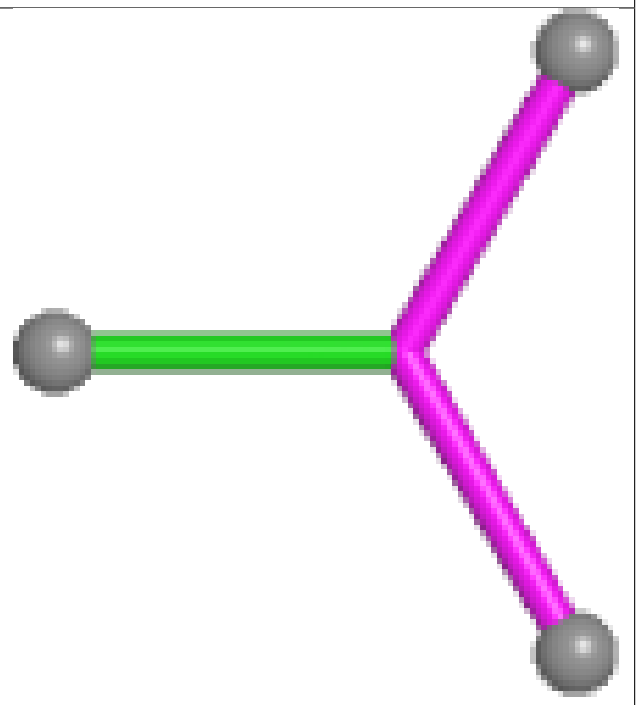

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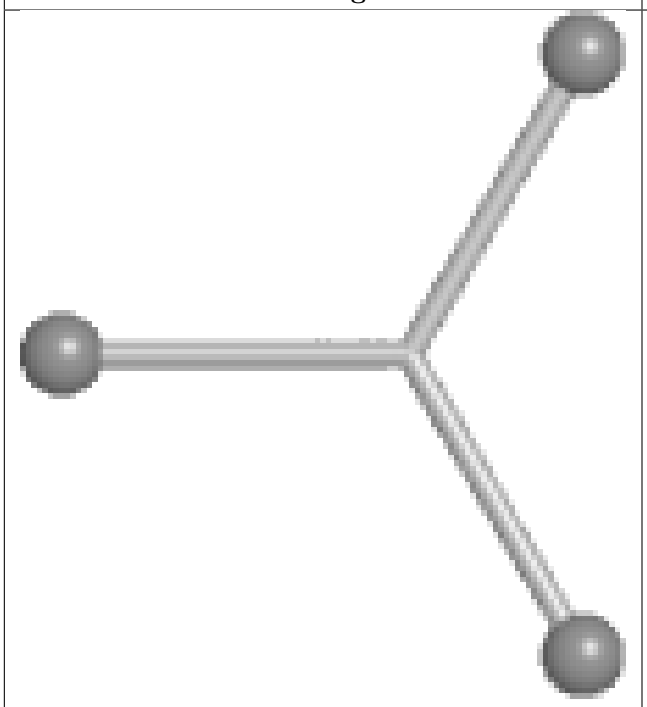

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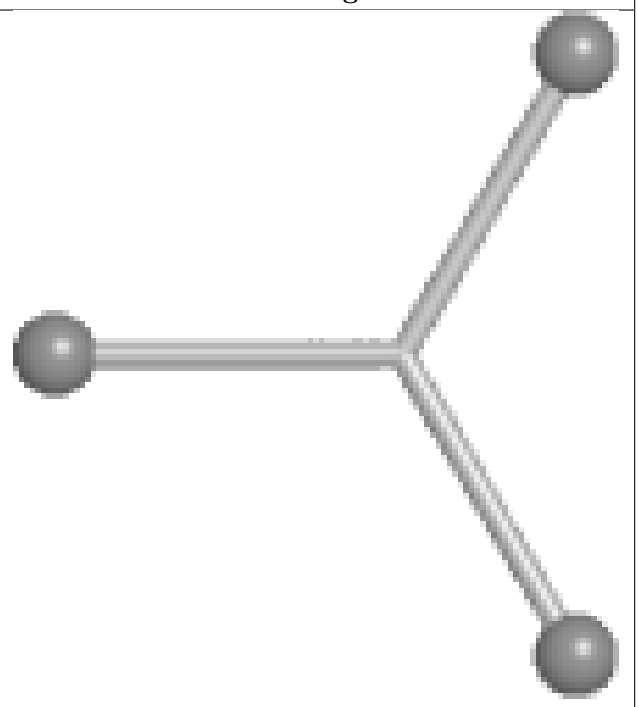

Rings

Ligand CL7 32 508



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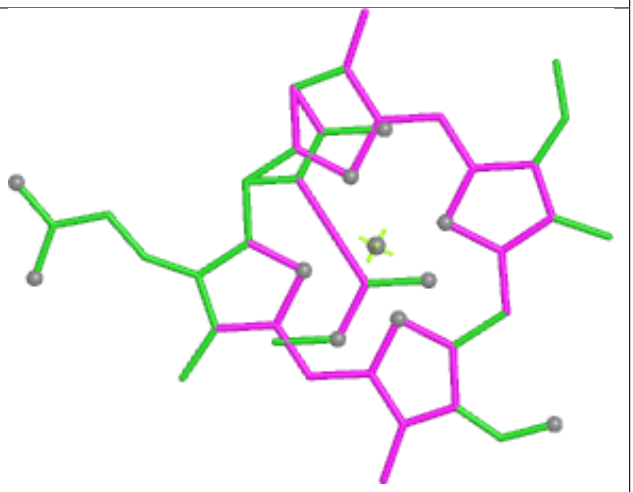

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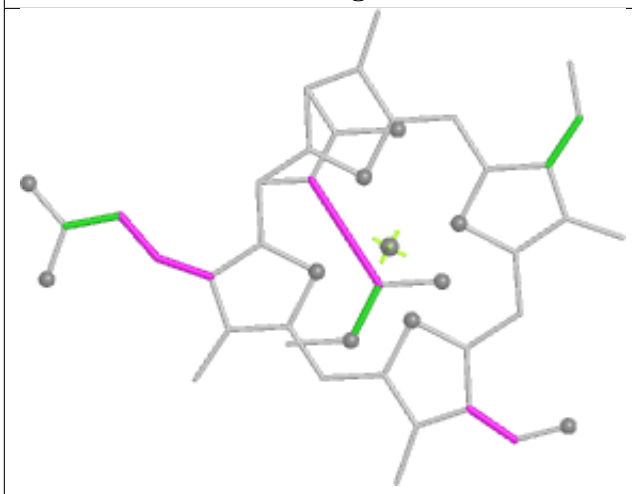

Torsions



Rings

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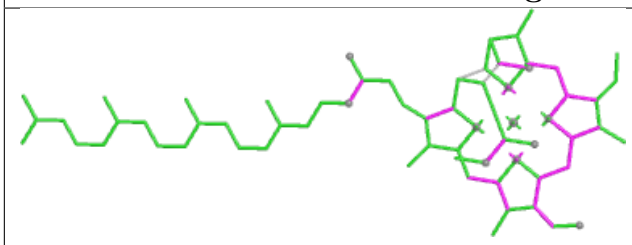

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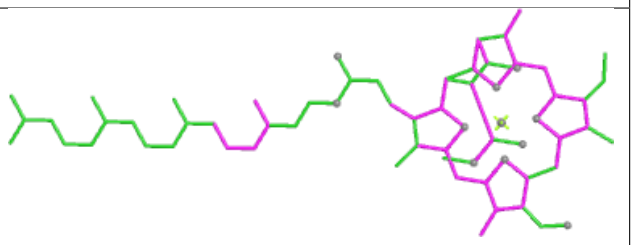

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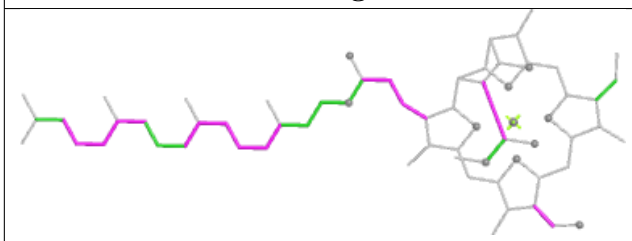

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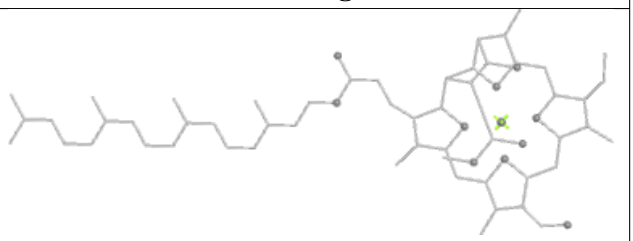

Rings

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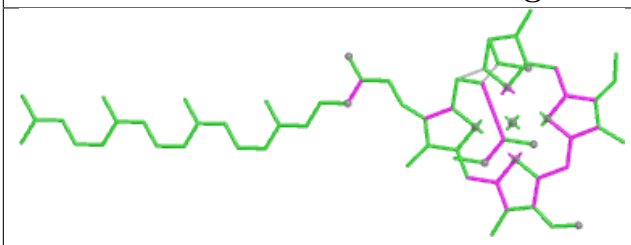

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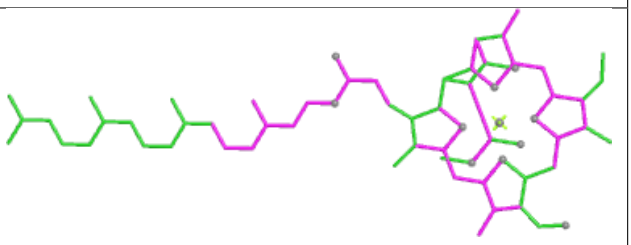

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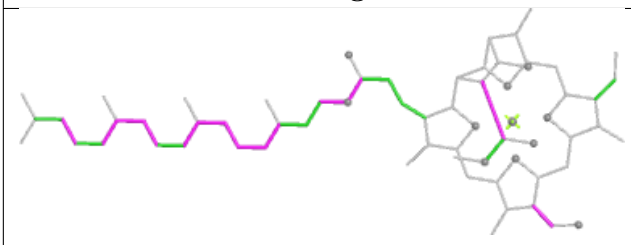

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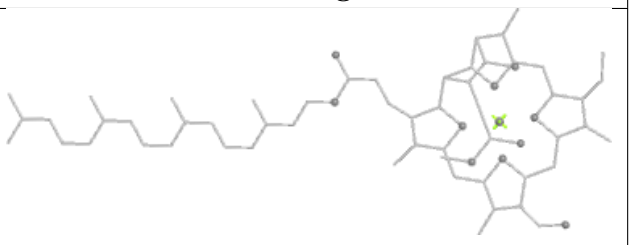

Rings

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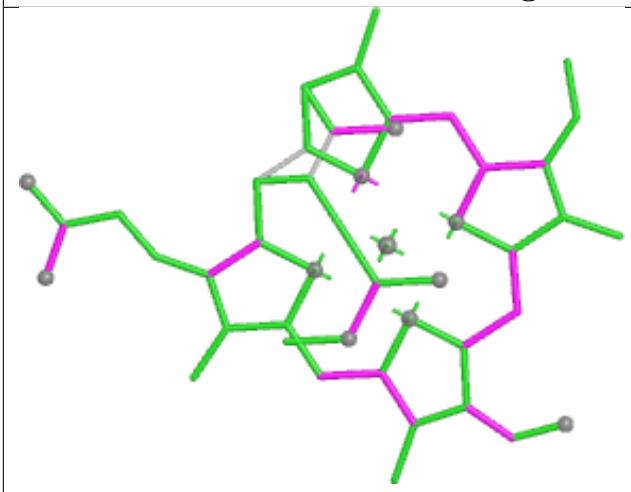
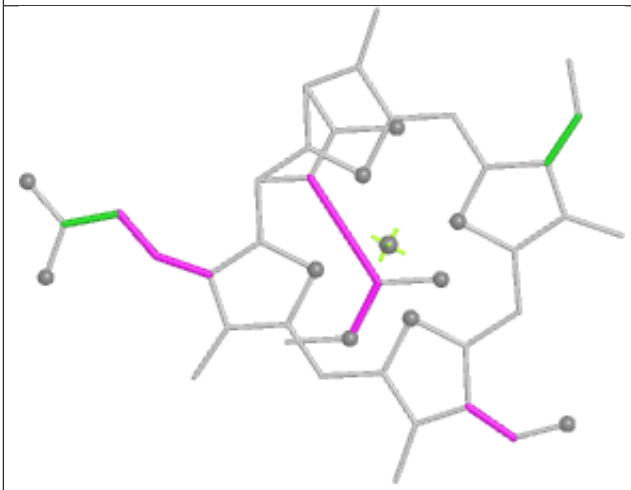


Bond lengths



Bond angles



Torsions



Rings

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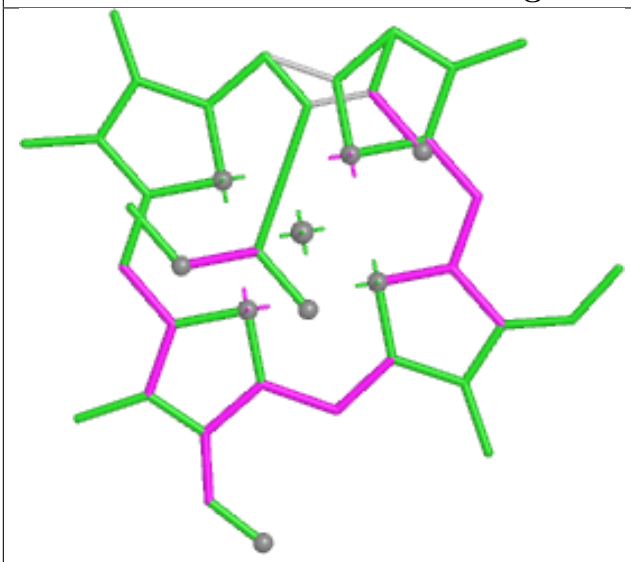

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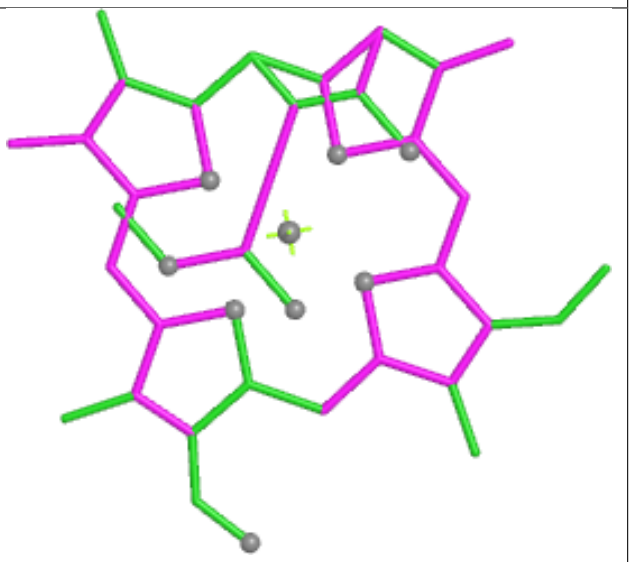

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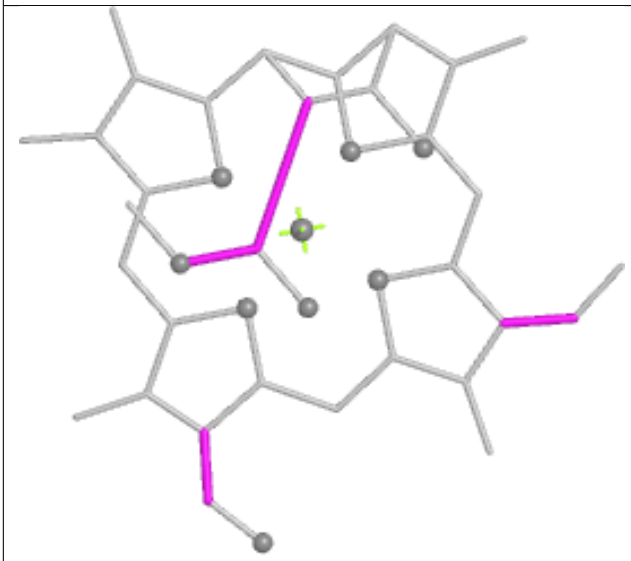

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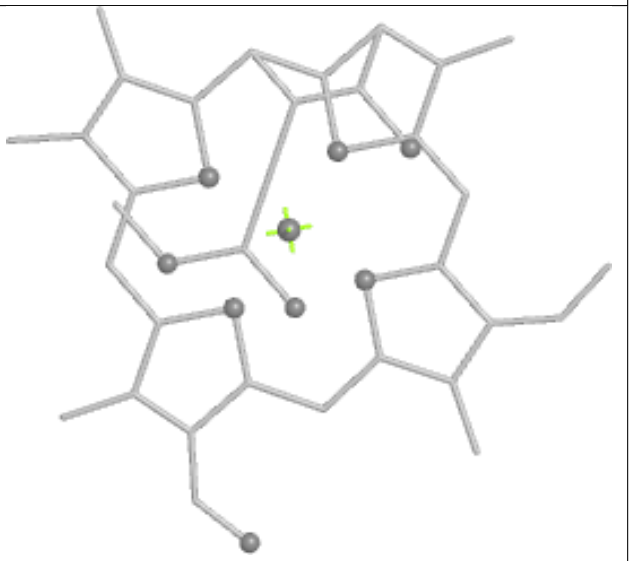
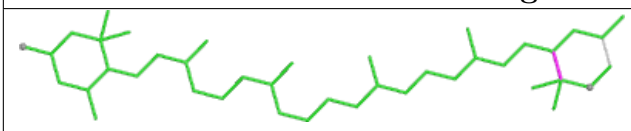


Rings

Ligand ZEX 44 418



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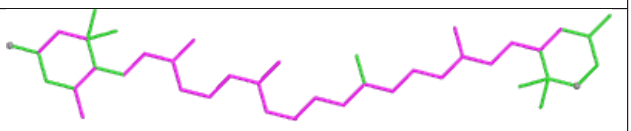

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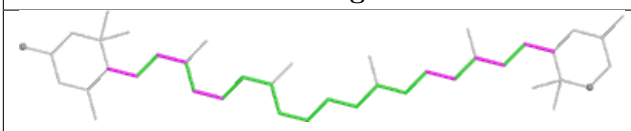

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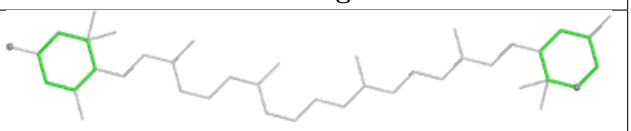
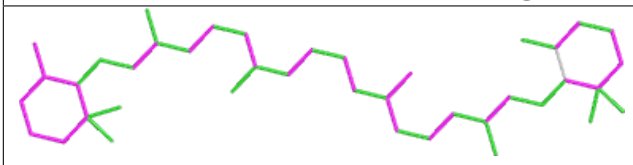


Rings

Ligand 8CT 2C 515



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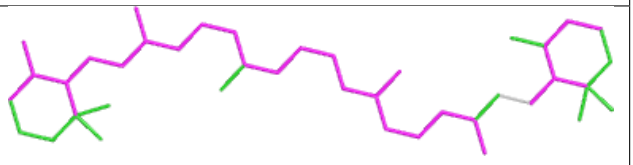

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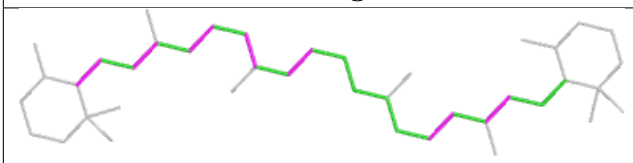

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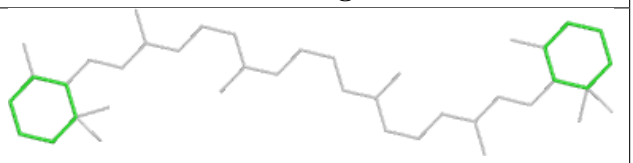
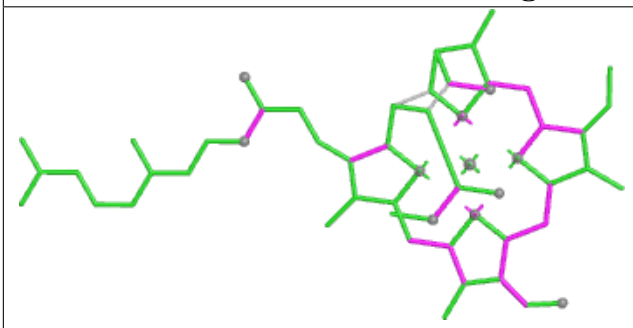


Rings

Ligand CL7 4C 504



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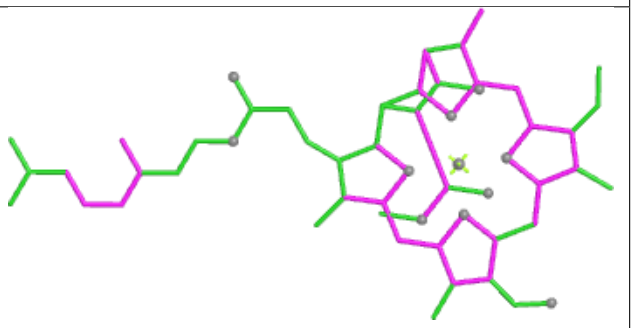

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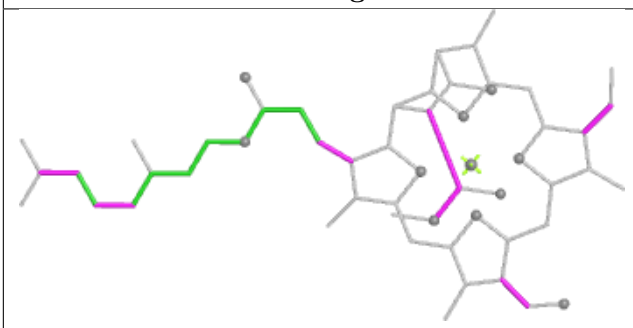

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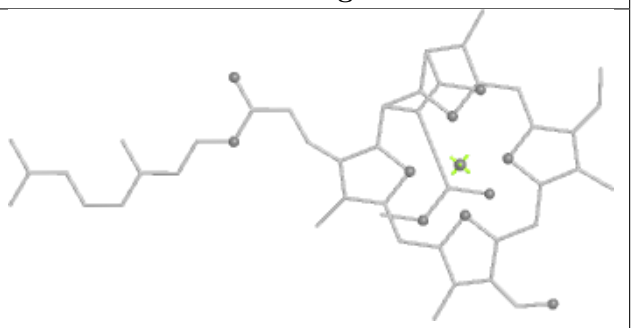

Rings

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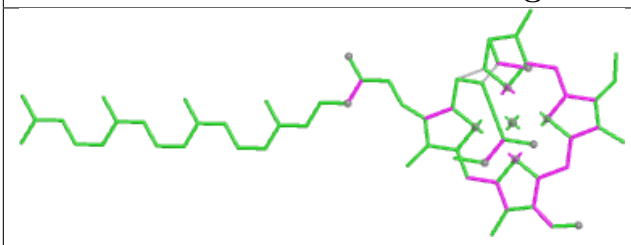

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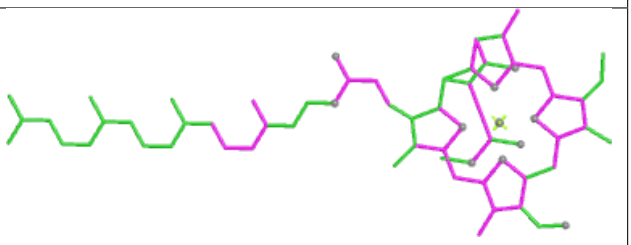

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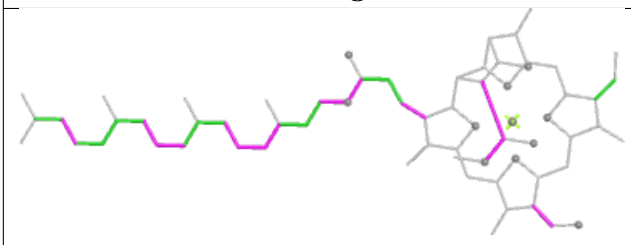

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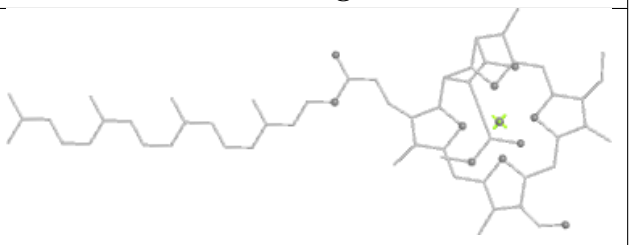
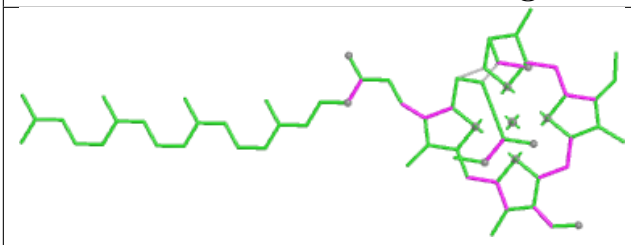


Rings

Ligand CL7 4A 401



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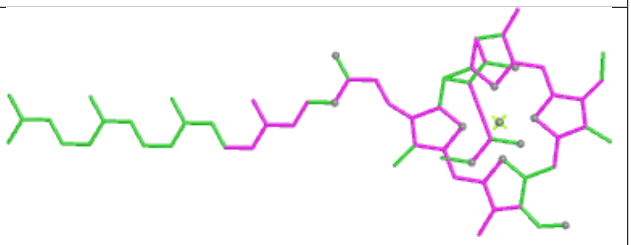

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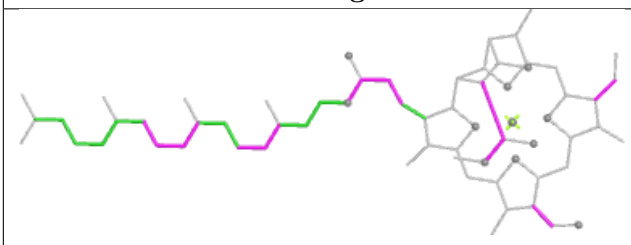

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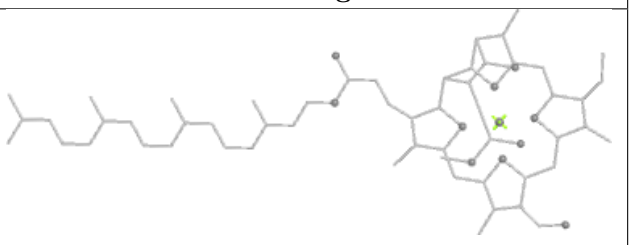
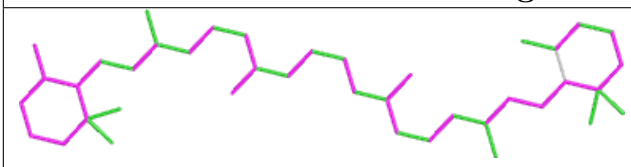


Rings

Ligand 8CT 3K 101



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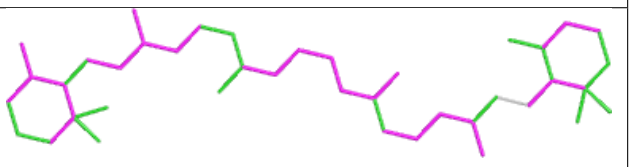

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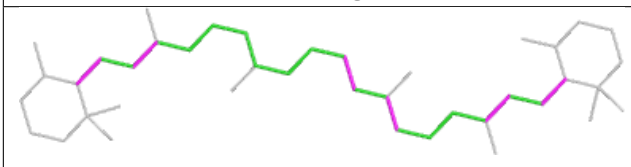

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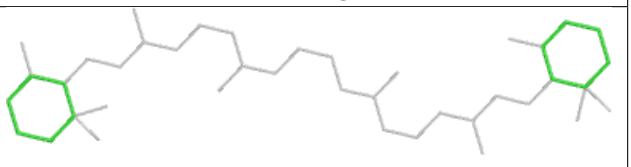
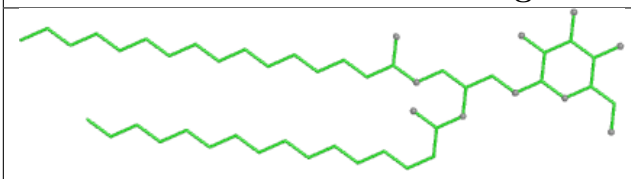


Rings

Ligand LMG 11 401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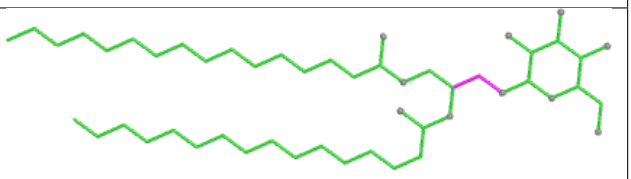
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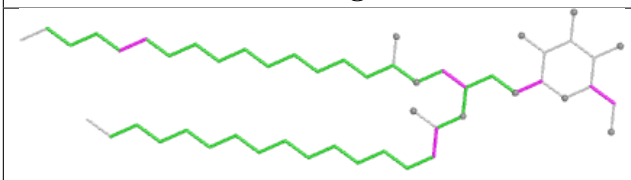
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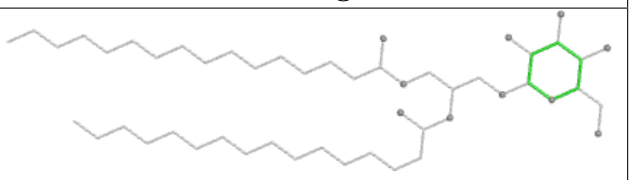
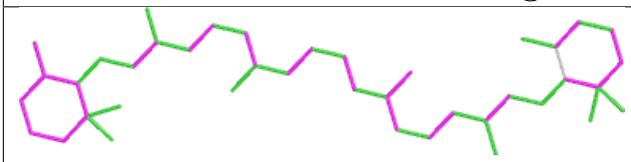

Rings

Ligand 8CT 24 402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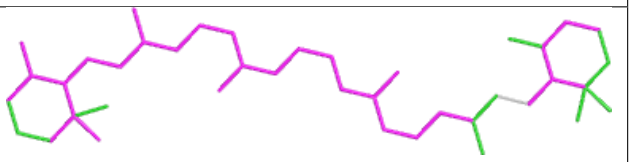
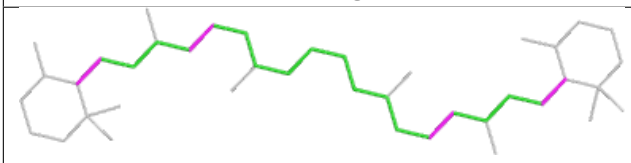

Bond angles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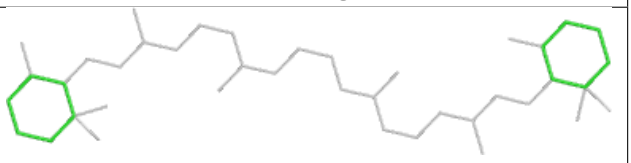
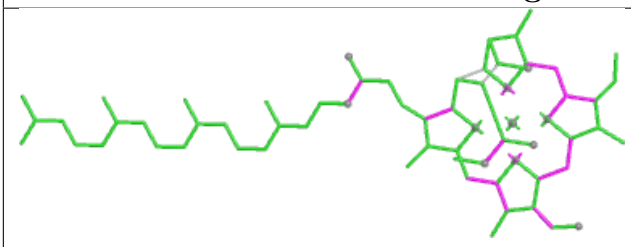
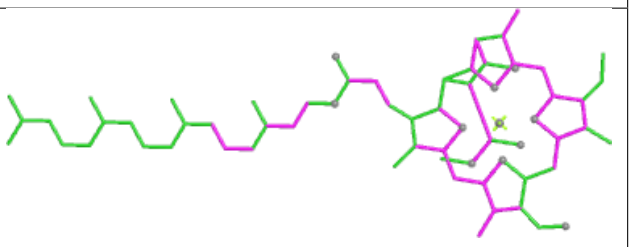
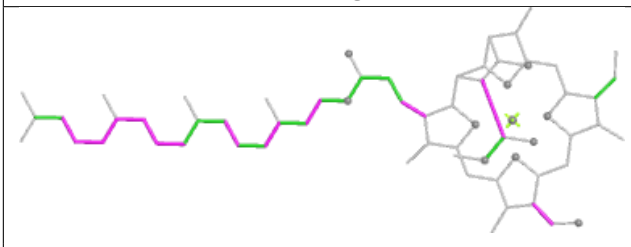
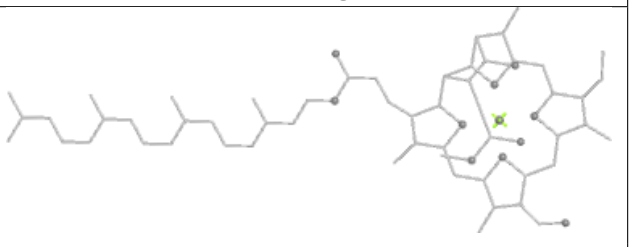

Rings

Ligand CL7 41 404

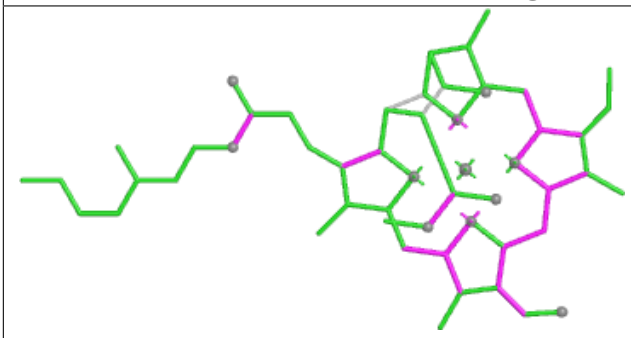

Bond lengths


Bond angles


Torsions


Rings

Ligand CL7 14 414



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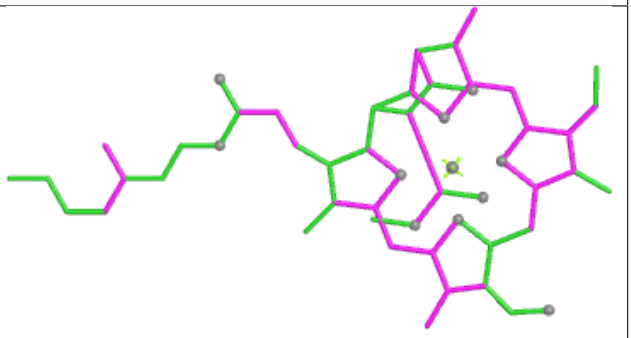

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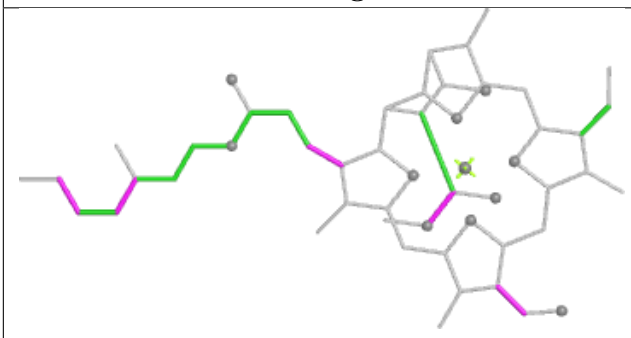

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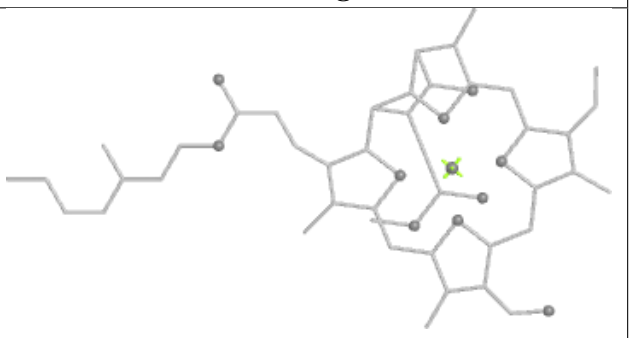
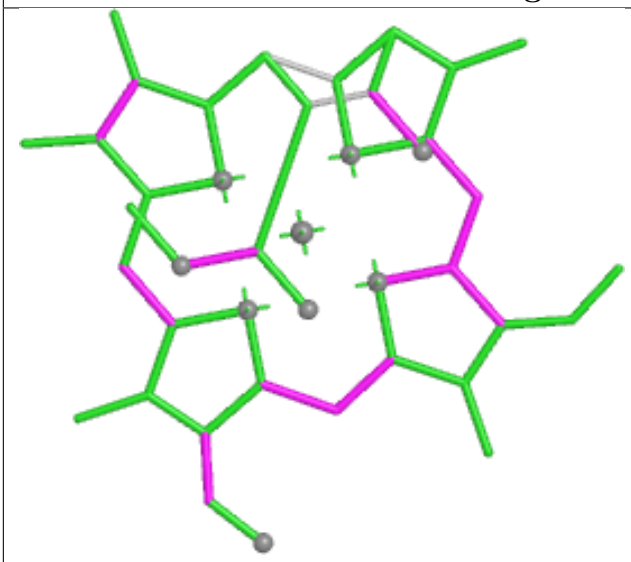


Rings

Ligand CL7 41 415



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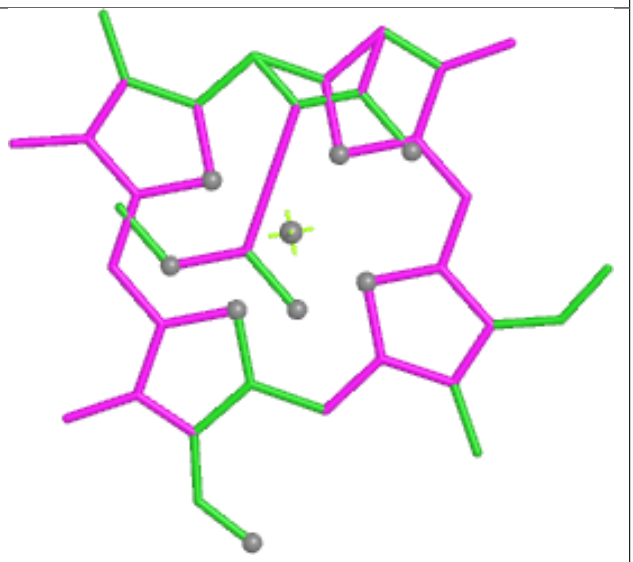

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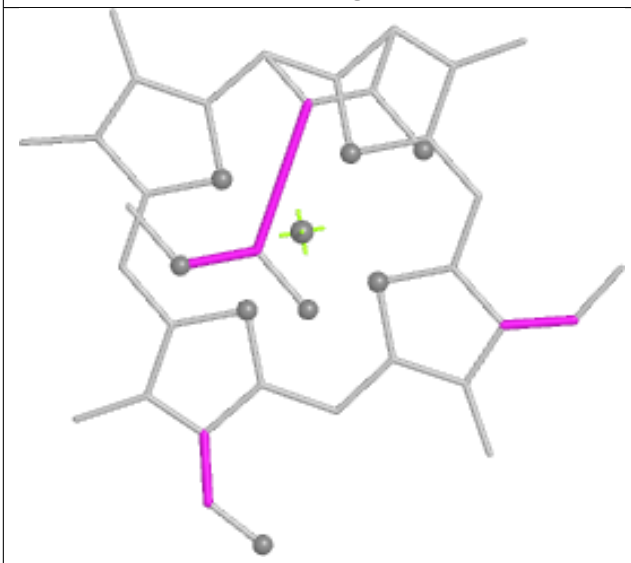

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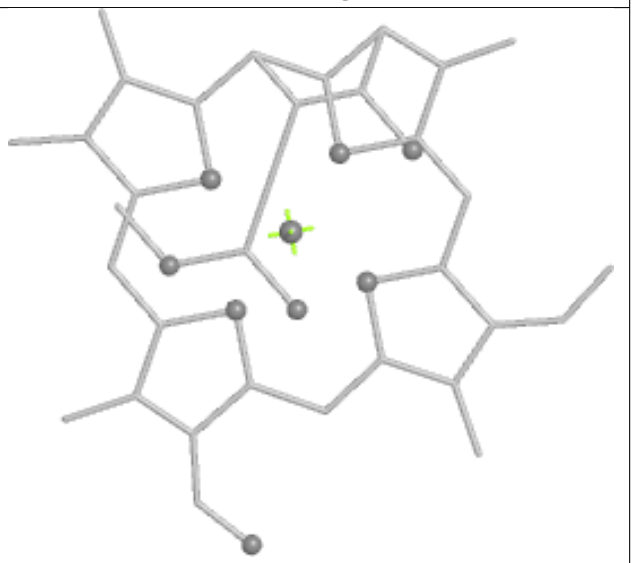
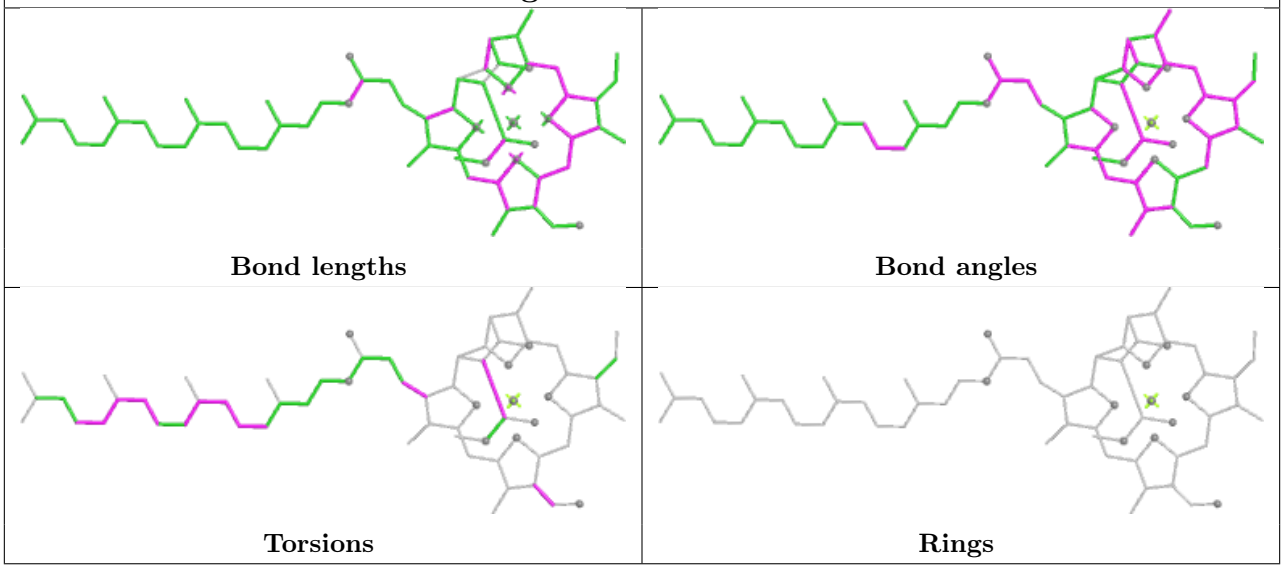


Rings

Ligand CL7 2B 613



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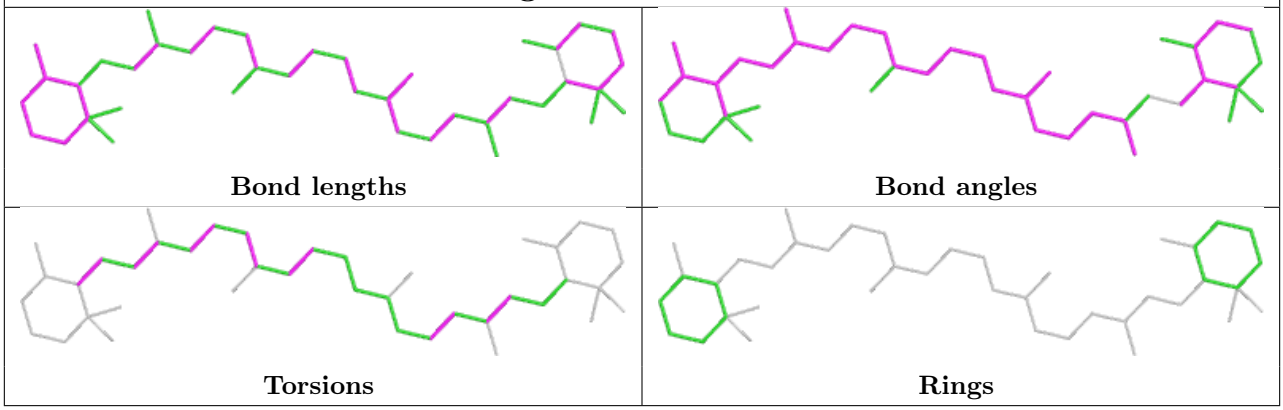

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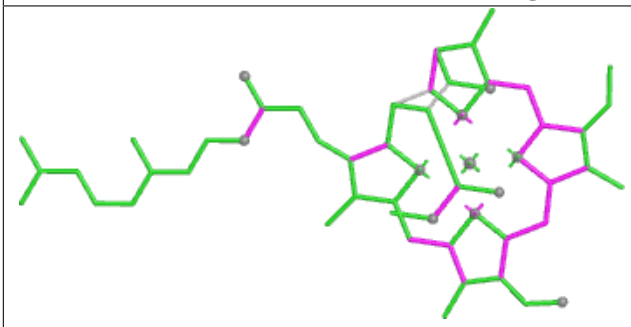

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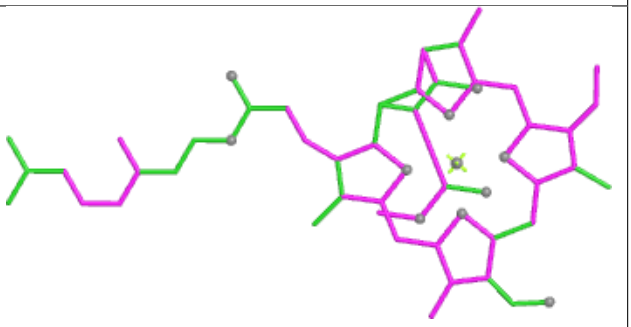

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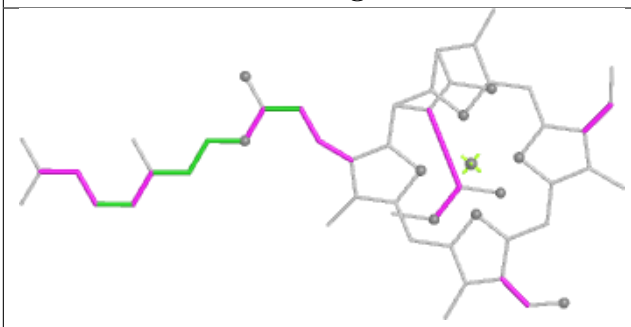

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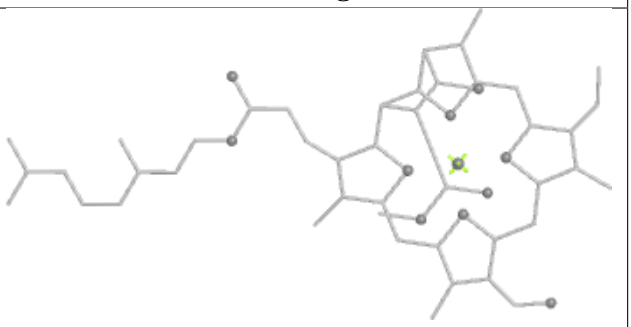

Rings

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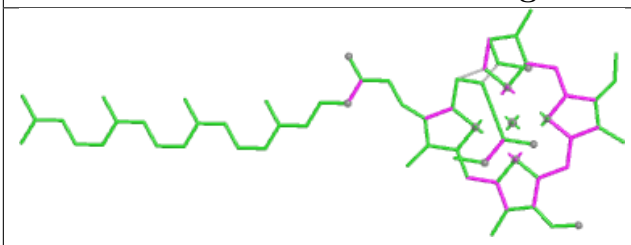

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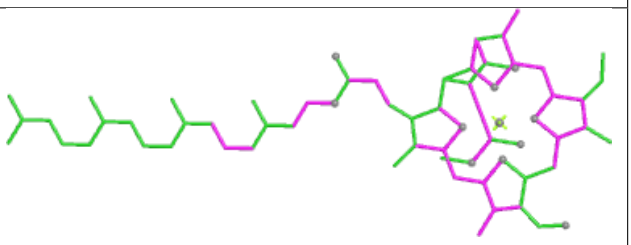

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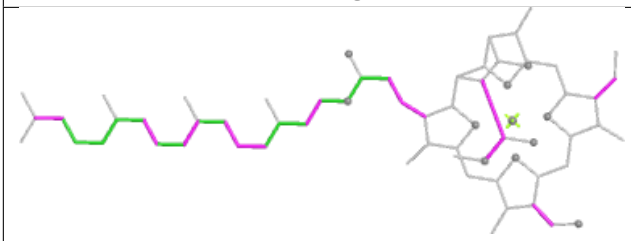

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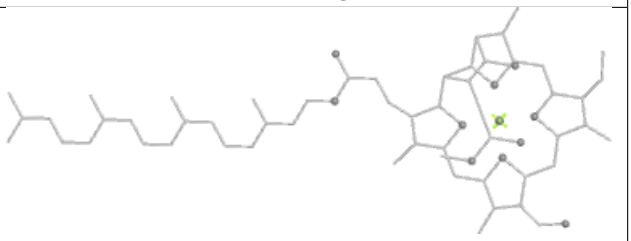

Rings

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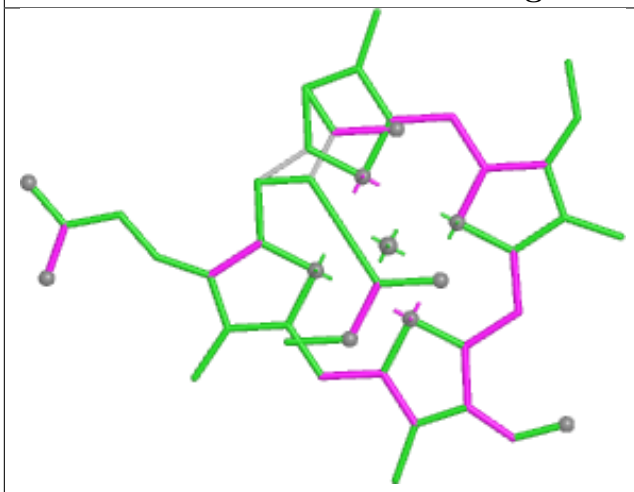

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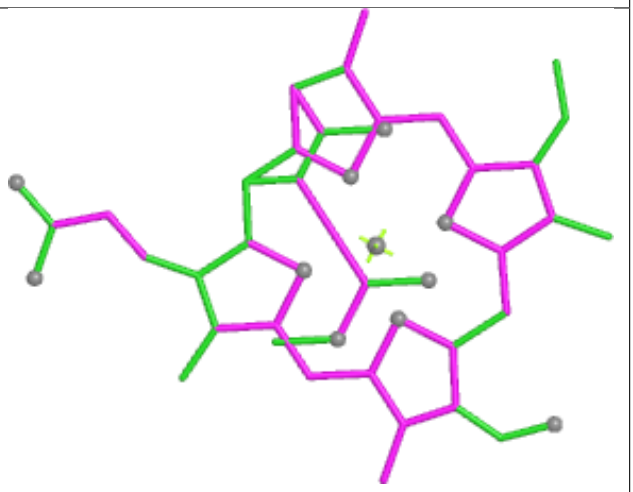

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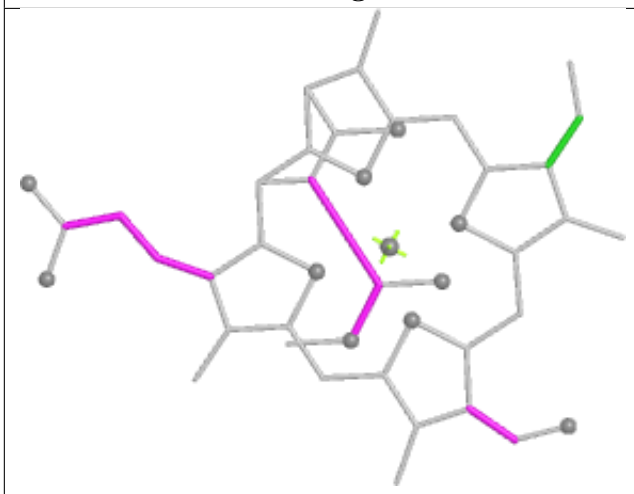

Torsions



Rings

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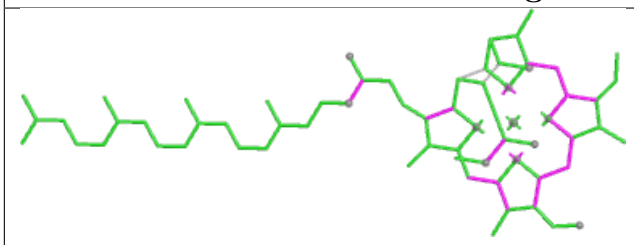

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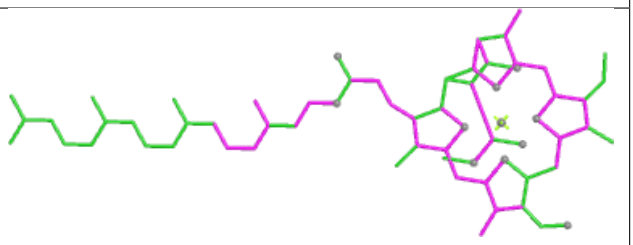

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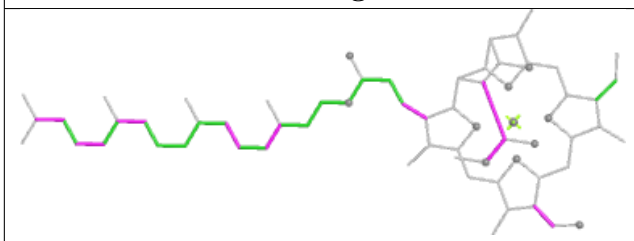

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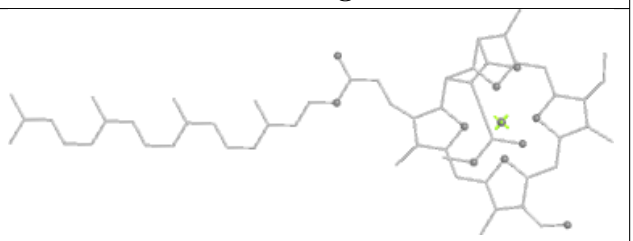

Rings

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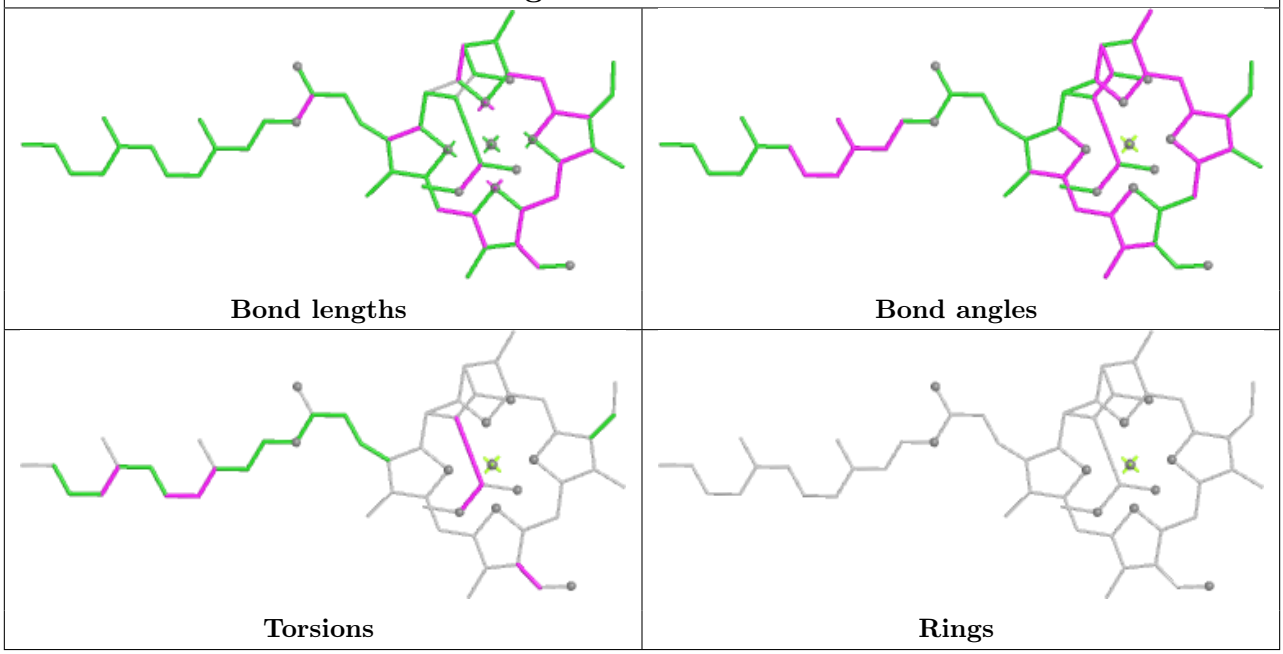

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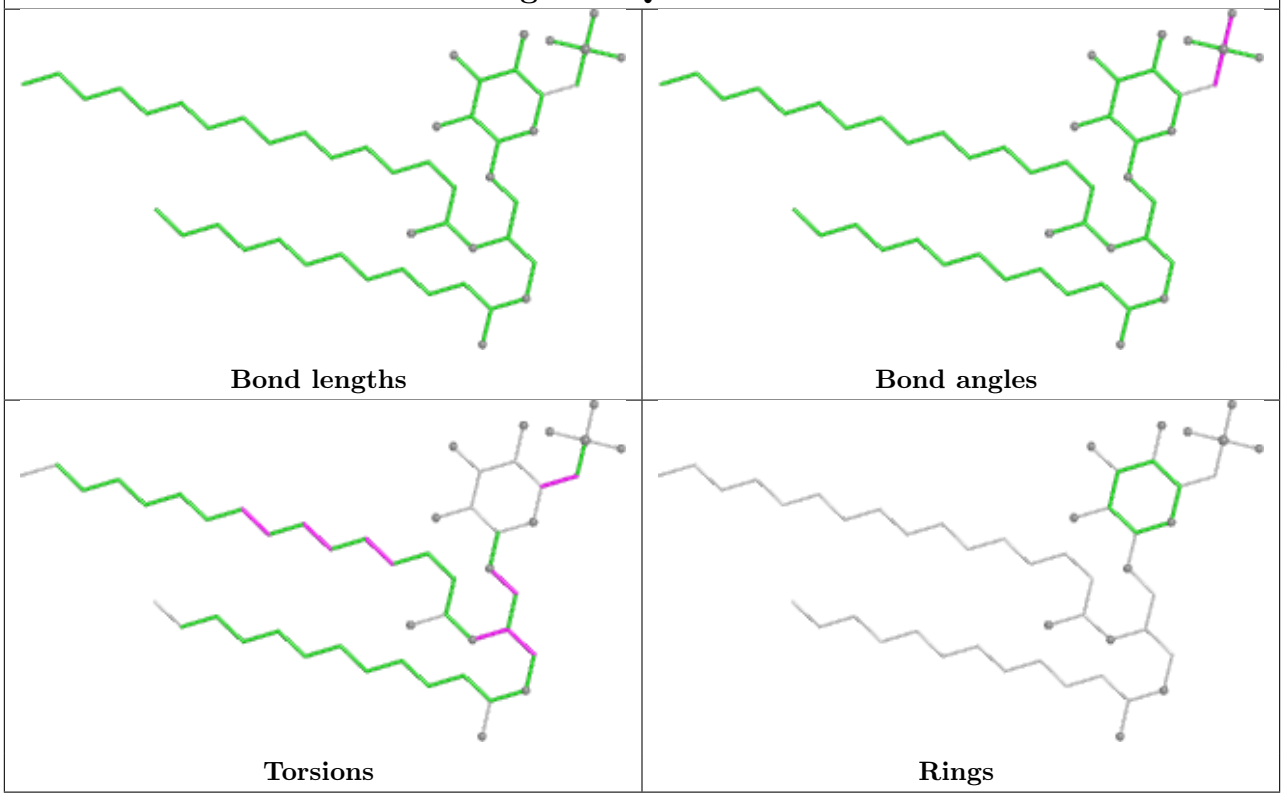

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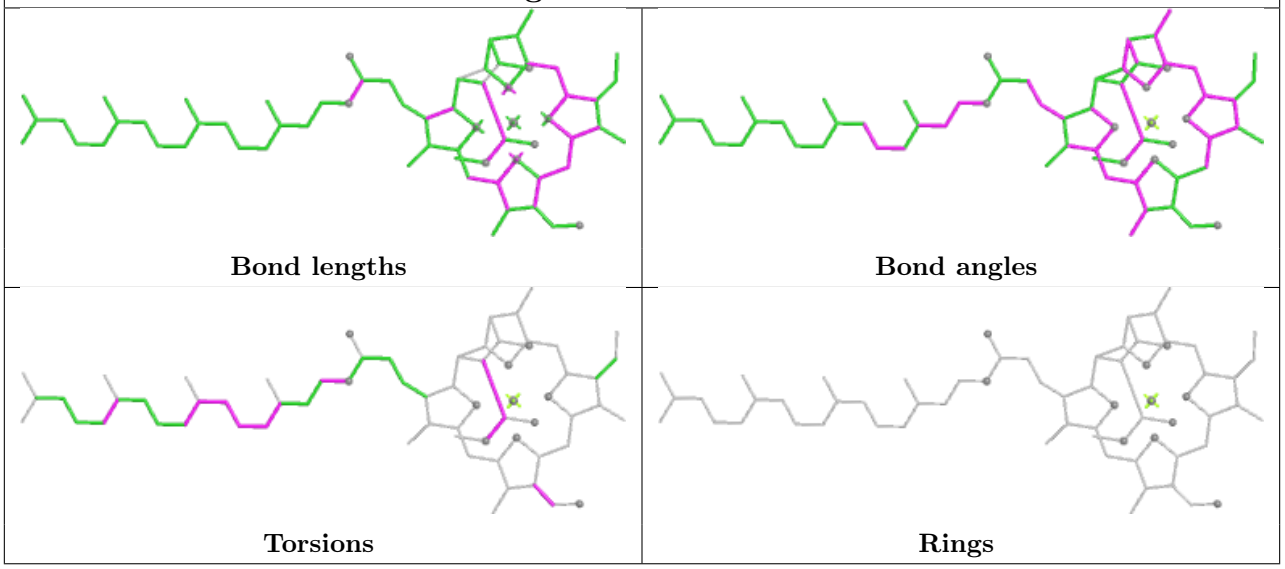

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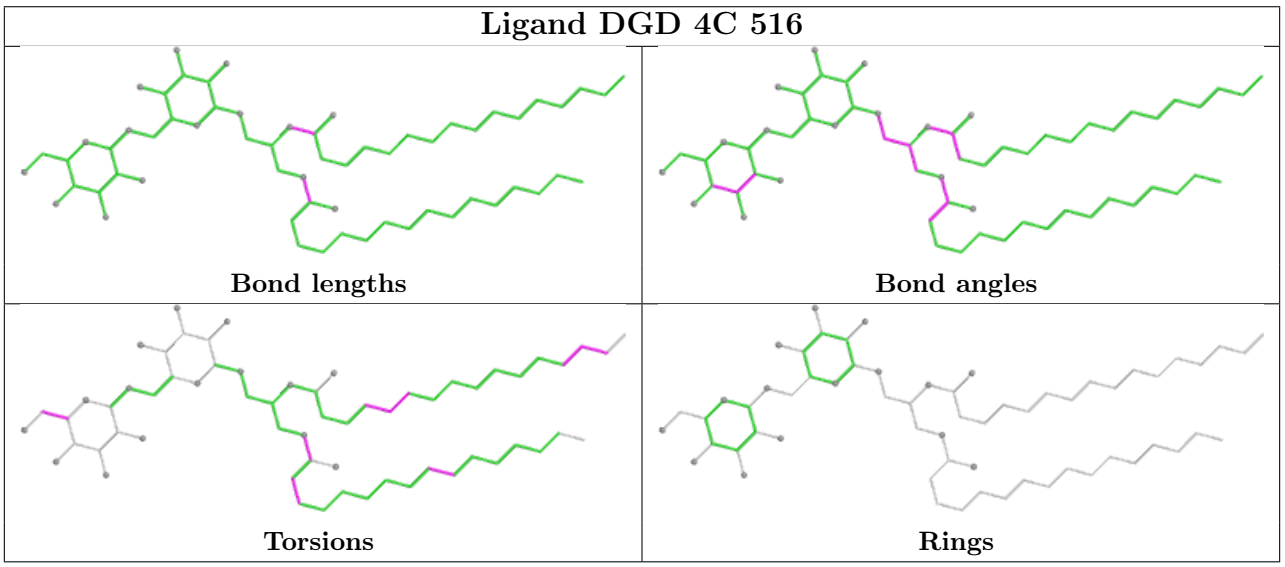

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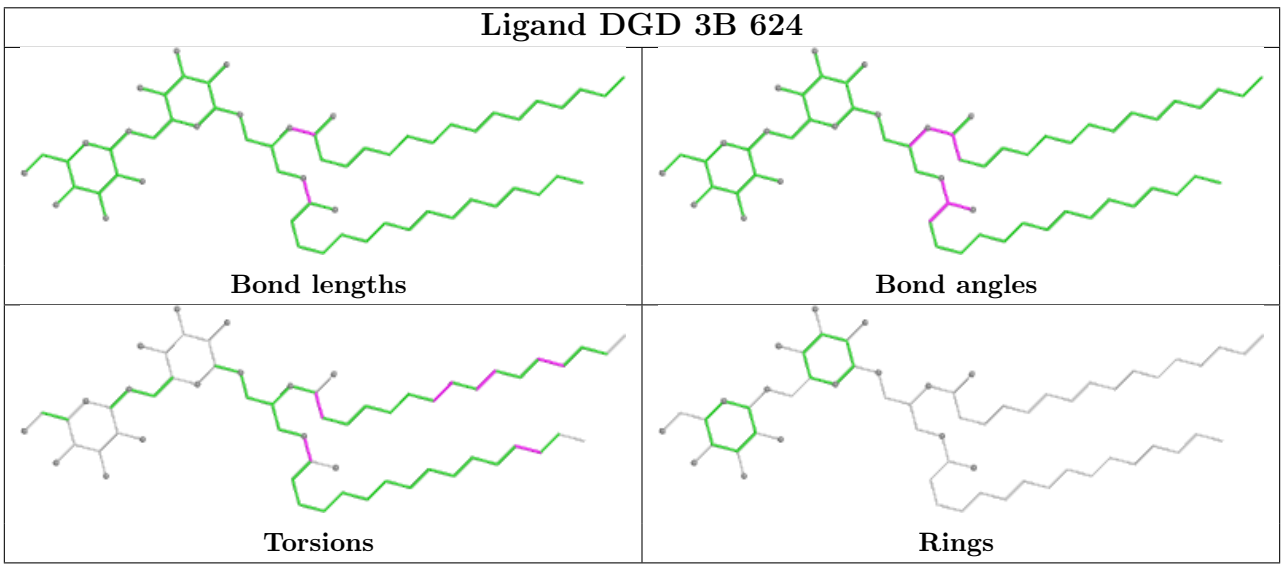

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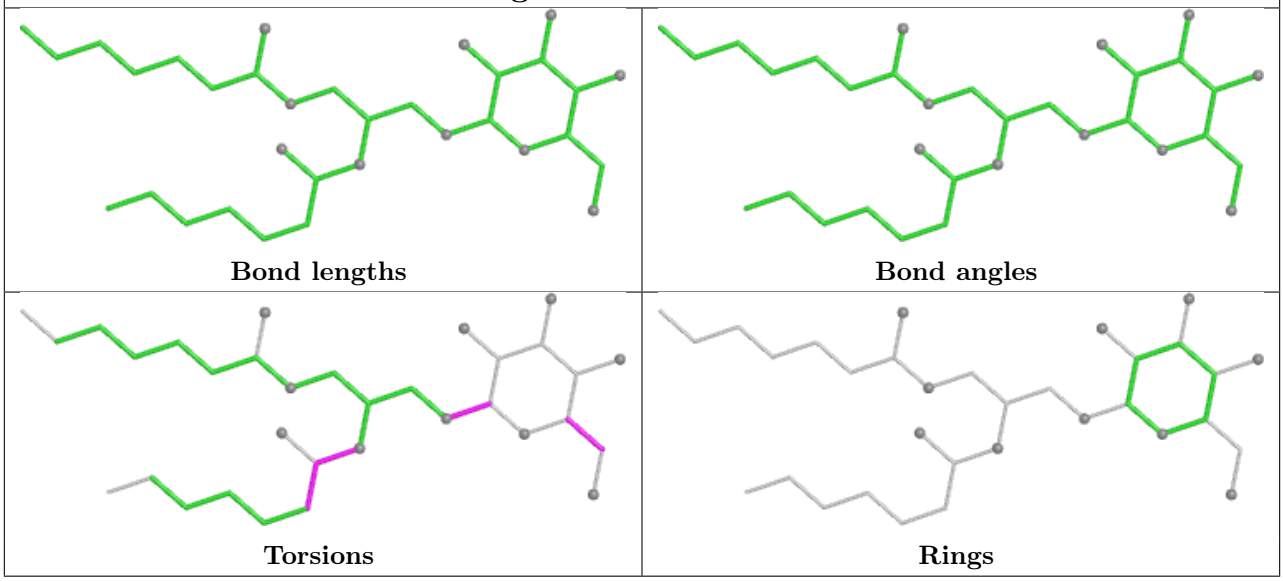

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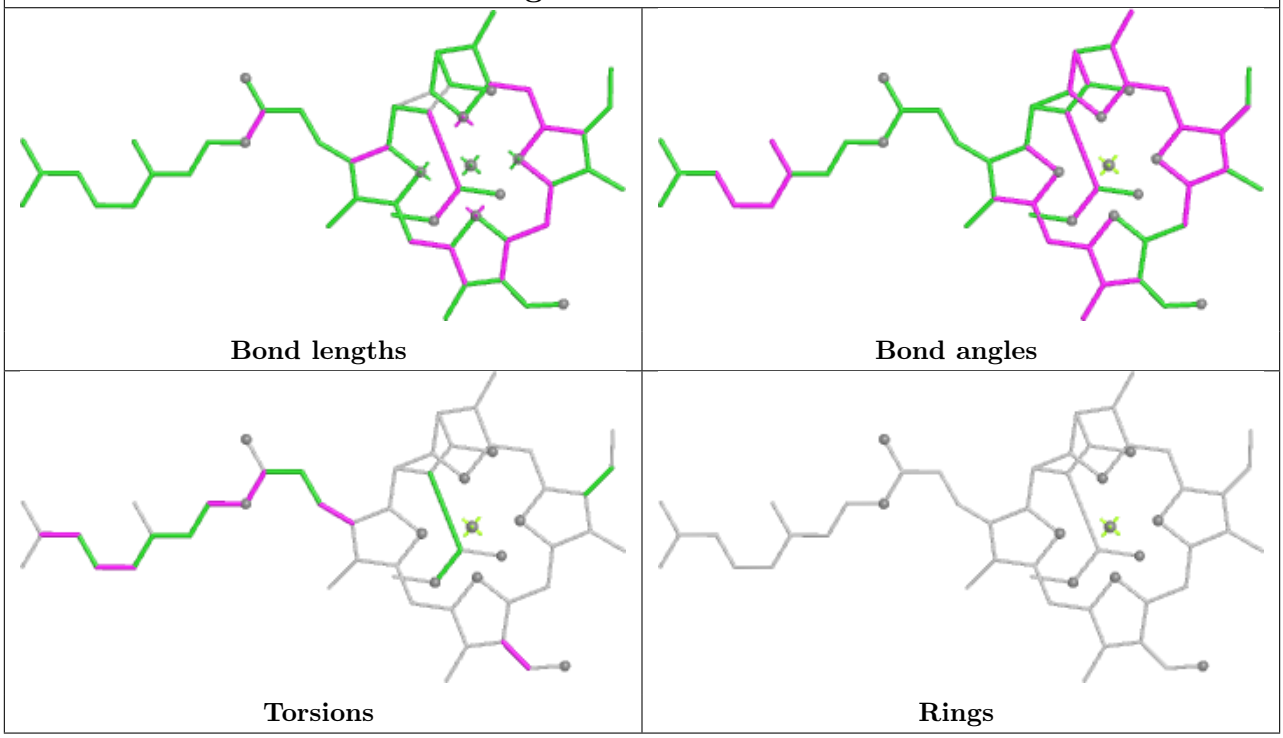

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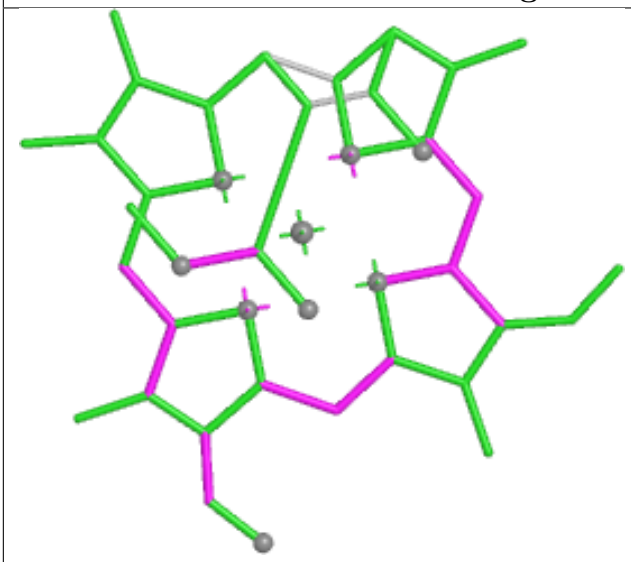
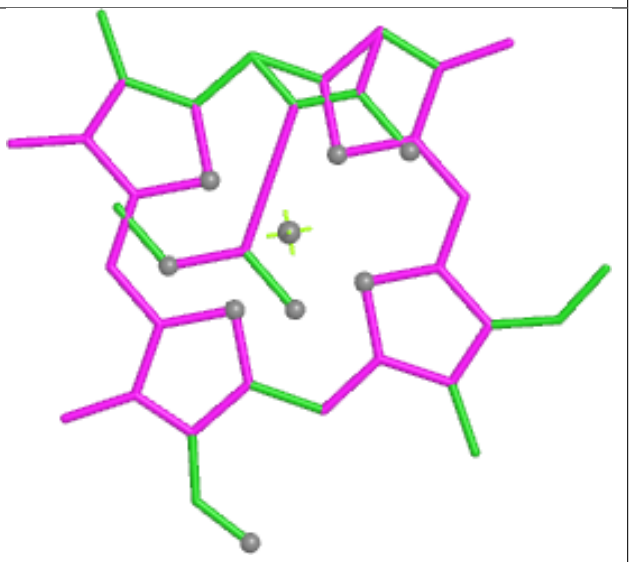
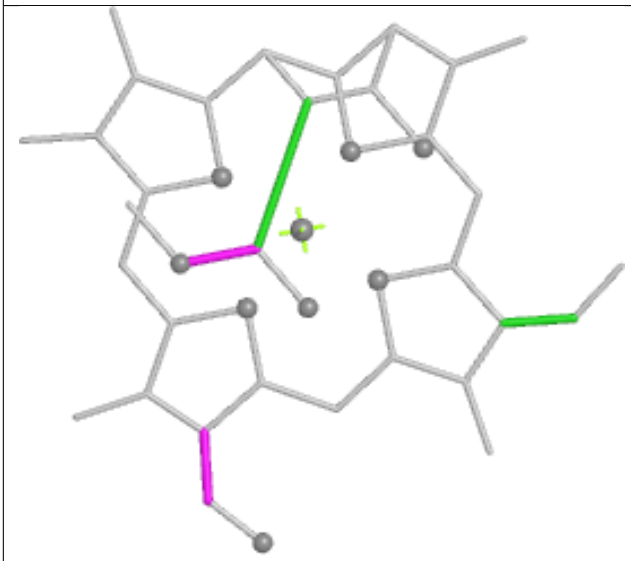


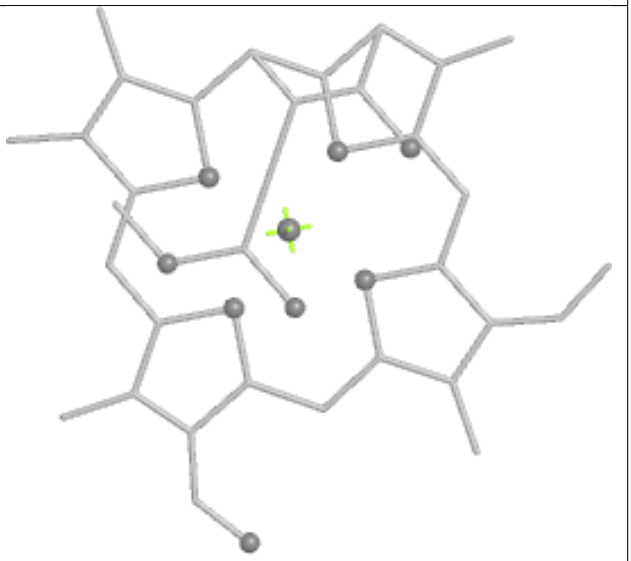
Bond lengths



Bond angles

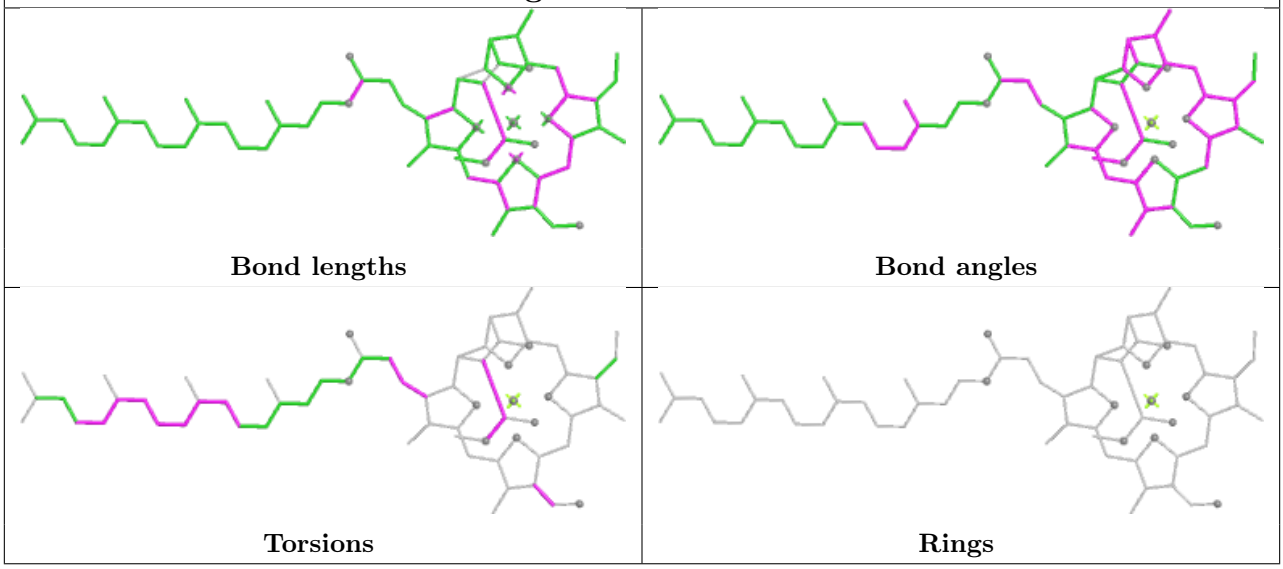


Torsions

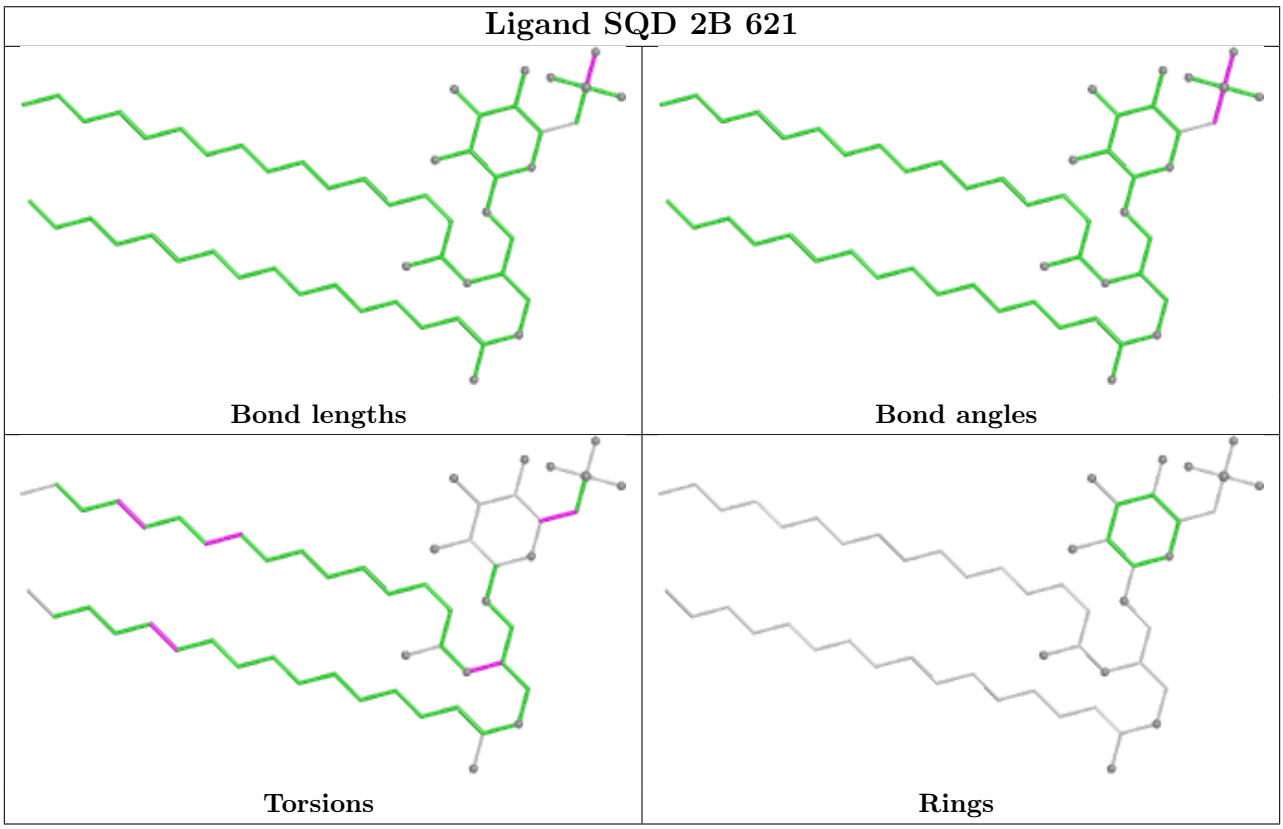


Rings

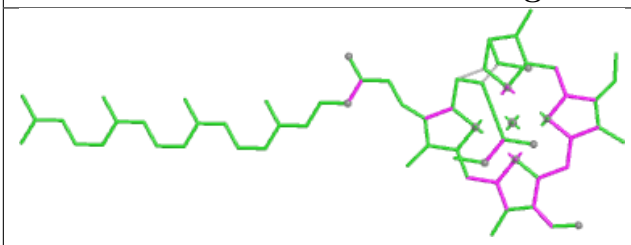
Ligand CL7 13 503



Ligand SQD 2B 621



Ligand CL7 22 516



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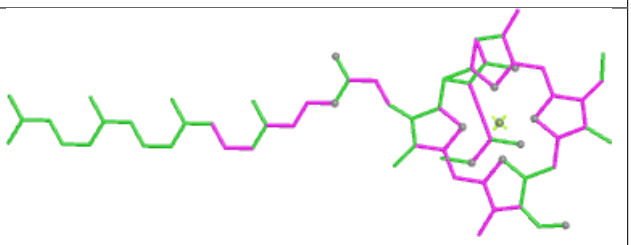
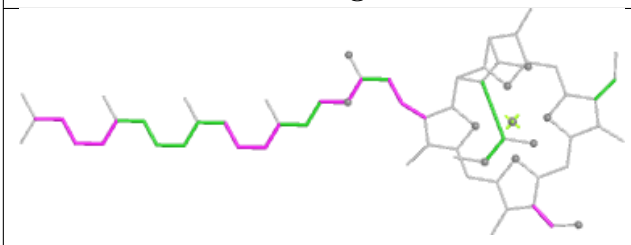


Bond angles



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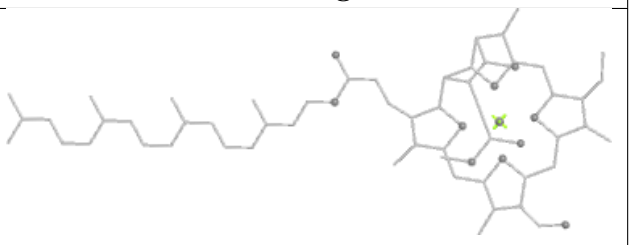

Rings

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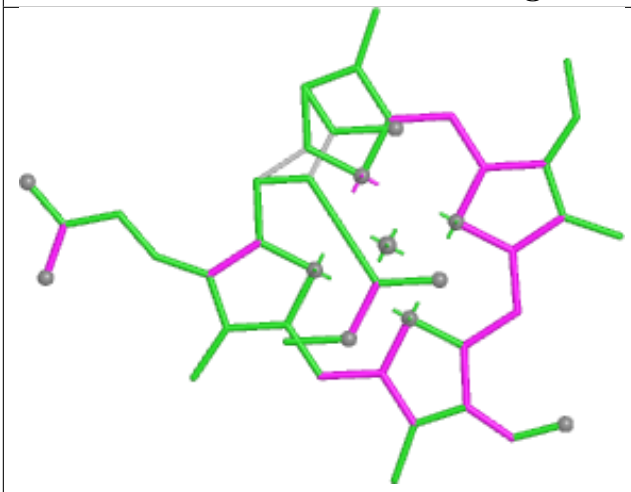

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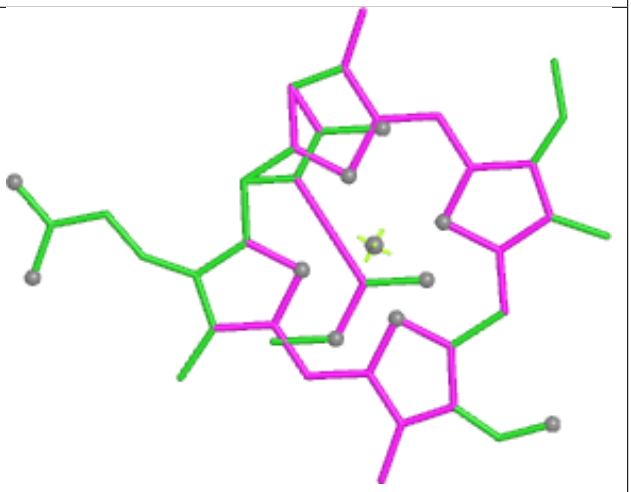
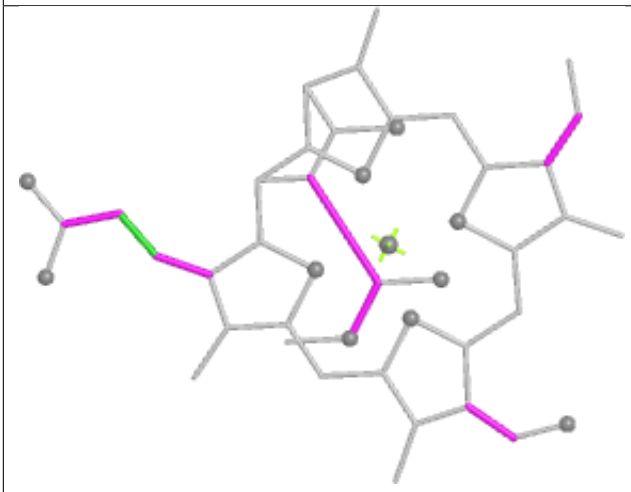


Bond angles

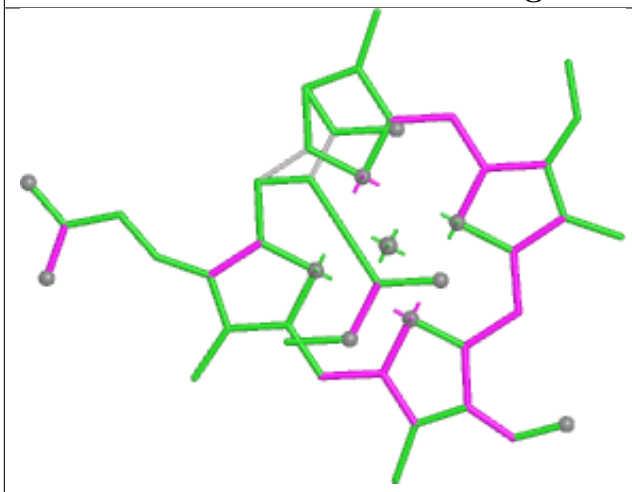


Torsions



Rings

Ligand CL7 24 410



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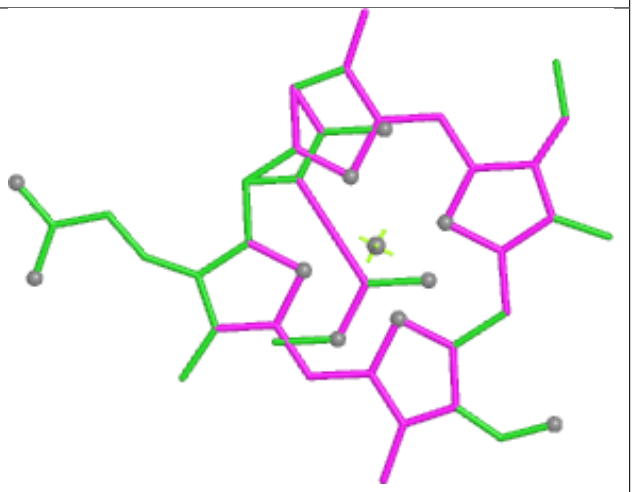
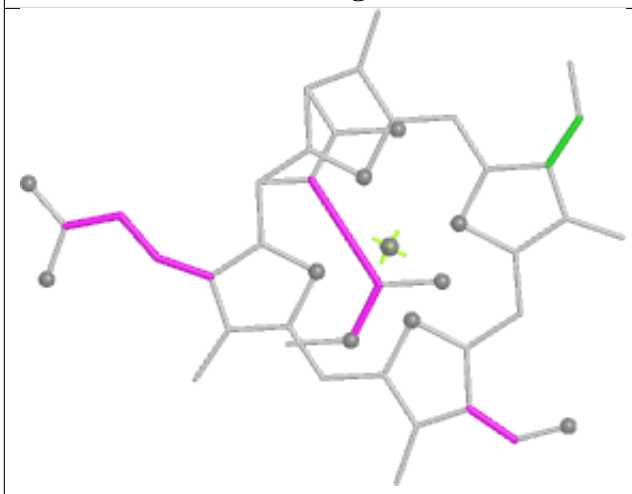


Bond angles

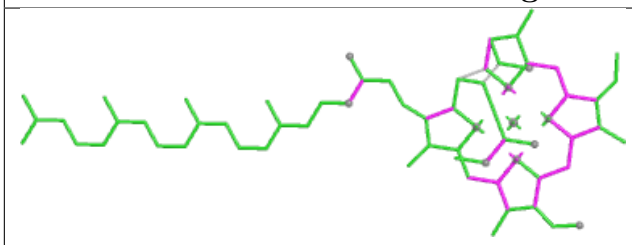


Torsions



Rings

Ligand CL7 1B 603



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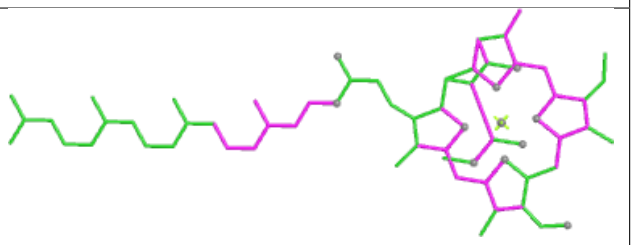
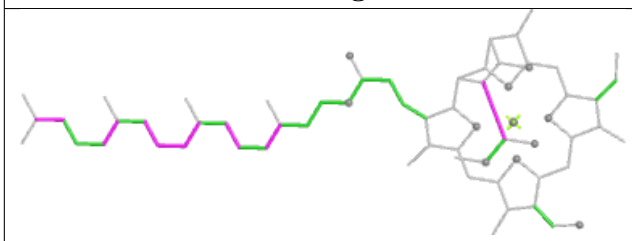


Bond angles



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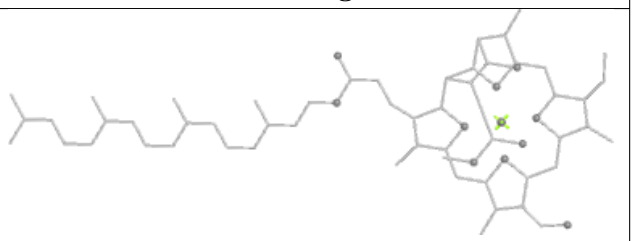
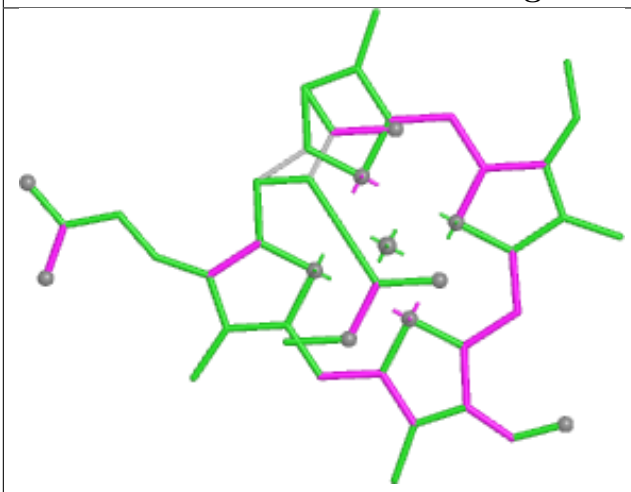


Rings

Ligand CL7 12 515



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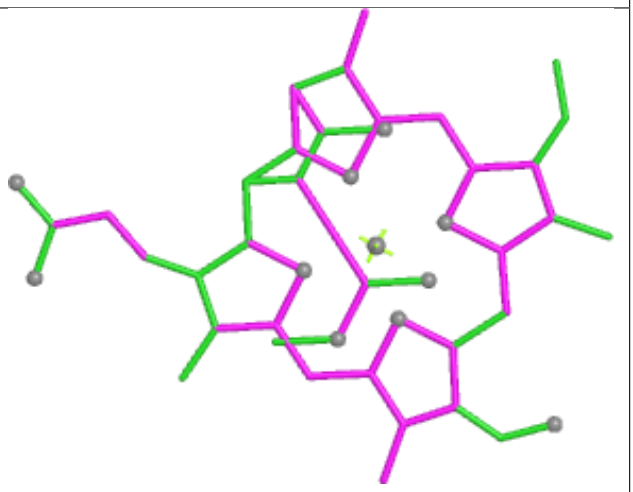
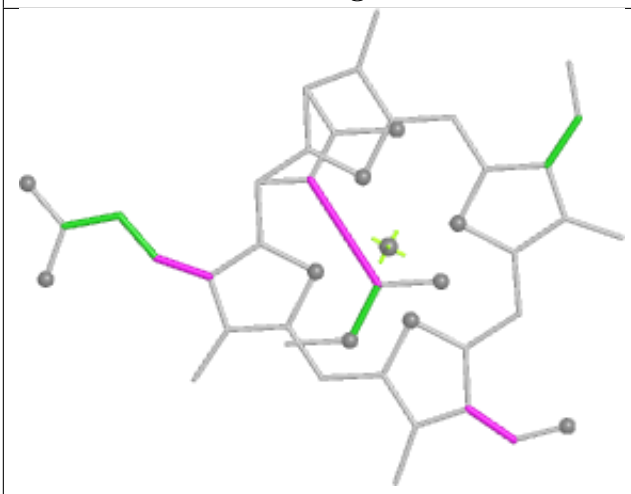


Bond angles

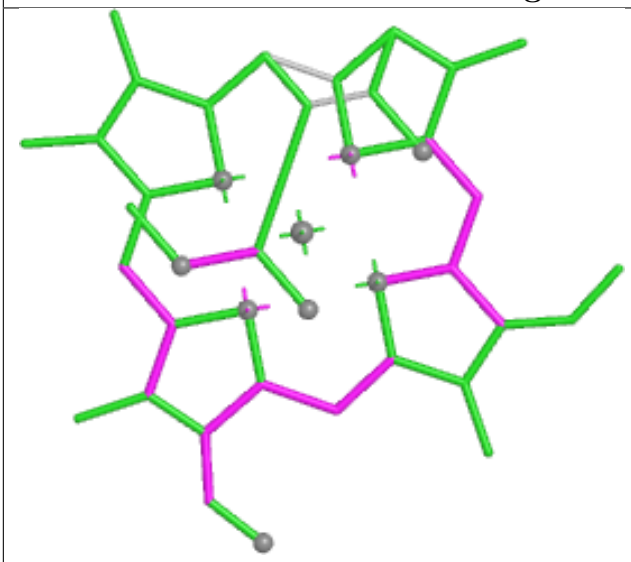


Torsions



Rings

Ligand CL7 44 407



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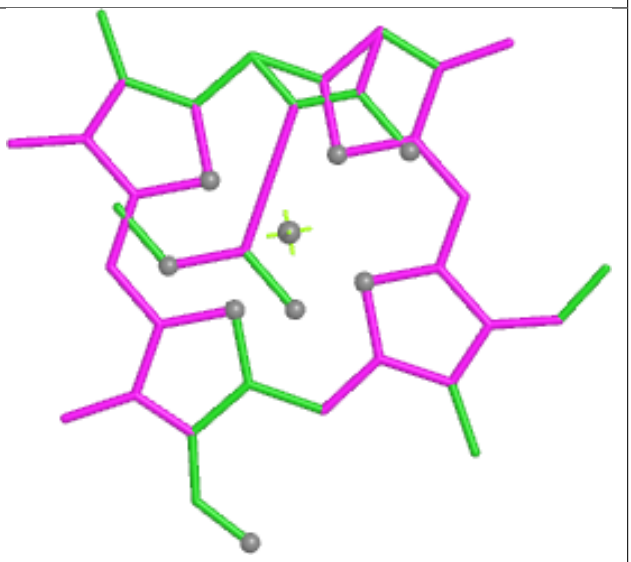

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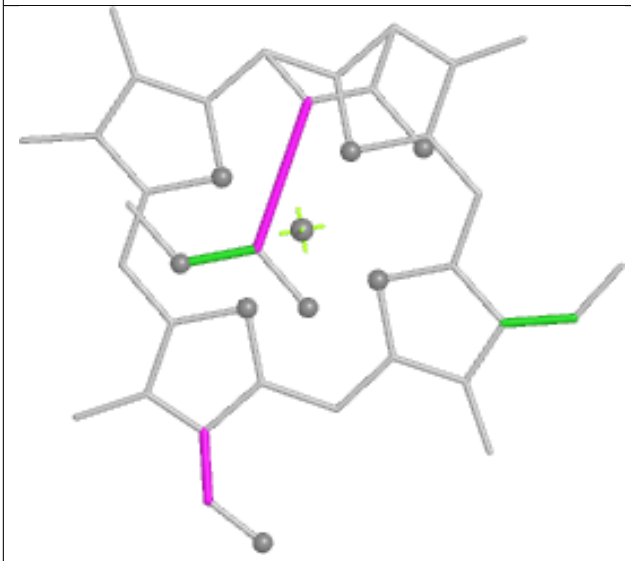
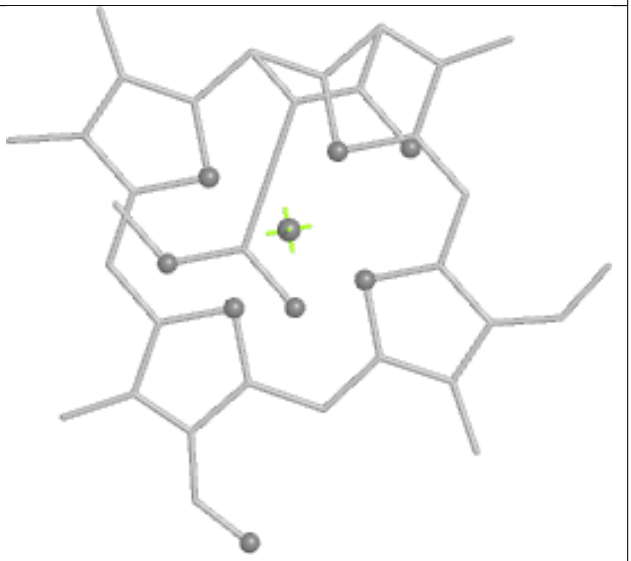
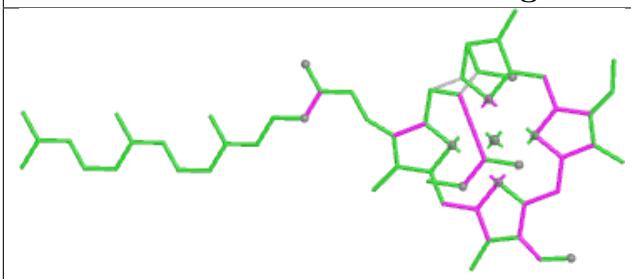


Torsions



Rings

Ligand CL7 1C 502



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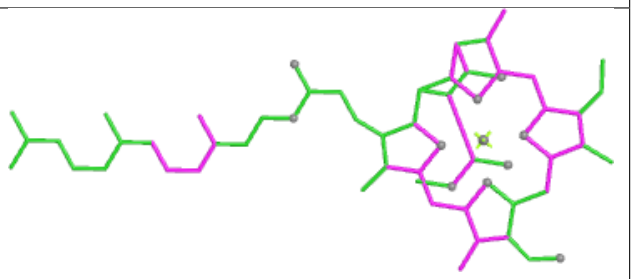

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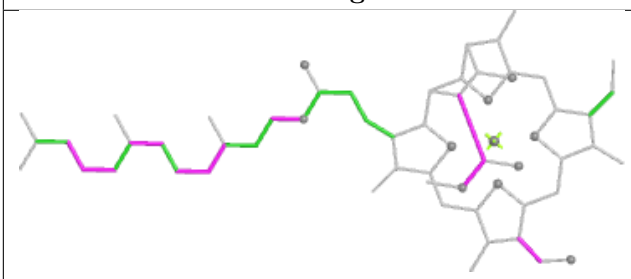

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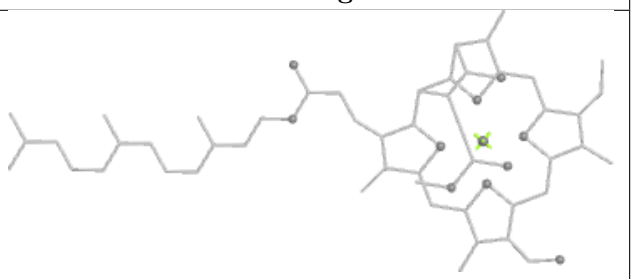
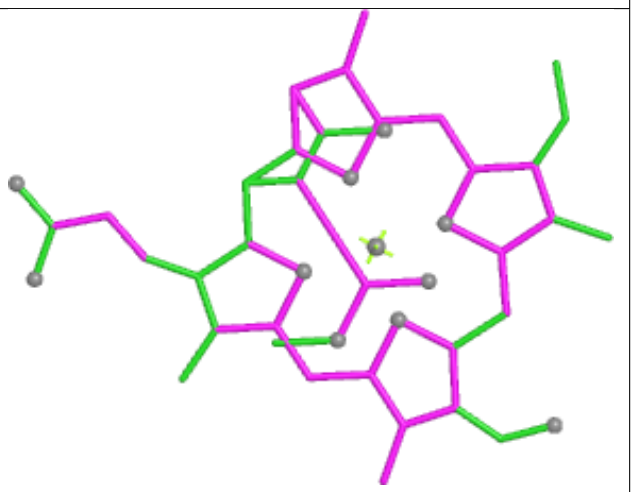


Rings

Ligand CL7 41 420



Bond lengths



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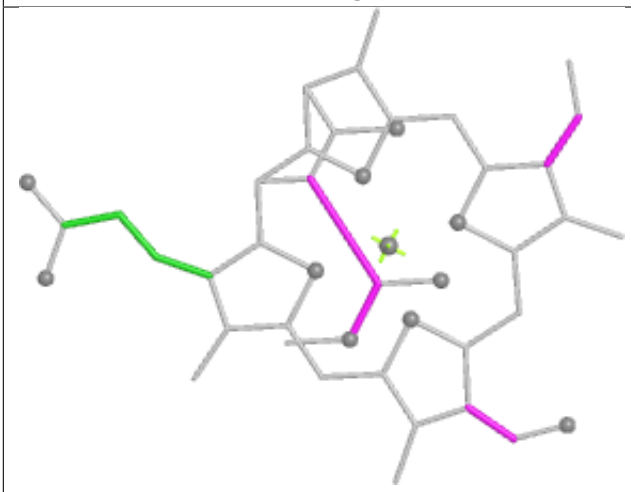

Torsions



Rings

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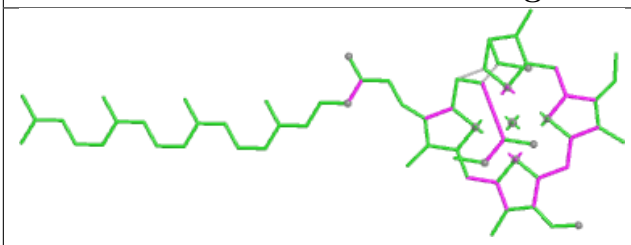

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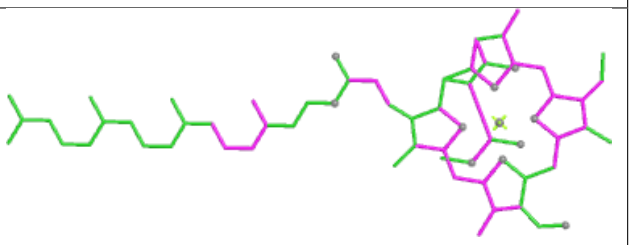

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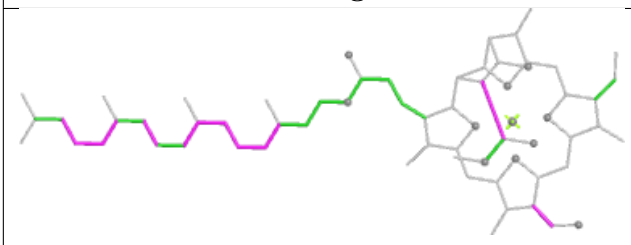

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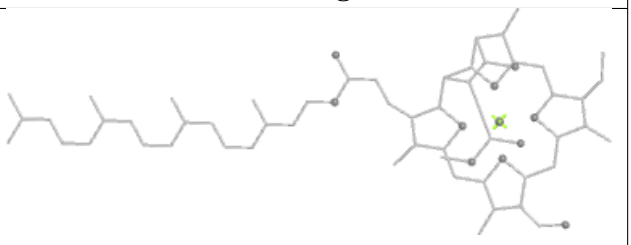
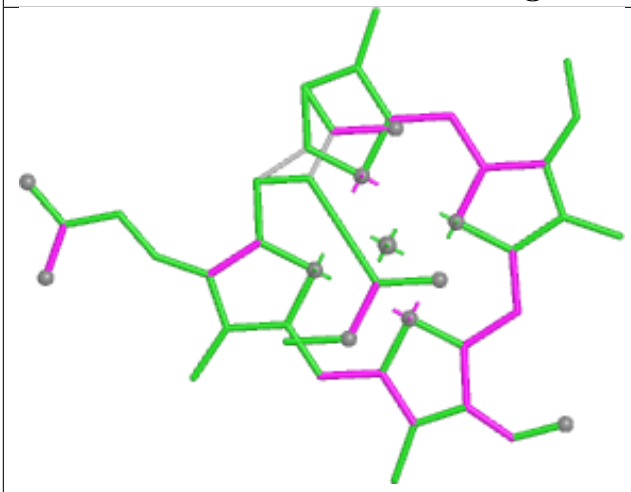


Rings

Ligand CL7 22 515



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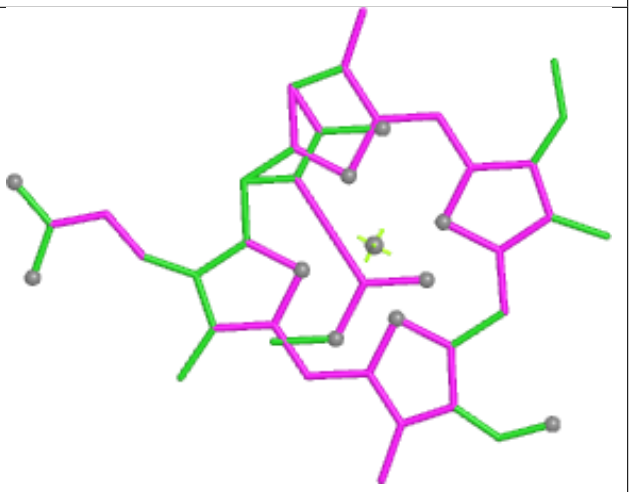

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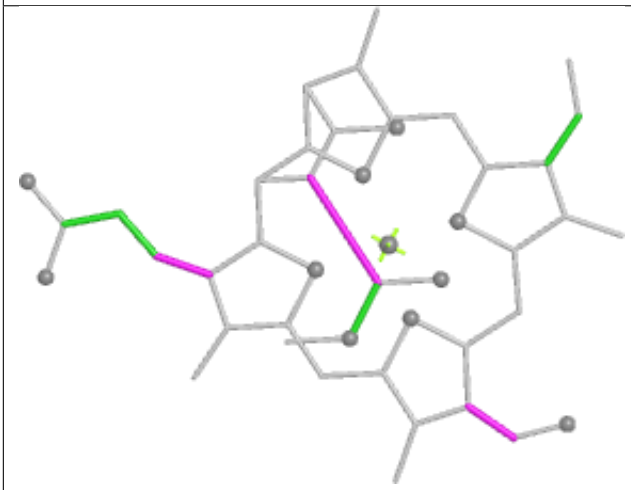
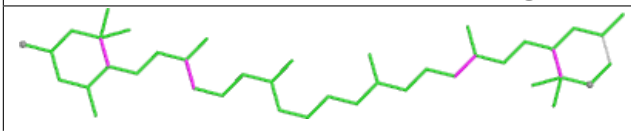


Torsions



Rings

Ligand ZEX 33 522



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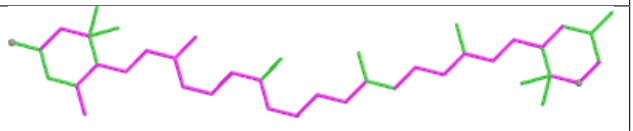

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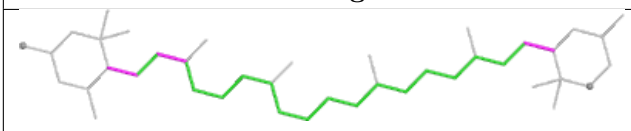

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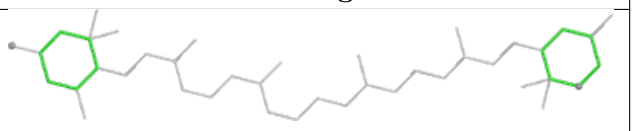
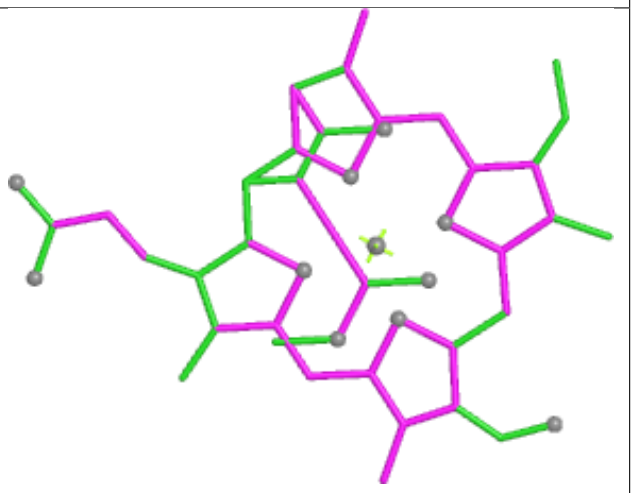


Rings

Ligand CL7 23 419



Bond lengths



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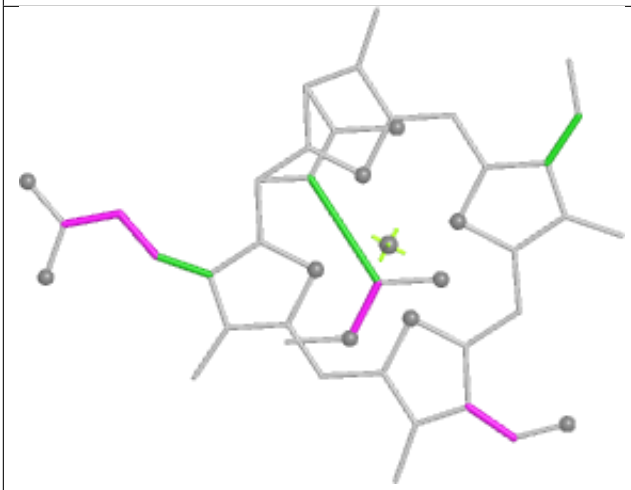
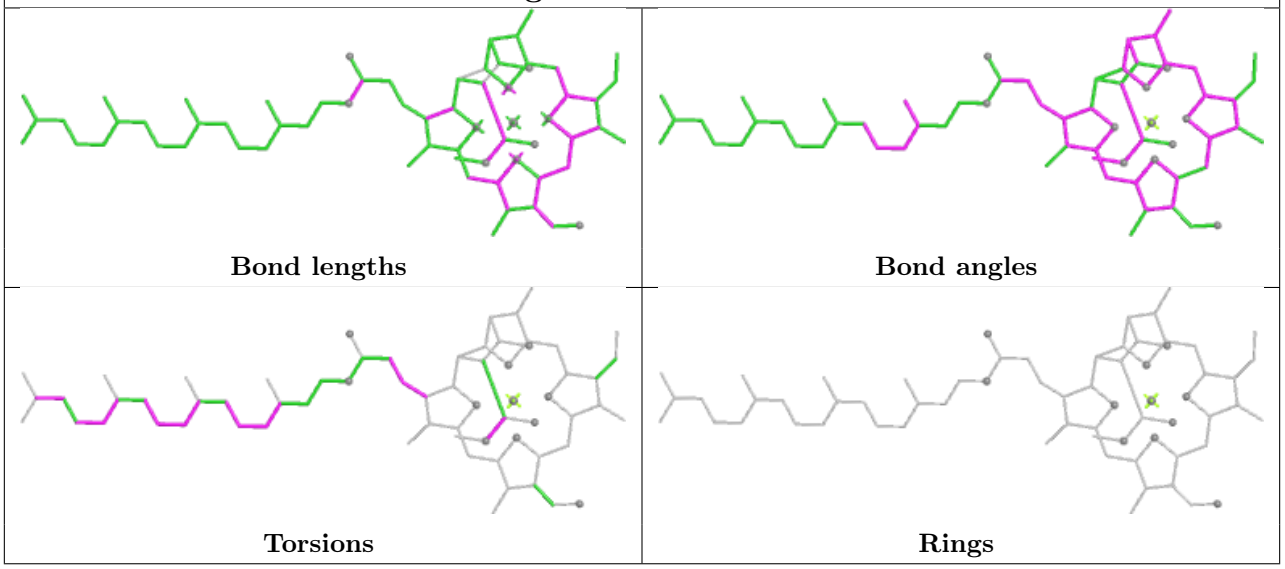


Torsions

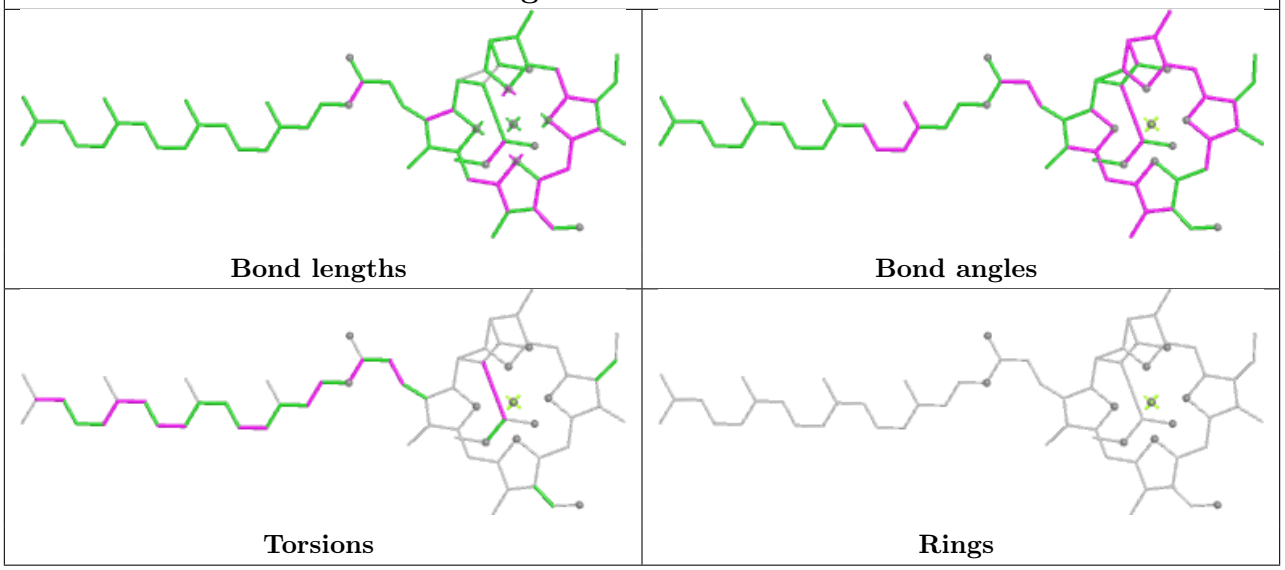


Rings

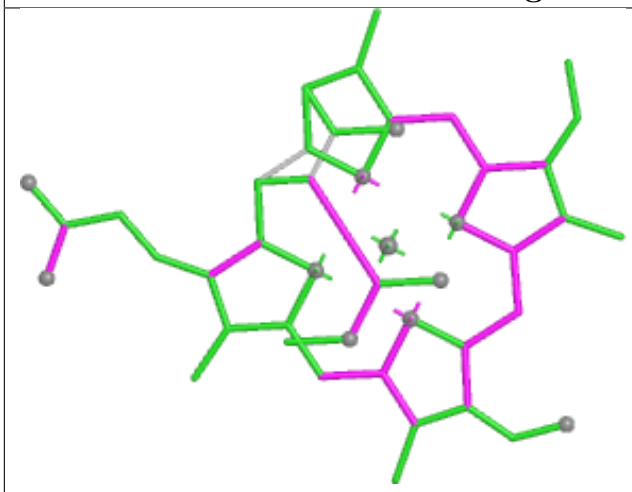
Ligand CL7 22 503



Ligand CL7 1B 610



Ligand CL7 43 414



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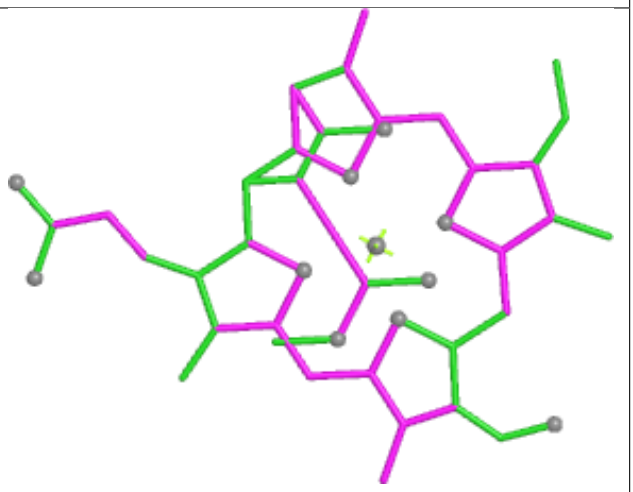

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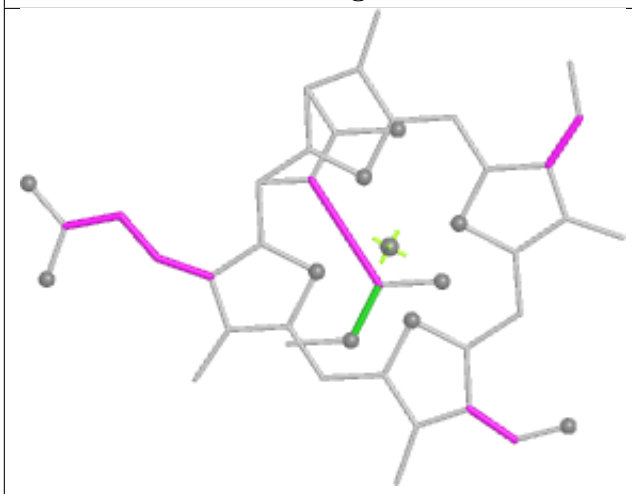
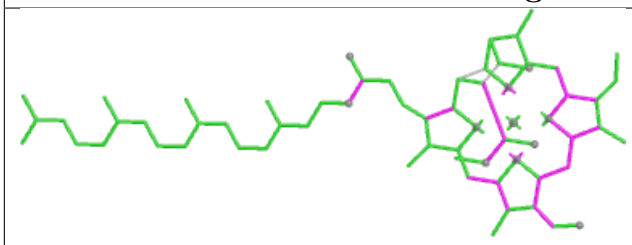


Torsions



Rings

Ligand CL7 32 503



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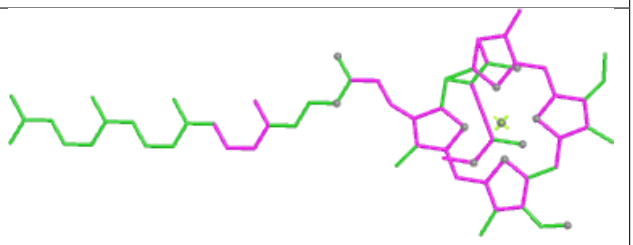

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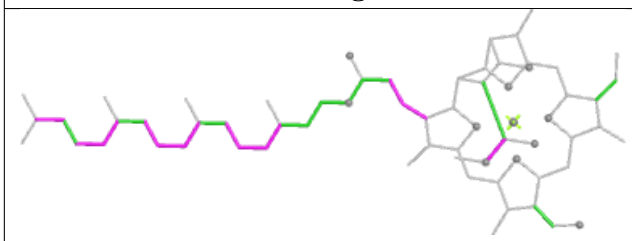

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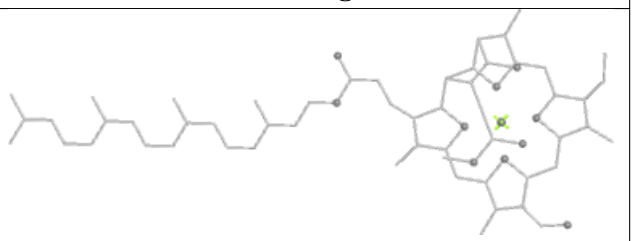
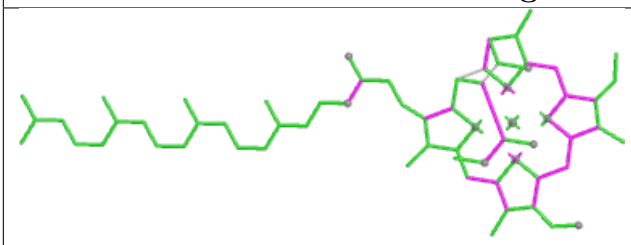


Rings

Ligand CL7 4B 612



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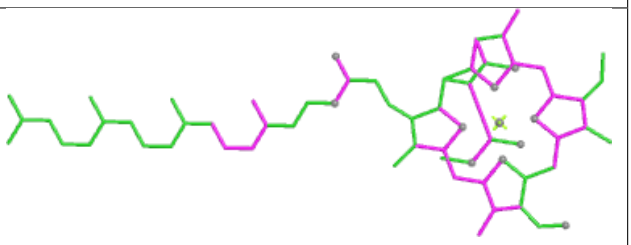

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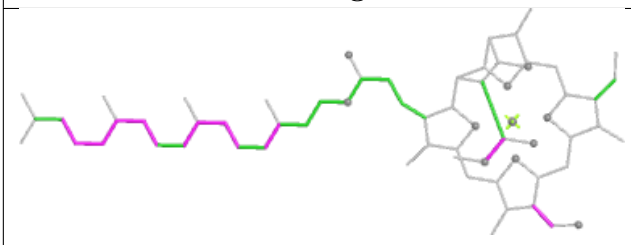

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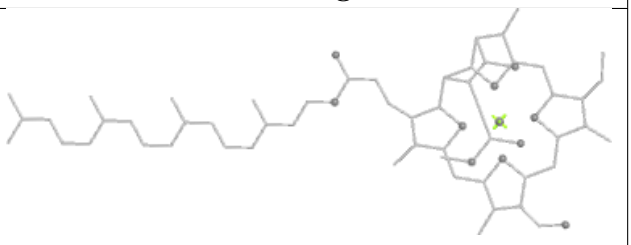
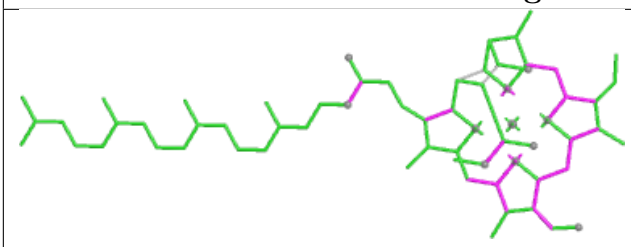


Rings

Ligand CL7 34 406



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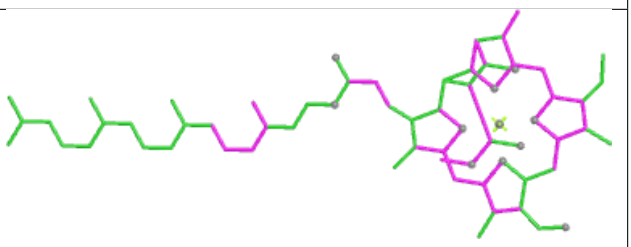

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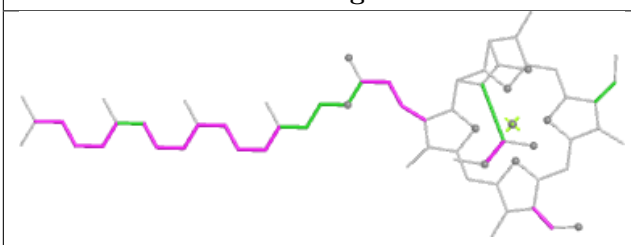

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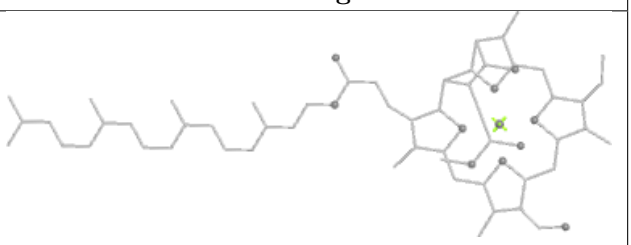
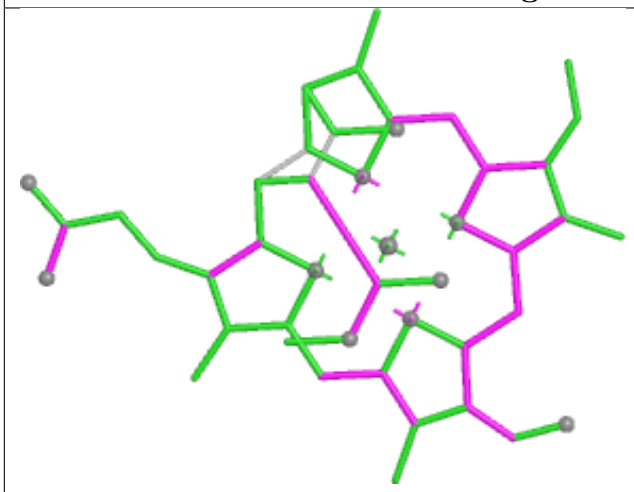


Rings

Ligand CL7 4B 617



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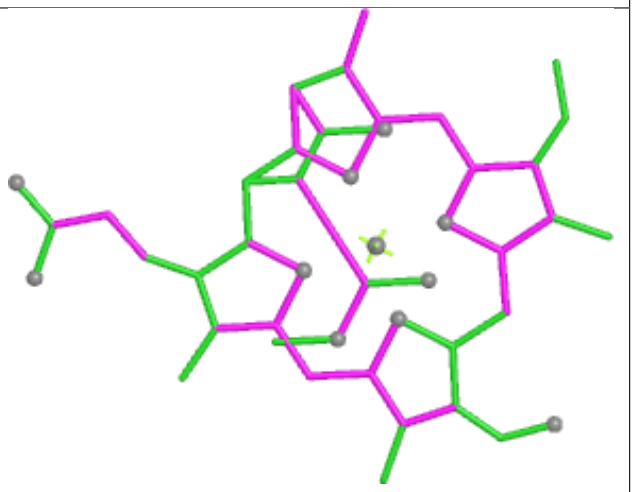

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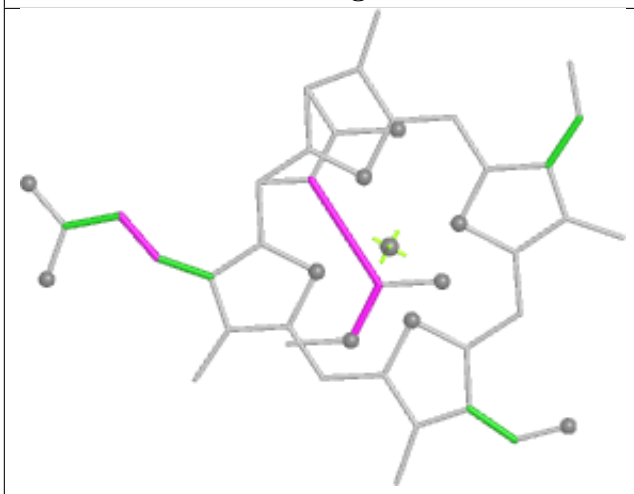
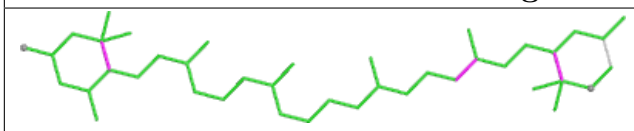


Torsions



Rings

Ligand ZEX 42 520



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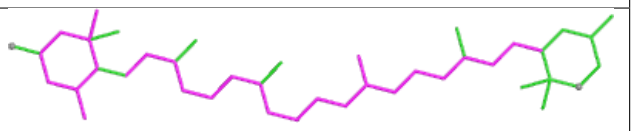

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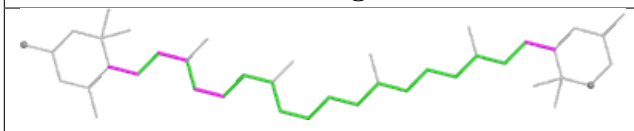

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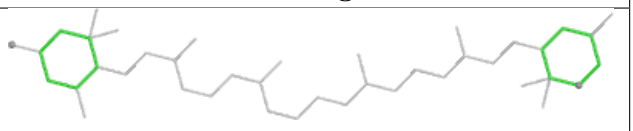
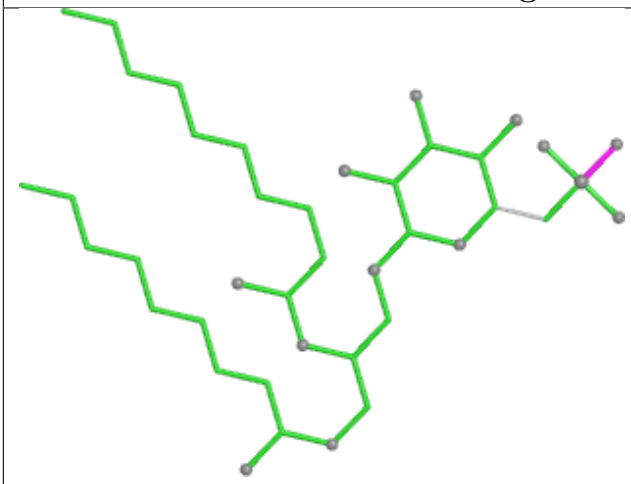


Rings

Ligand SQD 22 523



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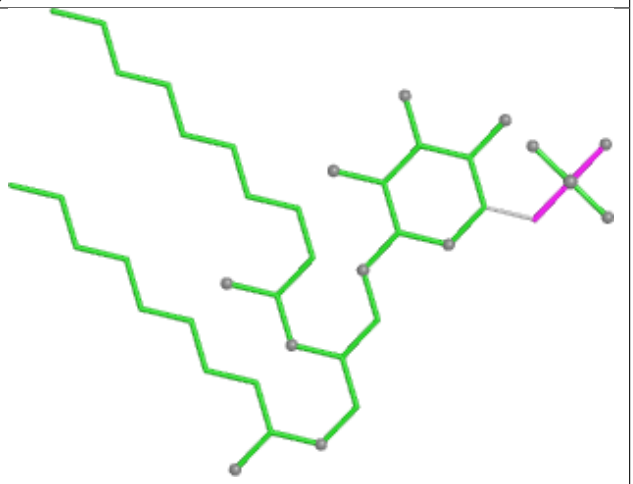
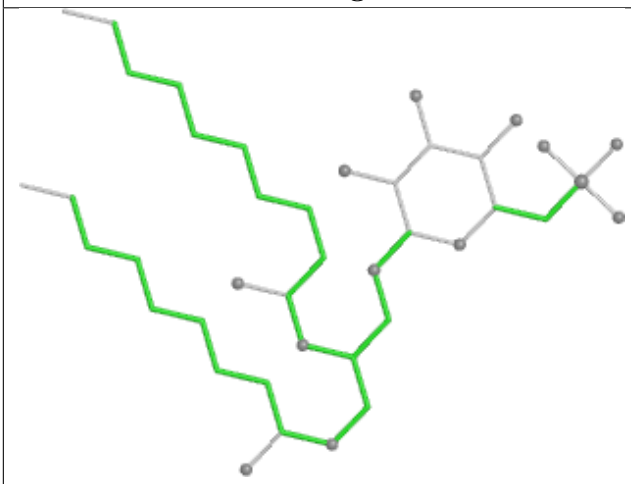


Bond angles



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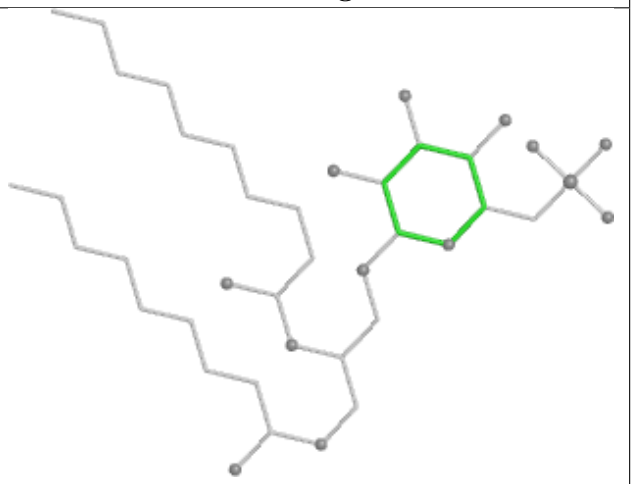
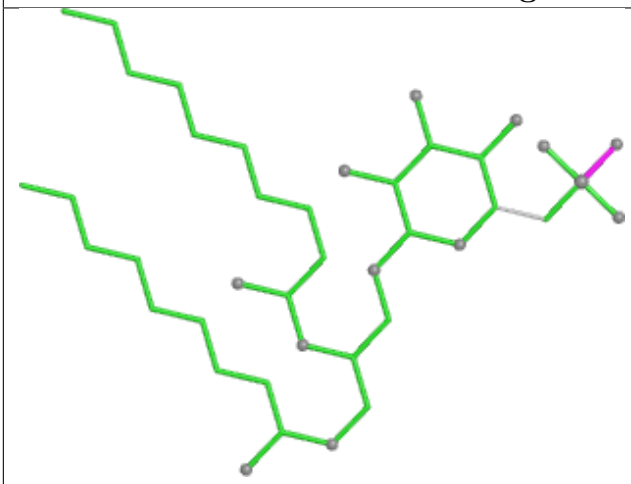


Rings

Ligand SQD 32 523



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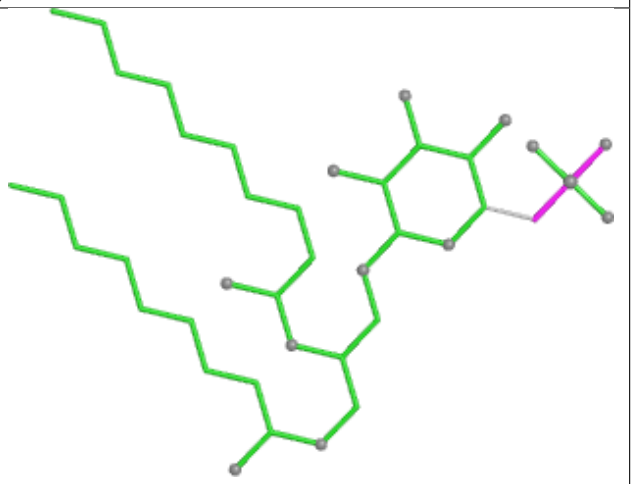
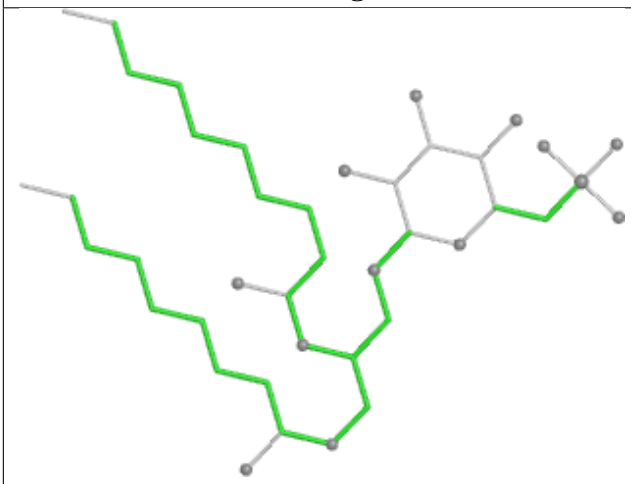


Bond angles



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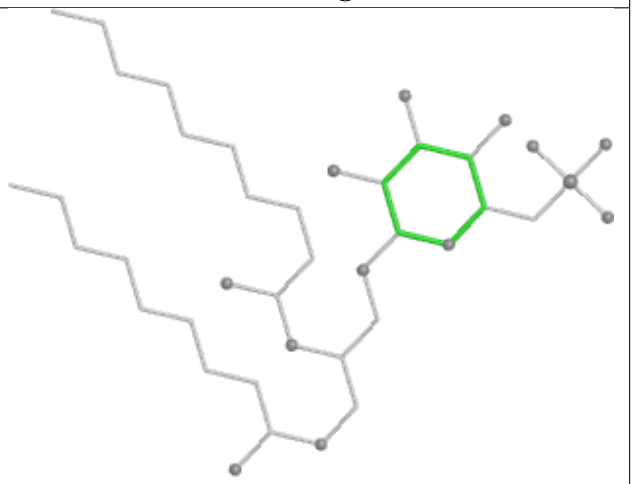
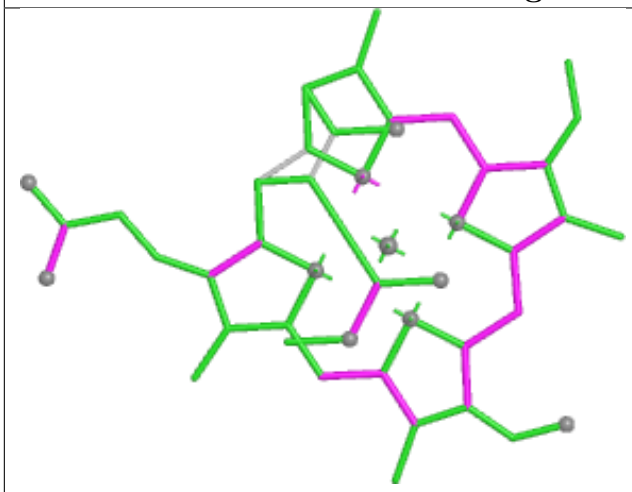


Rings

Ligand CL7 42 513



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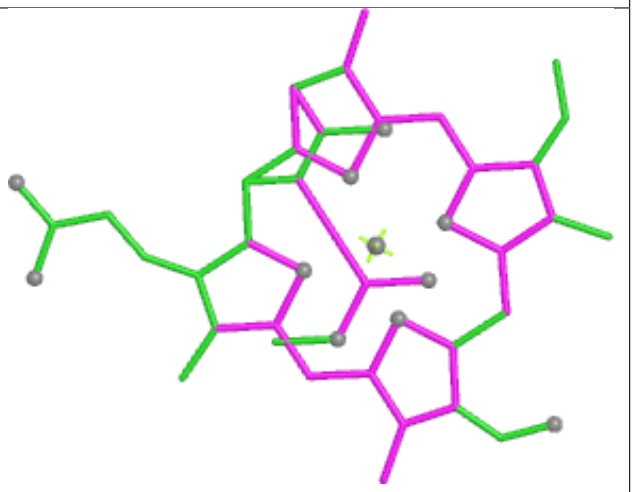
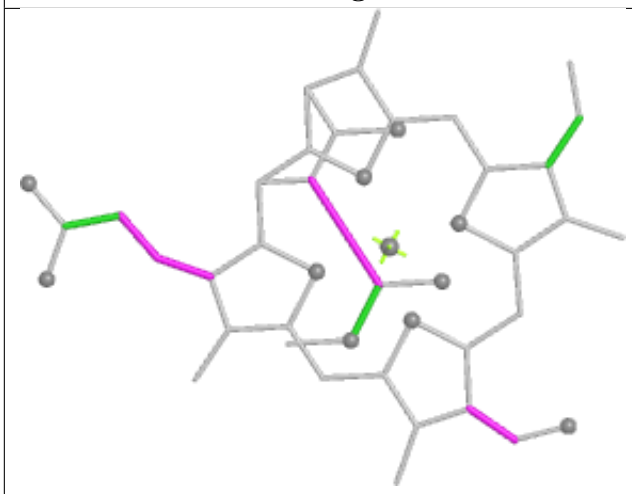


Bond angles

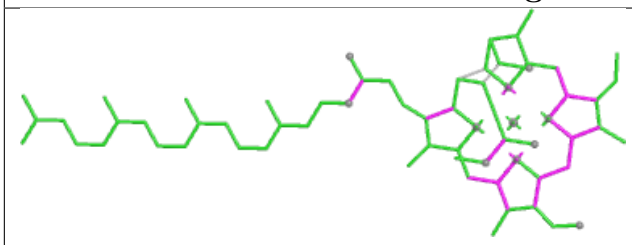


Torsions

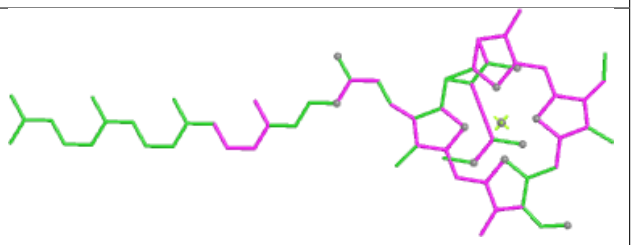


Rings

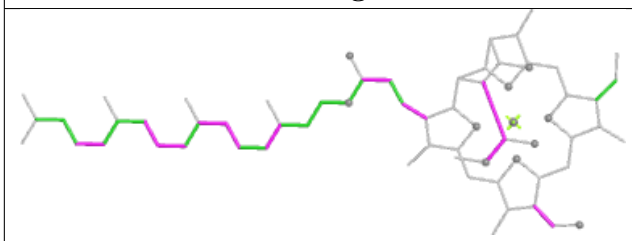
Ligand CL7 43 411



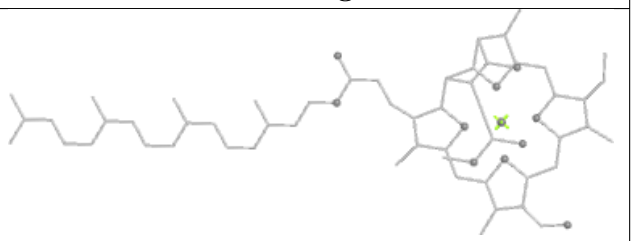
Bond lengths



Bond angles

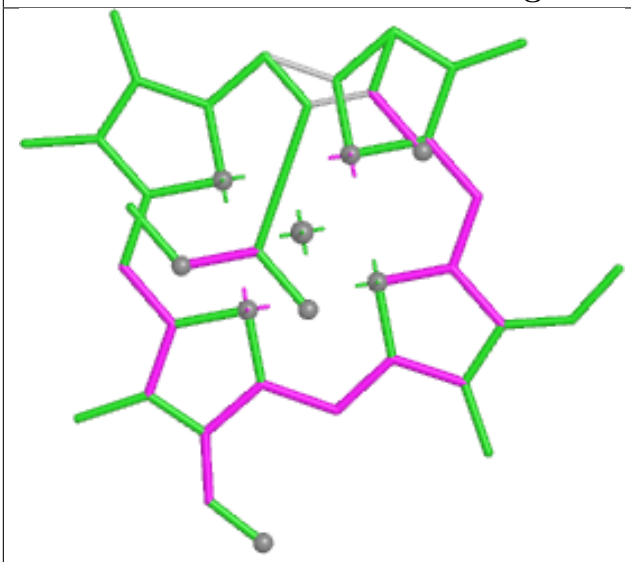


Torsions



Rings

Ligand CL7 11 407



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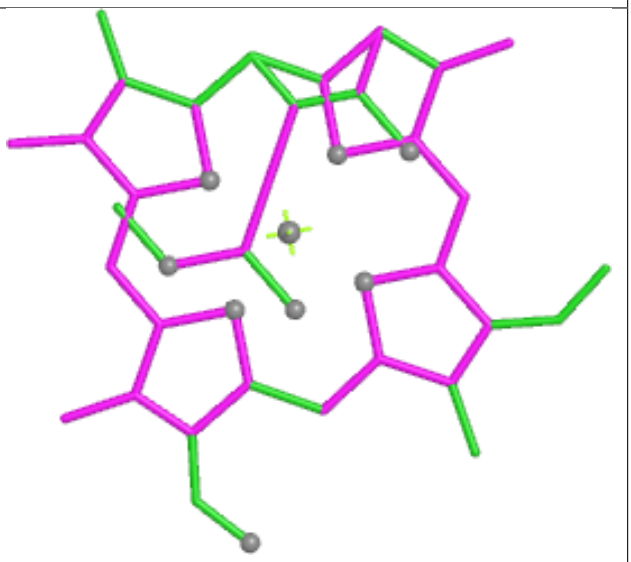

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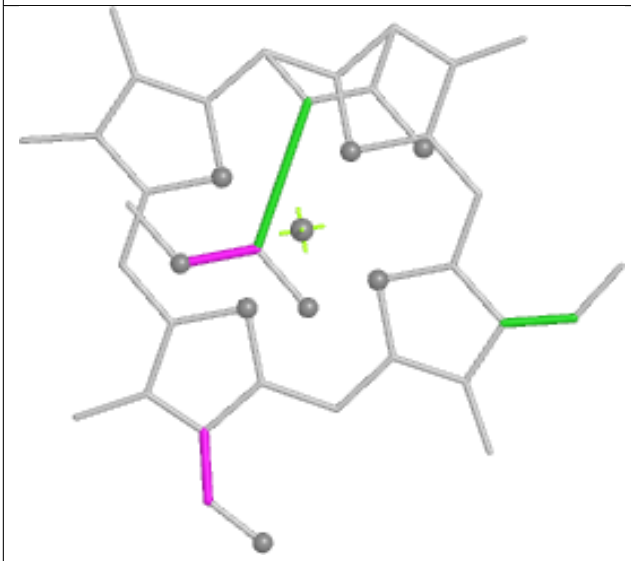

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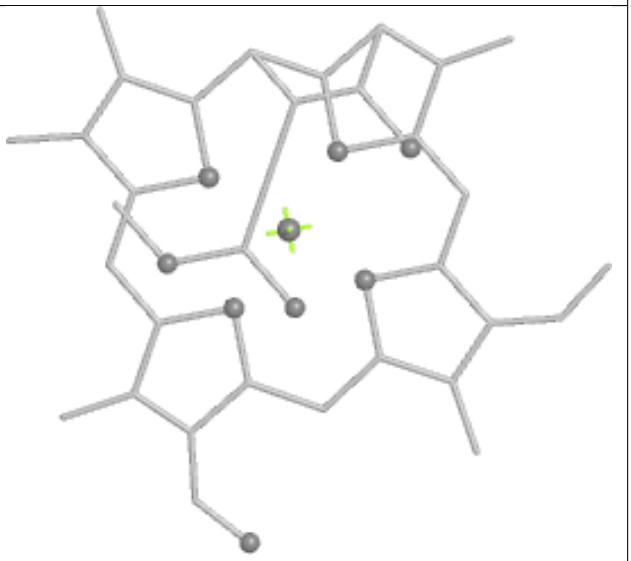
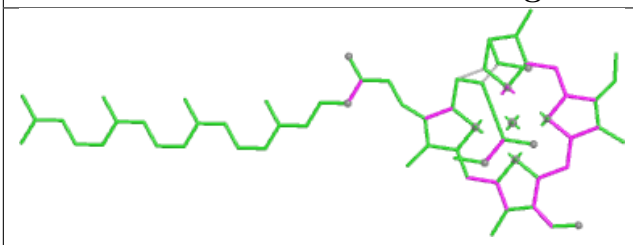


Rings

Ligand CL7 24 405



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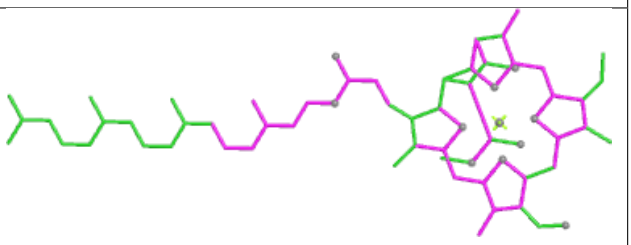

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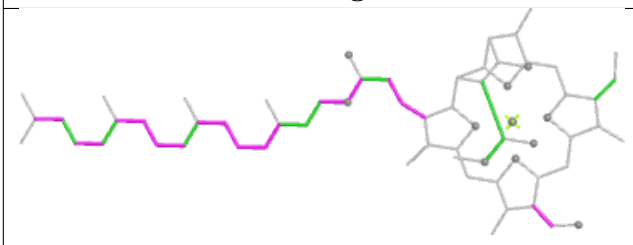

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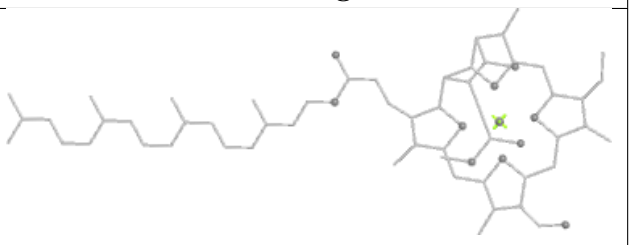
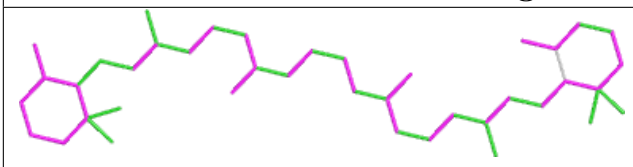


Rings

Ligand 8CT 4D 406



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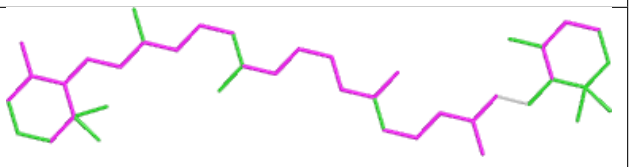

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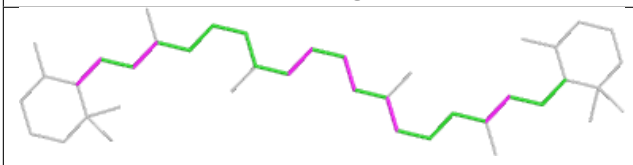

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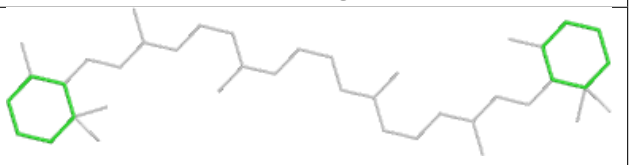
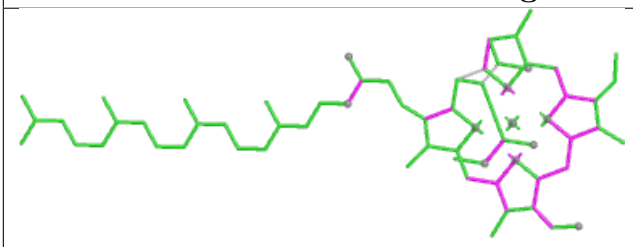


Rings

Ligand CL7 2B 609



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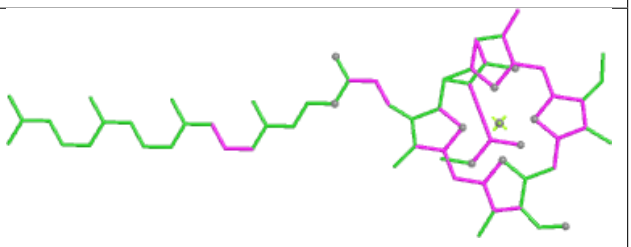

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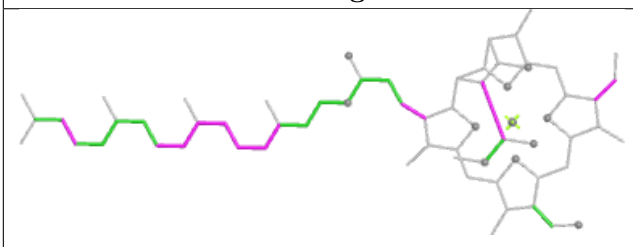

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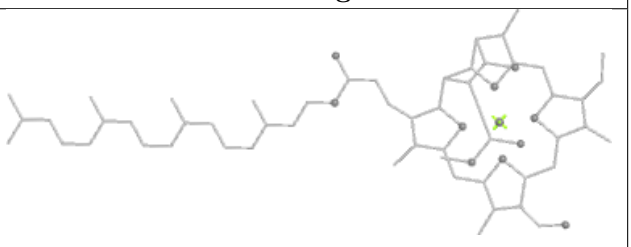

Rings

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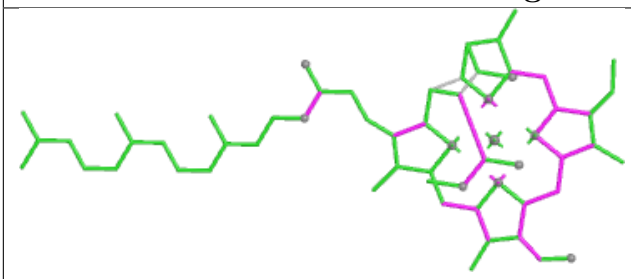

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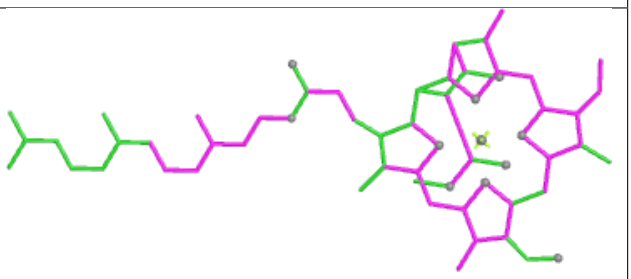

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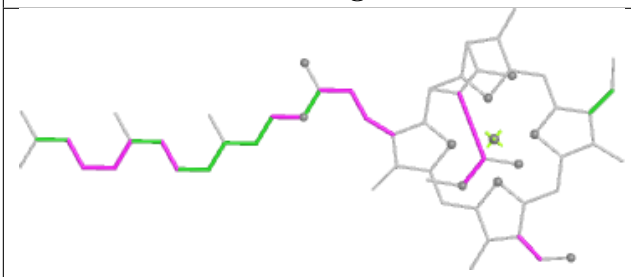

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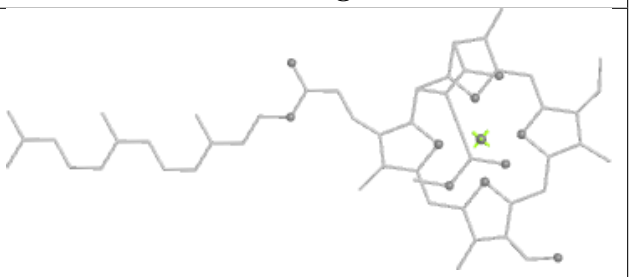

Rings

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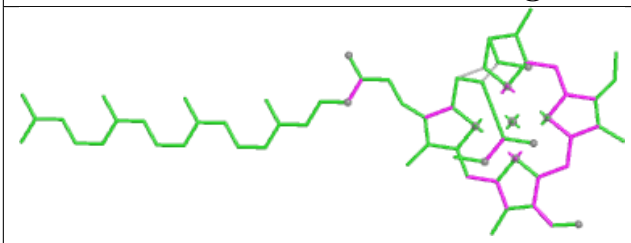

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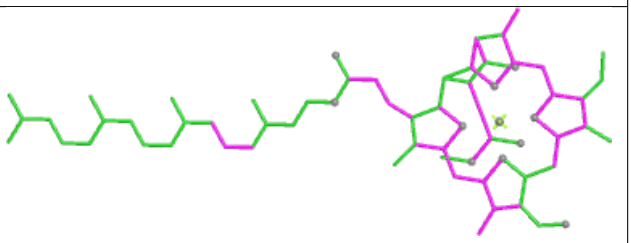
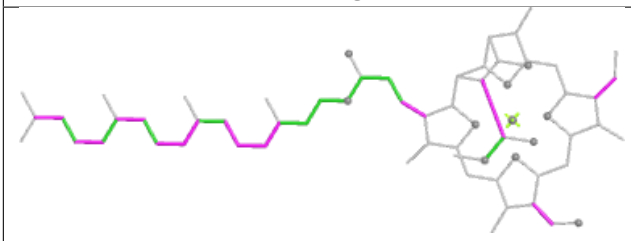


Bond angles



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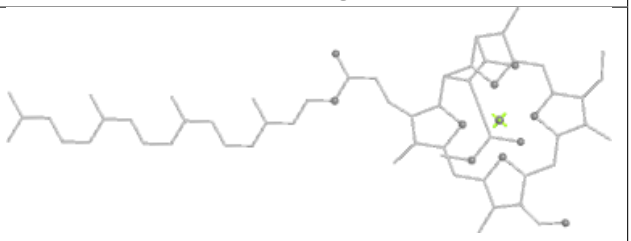
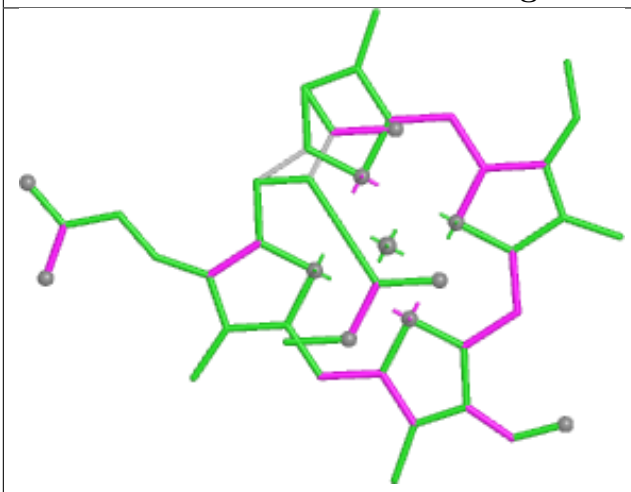


Rings

Ligand CL7 4B 623



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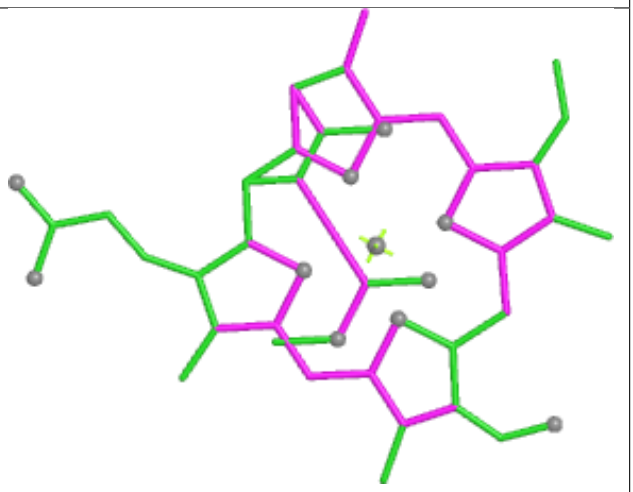

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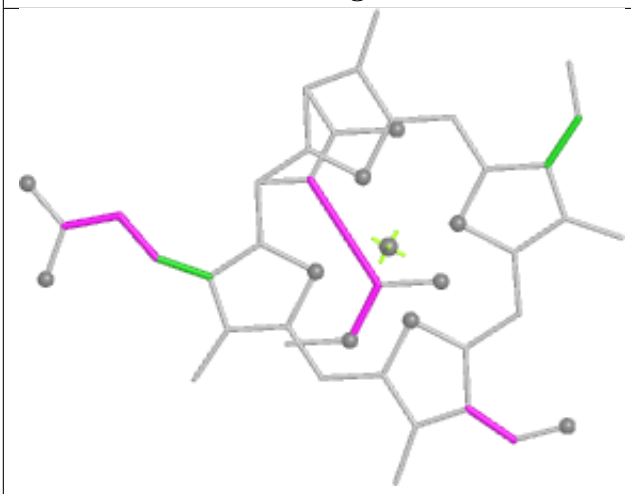
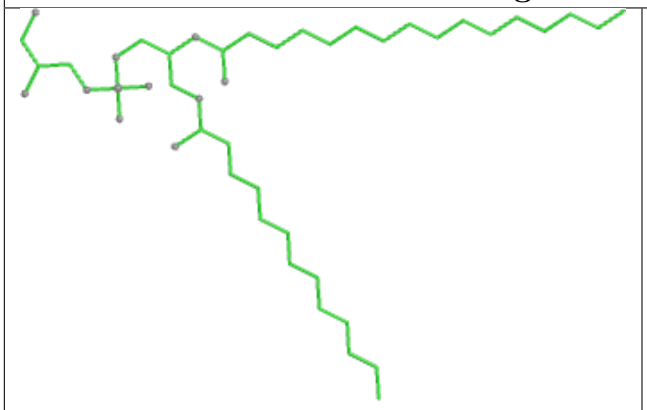


Torsions



Rings

Ligand LHG 4A 408



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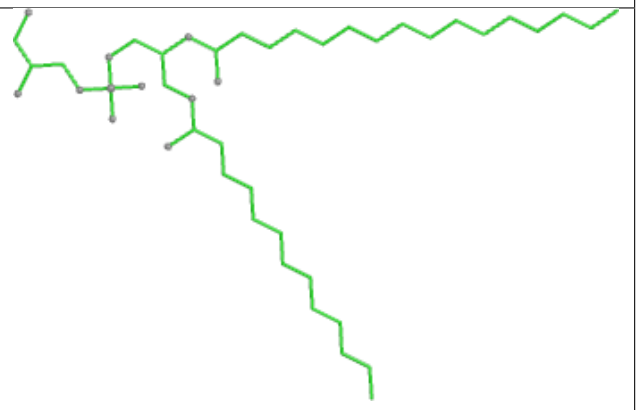

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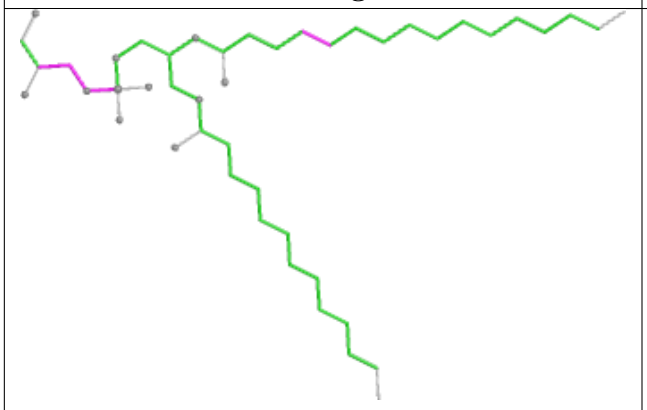

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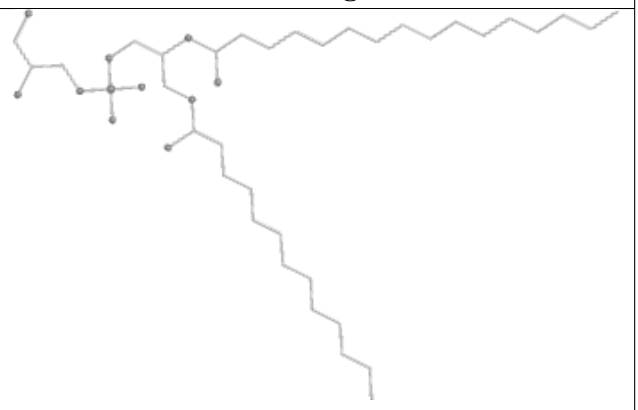
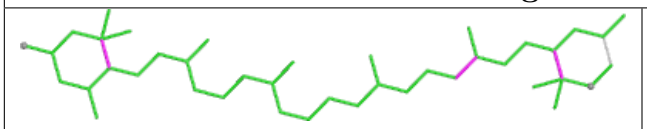


Rings

Ligand ZEX 42 524



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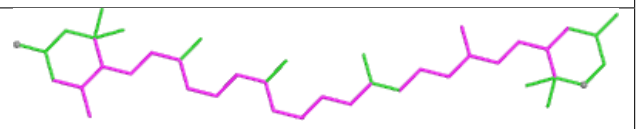

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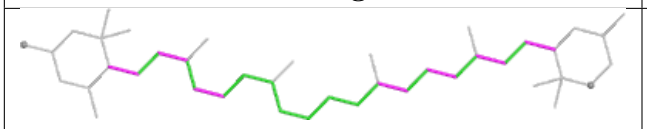

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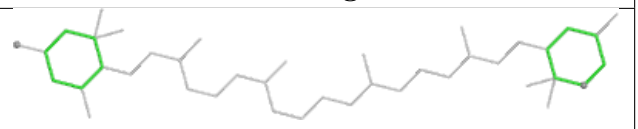
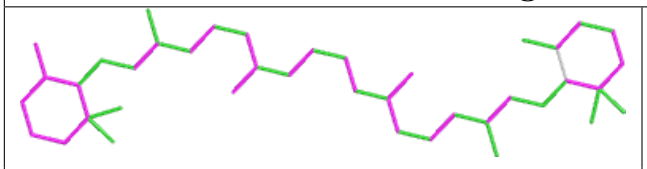


Rings

Ligand 8CT 4C 514



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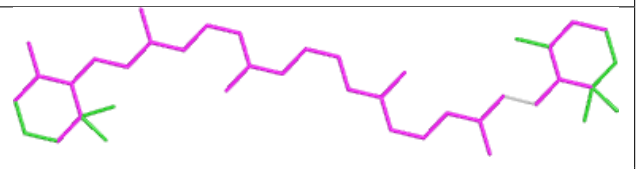

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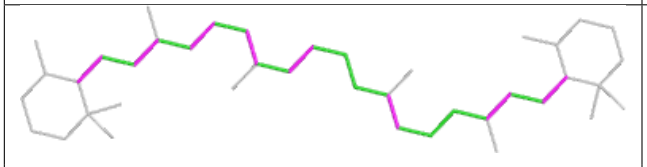

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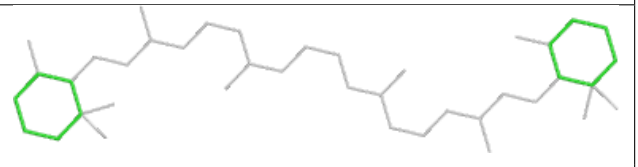
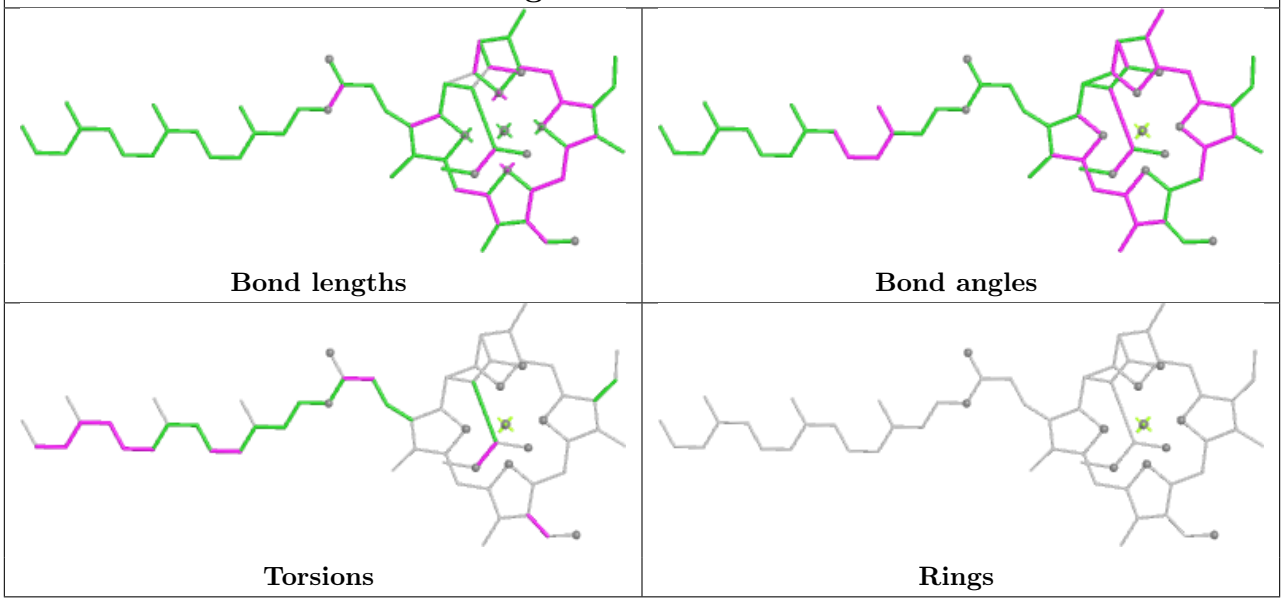


Rings

Ligand CL7 31 406



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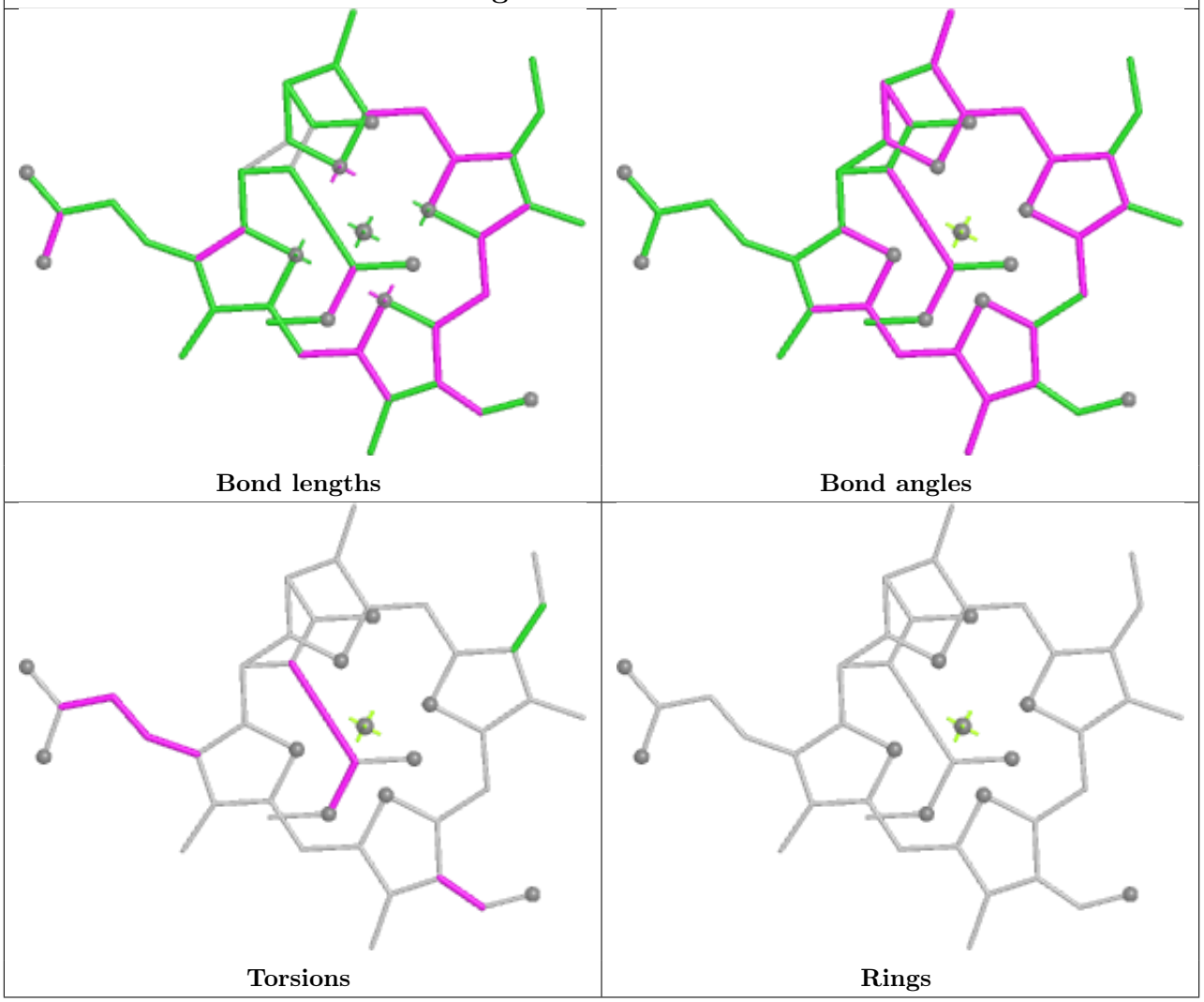

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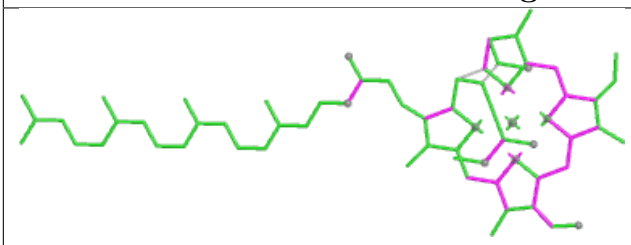

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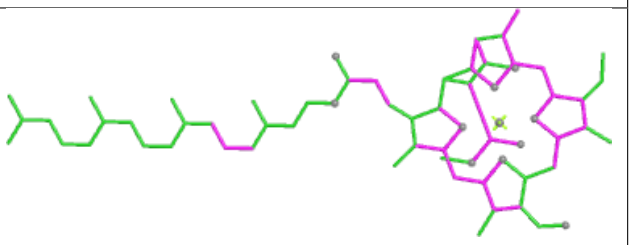
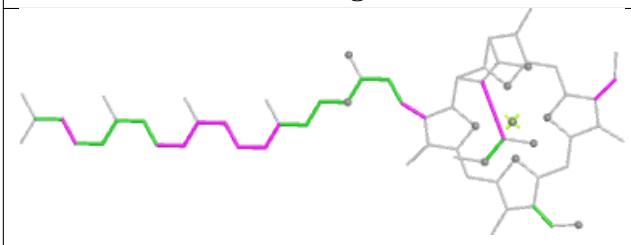


Bond angles



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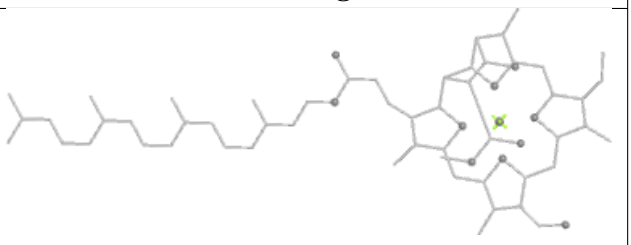
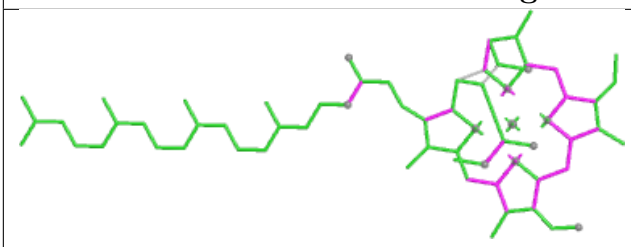


Rings

Ligand CL7 1B 612



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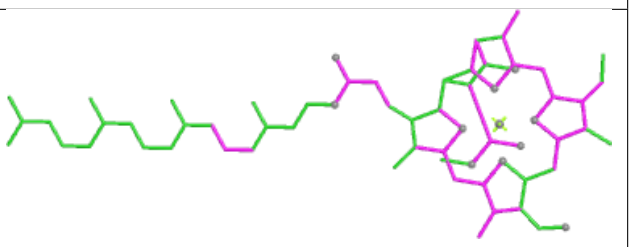
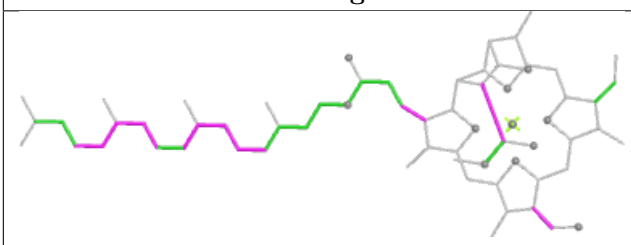


Bond angles



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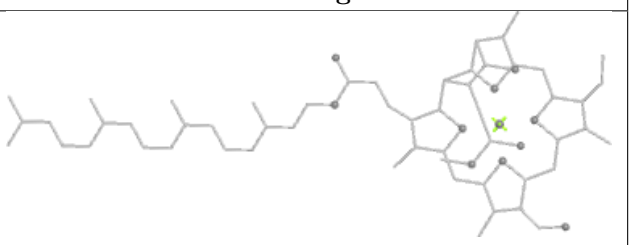
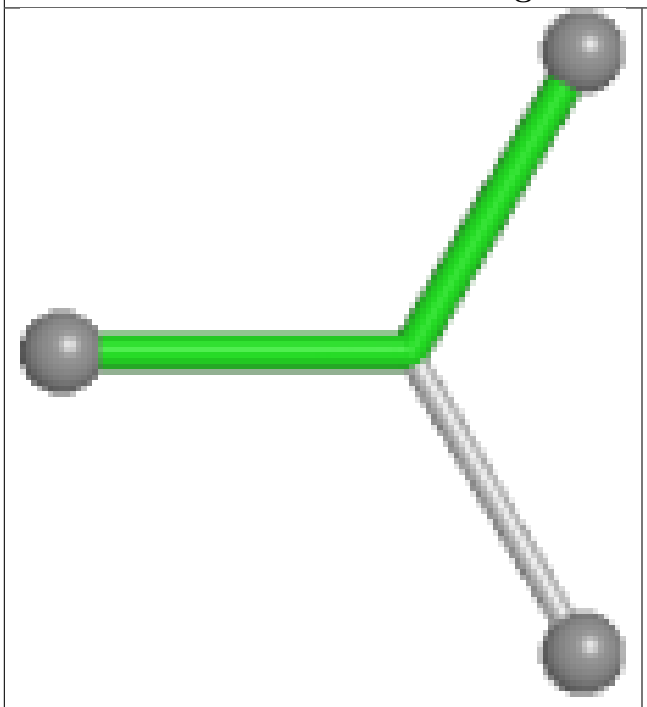


Rings

Ligand BCT 4D 403



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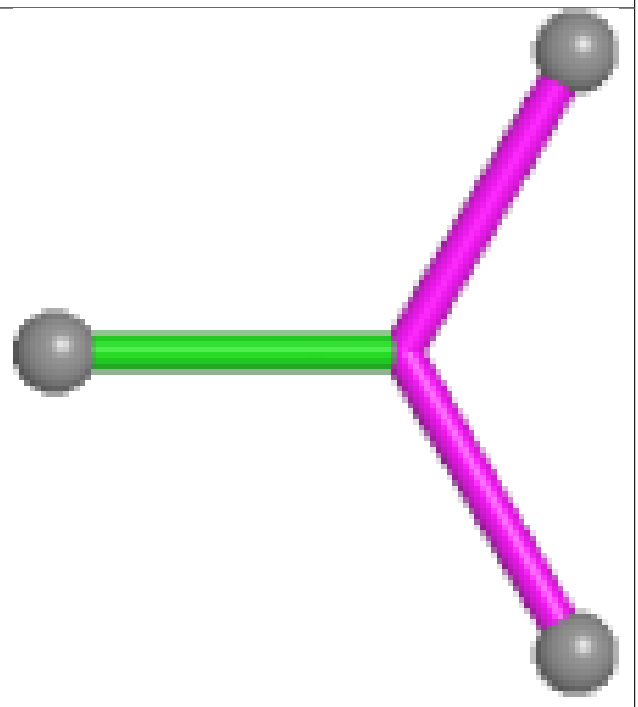
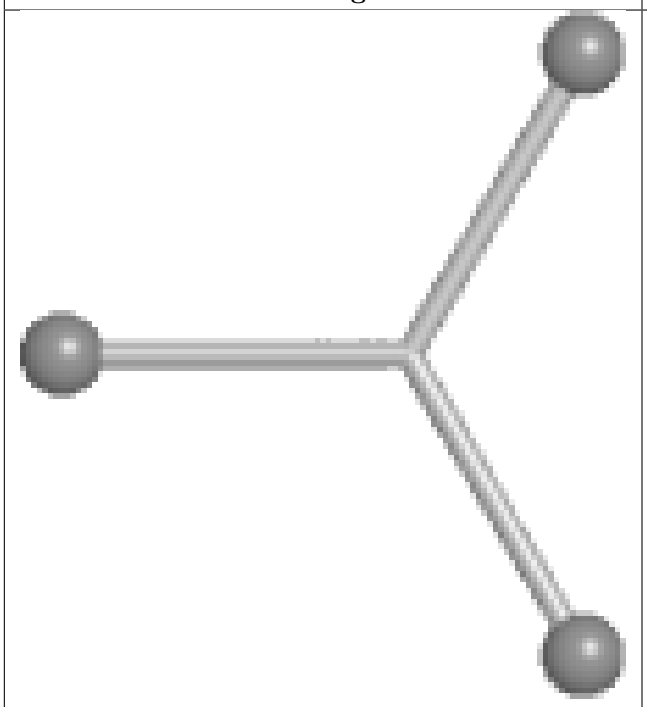


Bond angles



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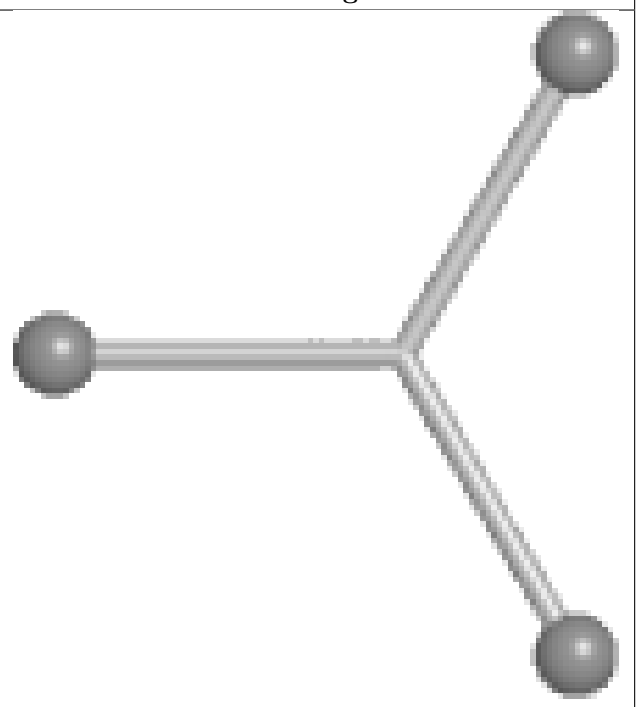
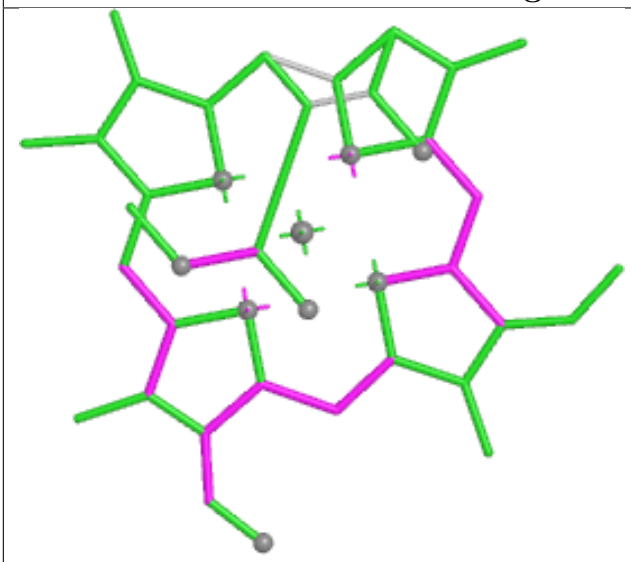


Rings

Ligand CL7 24 407



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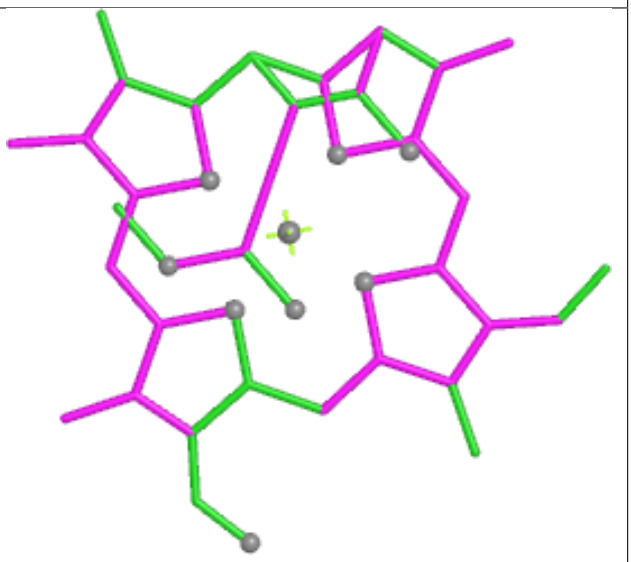
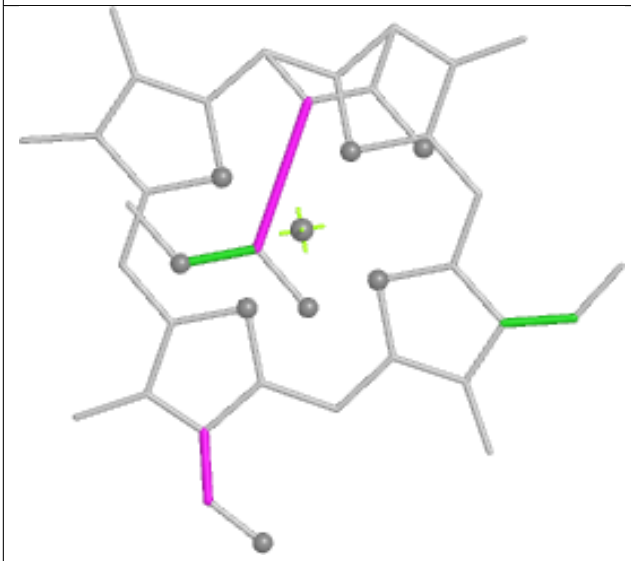
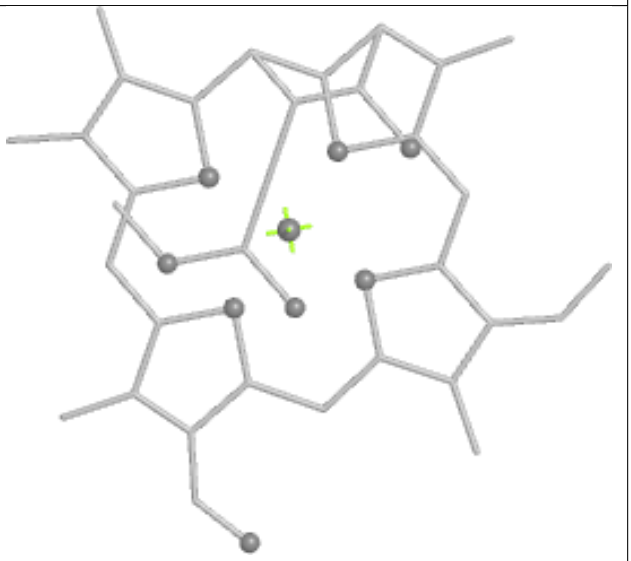


Bond angles

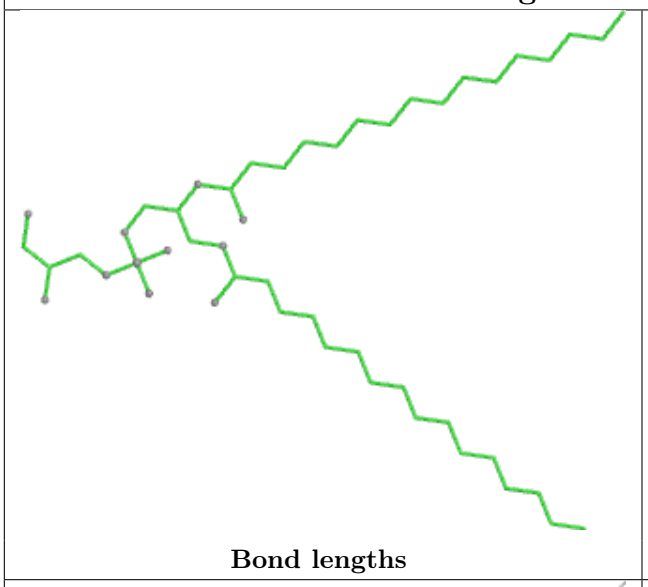


Torsions

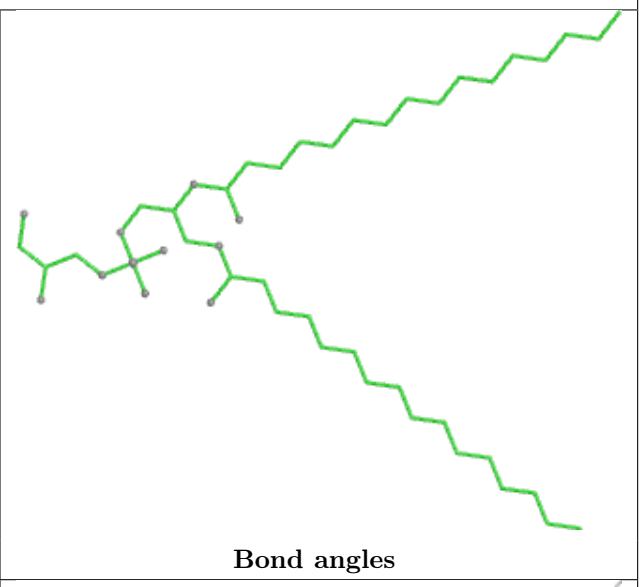


Rings

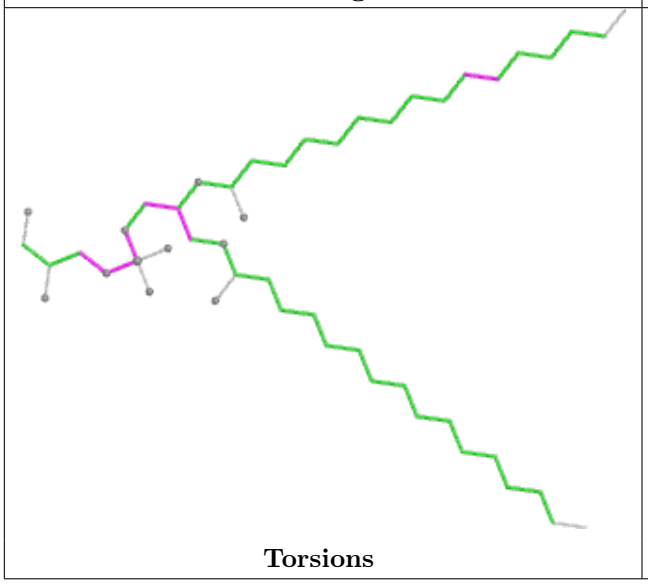
Ligand LHG 24 401



Bond lengths



Bond angles



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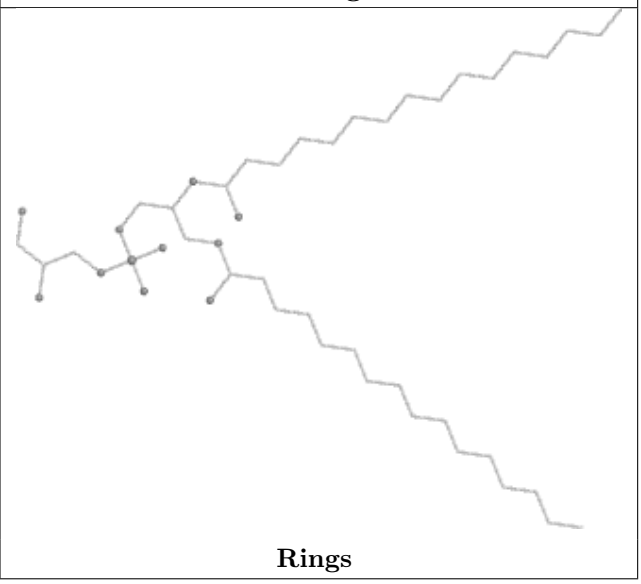
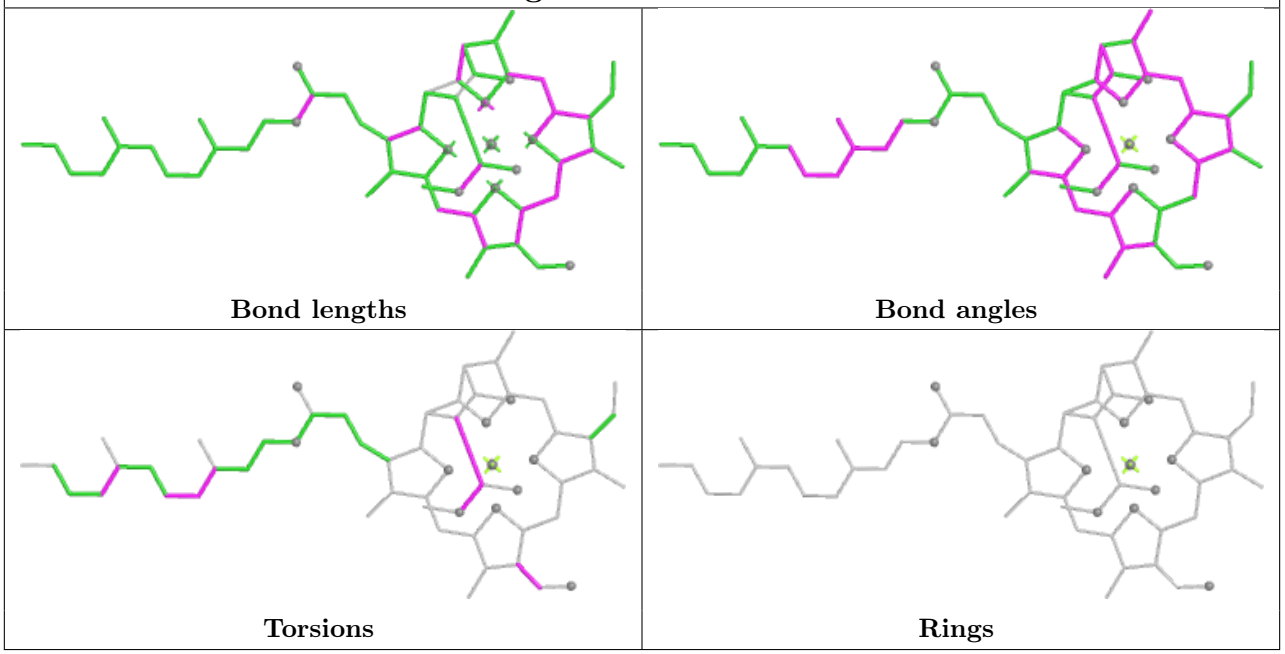


Rings

Ligand CL7 13 502



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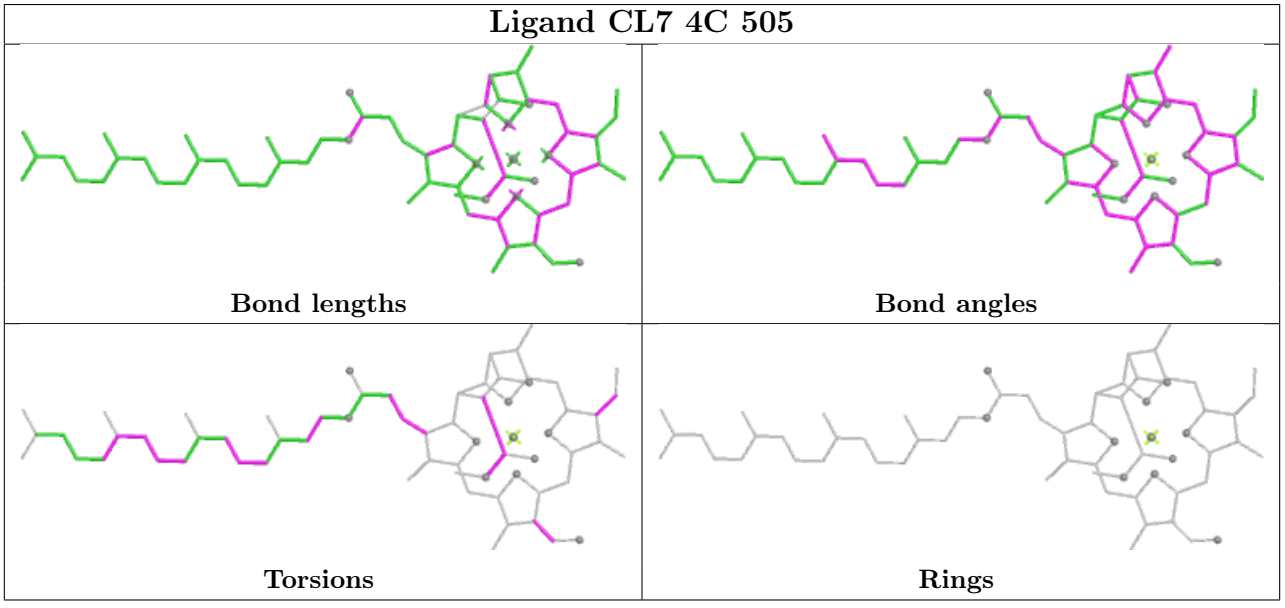
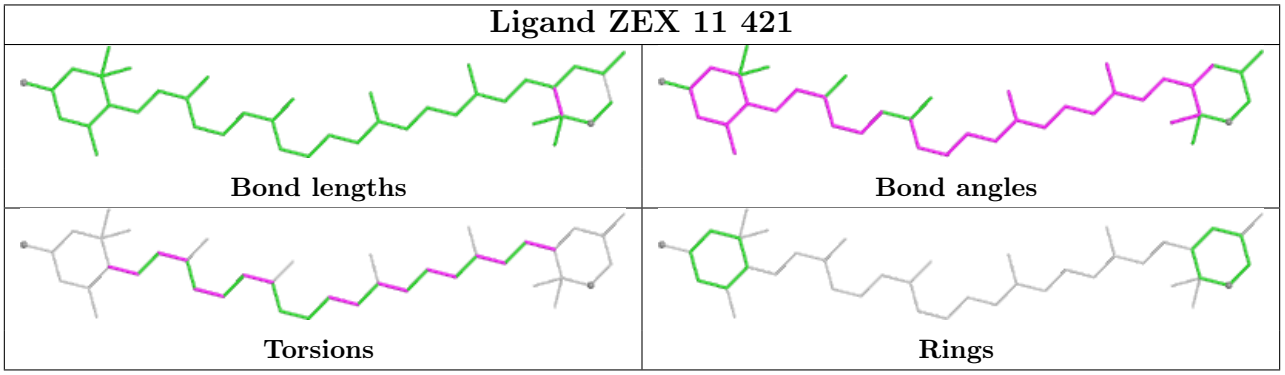
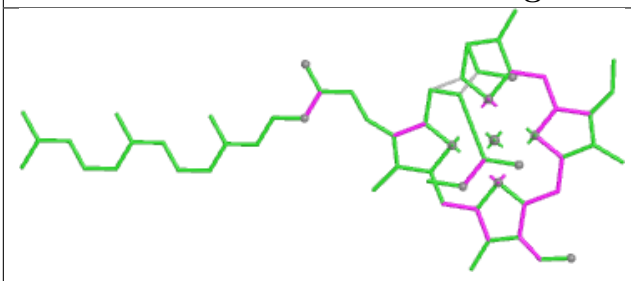


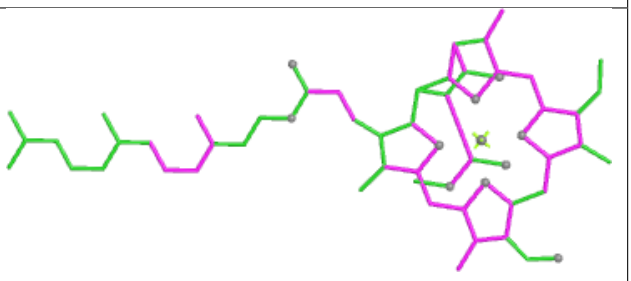
Ligand ZEX 11 421



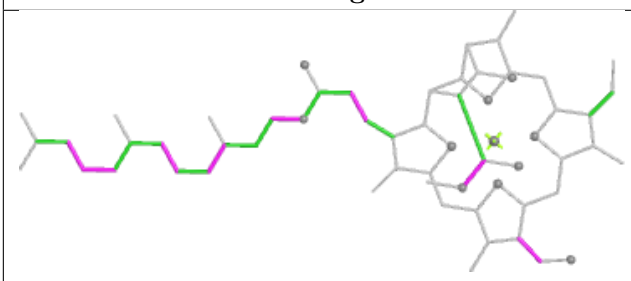
Ligand CL7 11 403



Bond lengths



Bond angles



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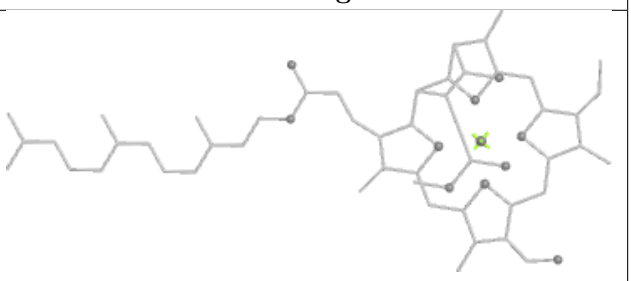
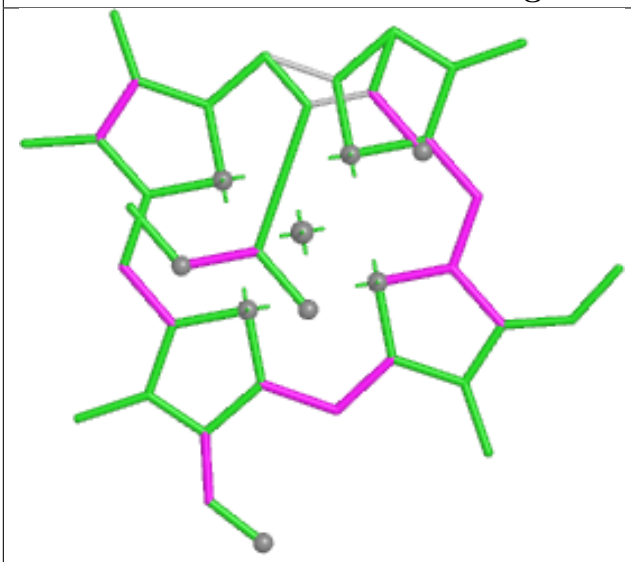


Rings

Ligand CL7 11 415



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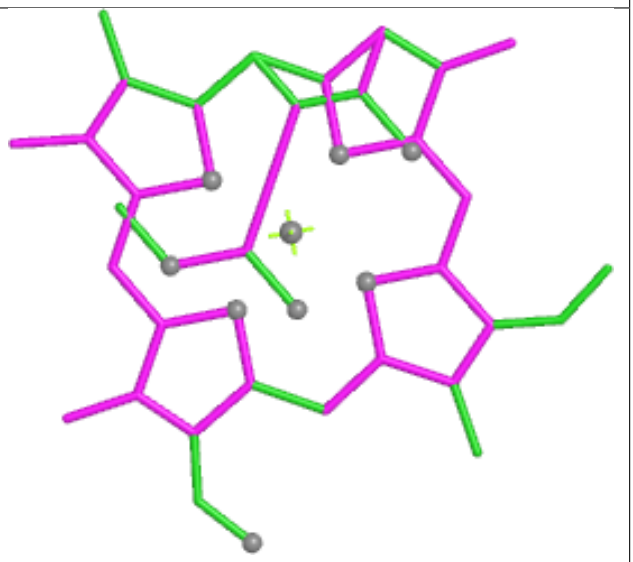
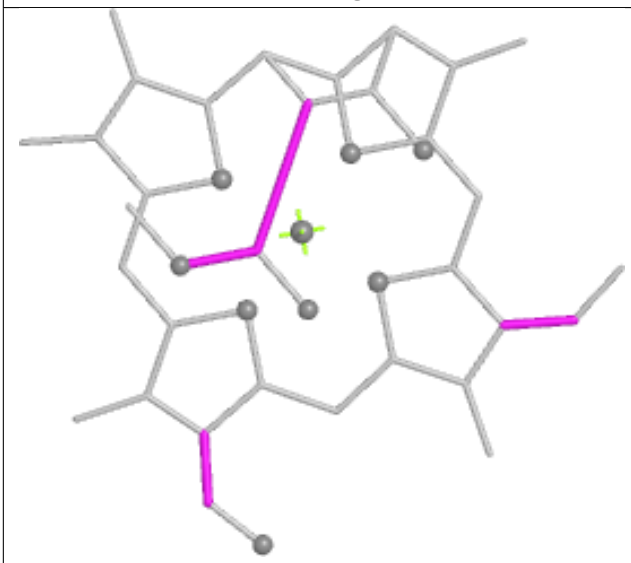


Bond angles



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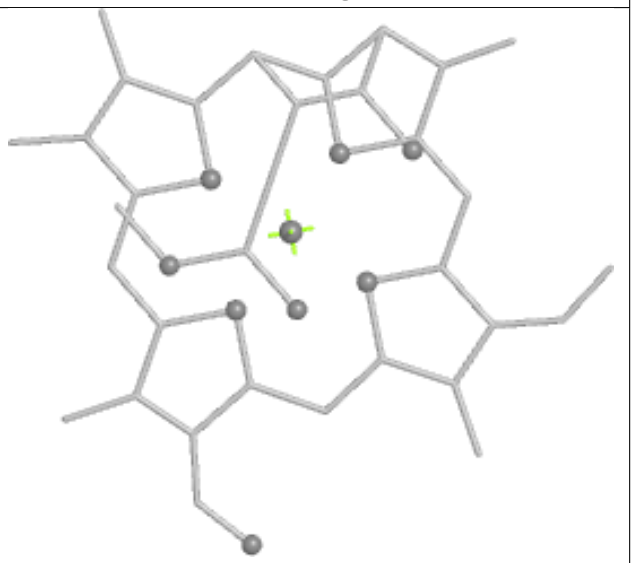
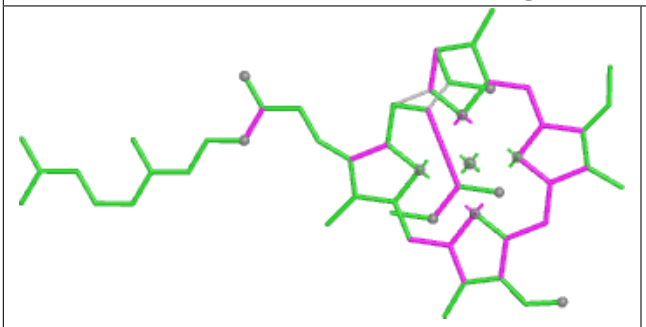


Rings

Ligand CL7 2B 614



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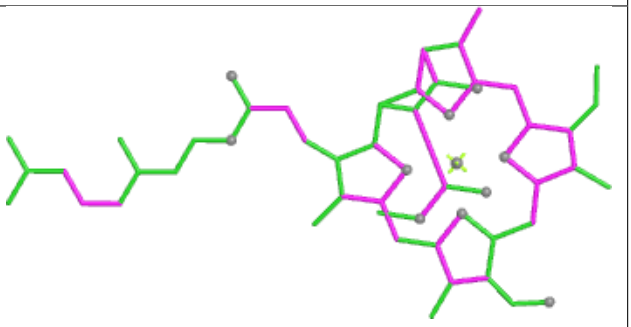
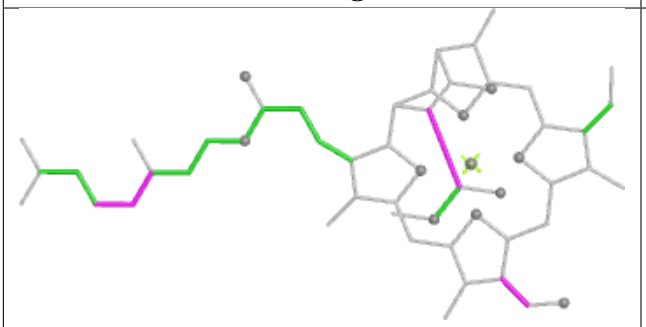


Bond angles



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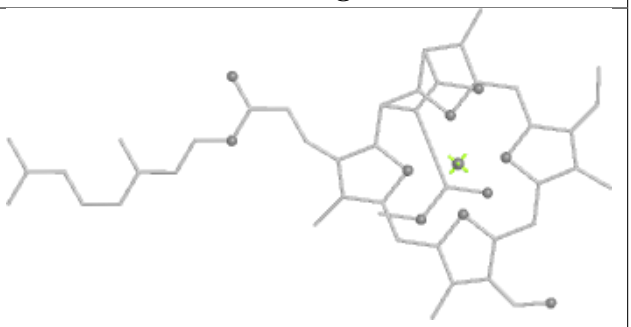
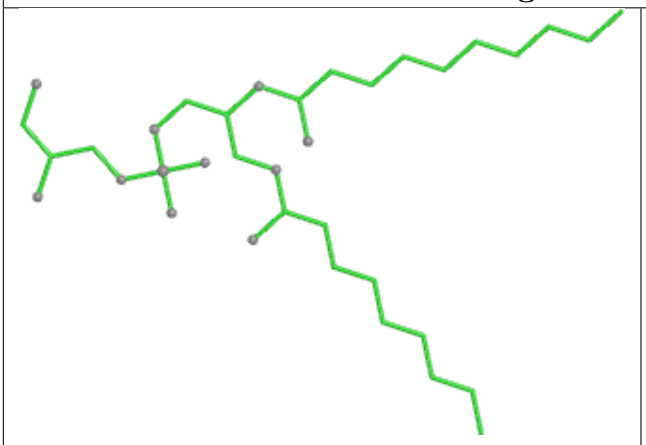


Rings

Ligand LHG 13 524



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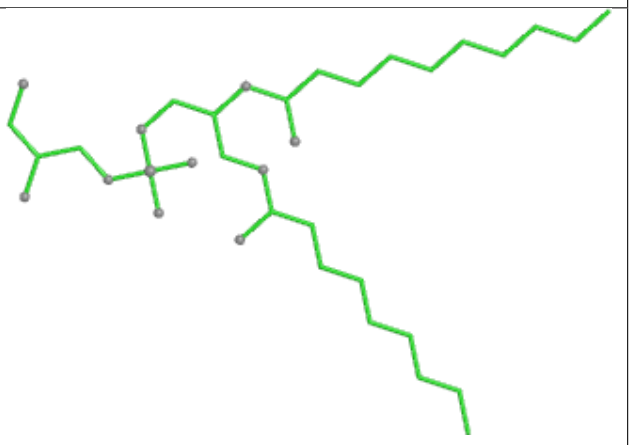
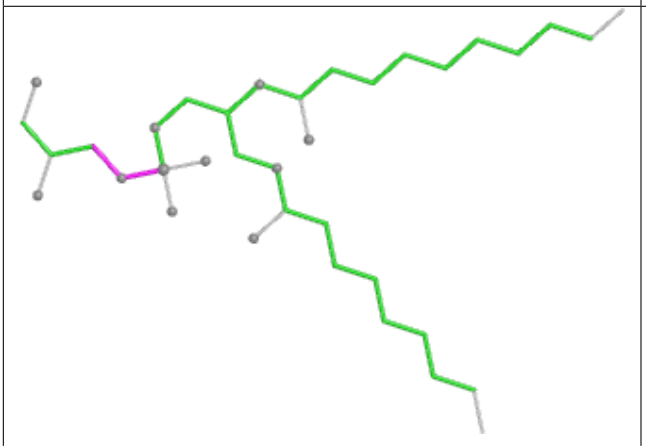


Bond angles



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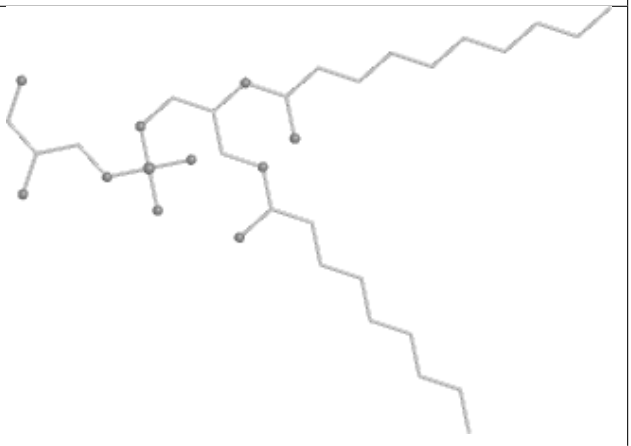
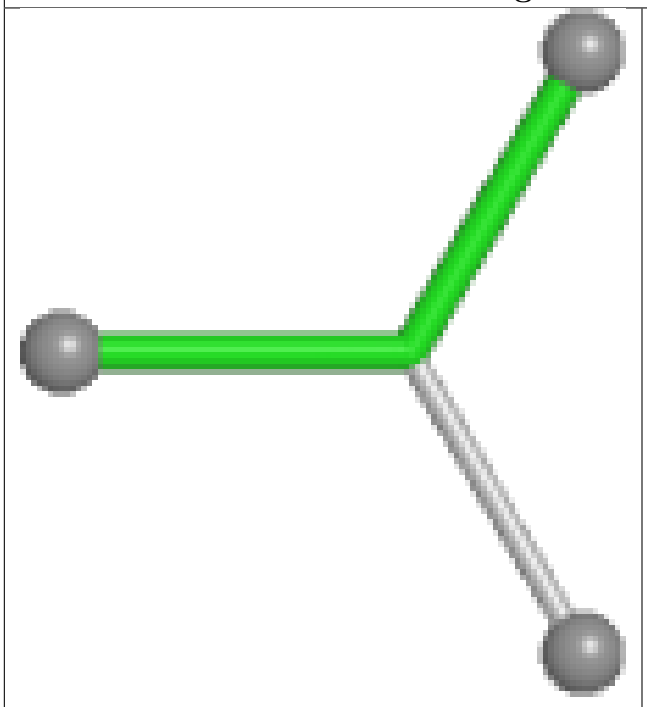


Rings

Ligand BCT 1D 403



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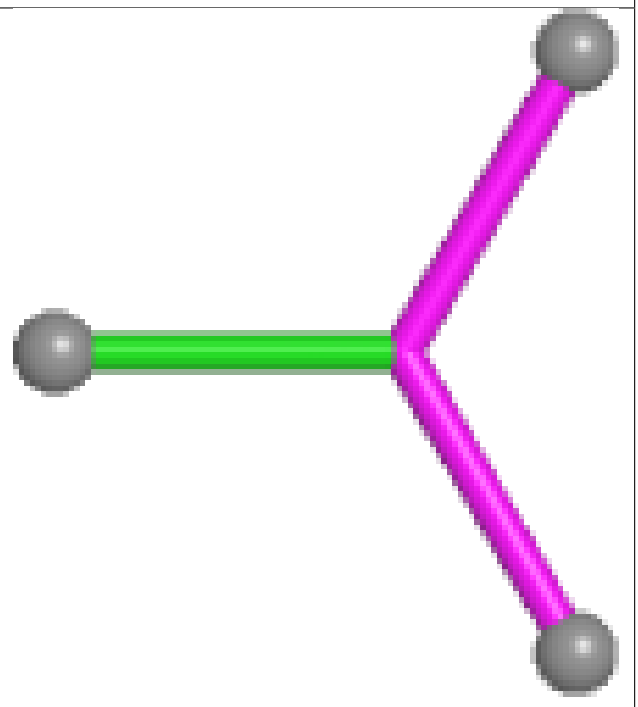
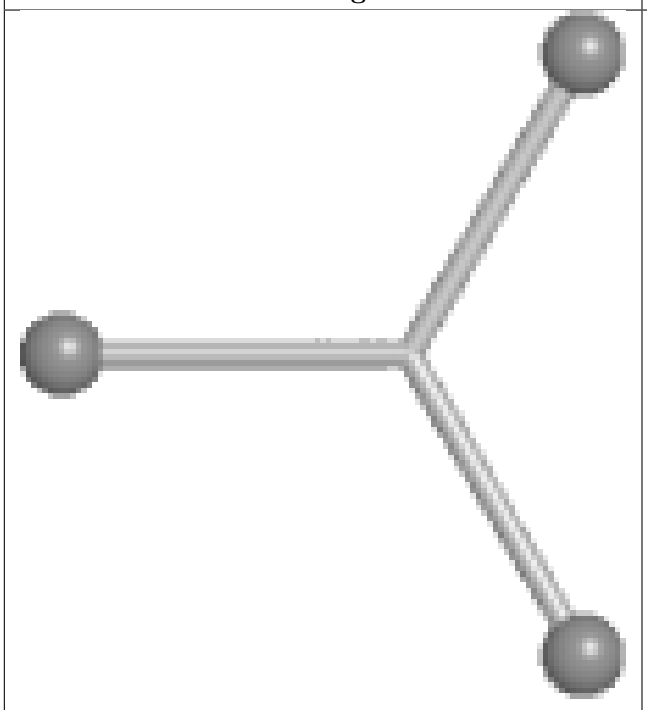


Bond angles



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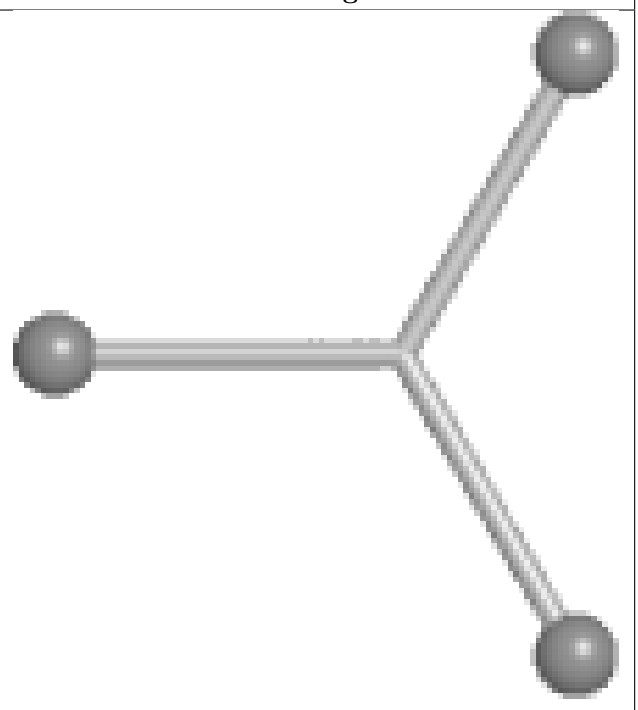
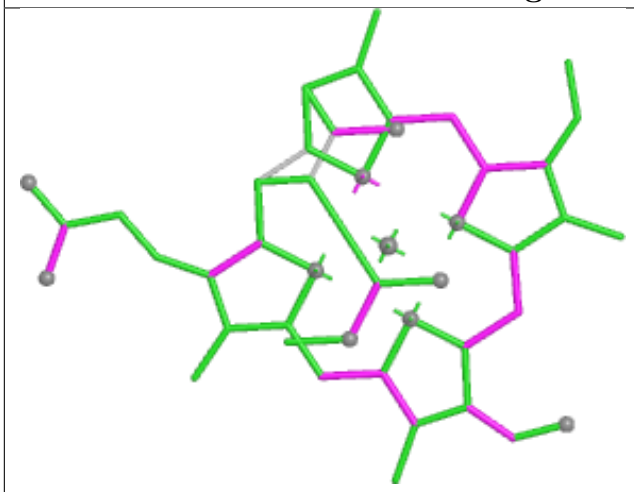


Rings

Ligand CL7 21 420



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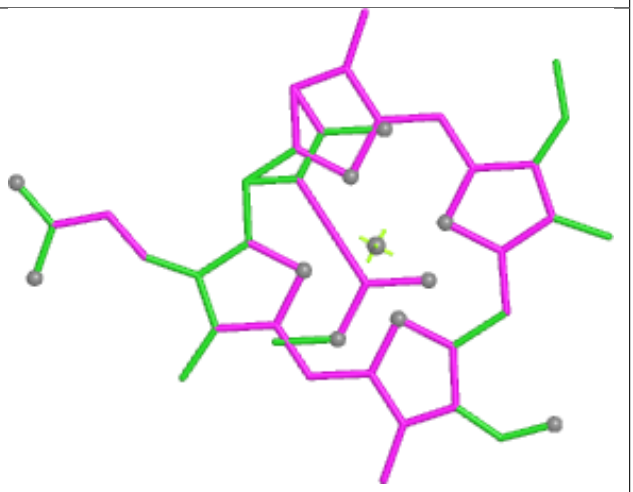
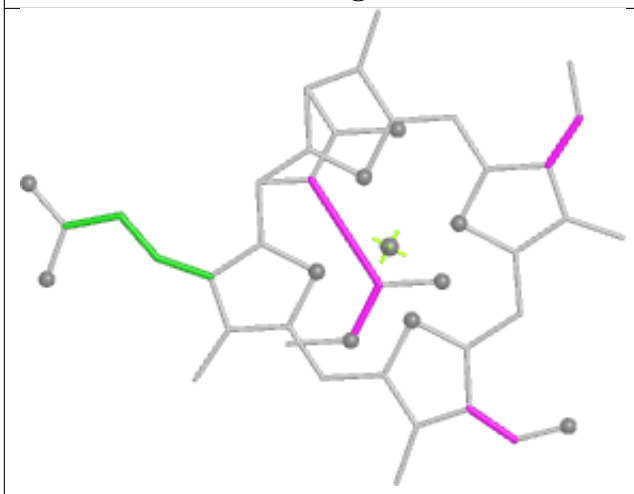


Bond angles

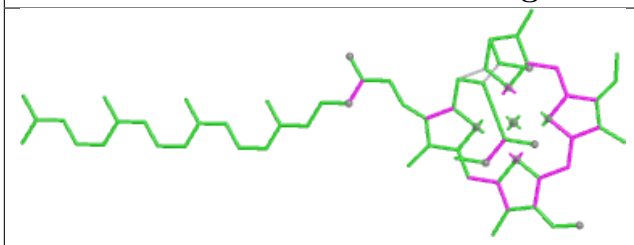


Torsions



Rings

Ligand CL7 4C 508



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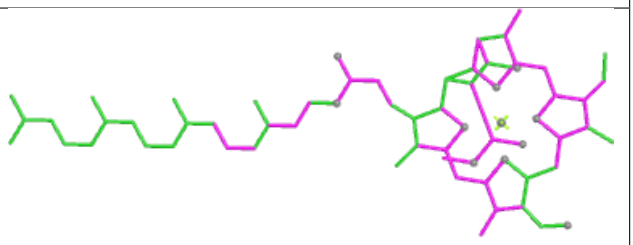
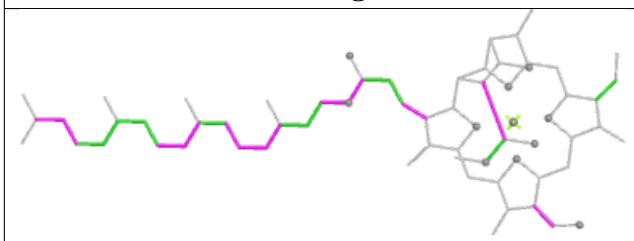


Bond angles



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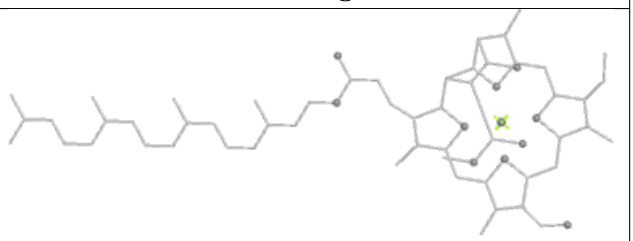
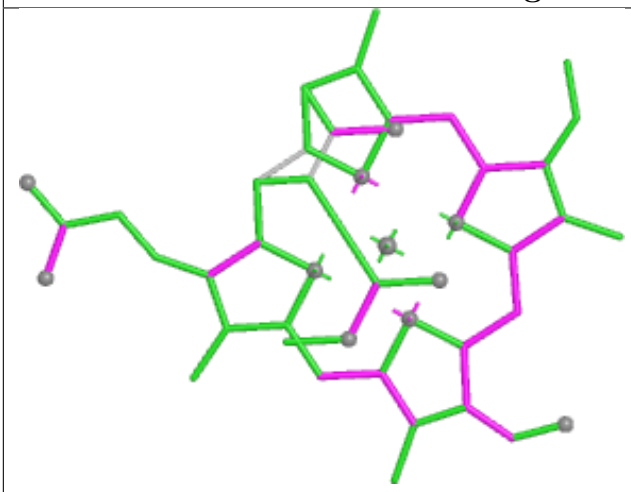


Rings

Ligand CL7 11 405



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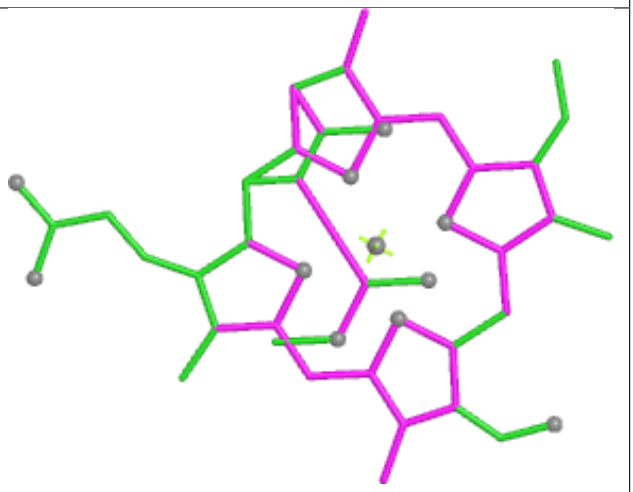
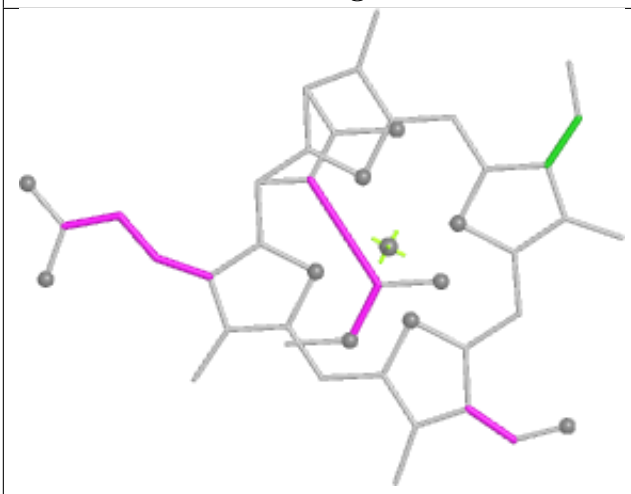


Bond angles

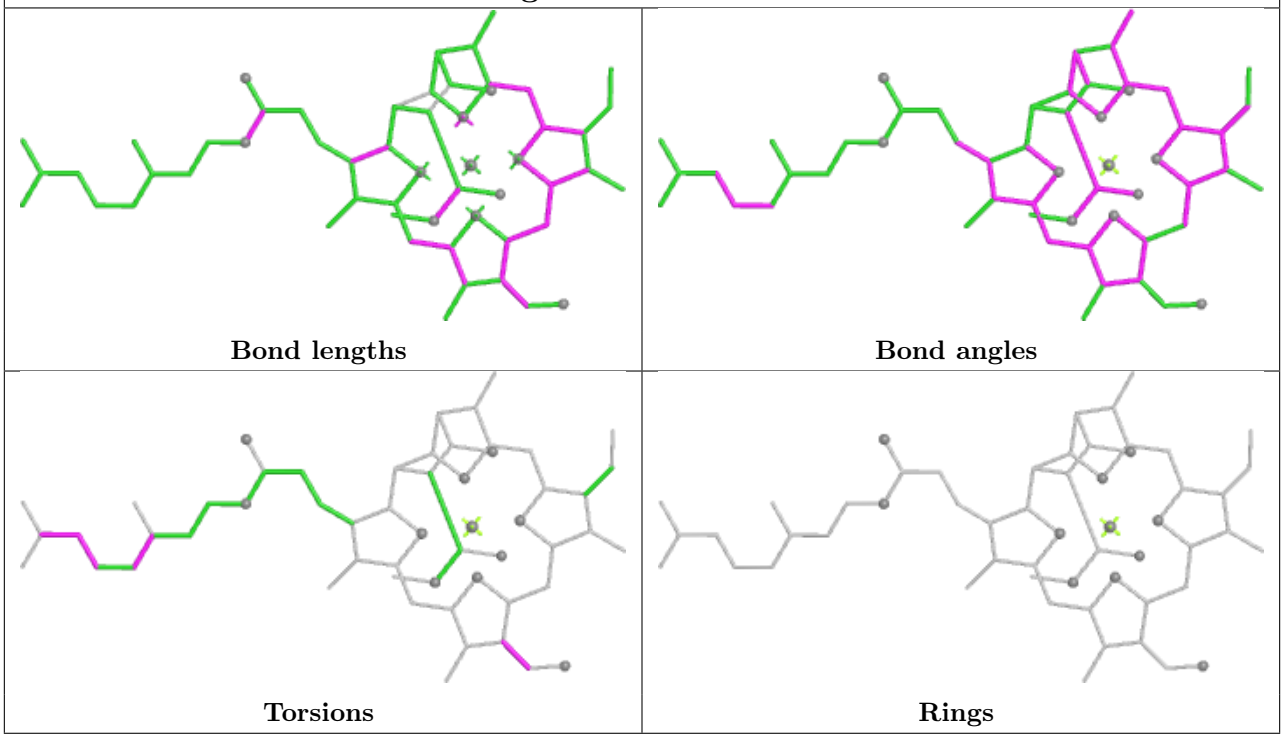


Torsions

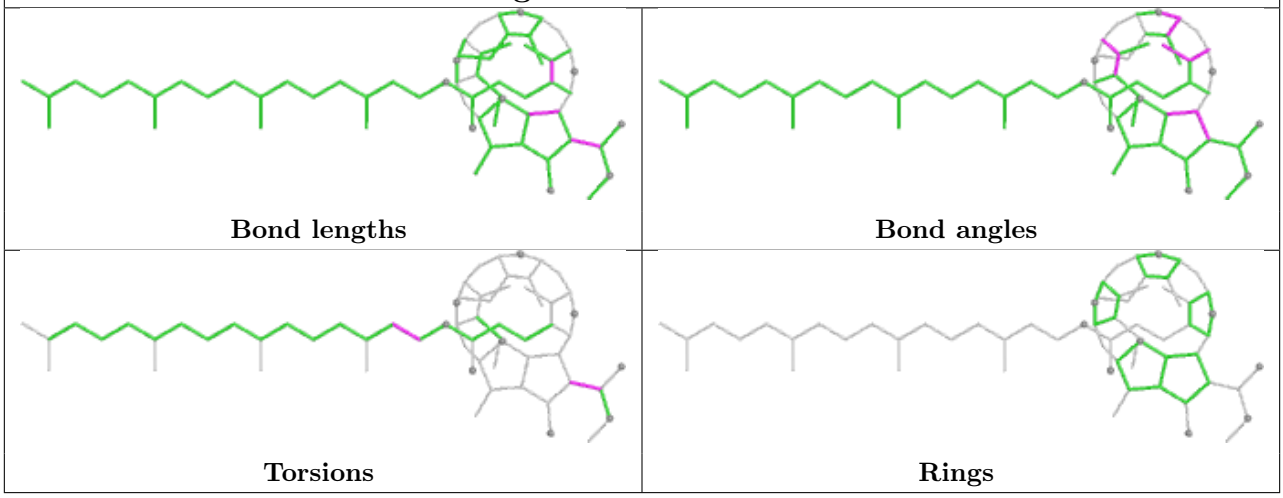


Rings

Ligand CL7 4B 607



Ligand PHO 3A 402



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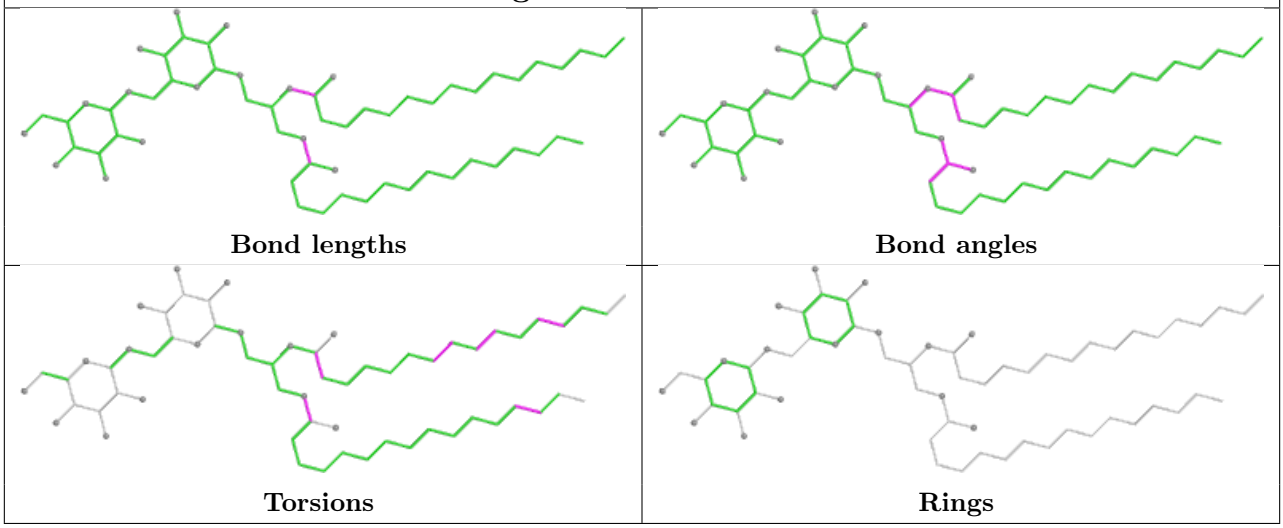

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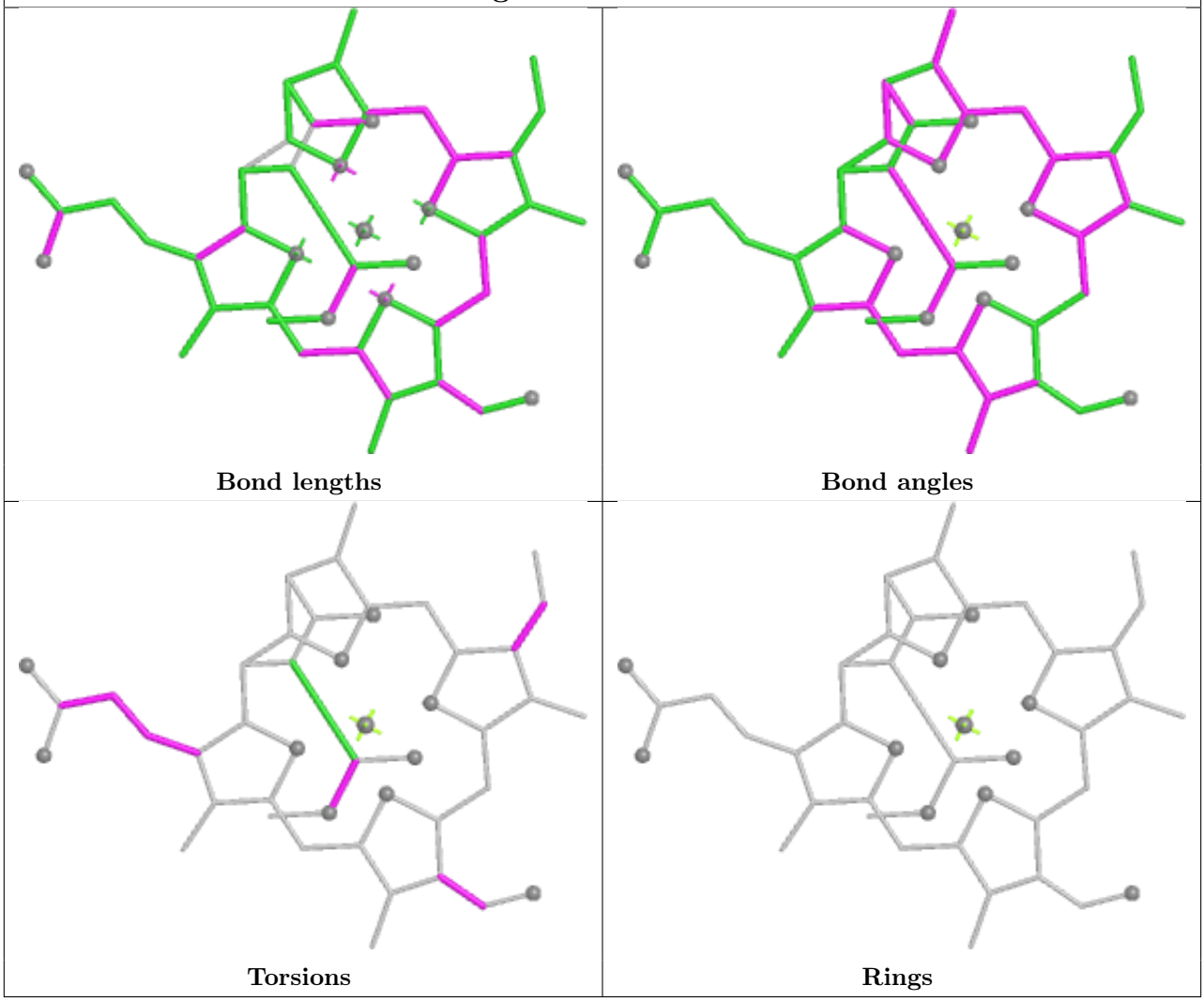

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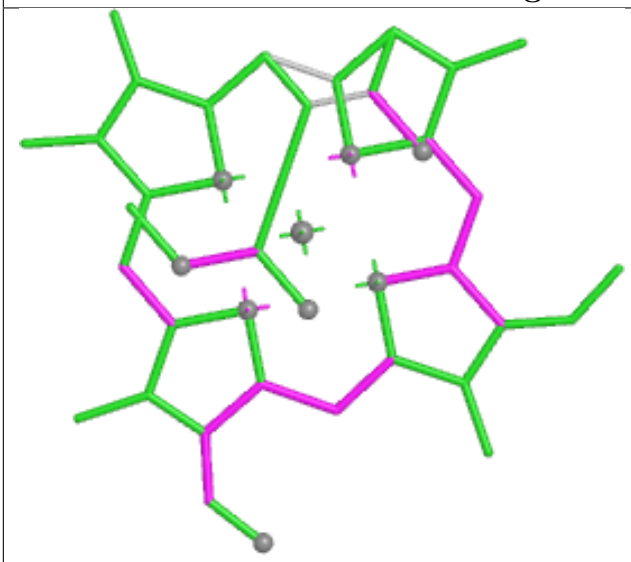
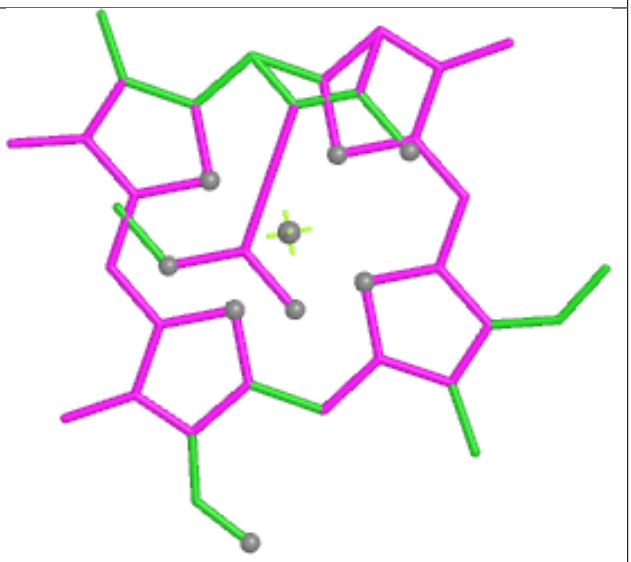
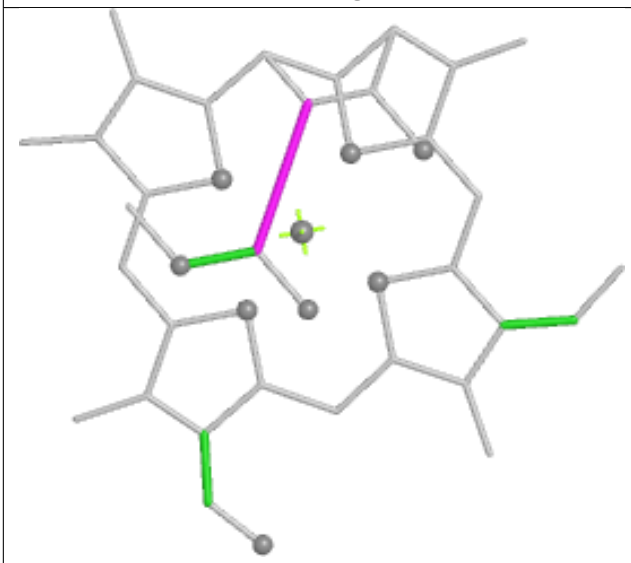


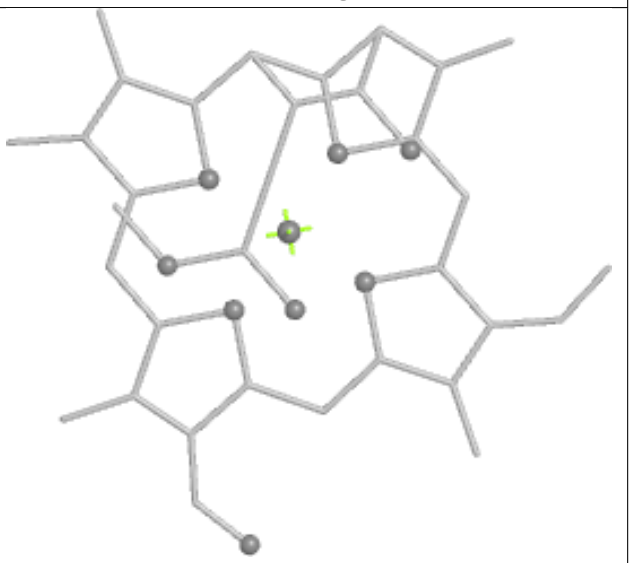
Bond lengths



Bond angles

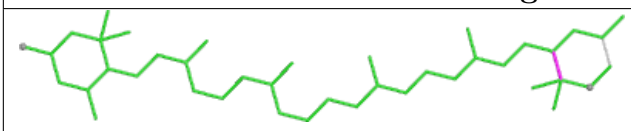


Torsions



Rings

Ligand ZEX 31 421



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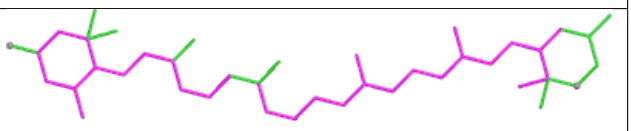
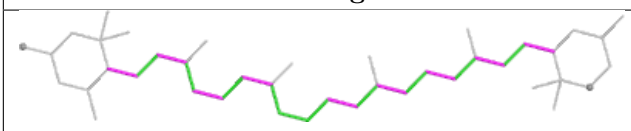


Bond angles



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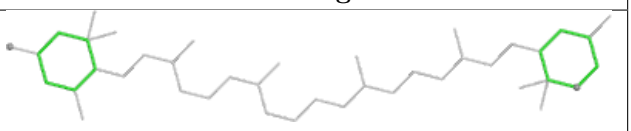
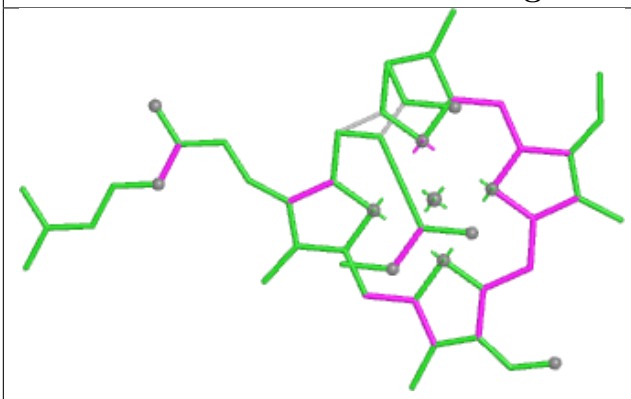


Rings

Ligand CL7 33 517



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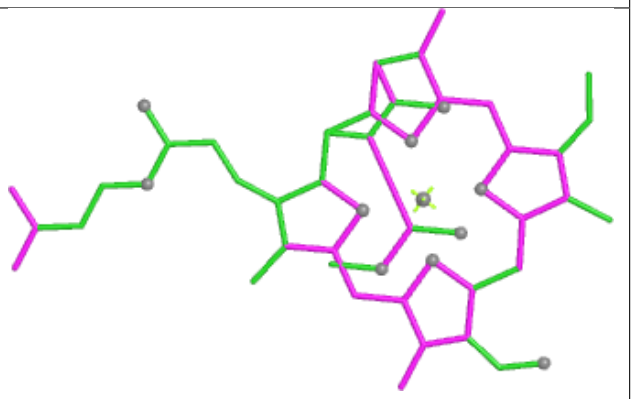
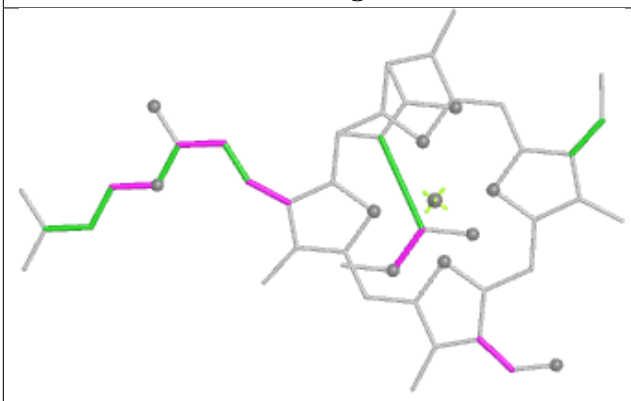


Bond angles



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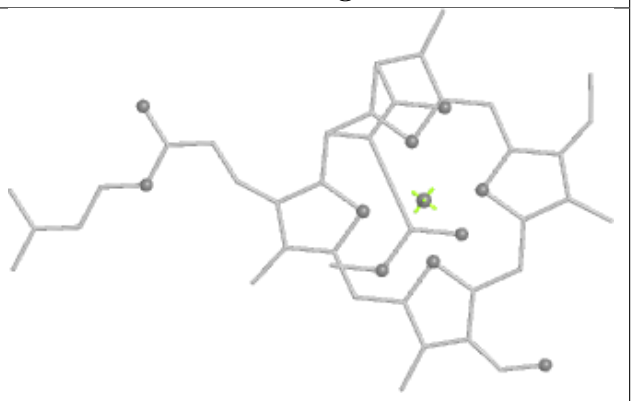
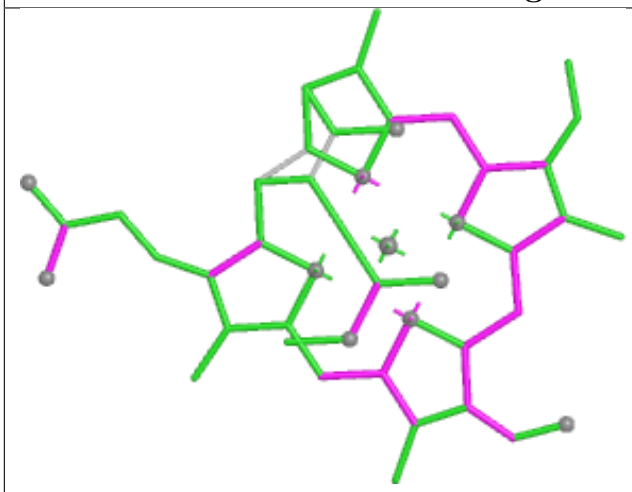


Rings

Ligand CL7 41 405



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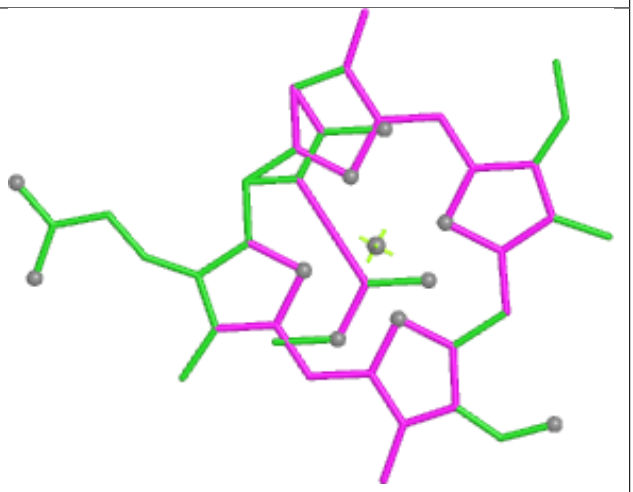
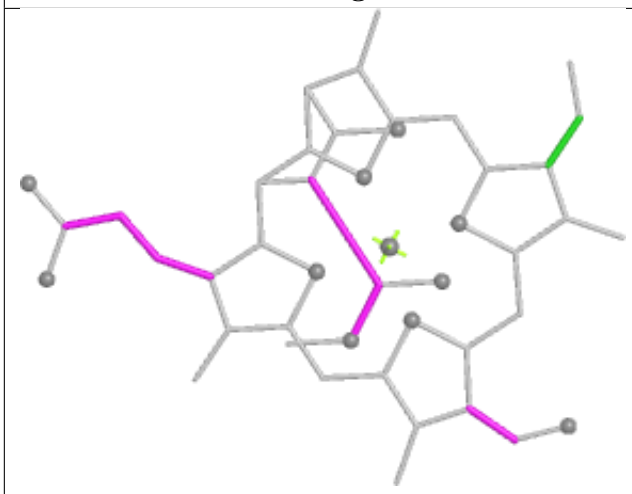


Bond angles

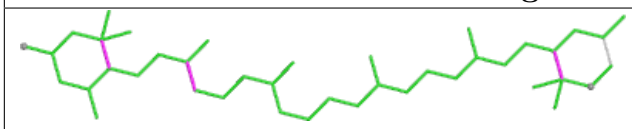


Torsions

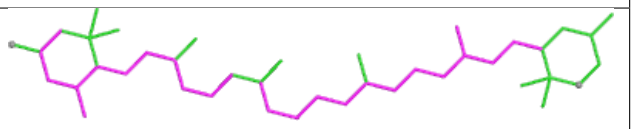


Rings

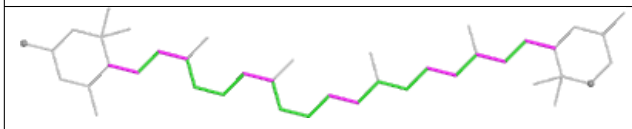
Ligand ZEX 32 519



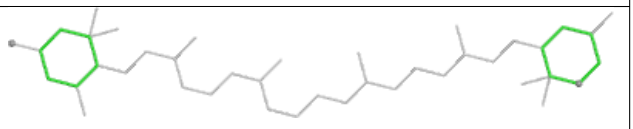
Bond lengths



Bond angles

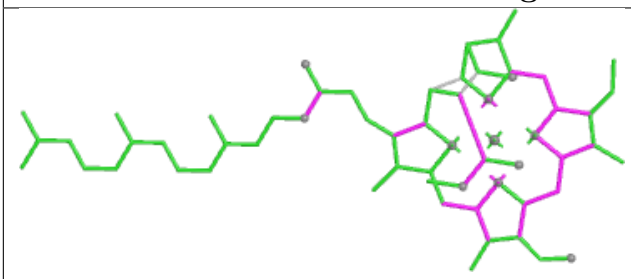


Torsions



Rings

Ligand CL7 3B 614



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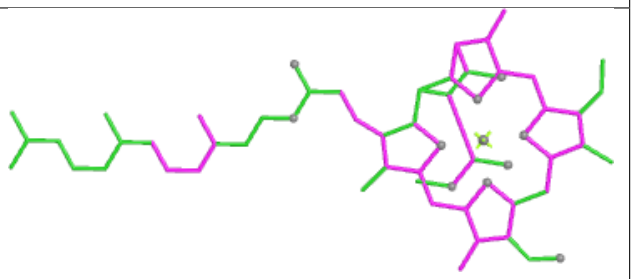

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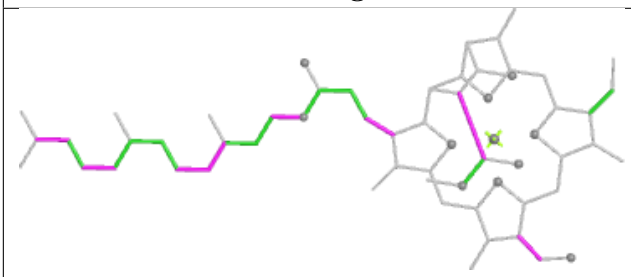

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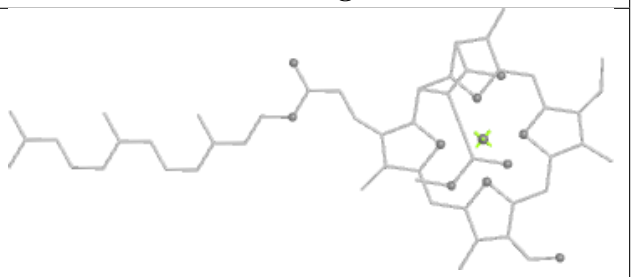
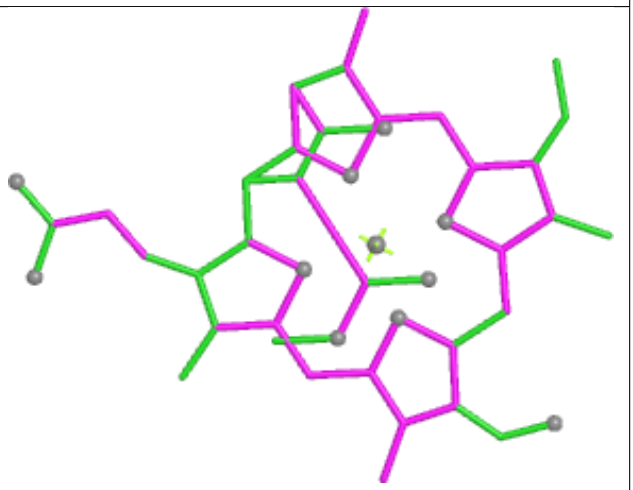


Rings

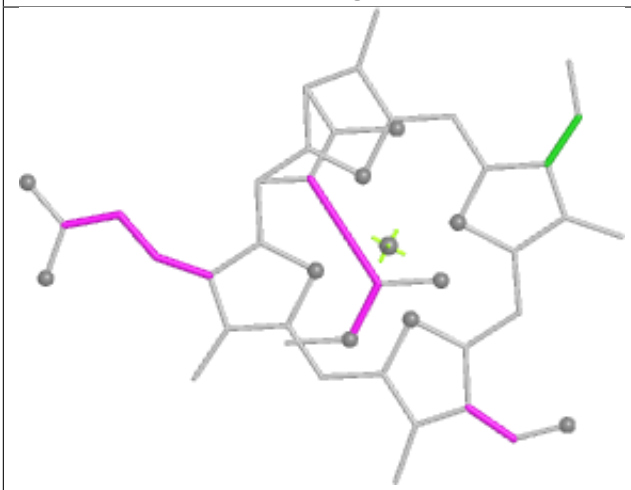
Ligand CL7 11 412



Bond lengths



Bond angles

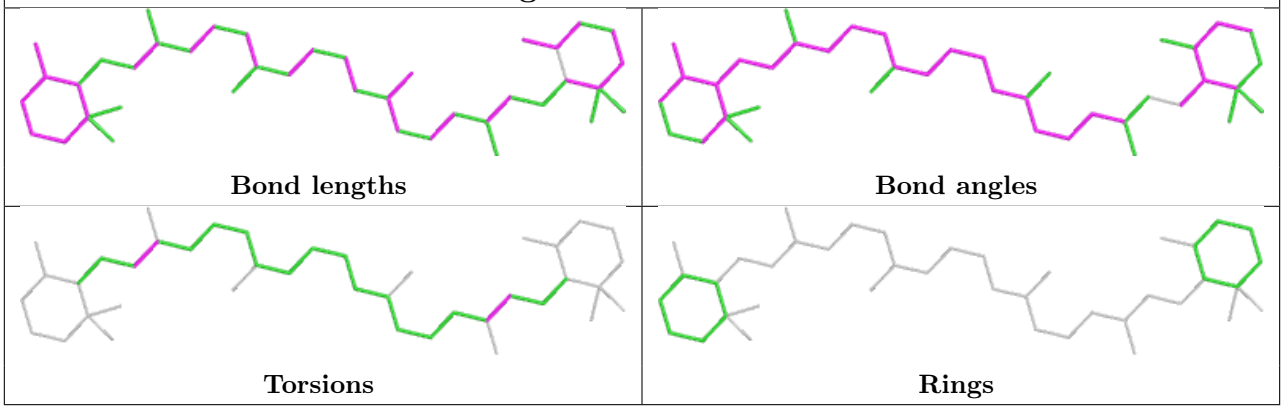


Torsions

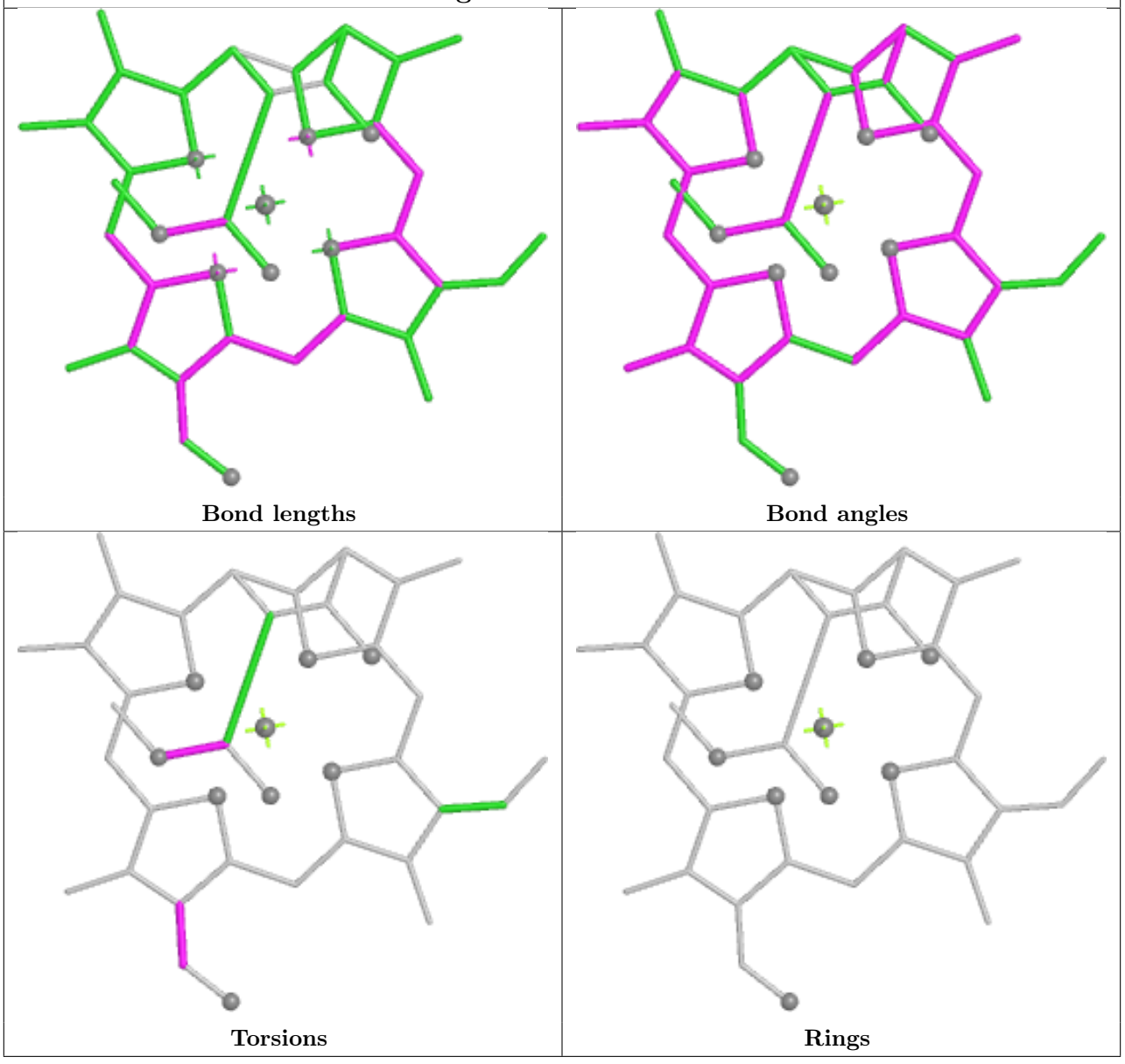


Rings

Ligand 8CT 2B 620



Ligand CL7 4C 512



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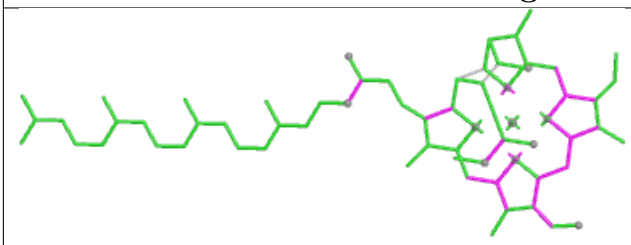

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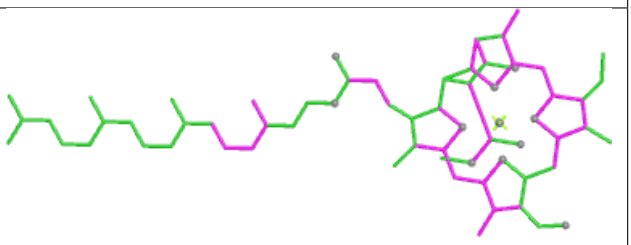

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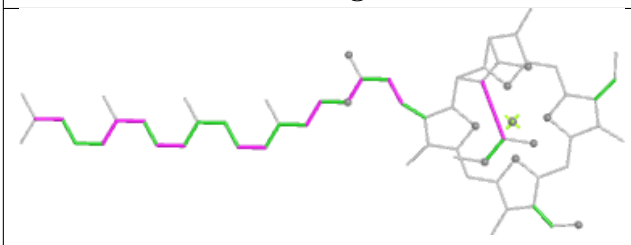

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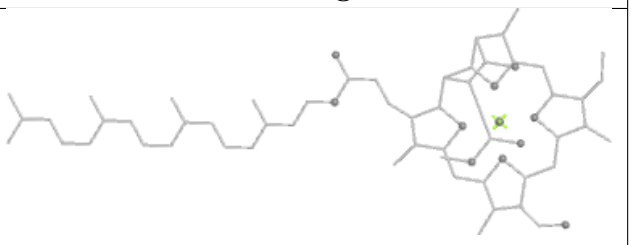
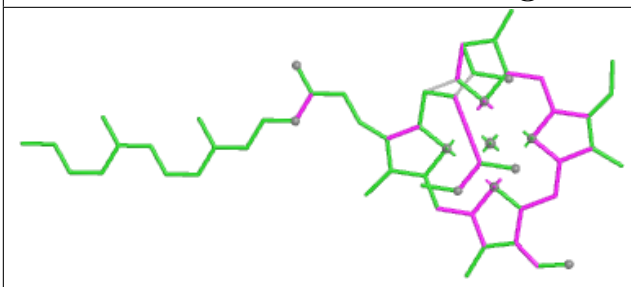


Rings

Ligand CL7 3D 404



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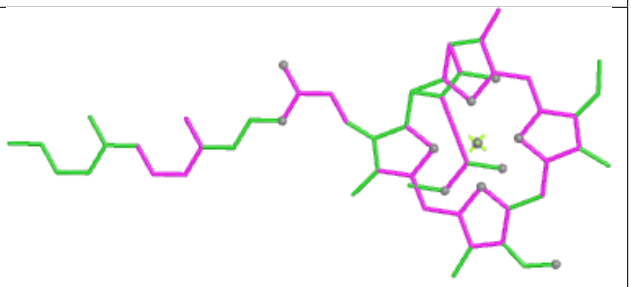

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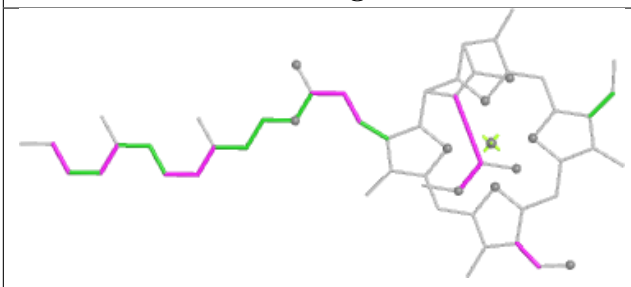

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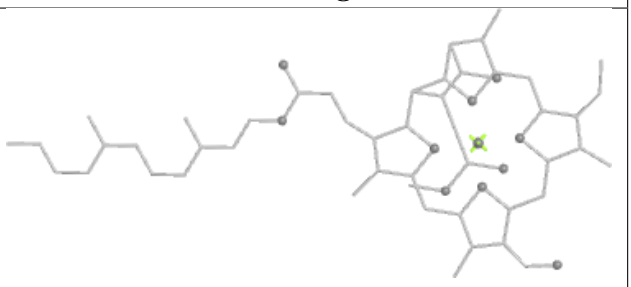
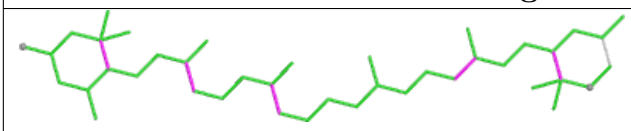


Rings

Ligand ZEX 23 401



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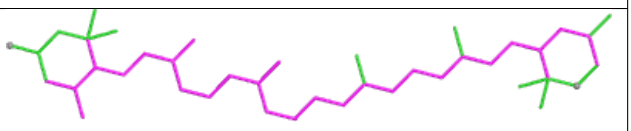

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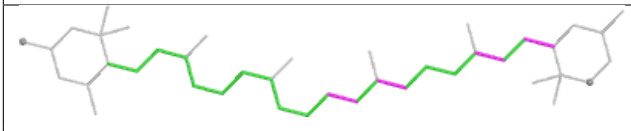

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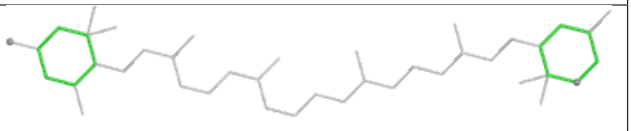
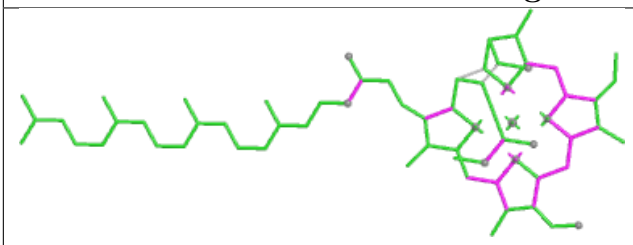


Rings

Ligand CL7 12 510



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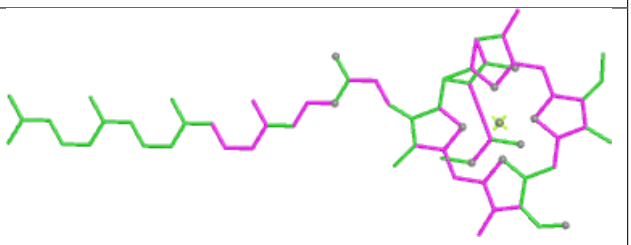
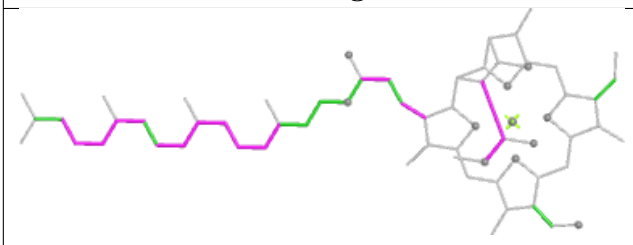


Bond angles



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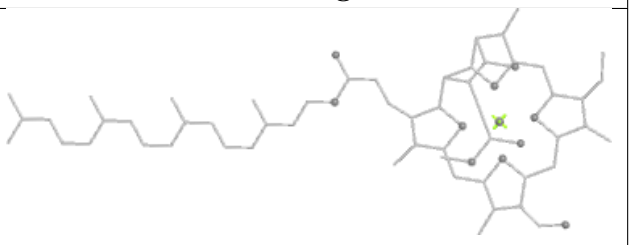
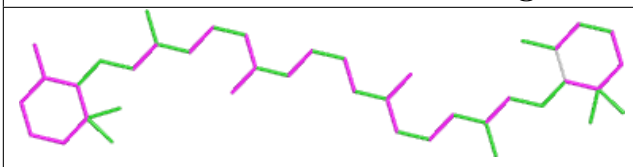


Rings

Ligand 8CT 3A 404



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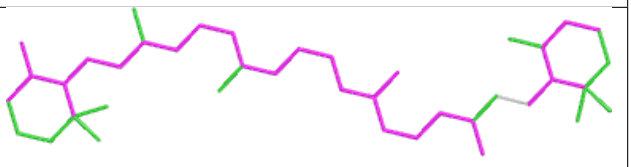

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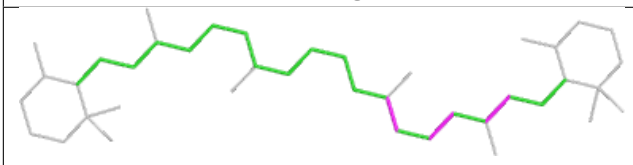

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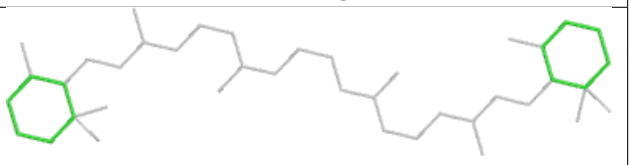
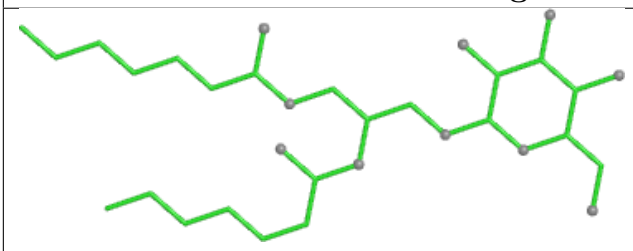


Rings

Ligand LMG 4D 410



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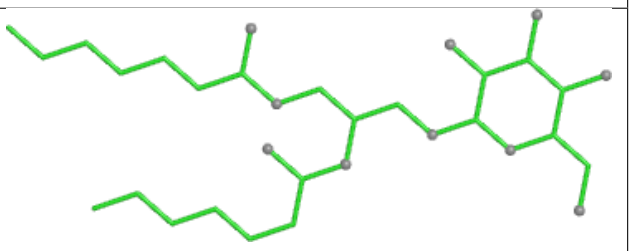
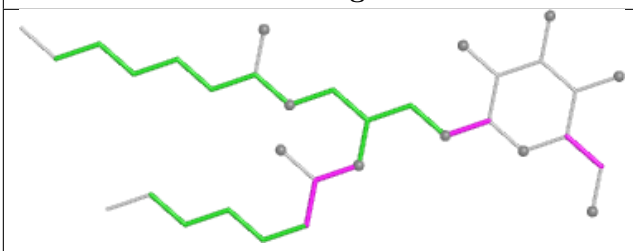


Bond angles



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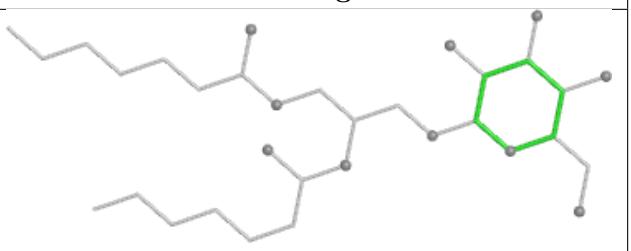
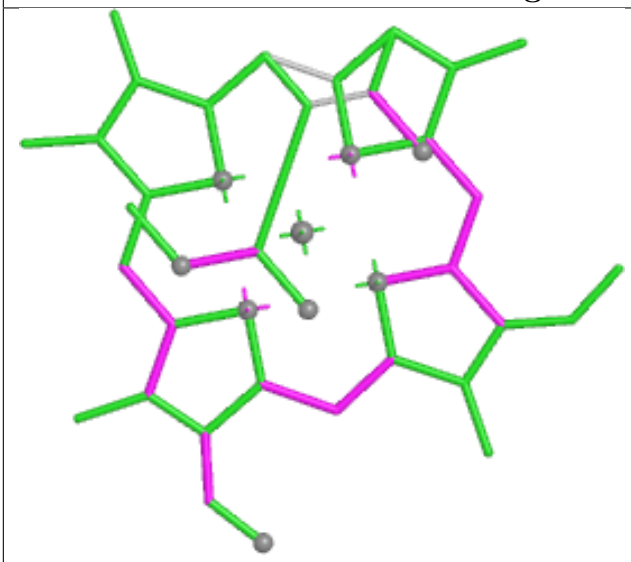


Rings

Ligand CL7 21 416



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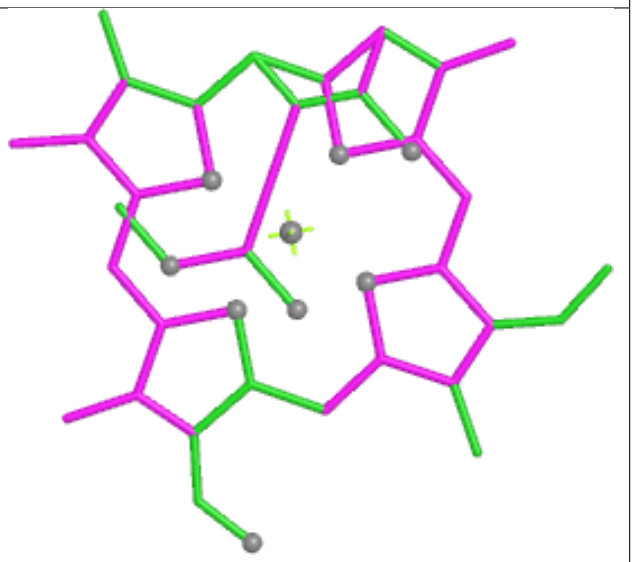

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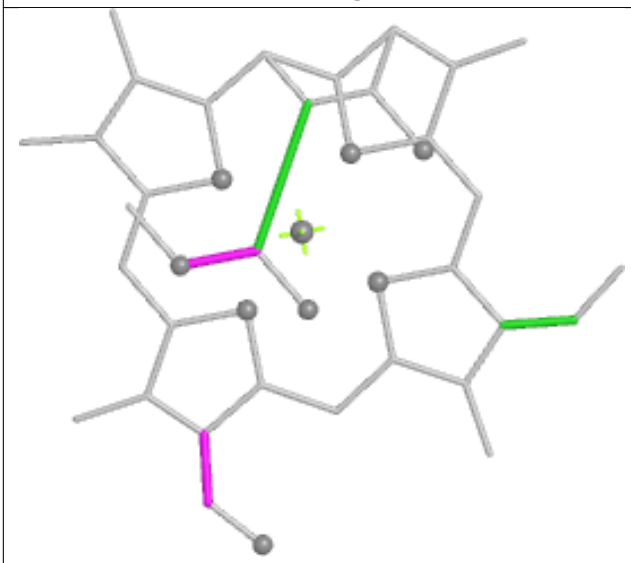

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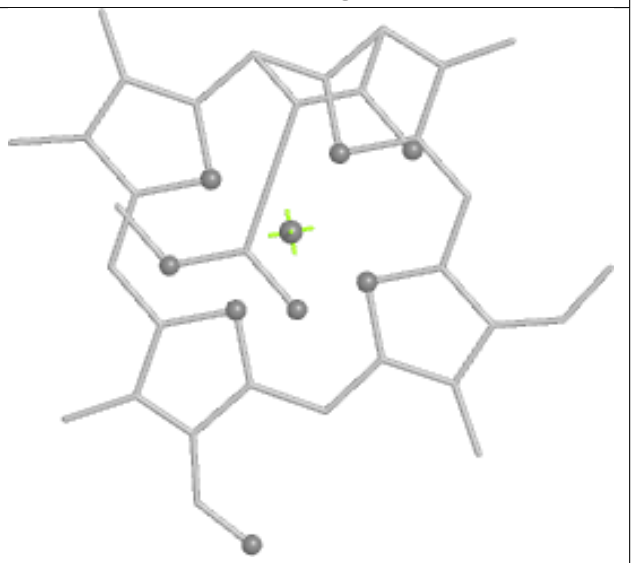
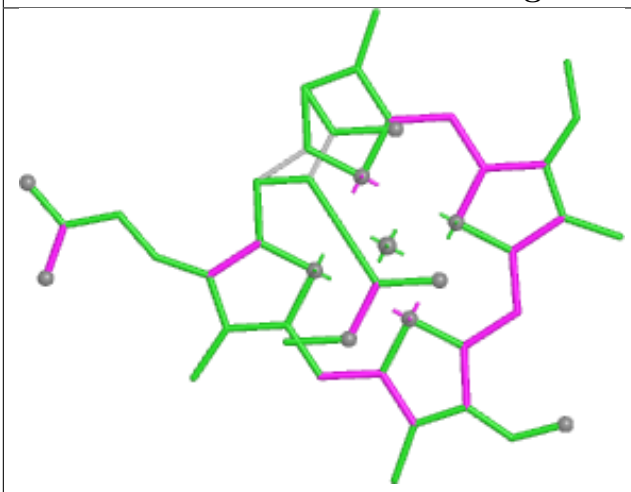


Rings

Ligand CL7 12 513



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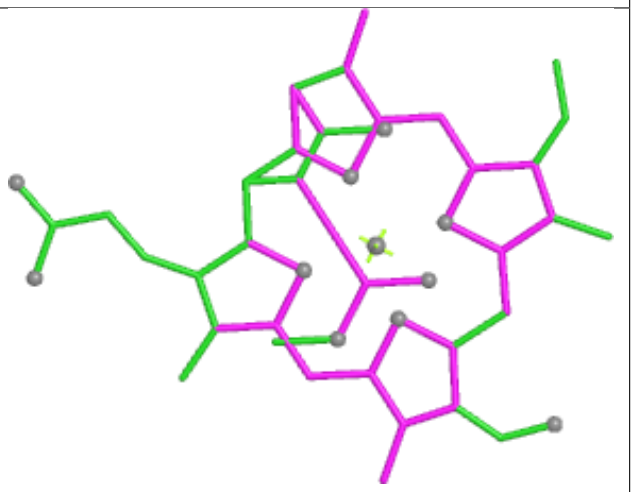
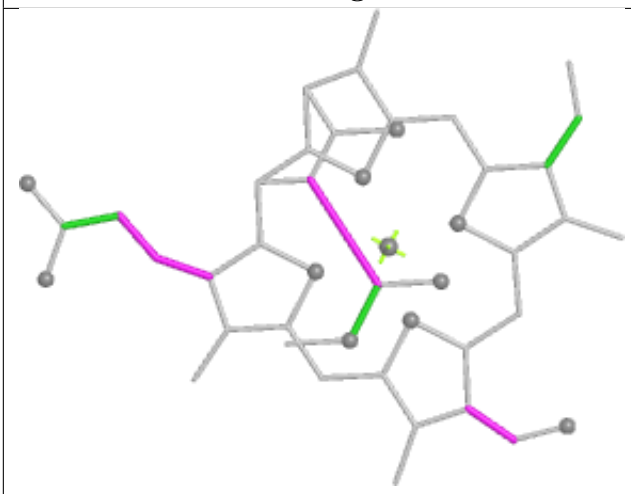


Bond angles

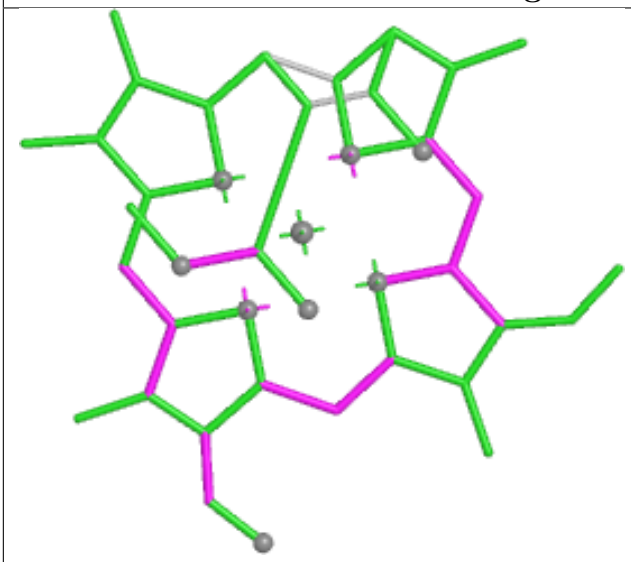


Torsions



Rings

Ligand CL7 13 515



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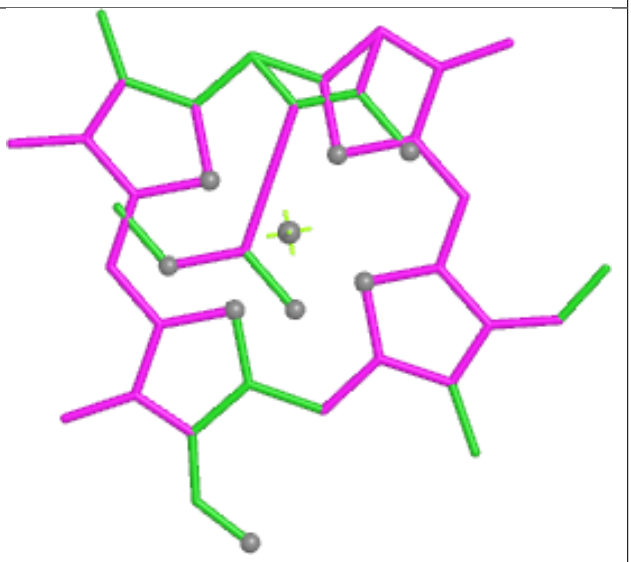
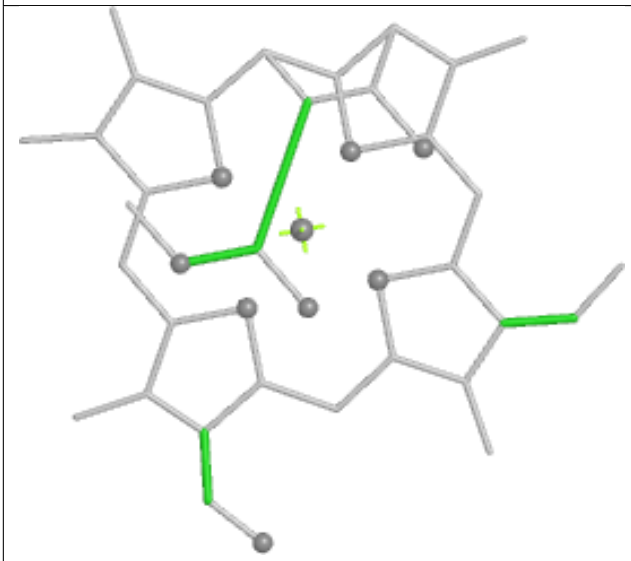


Bond angles



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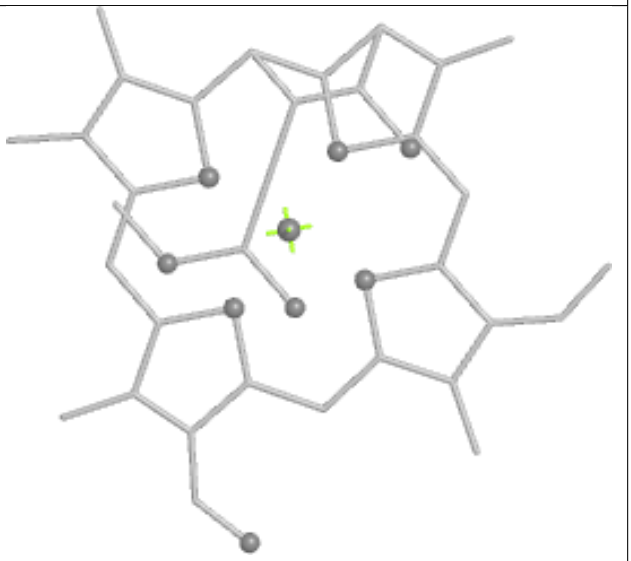
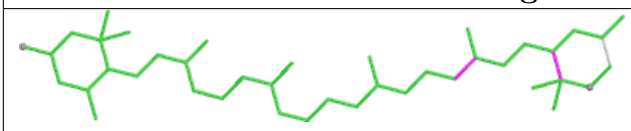


Rings

Ligand ZEX 31 422



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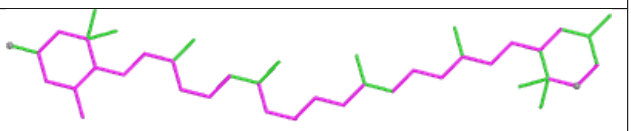
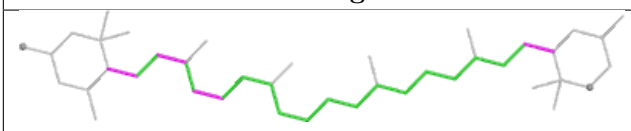


Bond angles



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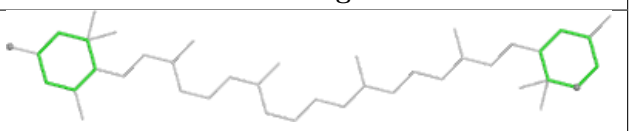
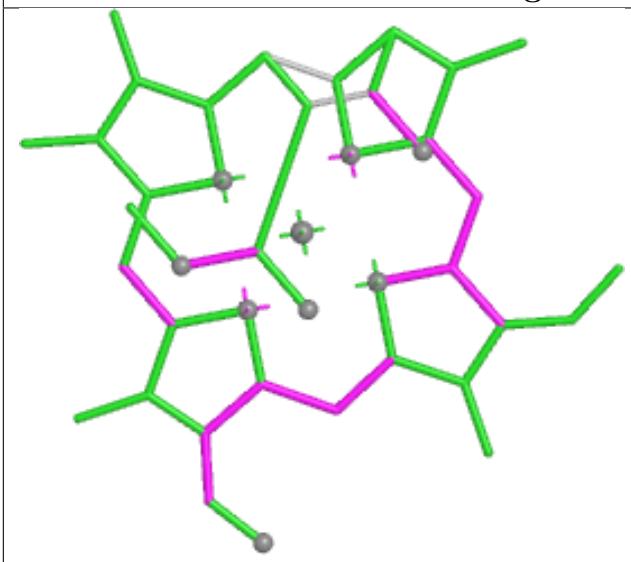


Rings

Ligand CL7 11 413



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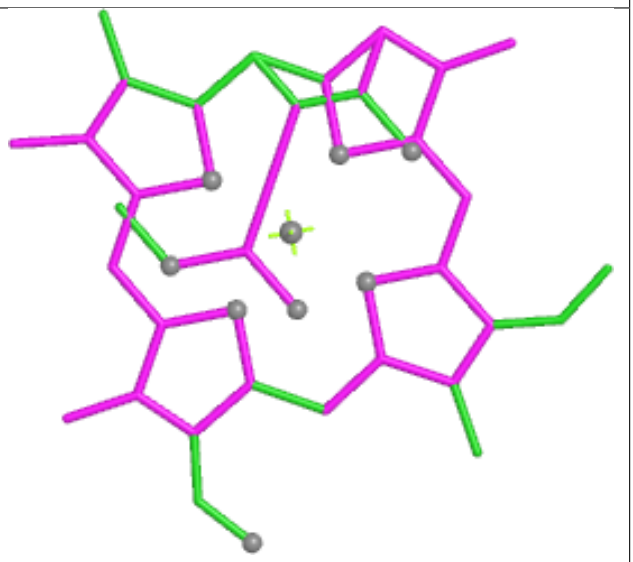
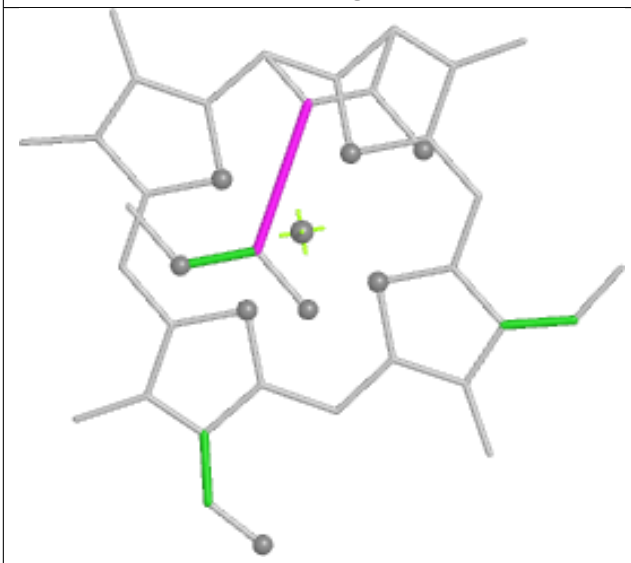


Bond angles



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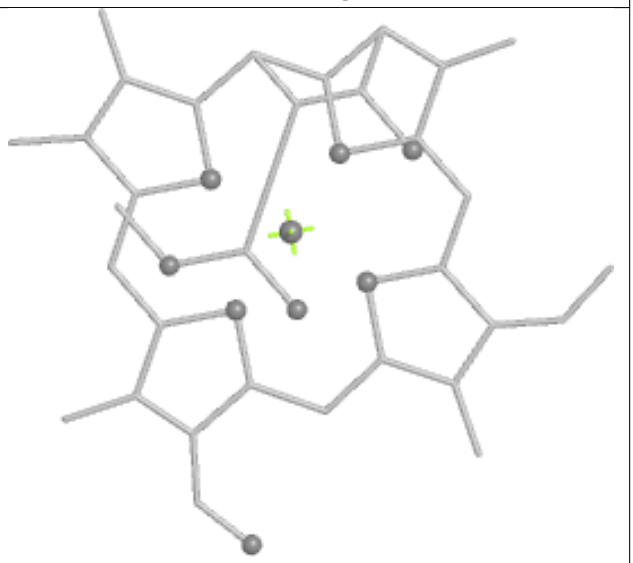
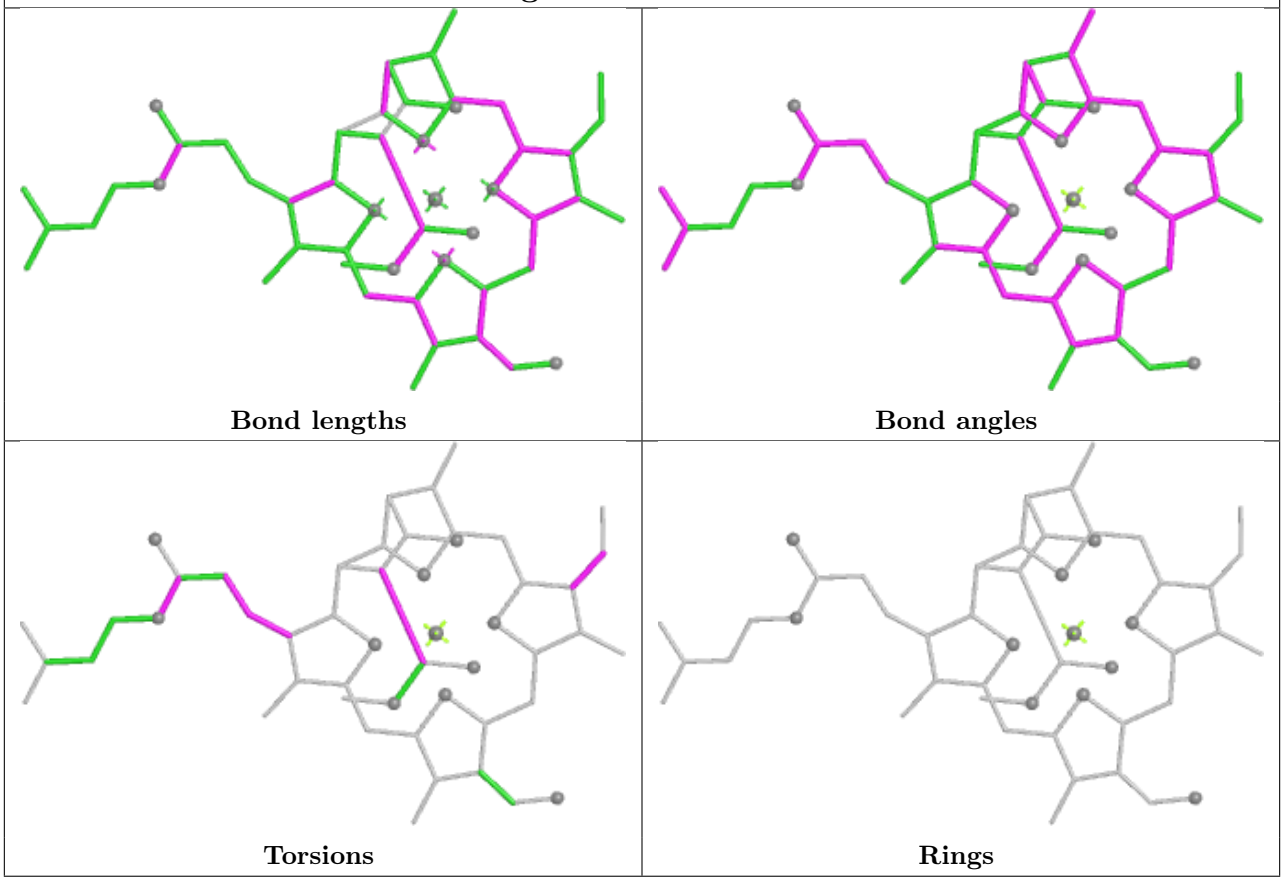
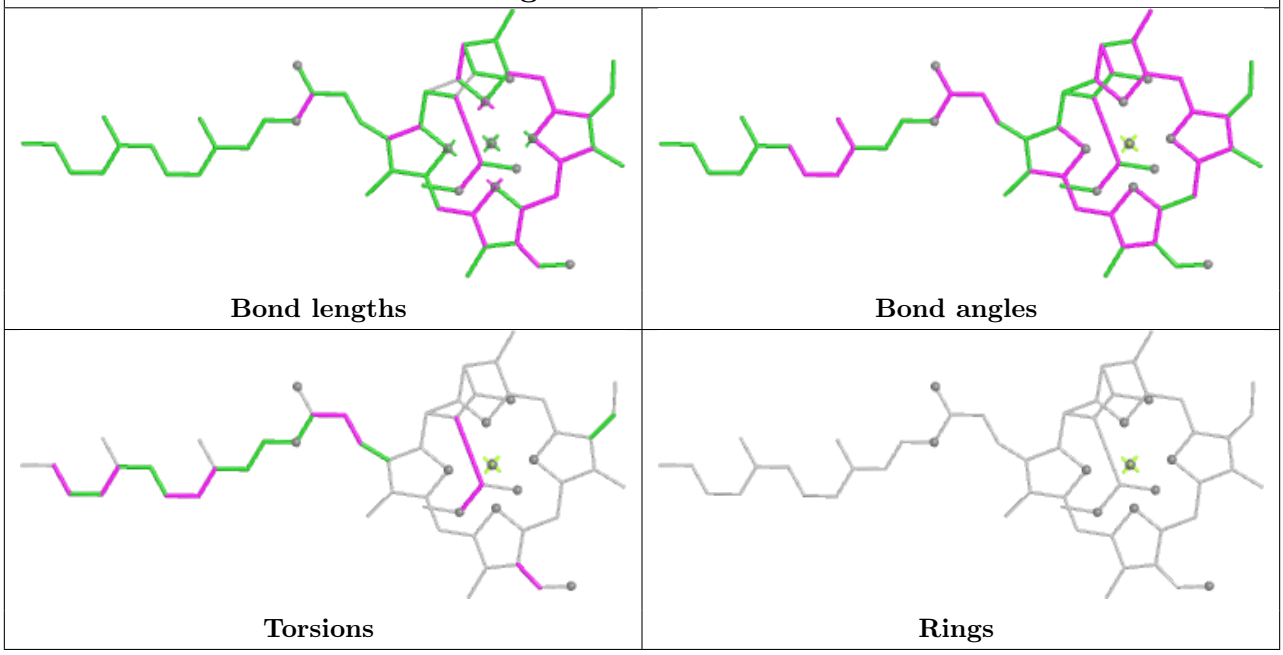


Rings

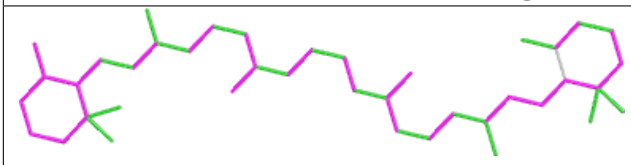
Ligand CL7 3B 615



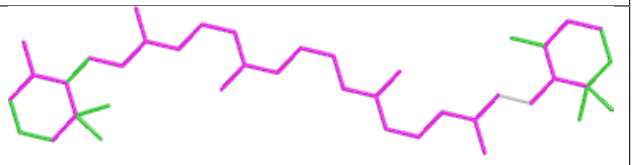
Ligand CL7 1D 404



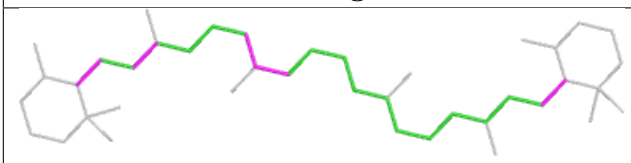
Ligand 8CT 3B 626



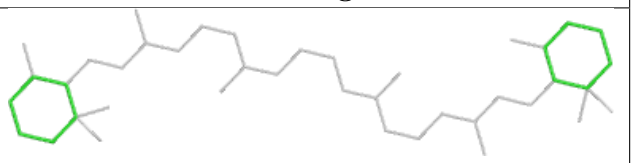
Bond lengths



Bond angles

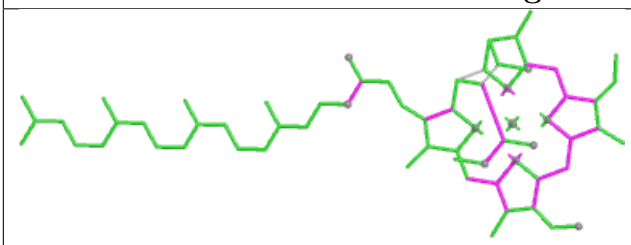


Torsions



Rings

Ligand CL7 23 412



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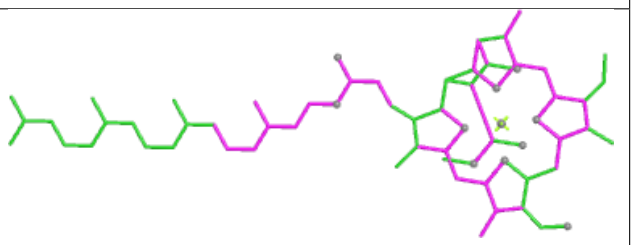

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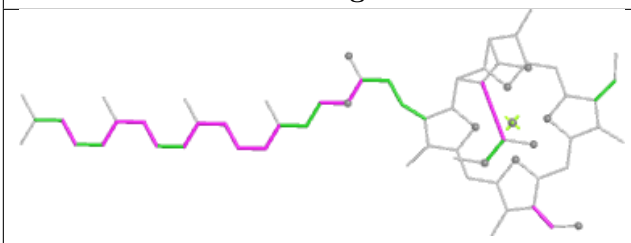

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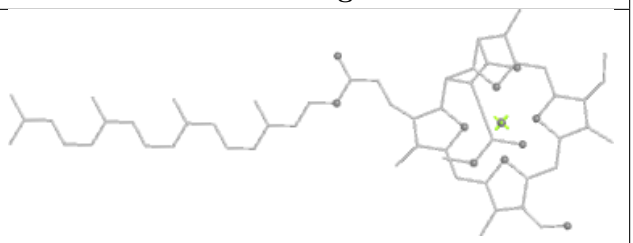
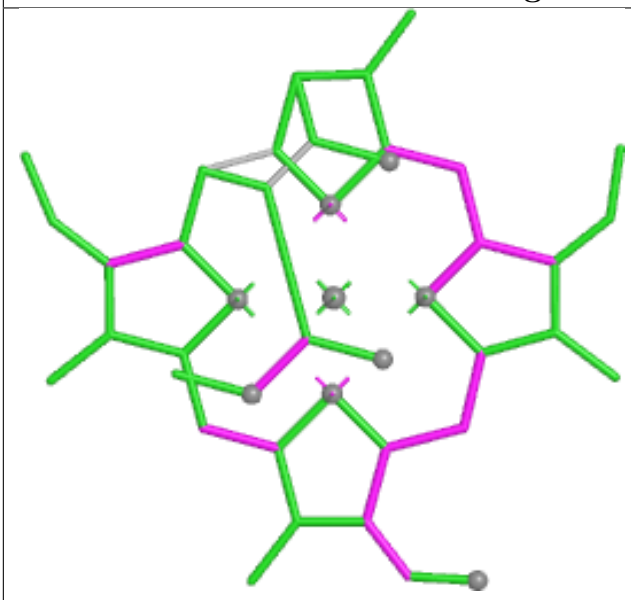


Rings

Ligand CL7 34 417



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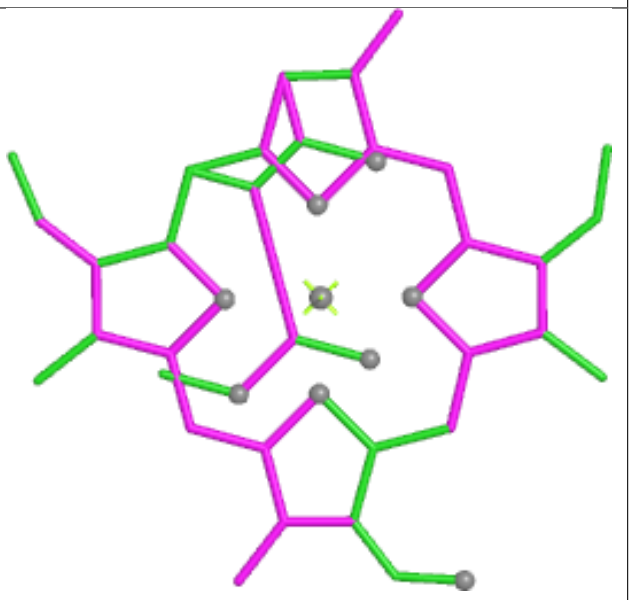

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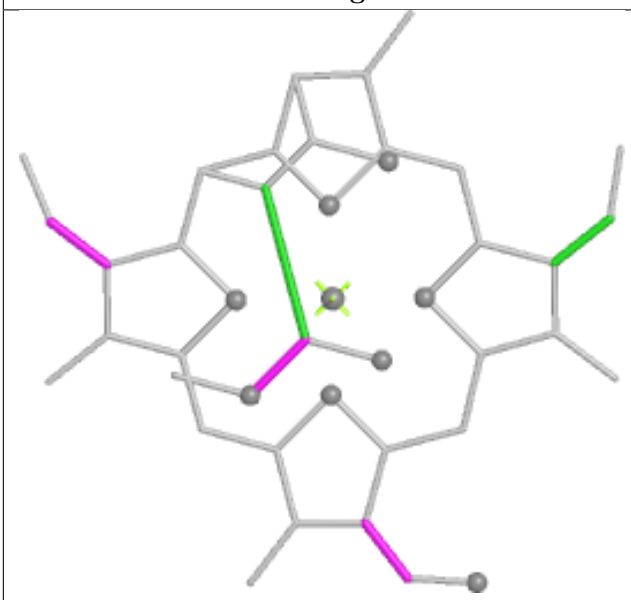

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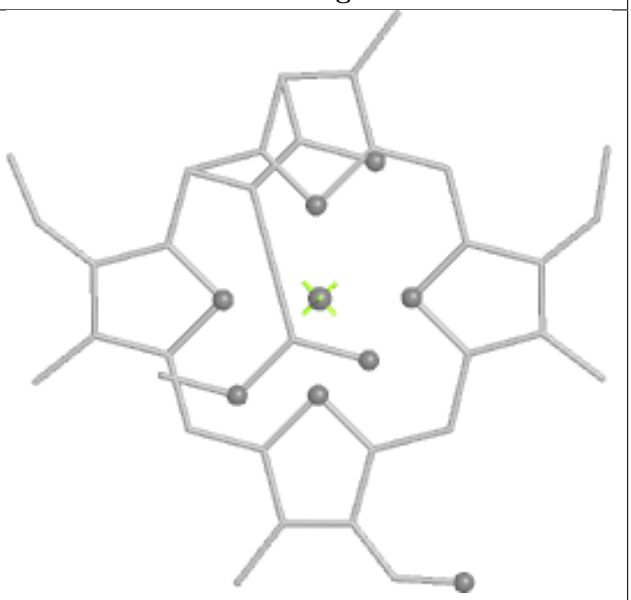

Rings

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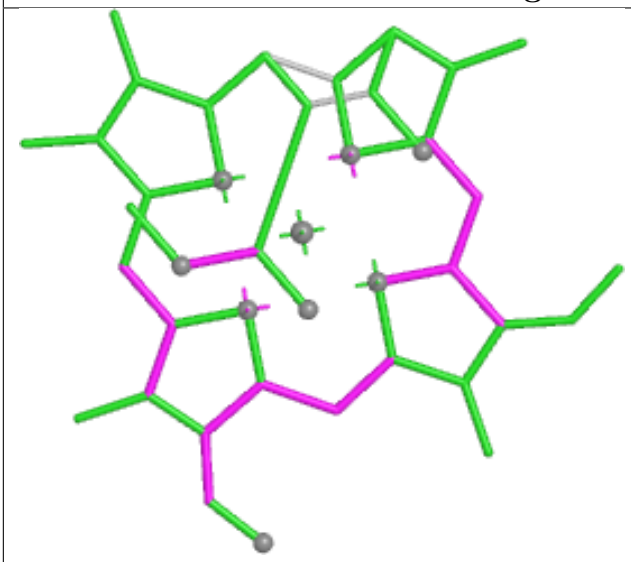

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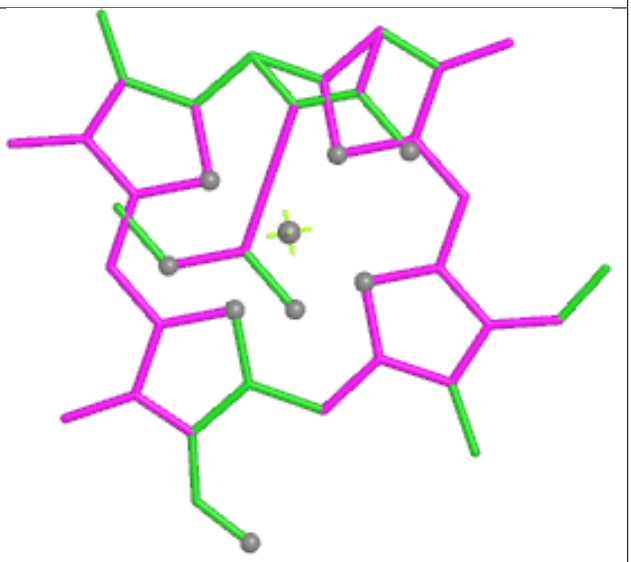

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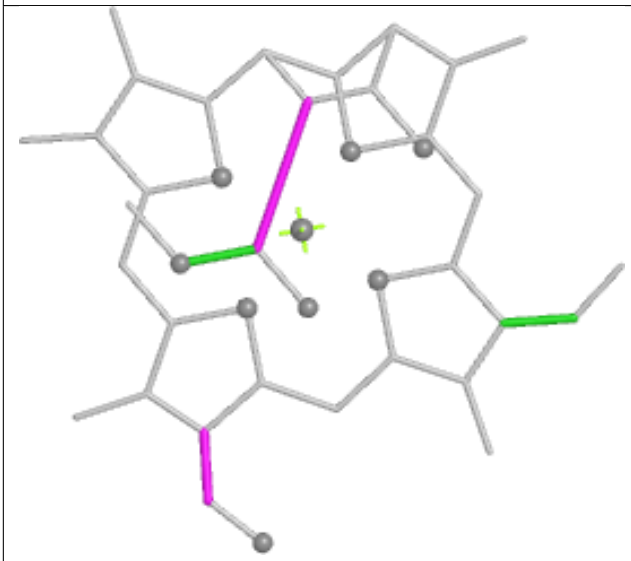

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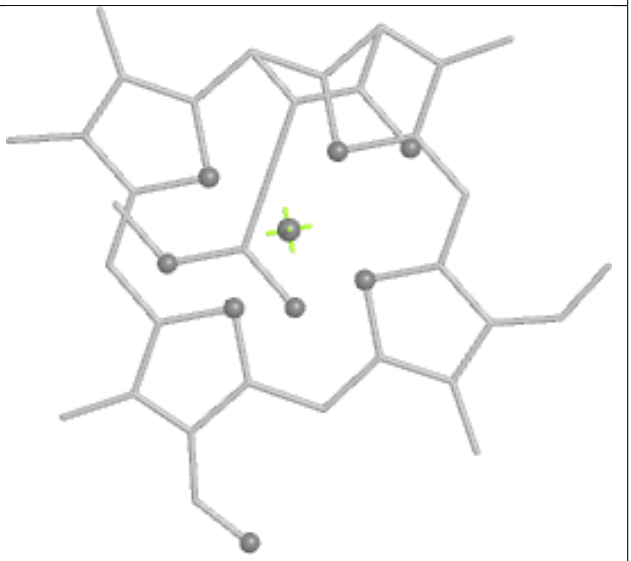

Rings

Ligand CL7 42 508



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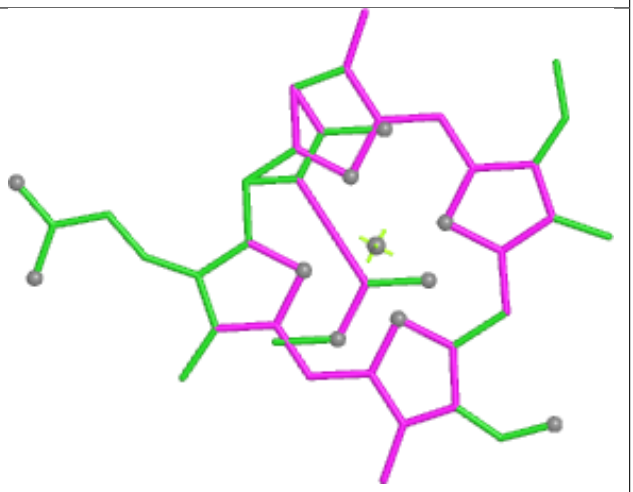

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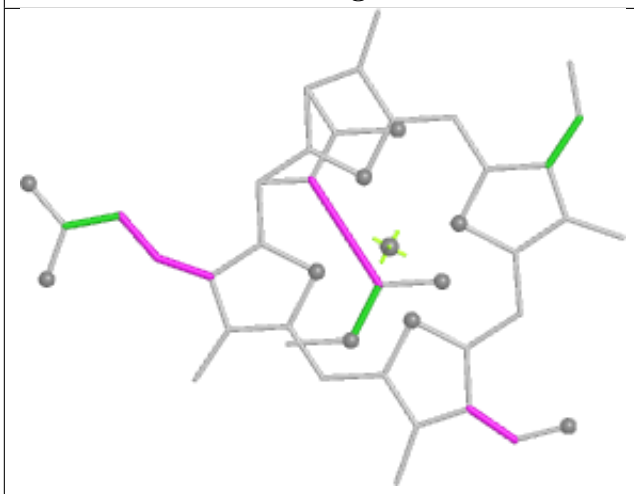

Torsions



Rings

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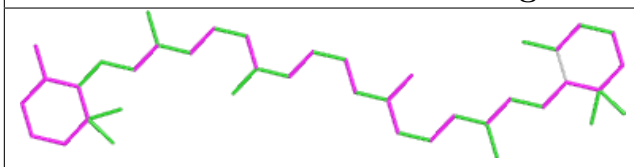

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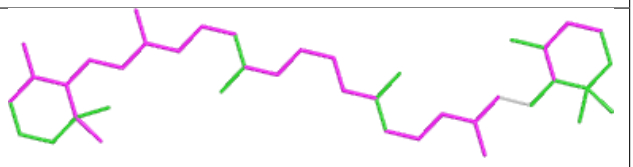

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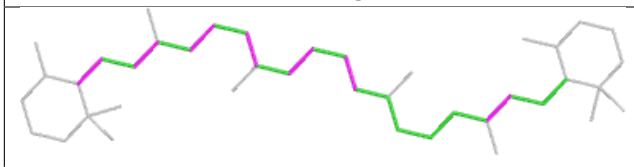

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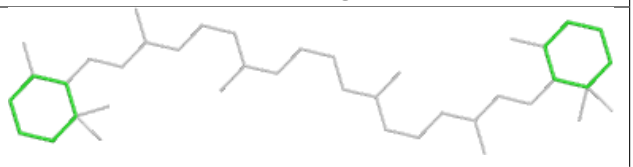

Rings

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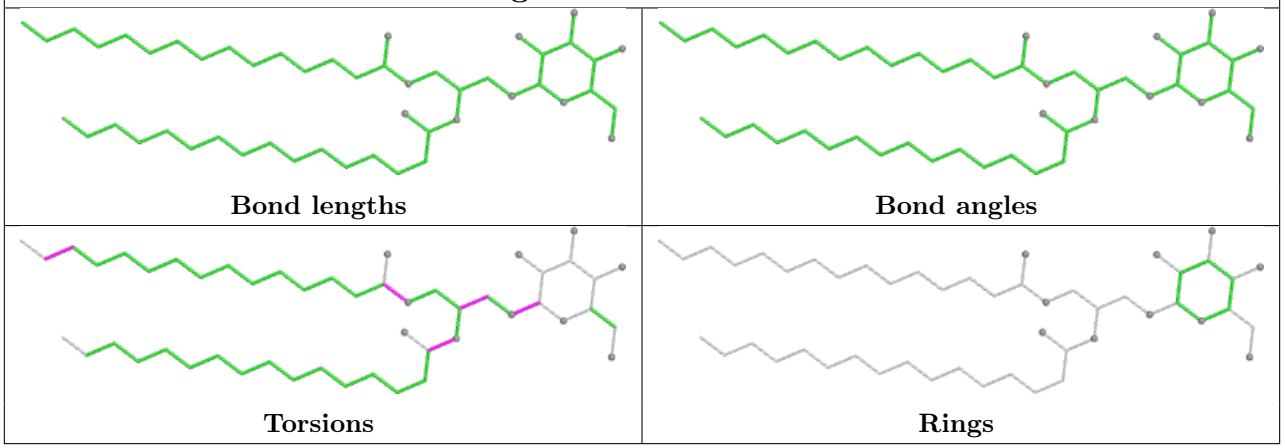

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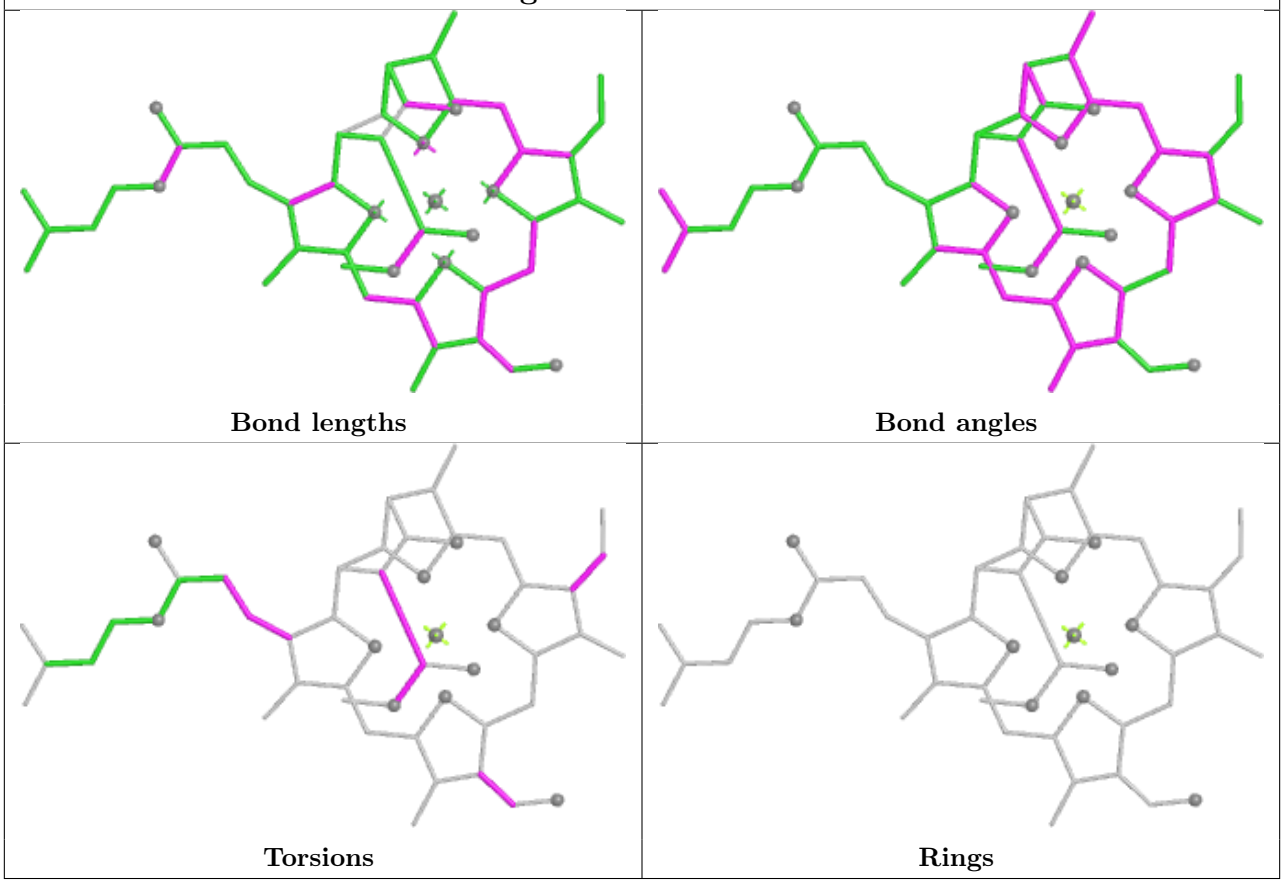

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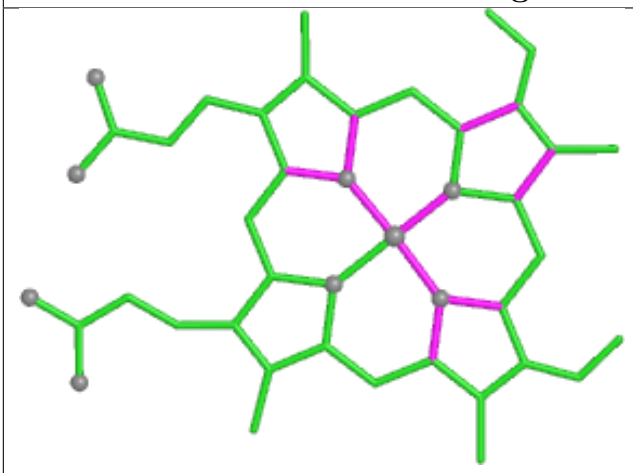

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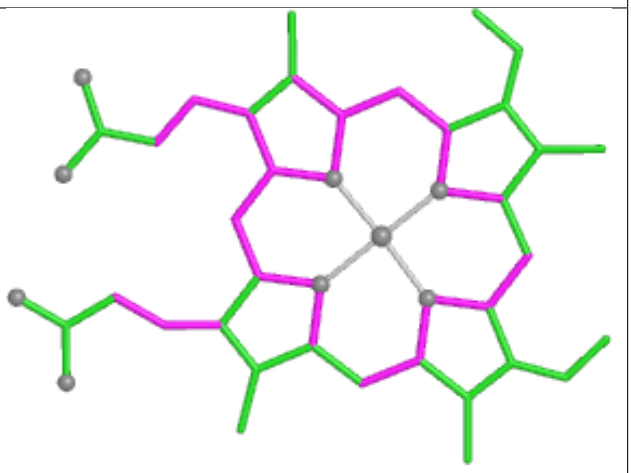

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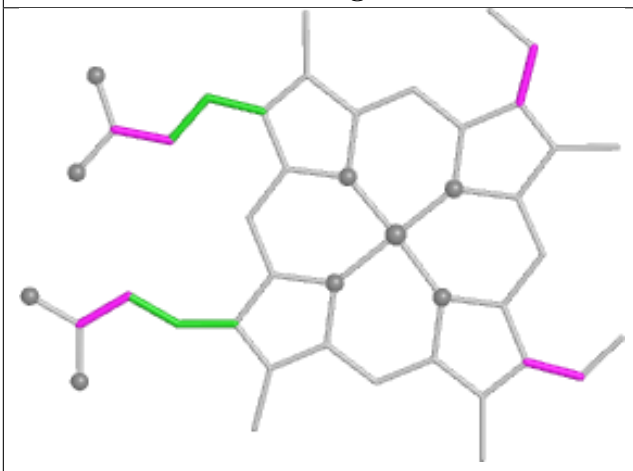

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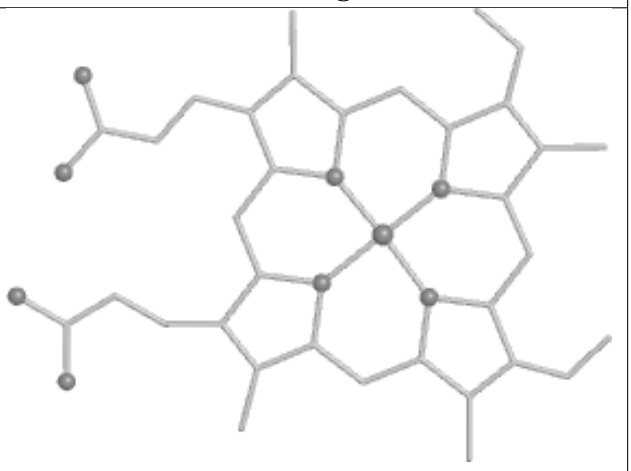
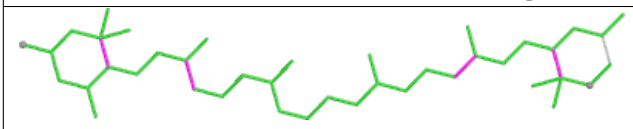


Rings

Ligand ZEX 43 423



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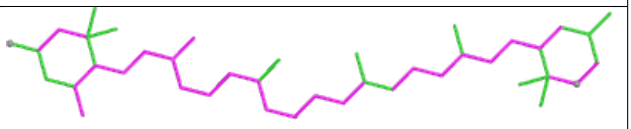

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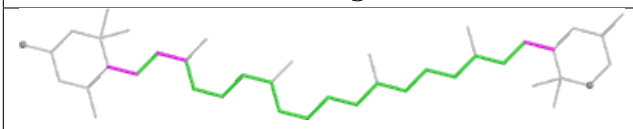

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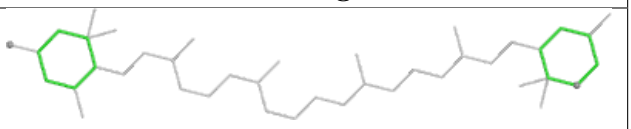

Rings

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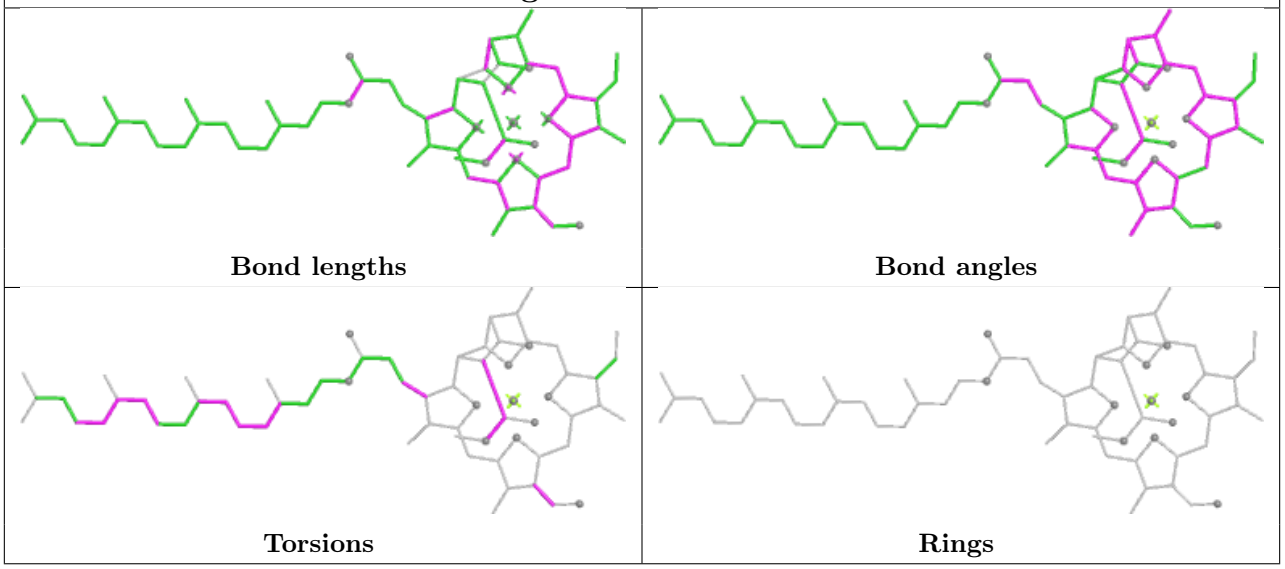

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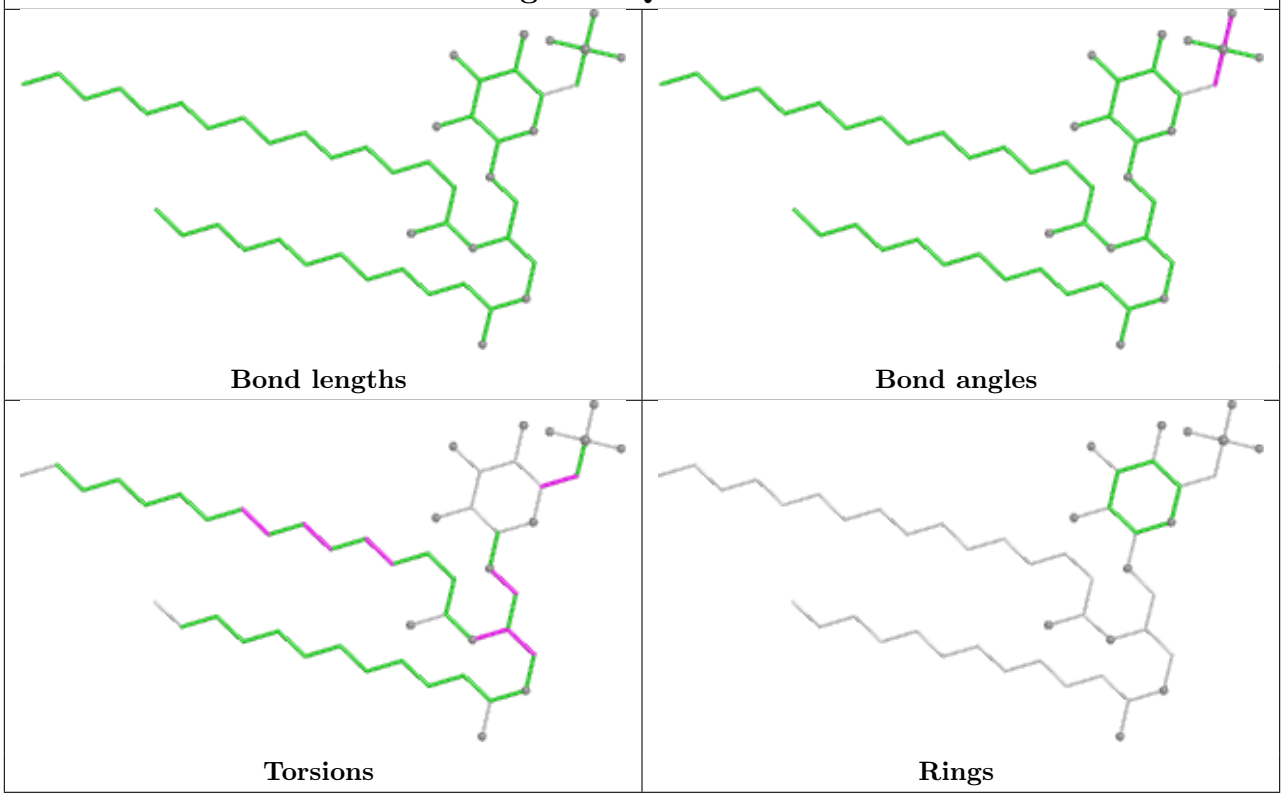

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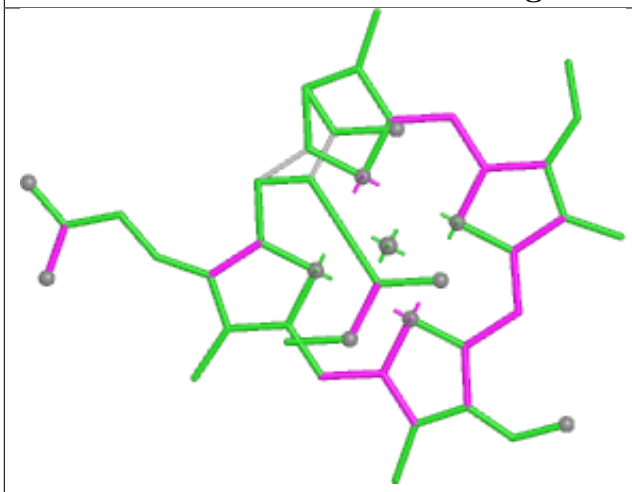

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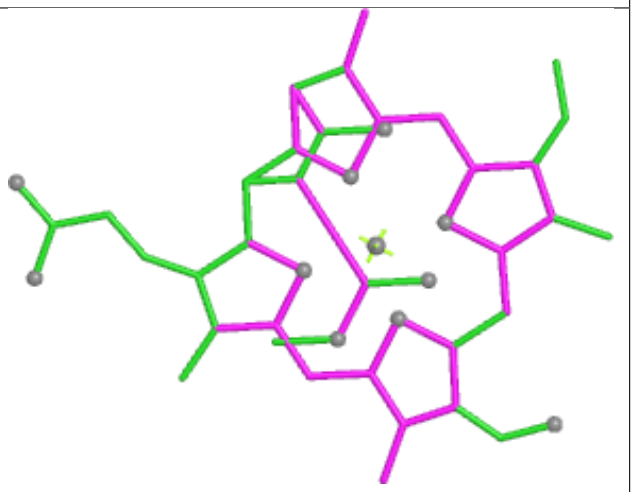

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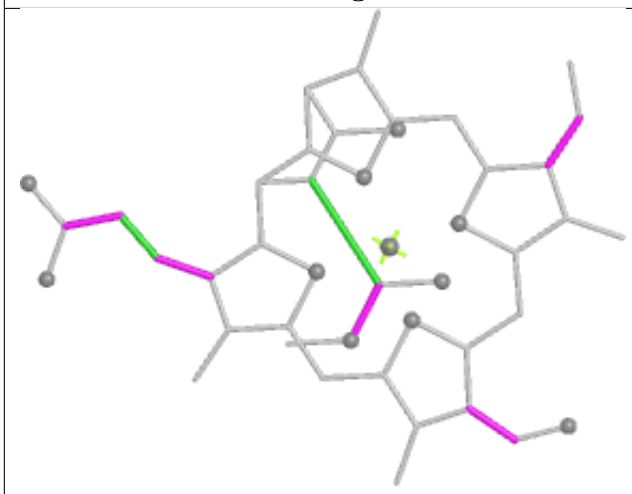

Torsions



Rings

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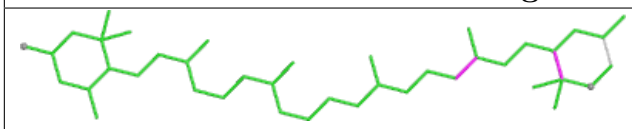

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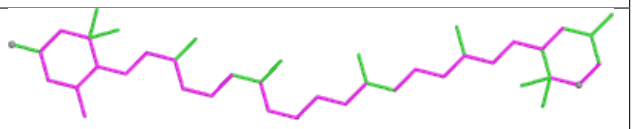

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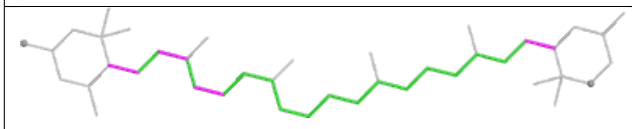

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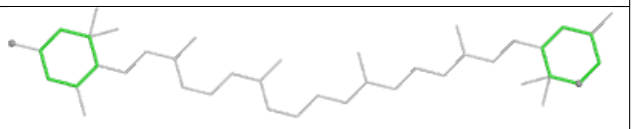

Rings

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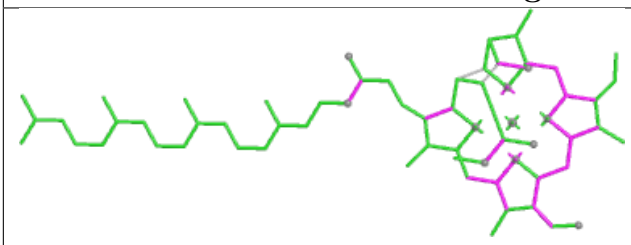

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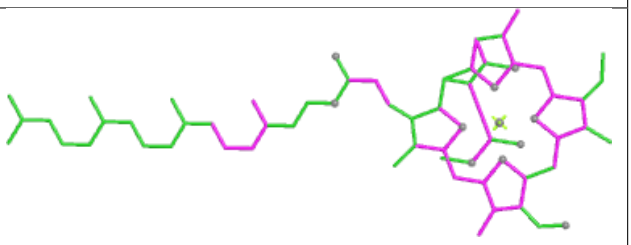
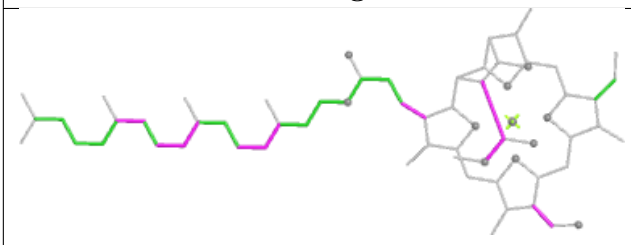


Bond angles



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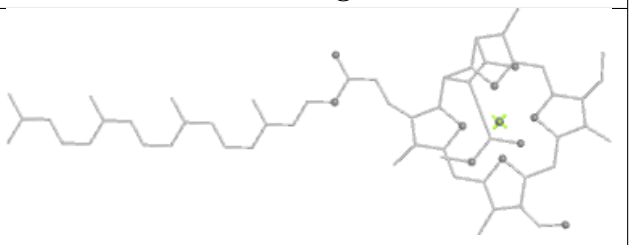
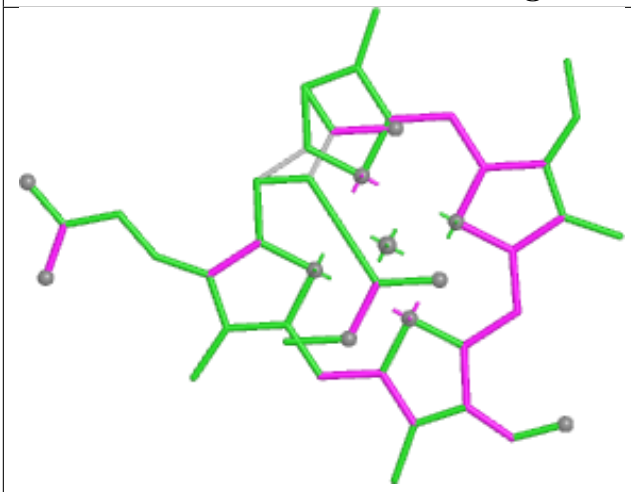


Rings

Ligand CL7 21 405



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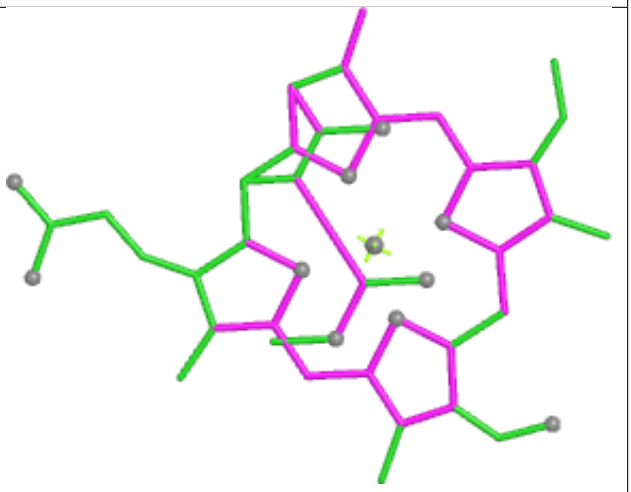


Bond angles

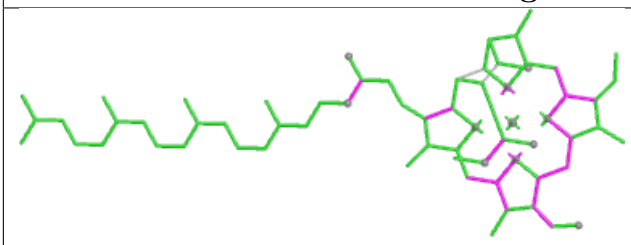


Torsions



Rings

Ligand CL7 2B 611



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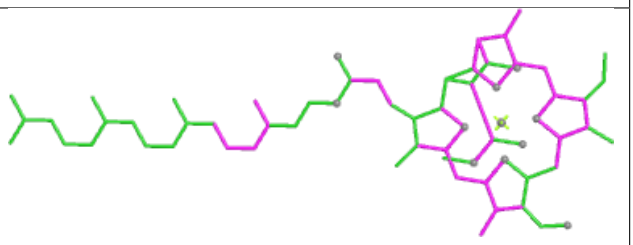
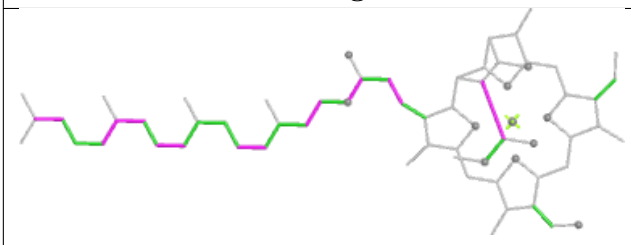


Bond angles



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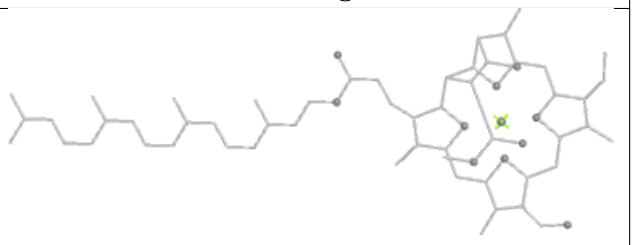
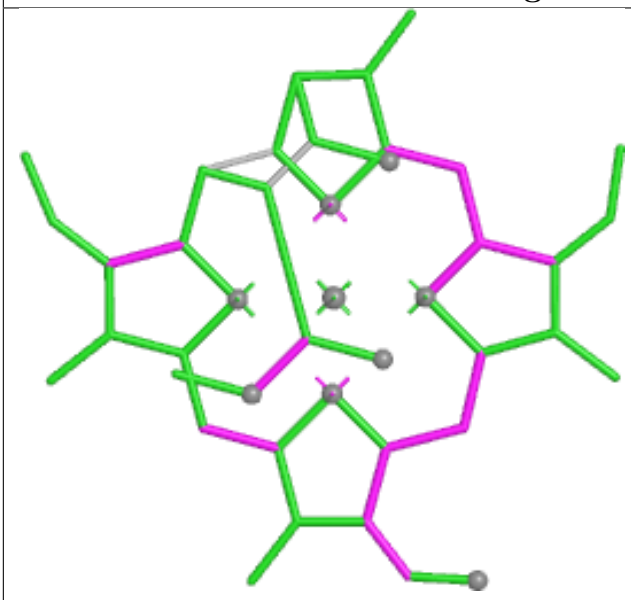


Rings

Ligand CL7 14 417



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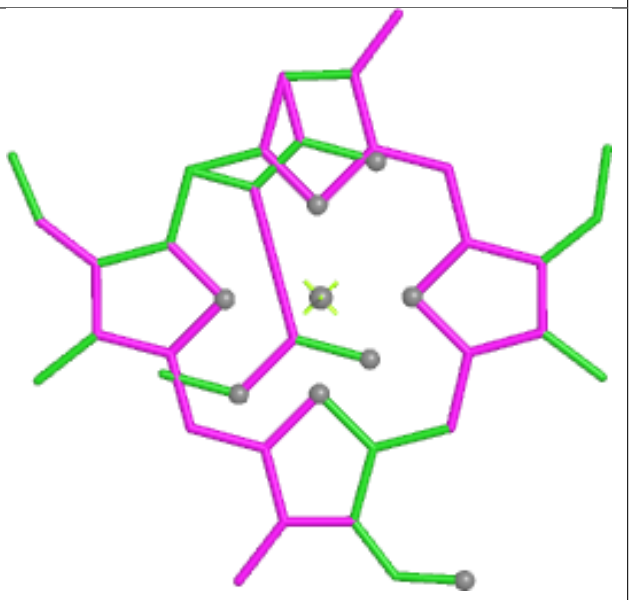
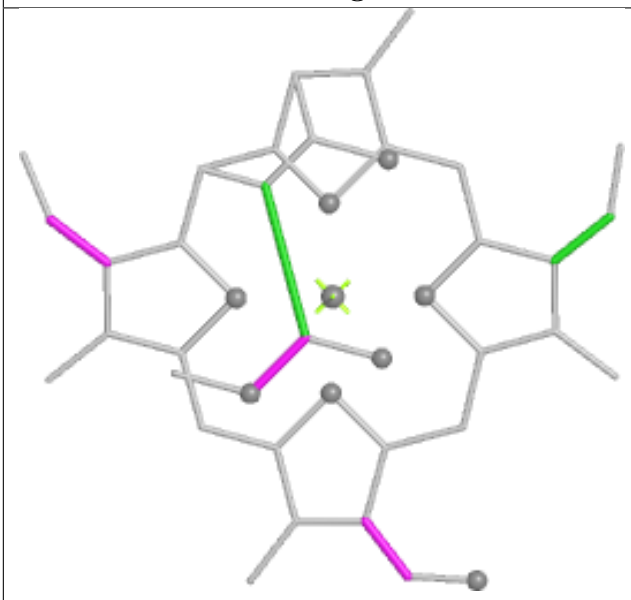


Bond angles



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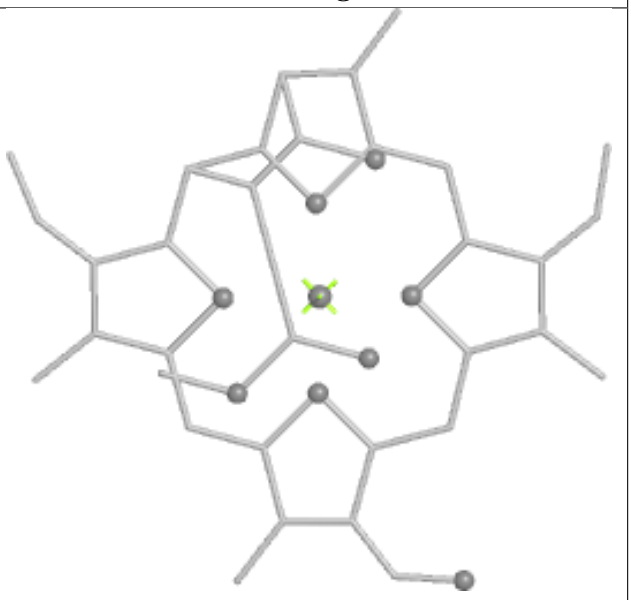
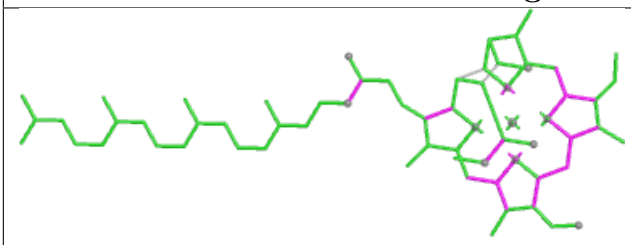


Rings

Ligand CL7 33 505



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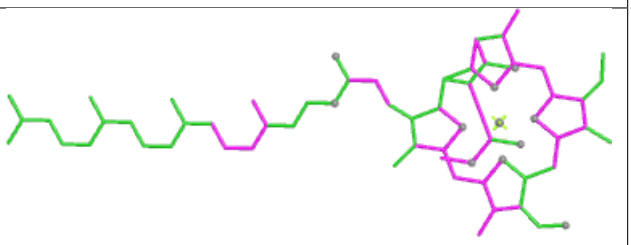
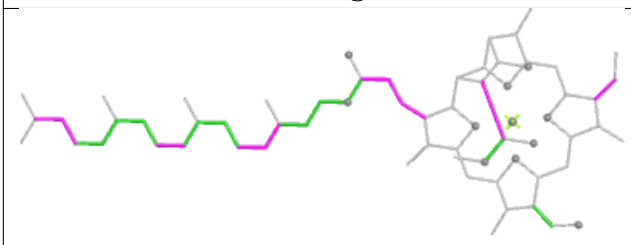


Bond angles



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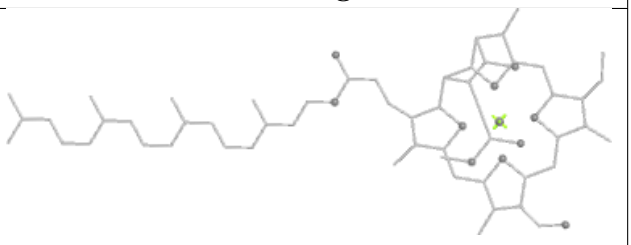

Rings

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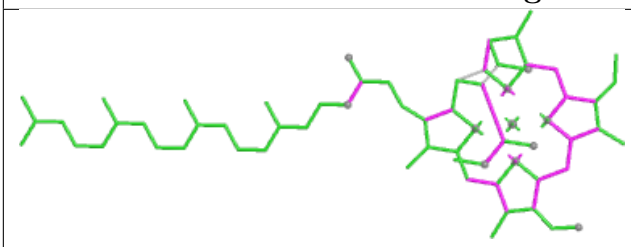
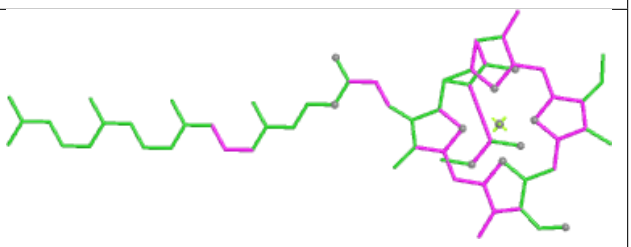
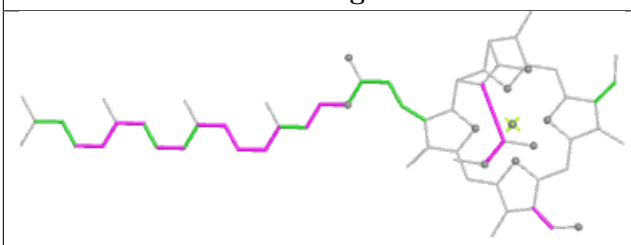


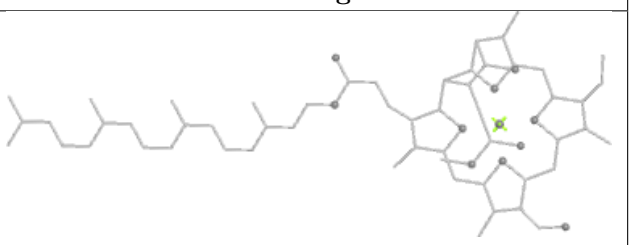
Bond lengths



Bond angles

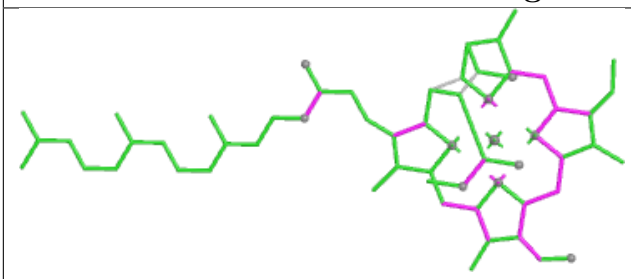


Torsions



Rings

Ligand CL7 31 403



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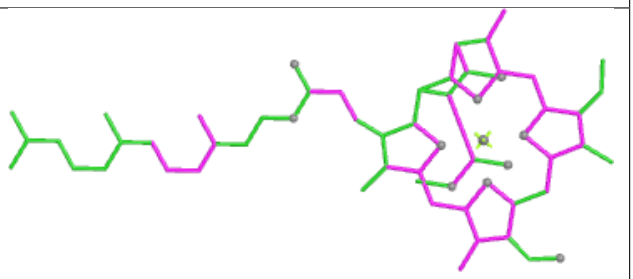
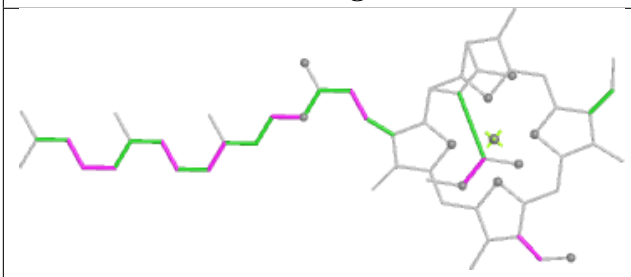


Bond angles



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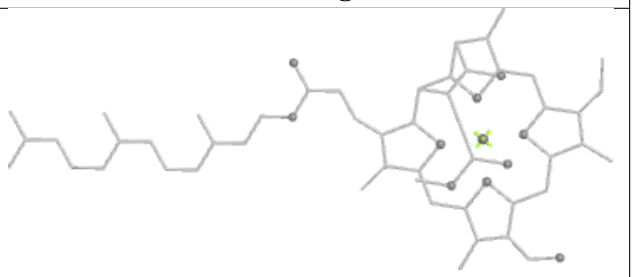
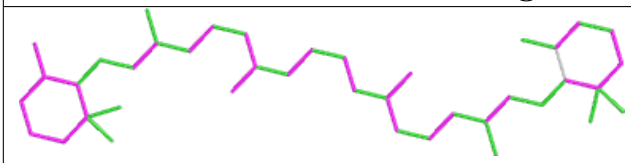
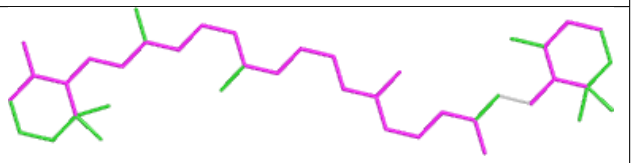


Rings

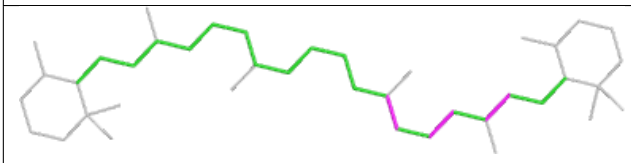
Ligand 8CT 4A 404



Bond lengths



Bond angles



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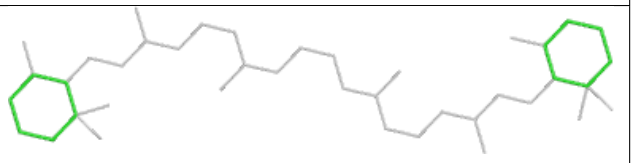
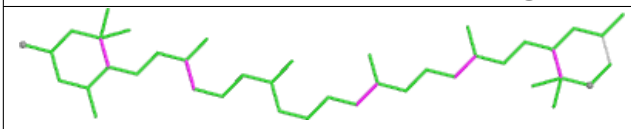


Rings

Ligand ZEX 42 522



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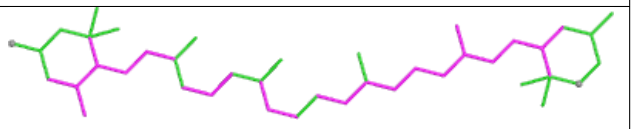

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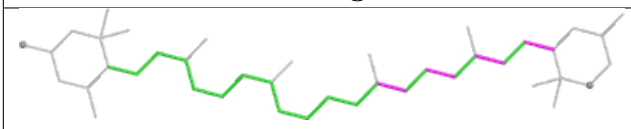

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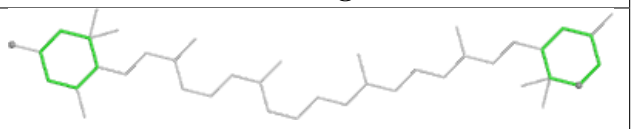
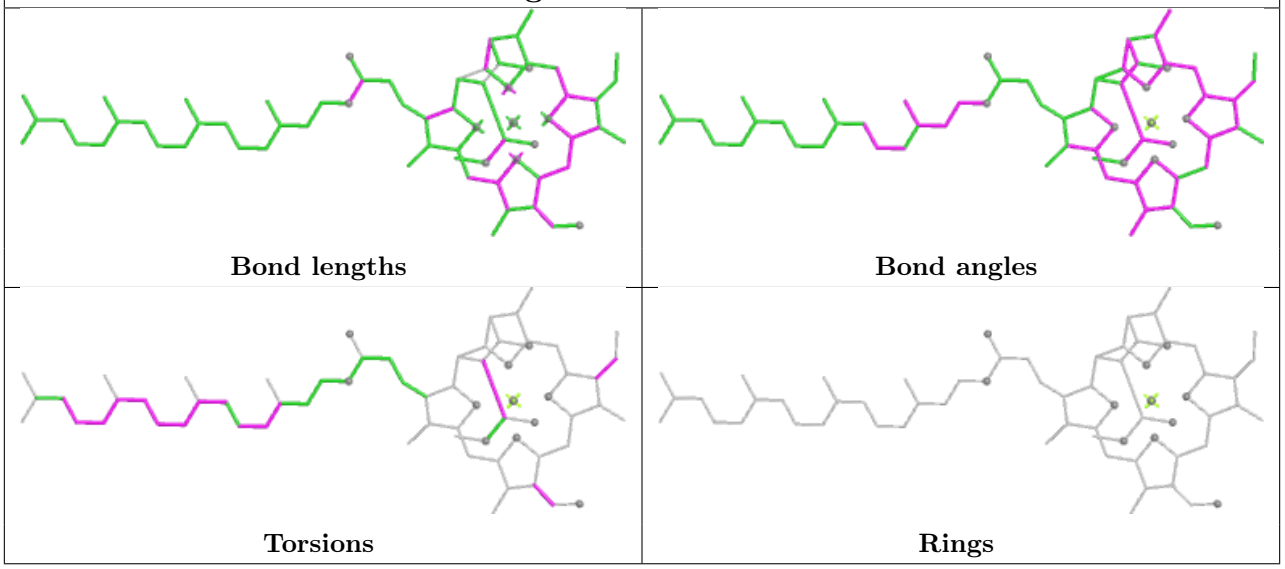


Rings

Ligand CL7 12 505



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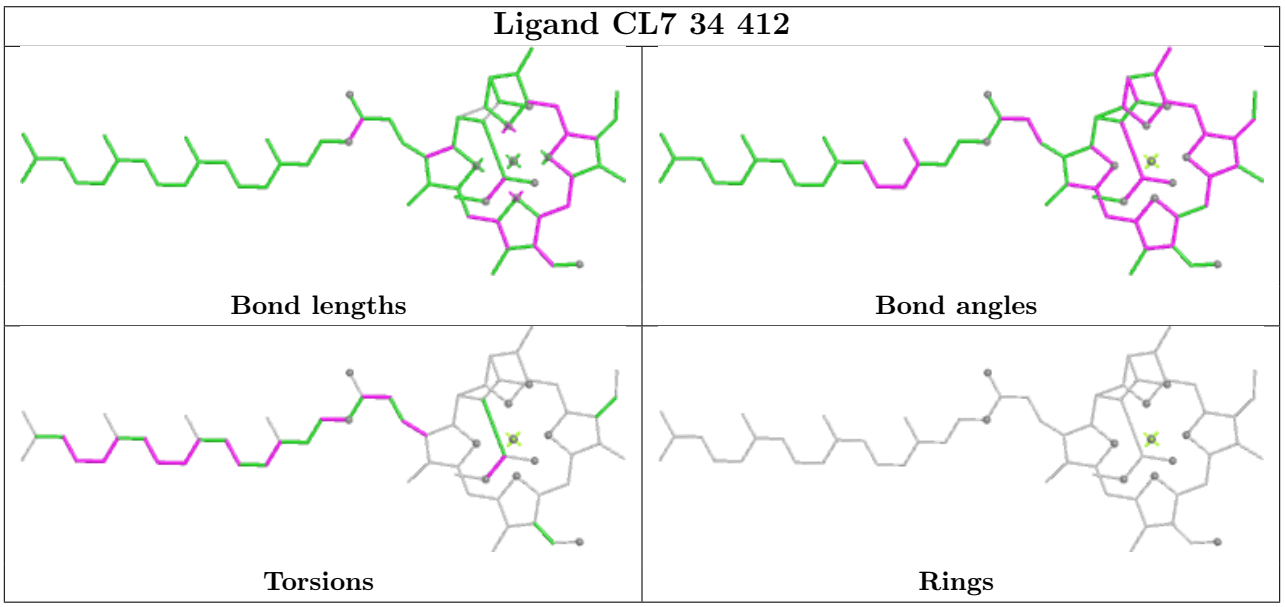

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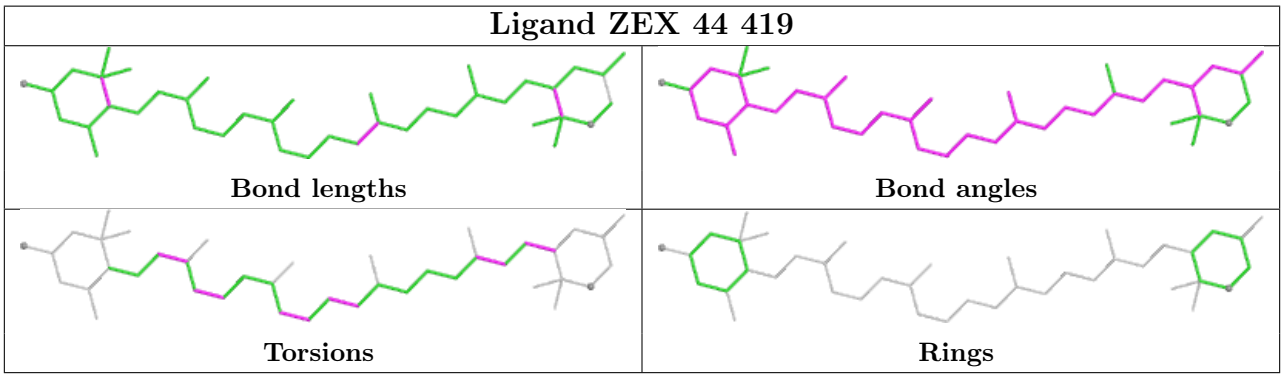
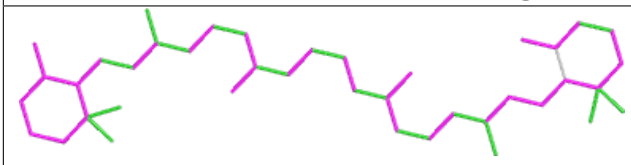
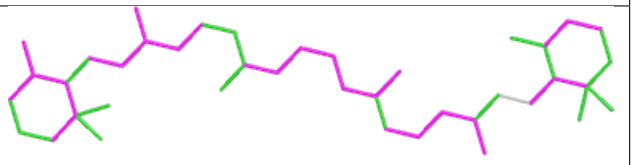
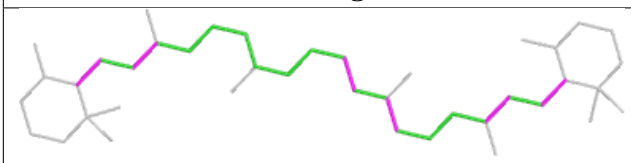
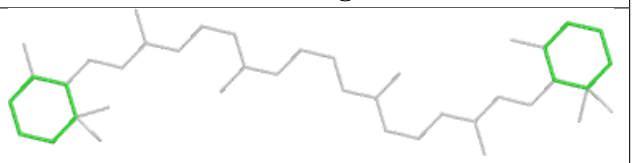


Ligand 8CT 4K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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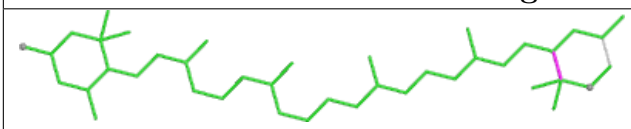
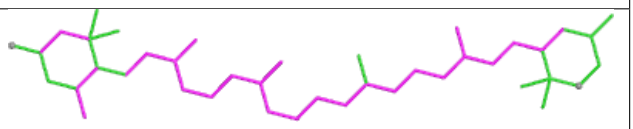
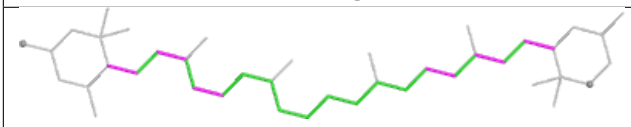
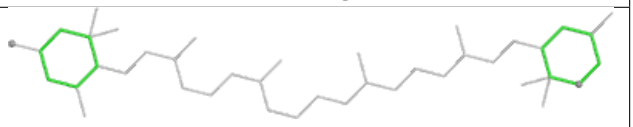
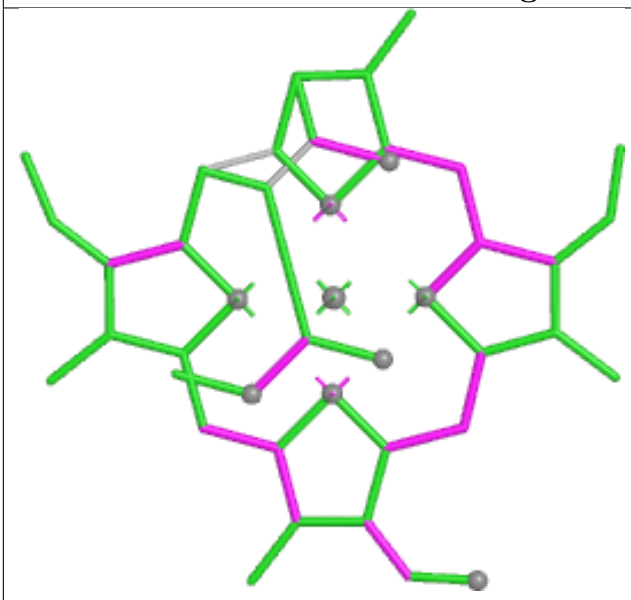
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CL7 1C 511



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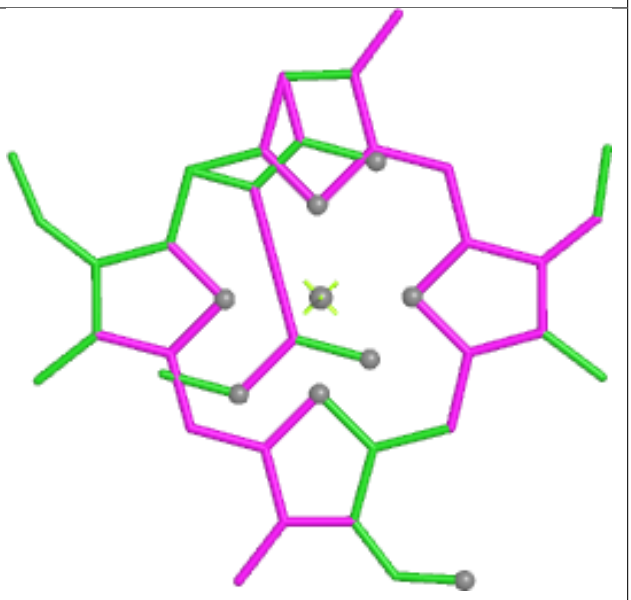
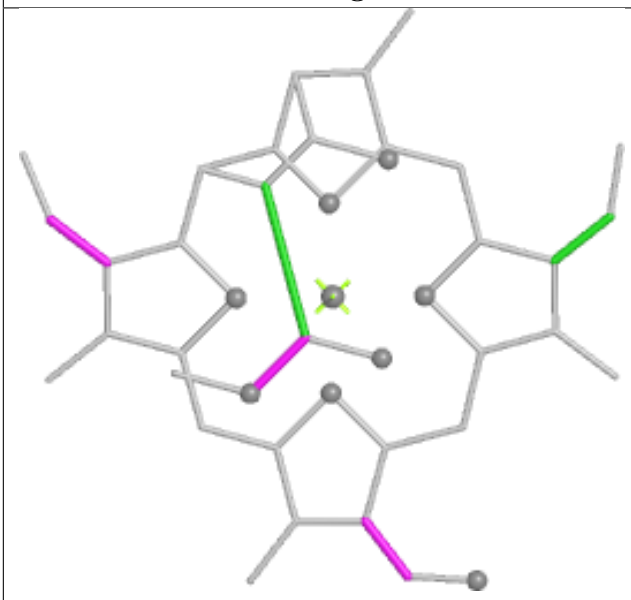


Bond angles



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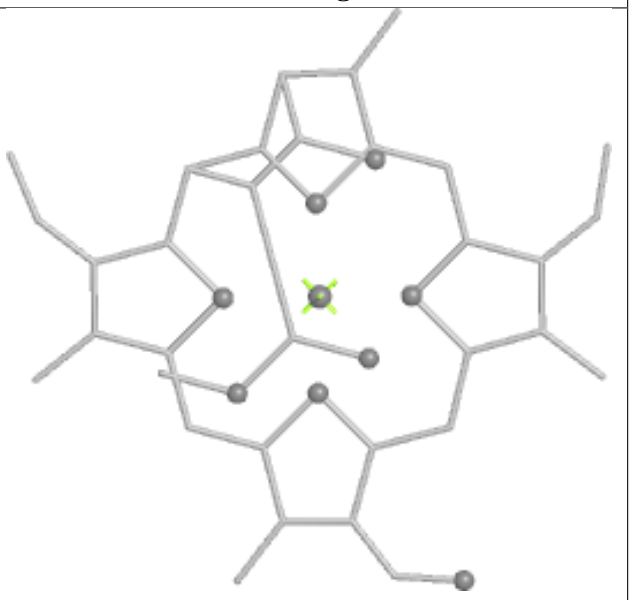
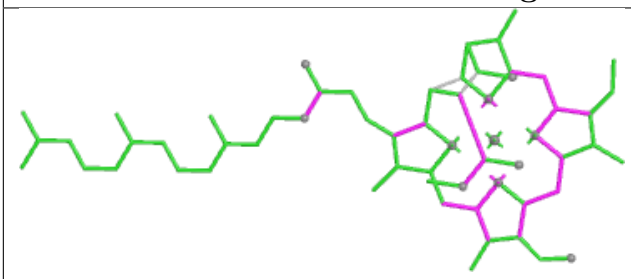


Rings

Ligand CL7 1C 506



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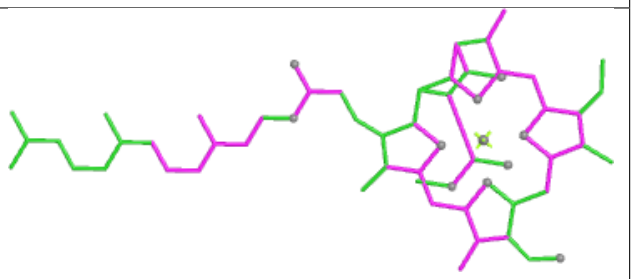
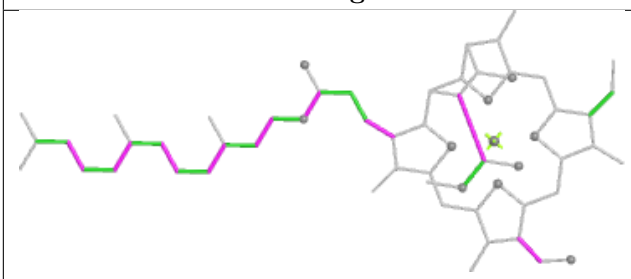


Bond angles



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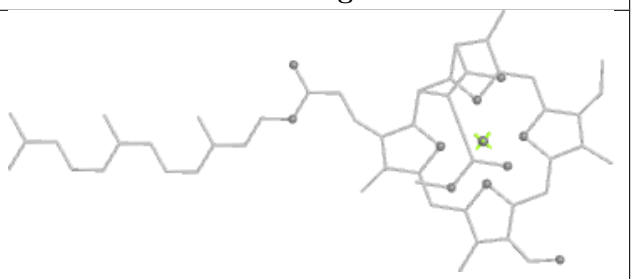
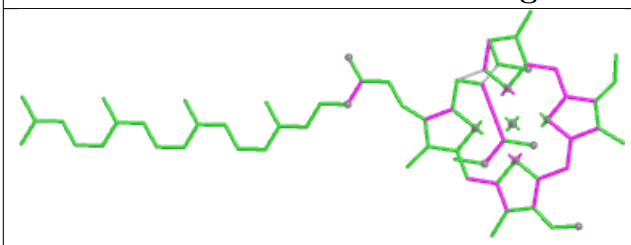


Rings

Ligand CL7 1B 609



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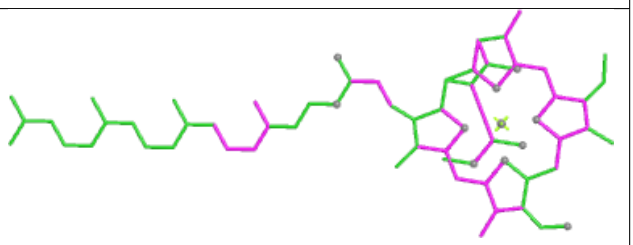
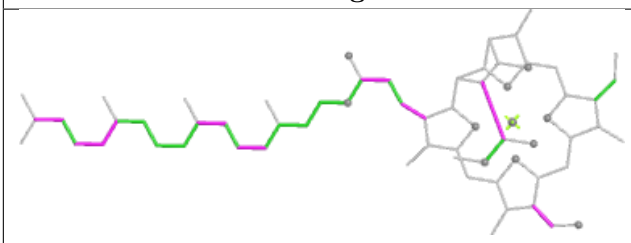


Bond angles



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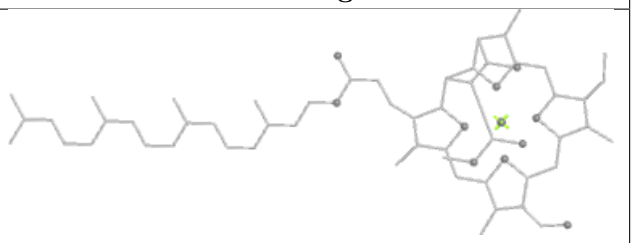
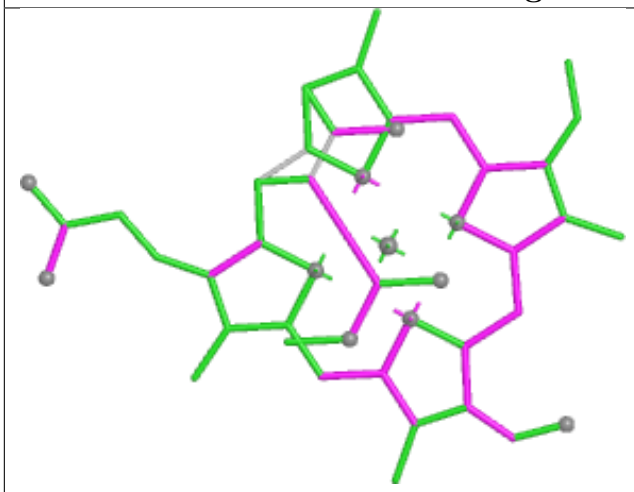


Rings

Ligand CL7 24 415



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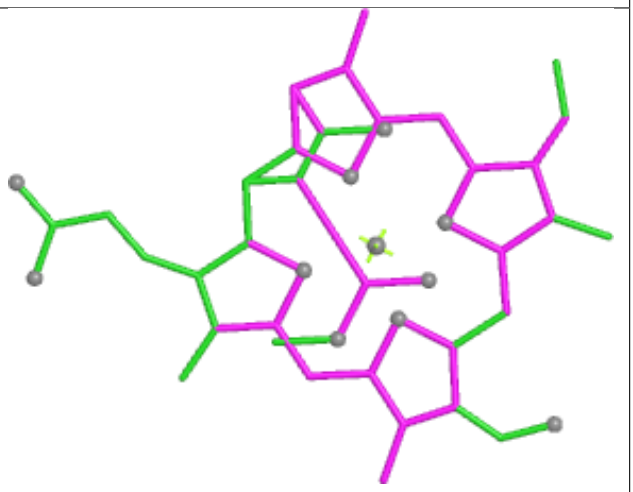
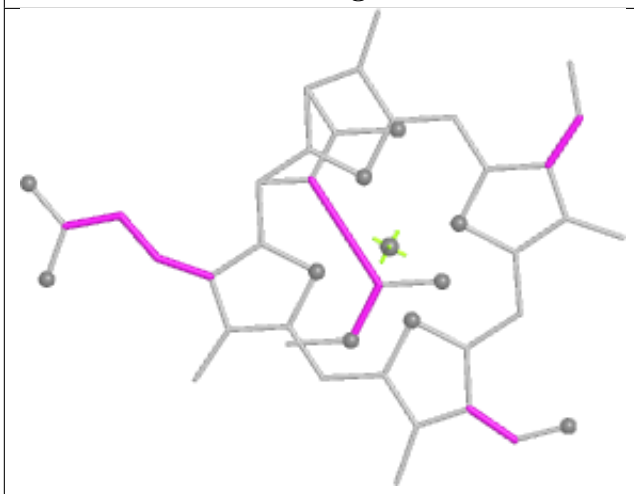


Bond angles

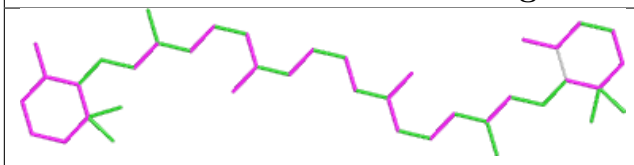


Torsions



Rings

Ligand 8CT 1B 619



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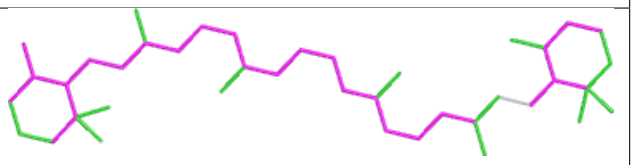

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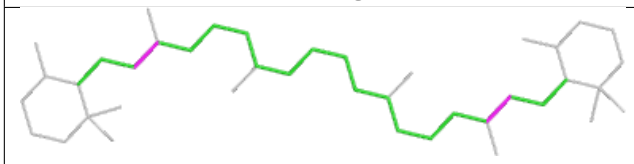

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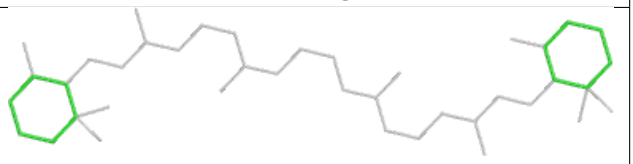
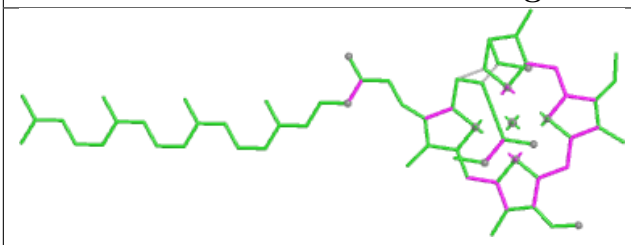


Rings

Ligand CL7 31 408



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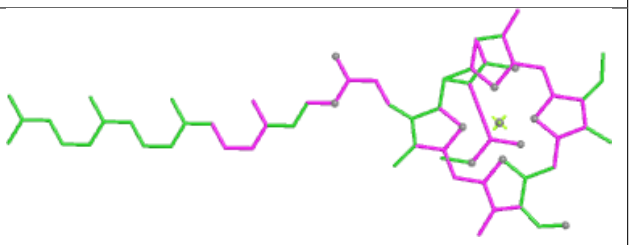
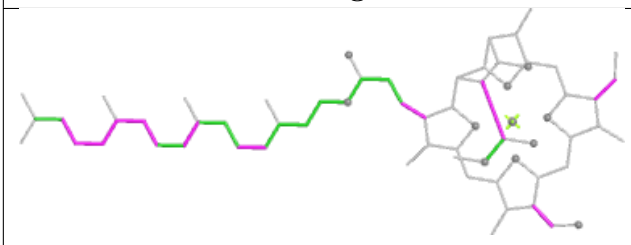


Bond angles



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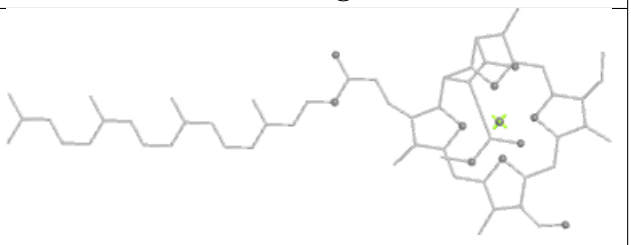
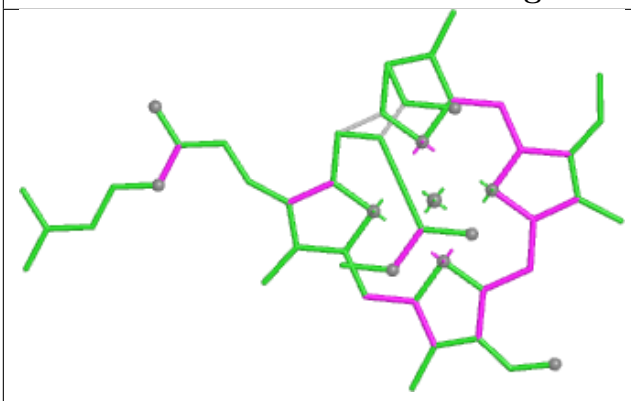


Rings

Ligand CL7 43 418



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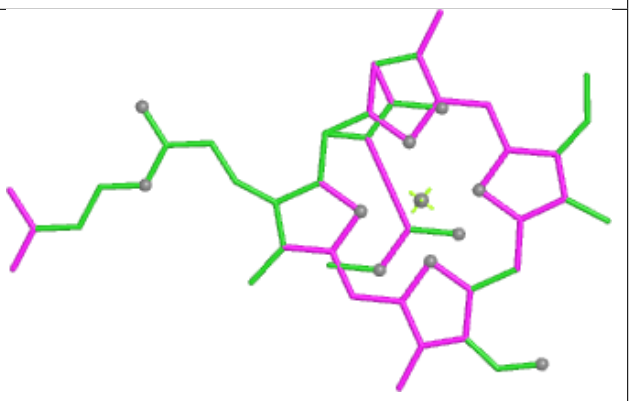
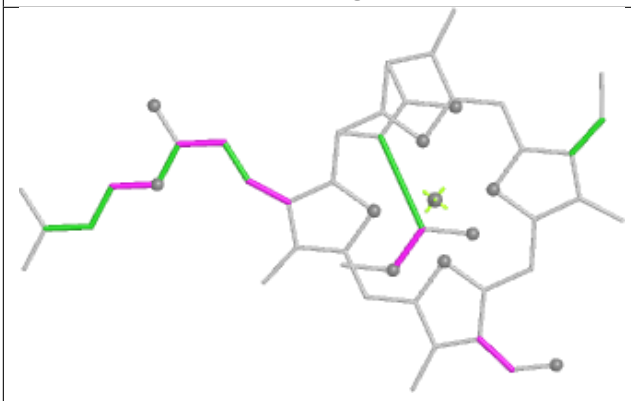


Bond angles



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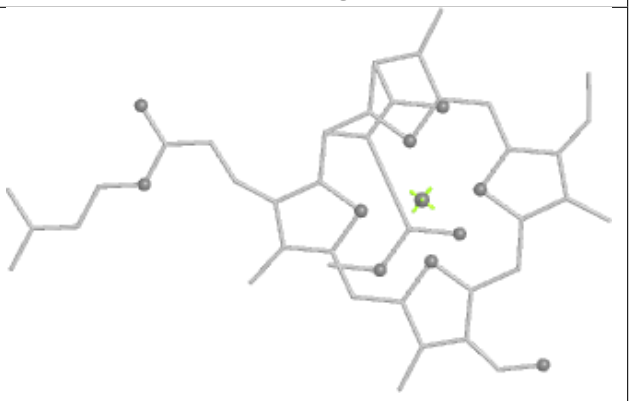
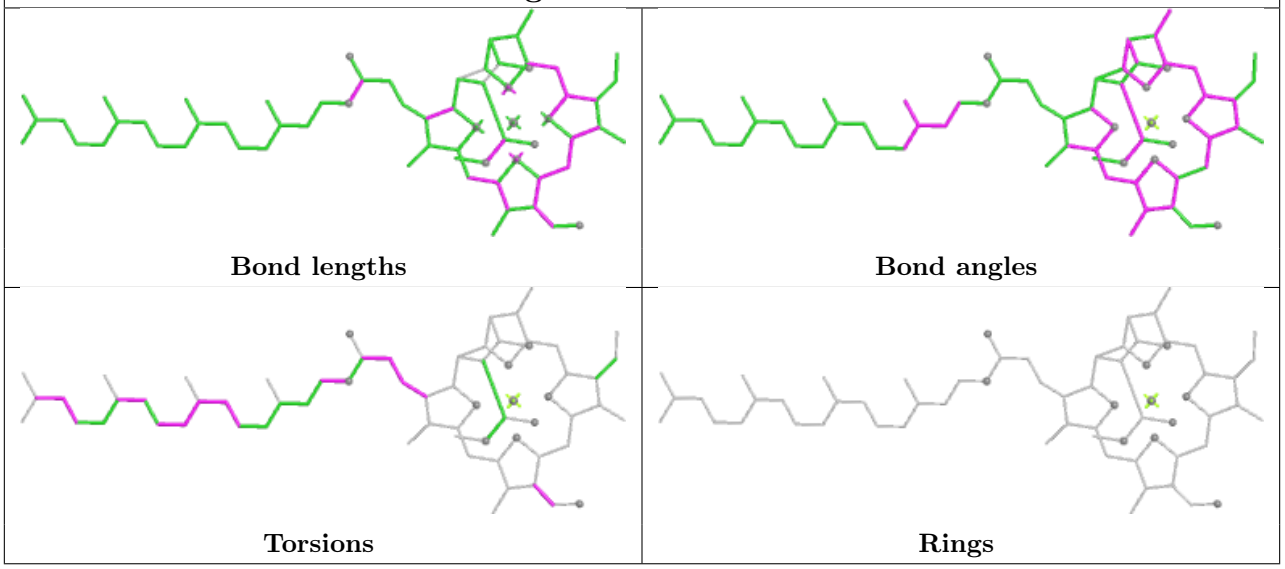
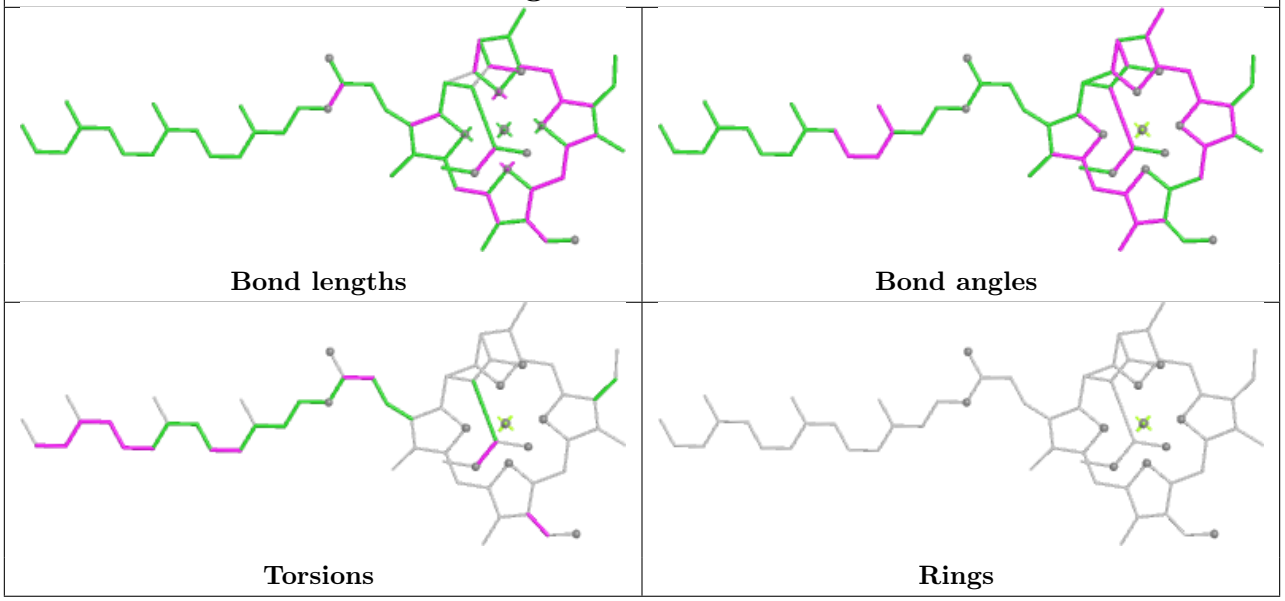


Rings

Ligand CL7 12 501



Ligand CL7 21 406



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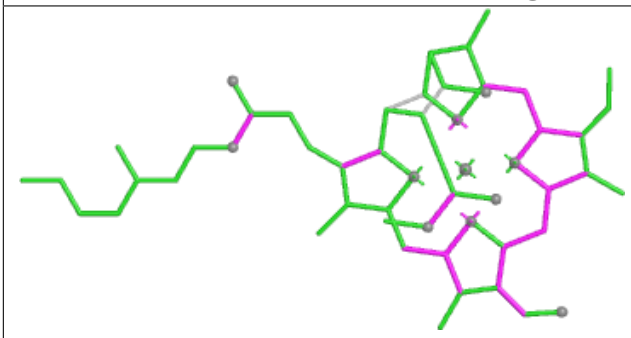

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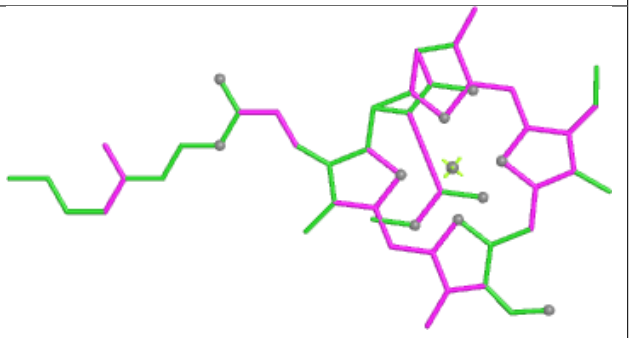
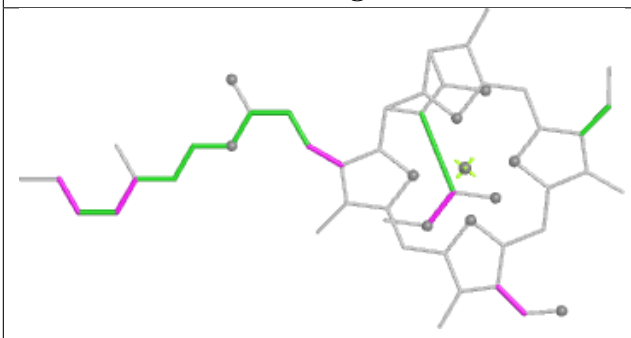


Bond angles



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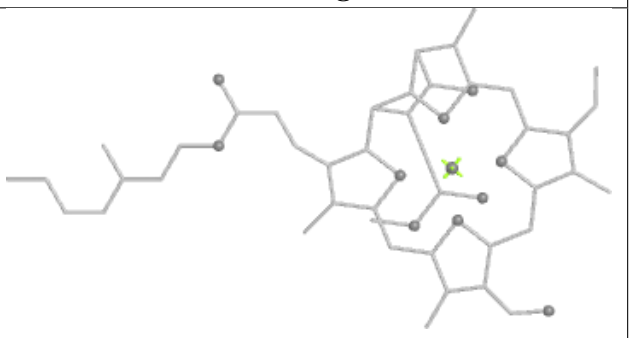
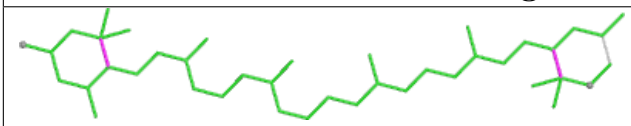


Rings

Ligand ZEX 33 520



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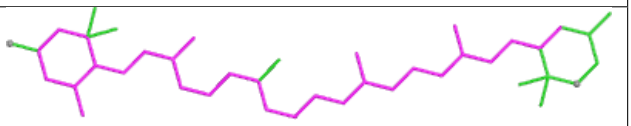
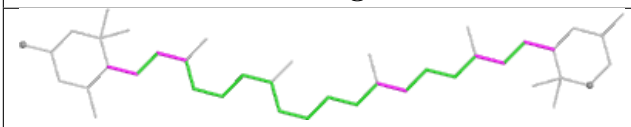


Bond angles



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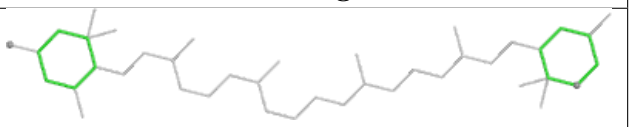
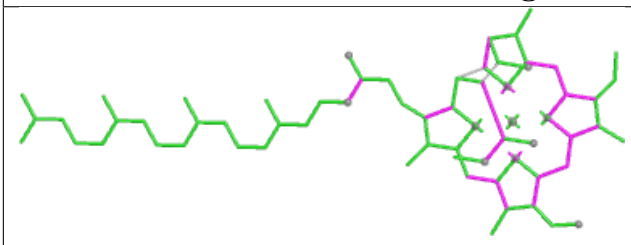


Rings

Ligand CL7 3B 611



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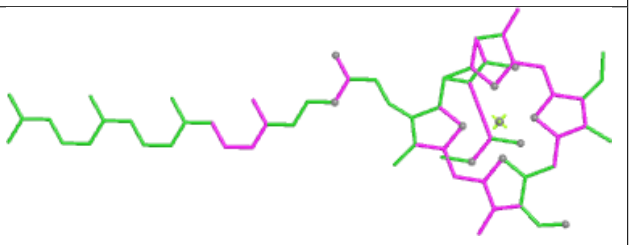

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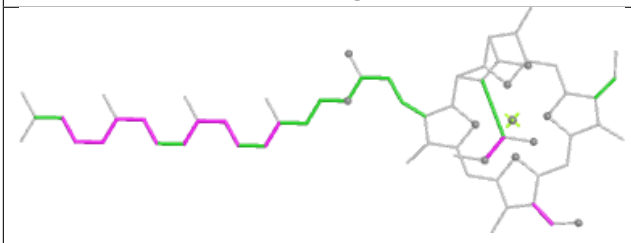

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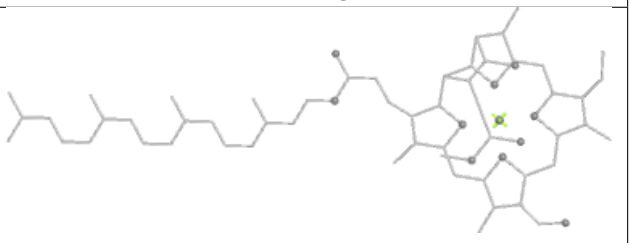
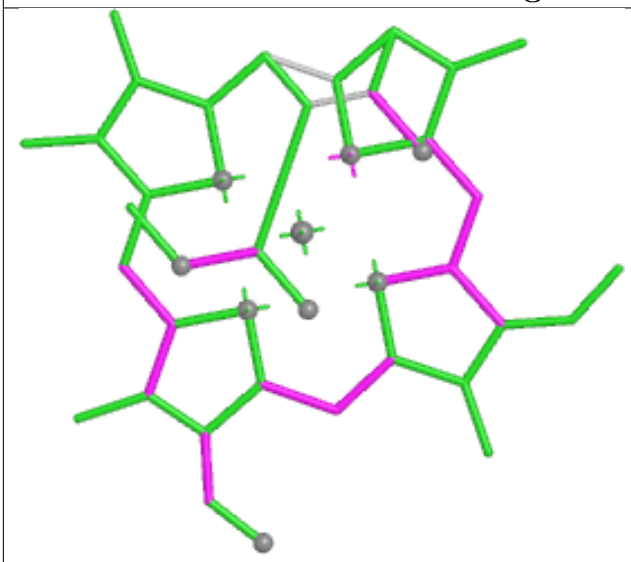


Rings

Ligand CL7 21 414



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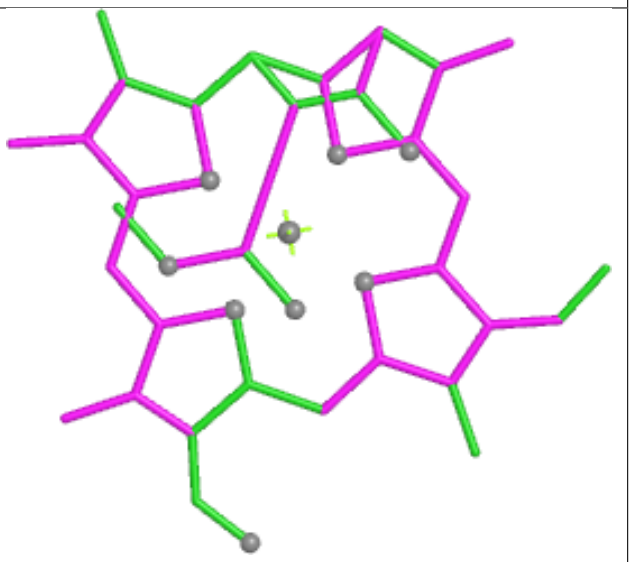

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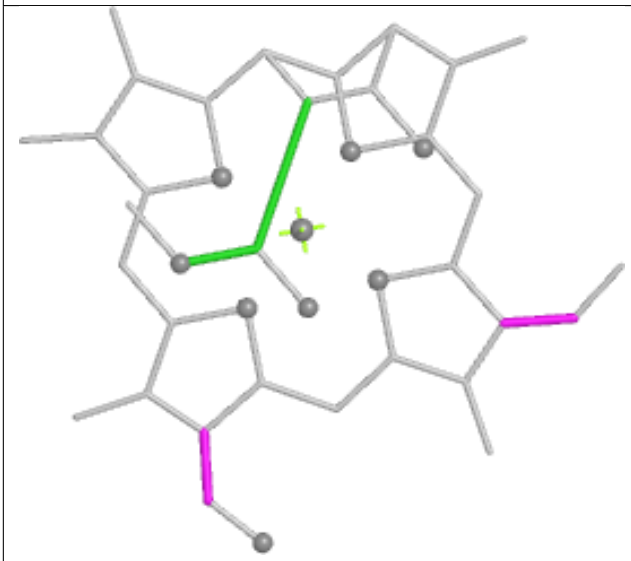

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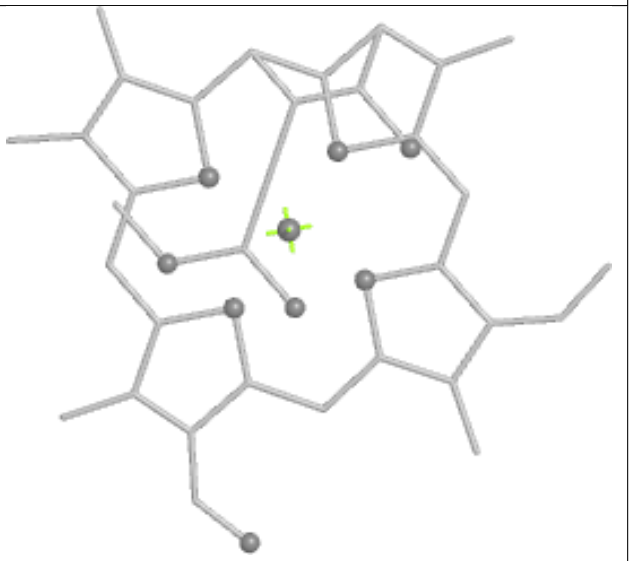
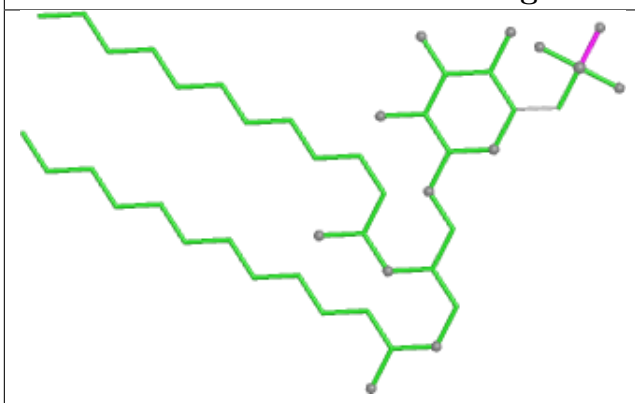


Rings

Ligand SQD 23 422



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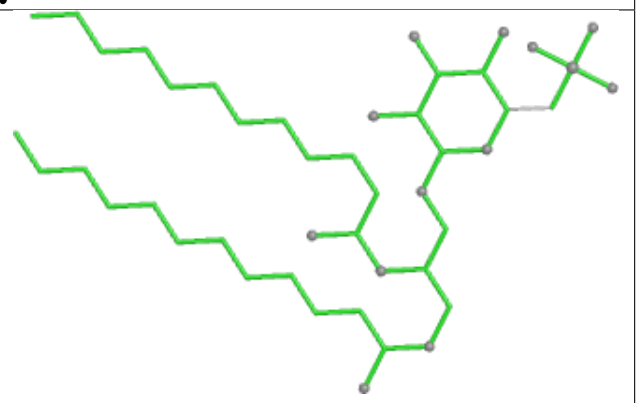

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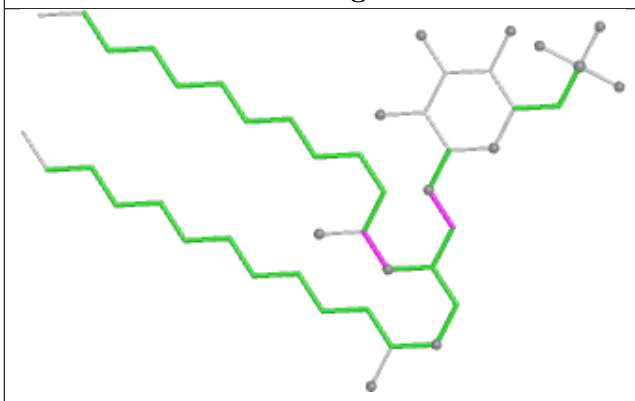

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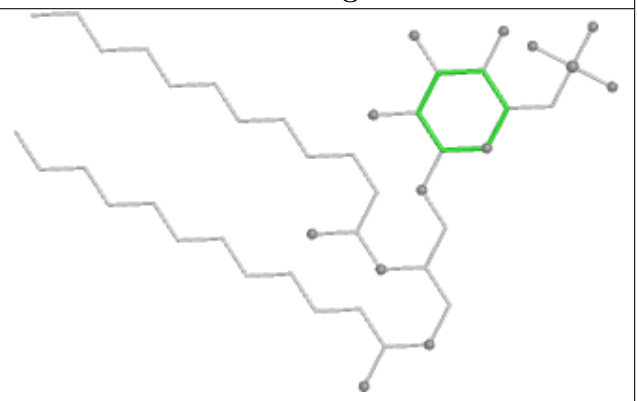
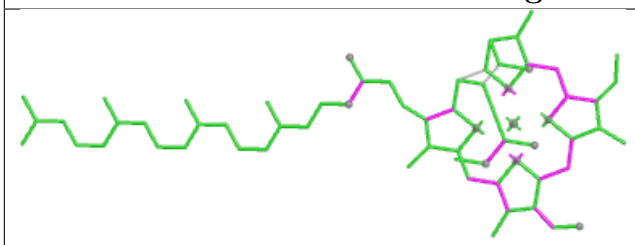


Rings

Ligand CL7 21 404



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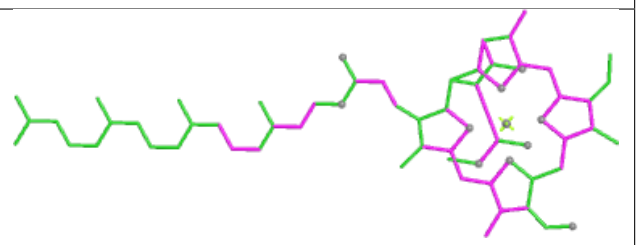

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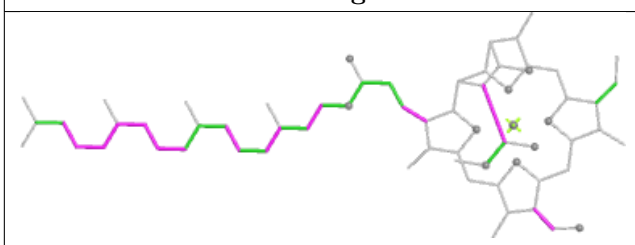

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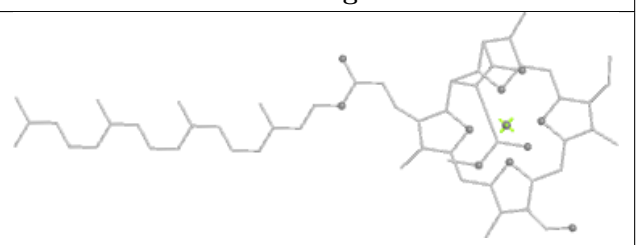

Rings

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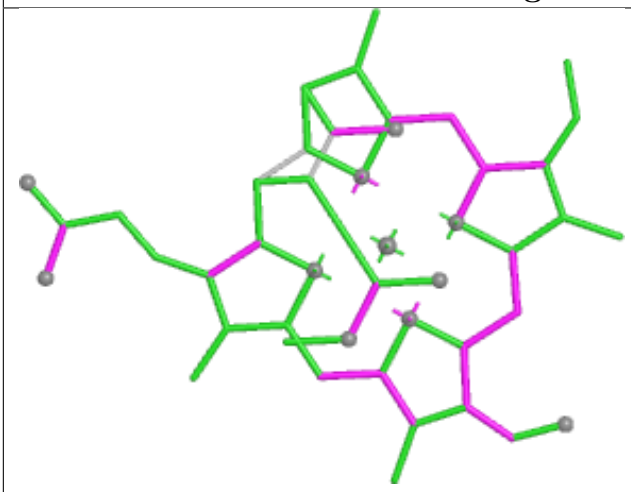

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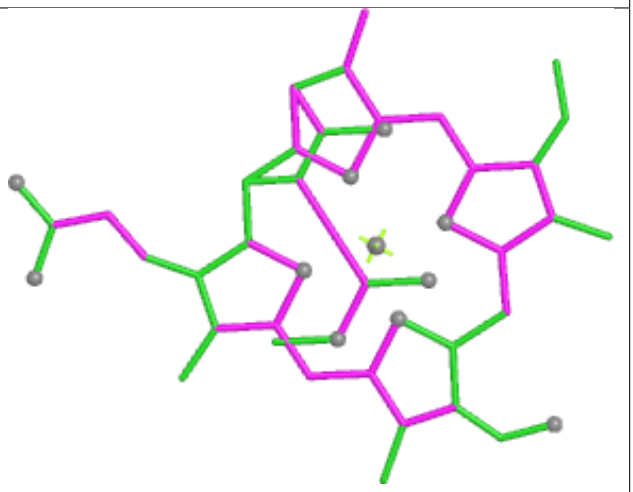

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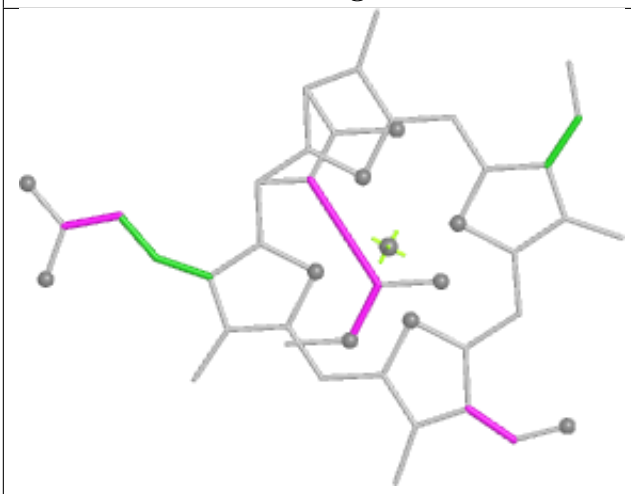
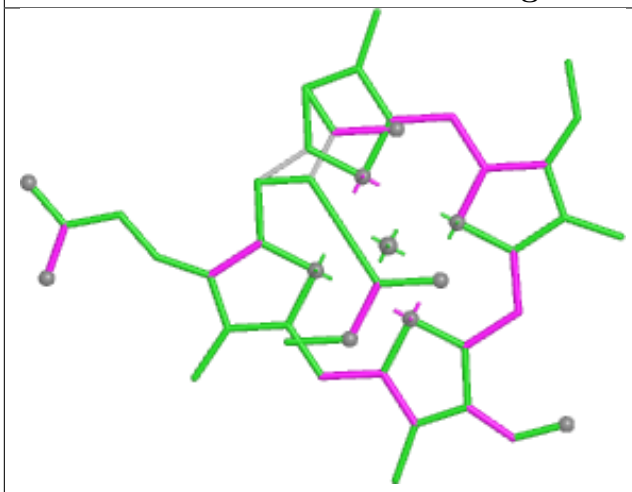


Torsions



Rings

Ligand CL7 1B 622



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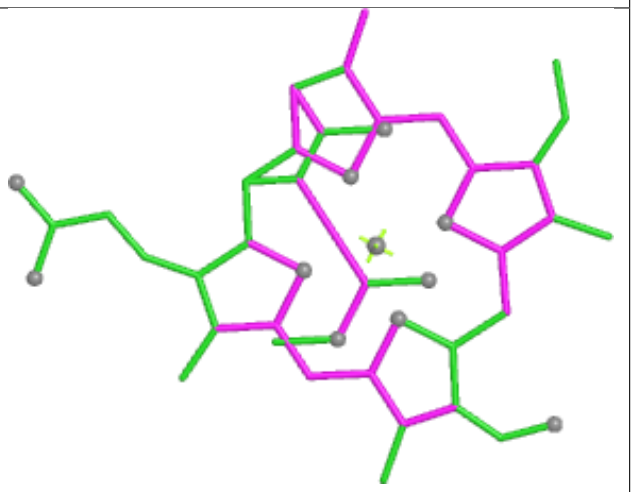

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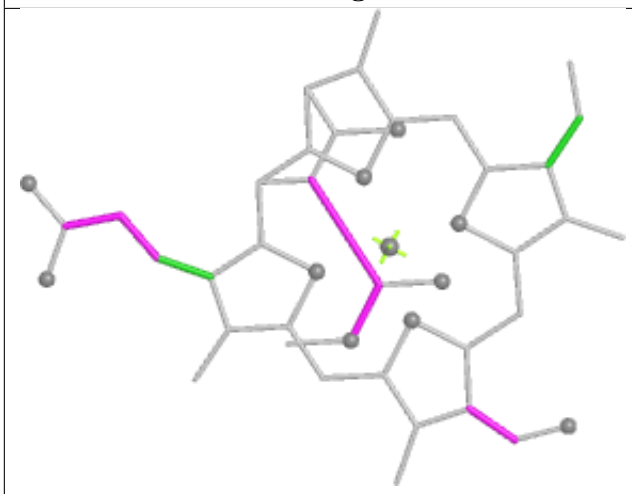

Torsions



Rings

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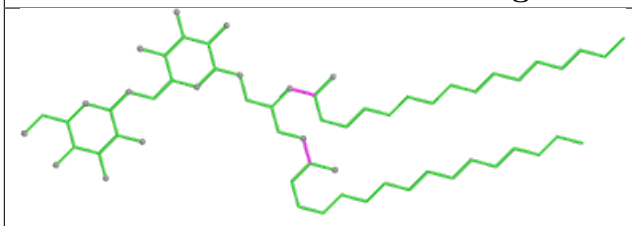

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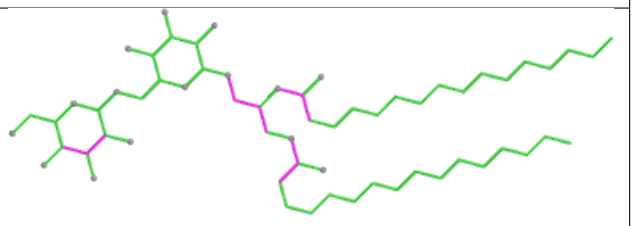

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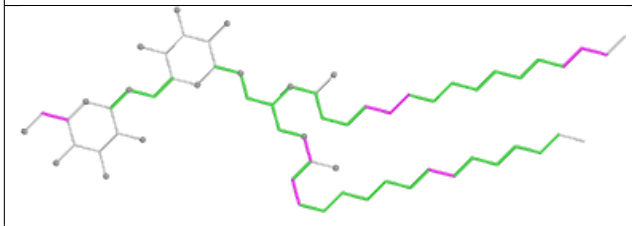

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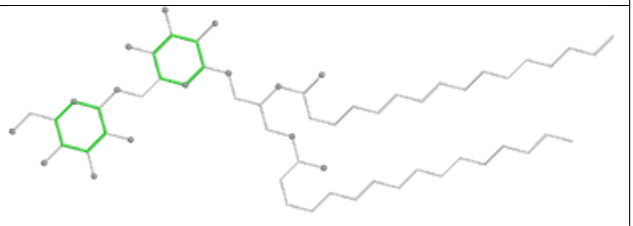
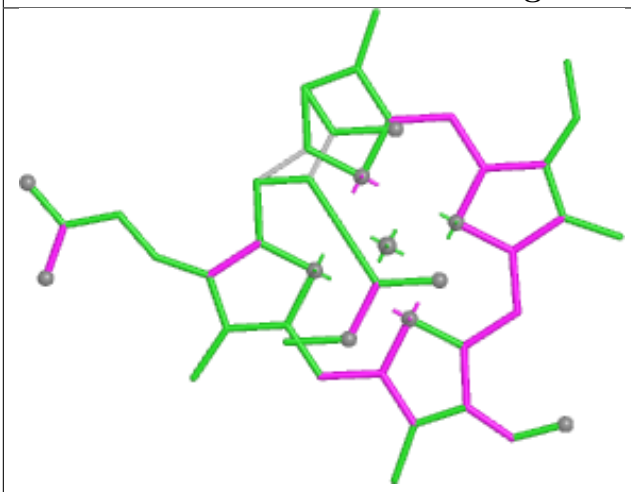


Rings

Ligand CL7 22 508



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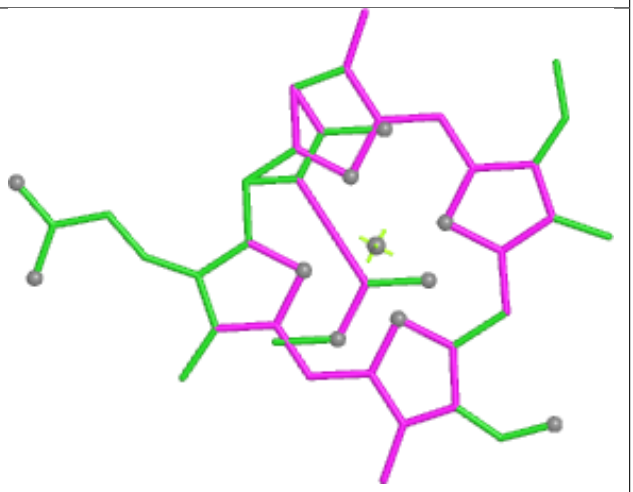

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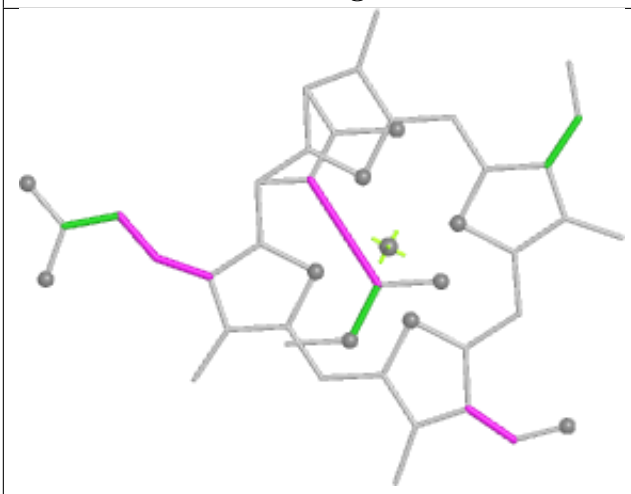

Torsions



Rings

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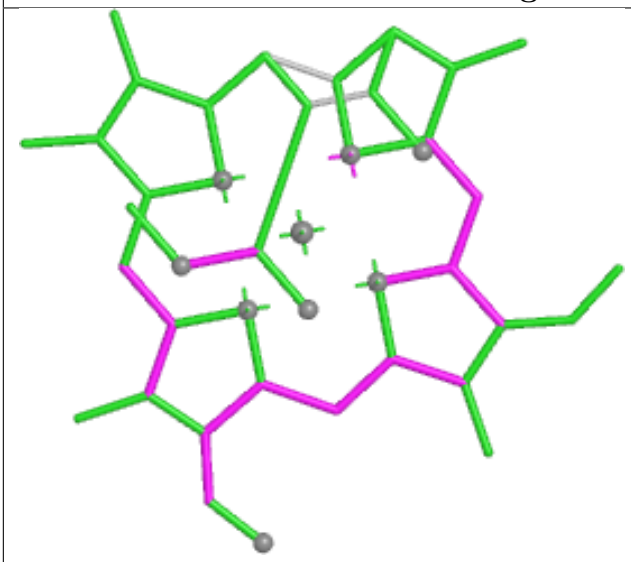

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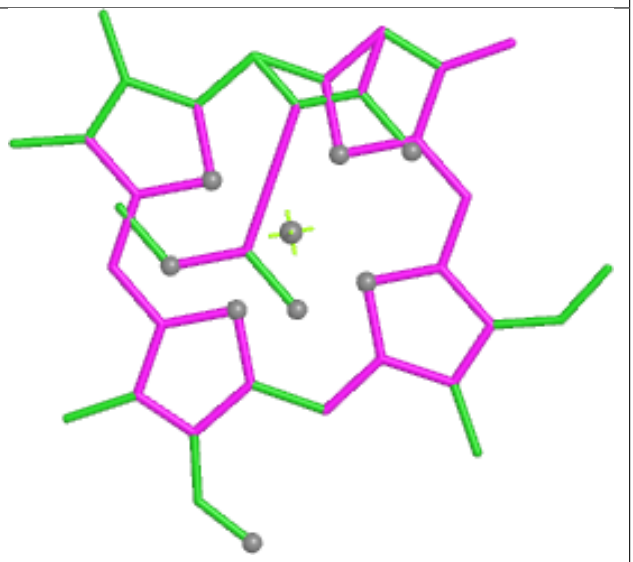

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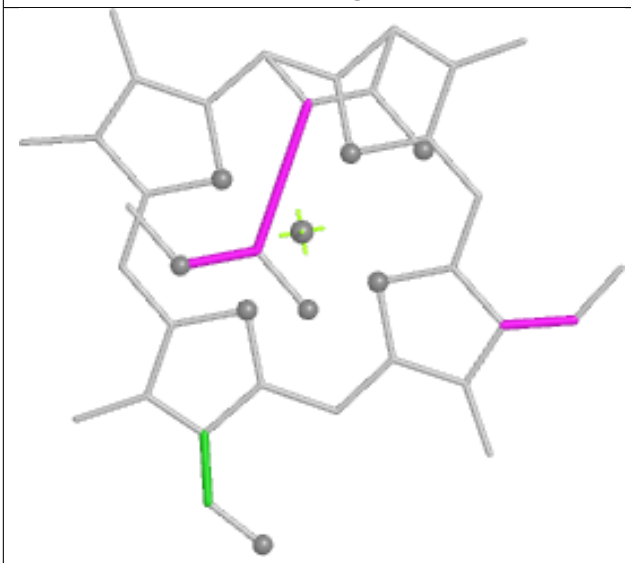

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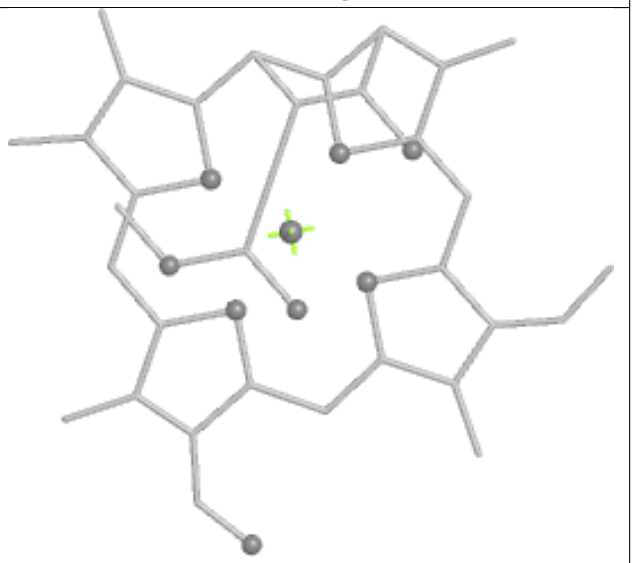

Rings

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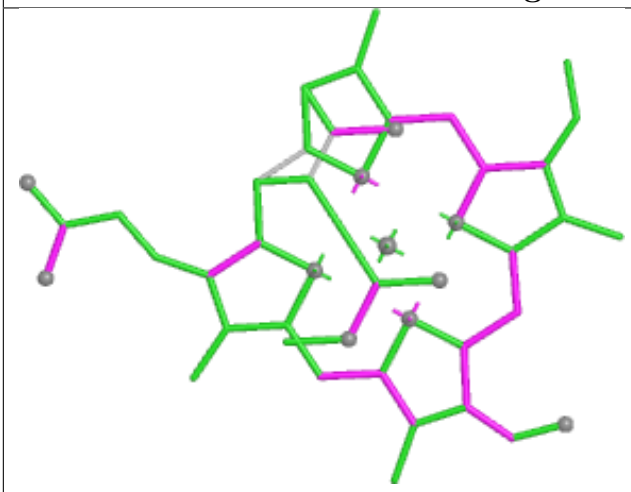

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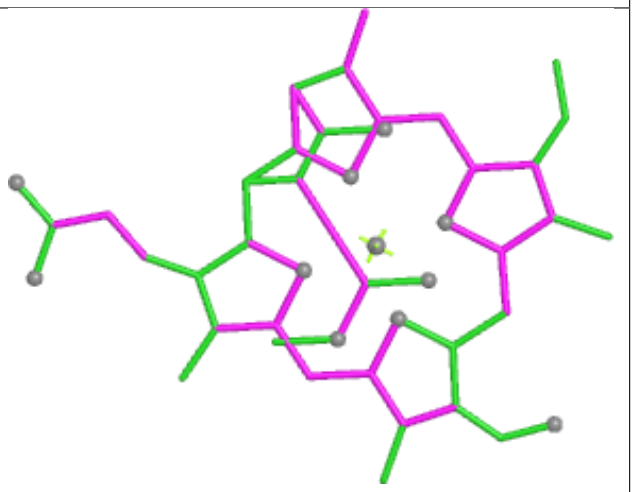

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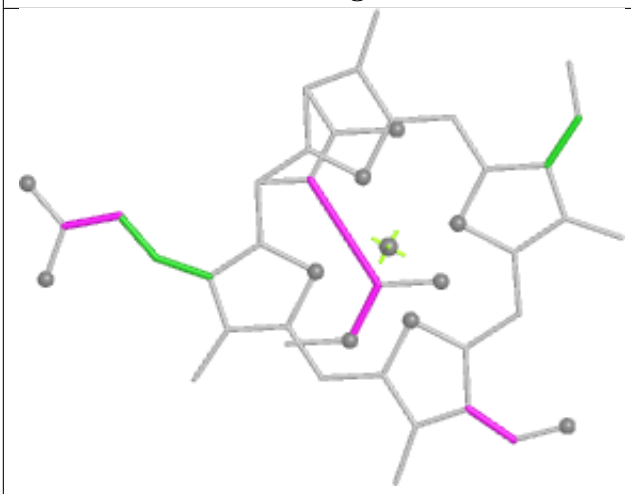

Torsions



Rings

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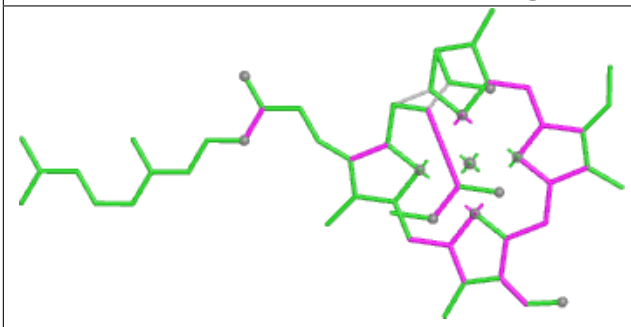

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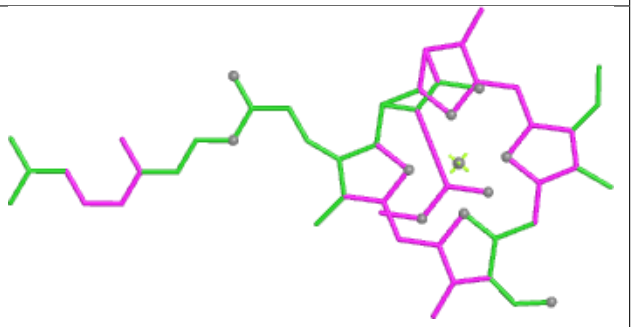

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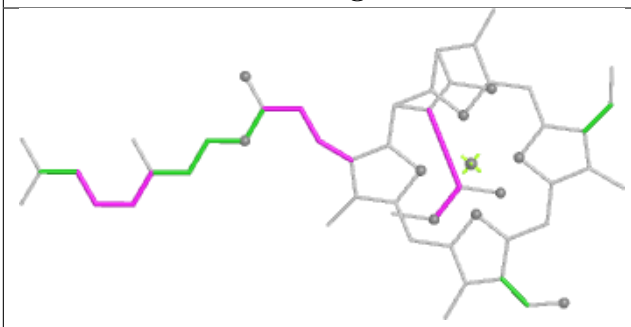

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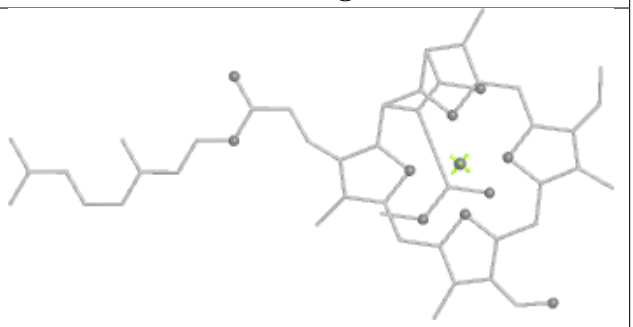

Rings

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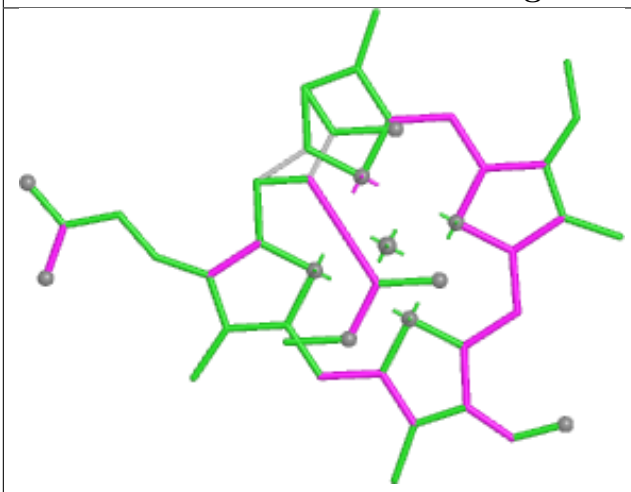

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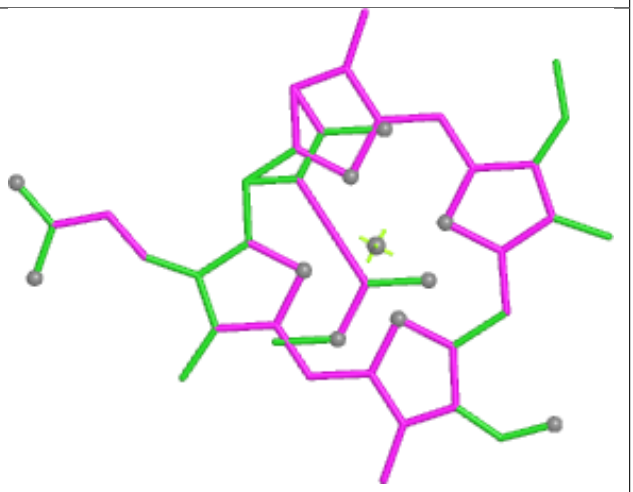

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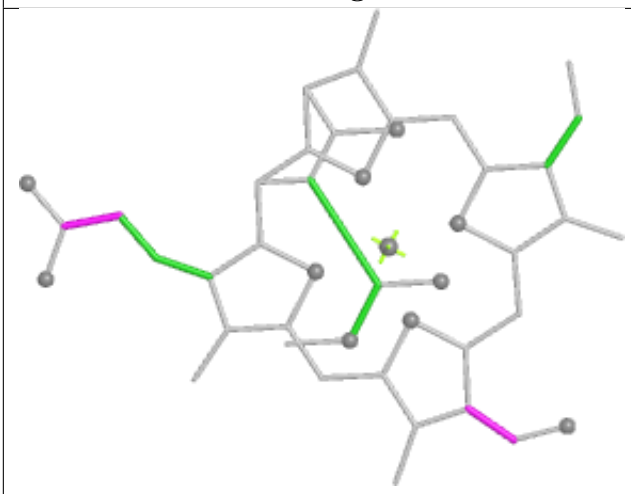

Torsions



Rings

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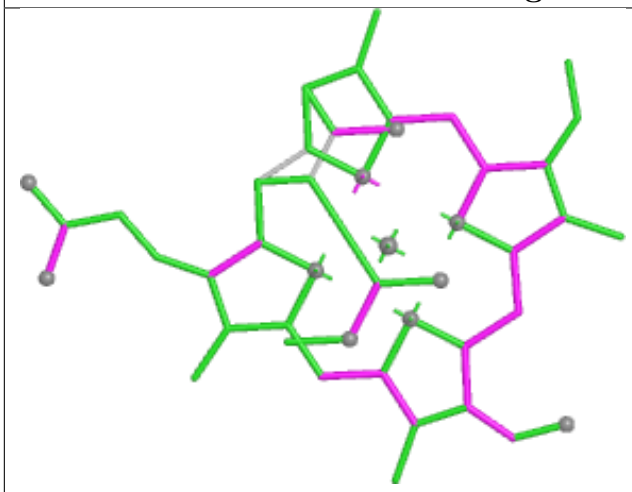

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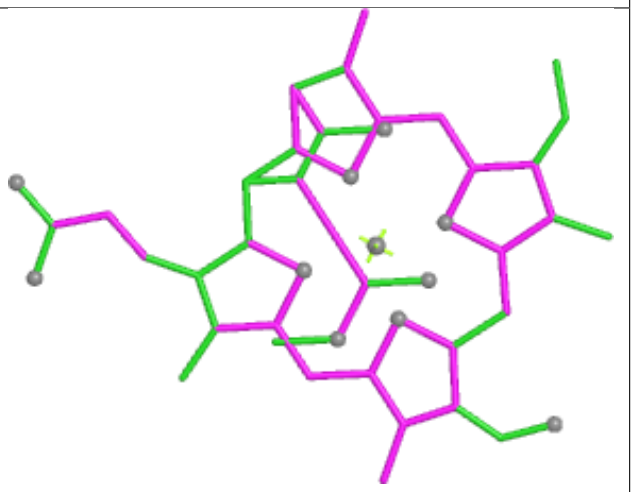
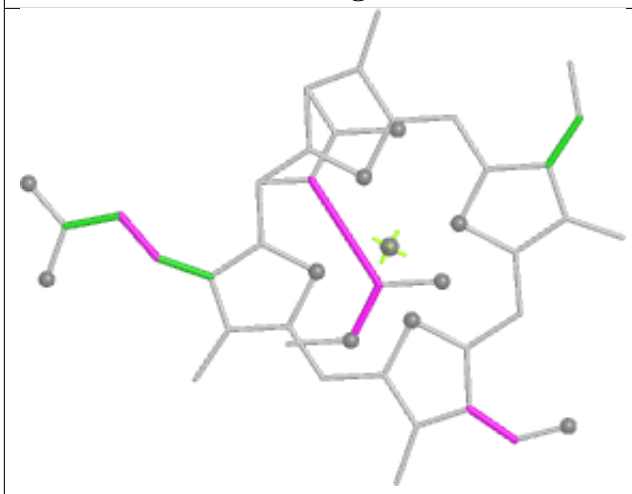


Bond angles

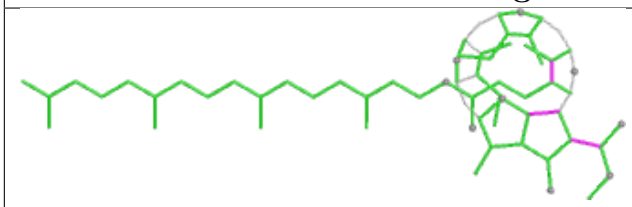


Torsions



Rings

Ligand PHO 4A 402



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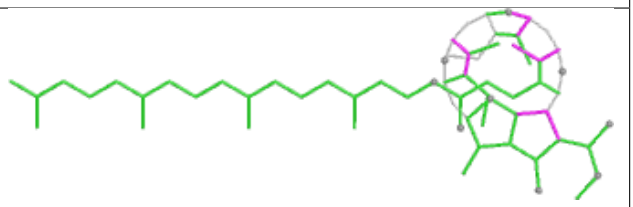
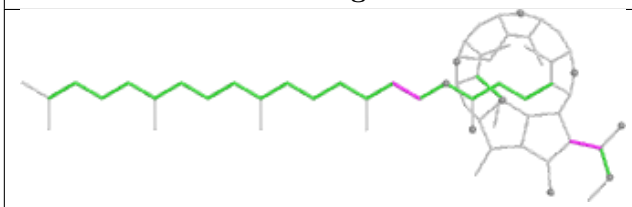


Bond angles



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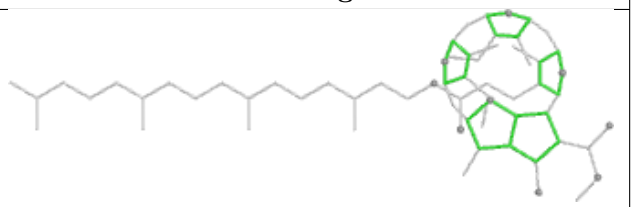
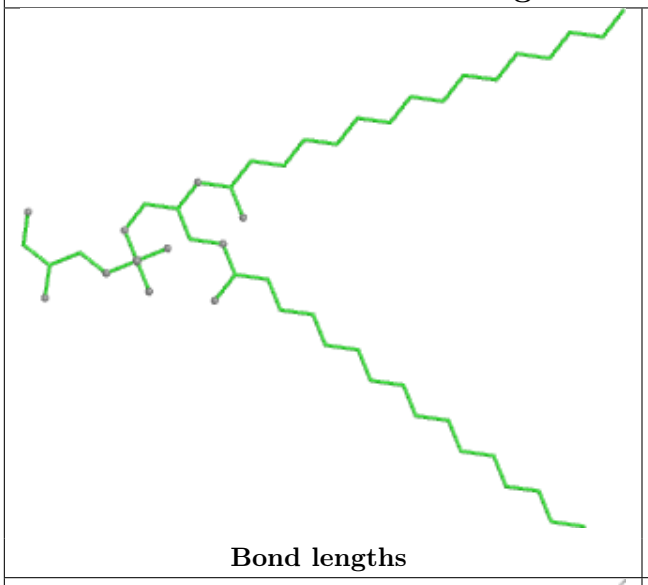


Rings

Ligand LHG 1D 409



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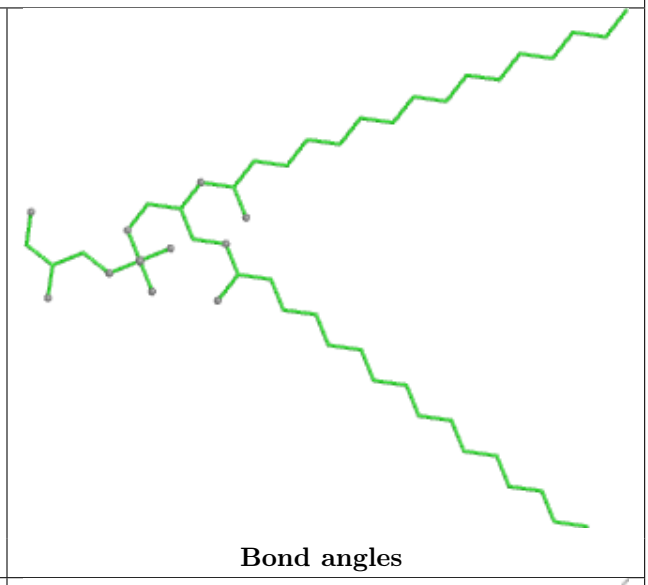

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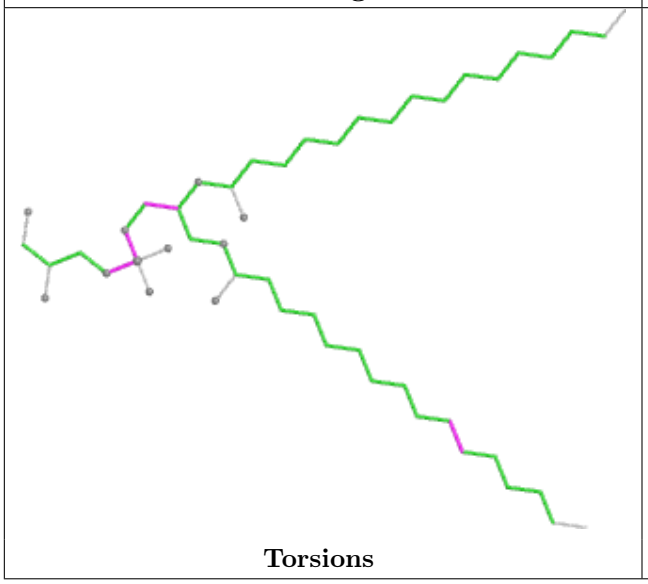

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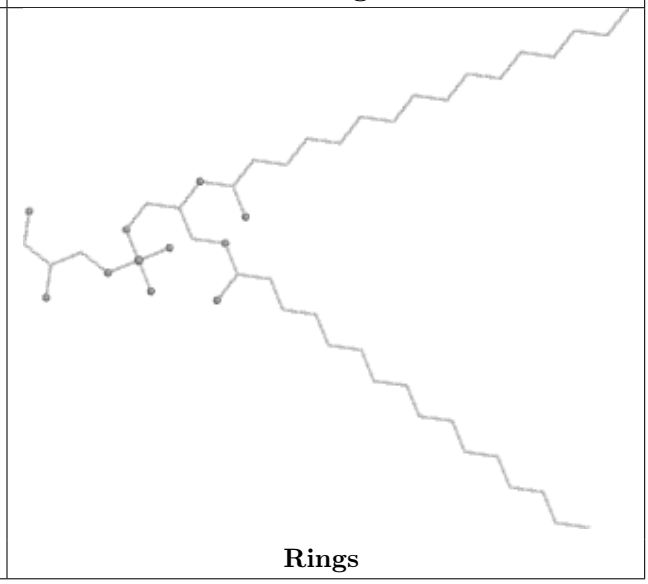
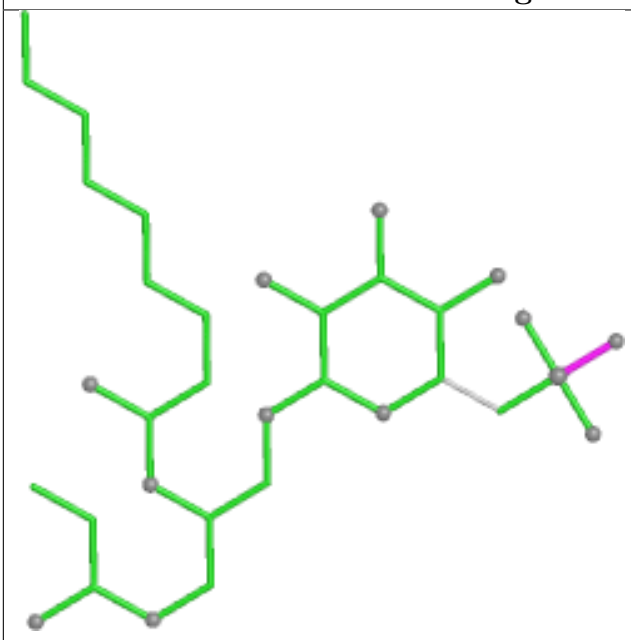


Rings

Ligand SQD 3A 406



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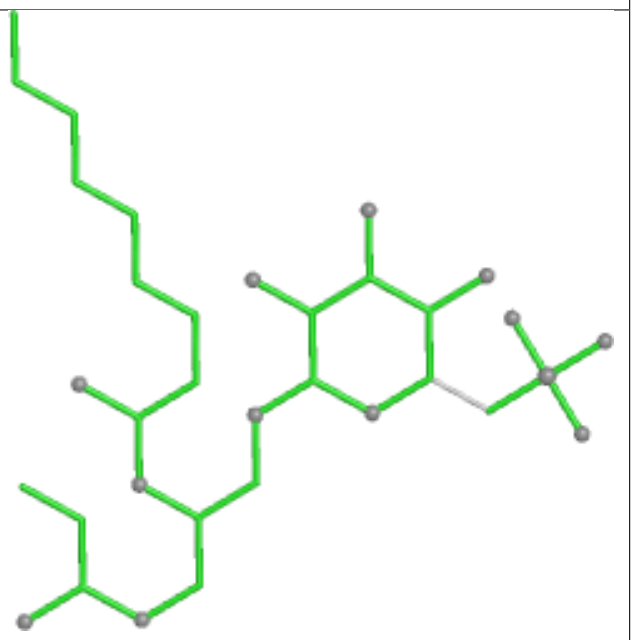

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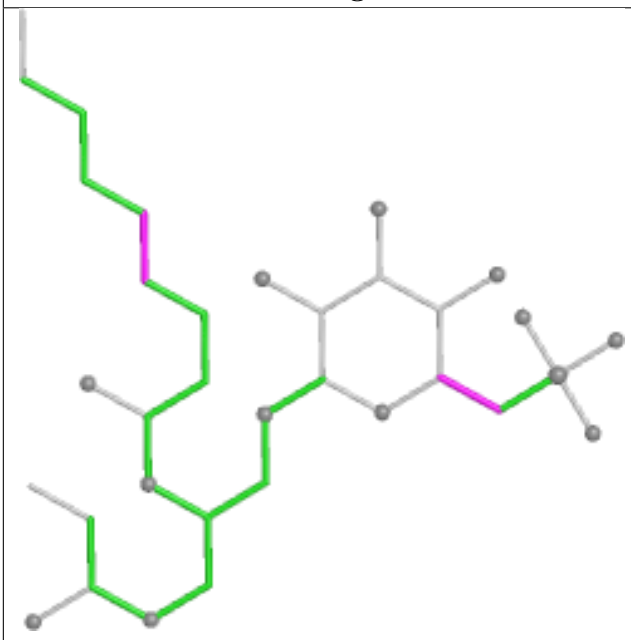
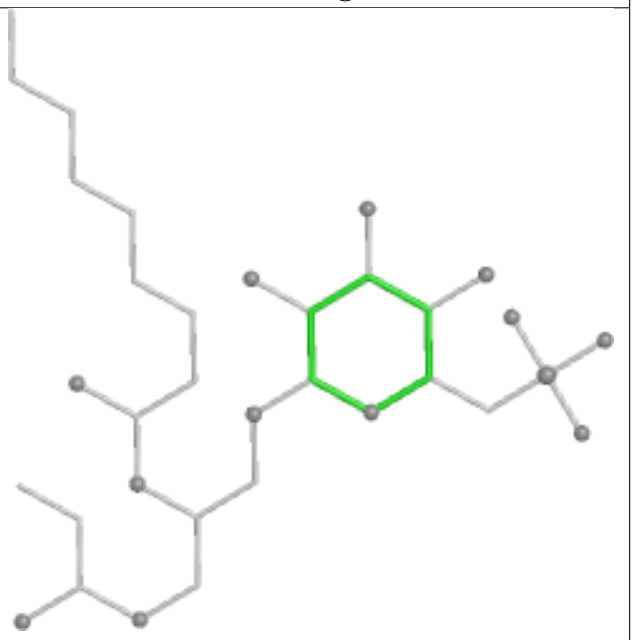
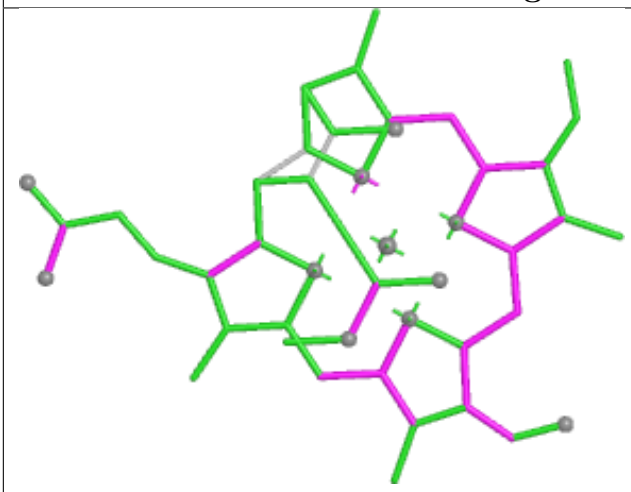


Torsions



Rings

Ligand CL7 23 407



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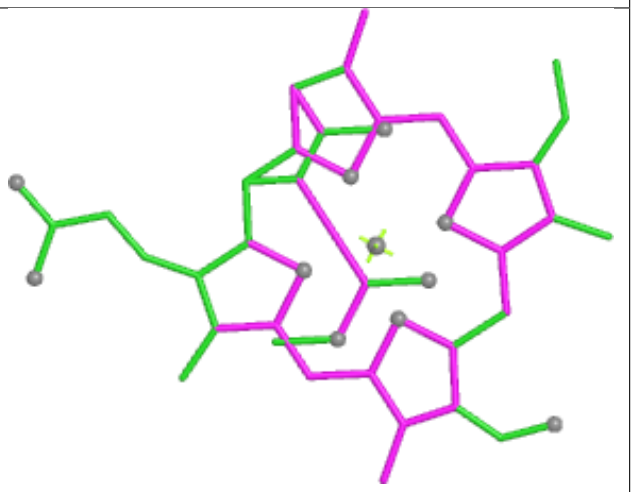

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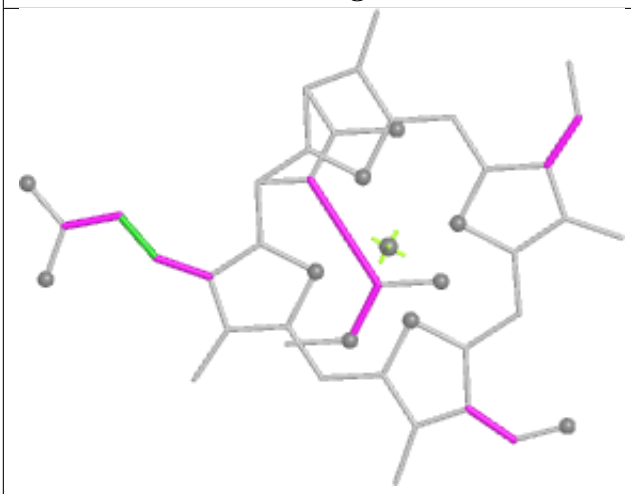
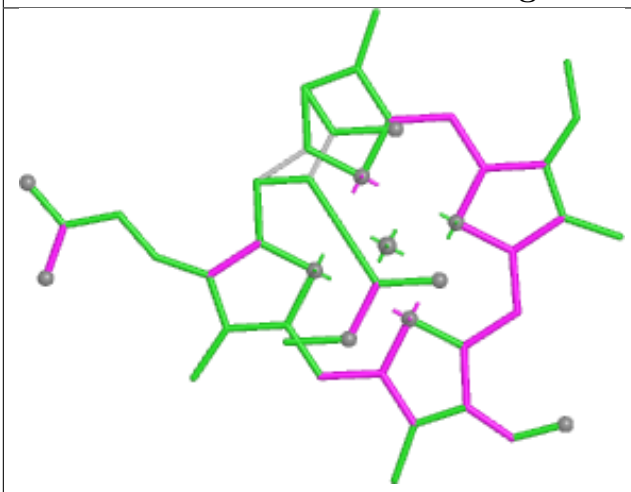


Torsions



Rings

Ligand CL7 1D 405



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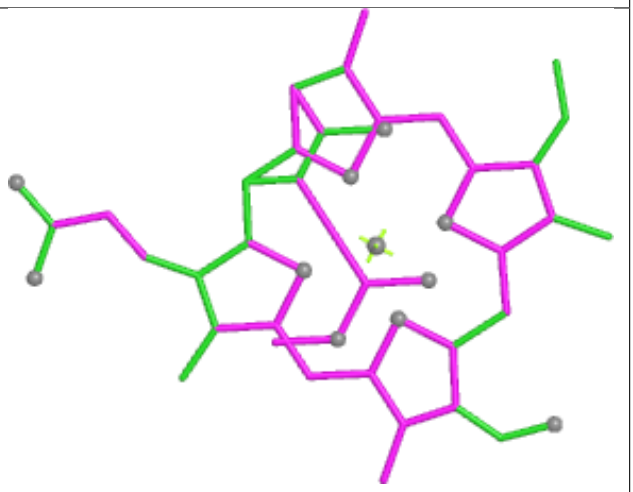

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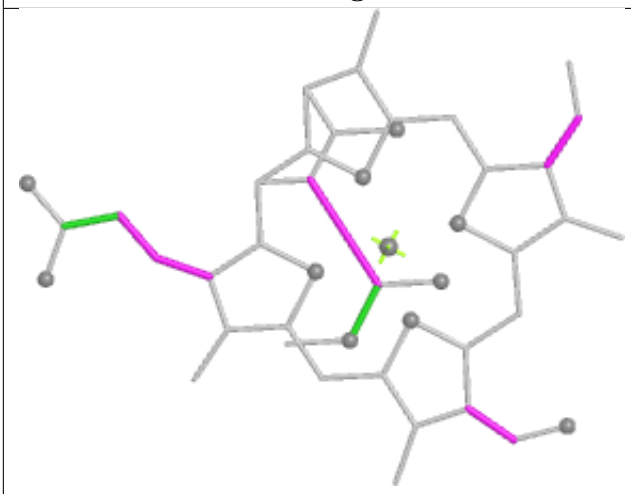

Torsions



Rings

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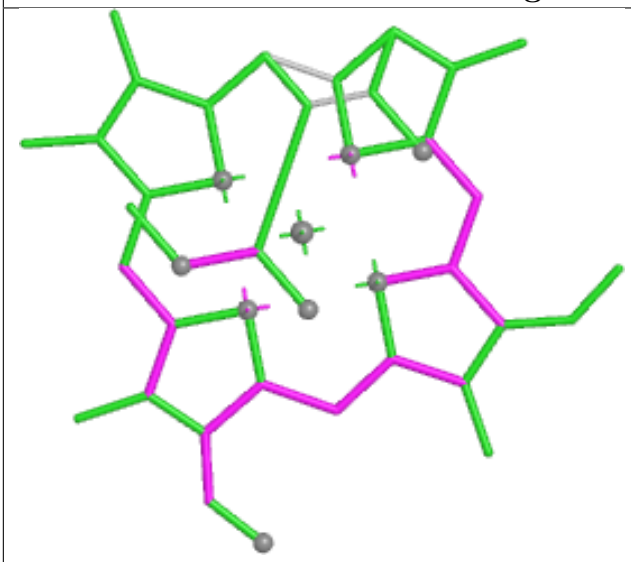

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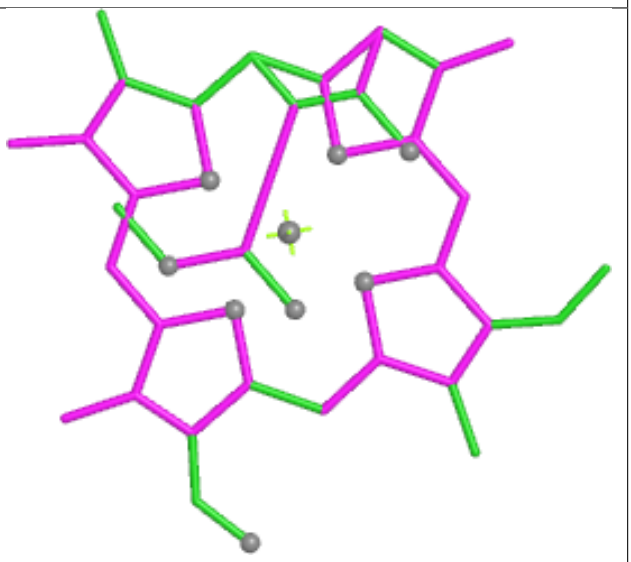

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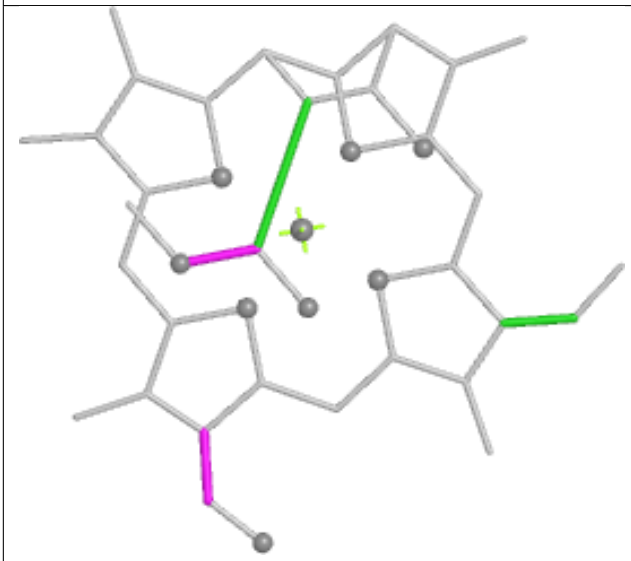

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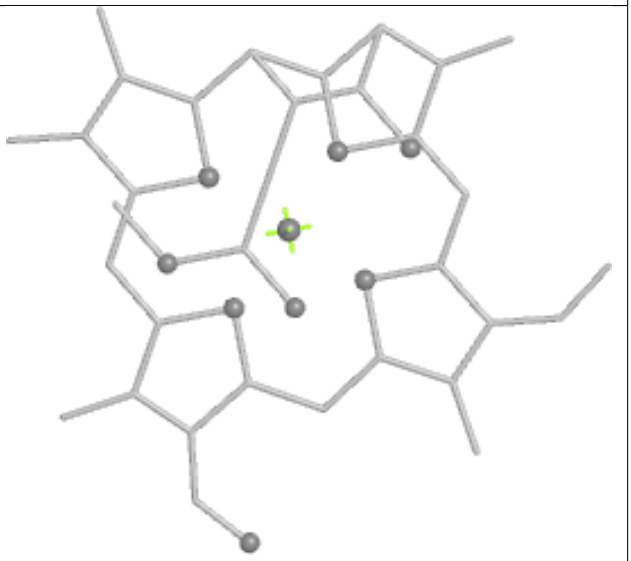
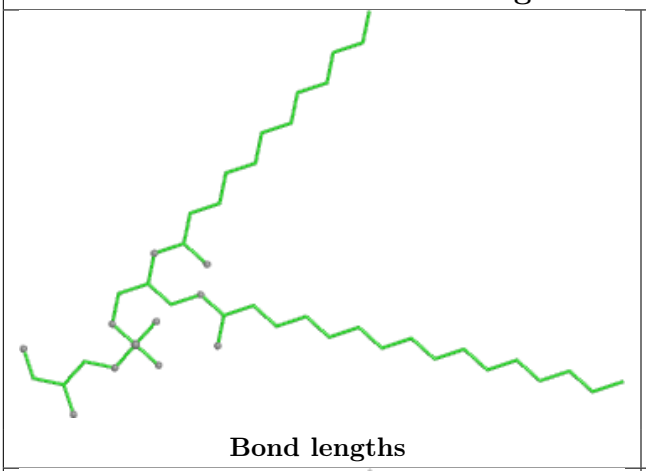


Rings

Ligand LHG 3B 623



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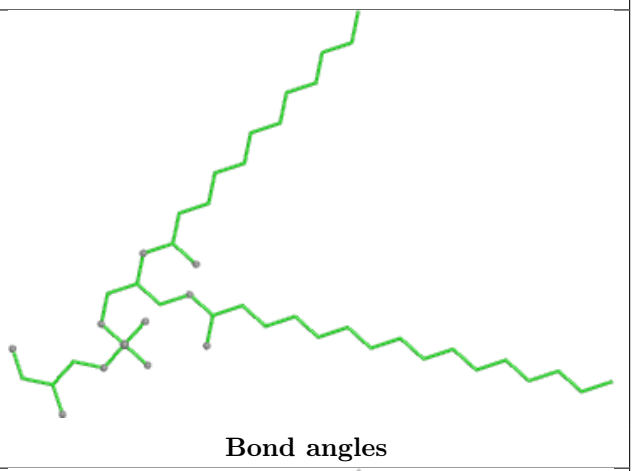

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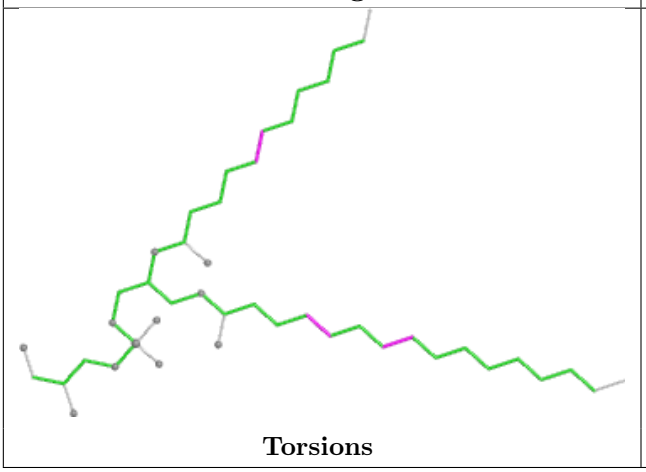

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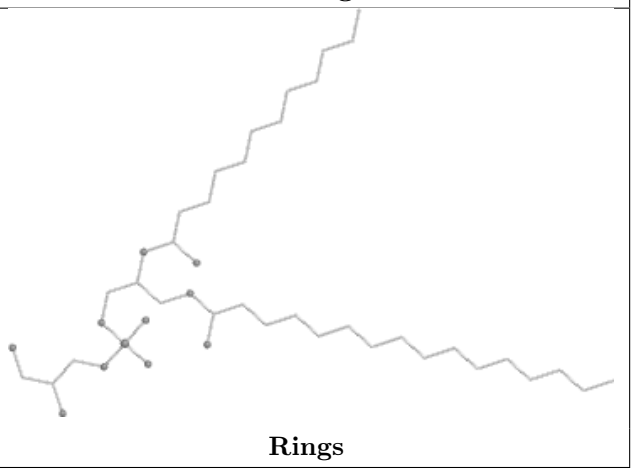
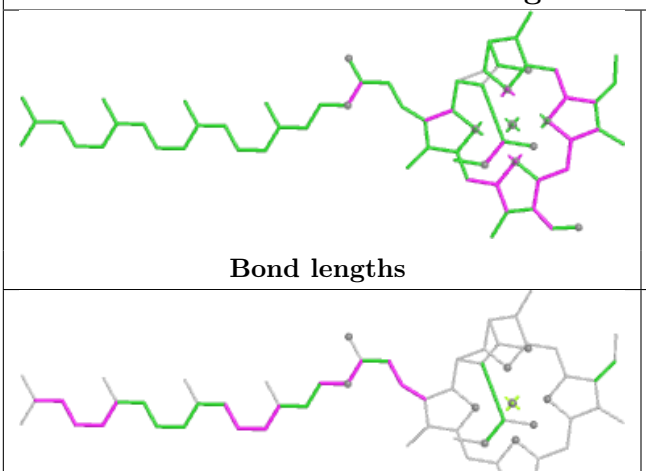


Rings

Ligand CL7 12 516



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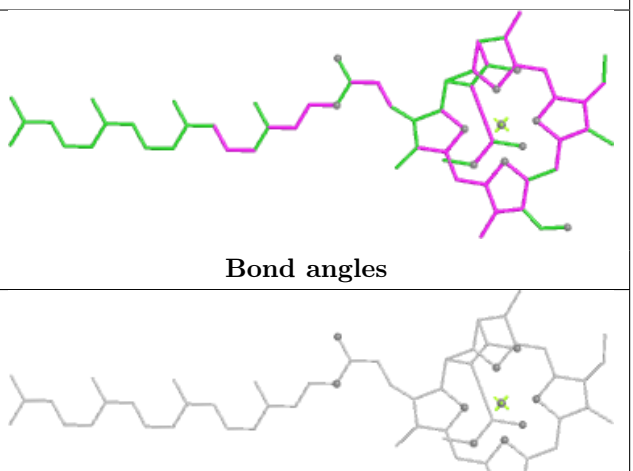

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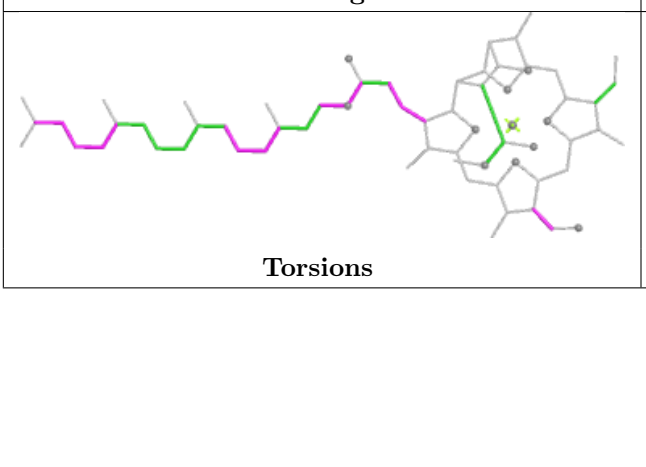

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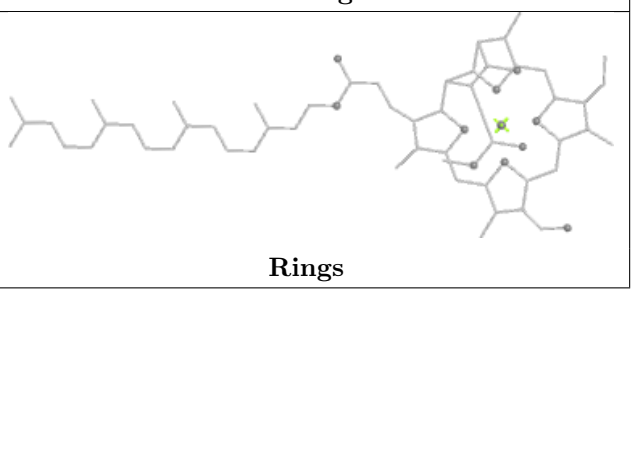
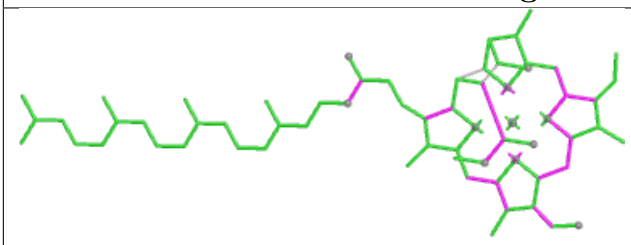


Rings

Ligand CL7 4C 503



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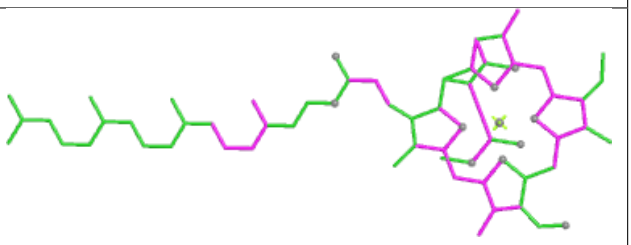

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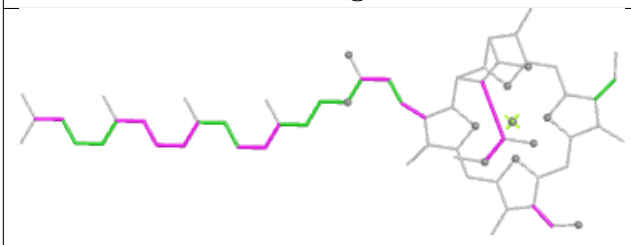

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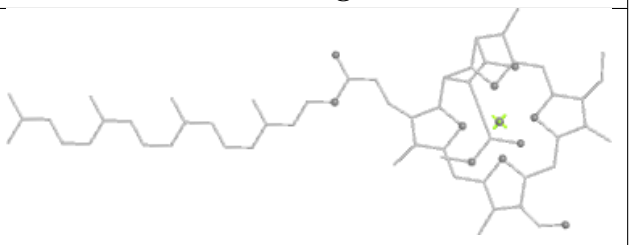
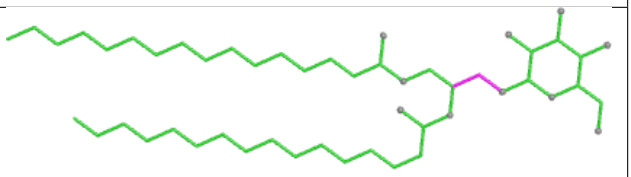


Rings

Ligand LMG 31 401



Bond lengths



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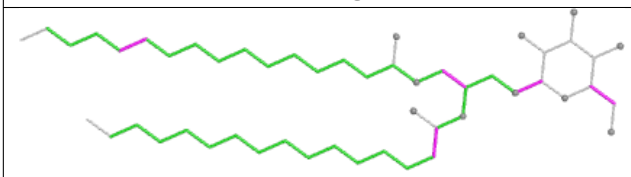

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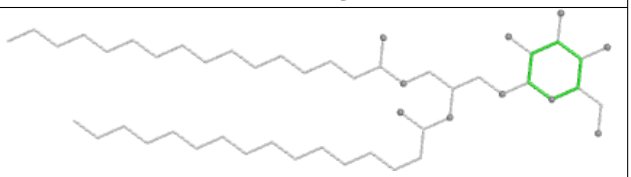
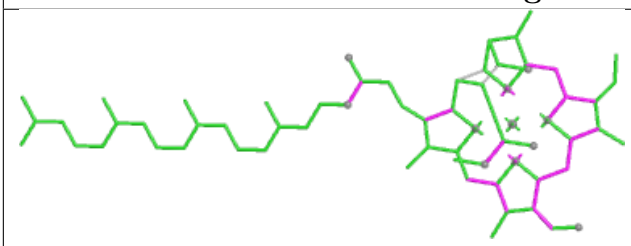


Rings

Ligand CL7 32 501



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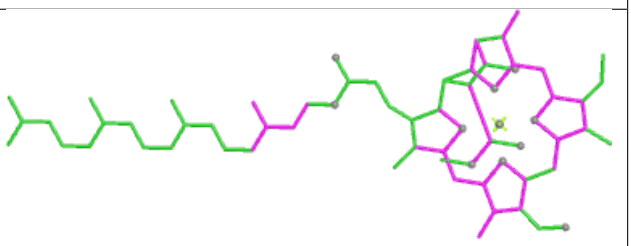

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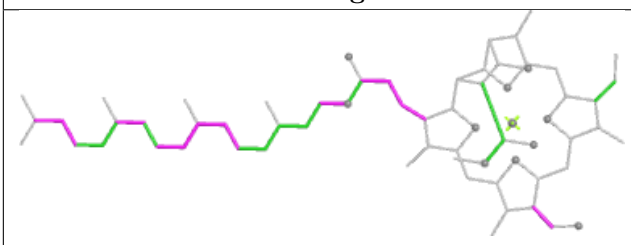

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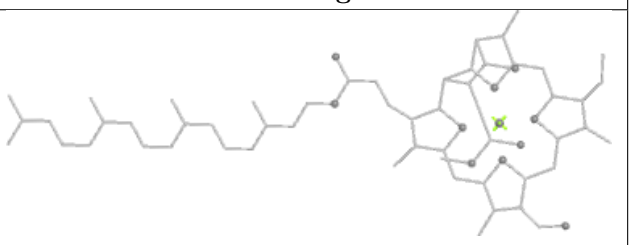

Rings

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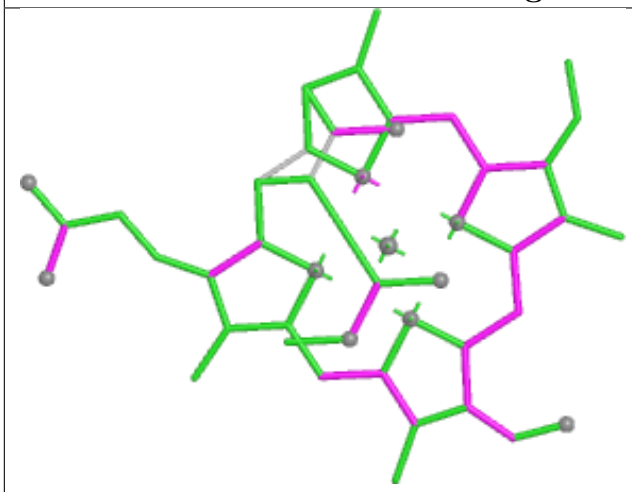

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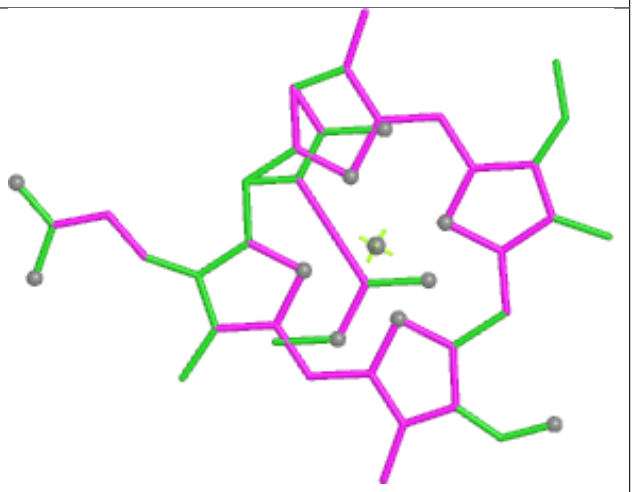

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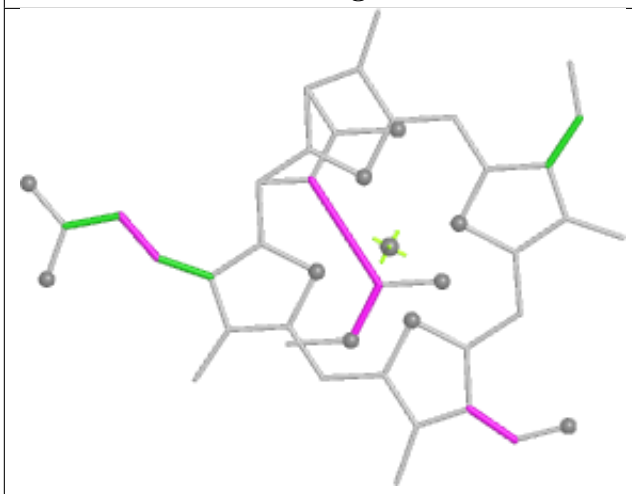
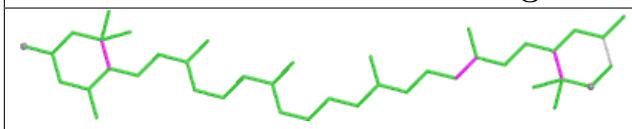


Torsions



Rings

Ligand ZEX 22 524



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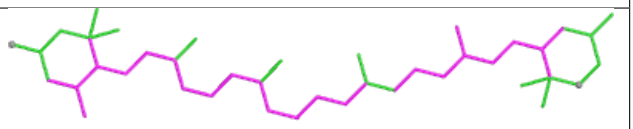

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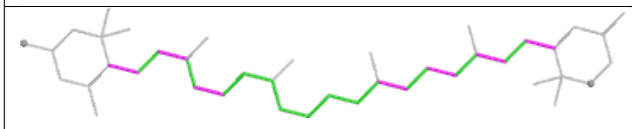

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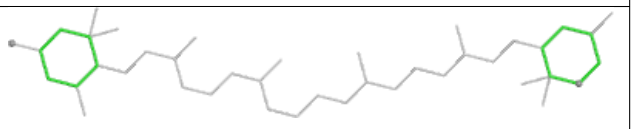
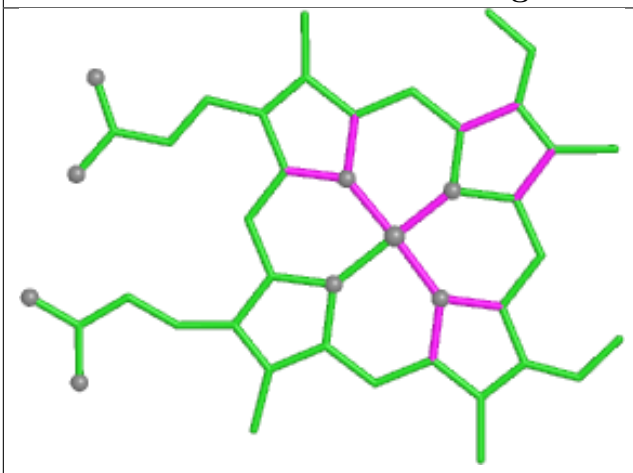


Rings

Ligand HEM 2F 101



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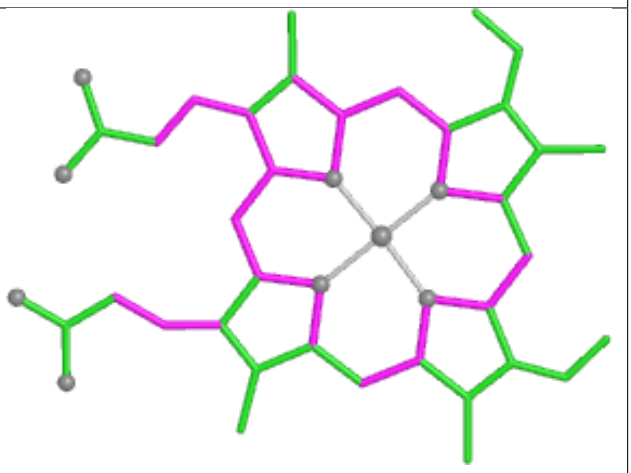

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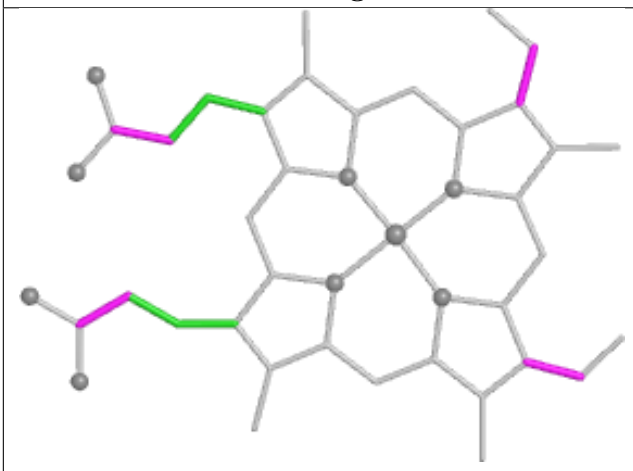

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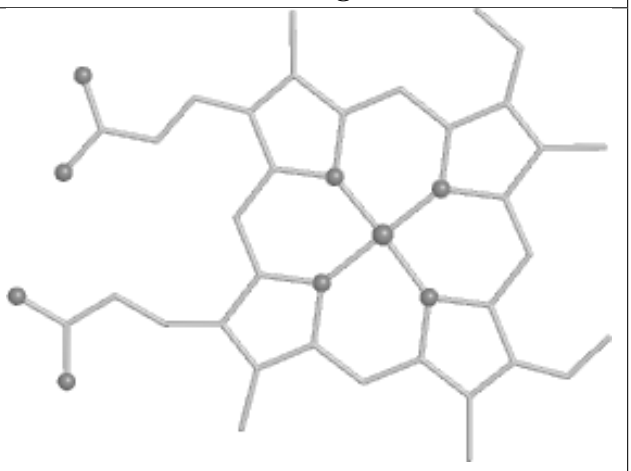
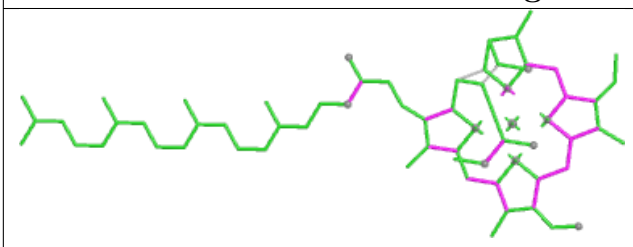


Rings

Ligand CL7 34 411



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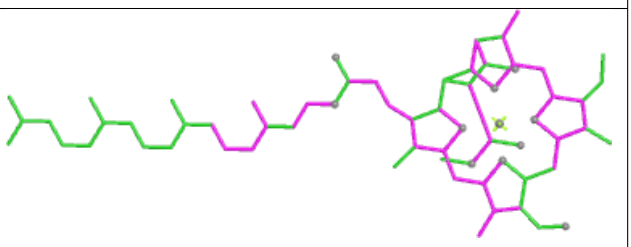

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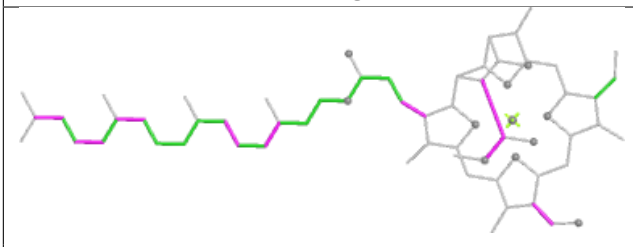

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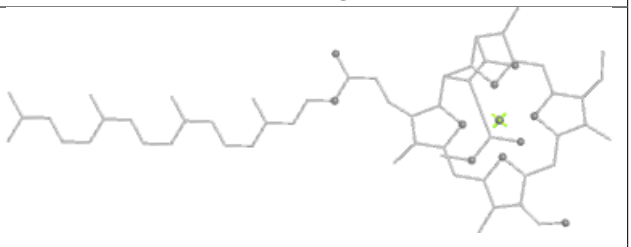
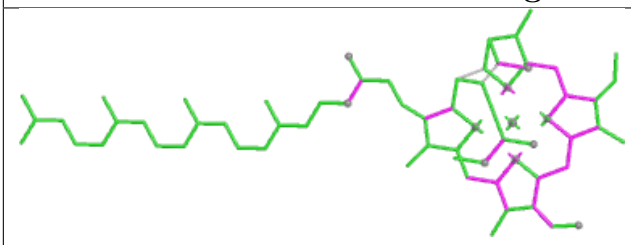


Rings

Ligand CL7 44 404



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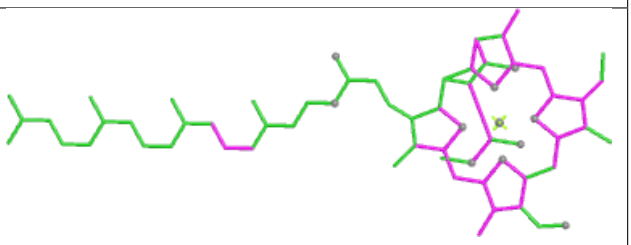
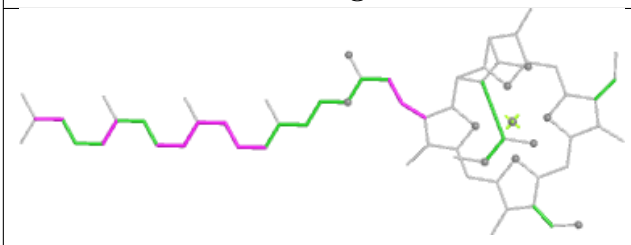


Bond angles



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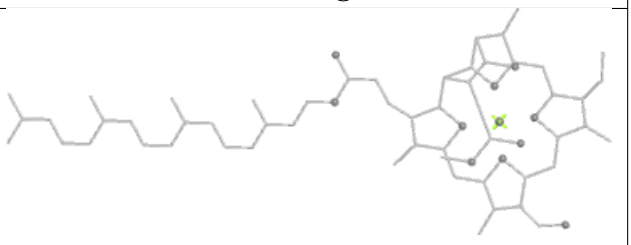
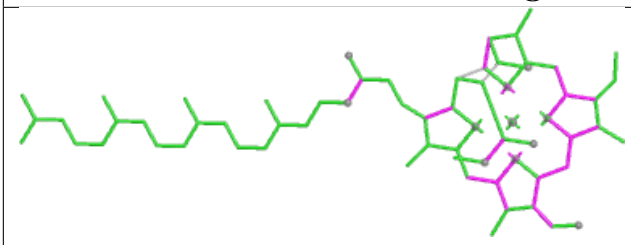


Rings

Ligand CL7 32 505



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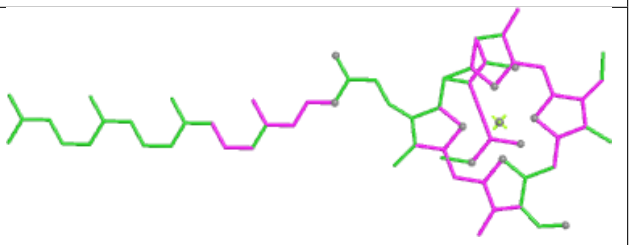
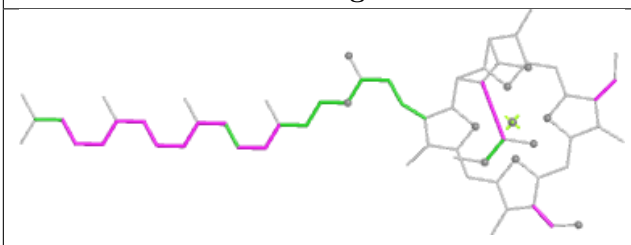


Bond angles



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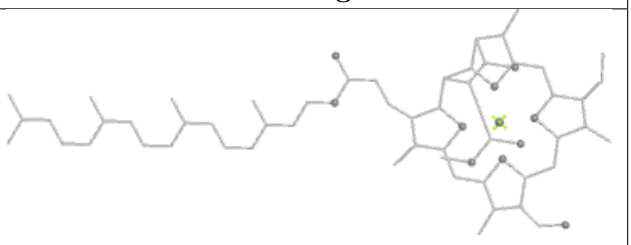
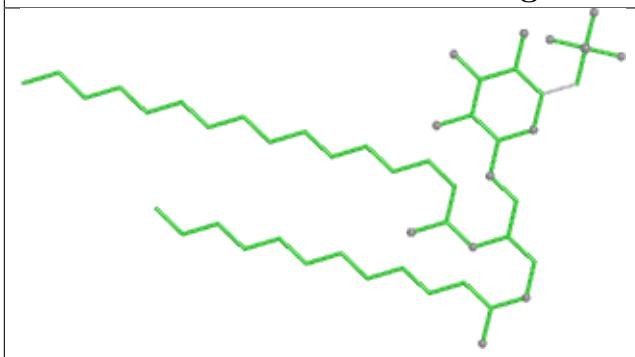


Rings

Ligand SQD 23 424



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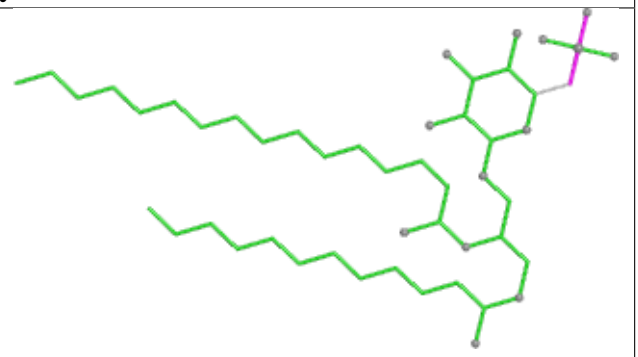
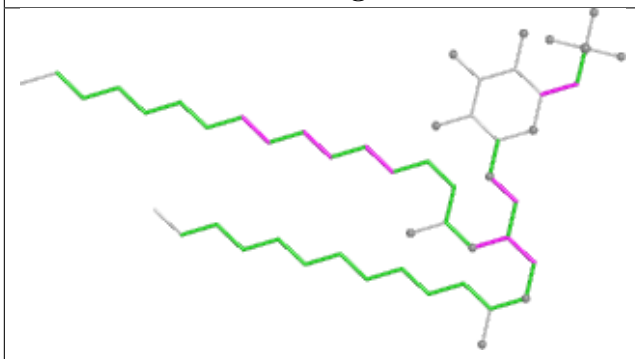
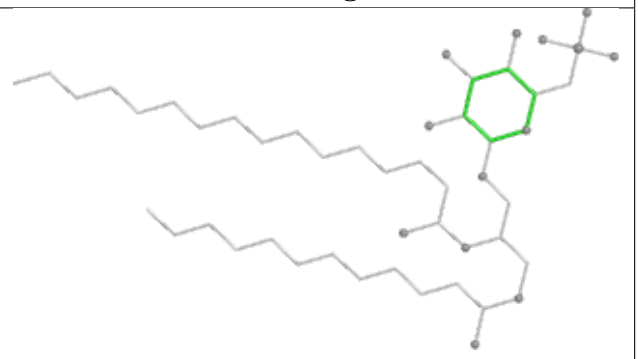


Bond angles

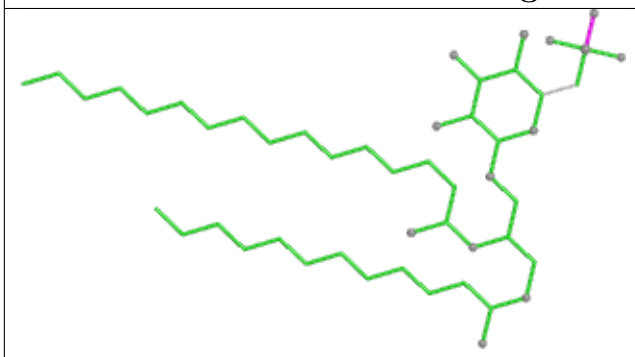


Torsions



Rings

Ligand SQD 12 521



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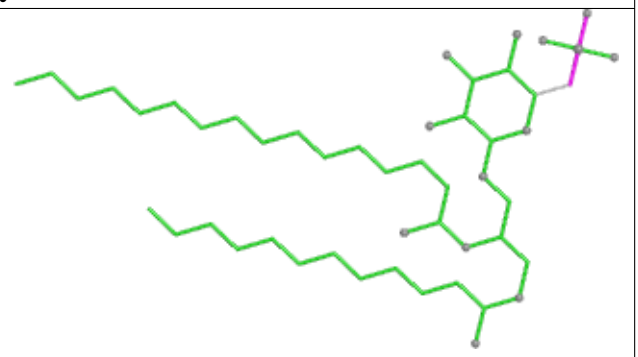
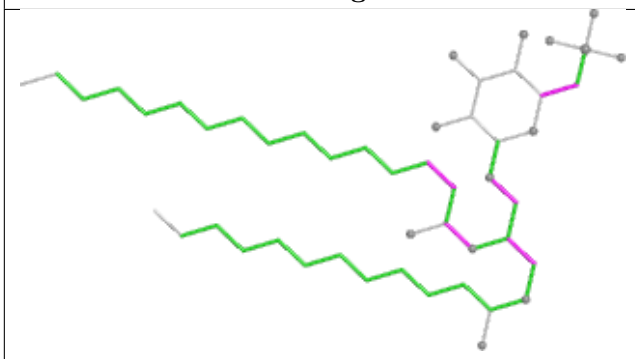


Bond angles



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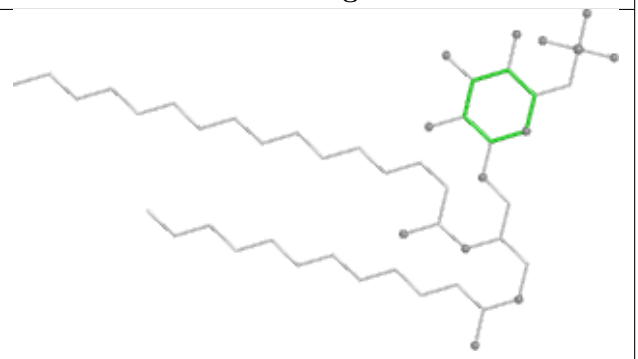
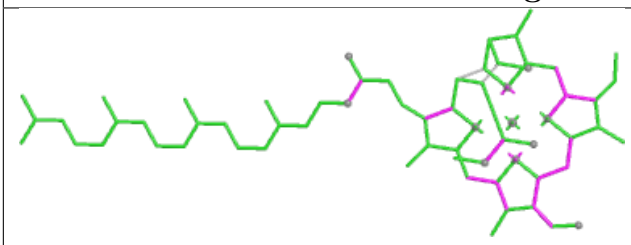


Rings

Ligand CL7 22 512



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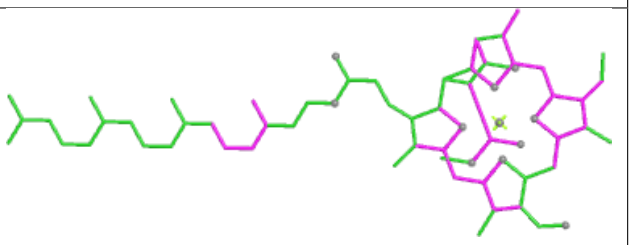

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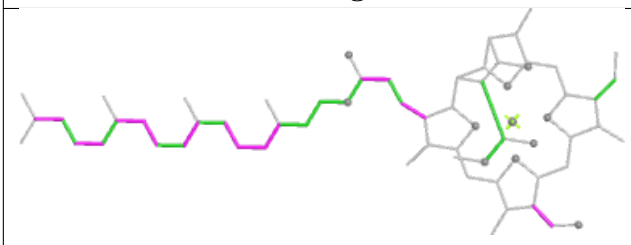

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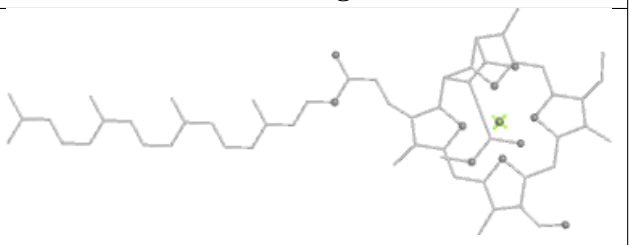

Rings

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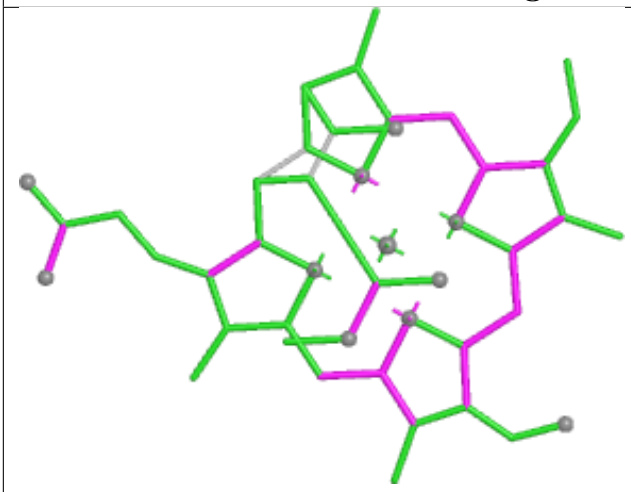

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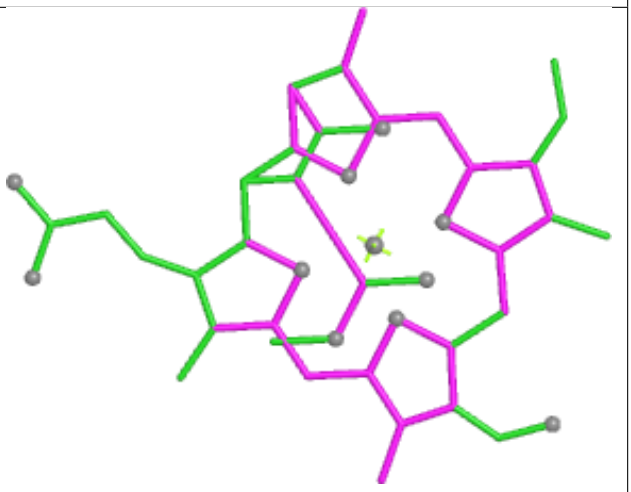

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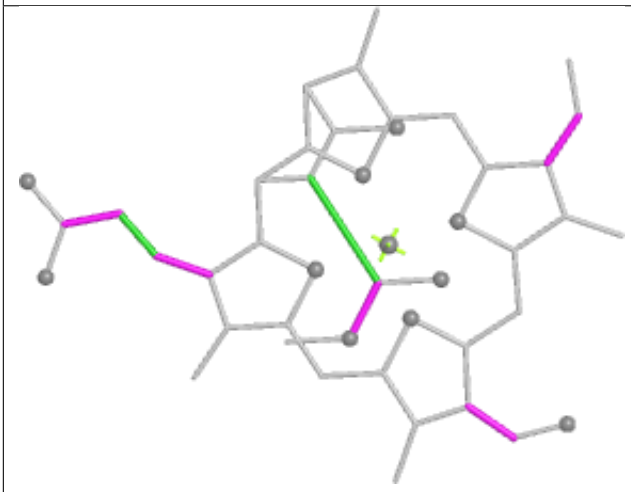
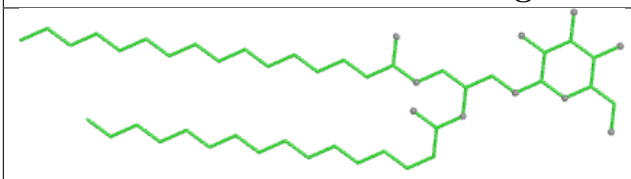


Torsions



Rings

Ligand LMG 41 401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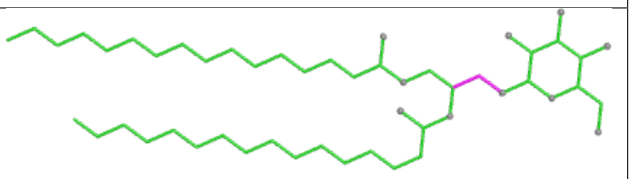
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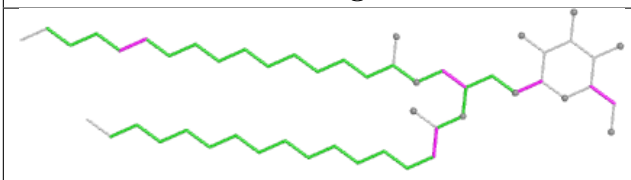
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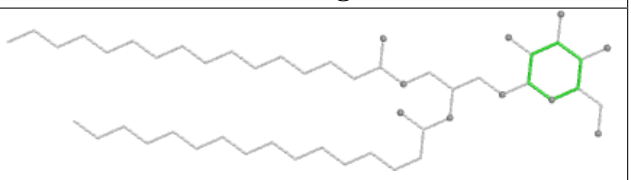
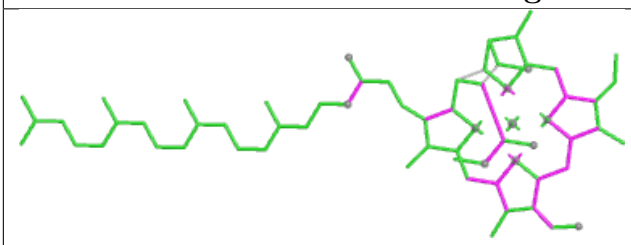

Rings

Ligand CL7 42 503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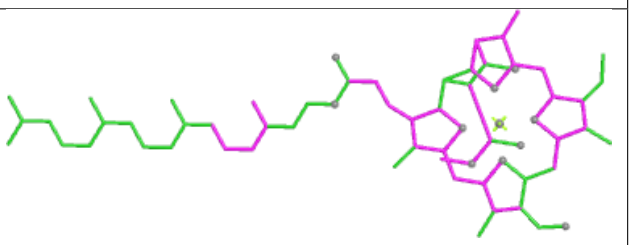
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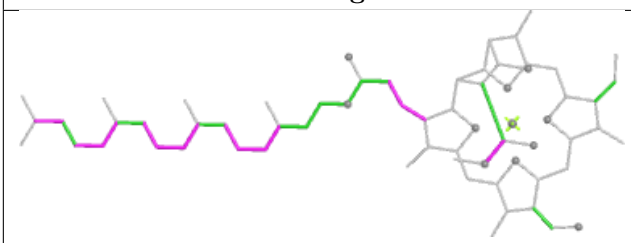
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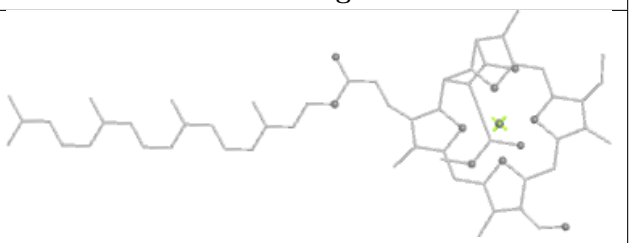
Rings

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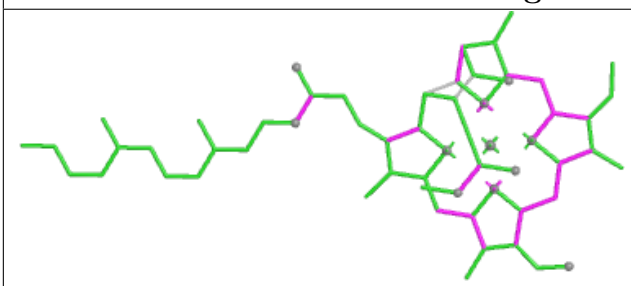
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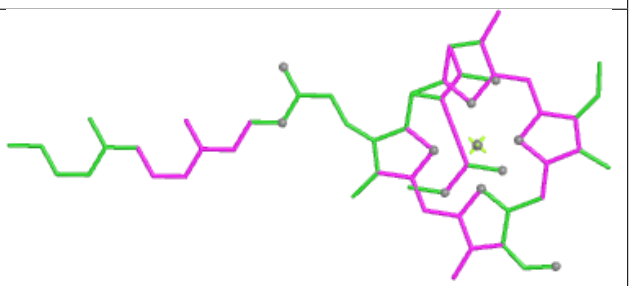
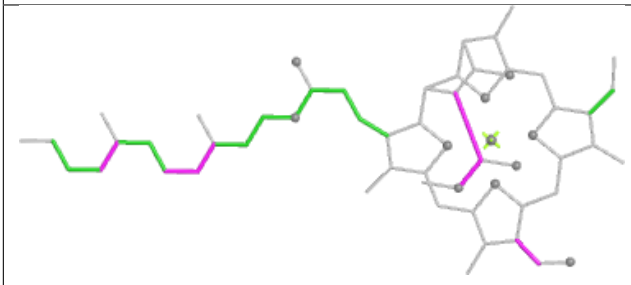

Bond angles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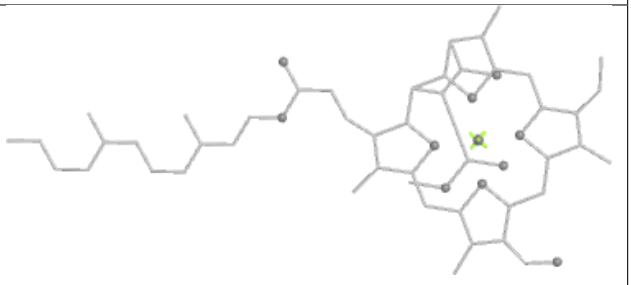
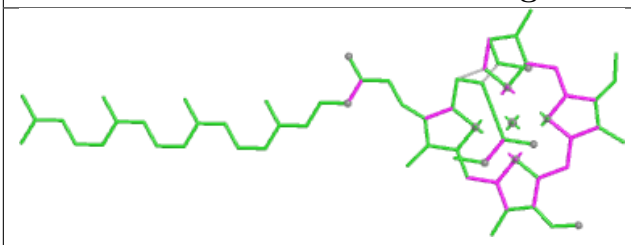

Rings

Ligand CL7 3B 603



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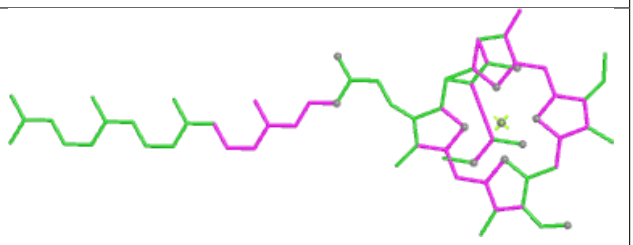
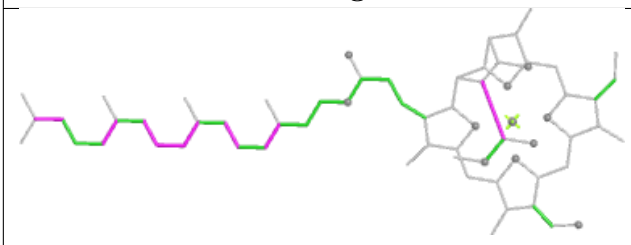


Bond angles



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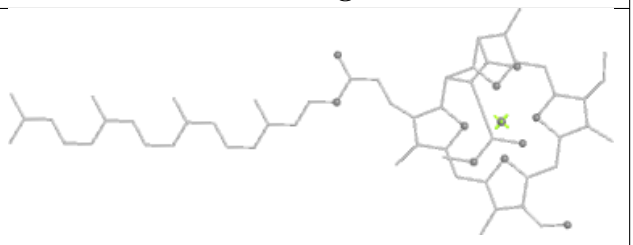
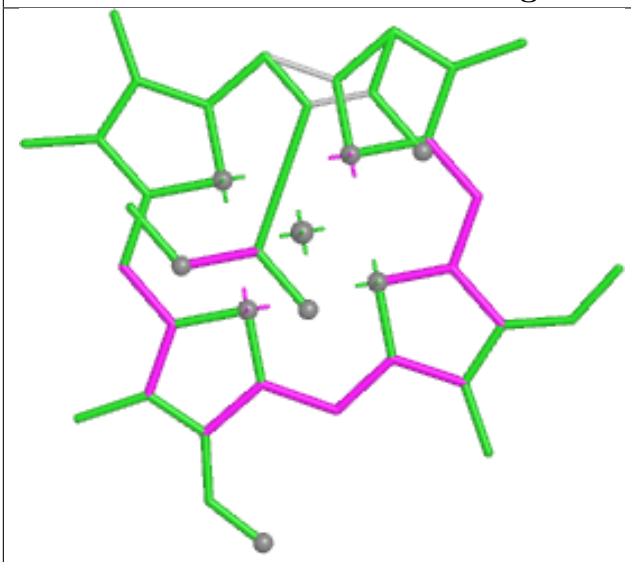


Rings

Ligand CL7 1C 517



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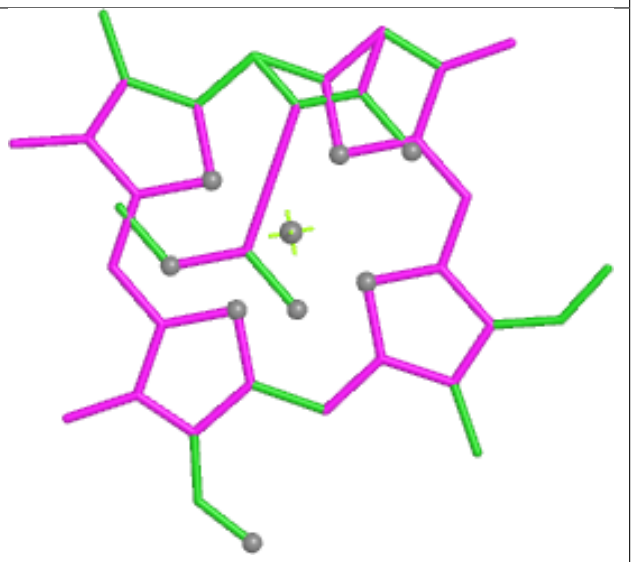

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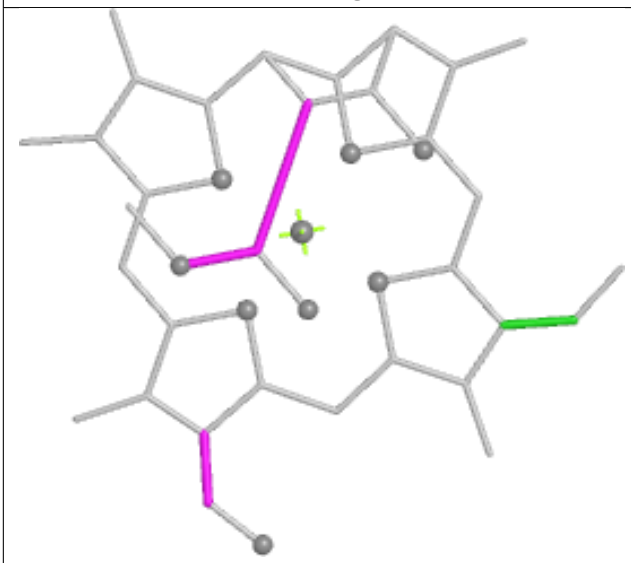

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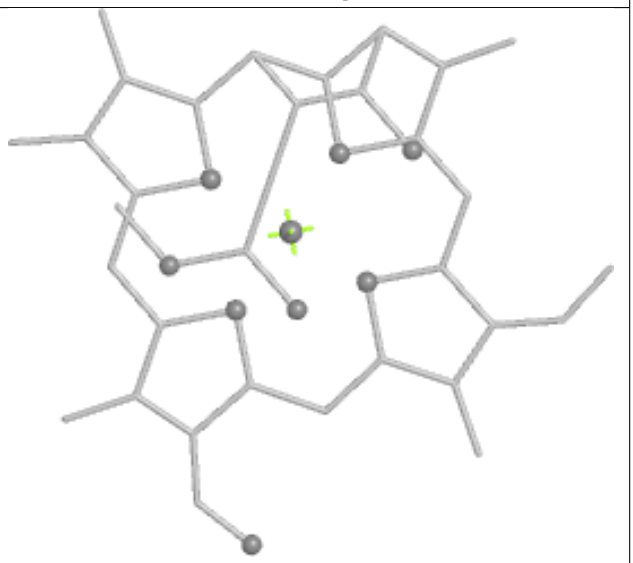
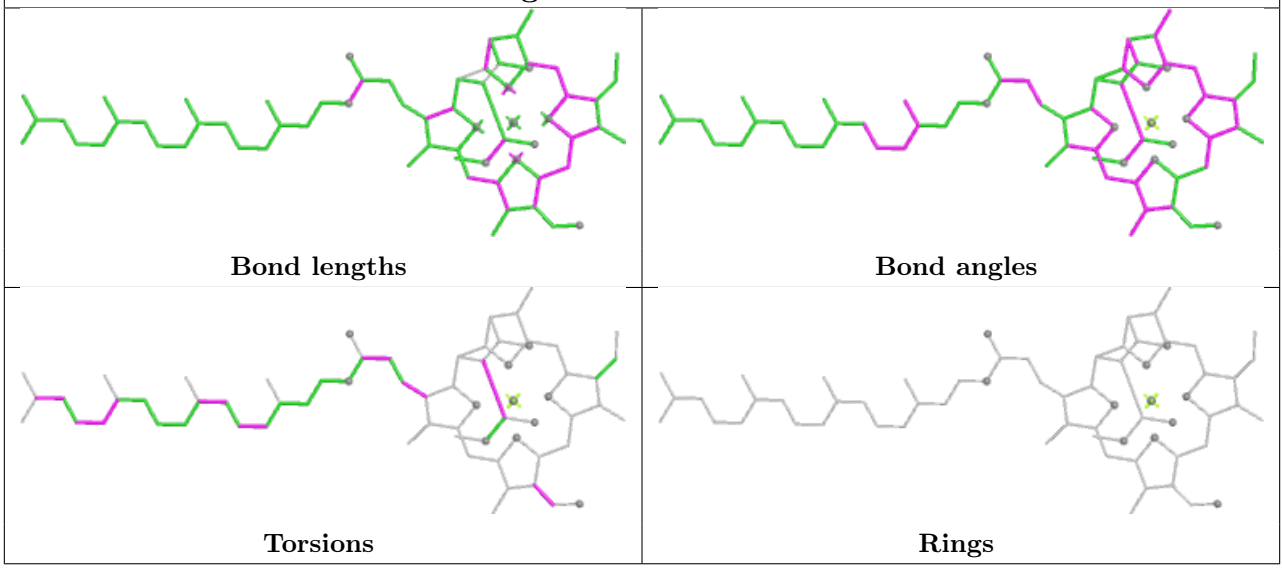


Rings

Ligand CL7 4B 610



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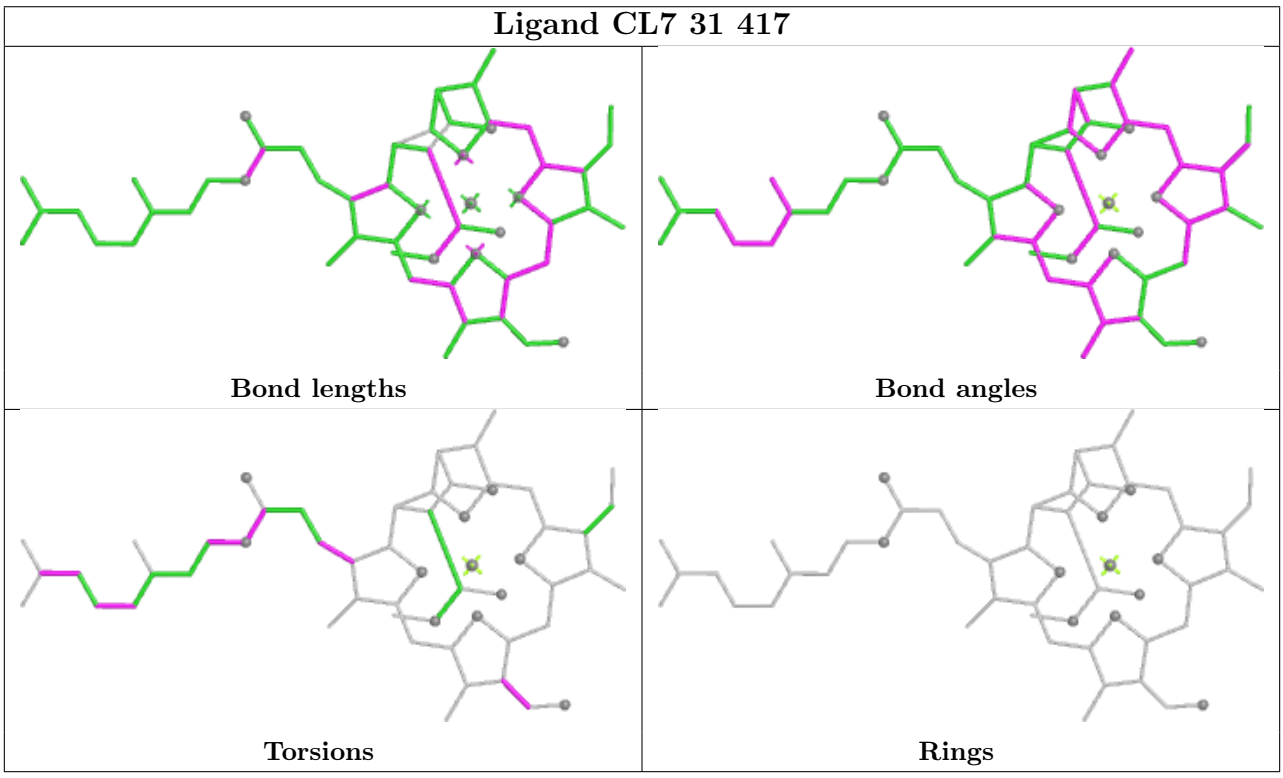

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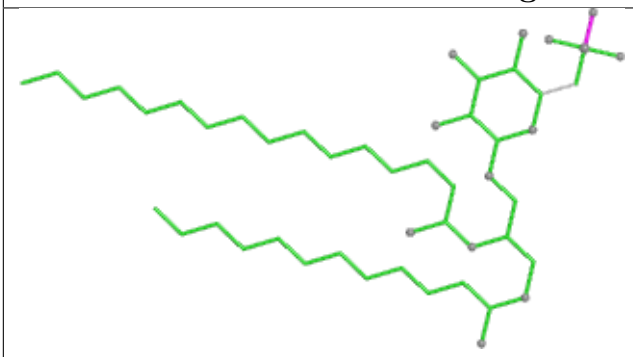

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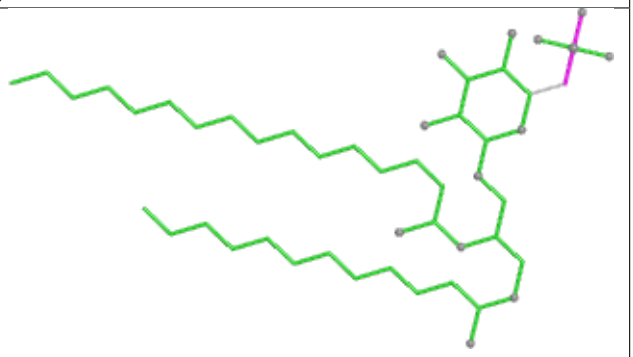
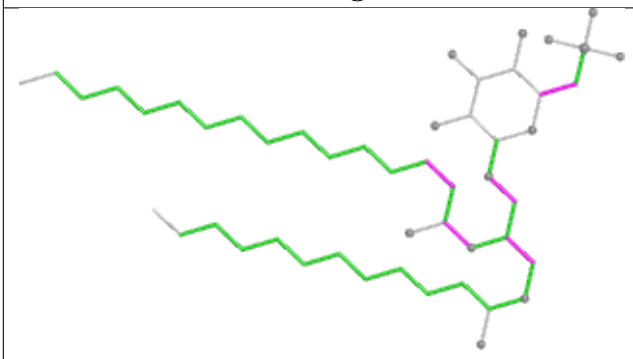


Bond angles



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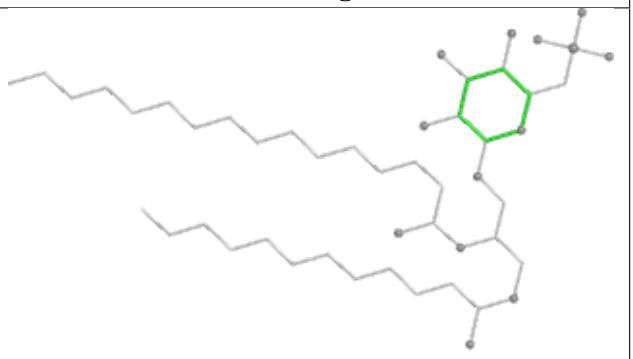

Rings

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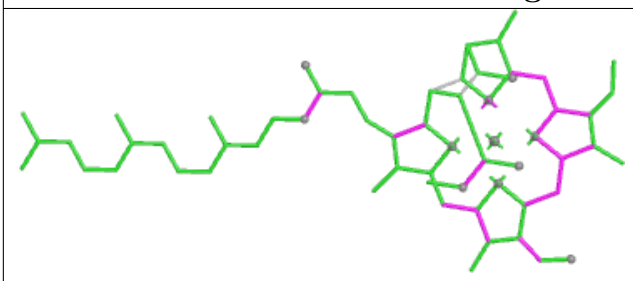

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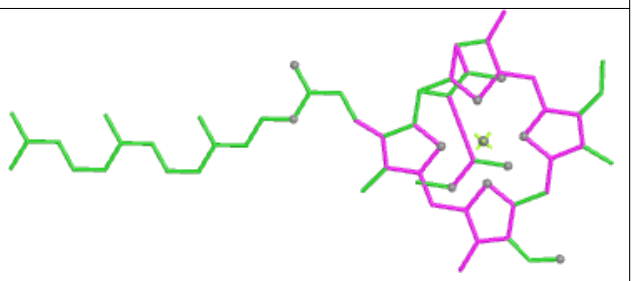
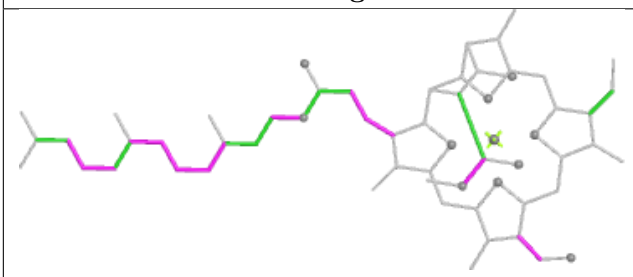


Bond angles



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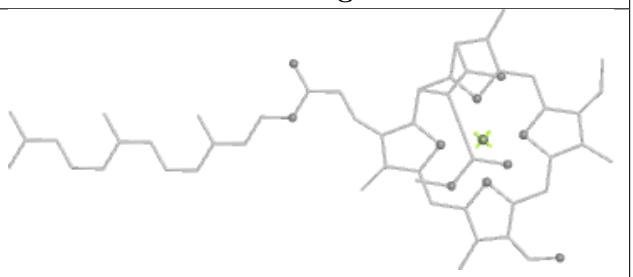
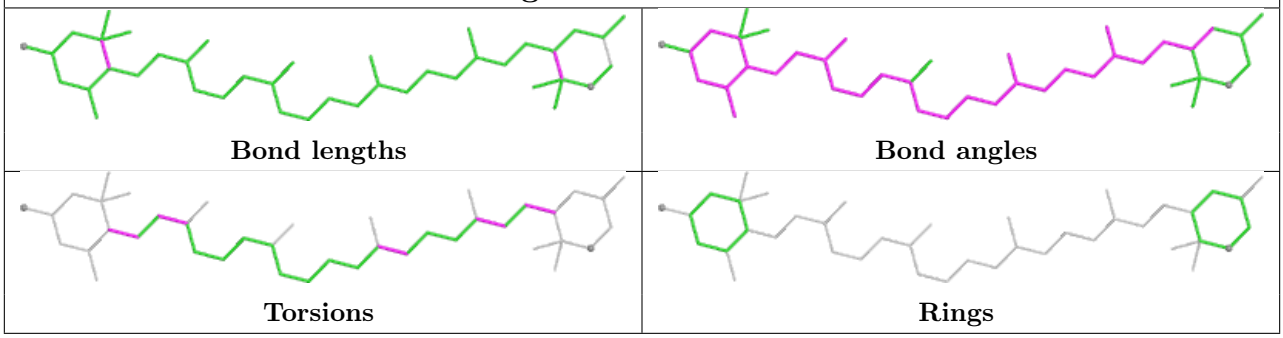


Rings

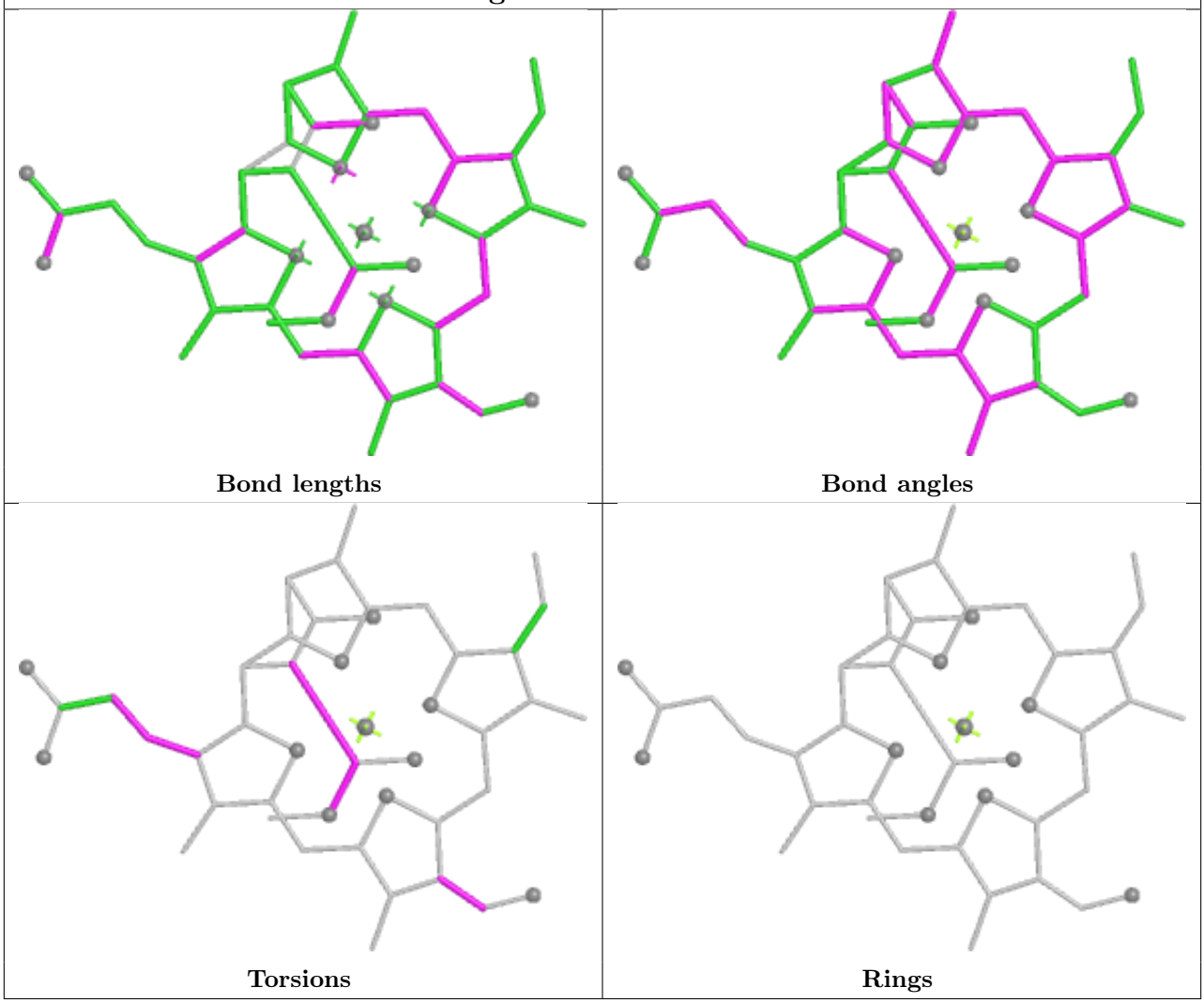
Ligand ZEX 13 520



Bond lengths | Bond angles

Torsions | Rings

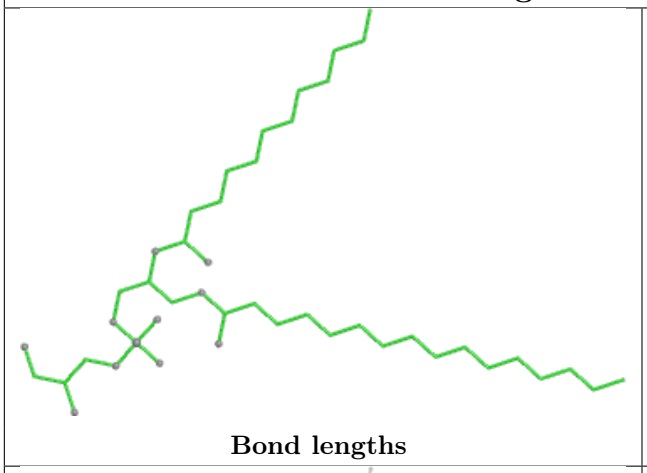
Ligand CL7 4C 513



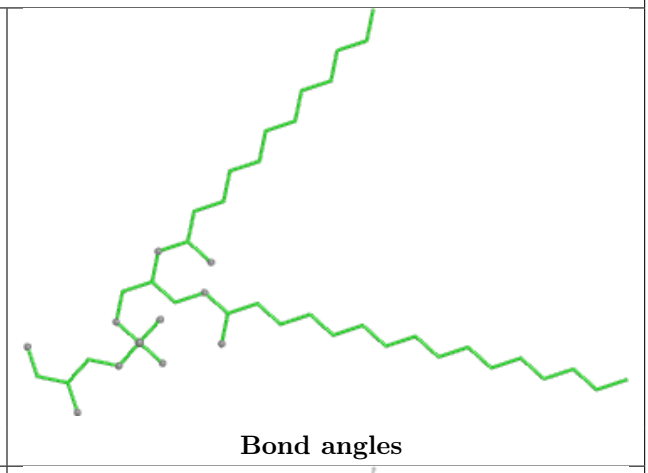
Bond lengths | Bond angles

Torsions | Rings

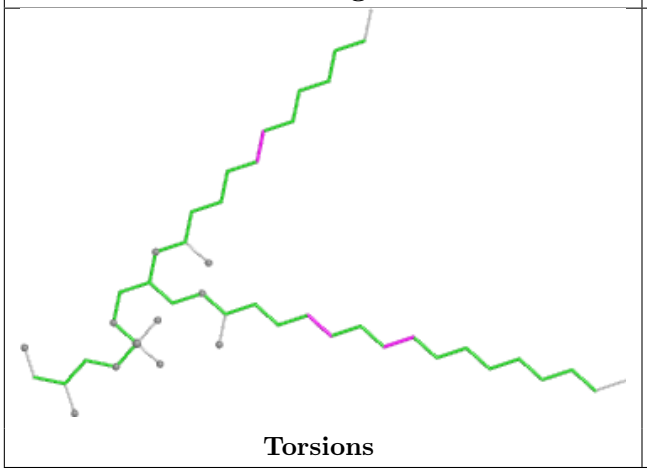
Ligand LHG 2B 624



Bond lengths



Bond angles



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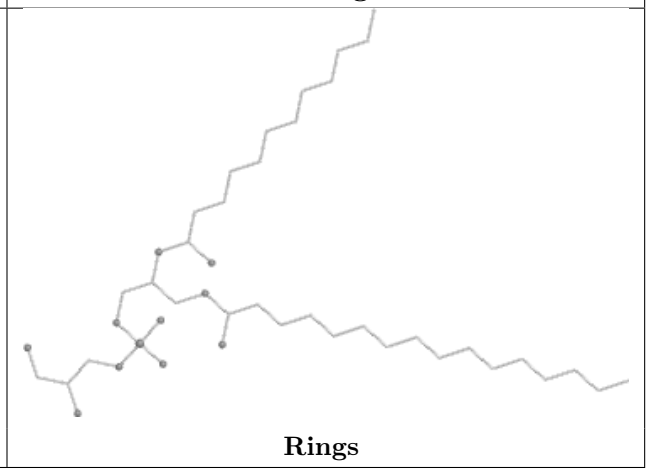
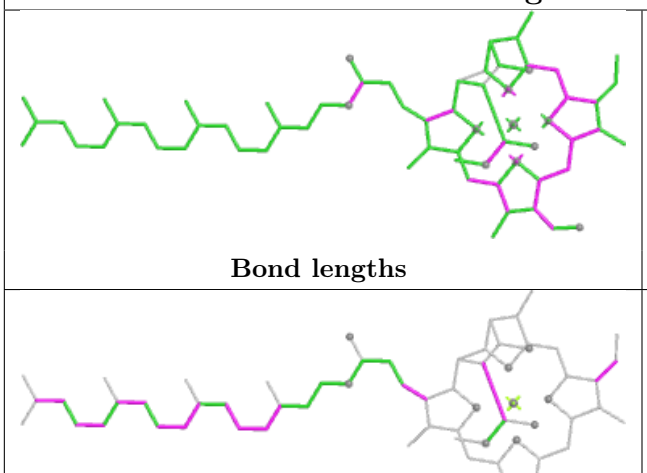
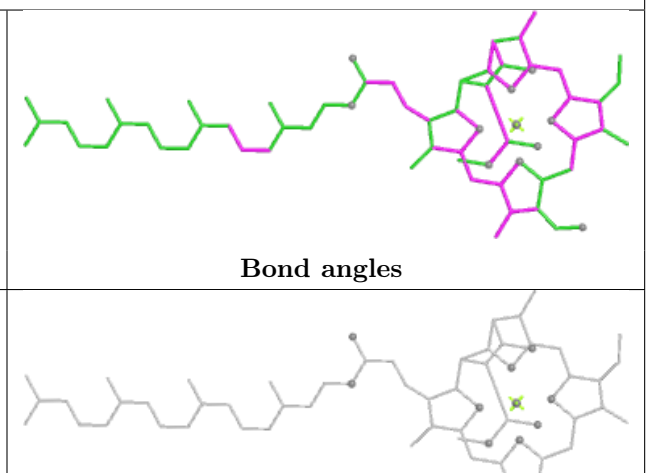


Rings

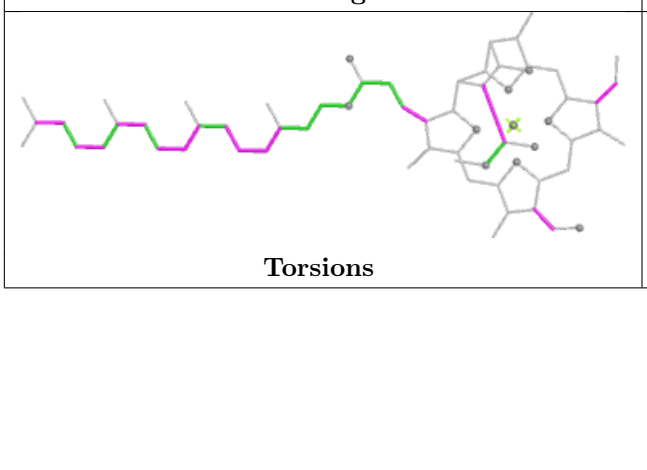
Ligand CL7 13 504



Bond lengths



Bond angles



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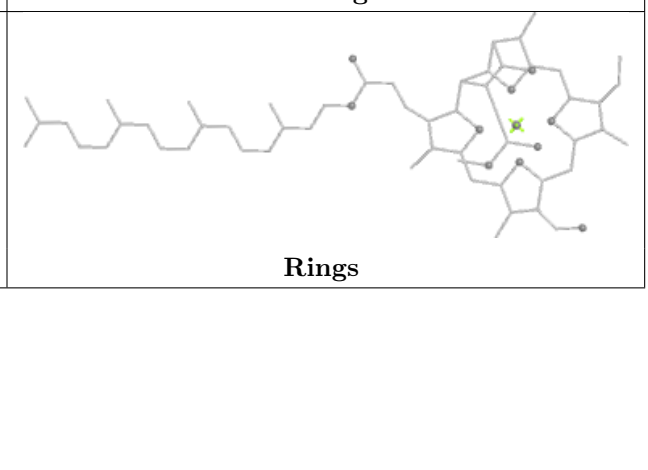
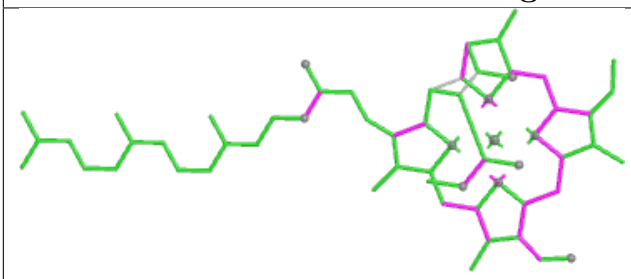


Rings

Ligand CL7 1B 602



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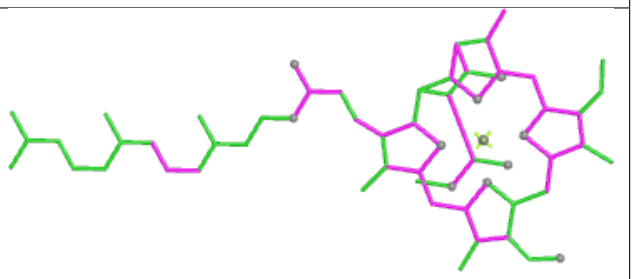
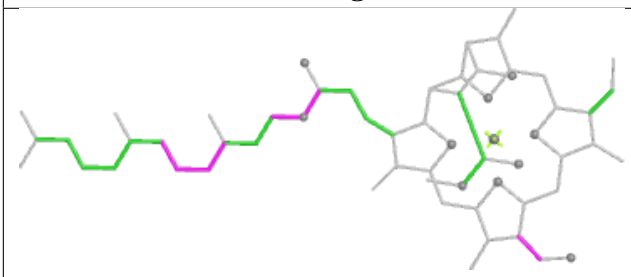


Bond angles



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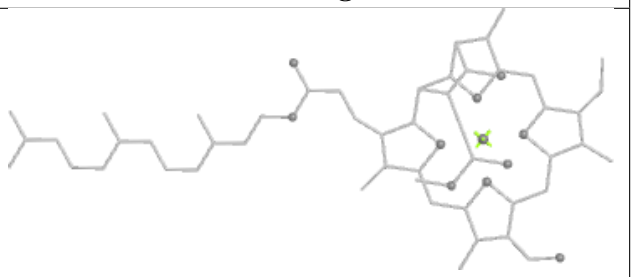
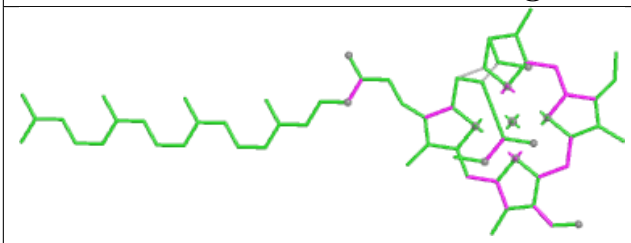


Rings

Ligand CL7 11 404



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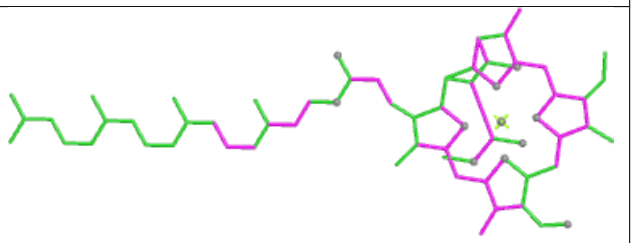
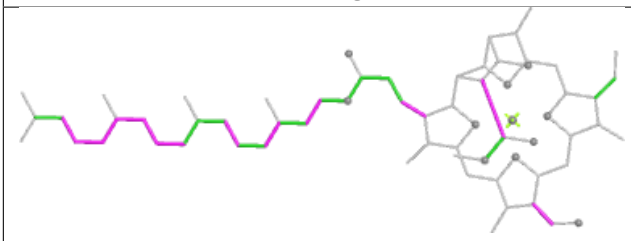
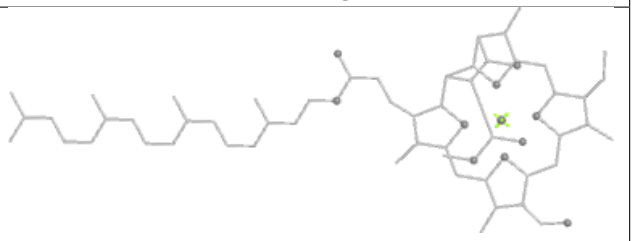


Bond angles



Torsions

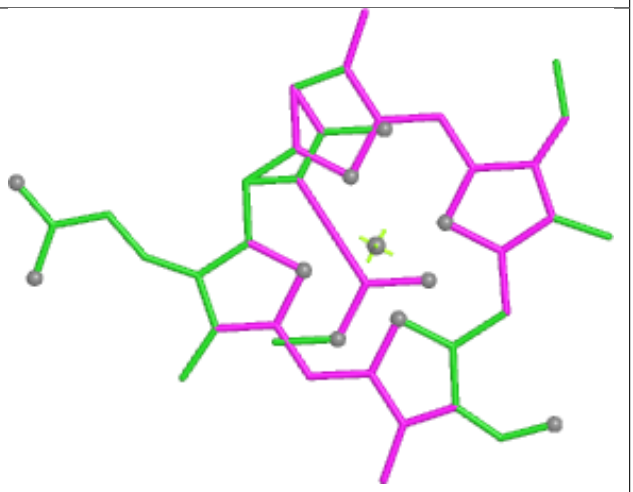


Rings

Ligand CL7 13 514



Bond lengths



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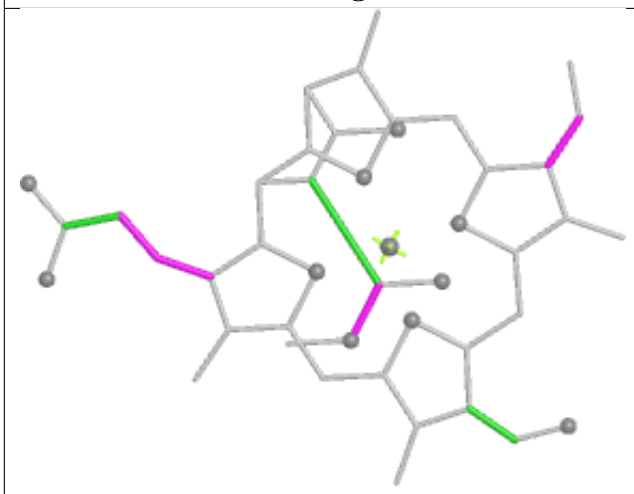
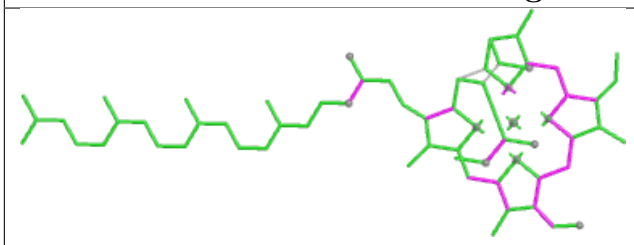


Torsions



Rings

Ligand CL7 14 412



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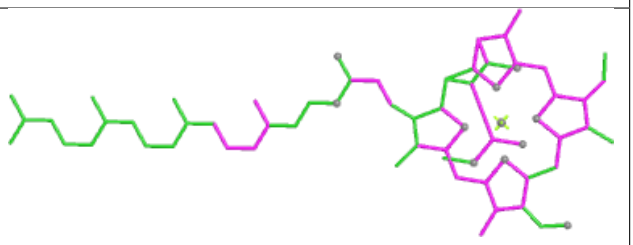

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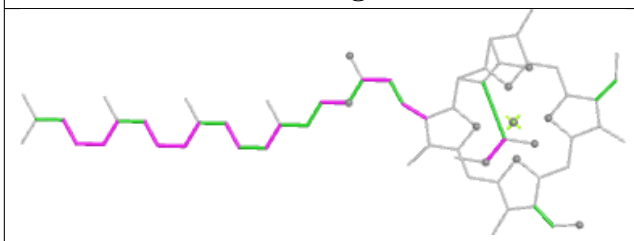

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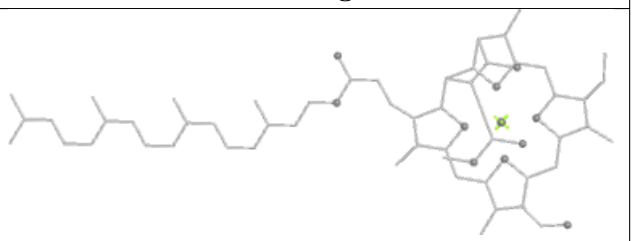
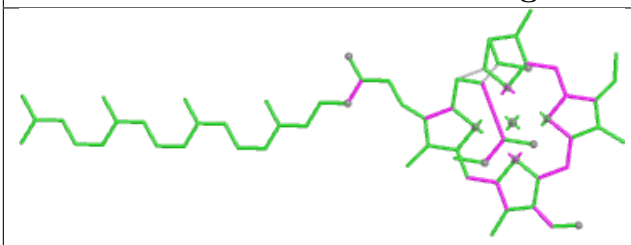


Rings

Ligand CL7 2C 503



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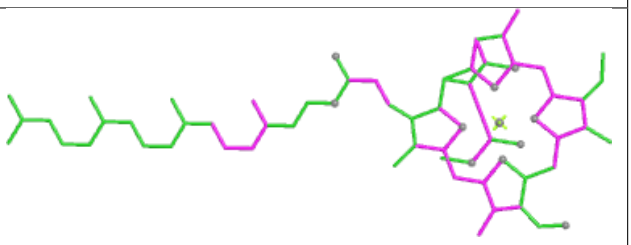

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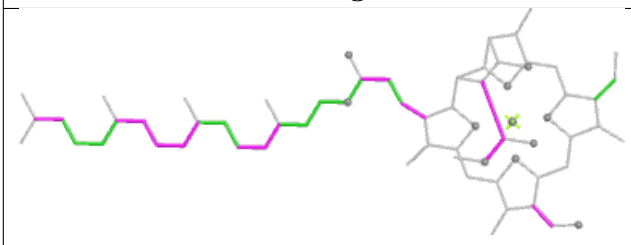

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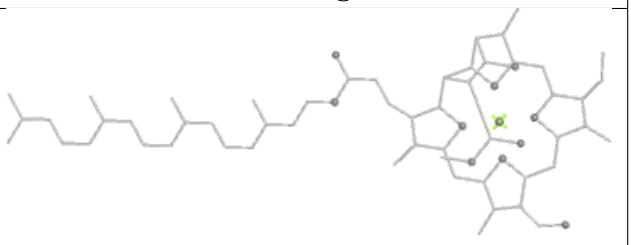
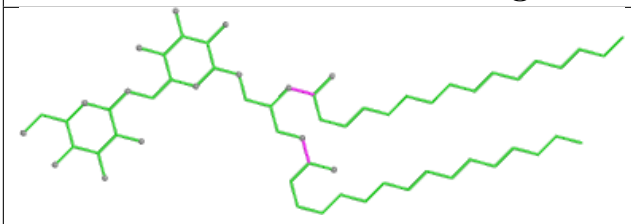


Rings

Ligand DGD 4B 625



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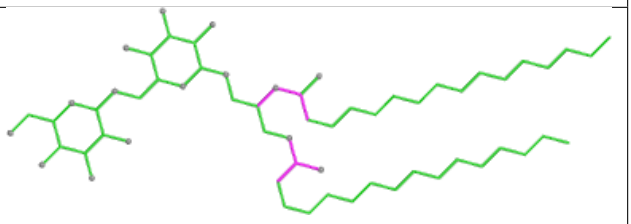

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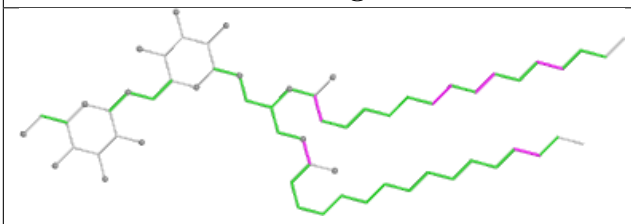

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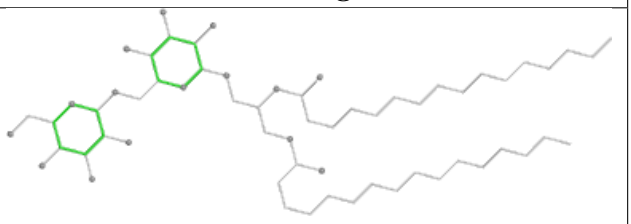
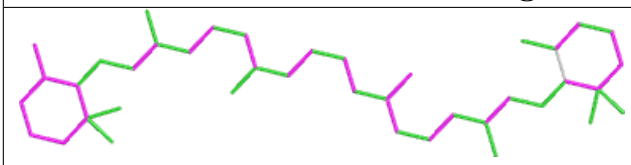


Rings

Ligand 8CT 1B 618



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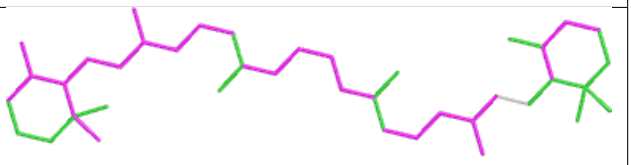

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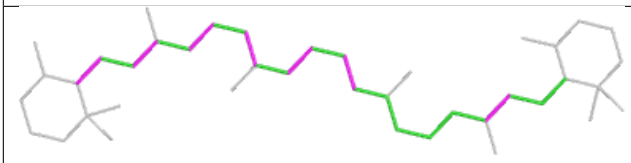

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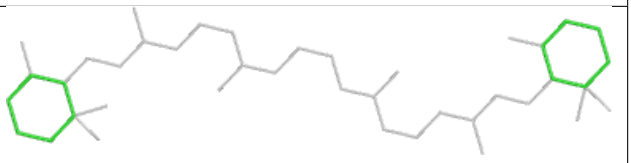
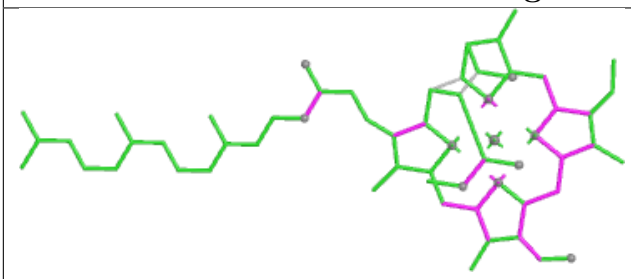


Rings

Ligand CL7 24 413



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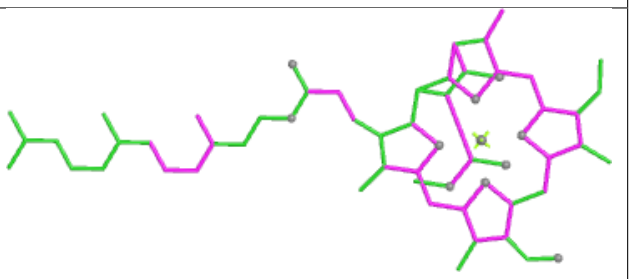

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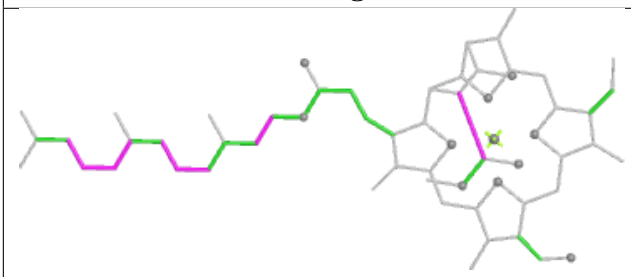

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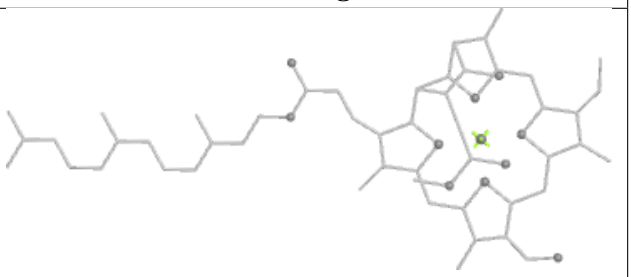

Rings

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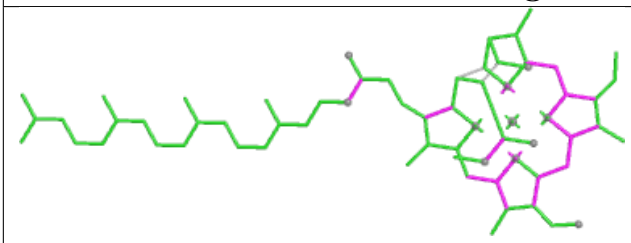

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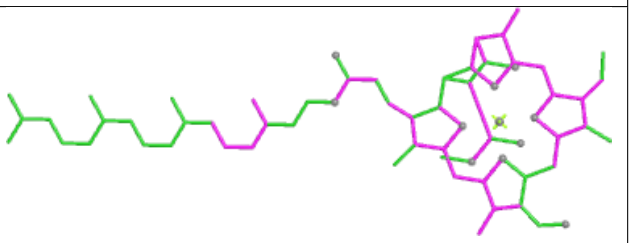

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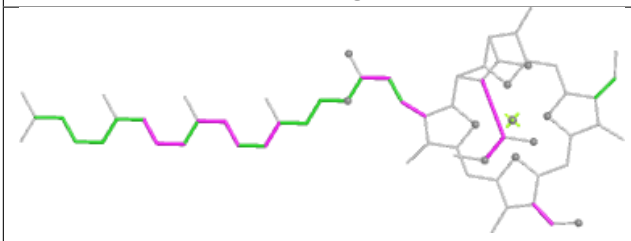

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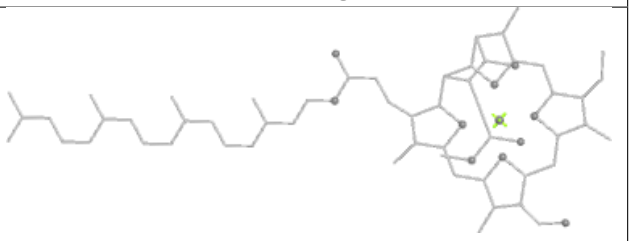

Rings

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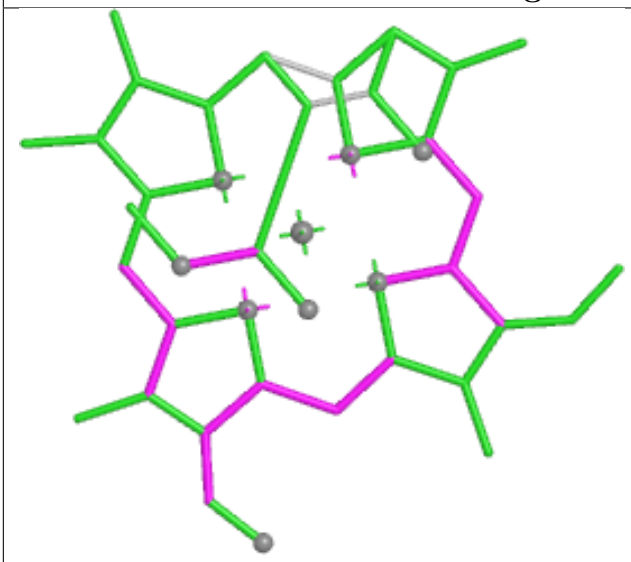

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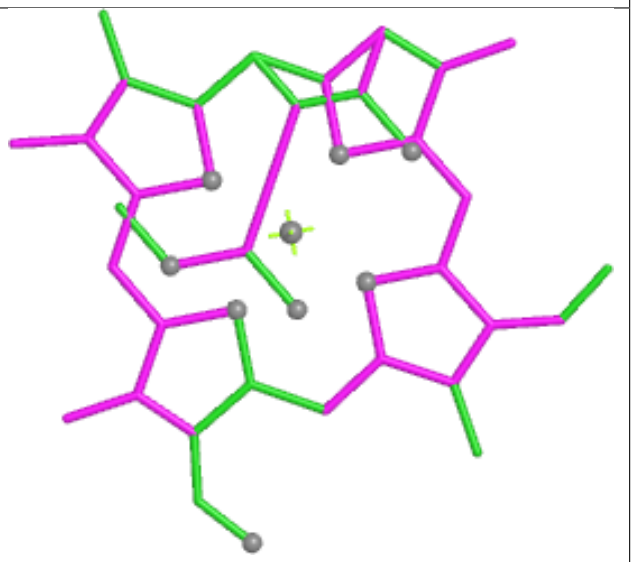

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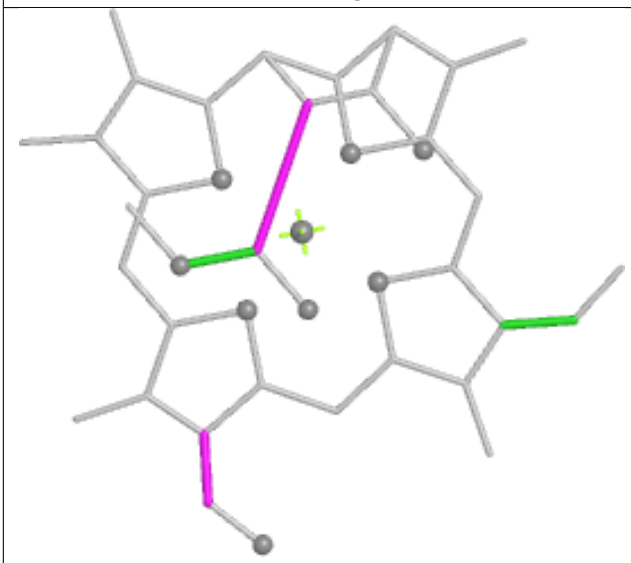

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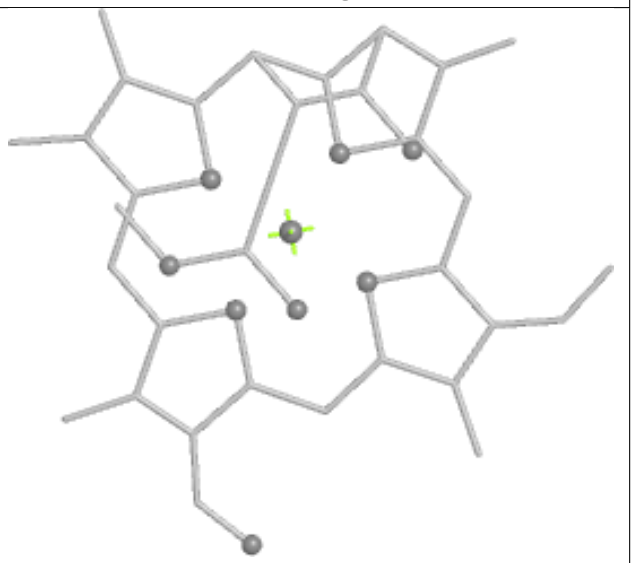
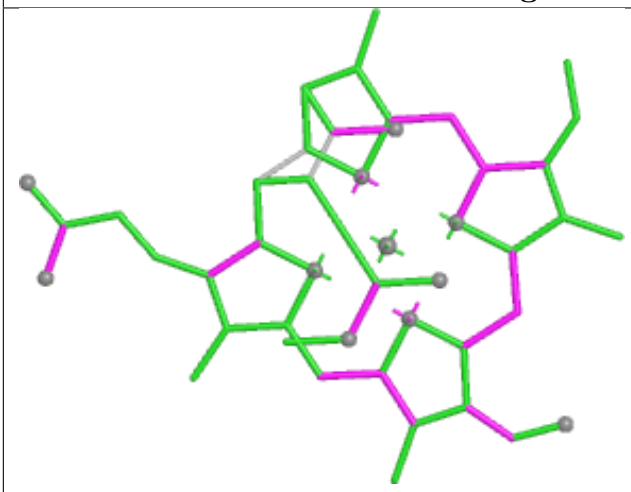


Rings

Ligand CL7 3B 622



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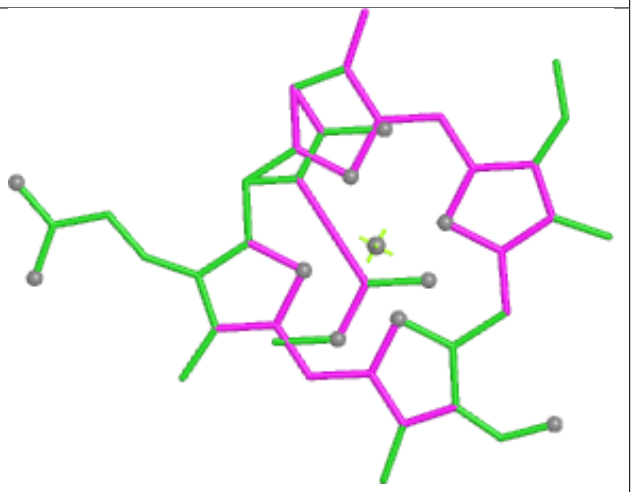

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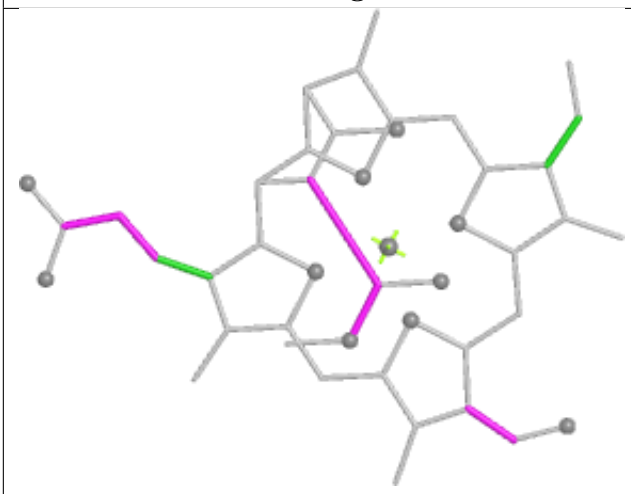
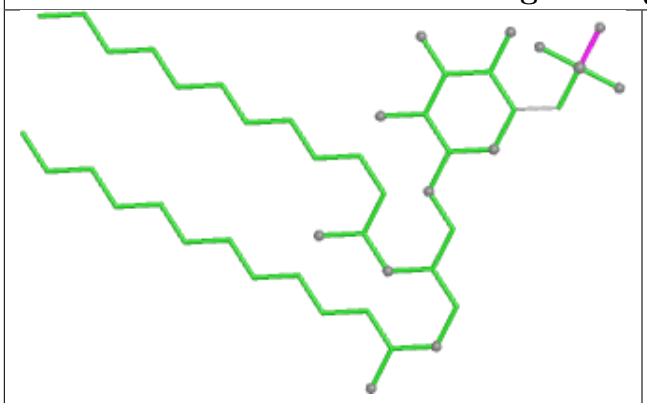


Torsions



Rings

Ligand SQD 13 521



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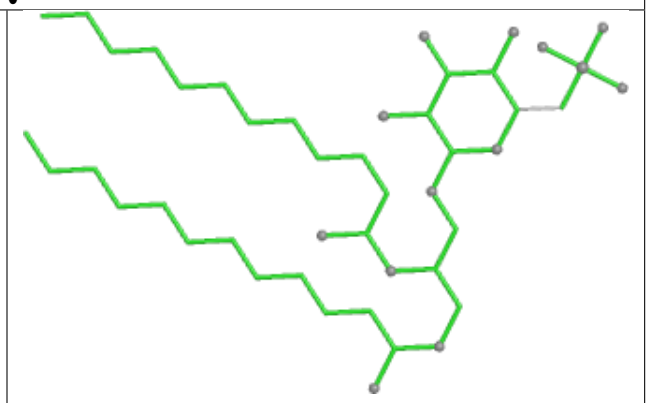

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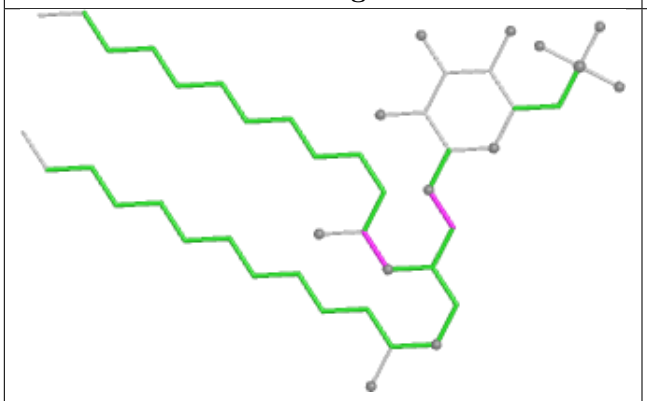

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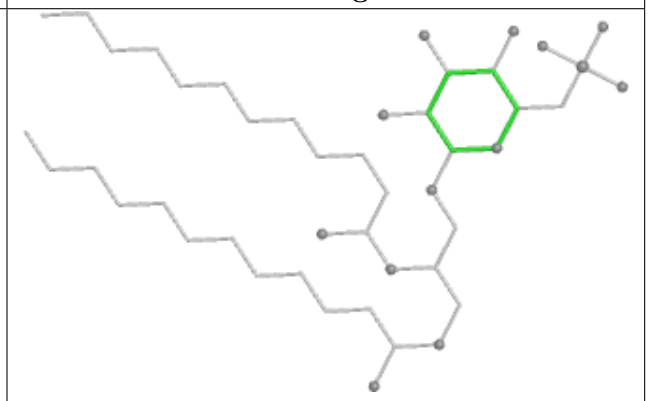

Rings

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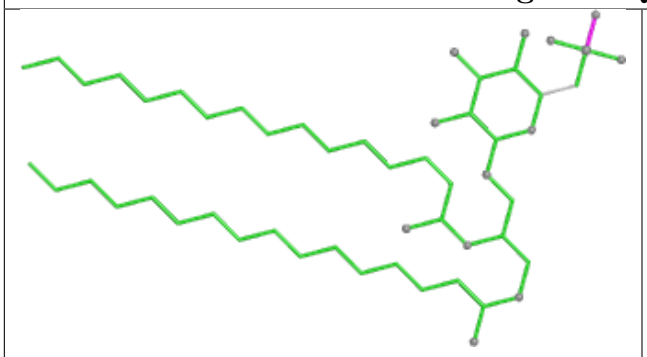

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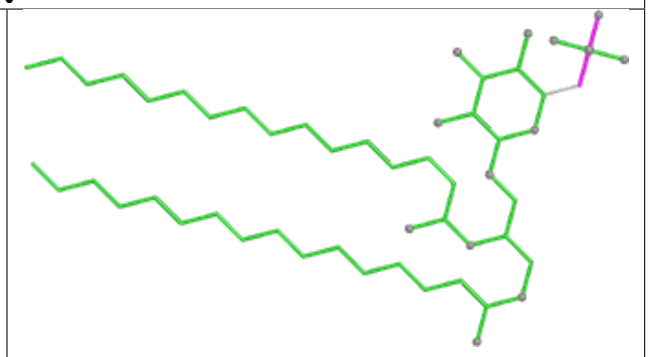

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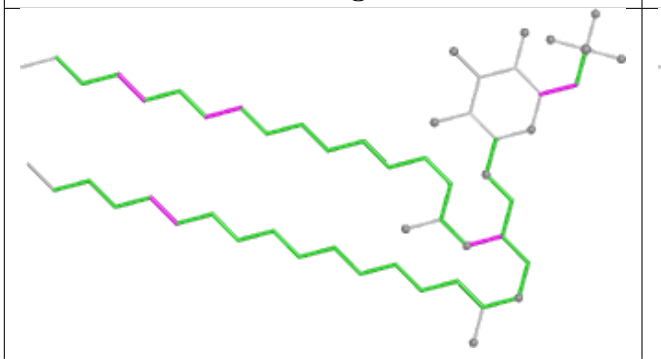

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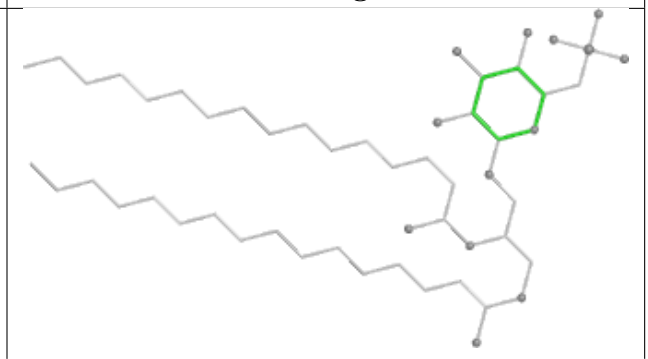

Rings

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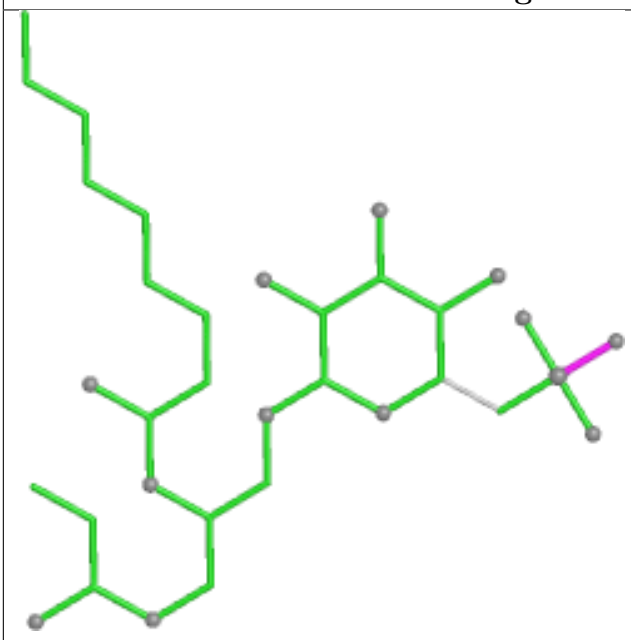

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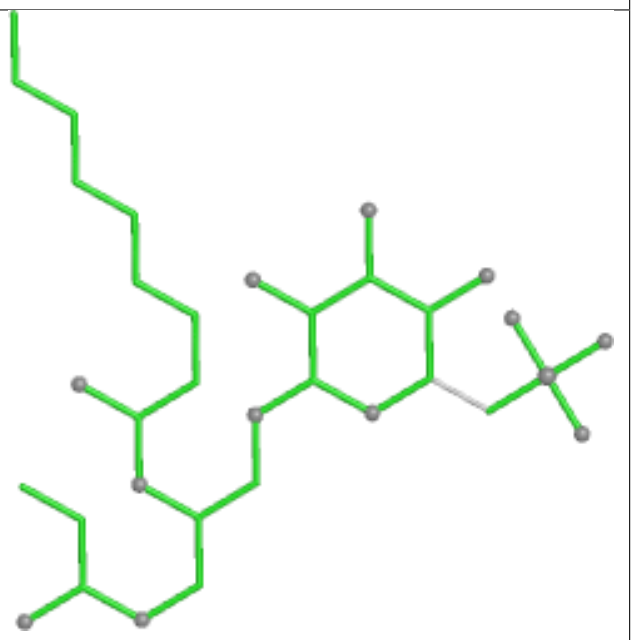

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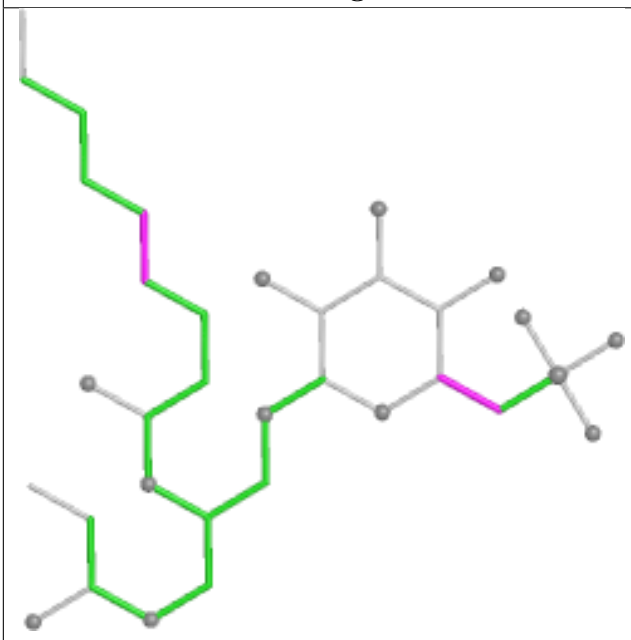

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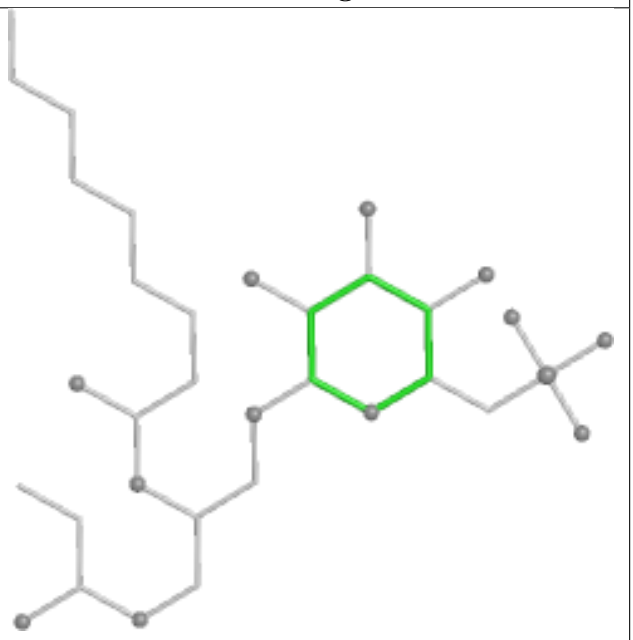
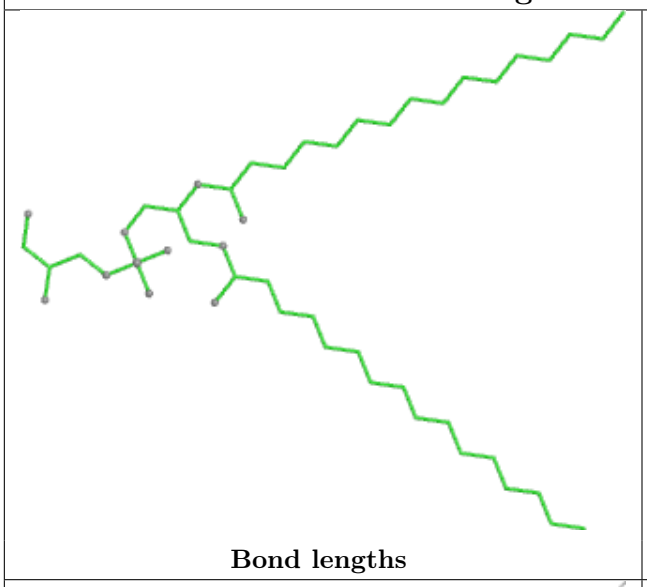


Rings

Ligand LHG 1B 625



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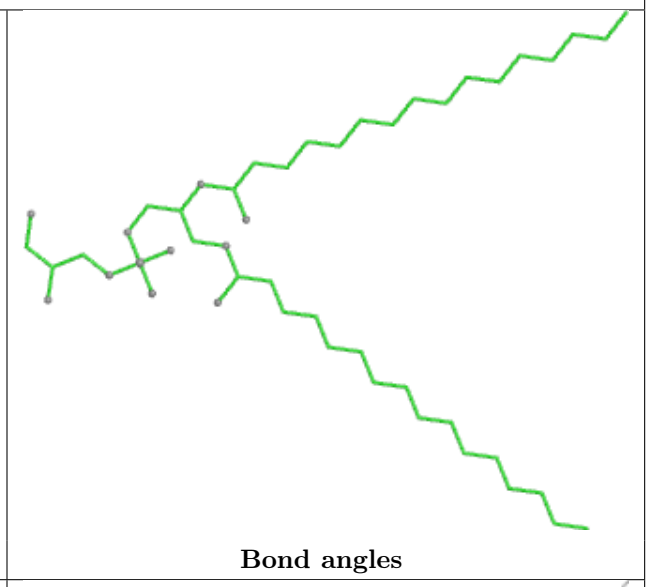
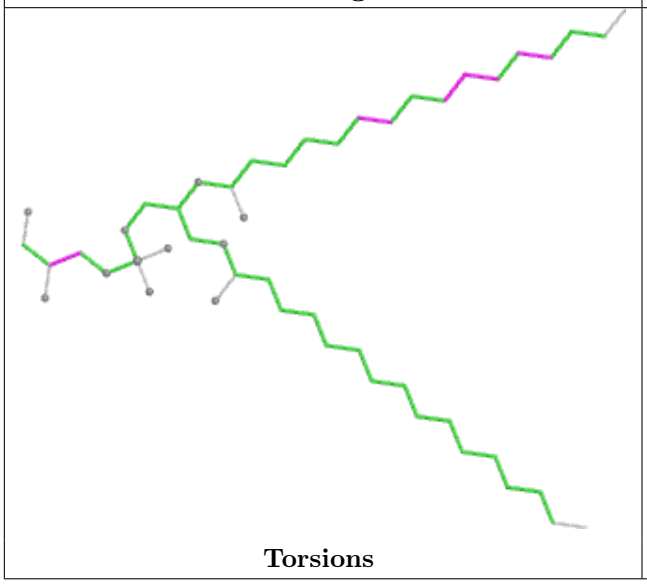


Bond angles



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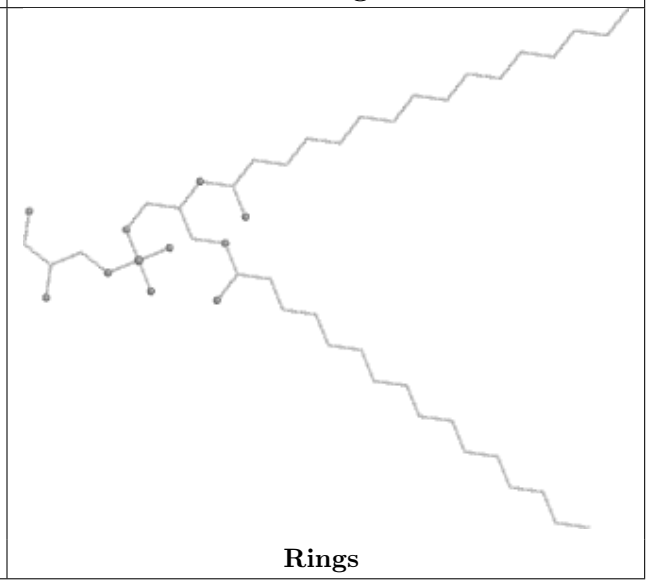
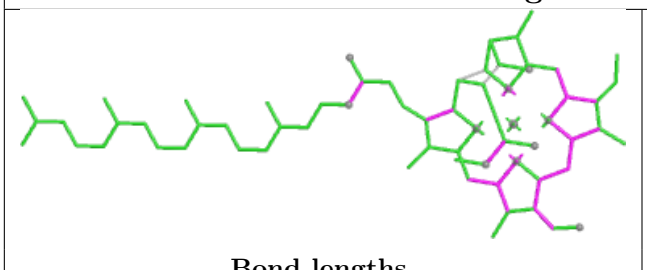


Rings

Ligand CL7 23 406



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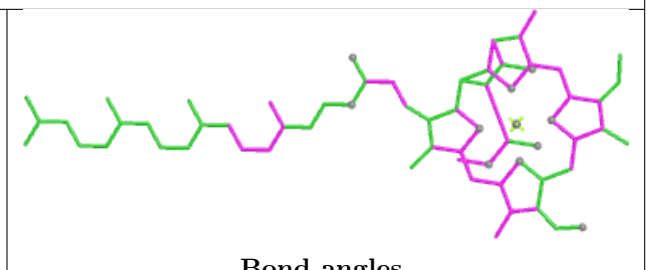
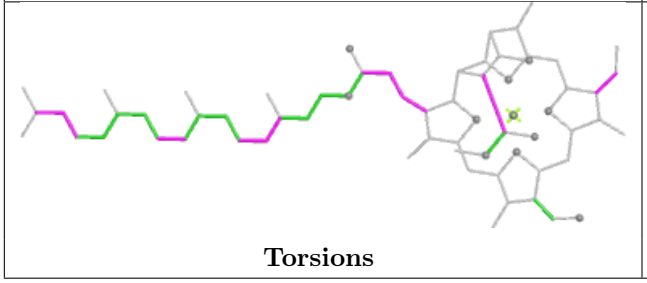


Bond angles



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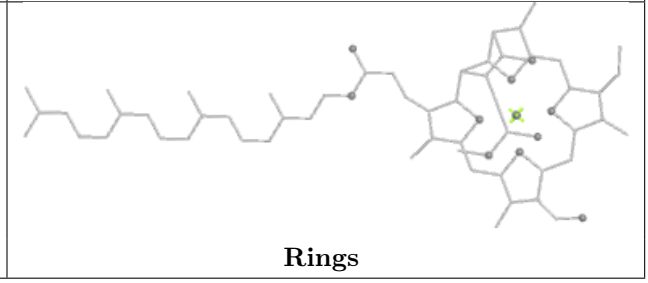
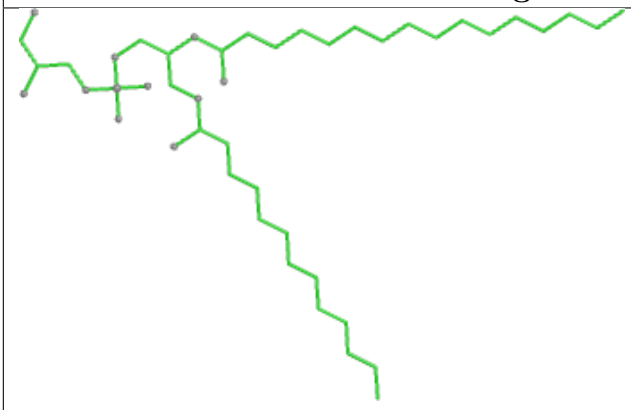


Rings

Ligand LHG 2A 408



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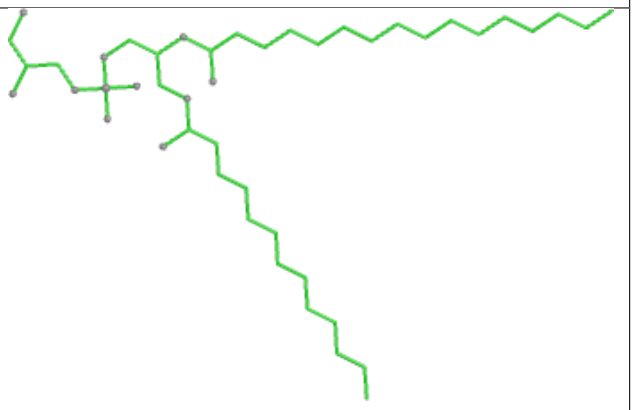
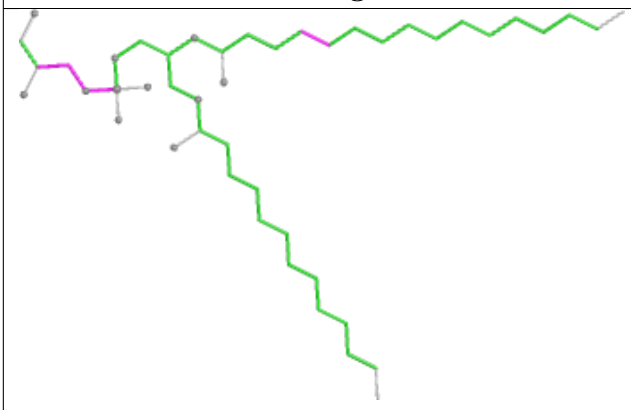
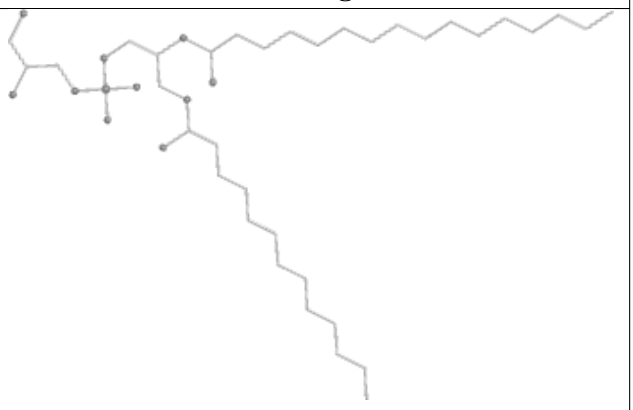


Bond angles

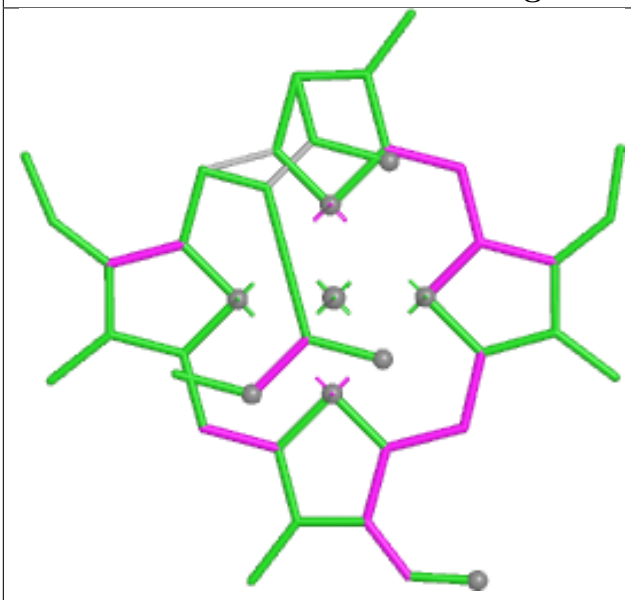


Torsions

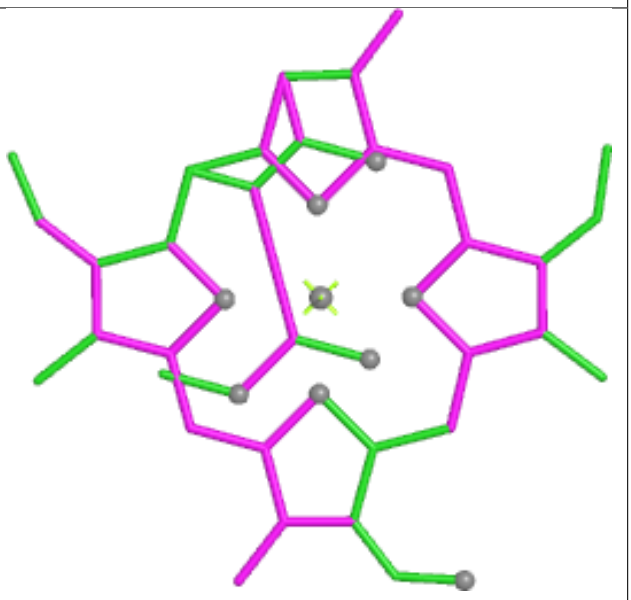


Rings

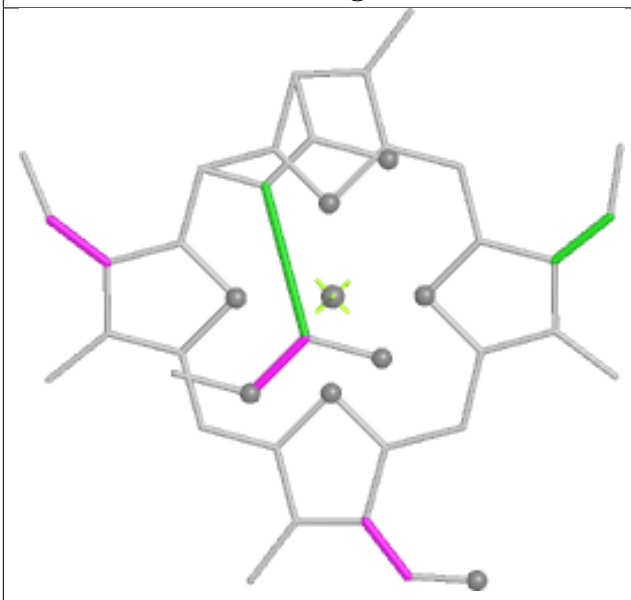
Ligand CL7 24 417



Bond lengths



Bond angles



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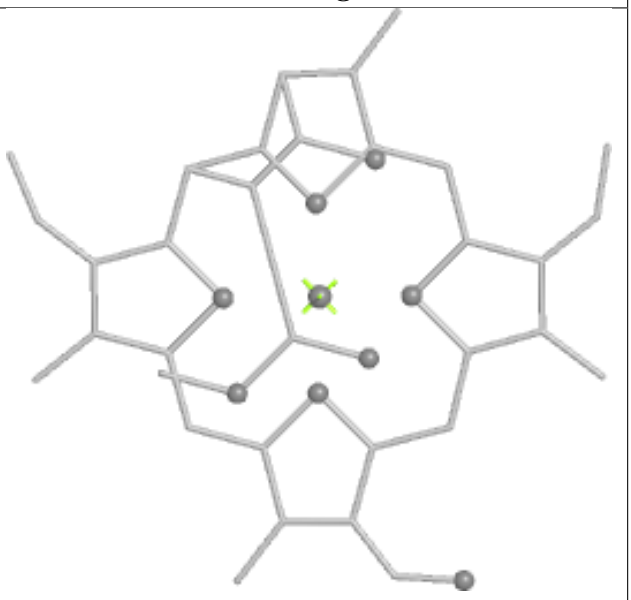
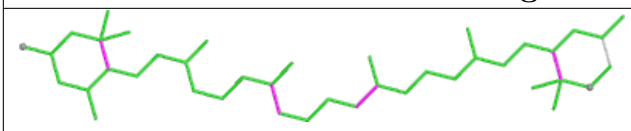


Rings

Ligand ZEX 24 403



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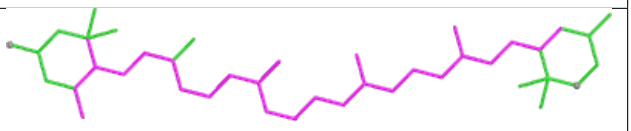
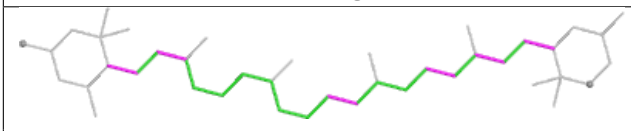


Bond angles



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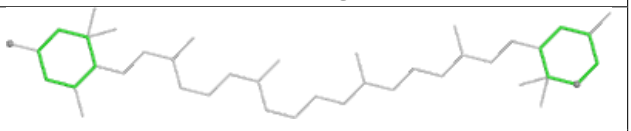
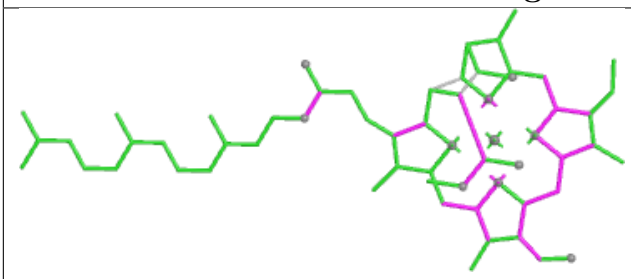


Rings

Ligand CL7 14 413



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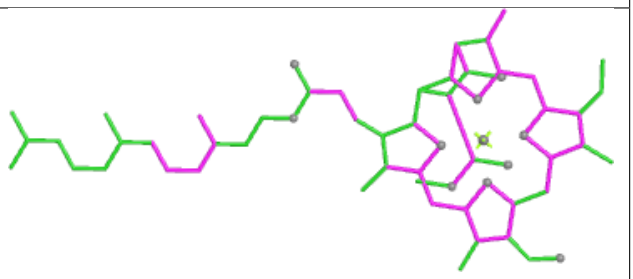
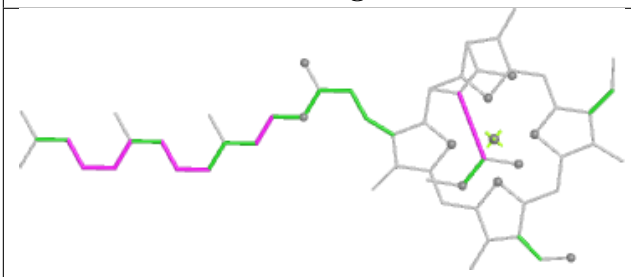


Bond angles



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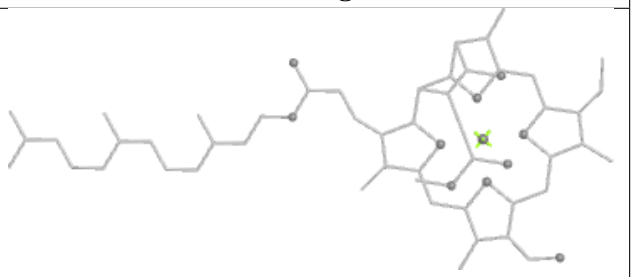
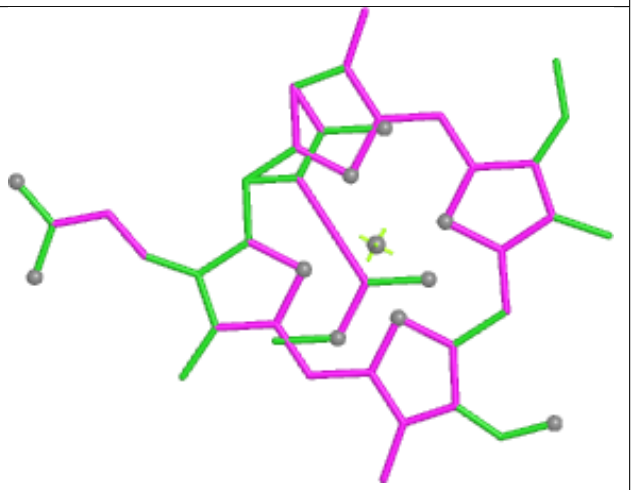


Rings

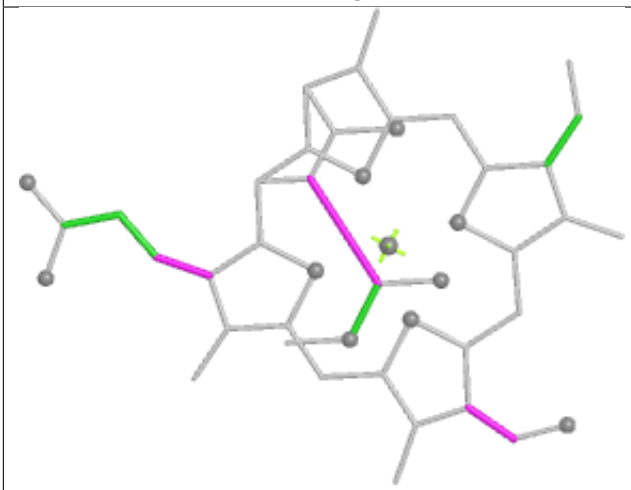
Ligand CL7 42 515



Bond lengths



Bond angles

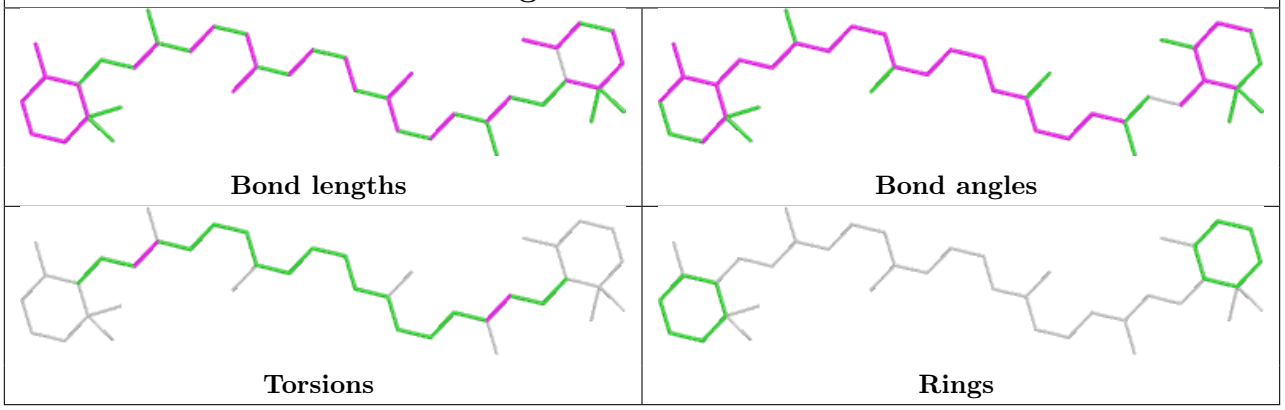


Torsions



Rings

Ligand 8CT 4B 620



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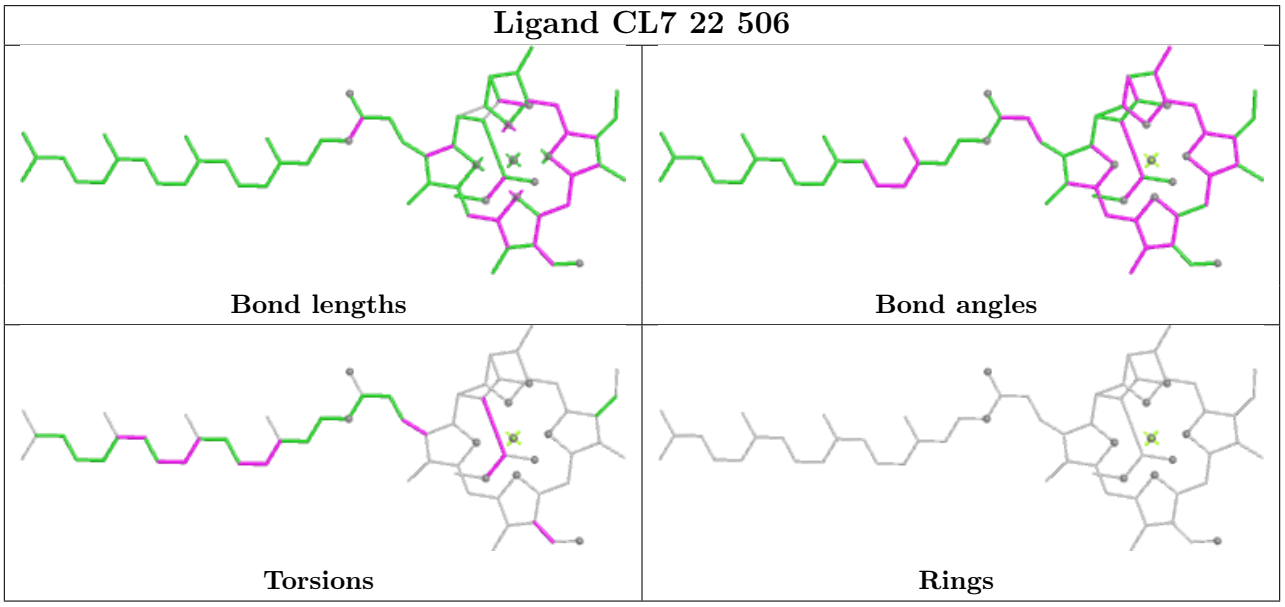

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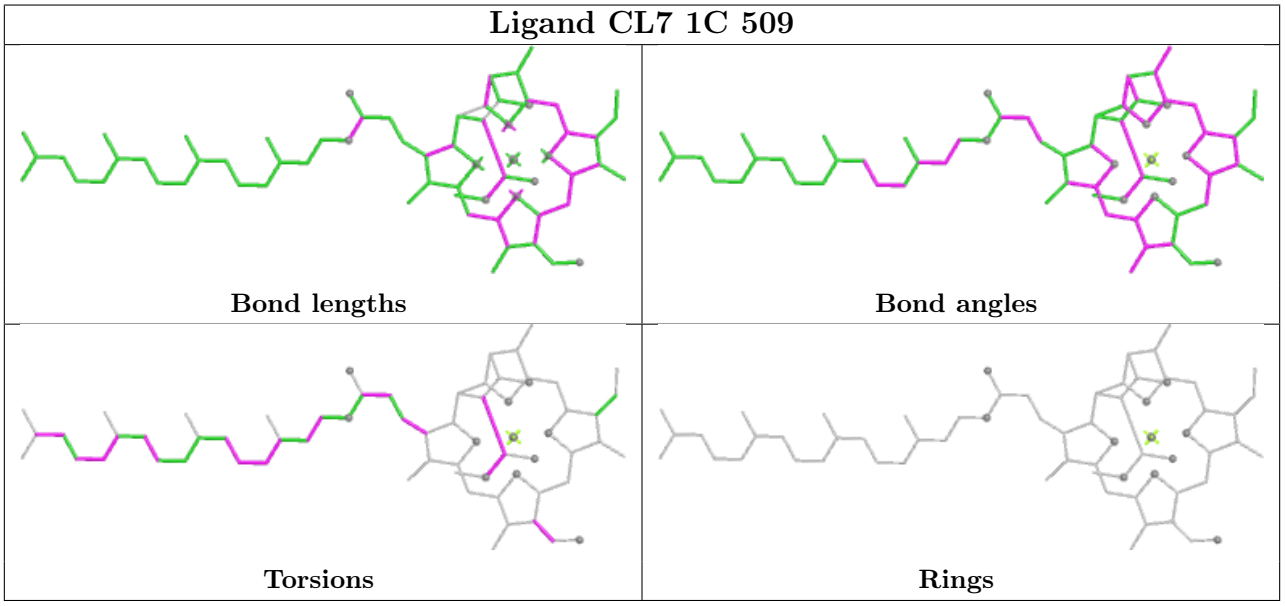

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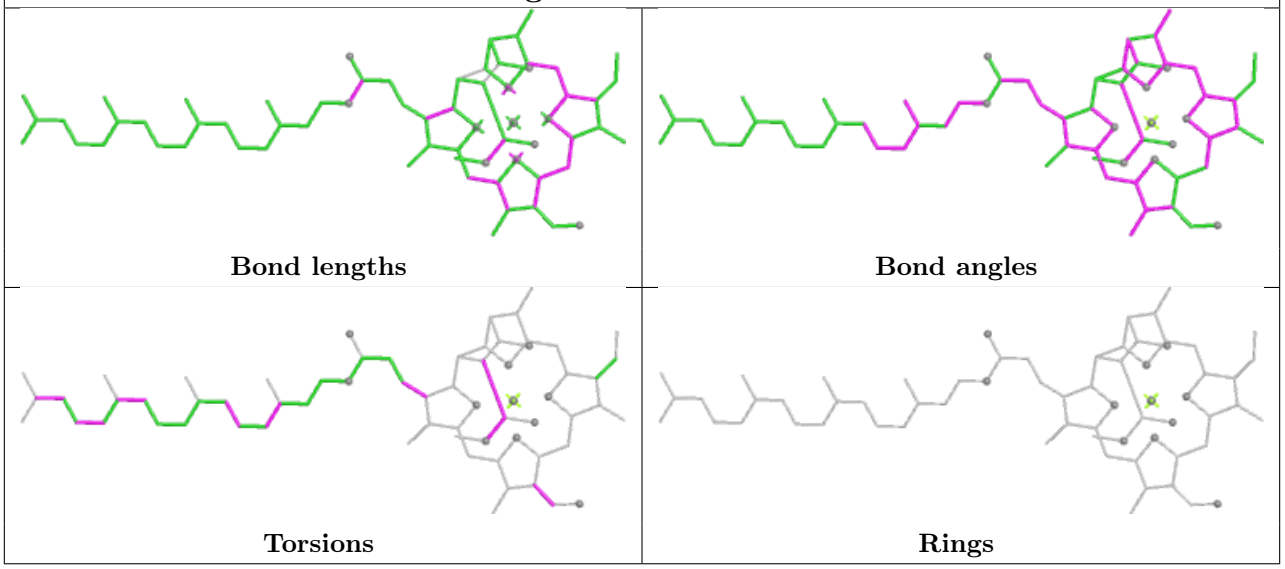

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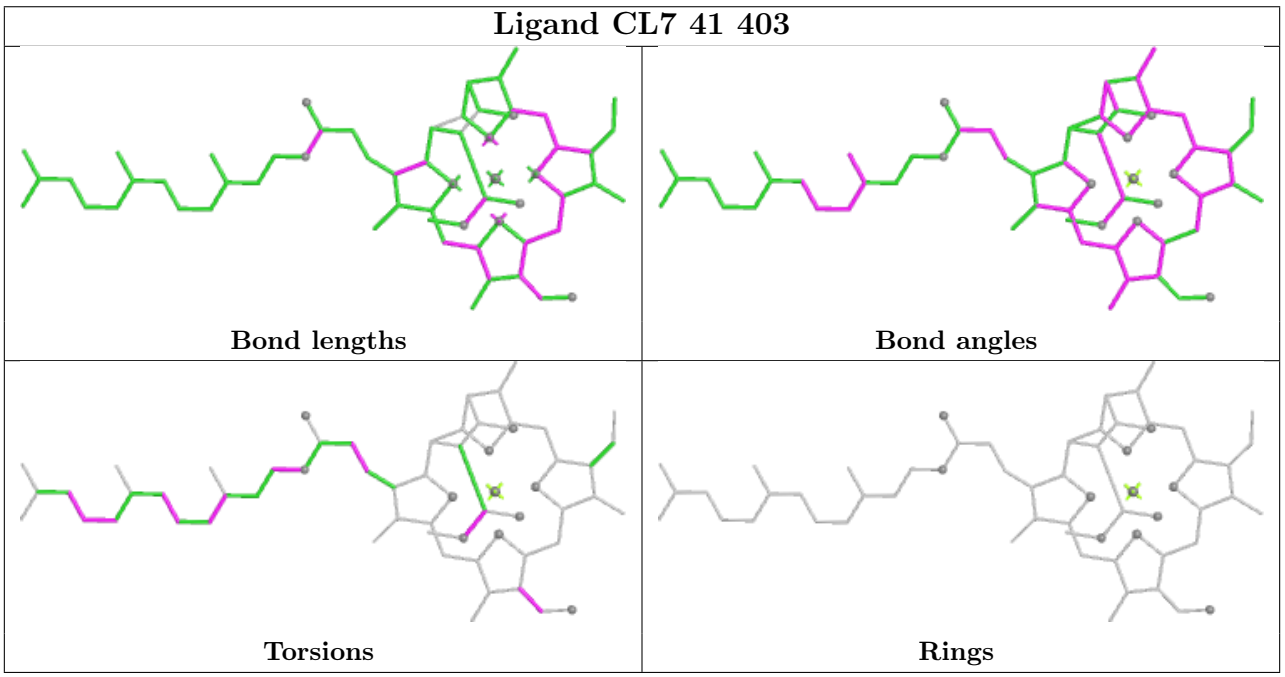
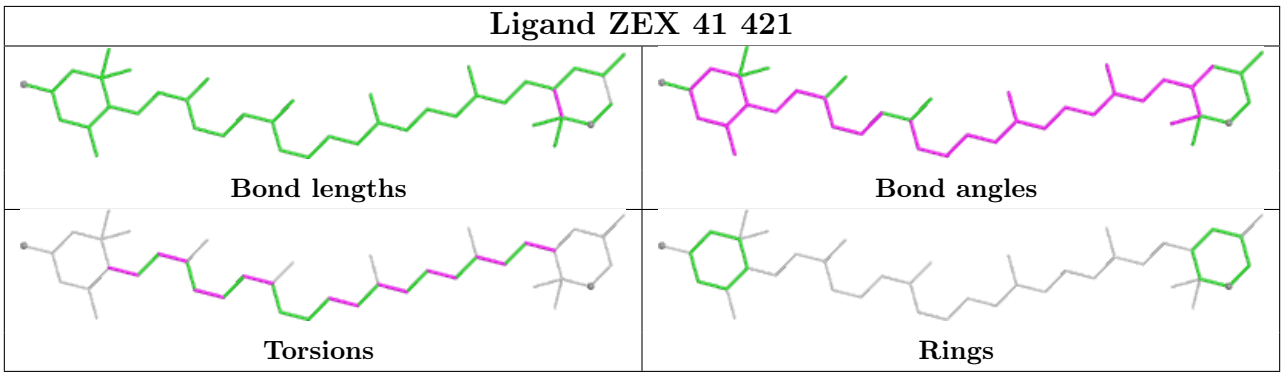


Ligand ZEX 41 421



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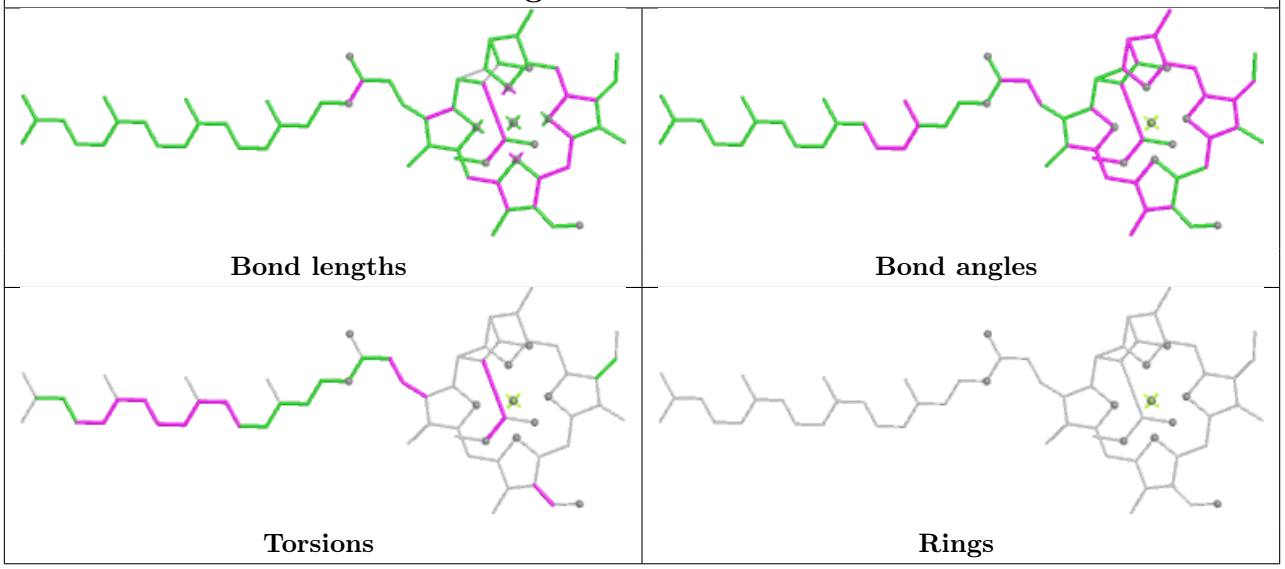

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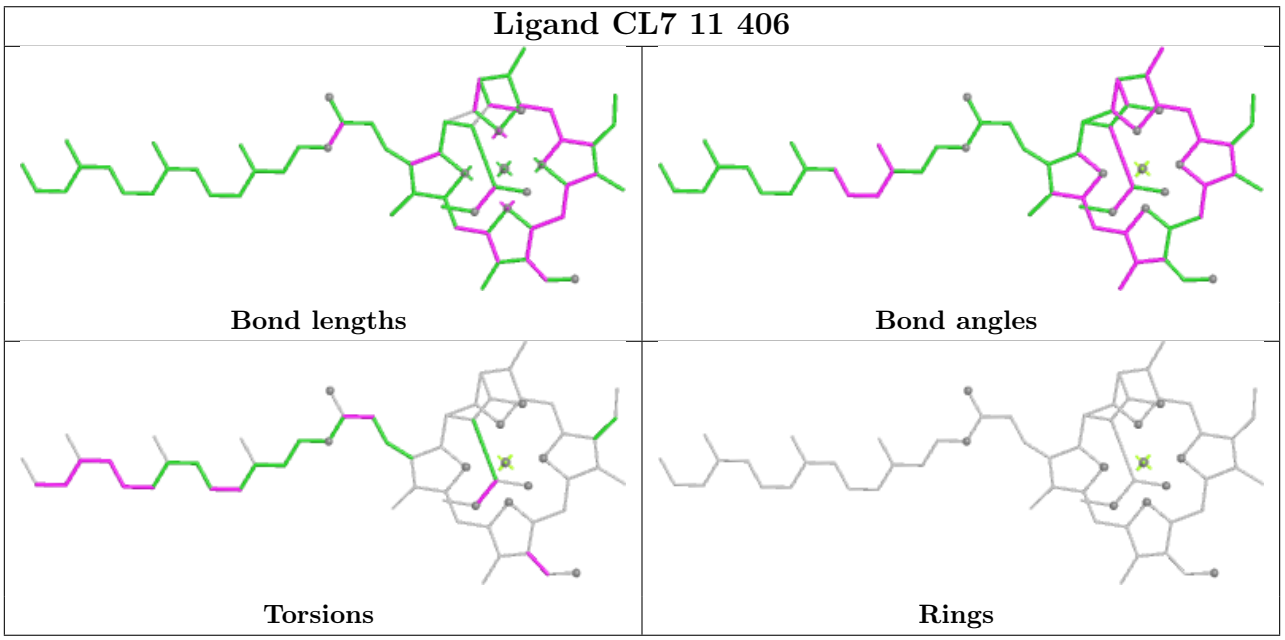

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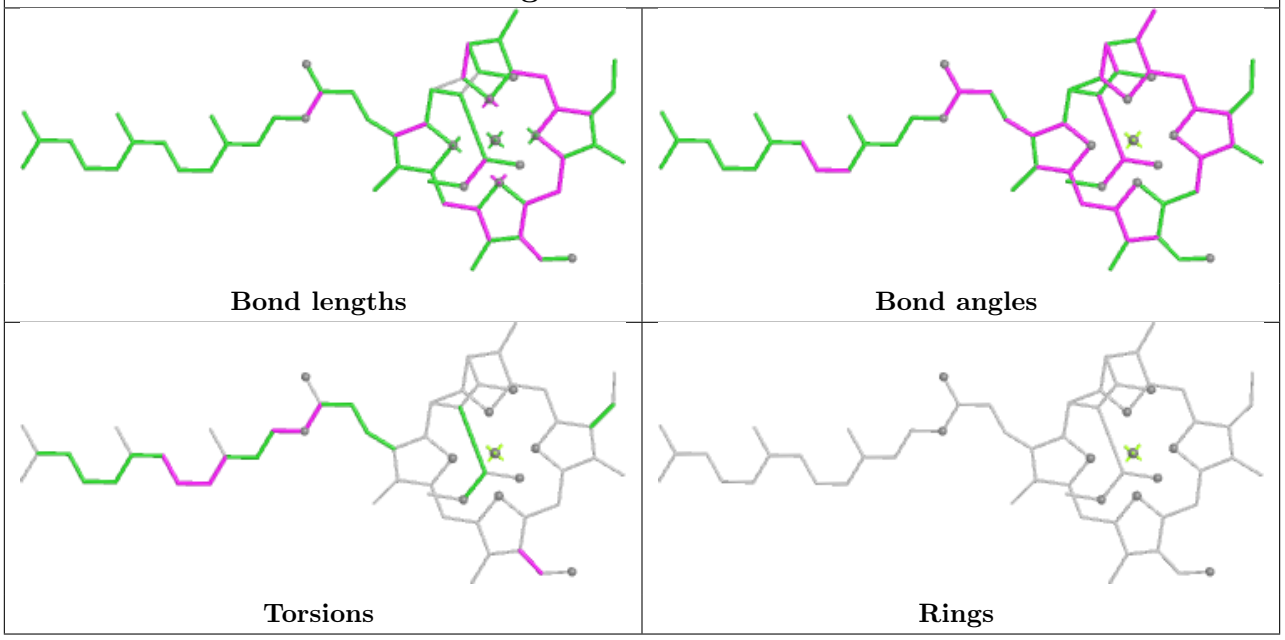

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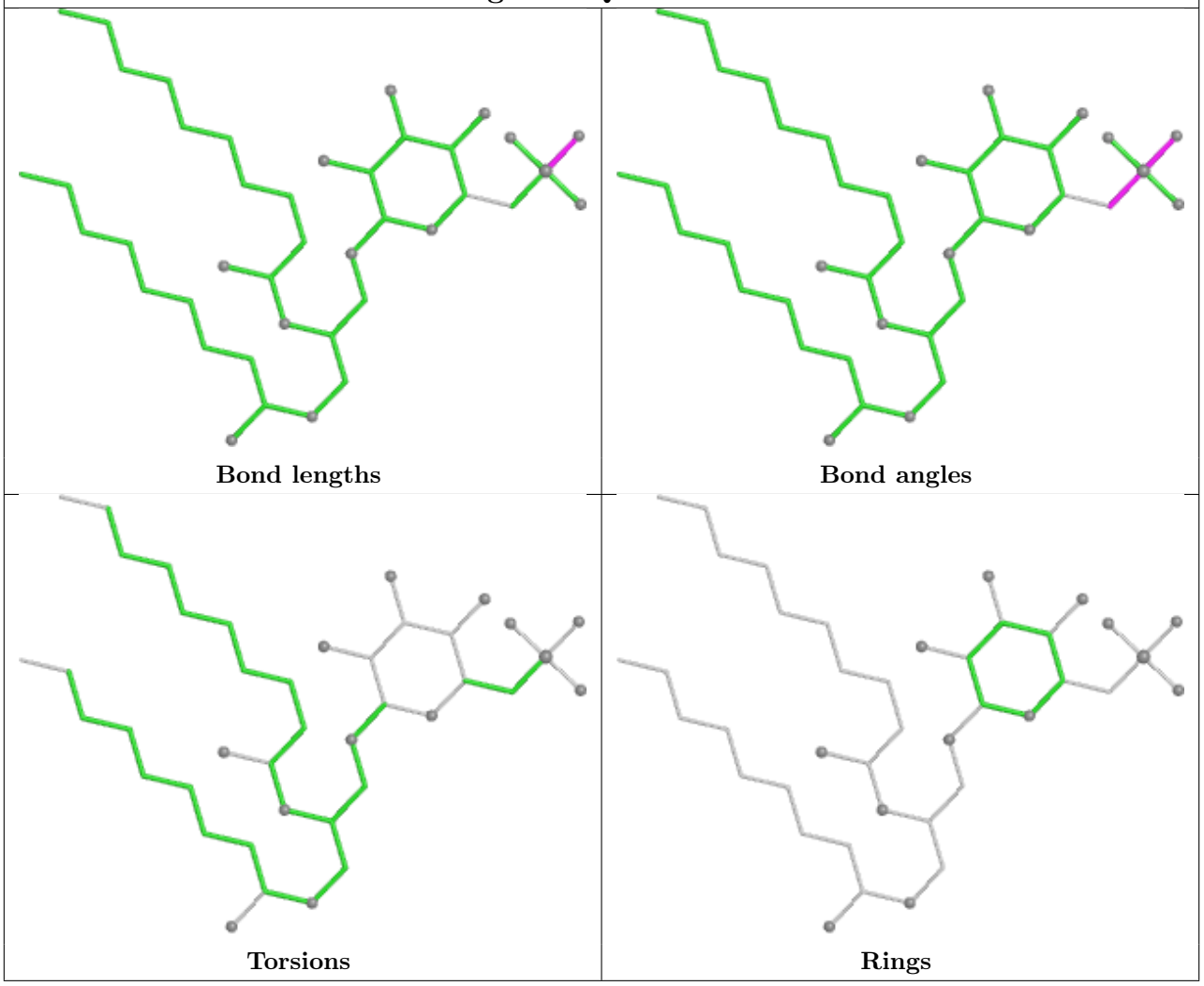

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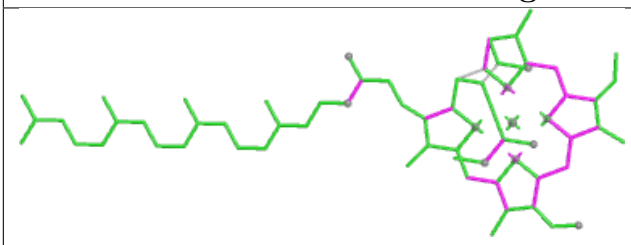
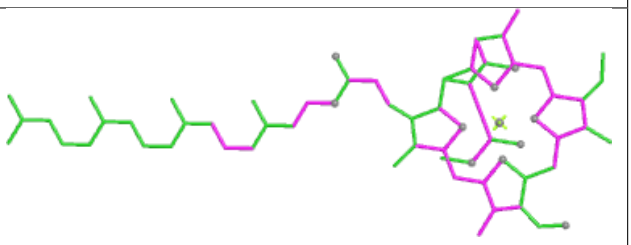
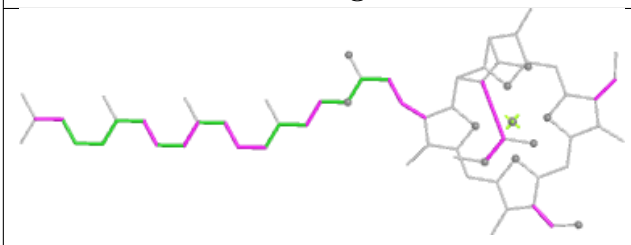


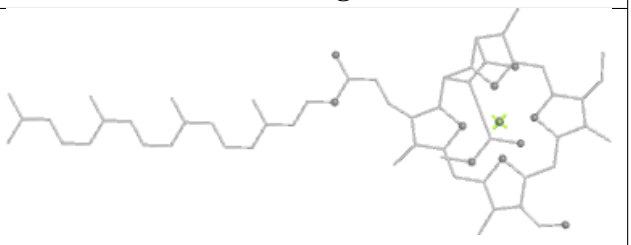
Bond lengths



Bond angles

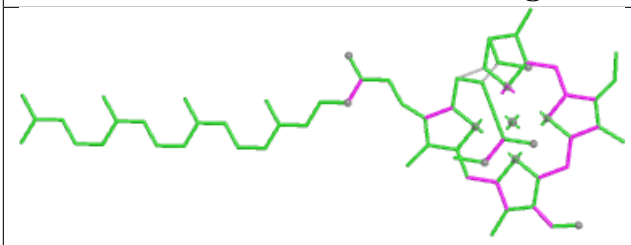


Torsions



Rings

Ligand CL7 22 518



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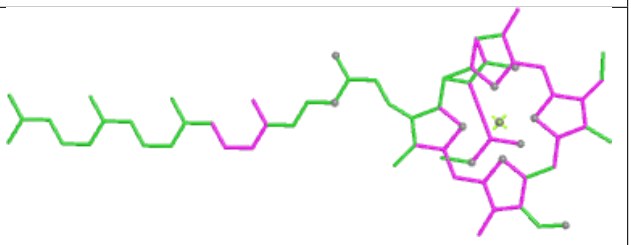
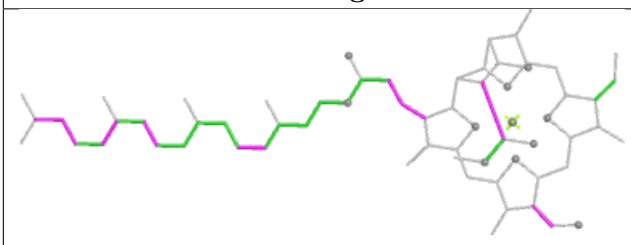


Bond angles



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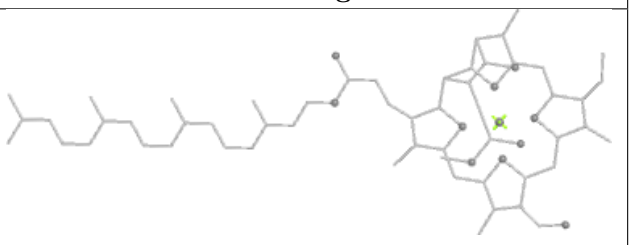
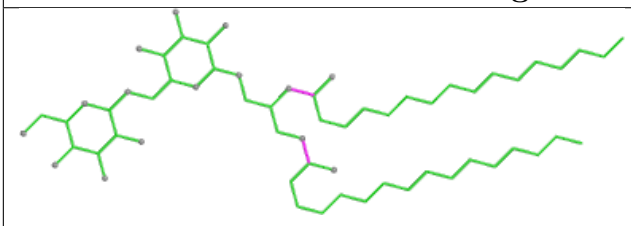


Rings

Ligand DGD 1B 624



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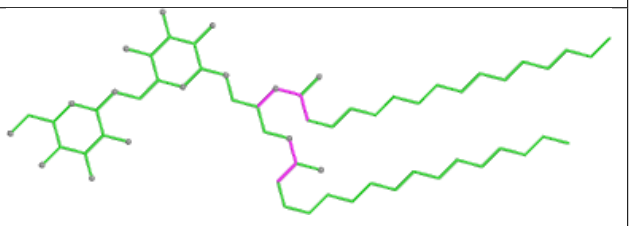
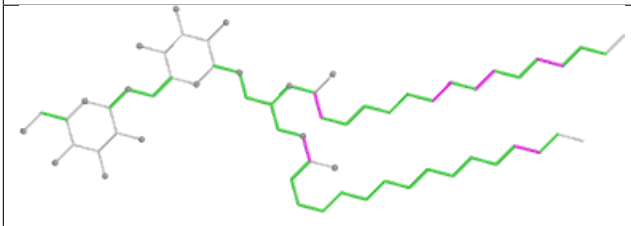
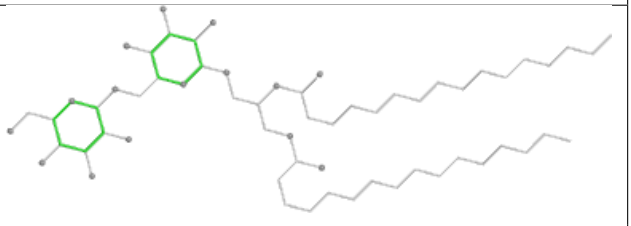


Bond angles

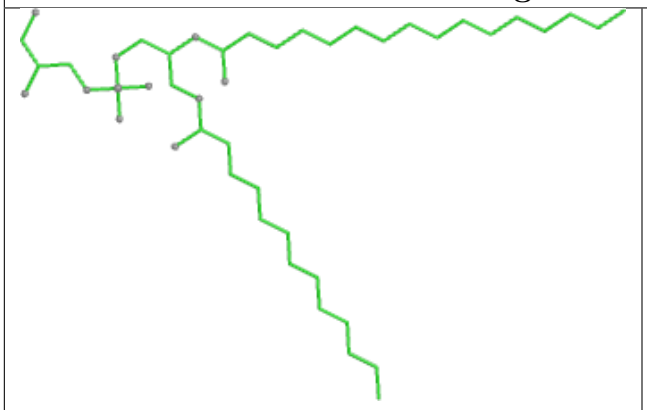


Torsions



Rings

Ligand LHG 1A 408



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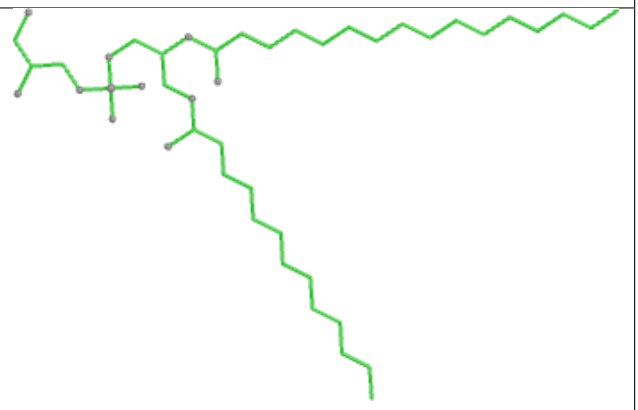
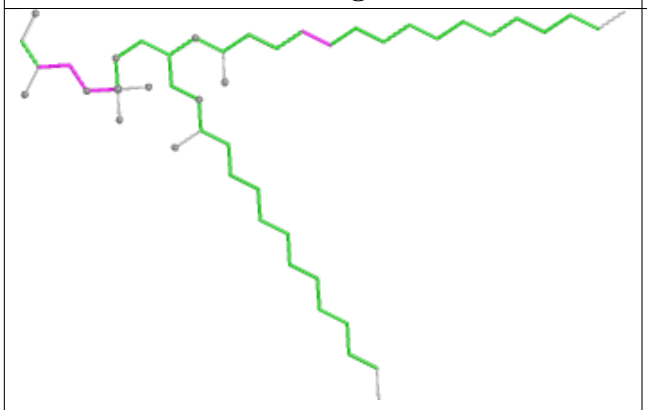


Bond angles



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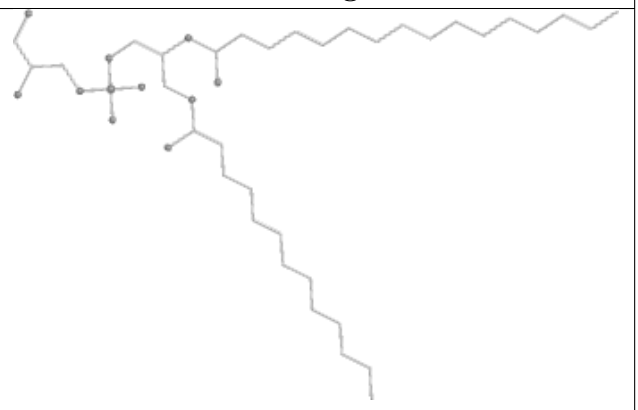
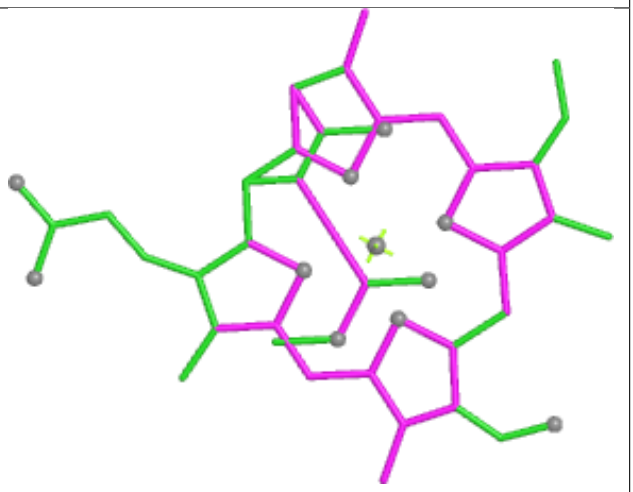


Rings

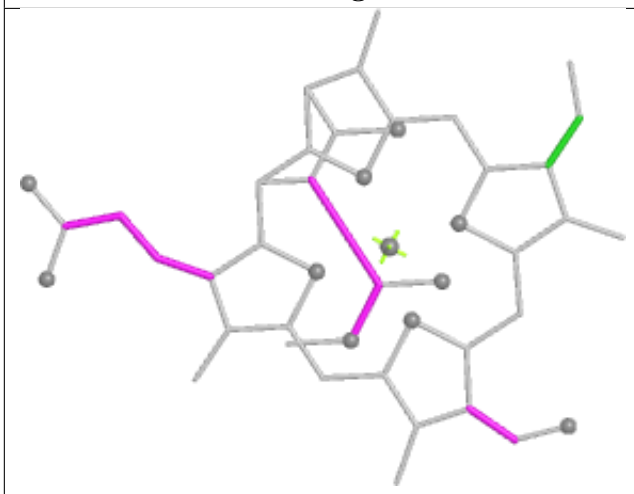
Ligand CL7 44 410



Bond lengths



Bond angles

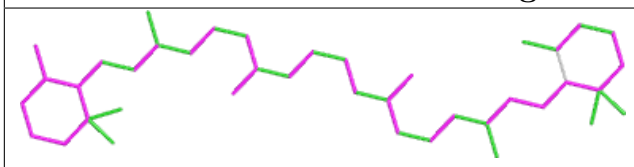


Torsions

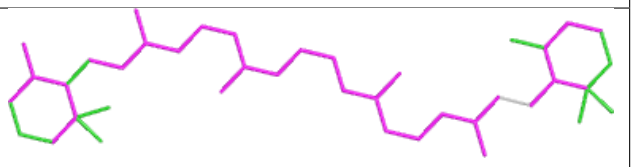


Rings

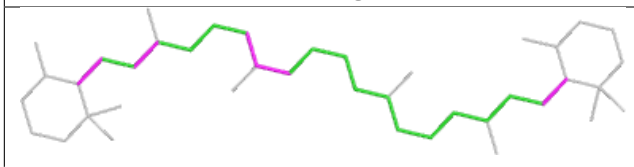
Ligand 8CT 1B 626



Bond lengths



Bond angles



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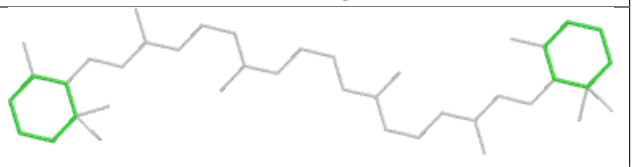
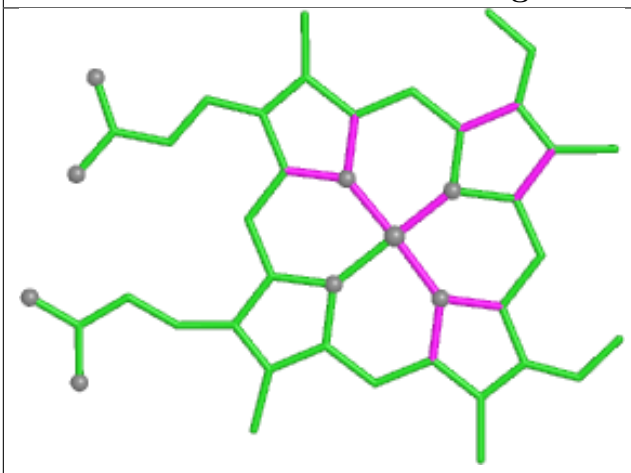
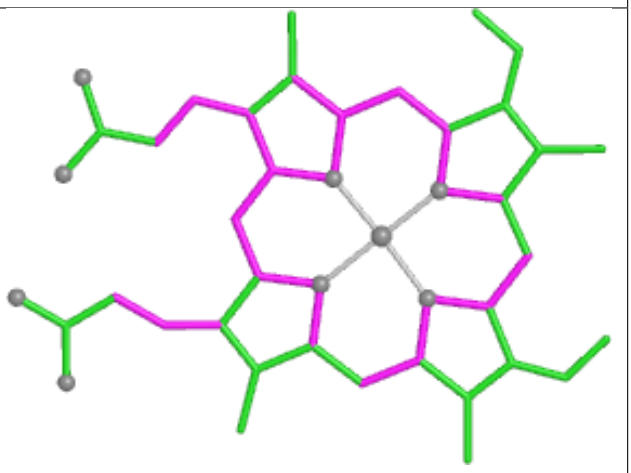


Rings

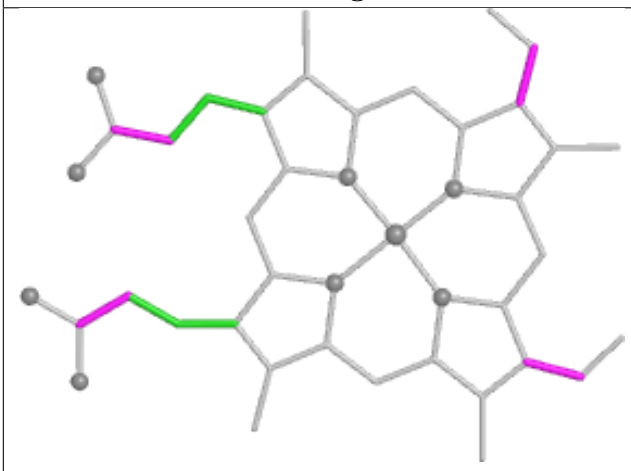
Ligand HEM 3F 101



Bond lengths



Bond angles



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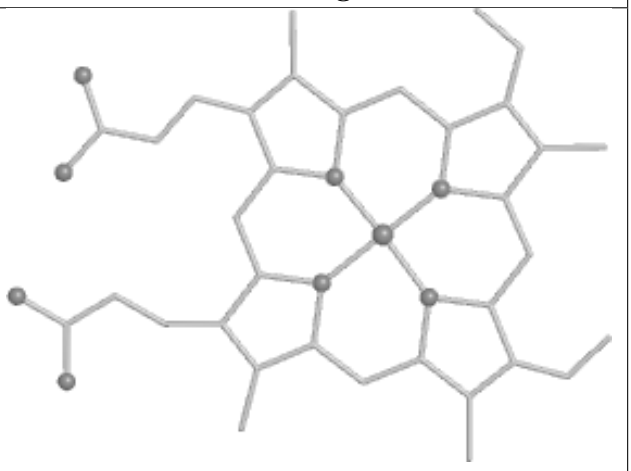
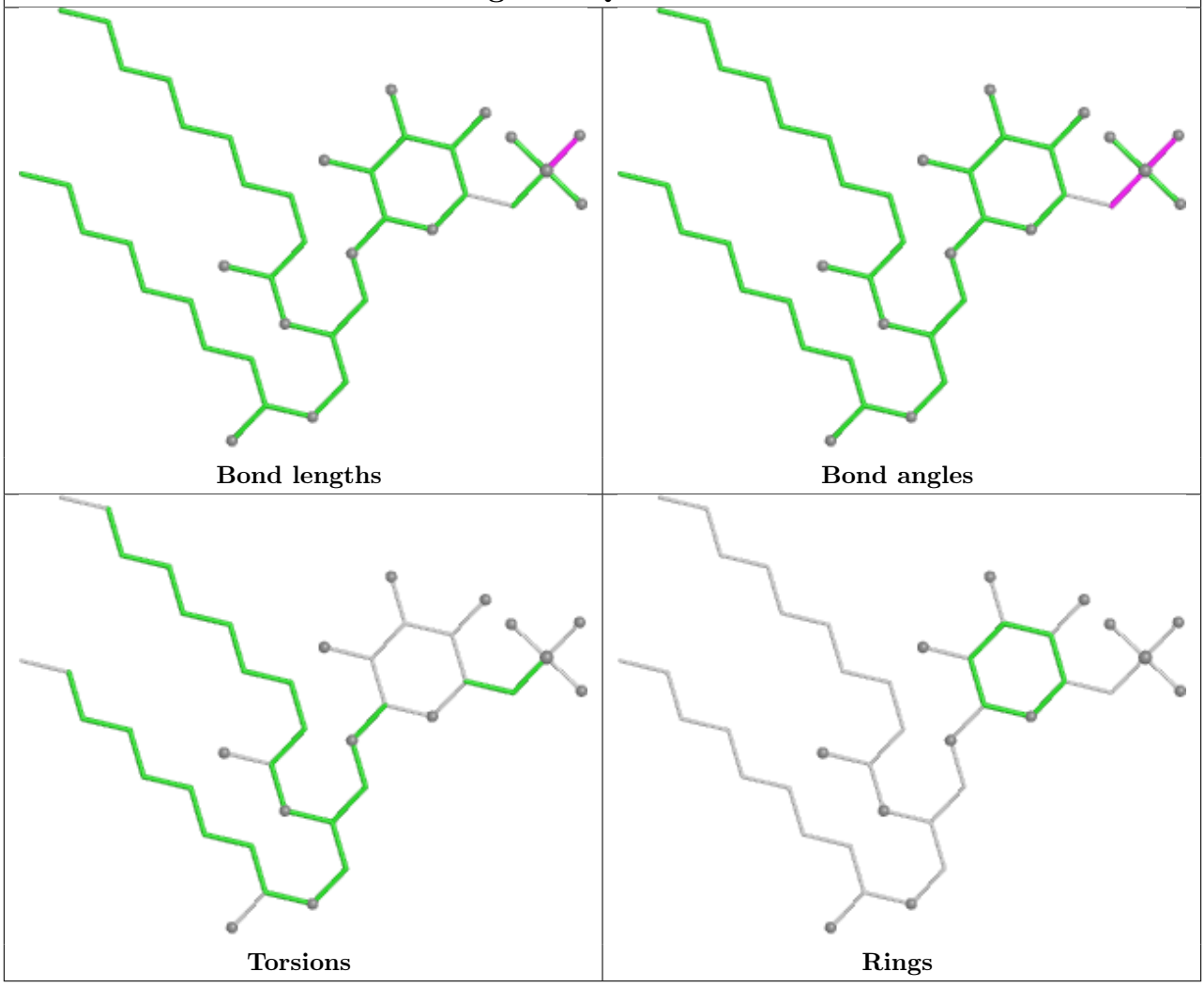
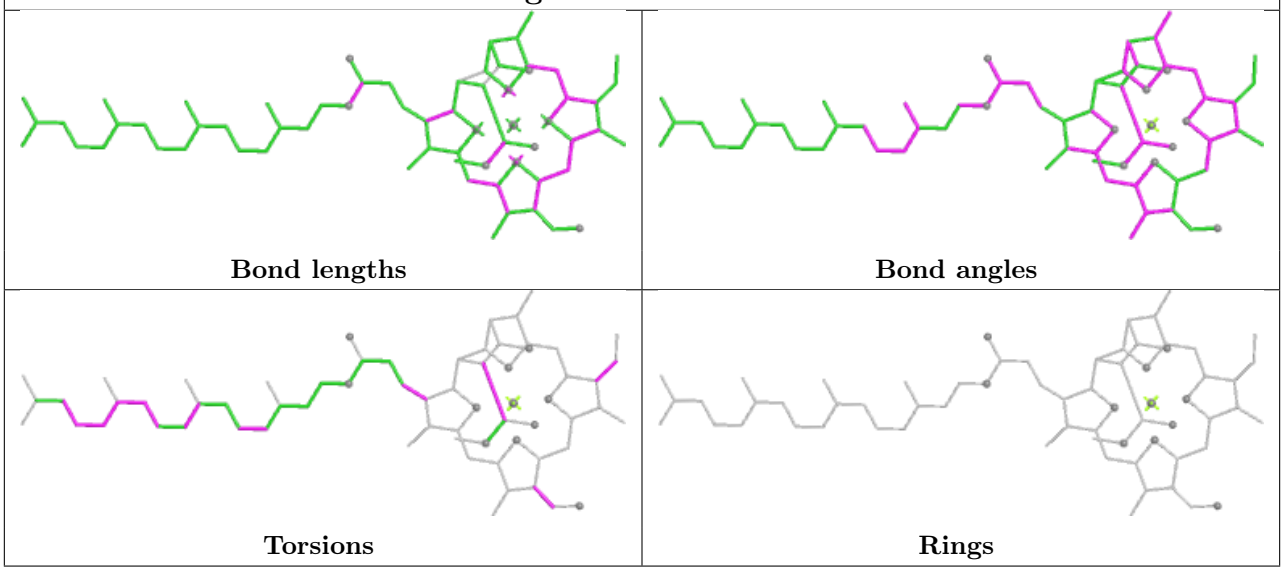


Rings

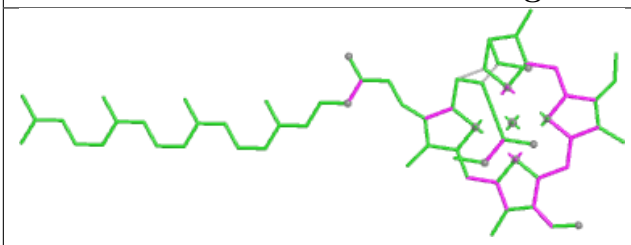
Ligand SQD 12 523



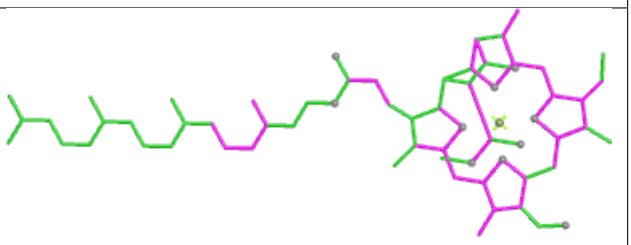
Ligand CL7 41 408



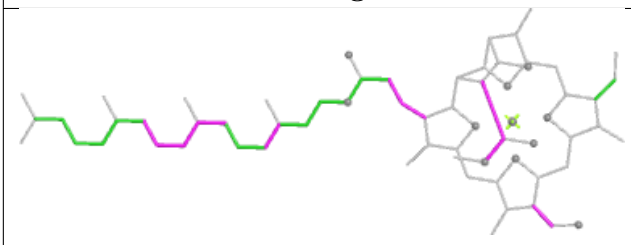
Ligand CL7 42 502



Bond lengths



Bond angles



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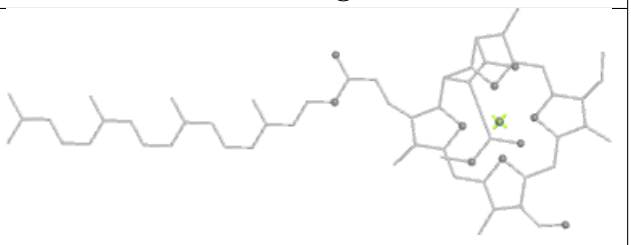

Rings

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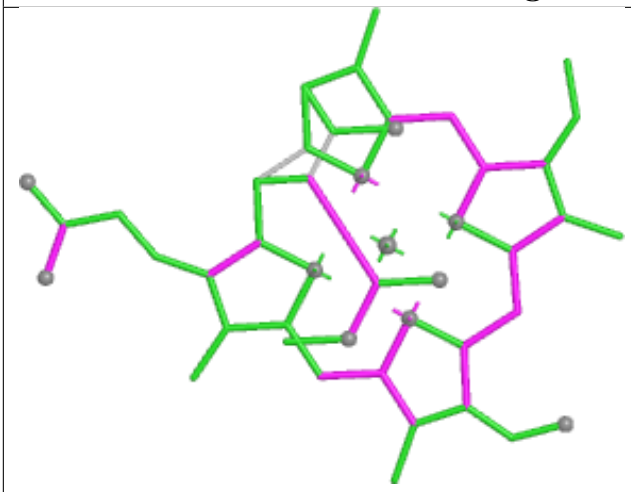


Bond lengths



Bond angles

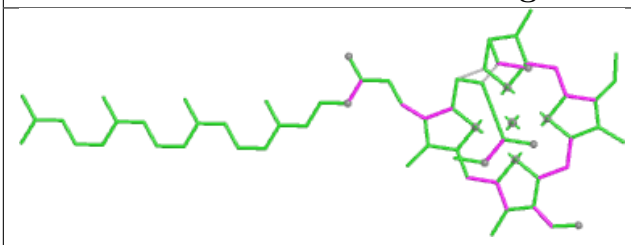


Torsions

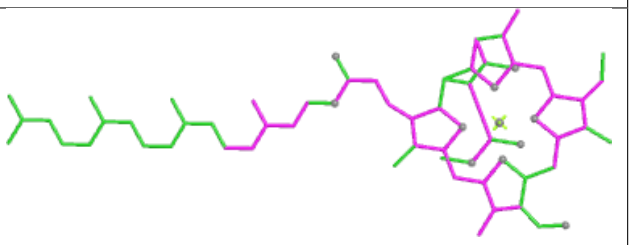


Rings

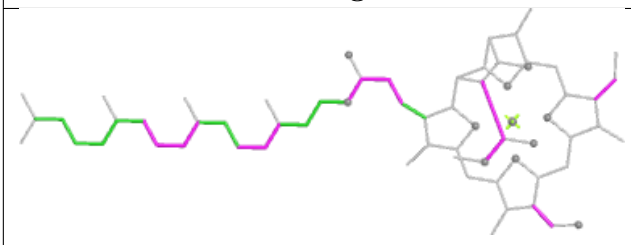
Ligand CL7 1A 401



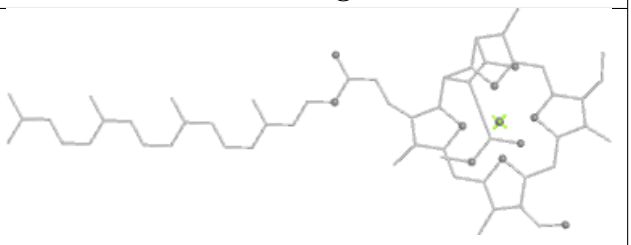
Bond lengths



Bond angles

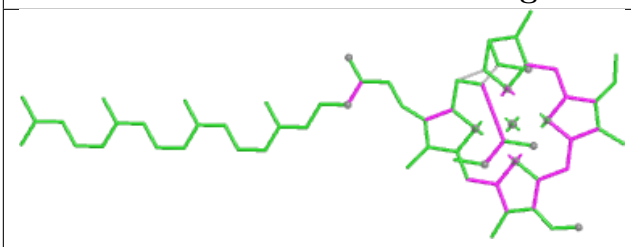


Torsions



Rings

Ligand CL7 1C 507



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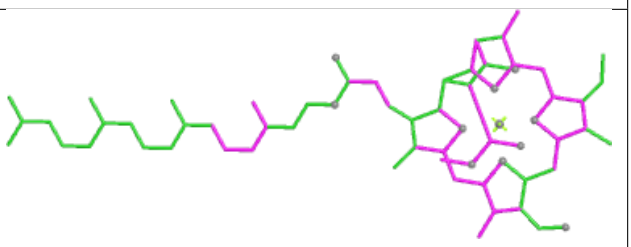

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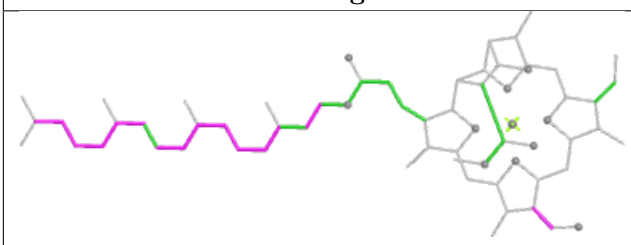

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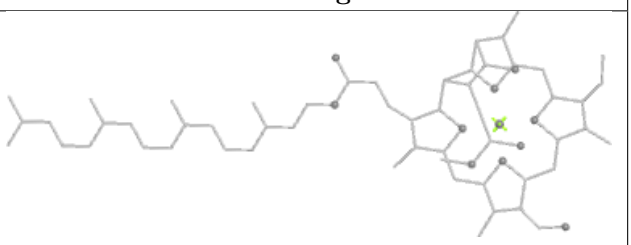
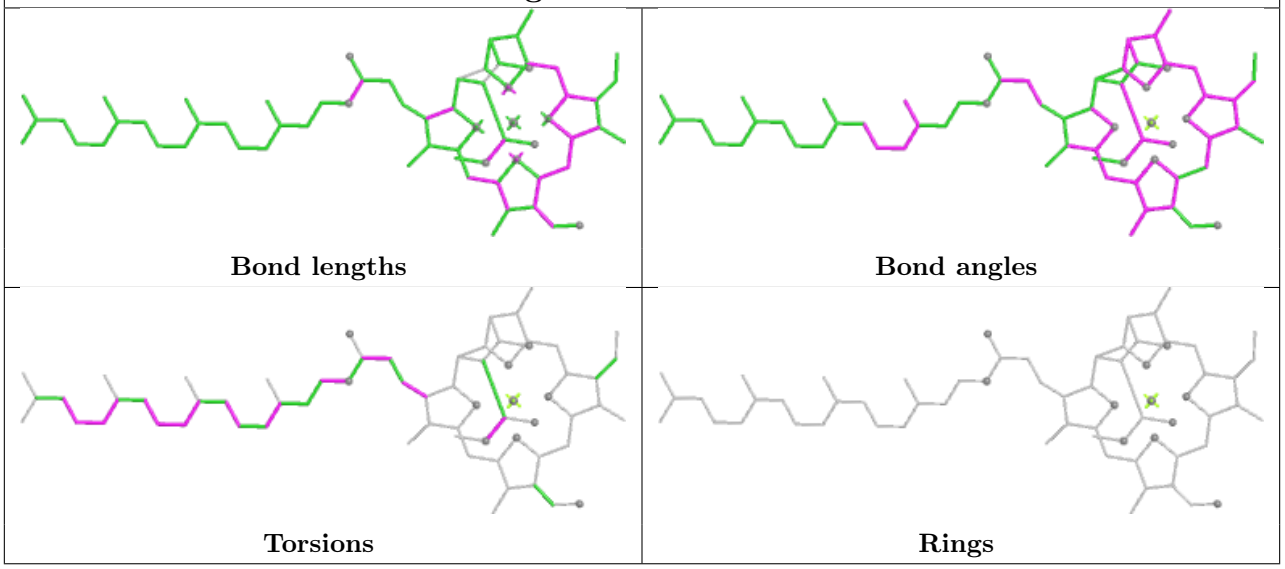
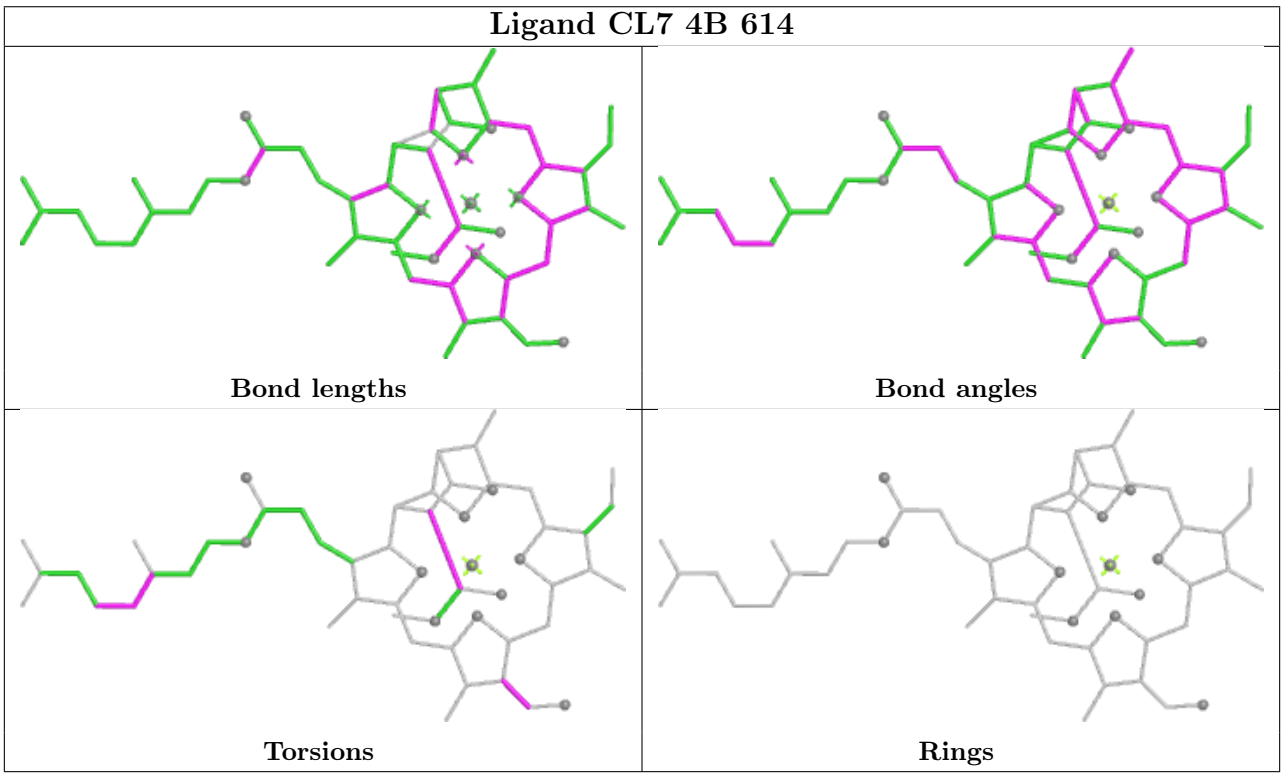


Rings

Ligand CL7 24 412



Ligand CL7 4B 614



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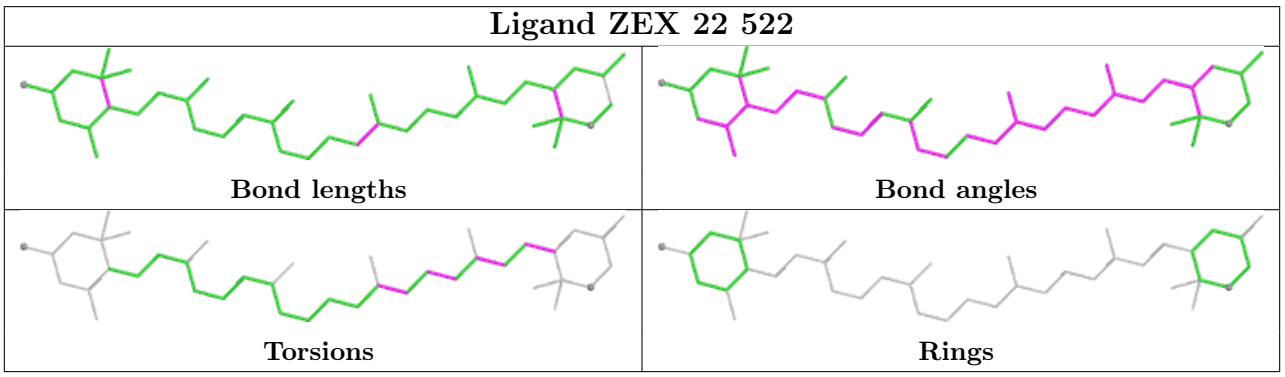
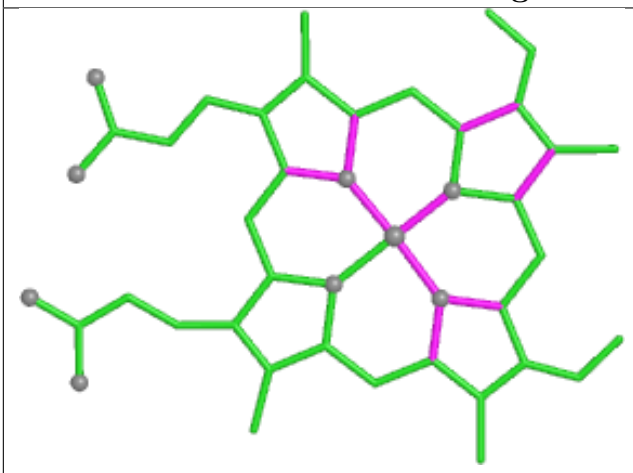


Ligand HEM 4F 101



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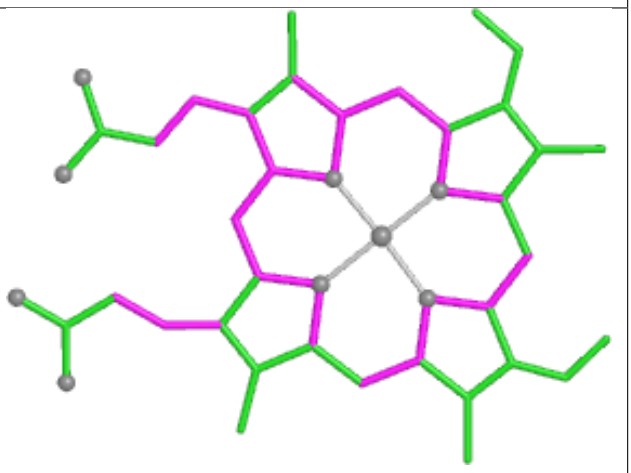
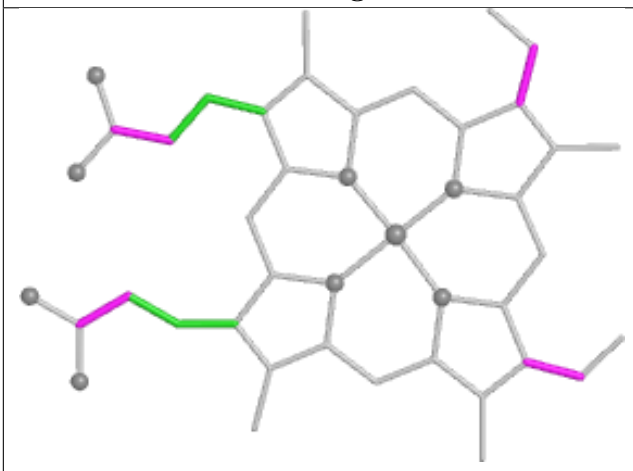


Bond angles



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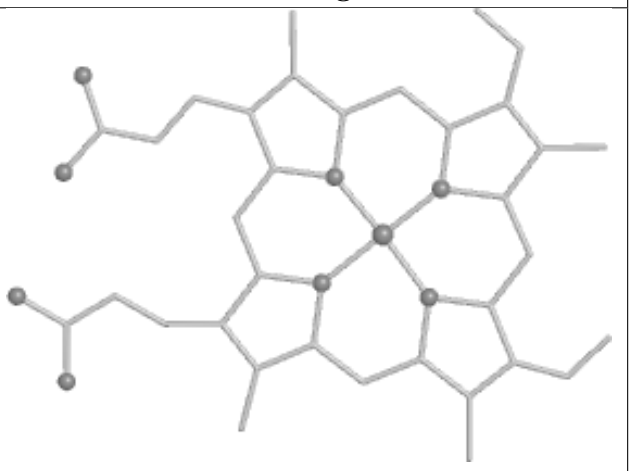

Rings

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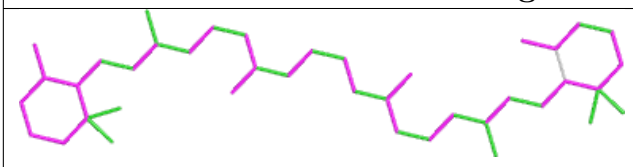

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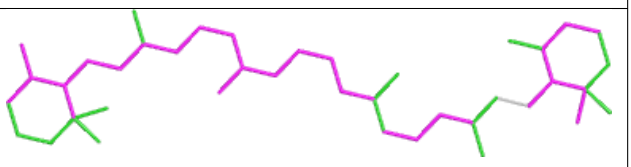
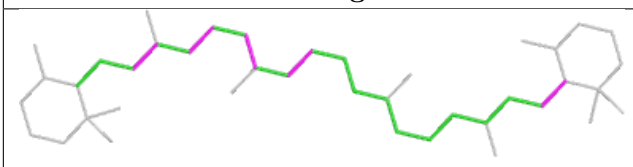


Bond angles



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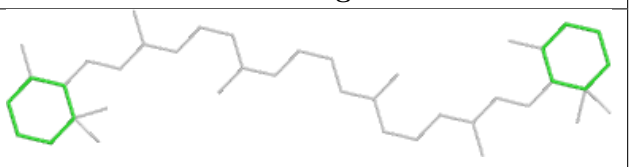
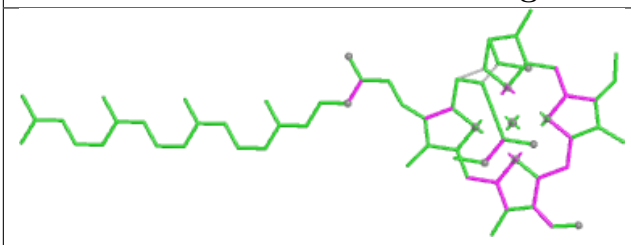


Rings

Ligand CL7 4C 501



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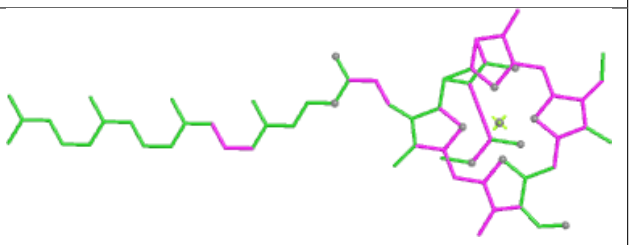

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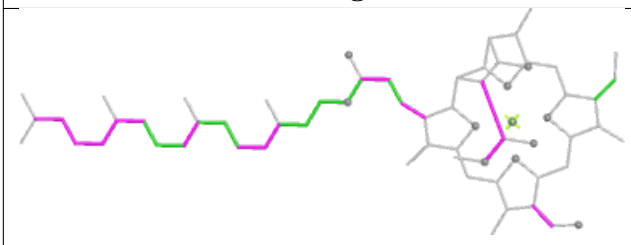

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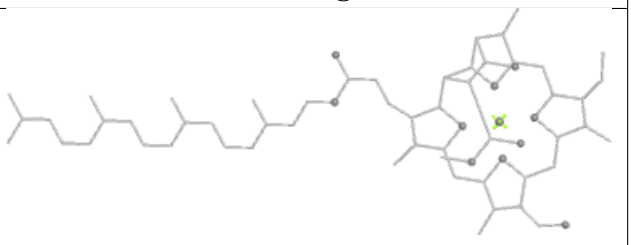
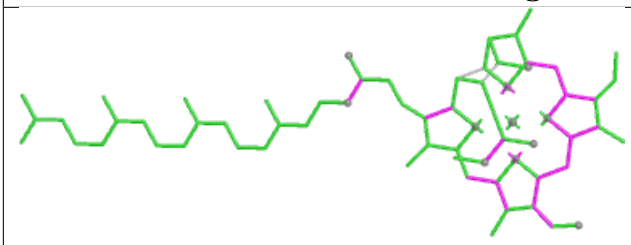


Rings

Ligand CL7 12 502



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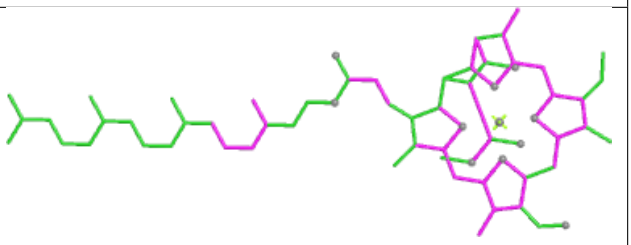
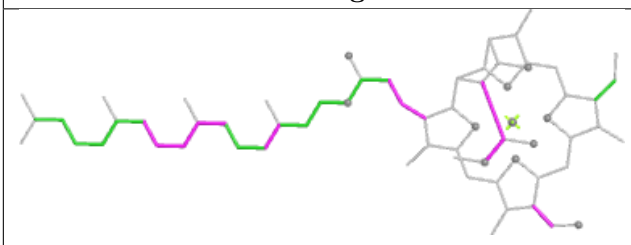


Bond angles



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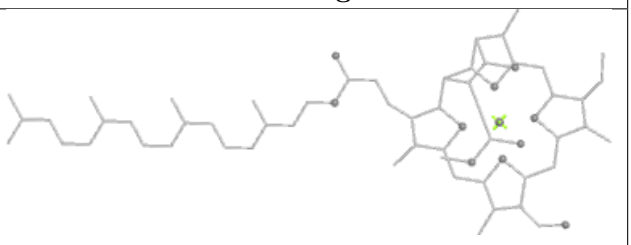
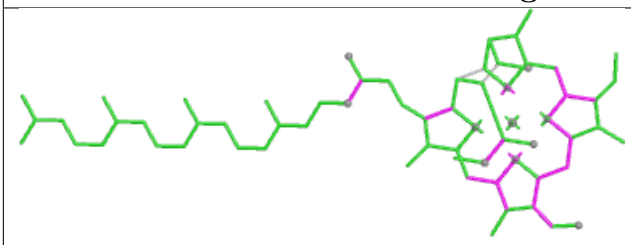


Rings

Ligand CL7 3C 501



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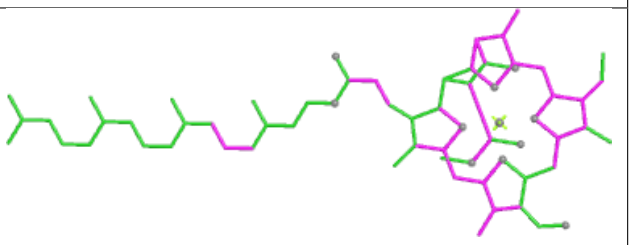

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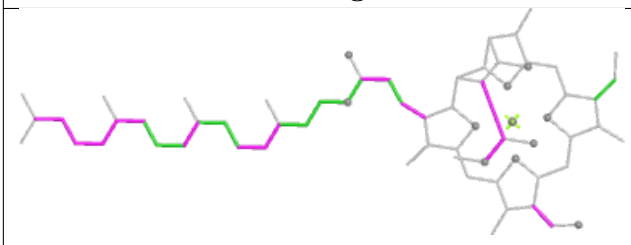

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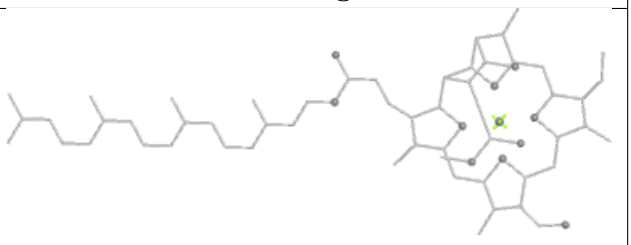
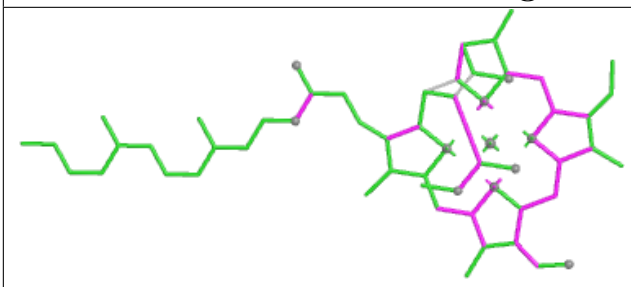


Rings

Ligand CL7 2D 404



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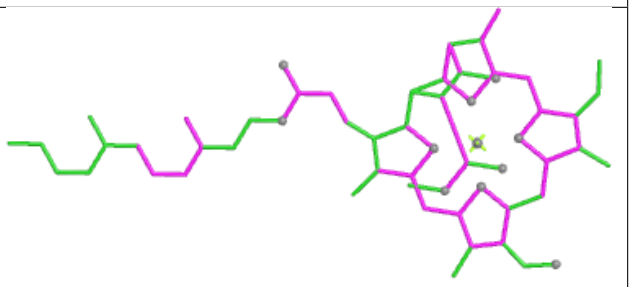

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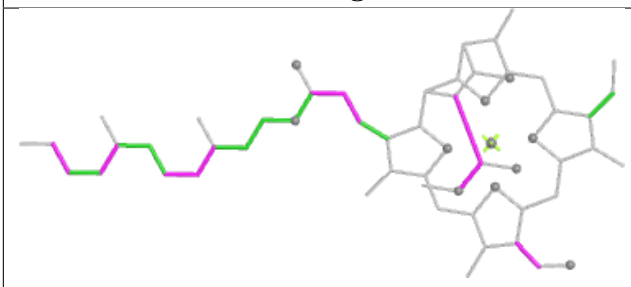

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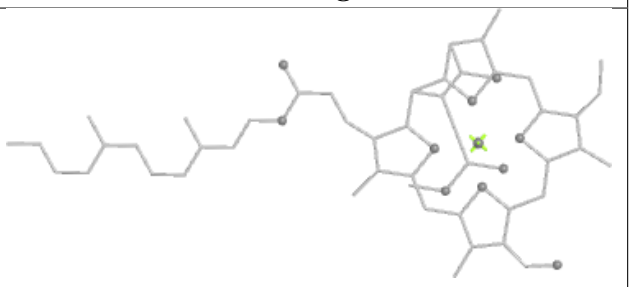
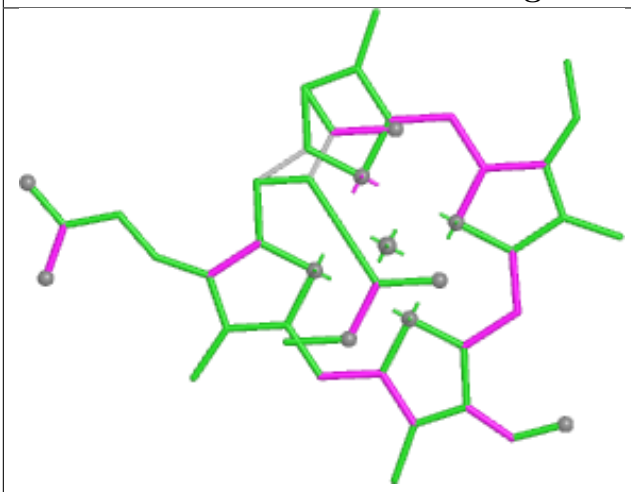


Rings

Ligand CL7 13 518



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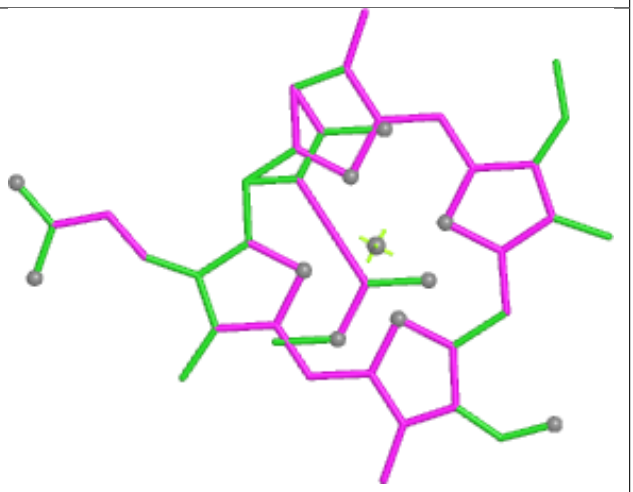
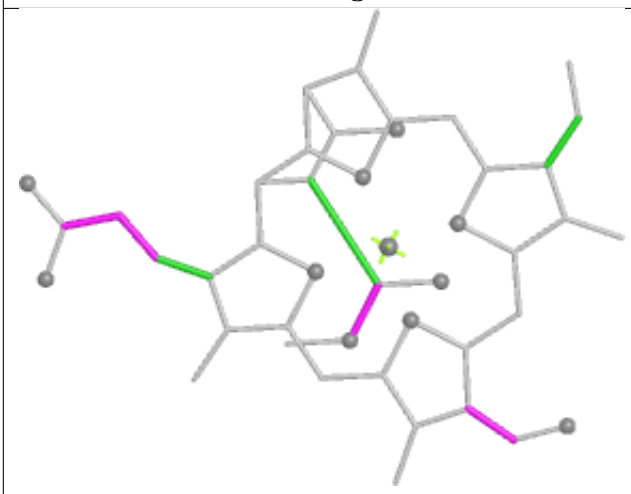


Bond angles

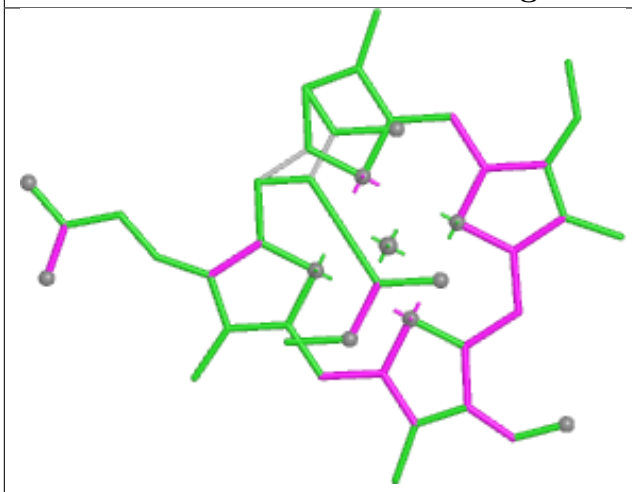


Torsions



Rings

Ligand CL7 2D 405



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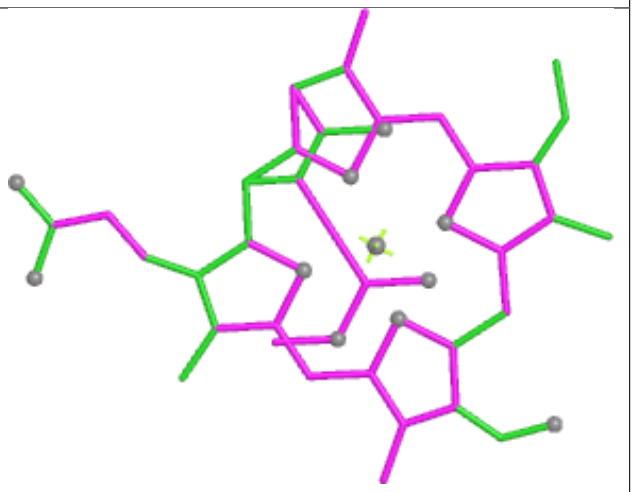

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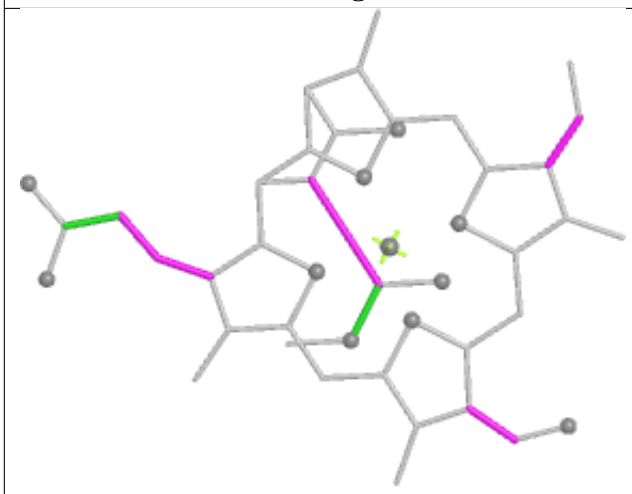
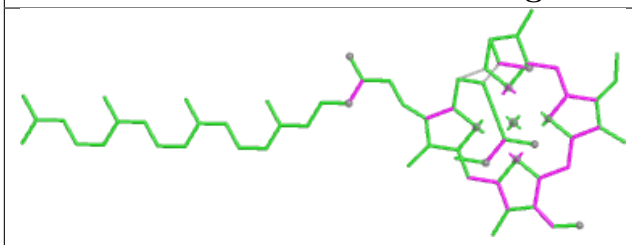


Torsions



Rings

Ligand CL7 11 410



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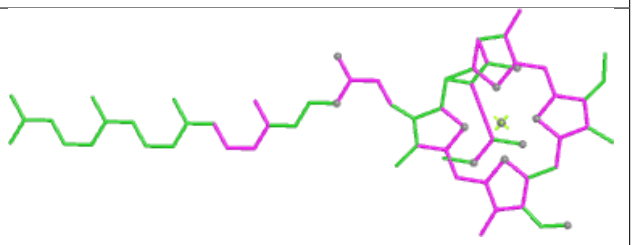

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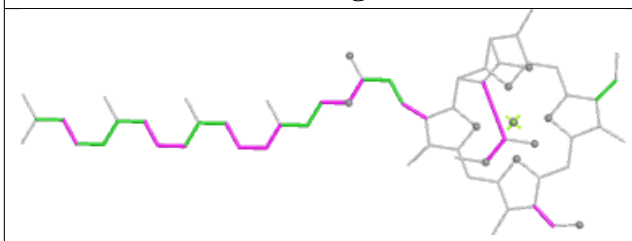

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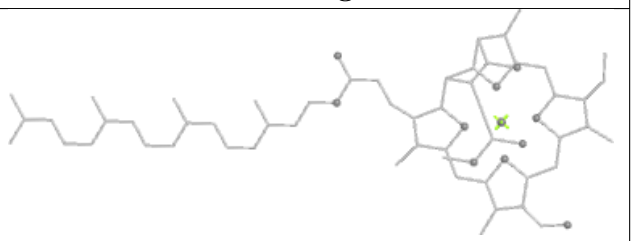
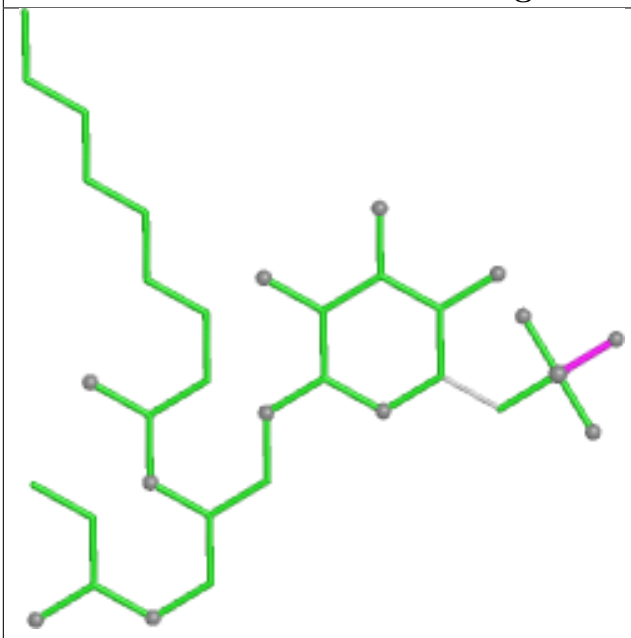


Rings

Ligand SQD 2A 406



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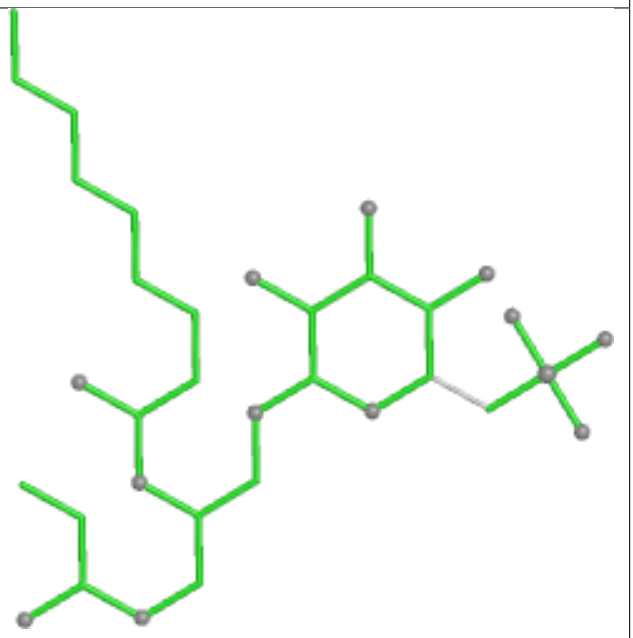

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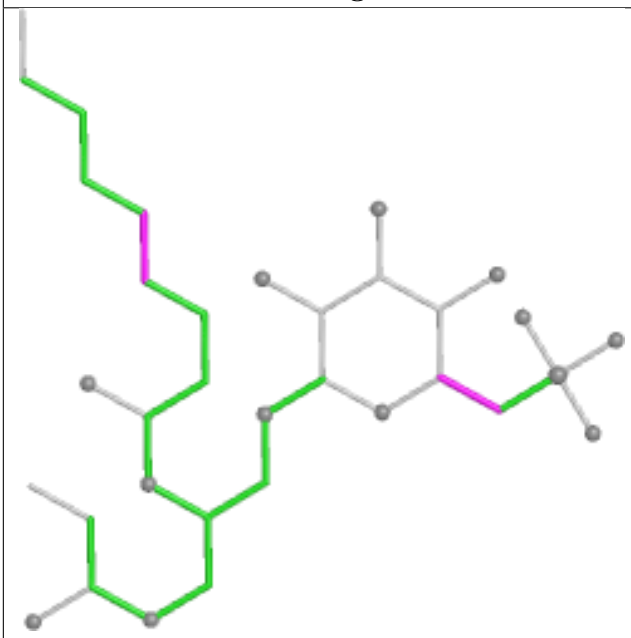

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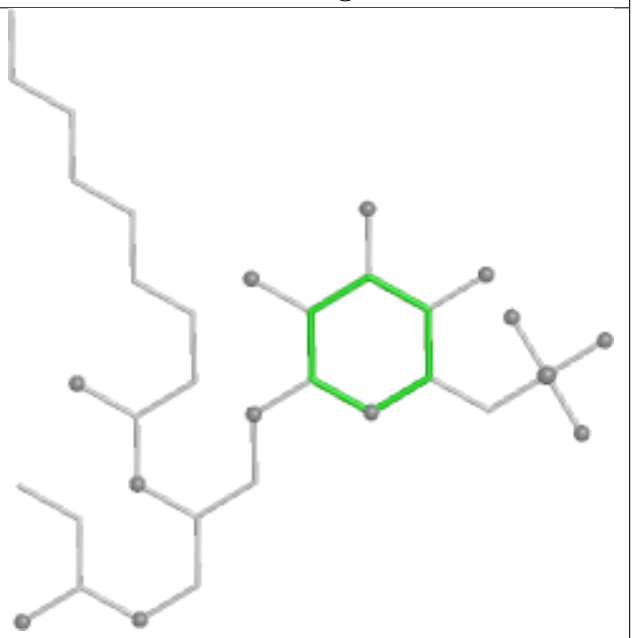
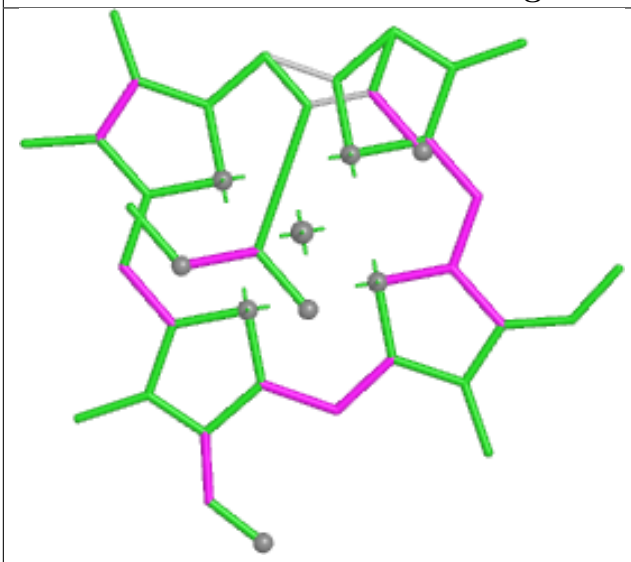


Rings

Ligand CL7 21 415



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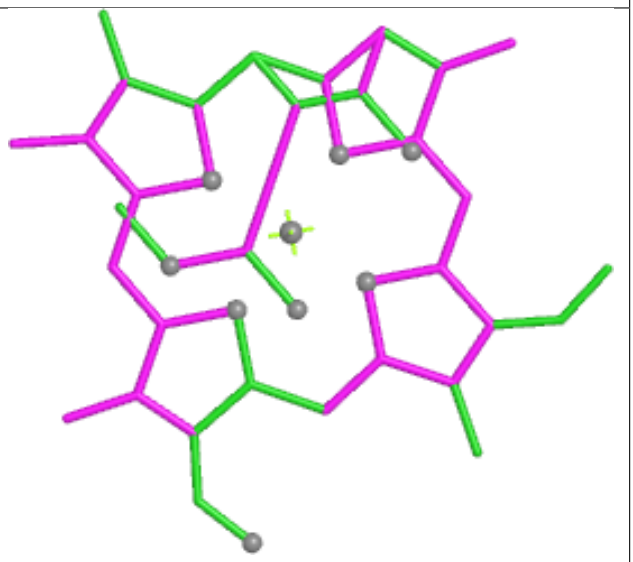
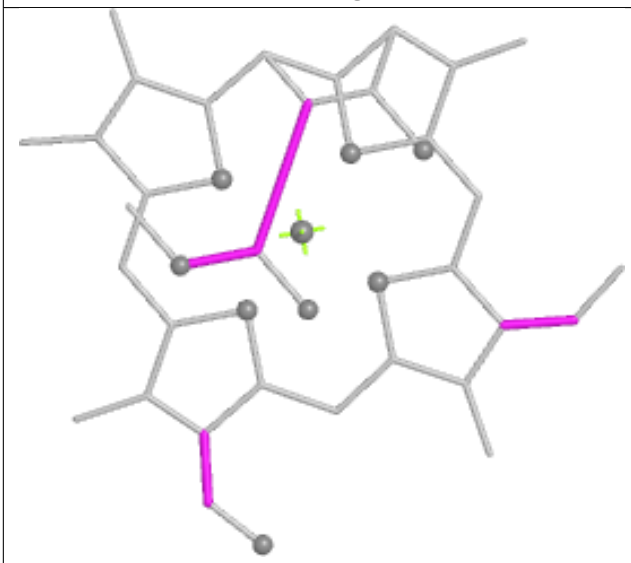


Bond angles



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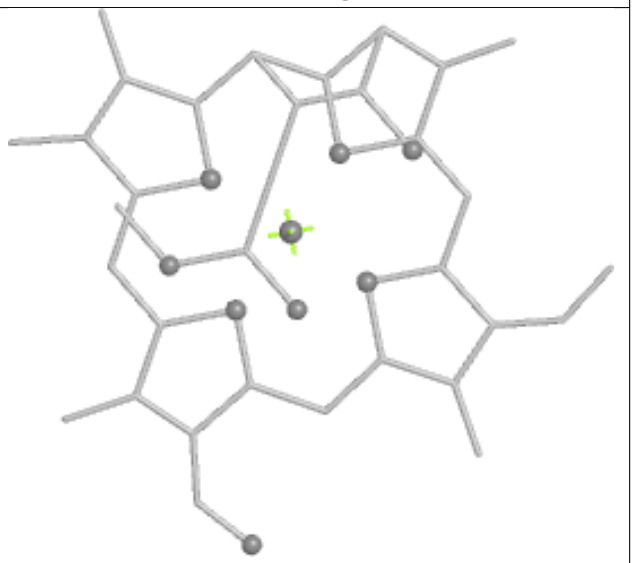
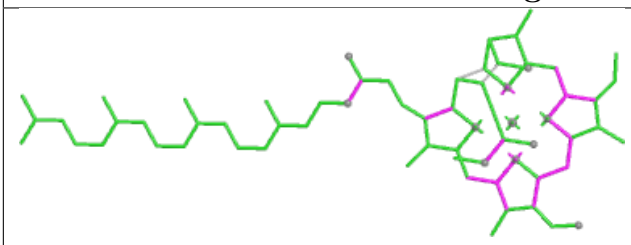


Rings

Ligand CL7 22 517



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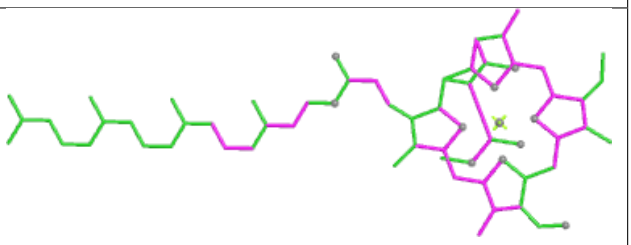
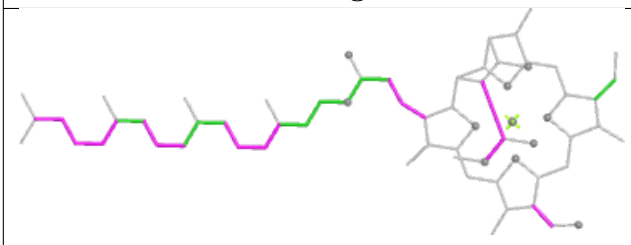


Bond angles



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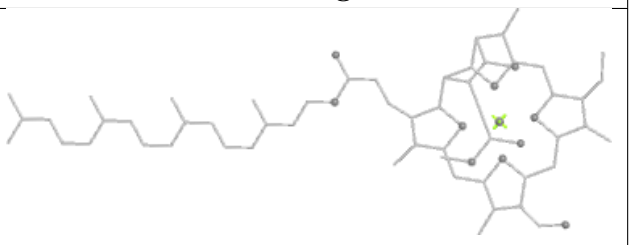
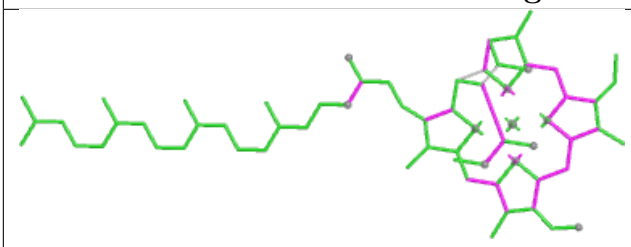
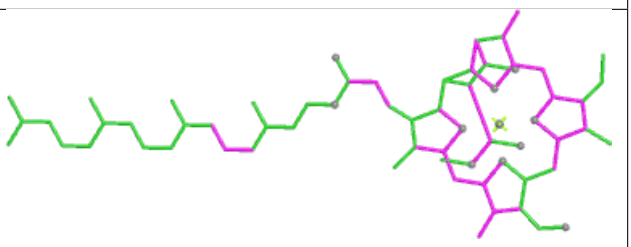


Rings

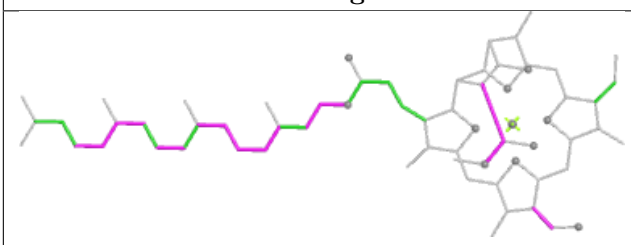
Ligand CL7 12 509



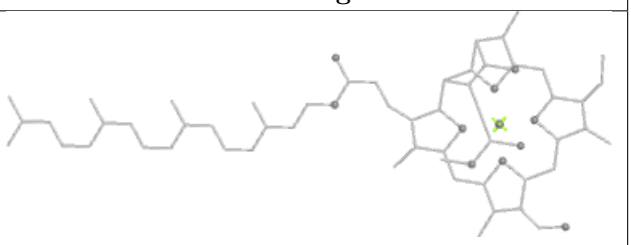
Bond lengths



Bond angles

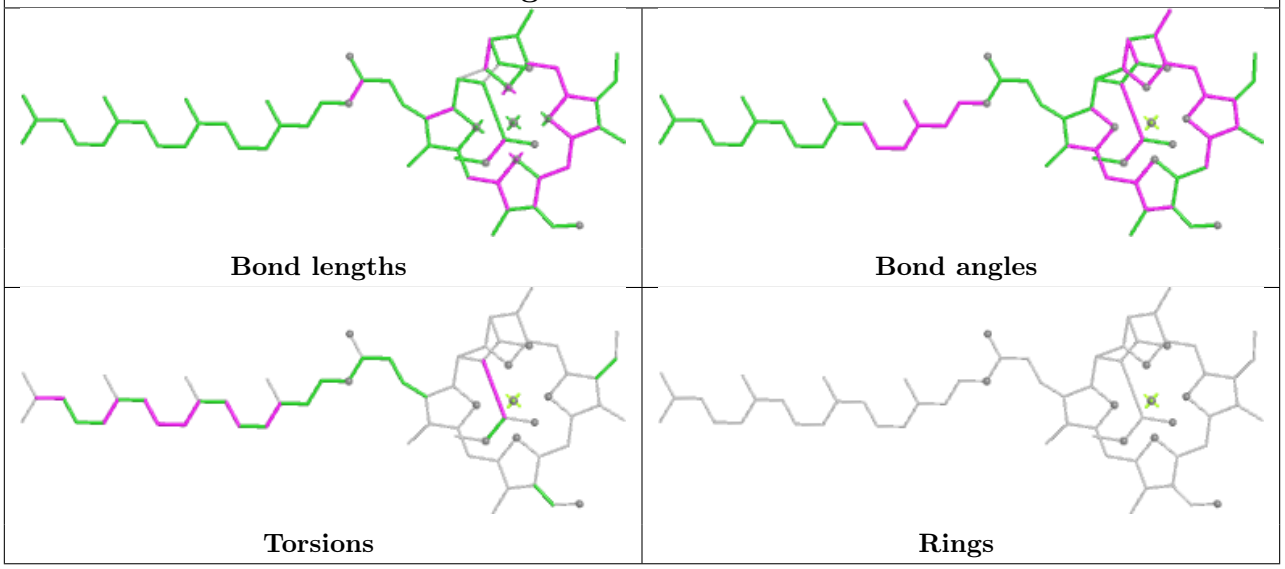


Torsions

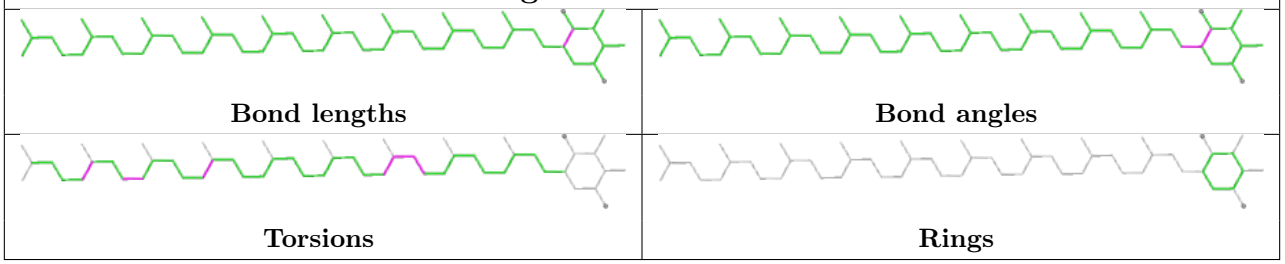


Rings

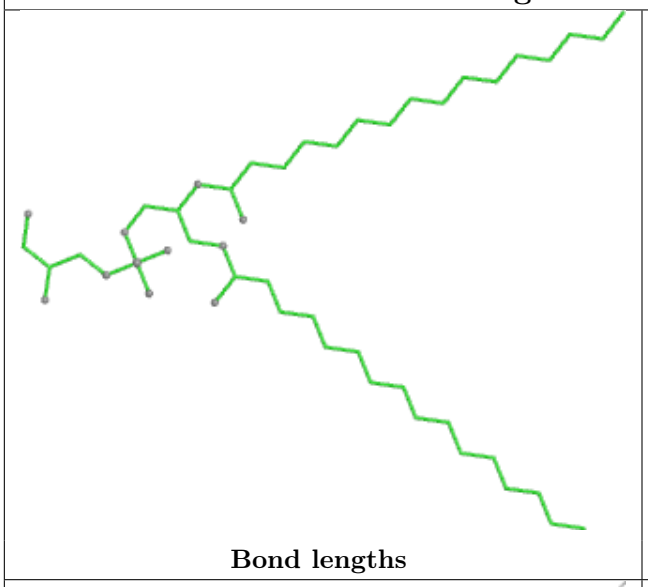
Ligand CL7 4B 604



Ligand PL9 3D 407



Ligand LHG 2D 409



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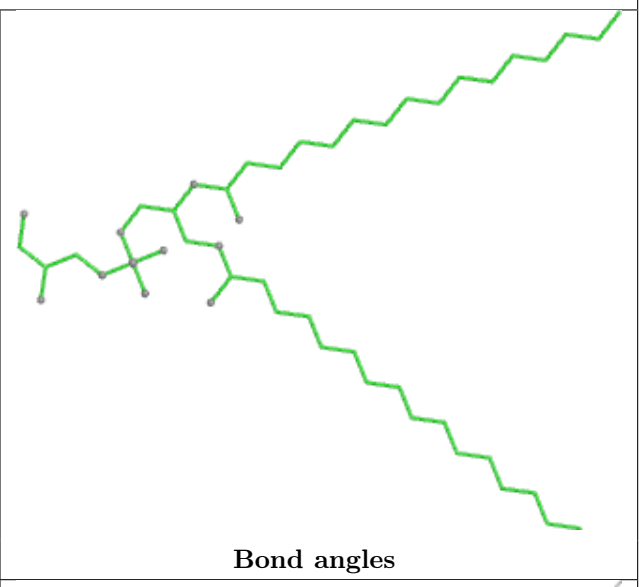
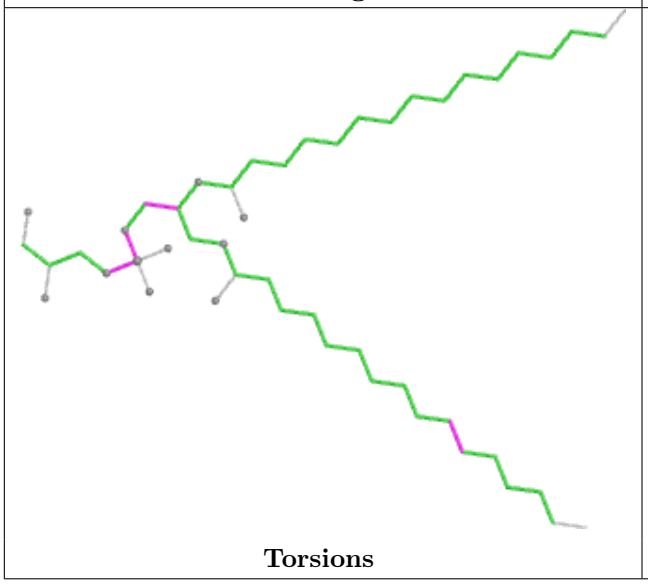


Bond angles



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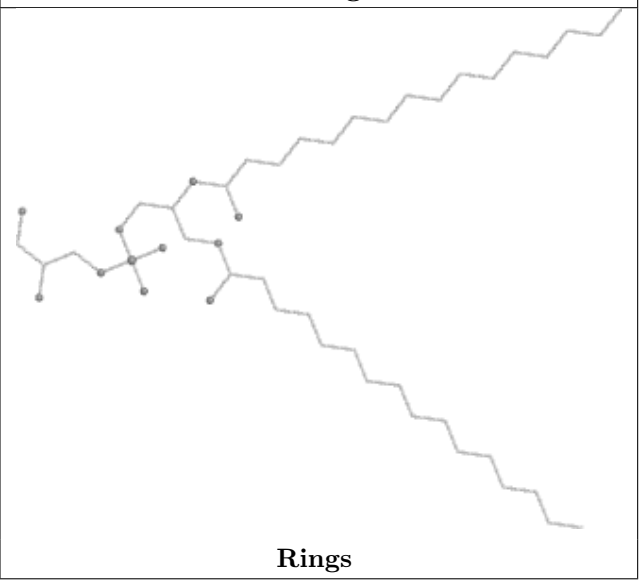
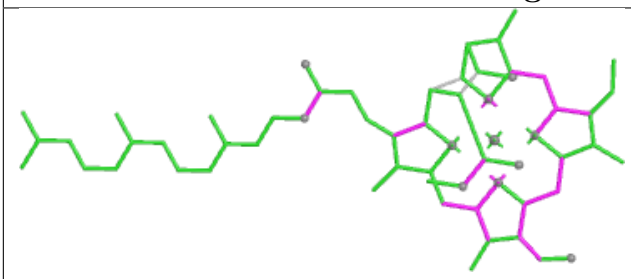


Rings

Ligand CL7 12 511



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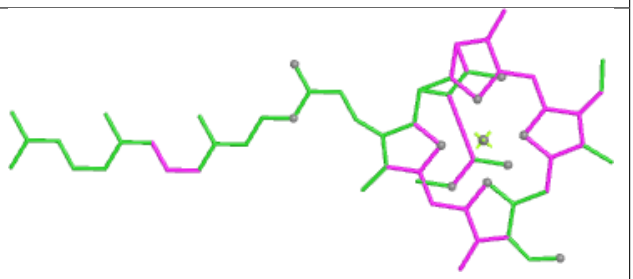
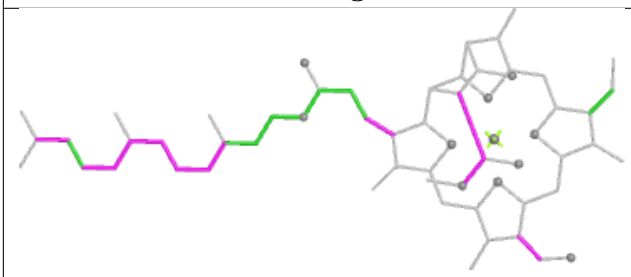


Bond angles



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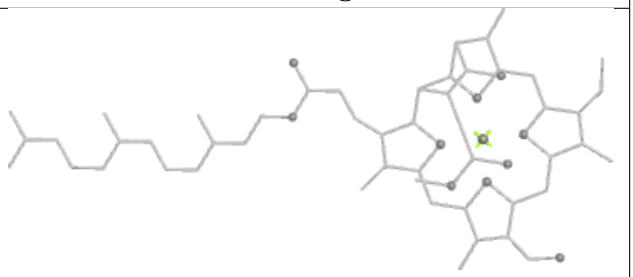
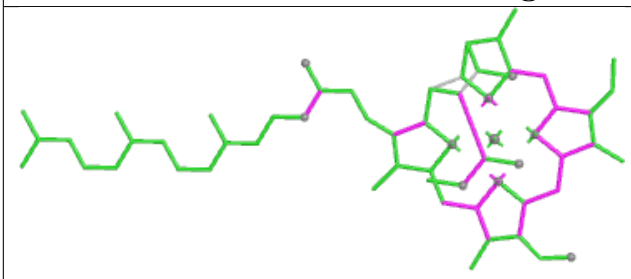


Rings

Ligand CL7 1B 614



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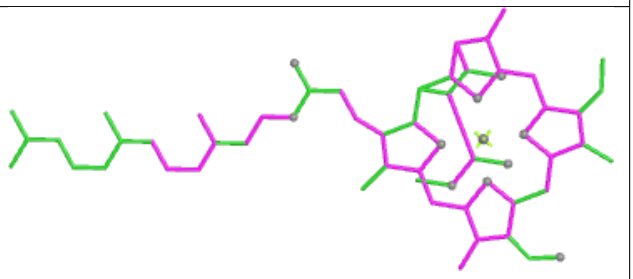
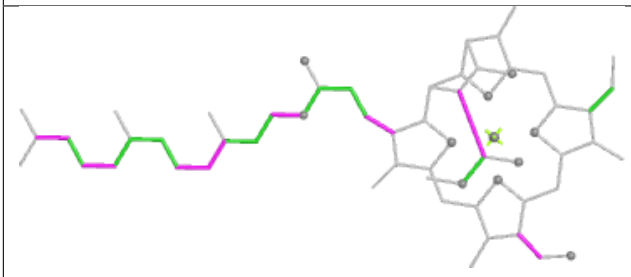


Bond angles



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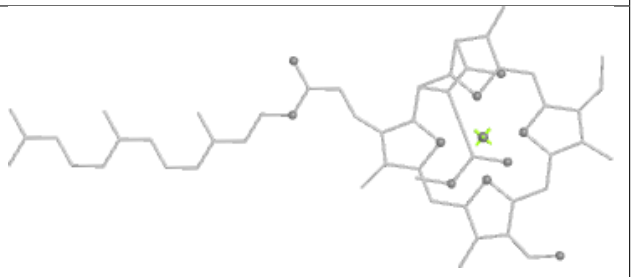
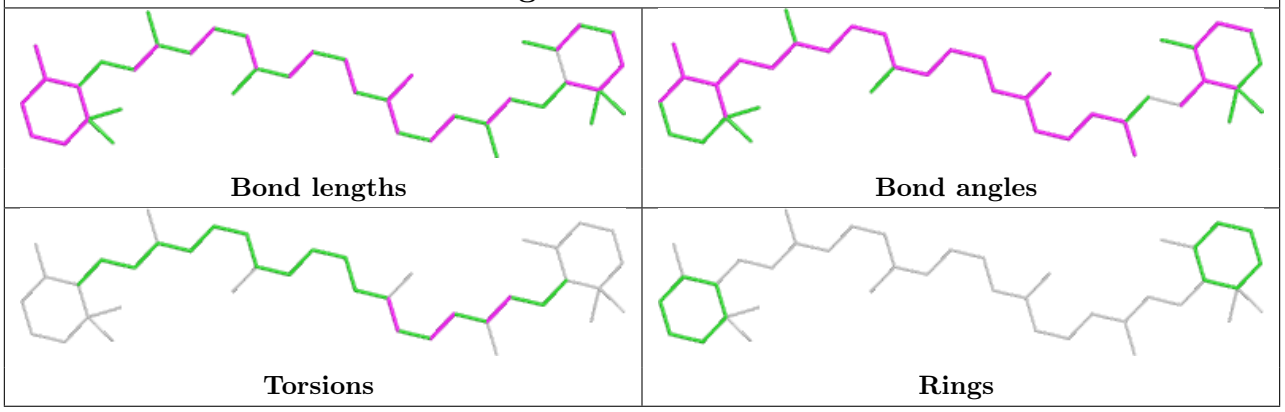


Rings

Ligand 8CT 2A 404



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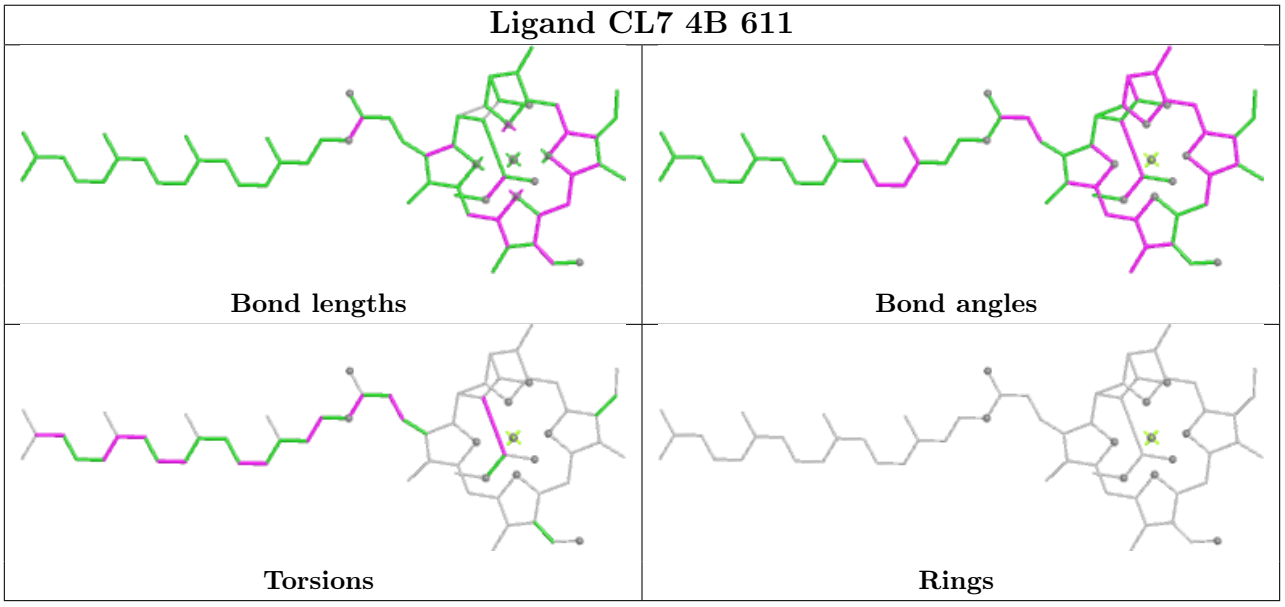
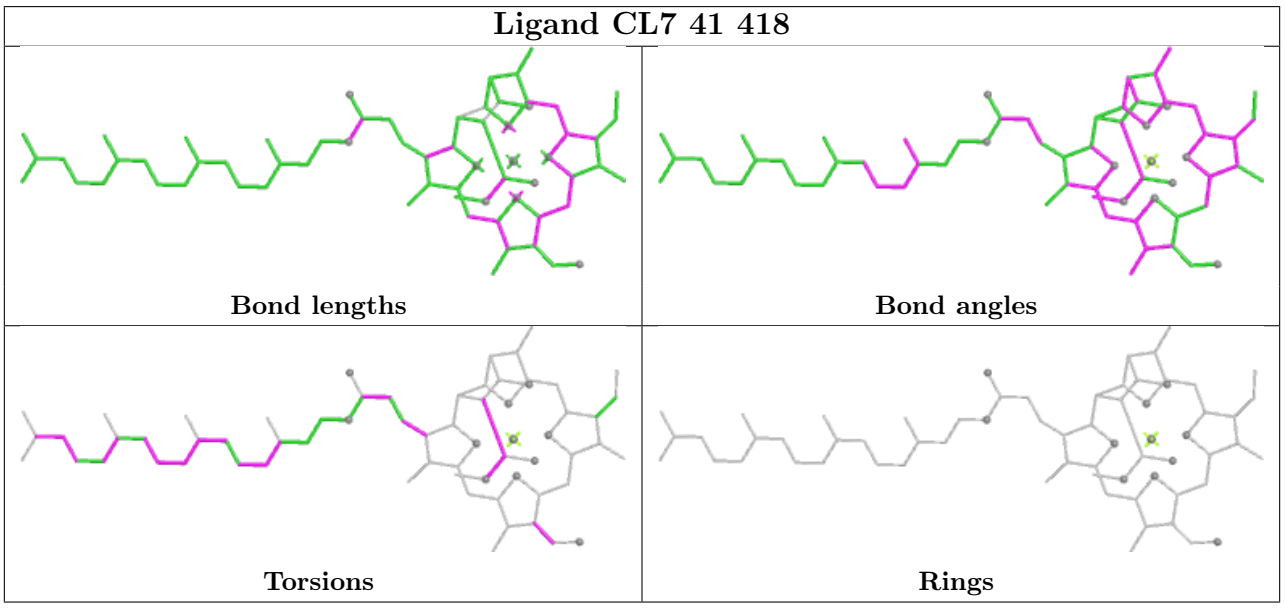
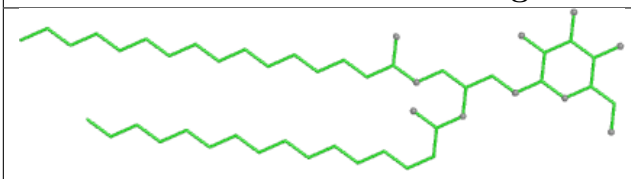


Ligand CL7 41 418



Ligand LMG 2B 622



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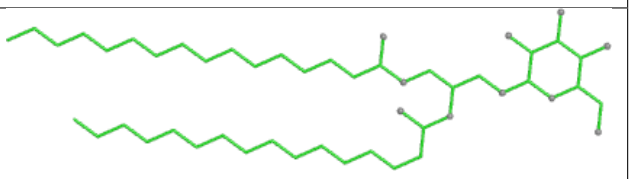
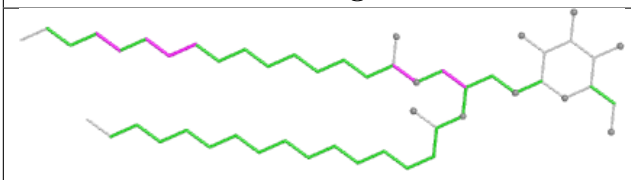


Bond angles



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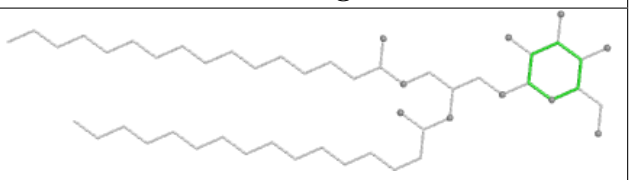
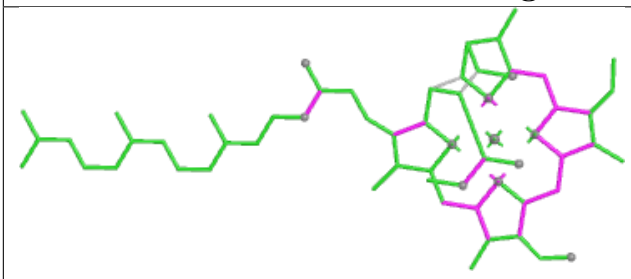


Rings

Ligand CL7 1B 607



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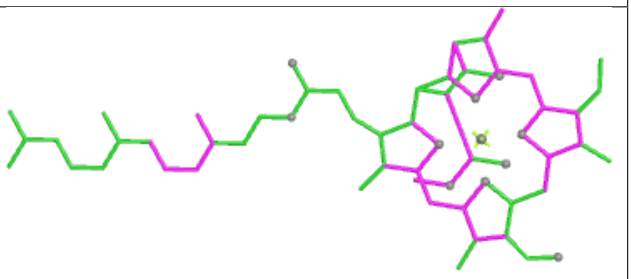
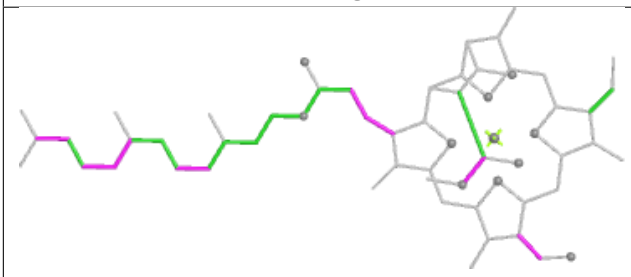


Bond angles



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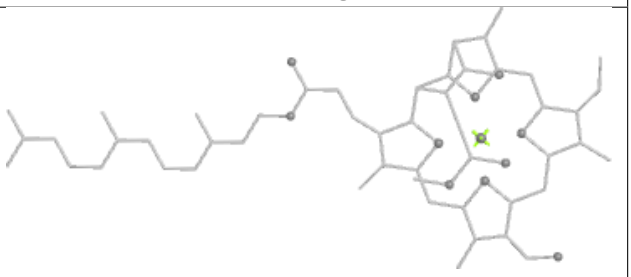
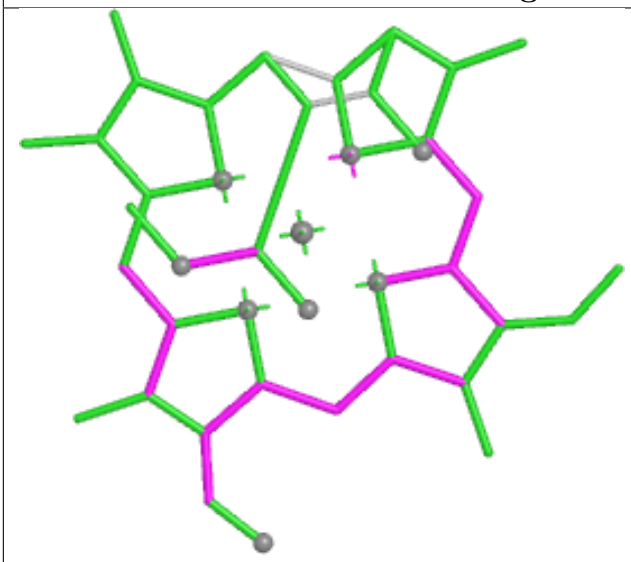


Rings

Ligand CL7 3B 601



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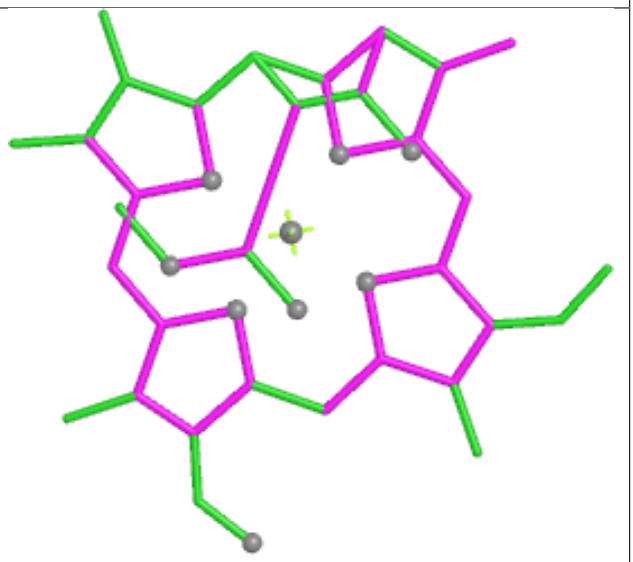

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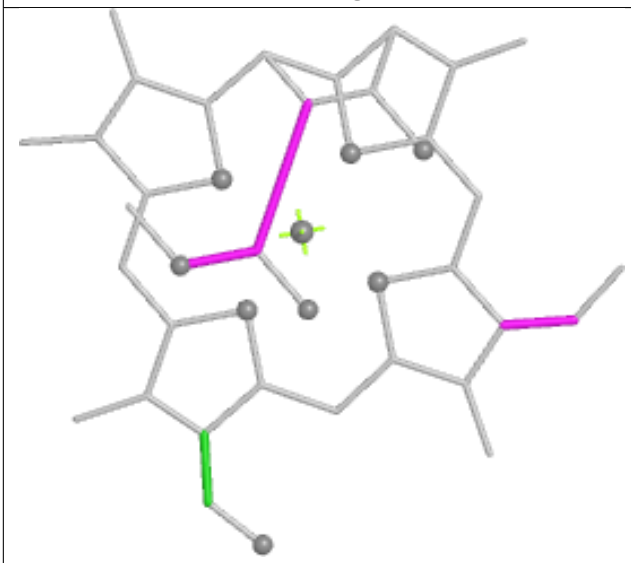

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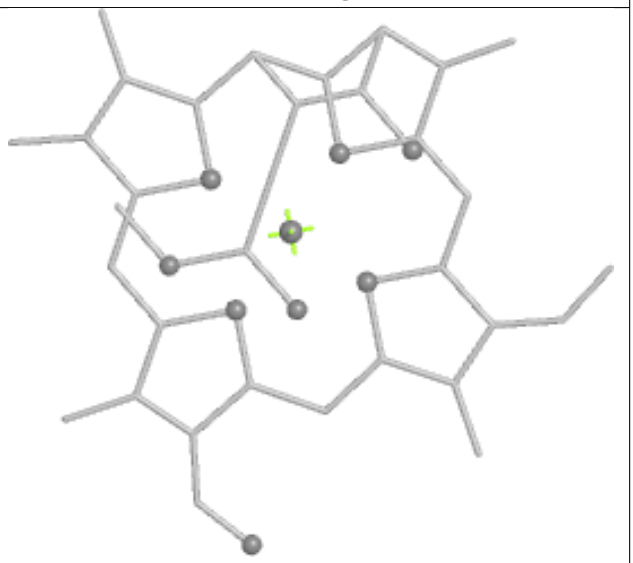

Rings

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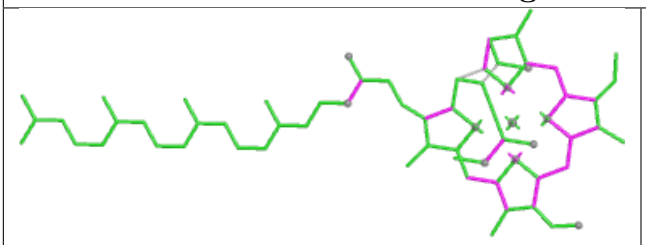

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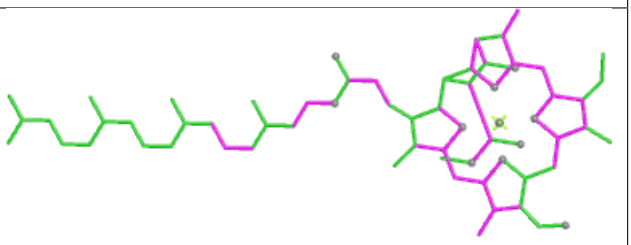

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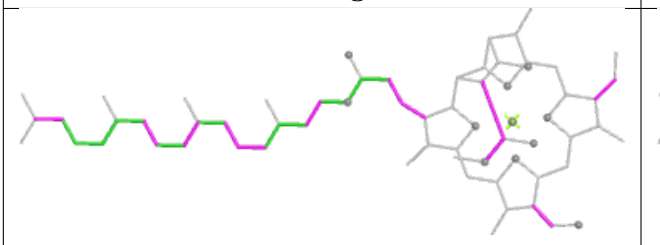

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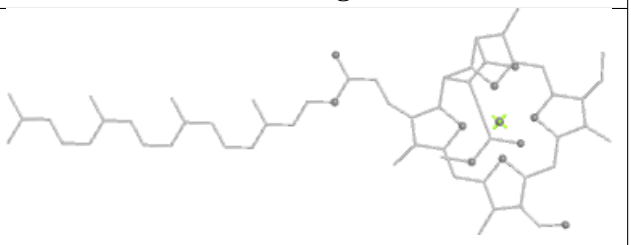
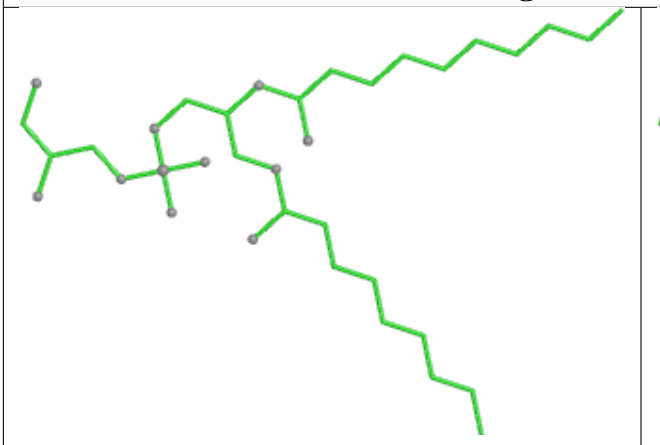


Rings

Ligand LHG 43 425



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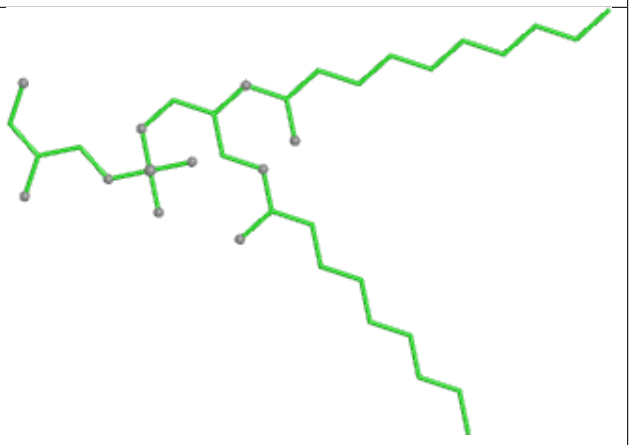

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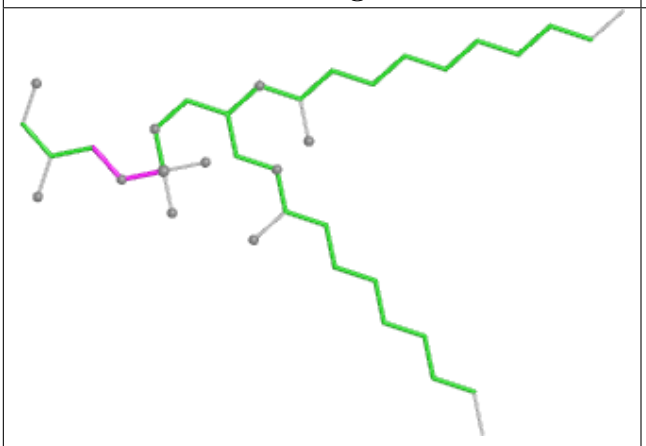

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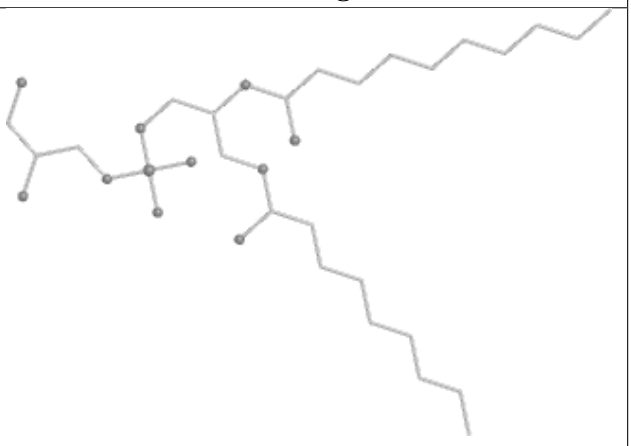
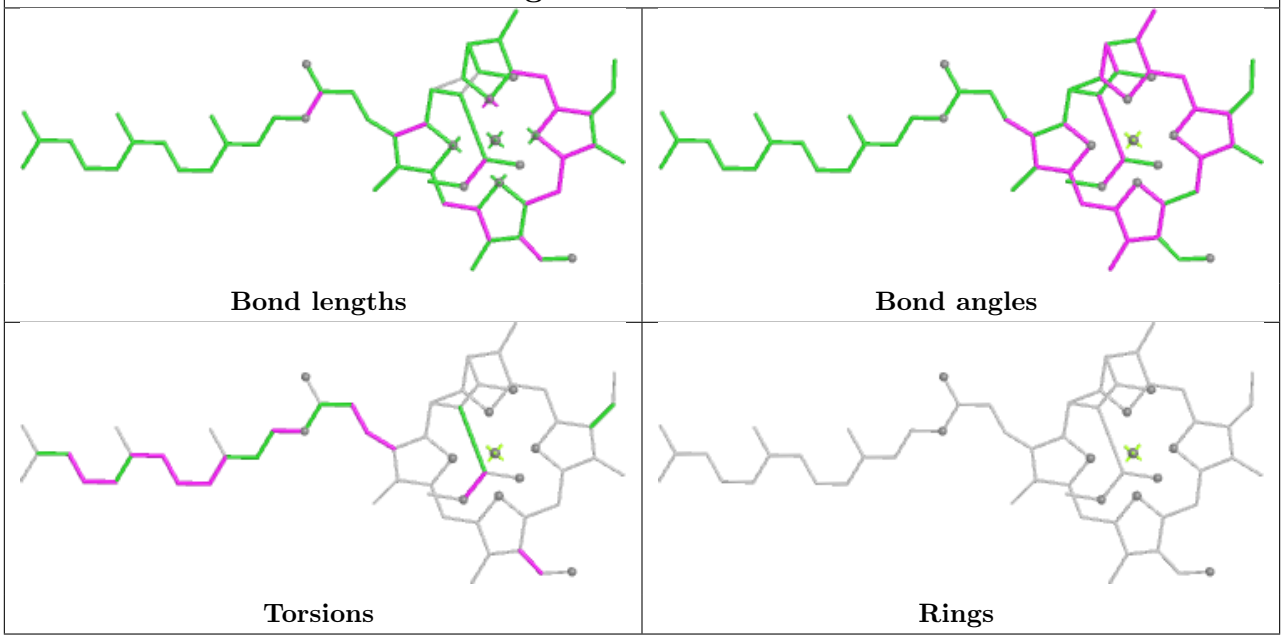
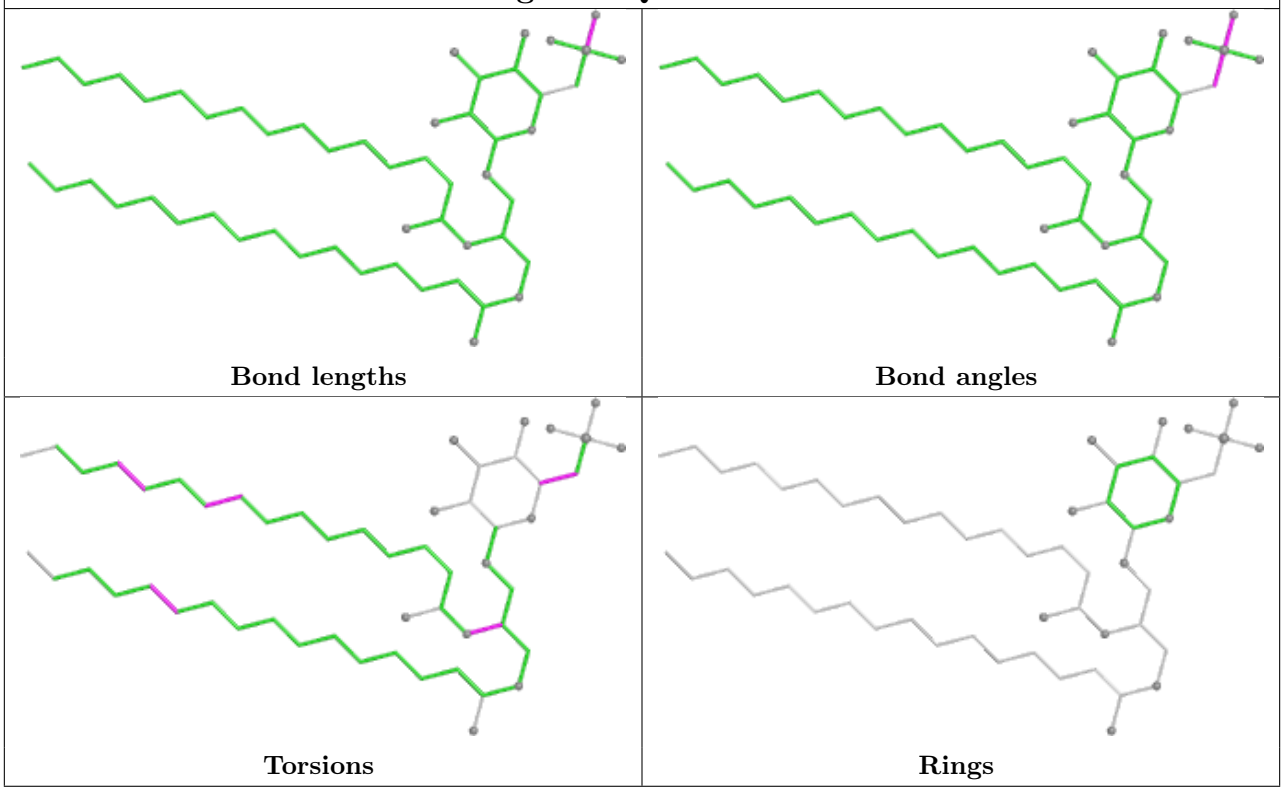


Rings

Ligand CL7 41 402



Ligand SQD 4B 621



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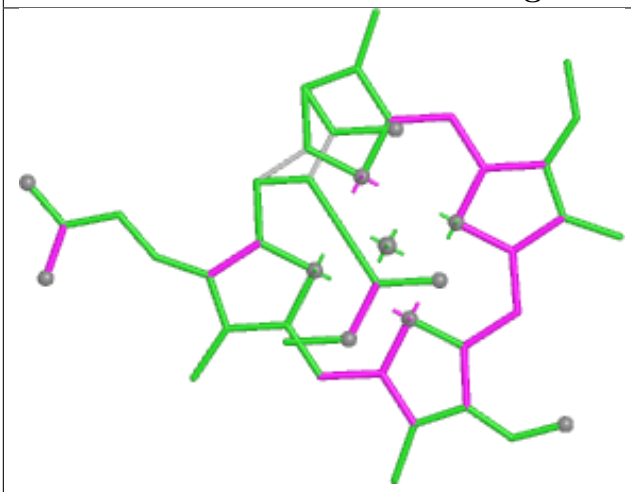

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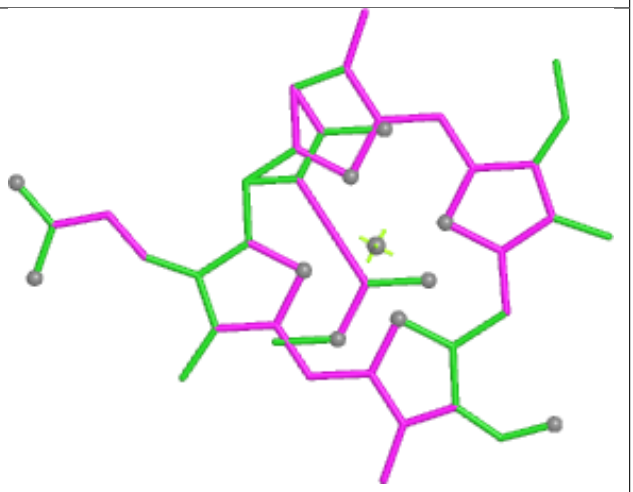
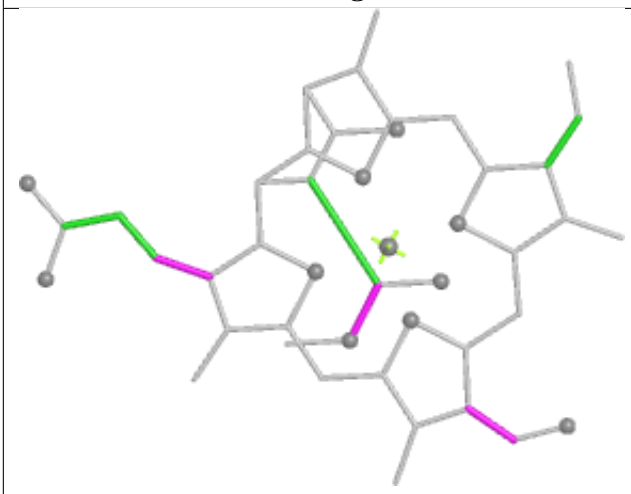


Bond angles

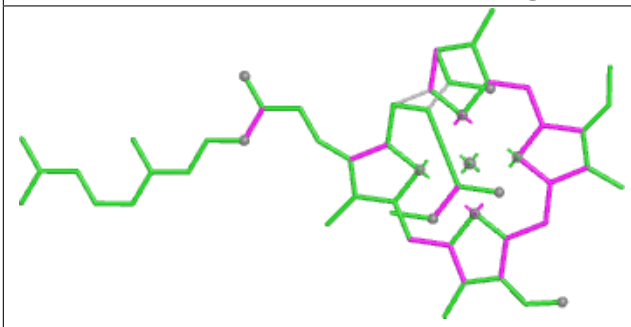


Torsions



Rings

Ligand CL7 23 417



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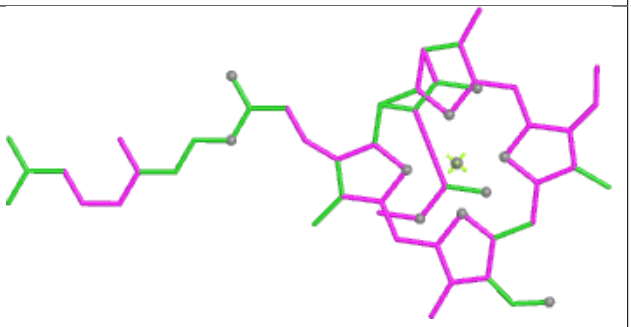
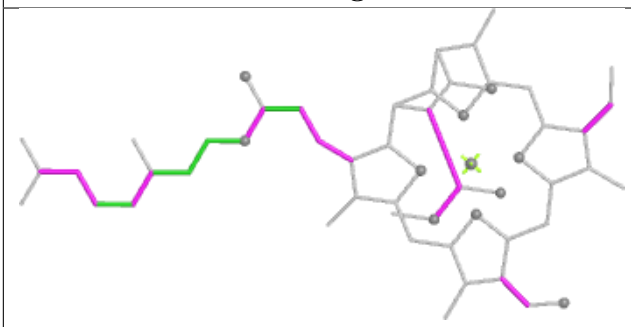


Bond angles



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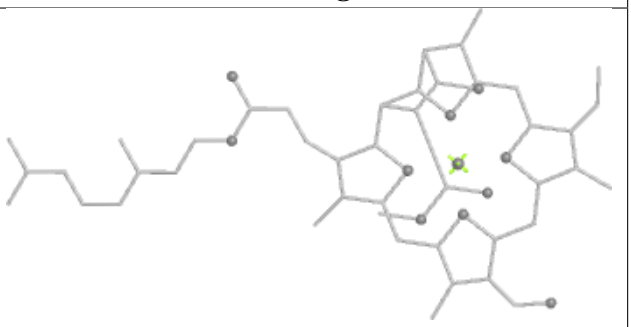
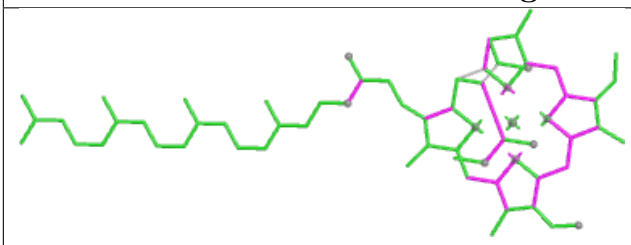


Rings

Ligand CL7 2C 505



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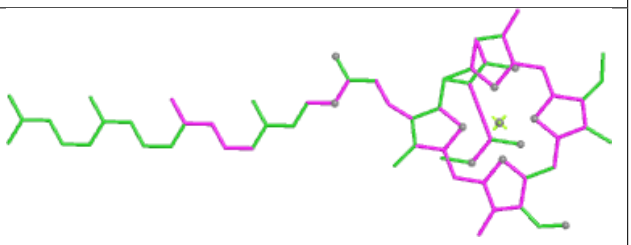
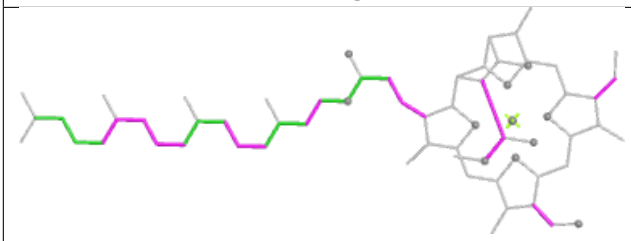


Bond angles



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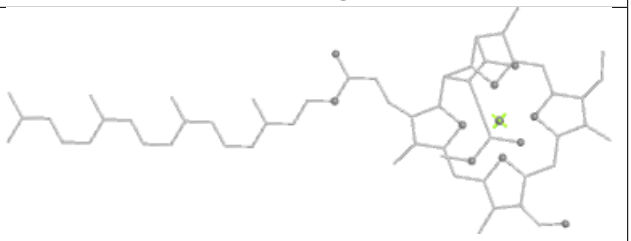
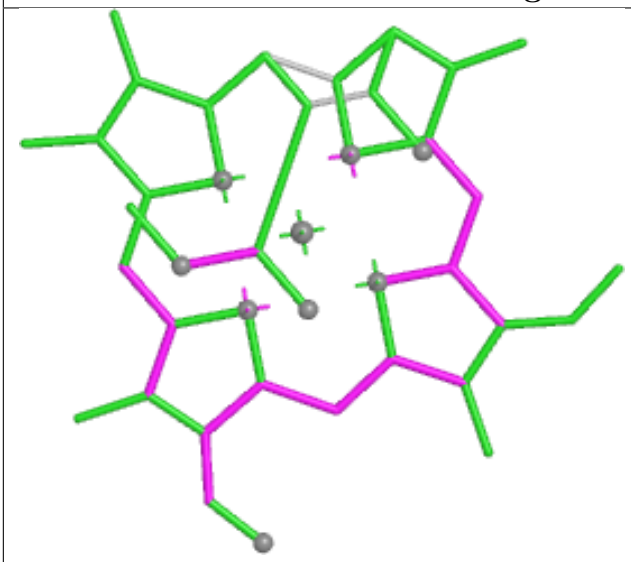


Rings

Ligand CL7 31 407



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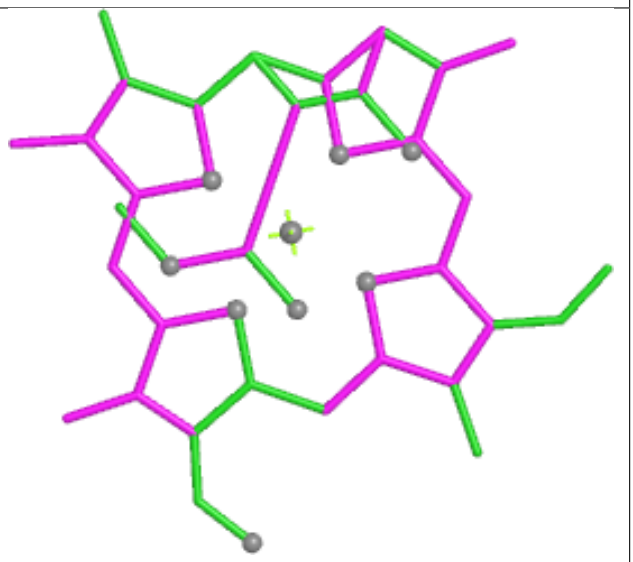
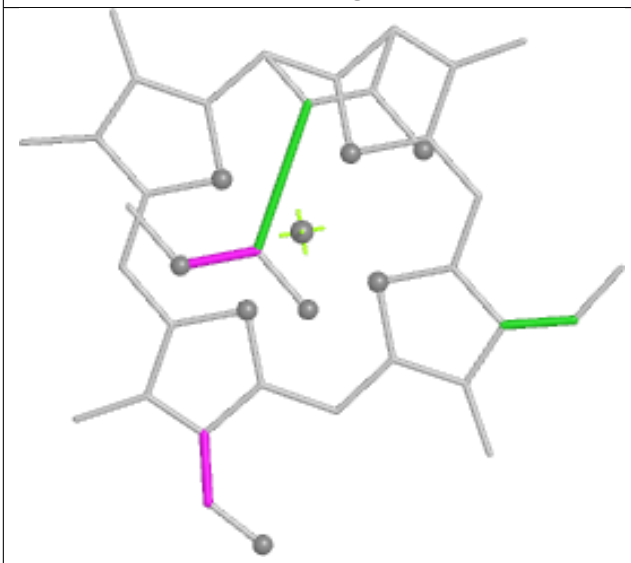


Bond angles



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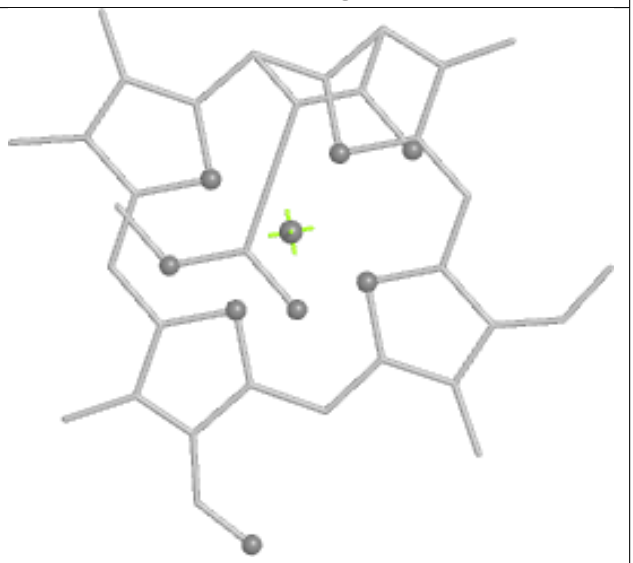
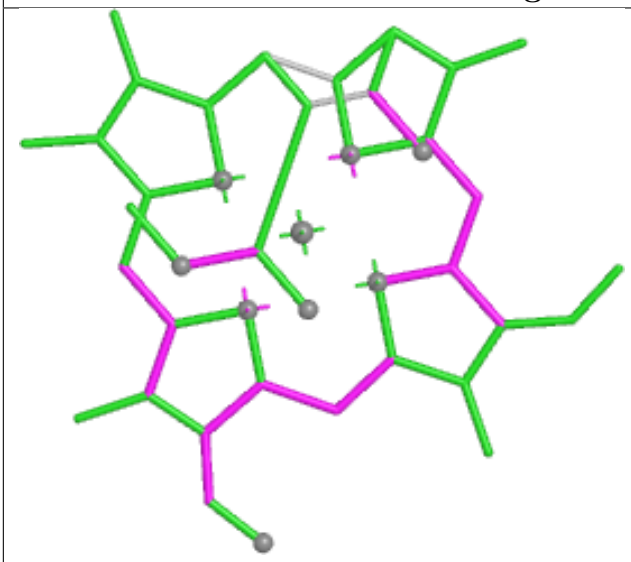


Rings

Ligand CL7 44 416



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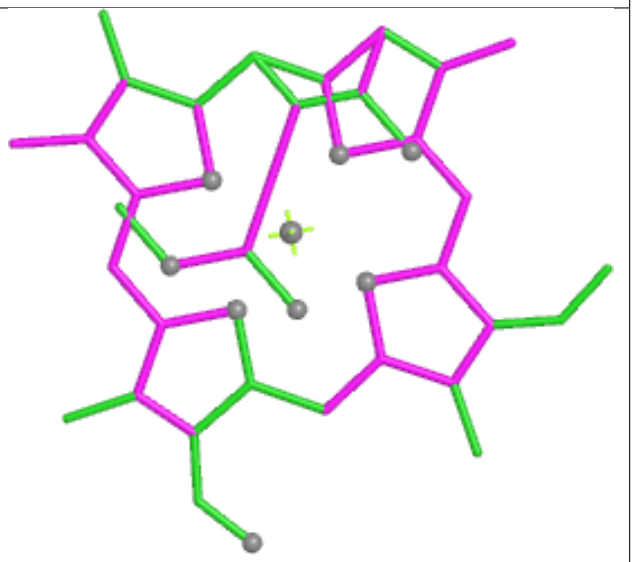
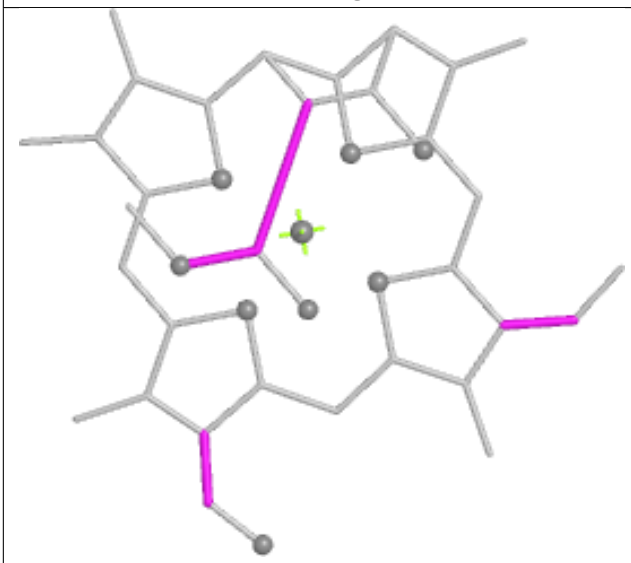
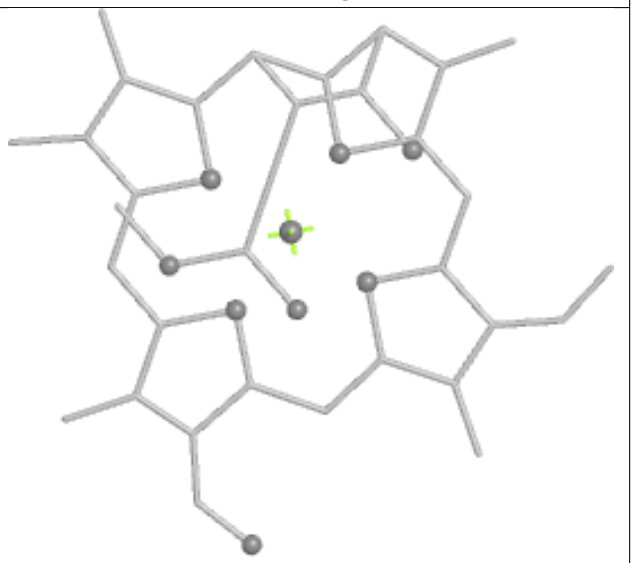


Bond angles

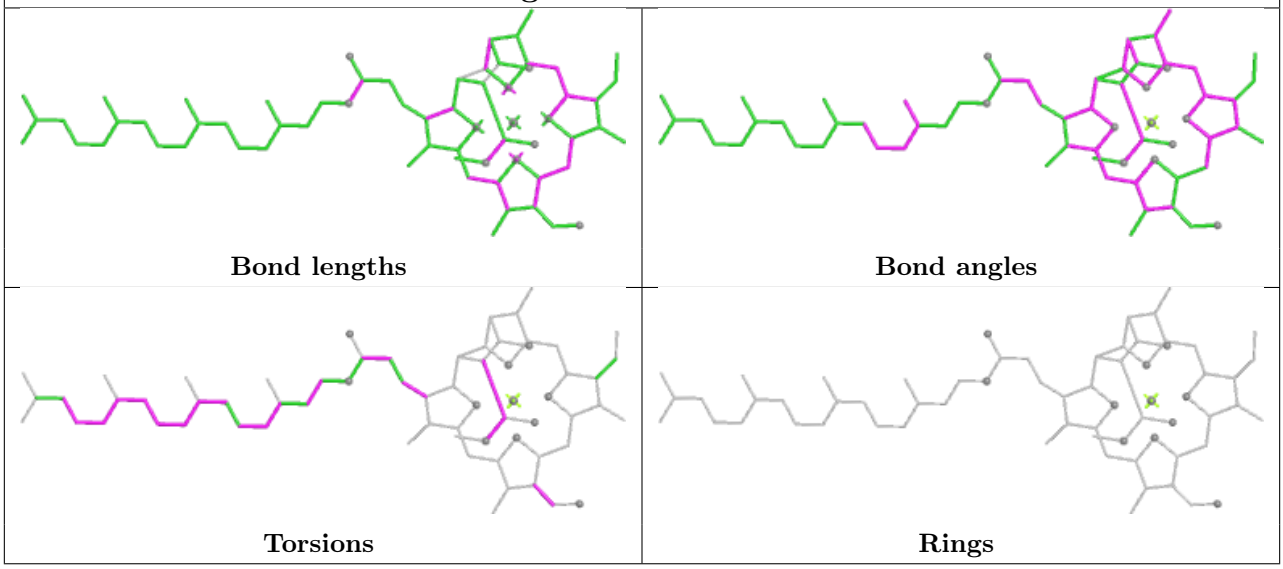


Torsions



Rings

Ligand CL7 2C 510



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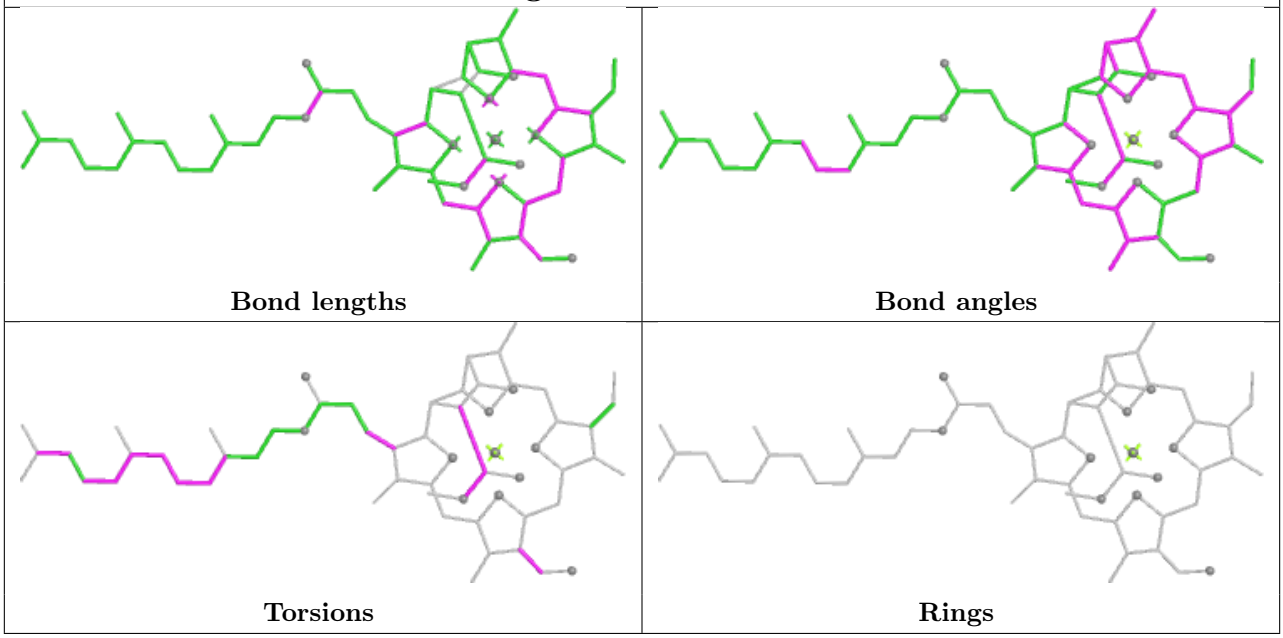

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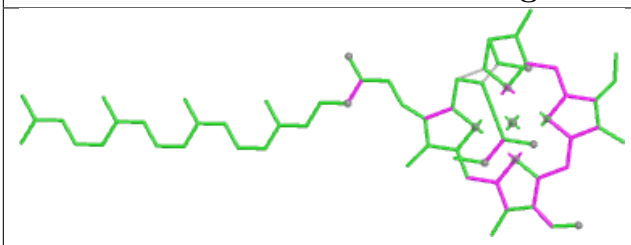
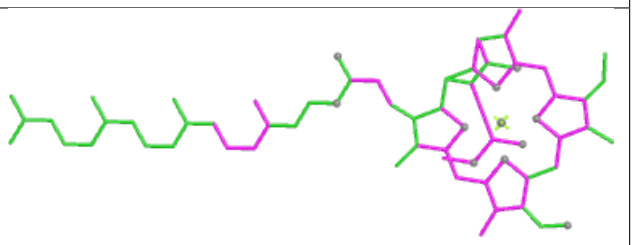
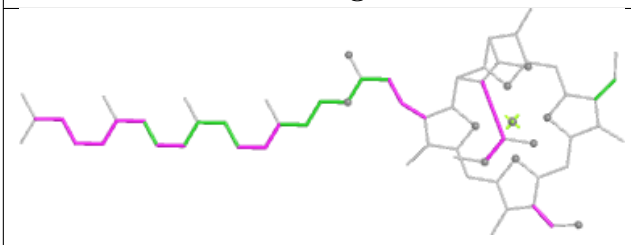


Bond lengths



Bond angles



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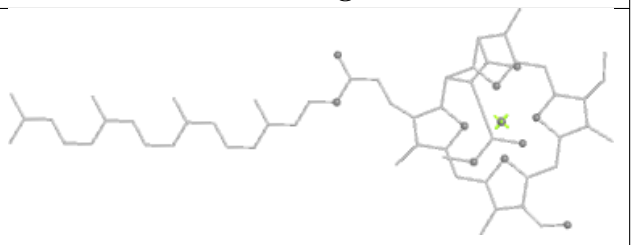
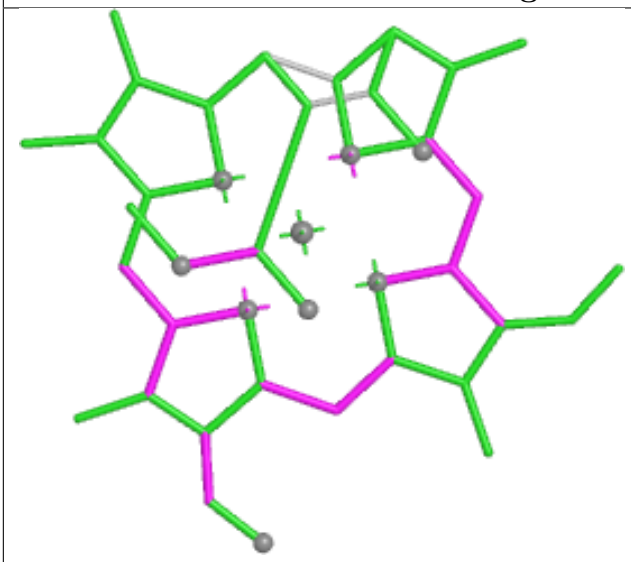


Rings

Ligand CL7 1C 512



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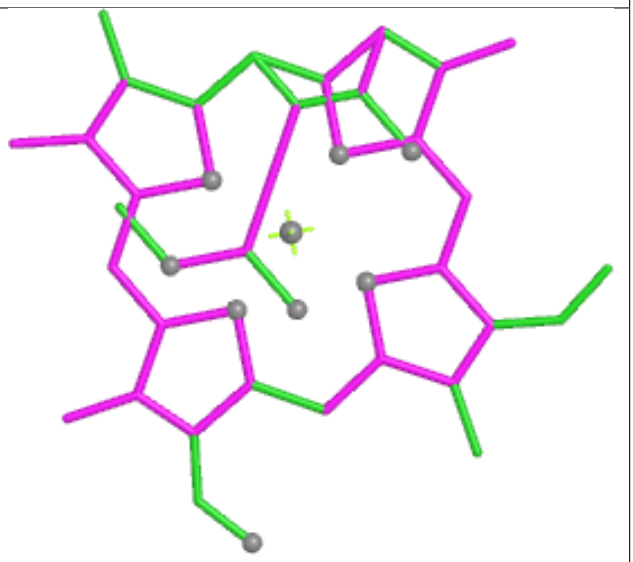
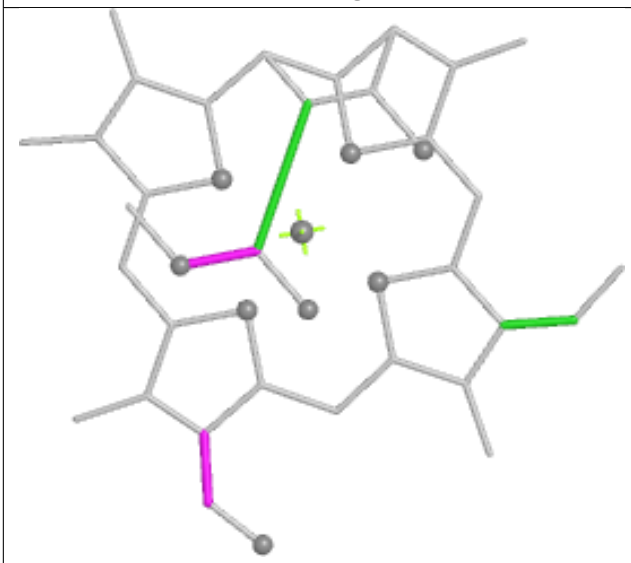


Bond angles



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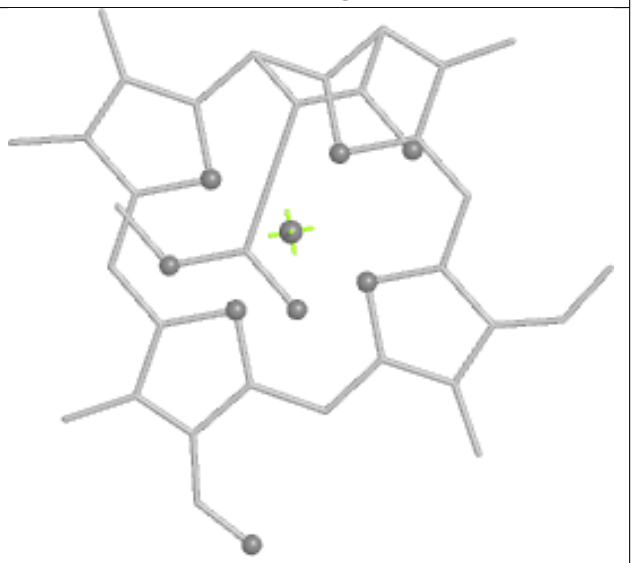
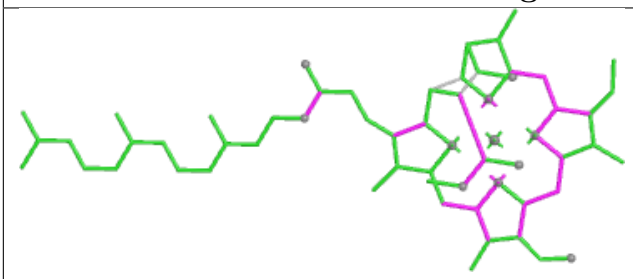


Rings

Ligand CL7 3C 506



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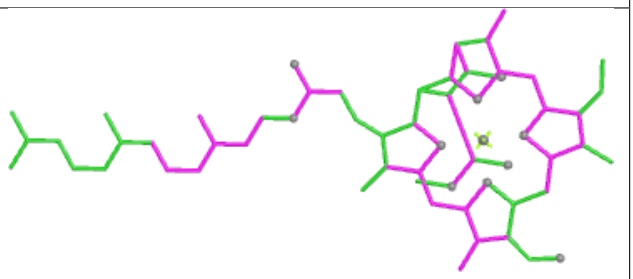

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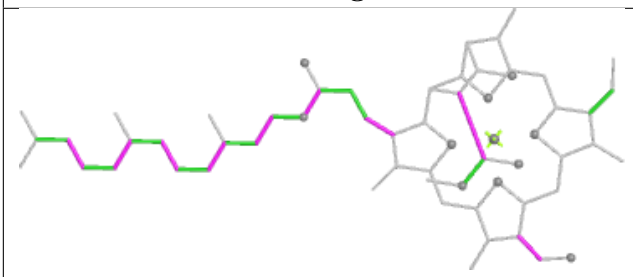

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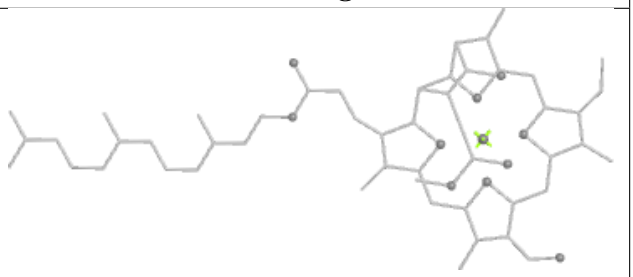
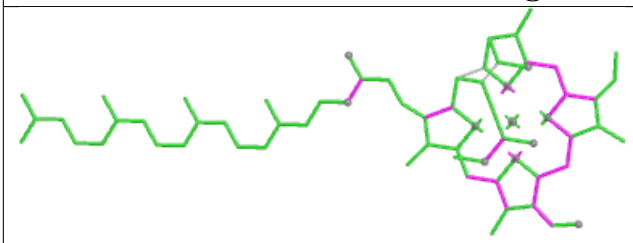


Rings

Ligand CL7 11 418



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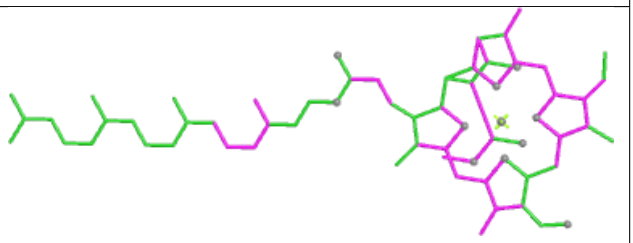

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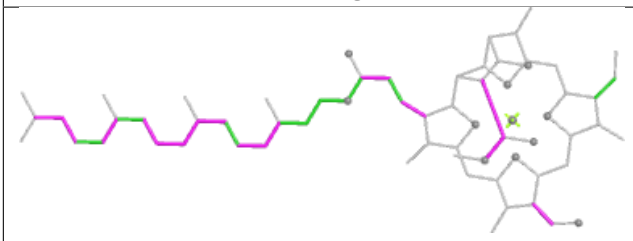

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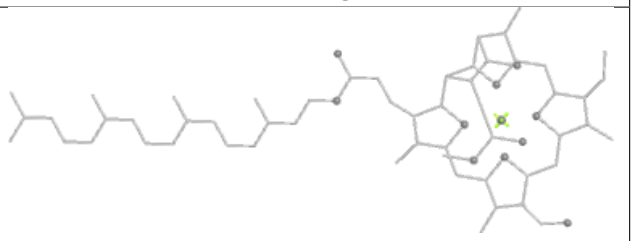
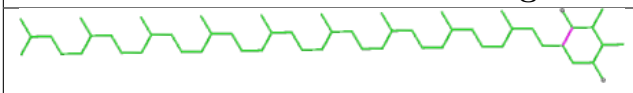


Rings

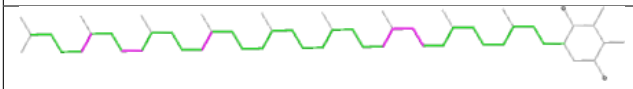
Ligand PL9 2D 407



Bond lengths



Bond angles



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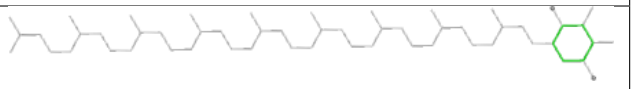
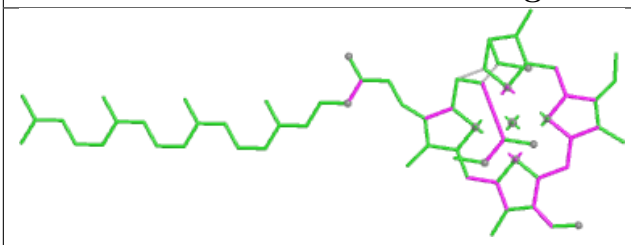


Rings

Ligand CL7 12 503



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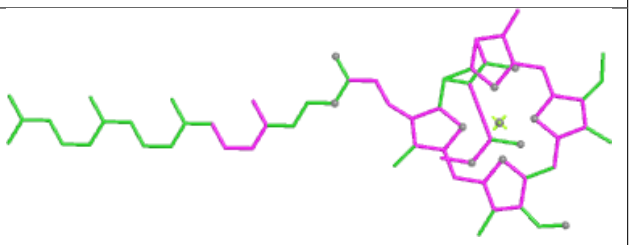
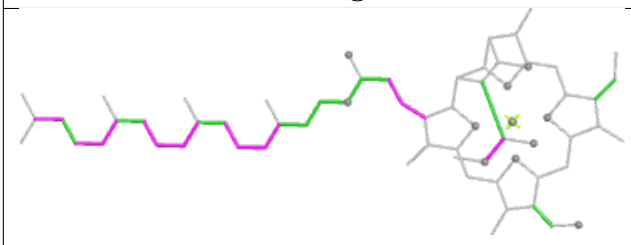


Bond angles



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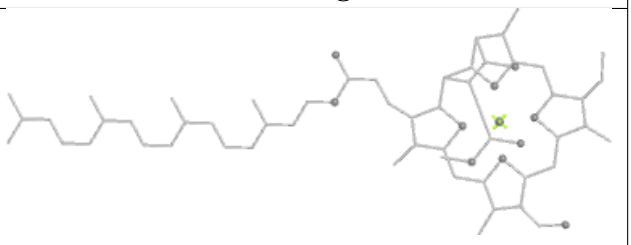
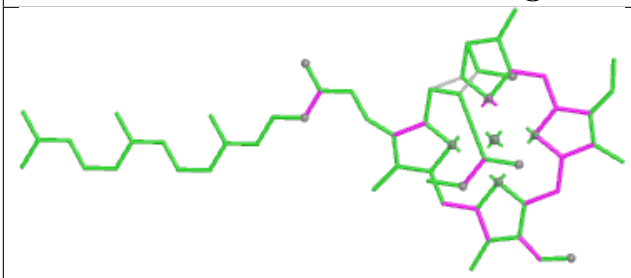


Rings

Ligand CL7 11 402



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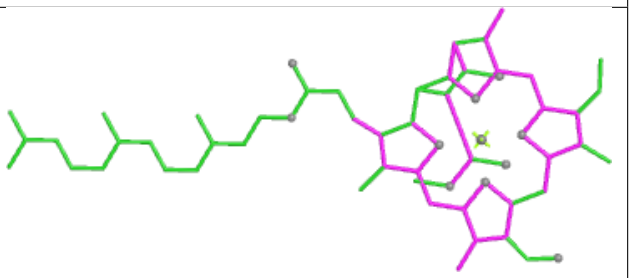
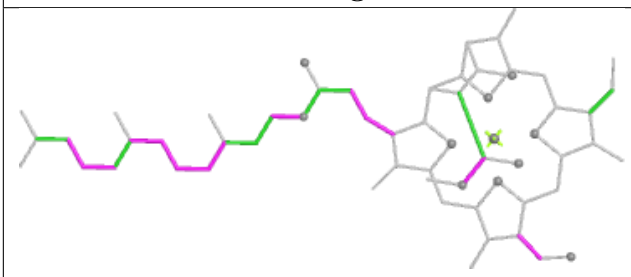


Bond angles



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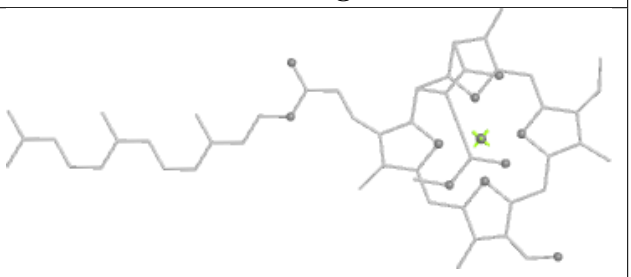

Rings

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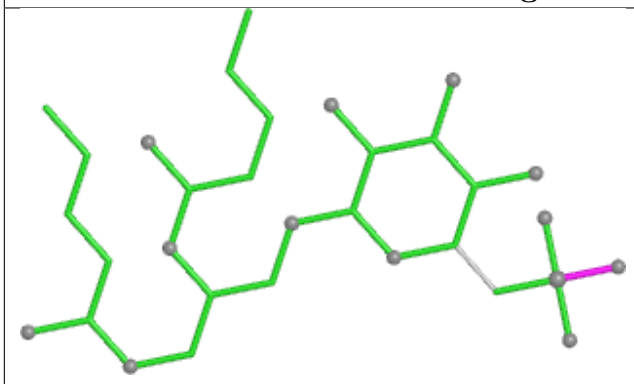

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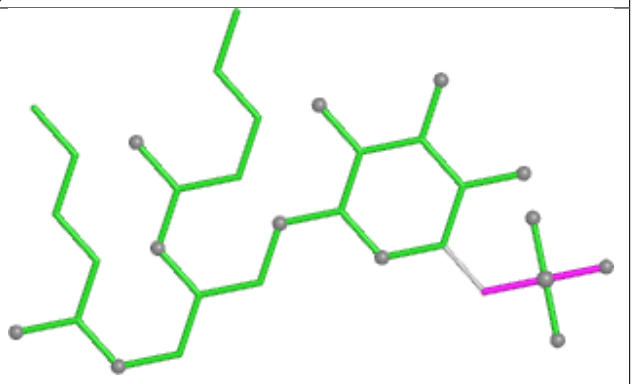

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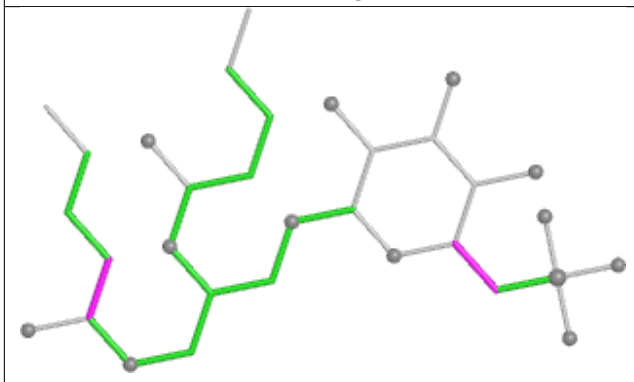

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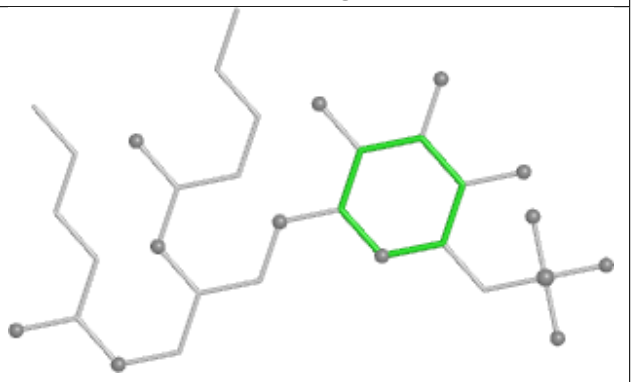
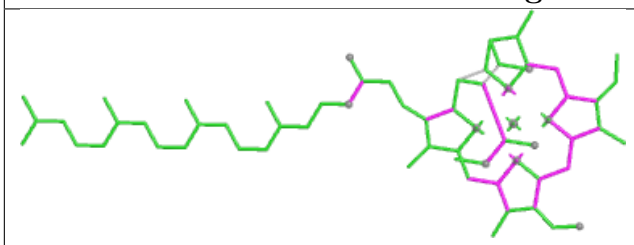


Rings

Ligand CL7 33 511



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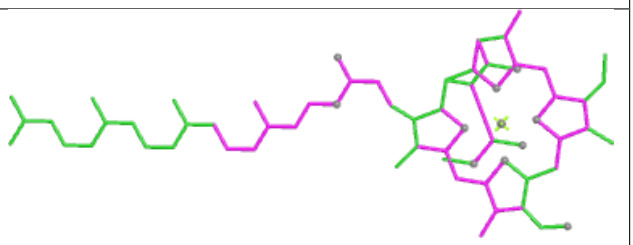

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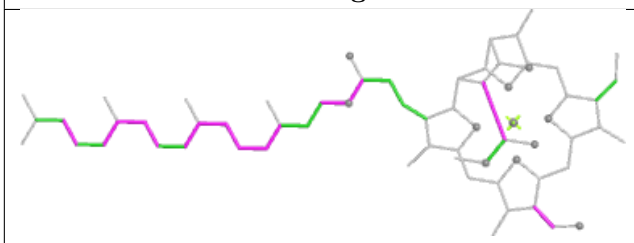

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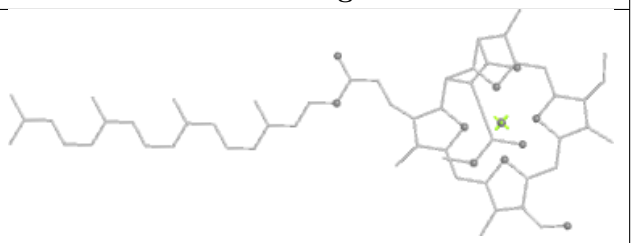
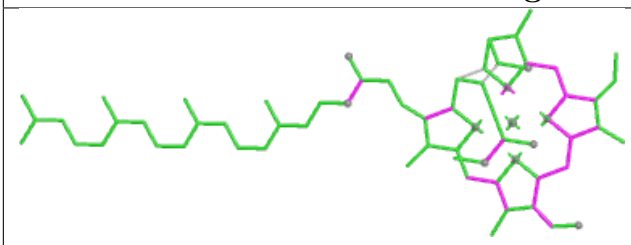


Rings

Ligand CL7 44 405



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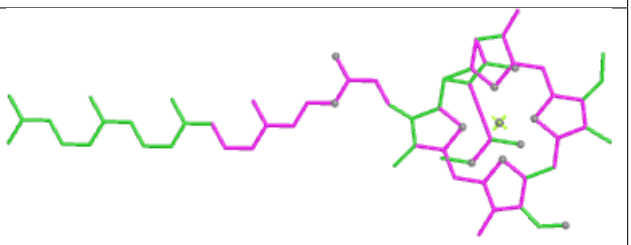
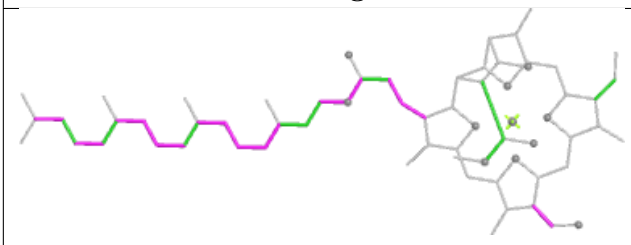


Bond angles



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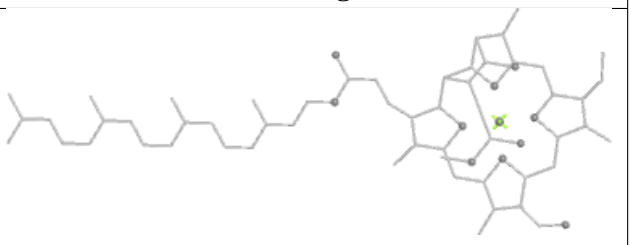
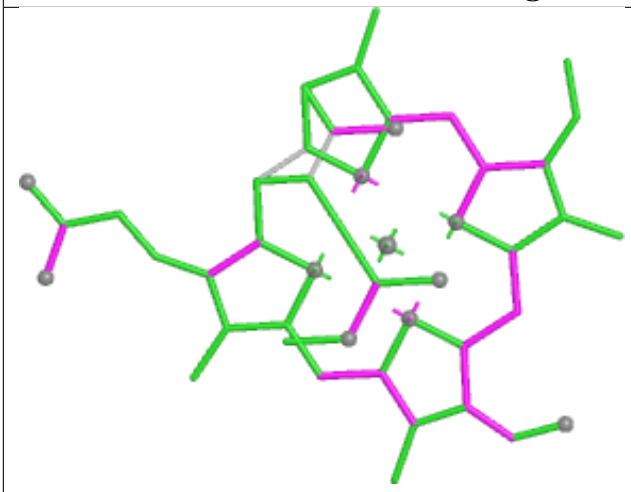


Rings

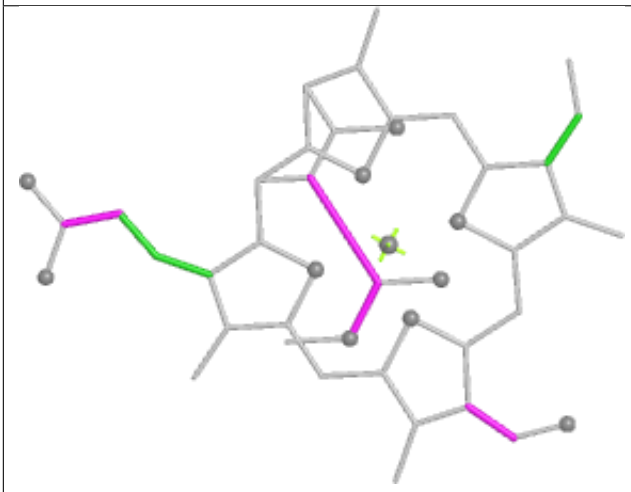
Ligand CL7 11 411



Bond lengths



Bond angles

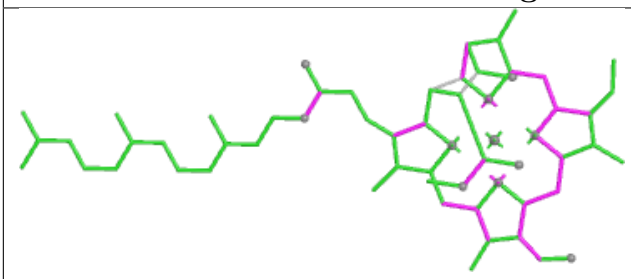


Torsions



Rings

Ligand CL7 2B 603



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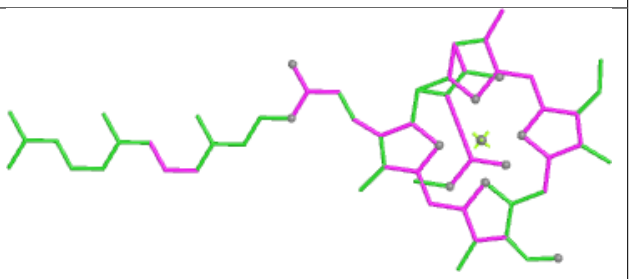
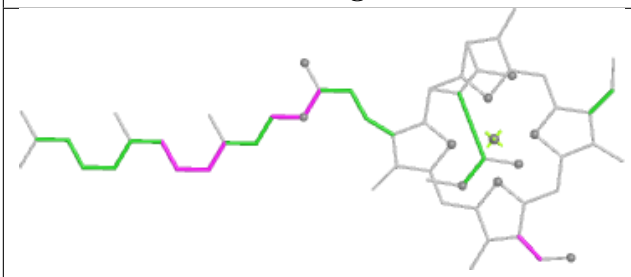


Bond angles



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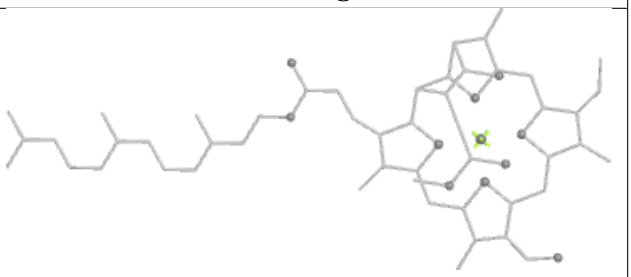
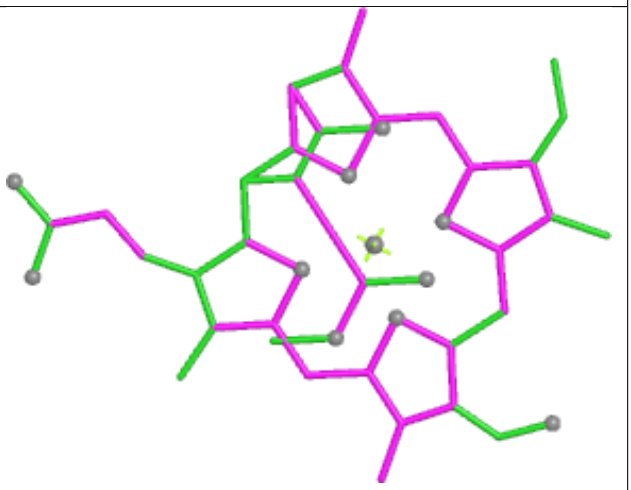


Rings

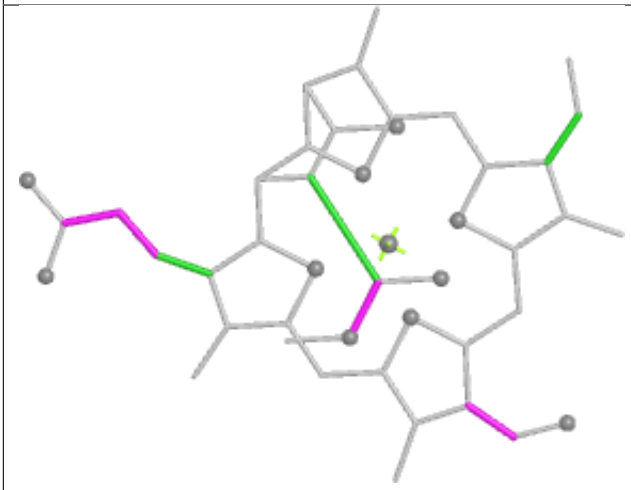
Ligand CL7 43 419



Bond lengths



Bond angles

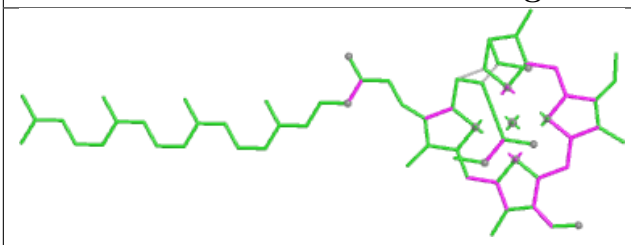


Torsions



Rings

Ligand CL7 43 405



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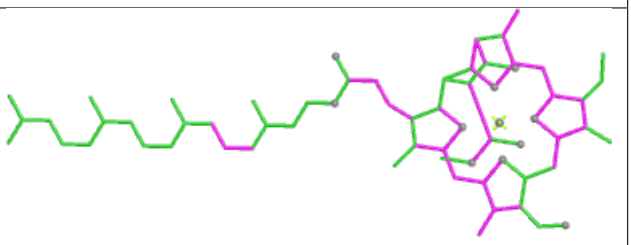
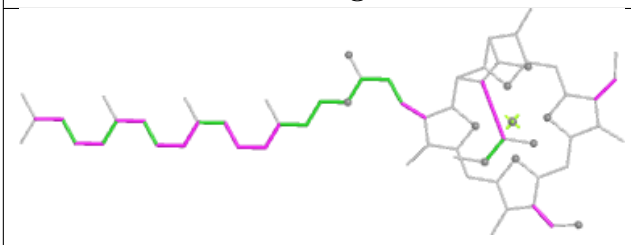


Bond angles



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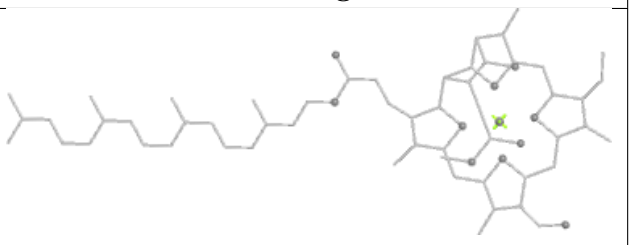
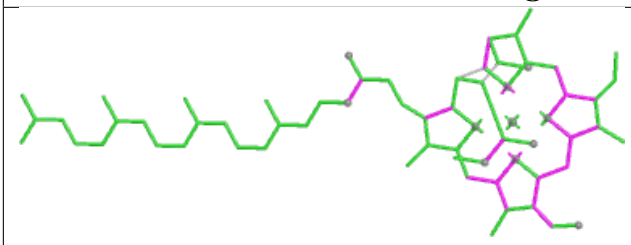


Rings

Ligand CL7 42 505



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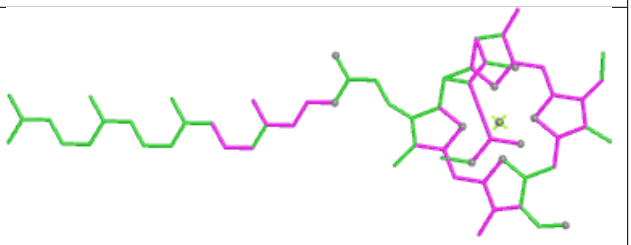
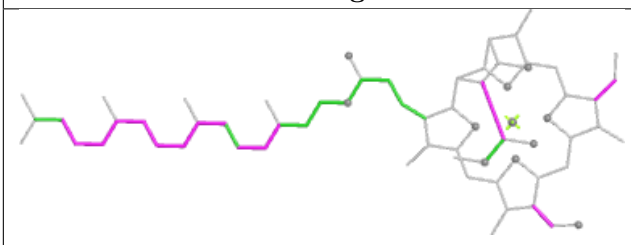
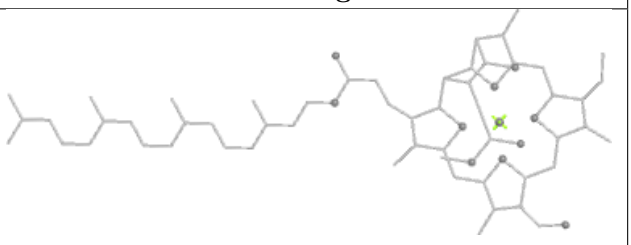


Bond angles

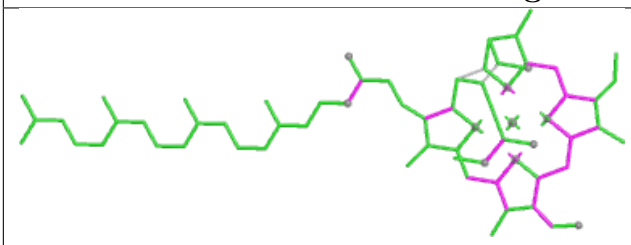


Torsions



Rings

Ligand CL7 42 510



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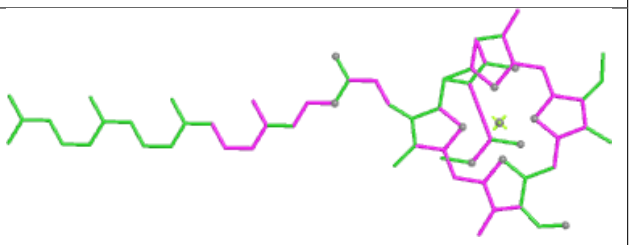
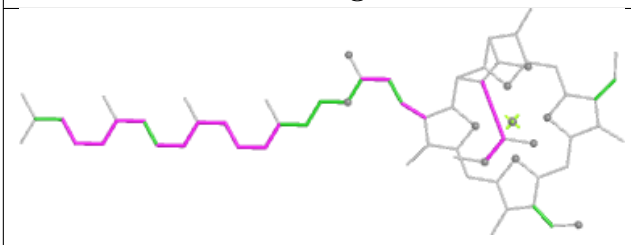


Bond angles



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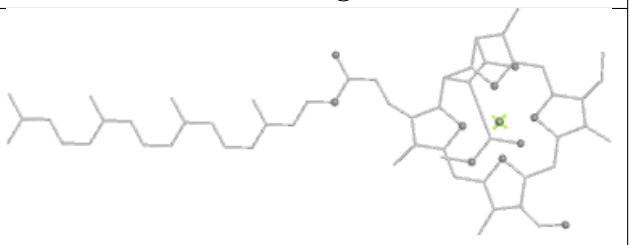
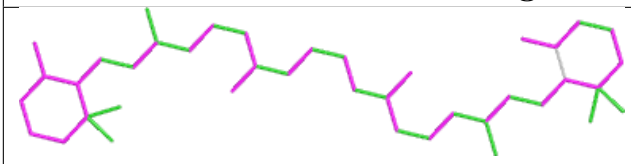


Rings

Ligand 8CT 2B 618



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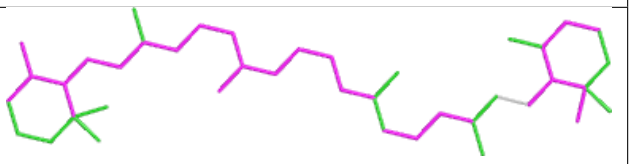

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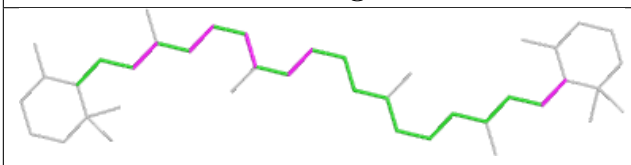

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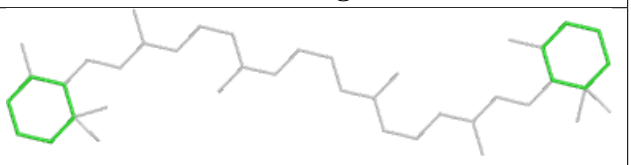
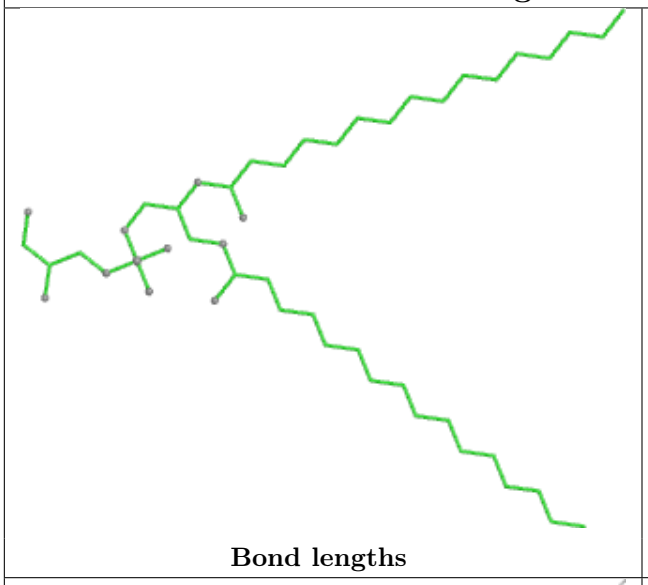


Rings

Ligand LHG 4D 409



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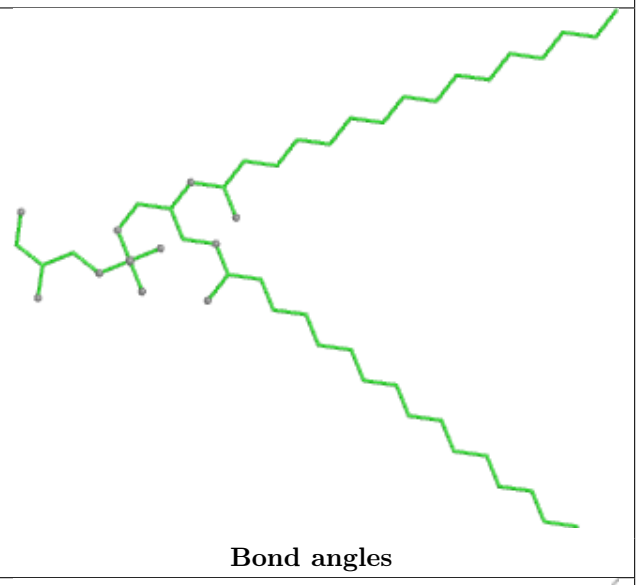

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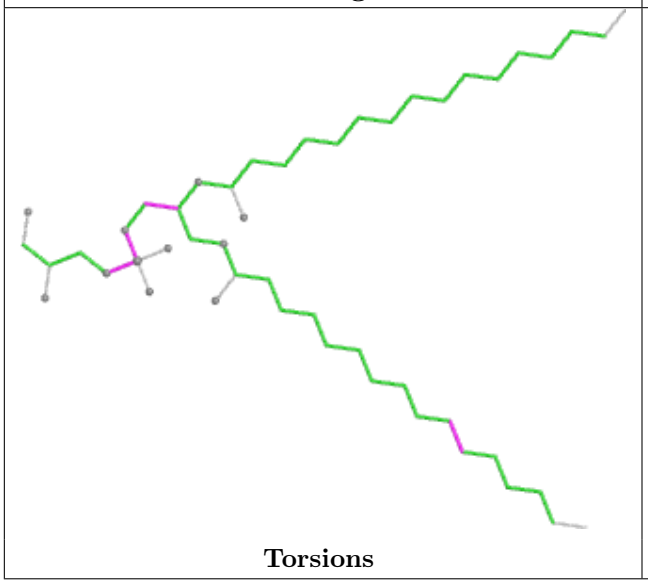

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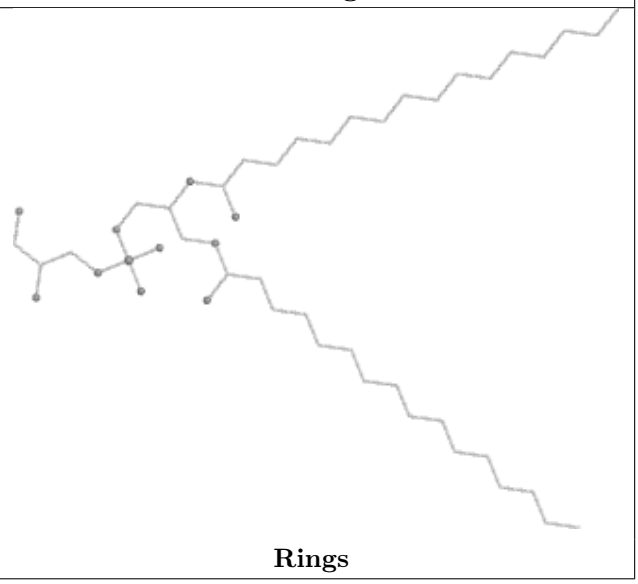
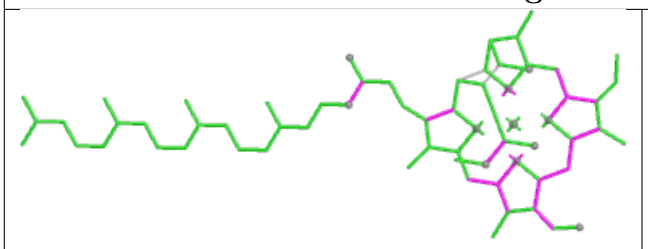


Rings

Ligand CL7 24 406



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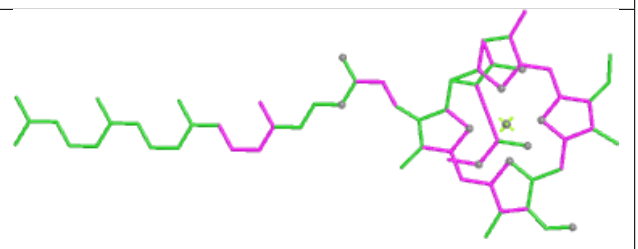

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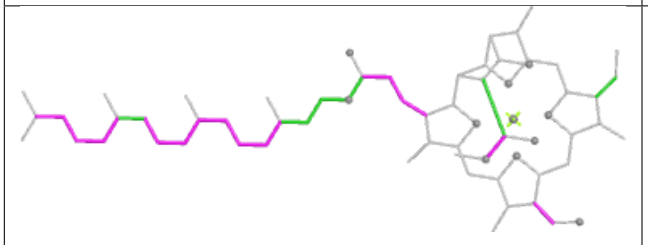

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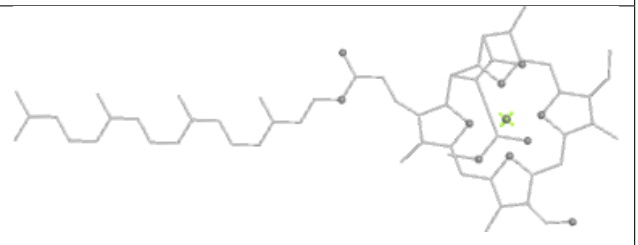
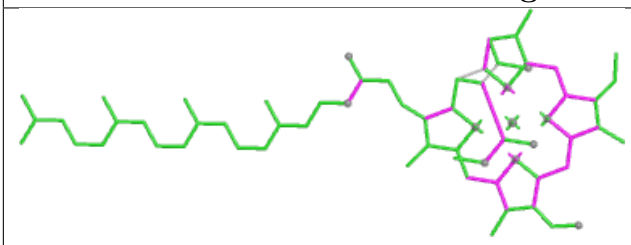


Rings

Ligand CL7 2C 509



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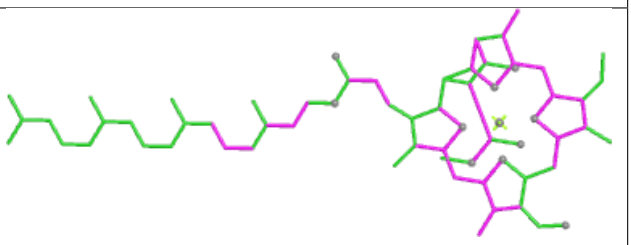

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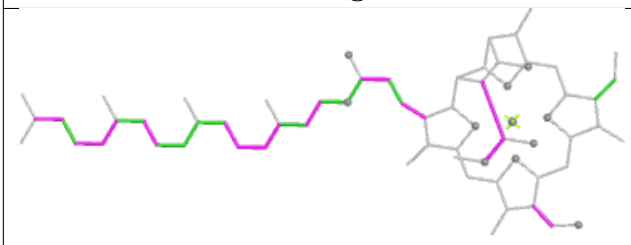

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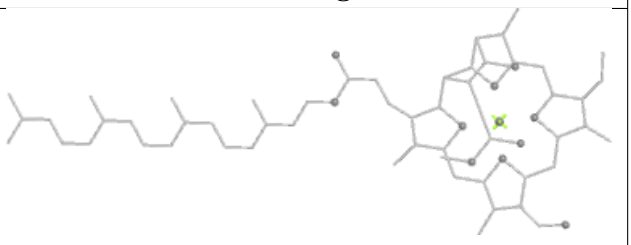

Rings

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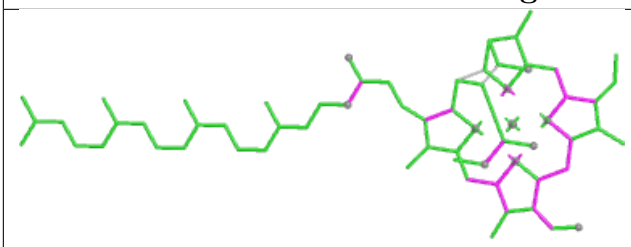

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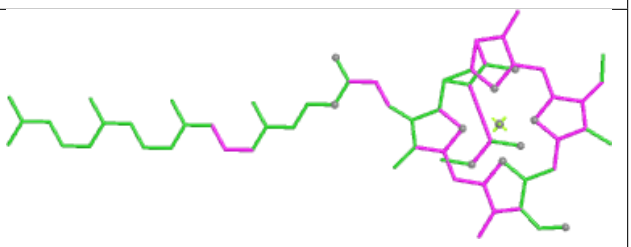

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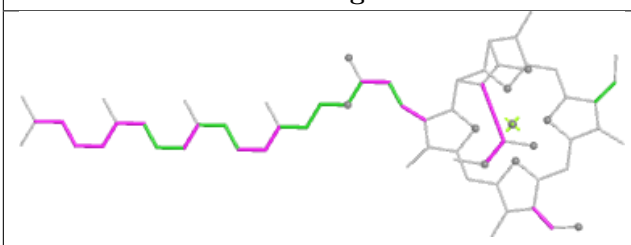

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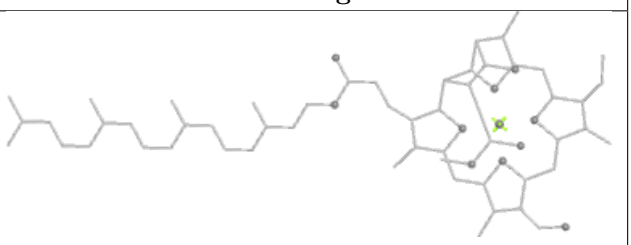
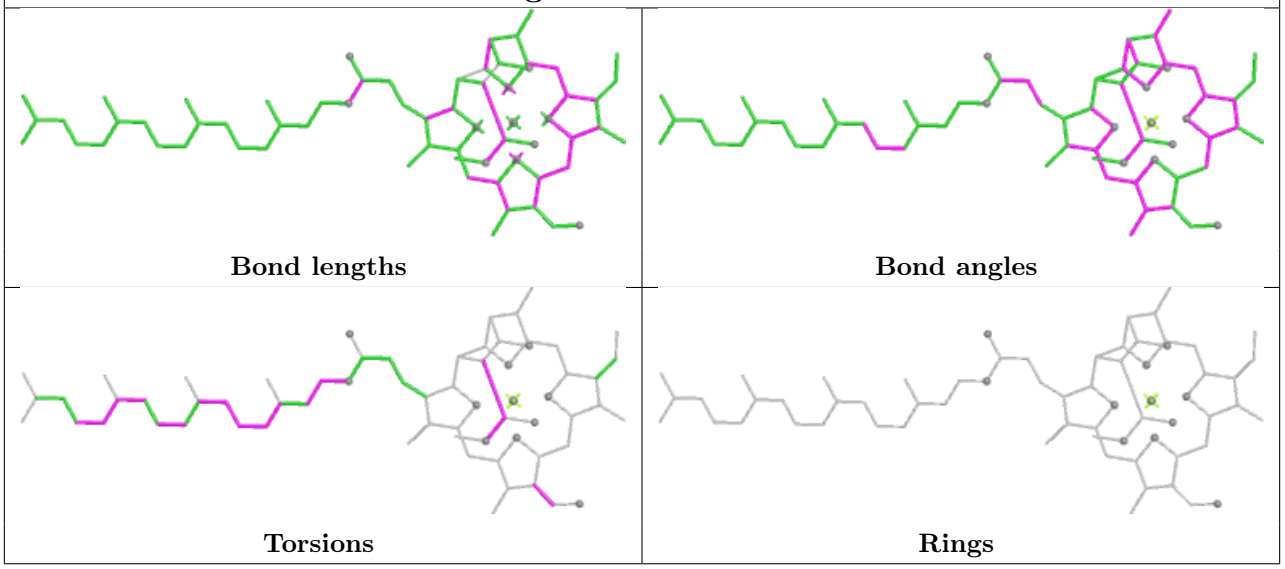


Rings

Ligand CL7 32 509



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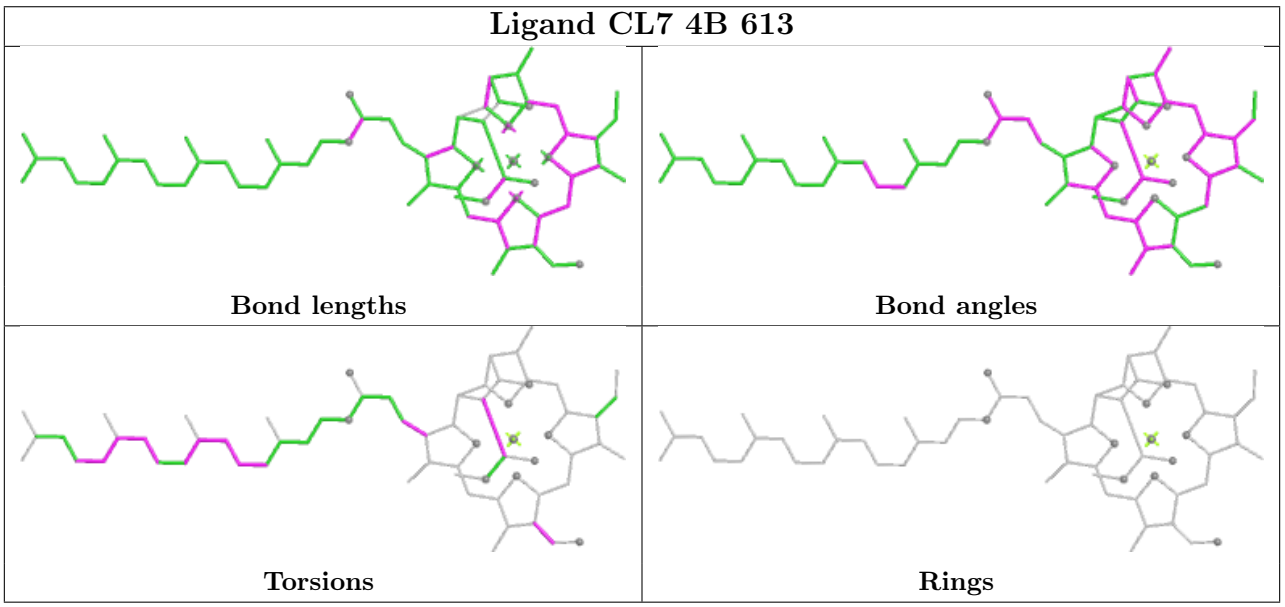

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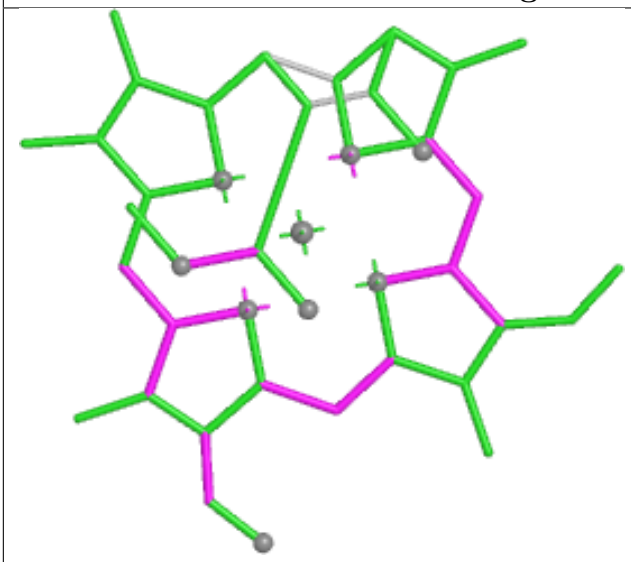

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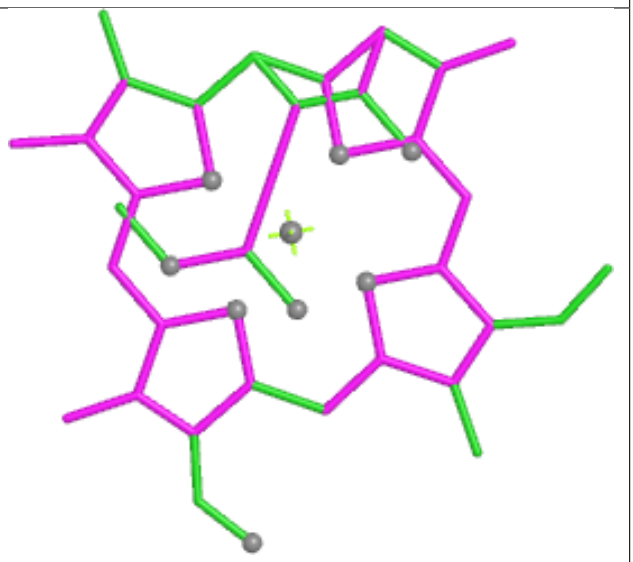

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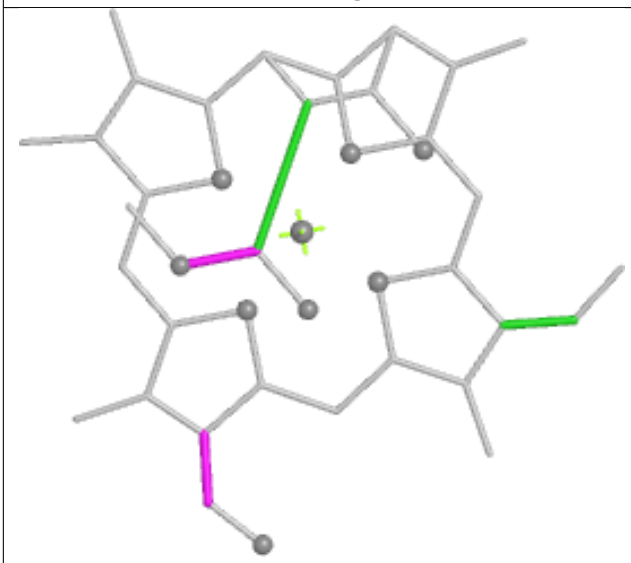

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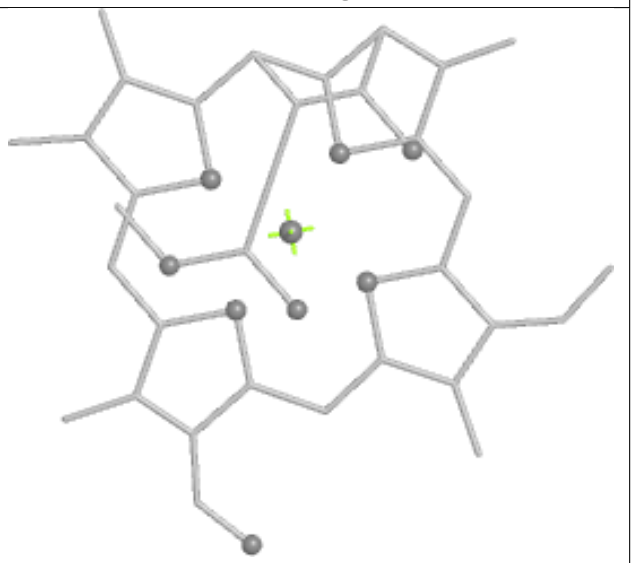
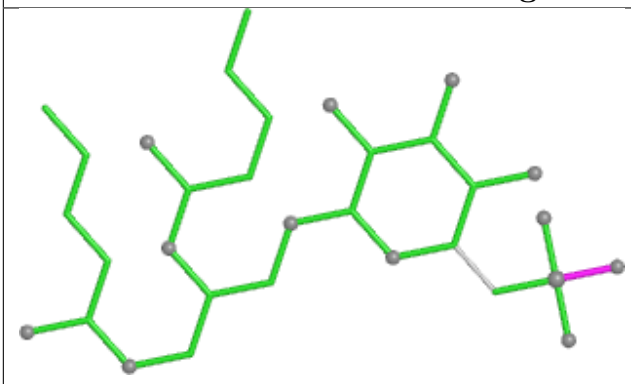


Rings

Ligand SQD 31 423



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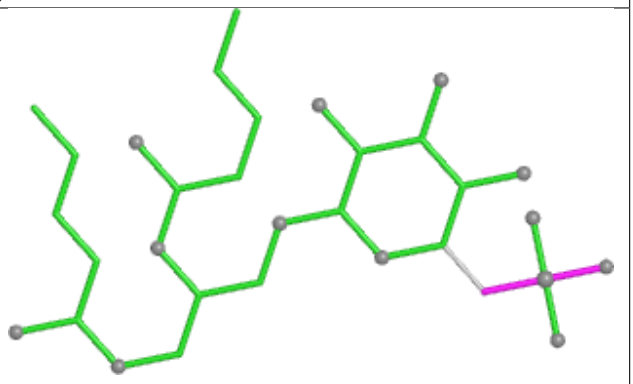

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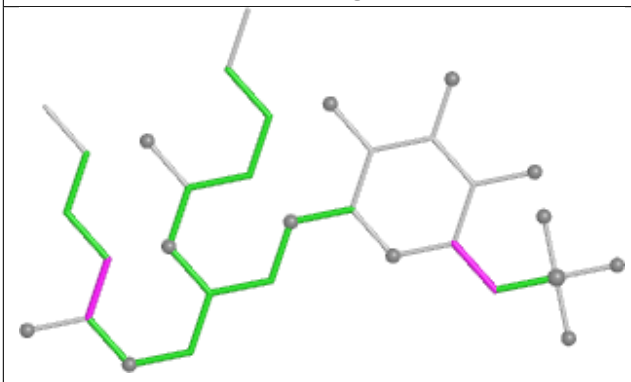

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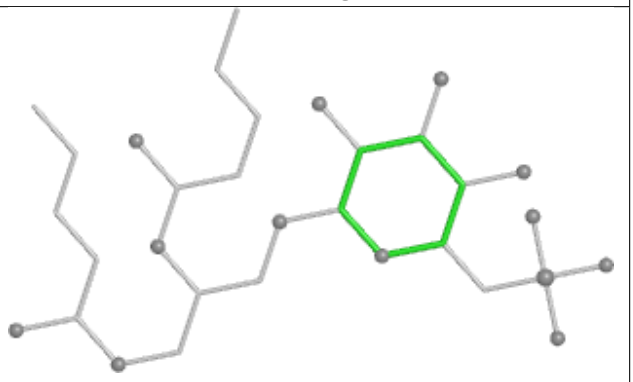
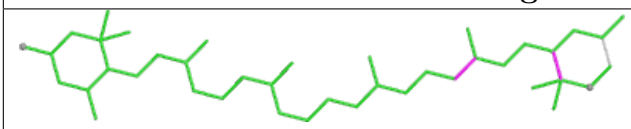


Rings

Ligand ZEX 11 422



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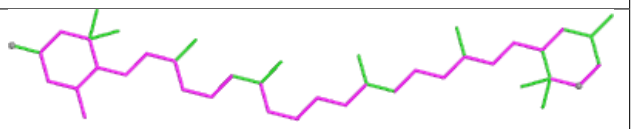

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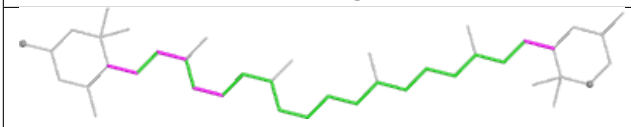

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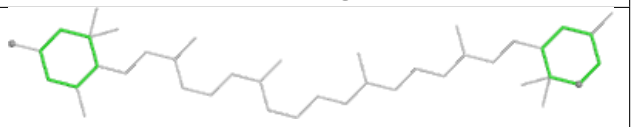
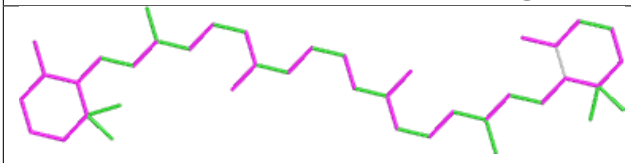


Rings

Ligand 8CT 1B 617



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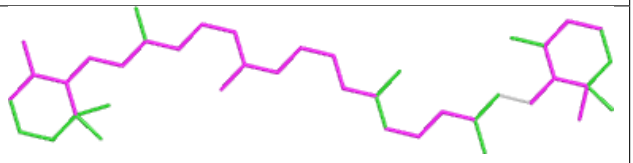
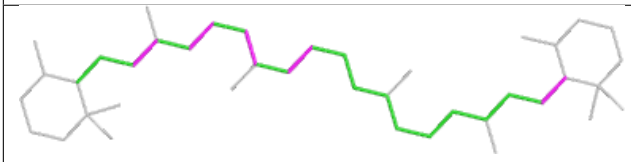


Bond angles



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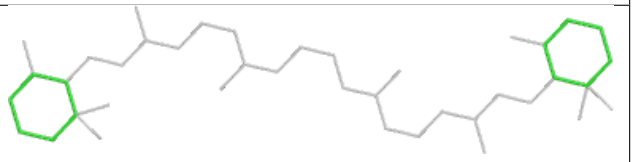
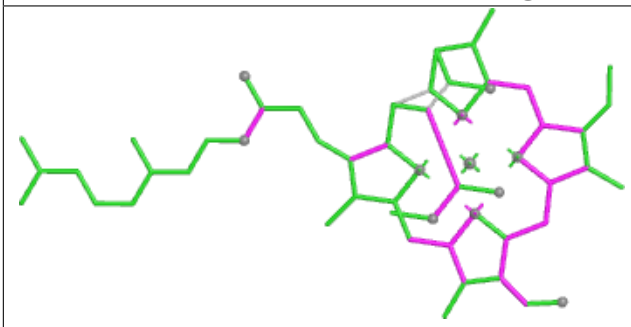


Rings

Ligand CL7 1A 403



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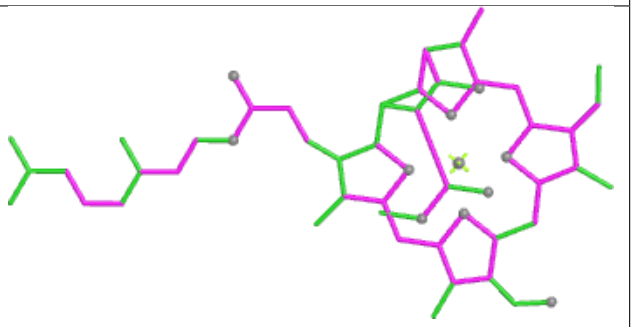

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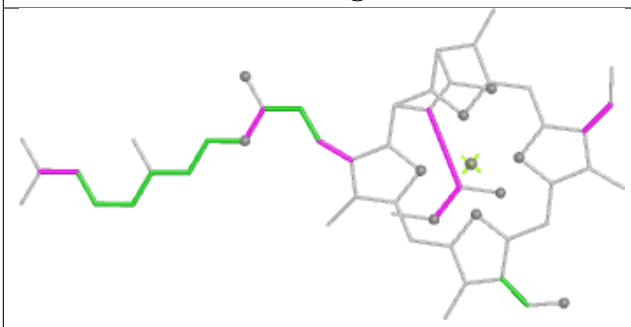

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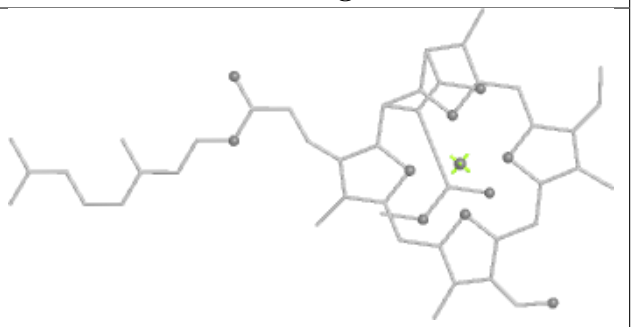
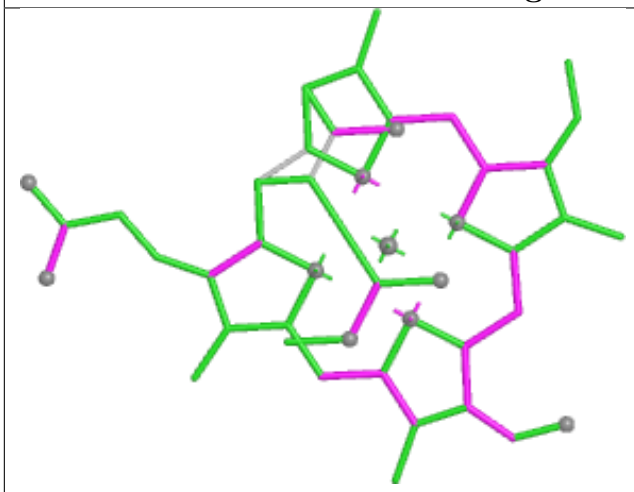


Rings

Ligand CL7 41 411



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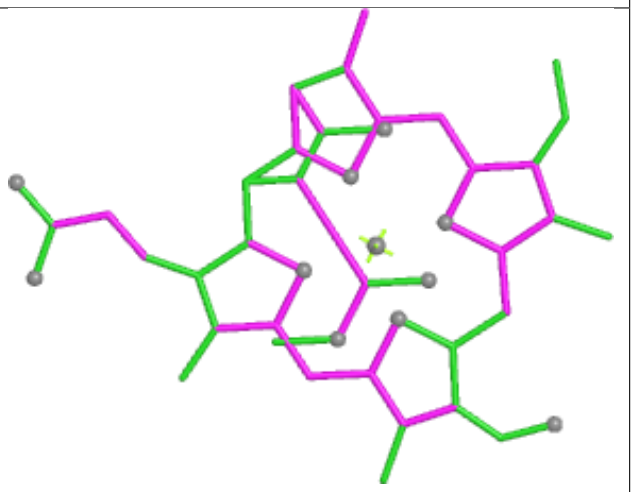
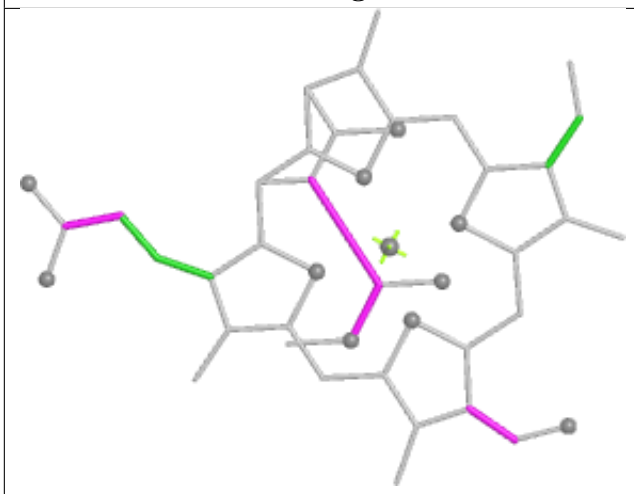


Bond angles

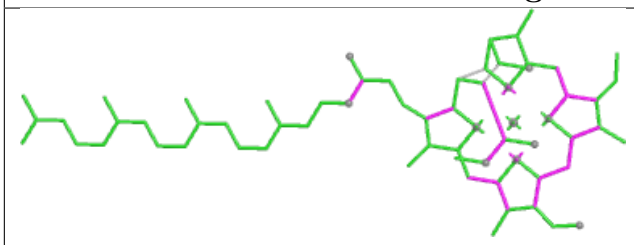


Torsions



Rings

Ligand CL7 33 507



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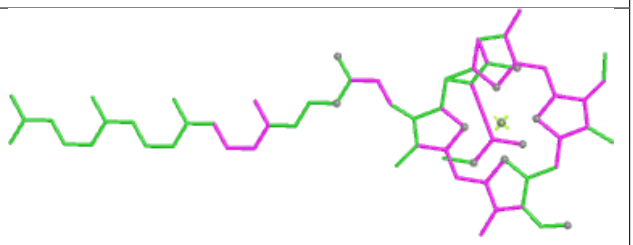
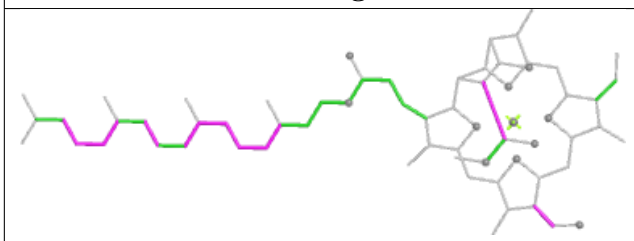


Bond angles



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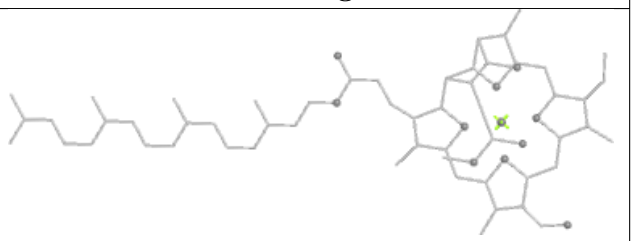
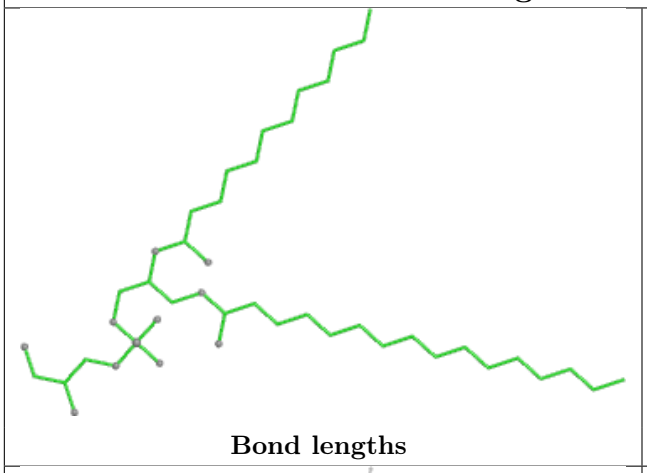


Rings

Ligand LHG 4B 624



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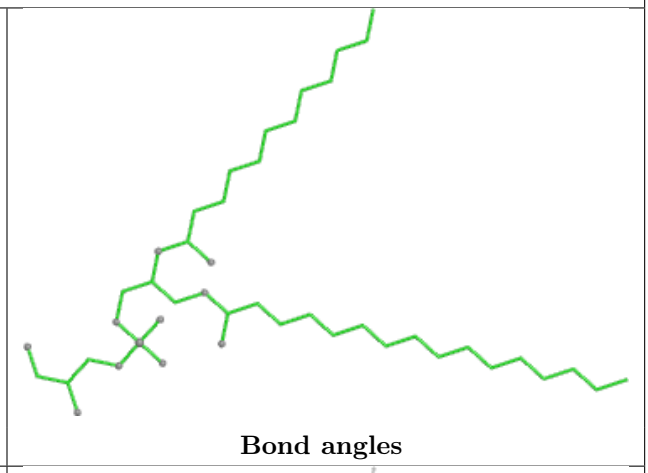
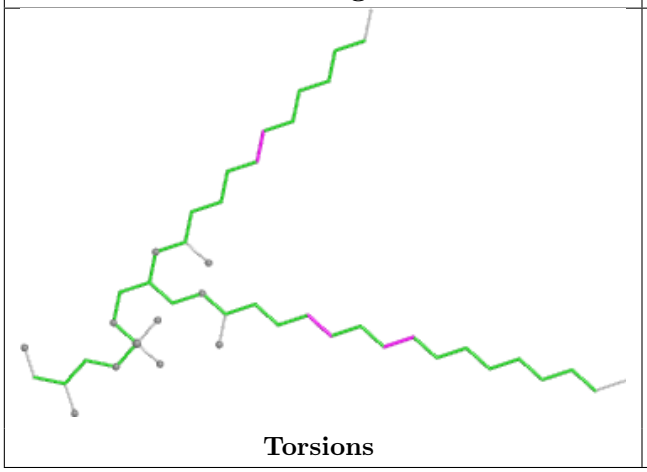


Bond angles



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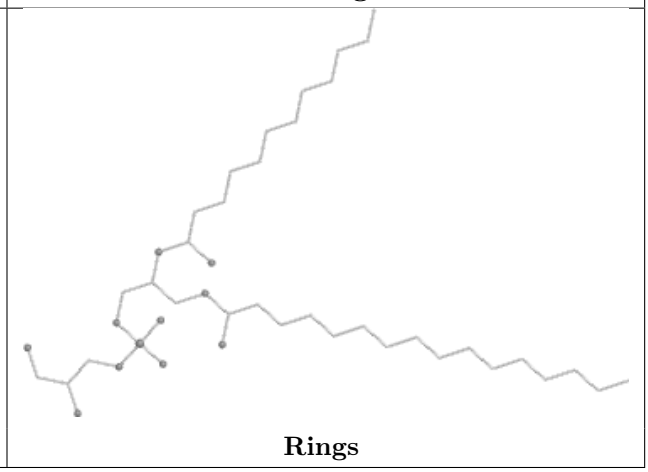
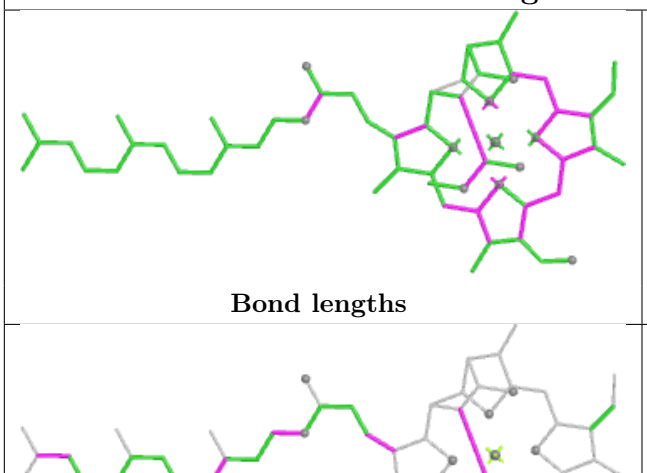


Rings

Ligand CL7 4B 615



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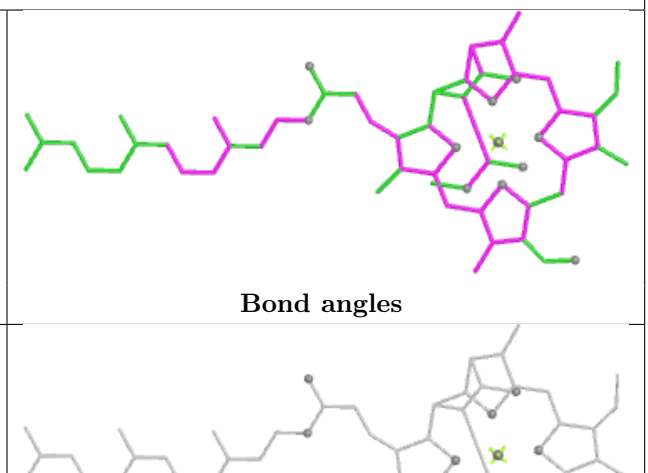
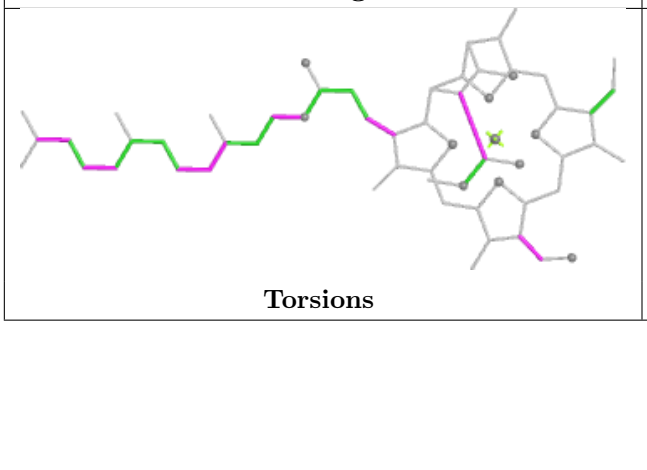
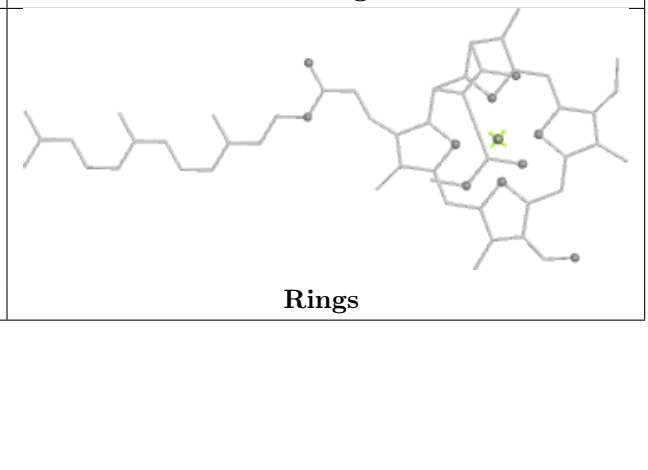


Bond angles

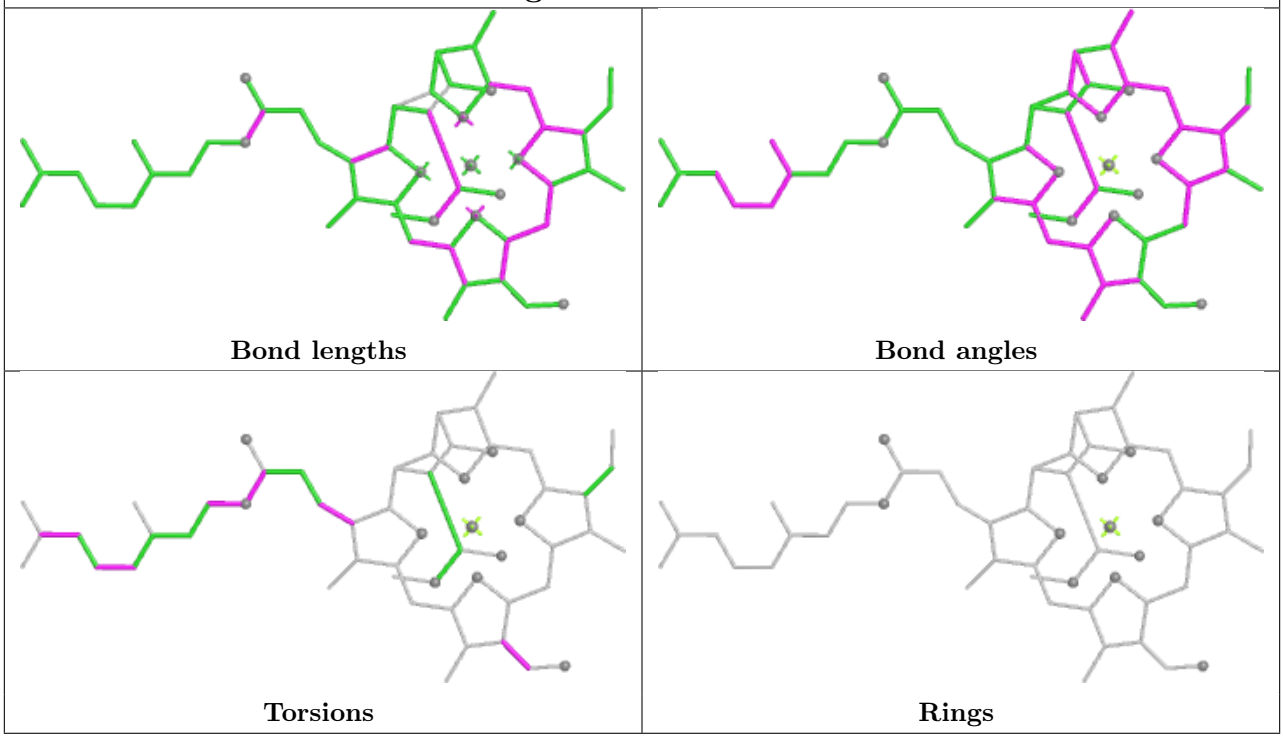


Torsions

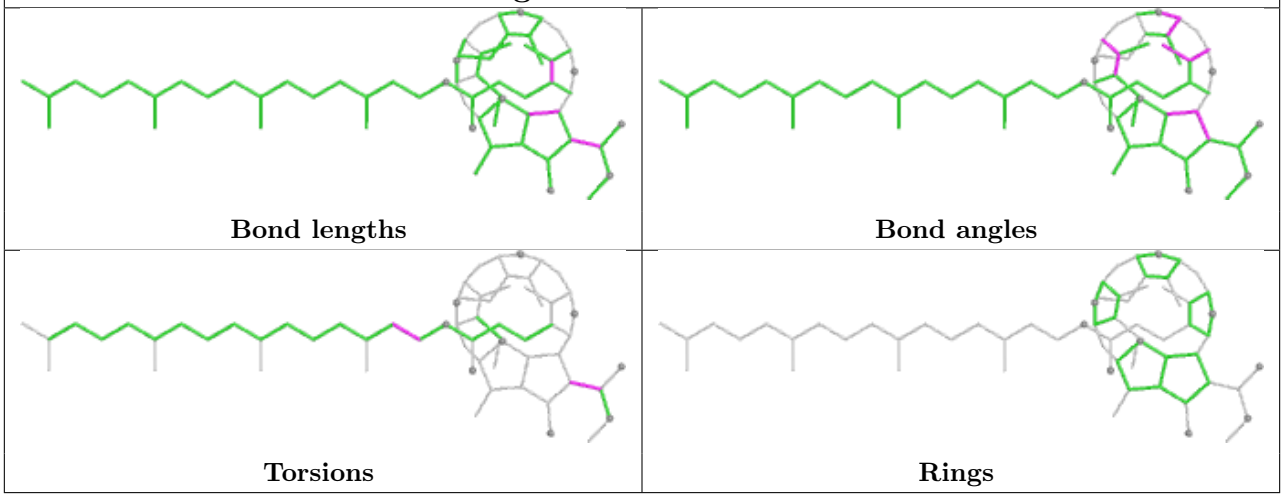


Rings

Ligand CL7 41 417



Ligand PHO 2A 402



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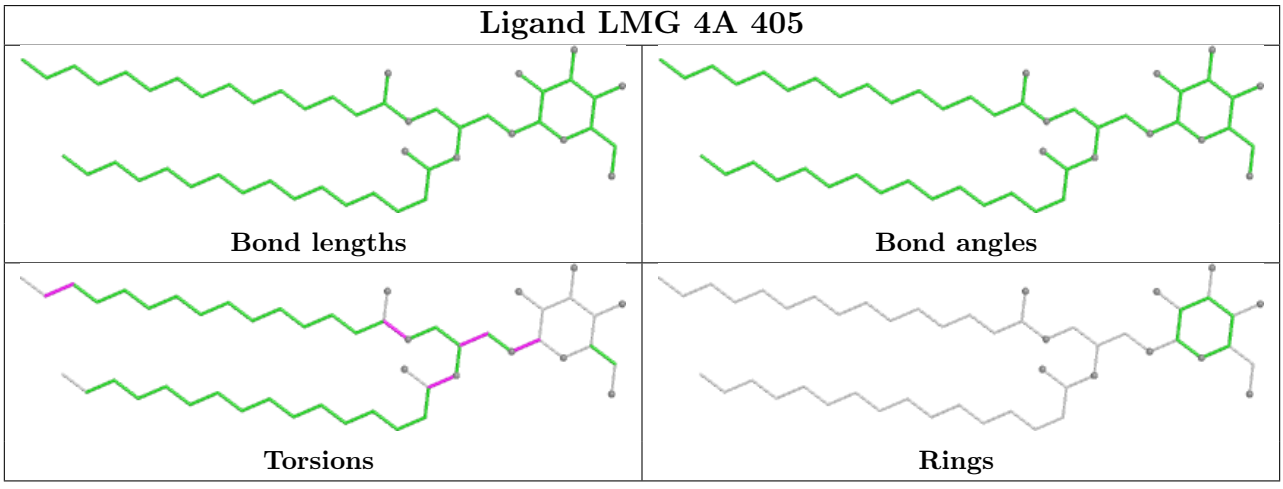
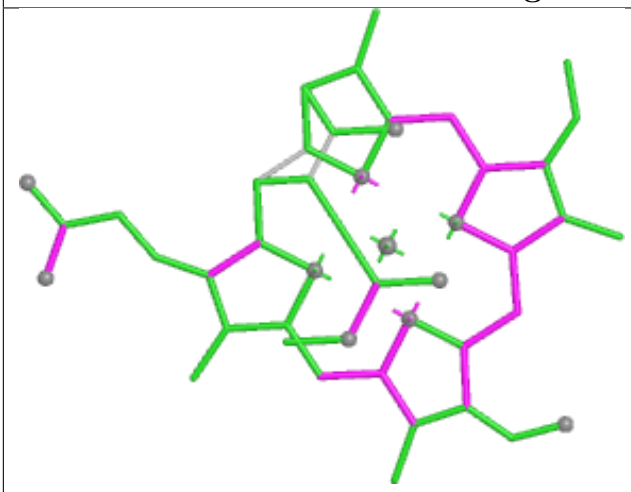


Ligand CL7 22 504



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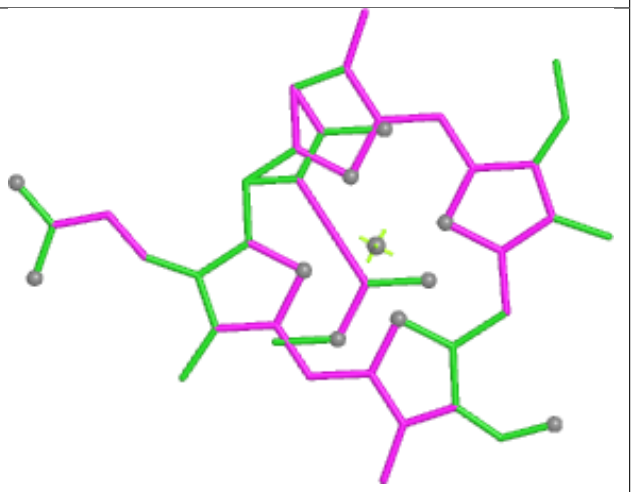

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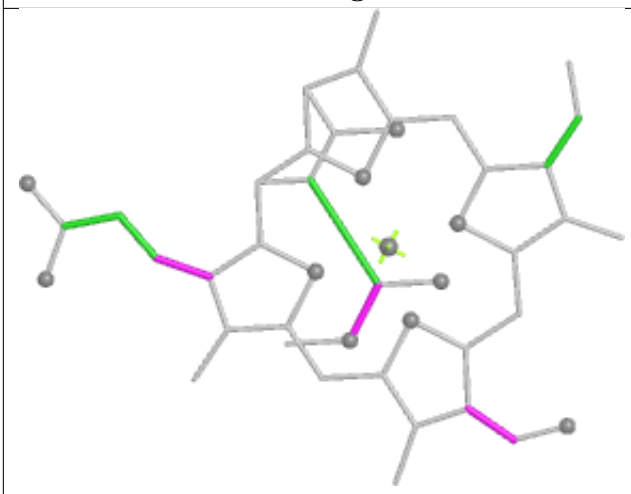
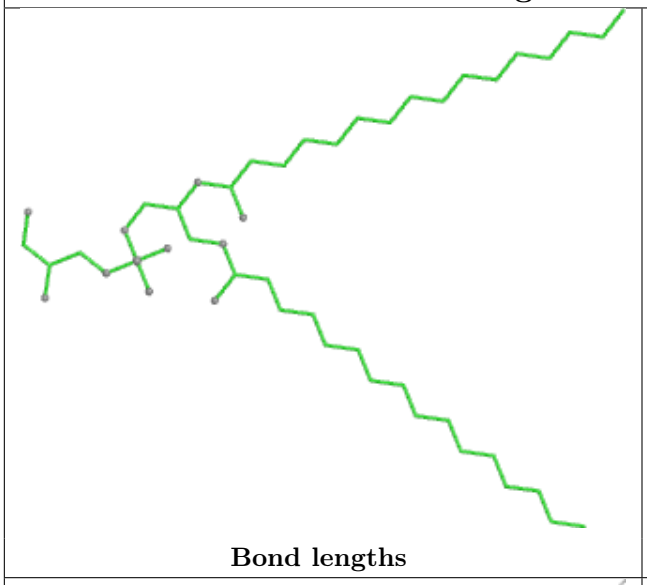


Torsions



Rings

Ligand LHG 3B 625



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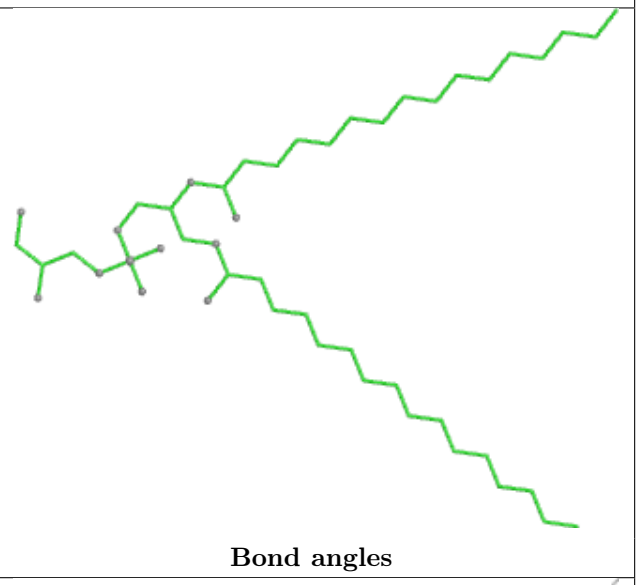

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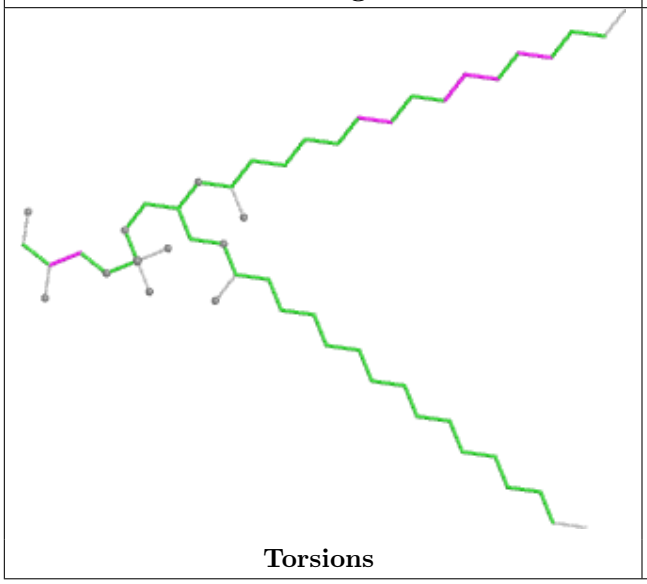

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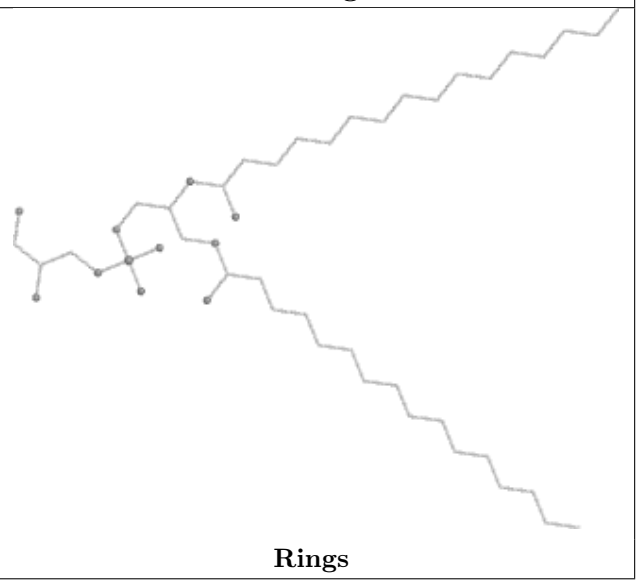
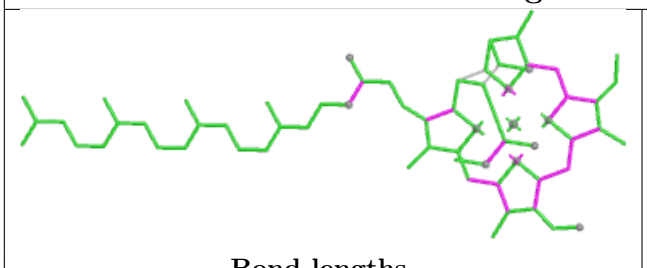


Rings

Ligand CL7 11 408



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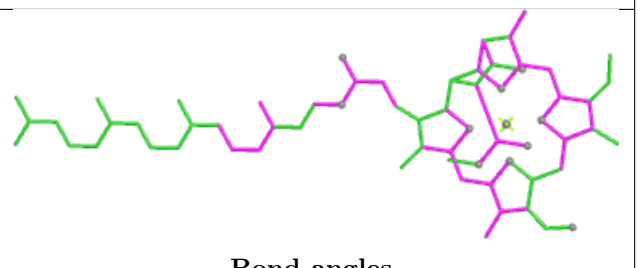

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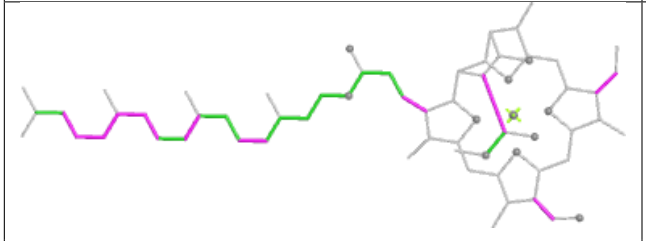

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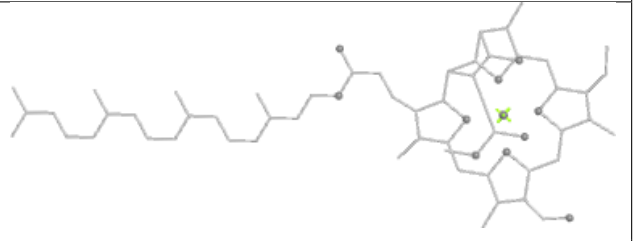
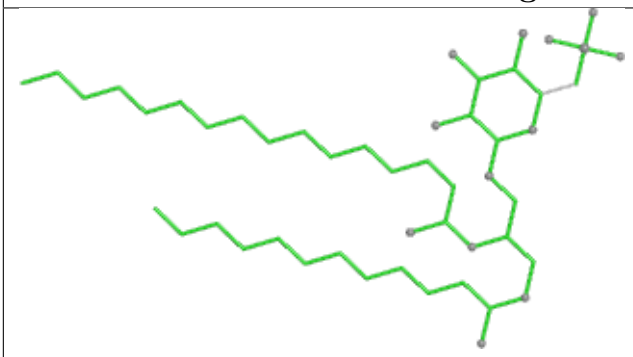


Rings

Ligand SQD 13 523



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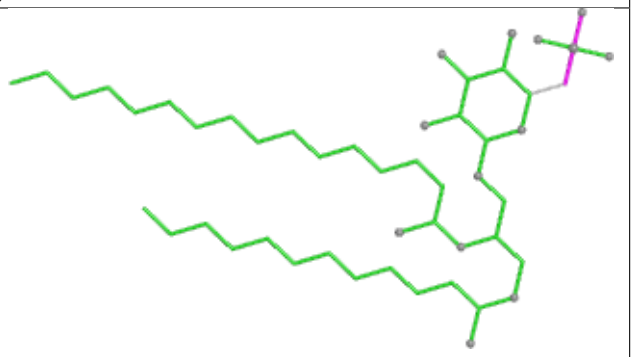

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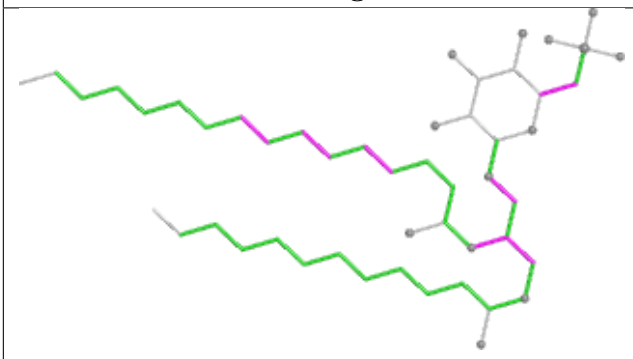

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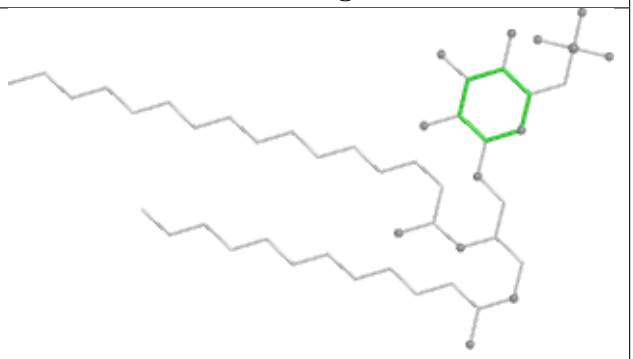
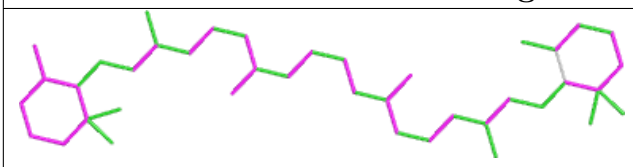


Rings

Ligand 8CT 1A 404



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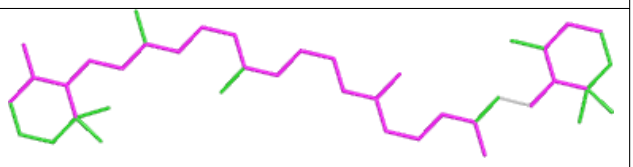
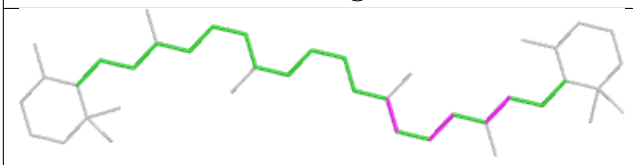


Bond angles



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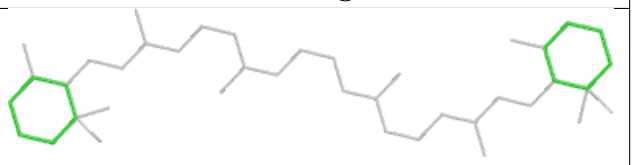
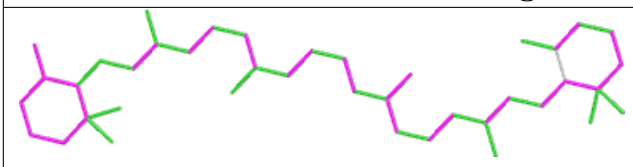


Rings

Ligand 8CT 3B 618



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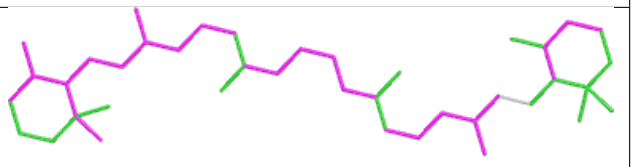

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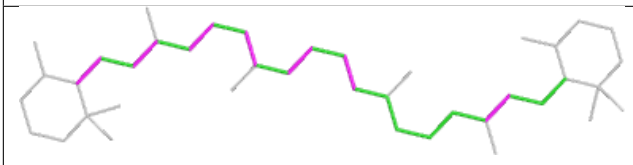

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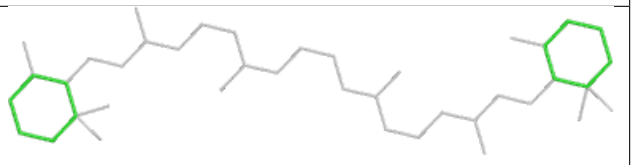
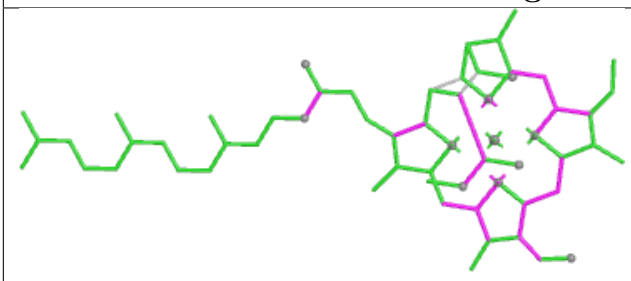


Rings

Ligand CL7 32 511



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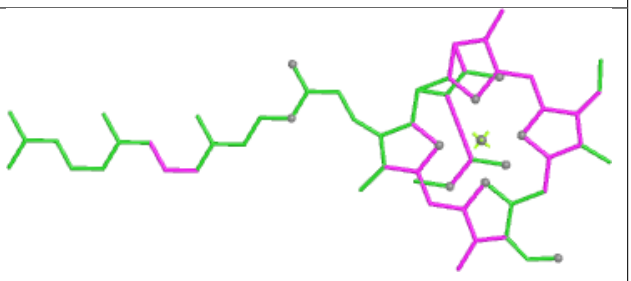

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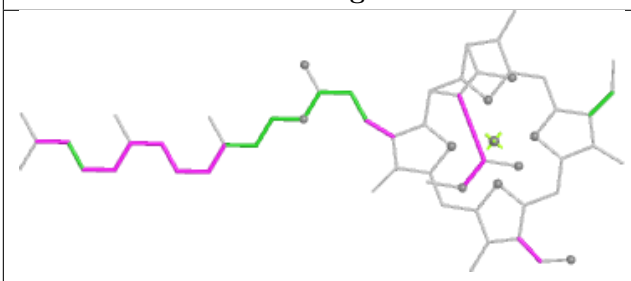

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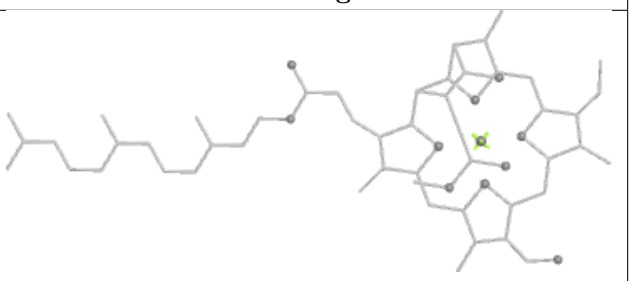
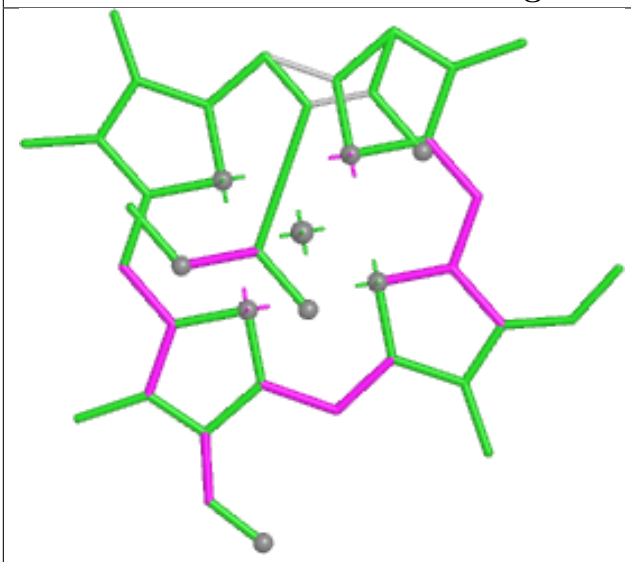


Rings

Ligand CL7 43 416



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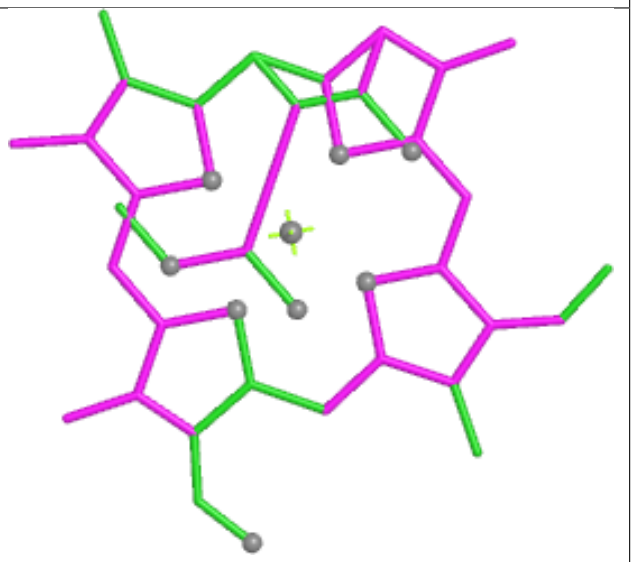

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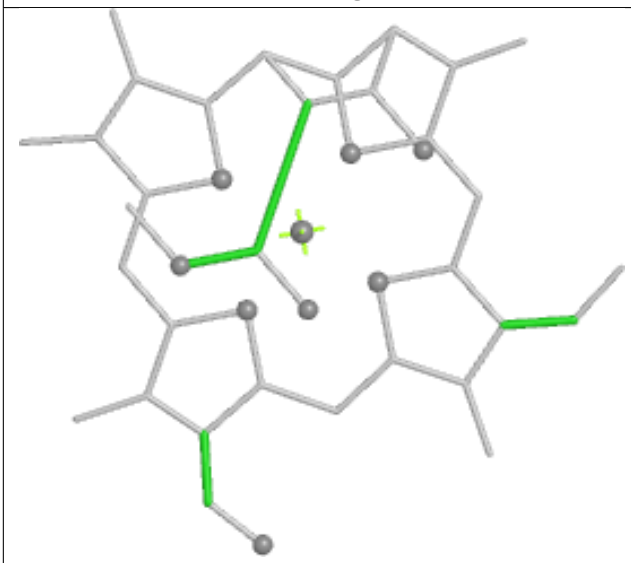

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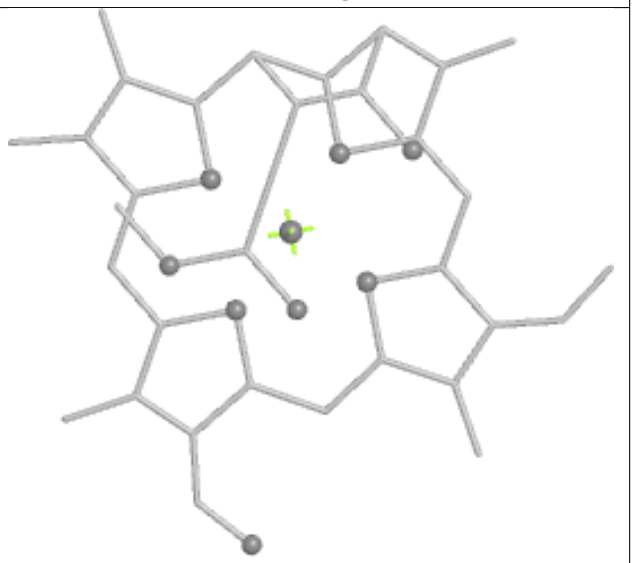
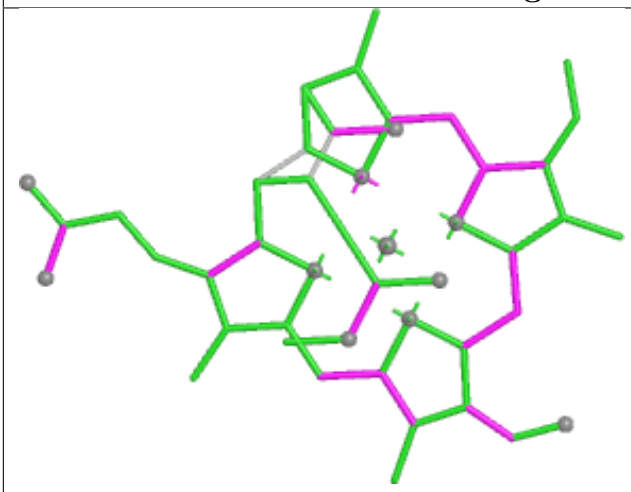


Rings

Ligand CL7 11 420



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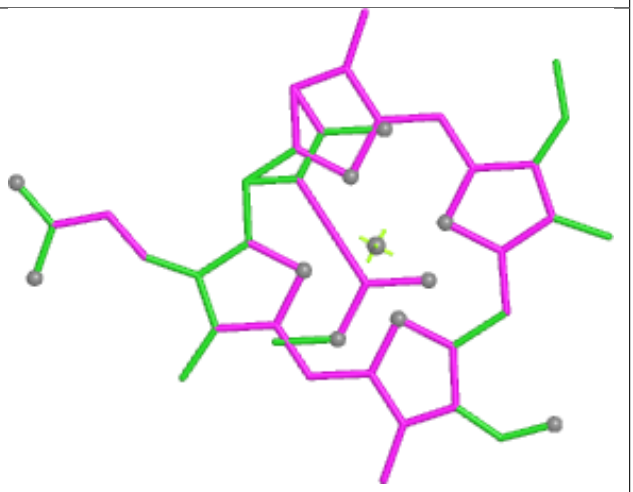

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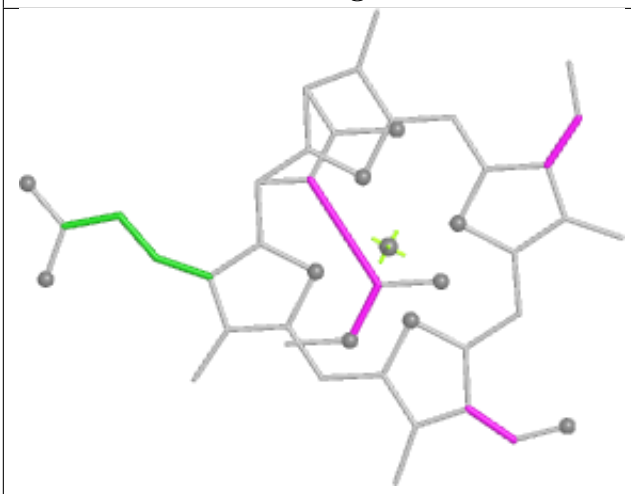
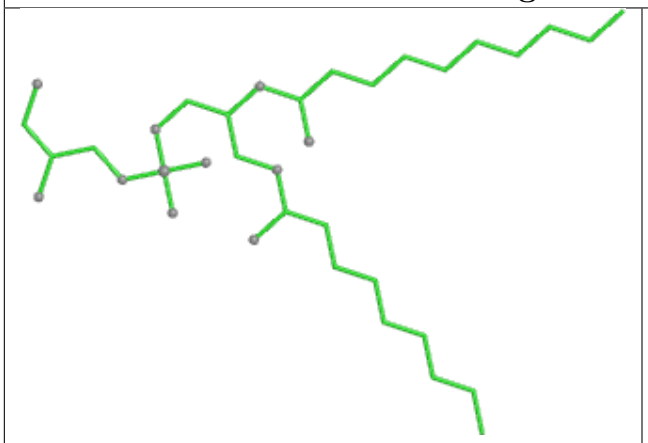


Torsions



Rings

Ligand LHG 33 524



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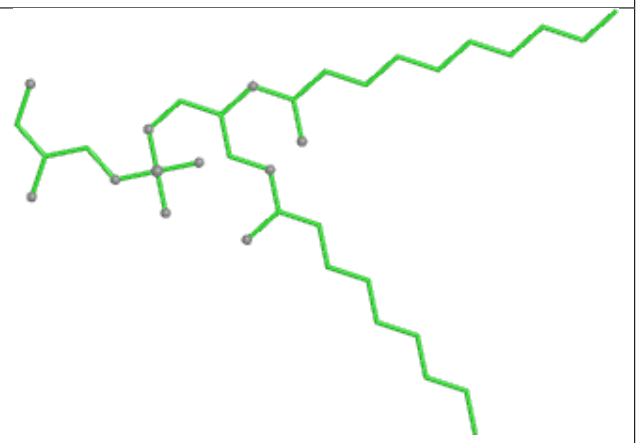

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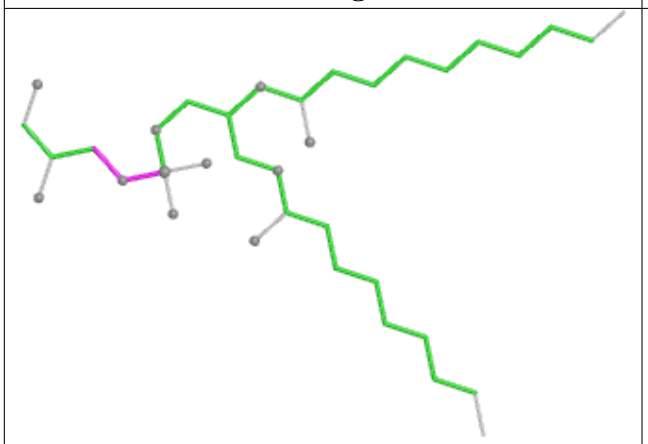

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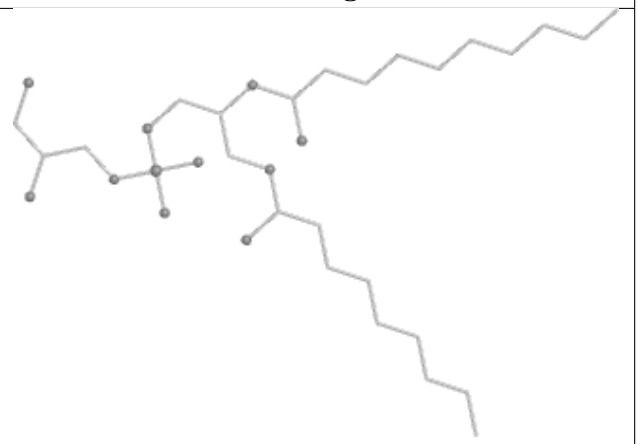
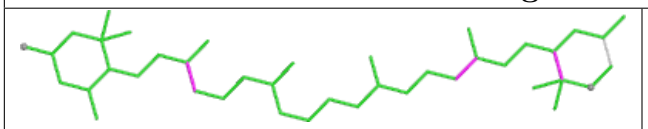


Rings

Ligand ZEX 13 519



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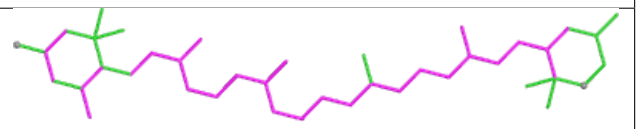
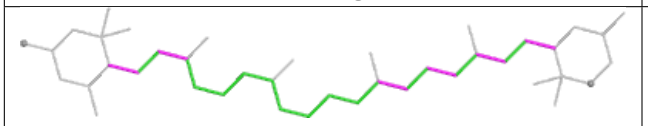


Bond angles



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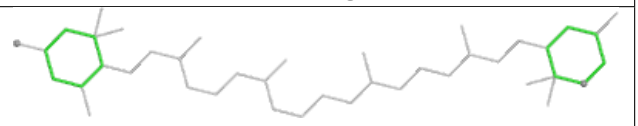
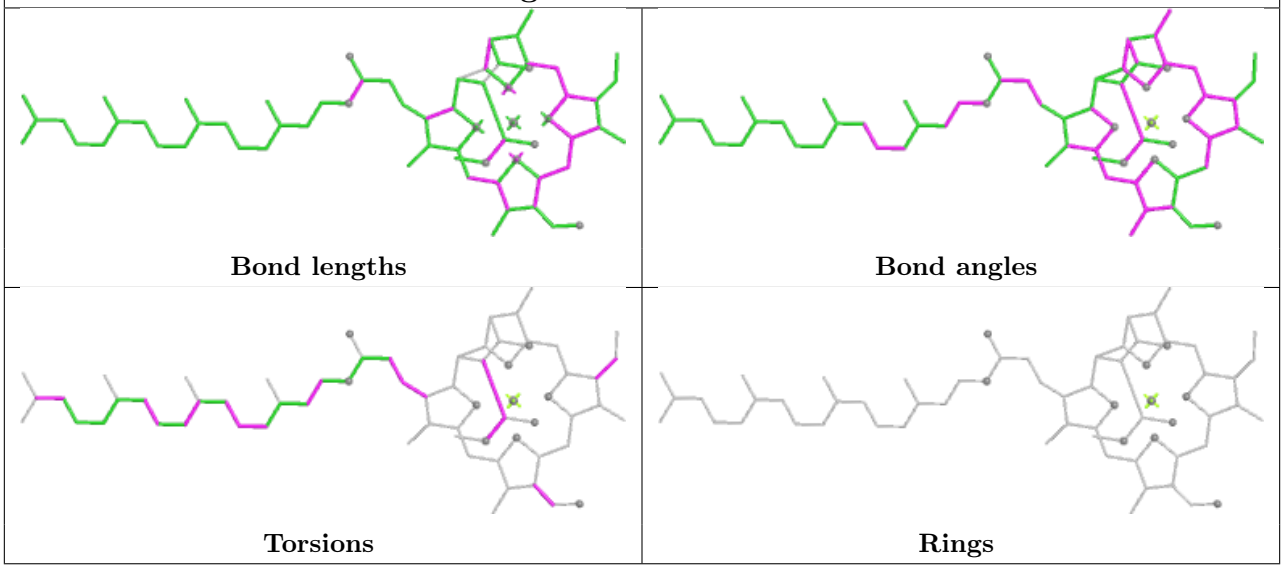
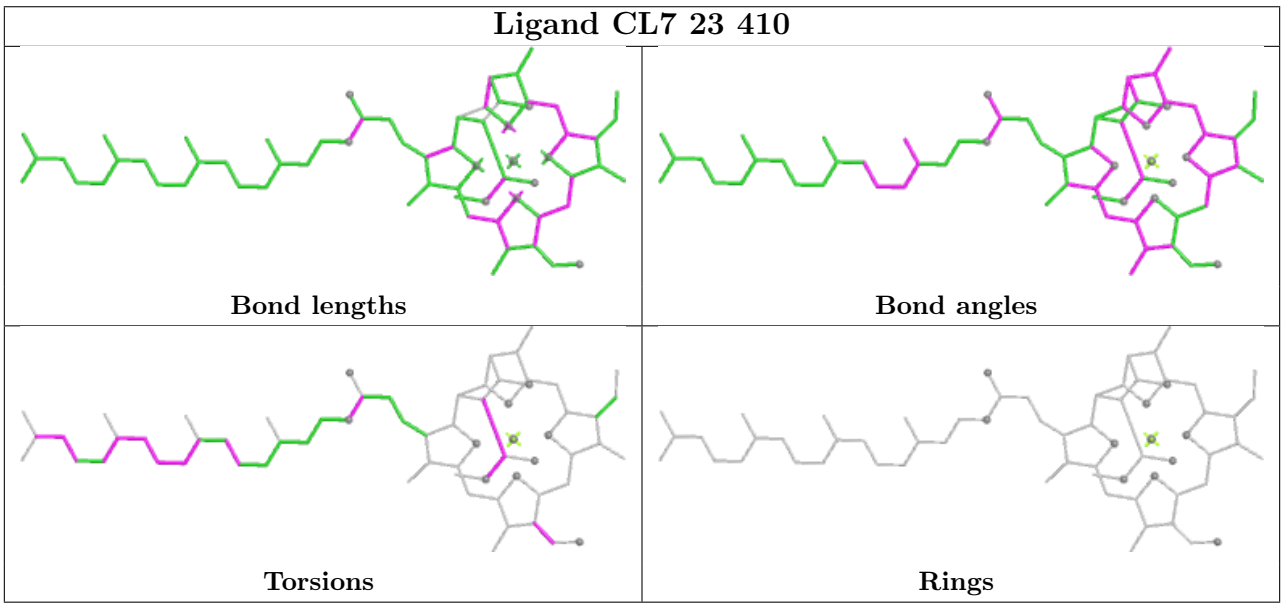


Rings

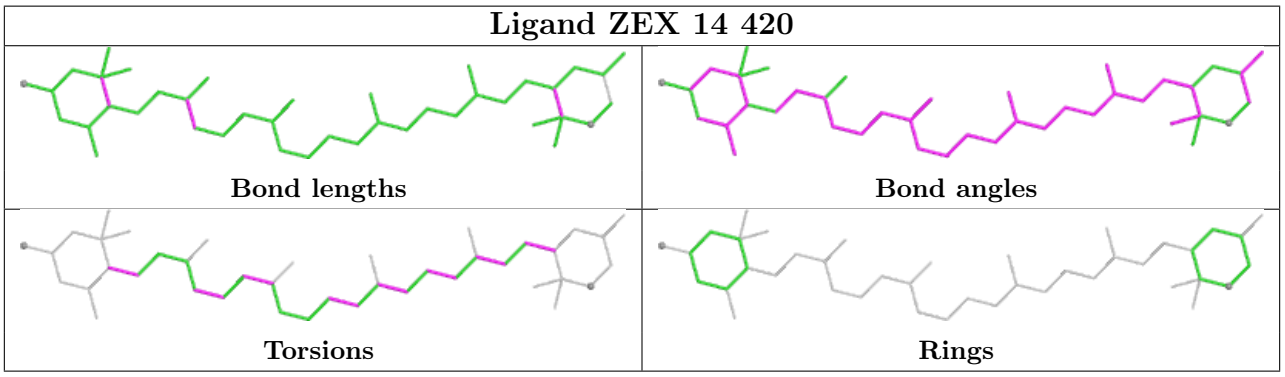
Ligand CL7 2A 407



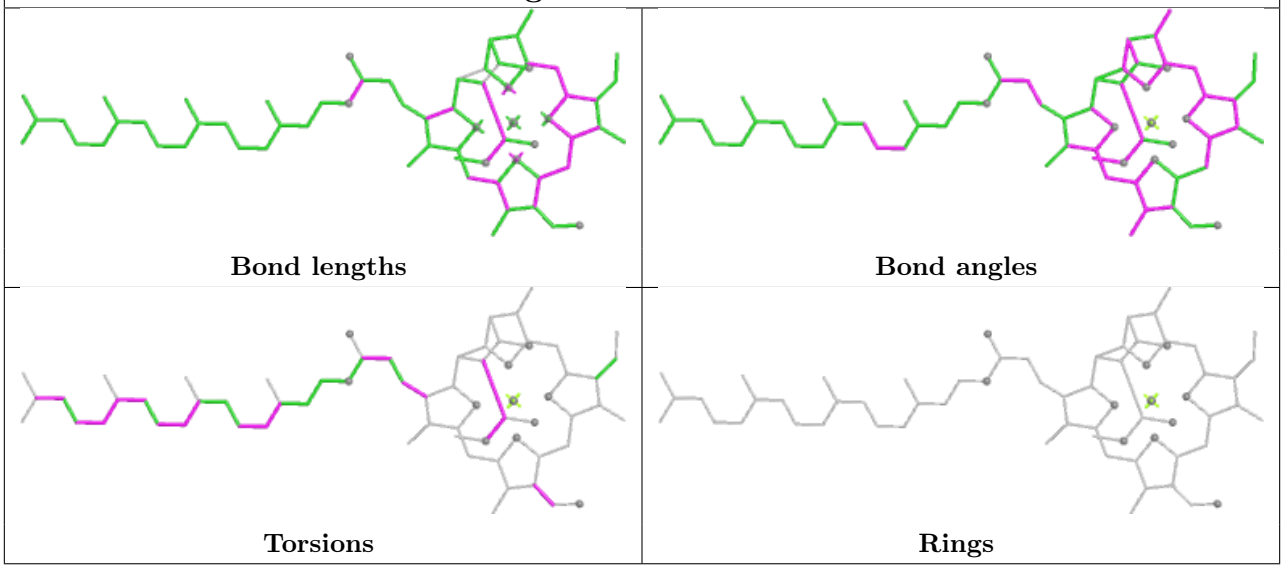
Ligand CL7 23 410



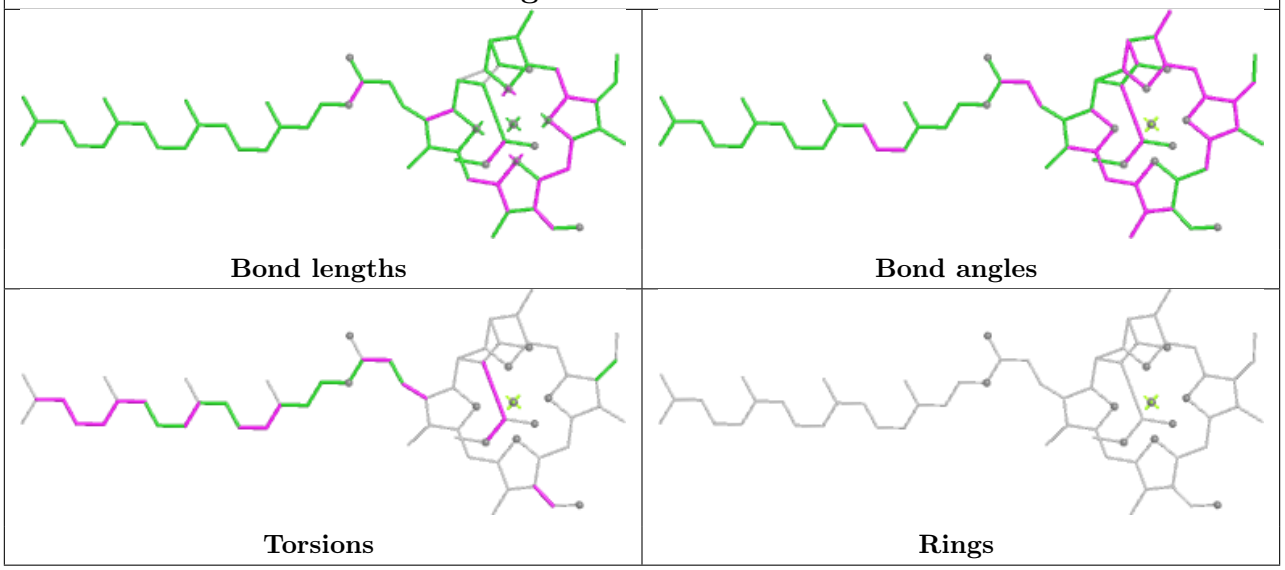
Ligand ZEX 14 420



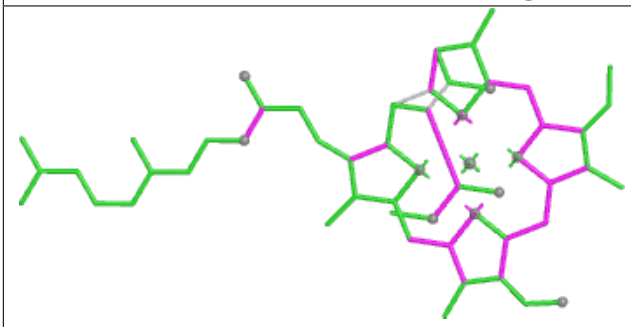
Ligand CL7 12 507



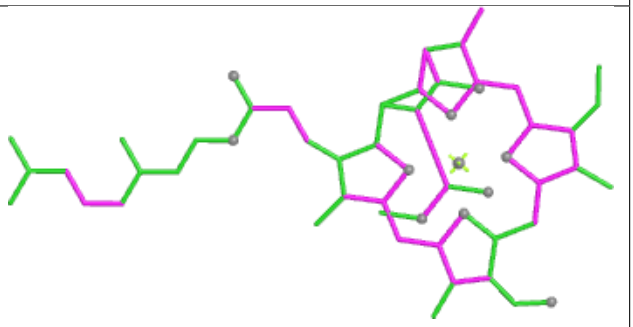
Ligand CL7 2C 501



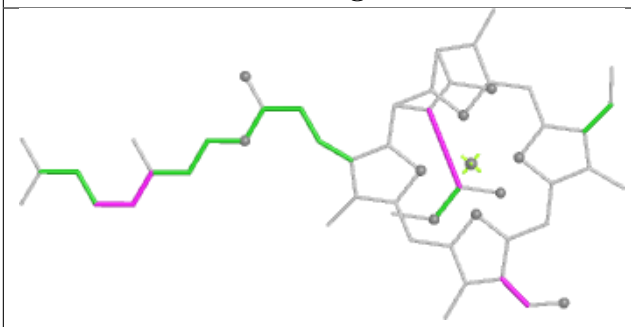
Ligand CL7 1B 613



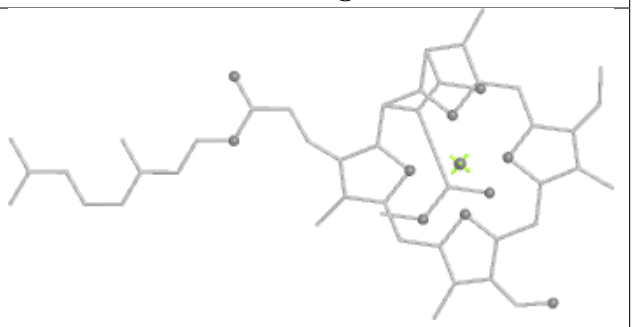
Bond lengths



Bond angles

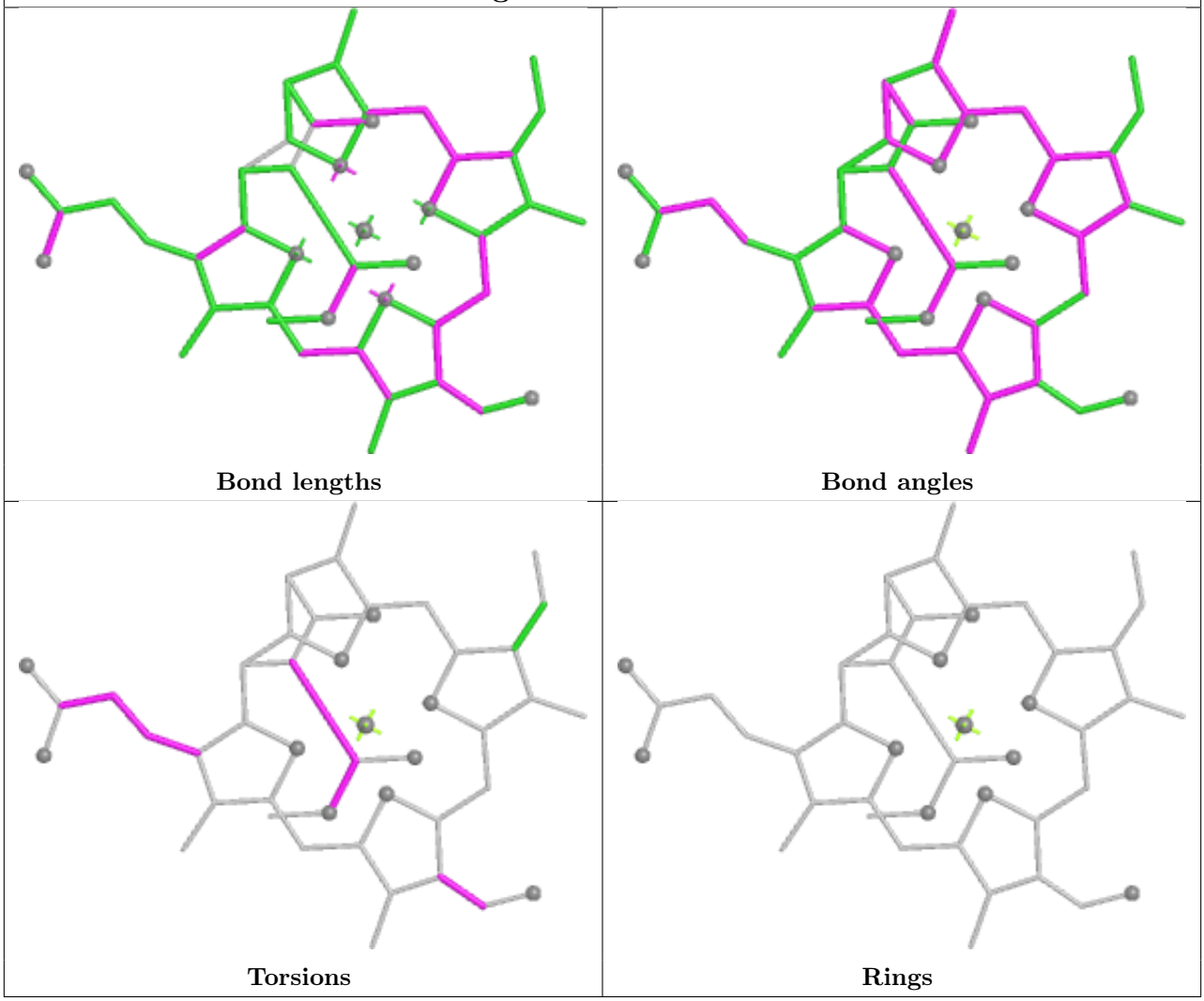


Torsions



Rings

Ligand CL7 21 412



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.

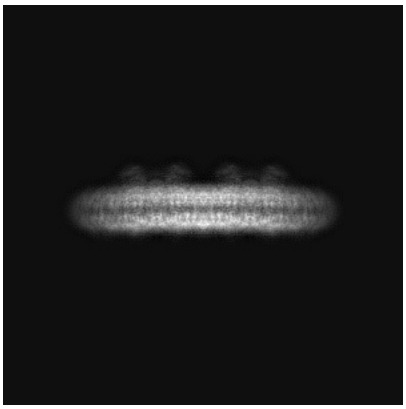
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33933. These allow visual inspection of the internal detail of the map and identification of artifacts.

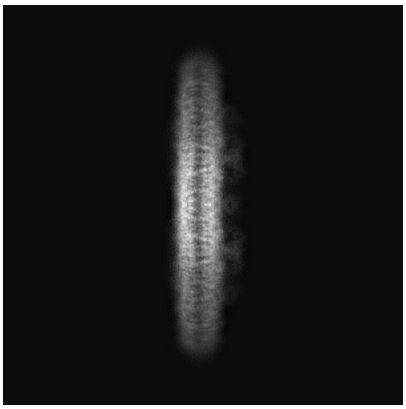
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

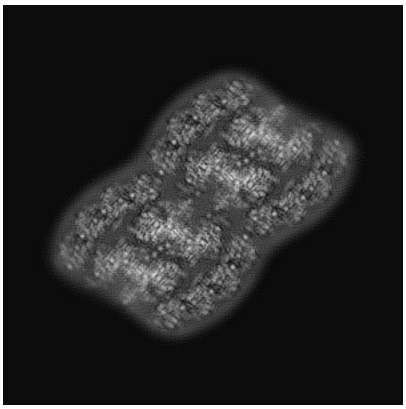
6.1.1 Primary map



X

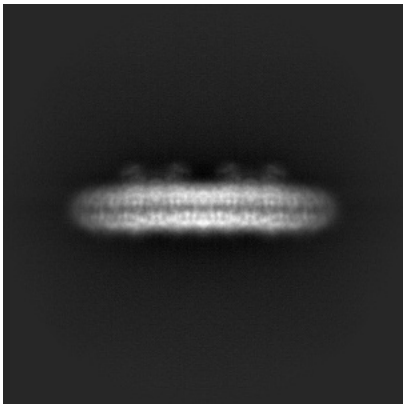


Y

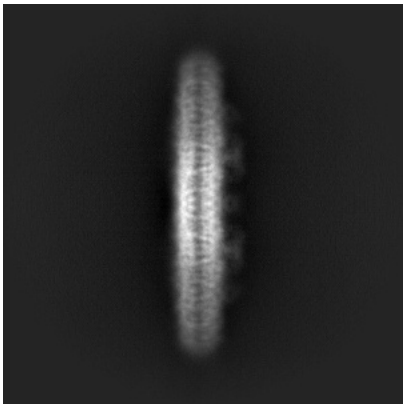


Z

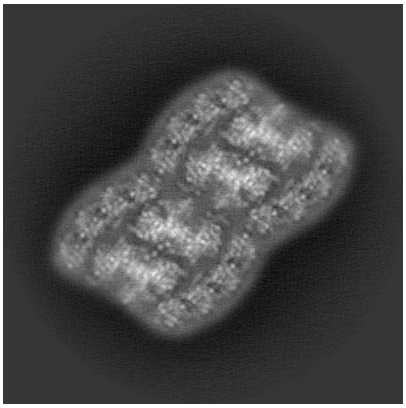
6.1.2 Raw map



X



Y

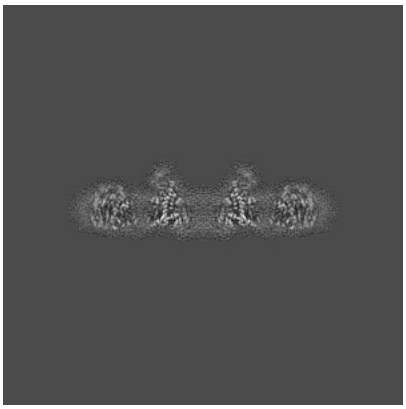


Z

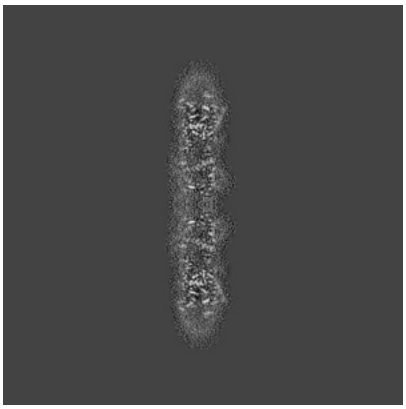
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

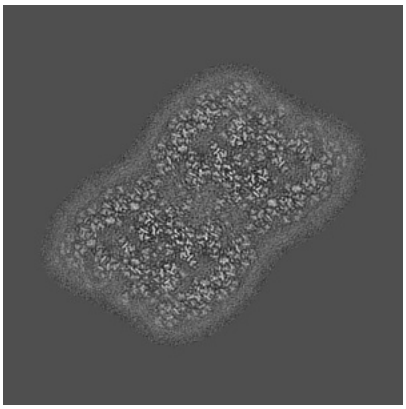
6.2.1 Primary map



X Index: 240

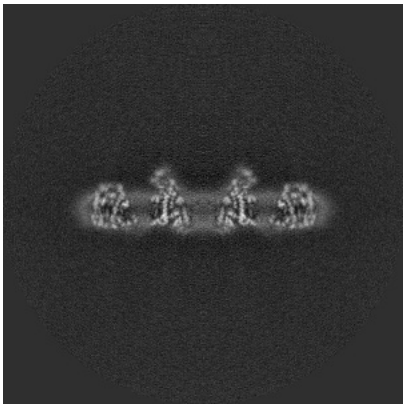


Y Index: 240

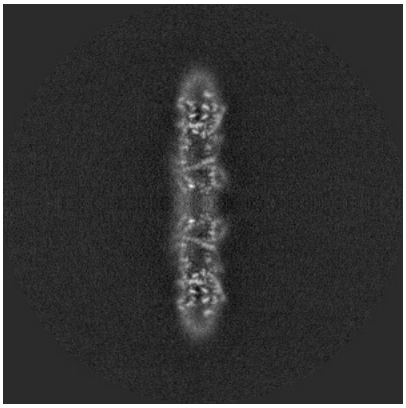


Z Index: 240

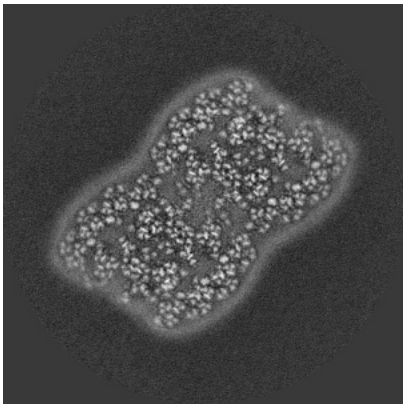
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

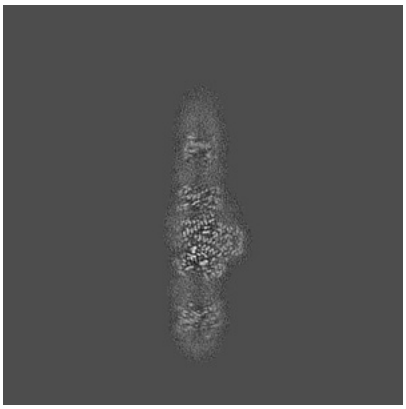
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

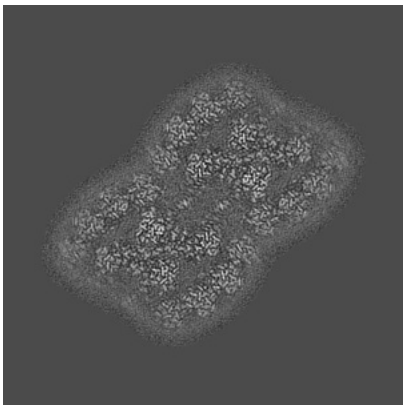
6.3.1 Primary map



X Index: 204

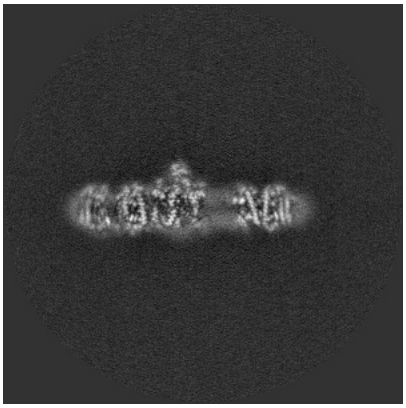


Y Index: 208

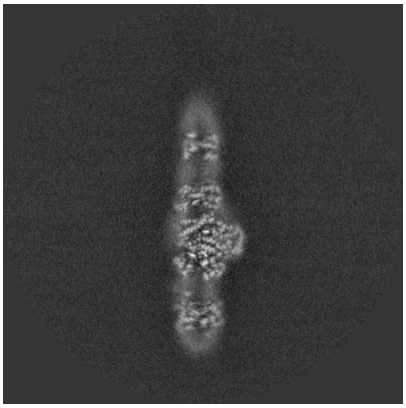


Z Index: 225

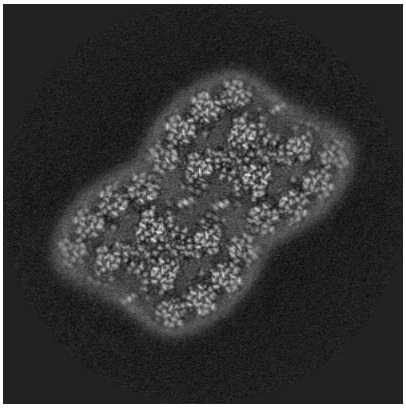
6.3.2 Raw map



X Index: 204



Y Index: 209

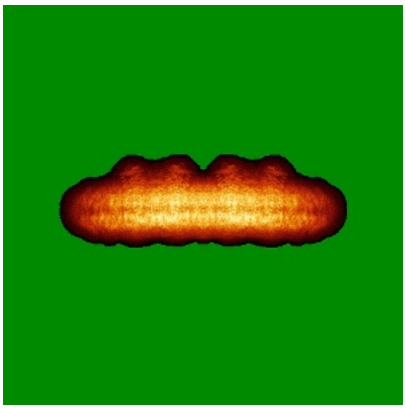


Z Index: 224

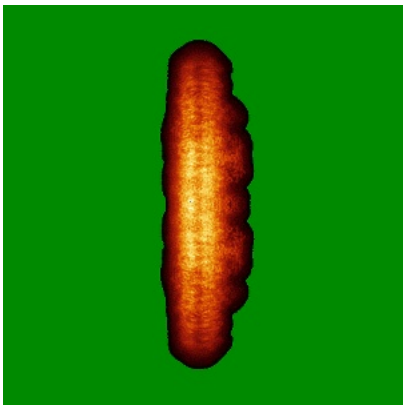
The images above show the largest variance slices of the map in three orthogonal directions.

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

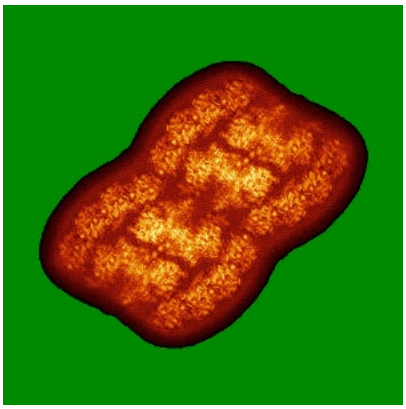
6.4.1 Primary map



X

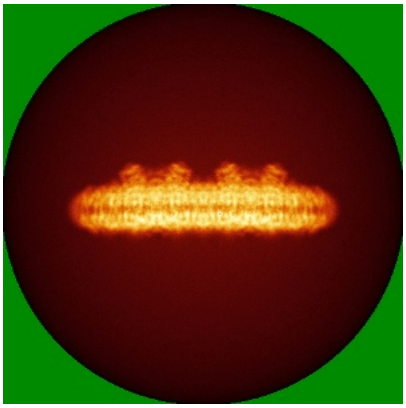


Y

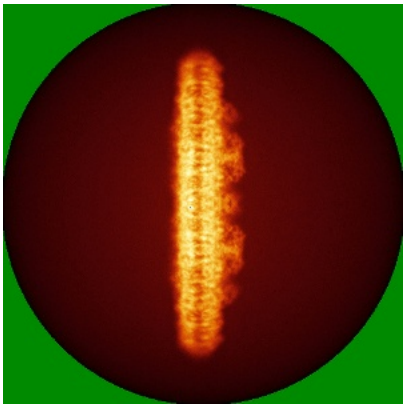


Z

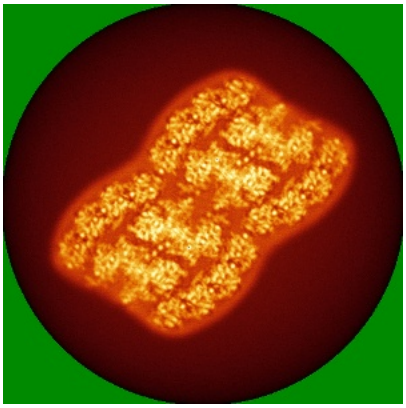
6.4.2 Raw map



X



Y

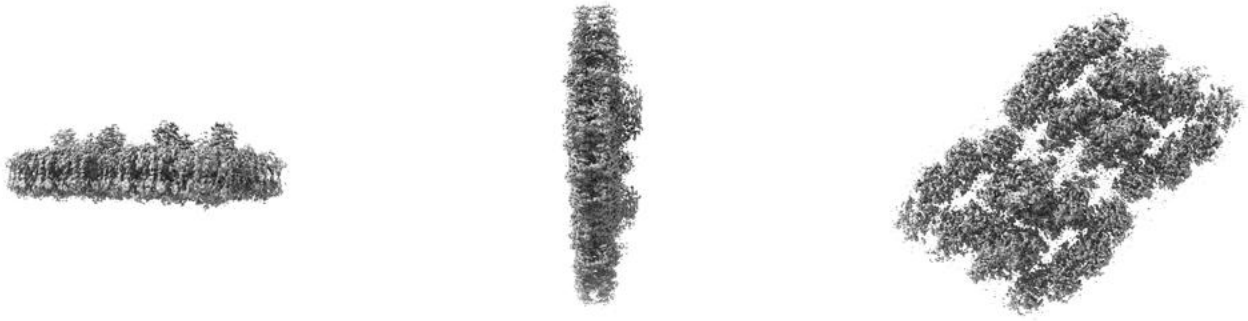


Z

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 0.0171. 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.

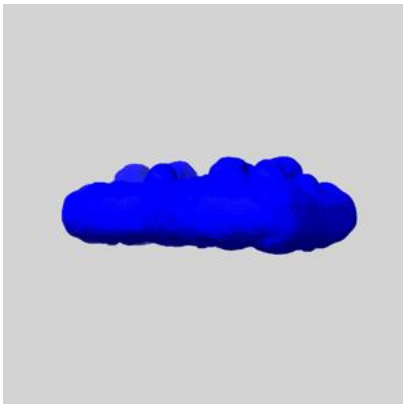
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

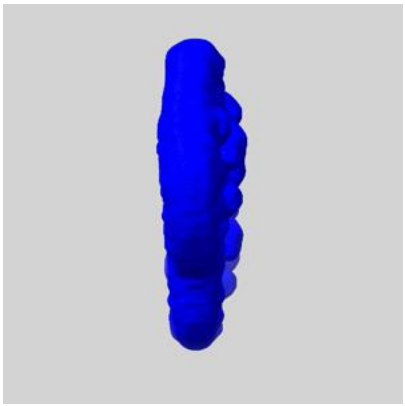
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

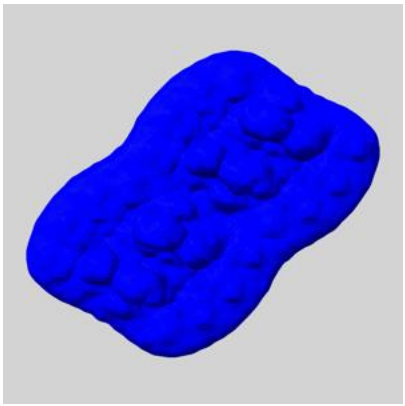
6.6.1 emd_33933_msk_1.map (i)



X



Y

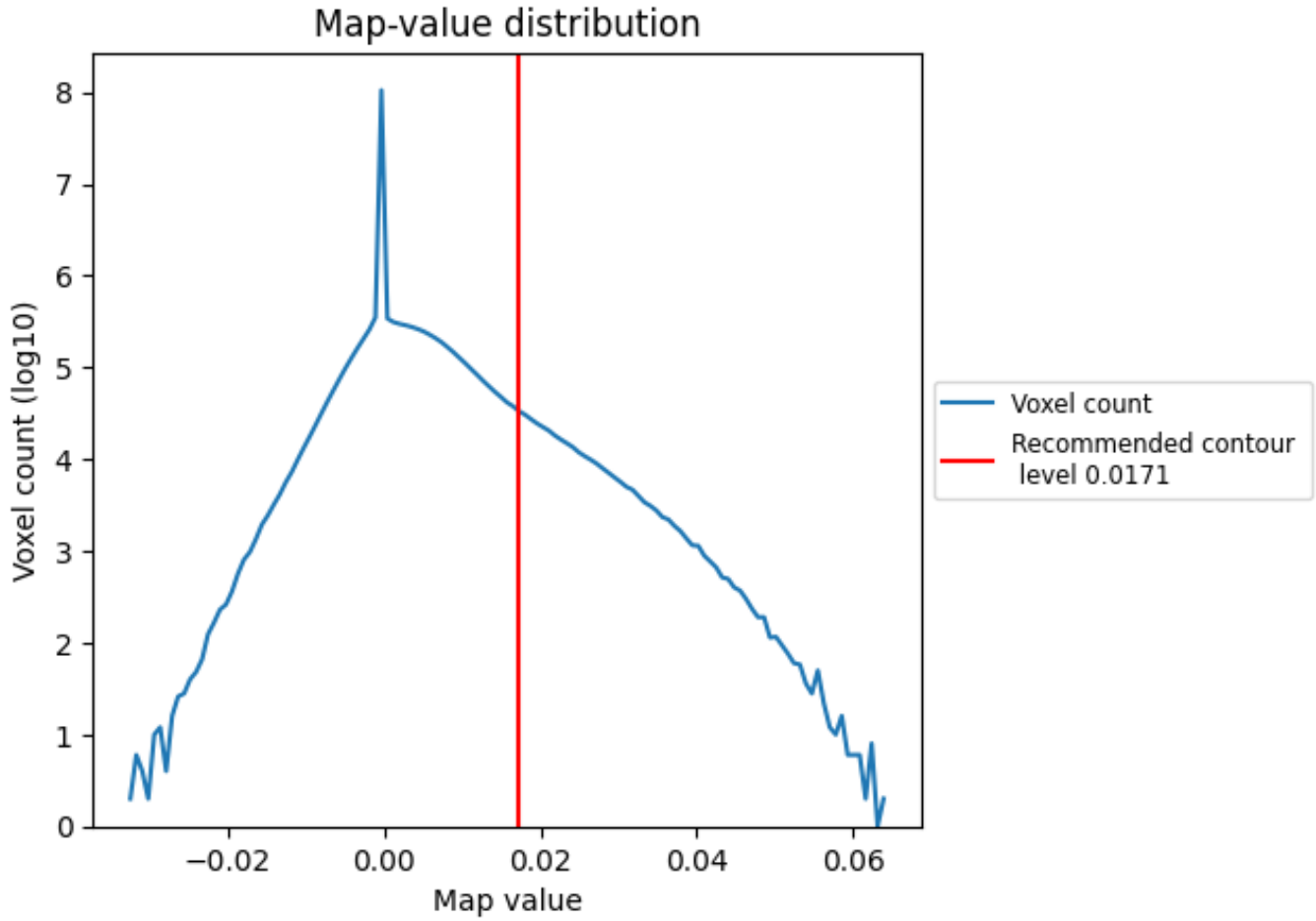


Z

7 Map analysis

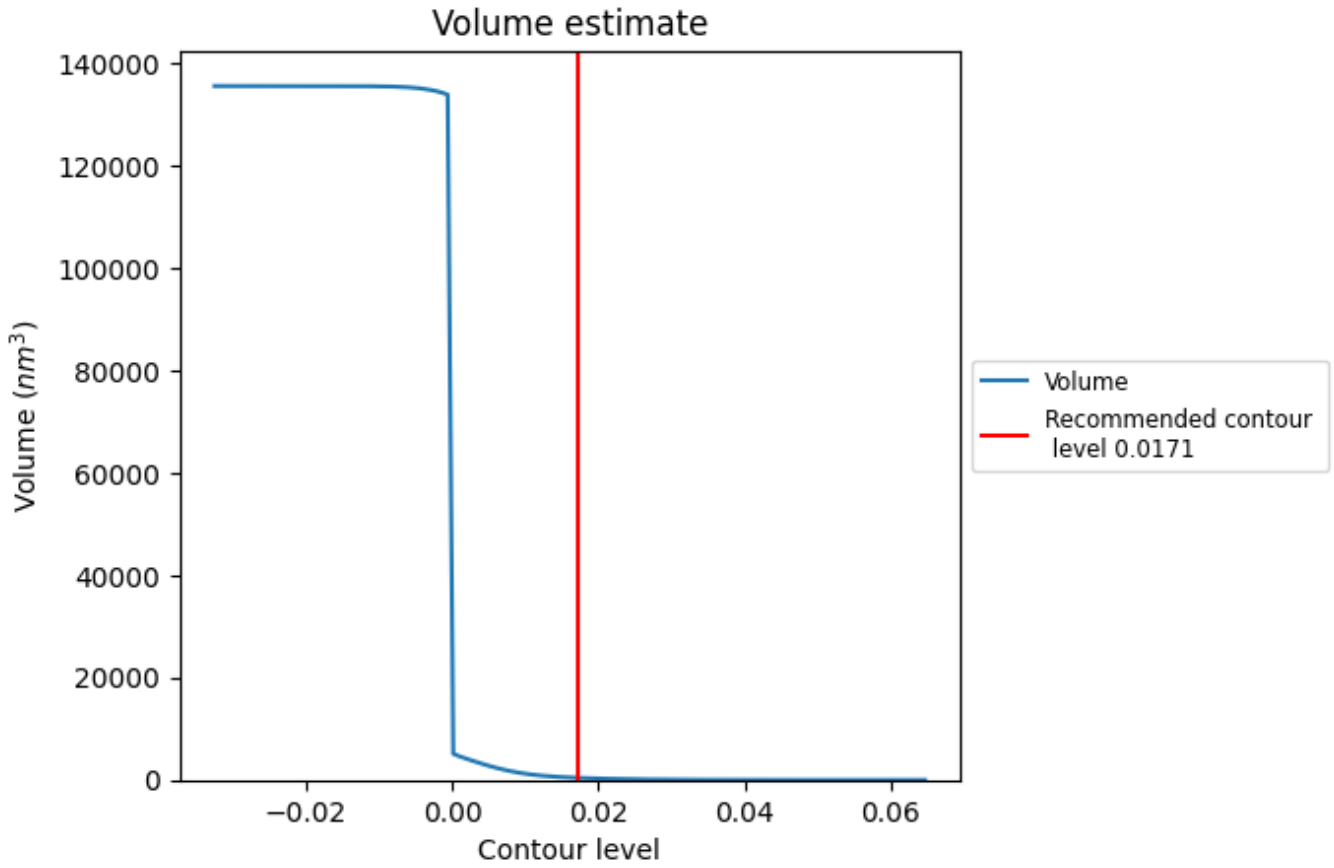
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

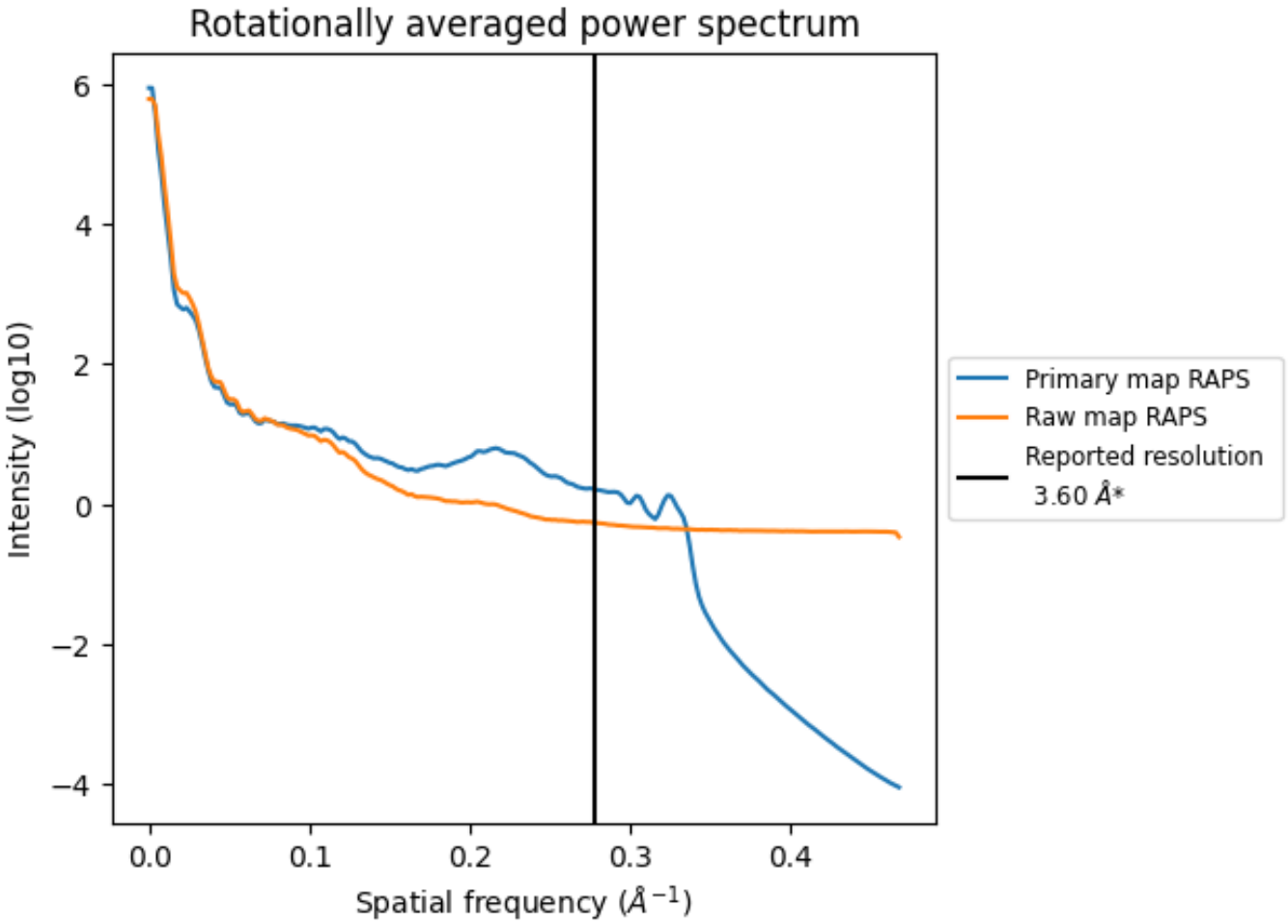
7.2 Volume estimate



The volume at the recommended contour level is 416 nm^3; this corresponds to an approximate mass of 376 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)

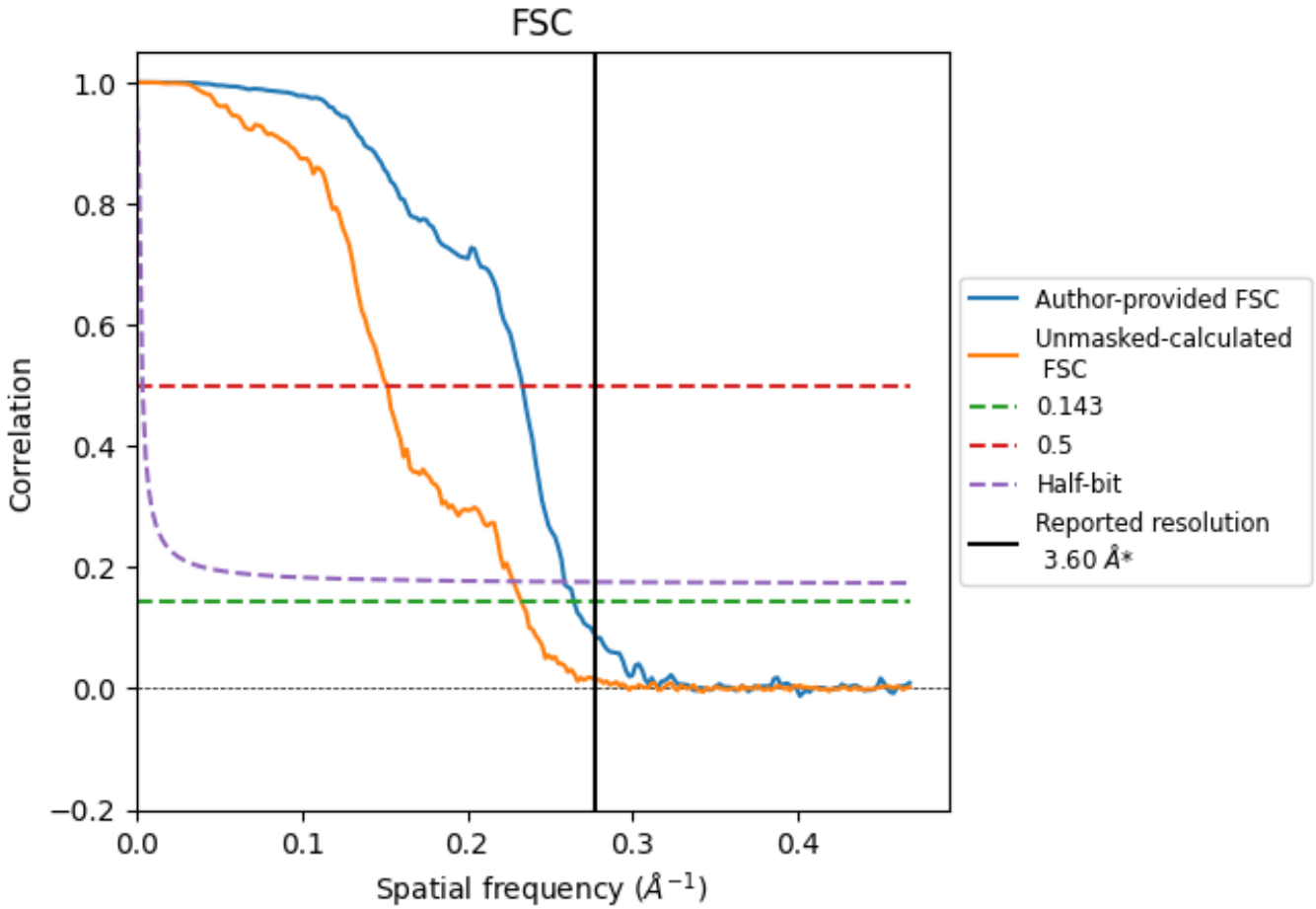


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

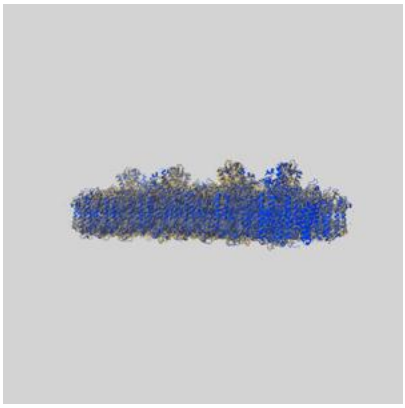
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.78	4.28	3.87
Unmasked-calculated*	4.30	6.59	4.39

*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 4.30 differs from the reported value 3.6 by more than 10 %

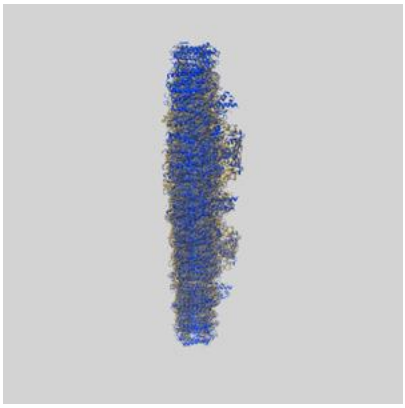
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33933 and PDB model 7YMM. Per-residue inclusion information can be found in section 3 on page 59.

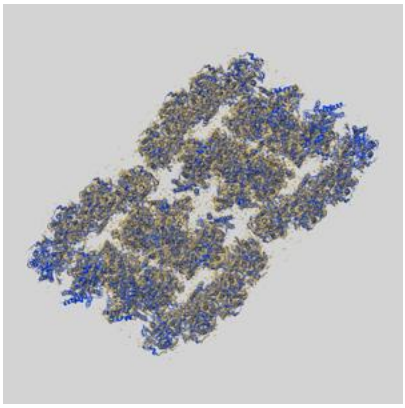
9.1 Map-model overlay



X



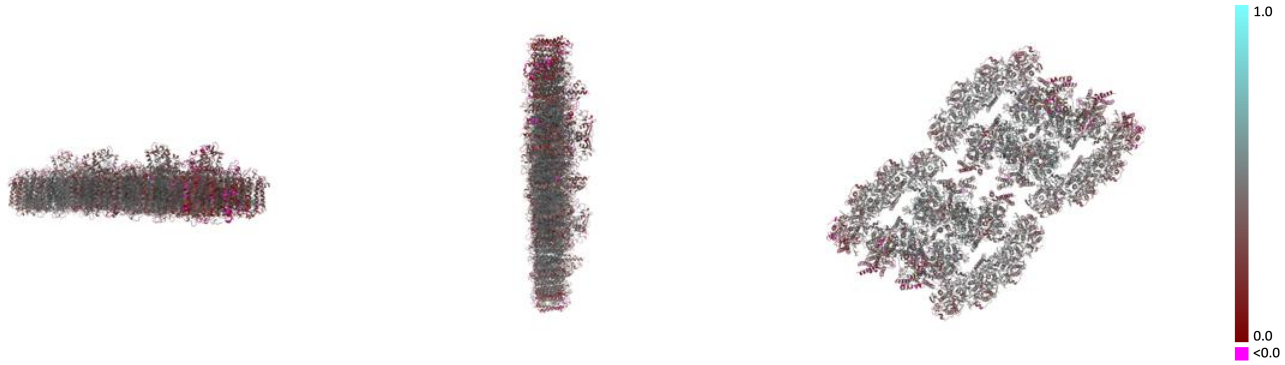
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

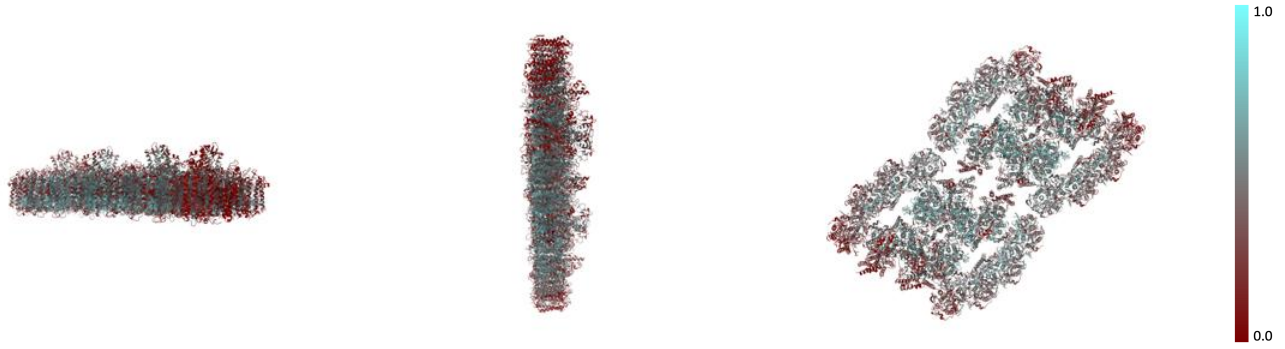
9.2 Q-score mapped to coordinate model



X Y Z

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

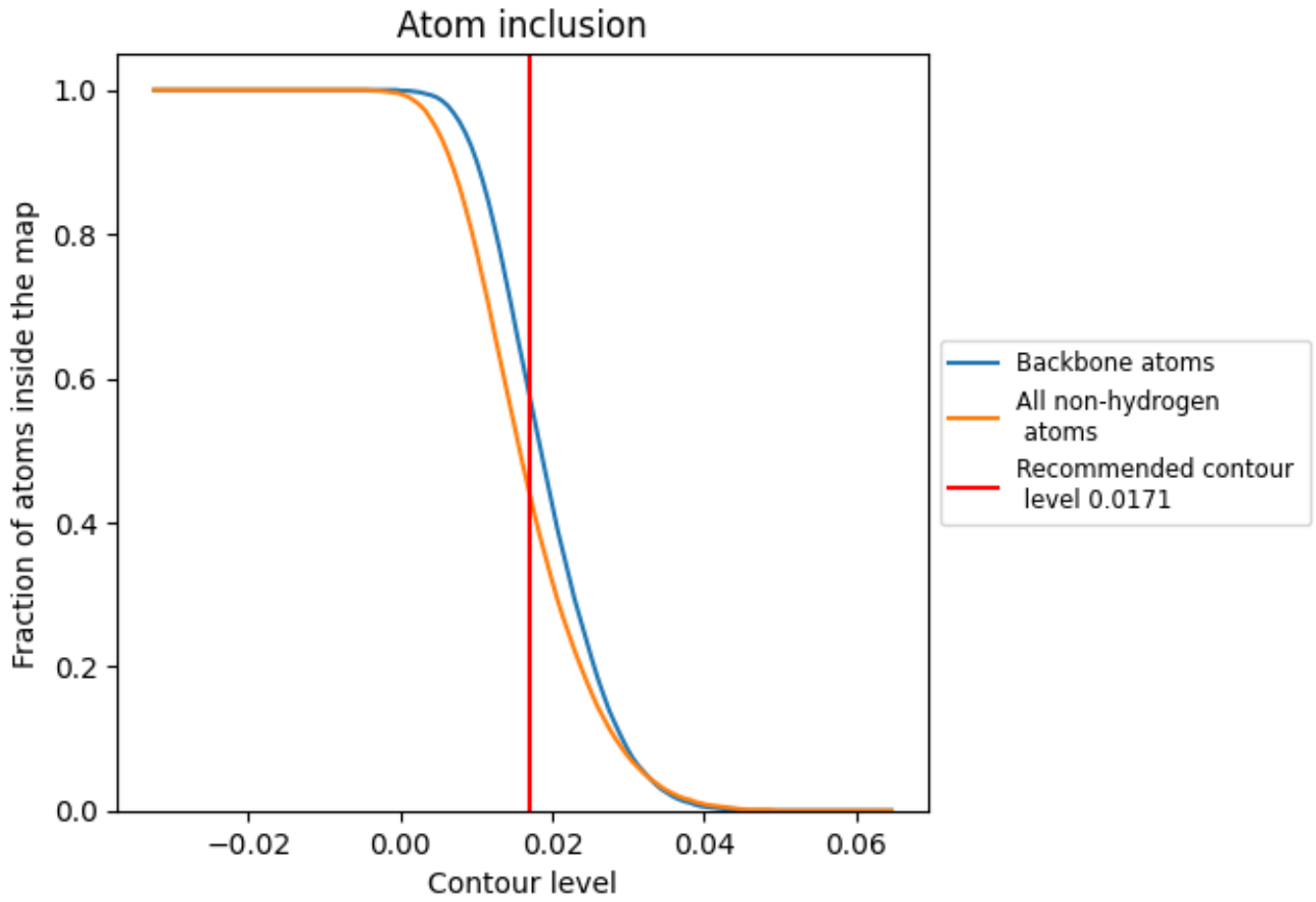
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0171).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 44% 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 (0.0171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4360	0.4150
11	0.1630	0.2740
12	0.3730	0.4020
13	0.4540	0.4310
14	0.2890	0.3650
1A	0.4920	0.4560
1B	0.4770	0.4460
1C	0.3450	0.3770
1D	0.4680	0.4410
1E	0.1260	0.1690
1F	0.1880	0.2640
1G	0.3900	0.3740
1H	0.3600	0.3920
1I	0.4510	0.4530
1K	0.0670	0.2420
1L	0.5750	0.4890
1M	0.4540	0.4280
1T	0.4120	0.4430
1X	0.1080	0.2590
1Y	0.0000	0.1200
1Z	0.0140	0.1310
21	0.4480	0.4060
22	0.4910	0.4500
23	0.4660	0.4370
24	0.4680	0.4210
2A	0.5940	0.4900
2B	0.5820	0.4800
2C	0.5220	0.4400
2D	0.6000	0.4840
2E	0.2790	0.2920
2F	0.4420	0.3740
2G	0.4240	0.4160
2H	0.5190	0.4680
2I	0.5920	0.4840
2K	0.2630	0.3470



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Chain	Atom inclusion	Q-score
2L	0.6180	0.5070
2M	0.5020	0.4500
2T	0.4870	0.4680
2X	0.2610	0.3470
2Y	0.1480	0.2450
2Z	0.1690	0.2230
31	0.4470	0.4050
32	0.4920	0.4480
33	0.4660	0.4380
34	0.4680	0.4210
3A	0.5950	0.4900
3B	0.5810	0.4800
3C	0.5230	0.4420
3D	0.5980	0.4840
3E	0.2770	0.2940
3F	0.4420	0.3720
3G	0.4240	0.4120
3H	0.5170	0.4680
3I	0.5960	0.4850
3K	0.2660	0.3490
3L	0.6140	0.5100
3M	0.5020	0.4520
3T	0.4870	0.4660
3X	0.2610	0.3460
3Y	0.1480	0.2410
3Z	0.1690	0.2290
41	0.1630	0.2750
42	0.3730	0.4020
43	0.4550	0.4300
44	0.2900	0.3640
4A	0.4930	0.4570
4B	0.4770	0.4450
4C	0.3460	0.3780
4D	0.4660	0.4410
4E	0.1240	0.1710
4F	0.1880	0.2690
4G	0.3760	0.3820
4H	0.3620	0.3910
4I	0.4440	0.4520
4K	0.0700	0.2420
4L	0.5750	0.4870
4M	0.4540	0.4300

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Chain	Atom inclusion	Q-score
4T	0.4120	0.4440
4X	0.1080	0.2570
4Y	0.0000	0.1250
4Z	0.0160	0.1280