



wwPDB EM Validation Summary Report ⓘ

Aug 13, 2026 – 03:48 AM 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

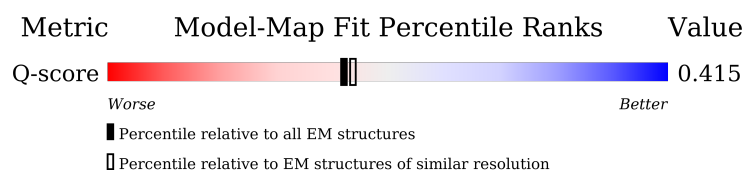
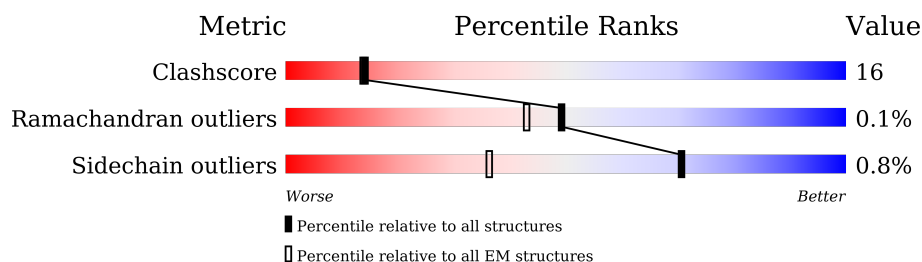
1 Overall quality at a glance

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 $\leq 5\%$. 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	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	
14	4Y	39	
15	1Z	62	
15	2Z	62	
15	3Z	62	
15	4Z	62	
16	12	352	
16	22	352	
16	32	352	
16	42	352	
17	1G	41	
17	2G	41	
17	3G	41	
17	4G	41	
18	11	356	
18	21	356	
18	31	356	
18	41	356	
19	13	349	
19	23	349	
19	33	349	
19	43	349	
20	14	353	
20	24	353	
20	34	353	

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Mol	Chain	Length	Quality of chain
20	44	353	71% 69% 24% 6%

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).



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

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

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

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

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

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

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

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

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

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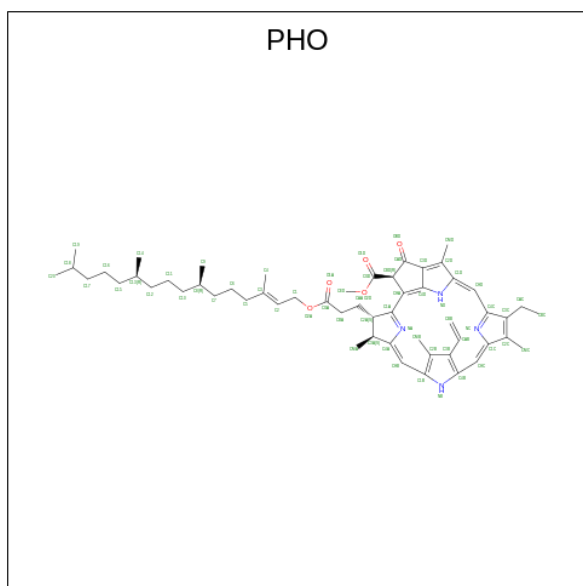
Mol	Chain	Residues	Atoms					AltConf
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 58	C 47	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43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

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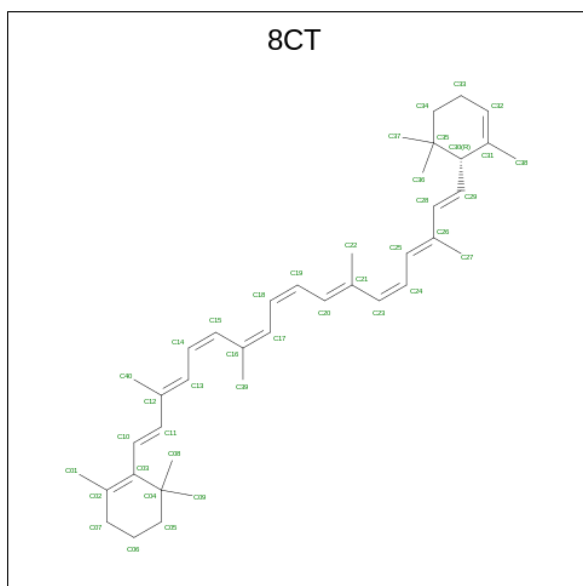
Mol	Chain	Residues	Atoms					AltConf
21	44	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	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	0
			64	55	4	5	
22	1D	1	Total	C	N	O	0
			64	55	4	5	
22	2A	1	Total	C	N	O	0
			64	55	4	5	
22	2D	1	Total	C	N	O	0
			64	55	4	5	
22	3A	1	Total	C	N	O	0
			64	55	4	5	
22	3D	1	Total	C	N	O	0
			64	55	4	5	
22	4A	1	Total	C	N	O	0
			64	55	4	5	
22	4D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 23 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



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

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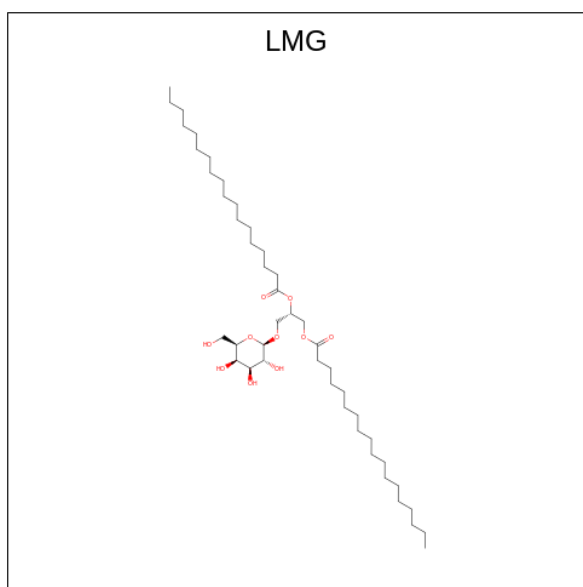
Mol	Chain	Residues	Atoms	AltConf
23	1B	1	Total C 40 40	0
23	1B	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1D	1	Total C 40 40	0
23	1K	1	Total C 40 40	0
23	14	1	Total C 40 40	0
23	2A	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	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: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



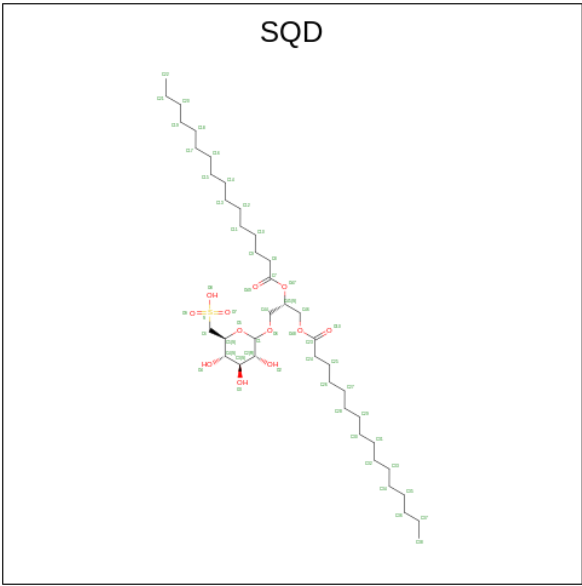
Mol	Chain	Residues	Atoms			AltConf
24	1A	1	Total	C	O	0
			50	40	10	
24	1B	1	Total	C	O	0
			51	41	10	
24	1D	1	Total	C	O	0
			33	23	10	
24	11	1	Total	C	O	0
			51	41	10	
24	2A	1	Total	C	O	0
			50	40	10	
24	2B	1	Total	C	O	0
			51	41	10	
24	2D	1	Total	C	O	0
			33	23	10	
24	21	1	Total	C	O	0
			51	41	10	
24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

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



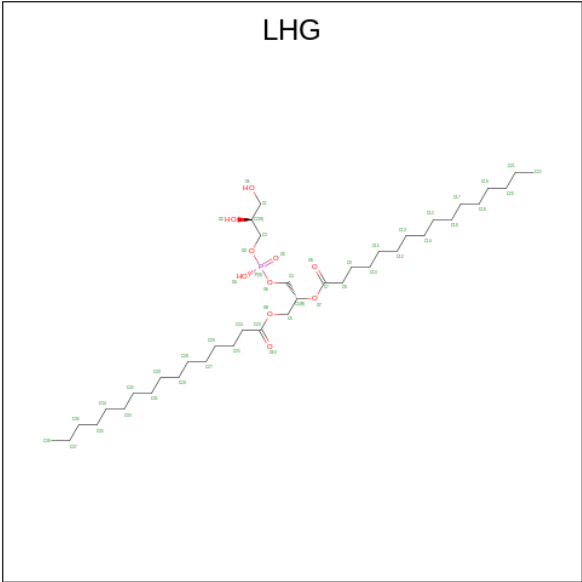
Mol	Chain	Residues	Atoms				AltConf
25	1A	1	Total	C	O	S	0
			34	21	12	1	
25	1B	1	Total	C	O	S	0
			54	41	12	1	
25	12	1	Total	C	O	S	0
			50	37	12	1	
25	12	1	Total	C	O	S	0
			41	28	12	1	
25	11	1	Total	C	O	S	0
			32	19	12	1	
25	13	1	Total	C	O	S	0
			46	33	12	1	
25	13	1	Total	C	O	S	0
			50	37	12	1	
25	2A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

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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: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



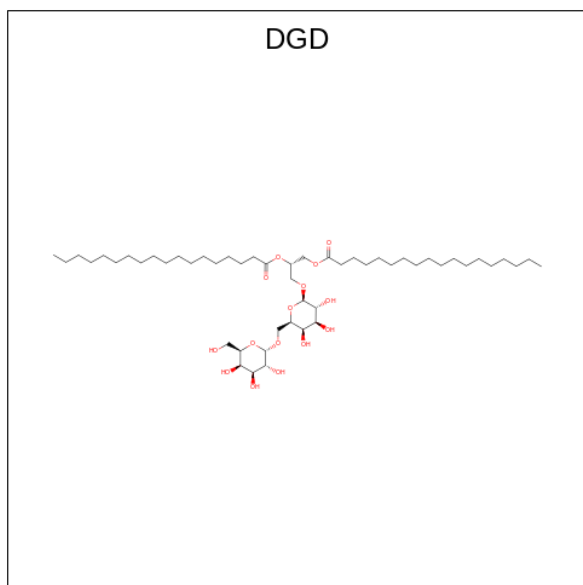
Mol	Chain	Residues	Atoms				AltConf
26	1A	1	Total	C	O	P	0
			46	35	10	1	
26	1B	1	Total	C	O	P	0
			45	34	10	1	
26	1B	1	Total	C	O	P	0
			49	38	10	1	
26	1D	1	Total	C	O	P	0
			49	38	10	1	
26	13	1	Total	C	O	P	0
			36	25	10	1	
26	14	1	Total	C	O	P	0
			49	38	10	1	
26	2A	1	Total	C	O	P	0
			46	35	10	1	
26	2B	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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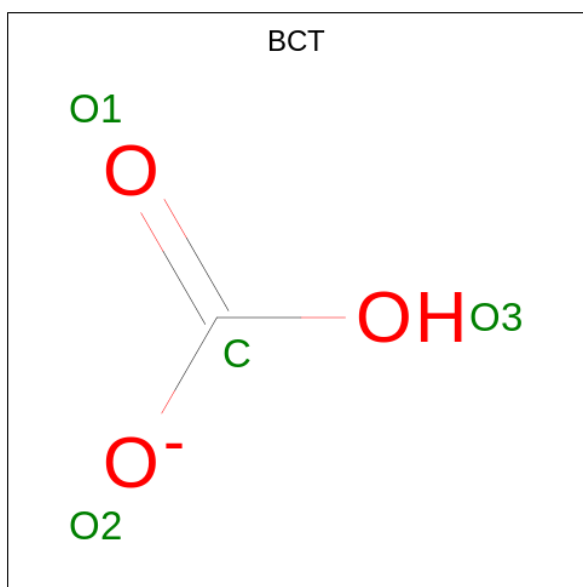
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Mol	Chain	Residues	Atoms			AltConf
27	1C	1	Total 62	C 47	O 15	0
27	2B	1	Total 62	C 47	O 15	0
27	2C	1	Total 62	C 47	O 15	0
27	3B	1	Total 62	C 47	O 15	0
27	3C	1	Total 62	C 47	O 15	0
27	4B	1	Total 62	C 47	O 15	0
27	4C	1	Total 62	C 47	O 15	0

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

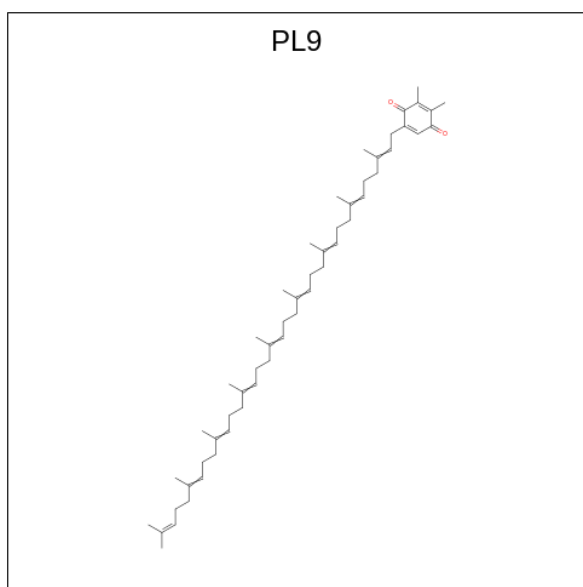
Mol	Chain	Residues	Atoms		AltConf
28	1D	1	Total 1	Fe 1	0
28	2D	1	Total 1	Fe 1	0
28	3D	1	Total 1	Fe 1	0
28	4D	1	Total 1	Fe 1	0

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



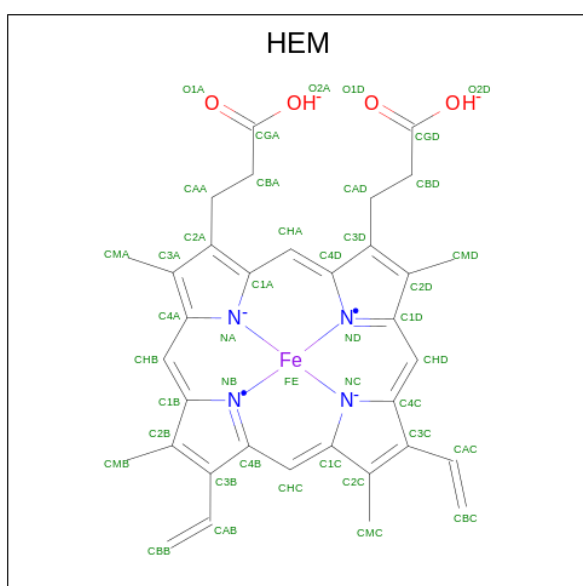
Mol	Chain	Residues	Atoms			AltConf
29	1D	1	Total	C	O	0
			4	1	3	
29	2D	1	Total	C	O	0
			4	1	3	
29	3D	1	Total	C	O	0
			4	1	3	
29	4D	1	Total	C	O	0
			4	1	3	

- 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: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



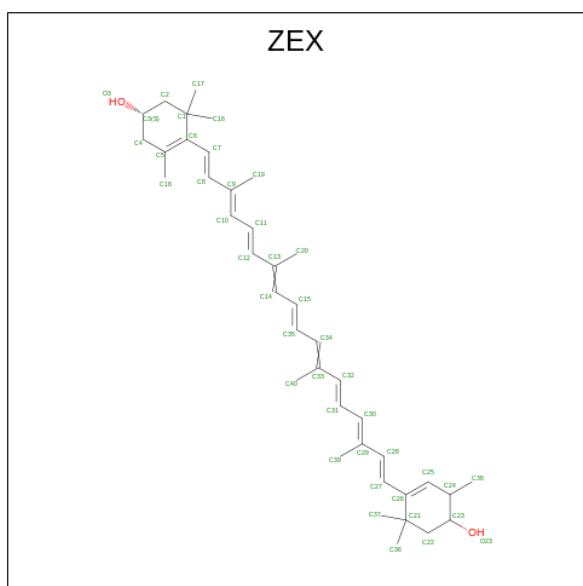
Mol	Chain	Residues	Atoms			AltConf
30	1D	1	Total	C	O	0
			55	53	2	
30	2D	1	Total	C	O	0
			55	53	2	
30	3D	1	Total	C	O	0
			55	53	2	
30	4D	1	Total	C	O	0
			55	53	2	

- 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 43	C 34	Fe 1	N 4	O 4	0
31	2F	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	3F	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	4F	1	Total 43	C 34	Fe 1	N 4	O 4	0

- 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: C₄₀H₅₆O₂) (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	0
			42	40	2	
32	13	1	Total	C	O	0
			42	40	2	
32	13	1	Total	C	O	0
			42	40	2	
32	13	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	21	1	Total	C	O	0
			42	40	2	
32	21	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	24	1	Total	C	O	0
			42	40	2	
32	24	1	Total	C	O	0
			42	40	2	
32	24	1	Total	C	O	0
			42	40	2	

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

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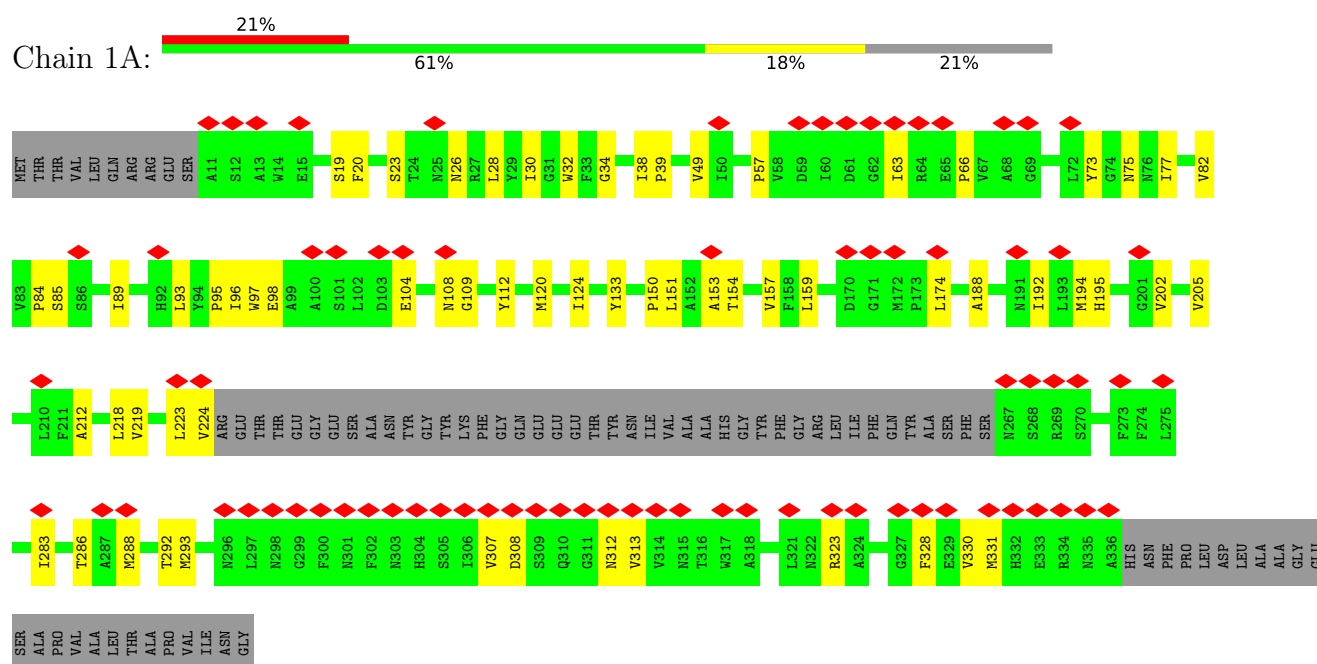
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Mol	Chain	Residues	Atoms			AltConf
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			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0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

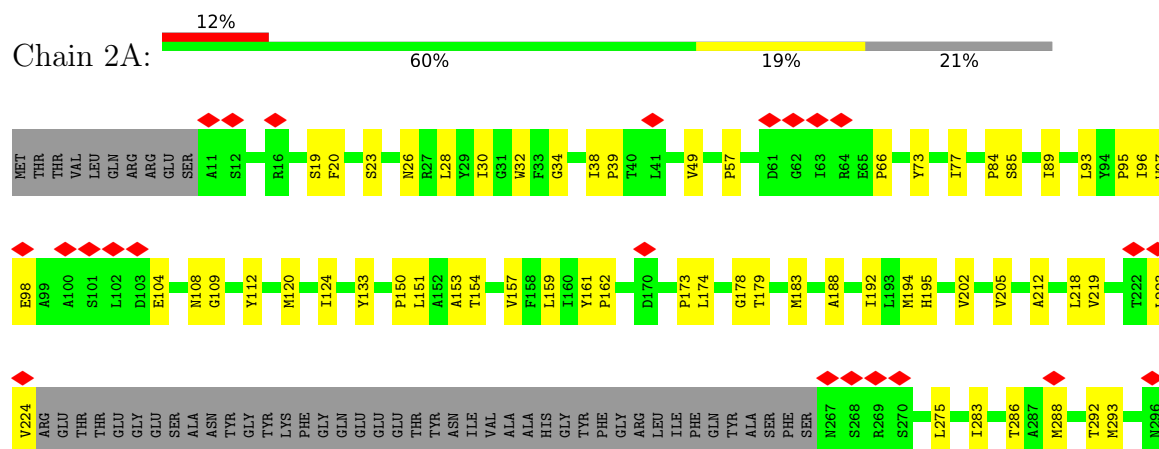
3 Residue-property plots

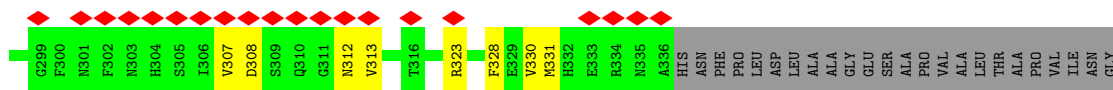
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

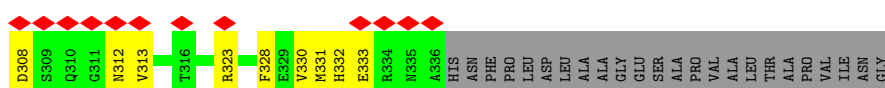
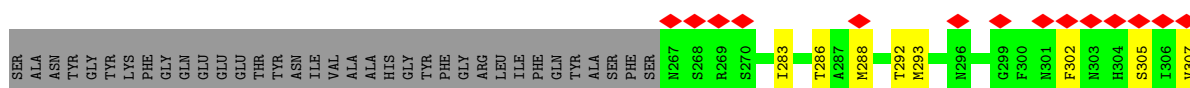
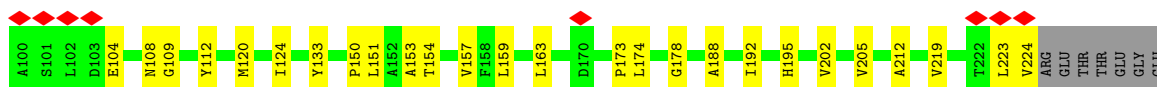
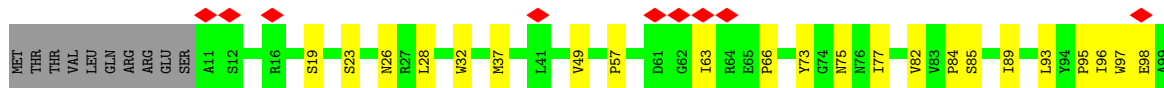


• Molecule 1: Photosystem II protein D1 2

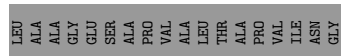
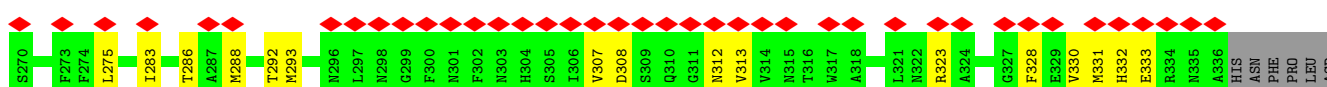
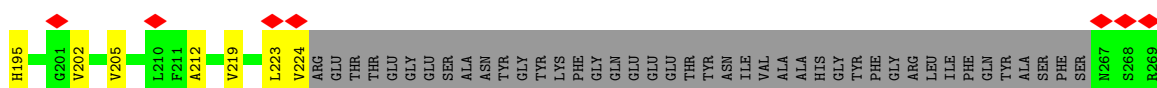
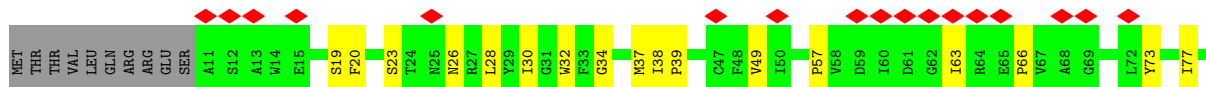




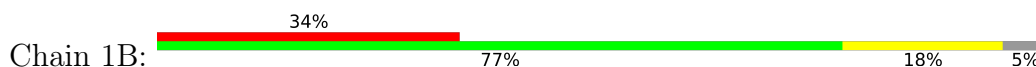
• Molecule 1: Photosystem II protein D1 2

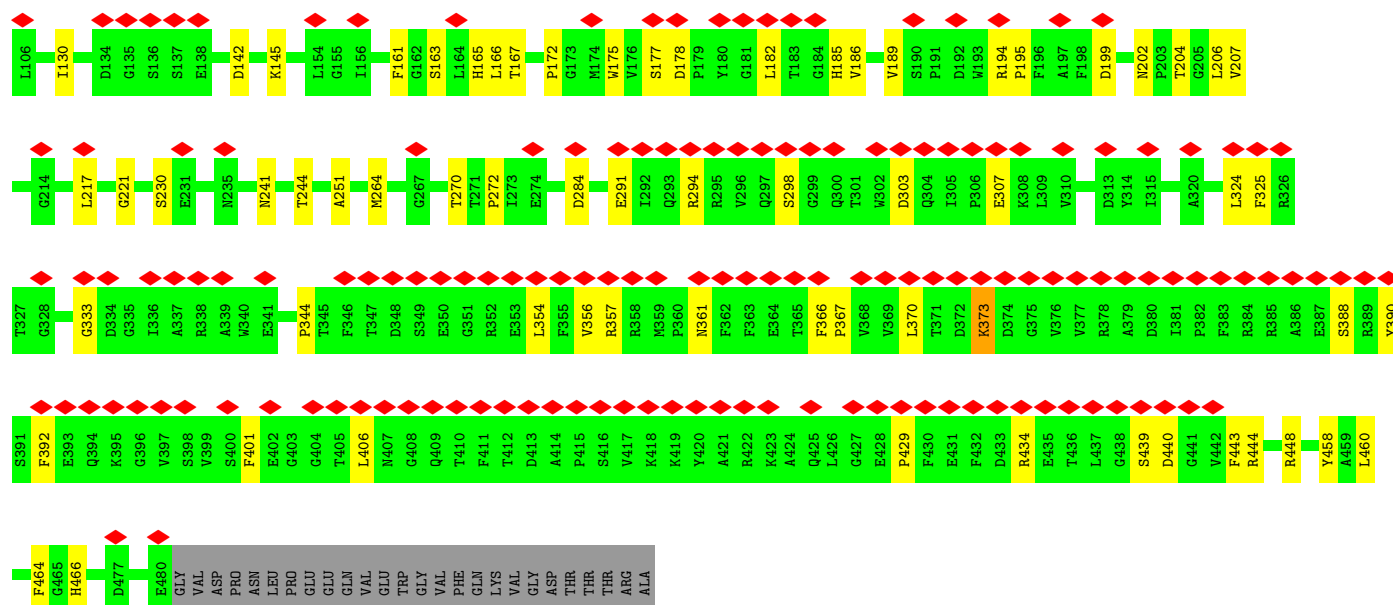


• Molecule 1: Photosystem II protein D1 2

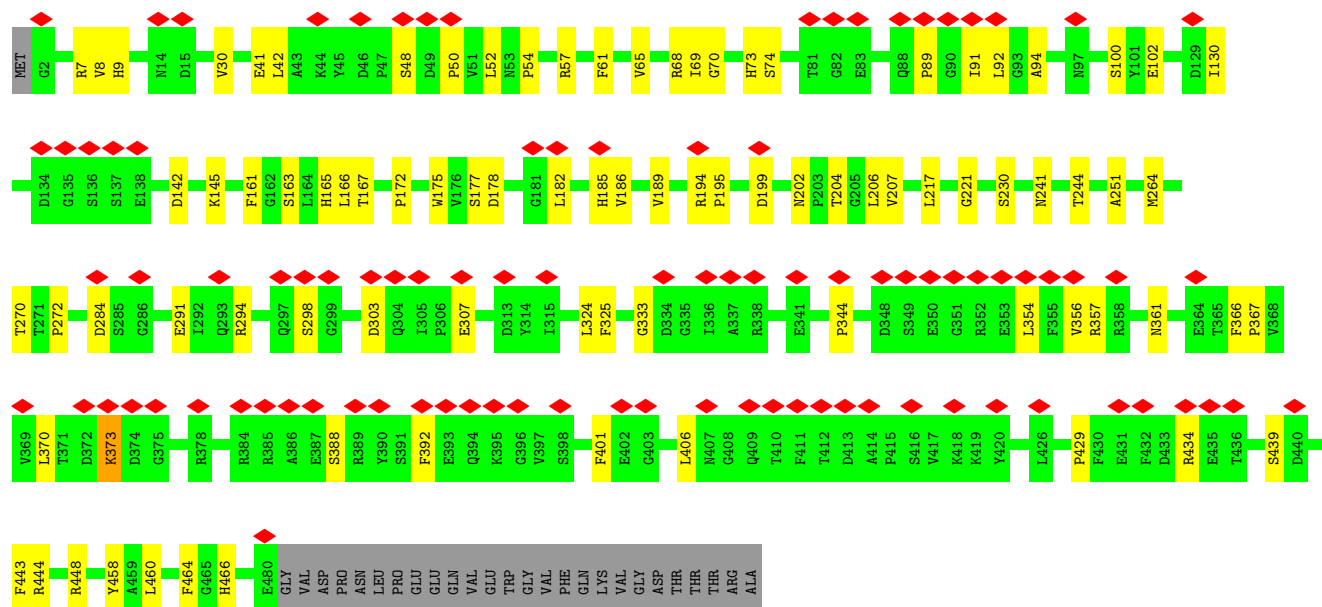
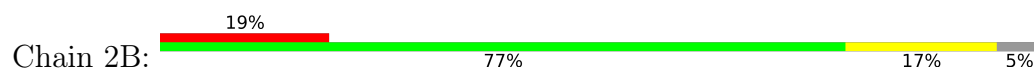


• Molecule 2: Photosystem II CP47 reaction center protein

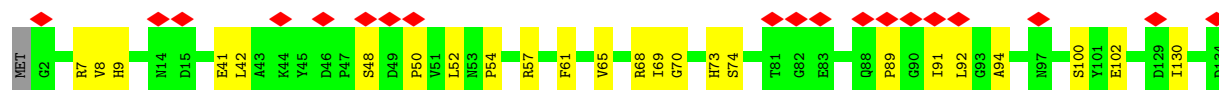
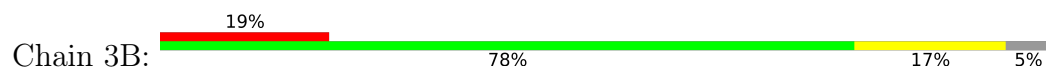


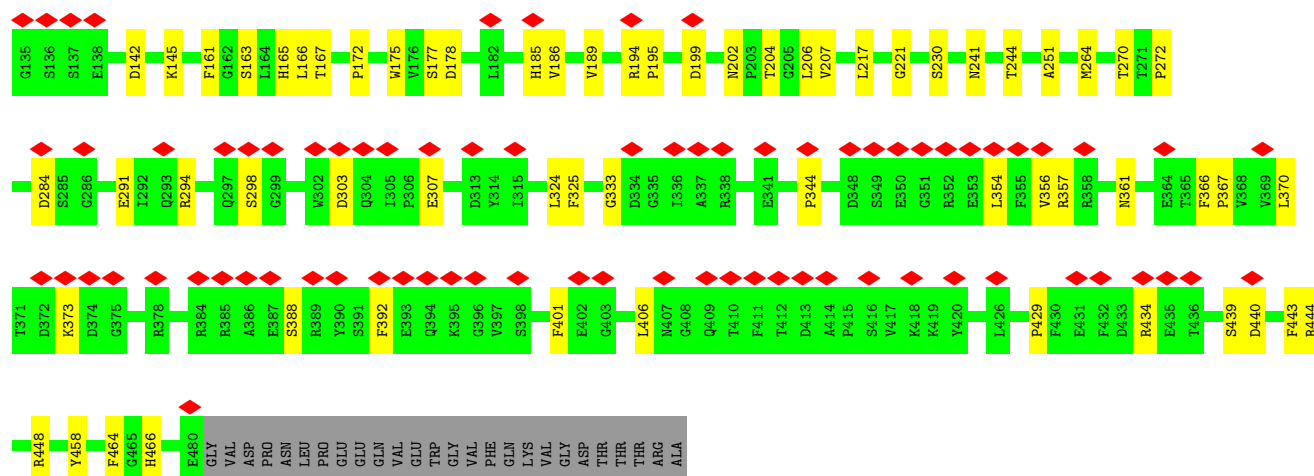


• Molecule 2: Photosystem II CP47 reaction center protein

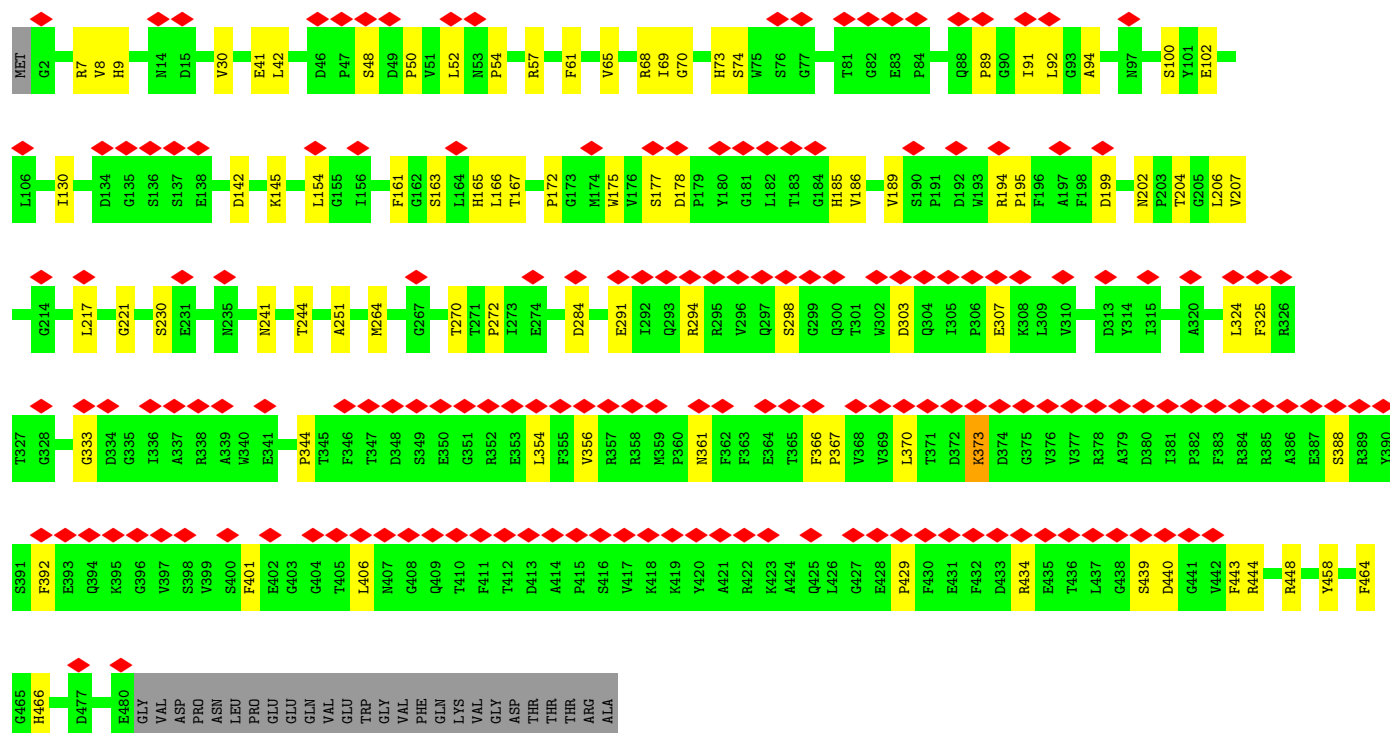
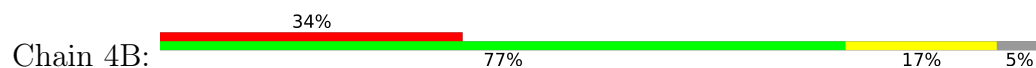


• Molecule 2: Photosystem II CP47 reaction center protein

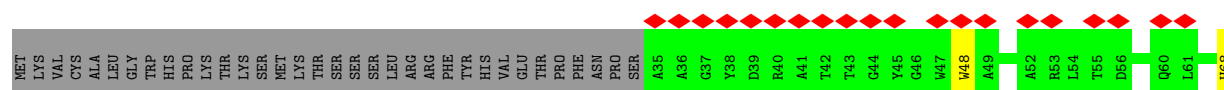


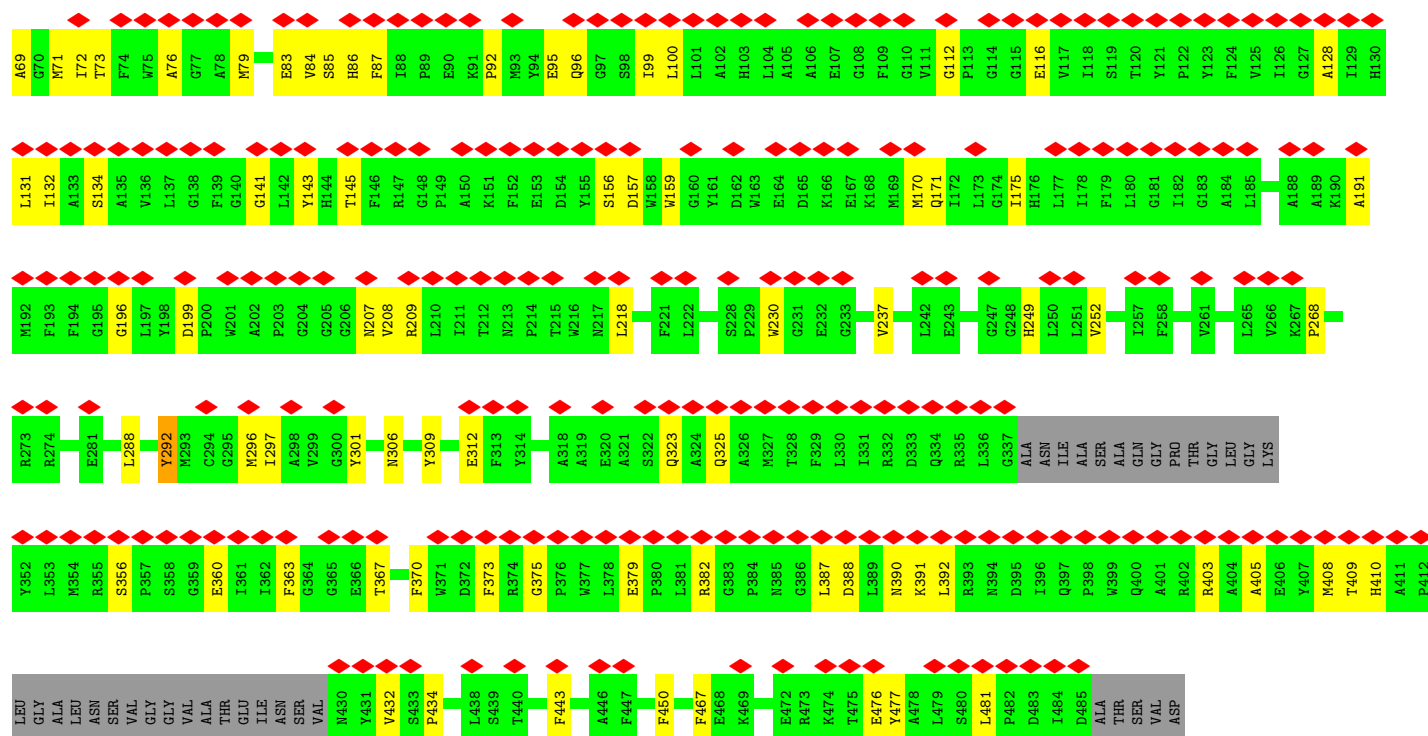


• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

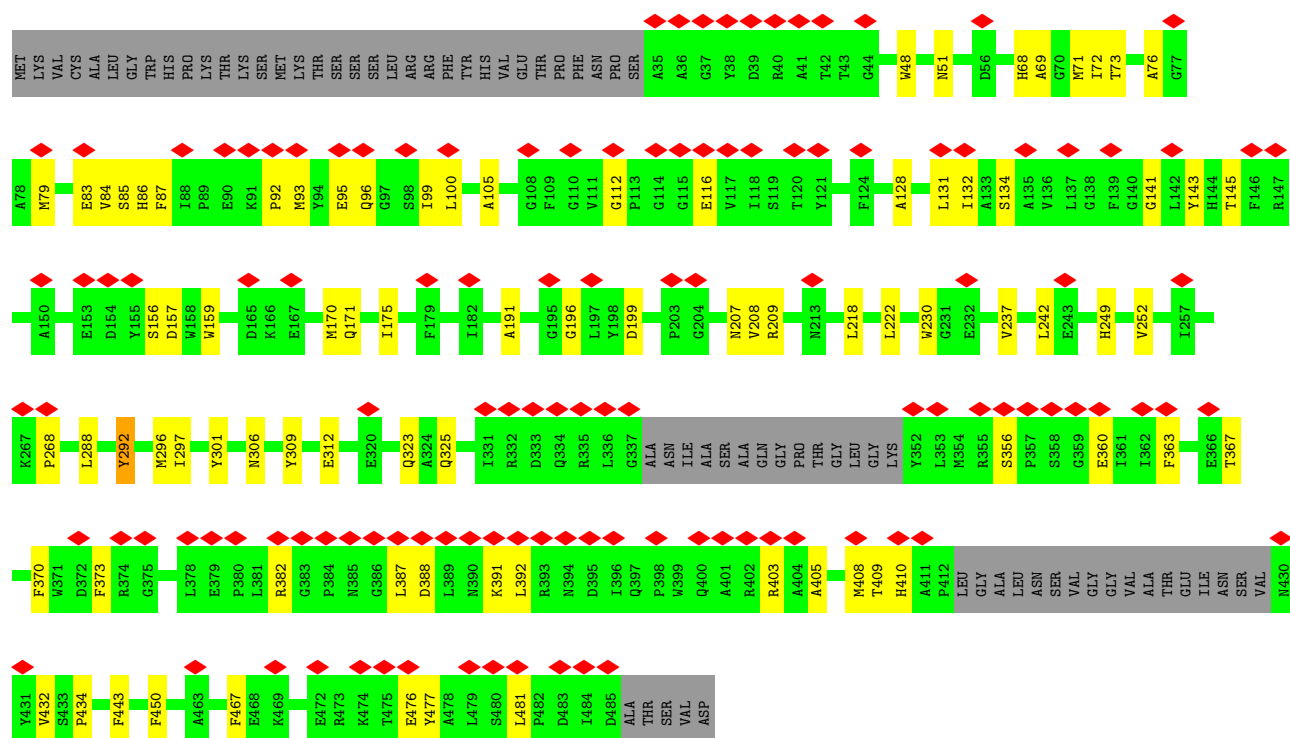
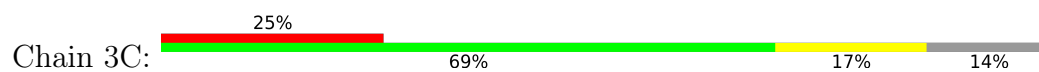




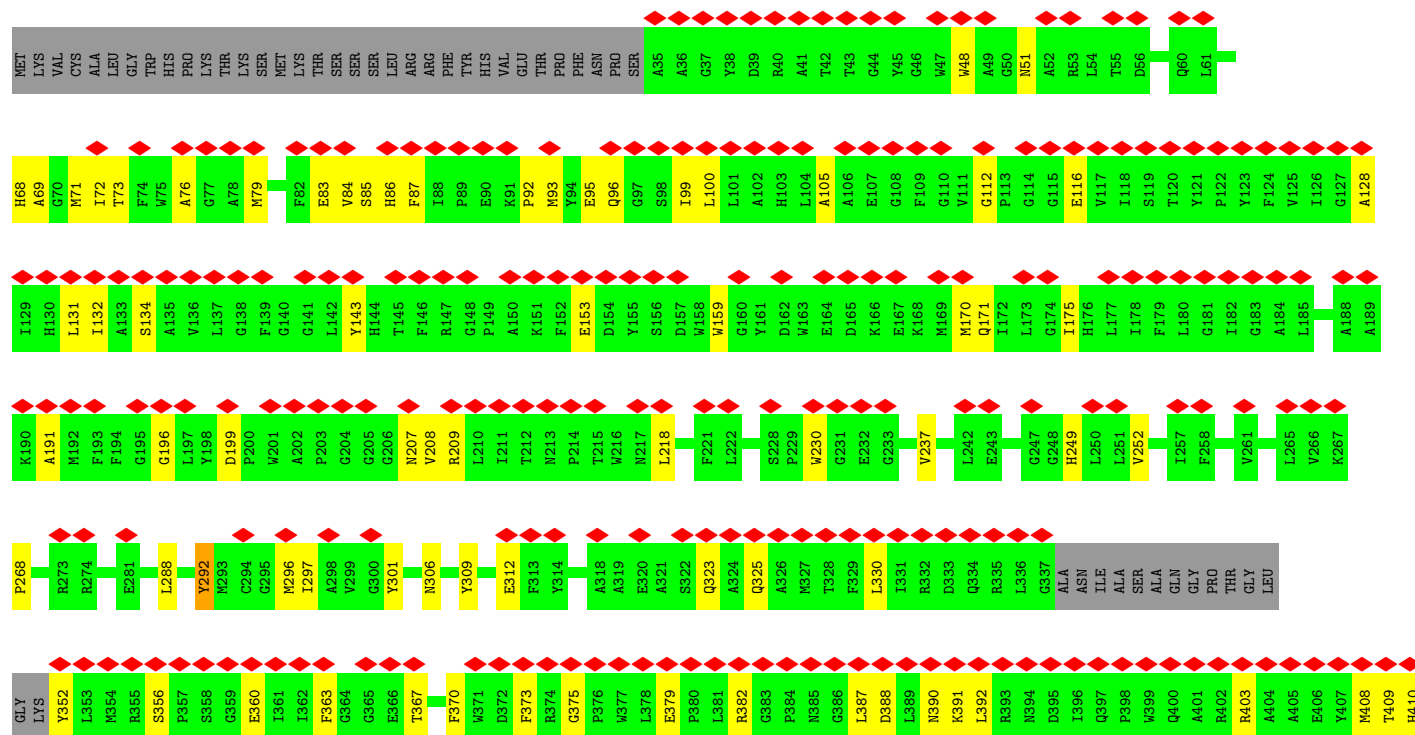
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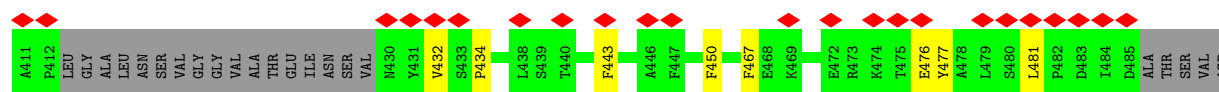


• Molecule 3: Photosystem II CP43 reaction center protein

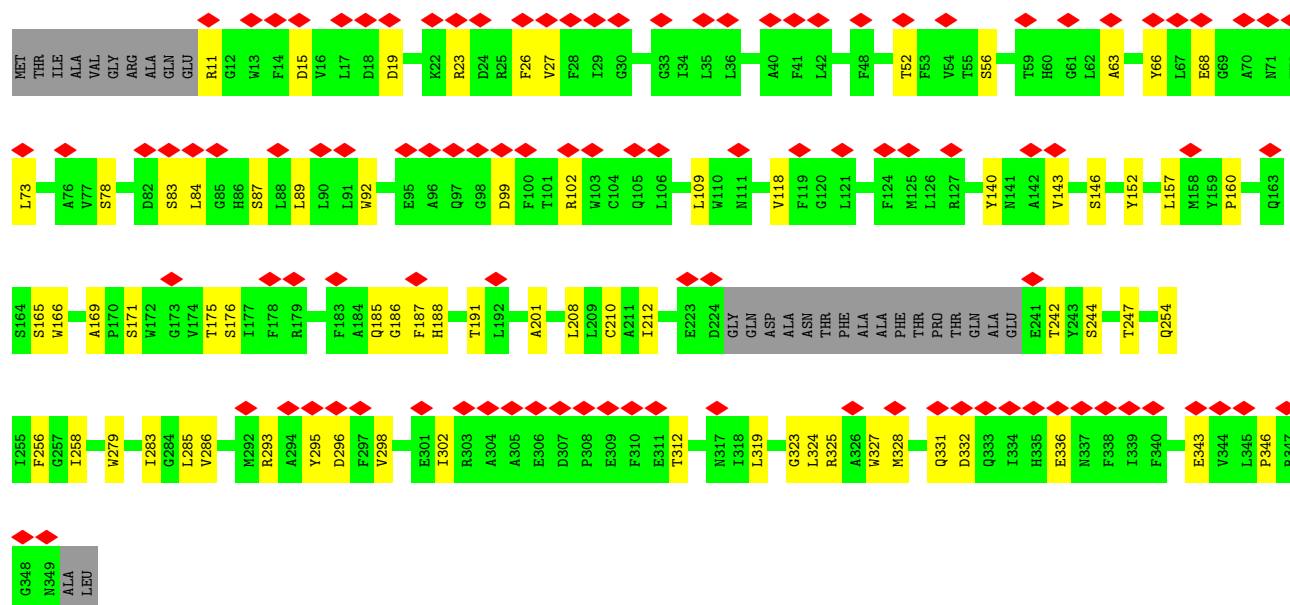
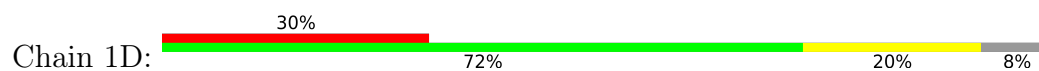


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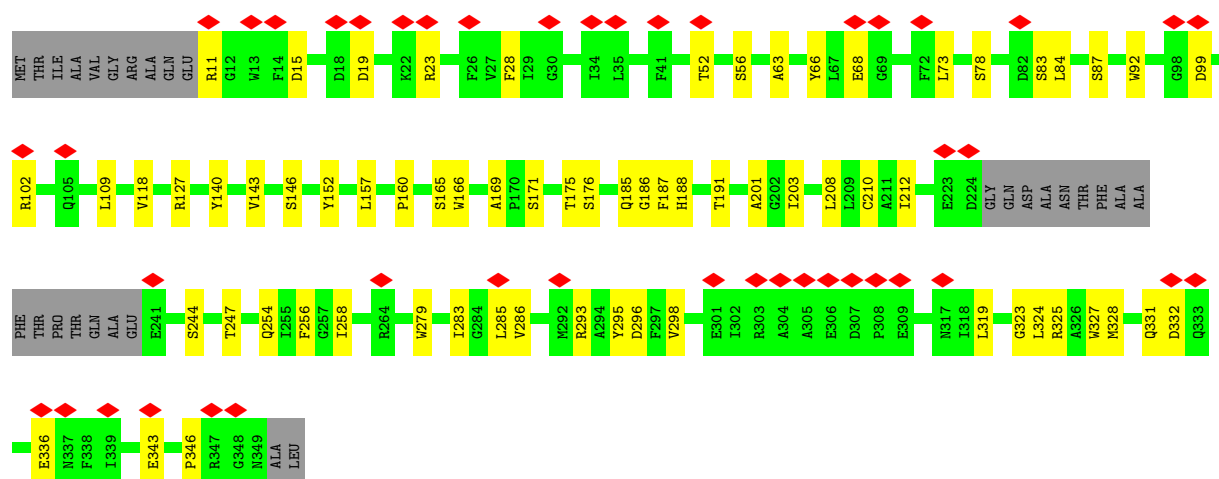
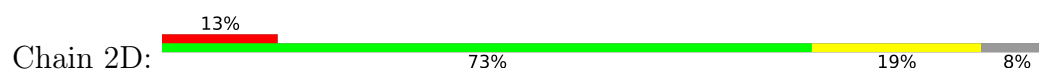




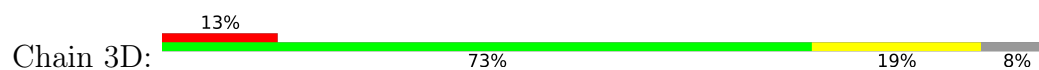
• Molecule 4: Photosystem II D2 protein 1

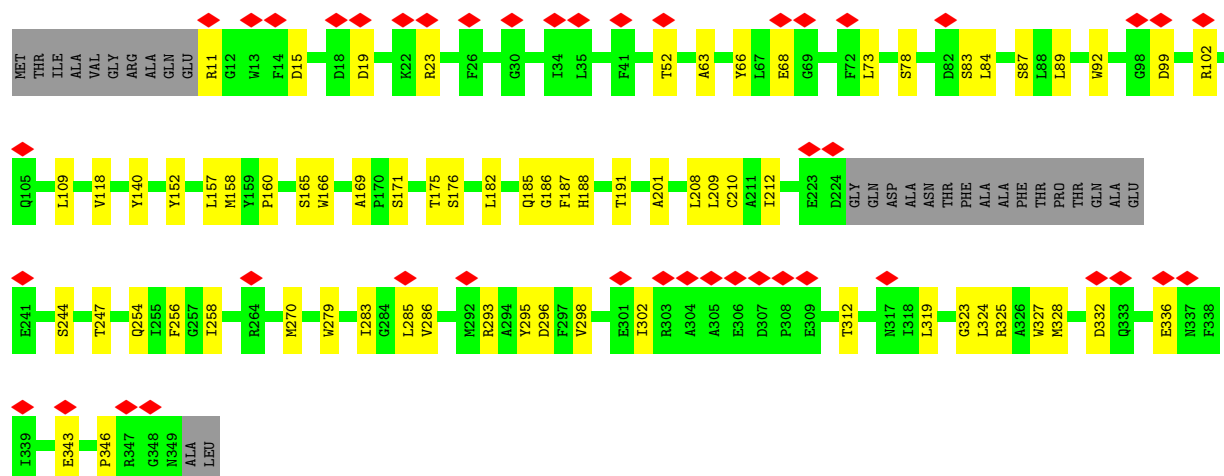


• Molecule 4: Photosystem II D2 protein 1

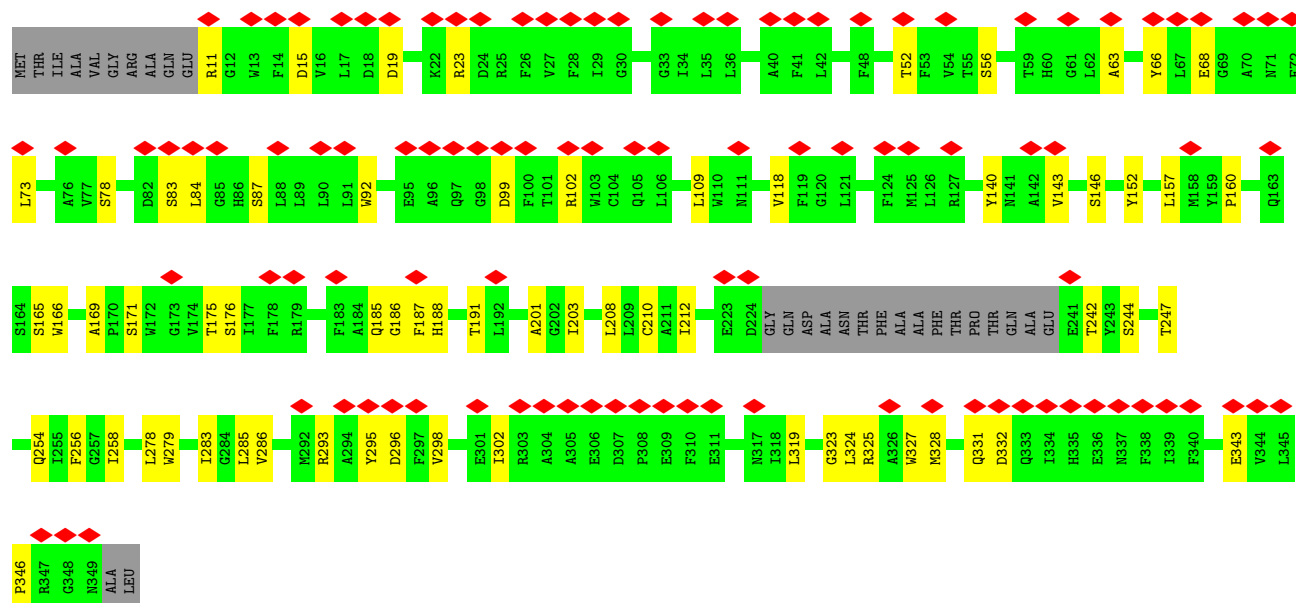
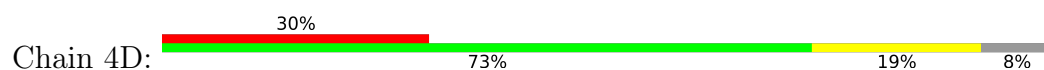


• Molecule 4: Photosystem II D2 protein 1

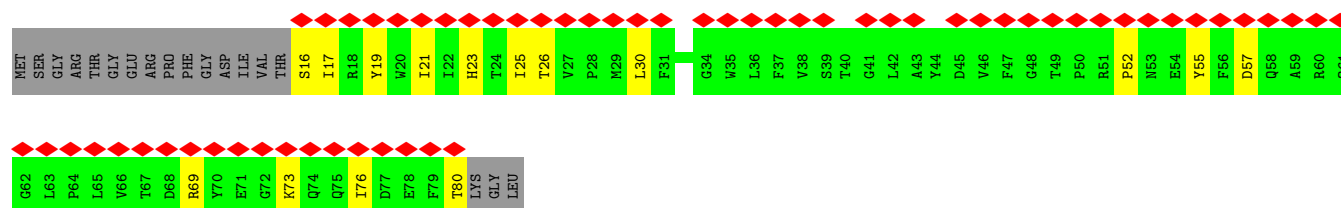
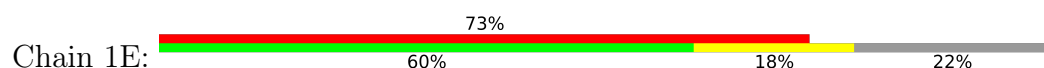




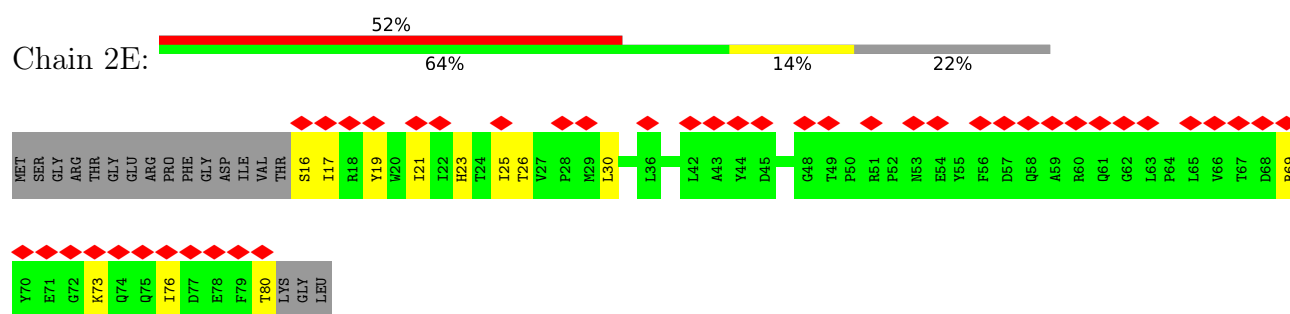
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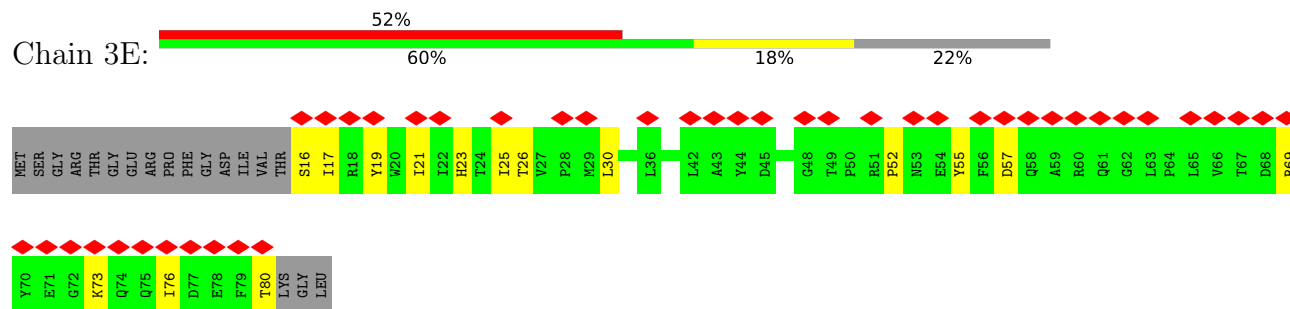
• Molecule 5: Cytochrome b559 subunit alpha



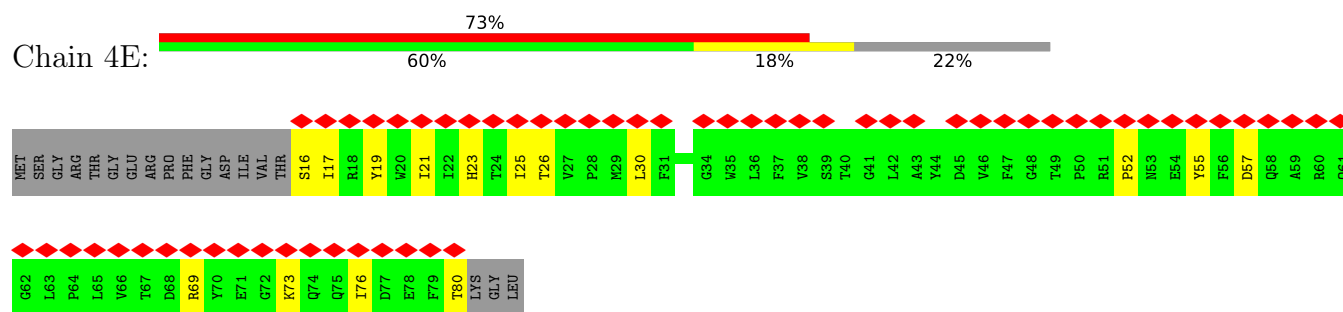
• Molecule 5: Cytochrome b559 subunit alpha



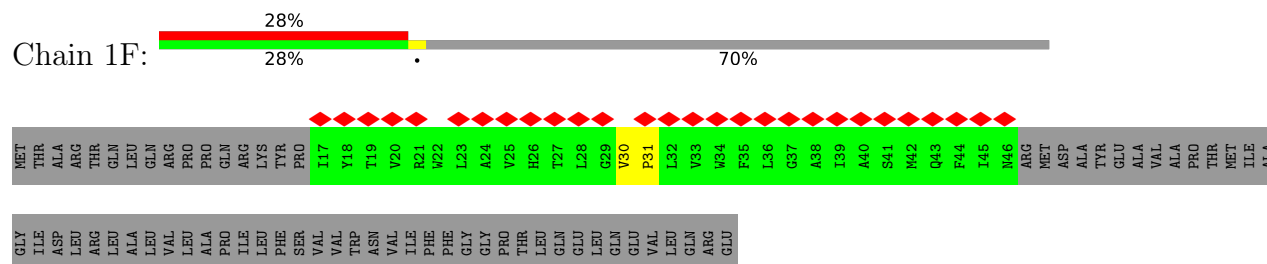
- Molecule 5: Cytochrome b559 subunit alpha



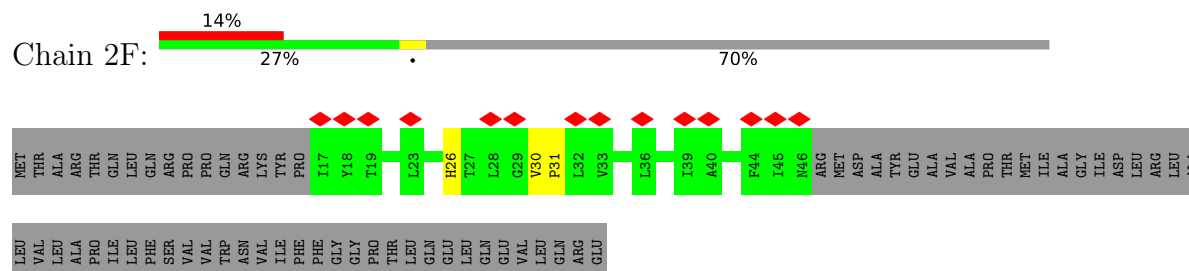
- Molecule 5: Cytochrome b559 subunit alpha



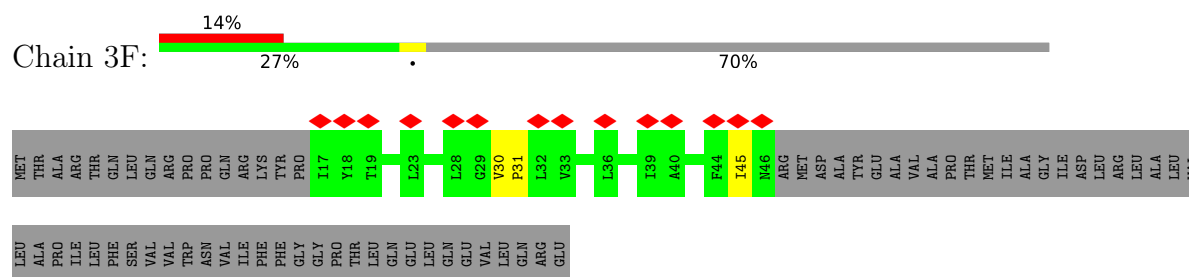
- Molecule 6: Photosystem II protein Y



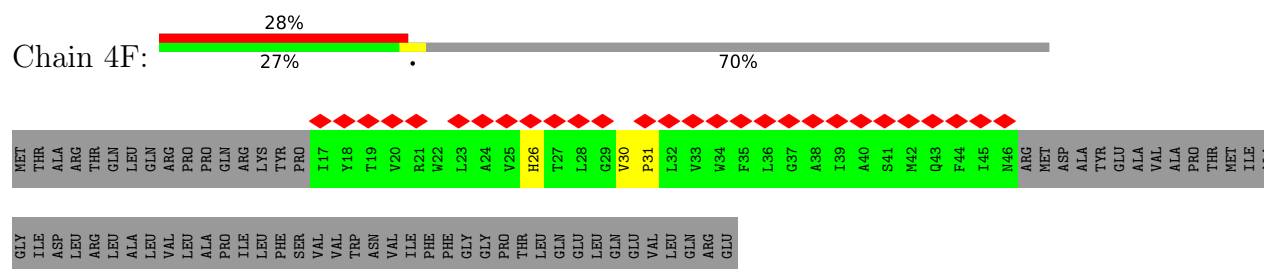
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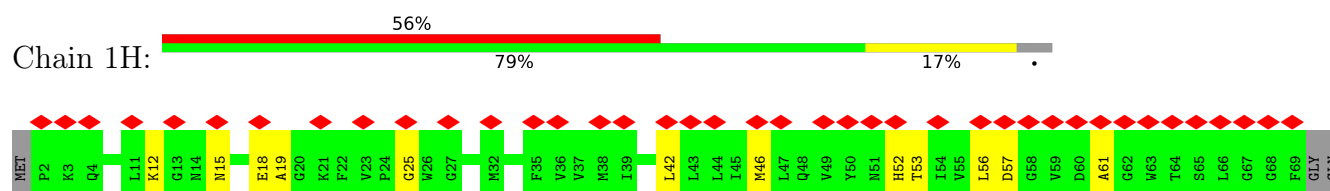
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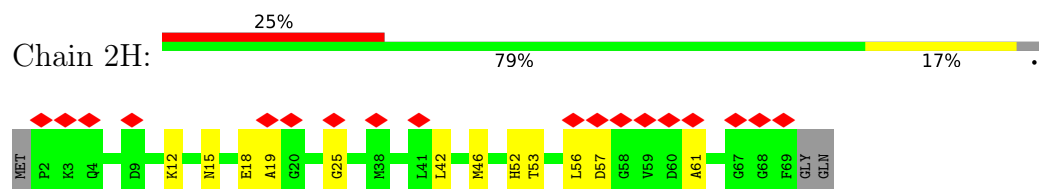
- Molecule 6: Photosystem II protein Y



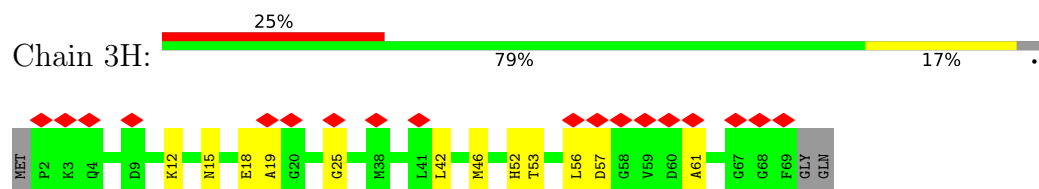
- Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



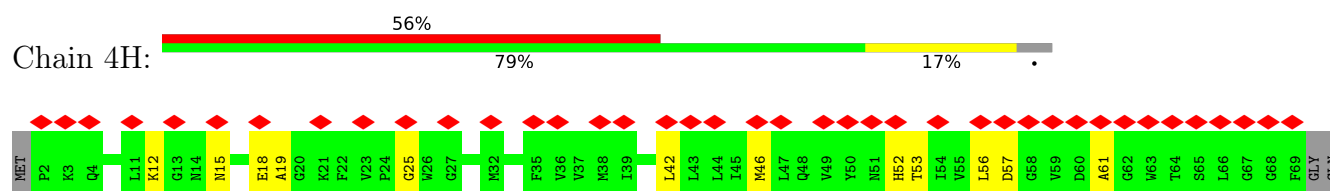
- Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



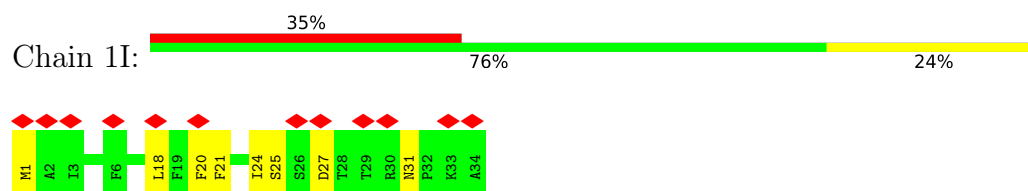
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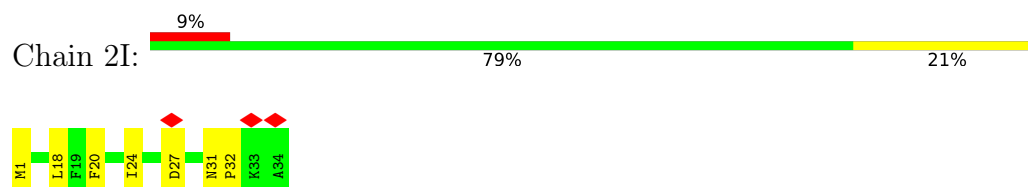
- Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



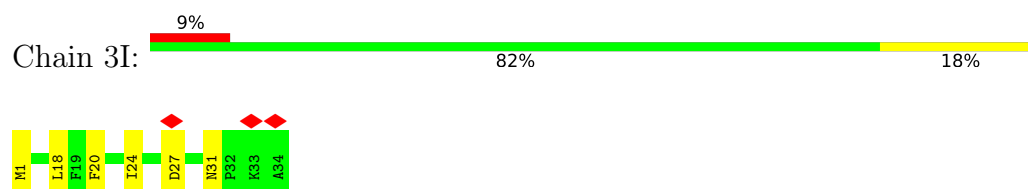
- Molecule 8: Photosystem II protein PsbI



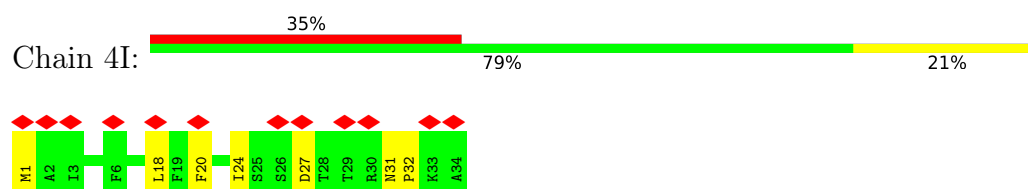
- Molecule 8: Photosystem II protein PsbI



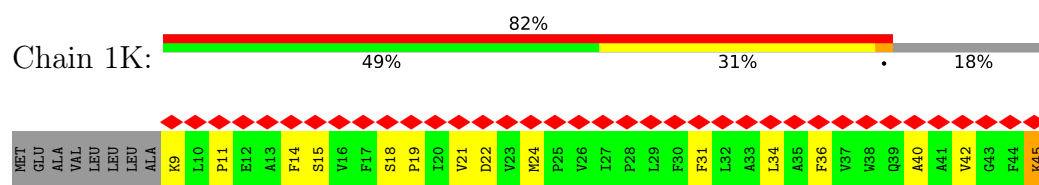
- Molecule 8: Photosystem II protein PsbI



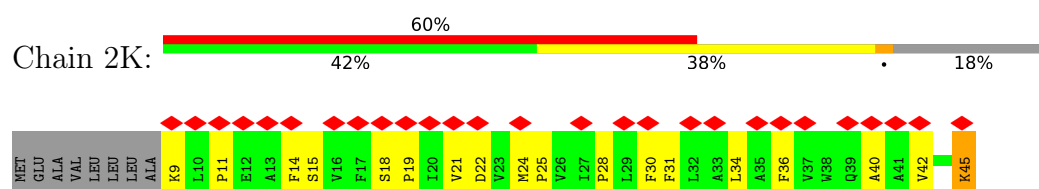
- Molecule 8: Photosystem II protein PsbI



- Molecule 9: Photosystem II reaction center protein K

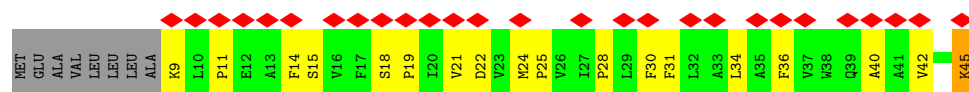


- Molecule 9: Photosystem II reaction center protein K

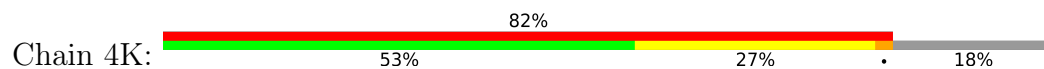


- Molecule 9: Photosystem II reaction center protein K

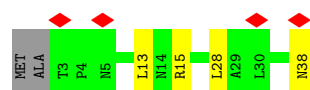
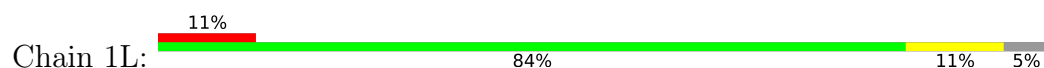




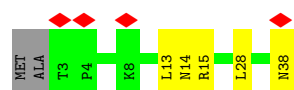
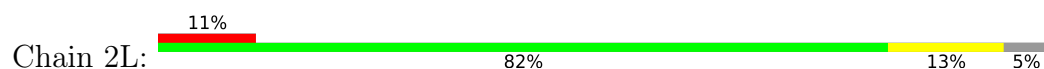
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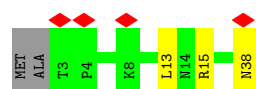
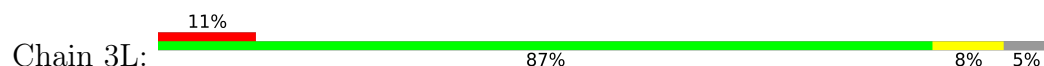
- Molecule 10: Photosystem II reaction center protein L



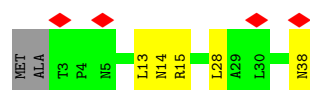
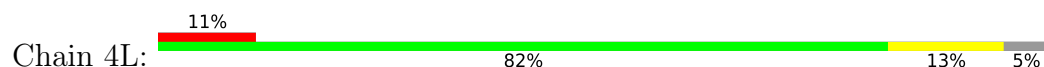
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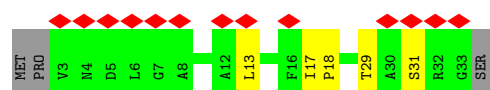
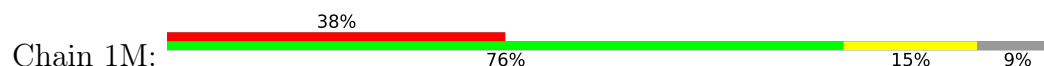
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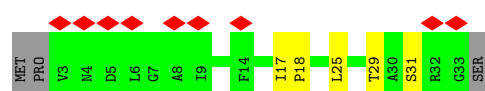
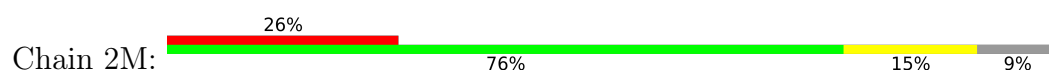
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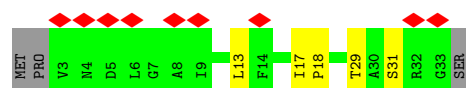
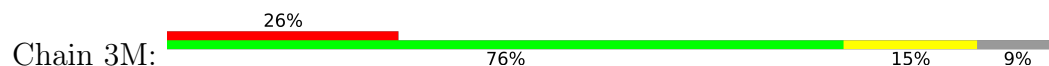
- Molecule 11: Photosystem II reaction center protein M



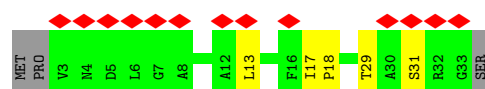
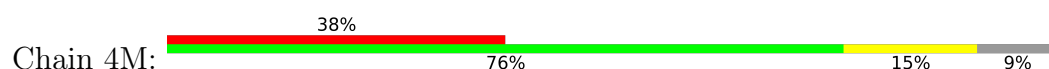
- Molecule 11: Photosystem II reaction center protein M



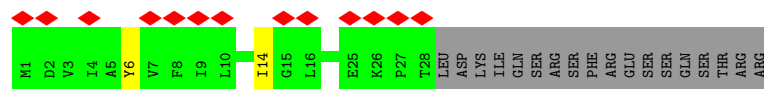
- Molecule 11: Photosystem II reaction center protein M



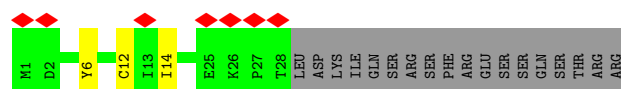
- Molecule 11: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein T



- Molecule 12: Photosystem II reaction center protein T



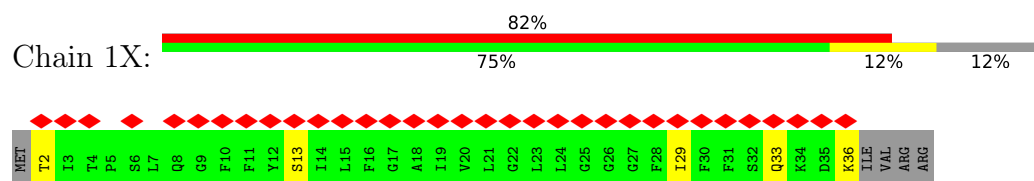
- Molecule 12: Photosystem II reaction center protein T



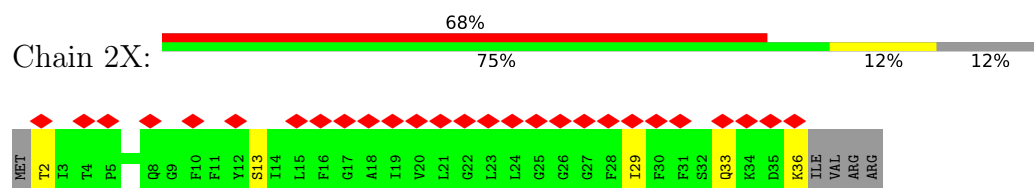
- Molecule 12: Photosystem II reaction center protein T



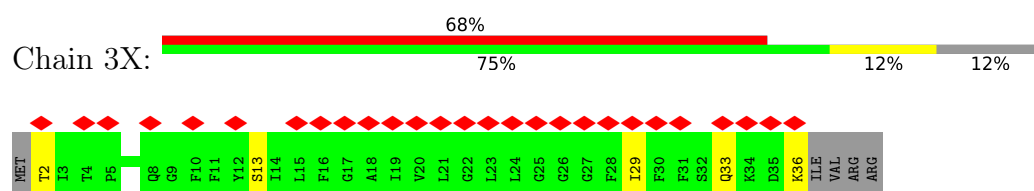
- Molecule 13: Photosystem II reaction center X protein



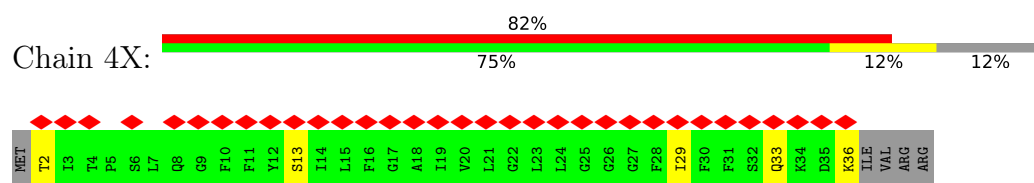
- Molecule 13: Photosystem II reaction center X protein



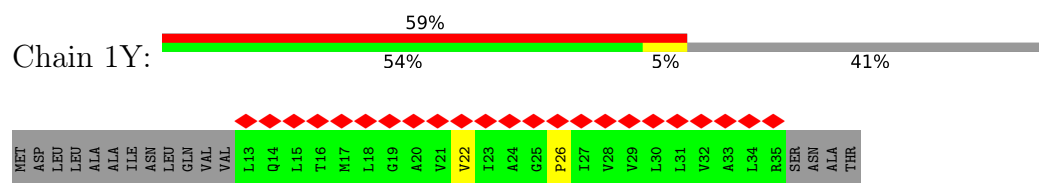
- Molecule 13: Photosystem II reaction center X protein



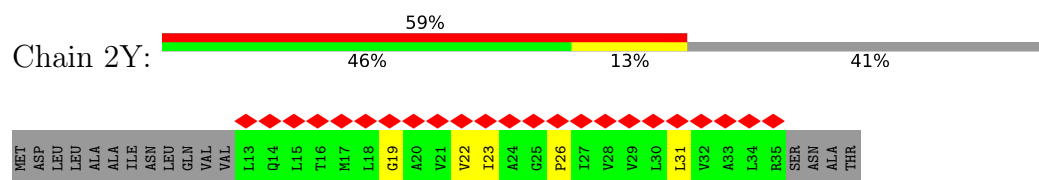
- Molecule 13: Photosystem II reaction center X protein



- Molecule 14: Photosystem II reaction center protein Ycf12



- Molecule 14: Photosystem II reaction center protein Ycf12



- Molecule 14: Photosystem II reaction center protein Ycf12

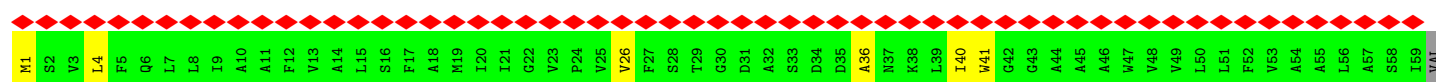
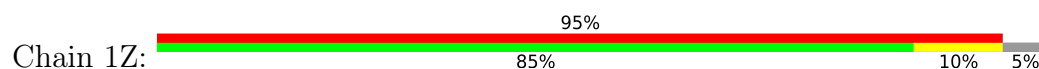




- Molecule 14: Photosystem II reaction center protein Ycf12

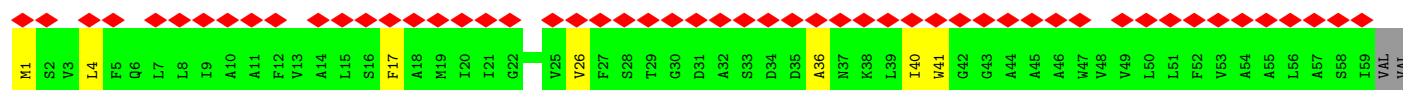
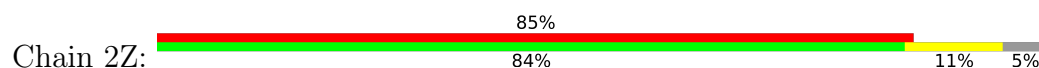


- Molecule 15: Photosystem II reaction center protein Z



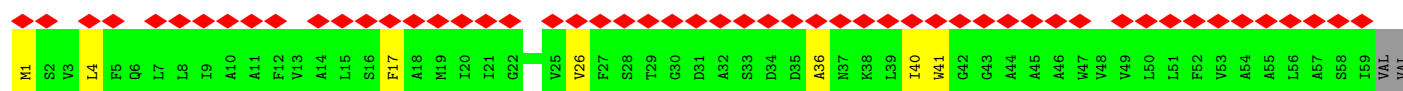
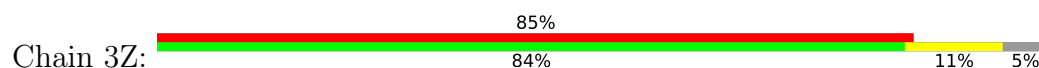
VAL
ILE

- Molecule 15: Photosystem II reaction center protein Z



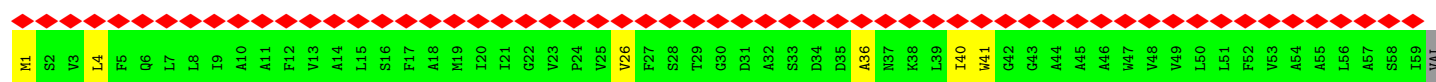
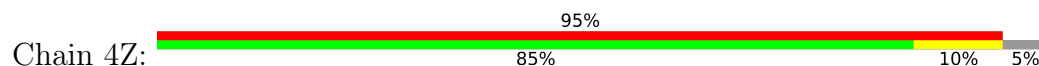
ILE

- Molecule 15: Photosystem II reaction center protein Z

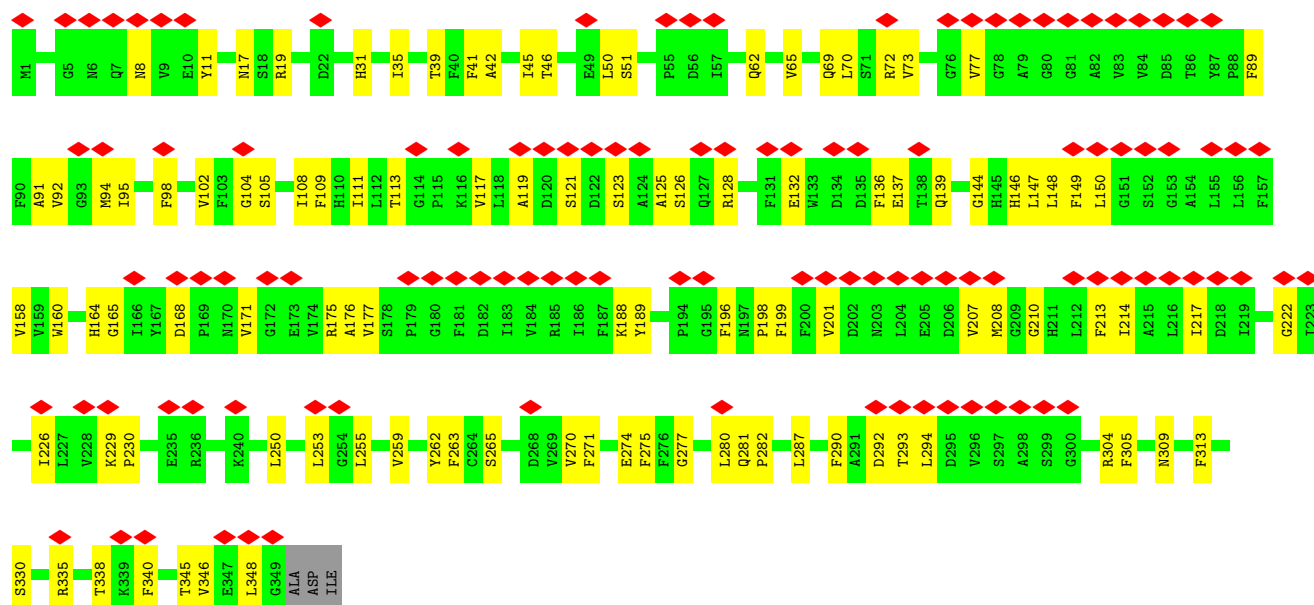


ILE

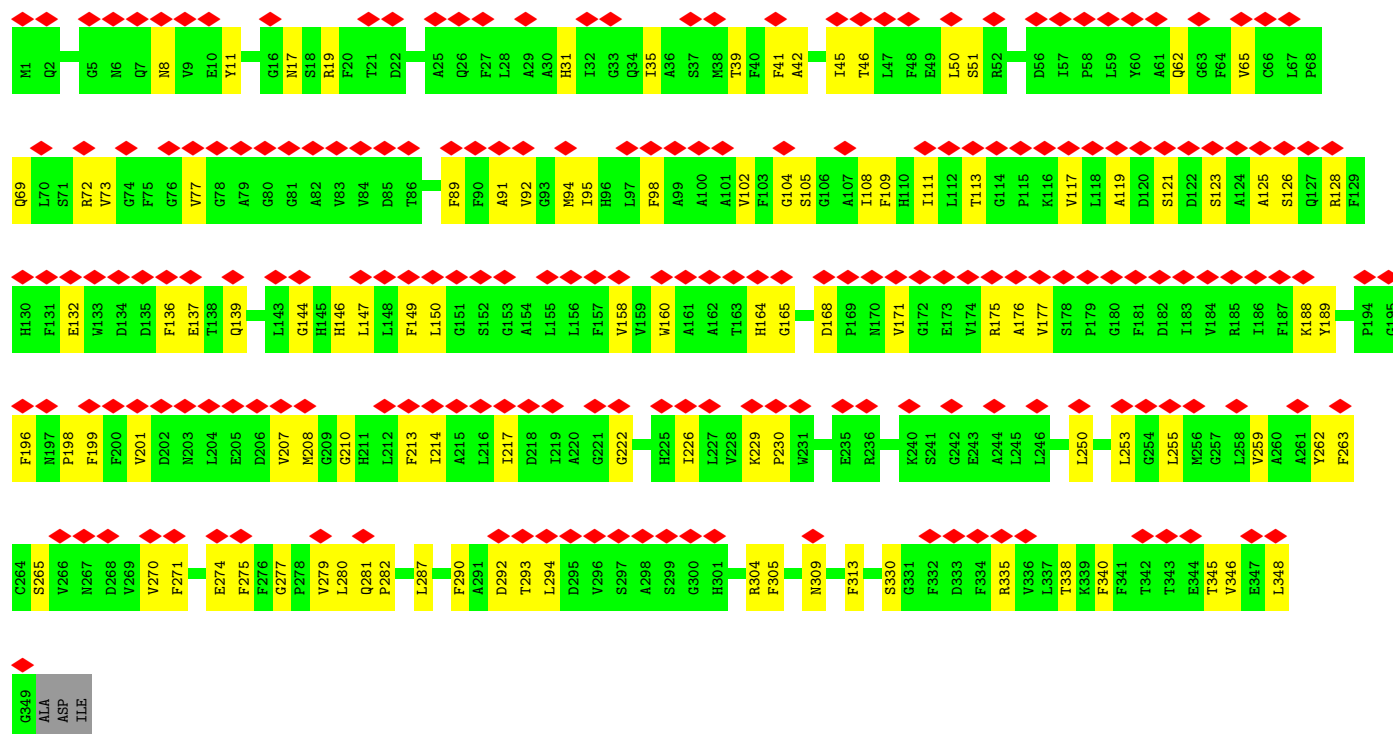
- Molecule 15: Photosystem II reaction center protein Z



VAL
ILE

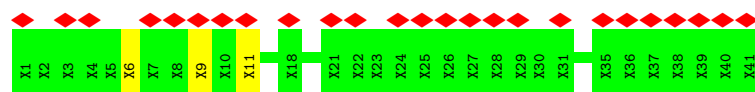


- Molecule 16: High light inducible protein

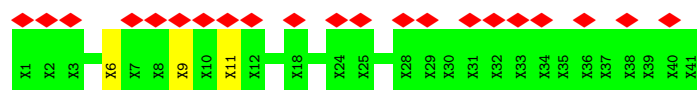


- Molecule 17: Unknown protein

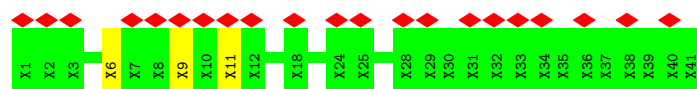




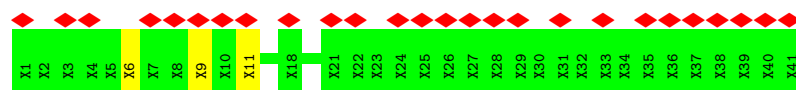
- Molecule 17: Unknown protein



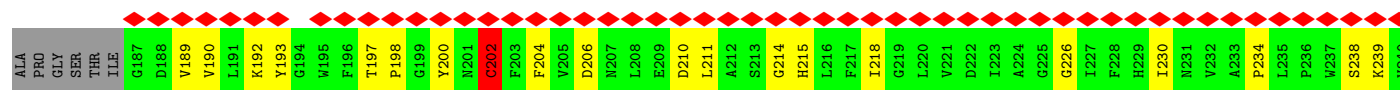
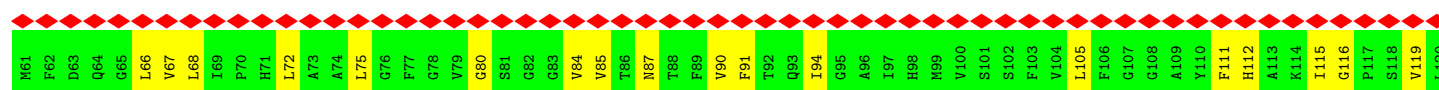
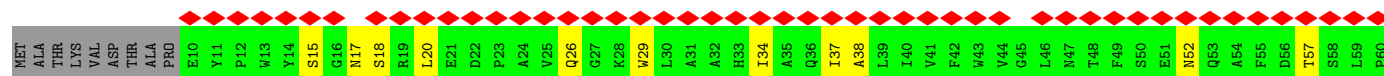
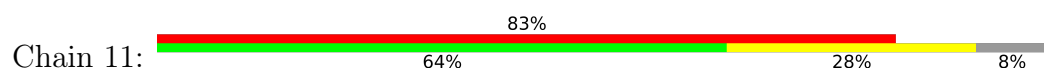
- Molecule 17: Unknown protein

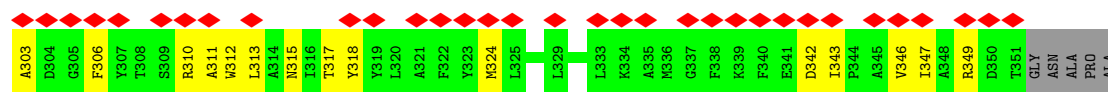


- Molecule 17: Unknown protein

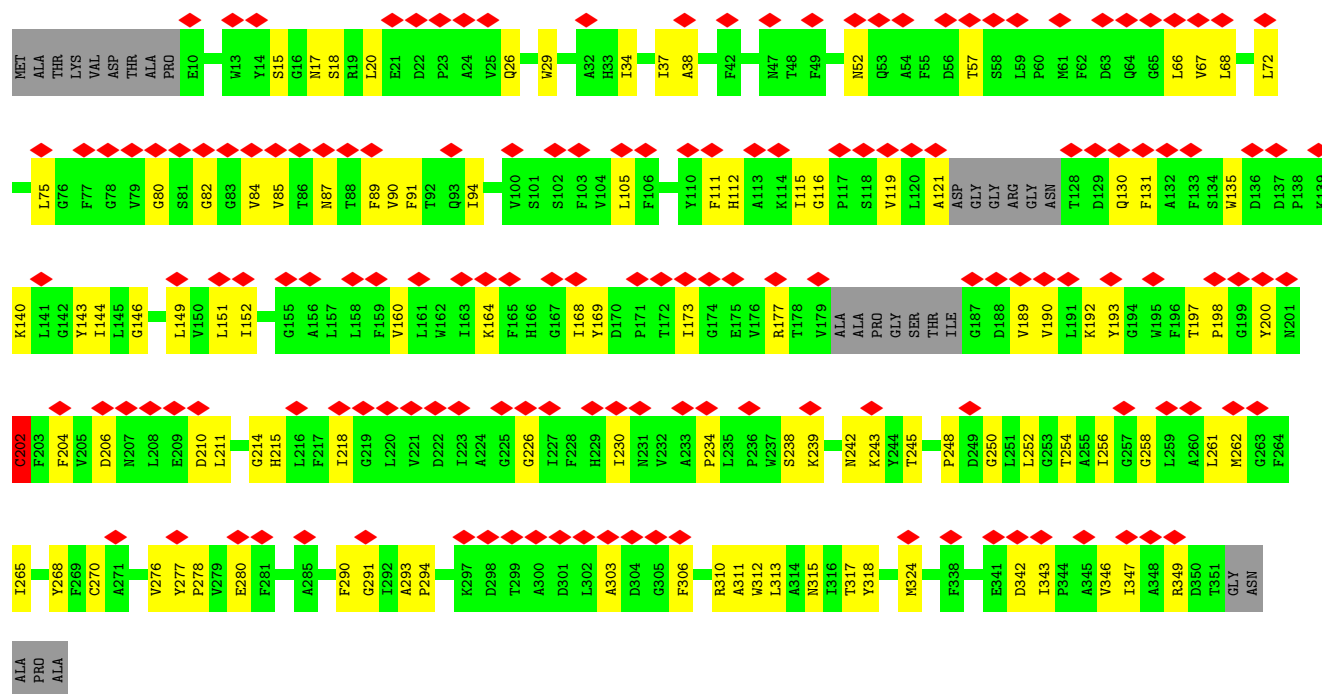
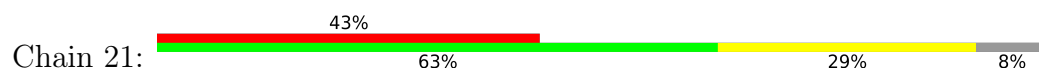


- Molecule 18: High light inducible protein

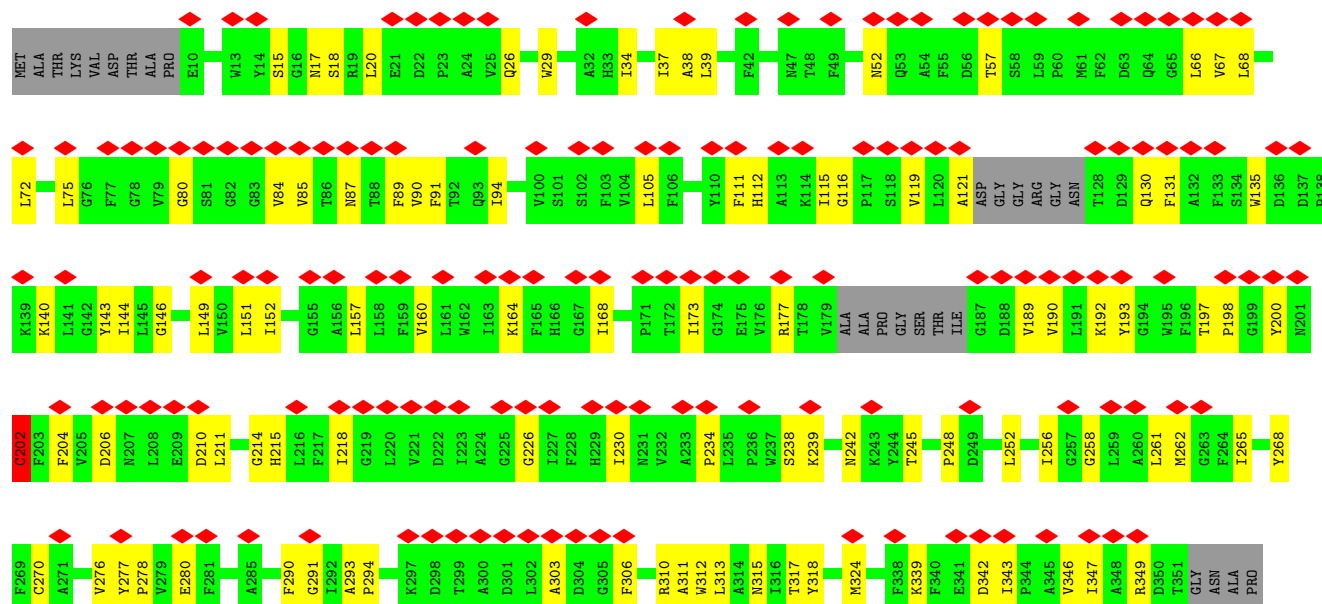
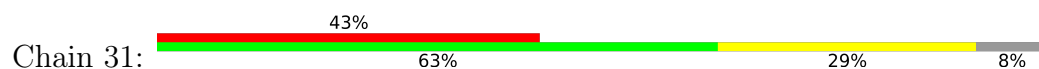




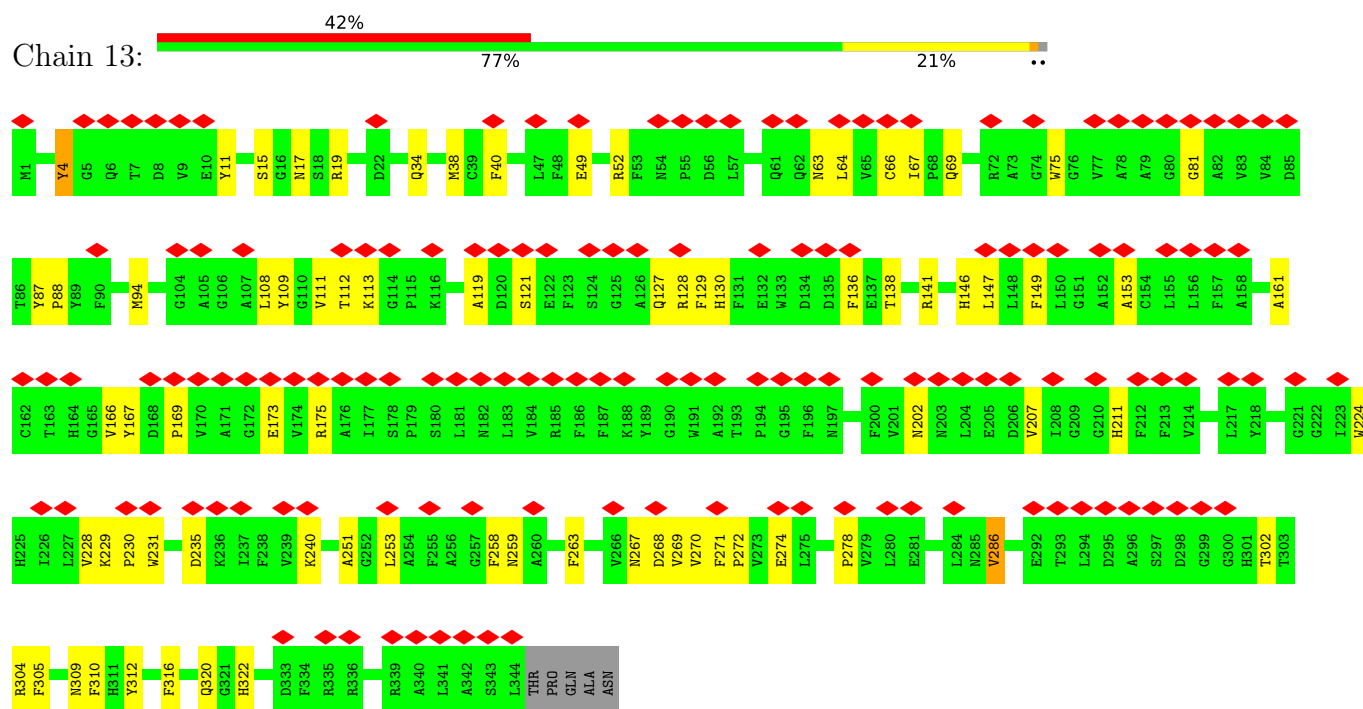
• Molecule 18: High light inducible protein



• Molecule 18: High light inducible protein

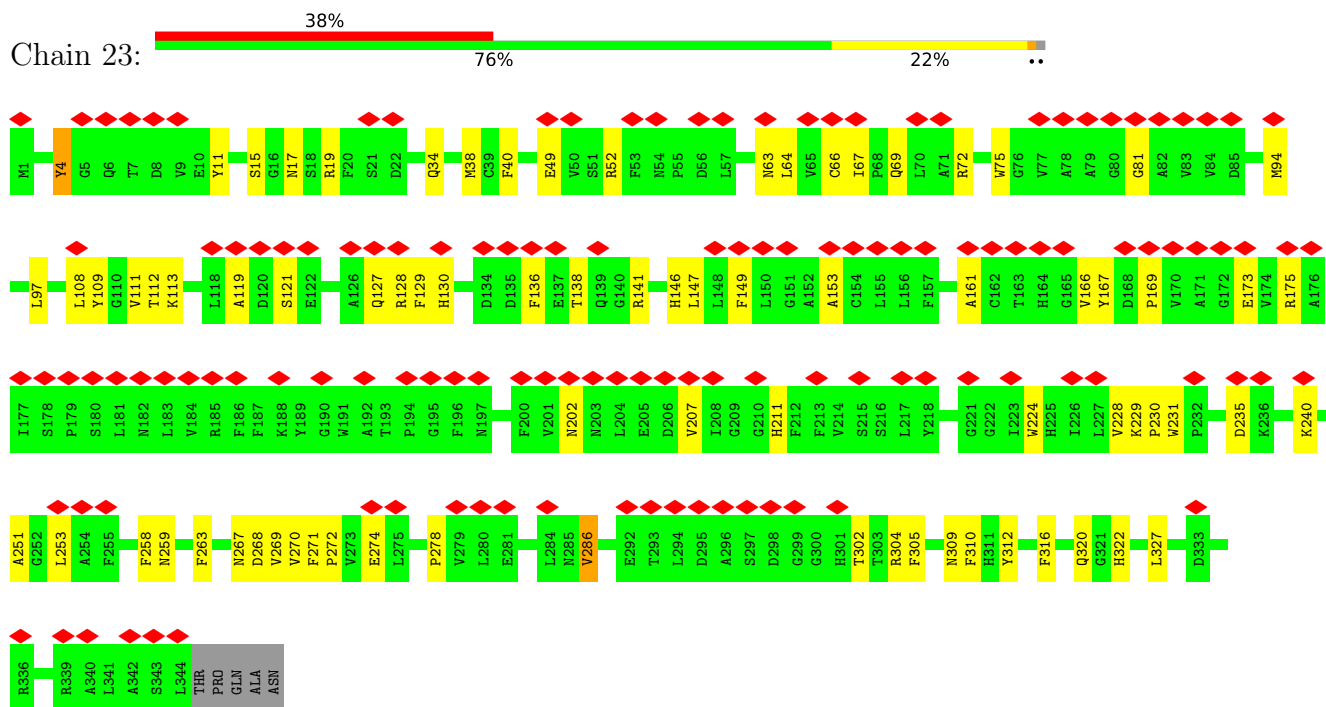


Chain 41:



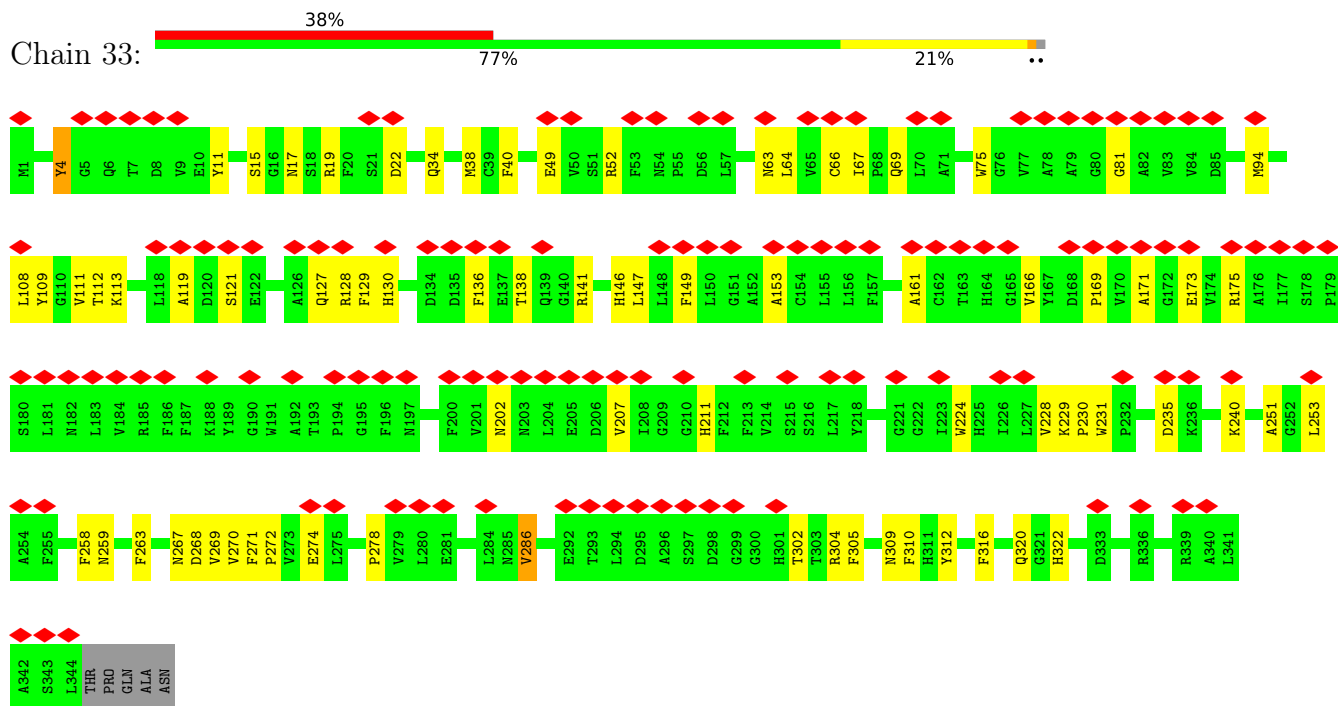
- Molecule 19: High light inducible protein

Chain 23:



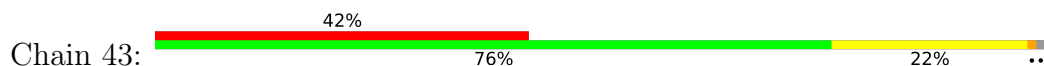
- Molecule 19: High light inducible protein

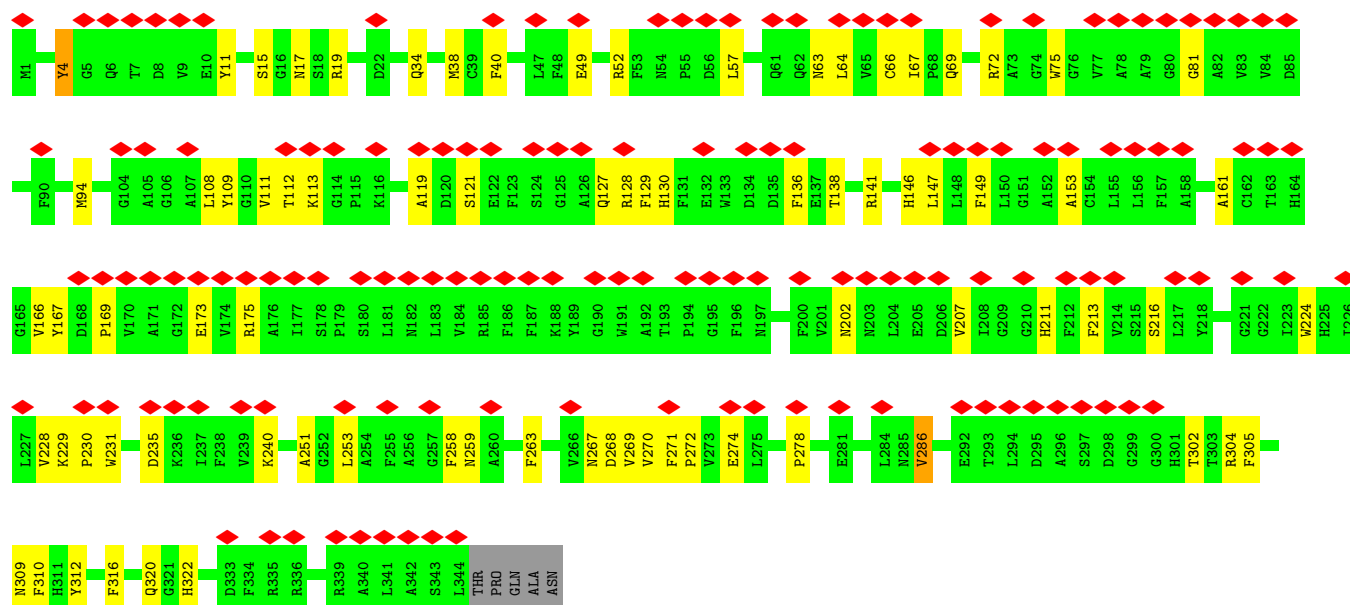
Chain 33:



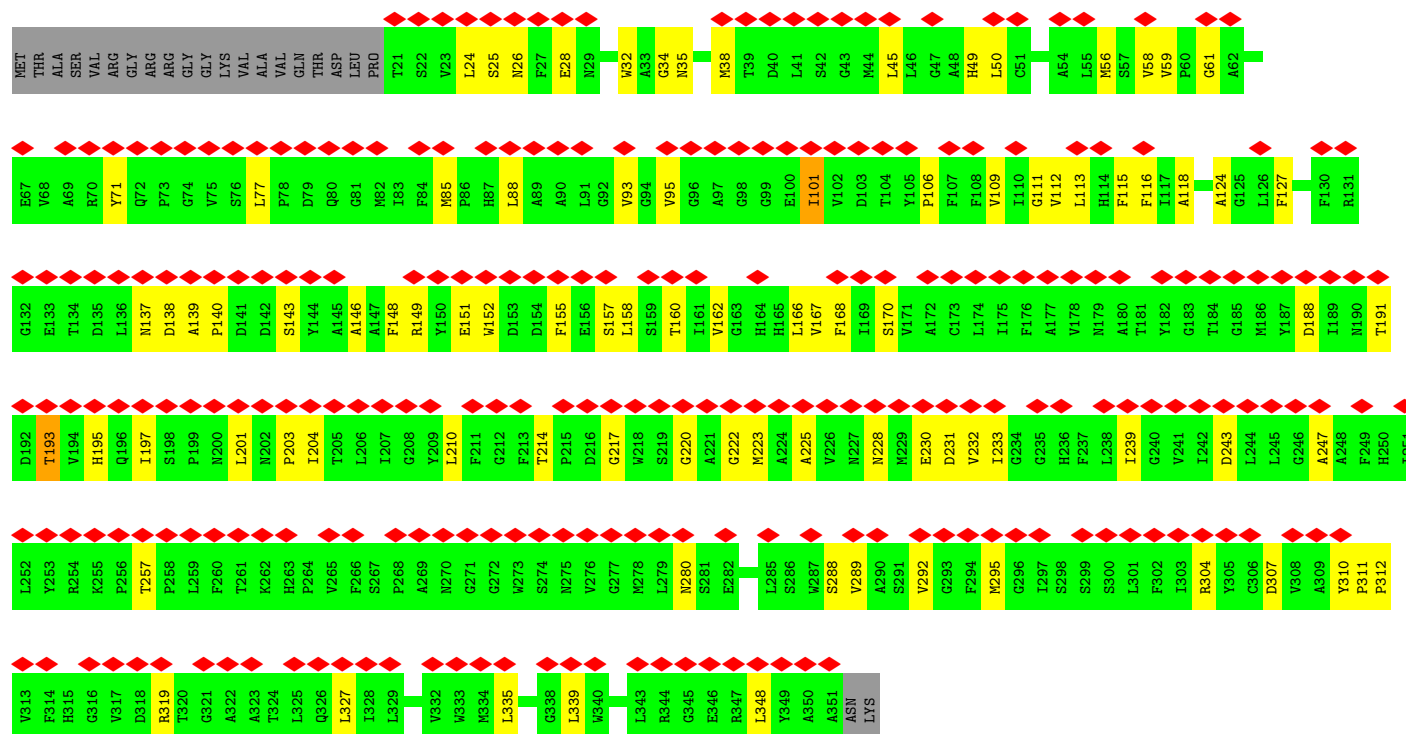
- Molecule 19: High light inducible protein

Chain 43:



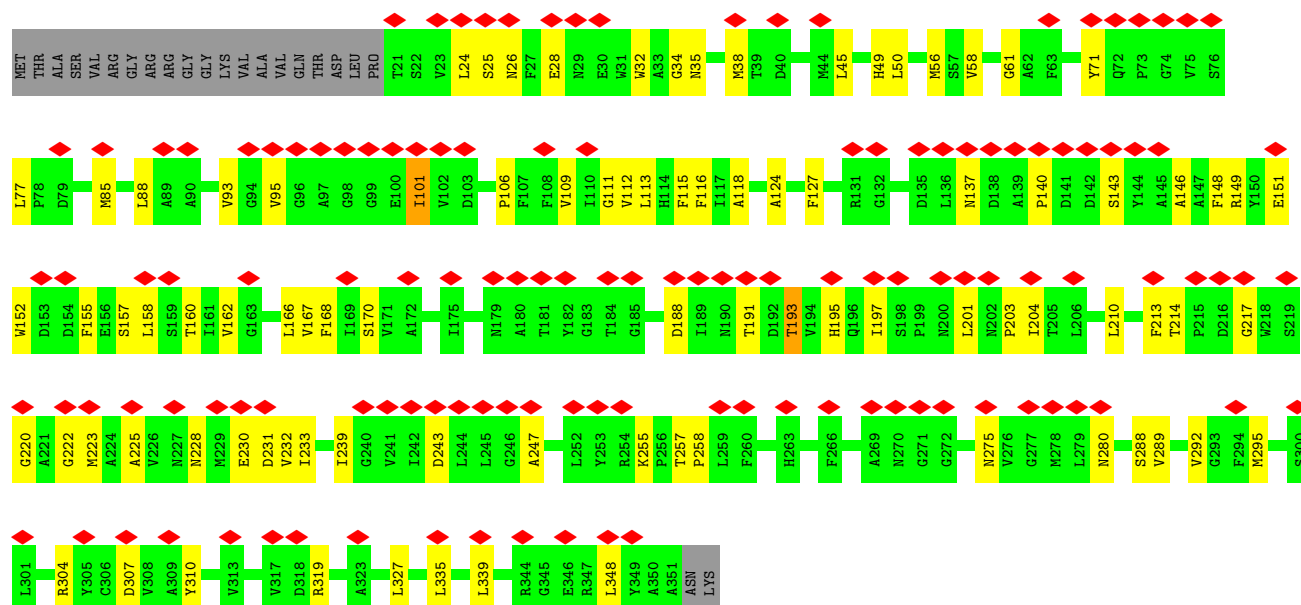


• Molecule 20: High light inducible protein

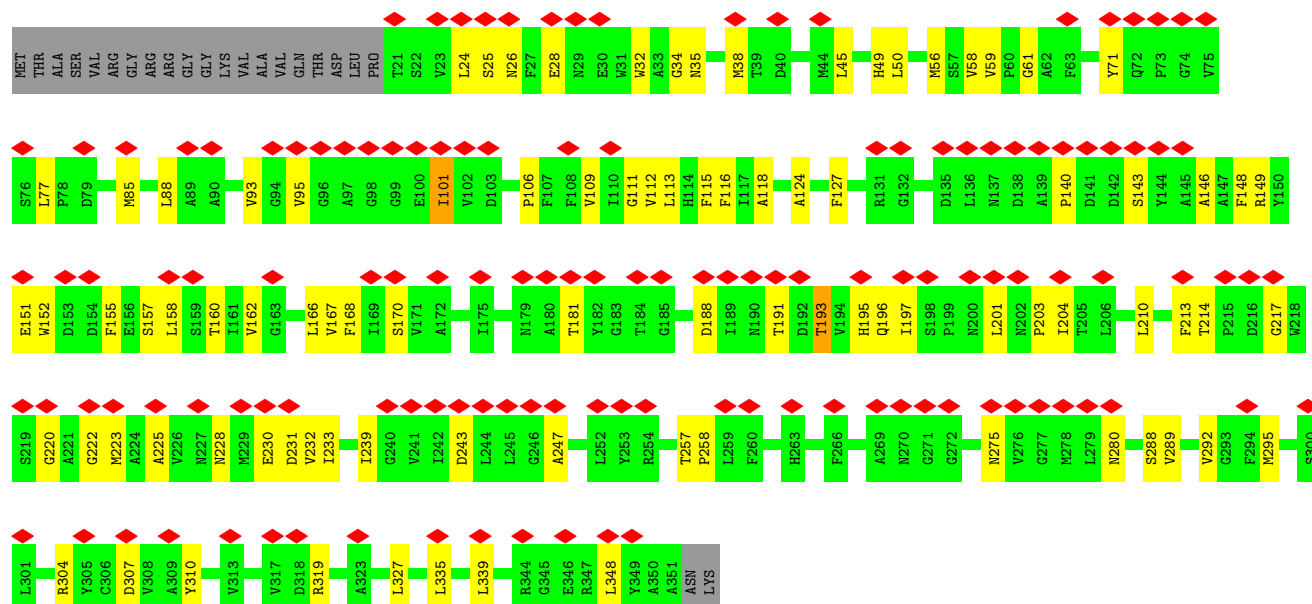


• Molecule 20: High light inducible protein

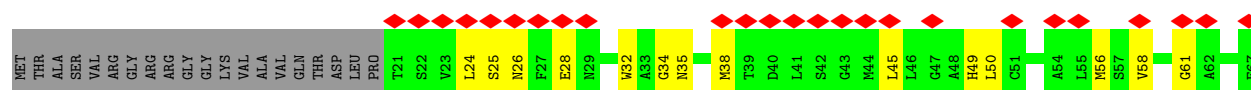




Chain 34: 37% 68% 25% 6%



Chain 44: 71% 69% 24% 6%





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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, FE2, LMG, PL9, 8CT, DGD, CL7, BCT, SQD, PHO, LHG, ZEX

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(°)	Ideal(°)
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

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 ⓘ

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 ⓘ

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	11	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.80	22 (39%)
21	CL7	23	415	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	42	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	20 (35%)
21	CL7	23	407	19	51,53,73	1.96	17 (33%)	56,89,113	2.75	19 (33%)
21	CL7	24	406	20	71,73,73	1.70	16 (22%)	80,113,113	2.35	21 (26%)
32	ZEX	24	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
21	CL7	3B	603	2	71,73,73	1.69	18 (25%)	80,113,113	2.35	21 (26%)
21	CL7	42	511	16	66,68,73	1.78	18 (27%)	74,107,113	2.40	21 (28%)
21	CL7	44	407	-	47,49,73	1.95	13 (27%)	51,84,113	2.82	20 (39%)
21	CL7	4A	407	-	71,73,73	1.67	17 (23%)	80,113,113	2.44	21 (26%)
21	CL7	3B	612	2	71,73,73	1.68	18 (25%)	80,113,113	2.39	23 (28%)
21	CL7	42	516	16	71,73,73	1.70	16 (22%)	80,113,113	2.39	23 (28%)
21	CL7	2C	512	3	47,49,73	1.92	13 (27%)	51,84,113	2.97	20 (39%)
26	LHG	2B	624	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	42	513	16	51,53,73	1.97	14 (27%)	56,89,113	2.84	21 (37%)
21	CL7	24	415	-	51,53,73	1.96	20 (39%)	56,89,113	2.87	21 (37%)
21	CL7	32	518	16	71,73,73	1.68	13 (18%)	80,113,113	2.33	22 (27%)
23	8CT	4B	620	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	11	412	18	51,53,73	1.96	16 (31%)	56,89,113	2.77	20 (35%)
24	LMG	4A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
22	PHO	3D	408	-	58,69,69	0.80	4 (6%)	56,99,99	1.27	5 (8%)
31	HEM	1F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.82	15 (22%)
21	CL7	42	518	16	71,73,73	1.68	13 (18%)	80,113,113	2.32	23 (28%)
21	CL7	32	509	-	71,73,73	1.68	18 (25%)	80,113,113	2.31	20 (25%)
24	LMG	2B	622	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	3B	601	-	47,49,73	1.94	13 (27%)	51,84,113	2.86	18 (35%)
21	CL7	4C	509	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	42	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.39	22 (27%)
21	CL7	31	405	-	51,53,73	1.97	18 (35%)	56,89,113	2.70	19 (33%)
21	CL7	42	503	-	71,73,73	1.69	18 (25%)	80,113,113	2.50	24 (30%)
21	CL7	23	418	19	56,58,73	1.89	16 (28%)	62,95,113	2.65	20 (32%)
25	SQD	23	424	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	32	517	16	71,73,73	1.68	15 (21%)	80,113,113	2.36	21 (26%)
32	ZEX	32	522	-	42,43,43	1.05	4 (9%)	55,60,60	2.47	17 (30%)
25	SQD	3B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
26	LHG	44	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	1B	616	2	51,53,73	1.97	18 (35%)	56,89,113	2.69	18 (32%)
30	PL9	3D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
29	BCT	2D	403	28	2,3,3	0.99	0	2,3,3	1.67	1 (50%)
21	CL7	43	418	19	56,58,73	1.88	16 (28%)	62,95,113	2.65	20 (32%)
21	CL7	12	512	16	71,73,73	1.69	14 (19%)	80,113,113	2.43	21 (26%)
32	ZEX	23	401	-	42,43,43	1.18	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	34	407	-	47,49,73	1.94	13 (27%)	51,84,113	2.81	20 (39%)
24	LMG	4B	622	-	51,51,55	0.24	0	59,59,63	0.33	0
26	LHG	24	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	32	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.36	22 (27%)
21	CL7	34	406	20	71,73,73	1.70	17 (23%)	80,113,113	2.35	21 (26%)
25	SQD	2A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
32	ZEX	23	421	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	33	515	-	47,49,73	1.94	12 (25%)	51,84,113	2.94	21 (41%)
21	CL7	1C	502	3	66,68,73	1.77	18 (27%)	74,107,113	2.45	19 (25%)
21	CL7	13	511	19	71,73,73	1.68	17 (23%)	80,113,113	2.55	24 (30%)
21	CL7	2B	606	2	71,73,73	1.67	18 (25%)	80,113,113	2.39	20 (25%)
23	8CT	2K	101	-	40,41,41	4.75	25 (62%)	50,56,56	2.65	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	ZEX	43	421	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	1D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
21	CL7	22	511	16	66,68,73	1.78	16 (24%)	74,107,113	2.40	21 (28%)
25	SQD	41	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
25	SQD	22	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	4B	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	19 (23%)
21	CL7	12	516	16	71,73,73	1.70	17 (23%)	80,113,113	2.39	24 (30%)
21	CL7	4C	512	3	47,49,73	1.92	14 (29%)	51,84,113	2.98	20 (39%)
32	ZEX	24	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	42	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.47	25 (31%)
21	CL7	24	412	20	71,73,73	1.69	17 (23%)	80,113,113	2.38	25 (31%)
21	CL7	31	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.71	18 (32%)
32	ZEX	12	522	-	42,43,43	1.04	4 (9%)	55,60,60	2.47	17 (30%)
21	CL7	41	418	18	71,73,73	1.67	15 (21%)	80,113,113	2.46	23 (28%)
23	8CT	2B	601	-	40,41,41	4.71	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	11	411	-	51,53,73	1.98	16 (31%)	56,89,113	2.71	18 (32%)
21	CL7	4C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.46	23 (28%)
21	CL7	13	503	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
21	CL7	43	405	-	71,73,73	1.69	17 (23%)	80,113,113	2.40	21 (26%)
21	CL7	3A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.60	23 (33%)
21	CL7	1D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)
21	CL7	23	402	19	71,73,73	1.69	17 (23%)	80,113,113	2.39	23 (28%)
21	CL7	1B	612	2	71,73,73	1.68	18 (25%)	80,113,113	2.37	23 (28%)
21	CL7	13	502	19	64,66,73	1.77	15 (23%)	71,104,113	2.40	22 (30%)
21	CL7	33	505	19	71,73,73	1.69	16 (22%)	80,113,113	2.39	21 (26%)
25	SQD	3A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
25	SQD	43	422	-	45,46,54	0.42	0	54,57,65	0.48	0
21	CL7	3C	503	3	71,73,73	1.68	16 (22%)	80,113,113	2.40	21 (26%)
21	CL7	31	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.46	24 (30%)
32	ZEX	41	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
32	ZEX	34	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	18 (32%)
21	CL7	43	402	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	23 (28%)
21	CL7	32	512	16	71,73,73	1.69	14 (19%)	80,113,113	2.42	21 (26%)
21	CL7	31	413	-	47,49,73	1.94	12 (25%)	51,84,113	2.97	22 (43%)
21	CL7	33	516	19	61,63,73	1.81	17 (27%)	68,101,113	2.55	25 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	13	504	-	71,73,73	1.69	17 (23%)	80,113,113	2.41	21 (26%)
21	CL7	2B	616	2	56,58,73	1.89	18 (32%)	62,95,113	2.69	21 (33%)
32	ZEX	24	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
32	ZEX	44	418	-	42,43,43	0.85	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	2C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.46	22 (27%)
26	LHG	4B	624	-	44,44,48	0.31	0	47,50,54	0.39	0
29	BCT	3D	403	28	2,3,3	1.00	0	2,3,3	1.66	1 (50%)
21	CL7	12	507	-	71,73,73	1.72	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	2B	607	2	61,63,73	1.81	16 (26%)	68,101,113	2.63	21 (30%)
21	CL7	4C	504	-	61,63,73	1.85	16 (26%)	68,101,113	2.54	19 (27%)
23	8CT	2D	406	-	40,41,41	4.63	23 (57%)	50,56,56	2.99	19 (38%)
32	ZEX	31	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.22	20 (36%)
21	CL7	2B	604	2	71,73,73	1.69	18 (25%)	80,113,113	2.37	21 (26%)
21	CL7	3C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.36	22 (27%)
21	CL7	43	404	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
21	CL7	43	419	19	51,53,73	1.98	14 (27%)	56,89,113	2.74	20 (35%)
21	CL7	24	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
21	CL7	3B	609	2	71,73,73	1.70	17 (23%)	80,113,113	2.33	20 (25%)
21	CL7	4B	615	2	66,68,73	1.78	18 (27%)	74,107,113	2.49	25 (33%)
23	8CT	4D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.98	19 (38%)
21	CL7	23	411	-	71,73,73	1.69	17 (23%)	80,113,113	2.37	24 (30%)
23	8CT	4A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	11	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.56	20 (29%)
25	SQD	23	422	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	2B	608	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	20 (27%)
21	CL7	2C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.35	21 (26%)
21	CL7	44	411	20	71,73,73	1.68	15 (21%)	80,113,113	2.41	23 (28%)
21	CL7	31	409	18	51,53,73	1.95	16 (31%)	56,89,113	2.72	20 (35%)
21	CL7	41	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.49	19 (25%)
21	CL7	4A	401	1	71,73,73	1.73	13 (18%)	80,113,113	2.47	25 (31%)
21	CL7	22	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.36	21 (26%)
29	BCT	1D	403	28	2,3,3	1.00	0	2,3,3	1.66	1 (50%)
21	CL7	22	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.32	20 (25%)
26	LHG	1D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	21	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.45	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	8CT	34	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
23	8CT	4B	619	-	40,41,41	4.69	21 (52%)	50,56,56	2.67	20 (40%)
21	CL7	22	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.37	22 (27%)
21	CL7	21	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.98	19 (37%)
24	LMG	31	401	-	51,51,55	0.22	0	59,59,63	0.42	1 (1%)
21	CL7	44	412	20	71,73,73	1.69	16 (22%)	80,113,113	2.37	24 (30%)
23	8CT	44	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	43	412	19	71,73,73	1.68	18 (25%)	80,113,113	2.54	24 (30%)
21	CL7	11	415	-	47,49,73	1.95	11 (23%)	51,84,113	2.97	20 (39%)
21	CL7	3A	407	-	71,73,73	1.68	17 (23%)	80,113,113	2.45	21 (26%)
21	CL7	3D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
21	CL7	33	508	19	71,73,73	1.71	18 (25%)	80,113,113	2.31	21 (26%)
21	CL7	41	409	18	51,53,73	1.96	16 (31%)	56,89,113	2.72	20 (35%)
21	CL7	42	512	16	71,73,73	1.69	14 (19%)	80,113,113	2.43	21 (26%)
32	ZEX	34	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
22	PHO	2A	402	-	58,69,69	0.83	3 (5%)	56,99,99	1.08	4 (7%)
21	CL7	23	405	-	71,73,73	1.69	17 (23%)	80,113,113	2.40	21 (26%)
21	CL7	1B	602	2	66,68,73	1.77	17 (25%)	74,107,113	2.51	21 (28%)
32	ZEX	12	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
23	8CT	1B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
32	ZEX	21	421	-	42,43,43	0.92	2 (4%)	55,60,60	2.23	20 (36%)
21	CL7	1C	512	3	47,49,73	1.93	13 (27%)	51,84,113	2.99	20 (39%)
21	CL7	13	509	19	71,73,73	1.68	16 (22%)	80,113,113	2.33	22 (27%)
23	8CT	2C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	31	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.40	21 (26%)
21	CL7	31	420	18	51,53,73	1.95	13 (25%)	56,89,113	2.80	21 (37%)
21	CL7	13	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	1B	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.32	20 (25%)
21	CL7	11	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.46	22 (27%)
21	CL7	12	518	16	71,73,73	1.69	13 (18%)	80,113,113	2.33	23 (28%)
21	CL7	2B	603	2	66,68,73	1.78	17 (25%)	74,107,113	2.51	22 (29%)
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%)
21	CL7	4B	604	2	71,73,73	1.69	18 (25%)	80,113,113	2.36	21 (26%)
21	CL7	1B	622	2	51,53,73	1.97	15 (29%)	56,89,113	2.78	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	22	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.72	19 (33%)
21	CL7	3A	401	1	71,73,73	1.74	14 (19%)	80,113,113	2.47	25 (31%)
32	ZEX	24	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	1B	613	2	61,63,73	1.83	19 (31%)	68,101,113	2.48	19 (27%)
21	CL7	23	406	19	71,73,73	1.69	17 (23%)	80,113,113	2.38	21 (26%)
23	8CT	4C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	33	507	-	71,73,73	1.68	15 (21%)	80,113,113	2.39	23 (28%)
21	CL7	2B	602	-	47,49,73	1.94	12 (25%)	51,84,113	2.87	18 (35%)
21	CL7	14	411	20	71,73,73	1.67	15 (21%)	80,113,113	2.41	23 (28%)
21	CL7	44	410	20	51,53,73	1.99	17 (33%)	56,89,113	2.71	19 (33%)
21	CL7	11	410	-	71,73,73	1.70	17 (23%)	80,113,113	2.33	23 (28%)
21	CL7	13	516	19	61,63,73	1.81	17 (27%)	68,101,113	2.56	25 (36%)
21	CL7	44	414	20	59,61,73	1.84	18 (30%)	65,98,113	2.66	21 (32%)
23	8CT	1B	618	-	40,41,41	4.69	20 (50%)	50,56,56	2.67	20 (40%)
21	CL7	31	412	18	51,53,73	1.96	16 (31%)	56,89,113	2.76	20 (35%)
21	CL7	24	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.86	18 (35%)
21	CL7	33	511	19	71,73,73	1.69	18 (25%)	80,113,113	2.55	24 (30%)
21	CL7	3B	607	-	66,68,73	1.76	17 (25%)	74,107,113	2.47	21 (28%)
32	ZEX	11	421	-	42,43,43	0.93	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	34	412	20	71,73,73	1.69	16 (22%)	80,113,113	2.36	23 (28%)
21	CL7	13	513	-	51,53,73	1.98	17 (33%)	56,89,113	2.72	18 (32%)
21	CL7	3B	604	2	71,73,73	1.68	18 (25%)	80,113,113	2.32	23 (28%)
21	CL7	33	502	19	64,66,73	1.77	15 (23%)	71,104,113	2.40	22 (30%)
21	CL7	21	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.49	19 (25%)
25	SQD	2B	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.53	1 (1%)
21	CL7	31	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.50	20 (27%)
21	CL7	21	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.80	22 (39%)
24	LMG	3A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	23	417	19	61,63,73	1.81	17 (27%)	68,101,113	2.56	25 (36%)
21	CL7	1C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.35	22 (27%)
21	CL7	3C	506	3	66,68,73	1.77	17 (25%)	74,107,113	2.51	23 (31%)
21	CL7	1B	608	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	20 (25%)
31	HEM	4F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.82	15 (22%)
32	ZEX	22	524	-	42,43,43	1.03	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	21	409	18	51,53,73	1.95	16 (31%)	56,89,113	2.72	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	1B	605	2	71,73,73	1.67	17 (23%)	80,113,113	2.40	20 (25%)
25	SQD	1B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.53	1 (1%)
21	CL7	22	512	16	71,73,73	1.68	14 (19%)	80,113,113	2.43	21 (26%)
21	CL7	24	417	20	48,50,73	1.94	13 (27%)	51,85,113	2.94	18 (35%)
21	CL7	44	406	20	71,73,73	1.70	15 (21%)	80,113,113	2.36	22 (27%)
21	CL7	3C	504	-	61,63,73	1.85	17 (27%)	68,101,113	2.54	19 (27%)
32	ZEX	13	520	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
32	ZEX	42	522	-	42,43,43	1.04	5 (11%)	55,60,60	2.47	15 (27%)
21	CL7	2B	610	2	71,73,73	1.69	17 (23%)	80,113,113	2.33	20 (25%)
21	CL7	3B	606	2	61,63,73	1.81	16 (26%)	68,101,113	2.63	21 (30%)
21	CL7	3B	615	2	56,58,73	1.89	18 (32%)	62,95,113	2.70	21 (33%)
22	PHO	4D	408	-	58,69,69	0.80	3 (5%)	56,99,99	1.27	5 (8%)
21	CL7	2C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
21	CL7	24	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.71	20 (35%)
23	8CT	3C	515	-	40,41,41	4.64	20 (50%)	50,56,56	3.06	22 (44%)
21	CL7	3C	509	3	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
21	CL7	23	408	-	71,73,73	1.68	15 (21%)	80,113,113	2.39	23 (28%)
21	CL7	43	417	19	61,63,73	1.81	18 (29%)	68,101,113	2.56	25 (36%)
21	CL7	14	405	-	71,73,73	1.70	16 (22%)	80,113,113	2.45	25 (31%)
26	LHG	2B	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	43	415	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	1A	407	-	71,73,73	1.68	17 (23%)	80,113,113	2.44	21 (26%)
32	ZEX	12	520	-	42,43,43	0.97	3 (7%)	55,60,60	2.19	17 (30%)
21	CL7	44	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.70	20 (35%)
21	CL7	3C	510	3	71,73,73	1.69	16 (22%)	80,113,113	2.38	21 (26%)
21	CL7	11	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.50	23 (28%)
23	8CT	4C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
23	8CT	1C	518	-	40,41,41	4.65	21 (52%)	50,56,56	2.71	20 (40%)
32	ZEX	12	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	11	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.77	18 (32%)
21	CL7	3C	517	3	47,49,73	1.93	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	44	409	-	66,68,73	1.76	18 (27%)	74,107,113	2.67	24 (32%)
21	CL7	1D	405	4	51,53,73	1.96	18 (35%)	56,89,113	2.77	22 (39%)
21	CL7	13	512	19	61,63,73	1.84	19 (31%)	68,101,113	2.58	23 (33%)
21	CL7	2C	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
25	SQD	2I	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
26	LHG	4B	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	34	405	-	71,73,73	1.70	16 (22%)	80,113,113	2.45	25 (31%)
23	8CT	3B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.91	18 (36%)
24	LMG	1A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
30	PL9	4D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
26	LHG	4A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
22	PHO	3A	402	-	58,69,69	0.84	3 (5%)	56,99,99	1.07	4 (7%)
23	8CT	1C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	24	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.67	25 (33%)
25	SQD	42	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	12	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.35	22 (27%)
23	8CT	4C	514	-	40,41,41	4.64	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	1B	607	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	20 (27%)
23	8CT	1A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
23	8CT	1B	626	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
32	ZEX	14	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
32	ZEX	21	422	-	42,43,43	0.95	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	42	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.72	19 (33%)
21	CL7	3D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)
26	LHG	3B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	23	409	19	71,73,73	1.70	18 (25%)	80,113,113	2.31	21 (26%)
26	LHG	34	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	14	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.68	25 (33%)
21	CL7	43	411	-	71,73,73	1.69	16 (22%)	80,113,113	2.37	24 (30%)
21	CL7	31	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.56	20 (29%)
21	CL7	1A	401	1	71,73,73	1.74	13 (18%)	80,113,113	2.46	25 (31%)
32	ZEX	42	520	-	42,43,43	0.98	3 (7%)	55,60,60	2.18	17 (30%)
32	ZEX	44	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
21	CL7	32	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.64	19 (33%)
21	CL7	43	403	19	64,66,73	1.78	17 (26%)	71,104,113	2.41	22 (30%)
32	ZEX	44	420	-	42,43,43	1.01	3 (7%)	55,60,60	2.20	18 (32%)
21	CL7	43	414	-	51,53,73	1.98	18 (35%)	56,89,113	2.74	18 (32%)
24	LMG	4D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
21	CL7	3C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.47	23 (28%)
21	CL7	4C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.37	26 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	41	407	18	47,49,73	1.94	14 (29%)	51,84,113	2.86	21 (41%)
32	ZEX	13	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
23	8CT	4K	101	-	40,41,41	4.76	25 (62%)	50,56,56	2.66	16 (32%)
21	CL7	32	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.38	22 (27%)
23	8CT	2C	514	-	40,41,41	4.65	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	44	415	-	51,53,73	1.96	20 (39%)	56,89,113	2.88	21 (37%)
21	CL7	12	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.31	20 (25%)
21	CL7	41	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.81	22 (39%)
21	CL7	24	408	20	51,53,73	1.97	16 (31%)	56,89,113	2.69	21 (37%)
23	8CT	2A	404	-	40,41,41	4.63	20 (50%)	50,56,56	2.97	20 (40%)
24	LMG	1D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
32	ZEX	33	525	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
32	ZEX	22	522	-	42,43,43	1.04	3 (7%)	55,60,60	2.47	17 (30%)
21	CL7	1C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
25	SQD	4B	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
21	CL7	43	416	-	47,49,73	1.93	12 (25%)	51,84,113	2.93	21 (41%)
25	SQD	32	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
25	SQD	33	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
27	DGD	2B	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	4C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
32	ZEX	44	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	1C	506	3	66,68,73	1.77	17 (25%)	74,107,113	2.51	23 (31%)
21	CL7	23	404	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
24	LMG	1B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	41	403	-	66,68,73	1.75	16 (24%)	74,107,113	2.51	22 (29%)
21	CL7	23	416	-	47,49,73	1.93	12 (25%)	51,84,113	2.93	21 (41%)
21	CL7	4B	613	2	71,73,73	1.68	18 (25%)	80,113,113	2.38	23 (28%)
32	ZEX	11	422	-	42,43,43	0.96	2 (4%)	55,60,60	2.23	18 (32%)
26	LHG	23	425	-	35,35,48	0.35	0	38,41,54	0.47	0
23	8CT	2B	619	-	40,41,41	4.70	20 (50%)	50,56,56	2.67	20 (40%)
21	CL7	44	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.85	18 (35%)
27	DGD	3C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	4B	617	2	51,53,73	1.97	18 (35%)	56,89,113	2.69	18 (32%)
27	DGD	2C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	41	408	-	71,73,73	1.66	15 (21%)	80,113,113	2.51	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	1B	614	2	66,68,73	1.78	18 (27%)	74,107,113	2.49	25 (33%)
21	CL7	11	407	18	47,49,73	1.95	15 (31%)	51,84,113	2.86	20 (39%)
21	CL7	21	415	-	47,49,73	1.94	11 (23%)	51,84,113	2.96	19 (37%)
21	CL7	31	415	-	47,49,73	1.94	11 (23%)	51,84,113	2.97	19 (37%)
21	CL7	3B	613	2	61,63,73	1.83	19 (31%)	68,101,113	2.48	19 (27%)
21	CL7	32	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.47	25 (31%)
32	ZEX	33	520	-	42,43,43	0.92	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	2B	623	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
21	CL7	43	406	19	71,73,73	1.70	17 (23%)	80,113,113	2.39	21 (26%)
21	CL7	4B	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.32	22 (27%)
21	CL7	34	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.43	21 (28%)
21	CL7	3D	405	4	51,53,73	1.95	18 (35%)	56,89,113	2.77	22 (39%)
21	CL7	14	416	20	47,49,73	1.96	14 (29%)	51,84,113	2.85	18 (35%)
21	CL7	43	409	19	71,73,73	1.70	18 (25%)	80,113,113	2.31	22 (27%)
32	ZEX	14	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.43	25 (45%)
32	ZEX	43	401	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	14	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.44	21 (28%)
26	LHG	13	524	-	35,35,48	0.34	0	38,41,54	0.47	0
21	CL7	1B	611	2	71,73,73	1.69	17 (23%)	80,113,113	2.34	20 (25%)
21	CL7	1C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
21	CL7	21	407	18	47,49,73	1.94	14 (29%)	51,84,113	2.87	20 (39%)
21	CL7	33	512	19	61,63,73	1.83	19 (31%)	68,101,113	2.59	23 (33%)
23	8CT	1D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	24	407	-	47,49,73	1.94	13 (27%)	51,84,113	2.81	20 (39%)
23	8CT	3A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	2A	401	1	71,73,73	1.73	13 (18%)	80,113,113	2.46	25 (31%)
21	CL7	12	501	16	71,73,73	1.68	16 (22%)	80,113,113	2.41	21 (26%)
21	CL7	14	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.70	21 (37%)
23	8CT	2B	620	-	40,41,41	4.58	21 (52%)	50,56,56	2.91	18 (36%)
21	CL7	3B	616	2	51,53,73	1.97	19 (37%)	56,89,113	2.70	18 (32%)
21	CL7	41	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.57	20 (29%)
25	SQD	12	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	22	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	21 (37%)
21	CL7	23	414	-	51,53,73	1.98	17 (33%)	56,89,113	2.73	18 (32%)
21	CL7	31	410	-	71,73,73	1.71	17 (23%)	80,113,113	2.34	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	HEM	2F	101	-	50,50,50	1.61	9 (18%)	66,82,82	1.81	15 (22%)
23	8CT	3D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	32	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.38	22 (27%)
32	ZEX	13	519	-	42,43,43	1.02	3 (7%)	55,60,60	2.58	17 (30%)
21	CL7	22	516	16	71,73,73	1.70	17 (23%)	80,113,113	2.39	23 (28%)
21	CL7	11	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.98	20 (39%)
21	CL7	31	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	4B	607	2	61,63,73	1.81	16 (26%)	68,101,113	2.64	22 (32%)
21	CL7	13	518	19	51,53,73	1.97	14 (27%)	56,89,113	2.75	20 (35%)
21	CL7	21	403	-	66,68,73	1.75	17 (25%)	74,107,113	2.51	22 (29%)
24	LMG	3D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
21	CL7	1B	615	2	56,58,73	1.89	17 (30%)	62,95,113	2.68	21 (33%)
26	LHG	43	425	-	35,35,48	0.34	0	38,41,54	0.47	0
21	CL7	43	408	-	71,73,73	1.68	15 (21%)	80,113,113	2.40	22 (27%)
21	CL7	13	506	19	51,53,73	1.97	18 (35%)	56,89,113	2.75	19 (33%)
21	CL7	3C	513	3	51,53,73	1.94	14 (27%)	56,89,113	2.90	19 (33%)
21	CL7	14	406	20	71,73,73	1.70	16 (22%)	80,113,113	2.35	21 (26%)
21	CL7	22	518	16	71,73,73	1.68	14 (19%)	80,113,113	2.33	23 (28%)
21	CL7	33	501	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	23 (28%)
32	ZEX	33	519	-	42,43,43	1.01	3 (7%)	55,60,60	2.58	17 (30%)
21	CL7	21	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.50	23 (28%)
21	CL7	4D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.61	20 (32%)
24	LMG	41	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
31	HEM	3F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.81	15 (22%)
21	CL7	3B	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.40	21 (26%)
21	CL7	22	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.37	22 (27%)
21	CL7	4B	606	2	71,73,73	1.68	18 (25%)	80,113,113	2.39	20 (25%)
32	ZEX	42	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	2B	613	2	71,73,73	1.68	18 (25%)	80,113,113	2.38	23 (28%)
21	CL7	2C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
21	CL7	44	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.33	21 (26%)
27	DGD	1C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	32	507	-	71,73,73	1.71	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	22	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.48	25 (31%)
21	CL7	21	405	-	51,53,73	1.97	18 (35%)	56,89,113	2.71	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	8CT	1C	514	-	40,41,41	4.63	21 (52%)	50,56,56	2.40	23 (46%)
26	LHG	3A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
32	ZEX	23	423	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	18 (32%)
21	CL7	2C	506	3	66,68,73	1.76	17 (25%)	74,107,113	2.50	23 (31%)
21	CL7	2D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)
21	CL7	14	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
21	CL7	1B	603	2	71,73,73	1.69	18 (25%)	80,113,113	2.36	21 (26%)
21	CL7	41	415	-	47,49,73	1.95	11 (23%)	51,84,113	2.97	19 (37%)
21	CL7	32	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.73	19 (33%)
21	CL7	1C	509	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	41	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.71	18 (32%)
27	DGD	1B	624	-	63,63,67	0.83	2 (3%)	77,77,81	1.00	3 (3%)
32	ZEX	42	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	42	501	16	71,73,73	1.67	16 (22%)	80,113,113	2.42	21 (26%)
21	CL7	24	414	20	59,61,73	1.85	18 (30%)	65,98,113	2.67	21 (32%)
23	8CT	2C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	31	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.51	23 (28%)
21	CL7	1C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.47	23 (28%)
21	CL7	34	414	20	59,61,73	1.84	18 (30%)	65,98,113	2.65	21 (32%)
21	CL7	13	508	19	71,73,73	1.70	18 (25%)	80,113,113	2.32	21 (26%)
21	CL7	2D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
25	SQD	11	423	-	31,32,54	0.49	1 (3%)	40,43,65	0.60	1 (2%)
26	LHG	1B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	22	507	-	71,73,73	1.71	17 (23%)	80,113,113	2.43	21 (26%)
26	LHG	2A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	4B	602	-	47,49,73	1.94	13 (27%)	51,84,113	2.87	18 (35%)
23	8CT	4B	601	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	13	505	19	71,73,73	1.69	17 (23%)	80,113,113	2.39	21 (26%)
21	CL7	41	412	18	51,53,73	1.95	16 (31%)	56,89,113	2.77	20 (35%)
25	SQD	32	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	1B	604	2	71,73,73	1.67	18 (25%)	80,113,113	2.32	23 (28%)
23	8CT	3B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.76	19 (38%)
21	CL7	32	504	-	51,53,73	1.99	17 (33%)	56,89,113	2.77	19 (33%)
21	CL7	14	414	20	59,61,73	1.84	17 (28%)	65,98,113	2.66	21 (32%)
21	CL7	22	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.63	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	8CT	3B	626	-	40,41,41	4.70	24 (60%)	50,56,56	3.24	21 (42%)
25	SQD	33	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
25	SQD	43	424	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	1C	504	-	61,63,73	1.85	17 (27%)	68,101,113	2.55	19 (27%)
21	CL7	12	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.64	19 (33%)
21	CL7	14	407	-	47,49,73	1.95	13 (27%)	51,84,113	2.81	20 (39%)
21	CL7	12	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.73	19 (33%)
25	SQD	13	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
26	LHG	4D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	12	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.38	22 (27%)
21	CL7	3B	622	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
21	CL7	34	417	20	48,50,73	1.93	13 (27%)	51,85,113	2.95	18 (35%)
21	CL7	14	412	20	71,73,73	1.69	15 (21%)	80,113,113	2.38	25 (31%)
21	CL7	1A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.62	23 (33%)
32	ZEX	23	420	-	42,43,43	1.02	4 (9%)	55,60,60	2.58	17 (30%)
32	ZEX	14	420	-	42,43,43	1.01	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	44	417	20	48,50,73	1.93	14 (29%)	51,85,113	2.94	18 (35%)
21	CL7	4C	510	3	71,73,73	1.69	14 (19%)	80,113,113	2.38	20 (25%)
24	LMG	21	401	-	51,51,55	0.22	0	59,59,63	0.42	1 (1%)
21	CL7	34	411	20	71,73,73	1.68	16 (22%)	80,113,113	2.41	23 (28%)
21	CL7	34	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.70	19 (33%)
32	ZEX	32	519	-	42,43,43	1.06	3 (7%)	55,60,60	2.50	16 (29%)
23	8CT	3C	514	-	40,41,41	4.65	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	22	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.77	19 (33%)
30	PL9	2D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	2C	504	-	61,63,73	1.85	17 (27%)	68,101,113	2.54	19 (27%)
21	CL7	2B	614	2	61,63,73	1.84	19 (31%)	68,101,113	2.48	18 (26%)
21	CL7	43	407	19	51,53,73	1.97	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	31	416	-	47,49,73	1.96	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	31	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.97	20 (39%)
21	CL7	2B	615	2	66,68,73	1.79	18 (27%)	74,107,113	2.49	25 (33%)
21	CL7	4A	403	1	61,63,73	1.87	19 (31%)	68,101,113	2.61	23 (33%)
32	ZEX	43	423	-	42,43,43	1.01	4 (9%)	55,60,60	2.39	17 (30%)
21	CL7	41	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.77	18 (32%)
21	CL7	33	518	19	51,53,73	1.98	13 (25%)	56,89,113	2.74	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	2C	517	3	47,49,73	1.92	13 (27%)	51,84,113	2.88	19 (37%)
21	CL7	4B	610	2	71,73,73	1.69	17 (23%)	80,113,113	2.32	20 (25%)
26	LHG	33	524	-	35,35,48	0.34	0	38,41,54	0.47	0
21	CL7	4C	506	3	66,68,73	1.77	17 (25%)	74,107,113	2.50	23 (31%)
21	CL7	41	405	-	51,53,73	1.97	17 (33%)	56,89,113	2.71	19 (33%)
32	ZEX	34	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
32	ZEX	33	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	4B	614	2	61,63,73	1.83	19 (31%)	68,101,113	2.47	18 (26%)
21	CL7	4B	603	2	66,68,73	1.78	17 (25%)	74,107,113	2.51	22 (29%)
21	CL7	2C	510	3	71,73,73	1.69	15 (21%)	80,113,113	2.38	21 (26%)
21	CL7	3C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
26	LHG	1A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	2B	617	2	51,53,73	1.97	18 (35%)	56,89,113	2.70	18 (32%)
21	CL7	11	405	-	51,53,73	1.97	17 (33%)	56,89,113	2.72	19 (33%)
21	CL7	32	516	16	71,73,73	1.70	17 (23%)	80,113,113	2.39	23 (28%)
21	CL7	4C	517	3	47,49,73	1.93	13 (27%)	51,84,113	2.88	19 (37%)
32	ZEX	14	403	-	42,43,43	1.02	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	1B	601	-	47,49,73	1.94	13 (27%)	51,84,113	2.86	18 (35%)
22	PHO	1A	402	-	58,69,69	0.83	3 (5%)	56,99,99	1.07	4 (7%)
21	CL7	14	415	-	51,53,73	1.97	20 (39%)	56,89,113	2.89	22 (39%)
25	SQD	12	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	22	502	16	71,73,73	1.69	17 (23%)	80,113,113	2.35	23 (28%)
21	CL7	32	501	16	71,73,73	1.68	16 (22%)	80,113,113	2.42	21 (26%)
21	CL7	4B	611	-	71,73,73	1.69	17 (23%)	80,113,113	2.46	22 (27%)
25	SQD	1A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	33	514	-	51,53,73	1.99	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	4C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.36	22 (27%)
23	8CT	3B	618	-	40,41,41	4.69	21 (52%)	50,56,56	2.66	20 (40%)
21	CL7	34	415	-	51,53,73	1.96	19 (37%)	56,89,113	2.87	20 (35%)
21	CL7	31	407	18	47,49,73	1.94	14 (29%)	51,84,113	2.87	19 (37%)
27	DGD	3B	624	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	1C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.83	18 (35%)
21	CL7	14	417	20	48,50,73	1.93	13 (27%)	51,85,113	2.94	19 (37%)
32	ZEX	43	420	-	42,43,43	1.01	4 (9%)	55,60,60	2.58	17 (30%)
21	CL7	12	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	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	20 (35%)
21	CL7	4B	616	2	56,58,73	1.90	17 (30%)	62,95,113	2.71	20 (32%)
21	CL7	32	513	16	51,53,73	1.96	15 (29%)	56,89,113	2.84	21 (37%)
21	CL7	43	413	19	61,63,73	1.84	19 (31%)	68,101,113	2.58	23 (33%)
21	CL7	2B	612	2	71,73,73	1.70	18 (25%)	80,113,113	2.35	21 (26%)
23	8CT	2B	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	1C	513	3	51,53,73	1.94	14 (27%)	56,89,113	2.90	19 (33%)
21	CL7	3C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.83	18 (35%)
21	CL7	12	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.38	22 (27%)
32	ZEX	31	422	-	42,43,43	0.96	2 (4%)	55,60,60	2.24	18 (32%)
25	SQD	4A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
25	SQD	31	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	31	403	-	66,68,73	1.76	16 (24%)	74,107,113	2.51	22 (29%)
27	DGD	4C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	21	412	18	51,53,73	1.95	16 (31%)	56,89,113	2.76	20 (35%)
21	CL7	11	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.39	21 (26%)
32	ZEX	32	520	-	42,43,43	0.97	3 (7%)	55,60,60	2.18	17 (30%)
21	CL7	1B	606	2	61,63,73	1.81	16 (26%)	68,101,113	2.63	21 (30%)
21	CL7	42	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.31	20 (25%)
21	CL7	11	403	-	66,68,73	1.76	16 (24%)	74,107,113	2.51	22 (29%)
26	LHG	14	401	-	48,48,48	0.29	0	51,54,54	0.34	0
21	CL7	2D	405	4	51,53,73	1.95	17 (33%)	56,89,113	2.77	22 (39%)
21	CL7	32	503	-	71,73,73	1.68	17 (23%)	80,113,113	2.50	25 (31%)
21	CL7	2C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.84	18 (35%)
21	CL7	21	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.57	20 (29%)
21	CL7	1C	503	3	71,73,73	1.68	15 (21%)	80,113,113	2.40	21 (26%)
21	CL7	3B	614	2	66,68,73	1.78	18 (27%)	74,107,113	2.49	24 (32%)
21	CL7	12	511	16	66,68,73	1.78	16 (24%)	74,107,113	2.40	21 (28%)
21	CL7	21	404	-	71,73,73	1.71	14 (19%)	80,113,113	2.39	21 (26%)
21	CL7	3C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.37	23 (28%)
21	CL7	42	510	16	71,73,73	1.68	18 (25%)	80,113,113	2.37	22 (27%)
21	CL7	1B	610	-	71,73,73	1.68	17 (23%)	80,113,113	2.46	22 (27%)
21	CL7	41	413	-	47,49,73	1.94	12 (25%)	51,84,113	2.98	22 (43%)
27	DGD	4B	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
24	LMG	2A	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	41	416	-	47,49,73	1.95	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	41	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	21	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.72	18 (32%)
21	CL7	2C	513	3	51,53,73	1.95	14 (27%)	56,89,113	2.91	19 (33%)
21	CL7	4D	405	4	51,53,73	1.96	18 (35%)	56,89,113	2.77	22 (39%)
21	CL7	33	517	19	56,58,73	1.88	15 (26%)	62,95,113	2.65	20 (32%)
21	CL7	11	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.50	19 (25%)
32	ZEX	34	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
21	CL7	12	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.48	26 (32%)
21	CL7	33	510	-	71,73,73	1.69	17 (23%)	80,113,113	2.37	24 (30%)
29	BCT	4D	403	28	2,3,3	0.99	0	2,3,3	1.66	1 (50%)
21	CL7	23	419	19	51,53,73	1.97	14 (27%)	56,89,113	2.74	20 (35%)
32	ZEX	22	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	3B	611	2	71,73,73	1.70	18 (25%)	80,113,113	2.34	20 (25%)
21	CL7	22	503	-	71,73,73	1.68	18 (25%)	80,113,113	2.51	25 (31%)
25	SQD	13	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	2C	503	3	71,73,73	1.68	16 (22%)	80,113,113	2.40	21 (26%)
21	CL7	12	503	-	71,73,73	1.69	17 (23%)	80,113,113	2.51	25 (31%)
21	CL7	34	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.85	18 (35%)
21	CL7	34	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.69	21 (37%)
23	8CT	3C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
21	CL7	42	507	-	71,73,73	1.72	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	4B	623	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
21	CL7	42	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.35	21 (26%)
21	CL7	33	504	-	71,73,73	1.69	17 (23%)	80,113,113	2.41	21 (26%)
21	CL7	41	410	-	71,73,73	1.70	17 (23%)	80,113,113	2.34	23 (28%)
32	ZEX	13	525	-	42,43,43	1.18	5 (11%)	55,60,60	2.44	18 (32%)
21	CL7	4B	612	2	71,73,73	1.70	18 (25%)	80,113,113	2.36	20 (25%)
21	CL7	33	509	19	71,73,73	1.68	15 (21%)	80,113,113	2.33	22 (27%)
21	CL7	2B	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.33	23 (28%)
21	CL7	1C	517	3	47,49,73	1.93	13 (27%)	51,84,113	2.89	19 (37%)
21	CL7	11	416	-	47,49,73	1.95	13 (27%)	51,84,113	2.88	19 (37%)
21	CL7	12	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.78	19 (33%)
21	CL7	23	413	19	61,63,73	1.83	18 (29%)	68,101,113	2.58	22 (32%)
26	LHG	1B	625	-	48,48,48	0.30	0	51,54,54	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	2A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.61	23 (33%)
21	CL7	42	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.35	23 (28%)
21	CL7	23	412	19	71,73,73	1.69	18 (25%)	80,113,113	2.55	24 (30%)
21	CL7	13	510	-	71,73,73	1.69	17 (23%)	80,113,113	2.37	24 (30%)
21	CL7	24	411	20	71,73,73	1.68	15 (21%)	80,113,113	2.41	23 (28%)
21	CL7	44	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.44	21 (28%)
21	CL7	11	413	-	47,49,73	1.94	13 (27%)	51,84,113	2.98	22 (43%)
21	CL7	32	511	16	66,68,73	1.78	17 (25%)	74,107,113	2.40	21 (28%)
21	CL7	1C	510	3	71,73,73	1.69	14 (19%)	80,113,113	2.38	21 (26%)
26	LHG	2D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	4D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.48	22 (30%)
21	CL7	4C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.84	18 (35%)
21	CL7	21	419	-	51,53,73	1.97	15 (29%)	56,89,113	2.78	18 (32%)
21	CL7	42	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.65	19 (33%)
21	CL7	31	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.78	18 (32%)
21	CL7	24	413	20	66,68,73	1.77	17 (25%)	74,107,113	2.44	21 (28%)
26	LHG	3B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	34	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.68	24 (32%)
25	SQD	42	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
22	PHO	2D	408	-	58,69,69	0.80	4 (6%)	56,99,99	1.28	4 (7%)
21	CL7	42	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	11	409	18	51,53,73	1.96	16 (31%)	56,89,113	2.72	20 (35%)
21	CL7	21	416	-	47,49,73	1.95	13 (27%)	51,84,113	2.87	19 (37%)
23	8CT	24	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	22	513	16	51,53,73	1.97	14 (27%)	56,89,113	2.84	21 (37%)
23	8CT	14	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.77	21 (42%)
21	CL7	14	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.70	19 (33%)
21	CL7	33	513	-	51,53,73	1.97	16 (31%)	56,89,113	2.72	18 (32%)
25	SQD	22	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
22	PHO	1D	408	-	58,69,69	0.80	4 (6%)	56,99,99	1.26	4 (7%)
21	CL7	4C	513	3	51,53,73	1.95	14 (27%)	56,89,113	2.91	19 (33%)
21	CL7	41	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.39	21 (26%)
24	LMG	11	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
21	CL7	33	506	19	51,53,73	1.97	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	34	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	13	507	-	71,73,73	1.68	15 (21%)	80,113,113	2.40	23 (28%)
21	CL7	3B	610	-	71,73,73	1.69	17 (23%)	80,113,113	2.46	21 (26%)
21	CL7	13	517	19	56,58,73	1.89	16 (28%)	62,95,113	2.65	20 (32%)
21	CL7	3B	602	2	66,68,73	1.78	17 (25%)	74,107,113	2.50	22 (29%)
21	CL7	4C	502	3	66,68,73	1.76	16 (24%)	74,107,113	2.45	19 (25%)
21	CL7	13	515	-	47,49,73	1.94	12 (25%)	51,84,113	2.92	21 (41%)
21	CL7	3B	608	2	71,73,73	1.69	19 (26%)	80,113,113	2.30	20 (25%)
21	CL7	33	503	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
22	PHO	4A	402	-	58,69,69	0.83	3 (5%)	56,99,99	1.08	4 (7%)
32	ZEX	22	520	-	42,43,43	0.99	3 (7%)	55,60,60	2.18	17 (30%)
21	CL7	11	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.43	20 (26%)
30	PL9	1D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	4C	503	3	71,73,73	1.68	15 (21%)	80,113,113	2.39	21 (26%)
24	LMG	2D	410	-	33,33,55	0.28	0	41,41,63	0.33	0
21	CL7	21	413	-	47,49,73	1.94	13 (27%)	51,84,113	2.97	22 (43%)
21	CL7	43	410	19	71,73,73	1.69	16 (22%)	80,113,113	2.34	22 (27%)
21	CL7	21	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	4B	608	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	21 (28%)
21	CL7	3C	502	3	66,68,73	1.77	17 (25%)	74,107,113	2.45	19 (25%)
32	ZEX	32	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	2B	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	20 (25%)
21	CL7	13	501	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	24 (30%)
21	CL7	21	410	-	71,73,73	1.69	16 (22%)	80,113,113	2.33	22 (27%)
21	CL7	41	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.98	19 (37%)
23	8CT	1K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.66	16 (32%)
23	8CT	3K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.66	16 (32%)
21	CL7	22	501	16	71,73,73	1.68	17 (23%)	80,113,113	2.42	21 (26%)
21	CL7	2C	502	3	66,68,73	1.77	17 (25%)	74,107,113	2.45	19 (25%)
23	8CT	1B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	24	405	-	71,73,73	1.70	16 (22%)	80,113,113	2.46	26 (32%)
32	ZEX	41	422	-	42,43,43	0.95	2 (4%)	55,60,60	2.24	18 (32%)
24	LMG	3B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	32	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	19 (33%)
23	8CT	4B	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	23	403	19	64,66,73	1.77	16 (25%)	71,104,113	2.41	22 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	44	405	-	71,73,73	1.69	16 (22%)	80,113,113	2.45	26 (32%)
21	CL7	2B	611	-	71,73,73	1.68	16 (22%)	80,113,113	2.46	22 (27%)
21	CL7	12	513	16	51,53,73	1.96	15 (29%)	56,89,113	2.83	21 (37%)
21	CL7	3C	512	3	47,49,73	1.92	12 (25%)	51,84,113	2.98	20 (39%)
26	LHG	3D	409	-	48,48,48	0.30	0	51,54,54	0.37	0

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	11	420	18	2/2/11/20	6/15/91/115	-
21	CL7	23	415	-	2/2/11/20	5/15/91/115	-
21	CL7	42	515	-	2/2/11/20	8/15/91/115	-
21	CL7	23	407	19	2/2/11/20	13/15/91/115	-
21	CL7	24	406	20	2/2/15/20	24/39/115/115	-
32	ZEX	24	419	-	-	9/29/67/67	0/2/2/2
21	CL7	3B	603	2	2/2/15/20	12/39/115/115	-
21	CL7	42	511	16	2/2/14/20	16/33/109/115	-
21	CL7	44	407	-	2/2/10/20	3/10/86/115	-
21	CL7	4A	407	-	2/2/15/20	16/39/115/115	-
21	CL7	3B	612	2	2/2/15/20	17/39/115/115	-
21	CL7	42	516	16	2/2/15/20	16/39/115/115	-
21	CL7	2C	512	3	2/2/10/20	4/10/86/115	-
26	LHG	2B	624	-	-	3/49/49/53	-
21	CL7	42	513	16	2/2/11/20	8/15/91/115	-
21	CL7	24	415	-	2/2/11/20	11/15/91/115	-
21	CL7	32	518	16	2/2/15/20	12/39/115/115	-
23	8CT	4B	620	-	-	4/29/63/63	0/2/2/2
21	CL7	11	412	18	2/2/11/20	10/15/91/115	-
24	LMG	4A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
22	PHO	3D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
31	HEM	1F	101	-	-	8/14/54/54	-
21	CL7	42	518	16	2/2/15/20	12/39/115/115	-
21	CL7	32	509	-	2/2/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	2B	622	-	-	7/46/66/70	0/1/1/1
21	CL7	3B	601	-	2/2/10/20	4/10/86/115	-
21	CL7	4C	509	3	2/2/15/20	20/39/115/115	-
21	CL7	42	506	16	2/2/15/20	14/39/115/115	-
21	CL7	31	405	-	2/2/11/20	10/15/91/115	-
21	CL7	42	503	-	2/2/15/20	17/39/115/115	-
21	CL7	23	418	19	2/2/12/20	9/21/97/115	-
25	SQD	23	424	-	-	7/45/65/69	0/1/1/1
21	CL7	32	517	16	2/2/15/20	21/39/115/115	-
32	ZEX	32	522	-	-	6/29/67/67	0/2/2/2
25	SQD	3B	620	-	-	5/49/69/69	0/1/1/1
26	LHG	44	401	-	-	8/53/53/53	-
21	CL7	1B	616	2	2/2/11/20	4/15/91/115	-
30	PL9	3D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	43	418	19	2/2/12/20	9/21/97/115	-
21	CL7	12	512	16	2/2/15/20	18/39/115/115	-
32	ZEX	23	401	-	-	7/29/67/67	0/2/2/2
21	CL7	34	407	-	2/2/10/20	3/10/86/115	-
24	LMG	4B	622	-	-	7/46/66/70	0/1/1/1
26	LHG	24	401	-	-	8/53/53/53	-
21	CL7	32	502	16	2/2/15/20	17/39/115/115	-
21	CL7	34	406	20	2/2/15/20	24/39/115/115	-
25	SQD	2A	406	-	-	3/29/49/69	0/1/1/1
32	ZEX	23	421	-	-	10/29/67/67	0/2/2/2
21	CL7	33	515	-	2/2/10/20	0/10/86/115	-
21	CL7	1C	502	3	2/2/14/20	12/33/109/115	-
21	CL7	13	511	19	2/2/15/20	19/39/115/115	-
21	CL7	2B	606	2	2/2/15/20	18/39/115/115	-
23	8CT	2K	101	-	-	10/29/63/63	0/2/2/2
32	ZEX	43	421	-	-	10/29/67/67	0/2/2/2
21	CL7	1D	404	4	2/2/13/20	13/31/107/115	-
21	CL7	22	511	16	2/2/14/20	16/33/109/115	-
25	SQD	41	423	-	-	3/27/47/69	0/1/1/1
25	SQD	22	523	-	-	0/36/56/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	4B	609	2	2/2/15/20	15/39/115/115	-
21	CL7	12	516	16	2/2/15/20	16/39/115/115	-
21	CL7	4C	512	3	2/2/10/20	4/10/86/115	-
32	ZEX	24	403	-	-	10/29/67/67	0/2/2/2
21	CL7	42	505	16	2/2/15/20	18/39/115/115	-
21	CL7	24	412	20	2/2/15/20	17/39/115/115	-
21	CL7	31	411	-	2/2/11/20	7/15/91/115	-
32	ZEX	12	522	-	-	6/29/67/67	0/2/2/2
21	CL7	41	418	18	2/2/15/20	22/39/115/115	-
23	8CT	2B	601	-	-	10/29/63/63	0/2/2/2
21	CL7	11	411	-	2/2/11/20	7/15/91/115	-
21	CL7	4C	507	-	2/2/15/20	17/39/115/115	-
21	CL7	13	503	-	2/2/15/20	20/39/115/115	-
21	CL7	43	405	-	2/2/15/20	16/39/115/115	-
21	CL7	3A	403	1	2/2/13/20	9/27/103/115	-
21	CL7	1D	402	-	2/2/12/20	9/21/97/115	-
21	CL7	23	402	19	2/2/15/20	21/39/115/115	-
21	CL7	1B	612	2	2/2/15/20	17/39/115/115	-
21	CL7	13	502	19	2/2/13/20	12/31/107/115	-
21	CL7	33	505	19	2/2/15/20	14/39/115/115	-
25	SQD	3A	406	-	-	3/29/49/69	0/1/1/1
25	SQD	43	422	-	-	3/41/61/69	0/1/1/1
21	CL7	3C	503	3	2/2/15/20	19/39/115/115	-
21	CL7	31	418	18	2/2/15/20	22/39/115/115	-
32	ZEX	41	421	-	-	14/29/67/67	0/2/2/2
32	ZEX	34	420	-	-	12/29/67/67	0/2/2/2
21	CL7	43	402	19	2/2/15/20	21/39/115/115	-
21	CL7	32	512	16	2/2/15/20	18/39/115/115	-
21	CL7	31	413	-	2/2/10/20	2/10/86/115	-
21	CL7	33	516	19	2/2/13/20	16/27/103/115	-
21	CL7	13	504	-	2/2/15/20	16/39/115/115	-
21	CL7	2B	616	2	2/2/12/20	8/21/97/115	-
32	ZEX	24	418	-	-	9/29/67/67	0/2/2/2
32	ZEX	44	418	-	-	9/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2C	507	-	2/2/15/20	17/39/115/115	-
26	LHG	4B	624	-	-	3/49/49/53	-
21	CL7	12	507	-	2/2/15/20	20/39/115/115	-
21	CL7	2B	607	2	2/2/13/20	5/27/103/115	-
21	CL7	4C	504	-	2/2/13/20	13/27/103/115	-
23	8CT	2D	406	-	-	10/29/63/63	0/2/2/2
32	ZEX	3I	421	-	-	14/29/67/67	0/2/2/2
21	CL7	2B	604	2	2/2/15/20	12/39/115/115	-
21	CL7	3C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	43	404	-	2/2/15/20	20/39/115/115	-
21	CL7	43	419	19	2/2/11/20	7/15/91/115	-
21	CL7	24	404	20	2/2/15/20	15/39/115/115	-
21	CL7	3B	609	2	2/2/15/20	14/39/115/115	-
21	CL7	4B	615	2	2/2/14/20	14/33/109/115	-
23	8CT	4D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	23	411	-	2/2/15/20	15/39/115/115	-
23	8CT	4A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	11	417	18	2/2/13/20	9/27/103/115	-
25	SQD	23	422	-	-	3/41/61/69	0/1/1/1
21	CL7	2B	608	-	2/2/14/20	11/33/109/115	-
21	CL7	2C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	44	411	20	2/2/15/20	14/39/115/115	-
21	CL7	31	409	18	2/2/11/20	6/15/91/115	-
21	CL7	41	402	18	2/2/14/20	16/33/109/115	-
21	CL7	4A	401	1	2/2/15/20	18/39/115/115	-
21	CL7	22	517	16	2/2/15/20	21/39/115/115	-
21	CL7	22	509	-	2/2/15/20	16/39/115/115	-
26	LHG	1D	409	-	-	7/53/53/53	-
21	CL7	21	418	18	2/2/15/20	22/39/115/115	-
23	8CT	34	402	-	-	4/29/63/63	0/2/2/2
23	8CT	4B	619	-	-	10/29/63/63	0/2/2/2
21	CL7	22	510	16	2/2/15/20	20/39/115/115	-
21	CL7	21	414	18	2/2/10/20	3/10/86/115	-
24	LMG	31	401	-	-	5/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	44	412	20	2/2/15/20	17/39/115/115	-
23	8CT	44	402	-	-	4/29/63/63	0/2/2/2
21	CL7	43	412	19	2/2/15/20	19/39/115/115	-
21	CL7	11	415	-	2/2/10/20	7/10/86/115	-
21	CL7	3A	407	-	2/2/15/20	16/39/115/115	-
21	CL7	3D	404	4	2/2/13/20	13/31/107/115	-
21	CL7	33	508	19	2/2/15/20	16/39/115/115	-
21	CL7	41	409	18	2/2/11/20	6/15/91/115	-
21	CL7	42	512	16	2/2/15/20	18/39/115/115	-
32	ZEX	34	403	-	-	10/29/67/67	0/2/2/2
22	PHO	2A	402	-	-	3/37/103/103	0/5/6/6
21	CL7	23	405	-	2/2/15/20	16/39/115/115	-
21	CL7	1B	602	2	2/2/14/20	9/33/109/115	-
32	ZEX	12	519	-	-	11/29/67/67	0/2/2/2
23	8CT	1B	619	-	-	4/29/63/63	0/2/2/2
32	ZEX	21	421	-	-	14/29/67/67	0/2/2/2
21	CL7	1C	512	3	2/2/10/20	4/10/86/115	-
21	CL7	13	509	19	2/2/15/20	17/39/115/115	-
23	8CT	2C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	31	404	-	2/2/15/20	15/39/115/115	-
21	CL7	31	420	18	2/2/11/20	6/15/91/115	-
21	CL7	13	514	-	2/2/11/20	5/15/91/115	-
21	CL7	1B	609	2	2/2/15/20	14/39/115/115	-
21	CL7	11	418	18	2/2/15/20	22/39/115/115	-
21	CL7	12	518	16	2/2/15/20	12/39/115/115	-
21	CL7	2B	603	2	2/2/14/20	9/33/109/115	-
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	-
21	CL7	4B	604	2	2/2/15/20	12/39/115/115	-
21	CL7	1B	622	2	2/2/11/20	8/15/91/115	-
21	CL7	22	514	-	2/2/11/20	9/15/91/115	-
21	CL7	3A	401	1	2/2/15/20	18/39/115/115	-
32	ZEX	24	420	-	-	12/29/67/67	0/2/2/2
21	CL7	1B	613	2	2/2/13/20	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	23	406	19	2/2/15/20	14/39/115/115	-
23	8CT	4C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	33	507	-	2/2/15/20	15/39/115/115	-
21	CL7	2B	602	-	2/2/10/20	4/10/86/115	-
21	CL7	14	411	20	2/2/15/20	14/39/115/115	-
21	CL7	44	410	20	2/2/11/20	9/15/91/115	-
21	CL7	11	410	-	2/2/15/20	17/39/115/115	-
21	CL7	13	516	19	2/2/13/20	16/27/103/115	-
21	CL7	44	414	20	2/2/12/20	8/25/101/115	-
23	8CT	1B	618	-	-	10/29/63/63	0/2/2/2
21	CL7	31	412	18	2/2/11/20	10/15/91/115	-
21	CL7	24	416	20	2/2/10/20	7/10/86/115	-
21	CL7	33	511	19	2/2/15/20	19/39/115/115	-
21	CL7	3B	607	-	2/2/14/20	11/33/109/115	-
32	ZEX	11	421	-	-	14/29/67/67	0/2/2/2
21	CL7	34	412	20	2/2/15/20	17/39/115/115	-
21	CL7	13	513	-	2/2/11/20	9/15/91/115	-
21	CL7	3B	604	2	2/2/15/20	17/39/115/115	-
21	CL7	33	502	19	2/2/13/20	12/31/107/115	-
21	CL7	21	402	18	2/2/14/20	16/33/109/115	-
25	SQD	2B	621	-	-	5/49/69/69	0/1/1/1
21	CL7	31	402	18	2/2/14/20	16/33/109/115	-
21	CL7	21	420	18	2/2/11/20	6/15/91/115	-
24	LMG	3A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	23	417	19	2/2/13/20	16/27/103/115	-
21	CL7	1C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	3C	506	3	2/2/14/20	15/33/109/115	-
21	CL7	1B	608	2	2/2/15/20	15/39/115/115	-
31	HEM	4F	101	-	-	8/14/54/54	-
32	ZEX	22	524	-	-	11/29/67/67	0/2/2/2
21	CL7	21	409	18	2/2/11/20	6/15/91/115	-
21	CL7	1B	605	2	2/2/15/20	18/39/115/115	-
25	SQD	1B	620	-	-	5/49/69/69	0/1/1/1
21	CL7	22	512	16	2/2/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	24	417	20	2/2/10/20	6/12/88/115	-
21	CL7	44	406	20	2/2/15/20	24/39/115/115	-
21	CL7	3C	504	-	2/2/13/20	13/27/103/115	-
32	ZEX	13	520	-	-	10/29/67/67	0/2/2/2
32	ZEX	42	522	-	-	6/29/67/67	0/2/2/2
21	CL7	2B	610	2	2/2/15/20	14/39/115/115	-
21	CL7	3B	606	2	2/2/13/20	5/27/103/115	-
21	CL7	3B	615	2	2/2/12/20	8/21/97/115	-
22	PHO	4D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	2C	505	3	2/2/15/20	16/39/115/115	-
21	CL7	24	410	20	2/2/11/20	9/15/91/115	-
23	8CT	3C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	3C	509	3	2/2/15/20	20/39/115/115	-
21	CL7	23	408	-	2/2/15/20	15/39/115/115	-
21	CL7	43	417	19	2/2/13/20	16/27/103/115	-
21	CL7	14	405	-	2/2/15/20	18/39/115/115	-
26	LHG	2B	626	-	-	6/53/53/53	-
21	CL7	43	415	-	2/2/11/20	5/15/91/115	-
21	CL7	1A	407	-	2/2/15/20	16/39/115/115	-
32	ZEX	12	520	-	-	6/29/67/67	0/2/2/2
21	CL7	44	408	20	2/2/11/20	4/15/91/115	-
21	CL7	3C	510	3	2/2/15/20	22/39/115/115	-
21	CL7	11	408	-	2/2/15/20	16/39/115/115	-
23	8CT	4C	515	-	-	10/29/63/63	0/2/2/2
23	8CT	1C	518	-	-	8/29/63/63	0/2/2/2
32	ZEX	12	524	-	-	11/29/67/67	0/2/2/2
21	CL7	11	419	-	2/2/11/20	9/15/91/115	-
21	CL7	3C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	44	409	-	2/2/14/20	17/33/109/115	-
21	CL7	1D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	13	512	19	2/2/13/20	12/27/103/115	-
21	CL7	2C	509	3	2/2/15/20	20/39/115/115	-
25	SQD	21	423	-	-	3/27/47/69	0/1/1/1
26	LHG	4B	626	-	-	6/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	34	405	-	2/2/15/20	18/39/115/115	-
23	8CT	3B	619	-	-	4/29/63/63	0/2/2/2
24	LMG	1A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
30	PL9	4D	407	-	-	9/53/73/73	0/1/1/1
26	LHG	4A	408	-	-	5/50/50/53	-
22	PHO	3A	402	-	-	3/37/103/103	0/5/6/6
23	8CT	1C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	24	409	-	2/2/14/20	17/33/109/115	-
25	SQD	42	521	-	-	7/45/65/69	0/1/1/1
21	CL7	12	502	16	2/2/15/20	17/39/115/115	-
23	8CT	4C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	1B	607	-	2/2/14/20	11/33/109/115	-
23	8CT	1A	404	-	-	5/29/63/63	0/2/2/2
23	8CT	1B	626	-	-	10/29/63/63	0/2/2/2
32	ZEX	14	418	-	-	9/29/67/67	0/2/2/2
32	ZEX	21	422	-	-	6/29/67/67	0/2/2/2
21	CL7	42	514	-	2/2/11/20	9/15/91/115	-
21	CL7	3D	402	-	2/2/12/20	9/21/97/115	-
26	LHG	3B	625	-	-	6/53/53/53	-
21	CL7	23	409	19	2/2/15/20	16/39/115/115	-
26	LHG	34	401	-	-	8/53/53/53	-
21	CL7	14	409	-	2/2/14/20	17/33/109/115	-
21	CL7	43	411	-	2/2/15/20	16/39/115/115	-
21	CL7	31	417	18	2/2/13/20	9/27/103/115	-
21	CL7	1A	401	1	2/2/15/20	18/39/115/115	-
32	ZEX	42	520	-	-	6/29/67/67	0/2/2/2
32	ZEX	44	419	-	-	9/29/67/67	0/2/2/2
21	CL7	32	508	16	2/2/11/20	5/15/91/115	-
21	CL7	43	403	19	2/2/13/20	12/31/107/115	-
32	ZEX	44	420	-	-	12/29/67/67	0/2/2/2
21	CL7	43	414	-	2/2/11/20	9/15/91/115	-
24	LMG	4D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	3C	507	-	2/2/15/20	17/39/115/115	-
21	CL7	4C	508	3	2/2/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	41	407	18	2/2/10/20	4/10/86/115	-
32	ZEX	13	522	-	-	5/29/67/67	0/2/2/2
23	8CT	4K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	32	506	16	2/2/15/20	14/39/115/115	-
23	8CT	2C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	44	415	-	2/2/11/20	11/15/91/115	-
21	CL7	12	509	-	2/2/15/20	16/39/115/115	-
21	CL7	41	420	18	2/2/11/20	6/15/91/115	-
21	CL7	24	408	20	2/2/11/20	4/15/91/115	-
23	8CT	2A	404	-	-	5/29/63/63	0/2/2/2
24	LMG	1D	410	-	-	6/28/48/70	0/1/1/1
32	ZEX	33	525	-	-	7/29/67/67	0/2/2/2
32	ZEX	22	522	-	-	6/29/67/67	0/2/2/2
21	CL7	1C	508	3	2/2/15/20	17/39/115/115	-
25	SQD	4B	621	-	-	5/49/69/69	0/1/1/1
21	CL7	43	416	-	2/2/10/20	0/10/86/115	-
25	SQD	32	521	-	-	7/45/65/69	0/1/1/1
25	SQD	33	521	-	-	3/41/61/69	0/1/1/1
27	DGD	2B	625	-	-	7/51/91/95	0/2/2/2
21	CL7	4C	505	3	2/2/15/20	16/39/115/115	-
32	ZEX	44	403	-	-	10/29/67/67	0/2/2/2
21	CL7	1C	506	3	2/2/14/20	15/33/109/115	-
21	CL7	23	404	-	2/2/15/20	20/39/115/115	-
24	LMG	1B	621	-	-	7/46/66/70	0/1/1/1
21	CL7	41	403	-	2/2/14/20	11/33/109/115	-
21	CL7	23	416	-	2/2/10/20	0/10/86/115	-
21	CL7	4B	613	2	2/2/15/20	17/39/115/115	-
32	ZEX	11	422	-	-	6/29/67/67	0/2/2/2
26	LHG	23	425	-	-	3/40/40/53	-
23	8CT	2B	619	-	-	10/29/63/63	0/2/2/2
21	CL7	44	416	20	2/2/10/20	7/10/86/115	-
27	DGD	3C	516	-	-	9/51/91/95	0/2/2/2
21	CL7	4B	617	2	2/2/11/20	4/15/91/115	-
27	DGD	2C	516	-	-	9/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	41	408	-	2/2/15/20	16/39/115/115	-
21	CL7	1B	614	2	2/2/14/20	14/33/109/115	-
21	CL7	11	407	18	2/2/10/20	4/10/86/115	-
21	CL7	21	415	-	2/2/10/20	7/10/86/115	-
21	CL7	31	415	-	2/2/10/20	7/10/86/115	-
21	CL7	3B	613	2	2/2/13/20	5/27/103/115	-
21	CL7	32	505	16	2/2/15/20	18/39/115/115	-
32	ZEX	33	520	-	-	10/29/67/67	0/2/2/2
21	CL7	2B	623	2	2/2/11/20	8/15/91/115	-
21	CL7	43	406	19	2/2/15/20	14/39/115/115	-
21	CL7	4B	605	2	2/2/15/20	17/39/115/115	-
21	CL7	34	413	20	2/2/14/20	7/33/109/115	-
21	CL7	3D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	14	416	20	2/2/10/20	7/10/86/115	-
21	CL7	43	409	19	2/2/15/20	16/39/115/115	-
32	ZEX	14	419	-	-	9/29/67/67	0/2/2/2
32	ZEX	43	401	-	-	7/29/67/67	0/2/2/2
21	CL7	14	413	20	2/2/14/20	7/33/109/115	-
26	LHG	13	524	-	-	3/40/40/53	-
21	CL7	1B	611	2	2/2/15/20	17/39/115/115	-
21	CL7	1C	505	3	2/2/15/20	16/39/115/115	-
21	CL7	21	407	18	2/2/10/20	4/10/86/115	-
21	CL7	33	512	19	2/2/13/20	12/27/103/115	-
23	8CT	1D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	24	407	-	2/2/10/20	3/10/86/115	-
23	8CT	3A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	2A	401	1	2/2/15/20	18/39/115/115	-
21	CL7	12	501	16	2/2/15/20	17/39/115/115	-
21	CL7	14	408	20	2/2/11/20	4/15/91/115	-
23	8CT	2B	620	-	-	4/29/63/63	0/2/2/2
21	CL7	3B	616	2	2/2/11/20	4/15/91/115	-
21	CL7	41	417	18	2/2/13/20	9/27/103/115	-
25	SQD	12	523	-	-	0/36/56/69	0/1/1/1
21	CL7	22	515	-	2/2/11/20	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	23	414	-	2/2/11/20	9/15/91/115	-
21	CL7	31	410	-	2/2/15/20	17/39/115/115	-
31	HEM	2F	101	-	-	8/14/54/54	-
23	8CT	3D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	32	510	16	2/2/15/20	20/39/115/115	-
32	ZEX	13	519	-	-	10/29/67/67	0/2/2/2
21	CL7	22	516	16	2/2/15/20	16/39/115/115	-
21	CL7	11	414	18	2/2/10/20	3/10/86/115	-
21	CL7	31	406	18	2/2/14/20	13/36/112/115	-
21	CL7	4B	607	2	2/2/13/20	5/27/103/115	-
21	CL7	13	518	19	2/2/11/20	7/15/91/115	-
21	CL7	21	403	-	2/2/14/20	11/33/109/115	-
24	LMG	3D	410	-	-	5/28/48/70	0/1/1/1
21	CL7	1B	615	2	2/2/12/20	8/21/97/115	-
26	LHG	43	425	-	-	3/40/40/53	-
21	CL7	43	408	-	2/2/15/20	15/39/115/115	-
21	CL7	13	506	19	2/2/11/20	13/15/91/115	-
21	CL7	3C	513	3	2/2/11/20	8/15/91/115	-
21	CL7	14	406	20	2/2/15/20	24/39/115/115	-
21	CL7	22	518	16	2/2/15/20	12/39/115/115	-
21	CL7	33	501	19	2/2/15/20	21/39/115/115	-
32	ZEX	33	519	-	-	10/29/67/67	0/2/2/2
21	CL7	21	408	-	2/2/15/20	16/39/115/115	-
21	CL7	4D	402	-	2/2/12/20	9/21/97/115	-
24	LMG	41	401	-	-	5/46/66/70	0/1/1/1
31	HEM	3F	101	-	-	8/14/54/54	-
21	CL7	3B	605	2	2/2/15/20	18/39/115/115	-
21	CL7	22	506	16	2/2/15/20	14/39/115/115	-
21	CL7	4B	606	2	2/2/15/20	18/39/115/115	-
32	ZEX	42	524	-	-	11/29/67/67	0/2/2/2
21	CL7	2B	613	2	2/2/15/20	17/39/115/115	-
21	CL7	2C	508	3	2/2/15/20	17/39/115/115	-
21	CL7	44	404	20	2/2/15/20	14/39/115/115	-
27	DGD	1C	516	-	-	9/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	32	507	-	2/2/15/20	20/39/115/115	-
21	CL7	22	505	16	2/2/15/20	18/39/115/115	-
21	CL7	21	405	-	2/2/11/20	10/15/91/115	-
23	8CT	1C	514	-	-	14/29/63/63	0/2/2/2
26	LHG	3A	408	-	-	5/50/50/53	-
32	ZEX	23	423	-	-	5/29/67/67	0/2/2/2
21	CL7	2C	506	3	2/2/14/20	15/33/109/115	-
21	CL7	2D	402	-	2/2/12/20	9/21/97/115	-
21	CL7	14	404	20	2/2/15/20	15/39/115/115	-
21	CL7	1B	603	2	2/2/15/20	12/39/115/115	-
21	CL7	41	415	-	2/2/10/20	7/10/86/115	-
21	CL7	32	514	-	2/2/11/20	9/15/91/115	-
21	CL7	1C	509	3	2/2/15/20	20/39/115/115	-
21	CL7	41	411	-	2/2/11/20	7/15/91/115	-
27	DGD	1B	624	-	-	7/51/91/95	0/2/2/2
32	ZEX	42	519	-	-	11/29/67/67	0/2/2/2
21	CL7	42	501	16	2/2/15/20	17/39/115/115	-
21	CL7	24	414	20	2/2/12/20	8/25/101/115	-
23	8CT	2C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	31	408	-	2/2/15/20	16/39/115/115	-
21	CL7	1C	507	-	2/2/15/20	17/39/115/115	-
21	CL7	34	414	20	2/2/12/20	8/25/101/115	-
21	CL7	13	508	19	2/2/15/20	16/39/115/115	-
21	CL7	2D	404	4	2/2/13/20	13/31/107/115	-
25	SQD	11	423	-	-	3/27/47/69	0/1/1/1
26	LHG	1B	623	-	-	3/49/49/53	-
21	CL7	22	507	-	2/2/15/20	20/39/115/115	-
26	LHG	2A	408	-	-	5/50/50/53	-
21	CL7	4B	602	-	2/2/10/20	4/10/86/115	-
23	8CT	4B	601	-	-	10/29/63/63	0/2/2/2
21	CL7	13	505	19	2/2/15/20	14/39/115/115	-
21	CL7	41	412	18	2/2/11/20	10/15/91/115	-
25	SQD	32	523	-	-	0/36/56/69	0/1/1/1
21	CL7	1B	604	2	2/2/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	8CT	3B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	32	504	-	2/2/11/20	6/15/91/115	-
21	CL7	14	414	20	2/2/12/20	8/25/101/115	-
21	CL7	22	508	16	2/2/11/20	5/15/91/115	-
23	8CT	3B	626	-	-	10/29/63/63	0/2/2/2
25	SQD	33	523	-	-	7/45/65/69	0/1/1/1
25	SQD	43	424	-	-	7/45/65/69	0/1/1/1
21	CL7	1C	504	-	2/2/13/20	13/27/103/115	-
21	CL7	12	508	16	2/2/11/20	5/15/91/115	-
21	CL7	14	407	-	2/2/10/20	3/10/86/115	-
21	CL7	12	514	-	2/2/11/20	9/15/91/115	-
25	SQD	13	521	-	-	3/41/61/69	0/1/1/1
26	LHG	4D	409	-	-	7/53/53/53	-
21	CL7	12	506	16	2/2/15/20	14/39/115/115	-
21	CL7	3B	622	2	2/2/11/20	8/15/91/115	-
21	CL7	34	417	20	2/2/10/20	6/12/88/115	-
21	CL7	14	412	20	2/2/15/20	17/39/115/115	-
21	CL7	1A	403	1	2/2/13/20	9/27/103/115	-
32	ZEX	23	420	-	-	10/29/67/67	0/2/2/2
32	ZEX	14	420	-	-	12/29/67/67	0/2/2/2
21	CL7	44	417	20	2/2/10/20	6/12/88/115	-
21	CL7	4C	510	3	2/2/15/20	22/39/115/115	-
24	LMG	21	401	-	-	5/46/66/70	0/1/1/1
21	CL7	34	411	20	2/2/15/20	14/39/115/115	-
21	CL7	34	410	20	2/2/11/20	9/15/91/115	-
32	ZEX	32	519	-	-	11/29/67/67	0/2/2/2
23	8CT	3C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	22	504	-	2/2/11/20	6/15/91/115	-
30	PL9	2D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	2C	504	-	2/2/13/20	13/27/103/115	-
21	CL7	2B	614	2	2/2/13/20	5/27/103/115	-
21	CL7	43	407	19	2/2/11/20	13/15/91/115	-
21	CL7	31	416	-	2/2/10/20	4/10/86/115	-
21	CL7	31	414	18	2/2/10/20	3/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2B	615	2	2/2/14/20	14/33/109/115	-
21	CL7	4A	403	1	2/2/13/20	9/27/103/115	-
32	ZEX	43	423	-	-	5/29/67/67	0/2/2/2
21	CL7	41	419	-	2/2/11/20	9/15/91/115	-
21	CL7	33	518	19	2/2/11/20	7/15/91/115	-
21	CL7	2C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	4B	610	2	2/2/15/20	14/39/115/115	-
26	LHG	33	524	-	-	3/40/40/53	-
21	CL7	4C	506	3	2/2/14/20	15/33/109/115	-
21	CL7	41	405	-	2/2/11/20	10/15/91/115	-
32	ZEX	34	418	-	-	9/29/67/67	0/2/2/2
32	ZEX	33	522	-	-	5/29/67/67	0/2/2/2
21	CL7	4B	614	2	2/2/13/20	5/27/103/115	-
21	CL7	4B	603	2	2/2/14/20	9/33/109/115	-
21	CL7	2C	510	3	2/2/15/20	22/39/115/115	-
21	CL7	3C	508	3	2/2/15/20	17/39/115/115	-
26	LHG	1A	408	-	-	5/50/50/53	-
21	CL7	2B	617	2	2/2/11/20	4/15/91/115	-
21	CL7	11	405	-	2/2/11/20	10/15/91/115	-
21	CL7	32	516	16	2/2/15/20	16/39/115/115	-
21	CL7	4C	517	3	2/2/10/20	5/10/86/115	-
32	ZEX	14	403	-	-	10/29/67/67	0/2/2/2
21	CL7	1B	601	-	2/2/10/20	4/10/86/115	-
22	PHO	1A	402	-	-	3/37/103/103	0/5/6/6
21	CL7	14	415	-	2/2/11/20	11/15/91/115	-
25	SQD	12	521	-	-	7/45/65/69	0/1/1/1
21	CL7	22	502	16	2/2/15/20	17/39/115/115	-
21	CL7	32	501	16	2/2/15/20	17/39/115/115	-
21	CL7	4B	611	-	2/2/15/20	11/39/115/115	-
25	SQD	1A	406	-	-	3/29/49/69	0/1/1/1
21	CL7	33	514	-	2/2/11/20	5/15/91/115	-
21	CL7	4C	501	3	2/2/15/20	20/39/115/115	-
23	8CT	3B	618	-	-	10/29/63/63	0/2/2/2
21	CL7	34	415	-	2/2/11/20	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	31	407	18	2/2/10/20	4/10/86/115	-
27	DGD	3B	624	-	-	7/51/91/95	0/2/2/2
21	CL7	1C	511	3	2/2/10/20	5/12/88/115	-
21	CL7	14	417	20	2/2/10/20	6/12/88/115	-
32	ZEX	43	420	-	-	10/29/67/67	0/2/2/2
21	CL7	12	517	16	2/2/15/20	21/39/115/115	-
21	CL7	12	515	-	2/2/11/20	8/15/91/115	-
21	CL7	4B	616	2	2/2/12/20	8/21/97/115	-
21	CL7	32	513	16	2/2/11/20	8/15/91/115	-
21	CL7	43	413	19	2/2/13/20	12/27/103/115	-
21	CL7	2B	612	2	2/2/15/20	17/39/115/115	-
23	8CT	2B	618	-	-	7/29/63/63	0/2/2/2
21	CL7	1C	513	3	2/2/11/20	8/15/91/115	-
21	CL7	3C	511	3	2/2/10/20	5/12/88/115	-
21	CL7	12	510	16	2/2/15/20	20/39/115/115	-
32	ZEX	31	422	-	-	6/29/67/67	0/2/2/2
25	SQD	4A	406	-	-	3/29/49/69	0/1/1/1
25	SQD	31	423	-	-	3/27/47/69	0/1/1/1
21	CL7	31	403	-	2/2/14/20	11/33/109/115	-
27	DGD	4C	516	-	-	9/51/91/95	0/2/2/2
21	CL7	21	412	18	2/2/11/20	10/15/91/115	-
21	CL7	11	404	-	2/2/15/20	15/39/115/115	-
32	ZEX	32	520	-	-	6/29/67/67	0/2/2/2
21	CL7	1B	606	2	2/2/13/20	5/27/103/115	-
21	CL7	42	509	-	2/2/15/20	16/39/115/115	-
21	CL7	11	403	-	2/2/14/20	11/33/109/115	-
26	LHG	14	401	-	-	8/53/53/53	-
21	CL7	2D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	32	503	-	2/2/15/20	17/39/115/115	-
21	CL7	2C	511	3	2/2/10/20	5/12/88/115	-
21	CL7	21	417	18	2/2/13/20	9/27/103/115	-
21	CL7	1C	503	3	2/2/15/20	19/39/115/115	-
21	CL7	3B	614	2	2/2/14/20	14/33/109/115	-
21	CL7	12	511	16	2/2/14/20	16/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	21	404	-	2/2/15/20	15/39/115/115	-
21	CL7	3C	505	3	2/2/15/20	16/39/115/115	-
21	CL7	42	510	16	2/2/15/20	20/39/115/115	-
21	CL7	1B	610	-	2/2/15/20	11/39/115/115	-
21	CL7	41	413	-	2/2/10/20	2/10/86/115	-
27	DGD	4B	625	-	-	7/51/91/95	0/2/2/2
24	LMG	2A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	41	416	-	2/2/10/20	4/10/86/115	-
21	CL7	41	406	18	2/2/14/20	13/36/112/115	-
21	CL7	21	411	-	2/2/11/20	7/15/91/115	-
21	CL7	2C	513	3	2/2/11/20	8/15/91/115	-
21	CL7	4D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	33	517	19	2/2/12/20	9/21/97/115	-
21	CL7	11	402	18	2/2/14/20	16/33/109/115	-
32	ZEX	34	419	-	-	9/29/67/67	0/2/2/2
21	CL7	12	505	16	2/2/15/20	18/39/115/115	-
21	CL7	33	510	-	2/2/15/20	15/39/115/115	-
21	CL7	23	419	19	2/2/11/20	7/15/91/115	-
32	ZEX	22	519	-	-	11/29/67/67	0/2/2/2
21	CL7	3B	611	2	2/2/15/20	17/39/115/115	-
21	CL7	22	503	-	2/2/15/20	17/39/115/115	-
25	SQD	13	523	-	-	7/45/65/69	0/1/1/1
21	CL7	2C	503	3	2/2/15/20	19/39/115/115	-
21	CL7	12	503	-	2/2/15/20	17/39/115/115	-
21	CL7	34	416	20	2/2/10/20	7/10/86/115	-
21	CL7	34	408	20	2/2/11/20	4/15/91/115	-
23	8CT	3C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	42	507	-	2/2/15/20	20/39/115/115	-
21	CL7	4B	623	2	2/2/11/20	8/15/91/115	-
21	CL7	42	517	16	2/2/15/20	21/39/115/115	-
21	CL7	33	504	-	2/2/15/20	16/39/115/115	-
21	CL7	41	410	-	2/2/15/20	17/39/115/115	-
32	ZEX	13	525	-	-	7/29/67/67	0/2/2/2
21	CL7	4B	612	2	2/2/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	33	509	19	2/2/15/20	17/39/115/115	-
21	CL7	2B	605	2	2/2/15/20	17/39/115/115	-
21	CL7	1C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	11	416	-	2/2/10/20	4/10/86/115	-
21	CL7	12	504	-	2/2/11/20	6/15/91/115	-
21	CL7	23	413	19	2/2/13/20	12/27/103/115	-
26	LHG	1B	625	-	-	6/53/53/53	-
21	CL7	2A	403	1	2/2/13/20	9/27/103/115	-
21	CL7	42	502	16	2/2/15/20	17/39/115/115	-
21	CL7	23	412	19	2/2/15/20	19/39/115/115	-
21	CL7	13	510	-	2/2/15/20	15/39/115/115	-
21	CL7	24	411	20	2/2/15/20	14/39/115/115	-
21	CL7	44	413	20	2/2/14/20	7/33/109/115	-
21	CL7	11	413	-	2/2/10/20	2/10/86/115	-
21	CL7	32	511	16	2/2/14/20	16/33/109/115	-
21	CL7	1C	510	3	2/2/15/20	22/39/115/115	-
26	LHG	2D	409	-	-	7/53/53/53	-
21	CL7	4D	404	4	2/2/13/20	13/31/107/115	-
21	CL7	4C	511	3	2/2/10/20	5/12/88/115	-
21	CL7	21	419	-	2/2/11/20	9/15/91/115	-
21	CL7	42	508	16	2/2/11/20	5/15/91/115	-
21	CL7	31	419	-	2/2/11/20	9/15/91/115	-
21	CL7	24	413	20	2/2/14/20	7/33/109/115	-
26	LHG	3B	623	-	-	3/49/49/53	-
21	CL7	34	409	-	2/2/14/20	17/33/109/115	-
25	SQD	42	523	-	-	0/36/56/69	0/1/1/1
22	PHO	2D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	42	504	-	2/2/11/20	6/15/91/115	-
21	CL7	11	409	18	2/2/11/20	6/15/91/115	-
21	CL7	21	416	-	2/2/10/20	4/10/86/115	-
23	8CT	24	402	-	-	4/29/63/63	0/2/2/2
21	CL7	22	513	16	2/2/11/20	8/15/91/115	-
23	8CT	14	402	-	-	4/29/63/63	0/2/2/2
21	CL7	14	410	20	2/2/11/20	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	33	513	-	2/2/11/20	9/15/91/115	-
25	SQD	22	521	-	-	7/45/65/69	0/1/1/1
22	PHO	1D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	4C	513	3	2/2/11/20	8/15/91/115	-
21	CL7	41	404	-	2/2/15/20	15/39/115/115	-
24	LMG	11	401	-	-	5/46/66/70	0/1/1/1
21	CL7	33	506	19	2/2/11/20	13/15/91/115	-
21	CL7	34	404	20	2/2/15/20	14/39/115/115	-
21	CL7	13	507	-	2/2/15/20	15/39/115/115	-
21	CL7	3B	610	-	2/2/15/20	11/39/115/115	-
21	CL7	13	517	19	2/2/12/20	9/21/97/115	-
21	CL7	3B	602	2	2/2/14/20	9/33/109/115	-
21	CL7	4C	502	3	2/2/14/20	12/33/109/115	-
21	CL7	13	515	-	2/2/10/20	0/10/86/115	-
21	CL7	3B	608	2	2/2/15/20	15/39/115/115	-
21	CL7	33	503	-	2/2/15/20	20/39/115/115	-
22	PHO	4A	402	-	-	3/37/103/103	0/5/6/6
32	ZEX	22	520	-	-	6/29/67/67	0/2/2/2
21	CL7	11	406	18	2/2/14/20	13/36/112/115	-
30	PL9	1D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	4C	503	3	2/2/15/20	19/39/115/115	-
24	LMG	2D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	21	413	-	2/2/10/20	2/10/86/115	-
21	CL7	43	410	19	2/2/15/20	17/39/115/115	-
21	CL7	21	406	18	2/2/14/20	13/36/112/115	-
21	CL7	4B	608	-	2/2/14/20	11/33/109/115	-
21	CL7	3C	502	3	2/2/14/20	12/33/109/115	-
32	ZEX	32	524	-	-	11/29/67/67	0/2/2/2
21	CL7	2B	609	2	2/2/15/20	15/39/115/115	-
21	CL7	13	501	19	2/2/15/20	21/39/115/115	-
21	CL7	21	410	-	2/2/15/20	17/39/115/115	-
21	CL7	41	414	18	2/2/10/20	3/10/86/115	-
23	8CT	1K	101	-	-	10/29/63/63	0/2/2/2
23	8CT	3K	101	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	22	501	16	2/2/15/20	17/39/115/115	-
21	CL7	2C	502	3	2/2/14/20	12/33/109/115	-
23	8CT	1B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	24	405	-	2/2/15/20	18/39/115/115	-
32	ZEX	41	422	-	-	6/29/67/67	0/2/2/2
24	LMG	3B	621	-	-	7/46/66/70	0/1/1/1
21	CL7	32	515	-	2/2/11/20	8/15/91/115	-
23	8CT	4B	618	-	-	7/29/63/63	0/2/2/2
21	CL7	23	403	19	2/2/13/20	12/31/107/115	-
21	CL7	44	405	-	2/2/15/20	18/39/115/115	-
21	CL7	2B	611	-	2/2/15/20	11/39/115/115	-
21	CL7	12	513	16	2/2/11/20	8/15/91/115	-
21	CL7	3C	512	3	2/2/10/20	4/10/86/115	-
26	LHG	3D	409	-	-	7/53/53/53	-

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(°)	Ideal(°)
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	11	420	CL7	6	0
21	23	415	CL7	2	0
21	42	515	CL7	2	0
21	23	407	CL7	5	0
21	24	406	CL7	13	0
32	24	419	ZEX	7	0
21	3B	603	CL7	6	0
21	42	511	CL7	7	0
21	44	407	CL7	6	0
21	4A	407	CL7	14	0
21	3B	612	CL7	3	0
21	42	516	CL7	6	0
21	2C	512	CL7	1	0
26	2B	624	LHG	6	0
21	42	513	CL7	6	0
21	24	415	CL7	4	0
21	32	518	CL7	10	0
21	11	412	CL7	2	0
24	4A	405	LMG	2	0
22	3D	408	PHO	4	0
31	1F	101	HEM	3	0
21	42	518	CL7	10	0
21	32	509	CL7	5	0
24	2B	622	LMG	5	0
21	4C	509	CL7	3	0
21	42	506	CL7	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	31	405	CL7	5	0
21	42	503	CL7	7	0
21	23	418	CL7	2	0
25	23	424	SQD	2	0
21	32	517	CL7	10	0
32	32	522	ZEX	17	0
25	3B	620	SQD	2	0
26	44	401	LHG	2	0
30	3D	407	PL9	7	0
21	43	418	CL7	2	0
21	12	512	CL7	8	0
32	23	401	ZEX	24	0
21	34	407	CL7	6	0
24	4B	622	LMG	6	0
26	24	401	LHG	2	0
21	32	502	CL7	8	0
21	34	406	CL7	13	0
25	2A	406	SQD	2	0
32	23	421	ZEX	10	0
21	33	515	CL7	2	0
21	1C	502	CL7	4	0
21	13	511	CL7	5	0
21	2B	606	CL7	7	0
32	43	421	ZEX	11	0
21	1D	404	CL7	6	0
21	22	511	CL7	8	0
25	41	423	SQD	1	0
21	4B	609	CL7	4	0
21	12	516	CL7	5	0
21	4C	512	CL7	1	0
32	24	403	ZEX	22	0
21	42	505	CL7	14	0
21	24	412	CL7	3	0
21	31	411	CL7	2	0
32	12	522	ZEX	18	0
21	41	418	CL7	6	0
21	11	411	CL7	2	0
21	4C	507	CL7	3	0
21	13	503	CL7	10	0
21	43	405	CL7	9	0
21	3A	403	CL7	2	0
21	23	402	CL7	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1B	612	CL7	3	0
21	13	502	CL7	7	0
21	33	505	CL7	18	0
25	3A	406	SQD	1	0
25	43	422	SQD	3	0
21	3C	503	CL7	8	0
21	31	418	CL7	7	0
32	41	421	ZEX	15	0
32	34	420	ZEX	10	0
21	43	402	CL7	9	0
21	32	512	CL7	7	0
21	31	413	CL7	6	0
21	33	516	CL7	5	0
21	13	504	CL7	8	0
21	2B	616	CL7	4	0
32	24	418	ZEX	10	0
32	44	418	ZEX	9	0
21	2C	507	CL7	5	0
26	4B	624	LHG	6	0
21	12	507	CL7	6	0
21	2B	607	CL7	6	0
21	4C	504	CL7	3	0
32	31	421	ZEX	15	0
21	2B	604	CL7	9	0
21	3C	501	CL7	4	0
21	43	404	CL7	11	0
21	43	419	CL7	3	0
21	24	404	CL7	6	0
21	3B	609	CL7	4	0
21	4B	615	CL7	2	0
21	23	411	CL7	4	0
21	11	417	CL7	3	0
25	23	422	SQD	4	0
21	2B	608	CL7	7	0
21	2C	501	CL7	5	0
21	44	411	CL7	8	0
21	31	409	CL7	3	0
21	41	402	CL7	10	0
21	4A	401	CL7	18	0
21	22	517	CL7	9	0
21	22	509	CL7	4	0
26	1D	409	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	21	418	CL7	7	0
21	22	510	CL7	6	0
21	21	414	CL7	8	0
24	31	401	LMG	3	0
21	44	412	CL7	2	0
21	43	412	CL7	5	0
21	3A	407	CL7	15	0
21	3D	404	CL7	6	0
21	33	508	CL7	14	0
21	41	409	CL7	4	0
21	42	512	CL7	7	0
32	34	403	ZEX	21	0
22	2A	402	PHO	3	0
21	23	405	CL7	8	0
21	1B	602	CL7	5	0
32	12	519	ZEX	3	0
32	21	421	ZEX	15	0
21	1C	512	CL7	1	0
21	13	509	CL7	9	0
23	2C	518	8CT	1	0
21	31	404	CL7	8	0
21	31	420	CL7	6	0
21	13	514	CL7	2	0
21	1B	609	CL7	4	0
21	11	418	CL7	6	0
21	12	518	CL7	11	0
21	2B	603	CL7	4	0
21	2A	407	CL7	14	0
21	23	410	CL7	10	0
21	4B	604	CL7	8	0
21	22	514	CL7	2	0
21	3A	401	CL7	19	0
32	24	420	ZEX	12	0
21	1B	613	CL7	2	0
21	23	406	CL7	17	0
23	4C	518	8CT	1	0
21	33	507	CL7	10	0
21	14	411	CL7	7	0
21	44	410	CL7	2	0
21	11	410	CL7	8	0
21	13	516	CL7	5	0
21	44	414	CL7	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	31	412	CL7	2	0
21	33	511	CL7	6	0
21	3B	607	CL7	8	0
32	11	421	ZEX	13	0
21	34	412	CL7	4	0
21	13	513	CL7	12	0
21	3B	604	CL7	10	0
21	33	502	CL7	7	0
21	21	402	CL7	10	0
25	2B	621	SQD	2	0
21	31	402	CL7	10	0
21	21	420	CL7	6	0
24	3A	405	LMG	2	0
21	23	417	CL7	5	0
21	1C	501	CL7	3	0
21	3C	506	CL7	4	0
21	1B	608	CL7	4	0
31	4F	101	HEM	4	0
32	22	524	ZEX	16	0
21	21	409	CL7	4	0
21	1B	605	CL7	7	0
25	1B	620	SQD	3	0
21	22	512	CL7	8	0
21	24	417	CL7	4	0
21	44	406	CL7	12	0
21	3C	504	CL7	3	0
32	13	520	ZEX	11	0
32	42	522	ZEX	19	0
21	2B	610	CL7	4	0
21	3B	606	CL7	5	0
21	3B	615	CL7	4	0
22	4D	408	PHO	3	0
21	2C	505	CL7	6	0
21	24	410	CL7	2	0
23	3C	515	8CT	1	0
21	3C	509	CL7	4	0
21	23	408	CL7	9	0
21	43	417	CL7	6	0
21	14	405	CL7	7	0
26	2B	626	LHG	2	0
21	43	415	CL7	2	0
21	1A	407	CL7	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	12	520	ZEX	33	0
21	44	408	CL7	4	0
21	3C	510	CL7	4	0
21	11	408	CL7	7	0
23	4C	515	8CT	1	0
23	1C	518	8CT	1	0
32	12	524	ZEX	16	0
21	44	409	CL7	2	0
21	1D	405	CL7	2	0
21	13	512	CL7	6	0
21	2C	509	CL7	2	0
25	21	423	SQD	1	0
26	4B	626	LHG	2	0
21	34	405	CL7	7	0
24	1A	405	LMG	2	0
30	4D	407	PL9	7	0
22	3A	402	PHO	3	0
23	1C	515	8CT	1	0
21	24	409	CL7	2	0
25	42	521	SQD	2	0
21	12	502	CL7	7	0
21	1B	607	CL7	8	0
32	14	418	ZEX	9	0
32	21	422	ZEX	21	0
21	42	514	CL7	2	0
26	3B	625	LHG	1	0
21	23	409	CL7	14	0
26	34	401	LHG	2	0
21	14	409	CL7	2	0
21	43	411	CL7	6	0
21	31	417	CL7	3	0
21	1A	401	CL7	18	0
32	42	520	ZEX	31	0
32	44	419	ZEX	9	0
21	32	508	CL7	3	0
21	43	403	CL7	8	0
32	44	420	ZEX	12	0
21	43	414	CL7	13	0
24	4D	410	LMG	1	0
21	3C	507	CL7	4	0
21	4C	508	CL7	5	0
21	41	407	CL7	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	13	522	ZEX	26	0
21	32	506	CL7	2	0
21	44	415	CL7	4	0
21	12	509	CL7	5	0
21	41	420	CL7	6	0
21	24	408	CL7	4	0
24	1D	410	LMG	1	0
32	33	525	ZEX	24	0
32	22	522	ZEX	18	0
21	1C	508	CL7	3	0
25	4B	621	SQD	3	0
21	43	416	CL7	2	0
25	32	521	SQD	1	0
25	33	521	SQD	4	0
27	2B	625	DGD	2	0
21	4C	505	CL7	6	0
32	44	403	ZEX	21	0
21	1C	506	CL7	5	0
21	23	404	CL7	11	0
24	1B	621	LMG	5	0
21	41	403	CL7	5	0
21	23	416	CL7	2	0
21	4B	613	CL7	6	0
32	11	422	ZEX	21	0
26	23	425	LHG	1	0
27	3C	516	DGD	5	0
27	2C	516	DGD	4	0
21	41	408	CL7	8	0
21	1B	614	CL7	2	0
21	11	407	CL7	3	0
21	3B	613	CL7	2	0
21	32	505	CL7	15	0
32	33	520	ZEX	11	0
21	43	406	CL7	18	0
21	4B	605	CL7	8	0
21	34	413	CL7	4	0
21	3D	405	CL7	2	0
21	43	409	CL7	14	0
32	14	419	ZEX	8	0
32	43	401	ZEX	24	0
21	14	413	CL7	5	0
26	13	524	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1B	611	CL7	4	0
21	1C	505	CL7	6	0
21	21	407	CL7	3	0
21	33	512	CL7	7	0
21	24	407	CL7	6	0
21	2A	401	CL7	17	0
21	12	501	CL7	5	0
21	14	408	CL7	4	0
21	41	417	CL7	6	0
21	22	515	CL7	3	0
21	23	414	CL7	12	0
21	31	410	CL7	7	0
31	2F	101	HEM	4	0
21	32	510	CL7	6	0
32	13	519	ZEX	16	0
21	22	516	CL7	6	0
21	11	414	CL7	2	0
21	31	406	CL7	13	0
21	4B	607	CL7	4	0
21	13	518	CL7	3	0
21	21	403	CL7	5	0
24	3D	410	LMG	1	0
21	1B	615	CL7	4	0
26	43	425	LHG	1	0
21	43	408	CL7	10	0
21	13	506	CL7	5	0
21	3C	513	CL7	3	0
21	14	406	CL7	13	0
21	22	518	CL7	11	0
21	33	501	CL7	8	0
32	33	519	ZEX	17	0
21	21	408	CL7	7	0
24	41	401	LMG	2	0
31	3F	101	HEM	3	0
21	3B	605	CL7	6	0
21	22	506	CL7	3	0
21	4B	606	CL7	6	0
32	42	524	ZEX	17	0
21	2B	613	CL7	5	0
21	2C	508	CL7	4	0
21	44	404	CL7	6	0
27	1C	516	DGD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	32	507	CL7	5	0
21	22	505	CL7	17	0
21	21	405	CL7	4	0
32	23	423	ZEX	26	0
21	2C	506	CL7	3	0
21	14	404	CL7	6	0
21	1B	603	CL7	7	0
21	32	514	CL7	2	0
21	1C	509	CL7	3	0
21	41	411	CL7	2	0
27	1B	624	DGD	2	0
32	42	519	ZEX	3	0
21	42	501	CL7	6	0
21	24	414	CL7	3	0
23	2C	515	8CT	1	0
21	31	408	CL7	7	0
21	1C	507	CL7	5	0
21	34	414	CL7	4	0
21	13	508	CL7	15	0
21	2D	404	CL7	7	0
25	11	423	SQD	1	0
26	1B	623	LHG	6	0
21	22	507	CL7	5	0
21	13	505	CL7	17	0
21	41	412	CL7	2	0
21	1B	604	CL7	9	0
21	32	504	CL7	3	0
21	14	414	CL7	4	0
21	22	508	CL7	3	0
25	33	523	SQD	1	0
25	43	424	SQD	2	0
21	1C	504	CL7	3	0
21	12	508	CL7	4	0
21	14	407	CL7	6	0
21	12	514	CL7	2	0
25	13	521	SQD	4	0
26	4D	409	LHG	3	0
21	12	506	CL7	2	0
21	34	417	CL7	4	0
21	14	412	CL7	3	0
21	1A	403	CL7	2	0
32	23	420	ZEX	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	14	420	ZEX	10	0
21	44	417	CL7	4	0
21	4C	510	CL7	3	0
24	21	401	LMG	2	0
21	34	411	CL7	8	0
21	34	410	CL7	2	0
32	32	519	ZEX	4	0
21	22	504	CL7	3	0
30	2D	407	PL9	7	0
21	2C	504	CL7	3	0
21	2B	614	CL7	2	0
21	43	407	CL7	5	0
21	31	416	CL7	1	0
21	31	414	CL7	8	0
21	2B	615	CL7	2	0
21	4A	403	CL7	2	0
32	43	423	ZEX	27	0
21	33	518	CL7	3	0
21	4B	610	CL7	4	0
26	33	524	LHG	1	0
21	4C	506	CL7	4	0
21	41	405	CL7	4	0
32	34	418	ZEX	9	0
32	33	522	ZEX	25	0
21	4B	614	CL7	2	0
21	4B	603	CL7	3	0
21	2C	510	CL7	4	0
21	3C	508	CL7	3	0
21	11	405	CL7	4	0
21	32	516	CL7	5	0
32	14	403	ZEX	22	0
22	1A	402	PHO	3	0
21	14	415	CL7	4	0
25	12	521	SQD	2	0
21	22	502	CL7	7	0
21	32	501	CL7	6	0
21	4B	611	CL7	1	0
25	1A	406	SQD	3	0
21	33	514	CL7	2	0
21	4C	501	CL7	4	0
21	34	415	CL7	4	0
21	31	407	CL7	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	3B	624	DGD	2	0
21	1C	511	CL7	1	0
21	14	417	CL7	4	0
32	43	420	ZEX	17	0
21	12	517	CL7	8	0
21	12	515	CL7	3	0
21	4B	616	CL7	4	0
21	32	513	CL7	6	0
21	43	413	CL7	8	0
21	2B	612	CL7	4	0
21	1C	513	CL7	3	0
21	3C	511	CL7	1	0
21	12	510	CL7	6	0
32	31	422	ZEX	22	0
25	4A	406	SQD	2	0
25	31	423	SQD	1	0
21	31	403	CL7	5	0
27	4C	516	DGD	4	0
21	21	412	CL7	2	0
21	11	404	CL7	7	0
32	32	520	ZEX	30	0
21	1B	606	CL7	5	0
21	42	509	CL7	7	0
21	11	403	CL7	4	0
26	14	401	LHG	2	0
21	2D	405	CL7	2	0
21	32	503	CL7	9	0
21	2C	511	CL7	1	0
21	21	417	CL7	5	0
21	1C	503	CL7	7	0
21	3B	614	CL7	2	0
21	12	511	CL7	8	0
21	21	404	CL7	8	0
21	3C	505	CL7	5	0
21	42	510	CL7	7	0
21	1B	610	CL7	3	0
21	41	413	CL7	6	0
27	4B	625	DGD	2	0
24	2A	405	LMG	2	0
21	41	416	CL7	1	0
21	41	406	CL7	14	0
21	21	411	CL7	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2C	513	CL7	3	0
21	4D	405	CL7	2	0
21	33	517	CL7	2	0
21	11	402	CL7	10	0
32	34	419	ZEX	8	0
21	12	505	CL7	15	0
21	33	510	CL7	5	0
21	23	419	CL7	3	0
32	22	519	ZEX	3	0
21	3B	611	CL7	5	0
21	22	503	CL7	5	0
25	13	523	SQD	2	0
21	2C	503	CL7	7	0
21	12	503	CL7	9	0
21	34	408	CL7	4	0
23	3C	518	8CT	1	0
21	42	507	CL7	5	0
21	42	517	CL7	10	0
21	33	504	CL7	9	0
21	41	410	CL7	6	0
32	13	525	ZEX	24	0
21	4B	612	CL7	4	0
21	33	509	CL7	8	0
21	2B	605	CL7	7	0
21	11	416	CL7	1	0
21	12	504	CL7	3	0
21	23	413	CL7	7	0
26	1B	625	LHG	1	0
21	2A	403	CL7	2	0
21	42	502	CL7	7	0
21	23	412	CL7	5	0
21	13	510	CL7	6	0
21	24	411	CL7	7	0
21	44	413	CL7	4	0
21	11	413	CL7	6	0
21	32	511	CL7	9	0
21	1C	510	CL7	4	0
26	2D	409	LHG	4	0
21	4D	404	CL7	7	0
21	4C	511	CL7	1	0
21	42	508	CL7	3	0
21	24	413	CL7	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	3B	623	LHG	6	0
21	34	409	CL7	2	0
22	2D	408	PHO	3	0
21	42	504	CL7	3	0
21	11	409	CL7	3	0
21	21	416	CL7	1	0
21	22	513	CL7	6	0
21	14	410	CL7	2	0
21	33	513	CL7	12	0
25	22	521	SQD	2	0
22	1D	408	PHO	4	0
21	4C	513	CL7	3	0
21	41	404	CL7	8	0
24	11	401	LMG	2	0
21	33	506	CL7	5	0
21	34	404	CL7	5	0
21	13	507	CL7	10	0
21	3B	610	CL7	1	0
21	13	517	CL7	2	0
21	3B	602	CL7	4	0
21	4C	502	CL7	3	0
21	13	515	CL7	2	0
21	3B	608	CL7	4	0
21	33	503	CL7	10	0
22	4A	402	PHO	3	0
32	22	520	ZEX	29	0
21	11	406	CL7	12	0
30	1D	407	PL9	7	0
21	4C	503	CL7	8	0
24	2D	410	LMG	1	0
21	21	413	CL7	6	0
21	43	410	CL7	8	0
21	21	406	CL7	13	0
21	4B	608	CL7	8	0
21	3C	502	CL7	3	0
32	32	524	ZEX	16	0
21	2B	609	CL7	4	0
21	13	501	CL7	8	0
21	21	410	CL7	7	0
21	41	414	CL7	2	0
21	22	501	CL7	7	0
21	2C	502	CL7	4	0

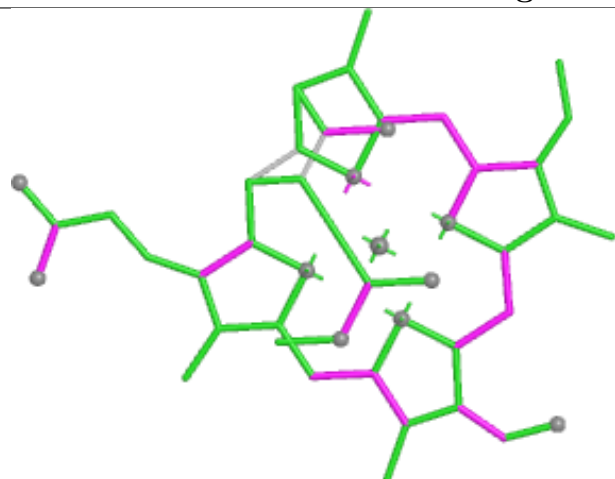
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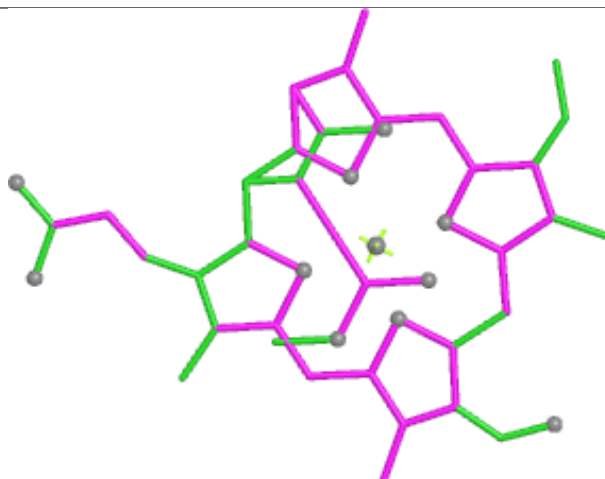
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	24	405	CL7	6	0
32	41	422	ZEX	23	0
24	3B	621	LMG	6	0
21	32	515	CL7	2	0
21	23	403	CL7	7	0
21	44	405	CL7	8	0
21	2B	611	CL7	3	0
21	12	513	CL7	6	0
21	3C	512	CL7	1	0
26	3D	409	LHG	3	0

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 than 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.

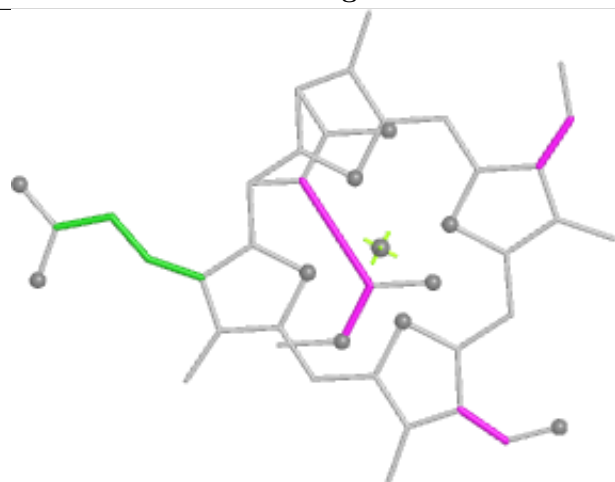
Ligand CL7 11 420



Bond lengths



Bond angles

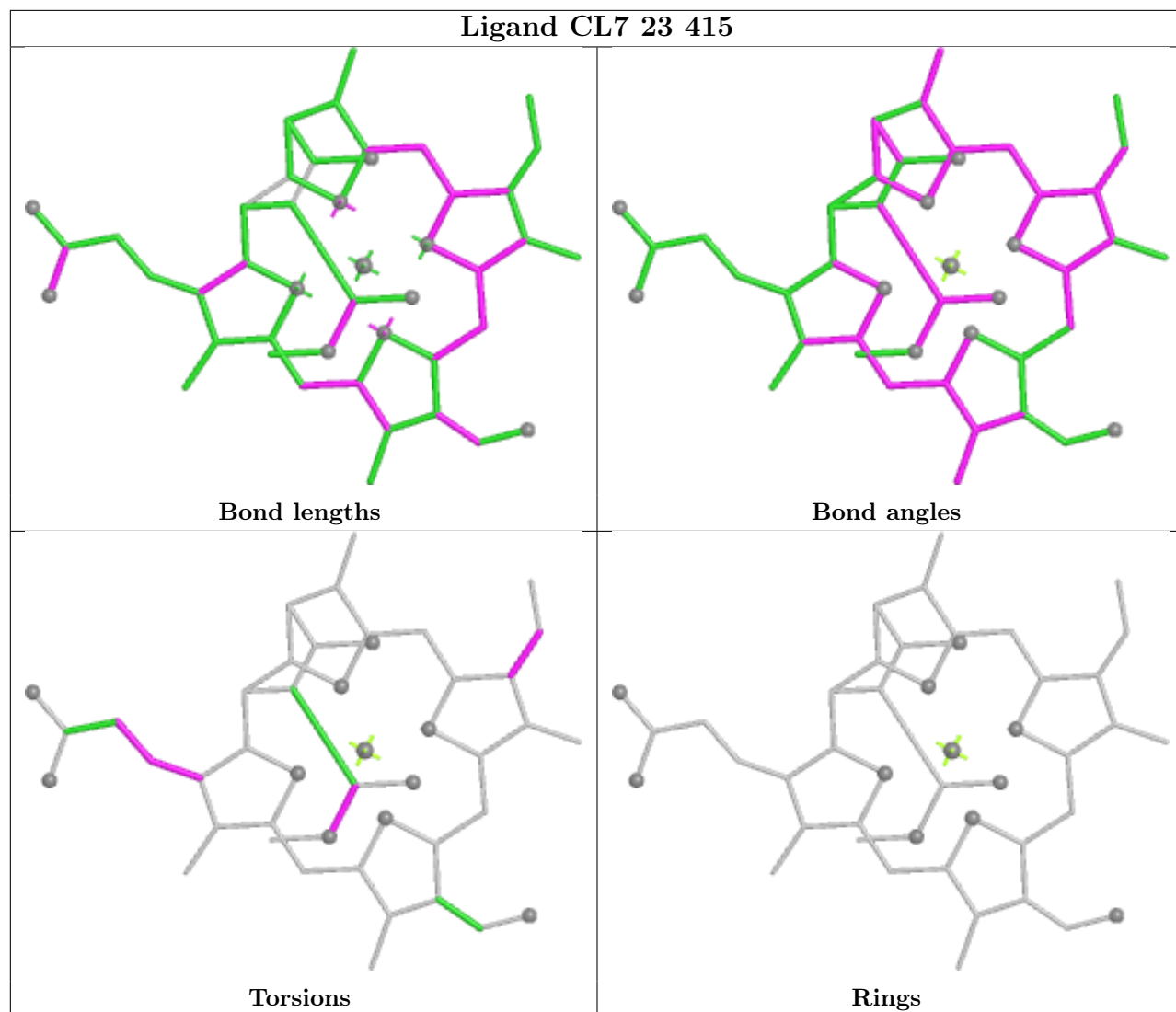


Torsions

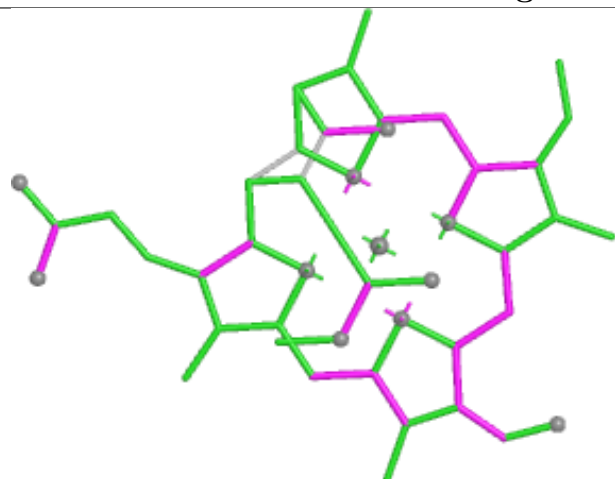


Rings

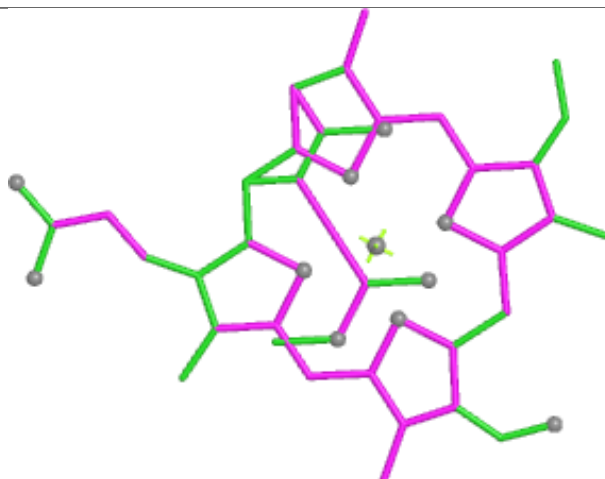
Ligand CL7 23 415



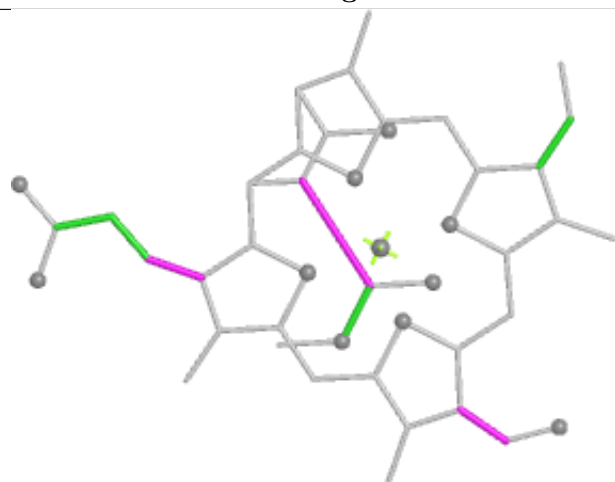
Ligand CL7 42 515



Bond lengths



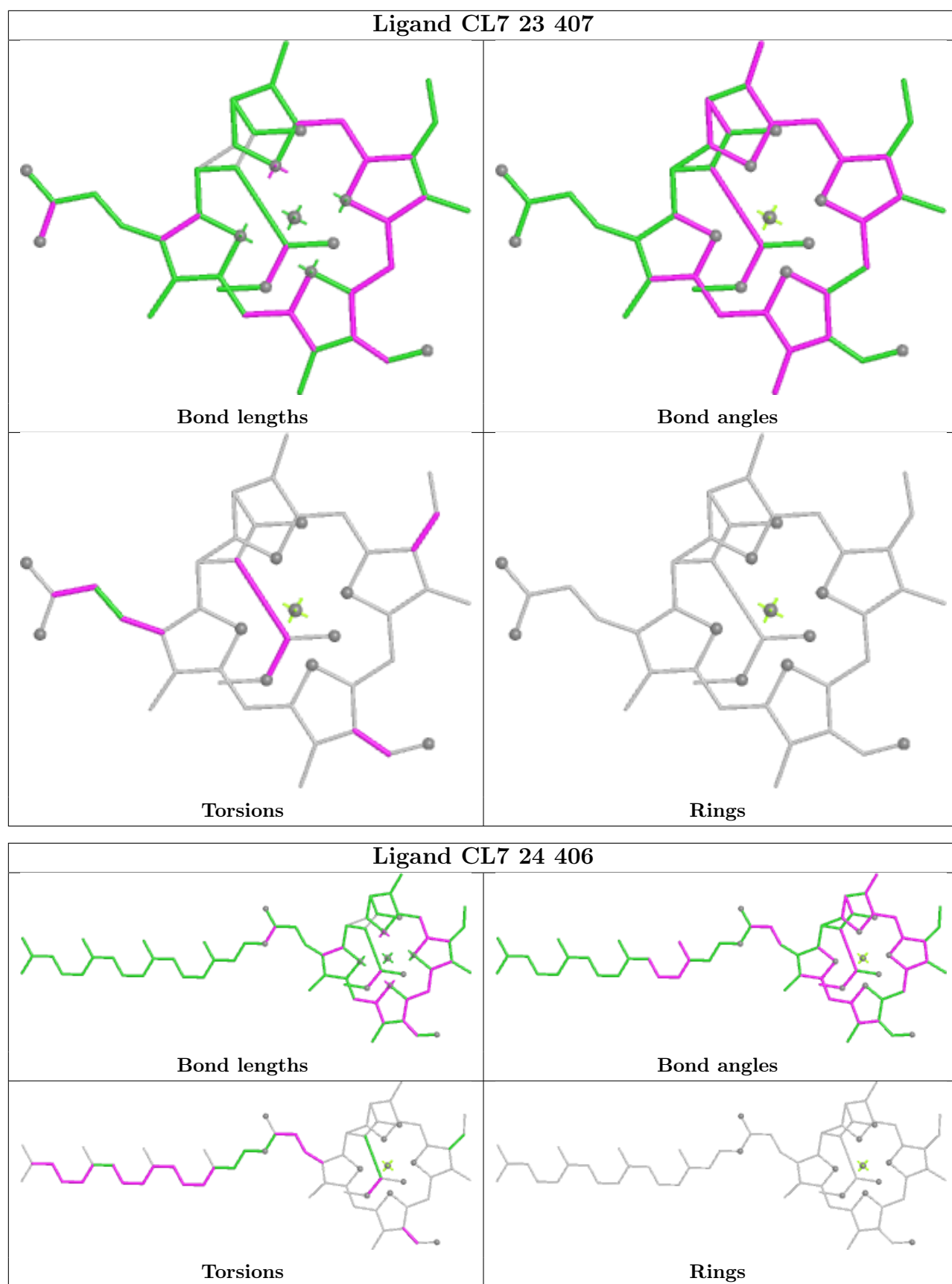
Bond angles

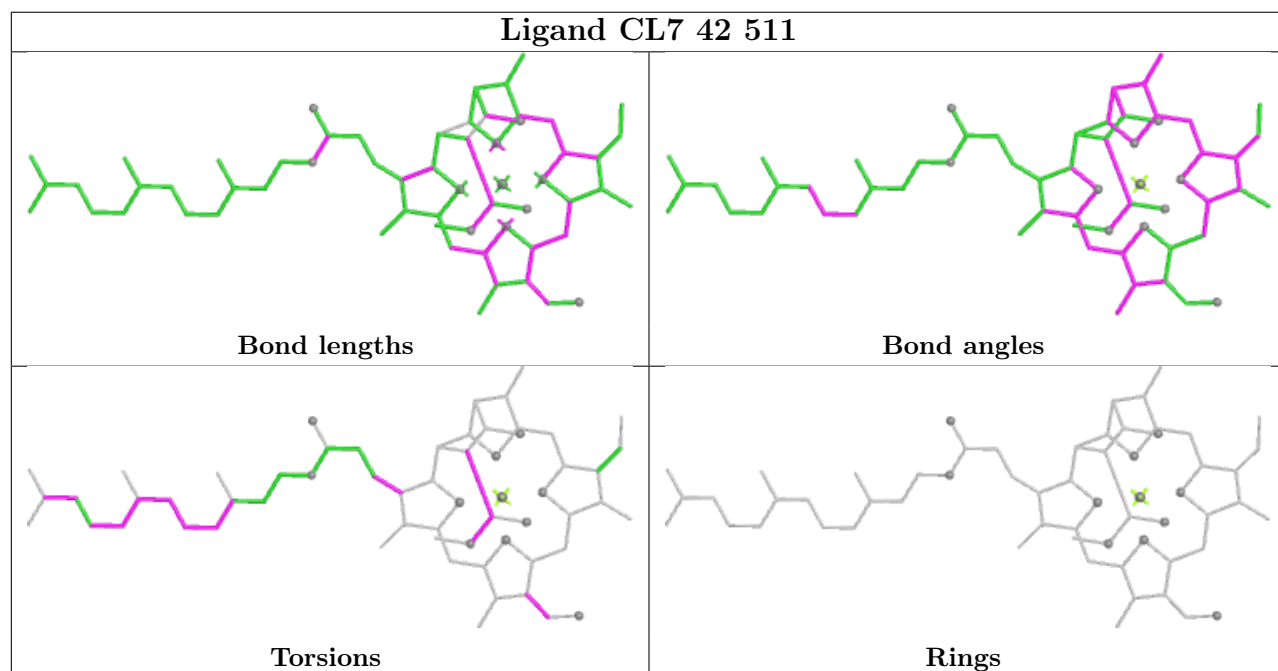
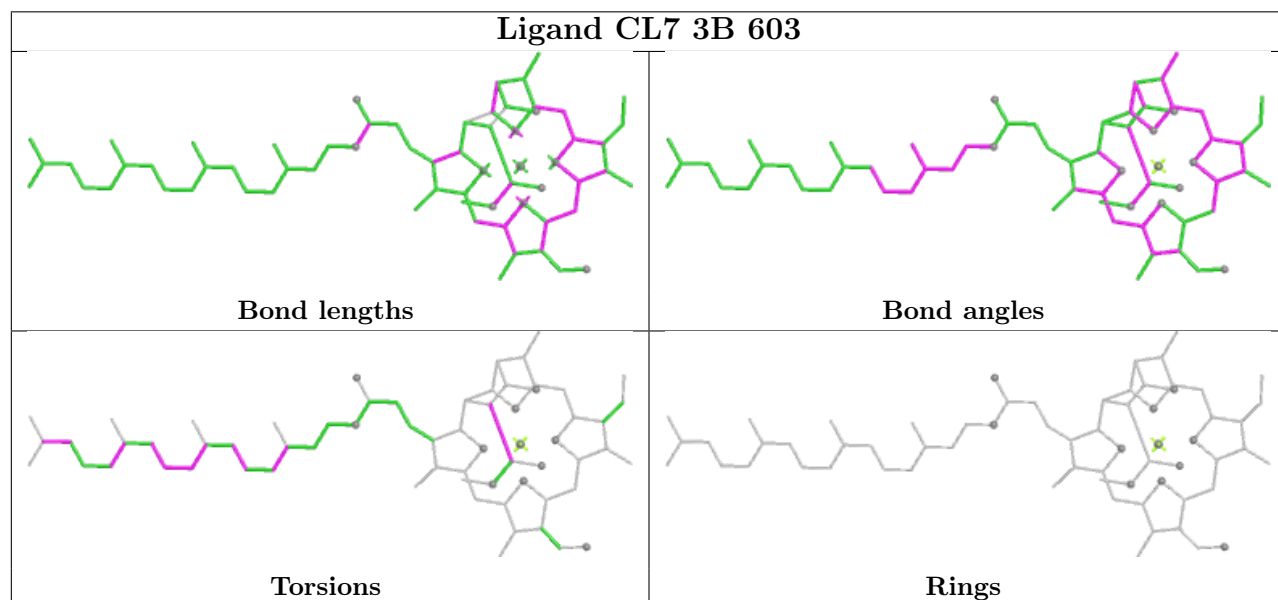
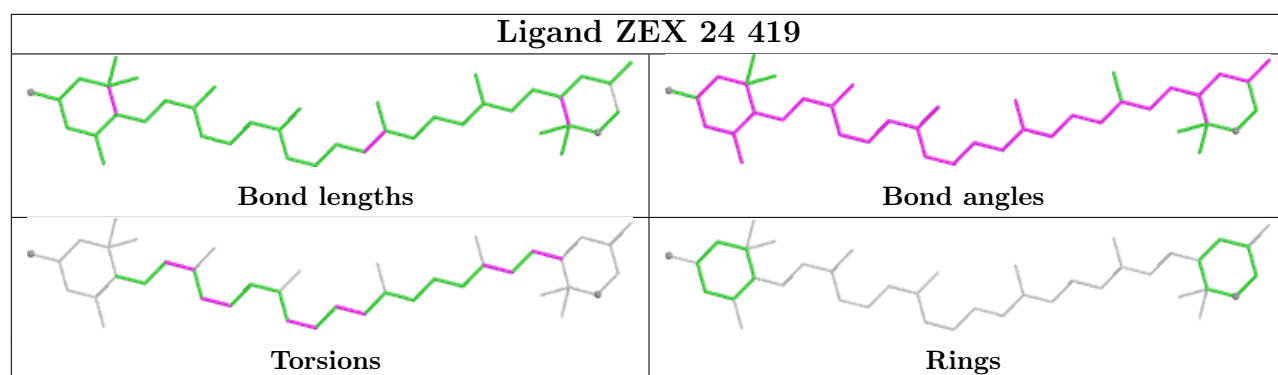


Torsions

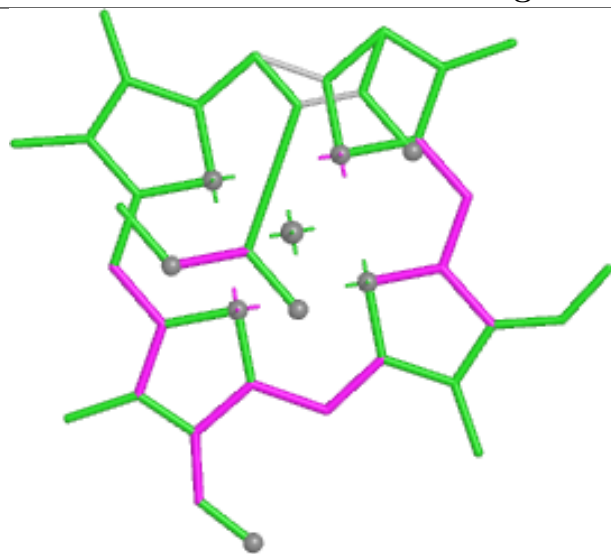


Rings

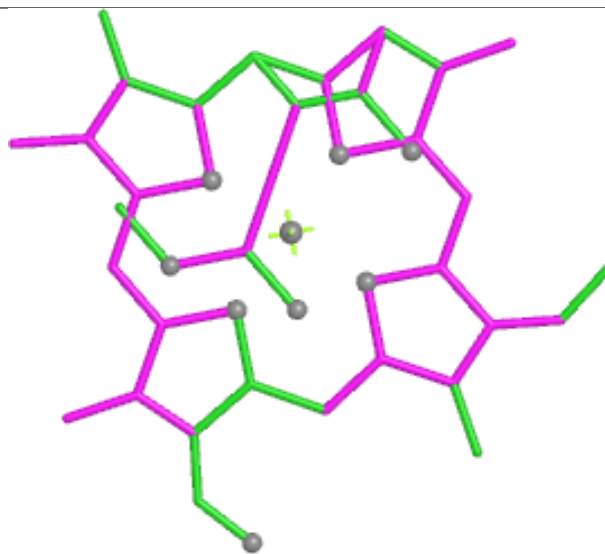




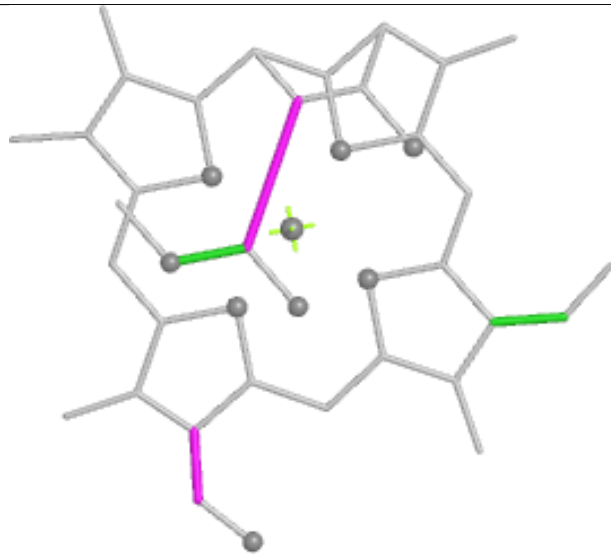
Ligand CL7 44 407



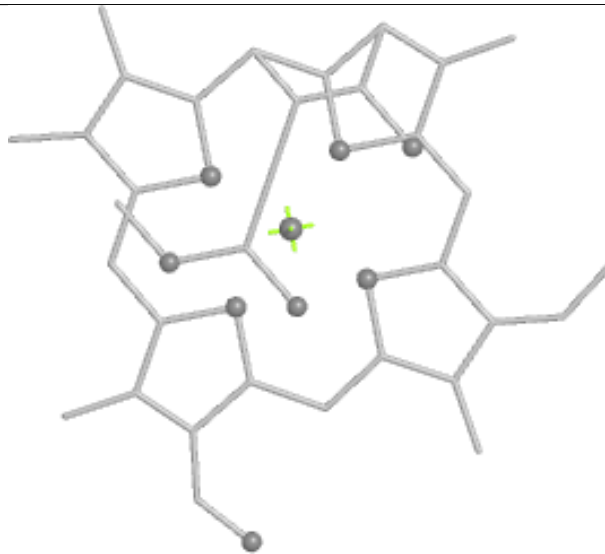
Bond lengths



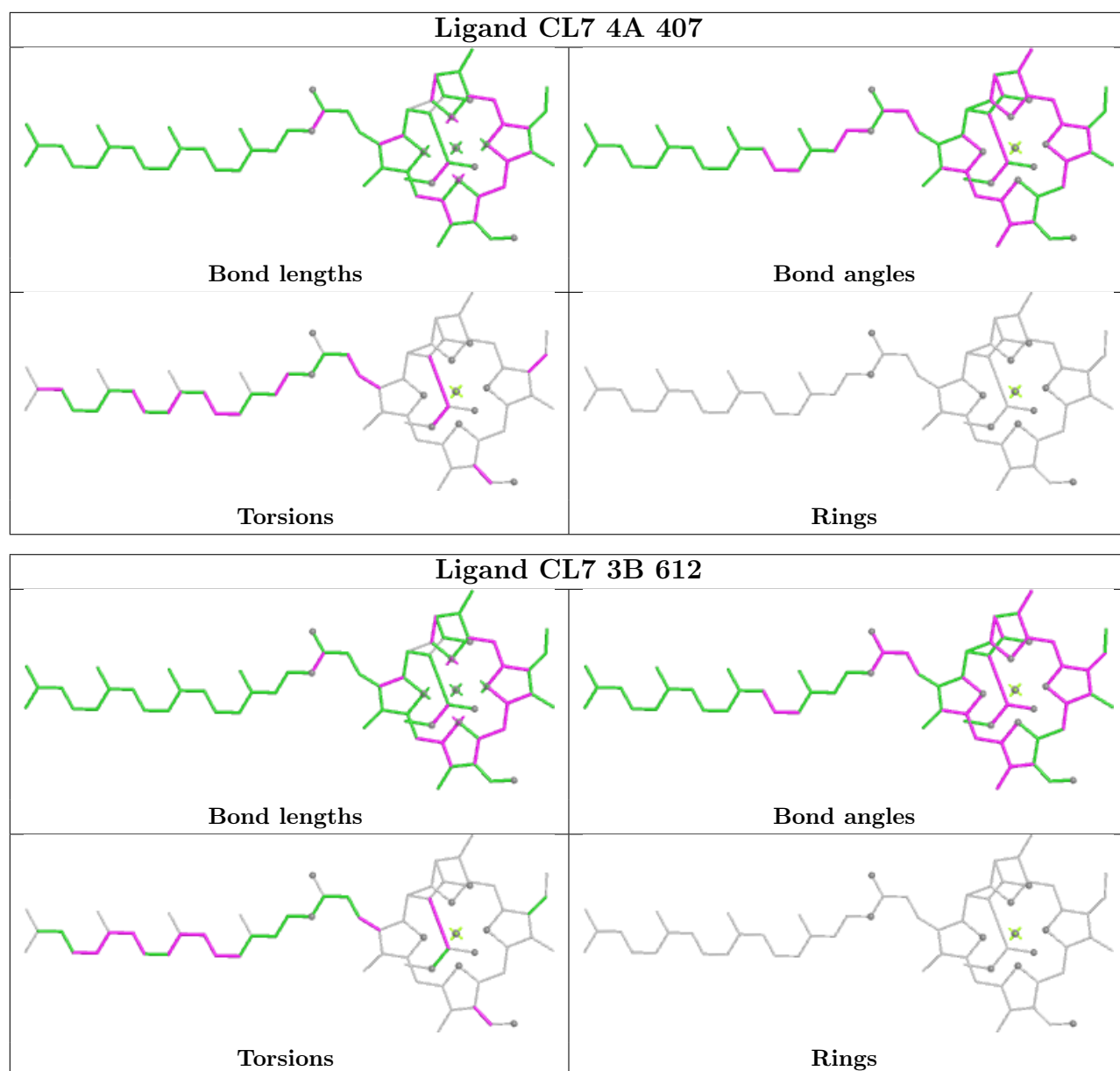
Bond angles

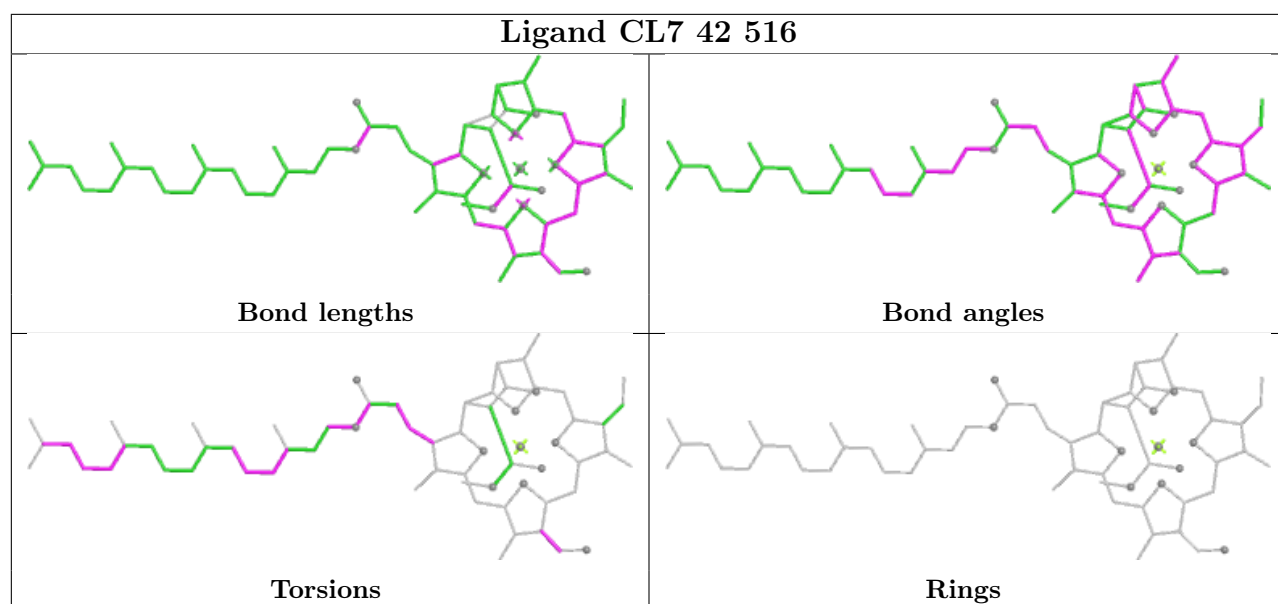


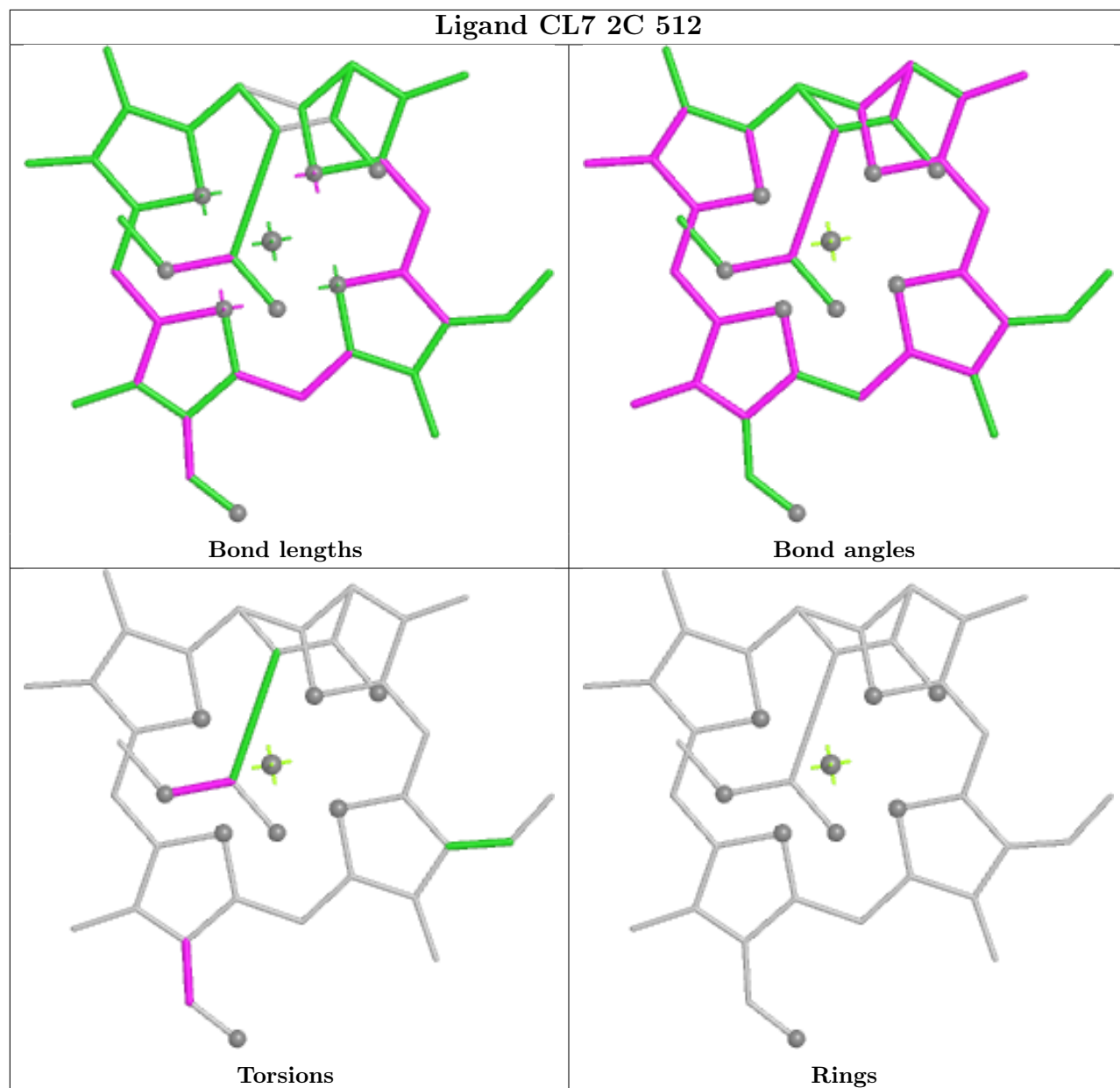
Torsions

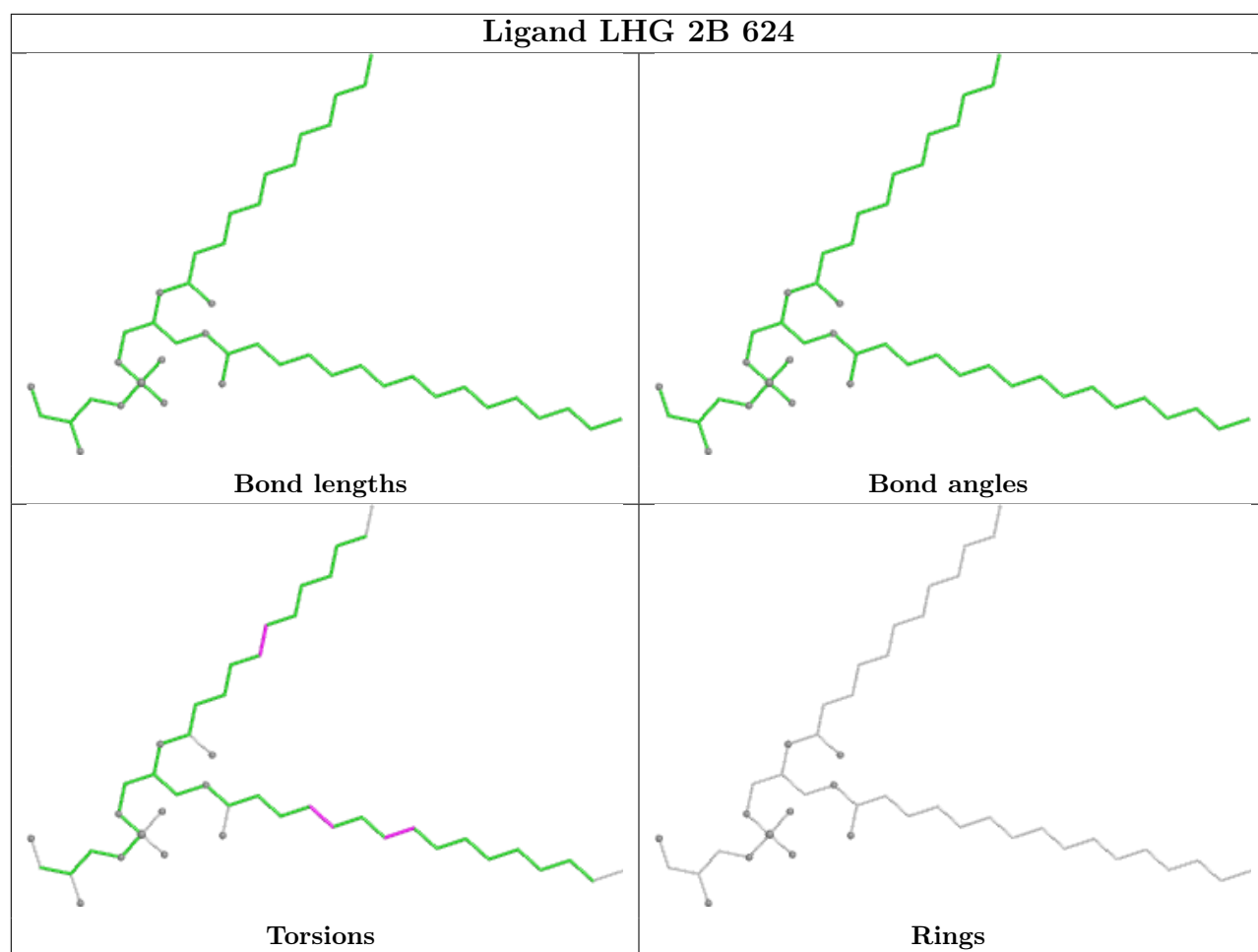


Rings

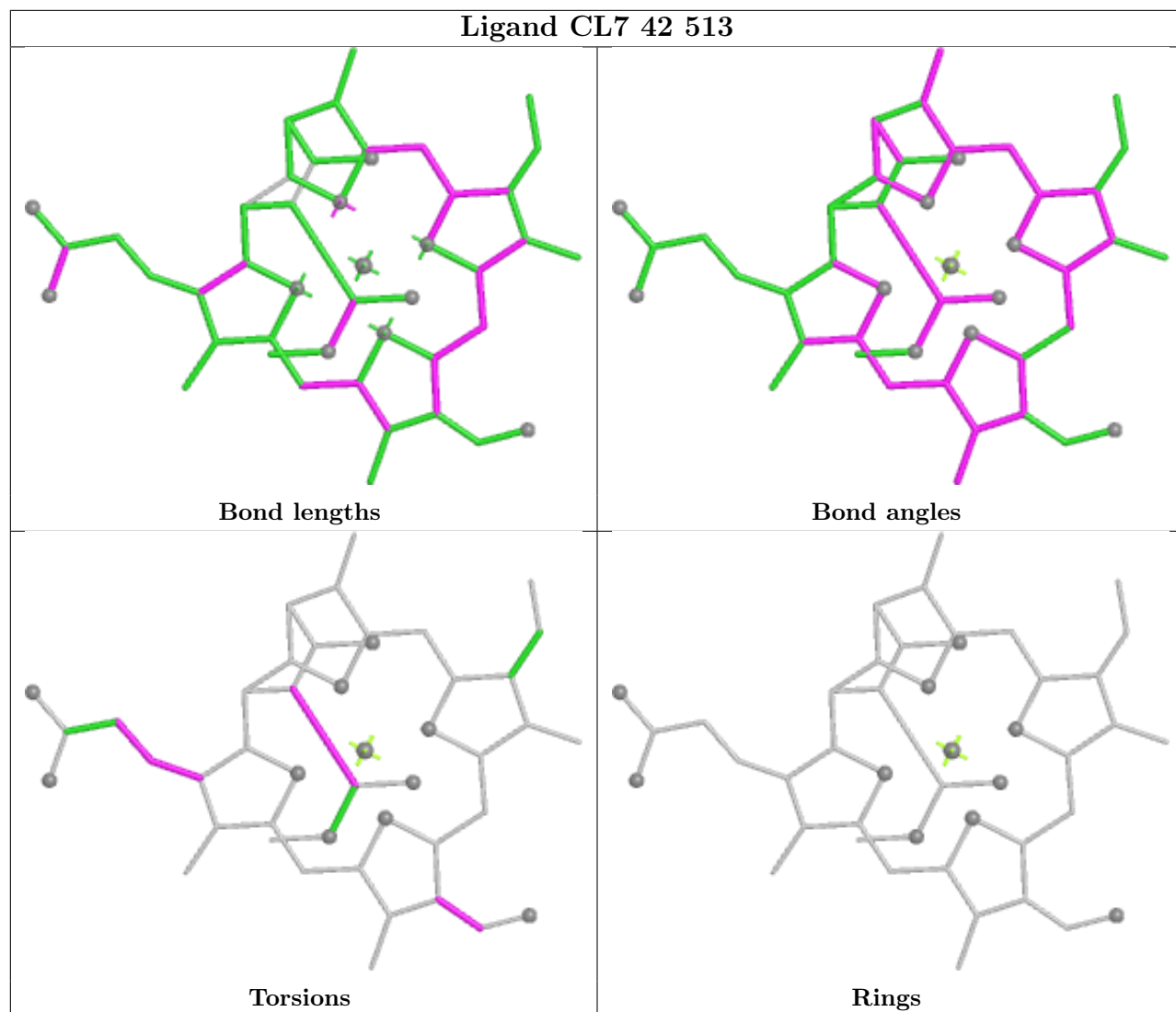


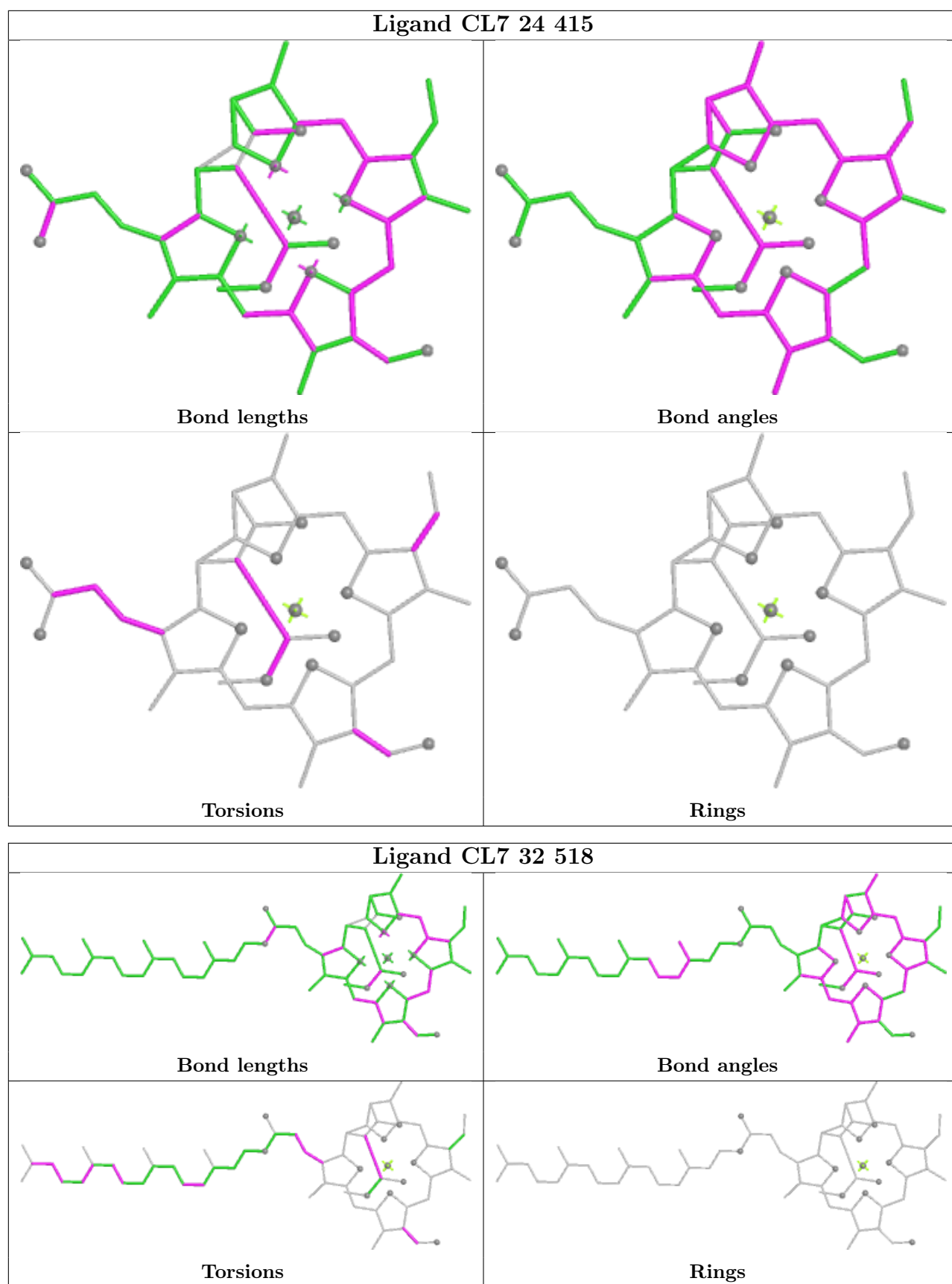


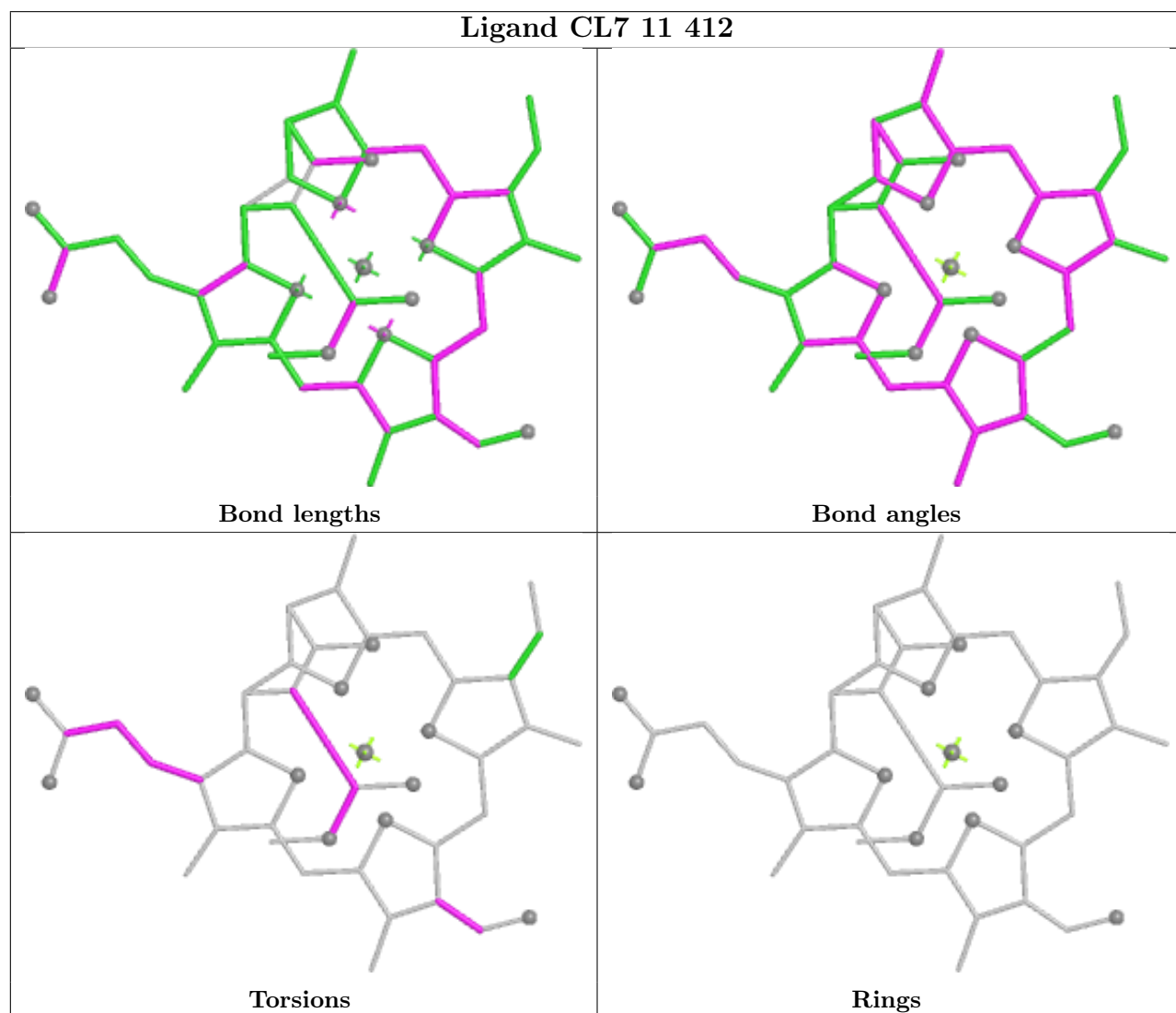
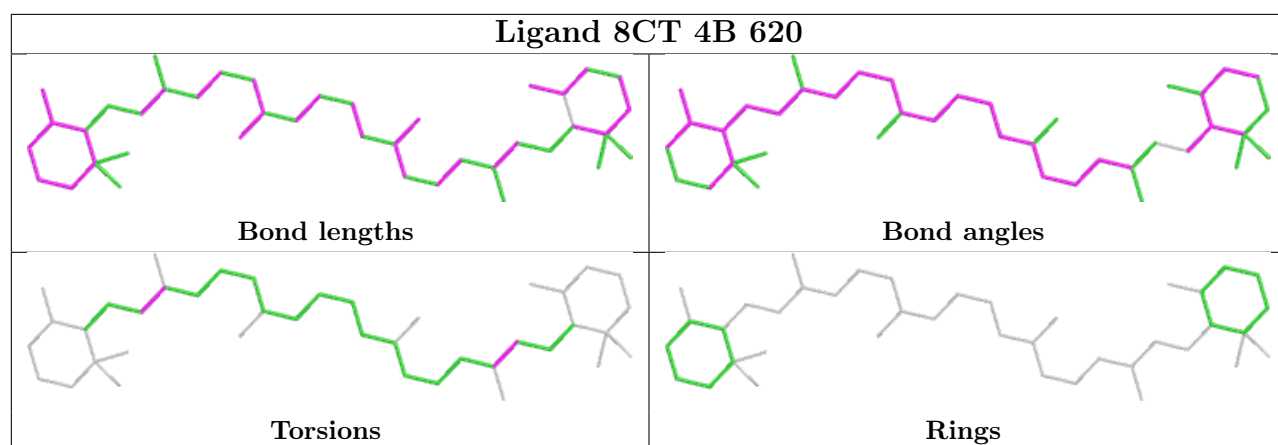


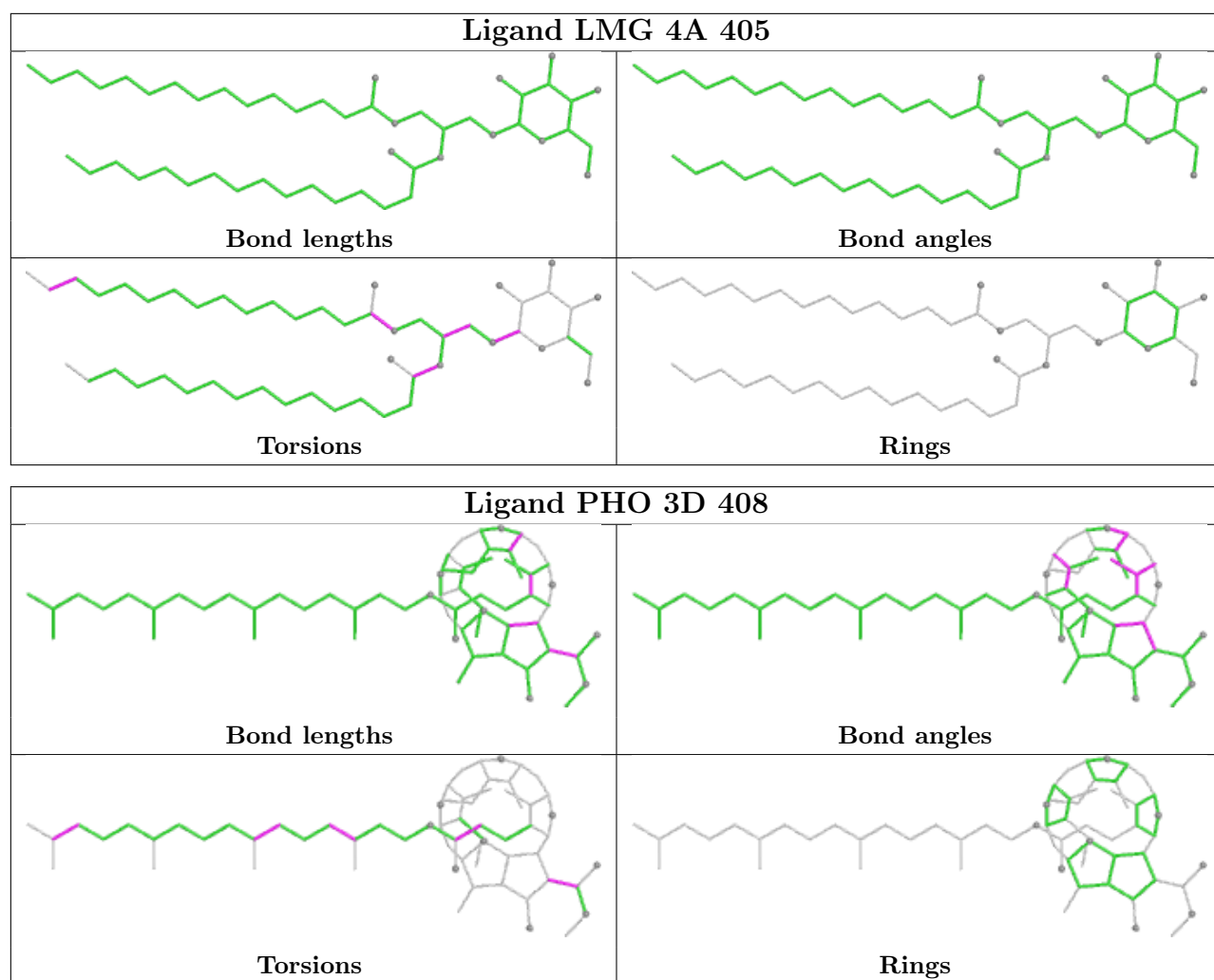


Ligand CL7 42 513

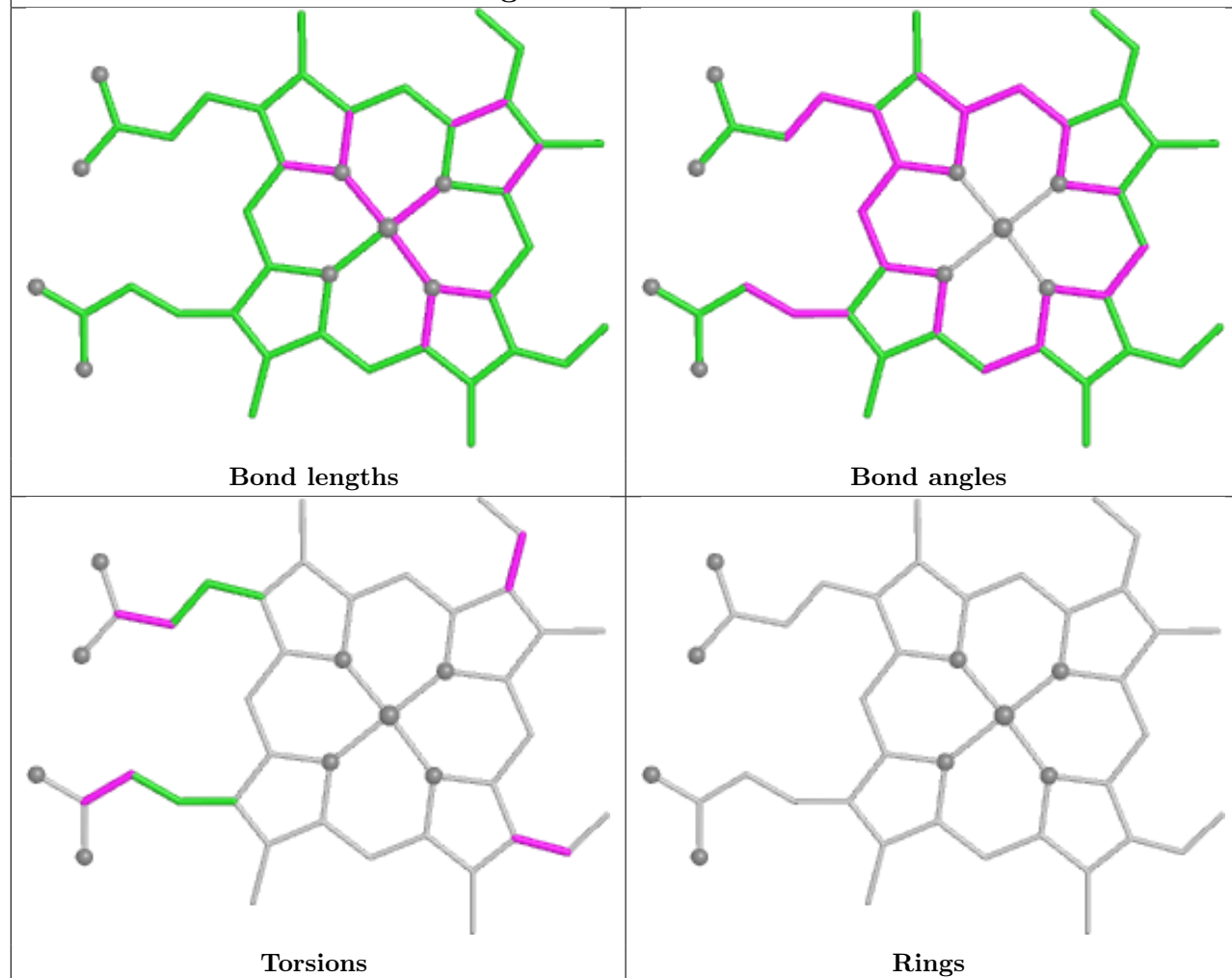




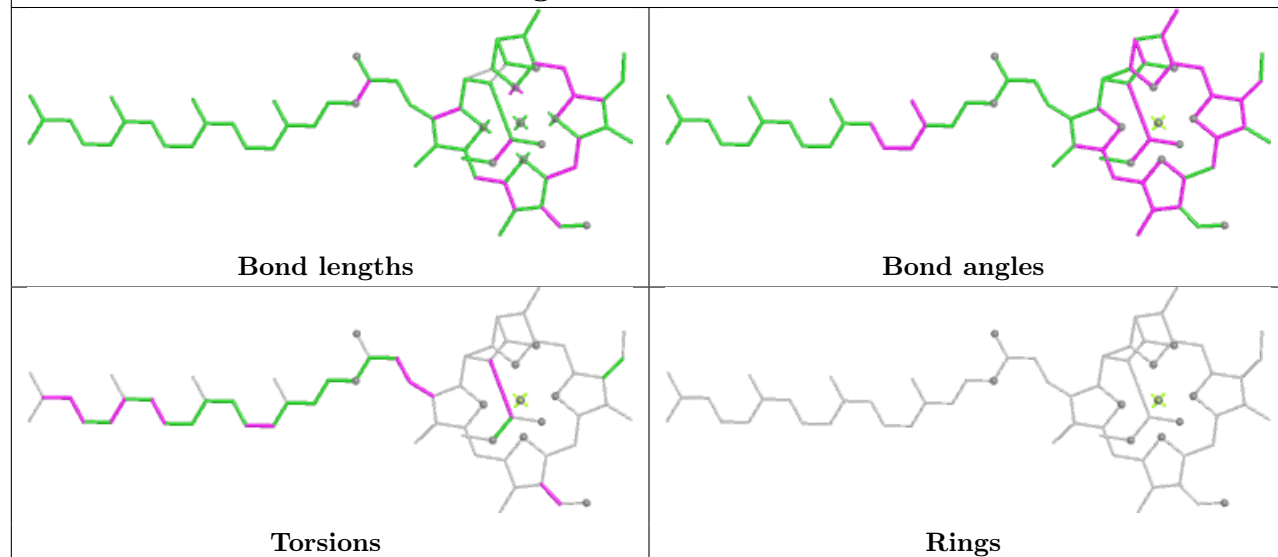


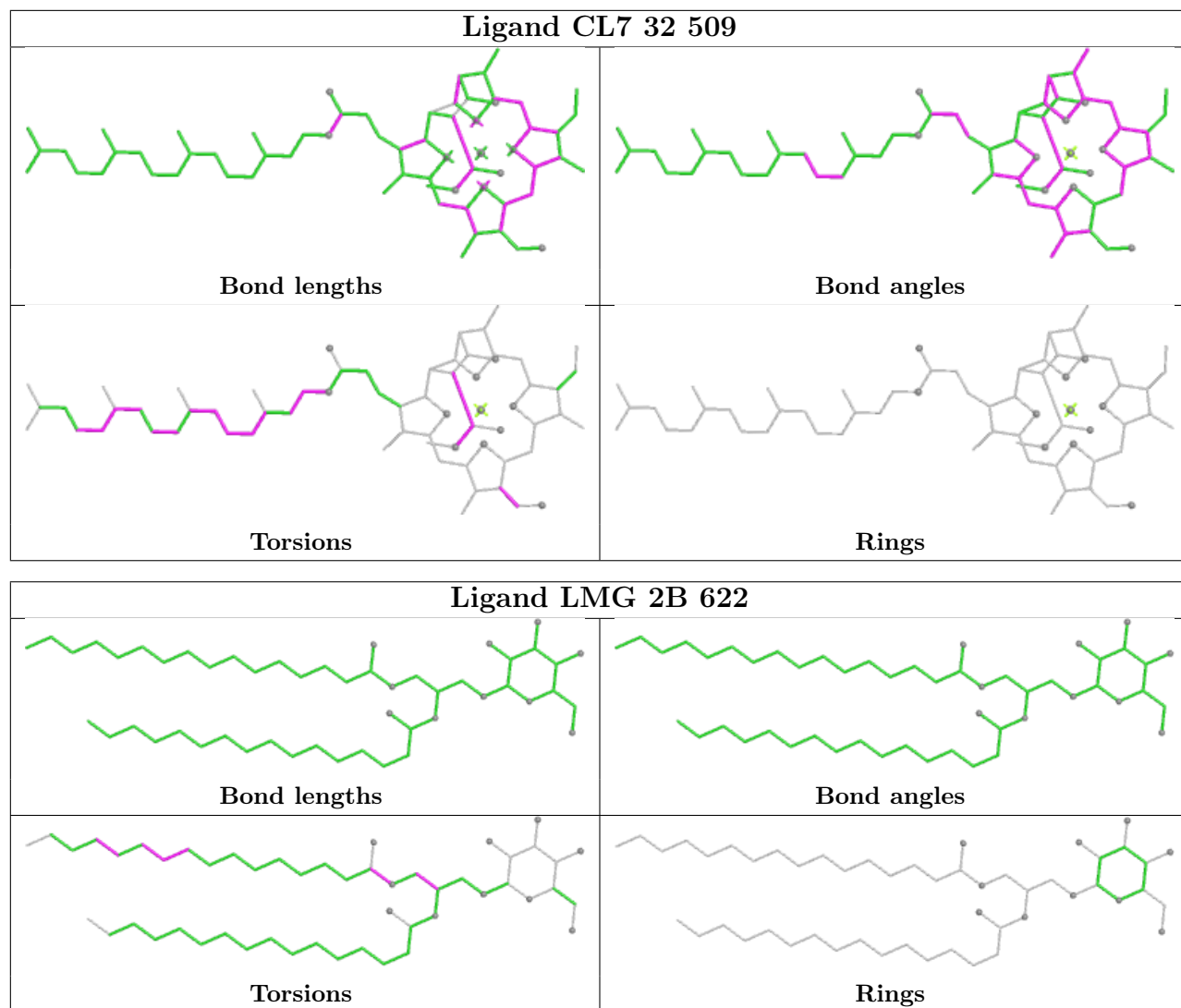


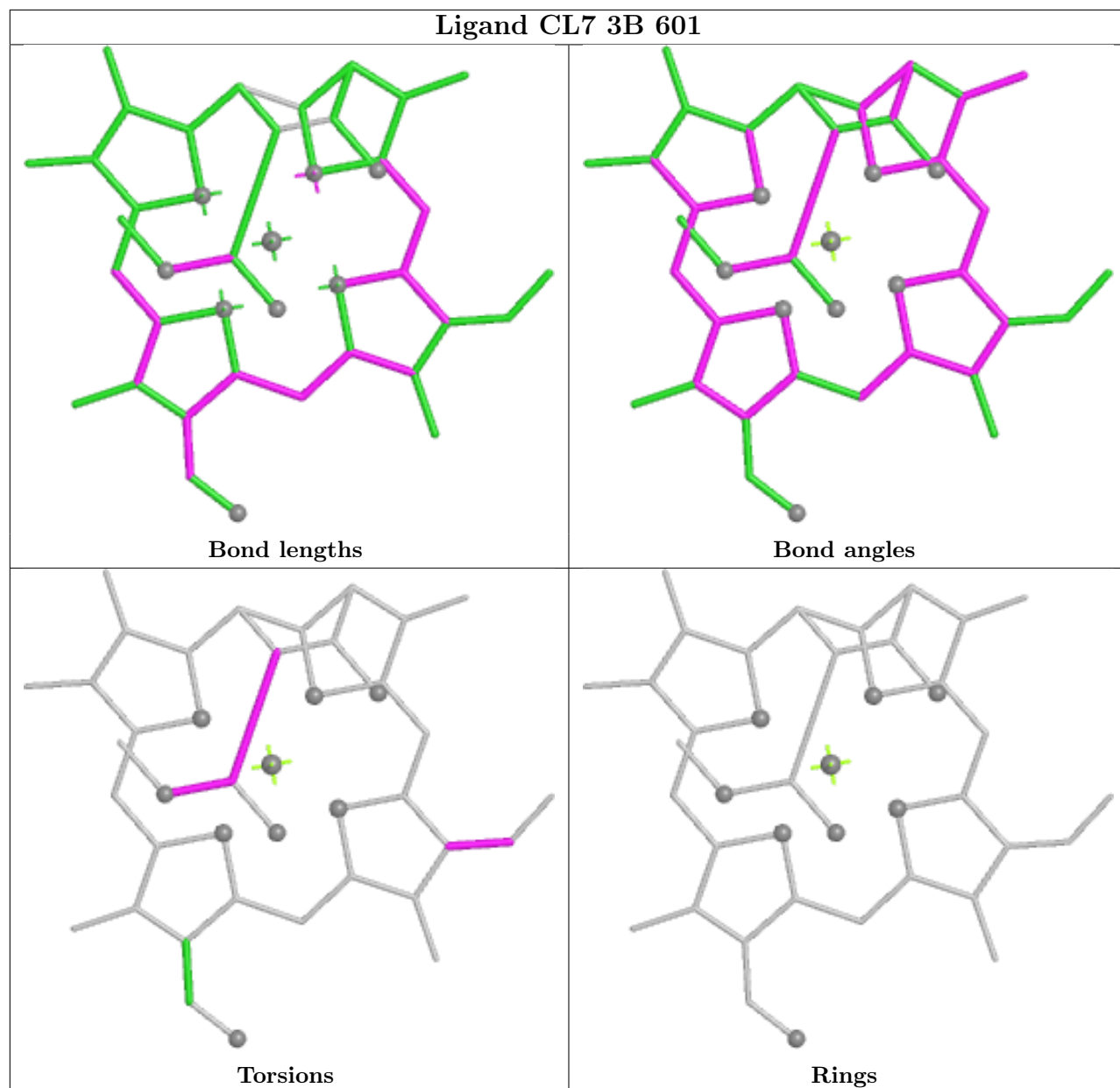
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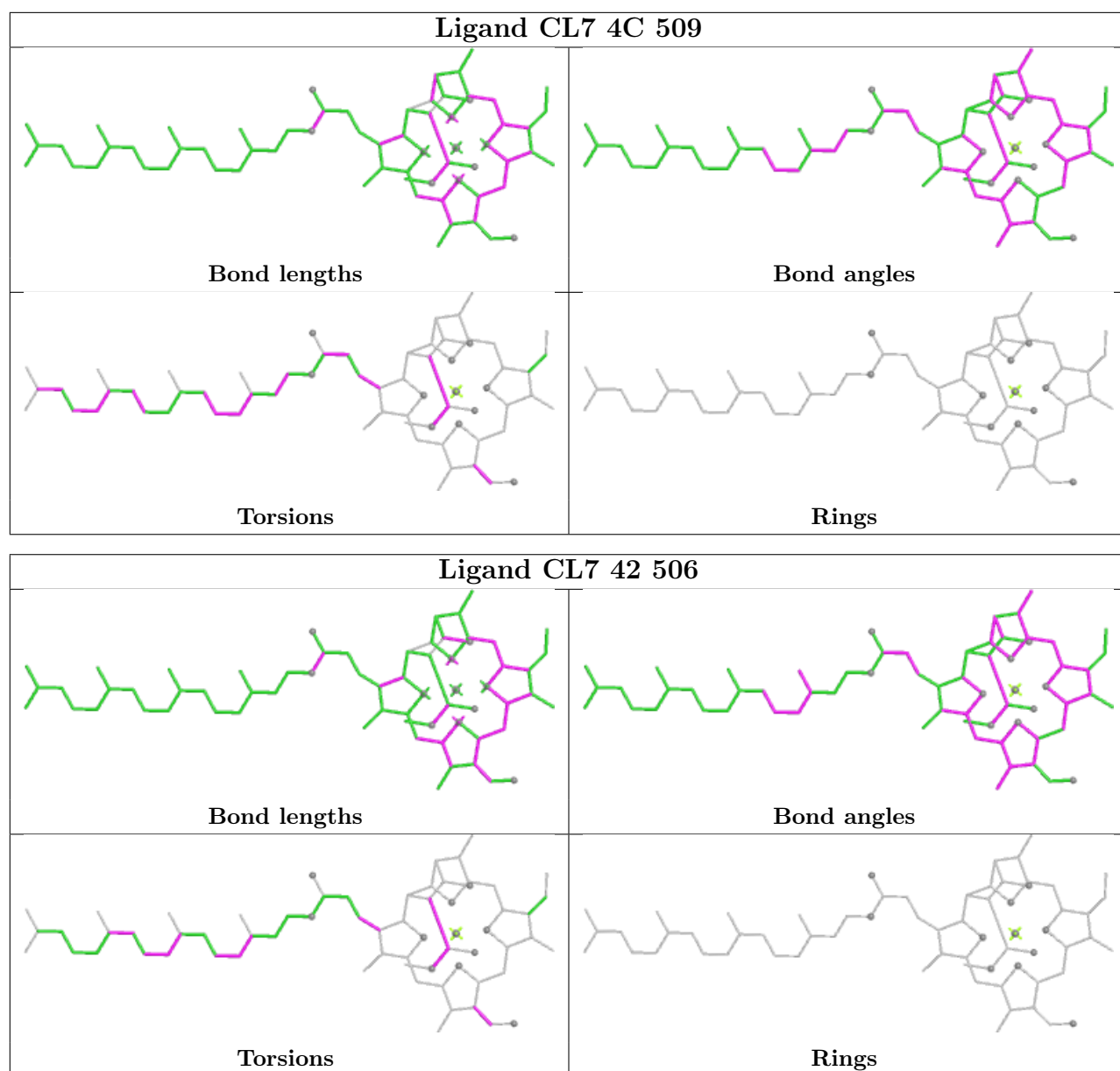


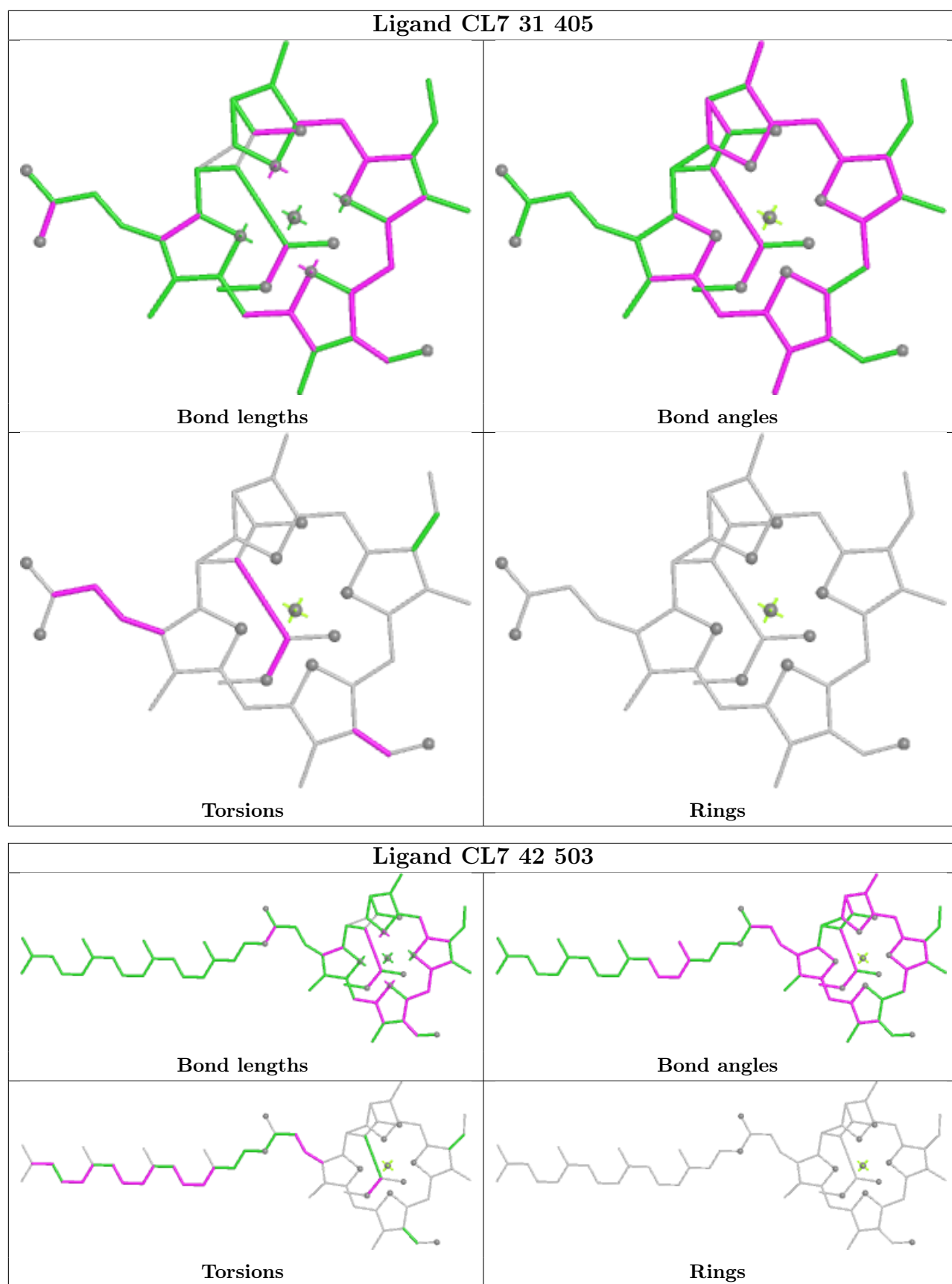
Ligand CL7 42 518



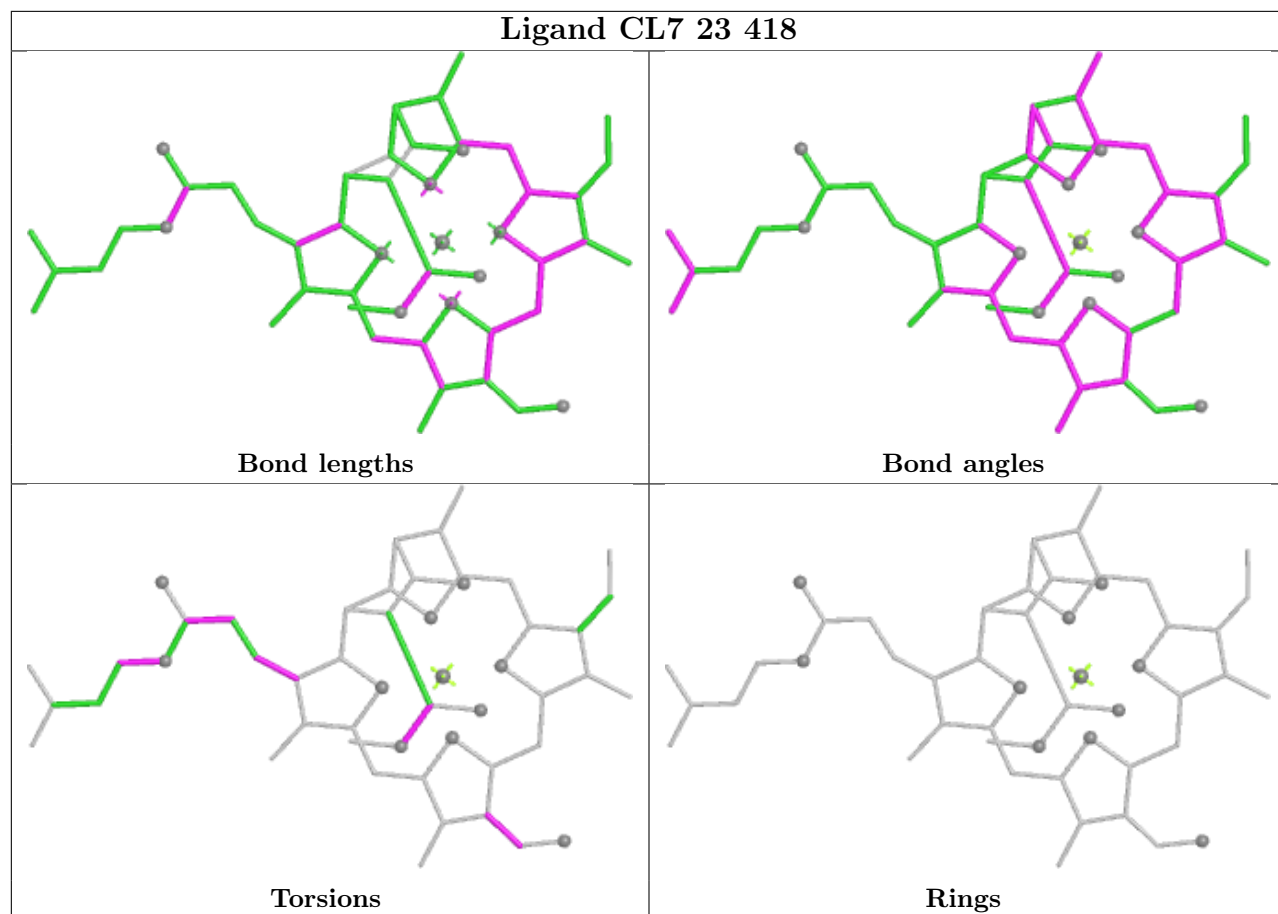




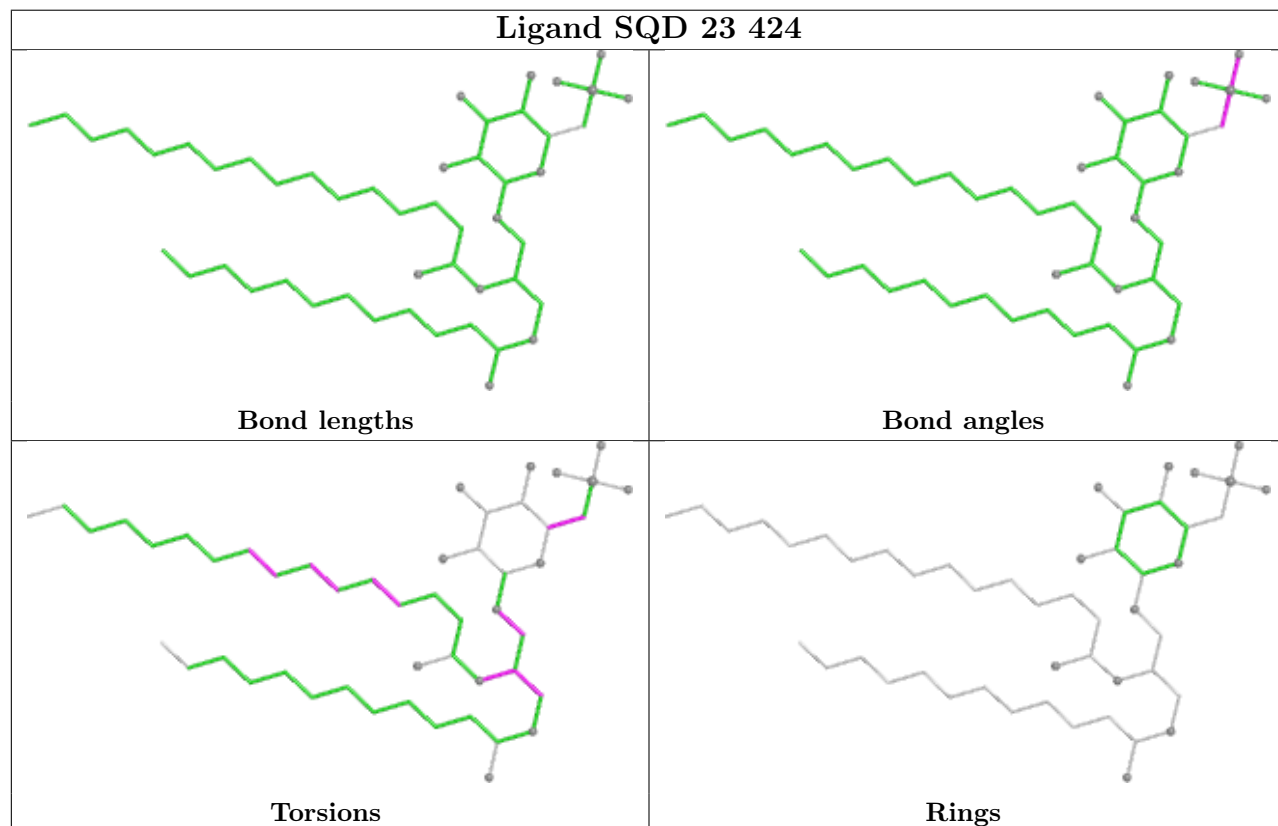


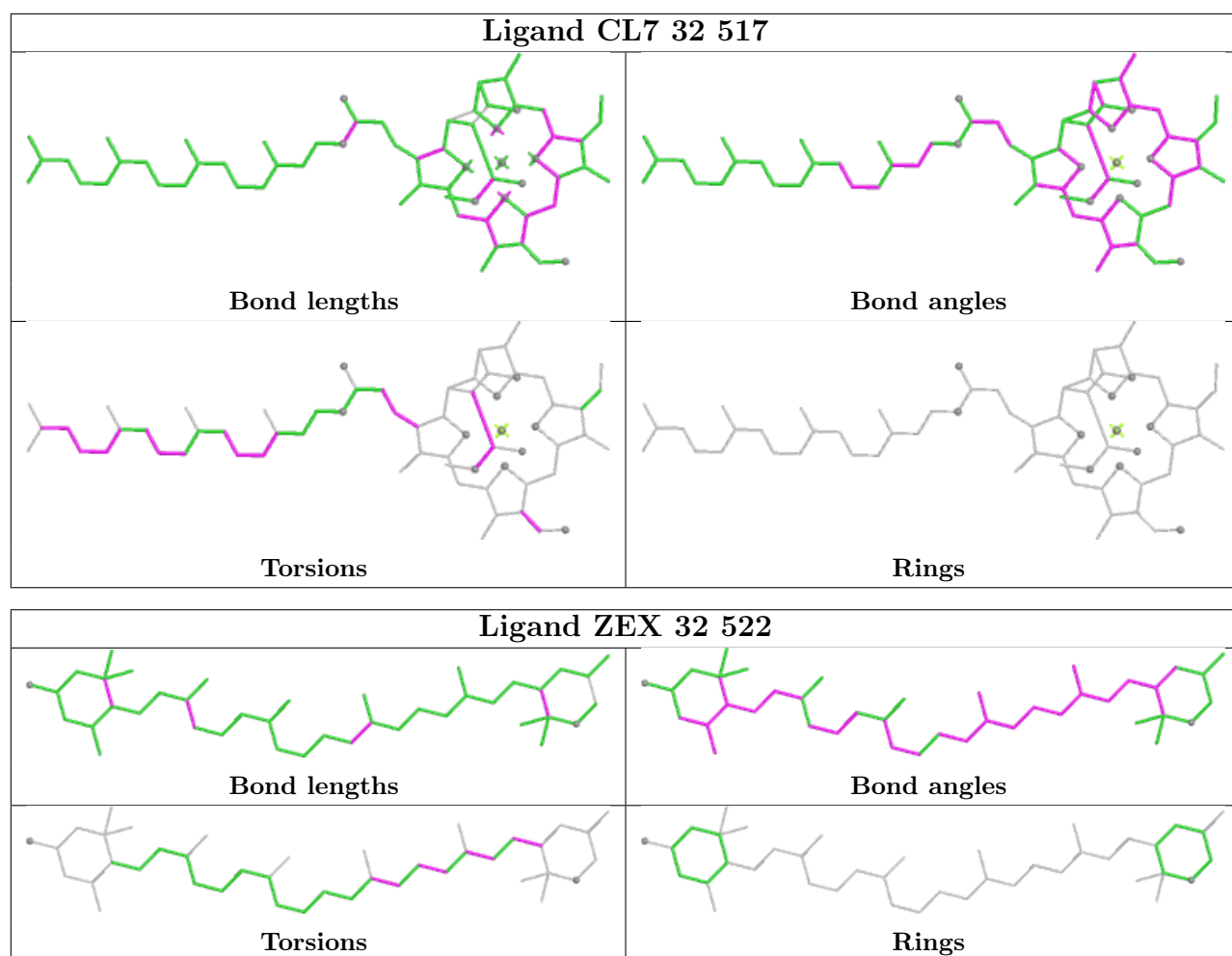


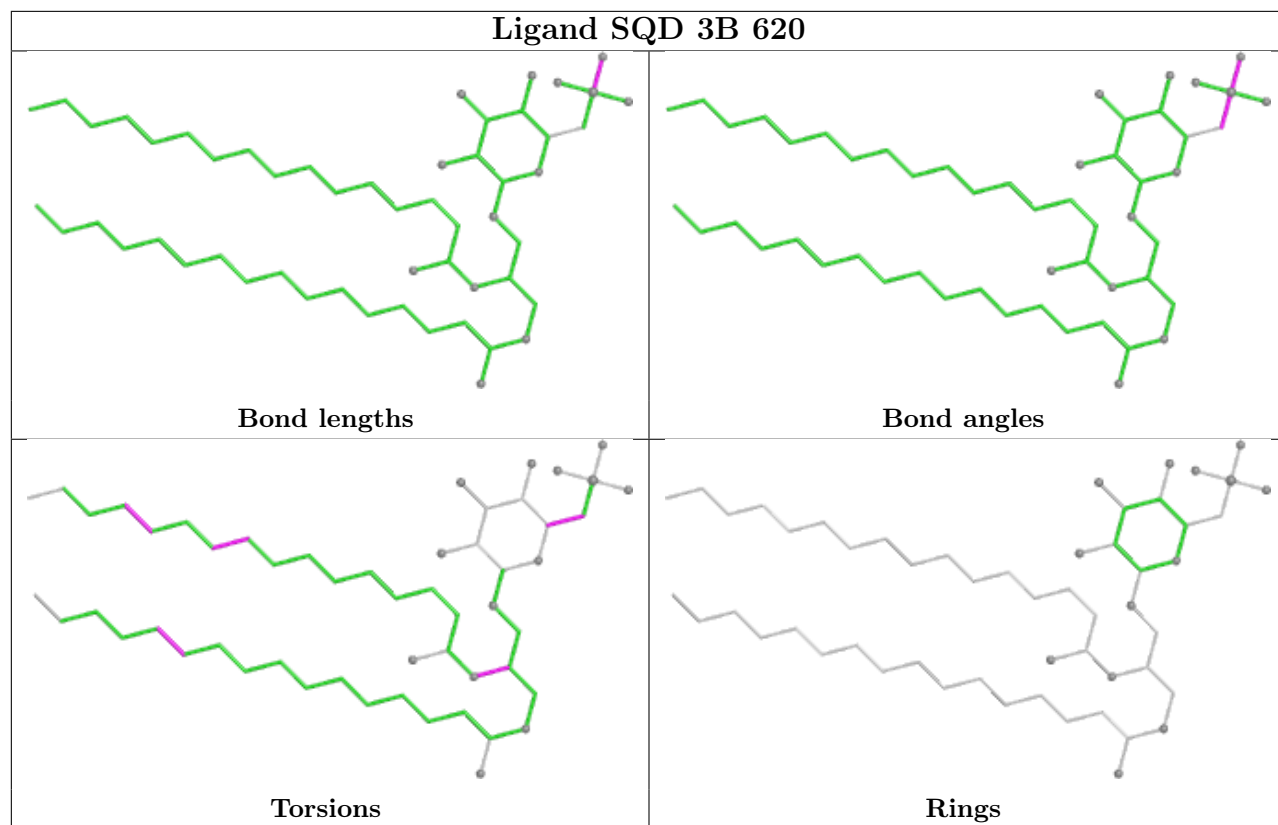
Ligand CL7 23 418

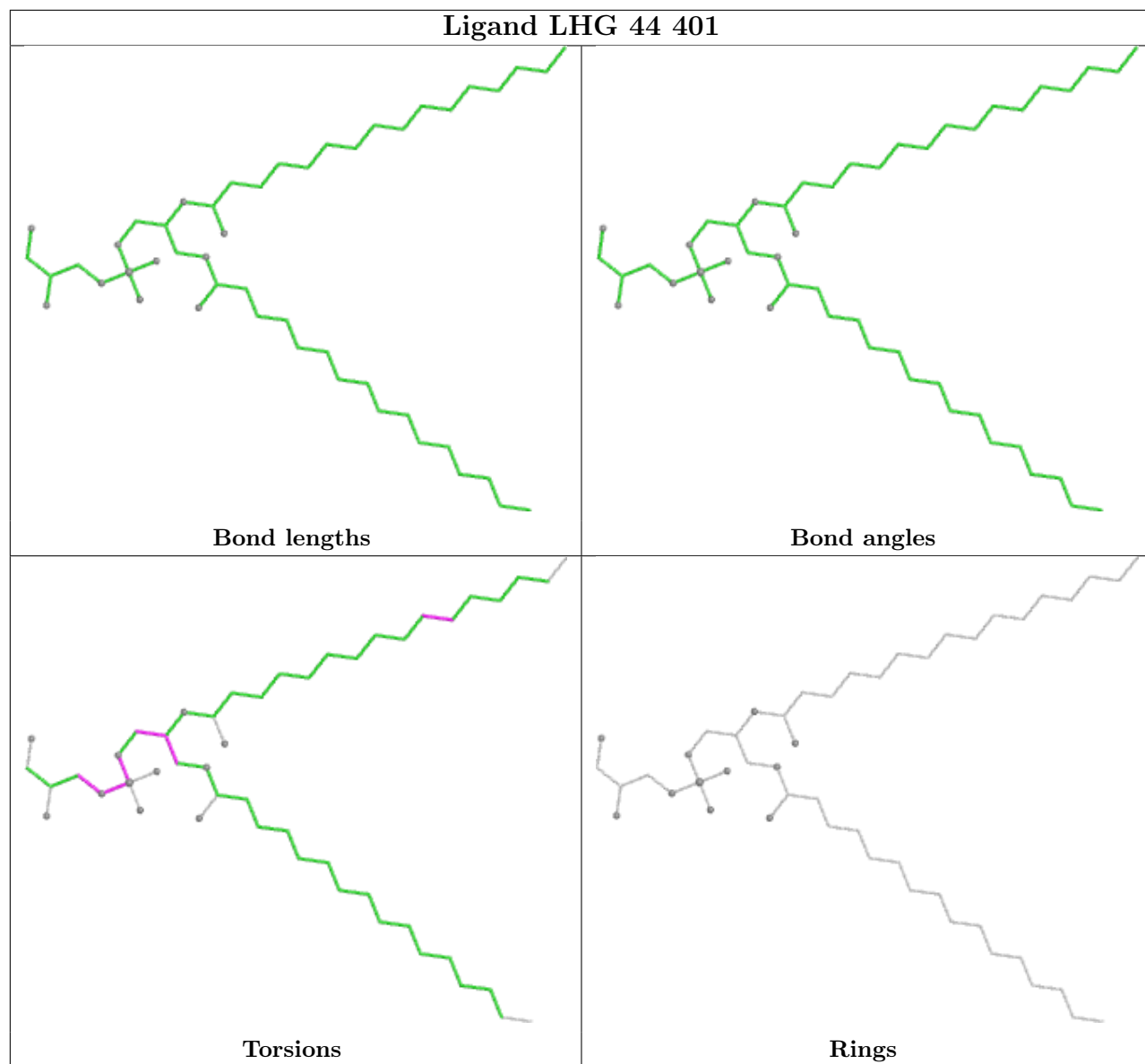


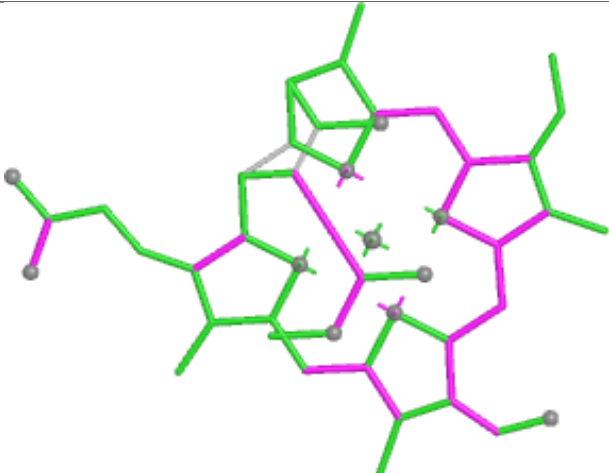
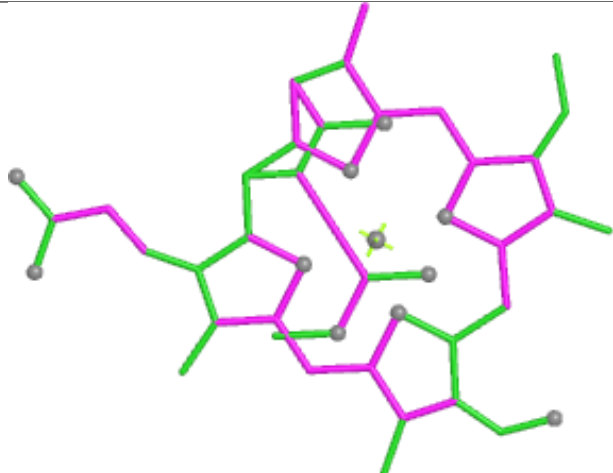
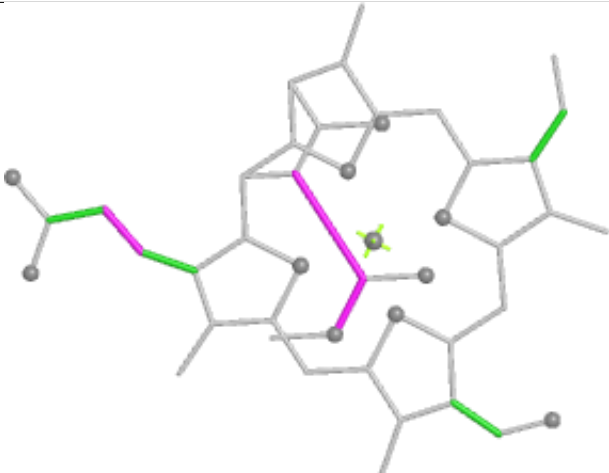
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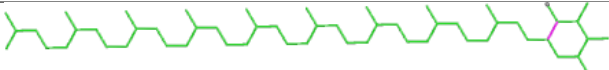
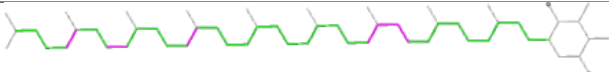
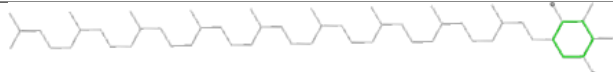


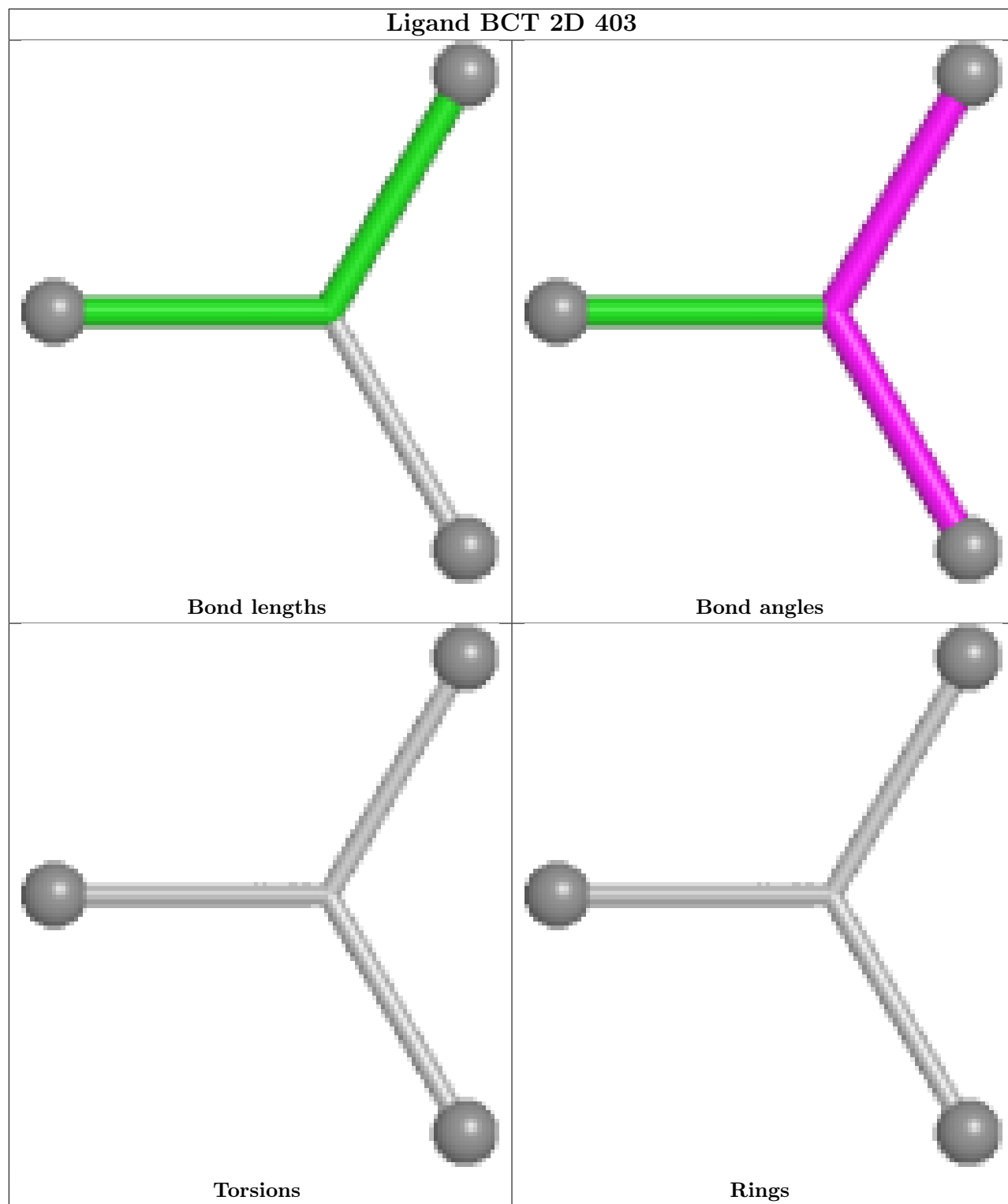




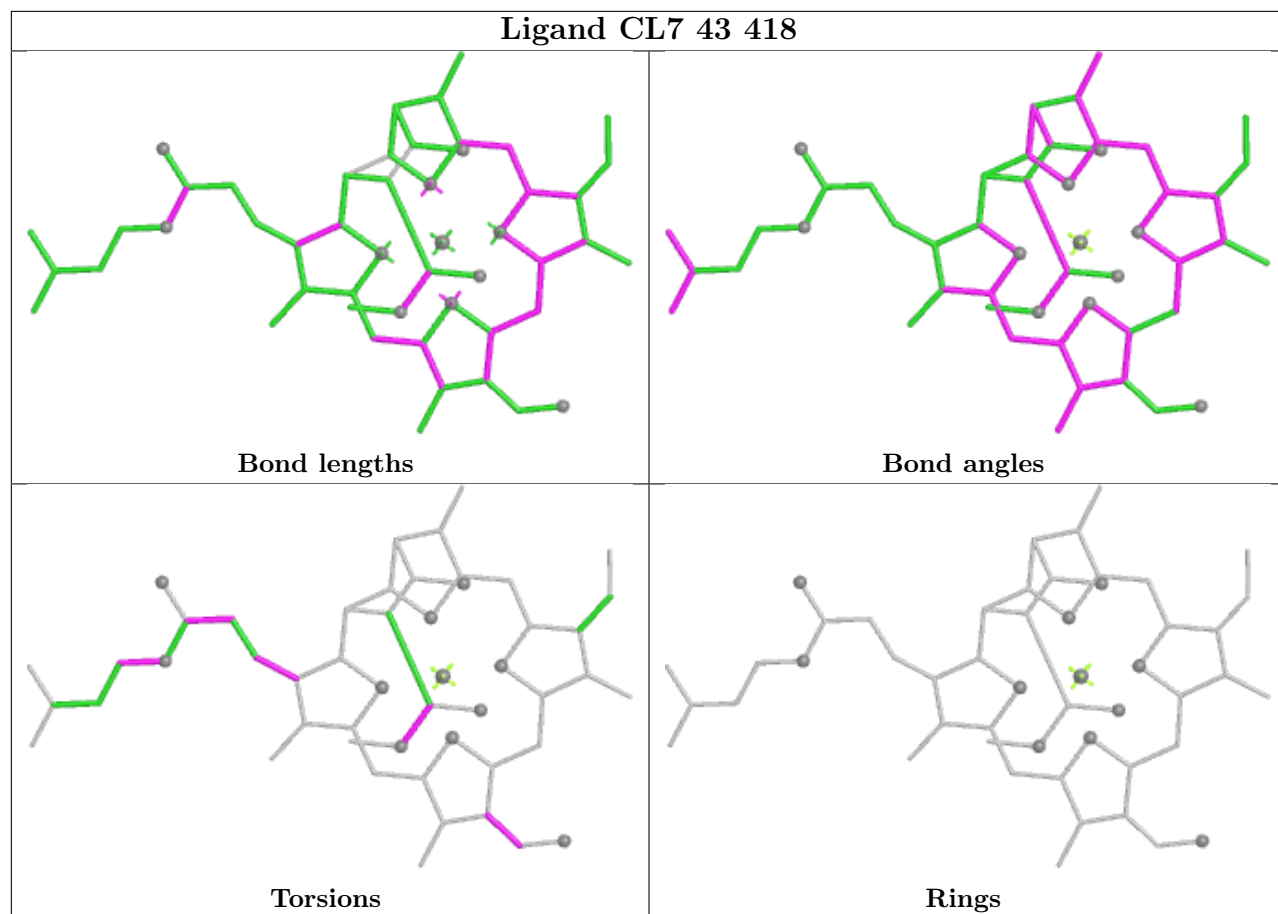


Ligand CL7 1B 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

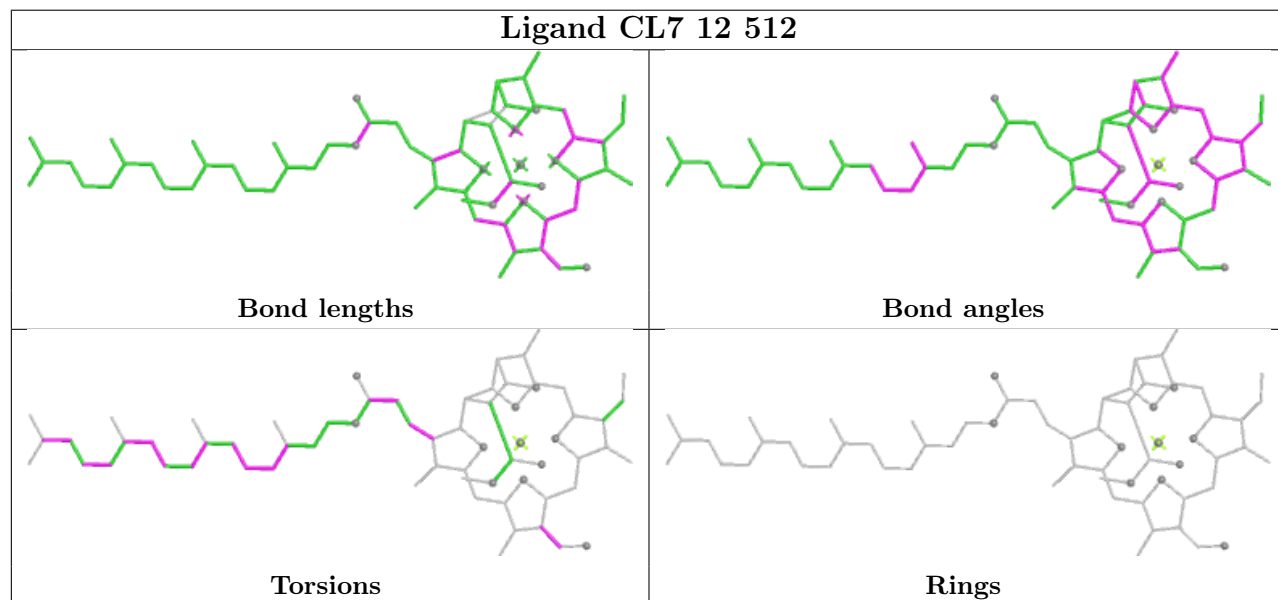
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Bond lengths	Bond angles
	
Torsions	Rings

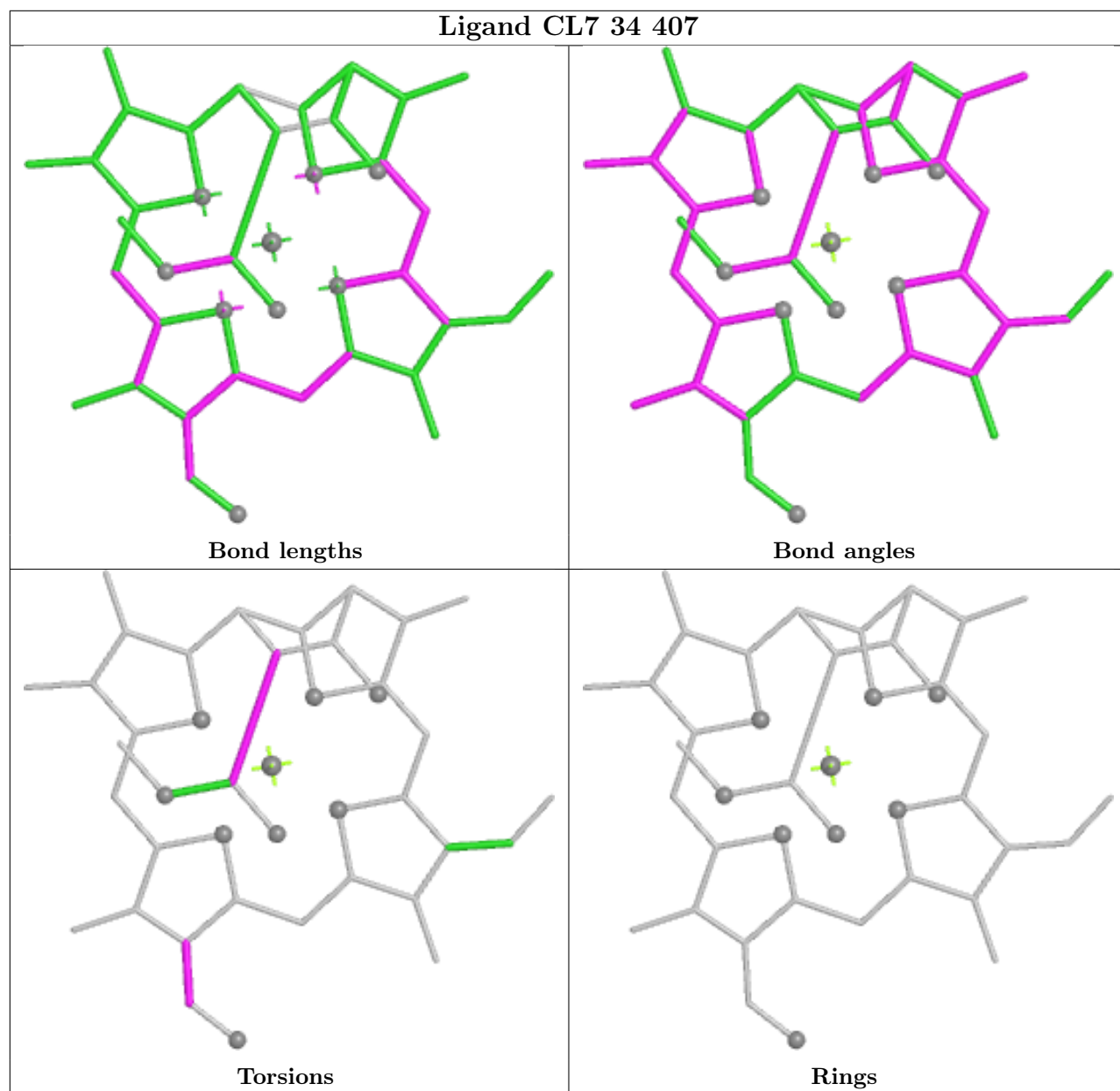
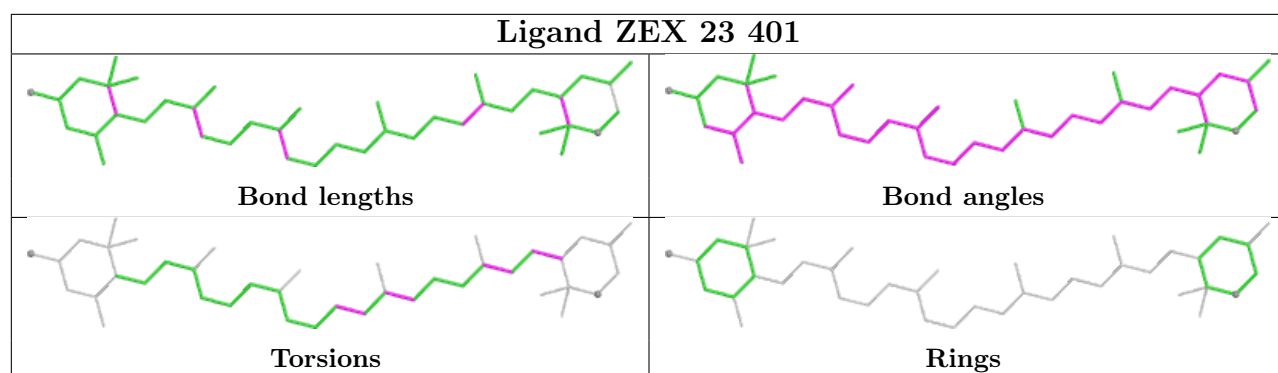


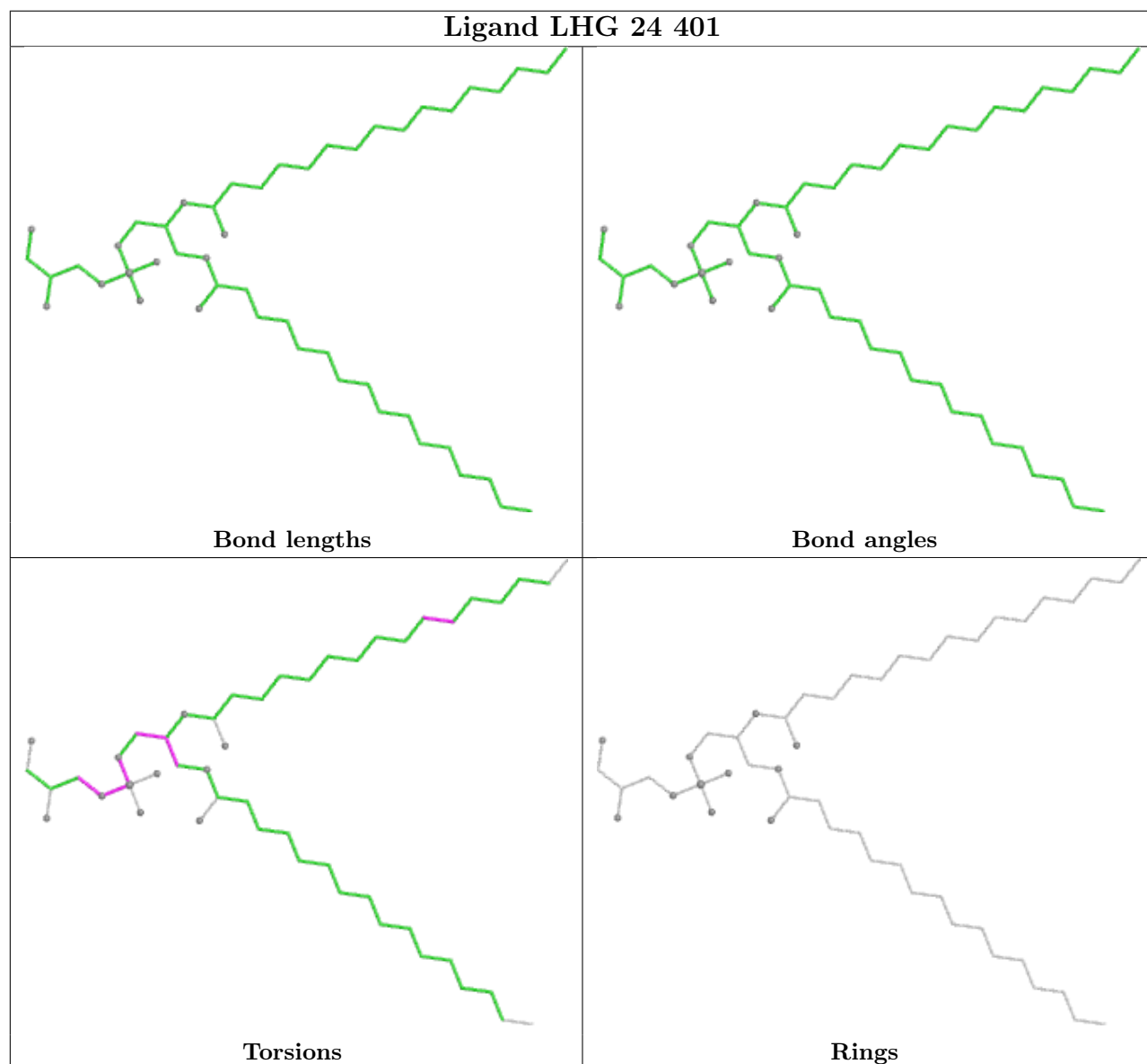
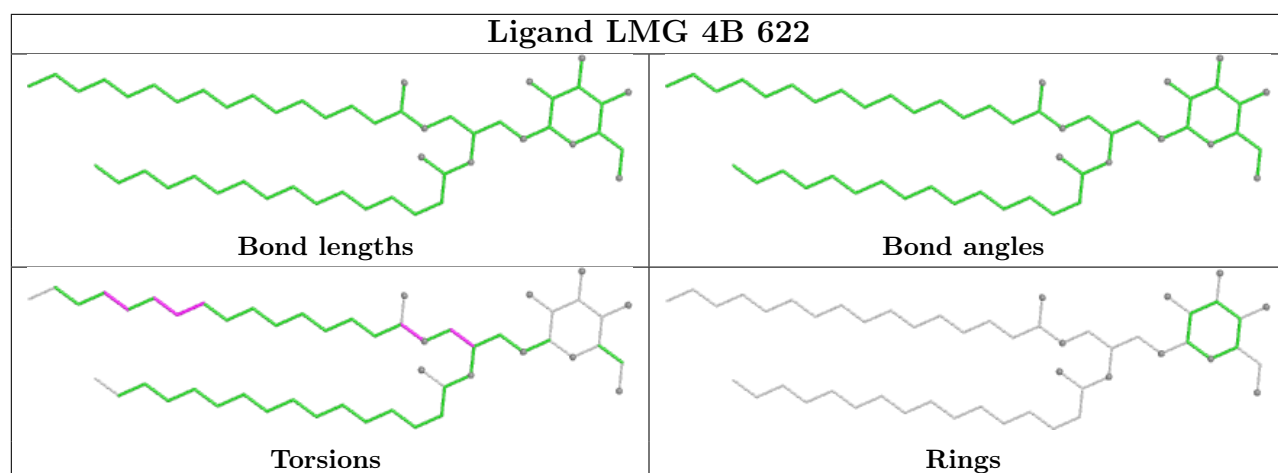
Ligand CL7 43 418

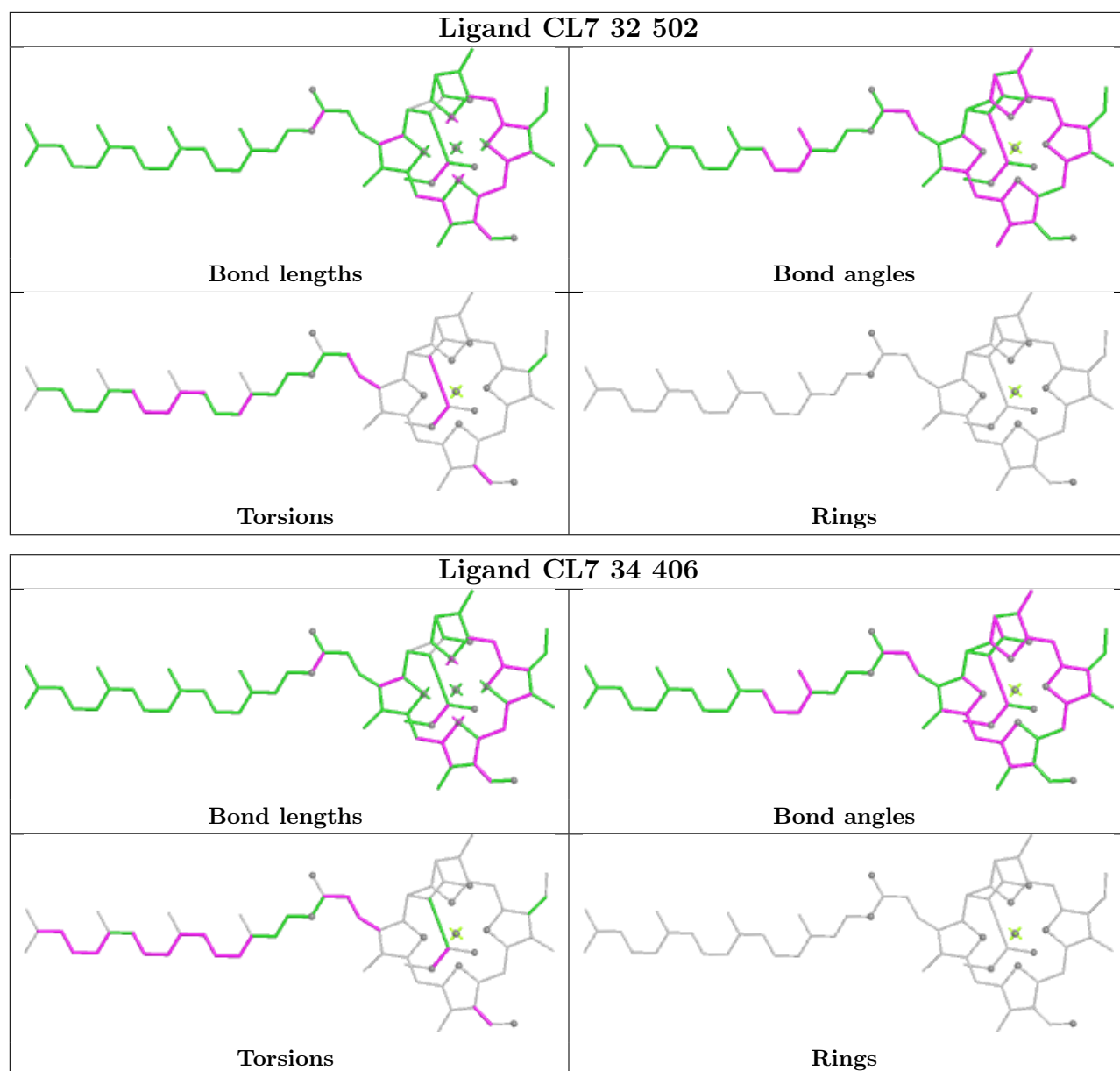


Ligand CL7 12 512

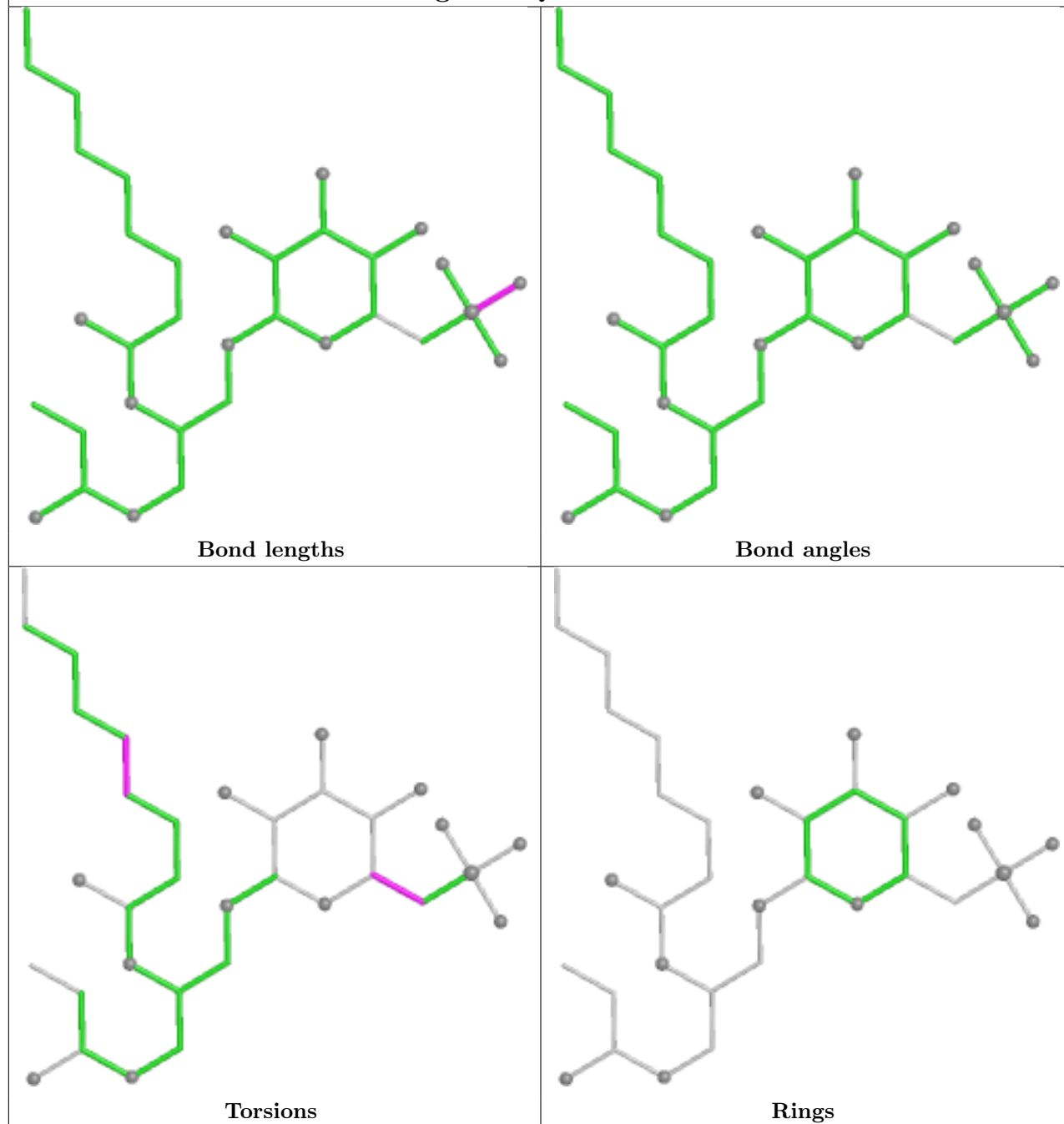




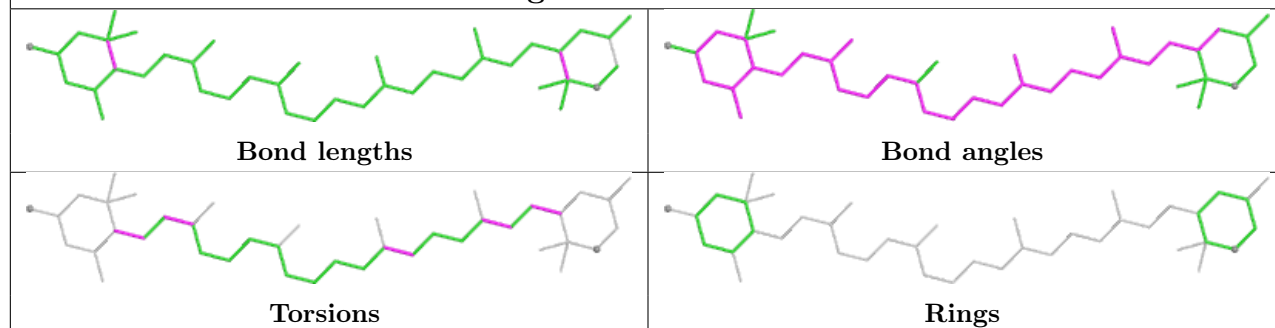




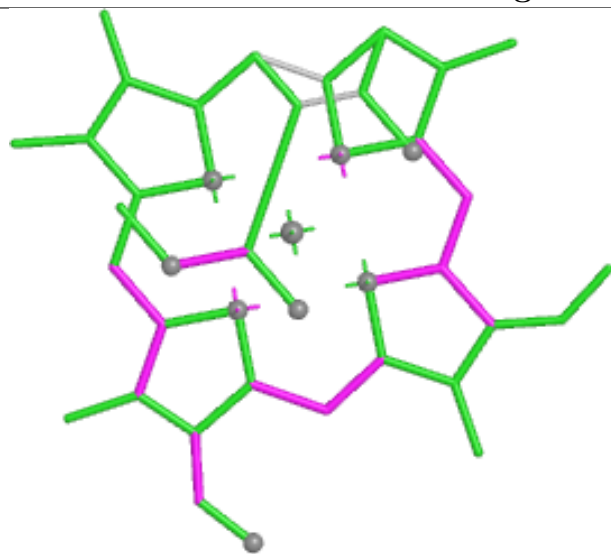
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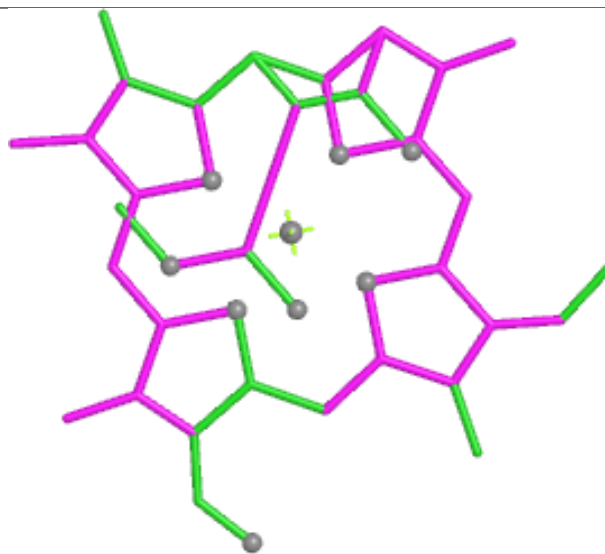
Ligand ZEX 23 421



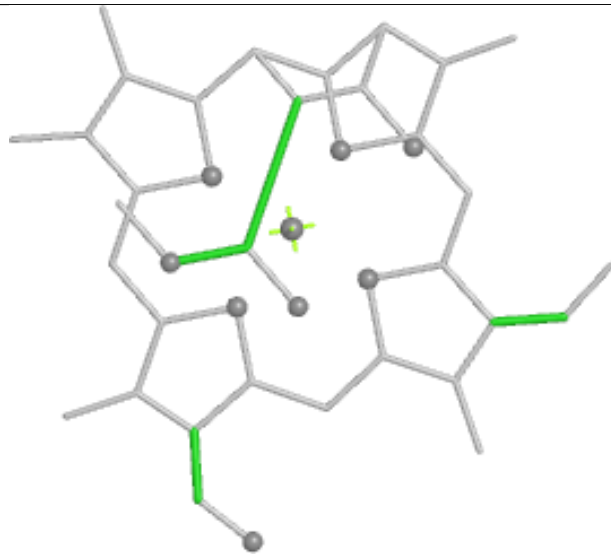
Ligand CL7 33 515



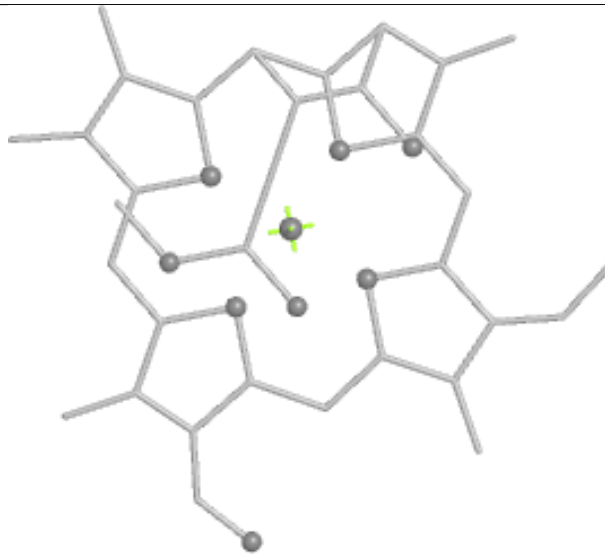
Bond lengths



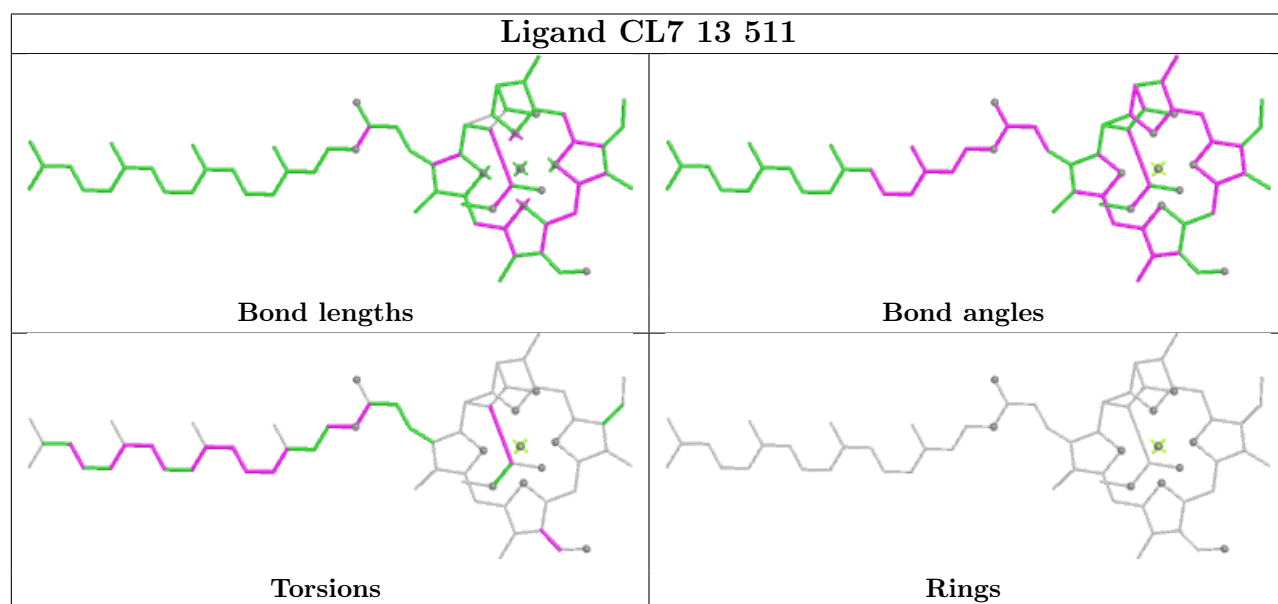
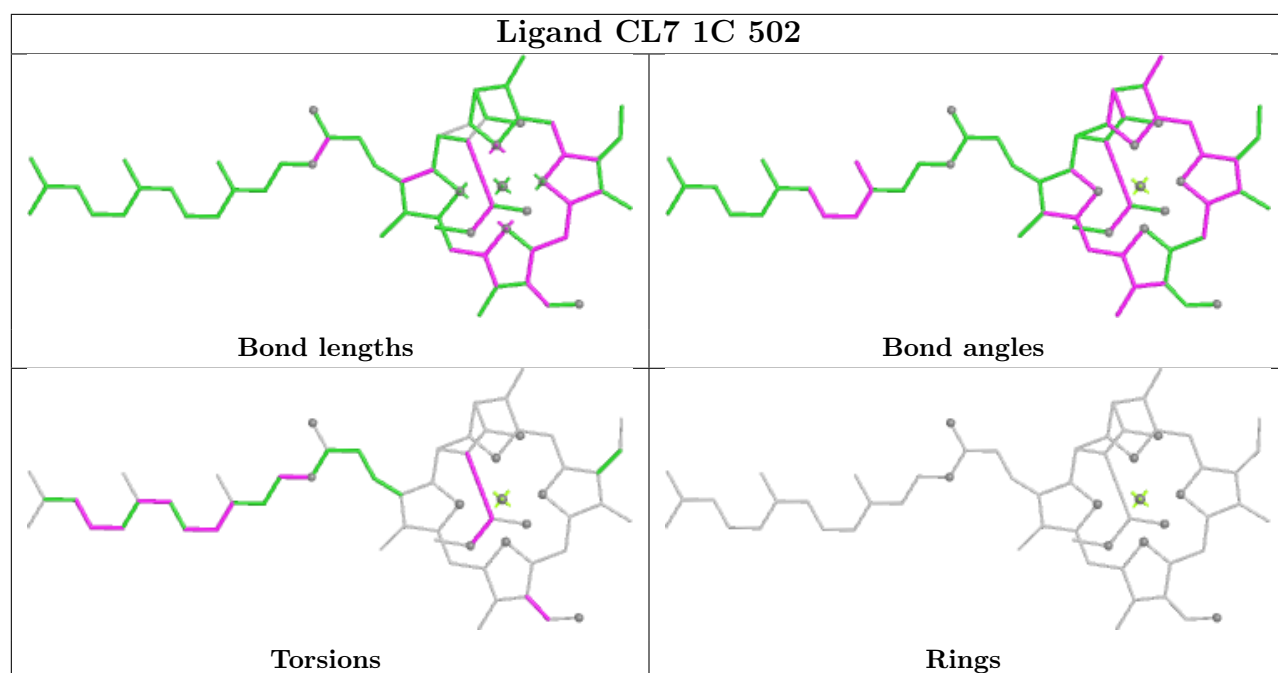
Bond angles

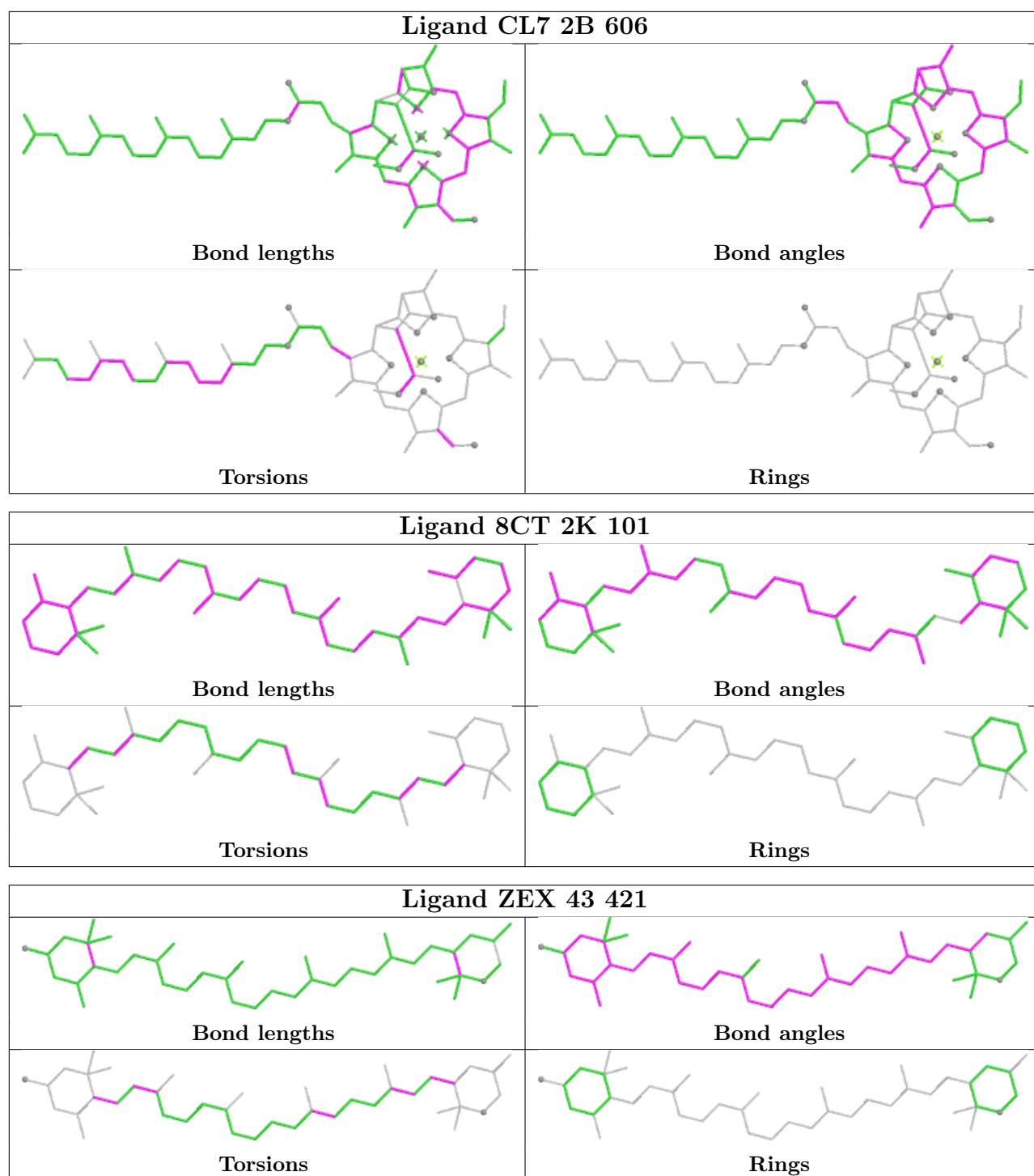


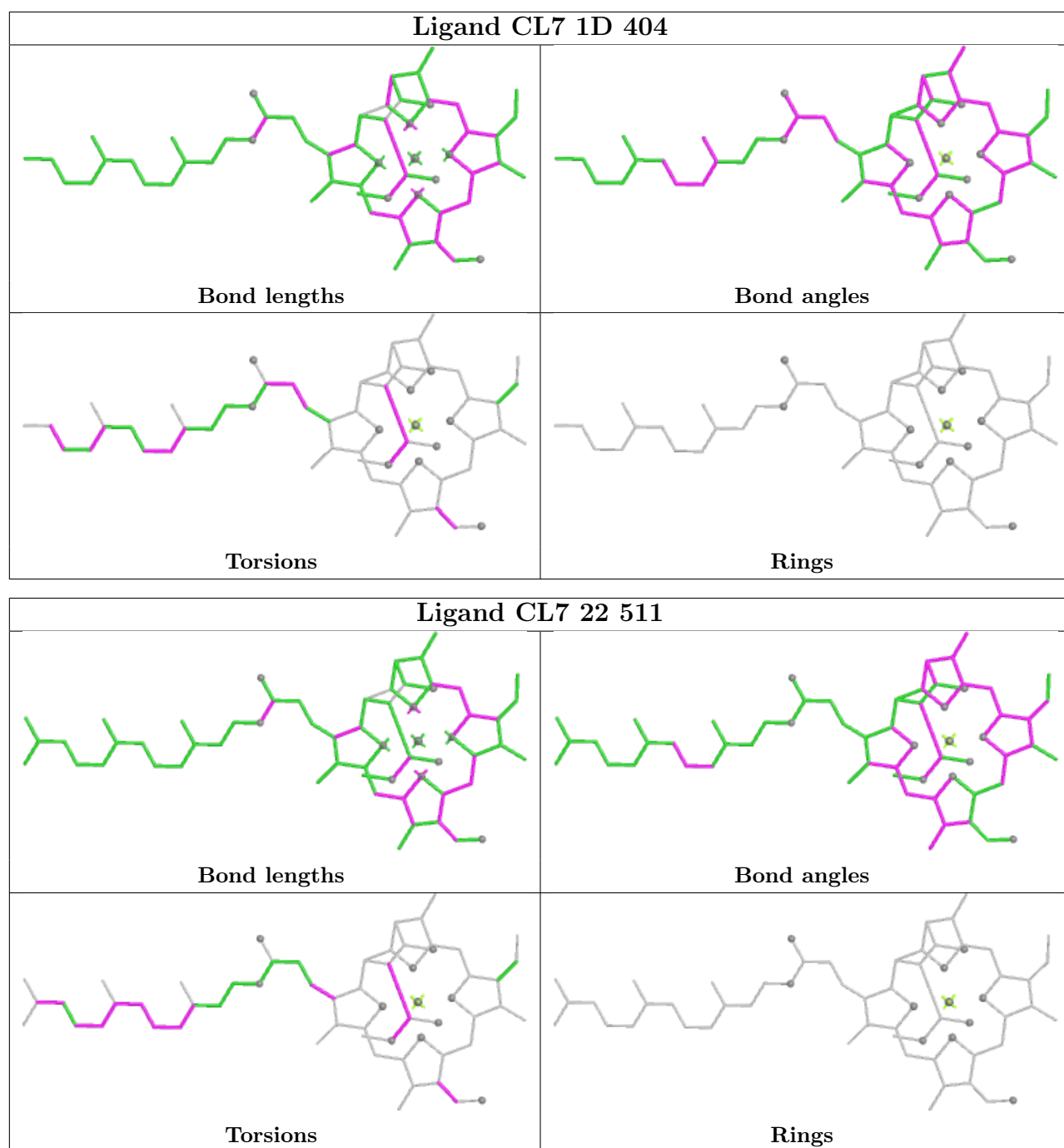
Torsions

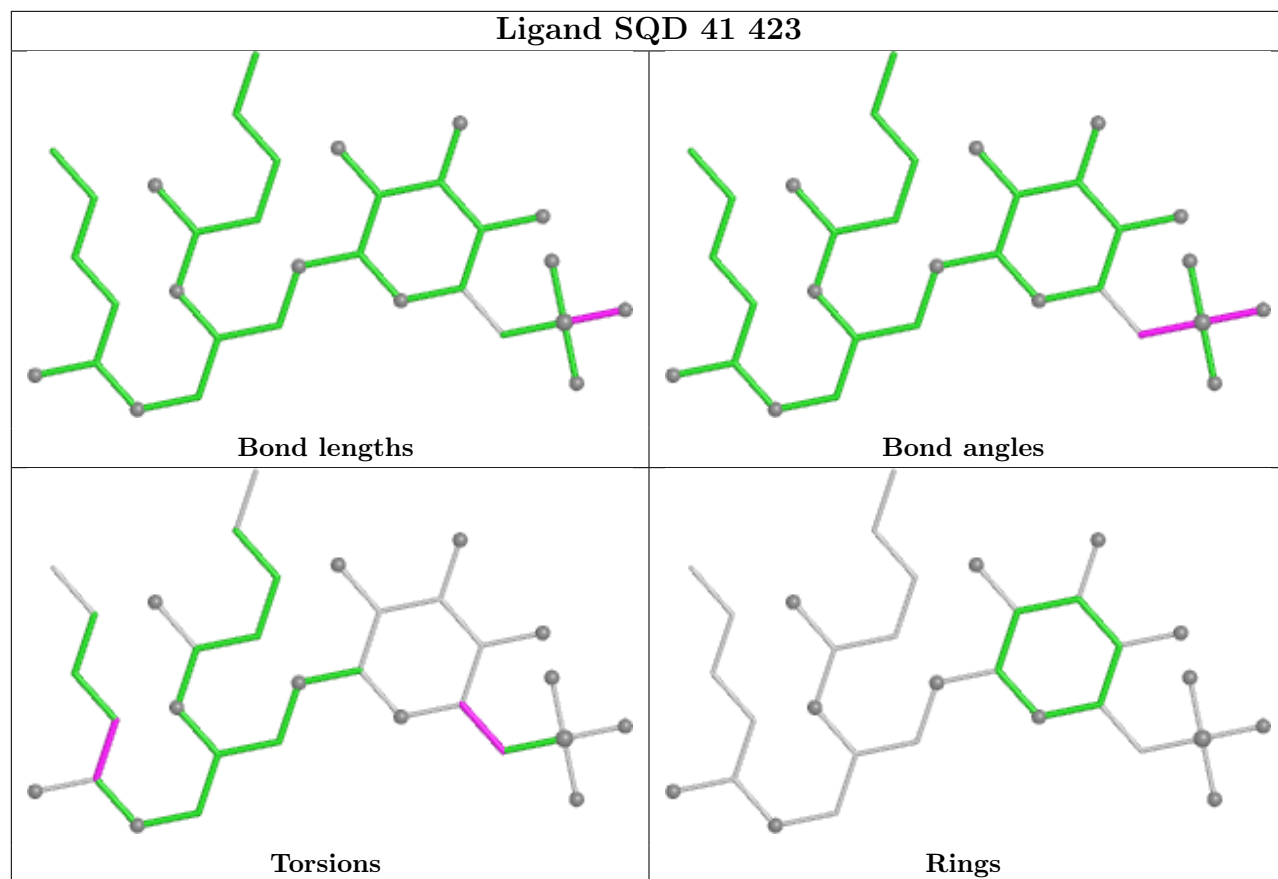


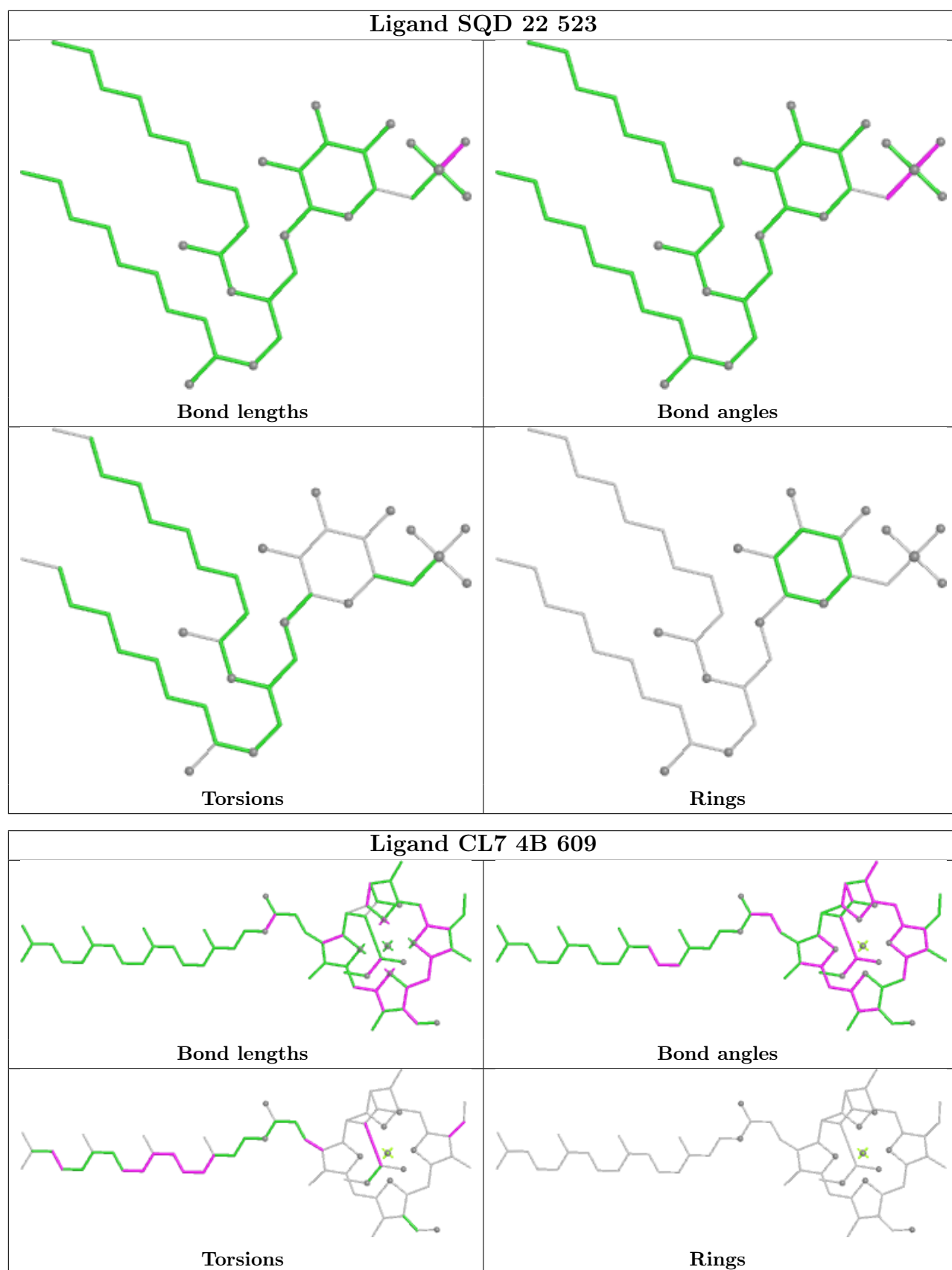
Rings

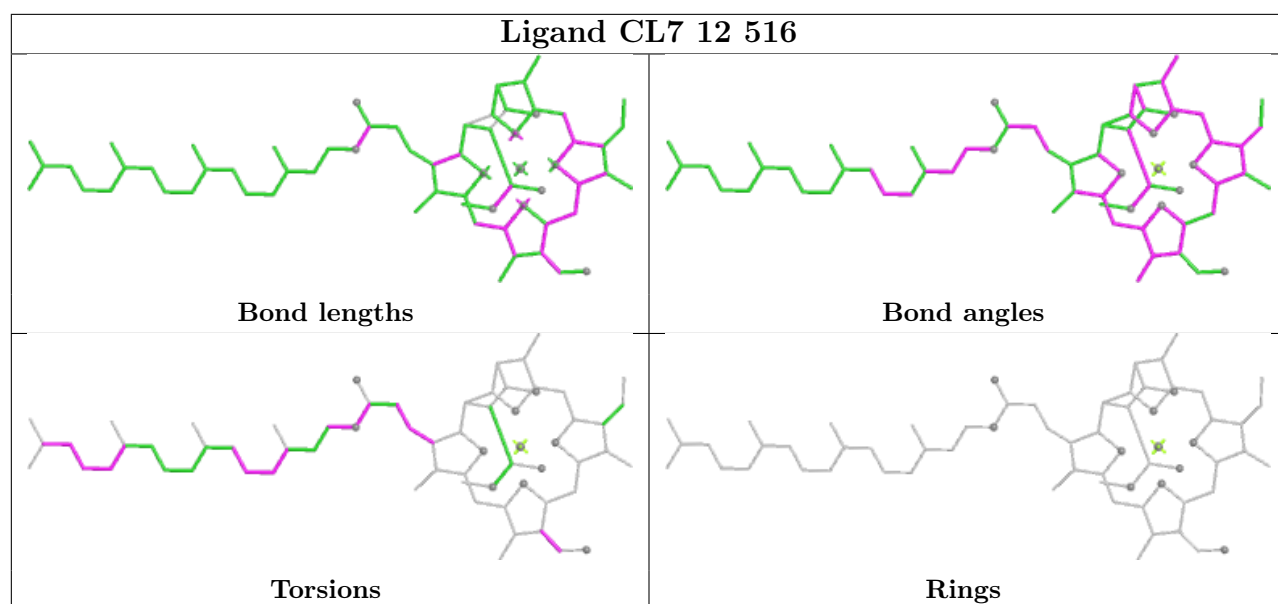


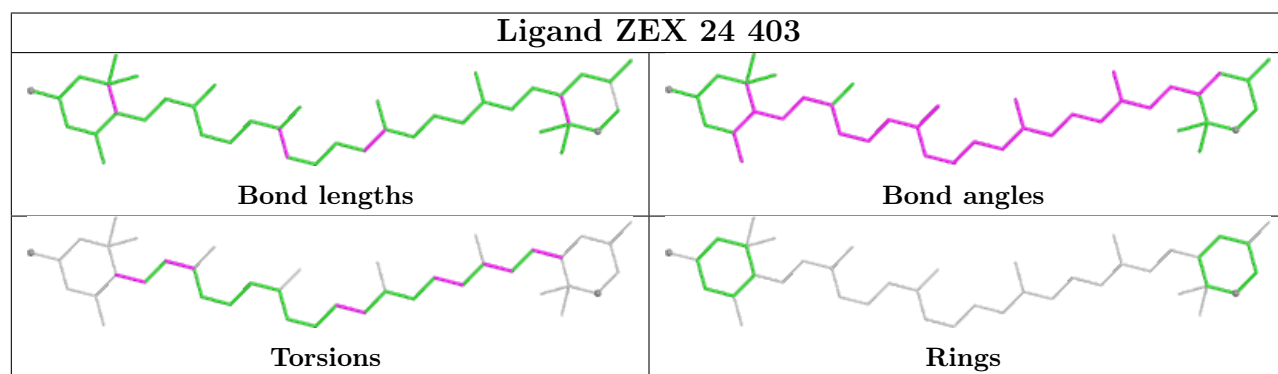
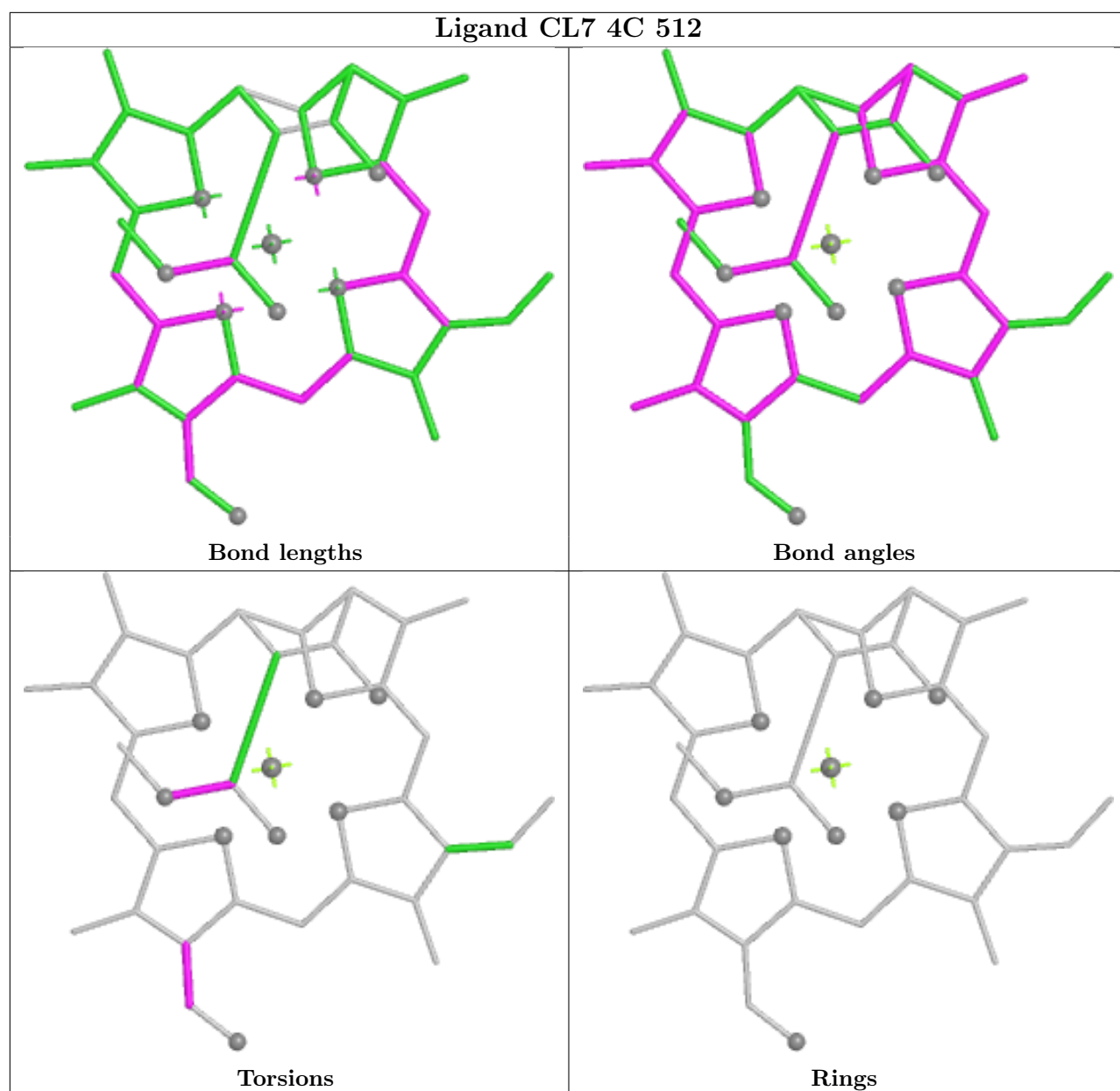


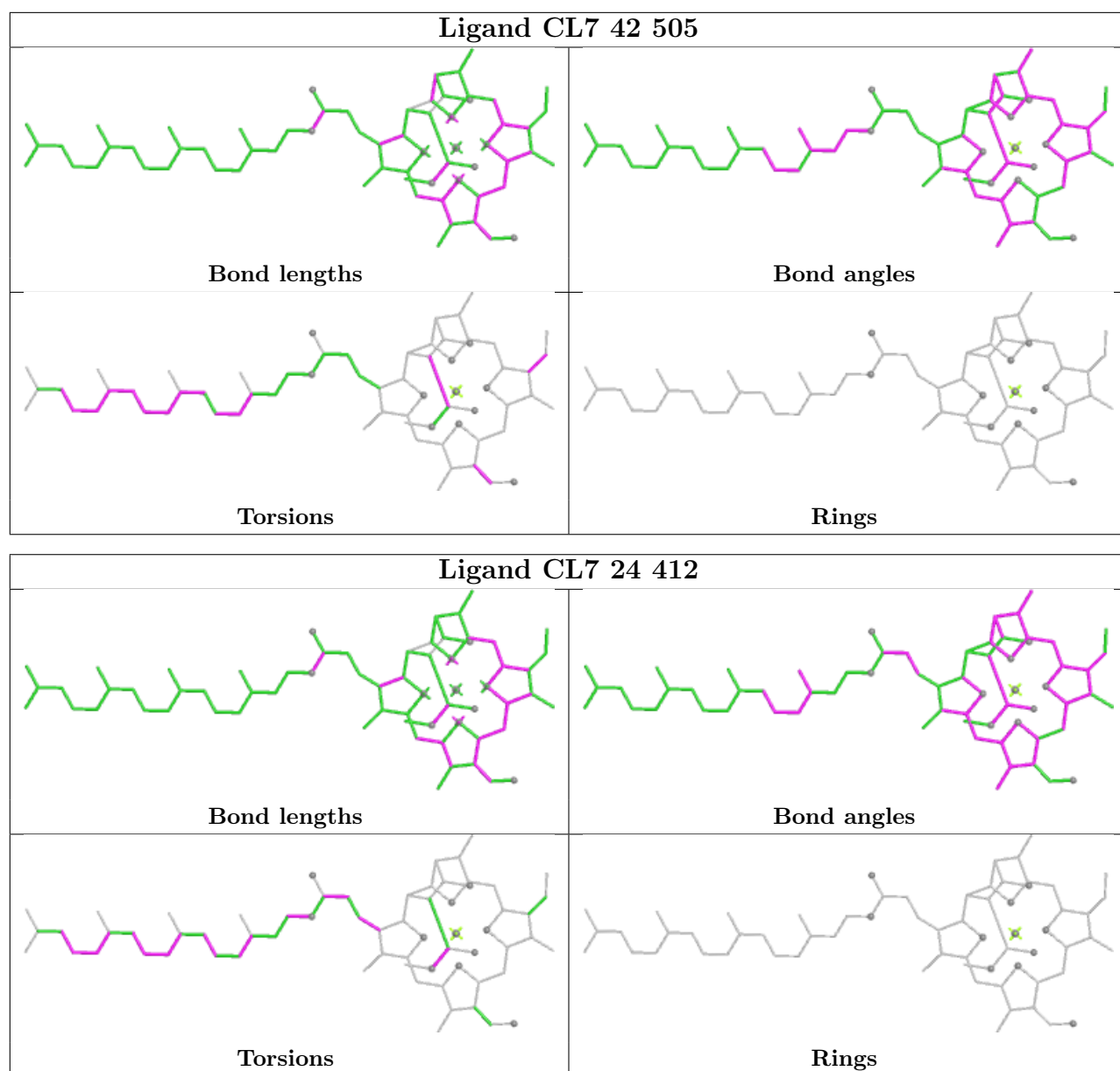




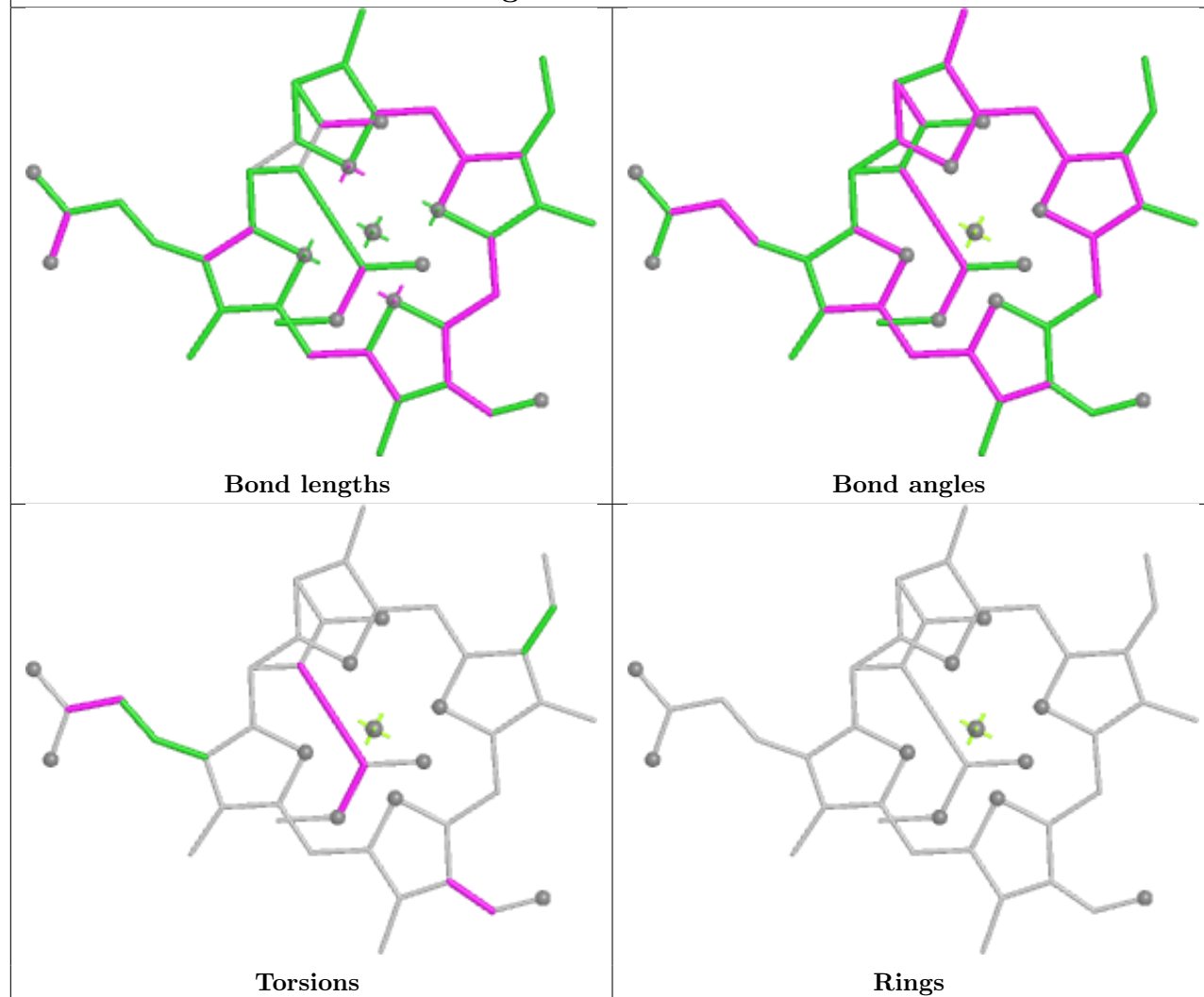




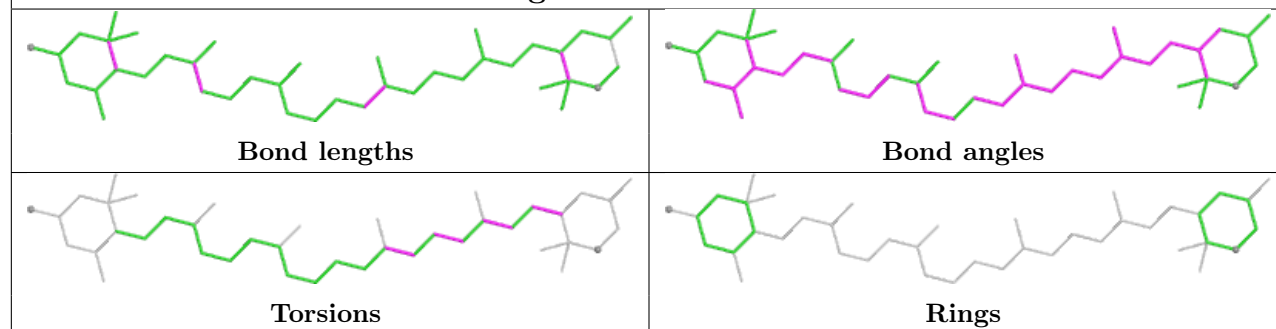


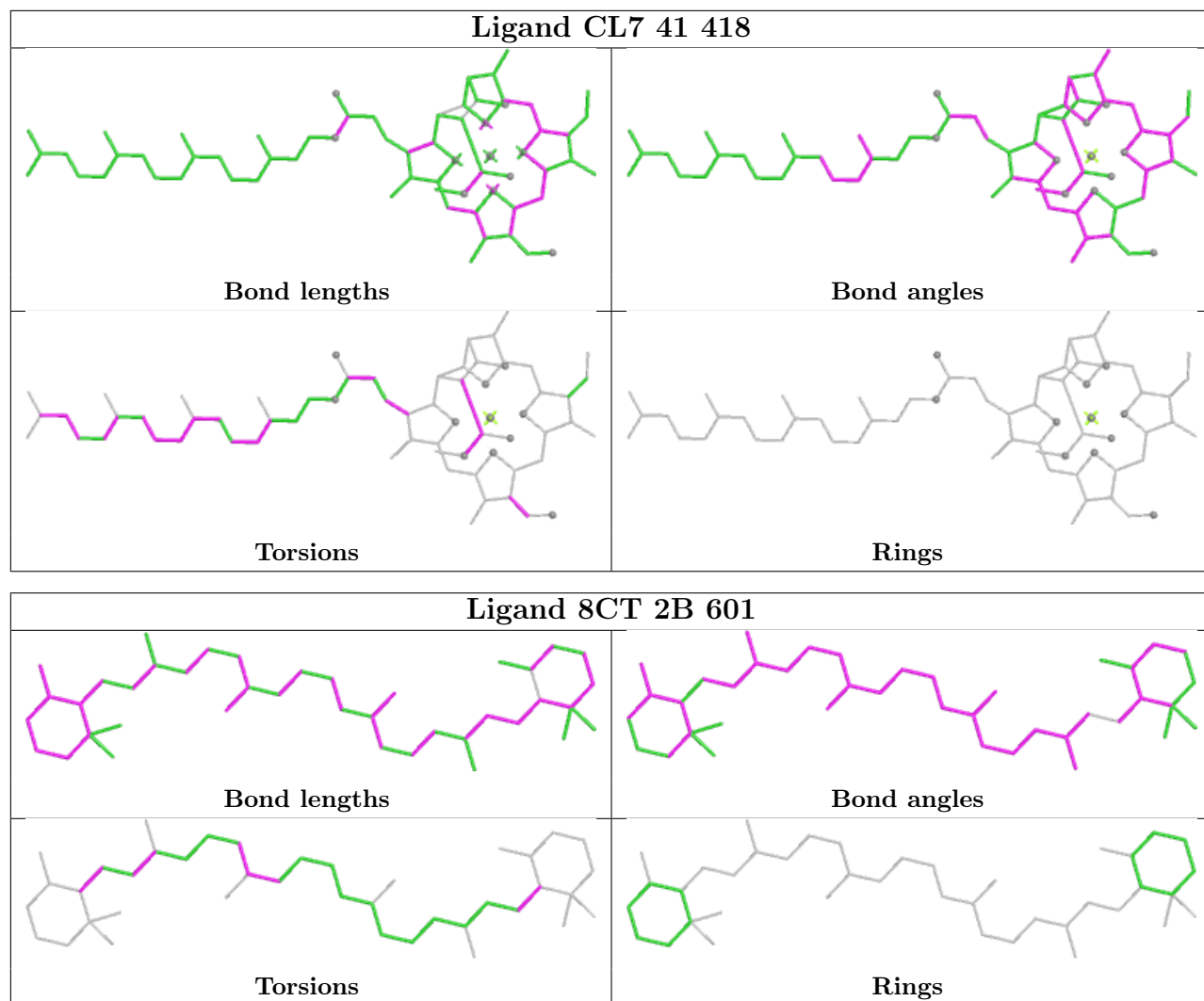


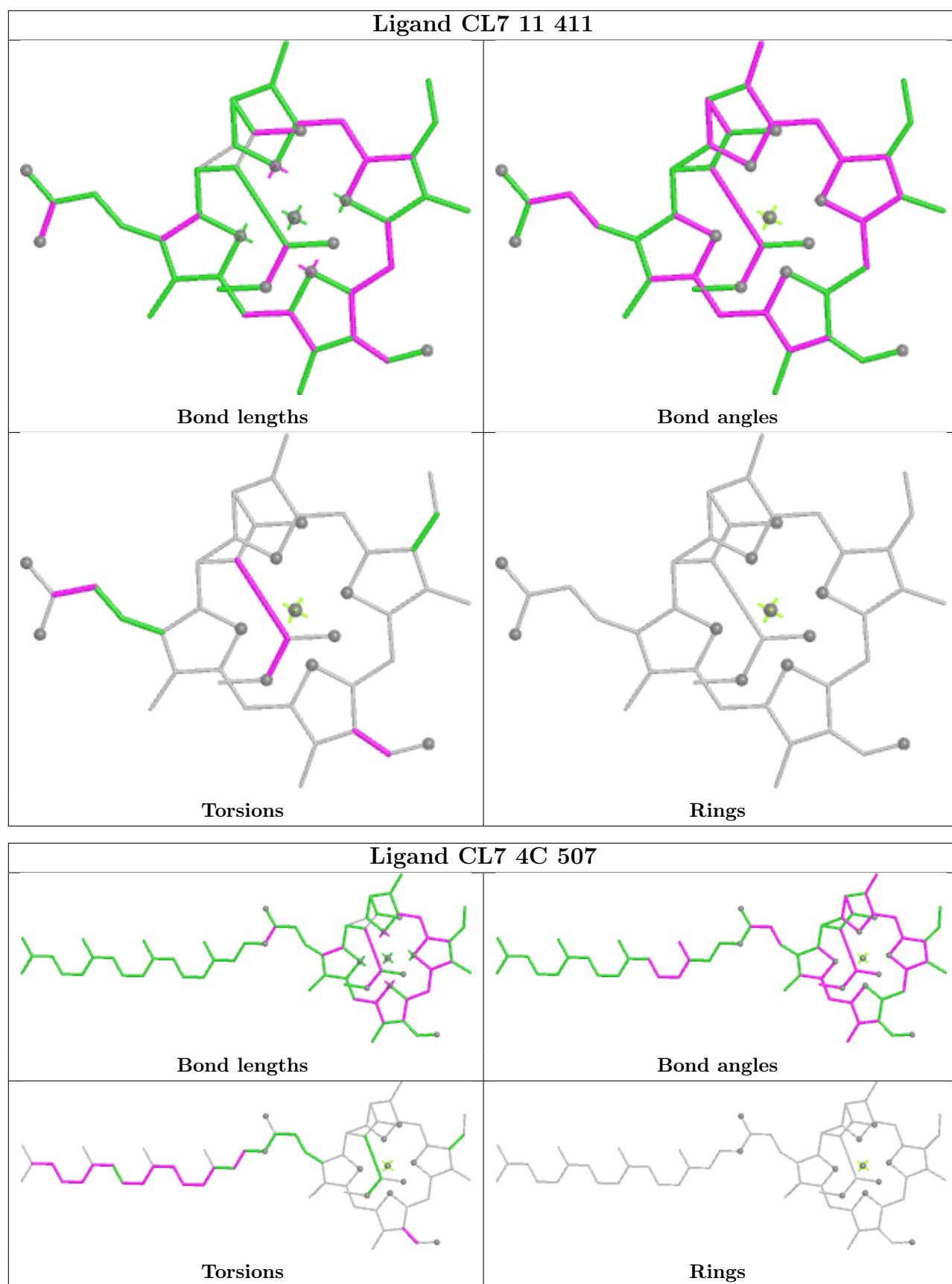
Ligand CL7 31 411

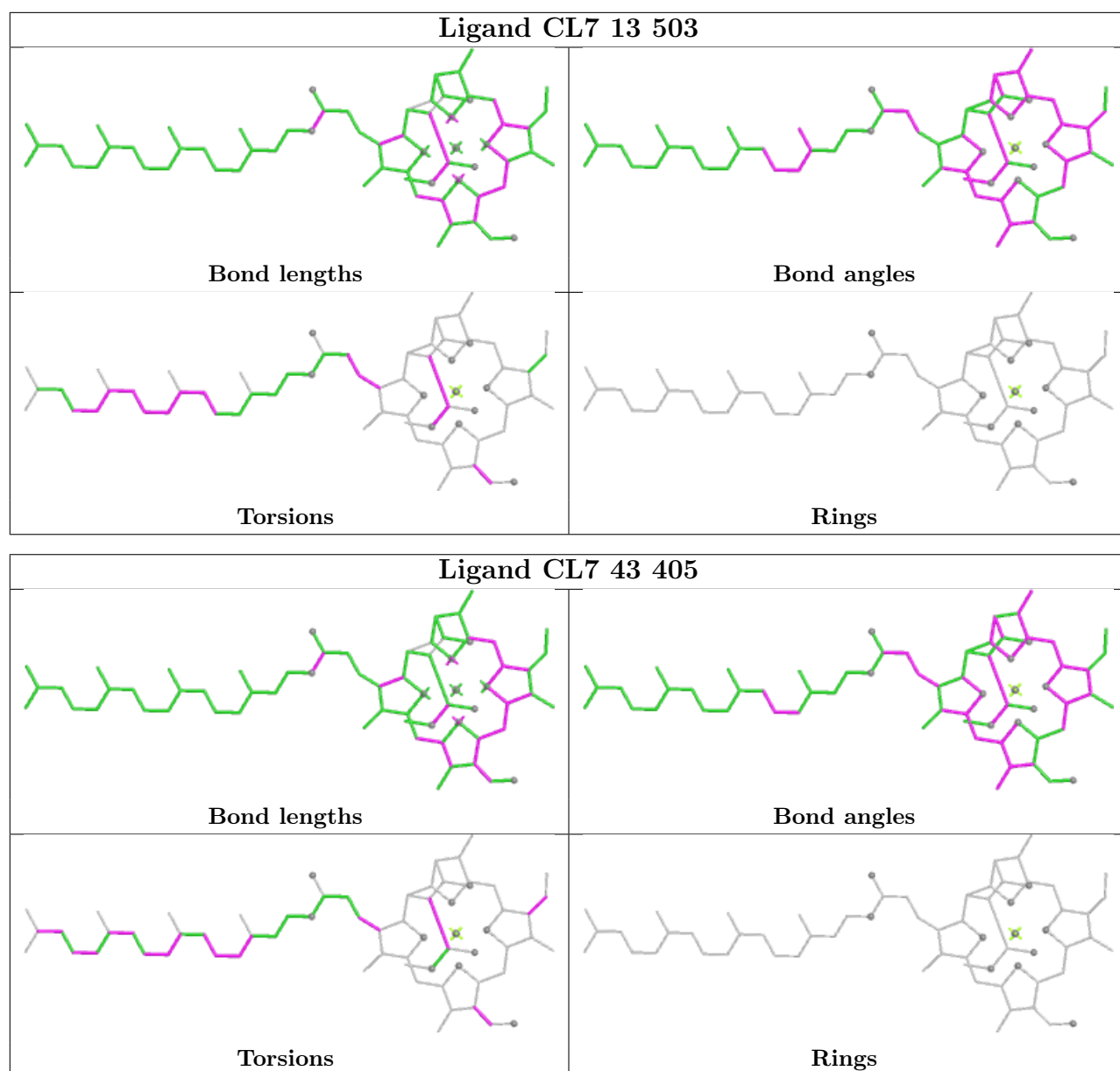


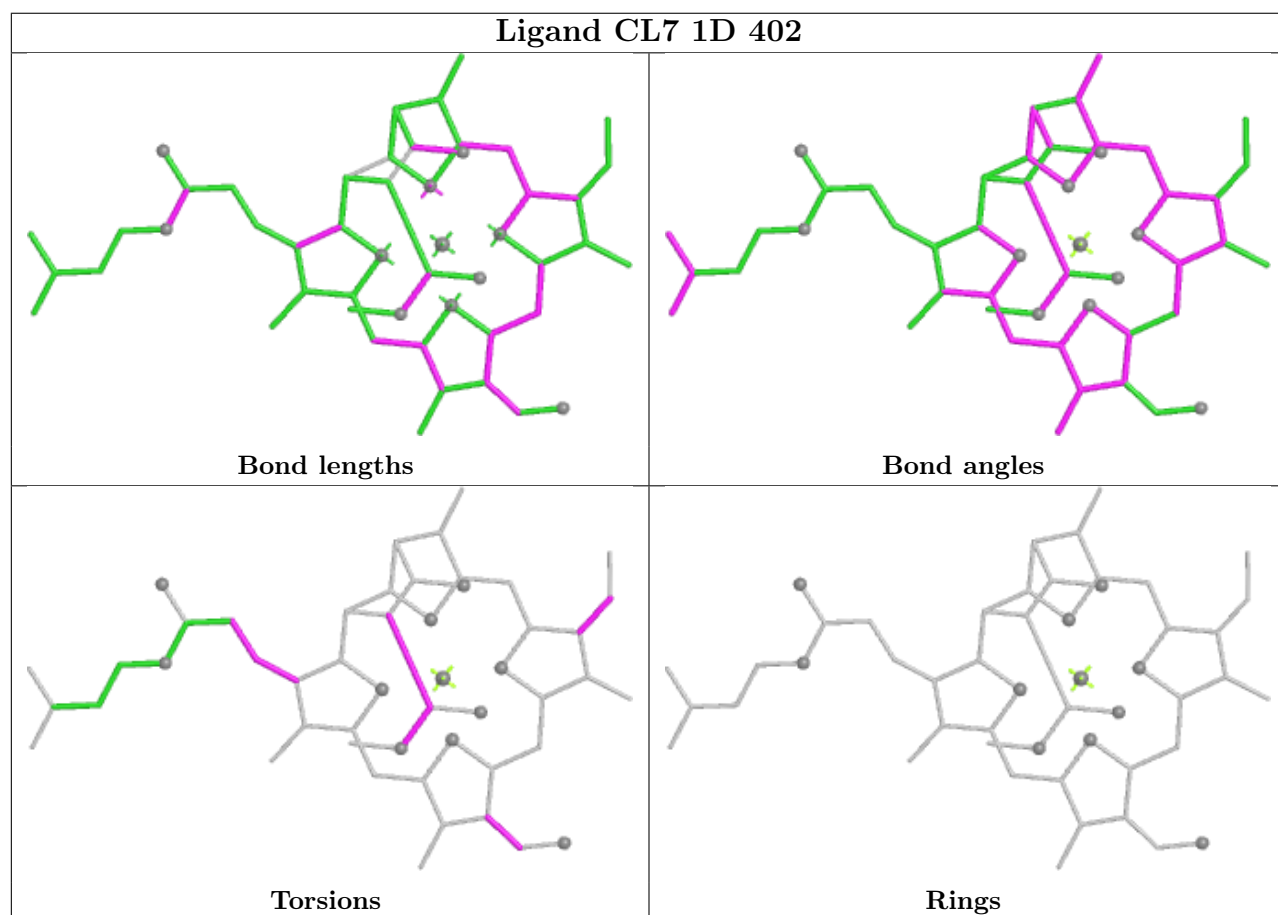
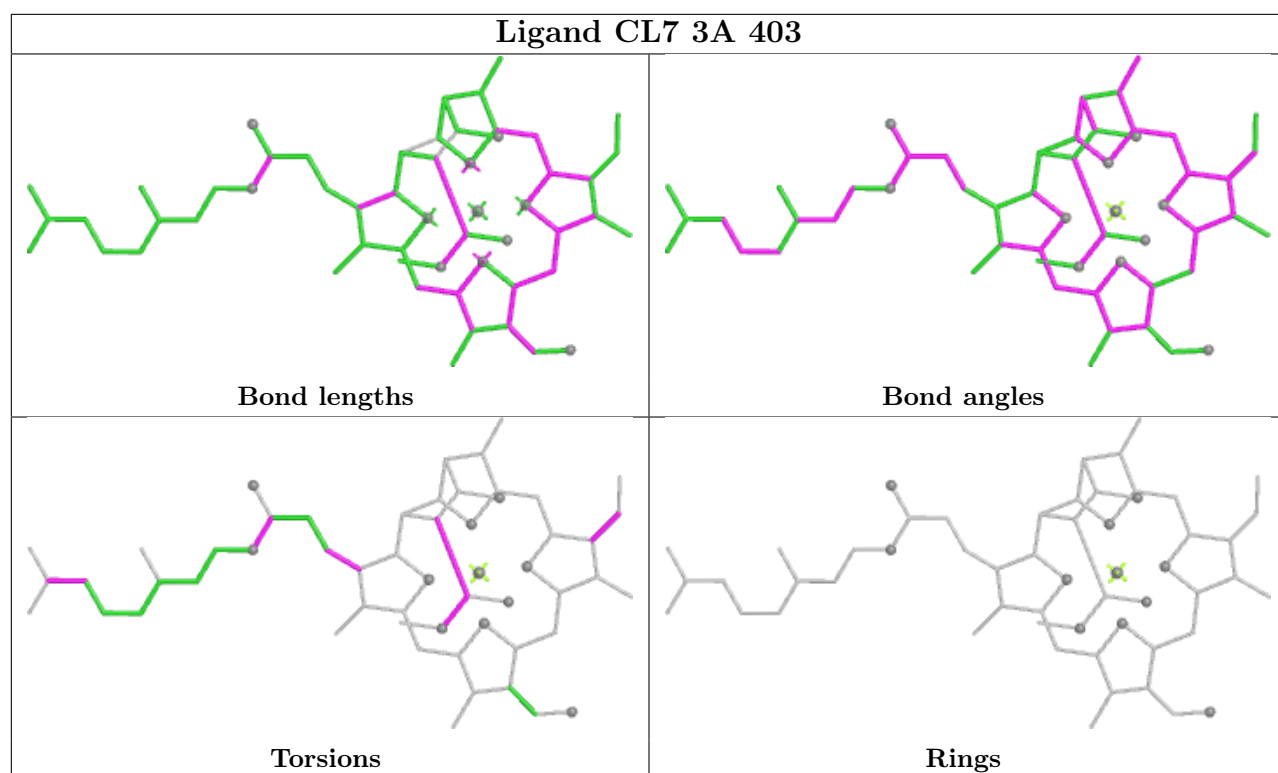
Ligand ZEX 12 522

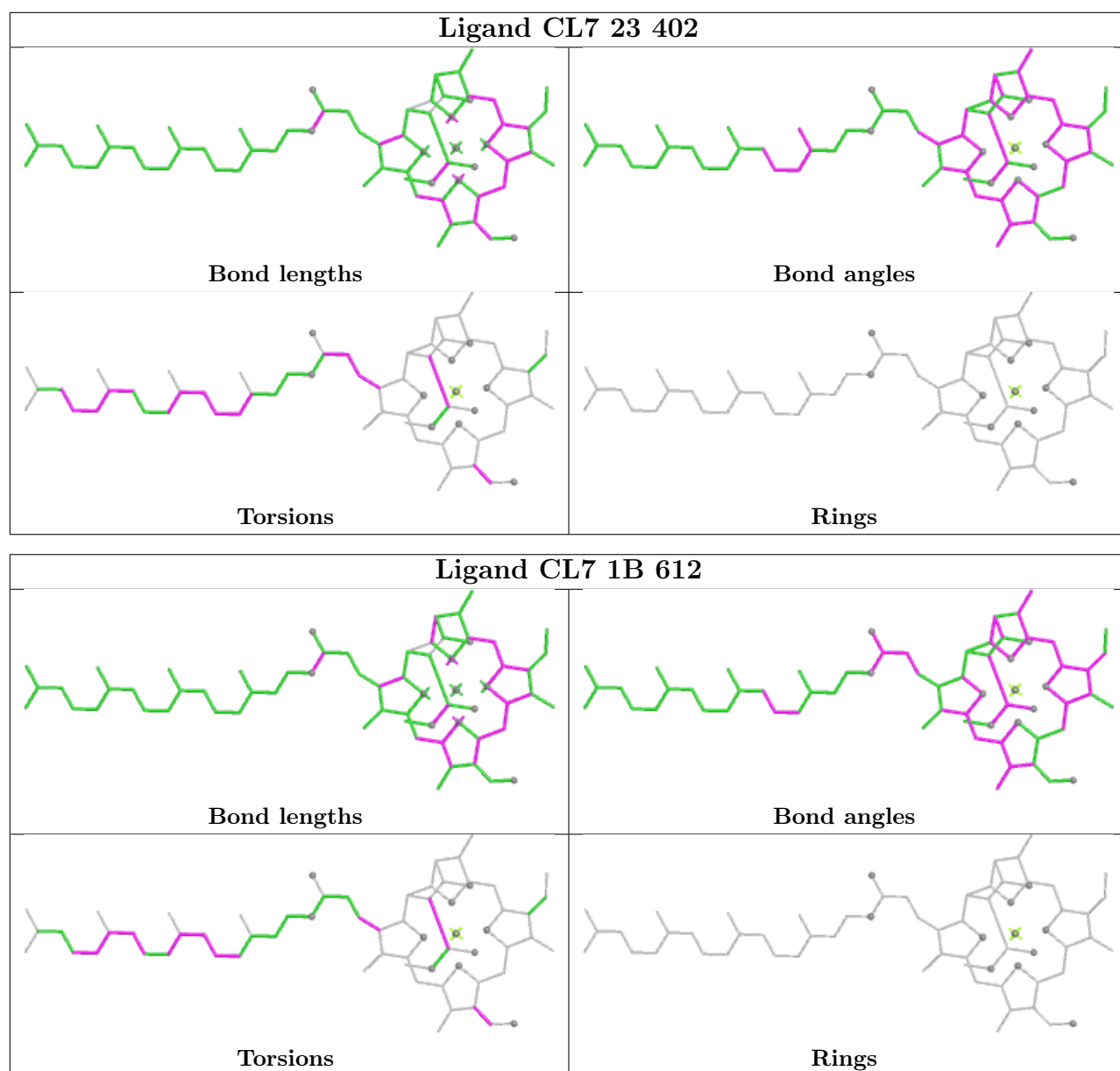


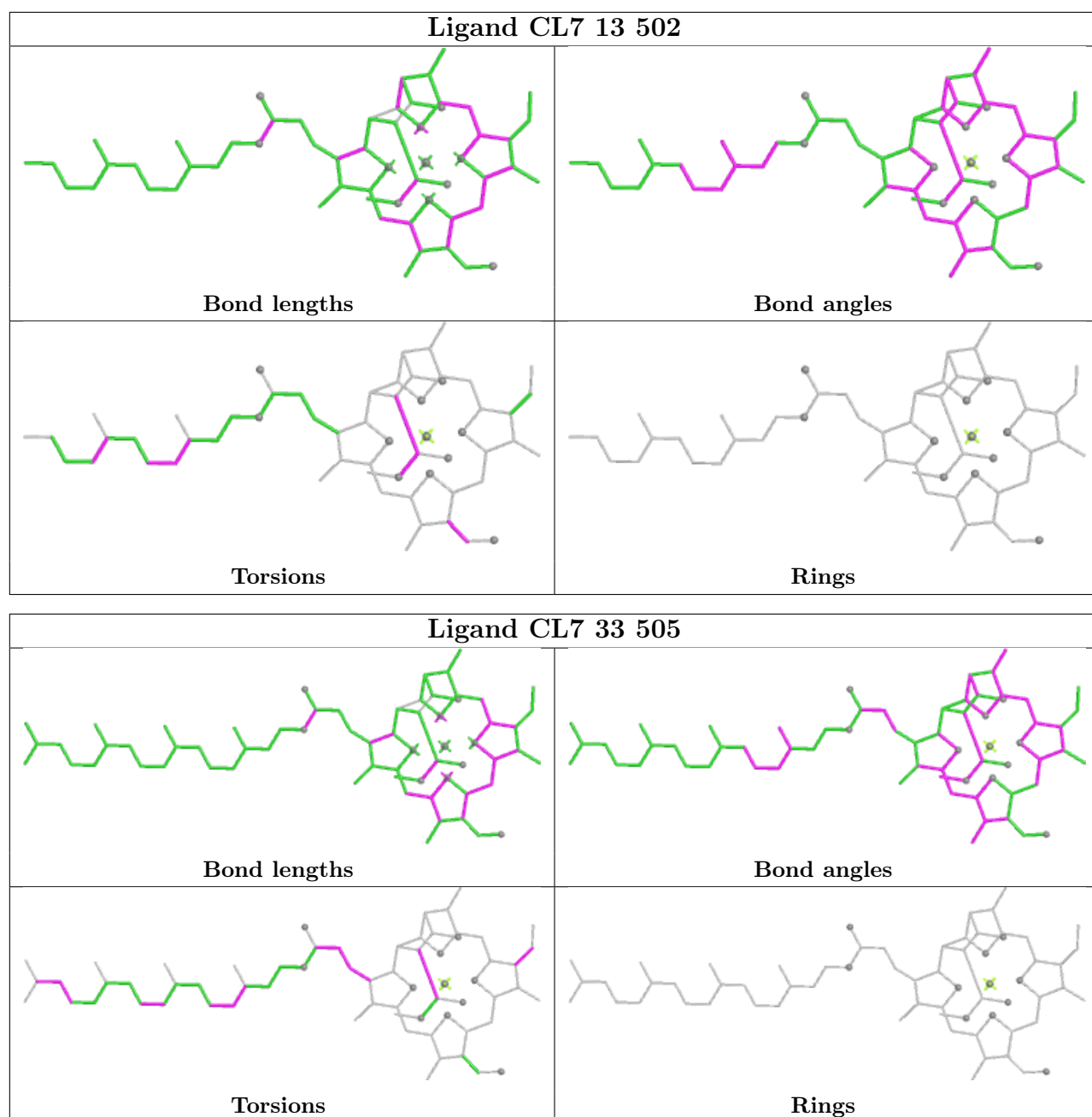


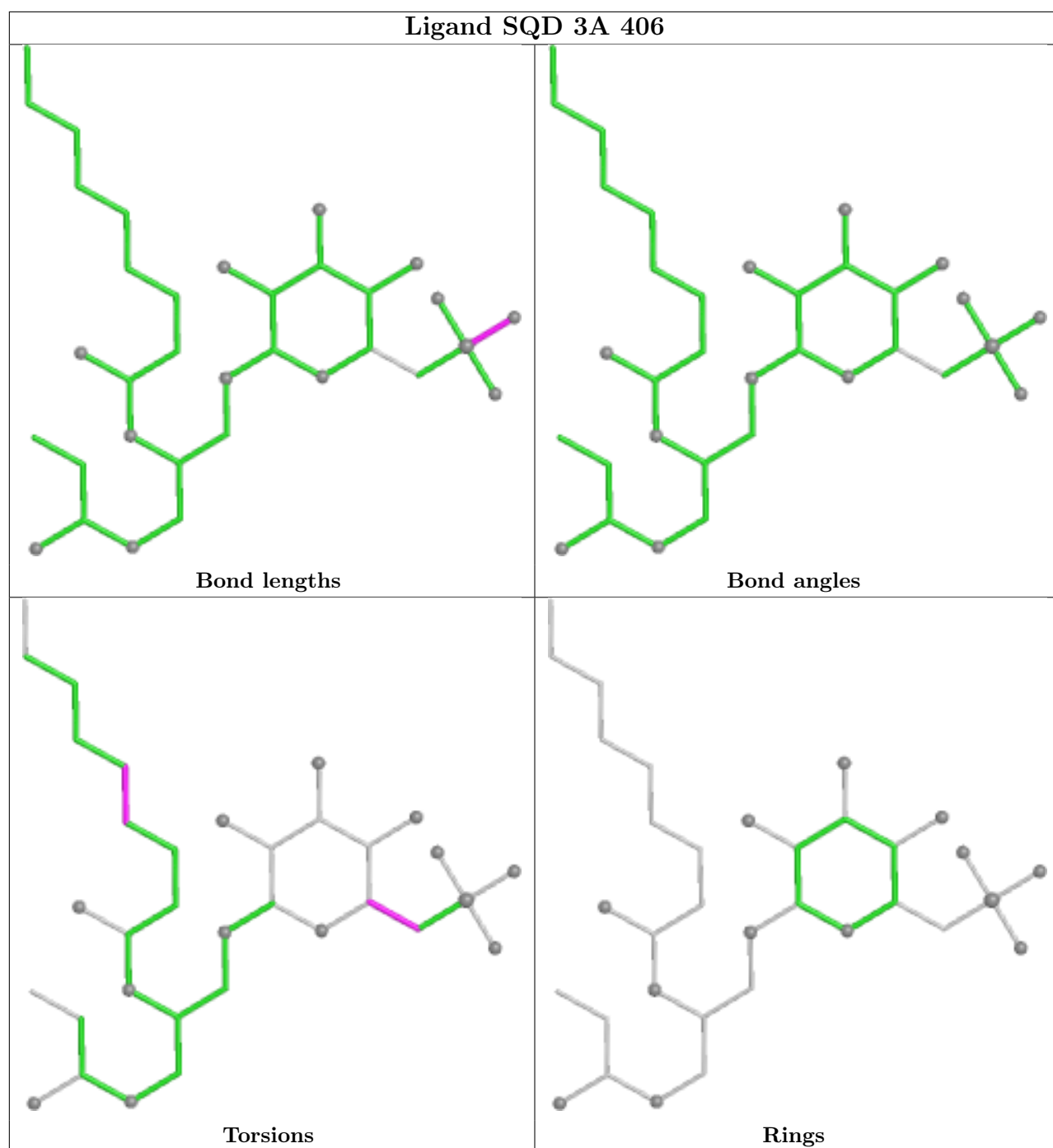


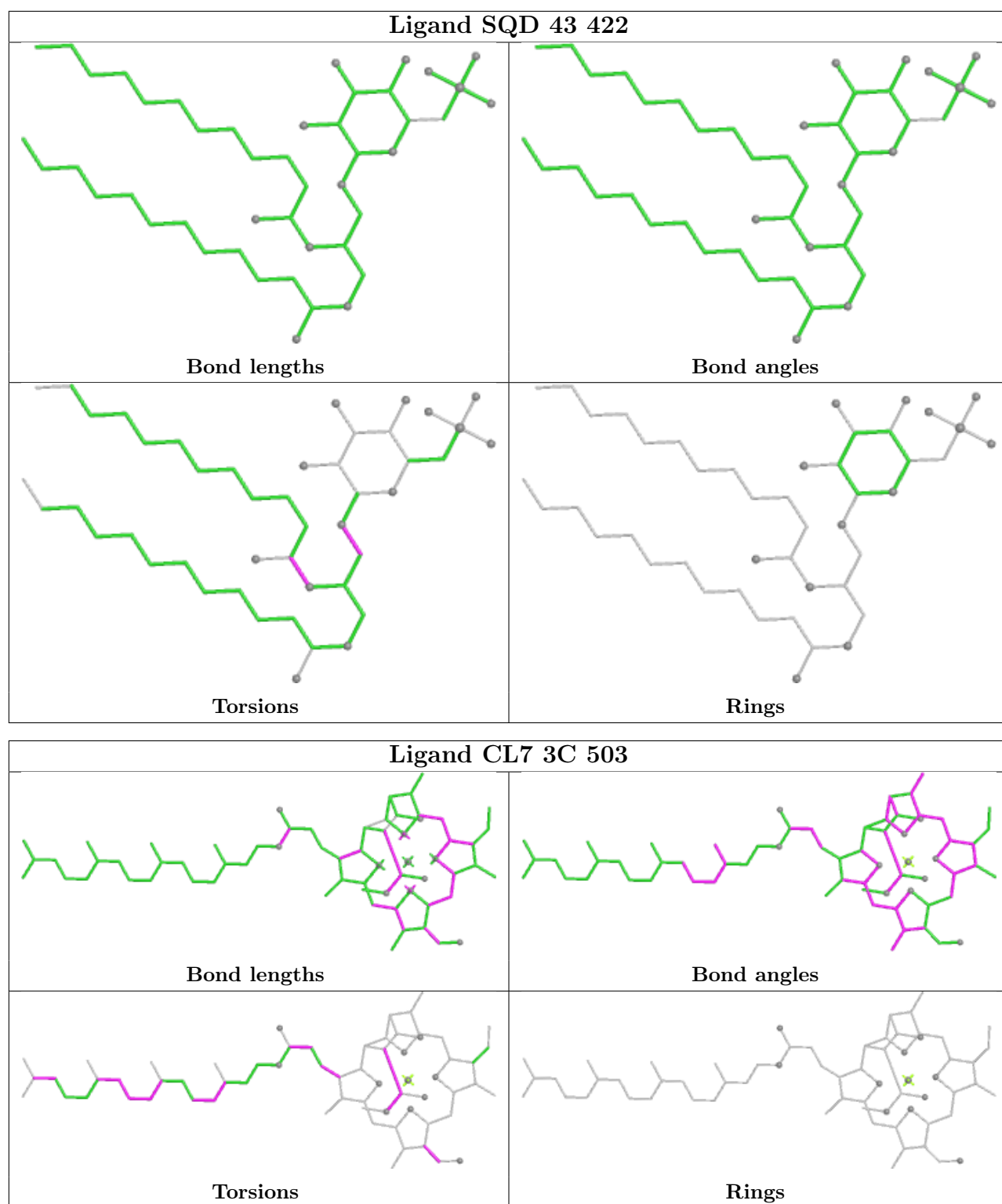


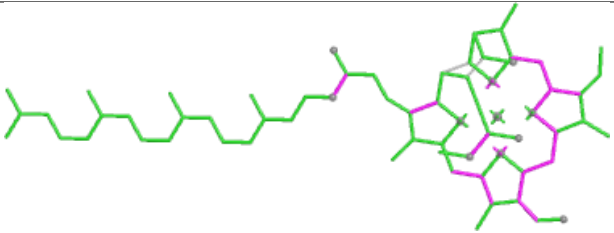
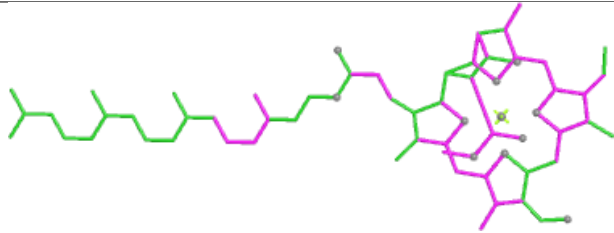
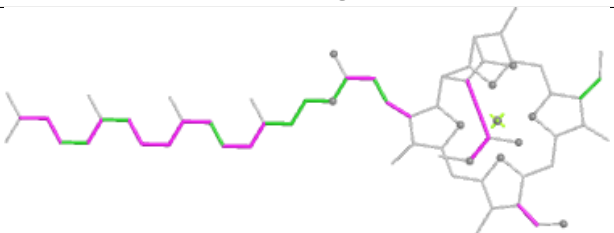
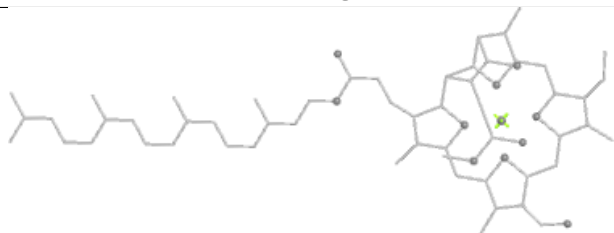


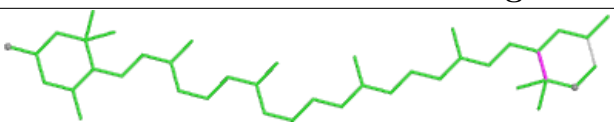
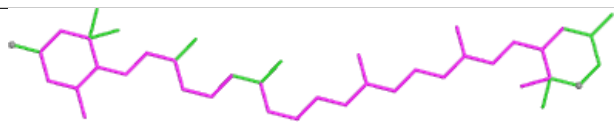
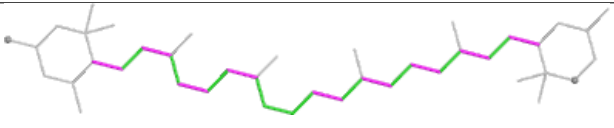
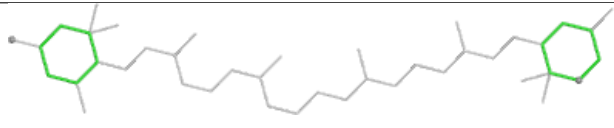


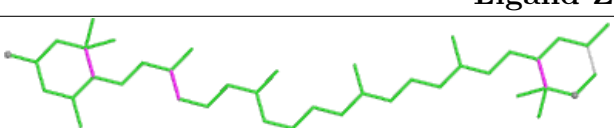
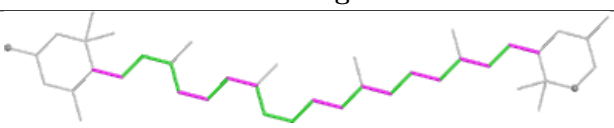
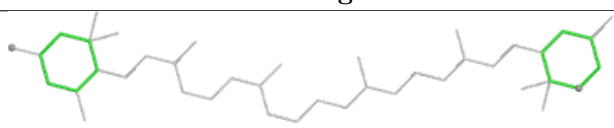


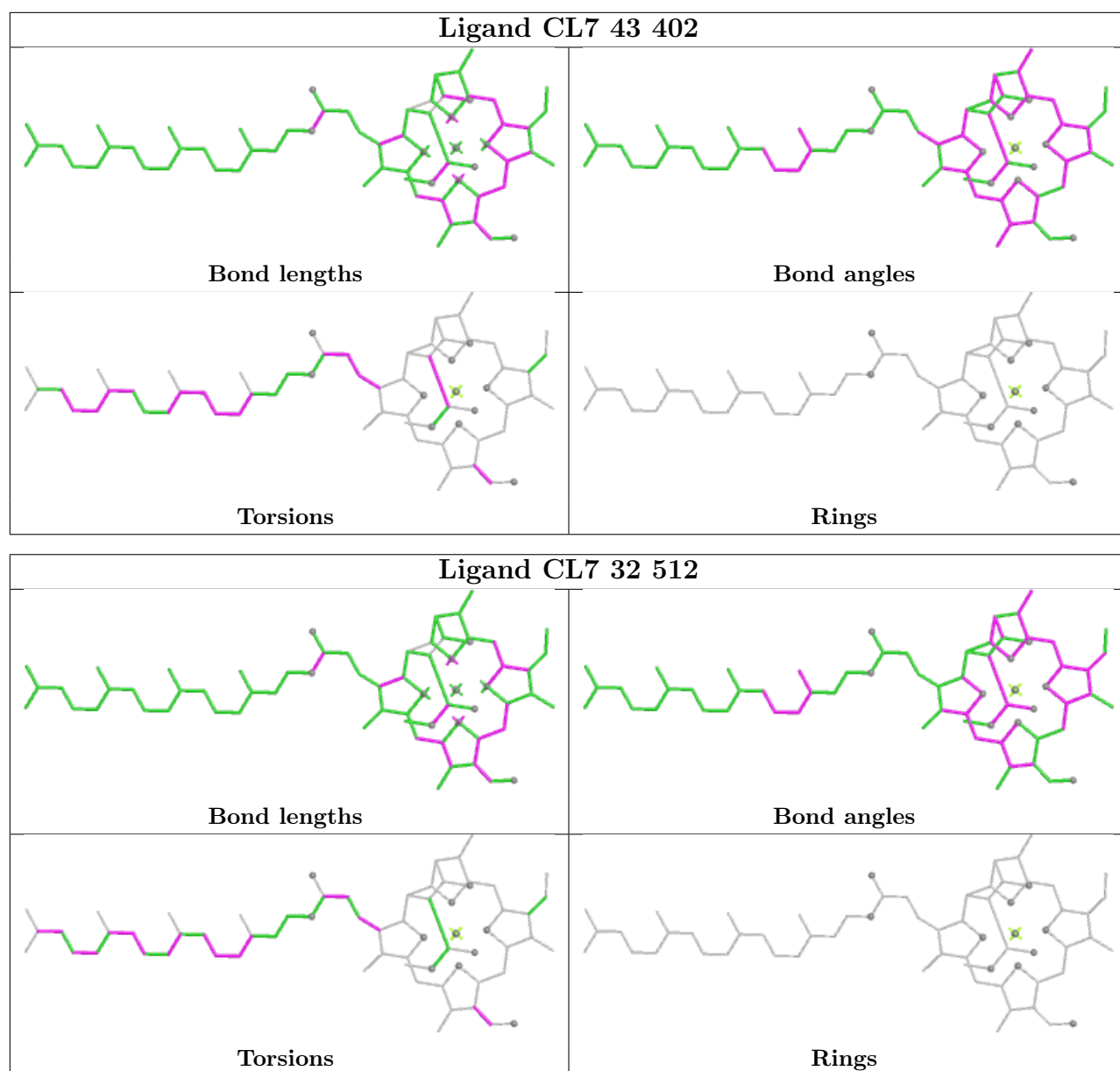




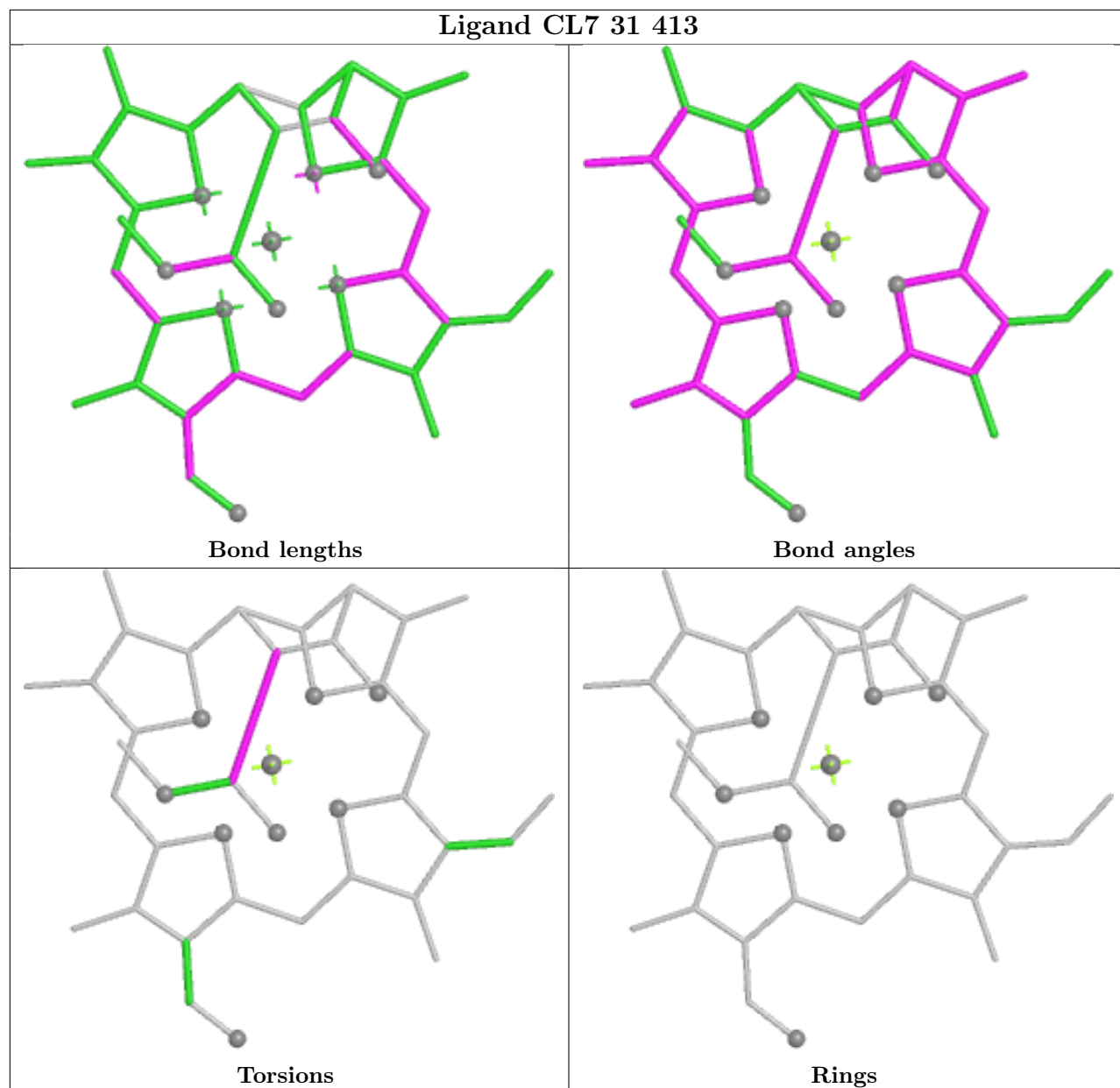
Ligand CL7 31 418	
	
Bond lengths	Bond angles
	
Torsions	Rings

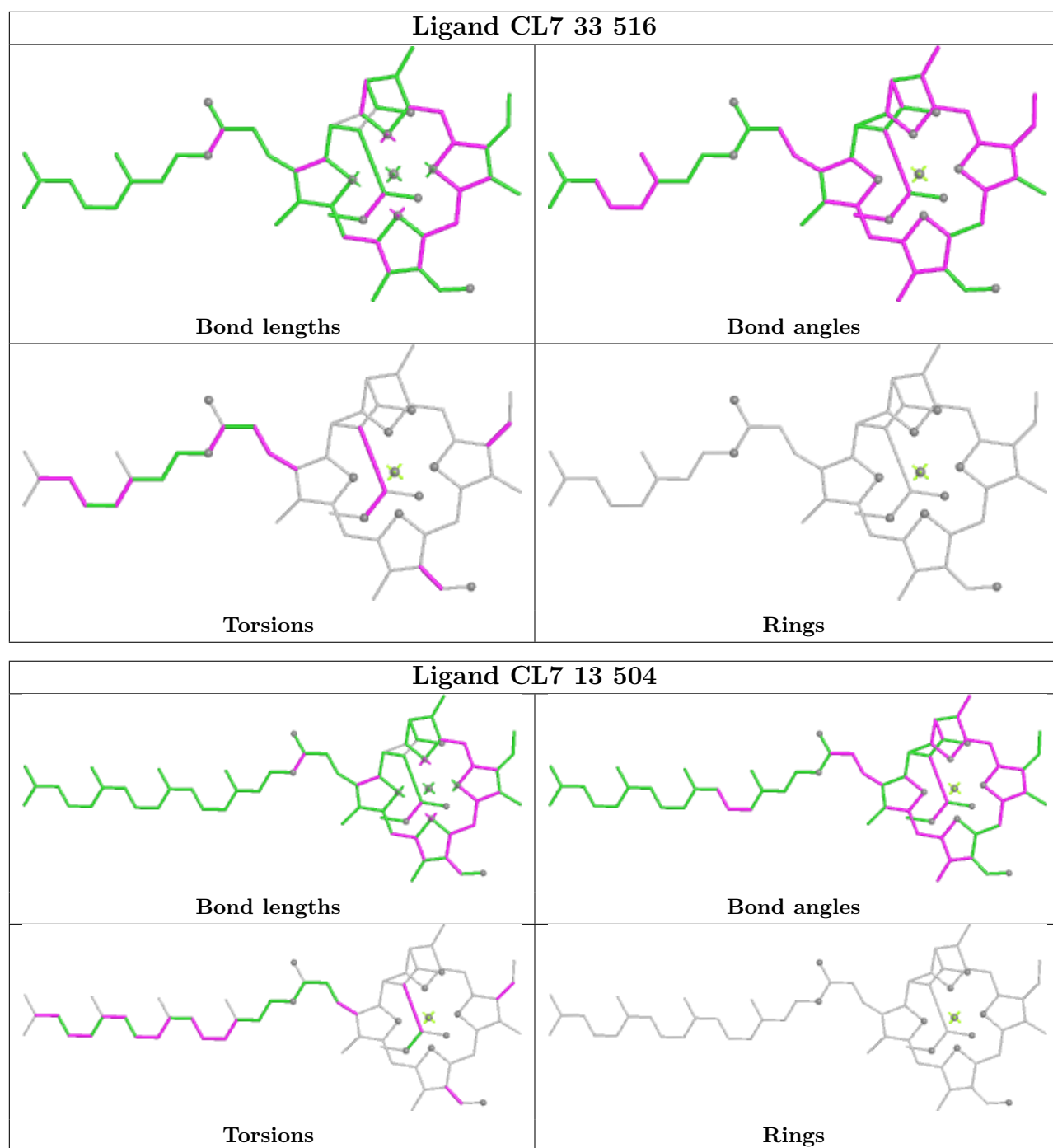
Ligand ZEX 41 421	
	
Bond lengths	Bond angles
	
Torsions	Rings

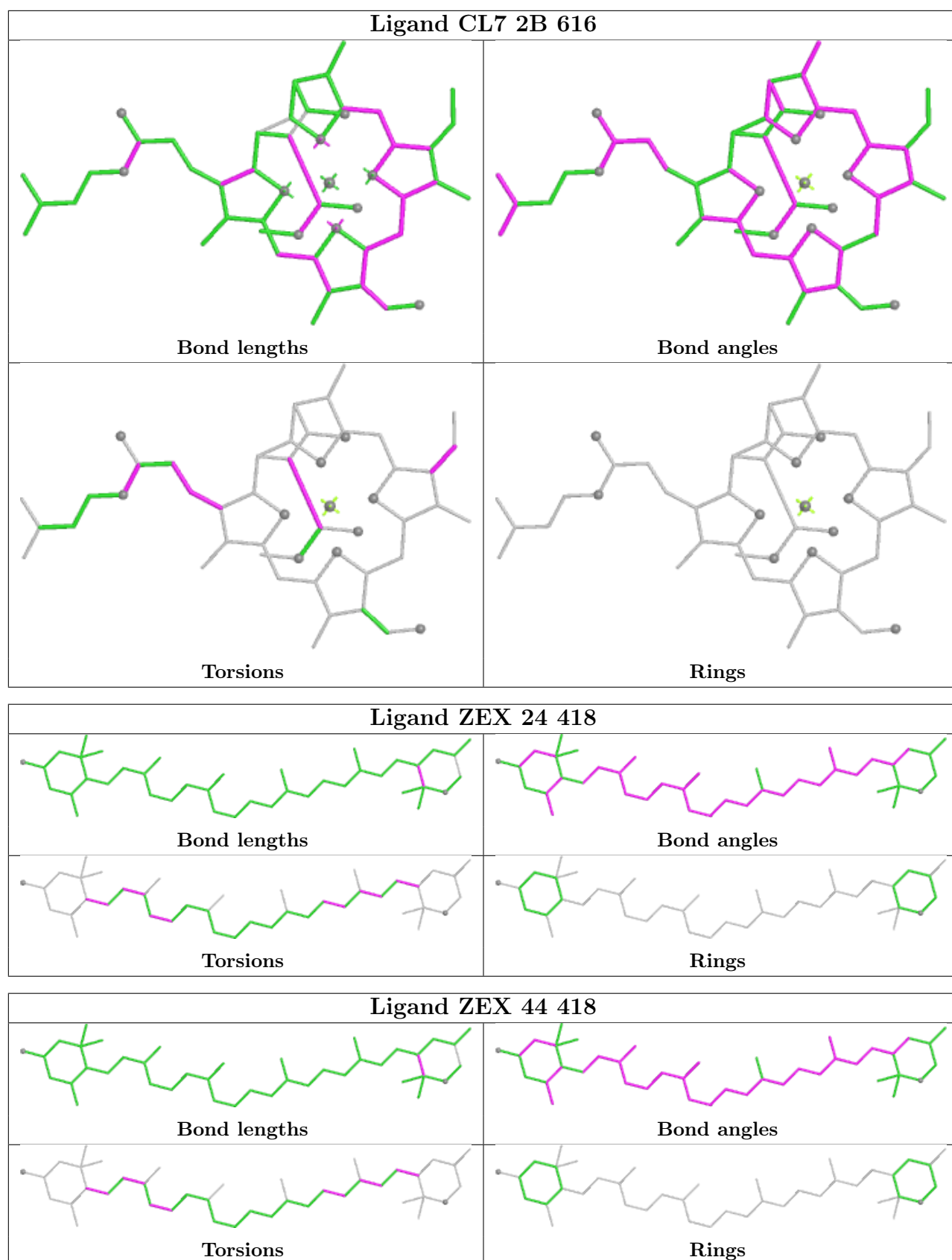
Ligand ZEX 34 420	
	
Bond lengths	Bond angles
	
Torsions	Rings

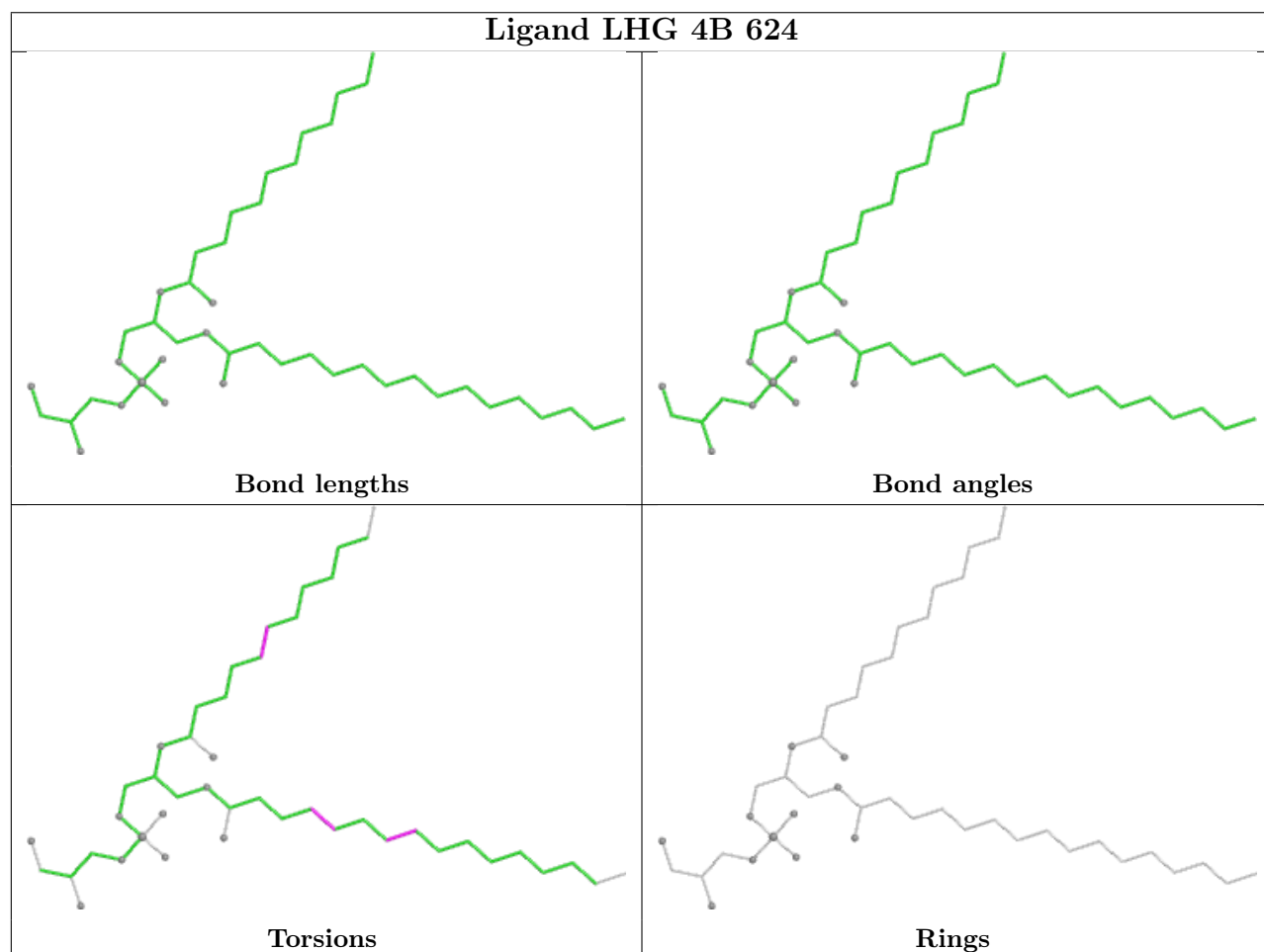
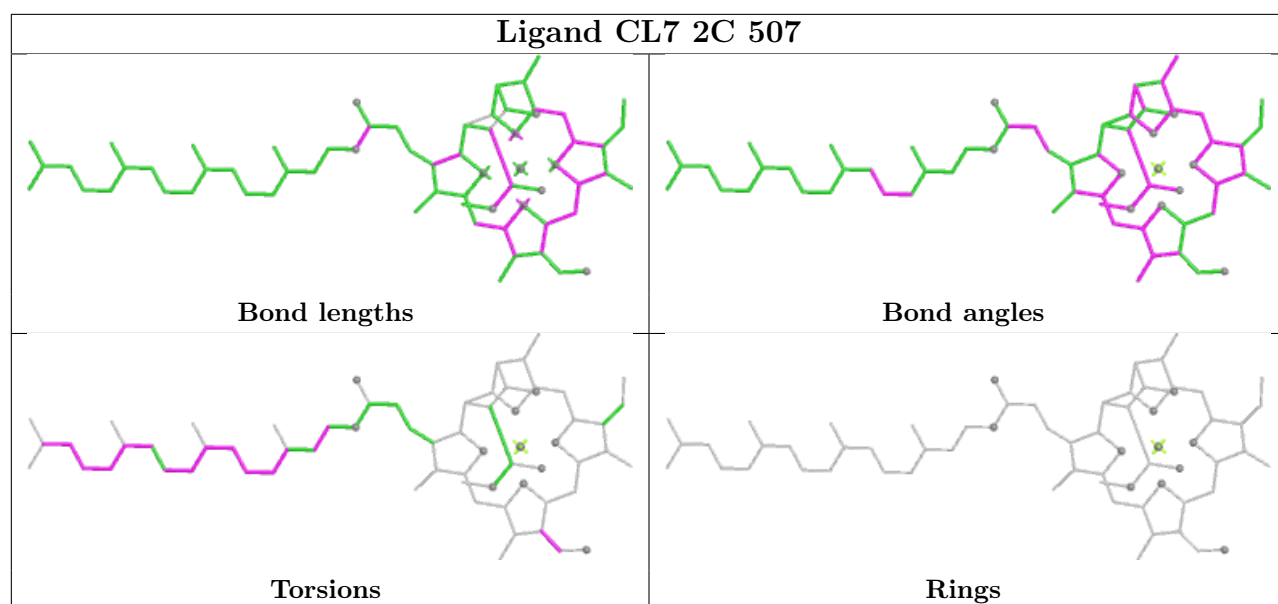


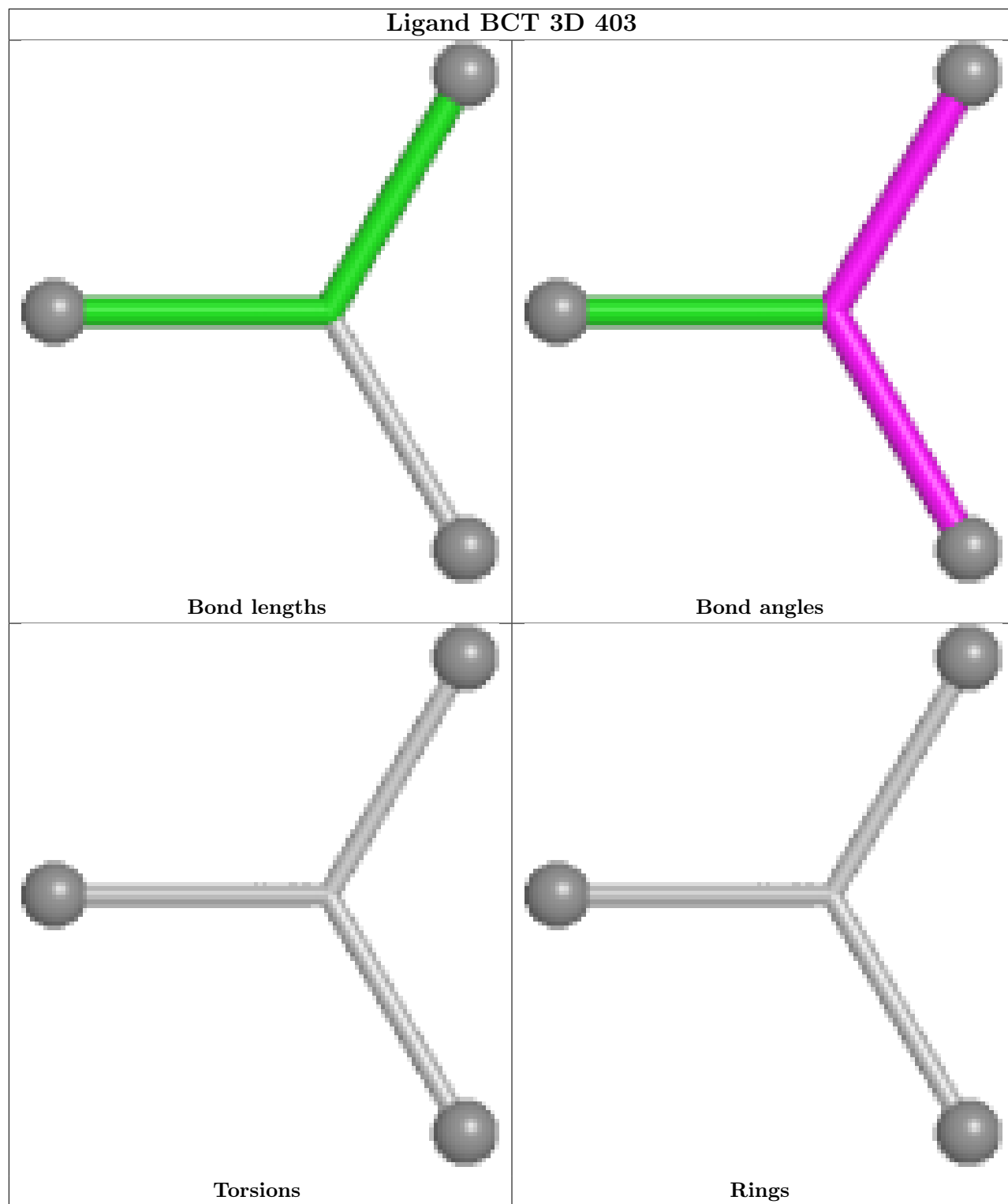
Ligand CL7 31 413

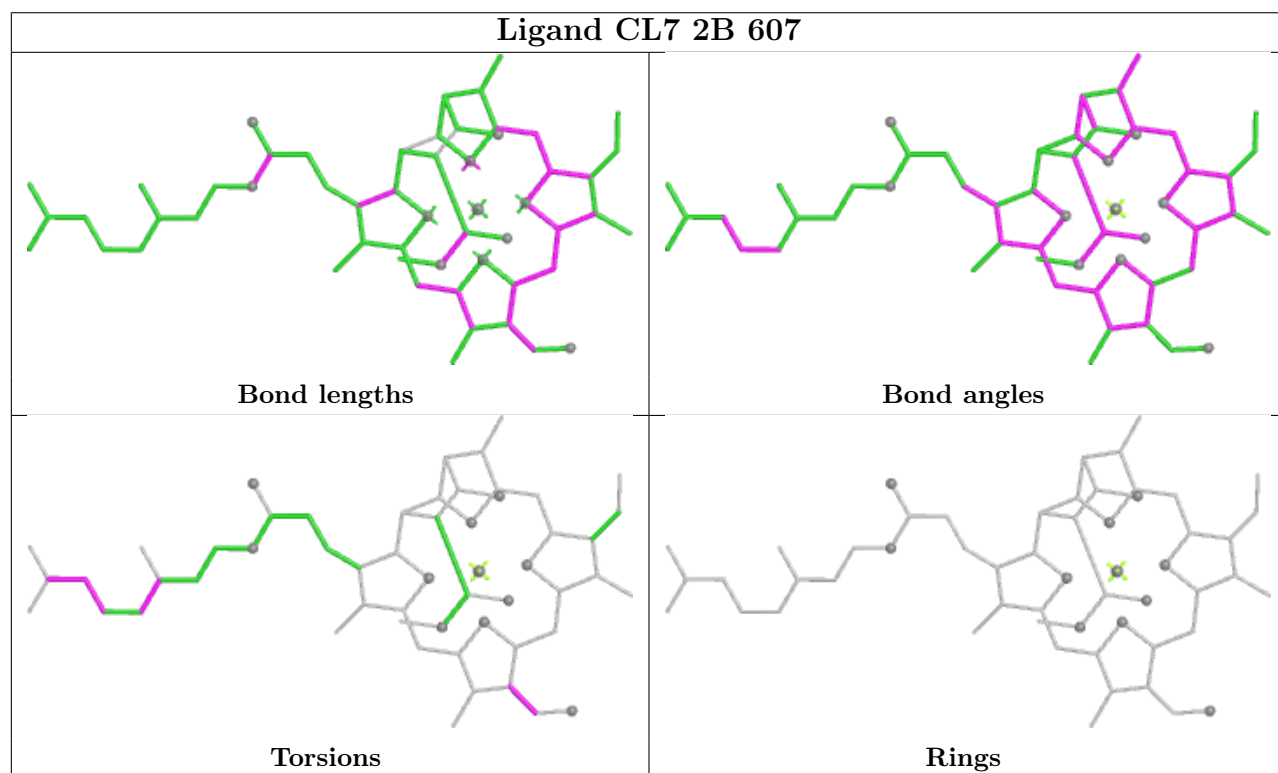
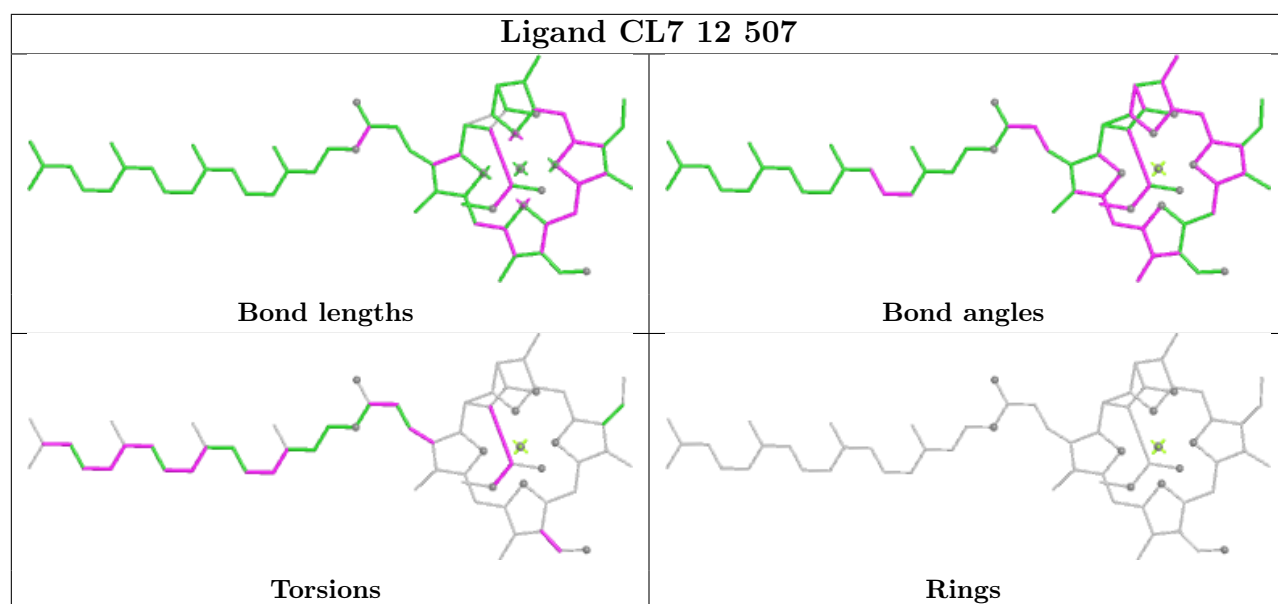


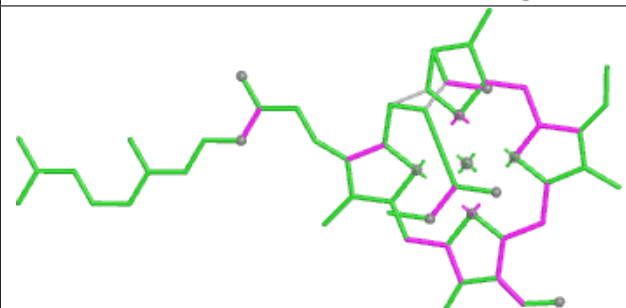
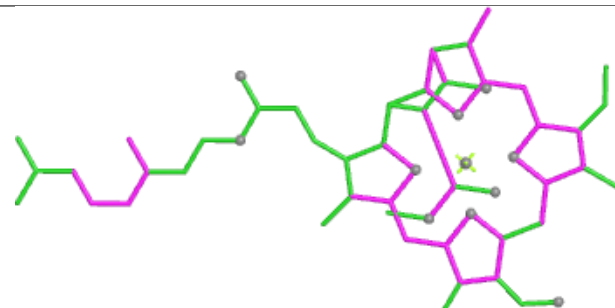
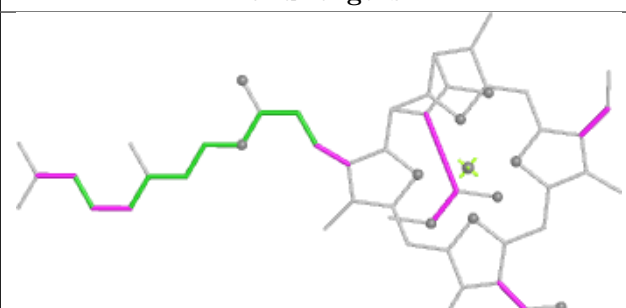
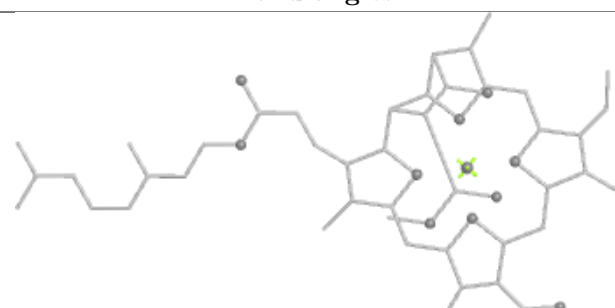


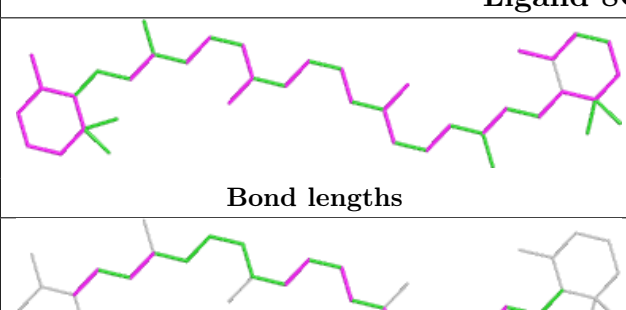
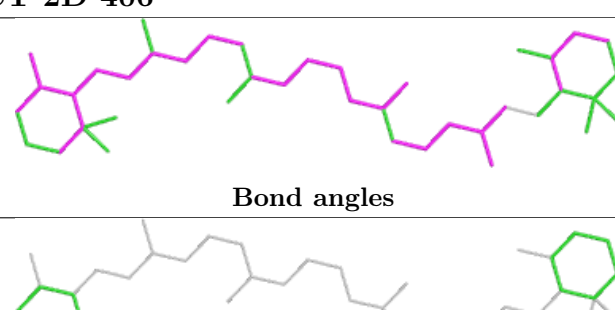
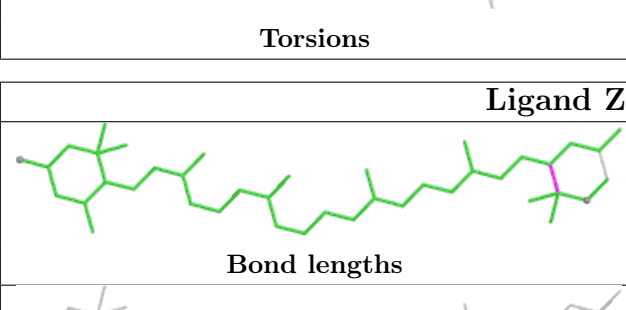
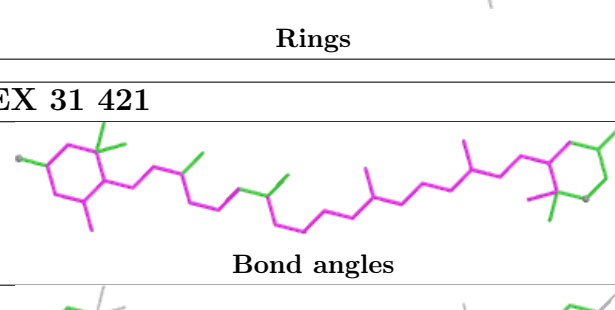


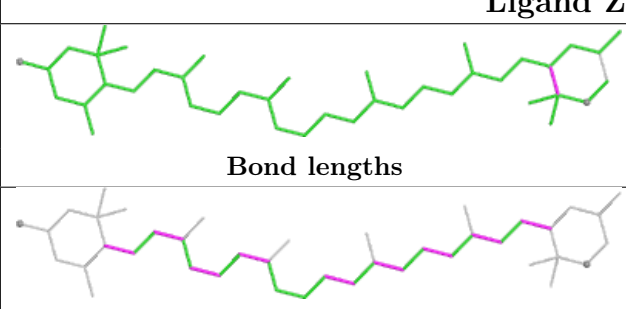
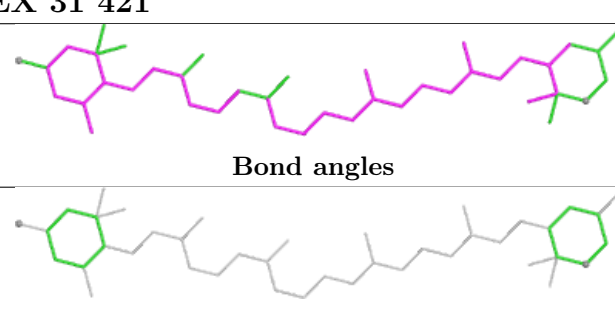
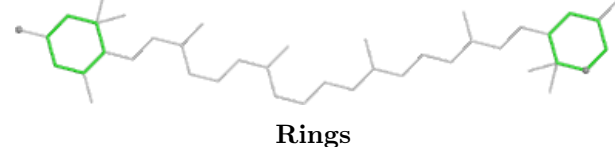


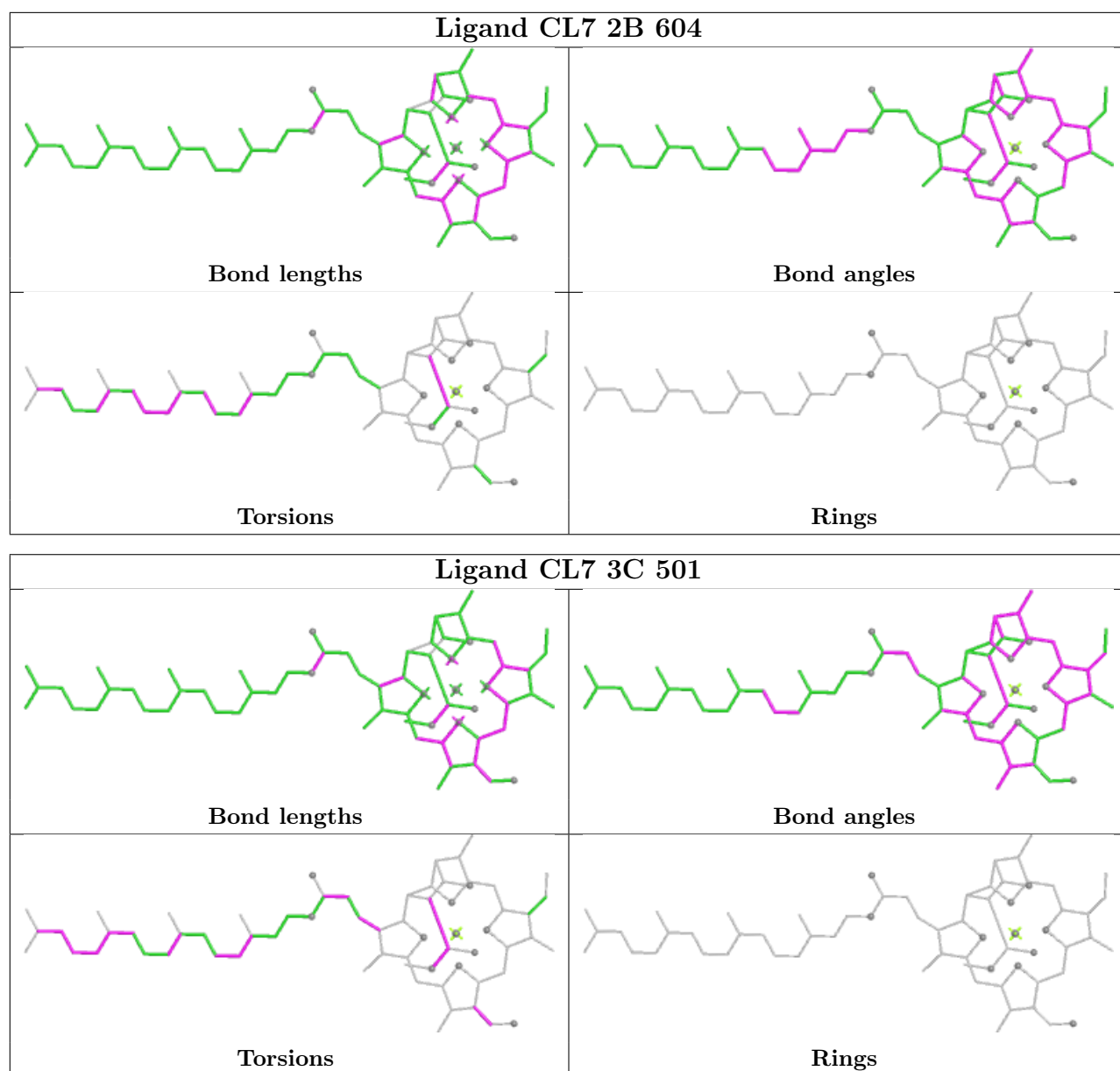


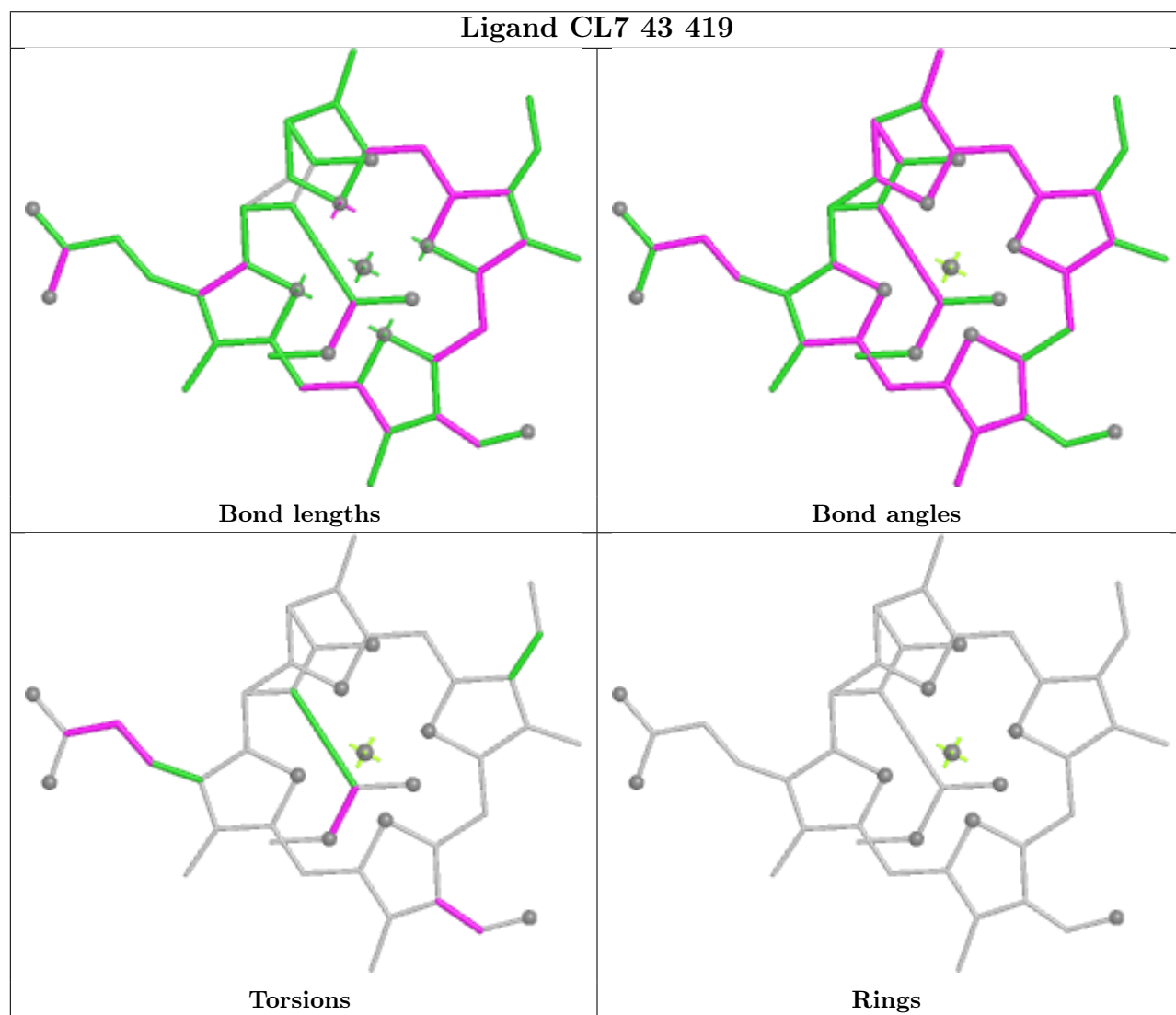
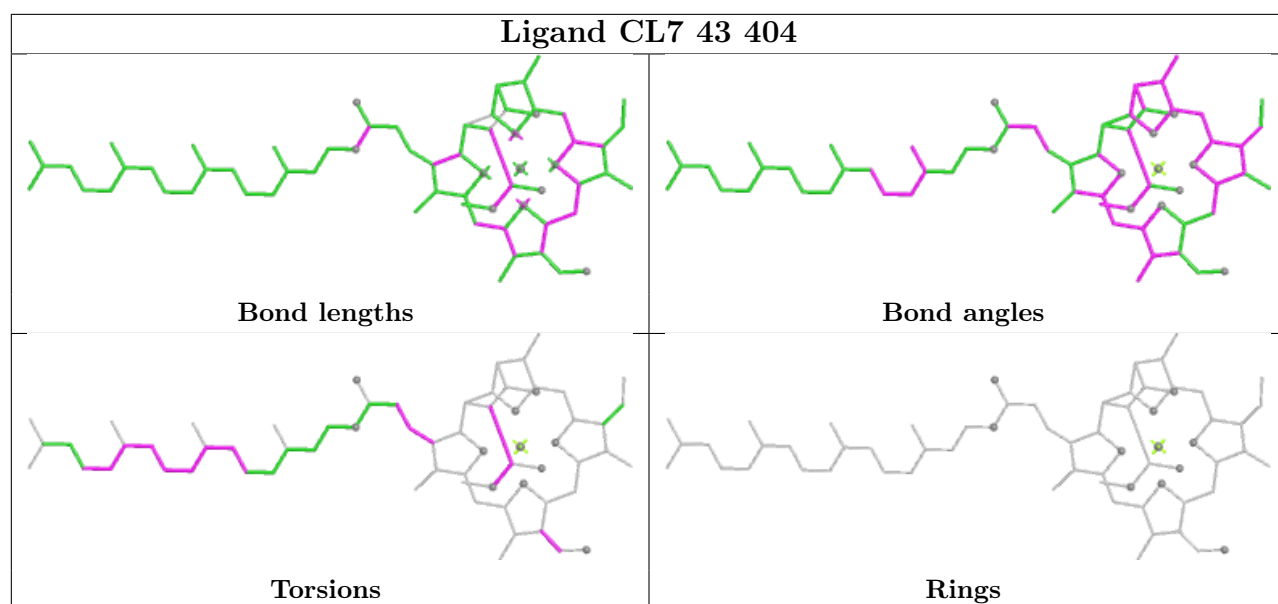


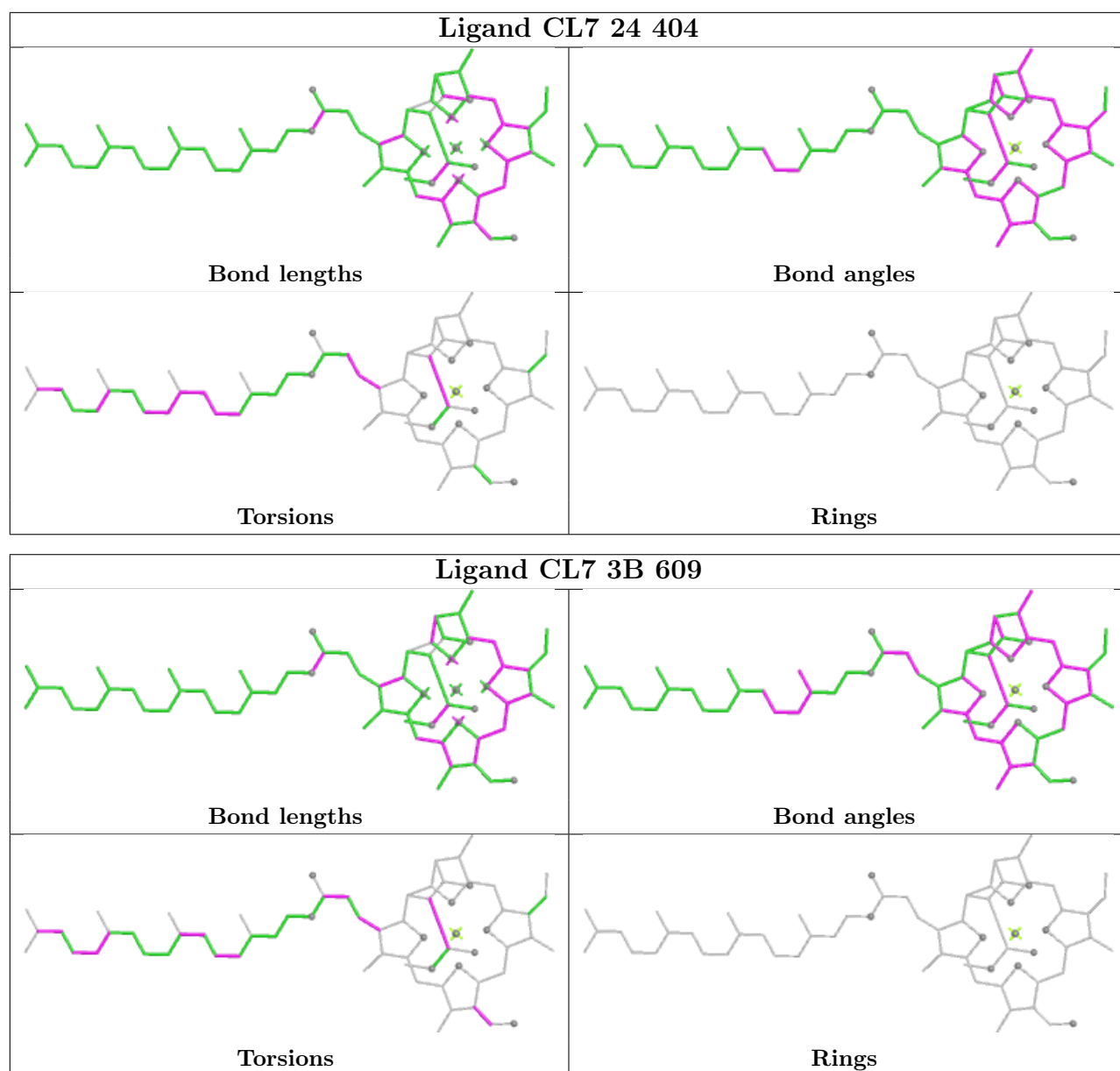
Ligand CL7 4C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

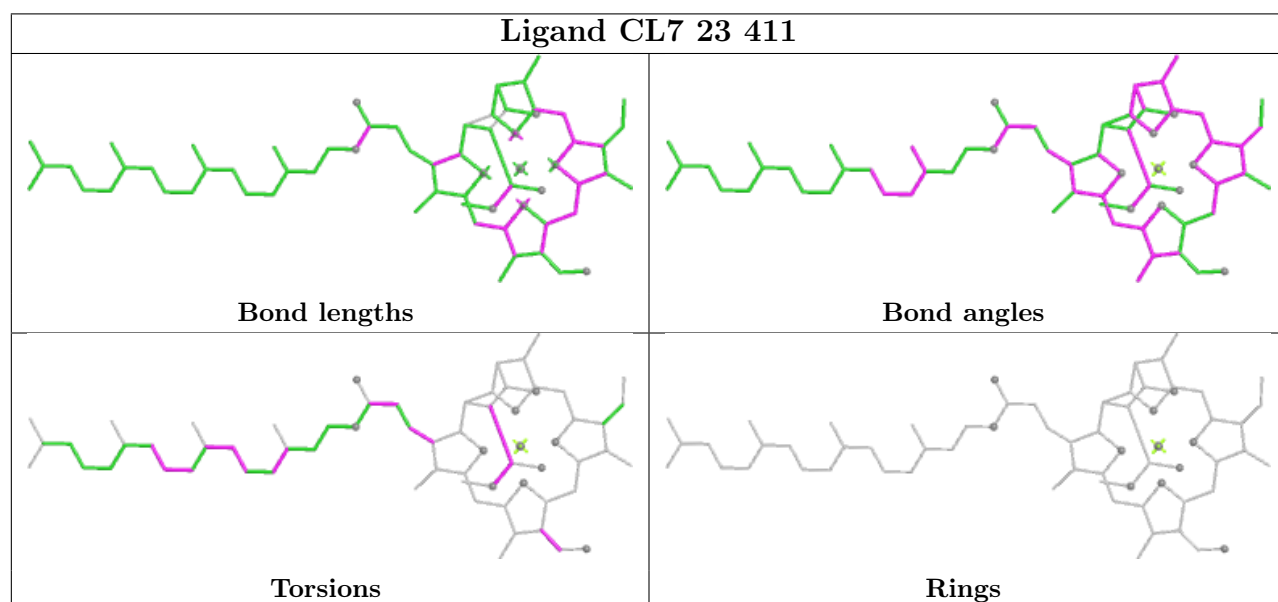
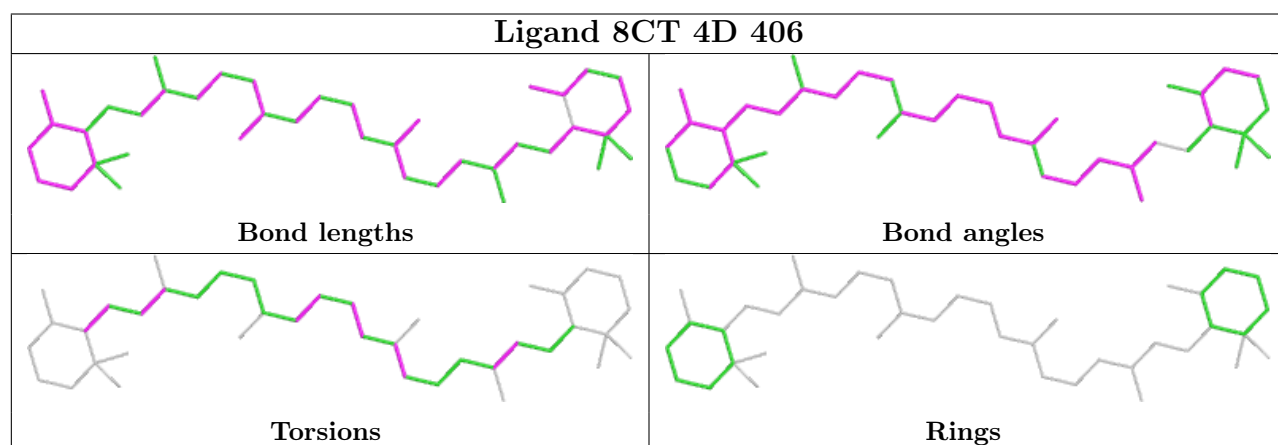
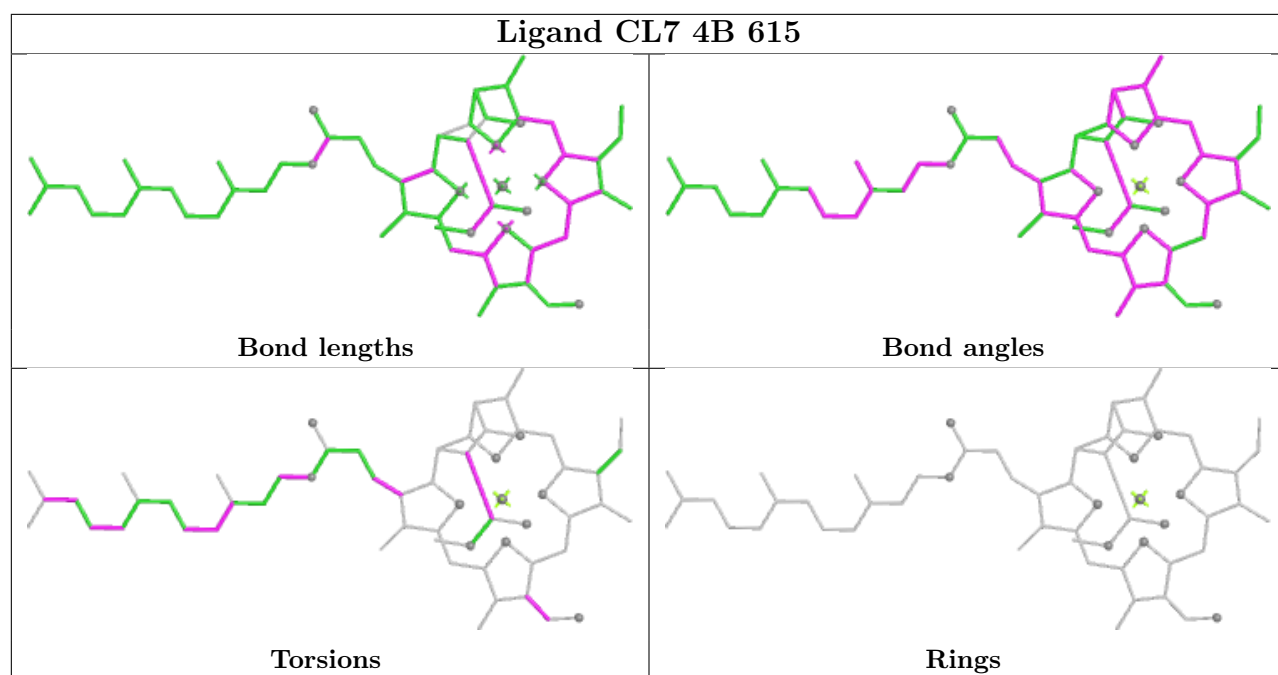
Ligand 8CT 2D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

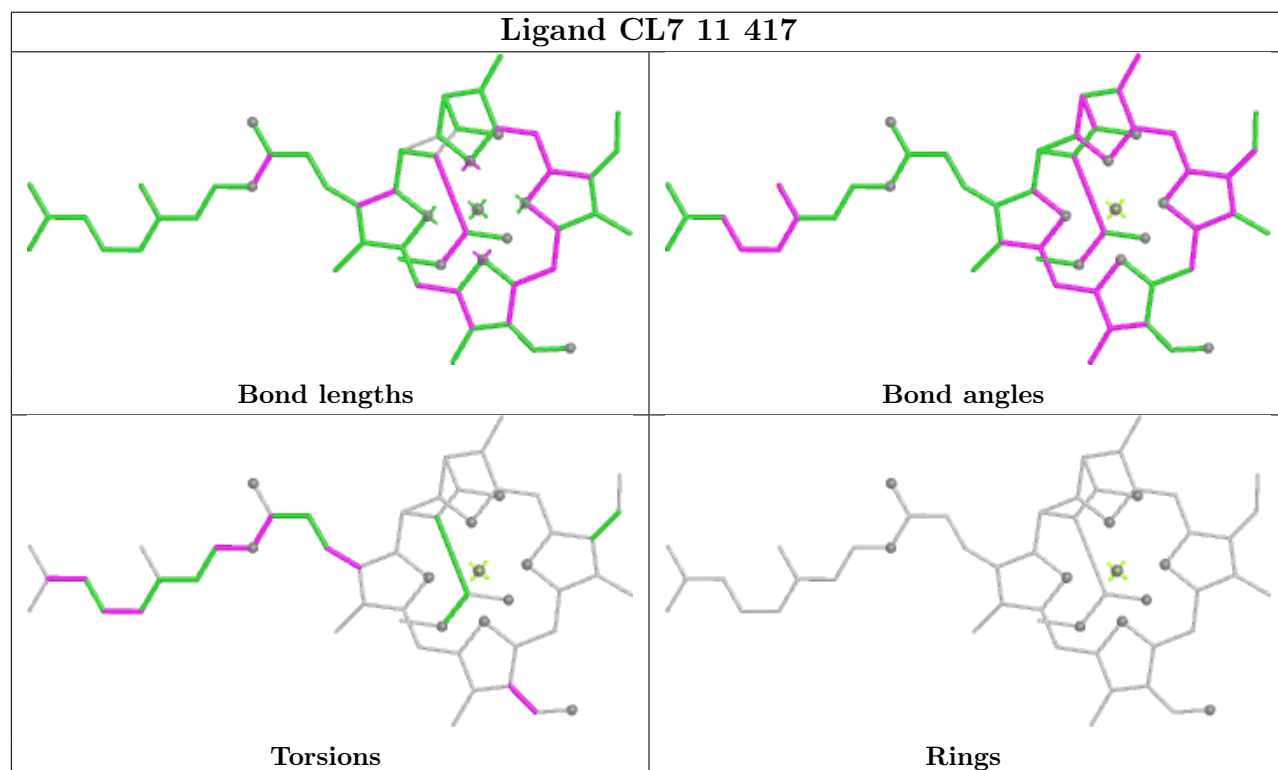
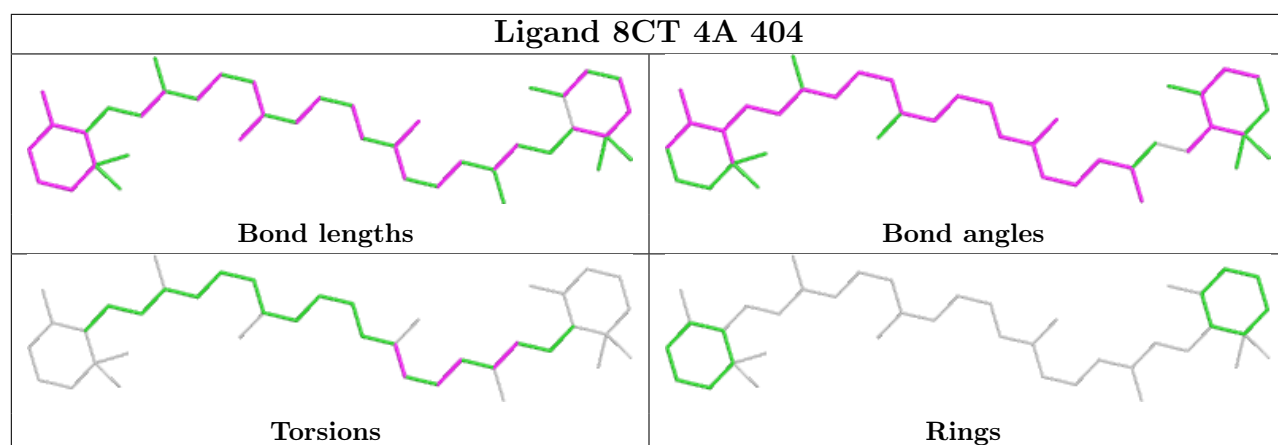
Ligand ZEX 31 421	
	
Bond lengths	Bond angles
	
Torsions	Rings

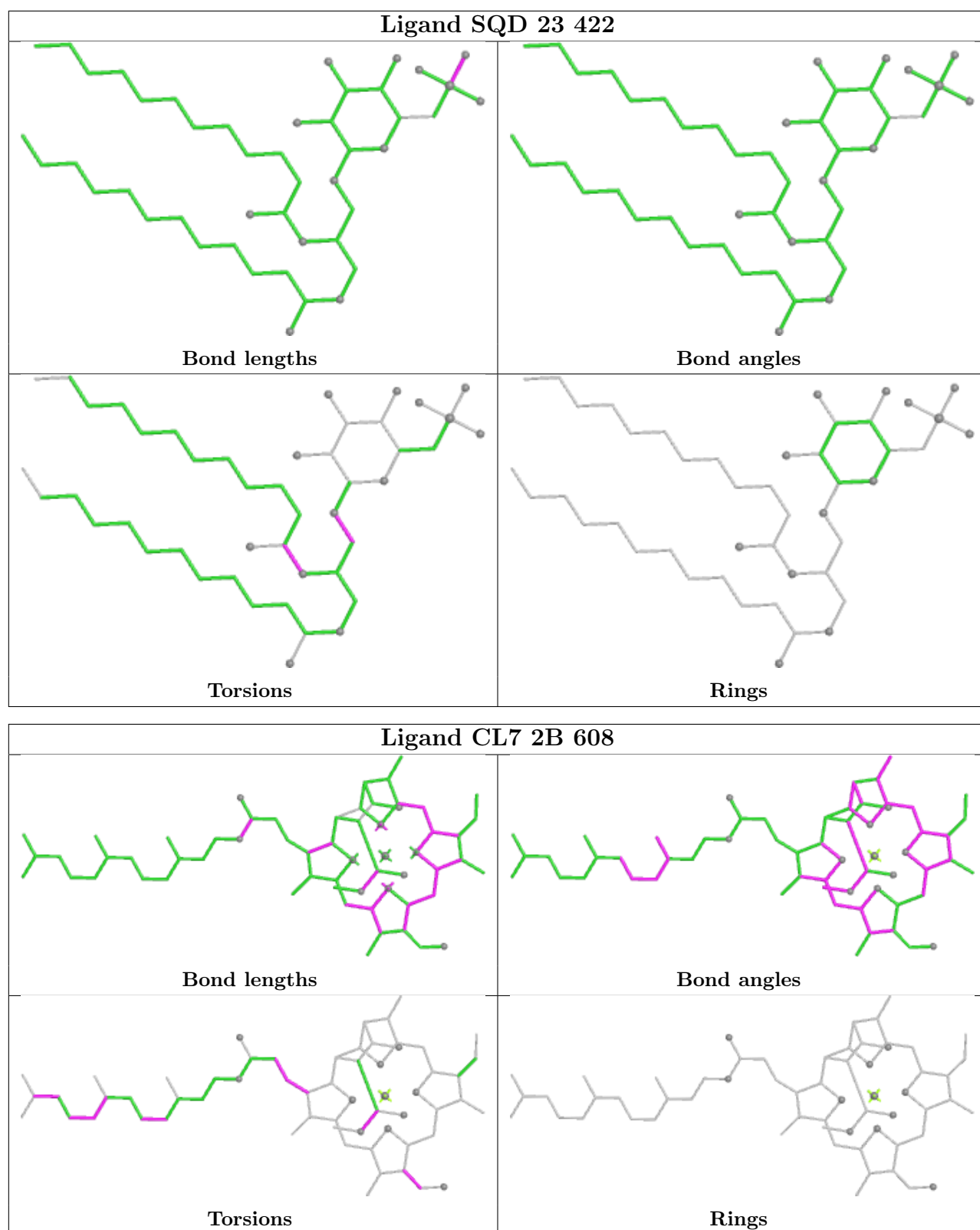


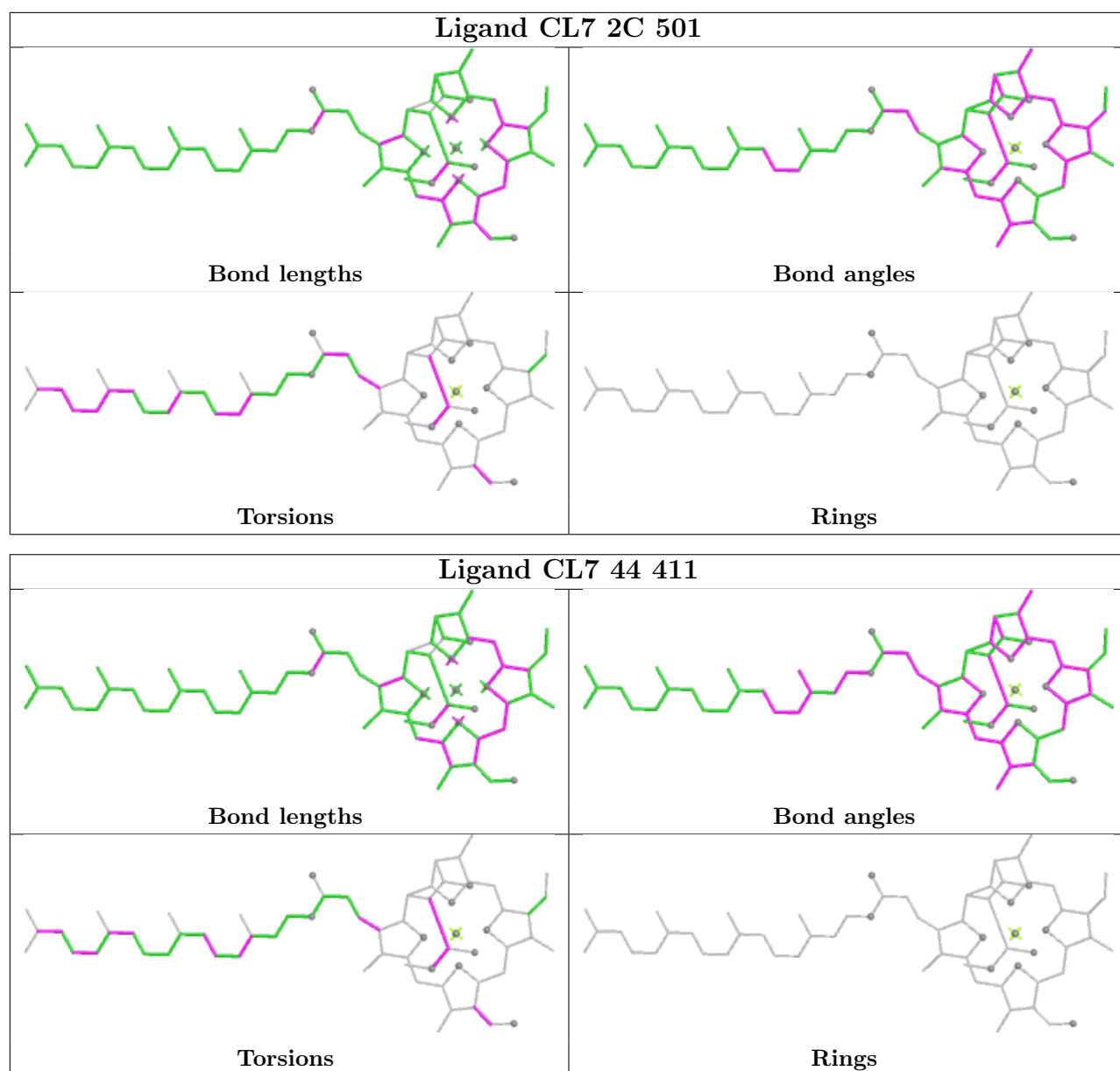




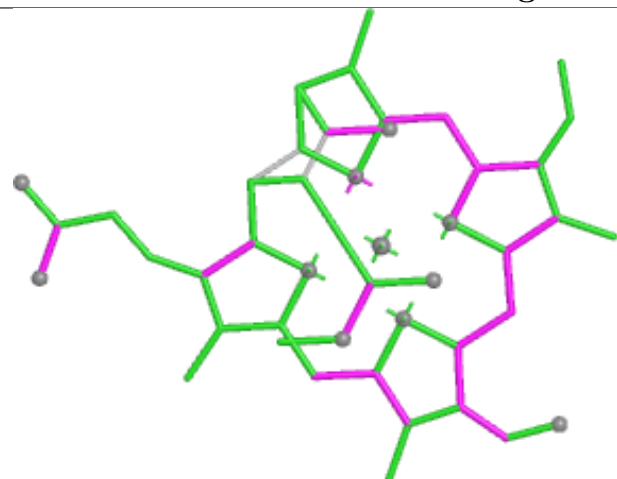




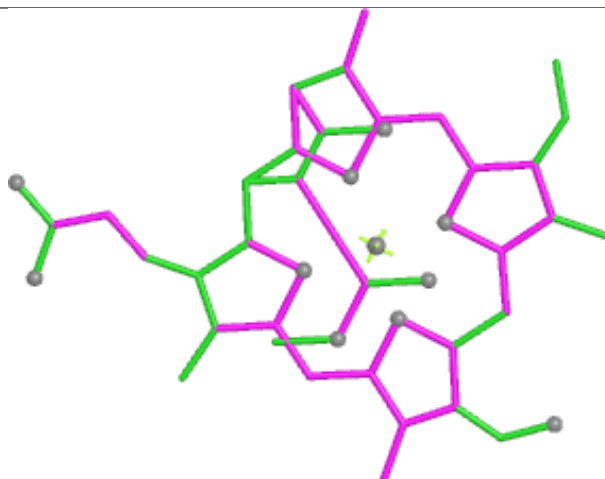




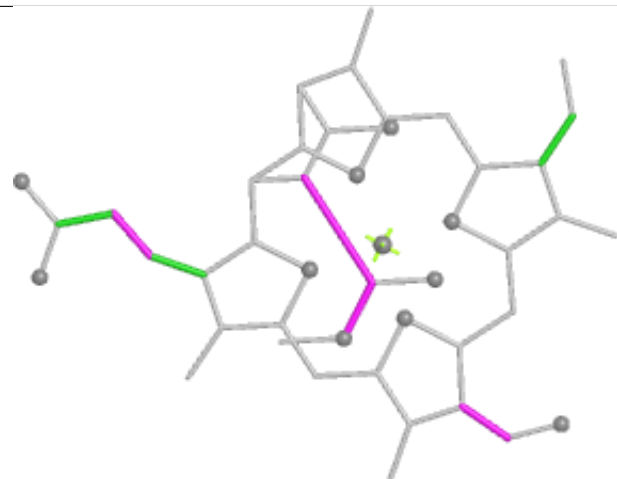
Ligand CL7 31 409



Bond lengths



Bond angles

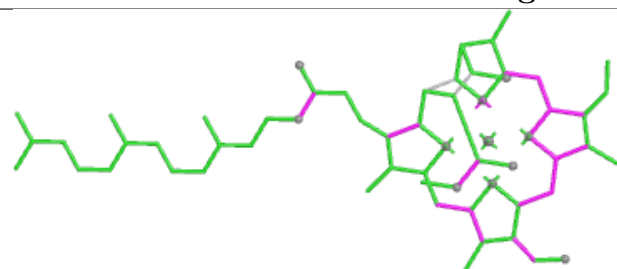


Torsions

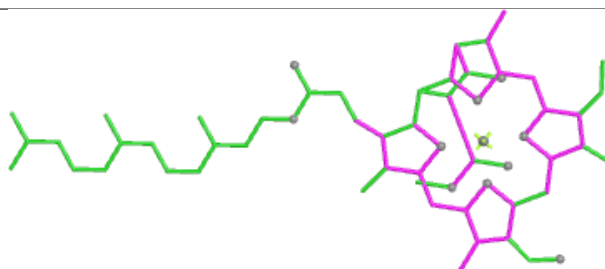


Rings

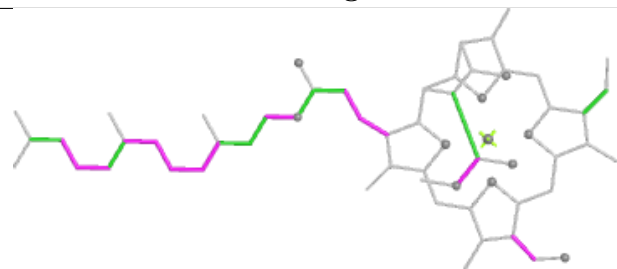
Ligand CL7 41 402



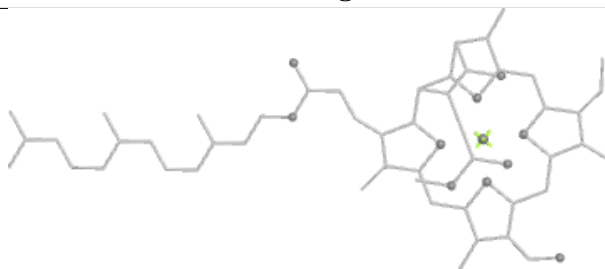
Bond lengths



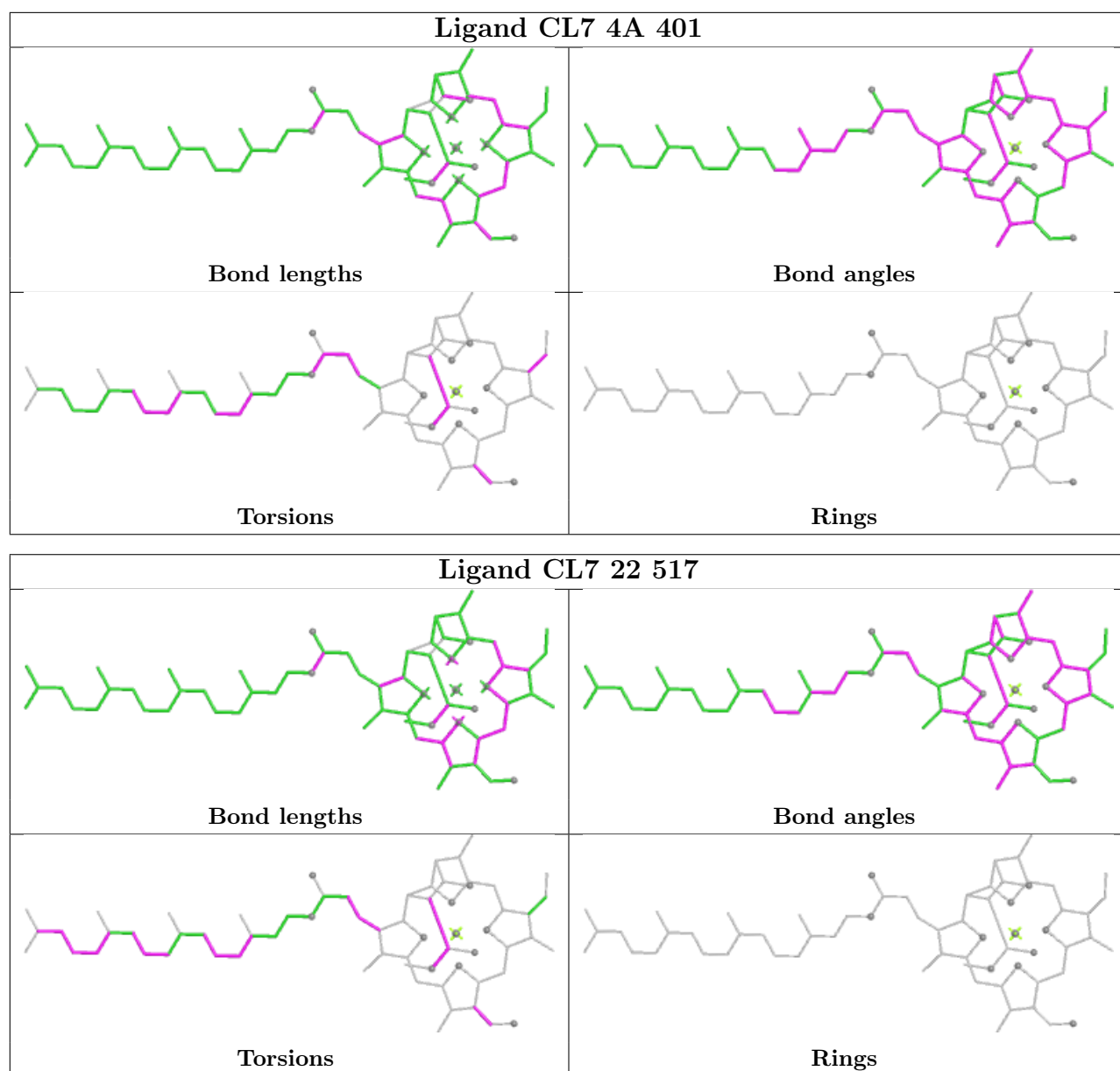
Bond angles

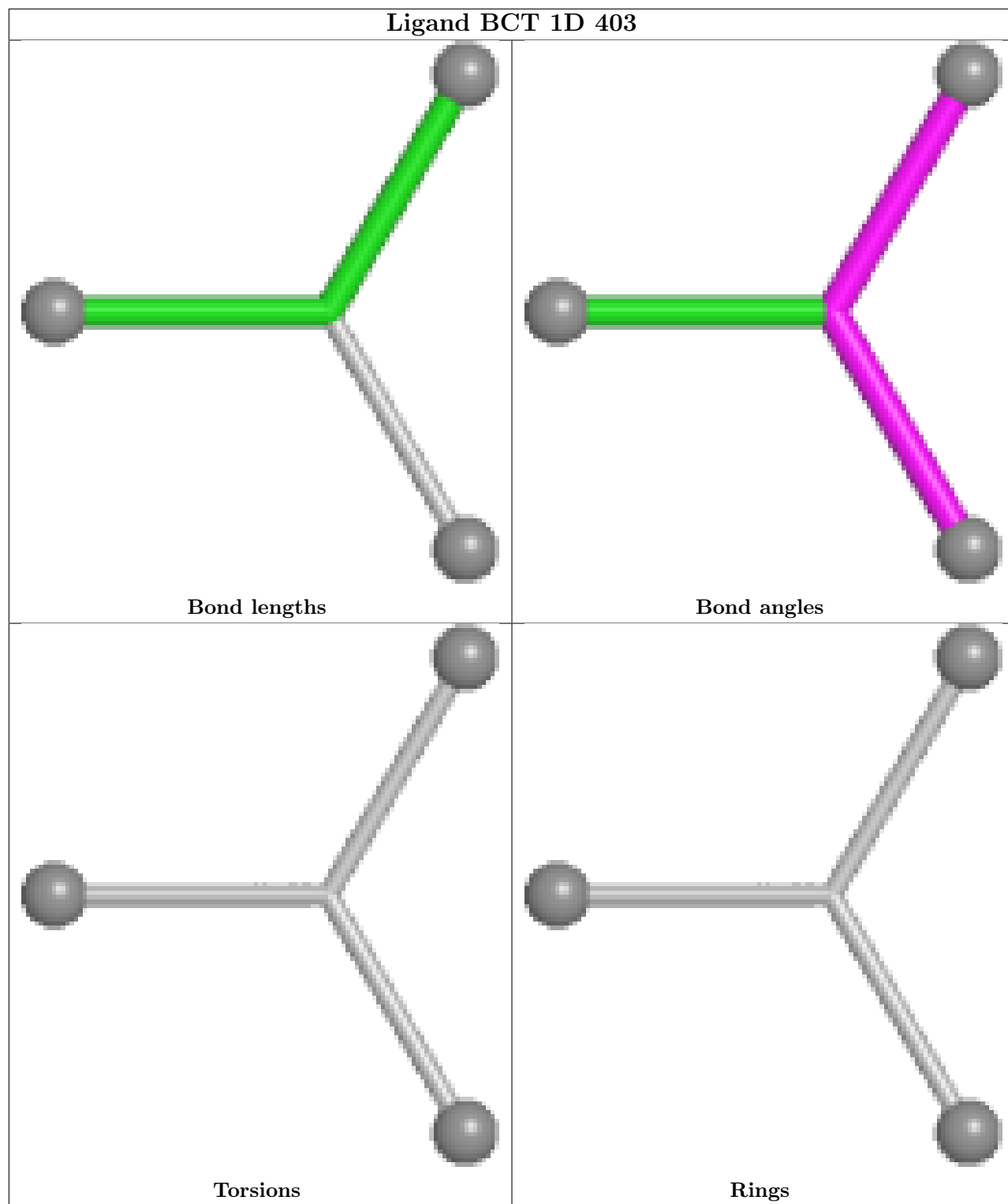


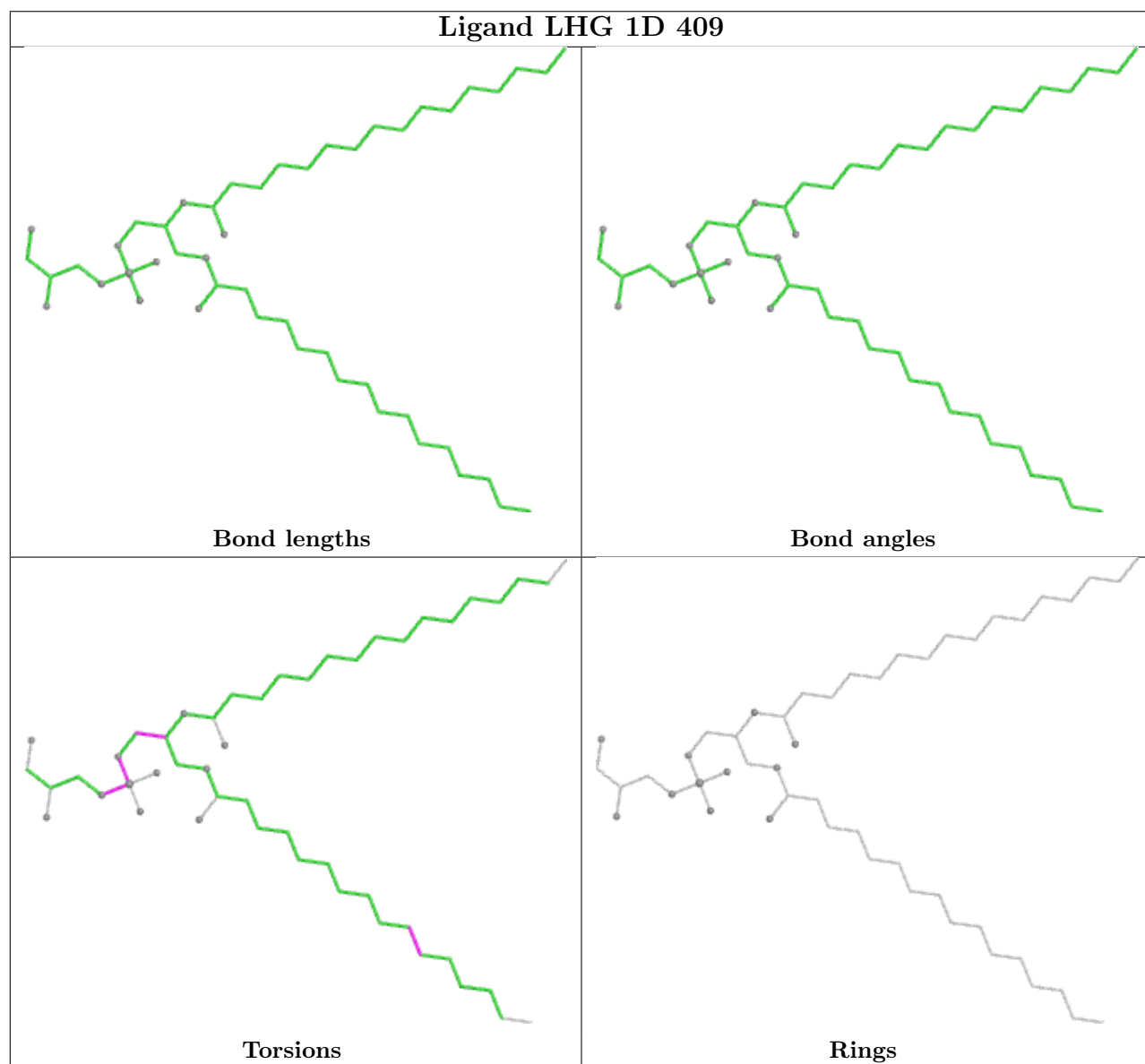
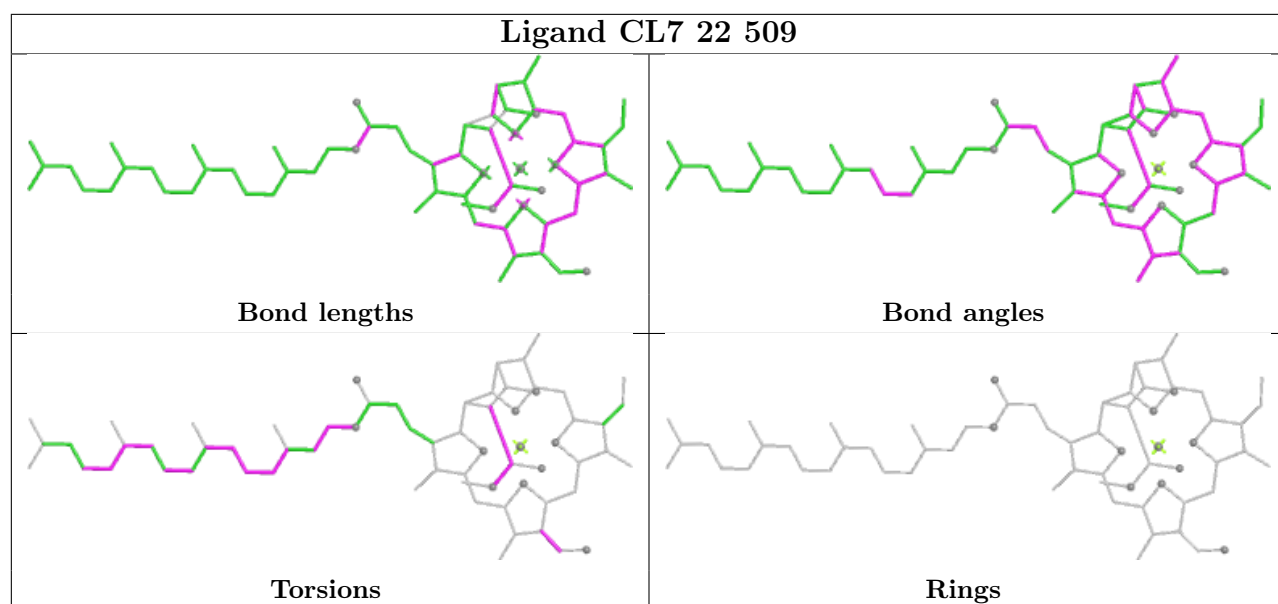
Torsions

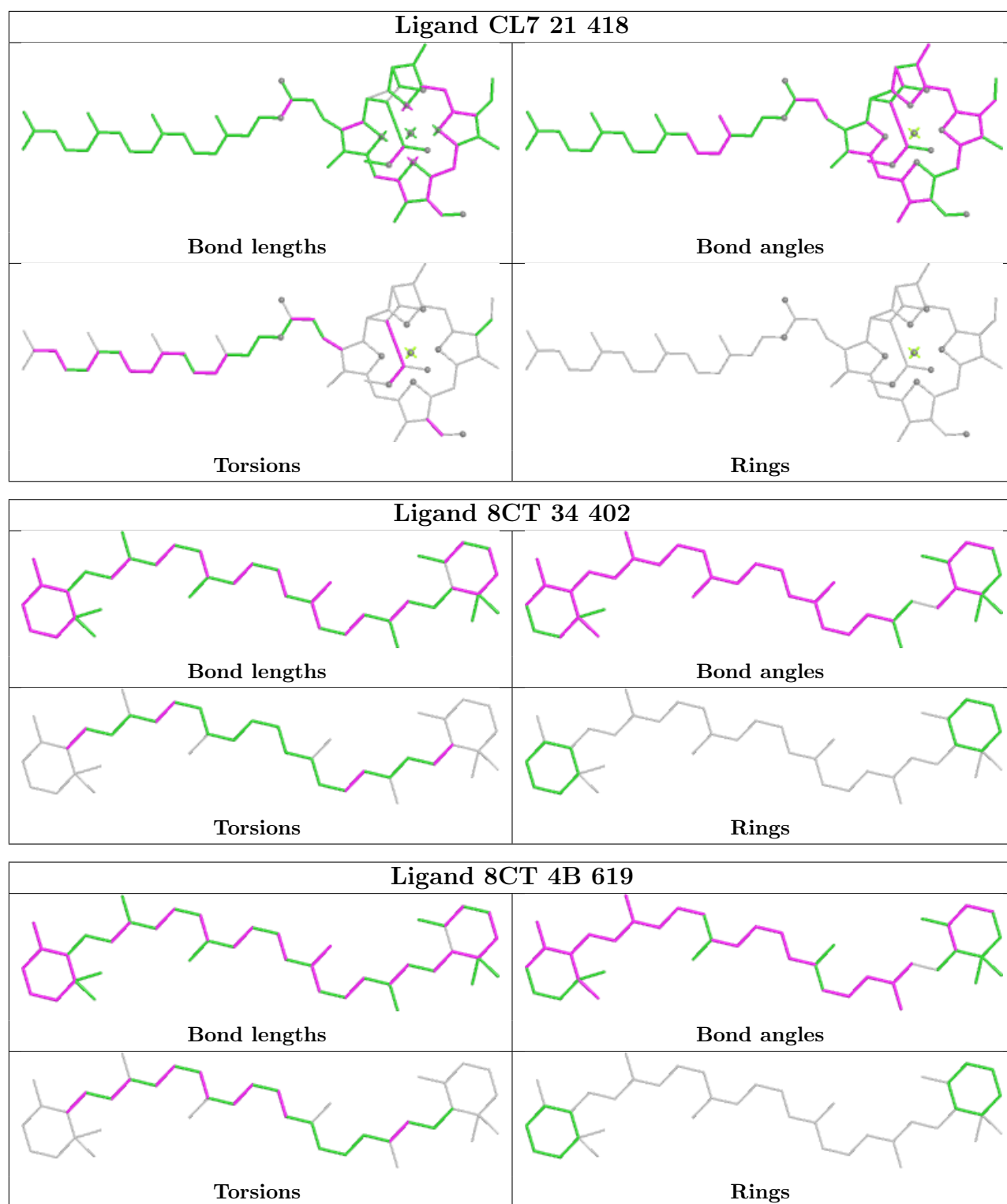


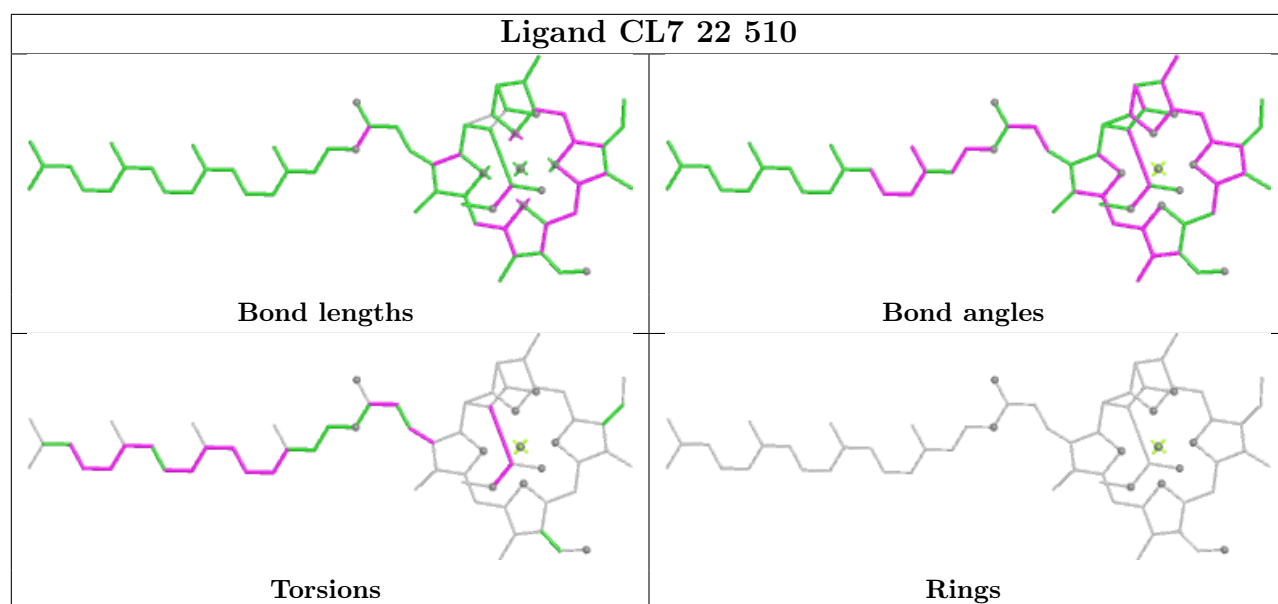
Rings

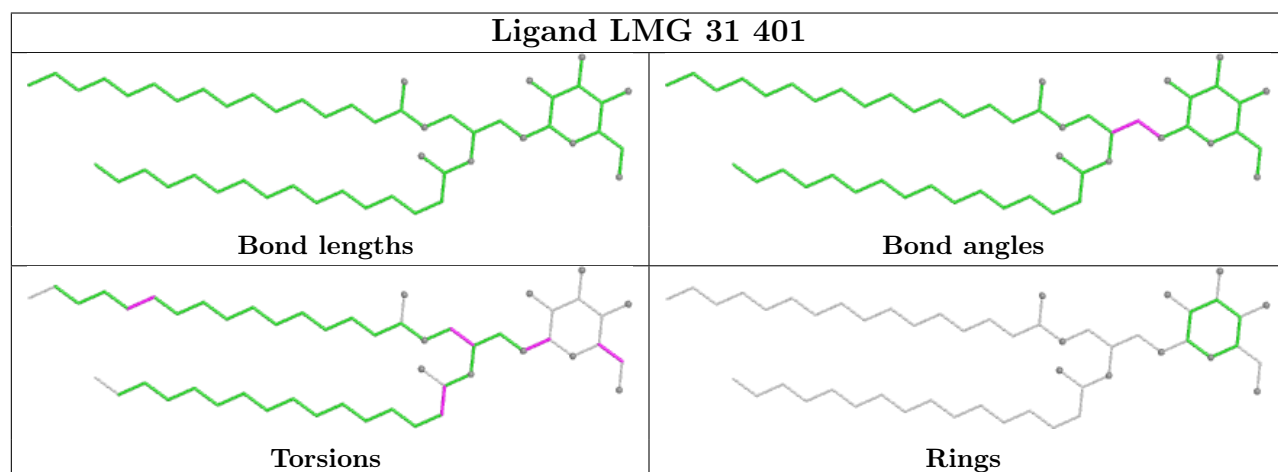
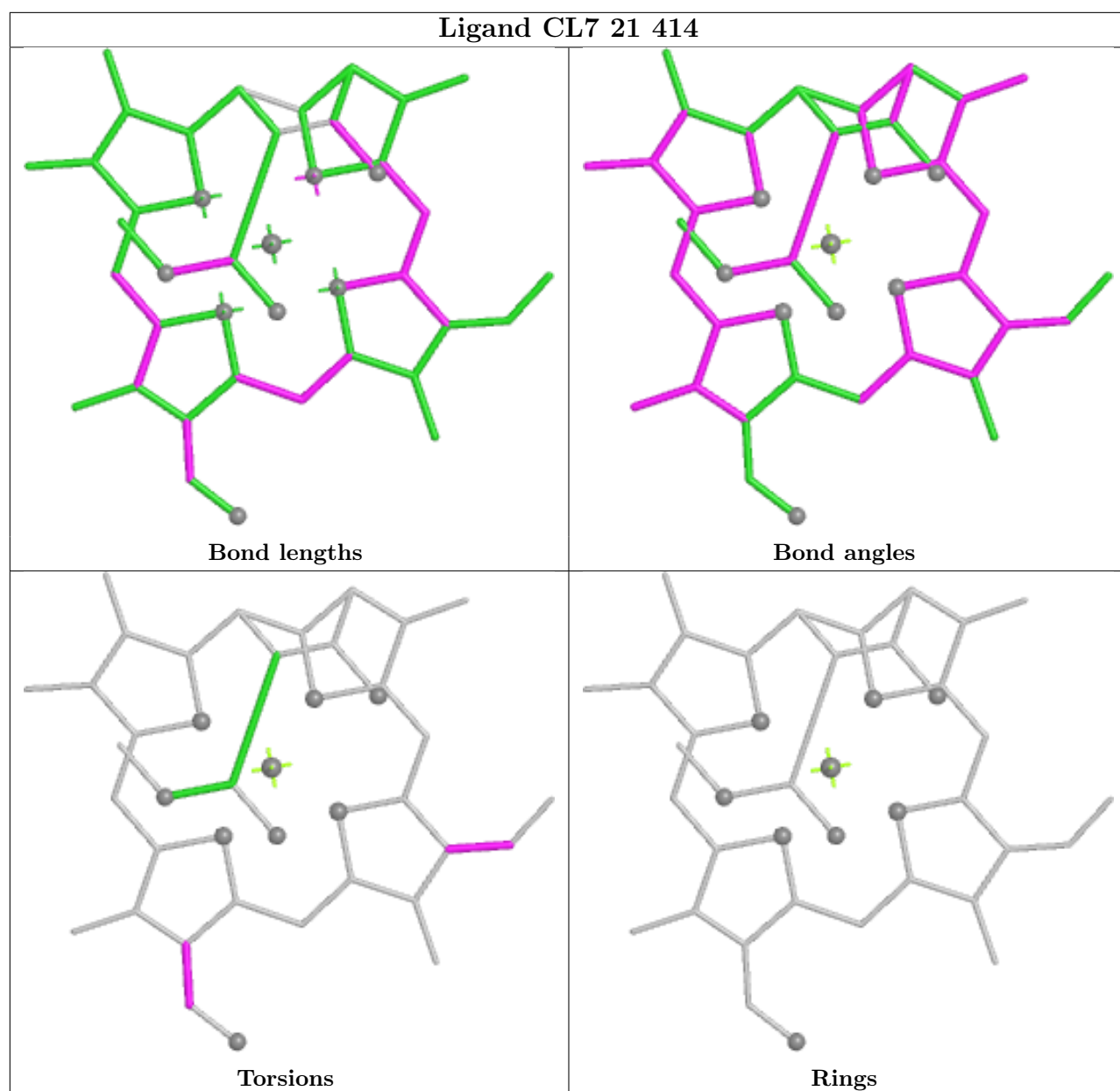


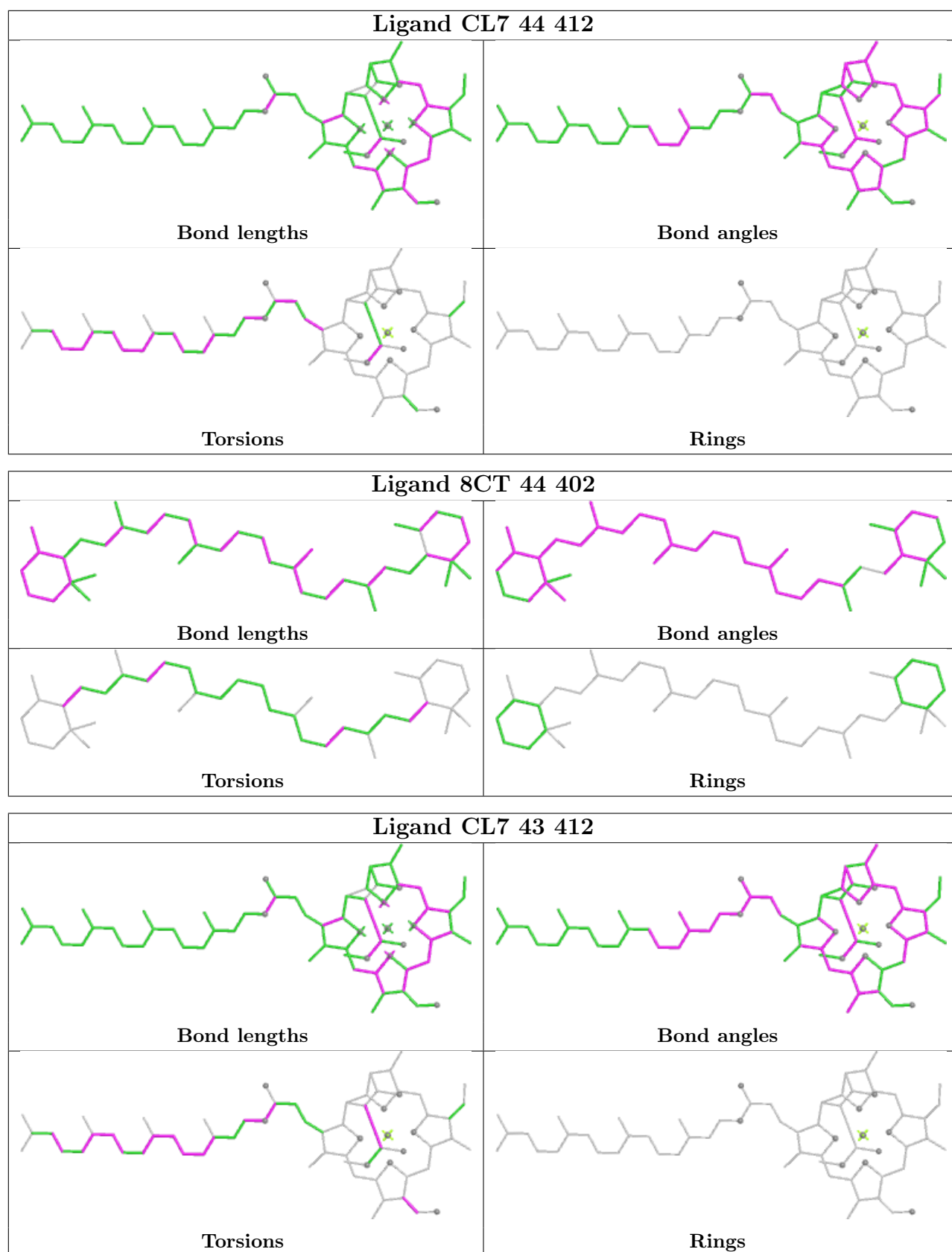




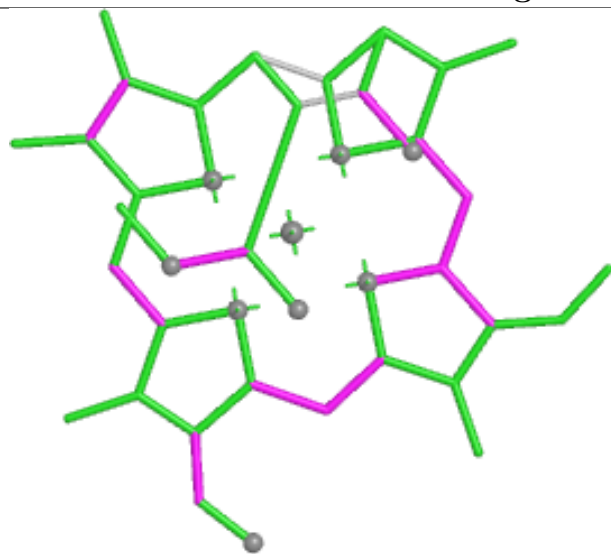




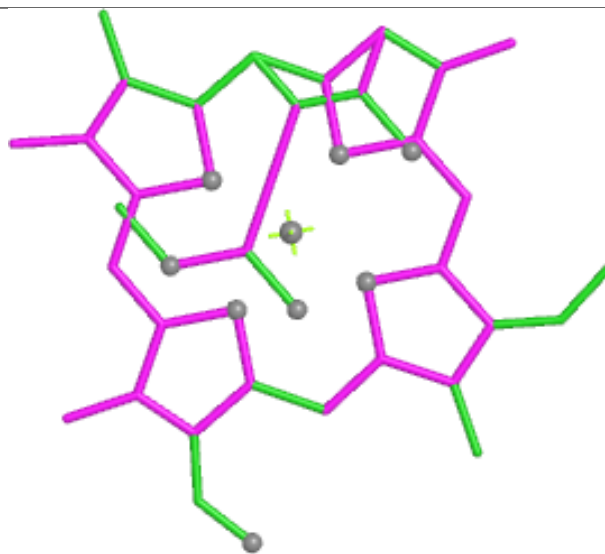




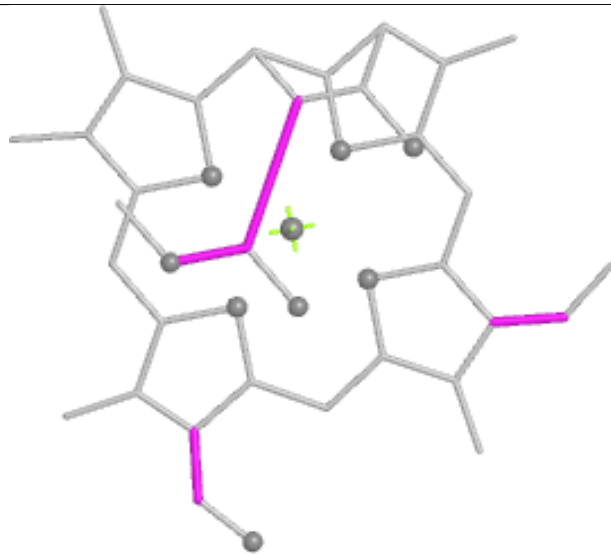
Ligand CL7 11 415



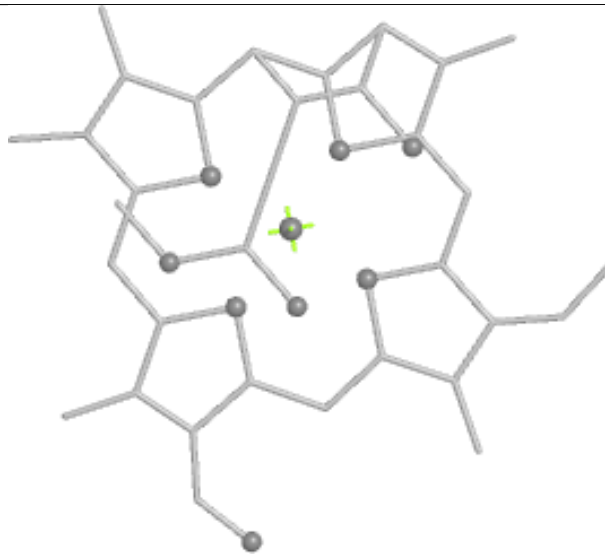
Bond lengths



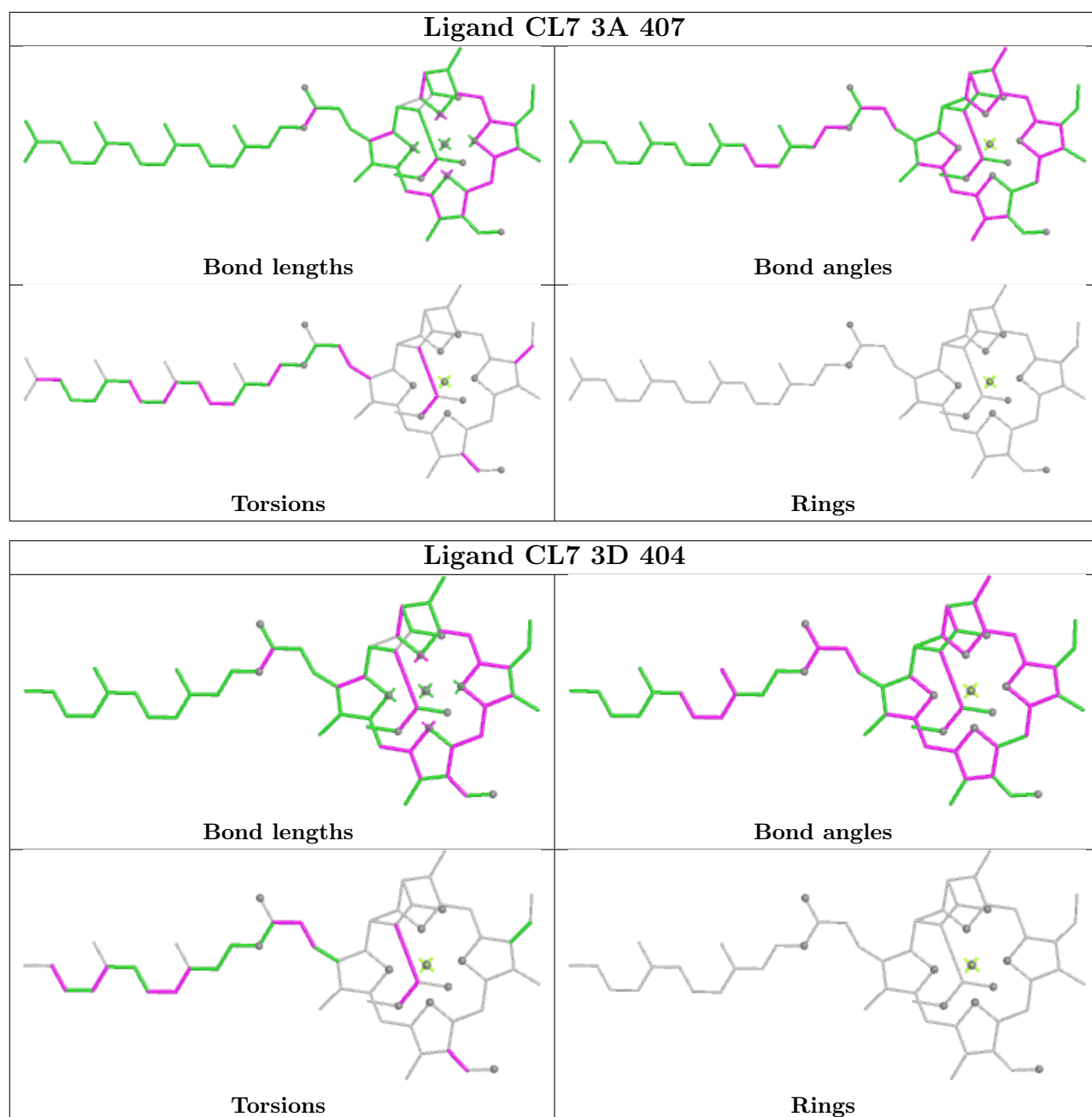
Bond angles

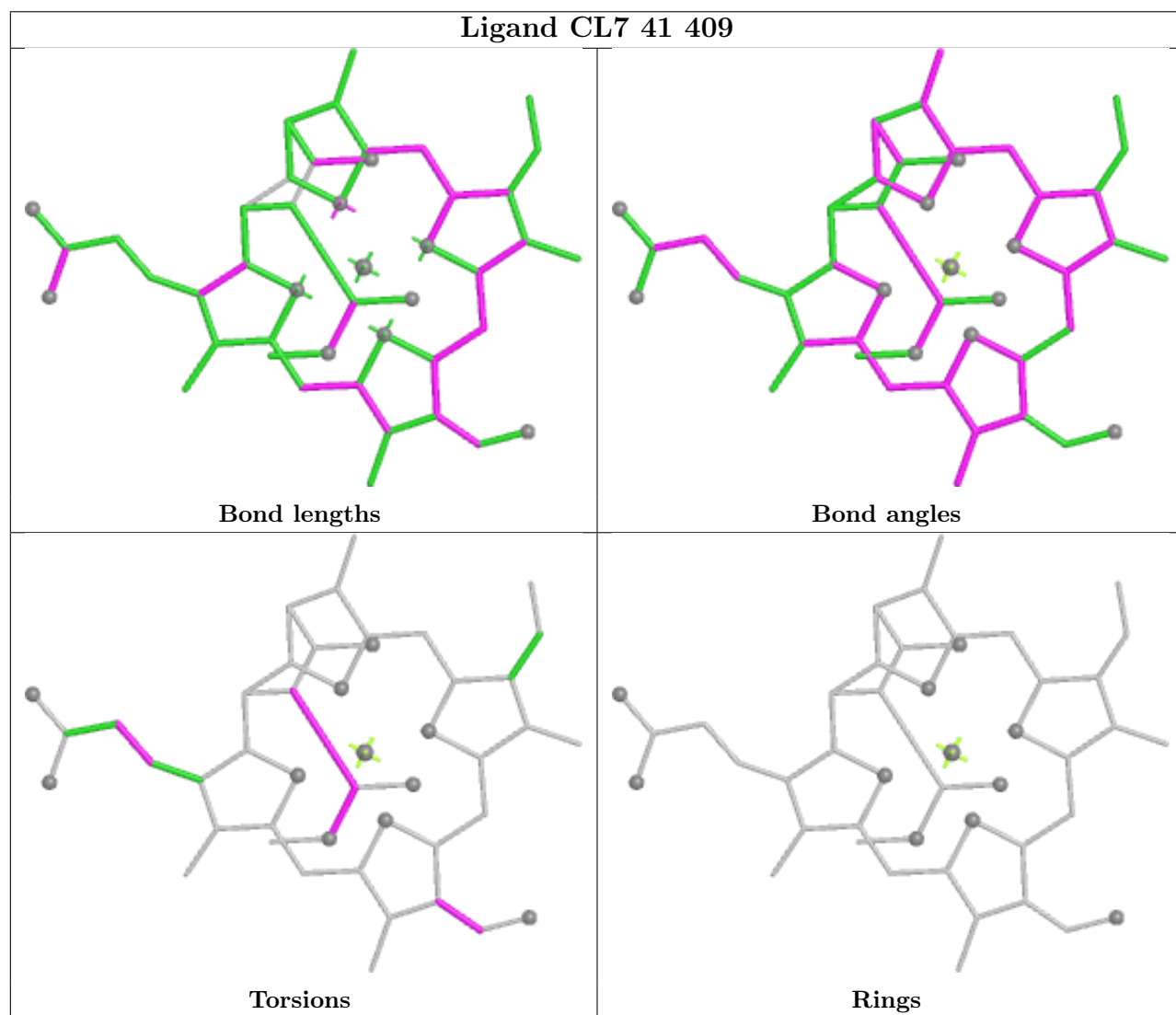
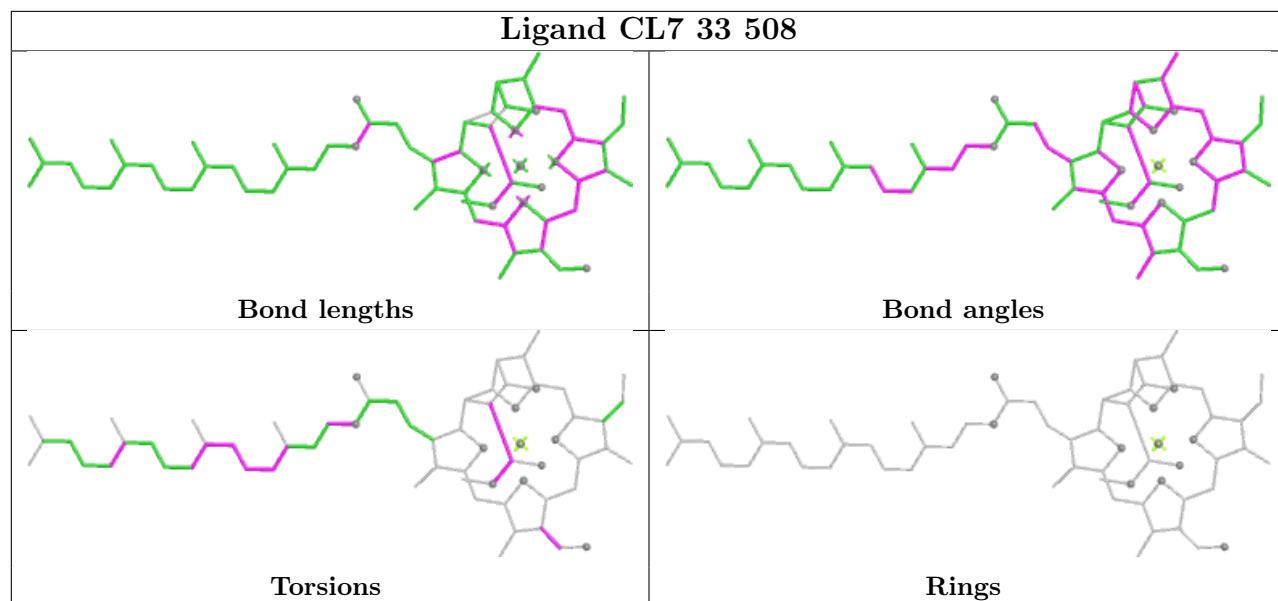


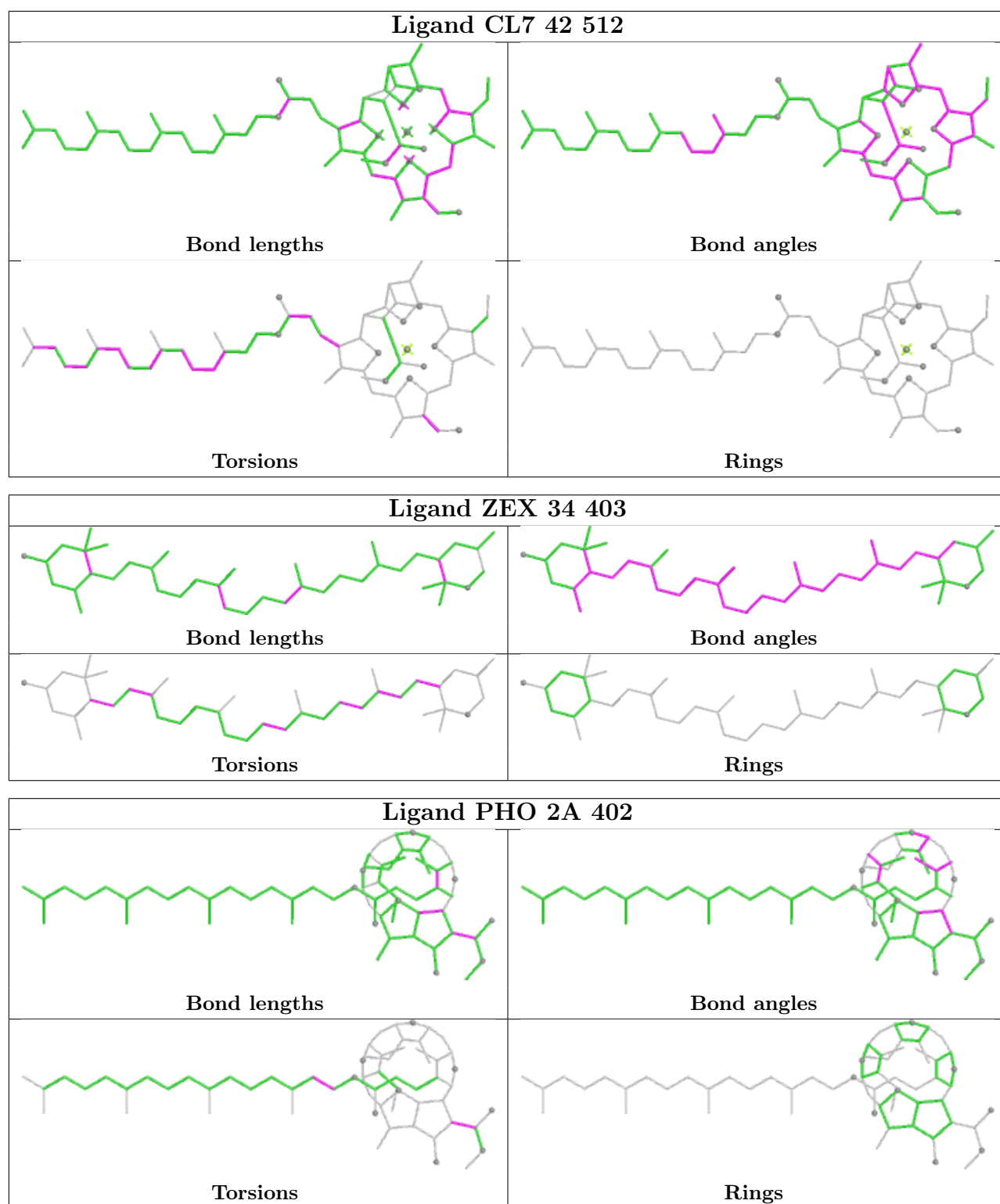
Torsions

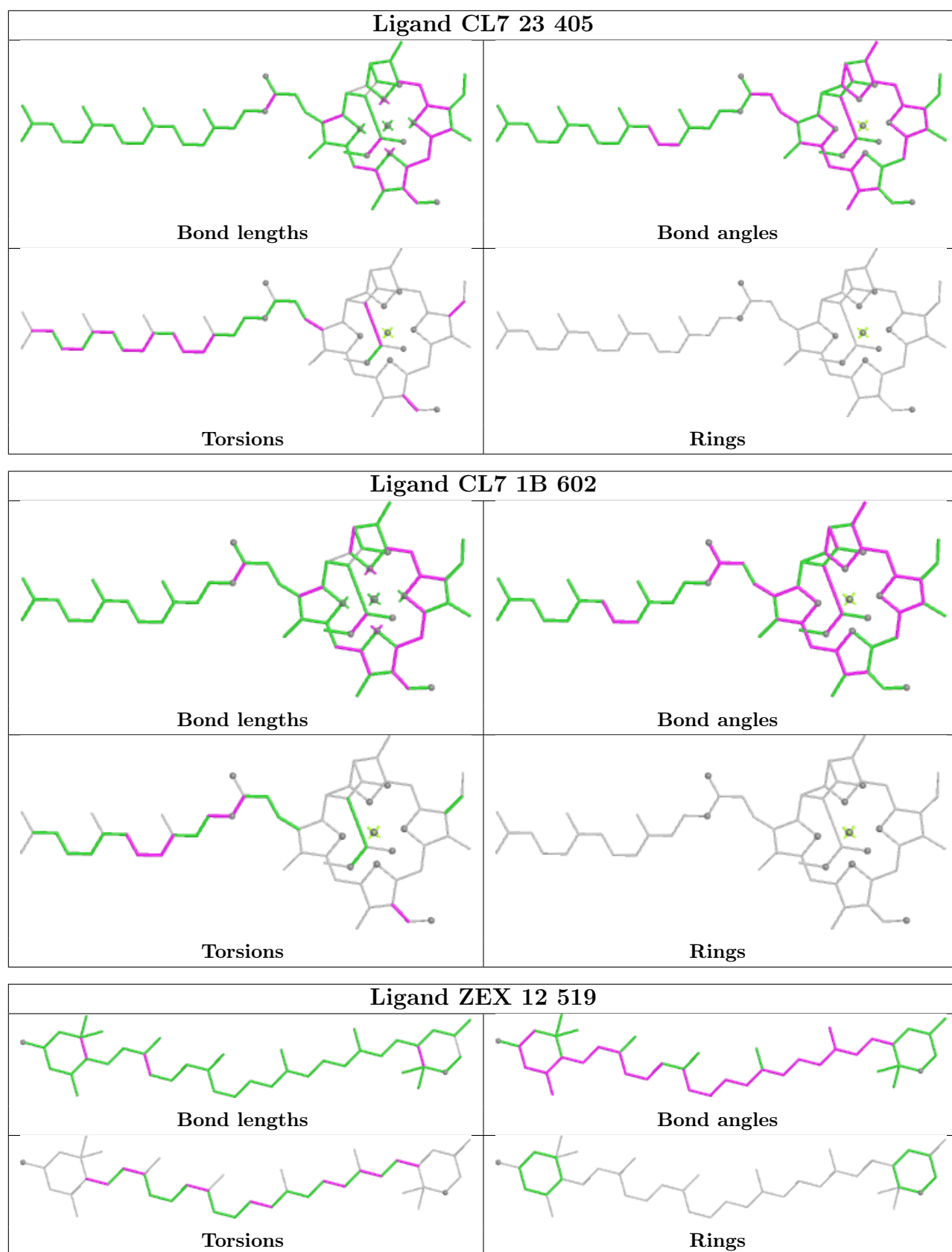


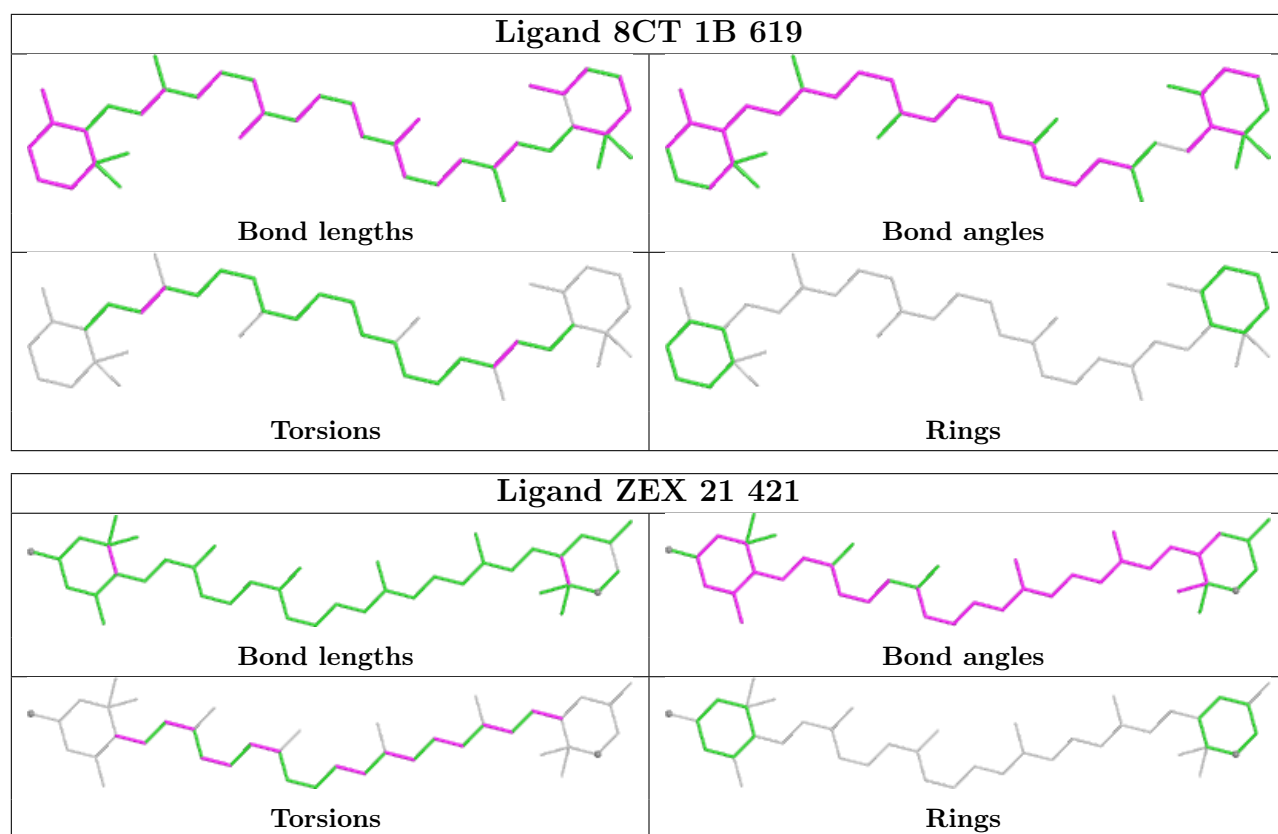
Rings

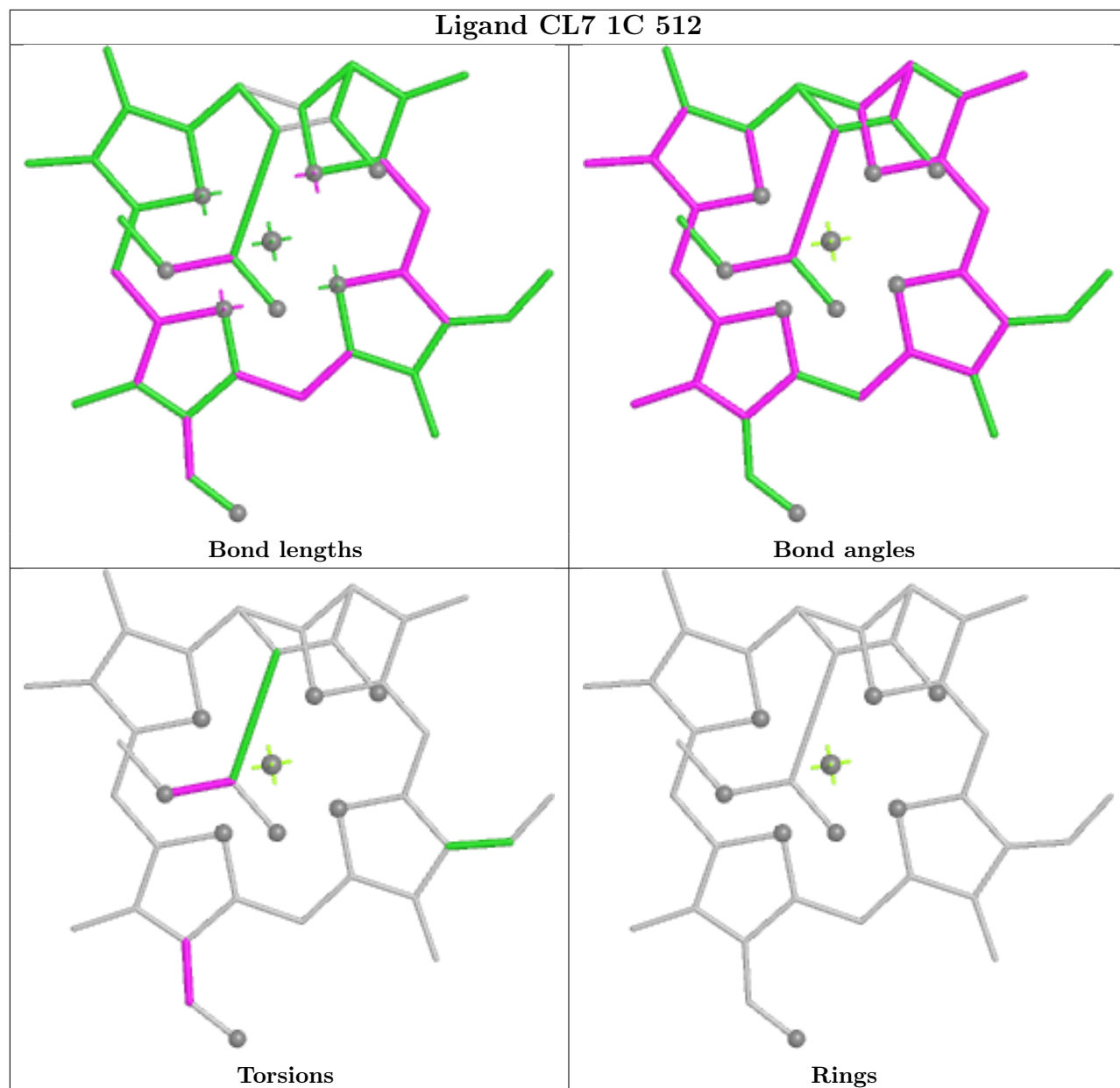


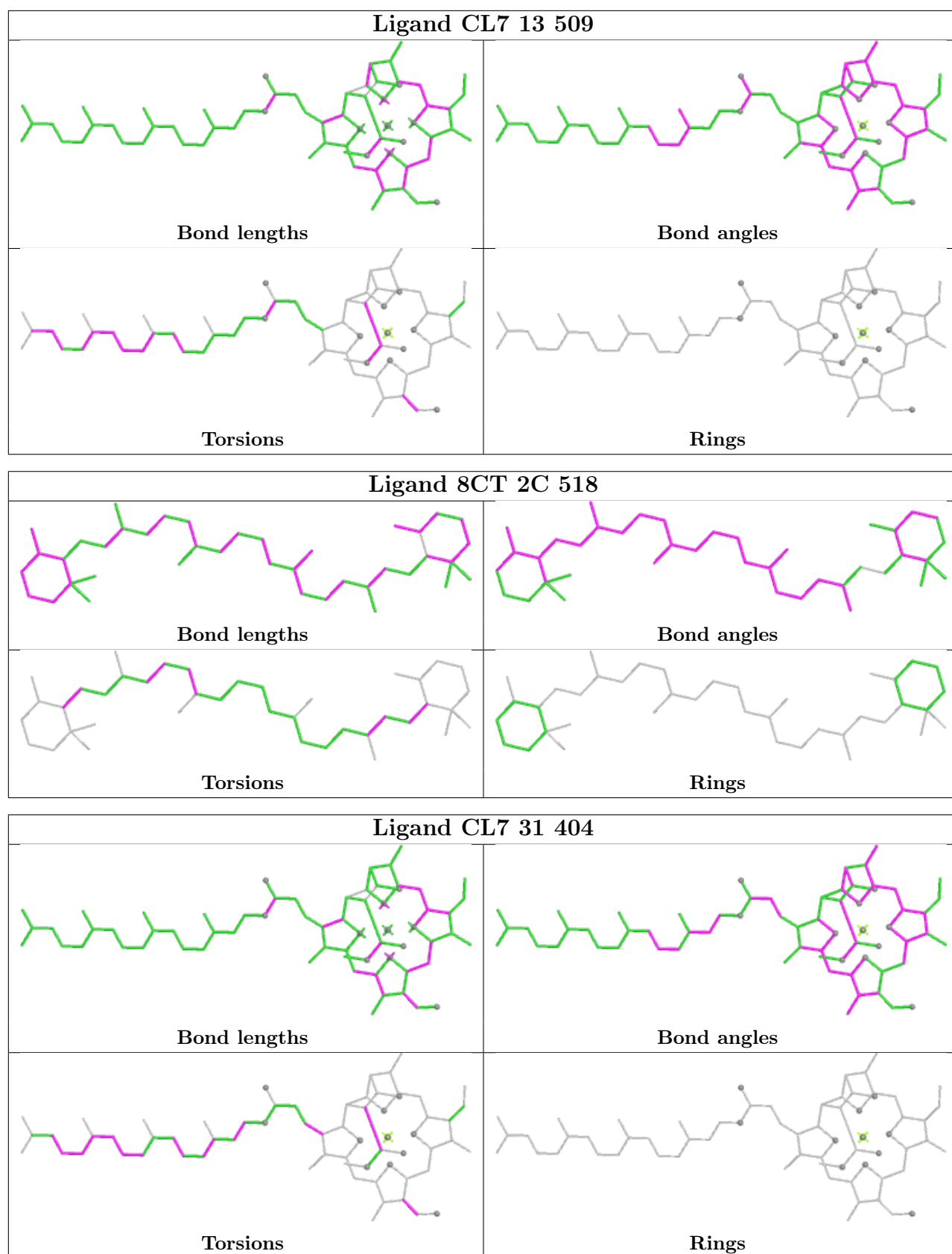








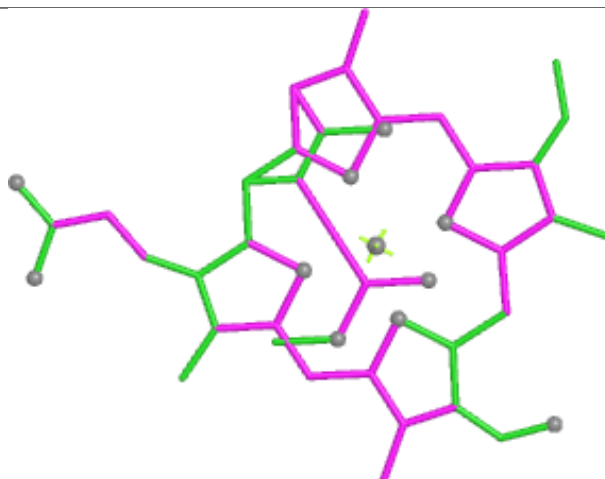




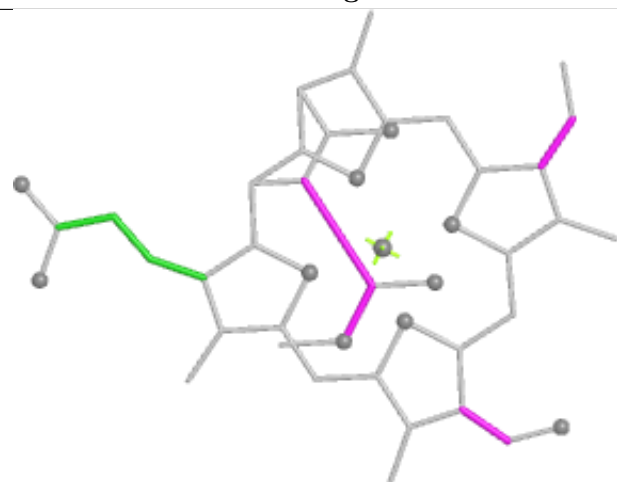
Ligand CL7 31 420



Bond lengths



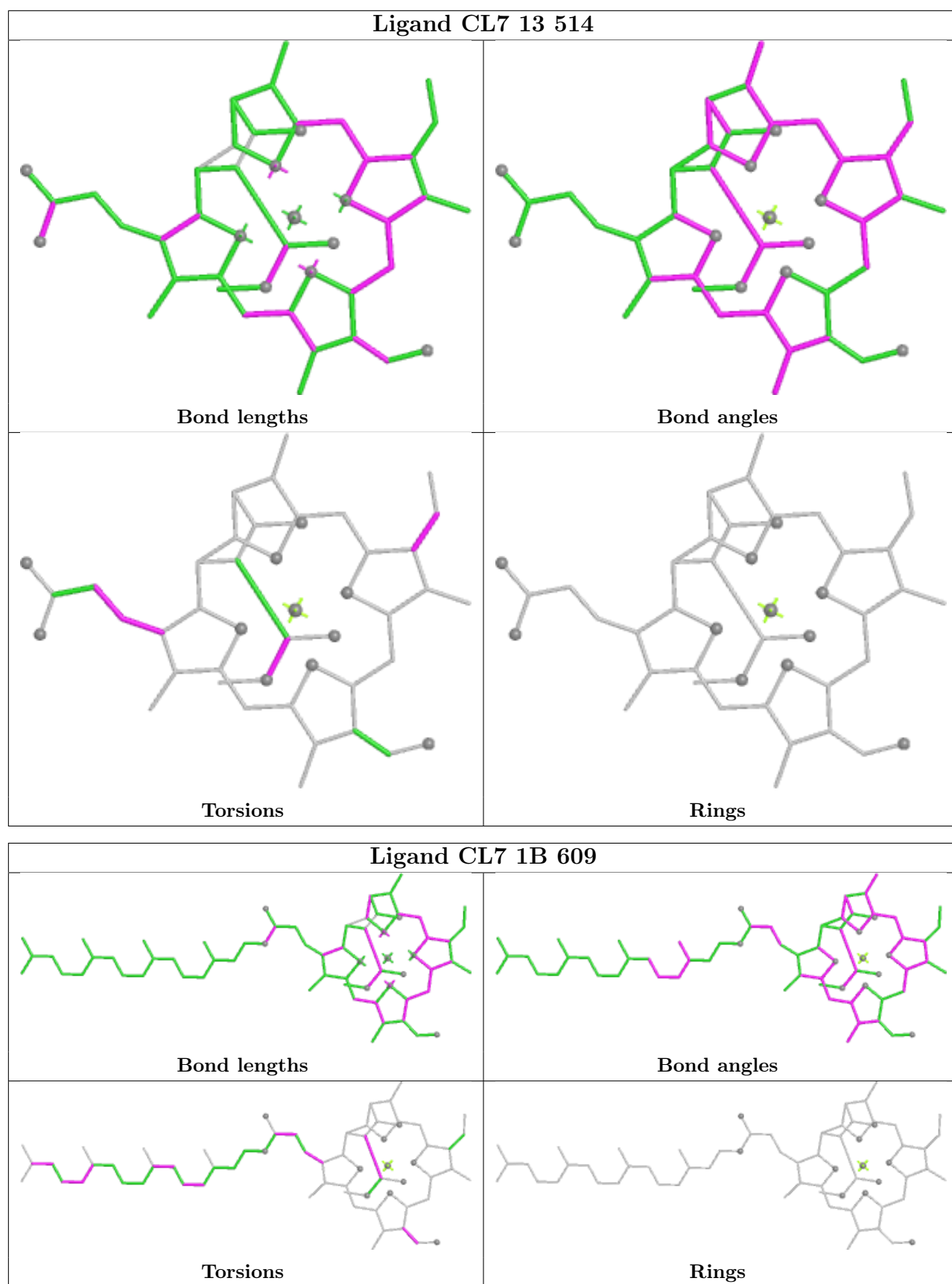
Bond angles

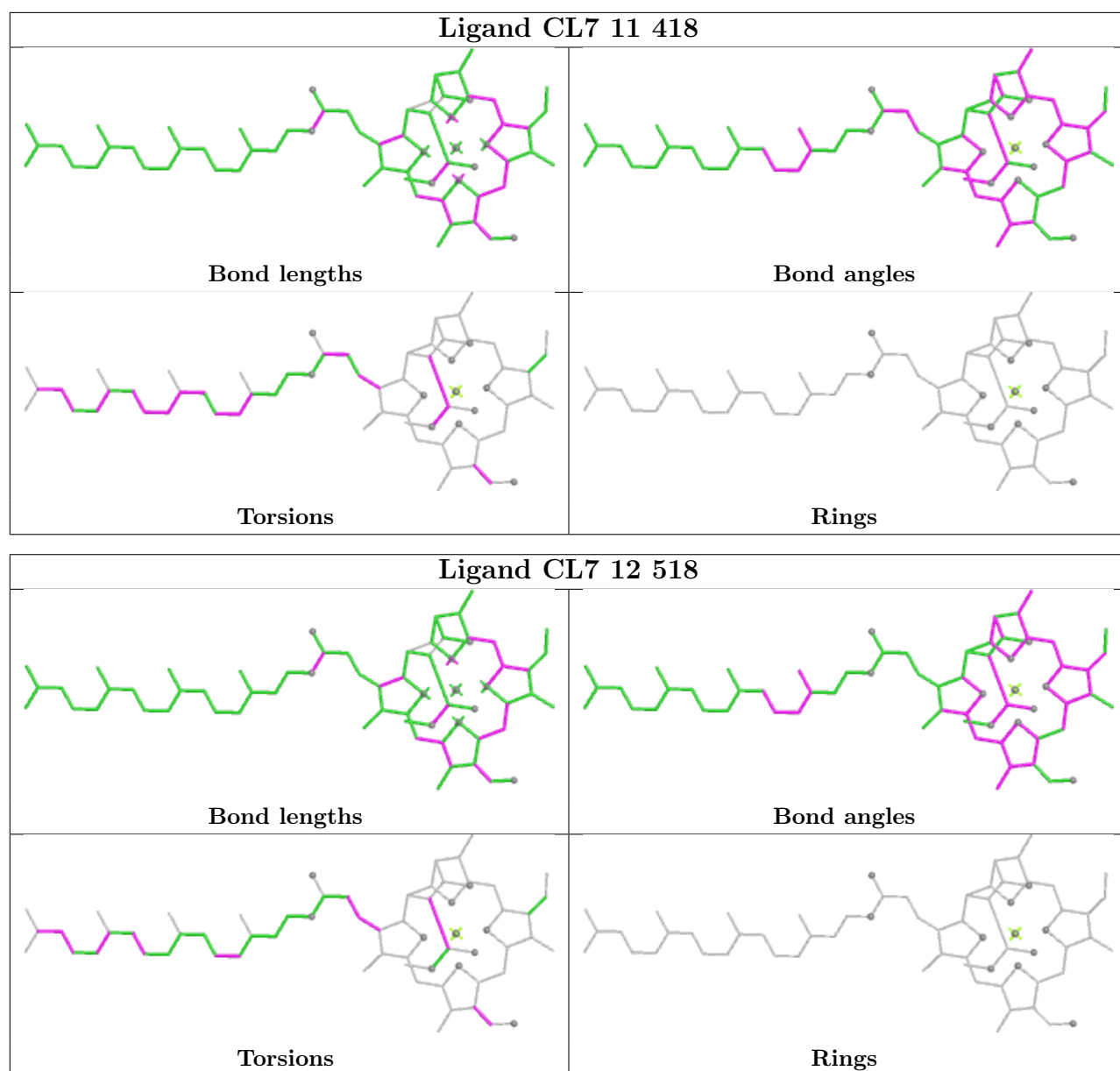


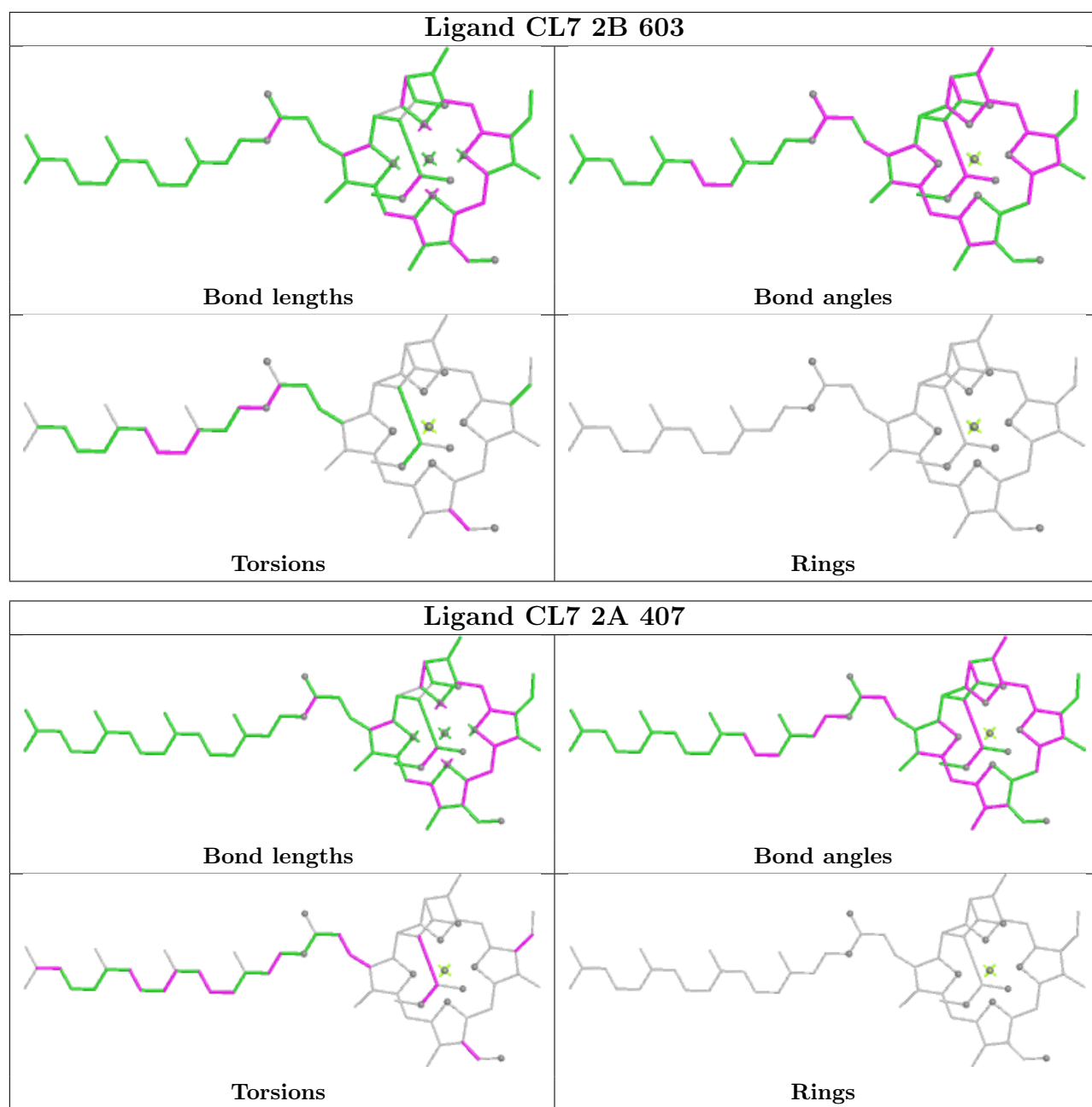
Torsions

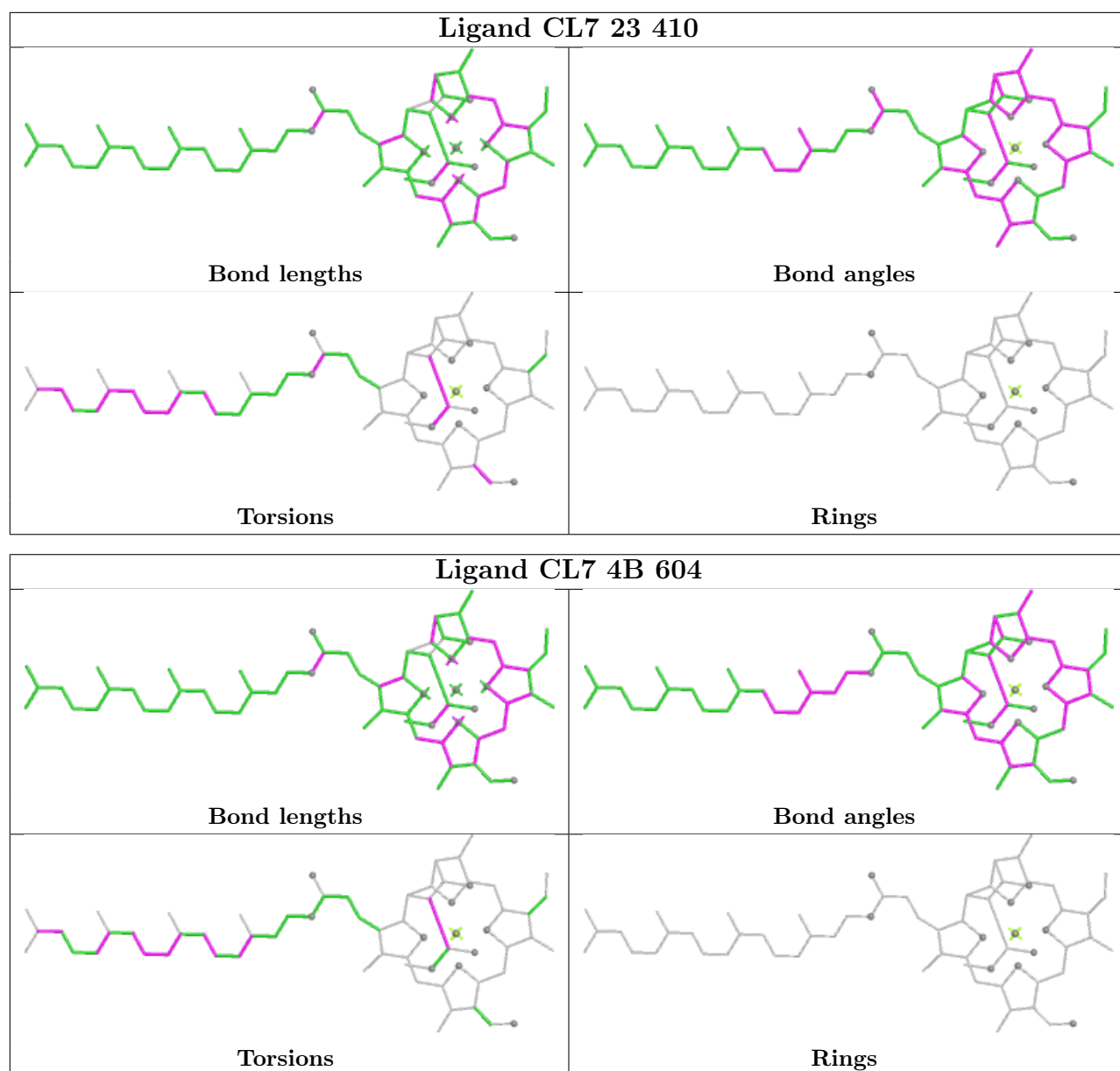


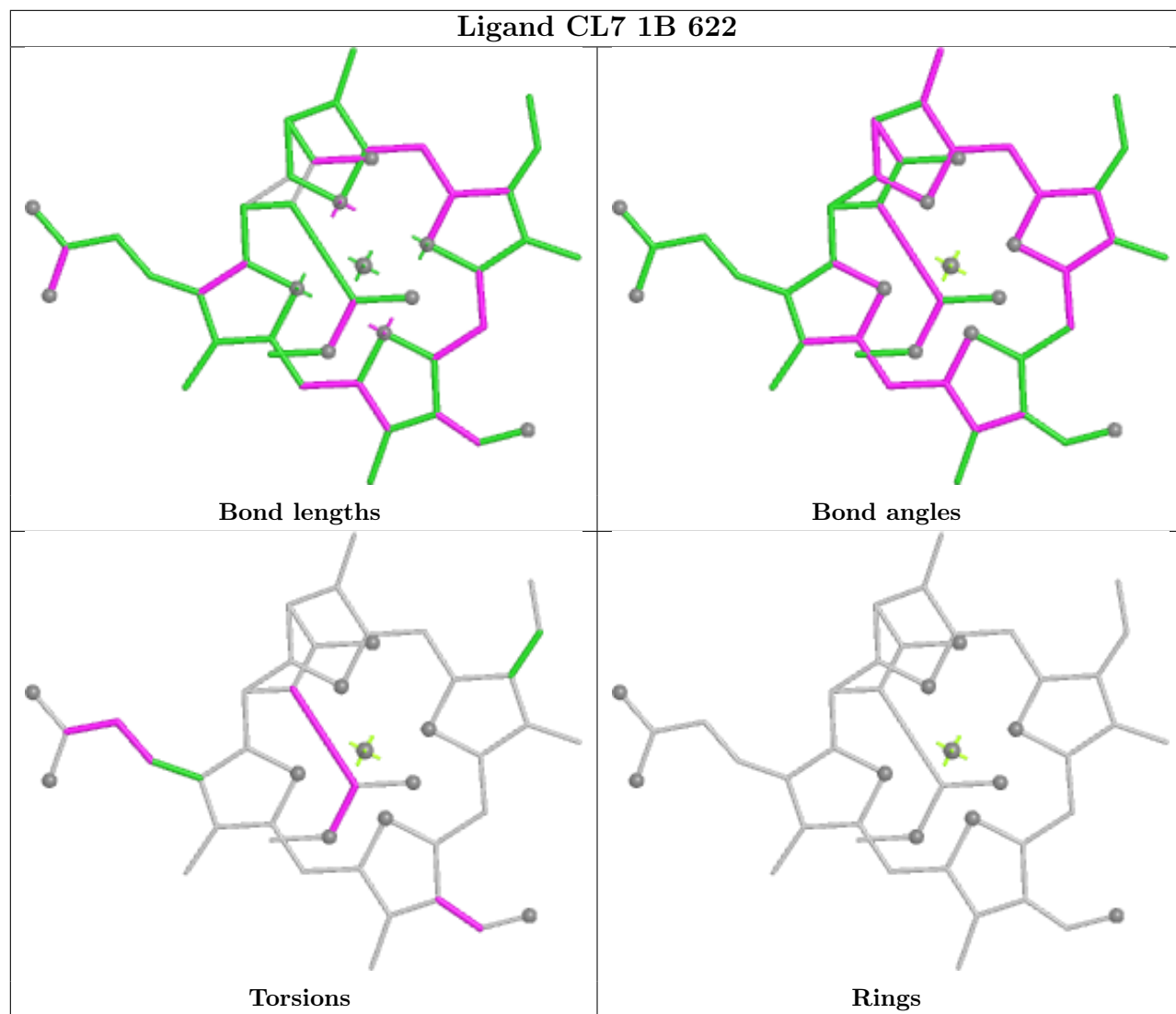
Rings



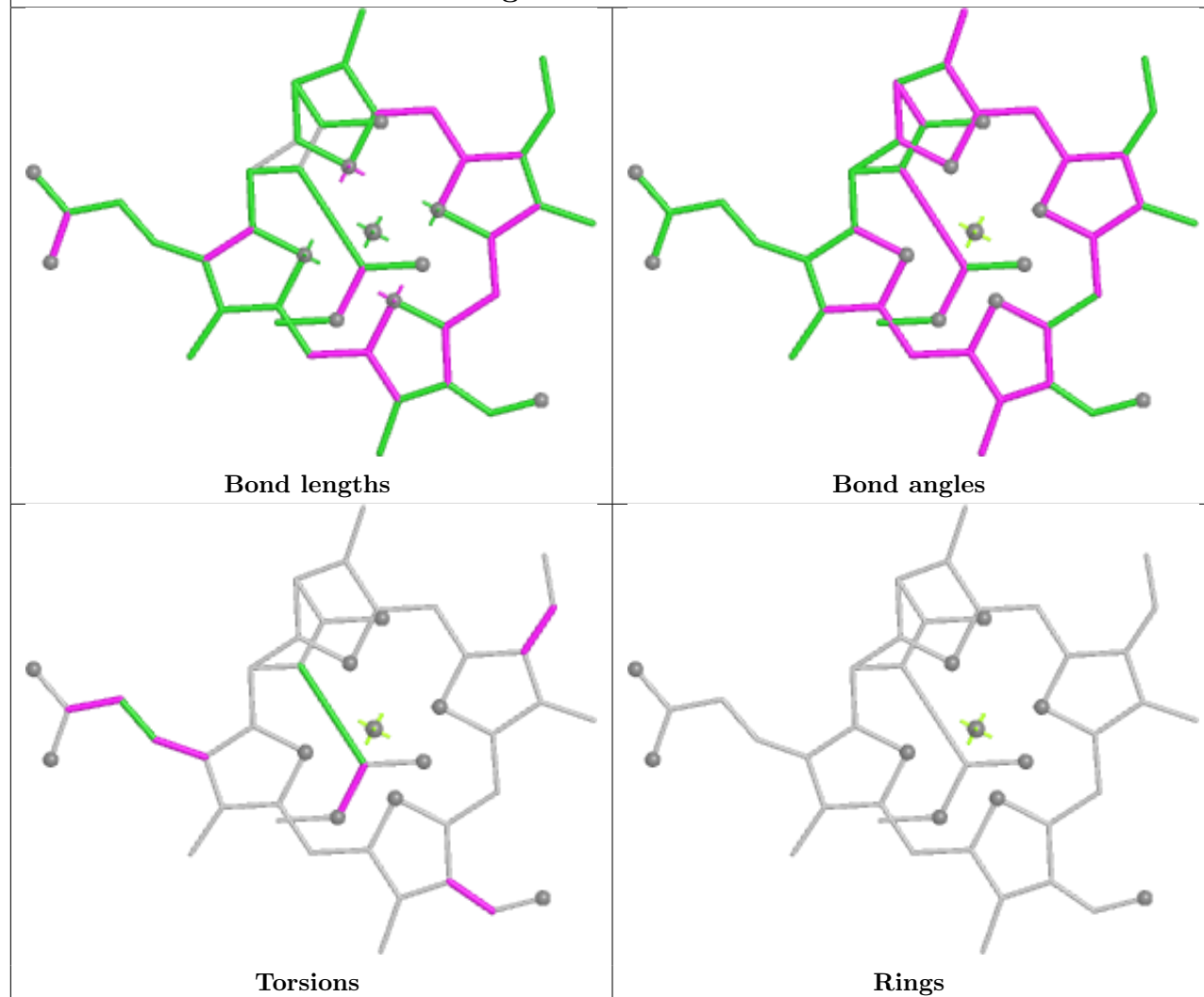




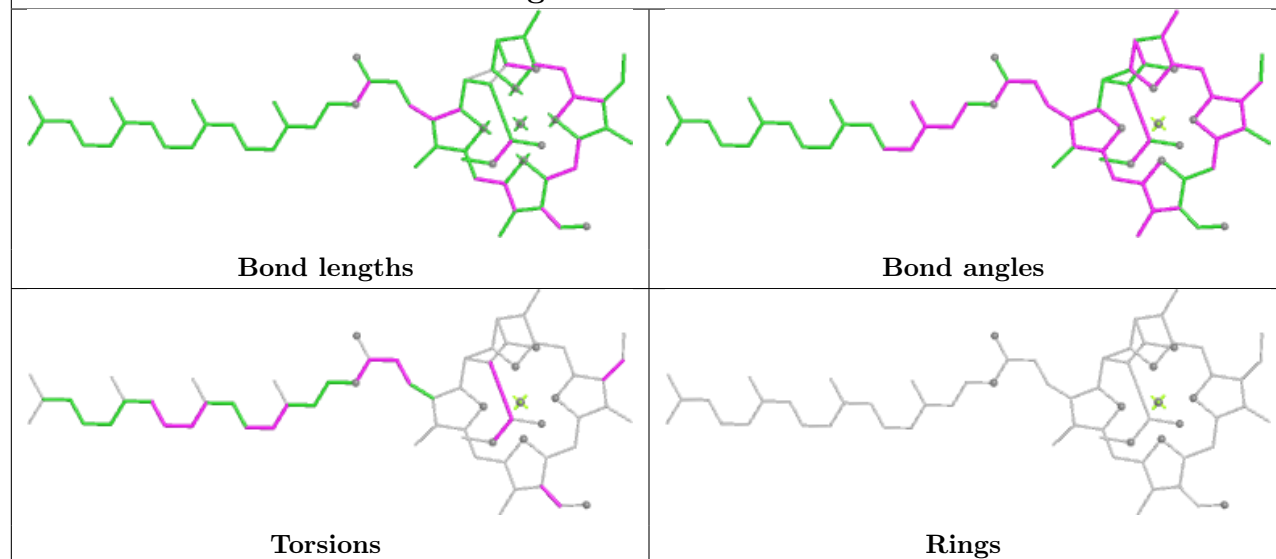


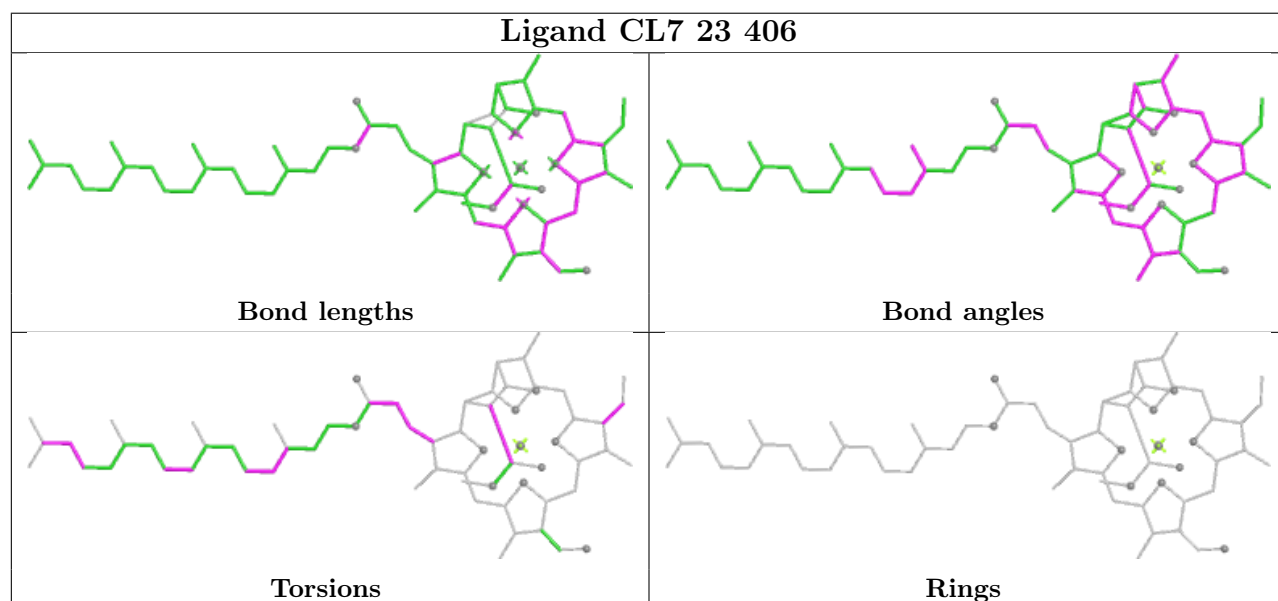
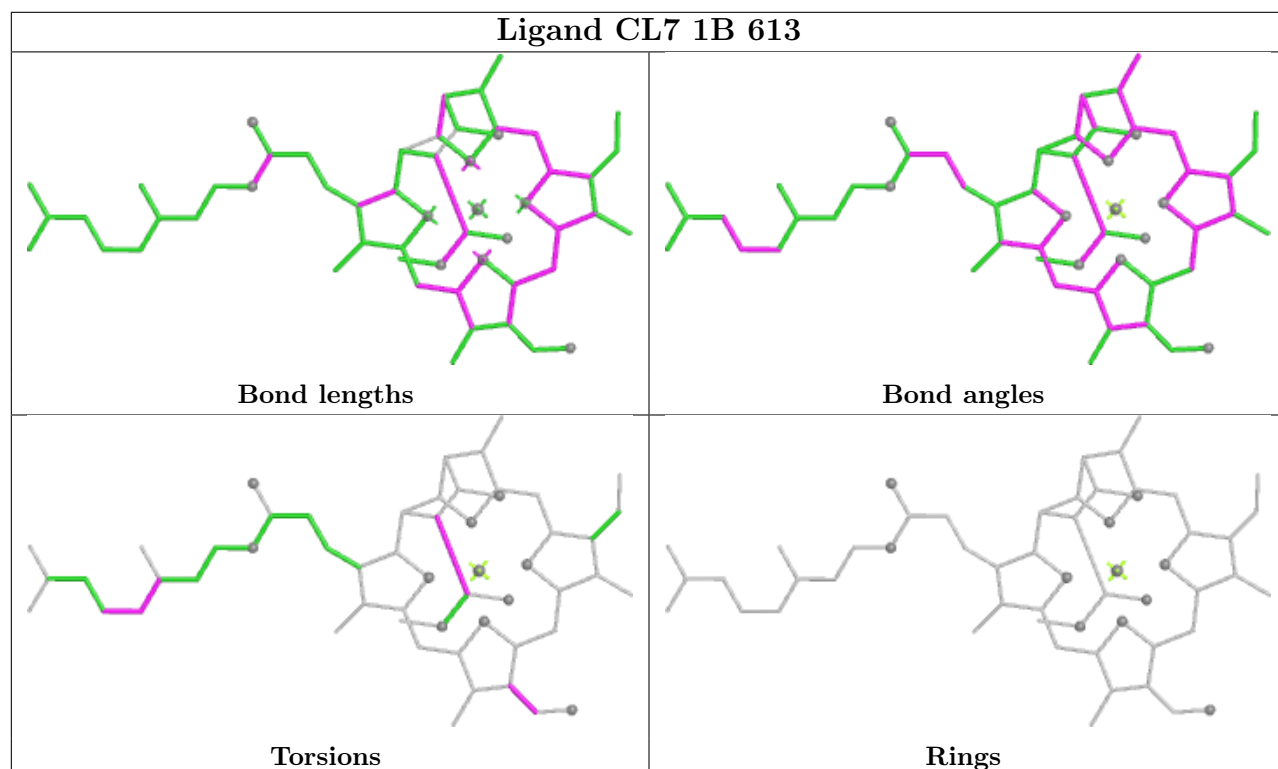
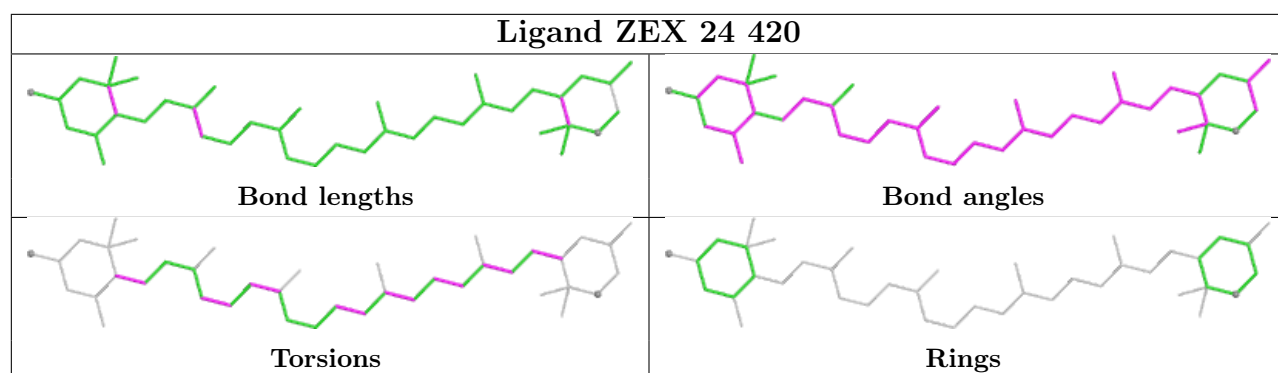


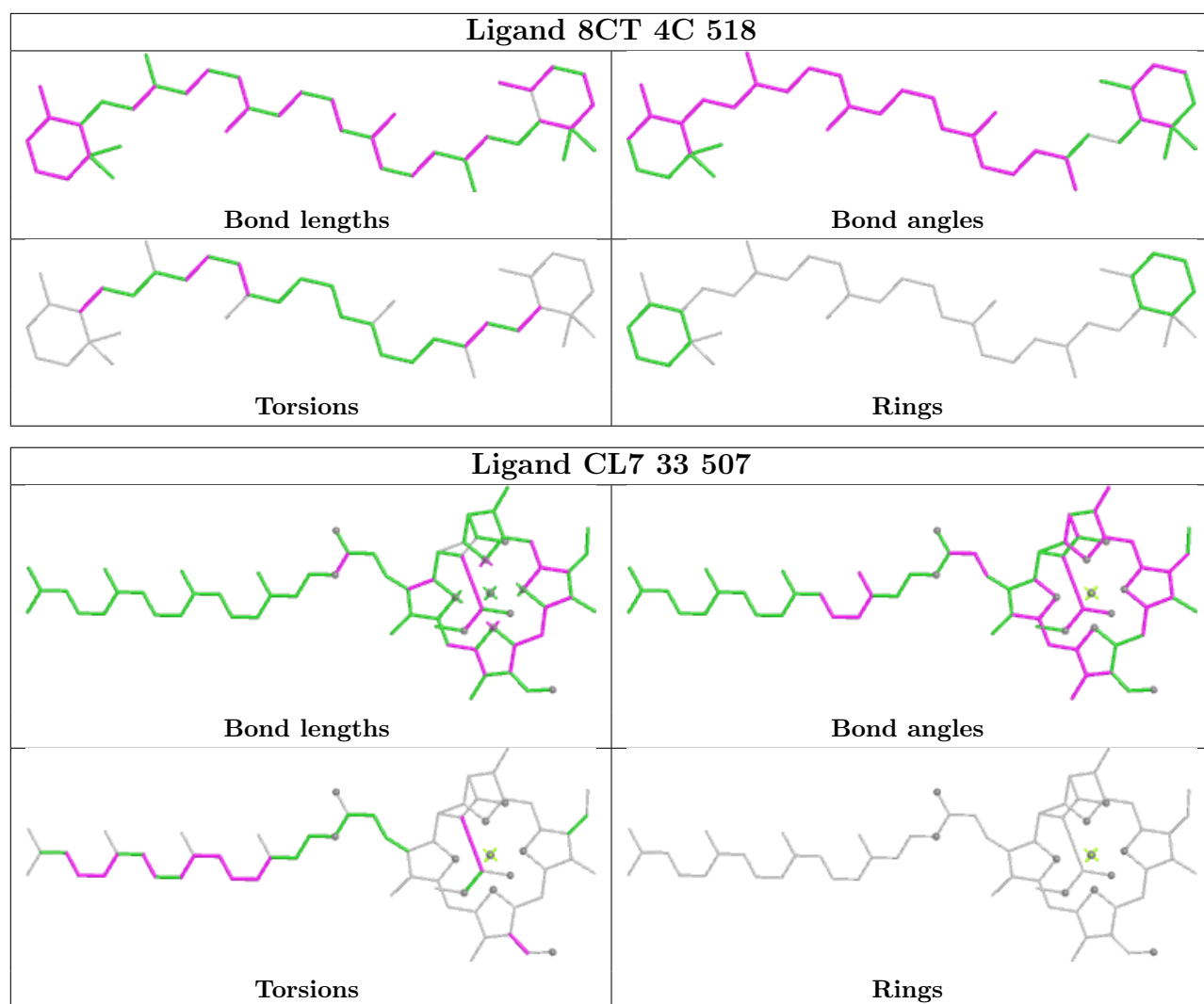
Ligand CL7 22 514

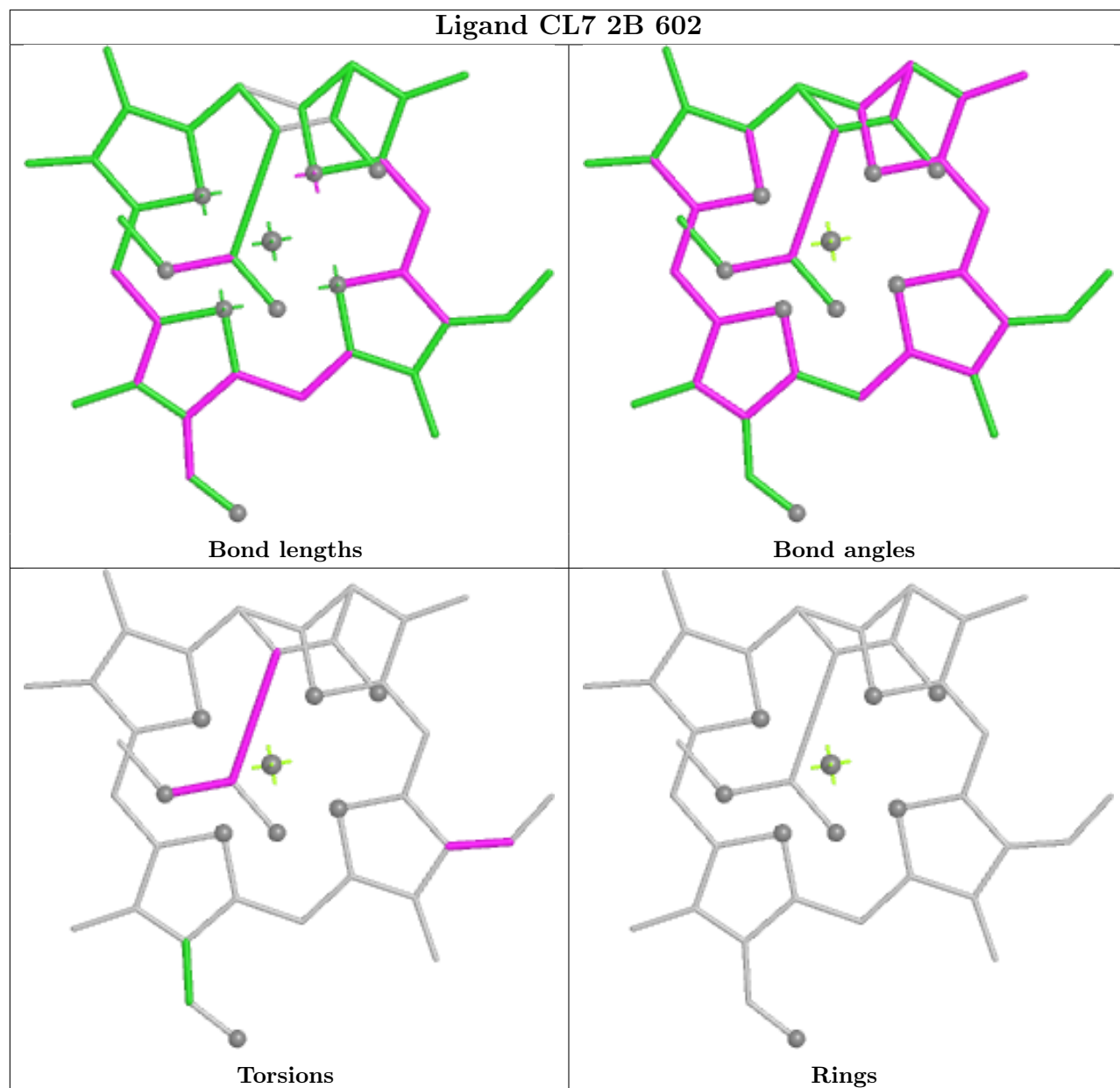


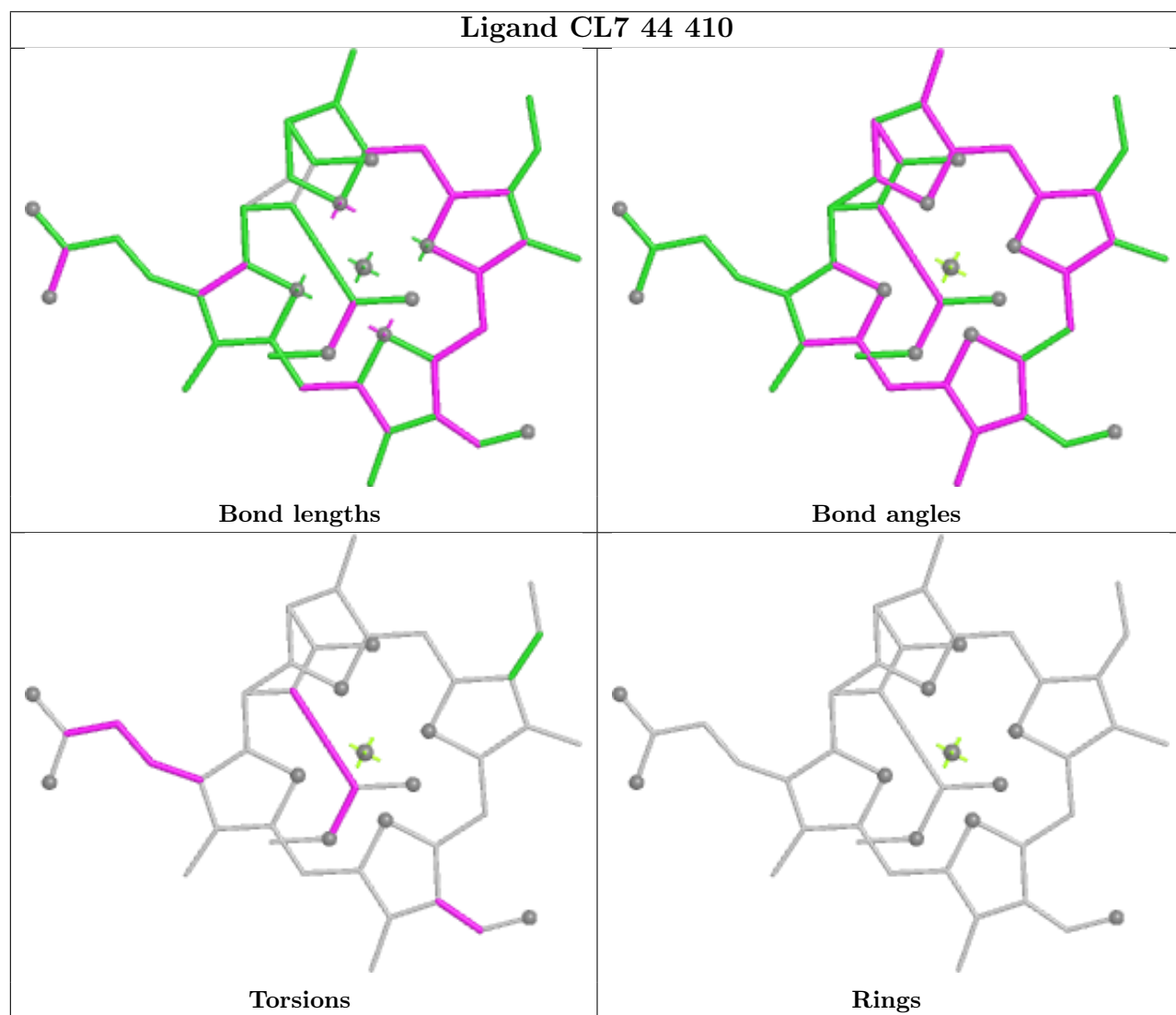
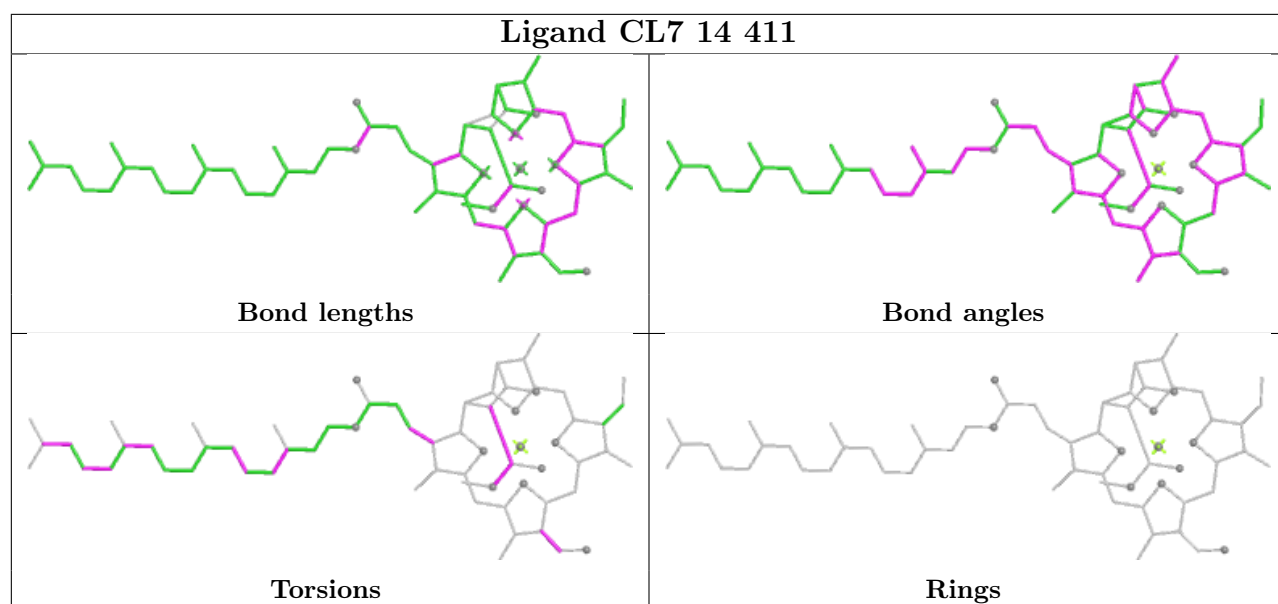
Ligand CL7 3A 401

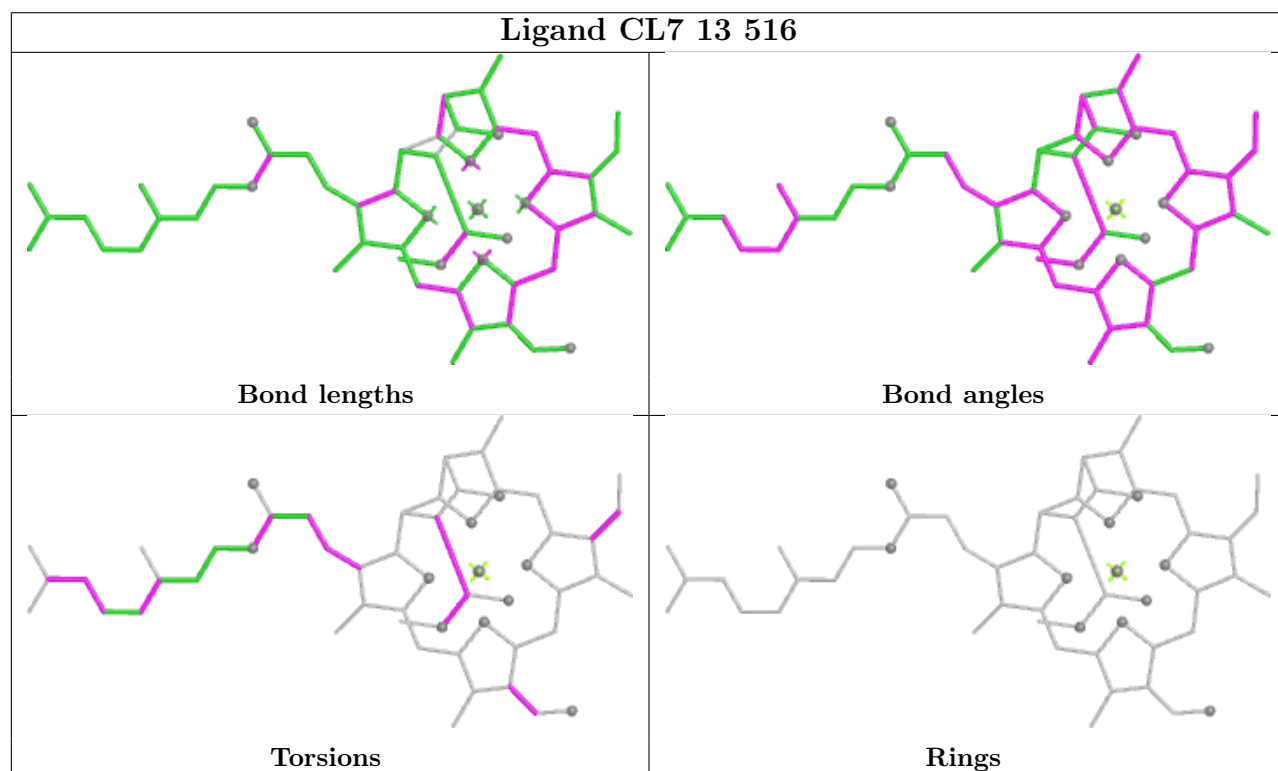
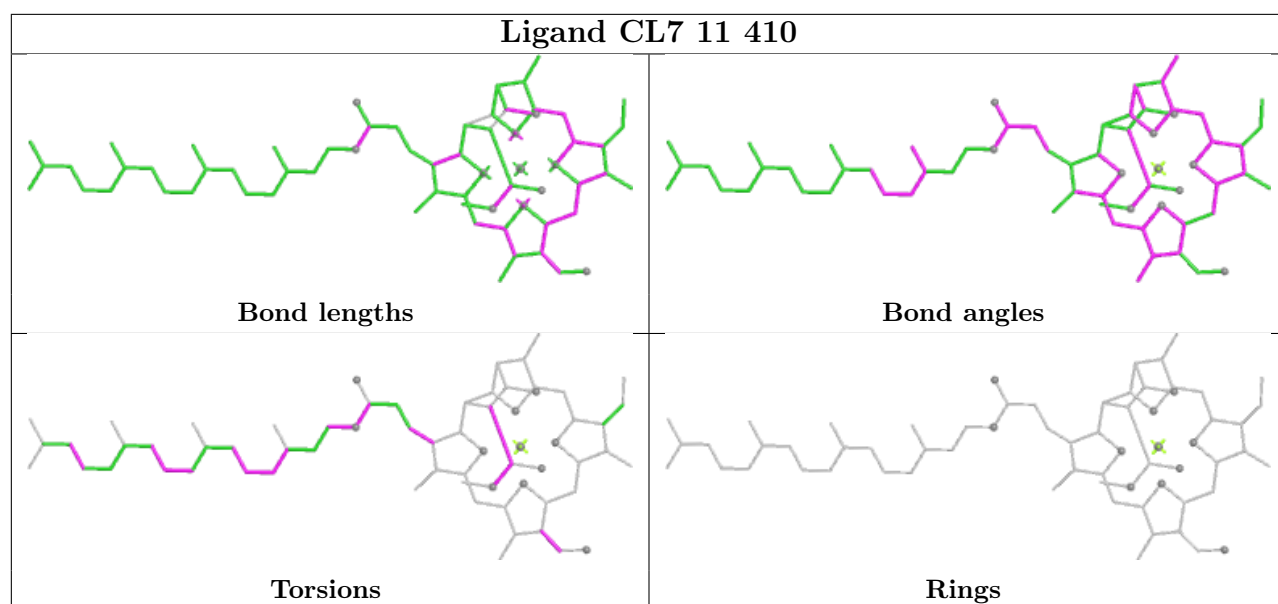


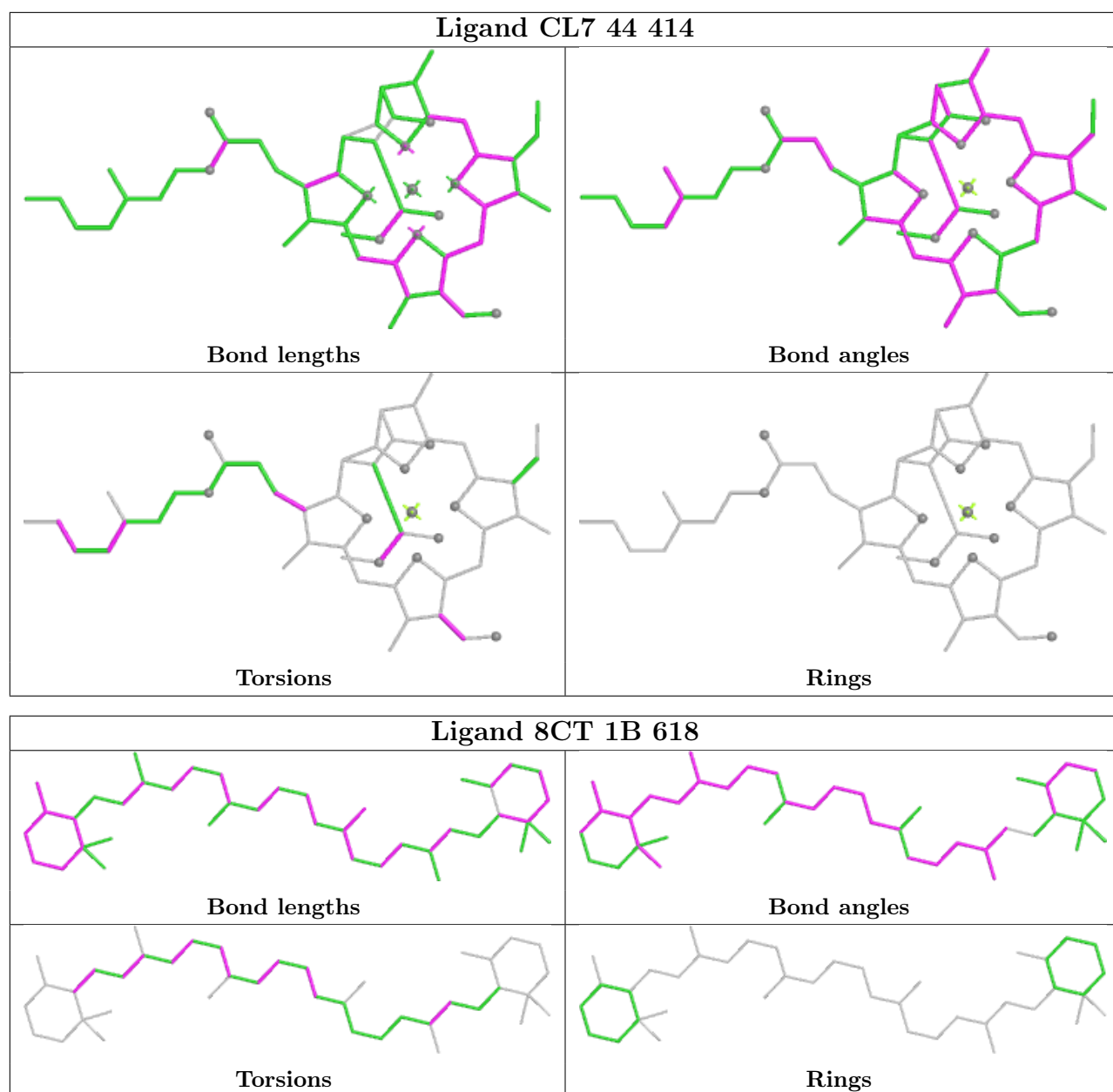




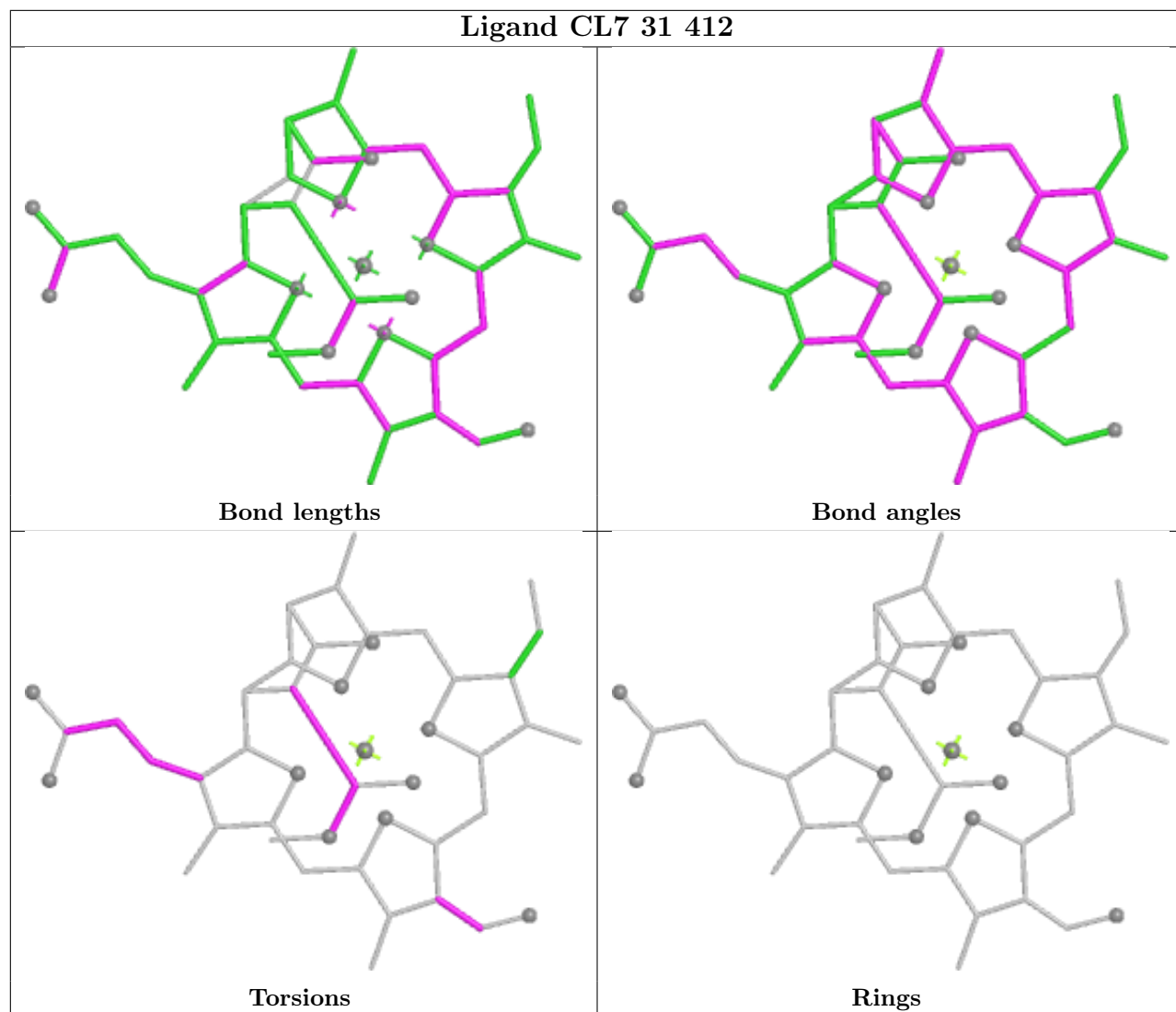




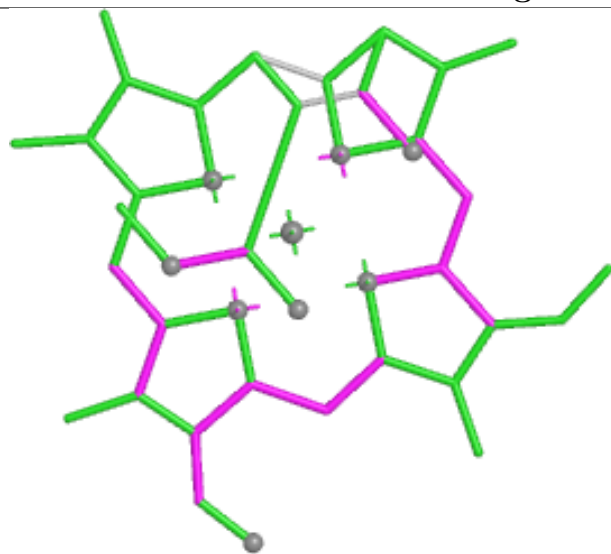




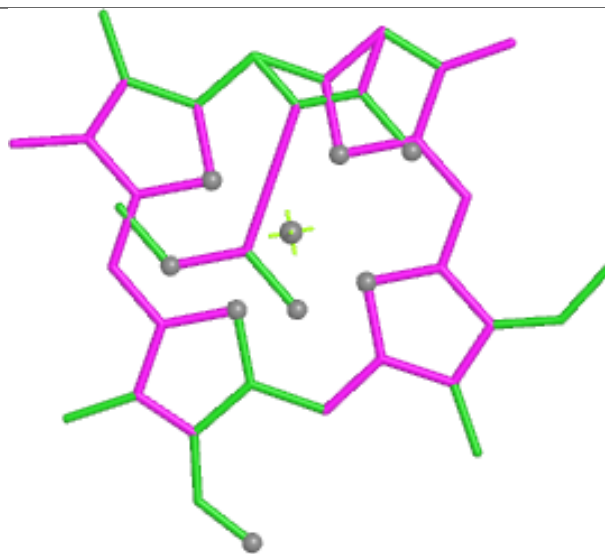
Ligand CL7 31 412



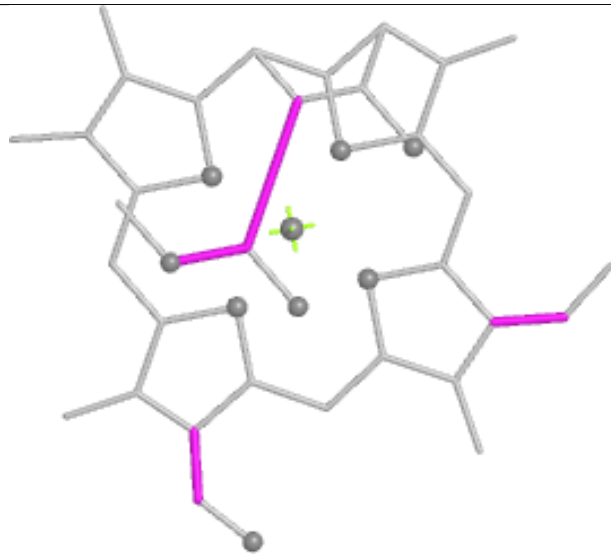
Ligand CL7 24 416



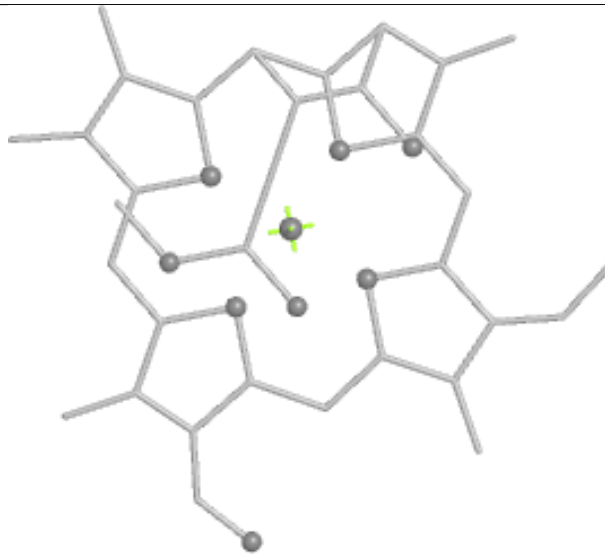
Bond lengths



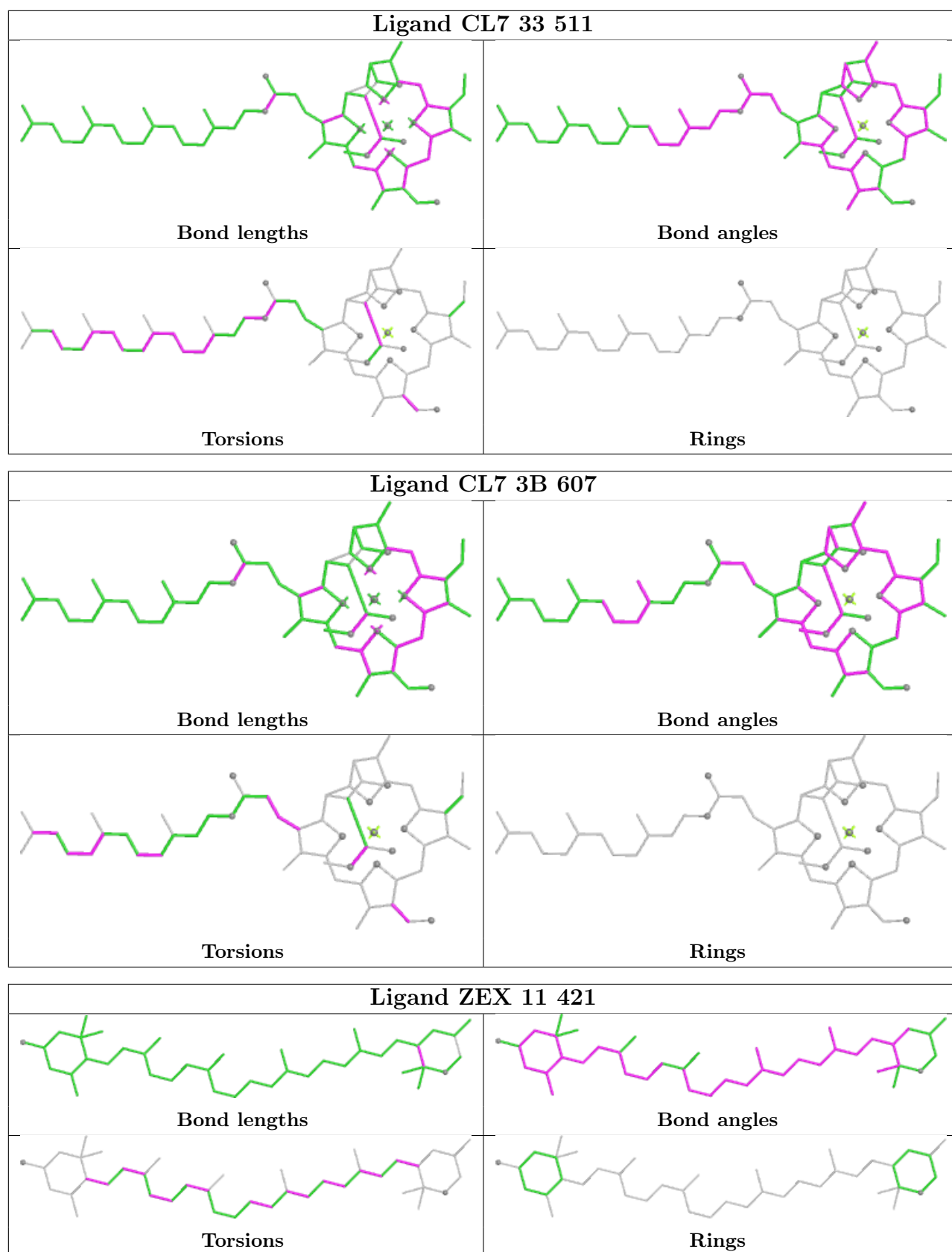
Bond angles

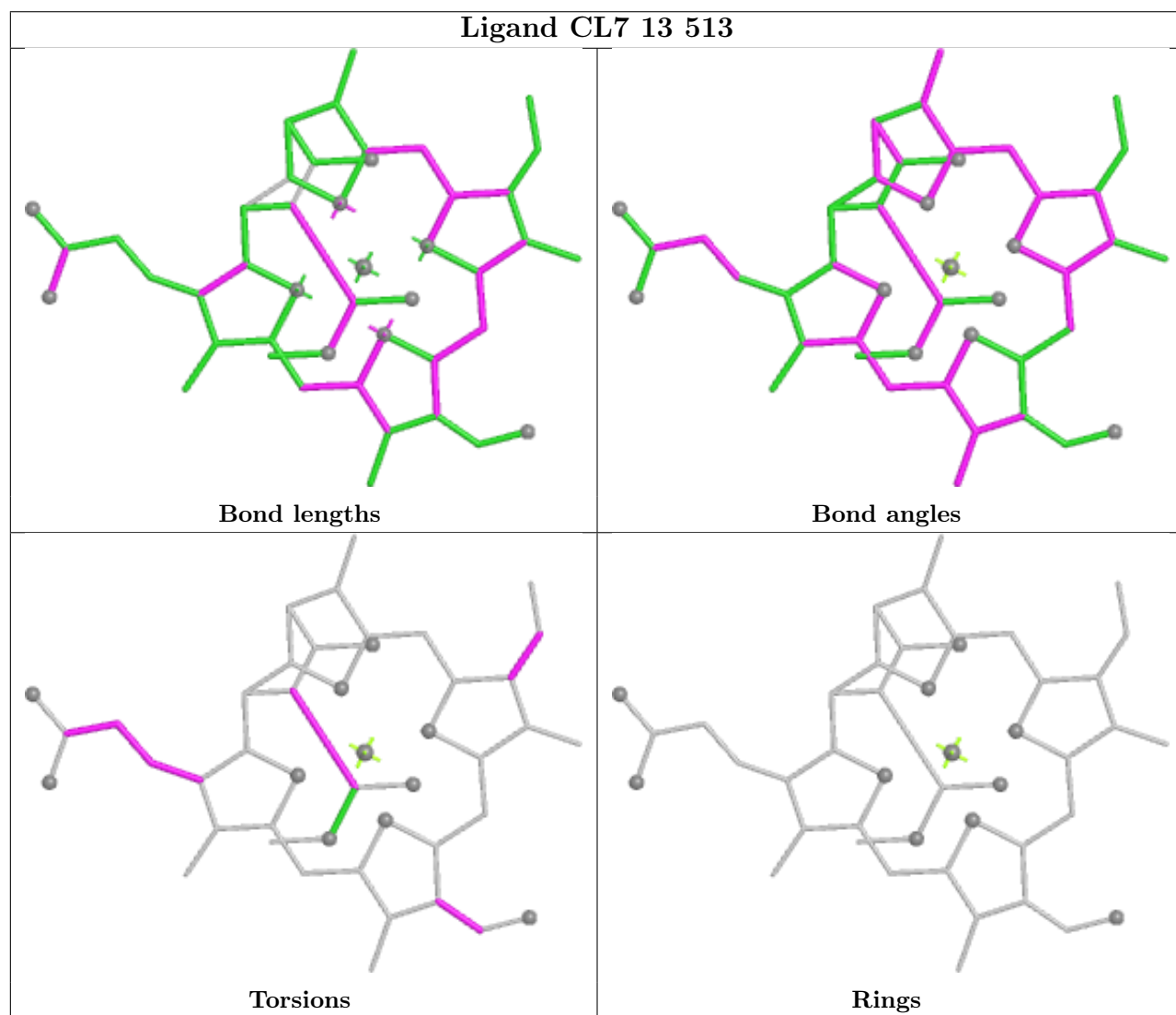
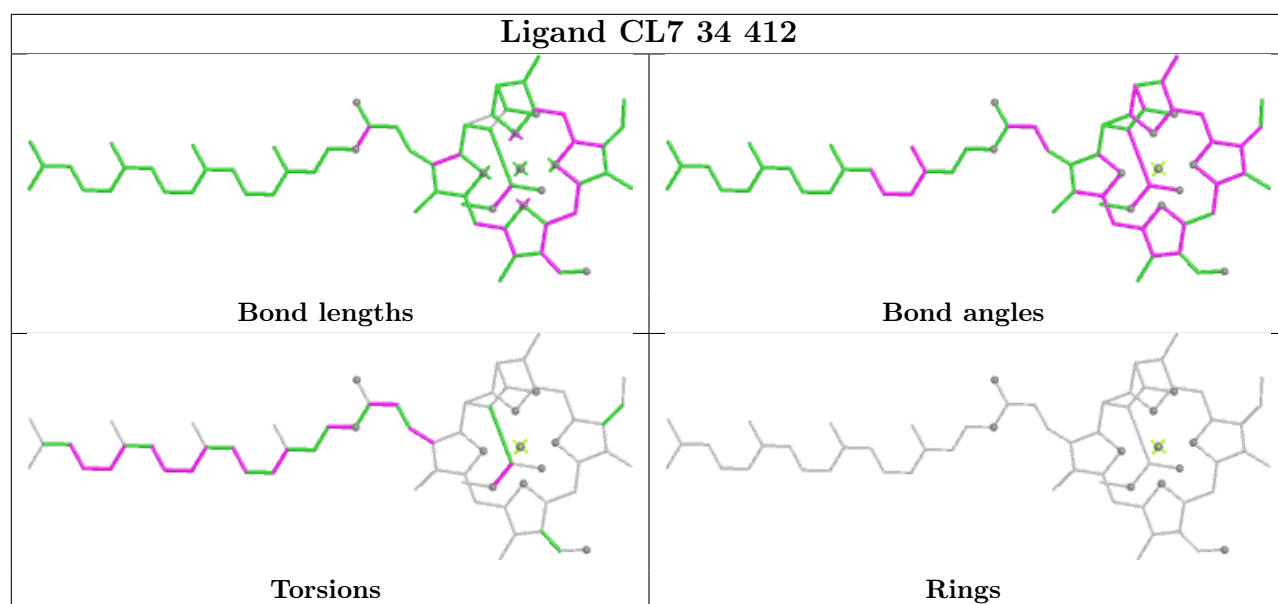


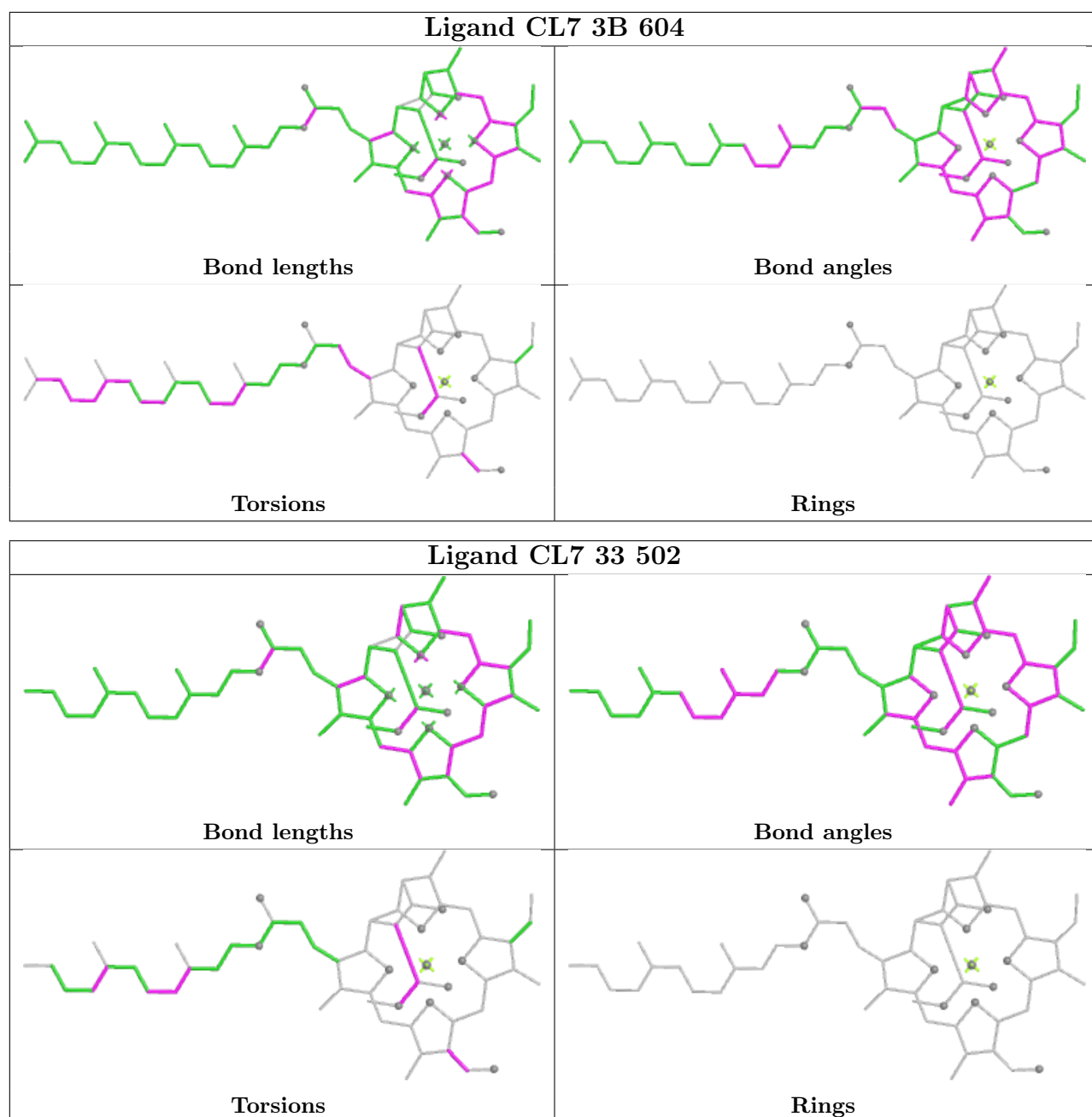
Torsions

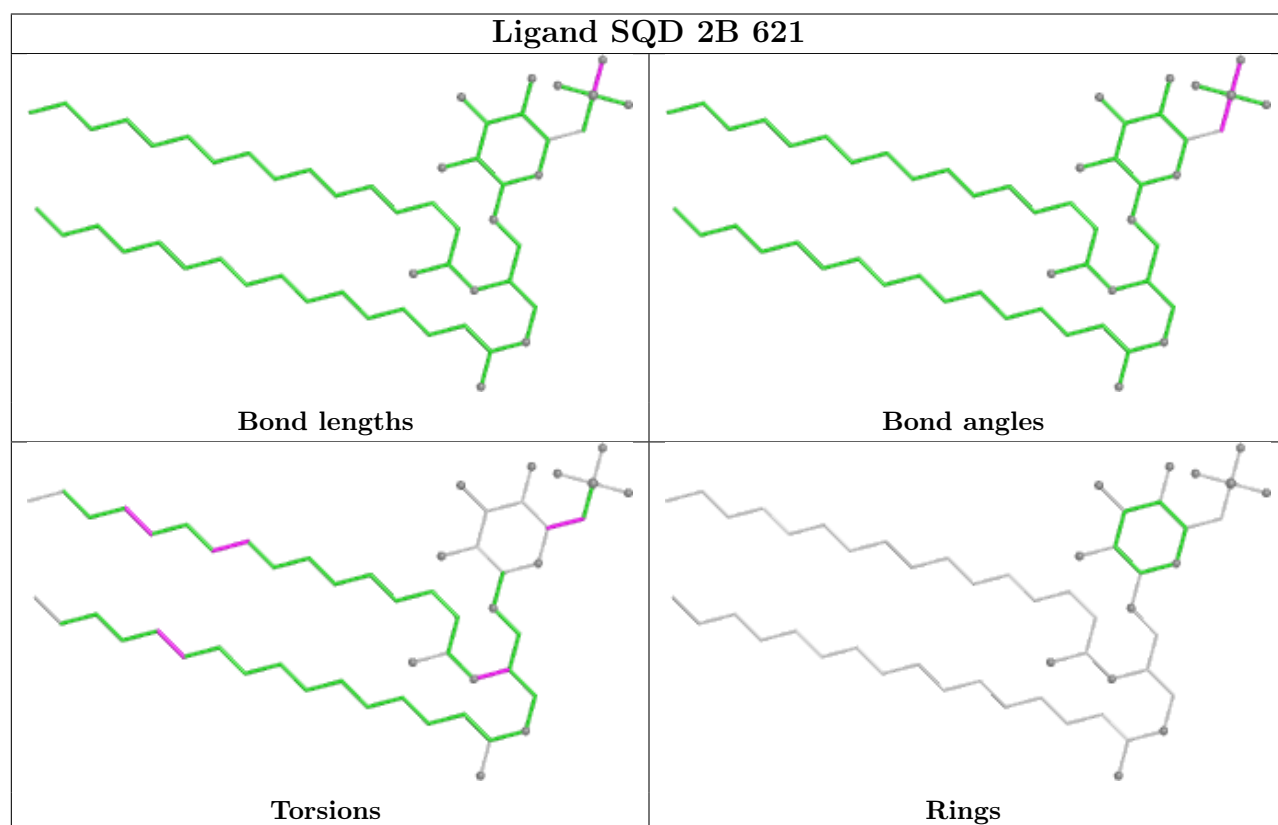
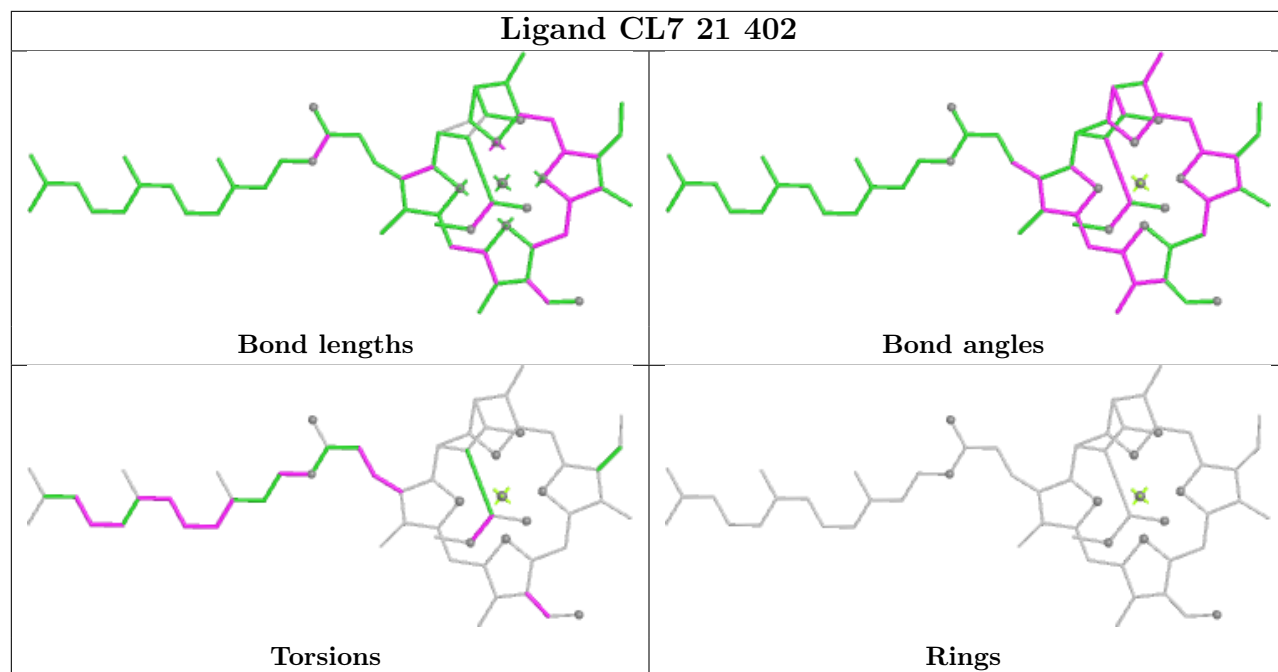


Rings

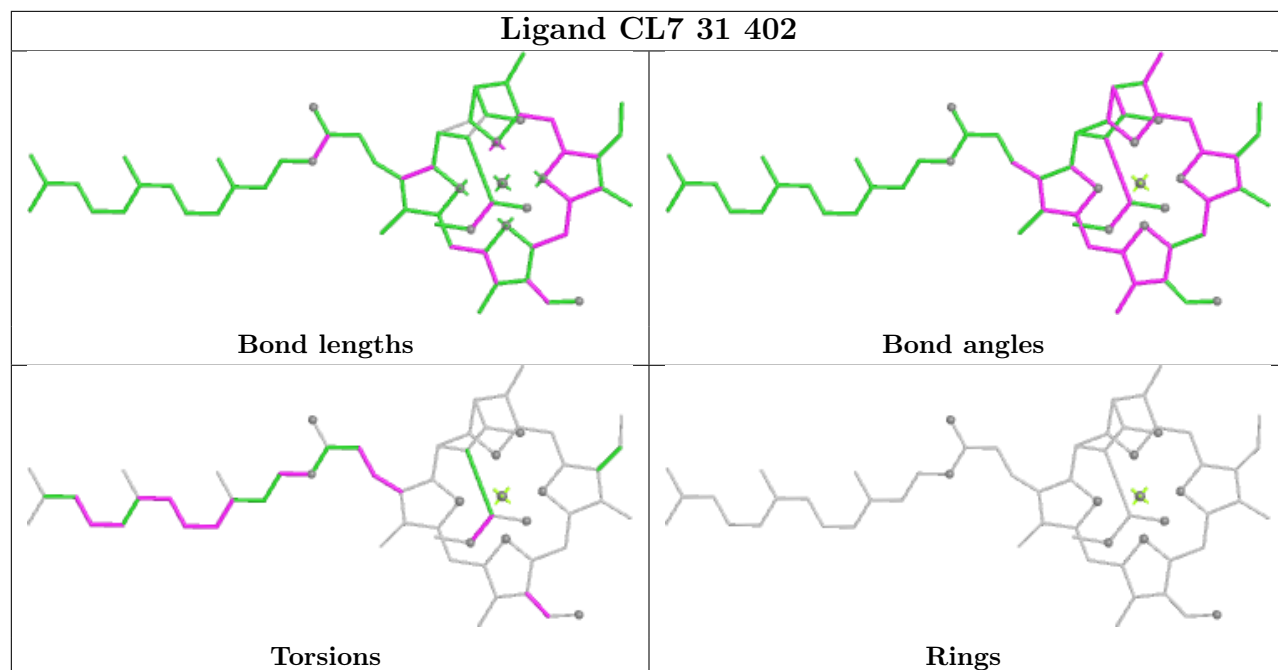




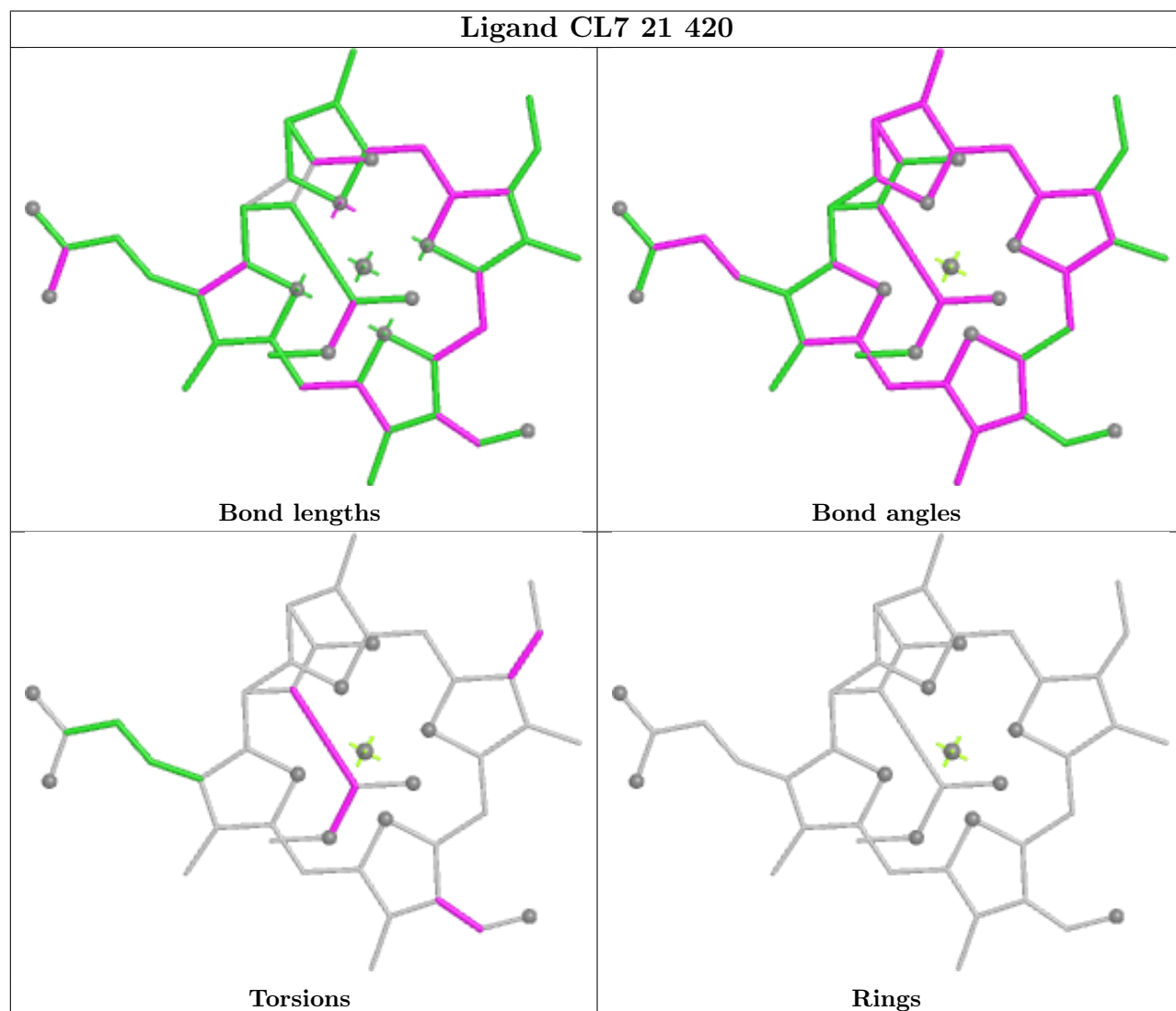


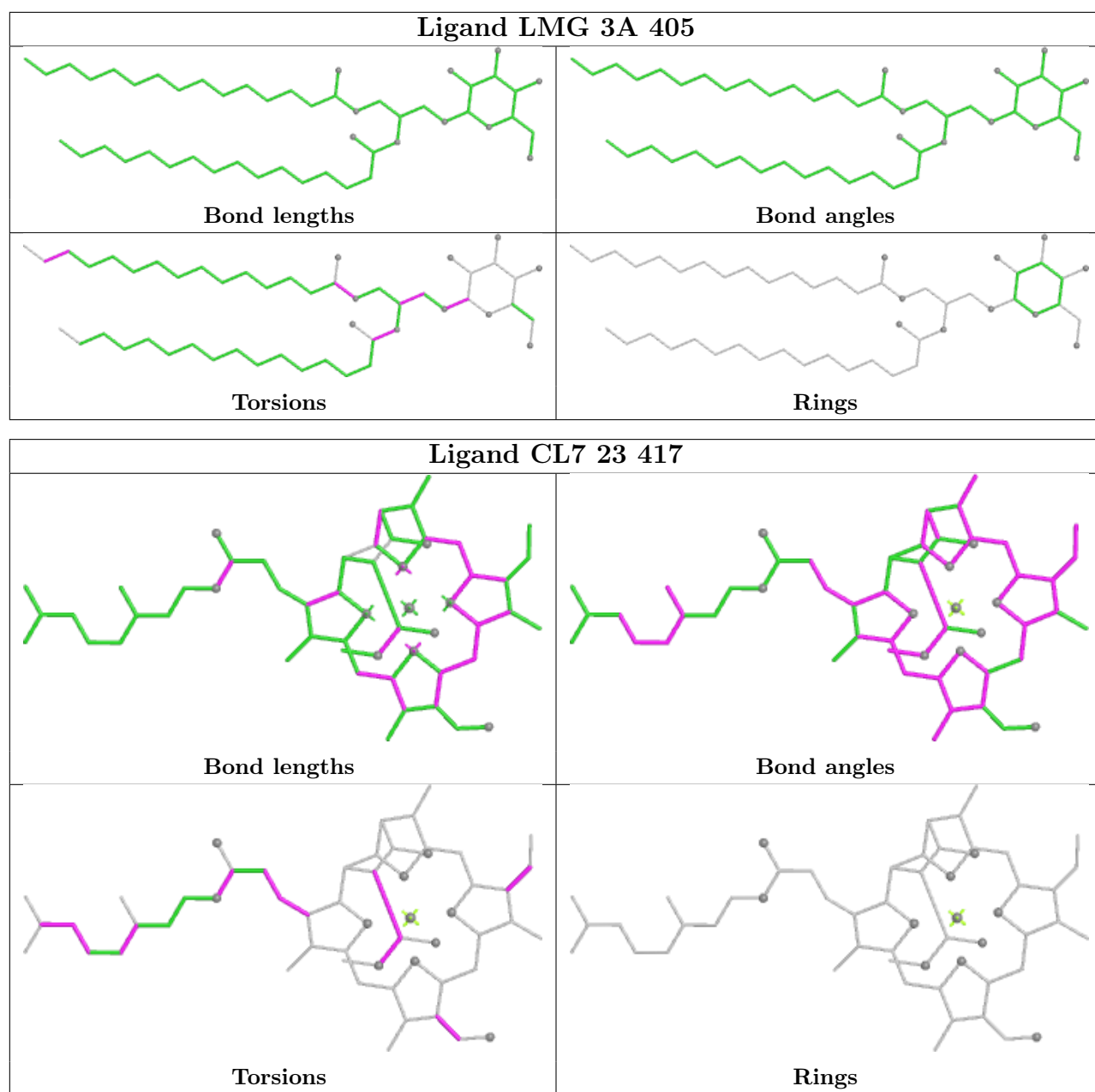


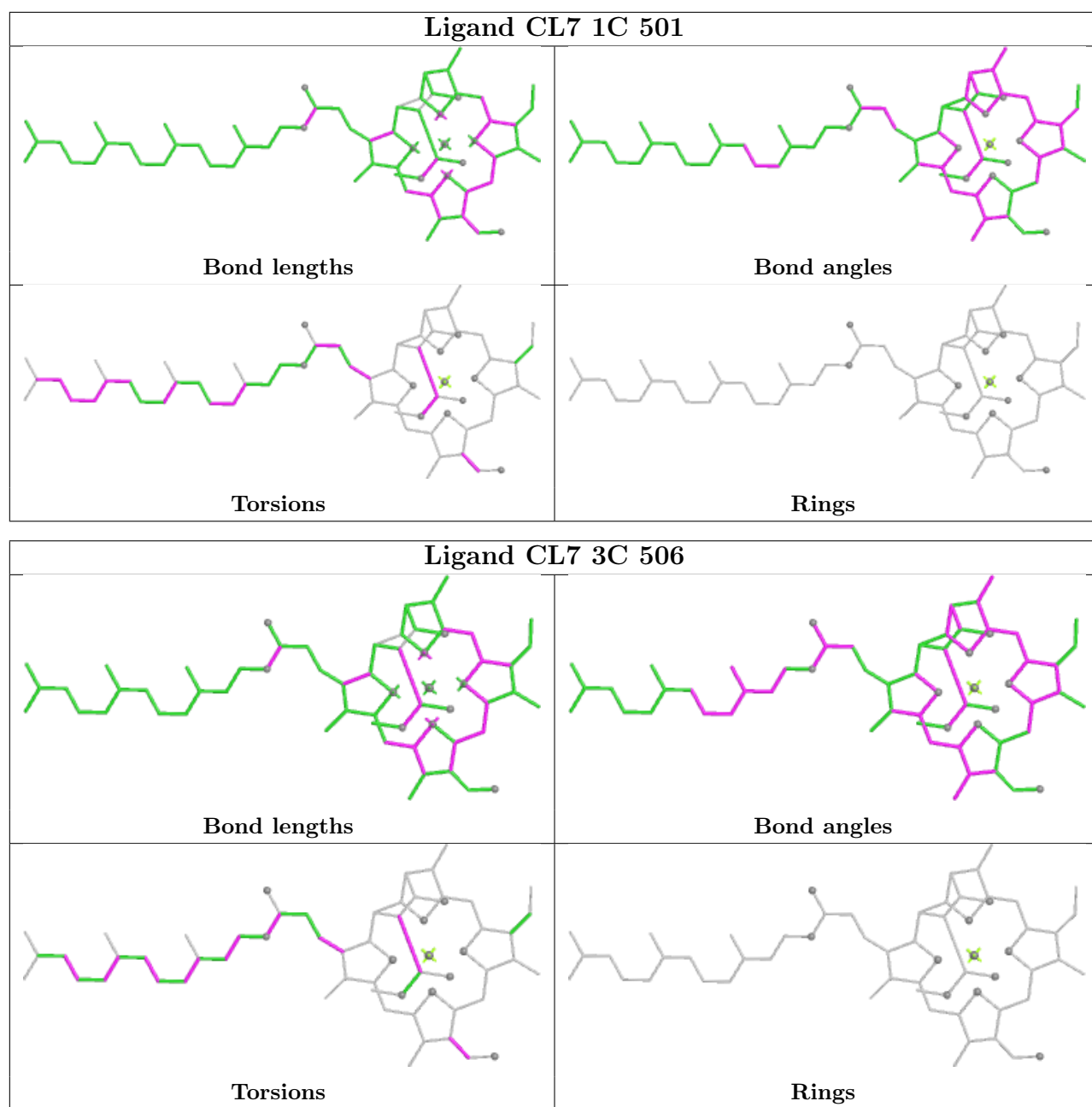
Ligand CL7 31 402

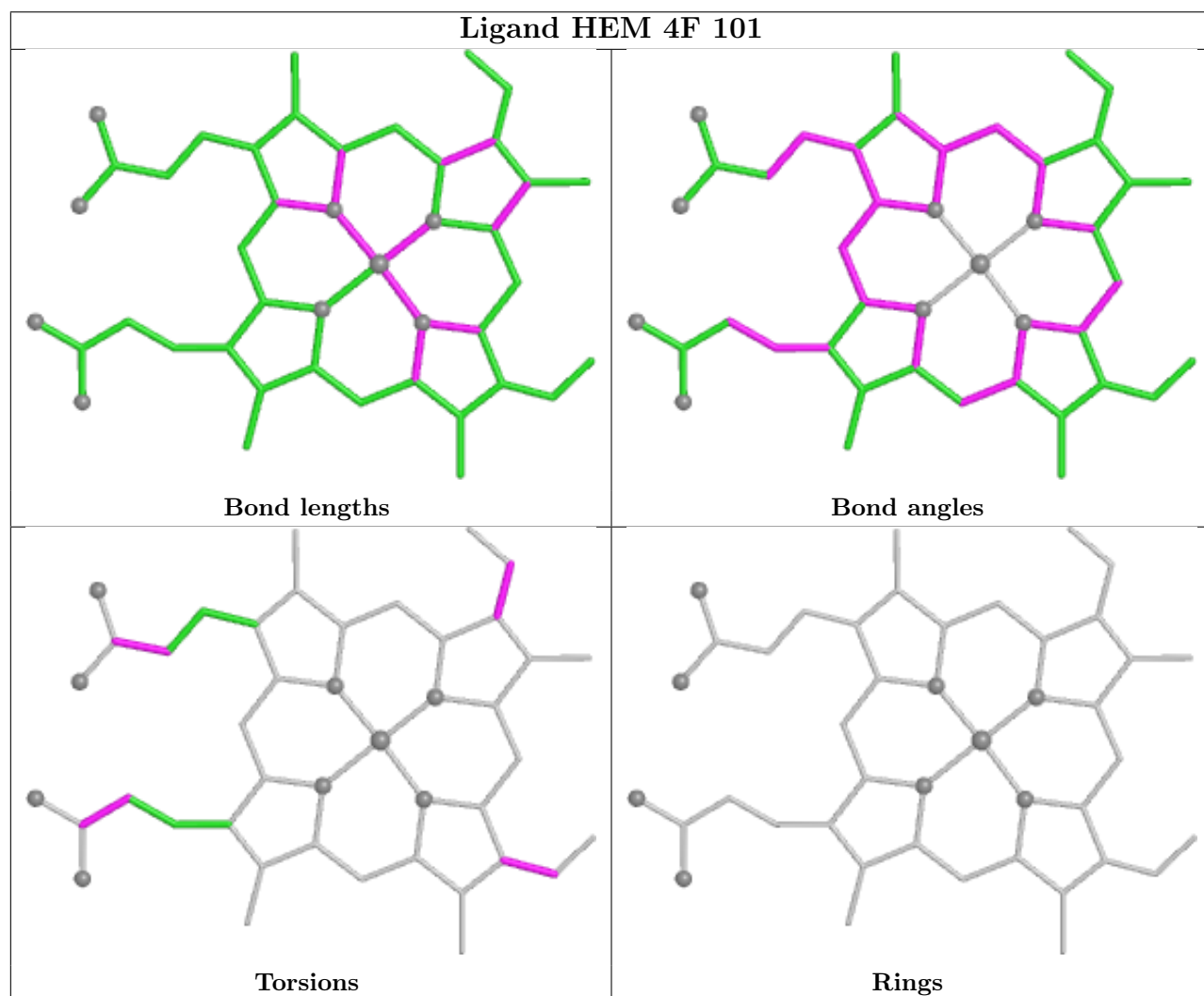
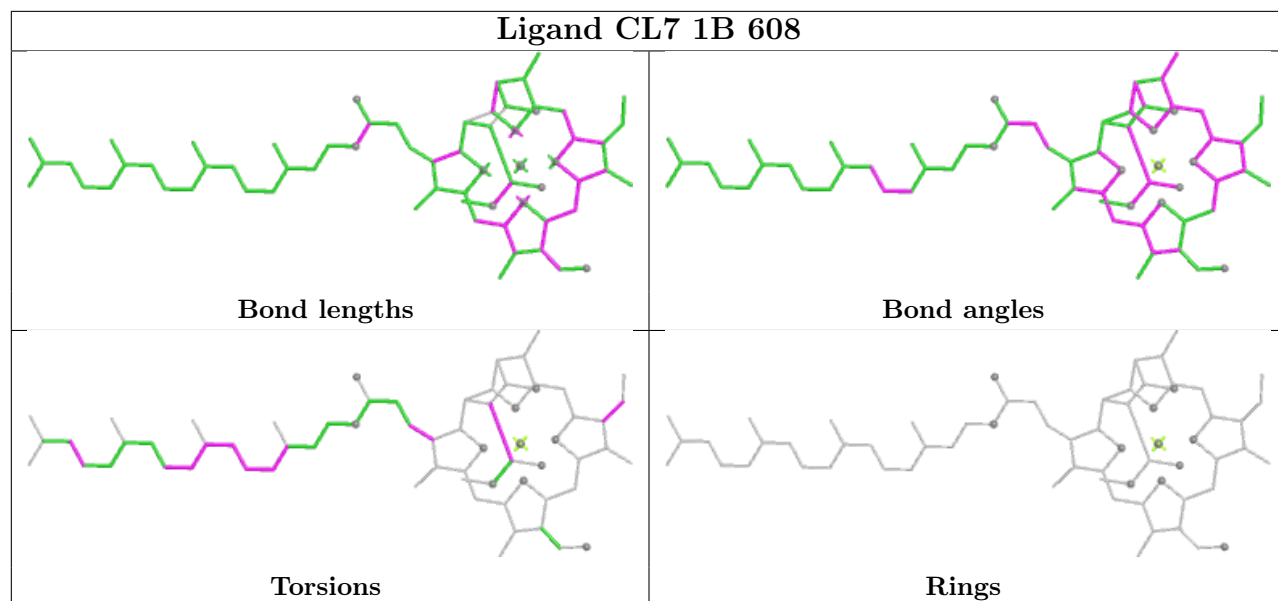


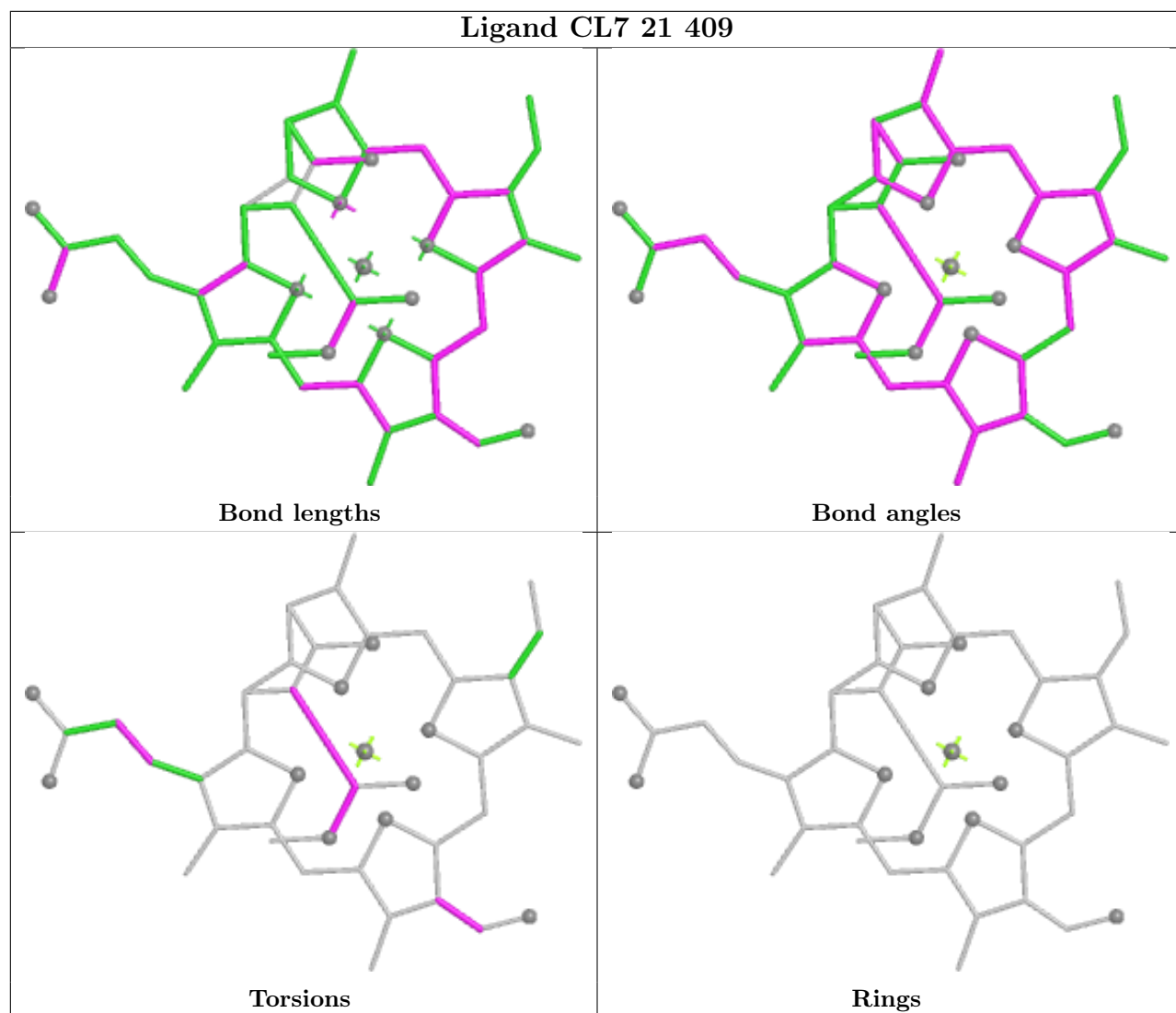
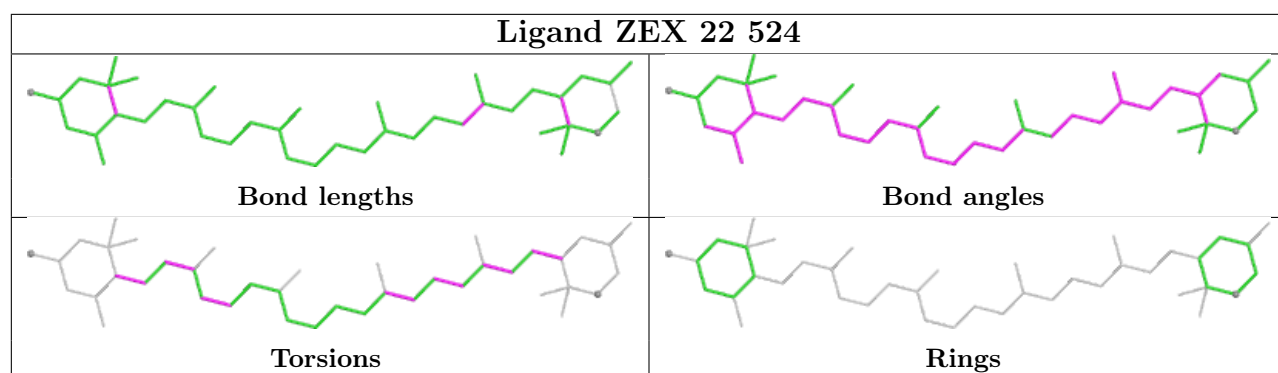
Ligand CL7 21 420

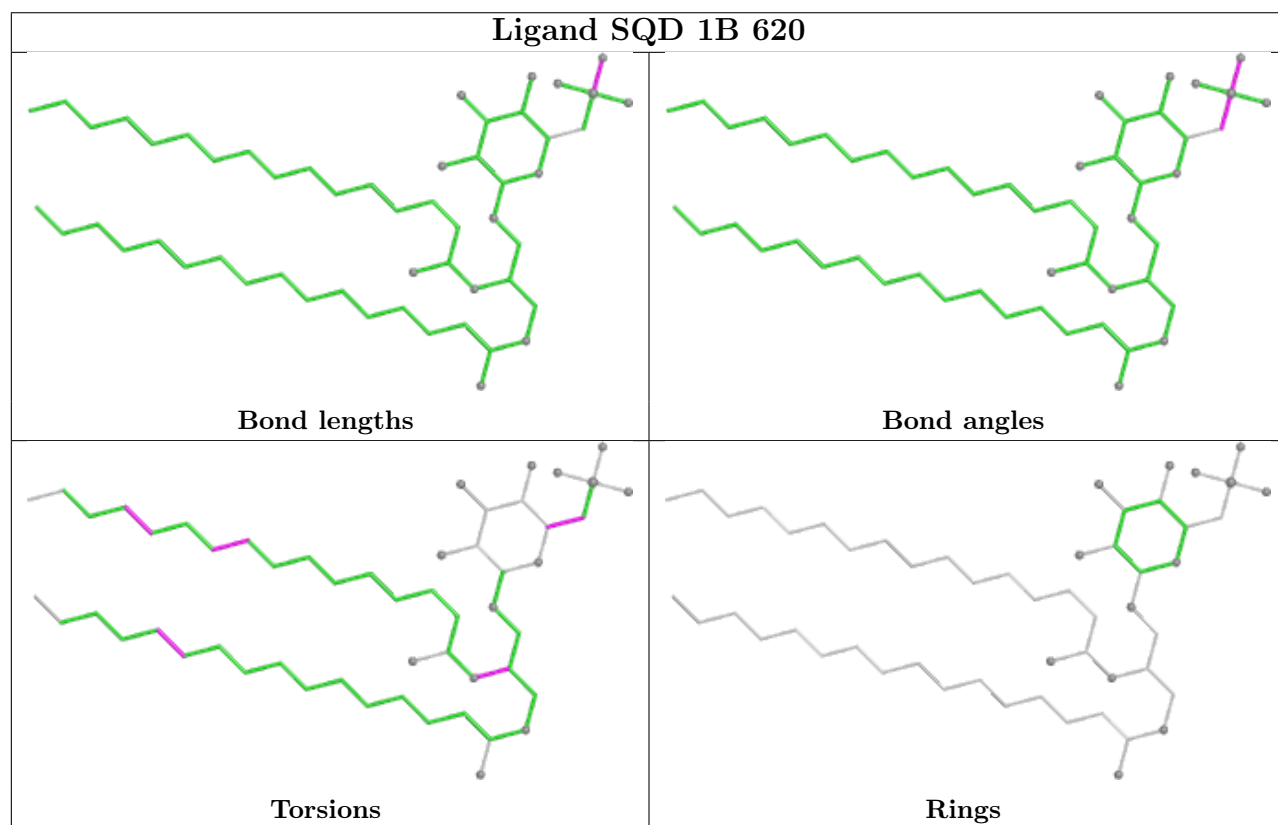
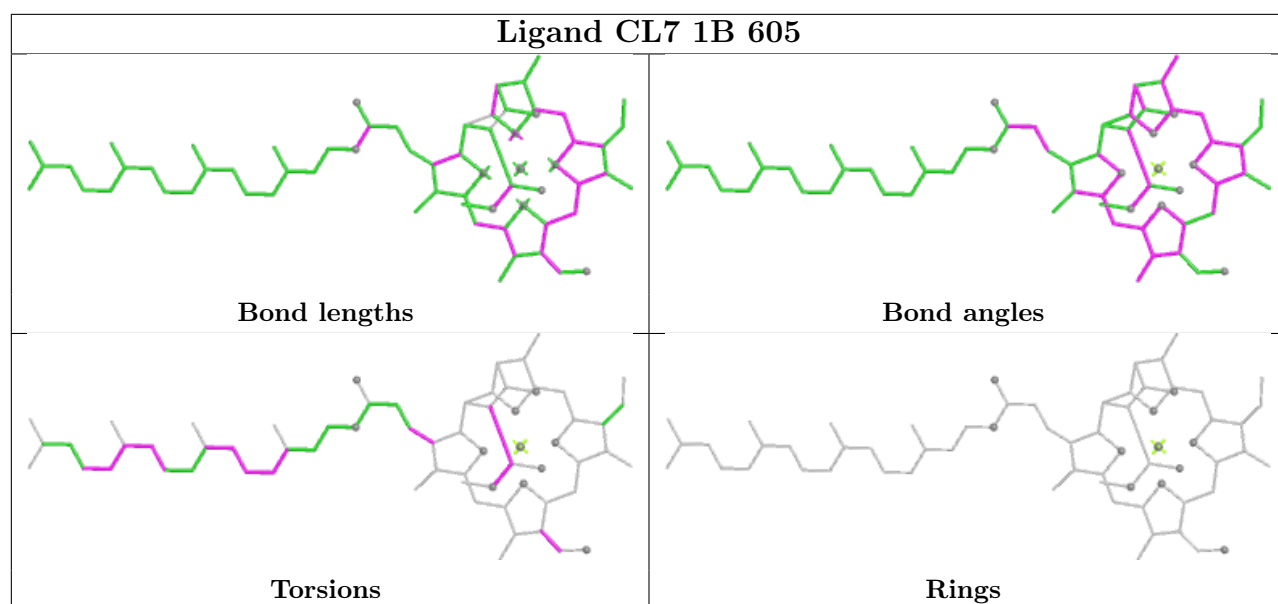


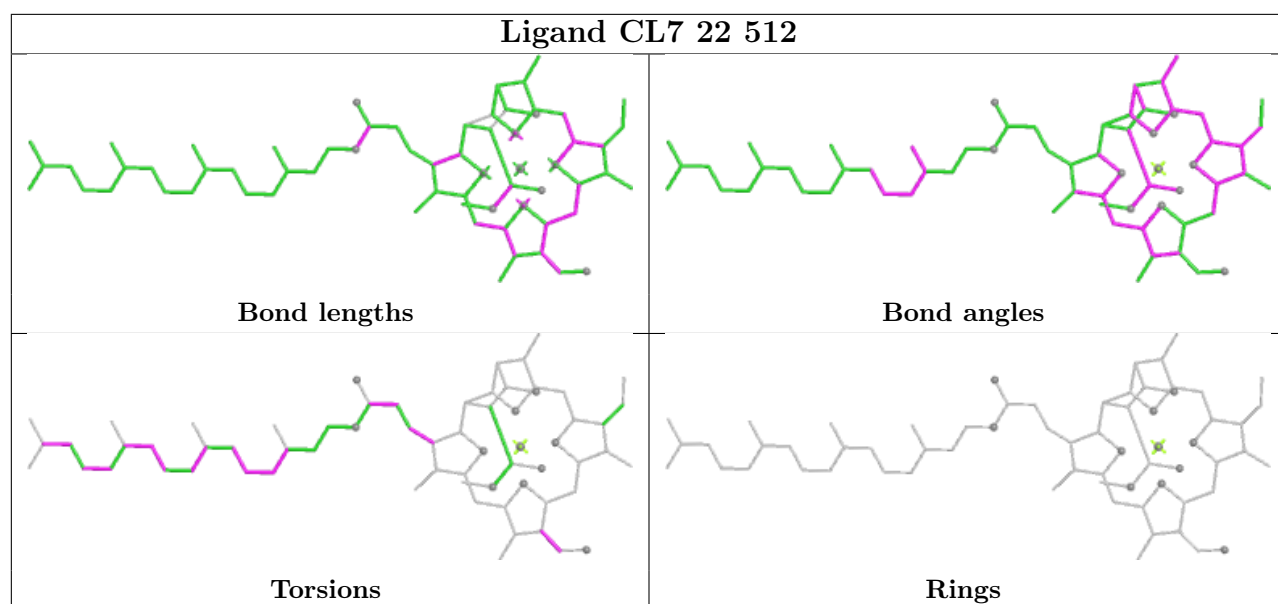


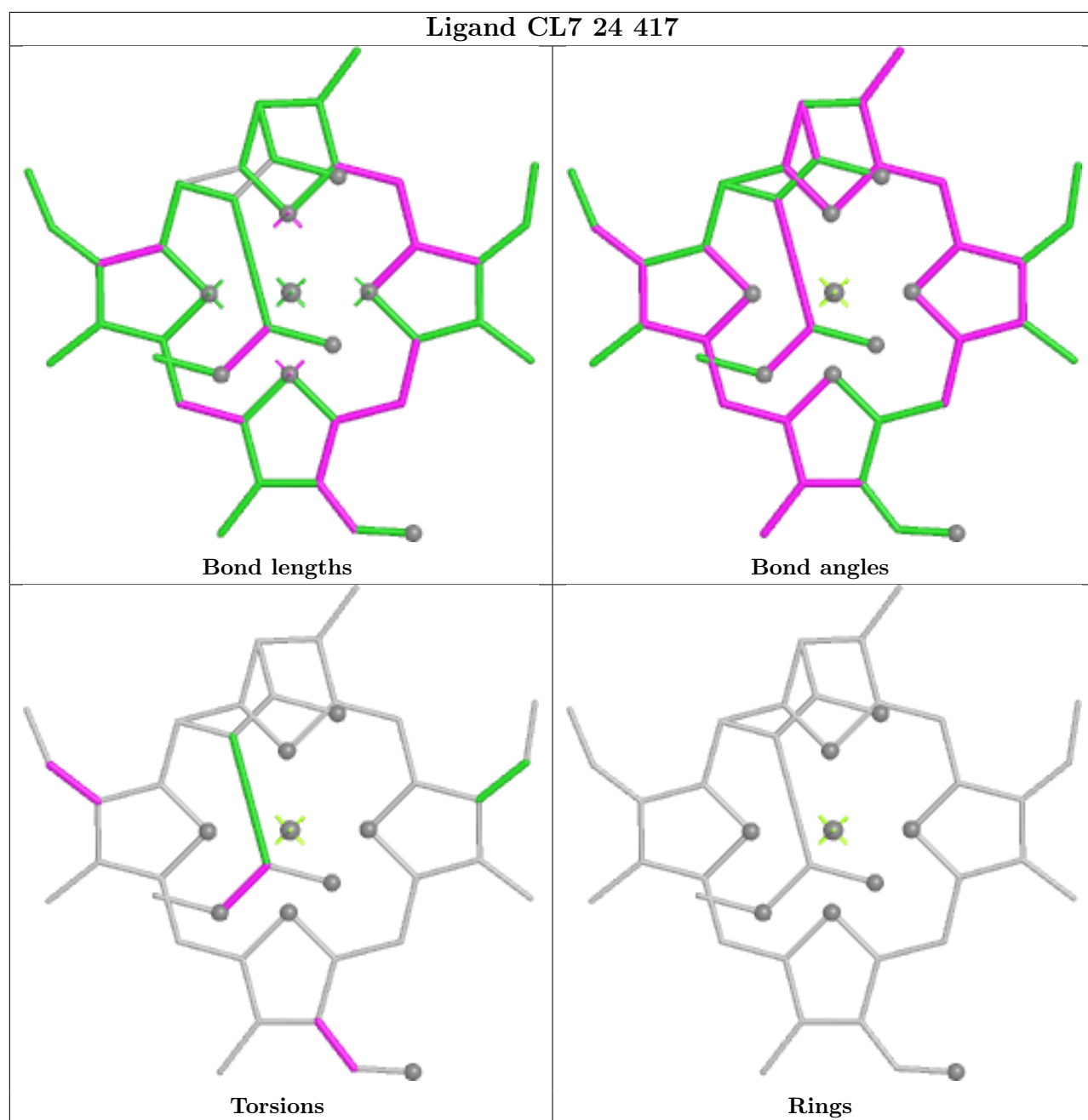


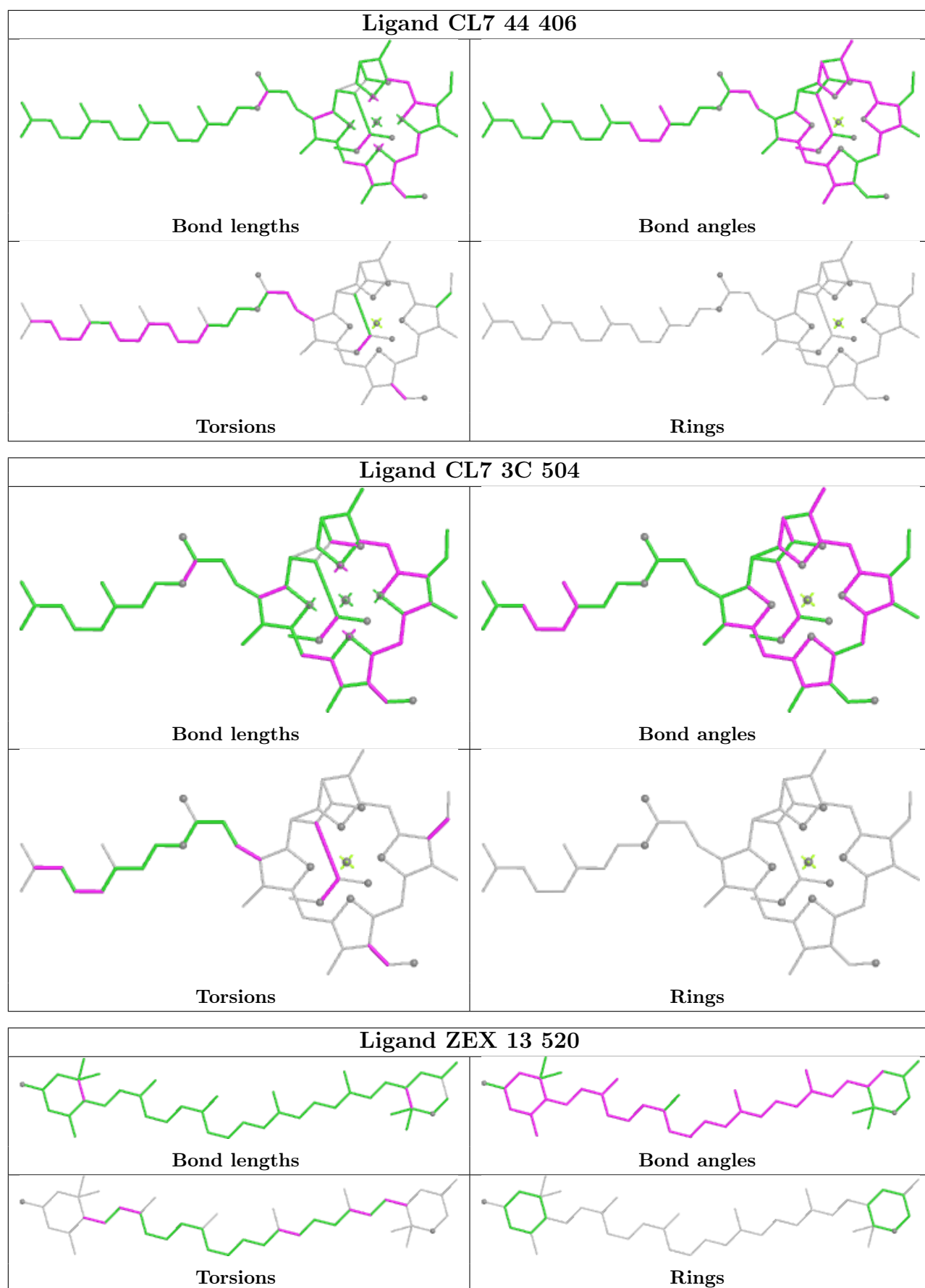


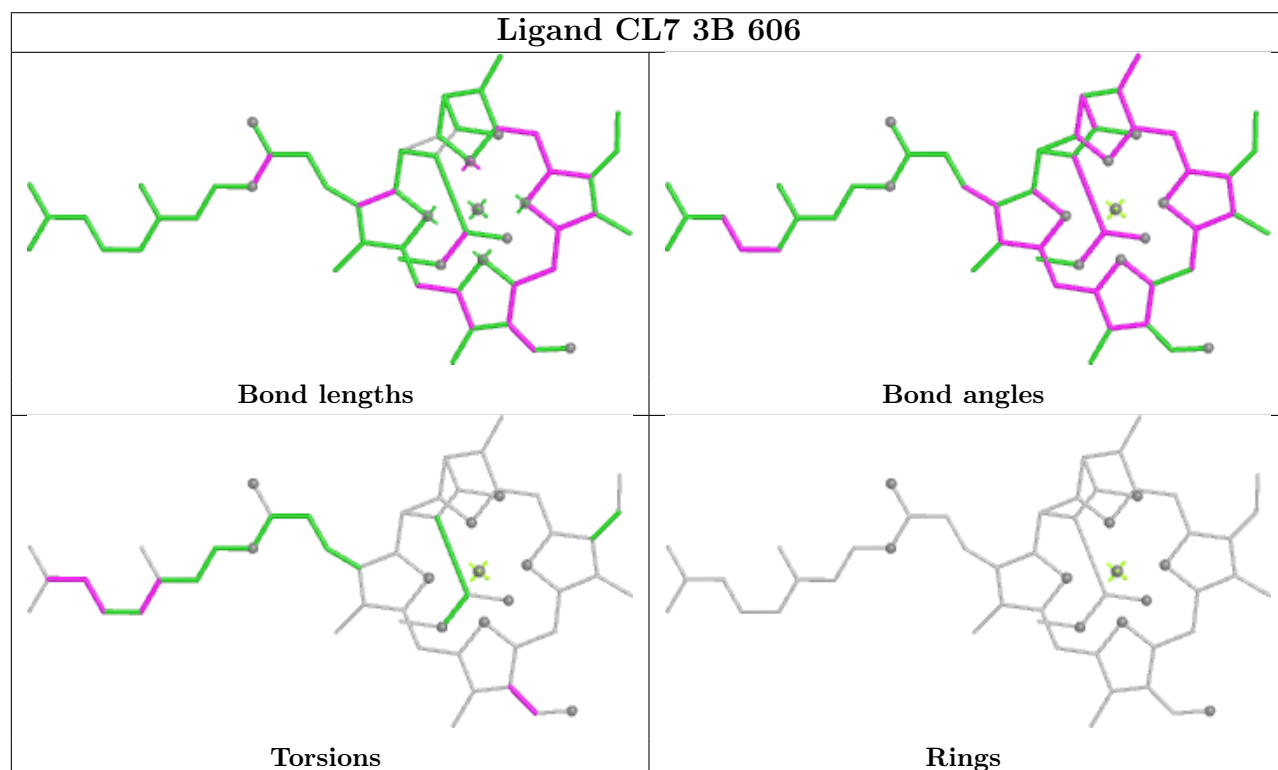
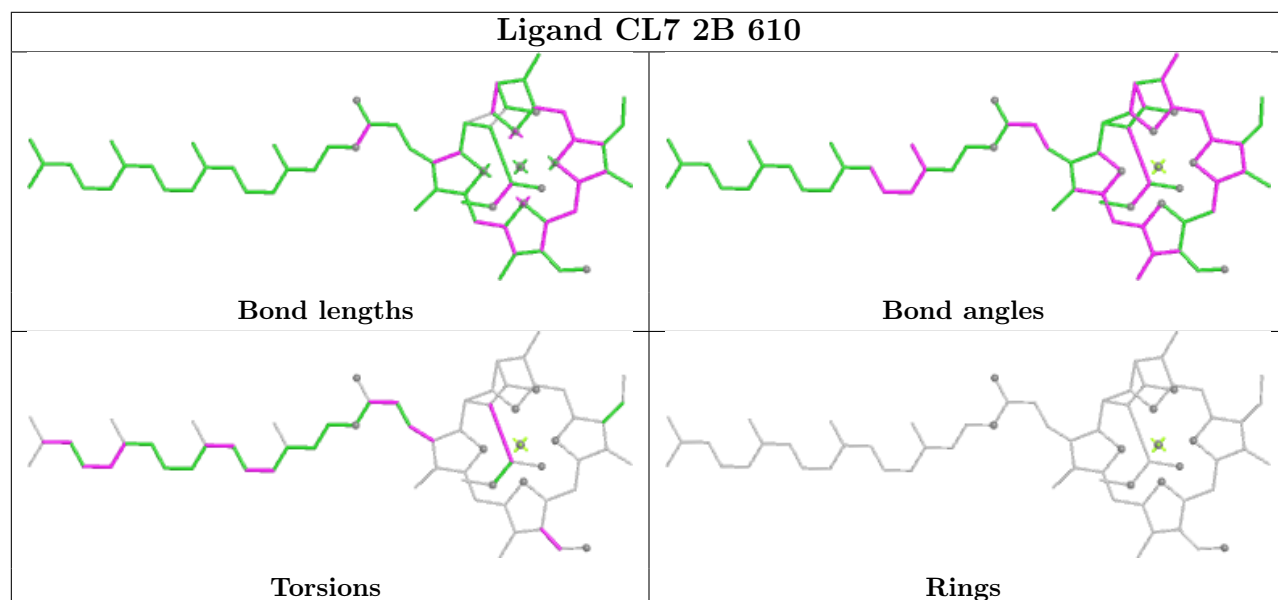
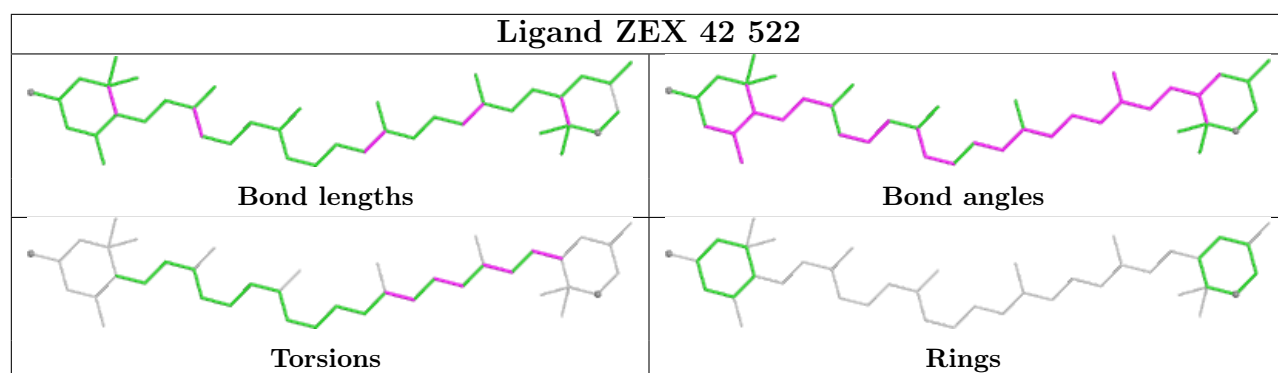


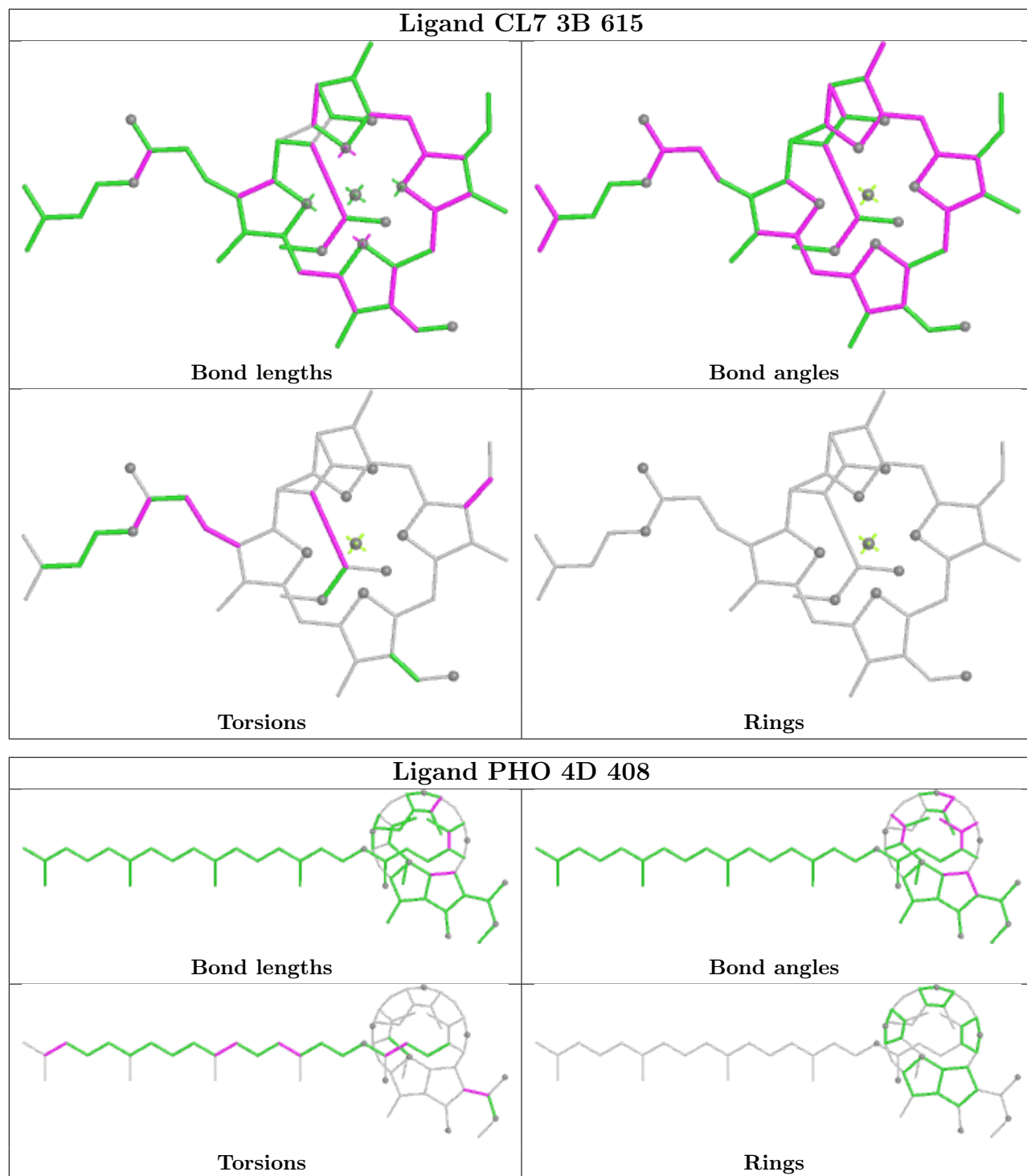


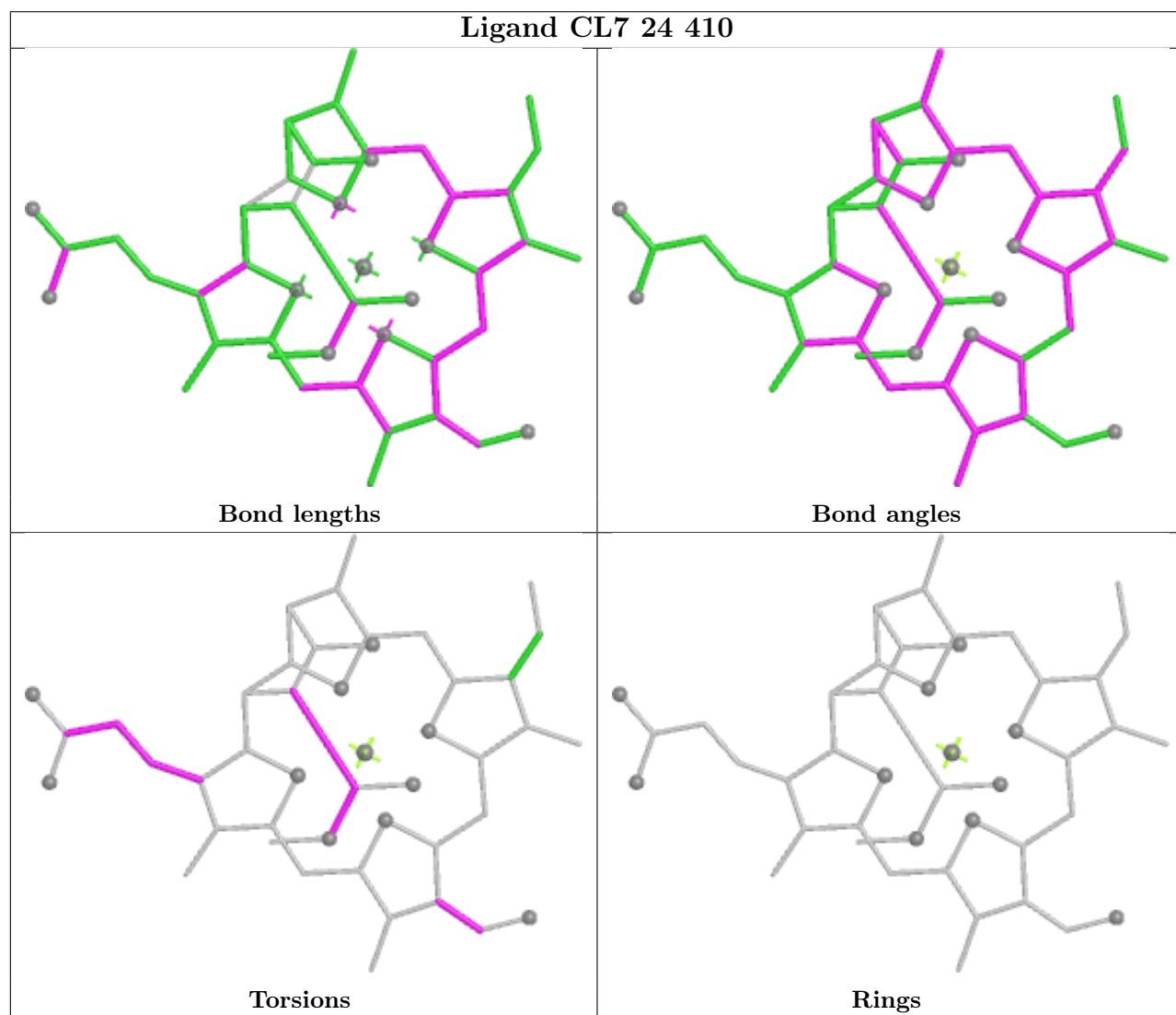
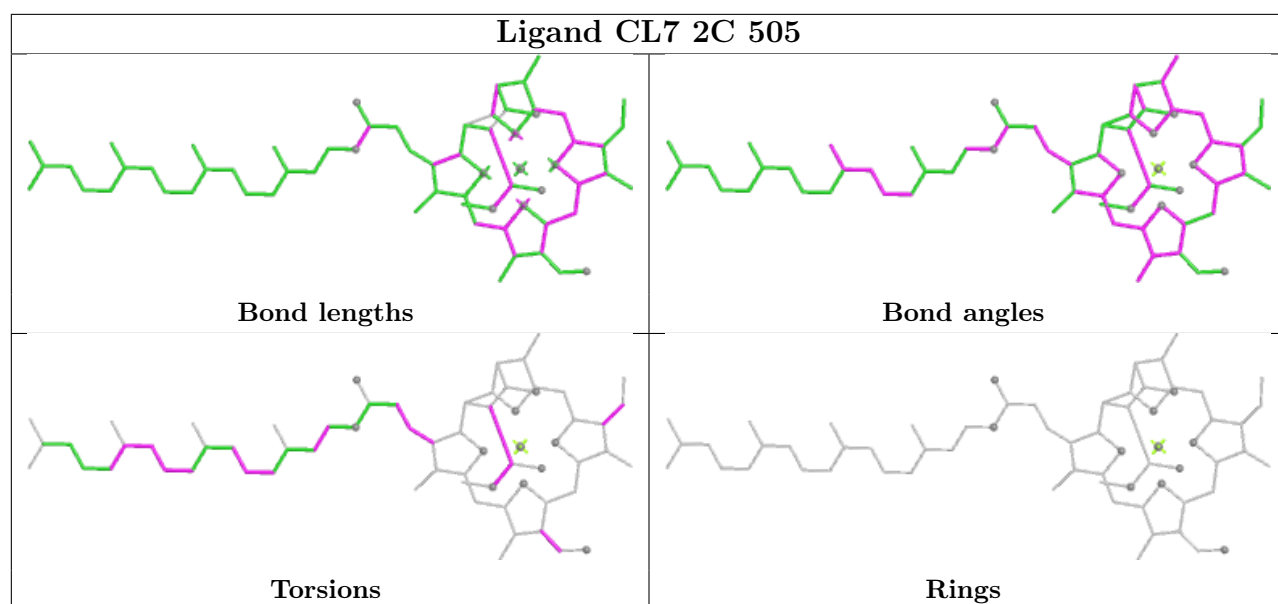


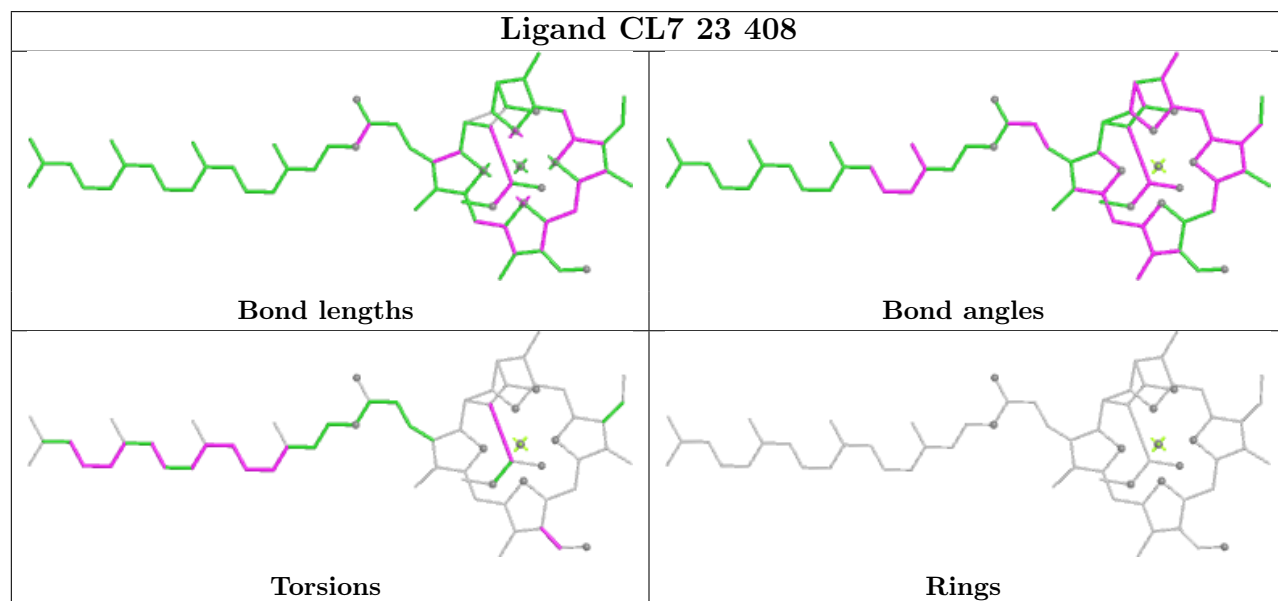
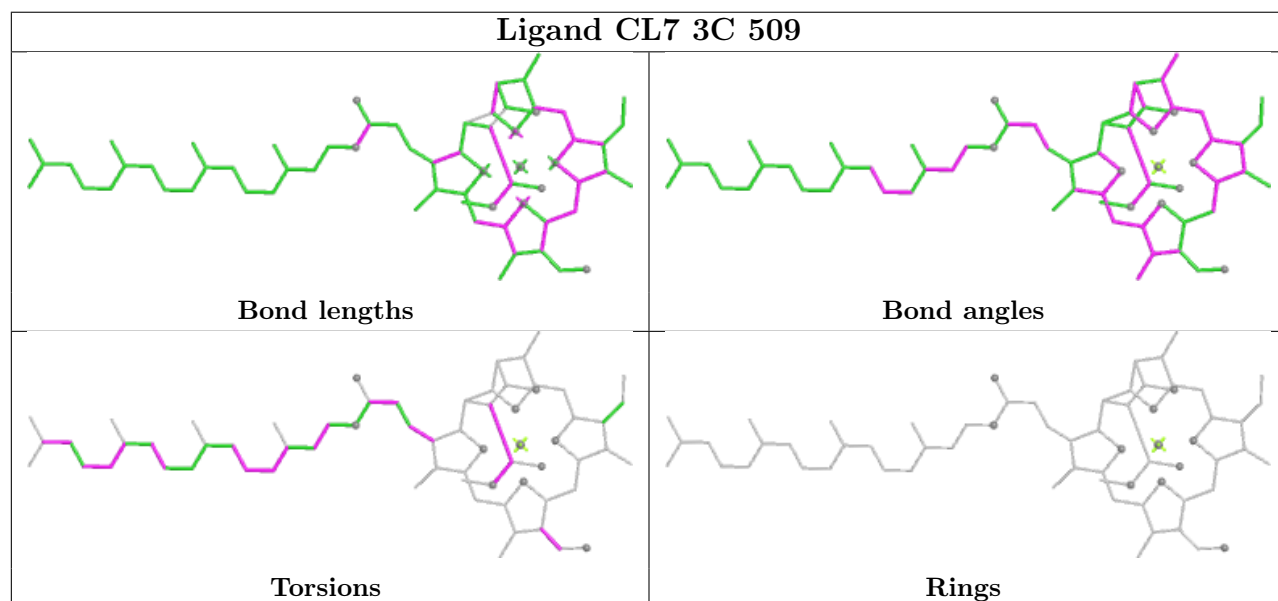
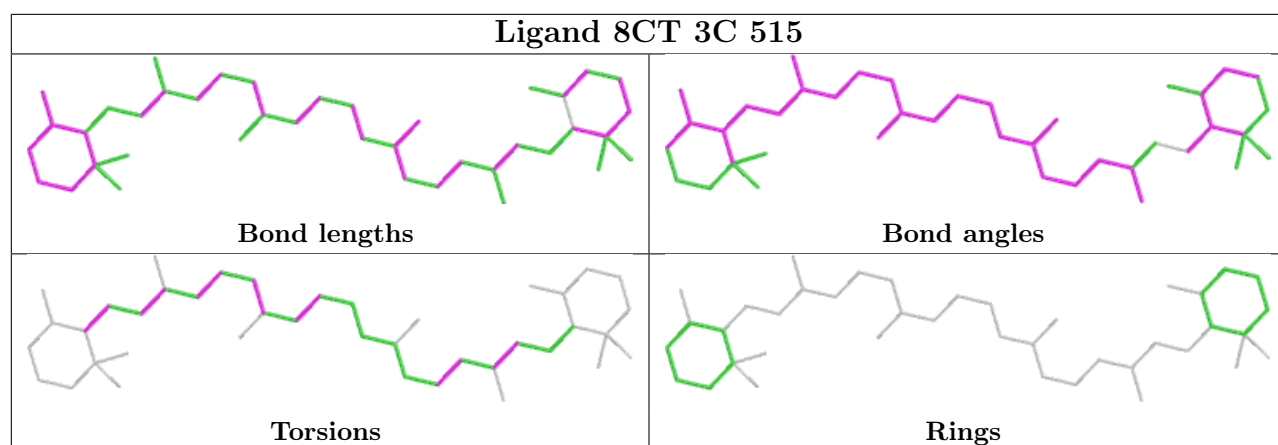


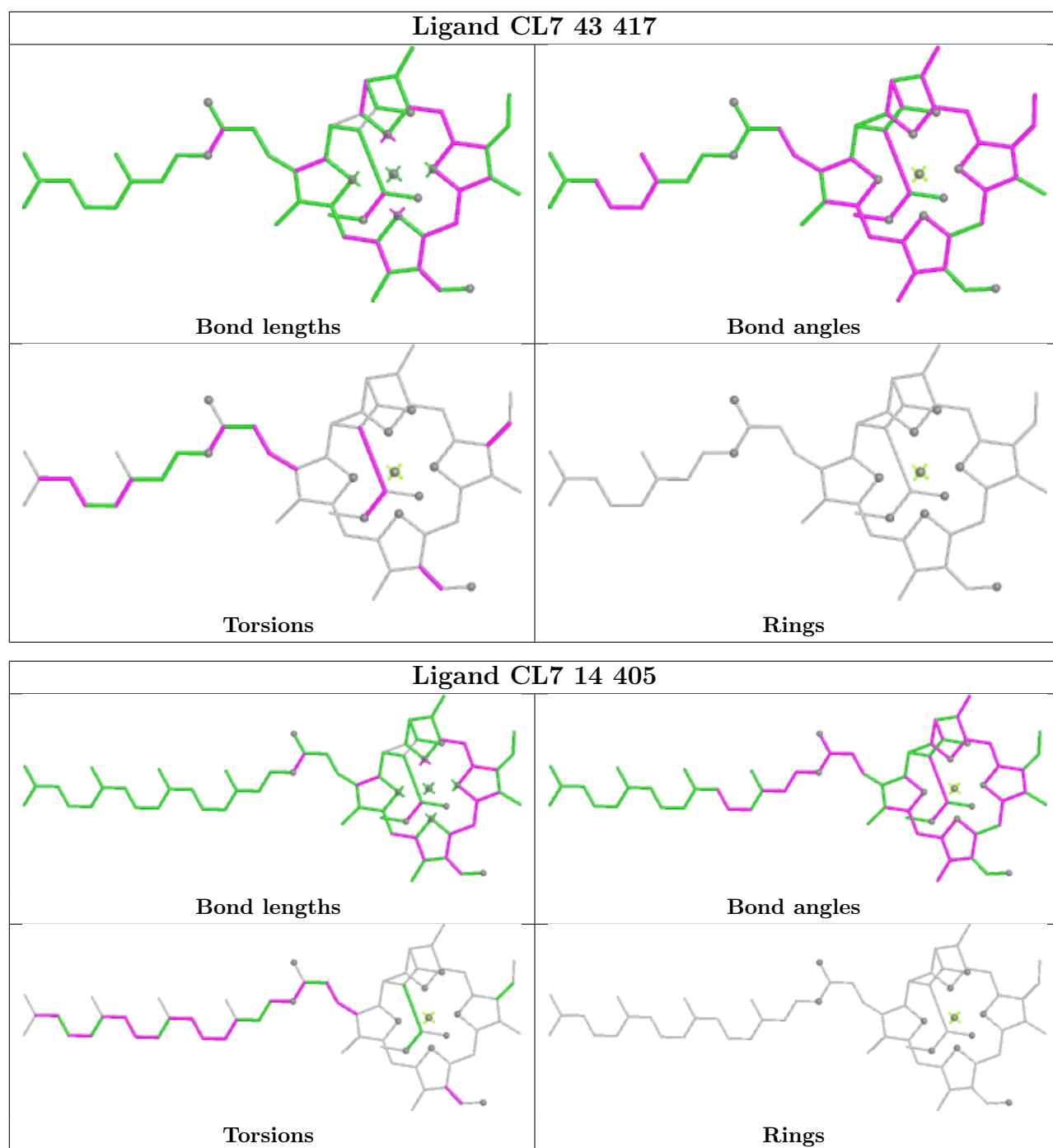


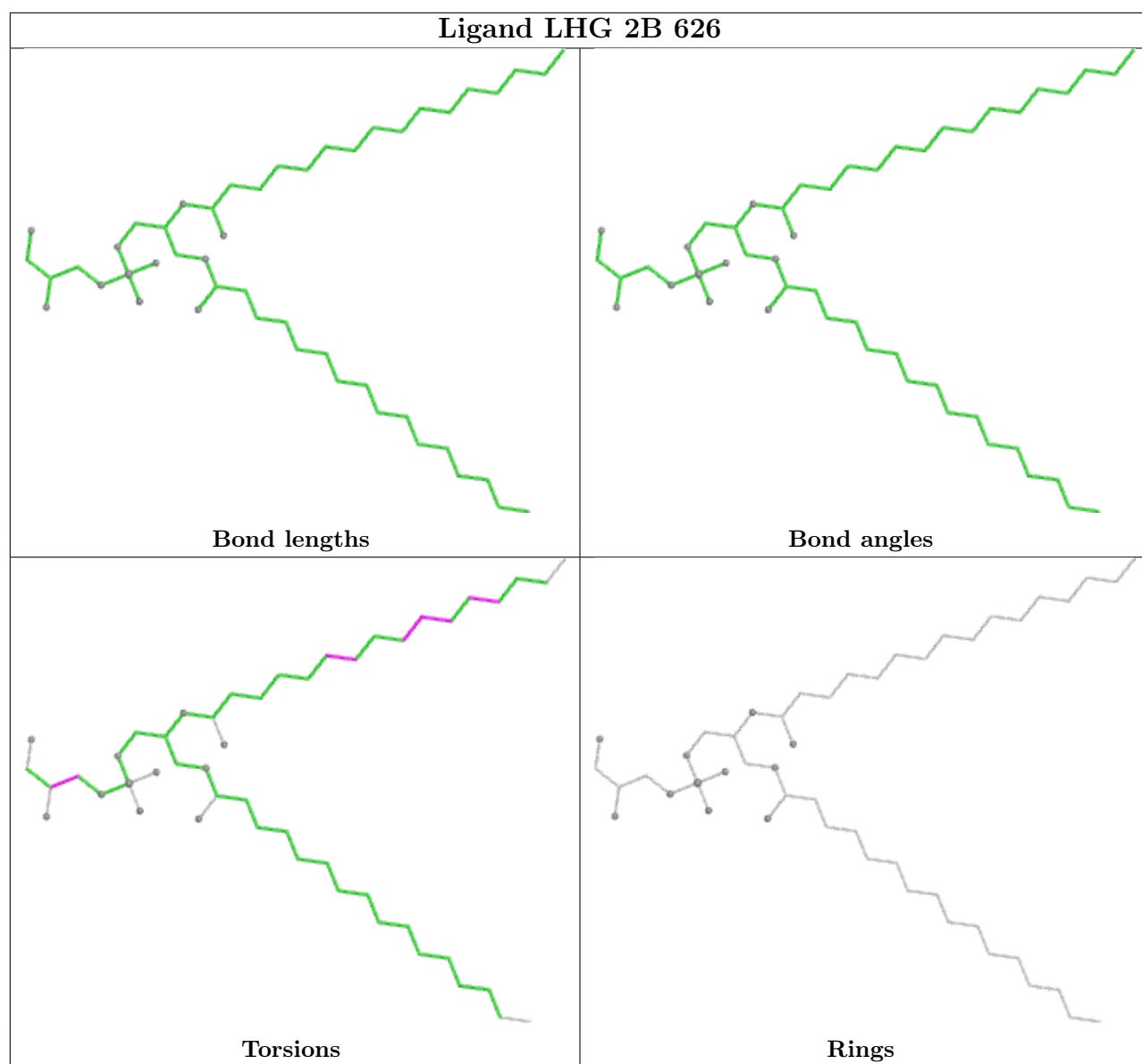


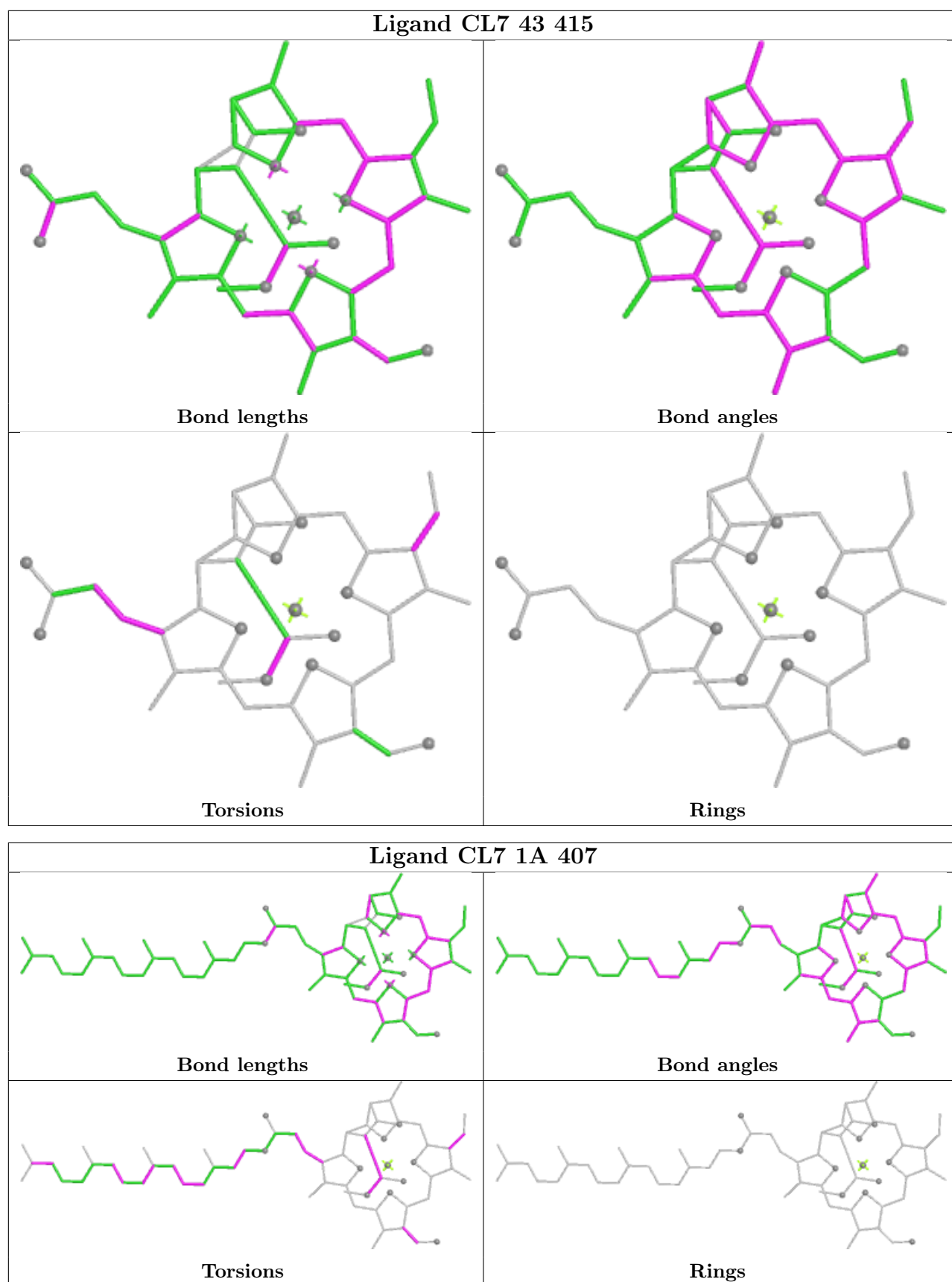


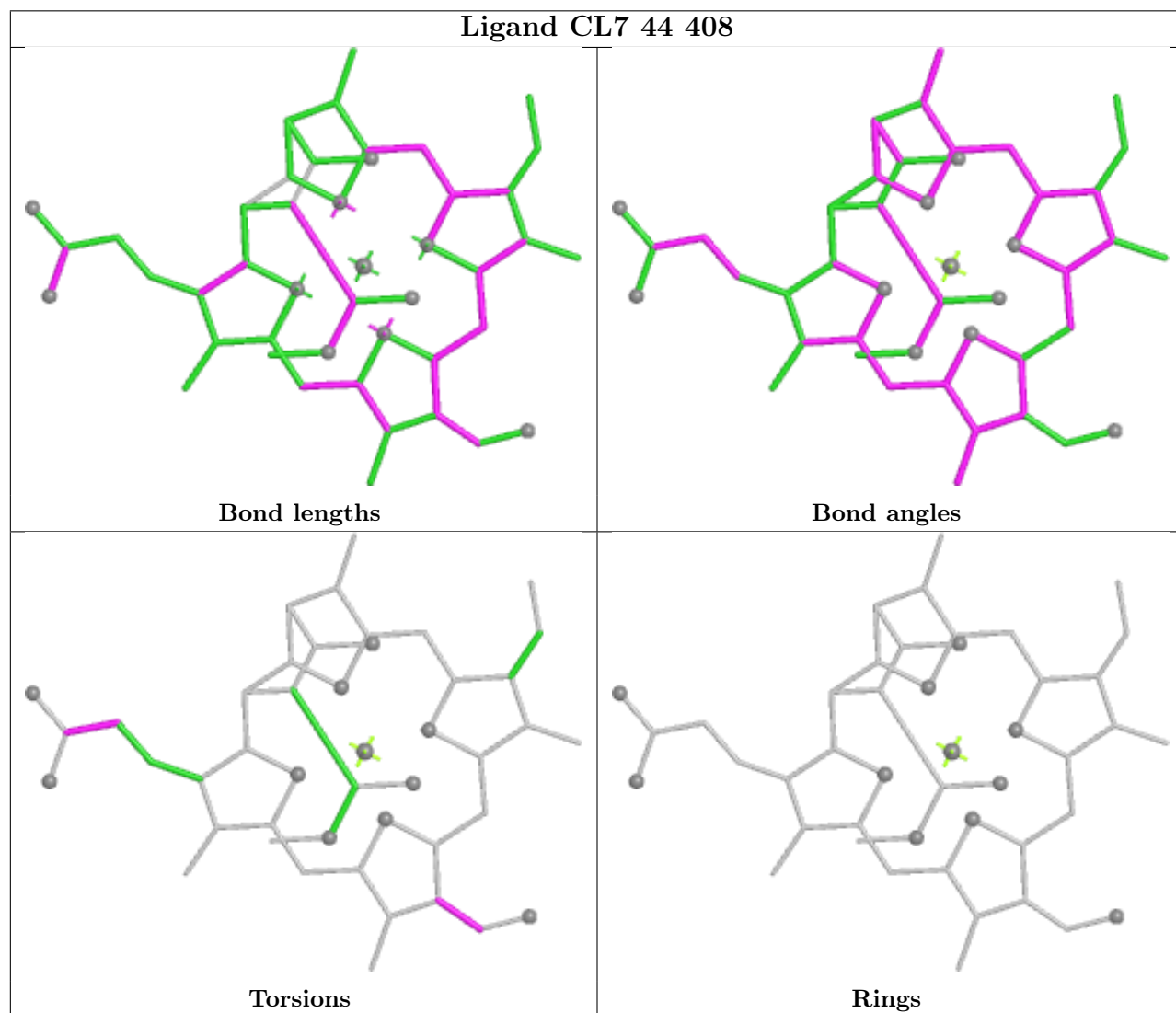
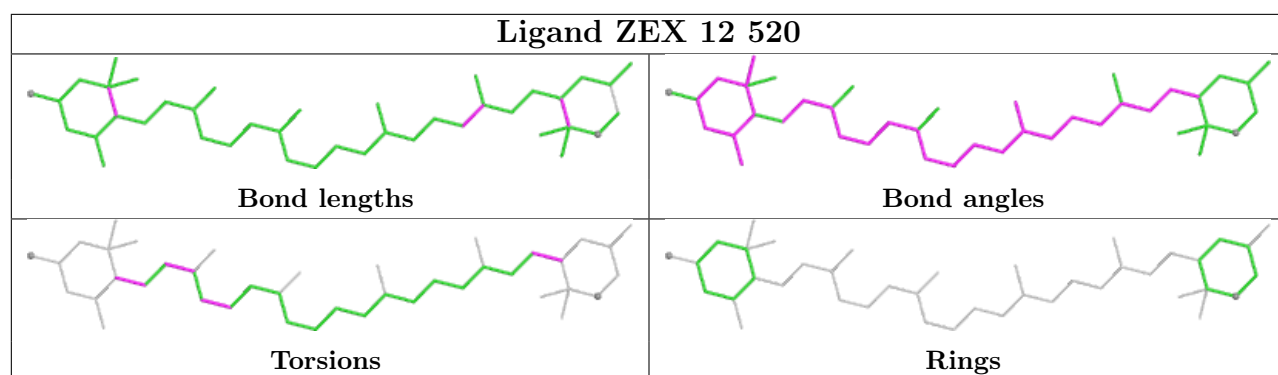


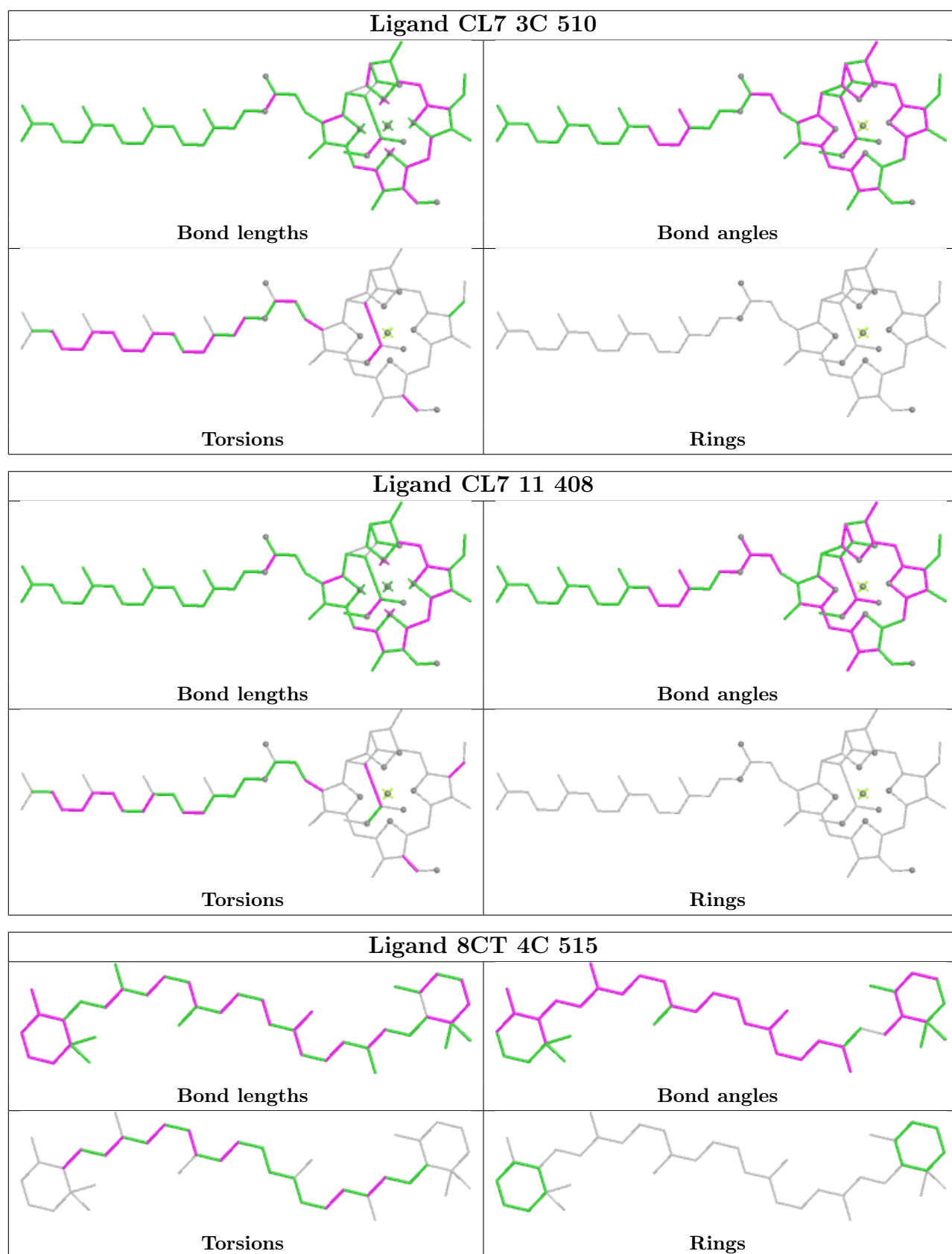


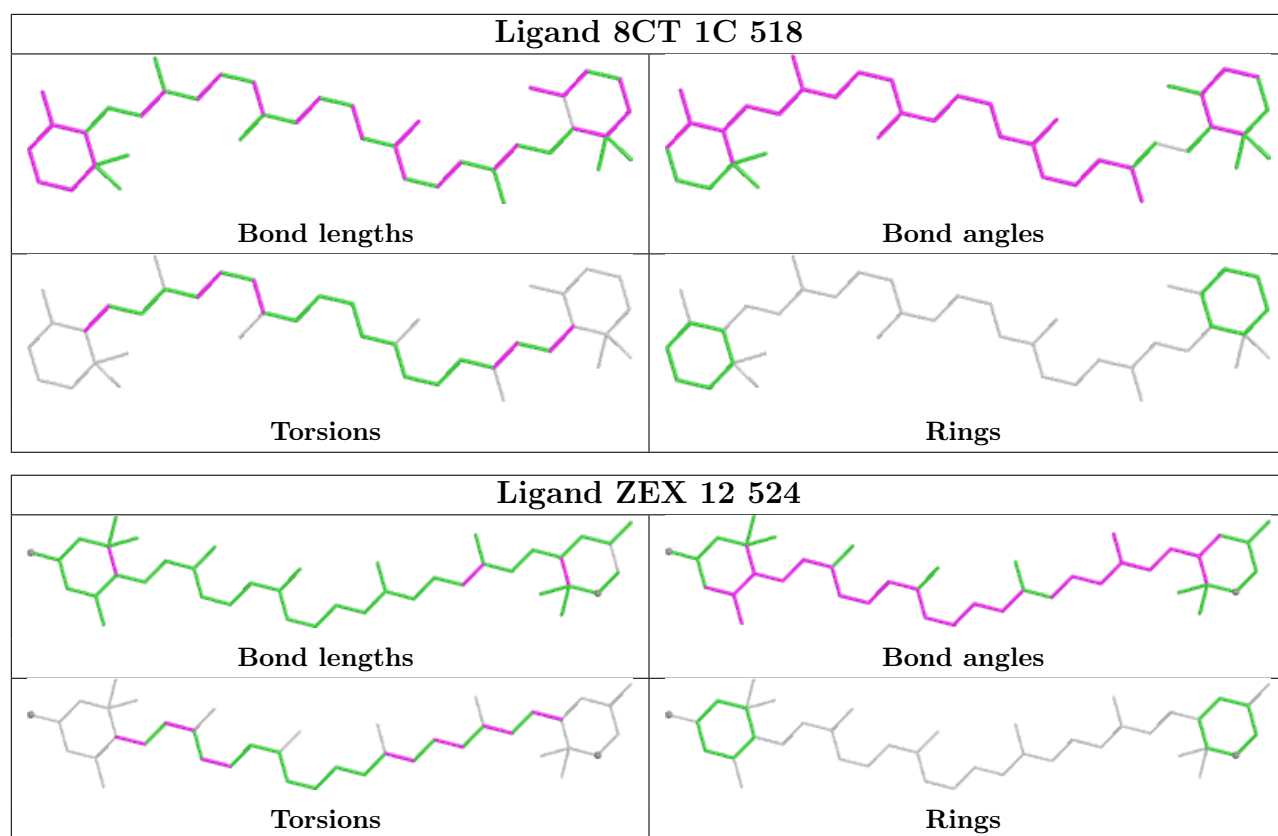








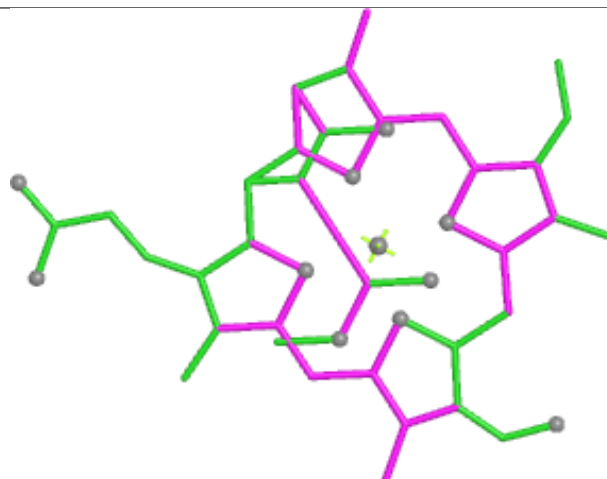




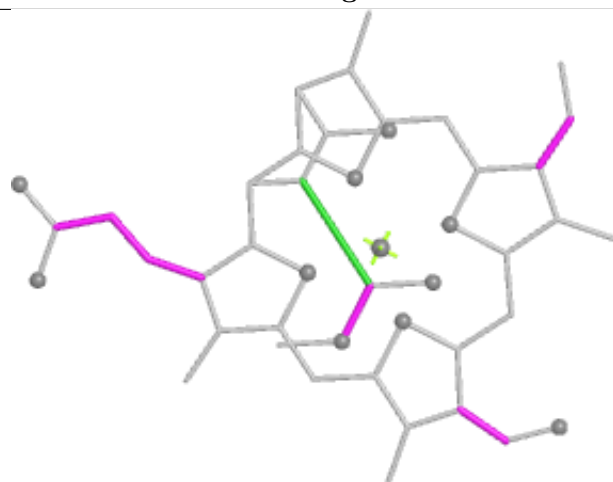
Ligand CL7 11 419



Bond lengths



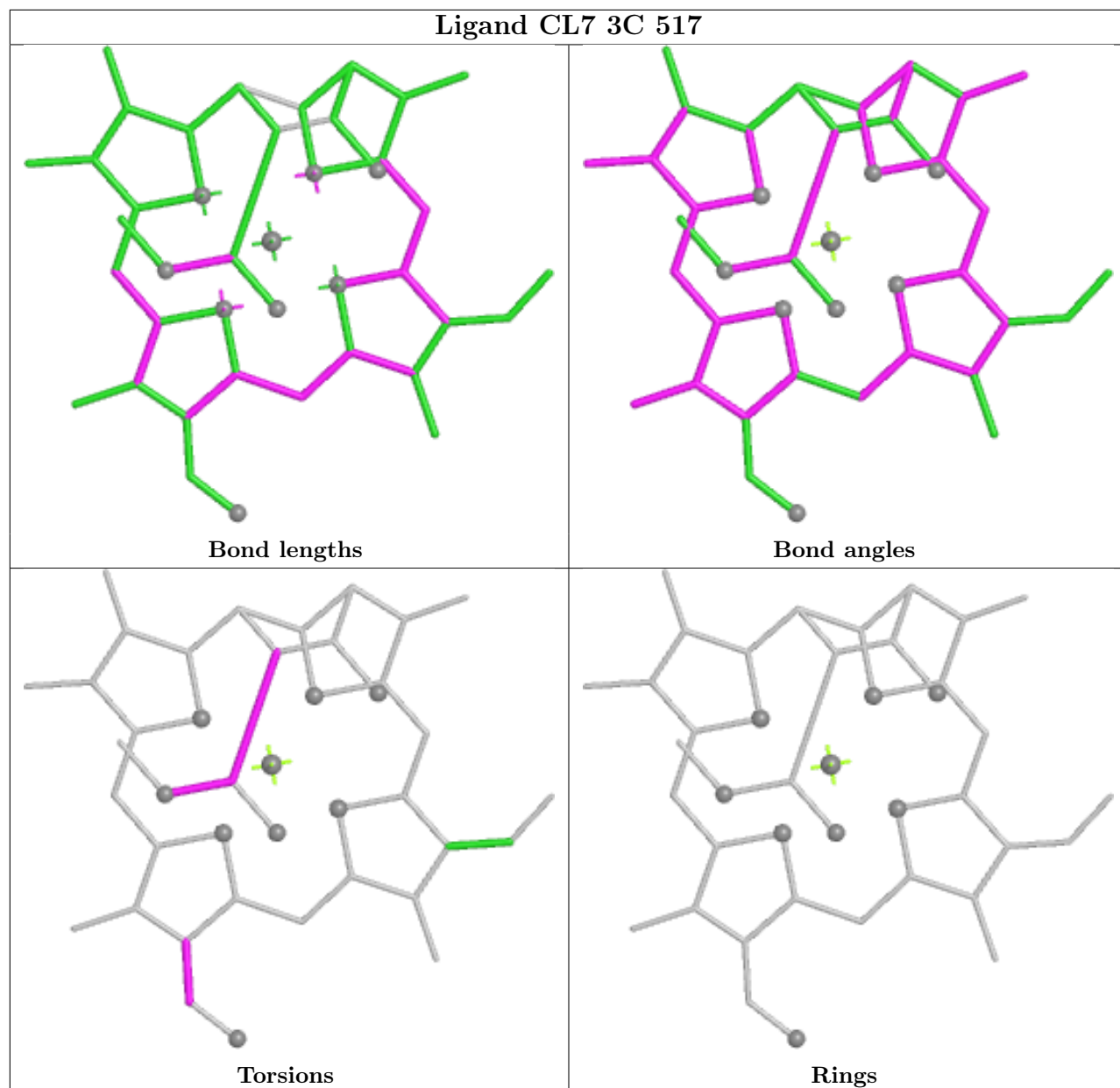
Bond angles



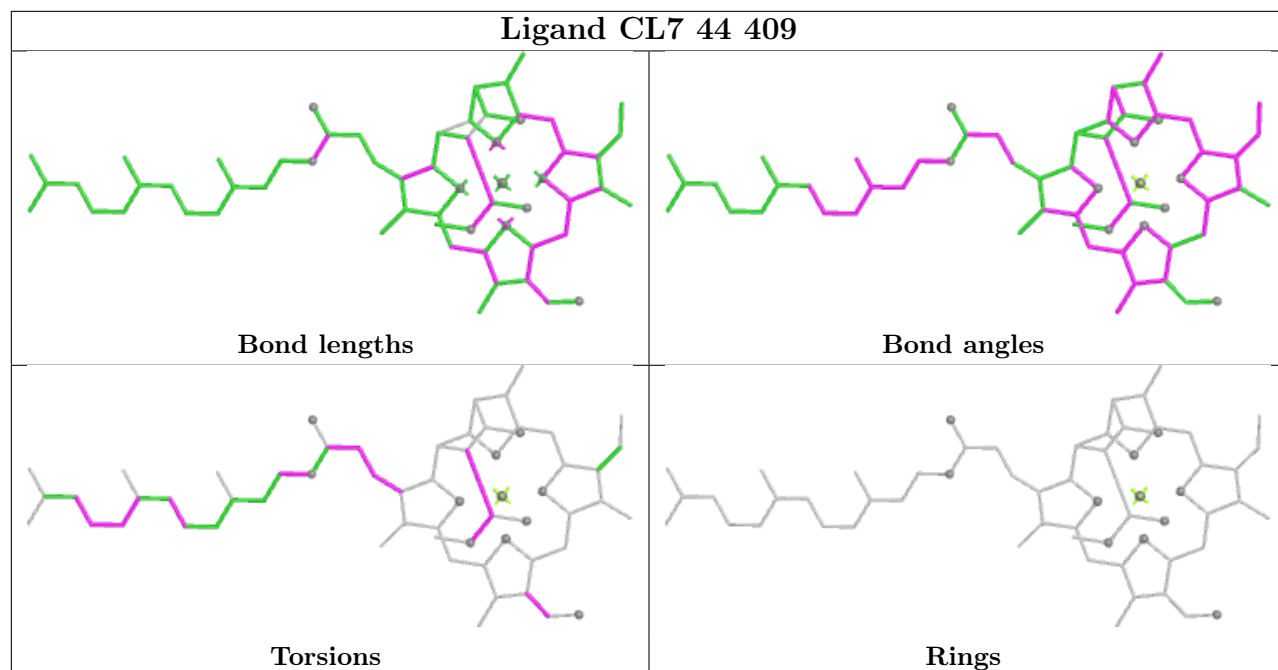
Torsions



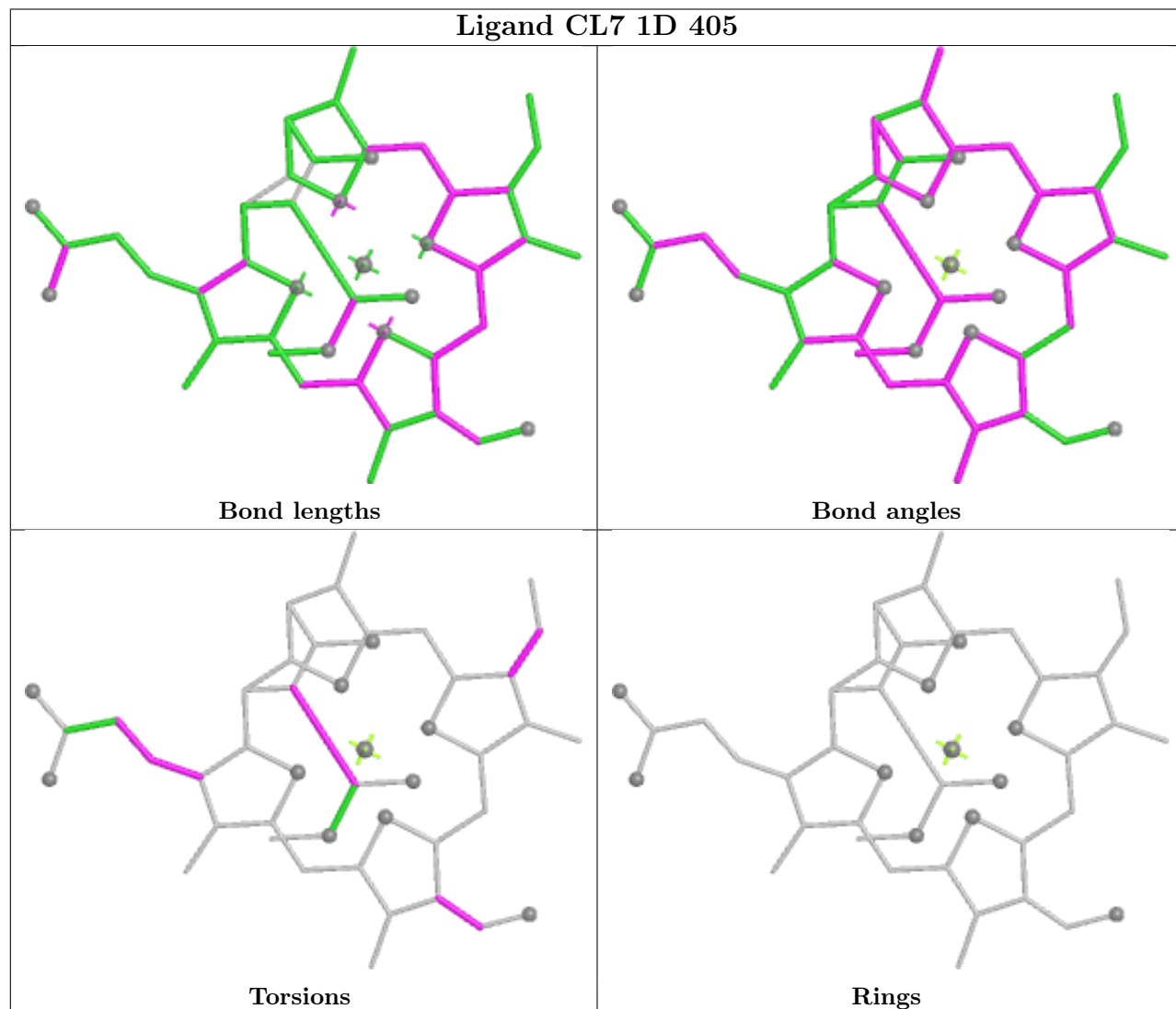
Rings

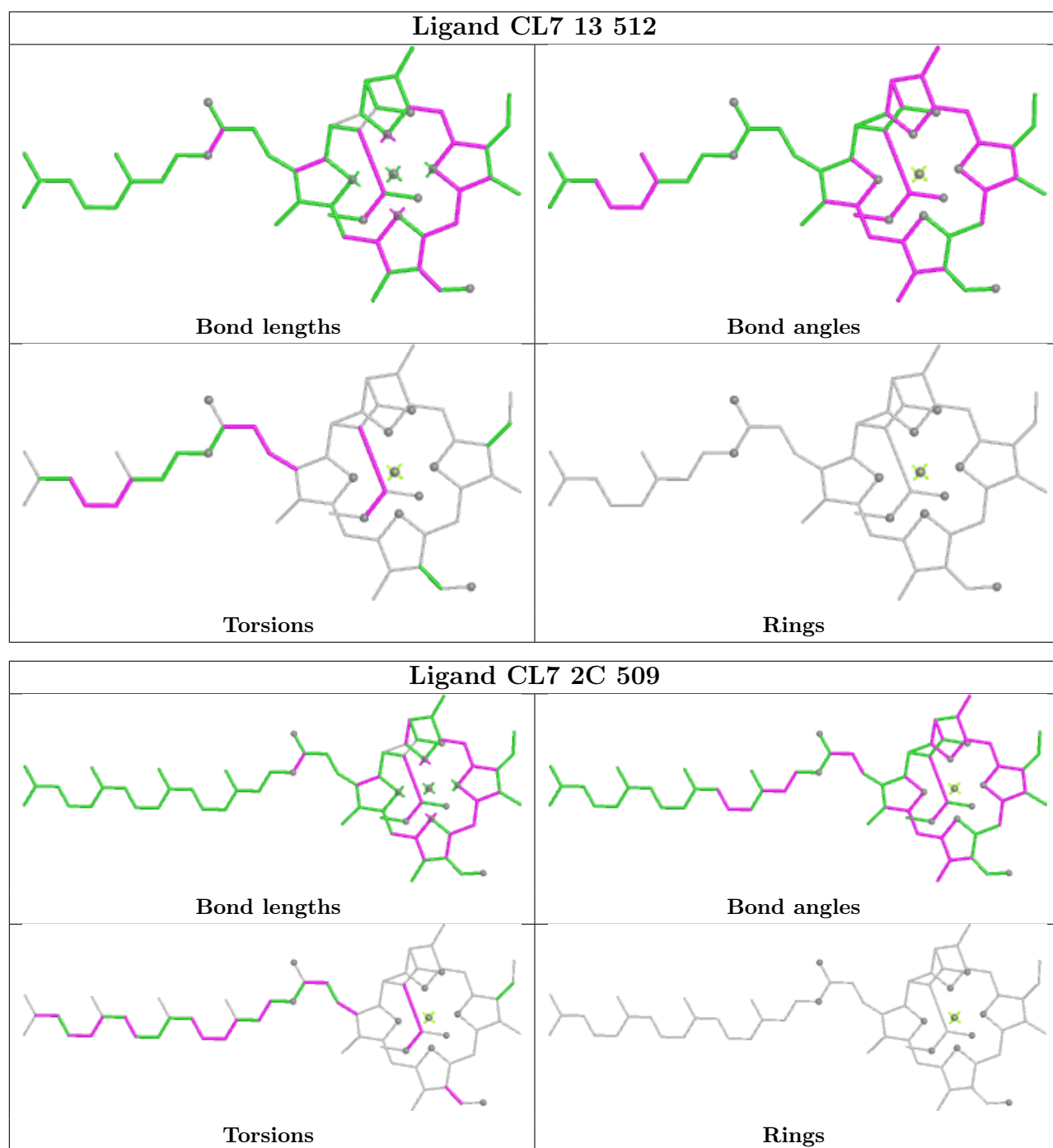


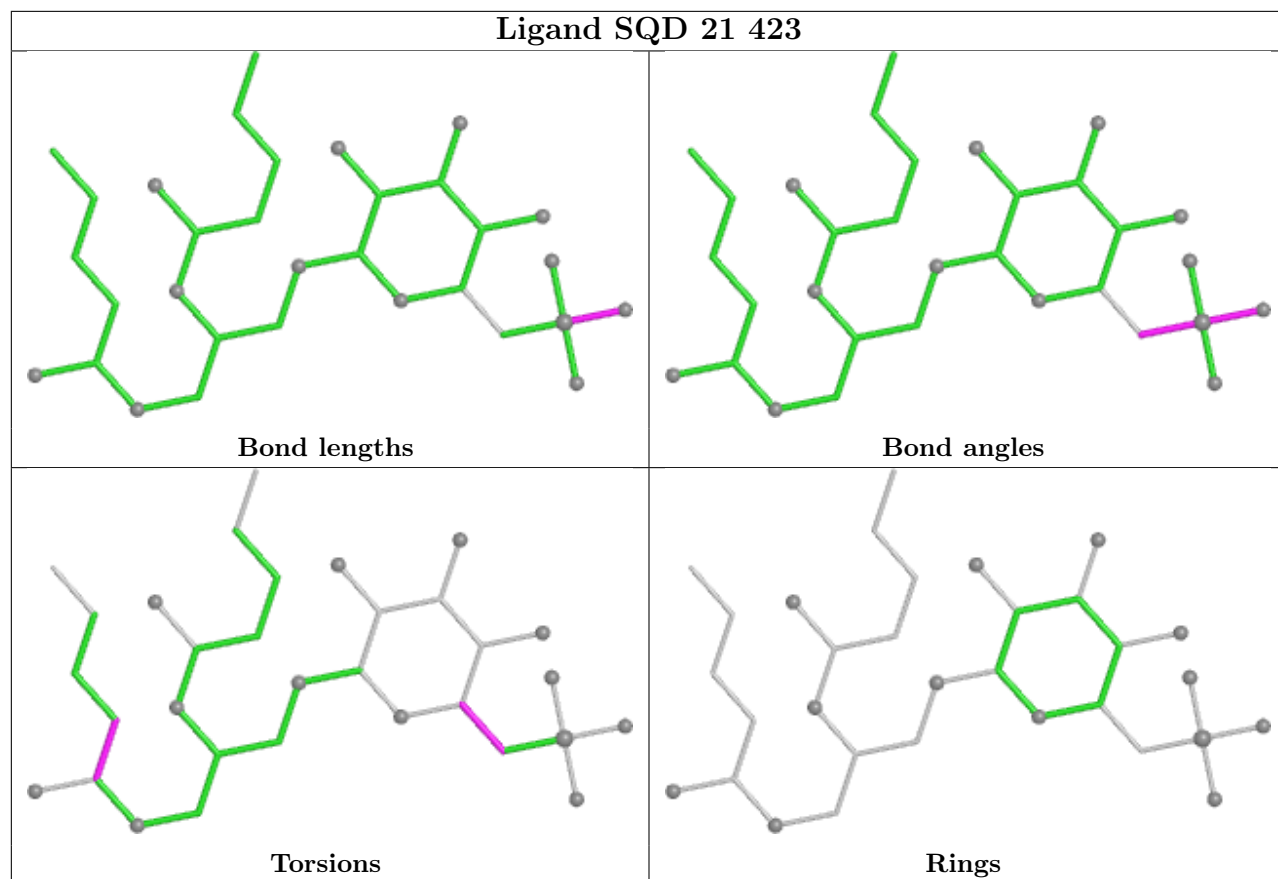
Ligand CL7 44 409

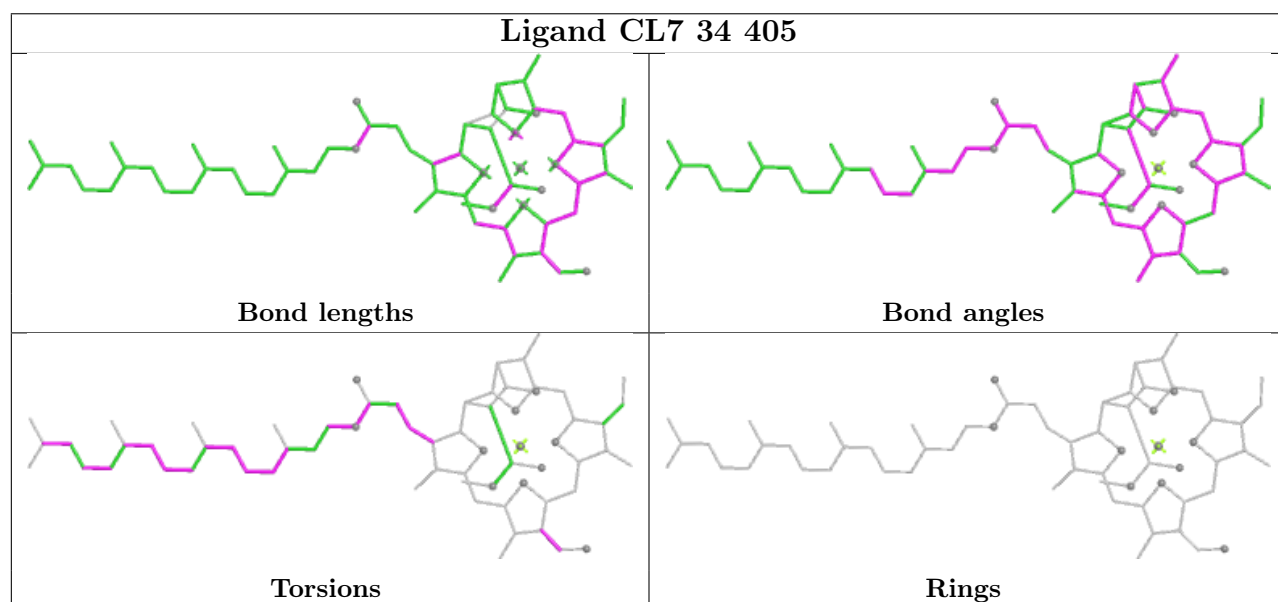
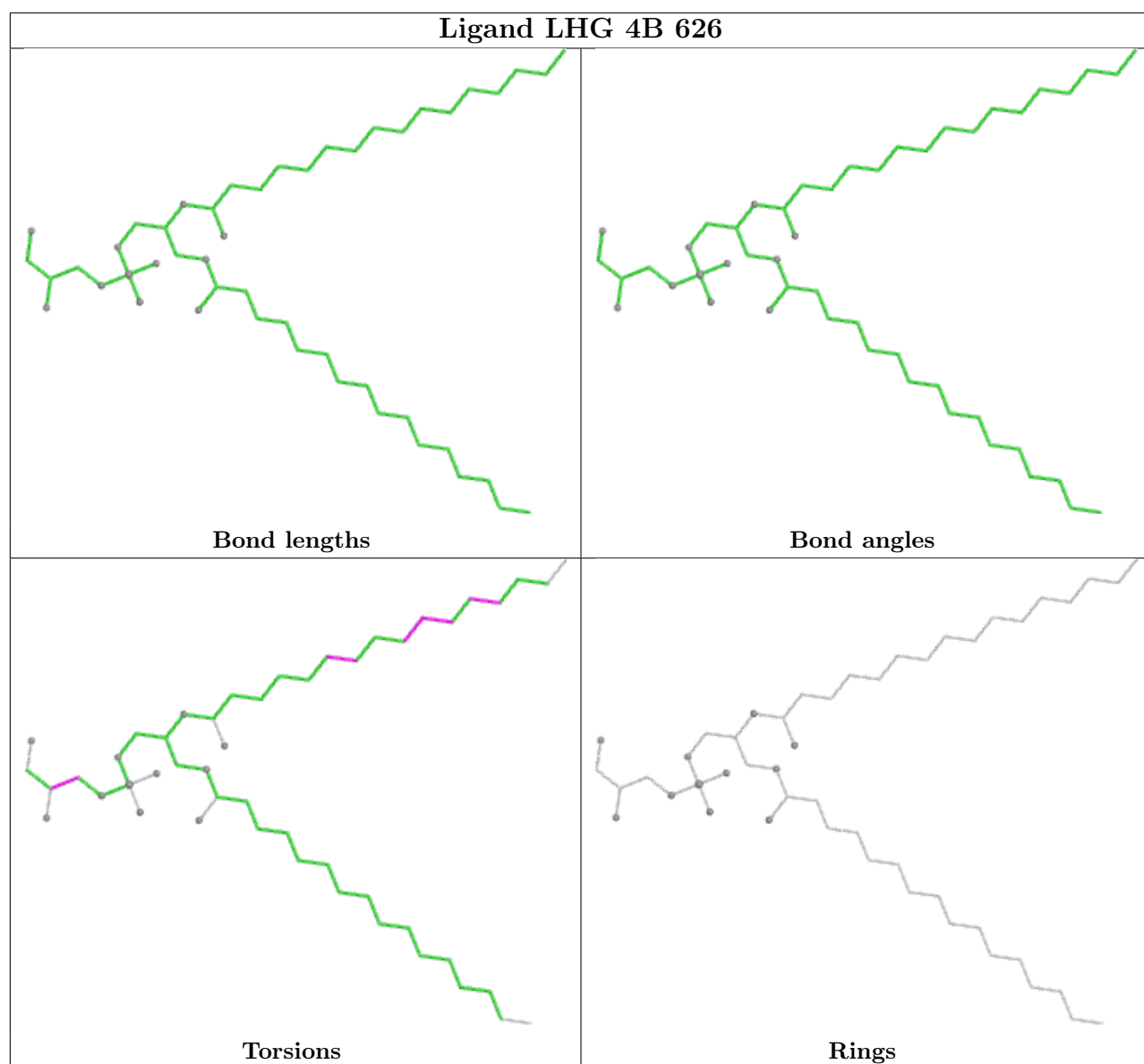


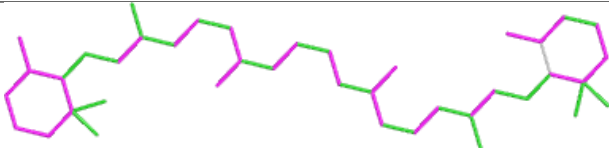
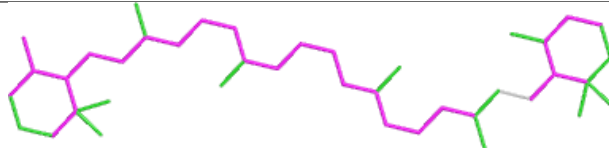
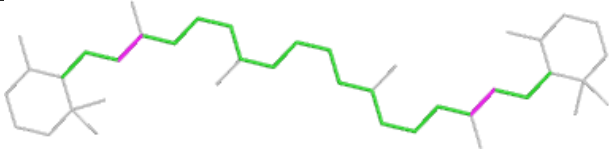
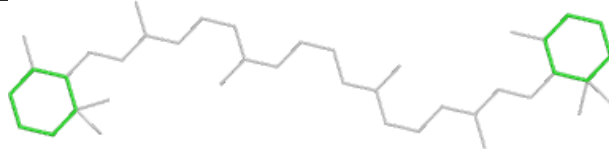
Ligand CL7 1D 405

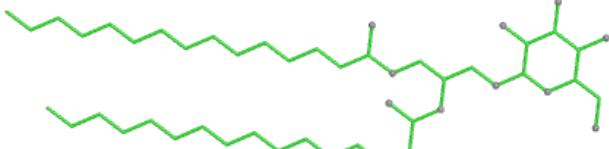
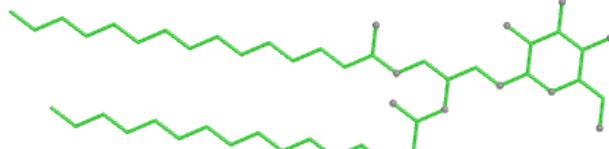
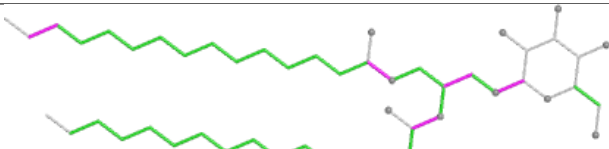
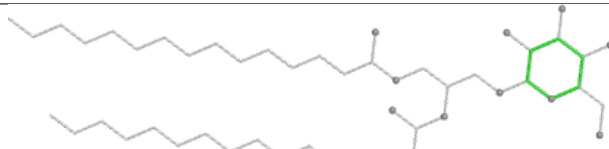


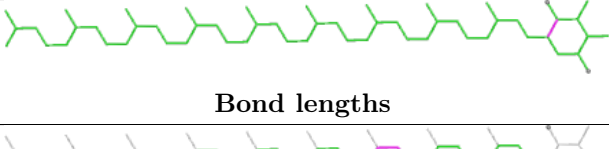
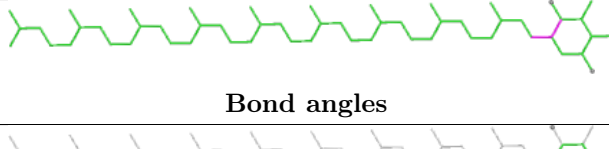
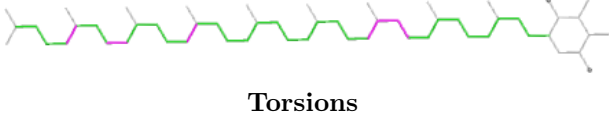
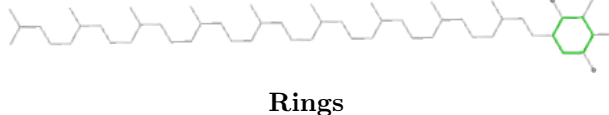


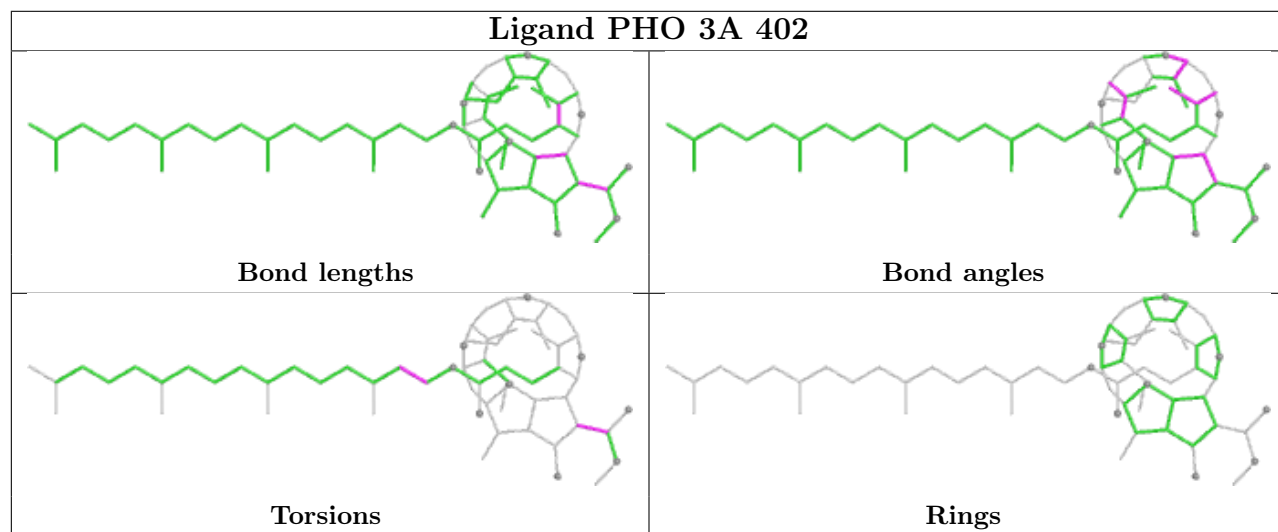
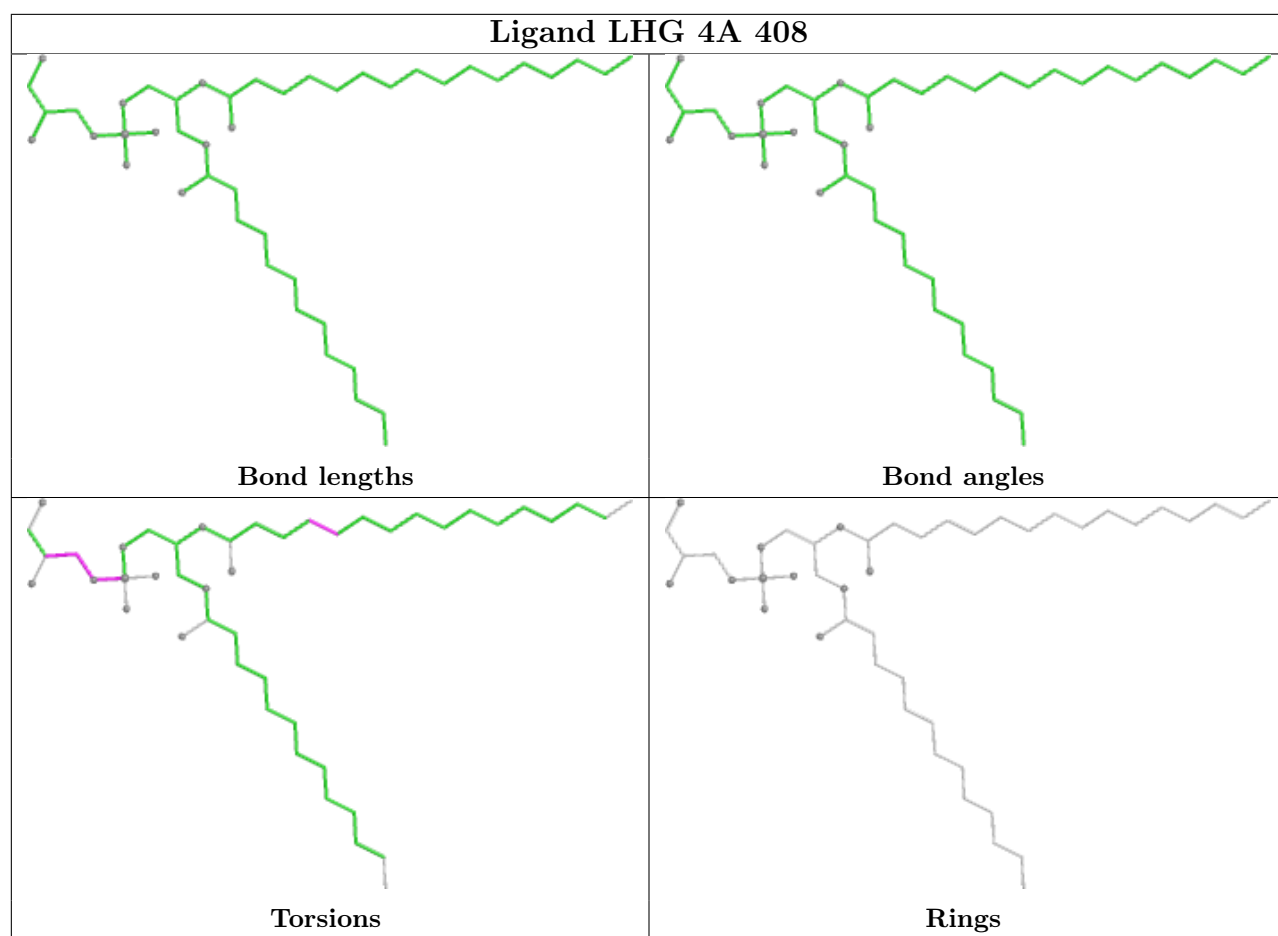


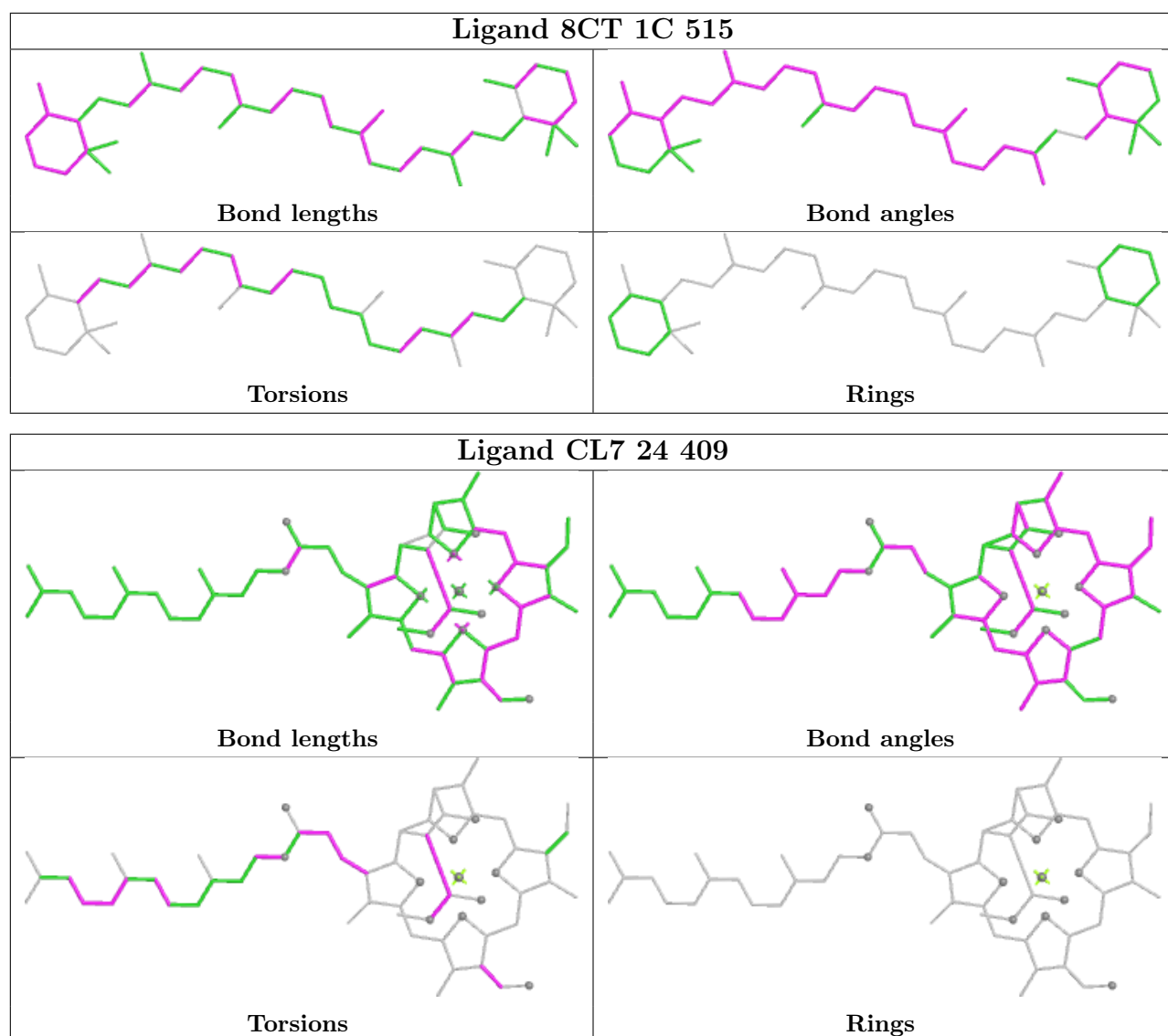


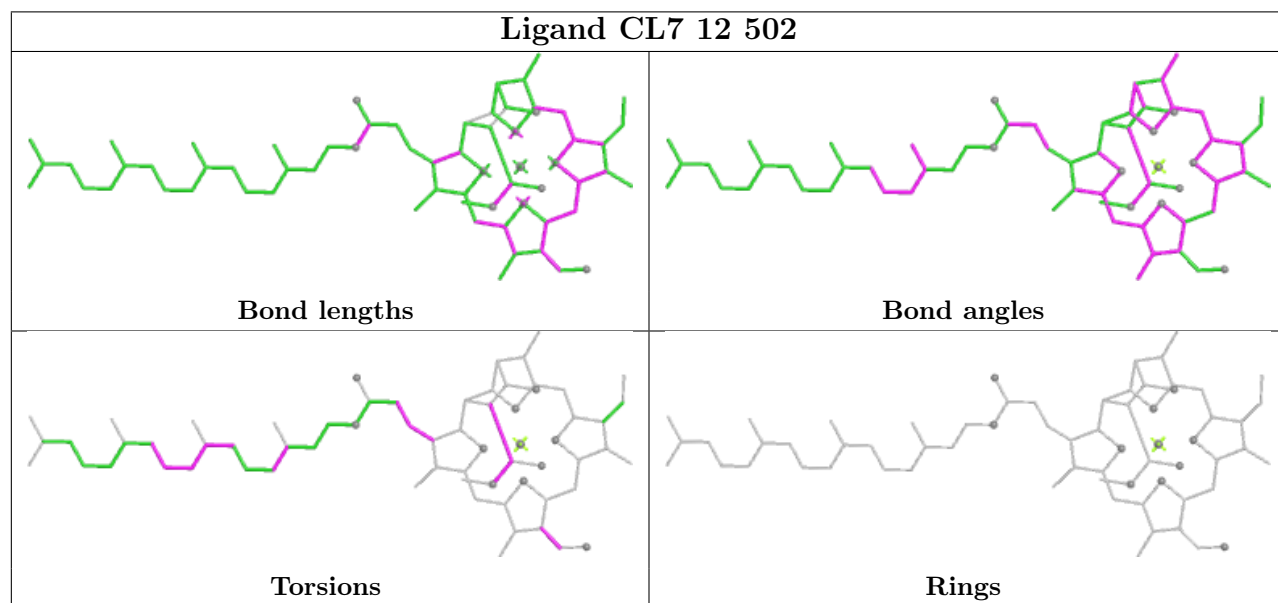
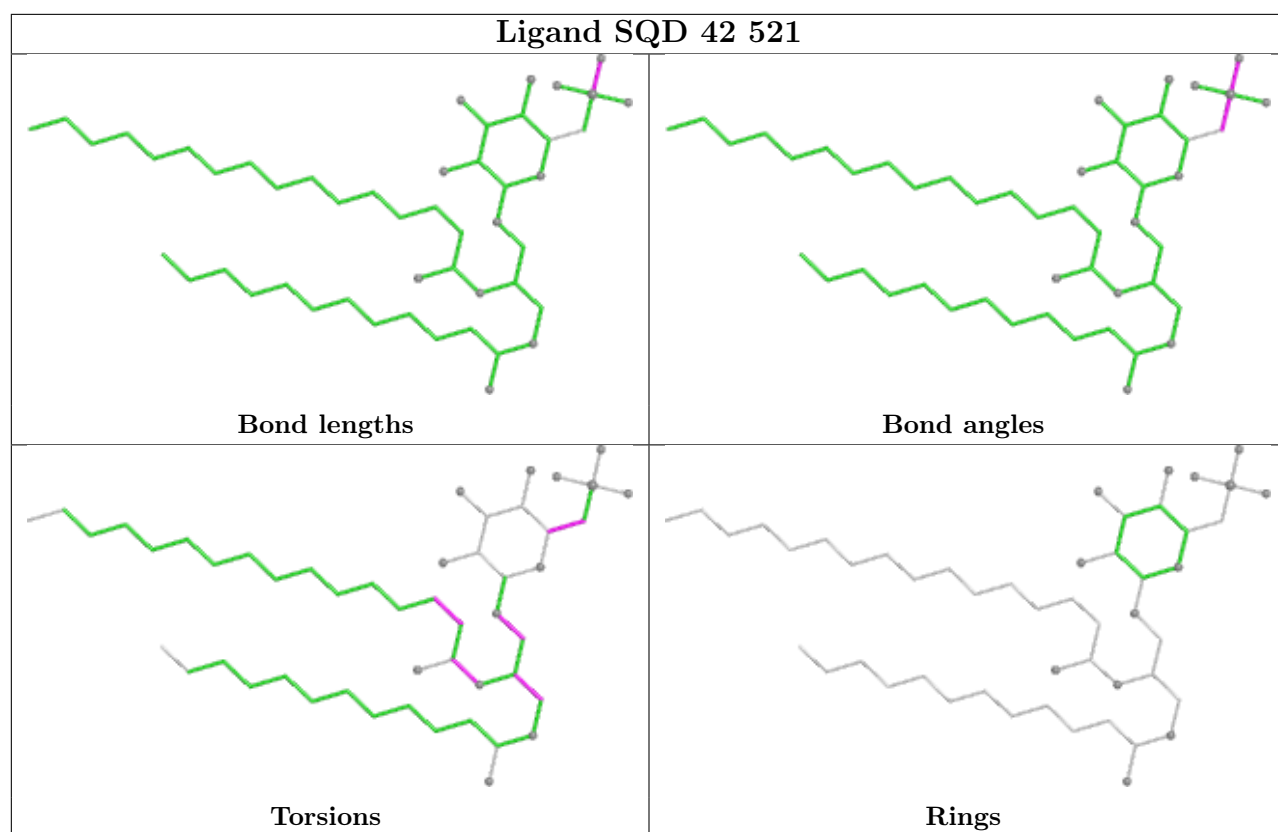
Ligand 8CT 3B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

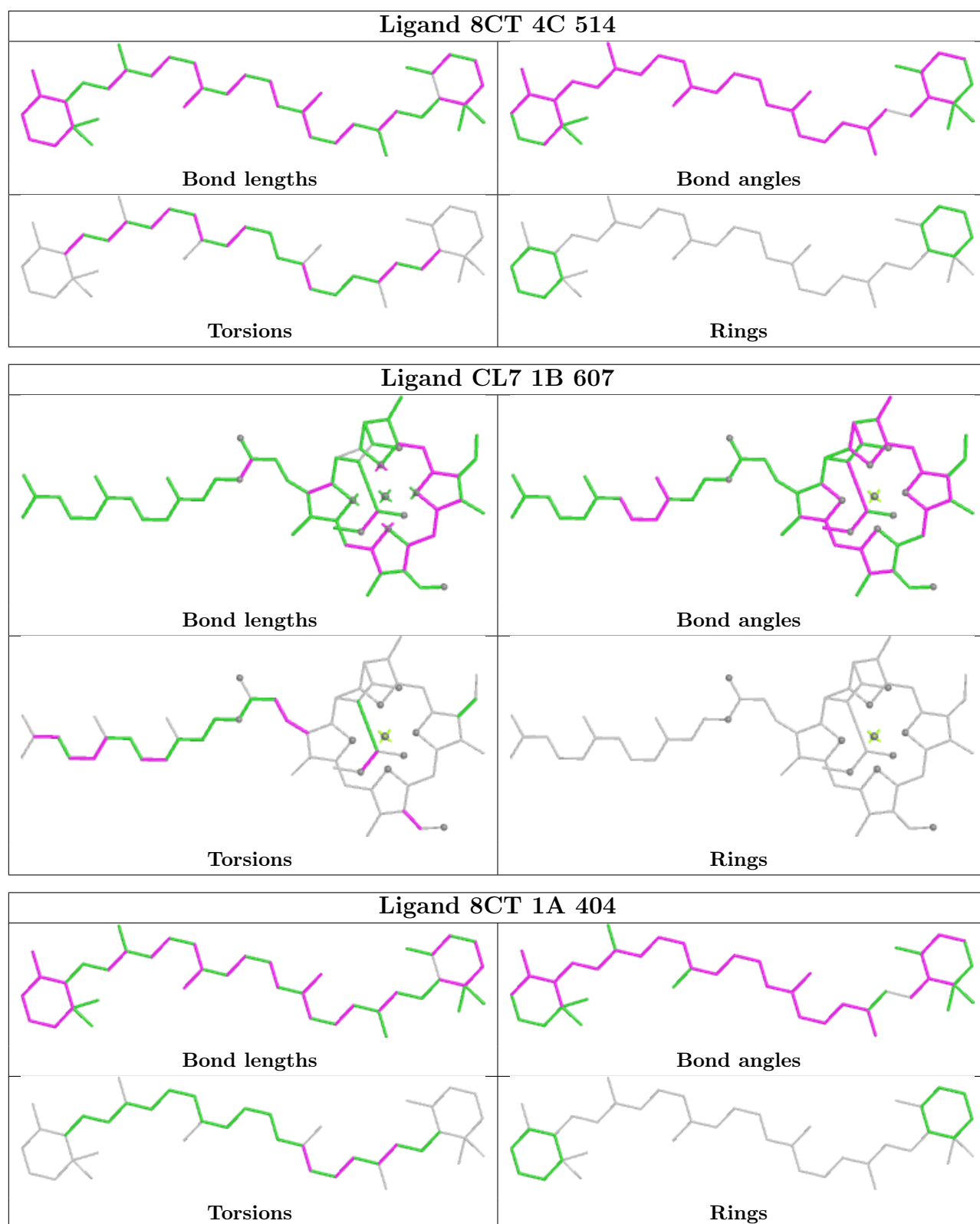
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Bond lengths	Bond angles
	
Torsions	Rings

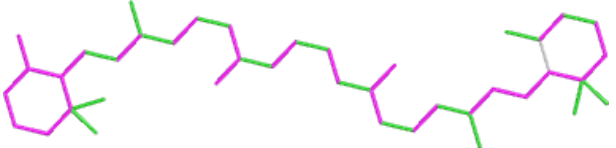
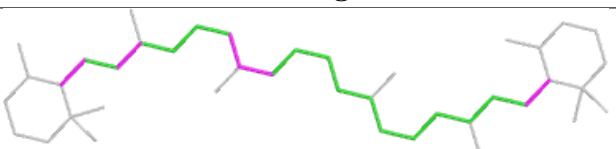
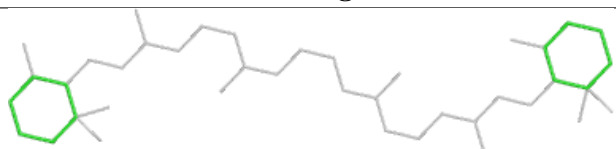
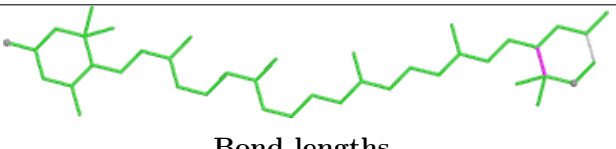
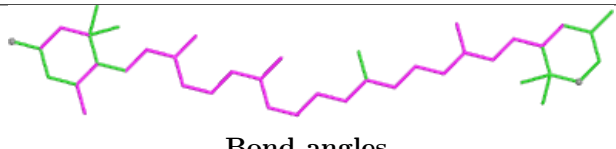
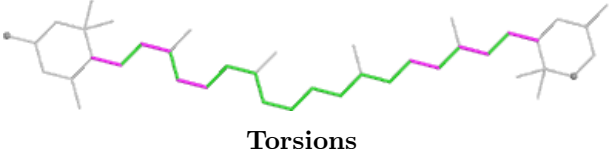
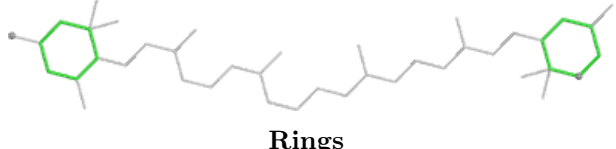
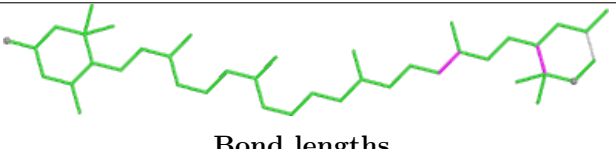
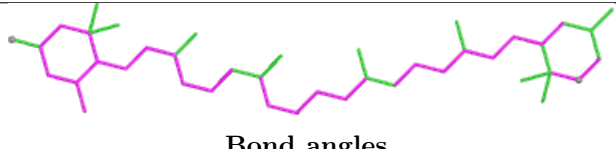
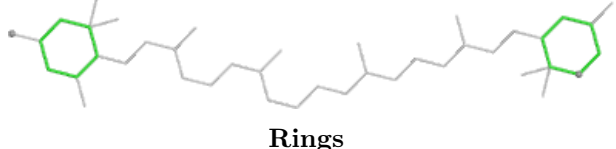
Ligand PL9 4D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings



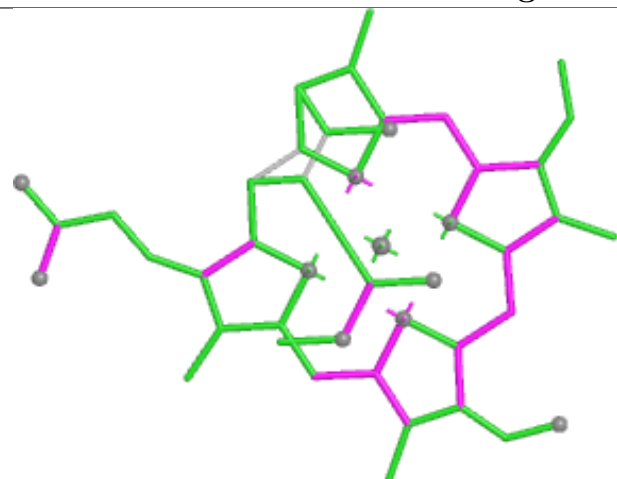




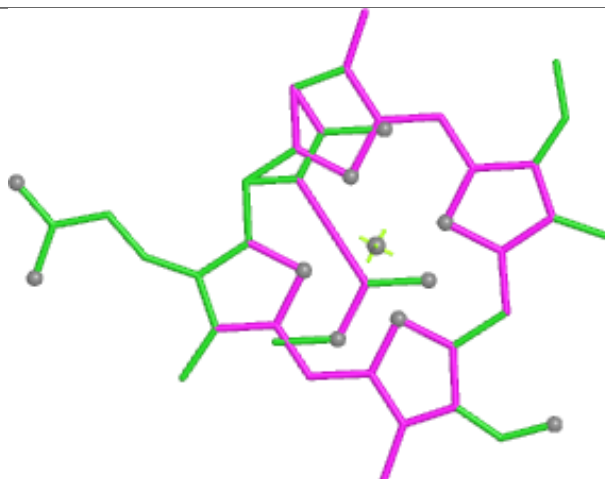


Ligand 8CT 1B 626	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand ZEX 14 418	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand ZEX 21 422	
 Bond lengths	 Bond angles
 Torsions	 Rings

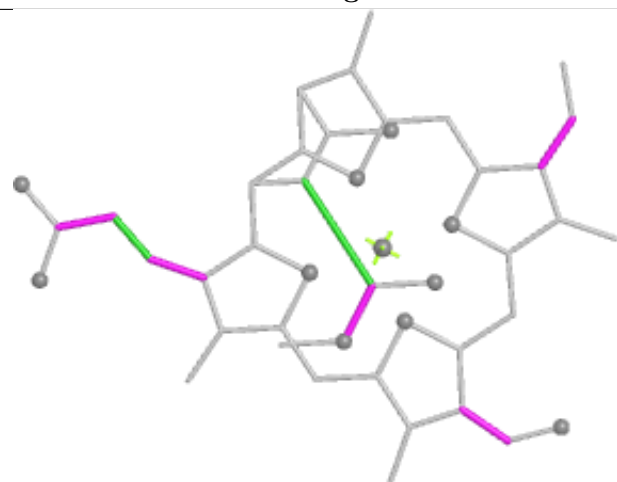
Ligand CL7 42 514



Bond lengths



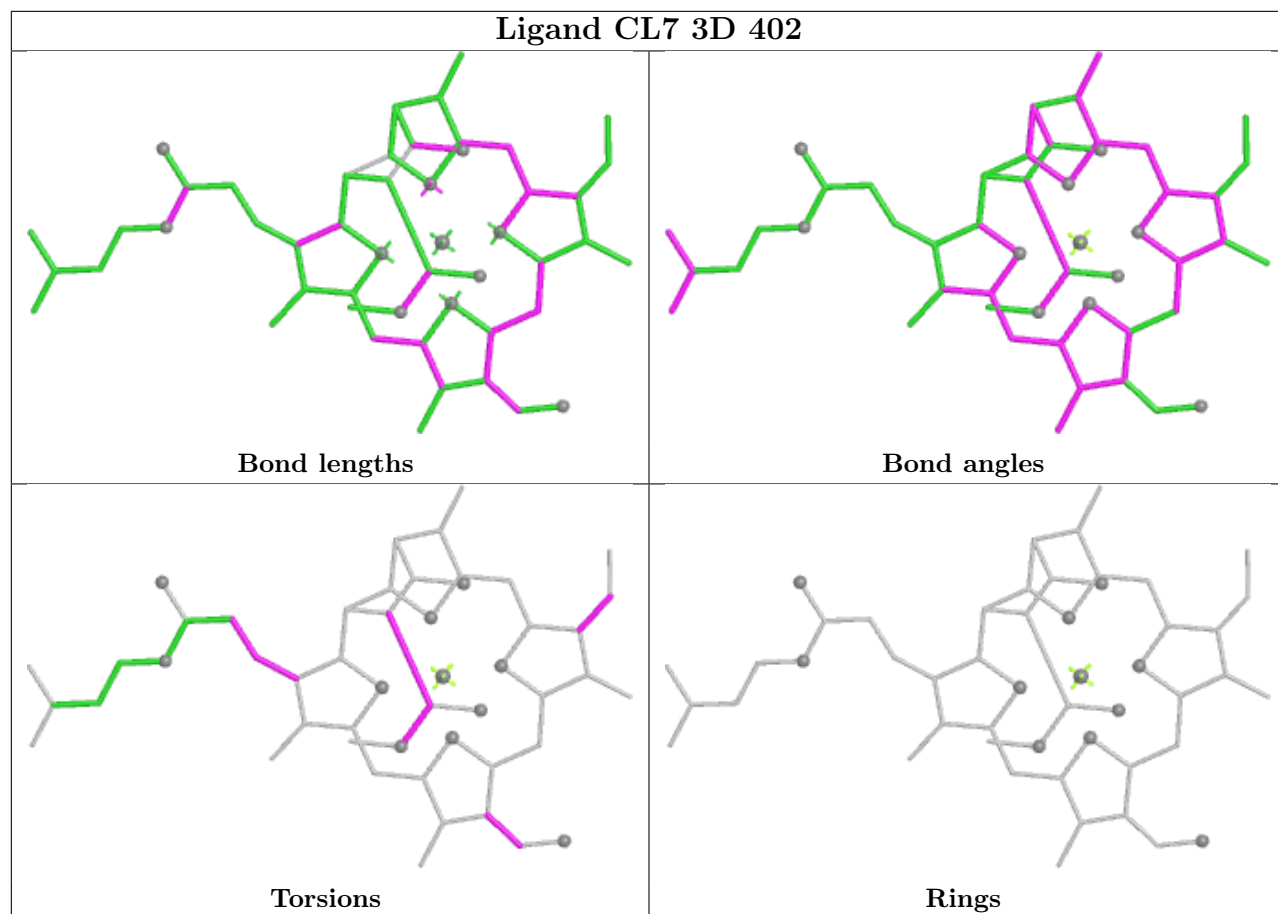
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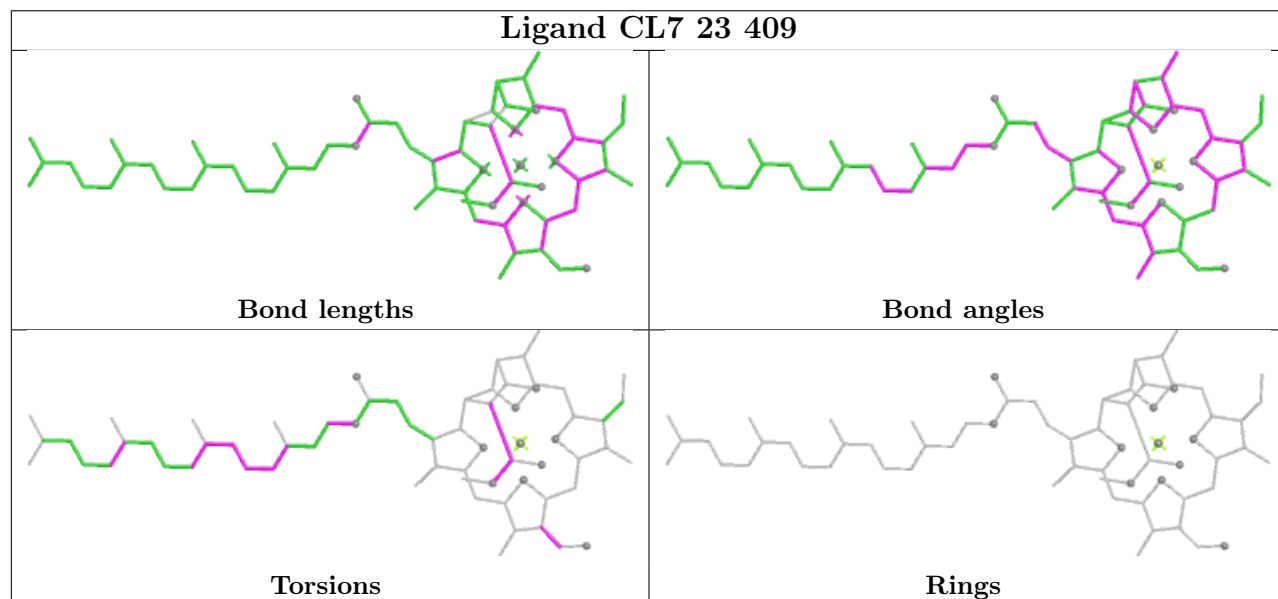
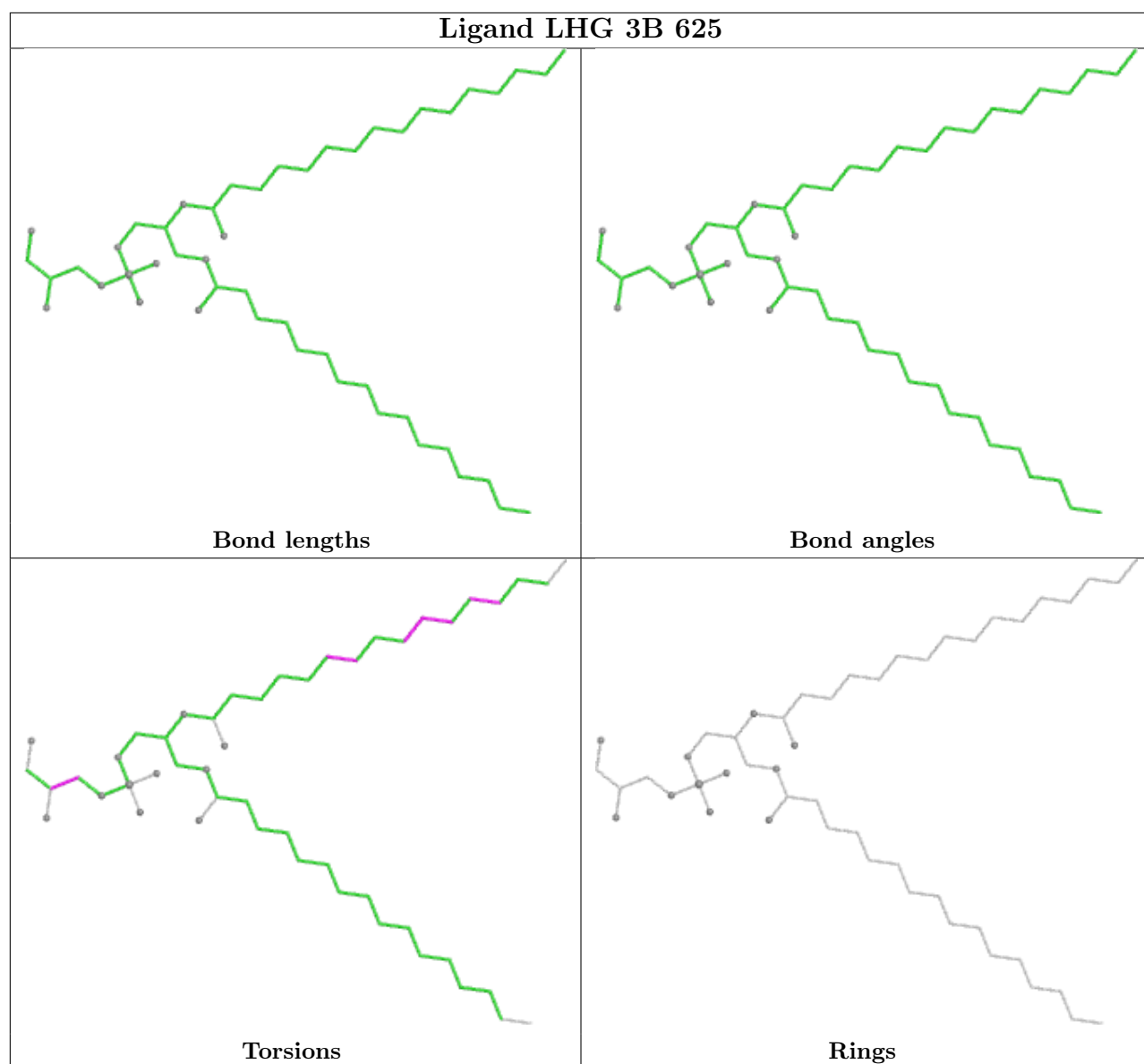


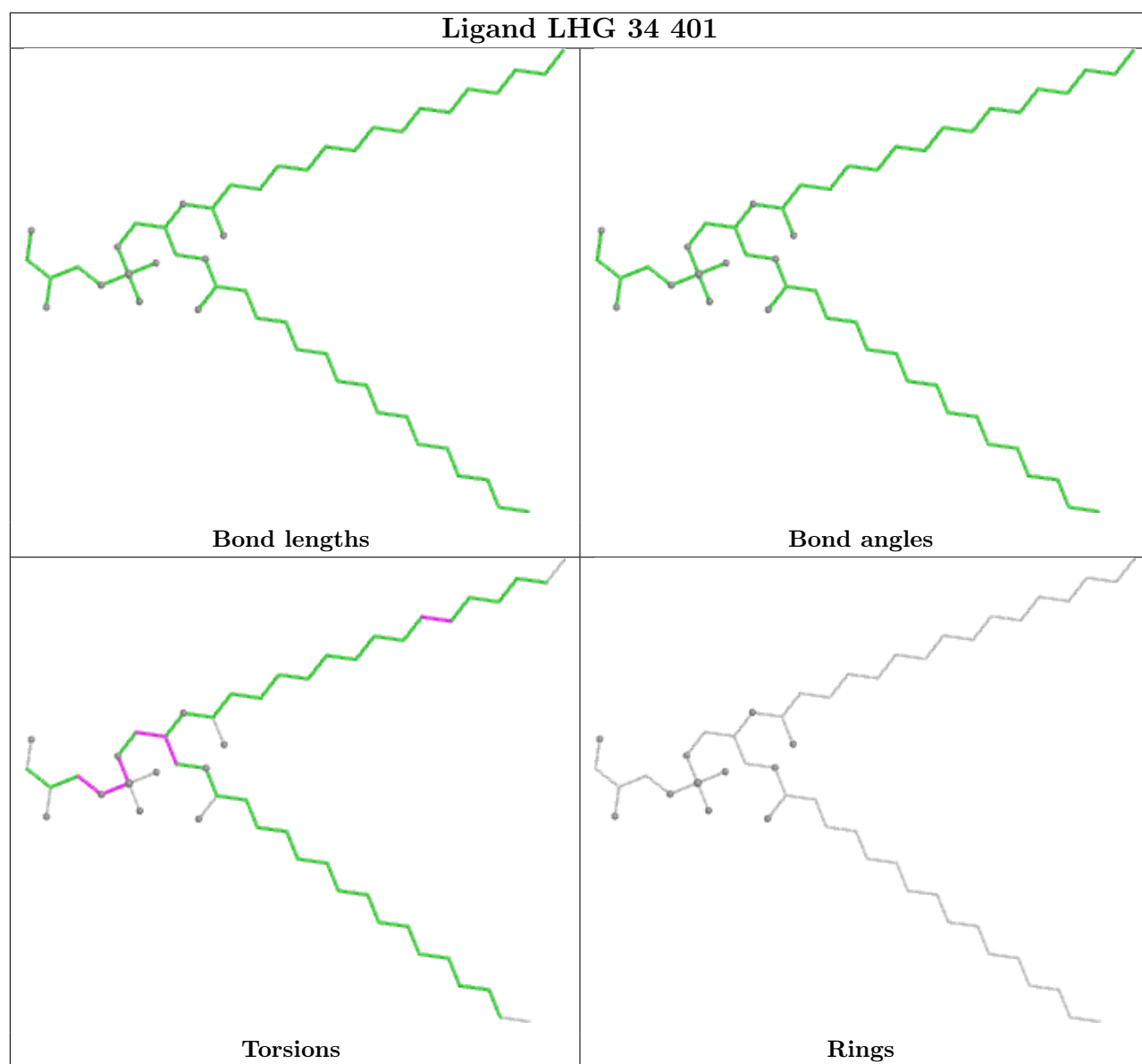
Torsions

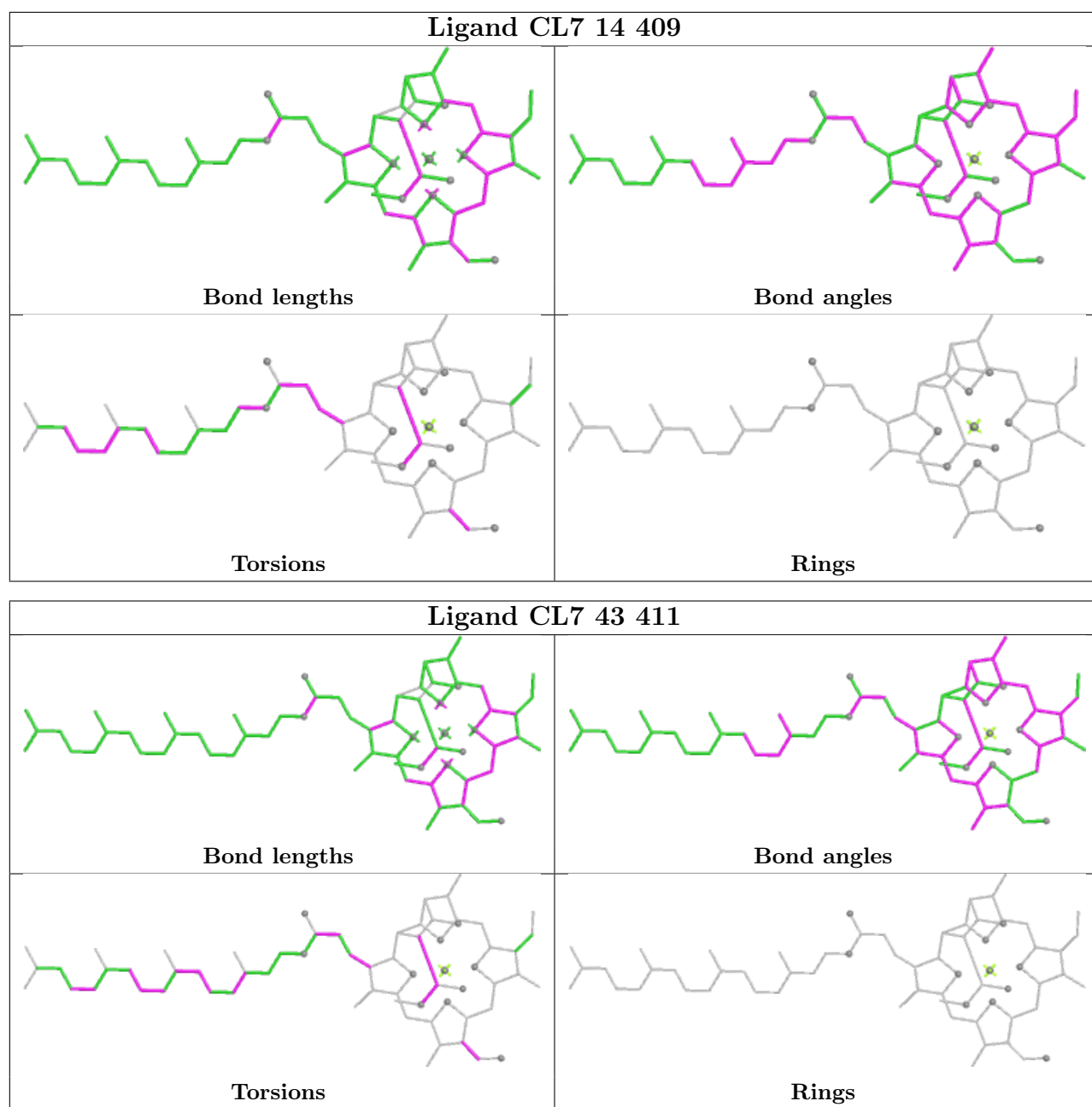


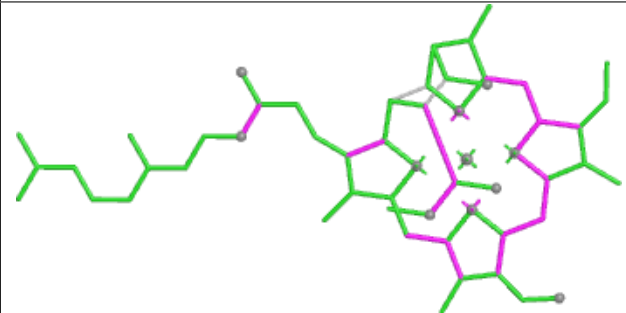
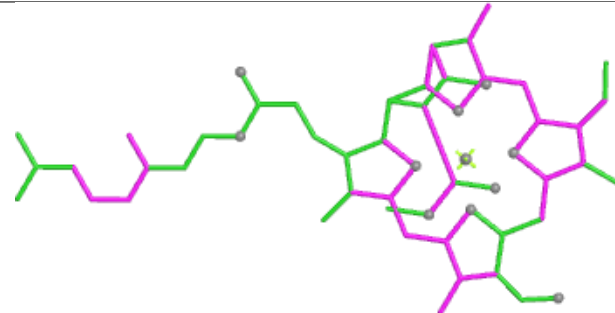
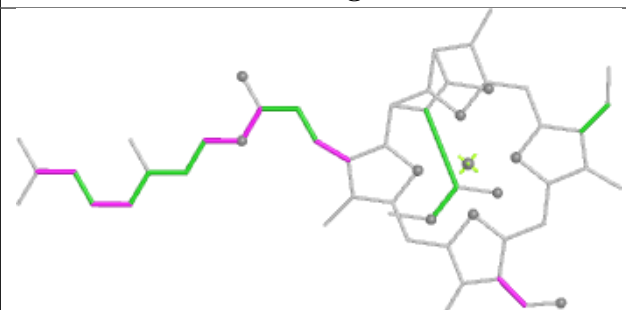
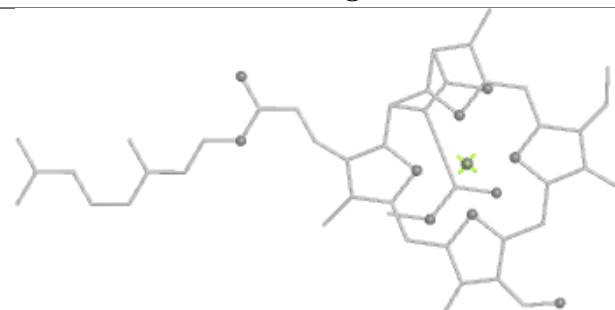
Rings

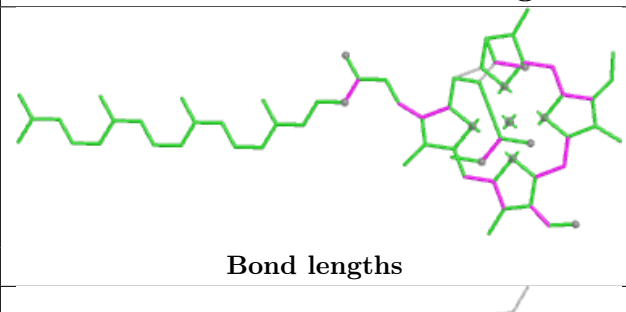
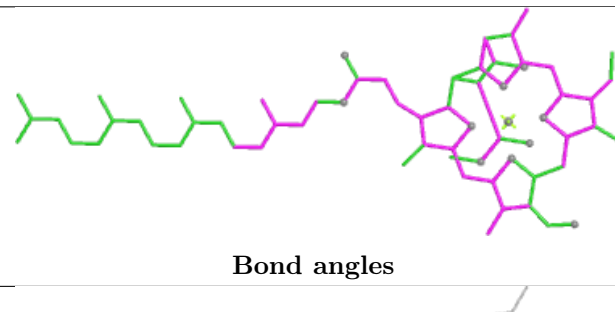
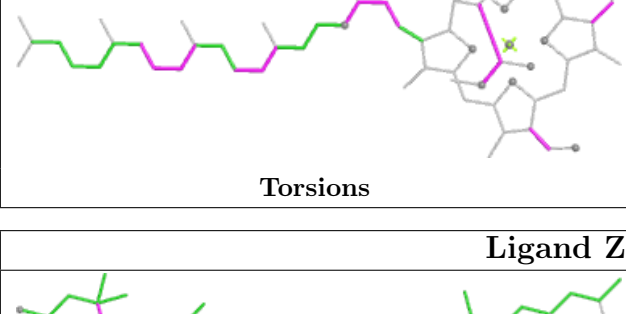


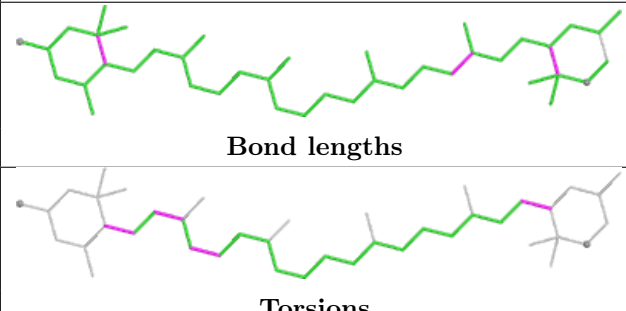
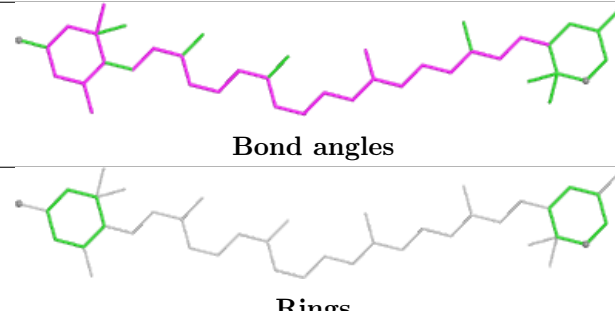
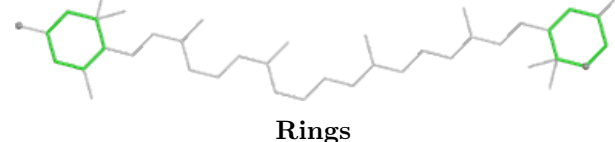


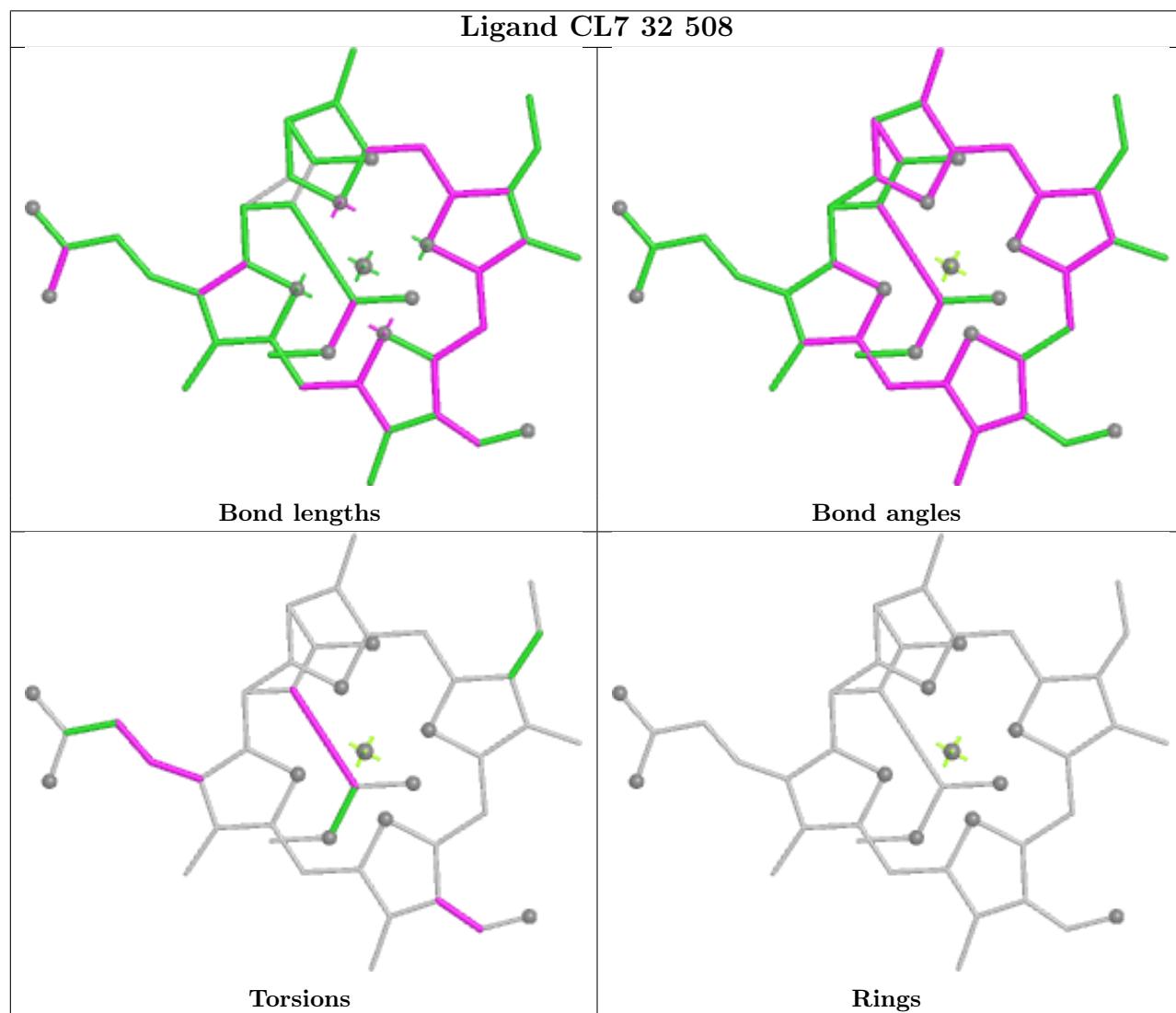
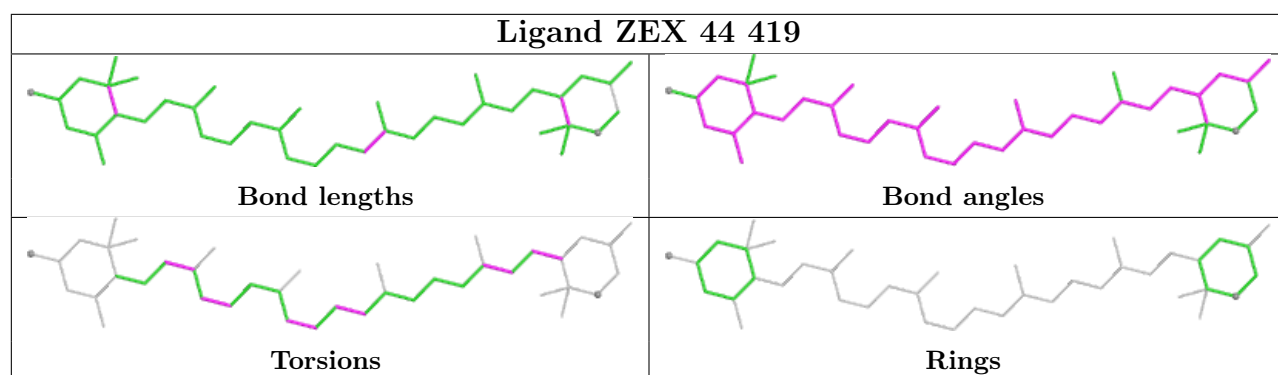


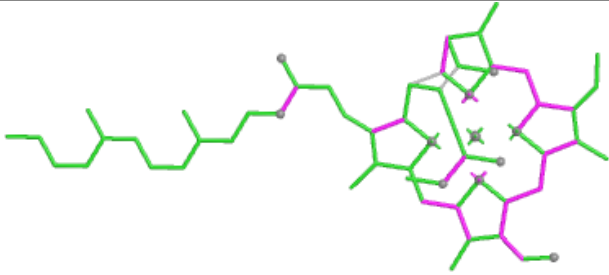
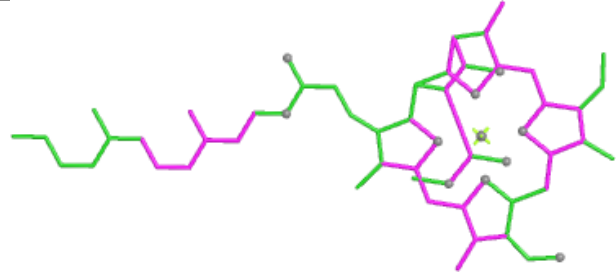
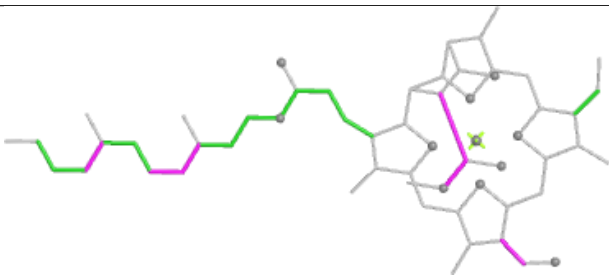
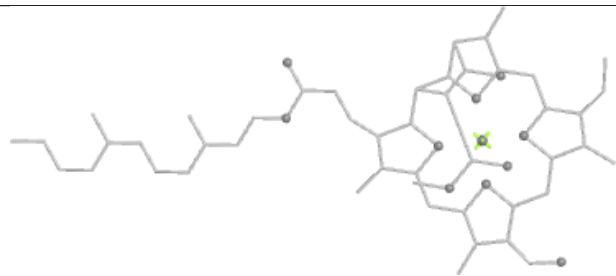


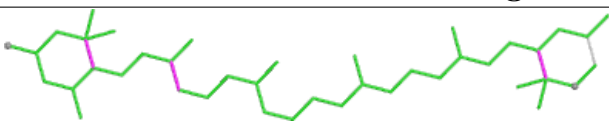
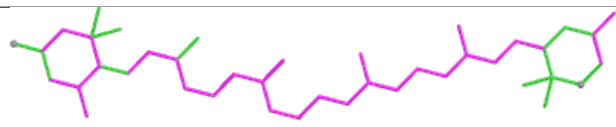
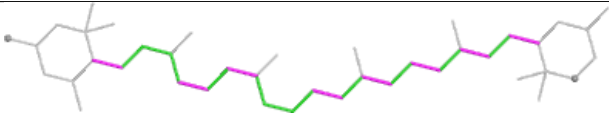
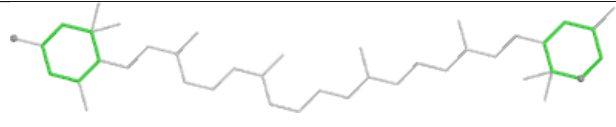
Ligand CL7 31 417	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CL7 1A 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

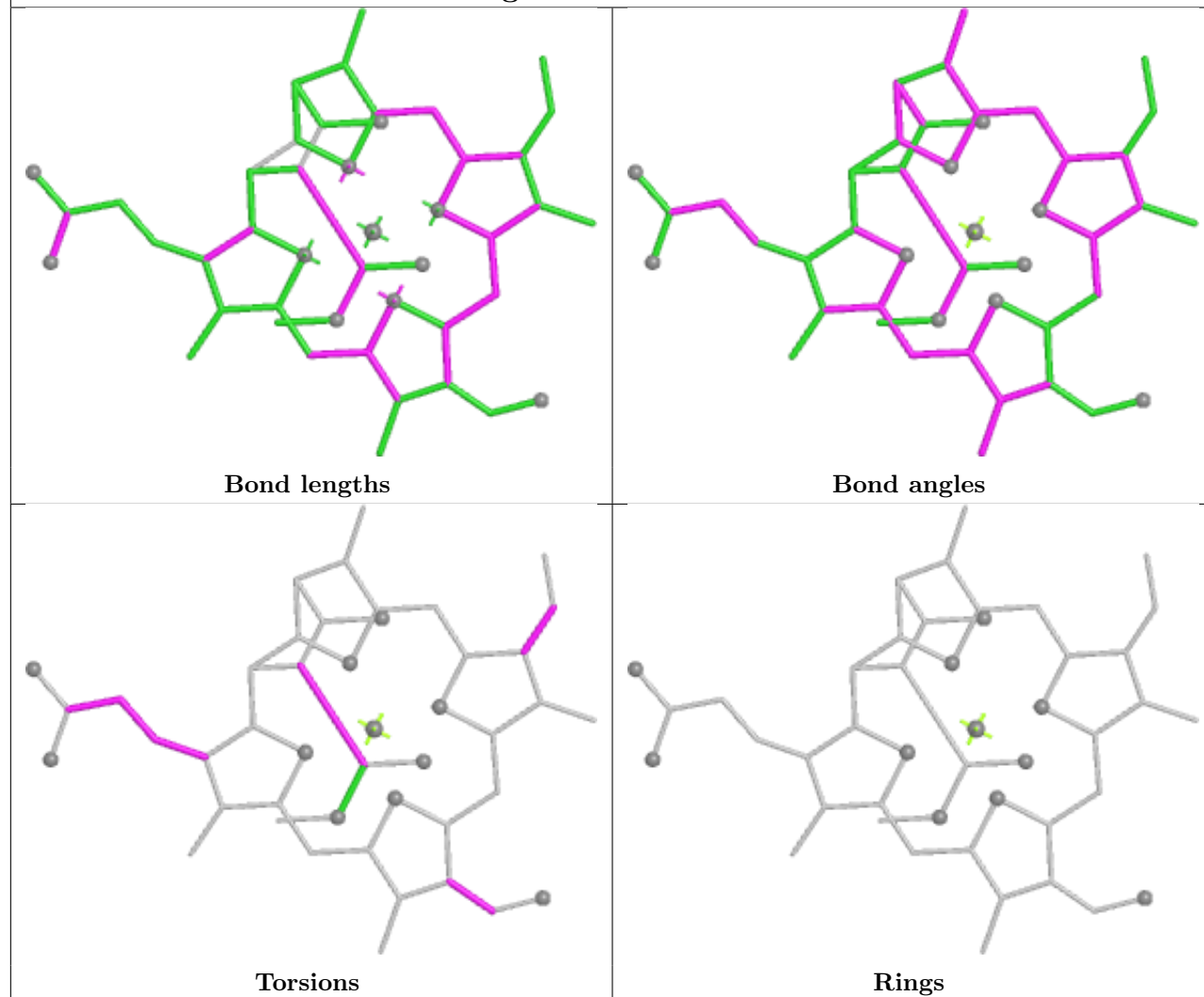
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Bond lengths	Bond angles
	
Torsions	Rings



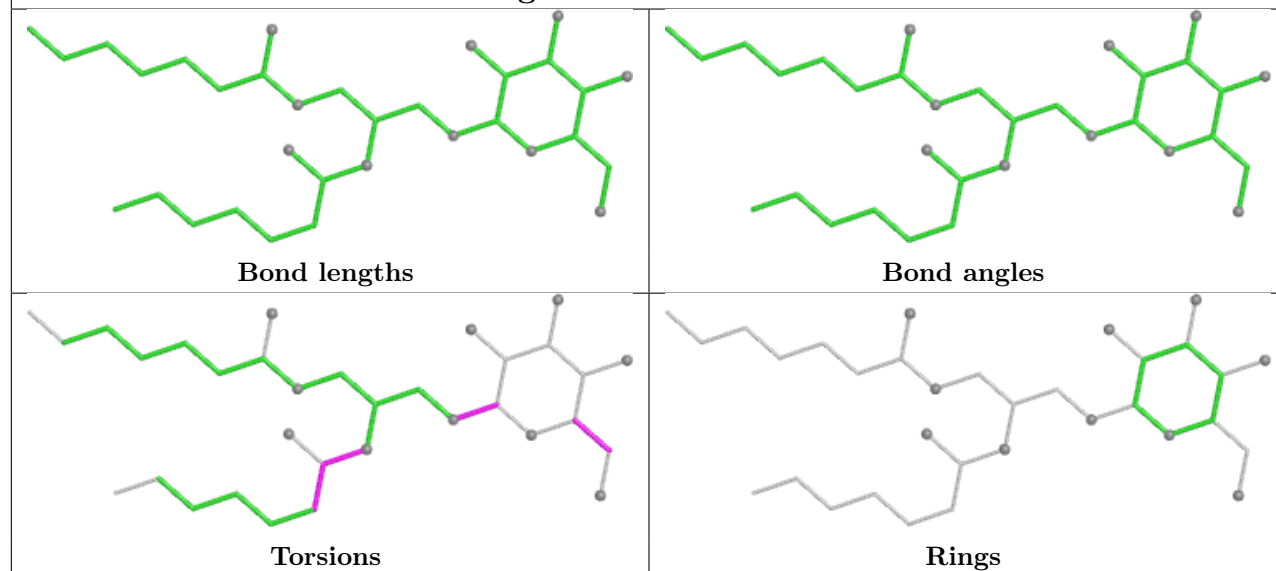
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Bond lengths	Bond angles
	
Torsions	Rings

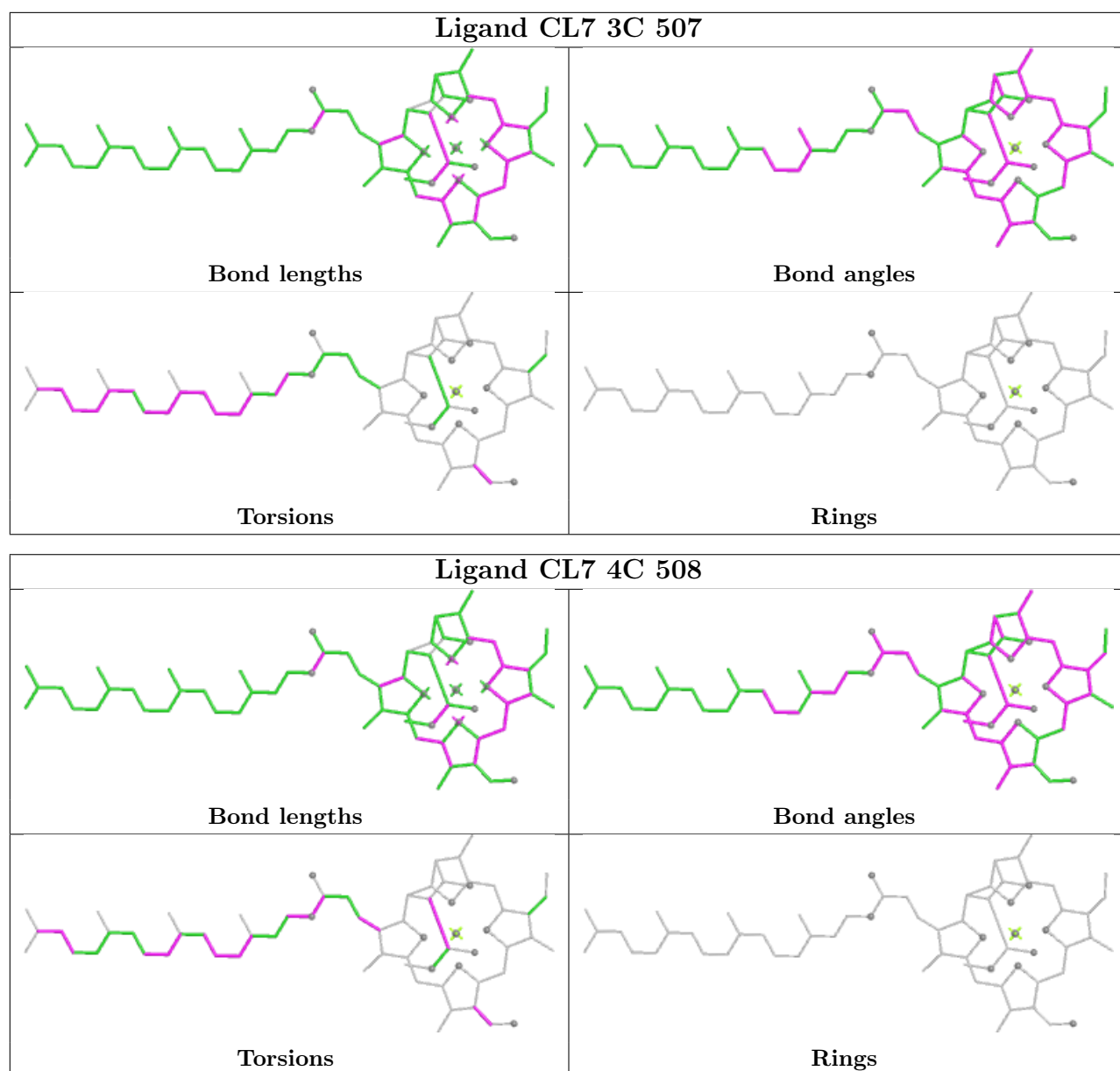
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CL7 43 414

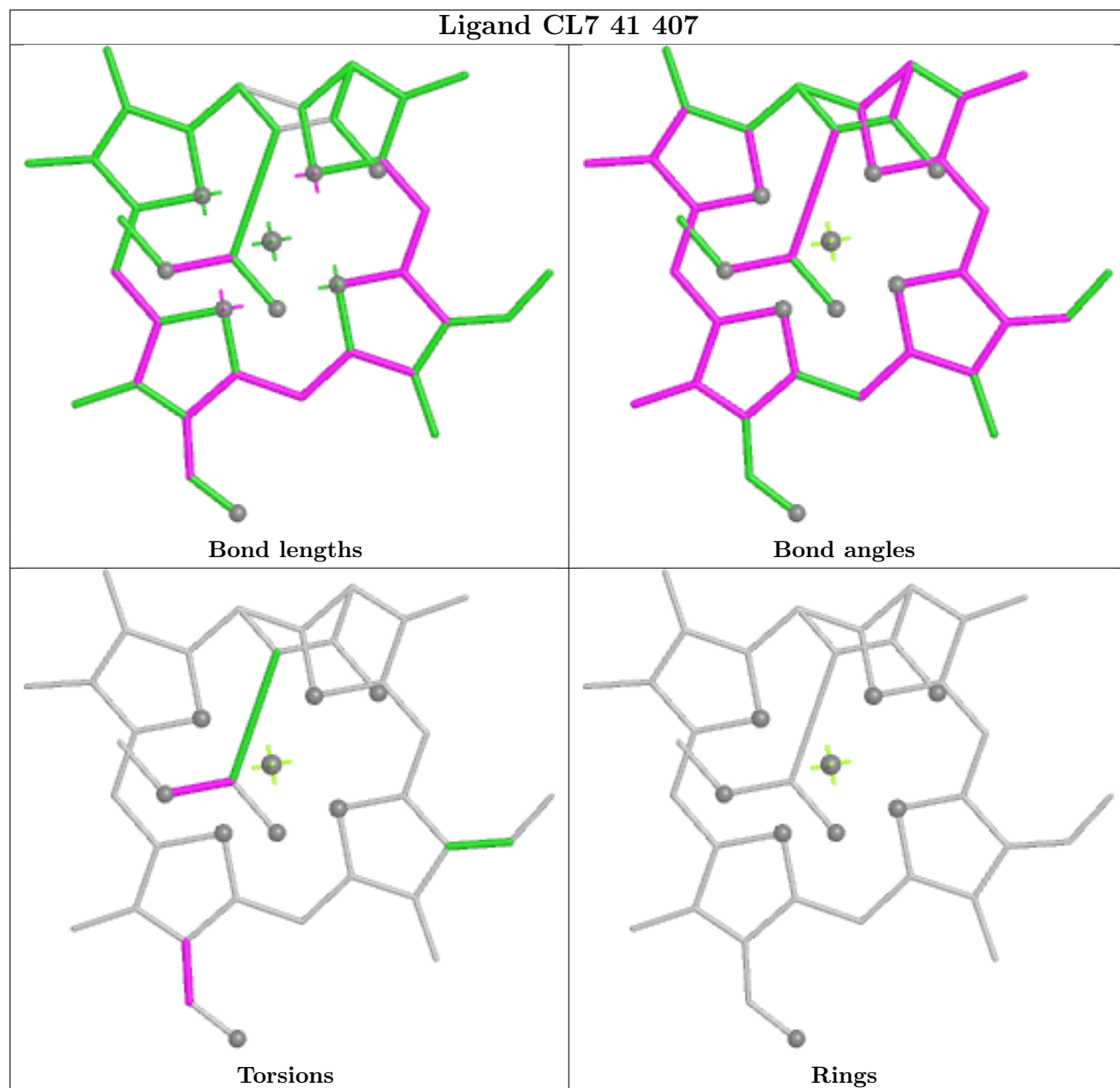


Ligand LMG 4D 410

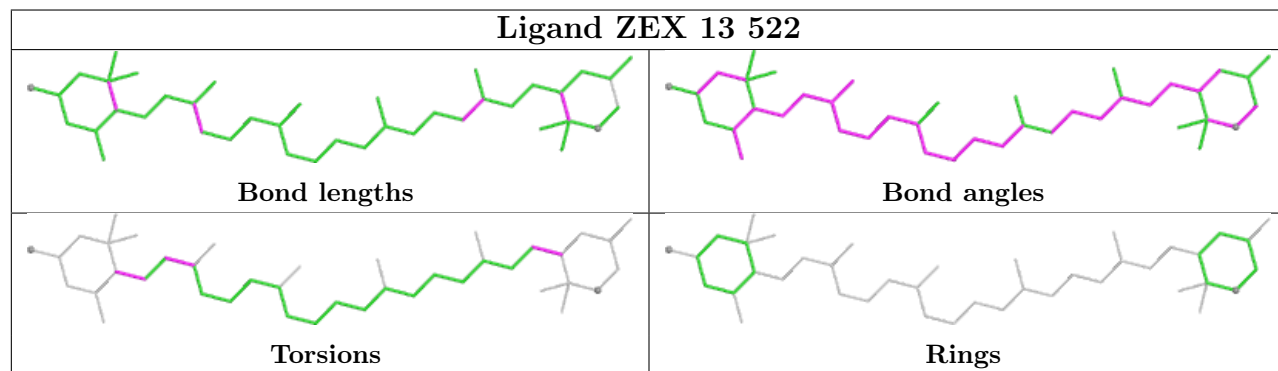


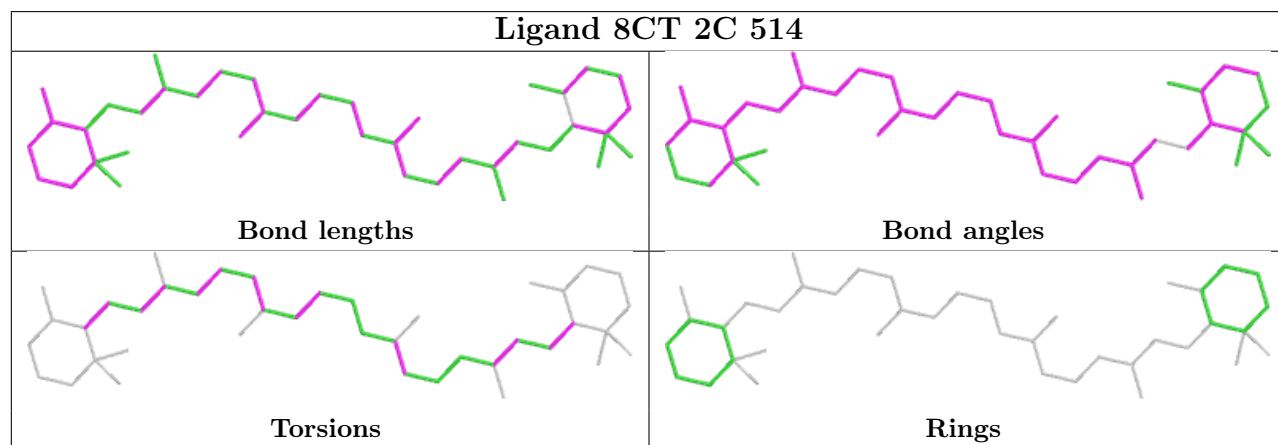
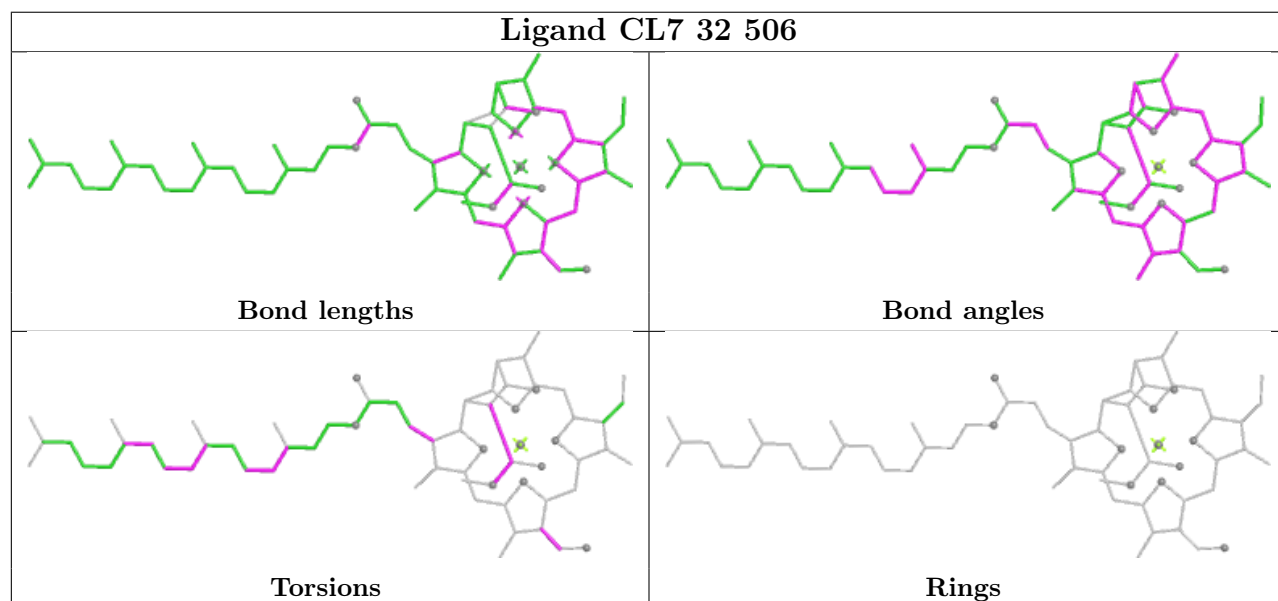
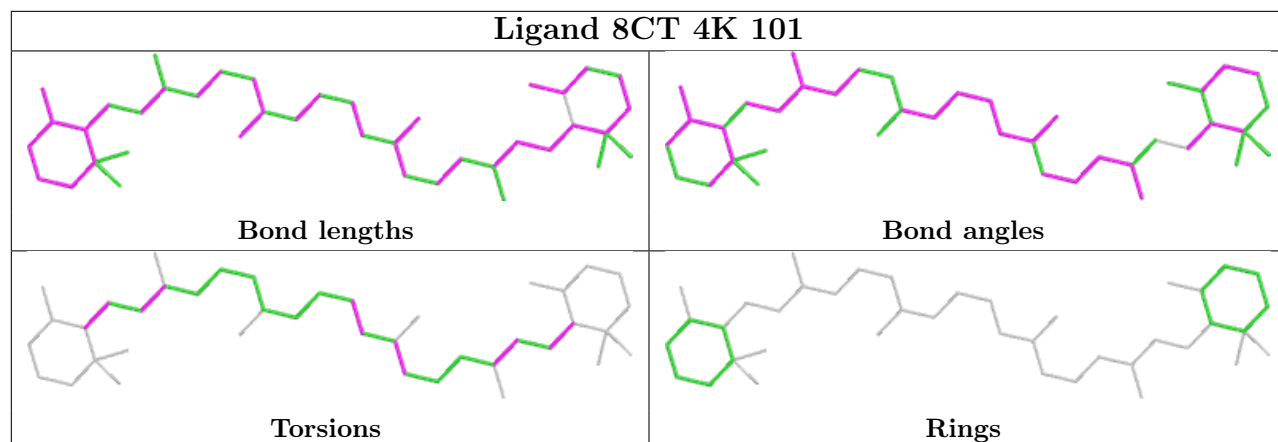


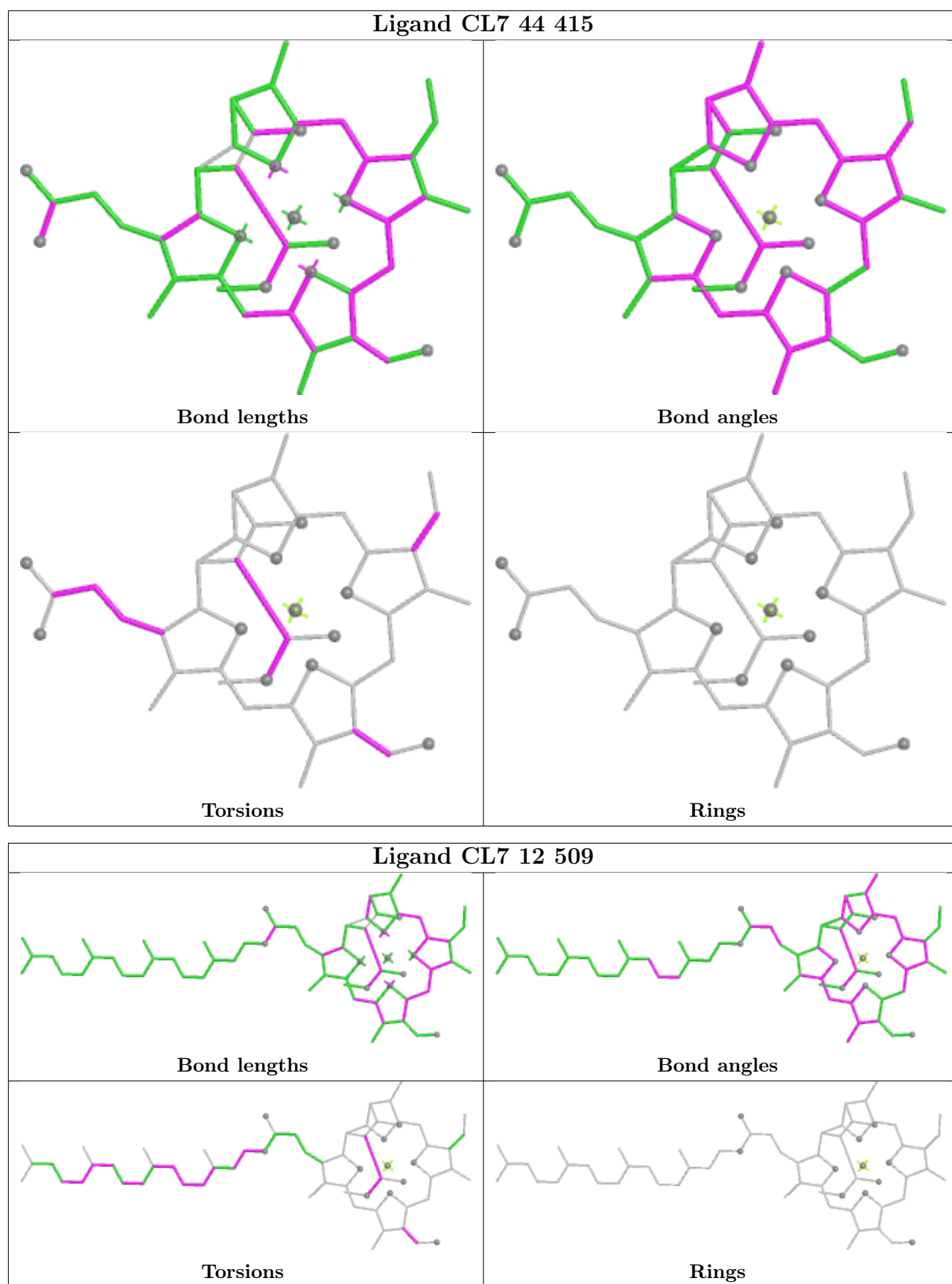
Ligand CL7 41 407



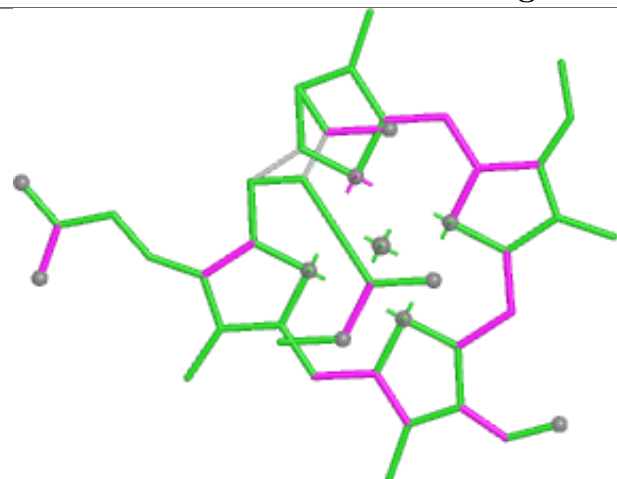
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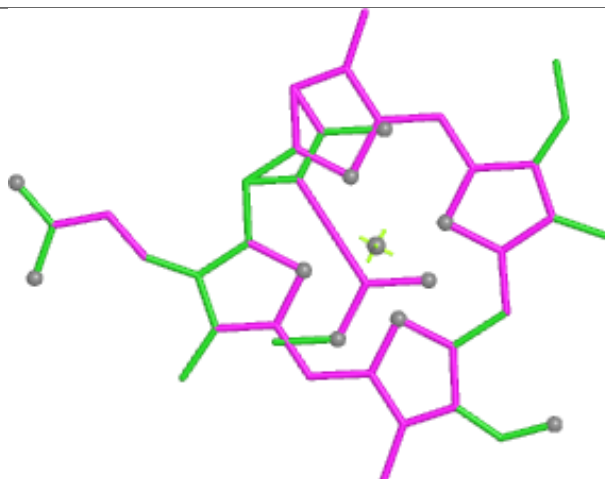




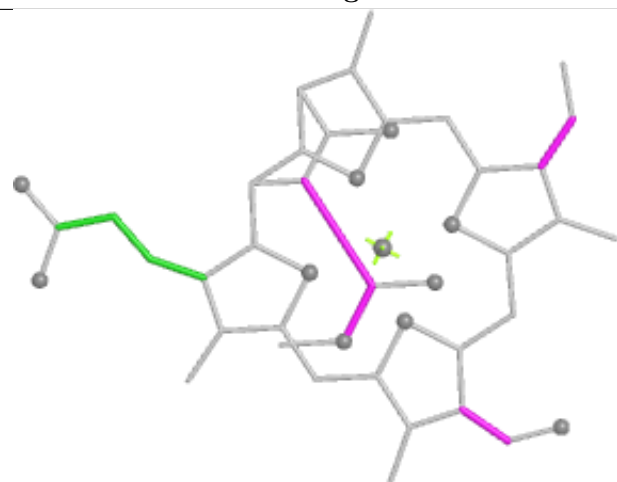
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Bond lengths



Bond angles

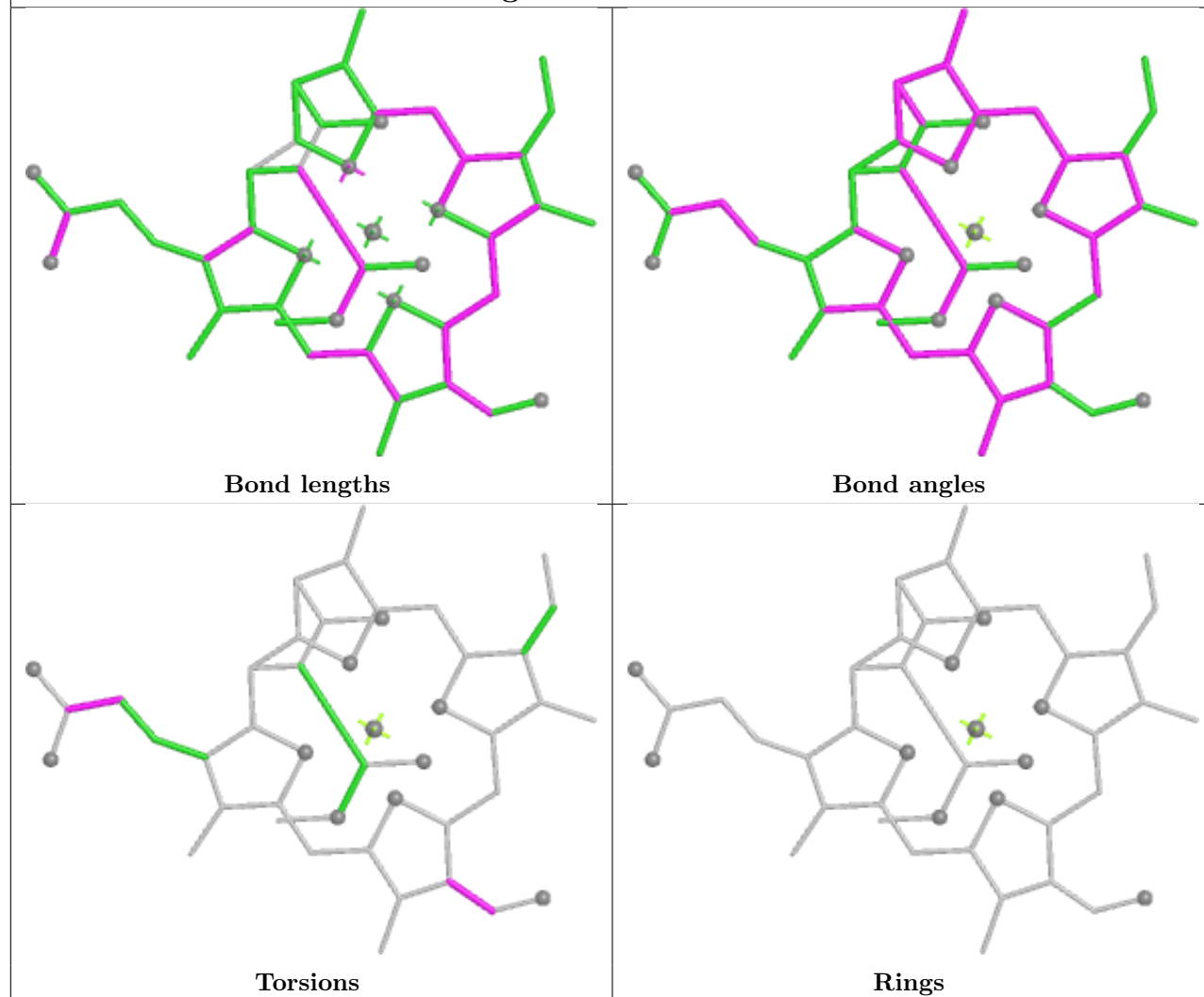


Torsions

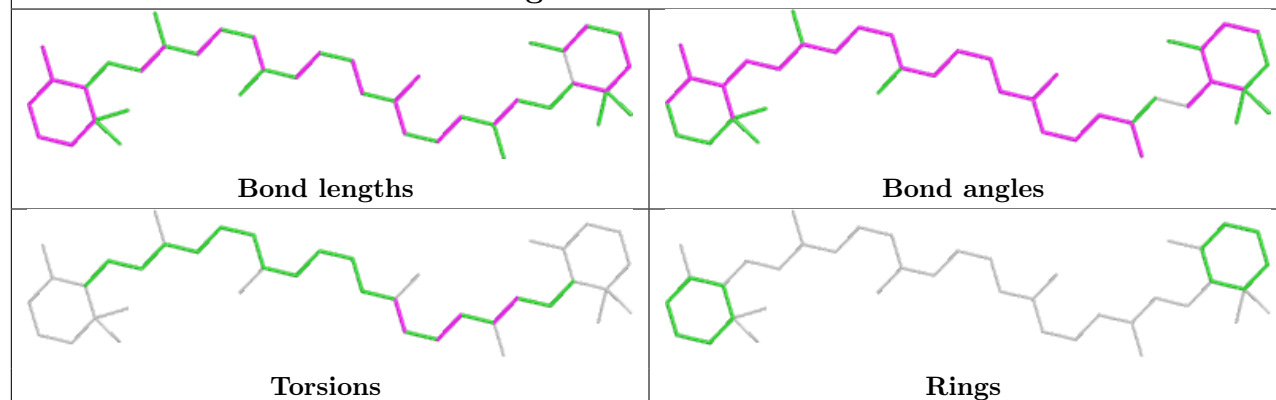


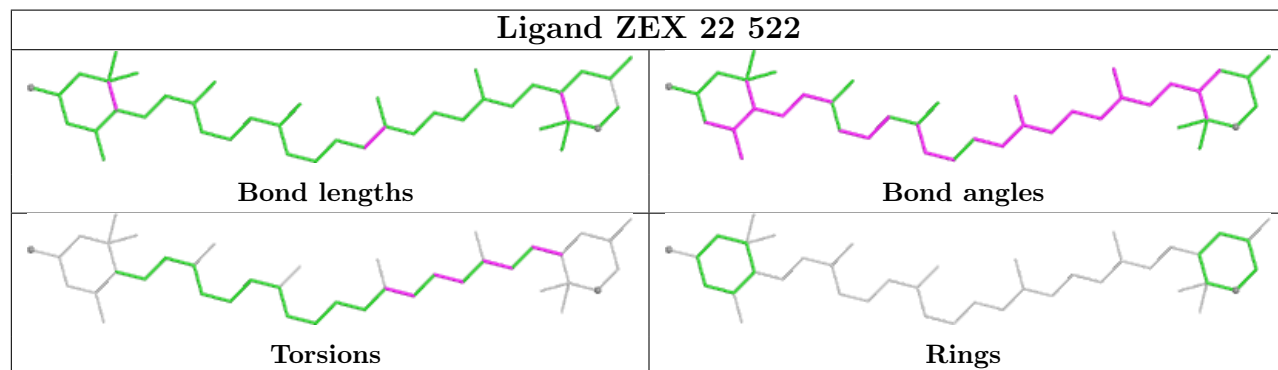
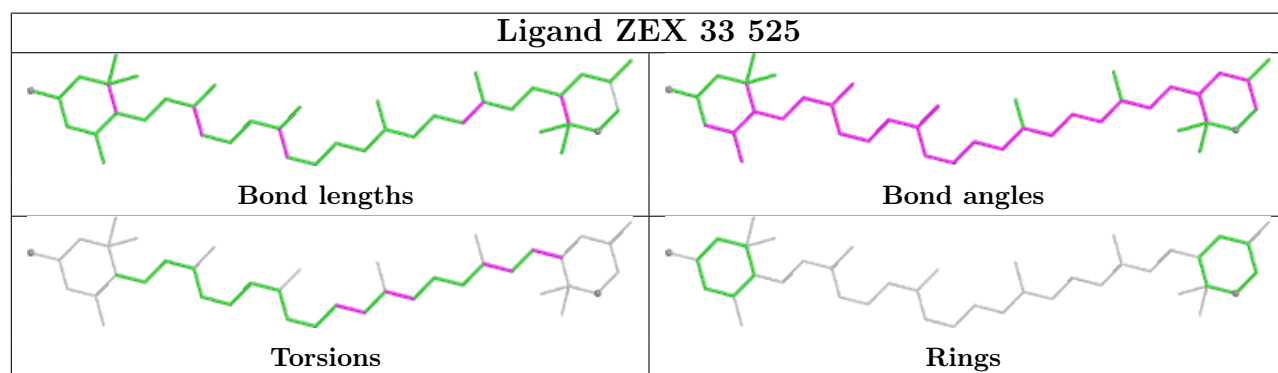
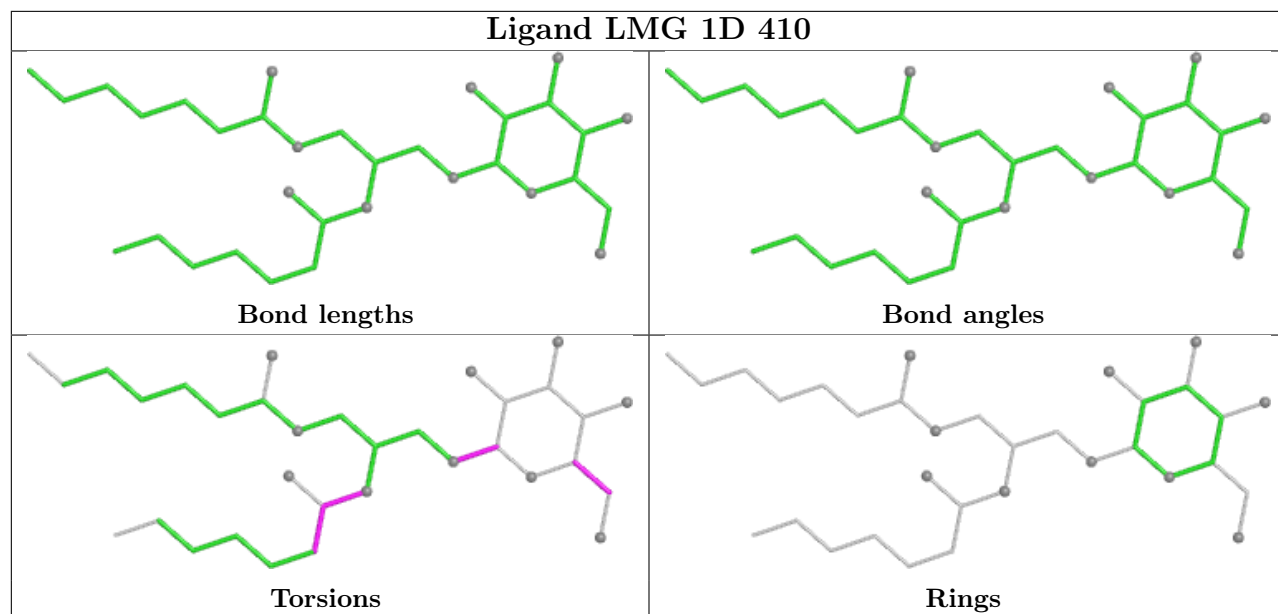
Rings

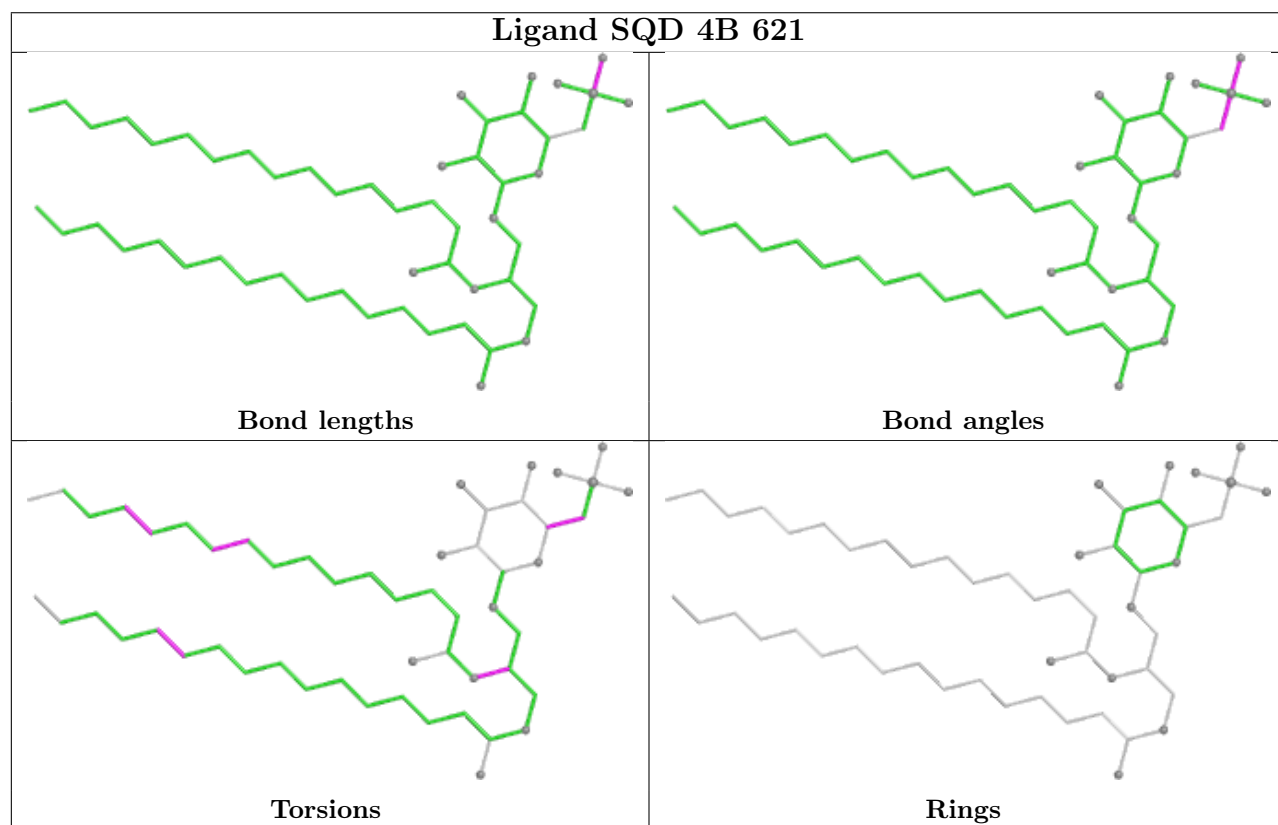
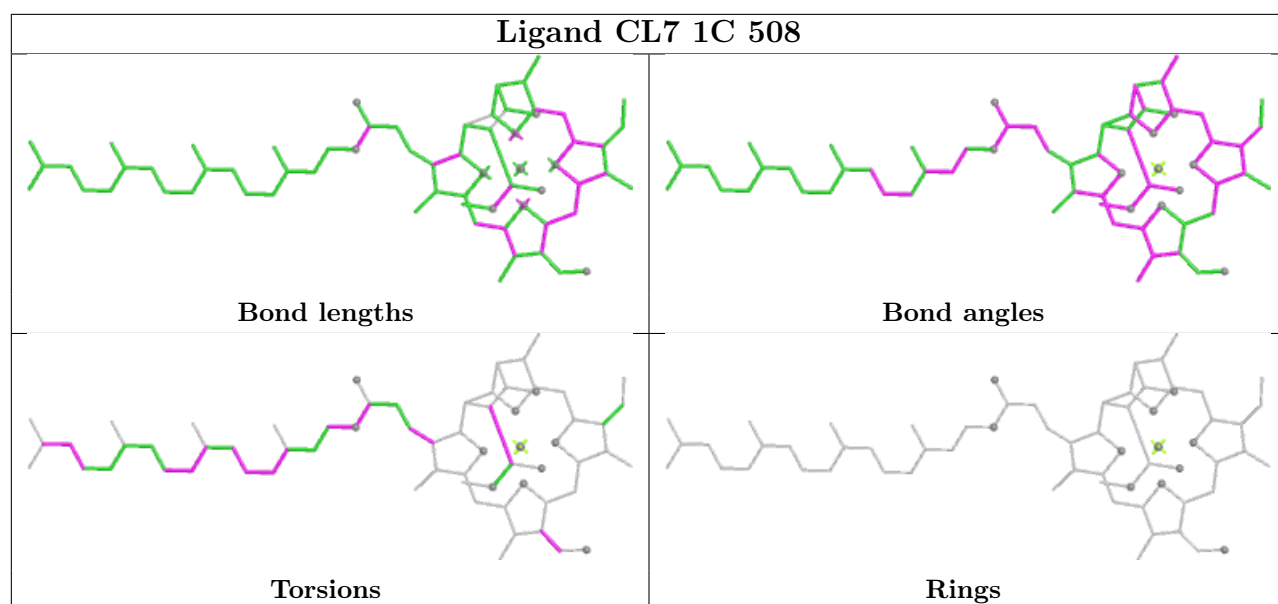
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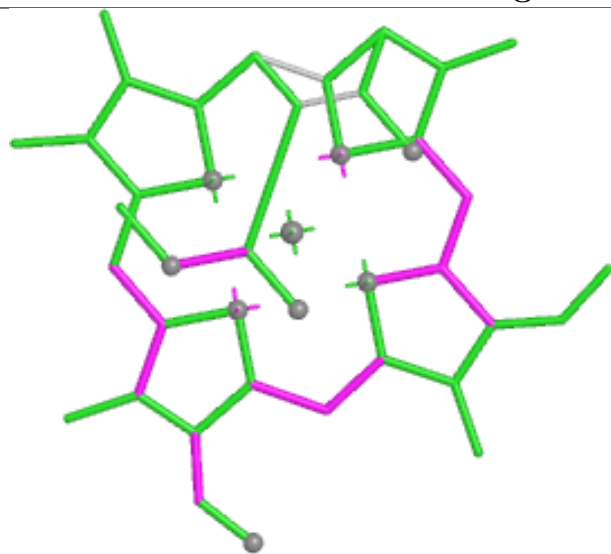
Ligand 8CT 2A 404



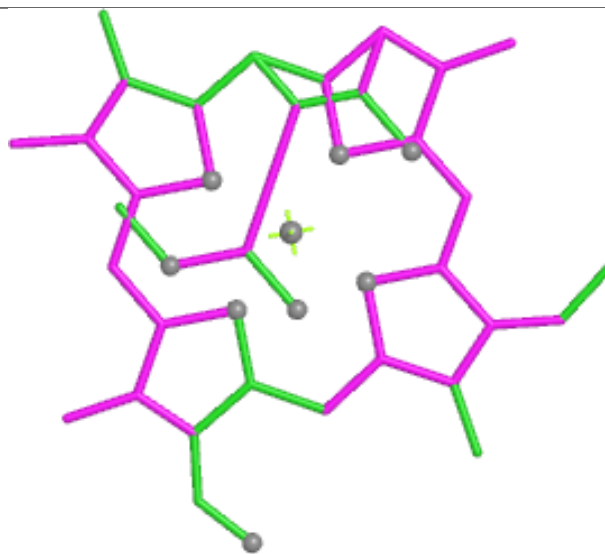




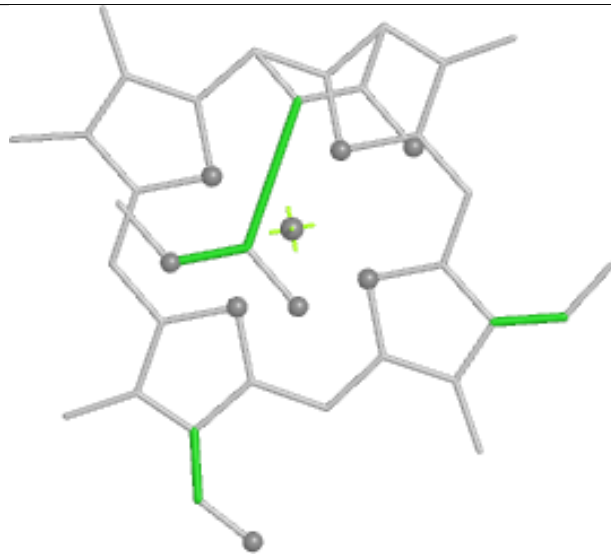
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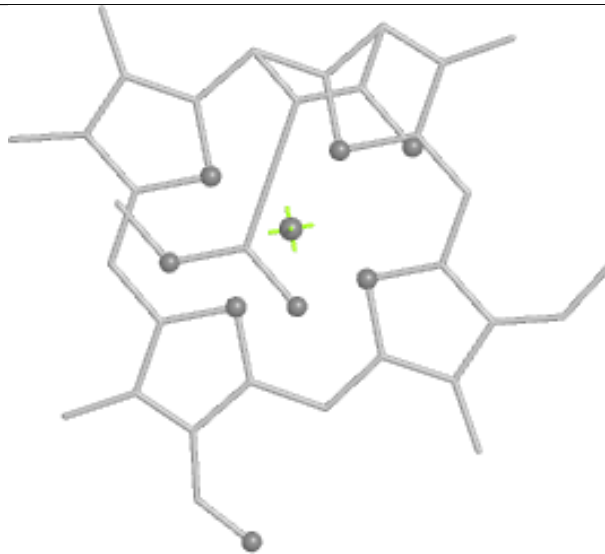
Bond lengths



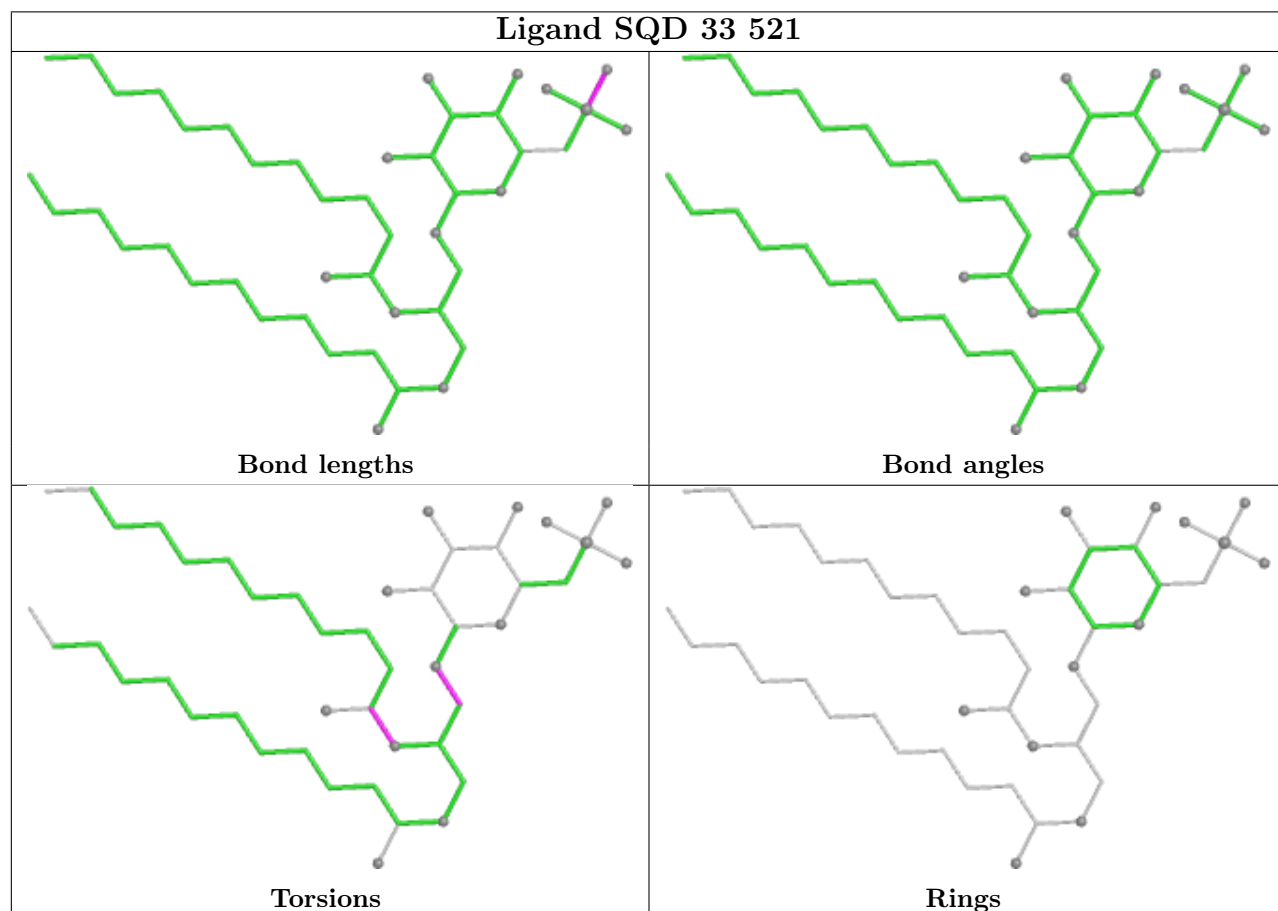
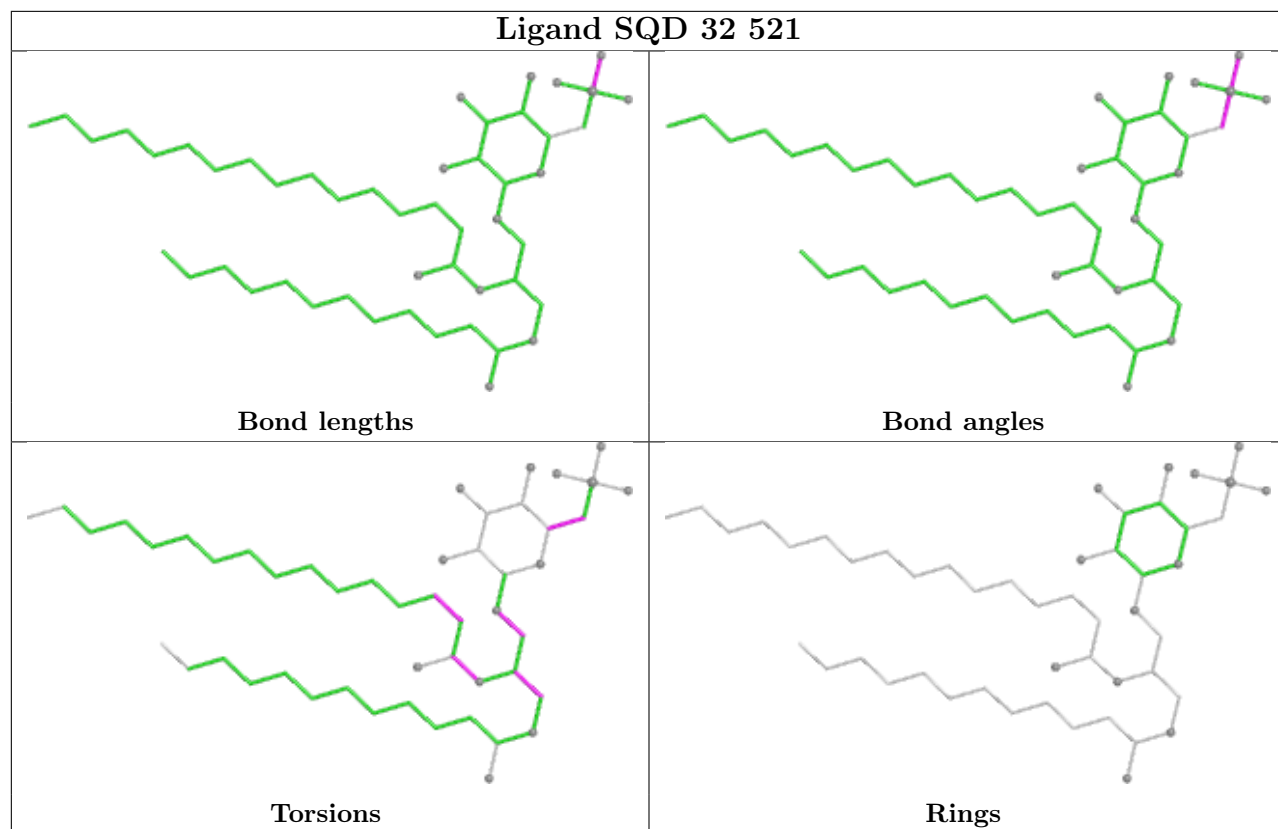
Bond angles

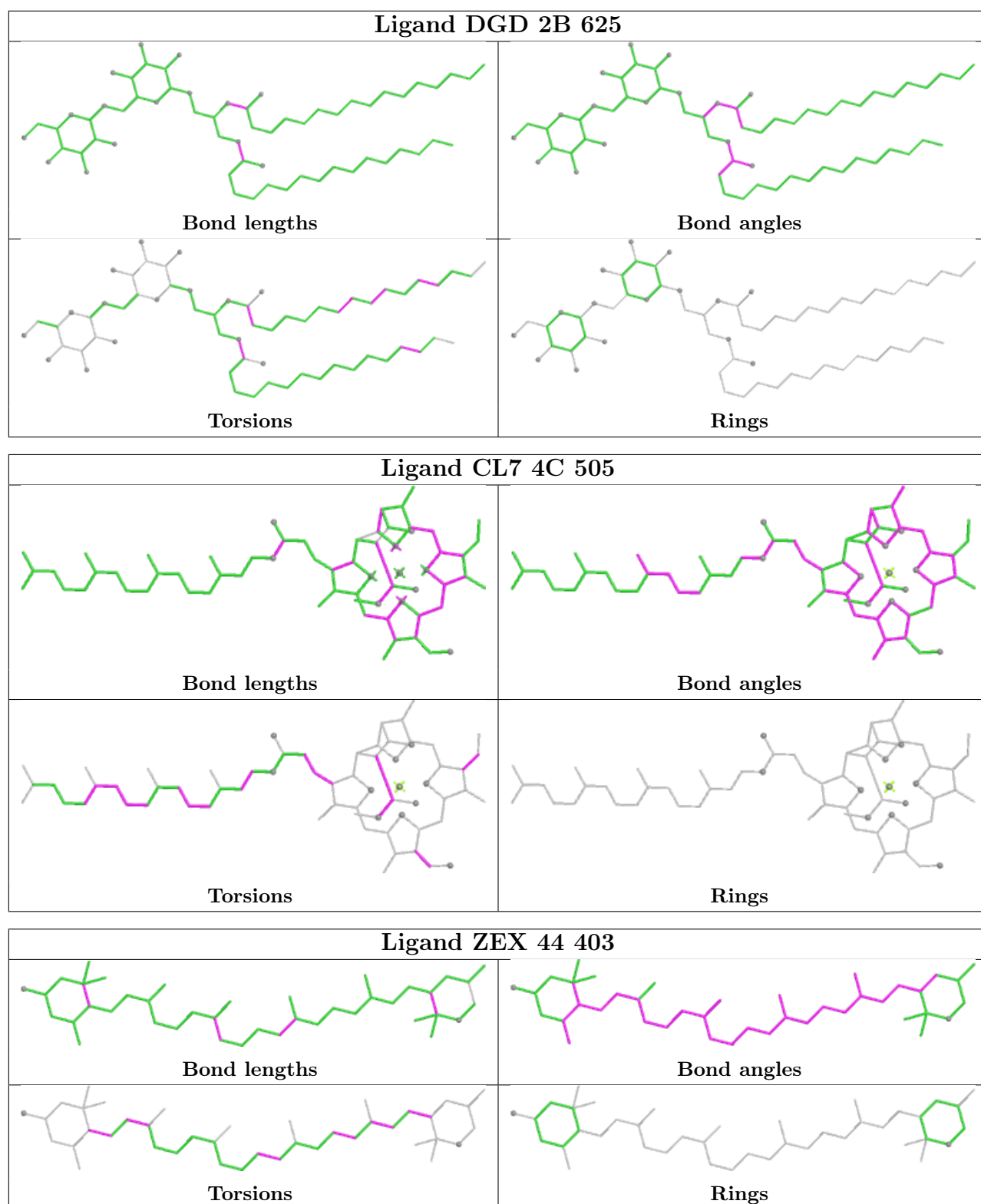


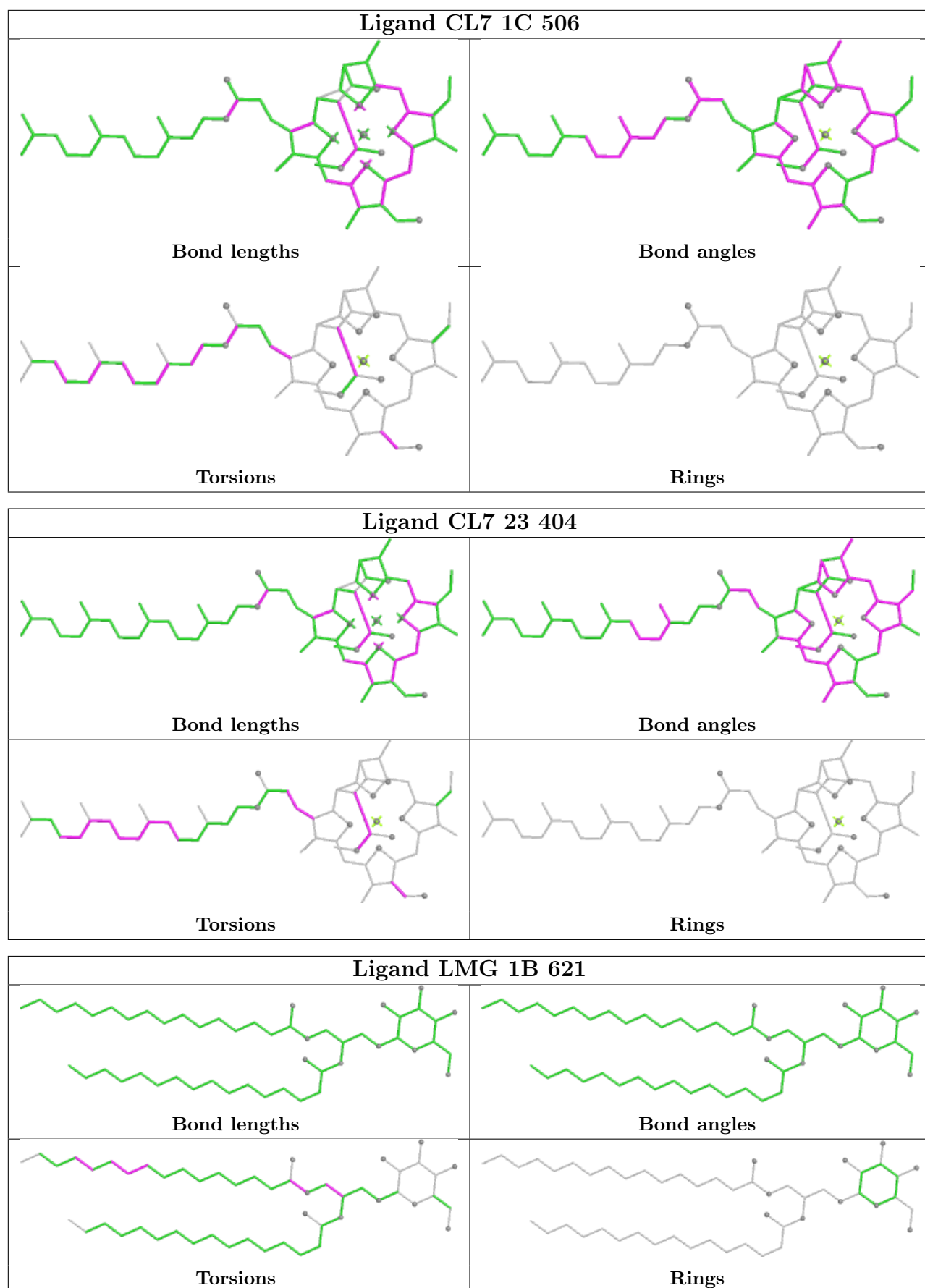
Torsions

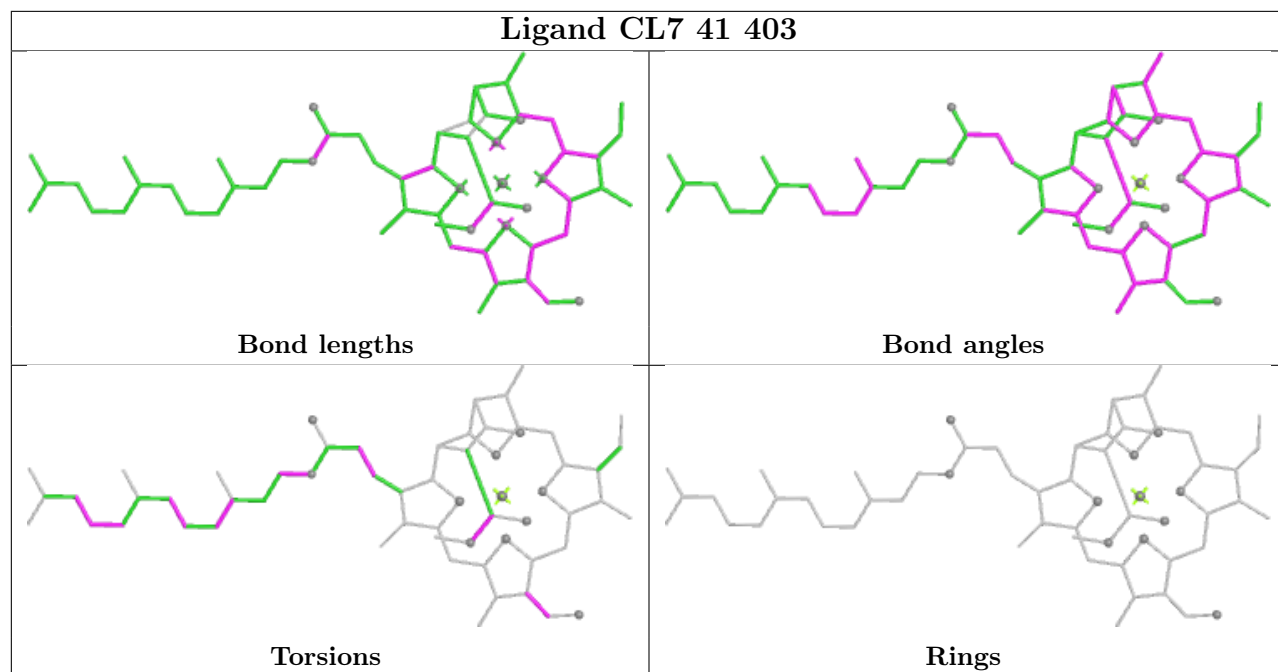


Rings

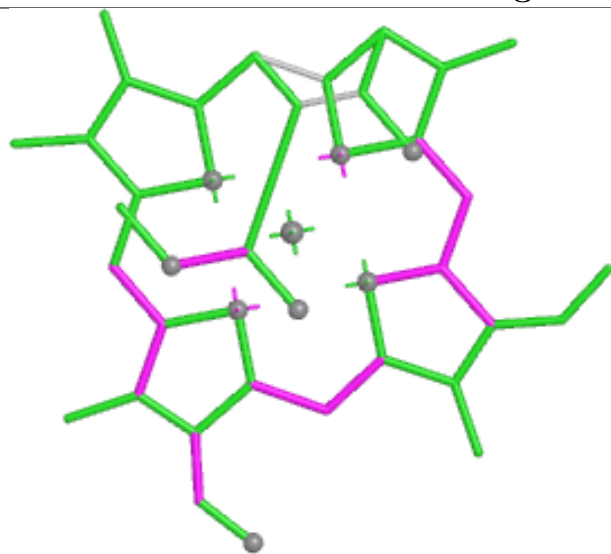




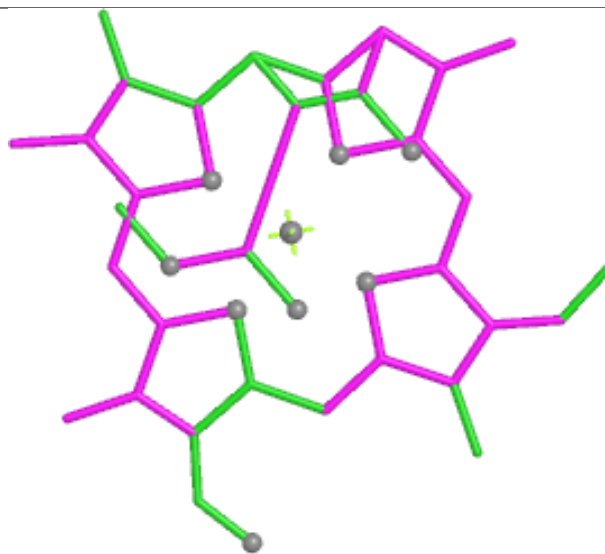




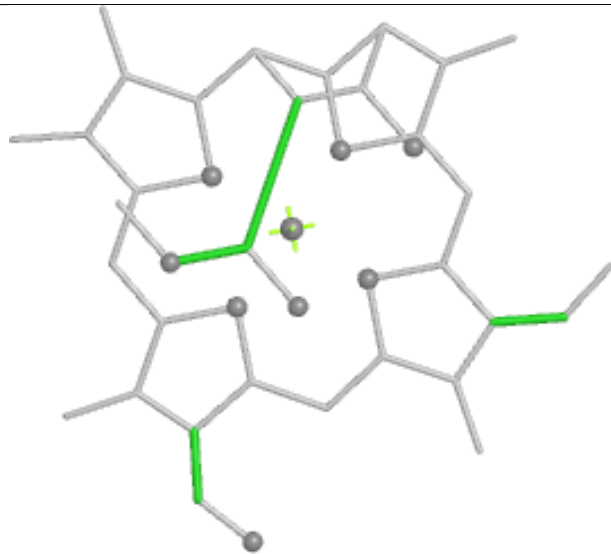
Ligand CL7 23 416



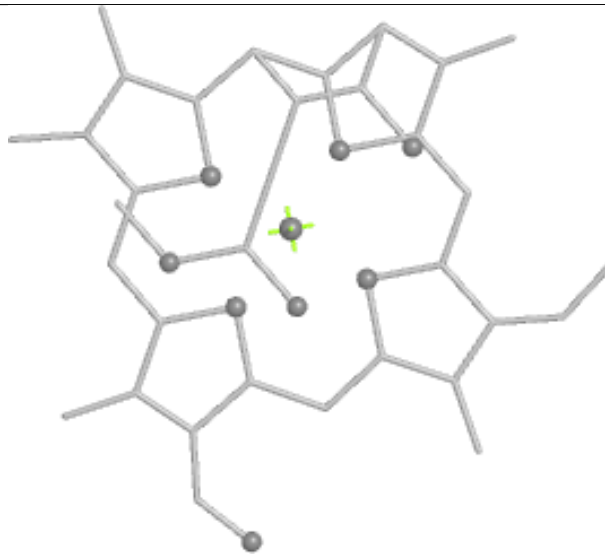
Bond lengths



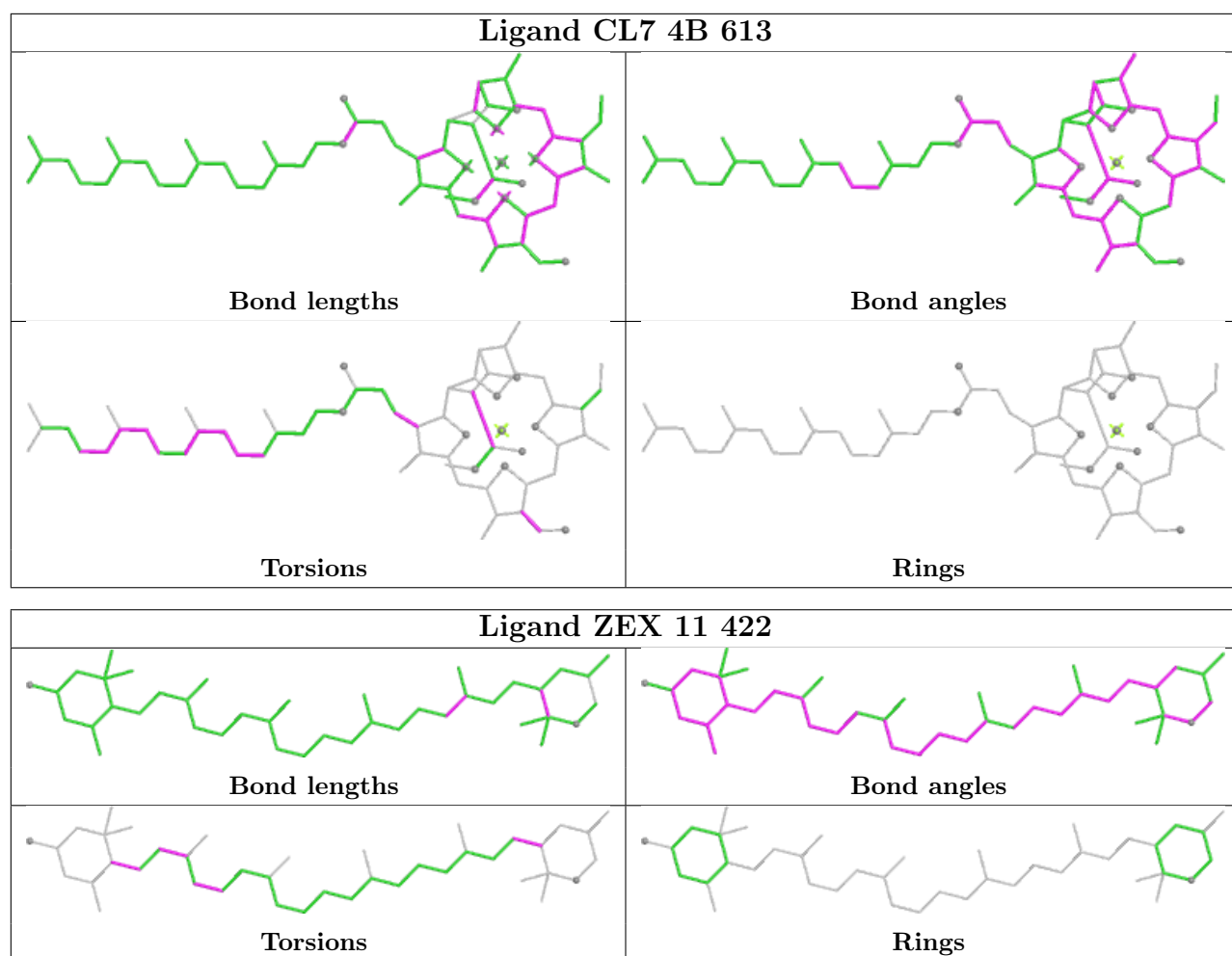
Bond angles

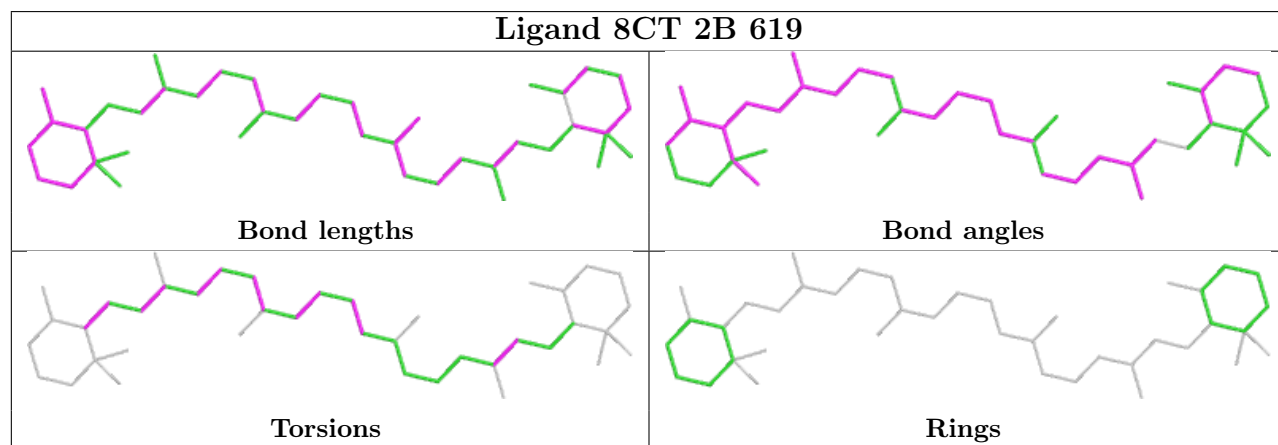
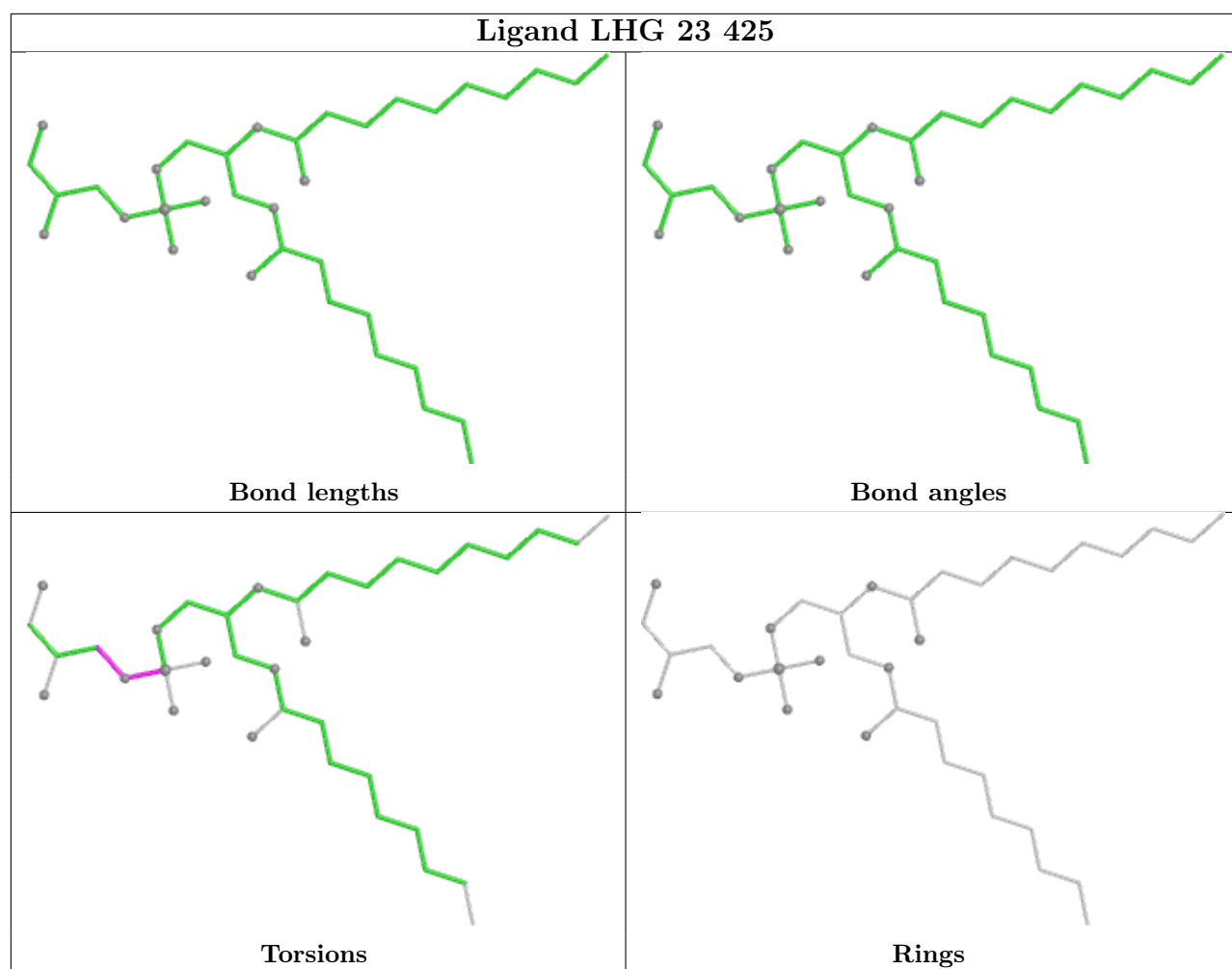


Torsions

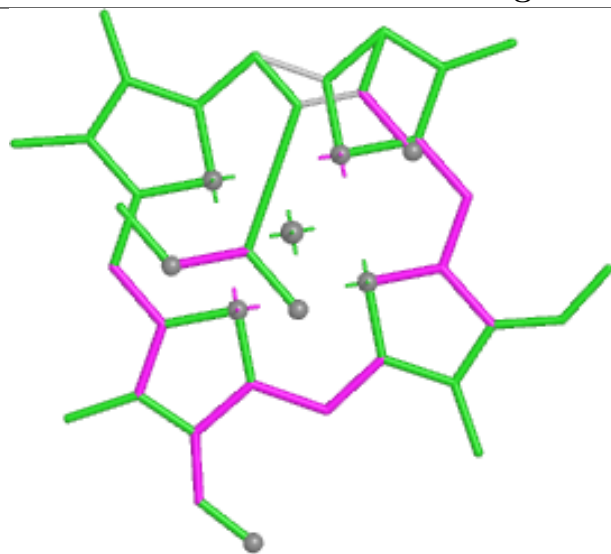


Rings

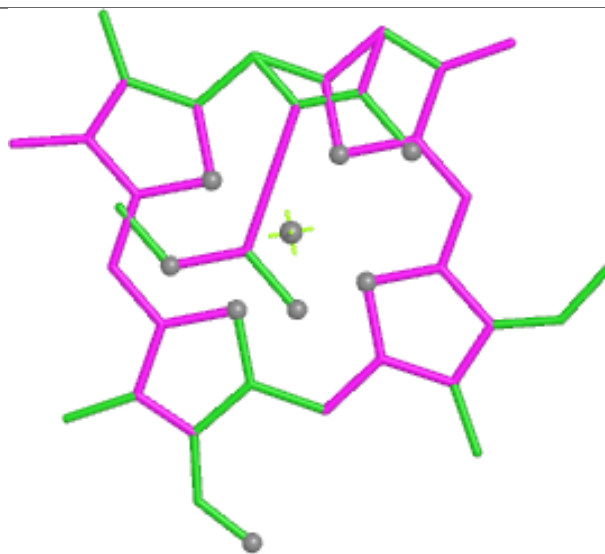




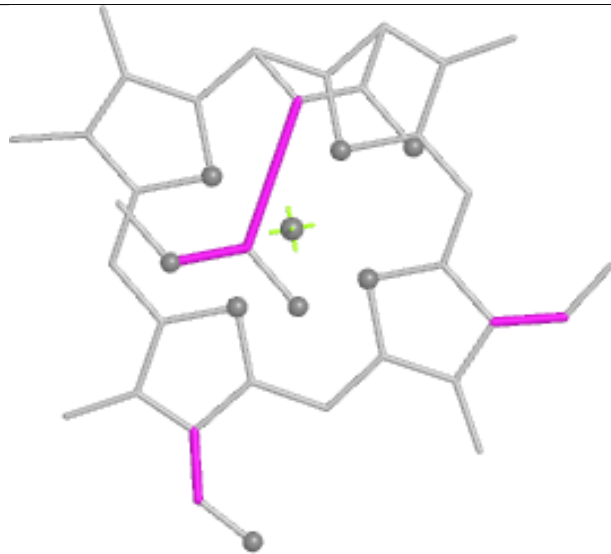
Ligand CL7 44 416



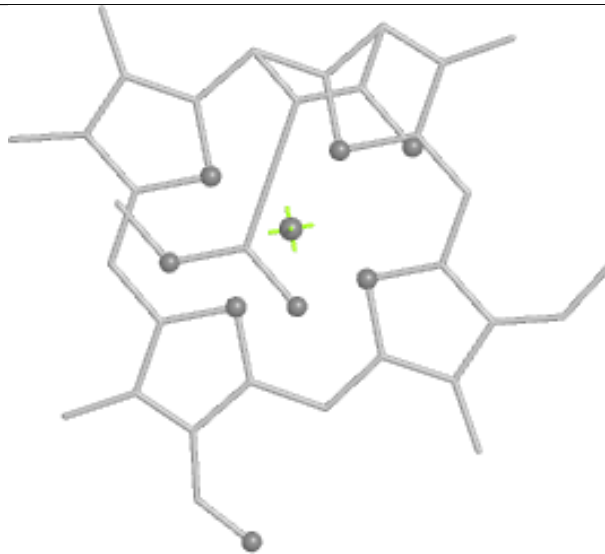
Bond lengths



Bond angles

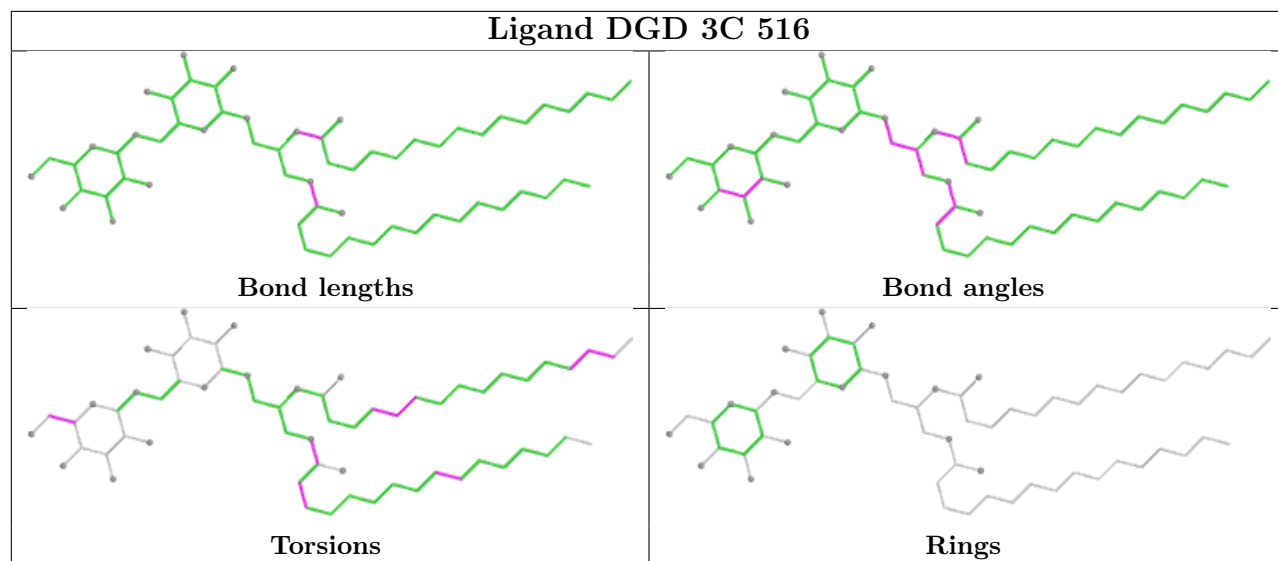


Torsions

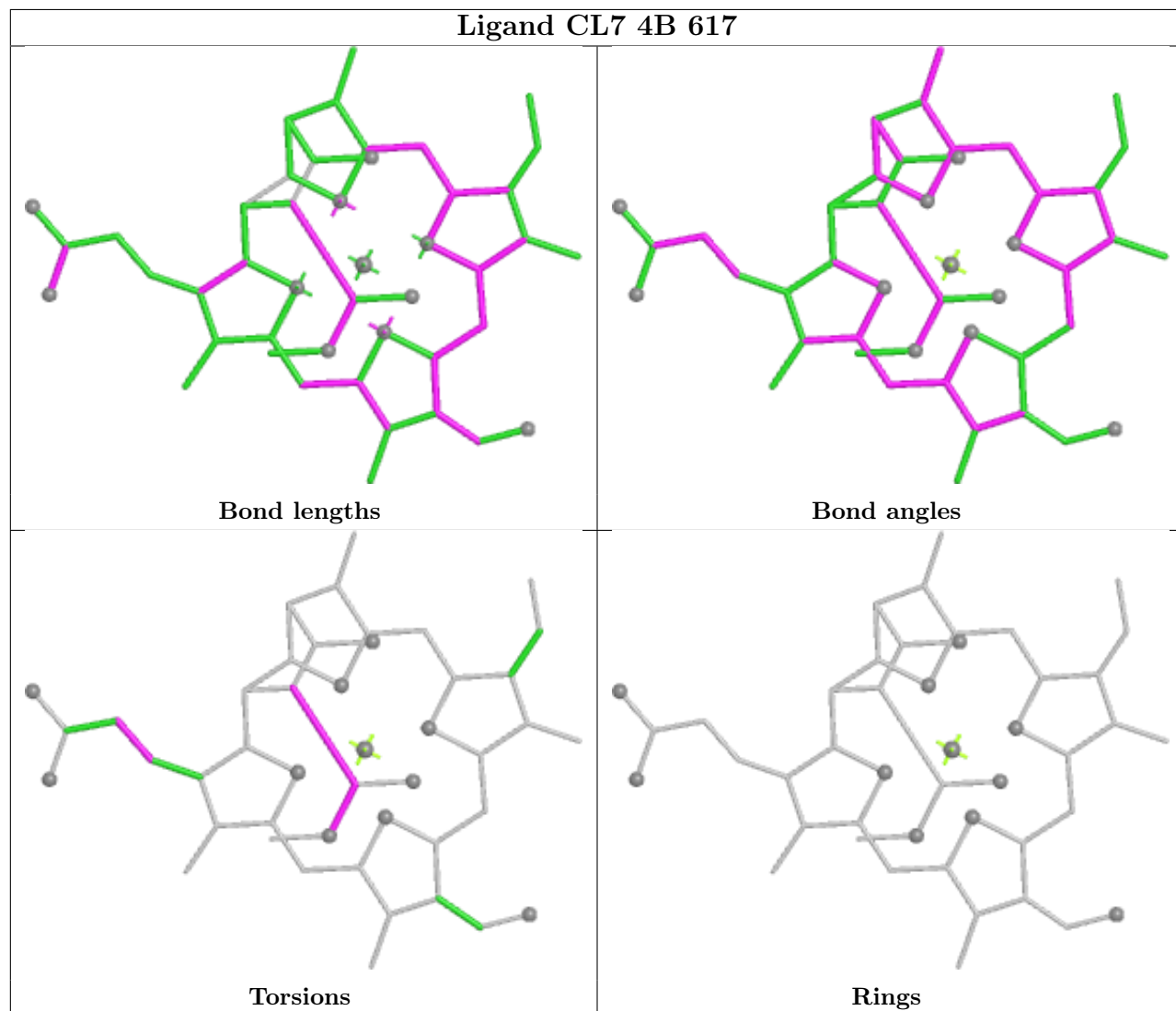


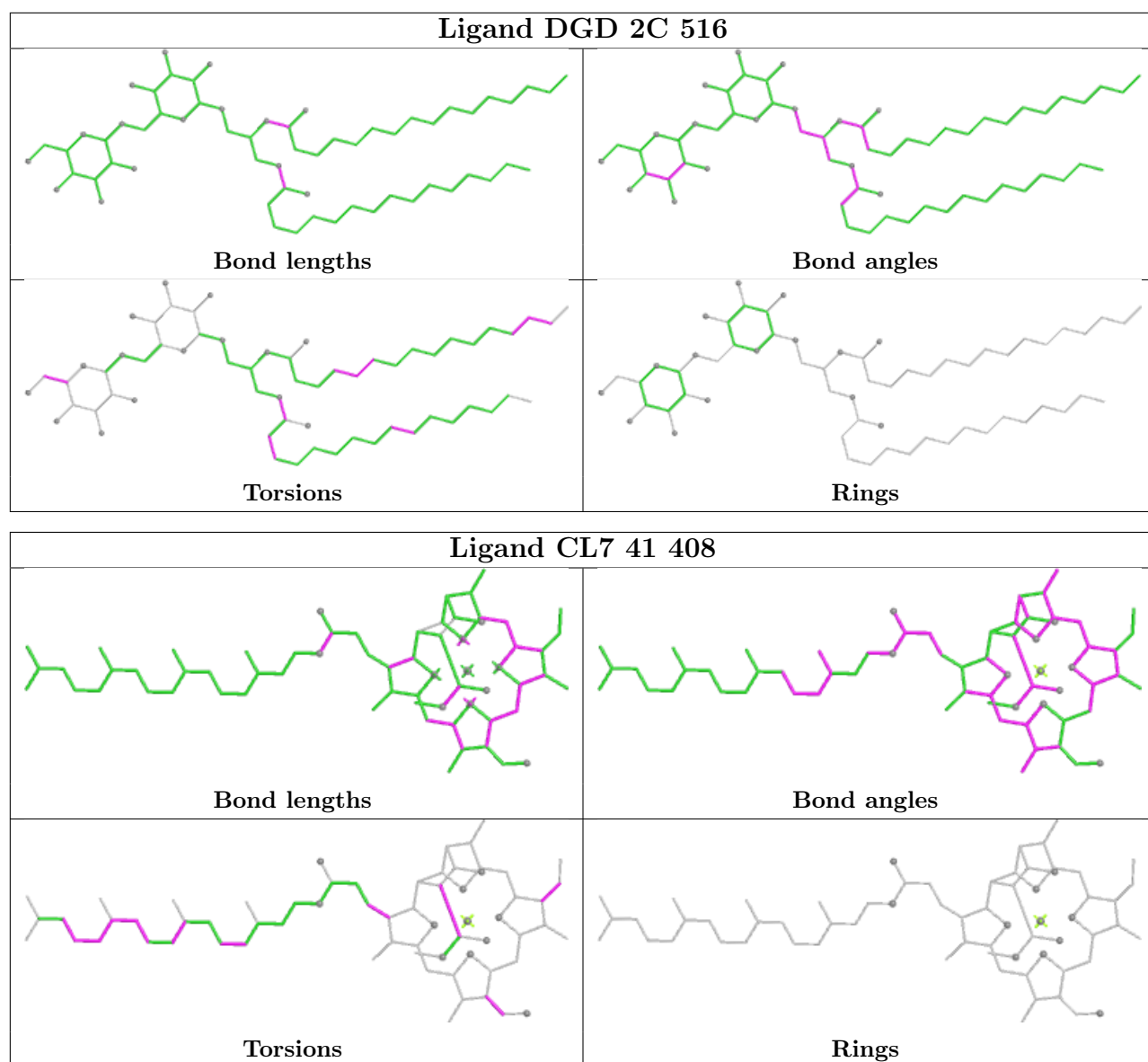
Rings

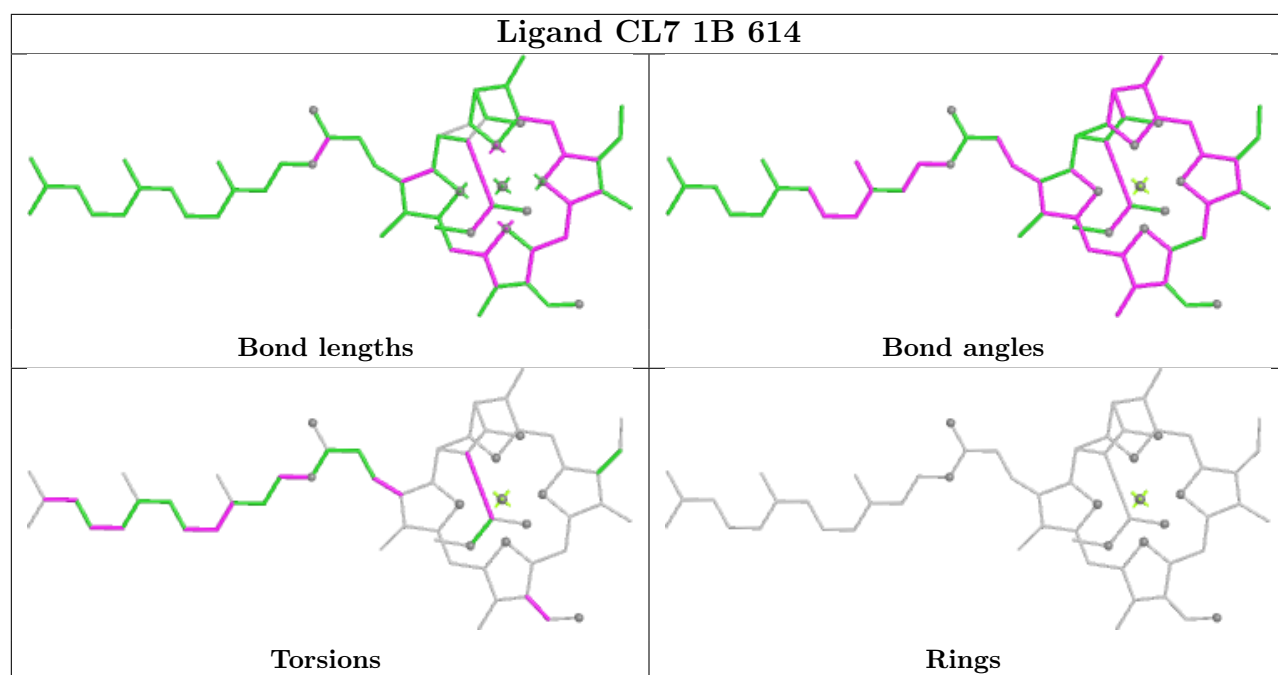
Ligand DGD 3C 516



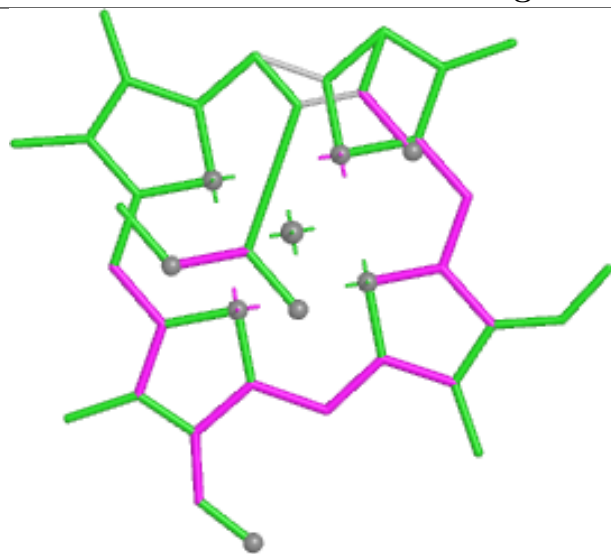
Ligand CL7 4B 617



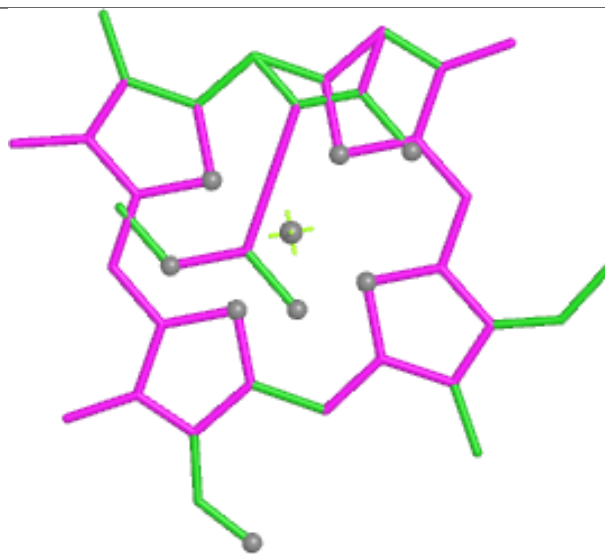




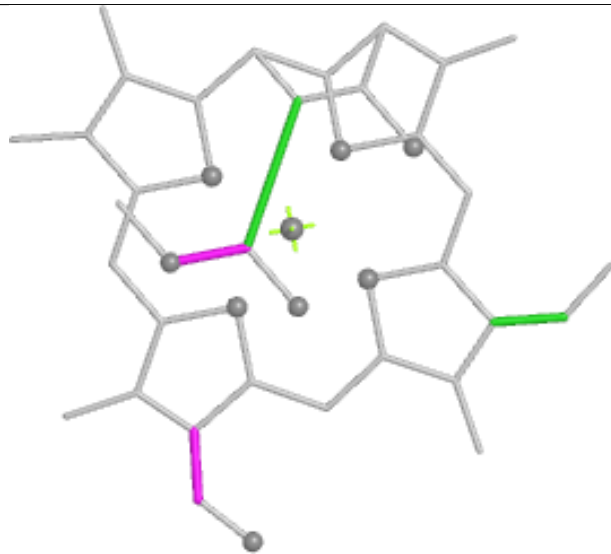
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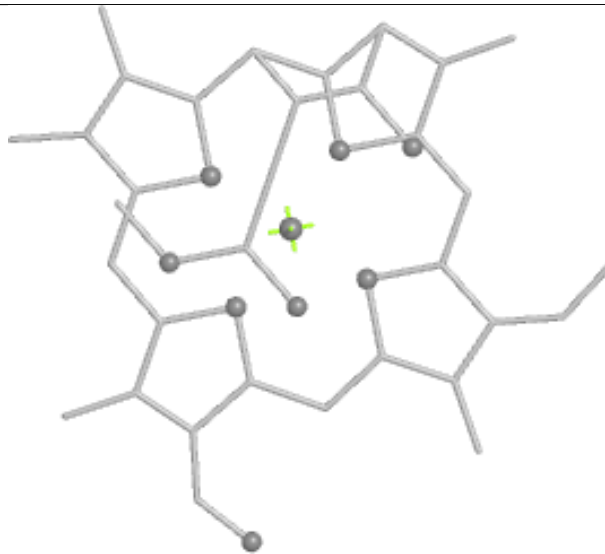
Bond lengths



Bond angles

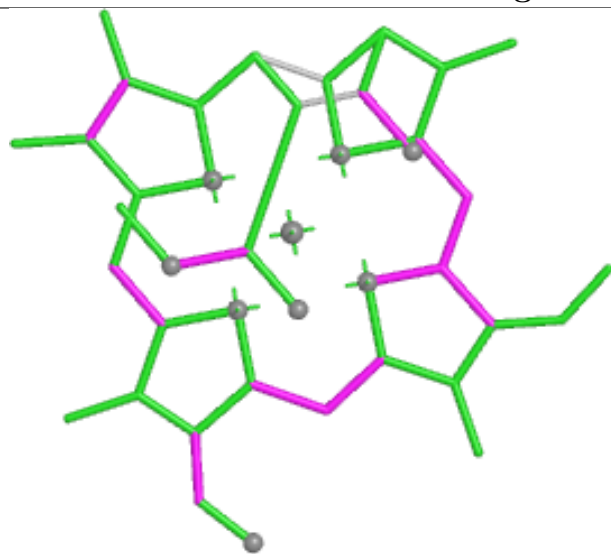


Torsions

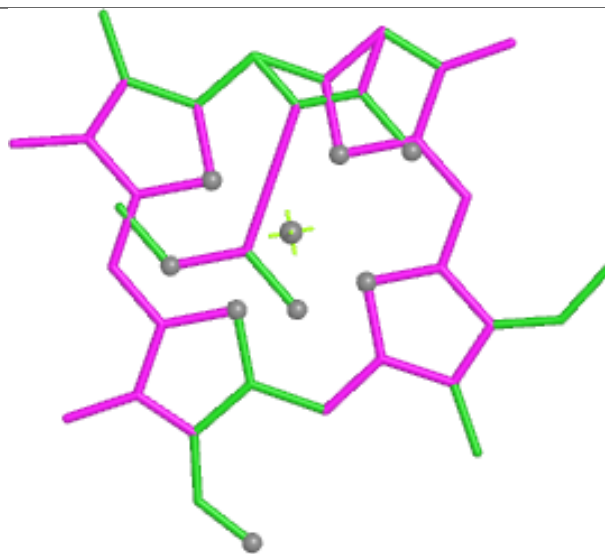


Rings

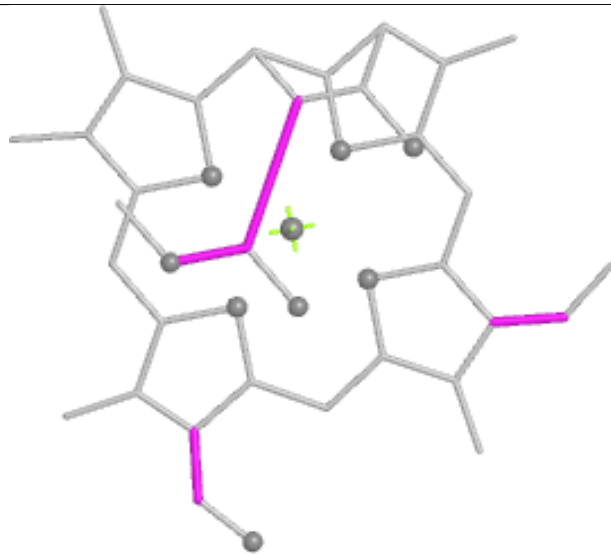
Ligand CL7 21 415



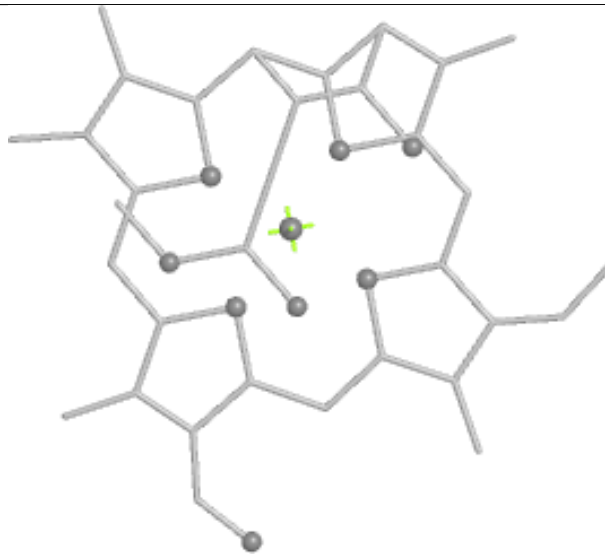
Bond lengths



Bond angles

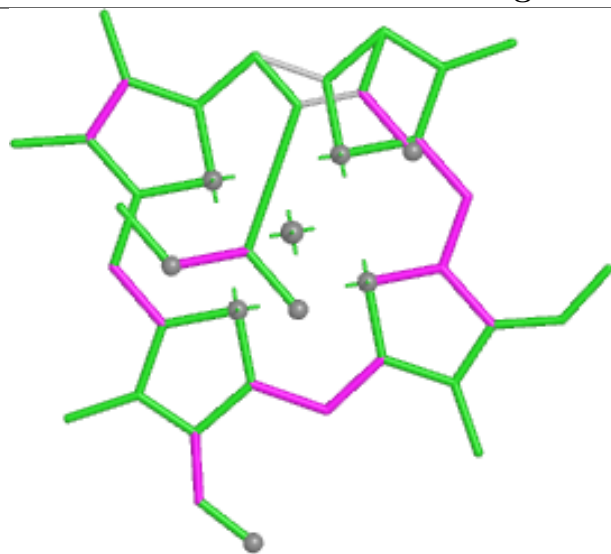


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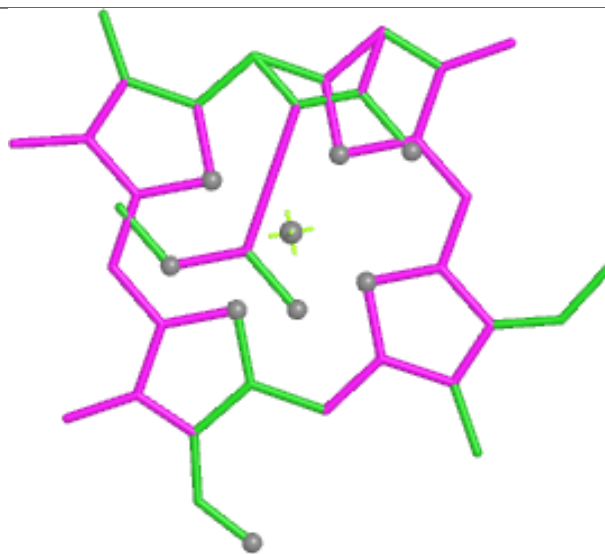


Rings

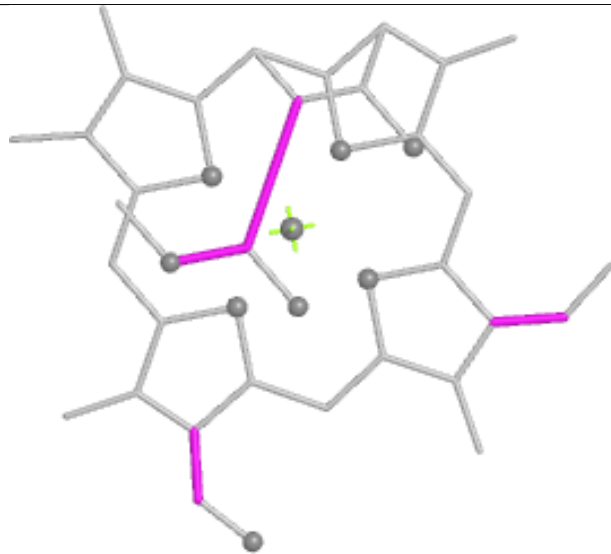
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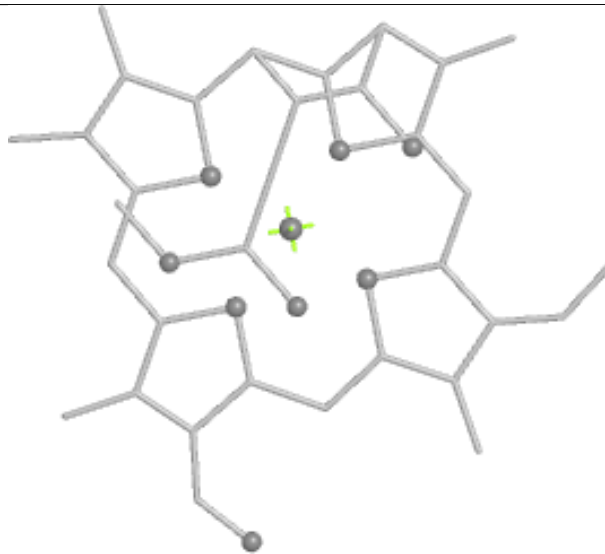
Bond lengths



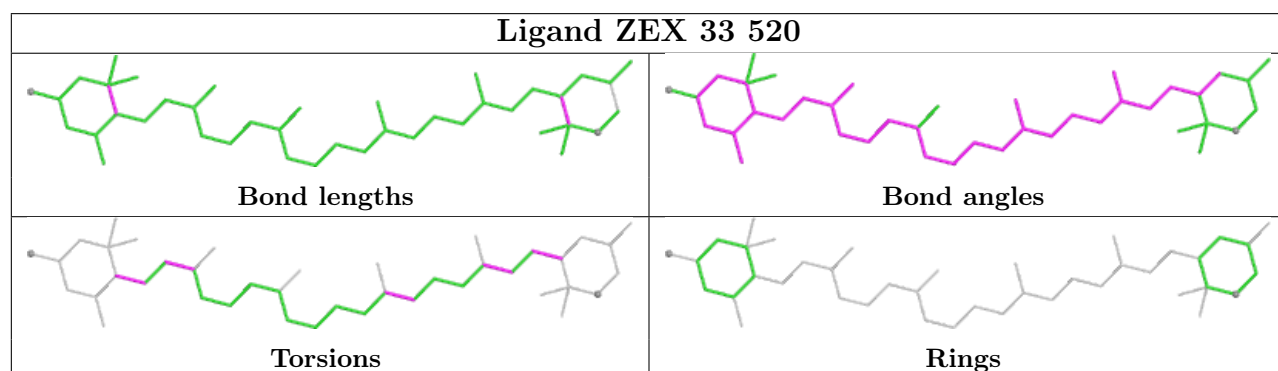
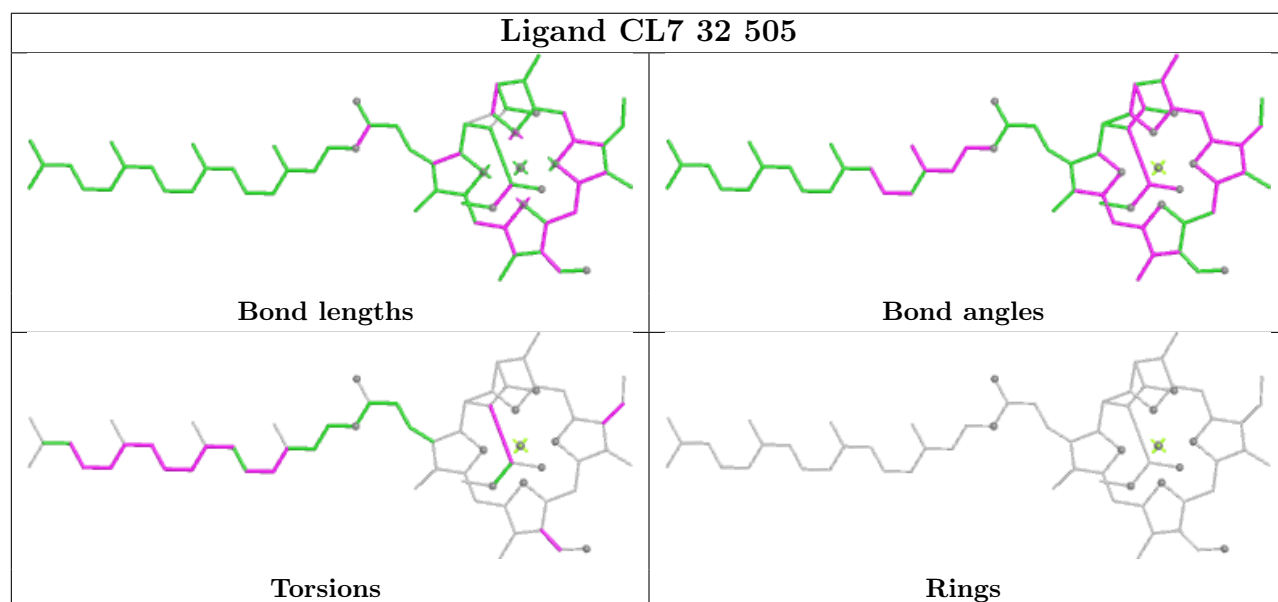
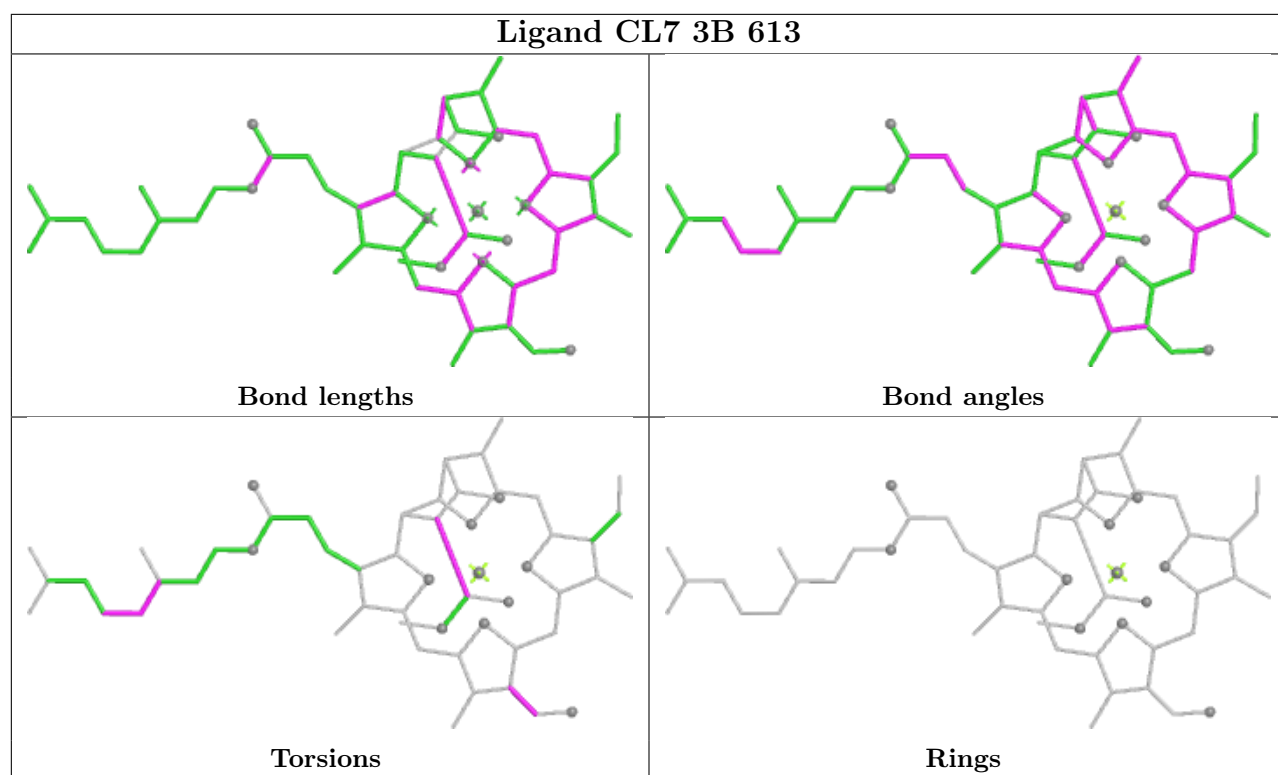
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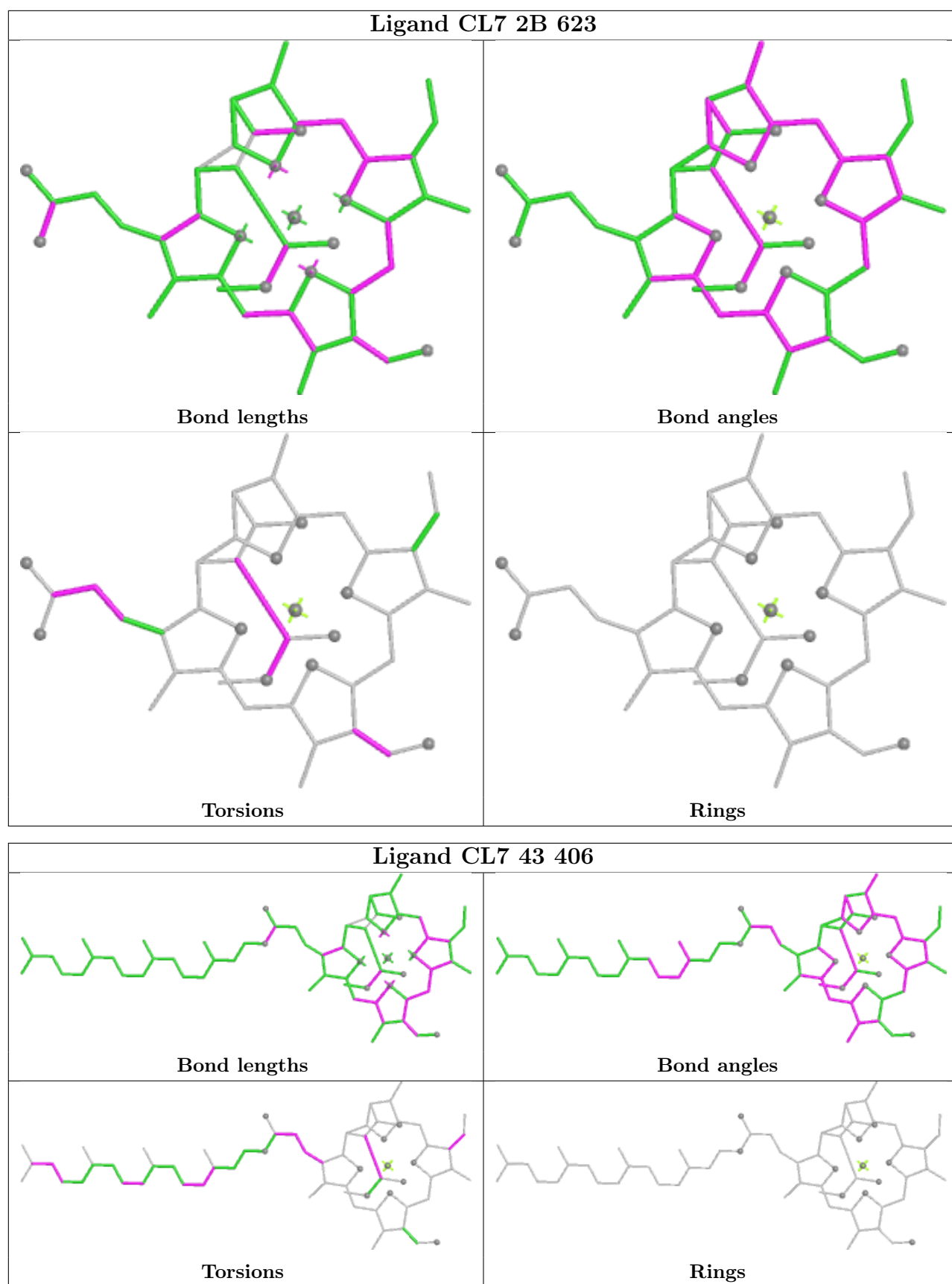


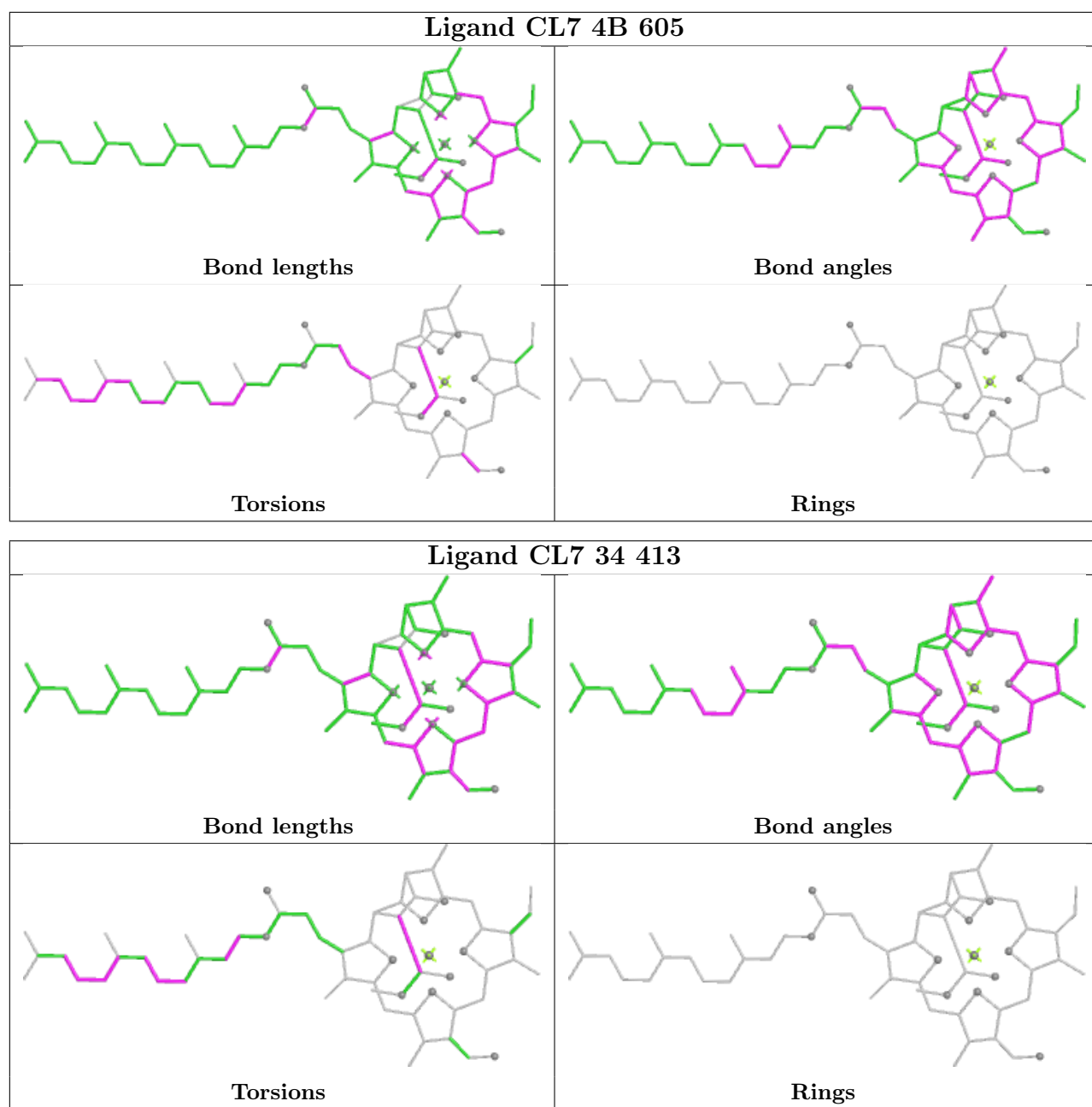
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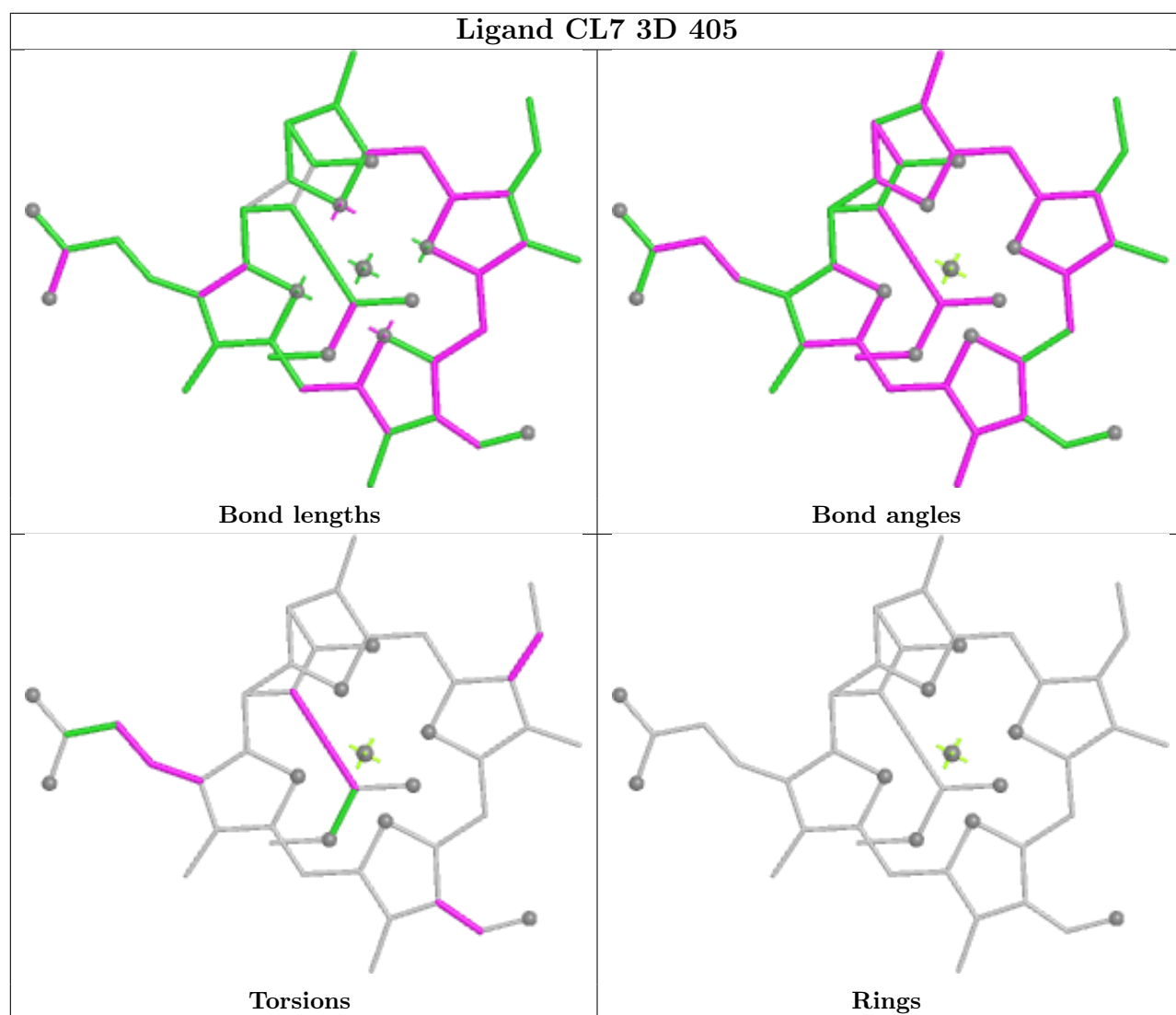


Rings

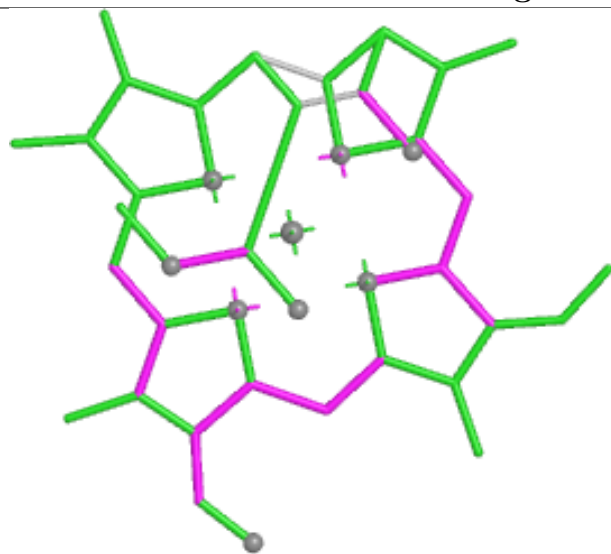




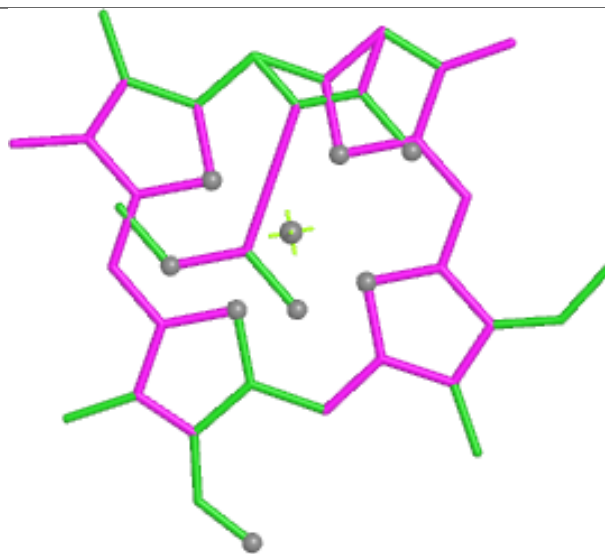




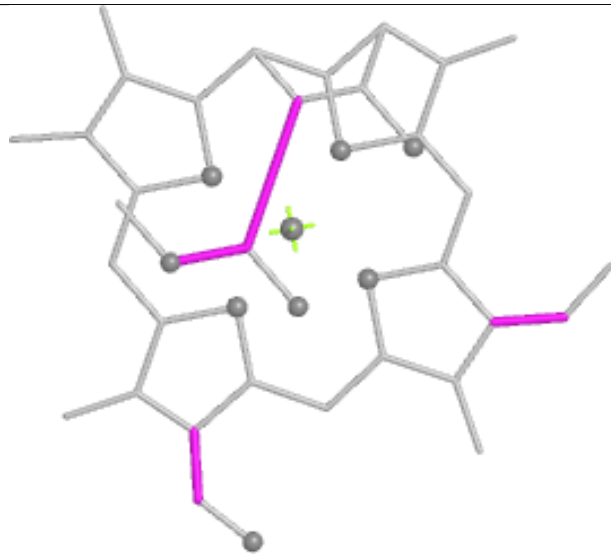
Ligand CL7 14 416



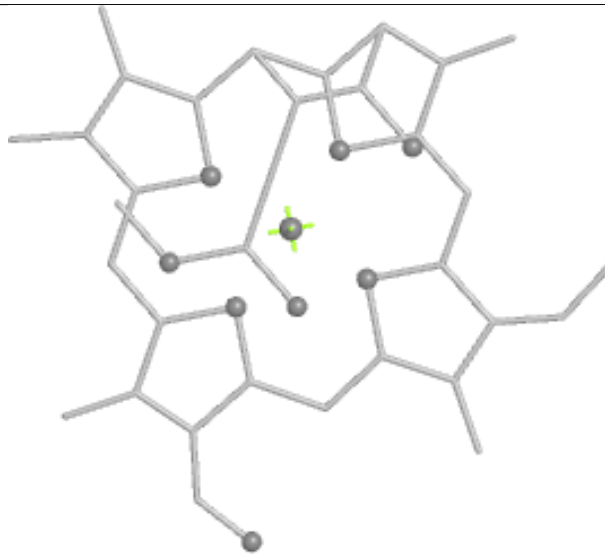
Bond lengths



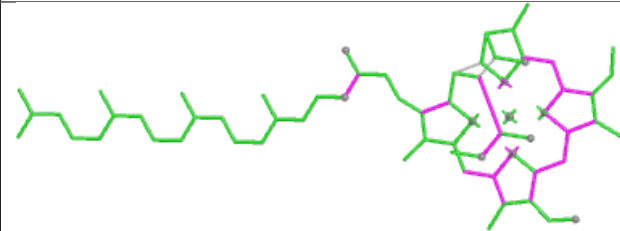
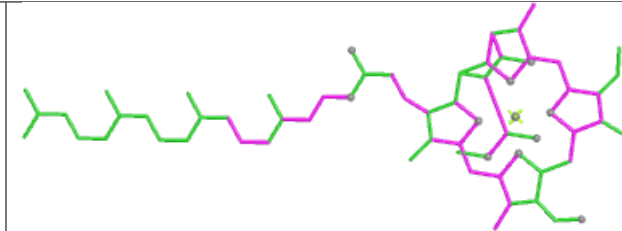
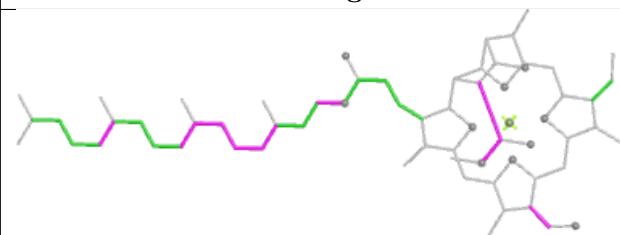
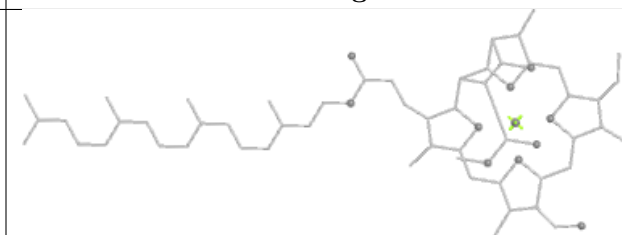
Bond angles

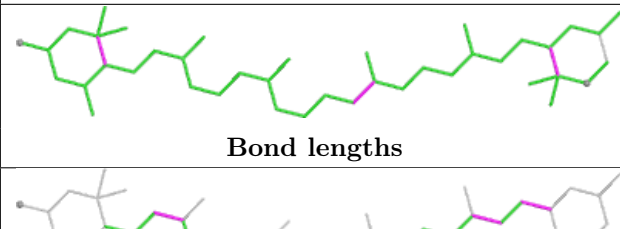
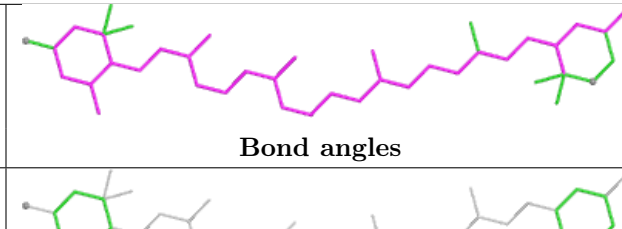
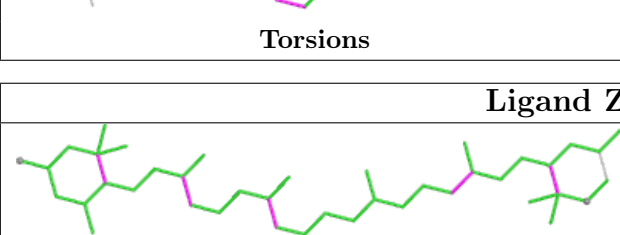


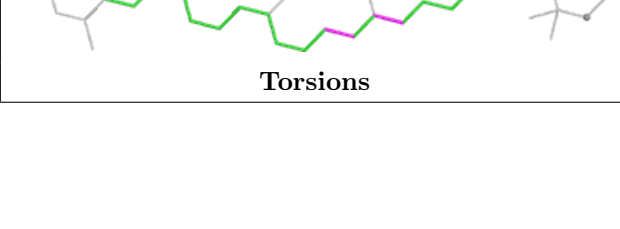
Torsions

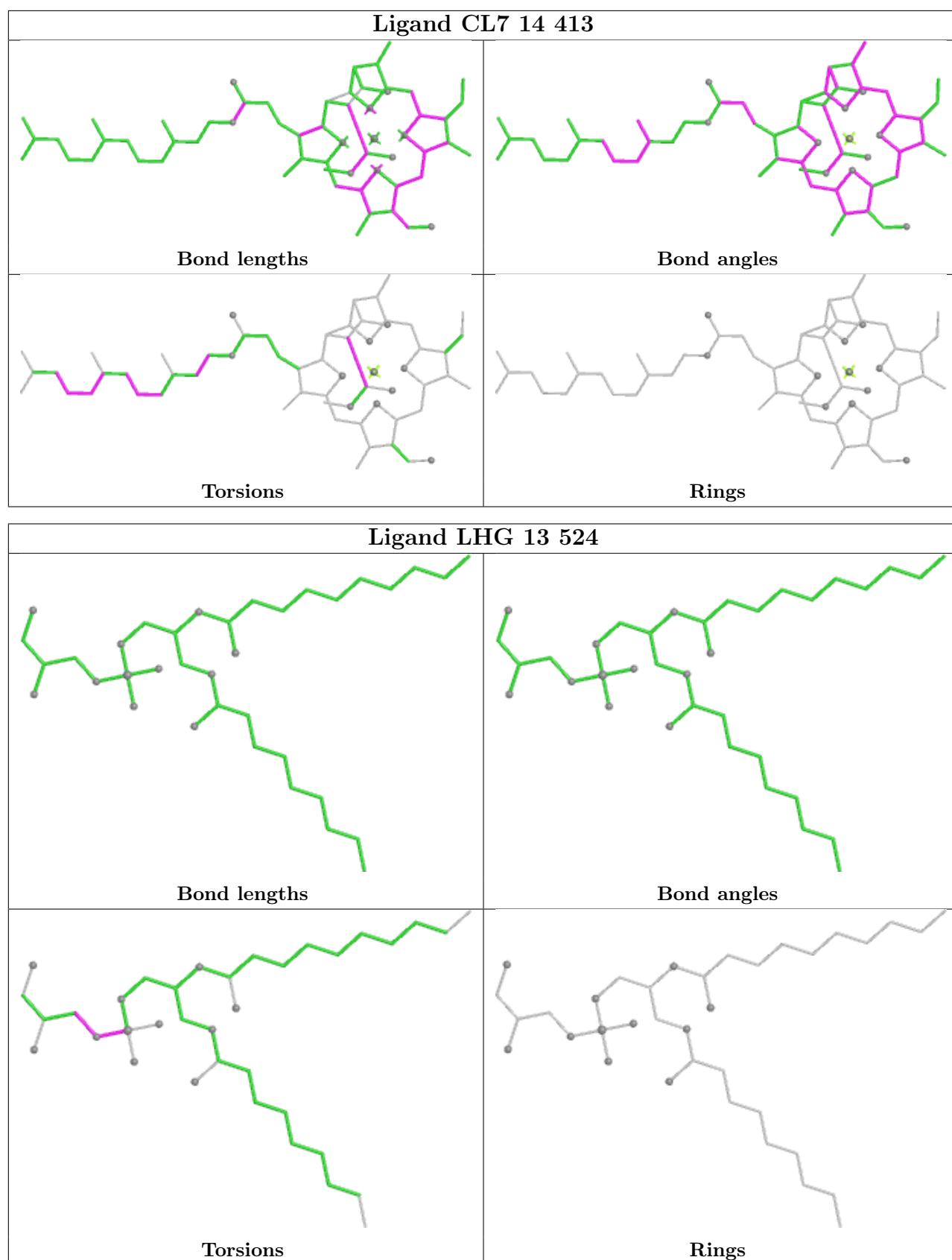


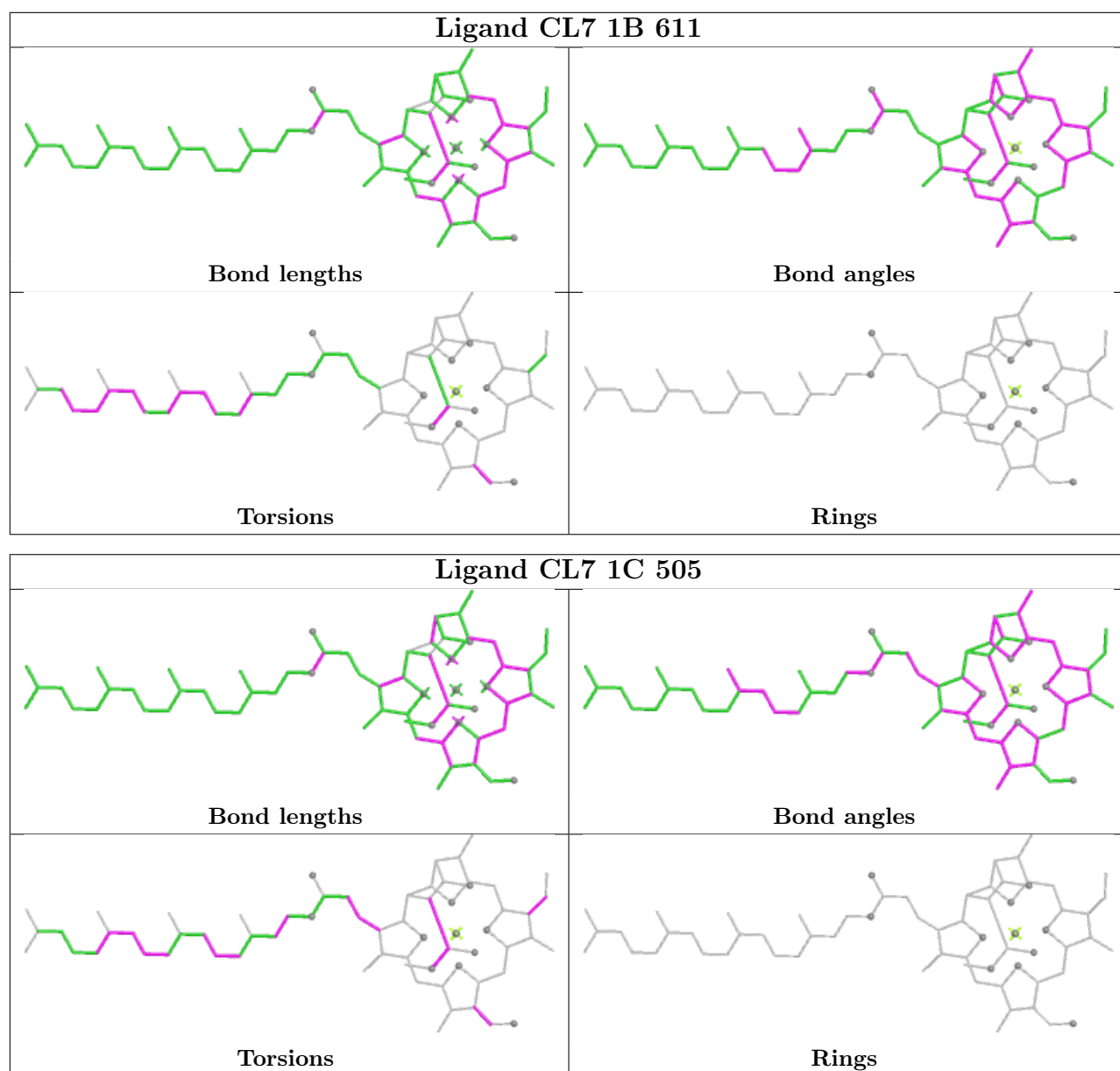
Rings

Ligand CL7 43 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

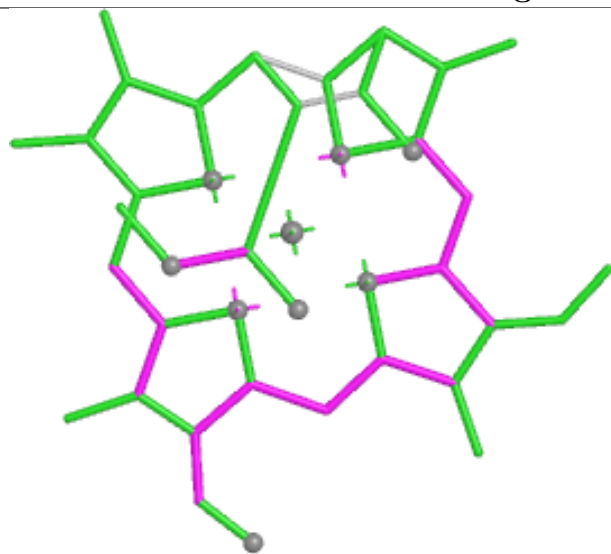
Ligand ZEX 14 419	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ZEX 43 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

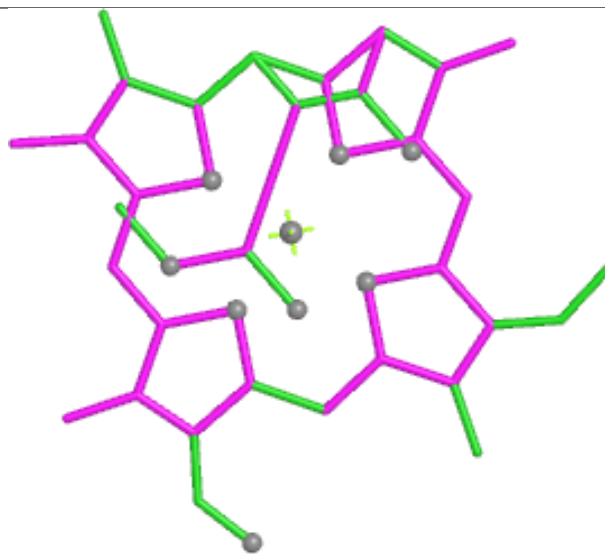




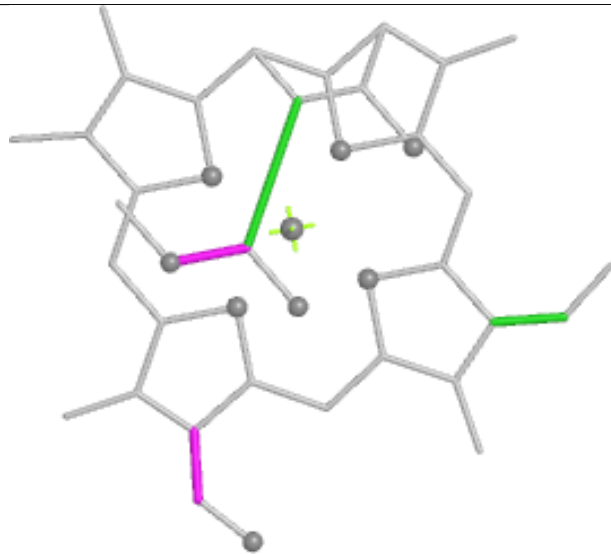
Ligand CL7 21 407



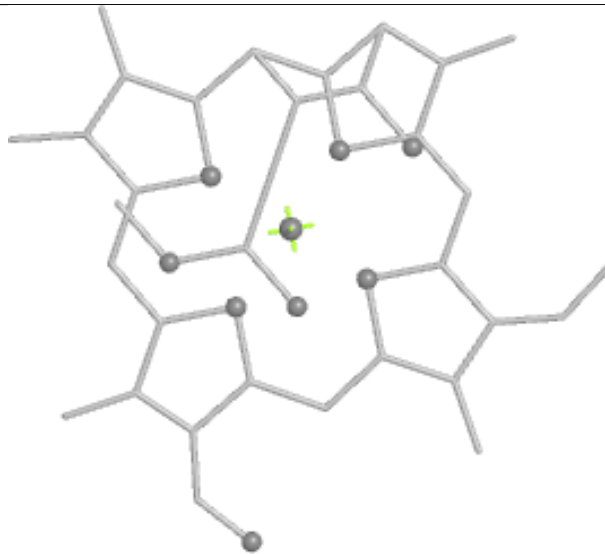
Bond lengths



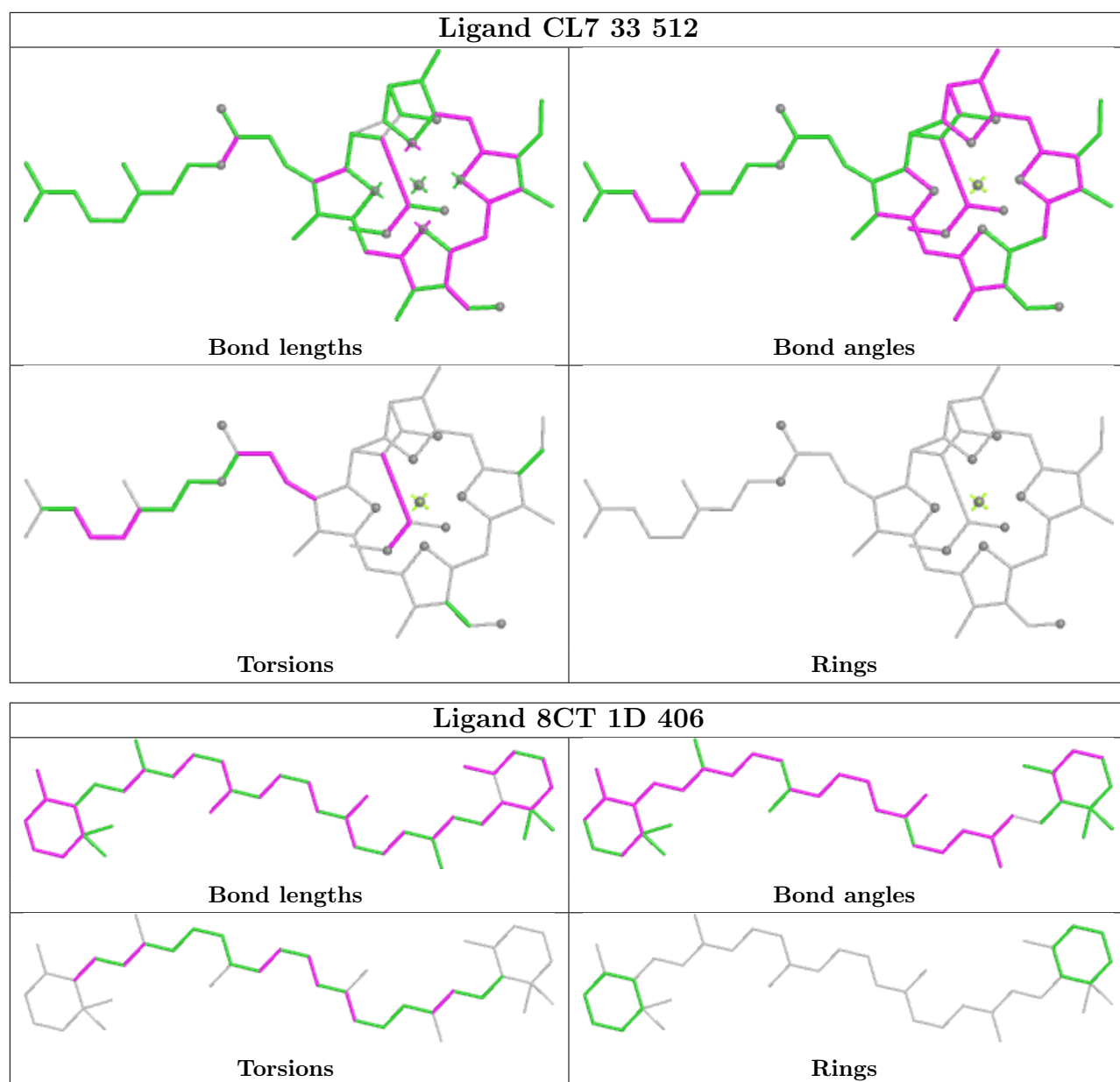
Bond angles



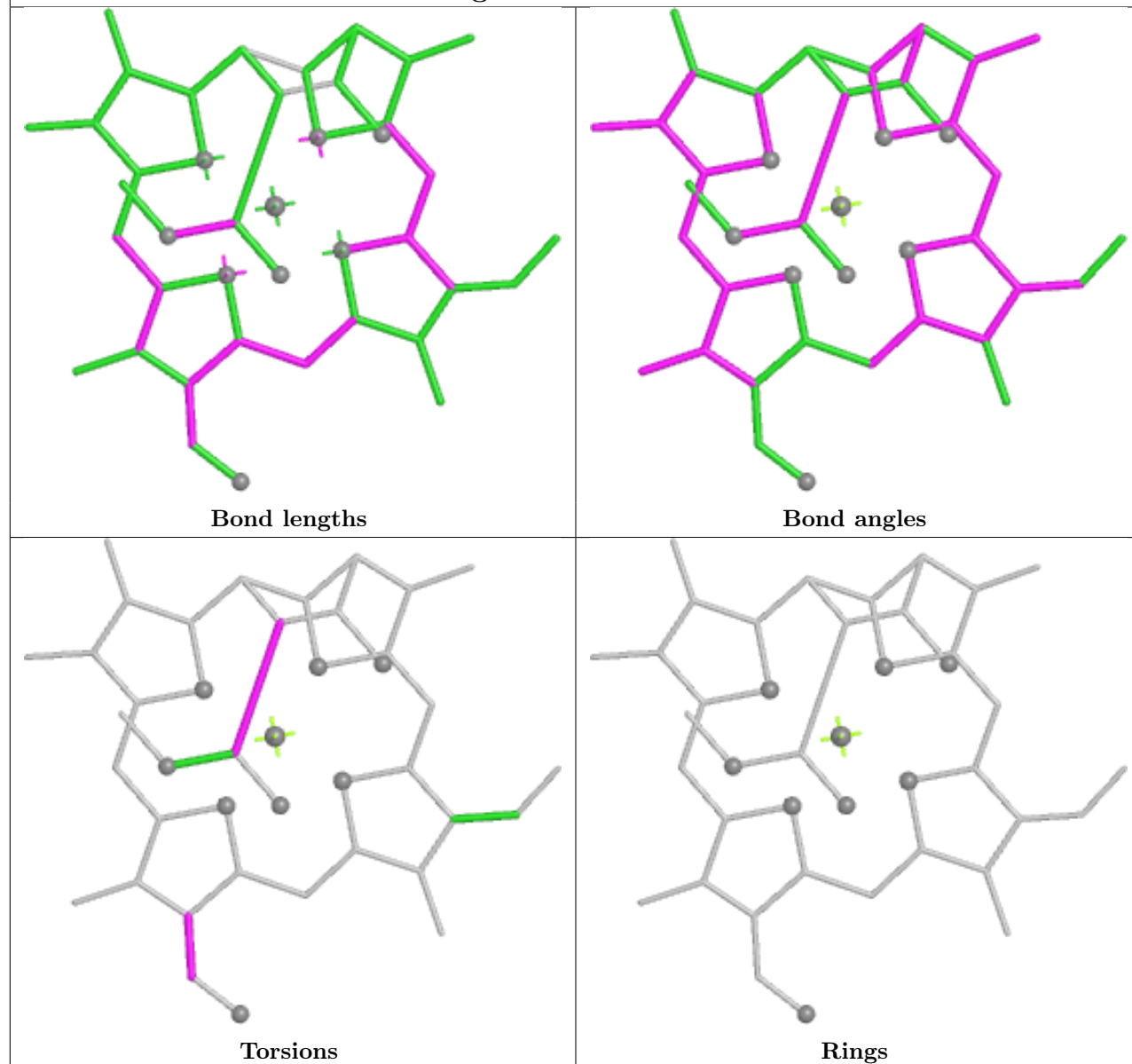
Torsions



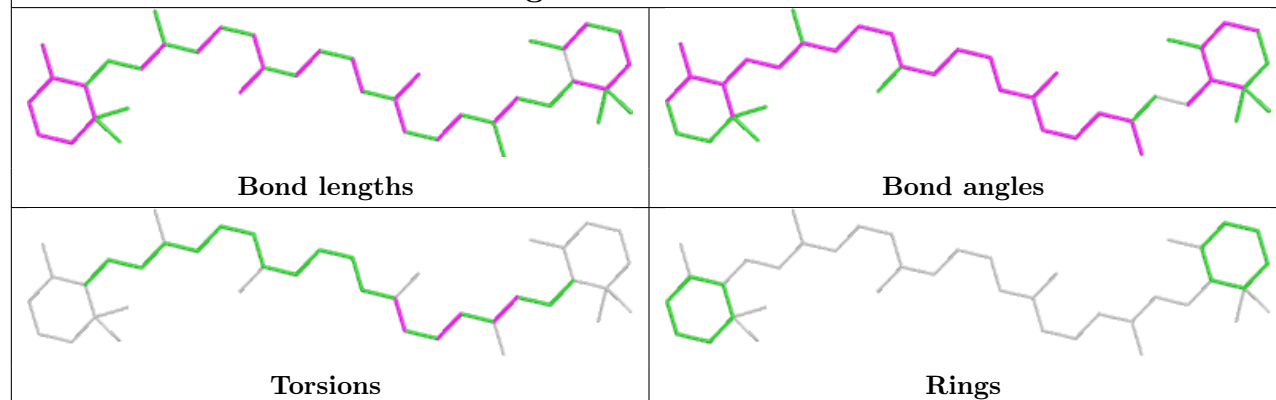
Rings

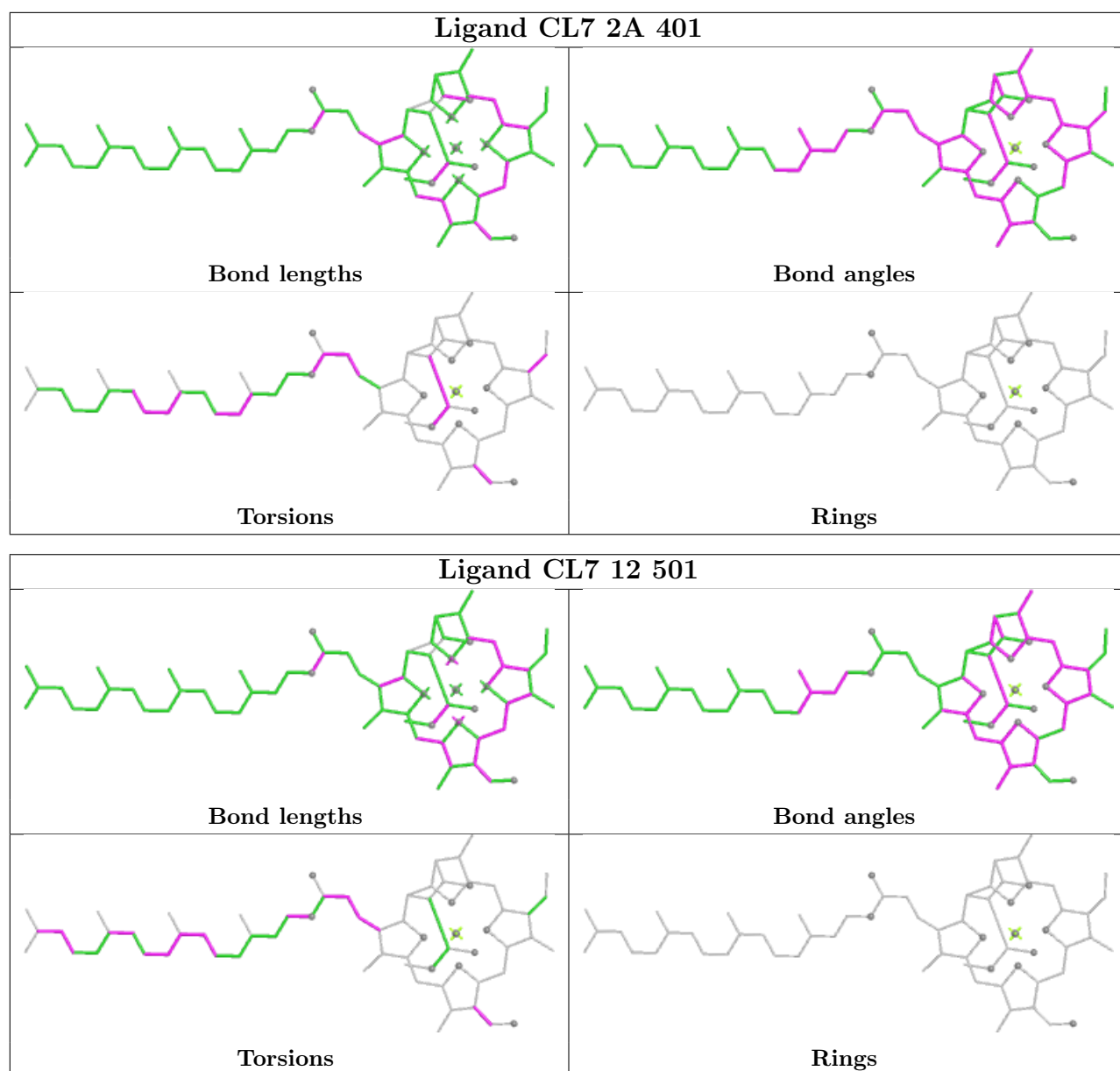


Ligand CL7 24 407

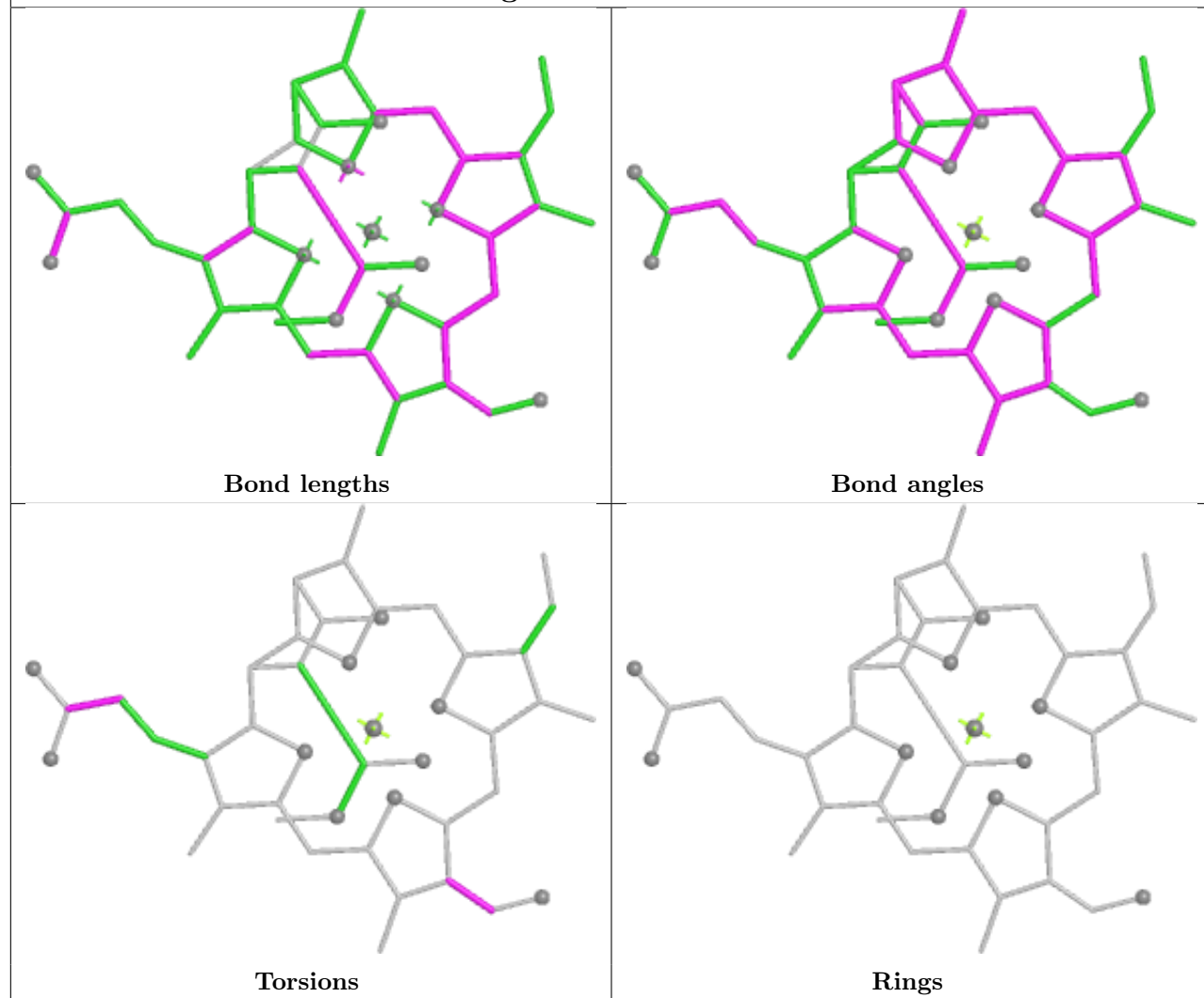


Ligand 8CT 3A 404

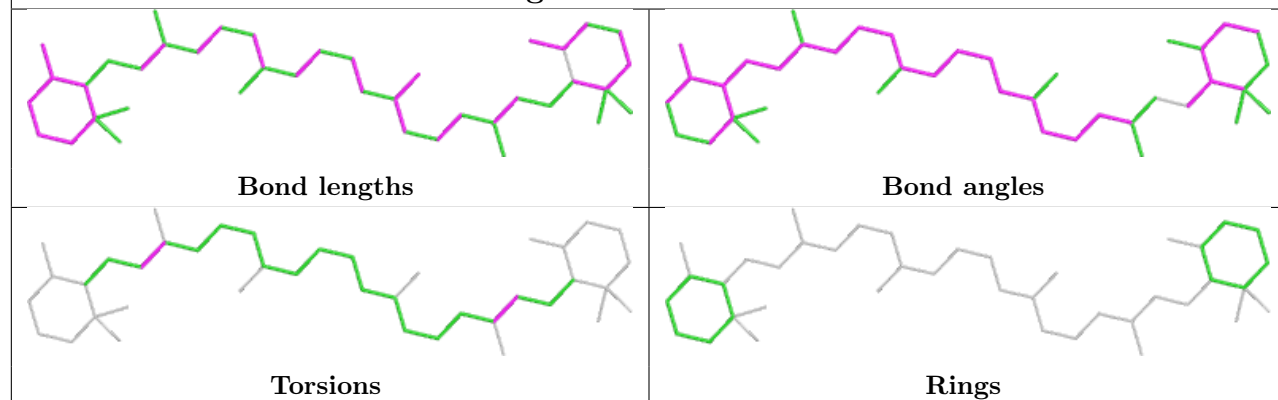


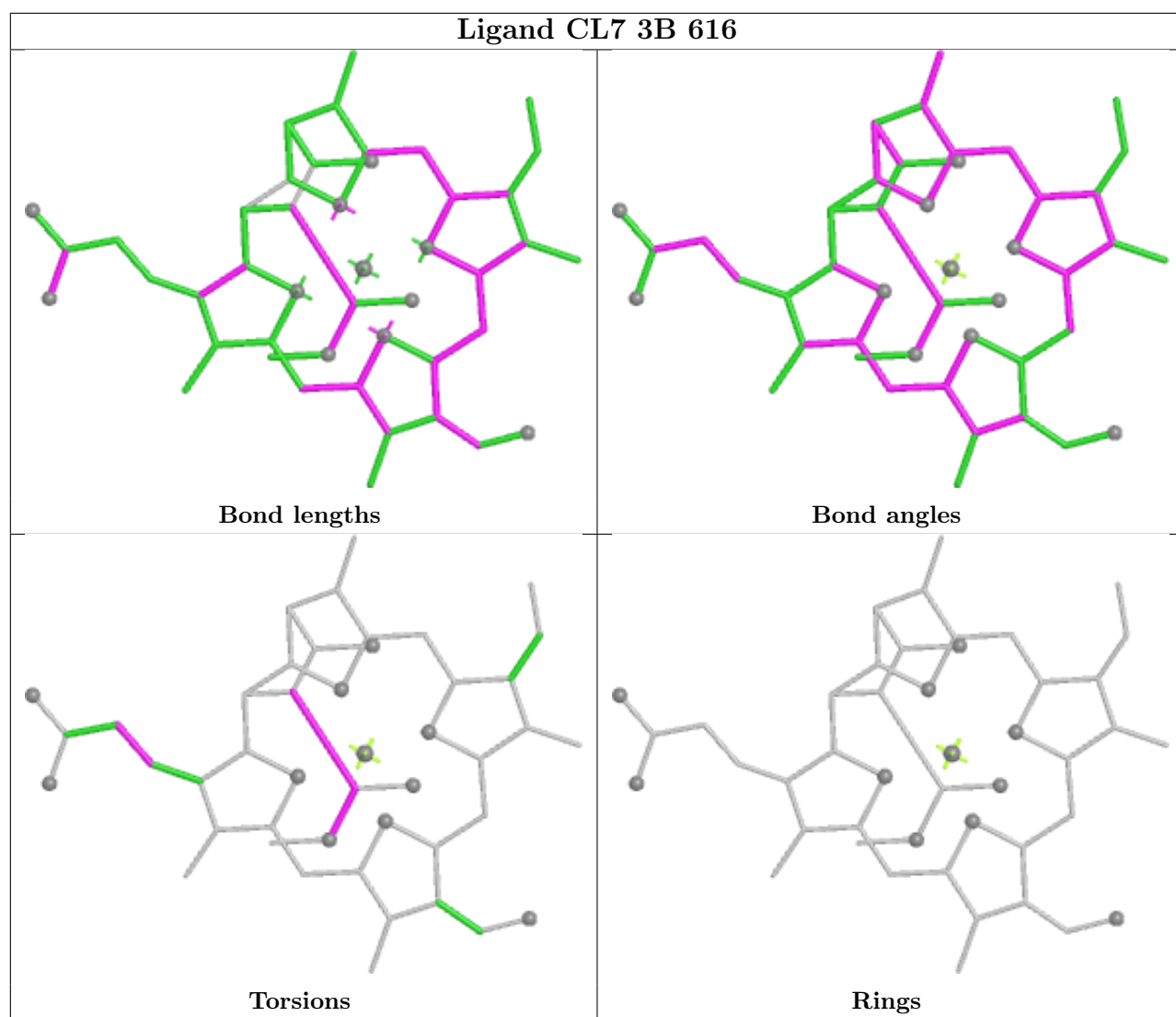


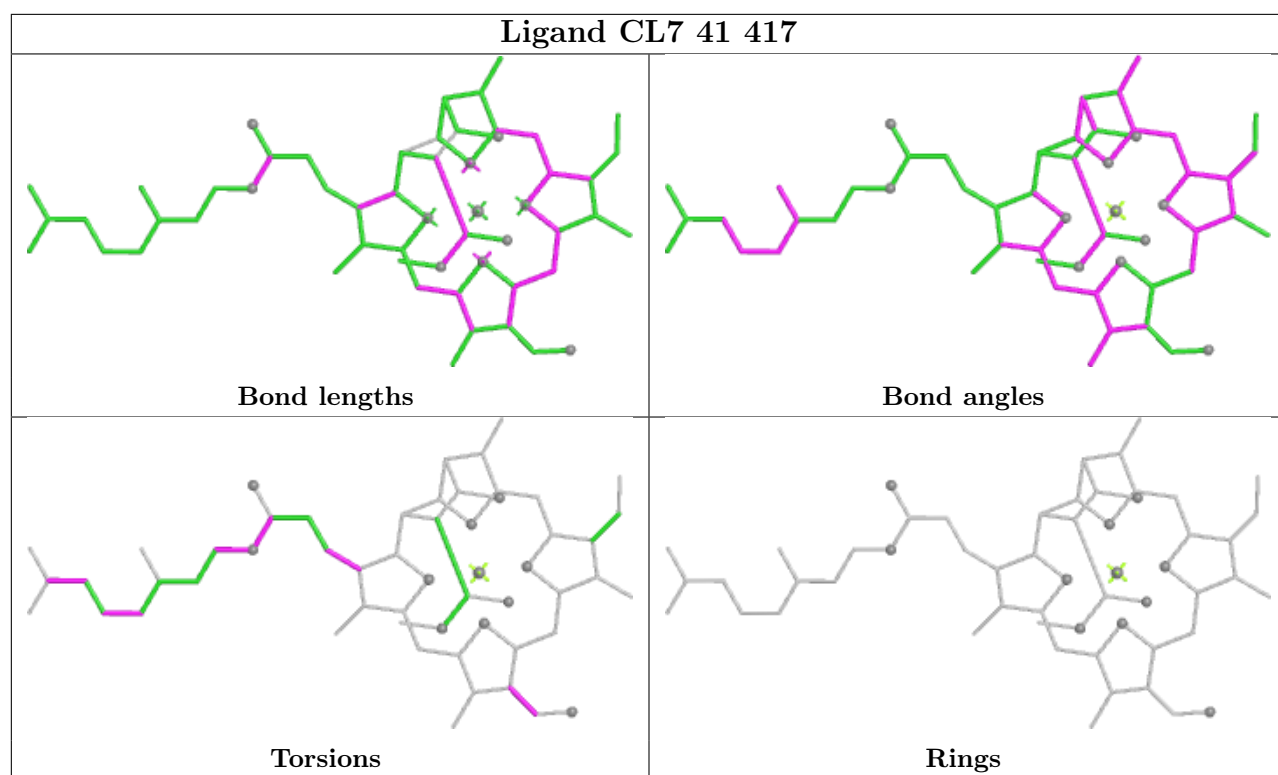
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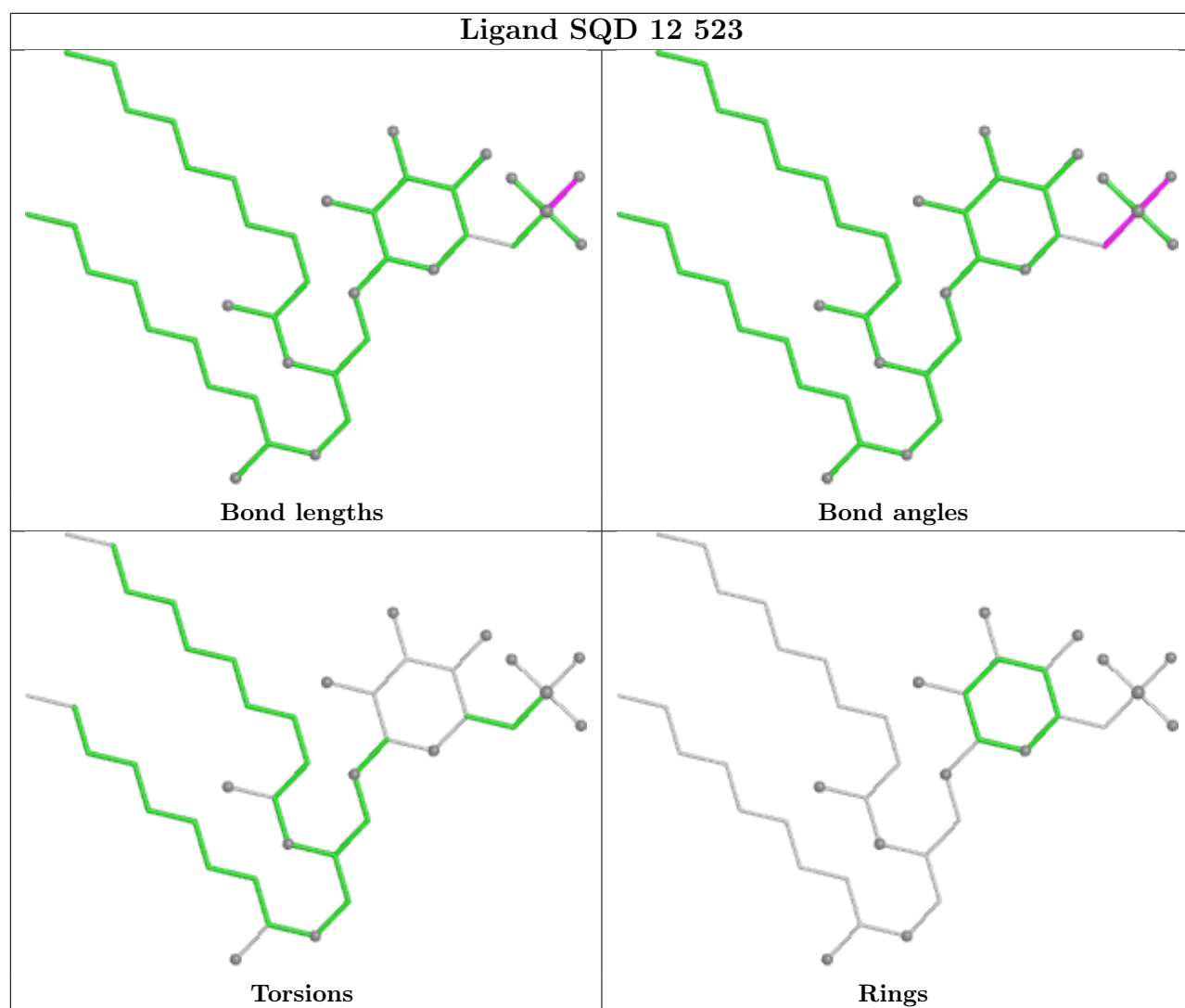


Ligand 8CT 2B 620

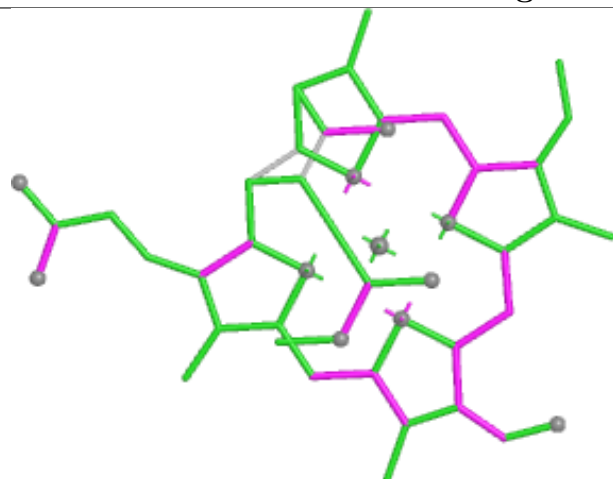




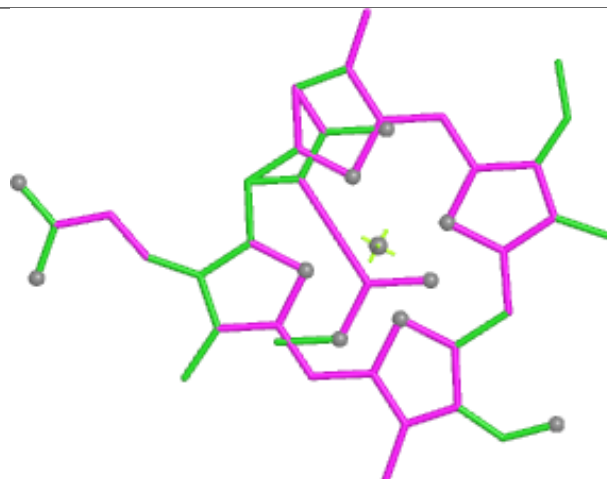




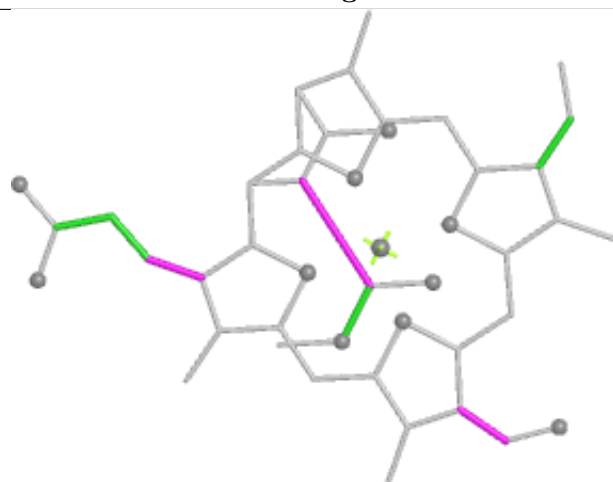
Ligand CL7 22 515



Bond lengths



Bond angles

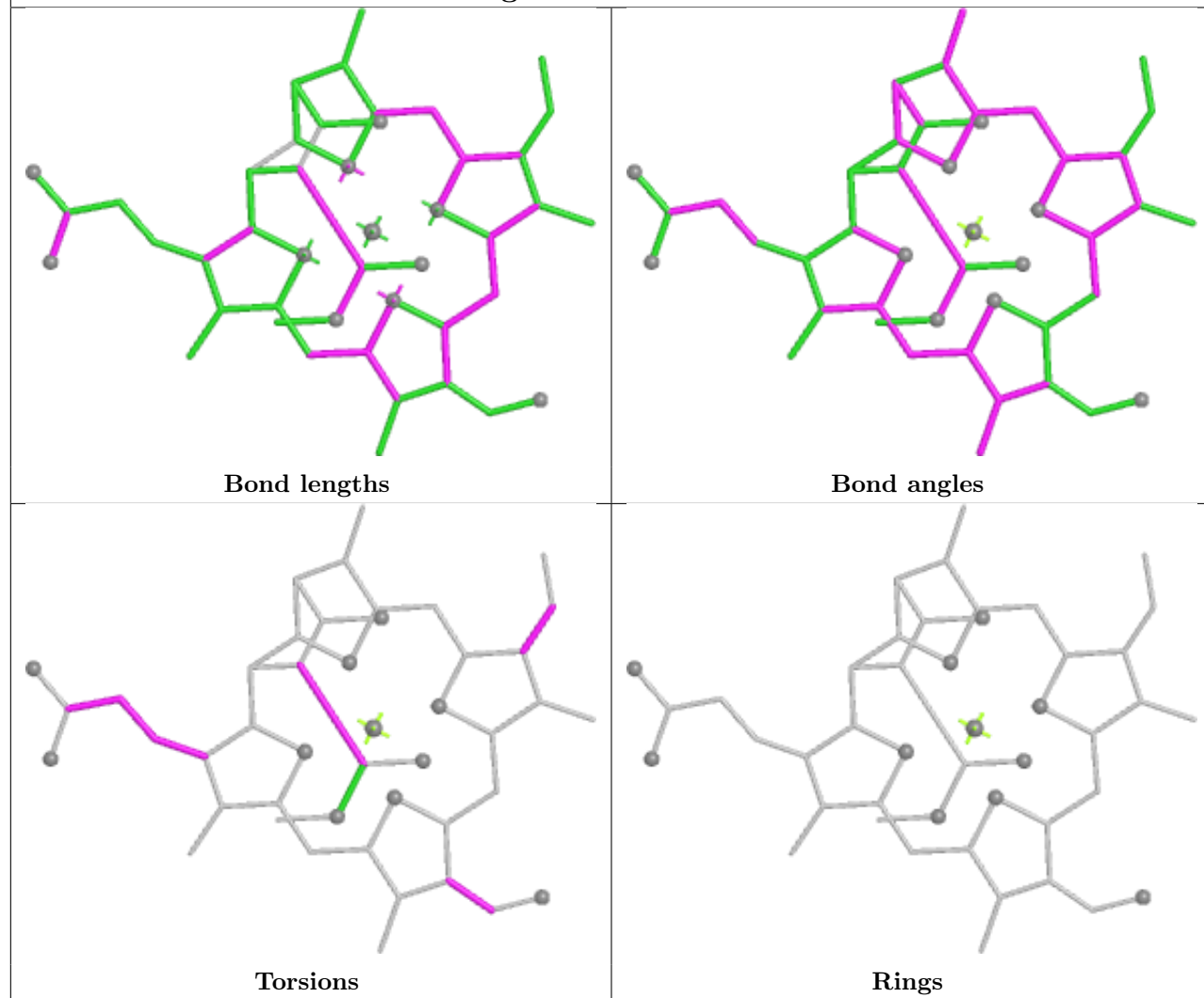


Torsions

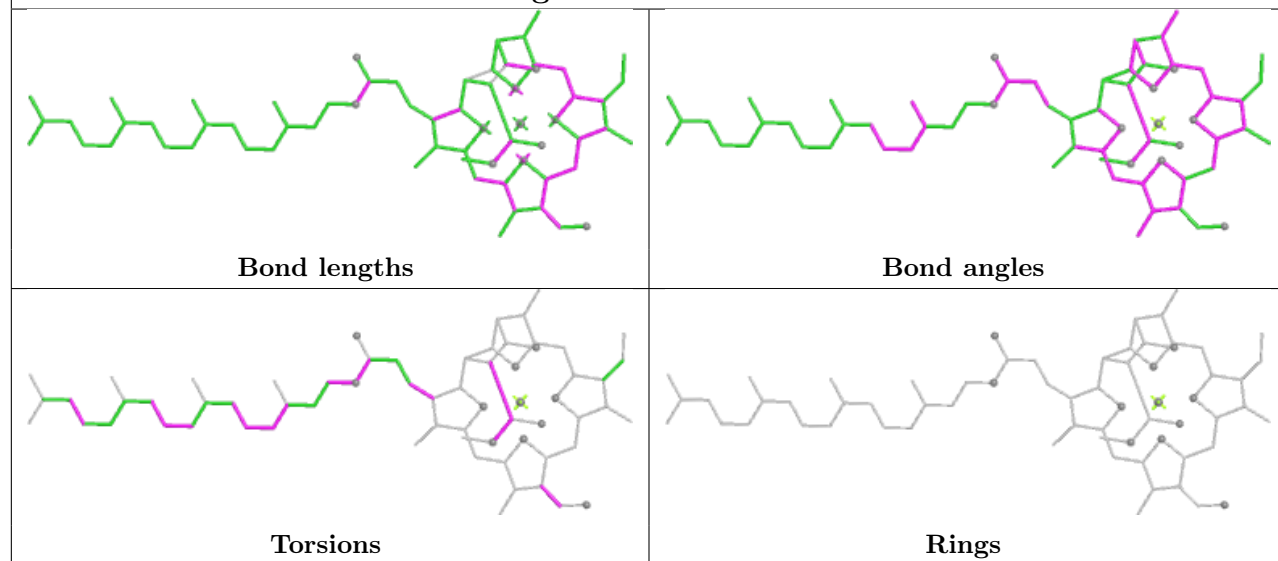


Rings

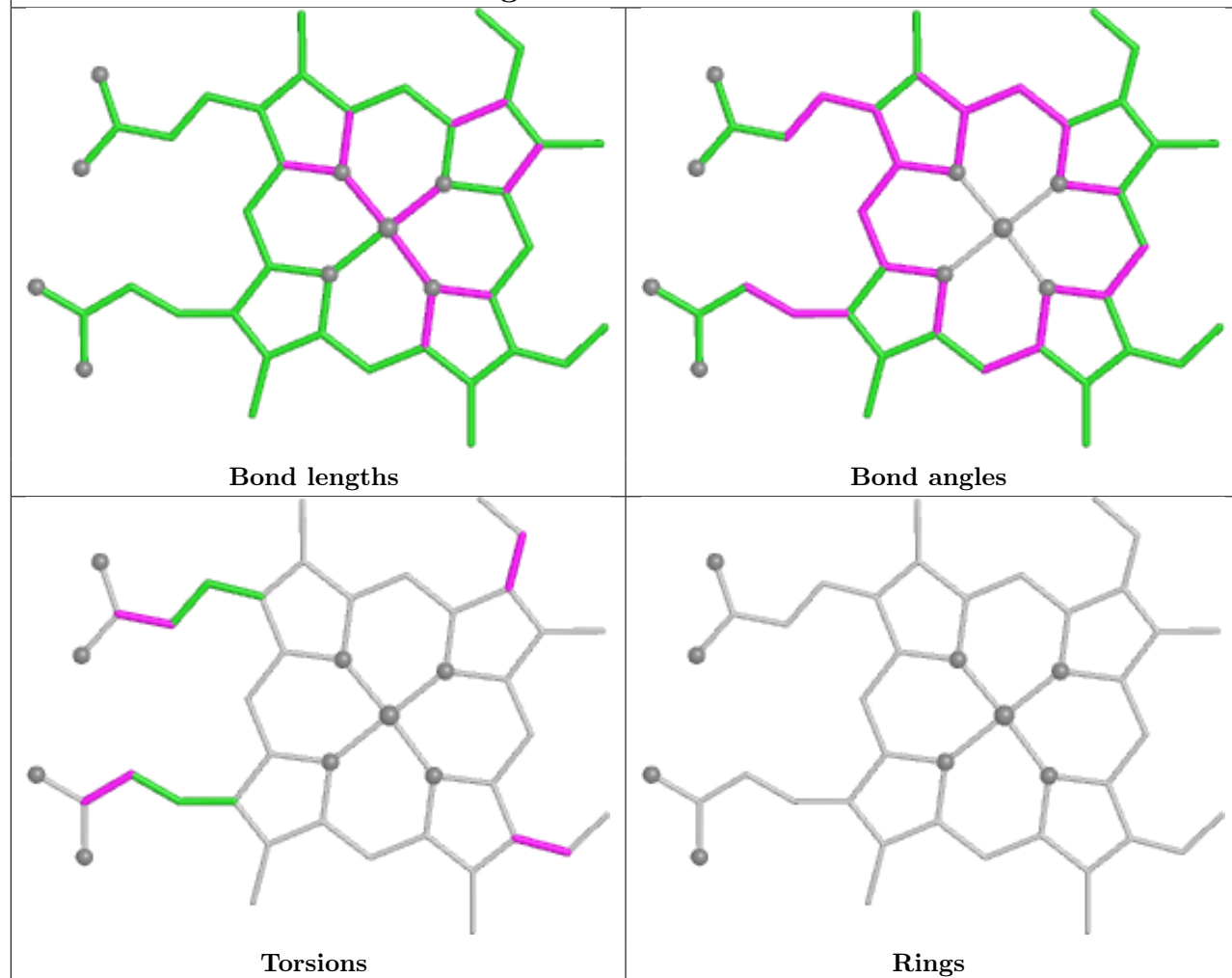
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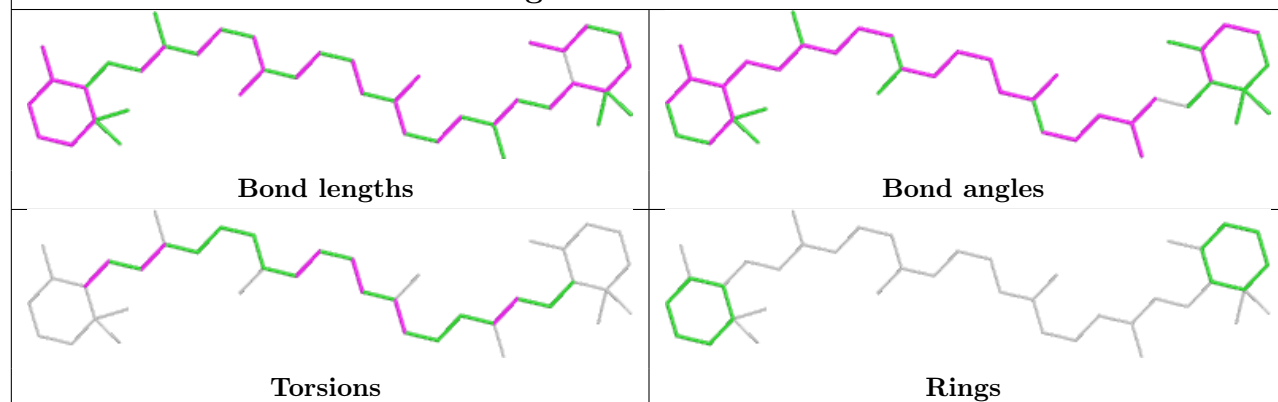
Ligand CL7 31 410

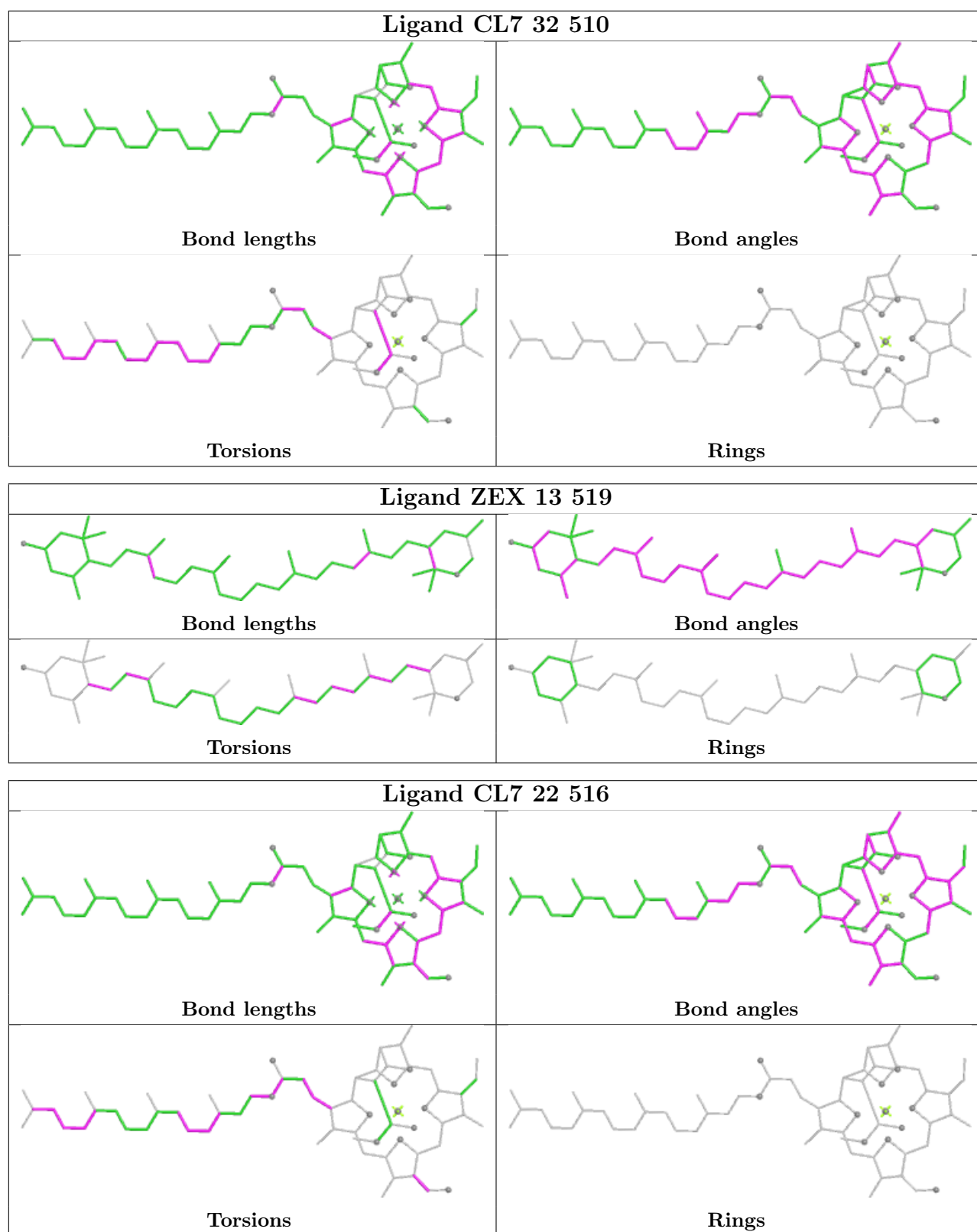


Ligand HEM 2F 101

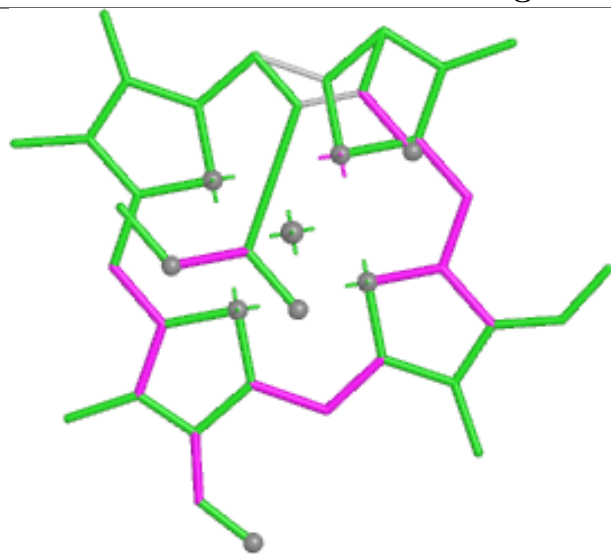


Ligand 8CT 3D 406

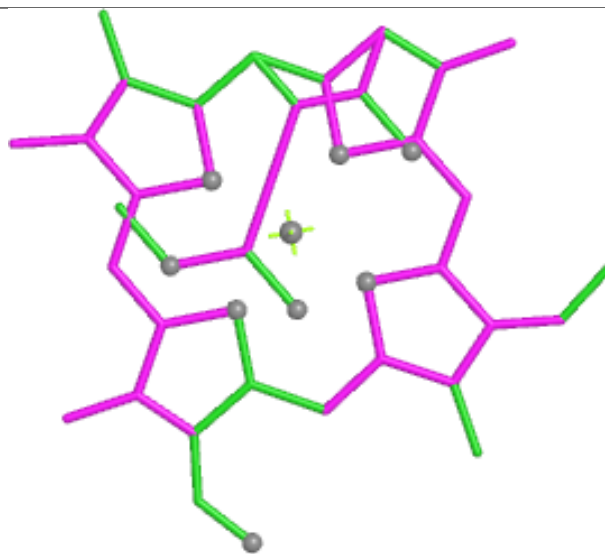




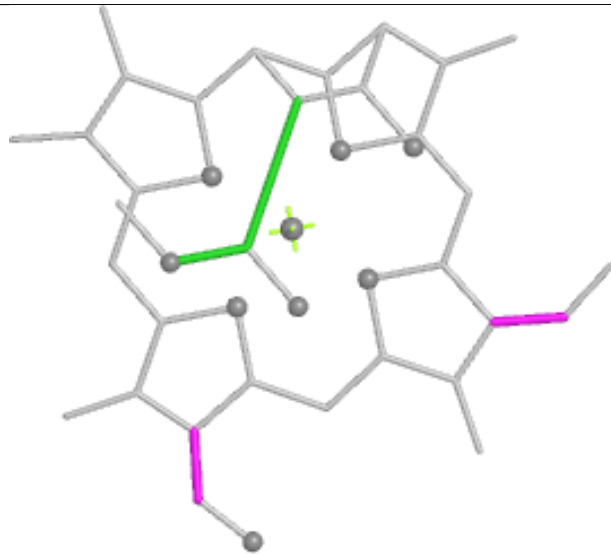
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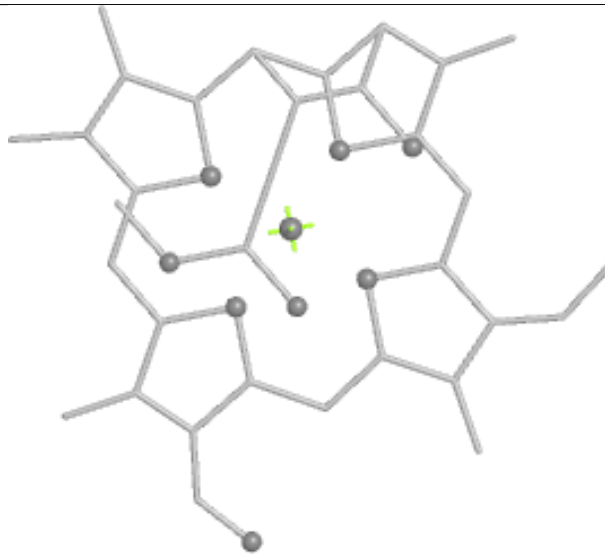
Bond lengths



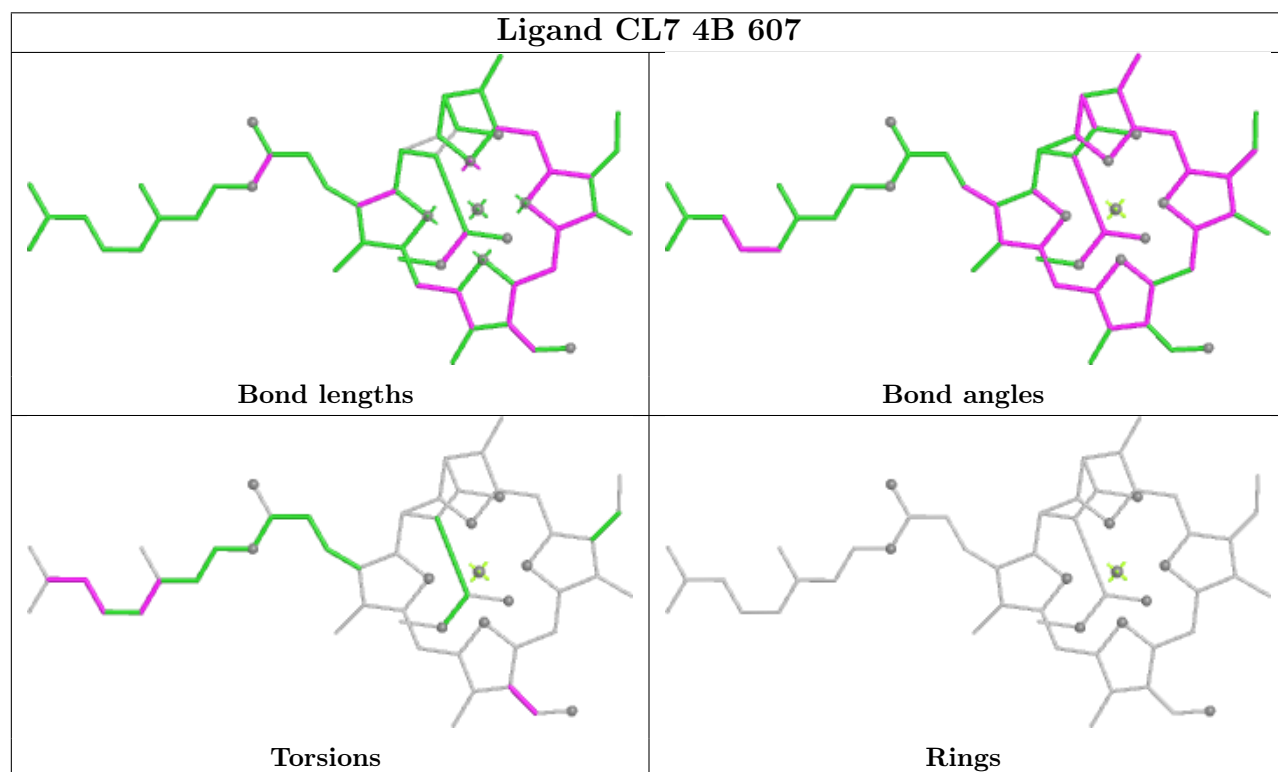
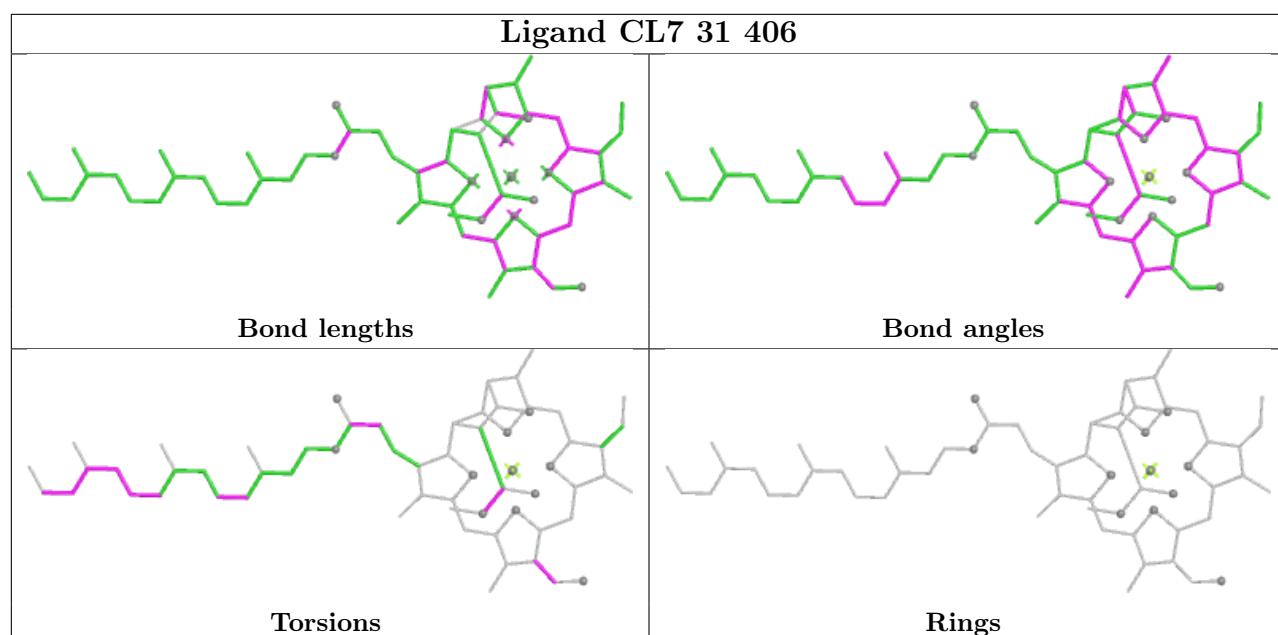
Bond angles



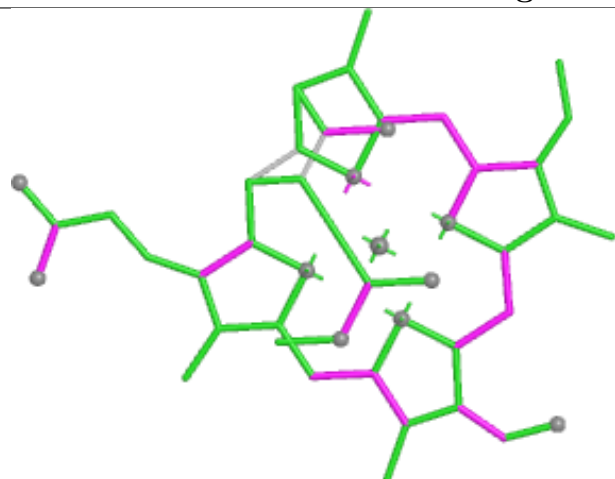
Torsions



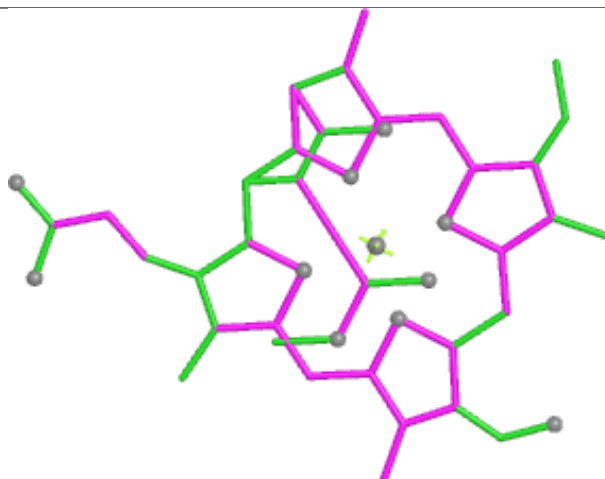
Rings



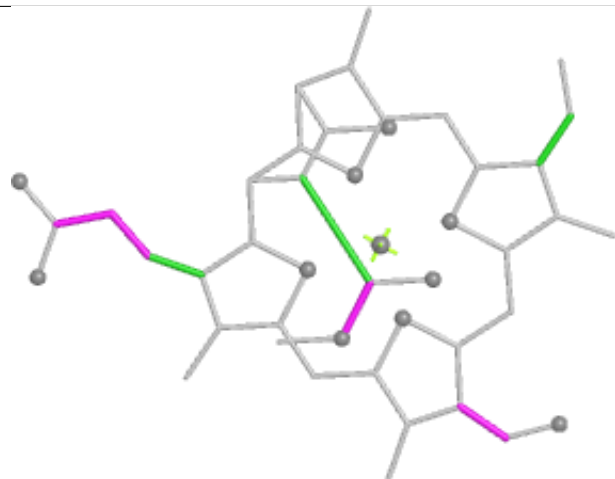
Ligand CL7 13 518



Bond lengths



Bond angles

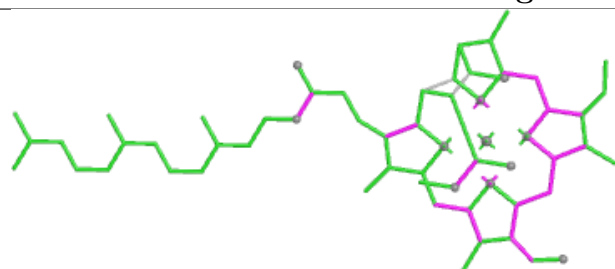


Torsions

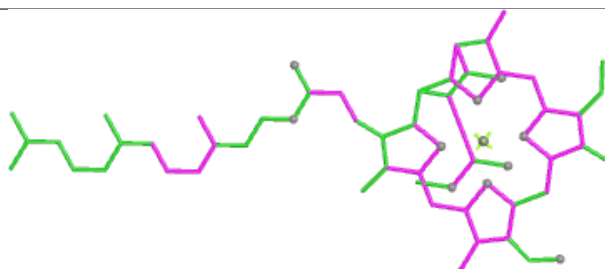


Rings

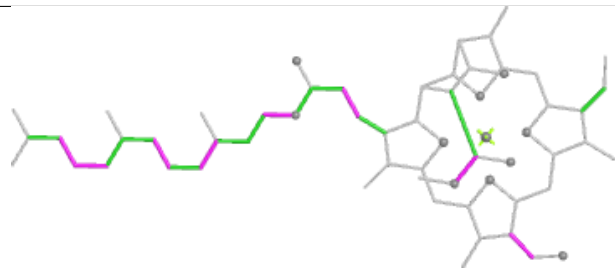
Ligand CL7 21 403



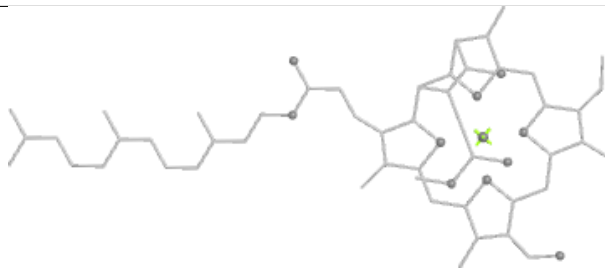
Bond lengths



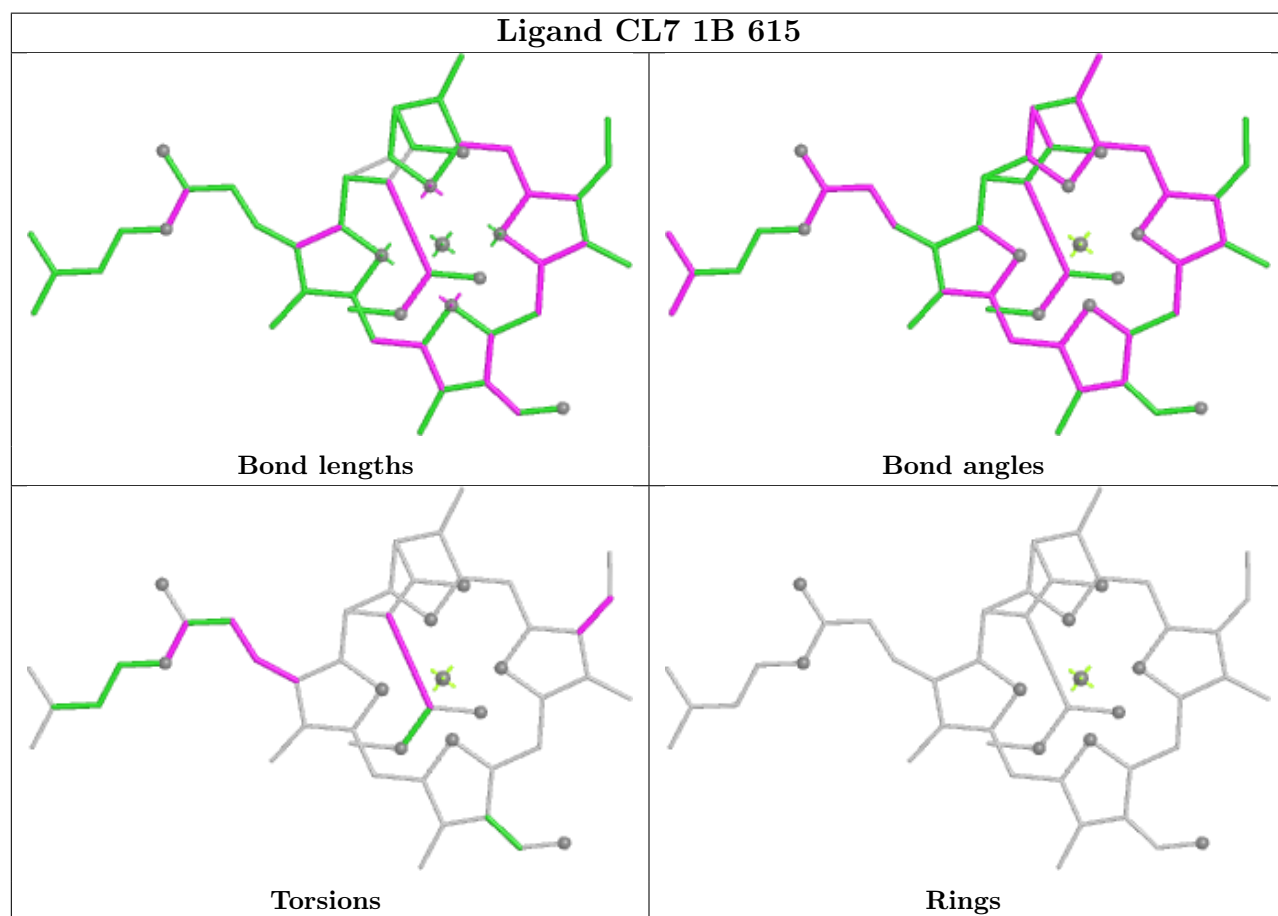
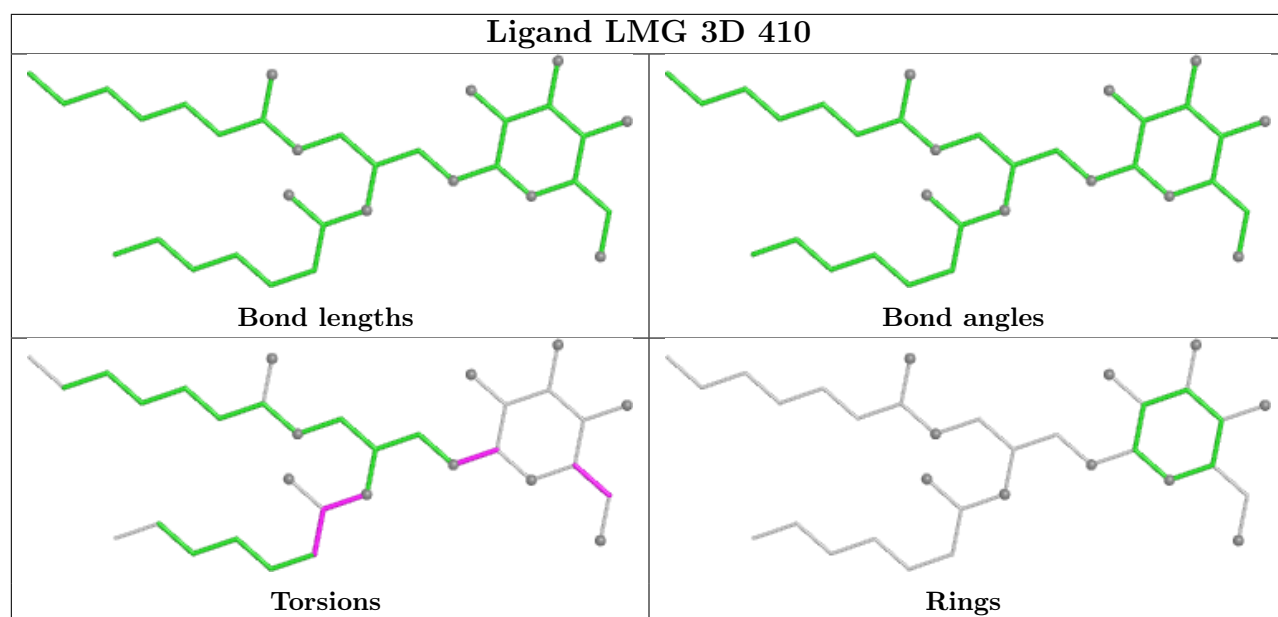
Bond angles

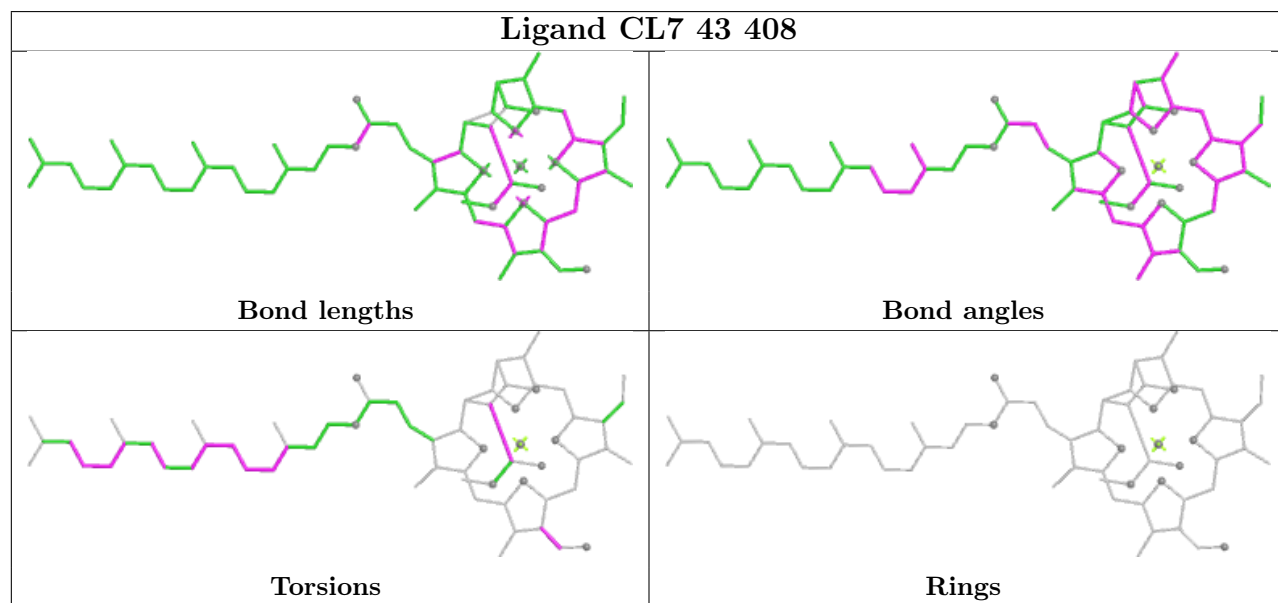
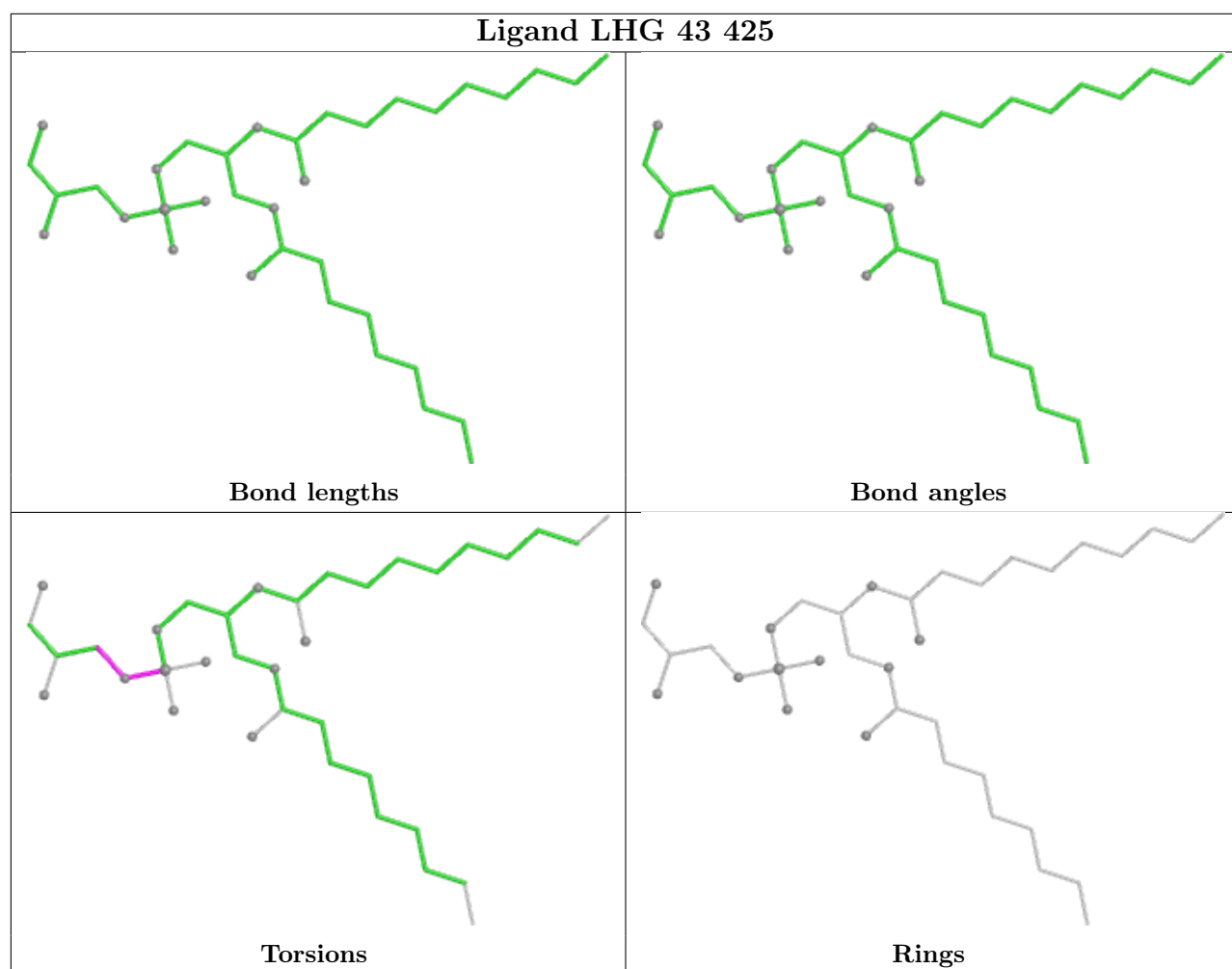


Torsions

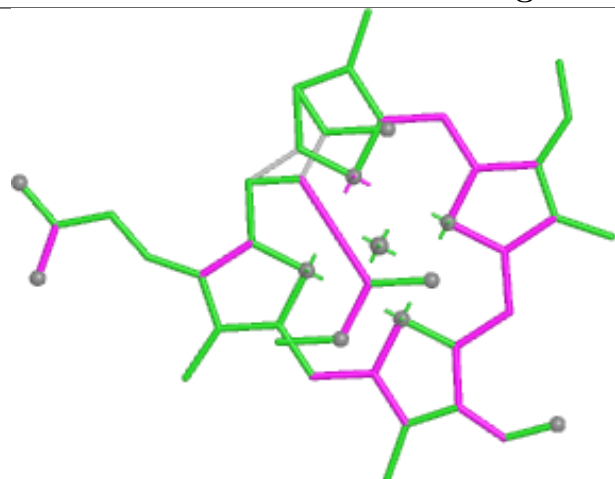


Rings

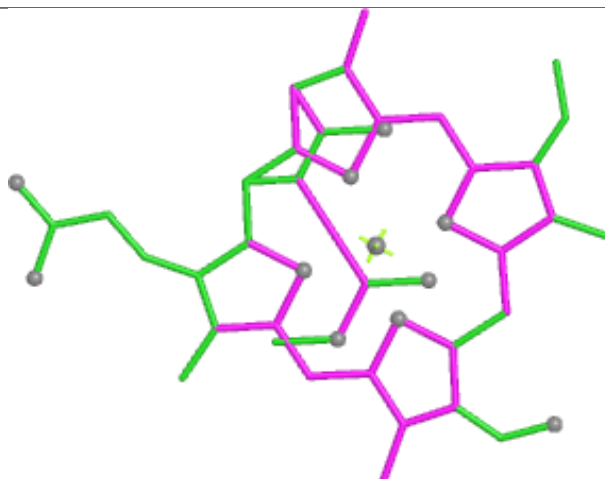




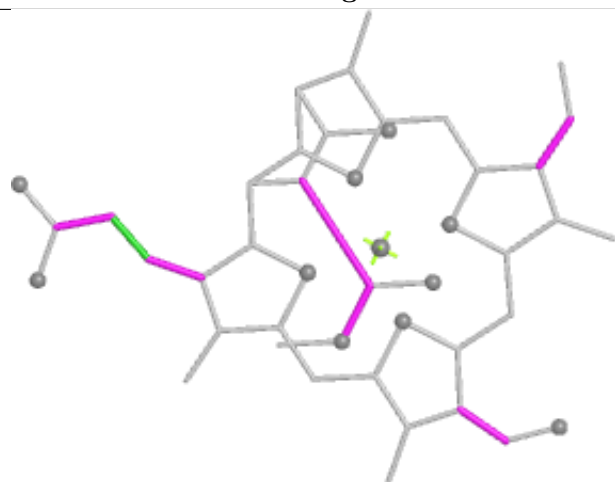
Ligand CL7 13 506



Bond lengths



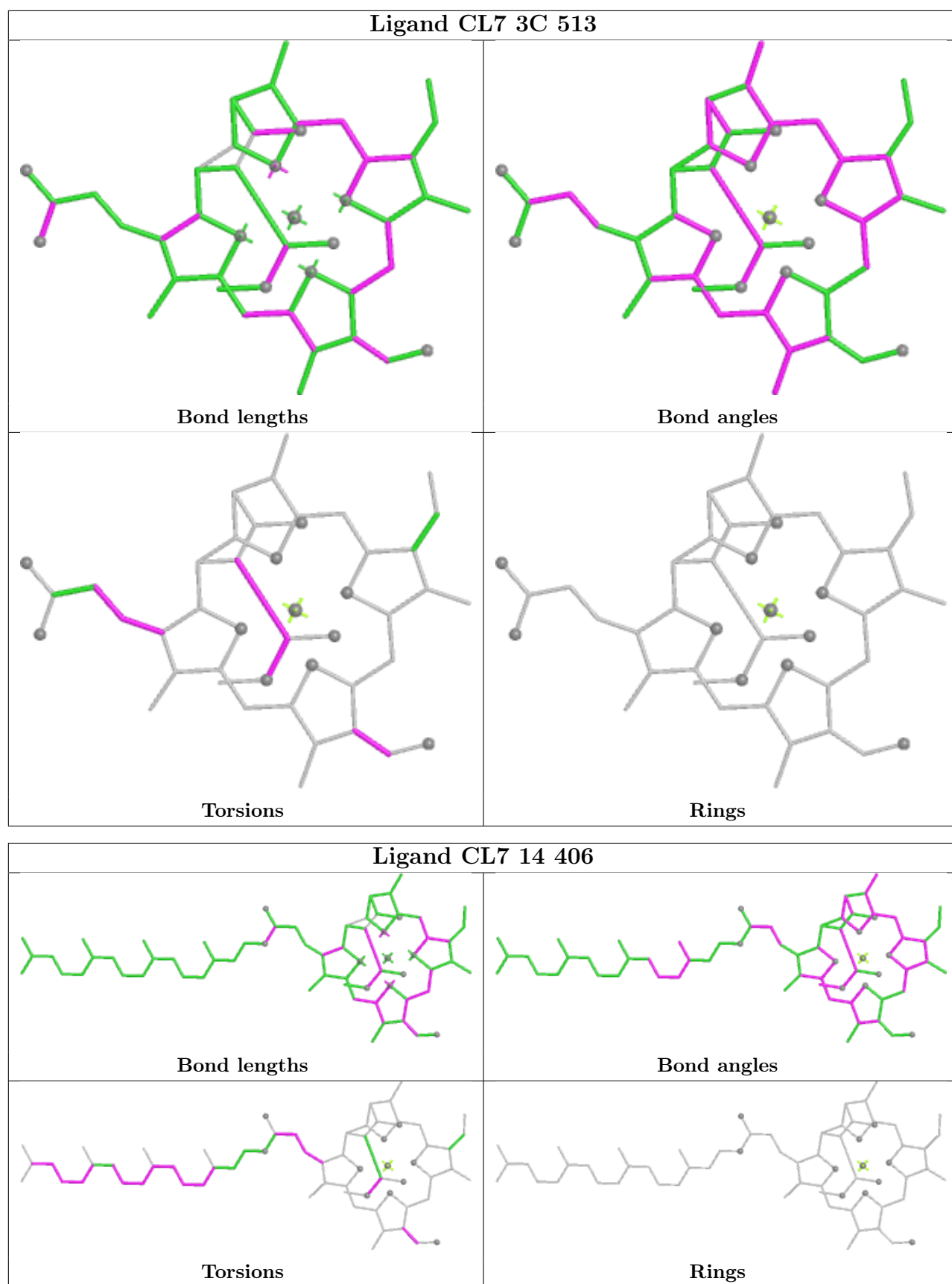
Bond angles

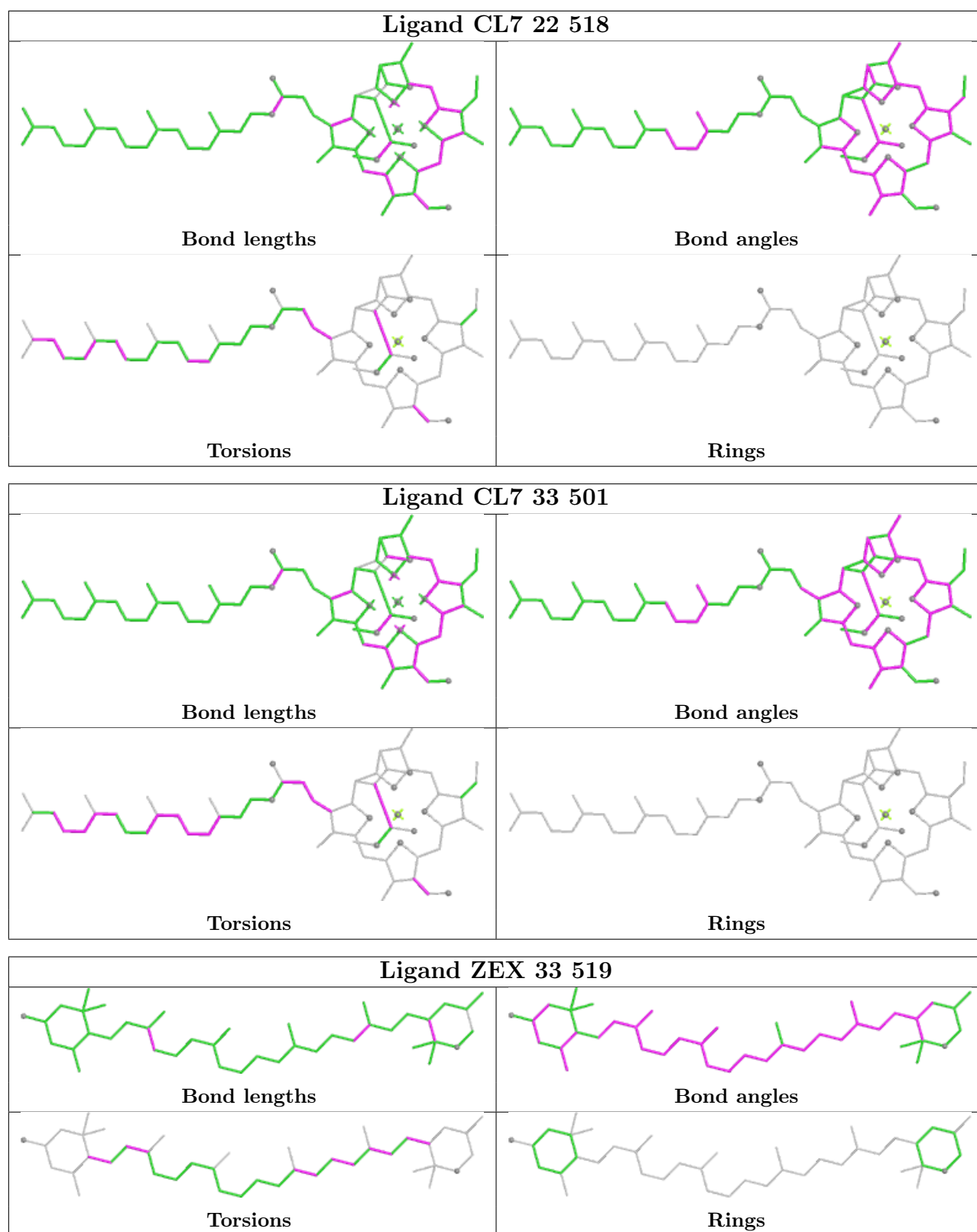


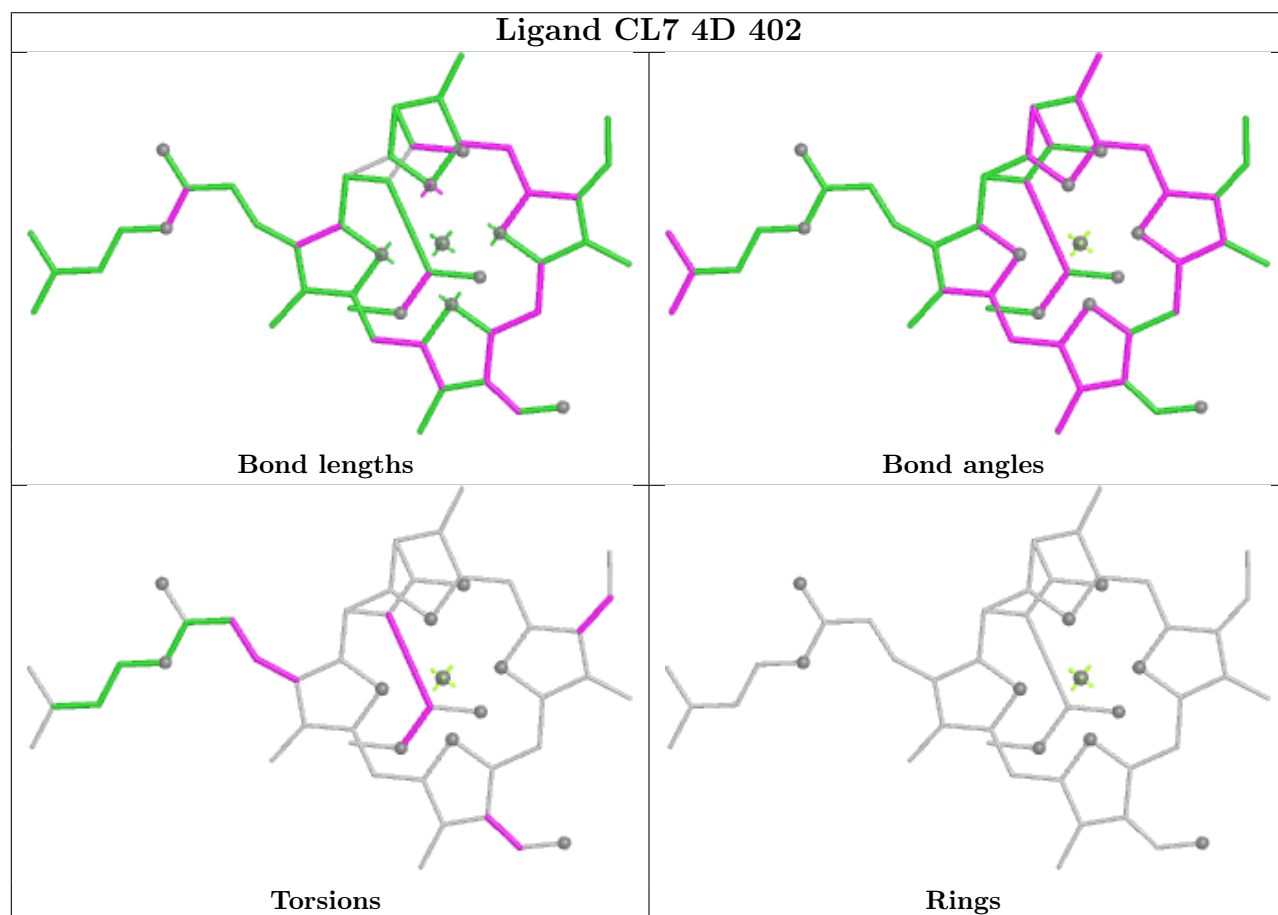
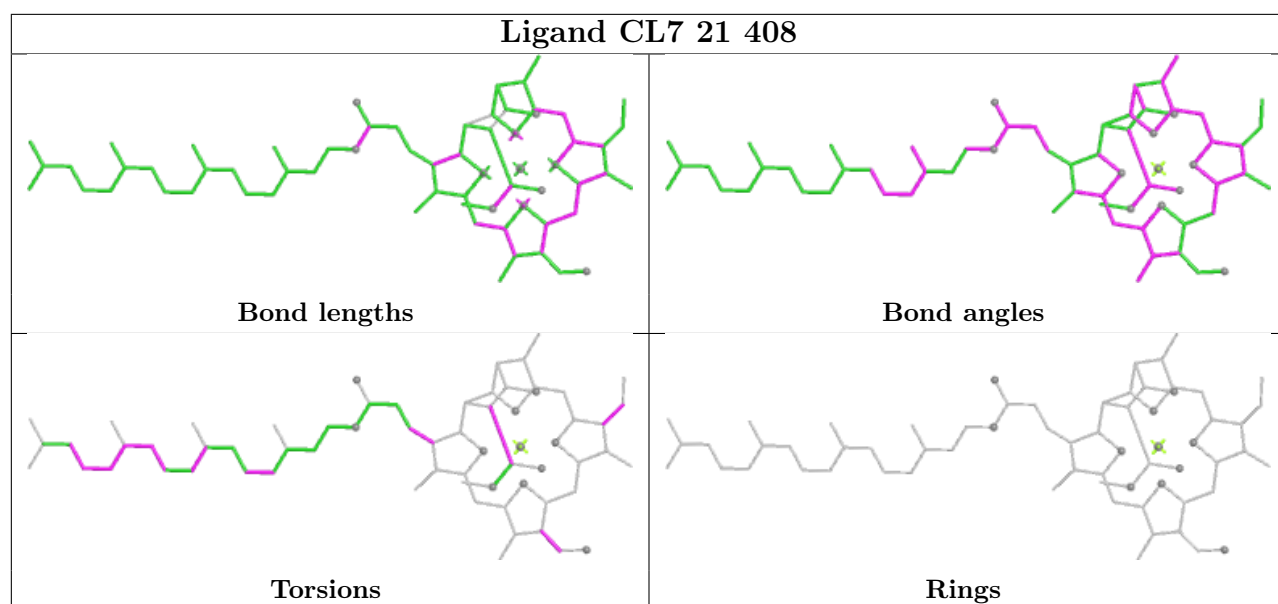
Torsions

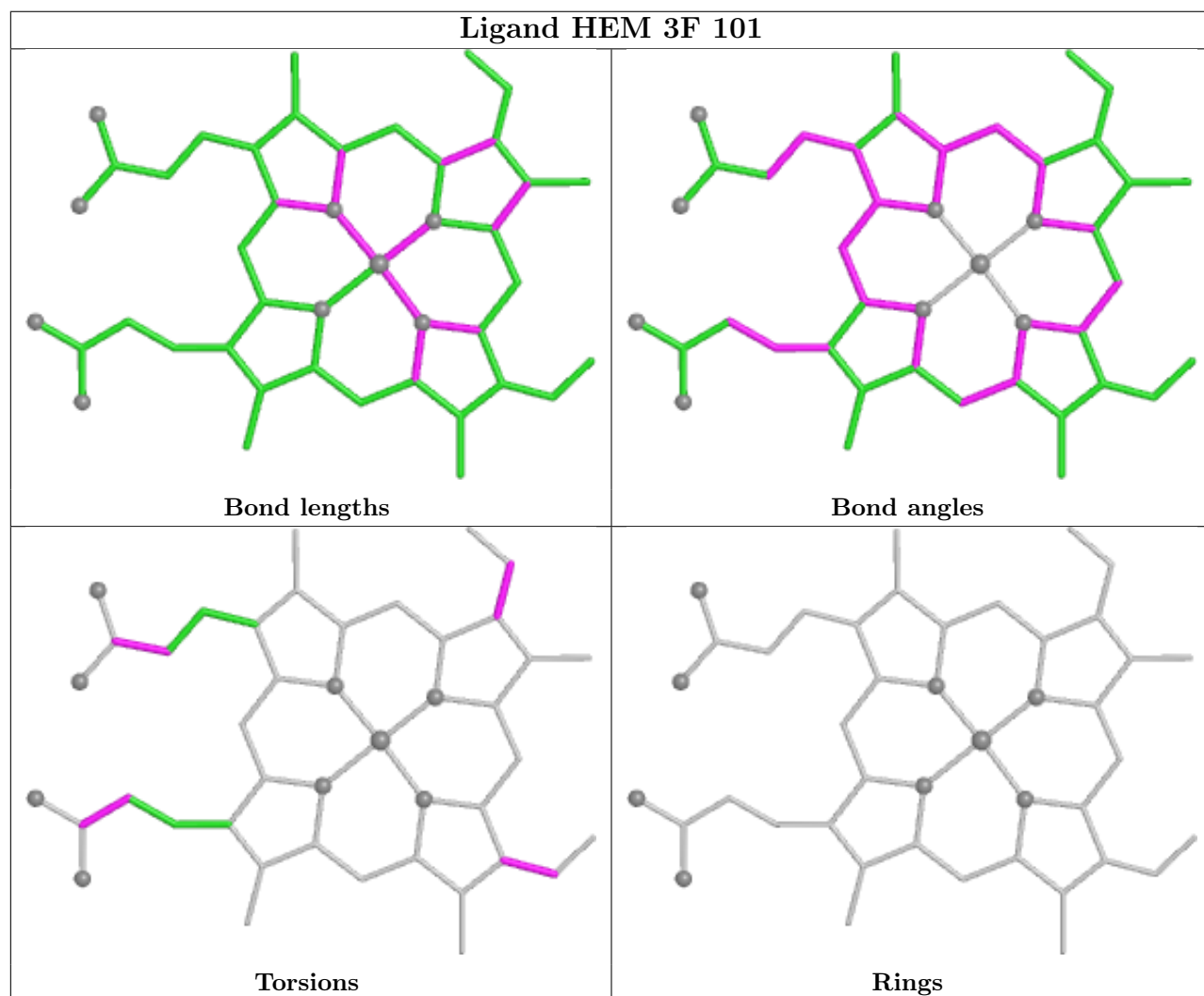
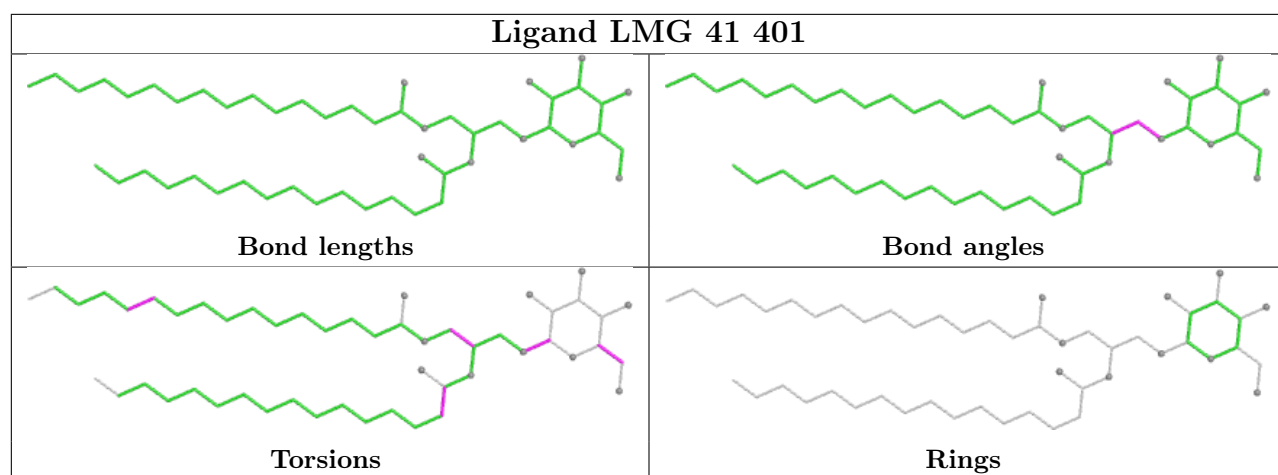


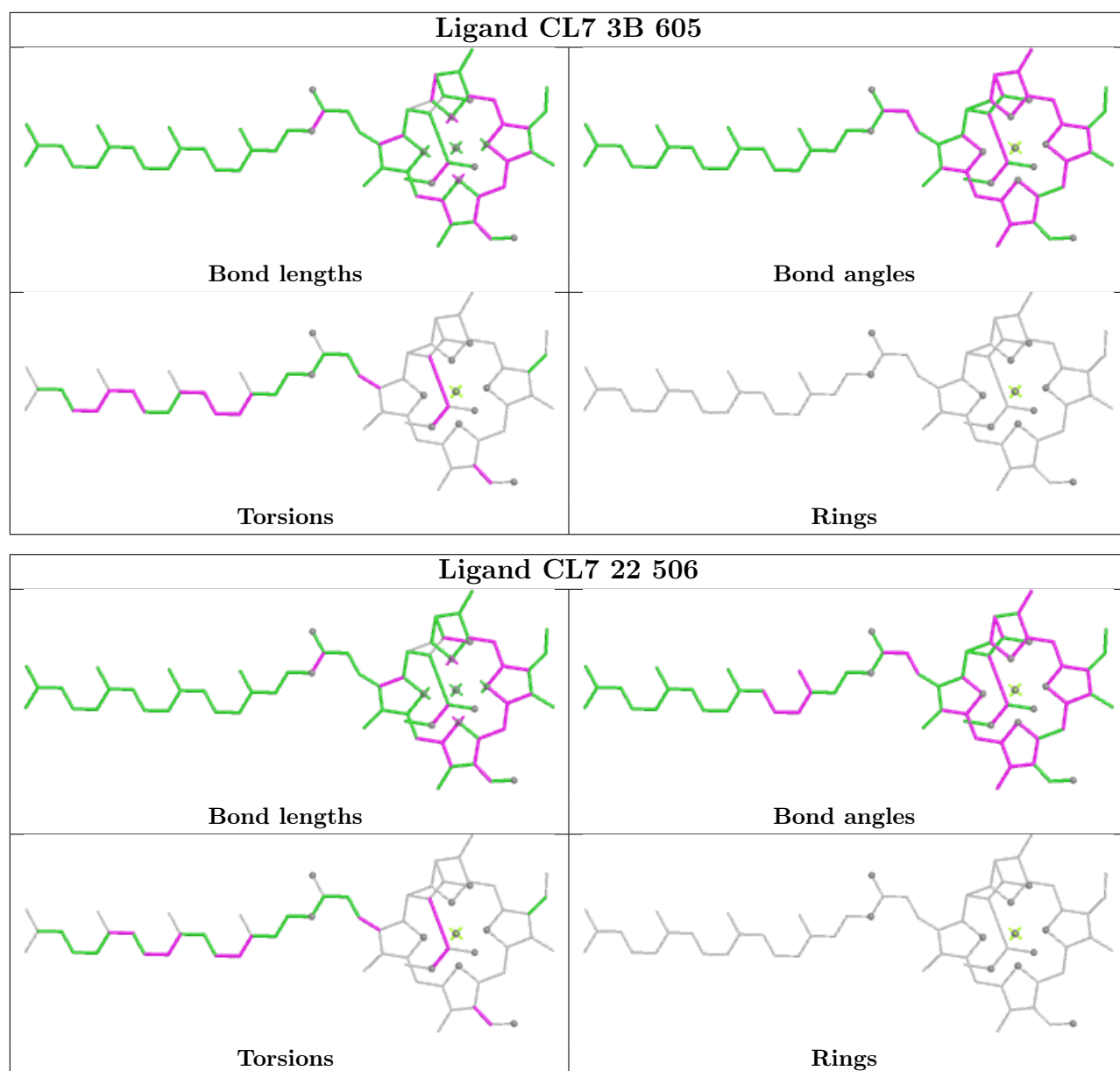
Rings

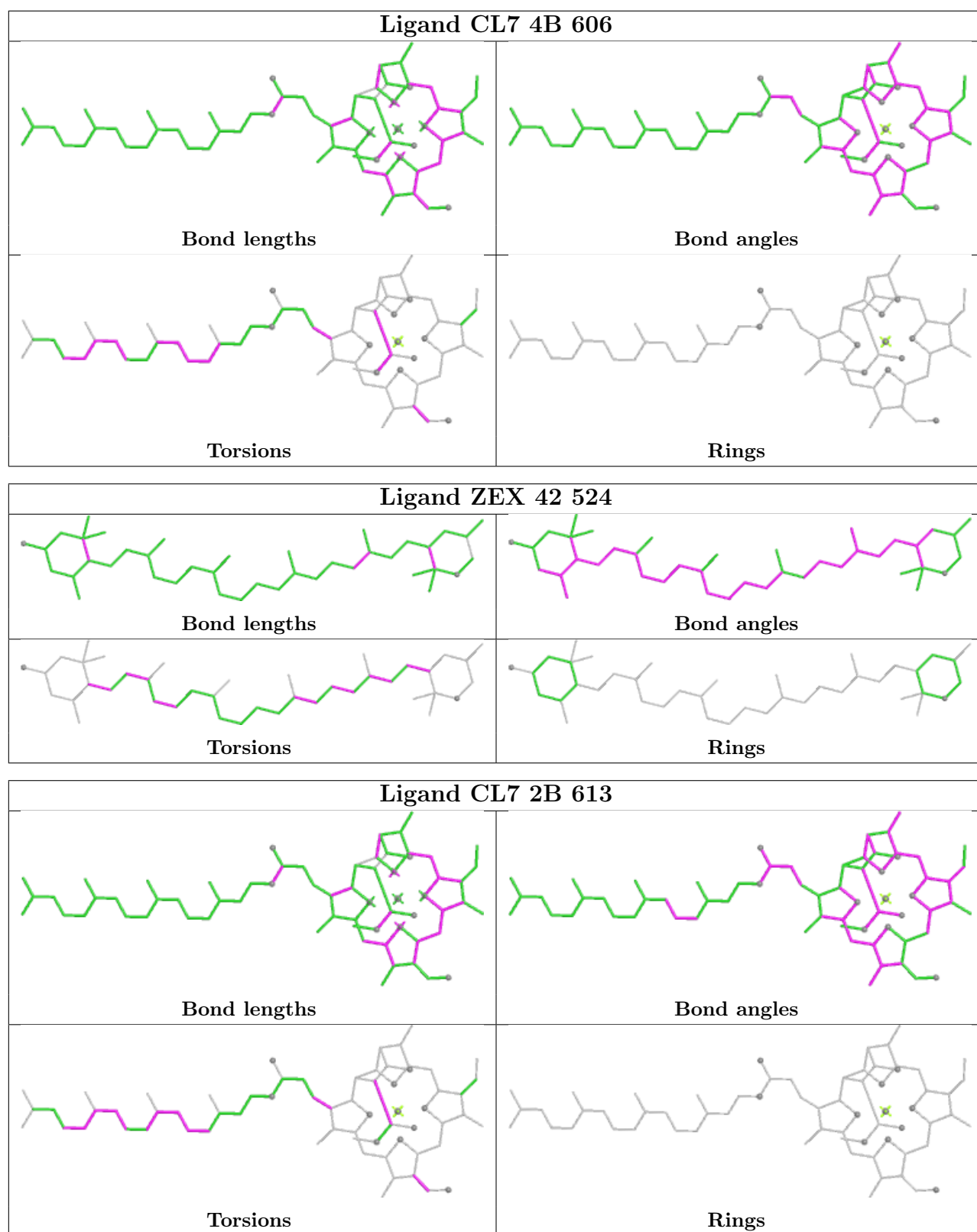


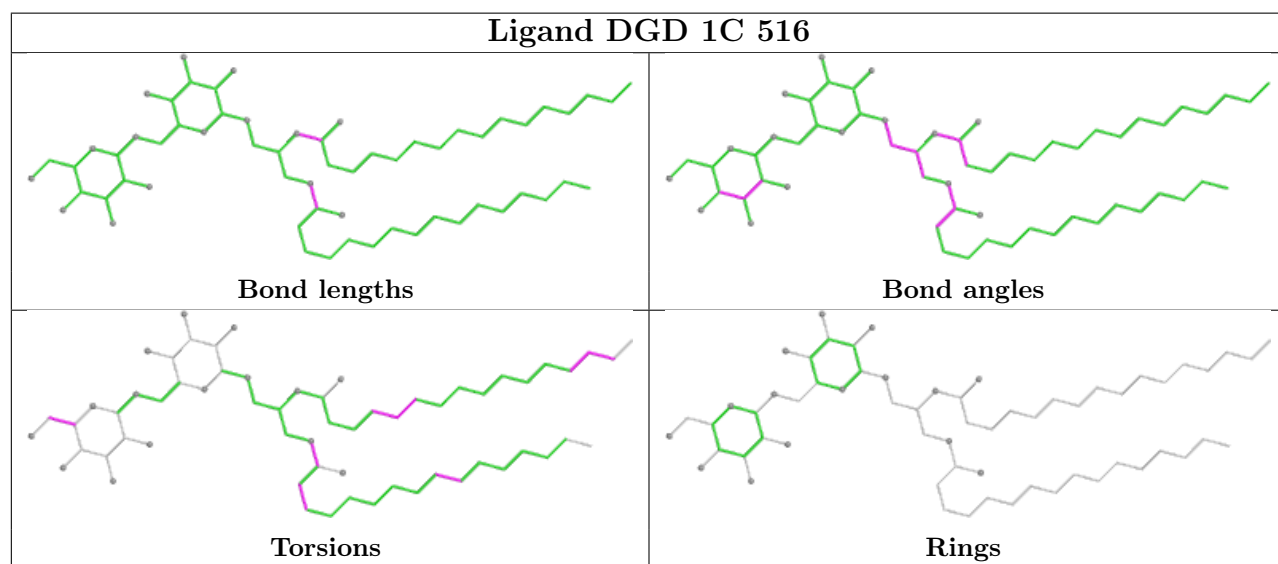
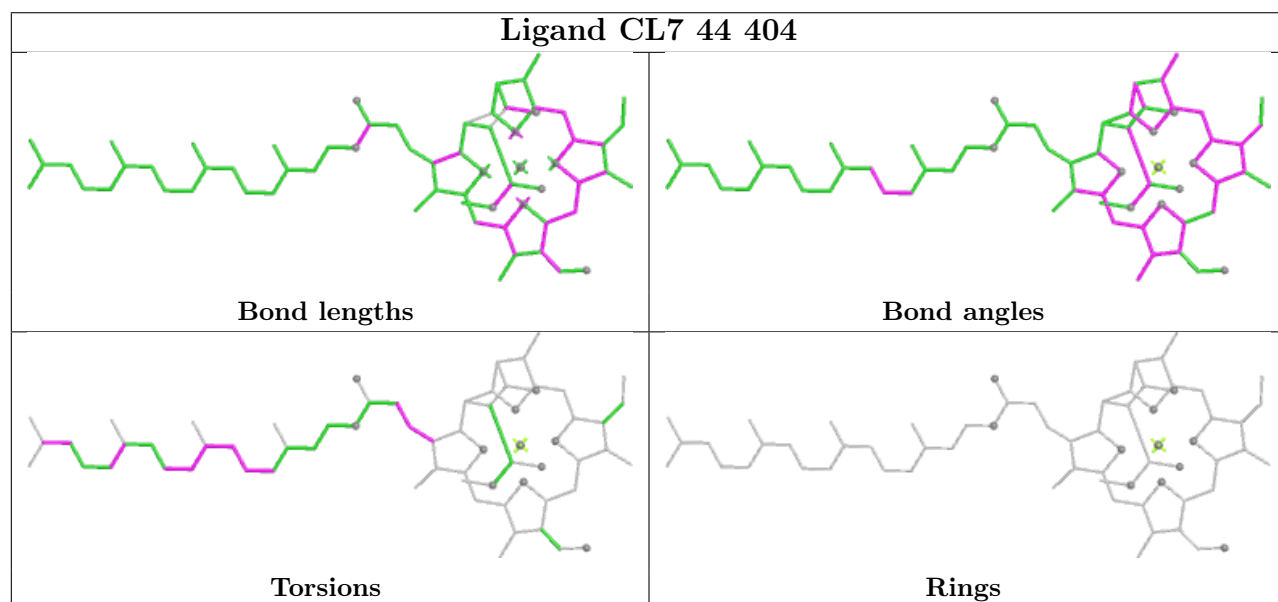
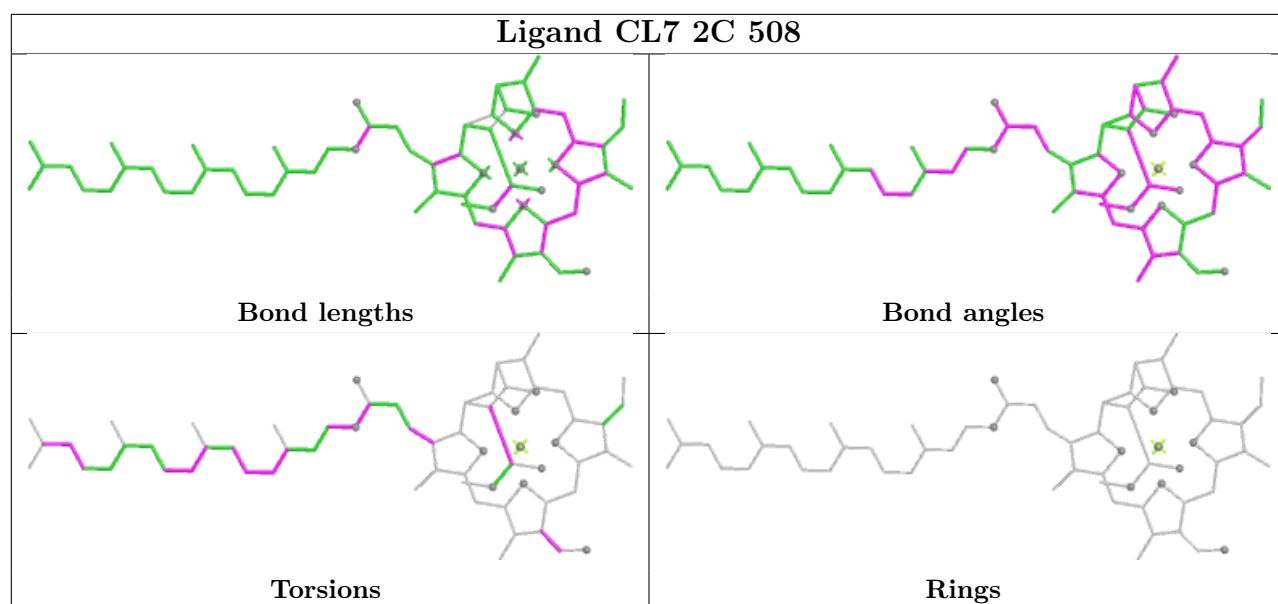


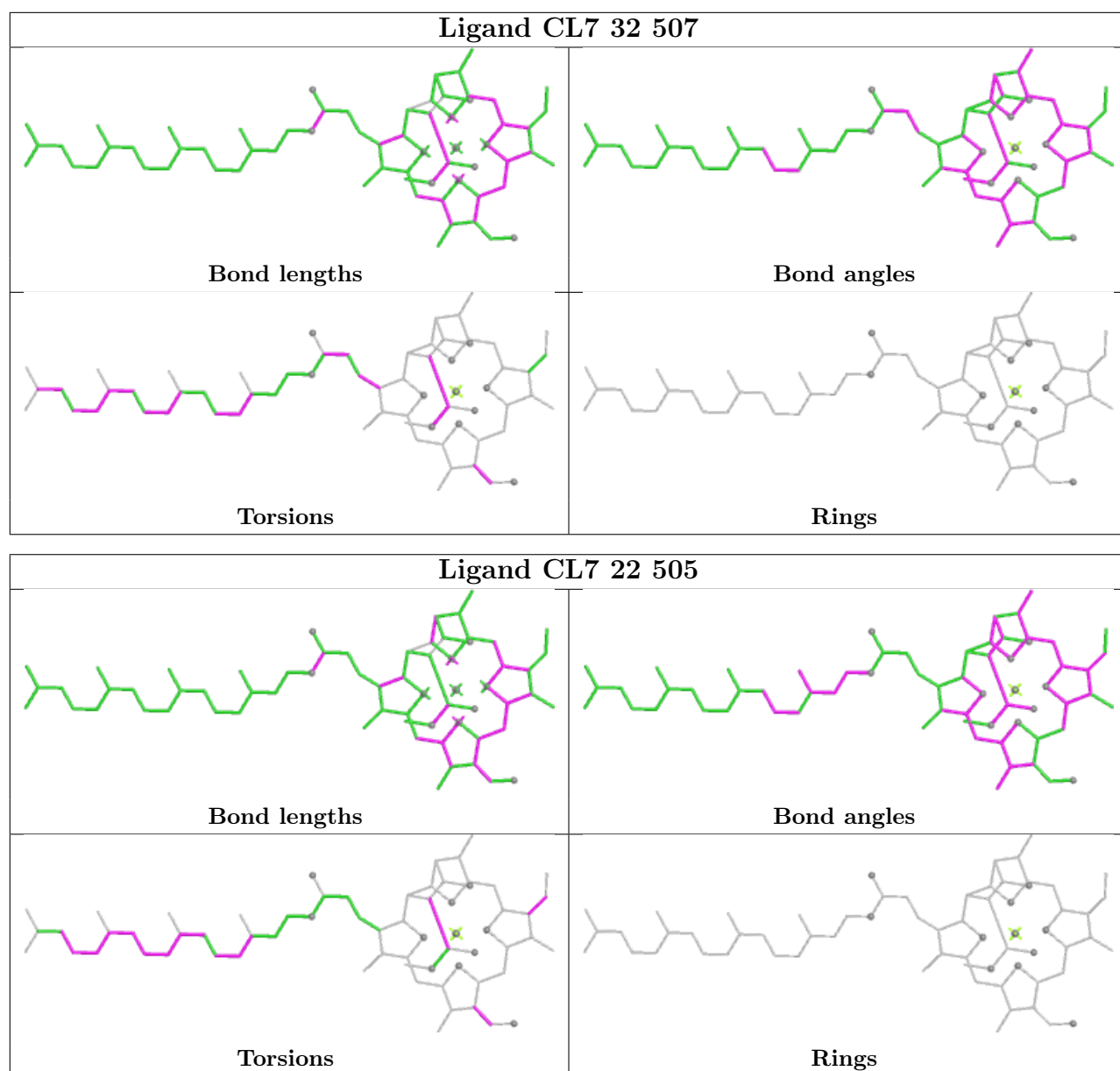




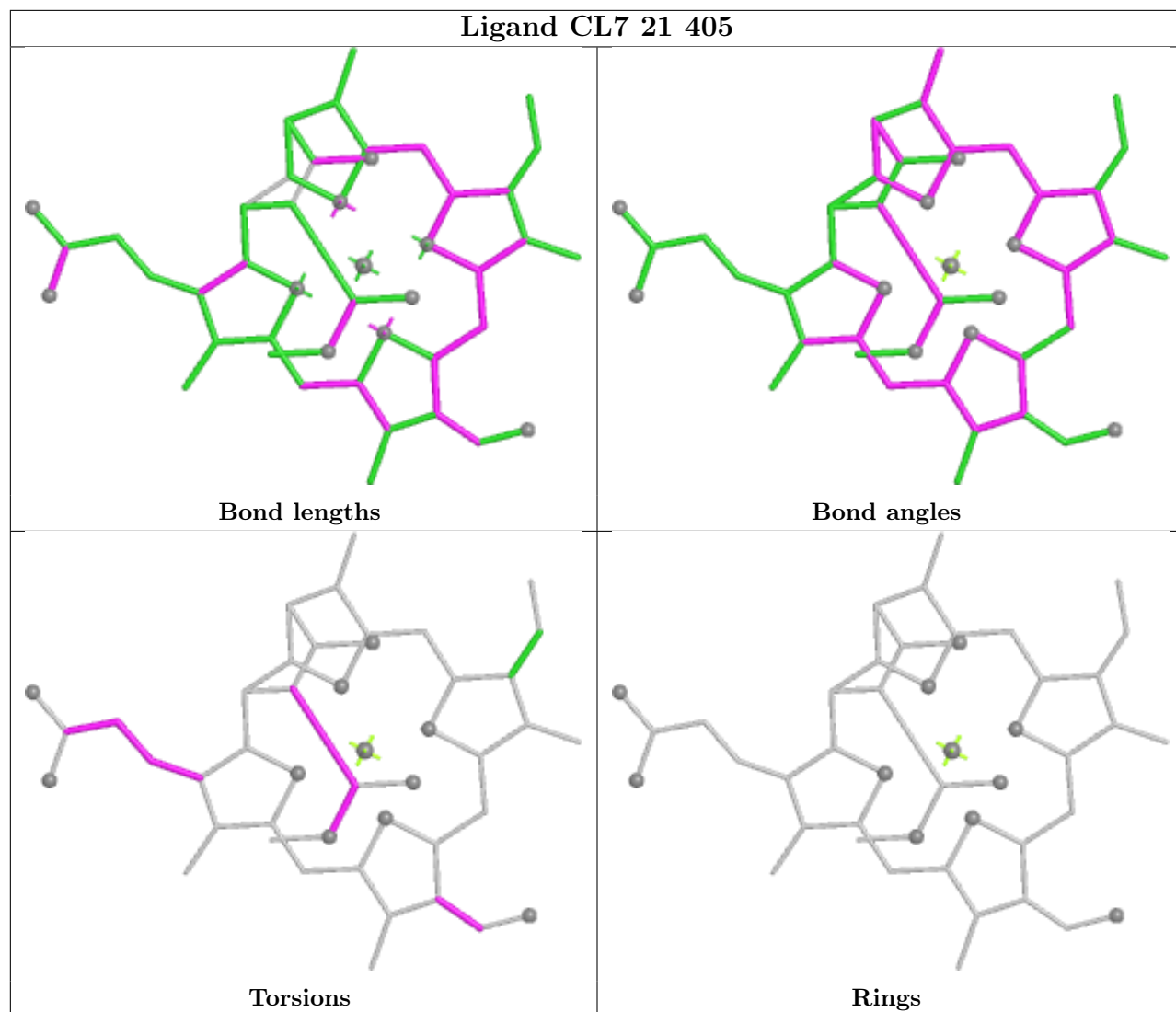




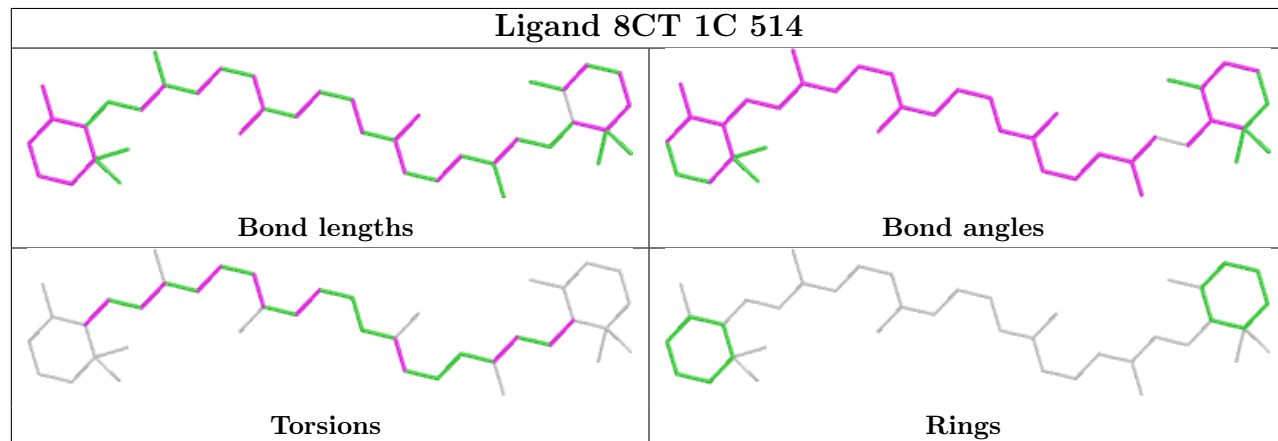


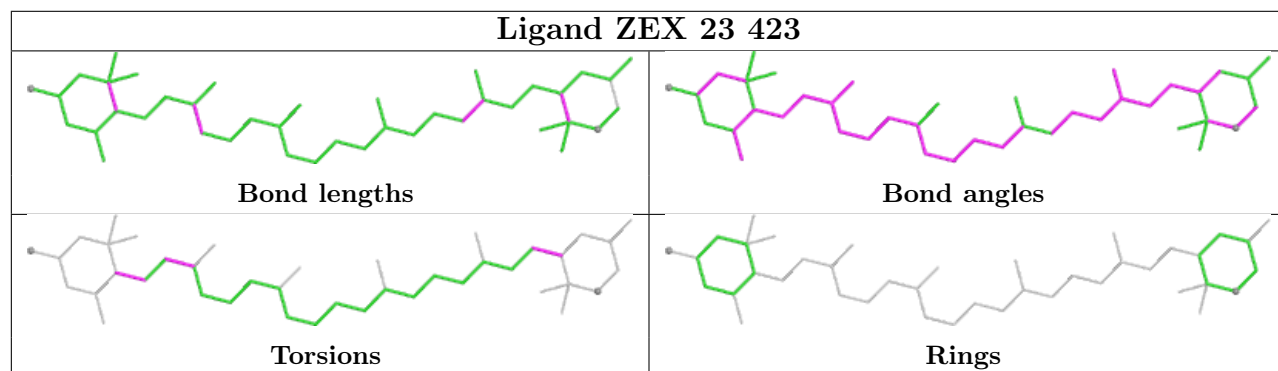
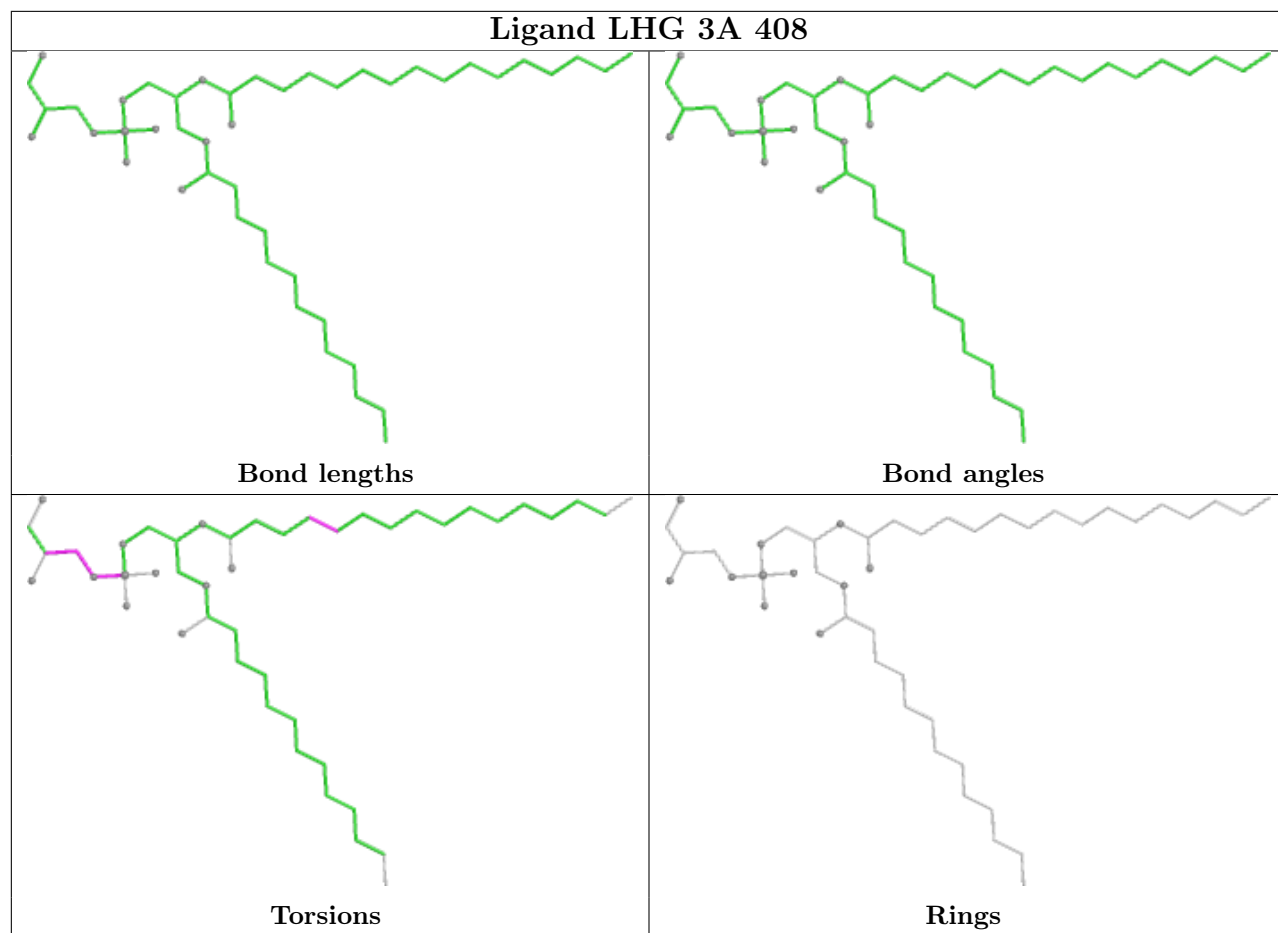


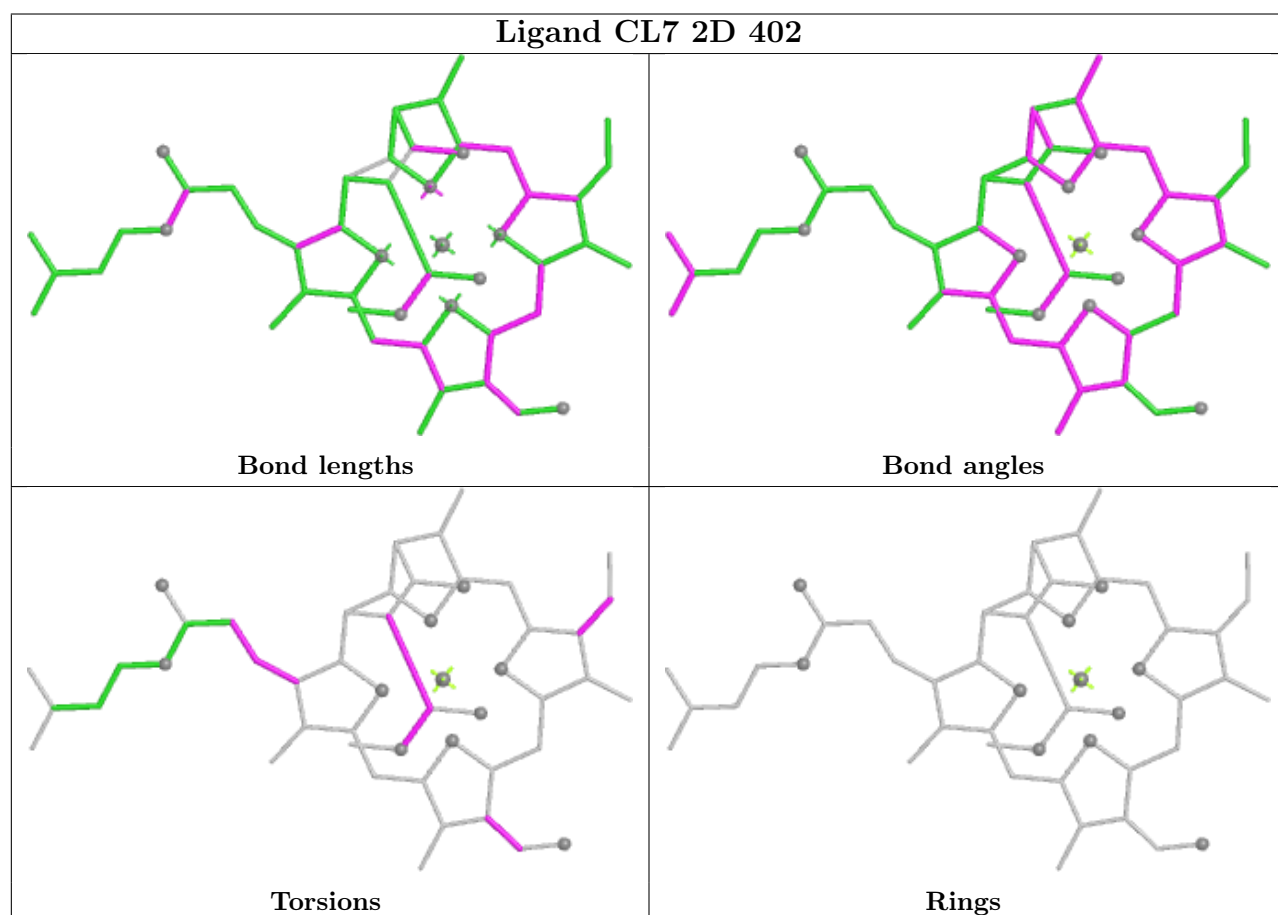
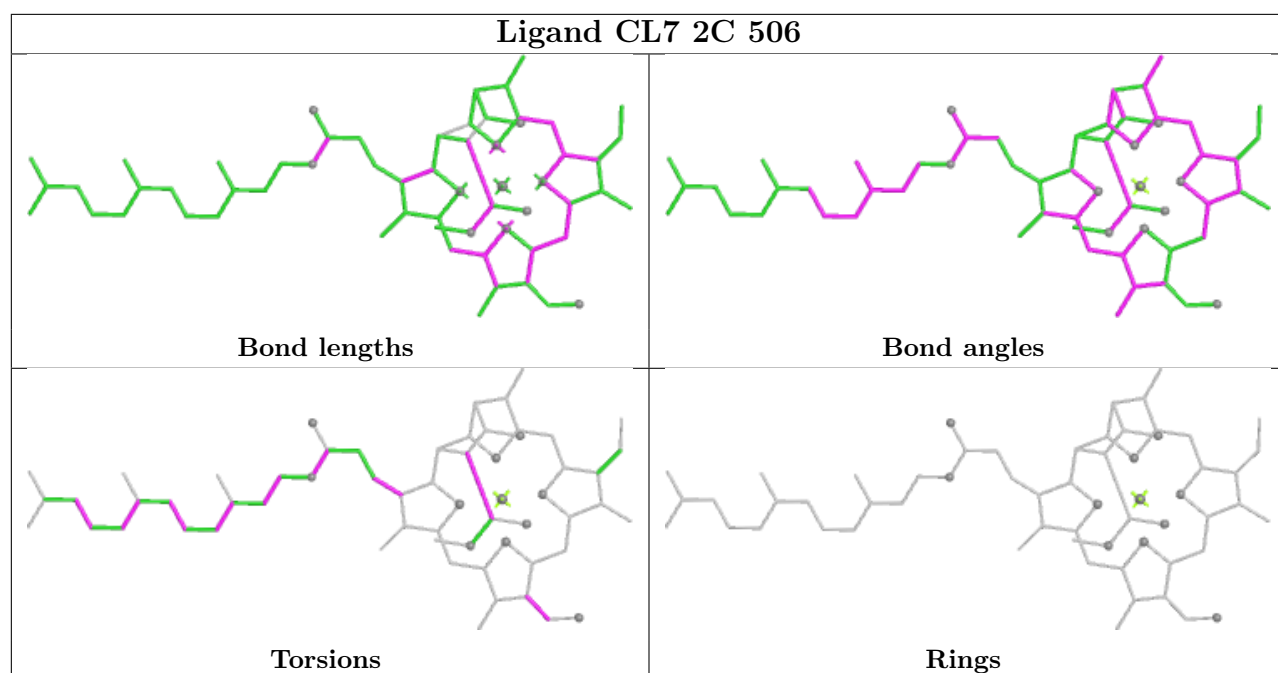
Ligand CL7 21 405

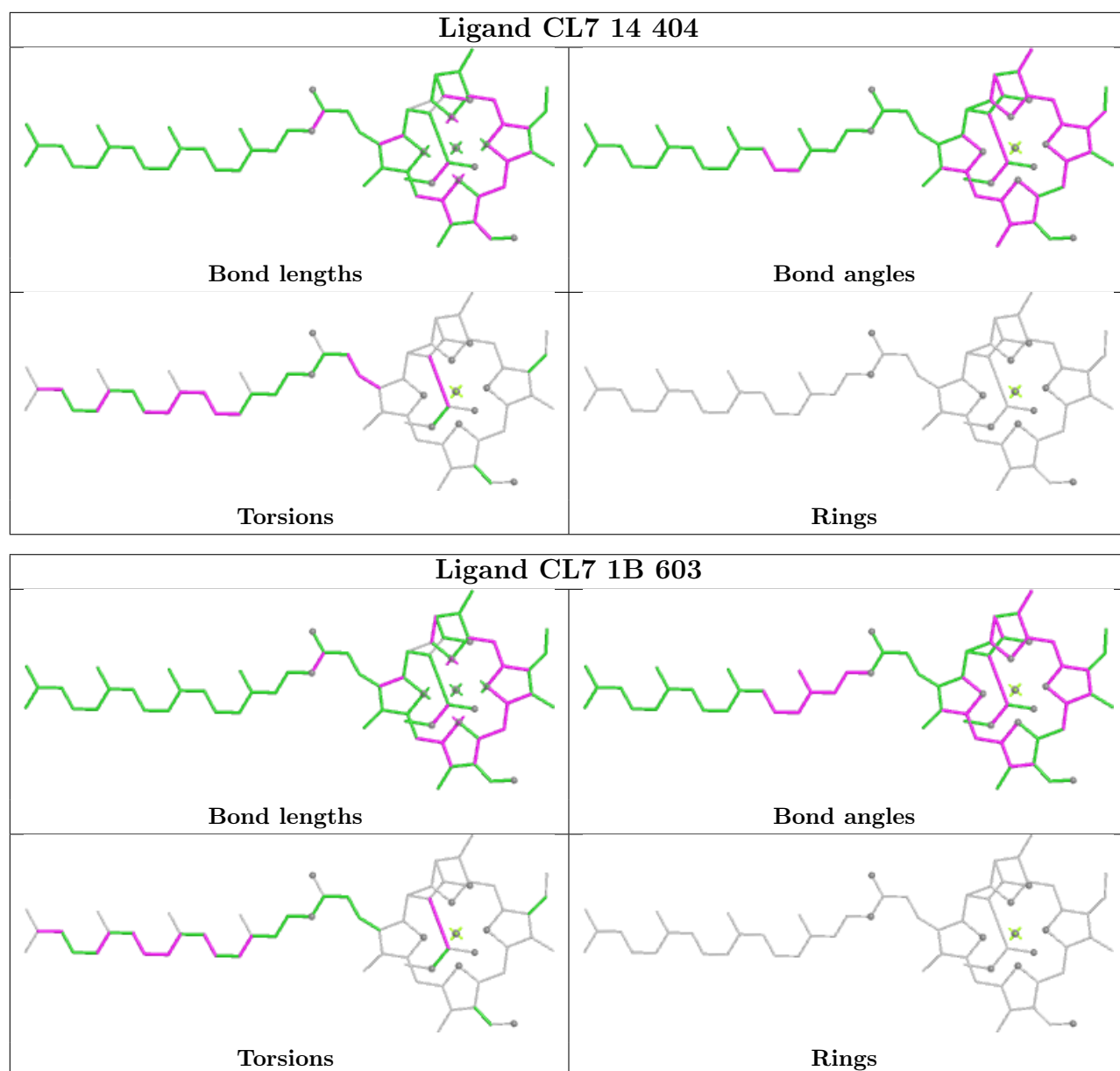


Ligand 8CT 1C 514

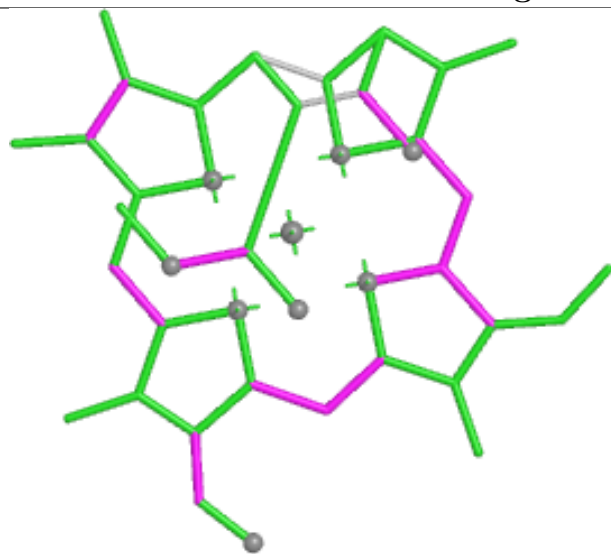




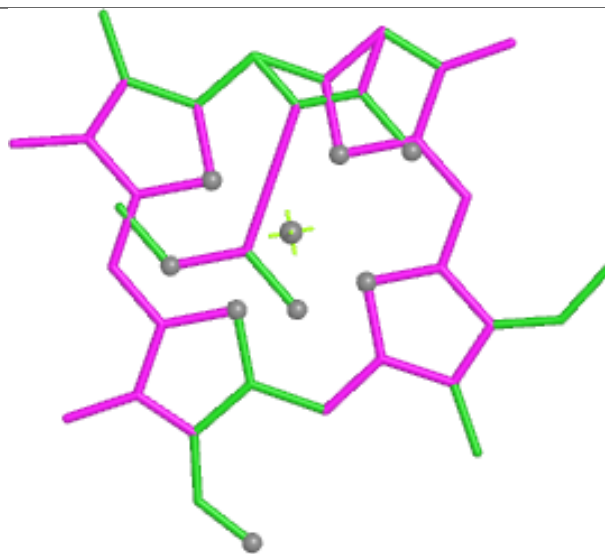




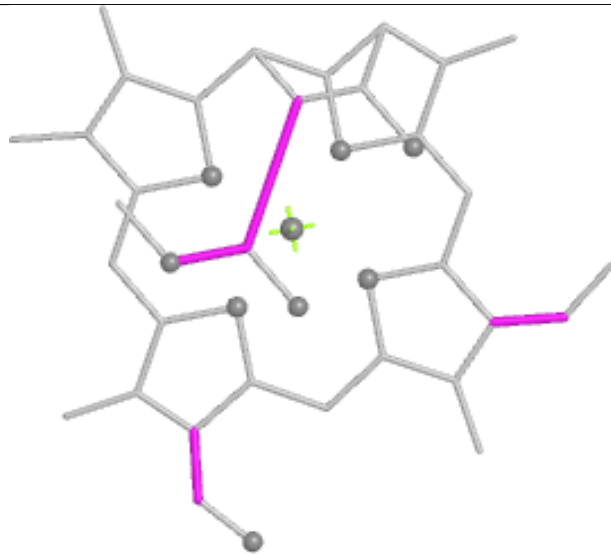
Ligand CL7 41 415



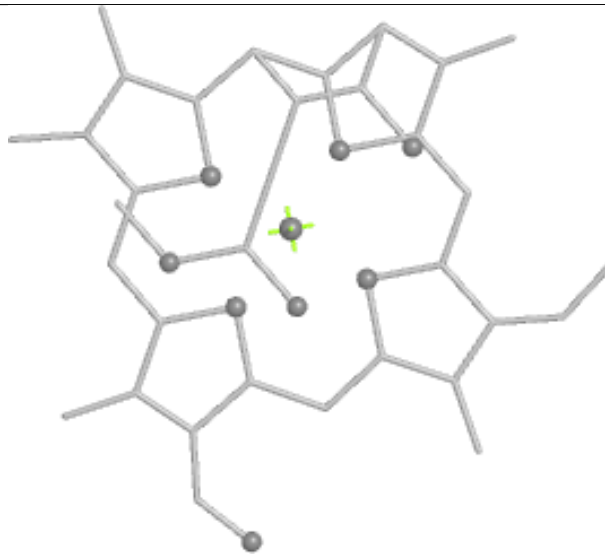
Bond lengths



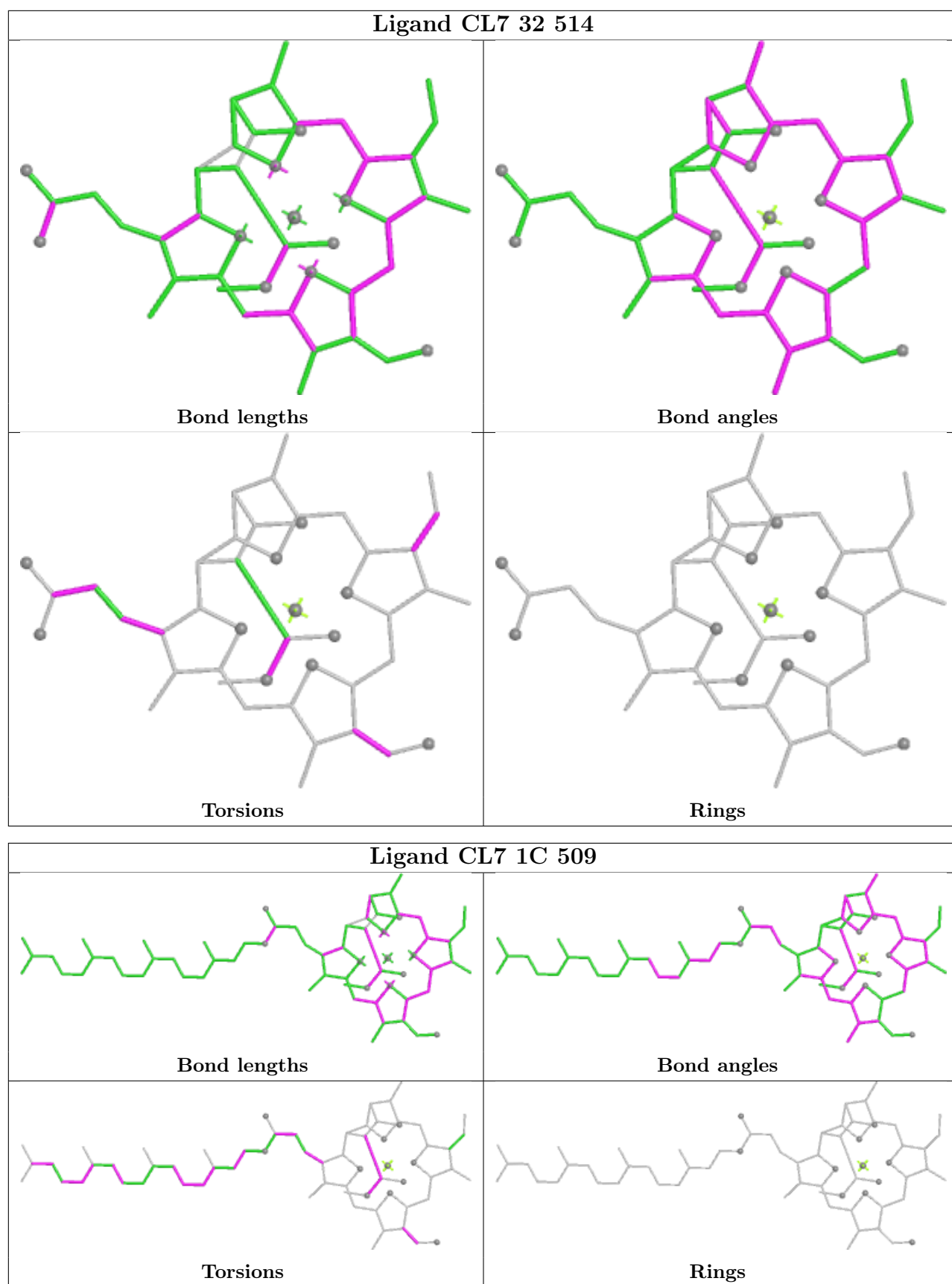
Bond angles



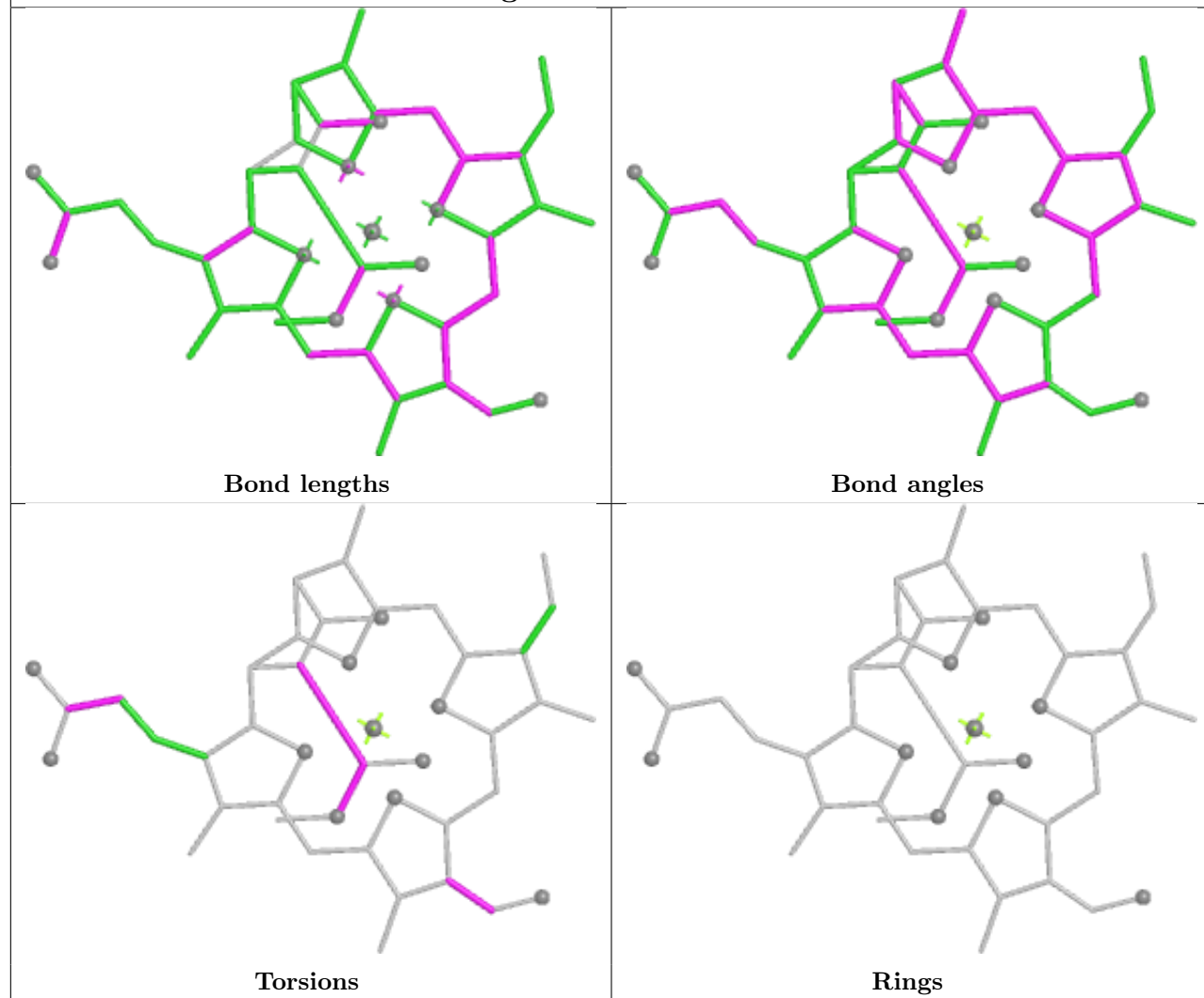
Torsions



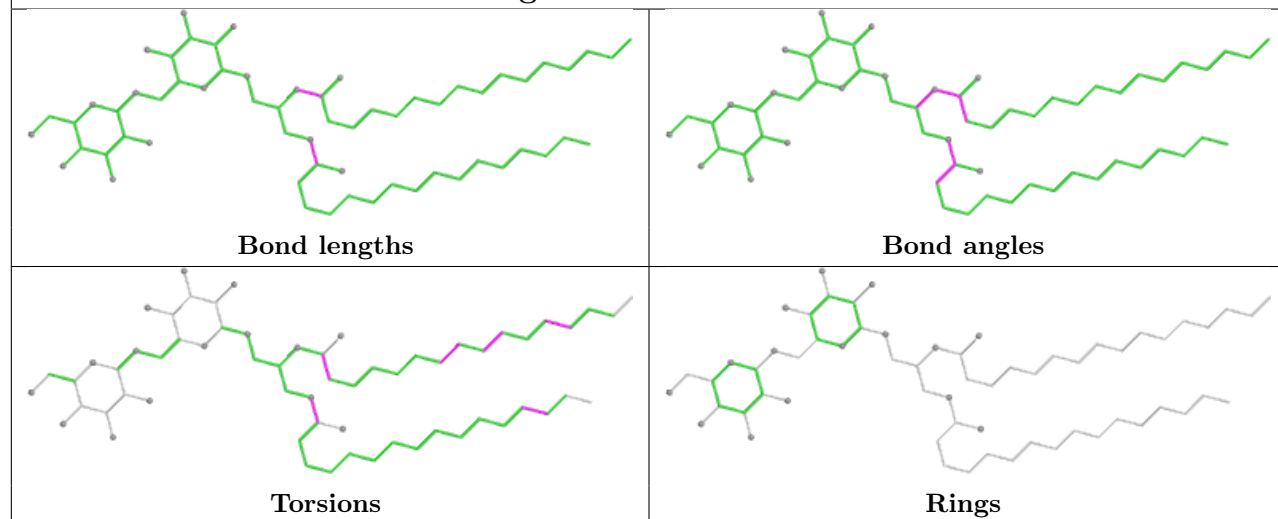
Rings

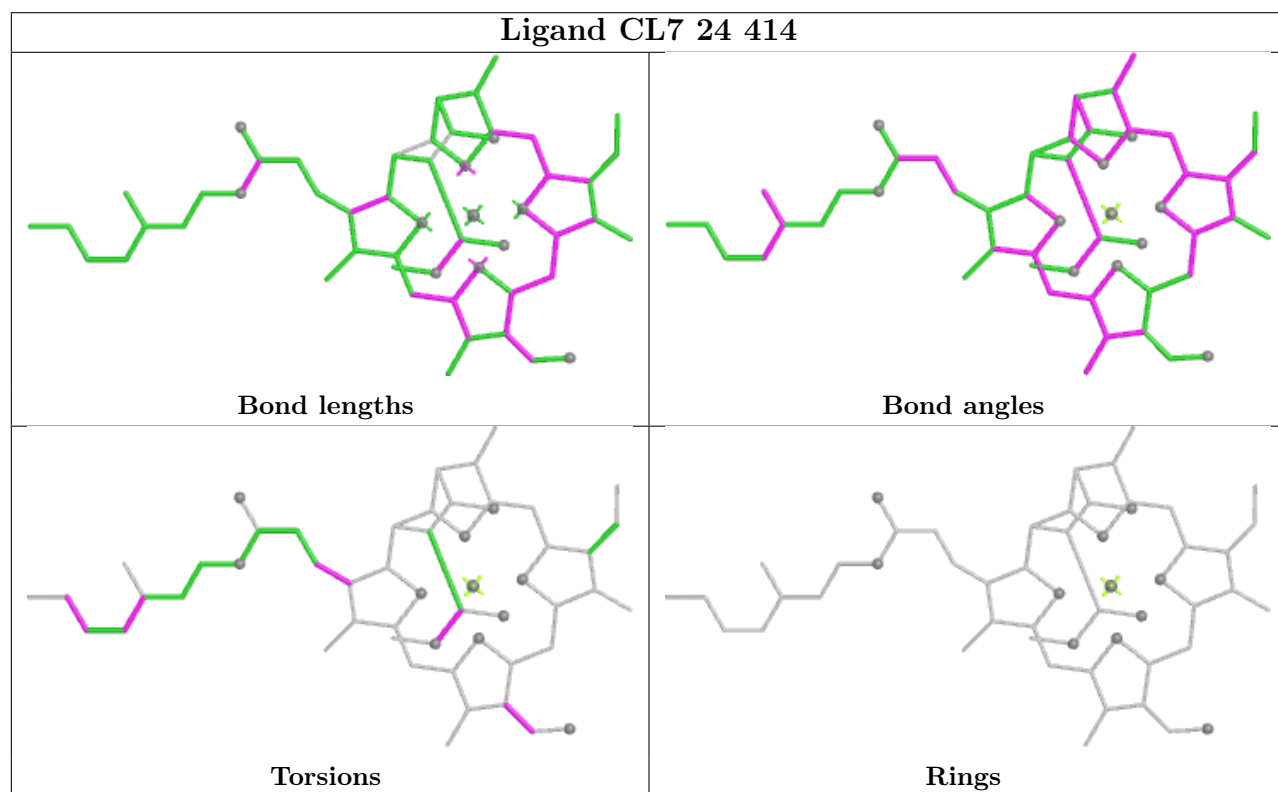
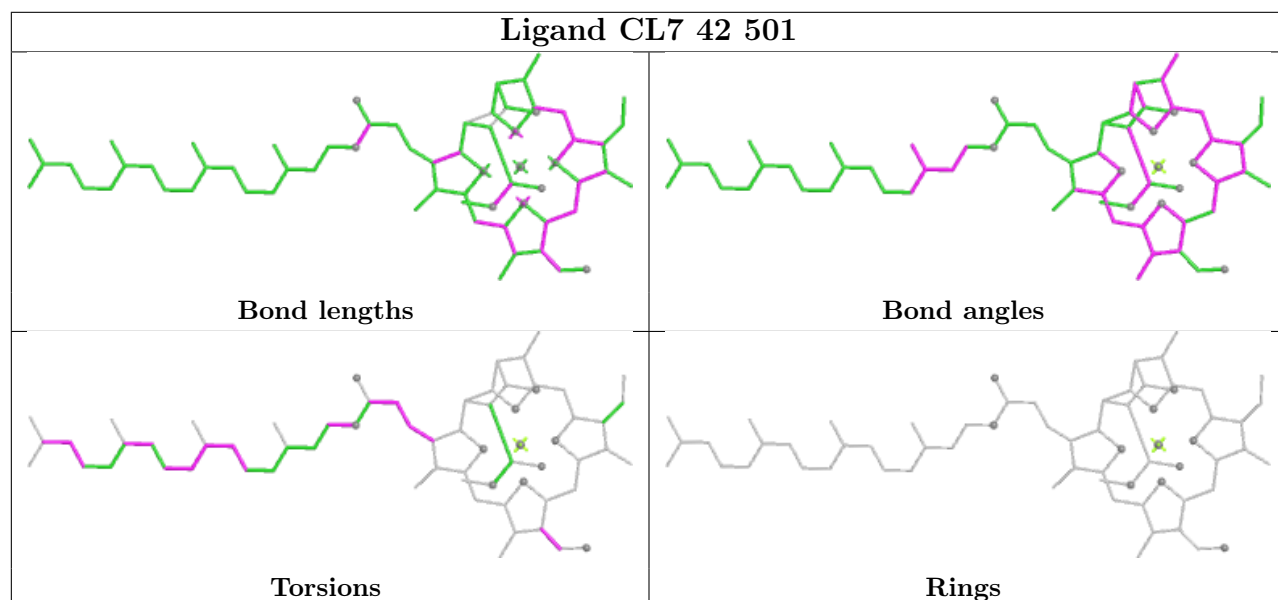
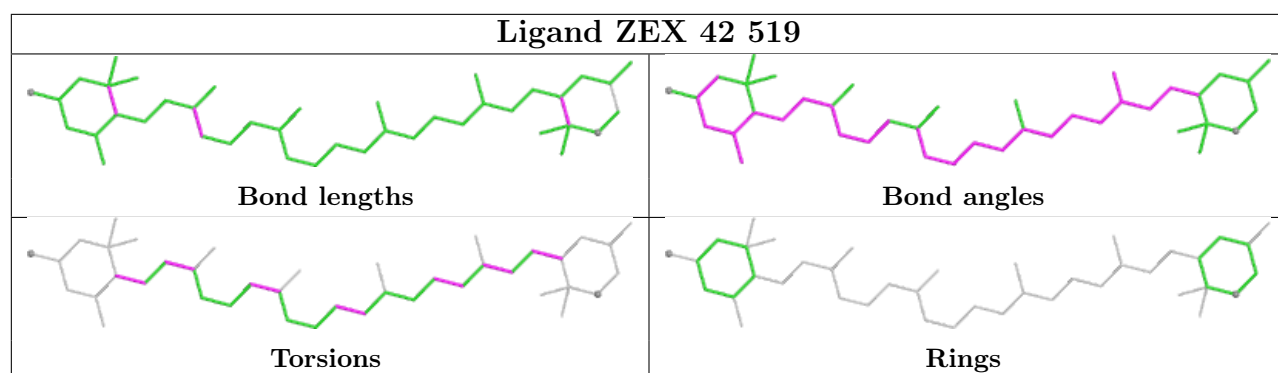


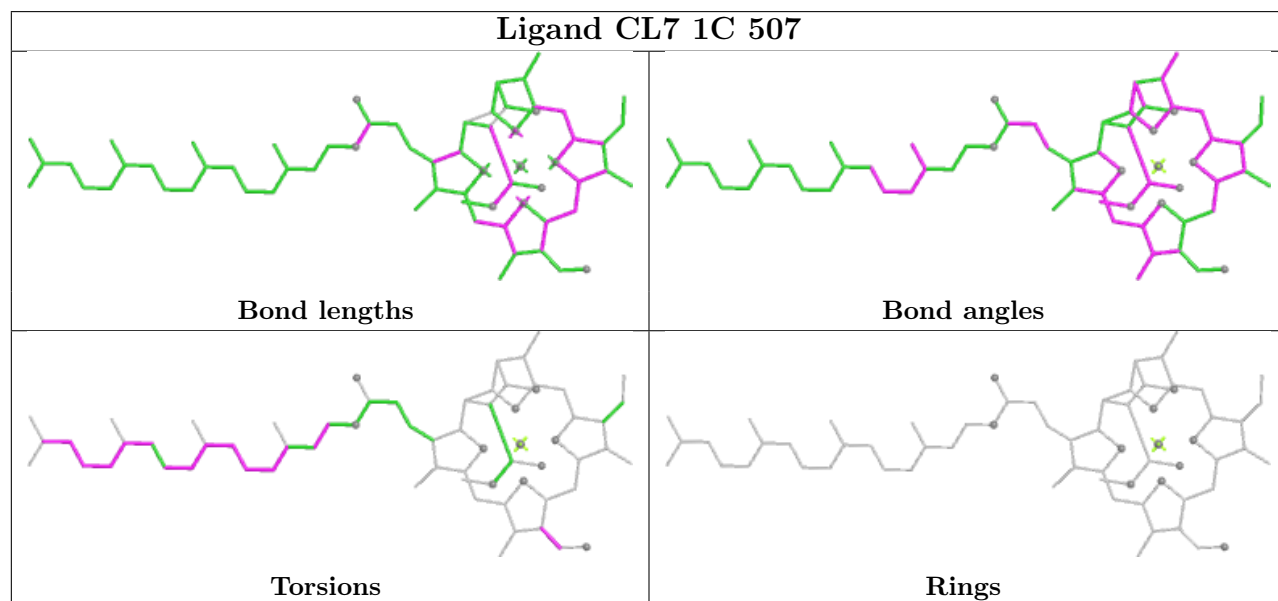
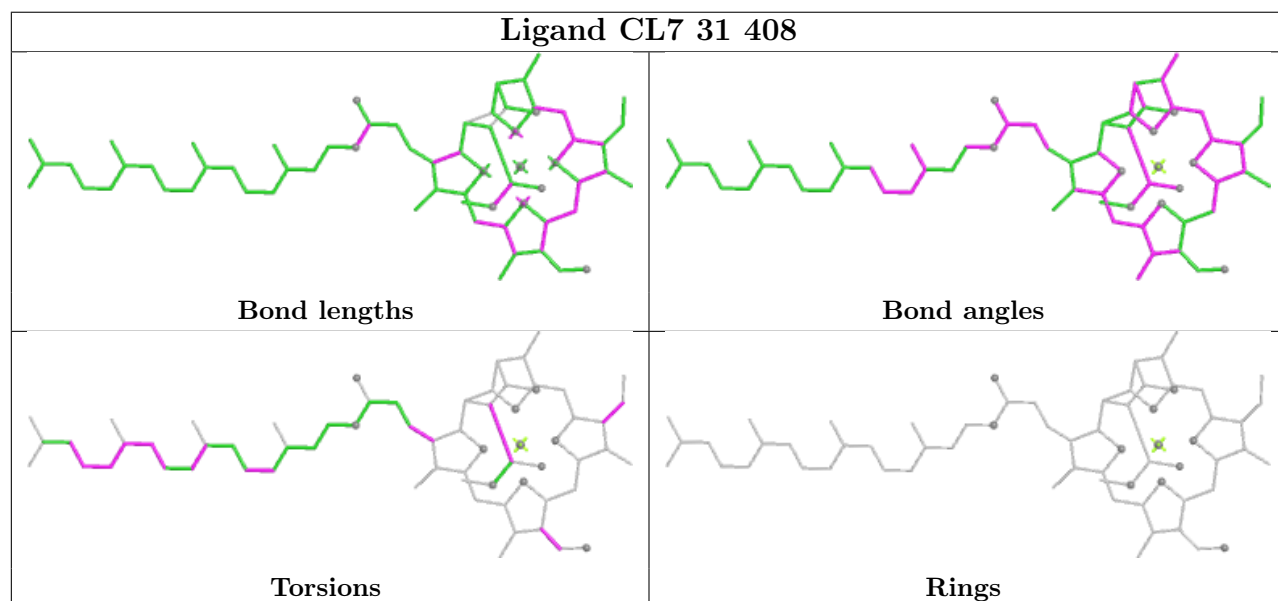
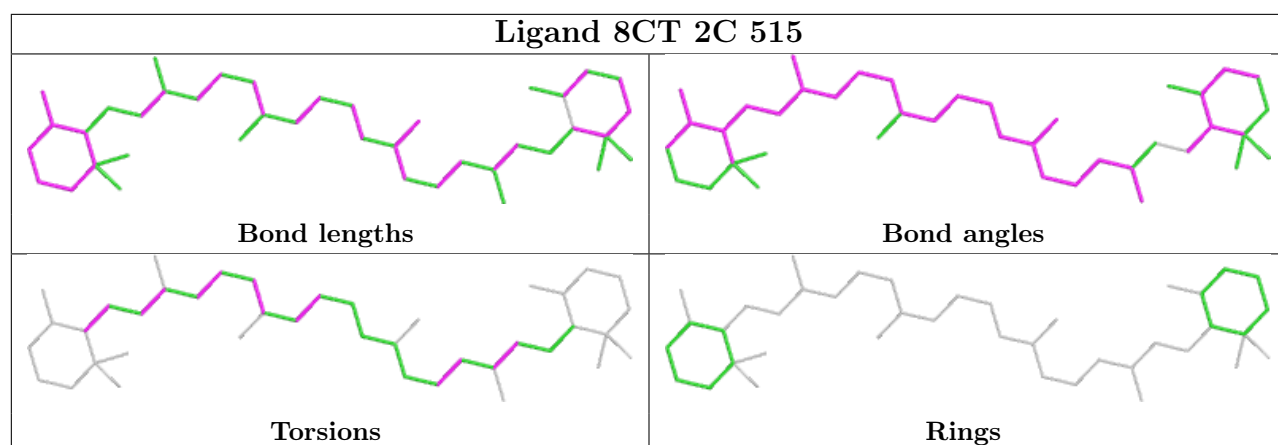
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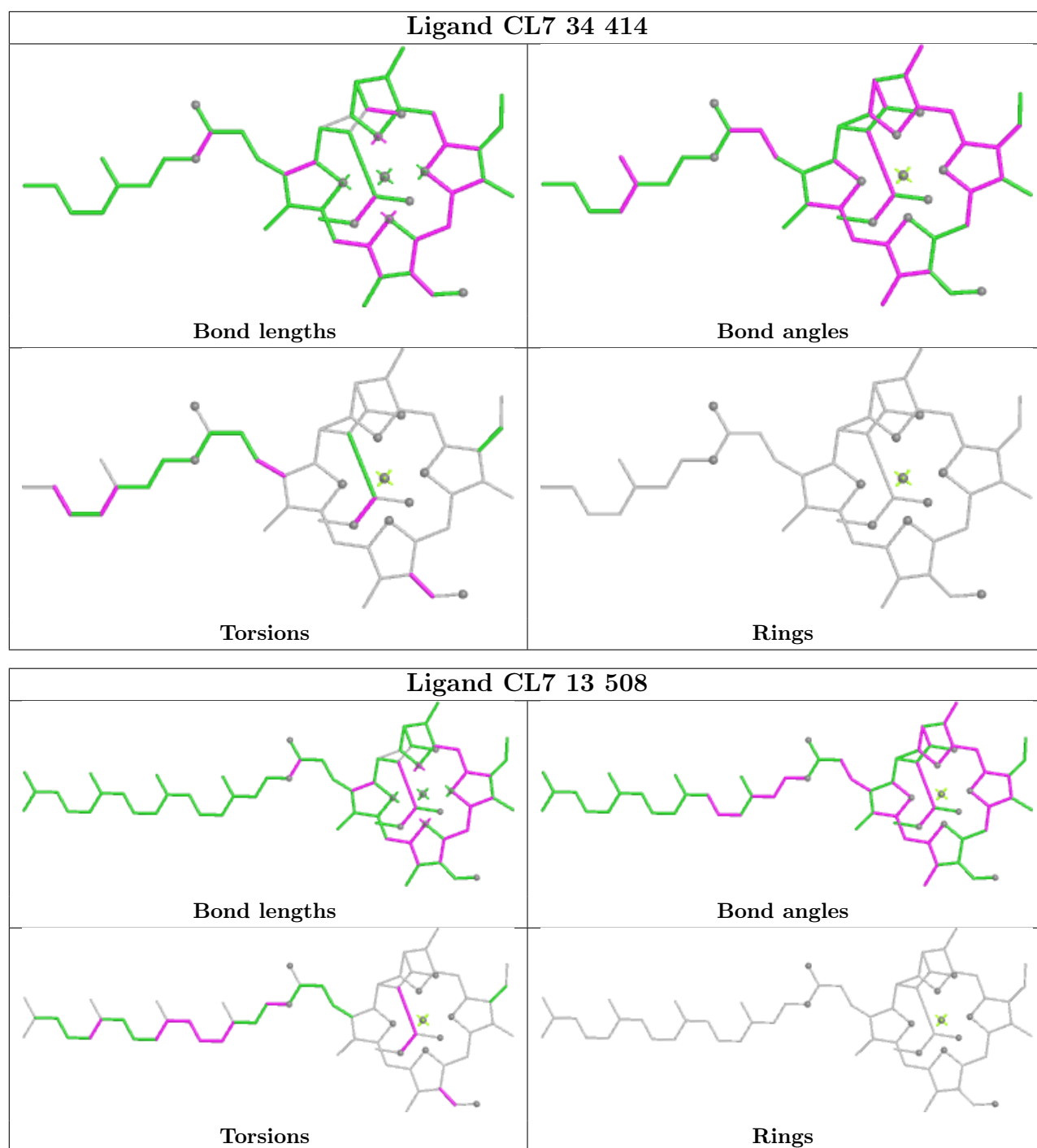


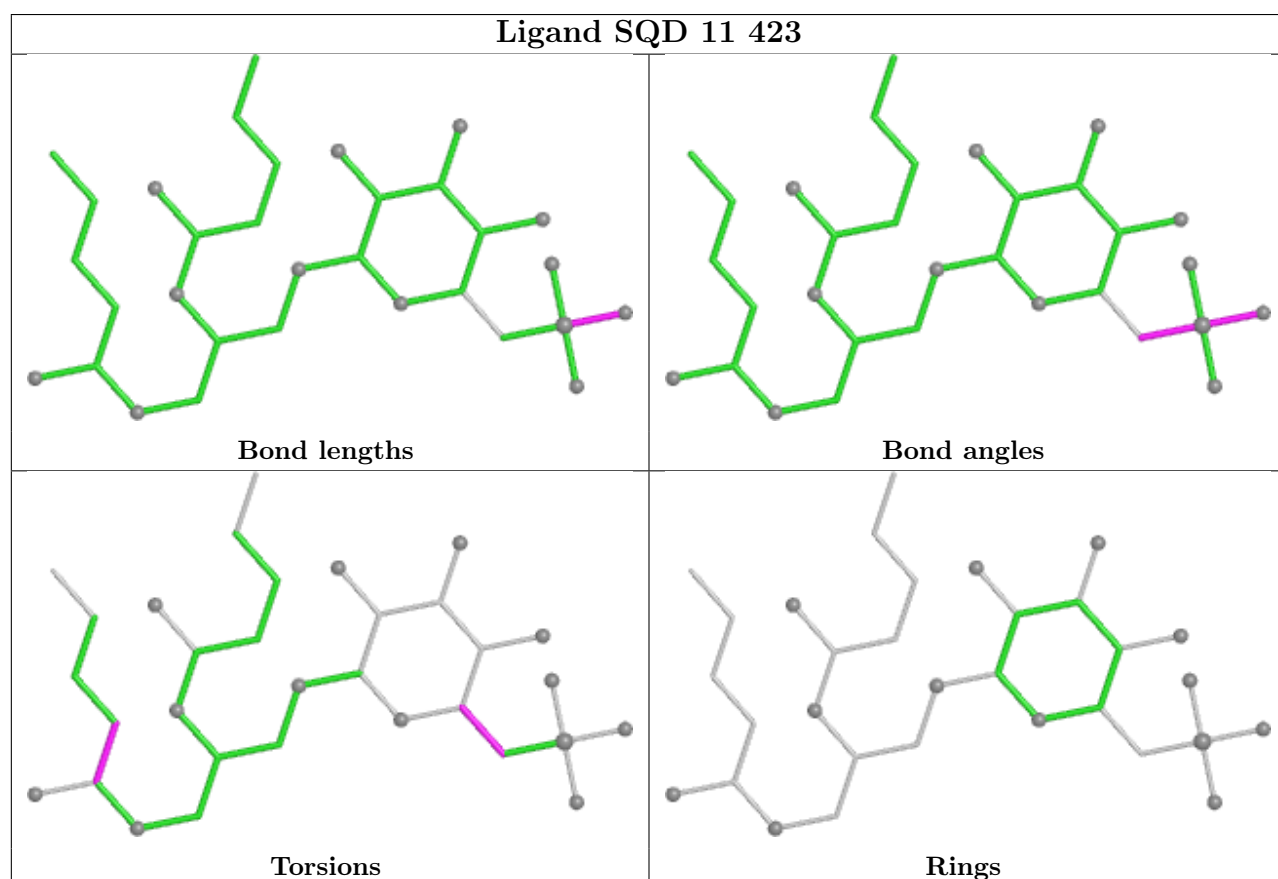
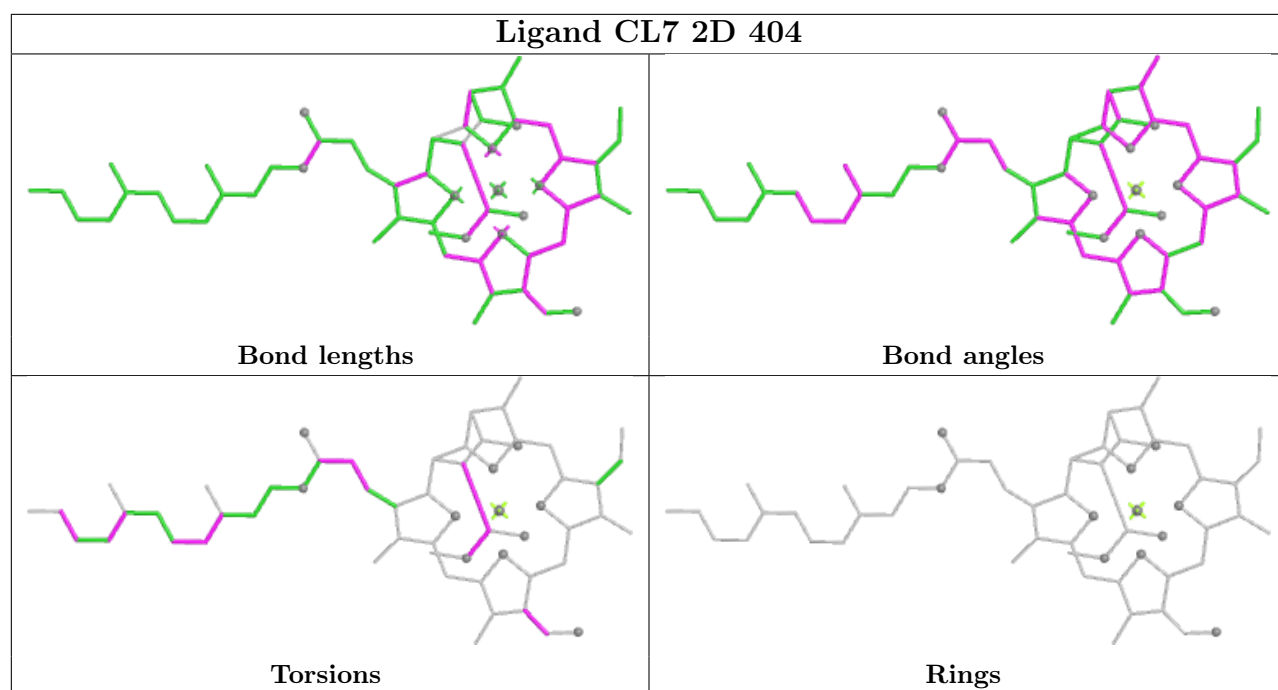
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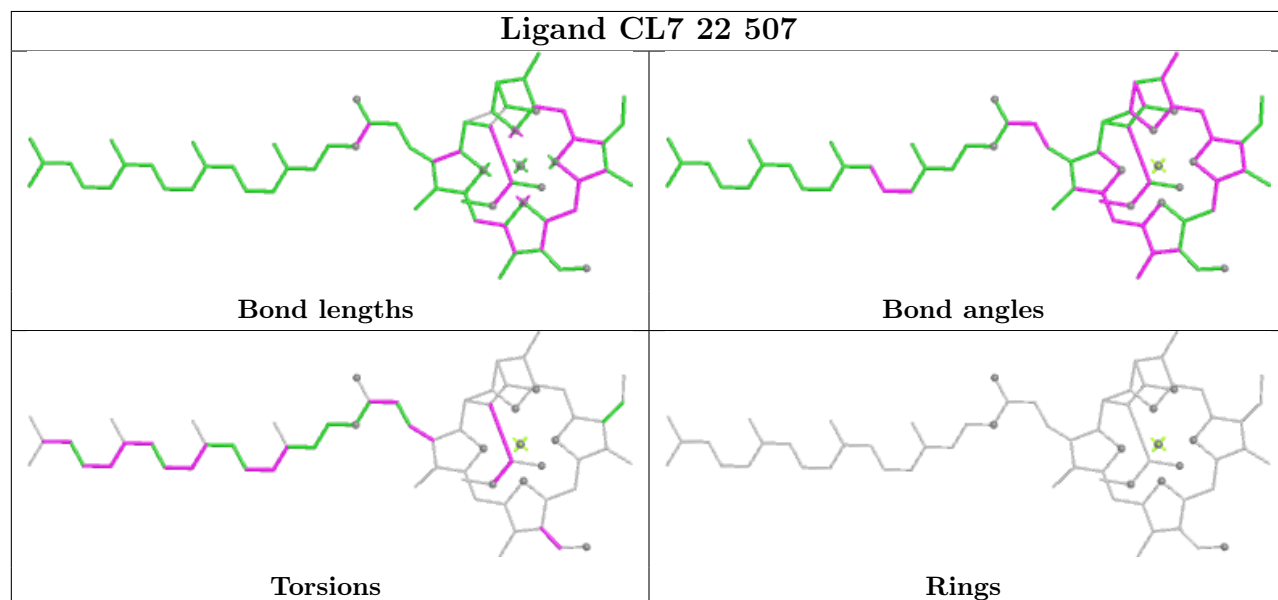
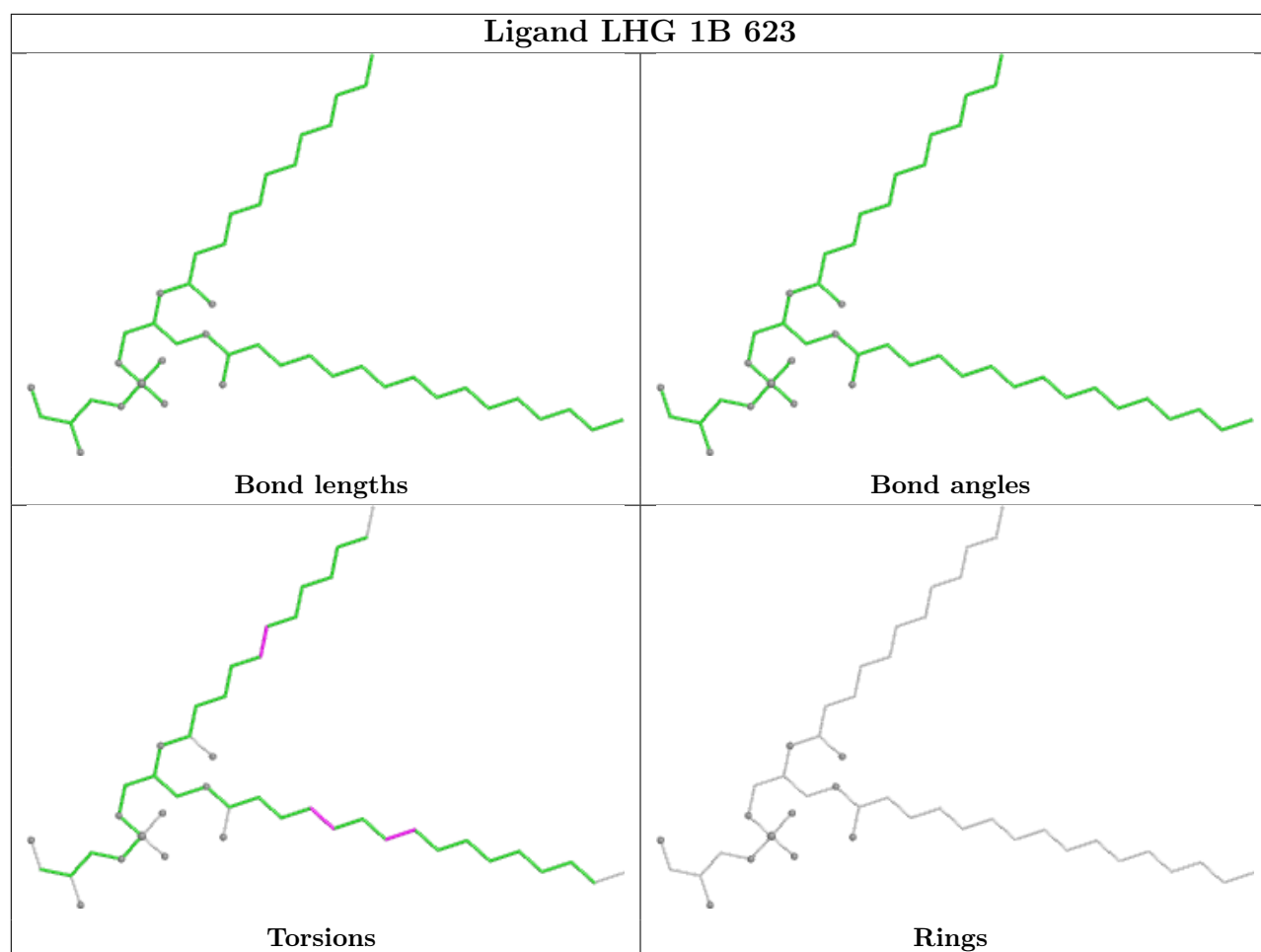


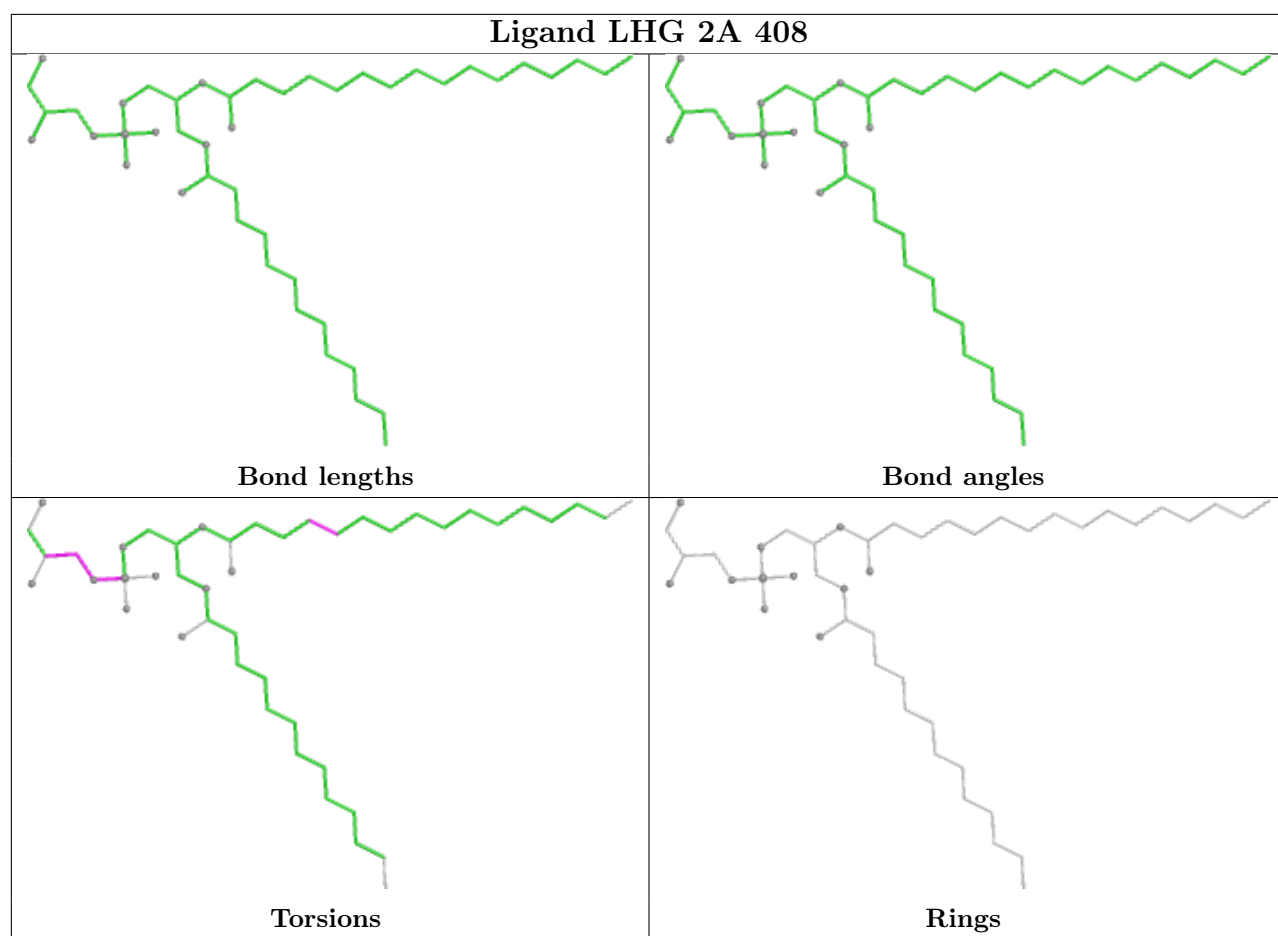


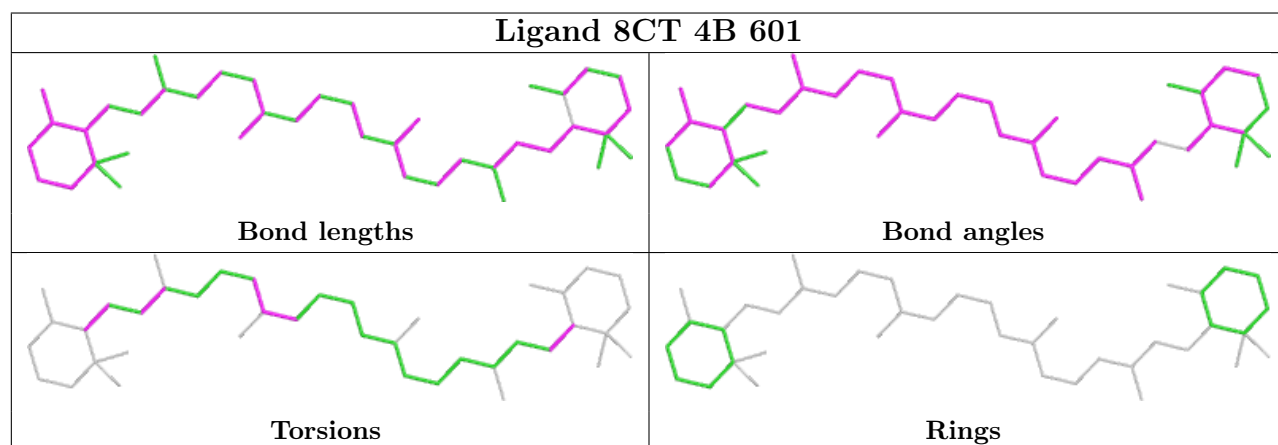
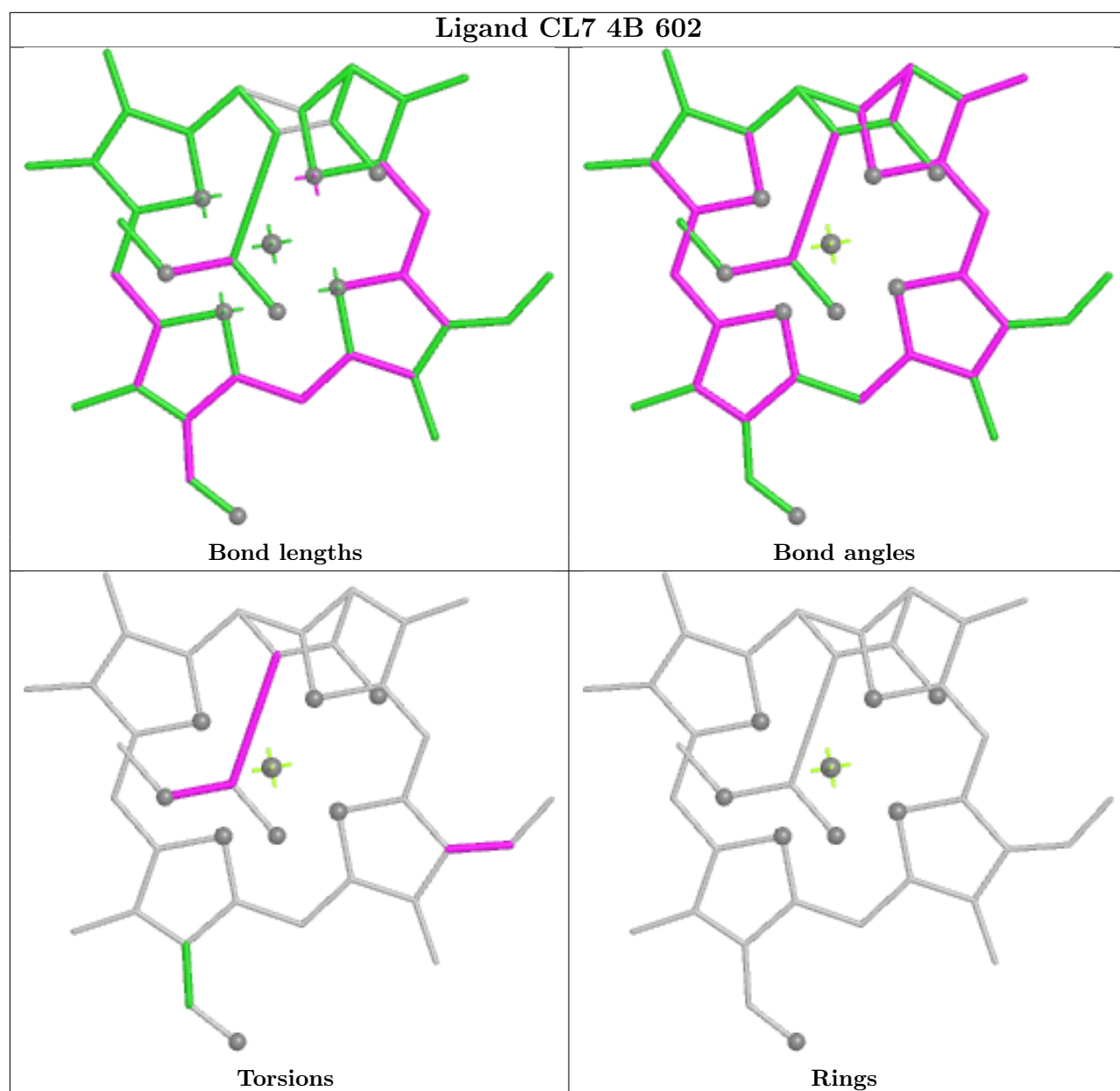


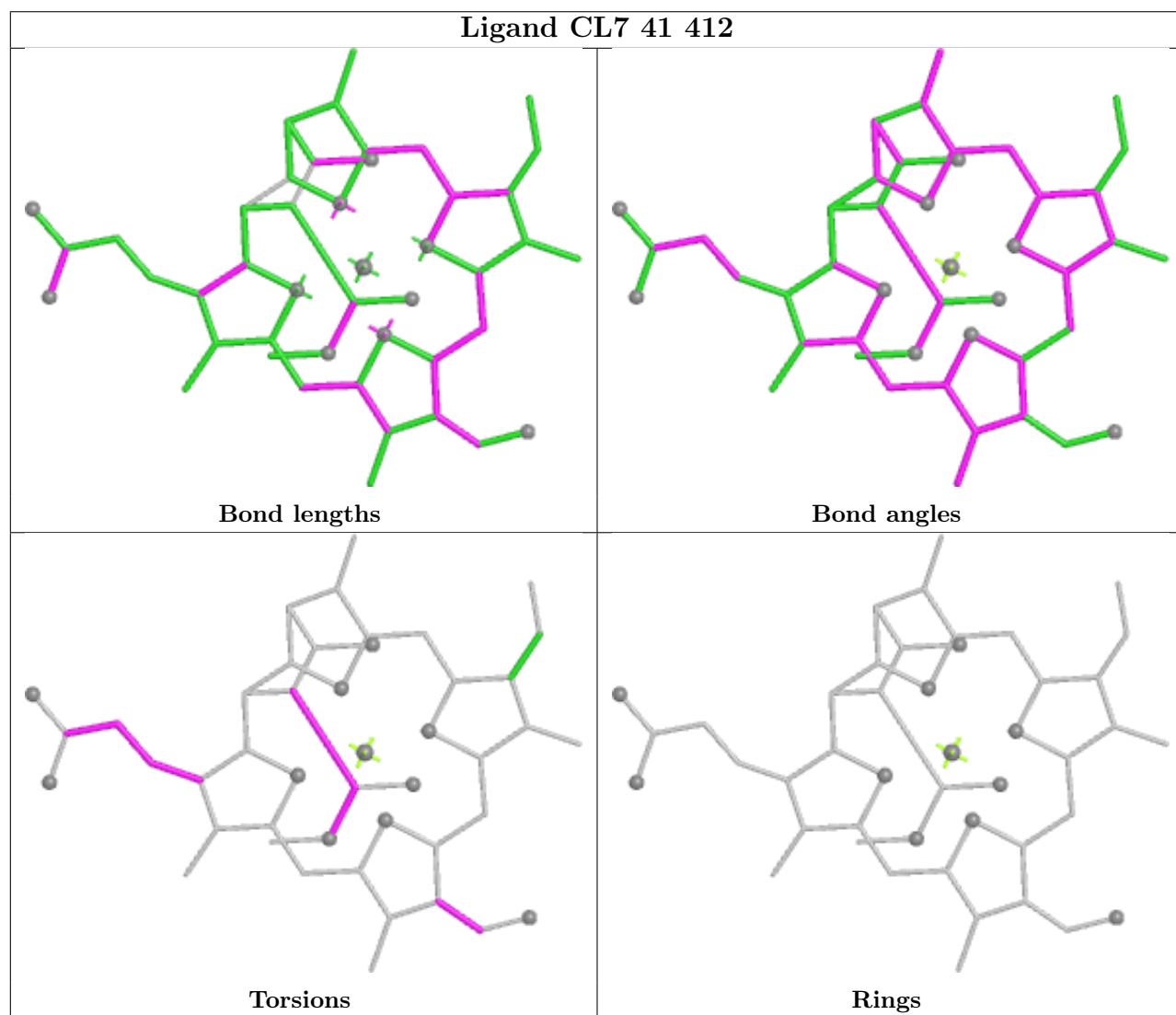
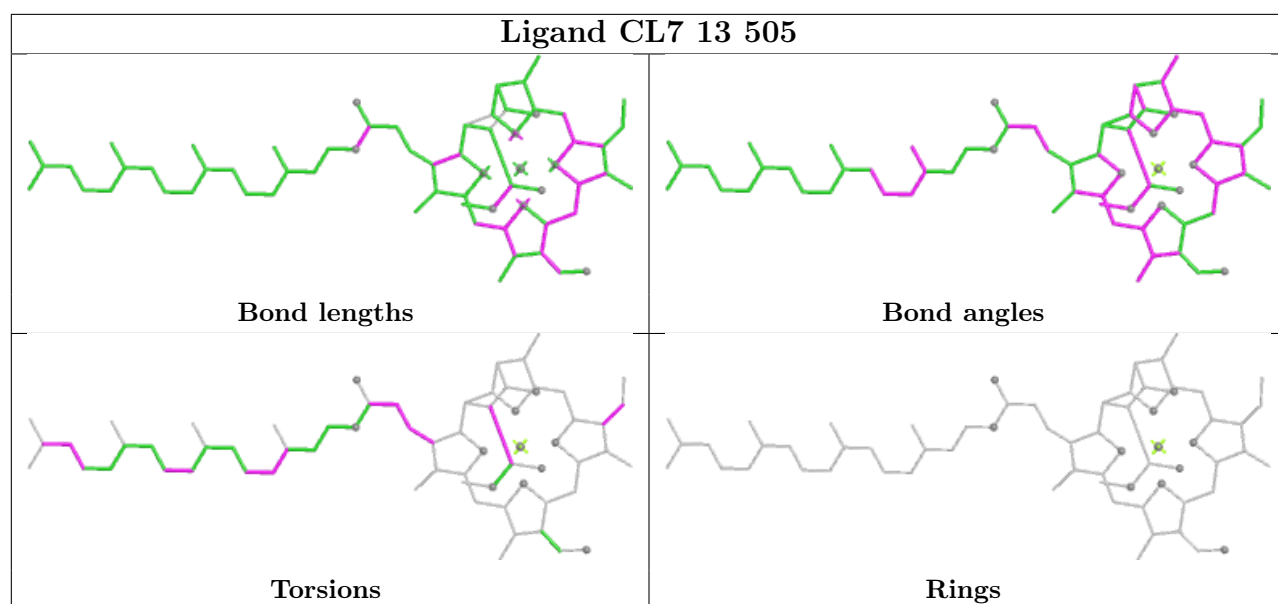


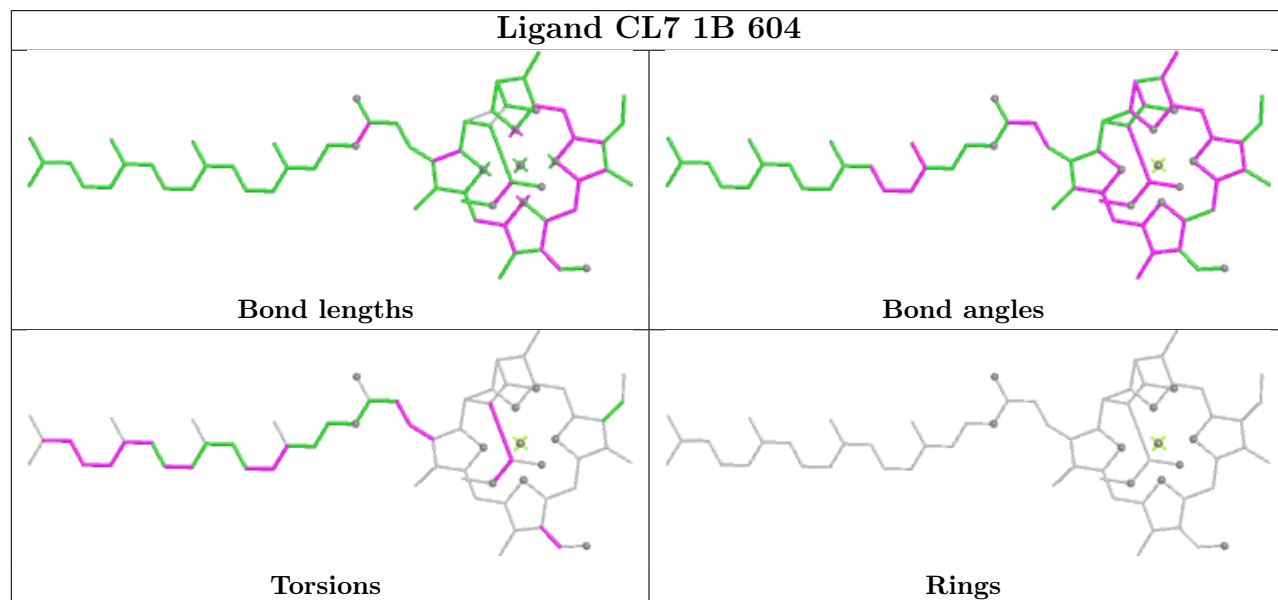
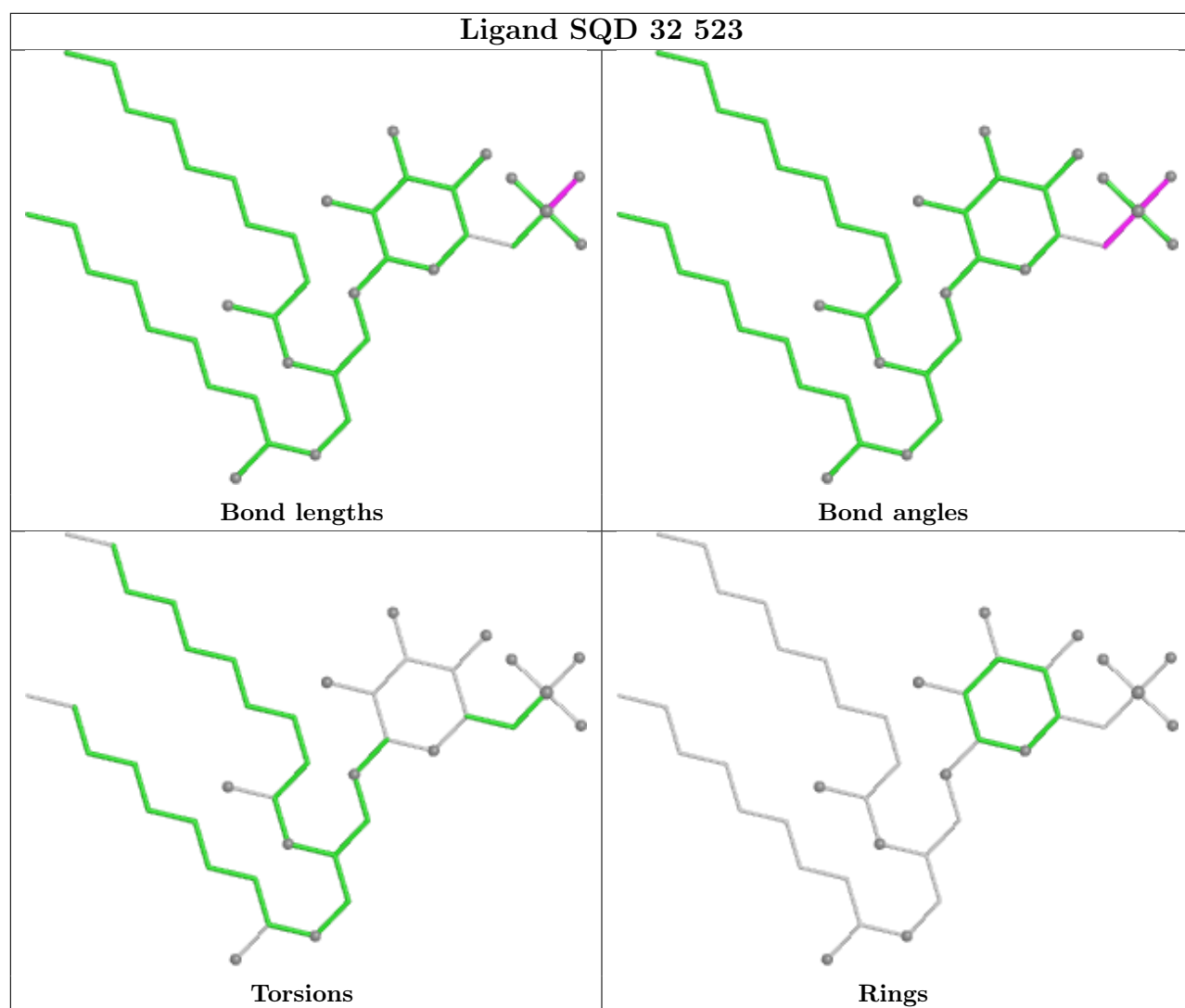


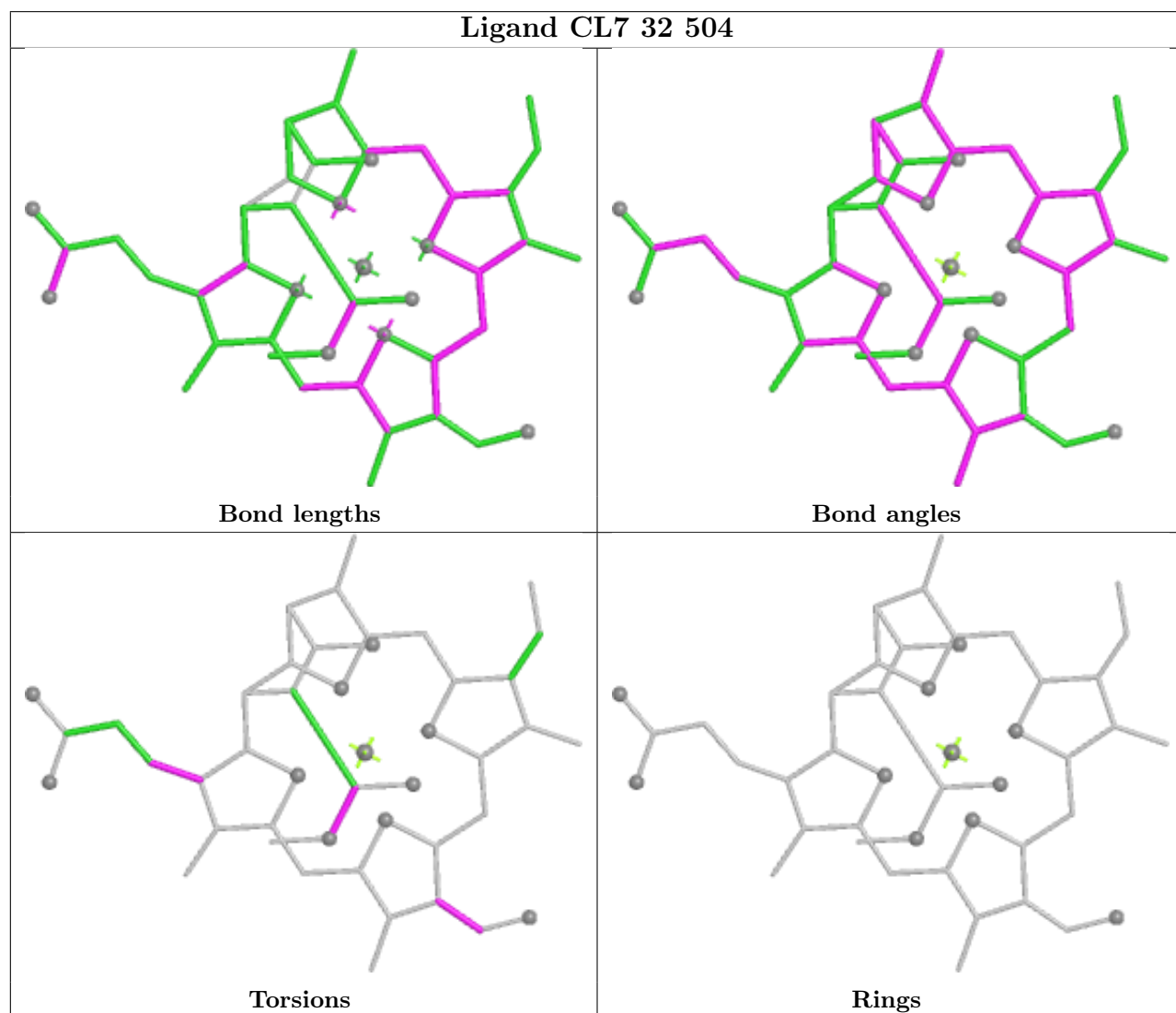
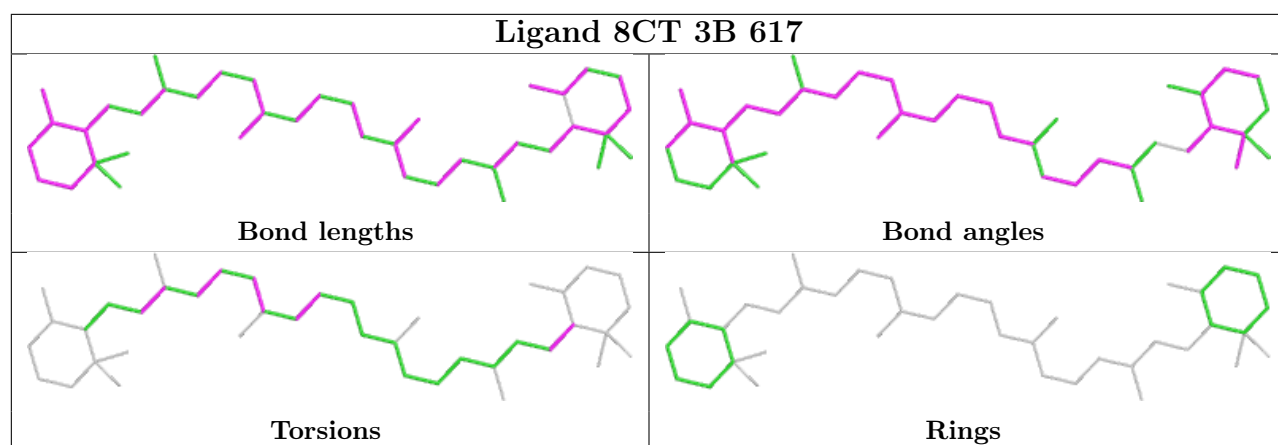


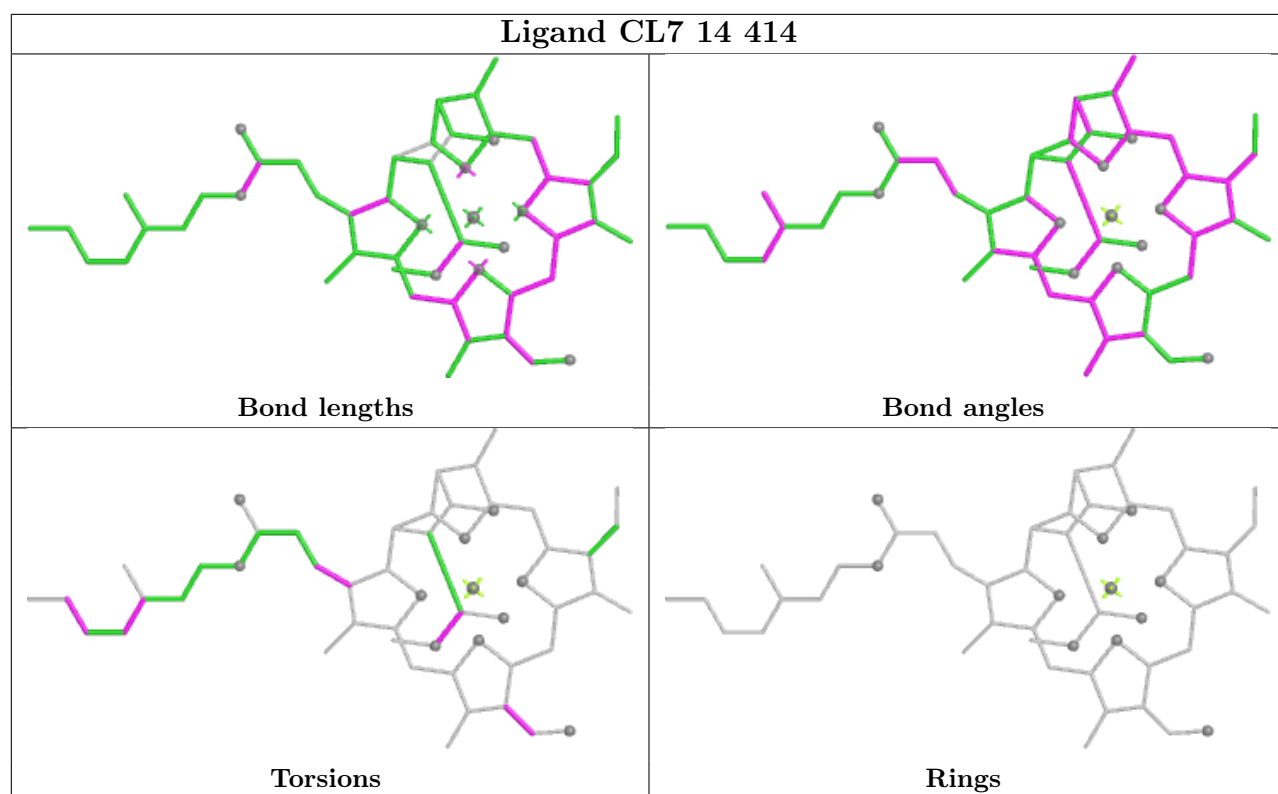




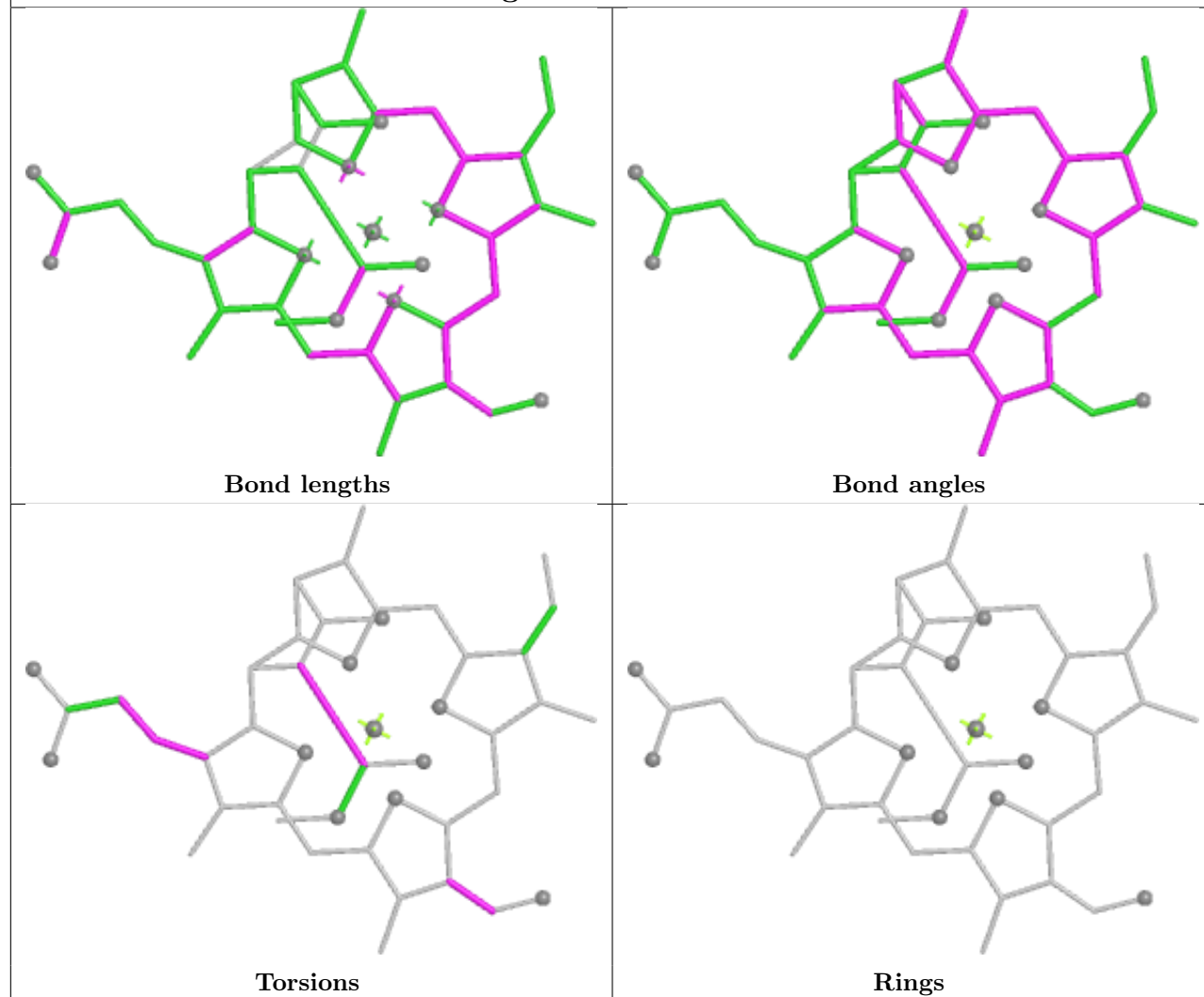




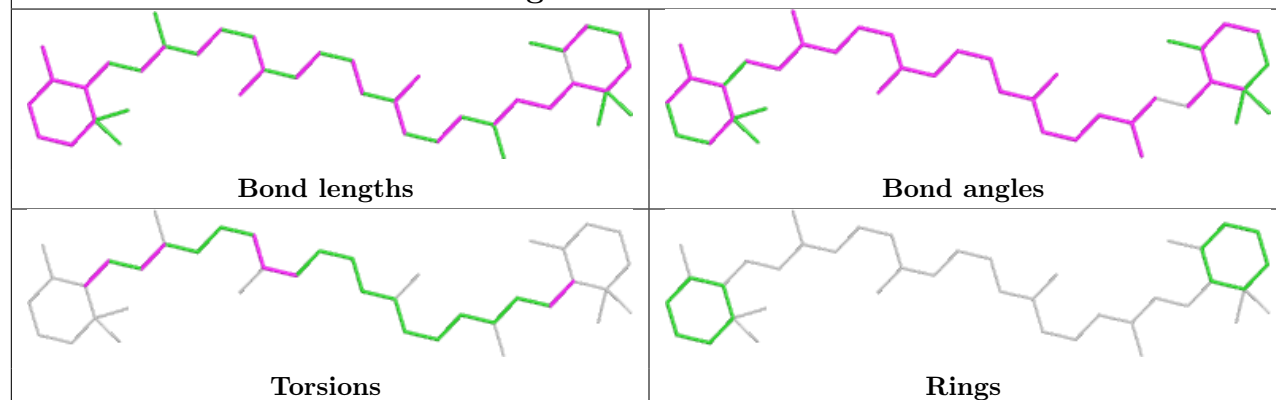


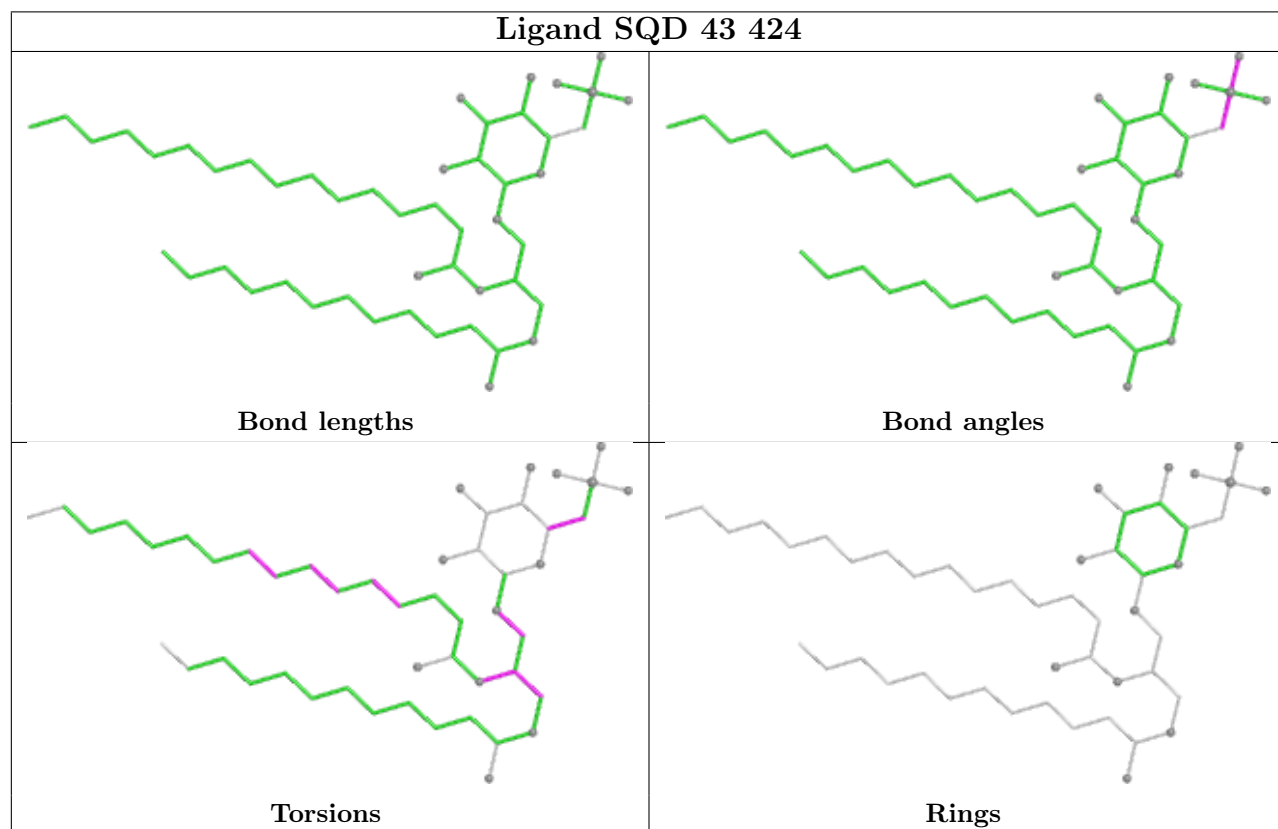
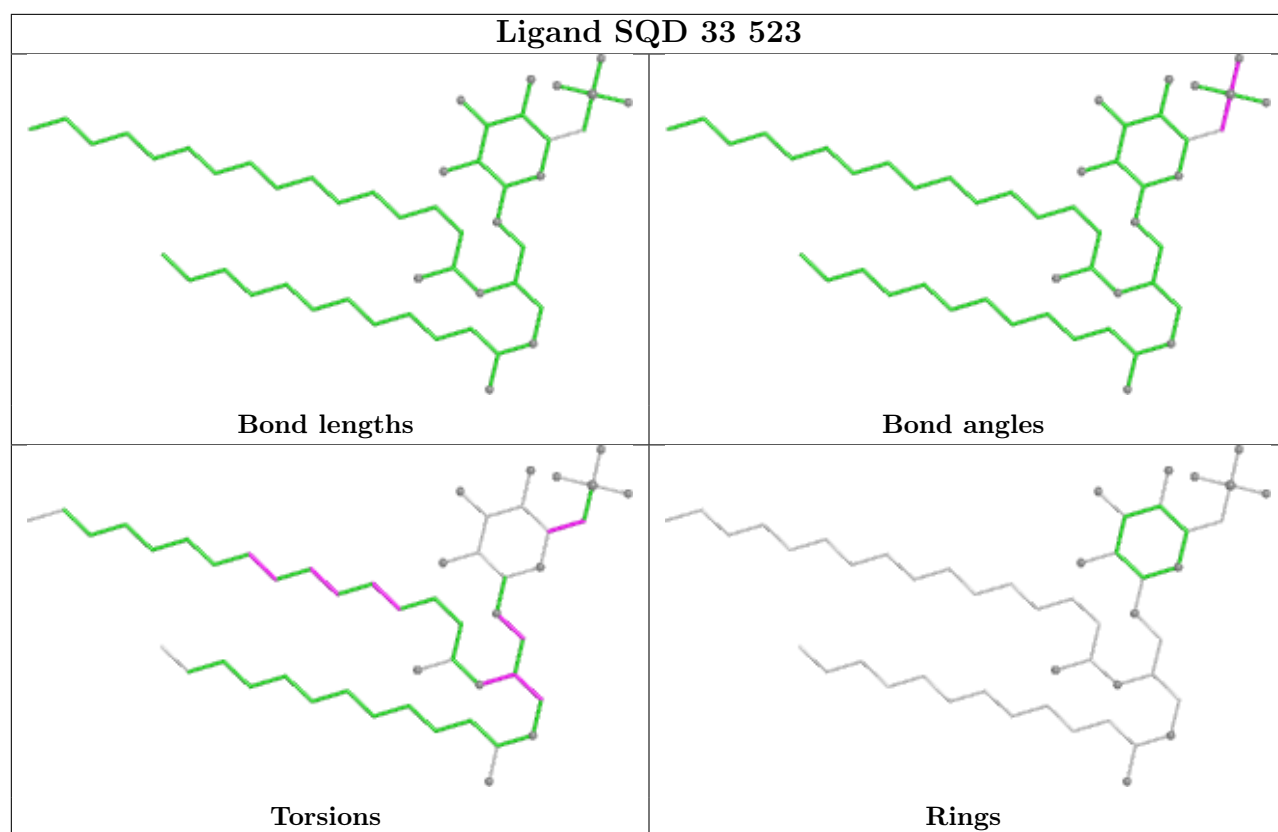


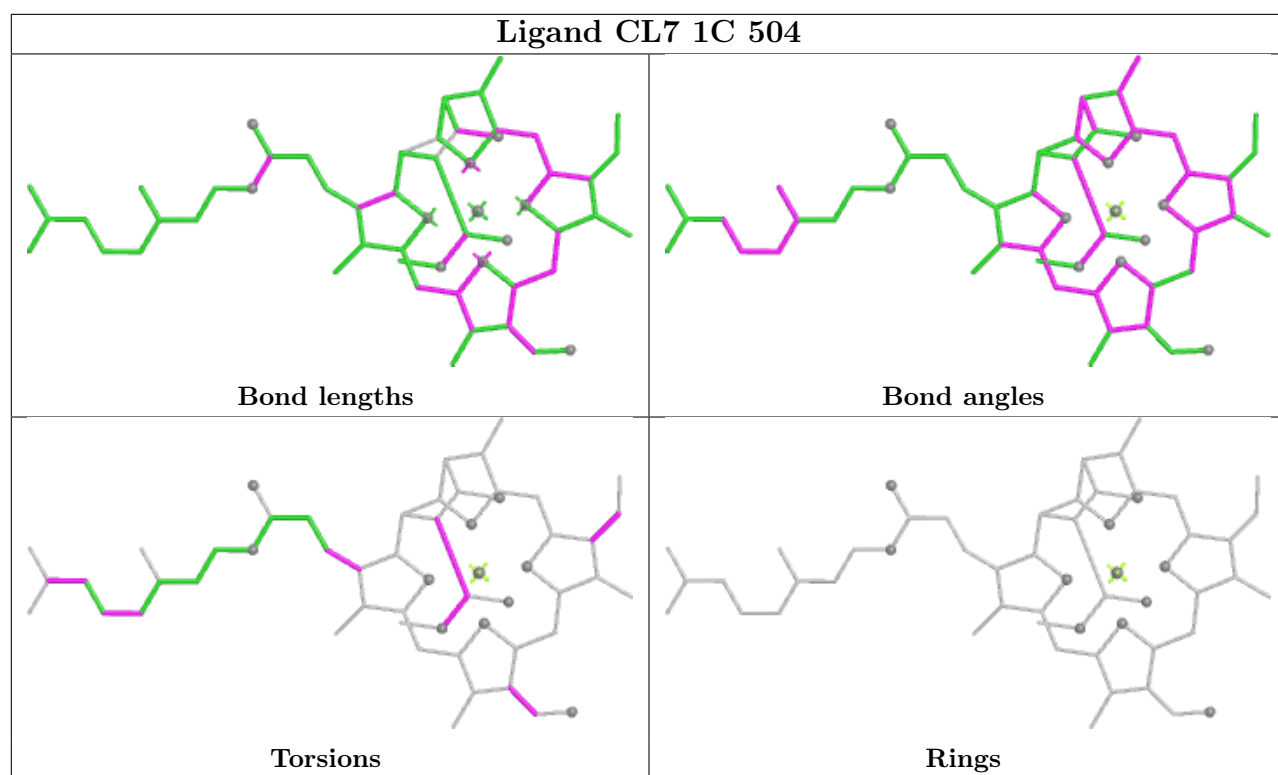
Ligand CL7 22 508



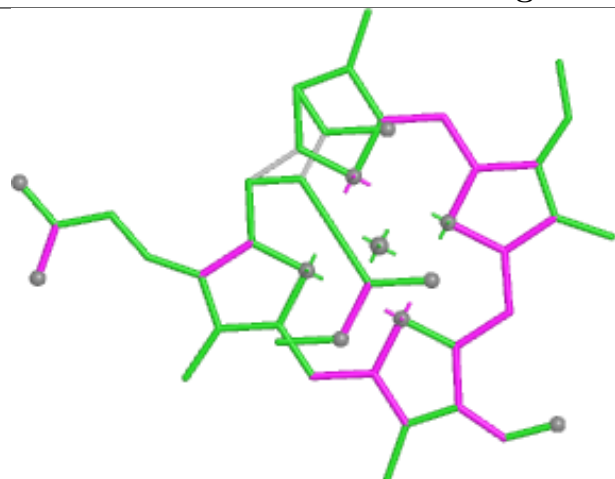
Ligand 8CT 3B 626



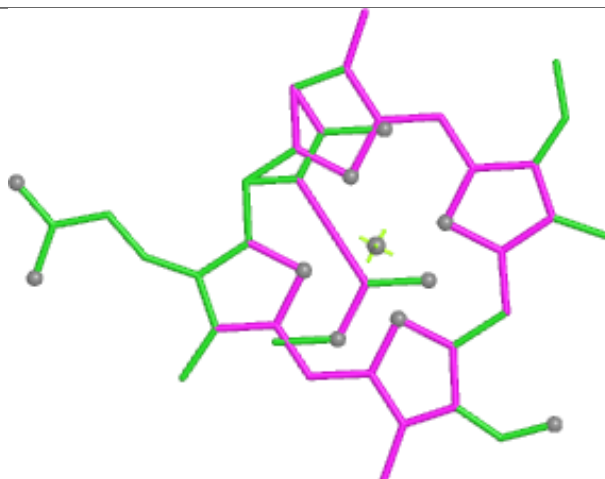




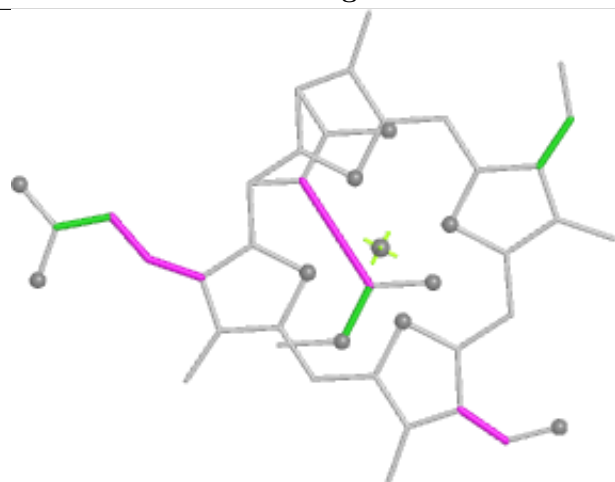
Ligand CL7 12 508



Bond lengths



Bond angles

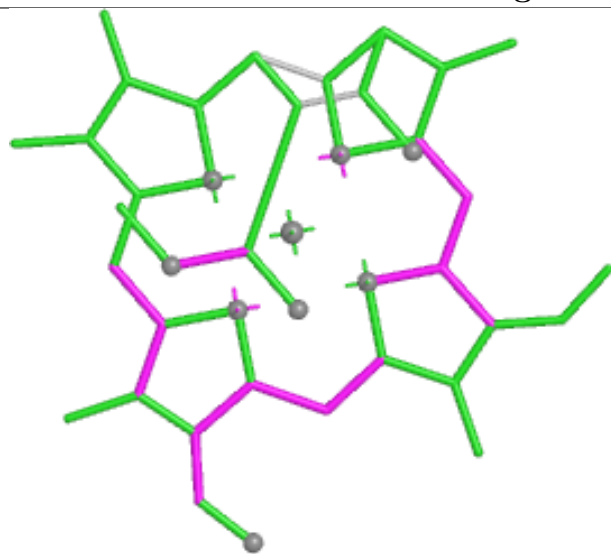


Torsions

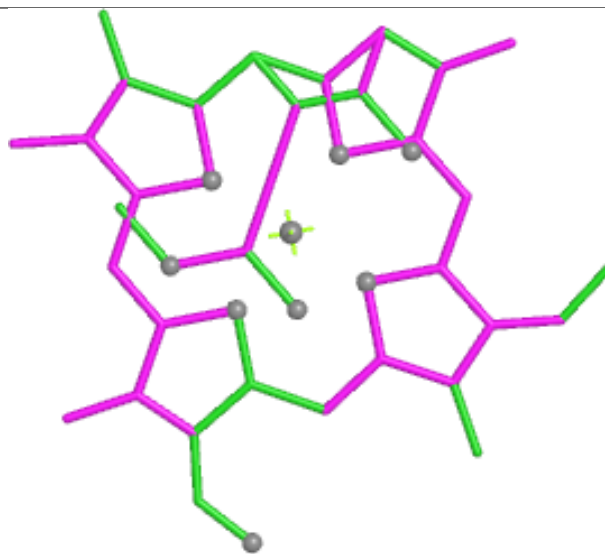


Rings

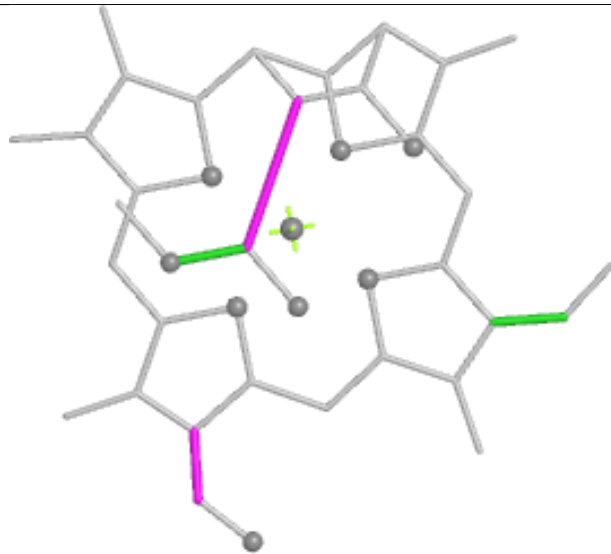
Ligand CL7 14 407



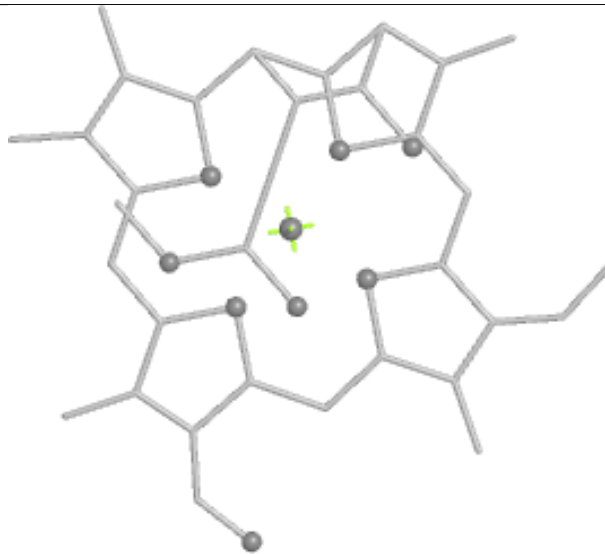
Bond lengths



Bond angles

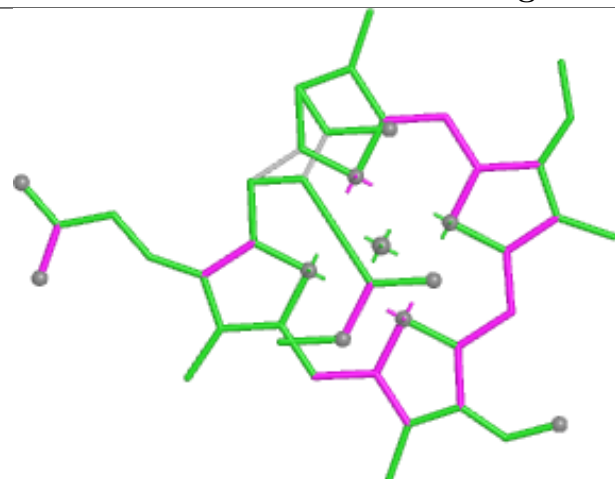


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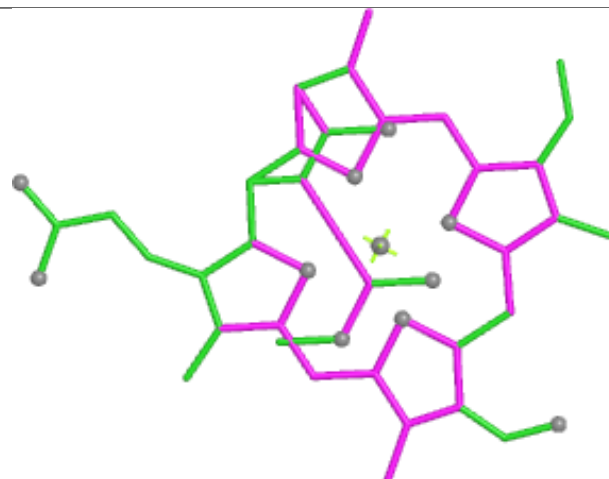


Rings

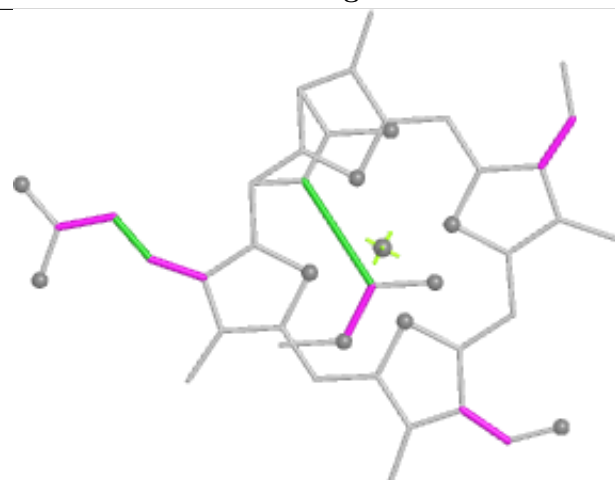
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Bond lengths



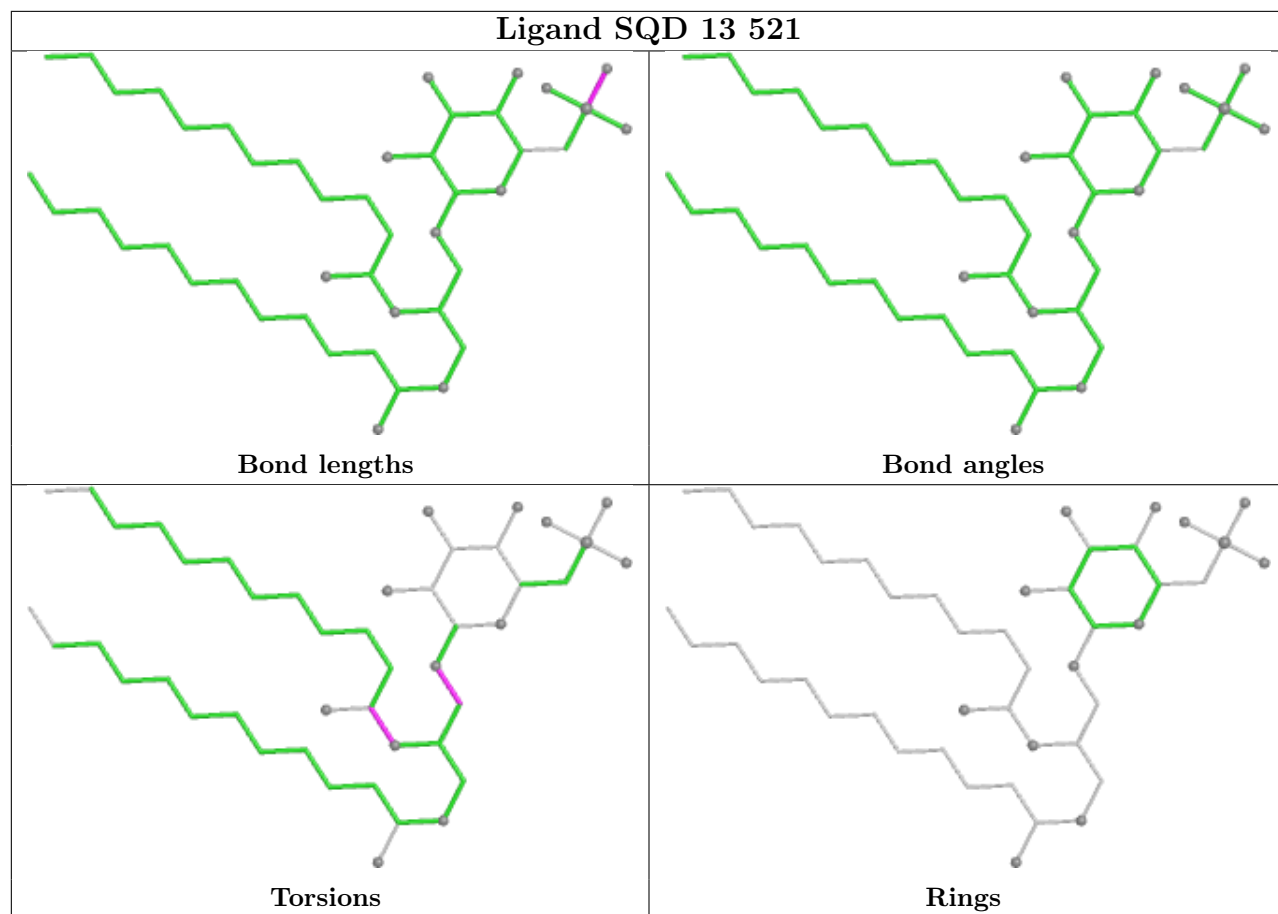
Bond angles

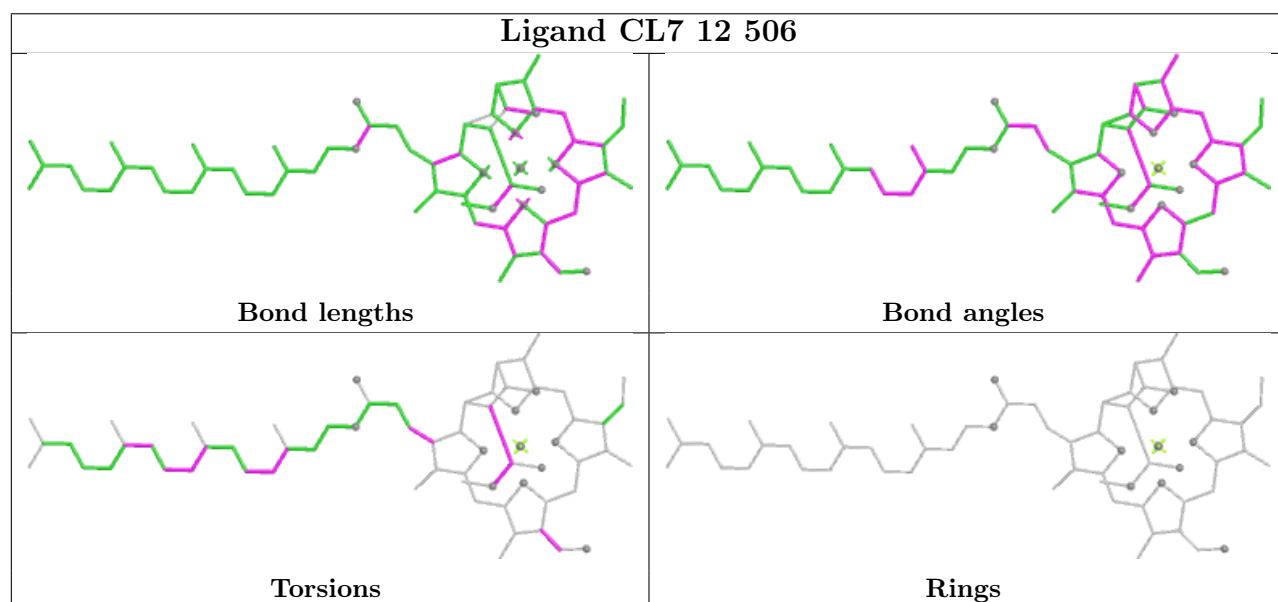
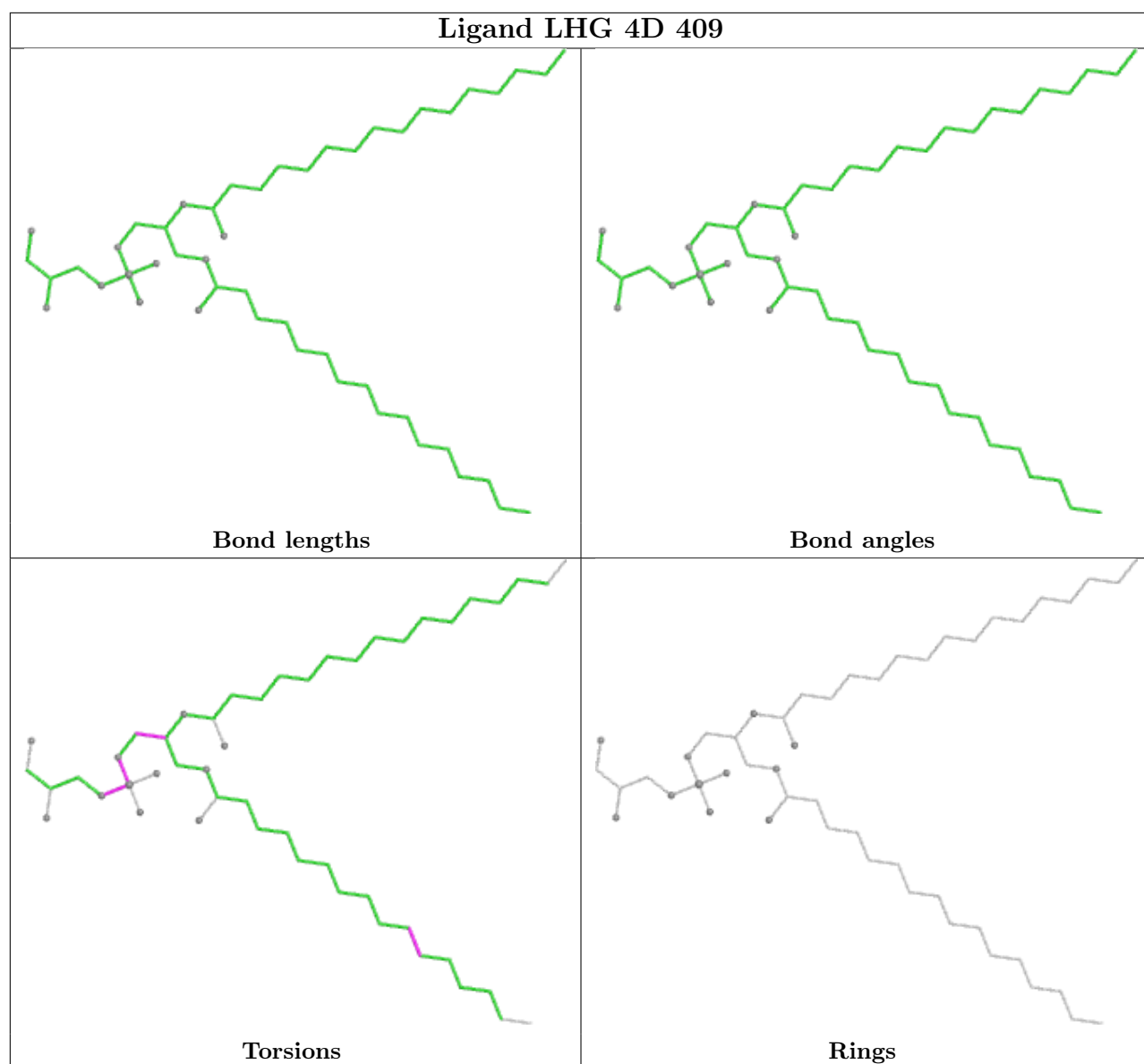


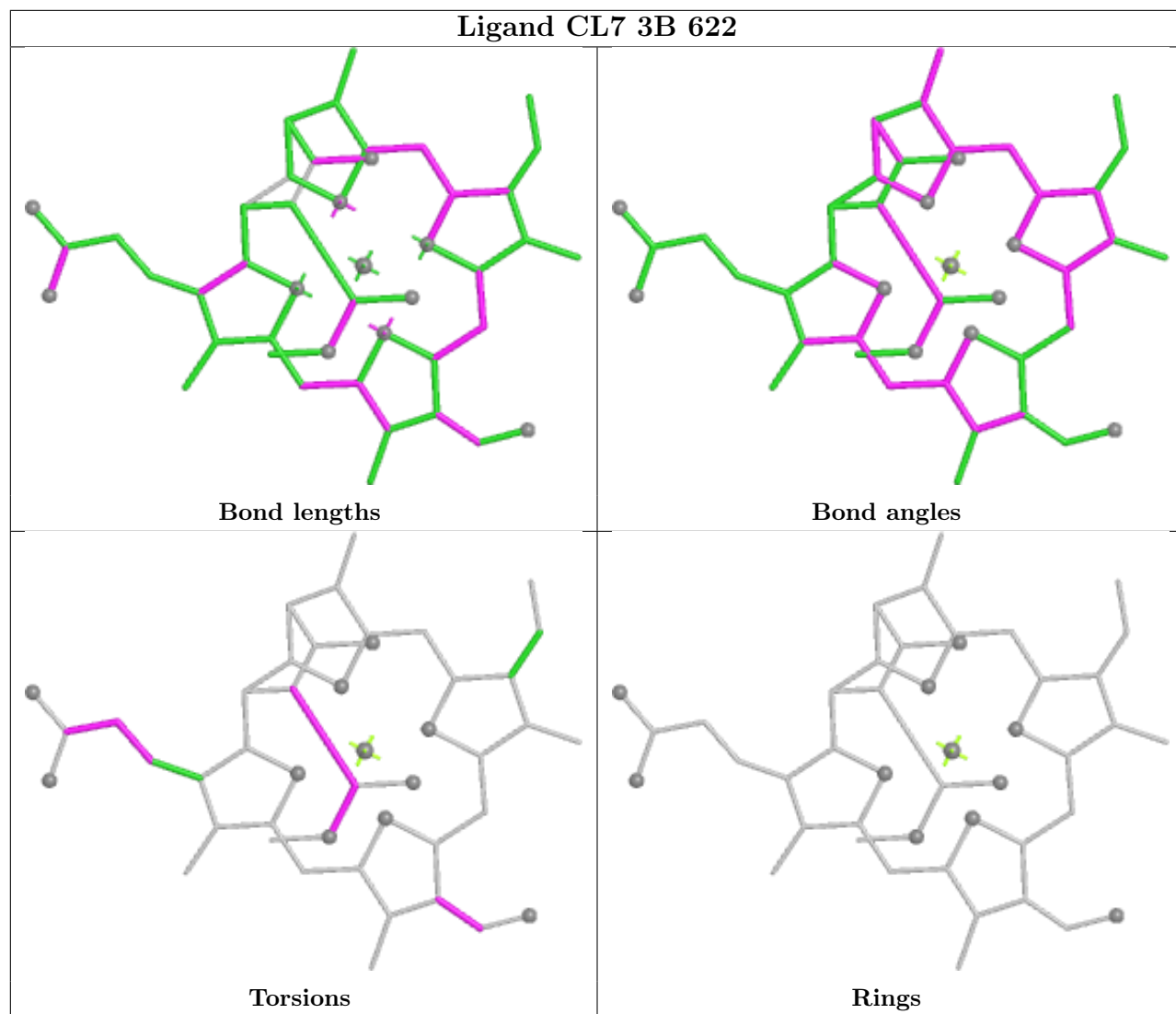
Torsions

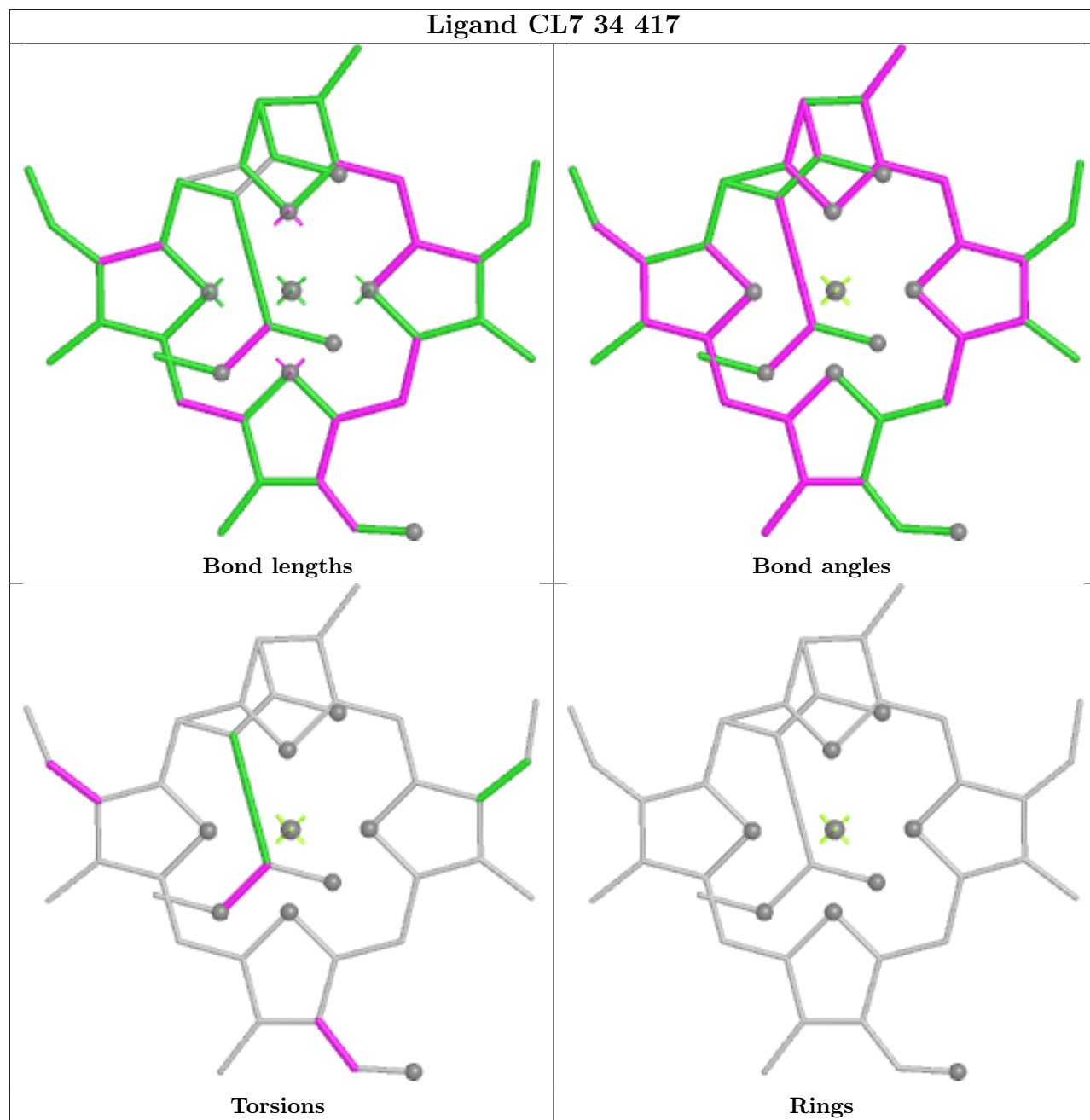


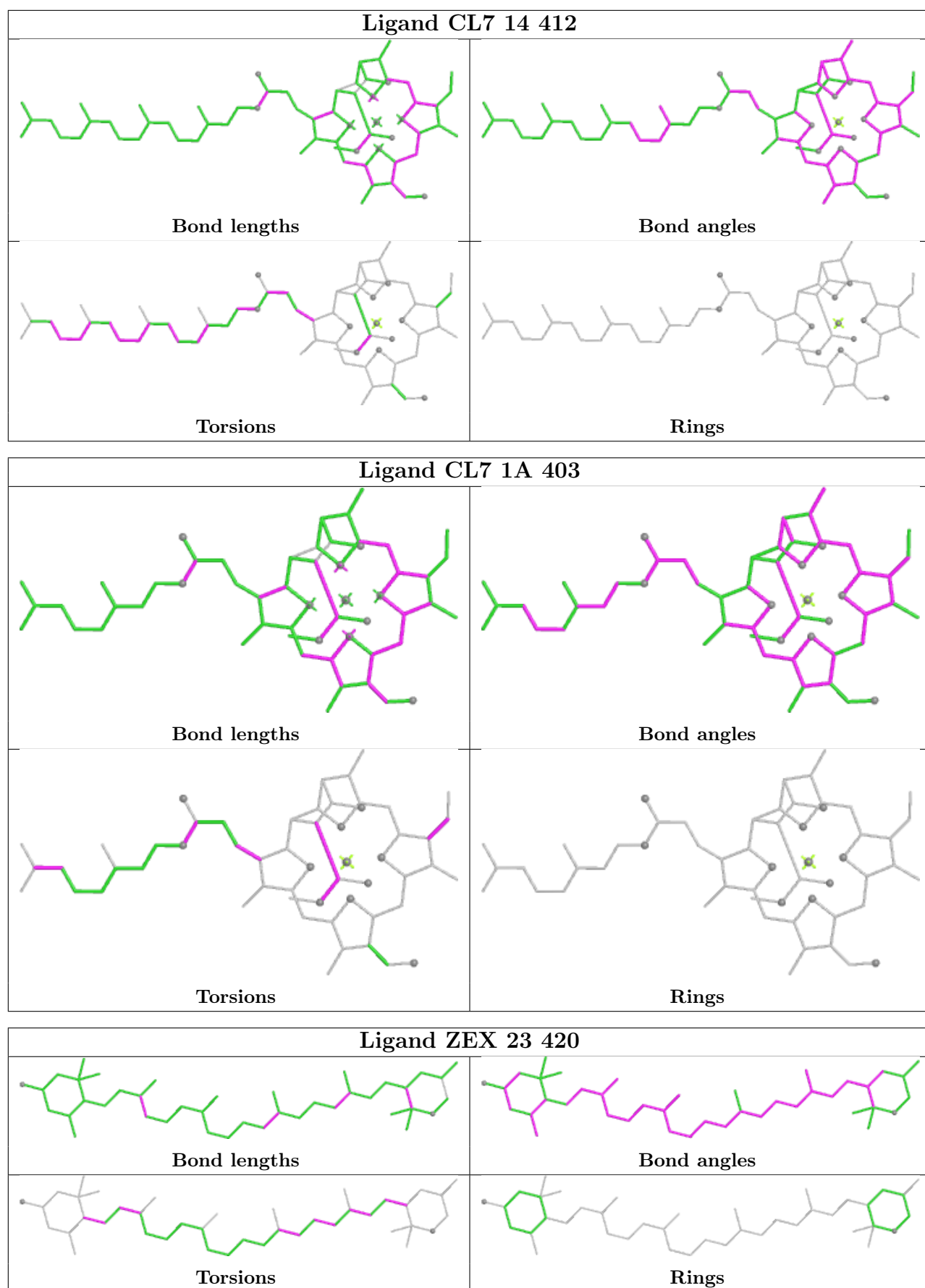
Rings

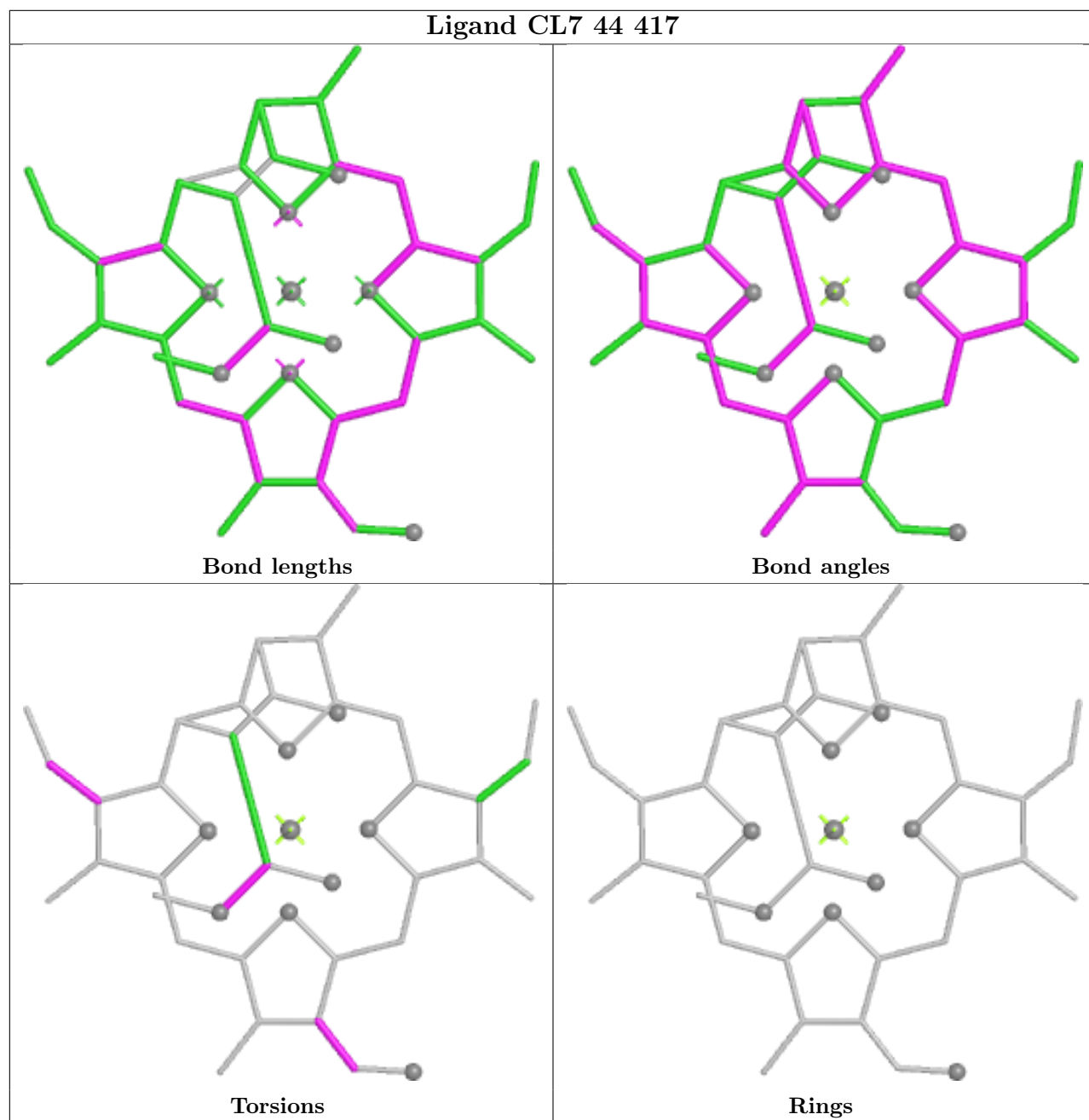
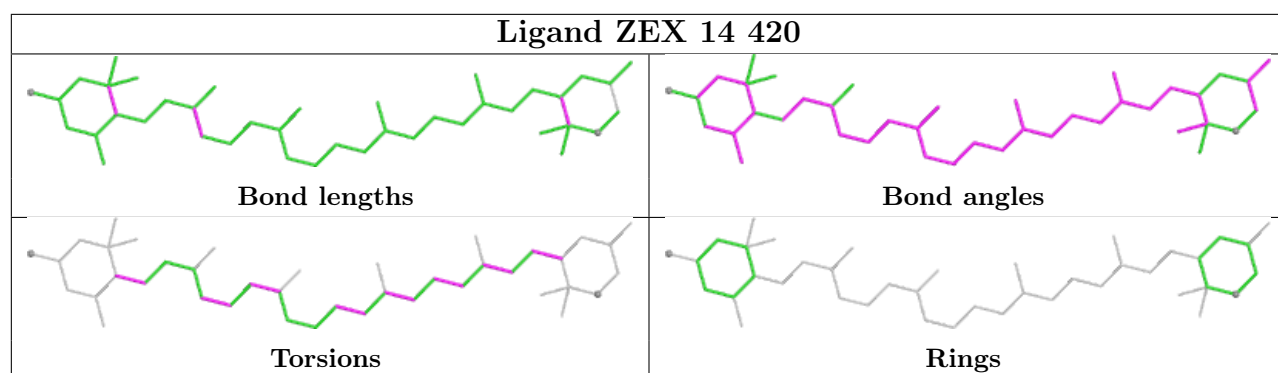


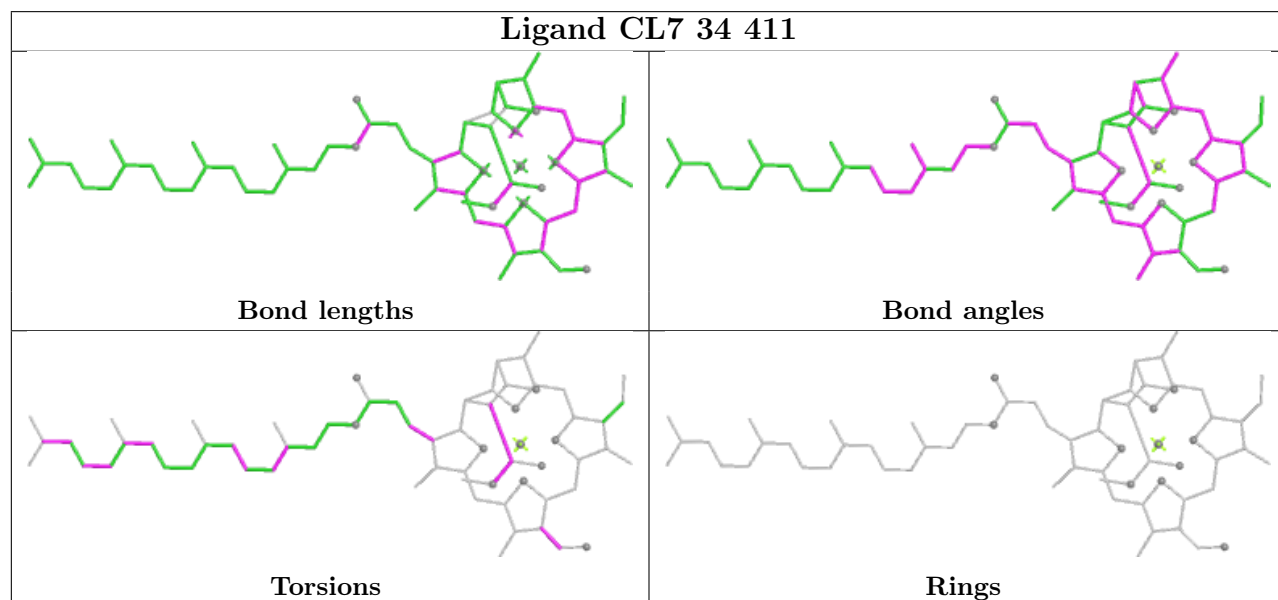
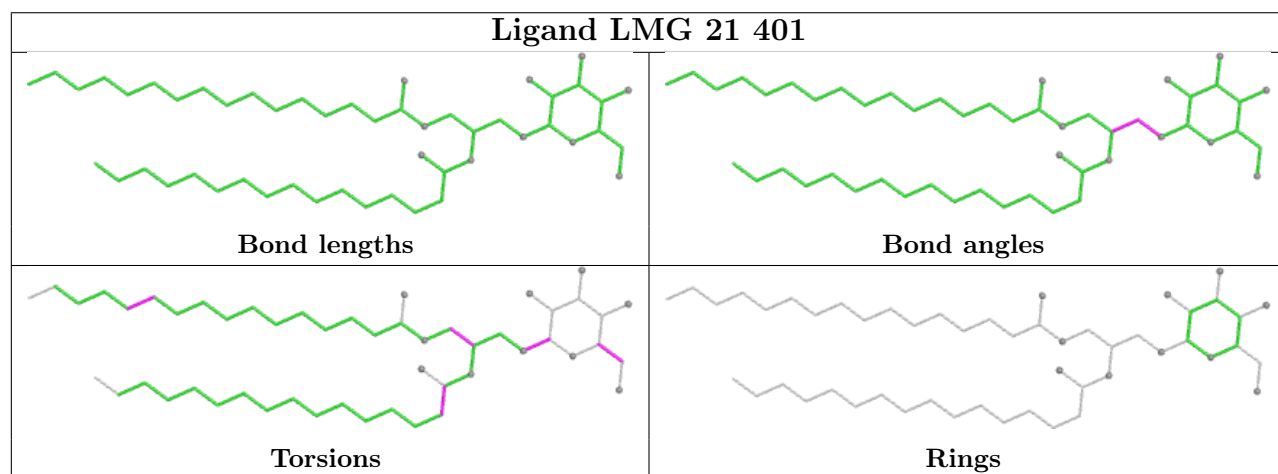
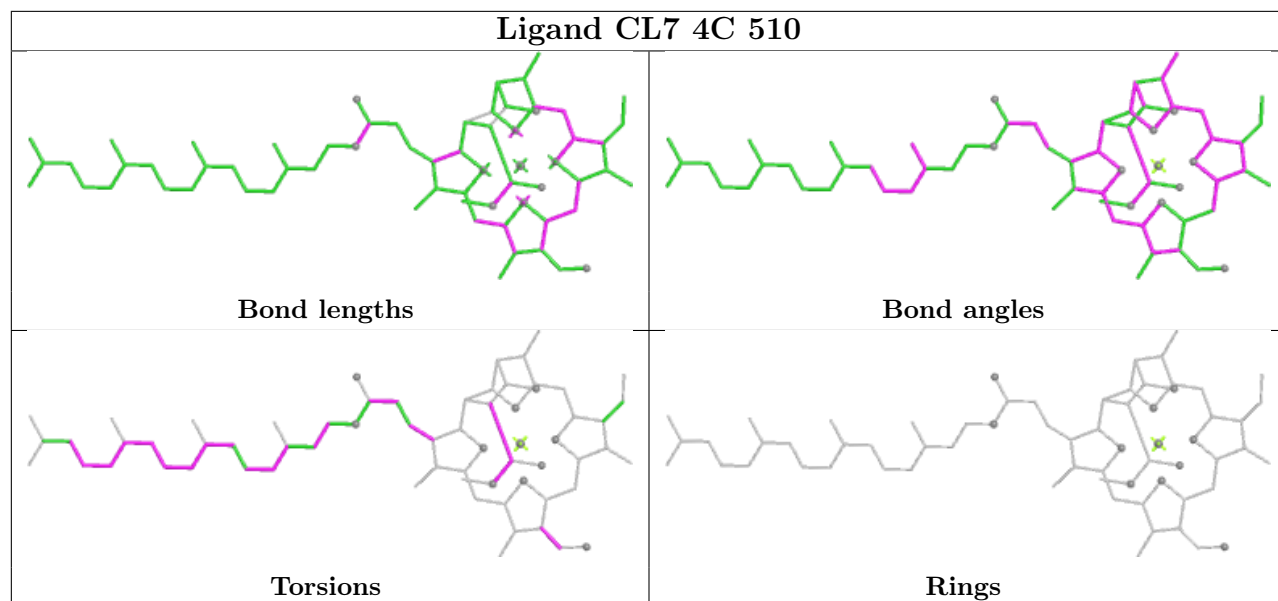




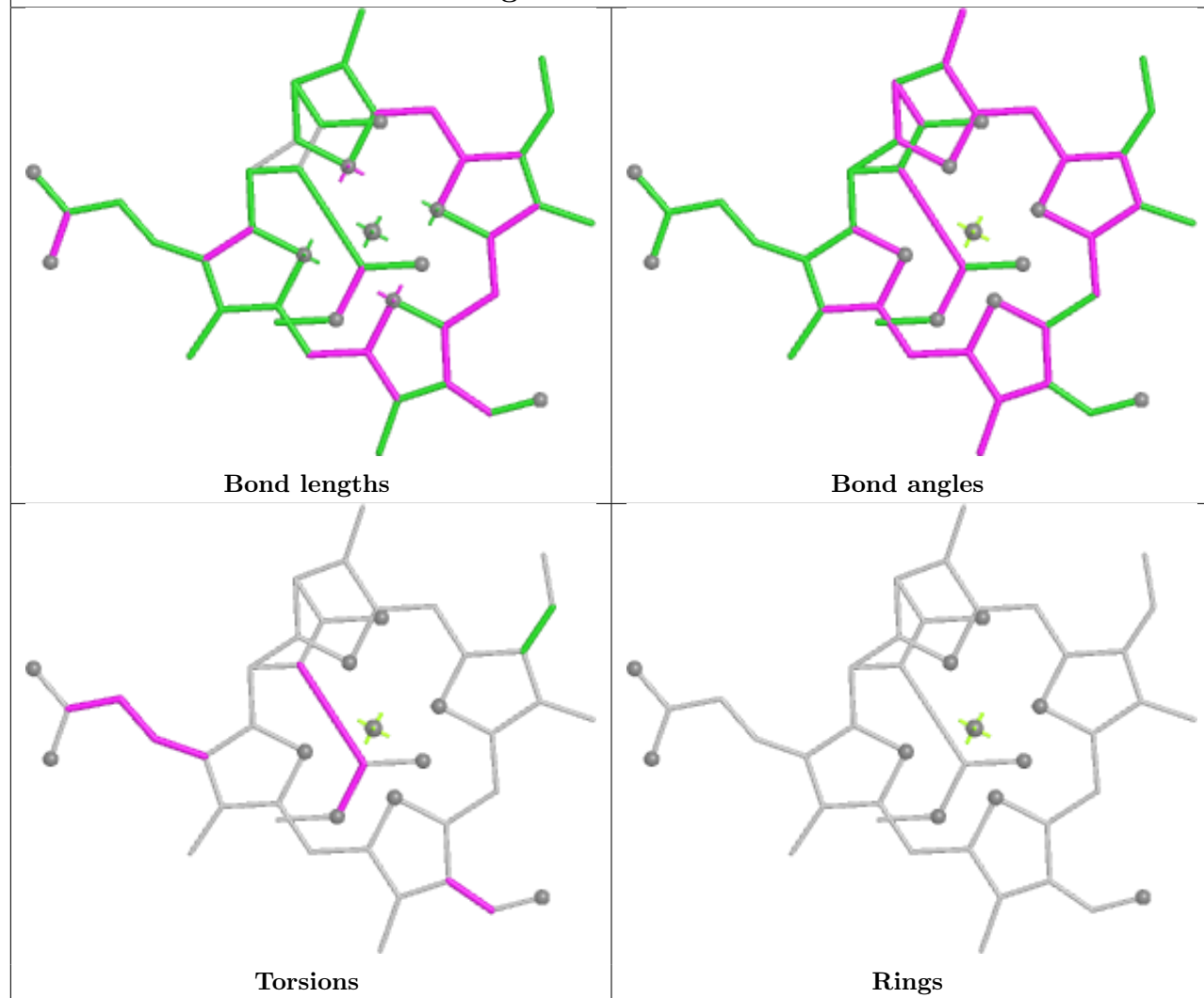




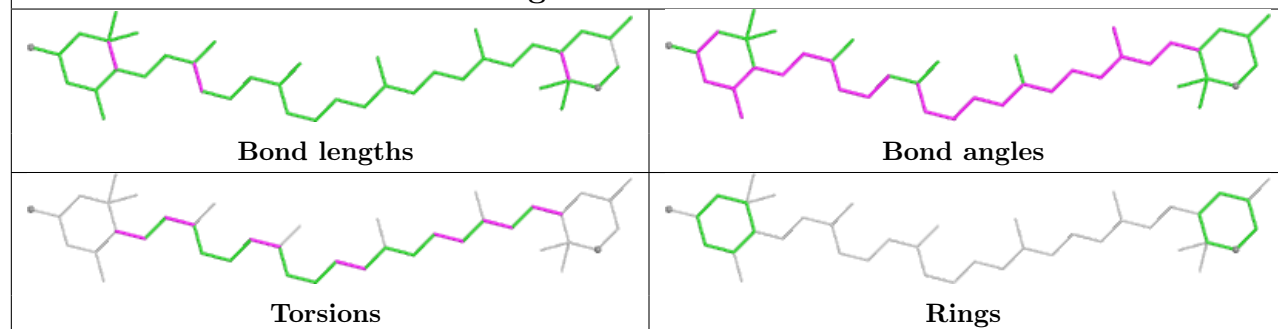


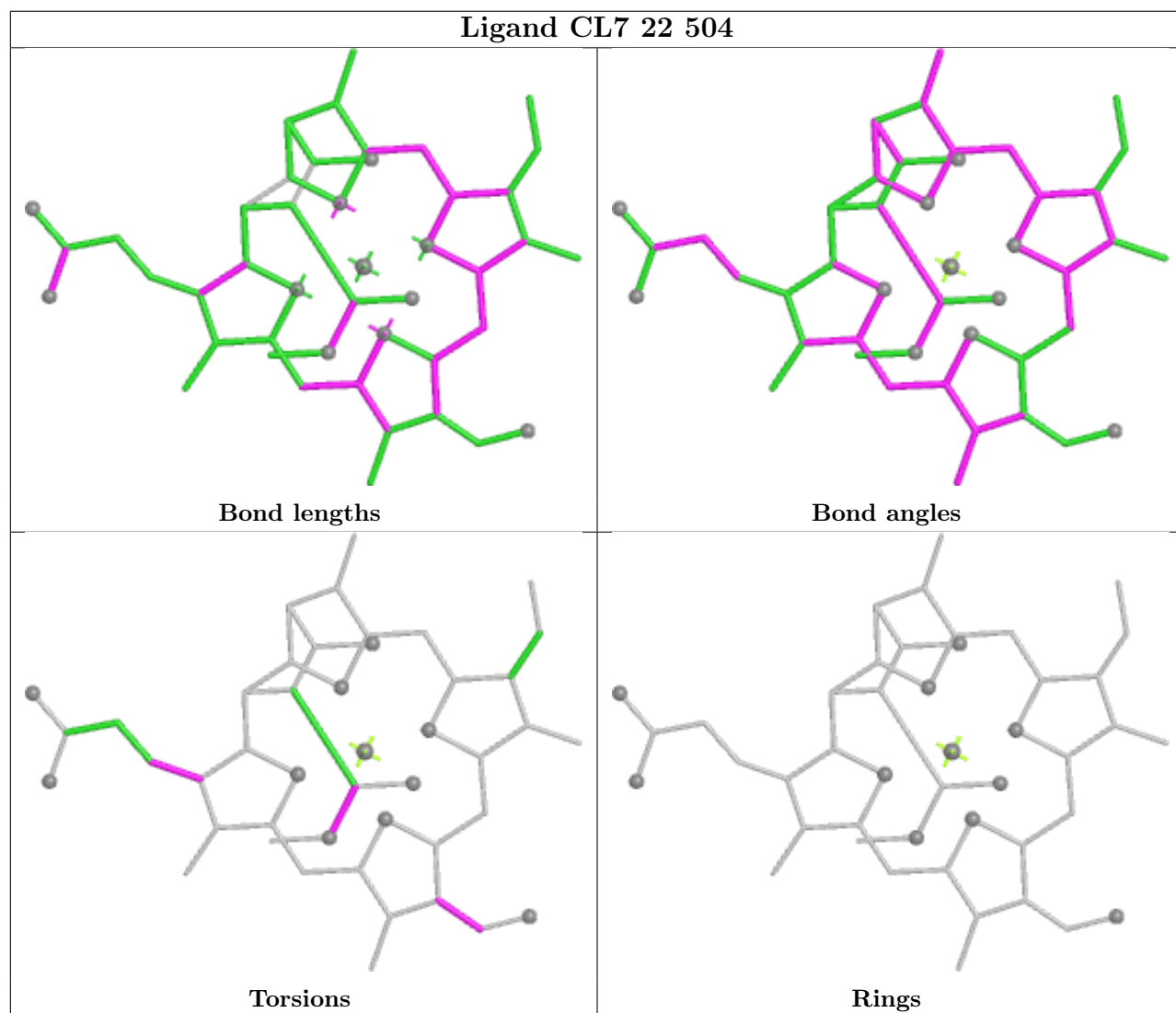
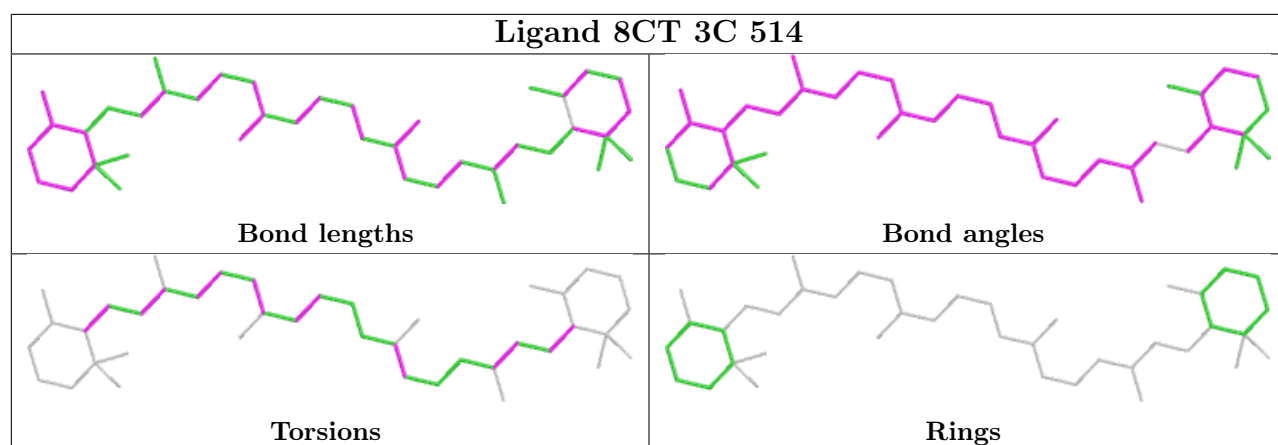


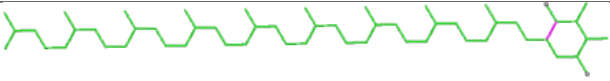
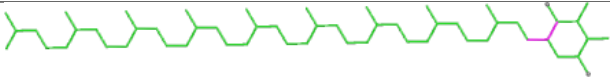
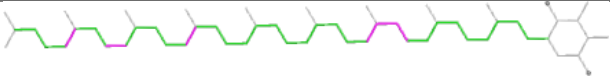
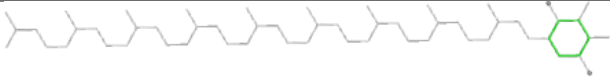
Ligand CL7 34 410

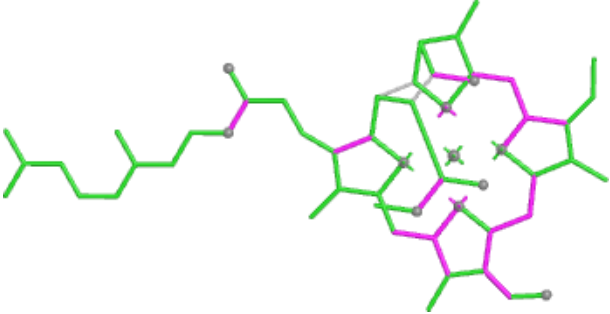
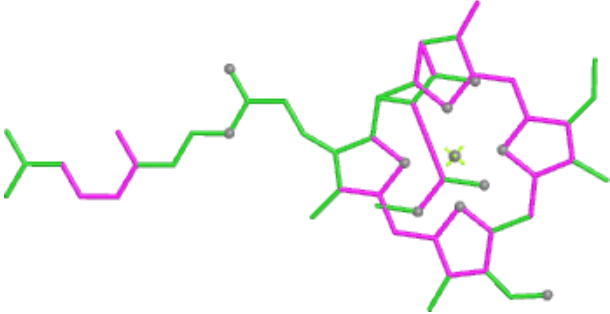
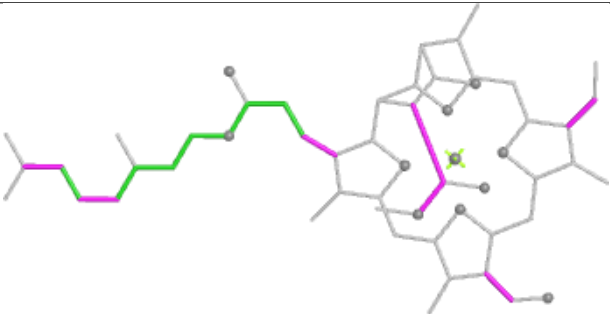
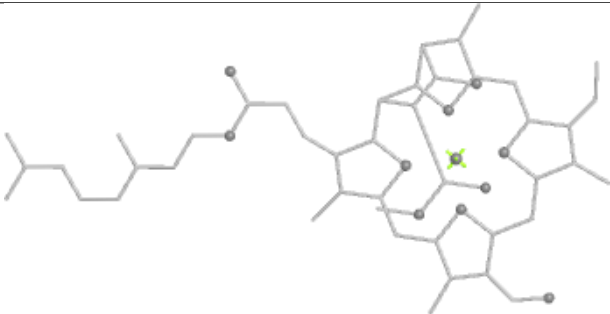


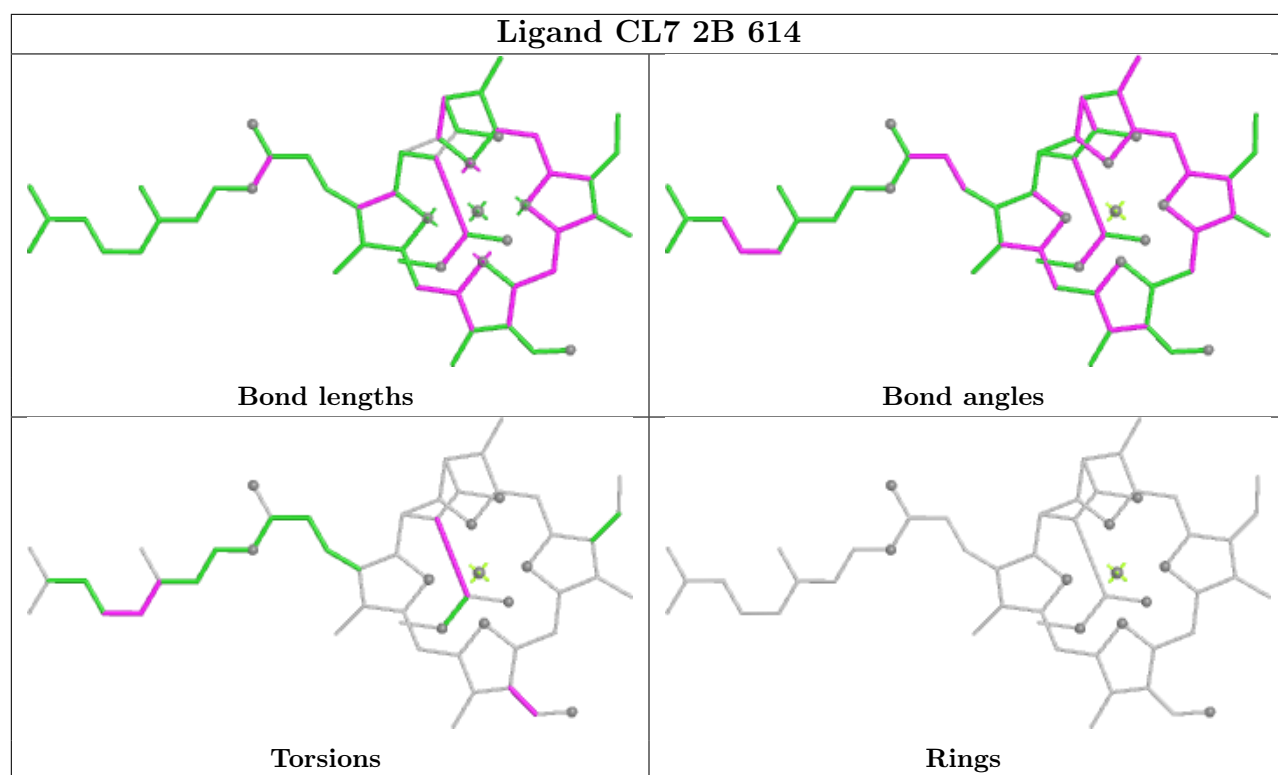
Ligand ZEX 32 519



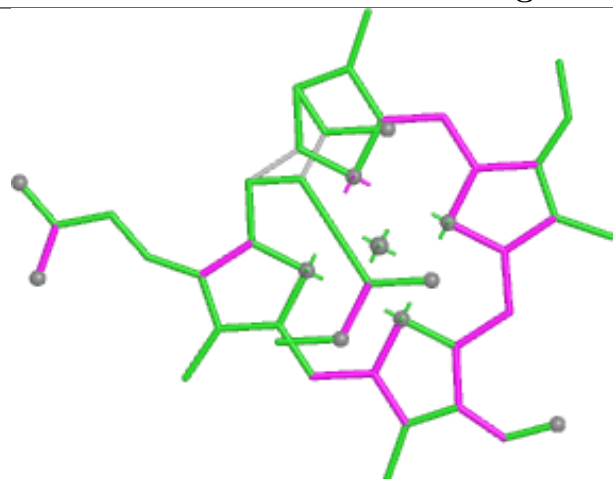


Ligand PL9 2D 407			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

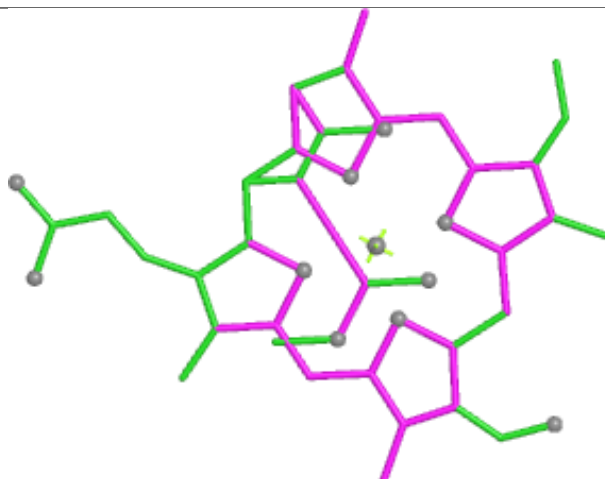
Ligand CL7 2C 504			
			
Bond lengths		Bond angles	
			
Torsions		Rings	



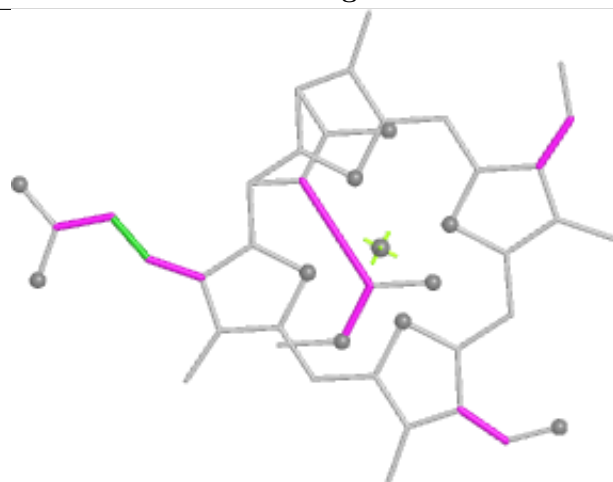
Ligand CL7 43 407



Bond lengths



Bond angles

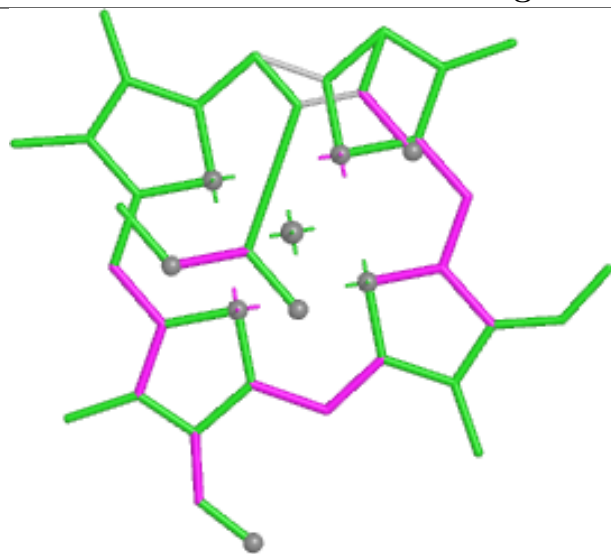


Torsions

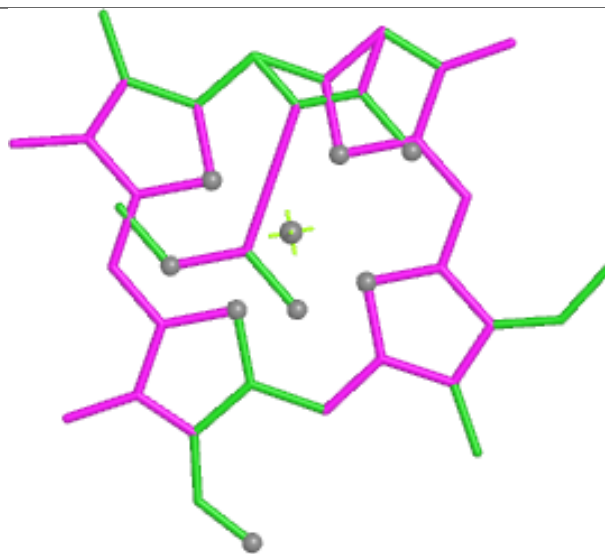


Rings

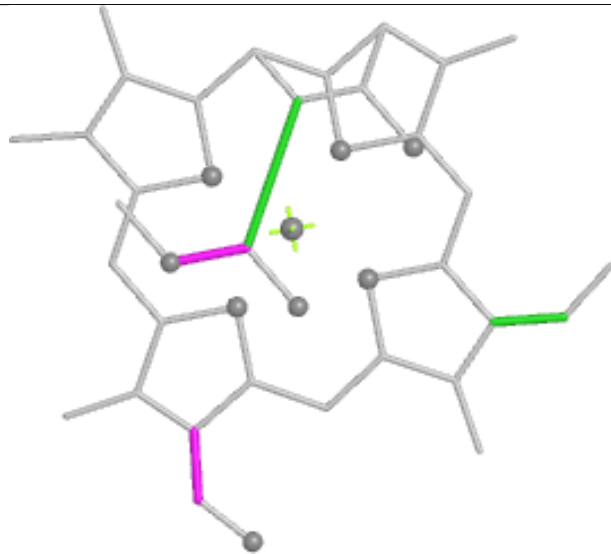
Ligand CL7 31 416



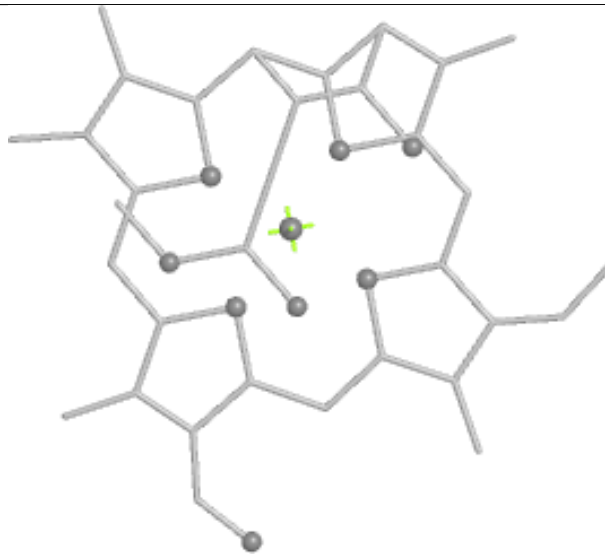
Bond lengths



Bond angles

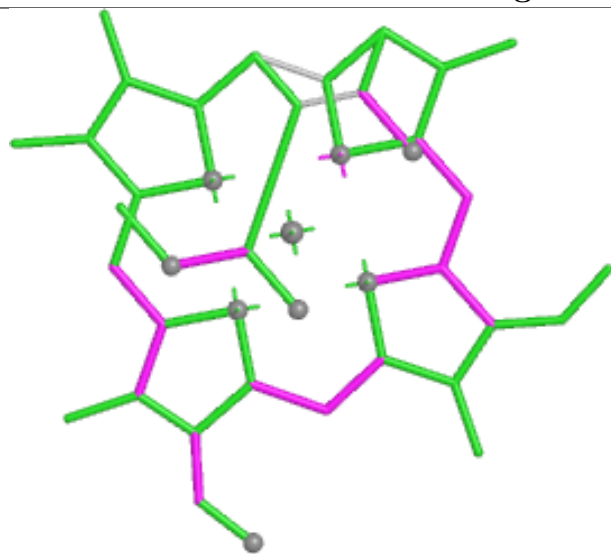


Torsions

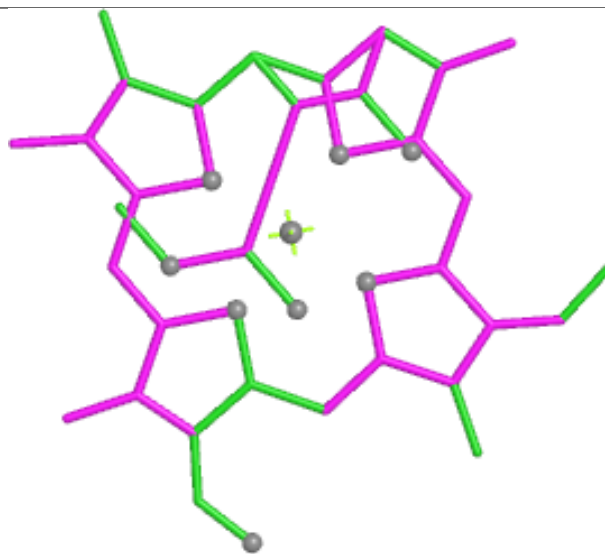


Rings

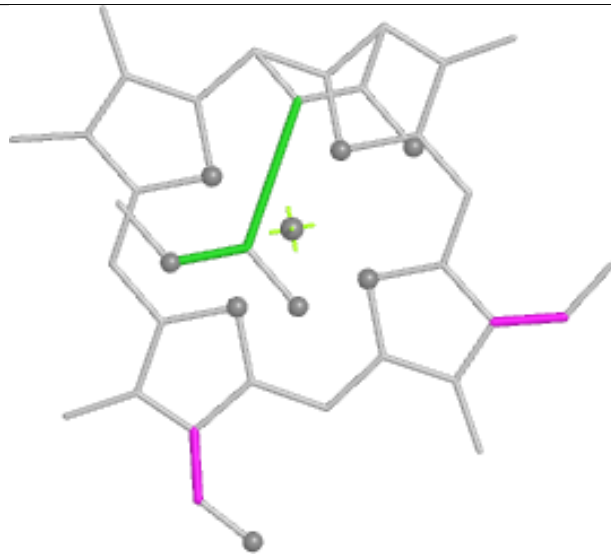
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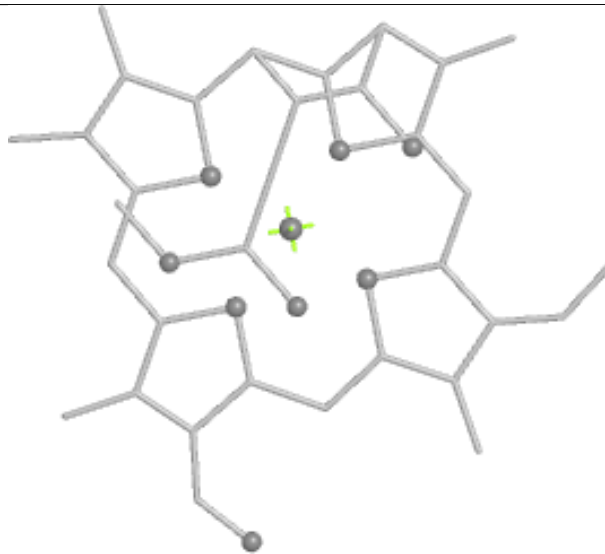
Bond lengths



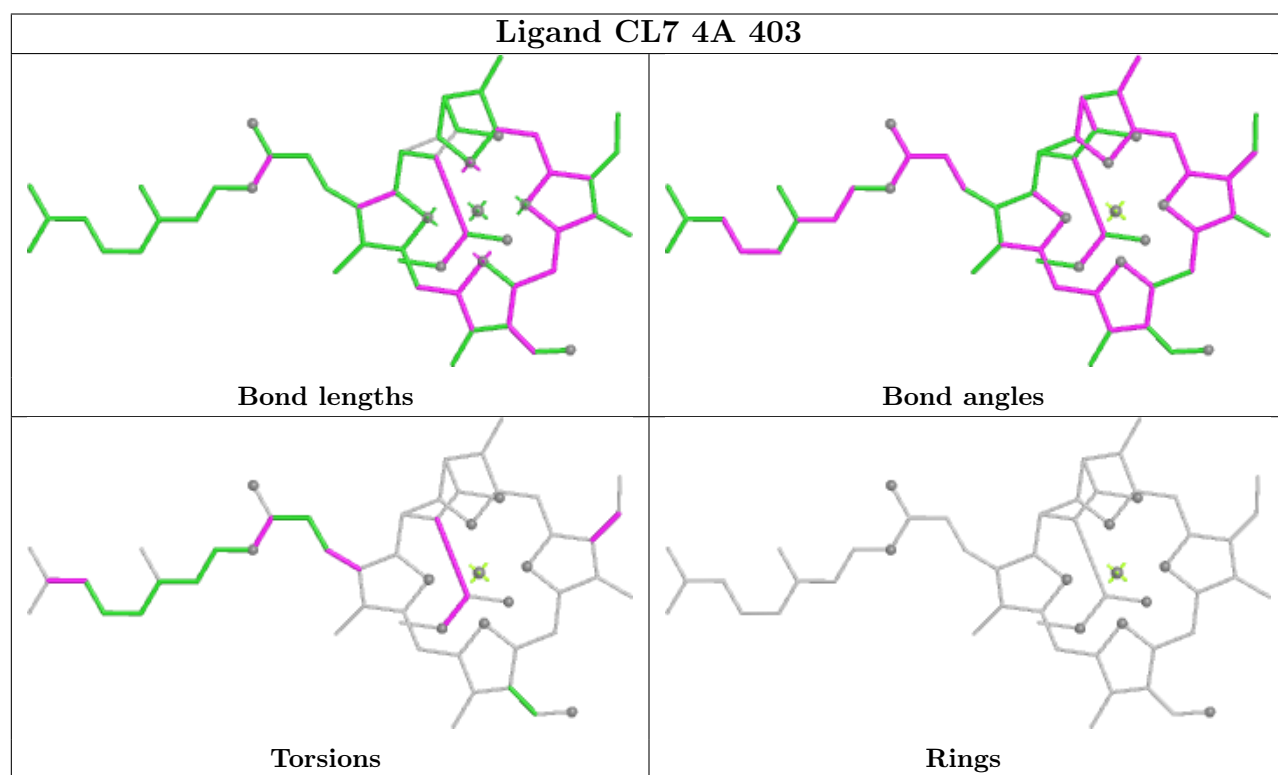
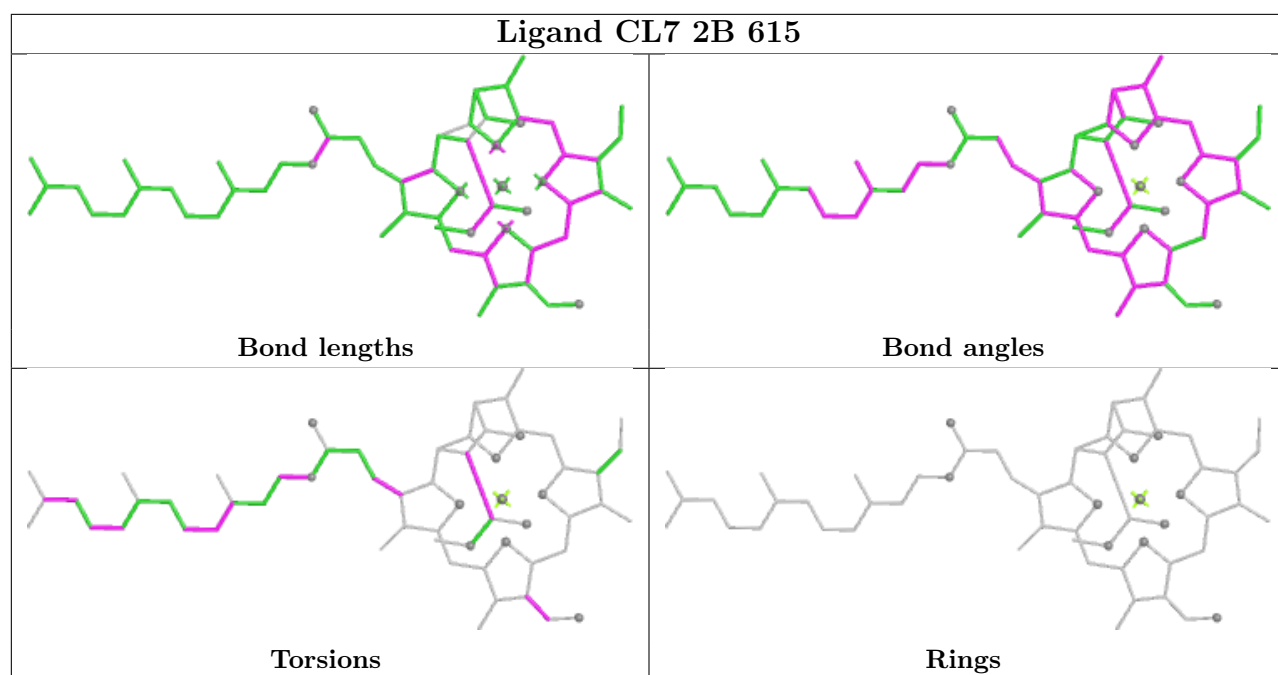
Bond angles

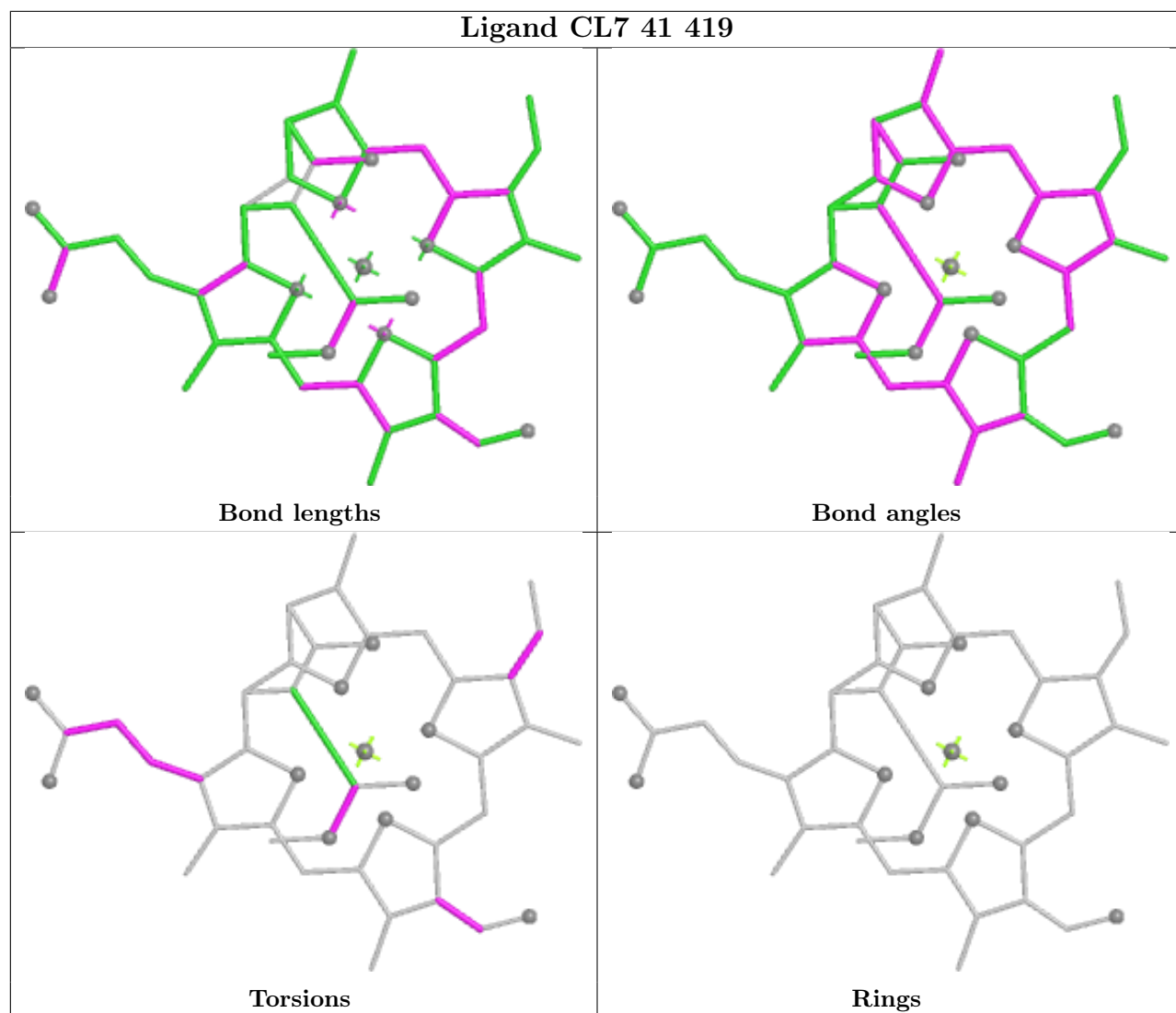
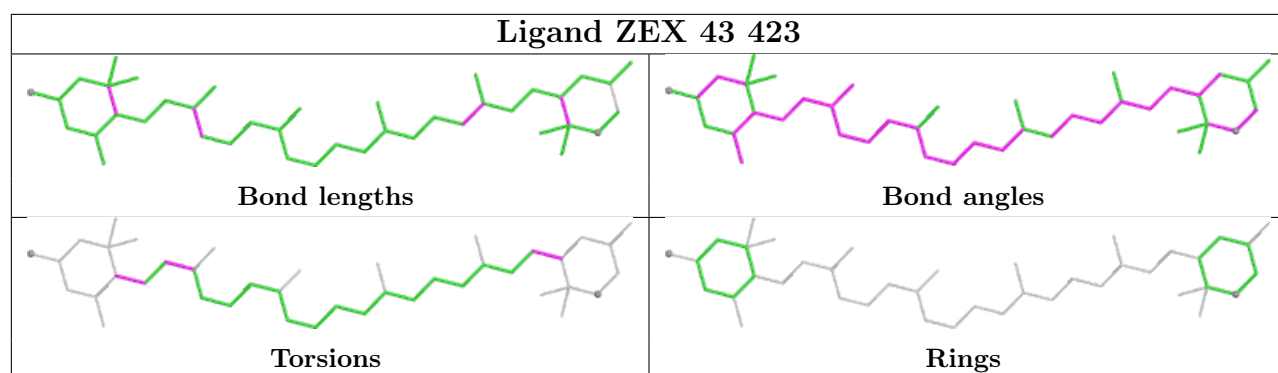


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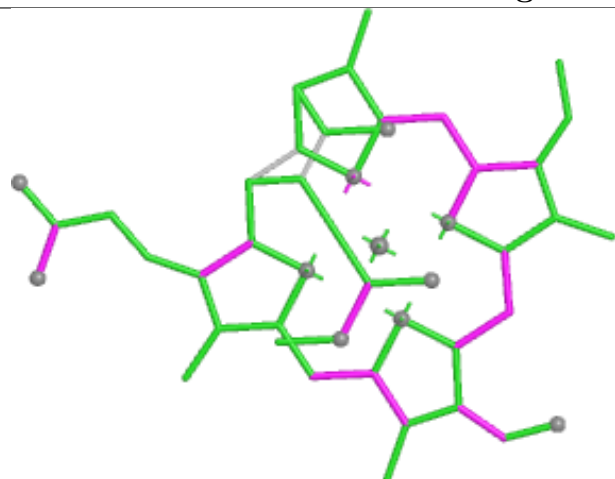


Rings

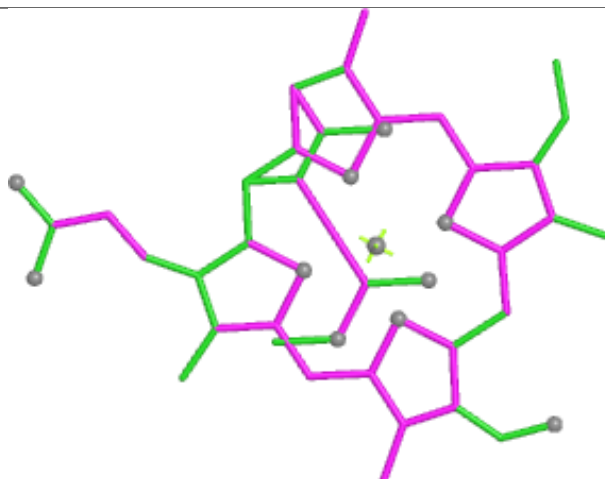




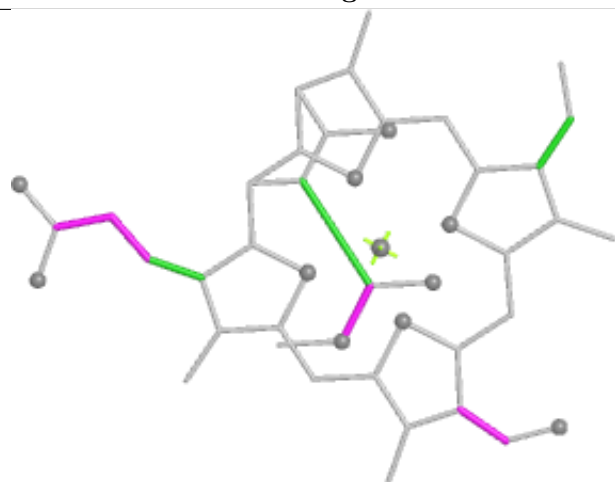
Ligand CL7 33 518



Bond lengths



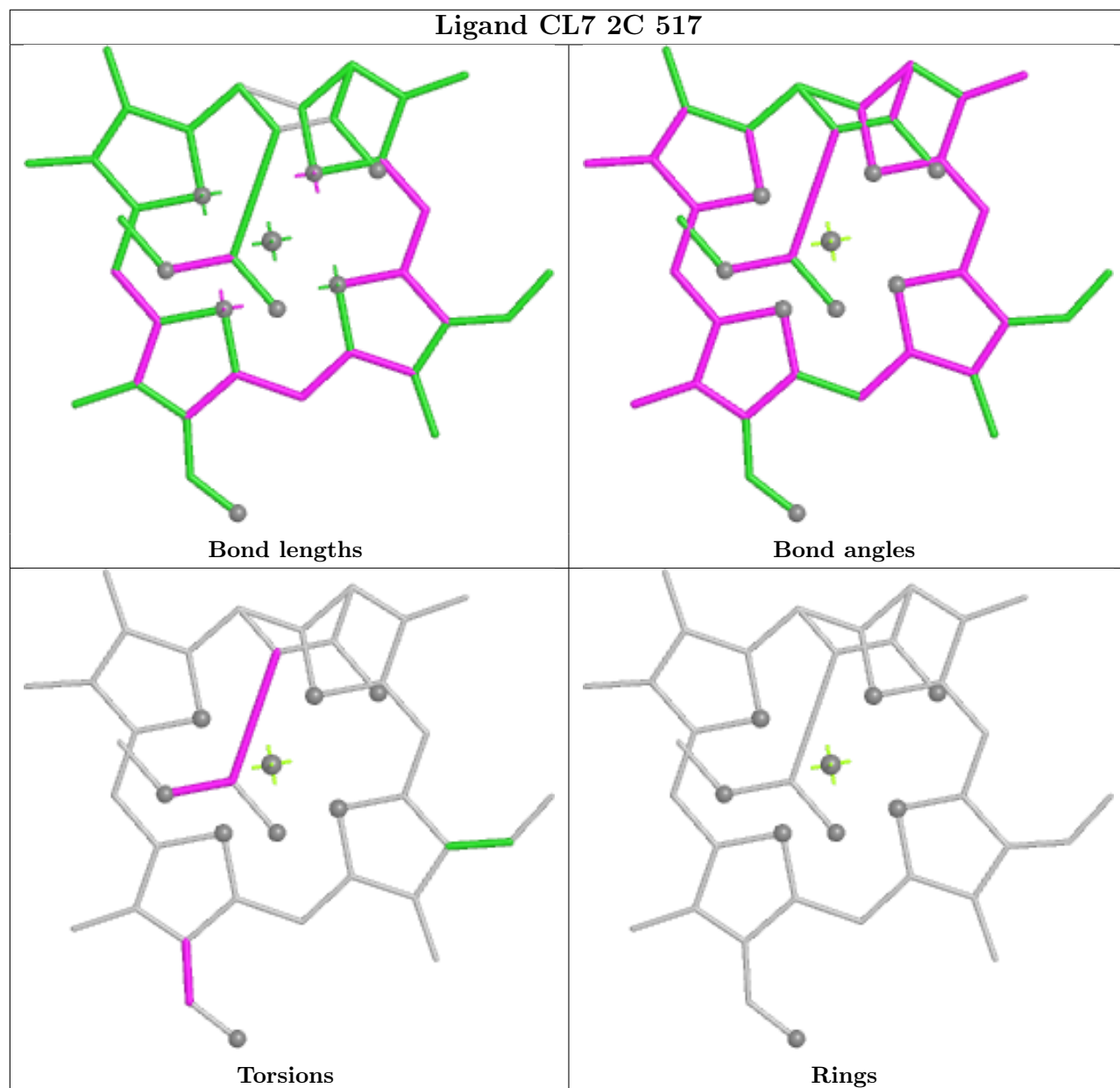
Bond angles

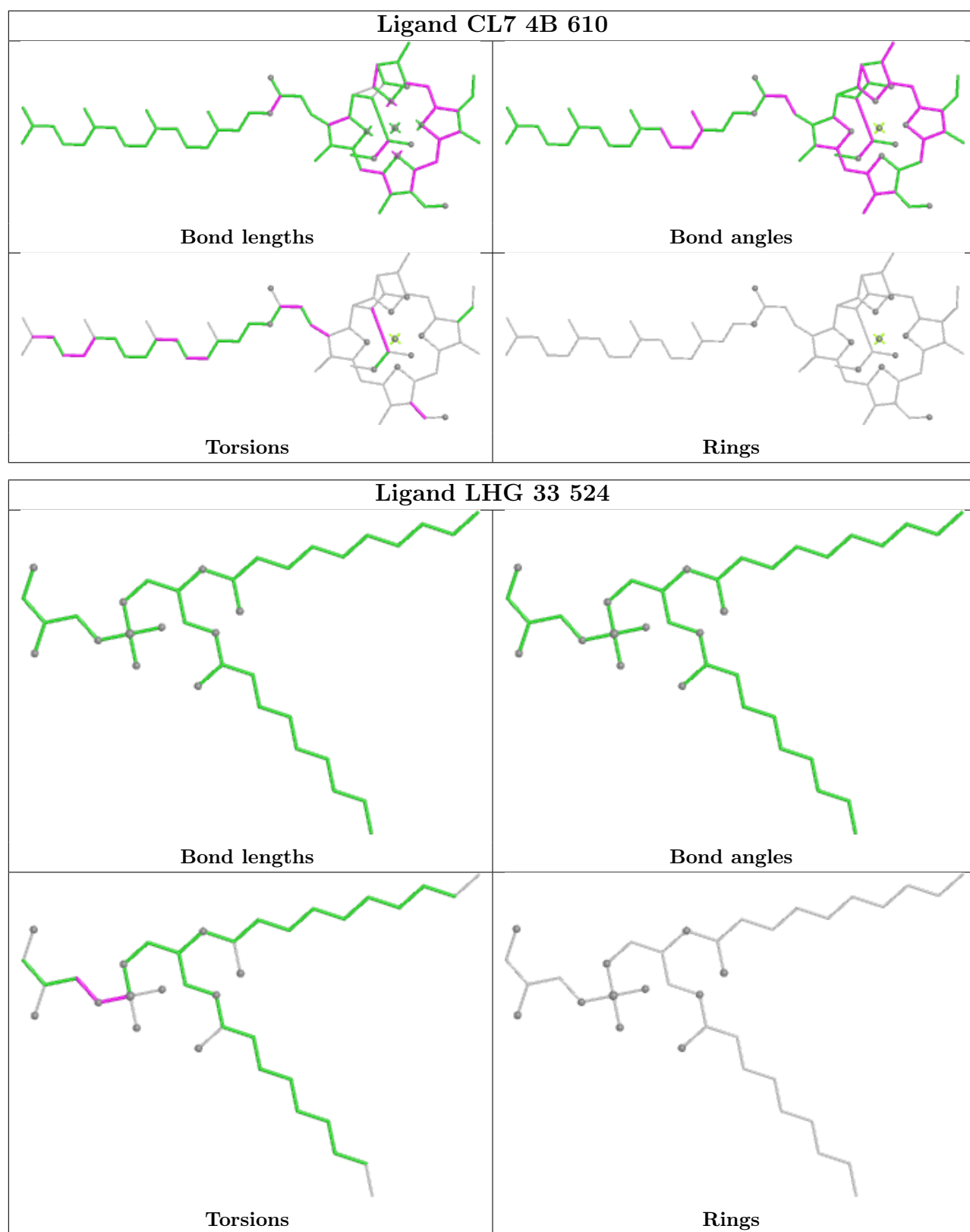


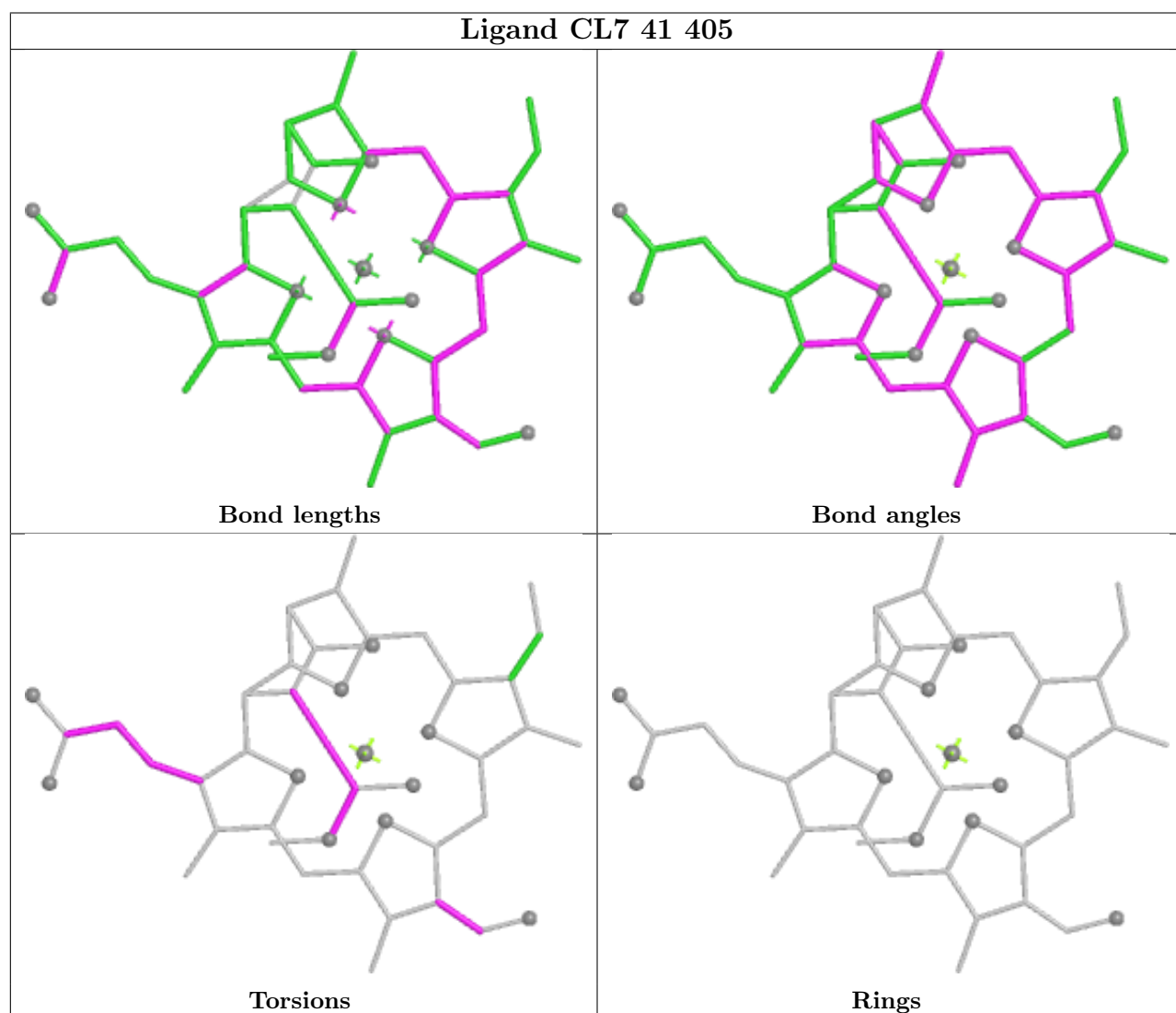
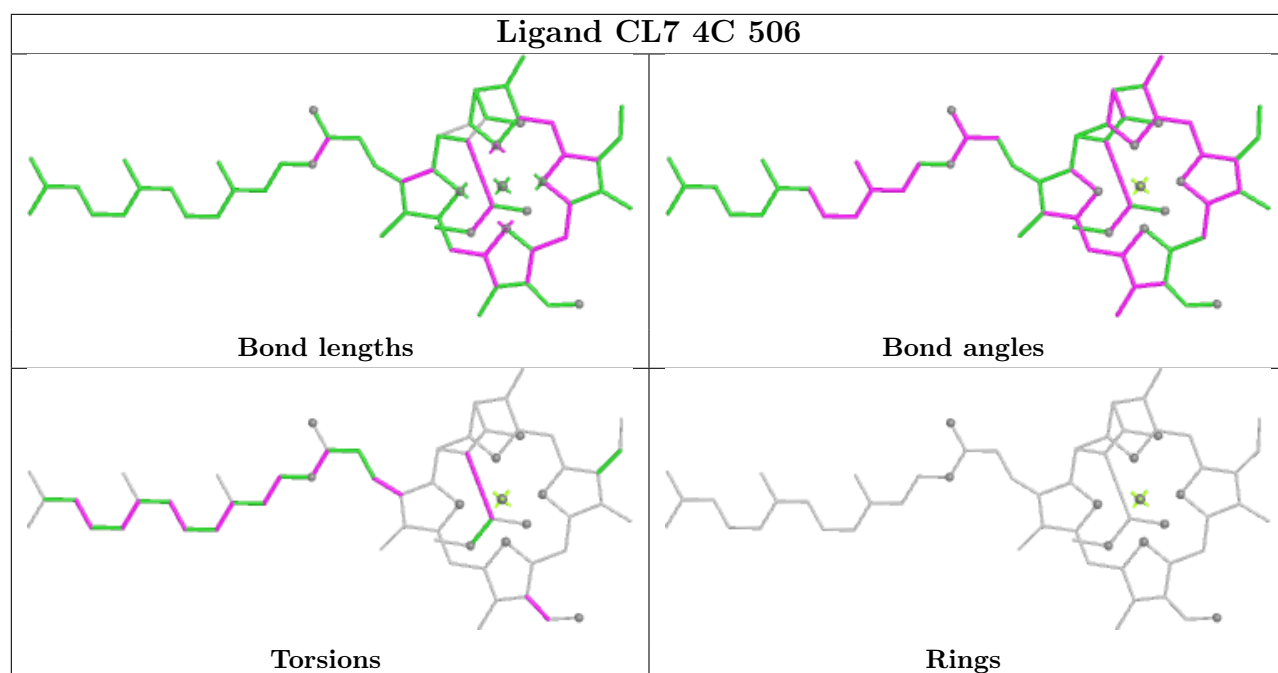
Torsions

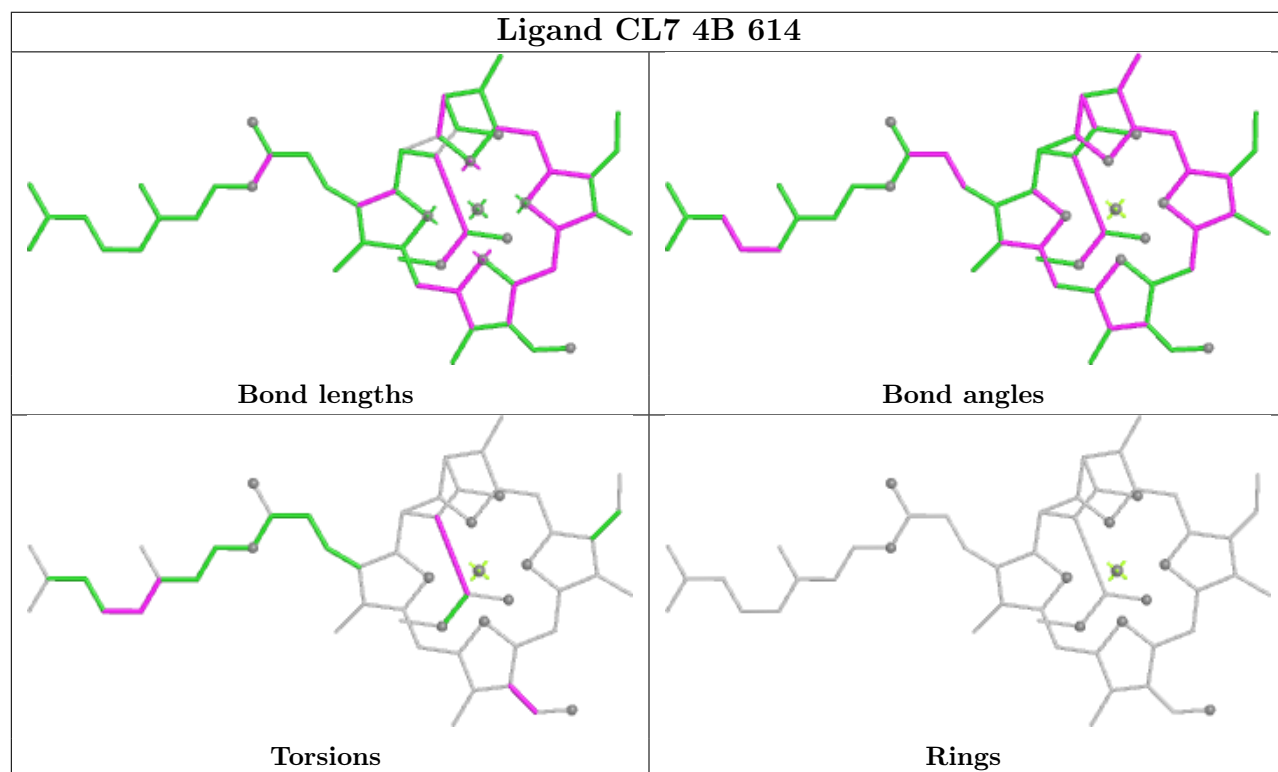
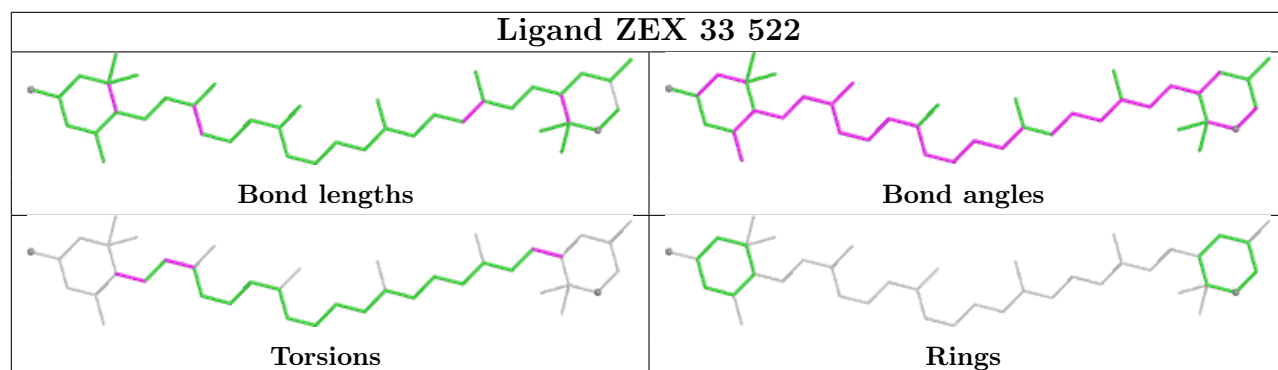
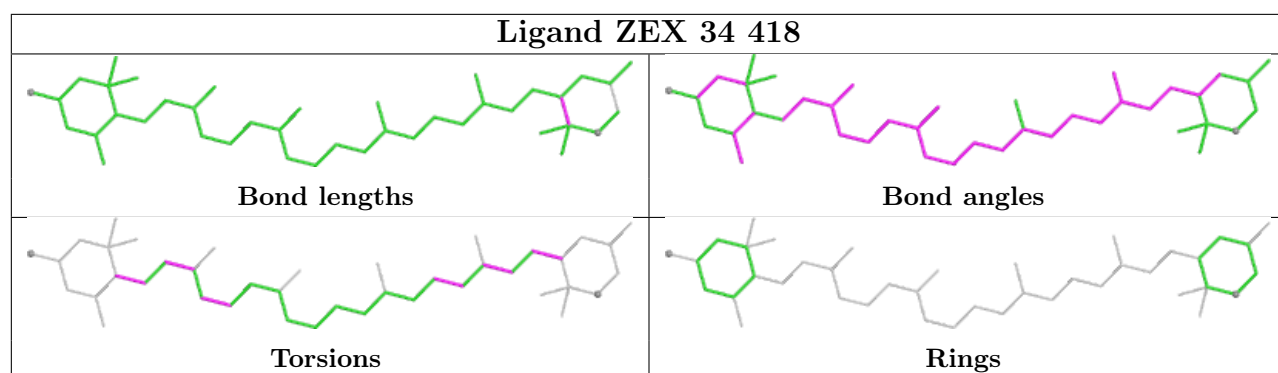


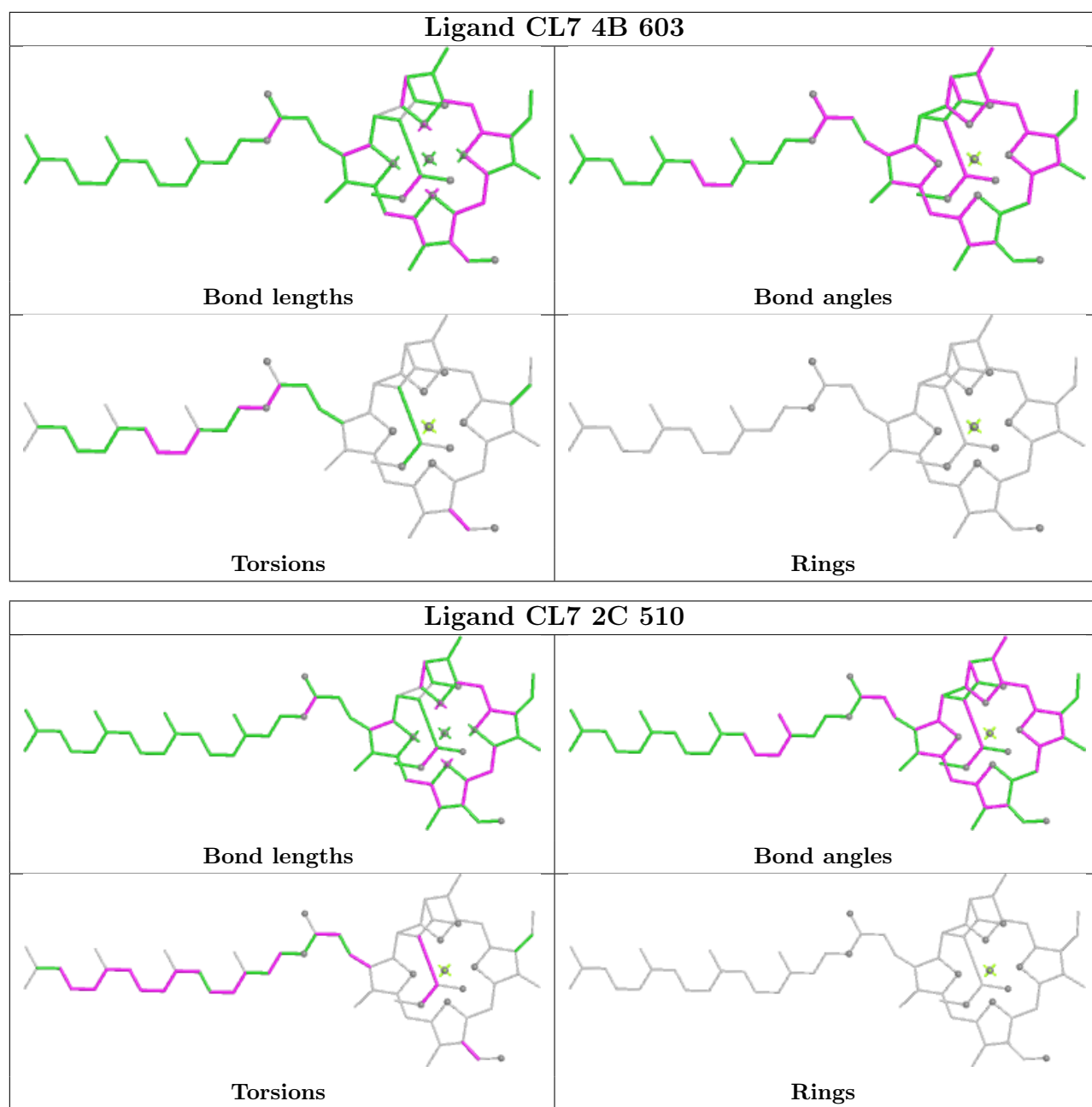
Rings

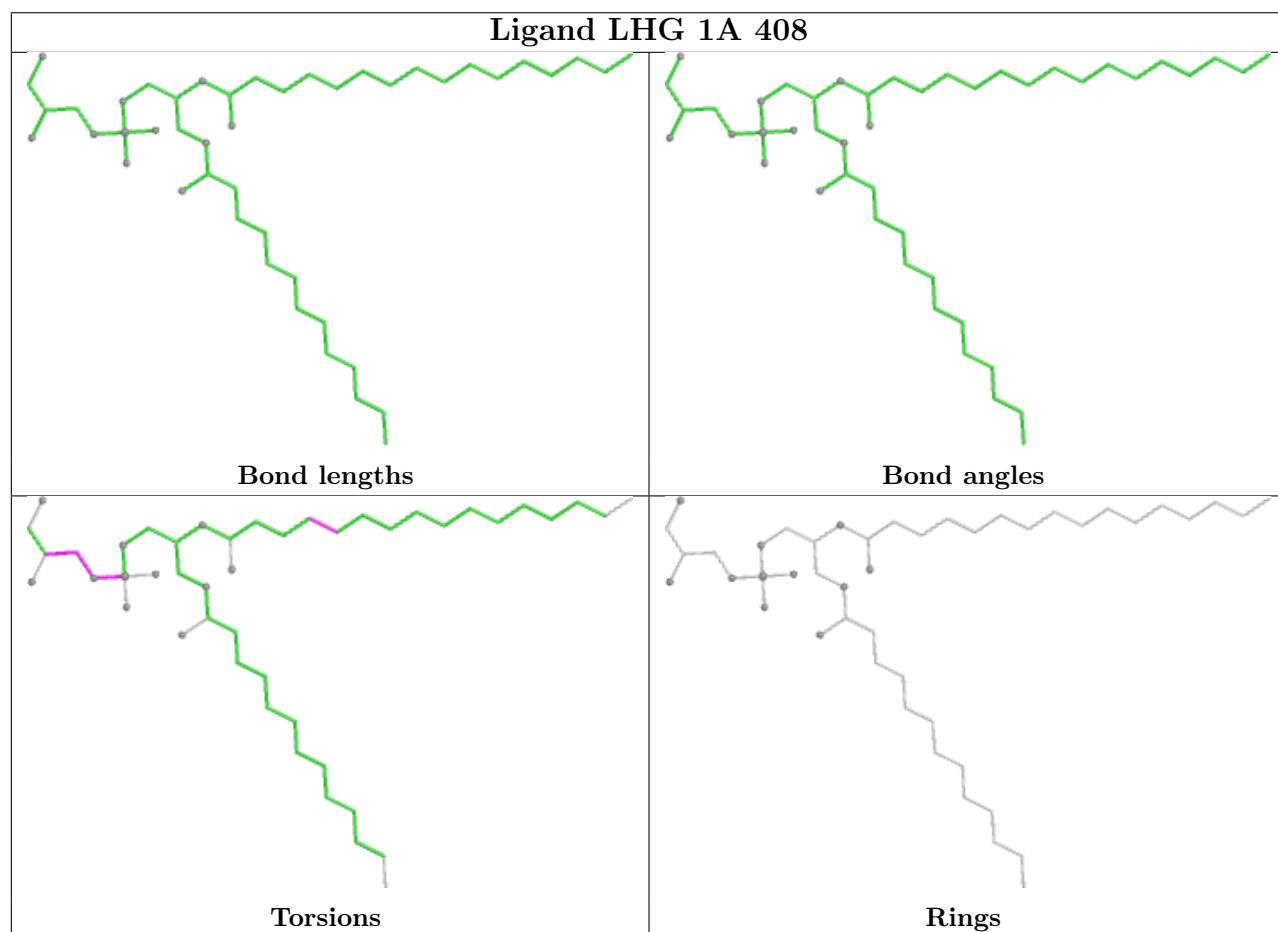
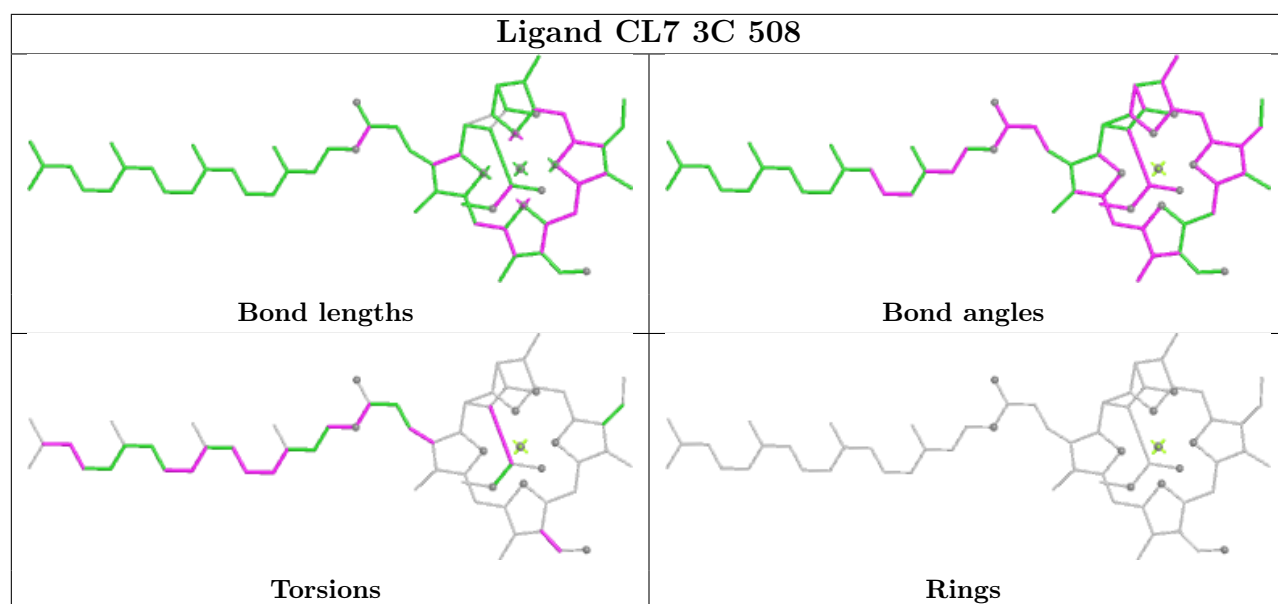


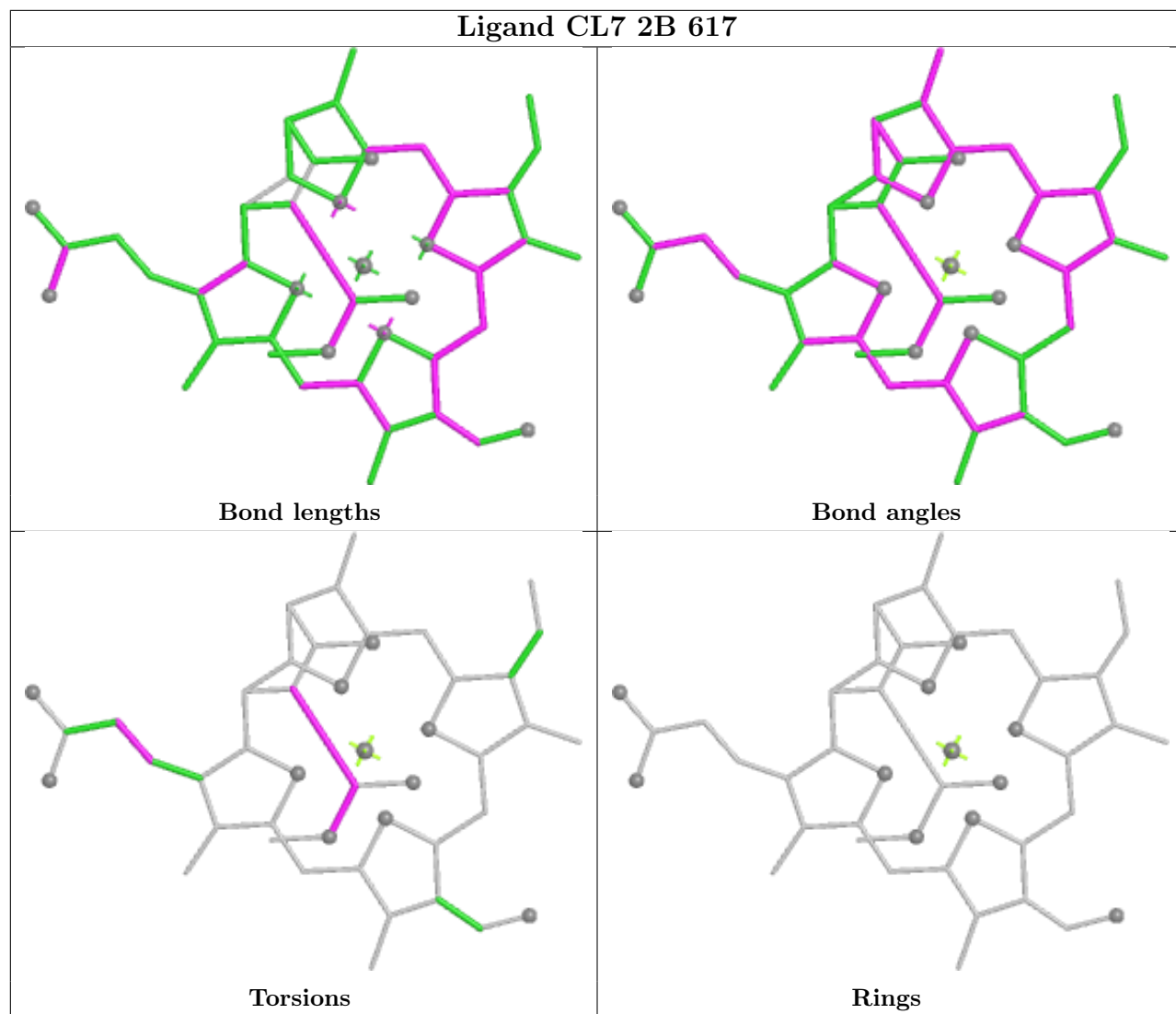


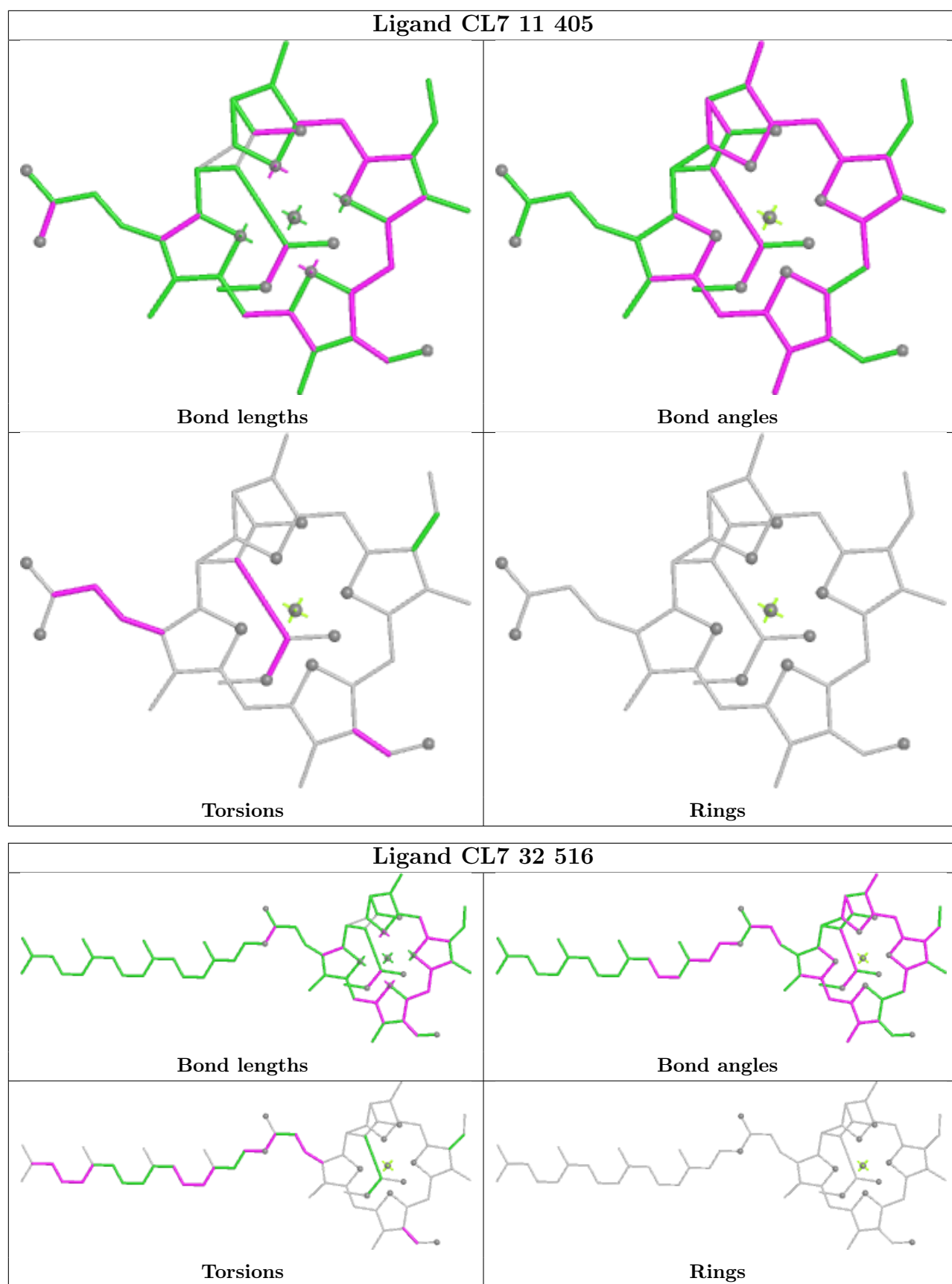


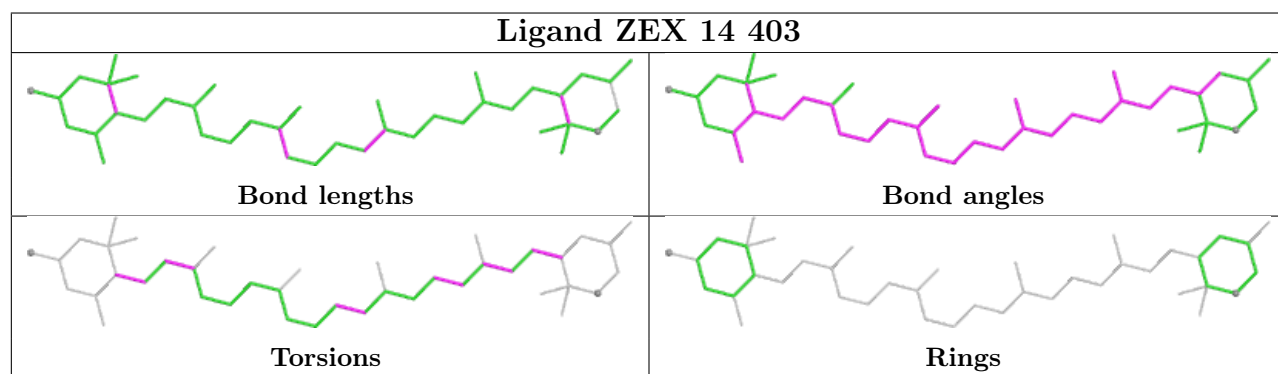
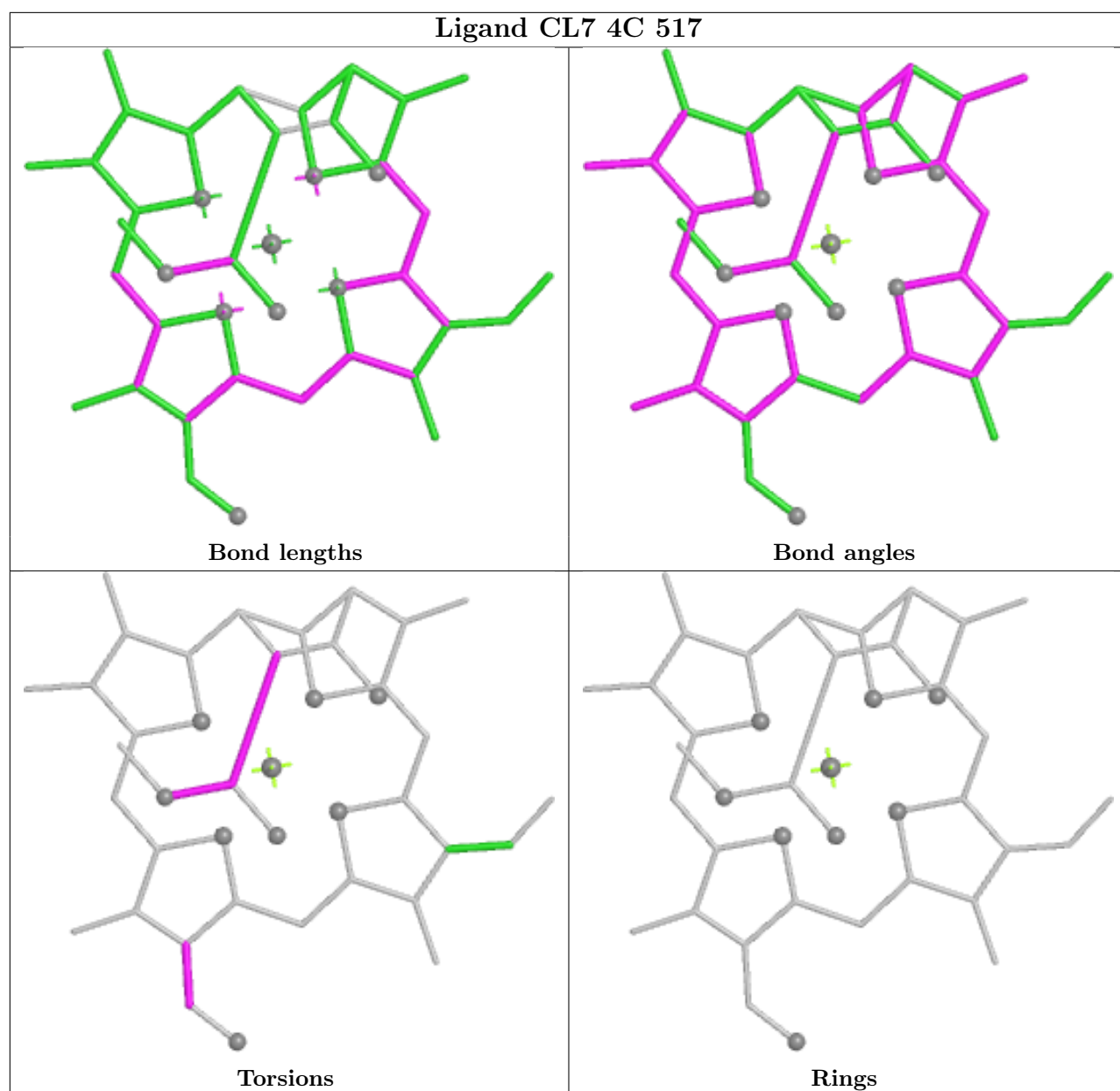


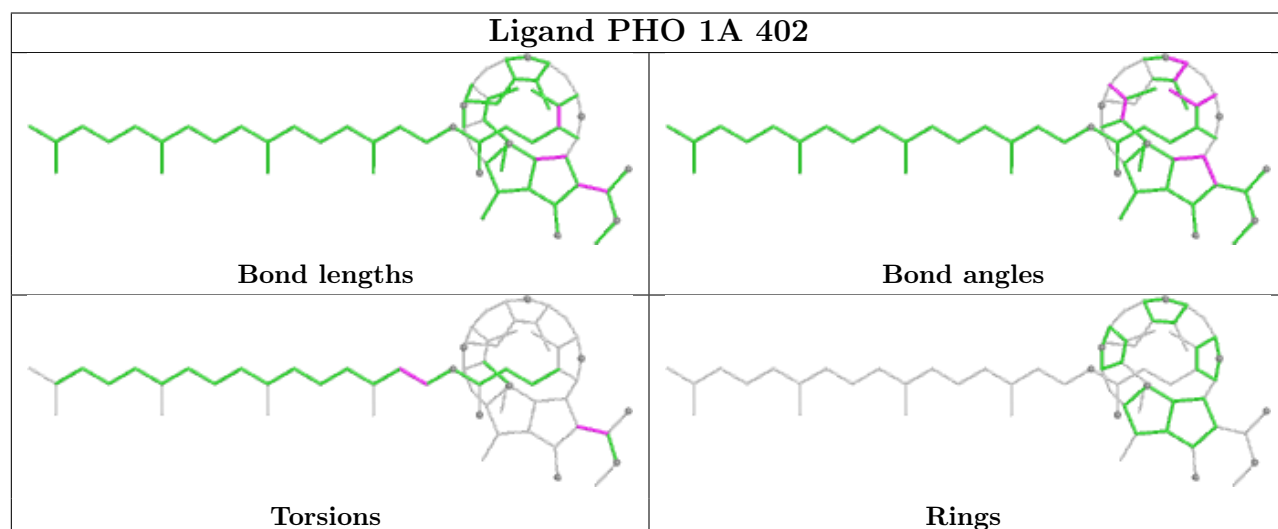
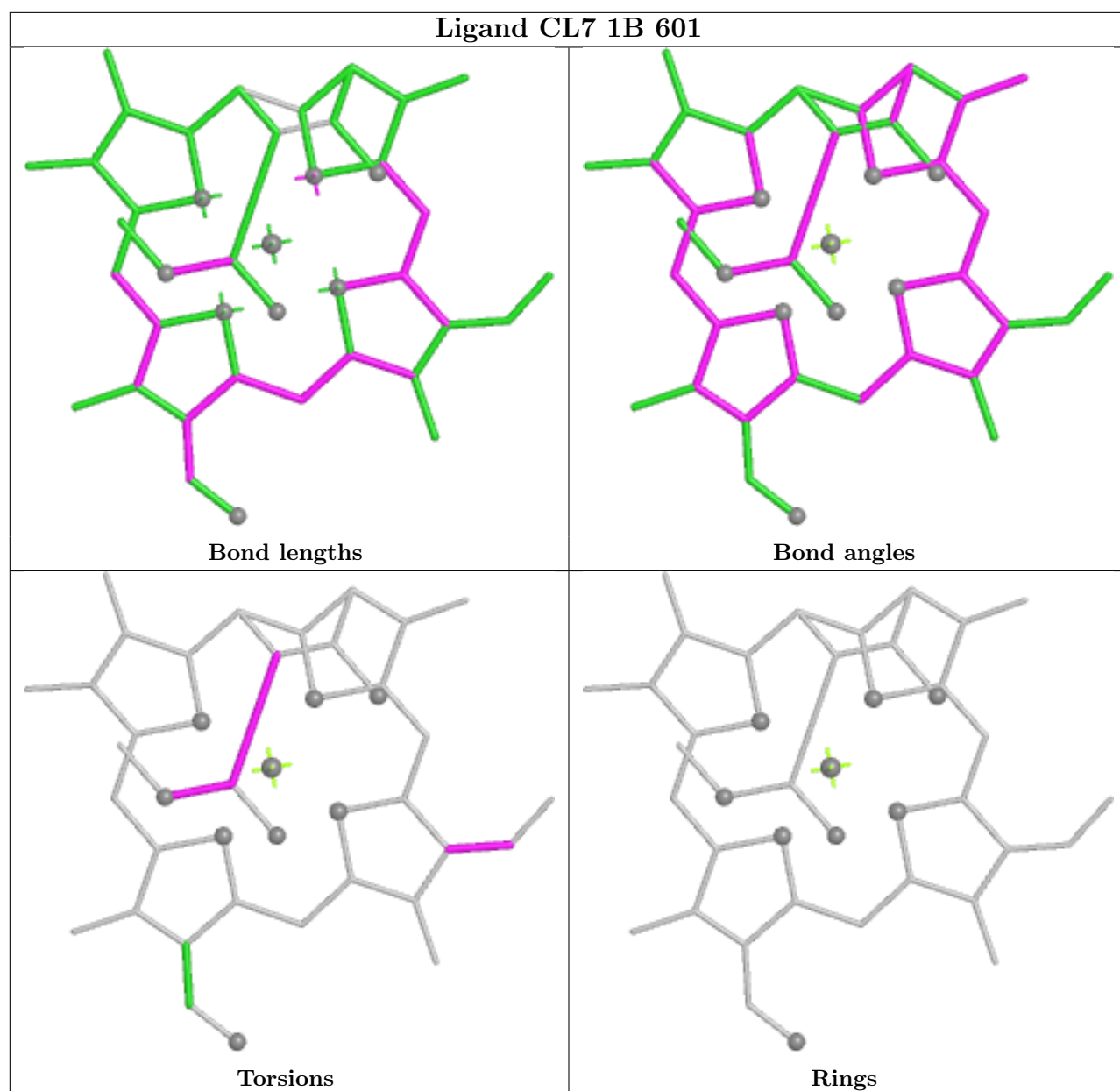




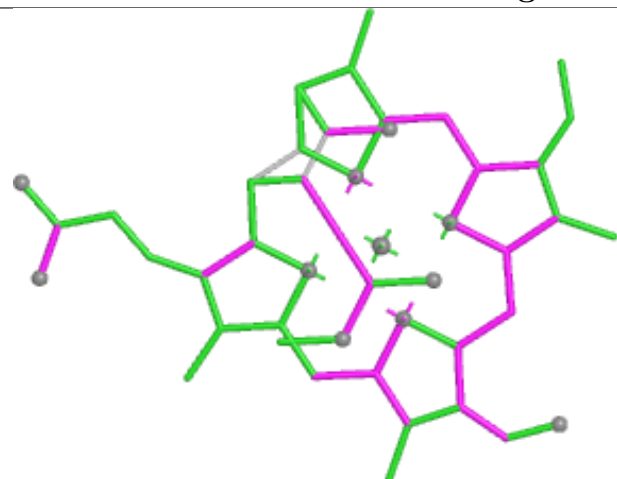




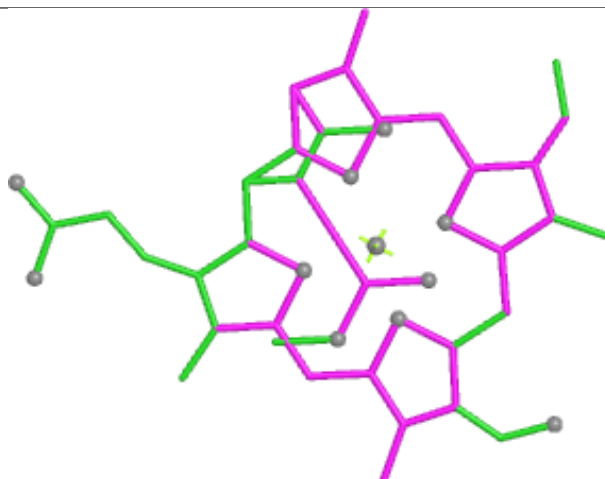




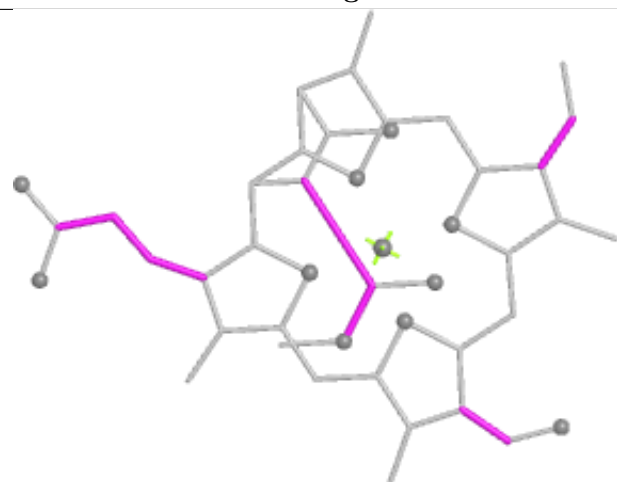
Ligand CL7 14 415



Bond lengths



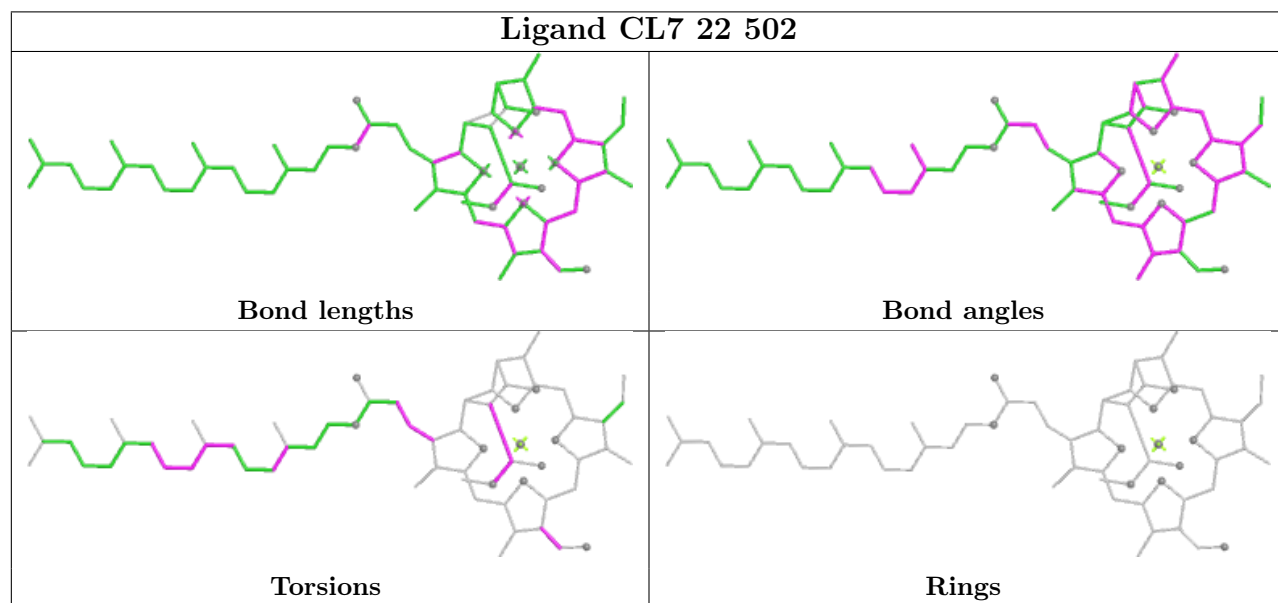
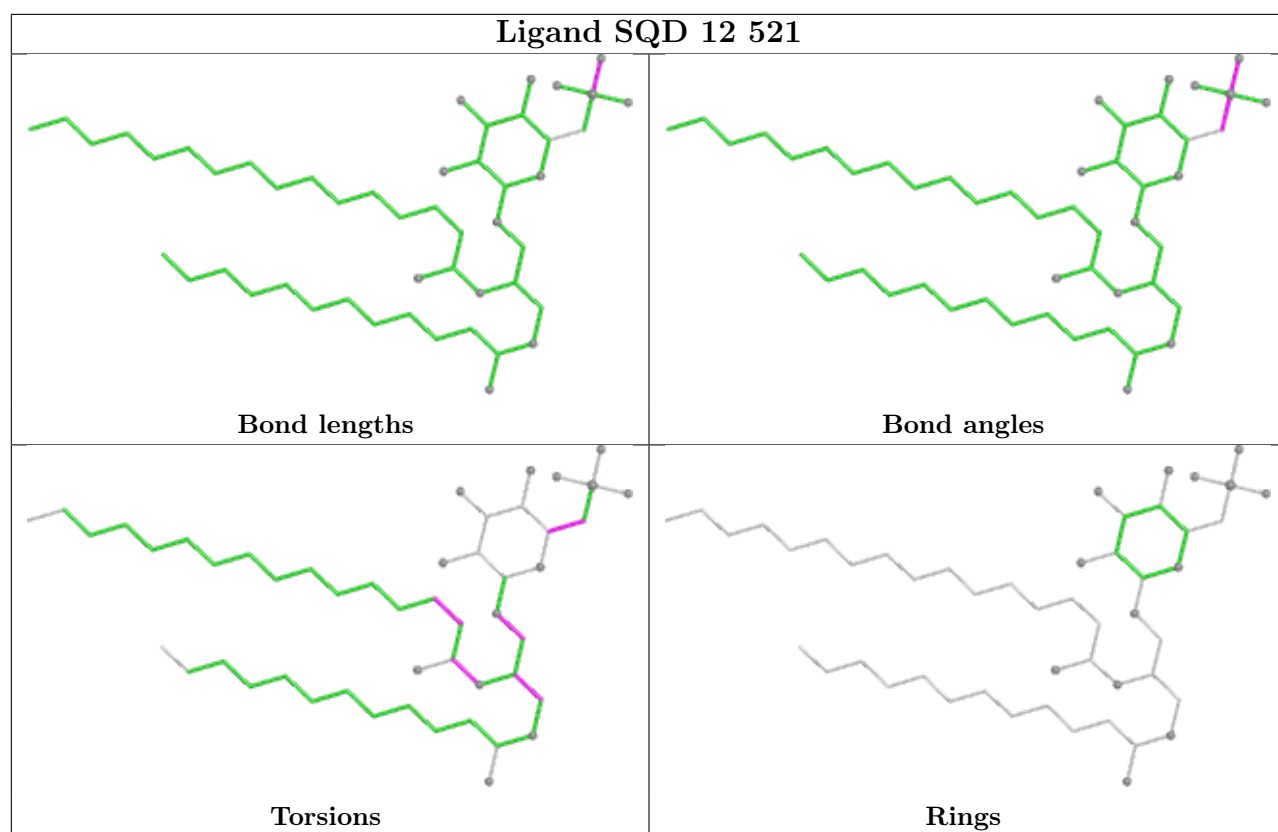
Bond angles

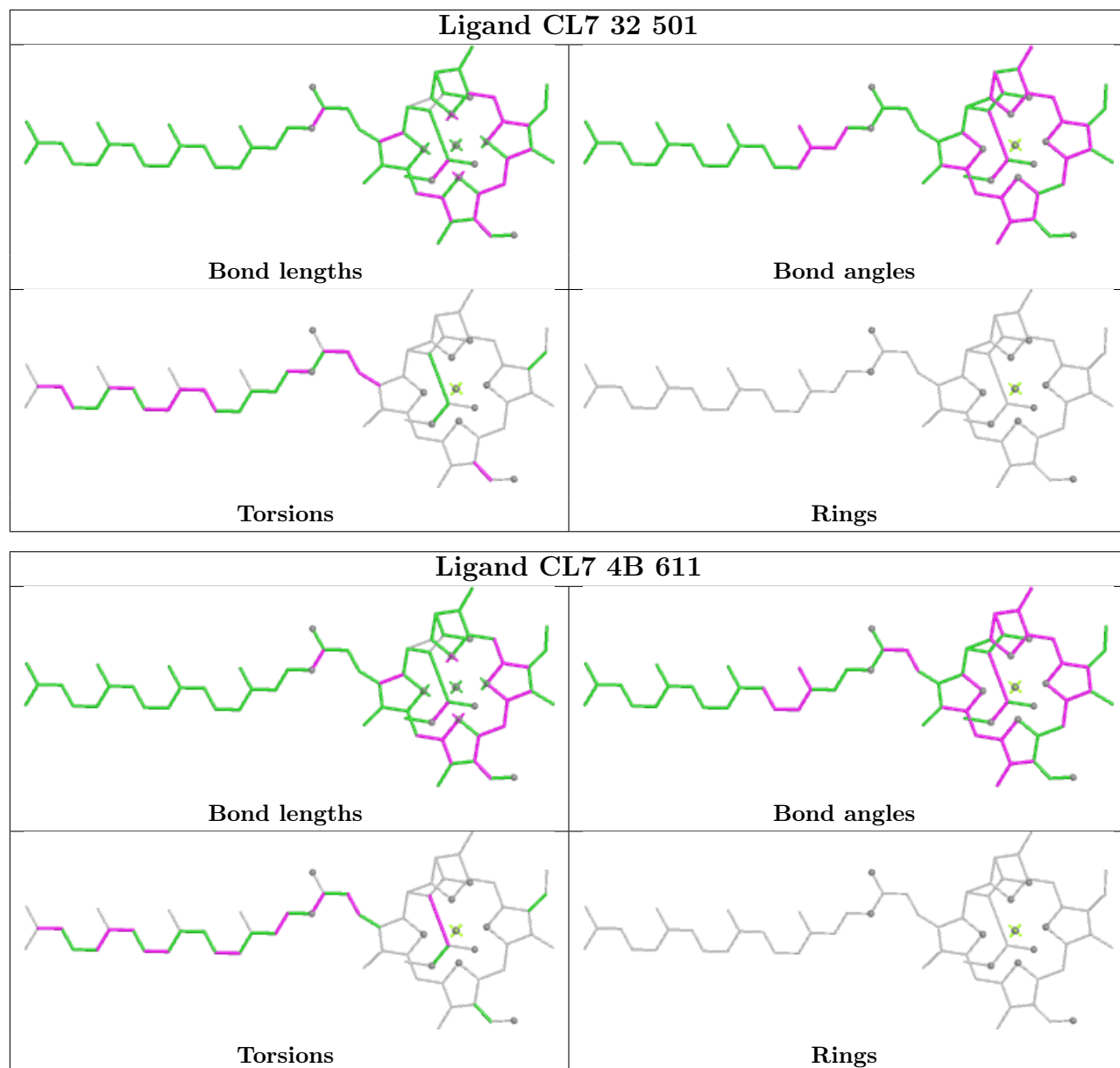


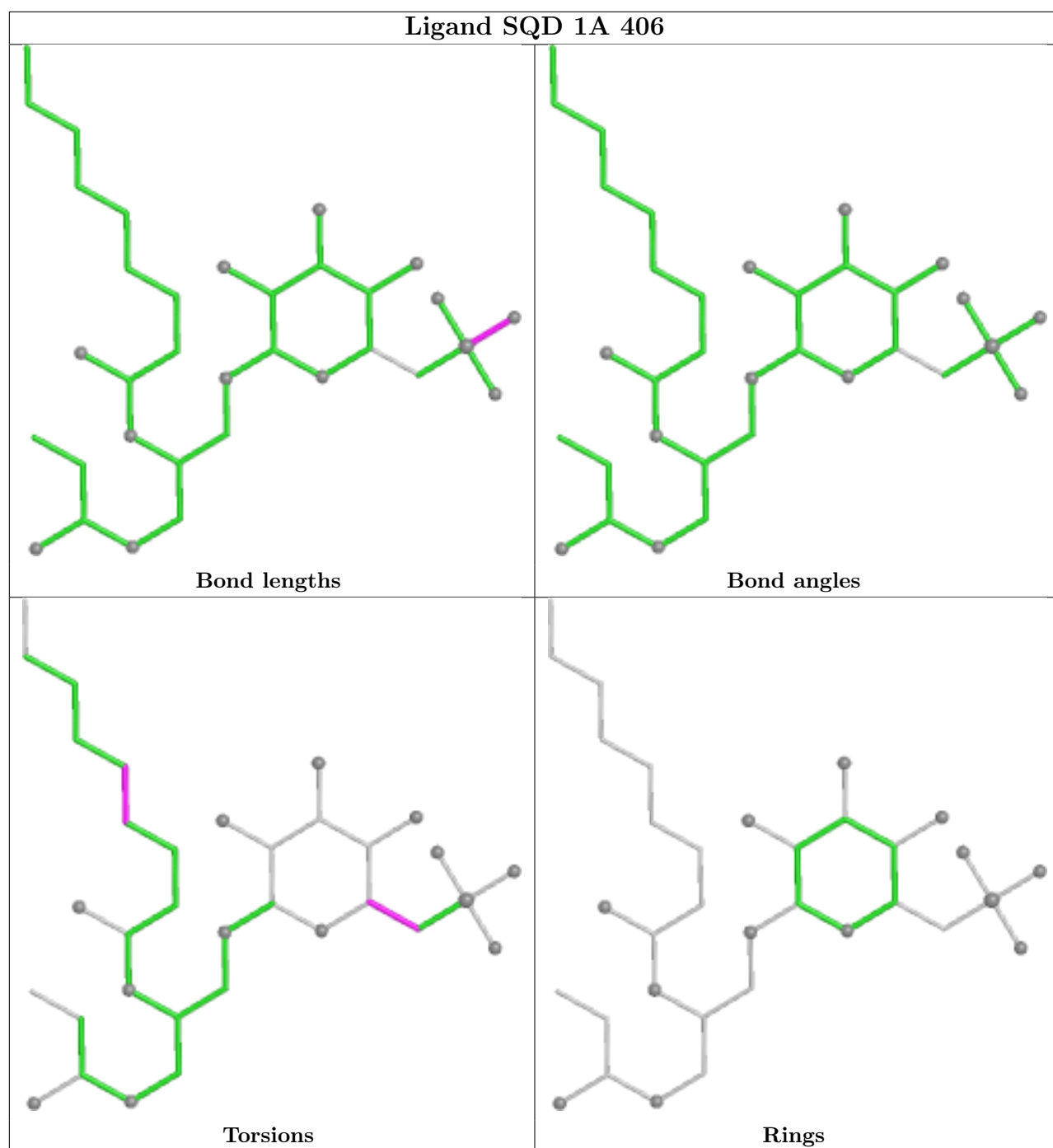
Torsions

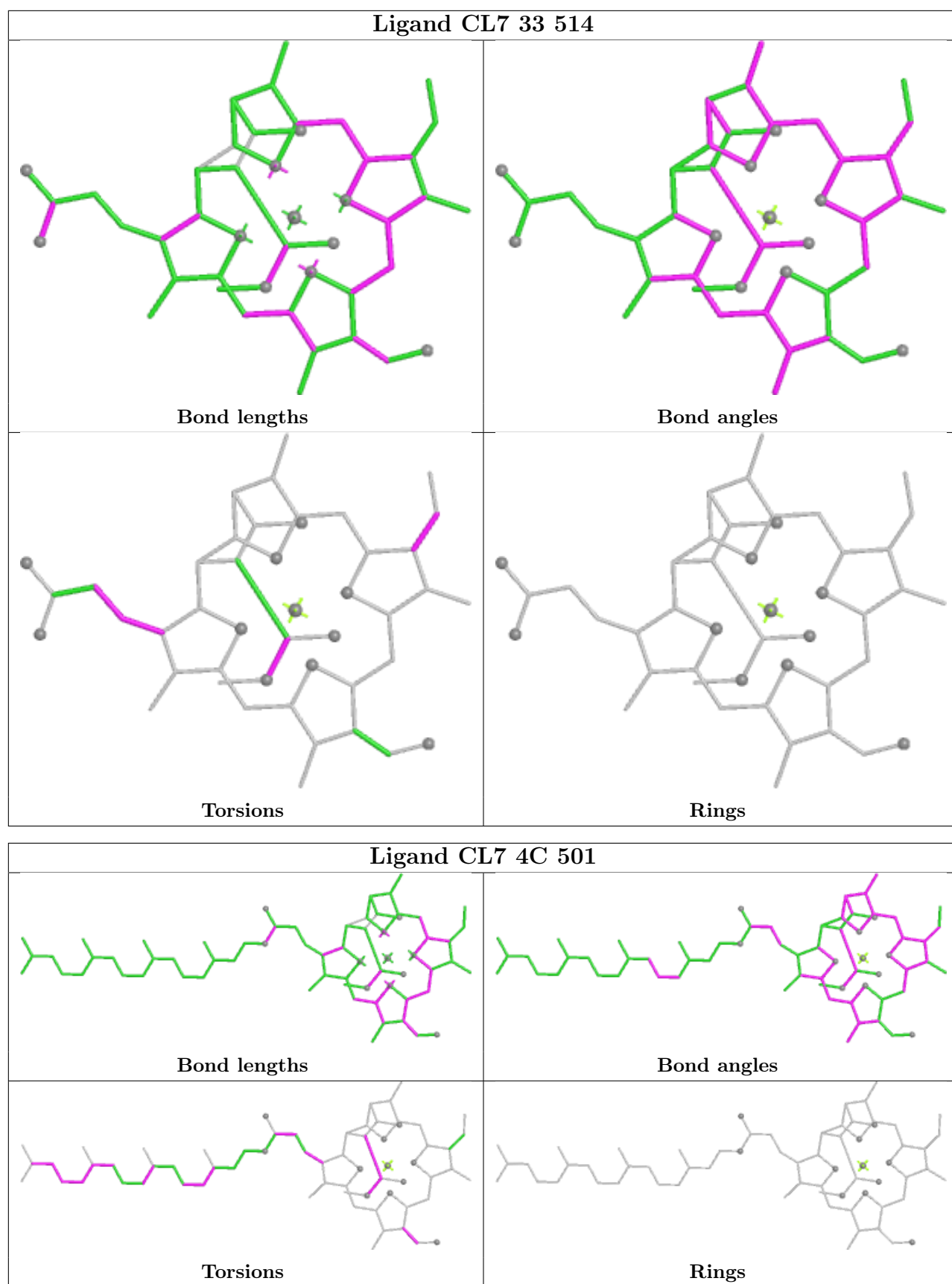


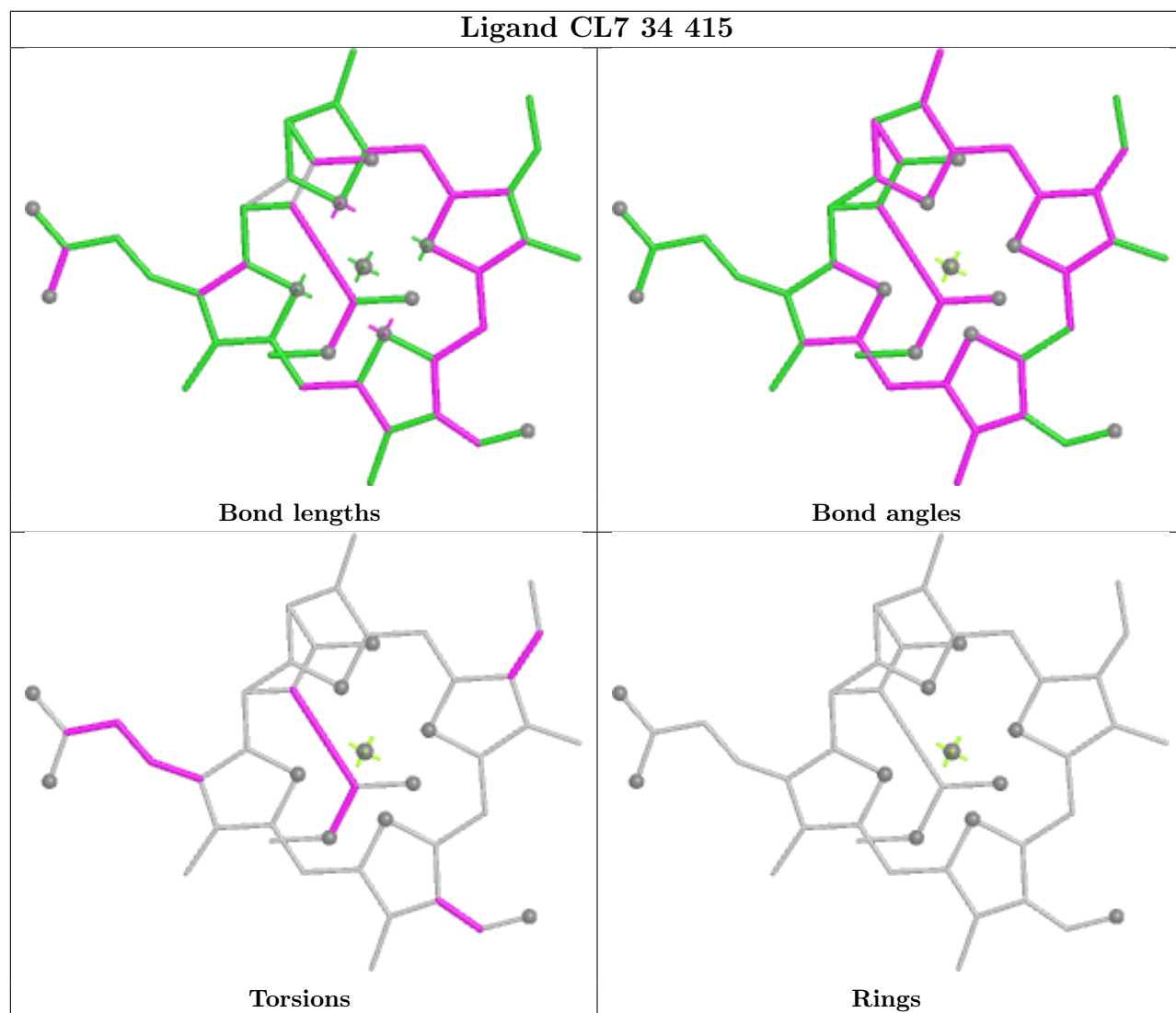
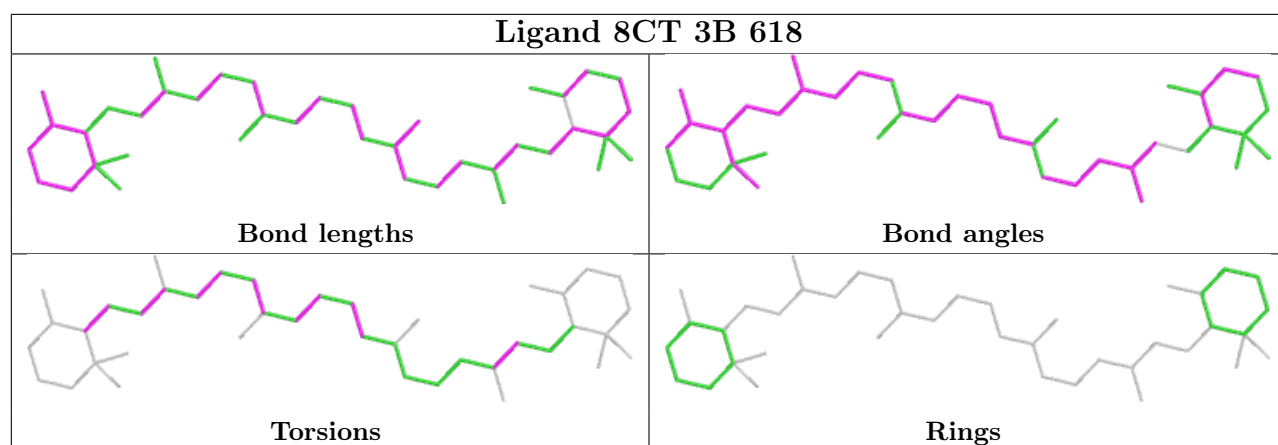
Rings



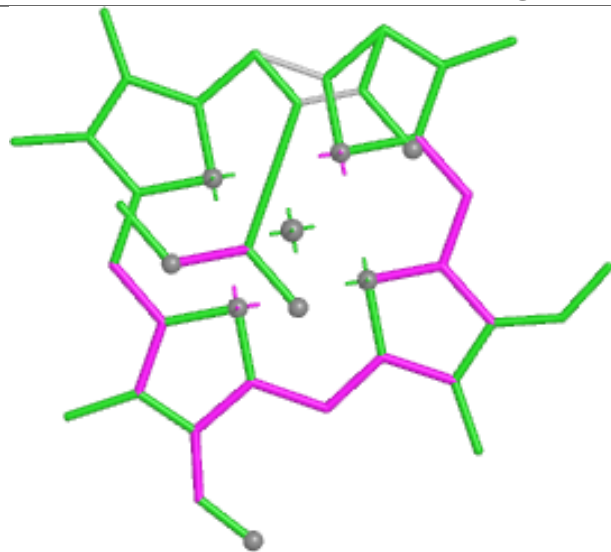




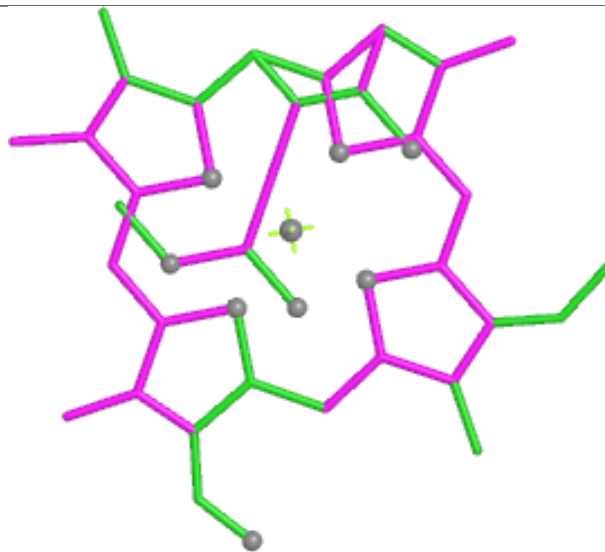




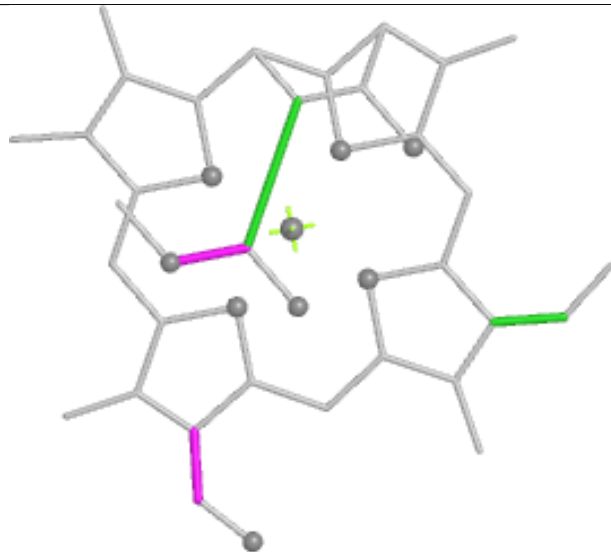
Ligand CL7 31 407



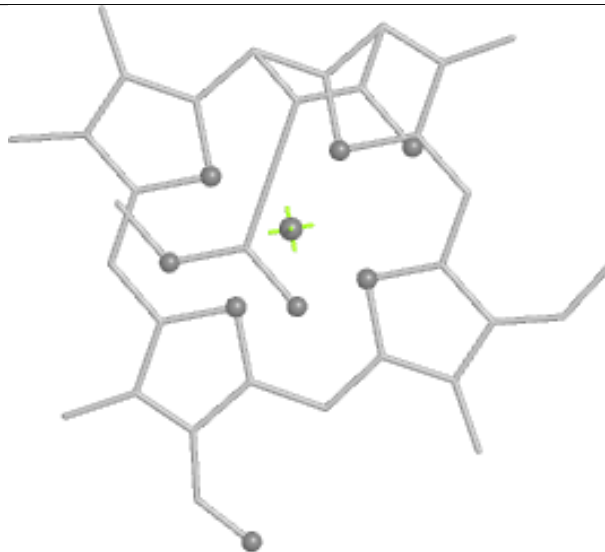
Bond lengths



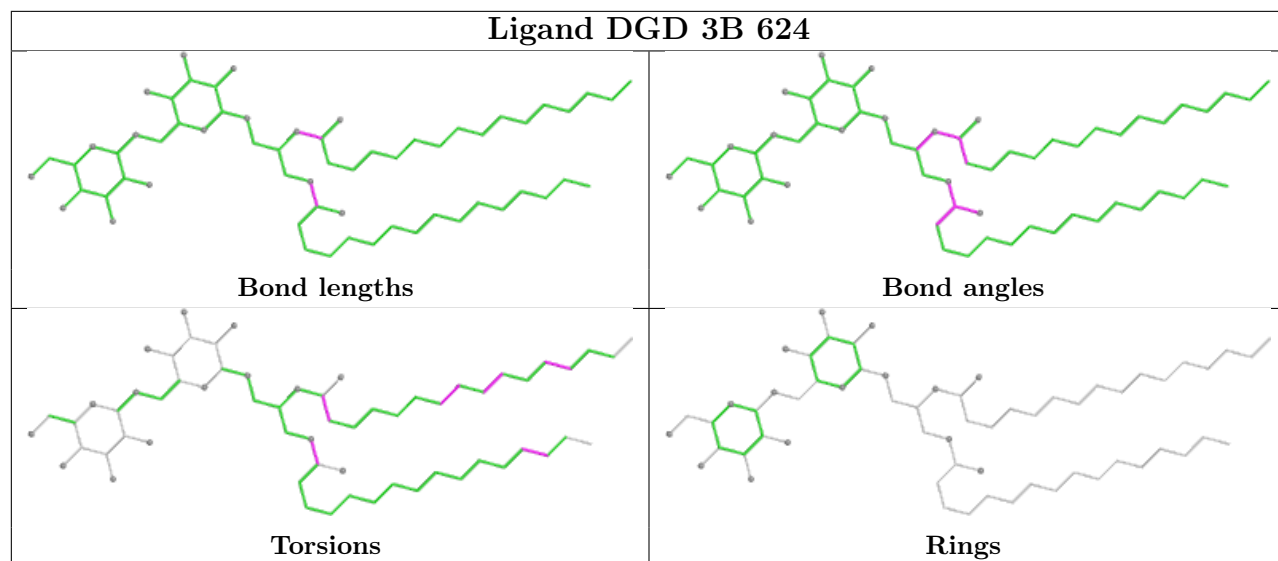
Bond angles

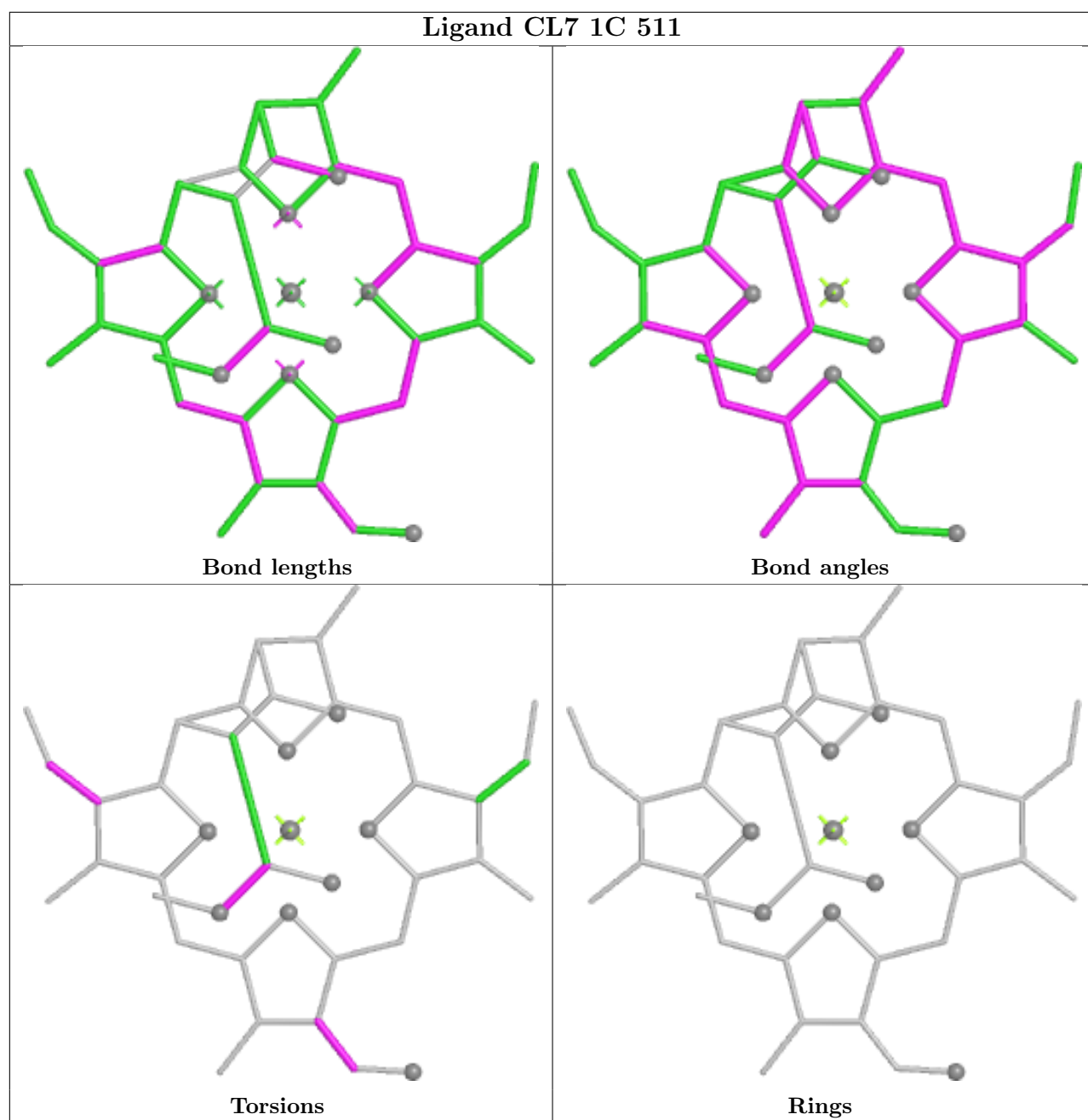


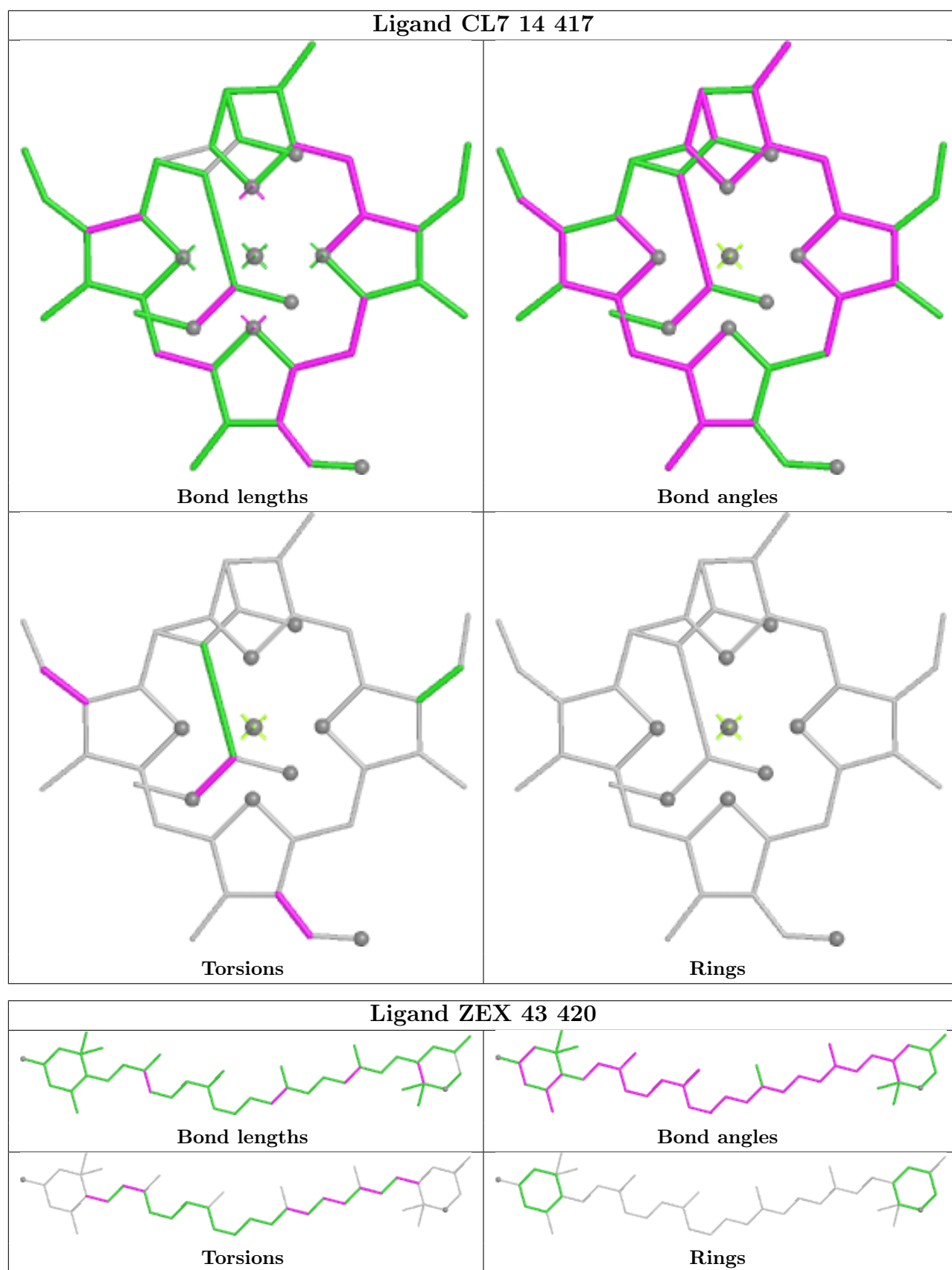
Torsions

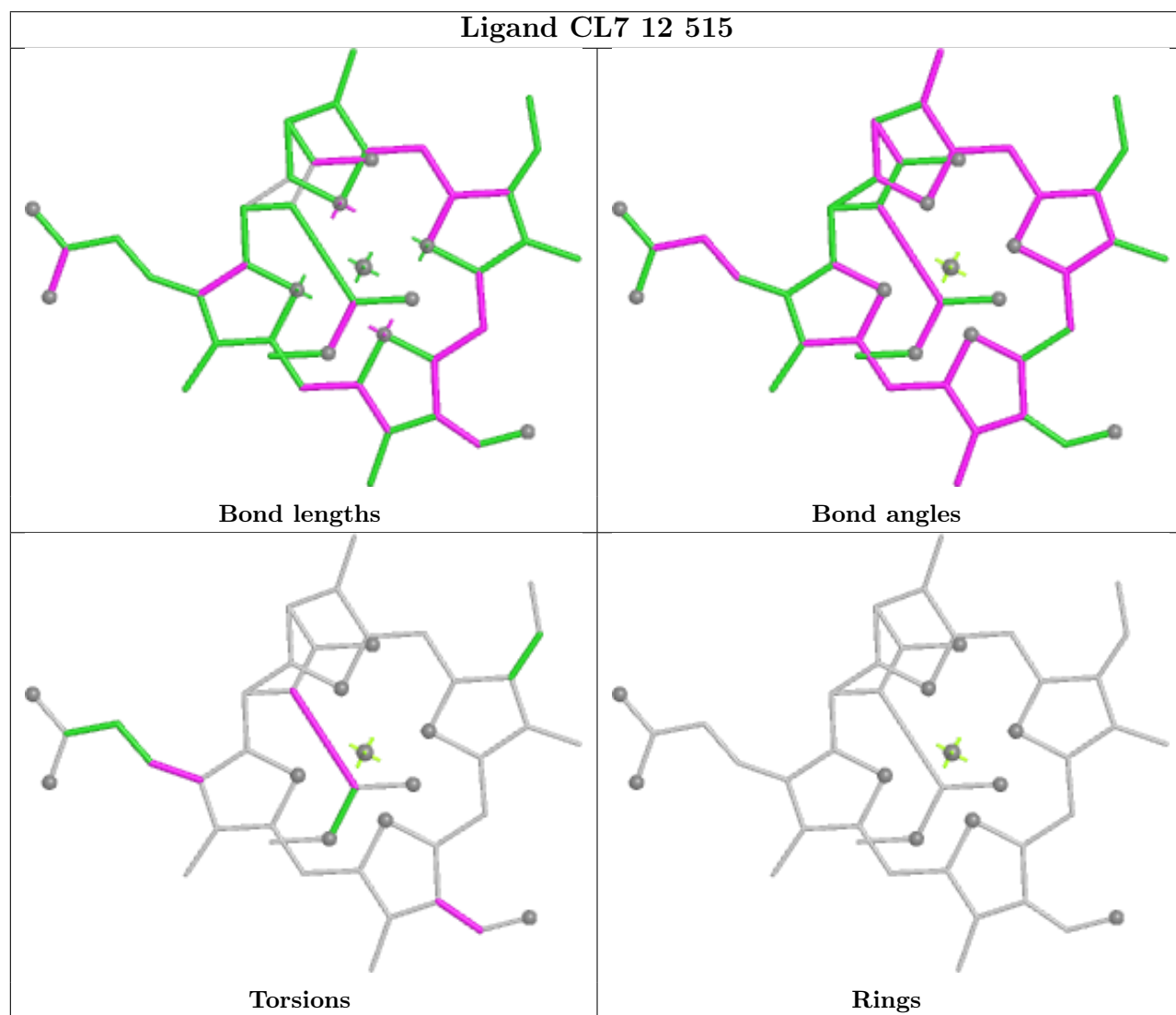
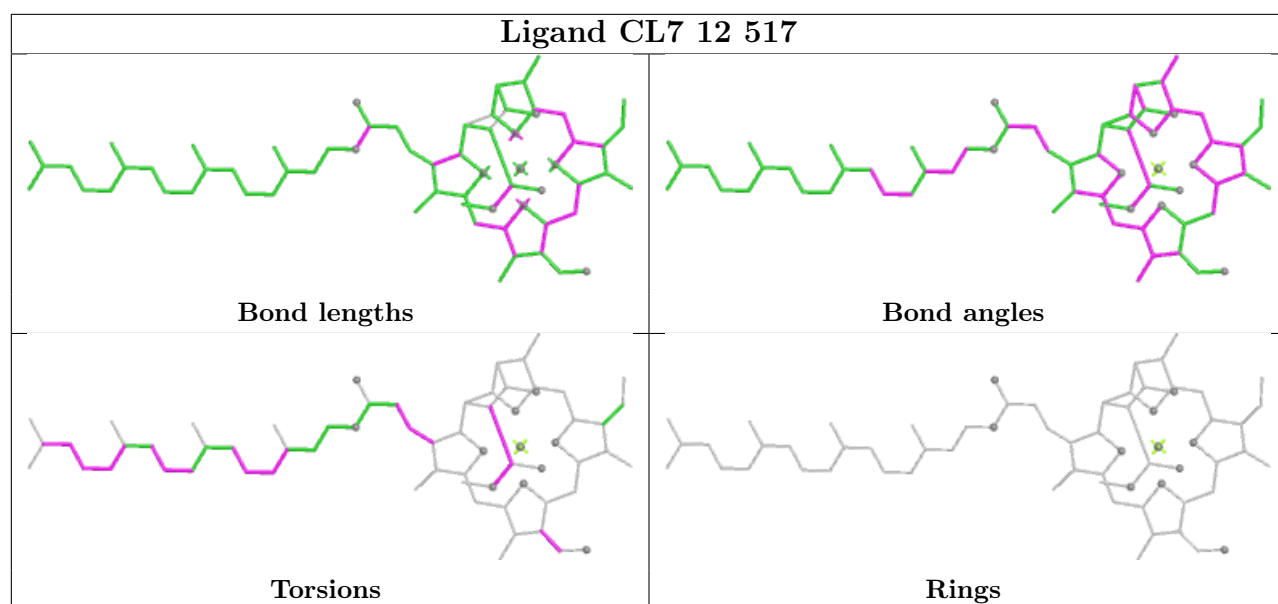


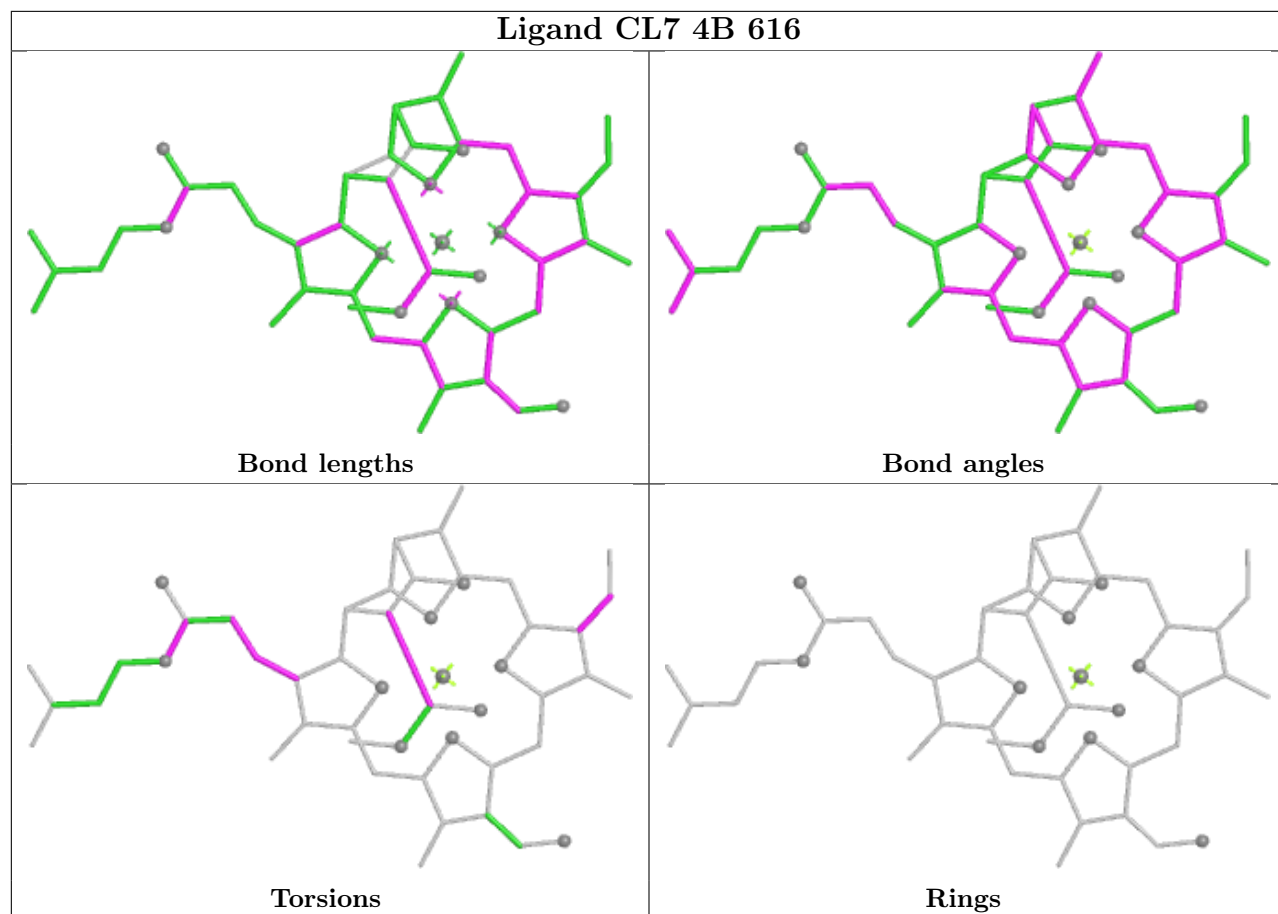
Rings



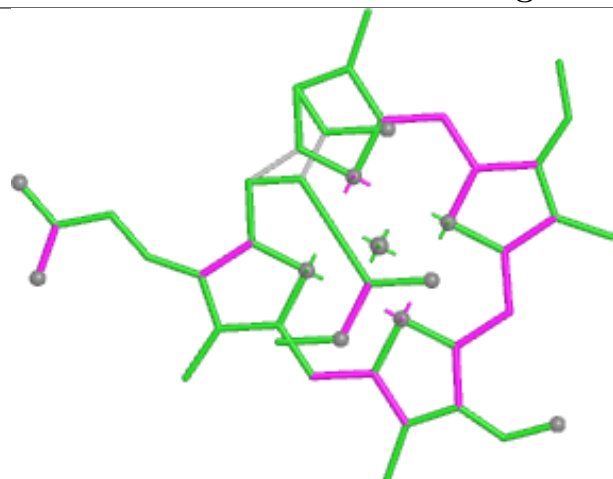




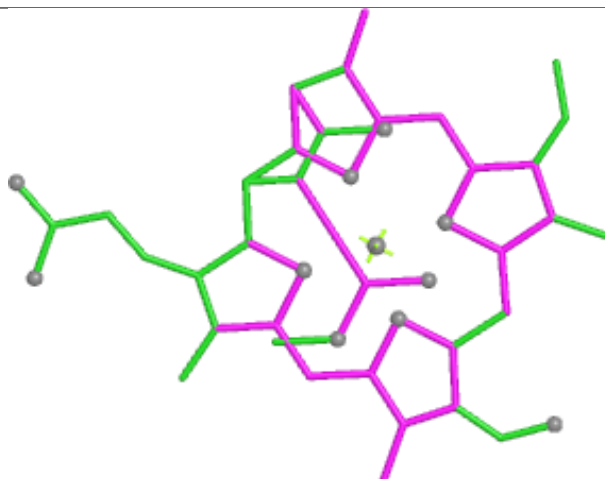




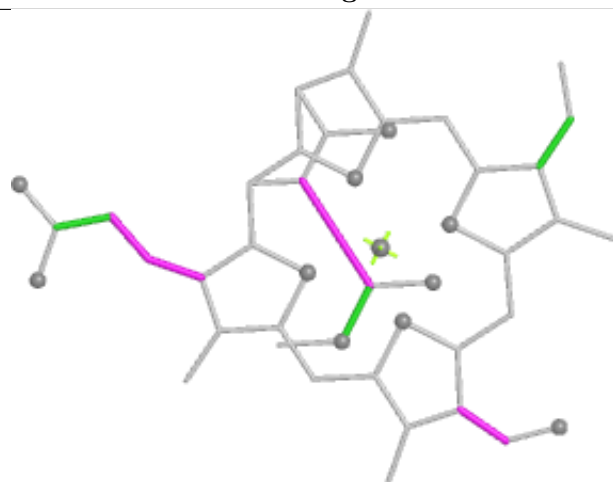
Ligand CL7 32 513



Bond lengths



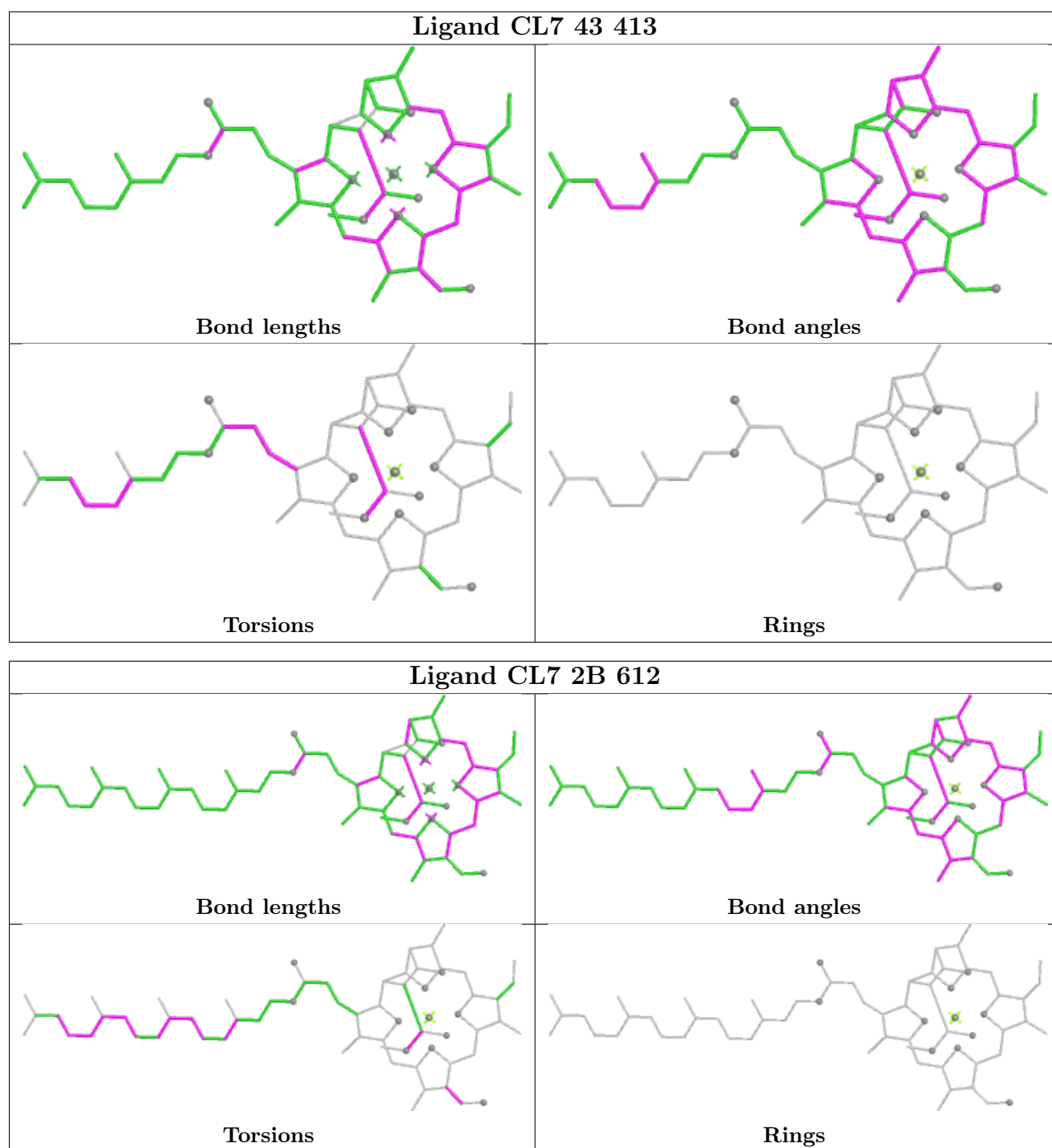
Bond angles

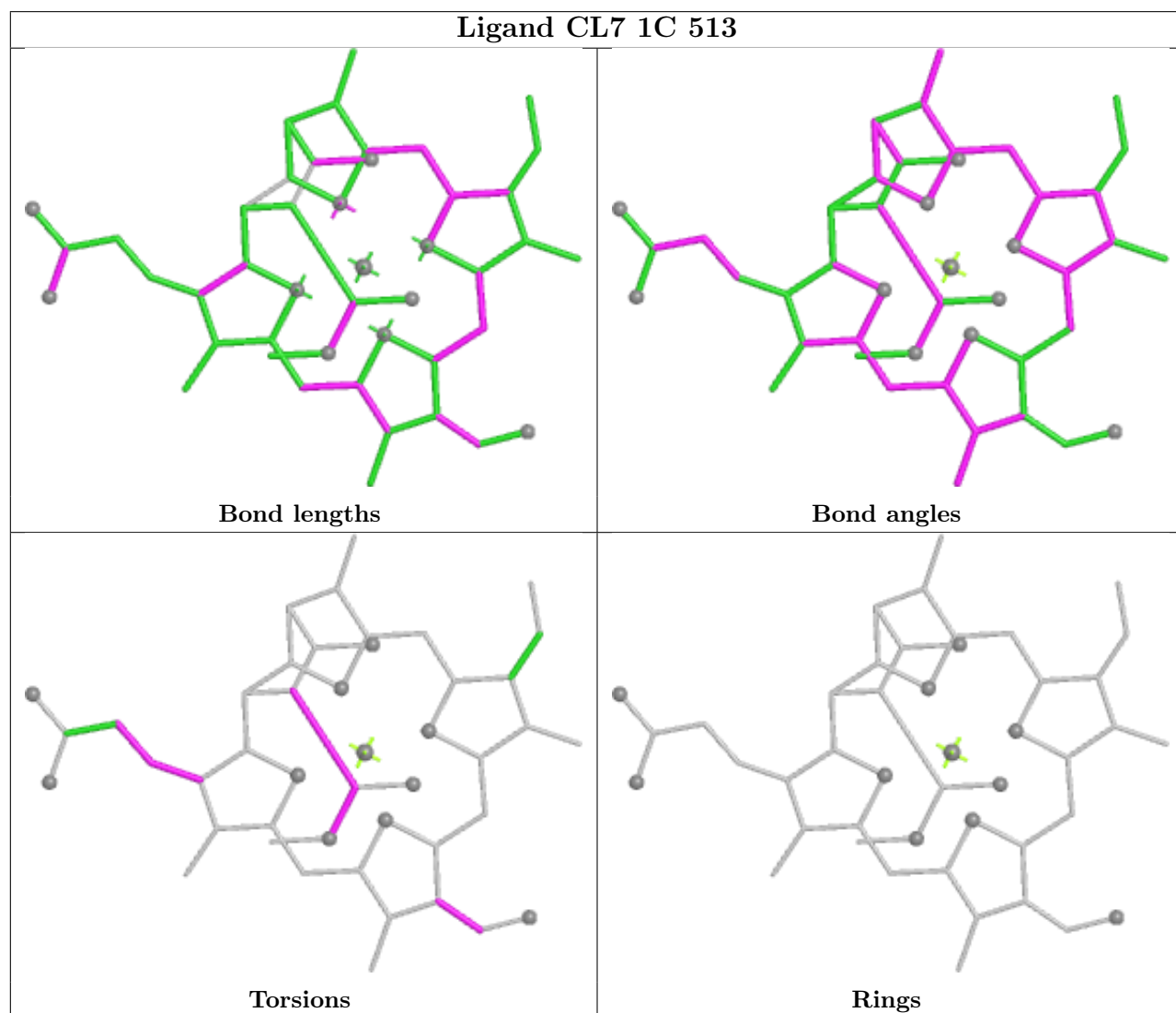
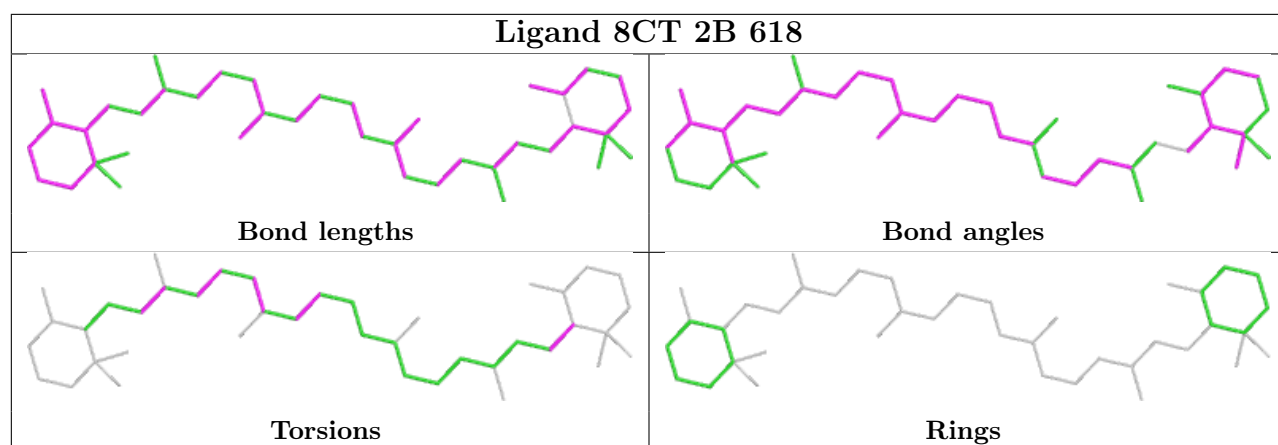


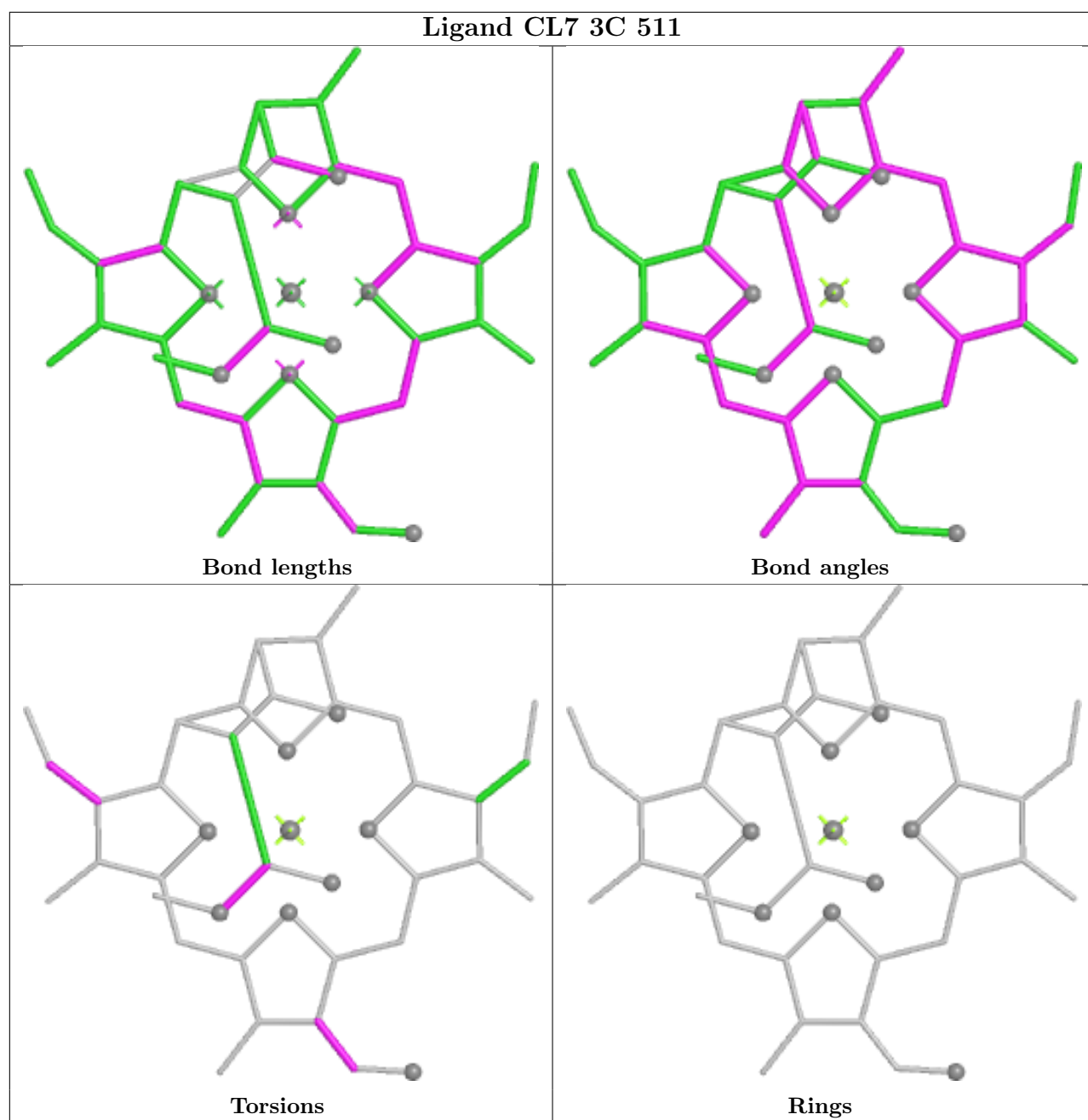
Torsions

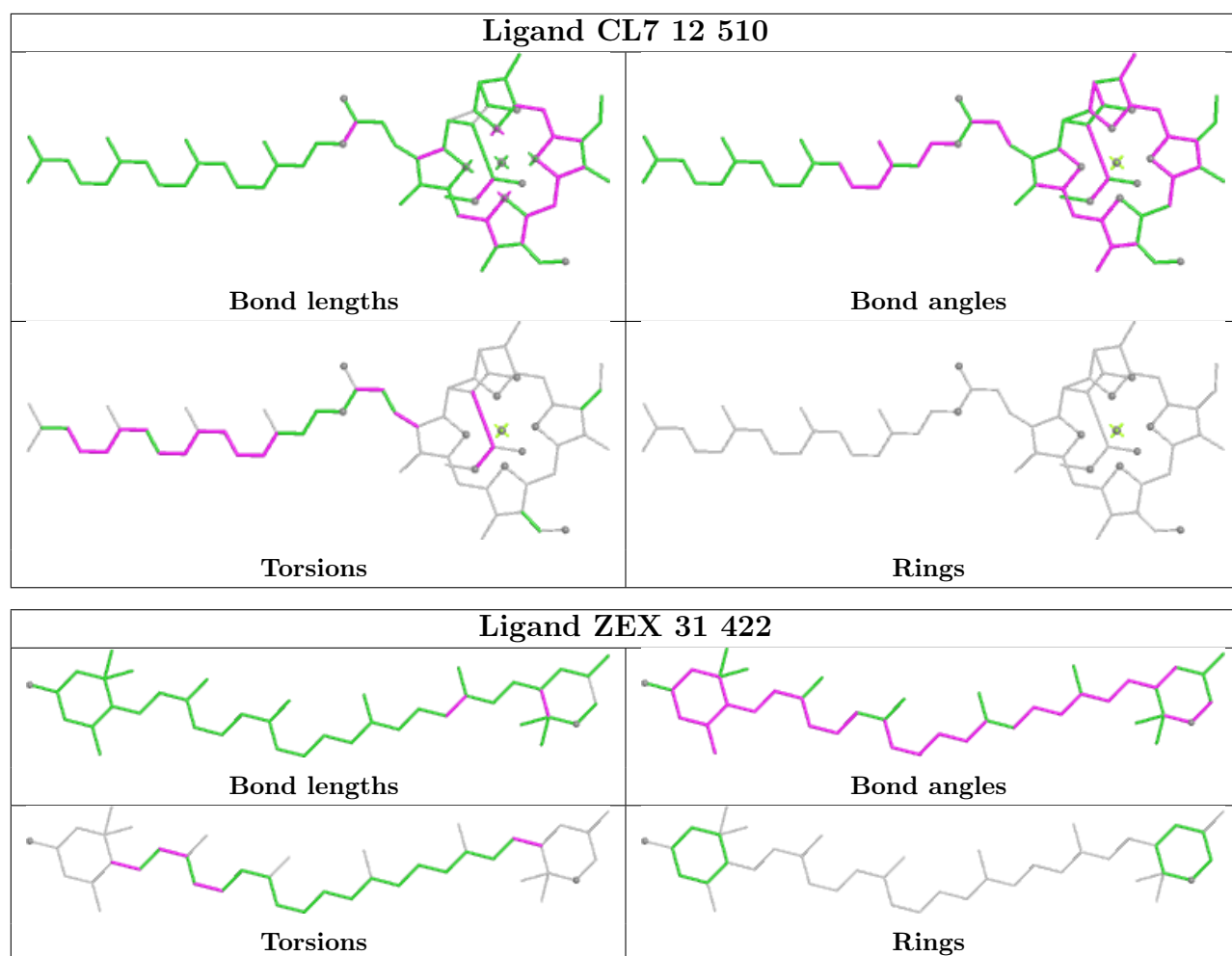


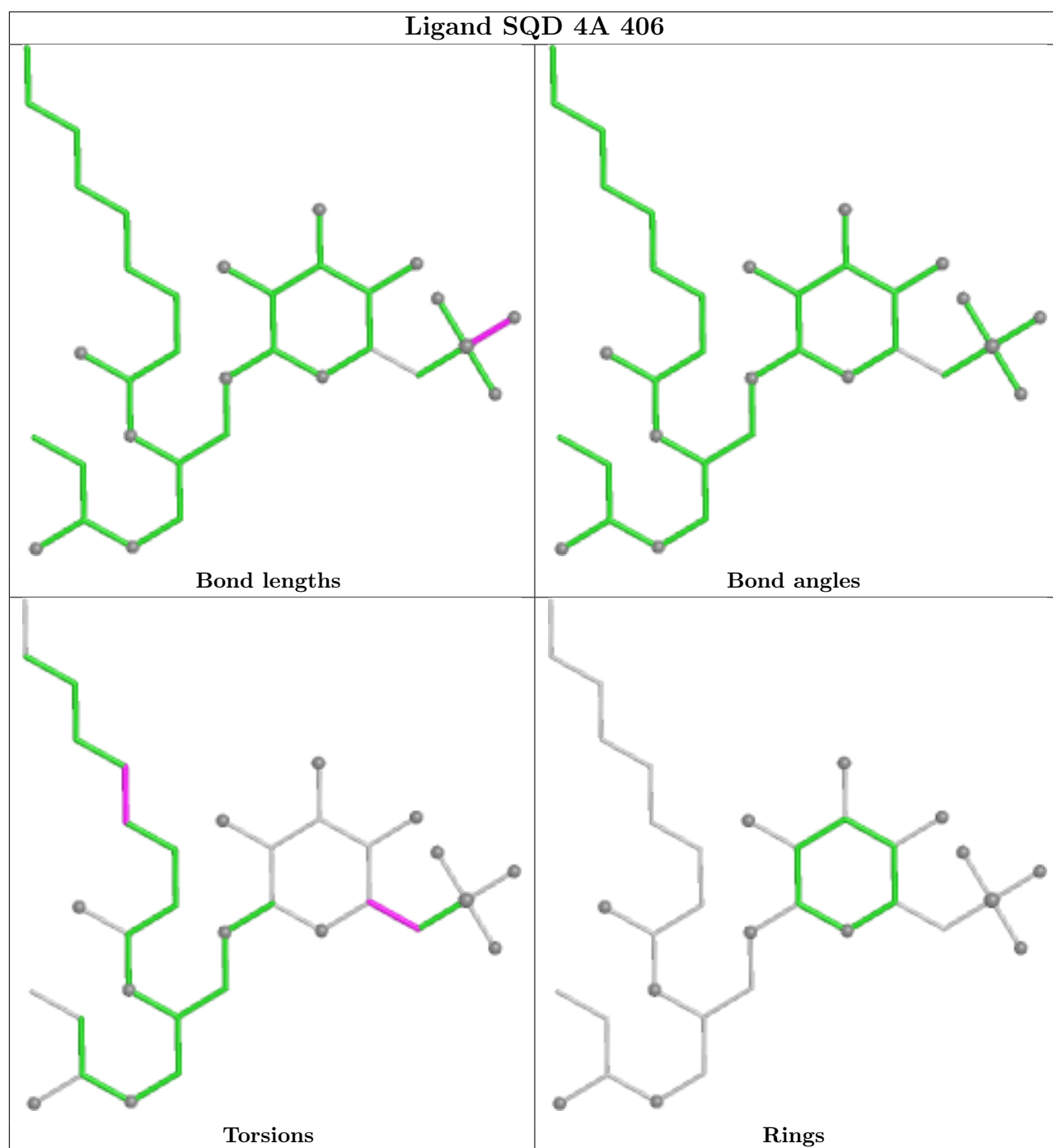
Rings

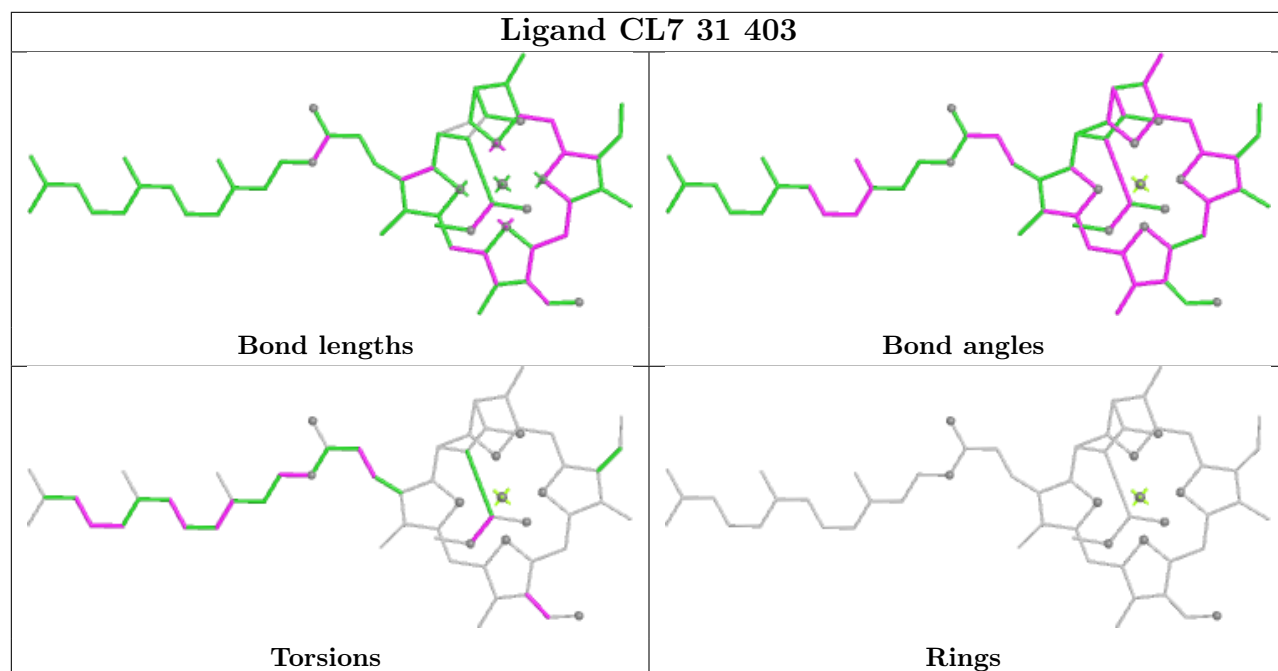
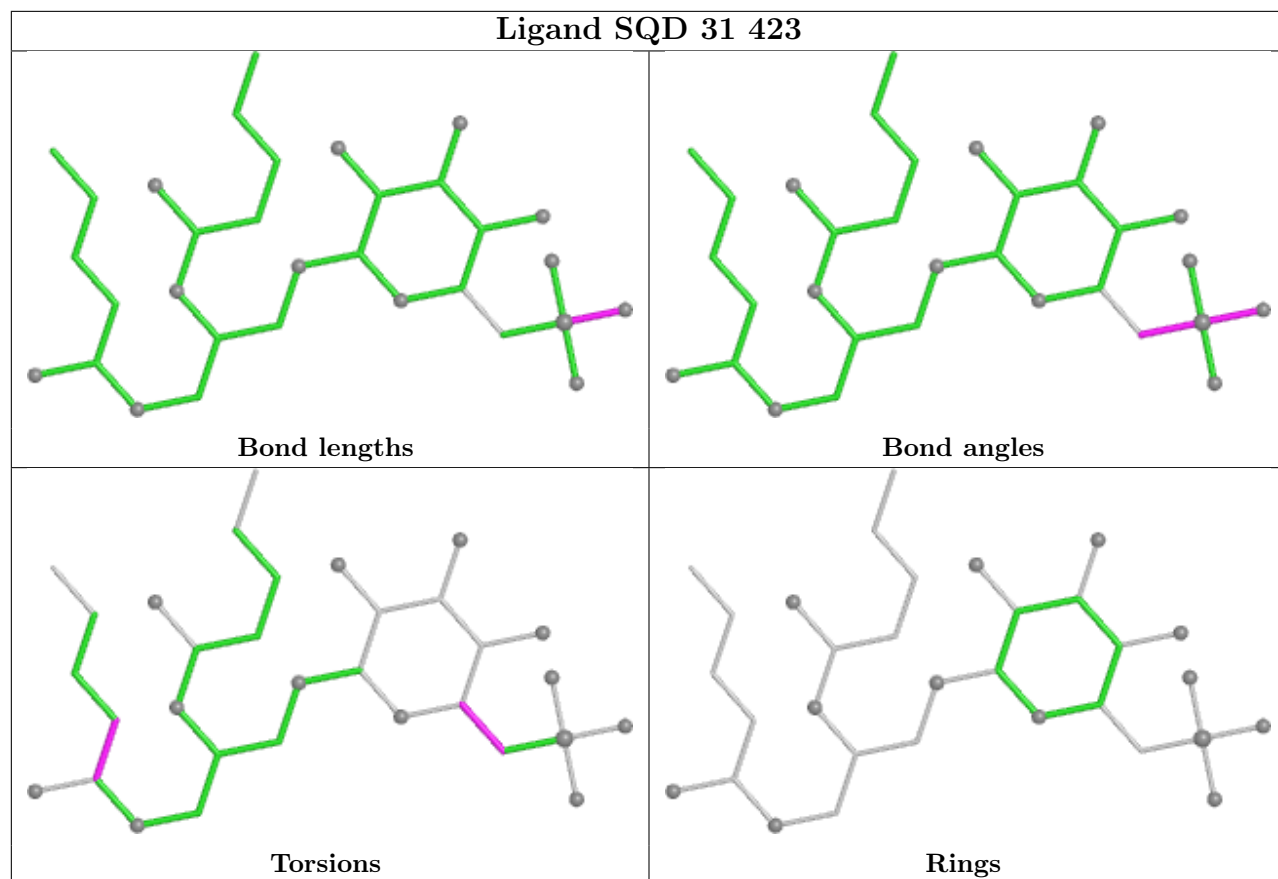


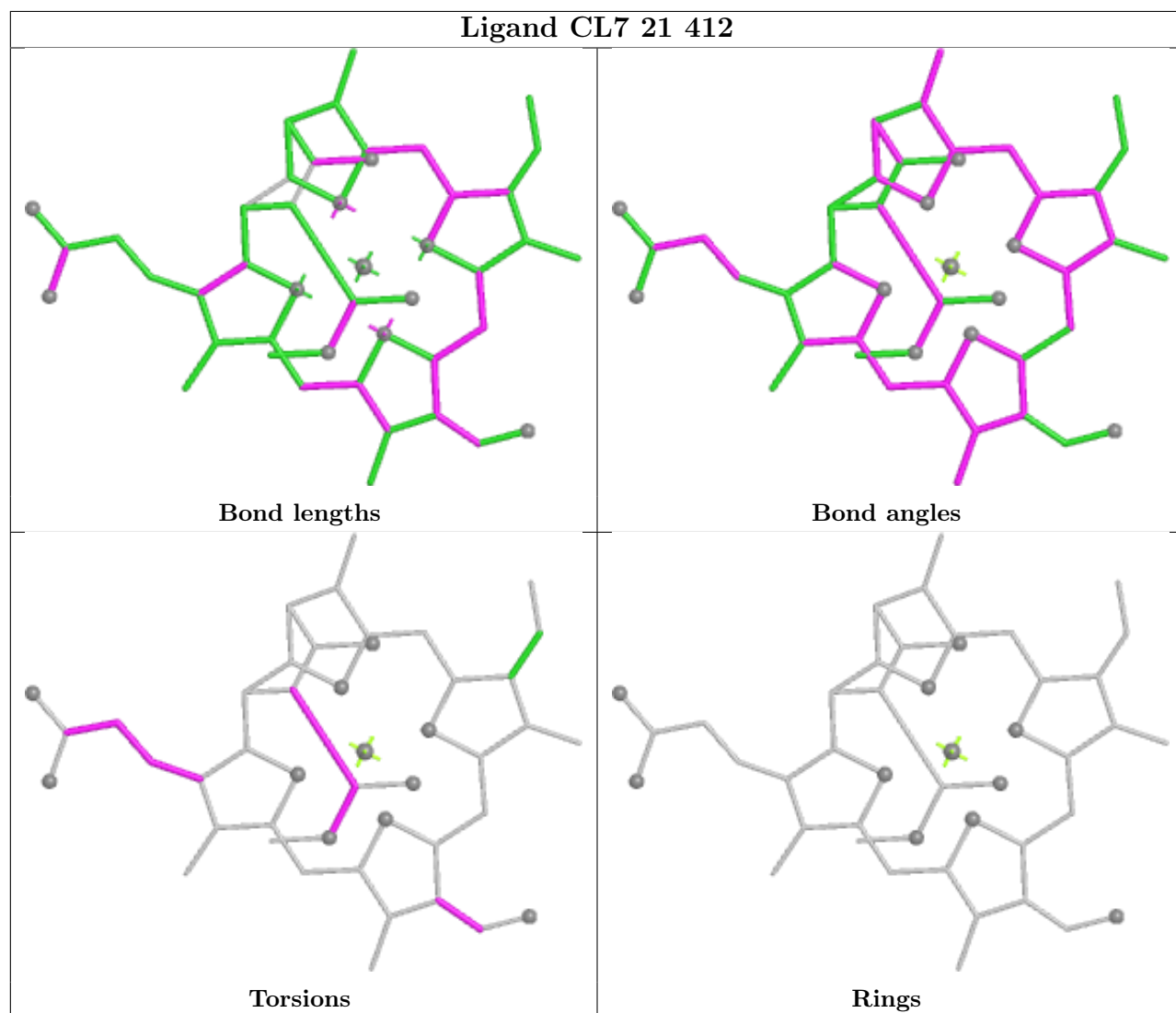
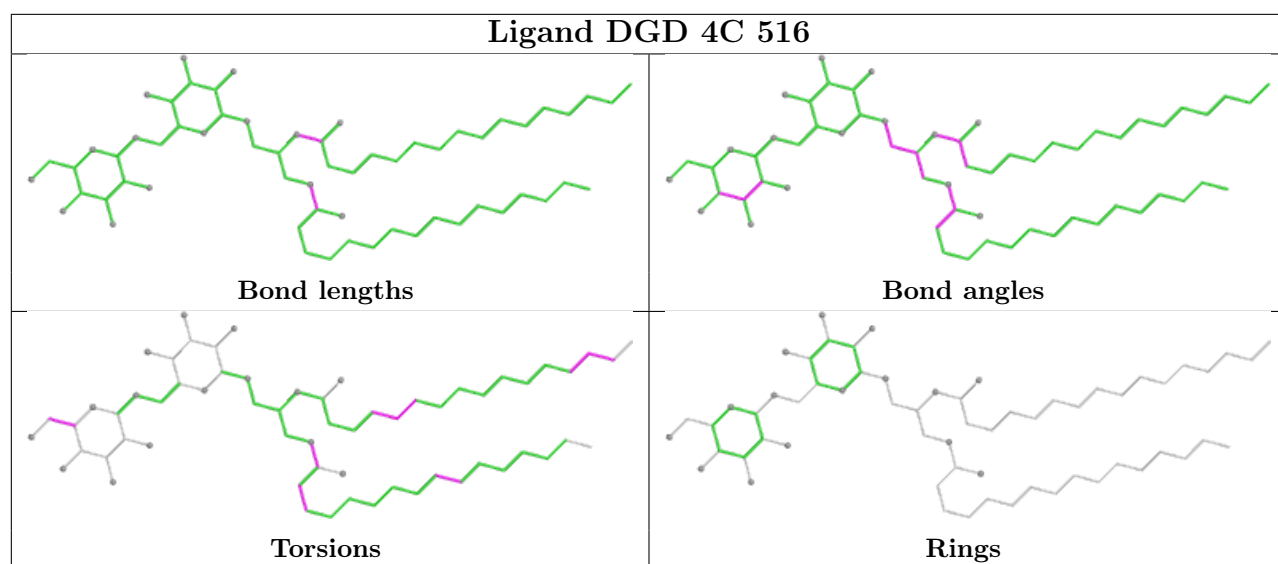


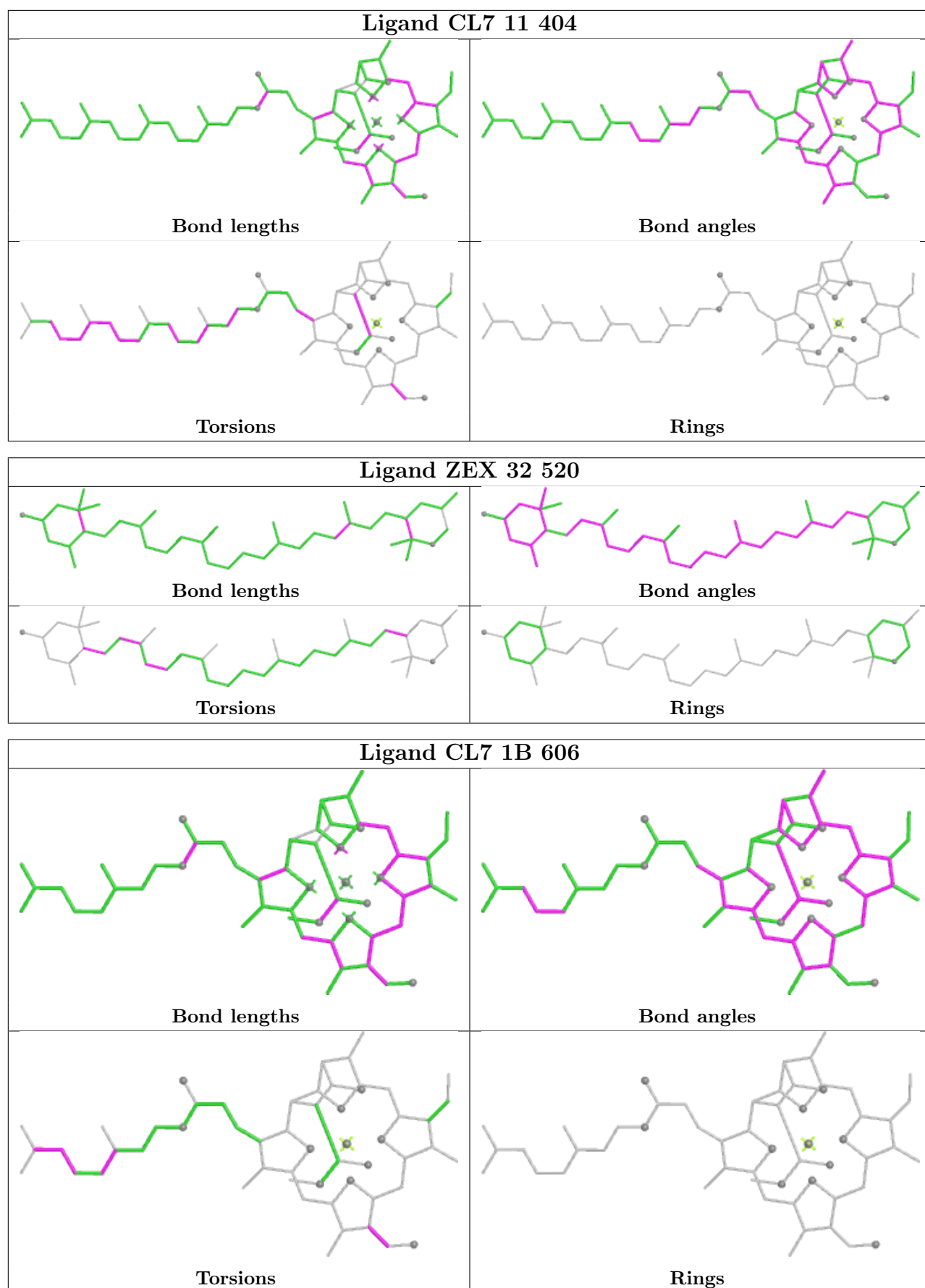


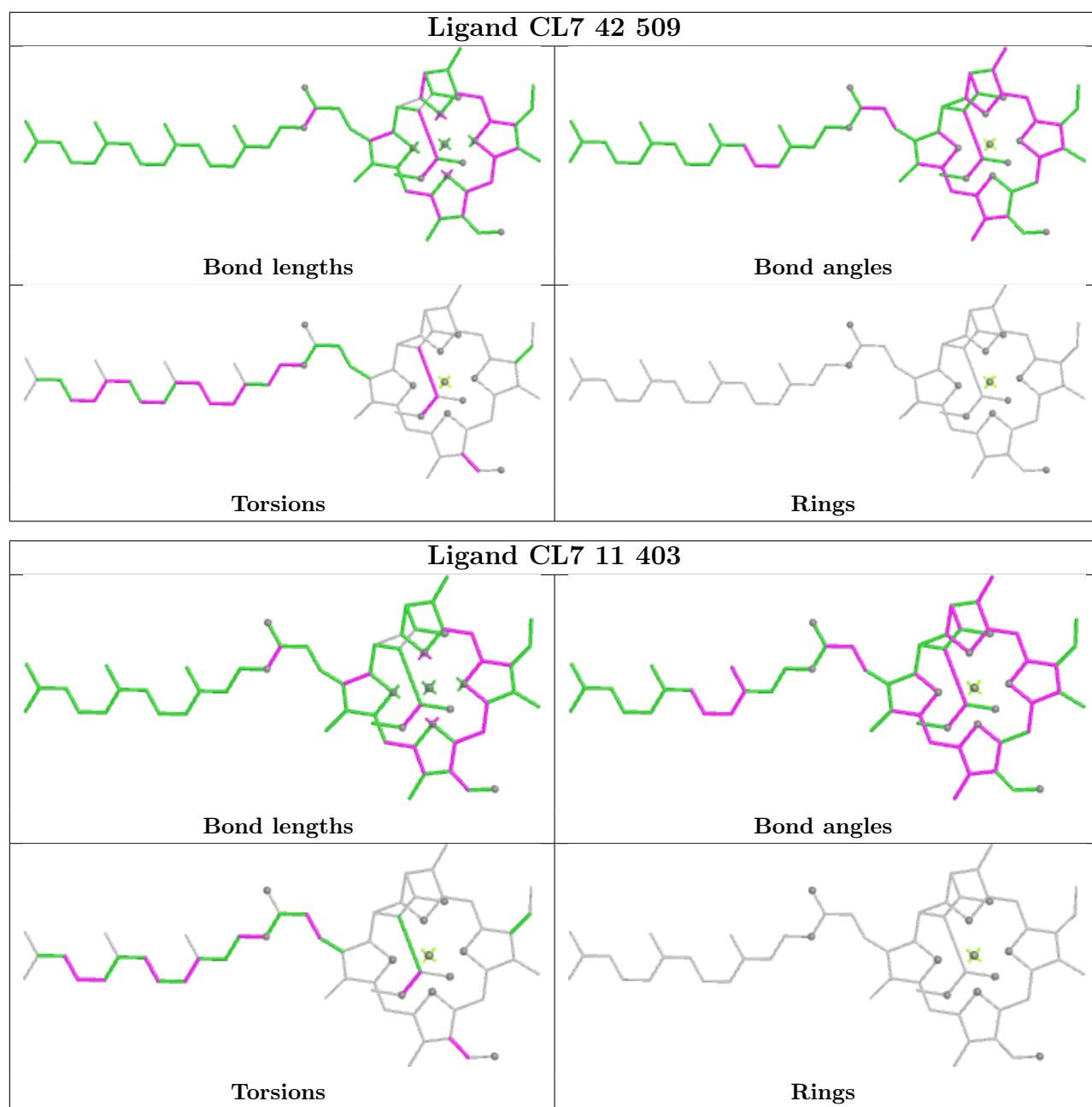


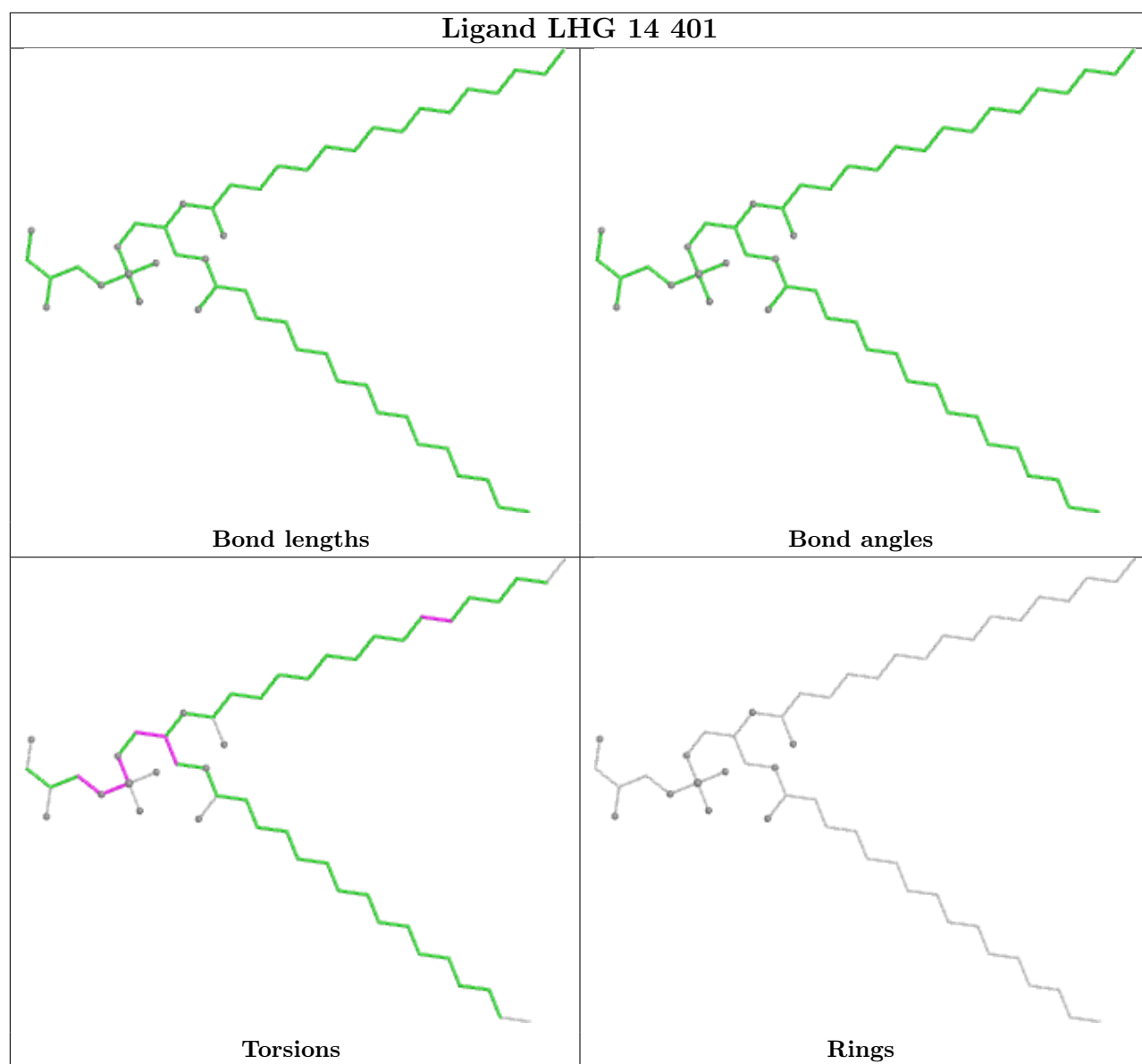


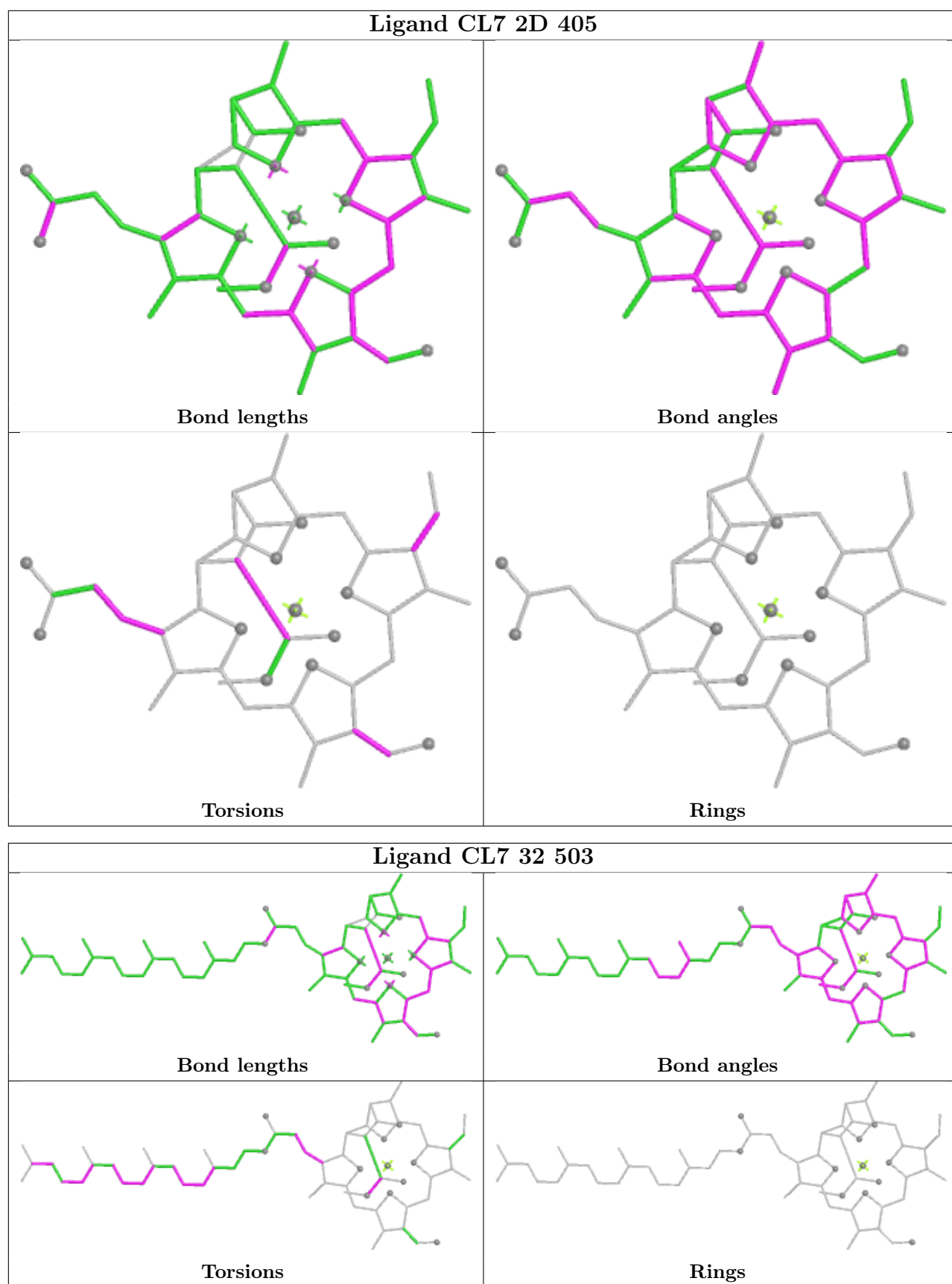


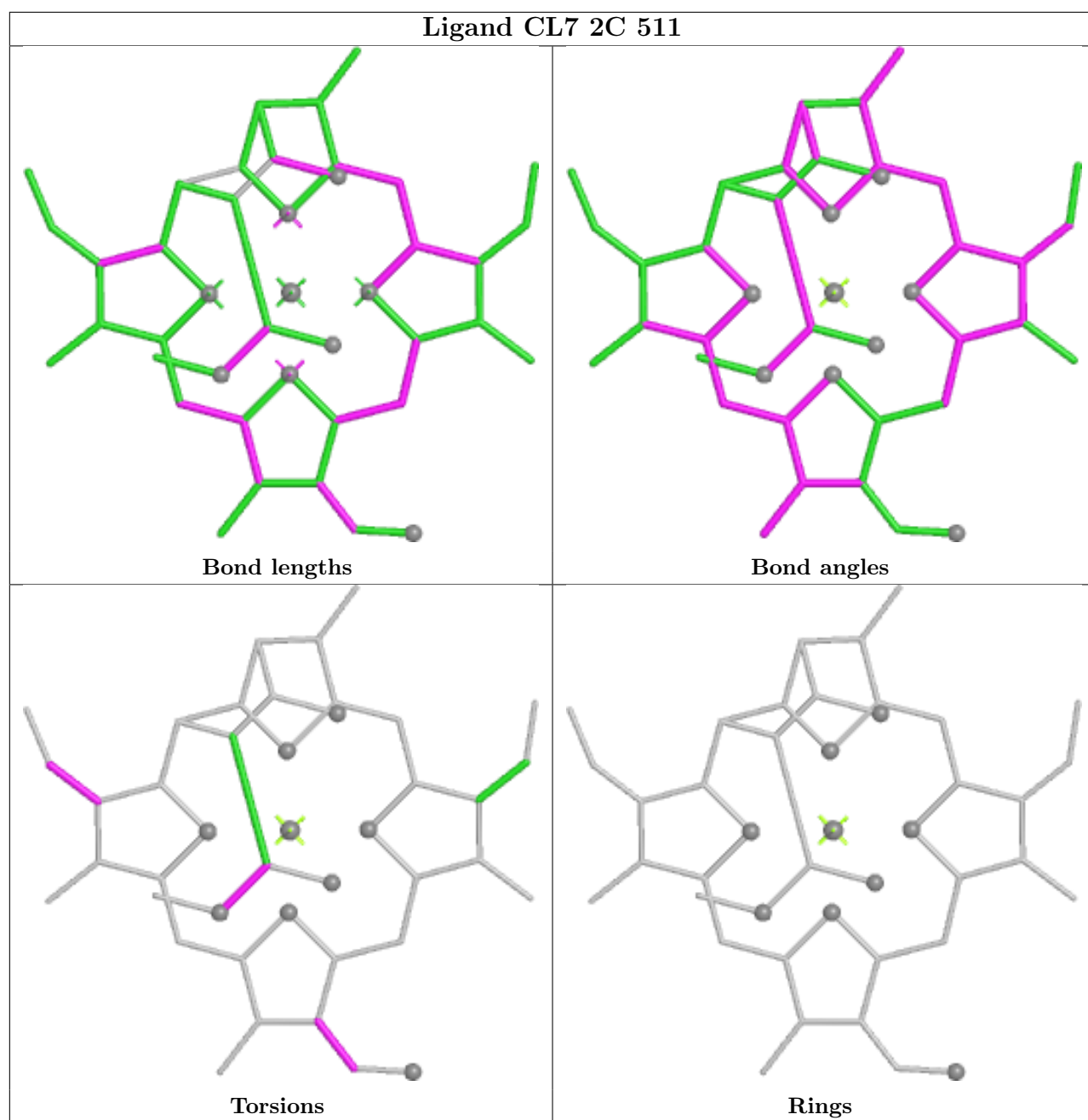


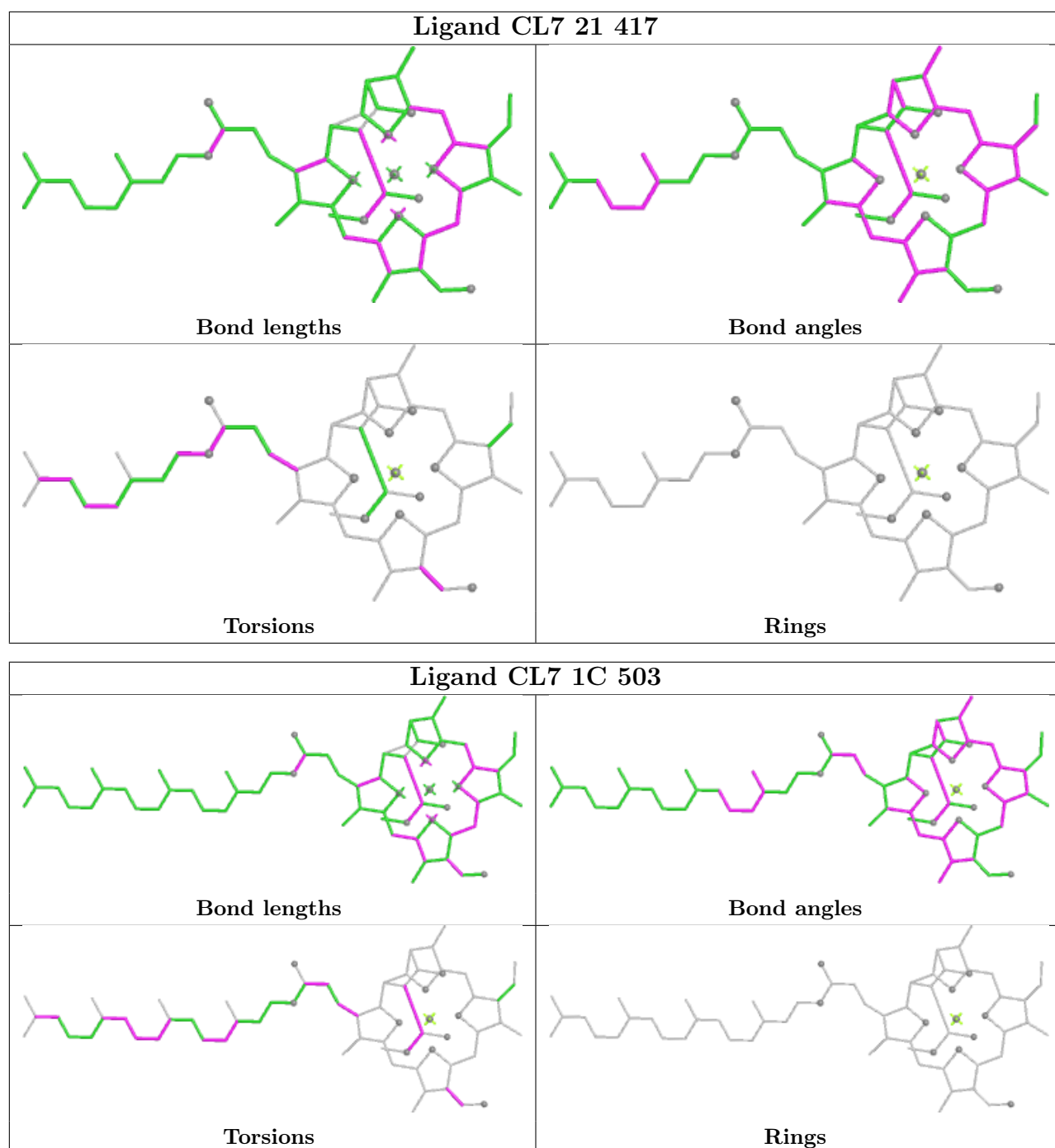


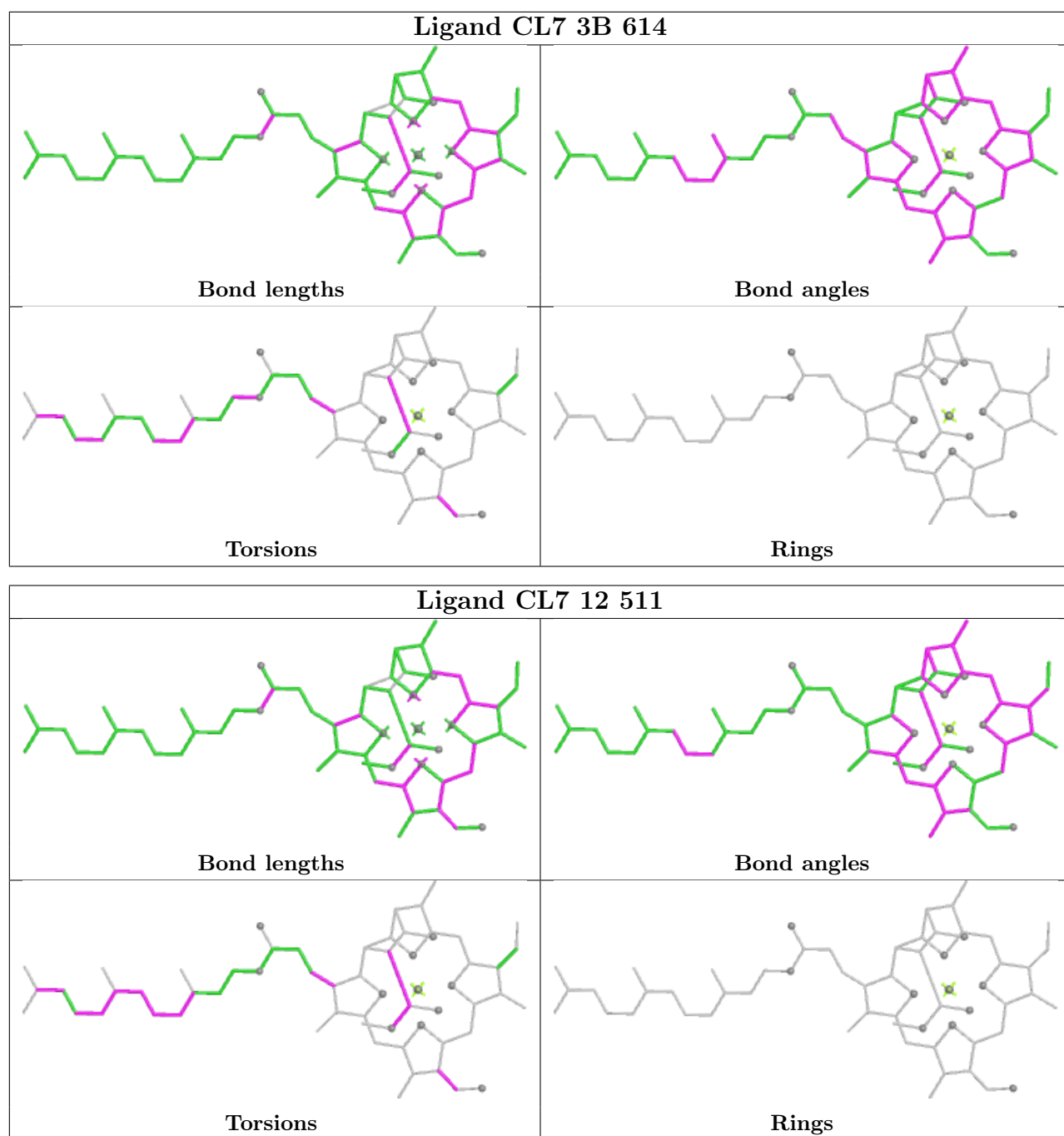


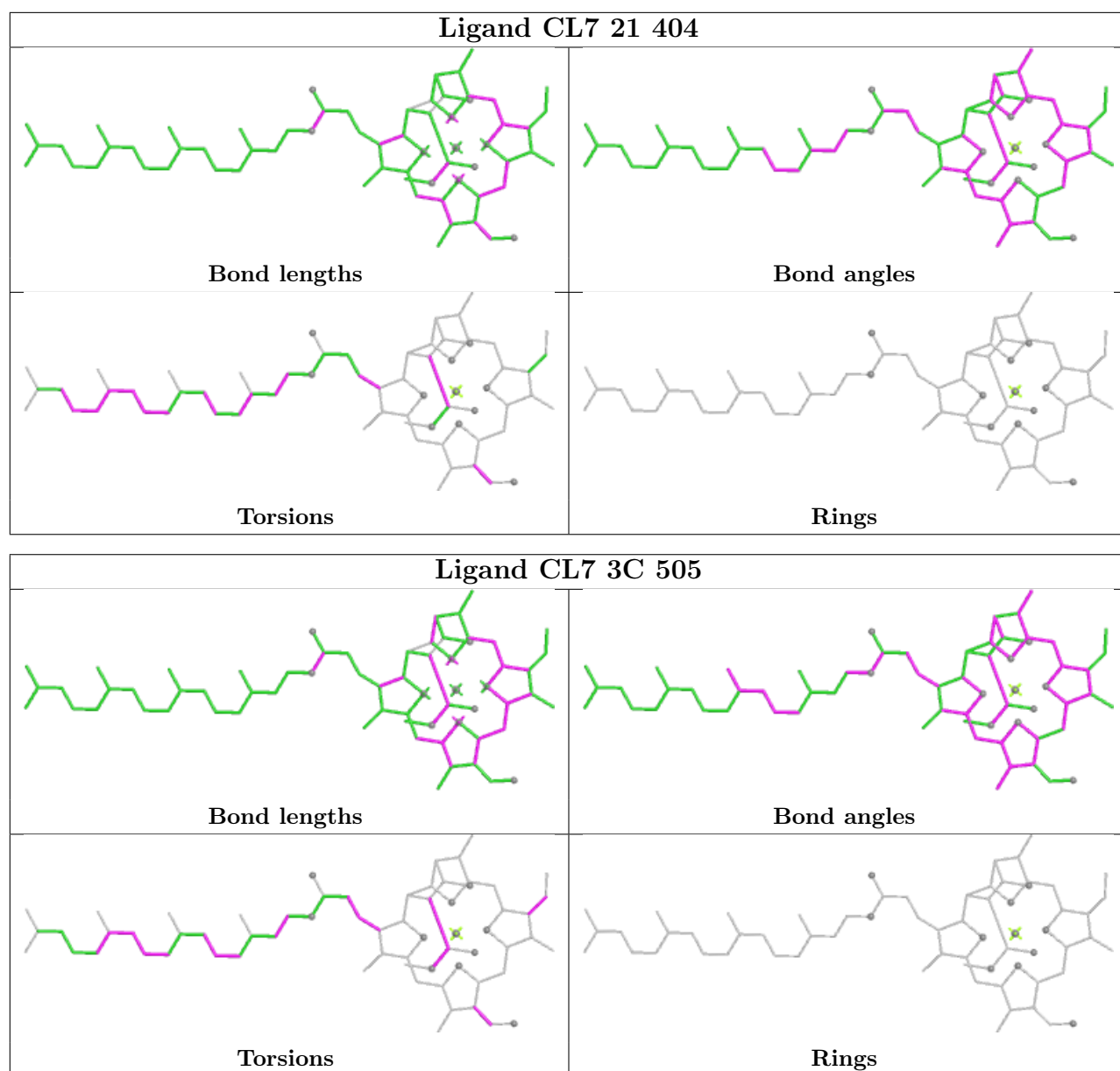


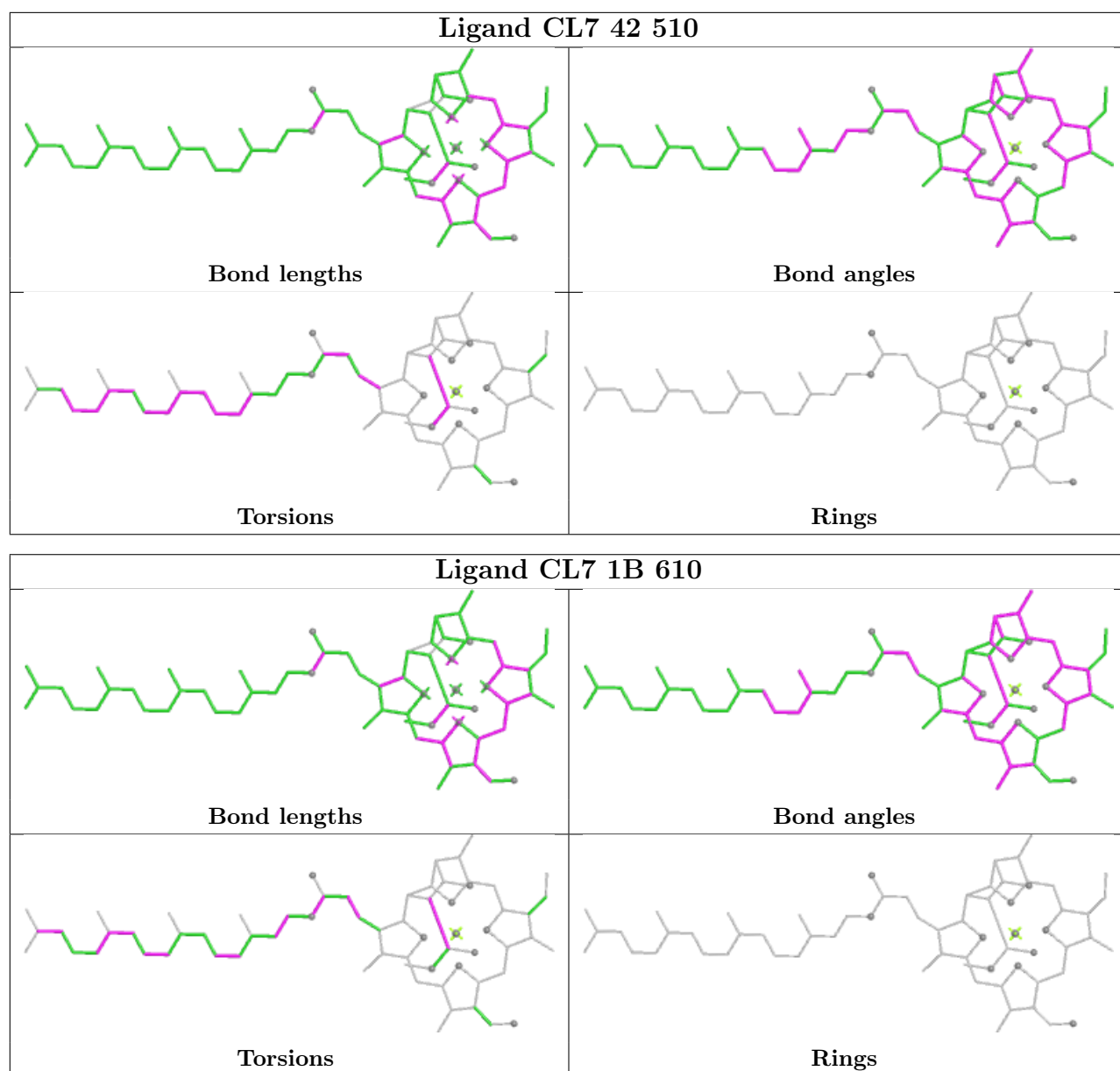




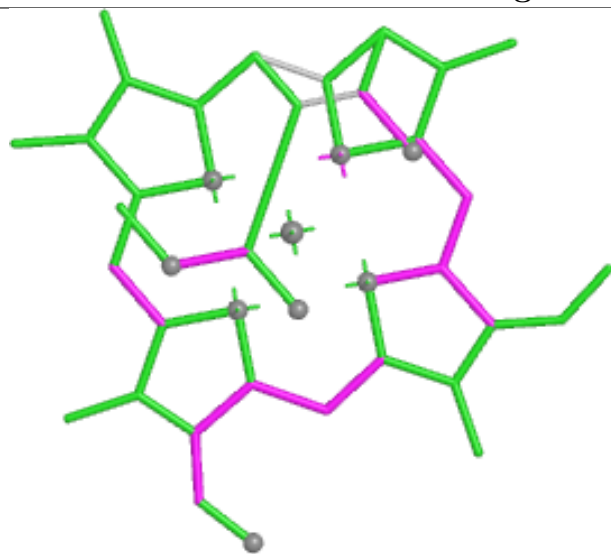




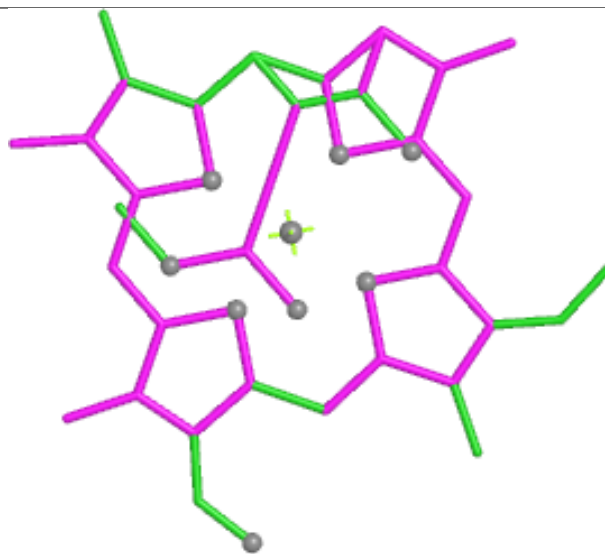




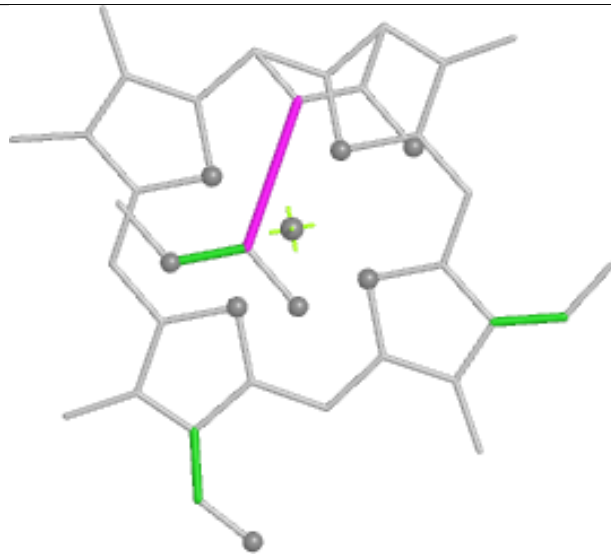
Ligand CL7 41 413



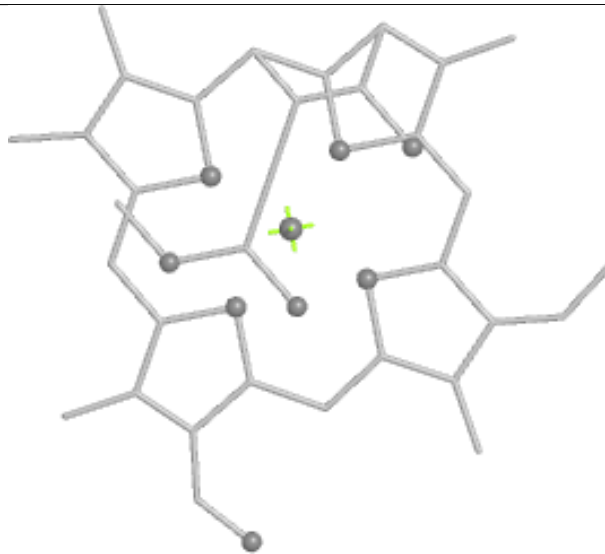
Bond lengths



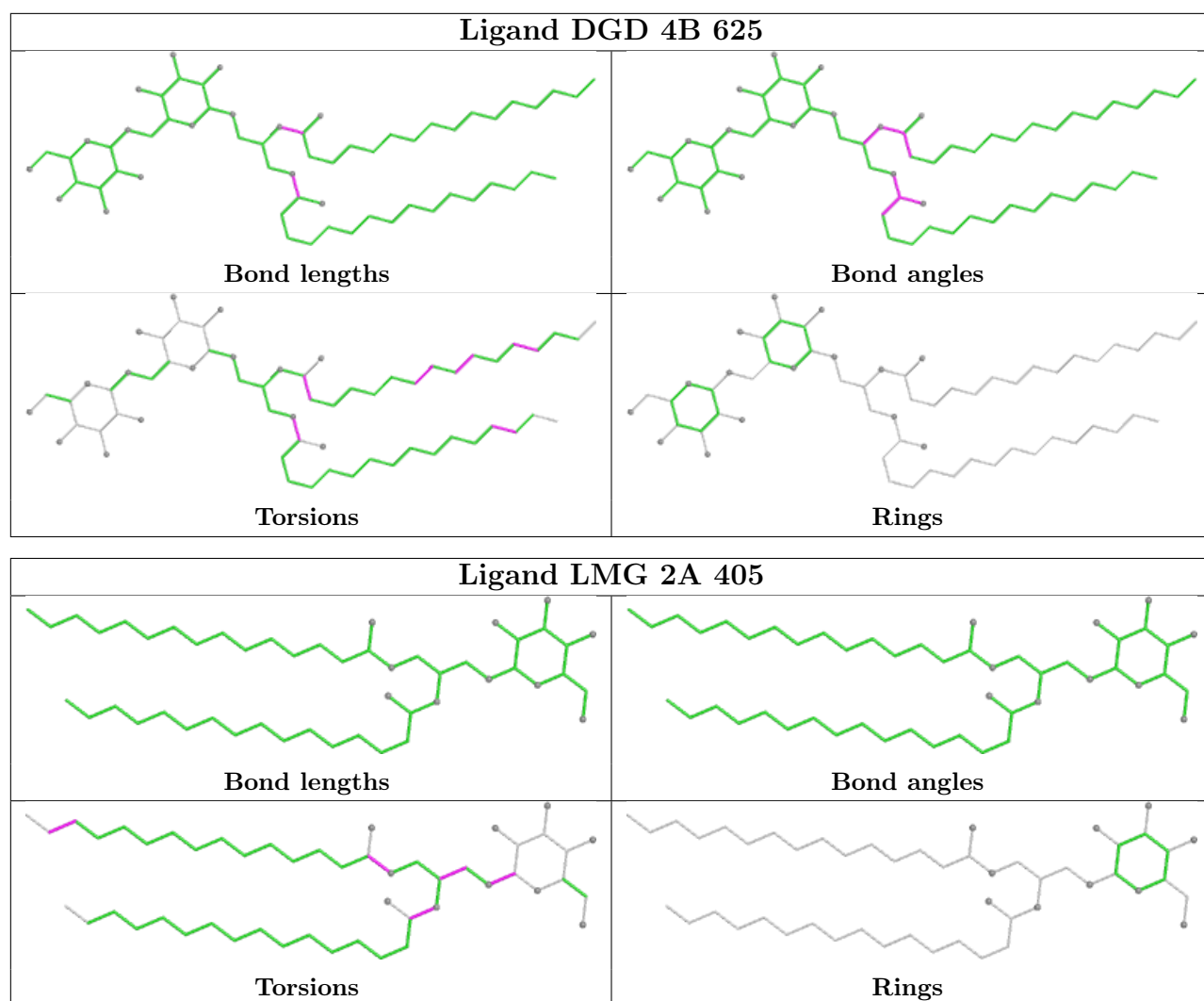
Bond angles



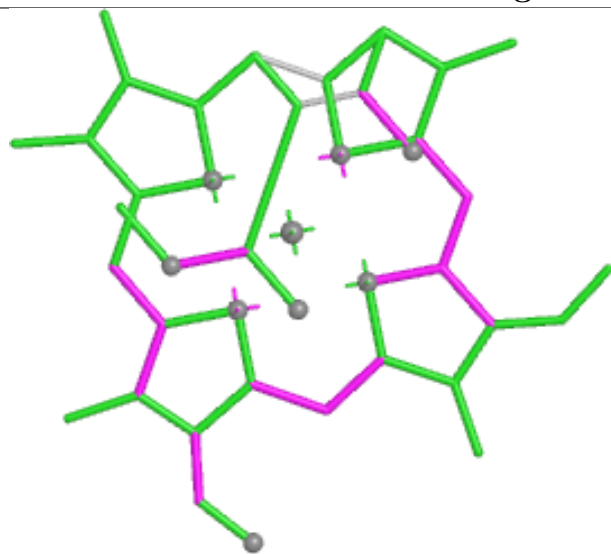
Torsions



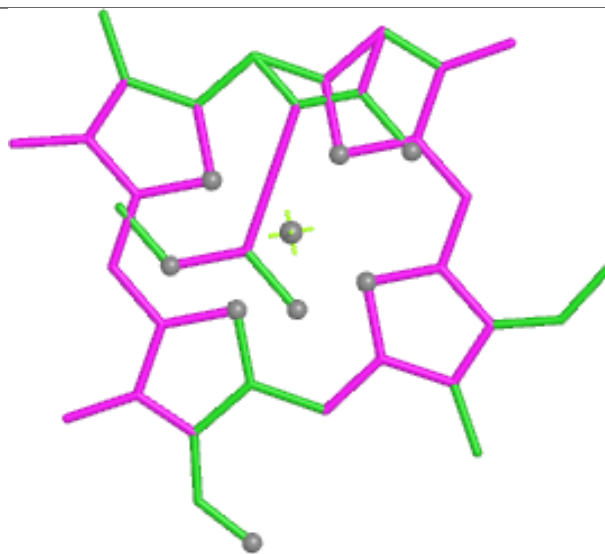
Rings



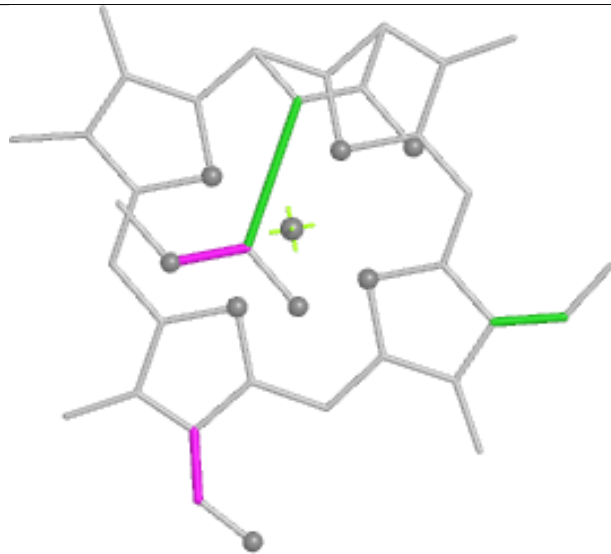
Ligand CL7 41 416



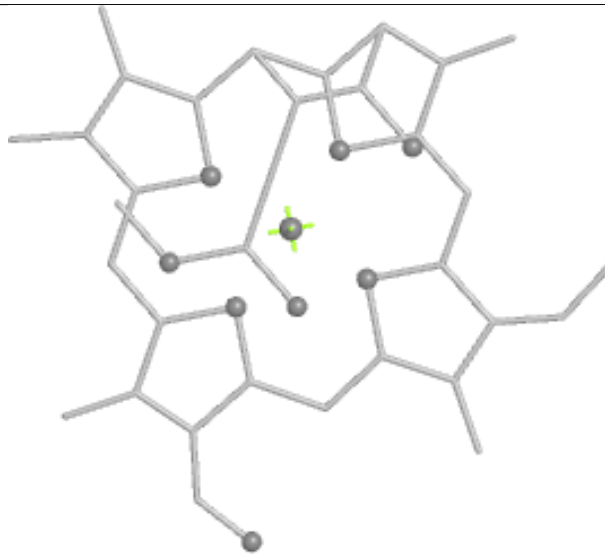
Bond lengths



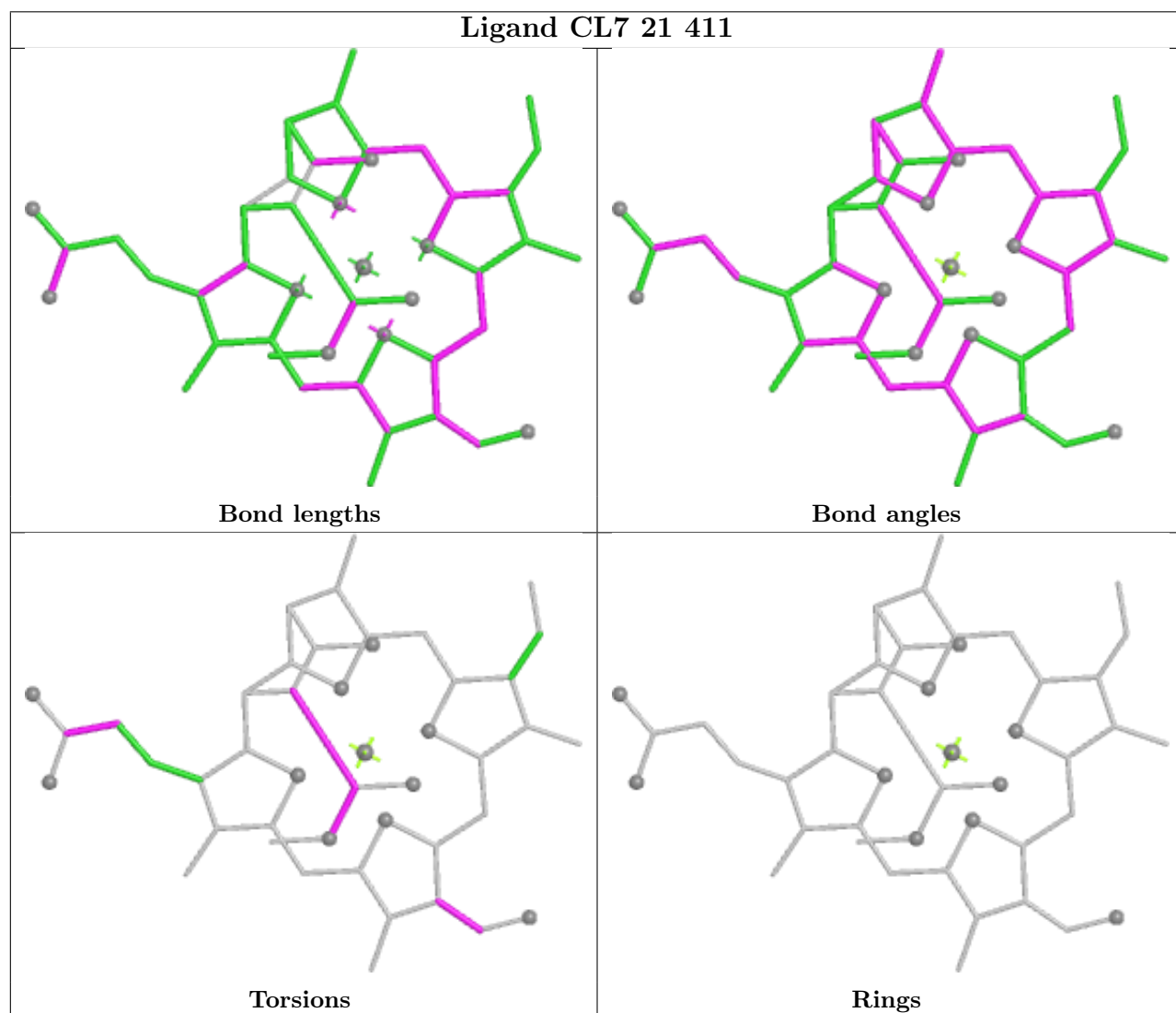
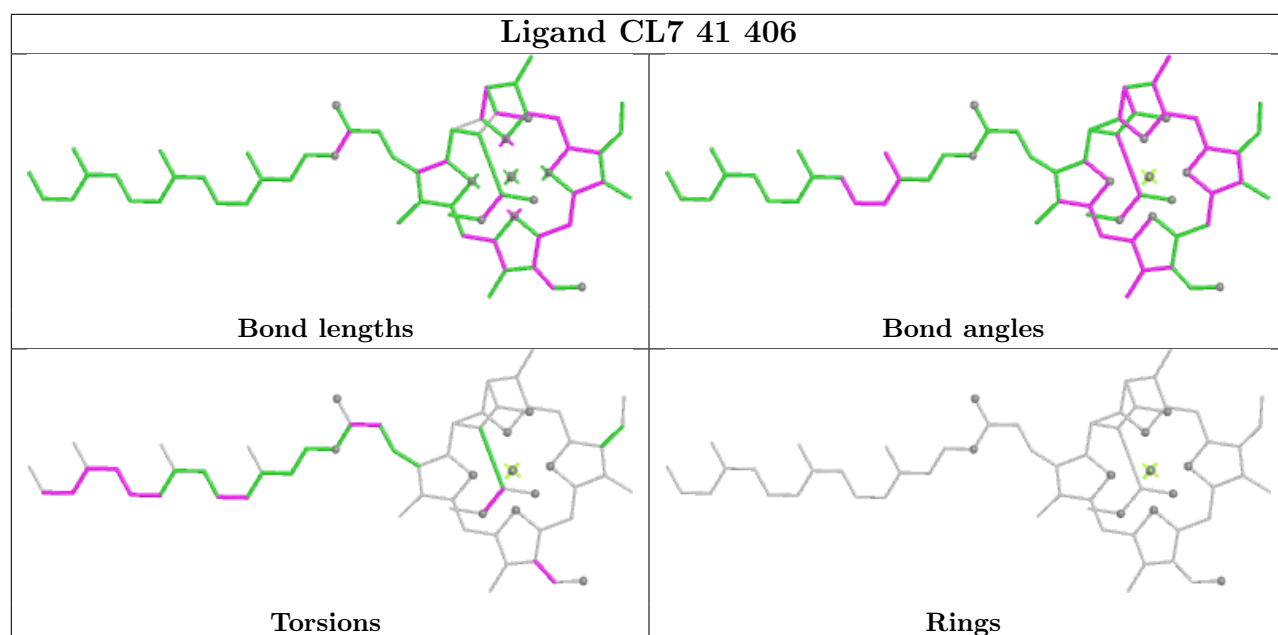
Bond angles

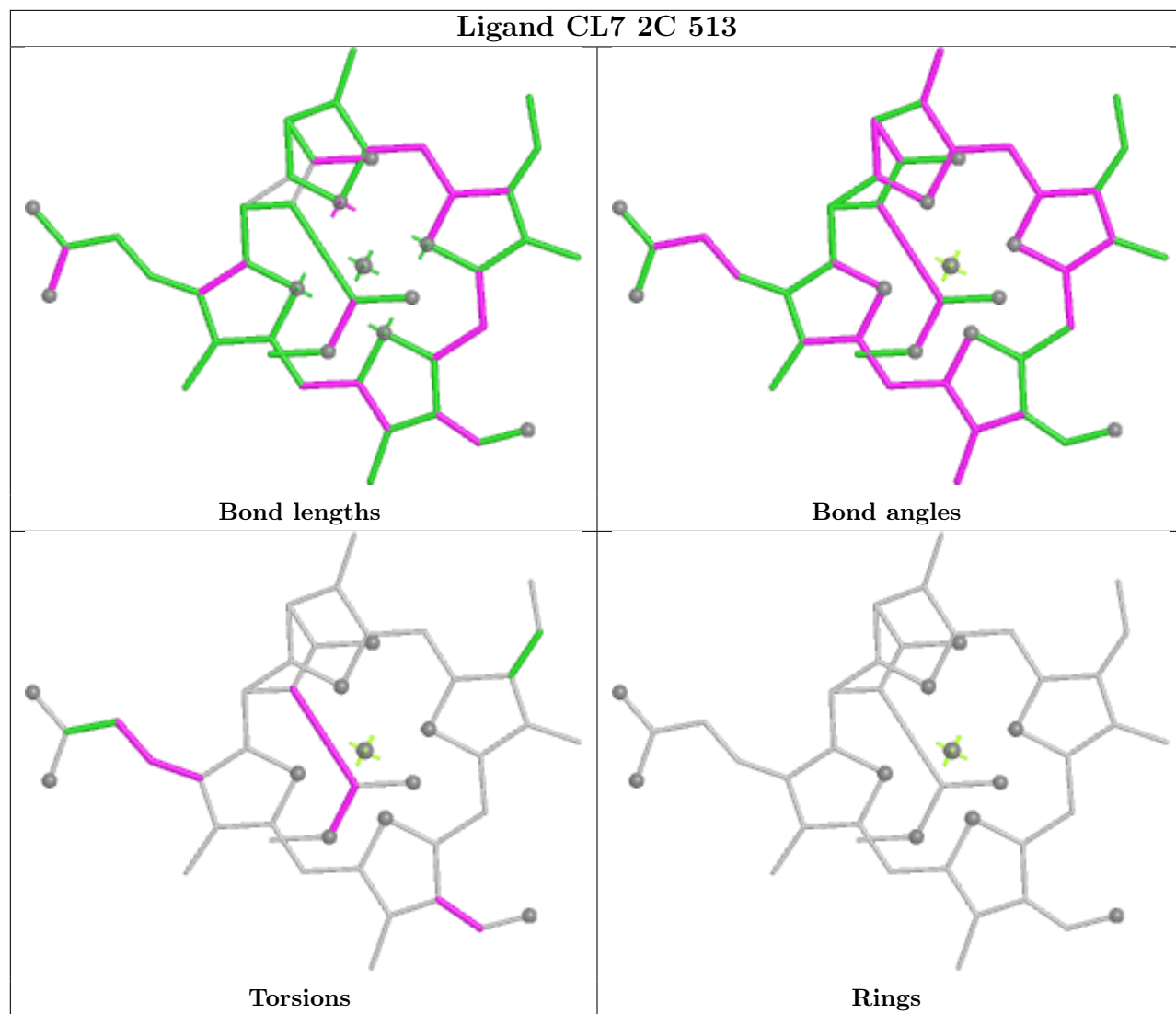


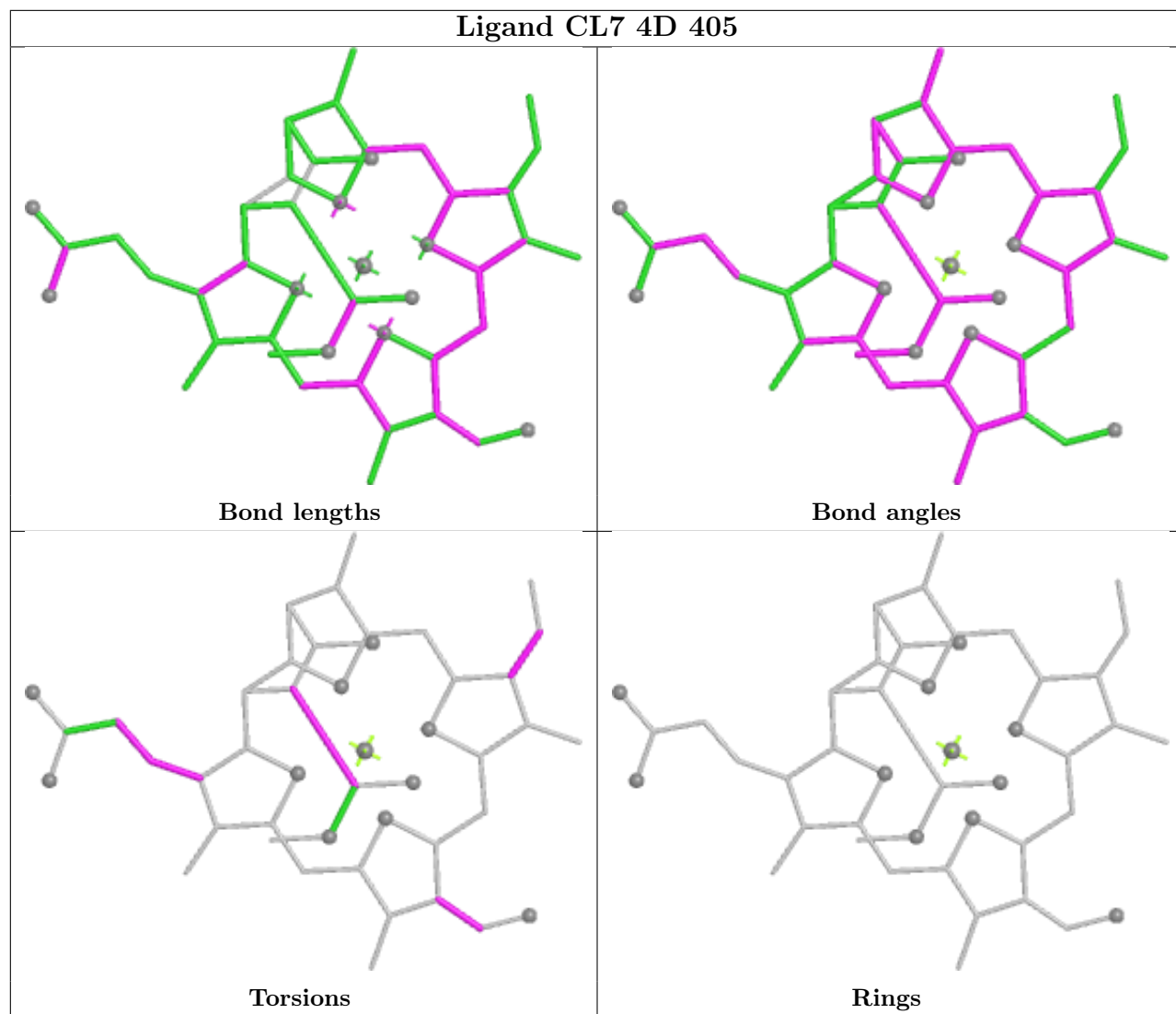
Torsions



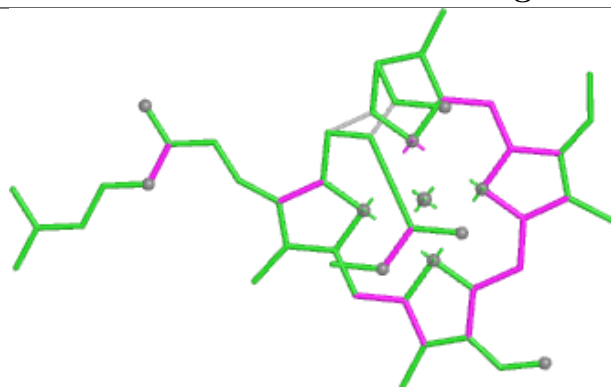
Rings



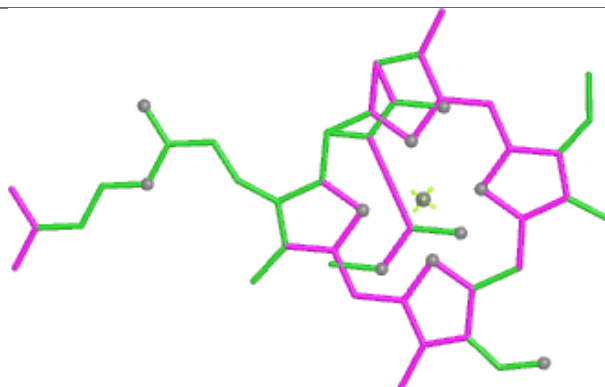




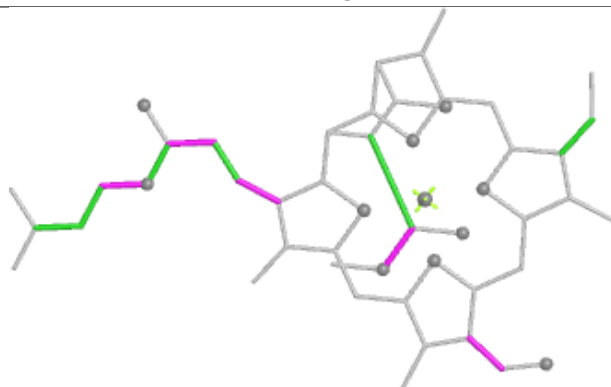
Ligand CL7 33 517



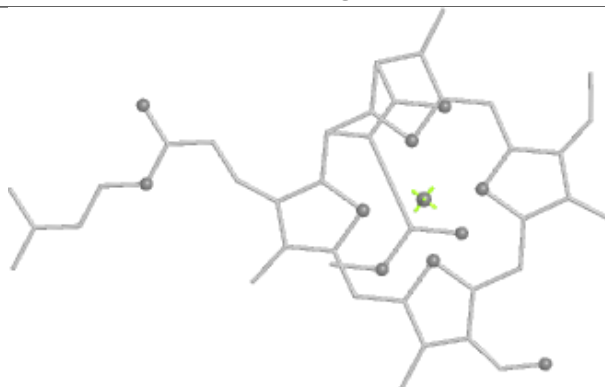
Bond lengths



Bond angles

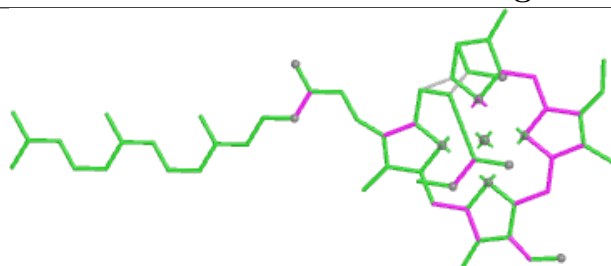


Torsions

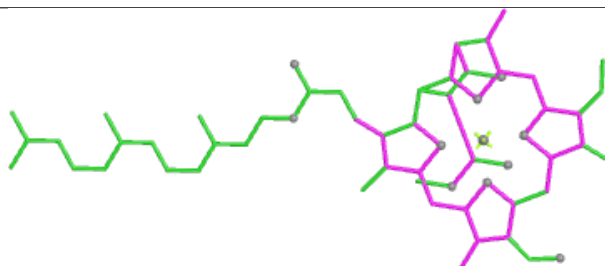


Rings

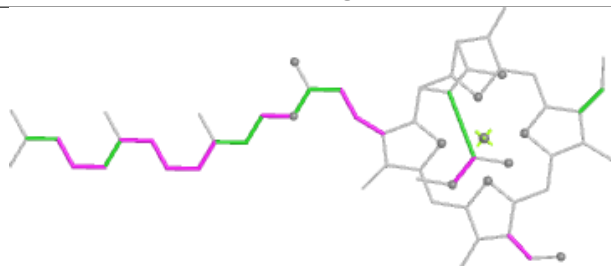
Ligand CL7 11 402



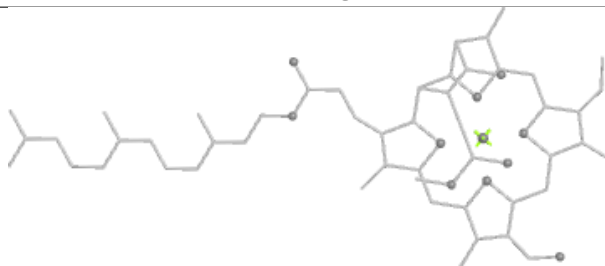
Bond lengths



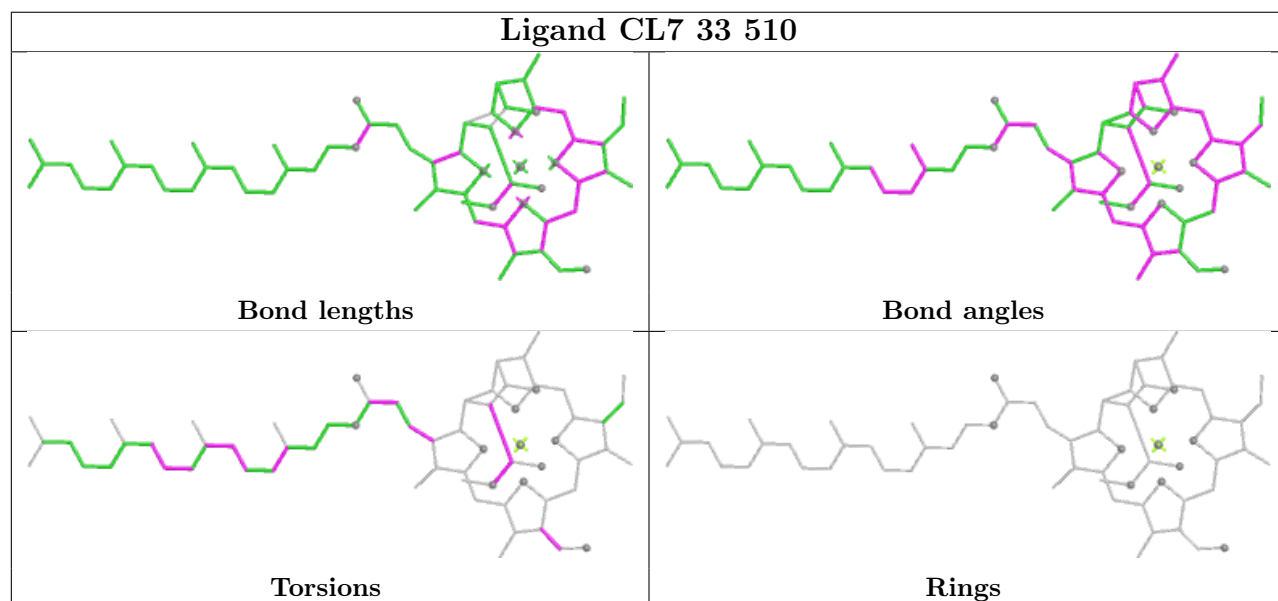
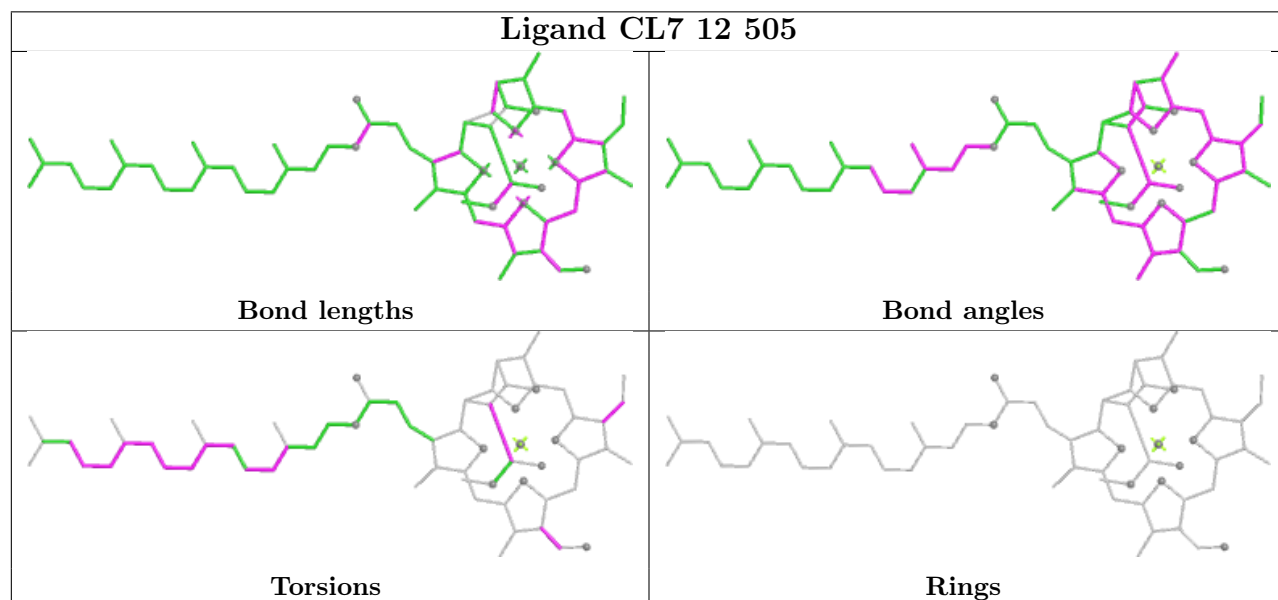
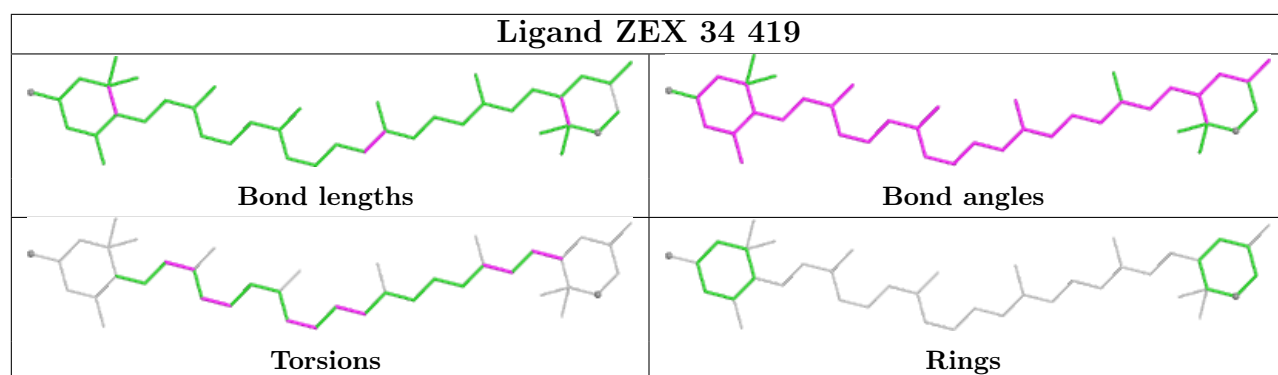
Bond angles

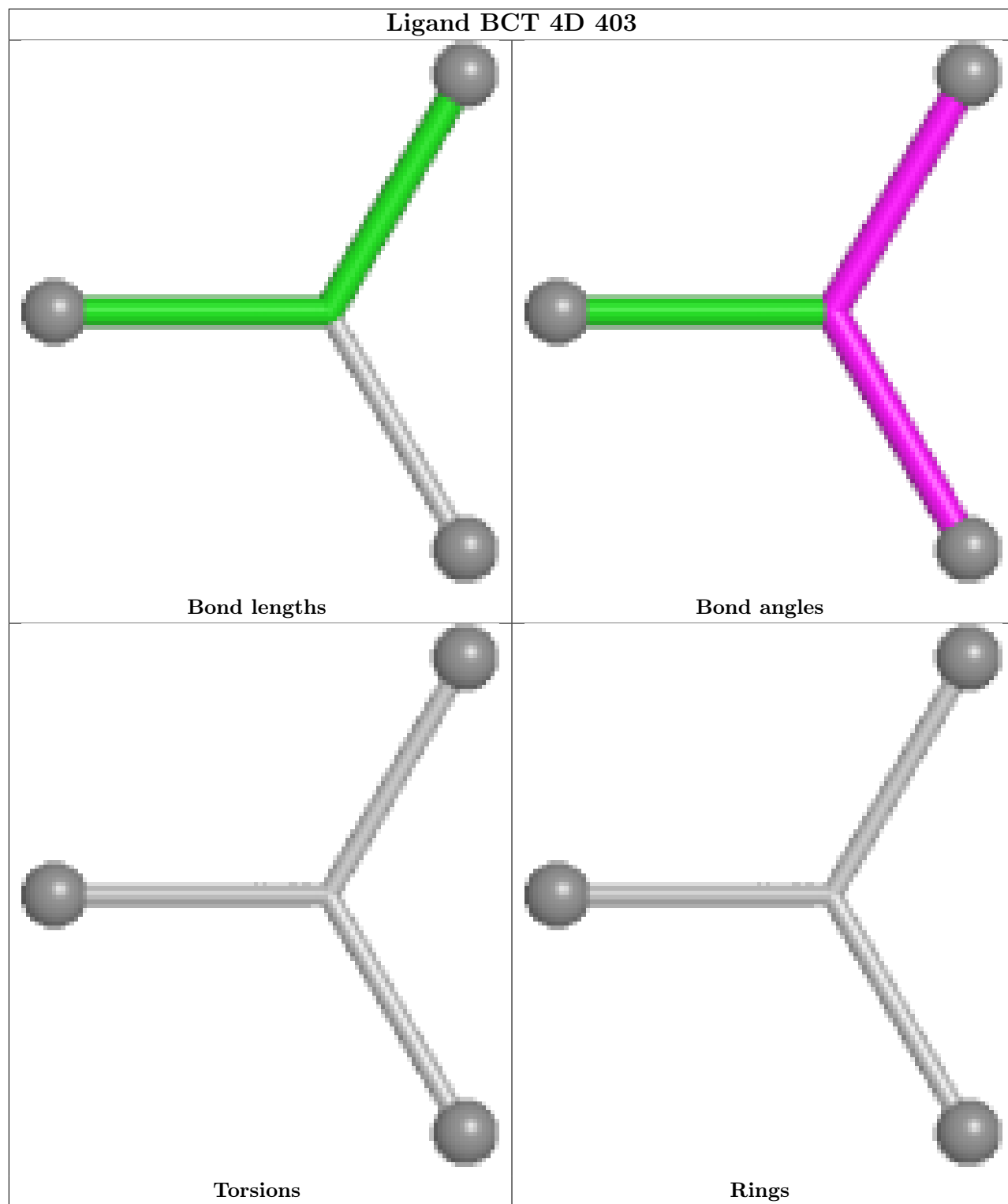


Torsions

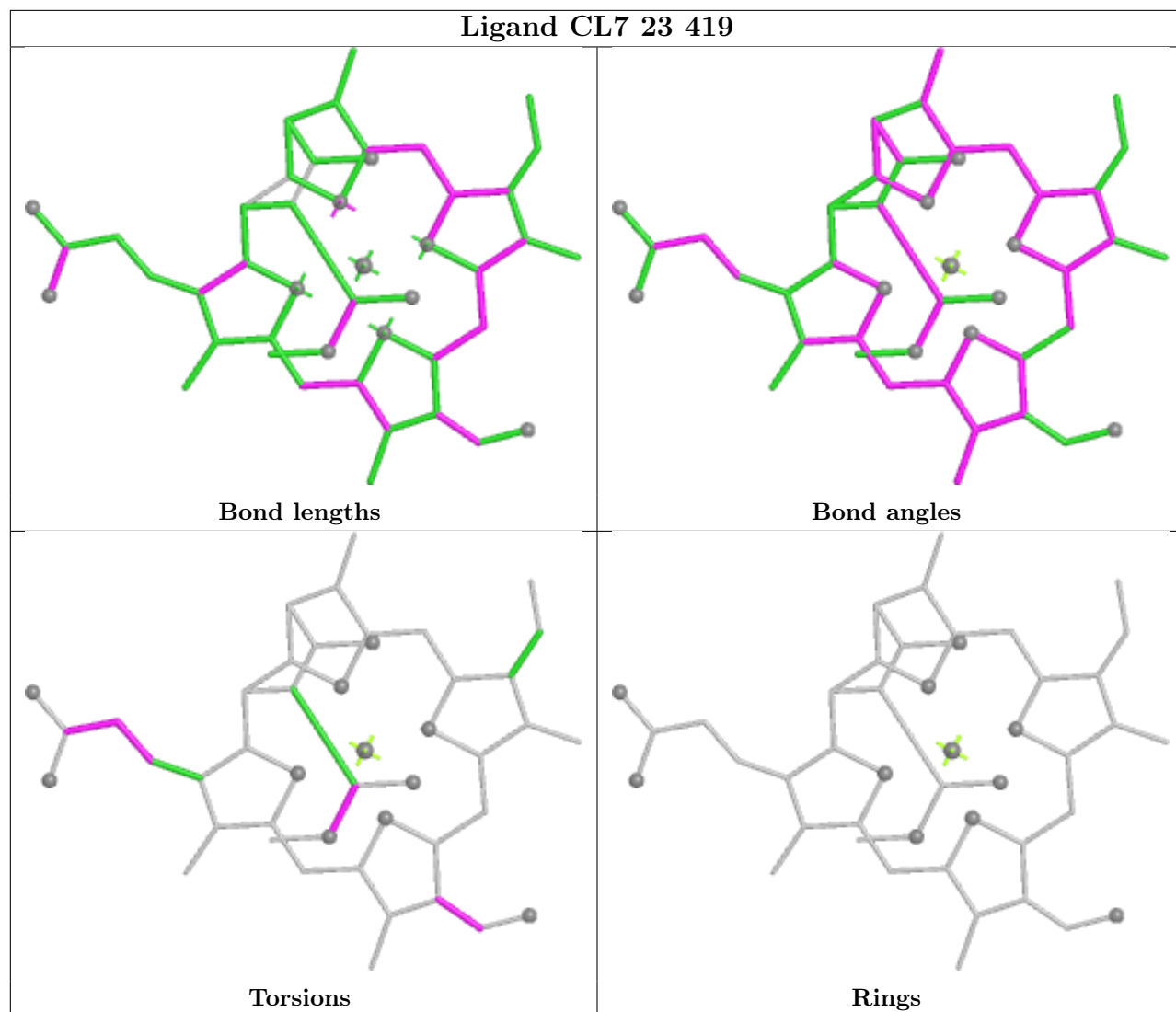


Rings

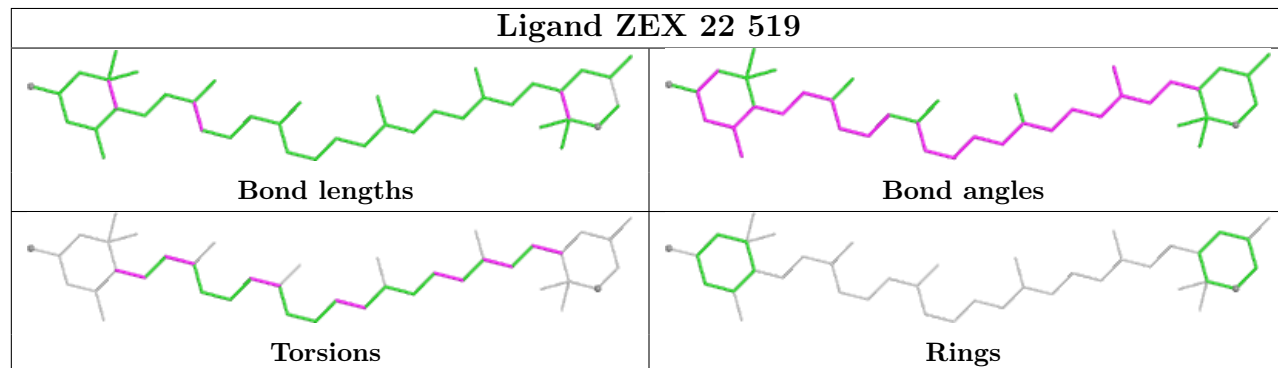


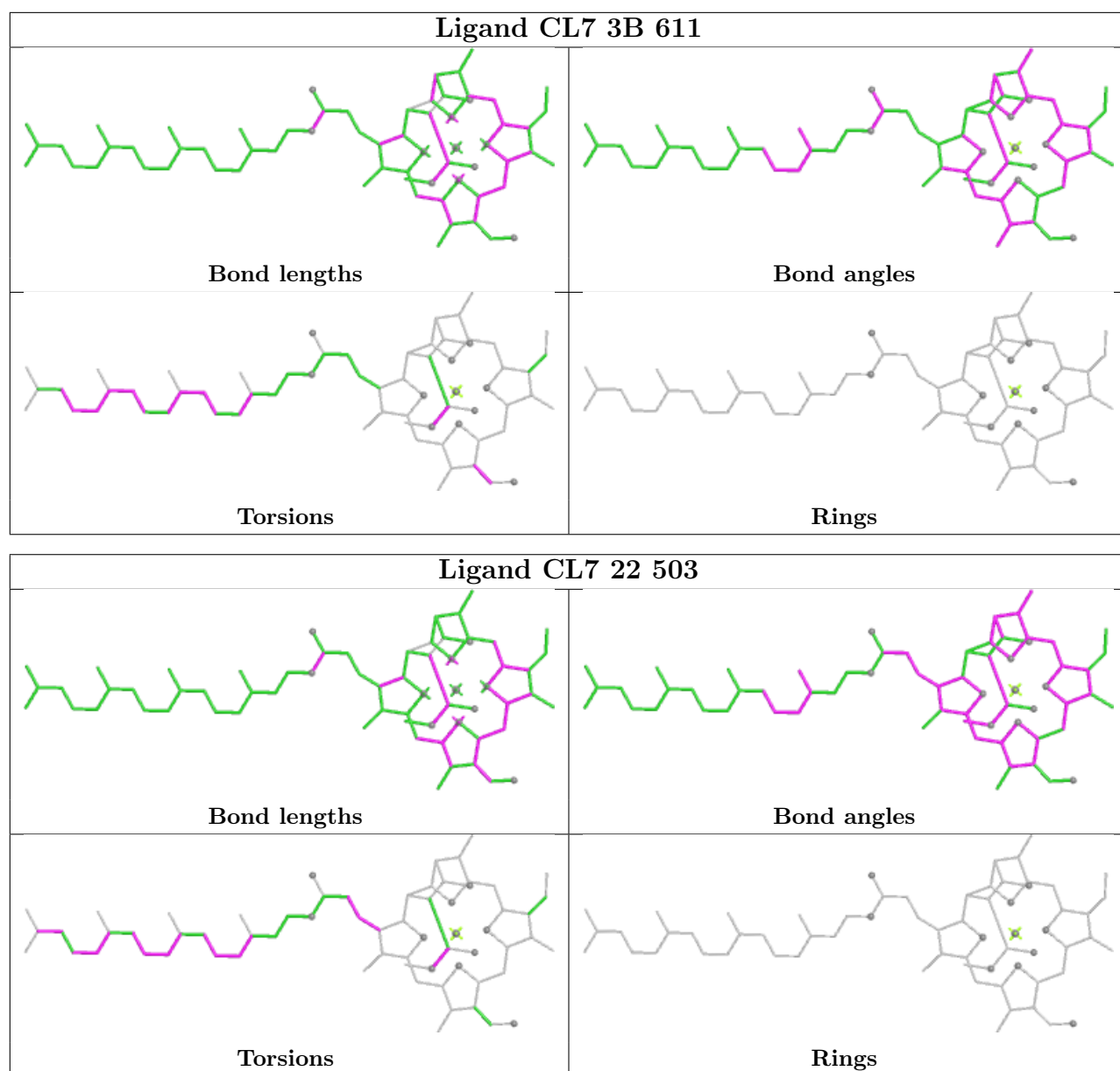


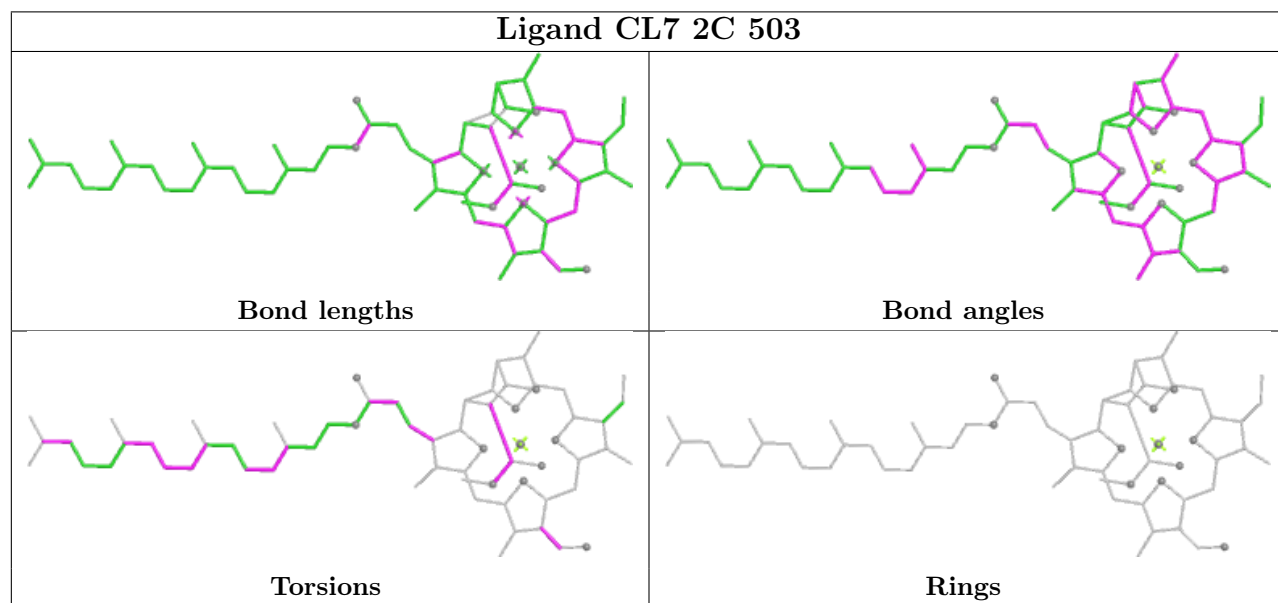
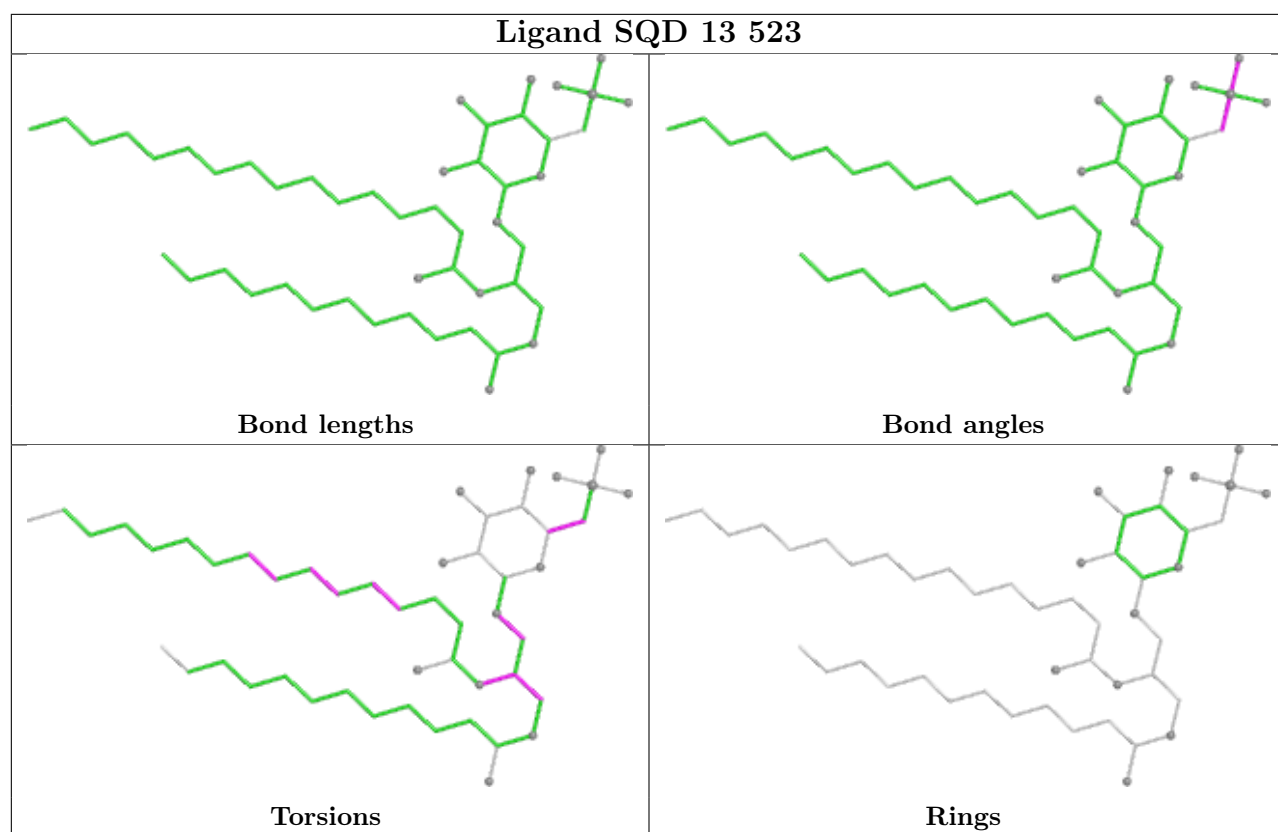
Ligand CL7 23 419

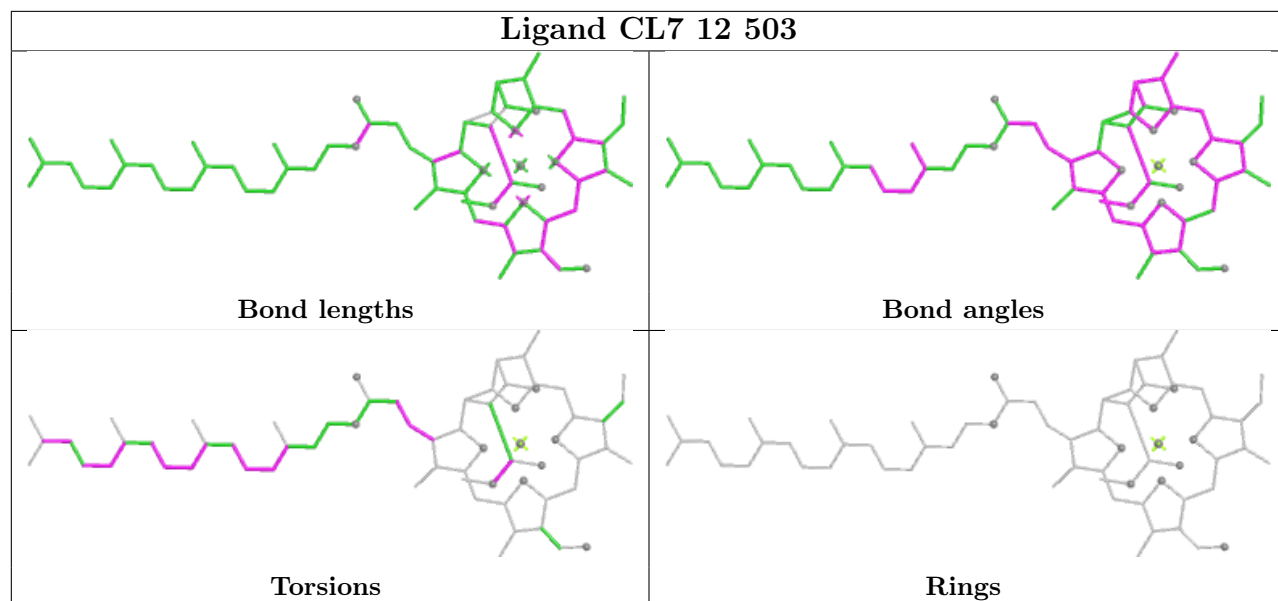


Ligand ZEX 22 519

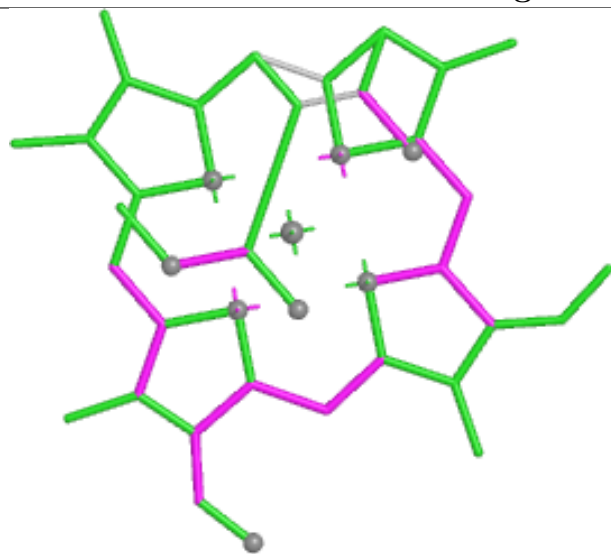




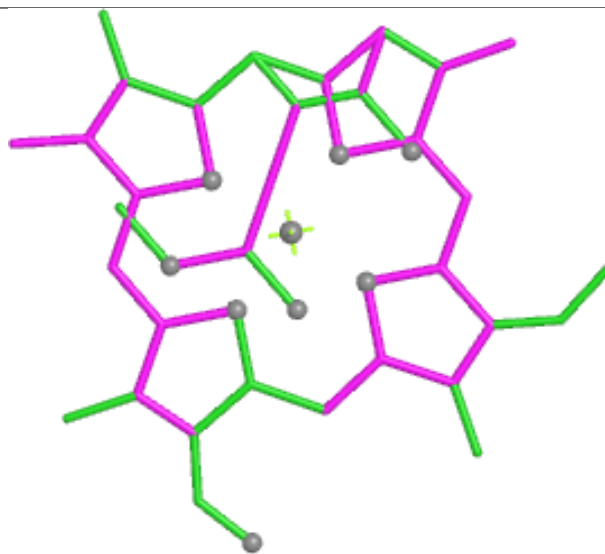




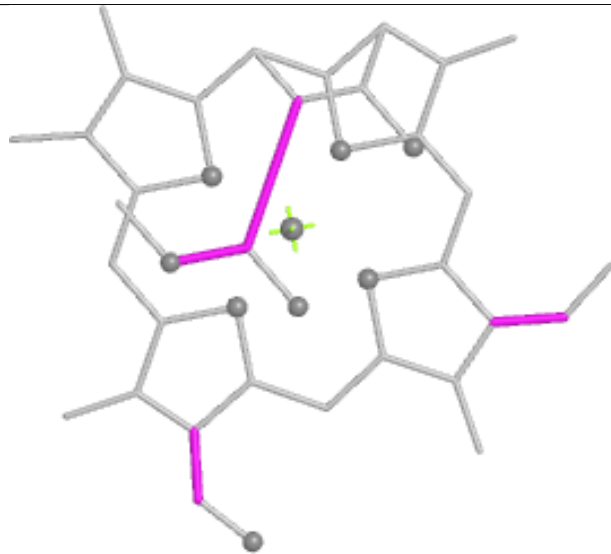
Ligand CL7 34 416



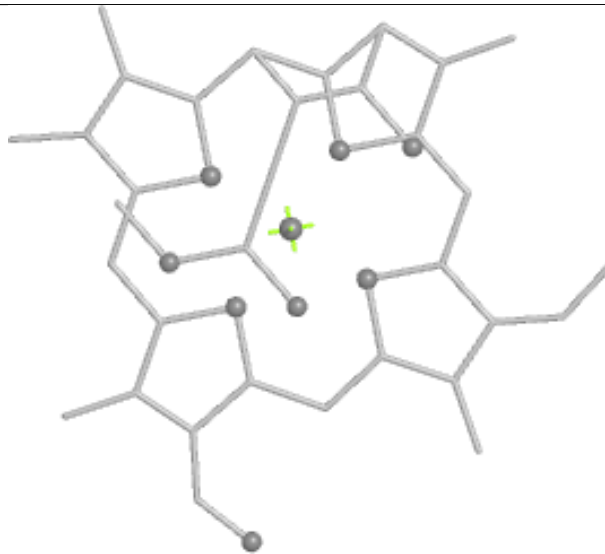
Bond lengths



Bond angles

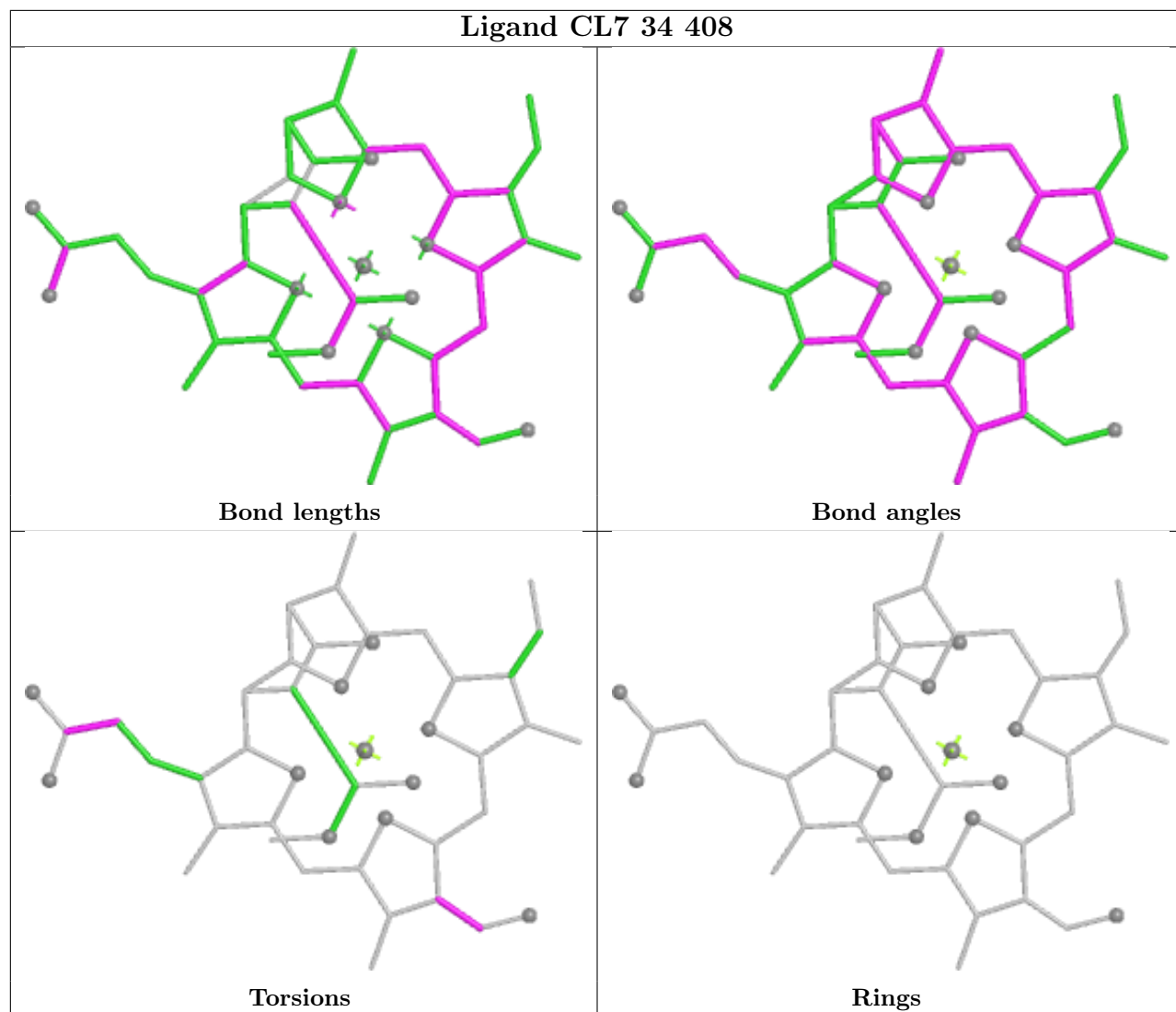


Torsions

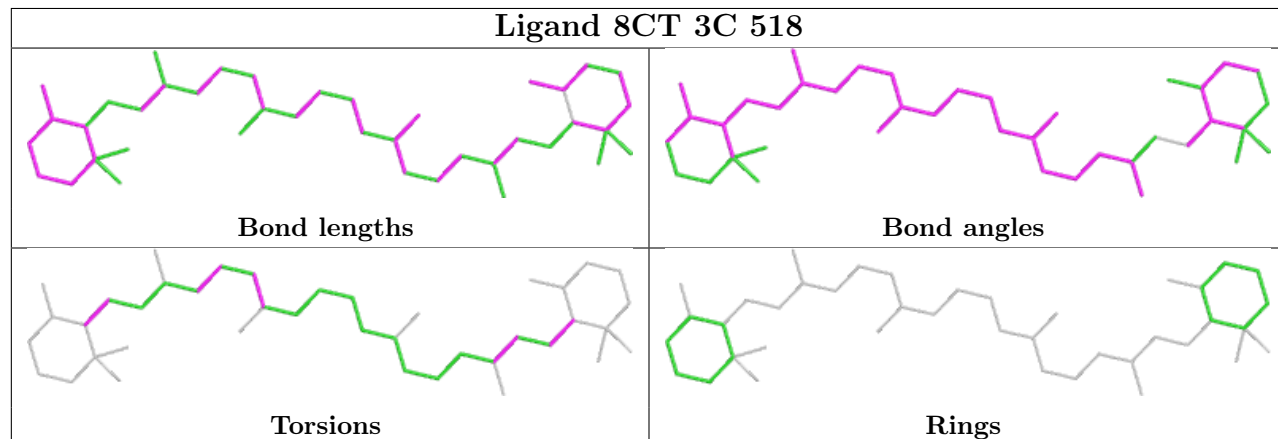


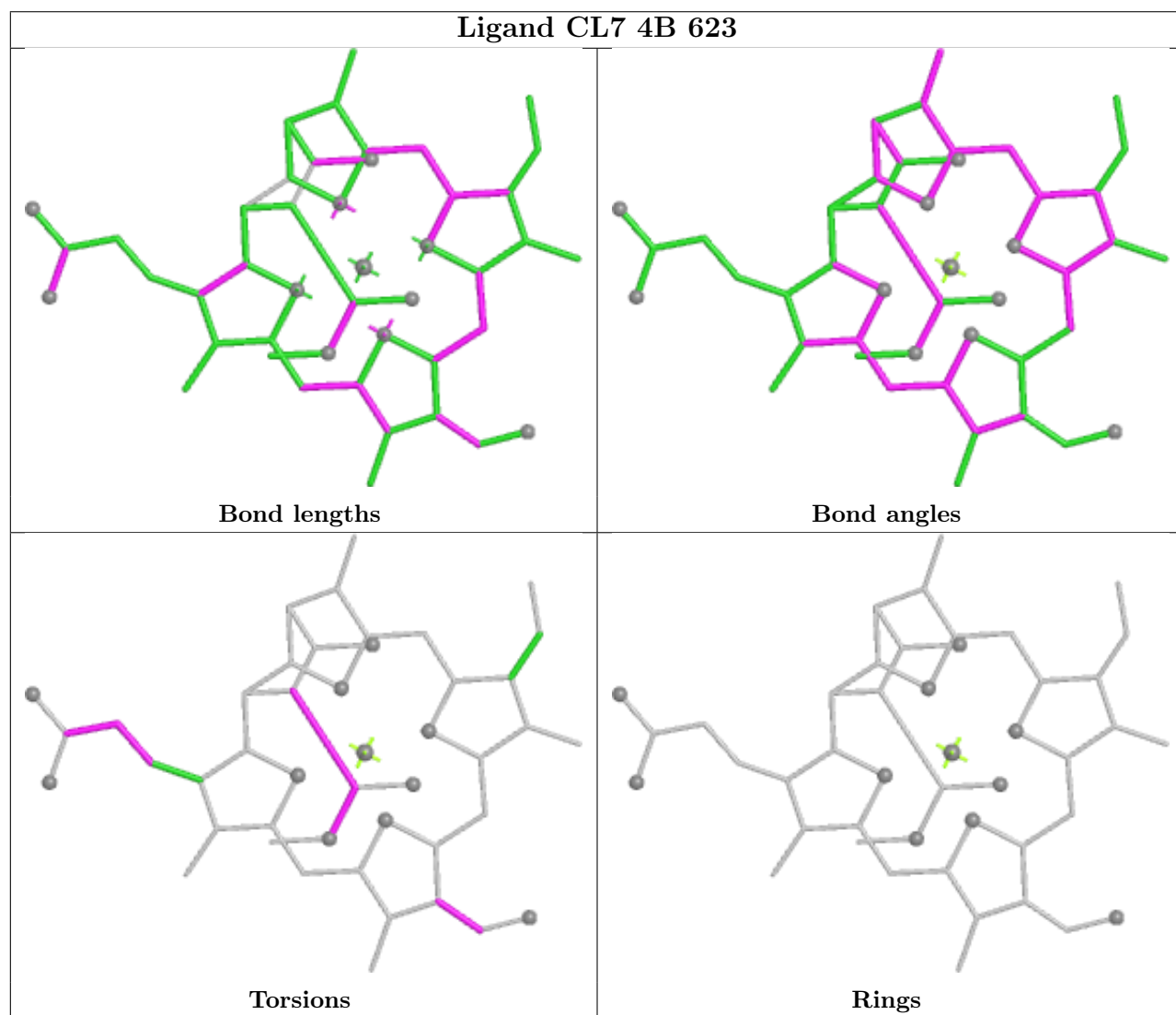
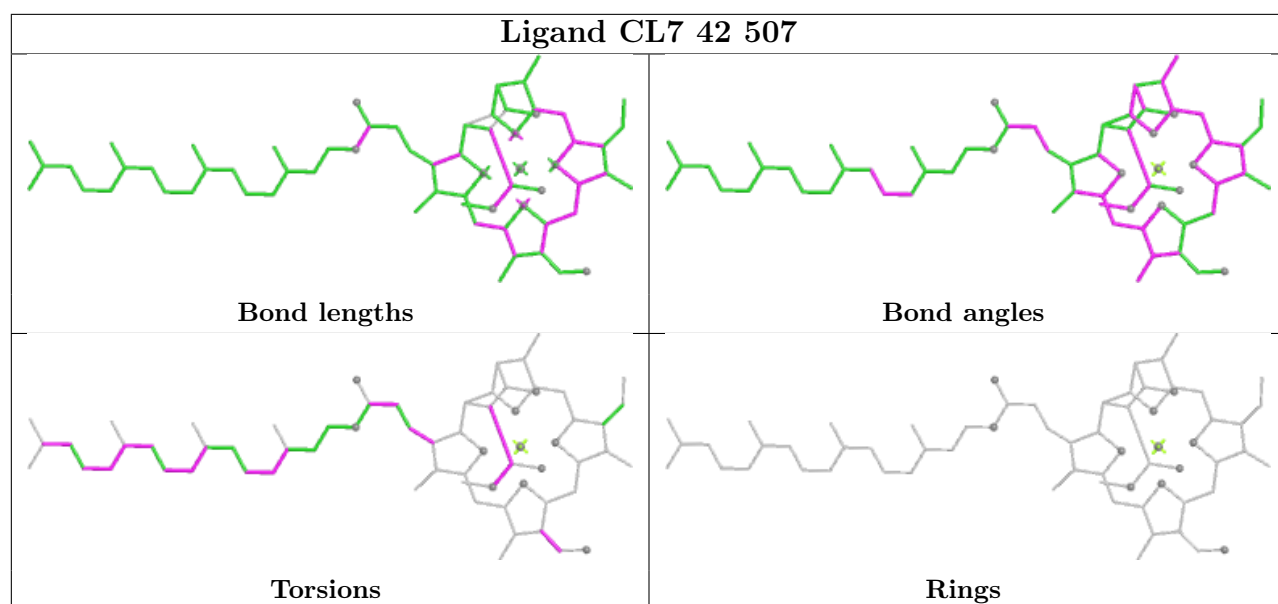
Rings

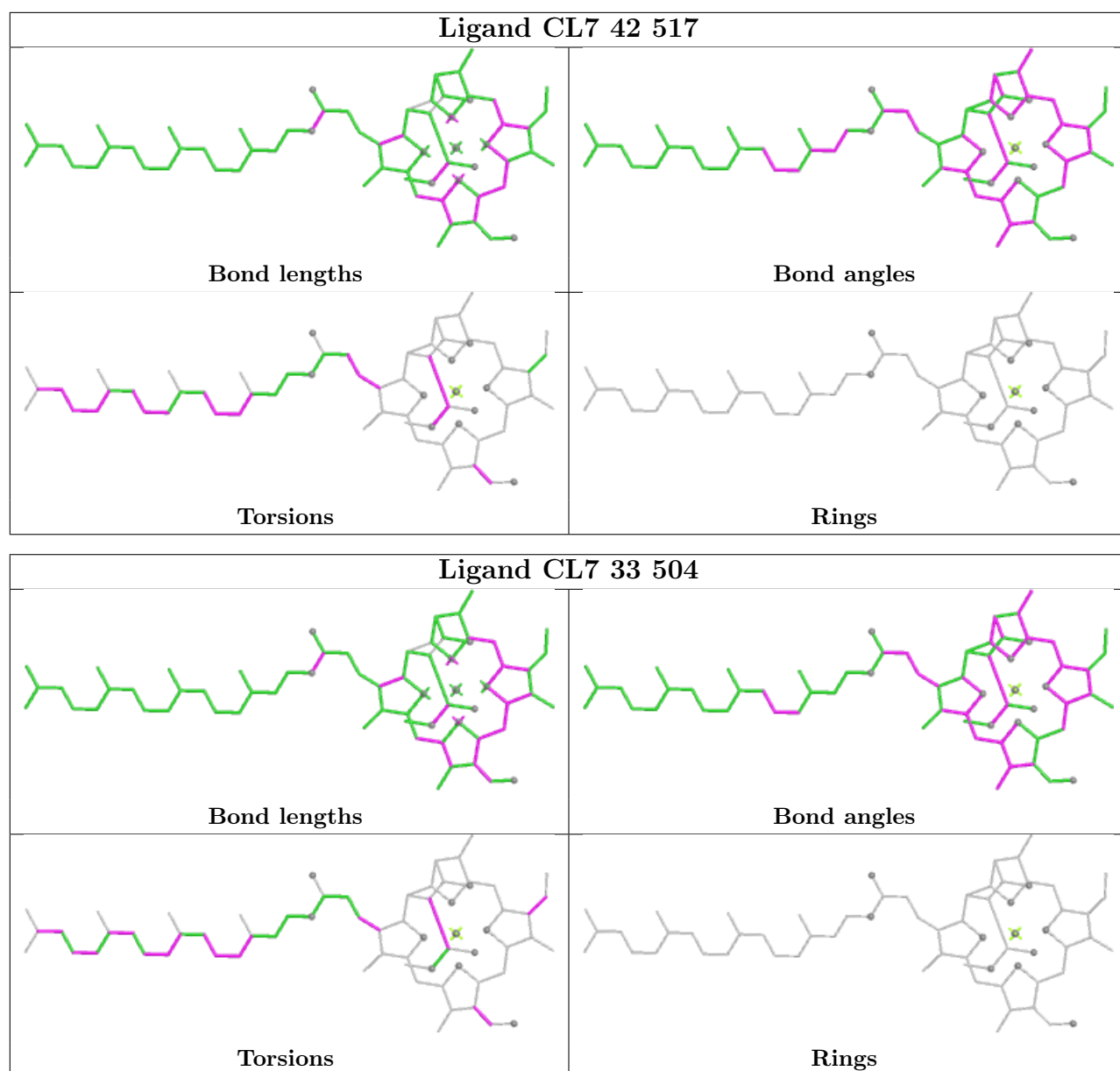
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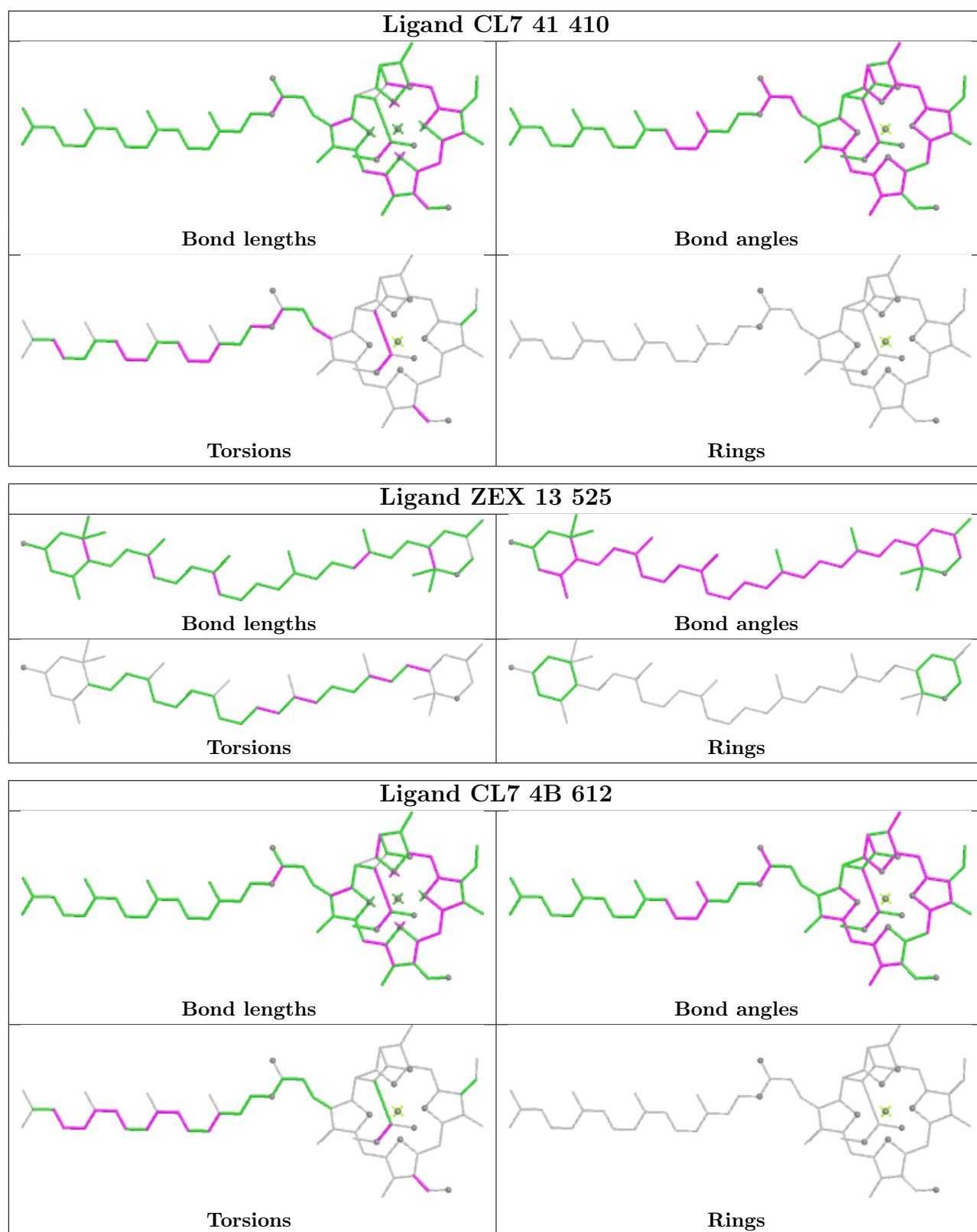


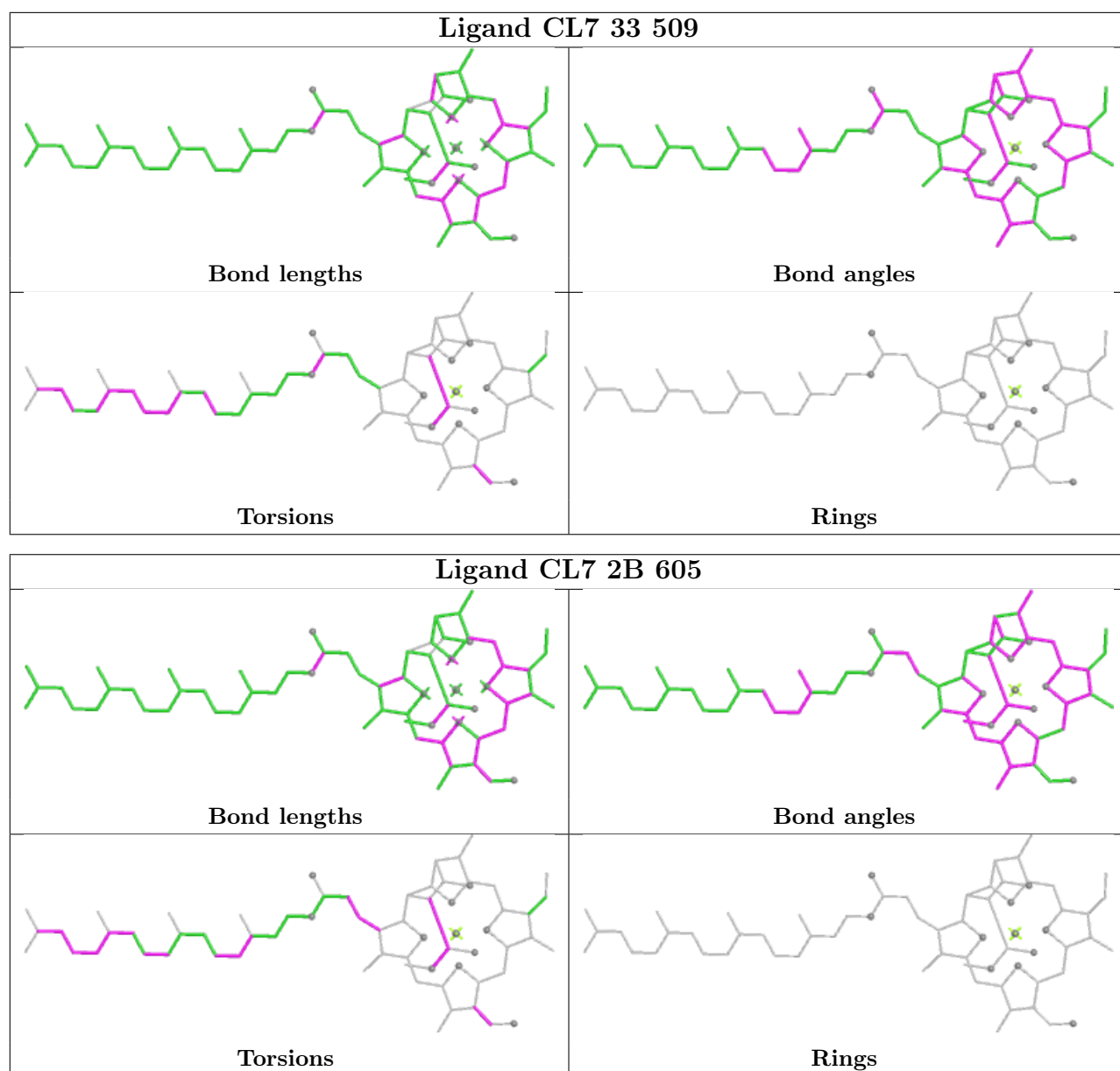
Ligand 8CT 3C 518

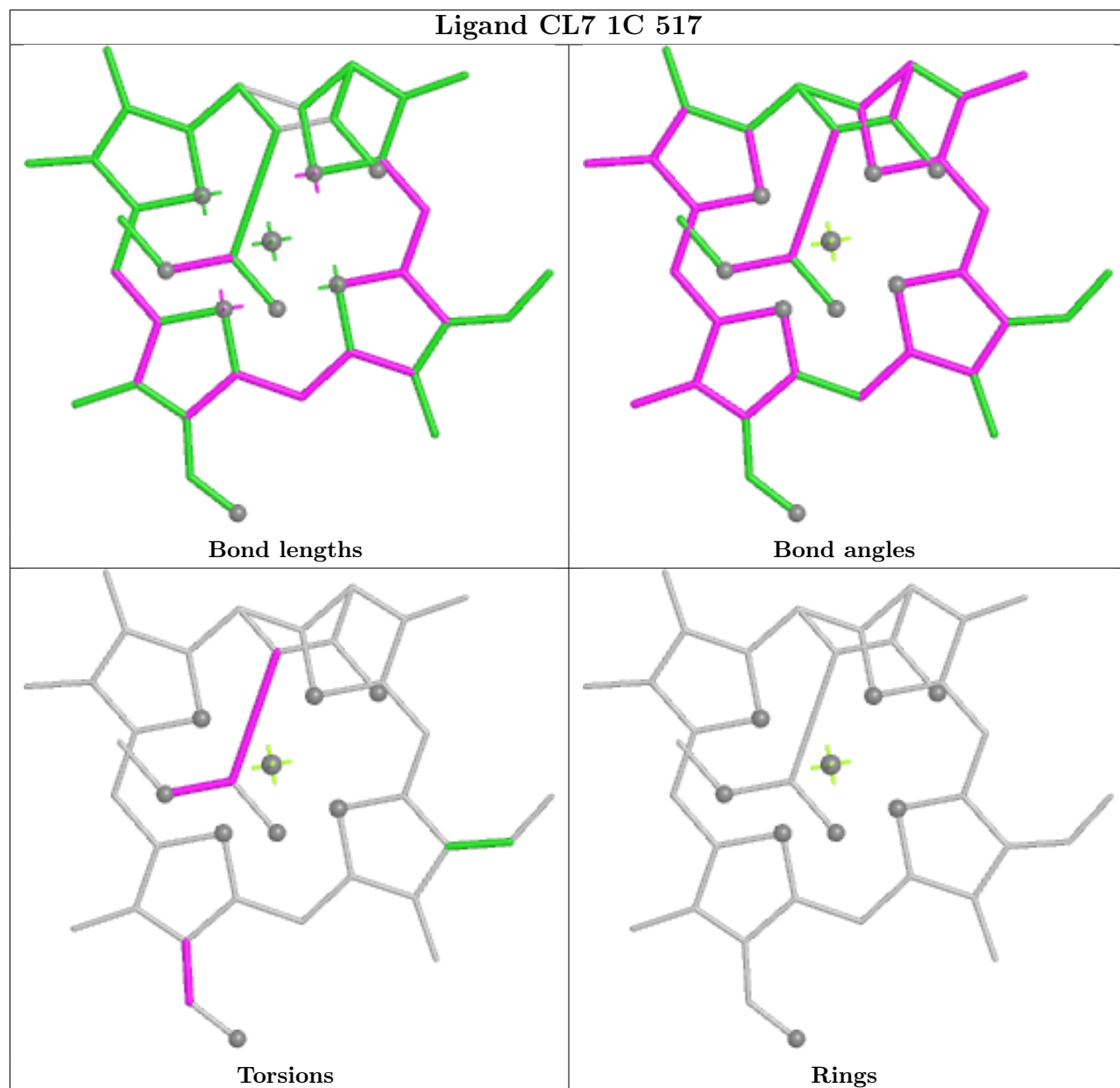




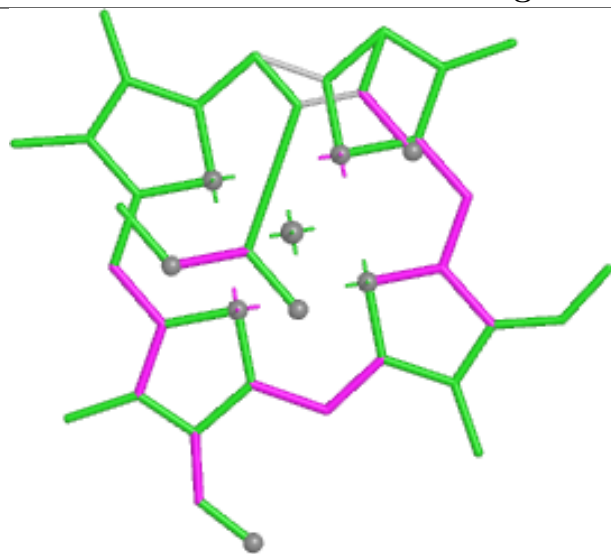




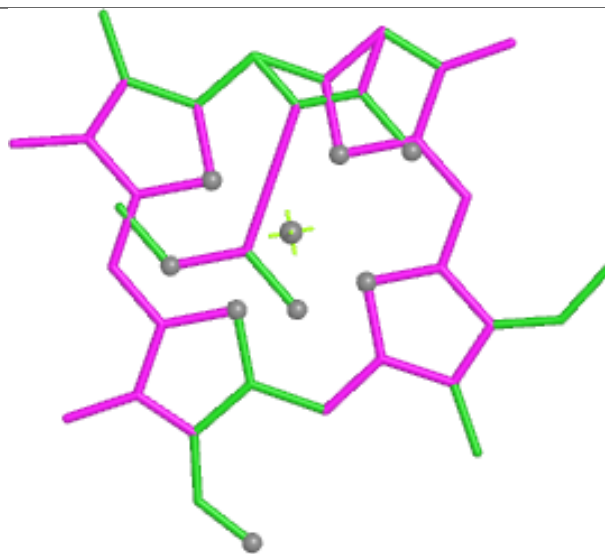




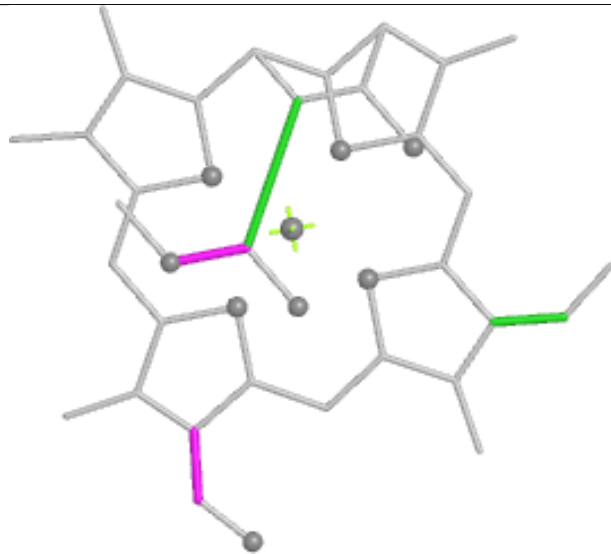
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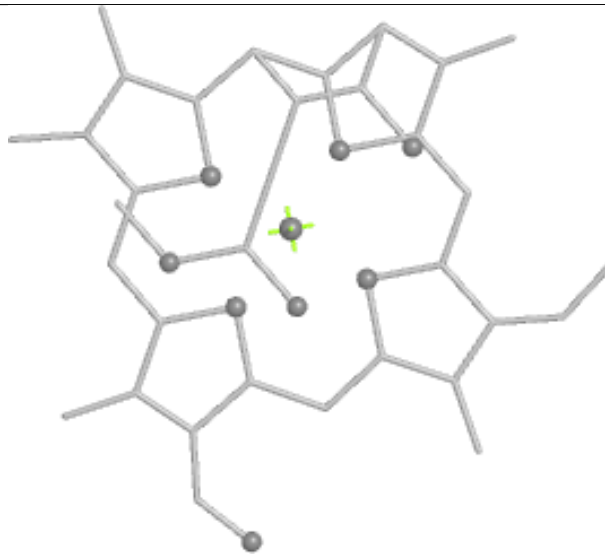
Bond lengths



Bond angles

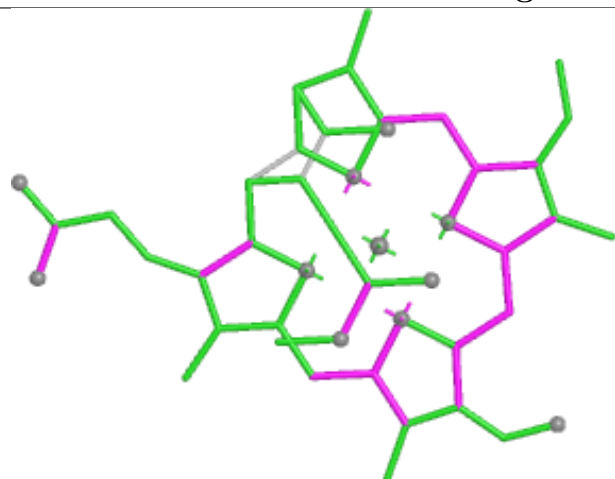


Torsions

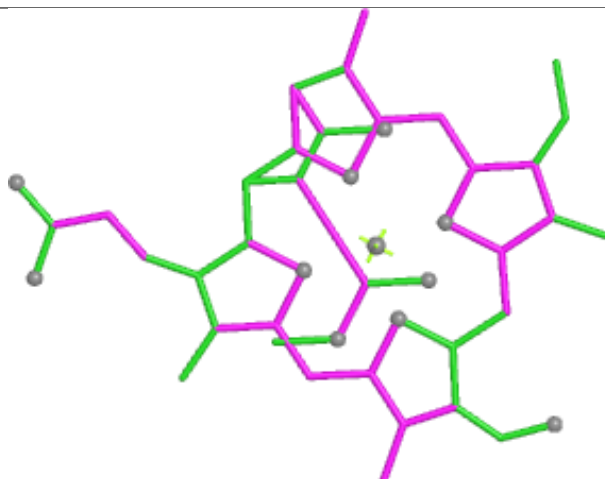


Rings

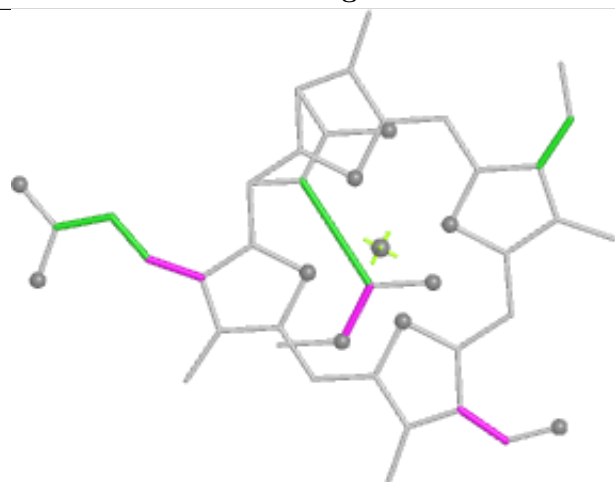
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Bond lengths



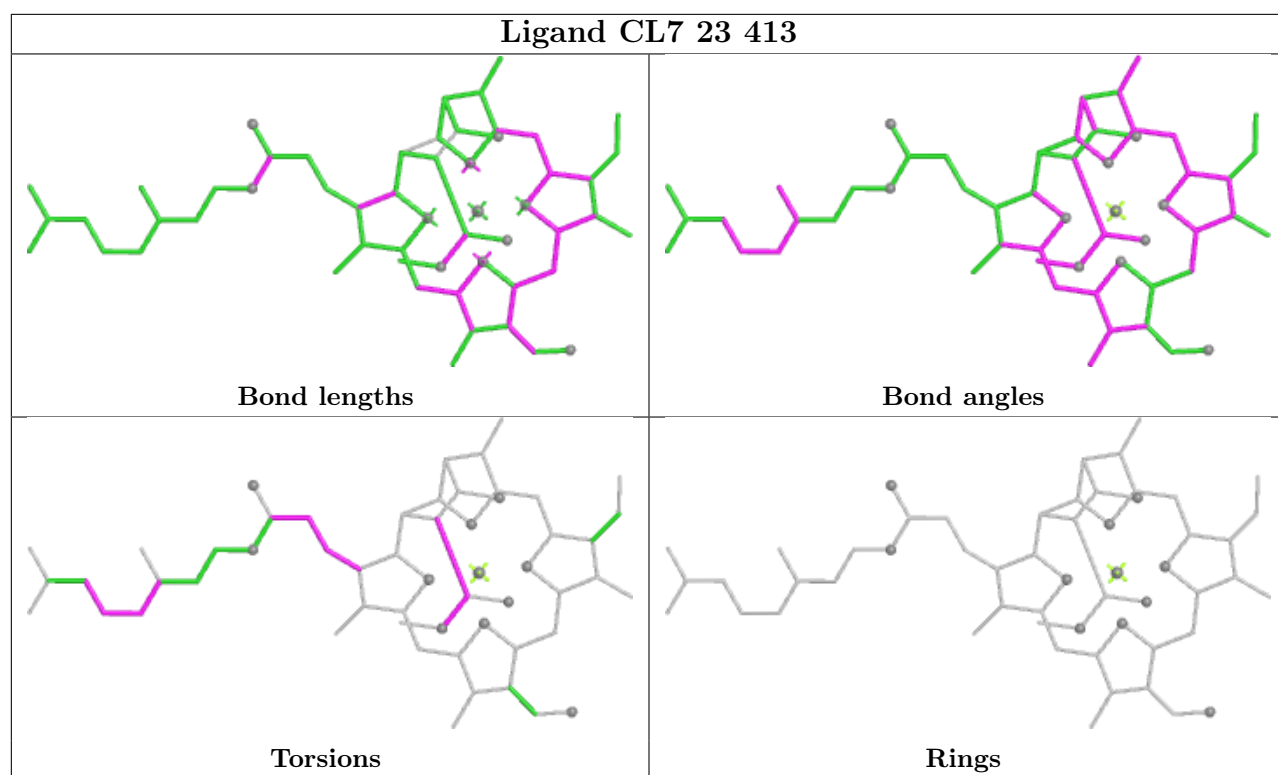
Bond angles

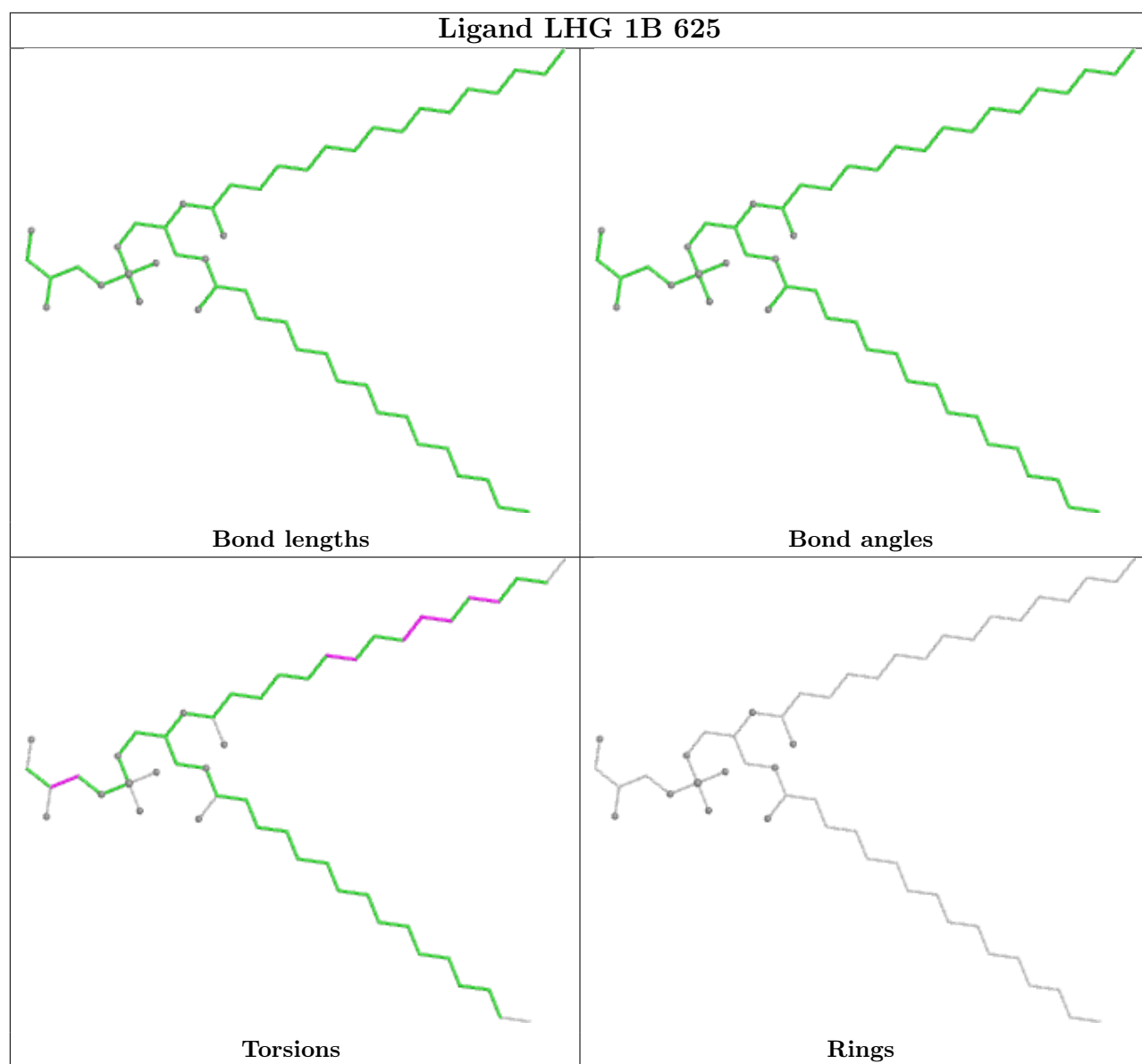


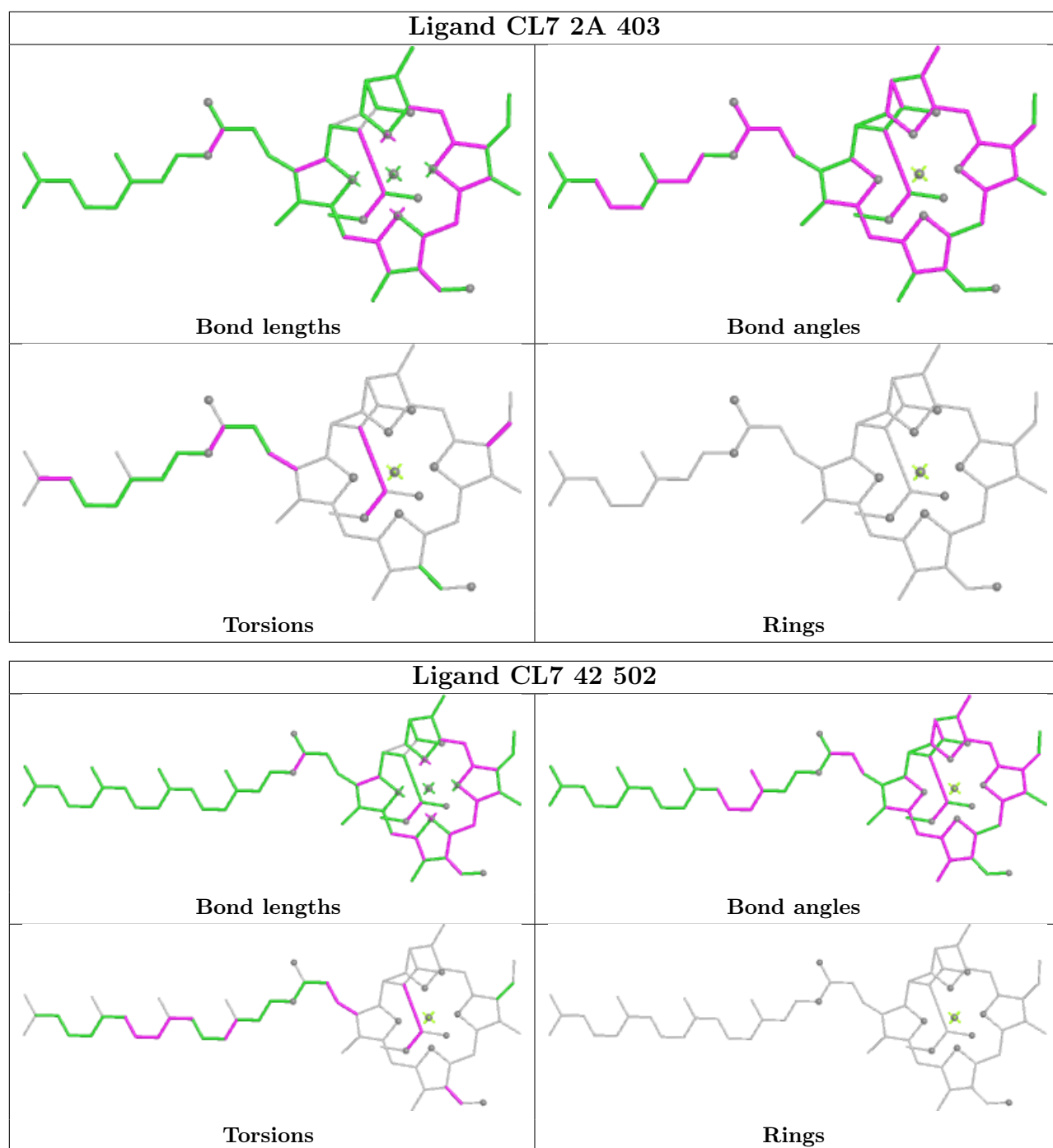
Torsions

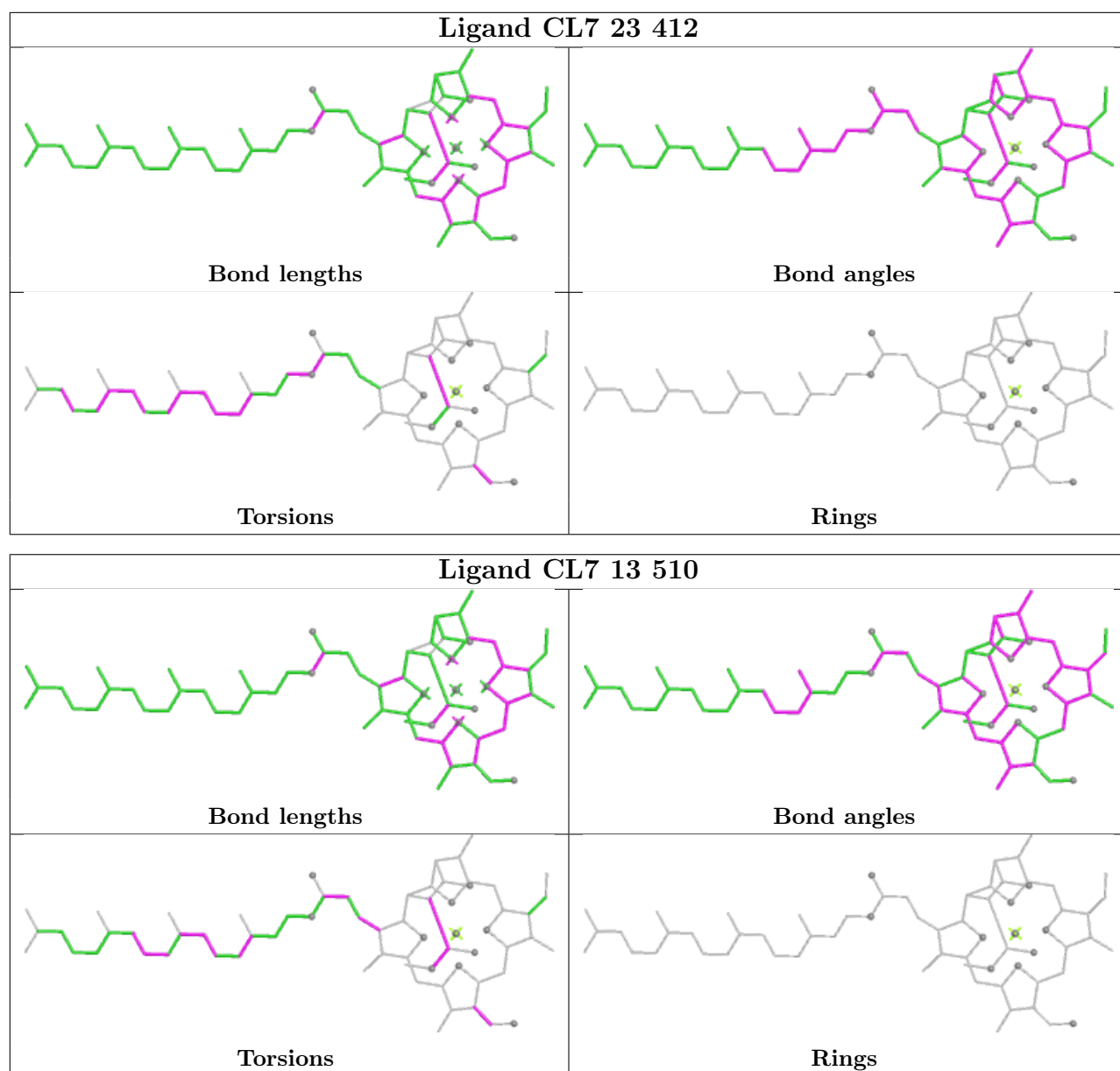


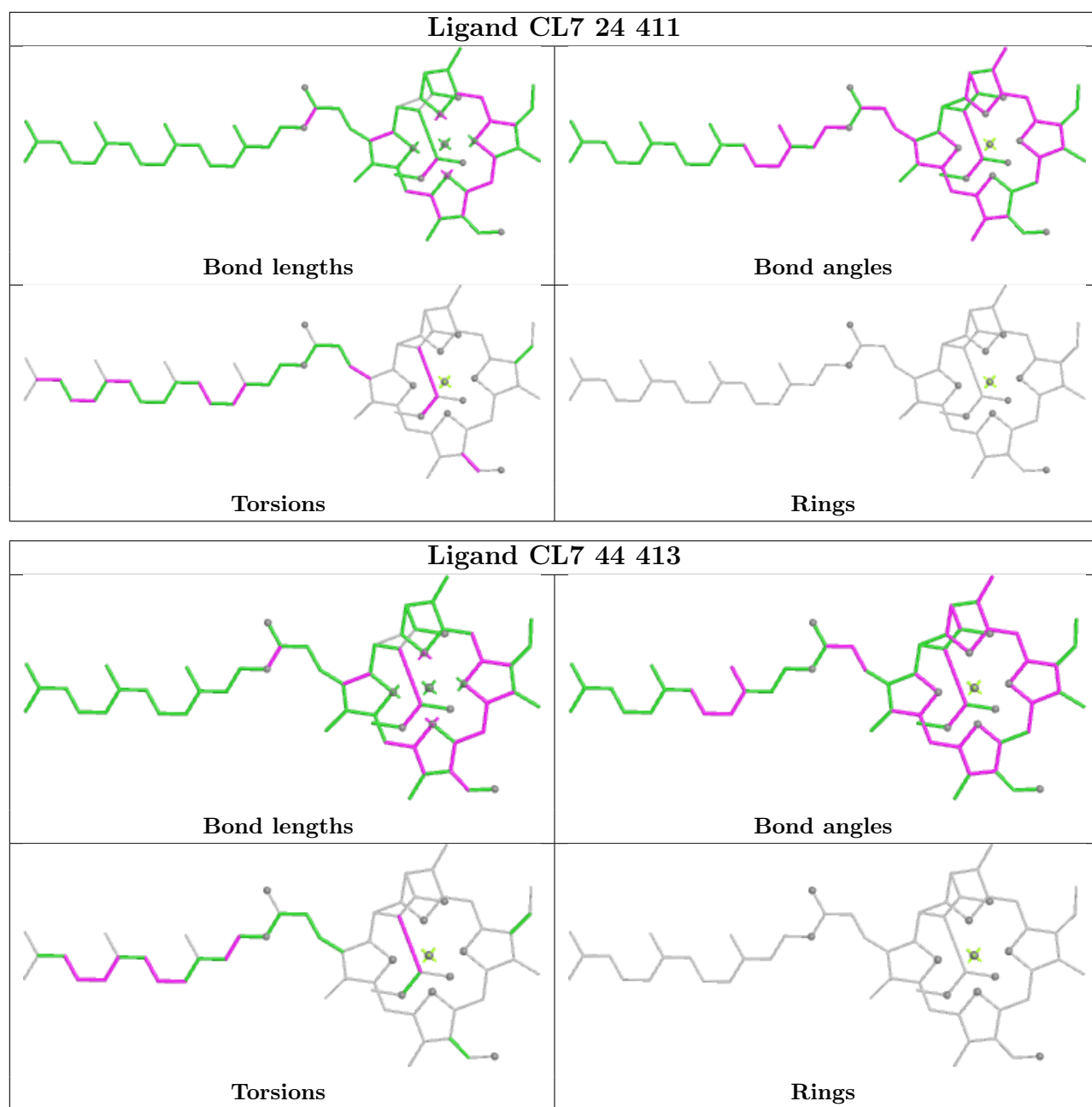
Rings



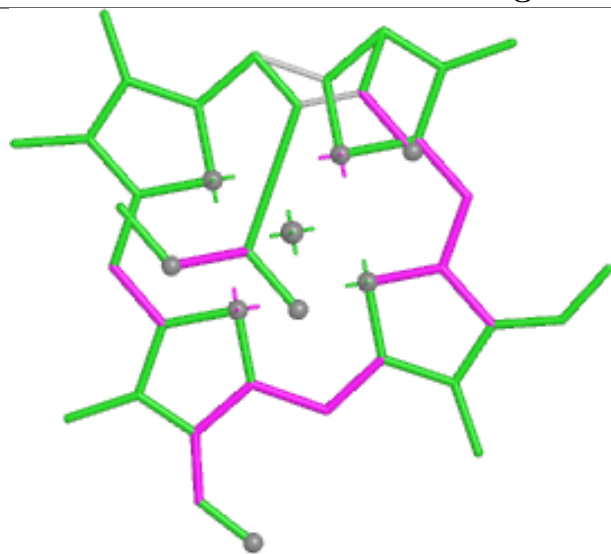




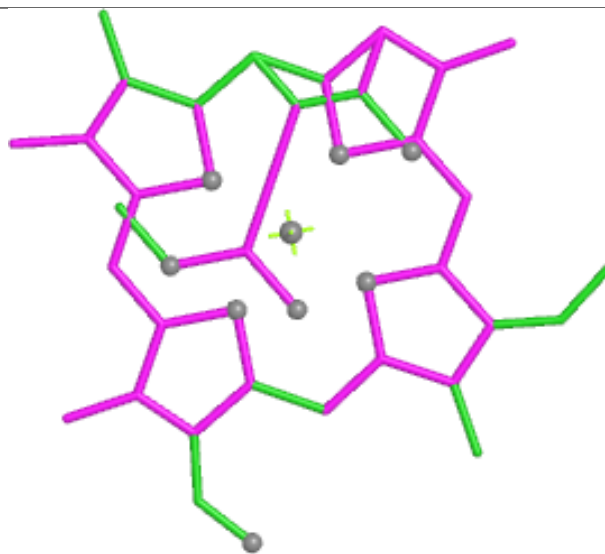




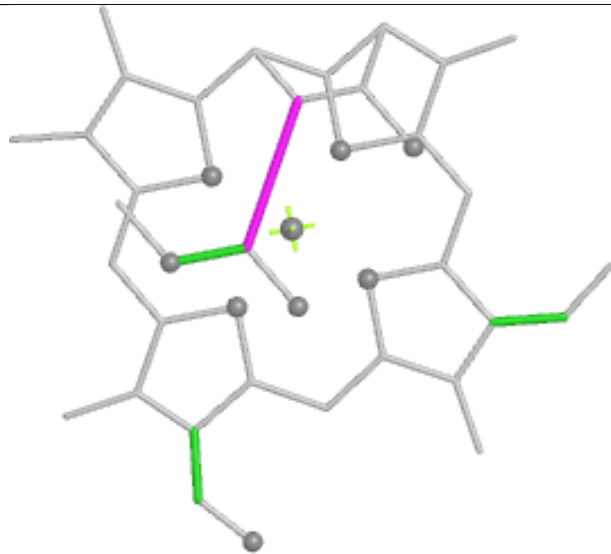
Ligand CL7 11 413



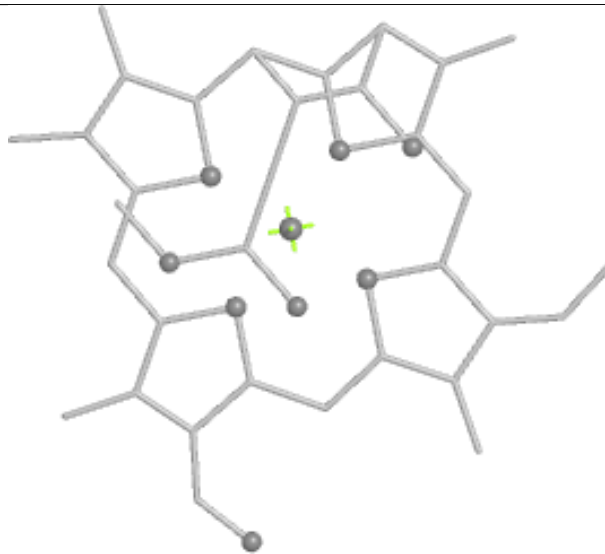
Bond lengths



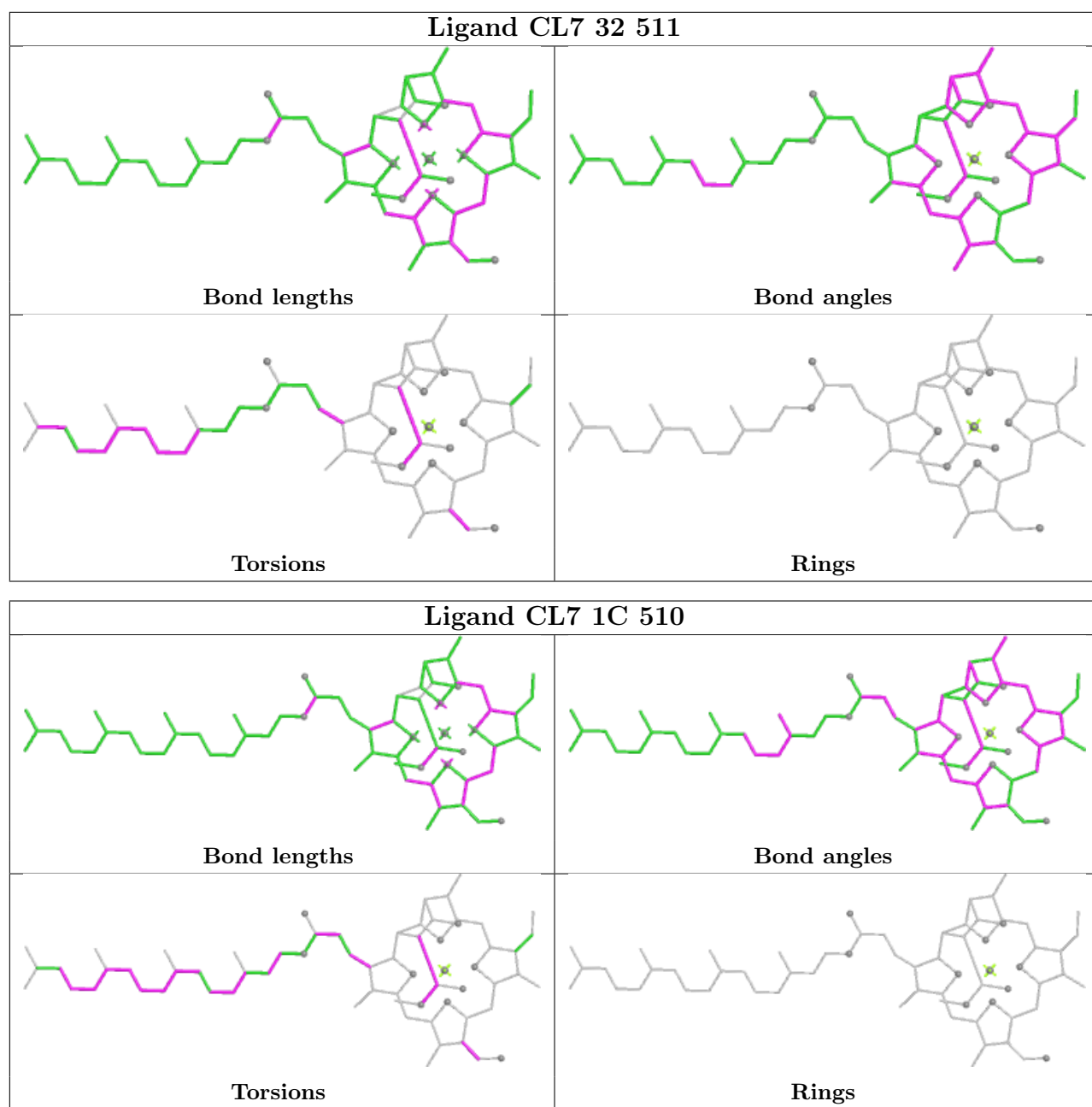
Bond angles

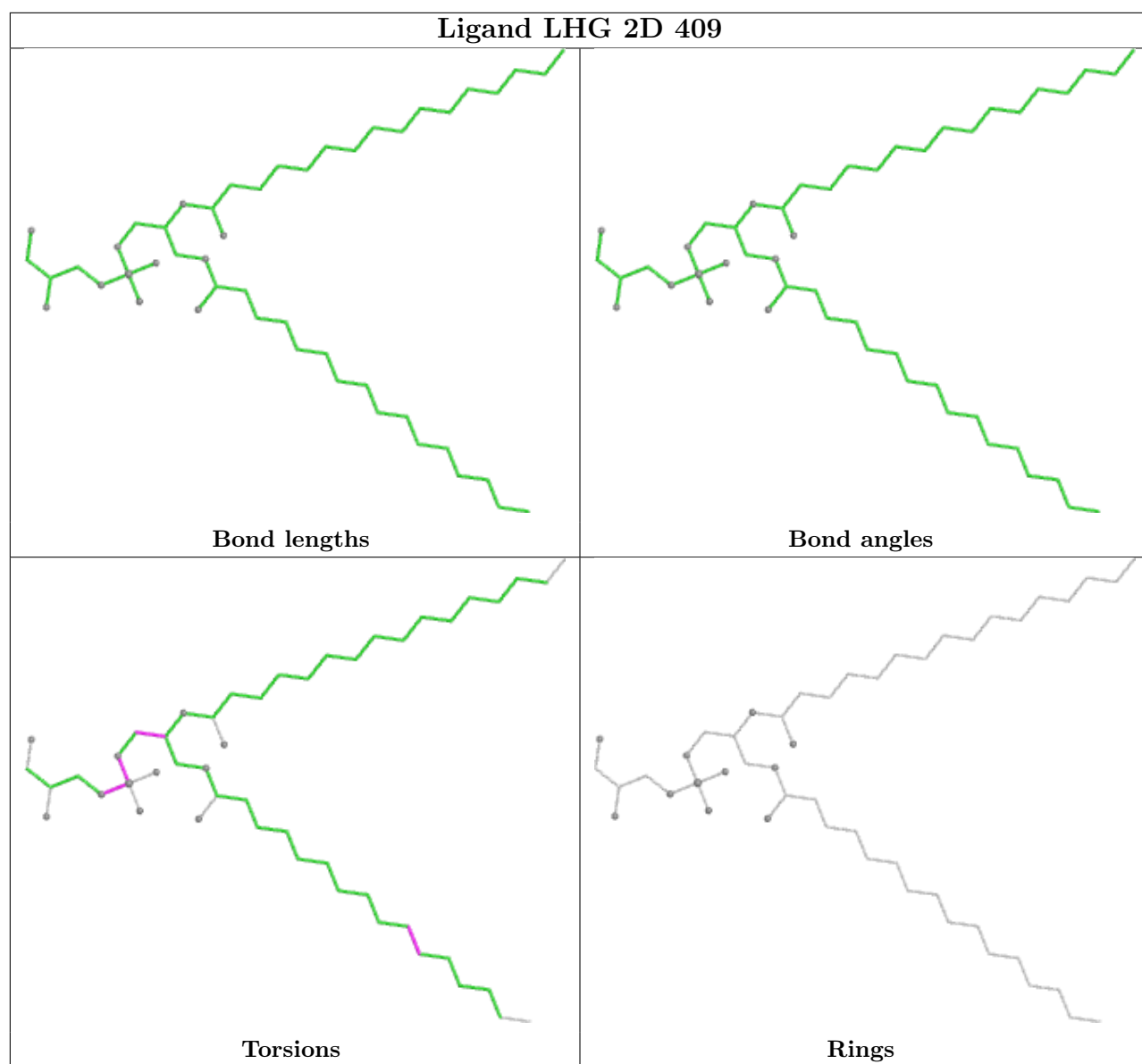


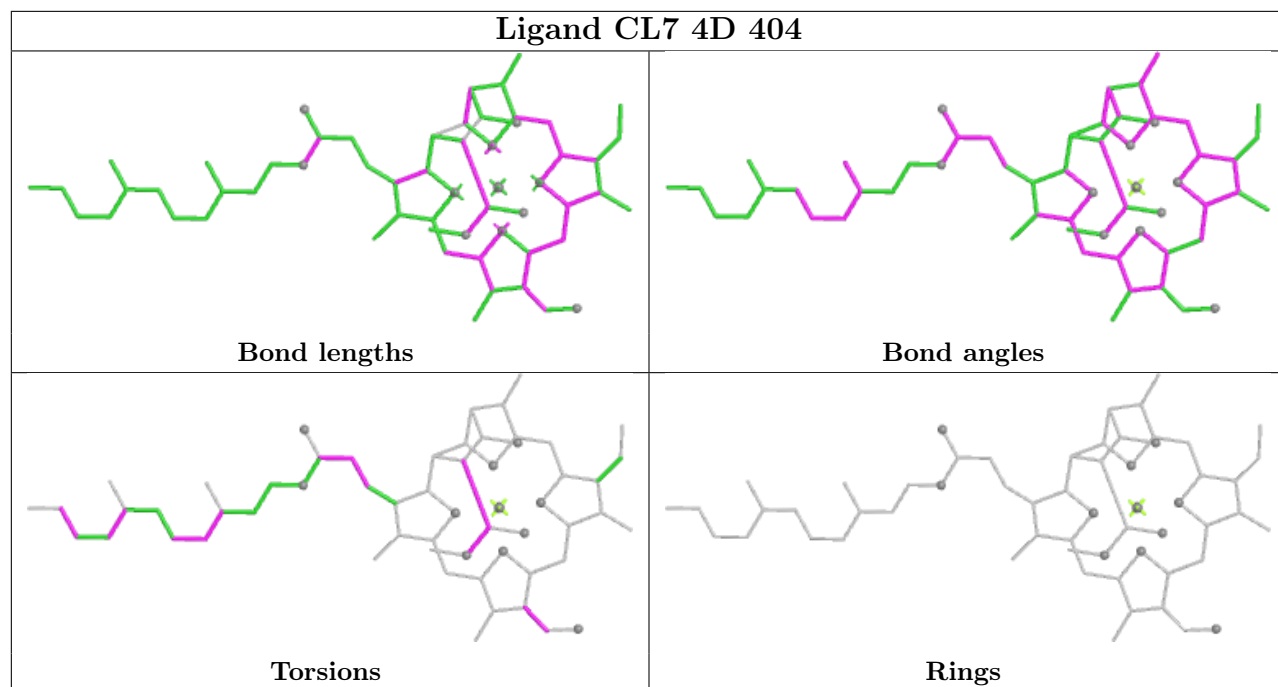
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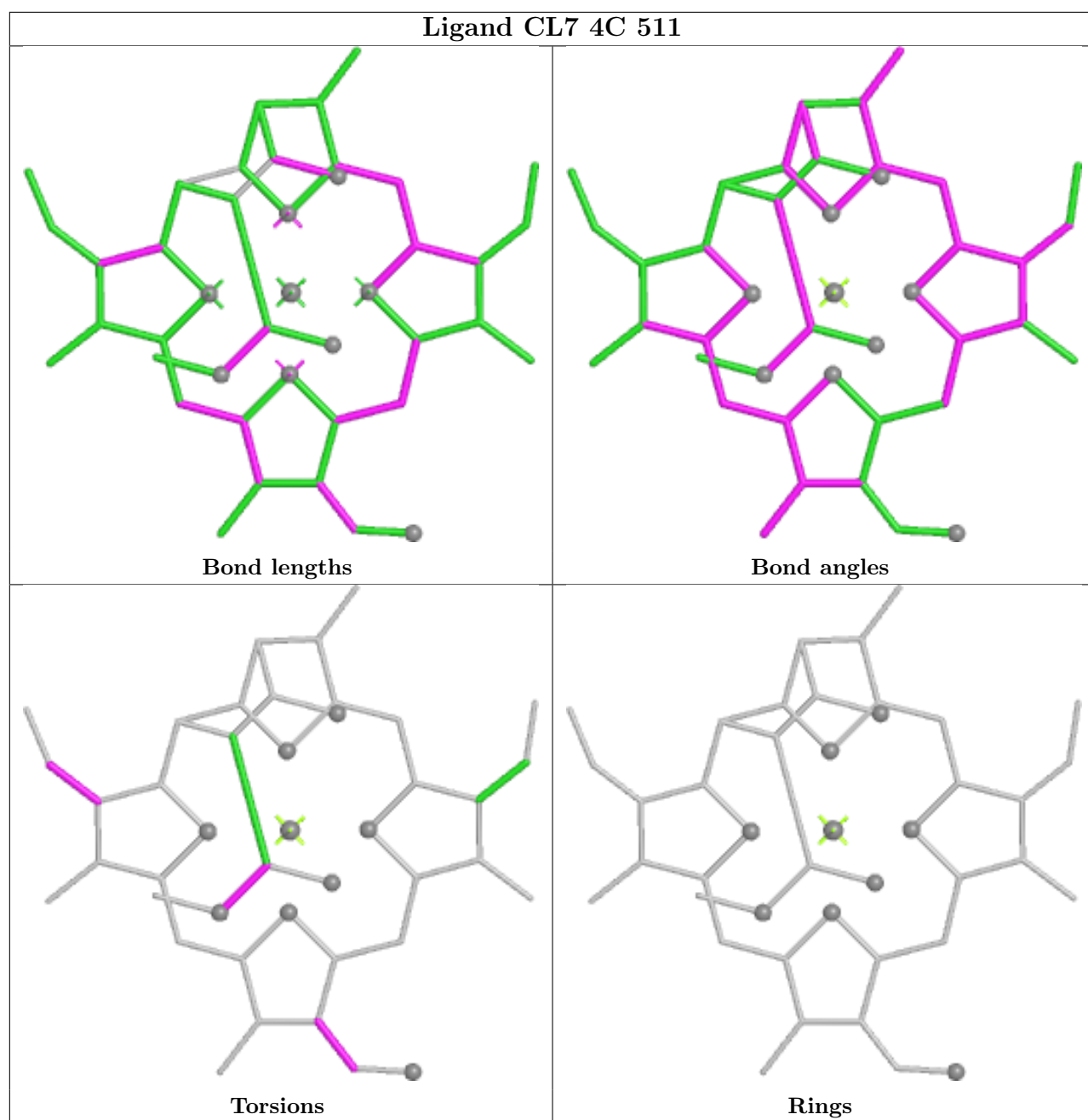


Rings

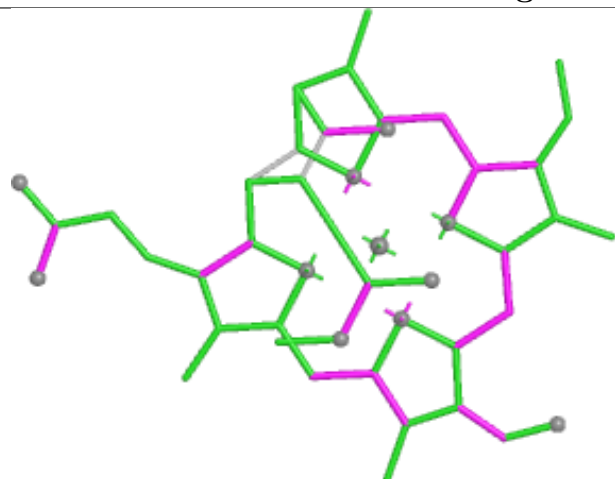




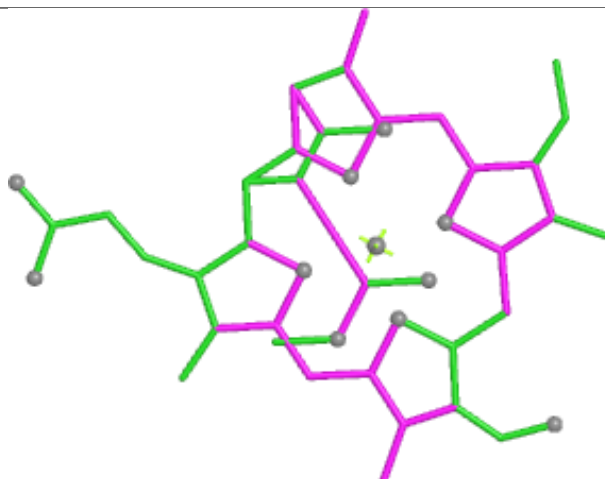




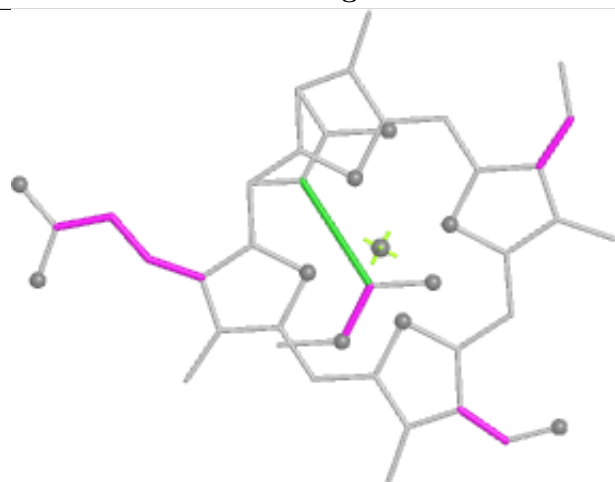
Ligand CL7 21 419



Bond lengths



Bond angles

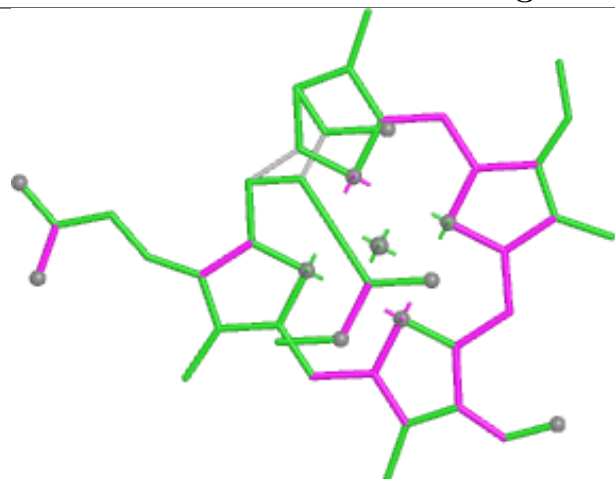


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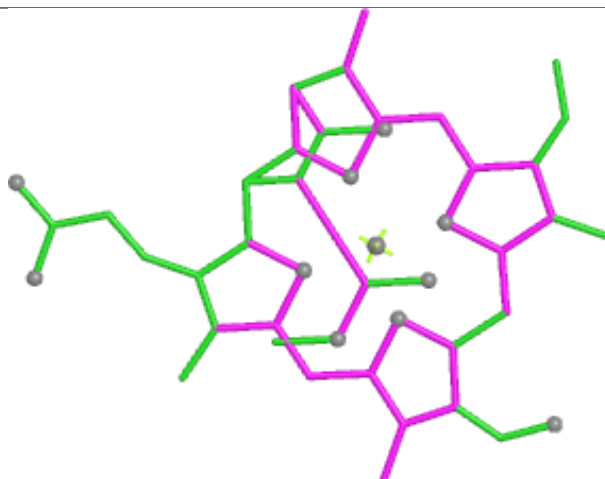


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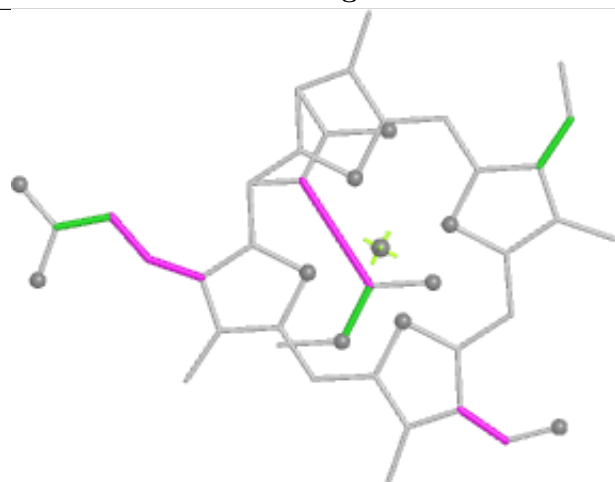
Ligand CL7 42 508



Bond lengths



Bond angles



Torsions

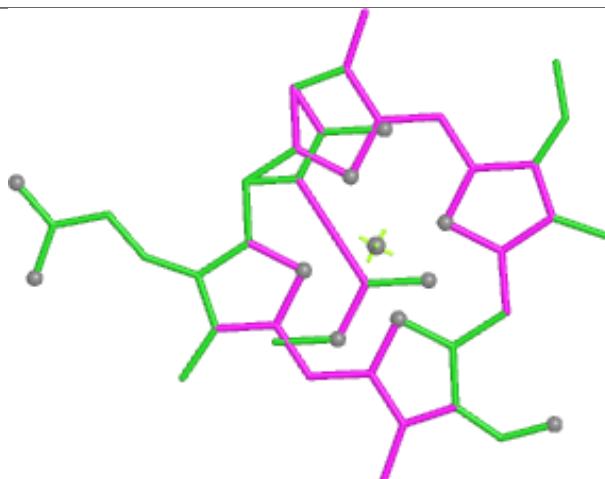


Rings

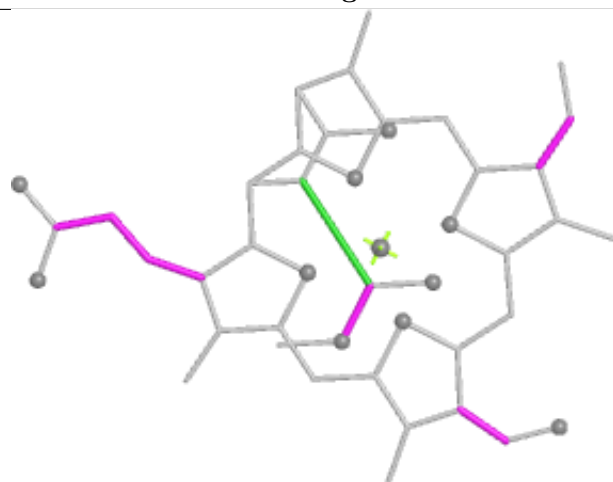
Ligand CL7 31 419



Bond lengths



Bond angles

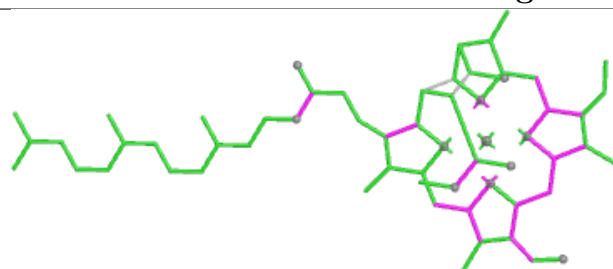


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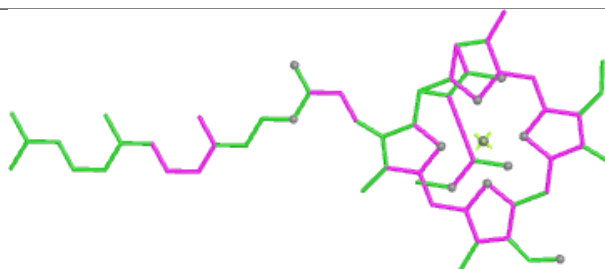


Rings

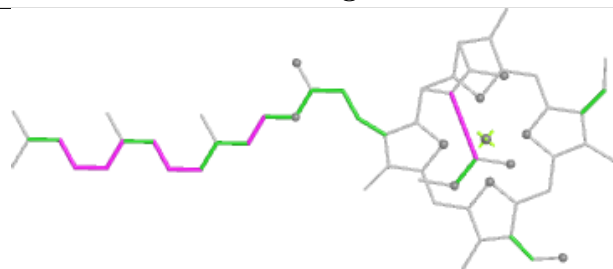
Ligand CL7 24 413



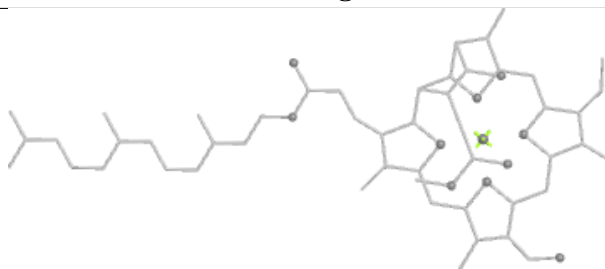
Bond lengths



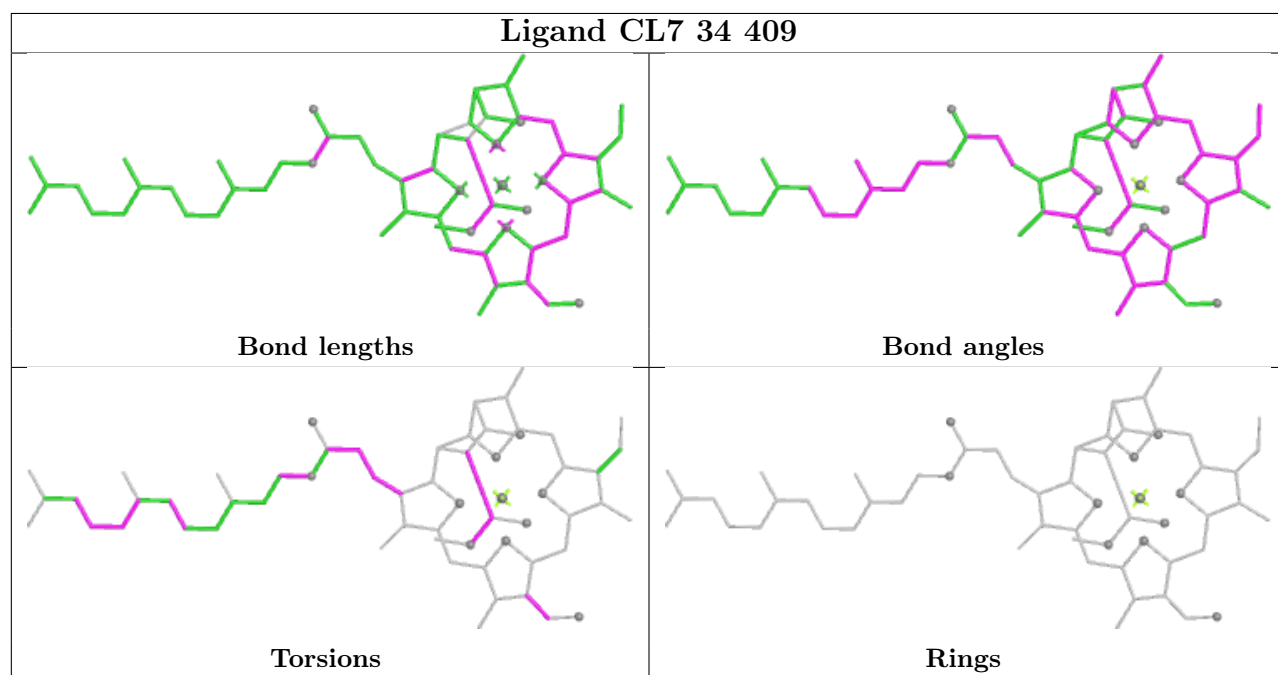
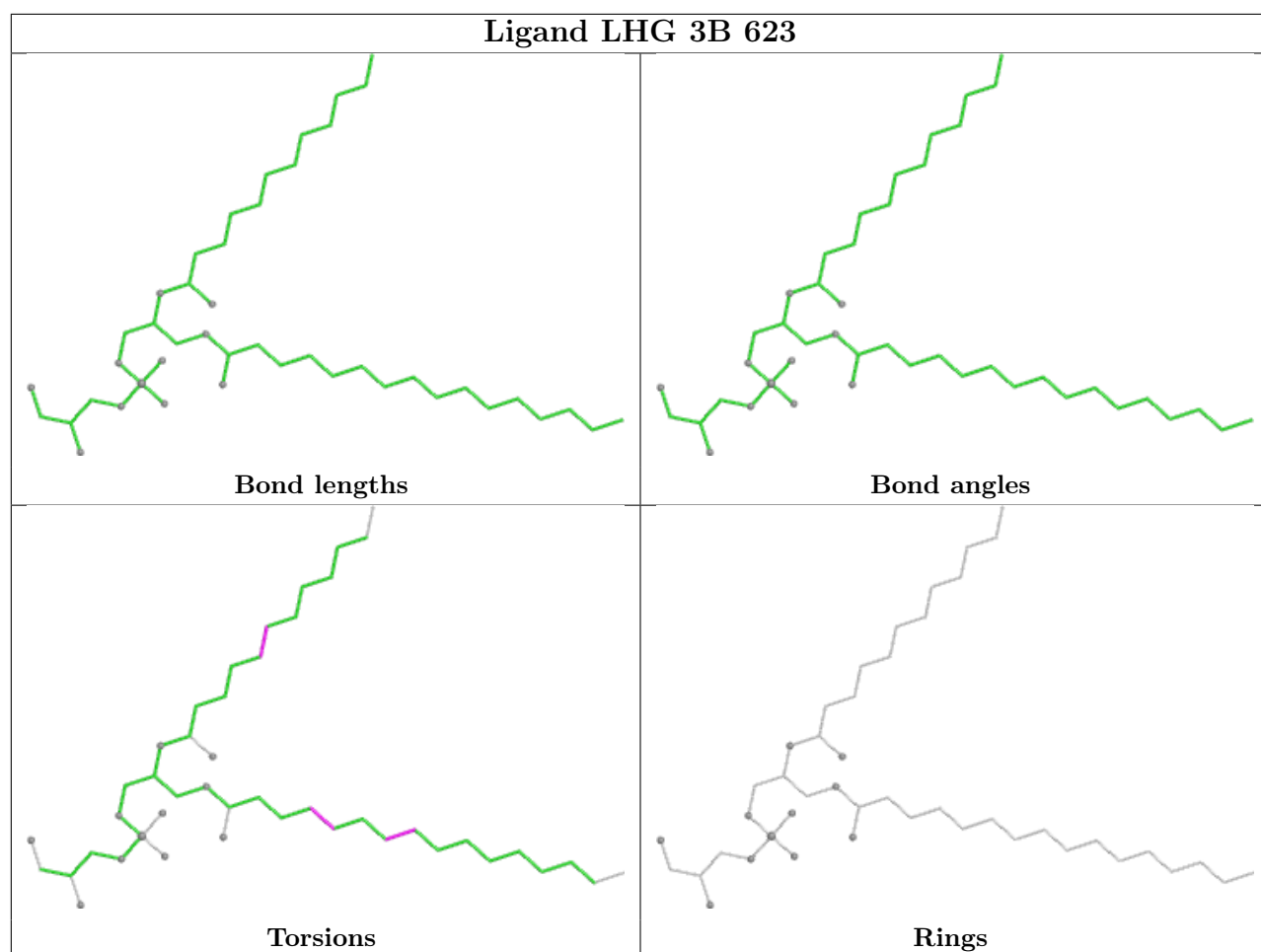
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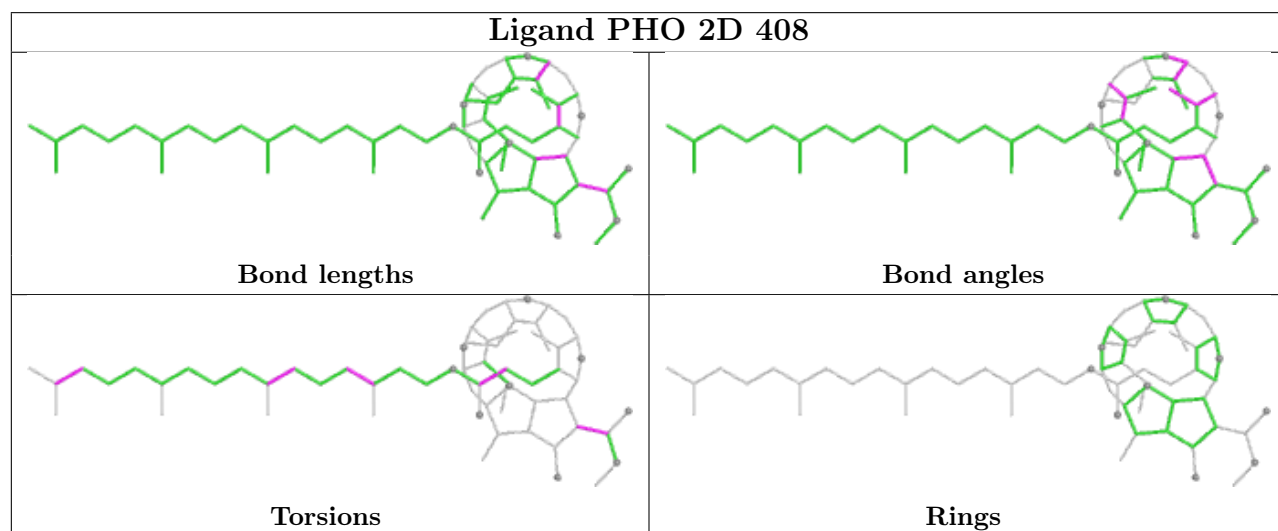
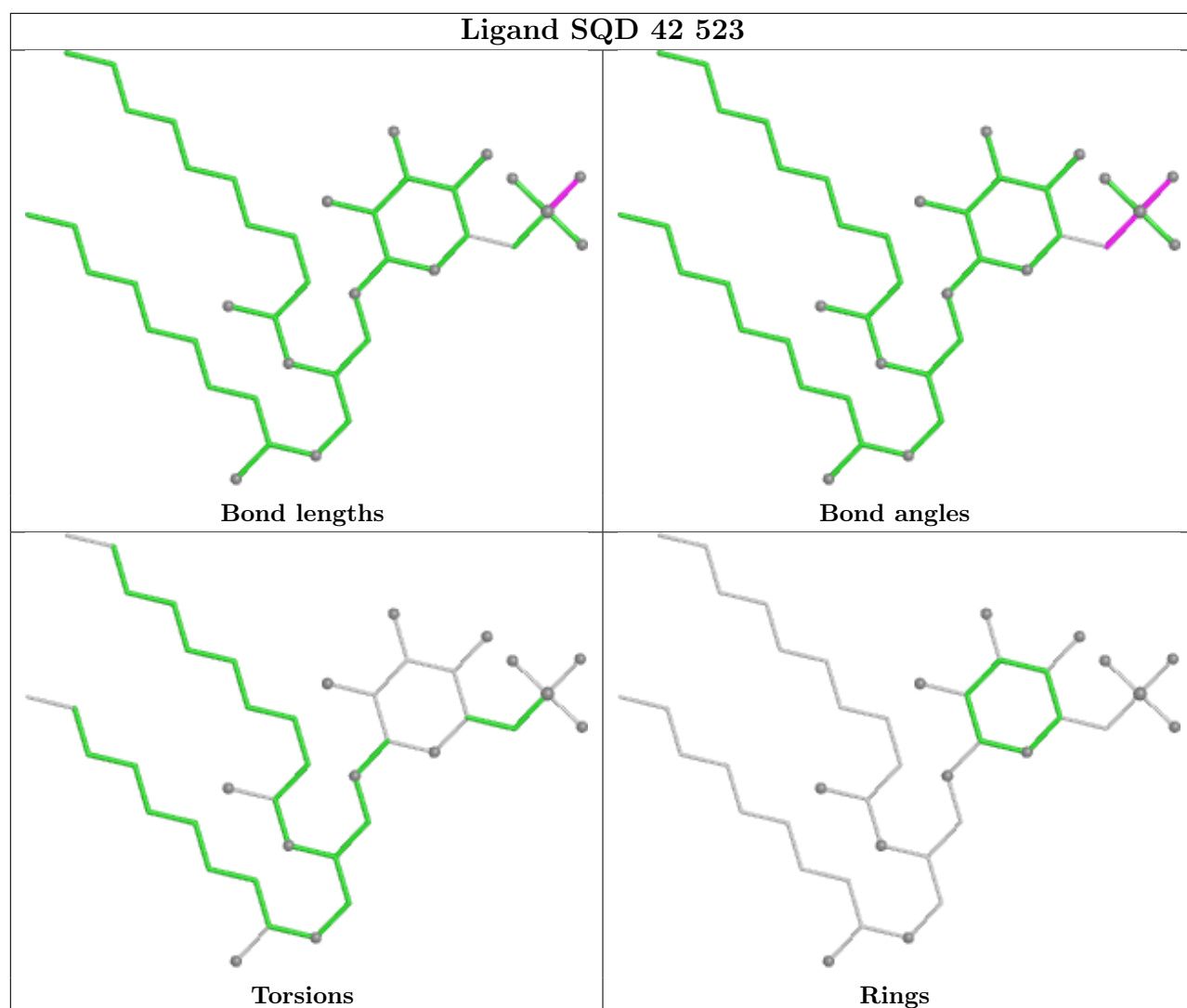


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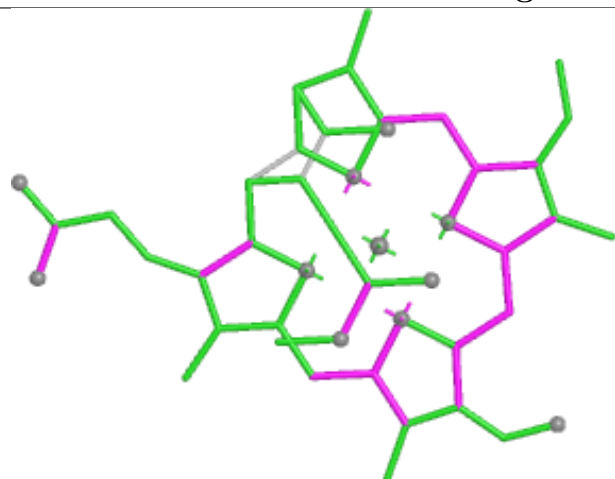


Rings

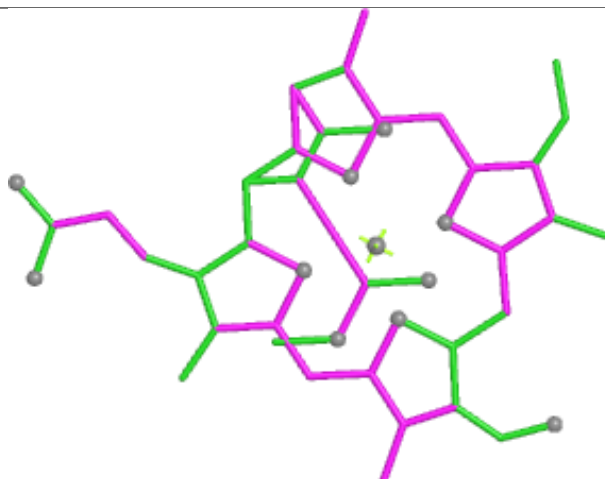




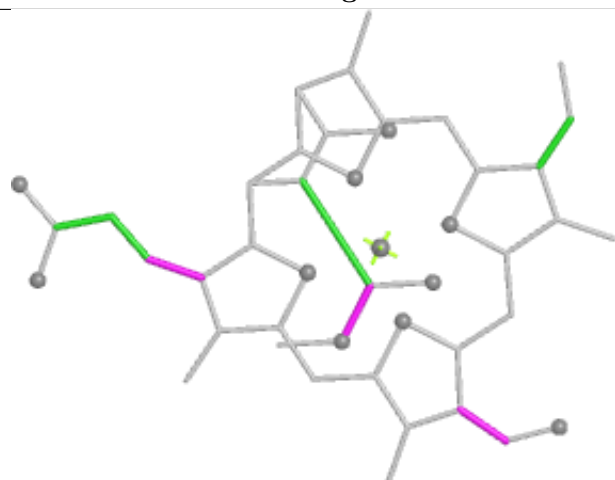
Ligand CL7 42 504



Bond lengths



Bond angles

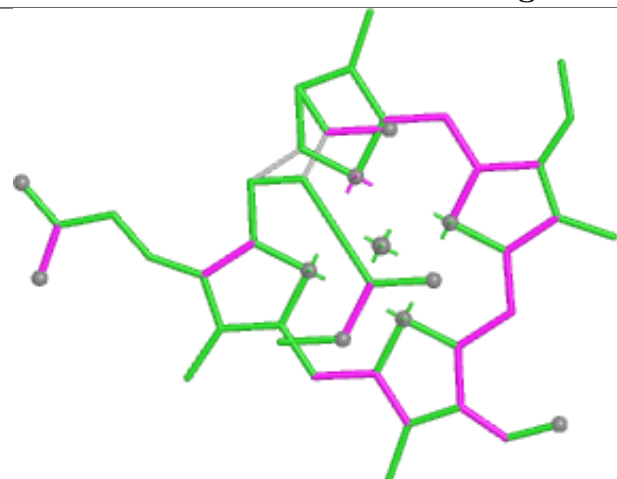


Torsions

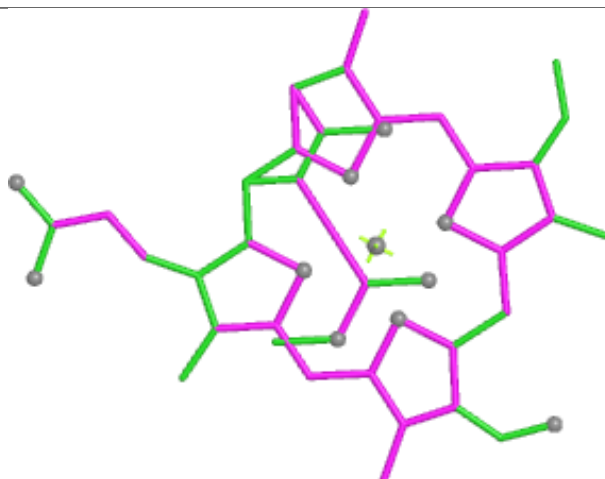


Rings

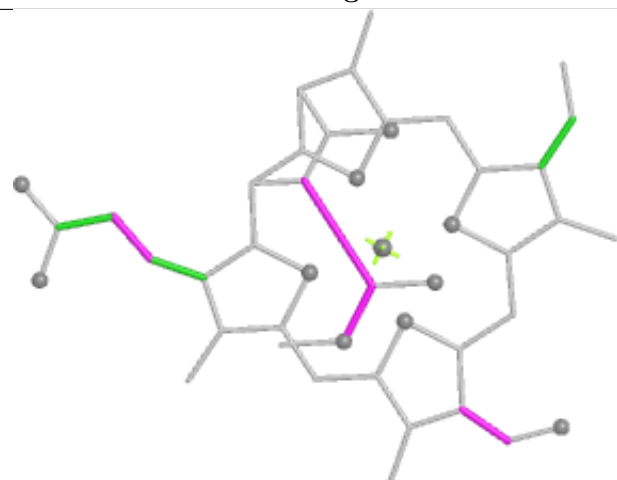
Ligand CL7 11 409



Bond lengths



Bond angles

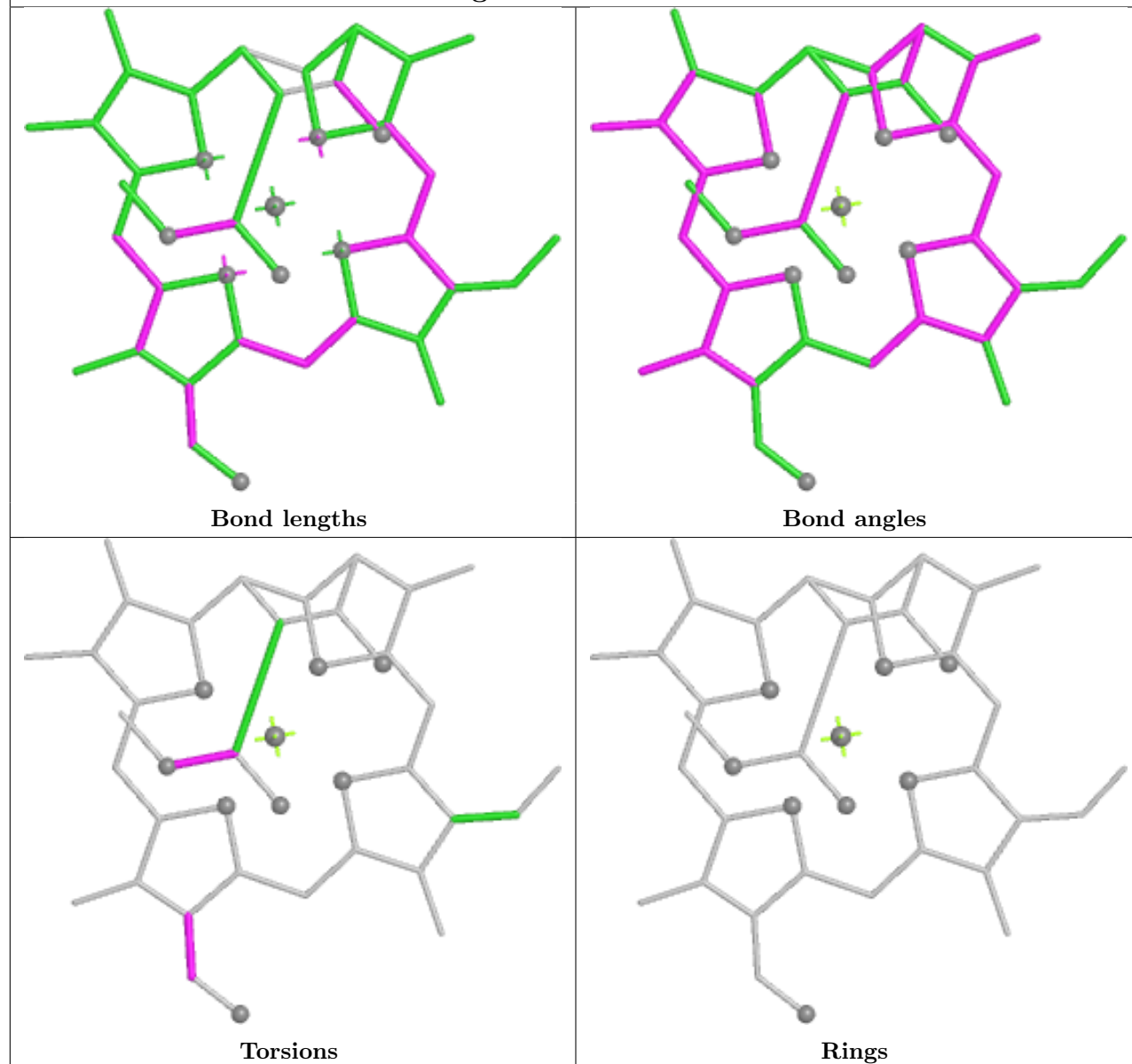


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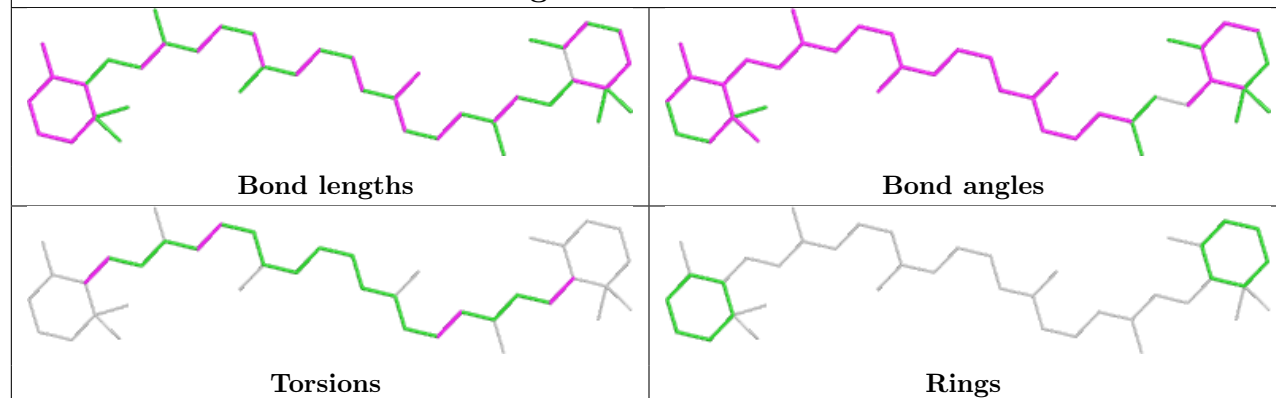


Rings

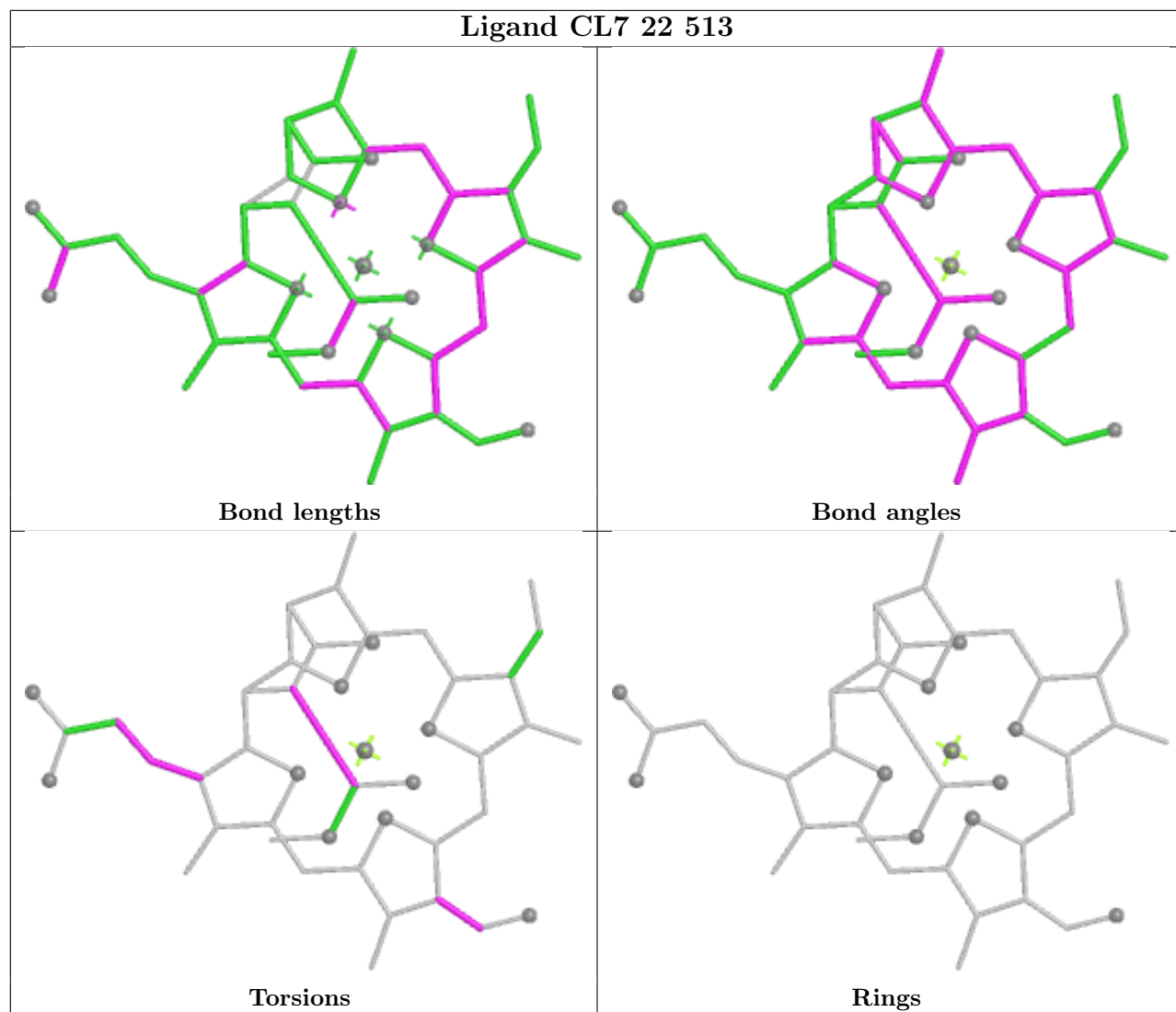
Ligand CL7 21 416



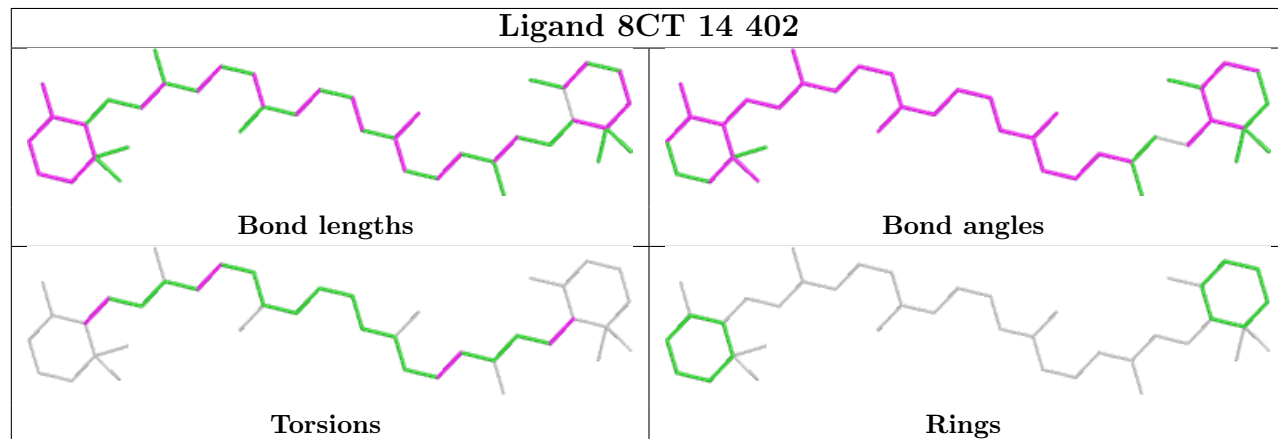
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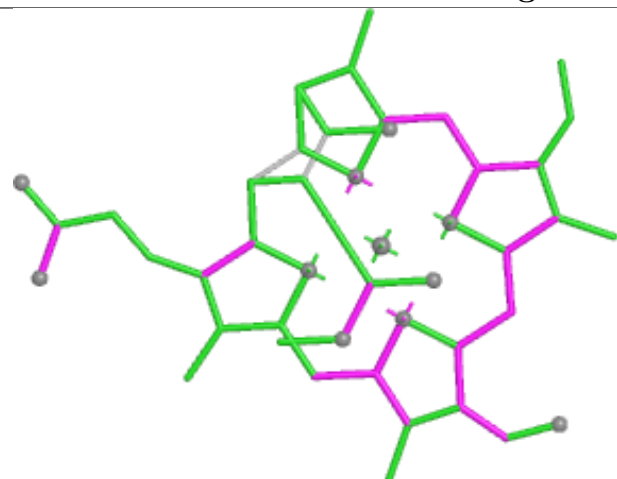
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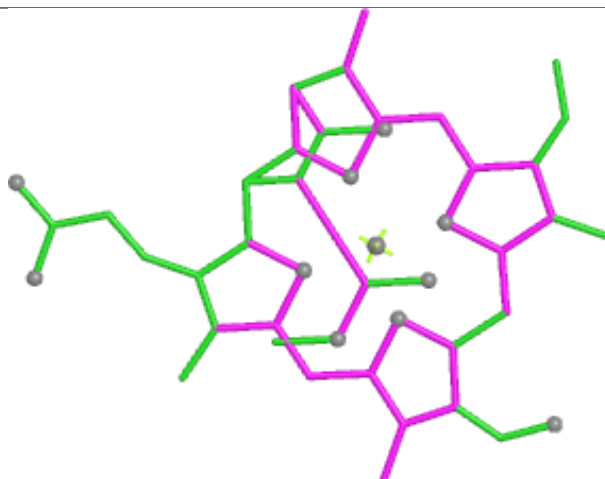
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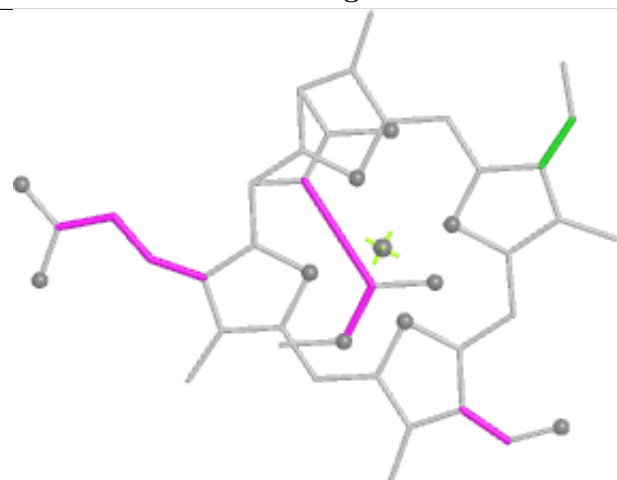
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Bond lengths



Bond angles

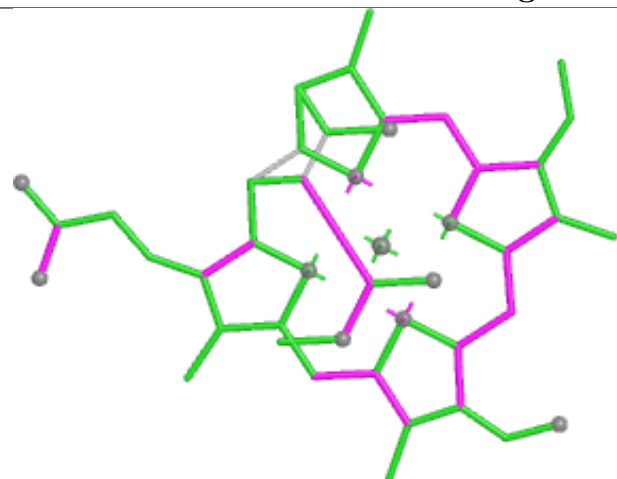


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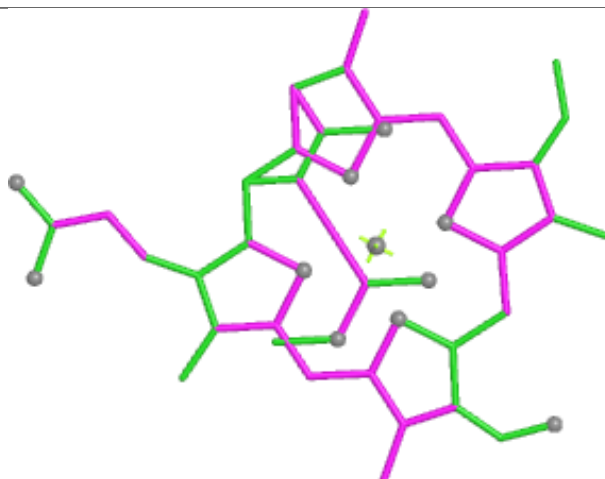


Rings

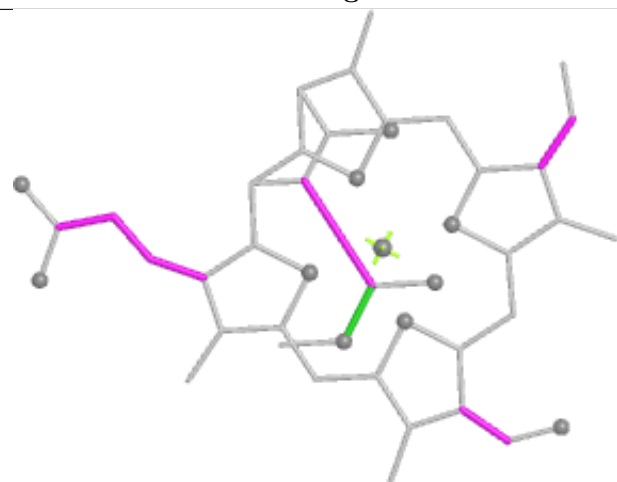
Ligand CL7 33 513



Bond lengths



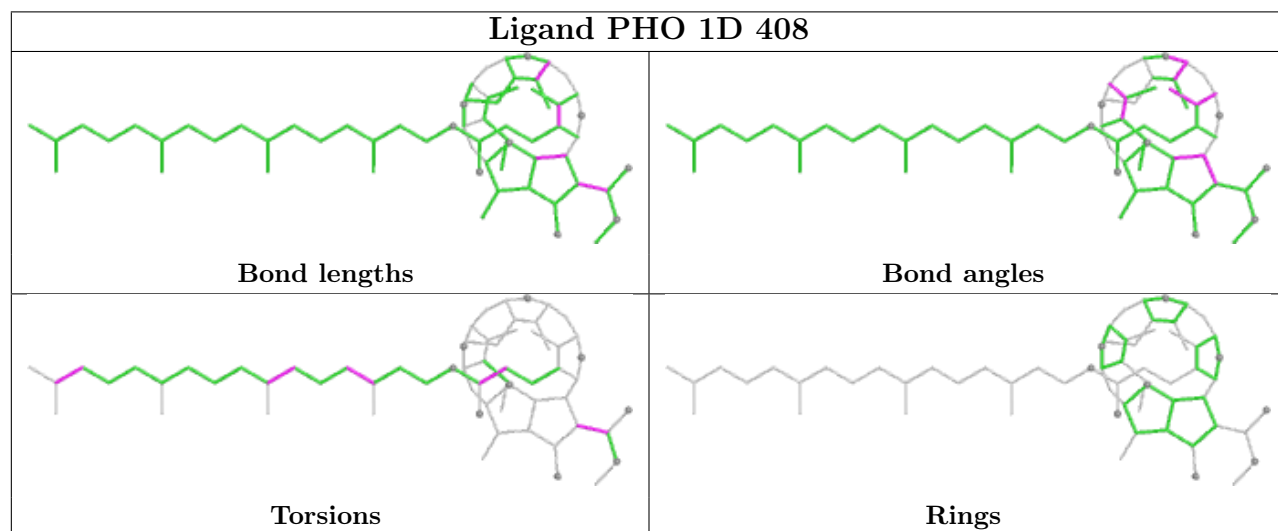
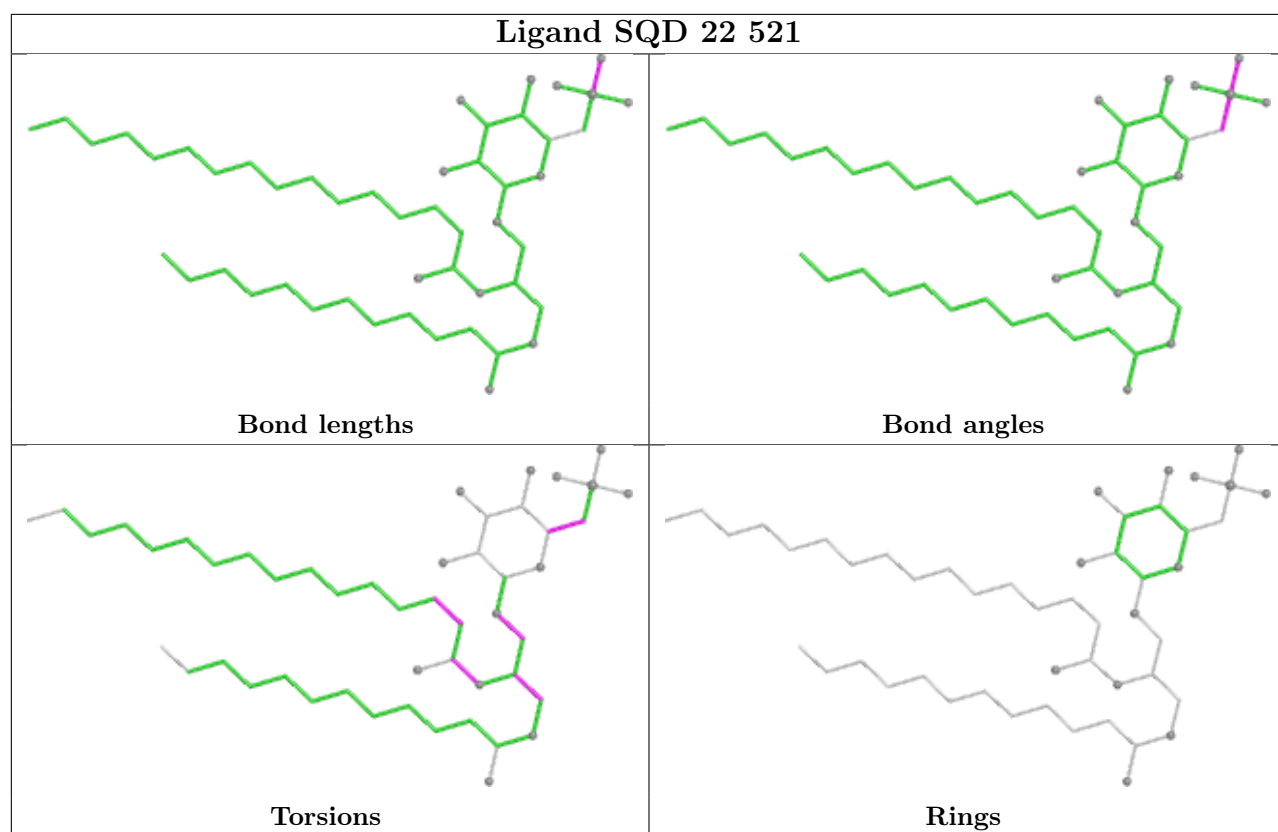
Bond angles

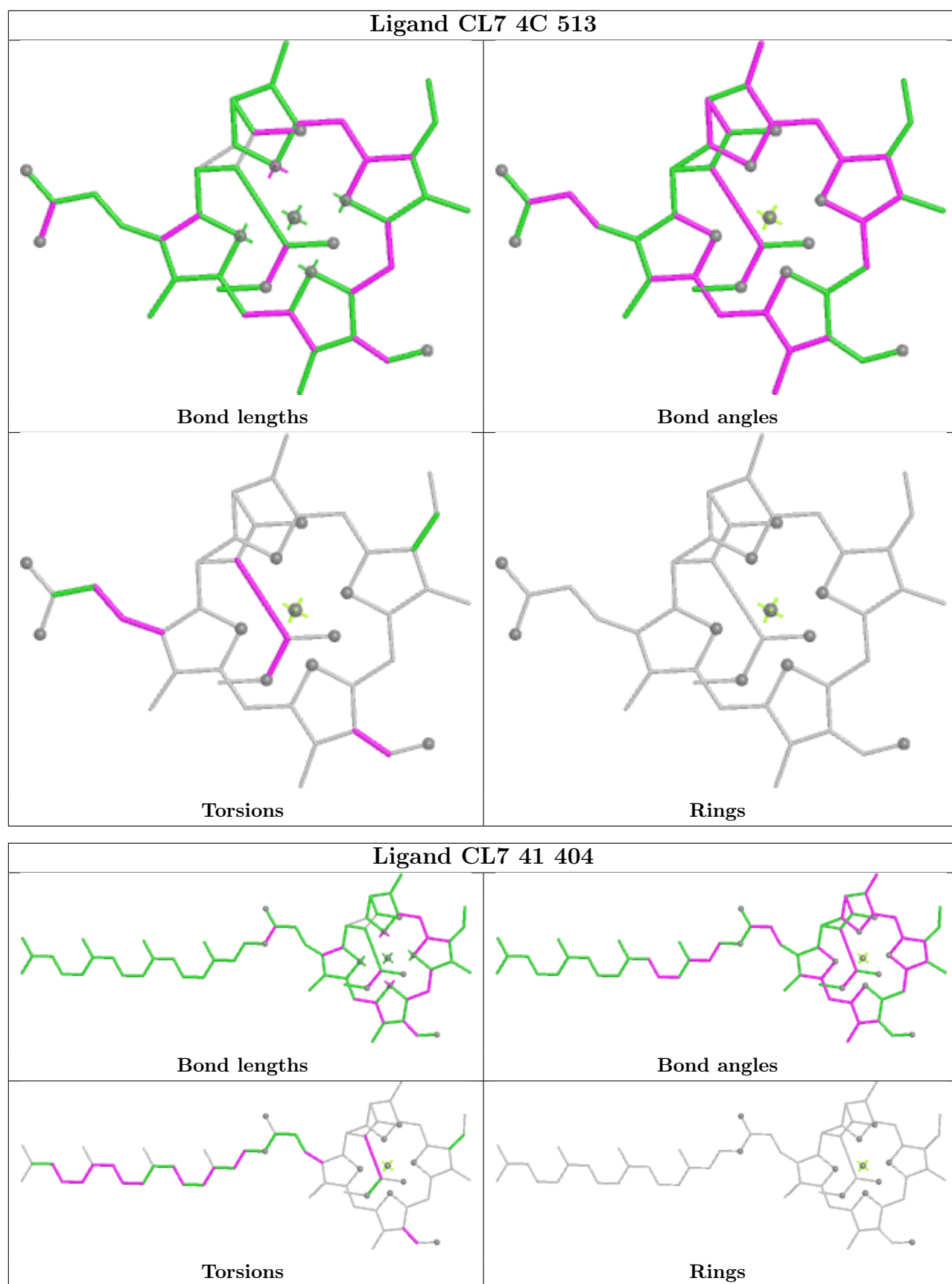


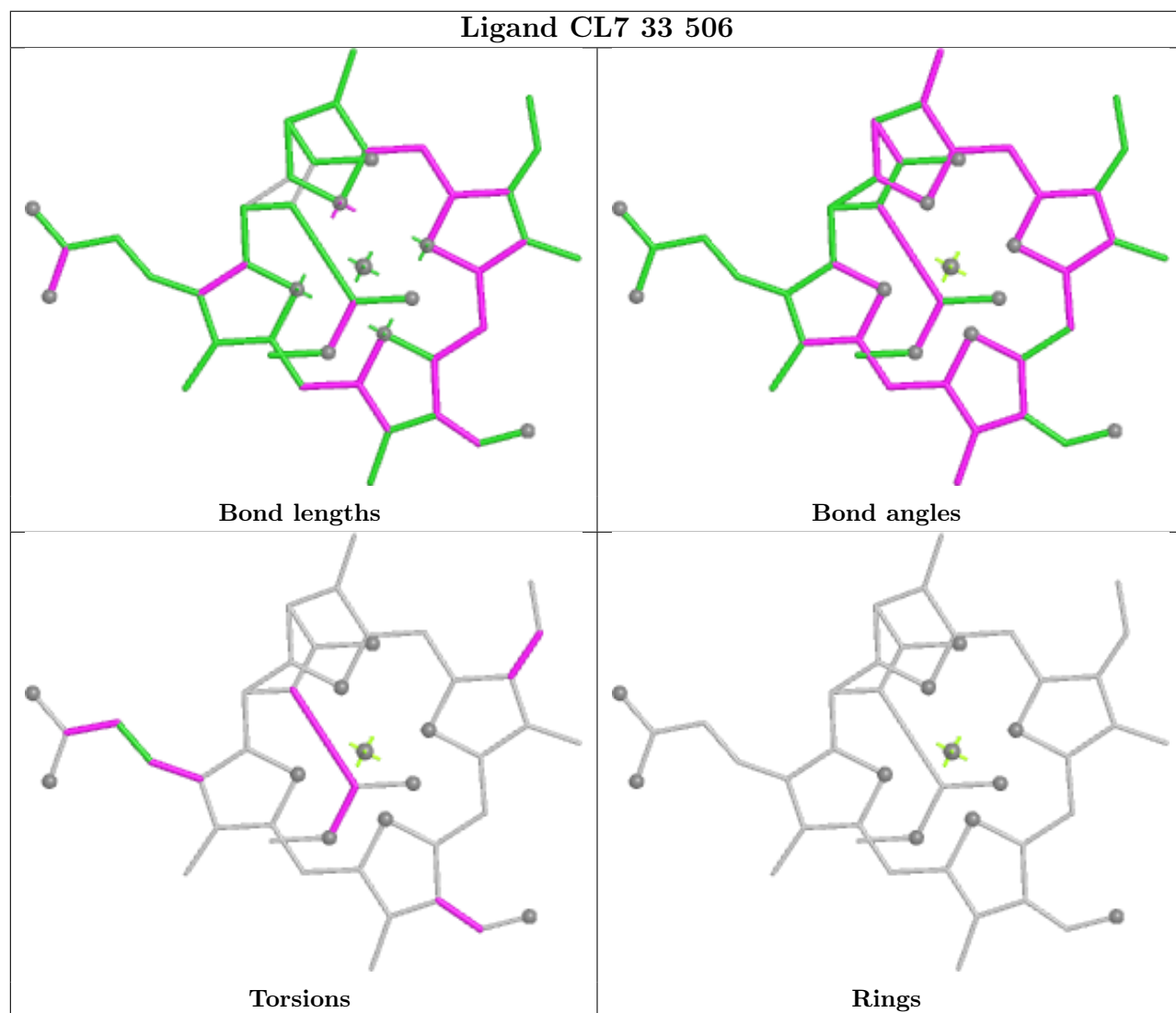
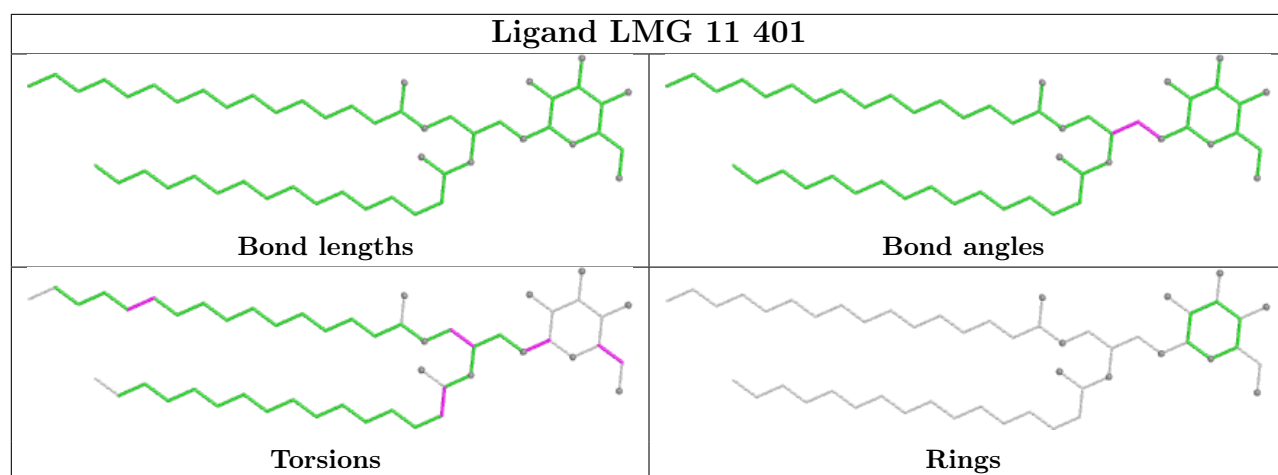
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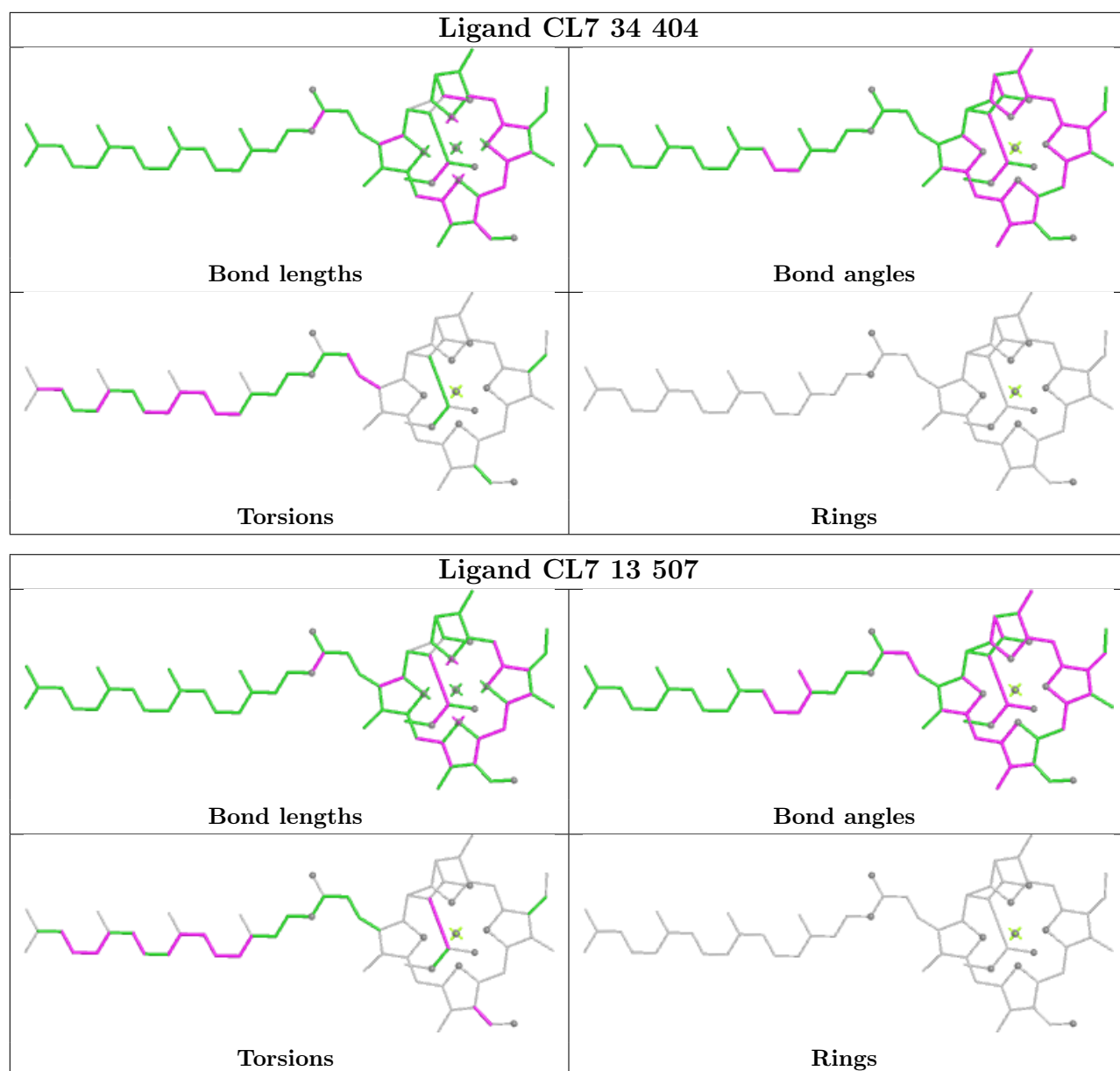


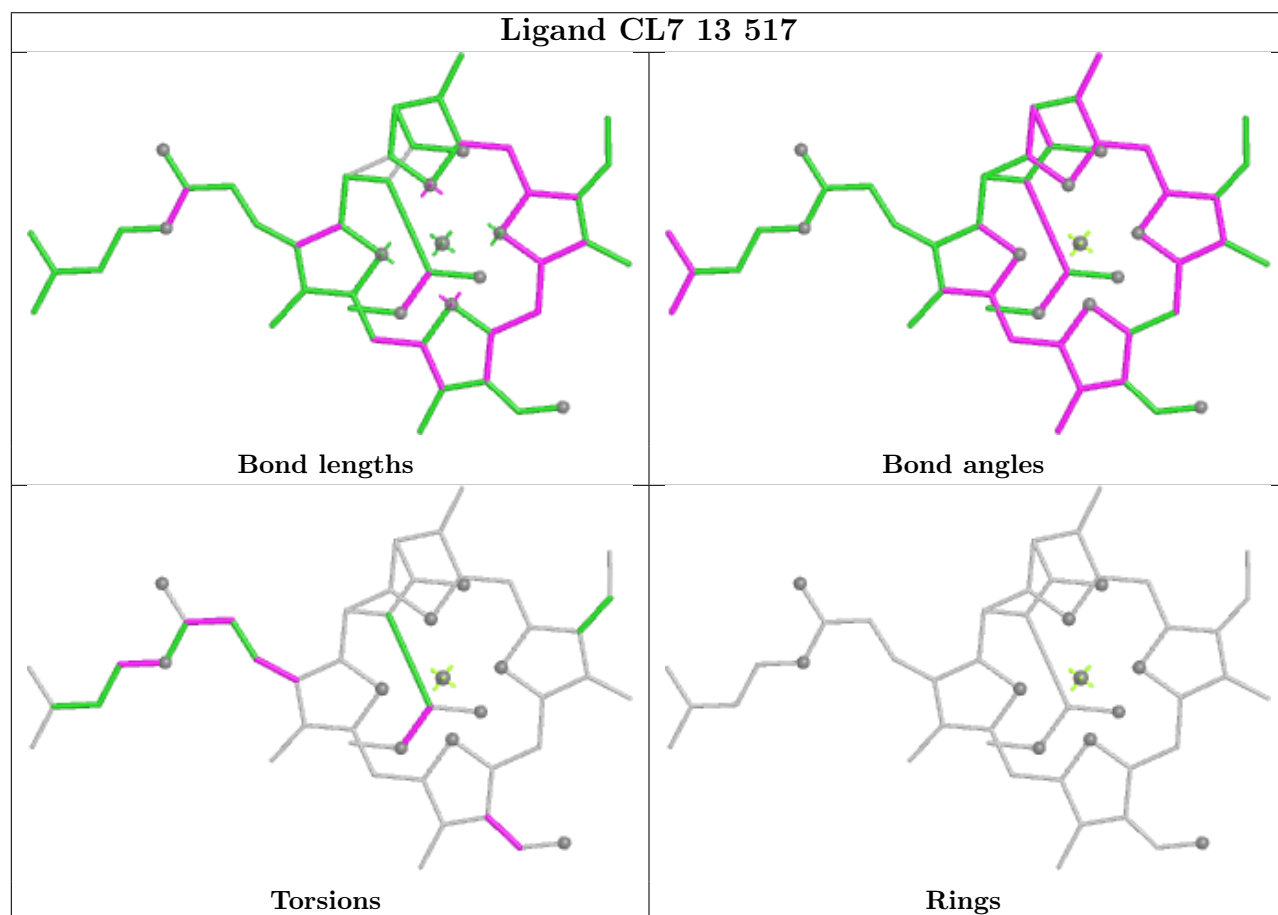
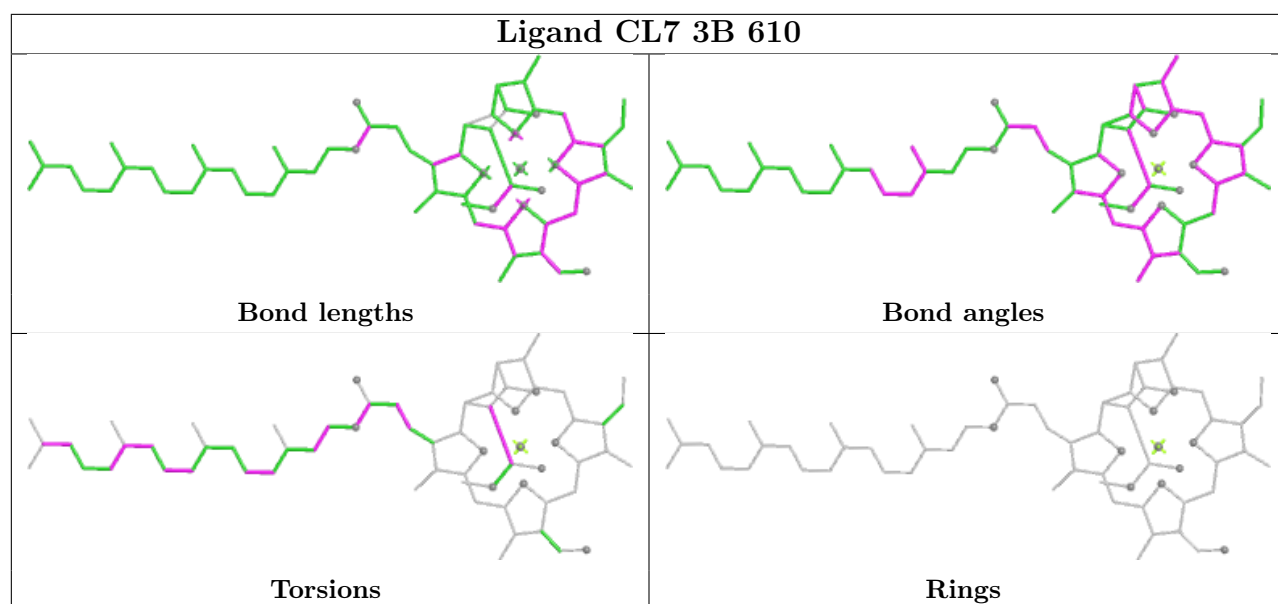
Rings

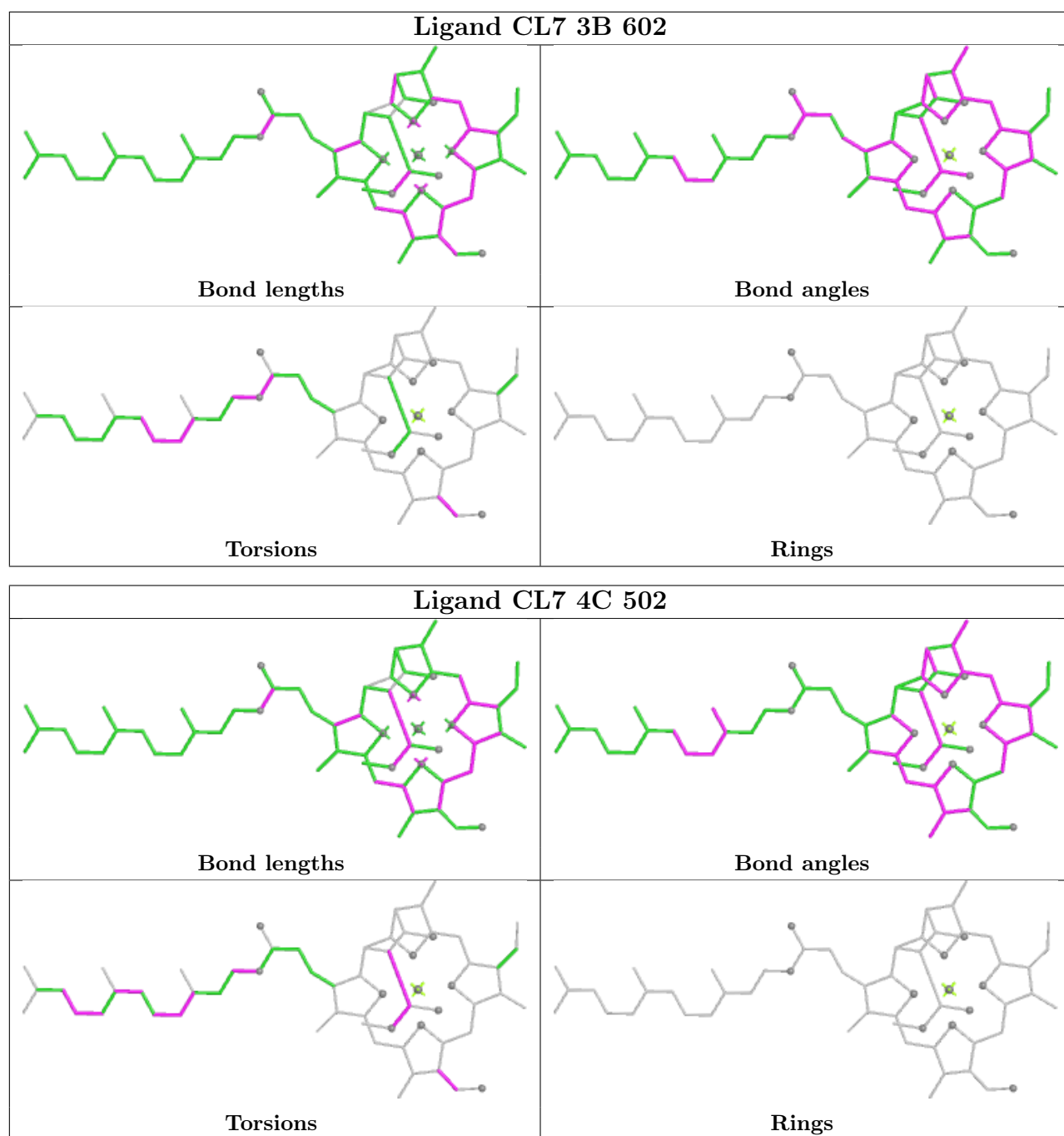




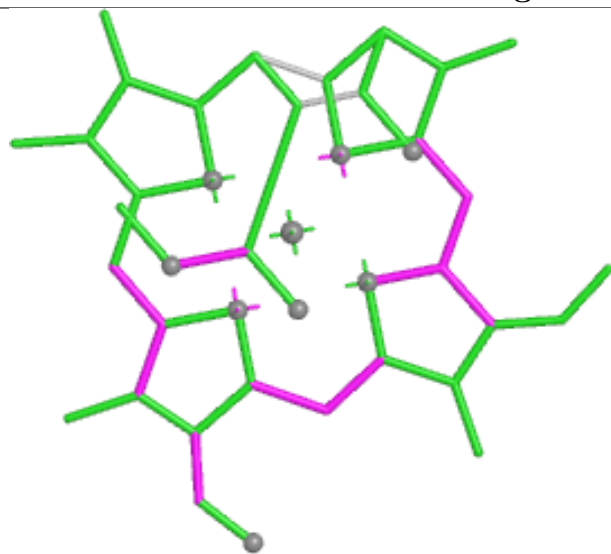




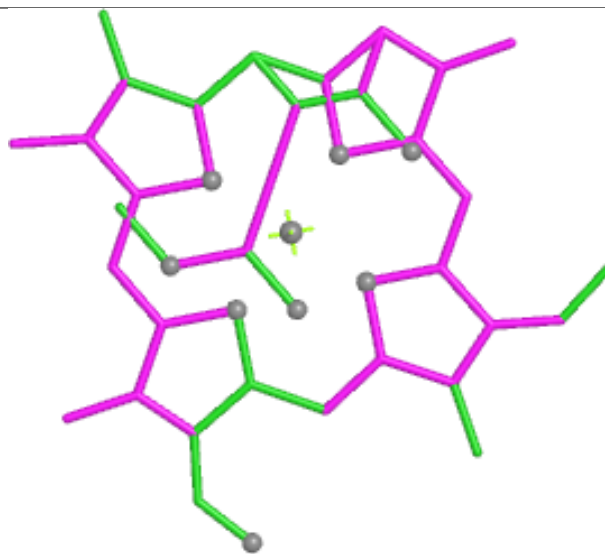




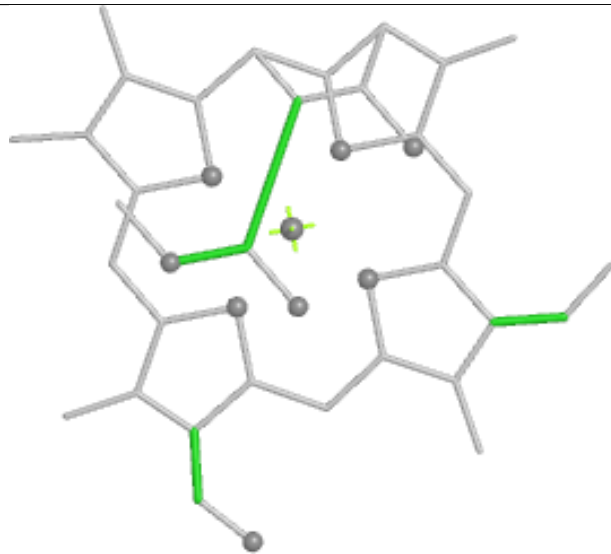
Ligand CL7 13 515



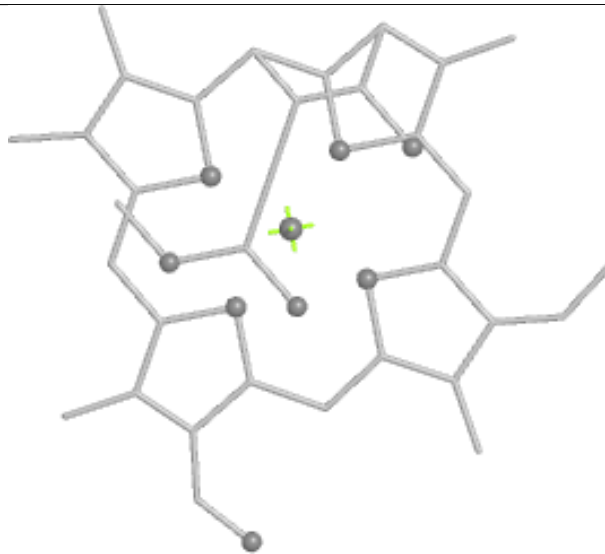
Bond lengths



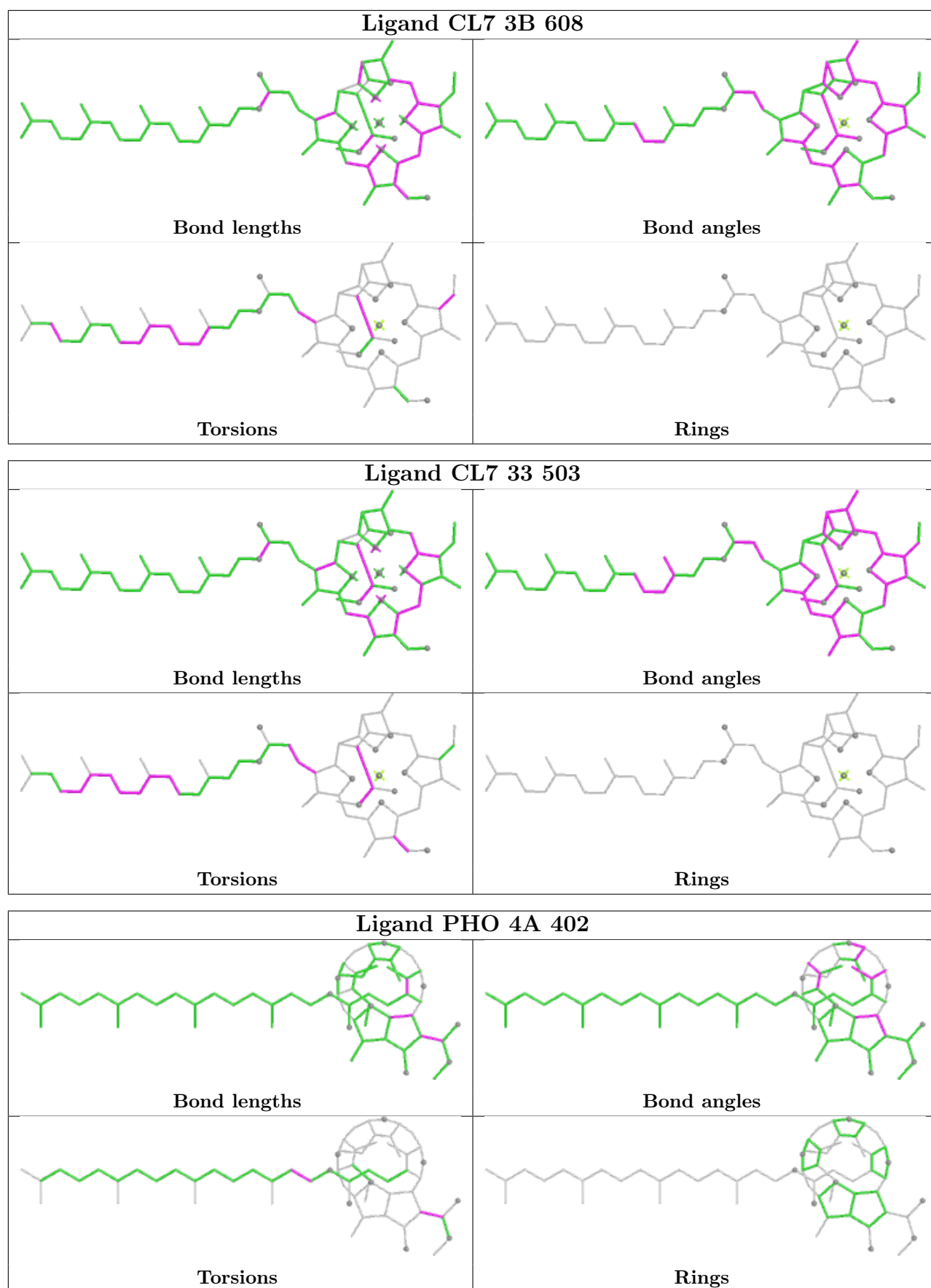
Bond angles

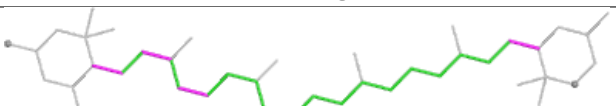


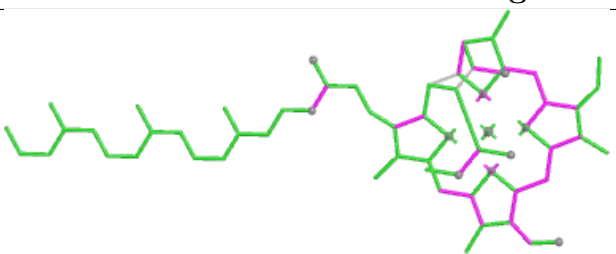
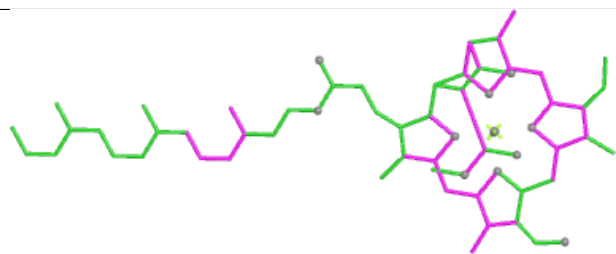
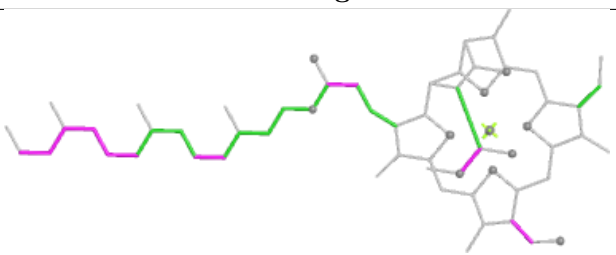
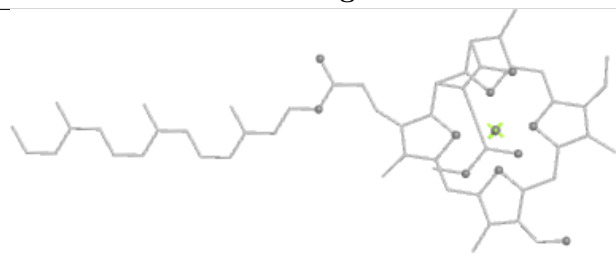
Torsions

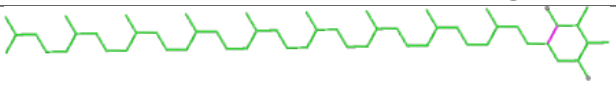
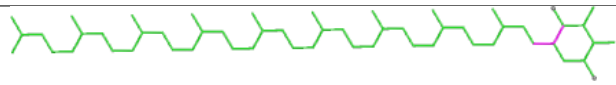
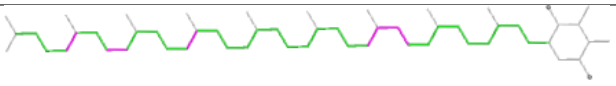
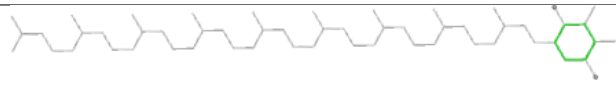


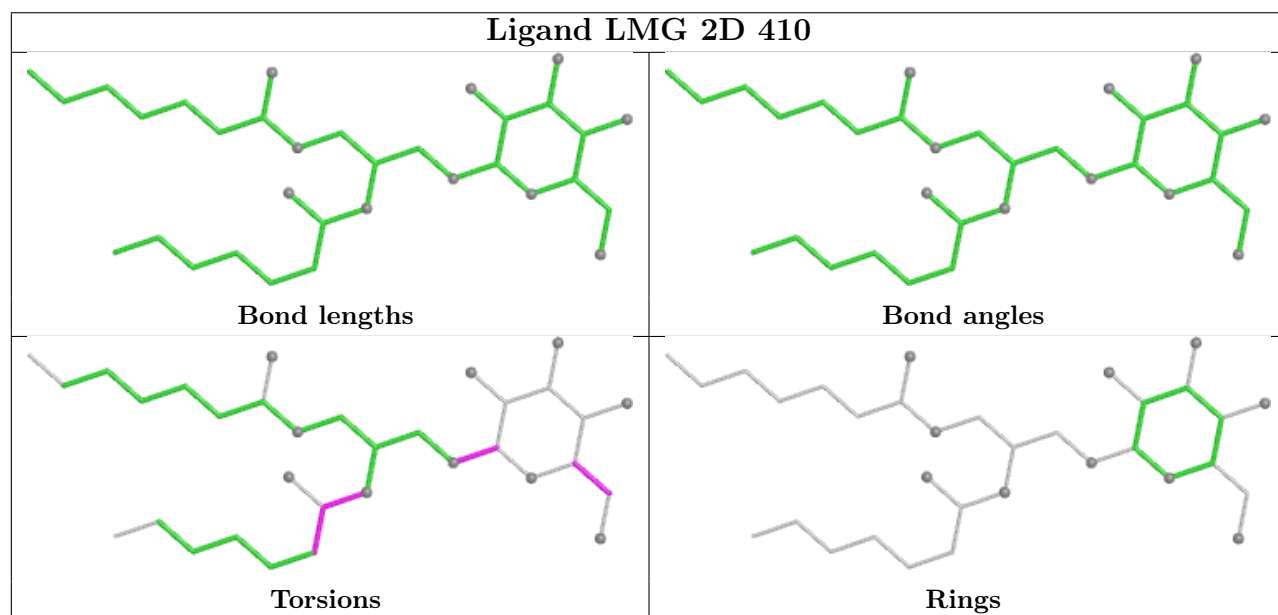
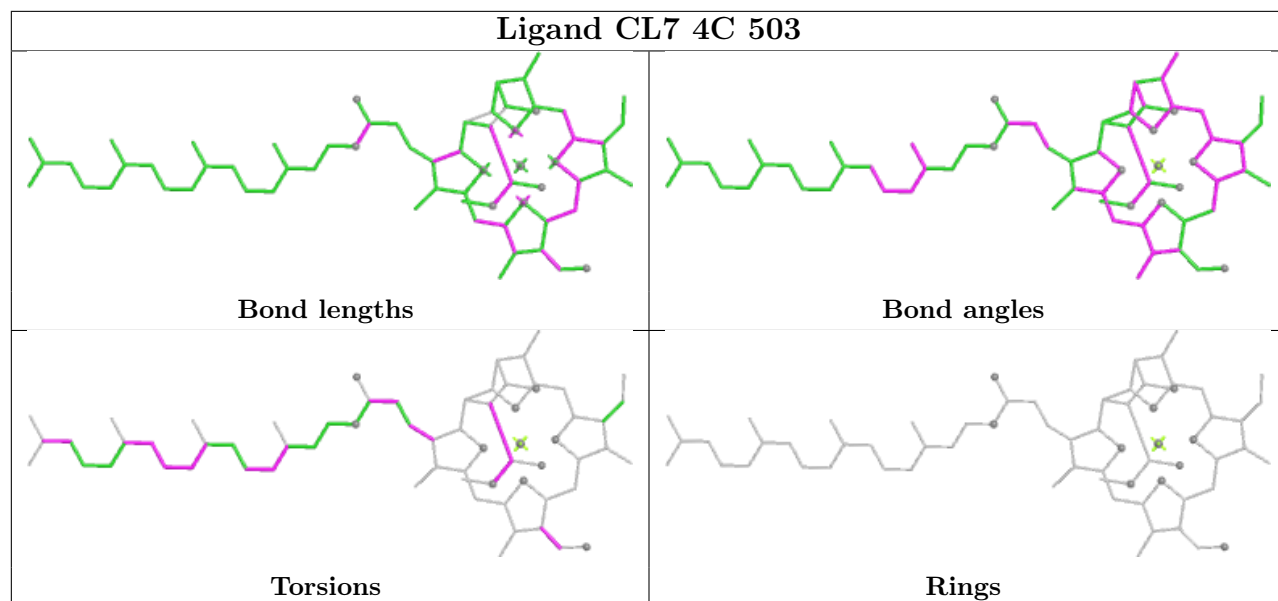
Rings



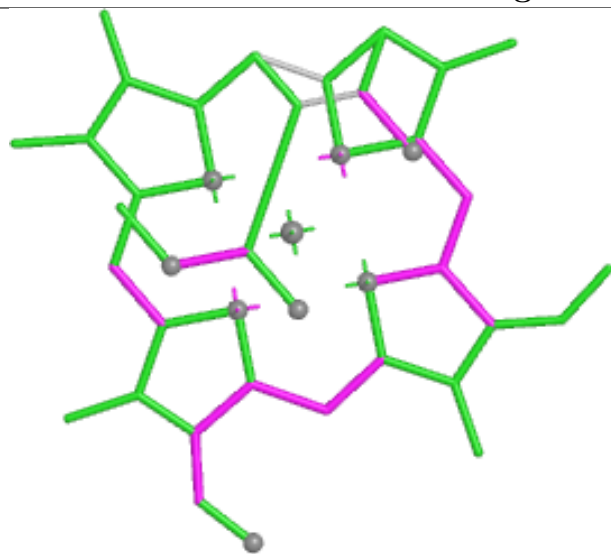
Ligand ZEX 22 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CL7 11 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

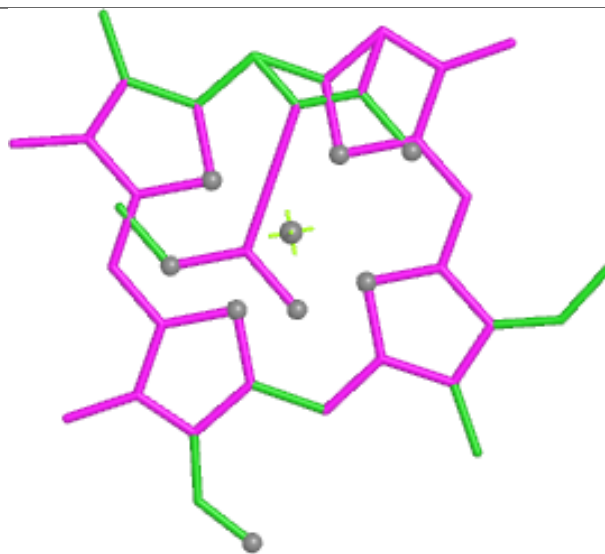
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Bond lengths	Bond angles
	
Torsions	Rings



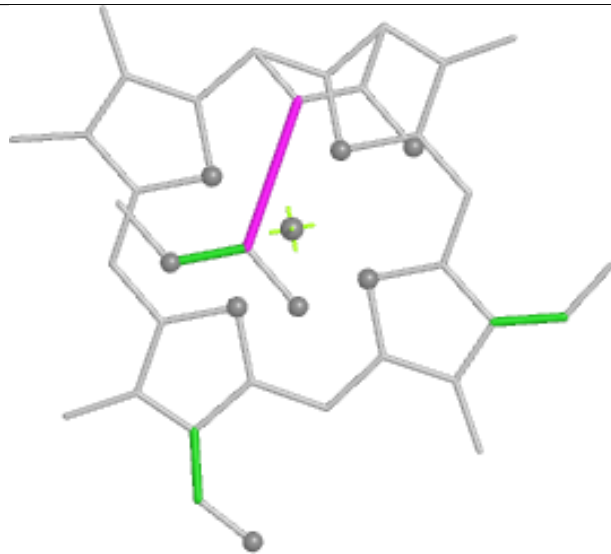
Ligand CL7 21 413



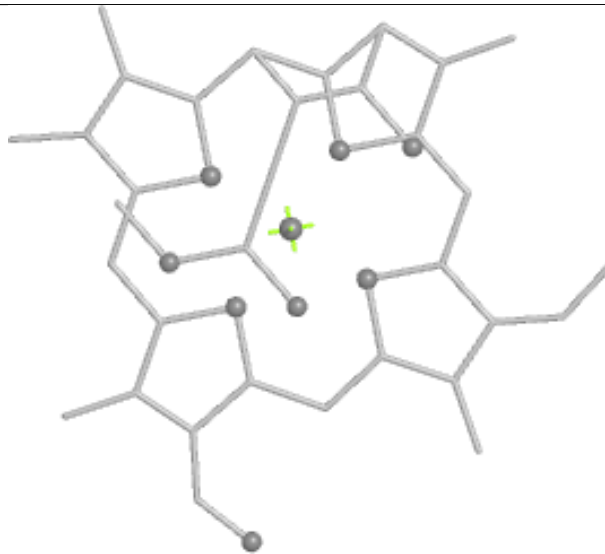
Bond lengths



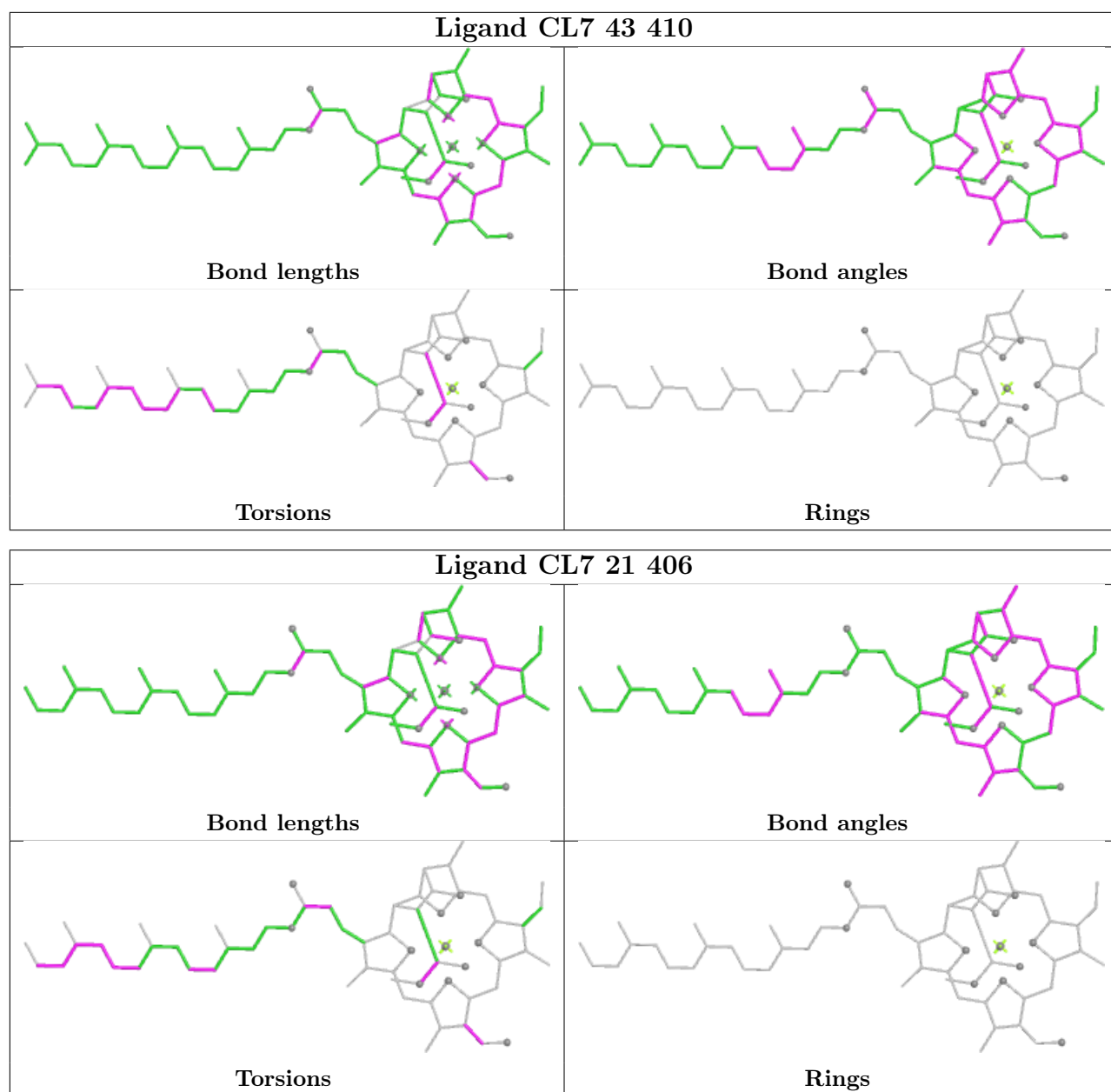
Bond angles

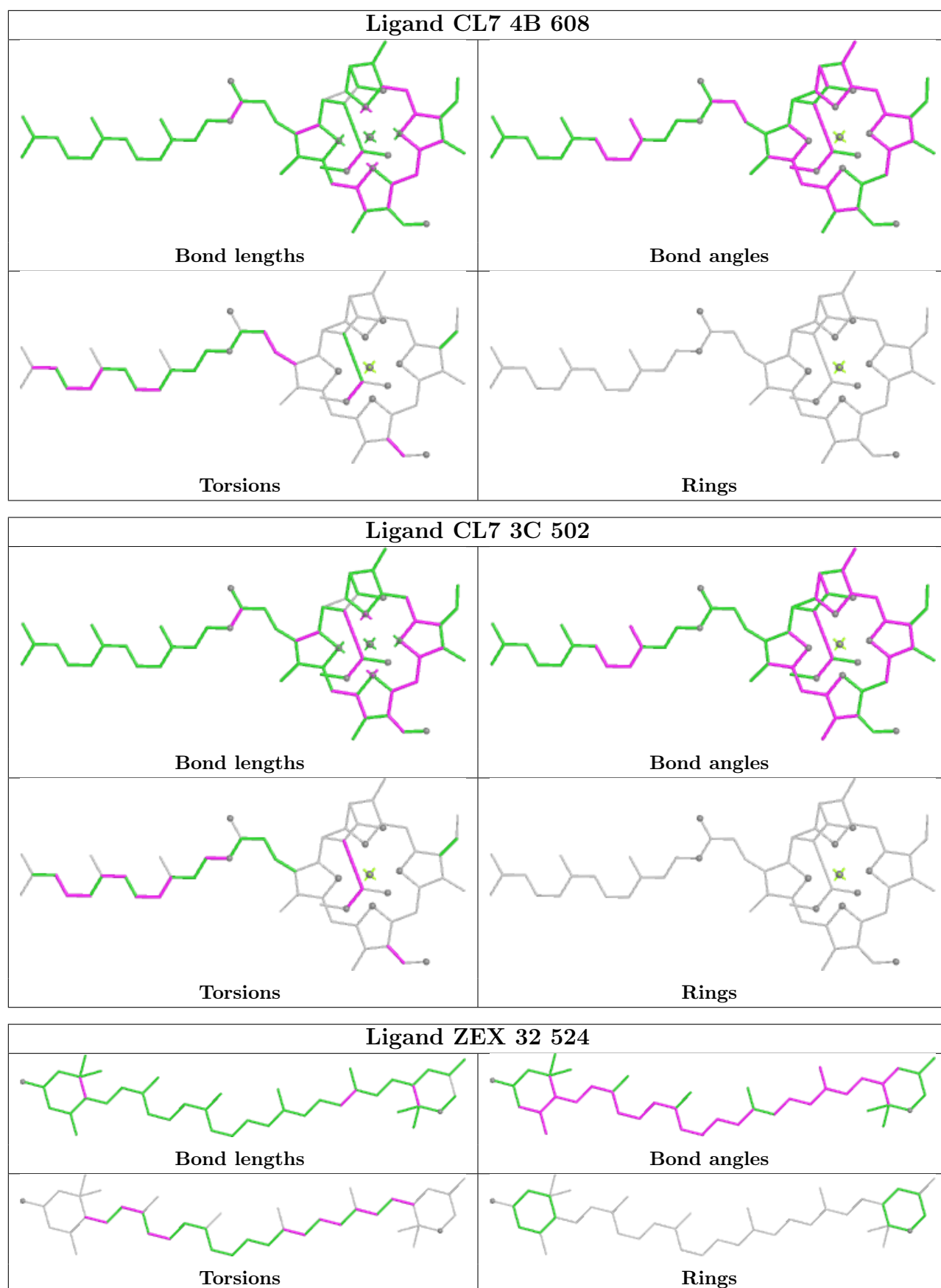


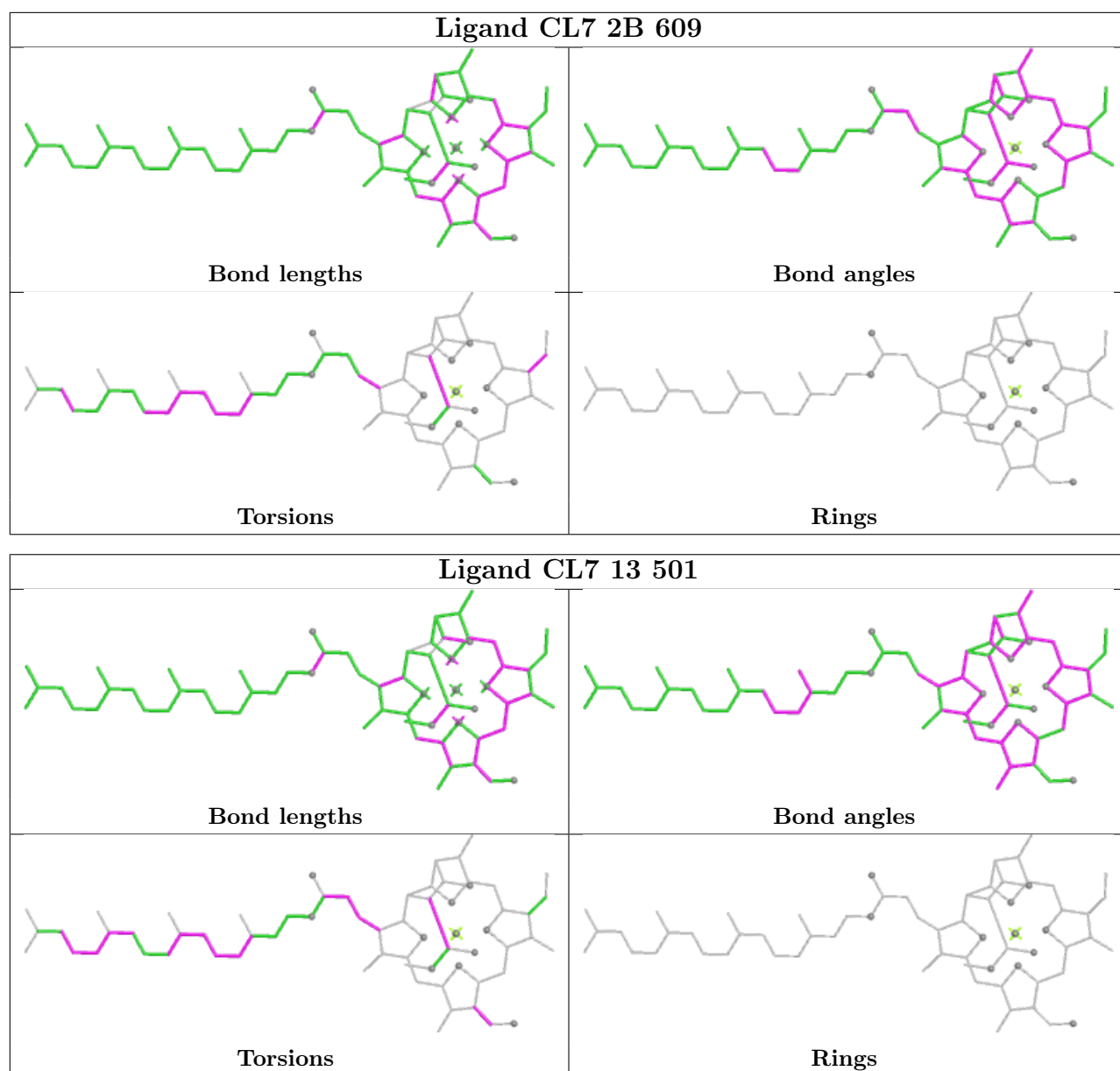
Torsions

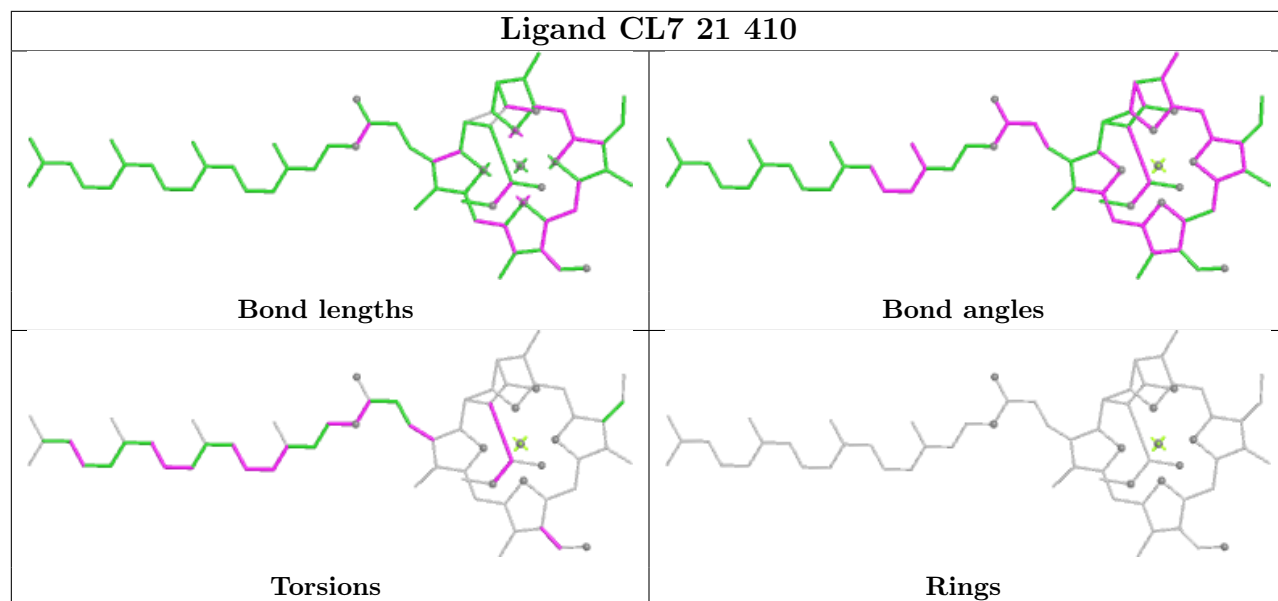


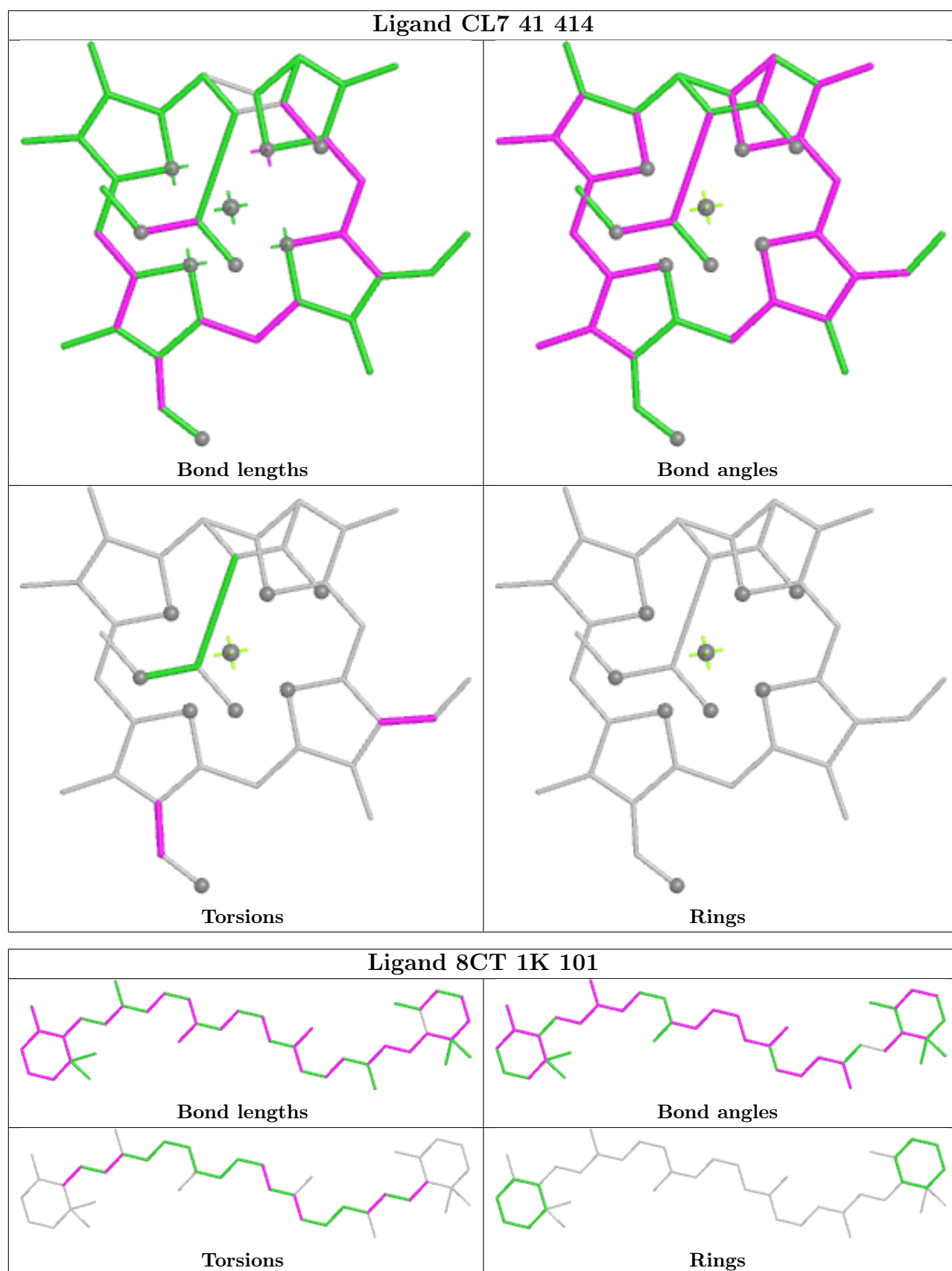
Rings

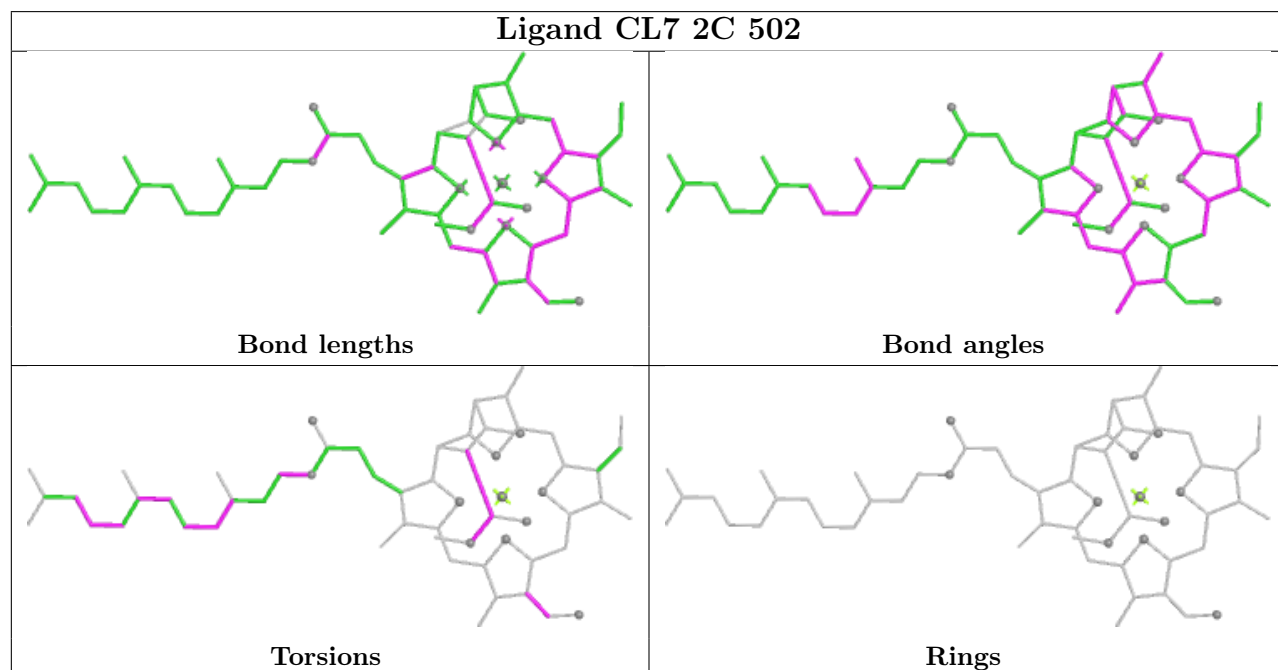
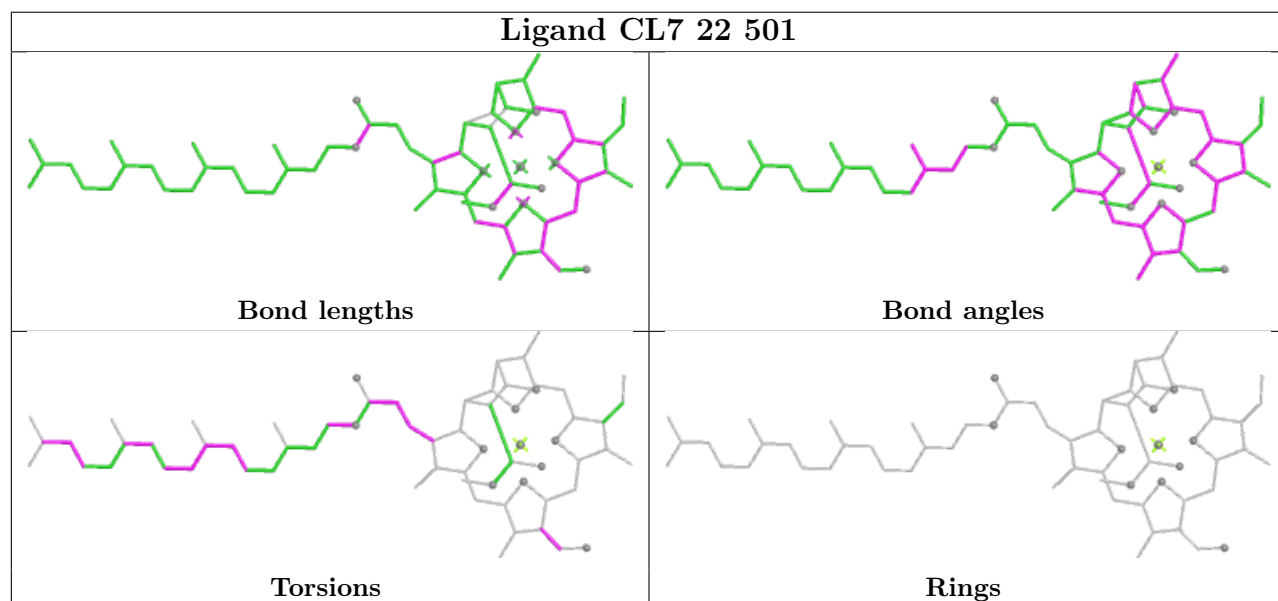
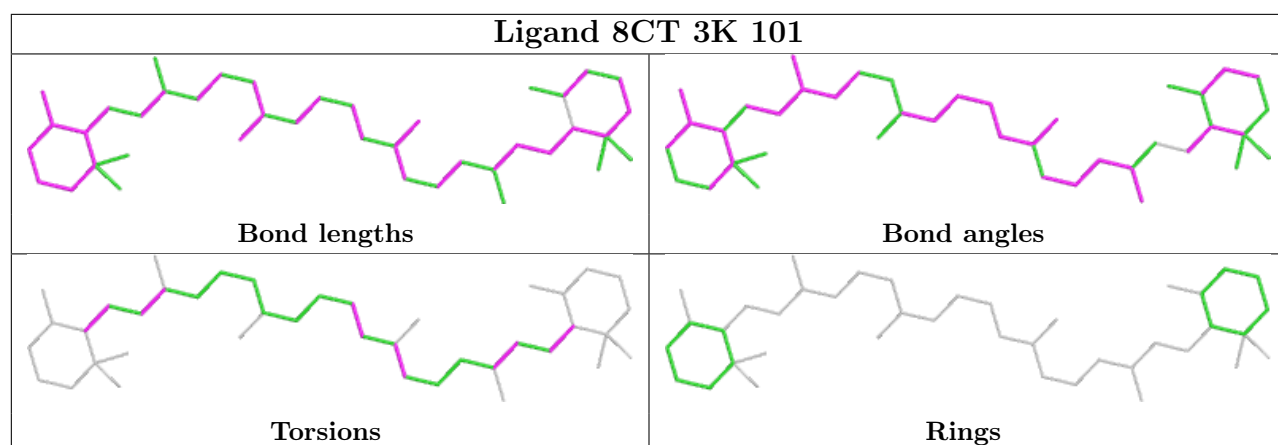


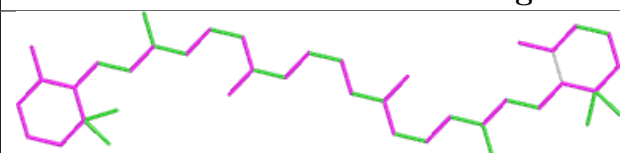
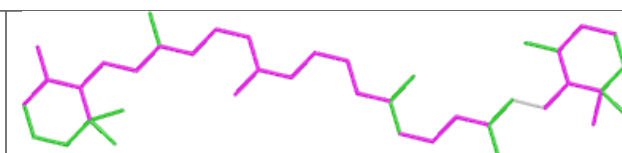
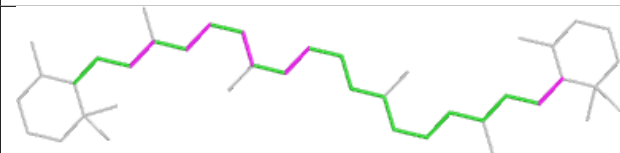
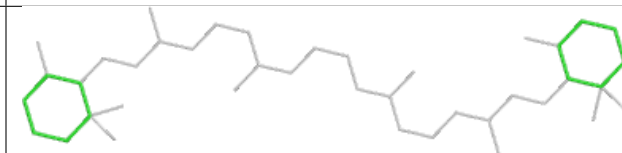
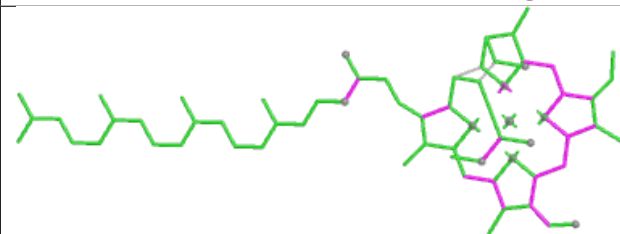
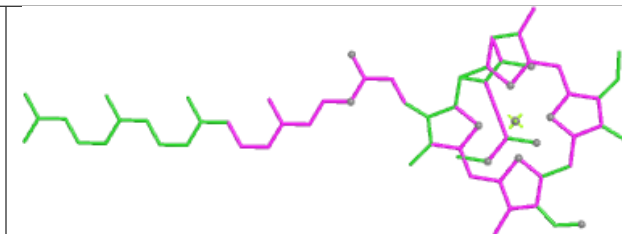
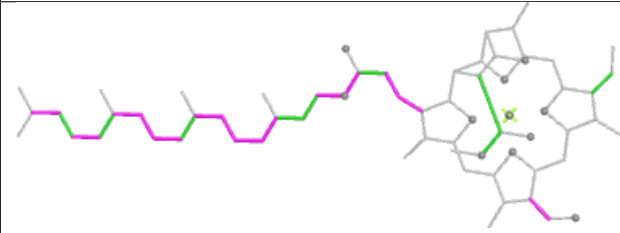
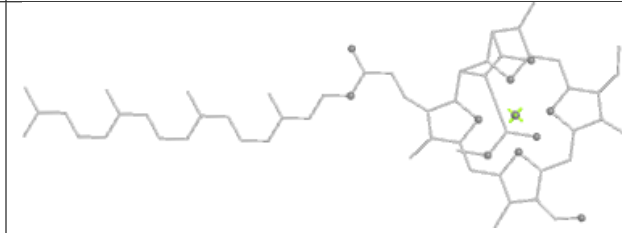
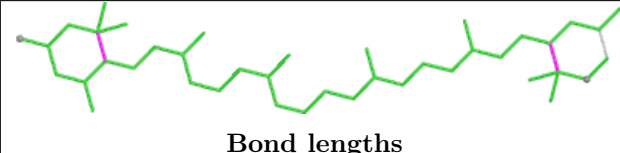
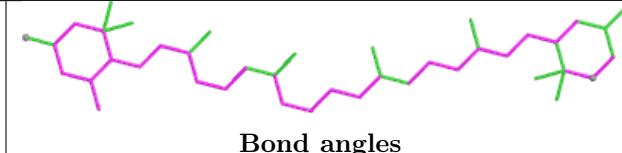
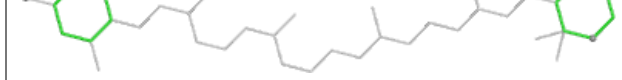


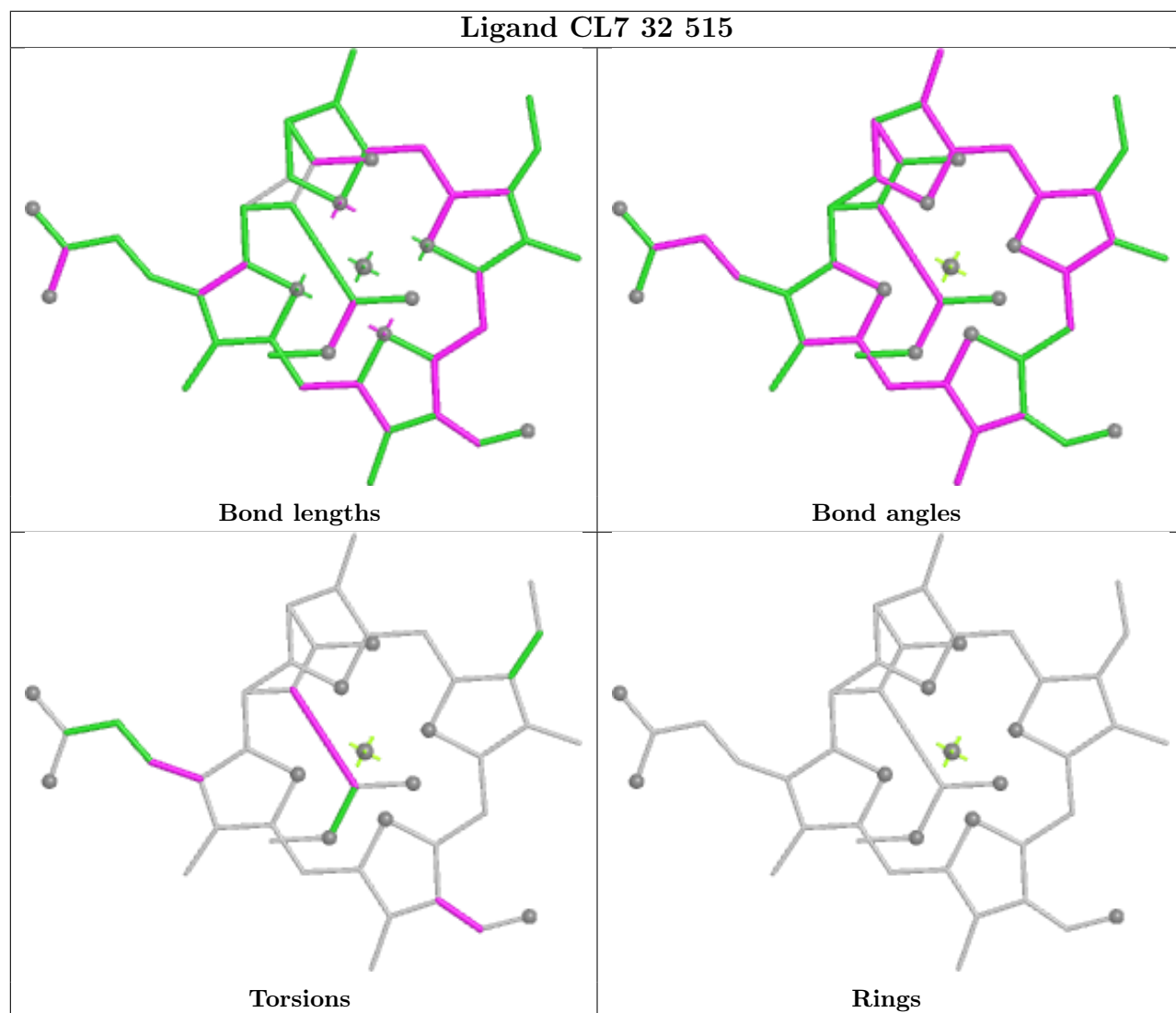
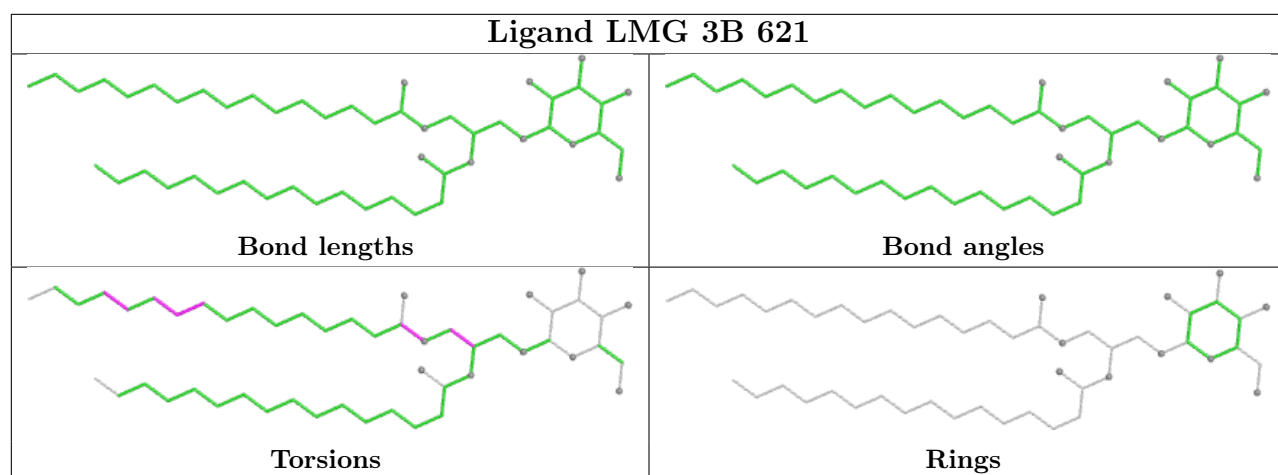


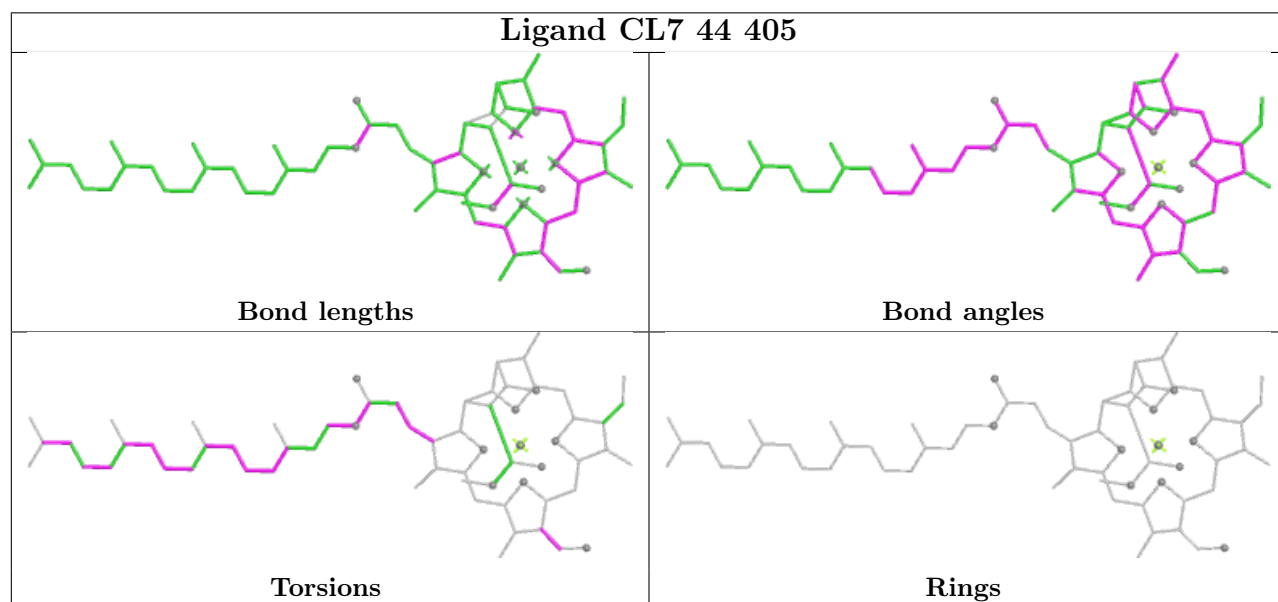
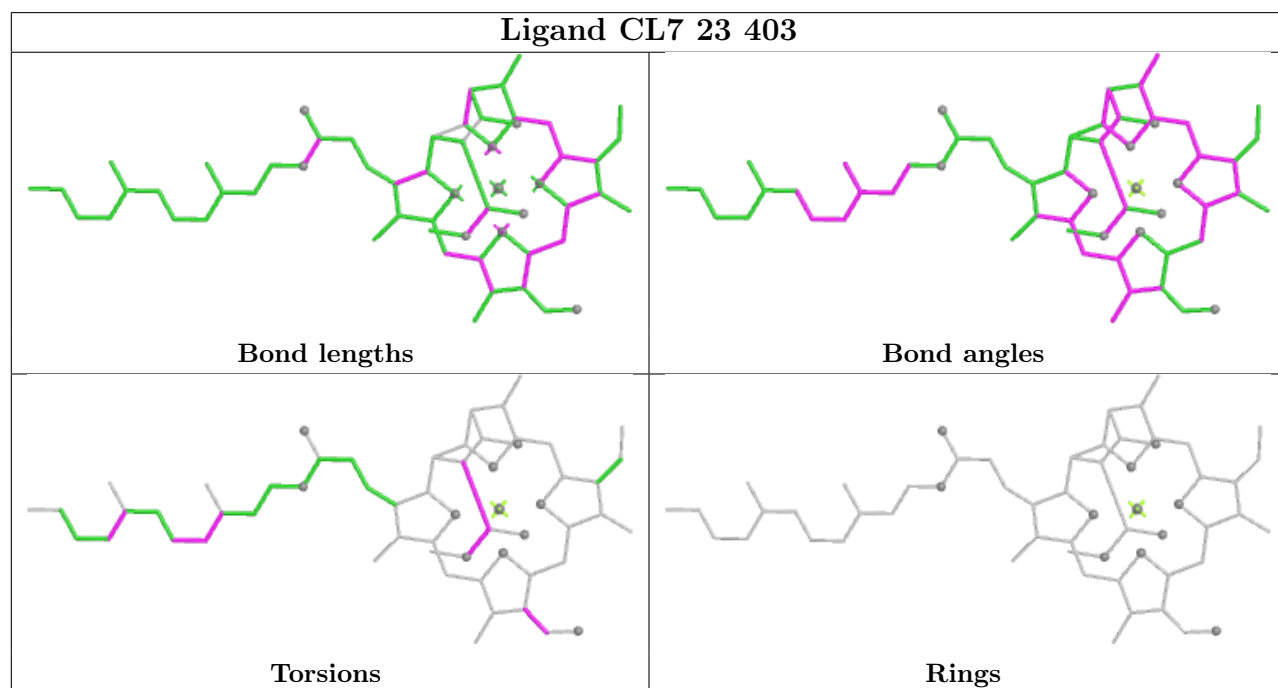
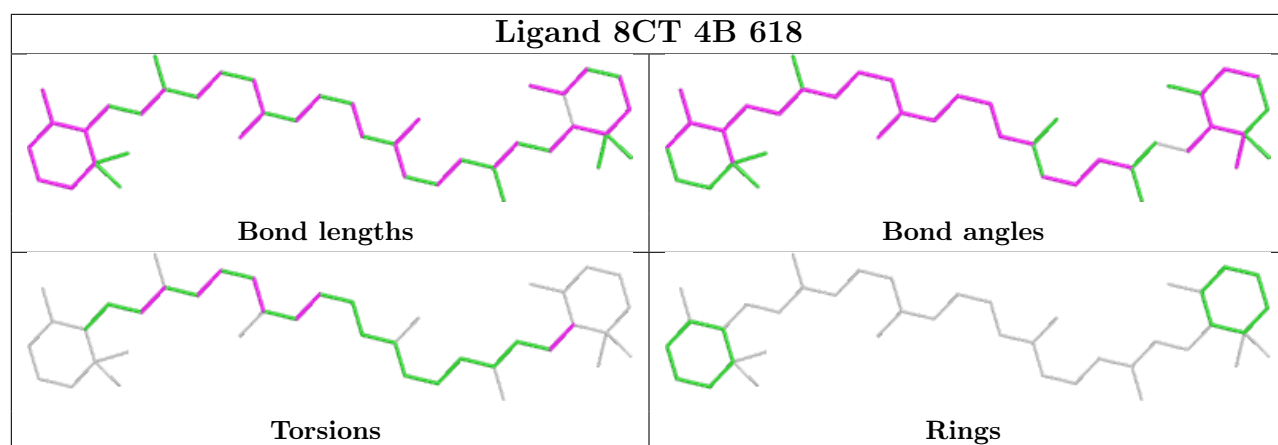


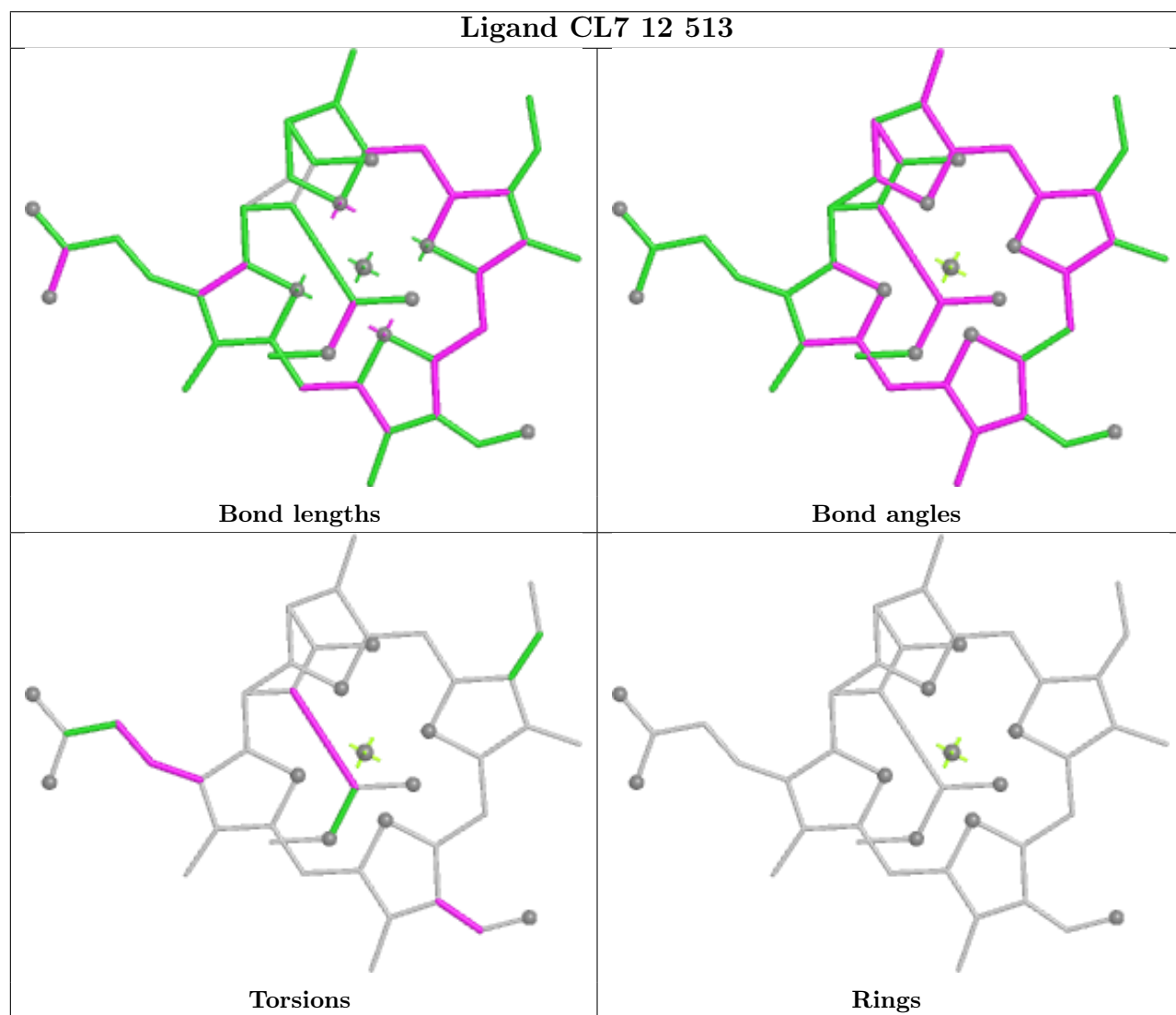
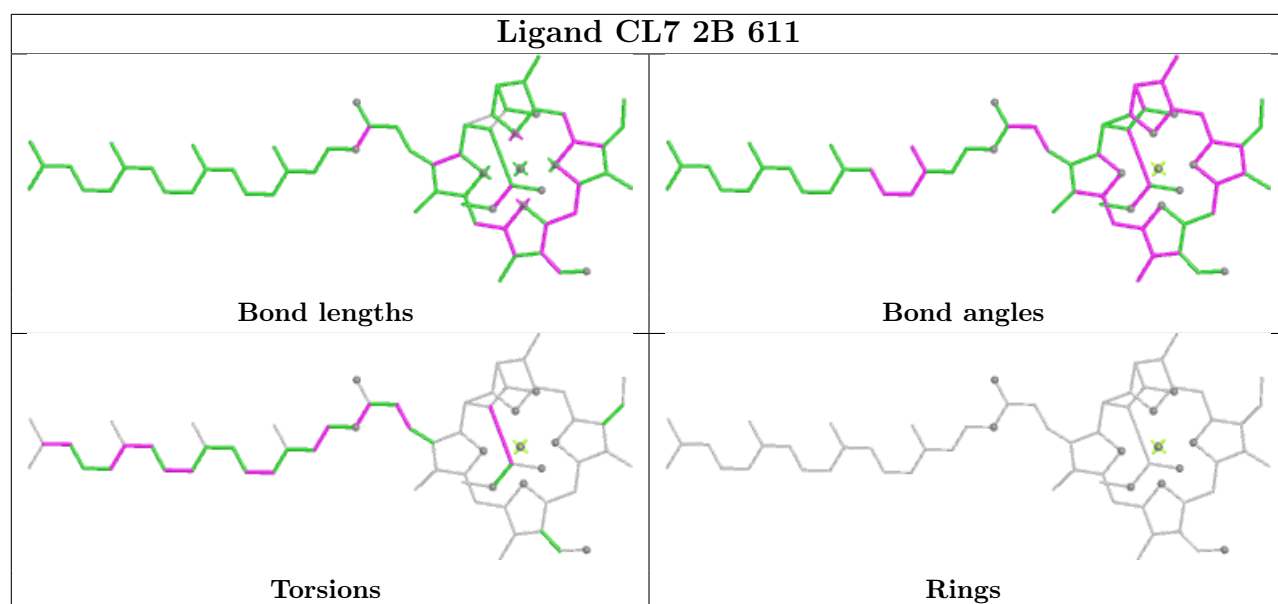


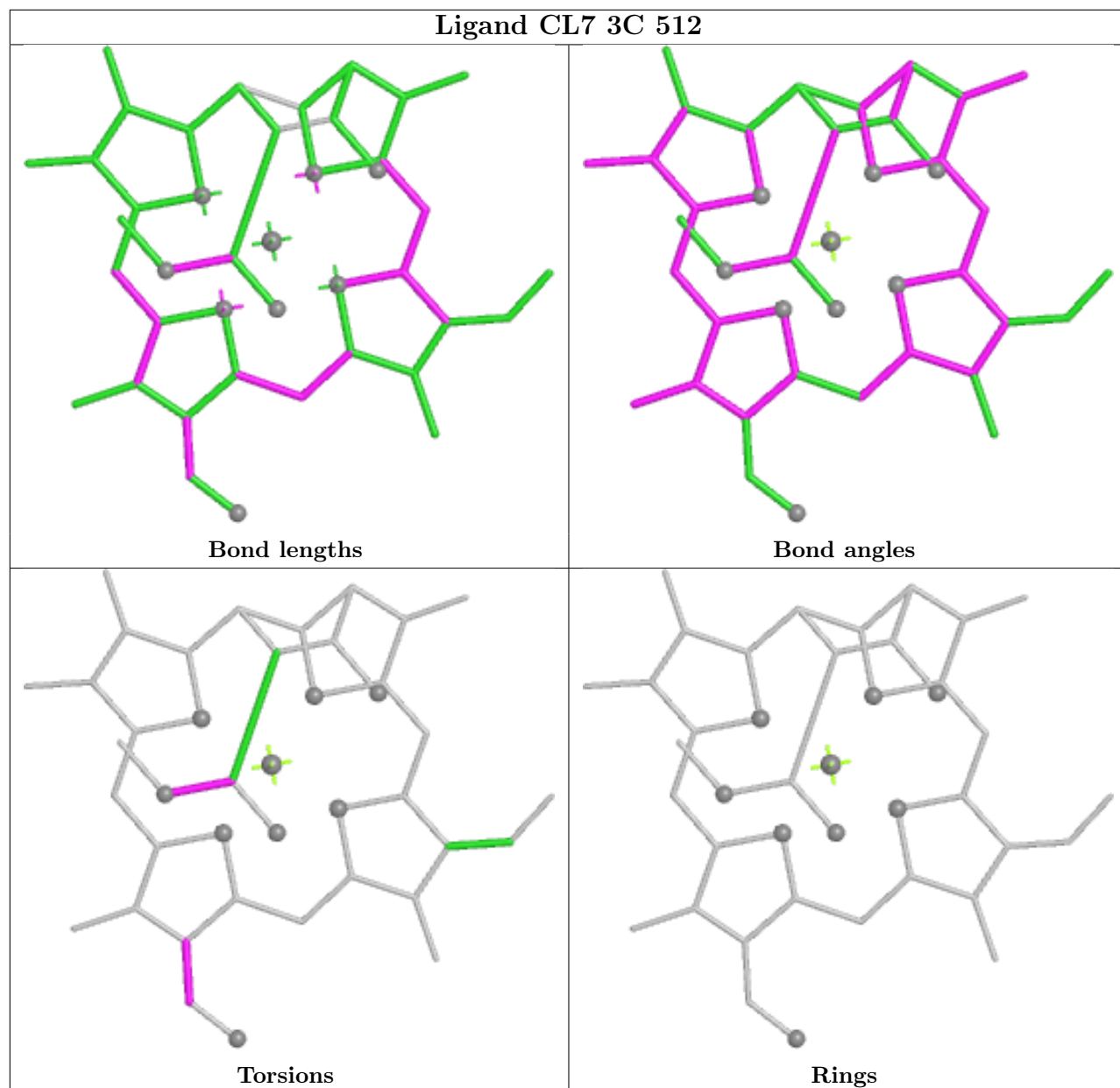


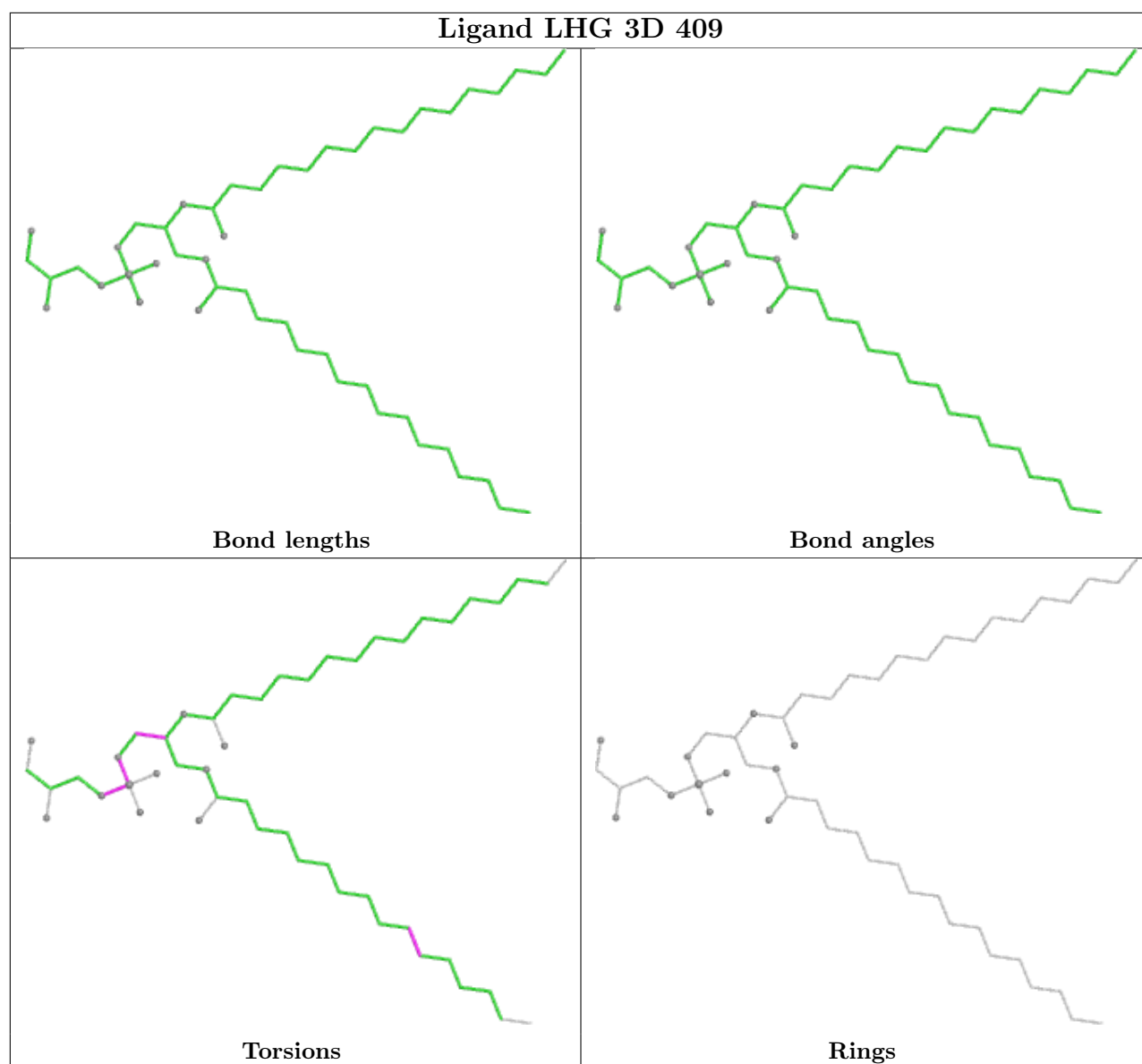
Ligand 8CT 1B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CL7 24 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand ZEX 41 422	
 Bond lengths	 Bond angles
 Torsions	 Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

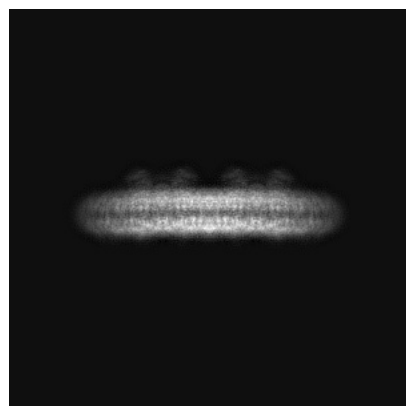
6 Map visualisation [i](#)

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

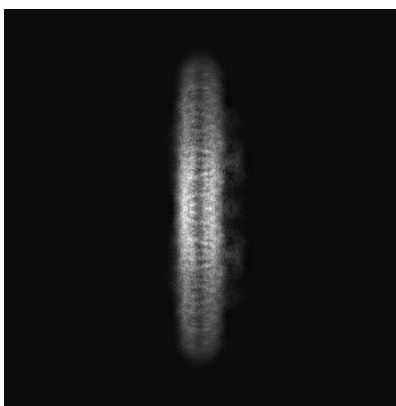
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

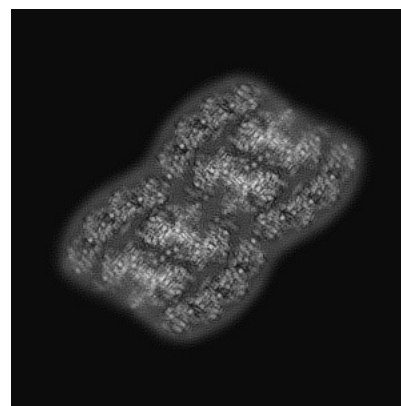
6.1.1 Primary map



X

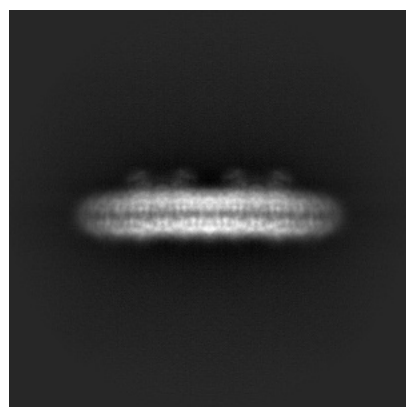


Y

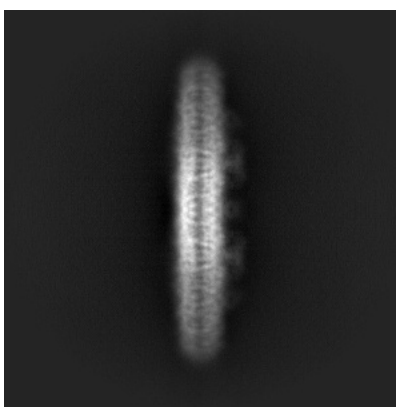


Z

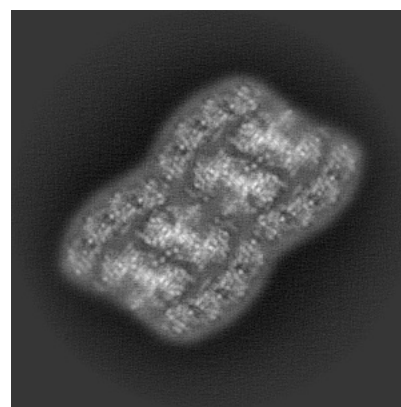
6.1.2 Raw map



X



Y

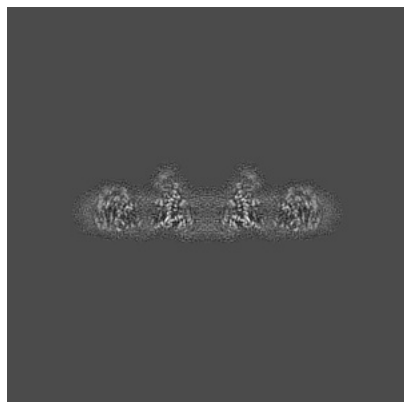


Z

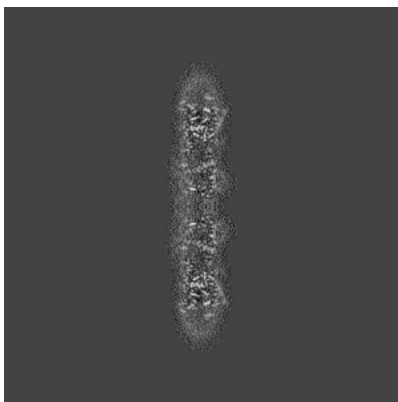
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

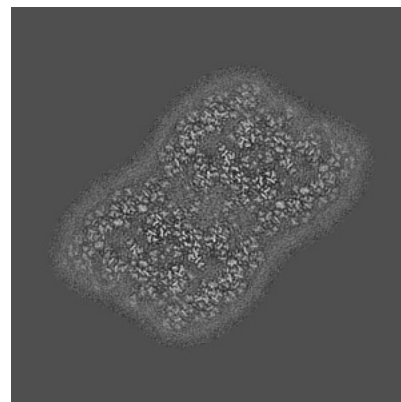
6.2.1 Primary map



X Index: 240

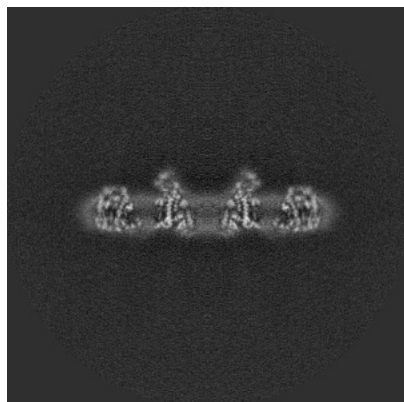


Y Index: 240

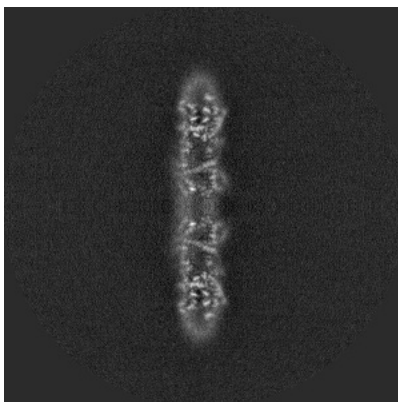


Z Index: 240

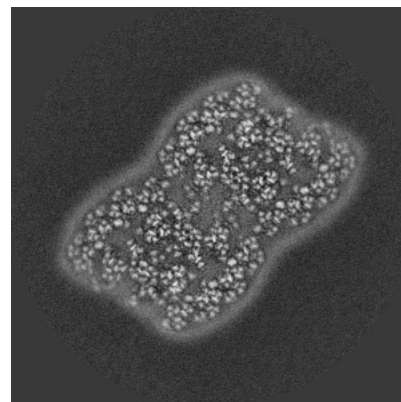
6.2.2 Raw map



X Index: 240



Y Index: 240

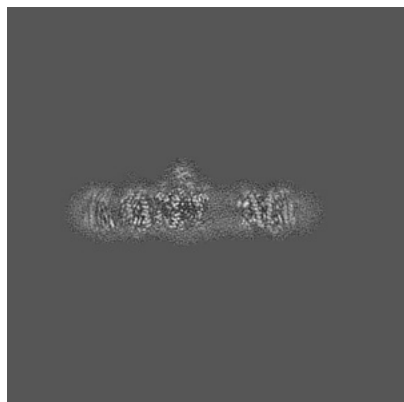


Z Index: 240

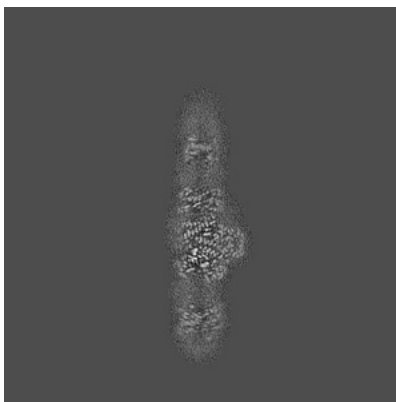
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

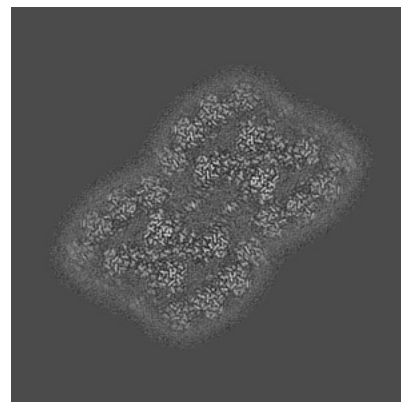
6.3.1 Primary map



X Index: 204

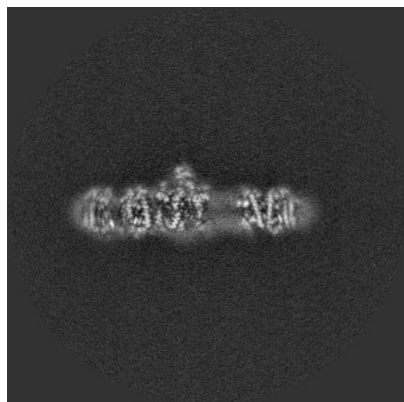


Y Index: 208

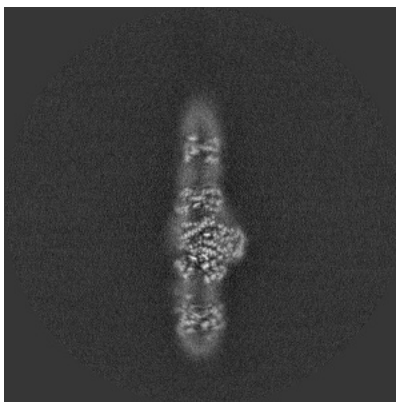


Z Index: 225

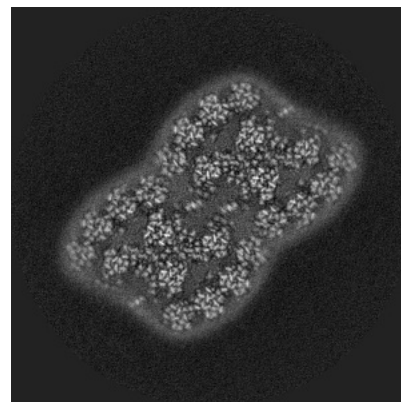
6.3.2 Raw map



X Index: 204



Y Index: 209

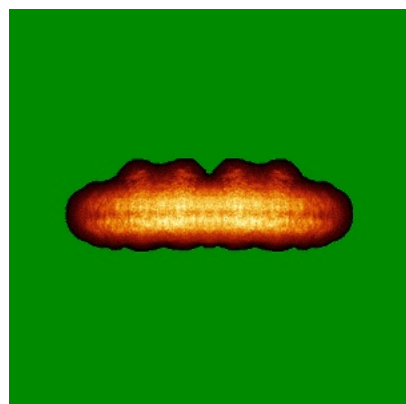


Z Index: 224

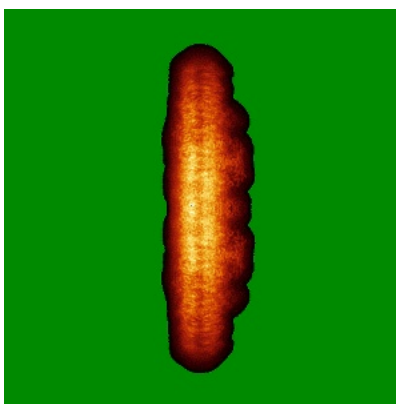
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

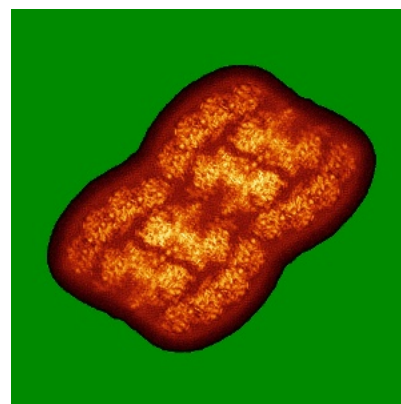
6.4.1 Primary map



X

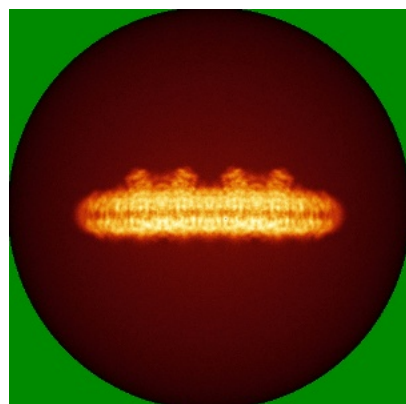


Y

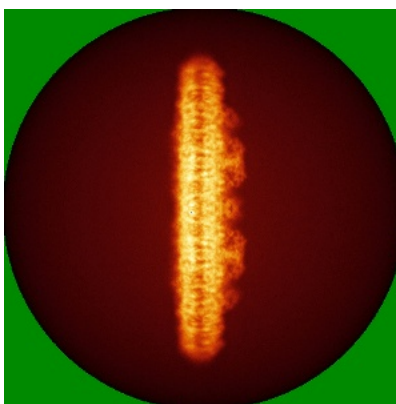


Z

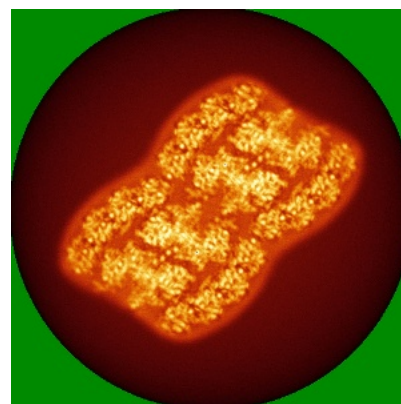
6.4.2 Raw map



X



Y

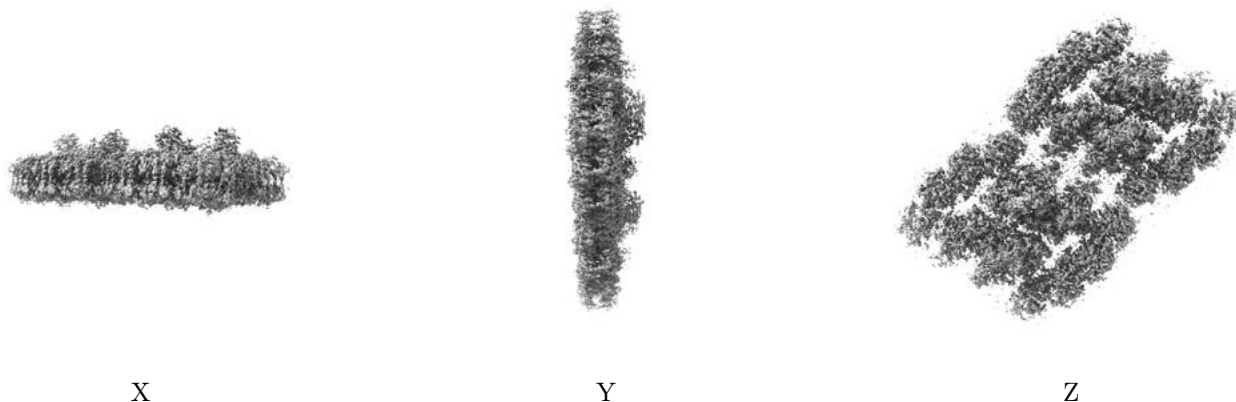


Z

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



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



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.

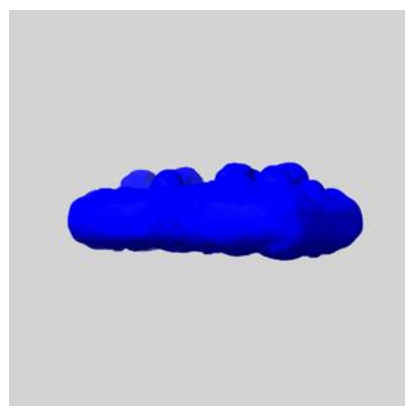
6.6 Mask visualisation [i](#)

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

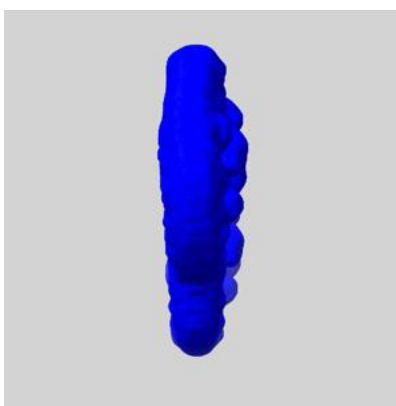
A mask typically either:

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

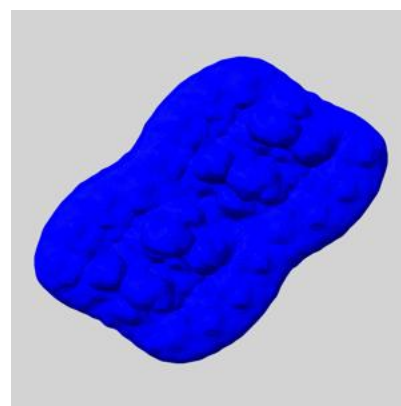
6.6.1 emd_33933_msk_1.map [i](#)



X



Y

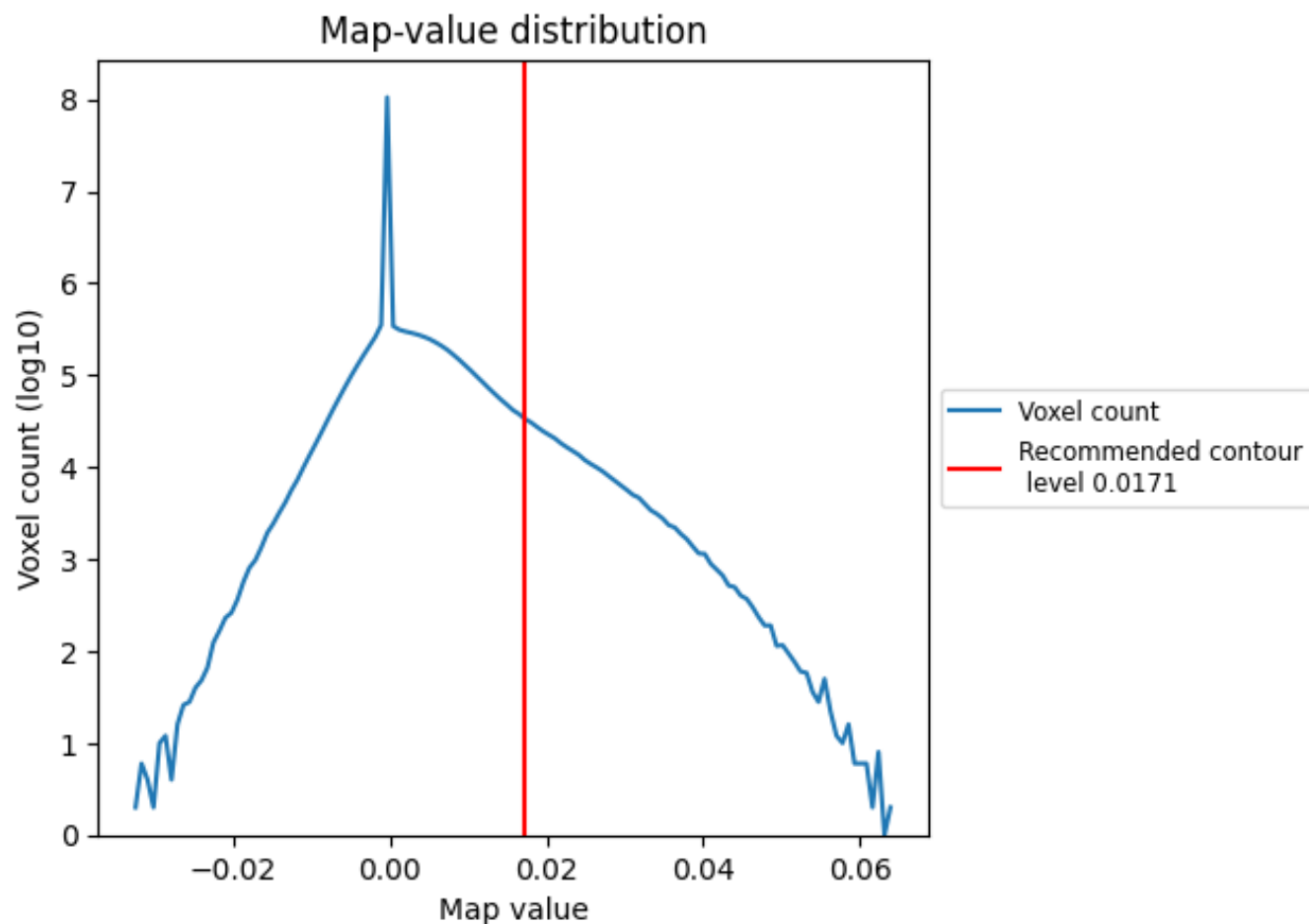


Z

7 Map analysis [i](#)

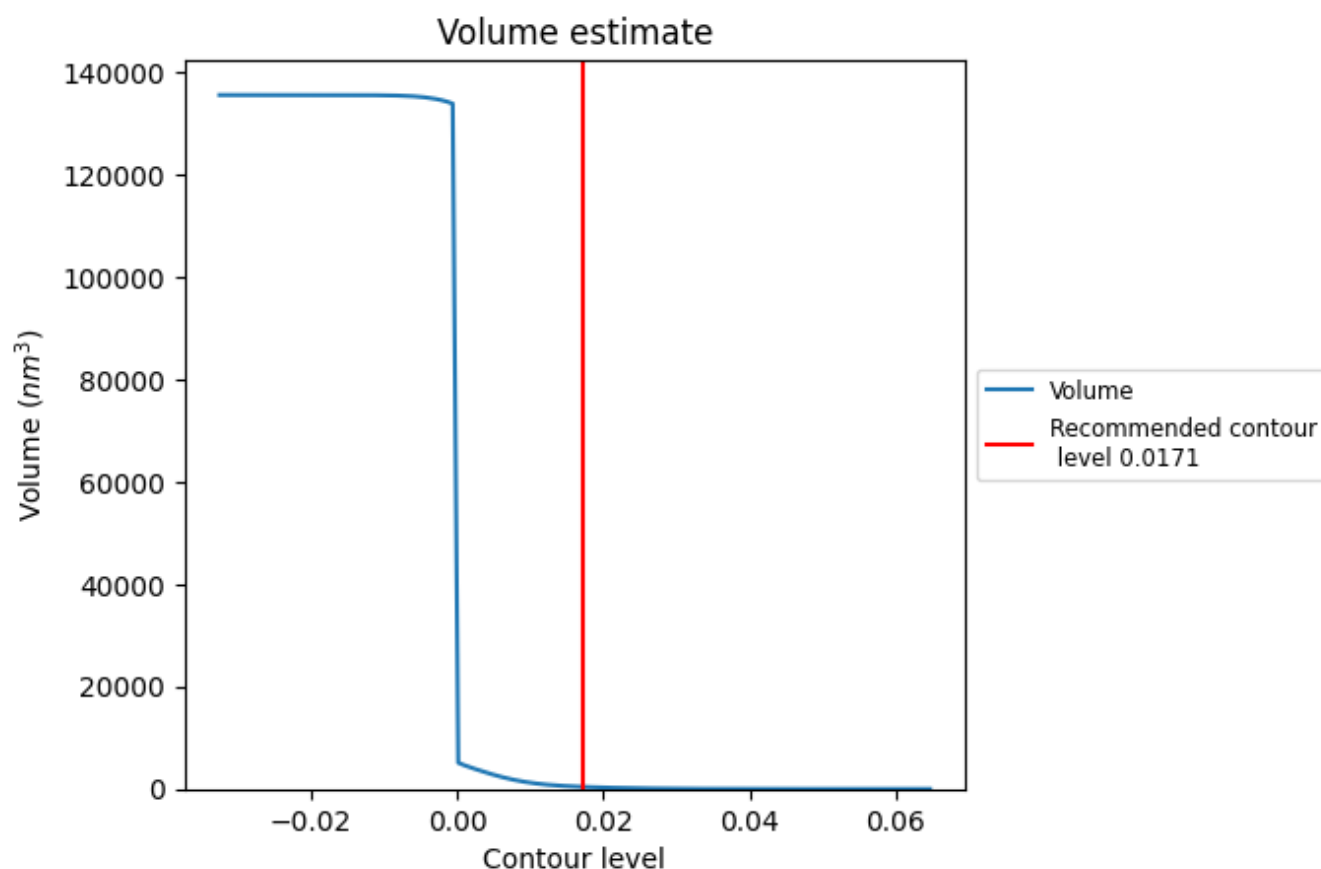
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

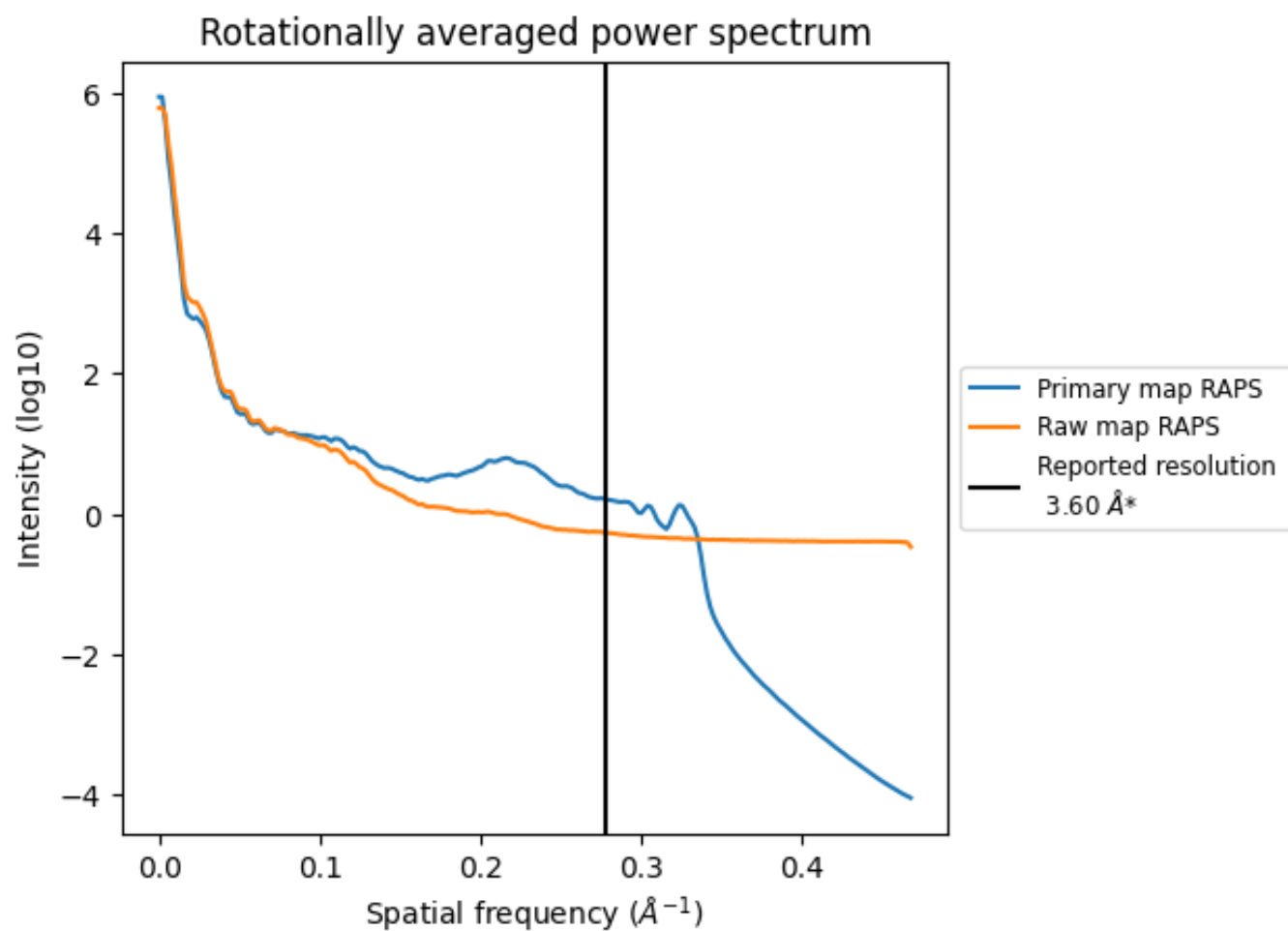
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

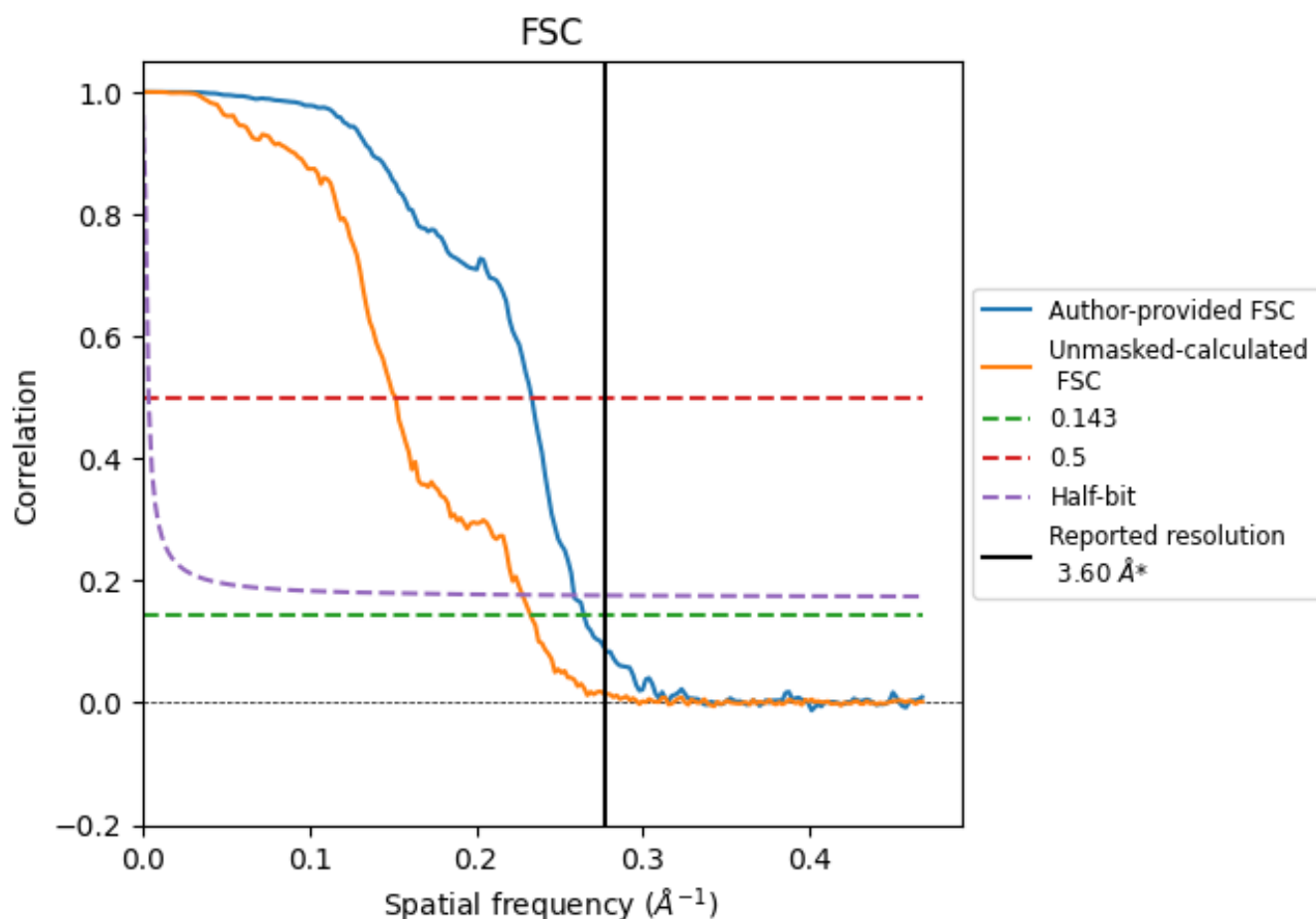


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

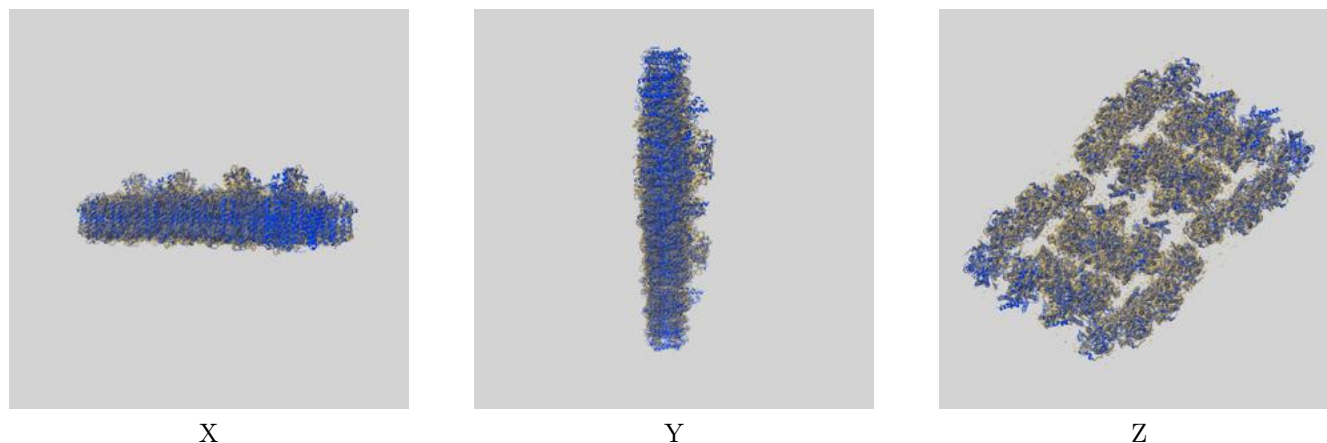
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.78	4.28	3.87
Unmasked-calculated*	4.30	6.59	4.39

*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 [i](#)

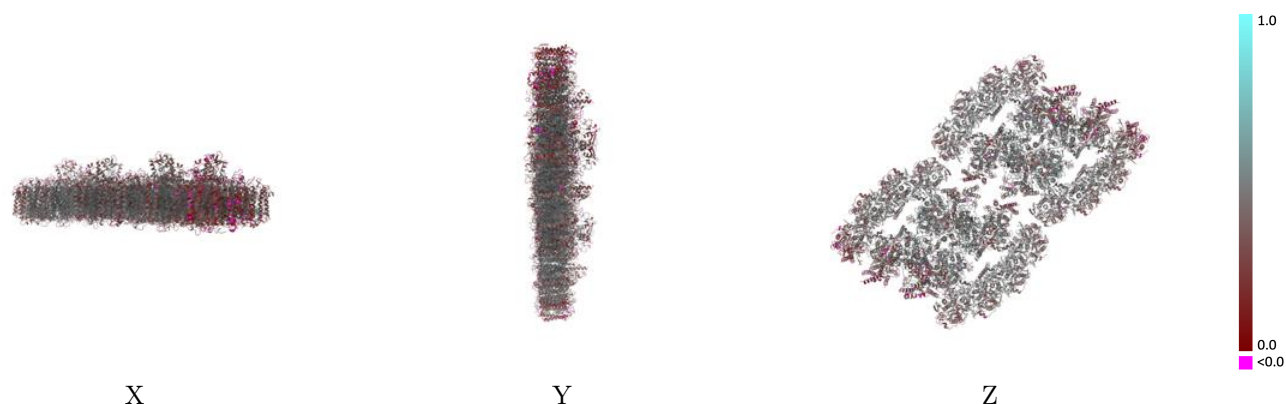
This section contains information regarding the fit between EMDB map EMD-33933 and PDB model 7YMM. Per-residue inclusion information can be found in section 3 on page 59.

9.1 Map-model overlay [i](#)



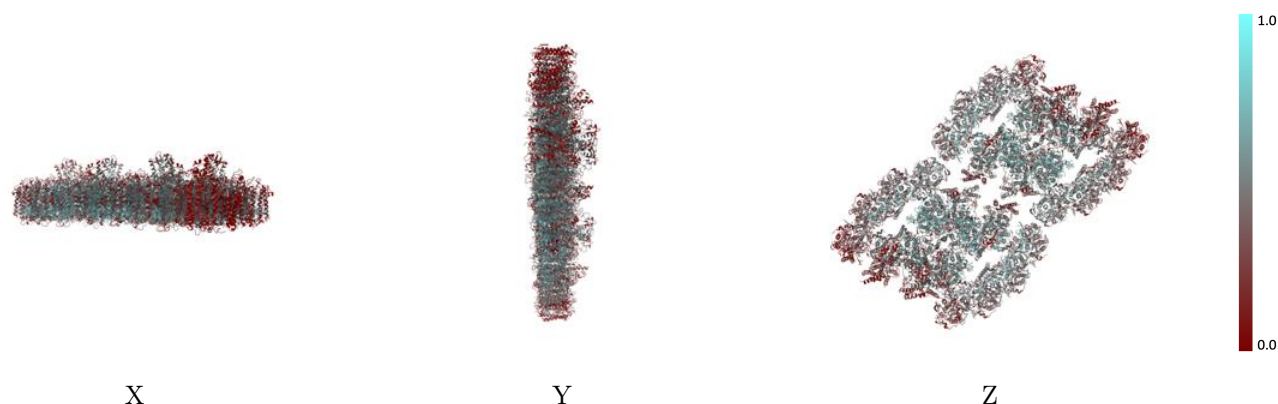
The images above show the 3D surface view of the map at the recommended contour level 0.0171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



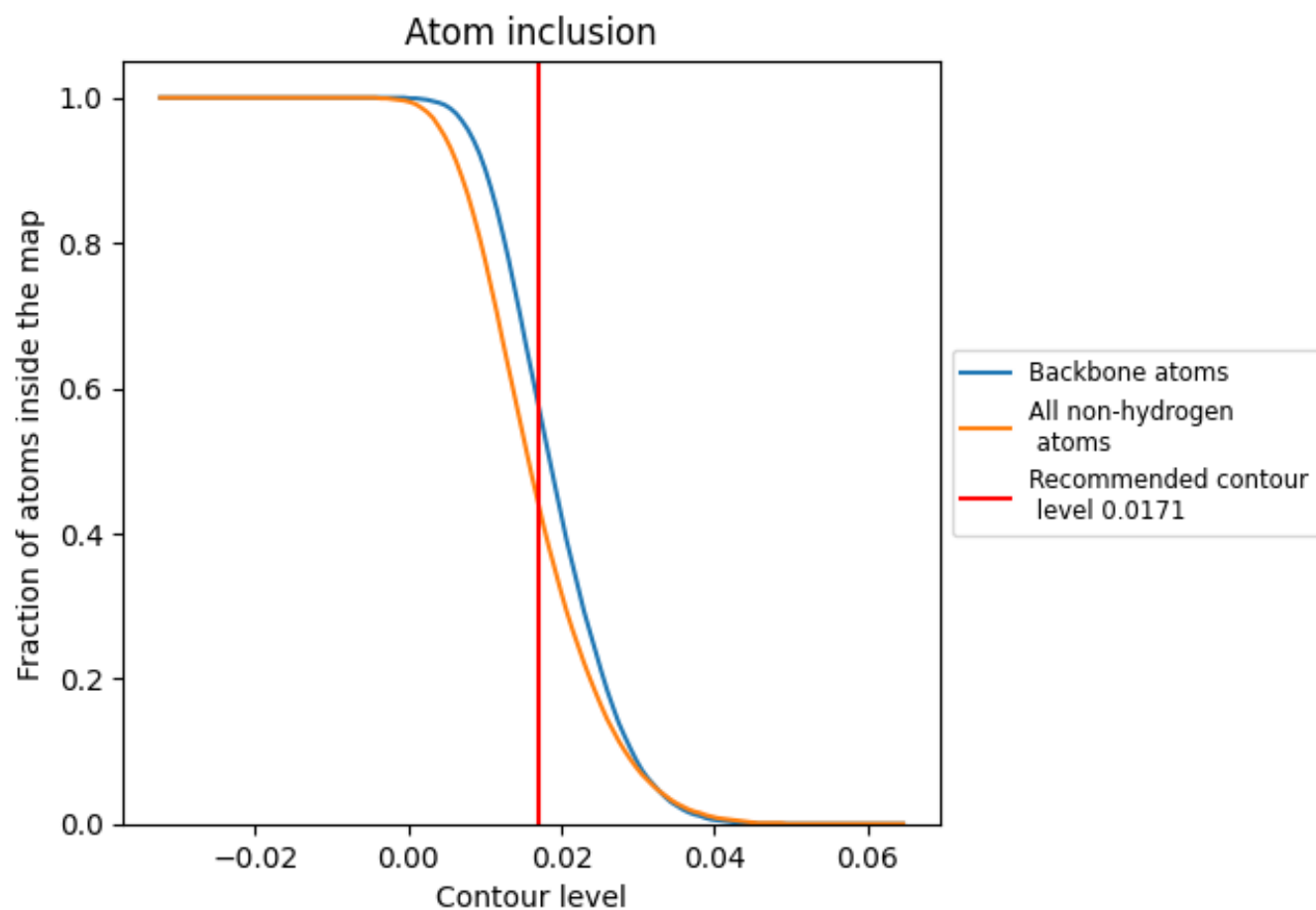
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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

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
3I	 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
4I	 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