



wwPDB EM Validation Summary Report ⓘ

Aug 26, 2024 – 01:24 PM JST

PDB ID : 7YMM
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:

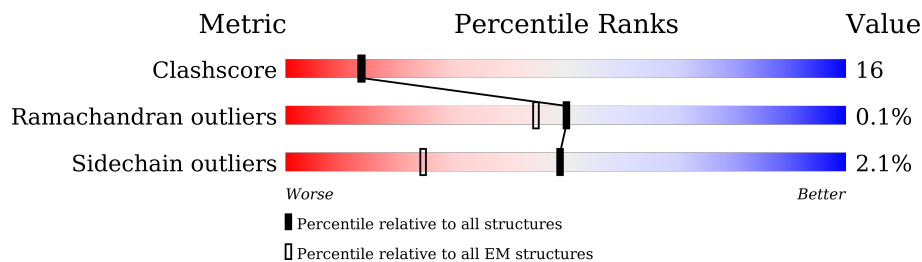
EMDB validation analysis : 0.0.1.dev112
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	2A	360	
1	3A	360	
1	4A	360	
2	1B	506	
2	2B	506	
2	3B	506	
2	4B	506	

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Mol	Chain	Length	Quality of chain
3	1C	490	53% 68% 17% 14%
3	2C	490	25% 69% 16% 14%
3	3C	490	25% 68% 17% 14%
3	4C	490	53% 69% 16% 14%
4	1D	351	30% 72% 19% 8%
4	2D	351	13% 72% 20% 8%
4	3D	351	13% 73% 19% 8%
4	4D	351	30% 72% 20% 8%
5	1E	83	73% 60% 17% 22%
5	2E	83	52% 63% 16% 22%
5	3E	83	52% 60% 17% 22%
5	4E	83	73% 60% 17% 22%
6	1F	99	28% 28% 70%
6	2F	99	14% 27% 70%
6	3F	99	14% 27% 70%
6	4F	99	28% 27% 70%
7	1H	71	56% 82% 14%
7	2H	71	25% 82% 14%
7	3H	71	25% 82% 14%
7	4H	71	56% 82% 14%
8	1I	34	35% 82% 18%
8	2I	34	9% 79% 21%
8	3I	34	9% 76% 24%
8	4I	34	35% 79% 21%
9	1K	45	82% 47% 33% 18%

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Mol	Chain	Length	Quality of chain
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% 51% 8% 41%
14	2Y	39	59% 44% 15% 41%
14	3Y	39	59% 49% 10% 41%
14	4Y	39	59% 46% 13% 41%
15	1Z	62	95% 84% 11% 5%
15	2Z	62	85% 82% 13% 5%

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Mol	Chain	Length	Quality of chain
15	3Z	62	85% 82% 13% 5%
15	4Z	62	95% 84% 11% 5%
16	12	352	57% 70% 29%
16	22	352	33% 70% 29%
16	32	352	32% 69% 30%
16	42	352	58% 70% 29%
17	1G	41	61% 93% 7%
17	2G	41	51% 93% 7%
17	3G	41	51% 93% 7%
17	4G	41	63% 93% 7%
18	11	356	83% 63% 30% 8%
18	21	356	43% 62% 30% 8%
18	31	356	43% 62% 30% 8%
18	41	356	83% 61% 31% 8%
19	13	349	42% 75% 23% ..
19	23	349	38% 75% 23% ..
19	33	349	38% 75% 23% ..
19	43	349	42% 75% 23% ..
20	14	353	71% 69% 25% 6%
20	24	353	36% 69% 25% 6%
20	34	353	37% 69% 25% 6%
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	-	-	-
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	-	-	-

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

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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	12	520	-	-	X	-
32	ZEX	13	522	-	-	X	-
32	ZEX	13	525	-	-	X	-
32	ZEX	14	403	-	-	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
			Total	C	N	O	S		
1	1A	284	2209	1450	361	381	17	0	0
1	2A	284	2209	1450	361	381	17	0	0
1	3A	284	2209	1450	361	381	17	0	0
1	4A	284	2209	1450	361	381	17	0	0

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

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

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

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

- 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		

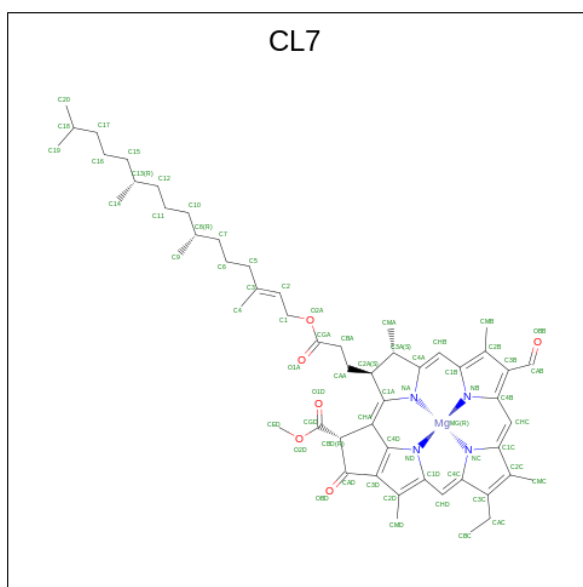
- Molecule 19 is a protein called High light inducible protein.

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 (three-letter code: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	21	1	60	49	1	4	6	0
21	21	1	60	49	1	4	6	0
21	21	1	65	54	1	4	6	0
21	21	1	45	34	1	4	6	0
21	21	1	62	51	1	4	6	0
21	21	1	41	32	1	4	4	0
21	21	1	65	54	1	4	6	0
21	21	1	45	34	1	4	6	0
21	21	1	65	54	1	4	6	0
21	21	1	45	34	1	4	6	0
21	21	1	45	34	1	4	6	0
21	21	1	41	32	1	4	4	0
21	21	1	41	32	1	4	4	0
21	21	1	41	32	1	4	4	0
21	21	1	41	32	1	4	4	0
21	21	1	55	44	1	4	6	0
21	21	1	65	54	1	4	6	0
21	21	1	45	34	1	4	6	0
21	21	1	45	34	1	4	6	0
21	23	1	65	54	1	4	6	0
21	23	1	58	47	1	4	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
			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
			Total	C	Mg	N	O	
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	
			Total	C	Mg	N		O
21	3B	1	65	54	1	4	6	0
21	3B	1	65	54	1	4	6	0
21	3B	1	65	54	1	4	6	0
21	3B	1	55	44	1	4	6	0
21	3B	1	60	49	1	4	6	0
21	3B	1	50	39	1	4	6	0
21	3B	1	45	34	1	4	6	0
21	3B	1	45	34	1	4	6	0
21	3C	1	65	54	1	4	6	0
21	3C	1	60	49	1	4	6	0
21	3C	1	65	54	1	4	6	0
21	3C	1	55	44	1	4	6	0
21	3C	1	65	54	1	4	6	0
21	3C	1	60	49	1	4	6	0
21	3C	1	65	54	1	4	6	0
21	3C	1	65	54	1	4	6	0
21	3C	1	65	54	1	4	6	0
21	3C	1	42	33	1	4	4	0
21	3C	1	41	32	1	4	4	0
21	3C	1	45	34	1	4	6	0

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

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

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Mol	Chain	Residues	Atoms				AltConf	
21	33	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			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
			Total	C	Mg	N	O	
21	34	1	45	34	1	4	6	0
21	34	1	60	49	1	4	6	0
21	34	1	45	34	1	4	6	0
21	34	1	65	54	1	4	6	0
21	34	1	65	54	1	4	6	0
21	34	1	60	49	1	4	6	0
21	34	1	53	42	1	4	6	0
21	34	1	45	34	1	4	6	0
21	34	1	41	32	1	4	4	0
21	34	1	42	33	1	4	4	0
21	4A	1	65	54	1	4	6	0
21	4A	1	55	44	1	4	6	0
21	4A	1	65	54	1	4	6	0
21	4B	1	41	32	1	4	4	0
21	4B	1	60	49	1	4	6	0
21	4B	1	65	54	1	4	6	0
21	4B	1	65	54	1	4	6	0
21	4B	1	65	54	1	4	6	0
21	4B	1	55	44	1	4	6	0
21	4B	1	60	49	1	4	6	0
21	4B	1	65	54	1	4	6	0

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

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

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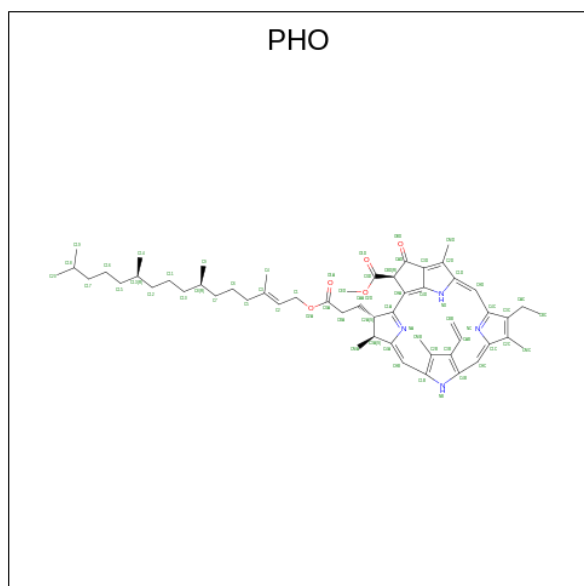
Mol	Chain	Residues	Atoms					AltConf
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	43	1	Total	C	Mg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

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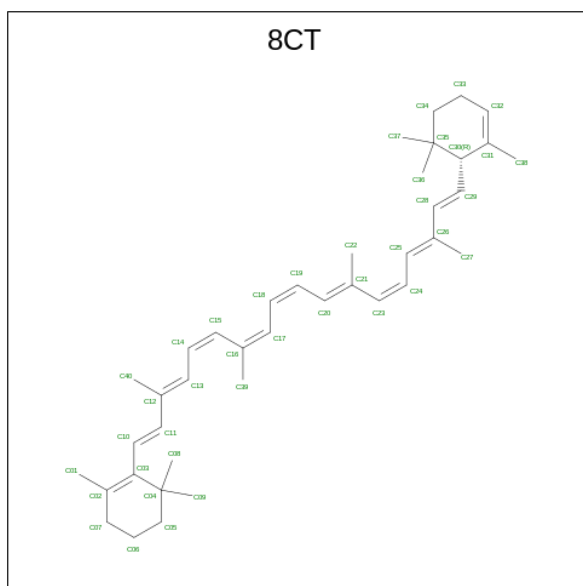
Mol	Chain	Residues	Atoms					AltConf
21	44	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg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

- Molecule 22 is PHEOPHYTIN A (three-letter code: 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 (three-letter code: 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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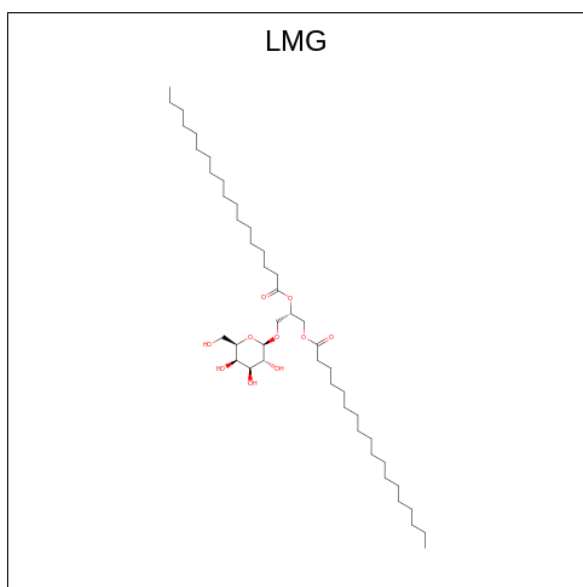
Mol	Chain	Residues	Atoms	AltConf
23	1B	1	Total C 40 40	0
23	1B	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1D	1	Total C 40 40	0
23	1K	1	Total C 40 40	0
23	14	1	Total C 40 40	0
23	2A	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	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 (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



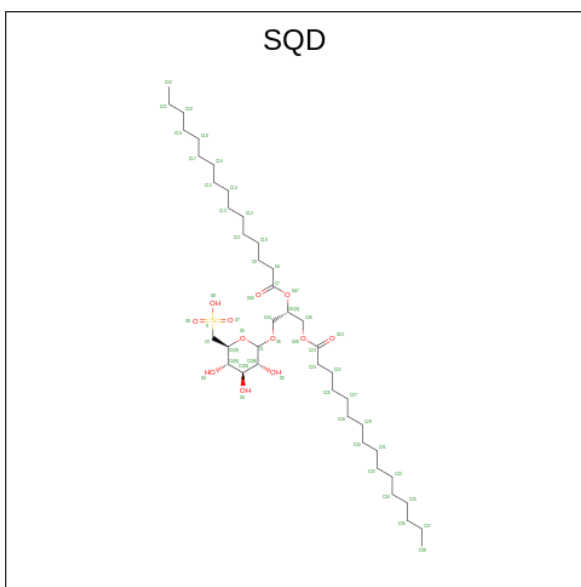
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	1A	1	50	40	10	0
24	1B	1	51	41	10	0
24	1D	1	33	23	10	0
24	11	1	51	41	10	0
24	2A	1	50	40	10	0
24	2B	1	51	41	10	0
24	2D	1	33	23	10	0
24	21	1	51	41	10	0
24	3A	1	50	40	10	0
24	3B	1	51	41	10	0
24	3D	1	33	23	10	0
24	31	1	51	41	10	0
24	4A	1	50	40	10	0
24	4B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

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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 (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



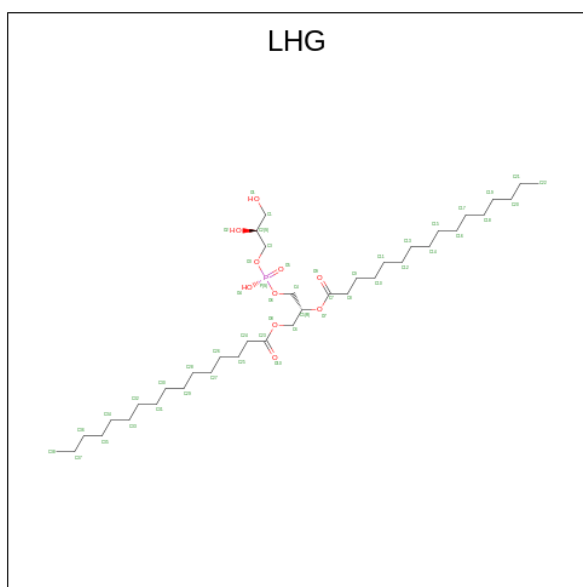
Mol	Chain	Residues	Atoms				AltConf
25	1A	1	Total	C	O	S	0
			34	21	12	1	
25	1B	1	Total	C	O	S	0
			54	41	12	1	
25	12	1	Total	C	O	S	0
			50	37	12	1	
25	12	1	Total	C	O	S	0
			41	28	12	1	
25	11	1	Total	C	O	S	0
			32	19	12	1	
25	13	1	Total	C	O	S	0
			46	33	12	1	
25	13	1	Total	C	O	S	0
			50	37	12	1	
25	2A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

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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



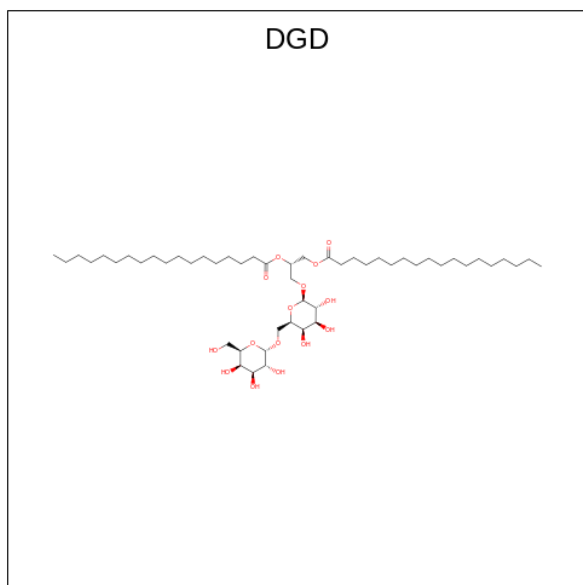
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
26	1A	1	46	35	10	1	0
26	1B	1	45	34	10	1	0
26	1B	1	49	38	10	1	0
26	1D	1	49	38	10	1	0
26	13	1	36	25	10	1	0
26	14	1	49	38	10	1	0
26	2A	1	46	35	10	1	0
26	2B	1	45	34	10	1	0
26	2B	1	49	38	10	1	0
26	2D	1	49	38	10	1	0
26	23	1	36	25	10	1	0
26	24	1	49	38	10	1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

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

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



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

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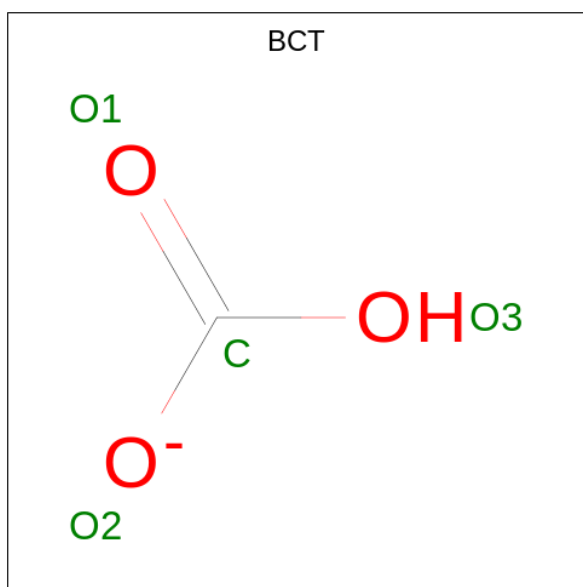
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Mol	Chain	Residues	Atoms			AltConf
27	1C	1	Total	C	O	0
			62	47	15	
27	2B	1	Total	C	O	0
			62	47	15	
27	2C	1	Total	C	O	0
			62	47	15	
27	3B	1	Total	C	O	0
			62	47	15	
27	3C	1	Total	C	O	0
			62	47	15	
27	4B	1	Total	C	O	0
			62	47	15	
27	4C	1	Total	C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

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

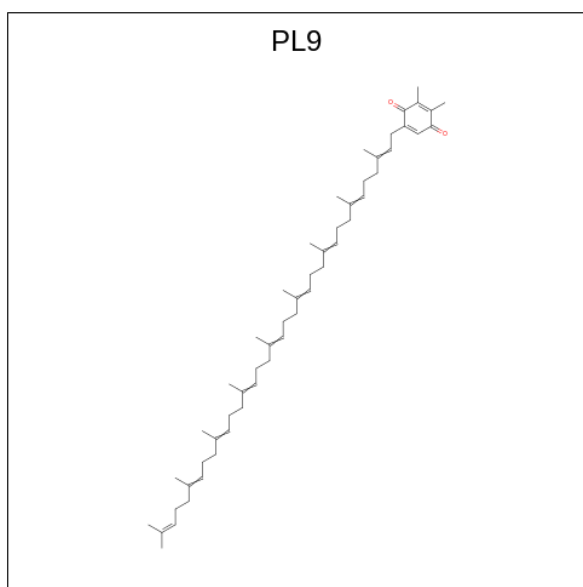
Mol	Chain	Residues	Atoms		AltConf
28	1D	1	Total	Fe	0
			1	1	
28	2D	1	Total	Fe	0
			1	1	
28	3D	1	Total	Fe	0
			1	1	
28	4D	1	Total	Fe	0
			1	1	

- Molecule 29 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃) (labeled as "Ligand of Interest" by depositor).



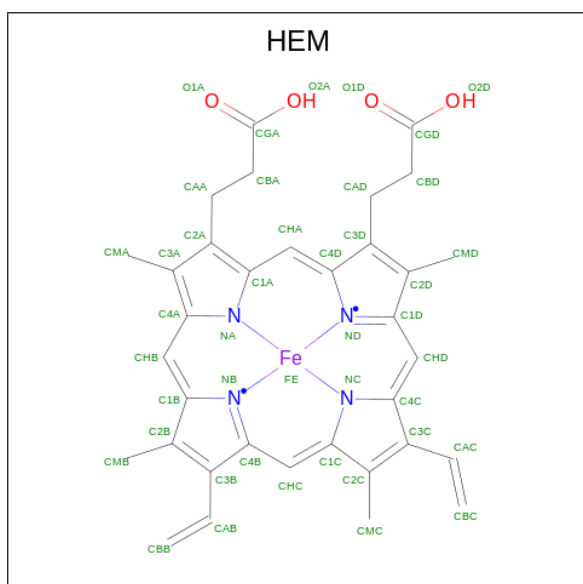
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	1D	1	4	1	3	0
29	2D	1	4	1	3	0
29	3D	1	4	1	3	0
29	4D	1	4	1	3	0

- 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 (three-letter code: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



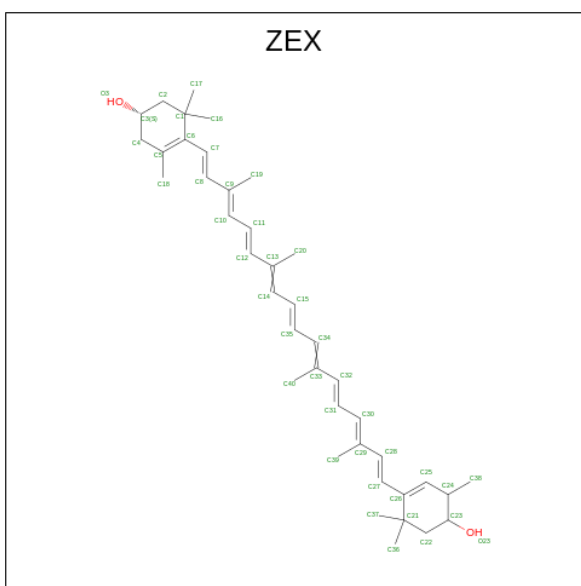
Mol	Chain	Residues	Atoms			AltConf
30	1D	1	Total	C	O	0
			55	53	2	
30	2D	1	Total	C	O	0
			55	53	2	
30	3D	1	Total	C	O	0
			55	53	2	
30	4D	1	Total	C	O	0
			55	53	2	

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



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

- Molecule 32 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: 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
			Total	C	O	
32	13	1	42	40	2	0
32	13	1	42	40	2	0
32	13	1	42	40	2	0
32	13	1	42	40	2	0
32	14	1	42	40	2	0
32	14	1	42	40	2	0
32	14	1	42	40	2	0
32	14	1	42	40	2	0
32	22	1	42	40	2	0
32	22	1	42	40	2	0
32	22	1	42	40	2	0
32	22	1	42	40	2	0
32	21	1	42	40	2	0
32	21	1	42	40	2	0
32	23	1	42	40	2	0
32	23	1	42	40	2	0
32	23	1	42	40	2	0
32	23	1	42	40	2	0
32	24	1	42	40	2	0
32	24	1	42	40	2	0
32	24	1	42	40	2	0

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

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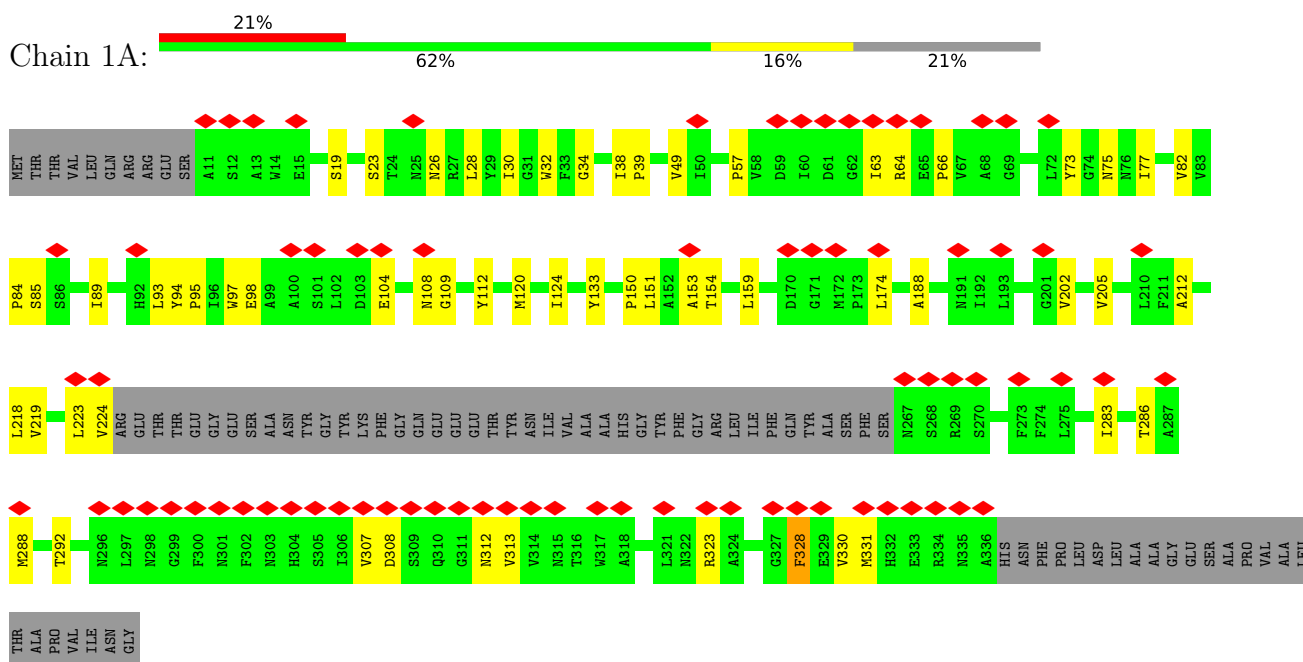
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	43	1	42	40	2	0
32	43	1	42	40	2	0
32	43	1	42	40	2	0
32	43	1	42	40	2	0
32	44	1	42	40	2	0
32	44	1	42	40	2	0
32	44	1	42	40	2	0
32	44	1	42	40	2	0

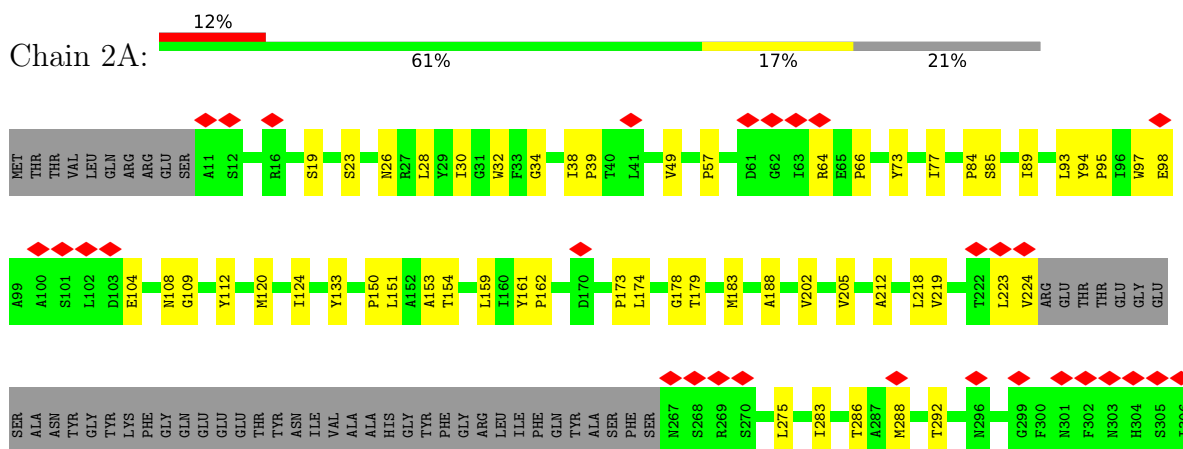
3 Residue-property plots [i](#)

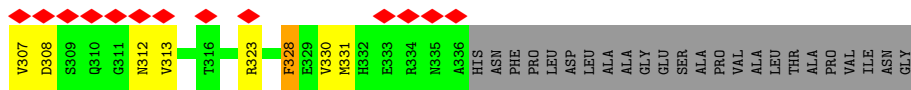
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem II protein D1 2

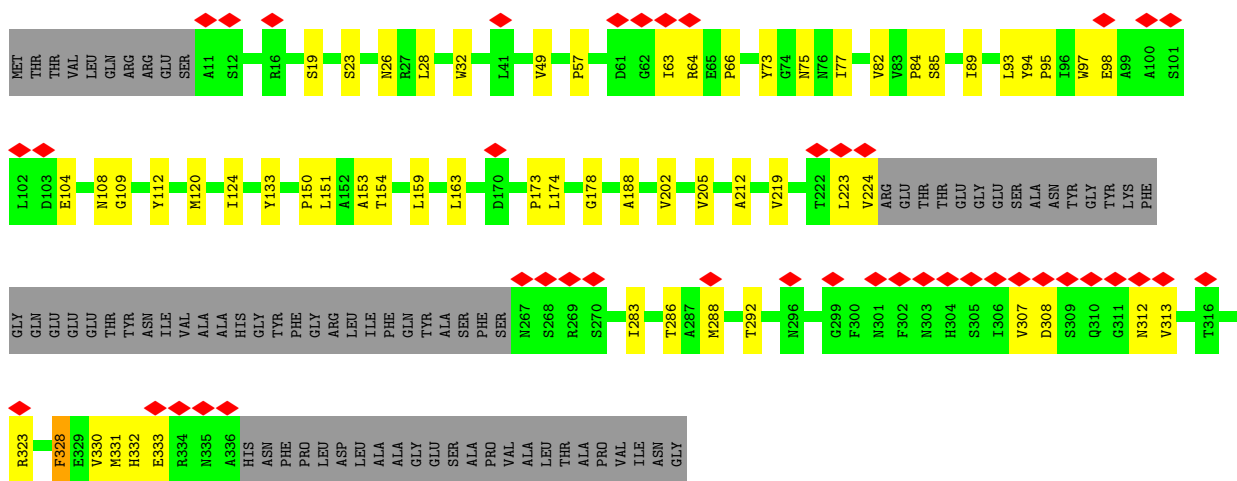


- Molecule 1: Photosystem II protein D1 2

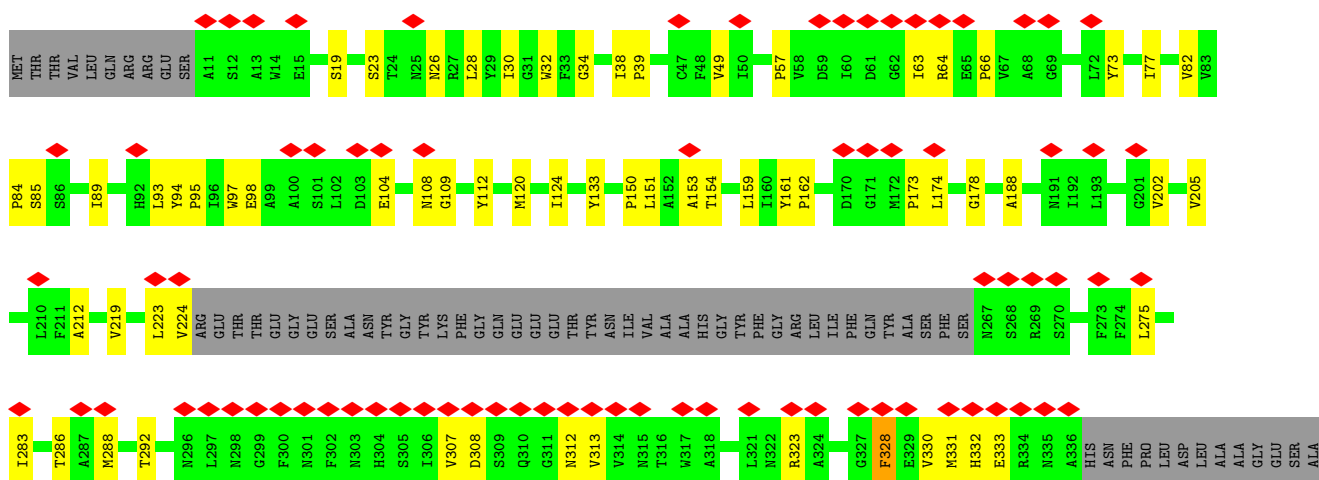




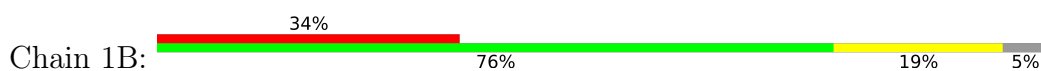
• Molecule 1: Photosystem II protein D1 2

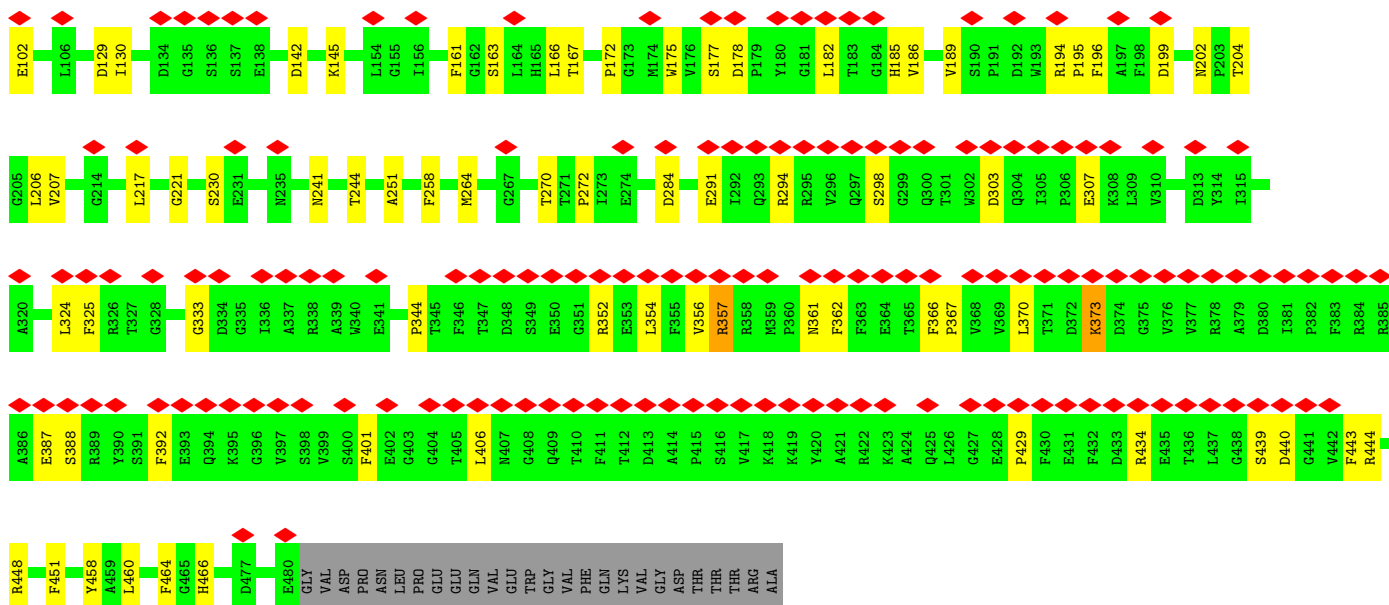


• Molecule 1: Photosystem II protein D1 2

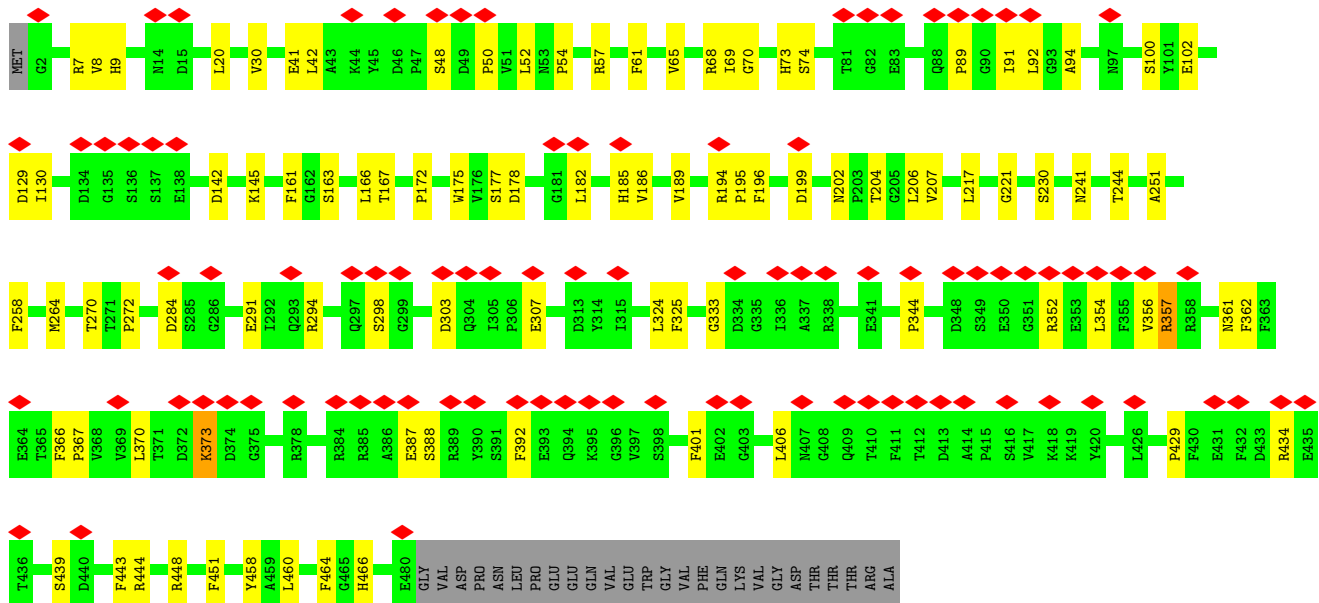
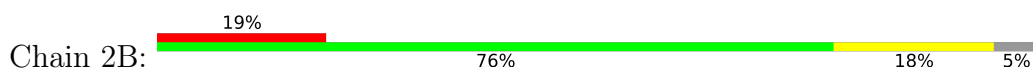


• Molecule 2: Photosystem II CP47 reaction center protein

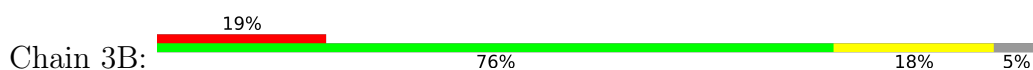


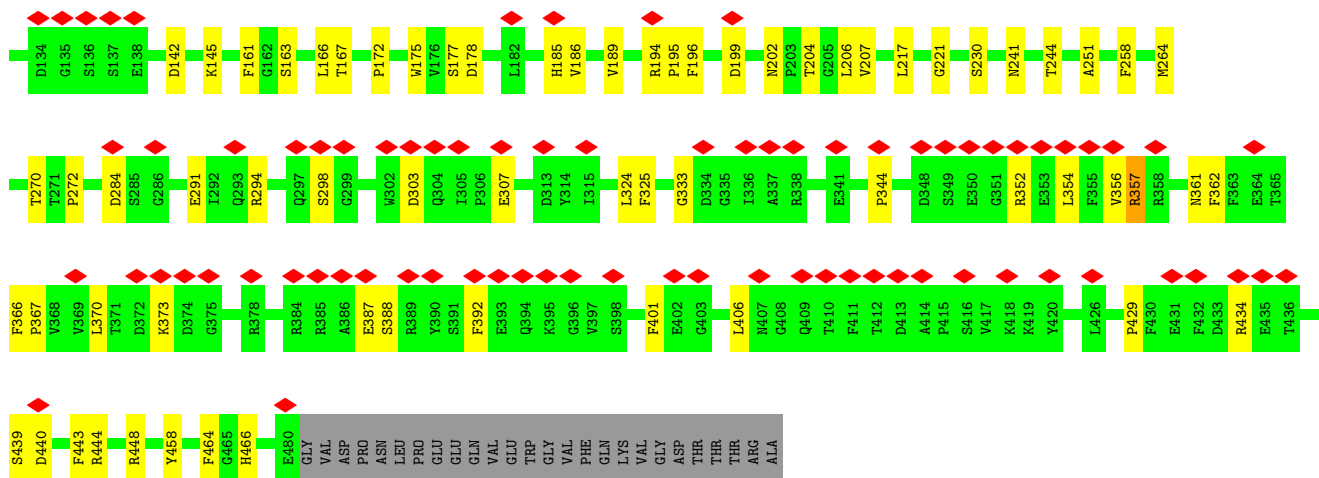


• Molecule 2: Photosystem II CP47 reaction center protein

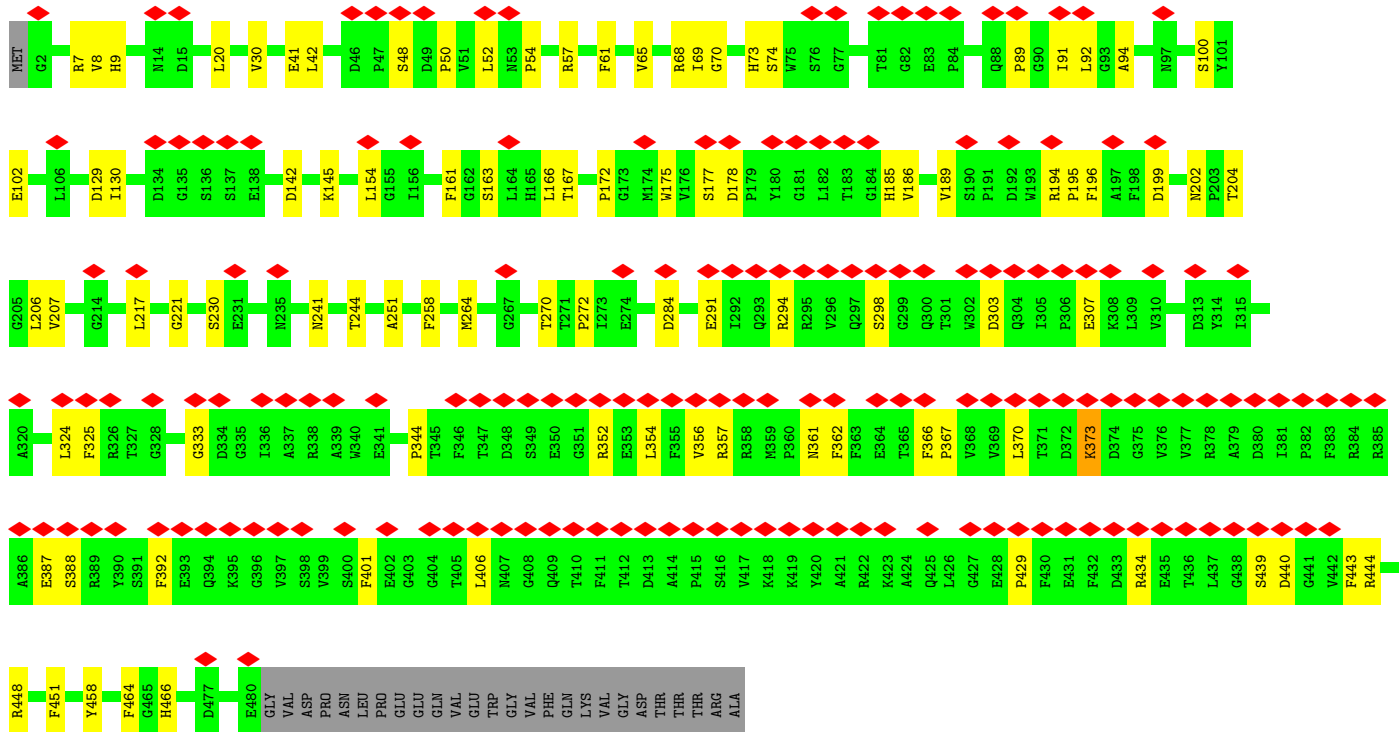
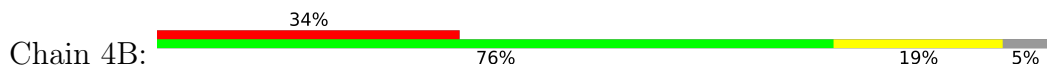


• Molecule 2: Photosystem II CP47 reaction center protein

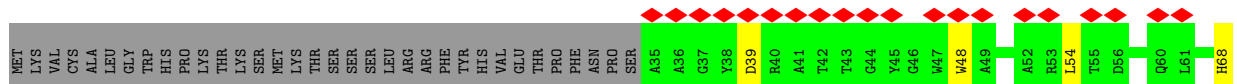


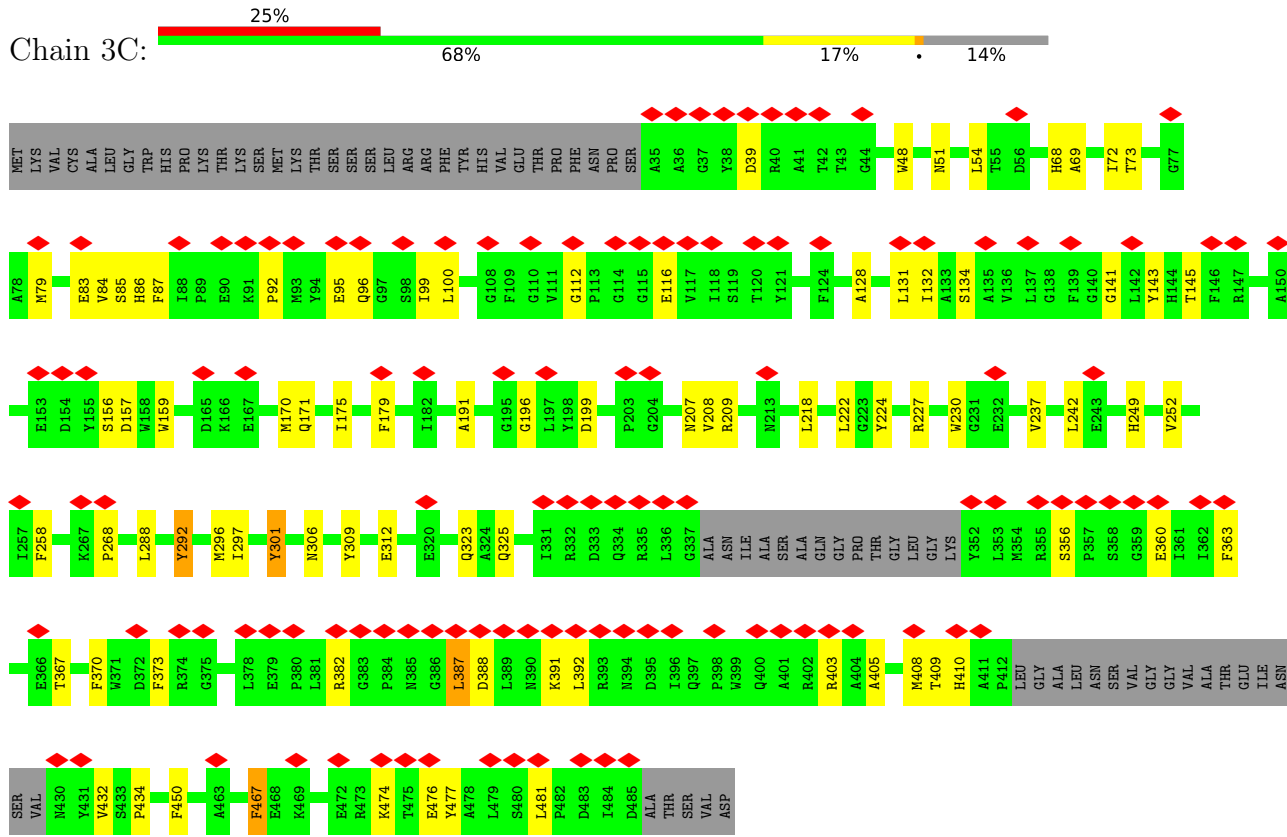


● Molecule 2: Photosystem II CP47 reaction center protein

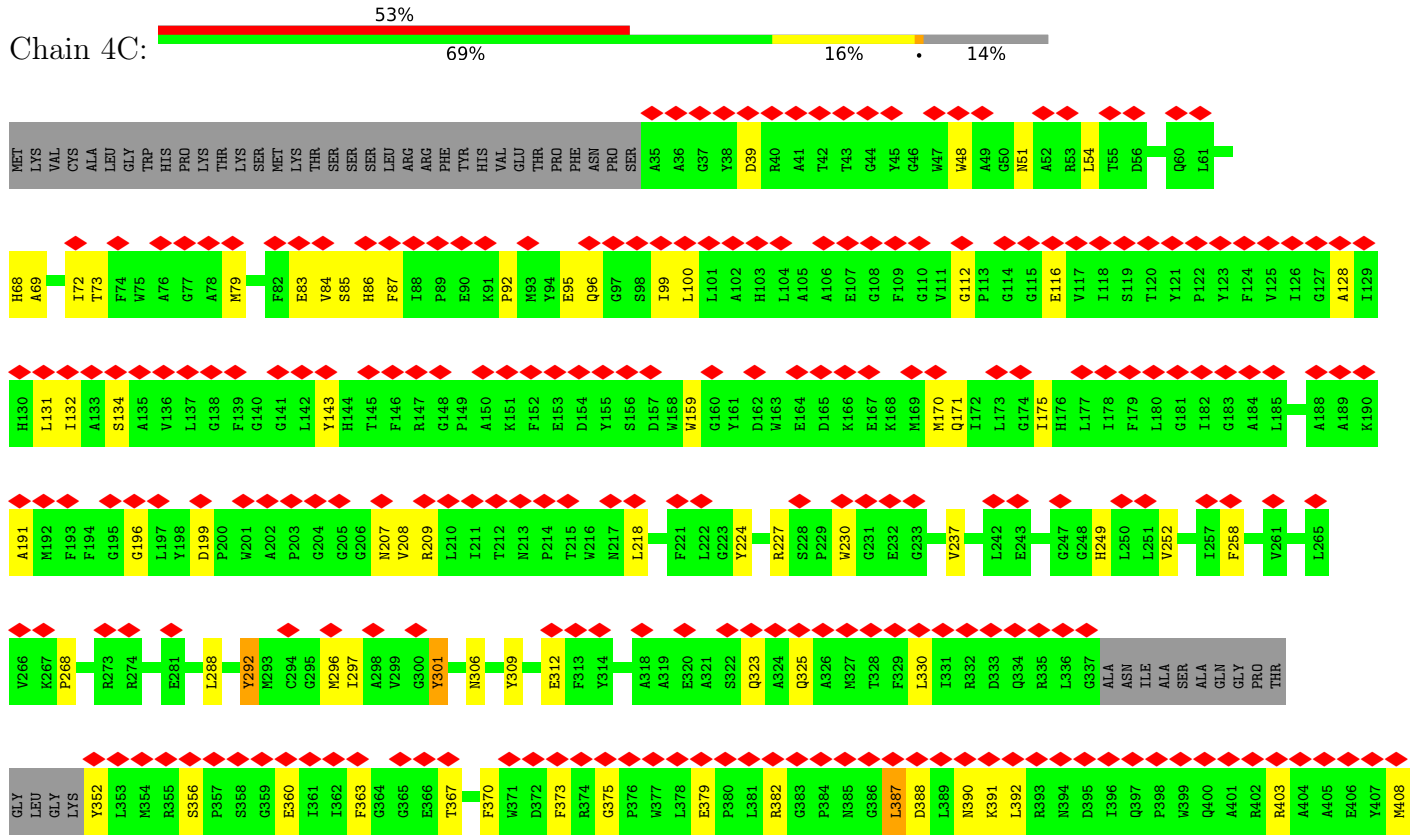


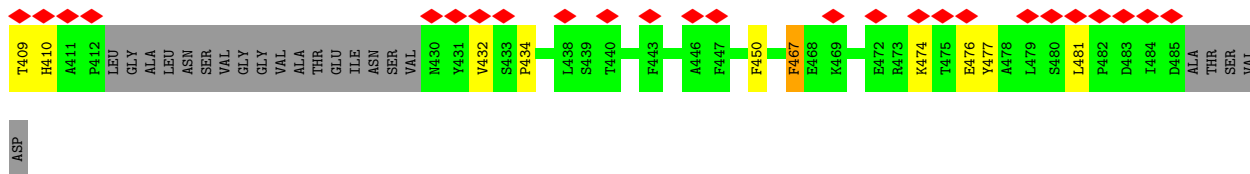
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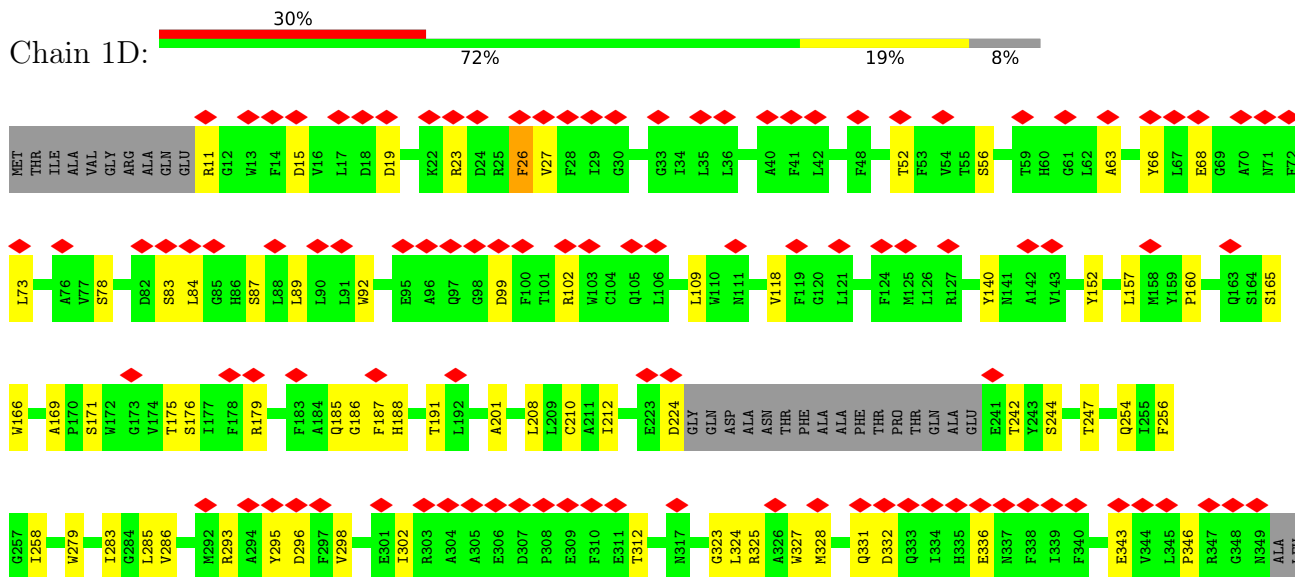


• Molecule 3: Photosystem II CP43 reaction center protein

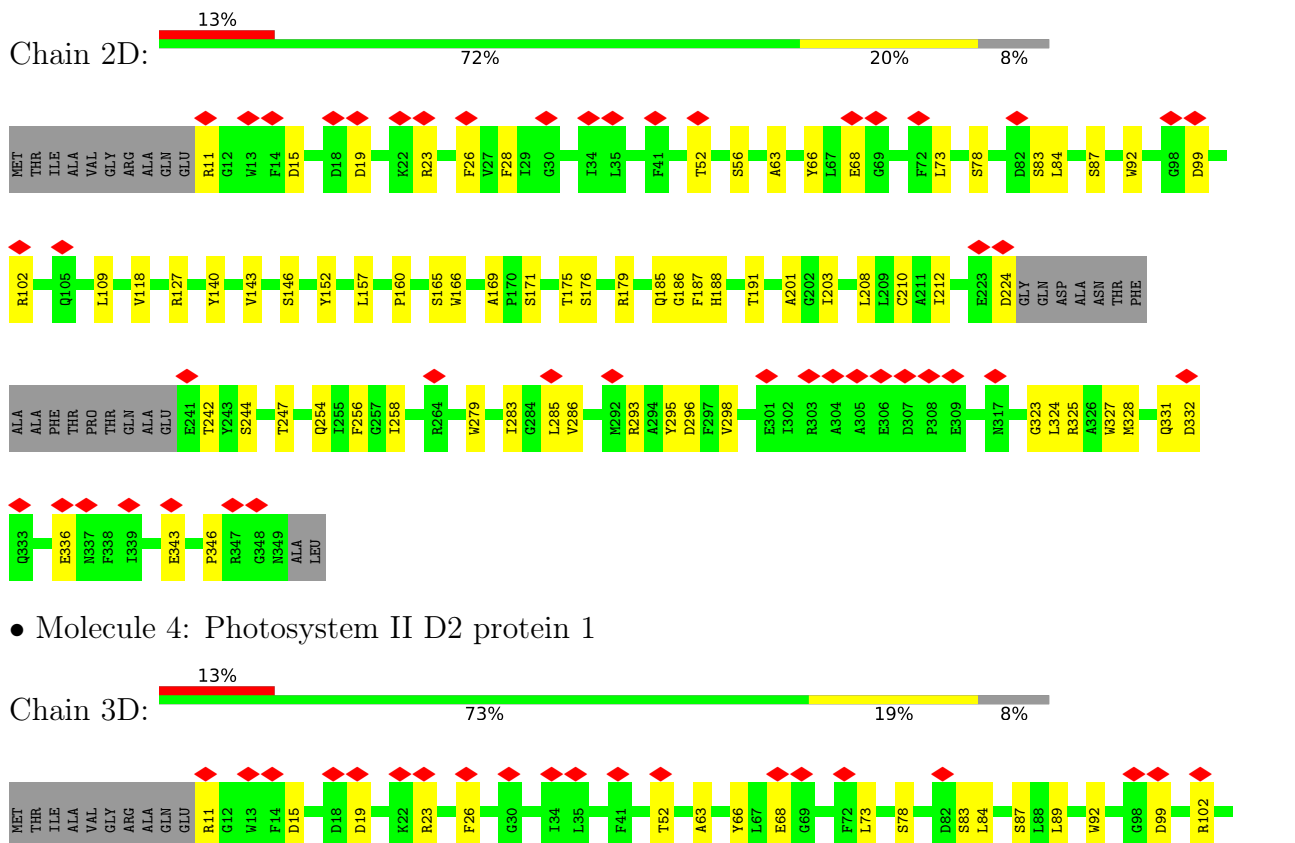


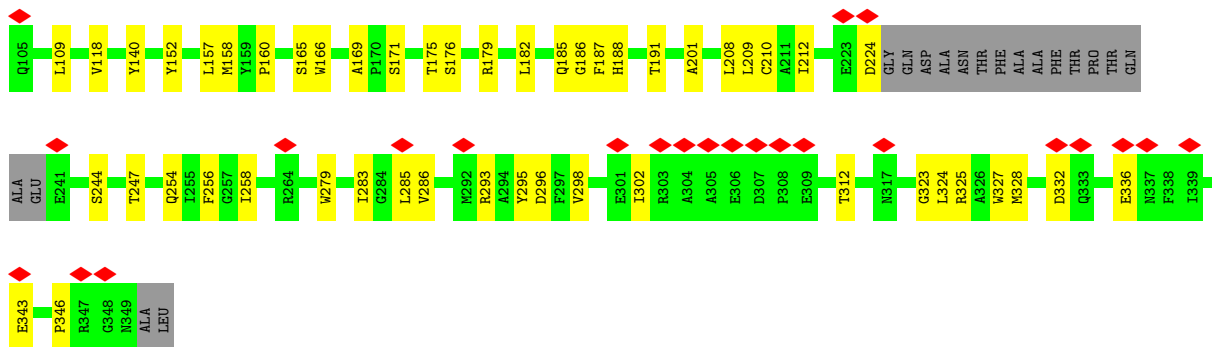


• Molecule 4: Photosystem II D2 protein 1

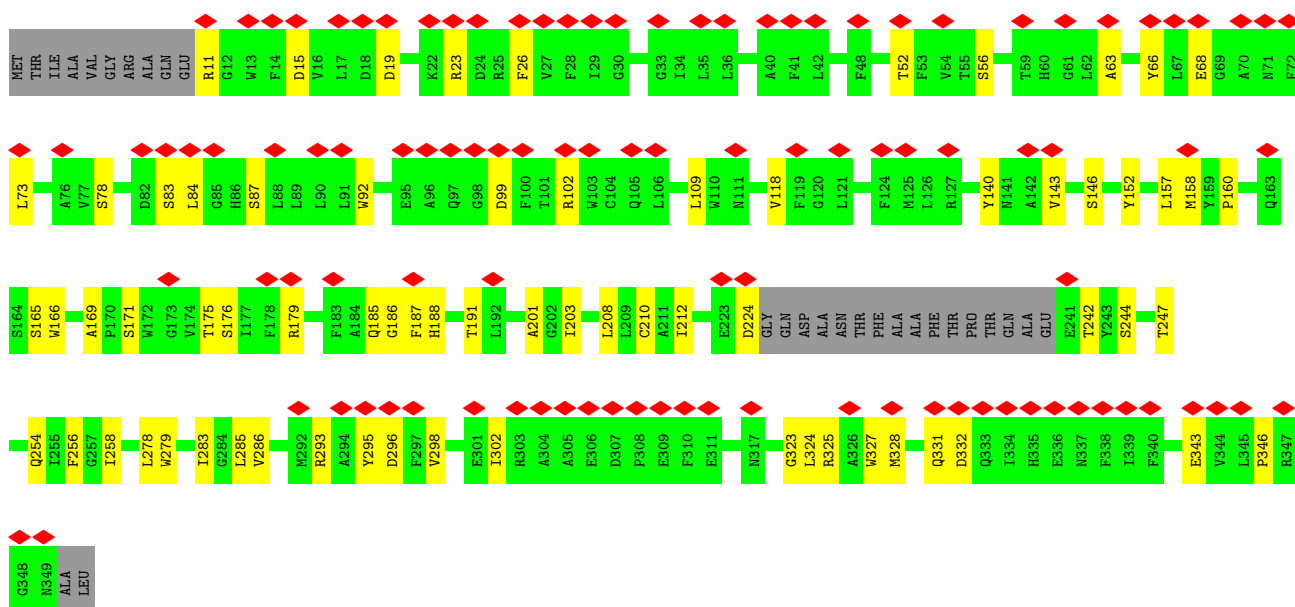
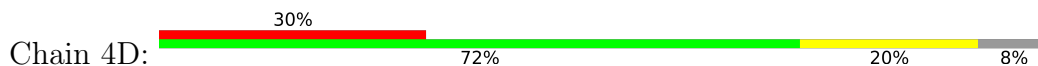


• Molecule 4: Photosystem II D2 protein 1

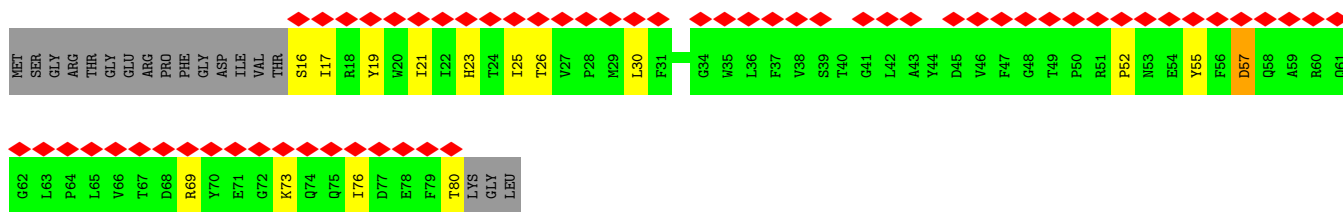
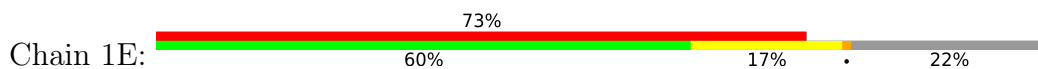




• Molecule 4: Photosystem II D2 protein 1

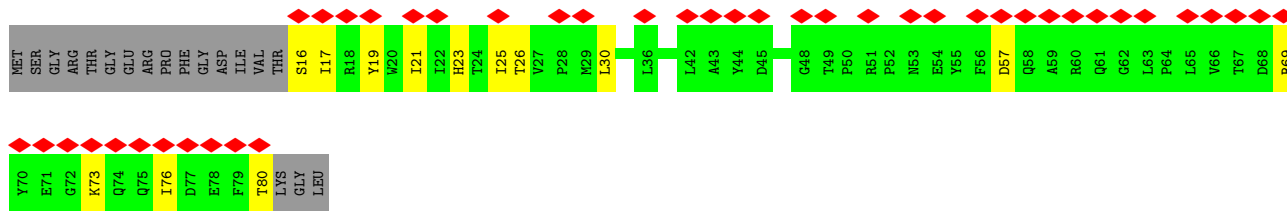


• Molecule 5: Cytochrome b559 subunit alpha

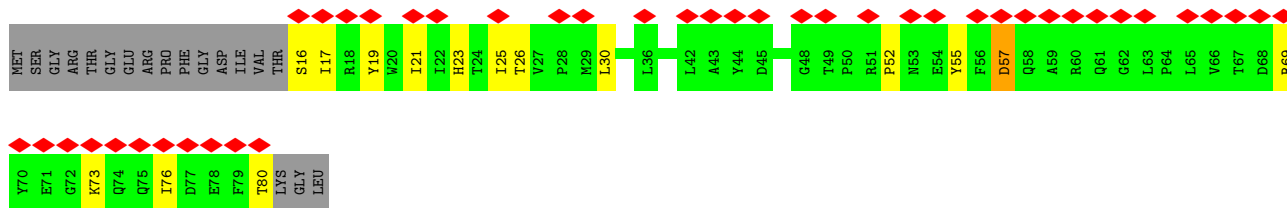


• Molecule 5: Cytochrome b559 subunit alpha

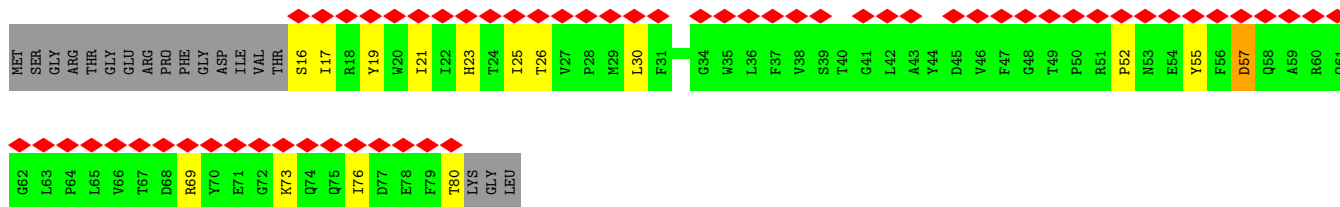
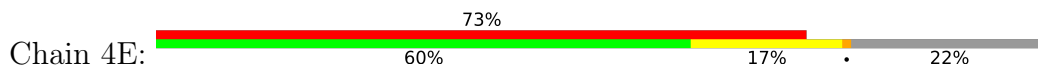




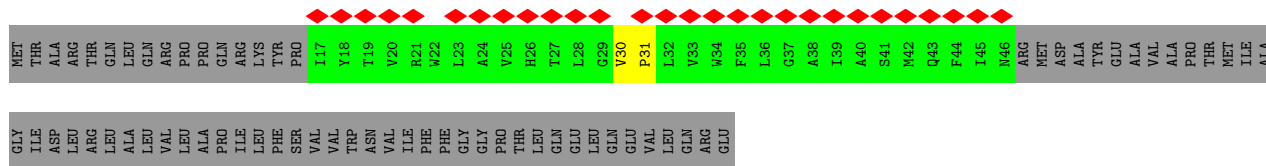
• Molecule 5: Cytochrome b559 subunit alpha



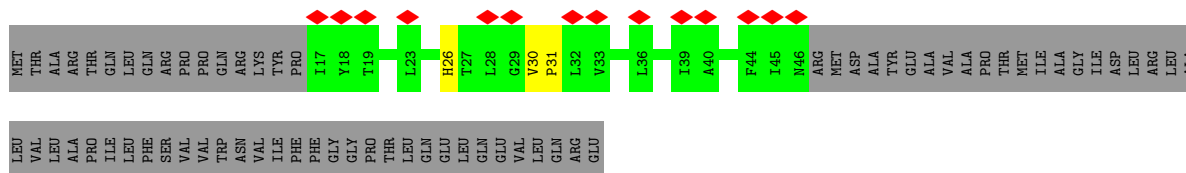
• Molecule 5: Cytochrome b559 subunit alpha



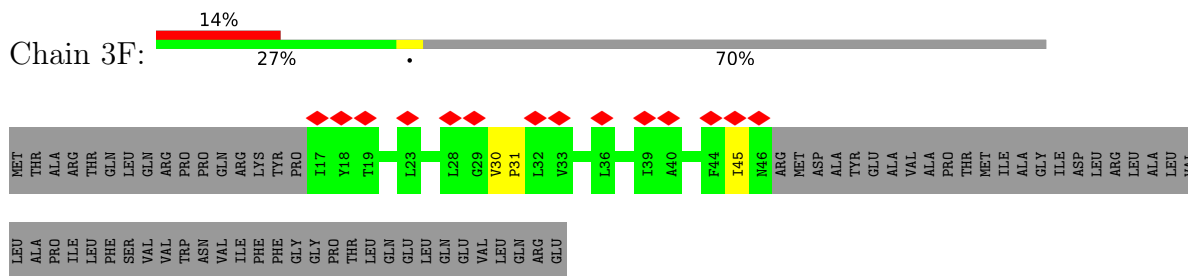
• Molecule 6: Photosystem II protein Y



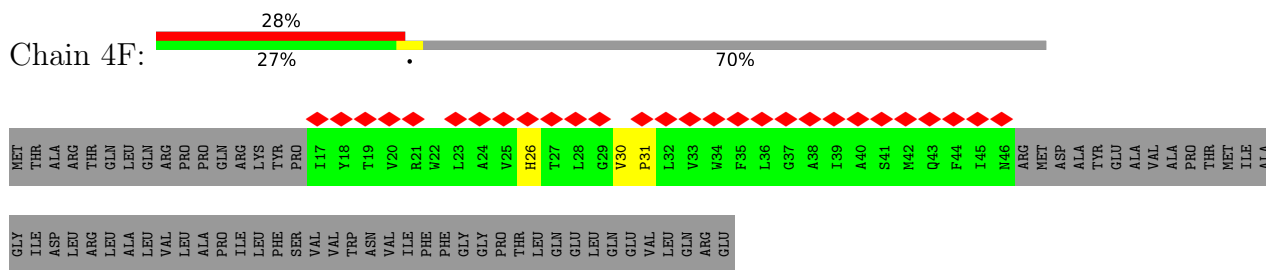
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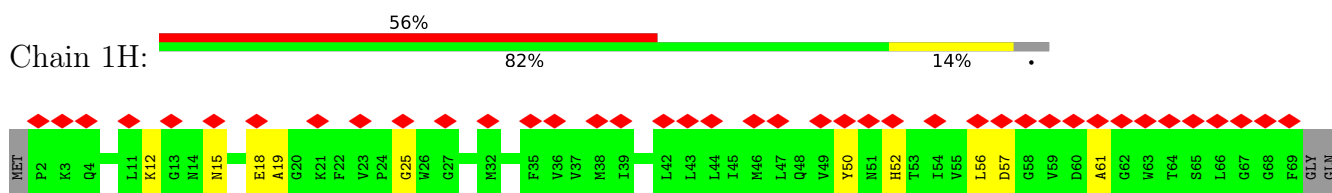
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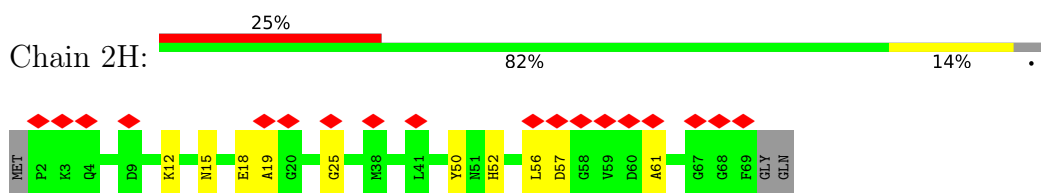
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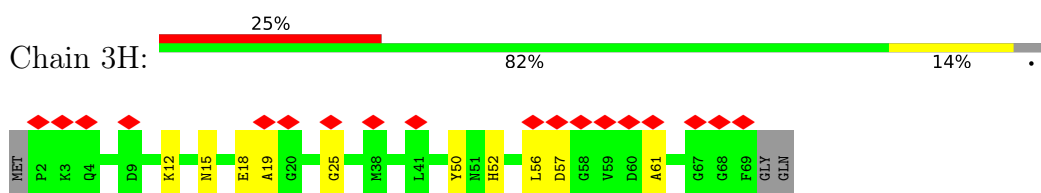
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



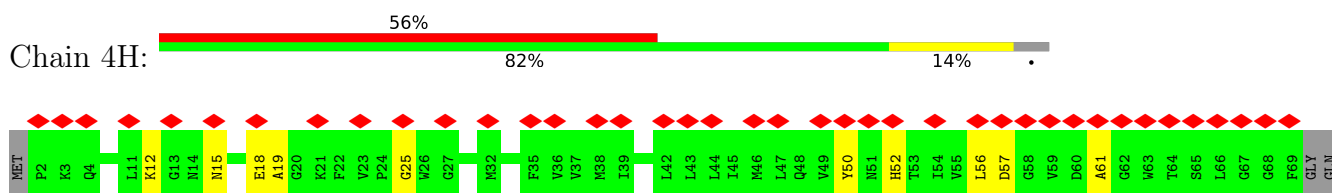
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



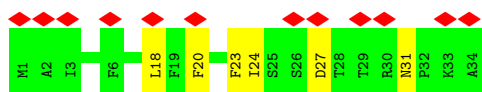
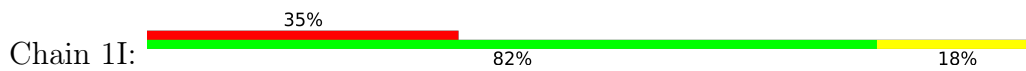
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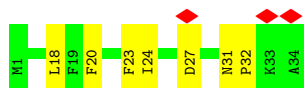
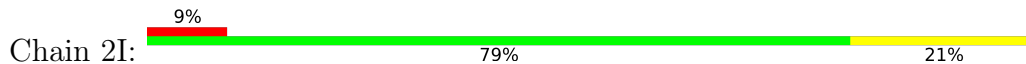
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



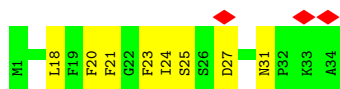
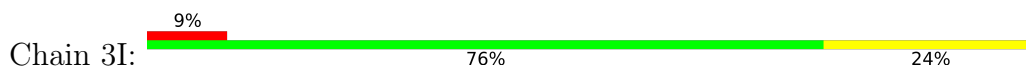
• Molecule 8: Photosystem II protein PsbI



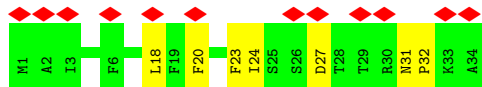
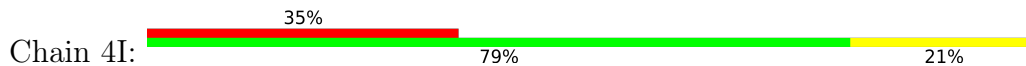
• Molecule 8: Photosystem II protein PsbI



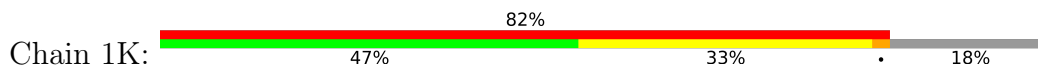
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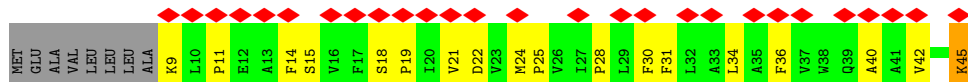
• Molecule 8: Photosystem II protein PsbI



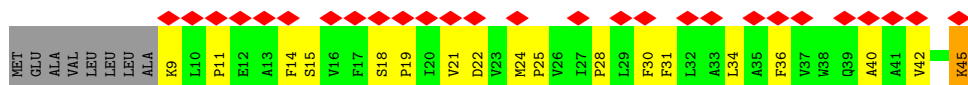
• Molecule 9: Photosystem II reaction center protein K



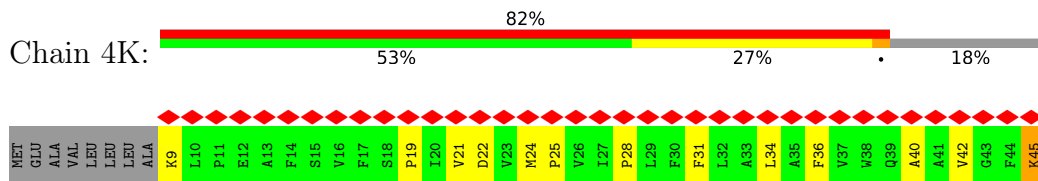
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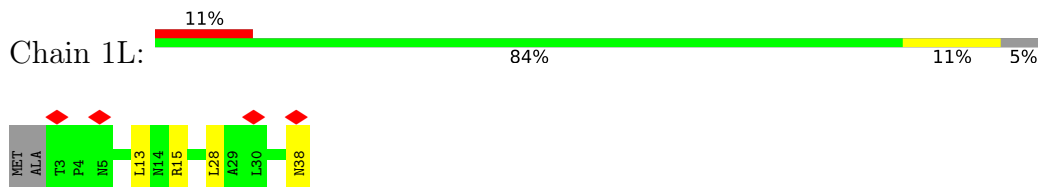
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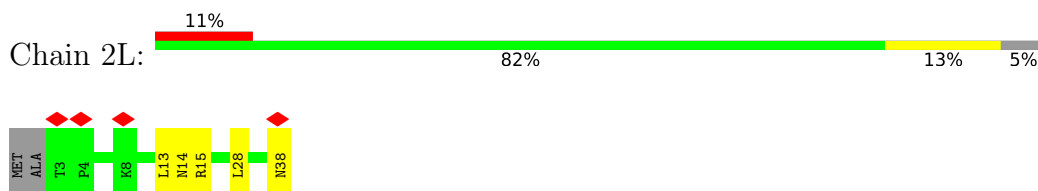
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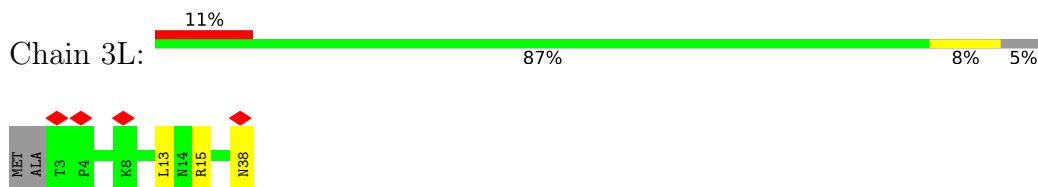
• Molecule 10: Photosystem II reaction center protein L



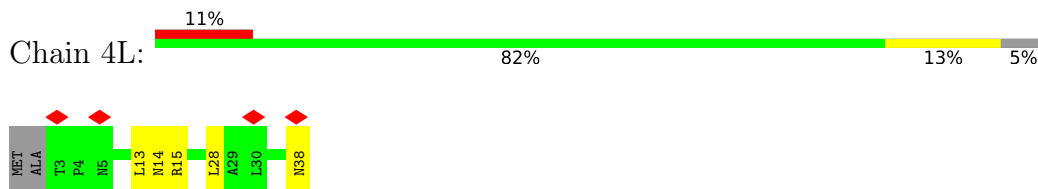
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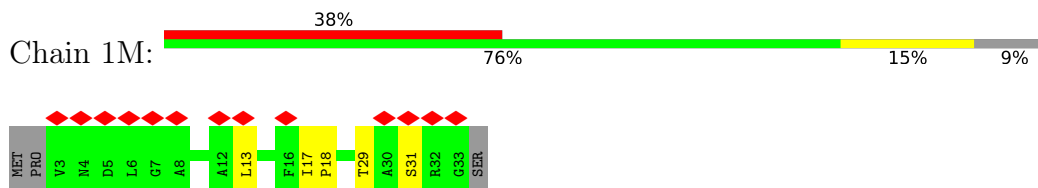
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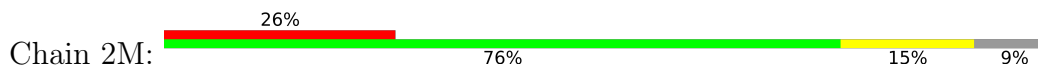
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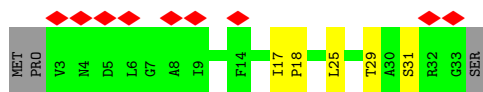


• Molecule 11: Photosystem II reaction center protein M

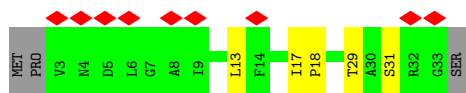
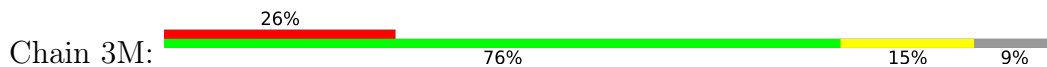


• Molecule 11: Photosystem II reaction center protein M

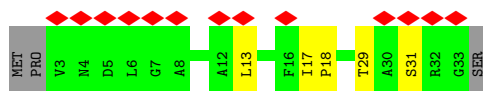
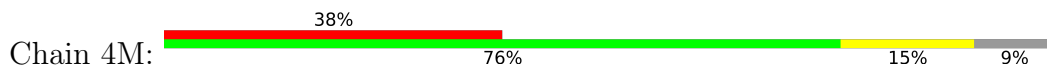




• Molecule 11: Photosystem II reaction center protein M



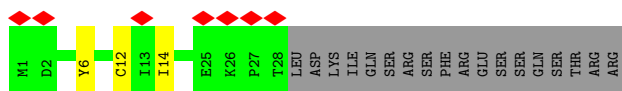
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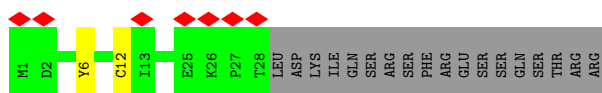
• Molecule 12: Photosystem II reaction center protein T



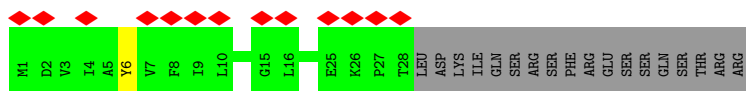
• Molecule 12: Photosystem II reaction center protein T



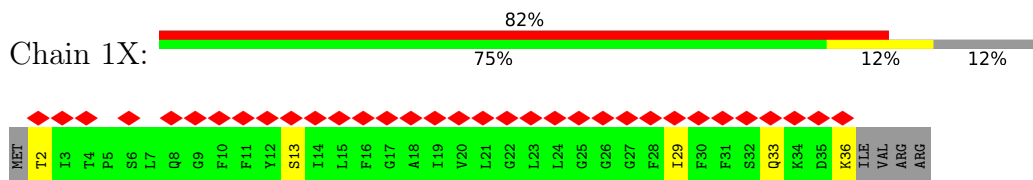
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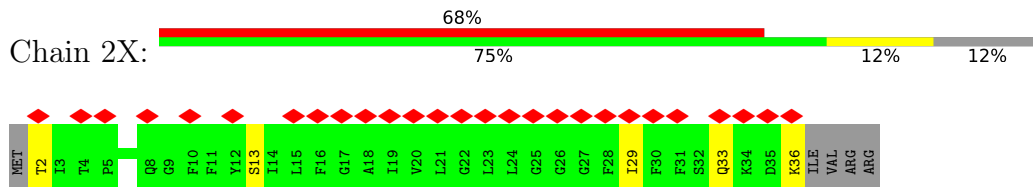
• Molecule 12: Photosystem II reaction center protein T



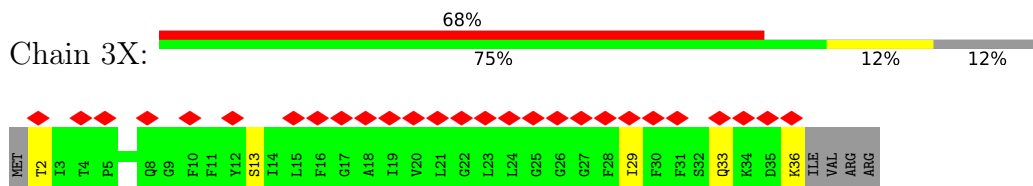
• Molecule 13: Photosystem II reaction center X protein



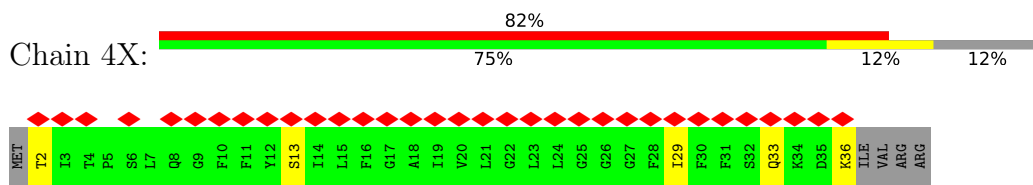
• Molecule 13: Photosystem II reaction center X protein



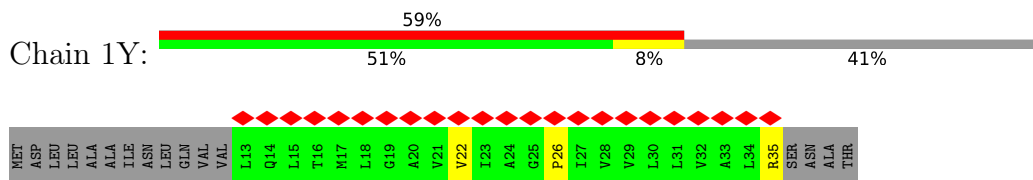
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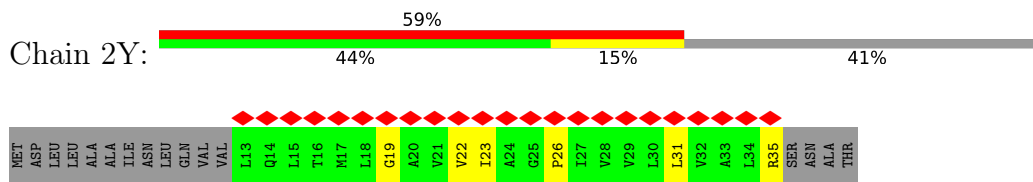
• Molecule 13: Photosystem II reaction center X protein



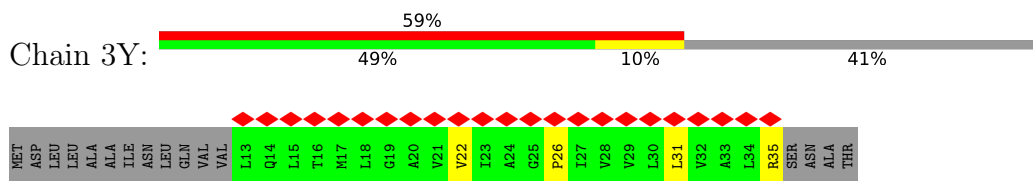
• Molecule 14: Photosystem II reaction center protein Ycf12



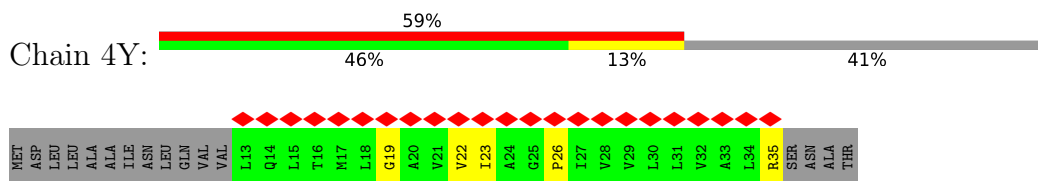
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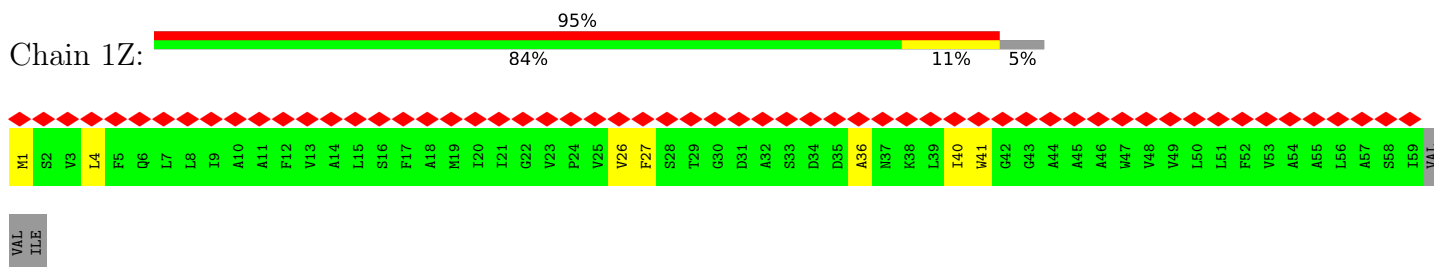
• Molecule 14: Photosystem II reaction center protein Ycf12



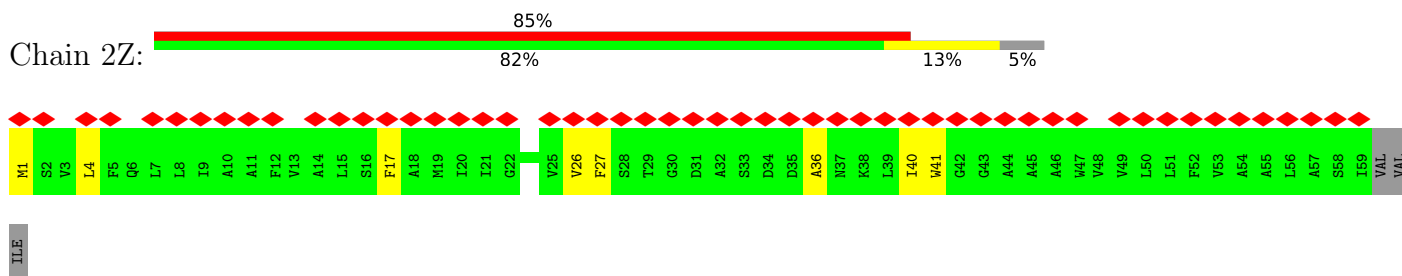
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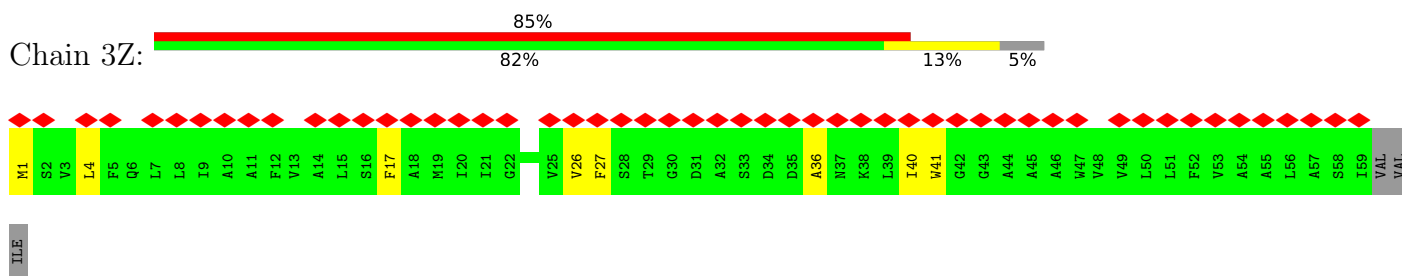
• Molecule 15: Photosystem II reaction center protein Z



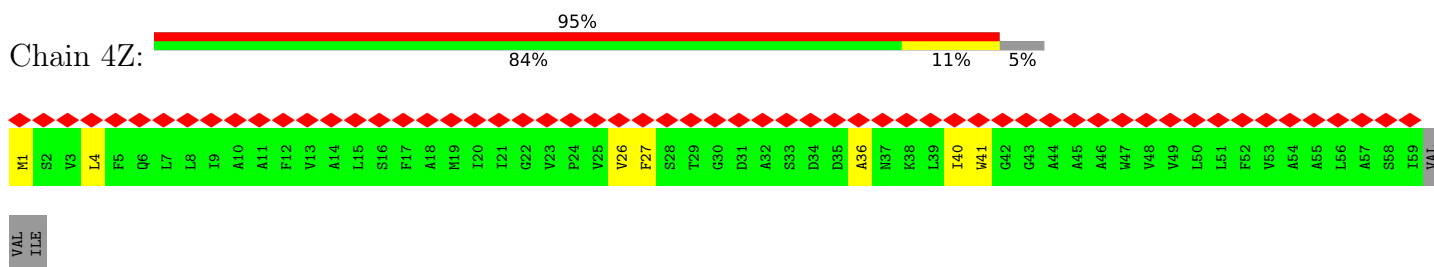
• Molecule 15: Photosystem II reaction center protein Z



• Molecule 15: Photosystem II reaction center protein Z

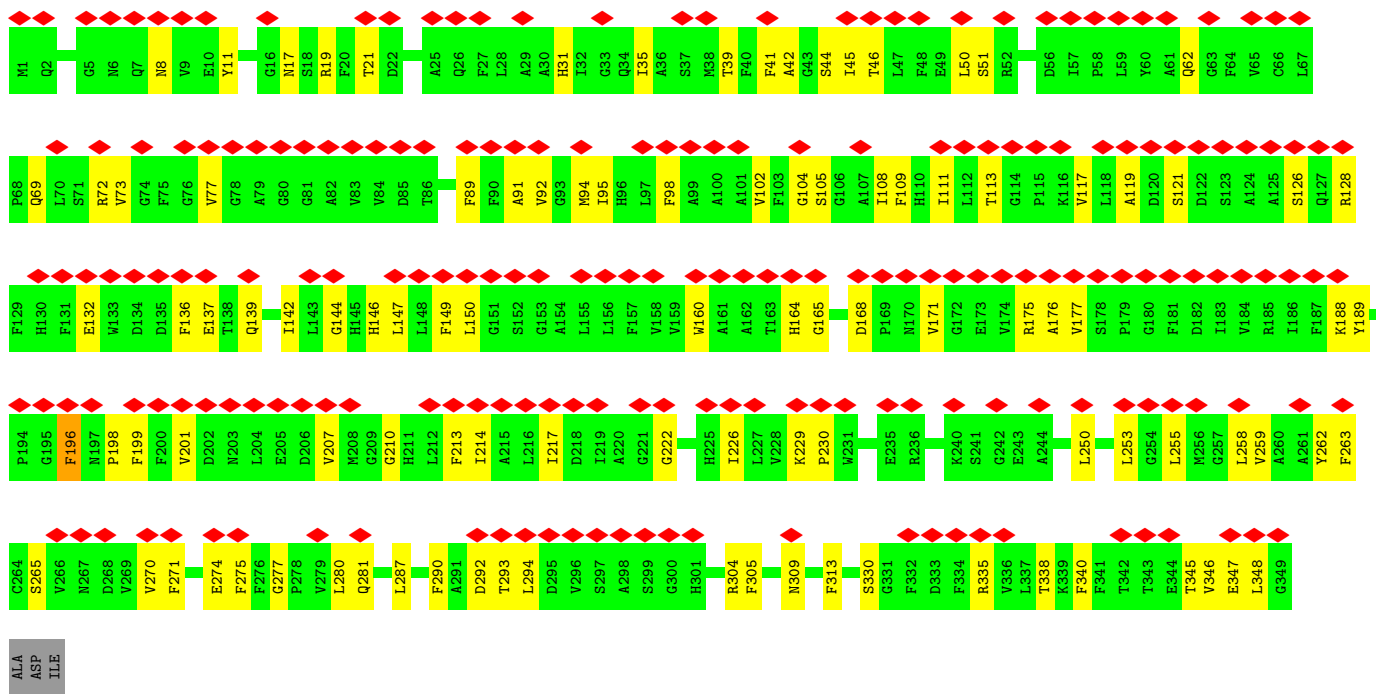


• Molecule 15: Photosystem II reaction center protein Z

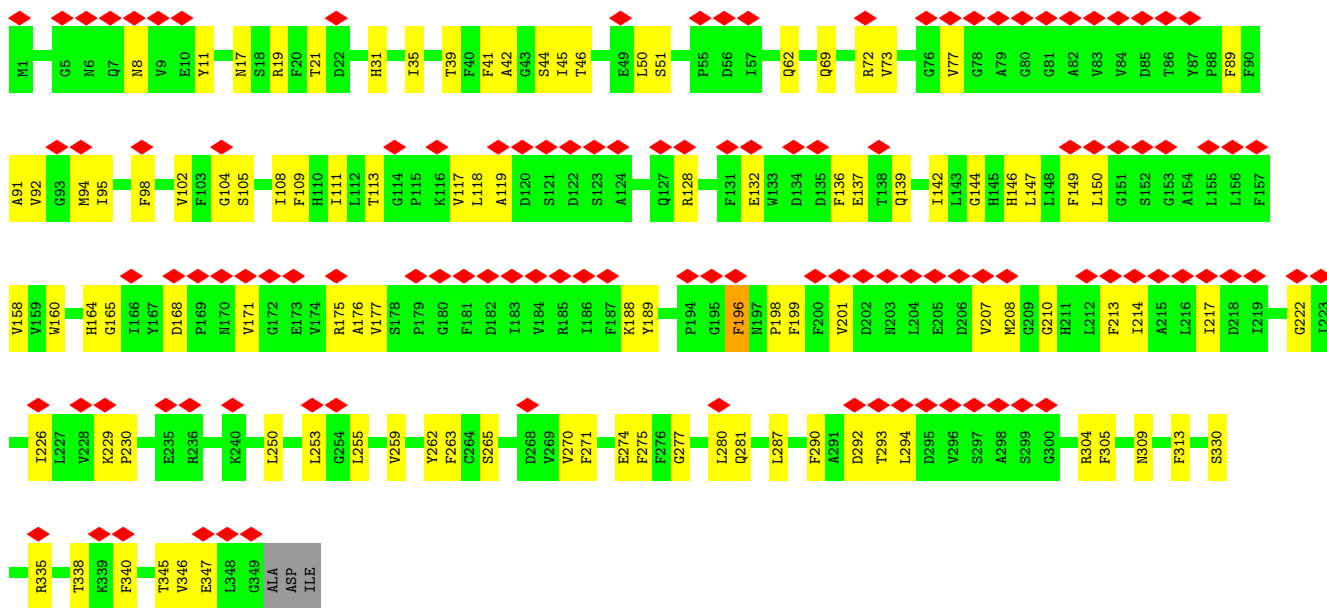


• Molecule 16: High light inducible protein

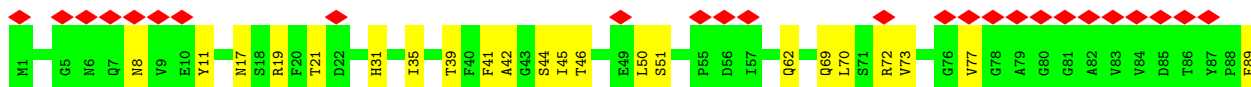


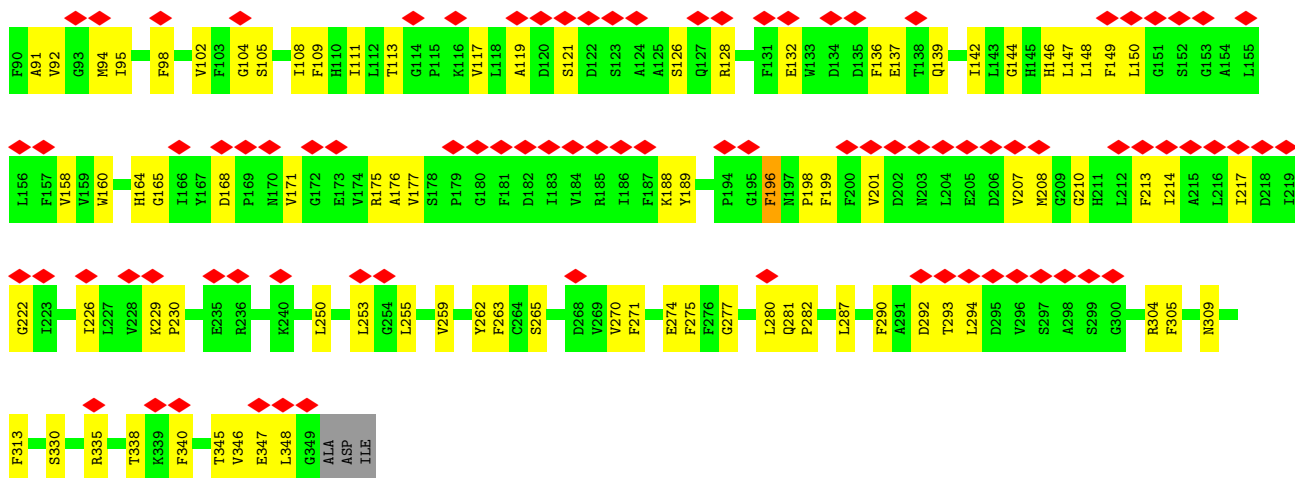


• Molecule 16: High light inducible protein

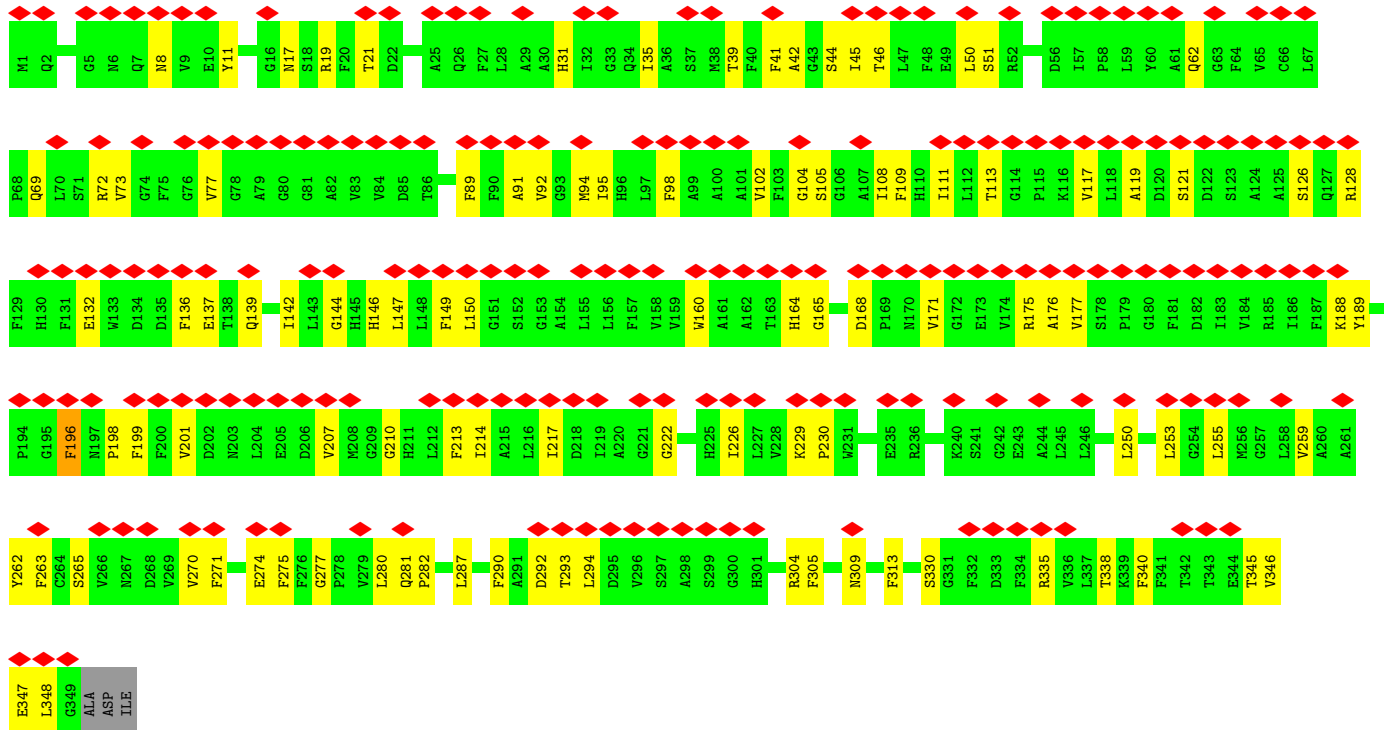


• Molecule 16: High light inducible protein

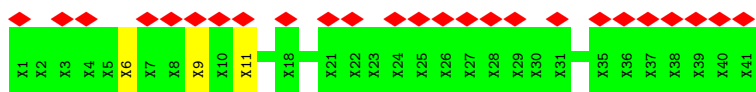




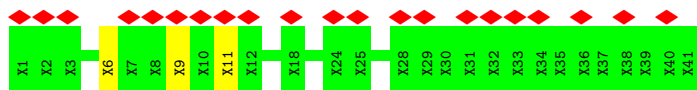
• Molecule 16: High light inducible protein



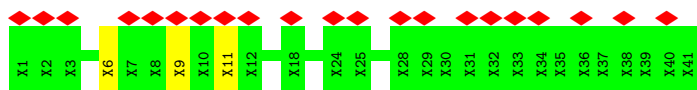
• Molecule 17: Unknown protein



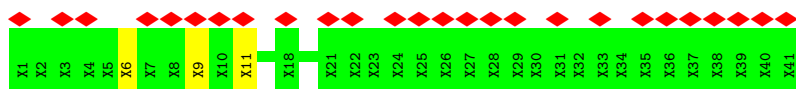
• Molecule 17: Unknown protein



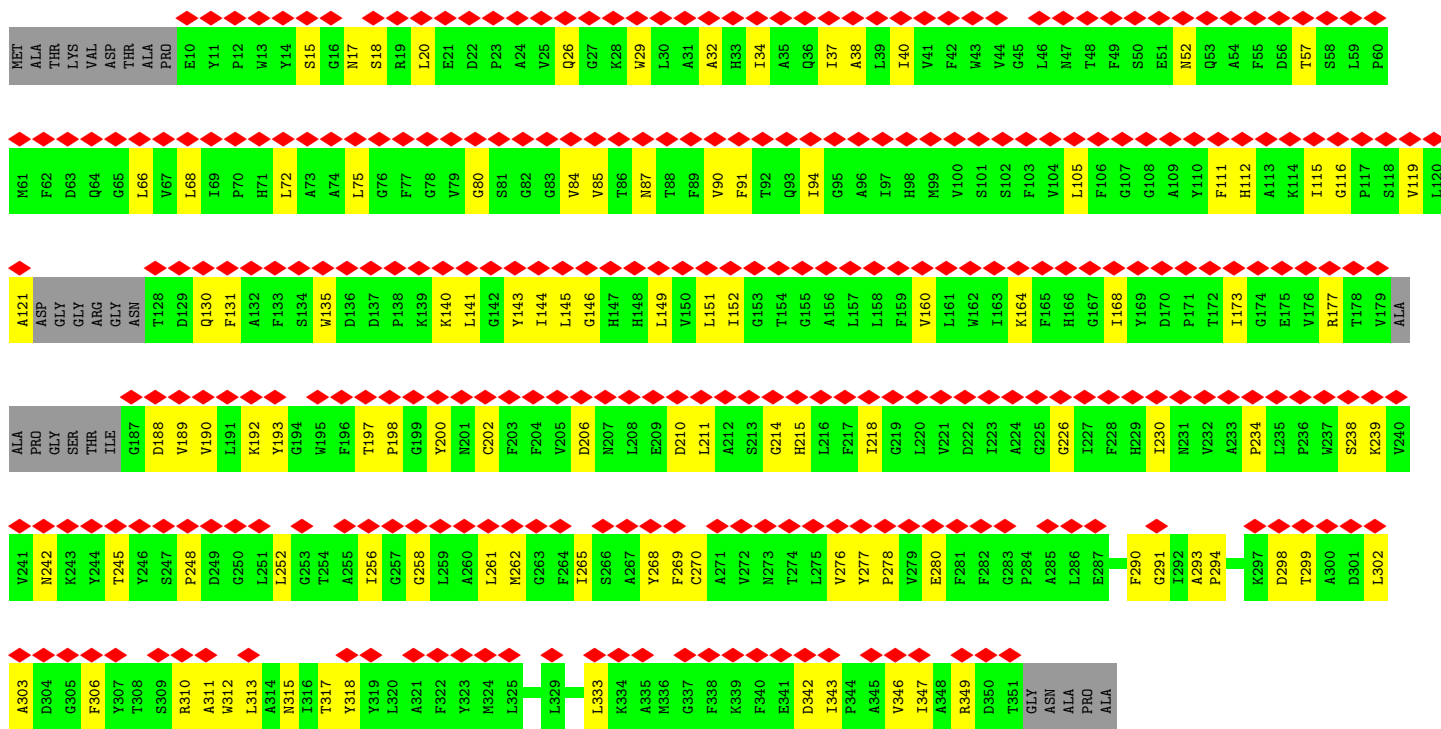
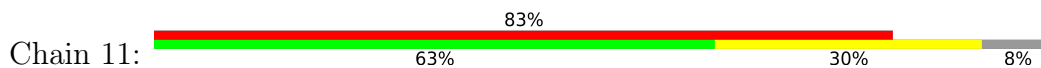
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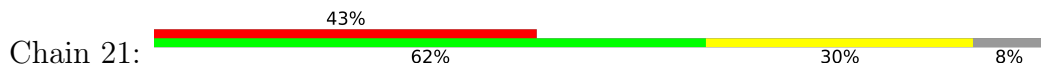
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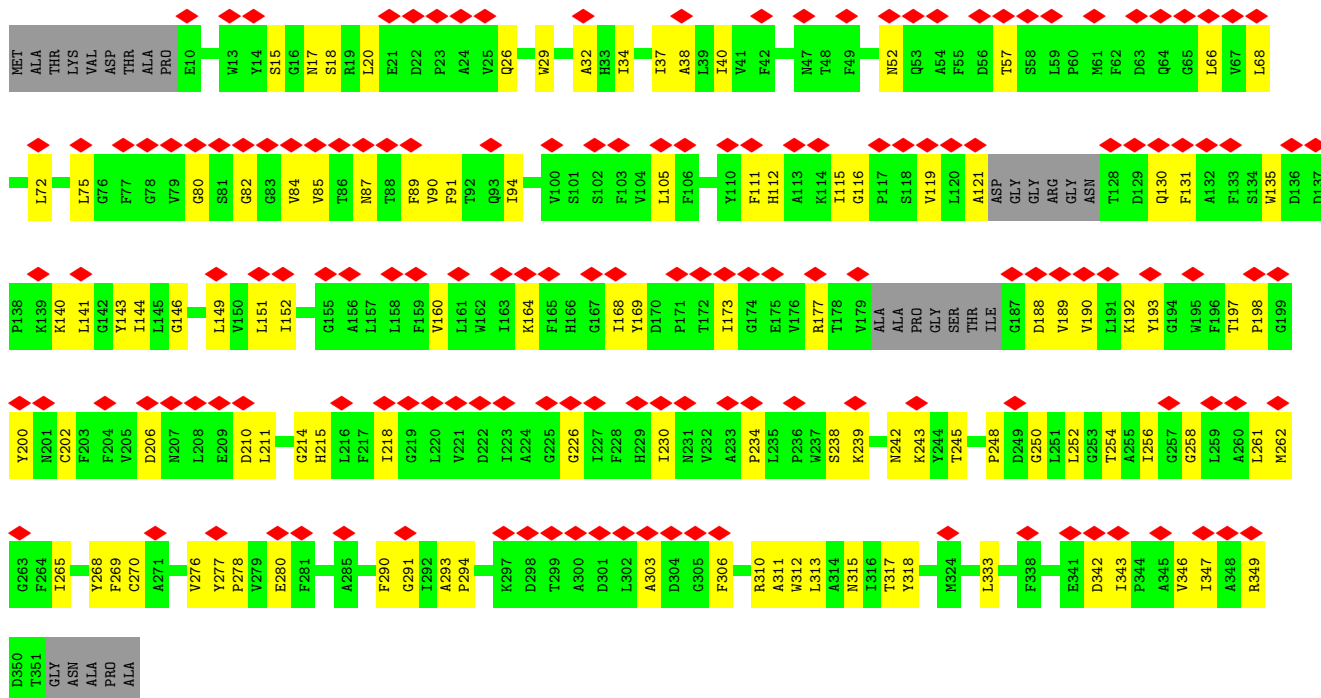


• Molecule 18: High light inducible protein

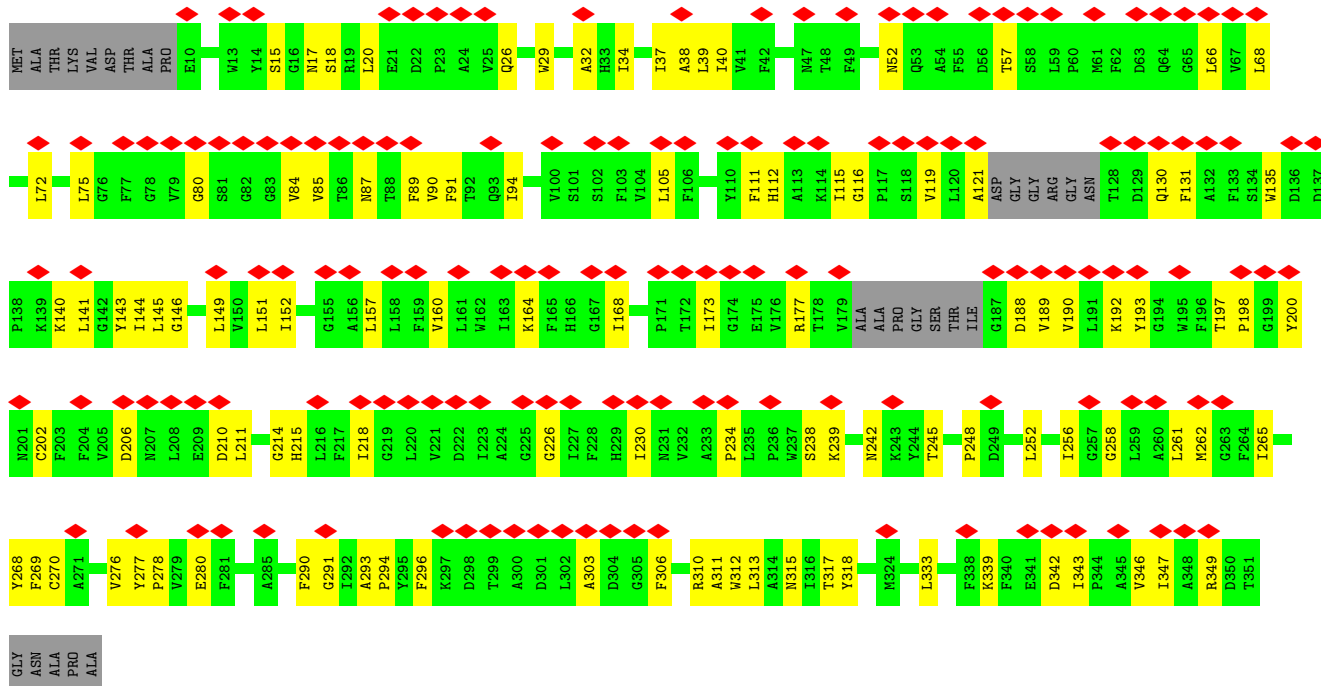
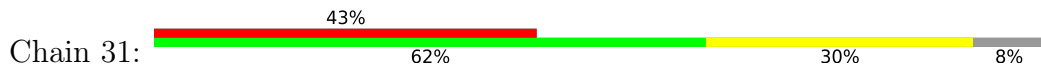


• Molecule 18: High light inducible protein

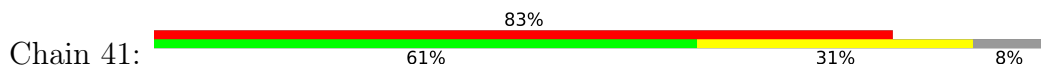


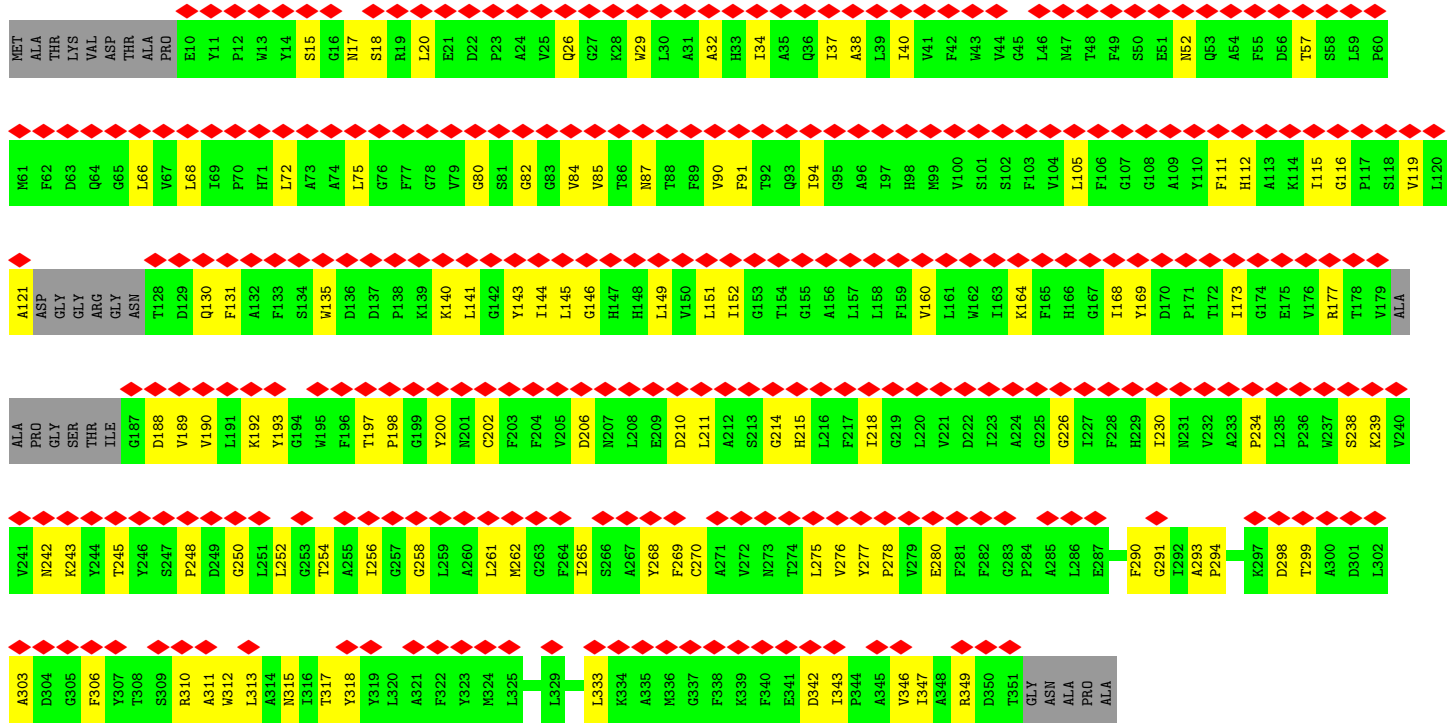


• Molecule 18: High light inducible protein

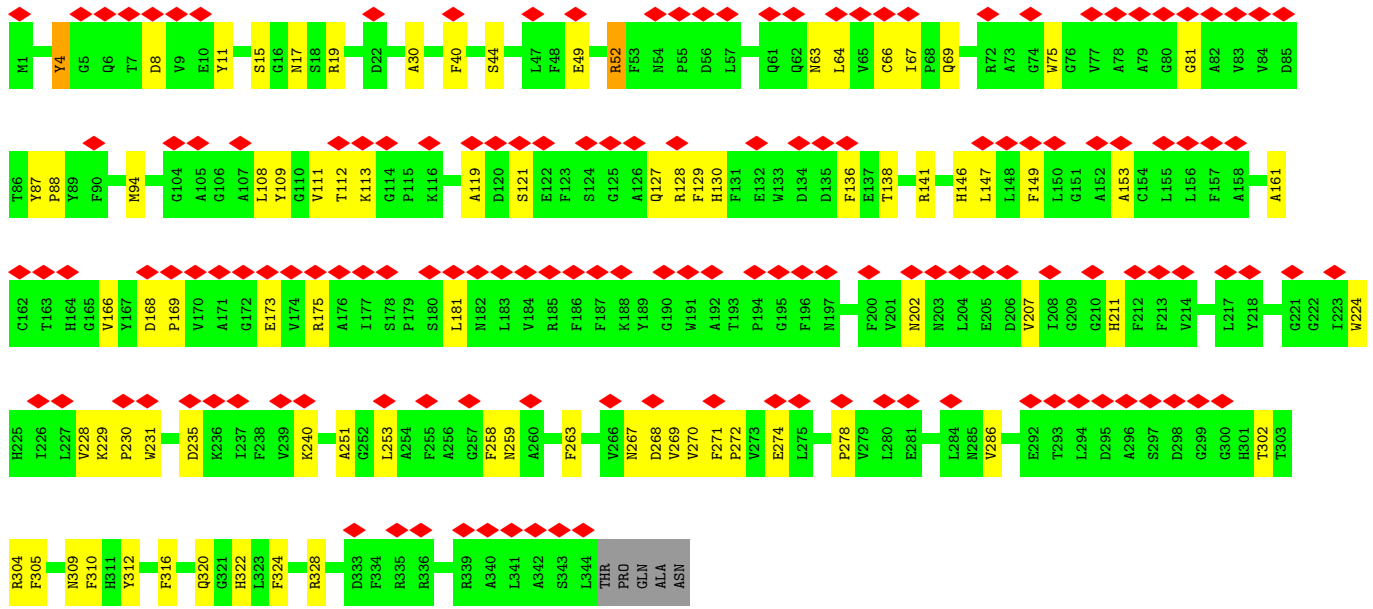
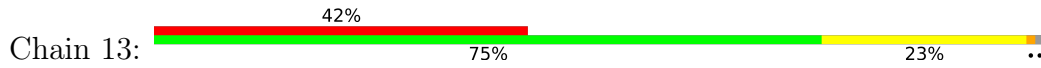


• Molecule 18: High light inducible protein

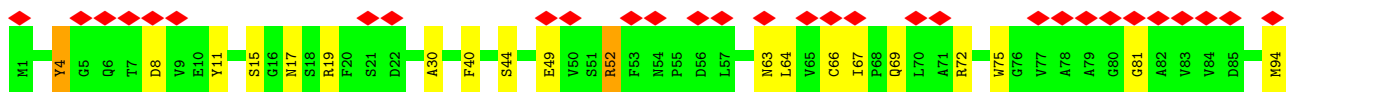
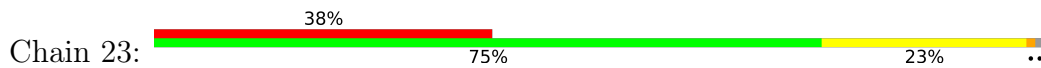


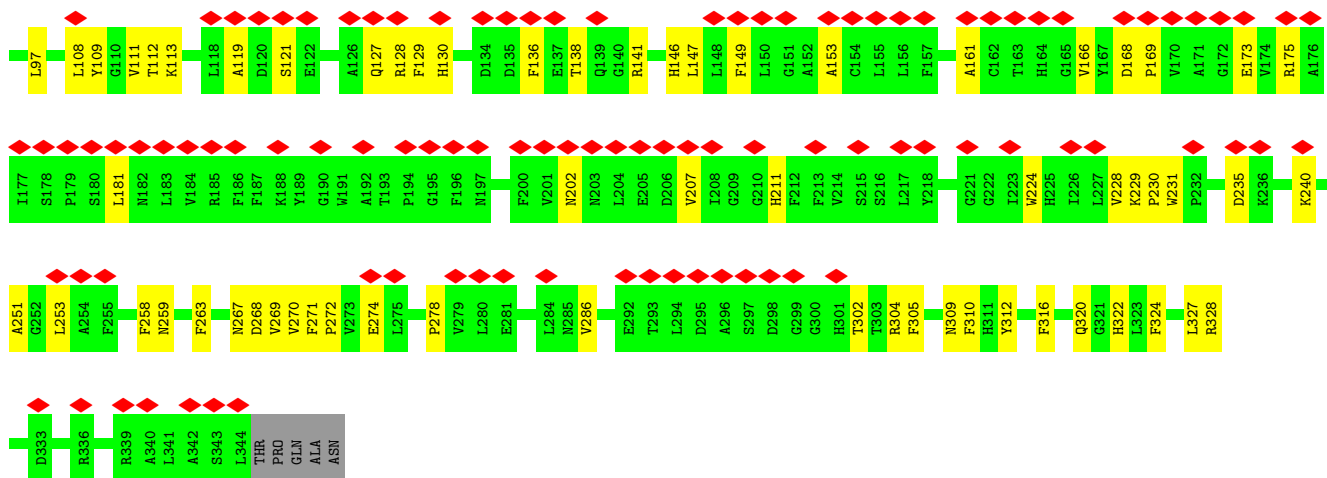


• Molecule 19: High light inducible protein

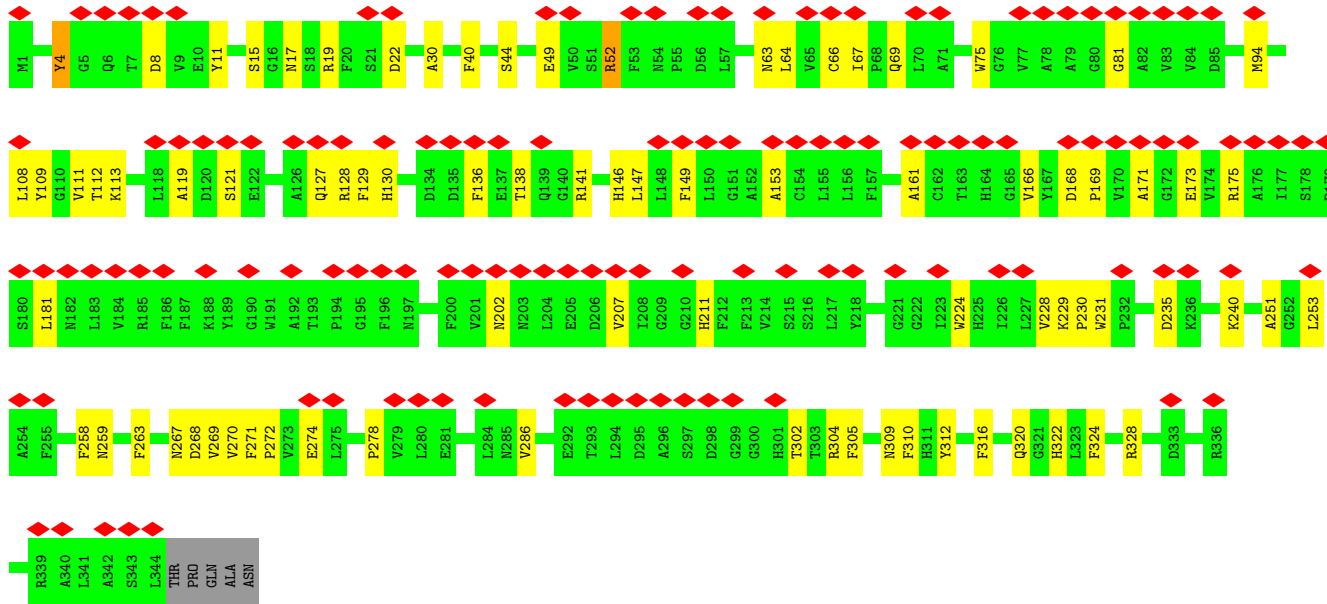
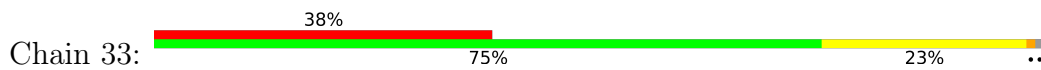


• Molecule 19: High light inducible protein

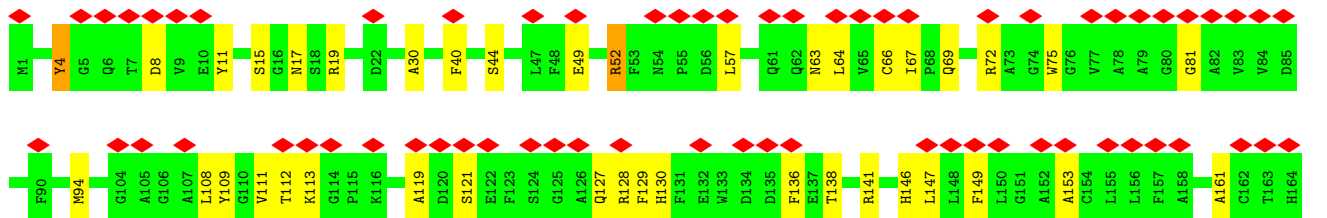
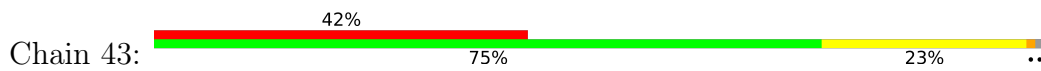


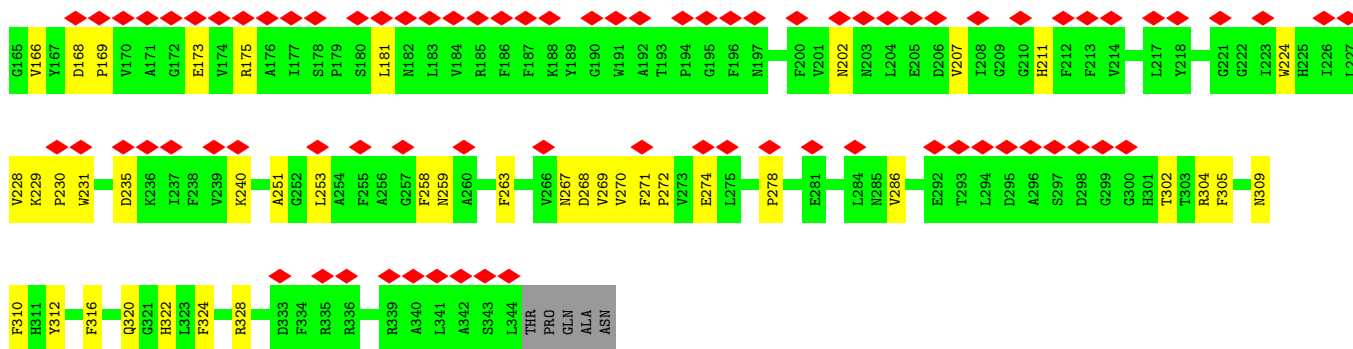


• Molecule 19: High light inducible protein

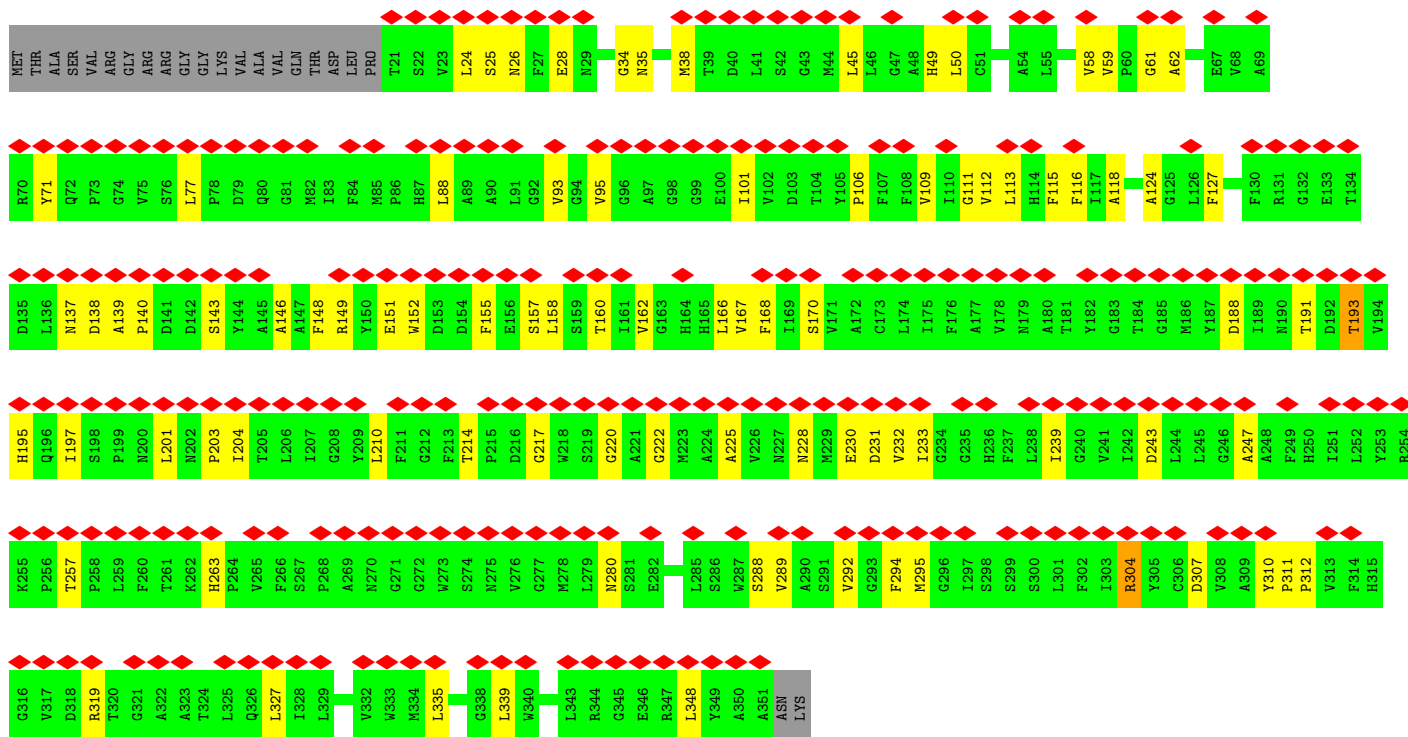


• Molecule 19: High light inducible protein

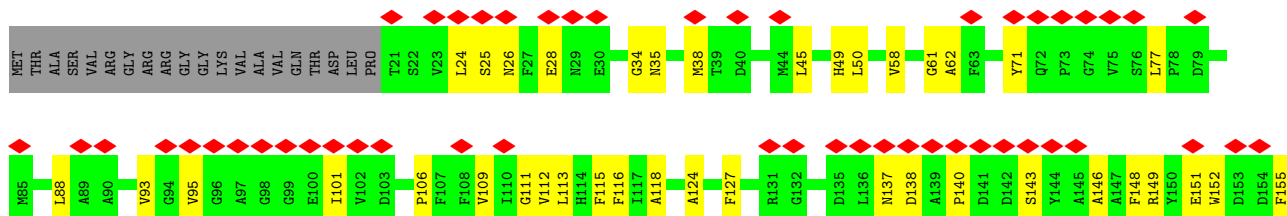


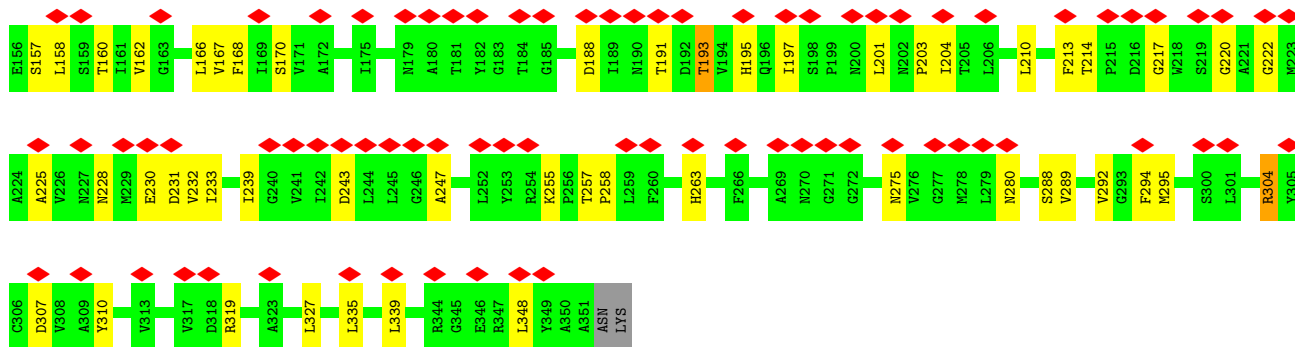


• Molecule 20: High light inducible protein

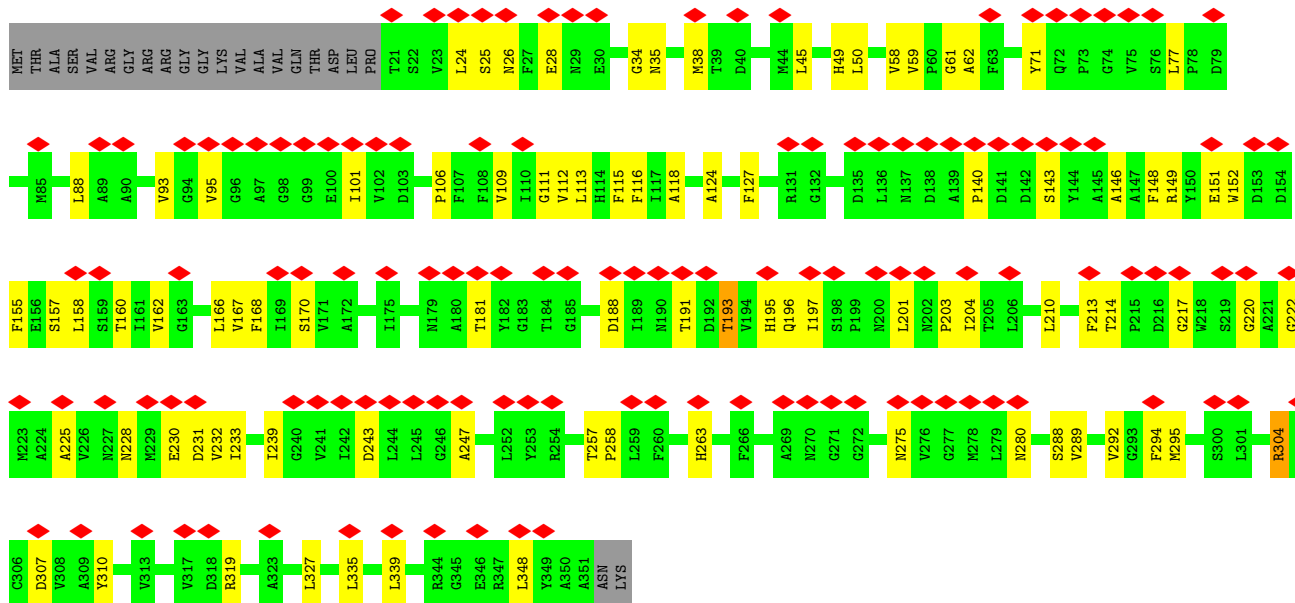


• Molecule 20: High light inducible protein

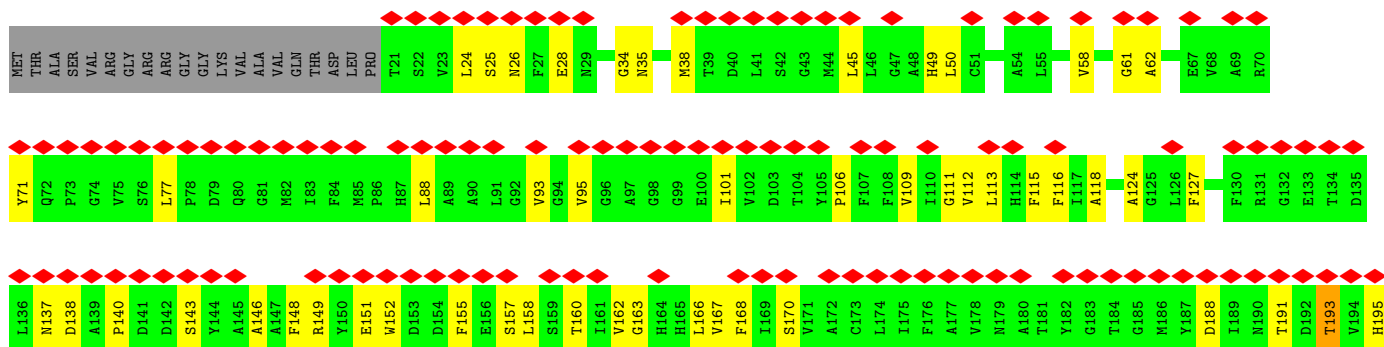




• Molecule 20: High light inducible protein



• Molecule 20: High light inducible protein



Q196	I197	S198	P199	N200	L201	N202	P203	I204	T205	L206	I207	G208	Y209	L210	F211	G212	F213	T214	P215	D216	G217	W218	S219	G220	A221	G222	M223	A224	A225	V226	N227	N228	M229	E230	D231	V232	I233	G234	G235	H236	F237	L238	I239	G240	V241	I242	D243	L244	L245	G246	A247	A248	F249	H250	I251	L252	Y253	R254	K255
P256	T257	P258	L259	F260	T261	R262	H263	P264	V265	F266	S267	P268	A269	N270	G271	G272	W273	S274	N275	V276	G277	M278	L279	N280	S281	E282	L283	I284	L285	S286	W287	S288	V289	V292	G293	F294	M295	G296	I297	S298	S299	S300	L301	F302	I303	R304	Y305	C306	D307	V308	A309	Y310	V313	F314	H315	G316	V317		
D318	R319	T320	G321	A322	A323	T324	L325	Q326	L327	I328	L329	V332	W333	M334	L335	G336	G337	G338	L339	W340	L343	R344	G345	E346	R347	L348	Y349	A350	A351	ASN	LYS																												

4 Experimental information

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 (\AA)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.47	0/2280	0.48	0/3112
1	2A	0.47	0/2280	0.48	0/3112
1	3A	0.47	0/2280	0.48	0/3112
1	4A	0.47	0/2280	0.48	0/3112
2	1B	0.46	0/3929	0.47	0/5360
2	2B	0.46	0/3929	0.47	0/5360
2	3B	0.46	0/3929	0.47	0/5360
2	4B	0.46	0/3929	0.47	0/5360
3	1C	0.43	0/3431	0.48	1/4669 (0.0%)
3	2C	0.43	0/3431	0.48	1/4669 (0.0%)
3	3C	0.43	0/3431	0.48	1/4669 (0.0%)
3	4C	0.43	0/3431	0.48	1/4669 (0.0%)
4	1D	0.45	0/2672	0.47	0/3641
4	2D	0.45	0/2672	0.47	0/3641
4	3D	0.45	0/2672	0.47	0/3641
4	4D	0.45	0/2672	0.47	0/3641
5	1E	0.34	0/555	0.44	0/757
5	2E	0.35	0/555	0.44	0/757
5	3E	0.35	0/555	0.44	0/757
5	4E	0.35	0/555	0.44	0/757
6	1F	0.37	0/250	0.42	0/343
6	2F	0.38	0/250	0.42	0/343
6	3F	0.37	0/250	0.42	0/343
6	4F	0.38	0/250	0.42	0/343
7	1H	0.37	0/534	0.49	0/729
7	2H	0.37	0/534	0.49	0/729
7	3H	0.38	0/534	0.49	0/729
7	4H	0.37	0/534	0.49	0/729
8	1I	0.49	0/290	0.43	0/391
8	2I	0.49	0/290	0.43	0/391
8	3I	0.49	0/290	0.43	0/391
8	4I	0.49	0/290	0.43	0/391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	1K	0.35	0/303	0.43	0/413
9	2K	0.35	0/303	0.43	0/413
9	3K	0.35	0/303	0.43	0/413
9	4K	0.35	0/303	0.43	0/413
10	1L	0.44	0/295	0.45	0/401
10	2L	0.44	0/295	0.45	0/401
10	3L	0.44	0/295	0.45	0/401
10	4L	0.44	0/295	0.45	0/401
11	1M	0.40	0/236	0.48	0/322
11	2M	0.40	0/236	0.48	0/322
11	3M	0.40	0/236	0.48	0/322
11	4M	0.41	0/236	0.48	0/322
12	1T	0.43	0/238	0.44	0/321
12	2T	0.42	0/238	0.44	0/321
12	3T	0.42	0/238	0.43	0/321
12	4T	0.43	0/238	0.43	0/321
13	1X	0.34	0/276	0.40	0/370
13	2X	0.34	0/276	0.40	0/370
13	3X	0.34	0/276	0.40	0/370
13	4X	0.34	0/276	0.40	0/370
14	1Y	0.26	0/164	0.42	0/224
14	2Y	0.26	0/164	0.42	0/224
14	3Y	0.26	0/164	0.42	0/224
14	4Y	0.26	0/164	0.42	0/224
15	1Z	0.29	0/438	0.38	0/599
15	2Z	0.29	0/438	0.38	0/599
15	3Z	0.29	0/438	0.38	0/599
15	4Z	0.29	0/438	0.38	0/599
16	12	0.44	0/2830	0.47	0/3855
16	22	0.44	0/2830	0.47	0/3855
16	32	0.44	0/2830	0.47	0/3855
16	42	0.44	0/2830	0.47	0/3855
18	11	0.37	0/2652	0.45	0/3618
18	21	0.37	0/2652	0.45	0/3618
18	31	0.37	0/2652	0.45	0/3618
18	41	0.37	0/2652	0.45	0/3618
19	13	0.46	0/2814	0.48	0/3841
19	23	0.46	0/2814	0.48	0/3841
19	33	0.46	0/2814	0.48	0/3841
19	43	0.46	0/2814	0.48	0/3841
20	14	0.39	0/2590	0.47	0/3537
20	24	0.38	0/2590	0.47	0/3537
20	34	0.39	0/2590	0.47	0/3537

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	44	0.39	0/2590	0.47	0/3537
All	All	0.43	0/107108	0.47	4/146012 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3C	387	LEU	CA-CB-CG	5.61	128.21	115.30
3	1C	387	LEU	CA-CB-CG	5.61	128.20	115.30
3	4C	387	LEU	CA-CB-CG	5.60	128.18	115.30
3	2C	387	LEU	CA-CB-CG	5.60	128.17	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	2209	0	2142	54	0
1	2A	2209	0	2142	55	0
1	3A	2209	0	2142	52	0
1	4A	2209	0	2142	56	0
2	1B	3794	0	3626	67	0
2	2B	3794	0	3626	68	0
2	3B	3794	0	3626	64	0
2	4B	3794	0	3626	66	0
3	1C	3313	0	3162	58	0
3	2C	3313	0	3162	56	0
3	3C	3313	0	3162	57	0
3	4C	3313	0	3162	56	0
4	1D	2583	0	2493	58	0
4	2D	2583	0	2493	57	0
4	3D	2583	0	2493	58	0
4	4D	2583	0	2493	58	0
5	1E	538	0	520	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	9	0
7	2H	519	0	518	9	0
7	3H	519	0	518	9	0
7	4H	519	0	518	9	0
8	1I	281	0	289	6	0
8	2I	281	0	289	7	0
8	3I	281	0	289	7	0
8	4I	281	0	289	7	0
9	1K	292	0	302	9	0
9	2K	292	0	302	11	0
9	3K	292	0	302	11	0
9	4K	292	0	302	8	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
15	3Z	429	0	450	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	4Z	429	0	450	3	0
16	12	2734	0	2611	106	0
16	22	2734	0	2611	103	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	100	0
18	21	2567	0	2508	108	0
18	31	2567	0	2508	110	0
18	41	2567	0	2508	104	0
19	13	2715	0	2580	77	0
19	23	2715	0	2580	79	0
19	33	2715	0	2580	80	0
19	43	2715	0	2580	77	0
20	14	2514	0	2436	79	0
20	24	2514	0	2436	91	0
20	34	2514	0	2436	89	0
20	44	2514	0	2436	78	0
21	11	972	0	822	84	0
21	12	1065	0	1050	110	0
21	13	1024	0	962	125	0
21	14	757	0	681	64	0
21	1A	185	0	187	32	0
21	1B	991	0	947	63	0
21	1C	799	0	763	46	0
21	1D	153	0	121	11	0
21	21	972	0	822	93	0
21	22	1065	0	1050	112	0
21	23	1024	0	962	126	0
21	24	757	0	681	62	0
21	2A	185	0	187	30	0
21	2B	991	0	947	64	0
21	2C	799	0	763	44	0
21	2D	153	0	121	12	0
21	31	972	0	821	92	0
21	32	1065	0	1050	111	0
21	33	1024	0	962	125	0
21	34	757	0	681	64	0
21	3A	185	0	187	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	3B	991	0	946	57	0
21	3C	799	0	763	44	0
21	3D	153	0	121	11	0
21	41	972	0	822	90	0
21	42	1065	0	1050	109	0
21	43	1024	0	962	132	0
21	44	757	0	681	63	0
21	4A	185	0	187	30	0
21	4B	991	0	947	60	0
21	4C	799	0	763	43	0
21	4D	153	0	121	12	0
22	1A	64	0	74	5	0
22	1D	64	0	74	5	0
22	2A	64	0	74	5	0
22	2D	64	0	74	4	0
22	3A	64	0	74	5	0
22	3D	64	0	74	5	0
22	4A	64	0	74	5	0
22	4D	64	0	74	4	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	1	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	1	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	1	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	1	0
23	4D	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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	0	0
25	22	91	0	113	2	0
25	23	96	0	123	6	0
25	2A	34	0	32	3	0
25	2B	54	0	78	2	0
25	31	32	0	28	0	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	0	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	1	0
26	1A	46	0	65	1	0
26	1B	94	0	137	7	0
26	1D	49	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	23	36	0	42	1	0
26	24	49	0	74	1	0
26	2A	46	0	65	1	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	1	0
26	3A	46	0	65	1	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	1	0
26	4A	46	0	65	1	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	3	0
27	3B	62	0	82	2	0
27	3C	62	0	82	4	0
27	4B	62	0	82	2	0
27	4C	62	0	82	3	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	69	0
32	13	168	0	224	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	14	168	0	224	51	0
32	21	84	0	112	36	0
32	22	168	0	224	65	0
32	23	168	0	224	80	0
32	24	168	0	224	53	0
32	31	84	0	112	36	0
32	32	168	0	224	68	0
32	33	168	0	224	80	0
32	34	168	0	224	50	0
32	41	84	0	112	37	0
32	42	168	0	224	69	0
32	43	168	0	224	82	0
32	44	168	0	224	53	0
All	All	136856	0	131770	4245	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 4245 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%)	37	67
18	21	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	37	67
18	31	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	37	67
18	41	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	37	67
19	13	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	37	67
19	23	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	37	67
19	33	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	37	67
19	43	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	37	67
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%)	50	79

5 of 8 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	232/292 (80%)	229 (99%)	3 (1%)	65	81
1	2A	232/292 (80%)	229 (99%)	3 (1%)	65	81
1	3A	232/292 (80%)	229 (99%)	3 (1%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4A	232/292 (80%)	229 (99%)	3 (1%)	65	81
2	1B	395/418 (94%)	385 (98%)	10 (2%)	42	66
2	2B	395/418 (94%)	385 (98%)	10 (2%)	42	66
2	3B	395/418 (94%)	385 (98%)	10 (2%)	42	66
2	4B	395/418 (94%)	385 (98%)	10 (2%)	42	66
3	1C	322/378 (85%)	313 (97%)	9 (3%)	38	64
3	2C	322/378 (85%)	313 (97%)	9 (3%)	38	64
3	3C	322/378 (85%)	313 (97%)	9 (3%)	38	64
3	4C	322/378 (85%)	313 (97%)	9 (3%)	38	64
4	1D	265/284 (93%)	261 (98%)	4 (2%)	60	78
4	2D	265/284 (93%)	261 (98%)	4 (2%)	60	78
4	3D	265/284 (93%)	261 (98%)	4 (2%)	60	78
4	4D	265/284 (93%)	261 (98%)	4 (2%)	60	78
5	1E	57/71 (80%)	56 (98%)	1 (2%)	54	74
5	2E	57/71 (80%)	56 (98%)	1 (2%)	54	74
5	3E	57/71 (80%)	56 (98%)	1 (2%)	54	74
5	4E	57/71 (80%)	56 (98%)	1 (2%)	54	74
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%)	54 (98%)	1 (2%)	54	74
7	2H	55/57 (96%)	54 (98%)	1 (2%)	54	74
7	3H	55/57 (96%)	54 (98%)	1 (2%)	54	74
7	4H	55/57 (96%)	54 (98%)	1 (2%)	54	74
8	1I	30/30 (100%)	29 (97%)	1 (3%)	33	61
8	2I	30/30 (100%)	29 (97%)	1 (3%)	33	61
8	3I	30/30 (100%)	29 (97%)	1 (3%)	33	61
8	4I	30/30 (100%)	29 (97%)	1 (3%)	33	61
9	1K	31/37 (84%)	30 (97%)	1 (3%)	34	61
9	2K	31/37 (84%)	30 (97%)	1 (3%)	34	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	3K	31/37 (84%)	30 (97%)	1 (3%)	34	61
9	4K	31/37 (84%)	30 (97%)	1 (3%)	34	61
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%)	17 (94%)	1 (6%)	17	47
14	2Y	18/31 (58%)	17 (94%)	1 (6%)	17	47
14	3Y	18/31 (58%)	17 (94%)	1 (6%)	17	47
14	4Y	18/31 (58%)	17 (94%)	1 (6%)	17	47
15	1Z	43/46 (94%)	42 (98%)	1 (2%)	45	68
15	2Z	43/46 (94%)	42 (98%)	1 (2%)	45	68
15	3Z	43/46 (94%)	42 (98%)	1 (2%)	45	68
15	4Z	43/46 (94%)	42 (98%)	1 (2%)	45	68
16	12	276/278 (99%)	270 (98%)	6 (2%)	47	69
16	22	276/278 (99%)	270 (98%)	6 (2%)	47	69
16	32	276/278 (99%)	270 (98%)	6 (2%)	47	69
16	42	276/278 (99%)	270 (98%)	6 (2%)	47	69
18	11	262/278 (94%)	258 (98%)	4 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	21	262/278 (94%)	258 (98%)	4 (2%)	60	78
18	31	262/278 (94%)	258 (98%)	4 (2%)	60	78
18	41	262/278 (94%)	258 (98%)	4 (2%)	60	78
19	13	269/273 (98%)	261 (97%)	8 (3%)	36	63
19	23	269/273 (98%)	261 (97%)	8 (3%)	36	63
19	33	269/273 (98%)	261 (97%)	8 (3%)	36	63
19	43	269/273 (98%)	261 (97%)	8 (3%)	36	63
20	14	260/277 (94%)	254 (98%)	6 (2%)	45	68
20	24	260/277 (94%)	254 (98%)	6 (2%)	45	68
20	34	260/277 (94%)	254 (98%)	6 (2%)	45	68
20	44	260/277 (94%)	254 (98%)	6 (2%)	45	68
All	All	10596/11880 (89%)	10372 (98%)	224 (2%)	49	71

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3B	129	ASP
20	44	204	ILE
15	3Z	27	PHE
20	44	28	GLU
15	4Z	27	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
16	32	62	GLN
20	34	195	HIS
20	44	195	HIS
19	33	34	GLN
20	34	275	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	4B	623	-	46,53,73	2.68	12 (26%)	41,89,113	2.58	13 (31%)
32	ZEX	33	525	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	13	508	-	66,73,73	2.21	14 (21%)	65,113,113	2.24	18 (27%)
25	SQD	22	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	23	408	-	66,73,73	2.16	13 (19%)	65,113,113	2.30	18 (27%)
21	CL7	14	405	-	66,73,73	2.21	14 (21%)	65,113,113	2.30	19 (29%)
21	CL7	34	406	-	66,73,73	2.21	12 (18%)	65,113,113	2.22	17 (26%)
21	CL7	32	508	-	46,53,73	2.60	13 (28%)	41,89,113	2.65	14 (34%)
21	CL7	22	501	-	66,73,73	2.17	13 (19%)	65,113,113	2.24	15 (23%)
23	8CT	1K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.66	16 (32%)
26	LHG	44	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	3C	503	-	66,73,73	2.20	14 (21%)	65,113,113	2.22	17 (26%)
23	8CT	4B	620	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
32	ZEX	24	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
32	ZEX	14	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.43	25 (45%)
21	CL7	33	517	19	51,58,73	2.48	13 (25%)	47,95,113	2.54	14 (29%)
21	CL7	4C	508	-	66,73,73	2.22	13 (19%)	65,113,113	2.28	21 (32%)
21	CL7	23	404	-	66,73,73	2.20	14 (21%)	65,113,113	2.29	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMG	2I	401	-	51,51,55	0.22	0	59,59,63	0.42	1 (1%)
30	PL9	2D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	44	410	-	46,53,73	2.62	13 (28%)	41,89,113	2.66	13 (31%)
21	CL7	3B	602	-	61,68,73	2.32	12 (19%)	59,107,113	2.39	18 (30%)
26	LHG	1B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
26	LHG	34	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	12	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.31	17 (26%)
21	CL7	2C	517	-	42,49,73	2.63	10 (23%)	36,84,113	2.84	14 (38%)
21	CL7	11	407	-	42,49,73	2.66	11 (26%)	36,84,113	2.81	15 (41%)
21	CL7	33	513	-	46,53,73	2.66	14 (30%)	41,89,113	2.67	13 (31%)
21	CL7	3C	511	3	43,50,73	2.69	11 (25%)	36,85,113	2.78	13 (36%)
23	8CT	2D	406	-	40,41,41	4.63	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	42	504	-	46,53,73	2.62	13 (28%)	41,89,113	2.62	14 (34%)
21	CL7	33	516	19	56,63,73	2.41	13 (23%)	53,101,113	2.42	19 (35%)
21	CL7	13	518	19	46,53,73	2.68	12 (26%)	41,89,113	2.67	14 (34%)
21	CL7	4A	401	-	66,73,73	2.27	14 (21%)	65,113,113	2.34	19 (29%)
21	CL7	41	402	-	61,68,73	2.31	14 (22%)	59,107,113	2.37	15 (25%)
21	CL7	13	512	-	56,63,73	2.39	14 (25%)	53,101,113	2.44	18 (33%)
21	CL7	4B	616	-	51,58,73	2.45	14 (27%)	47,95,113	2.64	16 (34%)
21	CL7	21	408	-	66,73,73	2.19	13 (19%)	65,113,113	2.30	19 (29%)
21	CL7	1C	511	3	43,50,73	2.70	11 (25%)	36,85,113	2.78	13 (36%)
21	CL7	22	515	-	46,53,73	2.62	12 (26%)	41,89,113	2.66	16 (39%)
21	CL7	41	406	-	63,70,73	2.26	12 (19%)	61,109,113	2.29	14 (22%)
21	CL7	41	403	-	61,68,73	2.29	12 (19%)	59,107,113	2.38	15 (25%)
25	SQD	13	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
32	ZEX	44	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
32	ZEX	42	520	-	42,43,43	0.98	3 (7%)	55,60,60	2.18	17 (30%)
21	CL7	11	416	-	42,49,73	2.73	10 (23%)	36,84,113	2.77	14 (38%)
21	CL7	14	410	-	46,53,73	2.62	13 (28%)	41,89,113	2.65	13 (31%)
21	CL7	2B	611	-	66,73,73	2.15	12 (18%)	65,113,113	2.31	15 (23%)
21	CL7	44	414	-	54,61,73	2.39	13 (24%)	50,98,113	2.53	16 (32%)
21	CL7	21	420	18	46,53,73	2.63	12 (26%)	41,89,113	2.75	14 (34%)
21	CL7	4B	615	-	61,68,73	2.30	15 (24%)	59,107,113	2.36	19 (32%)
21	CL7	1C	517	-	42,49,73	2.62	10 (23%)	36,84,113	2.84	14 (38%)
21	CL7	44	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.89	15 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	1D	405	-	46,53,73	2.58	13 (28%)	41,89,113	2.74	16 (39%)
21	CL7	41	410	-	66,73,73	2.24	13 (19%)	65,113,113	2.17	16 (24%)
21	CL7	11	406	-	63,70,73	2.27	12 (19%)	61,109,113	2.30	14 (22%)
21	CL7	4B	608	-	61,68,73	2.30	13 (21%)	59,107,113	2.27	17 (28%)
21	CL7	42	514	-	46,53,73	2.64	13 (28%)	41,89,113	2.69	12 (29%)
27	DGD	3B	624	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	4B	609	-	66,73,73	2.19	13 (19%)	65,113,113	2.17	14 (21%)
25	SQD	32	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	2C	503	-	66,73,73	2.20	14 (21%)	65,113,113	2.22	17 (26%)
31	HEM	3F	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
21	CL7	3B	603	-	66,73,73	2.22	13 (19%)	65,113,113	2.22	17 (26%)
21	CL7	32	504	-	46,53,73	2.63	13 (28%)	41,89,113	2.63	14 (34%)
21	CL7	1B	608	-	66,73,73	2.19	13 (19%)	65,113,113	2.18	15 (23%)
27	DGD	4C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	12	503	-	66,73,73	2.19	15 (22%)	65,113,113	2.39	19 (29%)
21	CL7	1D	402	-	51,58,73	2.54	12 (23%)	47,95,113	2.47	15 (31%)
21	CL7	23	416	-	42,49,73	2.65	10 (23%)	36,84,113	2.86	15 (41%)
21	CL7	3B	605	-	66,73,73	2.24	14 (21%)	65,113,113	2.22	15 (23%)
21	CL7	42	518	16	66,73,73	2.22	12 (18%)	65,113,113	2.16	17 (26%)
21	CL7	3C	513	-	46,53,73	2.62	12 (26%)	41,89,113	2.68	14 (34%)
21	CL7	22	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.19	16 (24%)
21	CL7	4C	504	-	56,63,73	2.43	12 (21%)	53,101,113	2.38	14 (26%)
32	ZEX	13	525	-	42,43,43	1.18	5 (11%)	55,60,60	2.44	18 (32%)
21	CL7	3C	504	-	56,63,73	2.42	13 (23%)	53,101,113	2.38	14 (26%)
21	CL7	12	515	-	46,53,73	2.63	12 (26%)	41,89,113	2.66	15 (36%)
21	CL7	31	409	-	46,53,73	2.61	13 (28%)	41,89,113	2.62	15 (36%)
21	CL7	4A	407	-	66,73,73	2.23	13 (19%)	65,113,113	2.29	16 (24%)
21	CL7	31	414	-	42,49,73	2.74	10 (23%)	36,84,113	2.92	15 (41%)
21	CL7	31	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.58	13 (31%)
21	CL7	12	511	16	61,68,73	2.33	12 (19%)	59,107,113	2.21	15 (25%)
21	CL7	14	414	-	54,61,73	2.39	13 (24%)	50,98,113	2.53	15 (30%)
21	CL7	2B	605	-	66,73,73	2.16	13 (19%)	65,113,113	2.23	17 (26%)
21	CL7	12	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.17	15 (23%)
21	CL7	3B	604	-	66,73,73	2.15	13 (19%)	65,113,113	2.22	18 (27%)
21	CL7	43	405	-	66,73,73	2.21	13 (19%)	65,113,113	2.24	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	1A	401	-	66,73,73	2.28	14 (21%)	65,113,113	2.33	19 (29%)
21	CL7	4D	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.36	17 (30%)
26	LHG	3B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
32	ZEX	22	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	44	408	-	46,53,73	2.66	14 (30%)	41,89,113	2.67	13 (31%)
21	CL7	2C	513	-	46,53,73	2.63	12 (26%)	41,89,113	2.69	14 (34%)
21	CL7	21	402	-	61,68,73	2.32	14 (22%)	59,107,113	2.37	15 (25%)
26	LHG	2B	626	-	48,48,48	0.30	0	51,54,54	0.34	0
23	8CT	4B	619	-	40,41,41	4.69	21 (52%)	50,56,56	2.67	20 (40%)
27	DGD	4B	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	34	417	20	43,50,73	2.67	11 (25%)	36,85,113	2.89	13 (36%)
21	CL7	23	407	-	46,53,73	2.58	14 (30%)	41,89,113	2.72	14 (34%)
21	CL7	4B	606	-	66,73,73	2.24	14 (21%)	65,113,113	2.22	15 (23%)
21	CL7	4C	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.24	16 (24%)
23	8CT	2A	404	-	40,41,41	4.63	20 (50%)	50,56,56	2.97	20 (40%)
27	DGD	2B	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
32	ZEX	23	423	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	18 (32%)
21	CL7	42	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.20	16 (24%)
21	CL7	21	411	-	46,53,73	2.65	12 (26%)	41,89,113	2.62	14 (34%)
22	PHO	3D	408	-	51,69,69	0.59	2 (3%)	47,99,99	0.87	2 (4%)
25	SQD	32	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	1B	611	-	66,73,73	2.18	14 (21%)	65,113,113	2.25	15 (23%)
21	CL7	13	516	19	56,63,73	2.42	13 (23%)	53,101,113	2.43	19 (35%)
21	CL7	42	508	-	46,53,73	2.59	14 (30%)	41,89,113	2.66	14 (34%)
23	8CT	34	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	2B	613	-	66,73,73	2.15	13 (19%)	65,113,113	2.28	18 (27%)
21	CL7	3A	403	-	56,63,73	2.40	14 (25%)	53,101,113	2.58	19 (35%)
21	CL7	12	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	19 (29%)
21	CL7	13	502	-	59,66,73	2.36	13 (22%)	56,104,113	2.26	17 (30%)
21	CL7	41	418	18	66,73,73	2.17	12 (18%)	65,113,113	2.31	20 (30%)
21	CL7	22	514	-	46,53,73	2.63	13 (28%)	41,89,113	2.68	12 (29%)
21	CL7	12	502	-	66,73,73	2.18	13 (19%)	65,113,113	2.25	17 (26%)
21	CL7	1B	604	-	66,73,73	2.15	13 (19%)	65,113,113	2.22	18 (27%)
21	CL7	1A	407	-	66,73,73	2.24	13 (19%)	65,113,113	2.30	16 (24%)
21	CL7	21	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.60	13 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCT	1D	403	28	2,3,3	1.00	0	2,3,3	1.66	1 (50%)
21	CL7	1B	602	-	61,68,73	2.31	12 (19%)	59,107,113	2.39	17 (28%)
21	CL7	22	505	-	66,73,73	2.23	13 (19%)	65,113,113	2.41	19 (29%)
21	CL7	43	411	-	66,73,73	2.18	13 (19%)	65,113,113	2.22	18 (27%)
26	LHG	1A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	41	405	-	46,53,73	2.63	13 (28%)	41,89,113	2.61	12 (29%)
21	CL7	23	413	-	56,63,73	2.38	13 (23%)	53,101,113	2.45	18 (33%)
21	CL7	34	405	-	66,73,73	2.21	14 (21%)	65,113,113	2.31	20 (30%)
21	CL7	4B	610	-	66,73,73	2.24	13 (19%)	65,113,113	2.15	15 (23%)
21	CL7	3A	401	-	66,73,73	2.27	15 (22%)	65,113,113	2.34	19 (29%)
26	LHG	1D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	11	412	-	46,53,73	2.59	12 (26%)	41,89,113	2.71	14 (34%)
21	CL7	14	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.89	15 (41%)
21	CL7	4B	611	-	66,73,73	2.16	13 (19%)	65,113,113	2.31	15 (23%)
21	CL7	22	503	-	66,73,73	2.18	15 (22%)	65,113,113	2.39	19 (29%)
23	8CT	4C	514	-	40,41,41	4.64	21 (52%)	50,56,56	2.40	23 (46%)
25	SQD	22	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
32	ZEX	14	420	-	42,43,43	1.01	3 (7%)	55,60,60	2.20	19 (34%)
32	ZEX	32	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	11	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.58	13 (31%)
21	CL7	1B	605	-	66,73,73	2.23	14 (21%)	65,113,113	2.22	15 (23%)
21	CL7	14	404	-	66,73,73	2.23	13 (19%)	65,113,113	2.20	16 (24%)
24	LMG	4D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
25	SQD	43	424	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	2B	604	-	66,73,73	2.21	13 (19%)	65,113,113	2.22	17 (26%)
21	CL7	4C	506	-	61,68,73	2.32	13 (21%)	59,107,113	2.39	18 (30%)
32	ZEX	24	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	23	415	-	46,53,73	2.64	14 (30%)	41,89,113	2.80	14 (34%)
21	CL7	32	501	-	66,73,73	2.17	12 (18%)	65,113,113	2.23	15 (23%)
21	CL7	11	411	-	46,53,73	2.65	12 (26%)	41,89,113	2.61	14 (34%)
23	8CT	2C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	22	511	16	61,68,73	2.33	12 (19%)	59,107,113	2.22	15 (25%)
21	CL7	11	417	18	56,63,73	2.41	14 (25%)	53,101,113	2.41	15 (28%)
21	CL7	4B	604	-	66,73,73	2.22	13 (19%)	65,113,113	2.22	17 (26%)
21	CL7	21	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.90	14 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	2D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	3I	408	-	66,73,73	2.19	13 (19%)	65,113,113	2.31	19 (29%)
32	ZEX	22	524	-	42,43,43	1.03	3 (7%)	55,60,60	2.51	17 (30%)
23	8CT	4C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	2D	405	-	46,53,73	2.58	13 (28%)	41,89,113	2.74	16 (39%)
23	8CT	2B	620	-	40,41,41	4.58	21 (52%)	50,56,56	2.91	18 (36%)
21	CL7	24	410	-	46,53,73	2.62	12 (26%)	41,89,113	2.65	14 (34%)
21	CL7	21	409	-	46,53,73	2.61	13 (28%)	41,89,113	2.62	15 (36%)
21	CL7	3I	412	-	46,53,73	2.59	12 (26%)	41,89,113	2.71	14 (34%)
21	CL7	1C	505	-	66,73,73	2.22	14 (21%)	65,113,113	2.25	17 (26%)
21	CL7	43	403	-	59,66,73	2.36	13 (22%)	56,104,113	2.26	17 (30%)
21	CL7	2C	505	-	66,73,73	2.22	14 (21%)	65,113,113	2.26	17 (26%)
21	CL7	22	508	-	46,53,73	2.60	13 (28%)	41,89,113	2.65	14 (34%)
21	CL7	33	506	-	46,53,73	2.58	13 (28%)	41,89,113	2.73	14 (34%)
32	ZEX	13	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
24	LMG	3B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
32	ZEX	21	421	-	42,43,43	0.92	2 (4%)	55,60,60	2.23	20 (36%)
21	CL7	33	515	-	42,49,73	2.66	10 (23%)	36,84,113	2.86	15 (41%)
25	SQD	42	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
27	DGD	1B	624	-	63,63,67	0.83	2 (3%)	77,77,81	1.00	3 (3%)
21	CL7	11	409	-	46,53,73	2.61	13 (28%)	41,89,113	2.62	15 (36%)
21	CL7	22	504	-	46,53,73	2.63	13 (28%)	41,89,113	2.63	14 (34%)
21	CL7	41	416	-	42,49,73	2.73	10 (23%)	36,84,113	2.76	14 (38%)
23	8CT	2K	101	-	40,41,41	4.75	25 (62%)	50,56,56	2.65	15 (30%)
32	ZEX	32	522	-	42,43,43	1.05	4 (9%)	55,60,60	2.47	17 (30%)
21	CL7	11	420	18	46,53,73	2.62	12 (26%)	41,89,113	2.75	14 (34%)
21	CL7	21	403	-	61,68,73	2.28	13 (21%)	59,107,113	2.38	15 (25%)
21	CL7	44	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.50	19 (32%)
21	CL7	33	505	-	66,73,73	2.16	13 (19%)	65,113,113	2.34	15 (23%)
25	SQD	3A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
26	LHG	23	425	-	35,35,48	0.35	0	38,41,54	0.47	0
32	ZEX	22	522	-	42,43,43	1.04	3 (7%)	55,60,60	2.47	17 (30%)
24	LMG	1A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	3D	405	-	46,53,73	2.57	13 (28%)	41,89,113	2.73	16 (39%)
21	CL7	33	503	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	23	417	19	56,63,73	2.42	13 (23%)	53,101,113	2.43	19 (35%)
32	ZEX	44	418	-	42,43,43	0.85	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	24	417	20	43,50,73	2.68	11 (25%)	36,85,113	2.89	13 (36%)
21	CL7	43	402	-	66,73,73	2.21	13 (19%)	65,113,113	2.23	18 (27%)
27	DGD	2C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	32	505	-	66,73,73	2.22	13 (19%)	65,113,113	2.41	19 (29%)
23	8CT	3C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
21	CL7	44	404	-	66,73,73	2.23	14 (21%)	65,113,113	2.20	16 (24%)
24	LMG	41	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
21	CL7	1D	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.36	17 (30%)
21	CL7	43	417	19	56,63,73	2.42	13 (23%)	53,101,113	2.43	19 (35%)
26	LHG	4A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	23	412	19	66,73,73	2.18	15 (22%)	65,113,113	2.43	19 (29%)
21	CL7	3B	609	-	66,73,73	2.25	14 (21%)	65,113,113	2.16	15 (23%)
21	CL7	2A	403	-	56,63,73	2.41	14 (25%)	53,101,113	2.58	18 (33%)
21	CL7	3C	507	-	66,73,73	2.17	14 (21%)	65,113,113	2.26	17 (26%)
25	SQD	2B	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.53	1 (1%)
29	BCT	2D	403	28	2,3,3	0.99	0	2,3,3	1.67	1 (50%)
23	8CT	24	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	21	412	-	46,53,73	2.59	12 (26%)	41,89,113	2.70	15 (36%)
21	CL7	44	413	20	61,68,73	2.27	14 (22%)	59,107,113	2.32	16 (27%)
21	CL7	12	517	16	66,73,73	2.17	11 (16%)	65,113,113	2.20	17 (26%)
21	CL7	13	511	19	66,73,73	2.18	15 (22%)	65,113,113	2.43	19 (29%)
21	CL7	1A	403	-	56,63,73	2.40	14 (25%)	53,101,113	2.58	19 (35%)
21	CL7	43	410	-	66,73,73	2.21	11 (16%)	65,113,113	2.20	16 (24%)
21	CL7	2C	512	-	42,49,73	2.56	9 (21%)	36,84,113	2.88	14 (38%)
21	CL7	43	413	-	56,63,73	2.39	14 (25%)	53,101,113	2.45	18 (33%)
21	CL7	32	509	-	66,73,73	2.20	14 (21%)	65,113,113	2.17	15 (23%)
24	LMG	11	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
21	CL7	22	518	16	66,73,73	2.23	13 (19%)	65,113,113	2.17	17 (26%)
21	CL7	2B	608	-	61,68,73	2.30	13 (21%)	59,107,113	2.26	16 (27%)
21	CL7	1B	609	-	66,73,73	2.24	15 (22%)	65,113,113	2.16	15 (23%)
21	CL7	2D	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.37	17 (30%)
21	CL7	33	509	-	66,73,73	2.20	11 (16%)	65,113,113	2.19	16 (24%)
21	CL7	1B	603	-	66,73,73	2.21	13 (19%)	65,113,113	2.22	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	ZEX	34	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	18 (32%)
32	ZEX	11	421	-	42,43,43	0.93	1 (2%)	55,60,60	2.23	20 (36%)
32	ZEX	33	520	-	42,43,43	0.92	2 (4%)	55,60,60	2.65	22 (40%)
32	ZEX	34	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
23	8CT	2C	514	-	40,41,41	4.65	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	31	416	-	42,49,73	2.73	10 (23%)	36,84,113	2.76	14 (38%)
26	LHG	1B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	24	408	-	46,53,73	2.66	14 (30%)	41,89,113	2.66	13 (31%)
21	CL7	4C	501	-	66,73,73	2.19	13 (19%)	65,113,113	2.20	15 (23%)
32	ZEX	33	519	-	42,43,43	1.01	3 (7%)	55,60,60	2.58	17 (30%)
26	LHG	43	425	-	35,35,48	0.34	0	38,41,54	0.47	0
21	CL7	2B	610	-	66,73,73	2.24	14 (21%)	65,113,113	2.16	15 (23%)
32	ZEX	12	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
23	8CT	3B	626	-	40,41,41	4.70	24 (60%)	50,56,56	3.24	21 (42%)
25	SQD	42	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	3C	512	-	42,49,73	2.56	9 (21%)	36,84,113	2.89	14 (38%)
26	LHG	4B	624	-	44,44,48	0.31	0	47,50,54	0.39	0
23	8CT	4B	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
23	8CT	4D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.98	19 (38%)
21	CL7	41	411	-	46,53,73	2.64	12 (26%)	41,89,113	2.61	14 (34%)
21	CL7	44	417	20	43,50,73	2.66	11 (25%)	36,85,113	2.88	13 (36%)
21	CL7	4B	617	-	46,53,73	2.62	14 (30%)	41,89,113	2.59	16 (39%)
21	CL7	33	514	-	46,53,73	2.63	14 (30%)	41,89,113	2.80	14 (34%)
21	CL7	34	408	-	46,53,73	2.66	15 (32%)	41,89,113	2.66	13 (31%)
21	CL7	31	407	-	42,49,73	2.65	11 (26%)	36,84,113	2.81	15 (41%)
21	CL7	23	409	-	66,73,73	2.20	14 (21%)	65,113,113	2.24	18 (27%)
21	CL7	24	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.89	15 (41%)
21	CL7	34	411	-	66,73,73	2.23	14 (21%)	65,113,113	2.21	17 (26%)
22	PHO	1D	408	-	51,69,69	0.59	2 (3%)	47,99,99	0.88	1 (2%)
21	CL7	1C	508	-	66,73,73	2.22	13 (19%)	65,113,113	2.28	21 (32%)
26	LHG	3D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
32	ZEX	42	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	44	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.88	14 (34%)
23	8CT	2B	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	3C	509	-	66,73,73	2.21	14 (21%)	65,113,113	2.22	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	1B	610	-	66,73,73	2.15	13 (19%)	65,113,113	2.32	15 (23%)
21	CL7	14	412	-	66,73,73	2.22	13 (19%)	65,113,113	2.21	18 (27%)
21	CL7	33	507	-	66,73,73	2.15	13 (19%)	65,113,113	2.30	18 (27%)
21	CL7	11	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.95	15 (41%)
21	CL7	4C	503	-	66,73,73	2.19	13 (19%)	65,113,113	2.22	17 (26%)
21	CL7	41	420	18	46,53,73	2.63	12 (26%)	41,89,113	2.76	14 (34%)
21	CL7	42	501	-	66,73,73	2.17	12 (18%)	65,113,113	2.23	15 (23%)
21	CL7	2C	507	-	66,73,73	2.17	14 (21%)	65,113,113	2.25	18 (27%)
21	CL7	13	507	-	66,73,73	2.16	13 (19%)	65,113,113	2.30	18 (27%)
21	CL7	2A	401	-	66,73,73	2.27	14 (21%)	65,113,113	2.34	19 (29%)
23	8CT	44	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
31	HEM	2F	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
23	8CT	1B	626	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
23	8CT	4A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	21	414	-	42,49,73	2.73	10 (23%)	36,84,113	2.93	14 (38%)
21	CL7	32	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	17 (26%)
21	CL7	41	404	-	66,73,73	2.27	12 (18%)	65,113,113	2.24	16 (24%)
21	CL7	34	404	-	66,73,73	2.23	13 (19%)	65,113,113	2.21	16 (24%)
22	PHO	1A	402	-	51,69,69	0.74	2 (3%)	47,99,99	0.74	1 (2%)
21	CL7	33	511	19	66,73,73	2.19	15 (22%)	65,113,113	2.43	19 (29%)
21	CL7	4B	602	-	42,49,73	2.67	11 (26%)	36,84,113	2.82	12 (33%)
22	PHO	2D	408	-	51,69,69	0.60	2 (3%)	47,99,99	0.88	1 (2%)
21	CL7	4B	607	-	56,63,73	2.42	14 (25%)	53,101,113	2.48	18 (33%)
21	CL7	44	405	-	66,73,73	2.20	14 (21%)	65,113,113	2.30	21 (32%)
21	CL7	13	515	-	42,49,73	2.65	10 (23%)	36,84,113	2.85	15 (41%)
32	ZEX	24	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	3B	615	-	51,58,73	2.44	14 (27%)	47,95,113	2.64	17 (36%)
32	ZEX	42	522	-	42,43,43	1.04	5 (11%)	55,60,60	2.47	15 (27%)
21	CL7	14	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.89	15 (36%)
23	8CT	2C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	4C	513	-	46,53,73	2.63	12 (26%)	41,89,113	2.69	14 (34%)
21	CL7	4A	403	-	56,63,73	2.41	14 (25%)	53,101,113	2.58	18 (33%)
21	CL7	32	510	16	66,73,73	2.18	13 (19%)	65,113,113	2.24	18 (27%)
23	8CT	1B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
21	CL7	1B	601	-	42,49,73	2.68	11 (26%)	36,84,113	2.82	12 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	41	408	-	66,73,73	2.18	13 (19%)	65,113,113	2.31	19 (29%)
21	CL7	2C	502	-	61,68,73	2.29	14 (22%)	59,107,113	2.30	15 (25%)
31	HEM	4F	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
26	LHG	2B	624	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	12	513	-	46,53,73	2.66	13 (28%)	41,89,113	2.66	15 (36%)
21	CL7	33	512	-	56,63,73	2.38	14 (25%)	53,101,113	2.44	18 (33%)
21	CL7	34	410	-	46,53,73	2.62	13 (28%)	41,89,113	2.66	13 (31%)
21	CL7	13	504	-	66,73,73	2.21	13 (19%)	65,113,113	2.24	17 (26%)
25	SQD	31	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	33	508	-	66,73,73	2.20	14 (21%)	65,113,113	2.23	18 (27%)
21	CL7	13	505	-	66,73,73	2.16	13 (19%)	65,113,113	2.34	15 (23%)
21	CL7	12	504	-	46,53,73	2.63	13 (28%)	41,89,113	2.64	14 (34%)
21	CL7	2D	402	-	51,58,73	2.55	12 (23%)	47,95,113	2.47	15 (31%)
21	CL7	23	411	-	66,73,73	2.18	13 (19%)	65,113,113	2.22	18 (27%)
21	CL7	42	505	-	66,73,73	2.22	13 (19%)	65,113,113	2.40	19 (29%)
24	LMG	3D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
21	CL7	3B	622	-	46,53,73	2.67	12 (26%)	41,89,113	2.58	13 (31%)
21	CL7	43	404	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	18 (27%)
23	8CT	2B	601	-	40,41,41	4.71	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	12	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.28	17 (26%)
21	CL7	11	402	-	61,68,73	2.32	14 (22%)	59,107,113	2.37	15 (25%)
21	CL7	11	403	-	61,68,73	2.29	12 (19%)	59,107,113	2.38	15 (25%)
21	CL7	13	509	-	66,73,73	2.20	11 (16%)	65,113,113	2.19	16 (24%)
21	CL7	2B	623	-	46,53,73	2.67	12 (26%)	41,89,113	2.57	13 (31%)
21	CL7	33	502	-	59,66,73	2.35	13 (22%)	56,104,113	2.25	17 (30%)
21	CL7	31	405	-	46,53,73	2.62	13 (28%)	41,89,113	2.58	12 (29%)
21	CL7	31	417	18	56,63,73	2.42	14 (25%)	53,101,113	2.41	15 (28%)
21	CL7	44	406	-	66,73,73	2.20	11 (16%)	65,113,113	2.22	17 (26%)
21	CL7	32	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.28	16 (24%)
21	CL7	11	410	-	66,73,73	2.23	13 (19%)	65,113,113	2.17	16 (24%)
25	SQD	33	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	2C	511	3	43,50,73	2.69	11 (25%)	36,85,113	2.78	12 (33%)
26	LHG	24	401	-	48,48,48	0.28	0	51,54,54	0.34	0
23	8CT	2B	619	-	40,41,41	4.70	20 (50%)	50,56,56	2.67	20 (40%)
25	SQD	1A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	ZEX	31	422	-	42,43,43	0.96	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	11	414	-	42,49,73	2.74	11 (26%)	36,84,113	2.93	15 (41%)
21	CL7	4C	512	-	42,49,73	2.56	9 (21%)	36,84,113	2.90	14 (38%)
21	CL7	24	414	-	54,61,73	2.40	13 (24%)	50,98,113	2.53	16 (32%)
21	CL7	41	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.91	14 (38%)
21	CL7	1C	502	-	61,68,73	2.30	14 (22%)	59,107,113	2.31	15 (25%)
21	CL7	13	514	-	46,53,73	2.63	14 (30%)	41,89,113	2.80	14 (34%)
21	CL7	3B	607	-	61,68,73	2.29	13 (21%)	59,107,113	2.26	17 (28%)
21	CL7	12	514	-	46,53,73	2.62	13 (28%)	41,89,113	2.69	12 (29%)
21	CL7	4B	605	-	66,73,73	2.15	13 (19%)	65,113,113	2.22	17 (26%)
21	CL7	4C	511	3	43,50,73	2.69	11 (25%)	36,85,113	2.78	13 (36%)
21	CL7	42	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.31	17 (26%)
21	CL7	43	412	19	66,73,73	2.18	15 (22%)	65,113,113	2.42	19 (29%)
21	CL7	23	406	-	66,73,73	2.16	13 (19%)	65,113,113	2.33	15 (23%)
21	CL7	12	518	16	66,73,73	2.23	12 (18%)	65,113,113	2.17	17 (26%)
21	CL7	24	407	-	42,49,73	2.65	10 (23%)	36,84,113	2.84	14 (38%)
21	CL7	14	408	-	46,53,73	2.66	15 (32%)	41,89,113	2.67	13 (31%)
21	CL7	3C	508	-	66,73,73	2.22	13 (19%)	65,113,113	2.28	21 (32%)
25	SQD	3B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
32	ZEX	14	403	-	42,43,43	1.02	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	3C	505	-	66,73,73	2.22	14 (21%)	65,113,113	2.26	17 (26%)
21	CL7	2B	602	-	42,49,73	2.66	10 (23%)	36,84,113	2.81	12 (33%)
21	CL7	14	417	20	43,50,73	2.66	11 (25%)	36,85,113	2.89	14 (38%)
21	CL7	3C	501	-	66,73,73	2.17	13 (19%)	65,113,113	2.19	15 (23%)
24	LMG	2A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
32	ZEX	23	420	-	42,43,43	1.02	4 (9%)	55,60,60	2.58	17 (30%)
32	ZEX	41	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	41	407	-	42,49,73	2.65	11 (26%)	36,84,113	2.81	16 (44%)
21	CL7	31	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.92	14 (38%)
24	LMG	4B	622	-	51,51,55	0.24	0	59,59,63	0.33	0
25	SQD	33	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	34	407	-	42,49,73	2.64	10 (23%)	36,84,113	2.85	14 (38%)
21	CL7	33	501	-	66,73,73	2.22	13 (19%)	65,113,113	2.23	18 (27%)
24	LMG	31	401	-	51,51,55	0.22	0	59,59,63	0.42	1 (1%)
24	LMG	2B	622	-	51,51,55	0.25	0	59,59,63	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	23	402	-	66,73,73	2.22	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	34	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.89	15 (41%)
32	ZEX	34	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
26	LHG	4B	626	-	48,48,48	0.30	0	51,54,54	0.34	0
30	PL9	4D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
23	8CT	14	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.77	21 (42%)
21	CL7	2B	603	-	61,68,73	2.32	12 (19%)	59,107,113	2.39	18 (30%)
21	CL7	2C	501	-	66,73,73	2.17	13 (19%)	65,113,113	2.19	15 (23%)
21	CL7	32	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.18	16 (24%)
23	8CT	3A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	23	403	-	59,66,73	2.36	13 (22%)	56,104,113	2.26	17 (30%)
21	CL7	21	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.94	15 (41%)
21	CL7	24	413	20	61,68,73	2.28	13 (21%)	59,107,113	2.32	16 (27%)
21	CL7	32	515	-	46,53,73	2.62	12 (26%)	41,89,113	2.66	15 (36%)
23	8CT	4K	101	-	40,41,41	4.76	25 (62%)	50,56,56	2.66	16 (32%)
21	CL7	1B	612	-	66,73,73	2.15	13 (19%)	65,113,113	2.27	18 (27%)
21	CL7	21	418	18	66,73,73	2.17	12 (18%)	65,113,113	2.31	19 (29%)
24	LMG	1B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	3B	612	-	66,73,73	2.15	13 (19%)	65,113,113	2.29	18 (27%)
25	SQD	41	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	12	508	-	46,53,73	2.59	14 (30%)	41,89,113	2.65	13 (31%)
32	ZEX	33	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
23	8CT	1D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	3A	407	-	66,73,73	2.24	13 (19%)	65,113,113	2.30	16 (24%)
21	CL7	4C	507	-	66,73,73	2.18	14 (21%)	65,113,113	2.26	18 (27%)
21	CL7	41	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.94	15 (41%)
32	ZEX	31	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.22	20 (36%)
23	8CT	1C	514	-	40,41,41	4.63	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	23	410	-	66,73,73	2.20	11 (16%)	65,113,113	2.19	16 (24%)
21	CL7	13	510	-	66,73,73	2.18	13 (19%)	65,113,113	2.22	18 (27%)
21	CL7	2A	407	-	66,73,73	2.24	13 (19%)	65,113,113	2.30	16 (24%)
27	DGD	1C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
23	8CT	4B	601	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	12	510	16	66,73,73	2.19	13 (19%)	65,113,113	2.24	18 (27%)
21	CL7	11	418	18	66,73,73	2.18	12 (18%)	65,113,113	2.32	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	SQD	4A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
30	PL9	3D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	42	502	-	66,73,73	2.18	13 (19%)	65,113,113	2.25	18 (27%)
21	CL7	42	510	16	66,73,73	2.18	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	24	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.87	14 (34%)
23	8CT	1C	518	-	40,41,41	4.65	21 (52%)	50,56,56	2.71	20 (40%)
25	SQD	12	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	2B	617	-	46,53,73	2.62	14 (30%)	41,89,113	2.59	16 (39%)
32	ZEX	43	421	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
23	8CT	3D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	11	405	-	46,53,73	2.64	13 (28%)	41,89,113	2.60	12 (29%)
21	CL7	3C	510	-	66,73,73	2.24	11 (16%)	65,113,113	2.20	18 (27%)
21	CL7	43	416	-	42,49,73	2.65	10 (23%)	36,84,113	2.86	15 (41%)
21	CL7	2C	508	-	66,73,73	2.21	13 (19%)	65,113,113	2.29	21 (32%)
21	CL7	32	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.24	19 (29%)
21	CL7	31	420	18	46,53,73	2.62	12 (26%)	41,89,113	2.75	14 (34%)
21	CL7	43	408	-	66,73,73	2.15	13 (19%)	65,113,113	2.30	17 (26%)
29	BCT	4D	403	28	2,3,3	0.99	0	2,3,3	1.66	1 (50%)
21	CL7	14	407	-	42,49,73	2.64	9 (21%)	36,84,113	2.84	14 (38%)
32	ZEX	12	520	-	42,43,43	0.97	3 (7%)	55,60,60	2.19	17 (30%)
21	CL7	3B	610	-	66,73,73	2.16	13 (19%)	65,113,113	2.31	15 (23%)
21	CL7	42	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.29	17 (26%)
25	SQD	23	422	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	21	416	-	42,49,73	2.72	10 (23%)	36,84,113	2.75	14 (38%)
26	LHG	4D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	1C	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.23	16 (24%)
21	CL7	1B	614	-	61,68,73	2.30	14 (22%)	59,107,113	2.36	19 (32%)
21	CL7	2C	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.24	16 (24%)
21	CL7	42	513	-	46,53,73	2.66	13 (28%)	41,89,113	2.67	15 (36%)
21	CL7	13	517	19	51,58,73	2.49	13 (25%)	47,95,113	2.54	14 (29%)
21	CL7	23	405	-	66,73,73	2.20	13 (19%)	65,113,113	2.25	17 (26%)
21	CL7	24	405	-	66,73,73	2.21	13 (19%)	65,113,113	2.31	20 (30%)
21	CL7	2B	607	-	56,63,73	2.42	14 (25%)	53,101,113	2.48	17 (32%)
21	CL7	4C	505	-	66,73,73	2.22	14 (21%)	65,113,113	2.24	17 (26%)
21	CL7	3B	606	-	56,63,73	2.42	14 (25%)	53,101,113	2.48	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	42	511	16	61,68,73	2.33	13 (21%)	59,107,113	2.22	15 (25%)
21	CL7	32	517	16	66,73,73	2.18	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	43	406	-	66,73,73	2.16	13 (19%)	65,113,113	2.34	15 (23%)
25	SQD	43	422	-	45,46,54	0.42	0	54,57,65	0.48	0
21	CL7	22	513	-	46,53,73	2.66	13 (28%)	41,89,113	2.67	15 (36%)
24	LMG	3A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
25	SQD	13	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
32	ZEX	32	519	-	42,43,43	1.06	3 (7%)	55,60,60	2.50	16 (29%)
25	SQD	12	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	13	501	-	66,73,73	2.22	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	22	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	19 (29%)
21	CL7	14	413	20	61,68,73	2.28	14 (22%)	59,107,113	2.33	16 (27%)
21	CL7	21	406	-	63,70,73	2.27	12 (19%)	61,109,113	2.30	14 (22%)
21	CL7	12	505	-	66,73,73	2.23	13 (19%)	65,113,113	2.41	19 (29%)
21	CL7	24	412	-	66,73,73	2.22	13 (19%)	65,113,113	2.21	18 (27%)
21	CL7	12	501	-	66,73,73	2.17	12 (18%)	65,113,113	2.23	15 (23%)
21	CL7	43	415	-	46,53,73	2.63	14 (30%)	41,89,113	2.81	14 (34%)
21	CL7	23	418	19	51,58,73	2.49	13 (25%)	47,95,113	2.54	14 (29%)
21	CL7	41	417	18	56,63,73	2.42	14 (25%)	53,101,113	2.41	15 (28%)
21	CL7	31	402	-	61,68,73	2.31	14 (22%)	59,107,113	2.38	15 (25%)
21	CL7	4B	614	-	56,63,73	2.38	14 (25%)	53,101,113	2.41	17 (32%)
22	PHO	2A	402	-	51,69,69	0.74	2 (3%)	47,99,99	0.74	1 (2%)
23	8CT	3C	515	-	40,41,41	4.64	20 (50%)	50,56,56	3.06	22 (44%)
32	ZEX	44	420	-	42,43,43	1.01	3 (7%)	55,60,60	2.20	18 (32%)
21	CL7	41	409	-	46,53,73	2.62	13 (28%)	41,89,113	2.62	15 (36%)
21	CL7	33	510	-	66,73,73	2.18	13 (19%)	65,113,113	2.22	18 (27%)
21	CL7	34	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.51	19 (32%)
21	CL7	2B	614	-	56,63,73	2.39	14 (25%)	53,101,113	2.42	17 (32%)
21	CL7	41	414	-	42,49,73	2.74	10 (23%)	36,84,113	2.93	14 (38%)
21	CL7	4B	603	-	61,68,73	2.32	12 (19%)	59,107,113	2.39	18 (30%)
21	CL7	34	414	-	54,61,73	2.39	13 (24%)	50,98,113	2.53	15 (30%)
21	CL7	22	509	-	66,73,73	2.21	14 (21%)	65,113,113	2.18	15 (23%)
21	CL7	41	412	-	46,53,73	2.60	12 (26%)	41,89,113	2.71	15 (36%)
21	CL7	34	412	-	66,73,73	2.21	12 (18%)	65,113,113	2.19	18 (27%)
21	CL7	3B	611	-	66,73,73	2.19	14 (21%)	65,113,113	2.25	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	2C	510	-	66,73,73	2.23	11 (16%)	65,113,113	2.19	18 (27%)
21	CL7	31	411	-	46,53,73	2.64	12 (26%)	41,89,113	2.61	14 (34%)
21	CL7	14	411	-	66,73,73	2.23	12 (18%)	65,113,113	2.21	17 (26%)
23	8CT	1C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
25	SQD	2A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	2C	504	-	56,63,73	2.42	12 (21%)	53,101,113	2.37	14 (26%)
32	ZEX	14	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
32	ZEX	34	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	22	517	16	66,73,73	2.18	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	4D	402	-	51,58,73	2.54	12 (23%)	47,95,113	2.47	15 (31%)
21	CL7	1B	607	-	61,68,73	2.30	13 (21%)	59,107,113	2.27	16 (27%)
21	CL7	13	506	-	46,53,73	2.59	15 (32%)	41,89,113	2.72	14 (34%)
21	CL7	2B	616	-	51,58,73	2.44	14 (27%)	47,95,113	2.63	17 (36%)
21	CL7	3B	614	-	61,68,73	2.30	14 (22%)	59,107,113	2.37	18 (30%)
21	CL7	32	502	-	66,73,73	2.19	13 (19%)	65,113,113	2.26	17 (26%)
21	CL7	12	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.19	16 (24%)
21	CL7	1C	507	-	66,73,73	2.18	14 (21%)	65,113,113	2.27	18 (27%)
21	CL7	32	503	-	66,73,73	2.18	15 (22%)	65,113,113	2.39	19 (29%)
21	CL7	1C	504	-	56,63,73	2.43	12 (21%)	53,101,113	2.38	14 (26%)
21	CL7	32	511	16	61,68,73	2.33	13 (21%)	59,107,113	2.22	15 (25%)
26	LHG	14	401	-	48,48,48	0.29	0	51,54,54	0.34	0
21	CL7	43	407	-	46,53,73	2.59	14 (30%)	41,89,113	2.73	14 (34%)
21	CL7	13	503	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	18 (27%)
21	CL7	43	418	19	51,58,73	2.49	13 (25%)	47,95,113	2.54	14 (29%)
21	CL7	42	515	-	46,53,73	2.62	12 (26%)	41,89,113	2.66	15 (36%)
21	CL7	22	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	17 (26%)
32	ZEX	23	421	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	4C	502	-	61,68,73	2.29	14 (22%)	59,107,113	2.30	15 (25%)
25	SQD	1B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.53	1 (1%)
23	8CT	4C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	4B	612	-	66,73,73	2.19	14 (21%)	65,113,113	2.27	15 (23%)
32	ZEX	13	519	-	42,43,43	1.02	3 (7%)	55,60,60	2.58	17 (30%)
21	CL7	14	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.51	20 (33%)
24	LMG	1D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
21	CL7	31	404	-	66,73,73	2.27	12 (18%)	65,113,113	2.25	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	3C	502	-	61,68,73	2.30	14 (22%)	59,107,113	2.30	15 (25%)
27	DGD	3C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
32	ZEX	41	422	-	42,43,43	0.95	2 (4%)	55,60,60	2.24	18 (32%)
23	8CT	1B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	33	504	-	66,73,73	2.20	13 (19%)	65,113,113	2.25	17 (26%)
21	CL7	21	407	-	42,49,73	2.66	11 (26%)	36,84,113	2.81	15 (41%)
21	CL7	1C	513	-	46,53,73	2.62	12 (26%)	41,89,113	2.68	14 (34%)
21	CL7	1B	615	-	51,58,73	2.44	14 (27%)	47,95,113	2.62	17 (36%)
21	CL7	1B	622	-	46,53,73	2.67	12 (26%)	41,89,113	2.57	13 (31%)
21	CL7	1C	510	-	66,73,73	2.23	11 (16%)	65,113,113	2.20	18 (27%)
21	CL7	3B	616	-	46,53,73	2.62	14 (30%)	41,89,113	2.60	16 (39%)
21	CL7	13	513	-	46,53,73	2.66	14 (30%)	41,89,113	2.66	13 (31%)
26	LHG	13	524	-	35,35,48	0.34	0	38,41,54	0.47	0
21	CL7	1C	503	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	17 (26%)
21	CL7	1B	606	-	56,63,73	2.43	14 (25%)	53,101,113	2.48	16 (30%)
21	CL7	24	406	-	66,73,73	2.21	12 (18%)	65,113,113	2.22	17 (26%)
21	CL7	42	517	16	66,73,73	2.18	12 (18%)	65,113,113	2.19	17 (26%)
21	CL7	31	406	-	63,70,73	2.27	12 (19%)	61,109,113	2.30	14 (22%)
21	CL7	32	513	-	46,53,73	2.65	13 (28%)	41,89,113	2.67	15 (36%)
32	ZEX	43	420	-	42,43,43	1.01	4 (9%)	55,60,60	2.58	17 (30%)
21	CL7	14	406	-	66,73,73	2.22	12 (18%)	65,113,113	2.22	17 (26%)
21	CL7	3B	608	-	66,73,73	2.19	13 (19%)	65,113,113	2.17	15 (23%)
26	LHG	33	524	-	35,35,48	0.34	0	38,41,54	0.47	0
21	CL7	41	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.57	13 (31%)
23	8CT	3B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.91	18 (36%)
21	CL7	23	414	-	46,53,73	2.66	14 (30%)	41,89,113	2.67	13 (31%)
21	CL7	4D	405	-	46,53,73	2.58	13 (28%)	41,89,113	2.73	16 (39%)
26	LHG	3B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	11	408	-	66,73,73	2.19	13 (19%)	65,113,113	2.31	19 (29%)
21	CL7	21	410	-	66,73,73	2.23	12 (18%)	65,113,113	2.17	16 (24%)
21	CL7	3D	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.36	17 (30%)
23	8CT	1A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
24	LMG	2D	410	-	33,33,55	0.28	0	41,41,63	0.33	0
32	ZEX	43	423	-	42,43,43	1.01	4 (9%)	55,60,60	2.39	17 (30%)
25	SQD	21	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	1B	616	-	46,53,73	2.61	14 (30%)	41,89,113	2.59	16 (39%)
23	8CT	3B	618	-	40,41,41	4.69	21 (52%)	50,56,56	2.66	20 (40%)
32	ZEX	13	520	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	1C	512	-	42,49,73	2.56	9 (21%)	36,84,113	2.91	14 (38%)
21	CL7	31	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.94	15 (41%)
21	CL7	21	404	-	66,73,73	2.28	12 (18%)	65,113,113	2.25	16 (24%)
21	CL7	11	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.91	14 (38%)
21	CL7	23	419	19	46,53,73	2.68	13 (28%)	41,89,113	2.66	14 (34%)
21	CL7	2B	612	-	66,73,73	2.19	14 (21%)	65,113,113	2.26	16 (24%)
32	ZEX	12	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	3B	613	-	56,63,73	2.38	14 (25%)	53,101,113	2.42	17 (32%)
32	ZEX	32	520	-	42,43,43	0.97	3 (7%)	55,60,60	2.18	17 (30%)
21	CL7	3B	601	-	42,49,73	2.66	11 (26%)	36,84,113	2.81	12 (33%)
23	8CT	3C	514	-	40,41,41	4.65	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	2B	606	-	66,73,73	2.24	14 (21%)	65,113,113	2.22	15 (23%)
21	CL7	3C	506	-	61,68,73	2.32	13 (21%)	59,107,113	2.40	18 (30%)
21	CL7	34	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.88	14 (34%)
32	ZEX	24	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
32	ZEX	44	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
21	CL7	44	412	-	66,73,73	2.22	12 (18%)	65,113,113	2.21	18 (27%)
21	CL7	21	405	-	46,53,73	2.63	14 (30%)	41,89,113	2.60	12 (29%)
21	CL7	43	419	19	46,53,73	2.68	13 (28%)	41,89,113	2.66	14 (34%)
22	PHO	4A	402	-	51,69,69	0.73	2 (3%)	47,99,99	0.74	1 (2%)
21	CL7	2B	615	-	61,68,73	2.31	14 (22%)	59,107,113	2.37	19 (32%)
25	SQD	11	423	-	31,32,54	0.49	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	31	403	-	61,68,73	2.30	12 (19%)	59,107,113	2.38	15 (25%)
22	PHO	3A	402	-	51,69,69	0.74	2 (3%)	47,99,99	0.74	1 (2%)
21	CL7	33	518	19	46,53,73	2.68	12 (26%)	41,89,113	2.66	14 (34%)
21	CL7	11	404	-	66,73,73	2.27	12 (18%)	65,113,113	2.25	16 (24%)
22	PHO	4D	408	-	51,69,69	0.59	1 (1%)	47,99,99	0.88	2 (4%)
21	CL7	22	510	16	66,73,73	2.19	14 (21%)	65,113,113	2.23	18 (27%)
23	8CT	1B	618	-	40,41,41	4.69	20 (50%)	50,56,56	2.67	20 (40%)
21	CL7	44	407	-	42,49,73	2.65	10 (23%)	36,84,113	2.85	14 (38%)
21	CL7	22	502	-	66,73,73	2.19	13 (19%)	65,113,113	2.25	18 (27%)
21	CL7	21	417	18	56,63,73	2.43	14 (25%)	53,101,113	2.41	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	32	514	-	46,53,73	2.63	13 (28%)	41,89,113	2.69	12 (29%)
21	CL7	42	503	-	66,73,73	2.18	15 (22%)	65,113,113	2.38	19 (29%)
21	CL7	2C	506	-	61,68,73	2.31	13 (21%)	59,107,113	2.38	18 (30%)
21	CL7	1B	613	-	56,63,73	2.38	14 (25%)	53,101,113	2.42	17 (32%)
21	CL7	3D	402	-	51,58,73	2.54	12 (23%)	47,95,113	2.47	15 (31%)
21	CL7	24	411	-	66,73,73	2.22	12 (18%)	65,113,113	2.21	17 (26%)
21	CL7	42	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	19 (29%)
23	8CT	3K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.66	16 (32%)
21	CL7	4C	517	-	42,49,73	2.63	10 (23%)	36,84,113	2.84	14 (38%)
21	CL7	24	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.51	20 (33%)
21	CL7	31	410	-	66,73,73	2.25	13 (19%)	65,113,113	2.18	16 (24%)
21	CL7	4B	613	-	66,73,73	2.16	13 (19%)	65,113,113	2.28	18 (27%)
32	ZEX	21	422	-	42,43,43	0.95	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	31	418	18	66,73,73	2.17	13 (19%)	65,113,113	2.31	21 (32%)
21	CL7	3C	517	-	42,49,73	2.63	10 (23%)	36,84,113	2.83	14 (38%)
21	CL7	32	518	16	66,73,73	2.23	12 (18%)	65,113,113	2.17	16 (24%)
21	CL7	4C	510	-	66,73,73	2.23	11 (16%)	65,113,113	2.19	17 (26%)
21	CL7	1C	506	-	61,68,73	2.32	13 (21%)	59,107,113	2.39	18 (30%)
32	ZEX	11	422	-	42,43,43	0.96	2 (4%)	55,60,60	2.23	18 (32%)
21	CL7	1C	501	-	66,73,73	2.18	13 (19%)	65,113,113	2.18	15 (23%)
21	CL7	43	414	-	46,53,73	2.66	15 (32%)	41,89,113	2.68	13 (31%)
21	CL7	44	411	-	66,73,73	2.22	12 (18%)	65,113,113	2.20	17 (26%)
32	ZEX	42	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
32	ZEX	22	520	-	42,43,43	0.99	3 (7%)	55,60,60	2.18	17 (30%)
21	CL7	42	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.17	15 (23%)
24	LMG	4A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
31	HEM	1F	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
23	8CT	3B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.76	19 (38%)
21	CL7	22	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.28	17 (26%)
32	ZEX	23	401	-	42,43,43	1.18	5 (11%)	55,60,60	2.43	18 (32%)
25	SQD	4B	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
21	CL7	2B	609	-	66,73,73	2.19	13 (19%)	65,113,113	2.17	15 (23%)
21	CL7	43	409	-	66,73,73	2.19	14 (21%)	65,113,113	2.23	18 (27%)
29	BCT	3D	403	28	2,3,3	1.00	0	2,3,3	1.66	1 (50%)
21	CL7	24	404	-	66,73,73	2.23	13 (19%)	65,113,113	2.20	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	3A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	34	413	20	61,68,73	2.27	14 (22%)	59,107,113	2.32	16 (27%)
32	ZEX	43	401	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
25	SQD	23	424	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
30	PL9	1D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
26	LHG	2A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
32	ZEX	12	522	-	42,43,43	1.04	4 (9%)	55,60,60	2.47	17 (30%)

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	4B	623	-	2/2/11/20	6/13/91/115	-
32	ZEX	33	525	-	-	7/29/67/67	0/2/2/2
21	CL7	13	508	-	2/2/15/20	14/37/115/115	-
25	SQD	22	521	-	-	7/45/65/69	0/1/1/1
21	CL7	23	408	-	2/2/15/20	13/37/115/115	-
21	CL7	14	405	-	2/2/15/20	16/37/115/115	-
21	CL7	34	406	-	2/2/15/20	22/37/115/115	-
21	CL7	32	508	-	2/2/11/20	3/13/91/115	-
21	CL7	22	501	-	2/2/15/20	15/37/115/115	-
23	8CT	1K	101	-	-	10/29/63/63	0/2/2/2
26	LHG	44	401	-	-	8/53/53/53	-
21	CL7	3C	503	-	2/2/15/20	17/37/115/115	-
23	8CT	4B	620	-	-	4/29/63/63	0/2/2/2
32	ZEX	24	420	-	-	12/29/67/67	0/2/2/2
32	ZEX	14	419	-	-	9/29/67/67	0/2/2/2
21	CL7	33	517	19	2/2/12/20	7/19/97/115	-
21	CL7	4C	508	-	2/2/15/20	15/37/115/115	-
21	CL7	23	404	-	2/2/15/20	18/37/115/115	-
24	LMG	21	401	-	-	5/46/66/70	0/1/1/1
30	PL9	2D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	44	410	-	2/2/11/20	7/13/91/115	-
21	CL7	3B	602	-	2/2/14/20	7/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	1B	623	-	-	3/49/49/53	-
26	LHG	34	401	-	-	8/53/53/53	-
21	CL7	12	507	-	2/2/15/20	18/37/115/115	-
21	CL7	2C	517	-	2/2/10/20	3/8/86/115	-
21	CL7	11	407	-	2/2/10/20	2/8/86/115	-
21	CL7	33	513	-	2/2/11/20	7/13/91/115	-
21	CL7	3C	511	3	2/2/10/20	3/10/88/115	-
23	8CT	2D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	42	504	-	2/2/11/20	4/13/91/115	-
21	CL7	33	516	19	2/2/13/20	14/25/103/115	-
21	CL7	13	518	19	2/2/11/20	5/13/91/115	-
21	CL7	4A	401	-	2/2/15/20	16/37/115/115	-
21	CL7	41	402	-	2/2/14/20	14/31/109/115	-
21	CL7	13	512	-	2/2/13/20	12/25/103/115	-
21	CL7	4B	616	-	2/2/12/20	8/19/97/115	-
21	CL7	21	408	-	2/2/15/20	14/37/115/115	-
21	CL7	1C	511	3	2/2/10/20	3/10/88/115	-
21	CL7	22	515	-	2/2/11/20	6/13/91/115	-
21	CL7	41	406	-	2/2/14/20	11/34/112/115	-
21	CL7	41	403	-	2/2/14/20	9/31/109/115	-
25	SQD	13	523	-	-	7/45/65/69	0/1/1/1
32	ZEX	44	403	-	-	10/29/67/67	0/2/2/2
32	ZEX	42	520	-	-	6/29/67/67	0/2/2/2
21	CL7	11	416	-	2/2/10/20	2/8/86/115	-
21	CL7	14	410	-	2/2/11/20	7/13/91/115	-
21	CL7	2B	611	-	2/2/15/20	11/37/115/115	-
21	CL7	44	414	-	2/2/12/20	6/23/101/115	-
21	CL7	21	420	18	2/2/11/20	4/13/91/115	-
21	CL7	4B	615	-	2/2/14/20	12/31/109/115	-
21	CL7	1C	517	-	2/2/10/20	3/8/86/115	-
21	CL7	44	416	-	2/2/10/20	5/8/86/115	-
21	CL7	1D	405	-	2/2/11/20	6/13/91/115	-
21	CL7	41	410	-	2/2/15/20	15/37/115/115	-
21	CL7	11	406	-	2/2/14/20	11/34/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	4B	608	-	2/2/14/20	9/31/109/115	-
21	CL7	42	514	-	2/2/11/20	7/13/91/115	-
27	DGD	3B	624	-	-	7/51/91/95	0/2/2/2
21	CL7	4B	609	-	2/2/15/20	15/37/115/115	-
25	SQD	32	521	-	-	7/45/65/69	0/1/1/1
21	CL7	2C	503	-	2/2/15/20	17/37/115/115	-
31	HEM	3F	101	-	-	6/12/54/54	-
21	CL7	3B	603	-	2/2/15/20	12/37/115/115	-
21	CL7	32	504	-	2/2/11/20	4/13/91/115	-
21	CL7	1B	608	-	2/2/15/20	15/37/115/115	-
27	DGD	4C	516	-	-	9/51/91/95	0/2/2/2
21	CL7	12	503	-	2/2/15/20	17/37/115/115	-
21	CL7	1D	402	-	2/2/12/20	7/19/97/115	-
21	CL7	23	416	-	2/2/10/20	0/8/86/115	-
21	CL7	3B	605	-	2/2/15/20	16/37/115/115	-
21	CL7	42	518	16	2/2/15/20	10/37/115/115	-
21	CL7	3C	513	-	2/2/11/20	6/13/91/115	-
21	CL7	22	506	-	2/2/15/20	12/37/115/115	-
21	CL7	4C	504	-	2/2/13/20	11/25/103/115	-
32	ZEX	13	525	-	-	7/29/67/67	0/2/2/2
21	CL7	3C	504	-	2/2/13/20	11/25/103/115	-
21	CL7	12	515	-	2/2/11/20	6/13/91/115	-
21	CL7	31	409	-	2/2/11/20	4/13/91/115	-
21	CL7	4A	407	-	2/2/15/20	14/37/115/115	-
21	CL7	31	414	-	2/2/10/20	1/8/86/115	-
21	CL7	31	419	-	2/2/11/20	7/13/91/115	-
21	CL7	12	511	16	2/2/14/20	14/31/109/115	-
21	CL7	14	414	-	2/2/12/20	6/23/101/115	-
21	CL7	2B	605	-	2/2/15/20	15/37/115/115	-
21	CL7	12	509	-	2/2/15/20	14/37/115/115	-
21	CL7	3B	604	-	2/2/15/20	15/37/115/115	-
21	CL7	43	405	-	2/2/15/20	14/37/115/115	-
21	CL7	1A	401	-	2/2/15/20	16/37/115/115	-
21	CL7	4D	404	-	2/2/13/20	11/29/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	3B	625	-	-	6/53/53/53	-
32	ZEX	22	519	-	-	11/29/67/67	0/2/2/2
21	CL7	44	408	-	2/2/11/20	2/13/91/115	-
21	CL7	2C	513	-	2/2/11/20	6/13/91/115	-
21	CL7	21	402	-	2/2/14/20	14/31/109/115	-
26	LHG	2B	626	-	-	6/53/53/53	-
23	8CT	4B	619	-	-	10/29/63/63	0/2/2/2
27	DGD	4B	625	-	-	7/51/91/95	0/2/2/2
21	CL7	34	417	20	2/2/10/20	4/10/88/115	-
21	CL7	23	407	-	2/2/11/20	11/13/91/115	-
21	CL7	4B	606	-	2/2/15/20	16/37/115/115	-
21	CL7	4C	509	-	2/2/15/20	18/37/115/115	-
23	8CT	2A	404	-	-	5/29/63/63	0/2/2/2
27	DGD	2B	625	-	-	7/51/91/95	0/2/2/2
32	ZEX	23	423	-	-	5/29/67/67	0/2/2/2
21	CL7	42	506	-	2/2/15/20	12/37/115/115	-
21	CL7	21	411	-	2/2/11/20	5/13/91/115	-
22	PHO	3D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
25	SQD	32	523	-	-	0/36/56/69	0/1/1/1
21	CL7	1B	611	-	2/2/15/20	15/37/115/115	-
21	CL7	13	516	19	2/2/13/20	14/25/103/115	-
21	CL7	42	508	-	2/2/11/20	3/13/91/115	-
23	8CT	34	402	-	-	4/29/63/63	0/2/2/2
21	CL7	2B	613	-	2/2/15/20	15/37/115/115	-
21	CL7	3A	403	-	2/2/13/20	9/25/103/115	-
21	CL7	12	516	-	2/2/15/20	14/37/115/115	-
21	CL7	13	502	-	2/2/13/20	10/29/107/115	-
21	CL7	41	418	18	2/2/15/20	20/37/115/115	-
21	CL7	22	514	-	2/2/11/20	7/13/91/115	-
21	CL7	12	502	-	2/2/15/20	15/37/115/115	-
21	CL7	1B	604	-	2/2/15/20	15/37/115/115	-
21	CL7	1A	407	-	2/2/15/20	14/37/115/115	-
21	CL7	21	419	-	2/2/11/20	7/13/91/115	-
21	CL7	1B	602	-	2/2/14/20	7/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	22	505	-	2/2/15/20	16/37/115/115	-
21	CL7	43	411	-	2/2/15/20	14/37/115/115	-
26	LHG	1A	408	-	-	5/50/50/53	-
21	CL7	41	405	-	2/2/11/20	9/13/91/115	-
21	CL7	23	413	-	2/2/13/20	12/25/103/115	-
21	CL7	34	405	-	2/2/15/20	16/37/115/115	-
21	CL7	4B	610	-	2/2/15/20	12/37/115/115	-
21	CL7	3A	401	-	2/2/15/20	16/37/115/115	-
26	LHG	1D	409	-	-	7/53/53/53	-
21	CL7	11	412	-	2/2/11/20	8/13/91/115	-
21	CL7	14	416	-	2/2/10/20	5/8/86/115	-
21	CL7	4B	611	-	2/2/15/20	11/37/115/115	-
21	CL7	22	503	-	2/2/15/20	17/37/115/115	-
23	8CT	4C	514	-	-	14/29/63/63	0/2/2/2
25	SQD	22	523	-	-	0/36/56/69	0/1/1/1
32	ZEX	14	420	-	-	12/29/67/67	0/2/2/2
32	ZEX	32	524	-	-	11/29/67/67	0/2/2/2
21	CL7	11	419	-	2/2/11/20	7/13/91/115	-
21	CL7	1B	605	-	2/2/15/20	16/37/115/115	-
21	CL7	14	404	-	2/2/15/20	15/37/115/115	-
24	LMG	4D	410	-	-	6/28/48/70	0/1/1/1
25	SQD	43	424	-	-	7/45/65/69	0/1/1/1
21	CL7	2B	604	-	2/2/15/20	12/37/115/115	-
21	CL7	4C	506	-	2/2/14/20	13/31/109/115	-
32	ZEX	24	418	-	-	9/29/67/67	0/2/2/2
21	CL7	23	415	-	2/2/11/20	5/13/91/115	-
21	CL7	32	501	-	2/2/15/20	15/37/115/115	-
21	CL7	11	411	-	2/2/11/20	5/13/91/115	-
23	8CT	2C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	22	511	16	2/2/14/20	14/31/109/115	-
21	CL7	11	417	18	2/2/13/20	7/25/103/115	-
21	CL7	4B	604	-	2/2/15/20	12/37/115/115	-
21	CL7	21	415	-	2/2/10/20	5/8/86/115	-
26	LHG	2D	409	-	-	7/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	31	408	-	2/2/15/20	14/37/115/115	-
32	ZEX	22	524	-	-	11/29/67/67	0/2/2/2
23	8CT	4C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	2D	405	-	2/2/11/20	6/13/91/115	-
23	8CT	2B	620	-	-	4/29/63/63	0/2/2/2
21	CL7	24	410	-	2/2/11/20	7/13/91/115	-
21	CL7	21	409	-	2/2/11/20	4/13/91/115	-
21	CL7	31	412	-	2/2/11/20	8/13/91/115	-
21	CL7	1C	505	-	2/2/15/20	14/37/115/115	-
21	CL7	43	403	-	2/2/13/20	10/29/107/115	-
21	CL7	2C	505	-	2/2/15/20	14/37/115/115	-
21	CL7	22	508	-	2/2/11/20	3/13/91/115	-
21	CL7	33	506	-	2/2/11/20	11/13/91/115	-
32	ZEX	13	522	-	-	5/29/67/67	0/2/2/2
24	LMG	3B	621	-	-	7/46/66/70	0/1/1/1
32	ZEX	21	421	-	-	14/29/67/67	0/2/2/2
21	CL7	33	515	-	2/2/10/20	0/8/86/115	-
25	SQD	42	521	-	-	7/45/65/69	0/1/1/1
27	DGD	1B	624	-	-	7/51/91/95	0/2/2/2
21	CL7	11	409	-	2/2/11/20	4/13/91/115	-
21	CL7	22	504	-	2/2/11/20	4/13/91/115	-
21	CL7	41	416	-	2/2/10/20	2/8/86/115	-
23	8CT	2K	101	-	-	10/29/63/63	0/2/2/2
32	ZEX	32	522	-	-	6/29/67/67	0/2/2/2
21	CL7	11	420	18	2/2/11/20	4/13/91/115	-
21	CL7	21	403	-	2/2/14/20	9/31/109/115	-
21	CL7	44	409	-	2/2/14/20	15/31/109/115	-
21	CL7	33	505	-	2/2/15/20	14/37/115/115	-
25	SQD	3A	406	-	-	3/29/49/69	0/1/1/1
26	LHG	23	425	-	-	3/40/40/53	-
32	ZEX	22	522	-	-	6/29/67/67	0/2/2/2
24	LMG	1A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	3D	405	-	2/2/11/20	6/13/91/115	-
21	CL7	33	503	-	2/2/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	23	417	19	2/2/13/20	14/25/103/115	-
32	ZEX	44	418	-	-	9/29/67/67	0/2/2/2
21	CL7	24	417	20	2/2/10/20	4/10/88/115	-
21	CL7	43	402	-	2/2/15/20	19/37/115/115	-
27	DGD	2C	516	-	-	9/51/91/95	0/2/2/2
21	CL7	32	505	-	2/2/15/20	16/37/115/115	-
23	8CT	3C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	44	404	-	2/2/15/20	14/37/115/115	-
24	LMG	41	401	-	-	5/46/66/70	0/1/1/1
21	CL7	1D	404	-	2/2/13/20	11/29/107/115	-
21	CL7	43	417	19	2/2/13/20	14/25/103/115	-
26	LHG	4A	408	-	-	5/50/50/53	-
21	CL7	23	412	19	2/2/15/20	17/37/115/115	-
21	CL7	3B	609	-	2/2/15/20	12/37/115/115	-
21	CL7	2A	403	-	2/2/13/20	9/25/103/115	-
21	CL7	3C	507	-	2/2/15/20	15/37/115/115	-
25	SQD	2B	621	-	-	5/49/69/69	0/1/1/1
23	8CT	24	402	-	-	4/29/63/63	0/2/2/2
21	CL7	21	412	-	2/2/11/20	8/13/91/115	-
21	CL7	44	413	20	2/2/14/20	7/31/109/115	-
21	CL7	12	517	16	2/2/15/20	19/37/115/115	-
21	CL7	13	511	19	2/2/15/20	17/37/115/115	-
21	CL7	1A	403	-	2/2/13/20	9/25/103/115	-
21	CL7	43	410	-	2/2/15/20	15/37/115/115	-
21	CL7	2C	512	-	2/2/10/20	2/8/86/115	-
21	CL7	43	413	-	2/2/13/20	12/25/103/115	-
21	CL7	32	509	-	2/2/15/20	14/37/115/115	-
24	LMG	11	401	-	-	5/46/66/70	0/1/1/1
21	CL7	22	518	16	2/2/15/20	10/37/115/115	-
21	CL7	2B	608	-	2/2/14/20	9/31/109/115	-
21	CL7	1B	609	-	2/2/15/20	12/37/115/115	-
21	CL7	2D	404	-	2/2/13/20	11/29/107/115	-
21	CL7	33	509	-	2/2/15/20	15/37/115/115	-
21	CL7	1B	603	-	2/2/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZEX	34	420	-	-	12/29/67/67	0/2/2/2
32	ZEX	11	421	-	-	14/29/67/67	0/2/2/2
32	ZEX	33	520	-	-	10/29/67/67	0/2/2/2
32	ZEX	34	419	-	-	9/29/67/67	0/2/2/2
23	8CT	2C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	31	416	-	2/2/10/20	2/8/86/115	-
26	LHG	1B	625	-	-	6/53/53/53	-
21	CL7	24	408	-	2/2/11/20	2/13/91/115	-
21	CL7	4C	501	-	2/2/15/20	18/37/115/115	-
32	ZEX	33	519	-	-	10/29/67/67	0/2/2/2
26	LHG	43	425	-	-	3/40/40/53	-
21	CL7	2B	610	-	2/2/15/20	12/37/115/115	-
32	ZEX	12	519	-	-	11/29/67/67	0/2/2/2
23	8CT	3B	626	-	-	10/29/63/63	0/2/2/2
25	SQD	42	523	-	-	0/36/56/69	0/1/1/1
21	CL7	3C	512	-	2/2/10/20	2/8/86/115	-
26	LHG	4B	624	-	-	3/49/49/53	-
23	8CT	4B	618	-	-	7/29/63/63	0/2/2/2
23	8CT	4D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	41	411	-	2/2/11/20	5/13/91/115	-
21	CL7	44	417	20	2/2/10/20	4/10/88/115	-
21	CL7	4B	617	-	2/2/11/20	4/13/91/115	-
21	CL7	33	514	-	2/2/11/20	5/13/91/115	-
21	CL7	34	408	-	2/2/11/20	2/13/91/115	-
21	CL7	31	407	-	2/2/10/20	2/8/86/115	-
21	CL7	23	409	-	2/2/15/20	14/37/115/115	-
21	CL7	24	416	-	2/2/10/20	5/8/86/115	-
21	CL7	34	411	-	2/2/15/20	12/37/115/115	-
22	PHO	1D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	1C	508	-	2/2/15/20	15/37/115/115	-
26	LHG	3D	409	-	-	7/53/53/53	-
32	ZEX	42	524	-	-	11/29/67/67	0/2/2/2
21	CL7	44	415	-	2/2/11/20	10/13/91/115	-
23	8CT	2B	618	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	3C	509	-	2/2/15/20	18/37/115/115	-
21	CL7	1B	610	-	2/2/15/20	11/37/115/115	-
21	CL7	14	412	-	2/2/15/20	17/37/115/115	-
21	CL7	33	507	-	2/2/15/20	13/37/115/115	-
21	CL7	11	413	-	2/2/10/20	2/8/86/115	-
21	CL7	4C	503	-	2/2/15/20	17/37/115/115	-
21	CL7	41	420	18	2/2/11/20	4/13/91/115	-
21	CL7	42	501	-	2/2/15/20	15/37/115/115	-
21	CL7	2C	507	-	2/2/15/20	15/37/115/115	-
21	CL7	13	507	-	2/2/15/20	13/37/115/115	-
21	CL7	2A	401	-	2/2/15/20	16/37/115/115	-
23	8CT	44	402	-	-	4/29/63/63	0/2/2/2
31	HEM	2F	101	-	-	6/12/54/54	-
23	8CT	1B	626	-	-	10/29/63/63	0/2/2/2
23	8CT	4A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	21	414	-	2/2/10/20	1/8/86/115	-
21	CL7	32	507	-	2/2/15/20	18/37/115/115	-
21	CL7	41	404	-	2/2/15/20	13/37/115/115	-
21	CL7	34	404	-	2/2/15/20	14/37/115/115	-
22	PHO	1A	402	-	-	3/37/103/103	0/5/6/6
21	CL7	33	511	19	2/2/15/20	17/37/115/115	-
21	CL7	4B	602	-	2/2/10/20	4/8/86/115	-
22	PHO	2D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	4B	607	-	2/2/13/20	4/25/103/115	-
21	CL7	44	405	-	2/2/15/20	16/37/115/115	-
21	CL7	13	515	-	2/2/10/20	0/8/86/115	-
32	ZEX	24	403	-	-	10/29/67/67	0/2/2/2
21	CL7	3B	615	-	2/2/12/20	8/19/97/115	-
32	ZEX	42	522	-	-	6/29/67/67	0/2/2/2
21	CL7	14	415	-	2/2/11/20	10/13/91/115	-
23	8CT	2C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	4C	513	-	2/2/11/20	6/13/91/115	-
21	CL7	4A	403	-	2/2/13/20	9/25/103/115	-
21	CL7	32	510	16	2/2/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	8CT	1B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	1B	601	-	2/2/10/20	4/8/86/115	-
21	CL7	41	408	-	2/2/15/20	14/37/115/115	-
21	CL7	2C	502	-	2/2/14/20	10/31/109/115	-
31	HEM	4F	101	-	-	6/12/54/54	-
26	LHG	2B	624	-	-	3/49/49/53	-
21	CL7	12	513	-	2/2/11/20	6/13/91/115	-
21	CL7	33	512	-	2/2/13/20	12/25/103/115	-
21	CL7	34	410	-	2/2/11/20	7/13/91/115	-
21	CL7	13	504	-	2/2/15/20	14/37/115/115	-
25	SQD	31	423	-	-	3/27/47/69	0/1/1/1
21	CL7	33	508	-	2/2/15/20	14/37/115/115	-
21	CL7	13	505	-	2/2/15/20	14/37/115/115	-
21	CL7	12	504	-	2/2/11/20	4/13/91/115	-
21	CL7	2D	402	-	2/2/12/20	7/19/97/115	-
21	CL7	23	411	-	2/2/15/20	13/37/115/115	-
21	CL7	42	505	-	2/2/15/20	16/37/115/115	-
24	LMG	3D	410	-	-	5/28/48/70	0/1/1/1
21	CL7	3B	622	-	2/2/11/20	6/13/91/115	-
21	CL7	43	404	-	2/2/15/20	18/37/115/115	-
23	8CT	2B	601	-	-	10/29/63/63	0/2/2/2
21	CL7	12	512	-	2/2/15/20	16/37/115/115	-
21	CL7	11	402	-	2/2/14/20	14/31/109/115	-
21	CL7	11	403	-	2/2/14/20	9/31/109/115	-
21	CL7	13	509	-	2/2/15/20	15/37/115/115	-
21	CL7	2B	623	-	2/2/11/20	6/13/91/115	-
21	CL7	33	502	-	2/2/13/20	10/29/107/115	-
21	CL7	31	405	-	2/2/11/20	9/13/91/115	-
21	CL7	31	417	18	2/2/13/20	7/25/103/115	-
21	CL7	44	406	-	2/2/15/20	22/37/115/115	-
21	CL7	32	512	-	2/2/15/20	16/37/115/115	-
21	CL7	11	410	-	2/2/15/20	15/37/115/115	-
25	SQD	33	523	-	-	7/45/65/69	0/1/1/1
21	CL7	2C	511	3	2/2/10/20	3/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	24	401	-	-	8/53/53/53	-
23	8CT	2B	619	-	-	10/29/63/63	0/2/2/2
25	SQD	1A	406	-	-	3/29/49/69	0/1/1/1
32	ZEX	31	422	-	-	6/29/67/67	0/2/2/2
21	CL7	11	414	-	2/2/10/20	1/8/86/115	-
21	CL7	4C	512	-	2/2/10/20	2/8/86/115	-
21	CL7	24	414	-	2/2/12/20	6/23/101/115	-
21	CL7	41	415	-	2/2/10/20	5/8/86/115	-
21	CL7	1C	502	-	2/2/14/20	10/31/109/115	-
21	CL7	13	514	-	2/2/11/20	5/13/91/115	-
21	CL7	3B	607	-	2/2/14/20	9/31/109/115	-
21	CL7	12	514	-	2/2/11/20	7/13/91/115	-
21	CL7	4B	605	-	2/2/15/20	15/37/115/115	-
21	CL7	4C	511	3	2/2/10/20	3/10/88/115	-
21	CL7	42	507	-	2/2/15/20	18/37/115/115	-
21	CL7	43	412	19	2/2/15/20	17/37/115/115	-
21	CL7	23	406	-	2/2/15/20	14/37/115/115	-
21	CL7	12	518	16	2/2/15/20	10/37/115/115	-
21	CL7	24	407	-	2/2/10/20	1/8/86/115	-
21	CL7	14	408	-	2/2/11/20	2/13/91/115	-
21	CL7	3C	508	-	2/2/15/20	15/37/115/115	-
25	SQD	3B	620	-	-	5/49/69/69	0/1/1/1
32	ZEX	14	403	-	-	10/29/67/67	0/2/2/2
21	CL7	3C	505	-	2/2/15/20	14/37/115/115	-
21	CL7	2B	602	-	2/2/10/20	4/8/86/115	-
21	CL7	14	417	20	2/2/10/20	4/10/88/115	-
21	CL7	3C	501	-	2/2/15/20	18/37/115/115	-
24	LMG	2A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
32	ZEX	23	420	-	-	10/29/67/67	0/2/2/2
32	ZEX	41	421	-	-	14/29/67/67	0/2/2/2
21	CL7	41	407	-	2/2/10/20	2/8/86/115	-
21	CL7	31	415	-	2/2/10/20	5/8/86/115	-
24	LMG	4B	622	-	-	7/46/66/70	0/1/1/1
25	SQD	33	521	-	-	3/41/61/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	34	407	-	2/2/10/20	1/8/86/115	-
21	CL7	33	501	-	2/2/15/20	19/37/115/115	-
24	LMG	31	401	-	-	5/46/66/70	0/1/1/1
24	LMG	2B	622	-	-	7/46/66/70	0/1/1/1
21	CL7	23	402	-	2/2/15/20	19/37/115/115	-
21	CL7	34	416	-	2/2/10/20	5/8/86/115	-
32	ZEX	34	403	-	-	10/29/67/67	0/2/2/2
26	LHG	4B	626	-	-	6/53/53/53	-
30	PL9	4D	407	-	-	9/53/73/73	0/1/1/1
23	8CT	14	402	-	-	4/29/63/63	0/2/2/2
21	CL7	2B	603	-	2/2/14/20	7/31/109/115	-
21	CL7	2C	501	-	2/2/15/20	18/37/115/115	-
21	CL7	32	506	-	2/2/15/20	12/37/115/115	-
23	8CT	3A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	23	403	-	2/2/13/20	10/29/107/115	-
21	CL7	21	413	-	2/2/10/20	2/8/86/115	-
21	CL7	24	413	20	2/2/14/20	7/31/109/115	-
21	CL7	32	515	-	2/2/11/20	6/13/91/115	-
23	8CT	4K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	1B	612	-	2/2/15/20	15/37/115/115	-
21	CL7	21	418	18	2/2/15/20	20/37/115/115	-
24	LMG	1B	621	-	-	7/46/66/70	0/1/1/1
21	CL7	3B	612	-	2/2/15/20	15/37/115/115	-
25	SQD	41	423	-	-	3/27/47/69	0/1/1/1
21	CL7	12	508	-	2/2/11/20	3/13/91/115	-
32	ZEX	33	522	-	-	5/29/67/67	0/2/2/2
23	8CT	1D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	3A	407	-	2/2/15/20	14/37/115/115	-
21	CL7	4C	507	-	2/2/15/20	15/37/115/115	-
21	CL7	41	413	-	2/2/10/20	2/8/86/115	-
32	ZEX	31	421	-	-	14/29/67/67	0/2/2/2
23	8CT	1C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	23	410	-	2/2/15/20	15/37/115/115	-
21	CL7	13	510	-	2/2/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2A	407	-	2/2/15/20	14/37/115/115	-
27	DGD	1C	516	-	-	9/51/91/95	0/2/2/2
23	8CT	4B	601	-	-	10/29/63/63	0/2/2/2
21	CL7	12	510	16	2/2/15/20	20/37/115/115	-
21	CL7	11	418	18	2/2/15/20	20/37/115/115	-
25	SQD	4A	406	-	-	3/29/49/69	0/1/1/1
30	PL9	3D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	42	502	-	2/2/15/20	15/37/115/115	-
21	CL7	42	510	16	2/2/15/20	20/37/115/115	-
21	CL7	24	415	-	2/2/11/20	10/13/91/115	-
23	8CT	1C	518	-	-	8/29/63/63	0/2/2/2
25	SQD	12	523	-	-	0/36/56/69	0/1/1/1
21	CL7	2B	617	-	2/2/11/20	4/13/91/115	-
32	ZEX	43	421	-	-	10/29/67/67	0/2/2/2
23	8CT	3D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	11	405	-	2/2/11/20	9/13/91/115	-
21	CL7	3C	510	-	2/2/15/20	20/37/115/115	-
21	CL7	43	416	-	2/2/10/20	0/8/86/115	-
21	CL7	2C	508	-	2/2/15/20	15/37/115/115	-
21	CL7	32	516	-	2/2/15/20	14/37/115/115	-
21	CL7	31	420	18	2/2/11/20	4/13/91/115	-
21	CL7	43	408	-	2/2/15/20	13/37/115/115	-
21	CL7	14	407	-	2/2/10/20	1/8/86/115	-
32	ZEX	12	520	-	-	6/29/67/67	0/2/2/2
21	CL7	3B	610	-	2/2/15/20	11/37/115/115	-
21	CL7	42	512	-	2/2/15/20	16/37/115/115	-
25	SQD	23	422	-	-	3/41/61/69	0/1/1/1
21	CL7	21	416	-	2/2/10/20	2/8/86/115	-
26	LHG	4D	409	-	-	7/53/53/53	-
21	CL7	1C	509	-	2/2/15/20	18/37/115/115	-
21	CL7	1B	614	-	2/2/14/20	12/31/109/115	-
21	CL7	2C	509	-	2/2/15/20	18/37/115/115	-
21	CL7	42	513	-	2/2/11/20	6/13/91/115	-
21	CL7	13	517	19	2/2/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	23	405	-	2/2/15/20	14/37/115/115	-
21	CL7	24	405	-	2/2/15/20	16/37/115/115	-
21	CL7	2B	607	-	2/2/13/20	4/25/103/115	-
21	CL7	4C	505	-	2/2/15/20	14/37/115/115	-
21	CL7	3B	606	-	2/2/13/20	4/25/103/115	-
21	CL7	42	511	16	2/2/14/20	14/31/109/115	-
21	CL7	32	517	16	2/2/15/20	19/37/115/115	-
21	CL7	43	406	-	2/2/15/20	14/37/115/115	-
25	SQD	43	422	-	-	3/41/61/69	0/1/1/1
21	CL7	22	513	-	2/2/11/20	6/13/91/115	-
24	LMG	3A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
25	SQD	13	521	-	-	3/41/61/69	0/1/1/1
32	ZEX	32	519	-	-	11/29/67/67	0/2/2/2
25	SQD	12	521	-	-	7/45/65/69	0/1/1/1
21	CL7	13	501	-	2/2/15/20	19/37/115/115	-
21	CL7	22	516	-	2/2/15/20	14/37/115/115	-
21	CL7	14	413	20	2/2/14/20	7/31/109/115	-
21	CL7	21	406	-	2/2/14/20	11/34/112/115	-
21	CL7	12	505	-	2/2/15/20	16/37/115/115	-
21	CL7	24	412	-	2/2/15/20	17/37/115/115	-
21	CL7	12	501	-	2/2/15/20	15/37/115/115	-
21	CL7	43	415	-	2/2/11/20	5/13/91/115	-
21	CL7	23	418	19	2/2/12/20	7/19/97/115	-
21	CL7	41	417	18	2/2/13/20	7/25/103/115	-
21	CL7	31	402	-	2/2/14/20	14/31/109/115	-
21	CL7	4B	614	-	2/2/13/20	4/25/103/115	-
22	PHO	2A	402	-	-	3/37/103/103	0/5/6/6
23	8CT	3C	515	-	-	10/29/63/63	0/2/2/2
32	ZEX	44	420	-	-	12/29/67/67	0/2/2/2
21	CL7	41	409	-	2/2/11/20	4/13/91/115	-
21	CL7	33	510	-	2/2/15/20	13/37/115/115	-
21	CL7	34	409	-	2/2/14/20	15/31/109/115	-
21	CL7	2B	614	-	2/2/13/20	4/25/103/115	-
21	CL7	41	414	-	2/2/10/20	1/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	4B	603	-	2/2/14/20	7/31/109/115	-
21	CL7	34	414	-	2/2/12/20	6/23/101/115	-
21	CL7	22	509	-	2/2/15/20	14/37/115/115	-
21	CL7	41	412	-	2/2/11/20	8/13/91/115	-
21	CL7	34	412	-	2/2/15/20	17/37/115/115	-
21	CL7	3B	611	-	2/2/15/20	15/37/115/115	-
21	CL7	2C	510	-	2/2/15/20	20/37/115/115	-
21	CL7	31	411	-	2/2/11/20	5/13/91/115	-
21	CL7	14	411	-	2/2/15/20	12/37/115/115	-
23	8CT	1C	515	-	-	10/29/63/63	0/2/2/2
25	SQD	2A	406	-	-	3/29/49/69	0/1/1/1
21	CL7	2C	504	-	2/2/13/20	11/25/103/115	-
32	ZEX	14	418	-	-	9/29/67/67	0/2/2/2
32	ZEX	34	418	-	-	9/29/67/67	0/2/2/2
21	CL7	22	517	16	2/2/15/20	19/37/115/115	-
21	CL7	4D	402	-	2/2/12/20	7/19/97/115	-
21	CL7	1B	607	-	2/2/14/20	9/31/109/115	-
21	CL7	13	506	-	2/2/11/20	11/13/91/115	-
21	CL7	2B	616	-	2/2/12/20	8/19/97/115	-
21	CL7	3B	614	-	2/2/14/20	12/31/109/115	-
21	CL7	32	502	-	2/2/15/20	15/37/115/115	-
21	CL7	12	506	-	2/2/15/20	12/37/115/115	-
21	CL7	1C	507	-	2/2/15/20	15/37/115/115	-
21	CL7	32	503	-	2/2/15/20	17/37/115/115	-
21	CL7	1C	504	-	2/2/13/20	11/25/103/115	-
21	CL7	32	511	16	2/2/14/20	14/31/109/115	-
26	LHG	14	401	-	-	8/53/53/53	-
21	CL7	43	407	-	2/2/11/20	11/13/91/115	-
21	CL7	13	503	-	2/2/15/20	18/37/115/115	-
21	CL7	43	418	19	2/2/12/20	7/19/97/115	-
21	CL7	42	515	-	2/2/11/20	6/13/91/115	-
21	CL7	22	507	-	2/2/15/20	18/37/115/115	-
32	ZEX	23	421	-	-	10/29/67/67	0/2/2/2
21	CL7	4C	502	-	2/2/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SQD	1B	620	-	-	5/49/69/69	0/1/1/1
23	8CT	4C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	4B	612	-	2/2/15/20	15/37/115/115	-
32	ZEX	13	519	-	-	10/29/67/67	0/2/2/2
21	CL7	14	409	-	2/2/14/20	15/31/109/115	-
24	LMG	1D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	31	404	-	2/2/15/20	13/37/115/115	-
21	CL7	3C	502	-	2/2/14/20	10/31/109/115	-
27	DGD	3C	516	-	-	9/51/91/95	0/2/2/2
32	ZEX	41	422	-	-	6/29/67/67	0/2/2/2
23	8CT	1B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	33	504	-	2/2/15/20	14/37/115/115	-
21	CL7	21	407	-	2/2/10/20	2/8/86/115	-
21	CL7	1C	513	-	2/2/11/20	6/13/91/115	-
21	CL7	1B	615	-	2/2/12/20	8/19/97/115	-
21	CL7	1B	622	-	2/2/11/20	6/13/91/115	-
21	CL7	1C	510	-	2/2/15/20	20/37/115/115	-
21	CL7	3B	616	-	2/2/11/20	4/13/91/115	-
21	CL7	13	513	-	2/2/11/20	7/13/91/115	-
26	LHG	13	524	-	-	3/40/40/53	-
21	CL7	1C	503	-	2/2/15/20	17/37/115/115	-
21	CL7	1B	606	-	2/2/13/20	4/25/103/115	-
21	CL7	24	406	-	2/2/15/20	22/37/115/115	-
21	CL7	42	517	16	2/2/15/20	19/37/115/115	-
21	CL7	31	406	-	2/2/14/20	11/34/112/115	-
21	CL7	32	513	-	2/2/11/20	6/13/91/115	-
32	ZEX	43	420	-	-	10/29/67/67	0/2/2/2
21	CL7	14	406	-	2/2/15/20	22/37/115/115	-
21	CL7	3B	608	-	2/2/15/20	15/37/115/115	-
26	LHG	33	524	-	-	3/40/40/53	-
21	CL7	41	419	-	2/2/11/20	7/13/91/115	-
23	8CT	3B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	23	414	-	2/2/11/20	7/13/91/115	-
21	CL7	4D	405	-	2/2/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	3B	623	-	-	3/49/49/53	-
21	CL7	11	408	-	2/2/15/20	14/37/115/115	-
21	CL7	21	410	-	2/2/15/20	15/37/115/115	-
21	CL7	3D	404	-	2/2/13/20	11/29/107/115	-
23	8CT	1A	404	-	-	5/29/63/63	0/2/2/2
24	LMG	2D	410	-	-	6/28/48/70	0/1/1/1
32	ZEX	43	423	-	-	5/29/67/67	0/2/2/2
25	SQD	21	423	-	-	3/27/47/69	0/1/1/1
21	CL7	1B	616	-	2/2/11/20	4/13/91/115	-
23	8CT	3B	618	-	-	10/29/63/63	0/2/2/2
32	ZEX	13	520	-	-	10/29/67/67	0/2/2/2
21	CL7	1C	512	-	2/2/10/20	2/8/86/115	-
21	CL7	31	413	-	2/2/10/20	2/8/86/115	-
21	CL7	21	404	-	2/2/15/20	13/37/115/115	-
21	CL7	11	415	-	2/2/10/20	5/8/86/115	-
21	CL7	23	419	19	2/2/11/20	5/13/91/115	-
21	CL7	2B	612	-	2/2/15/20	15/37/115/115	-
32	ZEX	12	524	-	-	11/29/67/67	0/2/2/2
21	CL7	3B	613	-	2/2/13/20	4/25/103/115	-
32	ZEX	32	520	-	-	6/29/67/67	0/2/2/2
21	CL7	3B	601	-	2/2/10/20	4/8/86/115	-
23	8CT	3C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	2B	606	-	2/2/15/20	16/37/115/115	-
21	CL7	3C	506	-	2/2/14/20	13/31/109/115	-
21	CL7	34	415	-	2/2/11/20	10/13/91/115	-
32	ZEX	24	419	-	-	9/29/67/67	0/2/2/2
32	ZEX	44	419	-	-	9/29/67/67	0/2/2/2
21	CL7	44	412	-	2/2/15/20	17/37/115/115	-
21	CL7	21	405	-	2/2/11/20	9/13/91/115	-
21	CL7	43	419	19	2/2/11/20	5/13/91/115	-
22	PHO	4A	402	-	-	3/37/103/103	0/5/6/6
21	CL7	2B	615	-	2/2/14/20	12/31/109/115	-
25	SQD	11	423	-	-	3/27/47/69	0/1/1/1
21	CL7	31	403	-	2/2/14/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PHO	3A	402	-	-	3/37/103/103	0/5/6/6
21	CL7	33	518	19	2/2/11/20	5/13/91/115	-
21	CL7	11	404	-	2/2/15/20	13/37/115/115	-
22	PHO	4D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	22	510	16	2/2/15/20	20/37/115/115	-
23	8CT	1B	618	-	-	10/29/63/63	0/2/2/2
21	CL7	44	407	-	2/2/10/20	1/8/86/115	-
21	CL7	22	502	-	2/2/15/20	15/37/115/115	-
21	CL7	21	417	18	2/2/13/20	7/25/103/115	-
21	CL7	32	514	-	2/2/11/20	7/13/91/115	-
21	CL7	42	503	-	2/2/15/20	17/37/115/115	-
21	CL7	2C	506	-	2/2/14/20	13/31/109/115	-
21	CL7	1B	613	-	2/2/13/20	4/25/103/115	-
21	CL7	3D	402	-	2/2/12/20	7/19/97/115	-
21	CL7	24	411	-	2/2/15/20	12/37/115/115	-
21	CL7	42	516	-	2/2/15/20	14/37/115/115	-
23	8CT	3K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	4C	517	-	2/2/10/20	3/8/86/115	-
21	CL7	24	409	-	2/2/14/20	15/31/109/115	-
21	CL7	31	410	-	2/2/15/20	15/37/115/115	-
21	CL7	4B	613	-	2/2/15/20	15/37/115/115	-
32	ZEX	21	422	-	-	6/29/67/67	0/2/2/2
21	CL7	31	418	18	2/2/15/20	20/37/115/115	-
21	CL7	3C	517	-	2/2/10/20	3/8/86/115	-
21	CL7	32	518	16	2/2/15/20	10/37/115/115	-
21	CL7	4C	510	-	2/2/15/20	20/37/115/115	-
21	CL7	1C	506	-	2/2/14/20	13/31/109/115	-
32	ZEX	11	422	-	-	6/29/67/67	0/2/2/2
21	CL7	1C	501	-	2/2/15/20	18/37/115/115	-
21	CL7	43	414	-	2/2/11/20	7/13/91/115	-
21	CL7	44	411	-	2/2/15/20	12/37/115/115	-
32	ZEX	42	519	-	-	11/29/67/67	0/2/2/2
32	ZEX	22	520	-	-	6/29/67/67	0/2/2/2
21	CL7	42	509	-	2/2/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	4A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
31	HEM	1F	101	-	-	6/12/54/54	-
23	8CT	3B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	22	512	-	2/2/15/20	16/37/115/115	-
32	ZEX	23	401	-	-	7/29/67/67	0/2/2/2
25	SQD	4B	621	-	-	5/49/69/69	0/1/1/1
21	CL7	2B	609	-	2/2/15/20	15/37/115/115	-
21	CL7	43	409	-	2/2/15/20	14/37/115/115	-
21	CL7	24	404	-	2/2/15/20	15/37/115/115	-
26	LHG	3A	408	-	-	5/50/50/53	-
21	CL7	34	413	20	2/2/14/20	7/31/109/115	-
32	ZEX	43	401	-	-	7/29/67/67	0/2/2/2
25	SQD	23	424	-	-	7/45/65/69	0/1/1/1
30	PL9	1D	407	-	-	9/53/73/73	0/1/1/1
26	LHG	2A	408	-	-	5/50/50/53	-
32	ZEX	12	522	-	-	6/29/67/67	0/2/2/2

The worst 5 of 6635 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 8780 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	NC
21	1A	401	CL7	NA
21	1A	403	CL7	NC
21	1A	403	CL7	NA
21	1A	407	CL7	NC

5 of 5870 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1A	403	CL7	O1A-CGA-O2A-C1
21	1A	403	CL7	CBA-CGA-O2A-C1
21	1A	403	CL7	C1A-C2A-CAA-CBA
21	1A	403	CL7	C3A-C2A-CAA-CBA
21	1A	407	CL7	C1A-C2A-CAA-CBA

There are no ring outliers.

552 monomers are involved in 2778 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	33	525	ZEX	24	0
21	13	508	CL7	15	0
25	22	521	SQD	2	0
21	23	408	CL7	9	0
21	14	405	CL7	6	0
21	34	406	CL7	13	0
21	32	508	CL7	4	0
21	22	501	CL7	8	0
26	44	401	LHG	1	0
21	3C	503	CL7	7	0
32	24	420	ZEX	12	0
32	14	419	ZEX	8	0
21	33	517	CL7	3	0
21	4C	508	CL7	6	0
21	23	404	CL7	11	0
24	21	401	LMG	2	0
30	2D	407	PL9	7	0
21	44	410	CL7	2	0
21	3B	602	CL7	4	0
26	1B	623	LHG	6	0
26	34	401	LHG	1	0
21	12	507	CL7	7	0
21	2C	517	CL7	1	0
21	11	407	CL7	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	33	513	CL7	12	0
21	3C	511	CL7	2	0
21	42	504	CL7	2	0
21	33	516	CL7	6	0
21	13	518	CL7	4	0
21	4A	401	CL7	20	0
21	41	402	CL7	9	0
21	13	512	CL7	6	0
21	4B	616	CL7	4	0
21	21	408	CL7	7	0
21	1C	511	CL7	2	0
21	22	515	CL7	2	0
21	41	406	CL7	15	0
21	41	403	CL7	6	0
25	13	523	SQD	2	0
32	44	403	ZEX	21	0
32	42	520	ZEX	30	0
21	11	416	CL7	2	0
21	14	410	CL7	2	0
21	2B	611	CL7	4	0
21	44	414	CL7	5	0
21	21	420	CL7	5	0
21	4B	615	CL7	2	0
21	1C	517	CL7	1	0
21	1D	405	CL7	2	0
21	41	410	CL7	5	0
21	11	406	CL7	13	0
21	4B	608	CL7	8	0
21	42	514	CL7	2	0
27	3B	624	DGD	2	0
21	4B	609	CL7	4	0
25	32	521	SQD	1	0
21	2C	503	CL7	6	0
31	3F	101	HEM	3	0
21	3B	603	CL7	6	0
21	32	504	CL7	2	0
21	1B	608	CL7	4	0
27	4C	516	DGD	3	0
21	12	503	CL7	8	0
21	1D	402	CL7	3	0
21	23	416	CL7	3	0
21	3B	605	CL7	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	42	518	CL7	11	0
21	3C	513	CL7	3	0
21	22	506	CL7	4	0
21	4C	504	CL7	4	0
32	13	525	ZEX	24	0
21	3C	504	CL7	4	0
21	12	515	CL7	2	0
21	31	409	CL7	3	0
21	4A	407	CL7	14	0
21	31	414	CL7	7	0
21	12	511	CL7	8	0
21	14	414	CL7	5	0
21	2B	605	CL7	8	0
21	12	509	CL7	7	0
21	3B	604	CL7	10	0
21	43	405	CL7	10	0
21	1A	401	CL7	20	0
21	4D	404	CL7	8	0
26	3B	625	LHG	1	0
32	22	519	ZEX	4	0
21	44	408	CL7	4	0
21	2C	513	CL7	3	0
21	21	402	CL7	9	0
26	2B	626	LHG	2	0
27	4B	625	DGD	2	0
21	34	417	CL7	5	0
21	23	407	CL7	5	0
21	4B	606	CL7	6	0
21	4C	509	CL7	4	0
27	2B	625	DGD	2	0
32	23	423	ZEX	27	0
21	42	506	CL7	3	0
21	21	411	CL7	3	0
22	3D	408	PHO	5	0
21	1B	611	CL7	4	0
21	13	516	CL7	6	0
21	42	508	CL7	4	0
21	2B	613	CL7	5	0
21	3A	403	CL7	2	0
21	12	516	CL7	6	0
21	13	502	CL7	7	0
21	41	418	CL7	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	22	514	CL7	2	0
21	12	502	CL7	8	0
21	1B	604	CL7	10	0
21	1A	407	CL7	16	0
21	1B	602	CL7	5	0
21	22	505	CL7	17	0
21	43	411	CL7	8	0
26	1A	408	LHG	1	0
21	41	405	CL7	4	0
21	23	413	CL7	7	0
21	34	405	CL7	6	0
21	4B	610	CL7	5	0
21	3A	401	CL7	21	0
26	1D	409	LHG	3	0
21	11	412	CL7	3	0
21	4B	611	CL7	2	0
21	22	503	CL7	5	0
32	14	420	ZEX	10	0
32	32	524	ZEX	17	0
21	1B	605	CL7	7	0
21	14	404	CL7	6	0
24	4D	410	LMG	1	0
25	43	424	SQD	2	0
21	2B	604	CL7	9	0
21	4C	506	CL7	5	0
32	24	418	ZEX	12	0
21	23	415	CL7	2	0
21	32	501	CL7	7	0
21	11	411	CL7	3	0
23	2C	515	8CT	1	0
21	22	511	CL7	8	0
21	11	417	CL7	4	0
21	4B	604	CL7	8	0
26	2D	409	LHG	4	0
21	31	408	CL7	7	0
32	22	524	ZEX	16	0
21	2D	405	CL7	2	0
21	24	410	CL7	2	0
21	21	409	CL7	4	0
21	31	412	CL7	3	0
21	1C	505	CL7	6	0
21	43	403	CL7	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2C	505	CL7	6	0
21	22	508	CL7	4	0
21	33	506	CL7	5	0
32	13	522	ZEX	27	0
24	3B	621	LMG	6	0
32	21	421	ZEX	16	0
21	33	515	CL7	3	0
25	42	521	SQD	2	0
27	1B	624	DGD	2	0
21	11	409	CL7	3	0
21	22	504	CL7	2	0
21	41	416	CL7	2	0
32	32	522	ZEX	17	0
21	11	420	CL7	6	0
21	21	403	CL7	6	0
21	44	409	CL7	3	0
21	33	505	CL7	19	0
25	3A	406	SQD	1	0
26	23	425	LHG	1	0
32	22	522	ZEX	17	0
24	1A	405	LMG	2	0
21	3D	405	CL7	2	0
21	33	503	CL7	10	0
21	23	417	CL7	6	0
32	44	418	ZEX	11	0
21	24	417	CL7	5	0
21	43	402	CL7	9	0
27	2C	516	DGD	3	0
21	32	505	CL7	15	0
21	44	404	CL7	6	0
24	41	401	LMG	2	0
21	1D	404	CL7	7	0
21	43	417	CL7	7	0
26	4A	408	LHG	1	0
21	23	412	CL7	6	0
21	3B	609	CL7	4	0
21	2A	403	CL7	2	0
21	3C	507	CL7	4	0
25	2B	621	SQD	2	0
21	21	412	CL7	3	0
21	44	413	CL7	5	0
21	12	517	CL7	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	13	511	CL7	6	0
21	1A	403	CL7	2	0
21	43	410	CL7	8	0
21	2C	512	CL7	1	0
21	43	413	CL7	8	0
21	32	509	CL7	7	0
24	11	401	LMG	2	0
21	22	518	CL7	12	0
21	2B	608	CL7	7	0
21	1B	609	CL7	5	0
21	2D	404	CL7	8	0
21	33	509	CL7	8	0
21	1B	603	CL7	7	0
32	34	420	ZEX	10	0
32	11	421	ZEX	14	0
32	33	520	ZEX	13	0
32	34	419	ZEX	8	0
21	31	416	CL7	2	0
26	1B	625	LHG	1	0
21	24	408	CL7	4	0
21	4C	501	CL7	3	0
32	33	519	ZEX	17	0
26	43	425	LHG	1	0
21	2B	610	CL7	5	0
32	12	519	ZEX	4	0
21	3C	512	CL7	2	0
26	4B	624	LHG	6	0
21	41	411	CL7	3	0
21	44	417	CL7	5	0
21	4B	617	CL7	1	0
21	33	514	CL7	2	0
21	34	408	CL7	4	0
21	31	407	CL7	3	0
21	23	409	CL7	14	0
21	34	411	CL7	7	0
22	1D	408	PHO	5	0
21	1C	508	CL7	4	0
26	3D	409	LHG	3	0
32	42	524	ZEX	17	0
21	44	415	CL7	4	0
21	3C	509	CL7	5	0
21	1B	610	CL7	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	14	412	CL7	4	0
21	33	507	CL7	10	0
21	11	413	CL7	5	0
21	4C	503	CL7	7	0
21	41	420	CL7	5	0
21	42	501	CL7	7	0
21	2C	507	CL7	5	0
21	13	507	CL7	10	0
21	2A	401	CL7	20	0
31	2F	101	HEM	4	0
21	21	414	CL7	7	0
21	32	507	CL7	6	0
21	41	404	CL7	9	0
21	34	404	CL7	5	0
22	1A	402	PHO	5	0
21	33	511	CL7	7	0
21	4B	602	CL7	1	0
22	2D	408	PHO	4	0
21	4B	607	CL7	4	0
21	44	405	CL7	7	0
21	13	515	CL7	3	0
32	24	403	ZEX	22	0
21	3B	615	CL7	4	0
32	42	522	ZEX	18	0
21	14	415	CL7	4	0
21	4C	513	CL7	3	0
21	4A	403	CL7	2	0
21	32	510	CL7	6	0
21	1B	601	CL7	1	0
21	41	408	CL7	8	0
21	2C	502	CL7	4	0
31	4F	101	HEM	4	0
26	2B	624	LHG	6	0
21	12	513	CL7	6	0
21	33	512	CL7	7	0
21	34	410	CL7	2	0
21	13	504	CL7	9	0
21	33	508	CL7	14	0
21	13	505	CL7	18	0
21	12	504	CL7	2	0
21	2D	402	CL7	3	0
21	23	411	CL7	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	42	505	CL7	14	0
24	3D	410	LMG	1	0
21	43	404	CL7	11	0
21	12	512	CL7	9	0
21	11	402	CL7	9	0
21	11	403	CL7	5	0
21	13	509	CL7	9	0
21	33	502	CL7	7	0
21	31	405	CL7	5	0
21	31	417	CL7	4	0
21	44	406	CL7	12	0
21	32	512	CL7	9	0
21	11	410	CL7	7	0
25	33	523	SQD	1	0
21	2C	511	CL7	2	0
26	24	401	LHG	1	0
25	1A	406	SQD	3	0
32	31	422	ZEX	21	0
21	11	414	CL7	2	0
21	4C	512	CL7	1	0
21	24	414	CL7	4	0
21	1C	502	CL7	4	0
21	13	514	CL7	2	0
21	3B	607	CL7	8	0
21	12	514	CL7	2	0
21	4B	605	CL7	9	0
21	4C	511	CL7	2	0
21	42	507	CL7	6	0
21	43	412	CL7	6	0
21	23	406	CL7	18	0
21	12	518	CL7	12	0
21	24	407	CL7	10	0
21	14	408	CL7	4	0
21	3C	508	CL7	4	0
25	3B	620	SQD	2	0
32	14	403	ZEX	22	0
21	3C	505	CL7	5	0
21	2B	602	CL7	1	0
21	14	417	CL7	5	0
21	3C	501	CL7	3	0
24	2A	405	LMG	2	0
32	23	420	ZEX	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	41	421	ZEX	15	0
21	41	407	CL7	3	0
24	4B	622	LMG	6	0
25	33	521	SQD	4	0
21	34	407	CL7	10	0
21	33	501	CL7	8	0
24	31	401	LMG	3	0
24	2B	622	LMG	5	0
21	23	402	CL7	10	0
32	34	403	ZEX	21	0
26	4B	626	LHG	2	0
30	4D	407	PL9	7	0
21	2B	603	CL7	4	0
21	2C	501	CL7	4	0
21	32	506	CL7	3	0
21	23	403	CL7	7	0
21	21	413	CL7	5	0
21	24	413	CL7	6	0
21	32	515	CL7	1	0
21	1B	612	CL7	3	0
21	21	418	CL7	8	0
24	1B	621	LMG	5	0
21	3B	612	CL7	3	0
21	12	508	CL7	4	0
32	33	522	ZEX	26	0
21	3A	407	CL7	15	0
21	4C	507	CL7	3	0
21	41	413	CL7	5	0
32	31	421	ZEX	15	0
21	23	410	CL7	10	0
21	13	510	CL7	8	0
21	2A	407	CL7	14	0
27	1C	516	DGD	5	0
21	12	510	CL7	6	0
21	11	418	CL7	7	0
25	4A	406	SQD	2	0
30	3D	407	PL9	7	0
21	42	502	CL7	8	0
21	42	510	CL7	7	0
21	24	415	CL7	4	0
21	2B	617	CL7	1	0
32	43	421	ZEX	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	11	405	CL7	4	0
21	3C	510	CL7	5	0
21	43	416	CL7	3	0
21	2C	508	CL7	5	0
21	32	516	CL7	6	0
21	31	420	CL7	6	0
21	43	408	CL7	10	0
21	14	407	CL7	10	0
32	12	520	ZEX	31	0
21	3B	610	CL7	1	0
21	42	512	CL7	9	0
25	23	422	SQD	4	0
21	21	416	CL7	2	0
26	4D	409	LHG	3	0
21	1C	509	CL7	4	0
21	1B	614	CL7	2	0
21	2C	509	CL7	3	0
21	42	513	CL7	6	0
21	13	517	CL7	3	0
21	23	405	CL7	9	0
21	24	405	CL7	5	0
21	2B	607	CL7	6	0
21	4C	505	CL7	6	0
21	3B	606	CL7	5	0
21	42	511	CL7	7	0
21	32	517	CL7	11	0
21	43	406	CL7	19	0
25	43	422	SQD	3	0
21	22	513	CL7	6	0
24	3A	405	LMG	2	0
25	13	521	SQD	4	0
32	32	519	ZEX	5	0
25	12	521	SQD	2	0
21	13	501	CL7	8	0
21	22	516	CL7	7	0
21	14	413	CL7	6	0
21	21	406	CL7	14	0
21	12	505	CL7	15	0
21	24	412	CL7	4	0
21	12	501	CL7	6	0
21	43	415	CL7	2	0
21	23	418	CL7	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	41	417	CL7	7	0
21	31	402	CL7	9	0
21	4B	614	CL7	2	0
22	2A	402	PHO	5	0
23	3C	515	8CT	1	0
32	44	420	ZEX	12	0
21	41	409	CL7	4	0
21	33	510	CL7	7	0
21	34	409	CL7	3	0
21	2B	614	CL7	2	0
21	41	414	CL7	2	0
21	4B	603	CL7	3	0
21	34	414	CL7	5	0
21	22	509	CL7	6	0
21	41	412	CL7	3	0
21	34	412	CL7	5	0
21	3B	611	CL7	5	0
21	2C	510	CL7	5	0
21	31	411	CL7	3	0
21	14	411	CL7	6	0
23	1C	515	8CT	1	0
25	2A	406	SQD	3	0
21	2C	504	CL7	4	0
32	14	418	ZEX	11	0
32	34	418	ZEX	11	0
21	22	517	CL7	10	0
21	4D	402	CL7	3	0
21	1B	607	CL7	8	0
21	13	506	CL7	5	0
21	2B	616	CL7	4	0
21	3B	614	CL7	2	0
21	32	502	CL7	9	0
21	12	506	CL7	3	0
21	1C	507	CL7	5	0
21	32	503	CL7	9	0
21	1C	504	CL7	4	0
21	32	511	CL7	9	0
26	14	401	LHG	1	0
21	43	407	CL7	5	0
21	13	503	CL7	10	0
21	43	418	CL7	3	0
21	42	515	CL7	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	22	507	CL7	6	0
32	23	421	ZEX	12	0
21	4C	502	CL7	3	0
25	1B	620	SQD	3	0
23	4C	515	8CT	1	0
21	4B	612	CL7	4	0
32	13	519	ZEX	16	0
21	14	409	CL7	3	0
24	1D	410	LMG	1	0
21	31	404	CL7	9	0
21	3C	502	CL7	3	0
27	3C	516	DGD	4	0
32	41	422	ZEX	22	0
21	33	504	CL7	10	0
21	21	407	CL7	2	0
21	1C	513	CL7	3	0
21	1B	615	CL7	4	0
21	1C	510	CL7	5	0
21	3B	616	CL7	1	0
21	13	513	CL7	12	0
26	13	524	LHG	1	0
21	1C	503	CL7	6	0
21	1B	606	CL7	5	0
21	24	406	CL7	13	0
21	42	517	CL7	11	0
21	31	406	CL7	13	0
21	32	513	CL7	6	0
32	43	420	ZEX	17	0
21	14	406	CL7	13	0
21	3B	608	CL7	4	0
26	33	524	LHG	1	0
21	23	414	CL7	12	0
21	4D	405	CL7	2	0
26	3B	623	LHG	6	0
21	11	408	CL7	7	0
21	21	410	CL7	6	0
21	3D	404	CL7	7	0
24	2D	410	LMG	1	0
32	43	423	ZEX	28	0
21	1B	616	CL7	1	0
32	13	520	ZEX	13	0
21	1C	512	CL7	2	0

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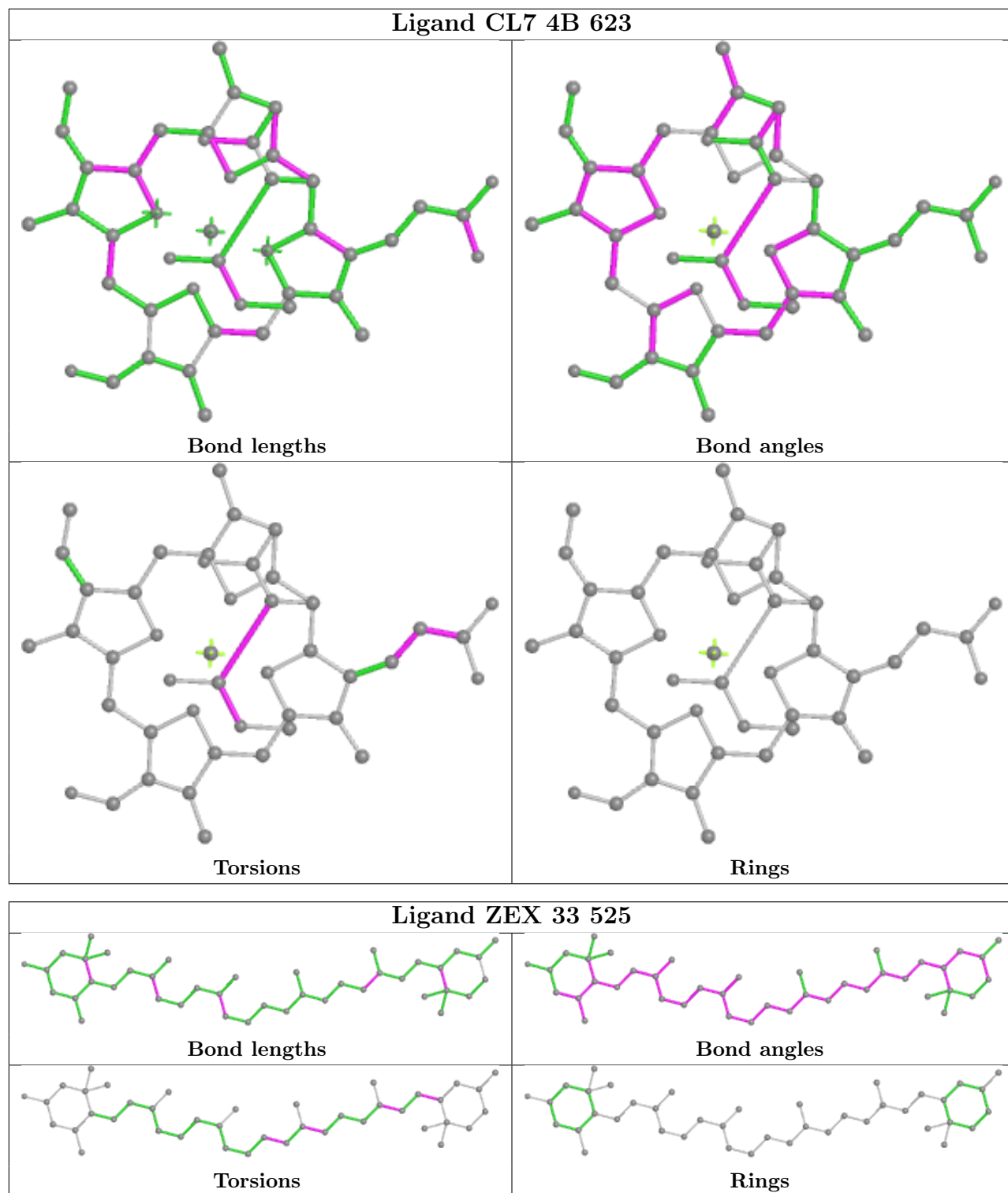
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	31	413	CL7	5	0
21	21	404	CL7	9	0
21	23	419	CL7	4	0
21	2B	612	CL7	4	0
32	12	524	ZEX	16	0
21	3B	613	CL7	2	0
32	32	520	ZEX	29	0
21	3B	601	CL7	1	0
21	2B	606	CL7	7	0
21	3C	506	CL7	5	0
21	34	415	CL7	4	0
32	24	419	ZEX	7	0
32	44	419	ZEX	9	0
21	44	412	CL7	3	0
21	21	405	CL7	4	0
21	43	419	CL7	4	0
22	4A	402	PHO	5	0
21	2B	615	CL7	2	0
21	31	403	CL7	6	0
22	3A	402	PHO	5	0
21	33	518	CL7	4	0
21	11	404	CL7	8	0
22	4D	408	PHO	4	0
21	22	510	CL7	6	0
21	44	407	CL7	10	0
21	22	502	CL7	8	0
21	21	417	CL7	6	0
21	32	514	CL7	2	0
21	42	503	CL7	7	0
21	2C	506	CL7	4	0
21	1B	613	CL7	2	0
21	3D	402	CL7	3	0
21	24	411	CL7	6	0
21	42	516	CL7	7	0
21	4C	517	CL7	1	0
21	24	409	CL7	3	0
21	31	410	CL7	6	0
21	4B	613	CL7	6	0
32	21	422	ZEX	20	0
21	31	418	CL7	8	0
21	3C	517	CL7	1	0
21	32	518	CL7	11	0

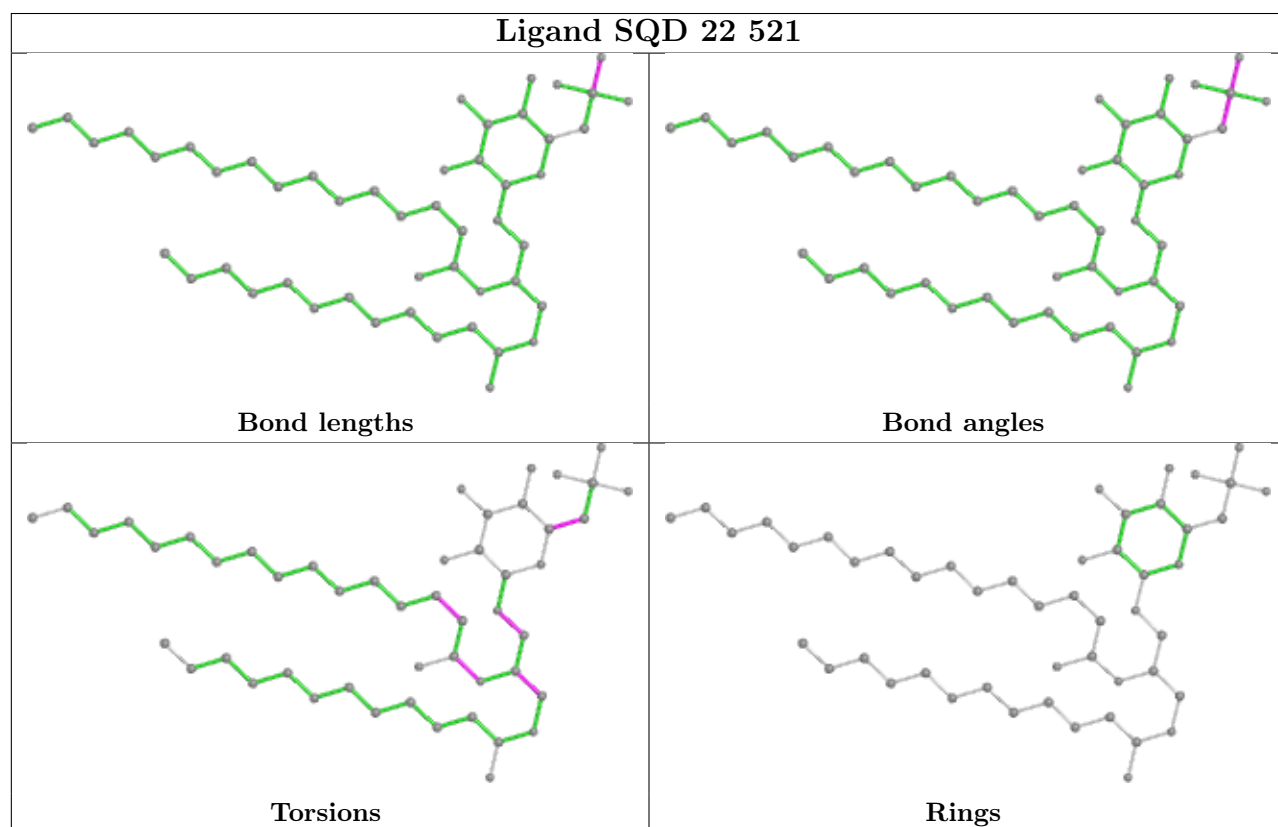
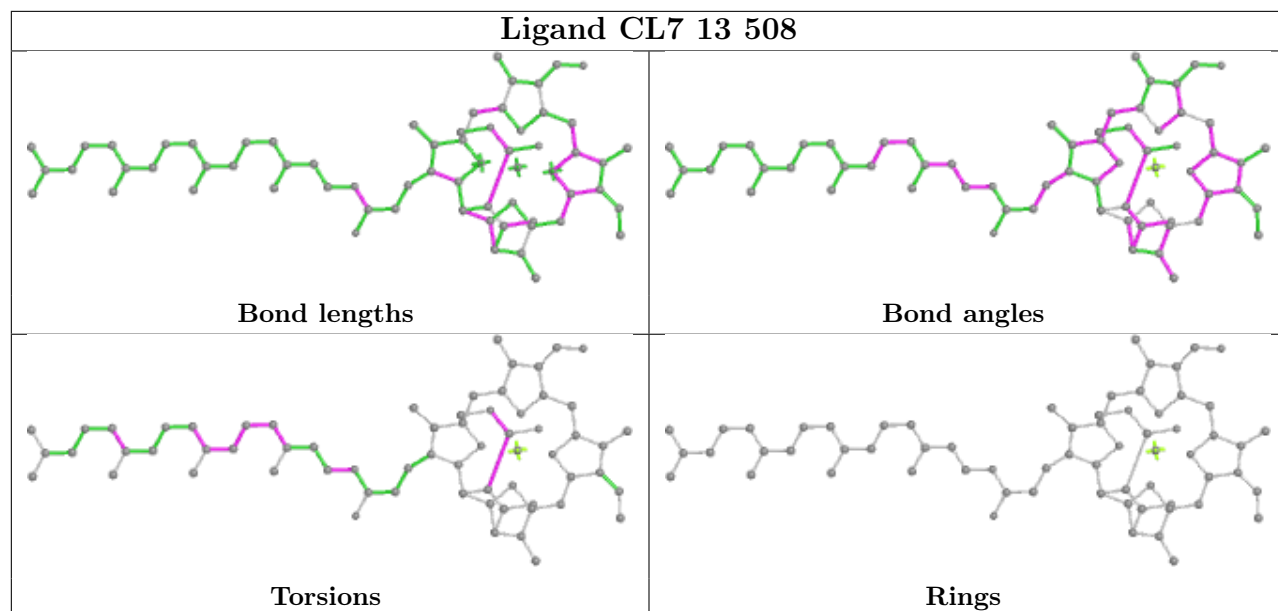
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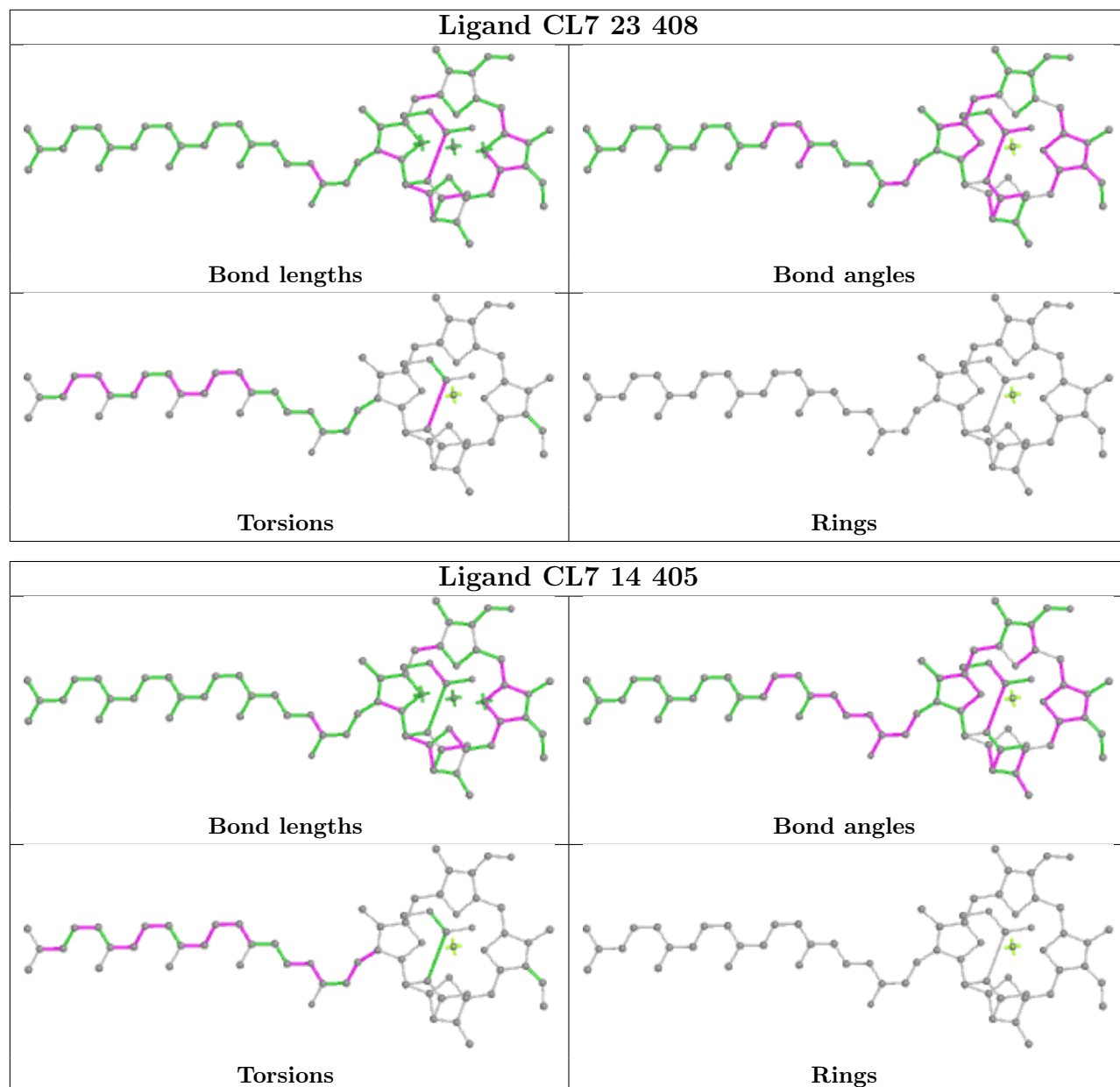
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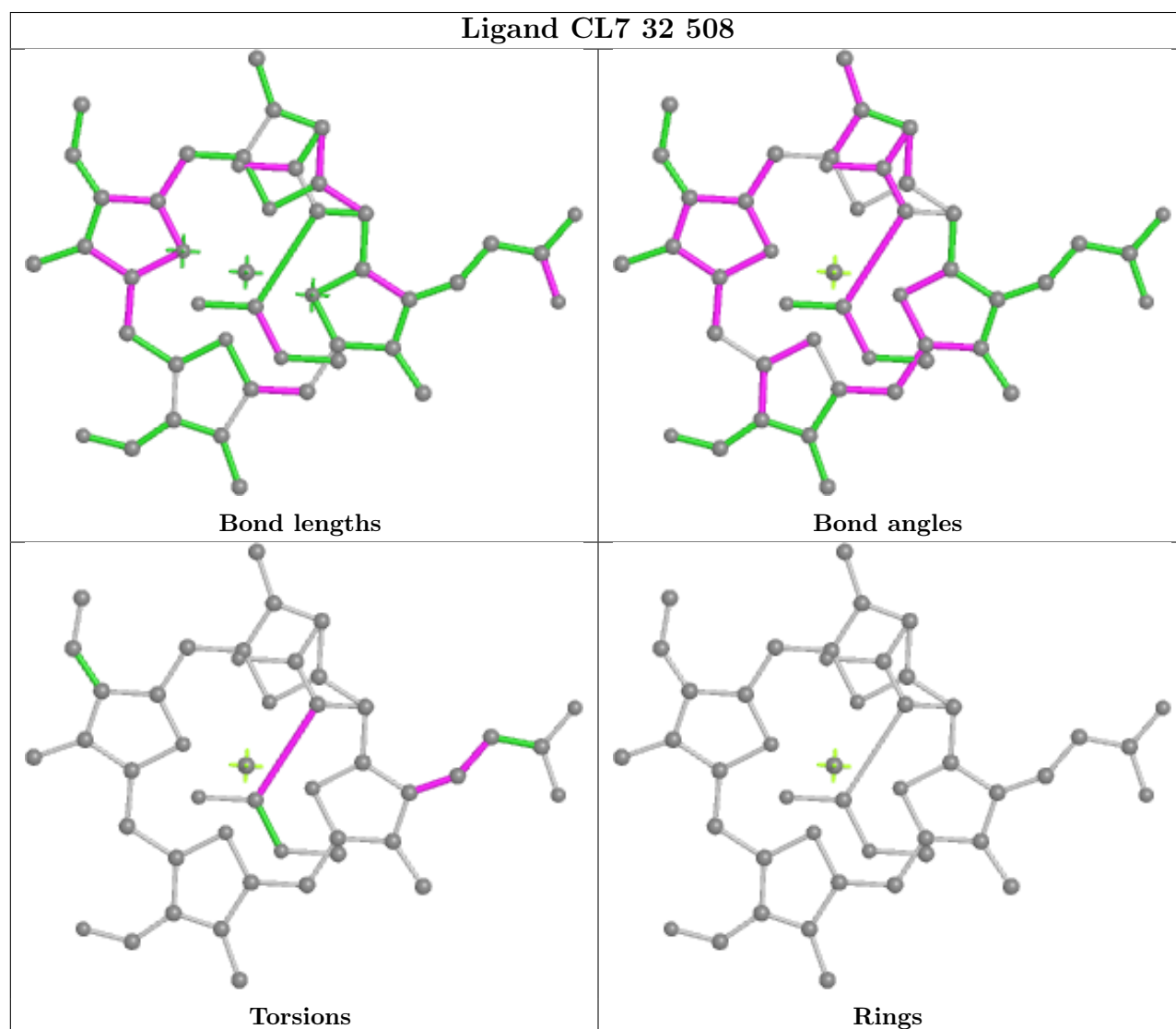
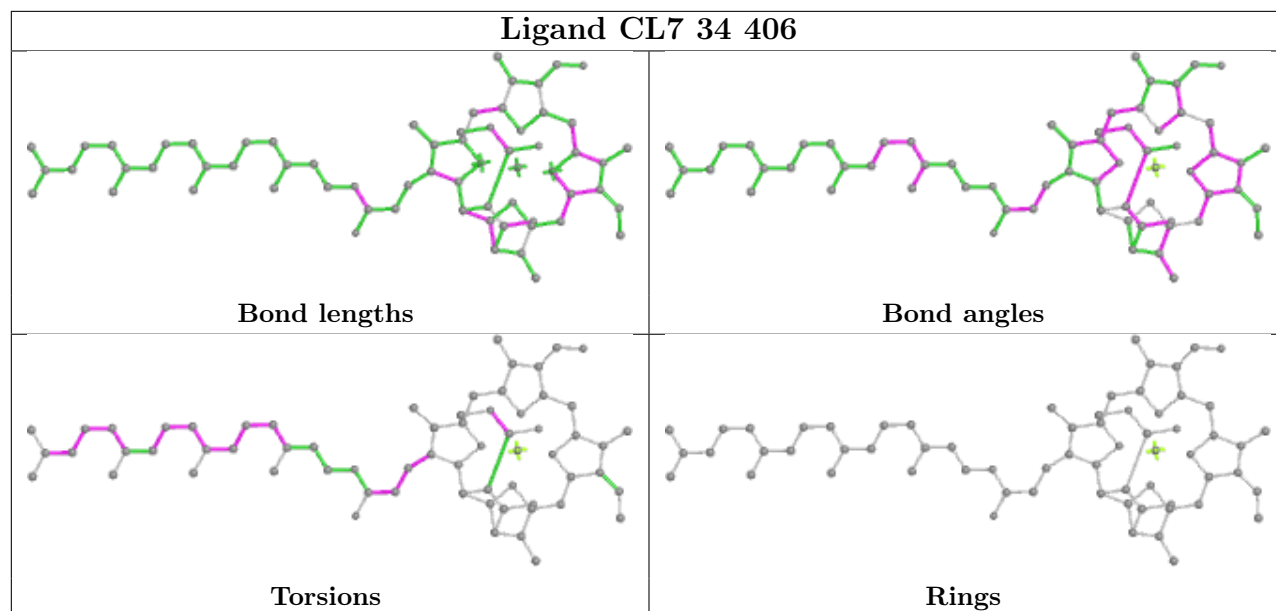
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	4C	510	CL7	4	0
21	1C	506	CL7	6	0
32	11	422	ZEX	20	0
21	1C	501	CL7	3	0
21	43	414	CL7	13	0
21	44	411	CL7	7	0
32	42	519	ZEX	4	0
32	22	520	ZEX	28	0
21	42	509	CL7	9	0
24	4A	405	LMG	2	0
31	1F	101	HEM	3	0
21	22	512	CL7	10	0
32	23	401	ZEX	24	0
25	4B	621	SQD	3	0
21	2B	609	CL7	4	0
21	43	409	CL7	14	0
21	24	404	CL7	6	0
26	3A	408	LHG	1	0
21	34	413	CL7	5	0
32	43	401	ZEX	24	0
25	23	424	SQD	2	0
30	1D	407	PL9	7	0
26	2A	408	LHG	1	0
32	12	522	ZEX	18	0

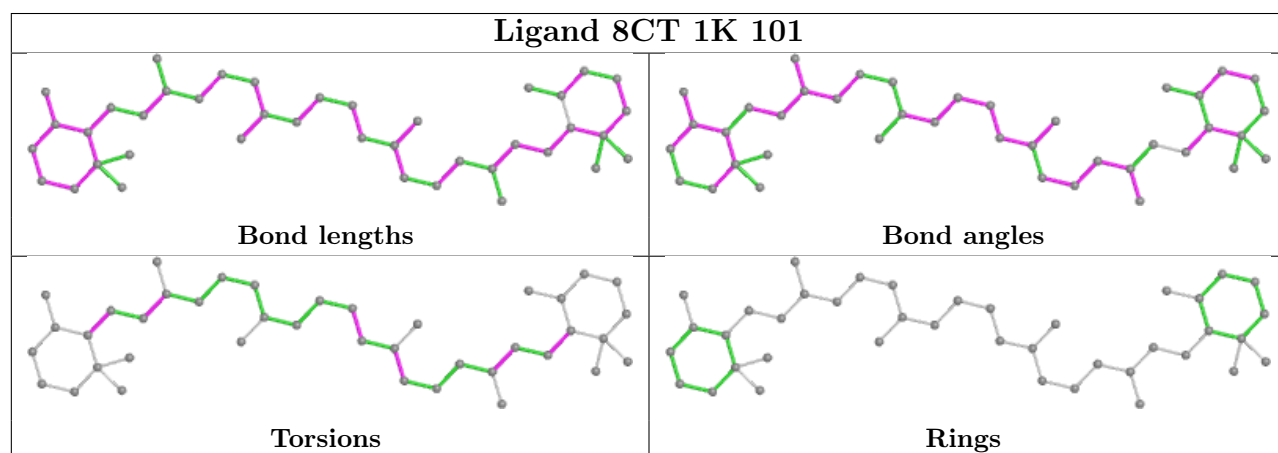
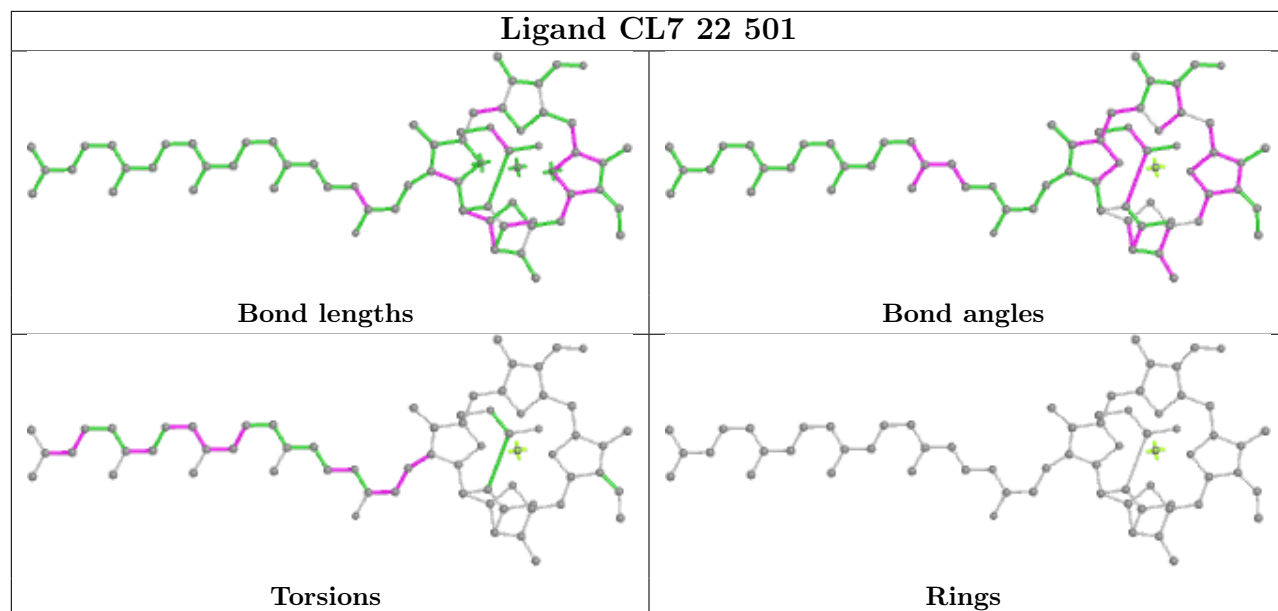
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

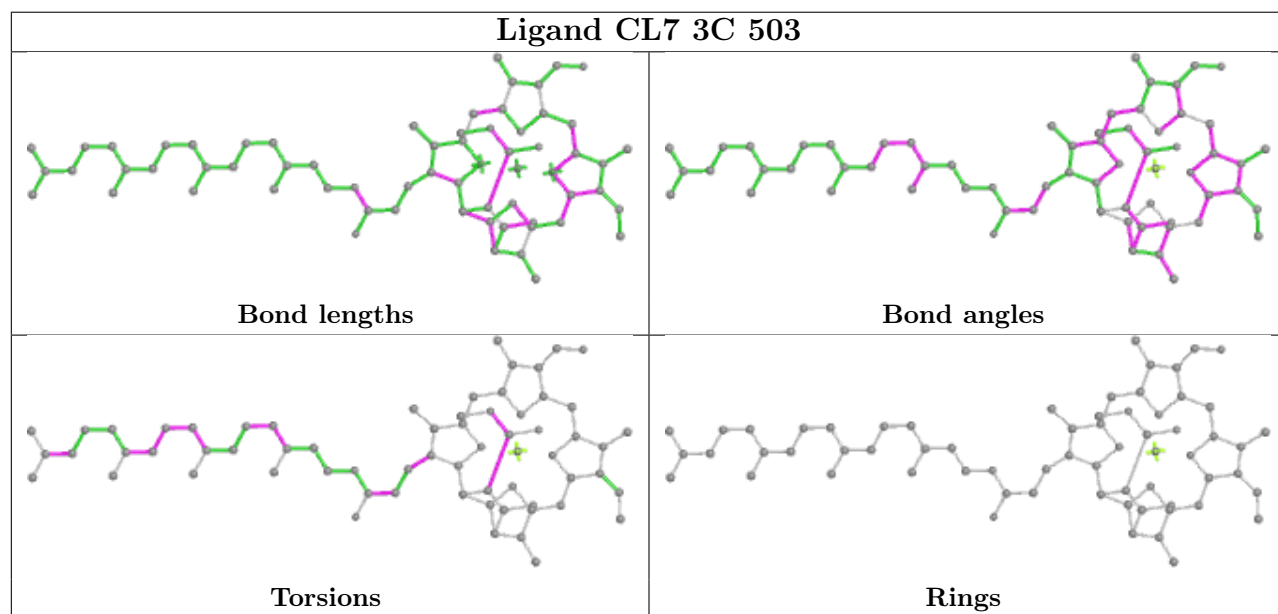
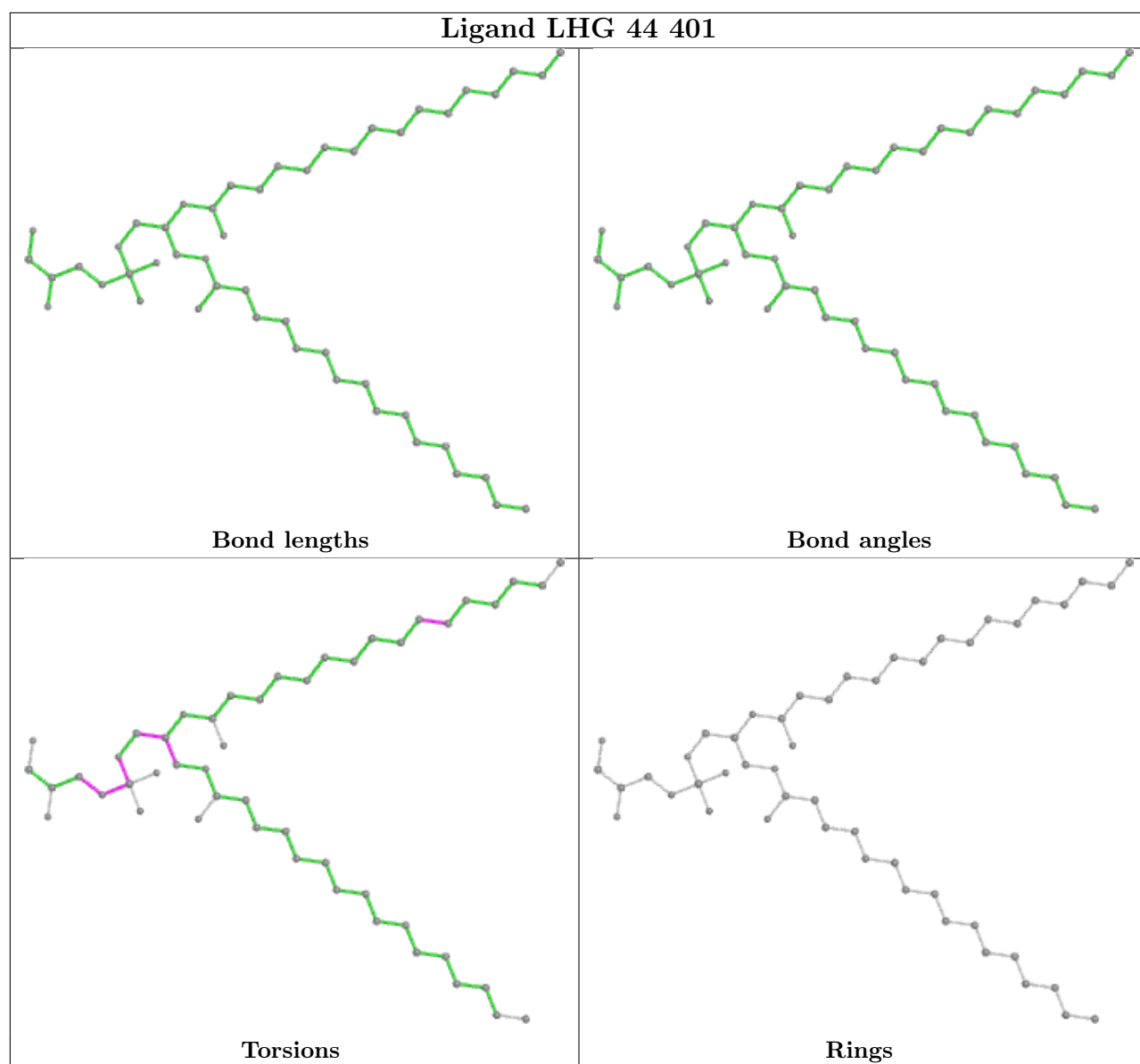


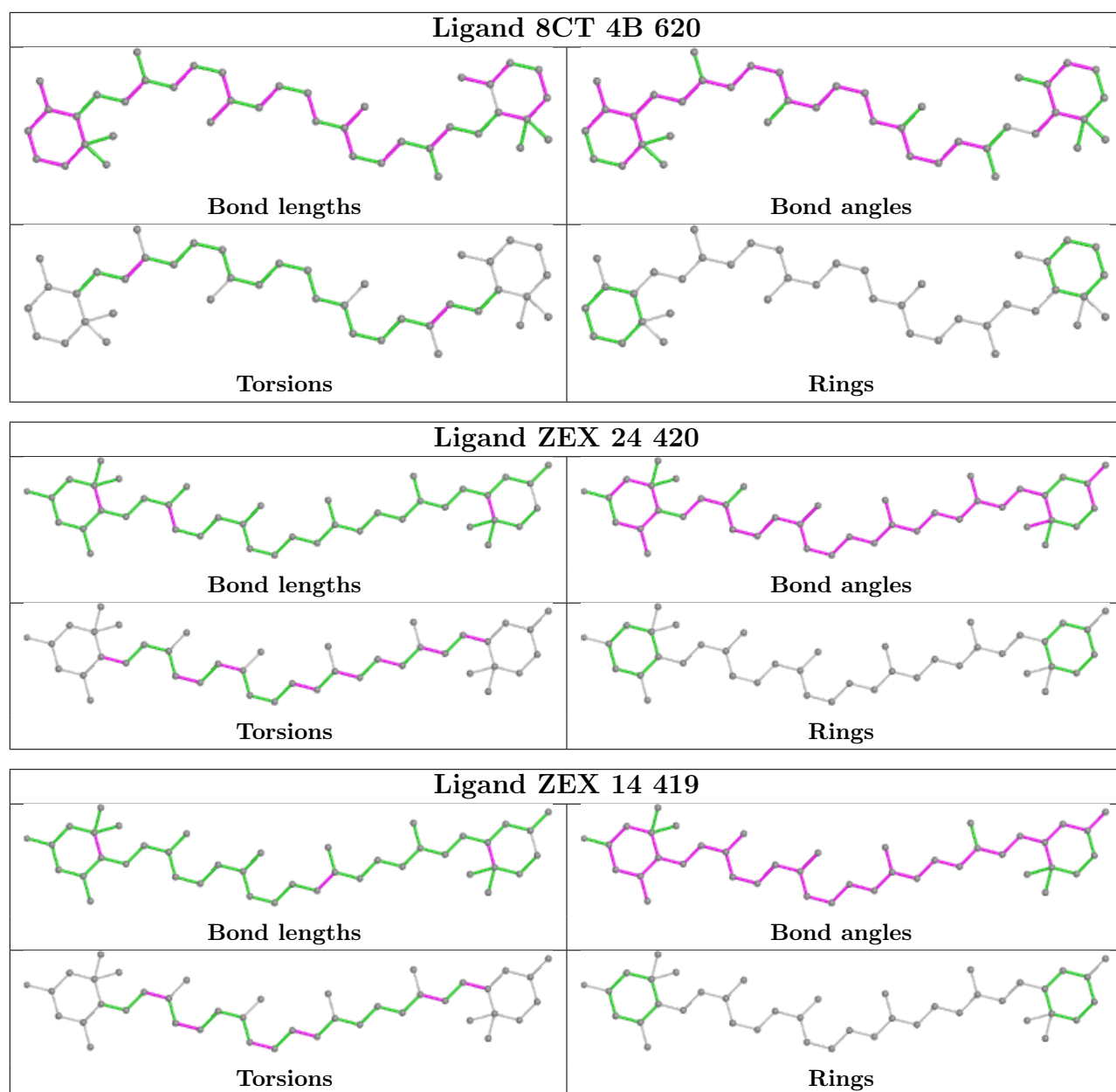


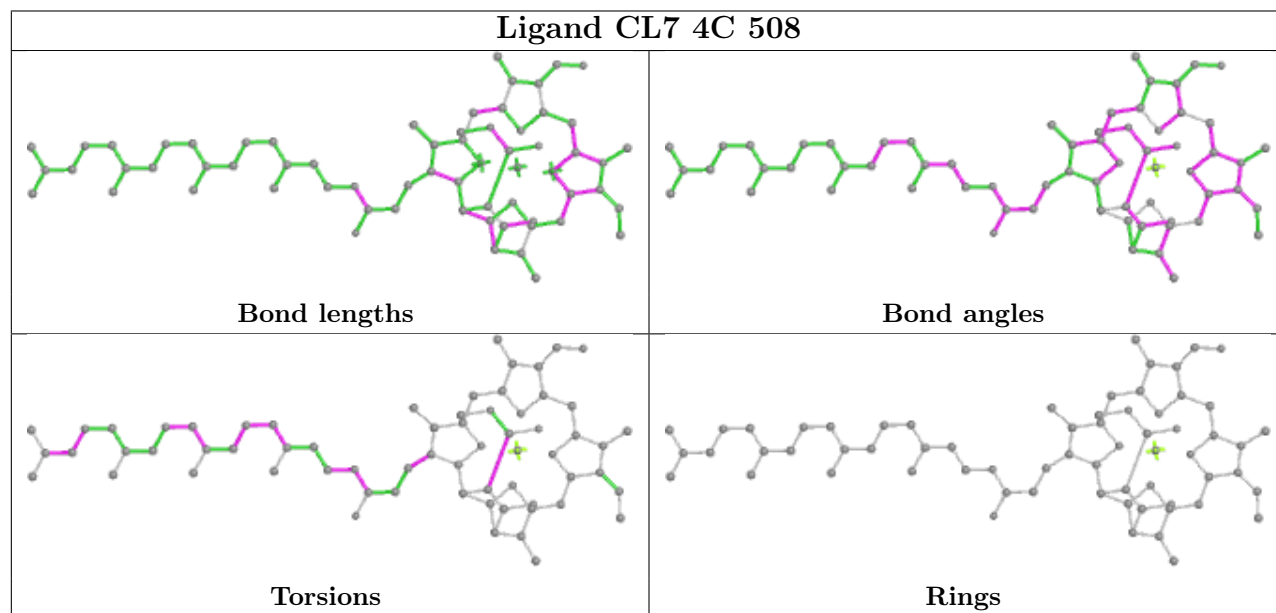
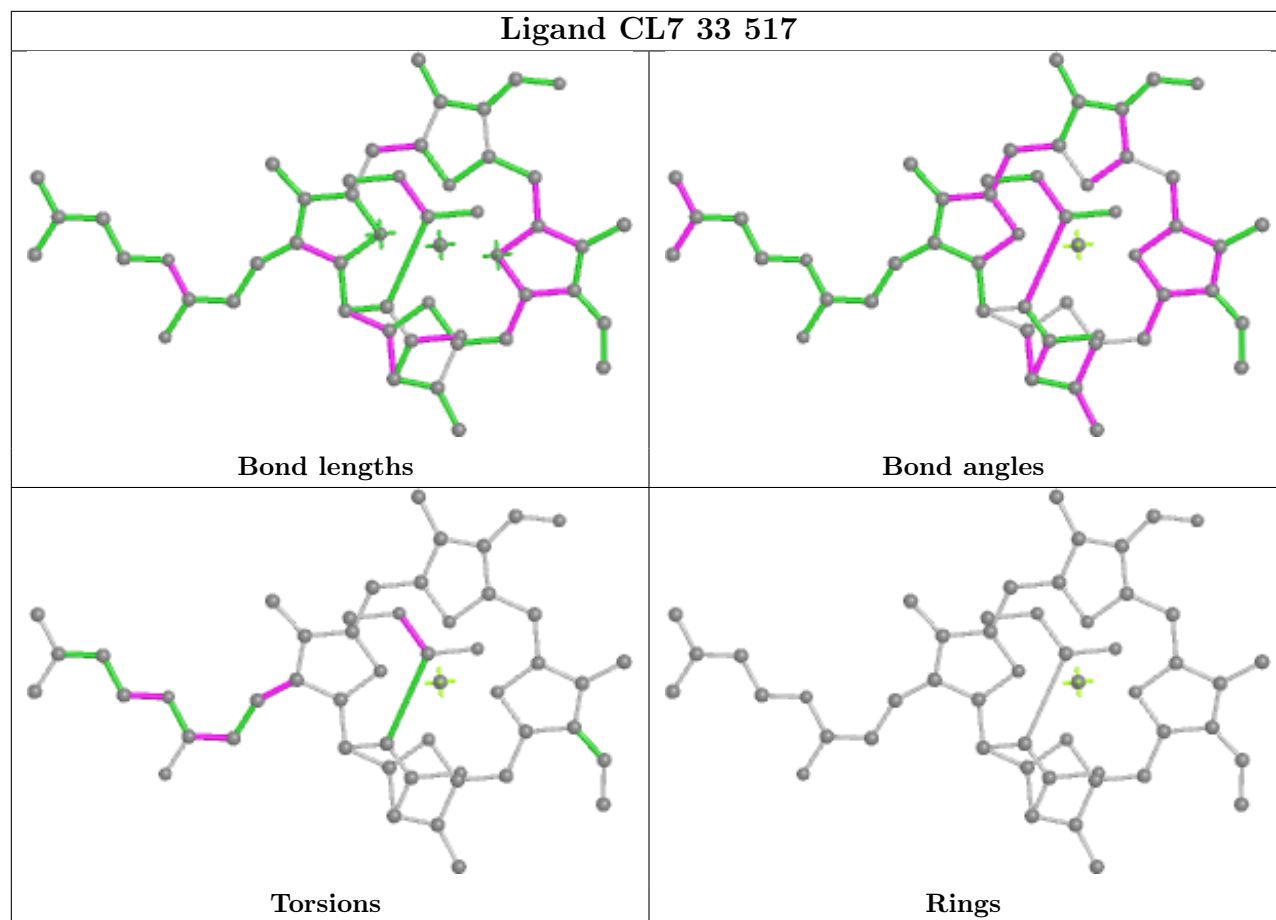


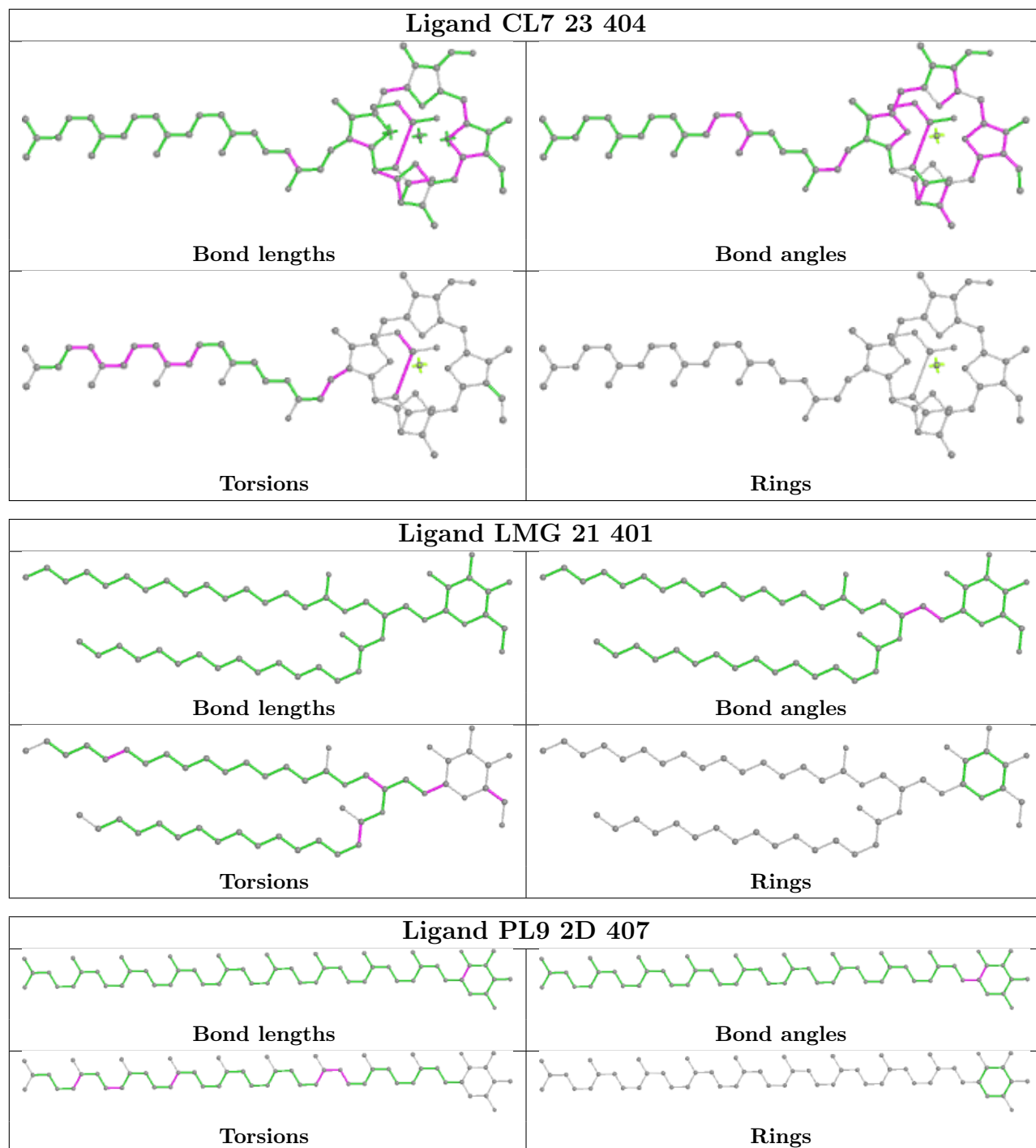


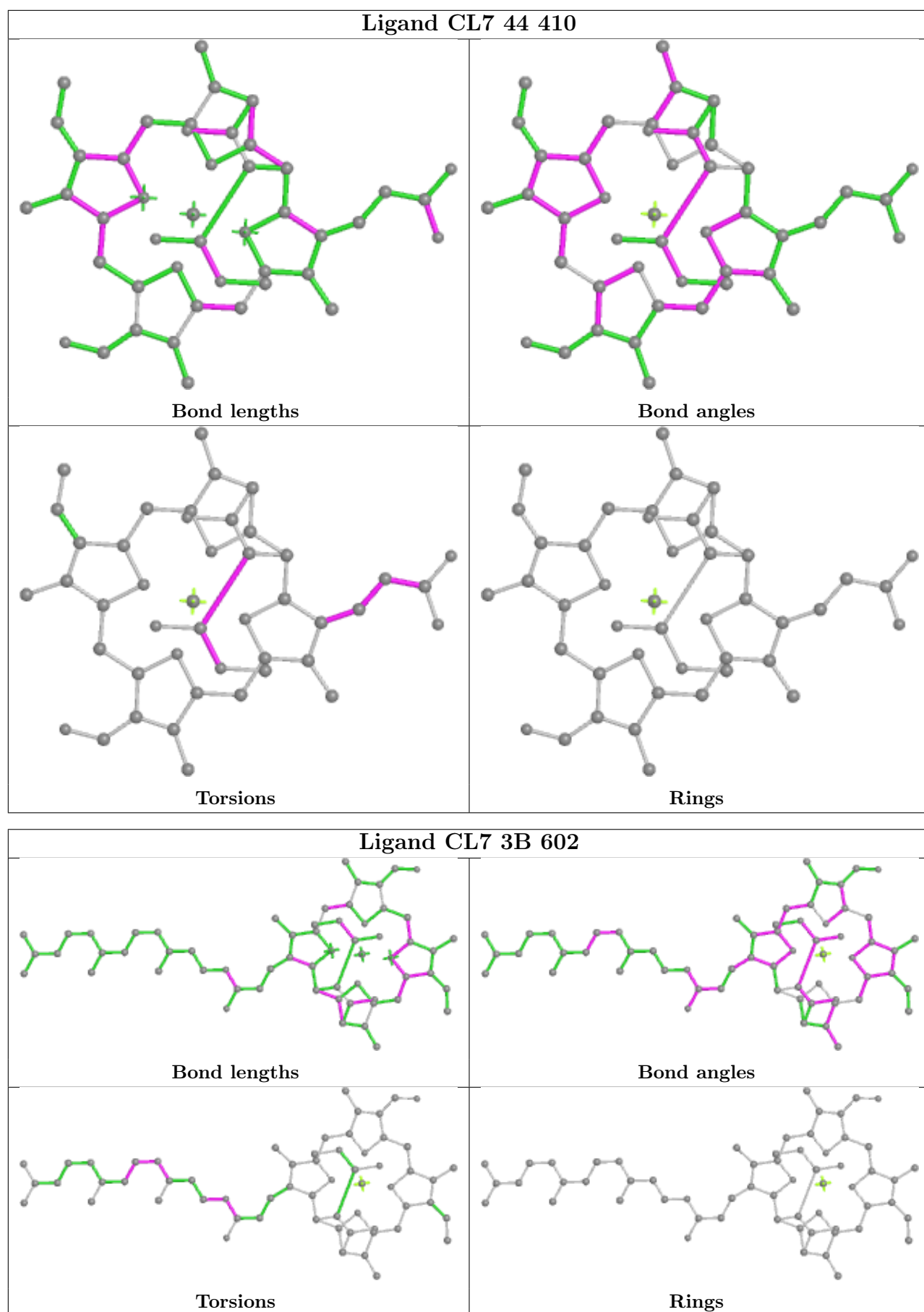


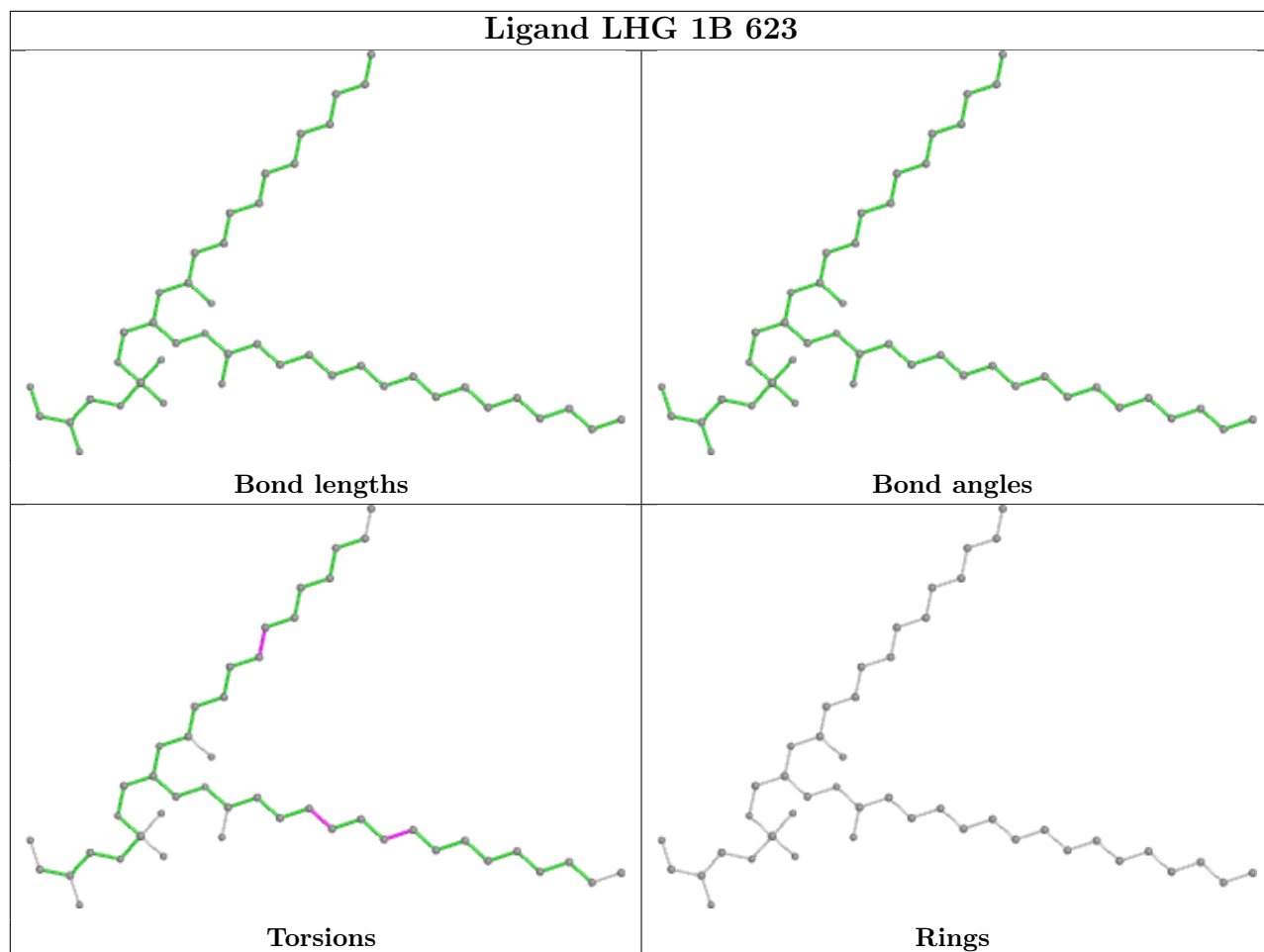


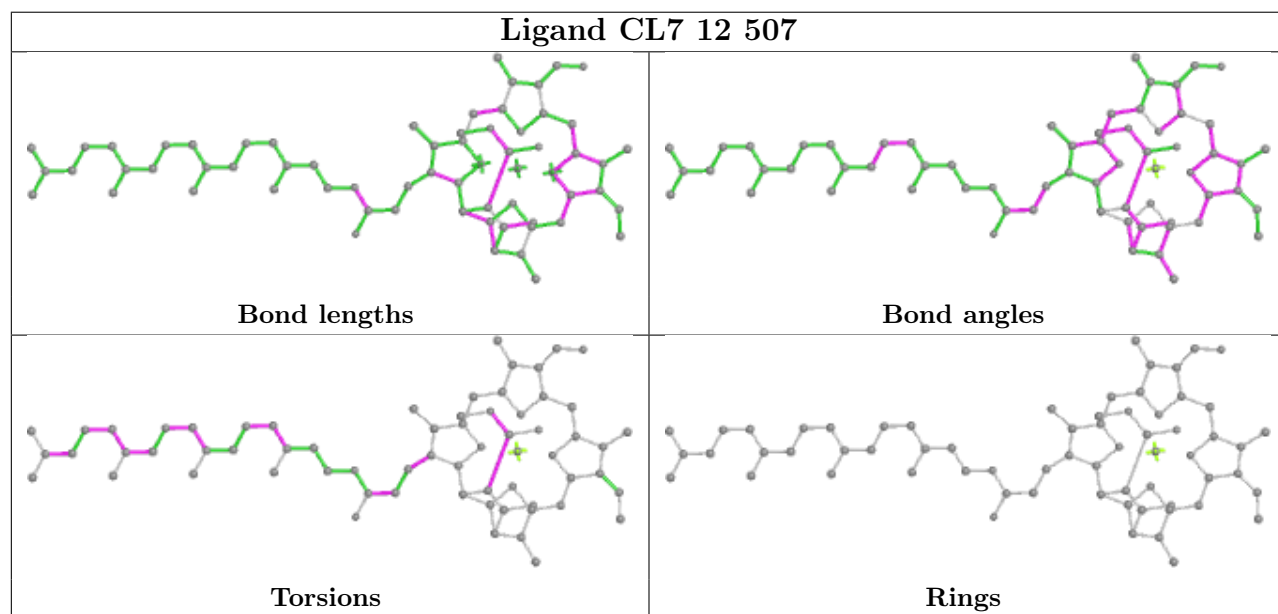
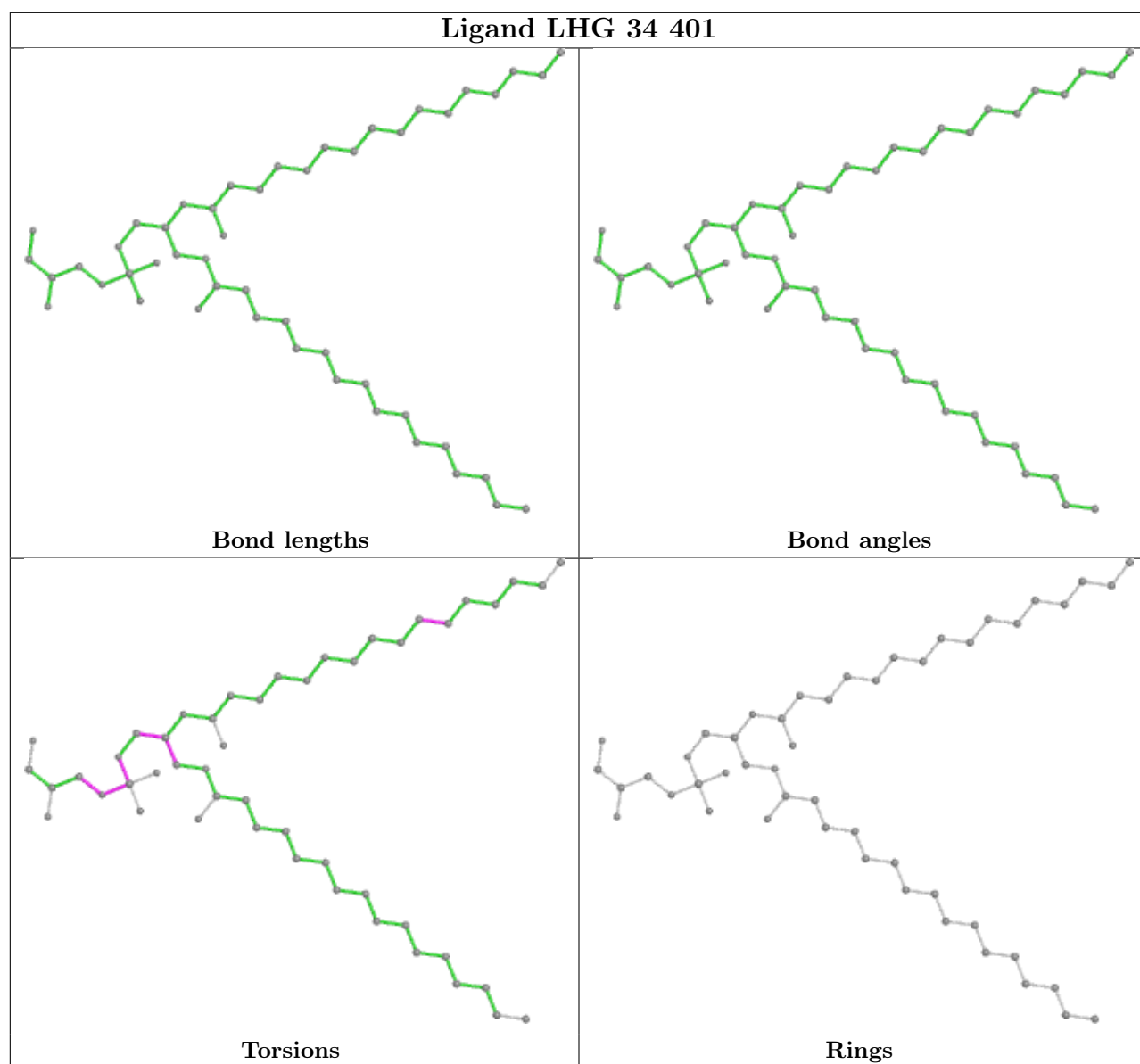


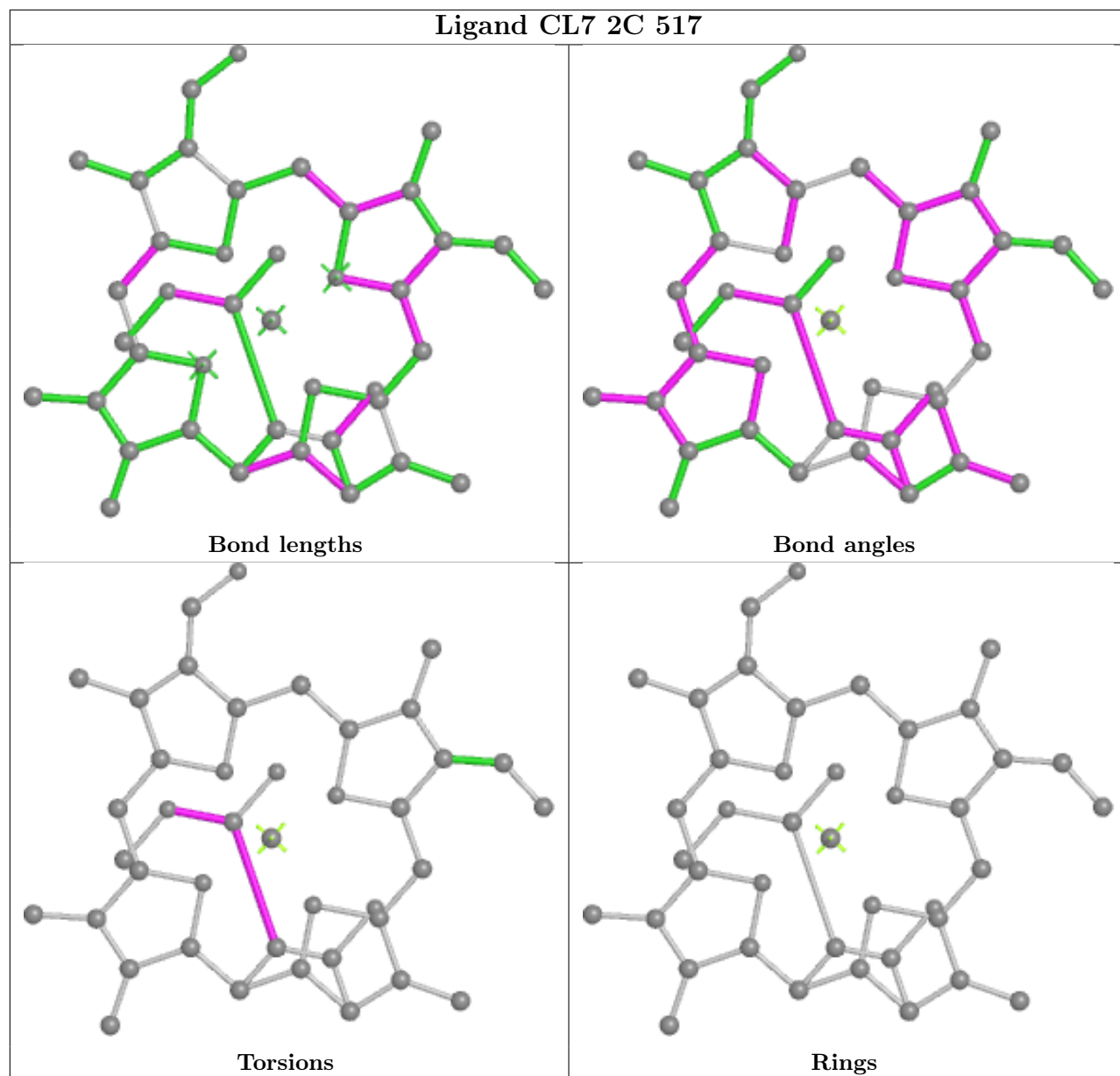


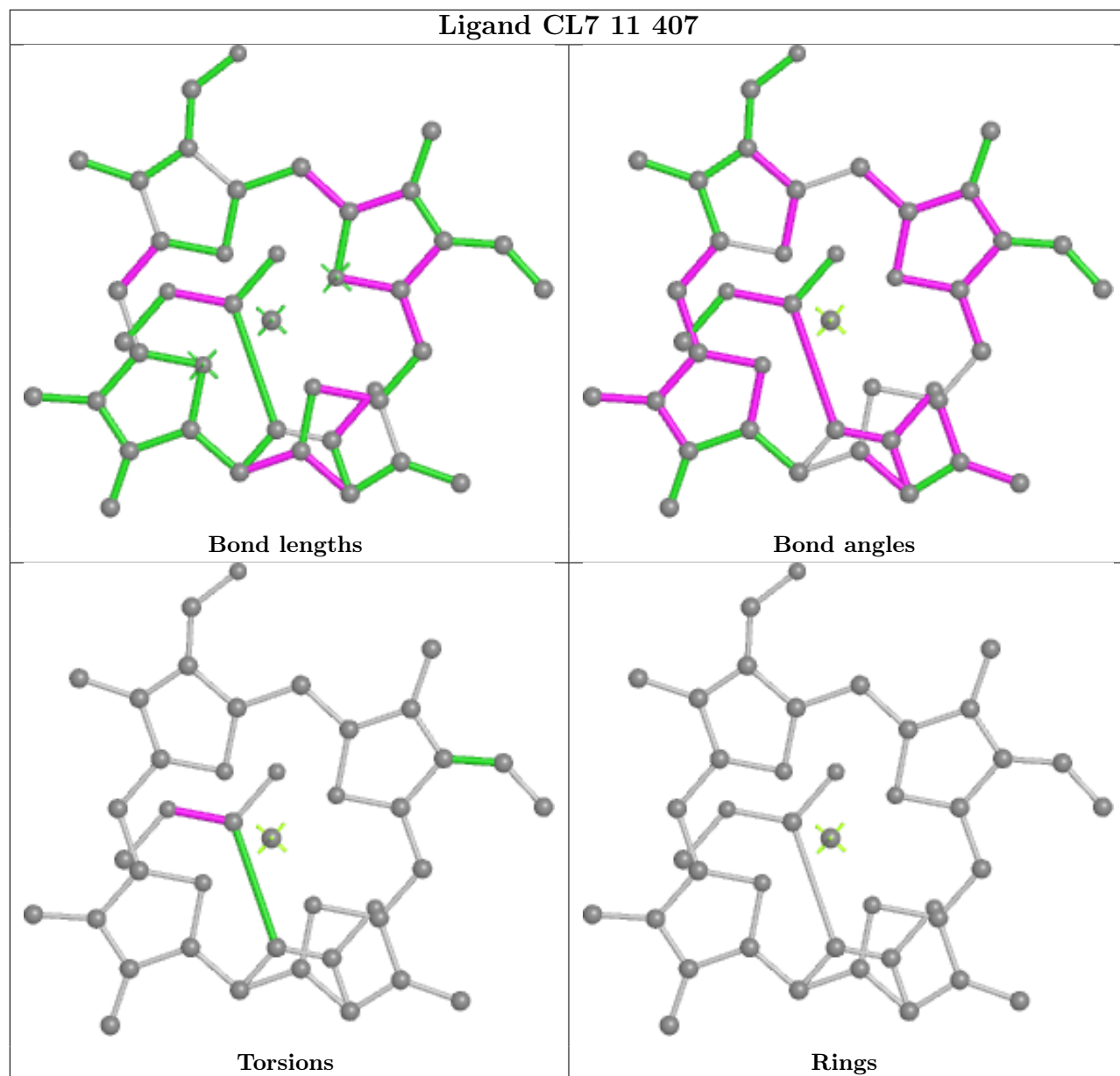


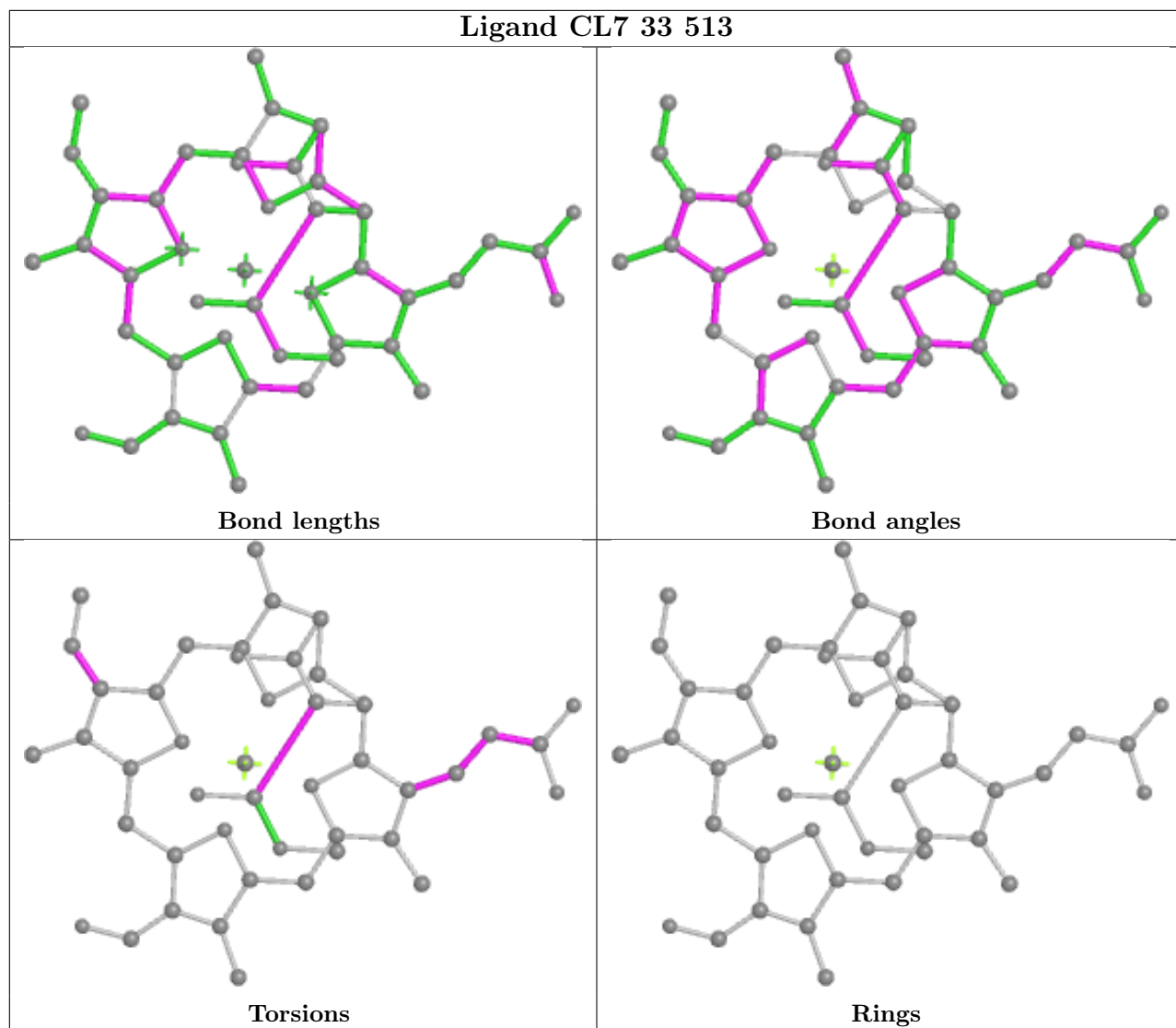


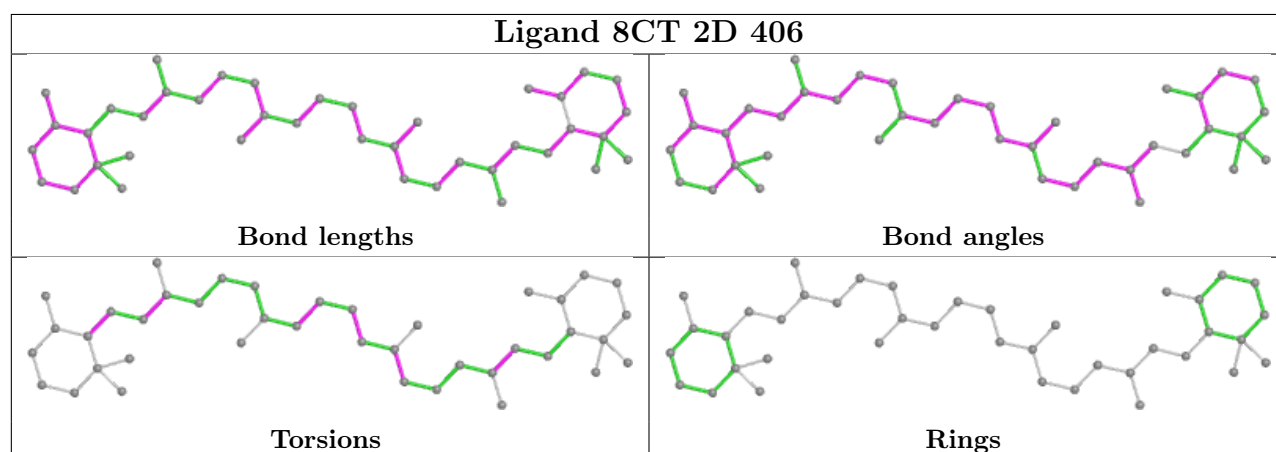
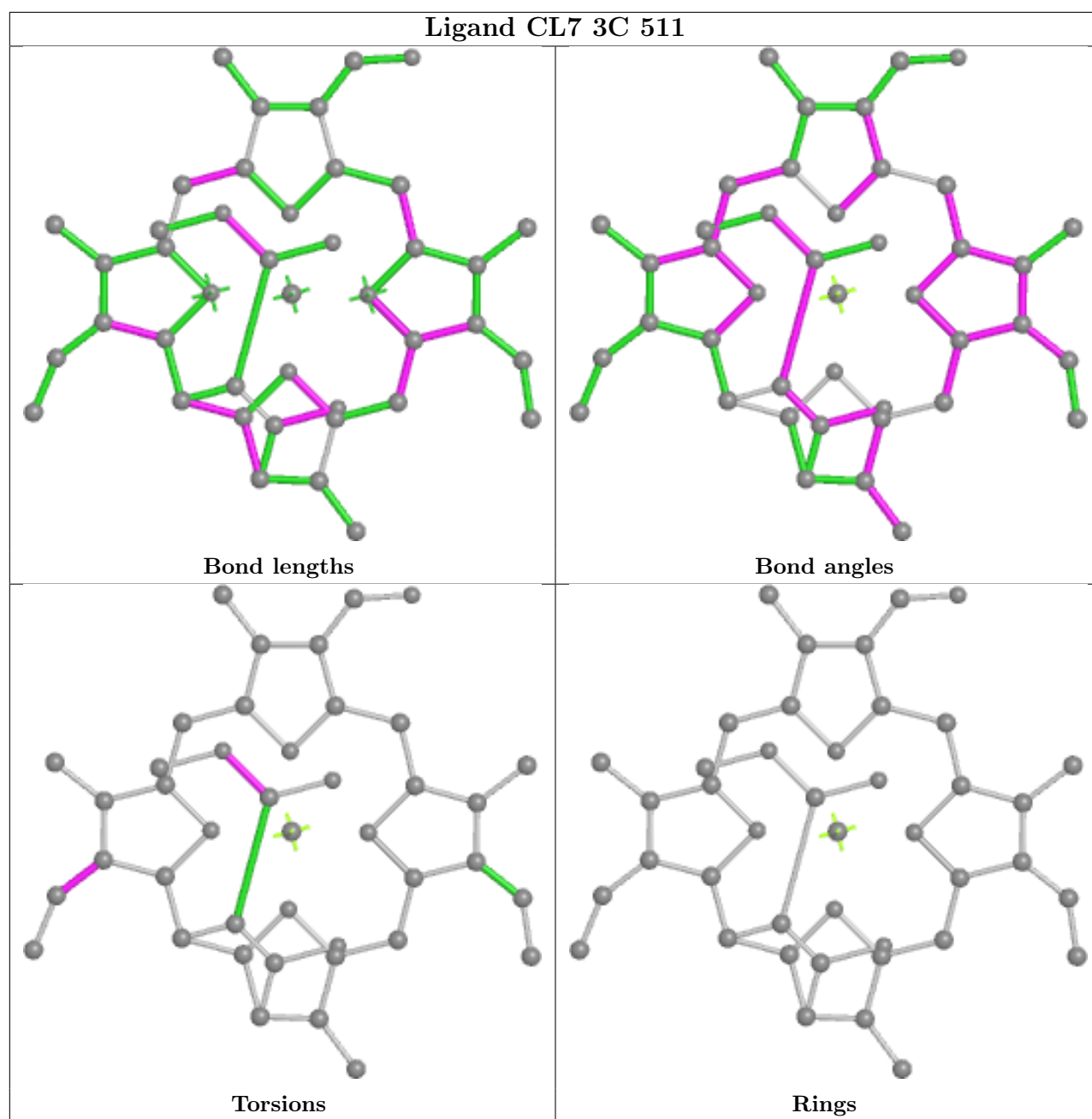


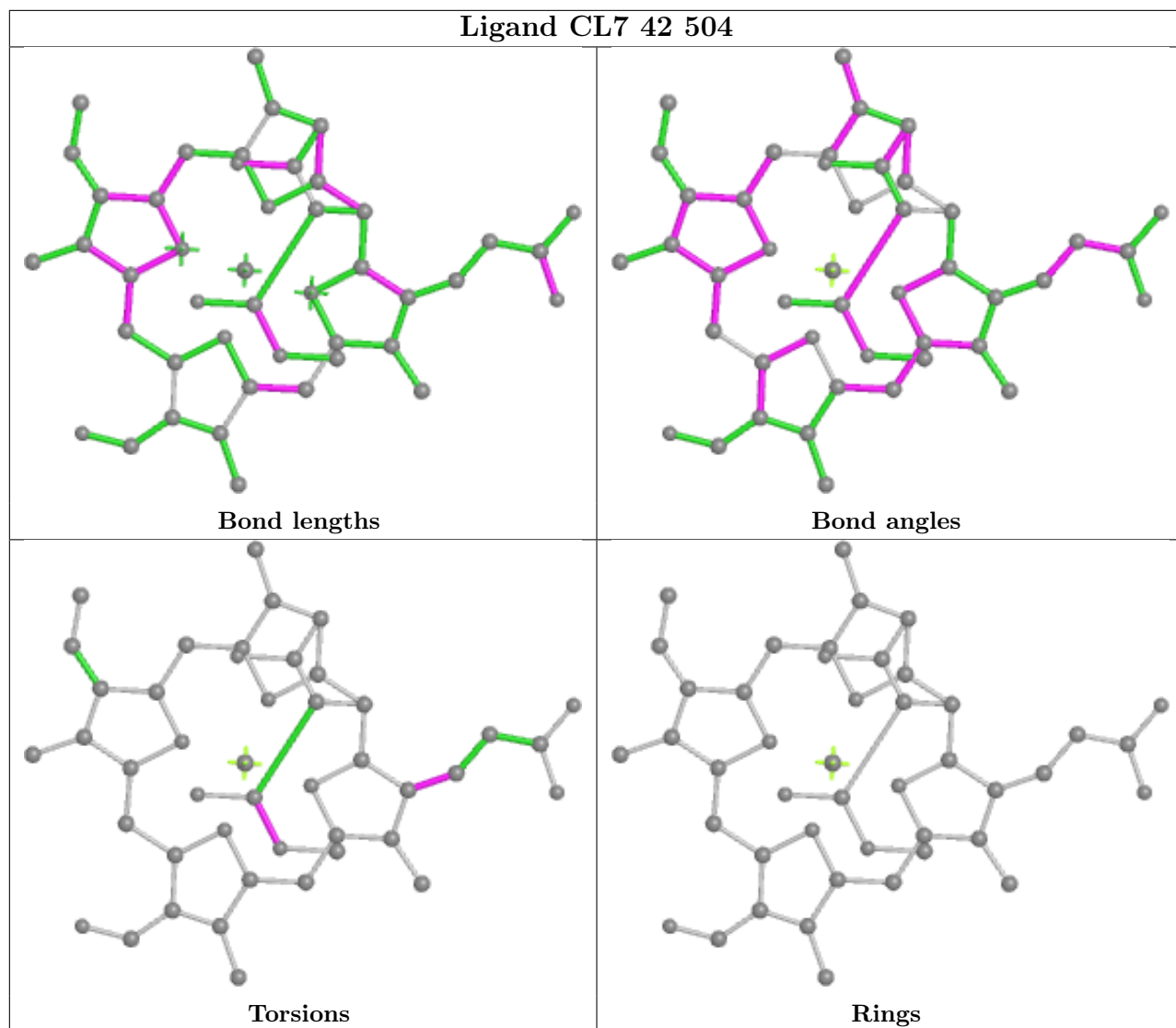


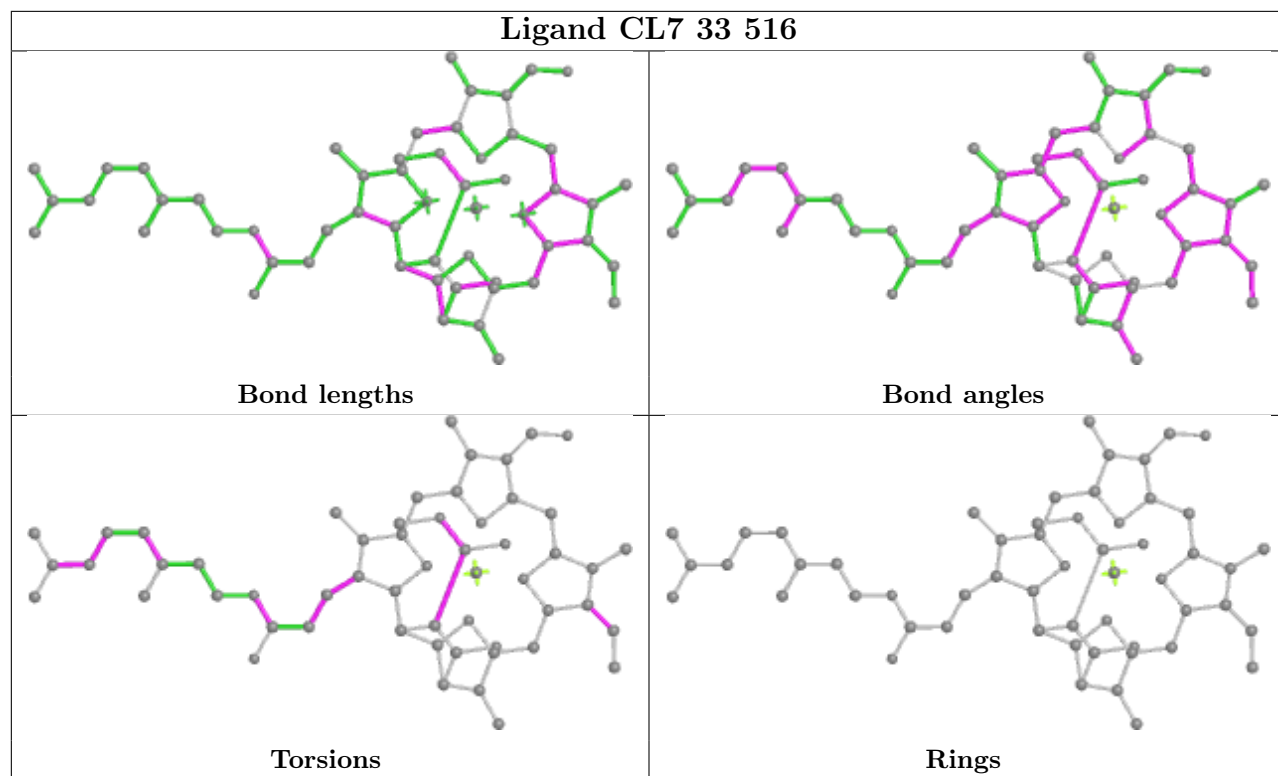


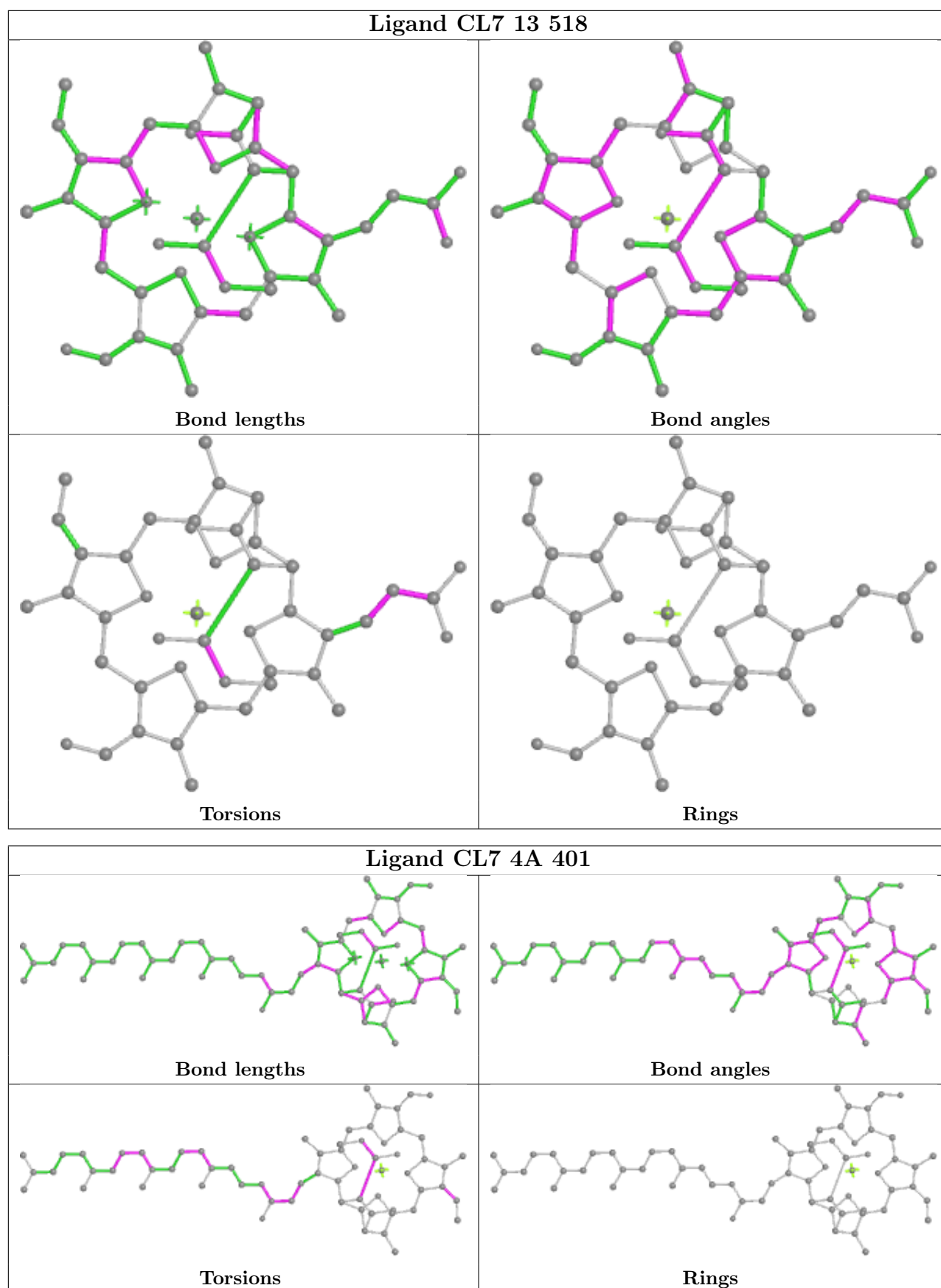


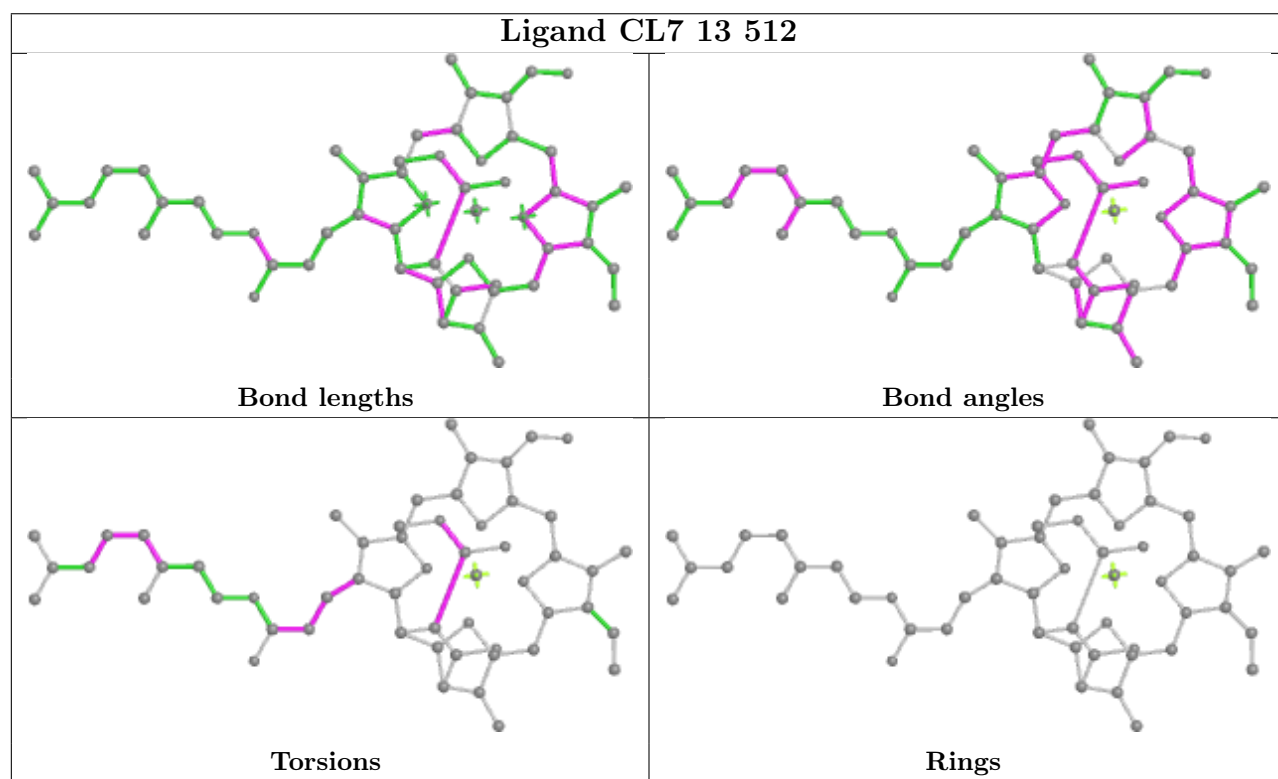
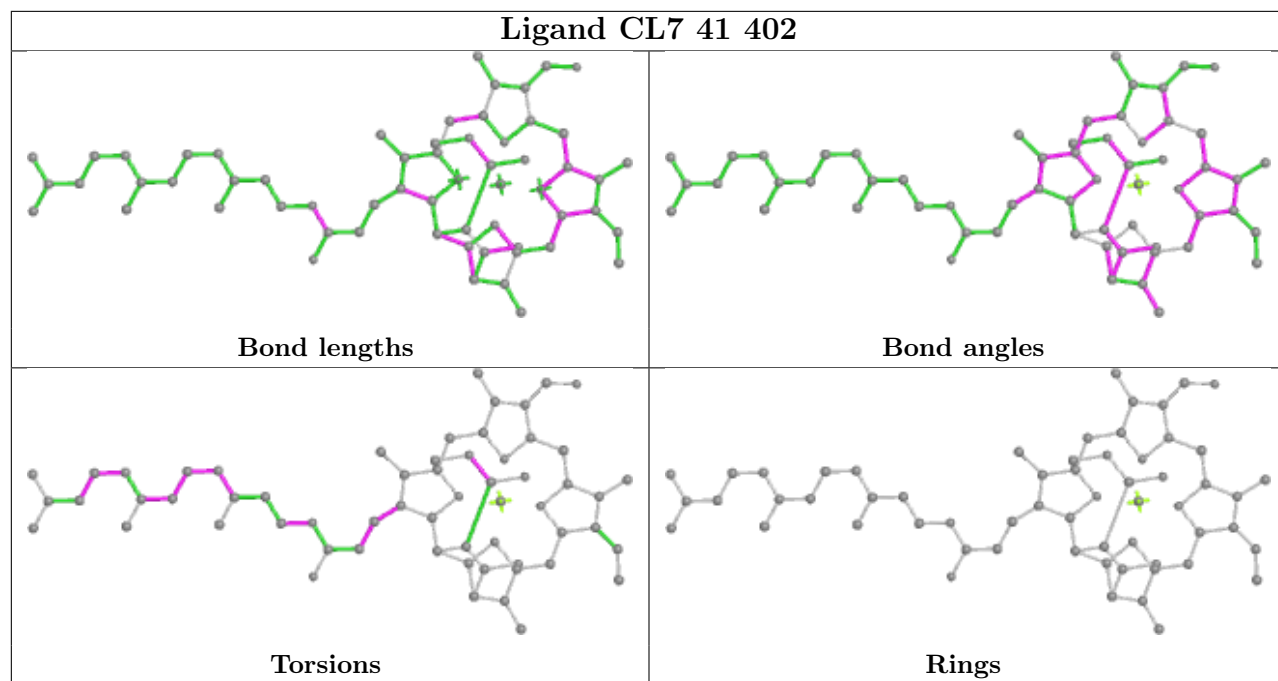


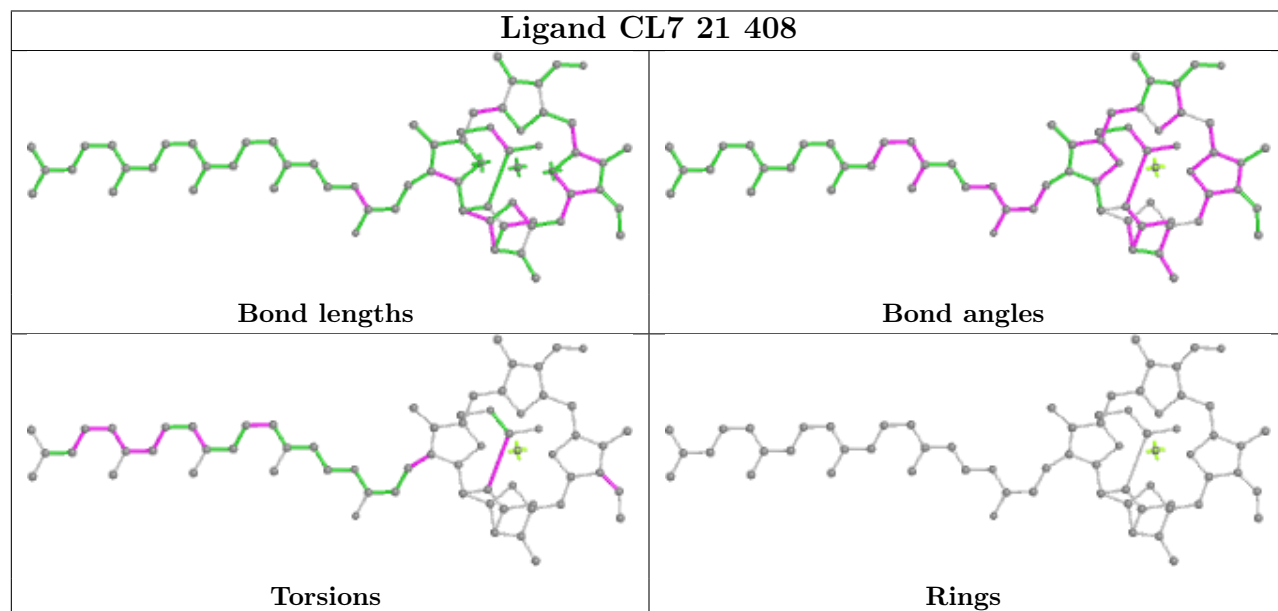
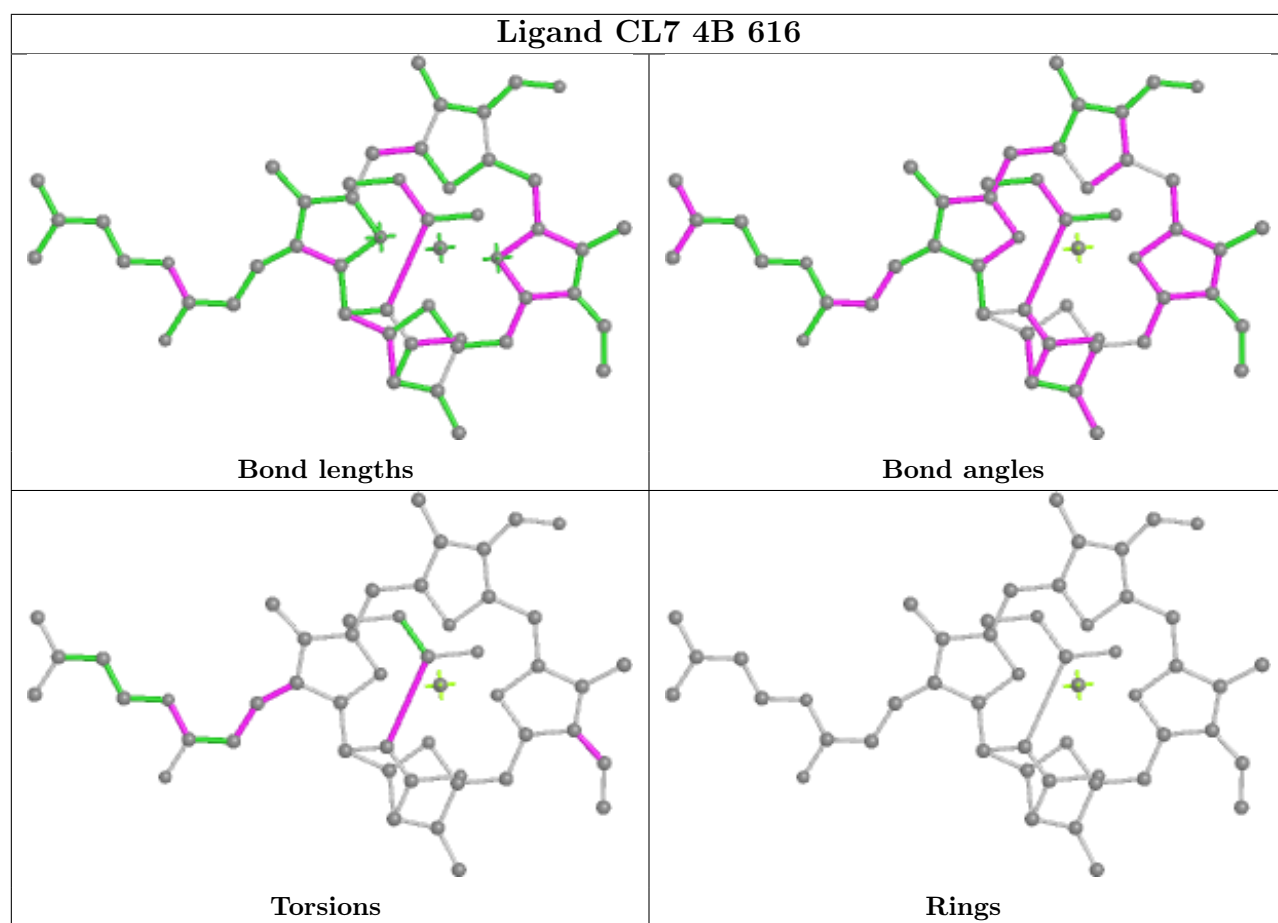


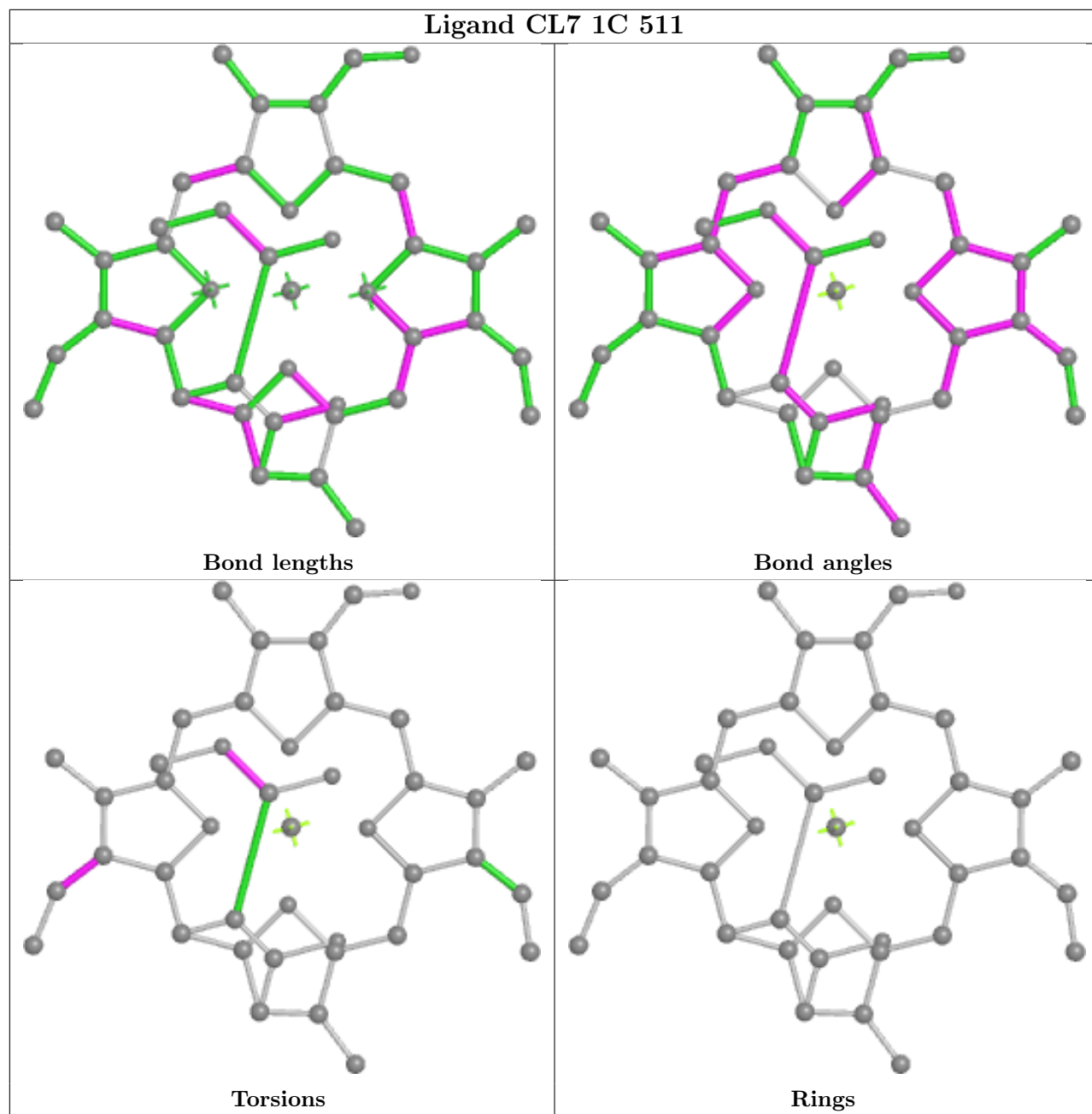


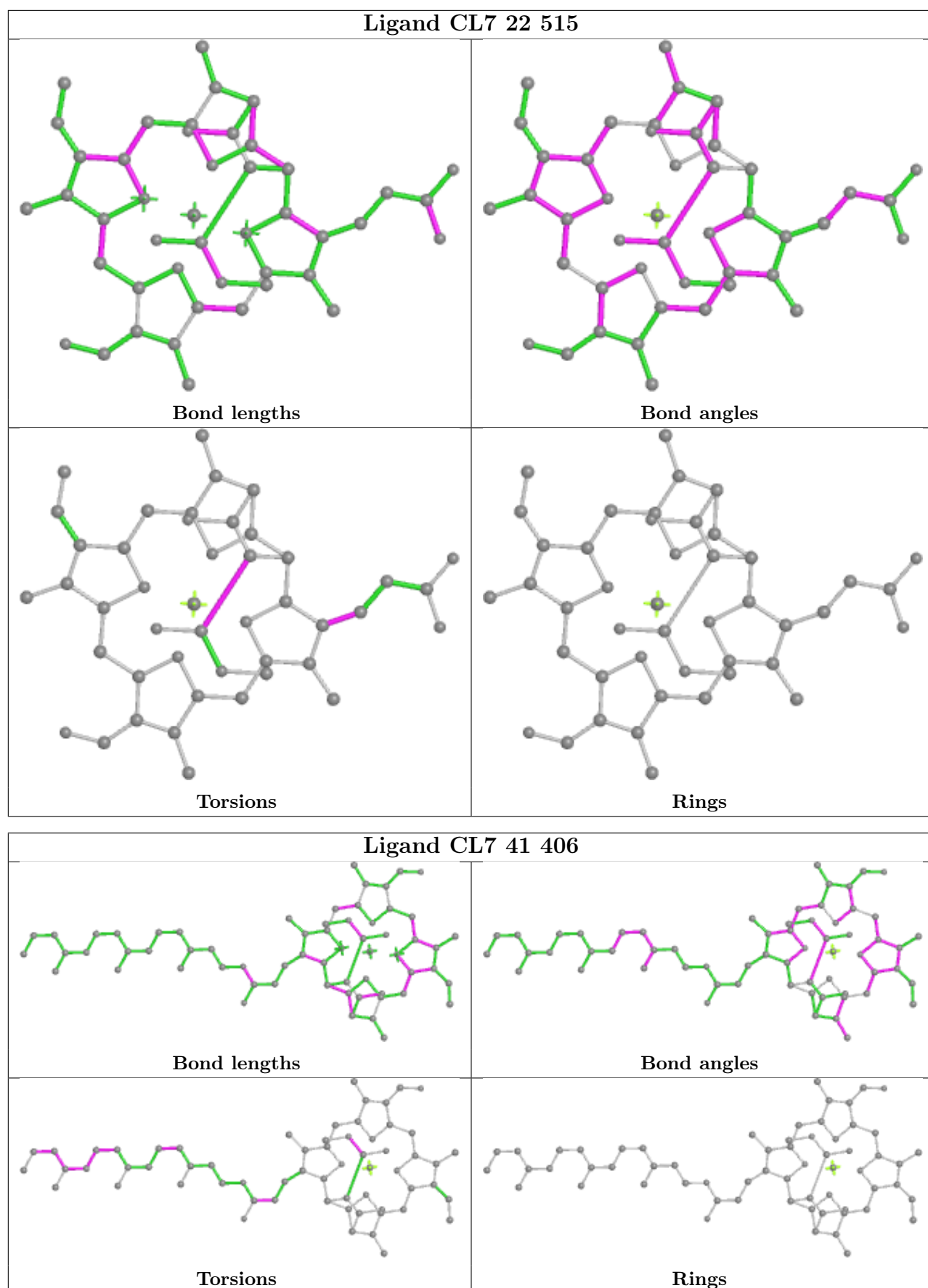


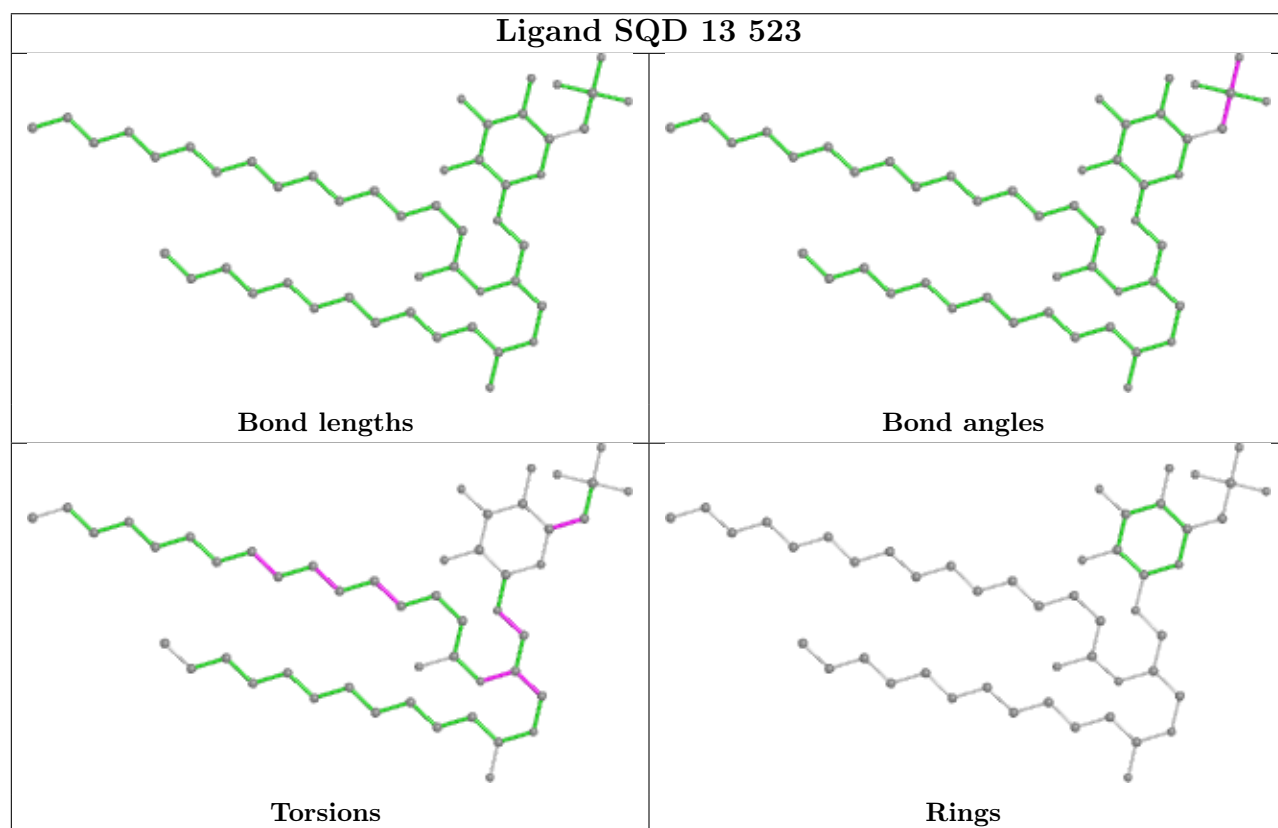
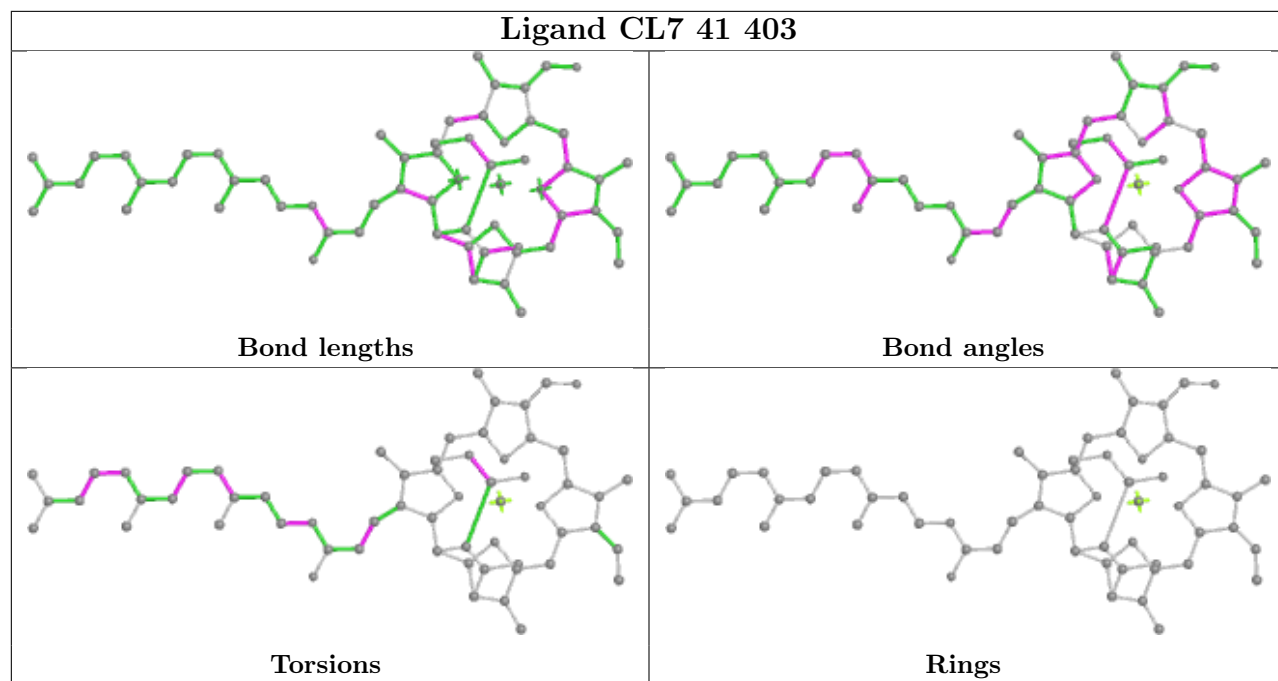


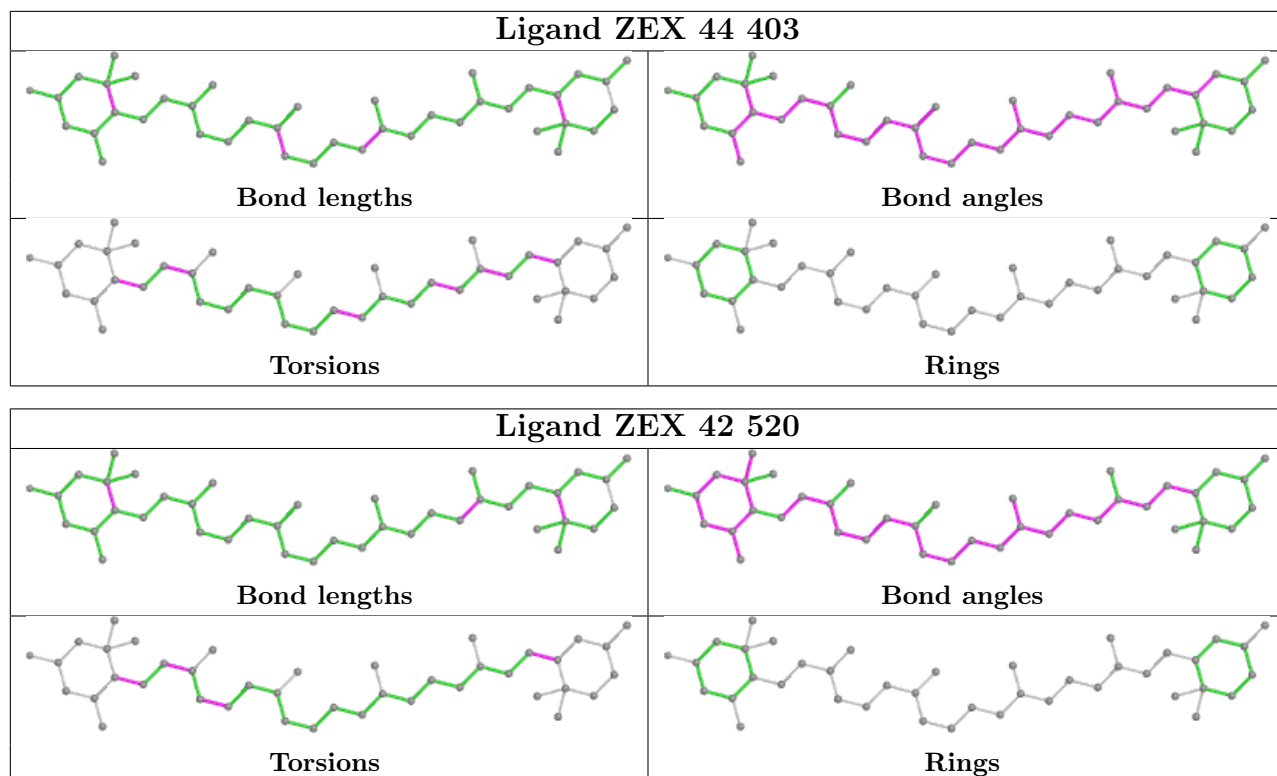


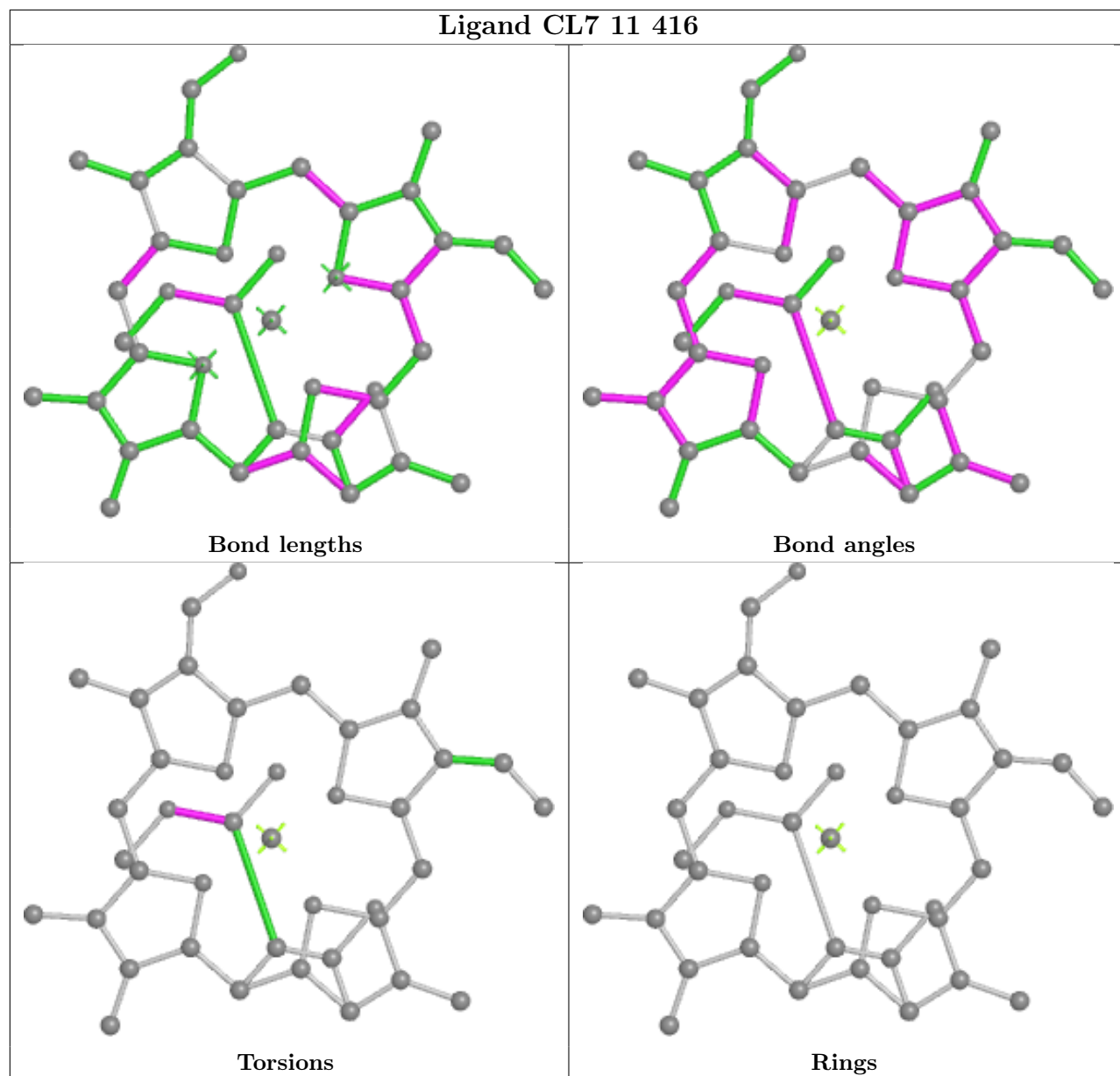


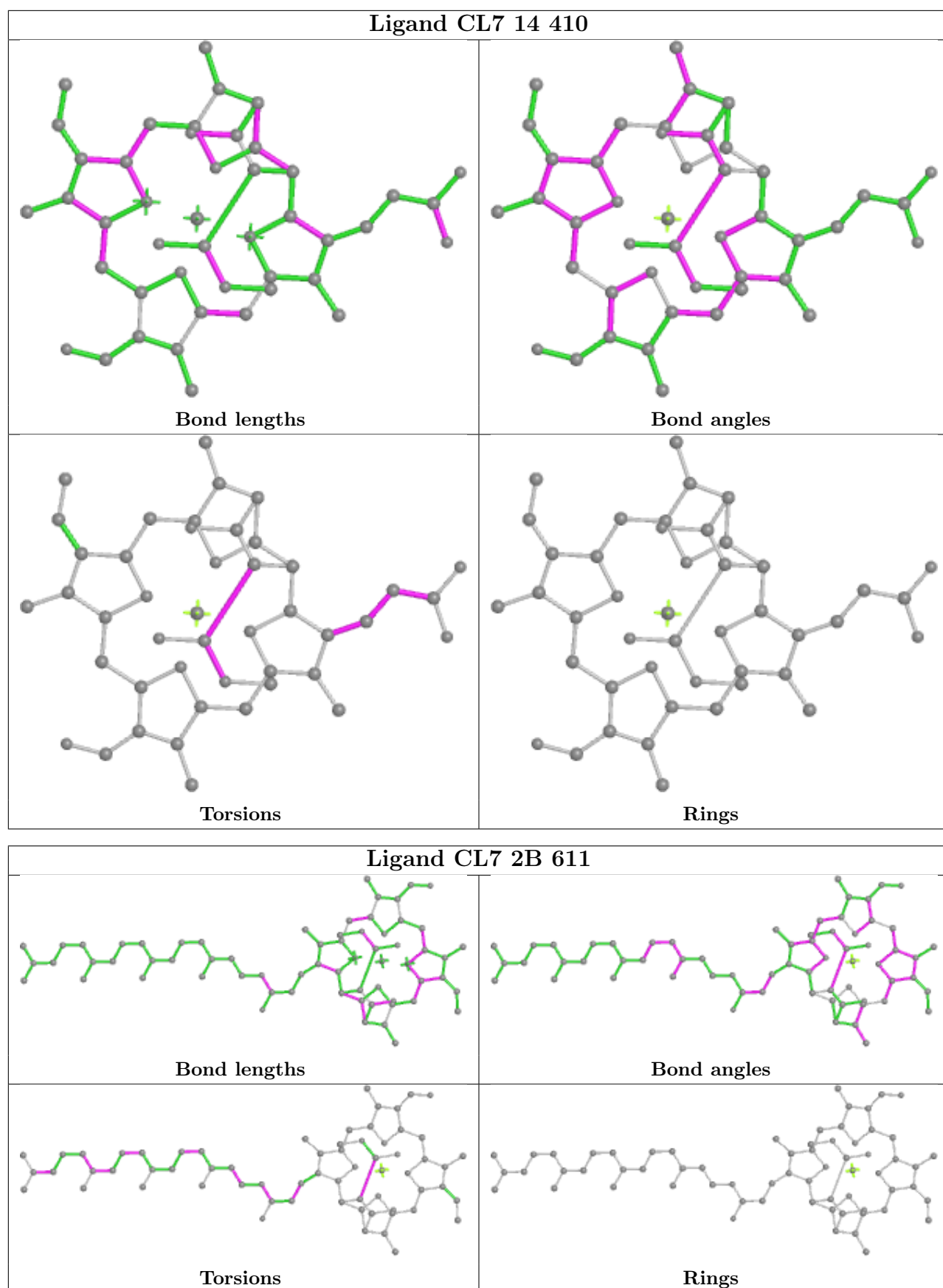


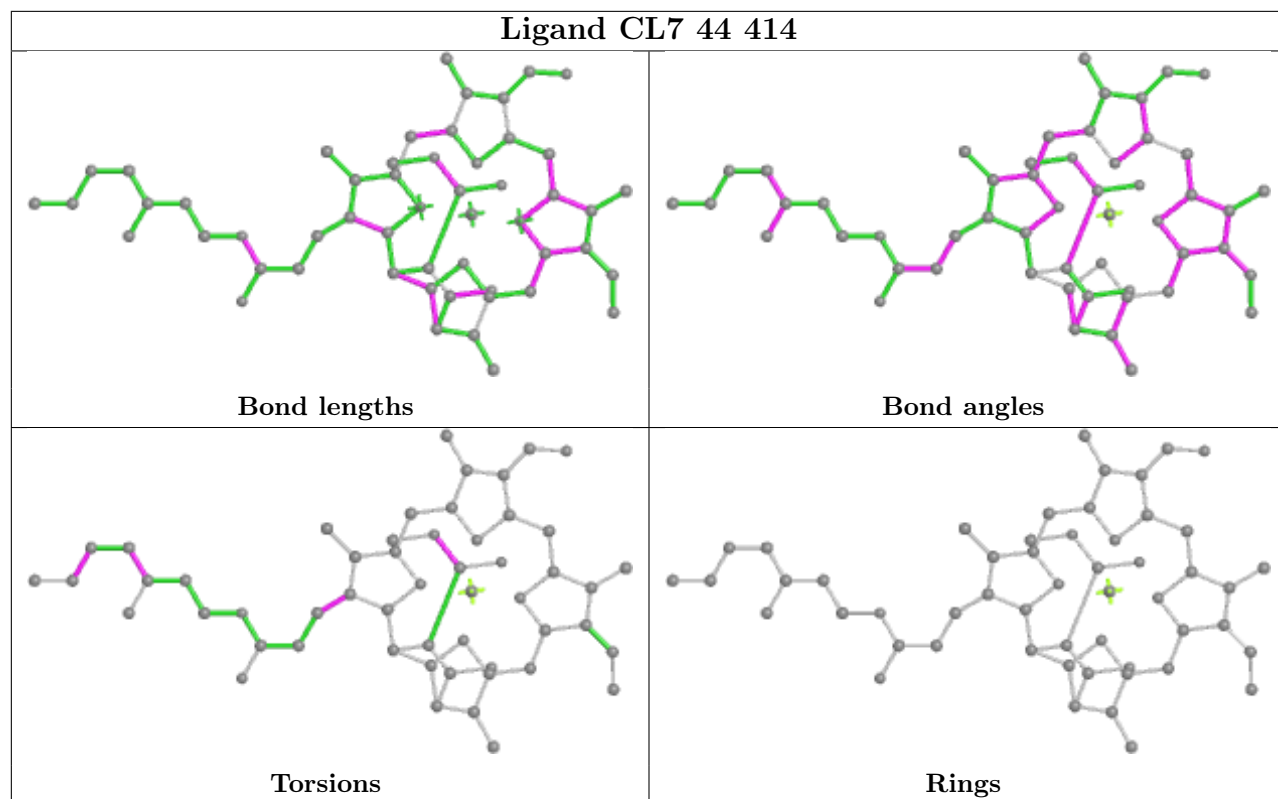


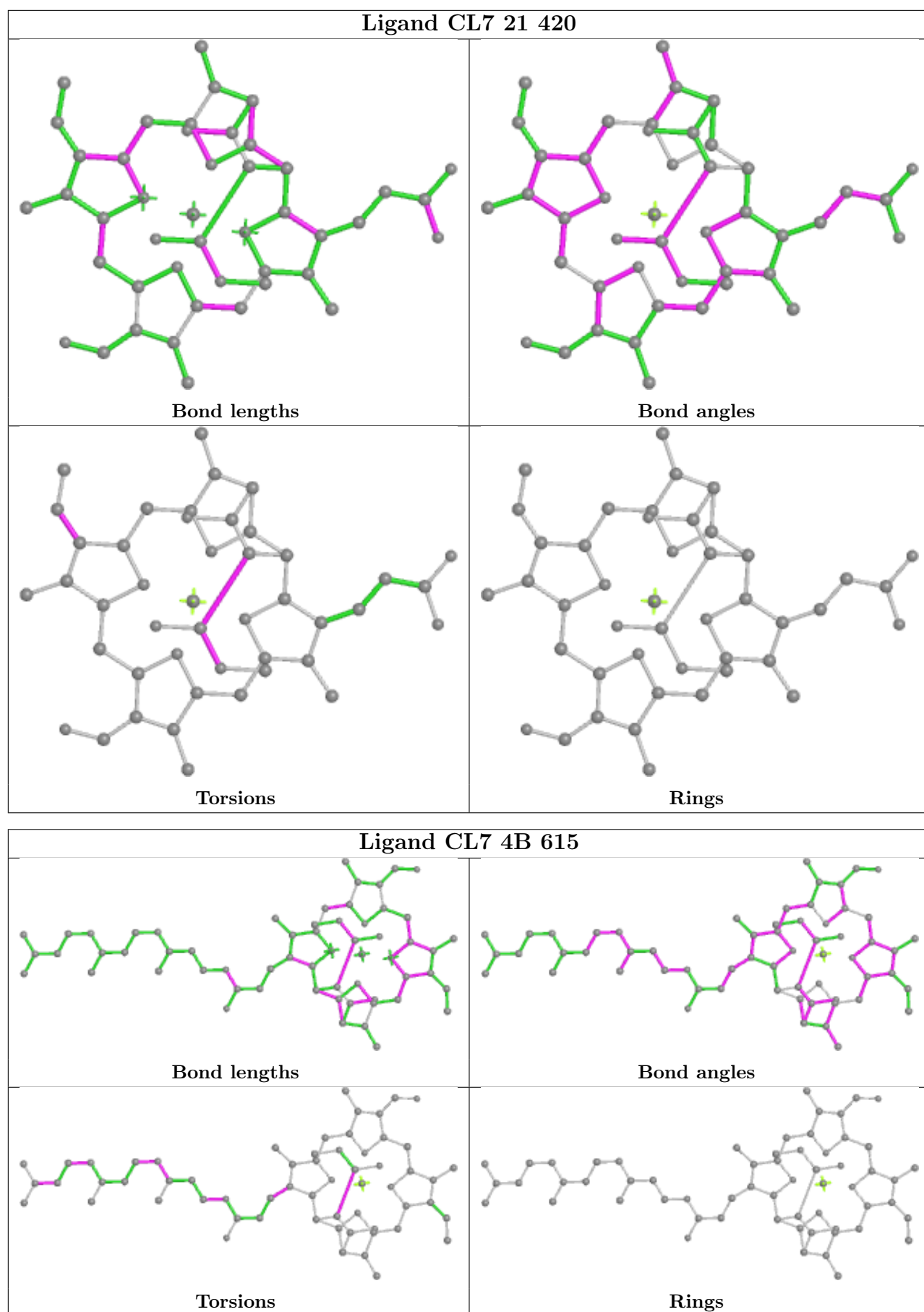


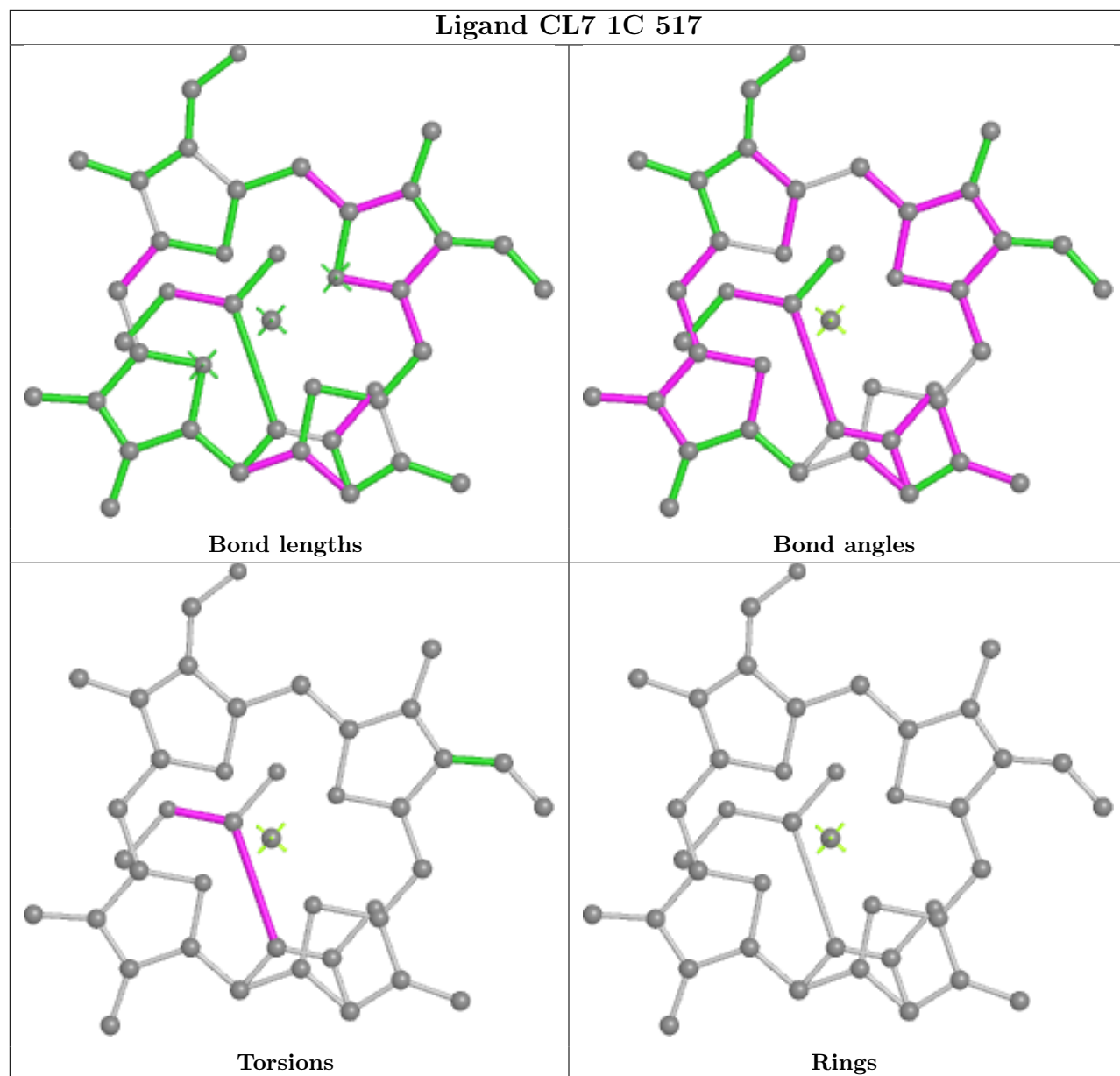


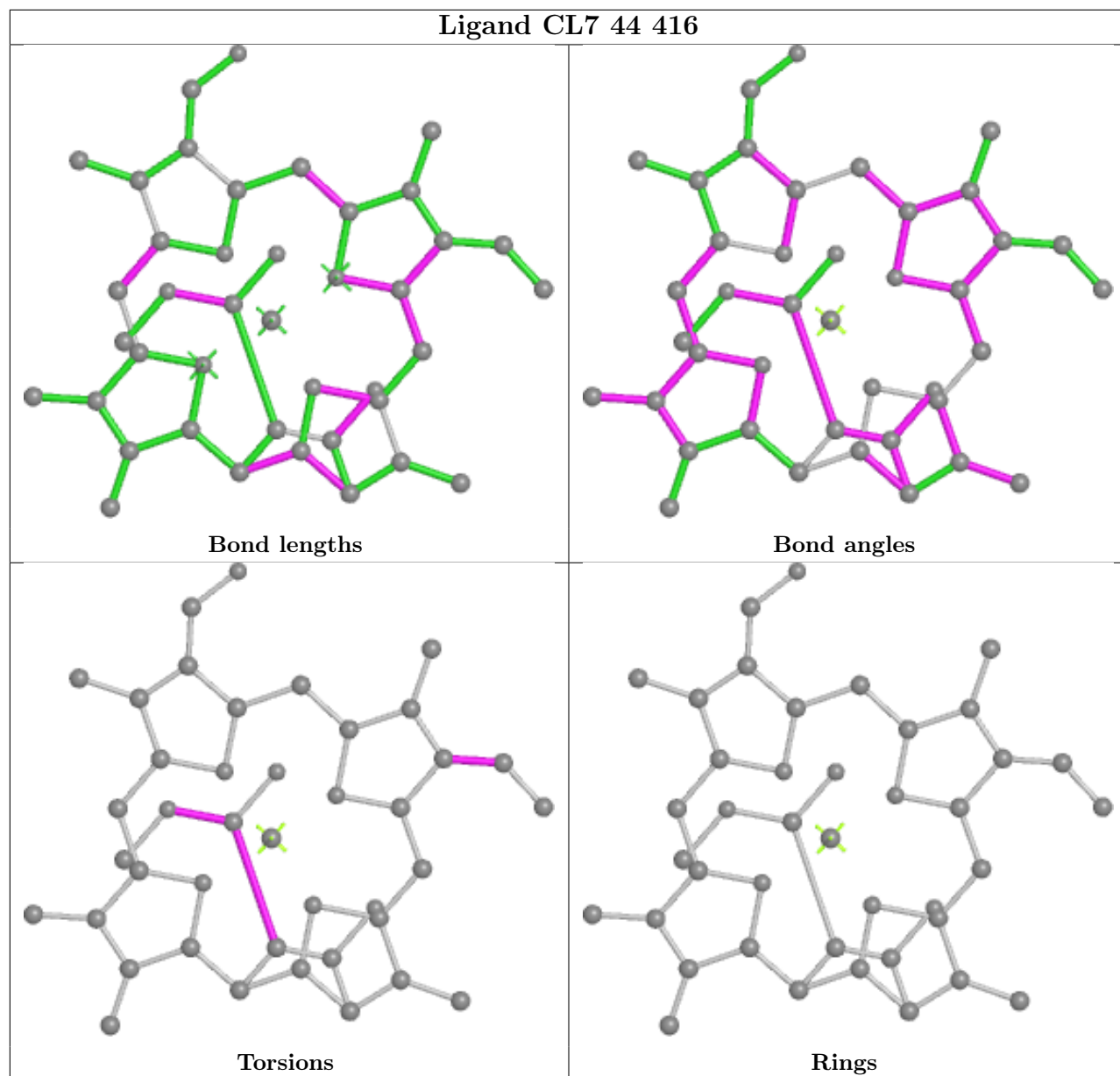


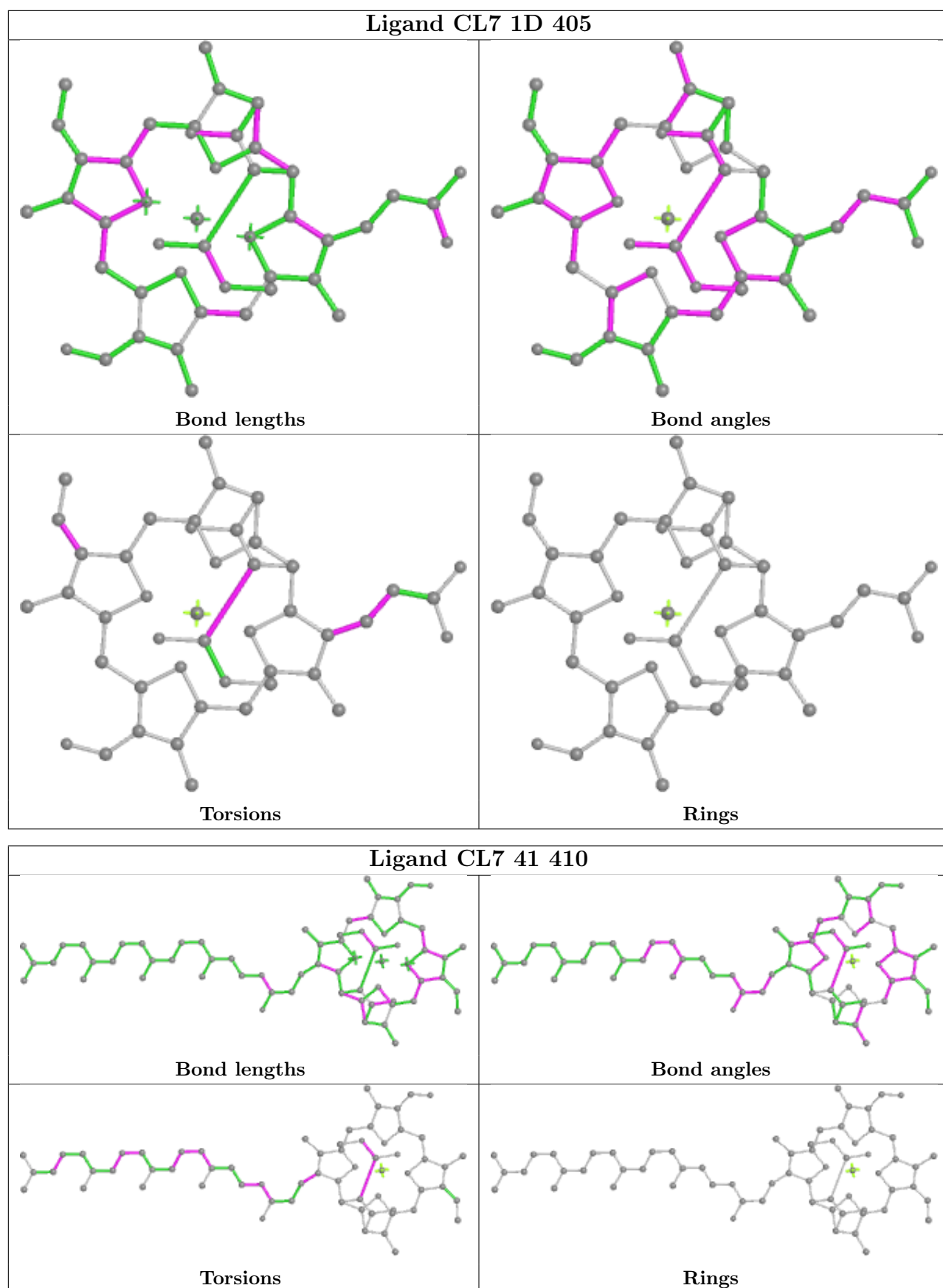


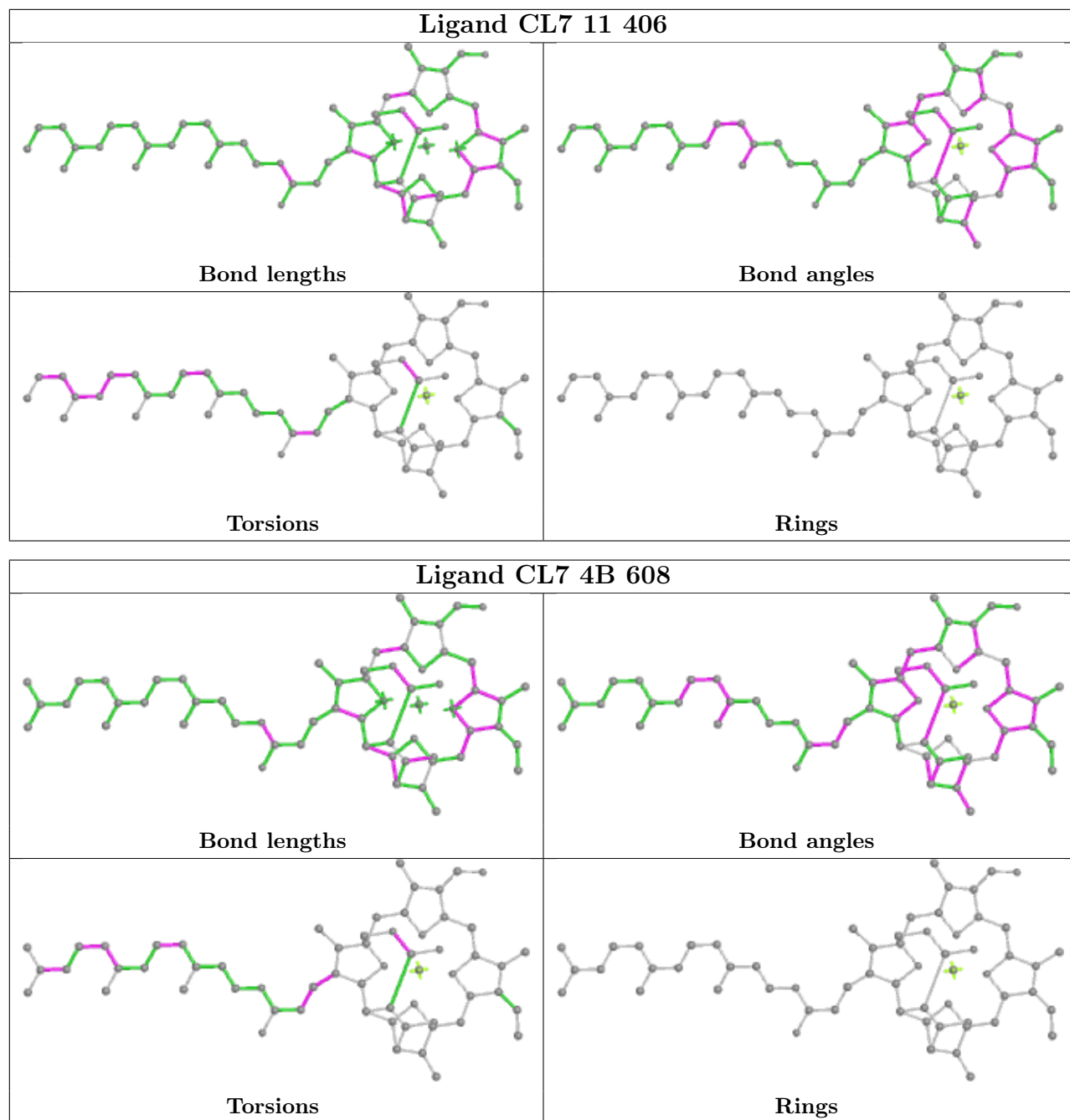


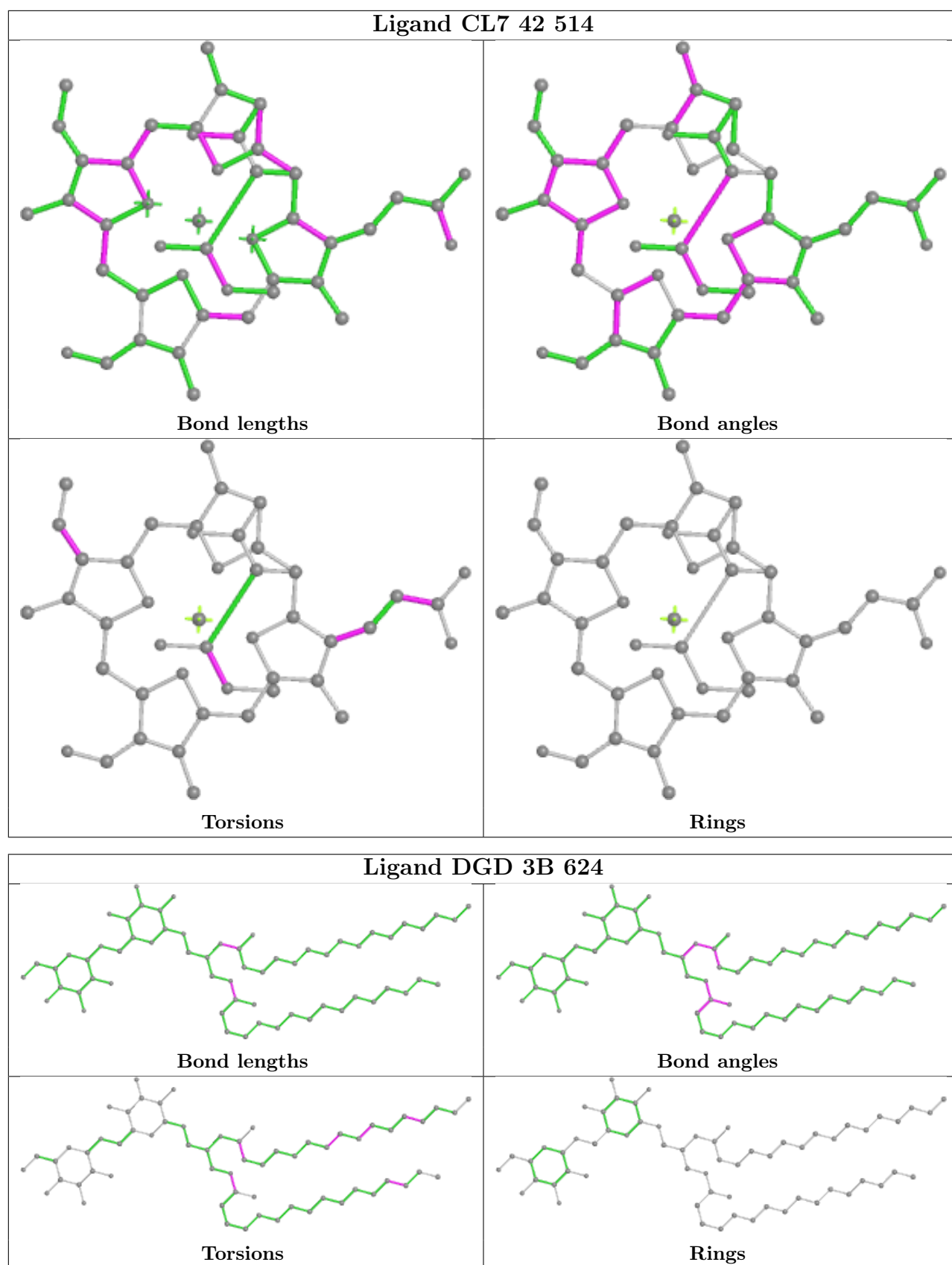


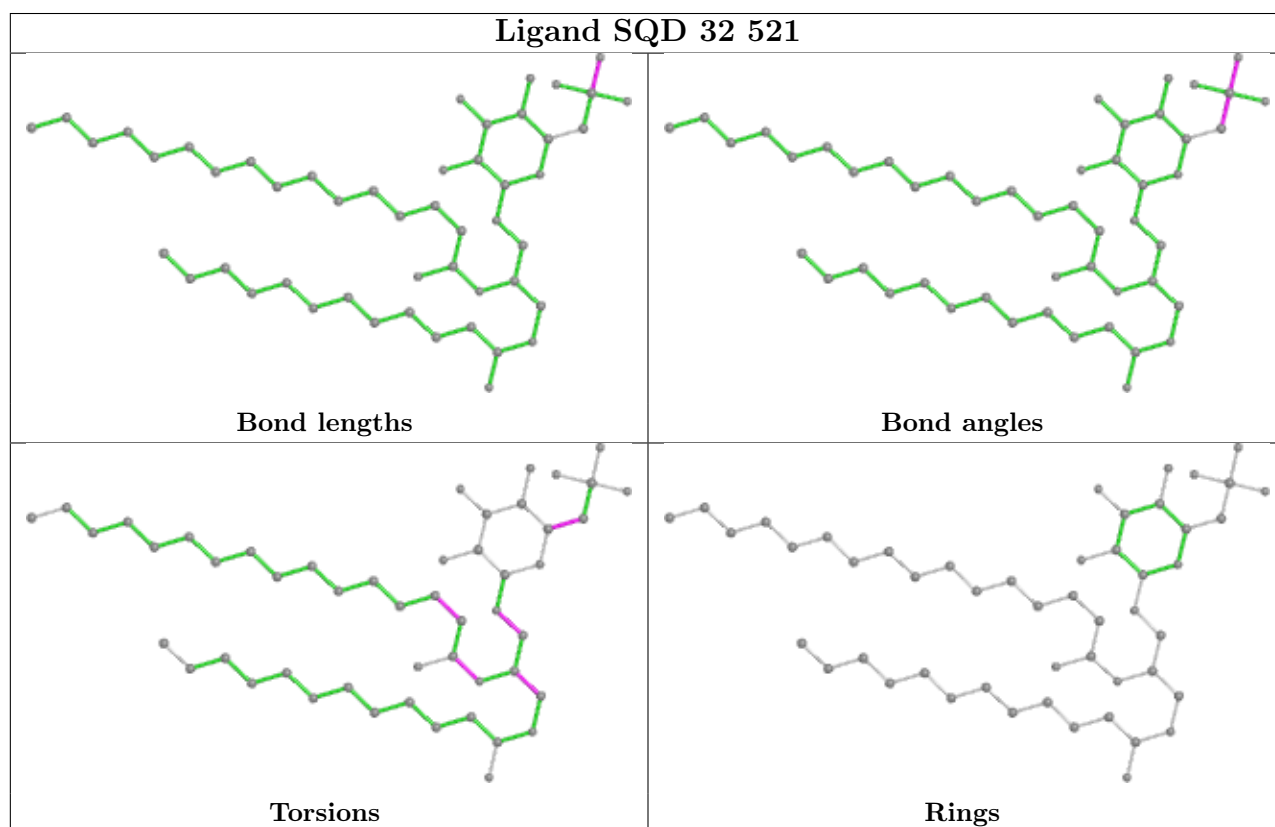
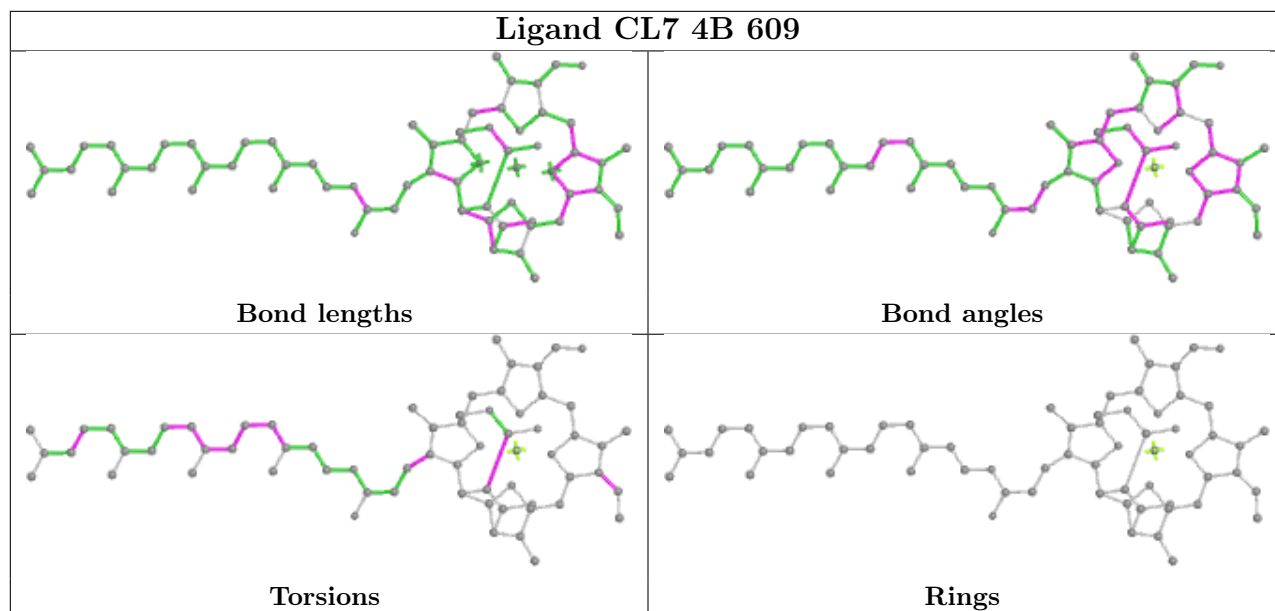


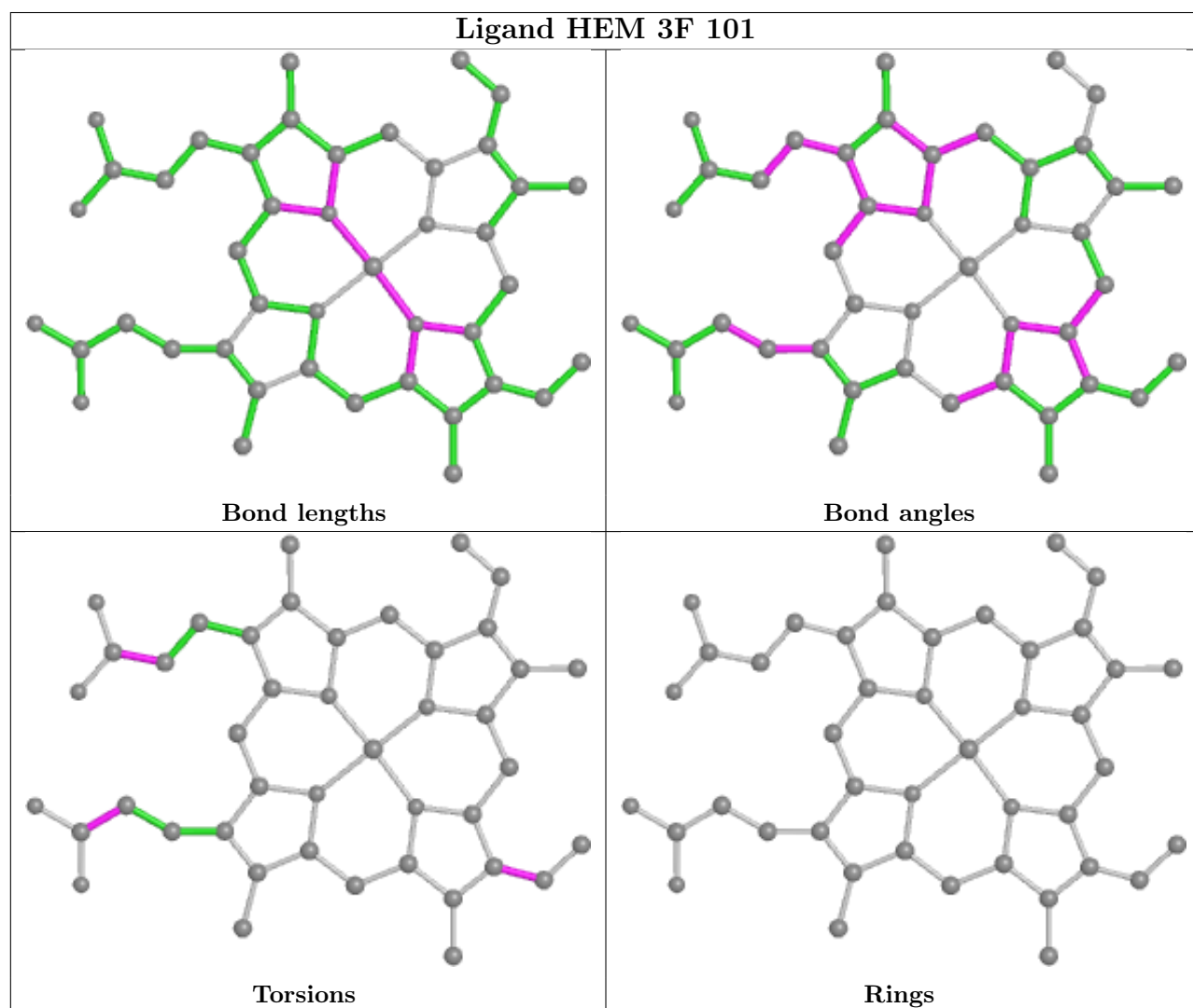
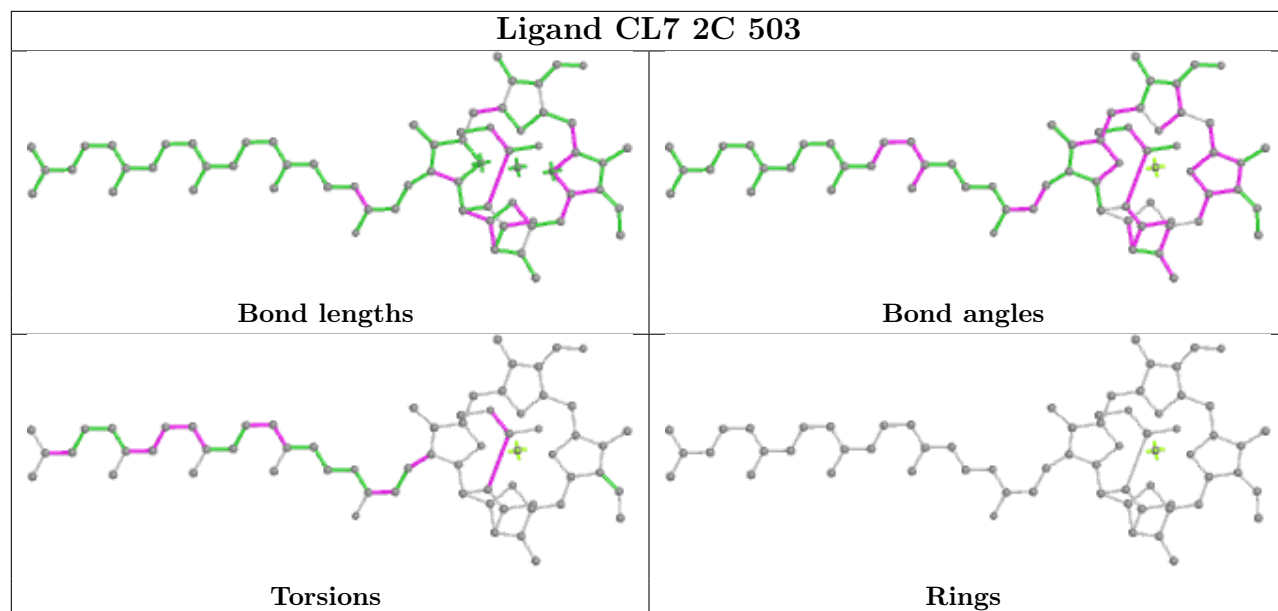


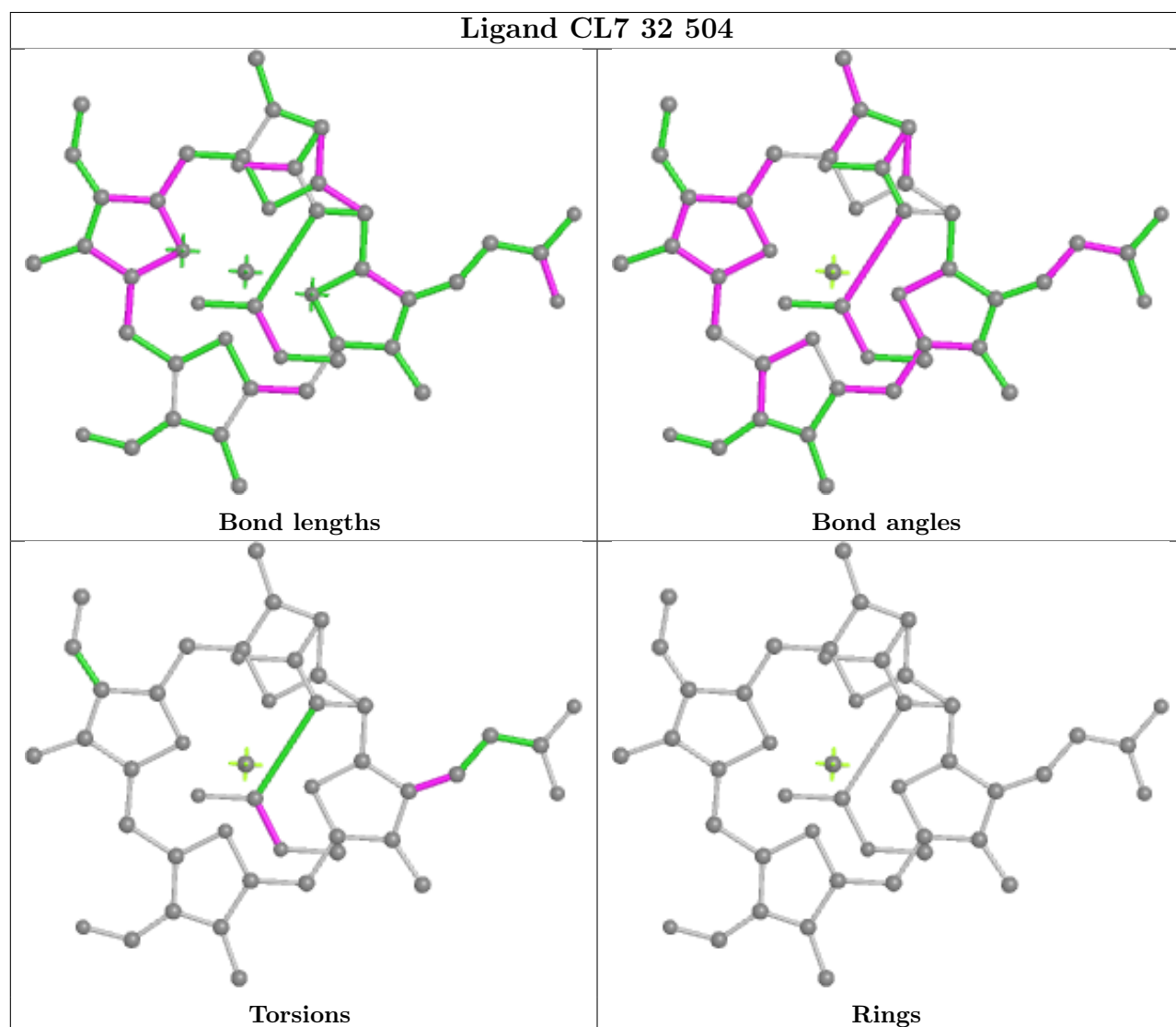
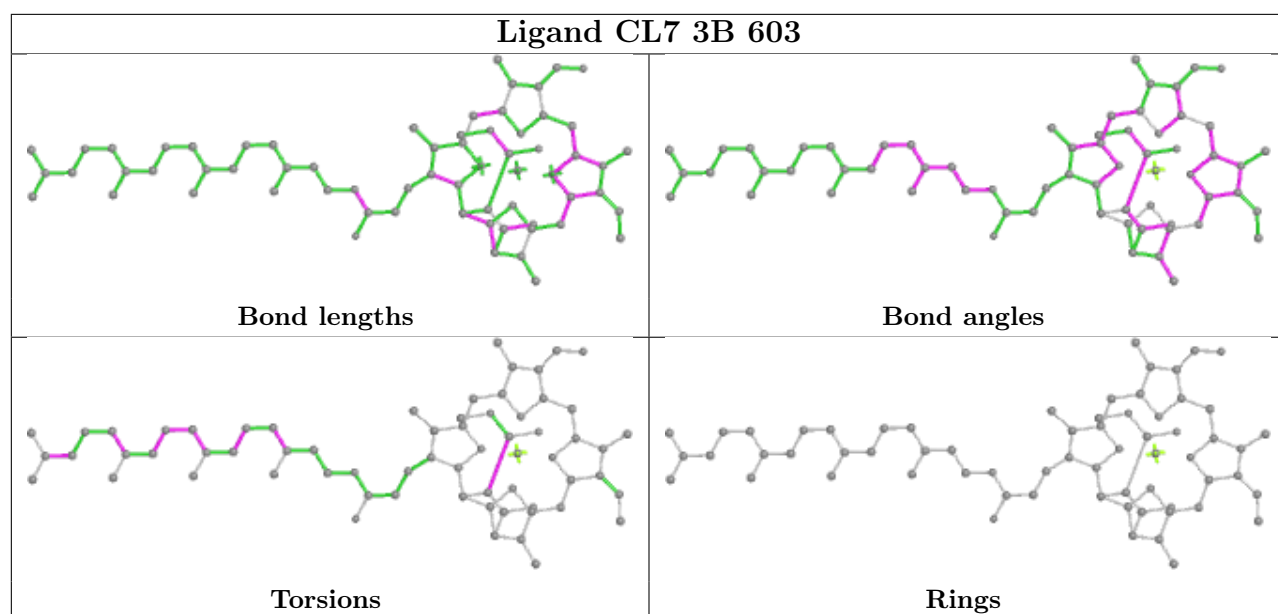


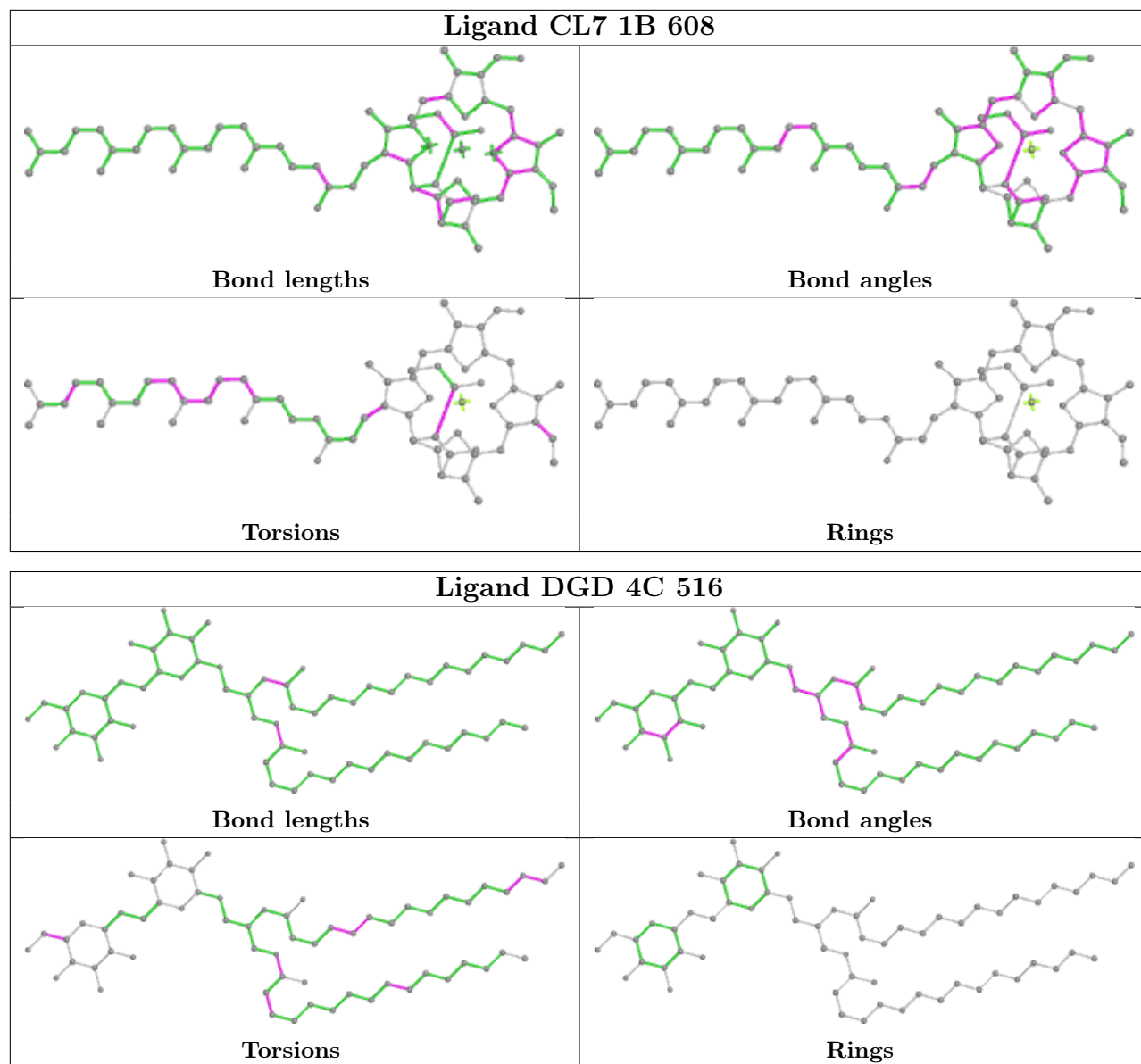


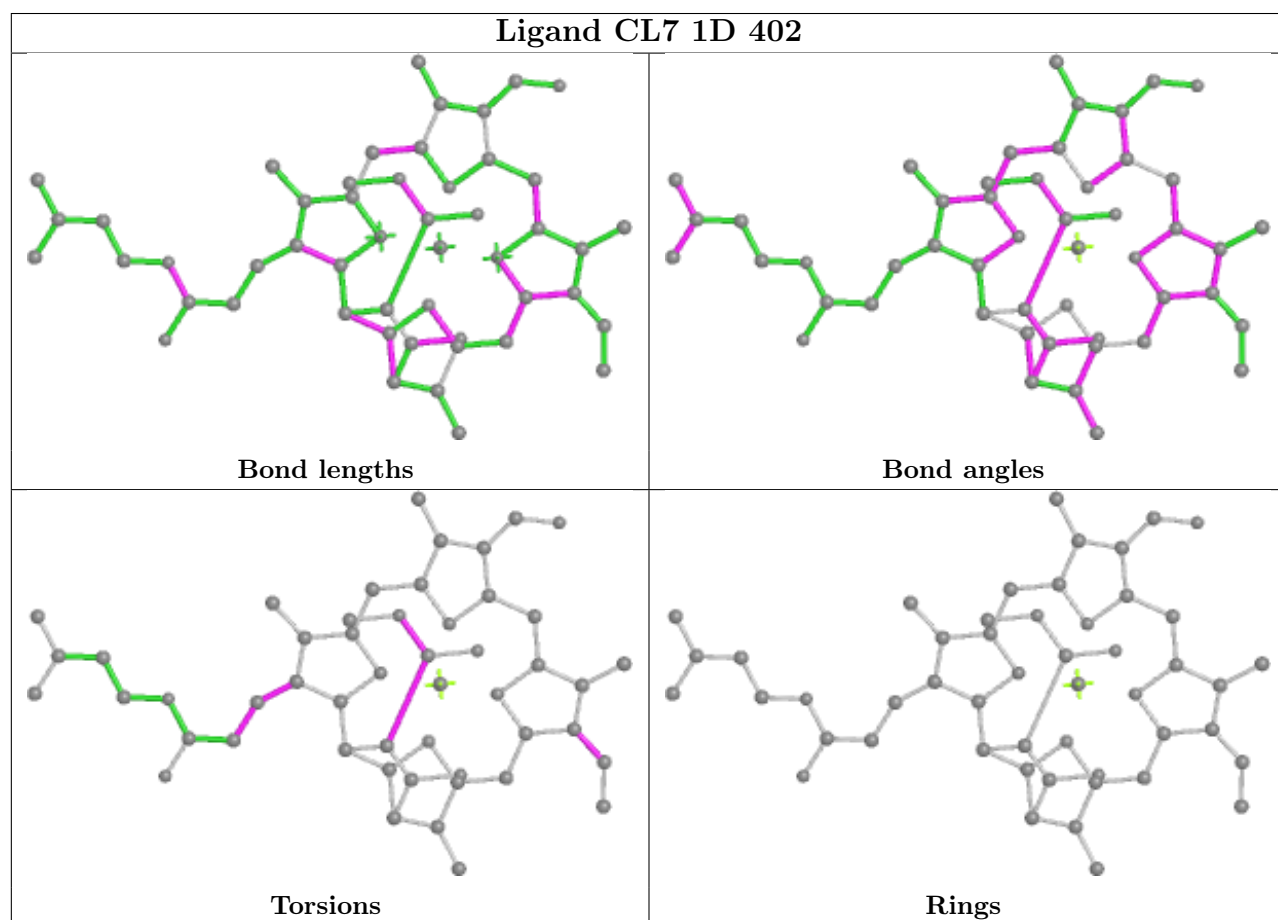
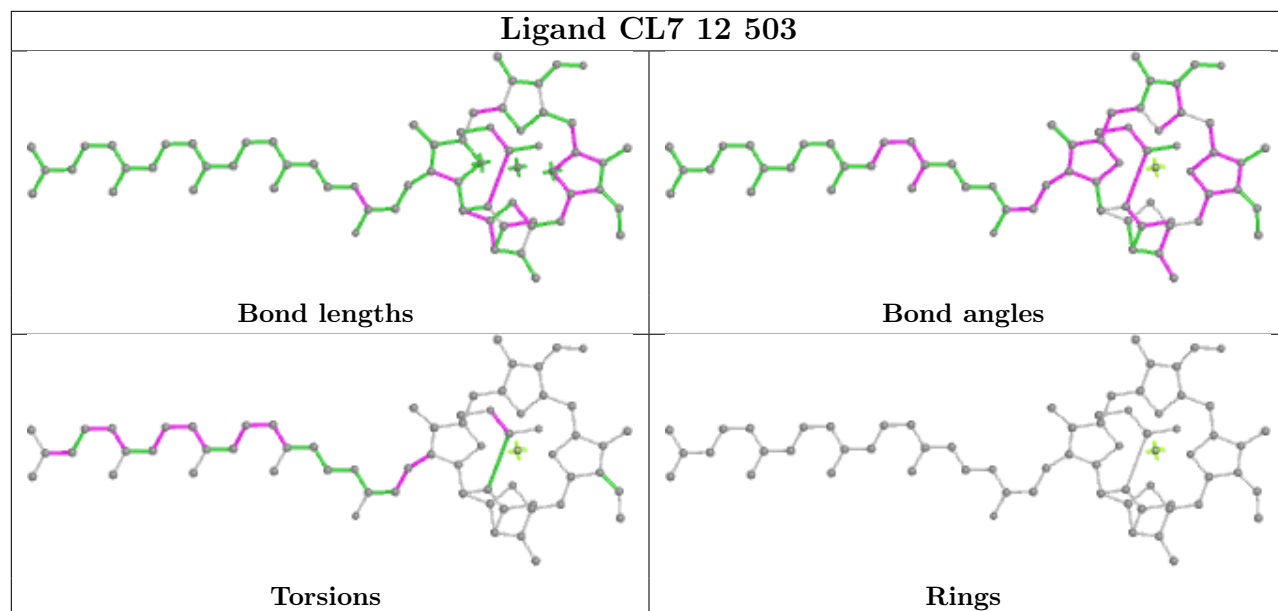


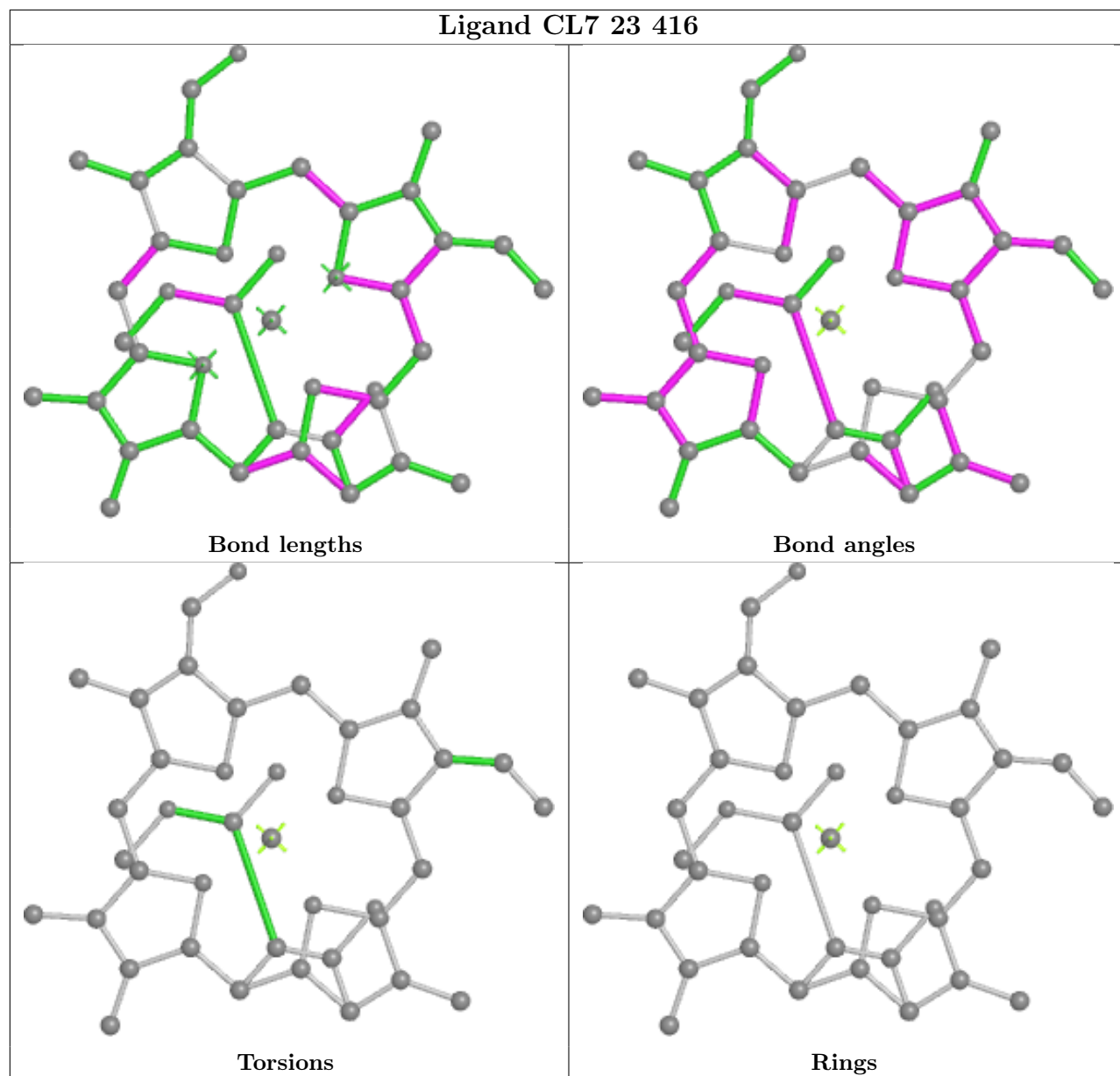


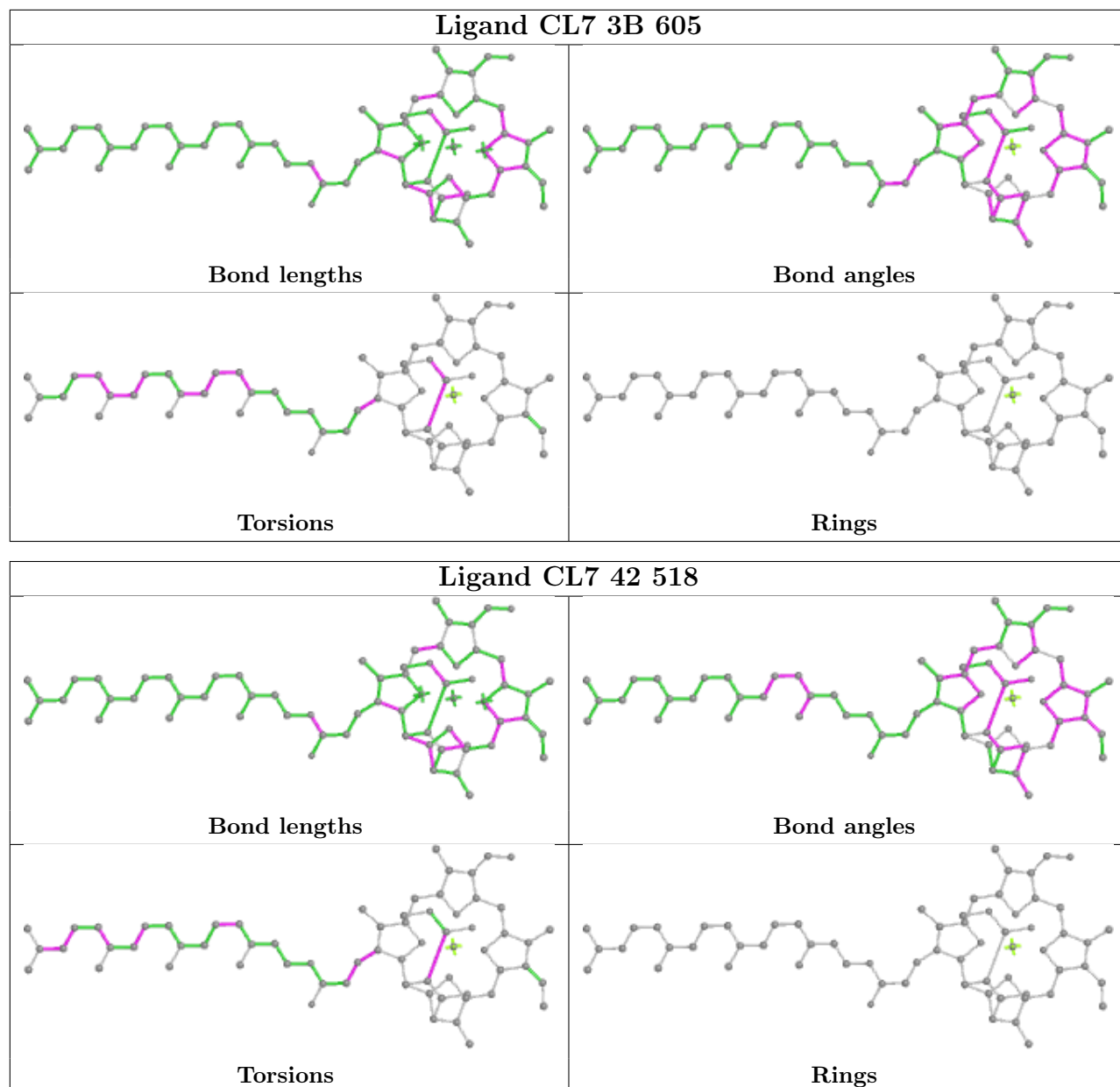


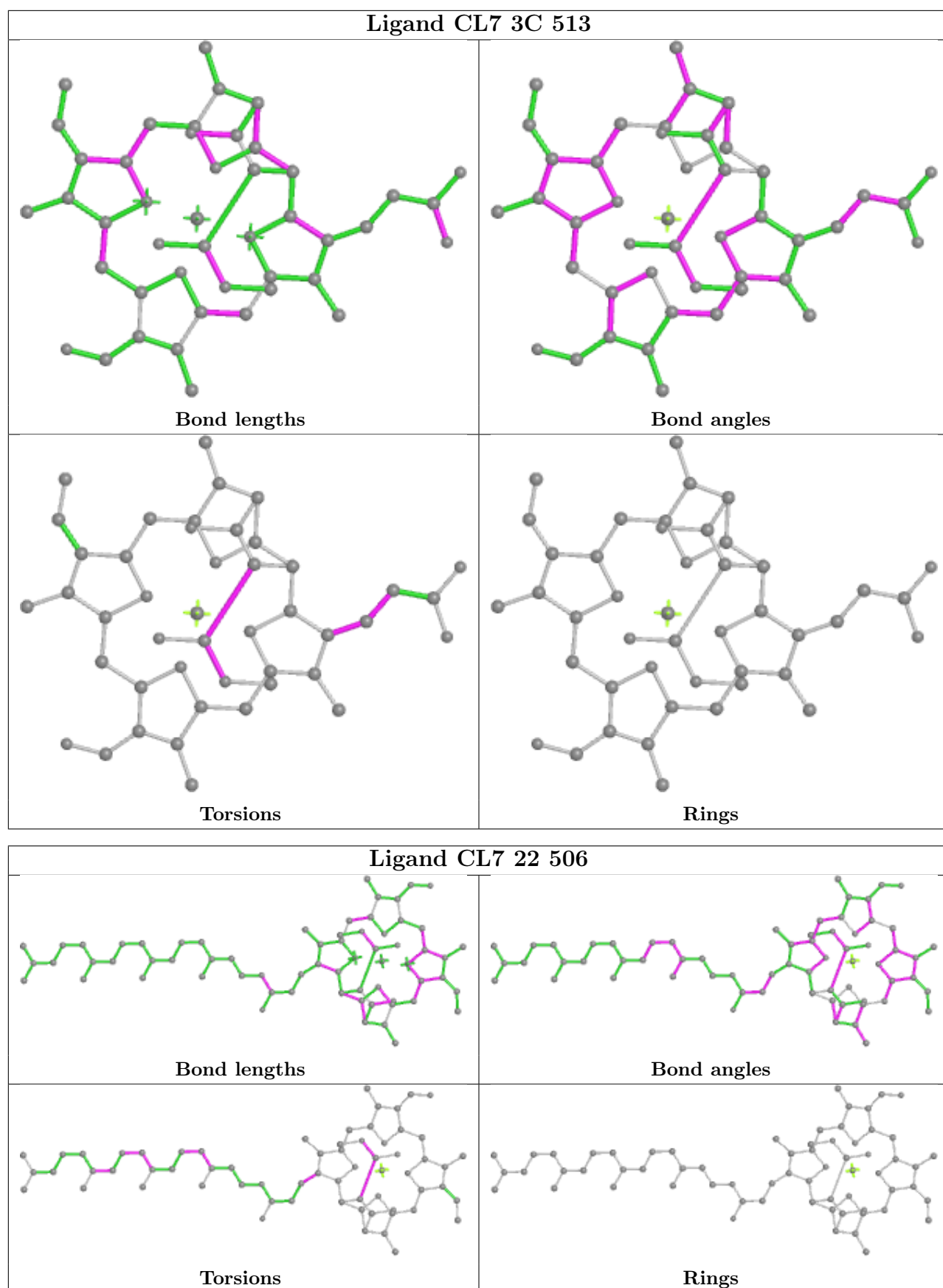


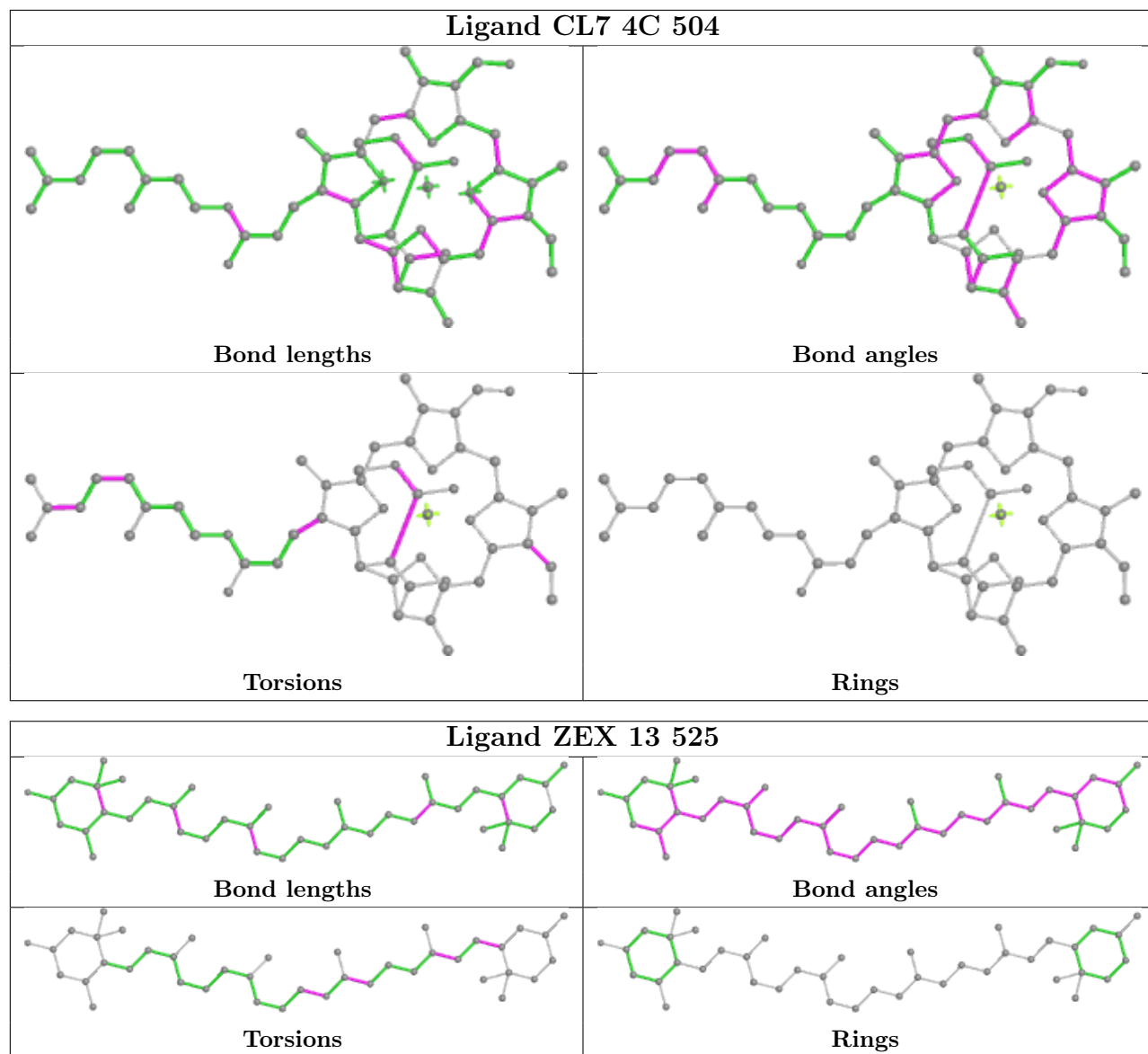


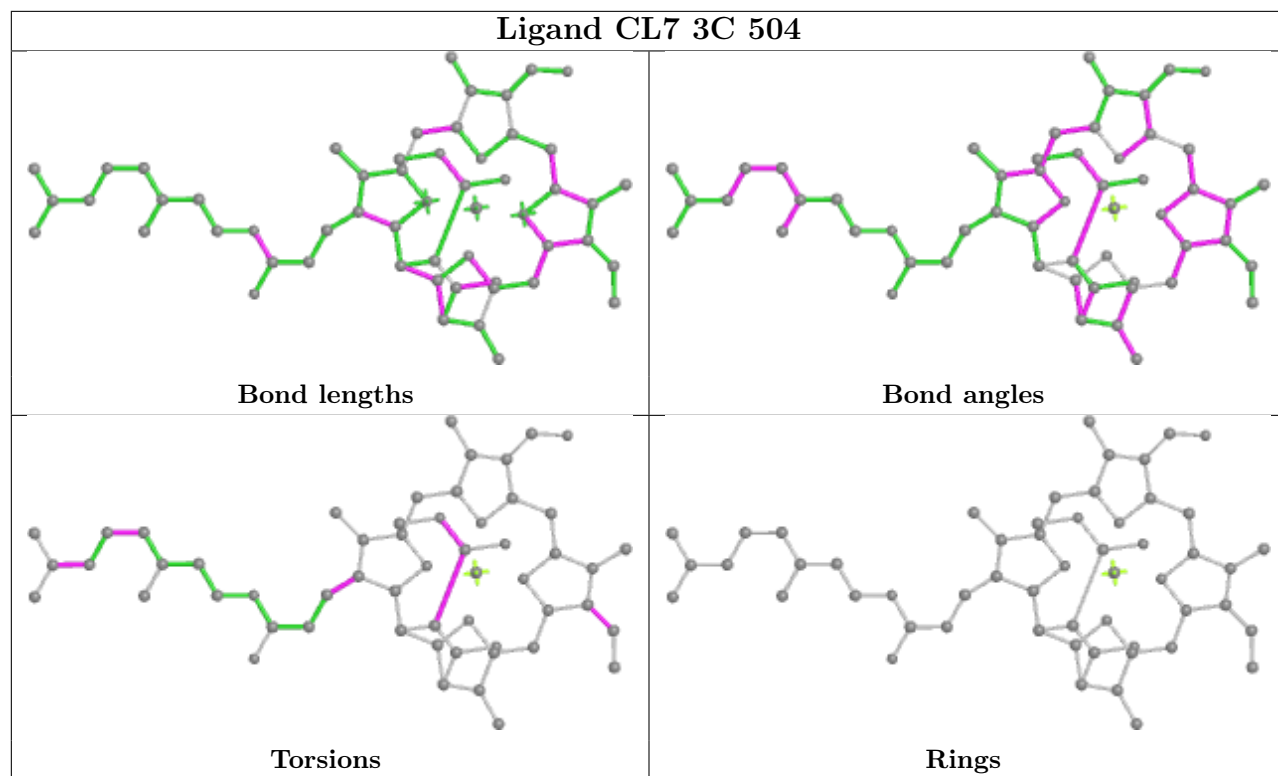


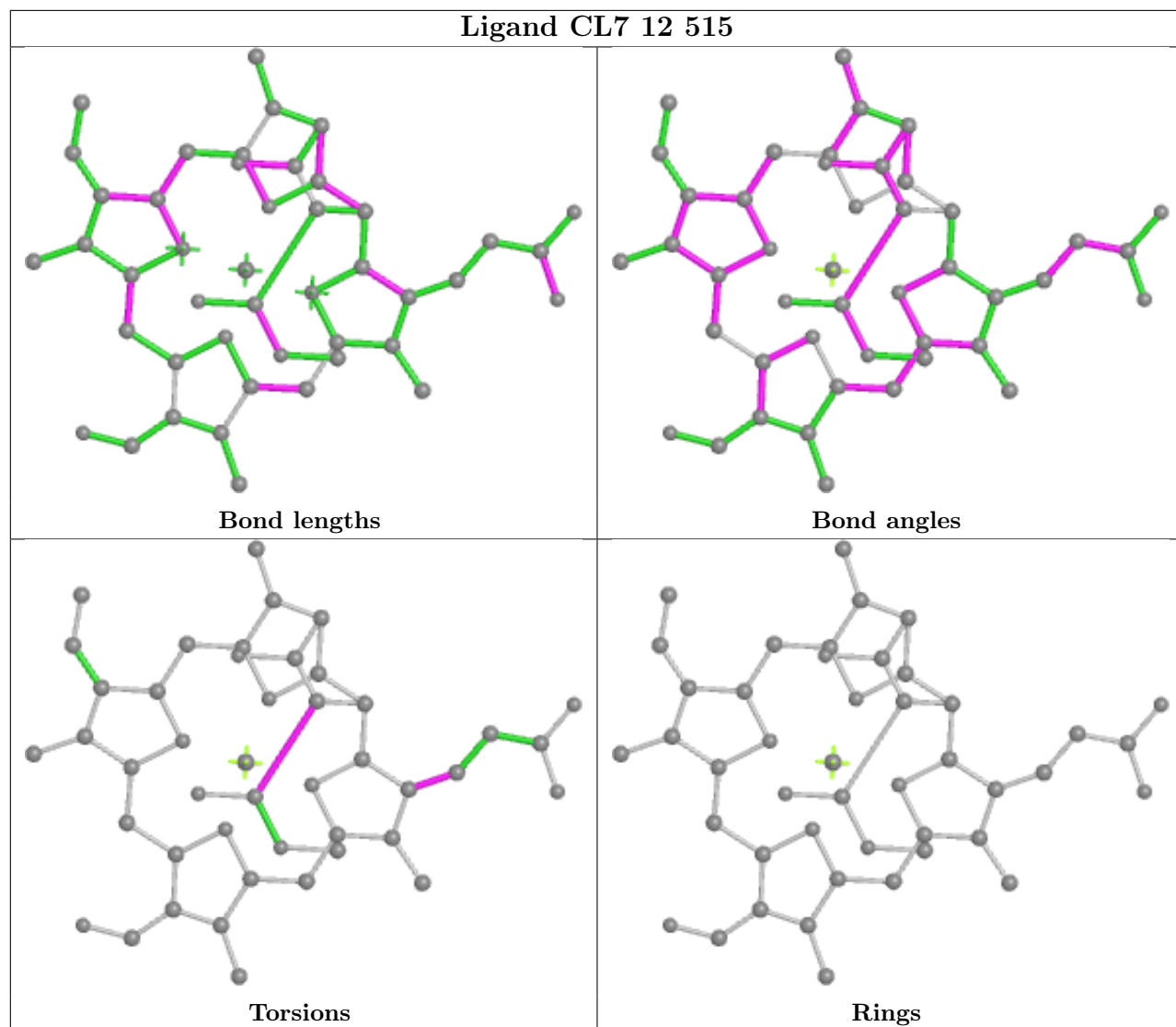


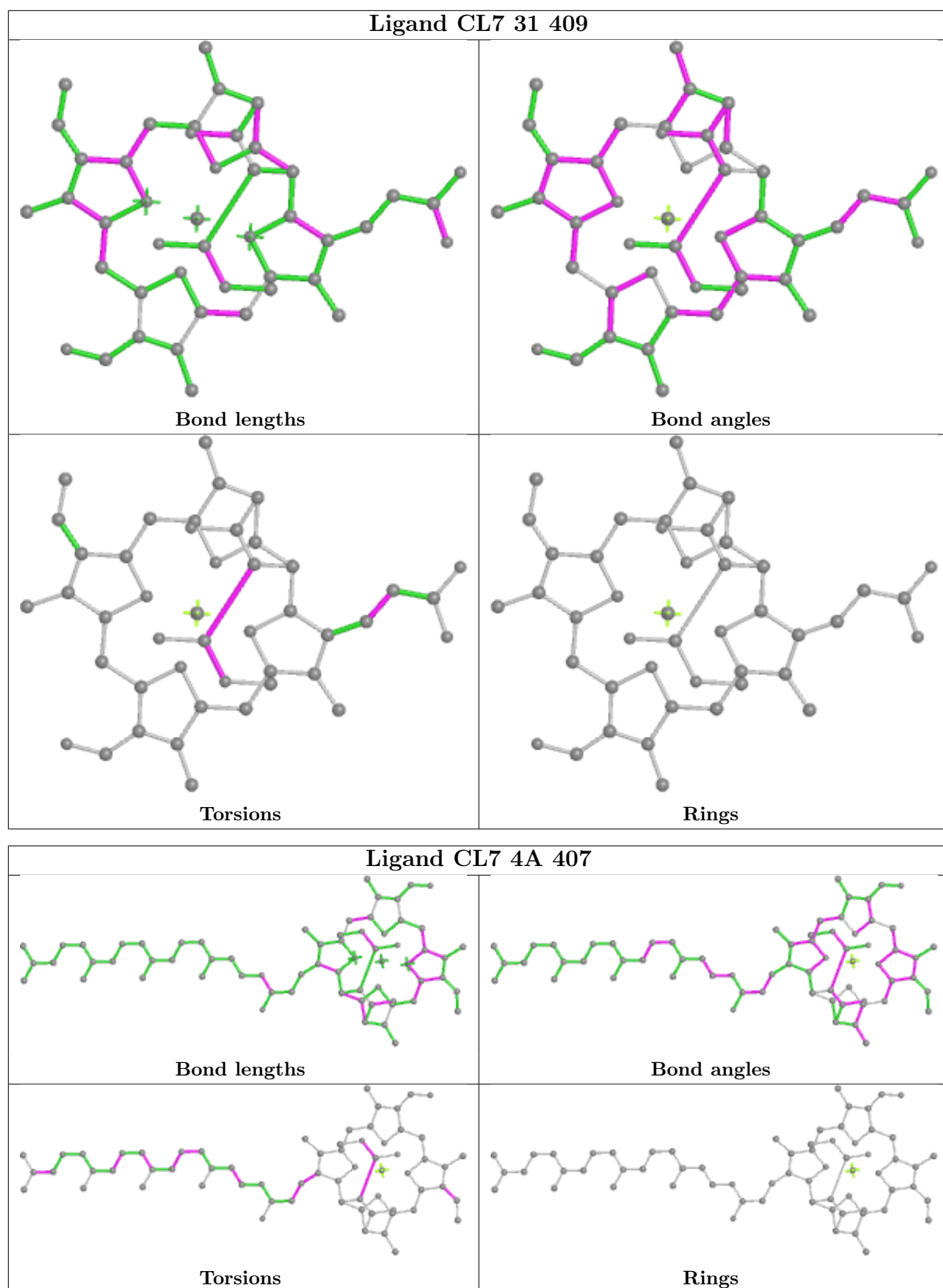


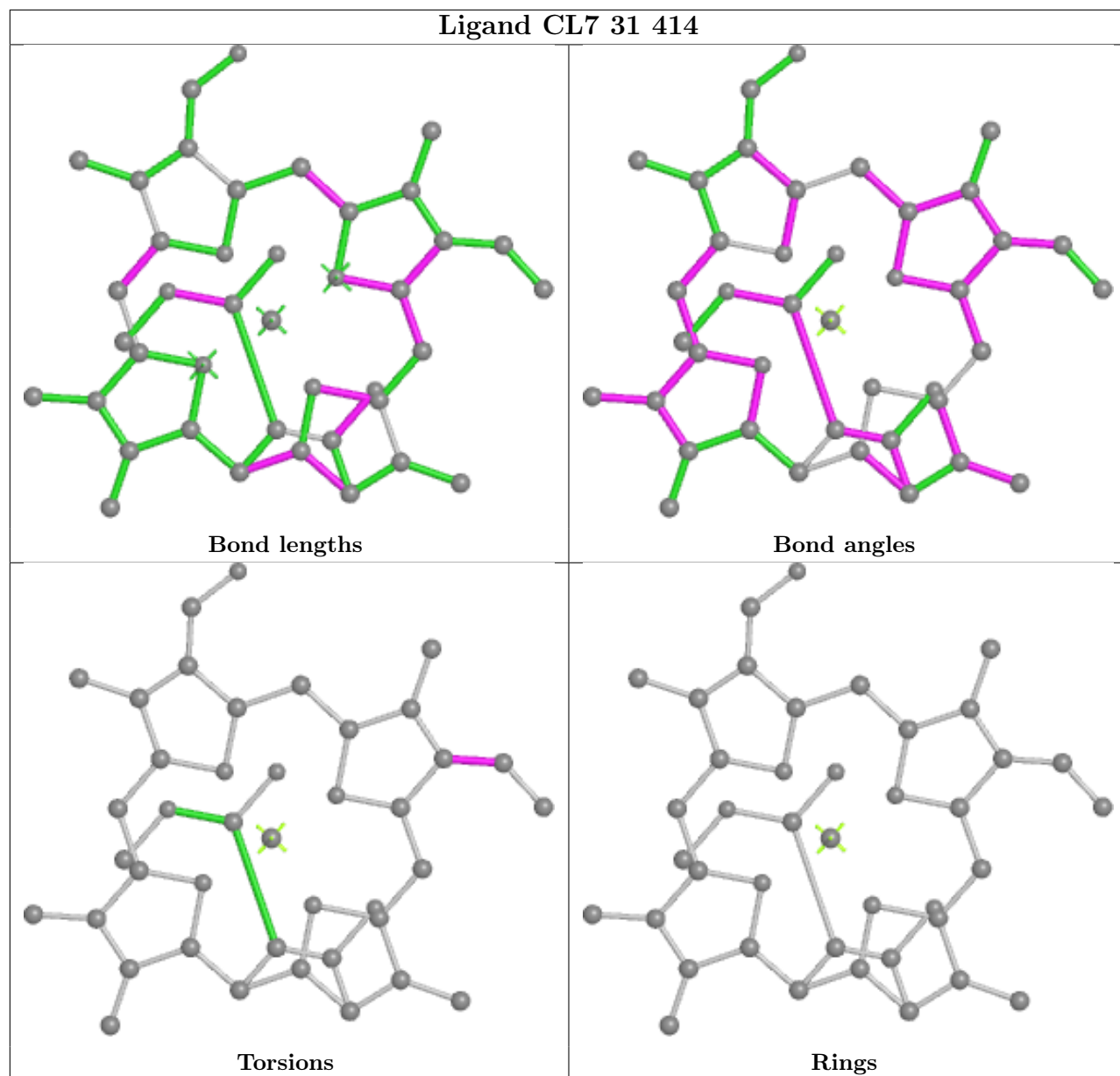


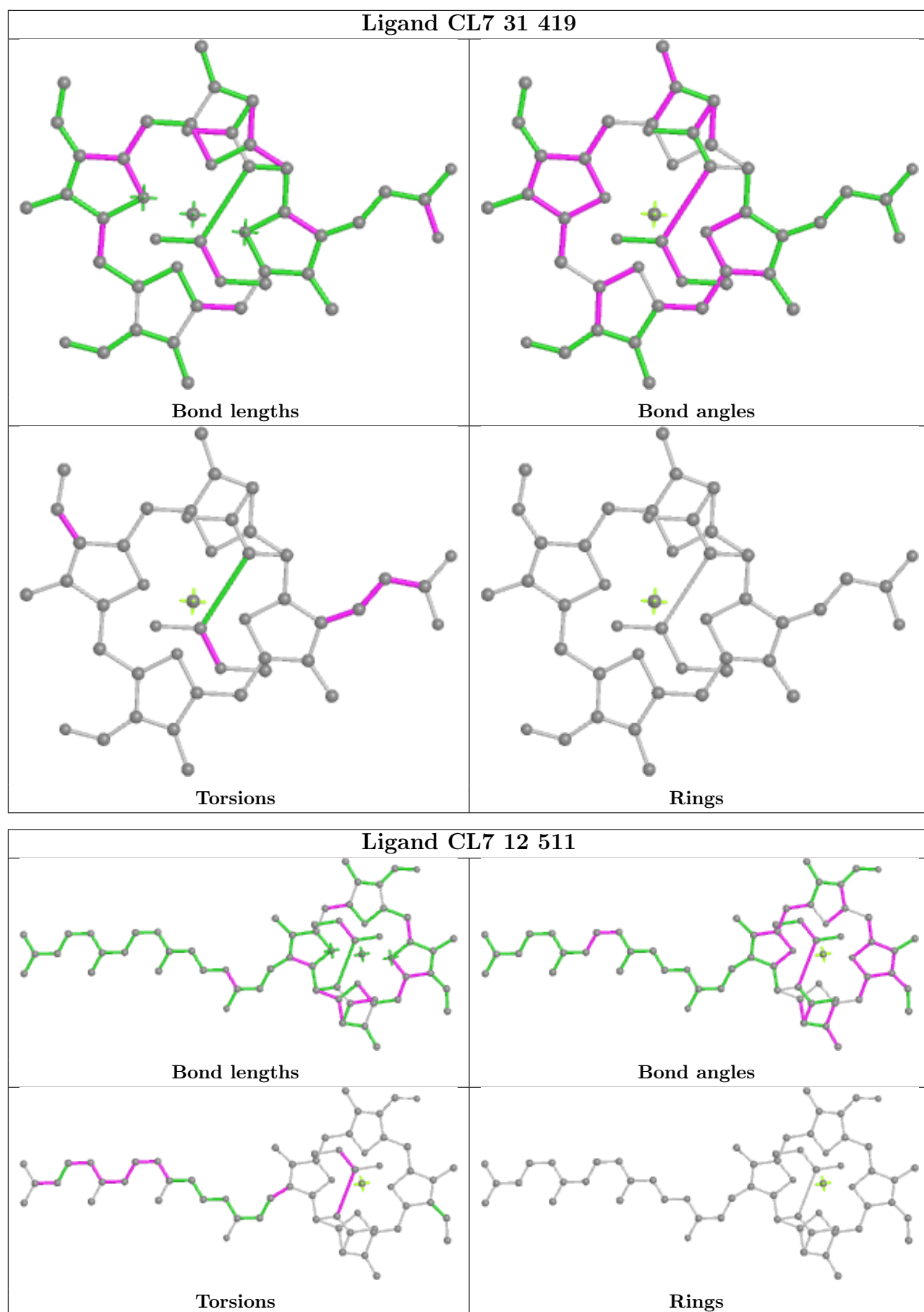


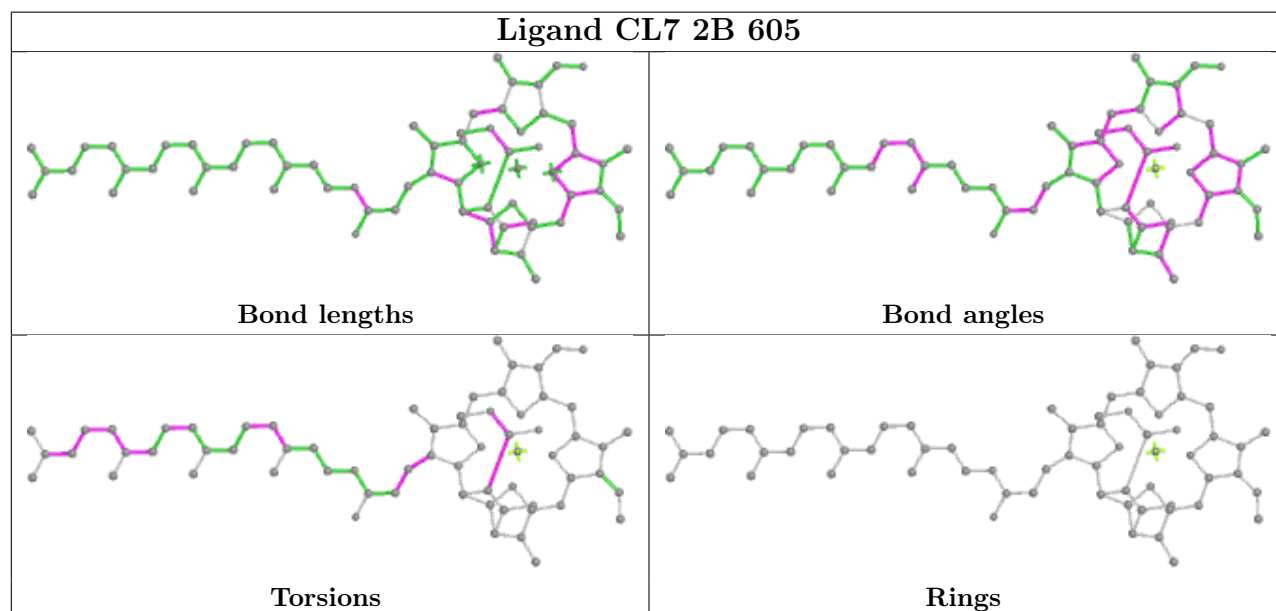
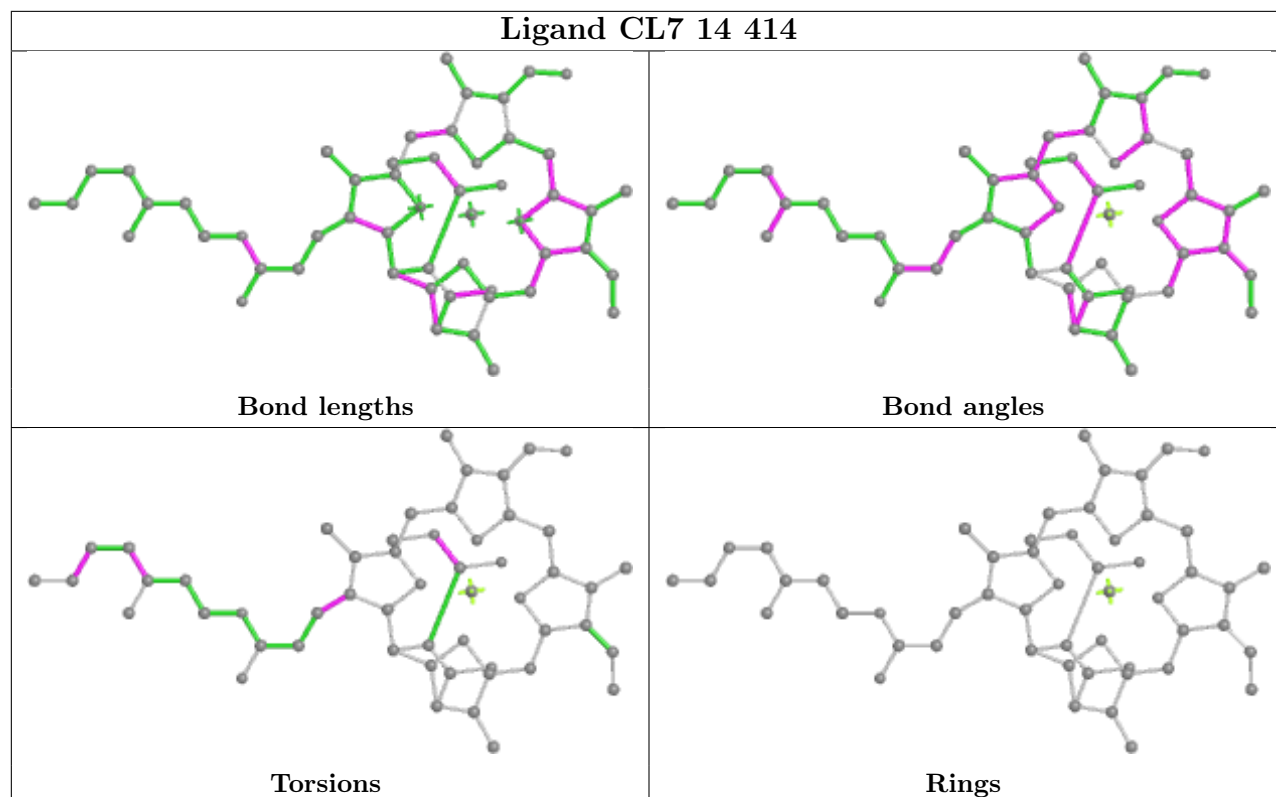


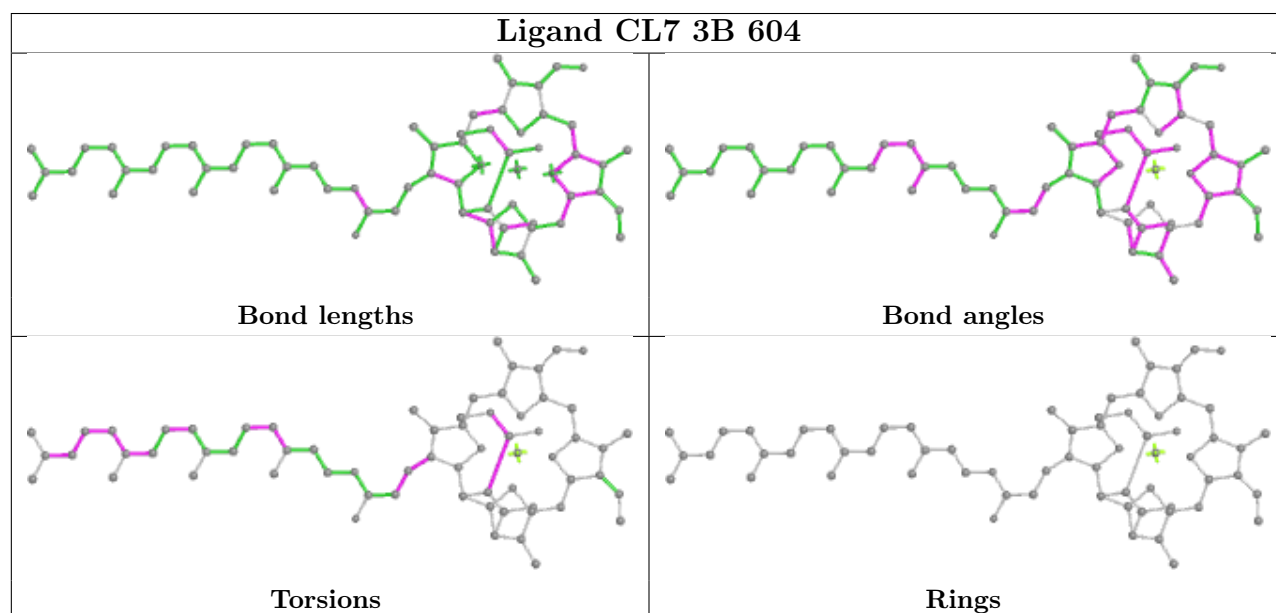
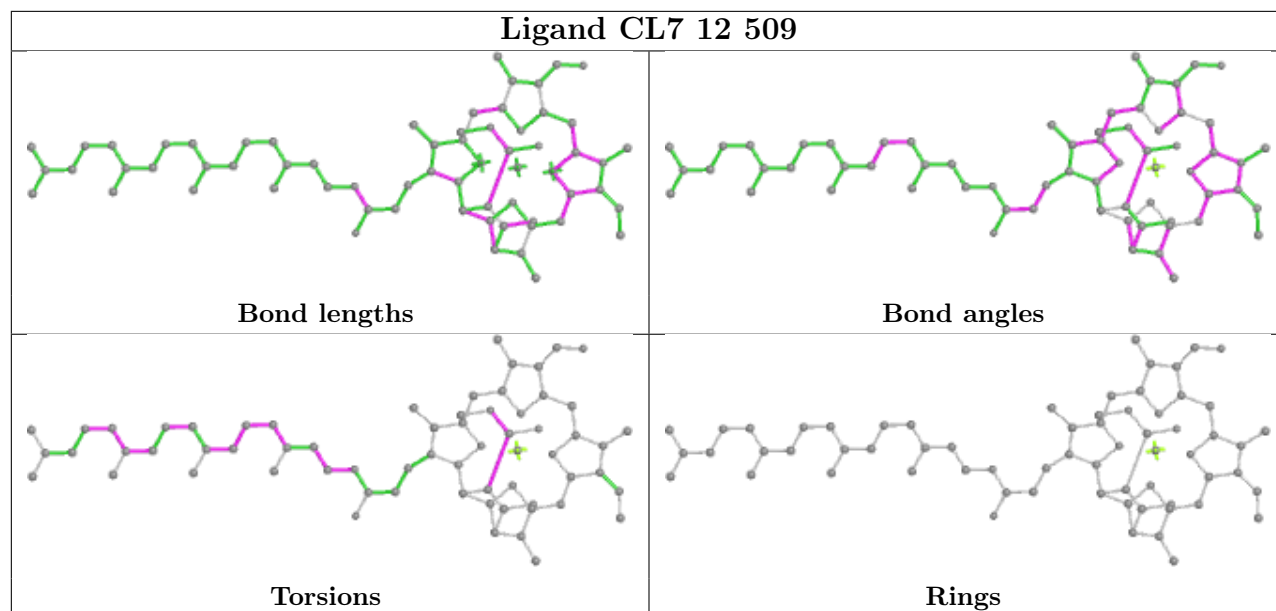


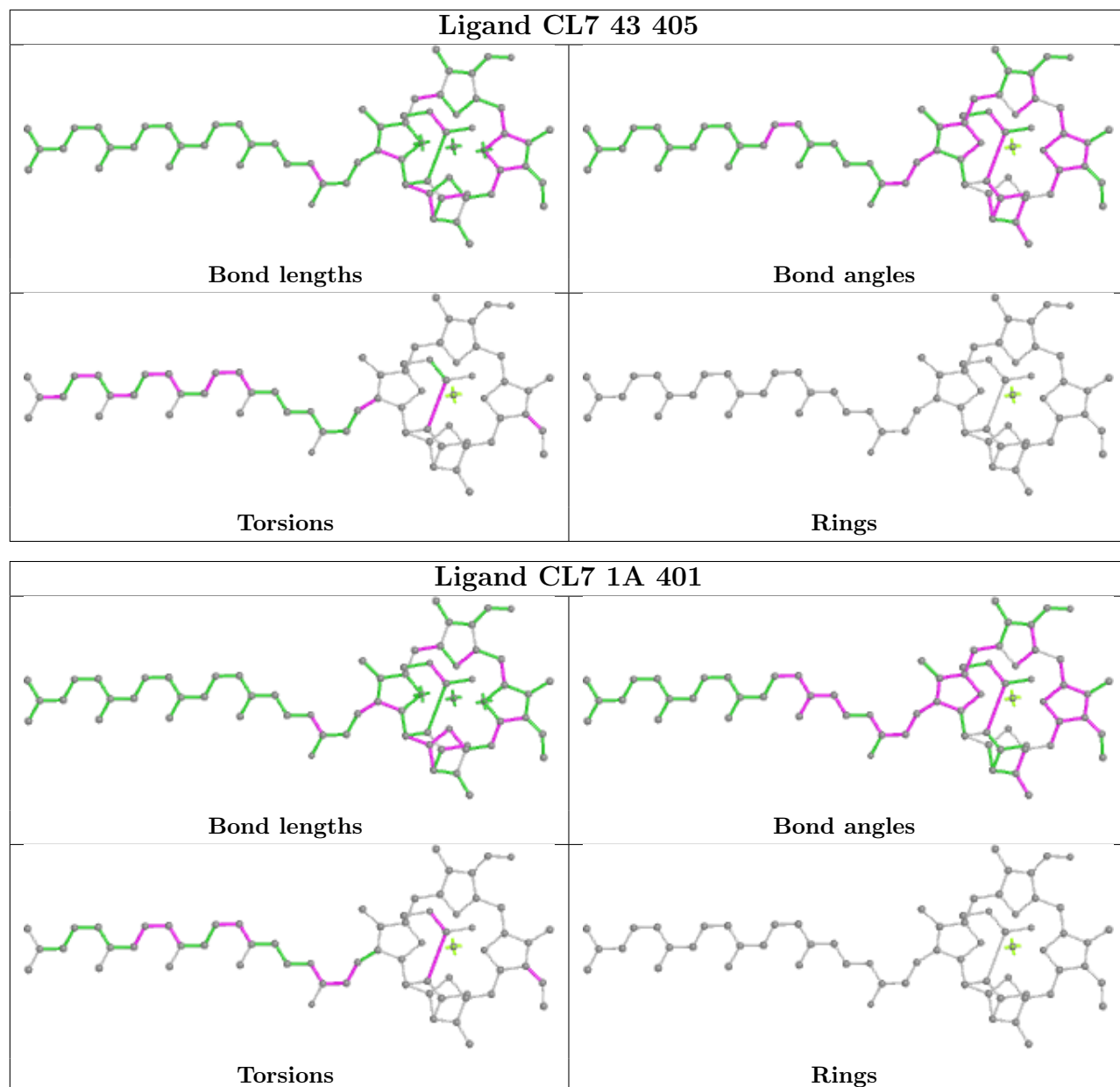


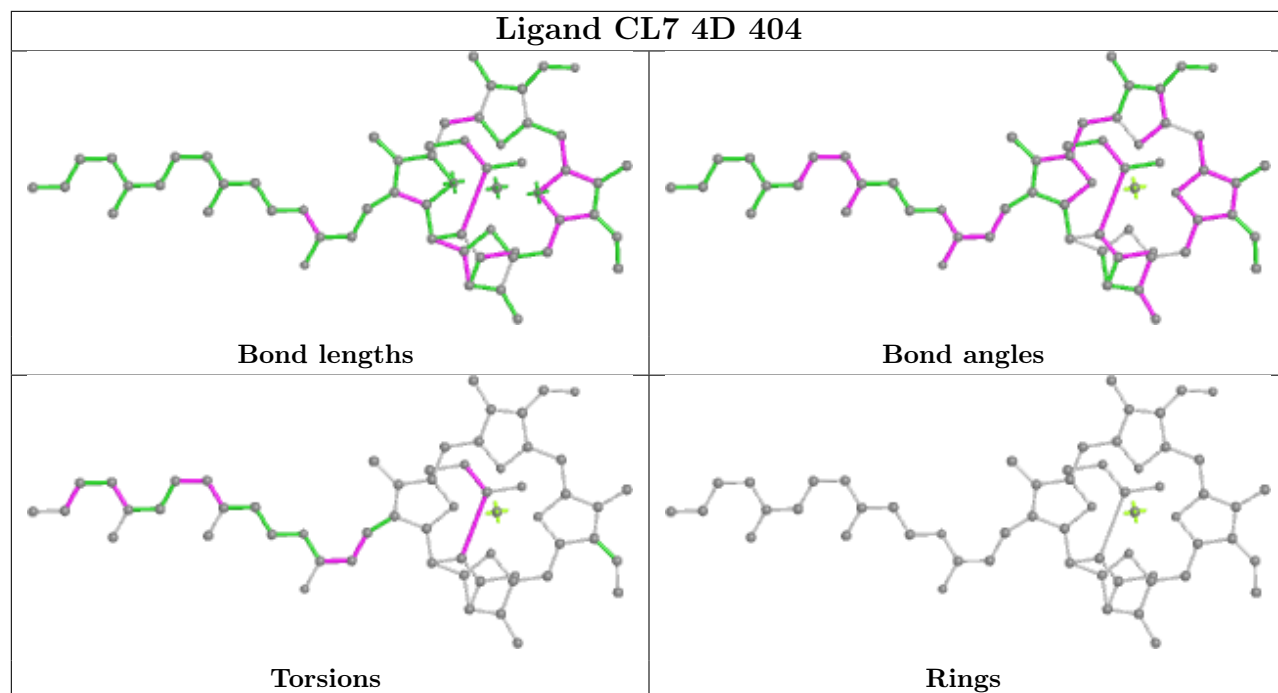


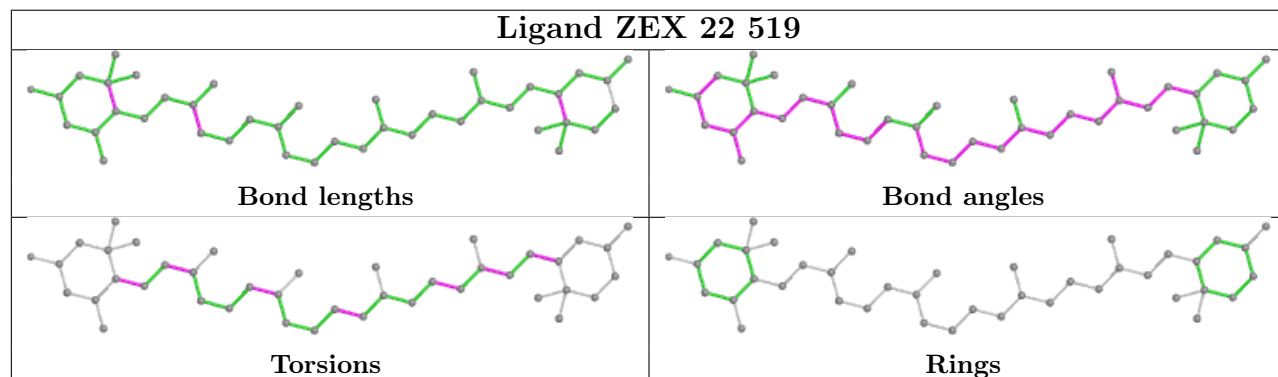
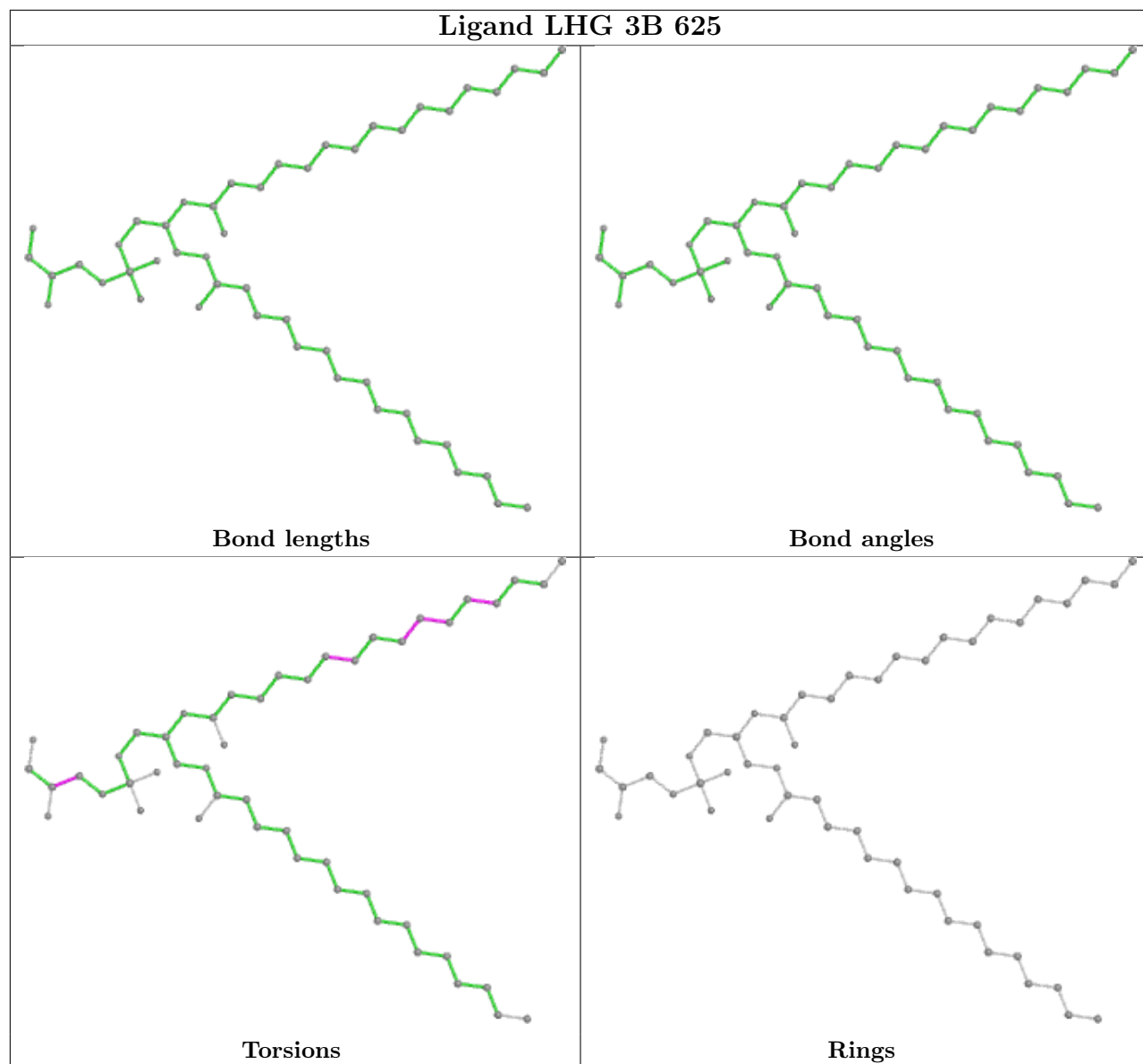


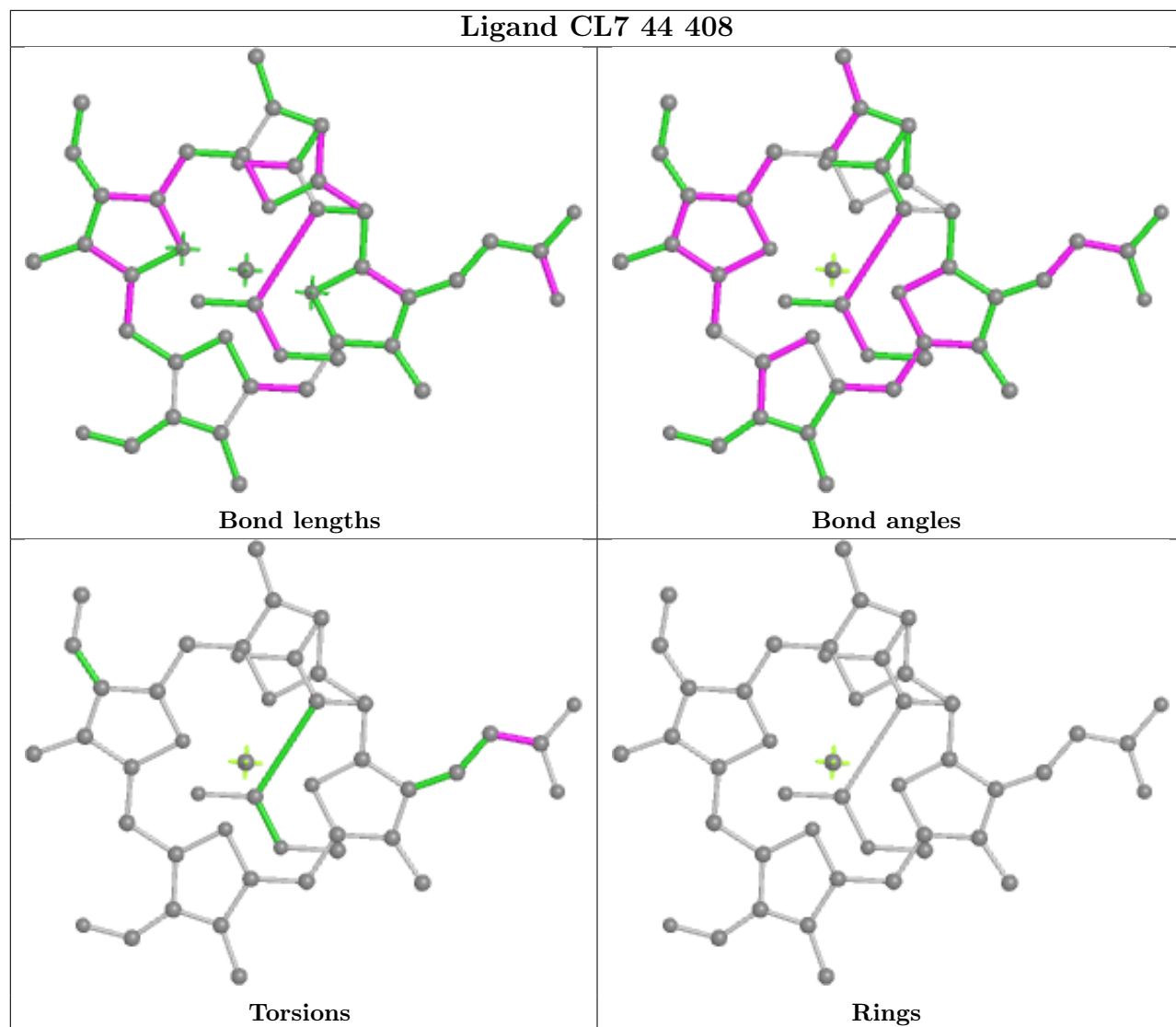


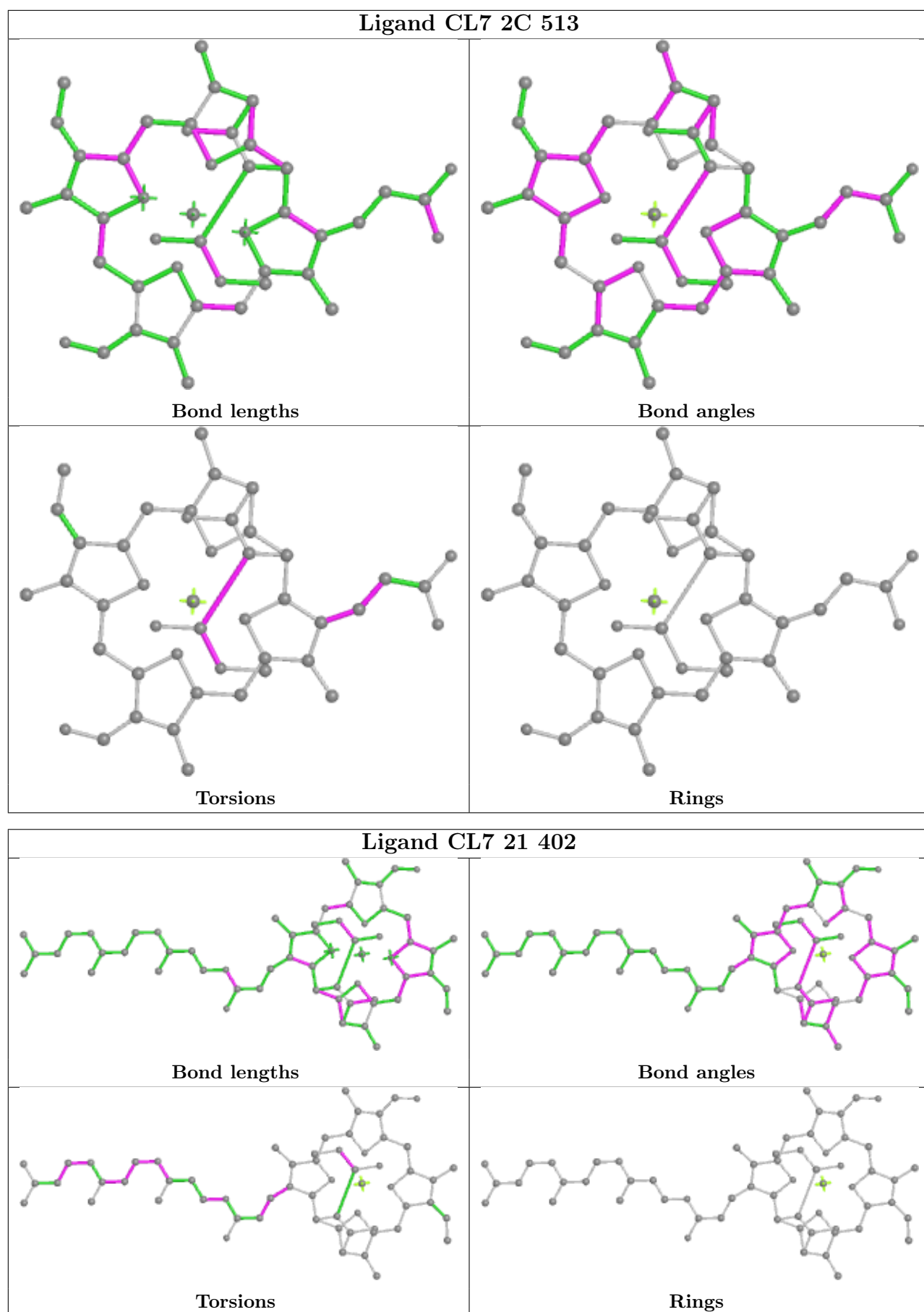


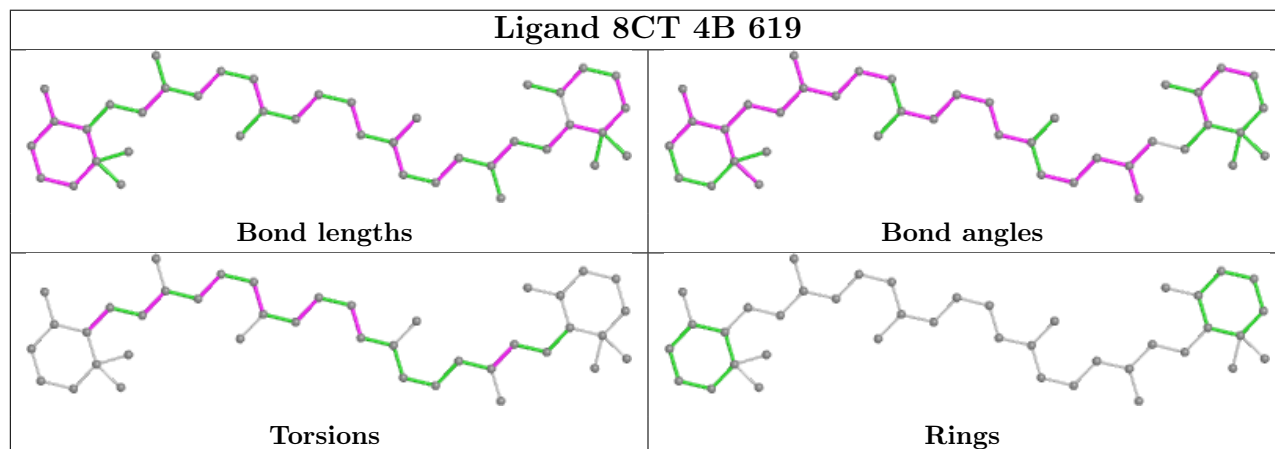
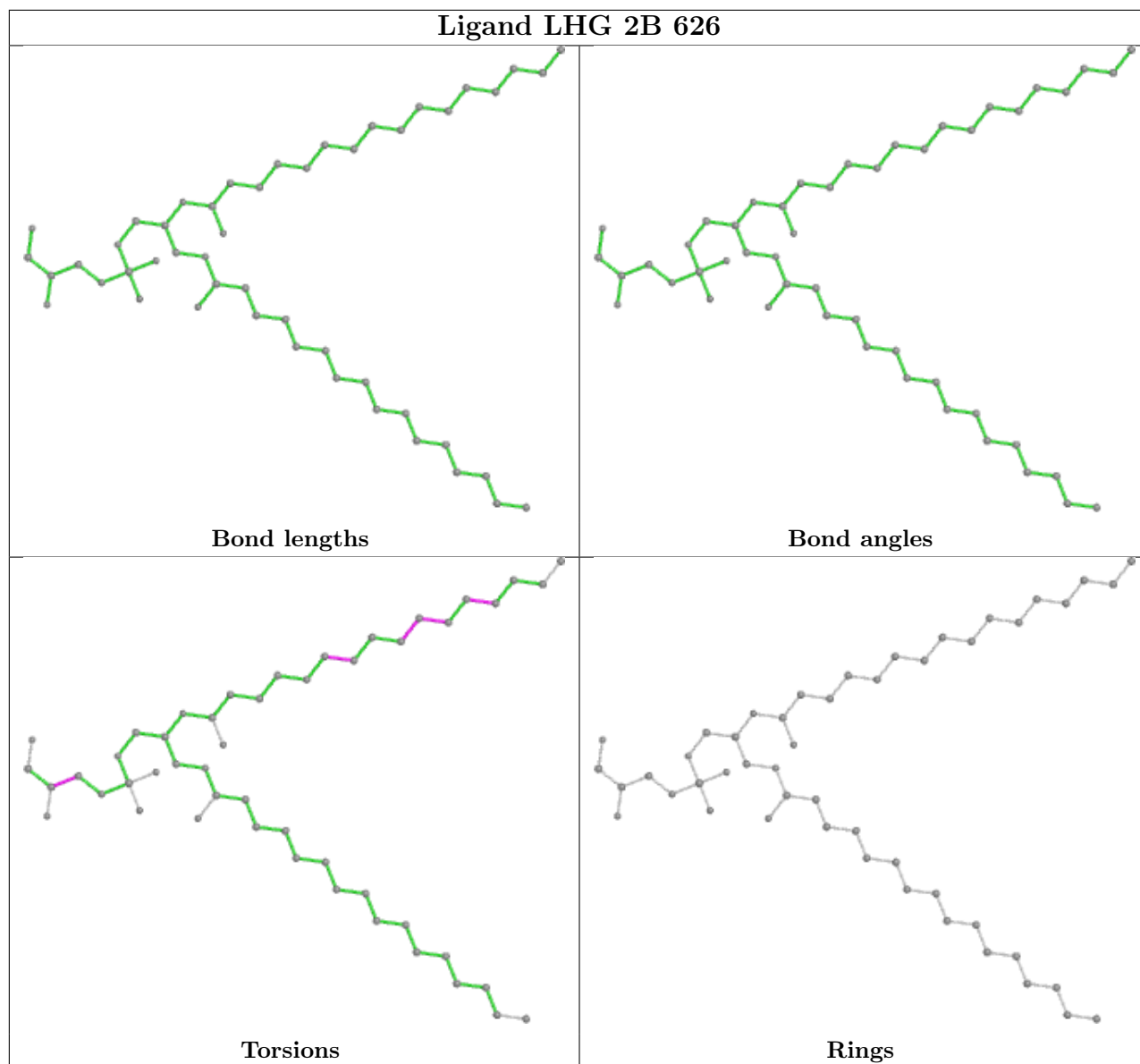


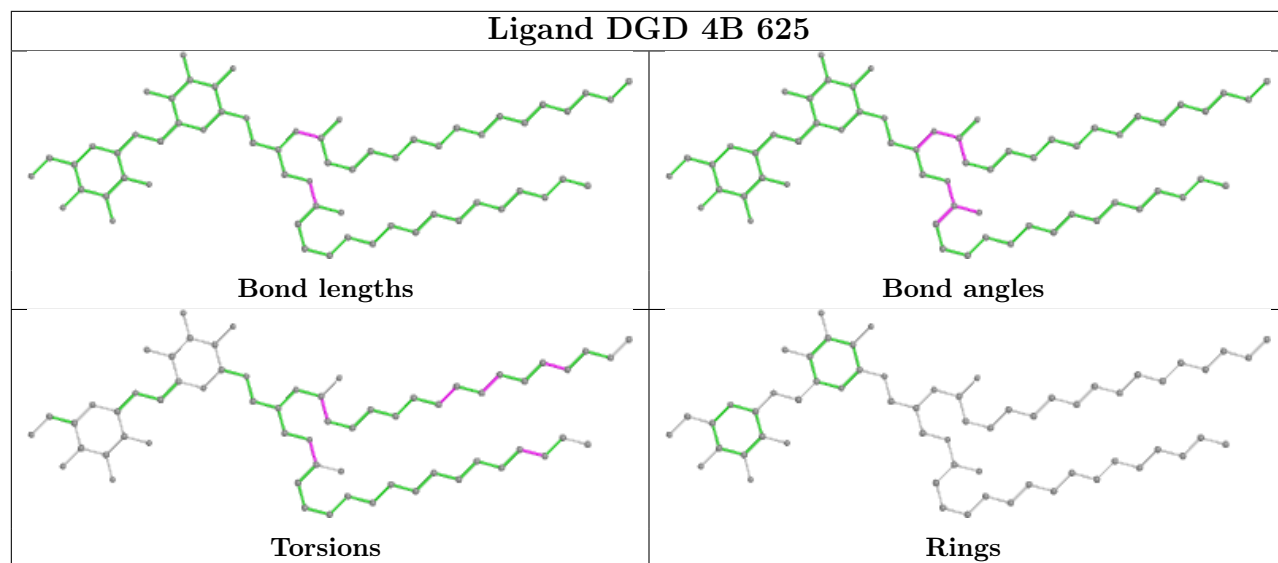


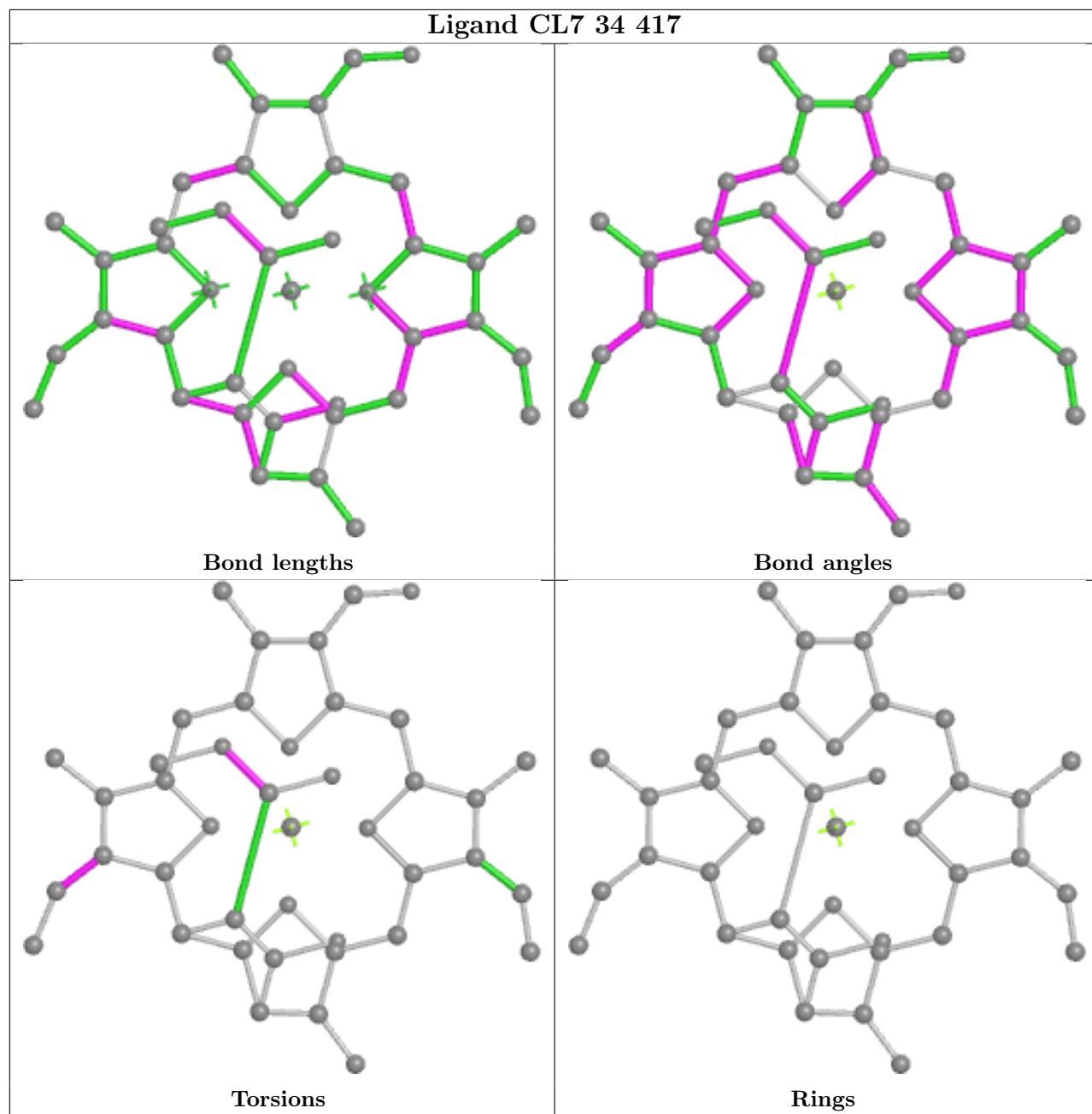


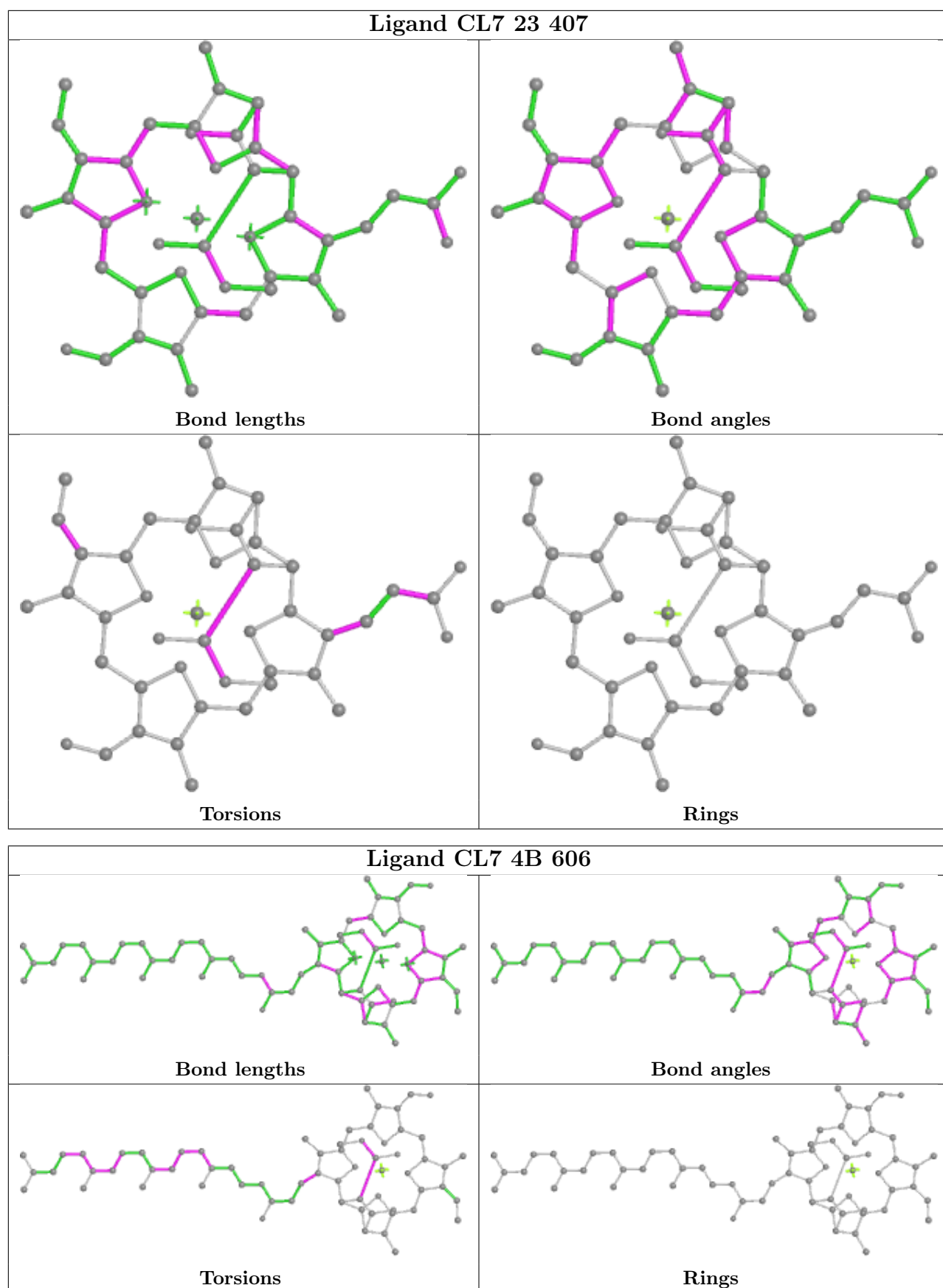


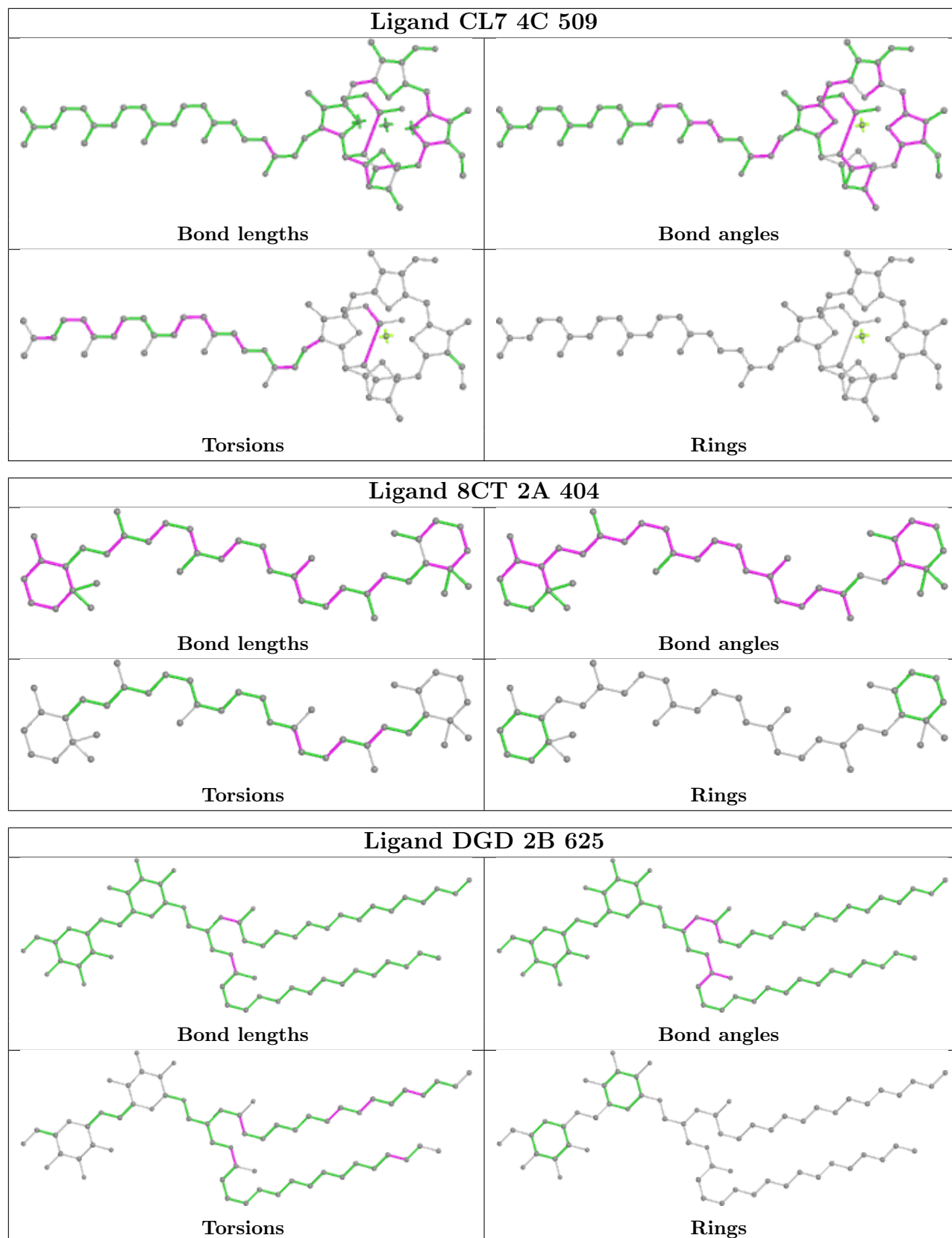


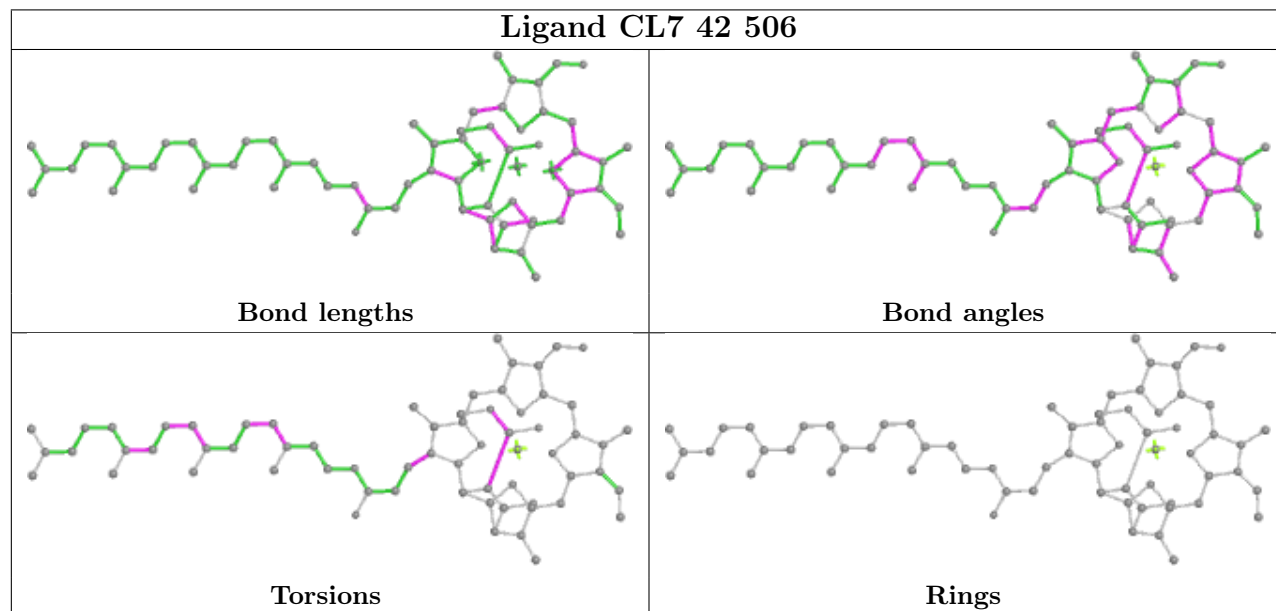
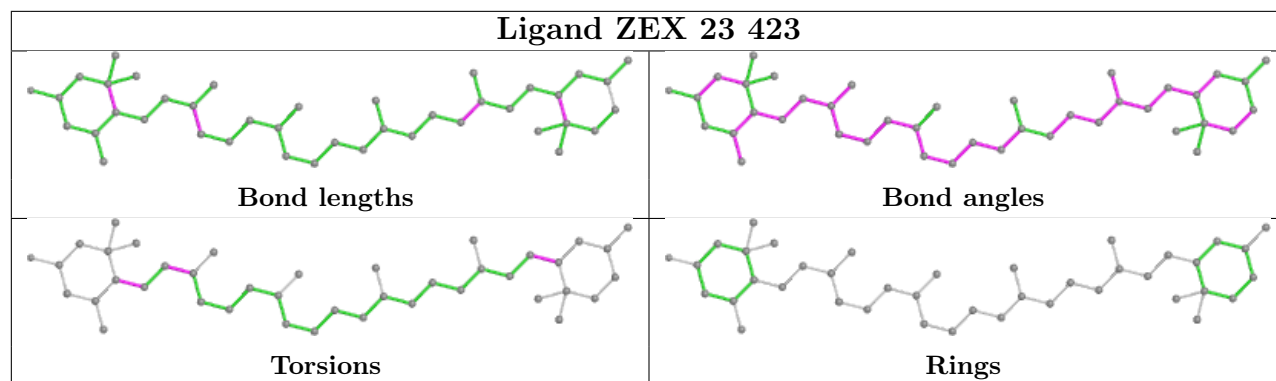


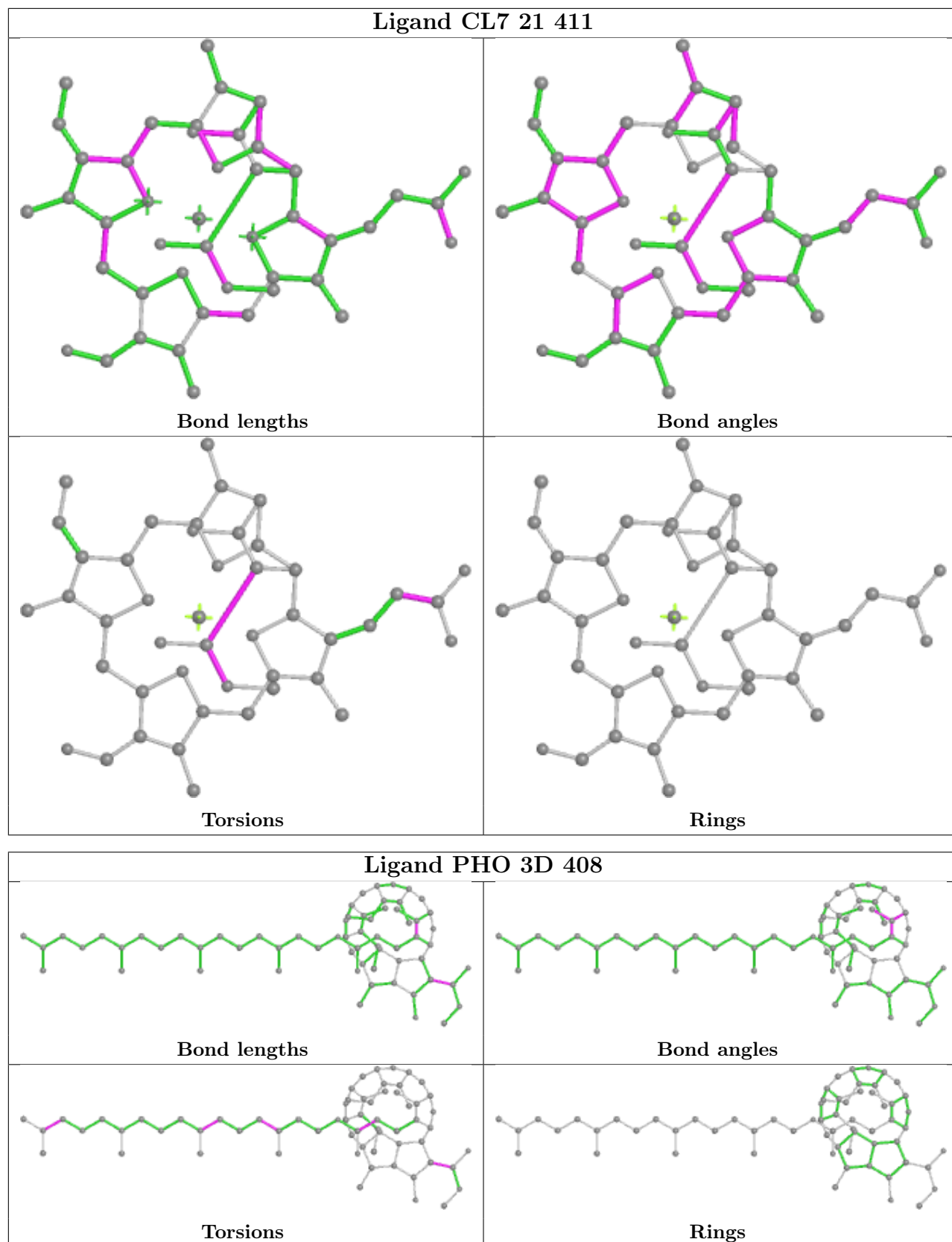


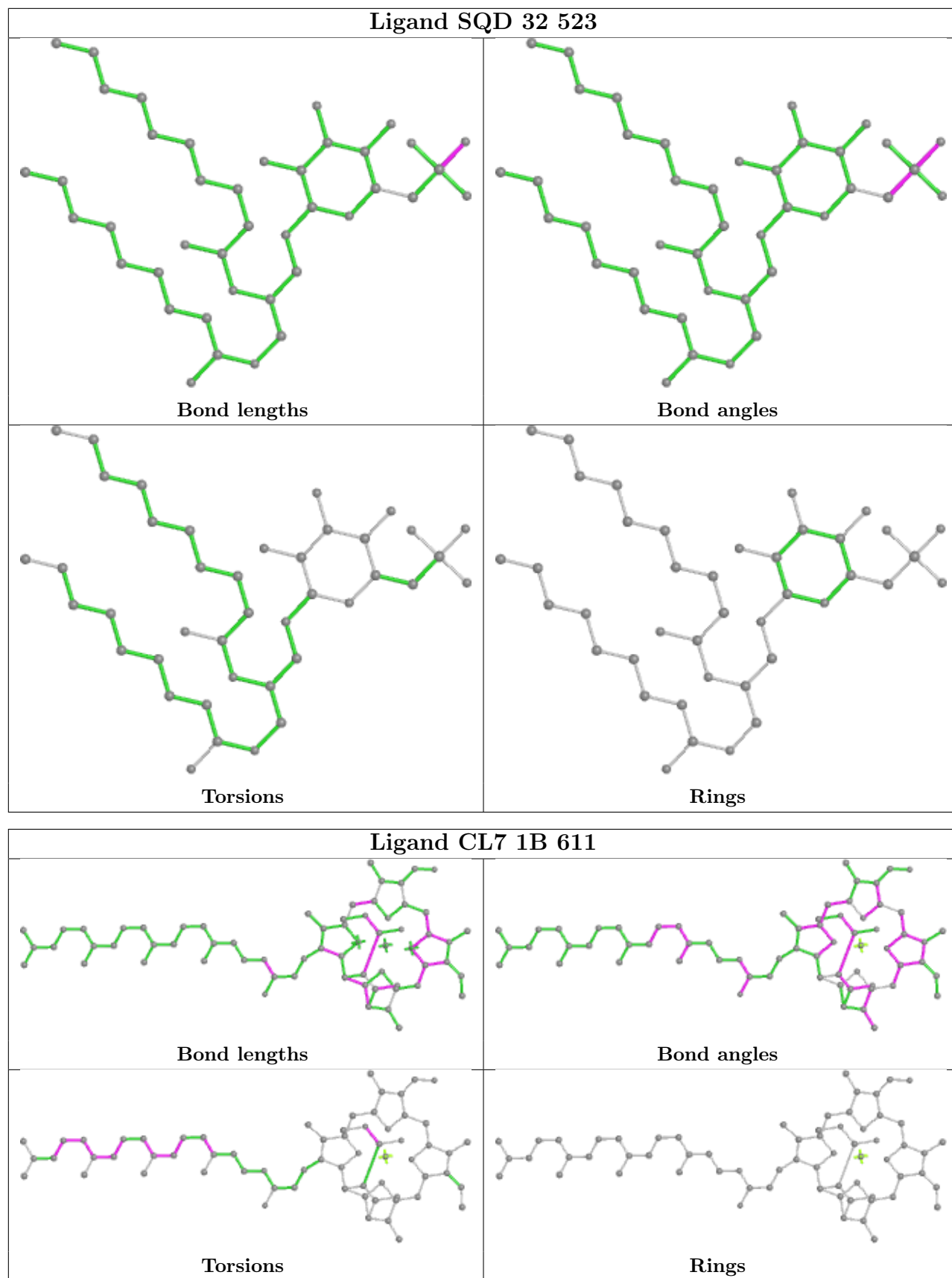


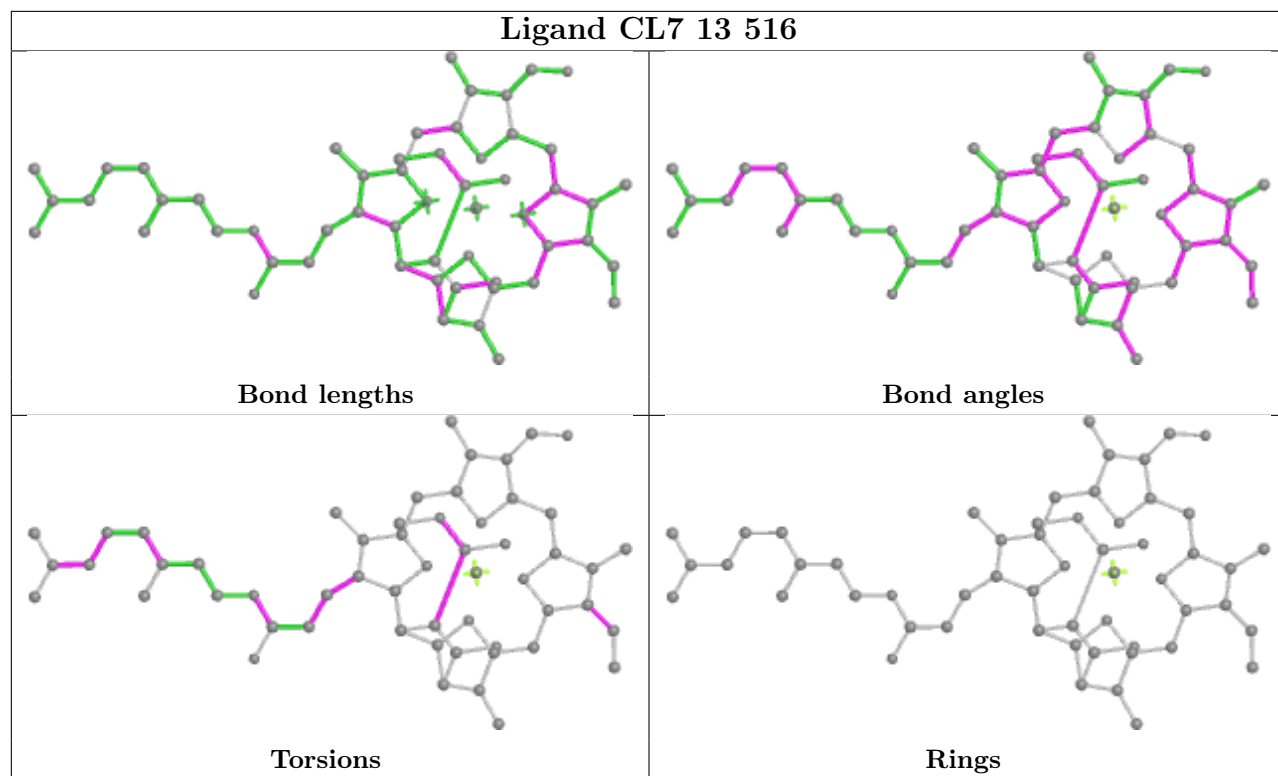


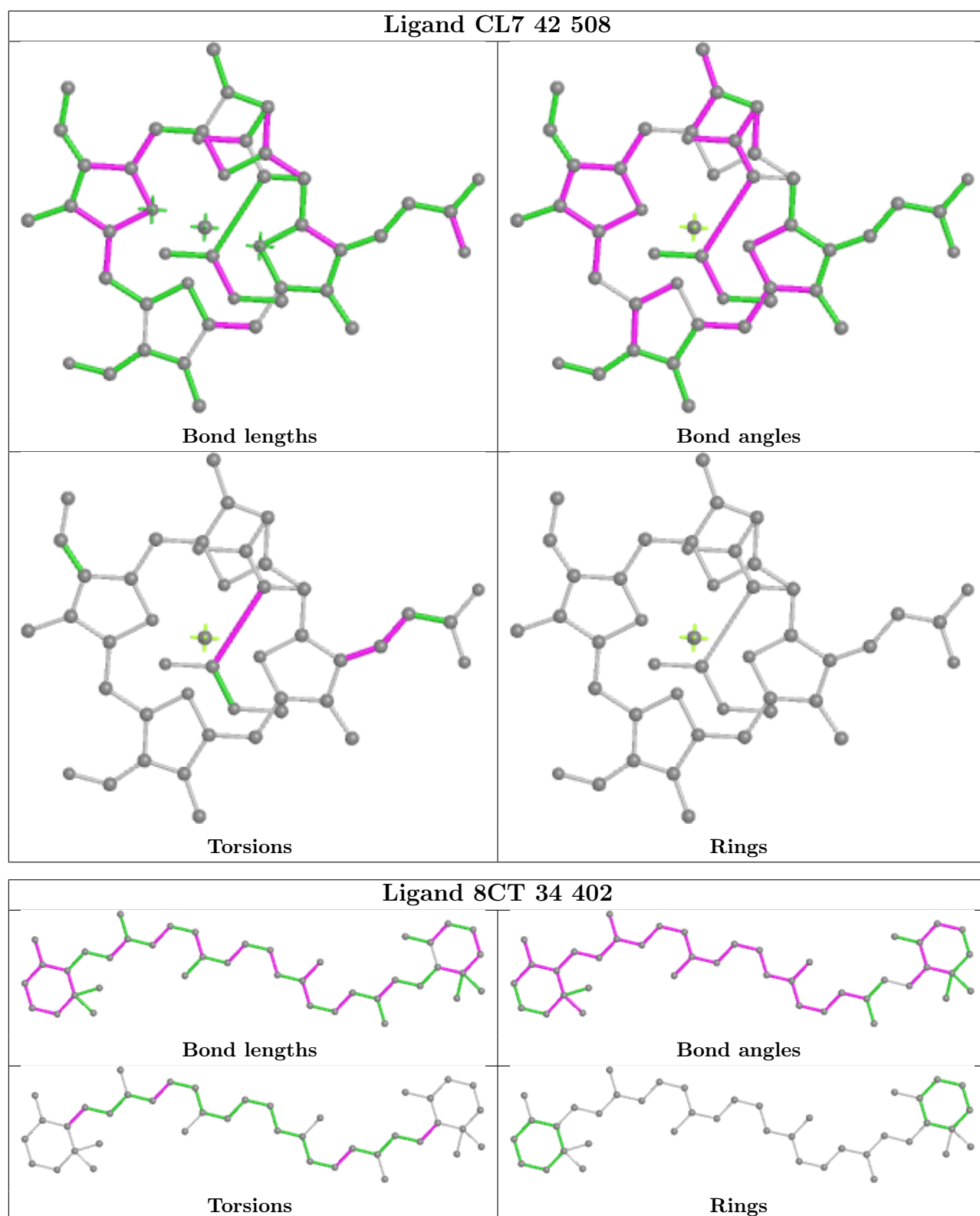


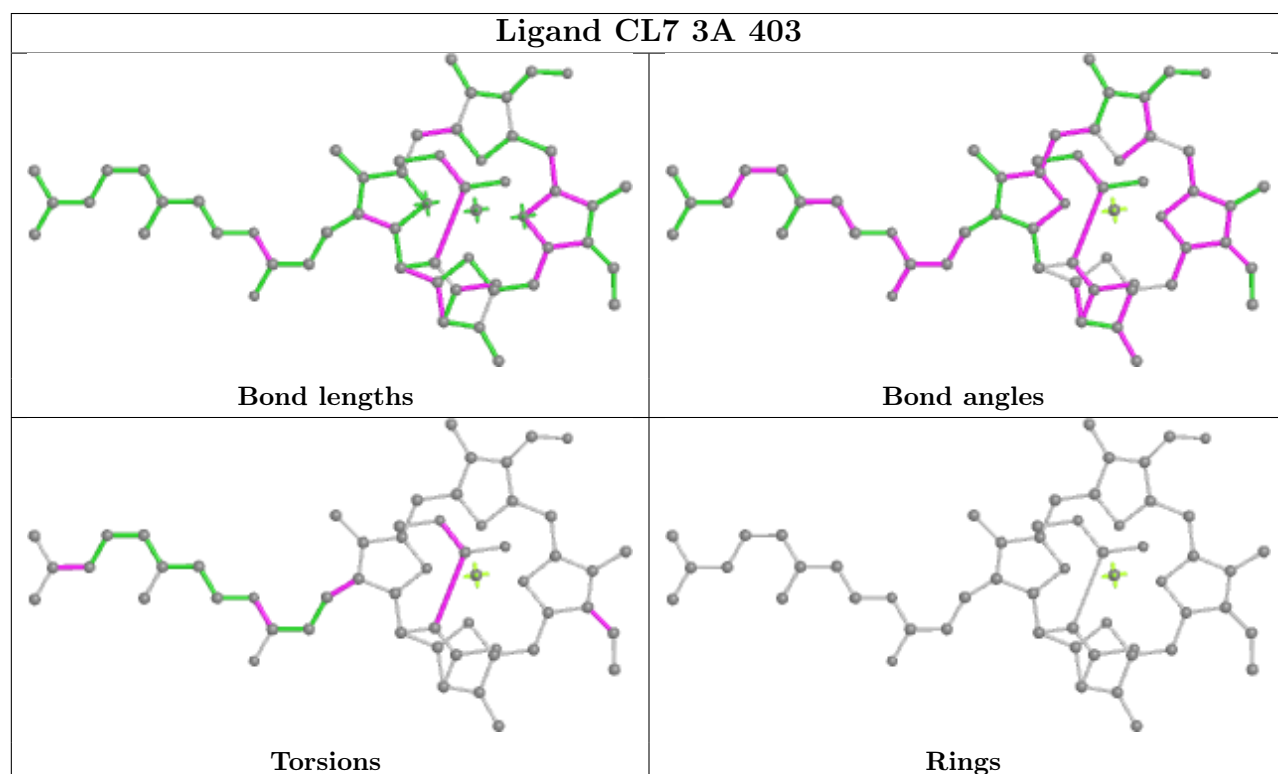
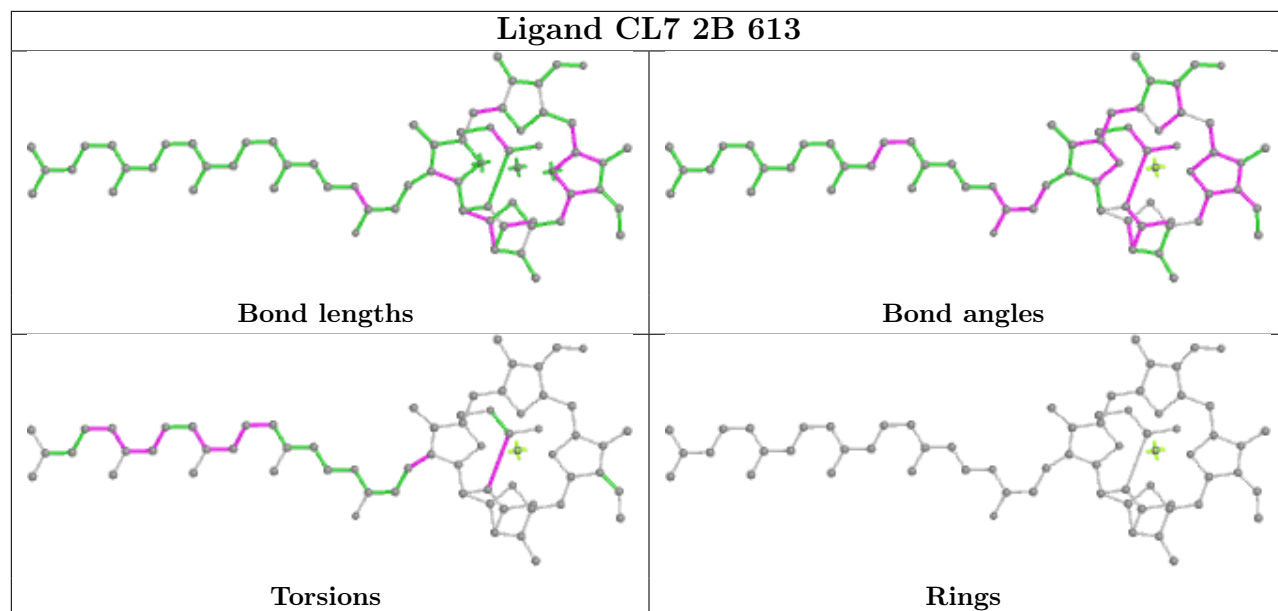


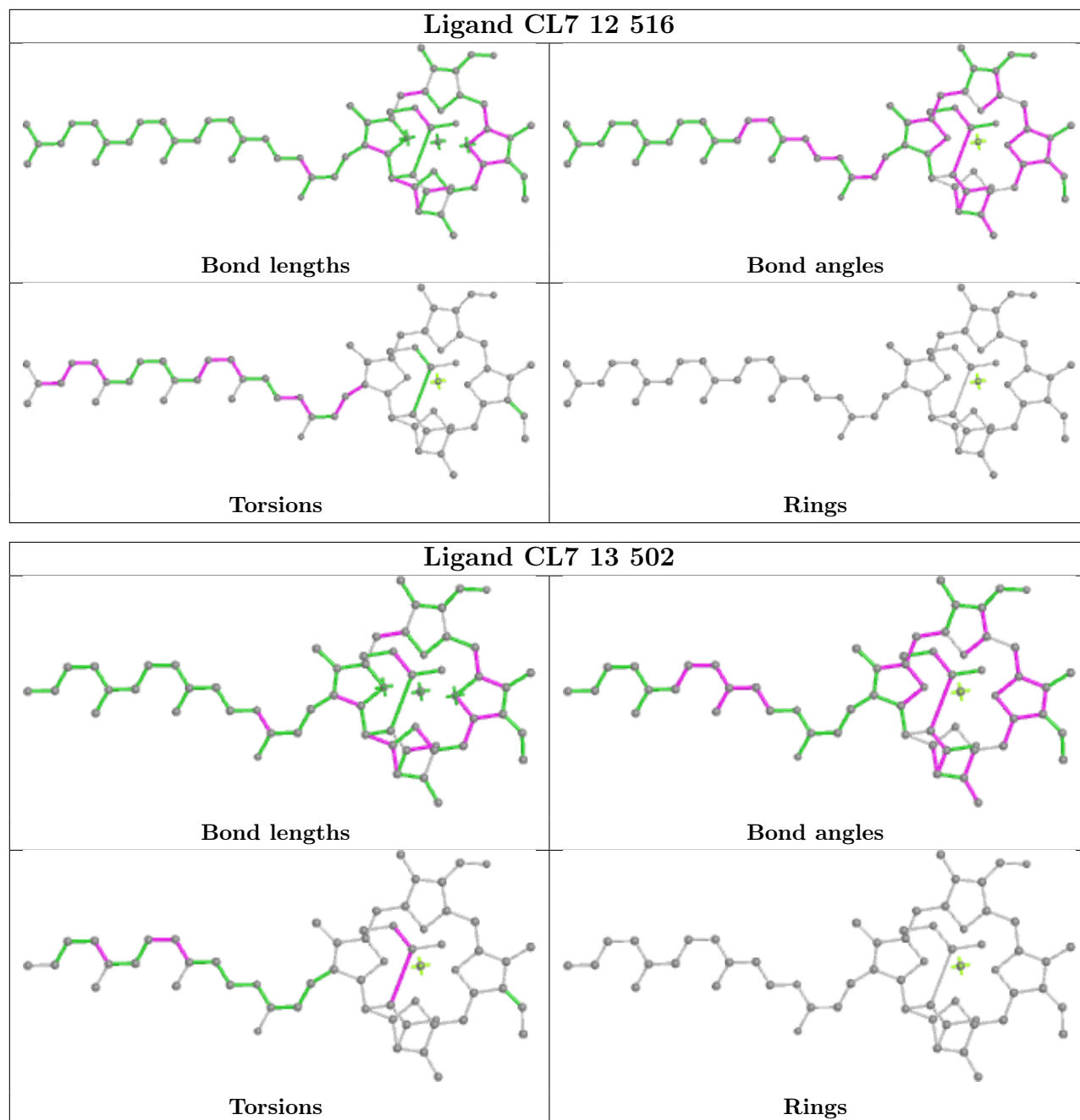


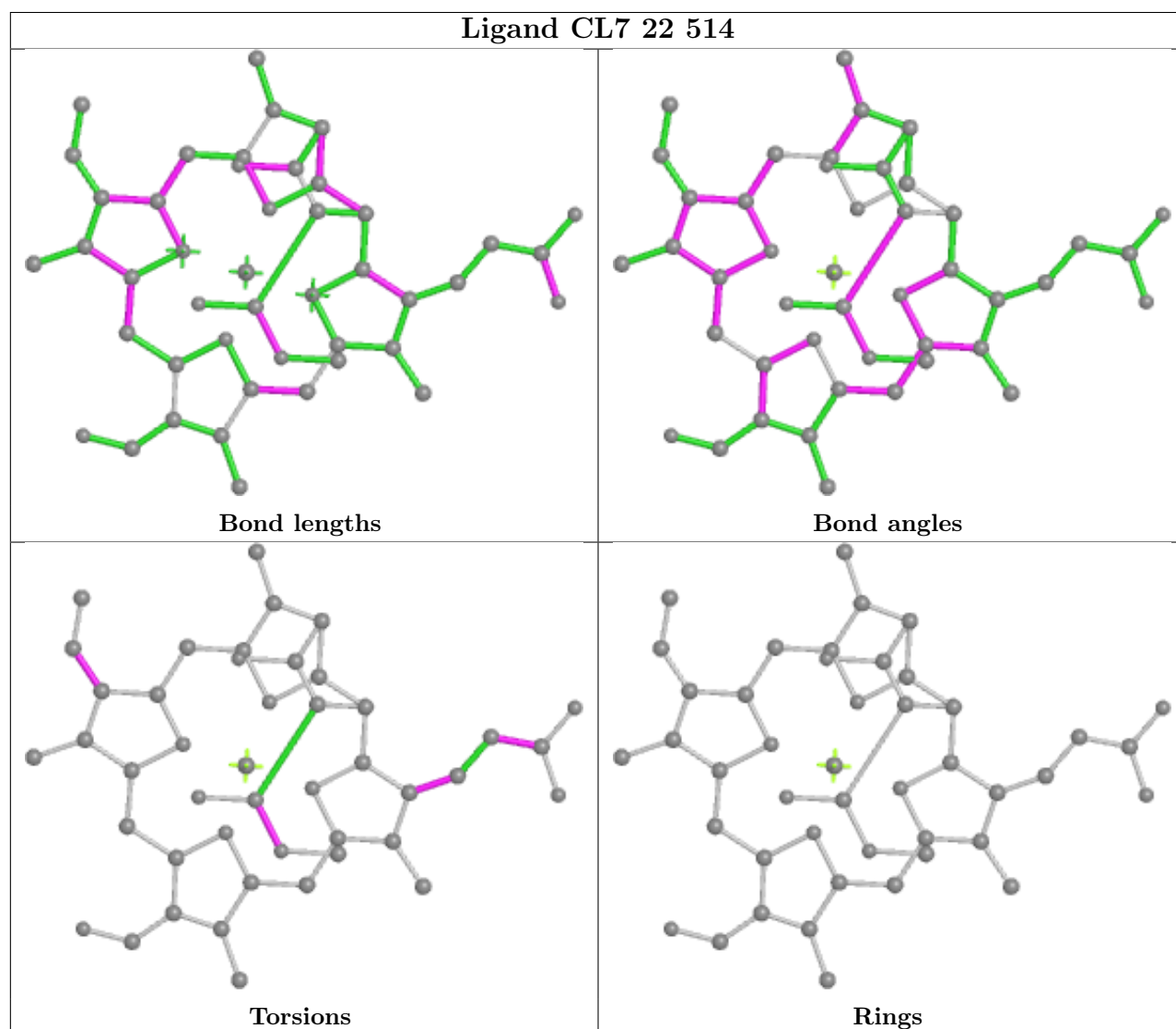
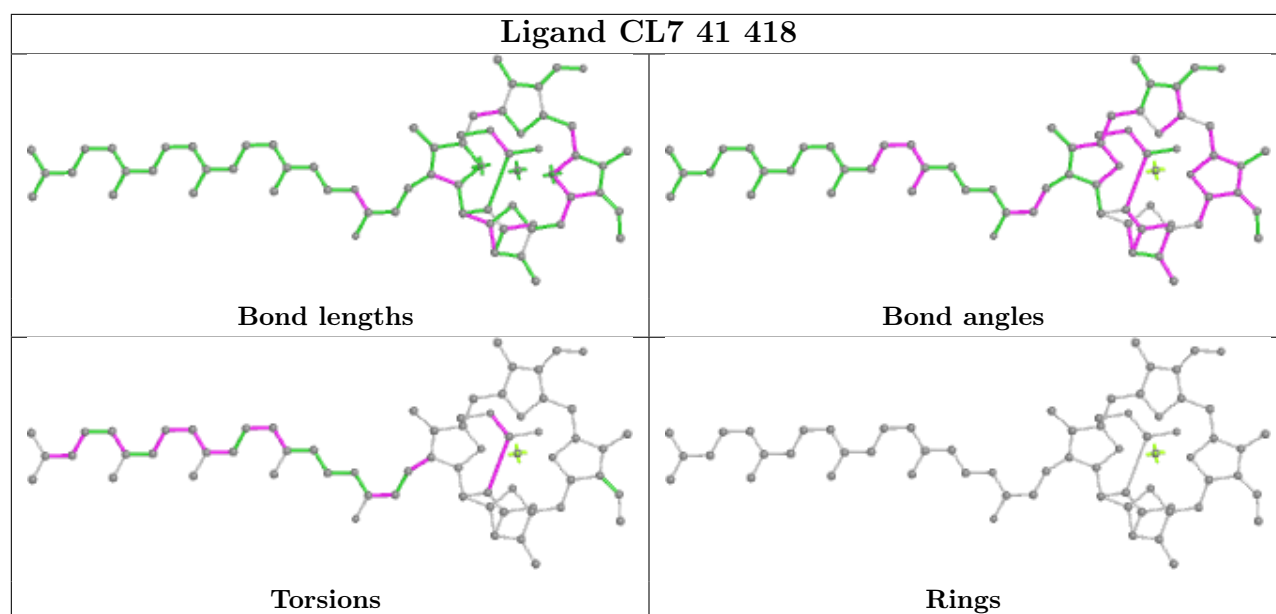


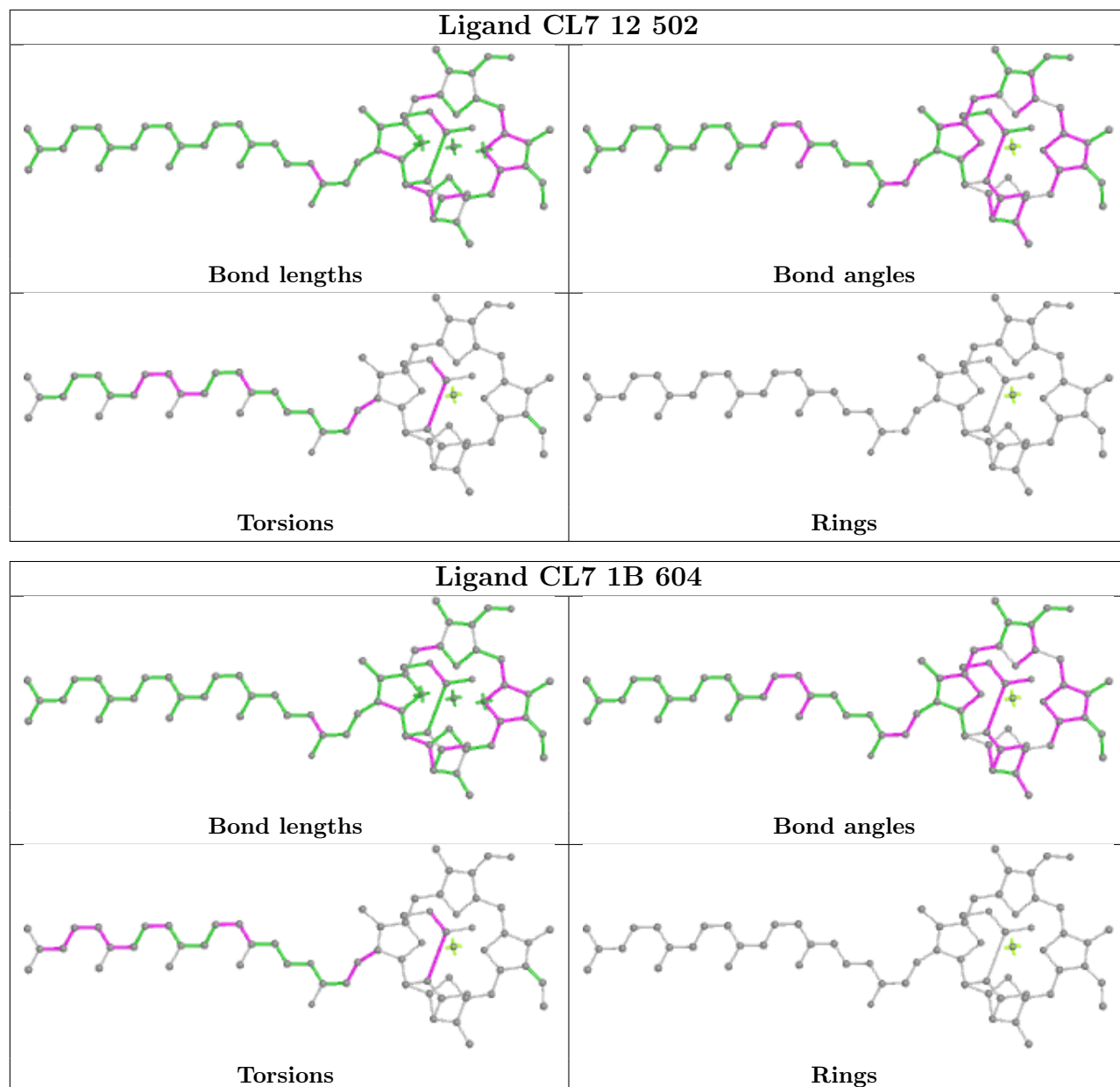


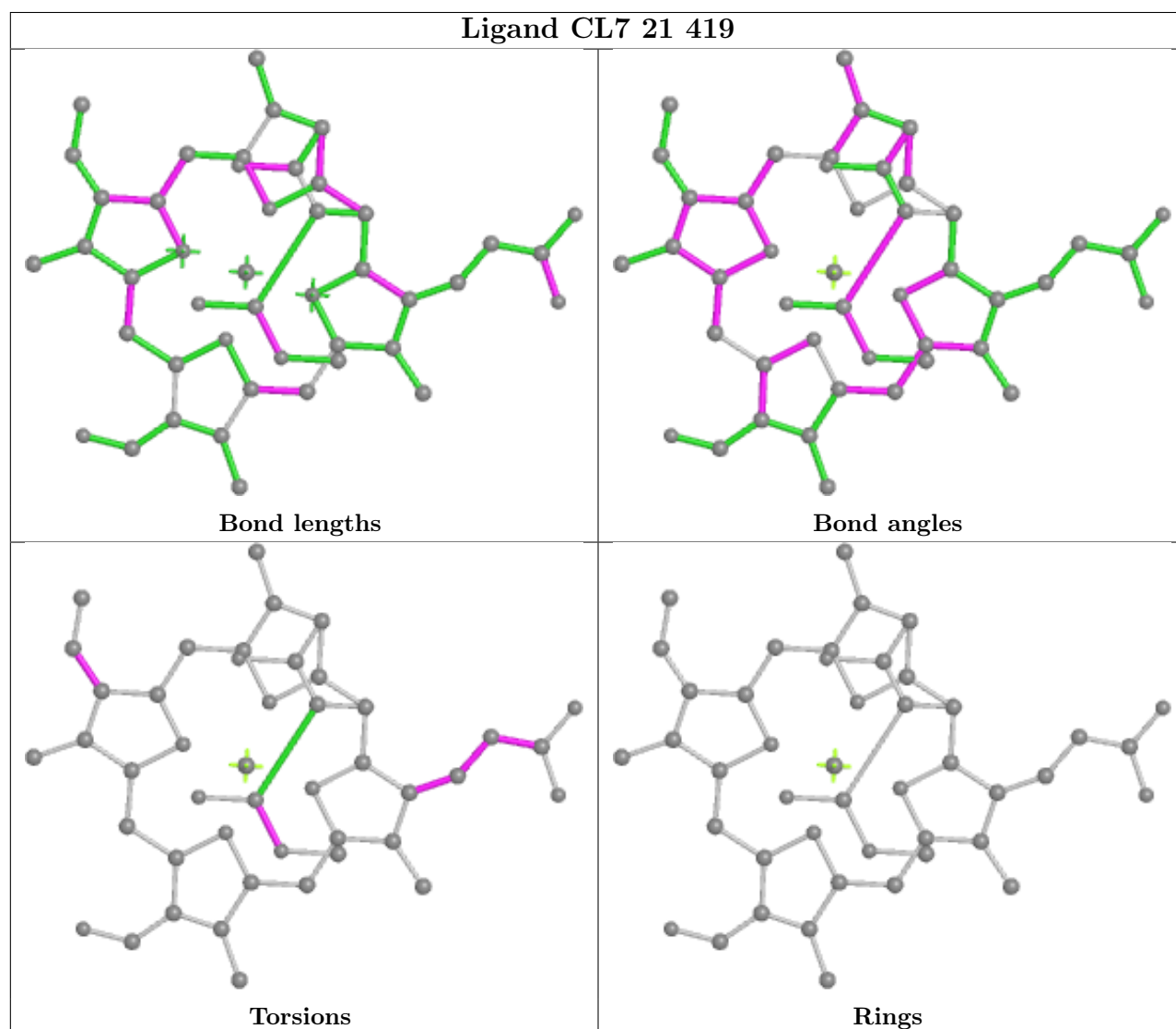
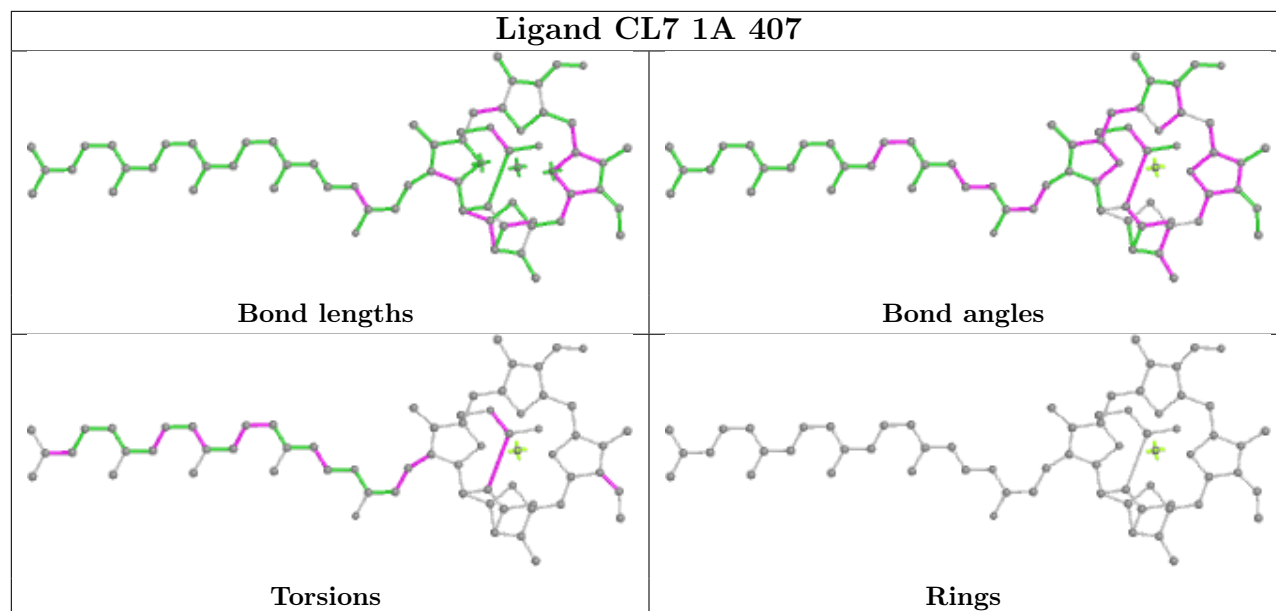


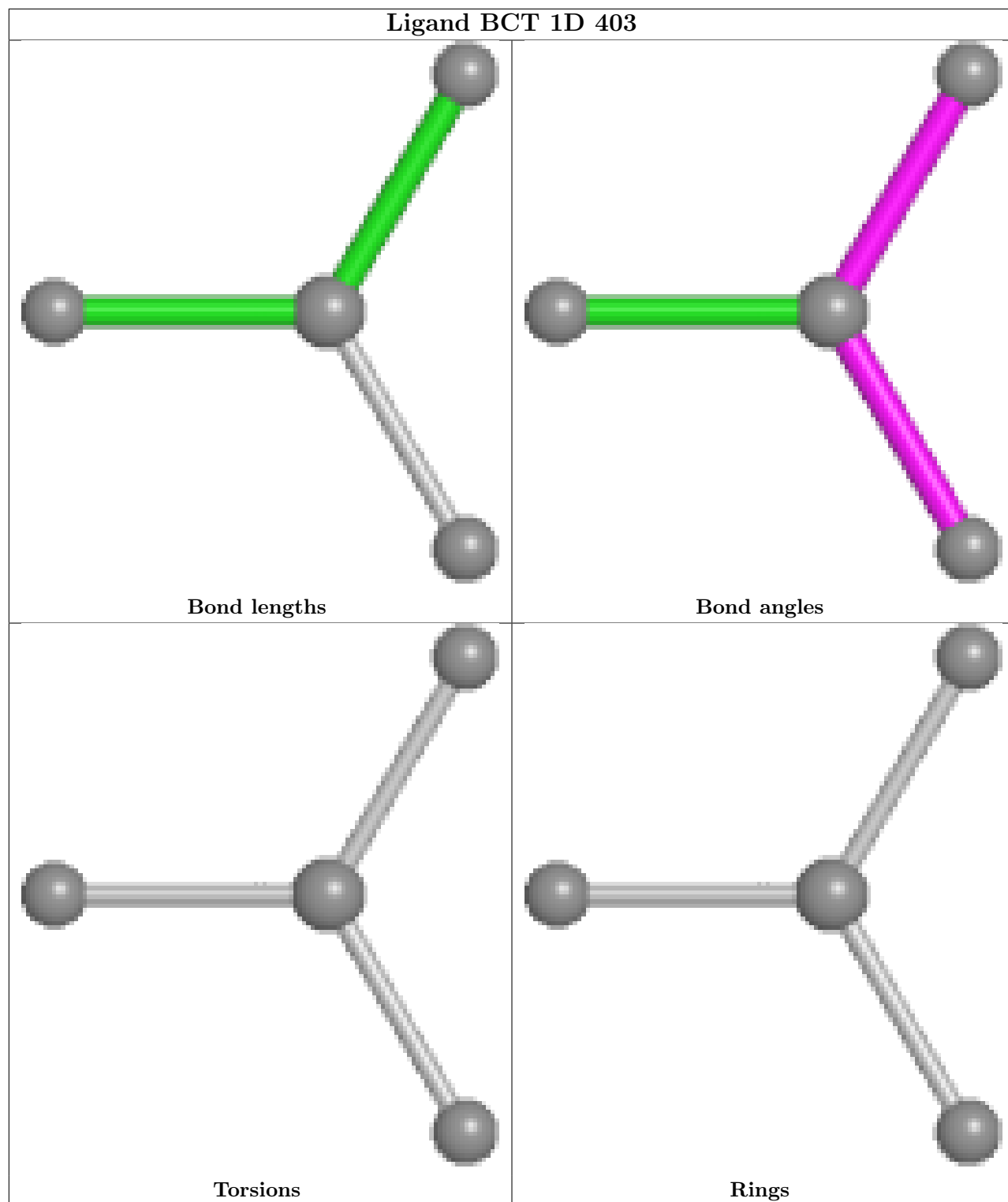


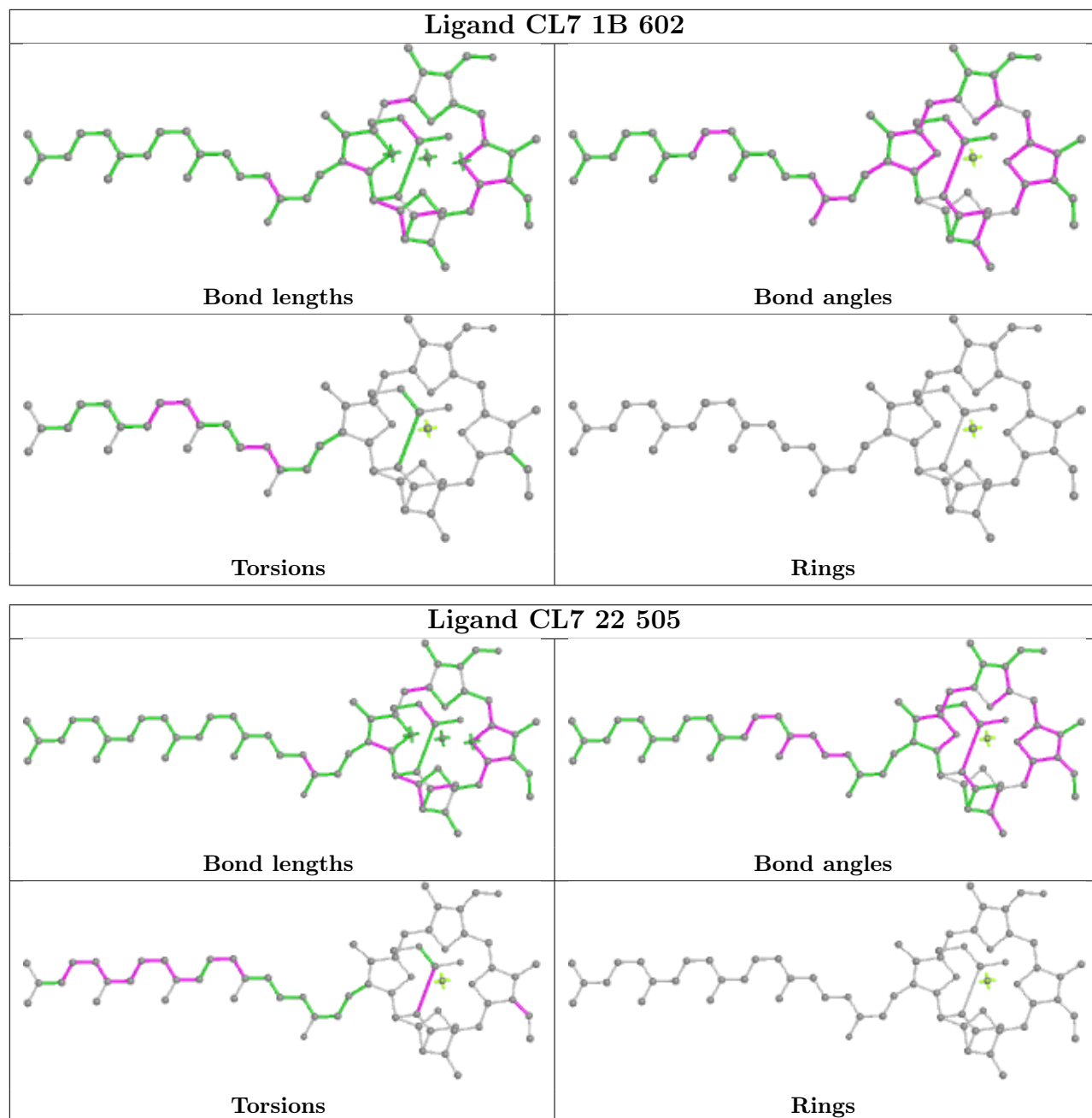


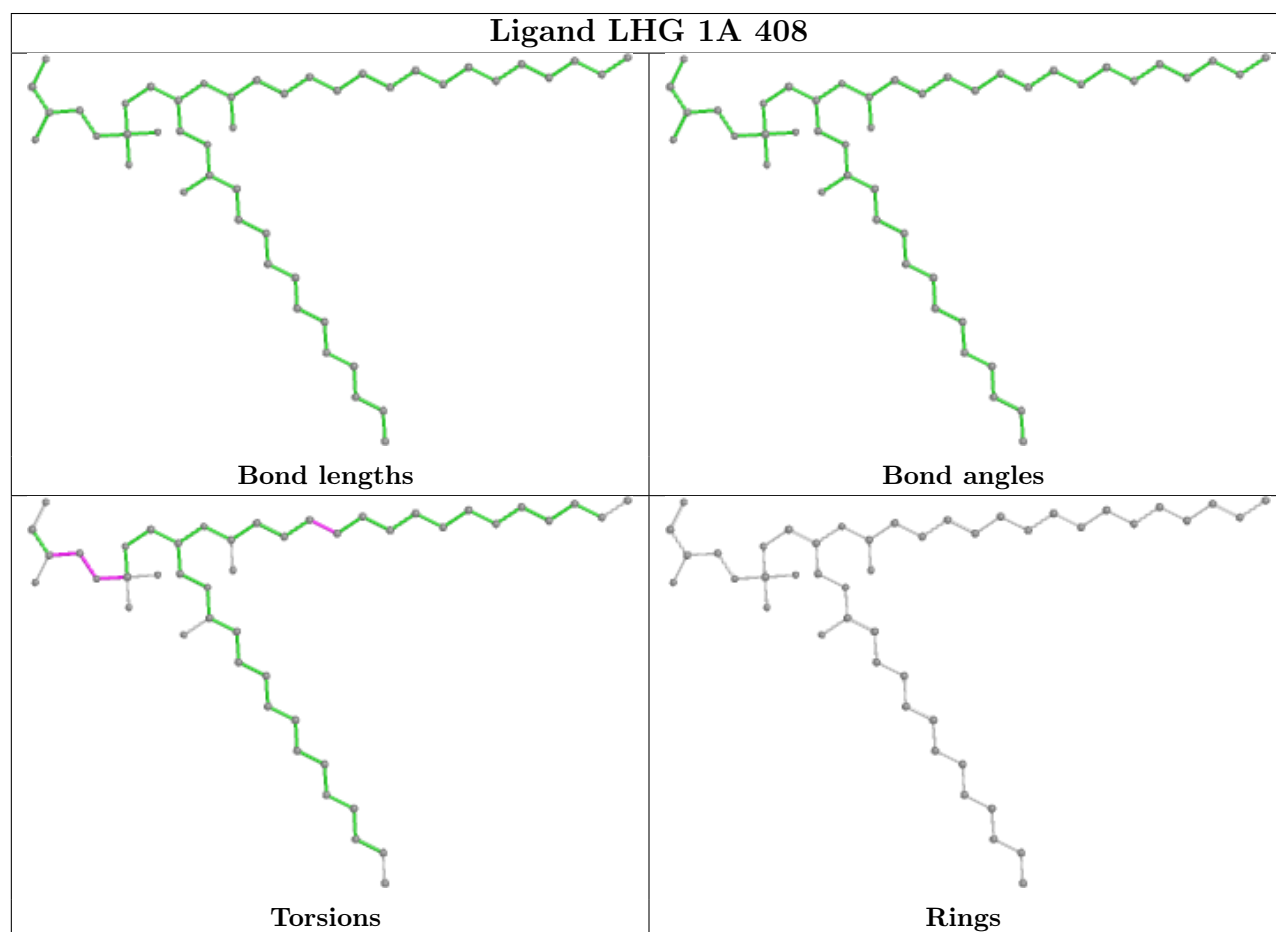
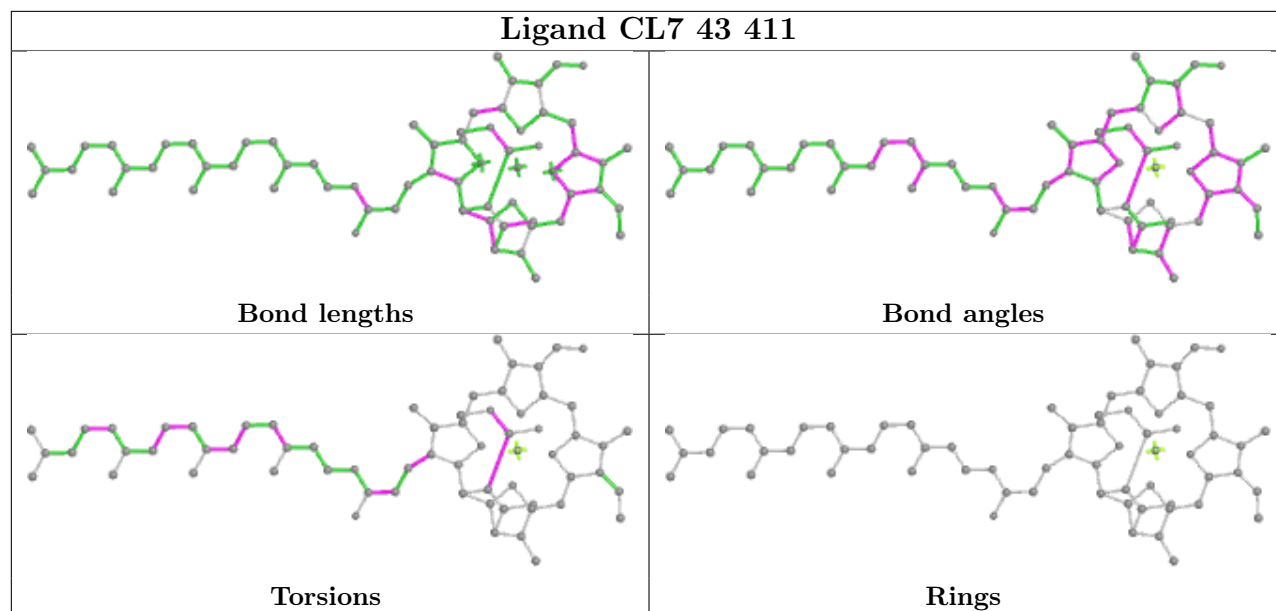


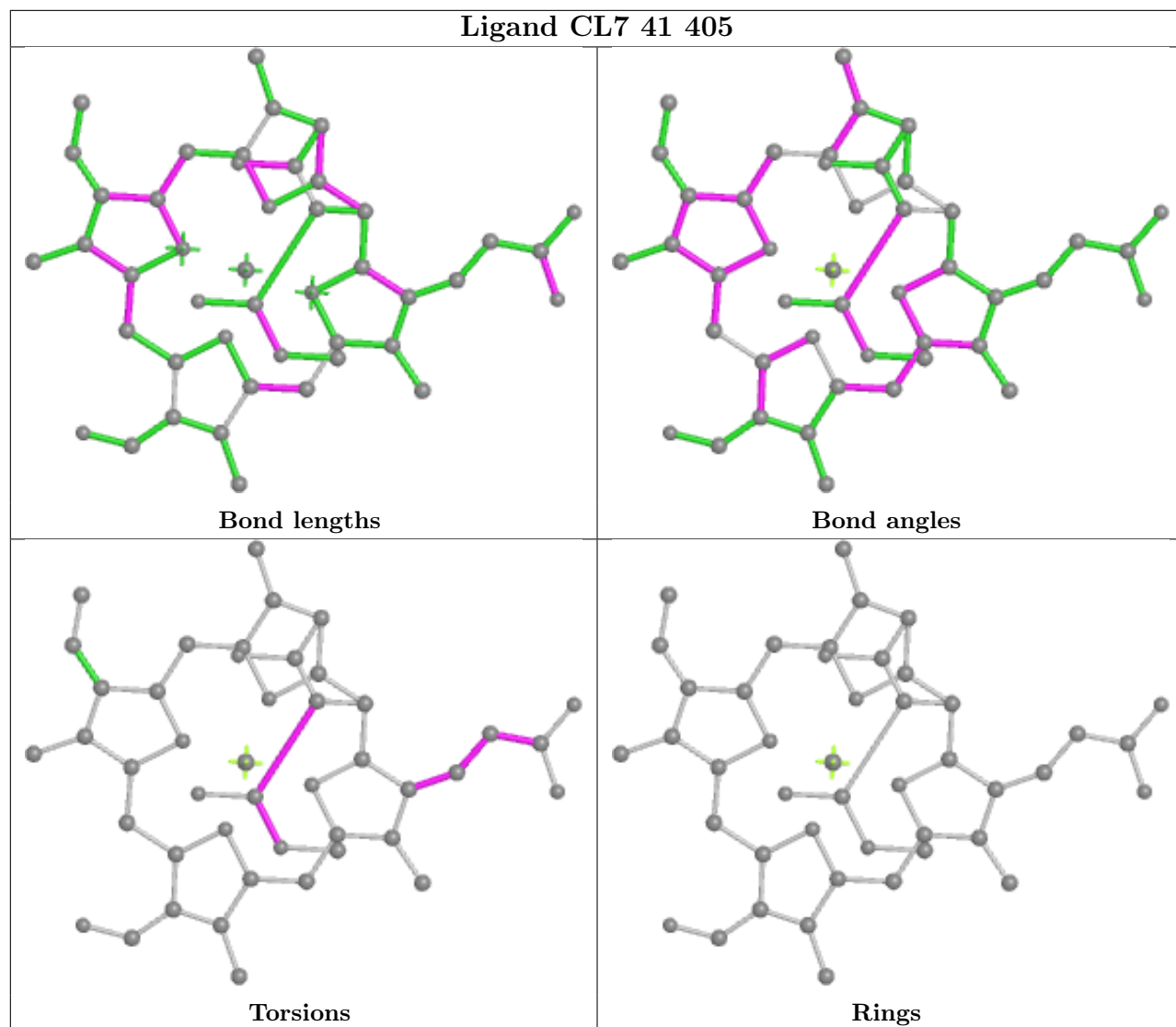


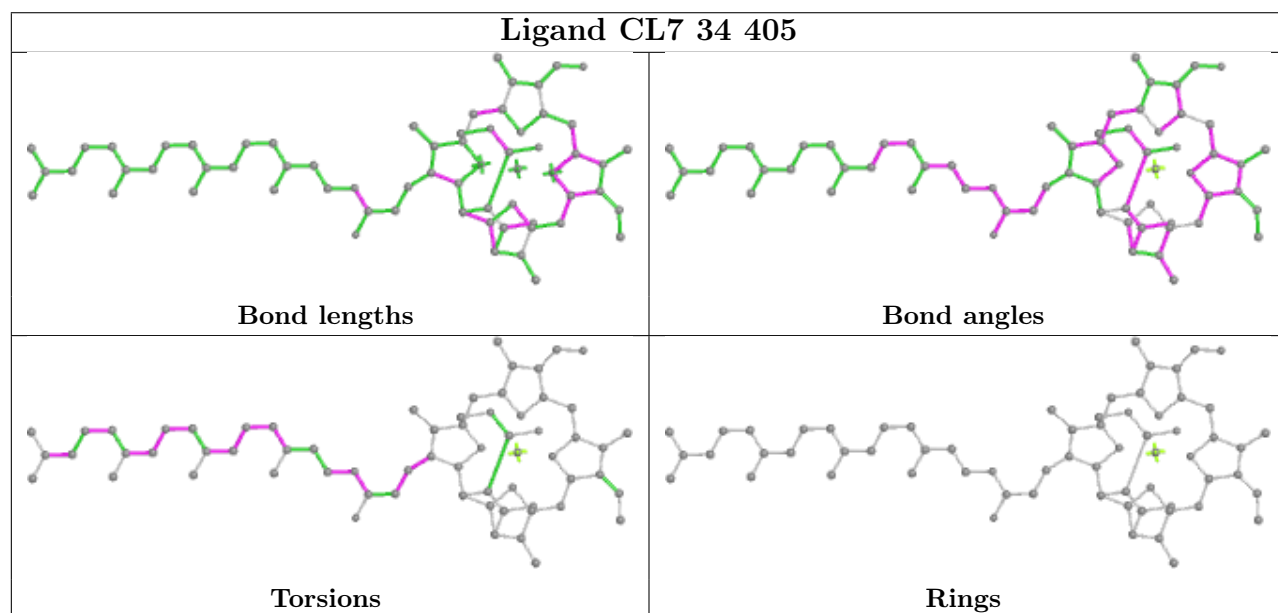
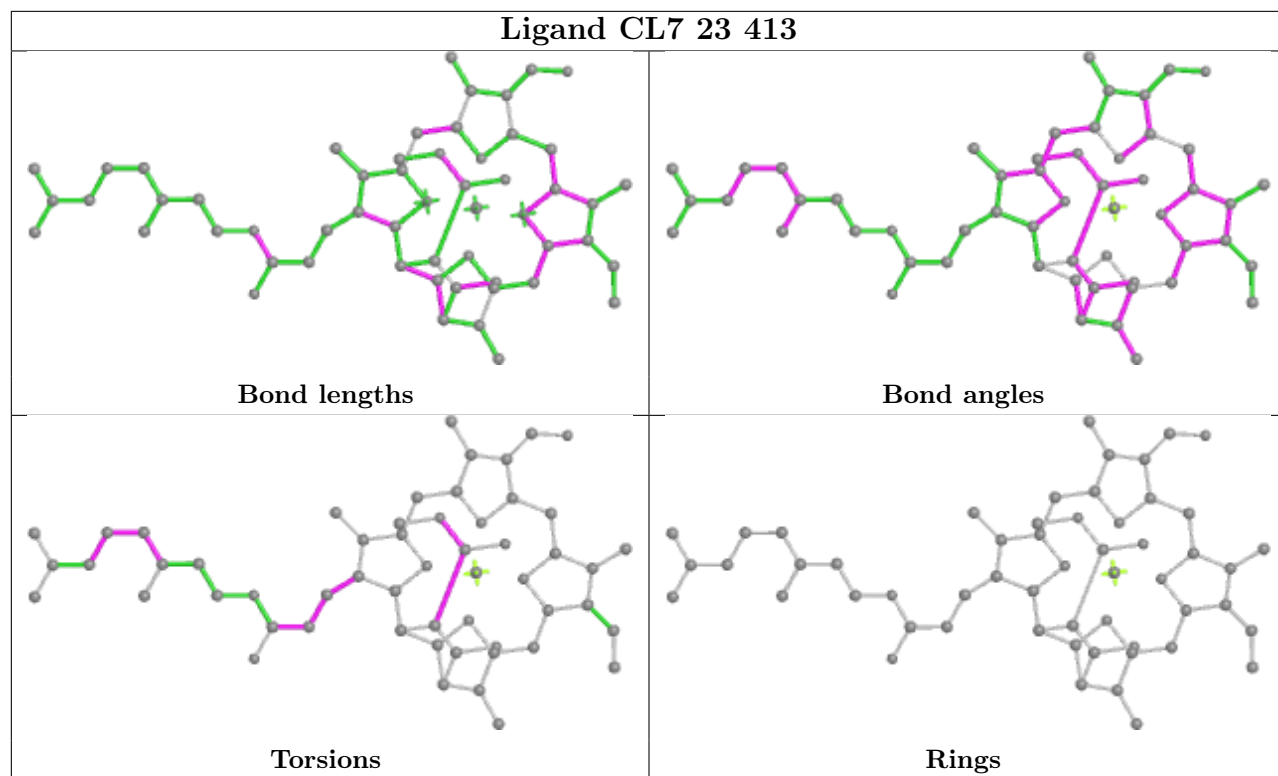


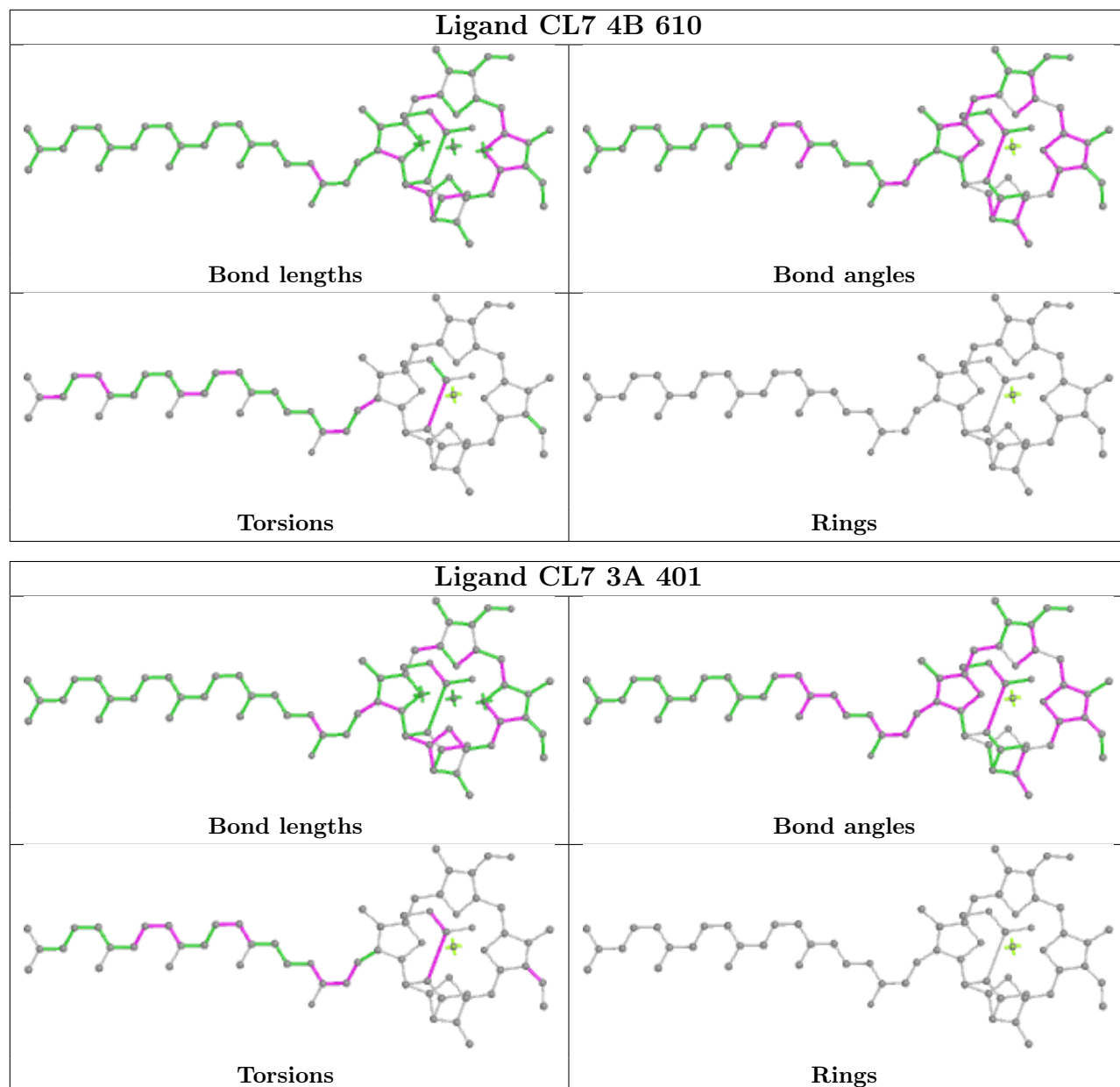


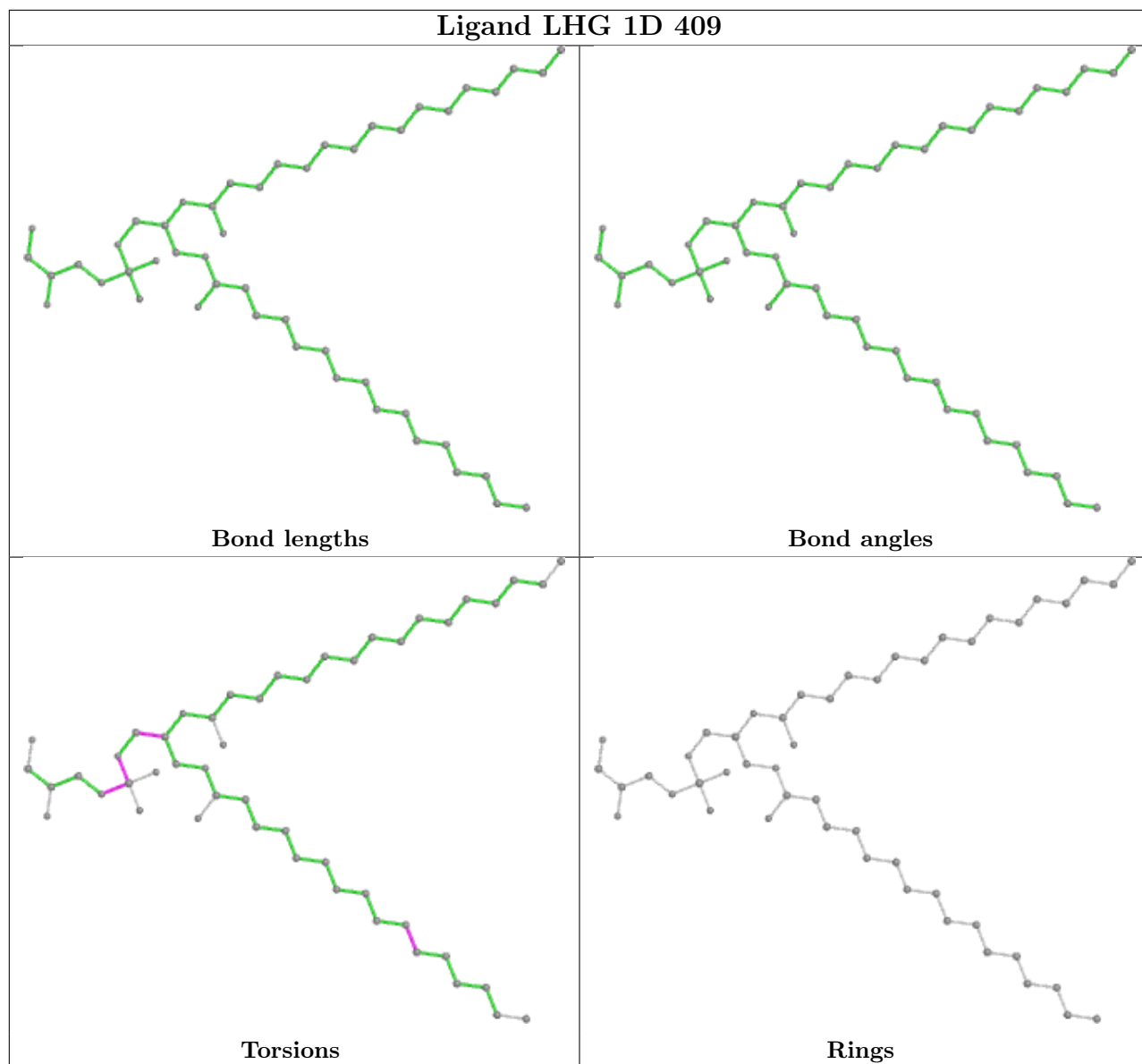


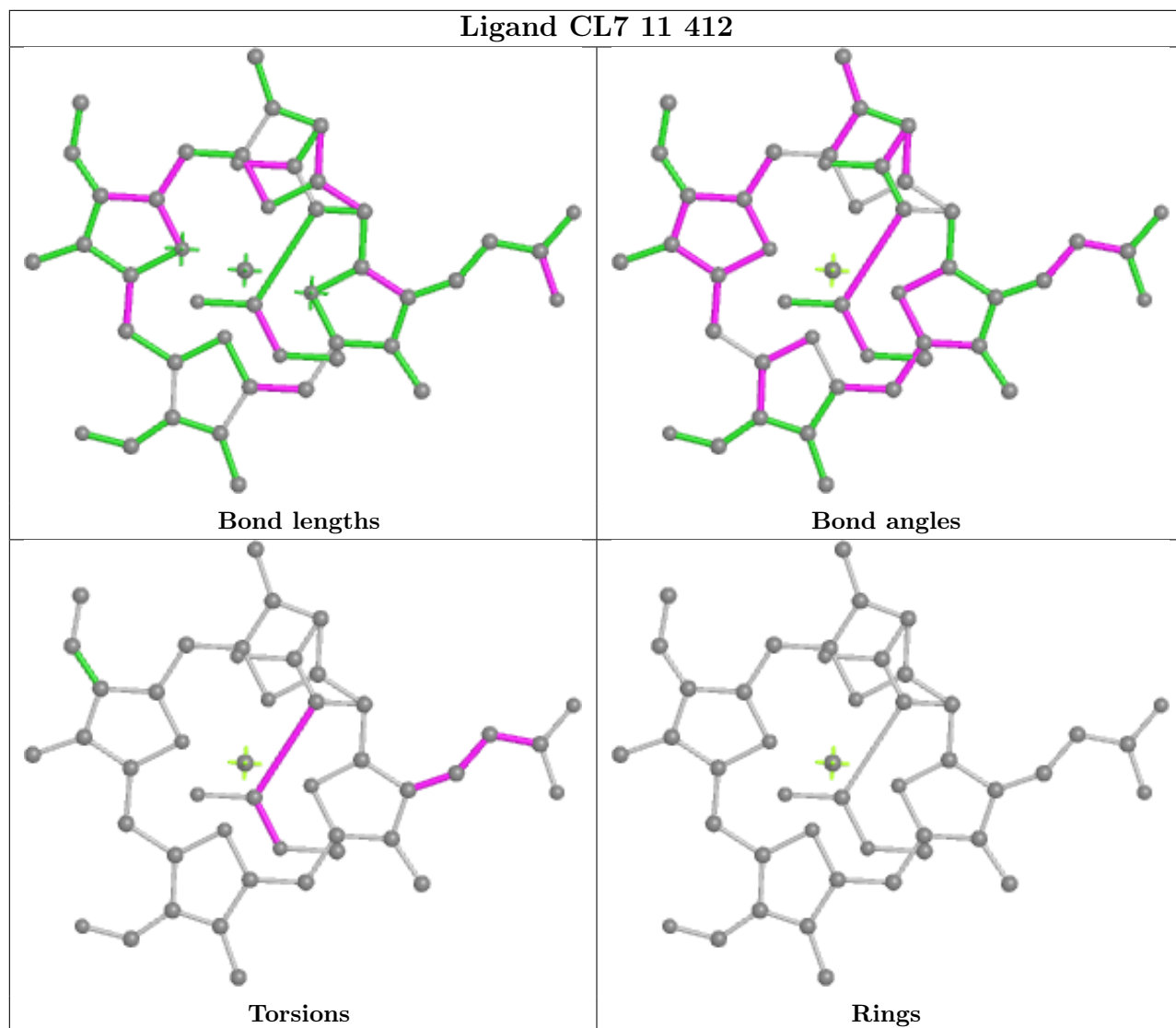


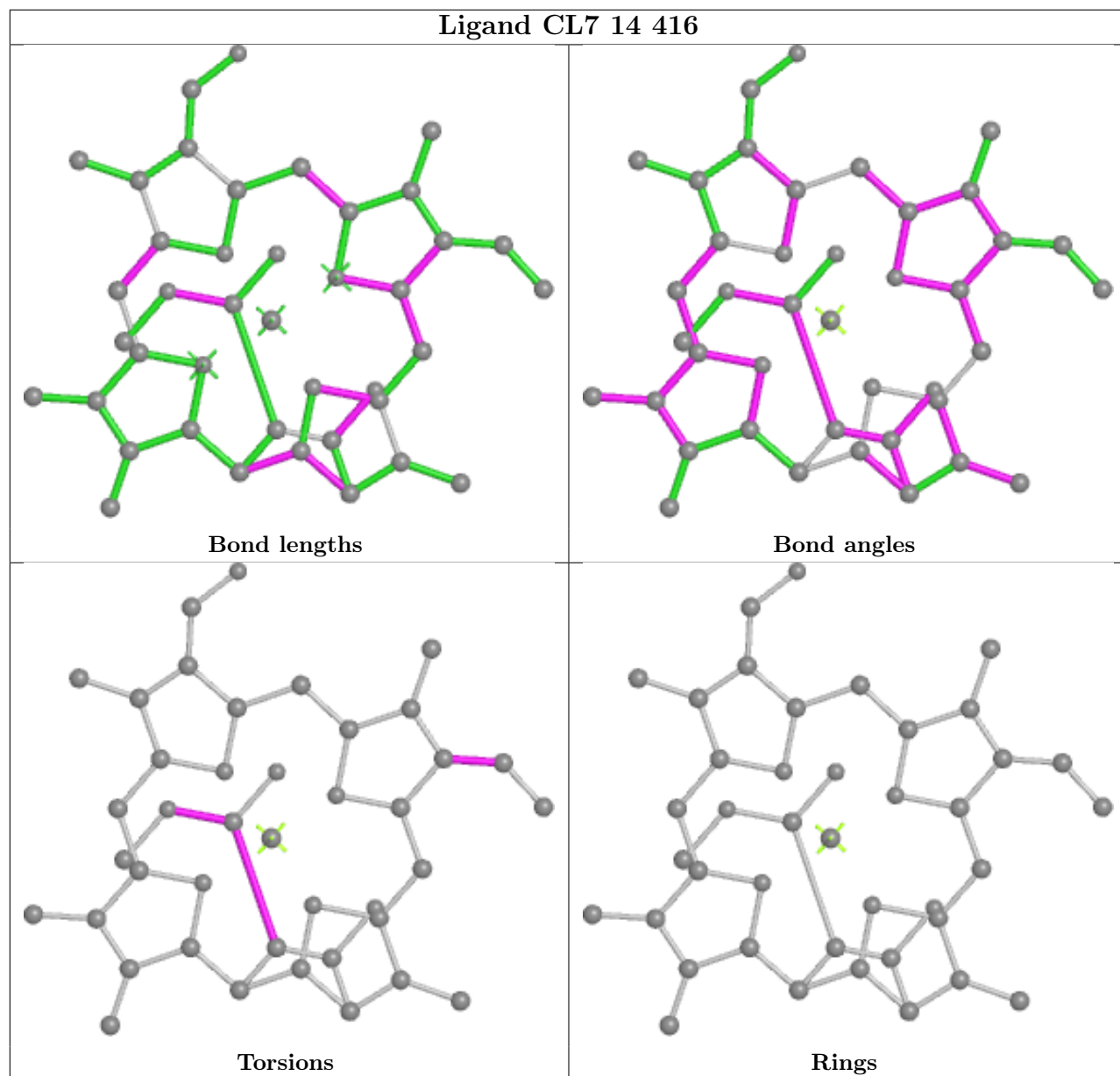


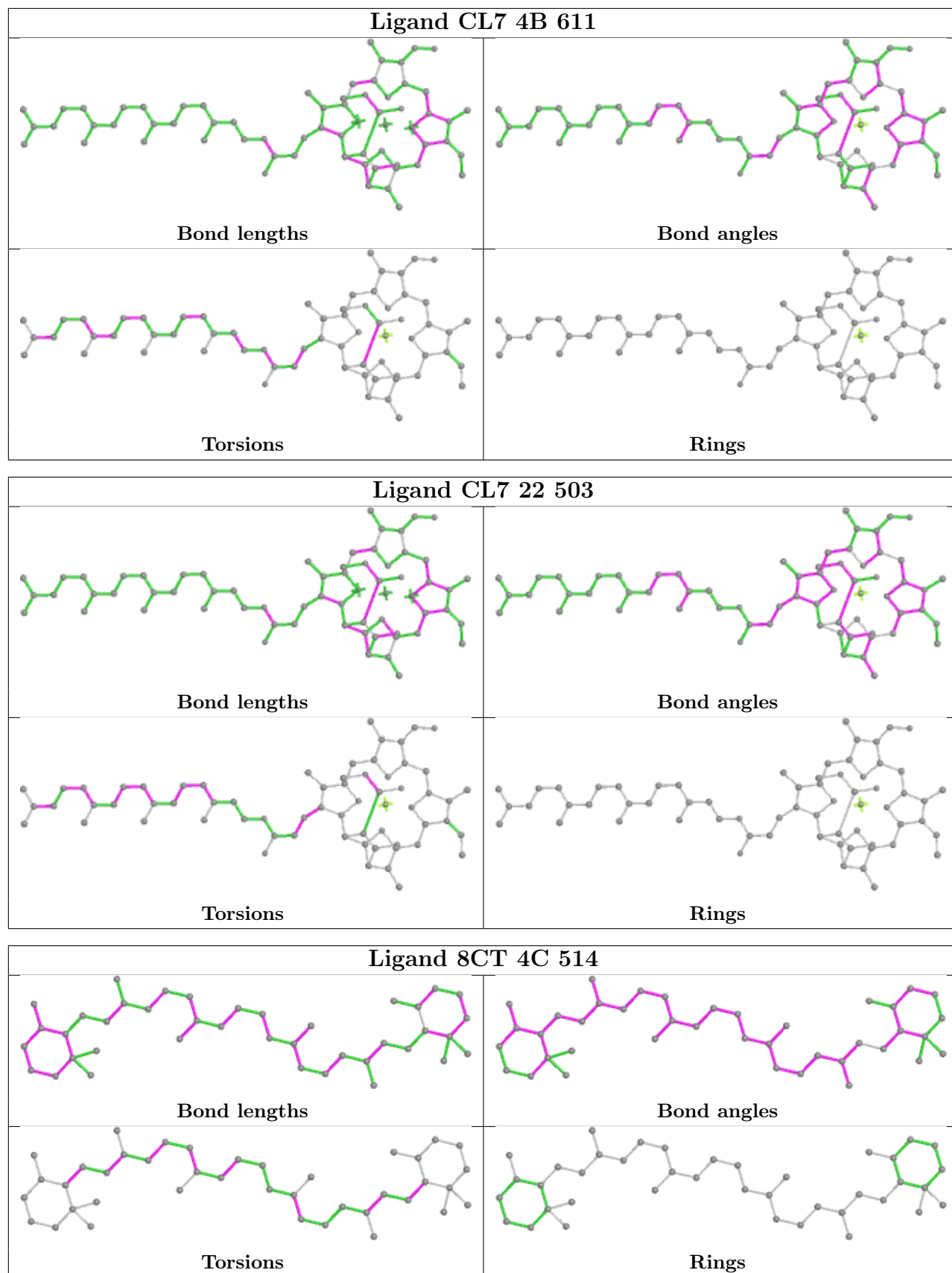


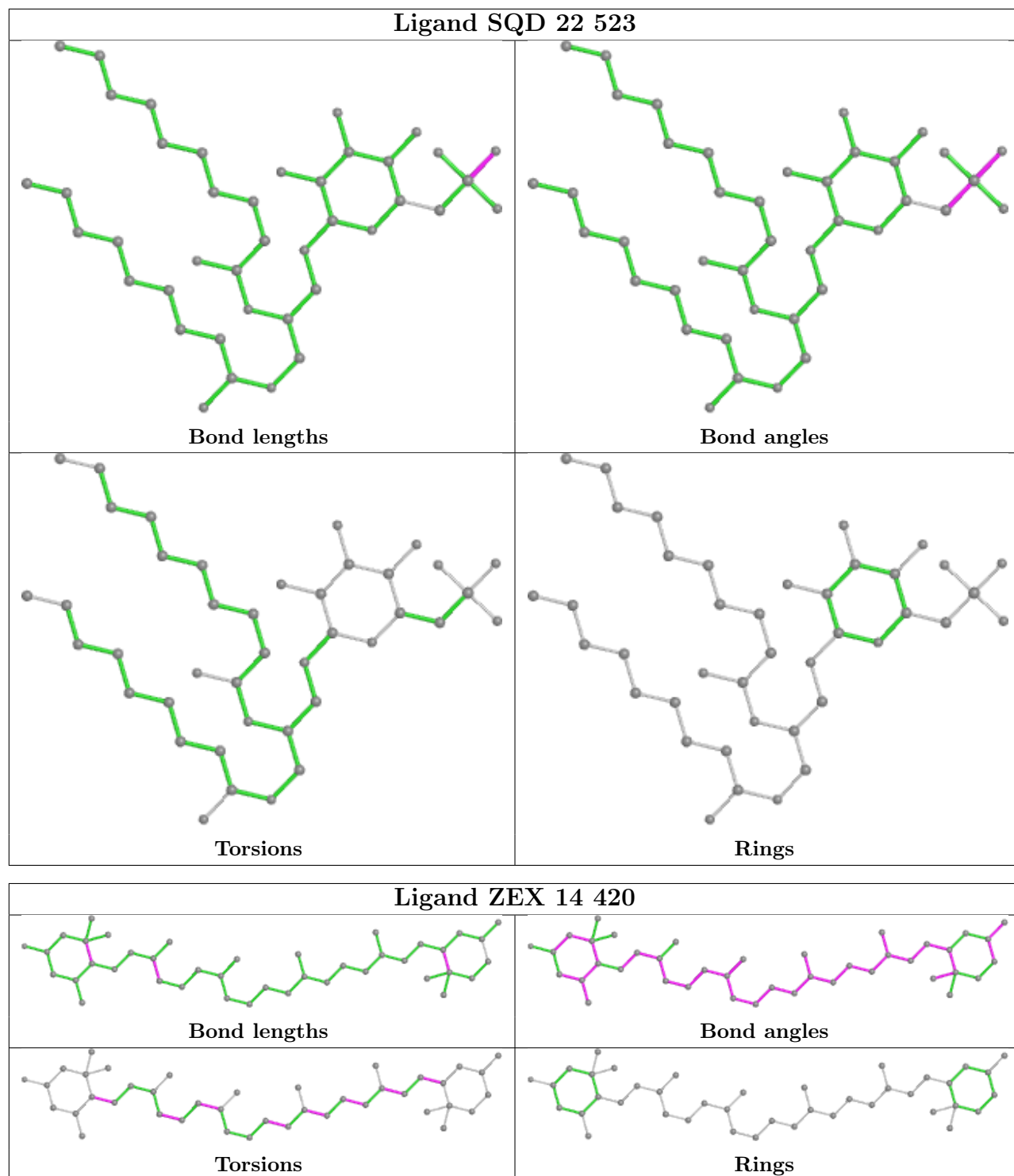


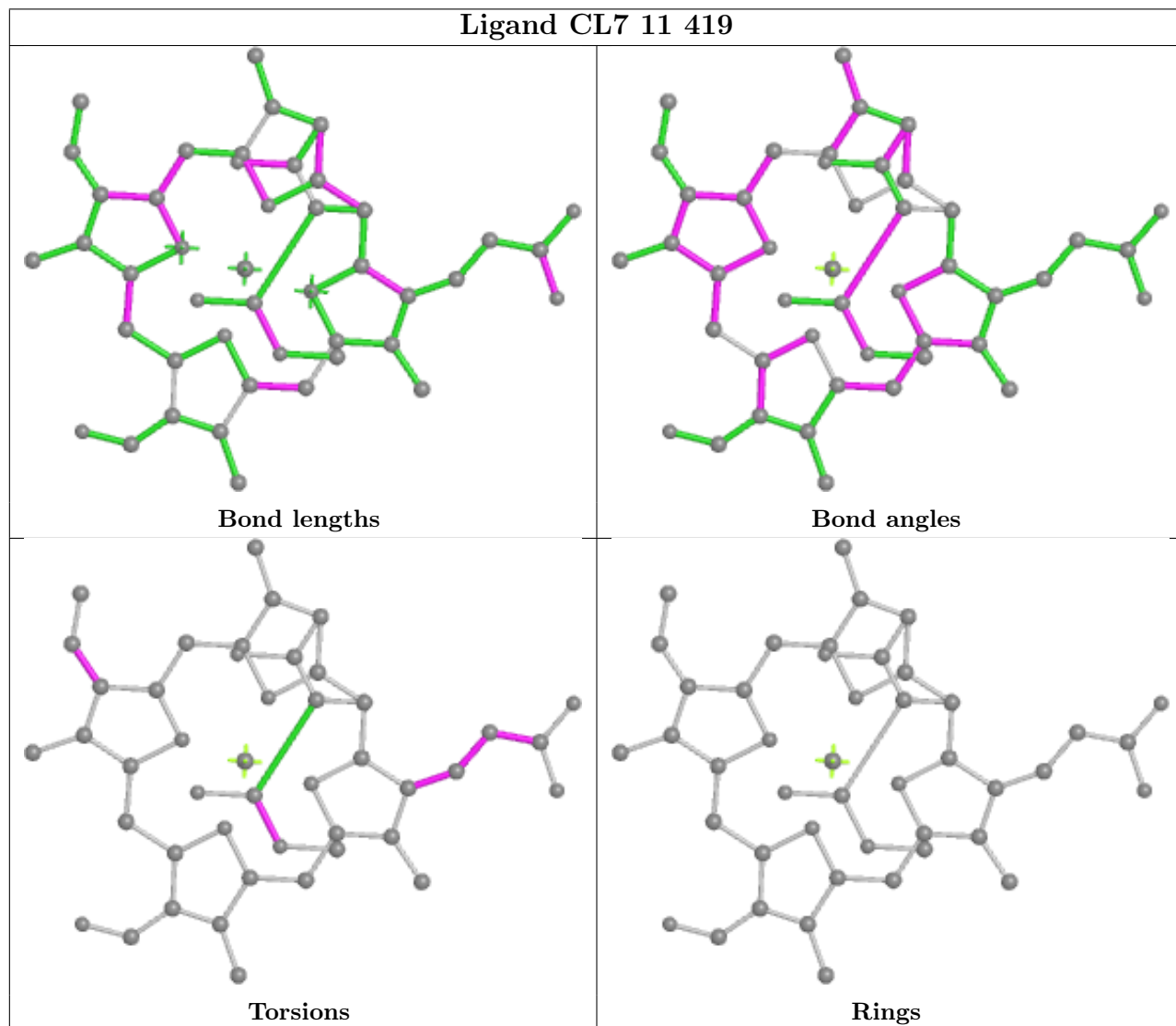
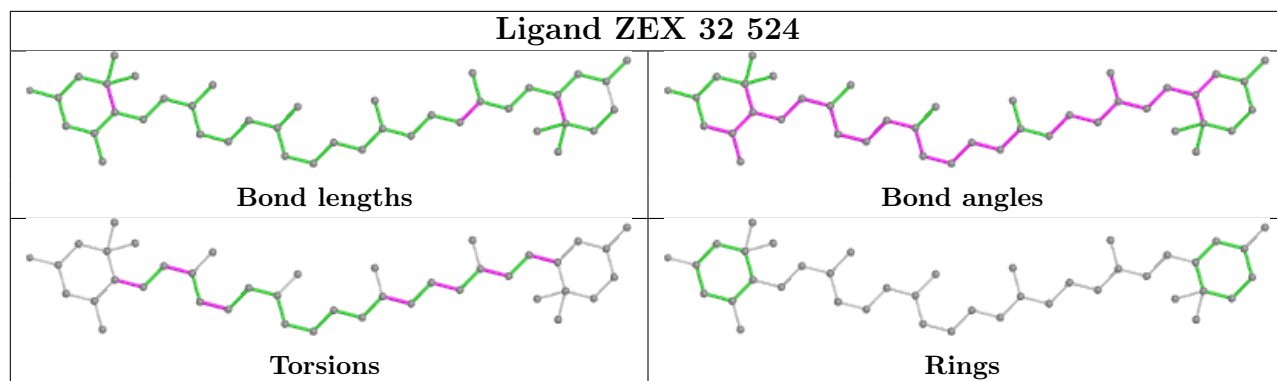


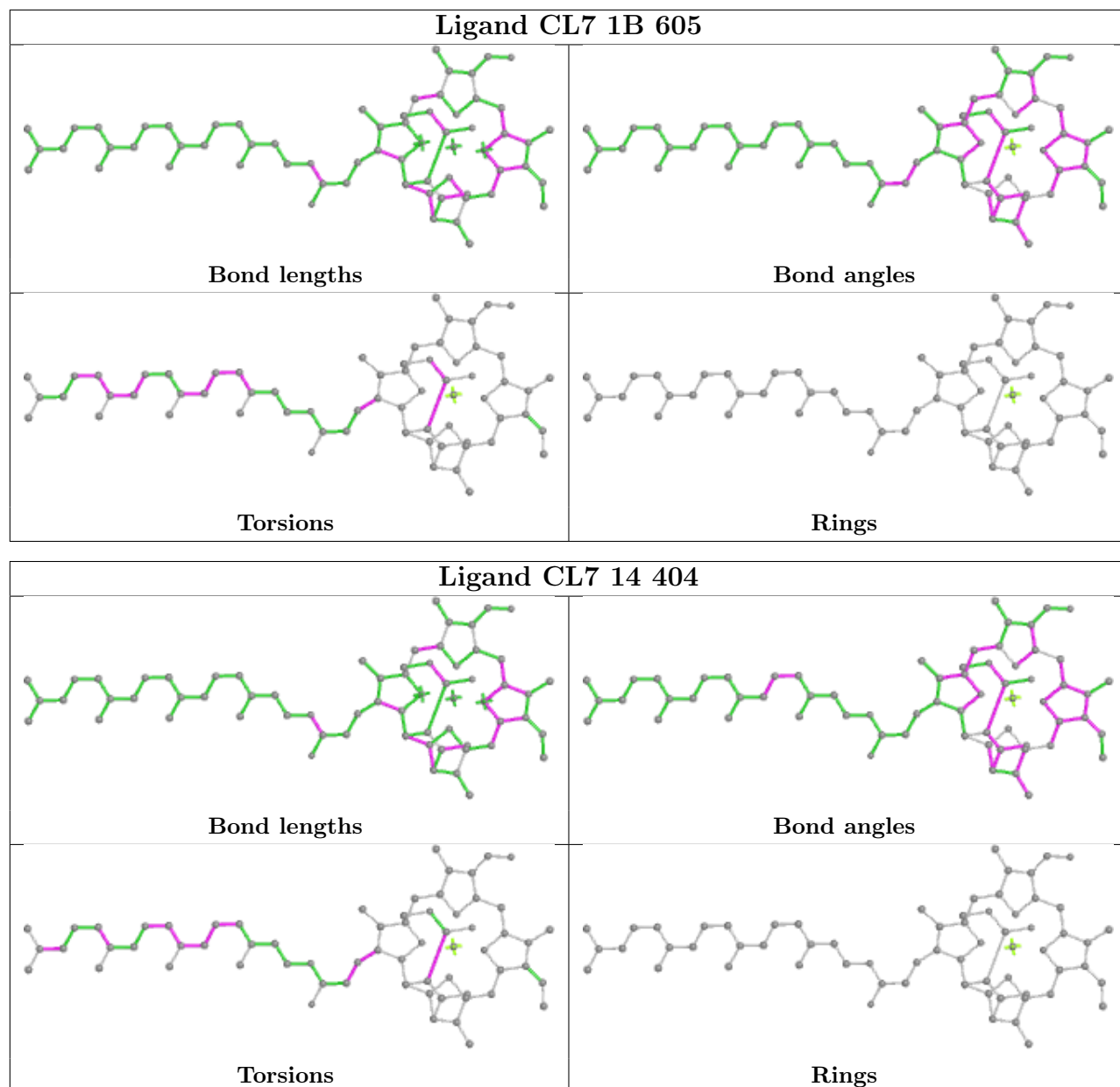


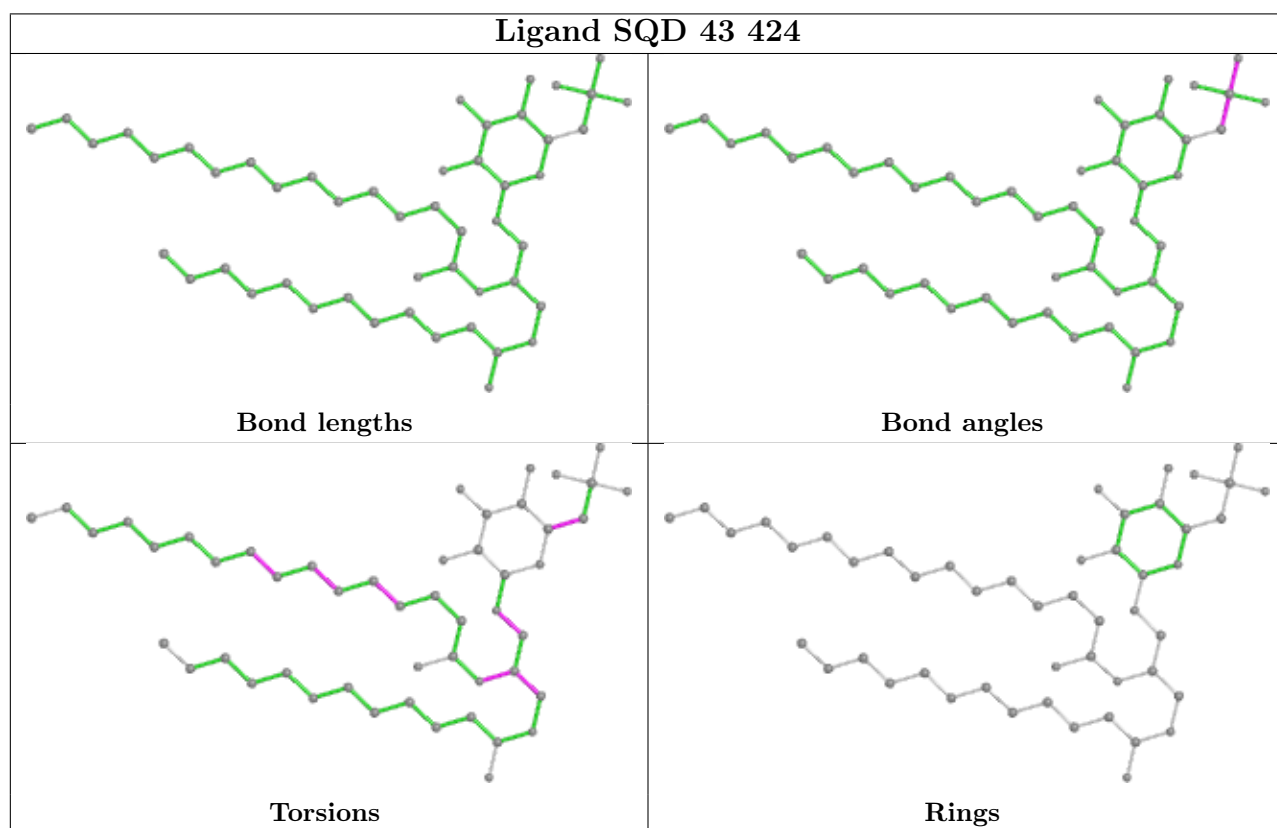
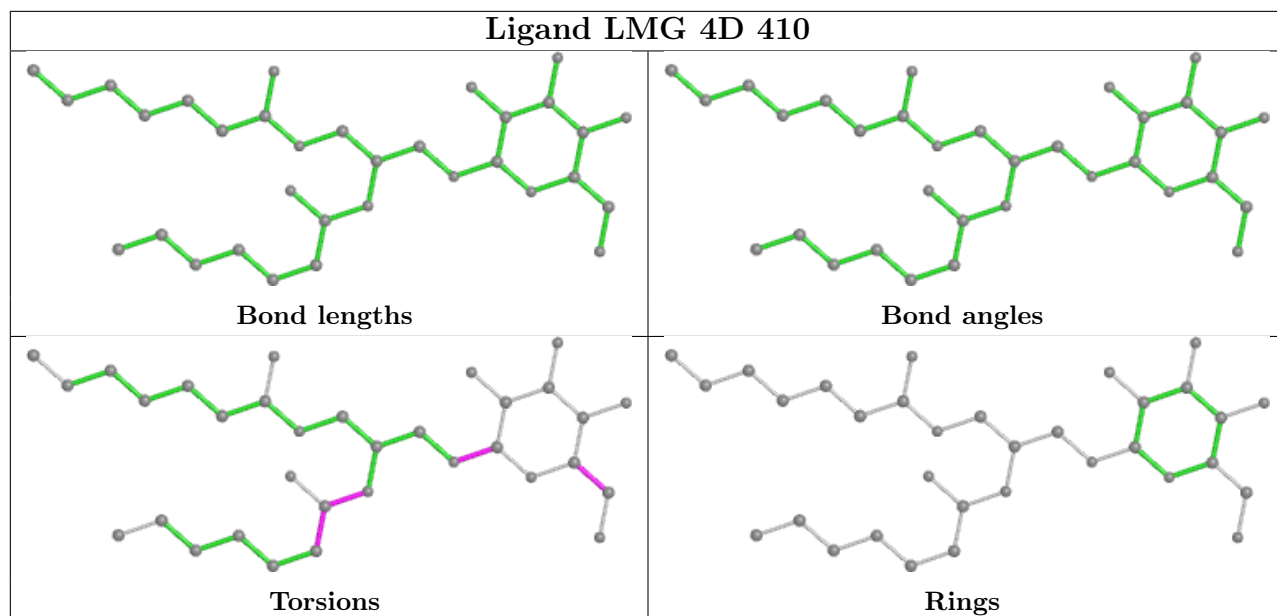


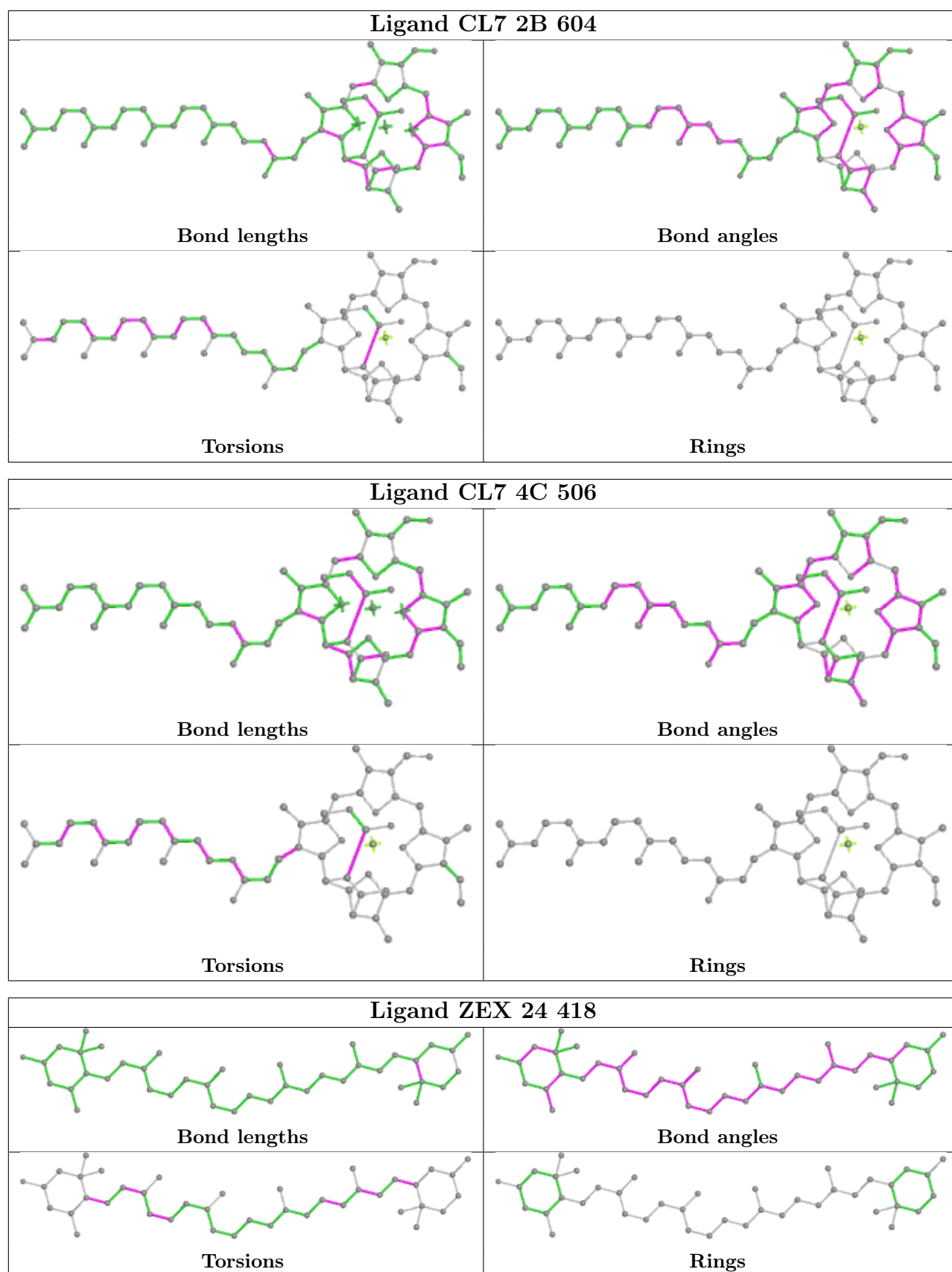


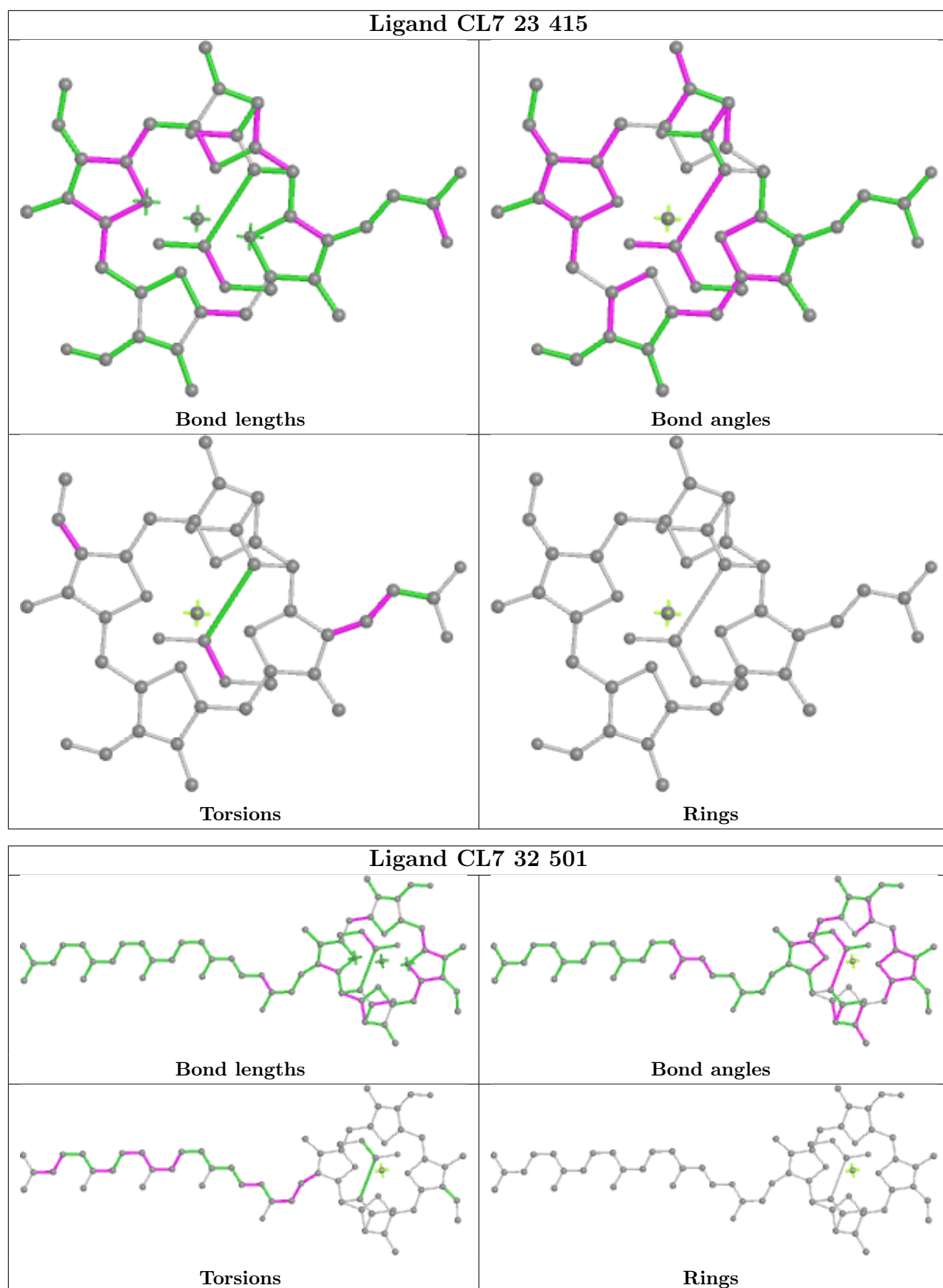


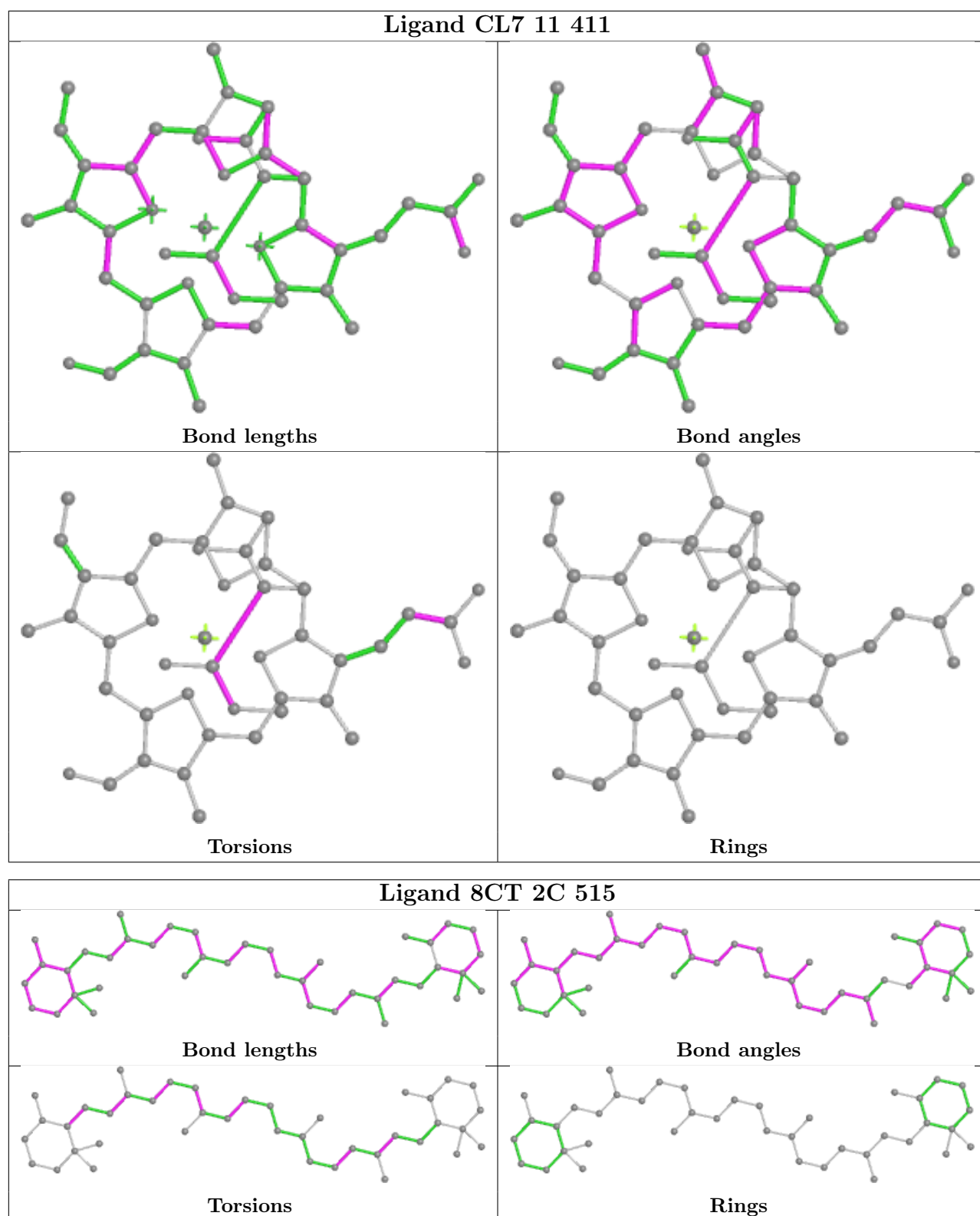


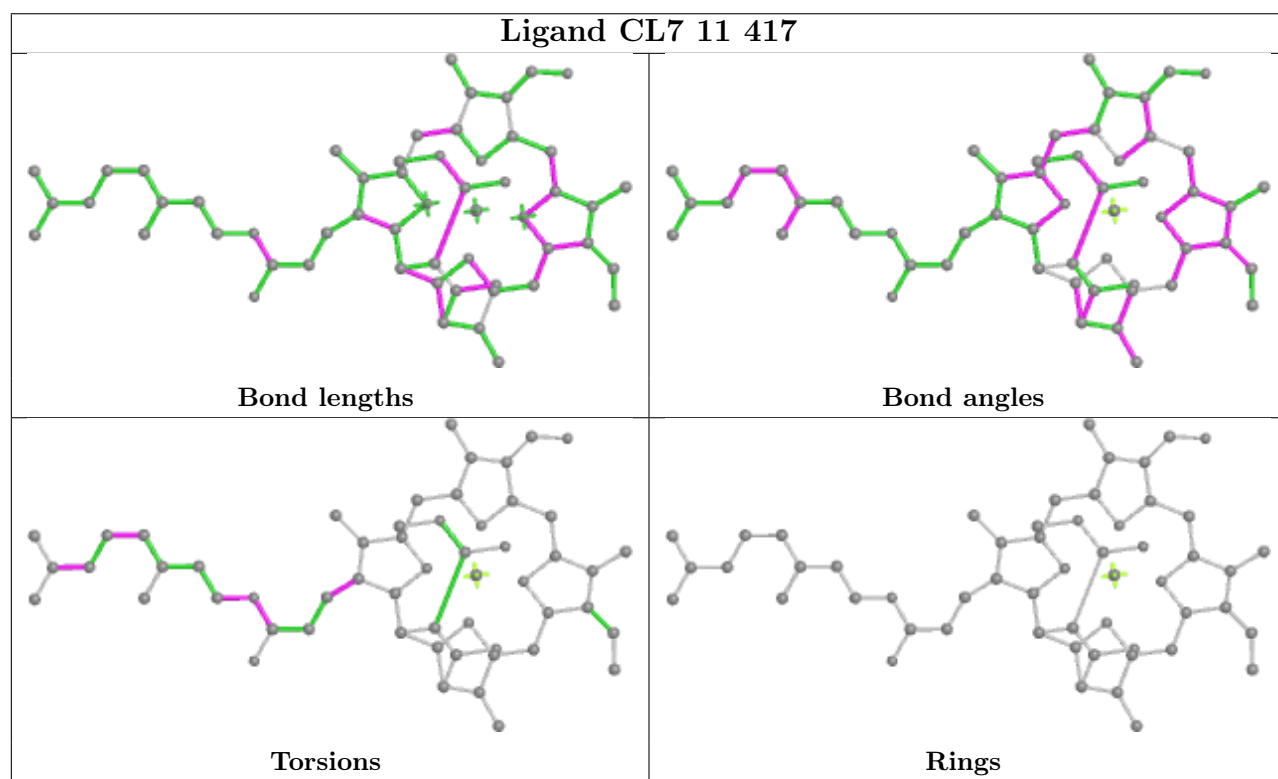
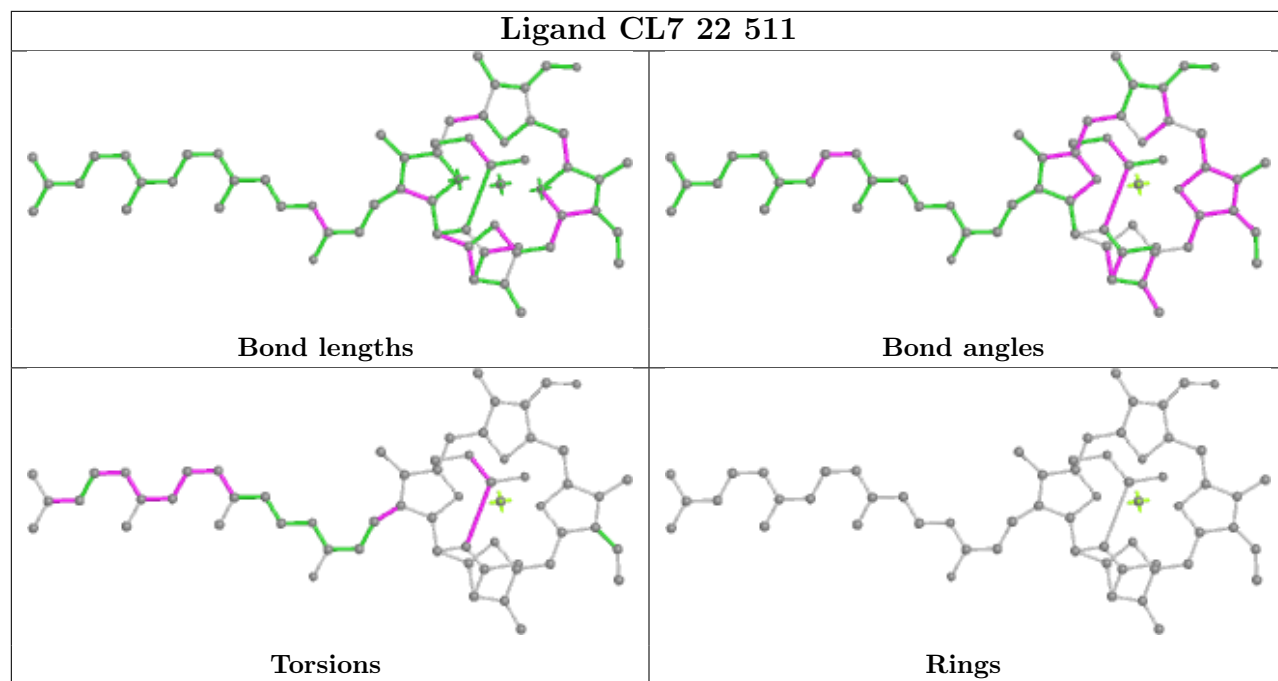


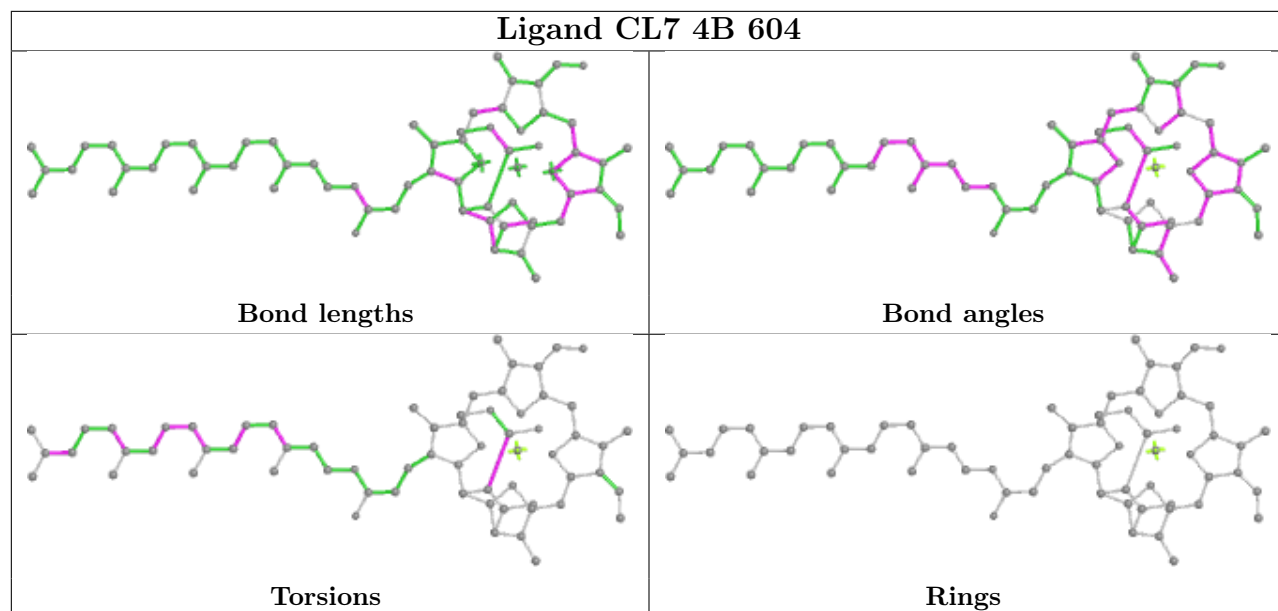


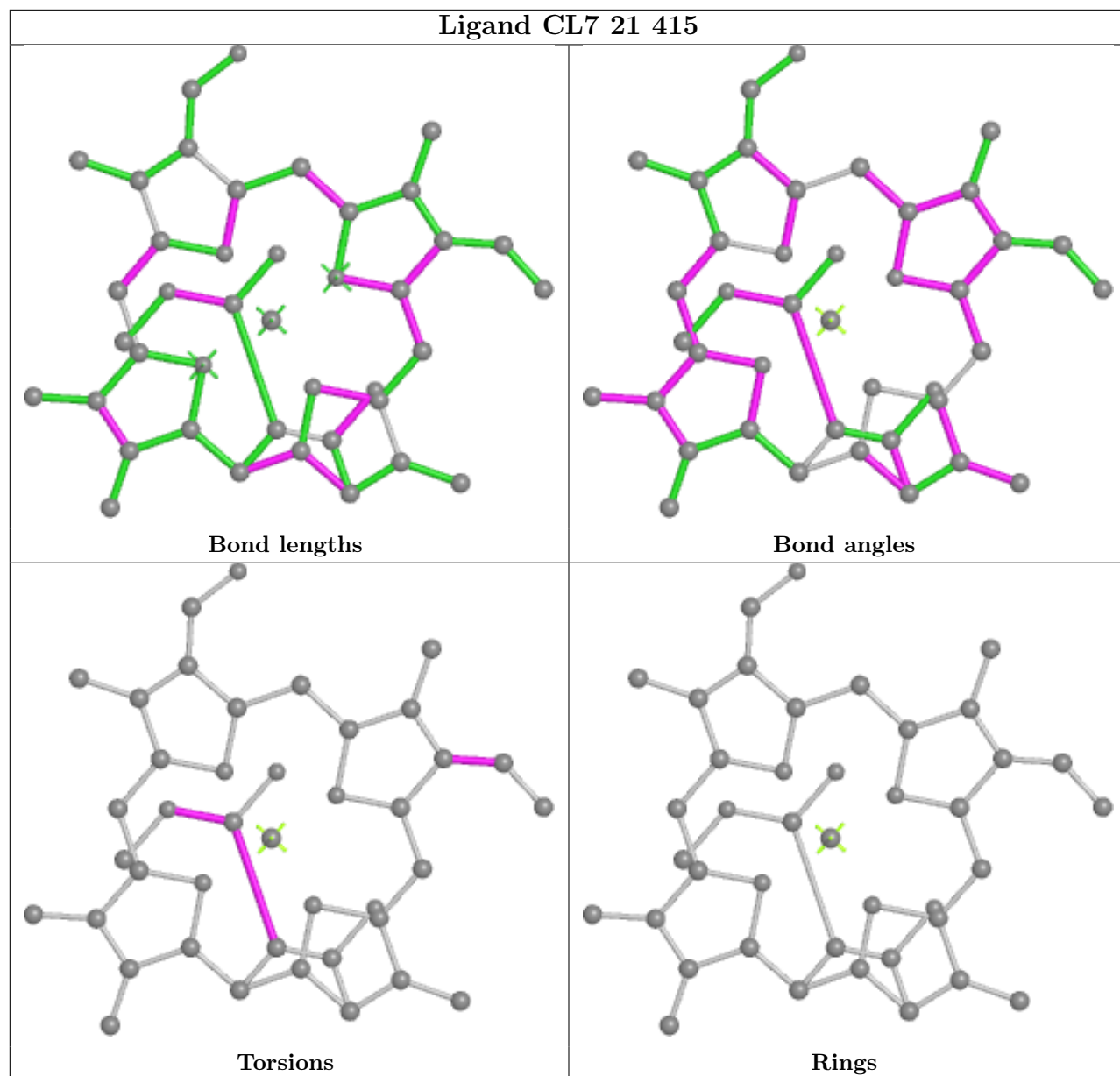


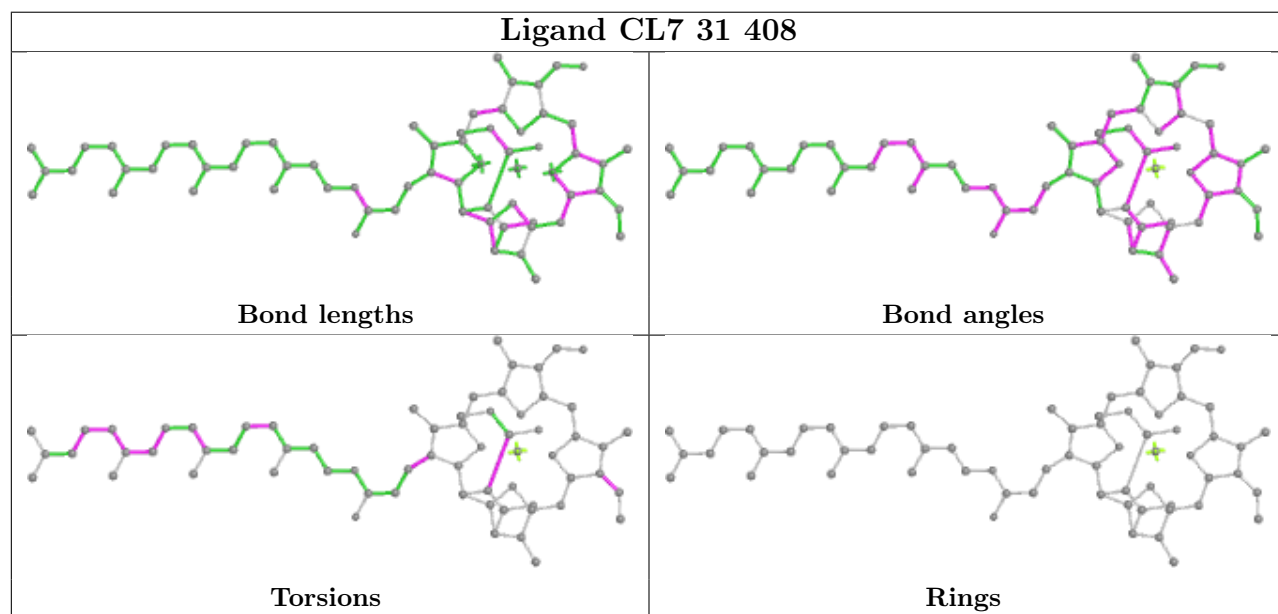
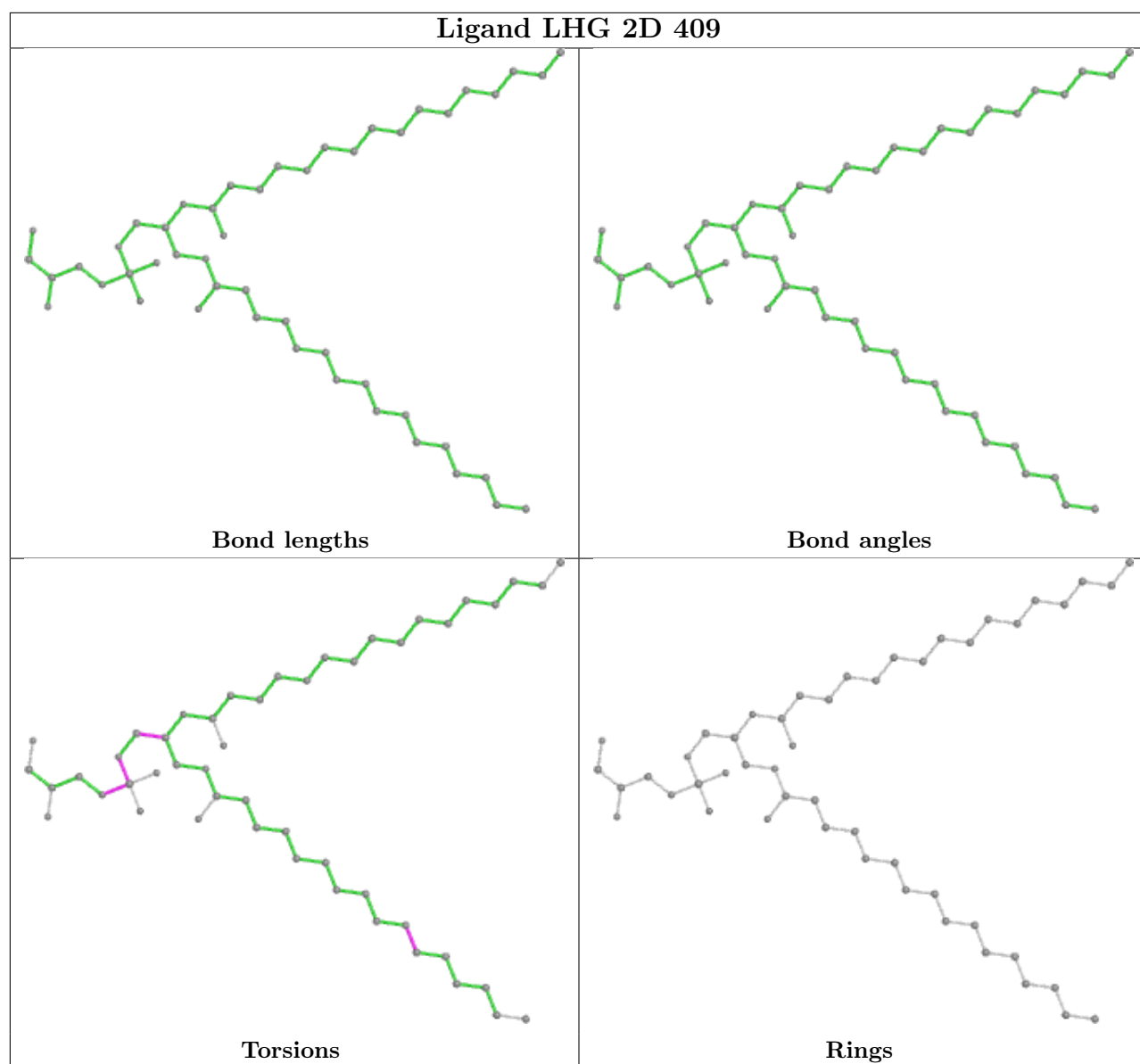


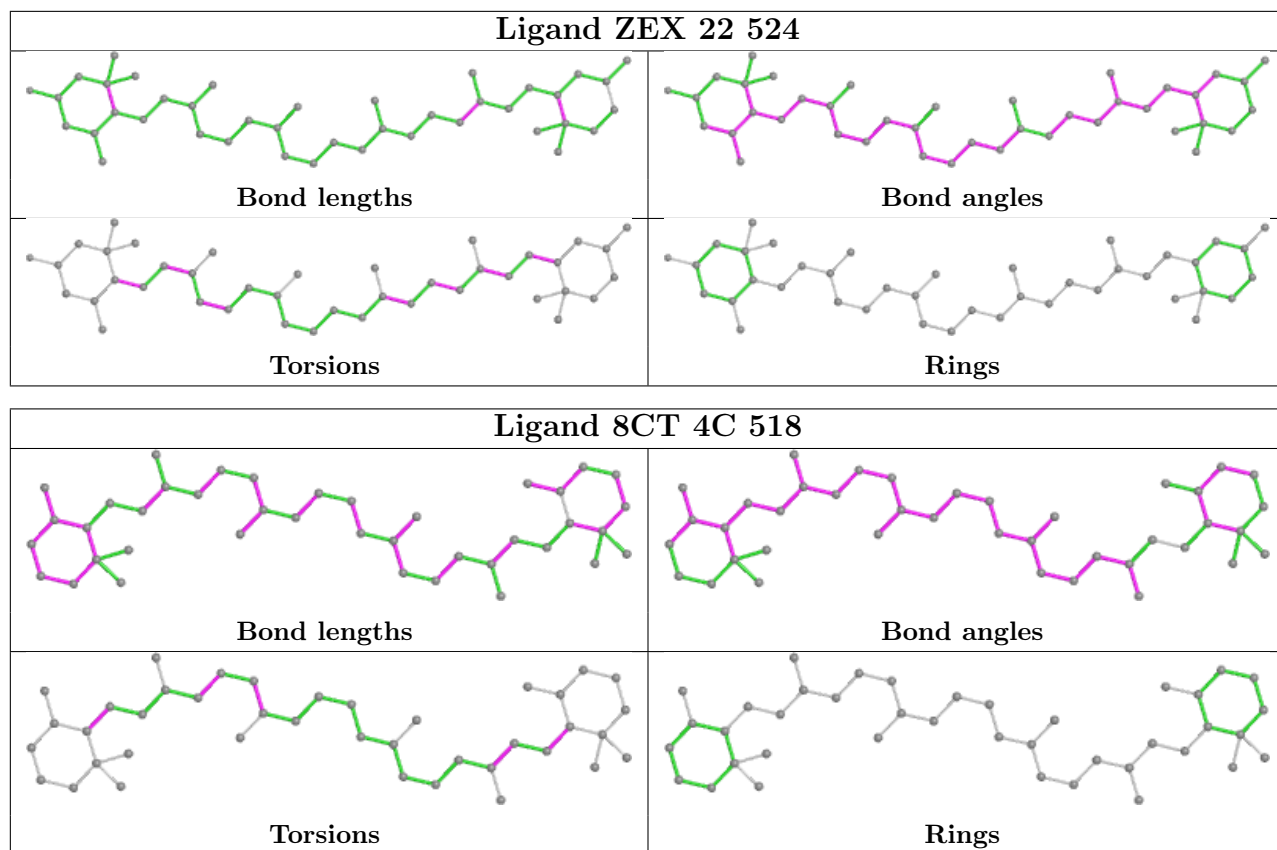


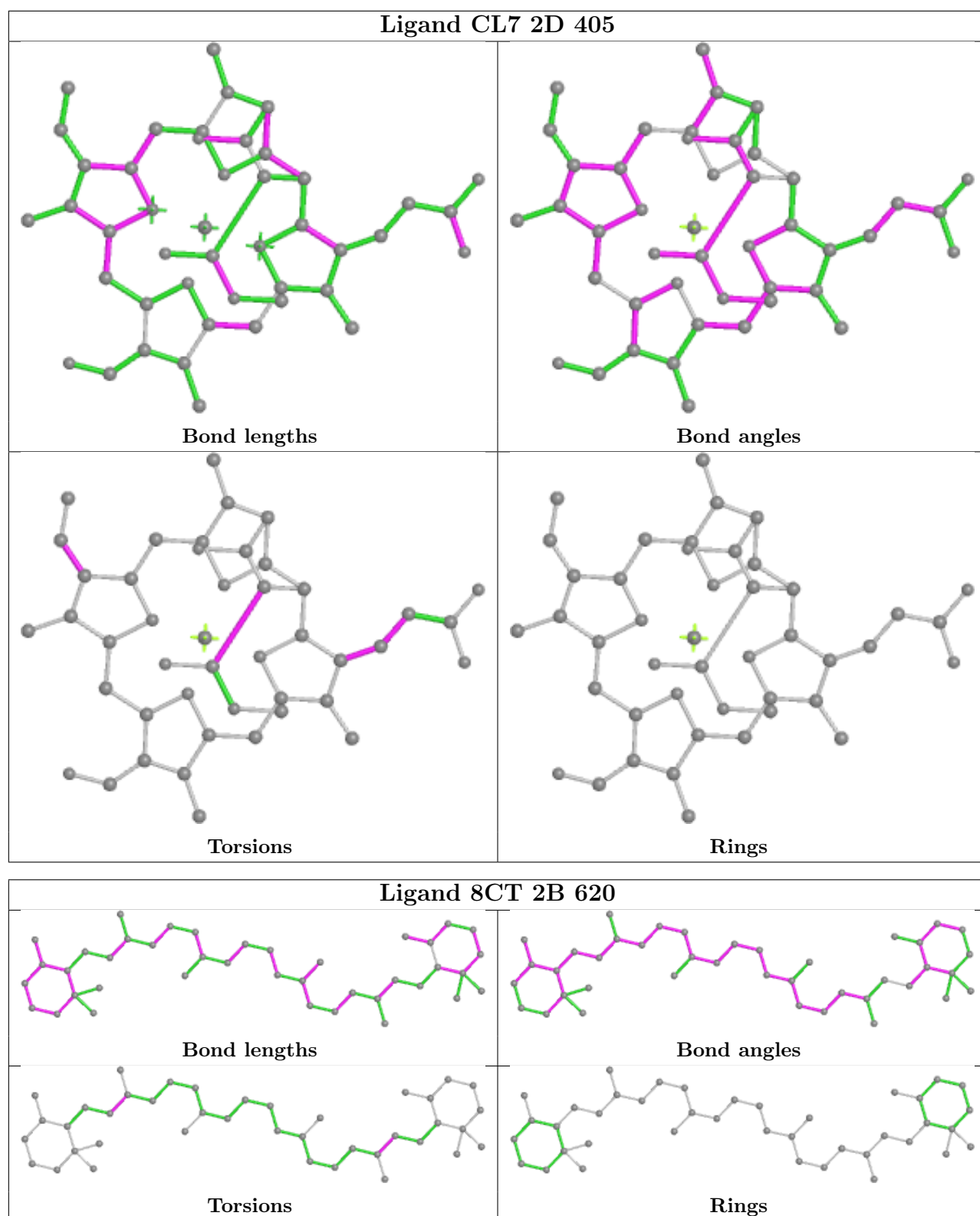


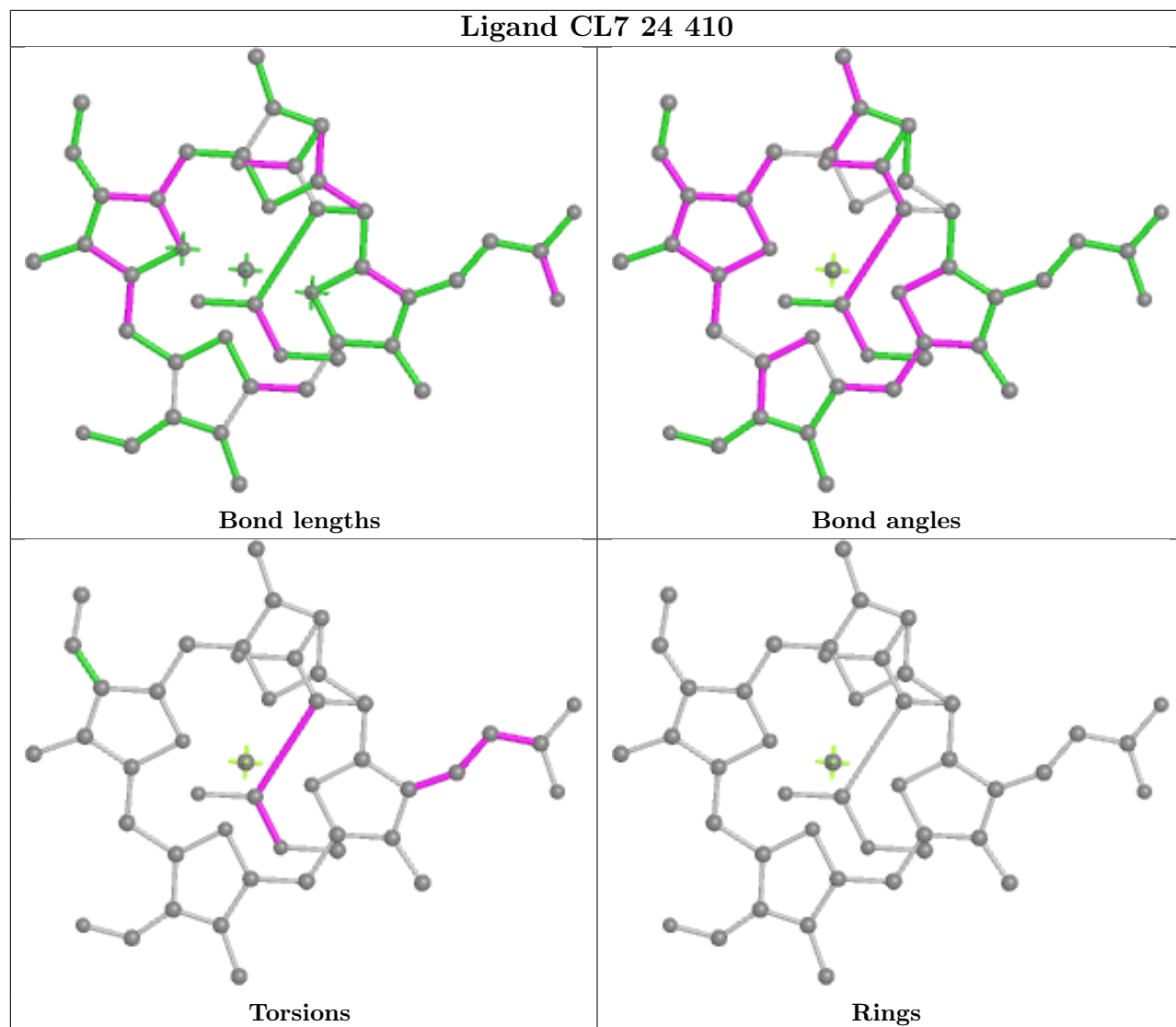


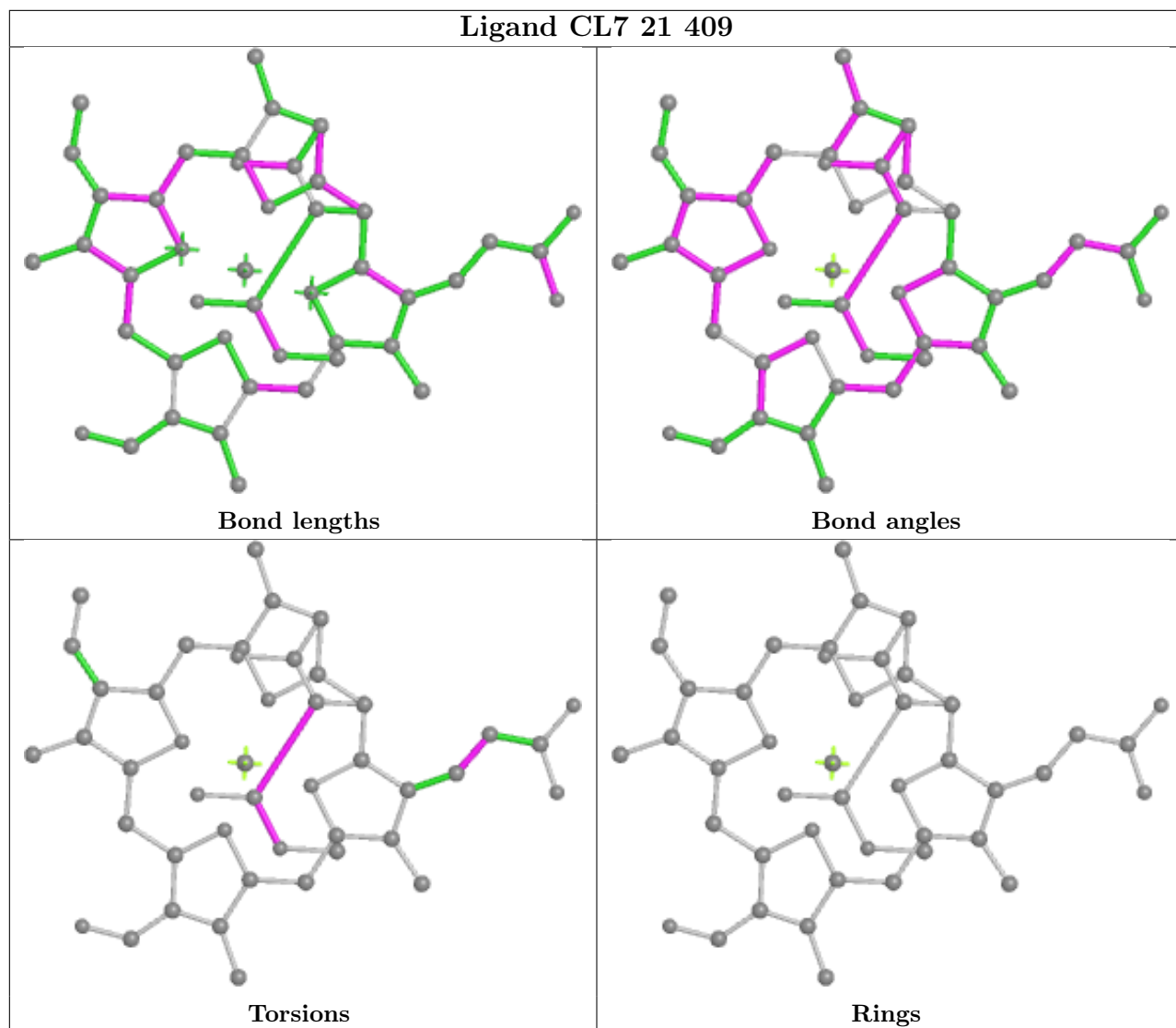


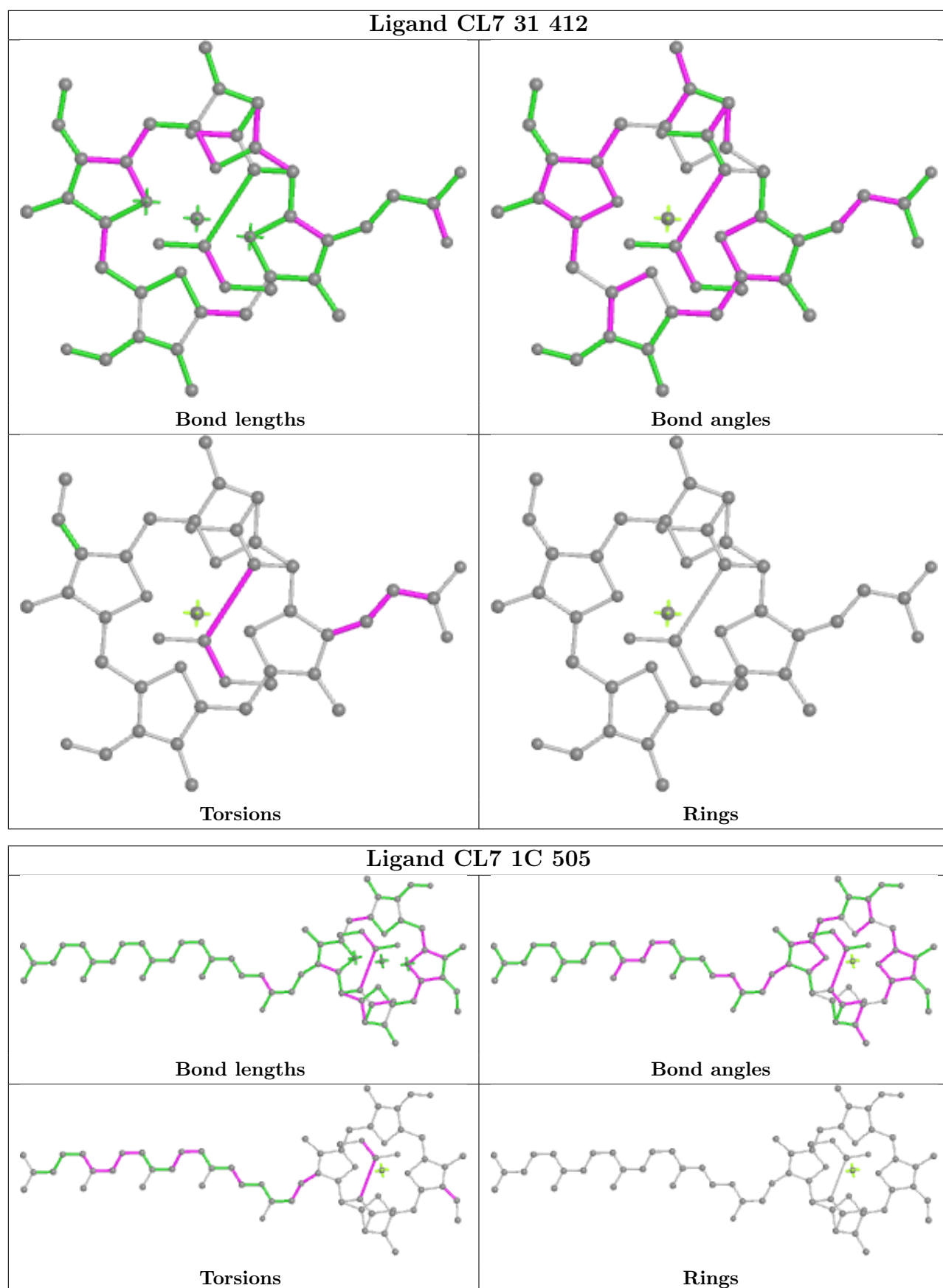


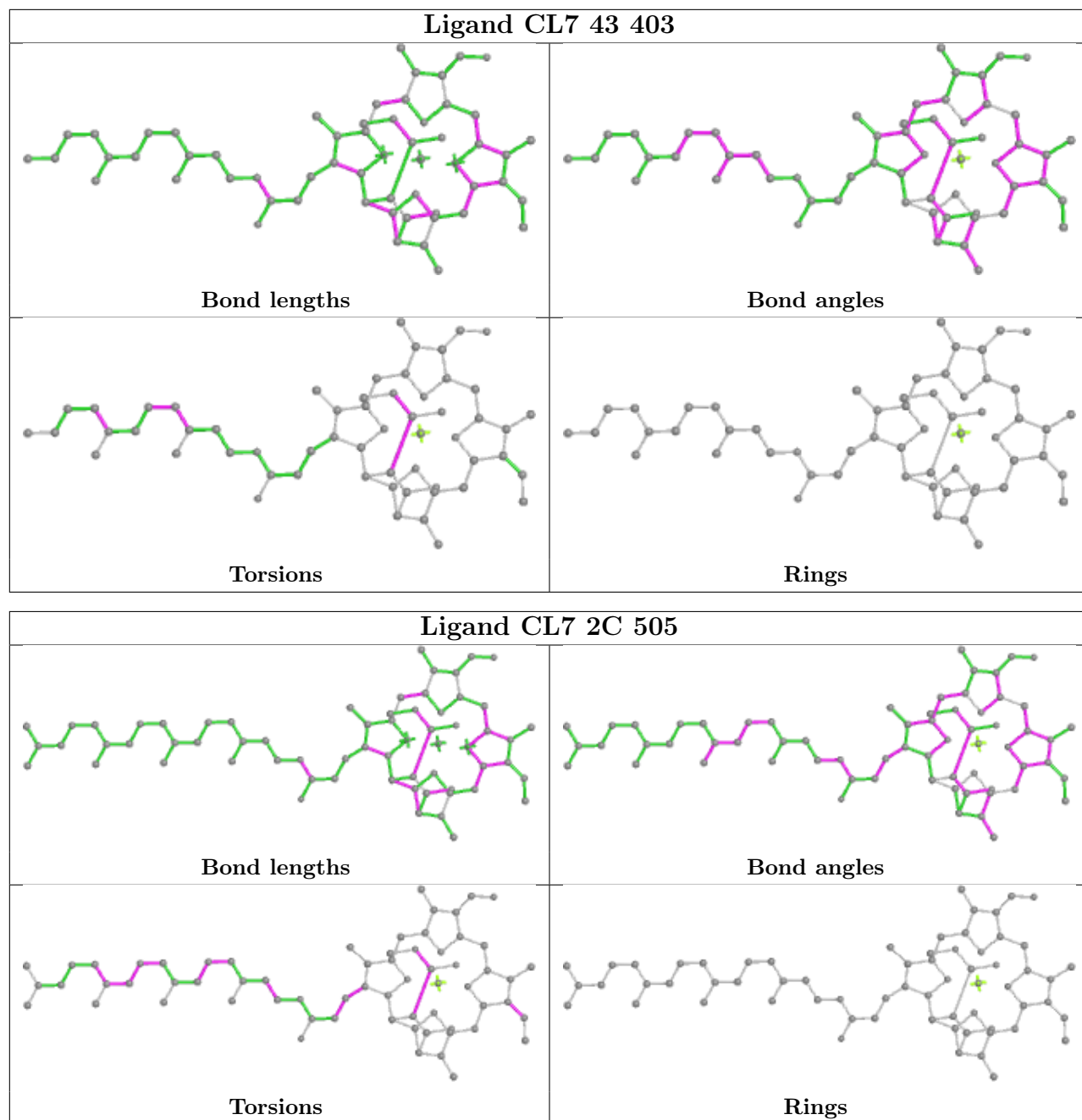


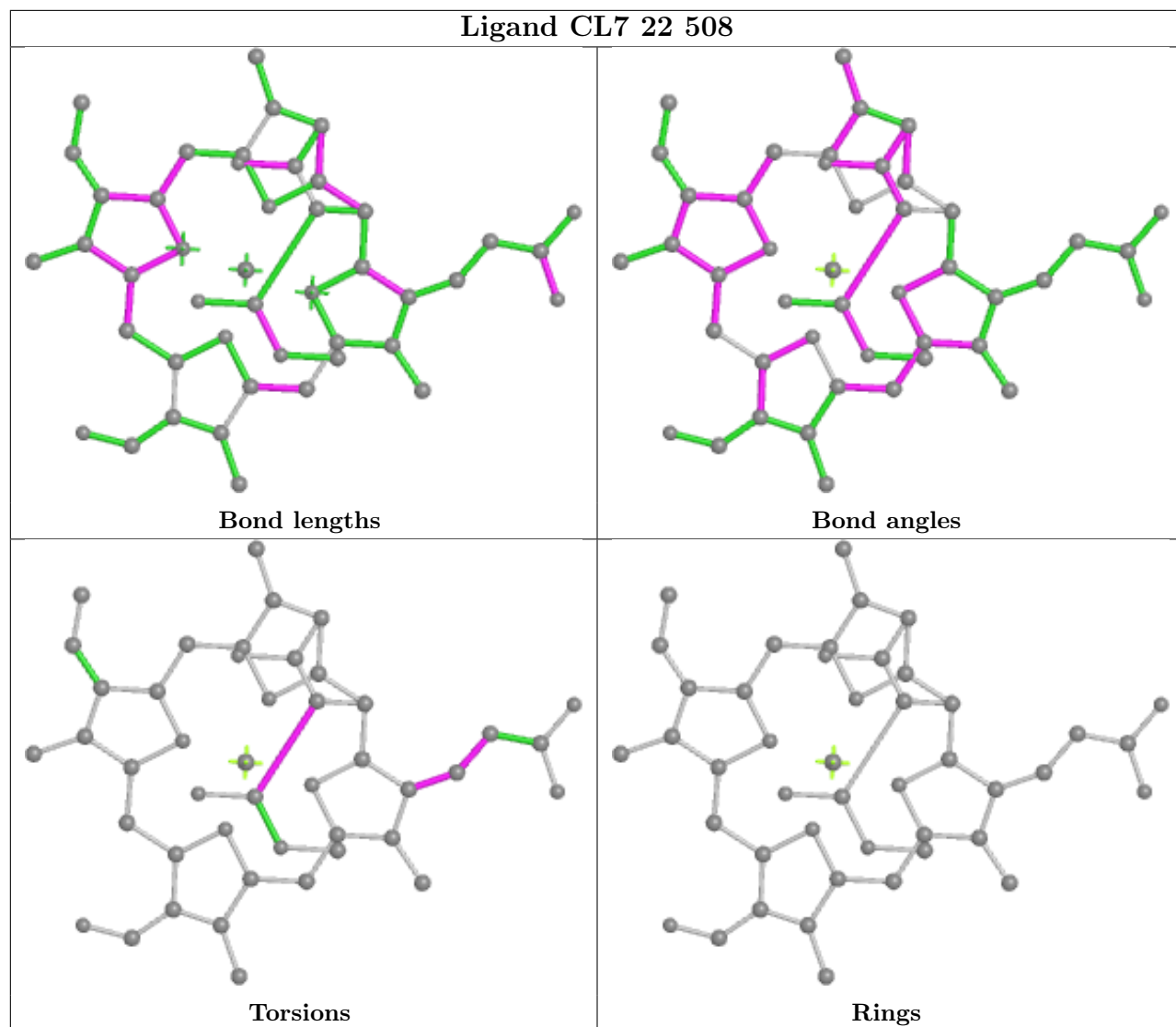


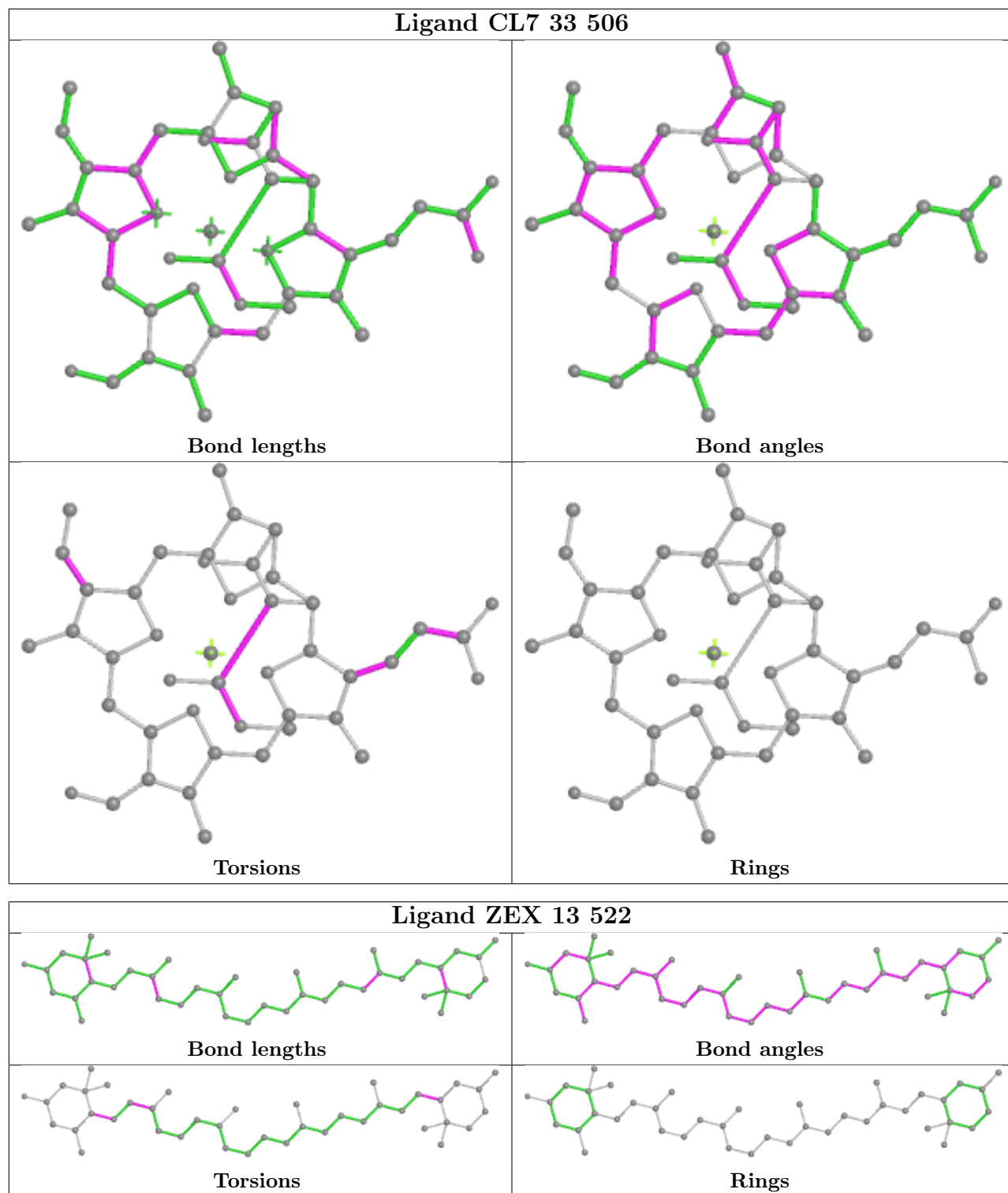


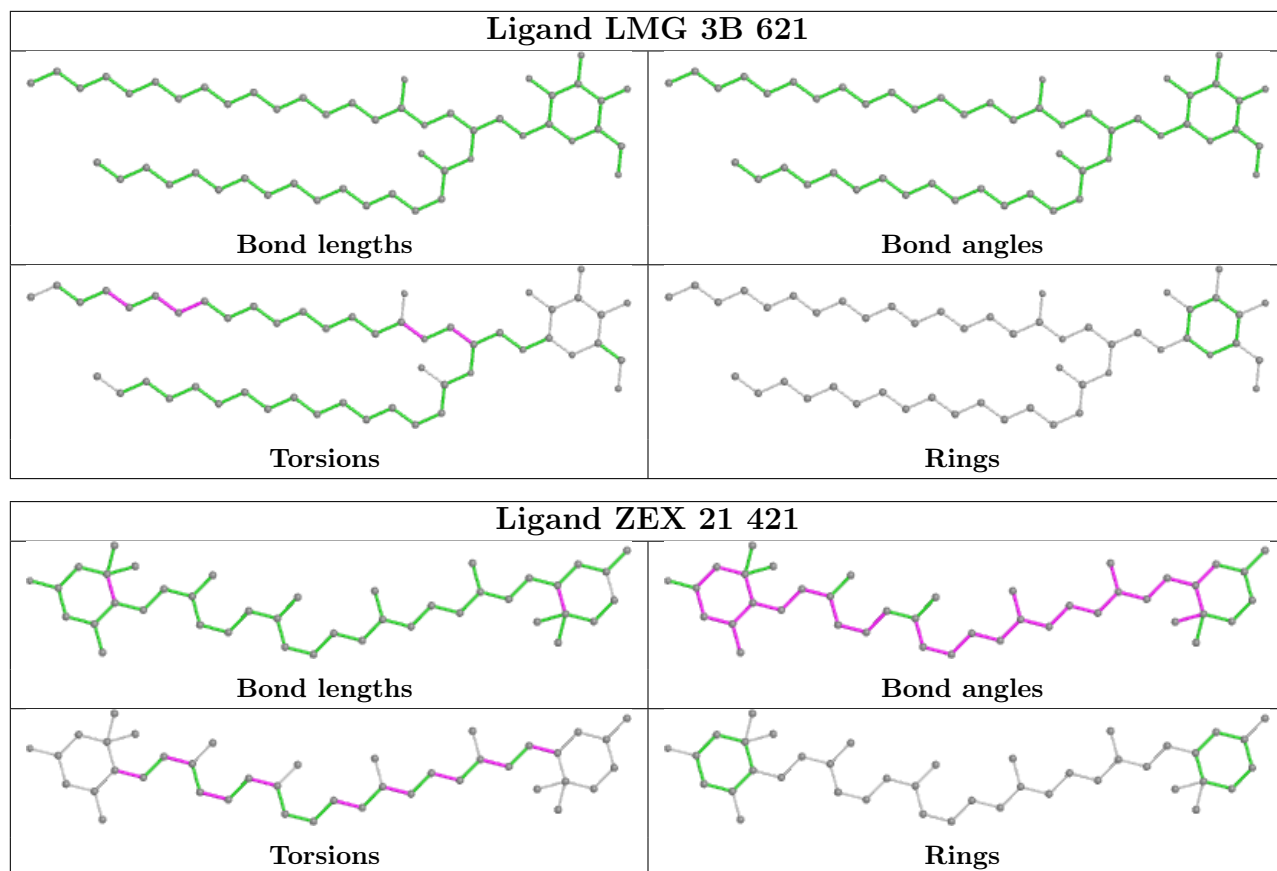


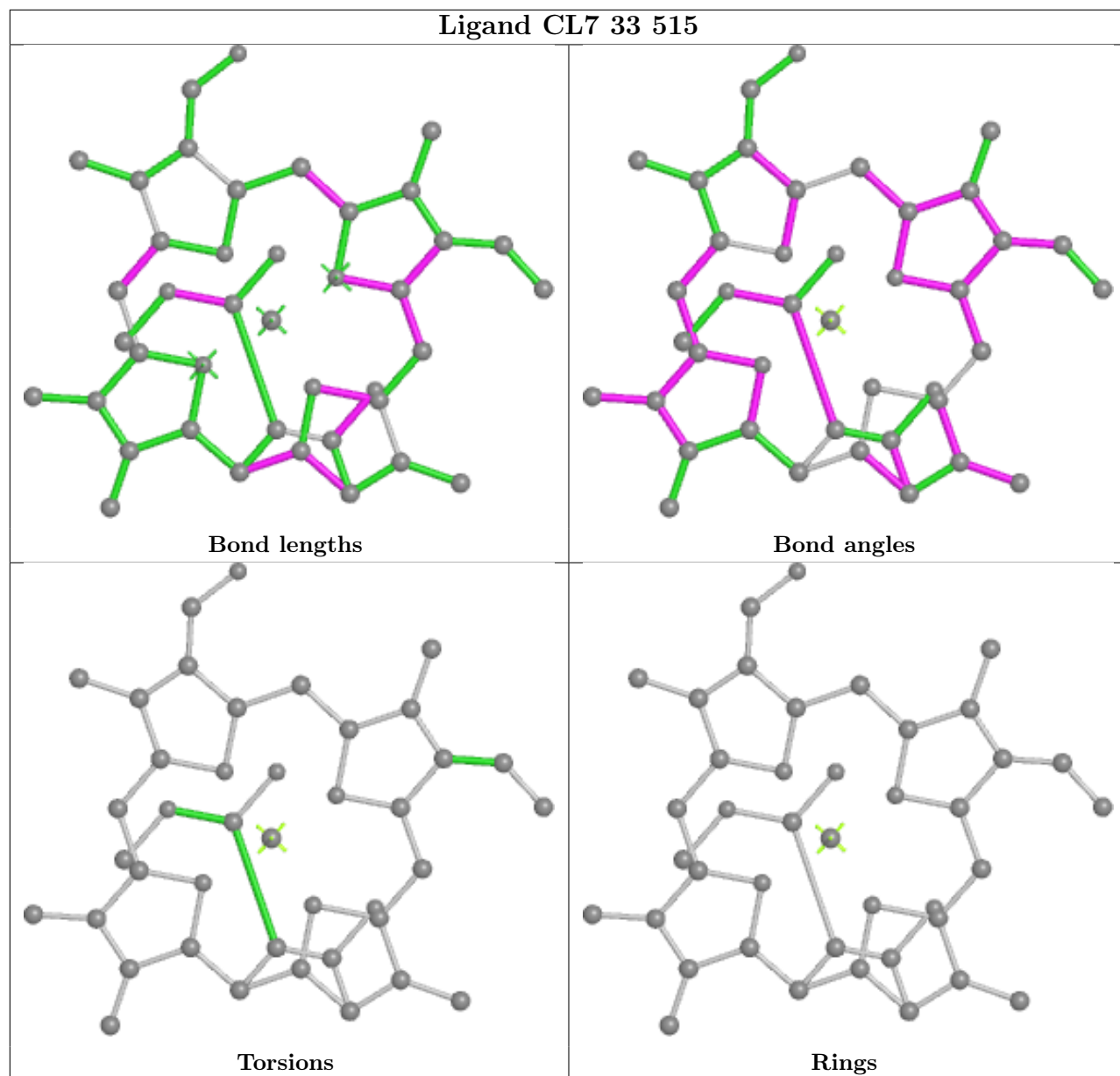


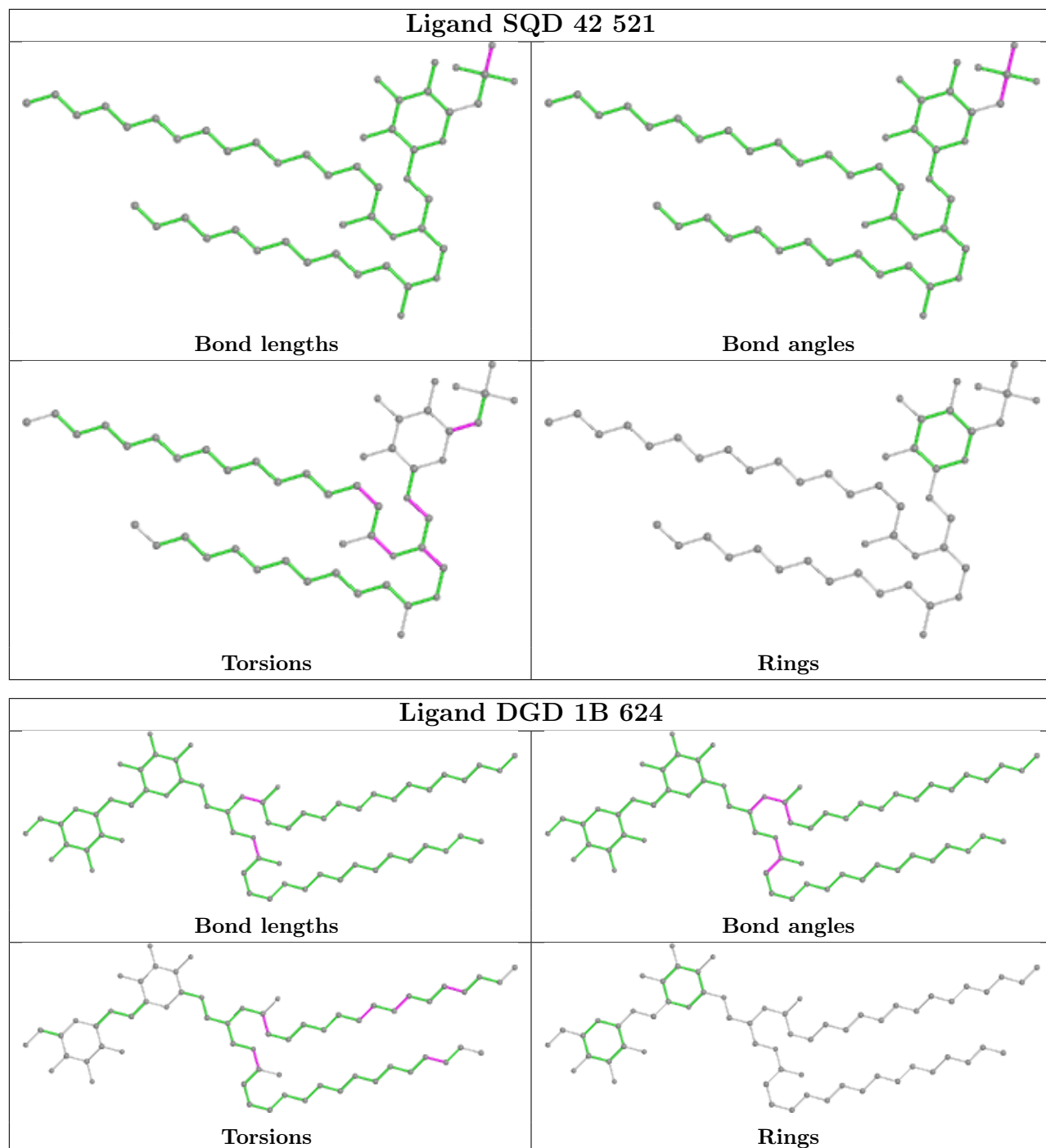


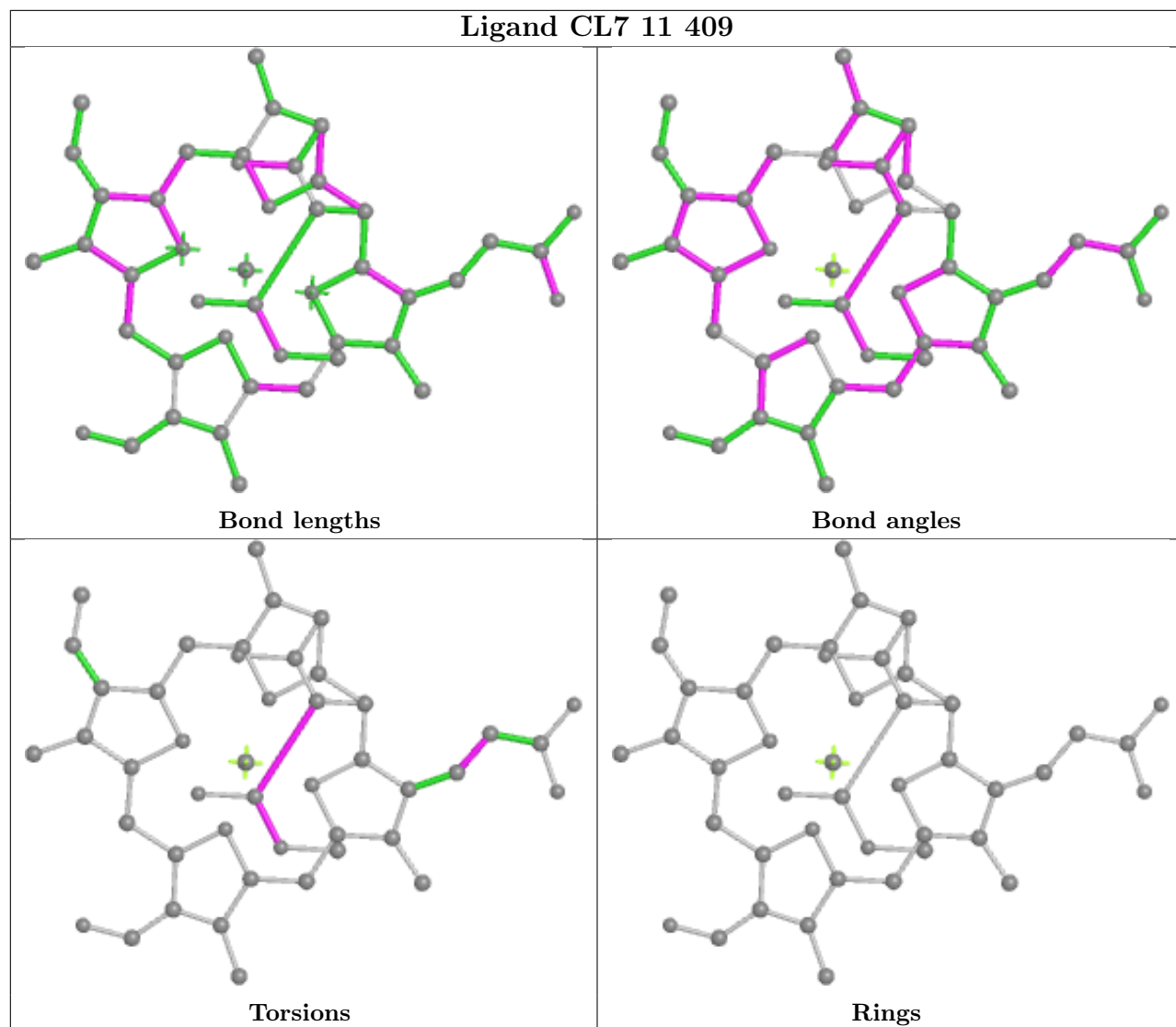


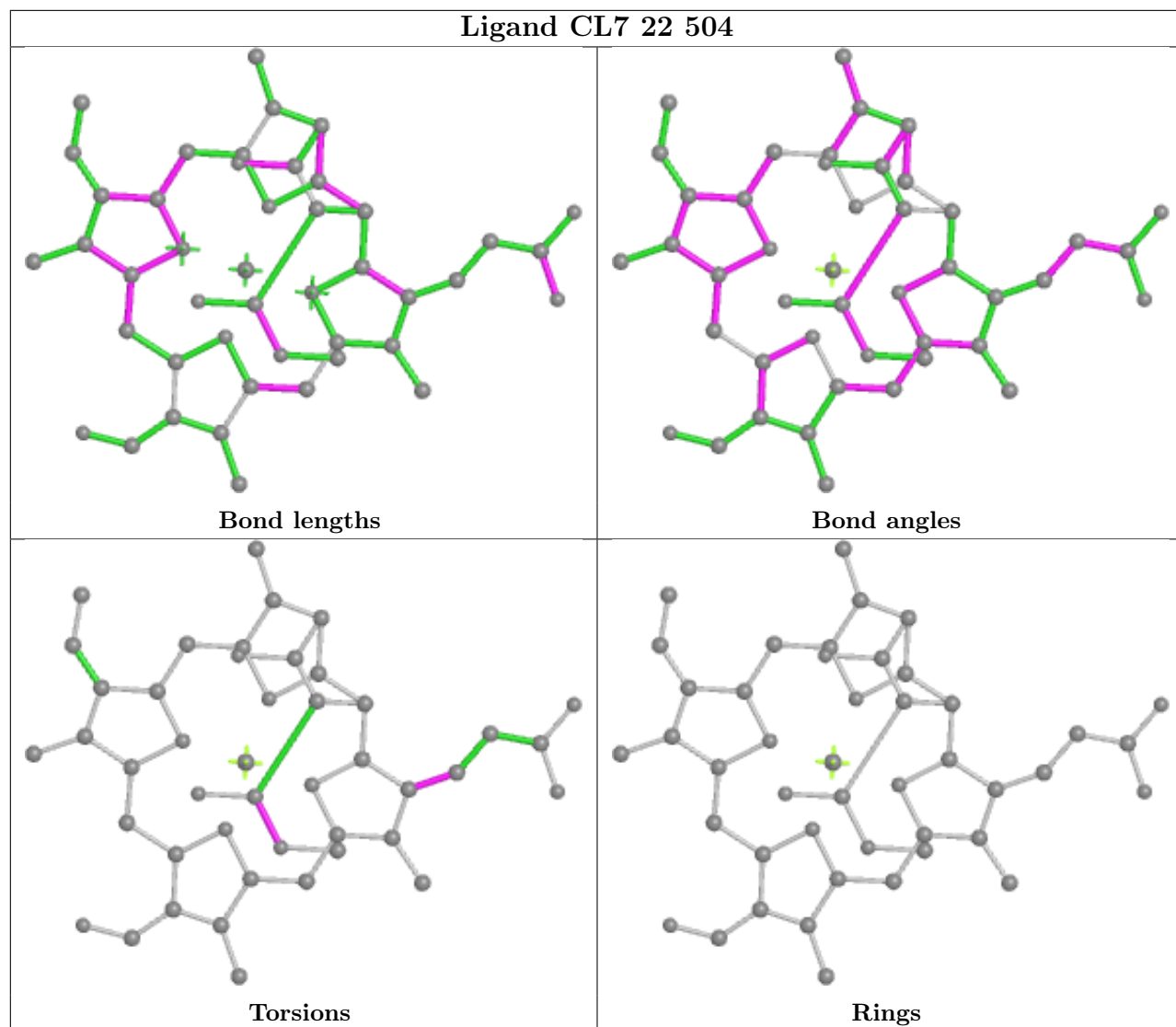


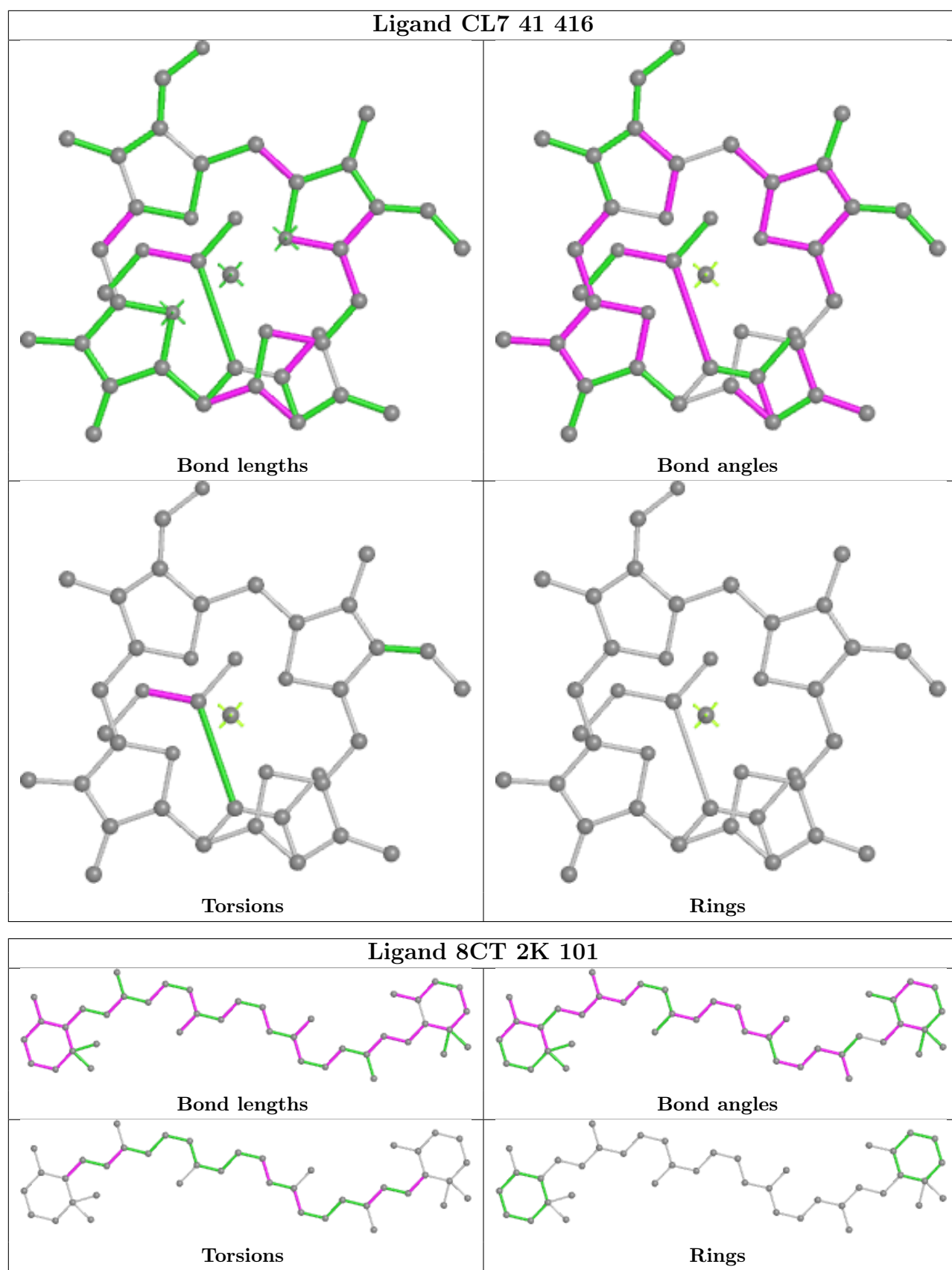


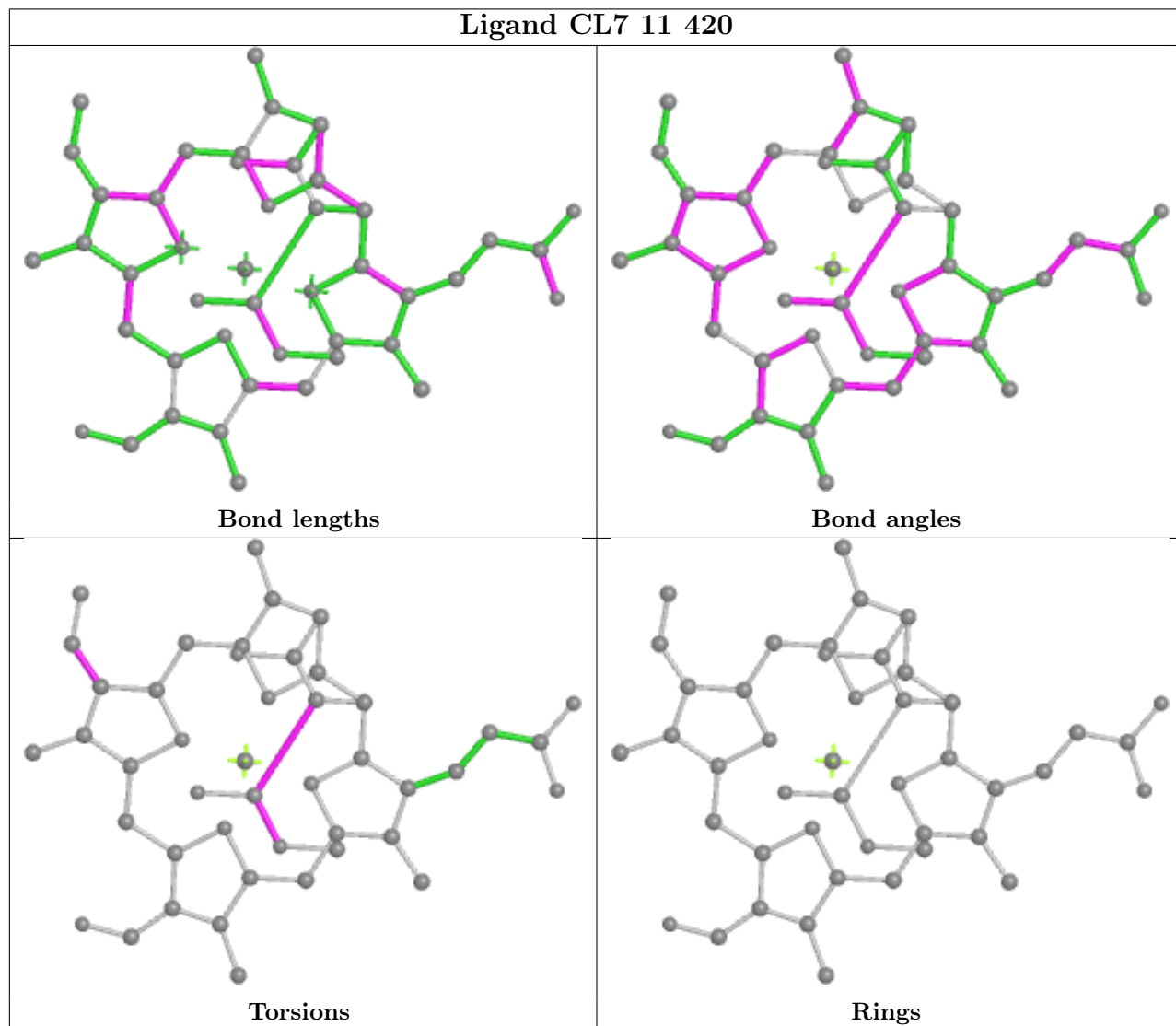
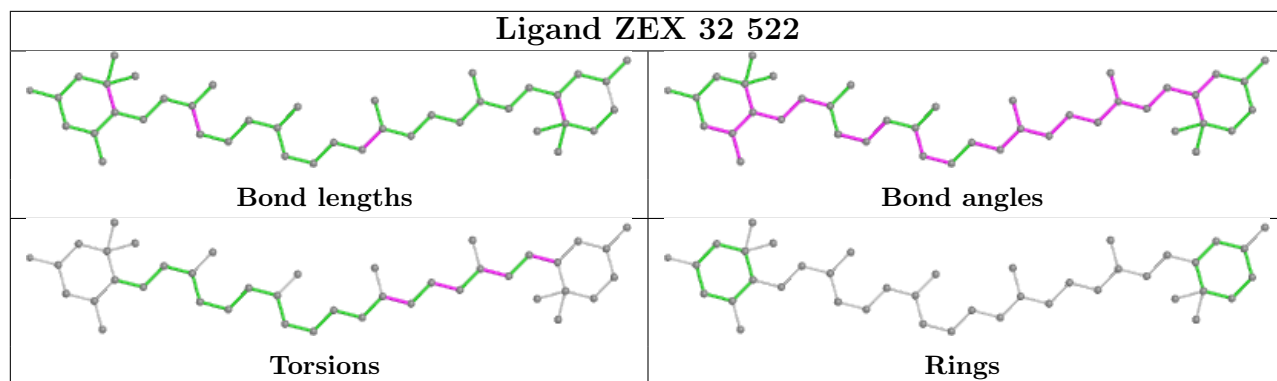


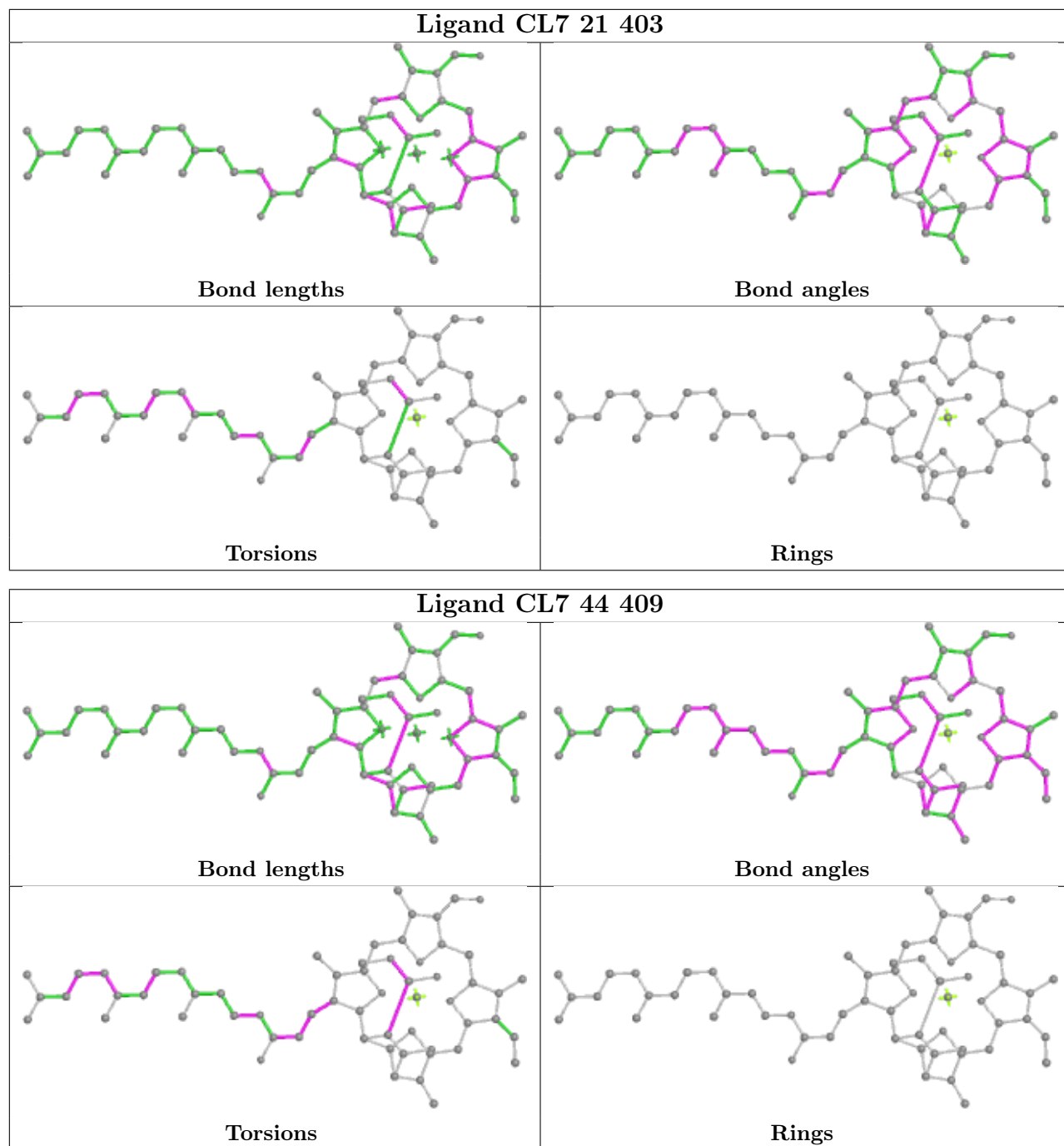


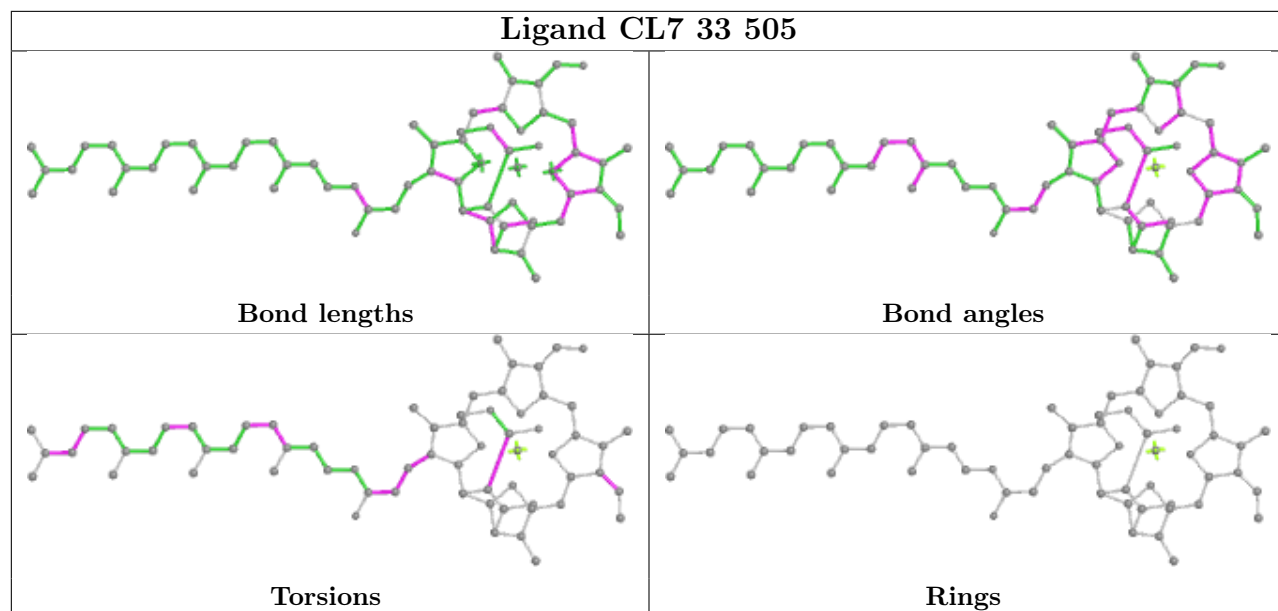


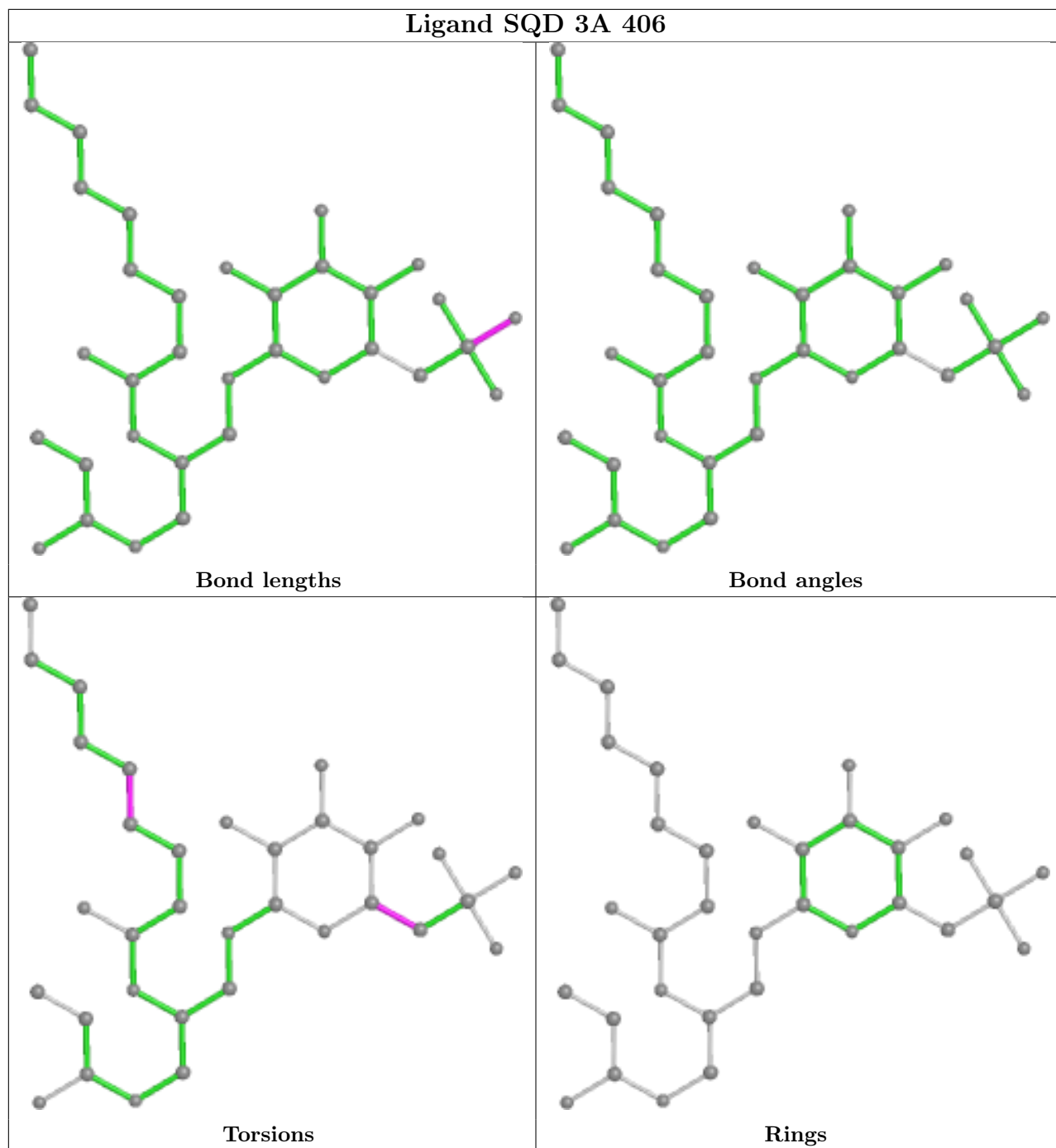


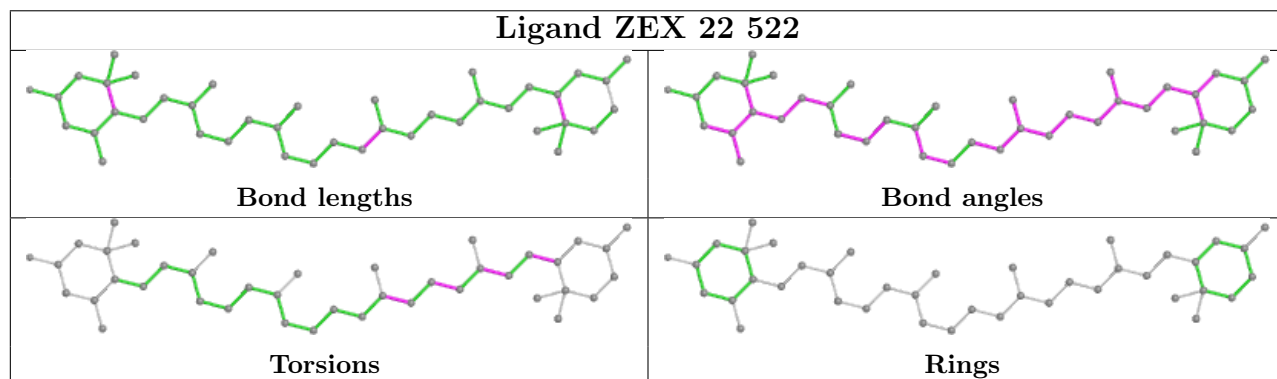
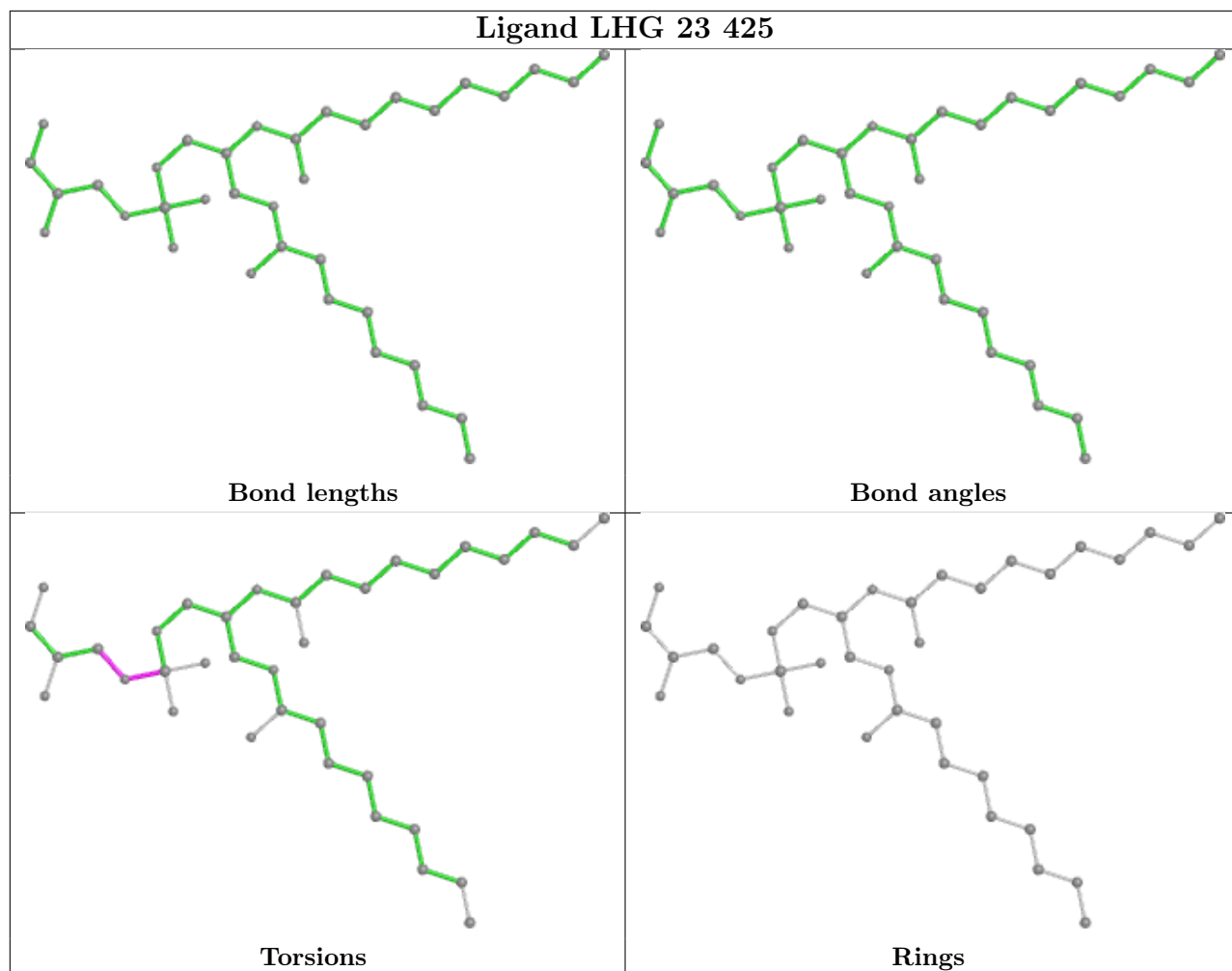


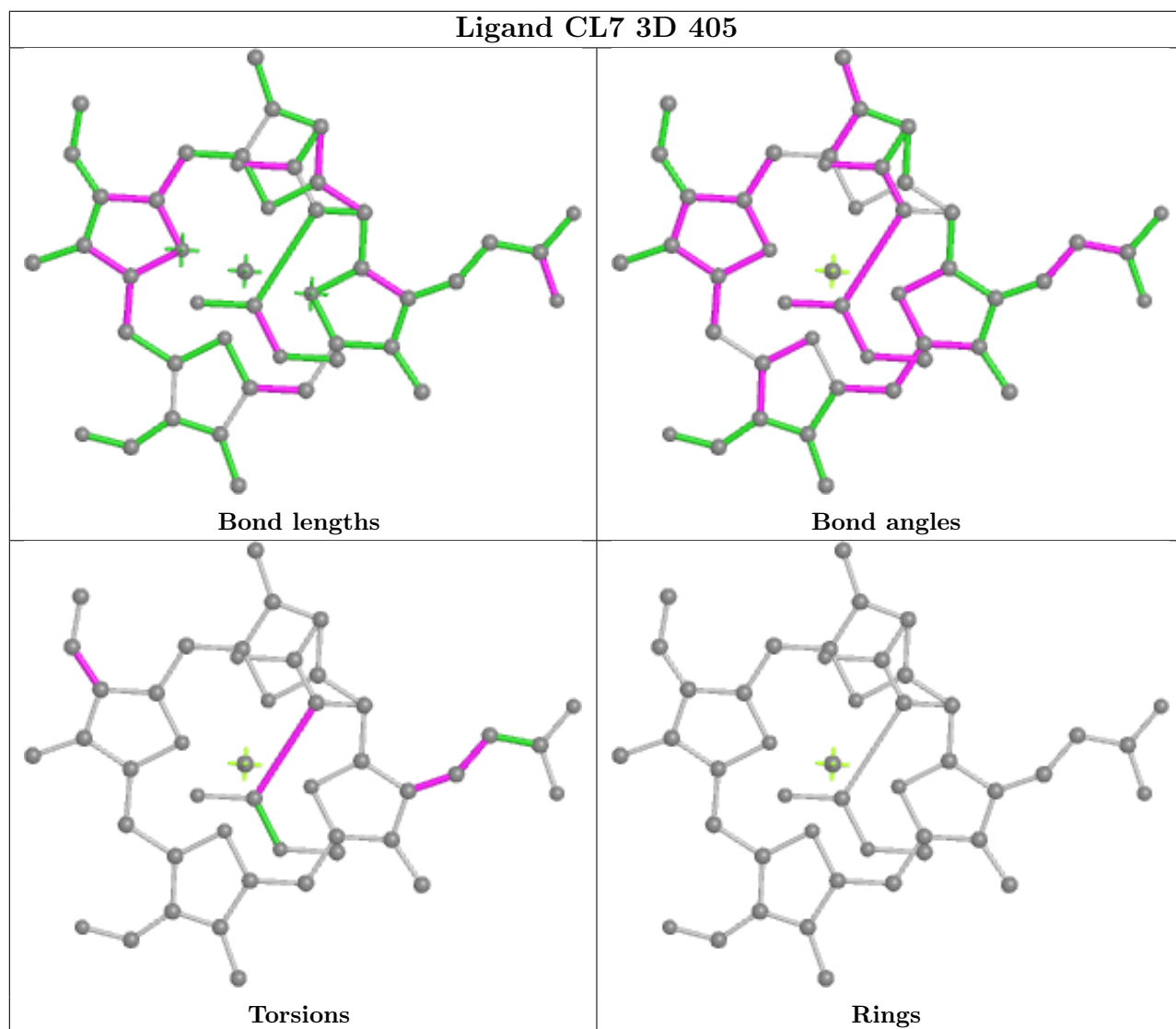
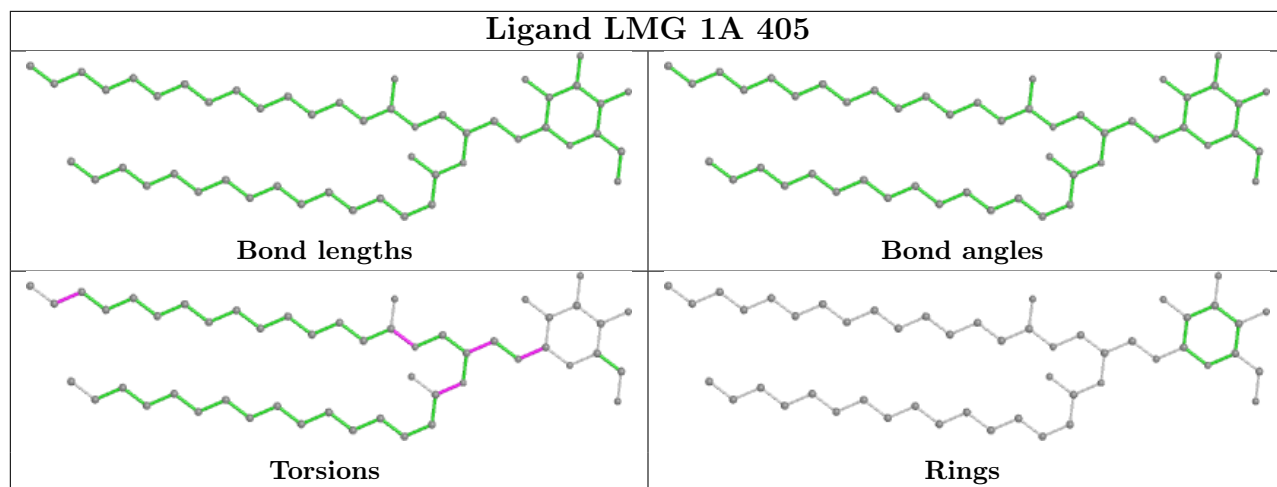


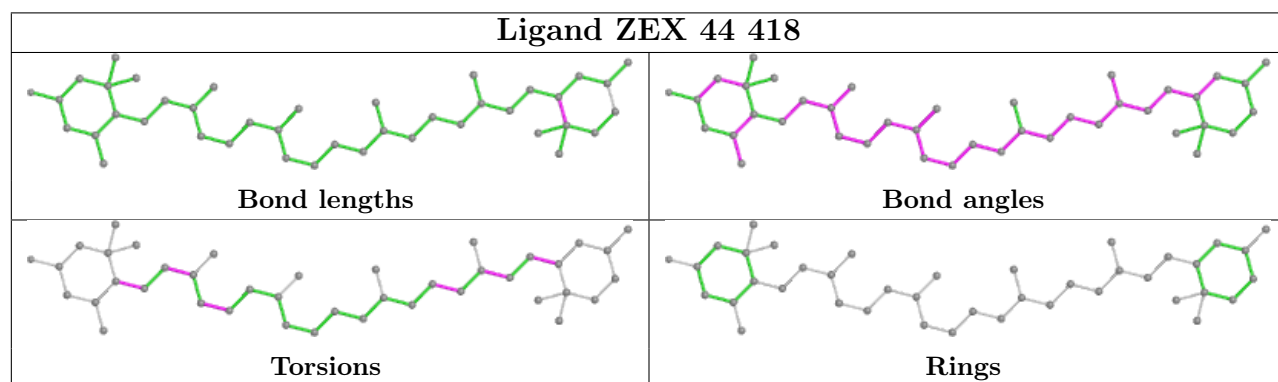
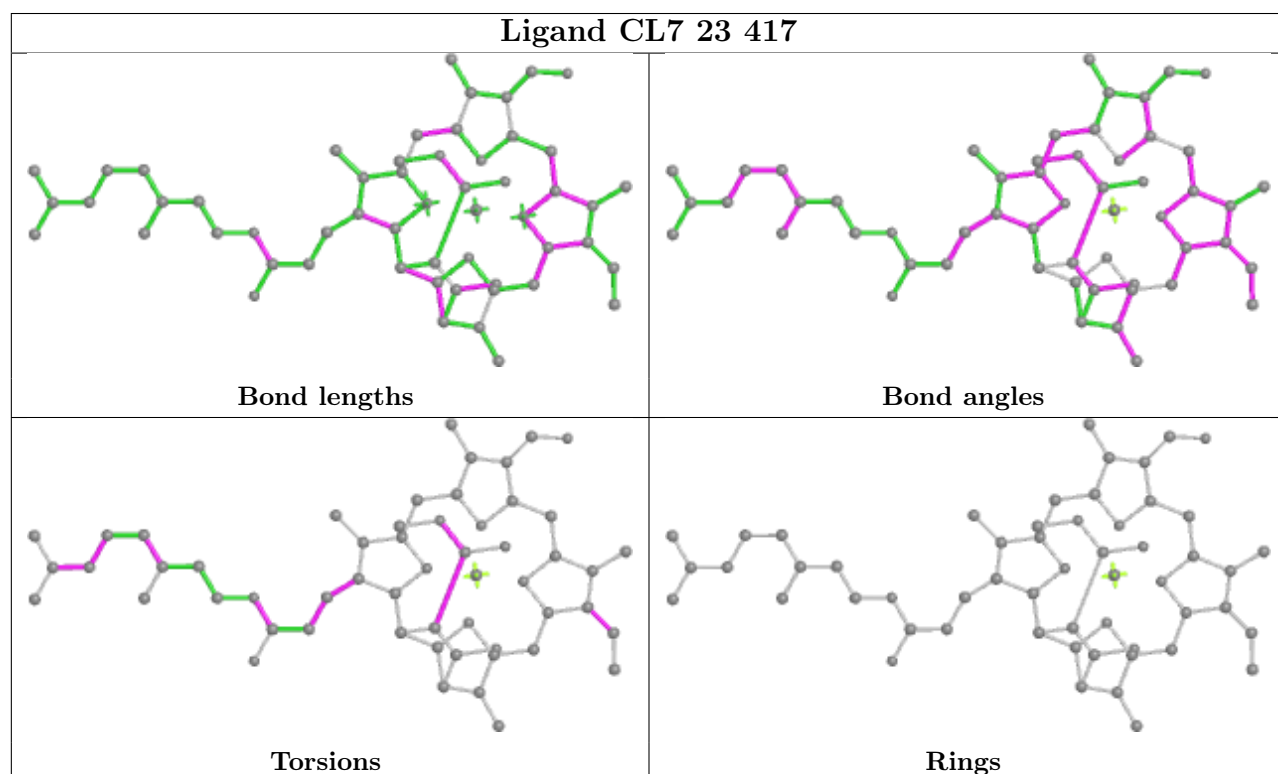
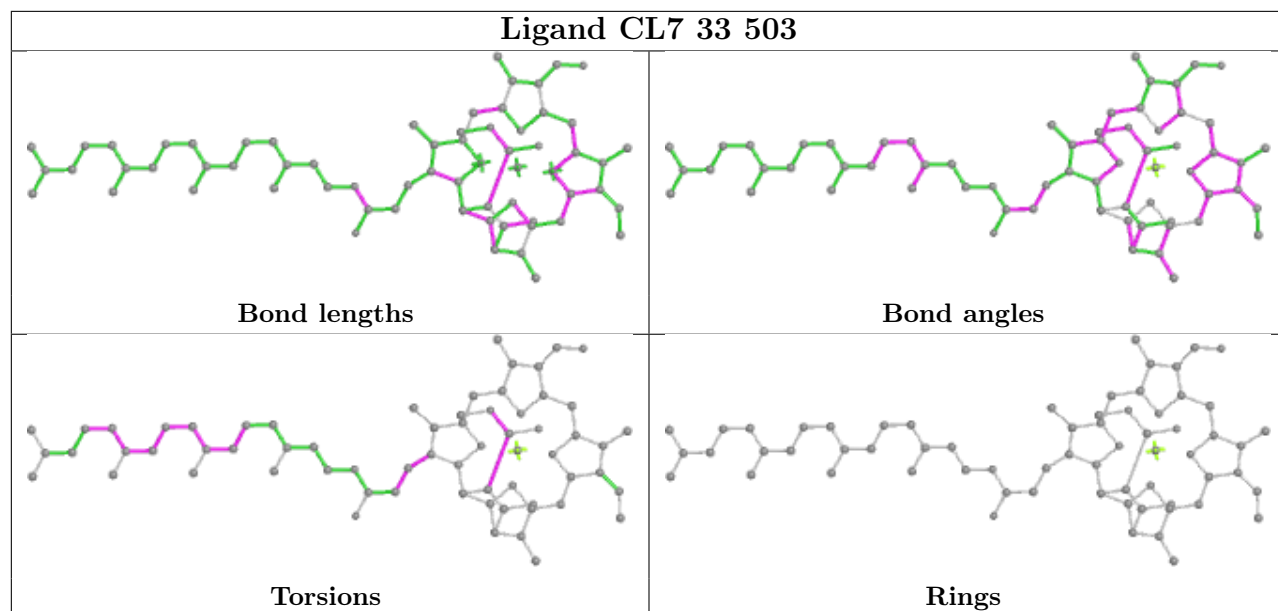


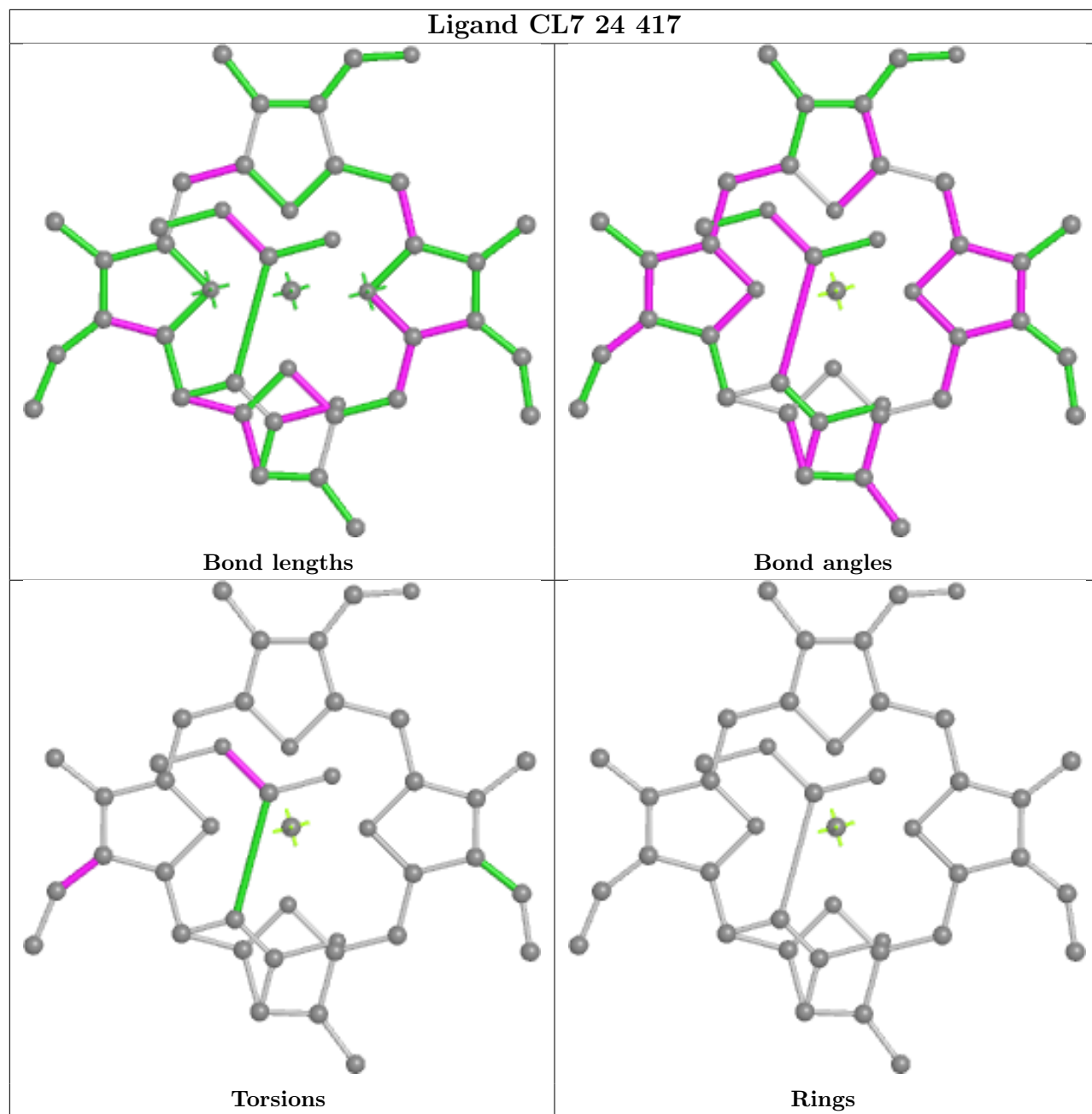


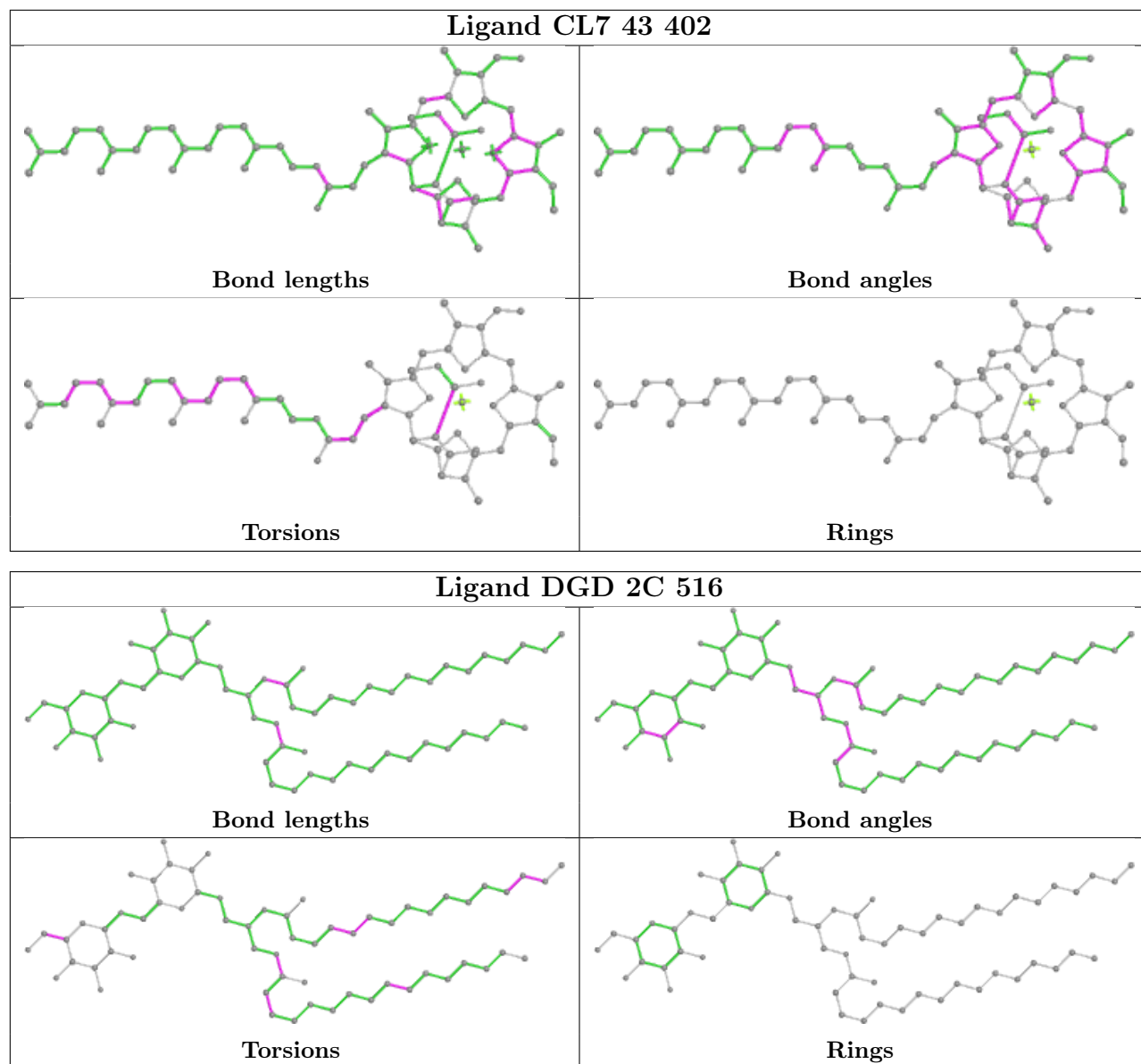


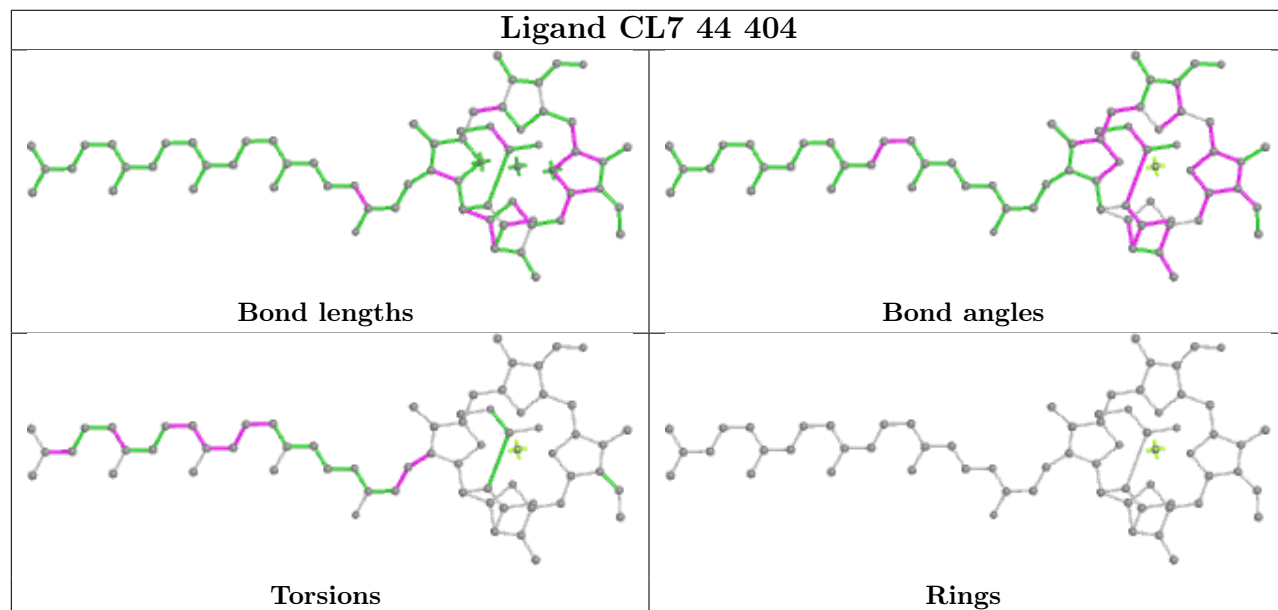
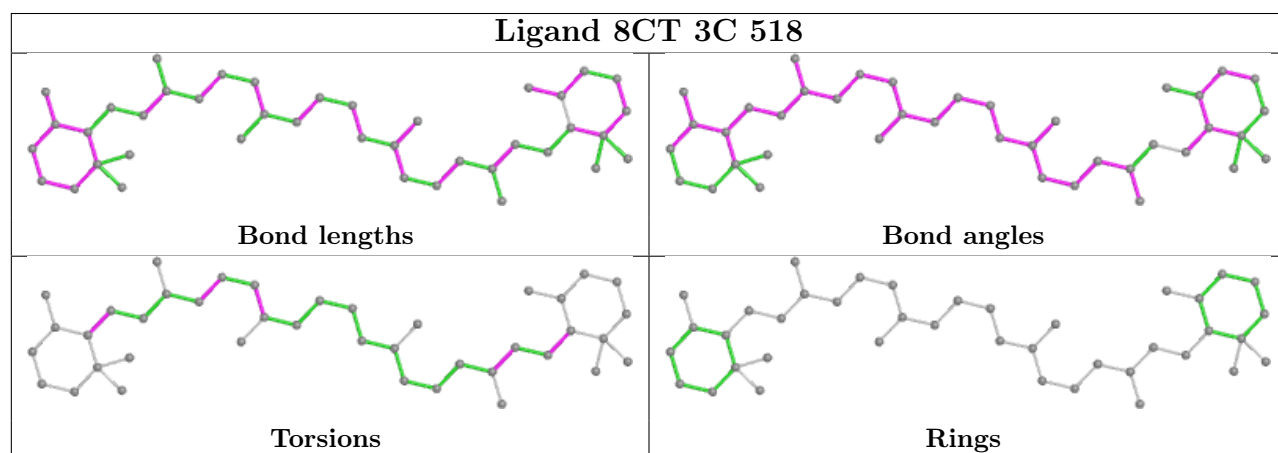
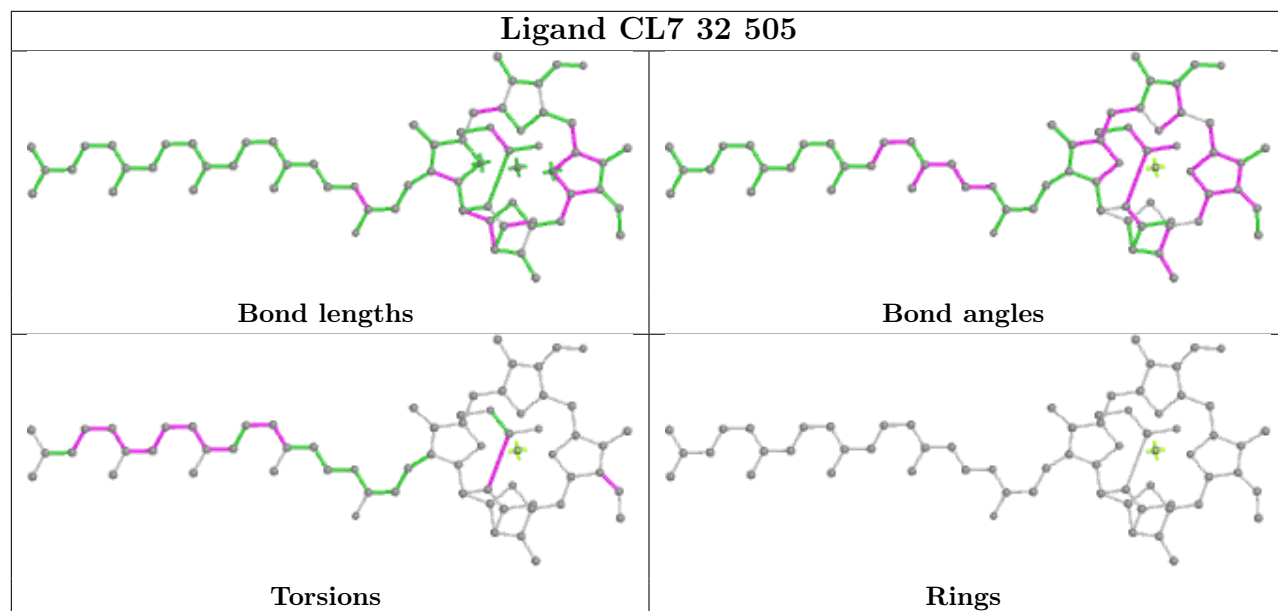


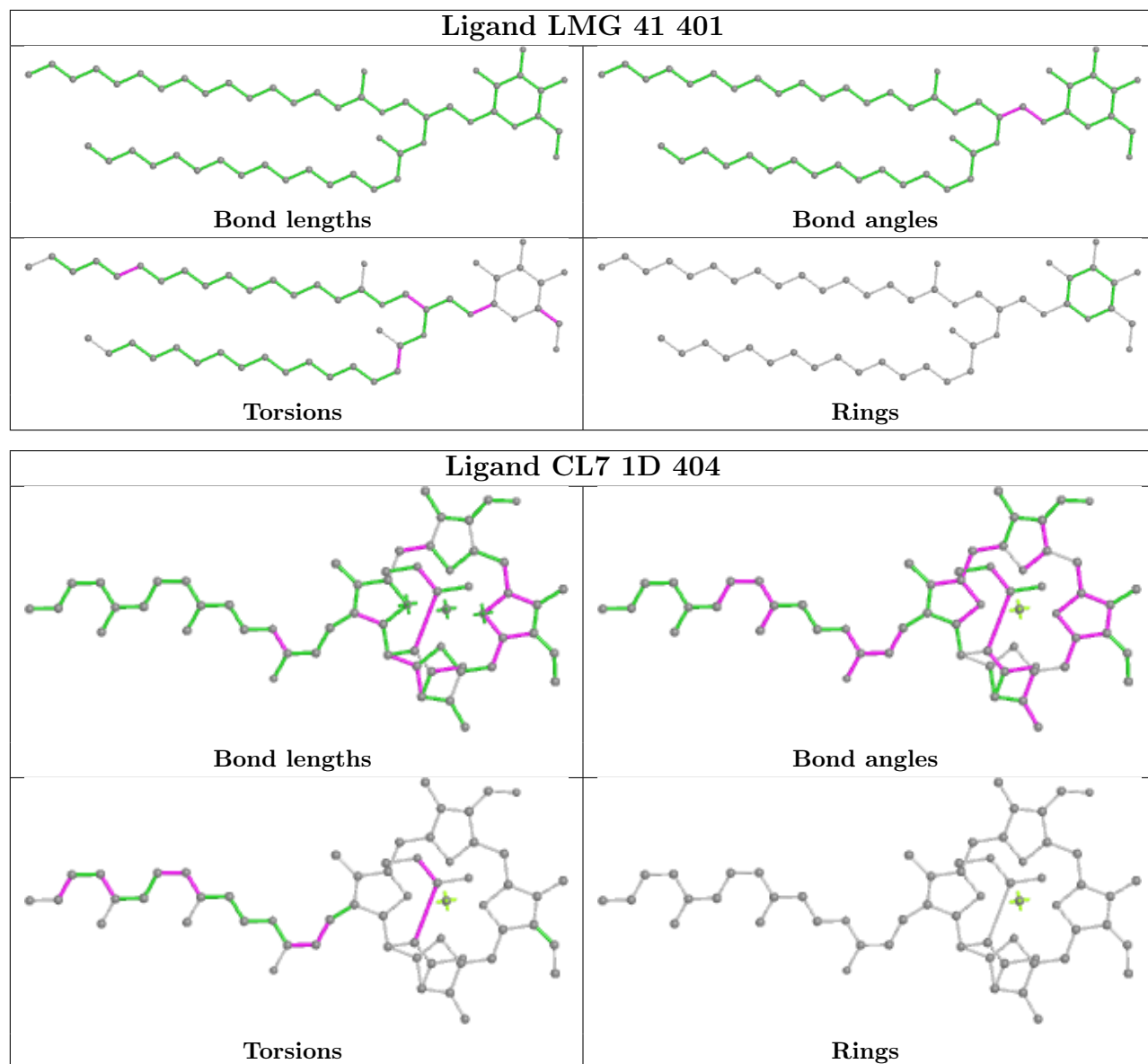


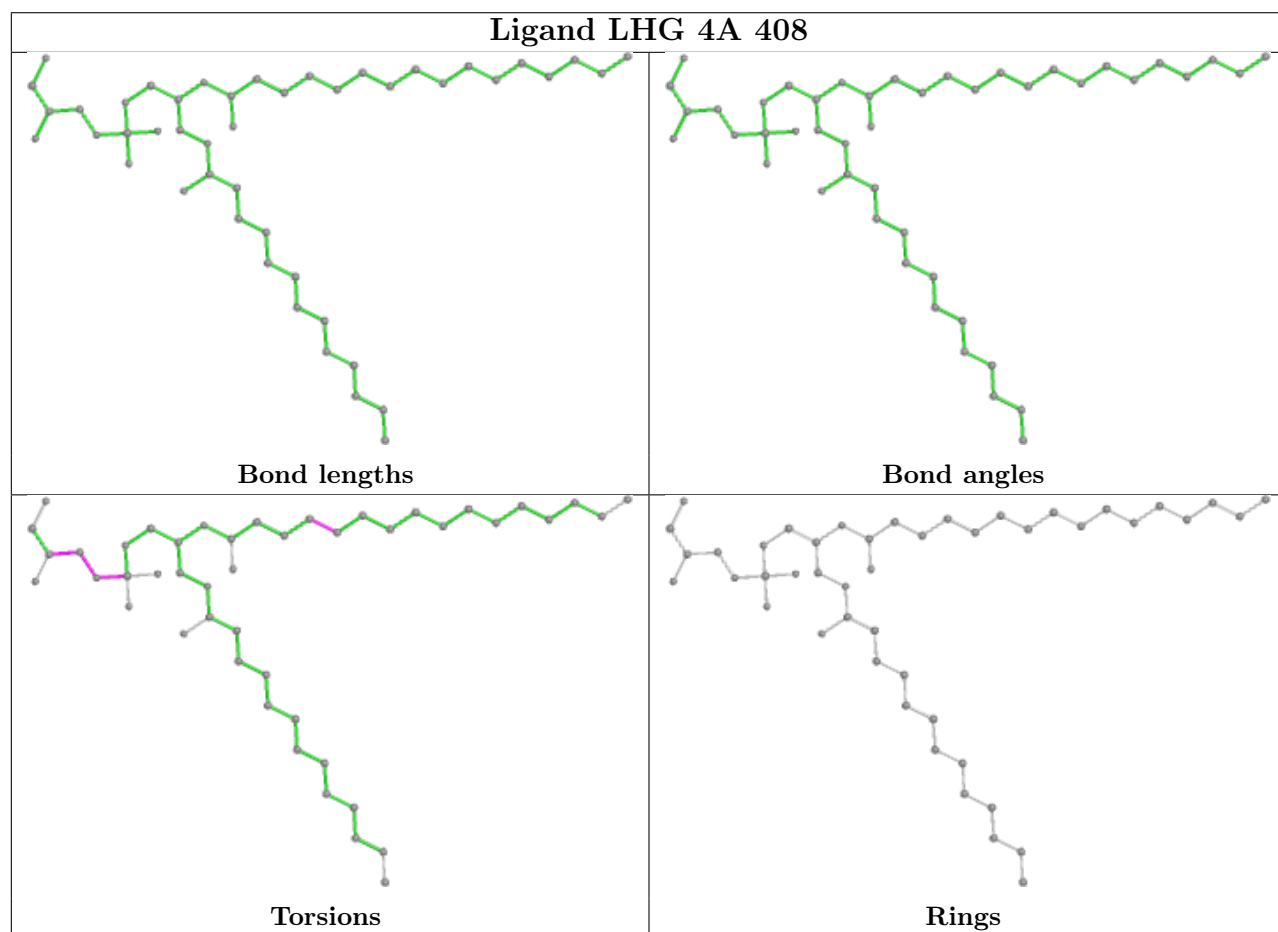
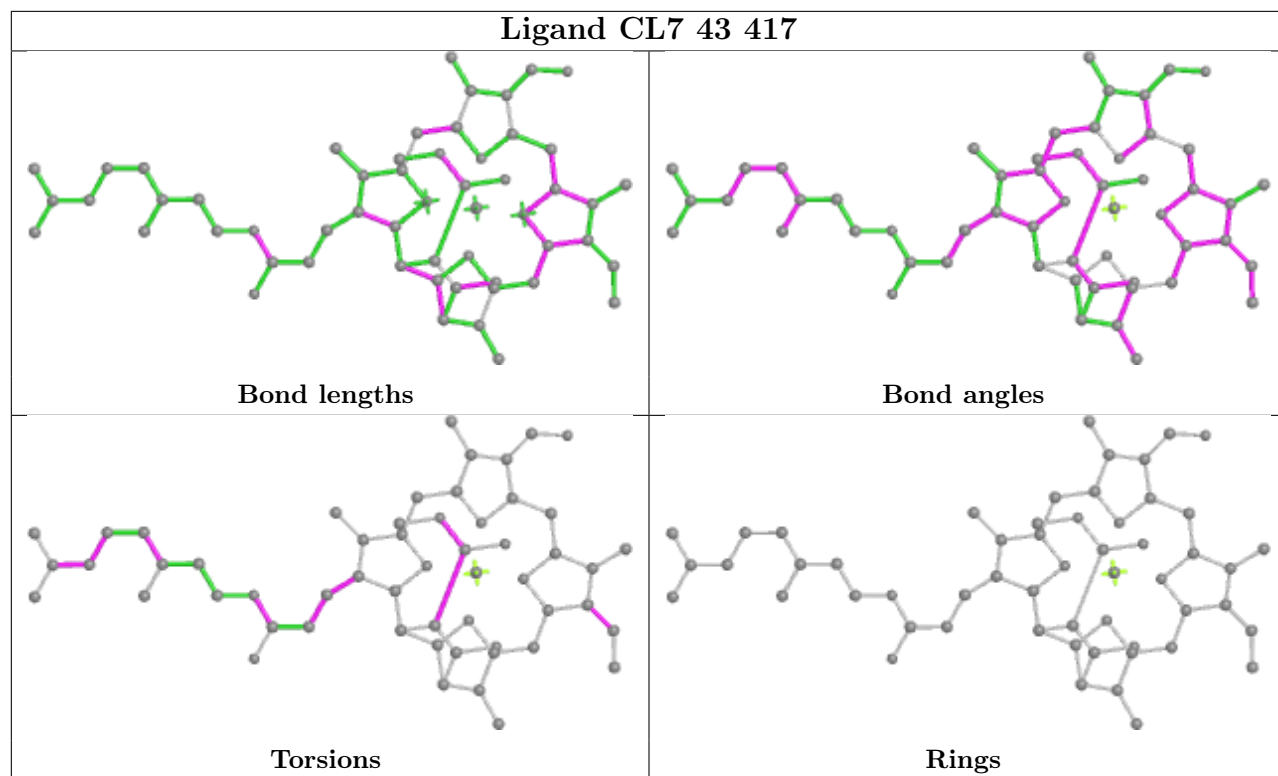


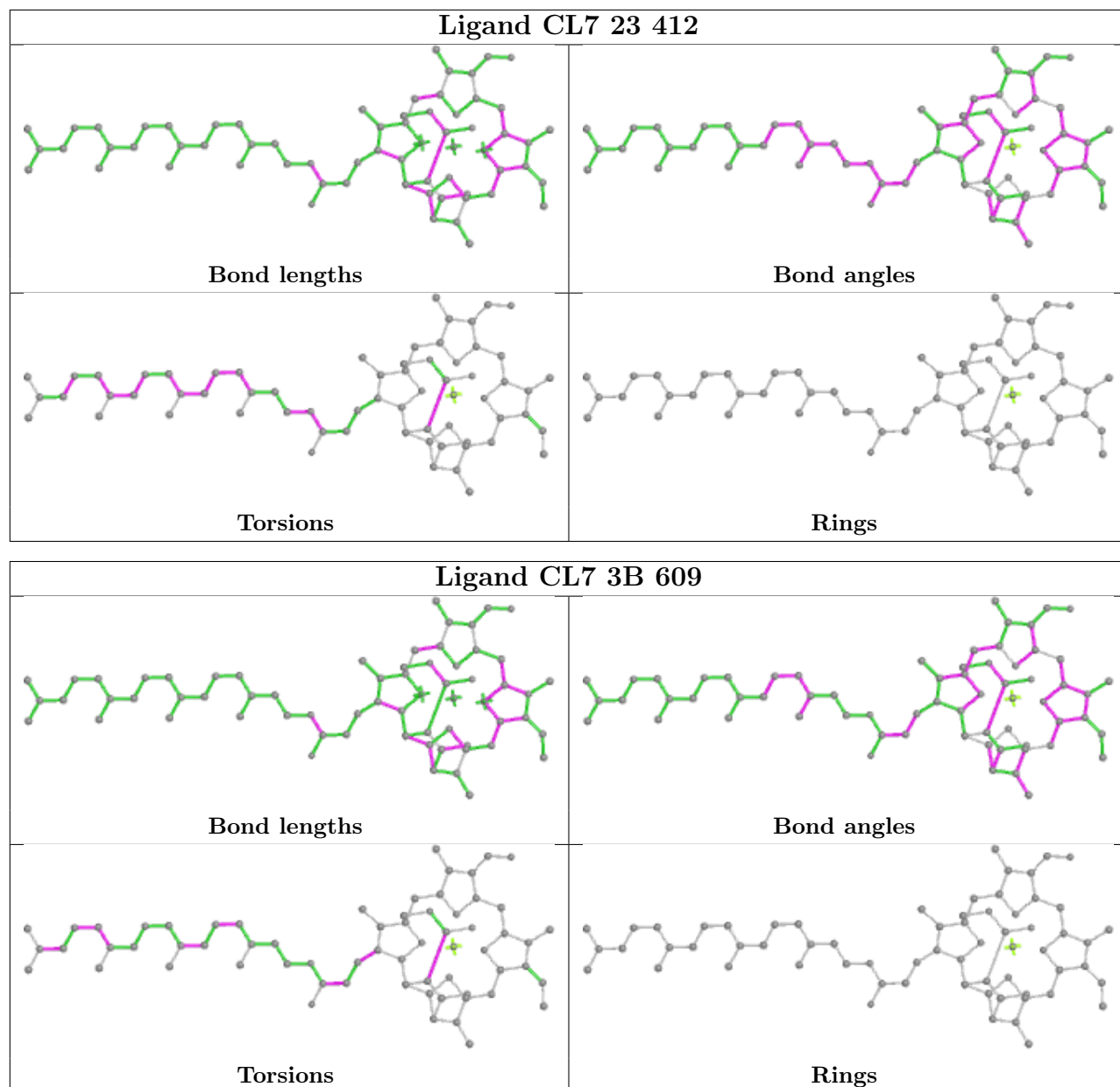


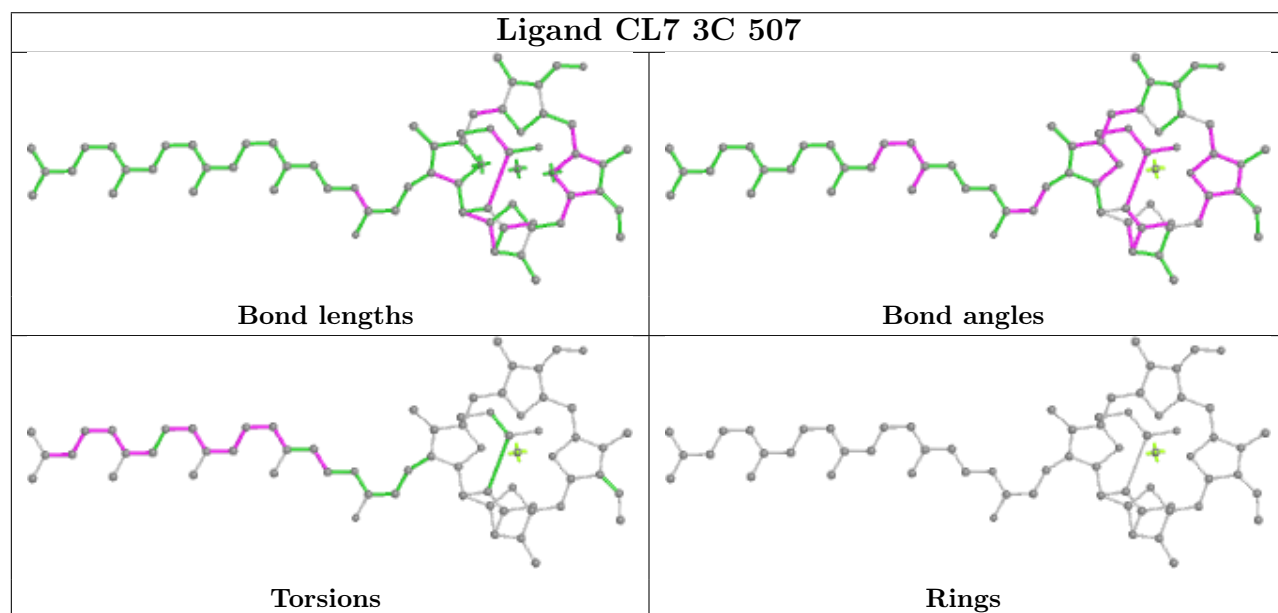
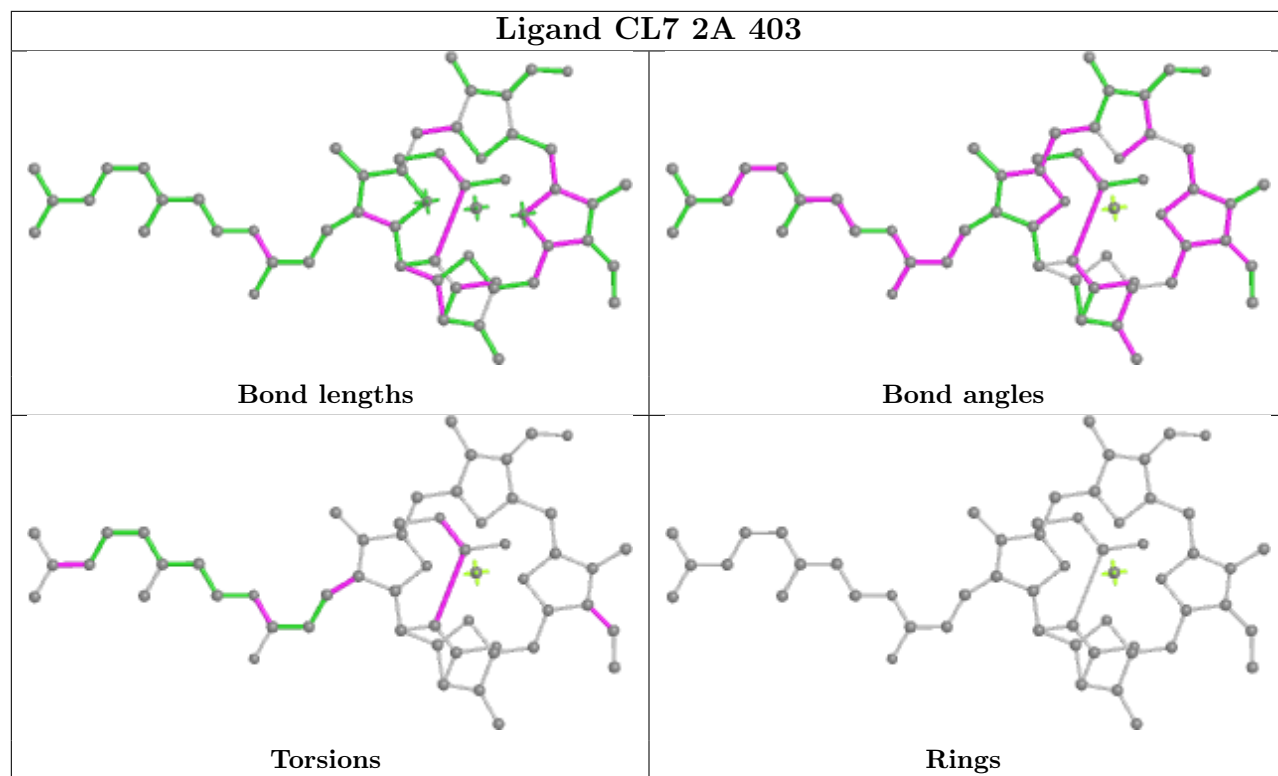


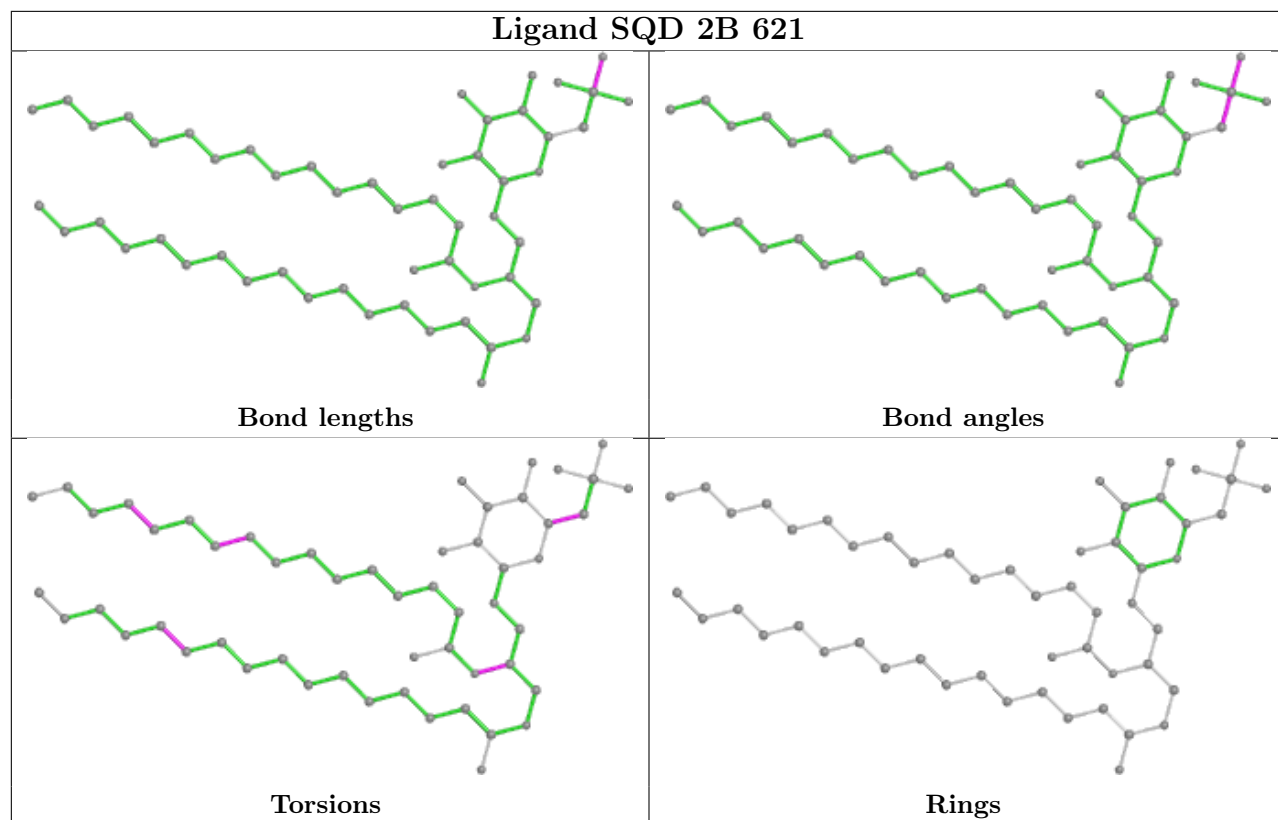


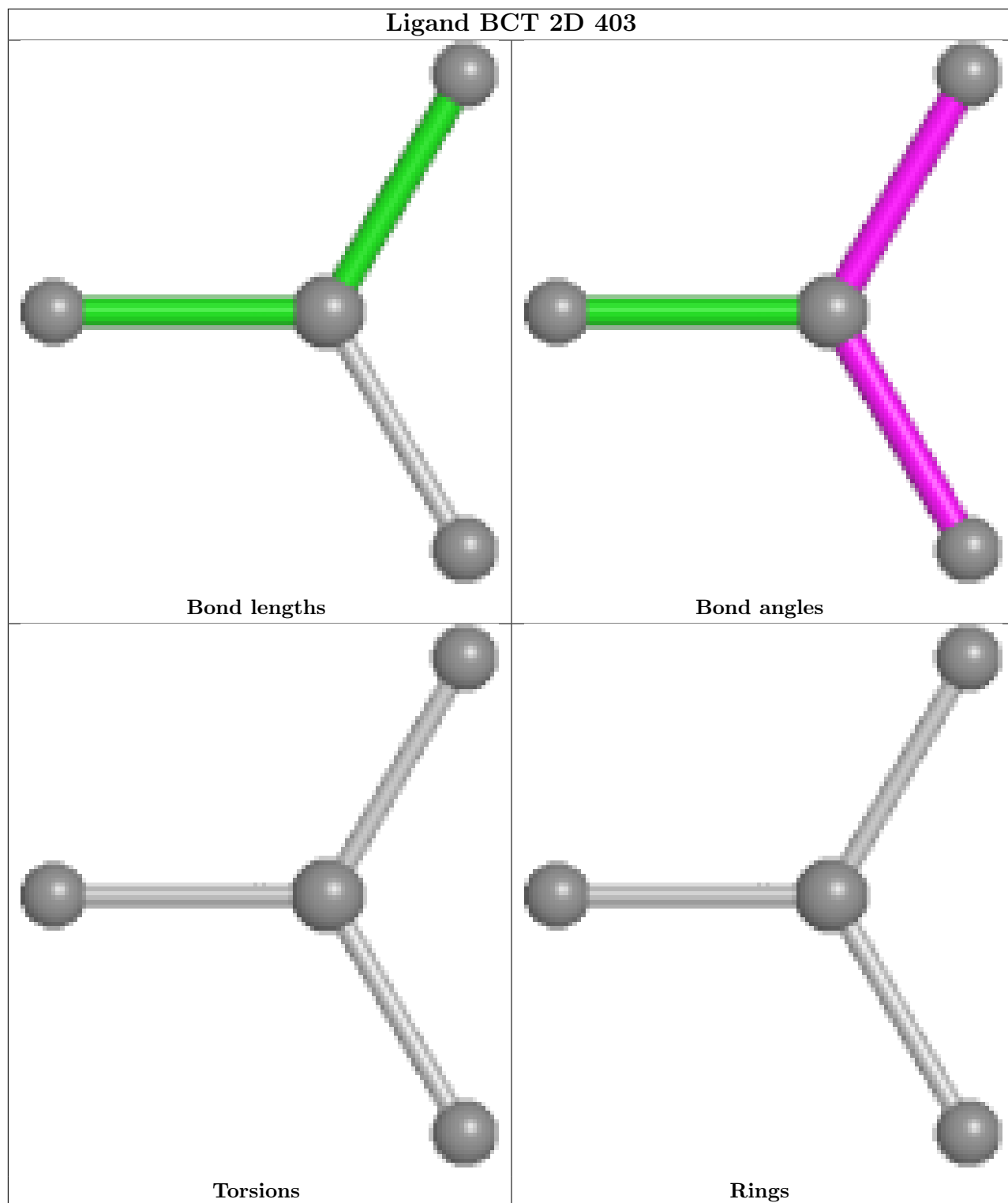


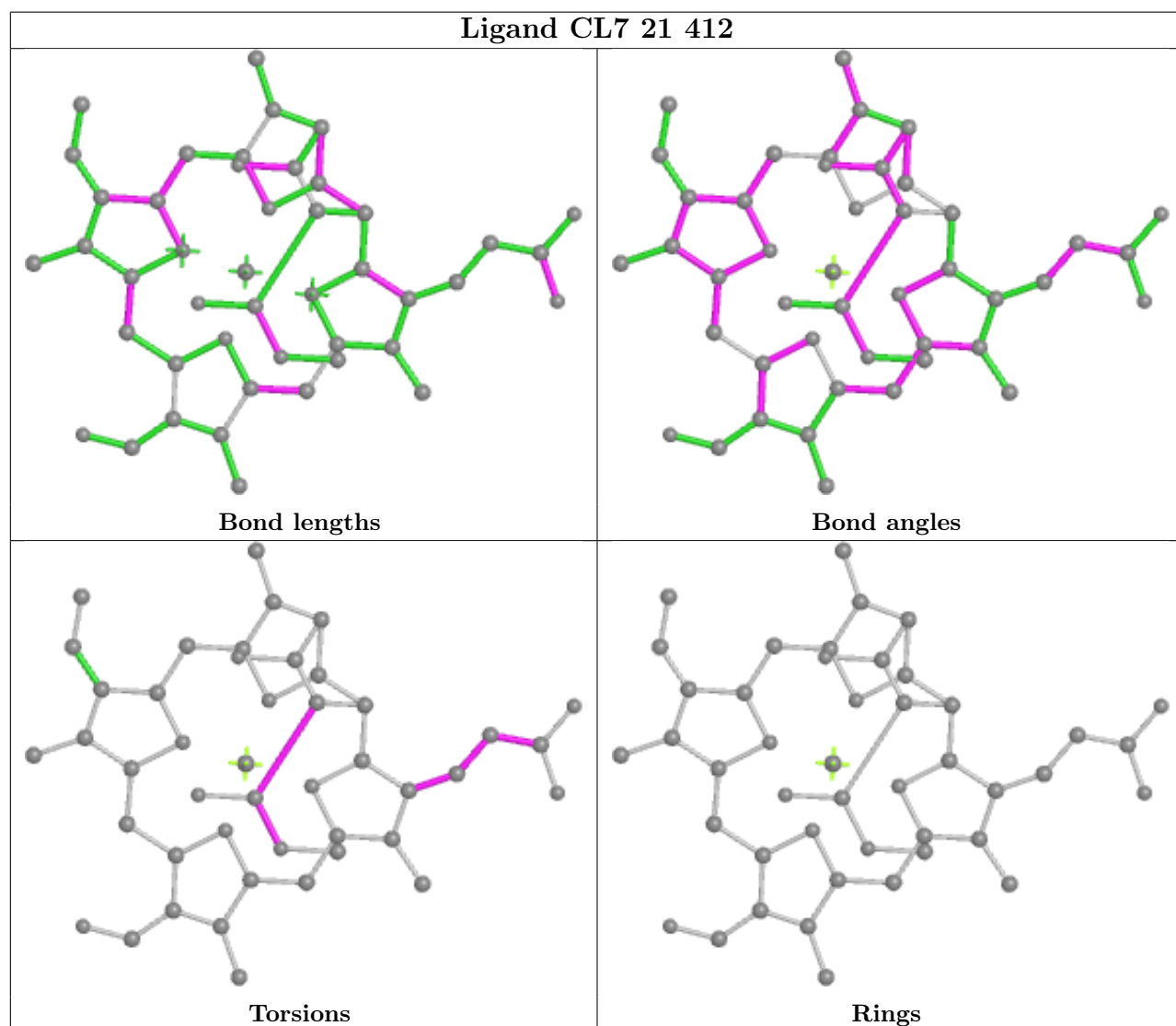
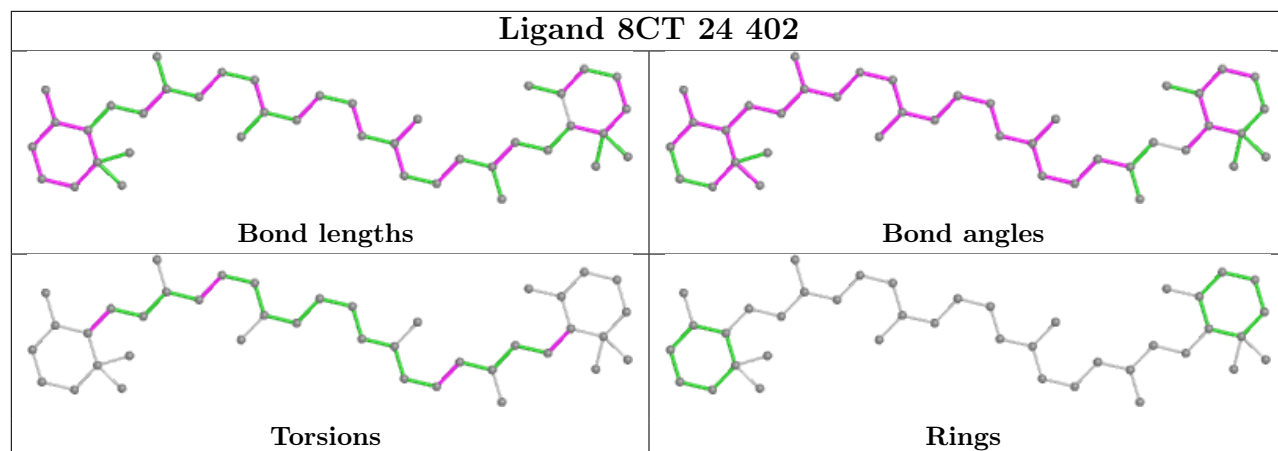


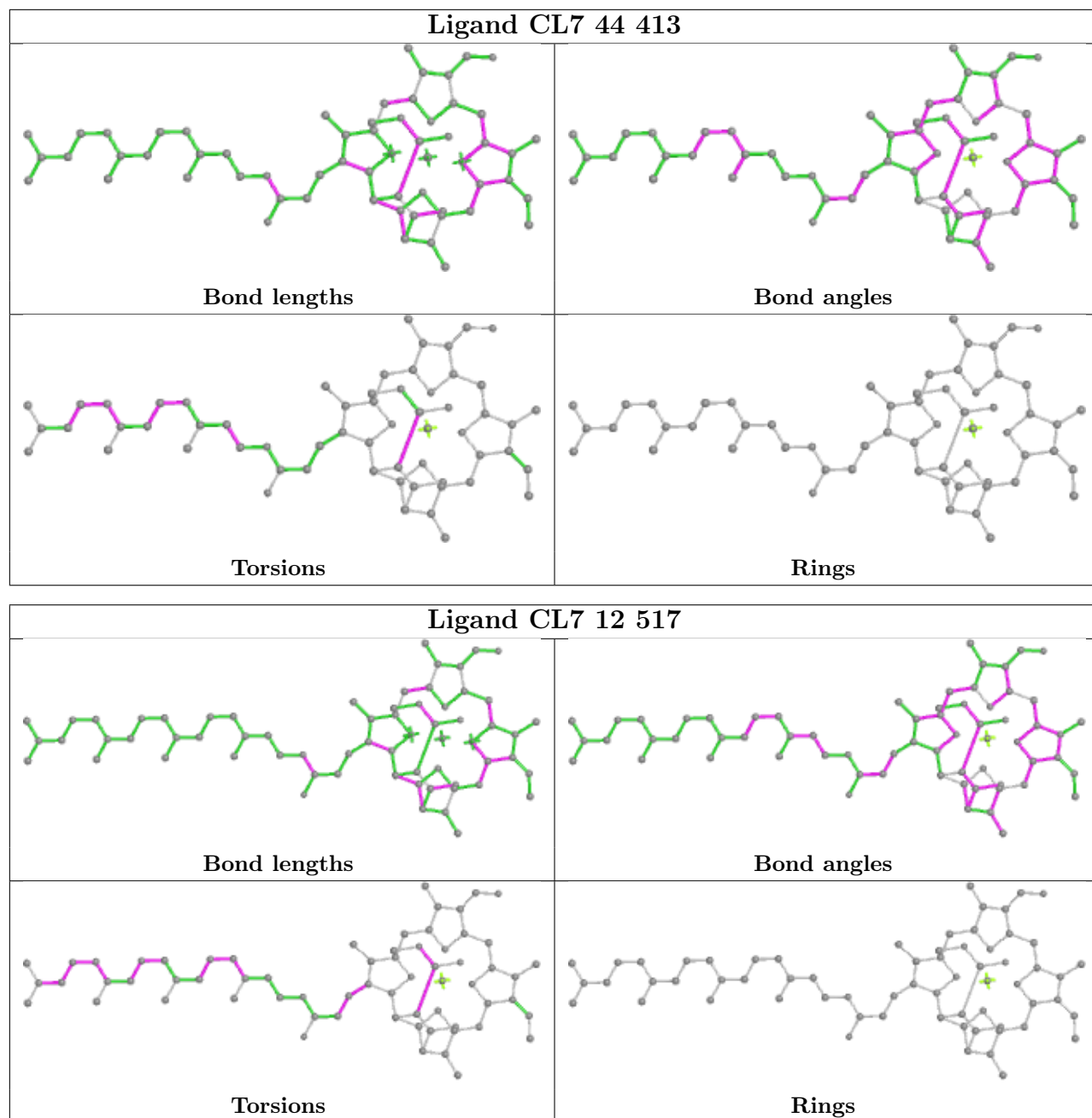


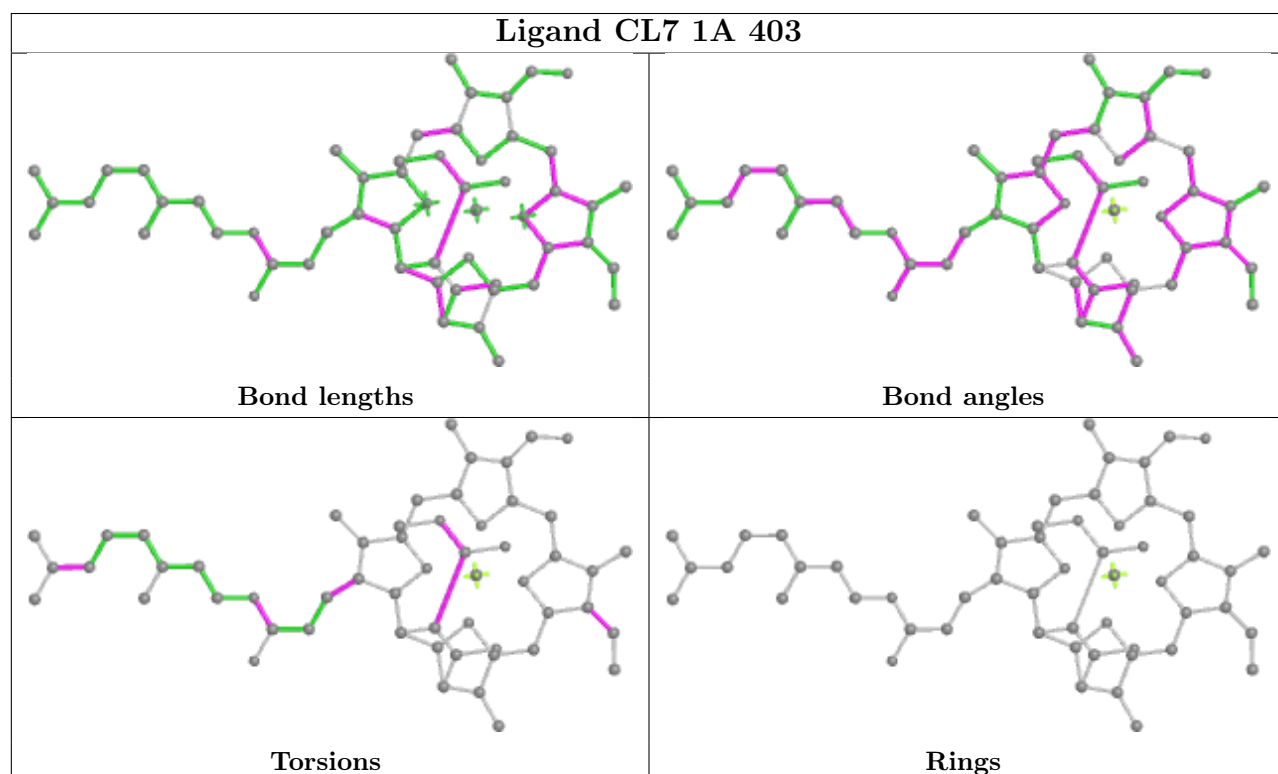
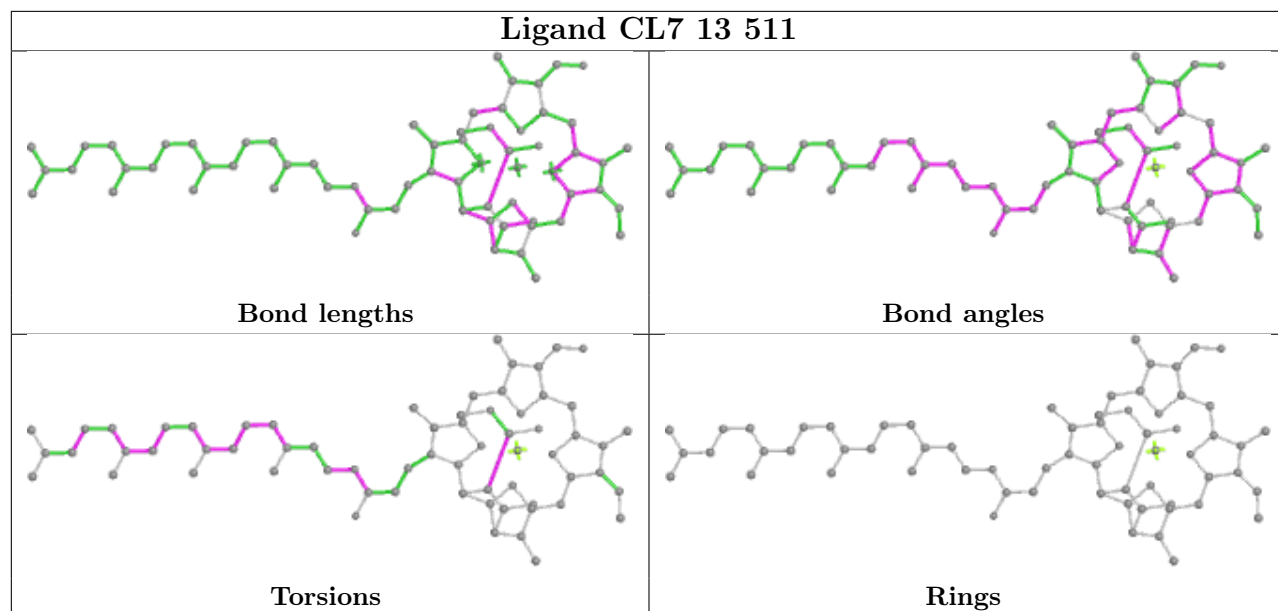


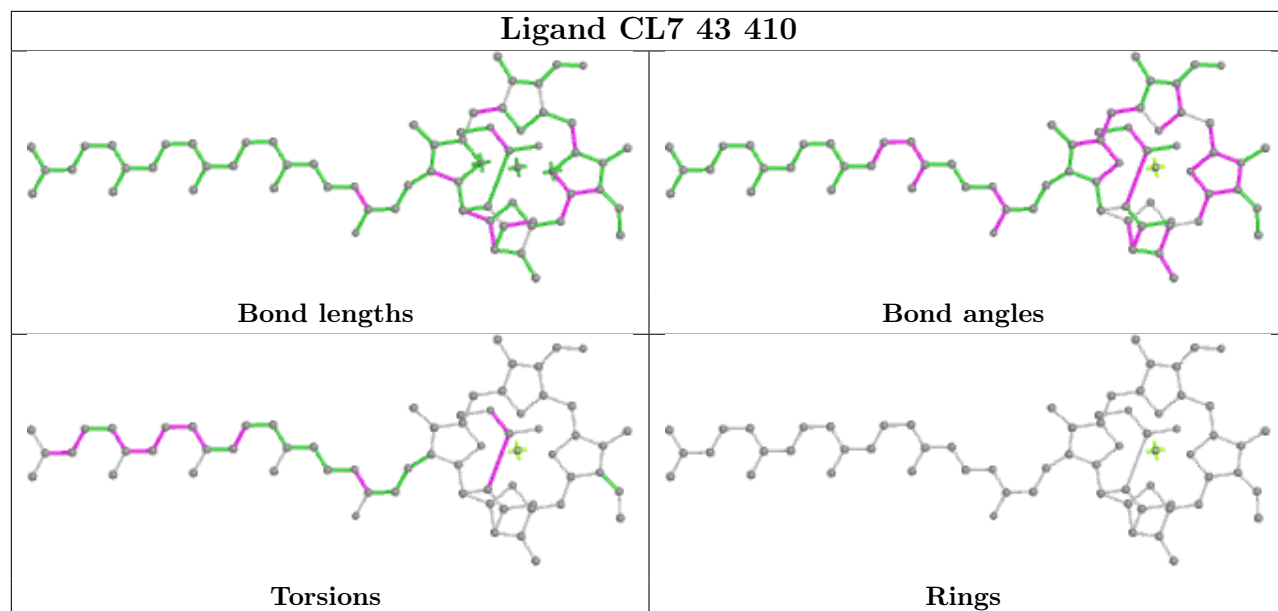


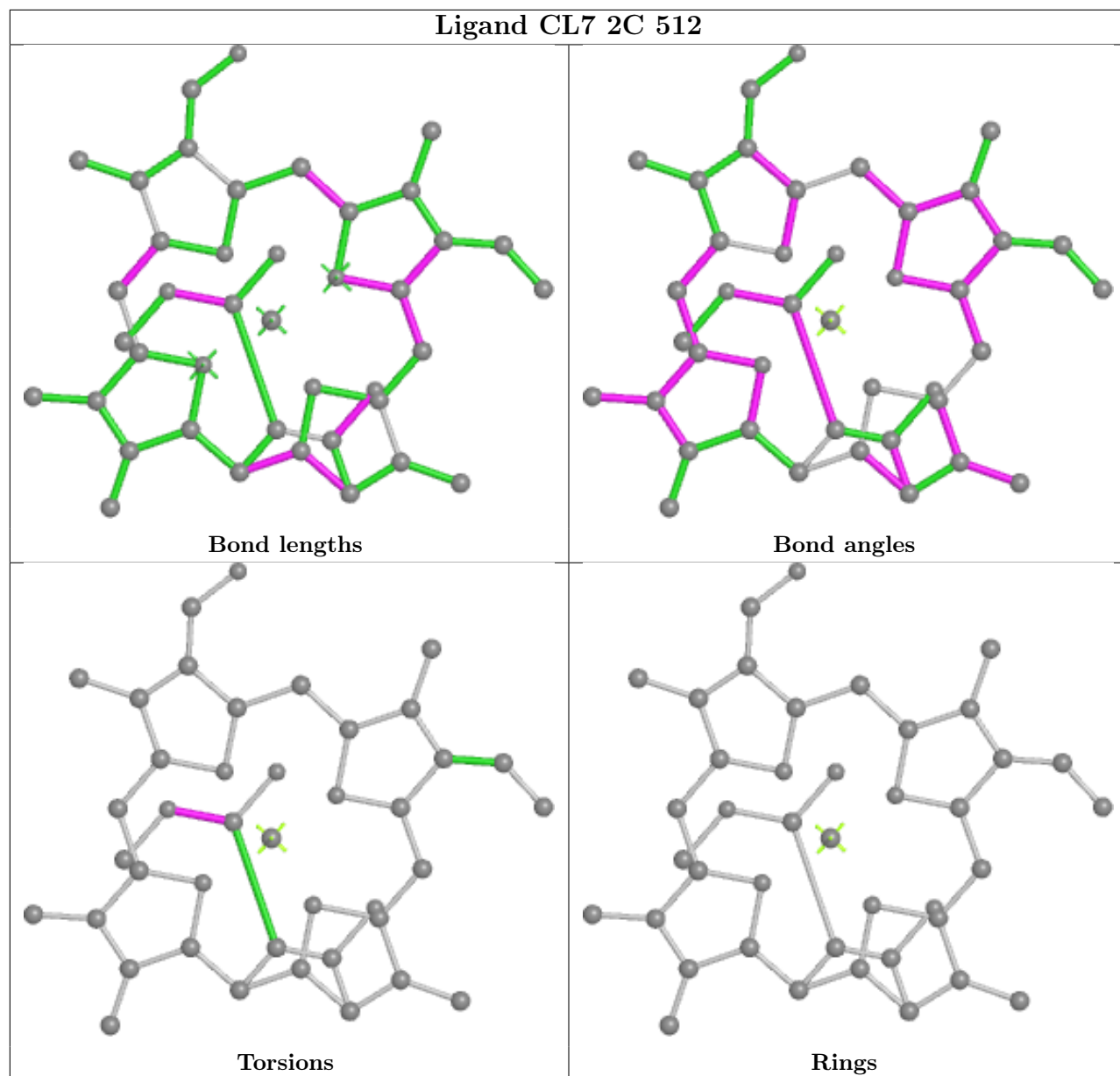


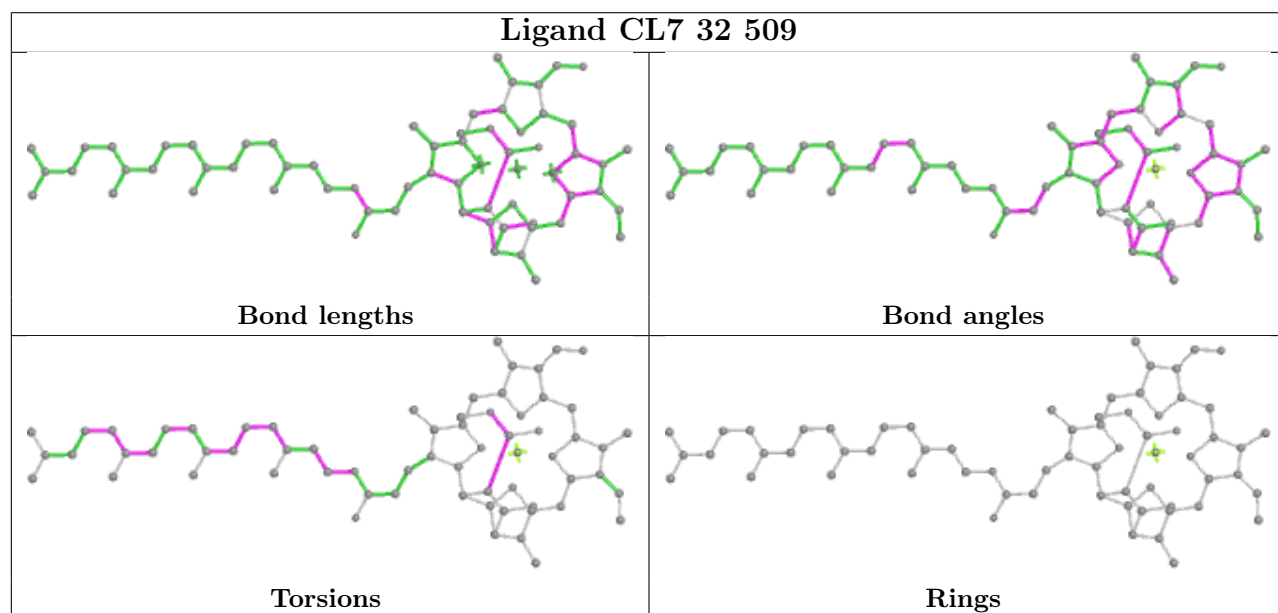
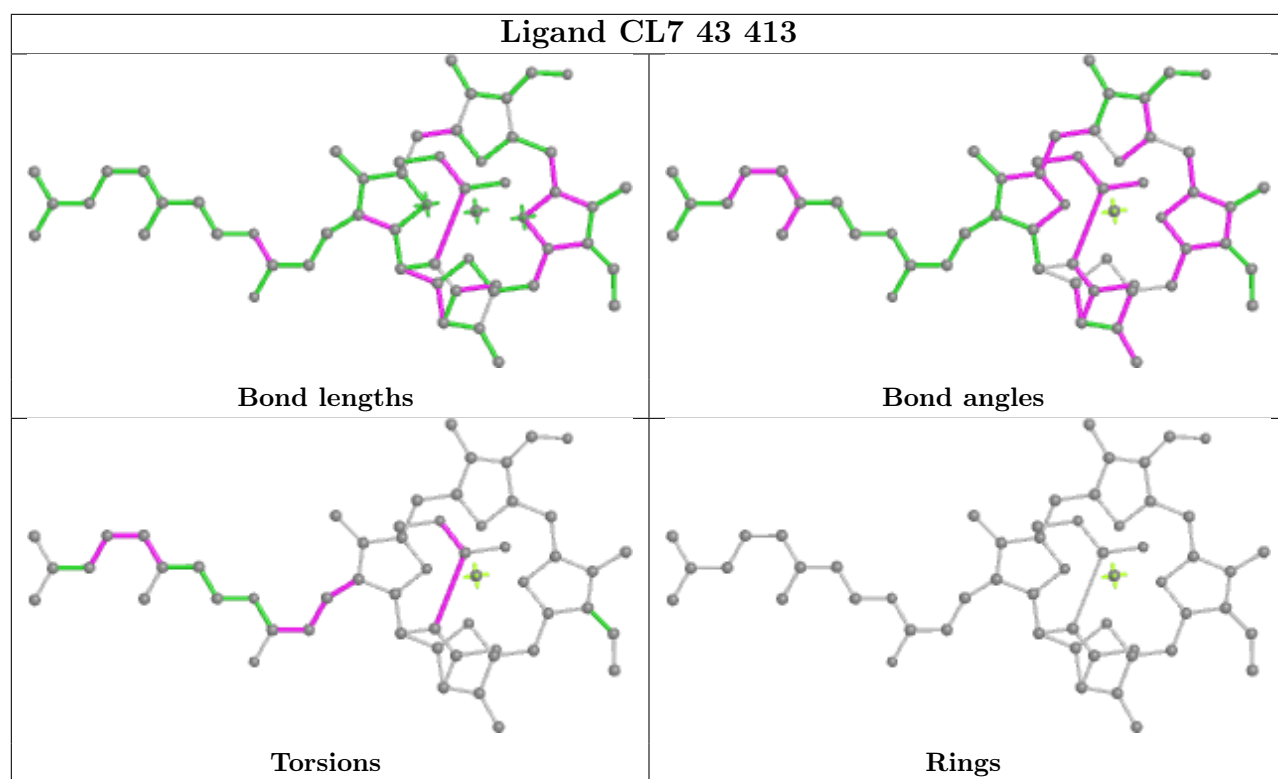


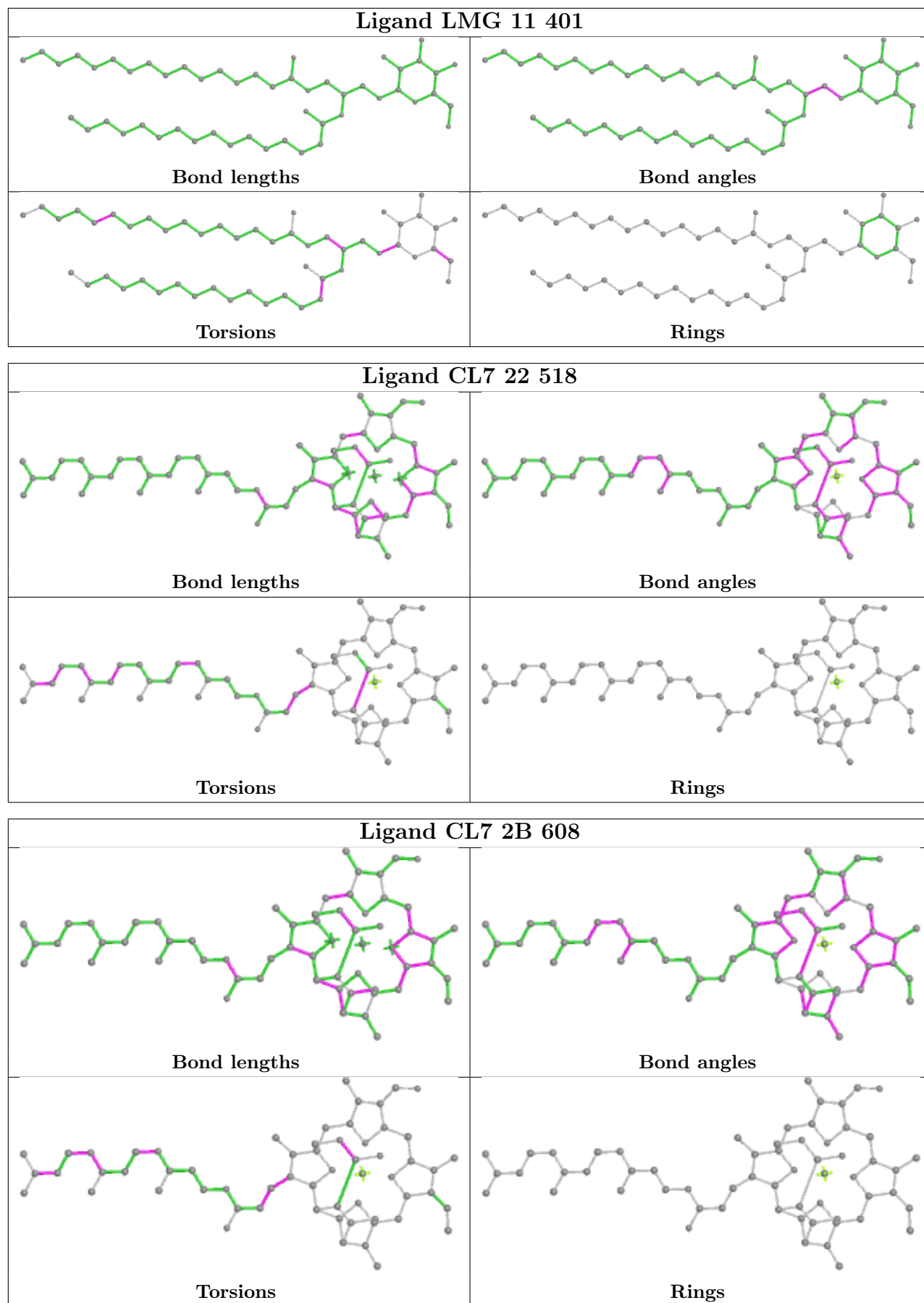


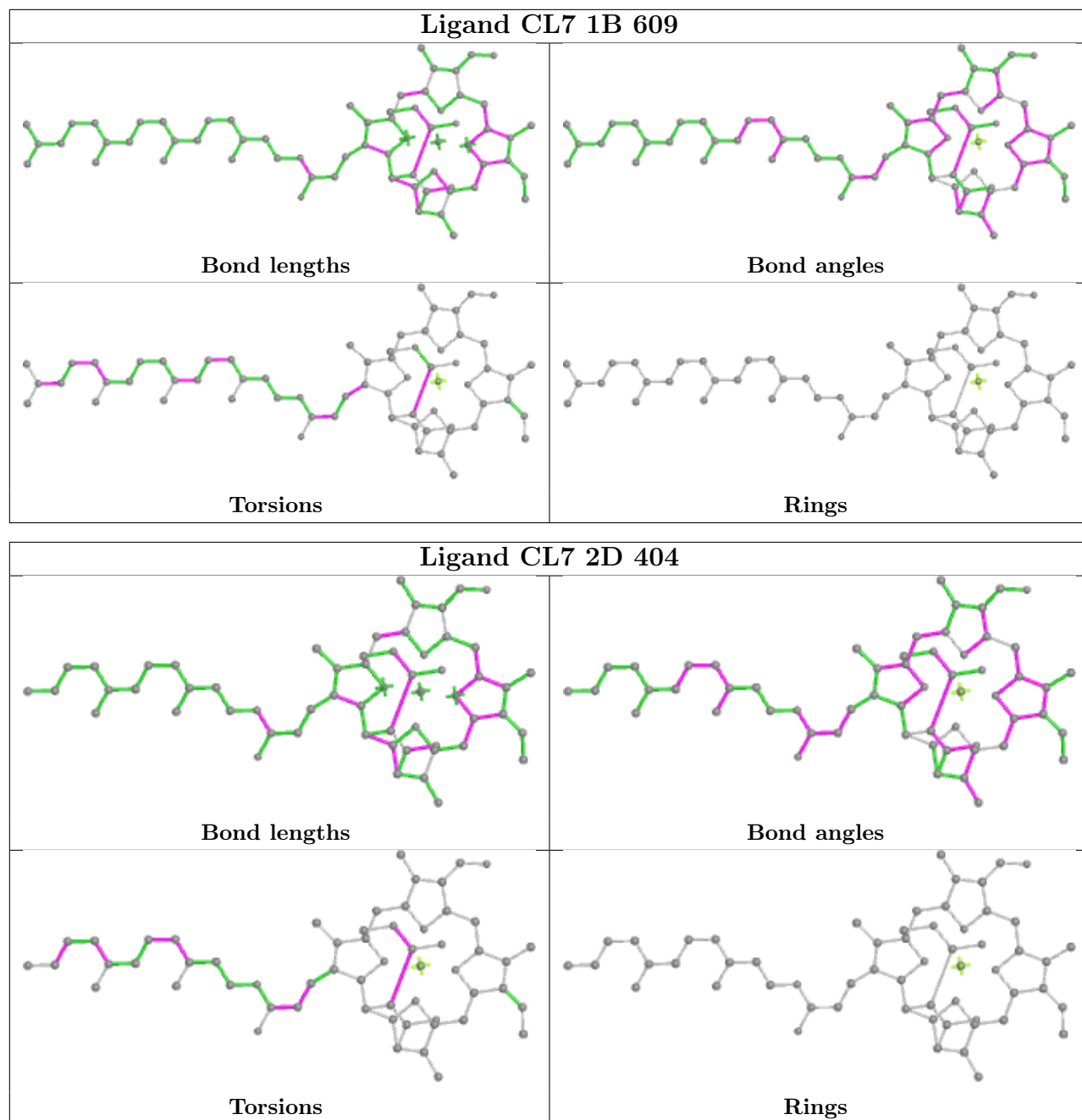


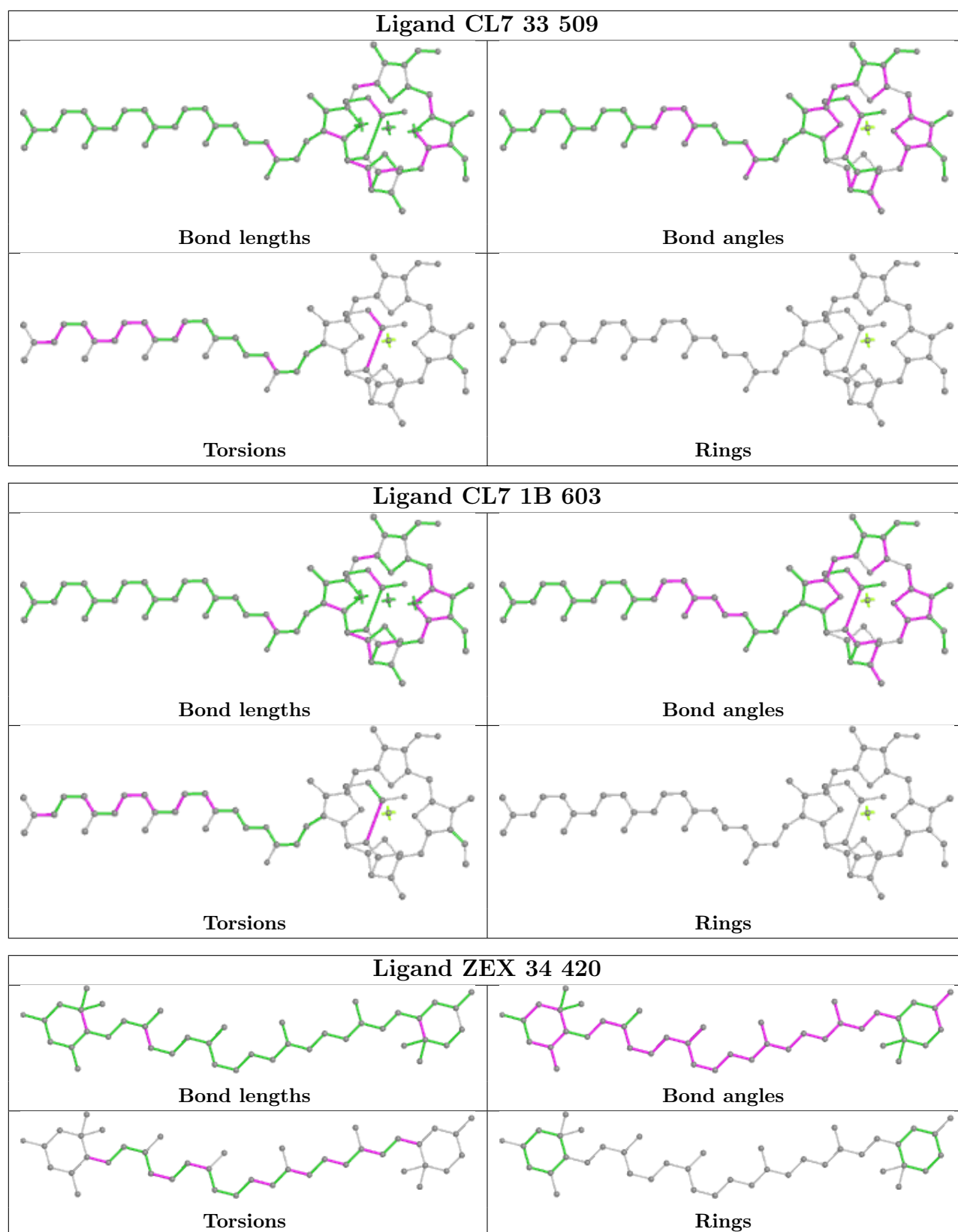


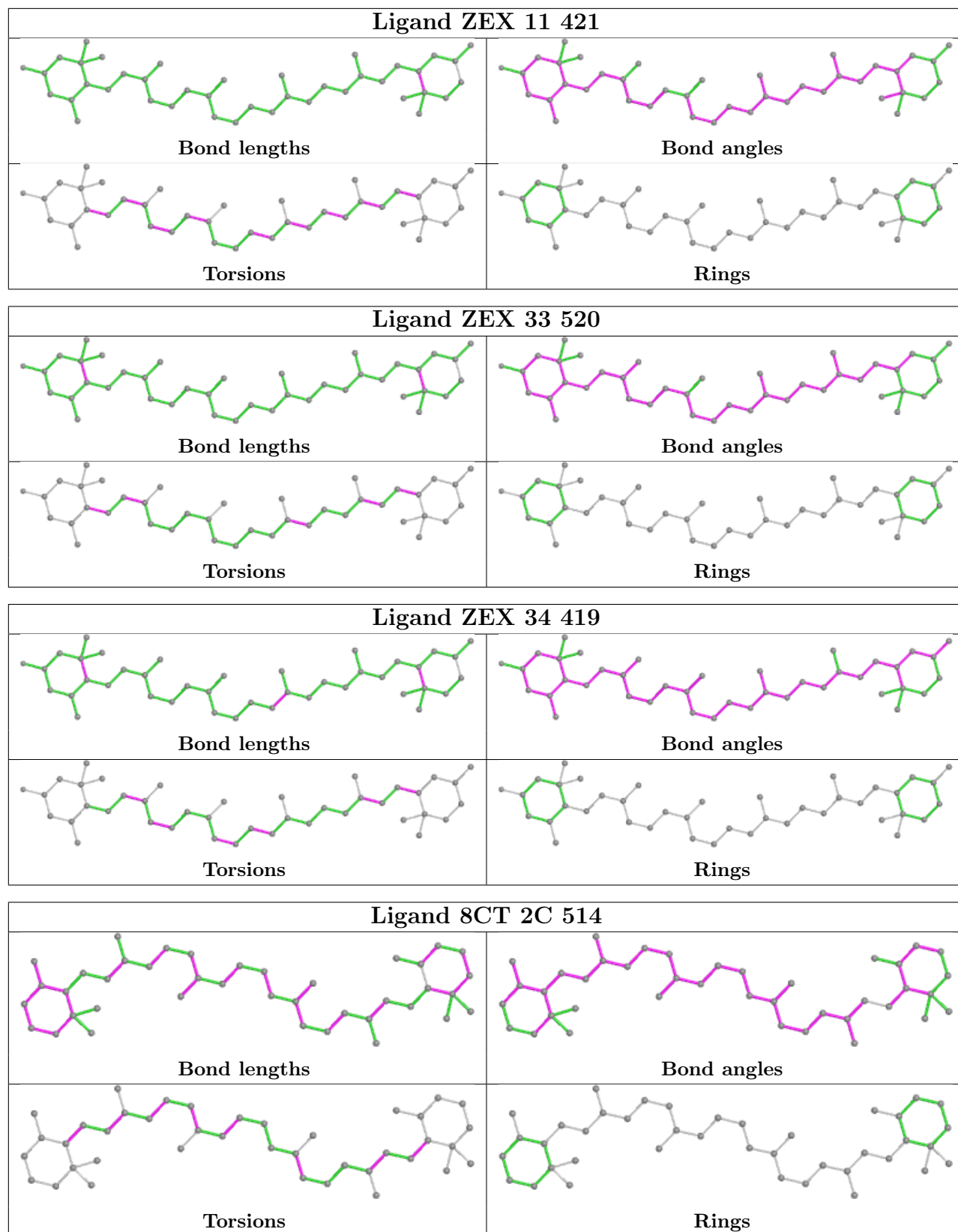


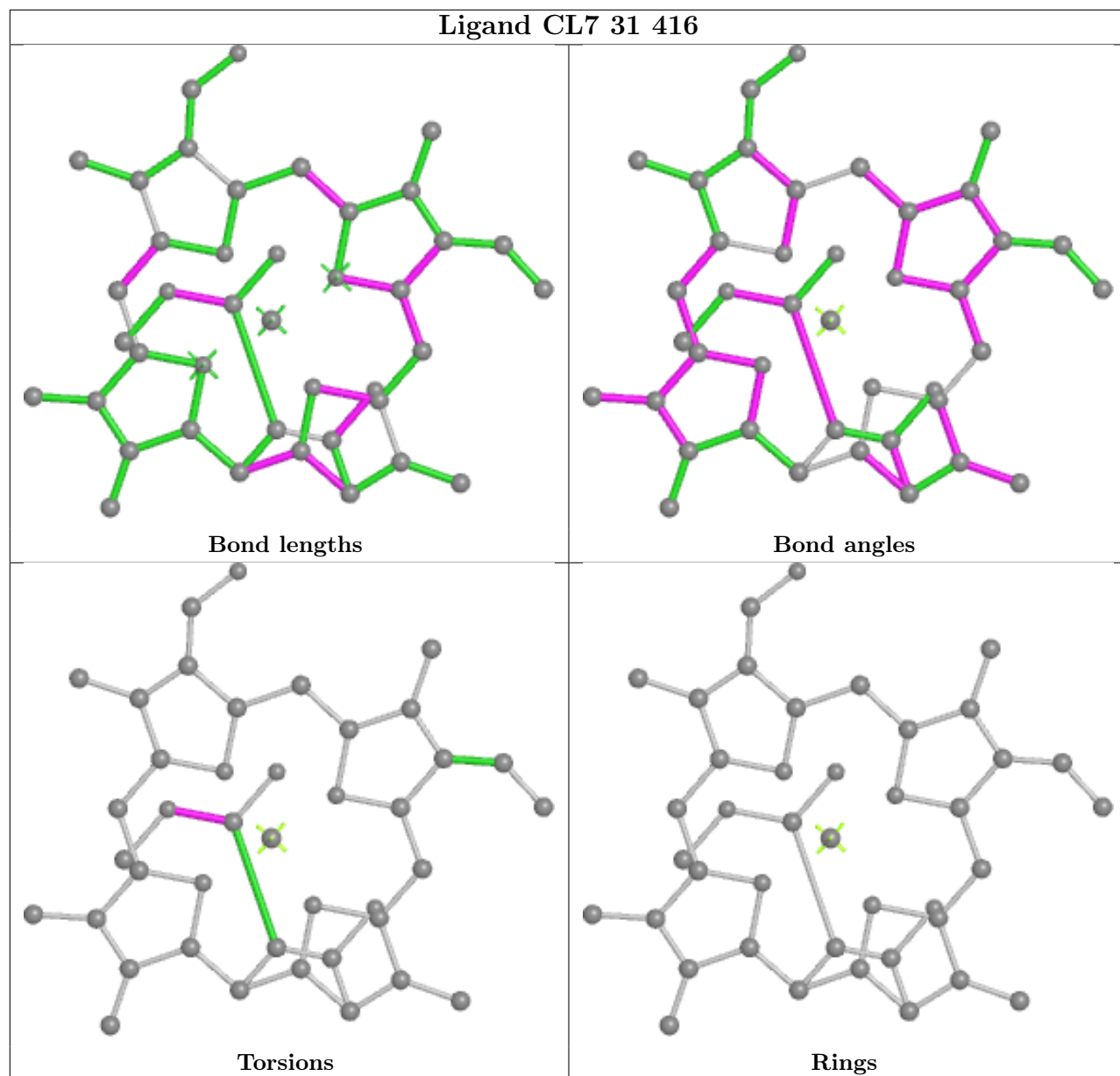


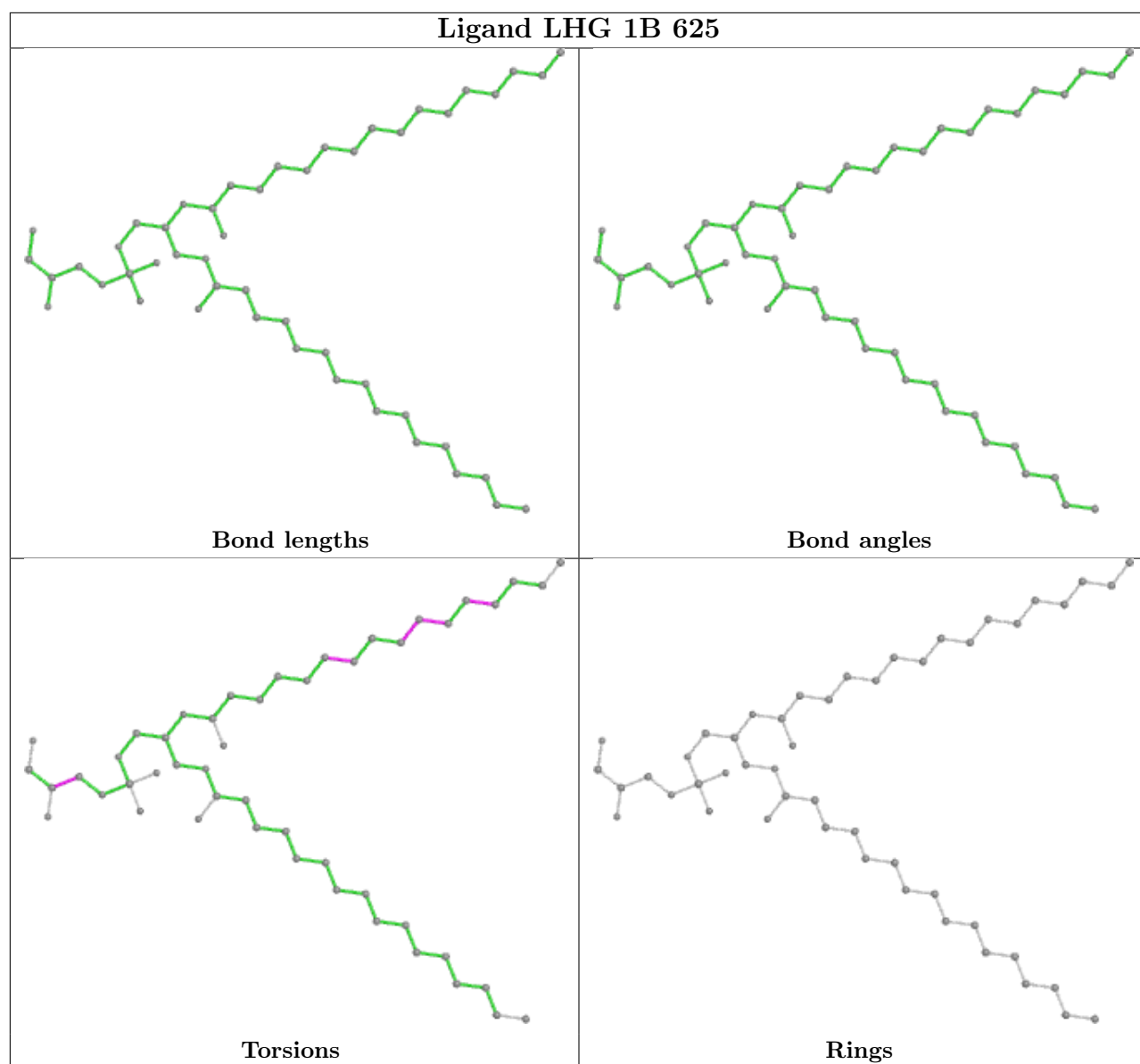


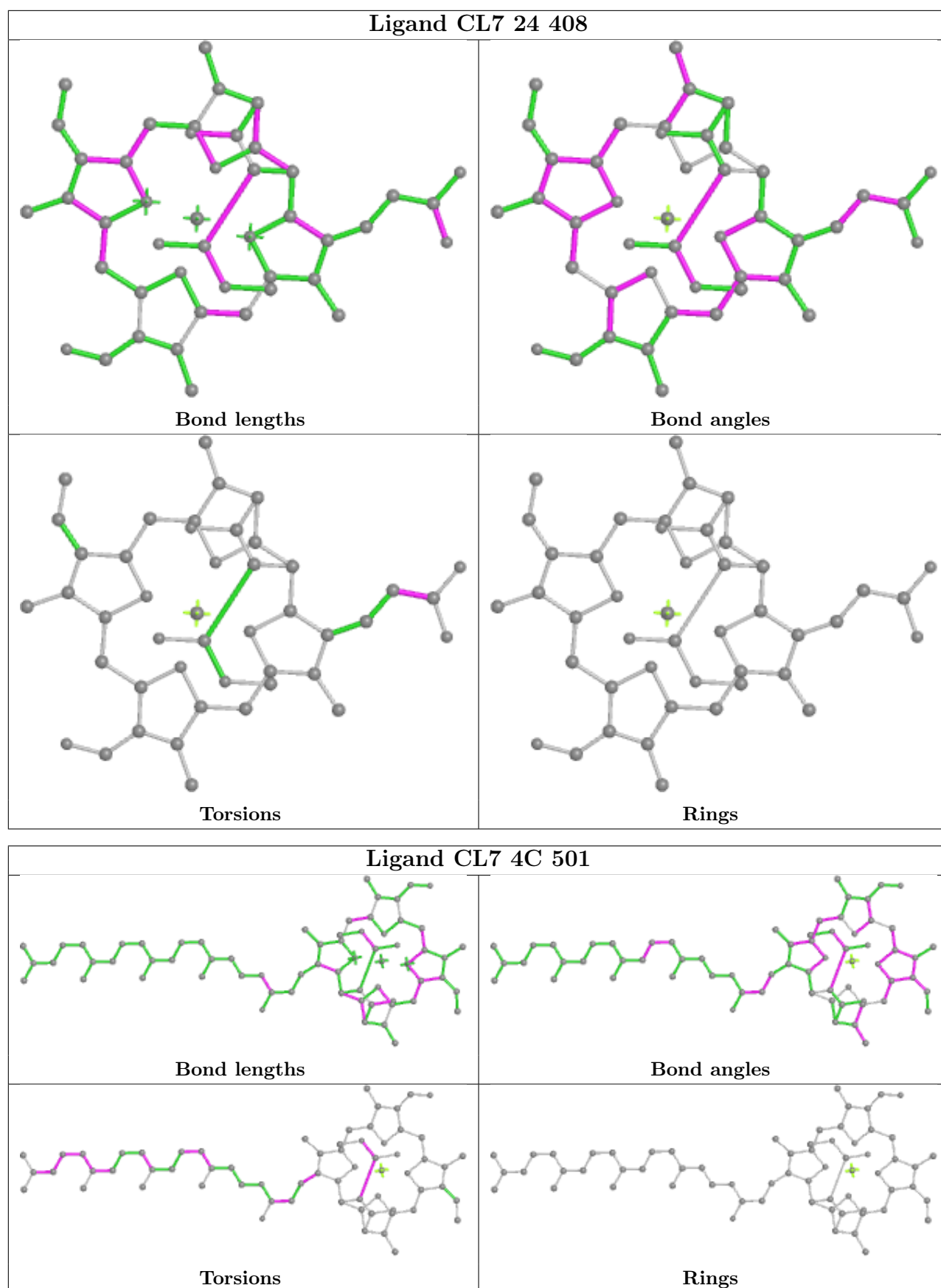


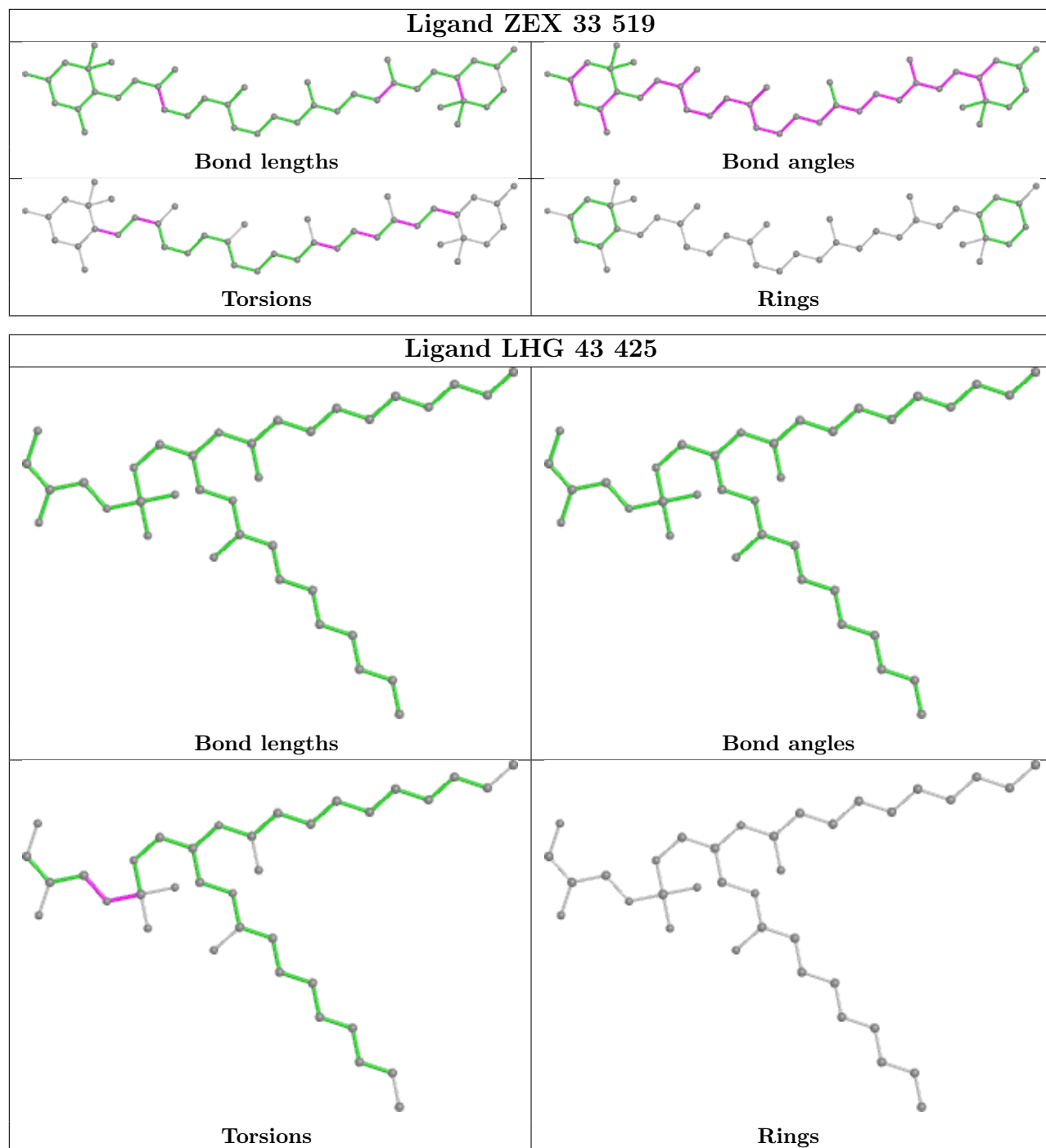


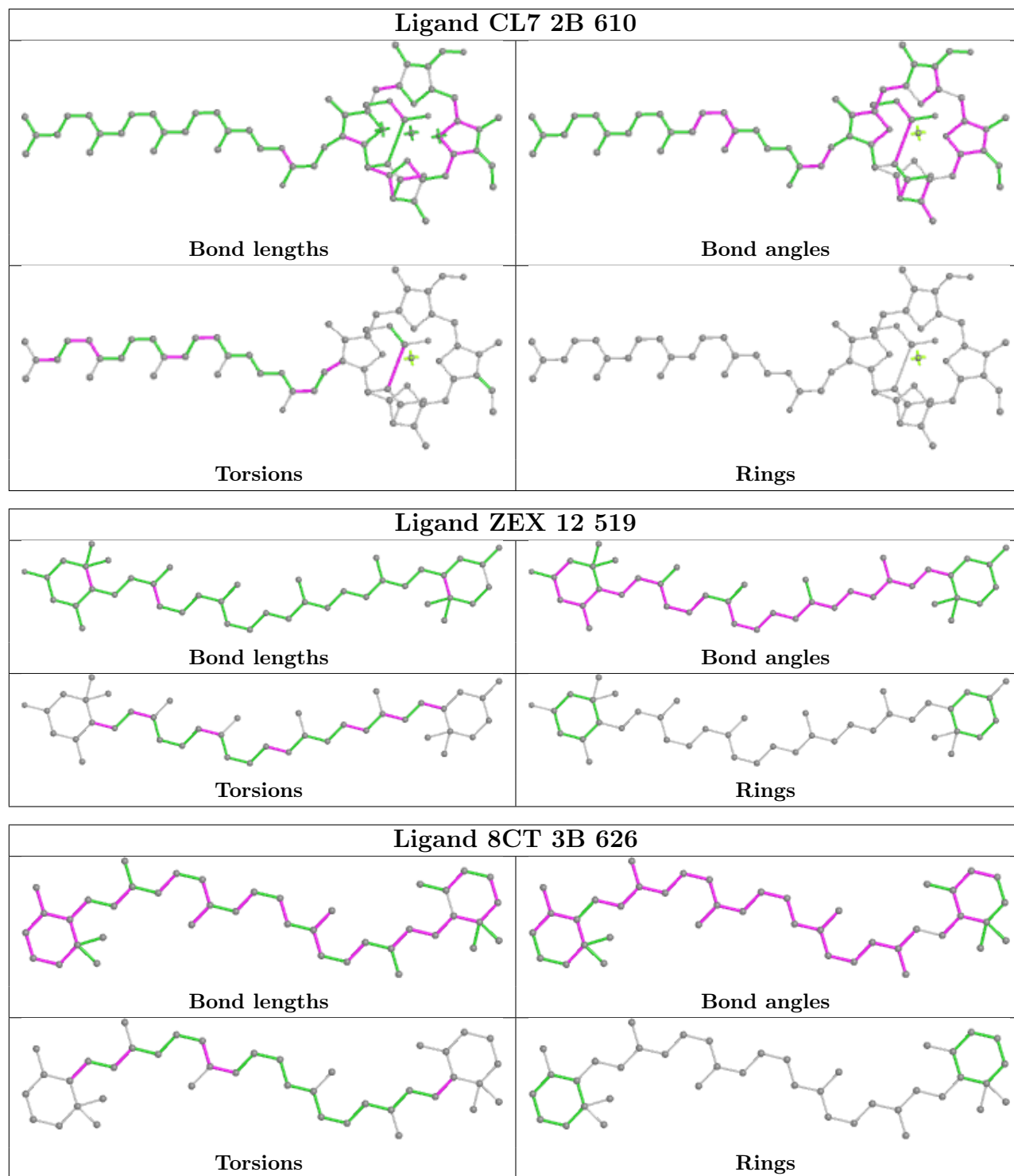


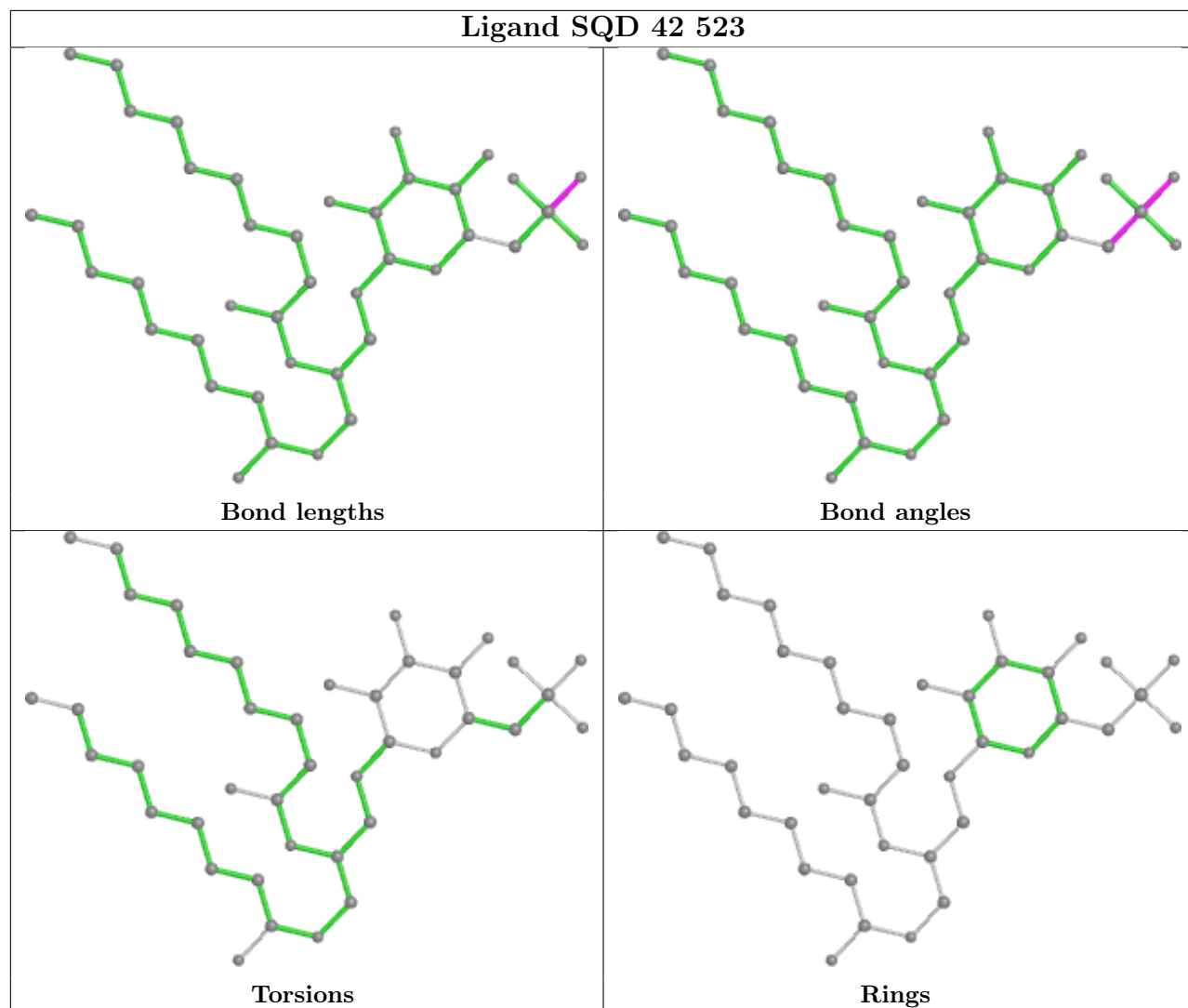


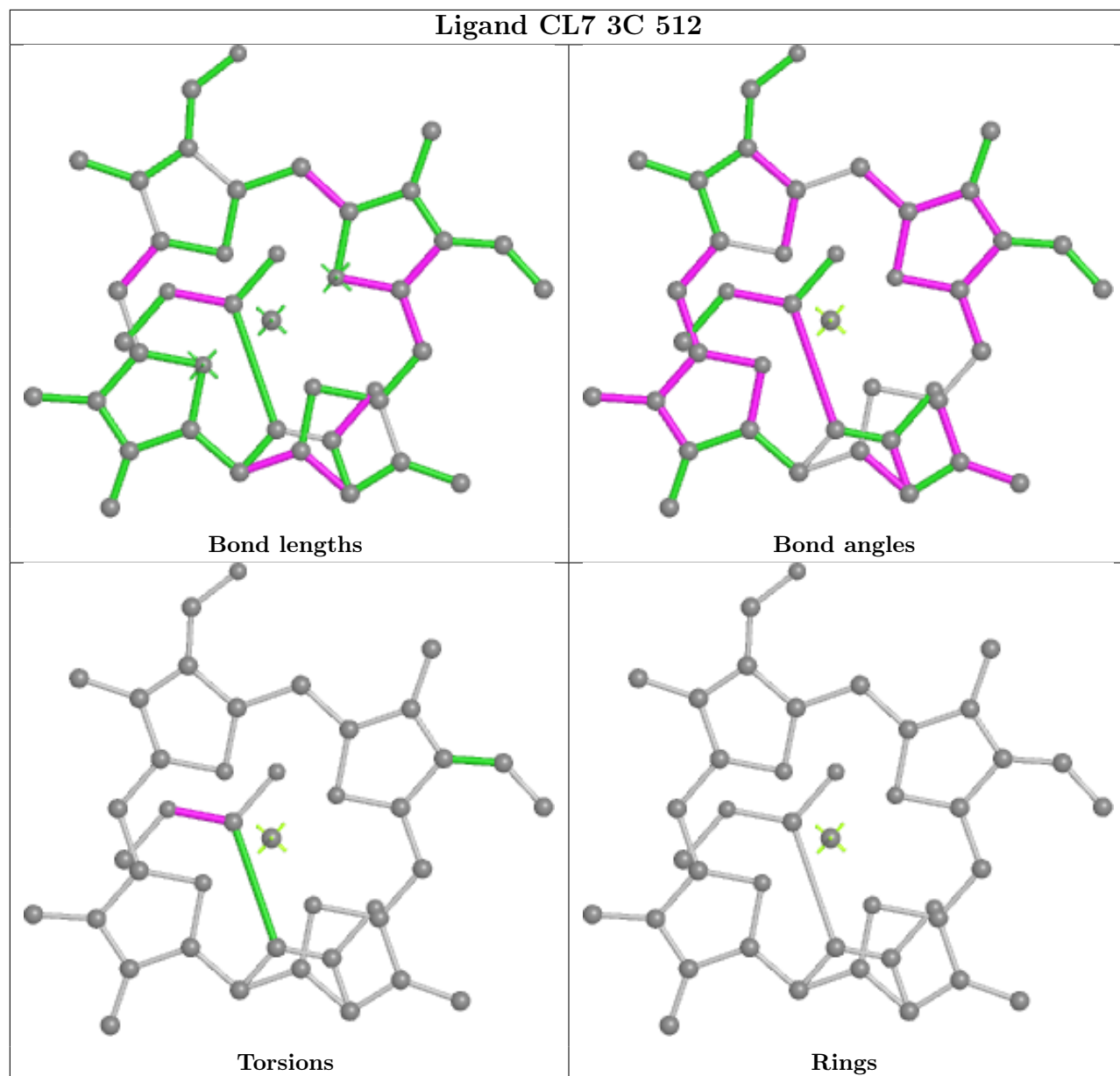


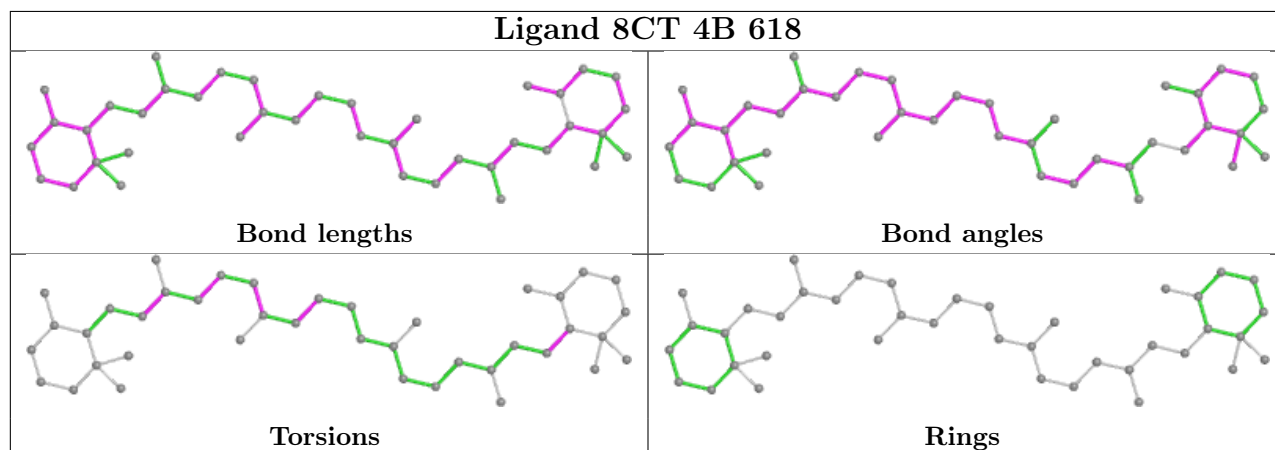
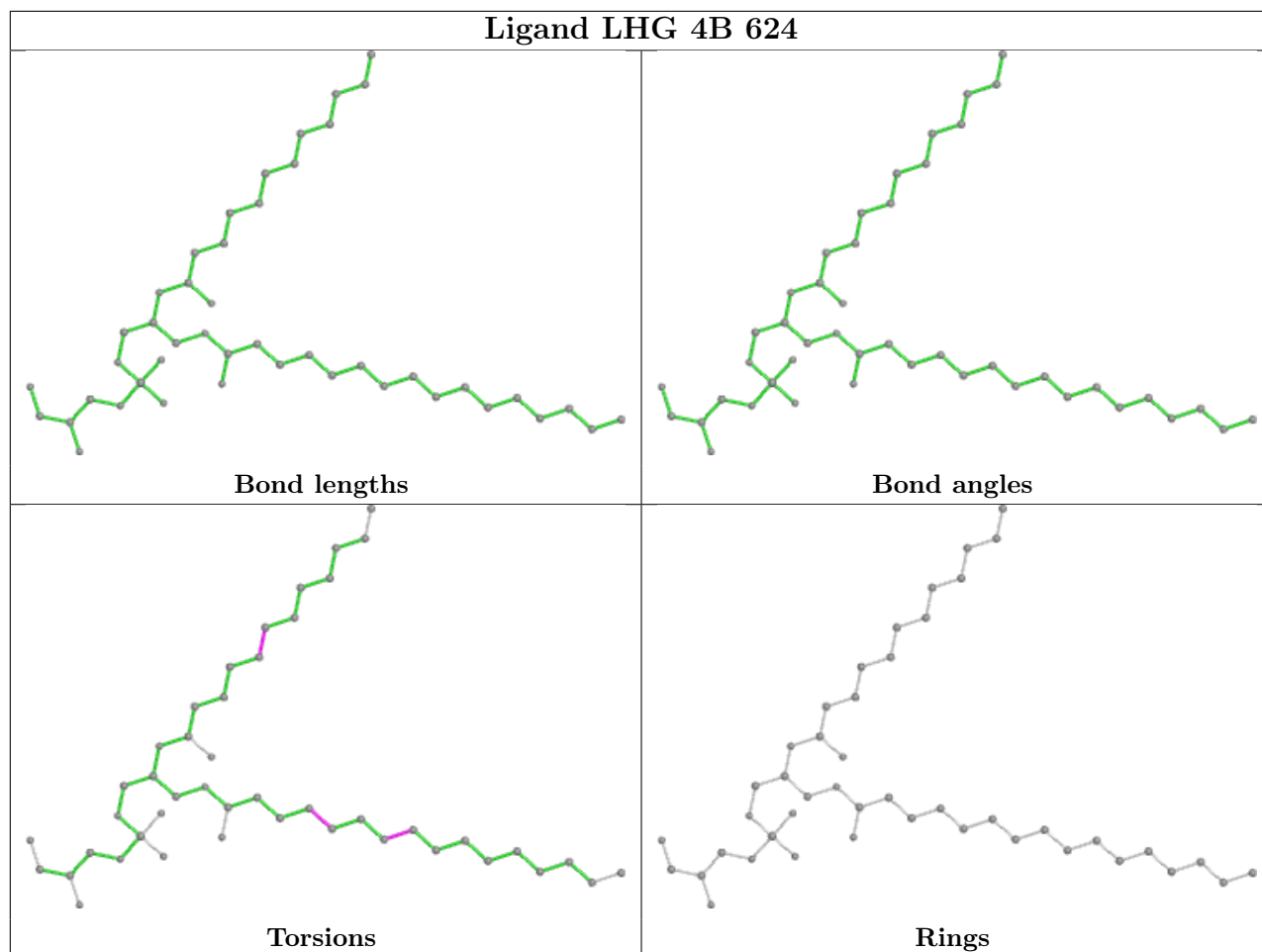


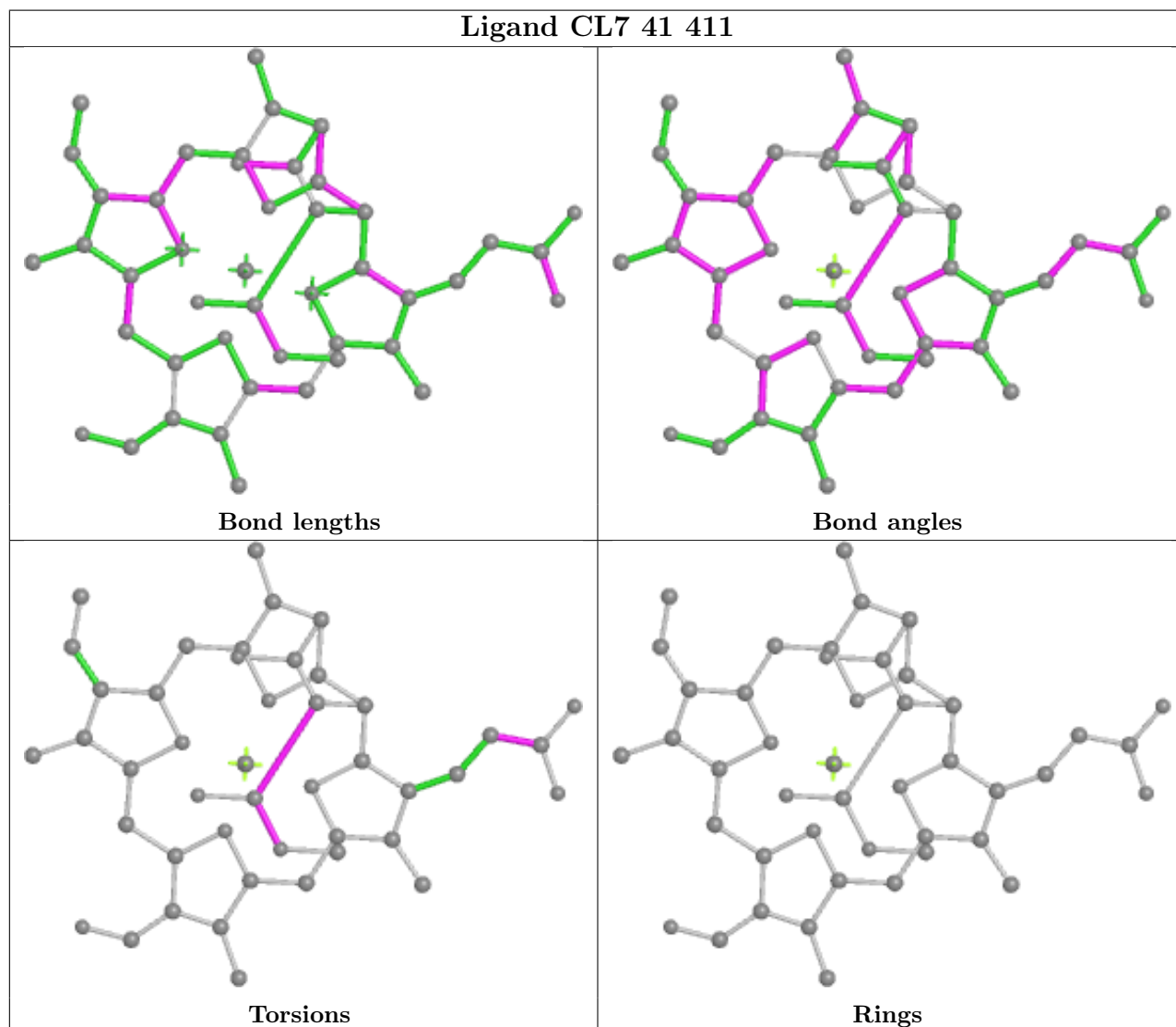
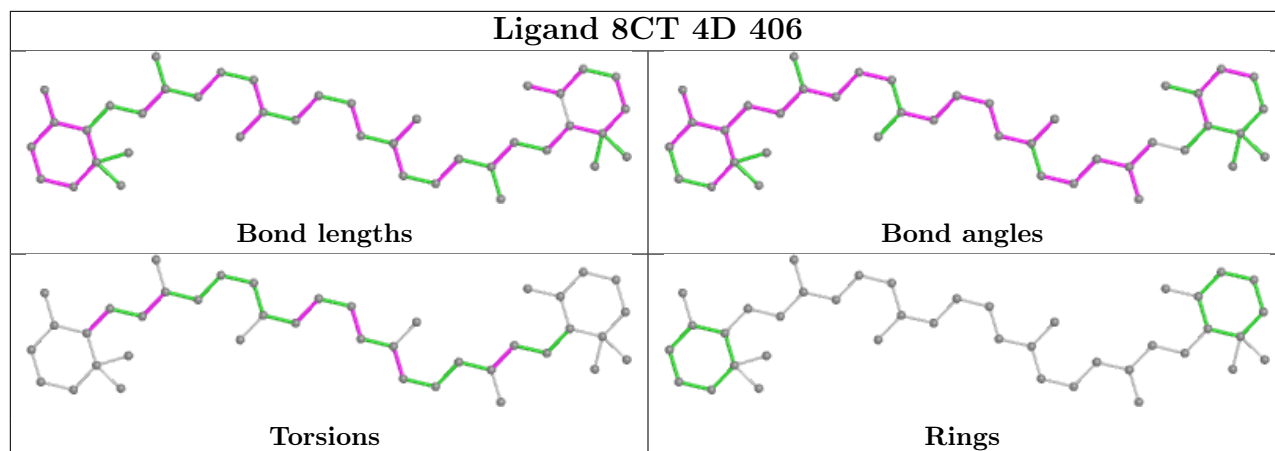


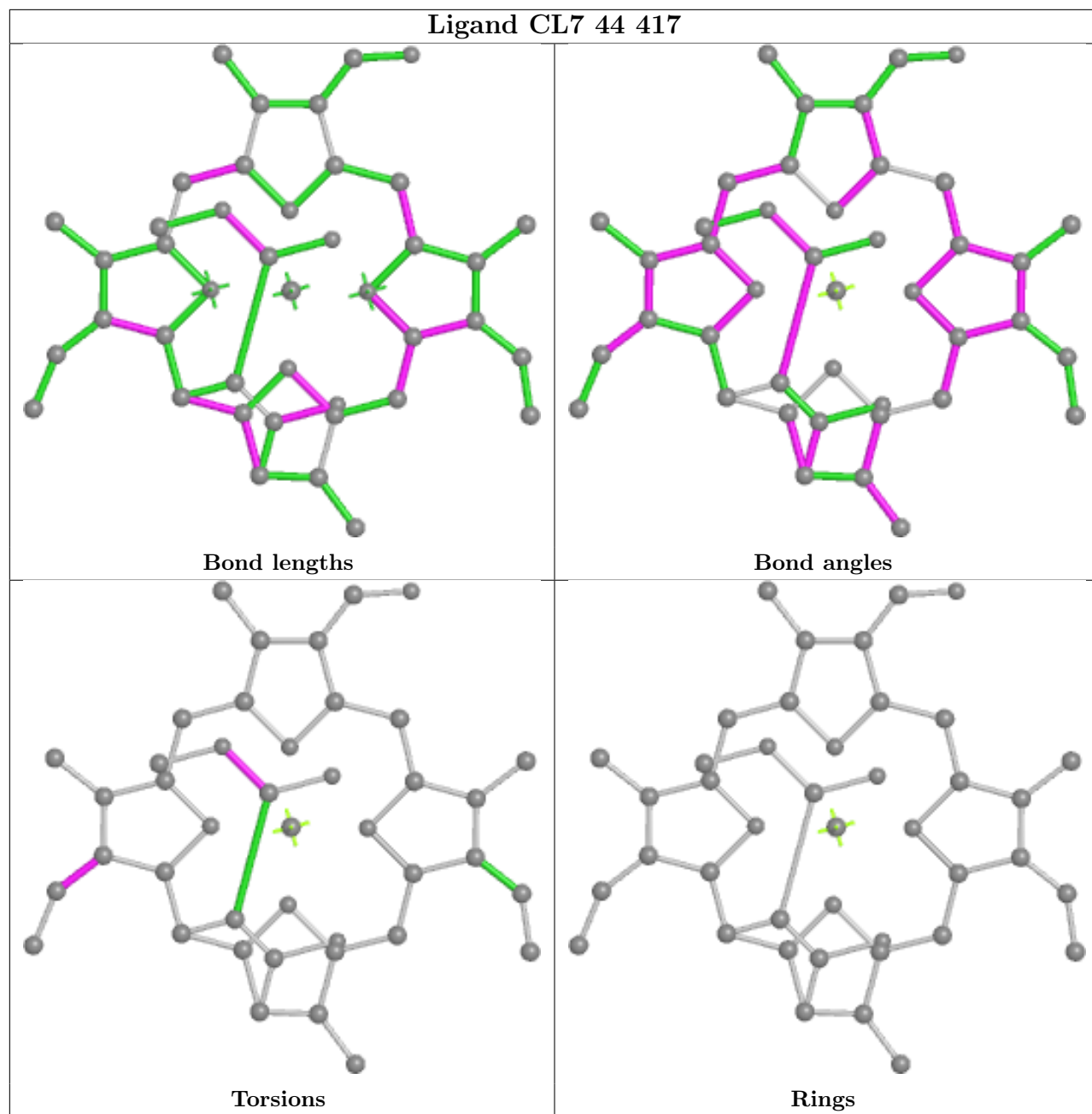


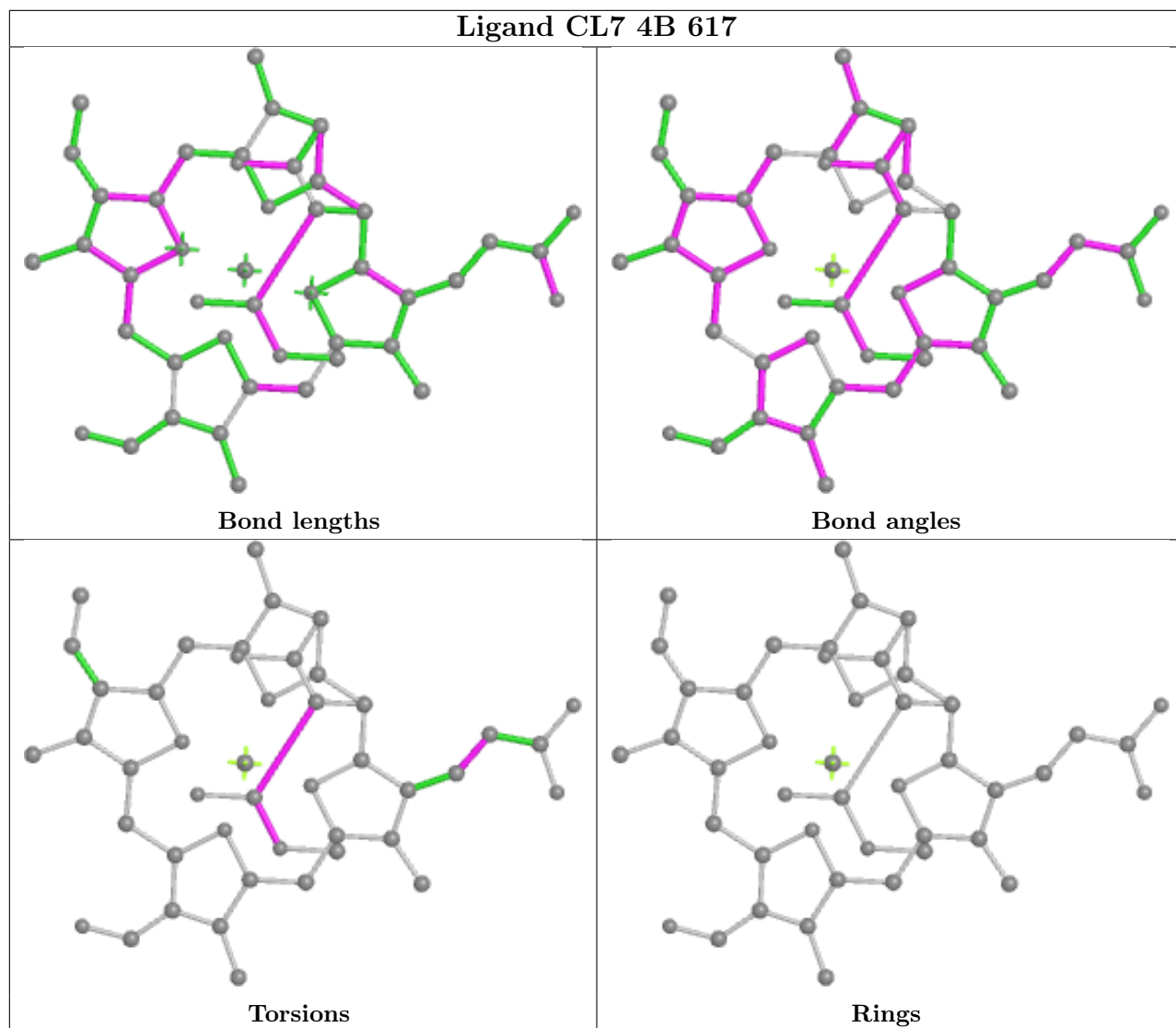


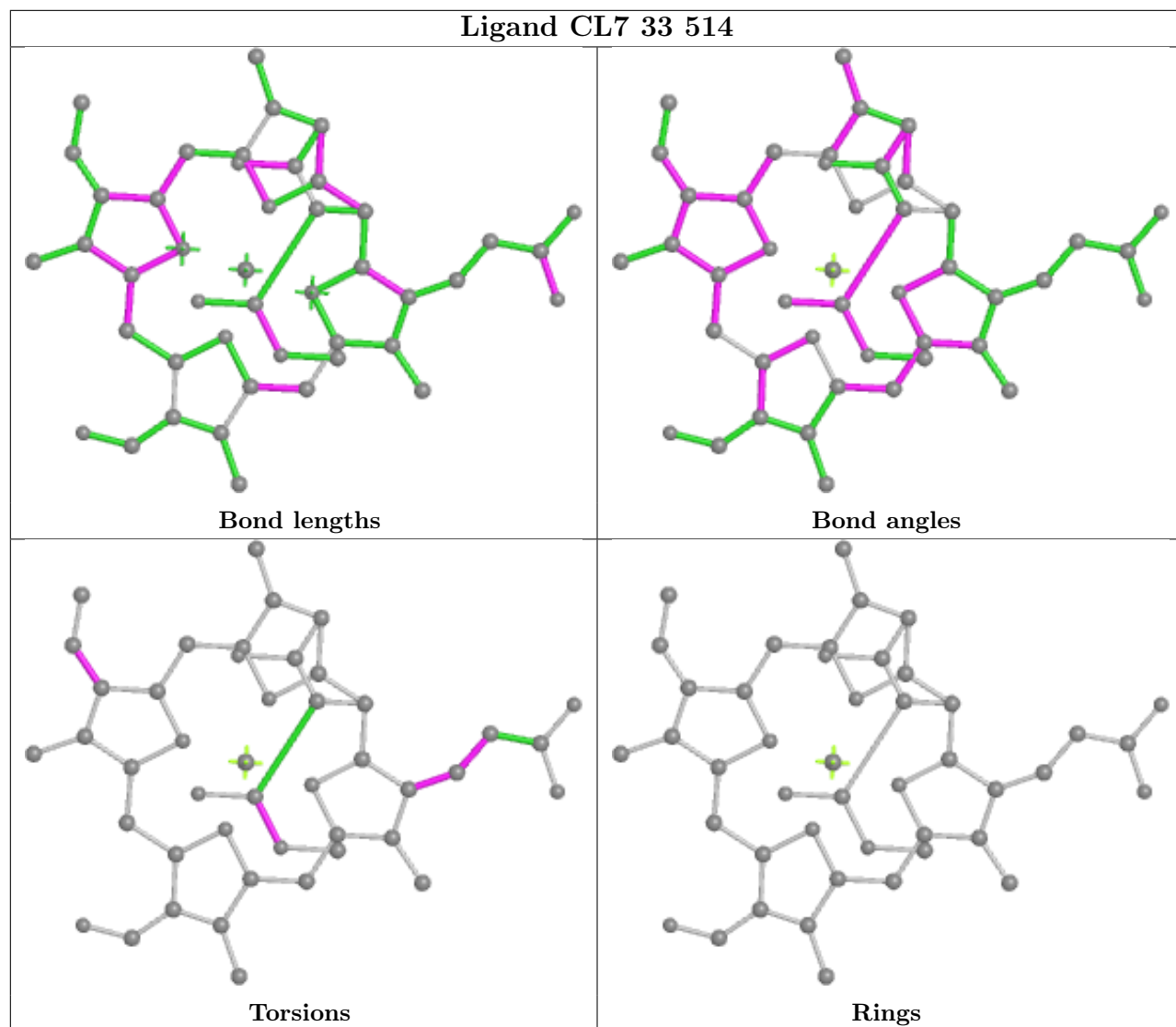


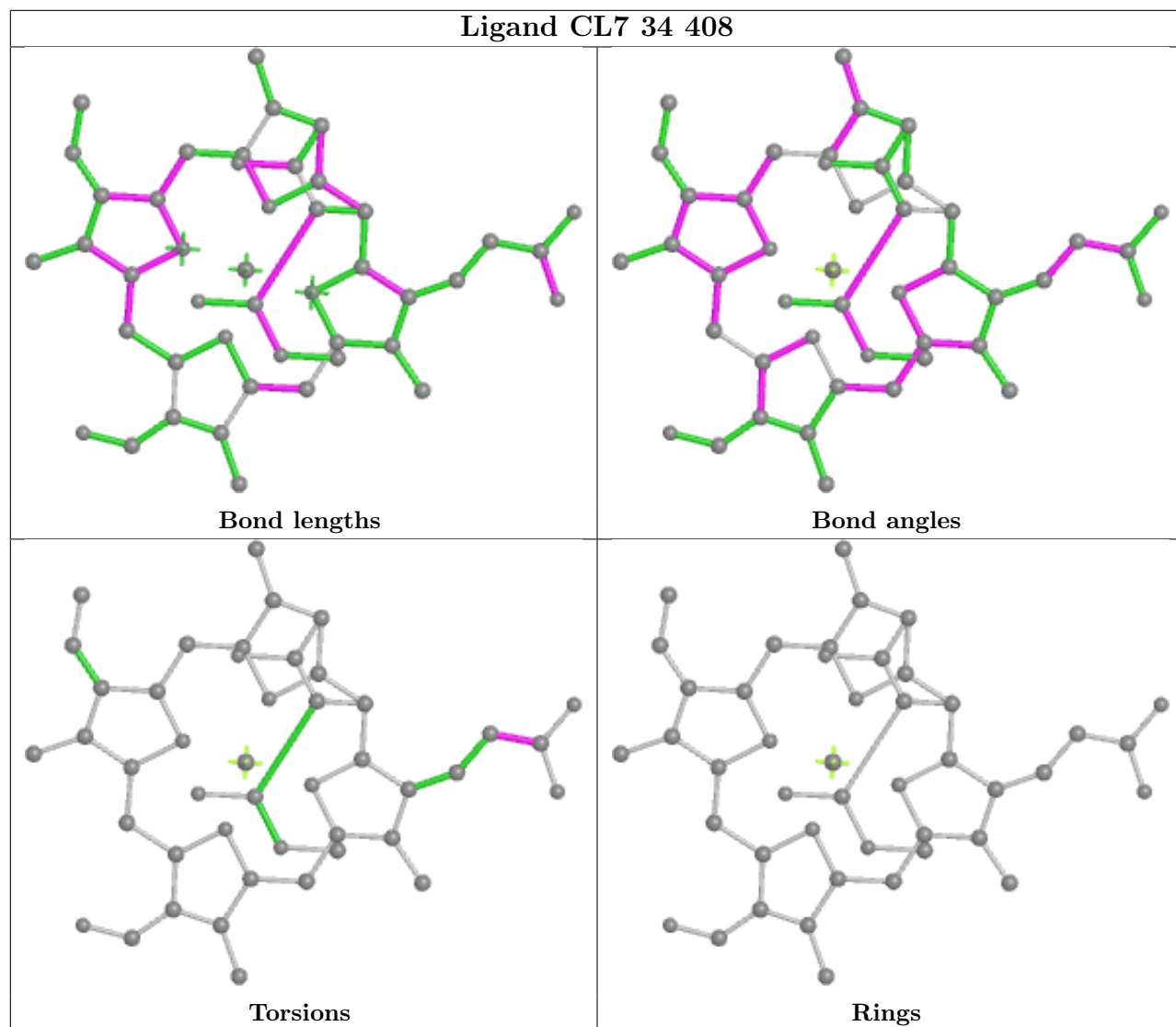


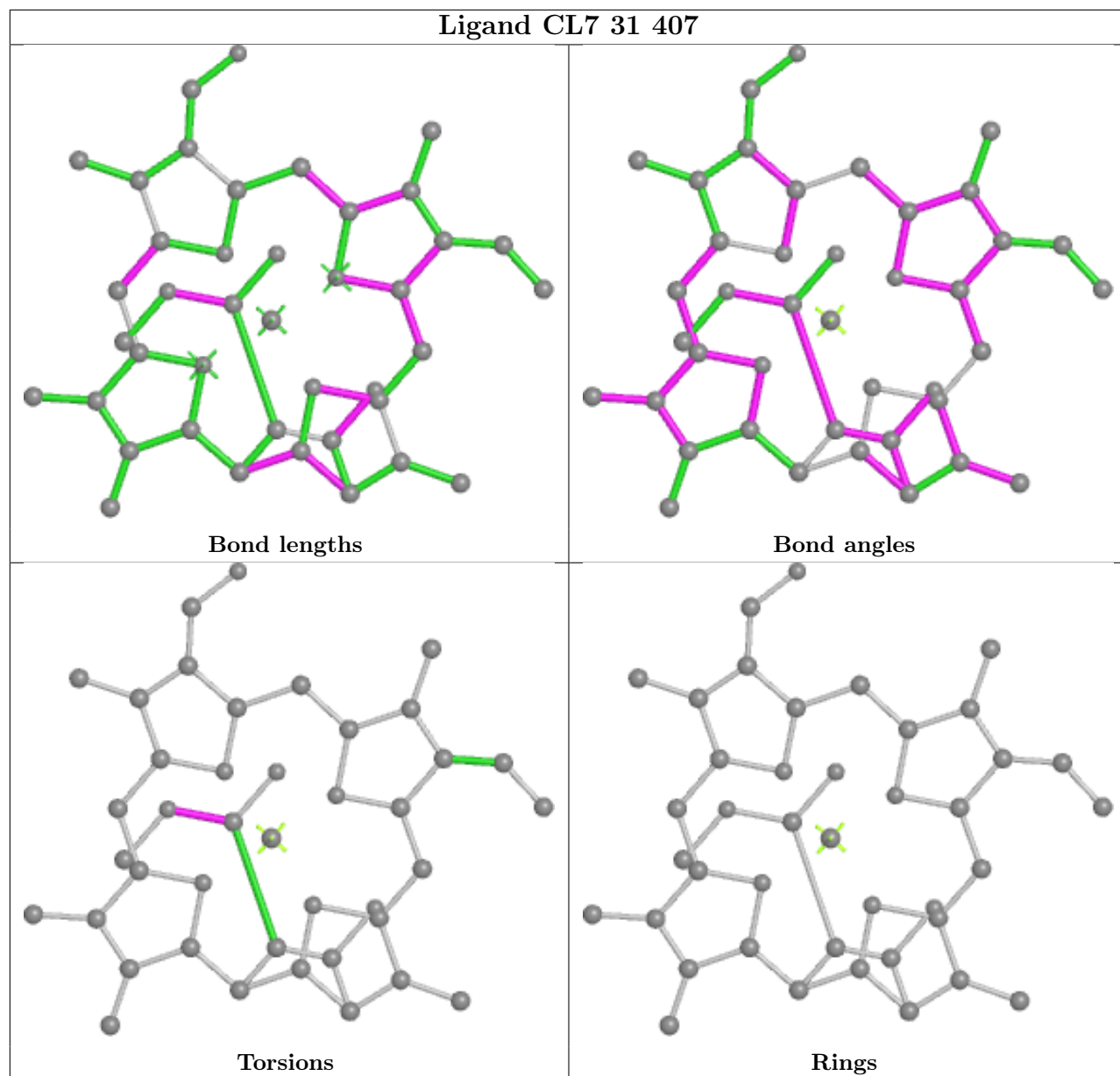


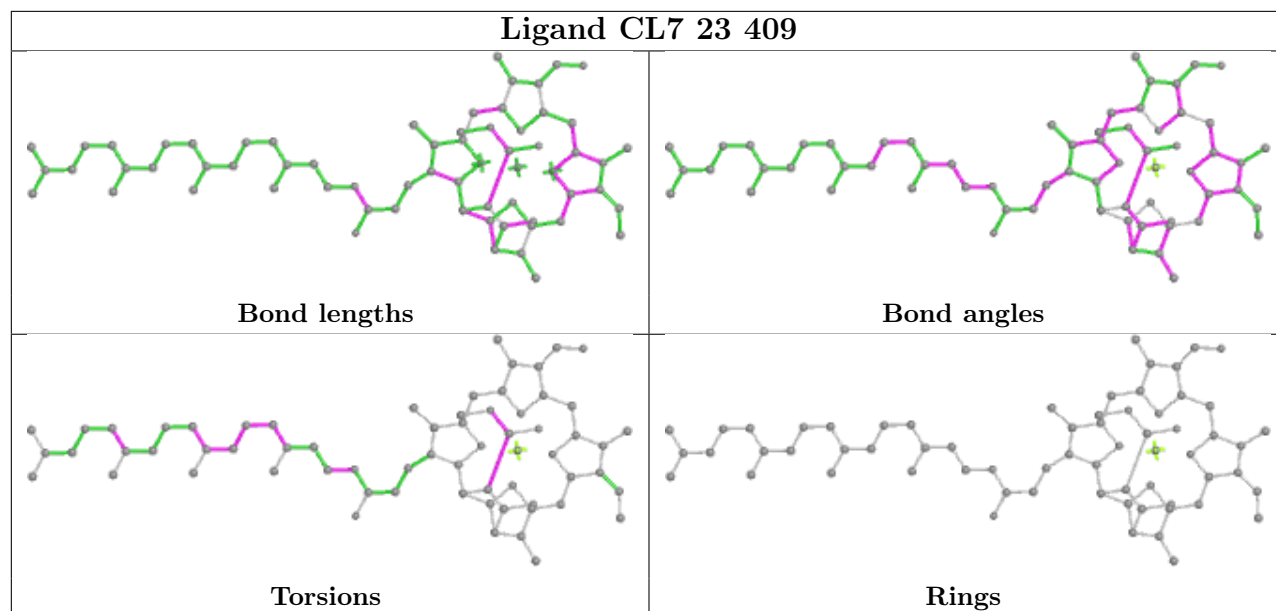


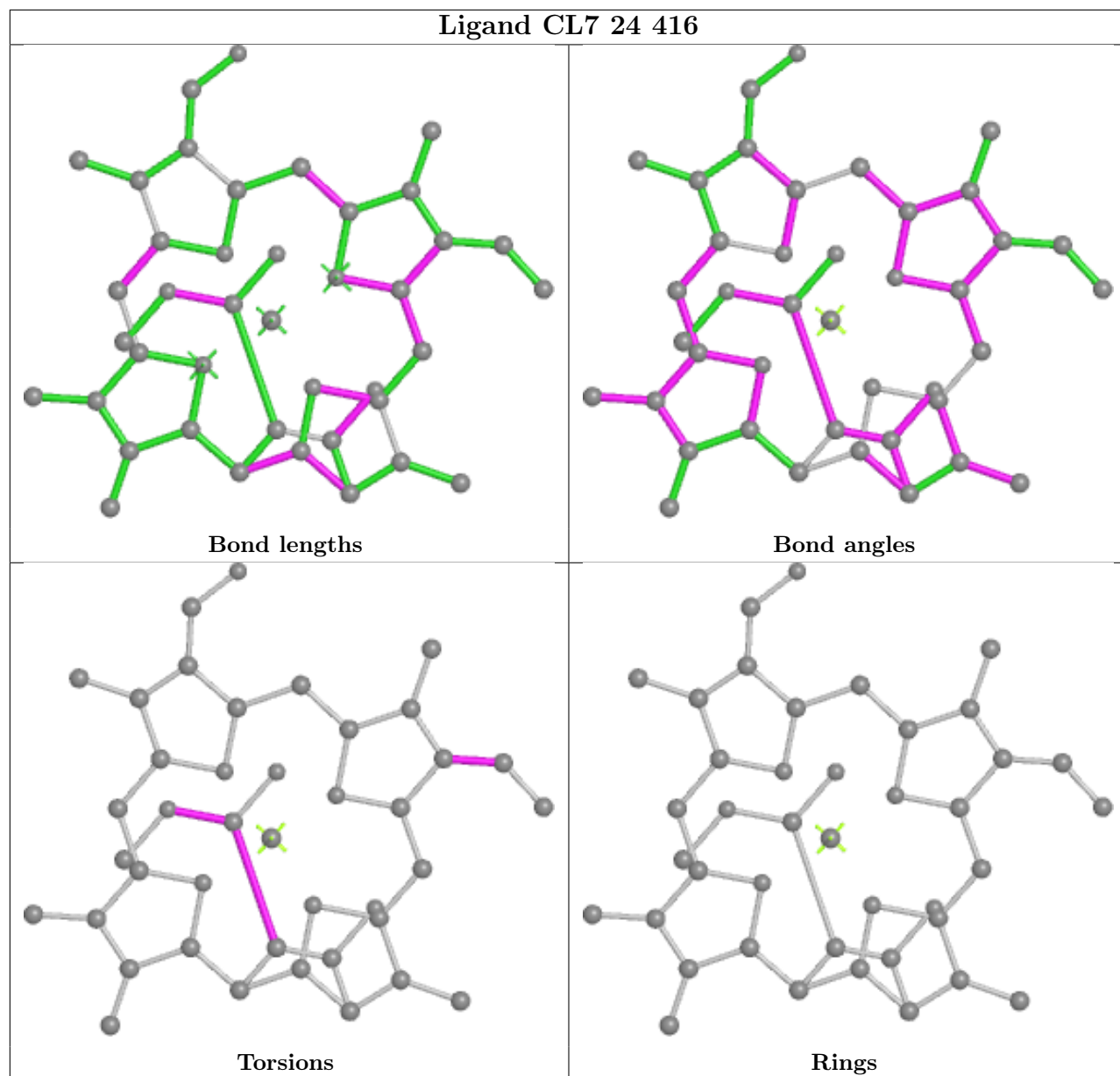


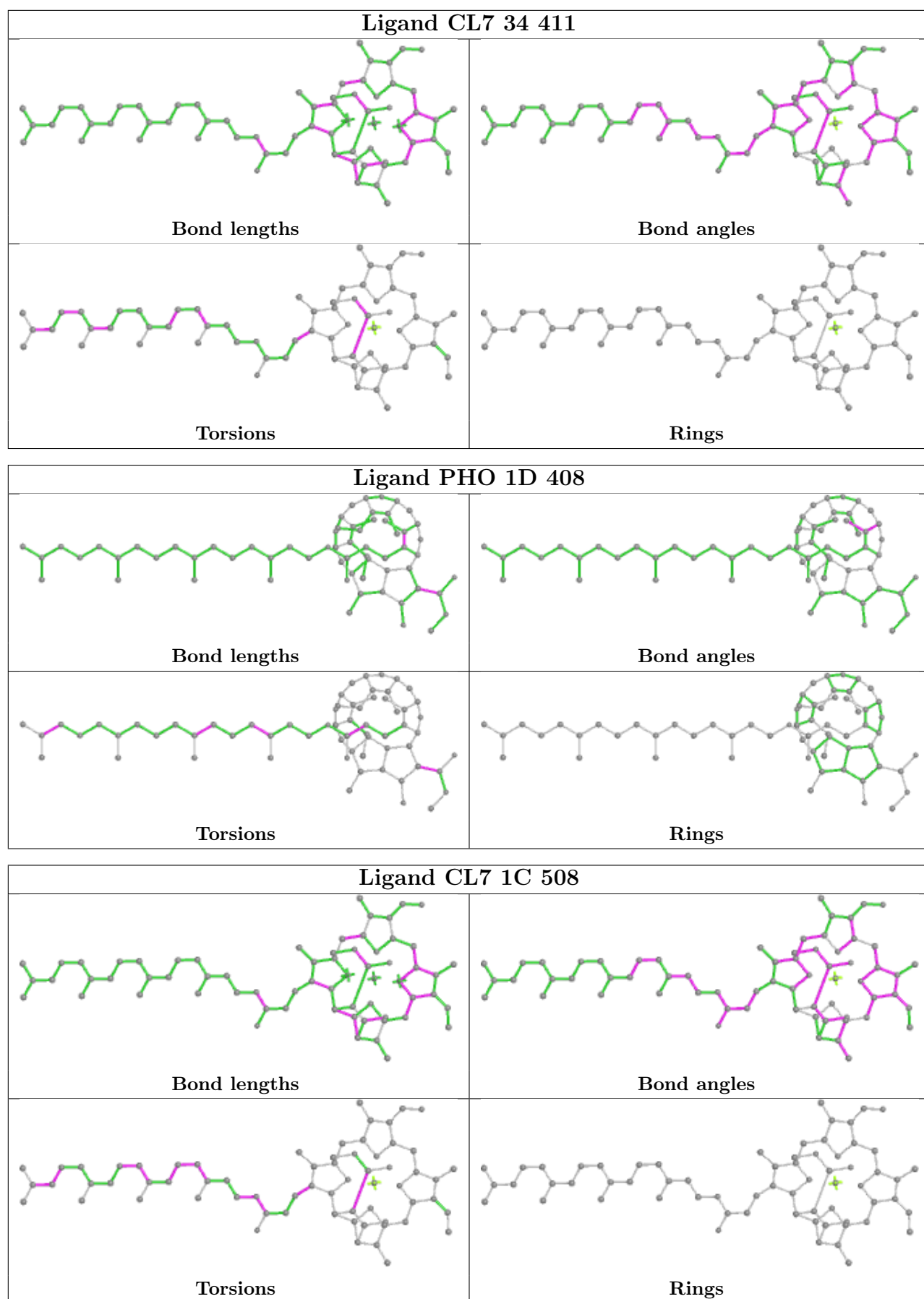


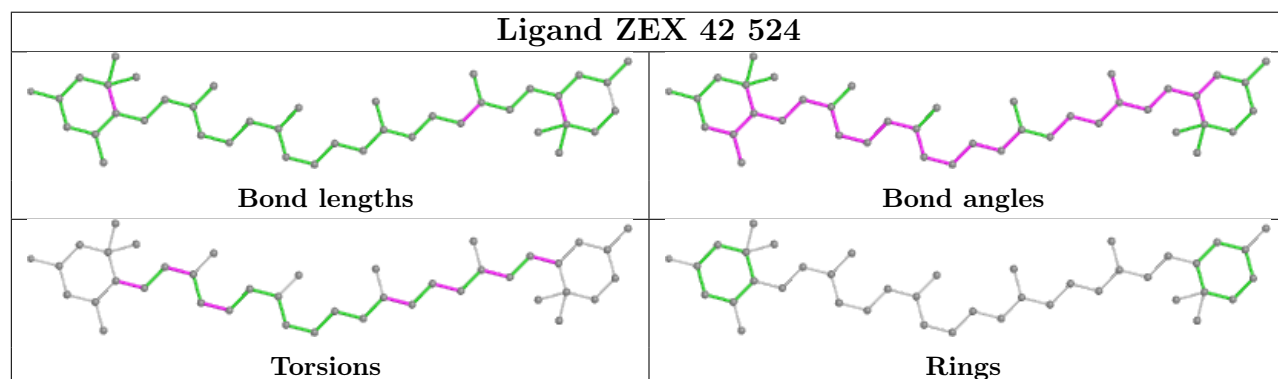
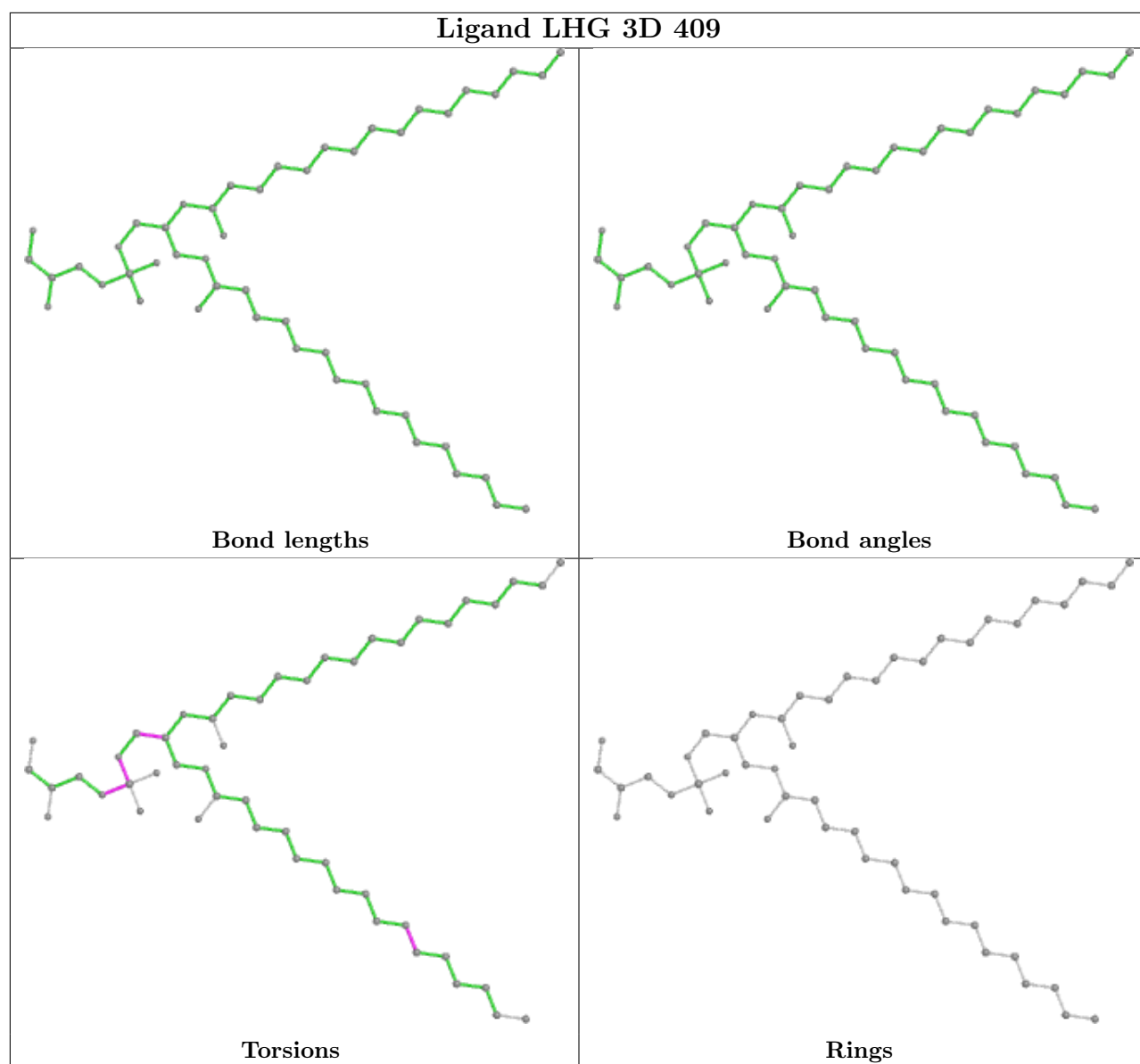


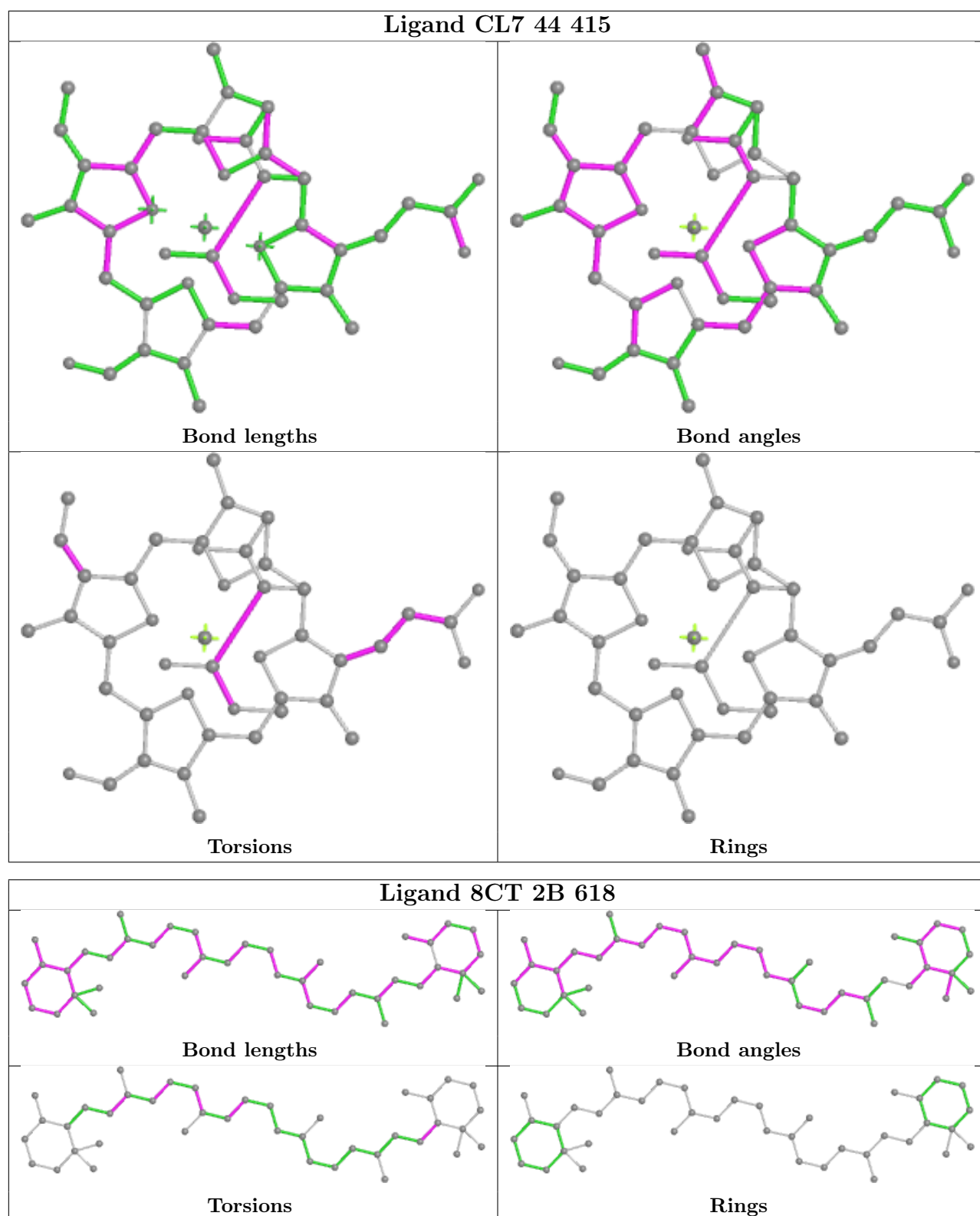


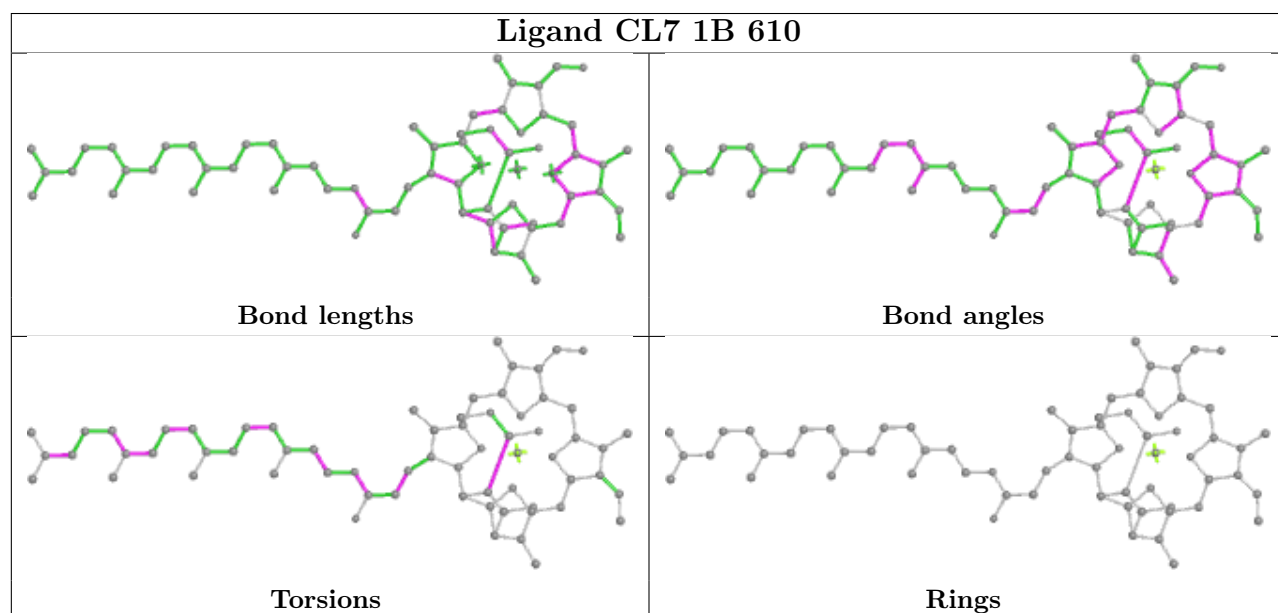
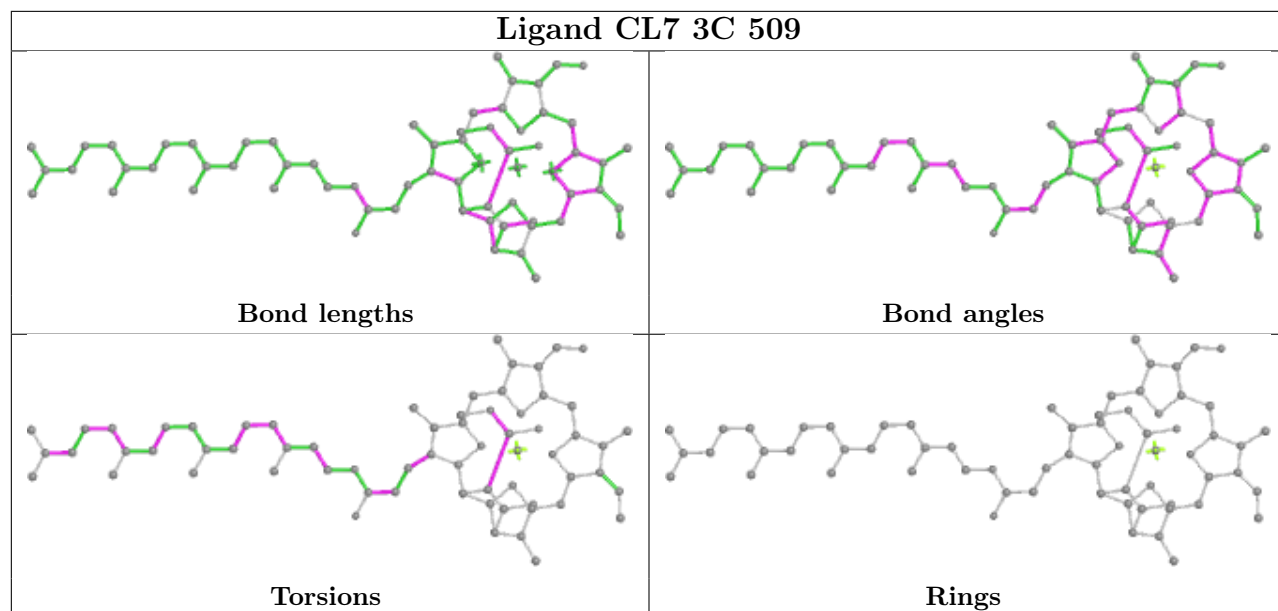


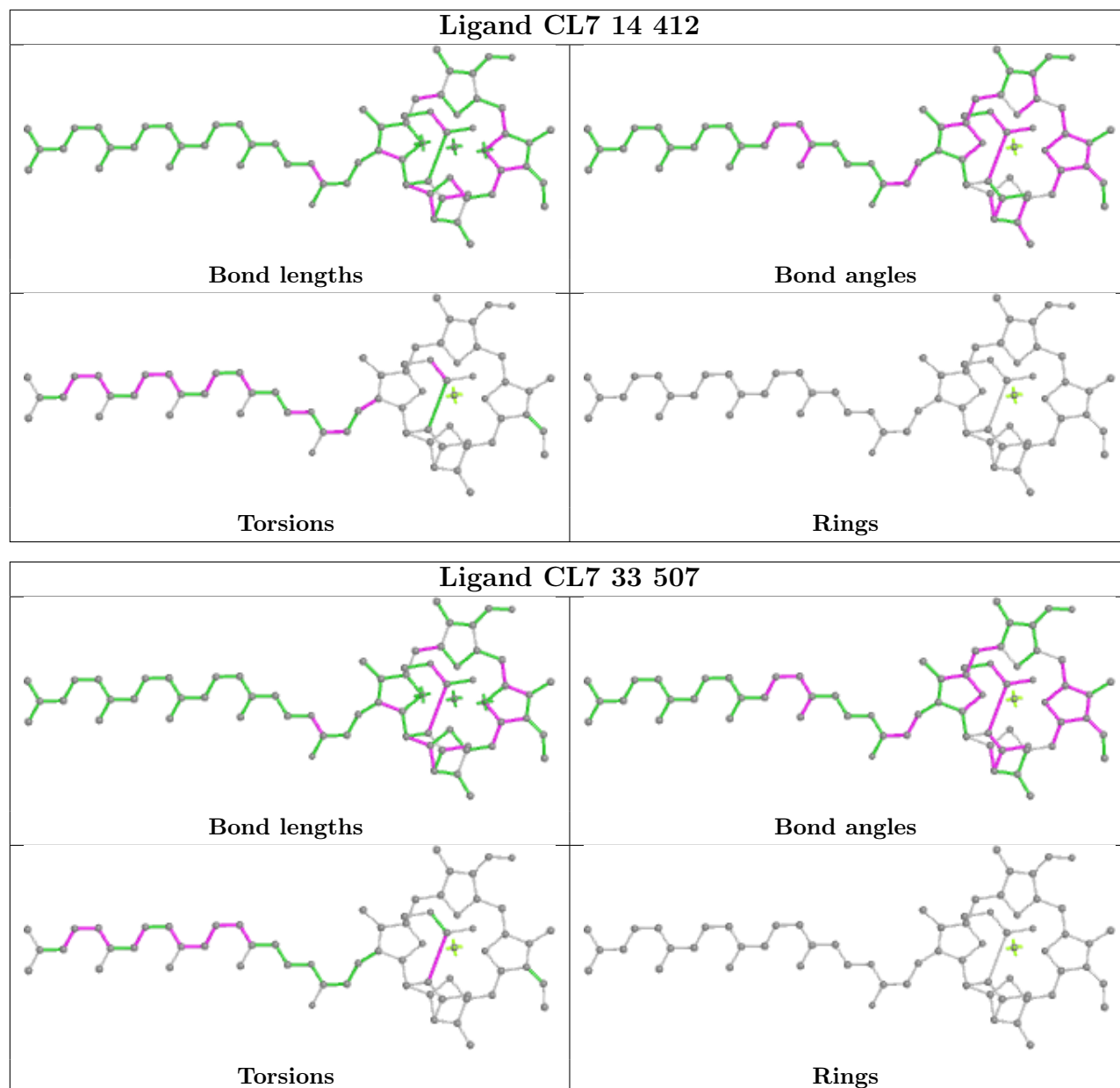


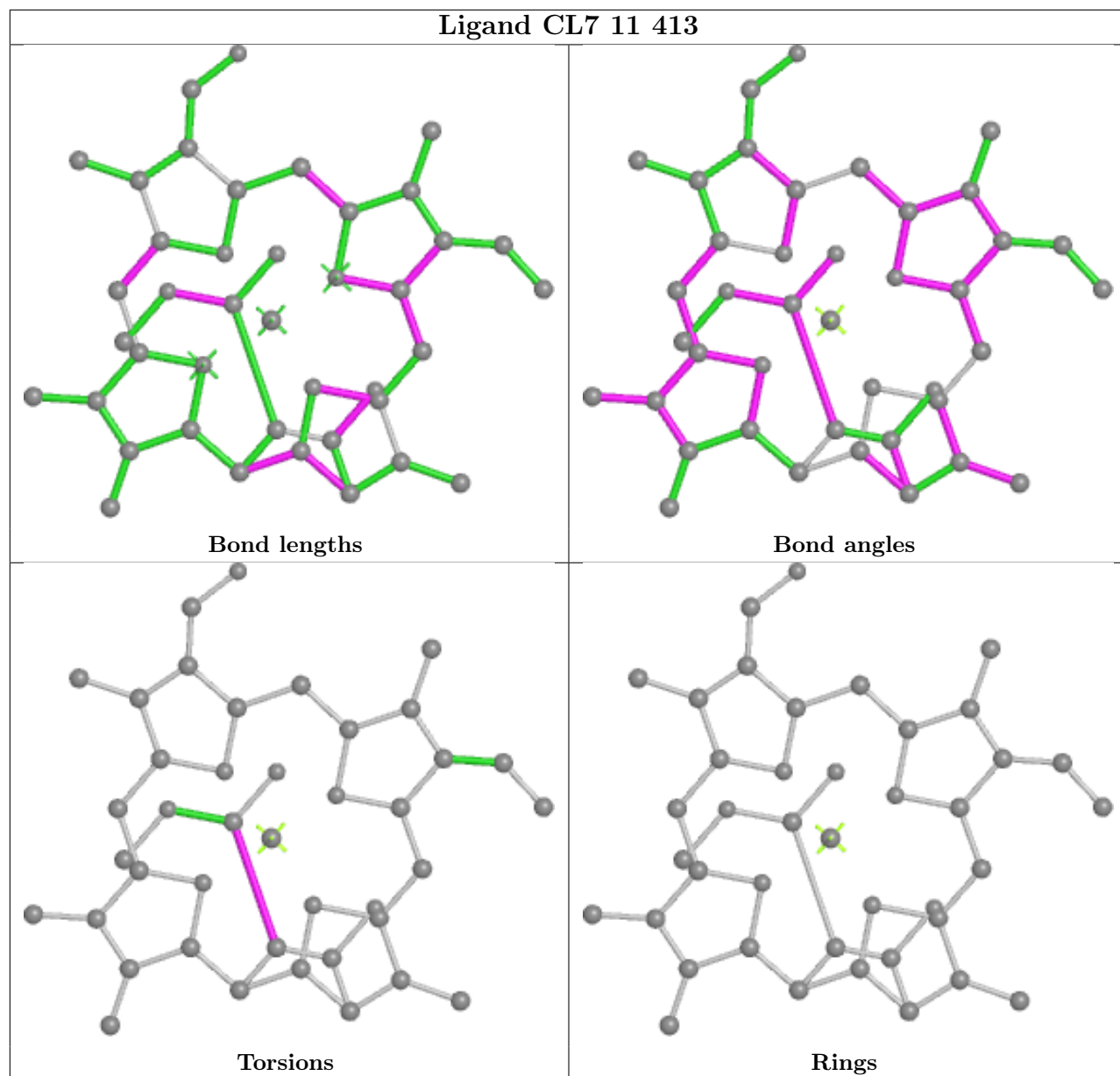


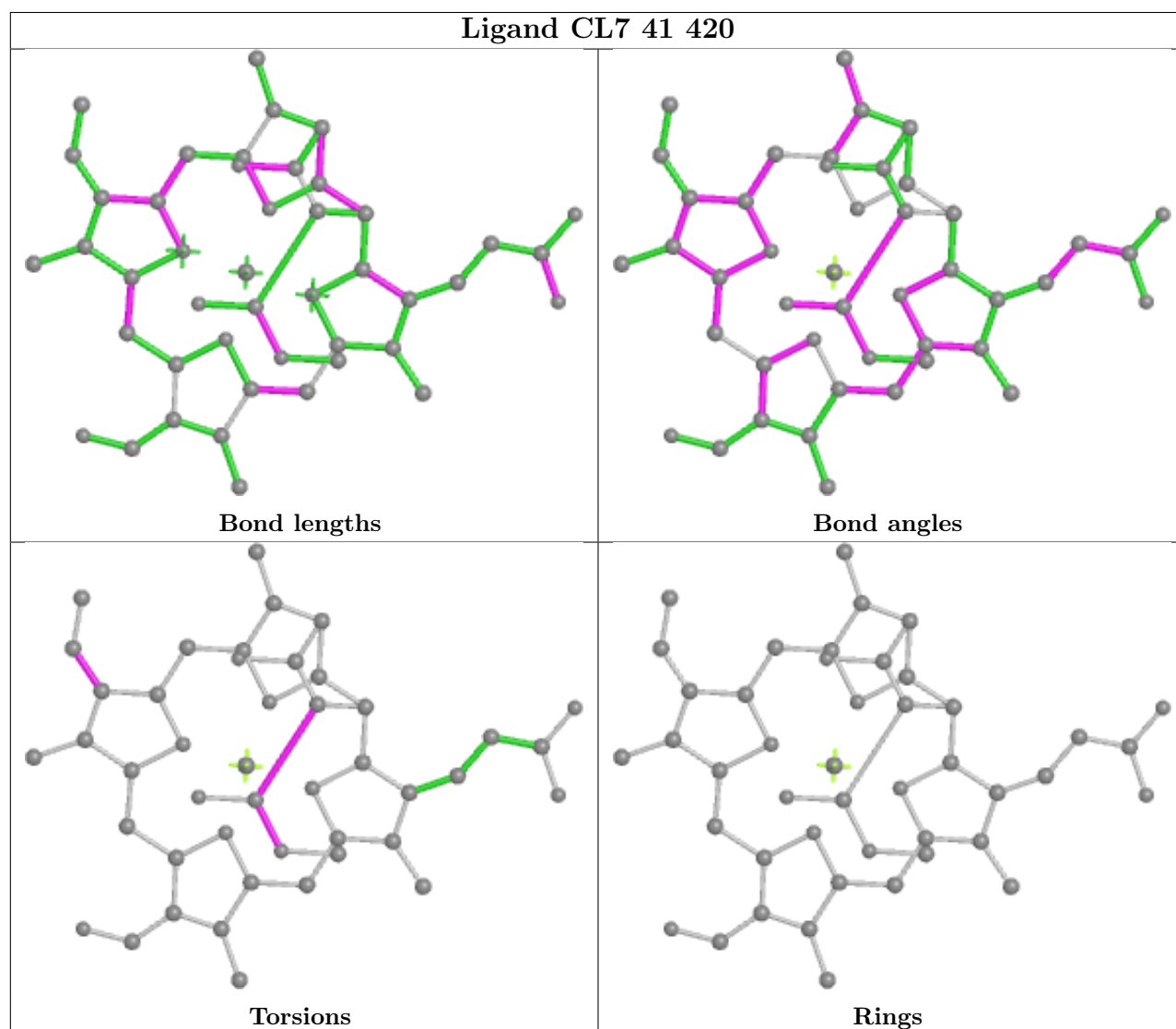
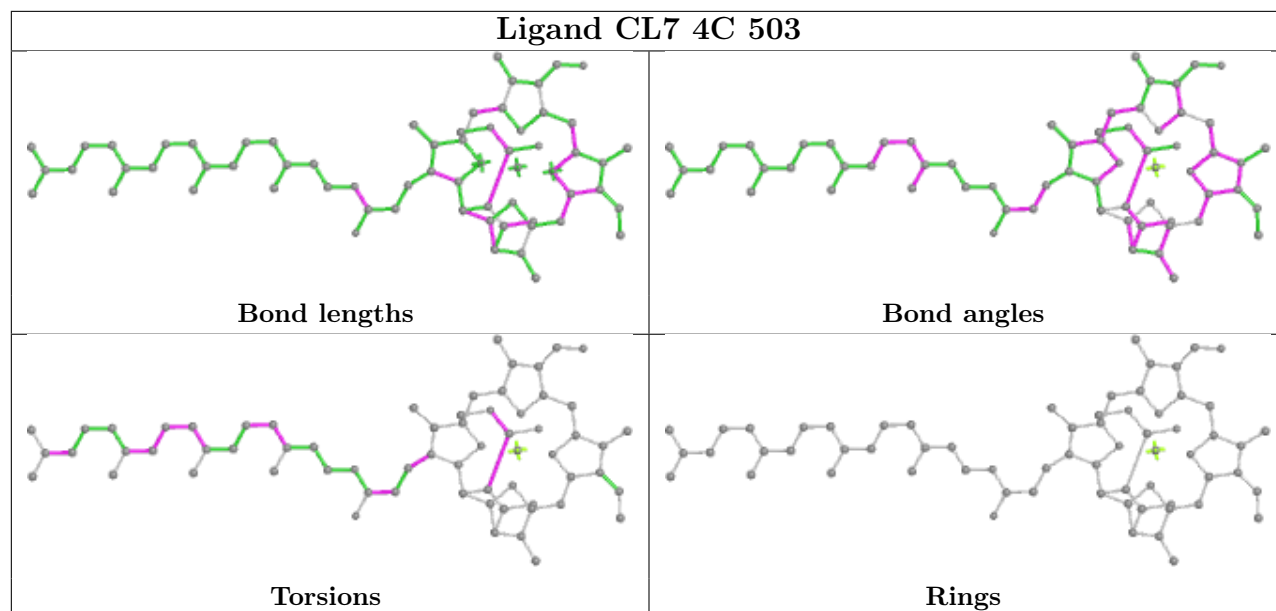


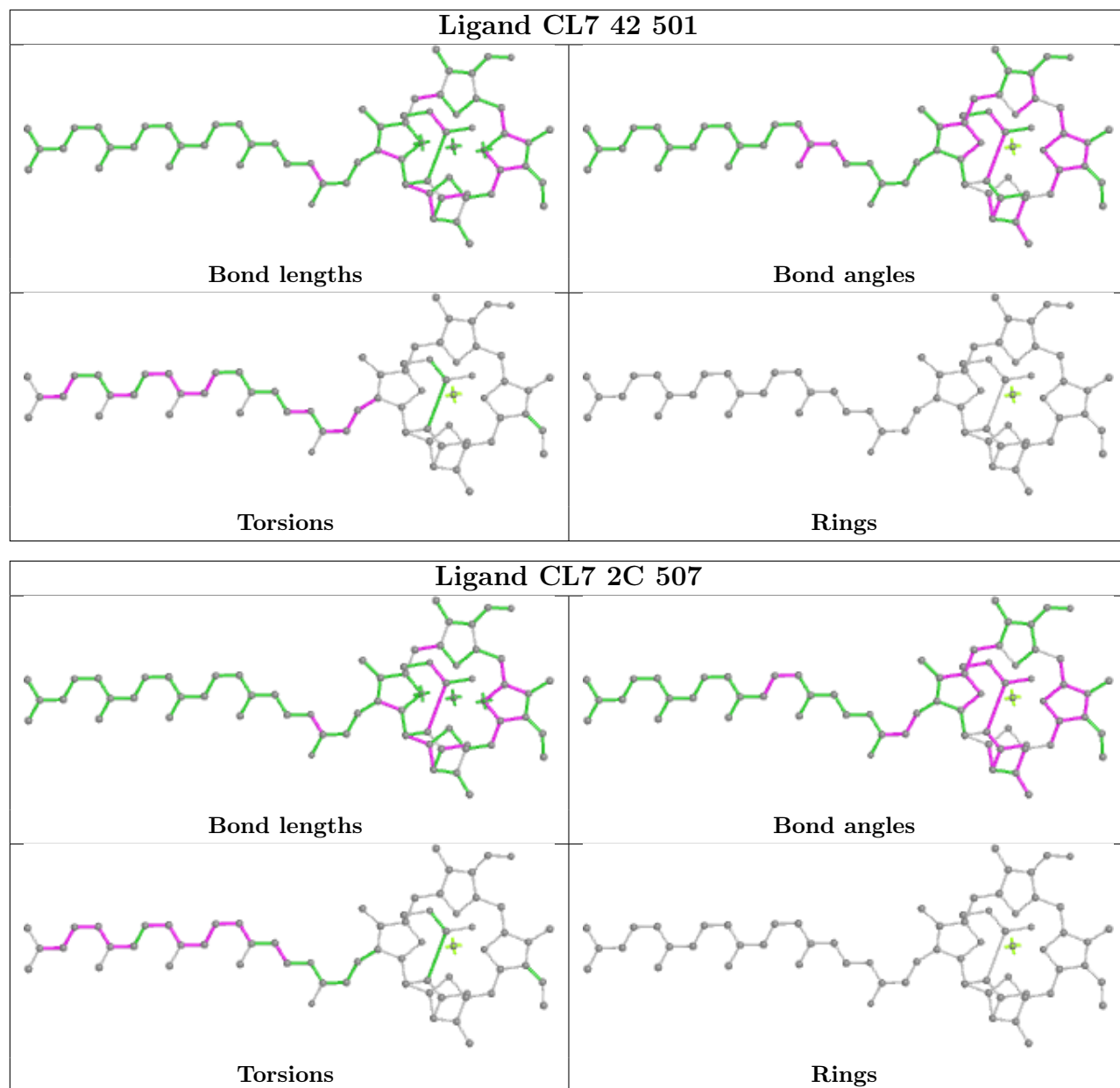


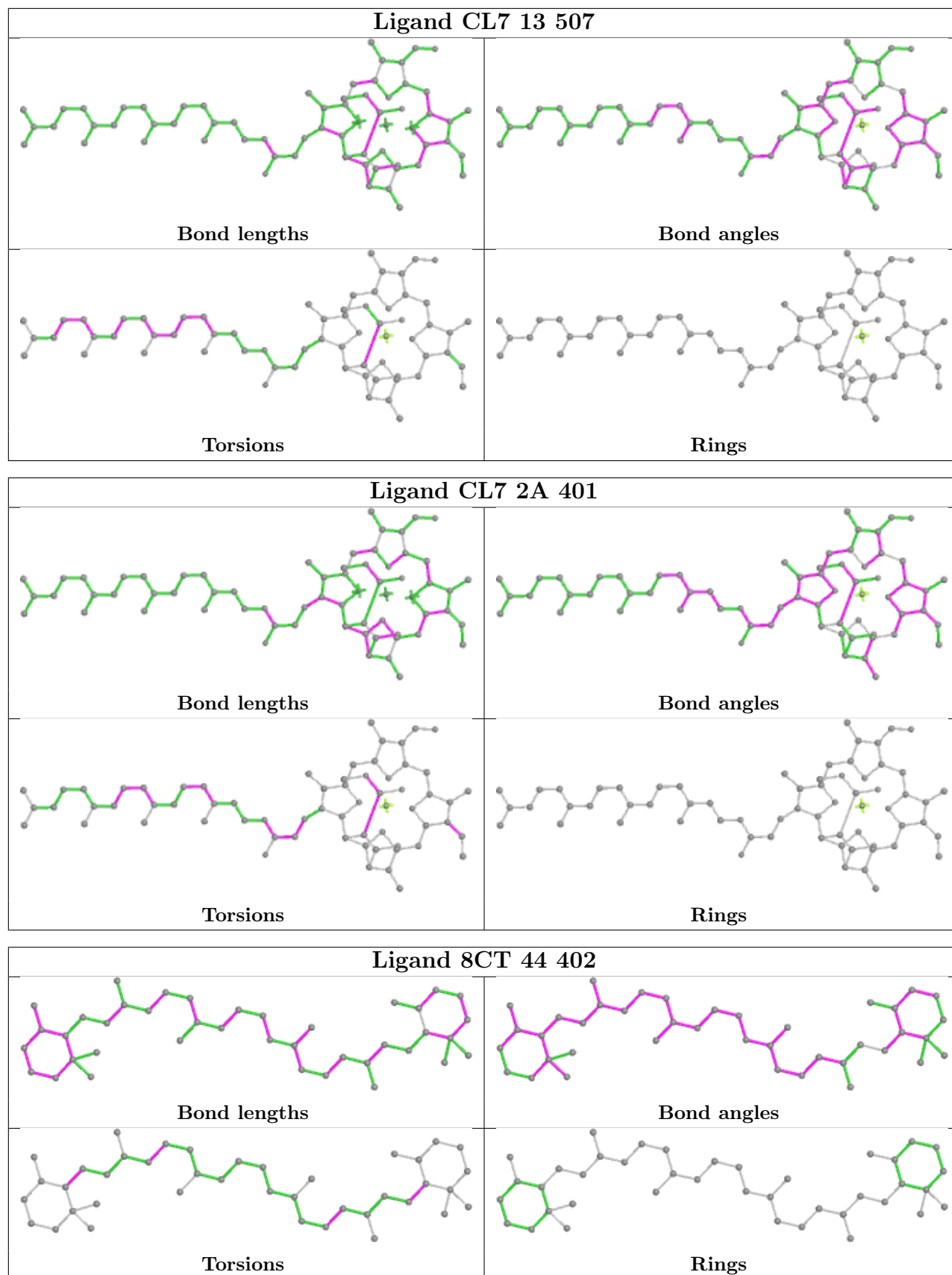


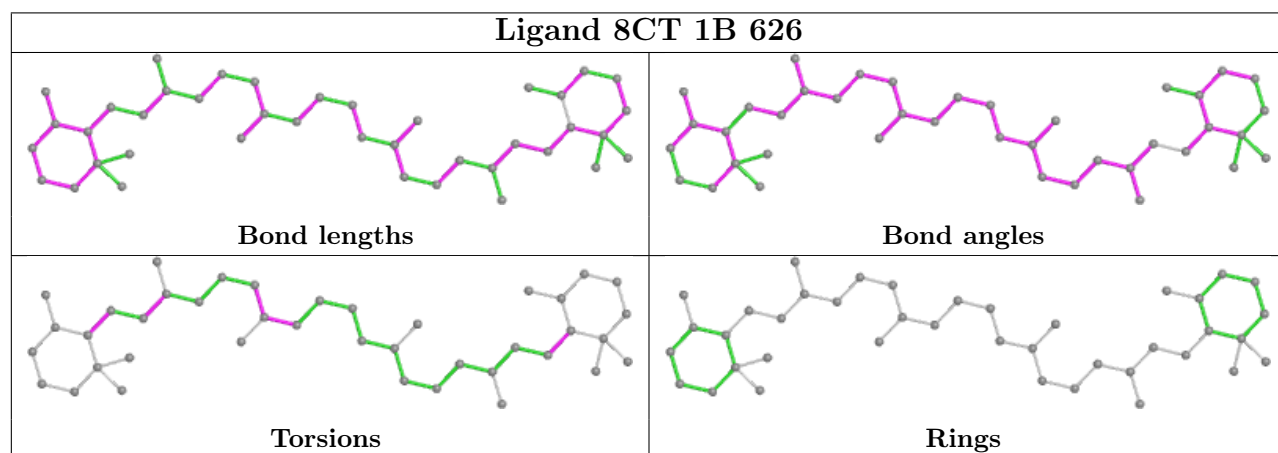
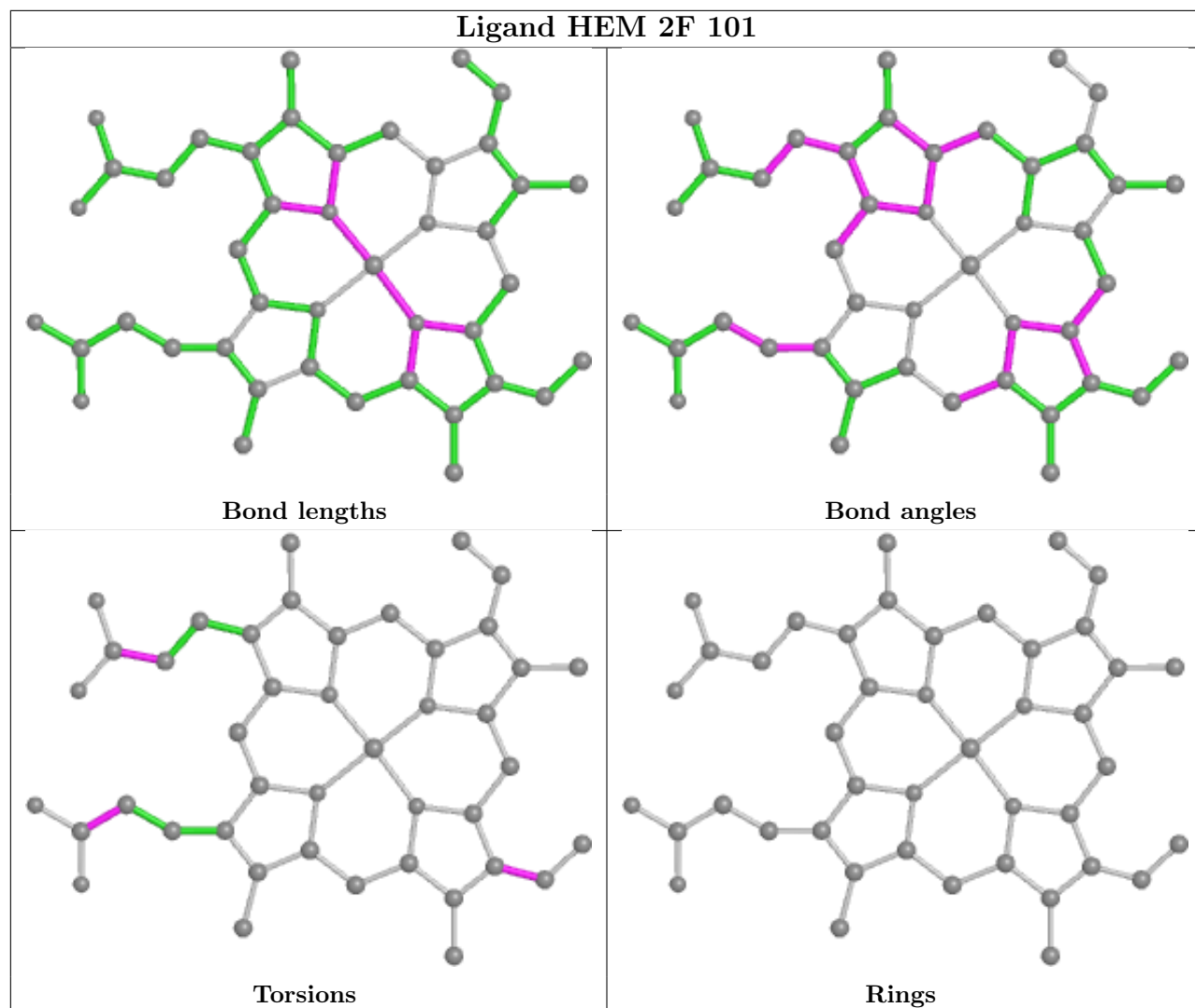


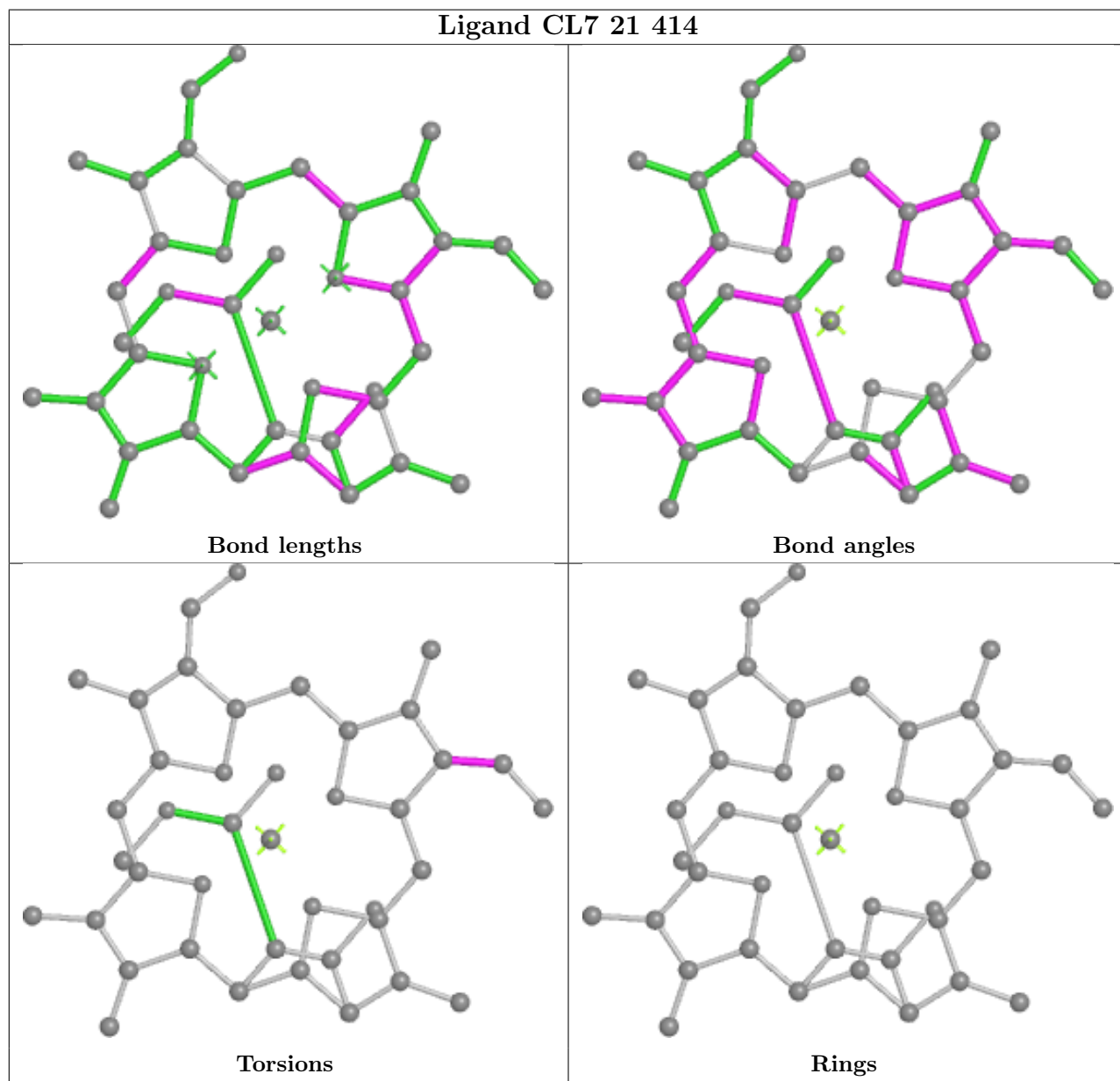
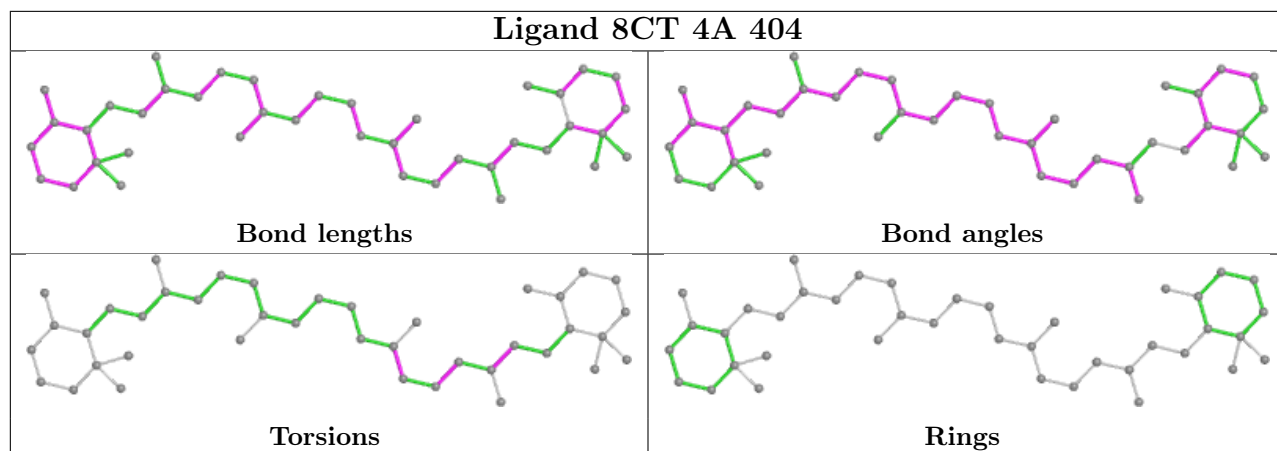


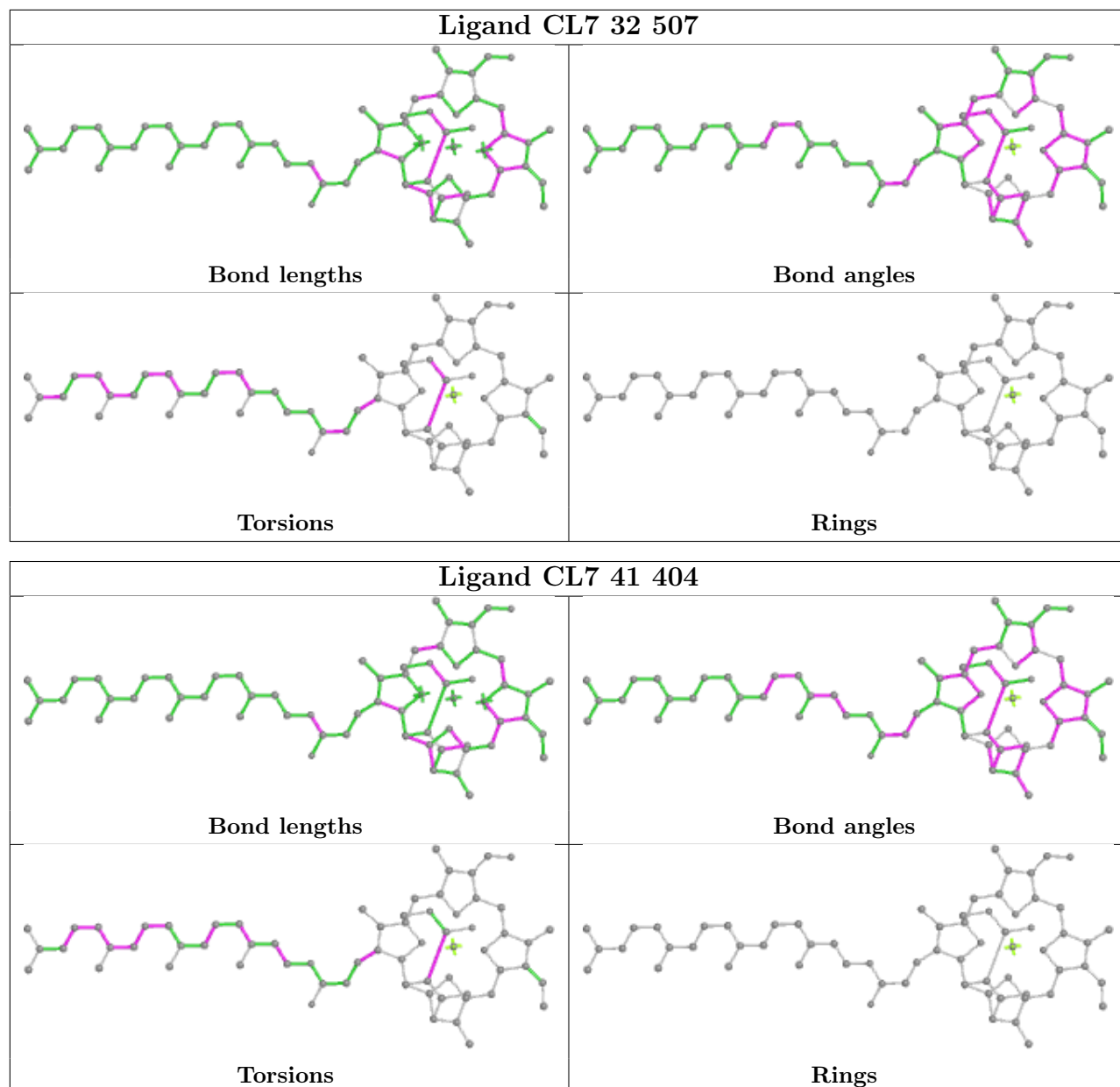


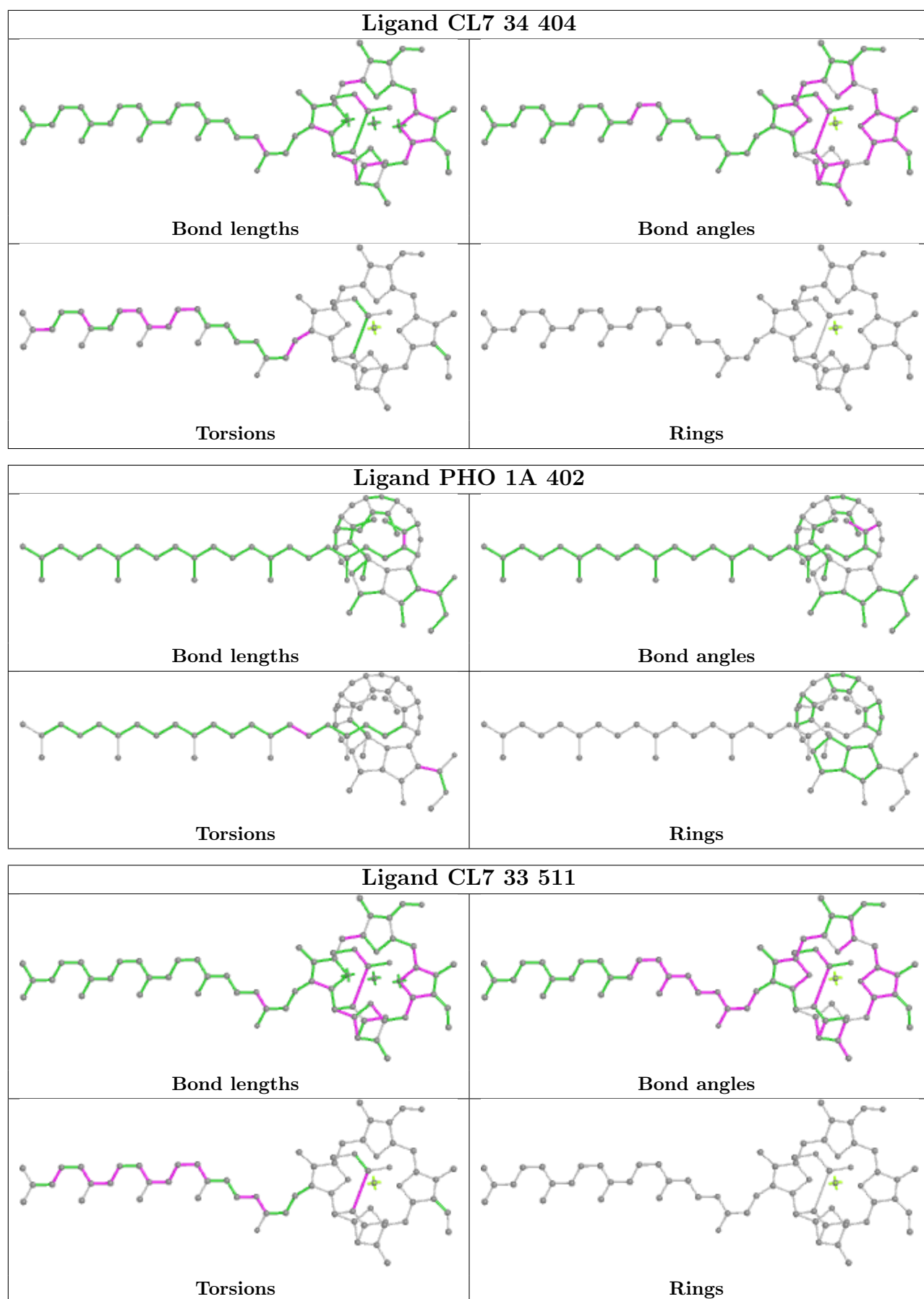


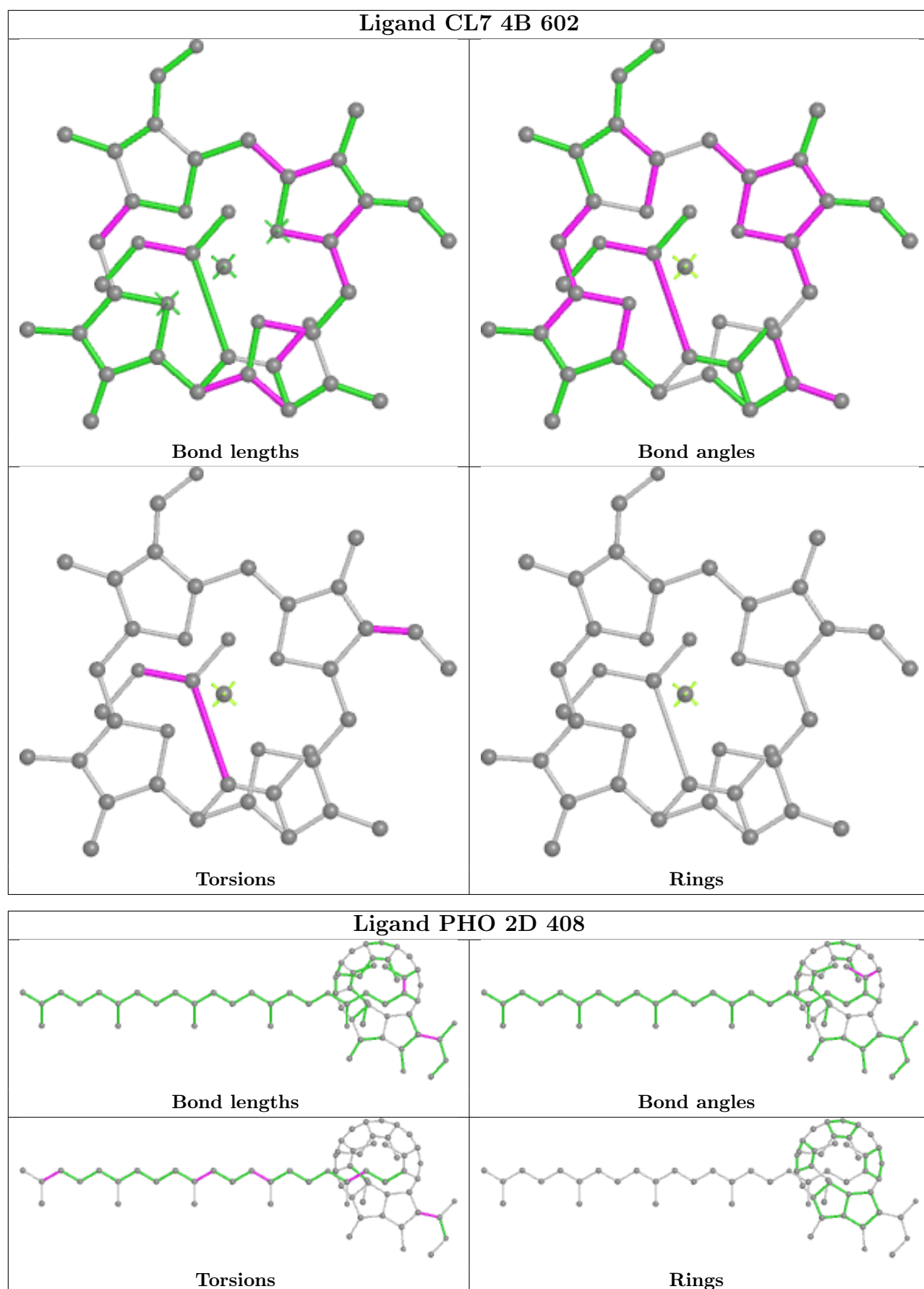


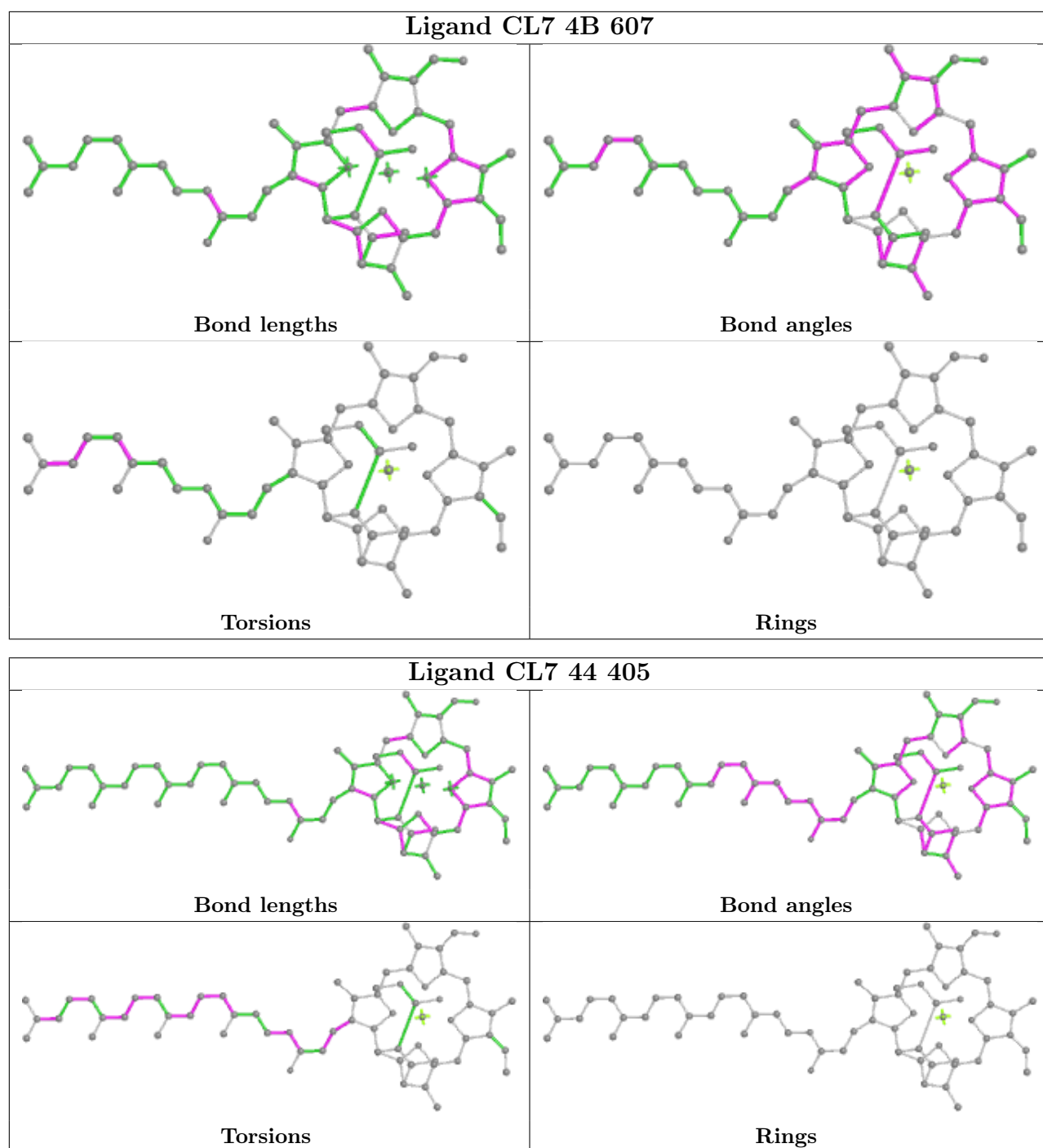


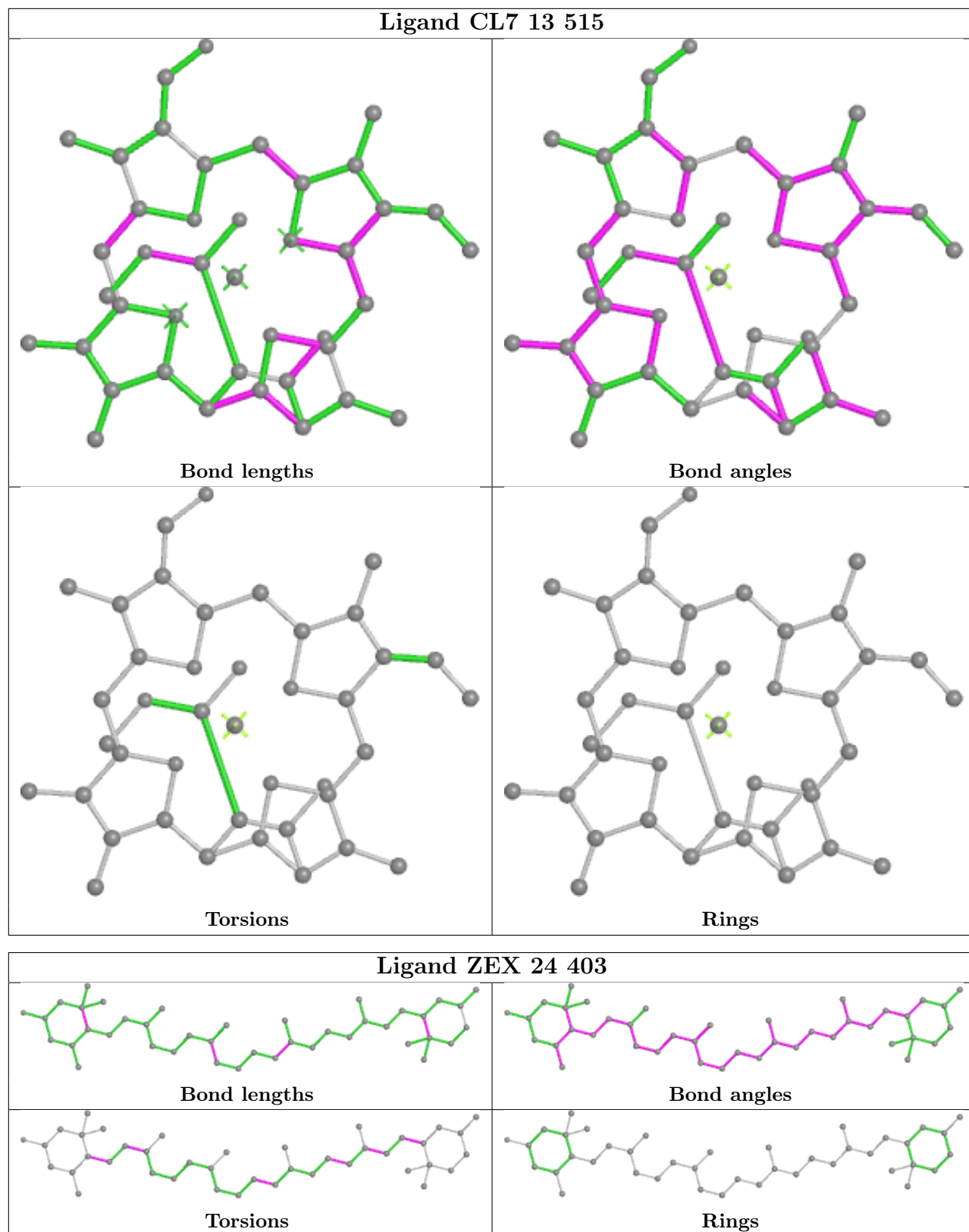


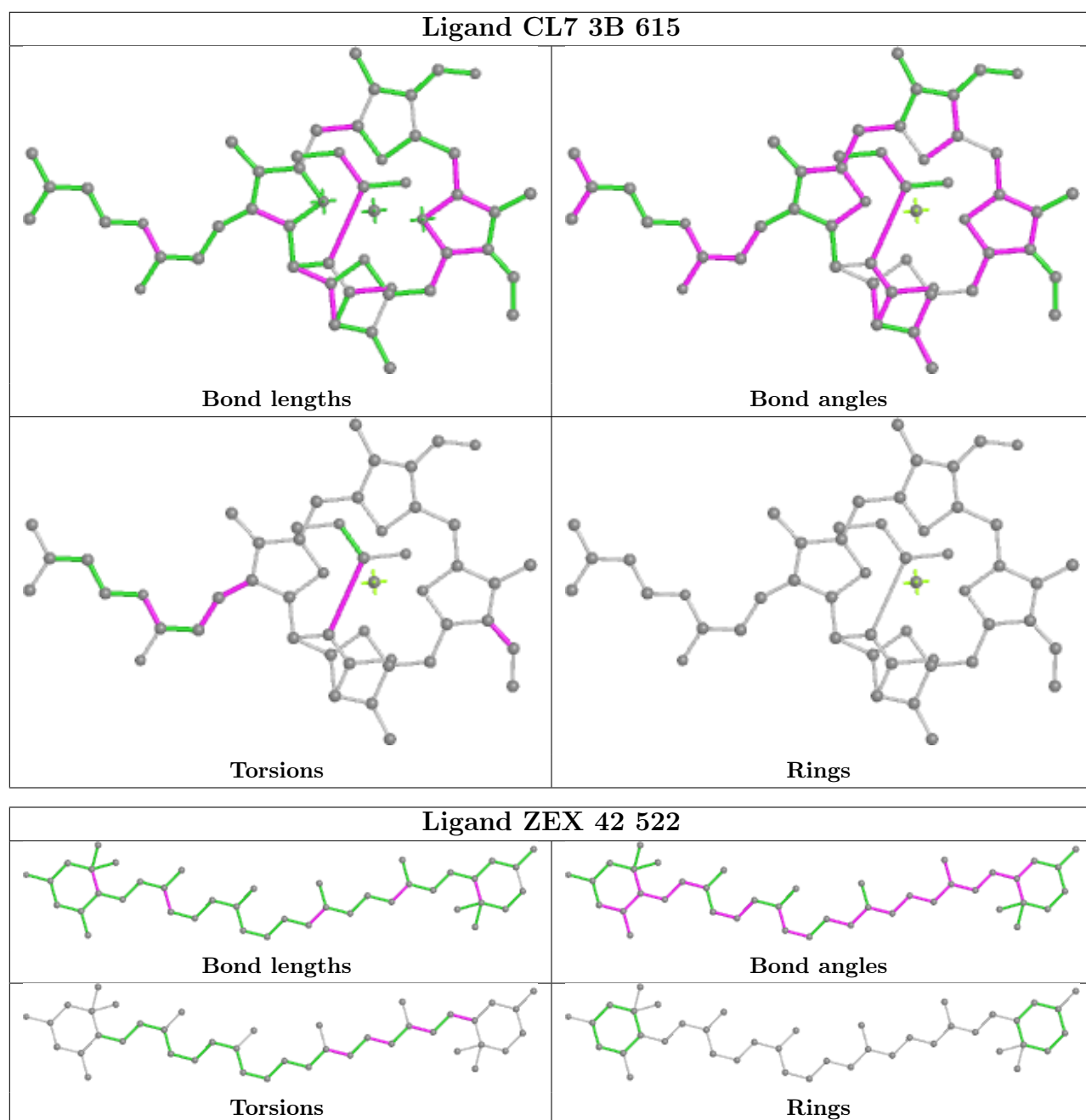


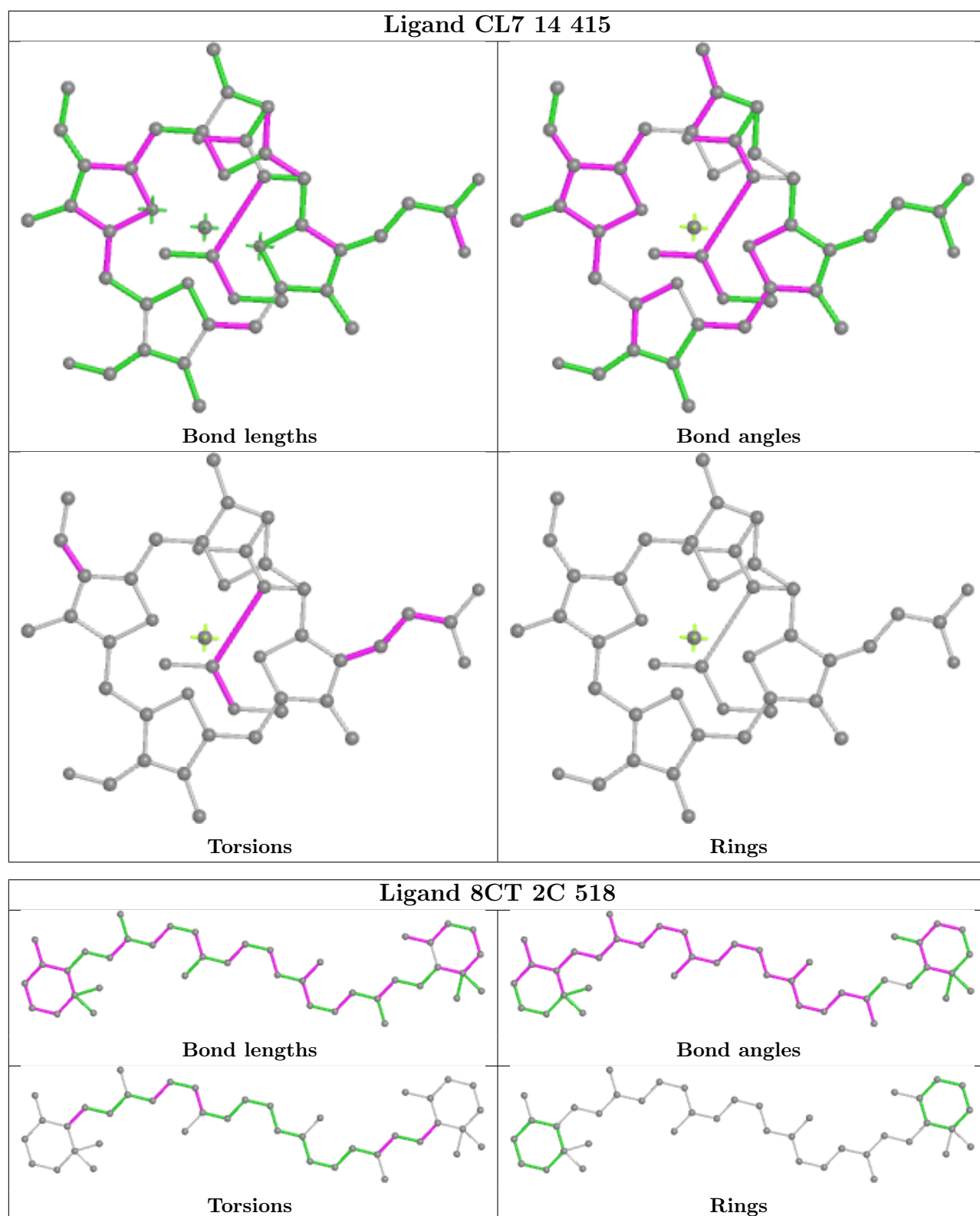


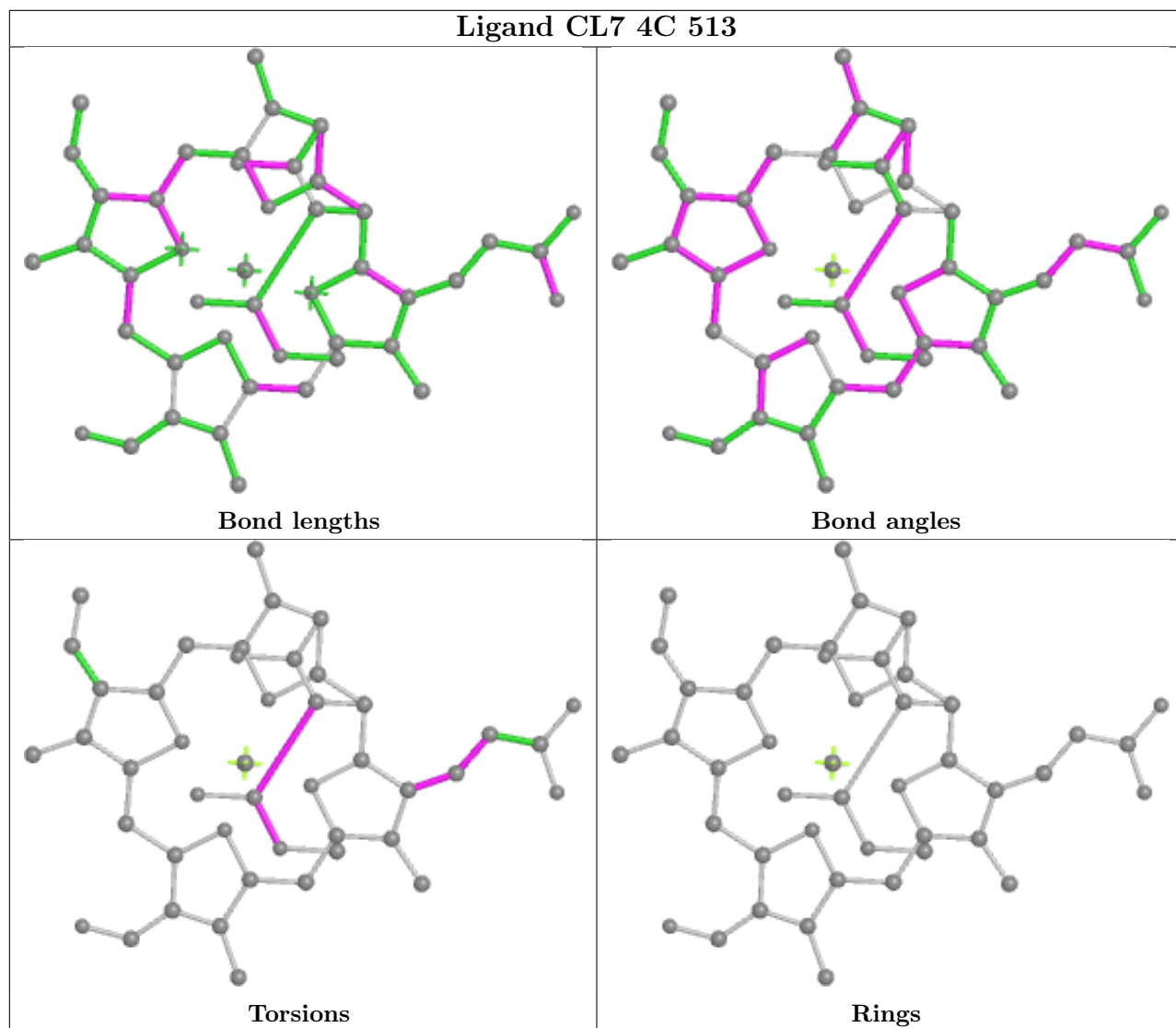


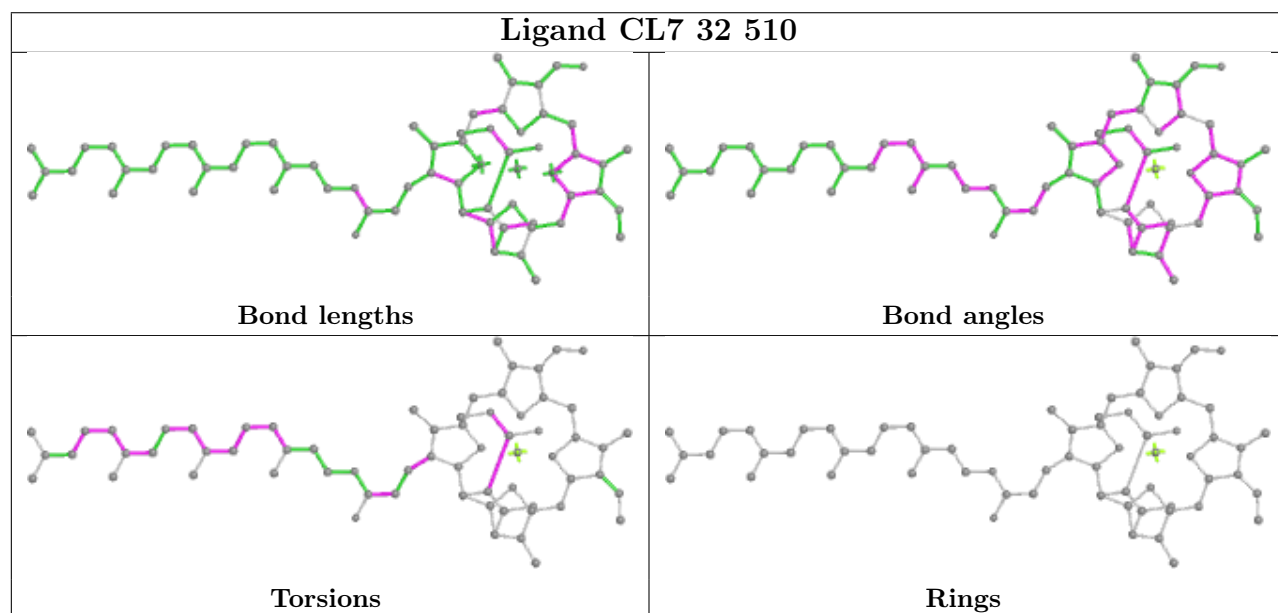
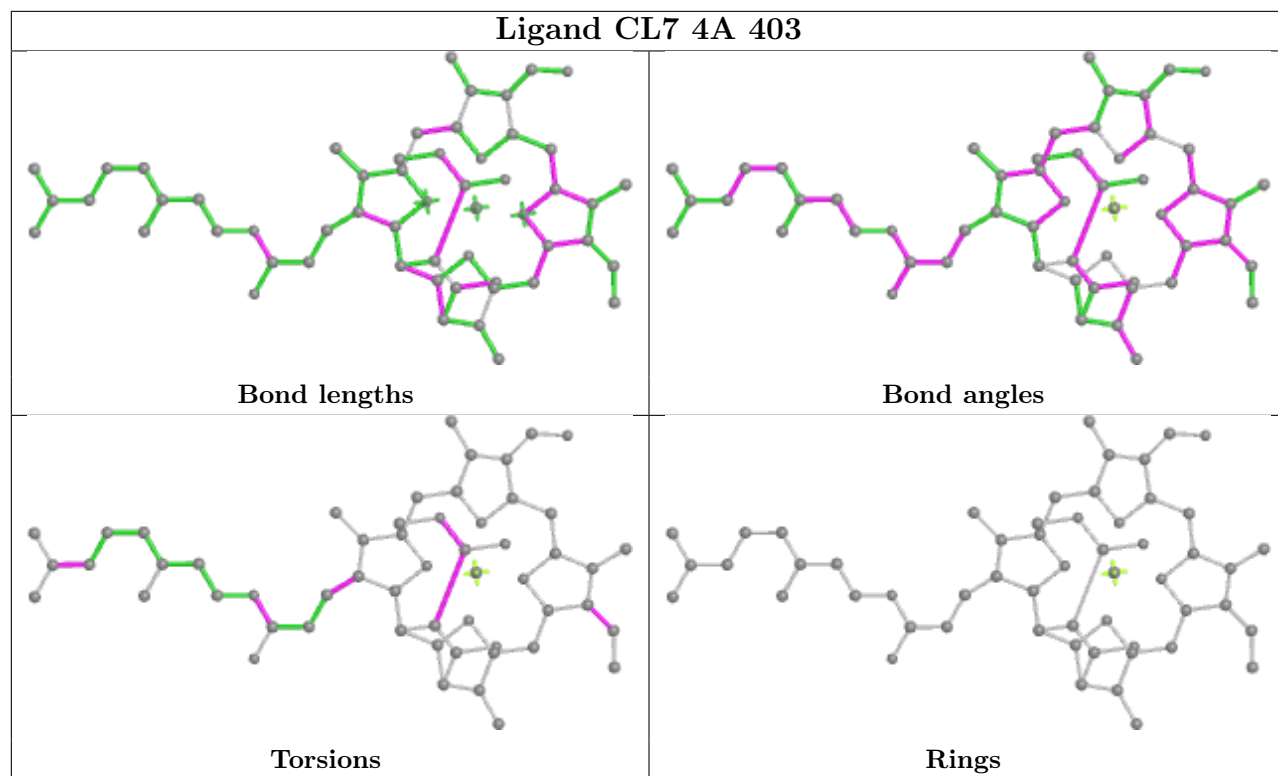


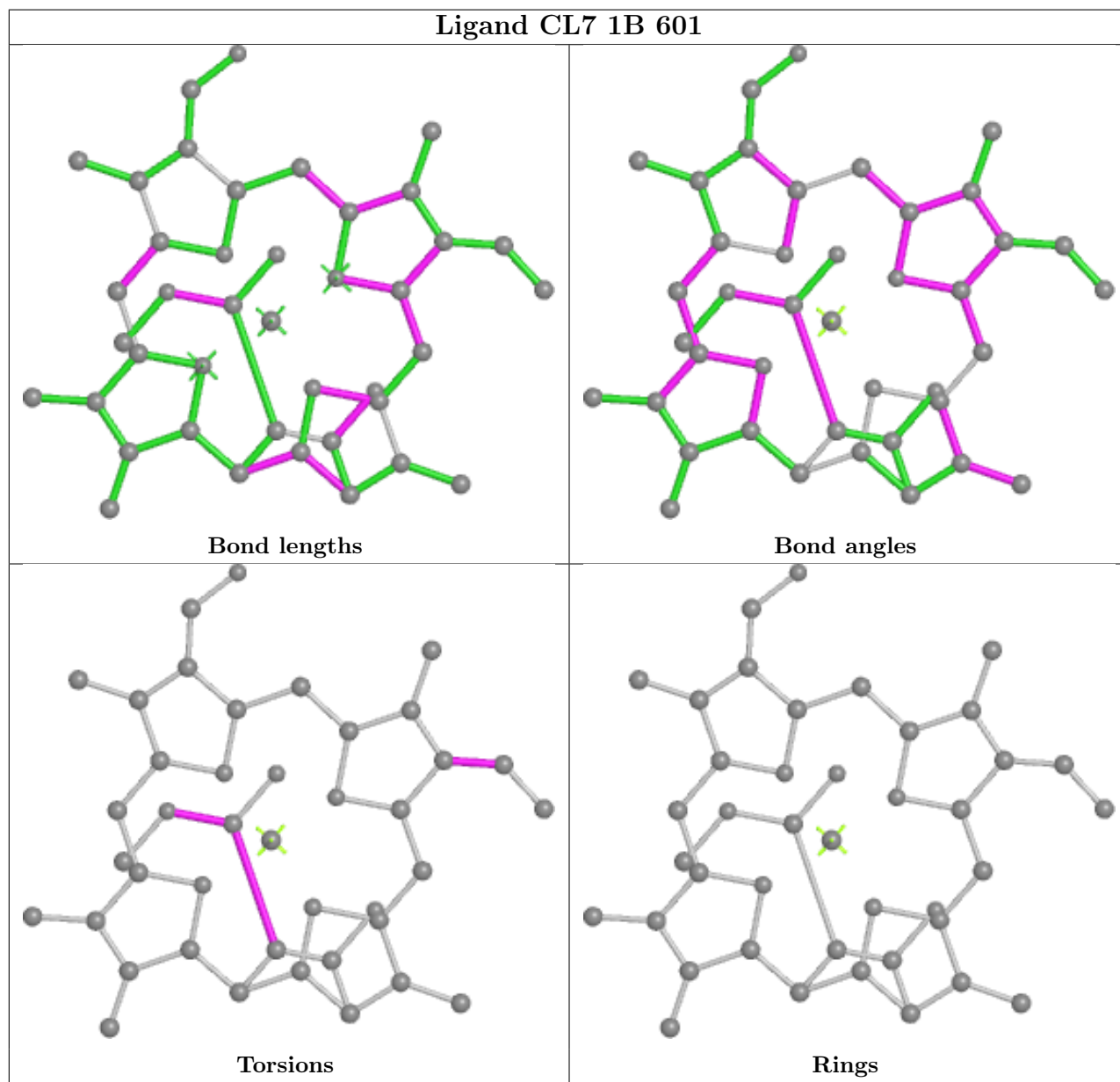
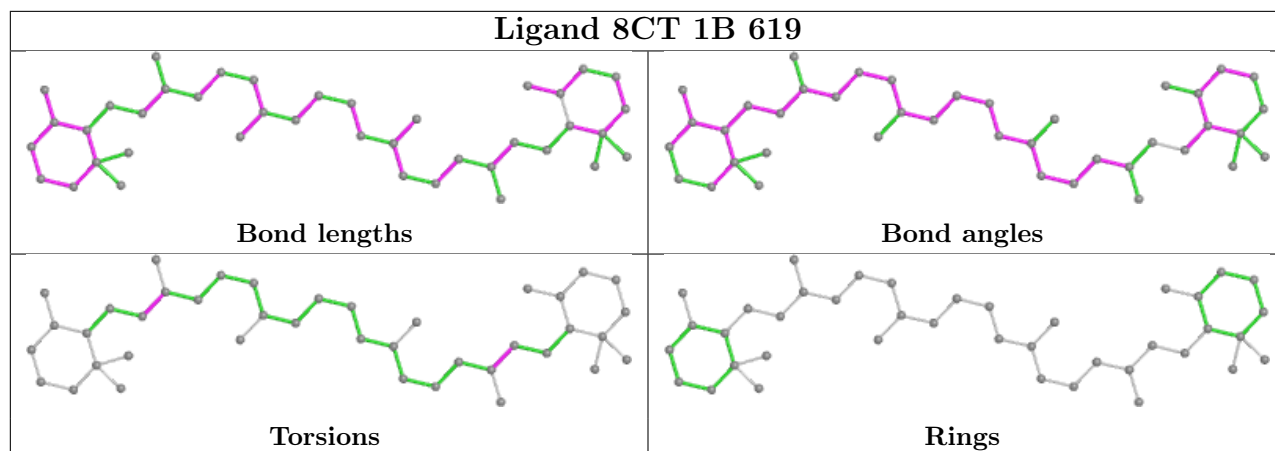


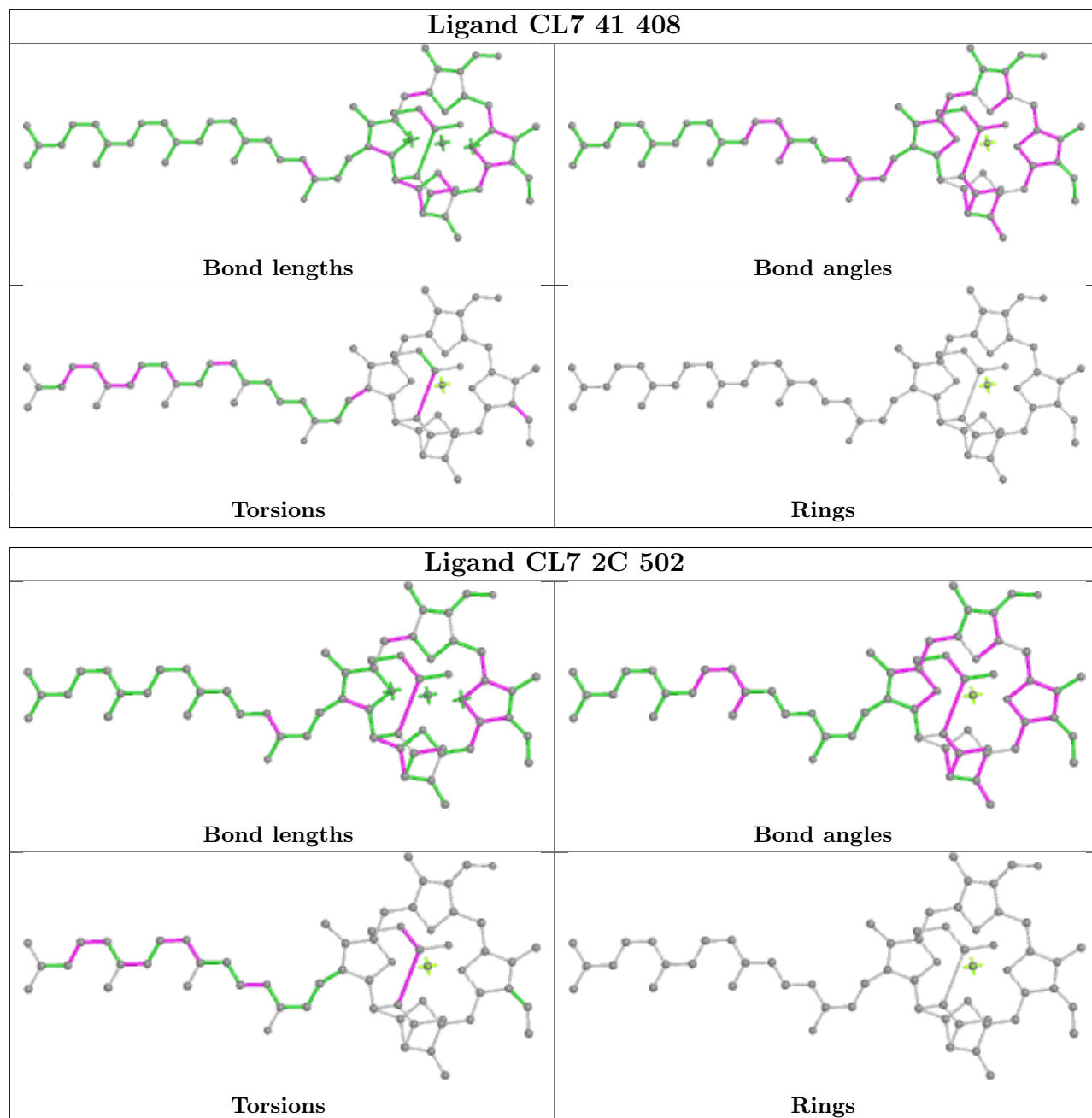


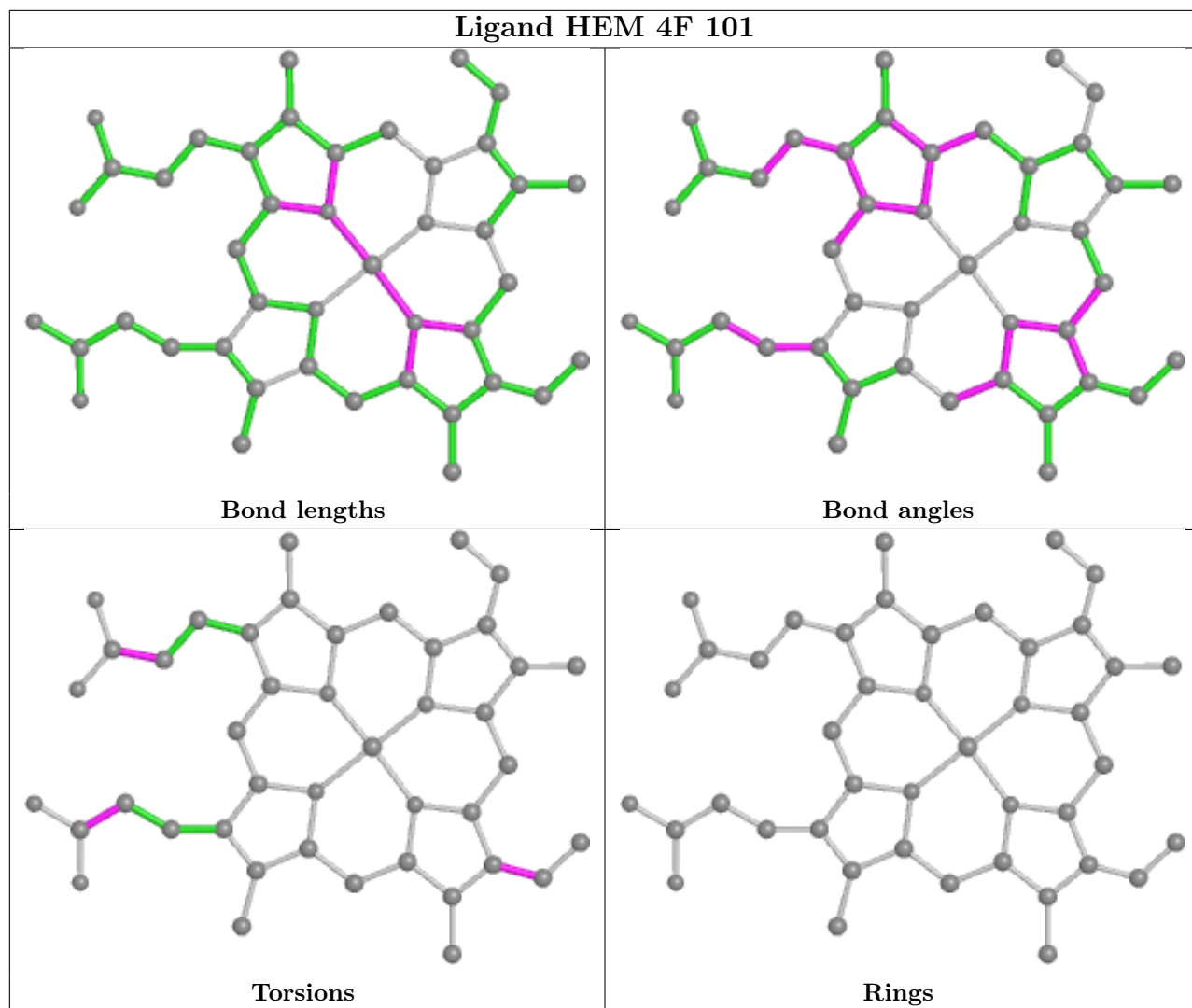


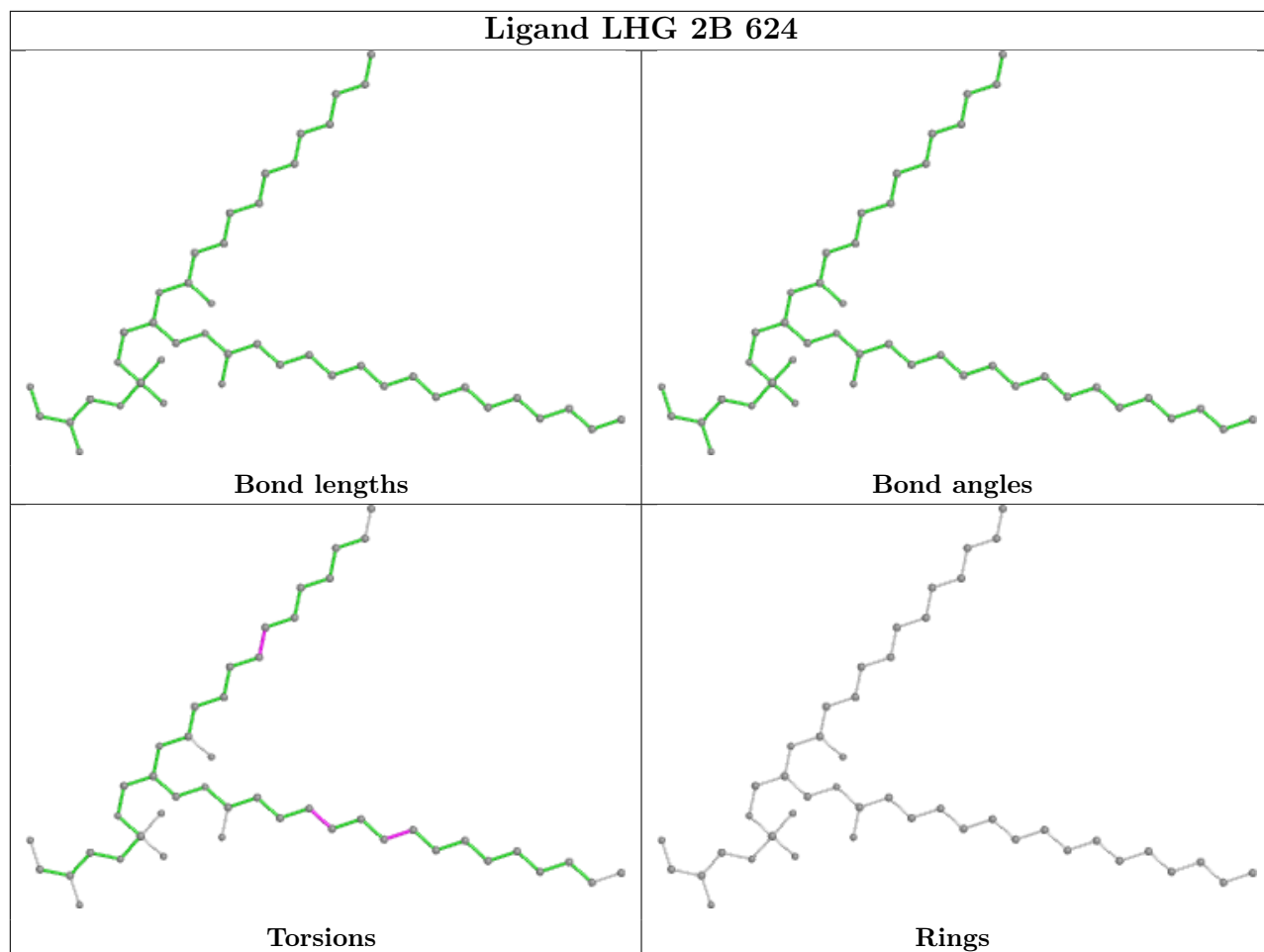


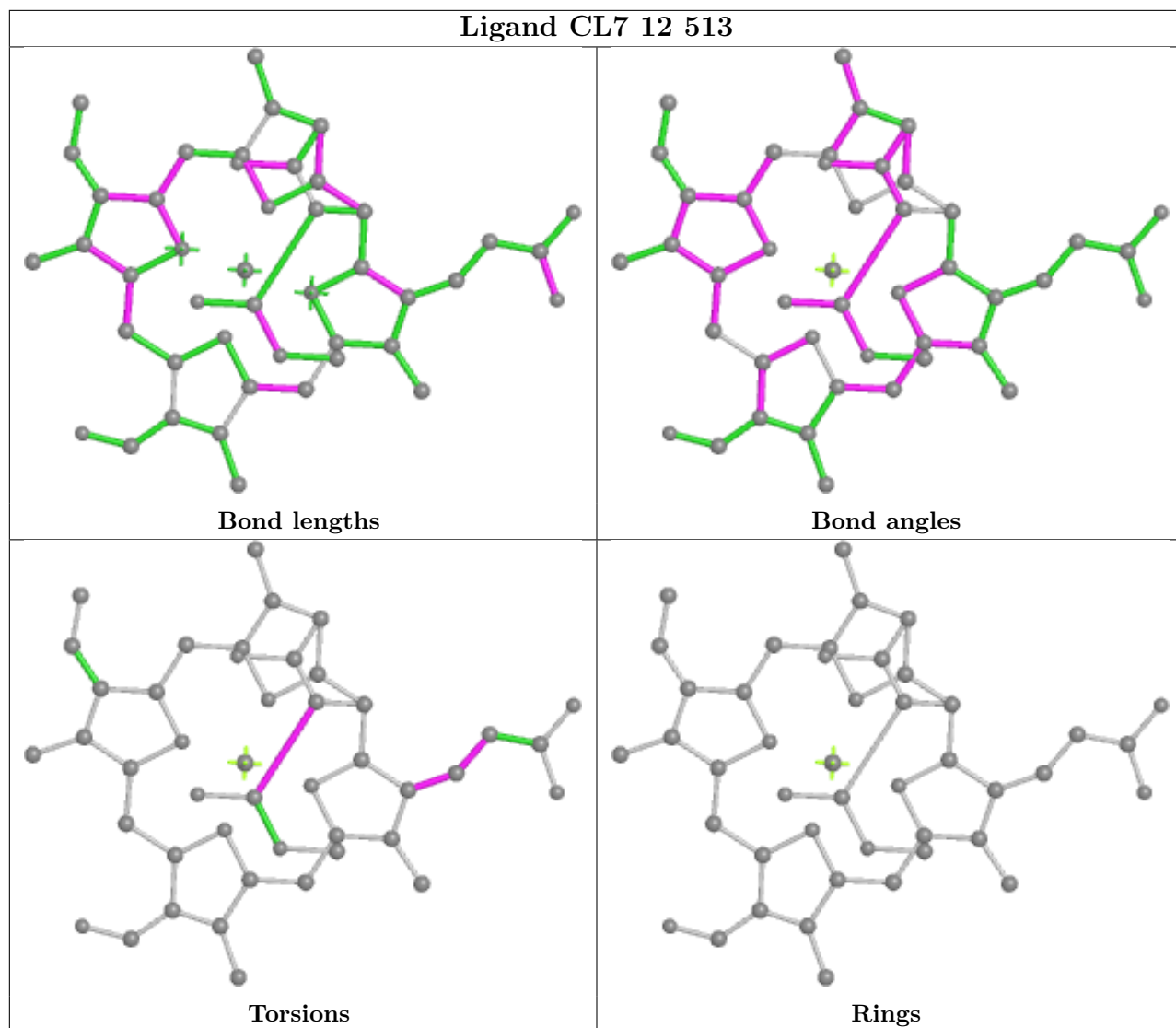


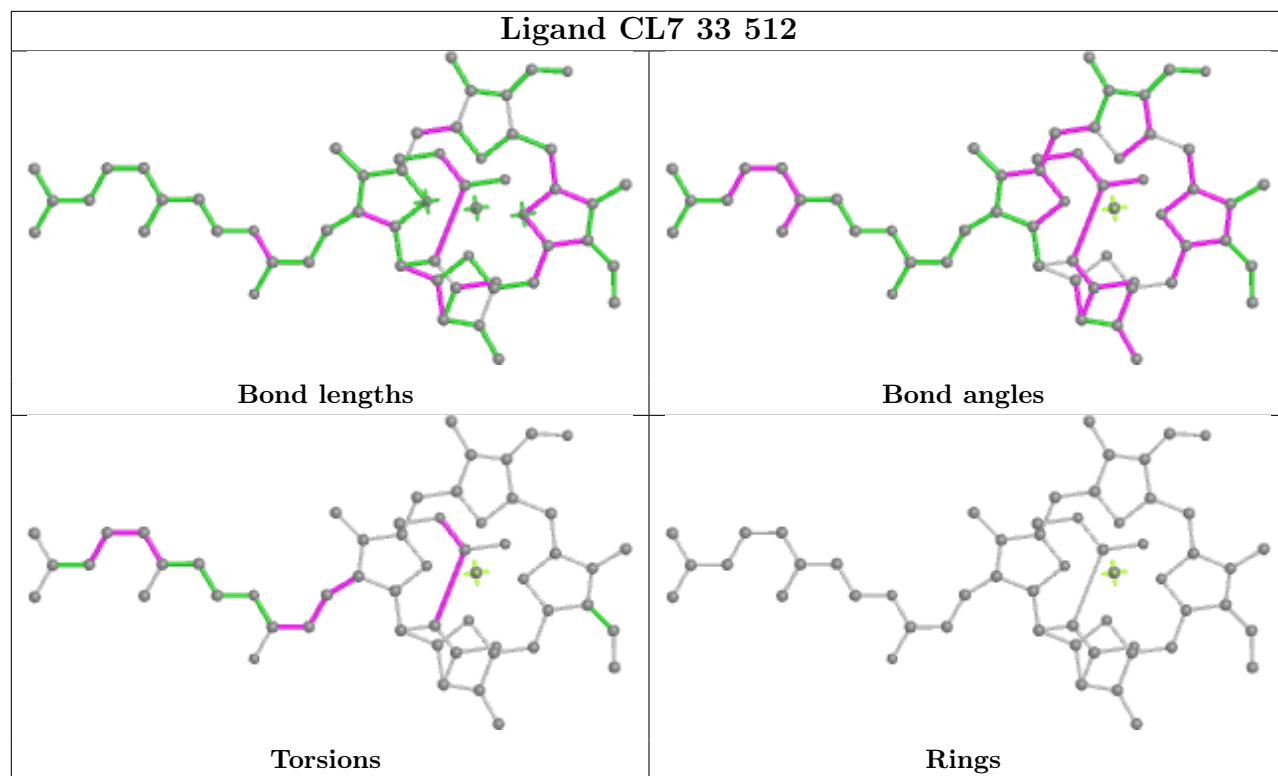


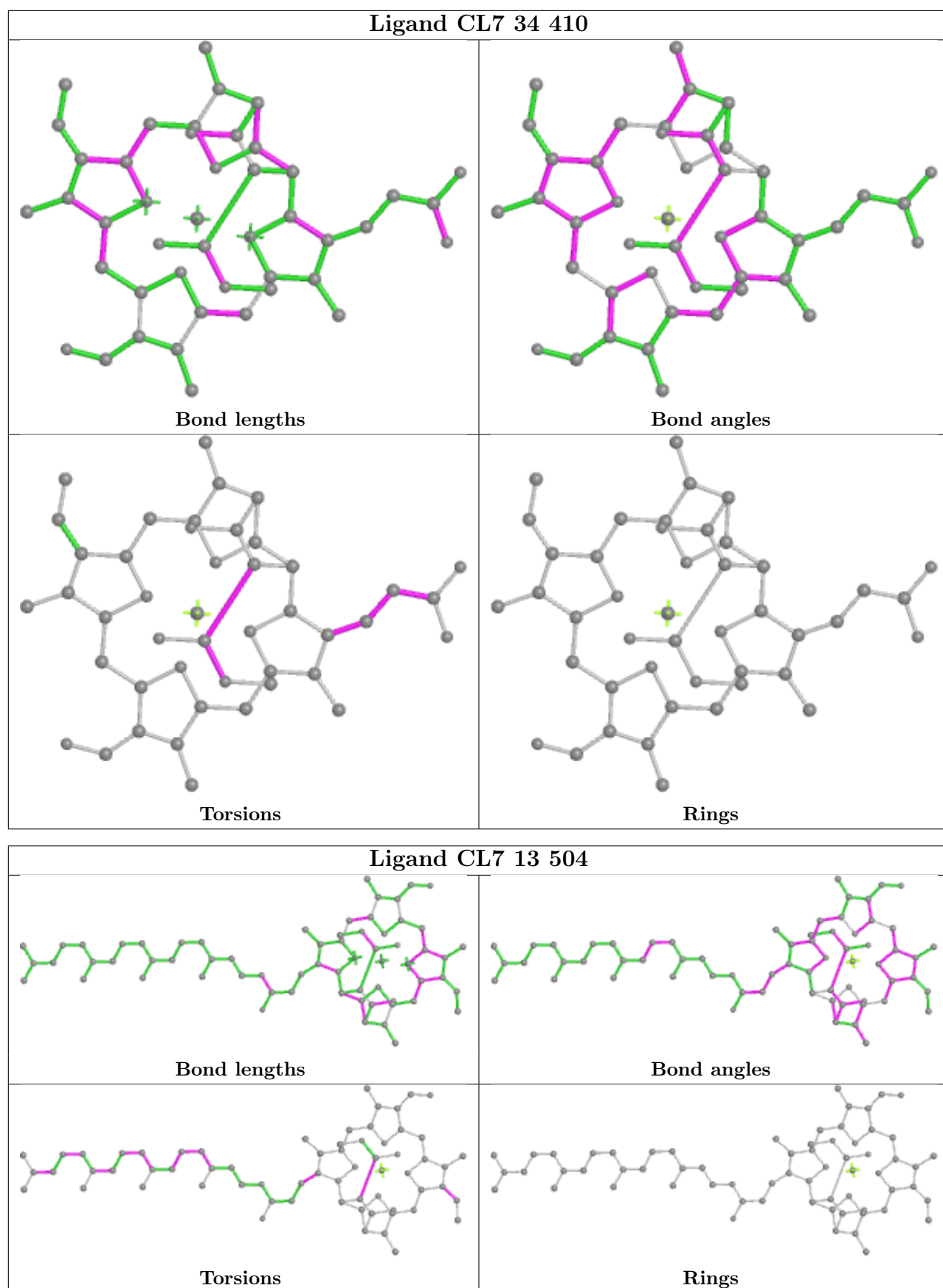


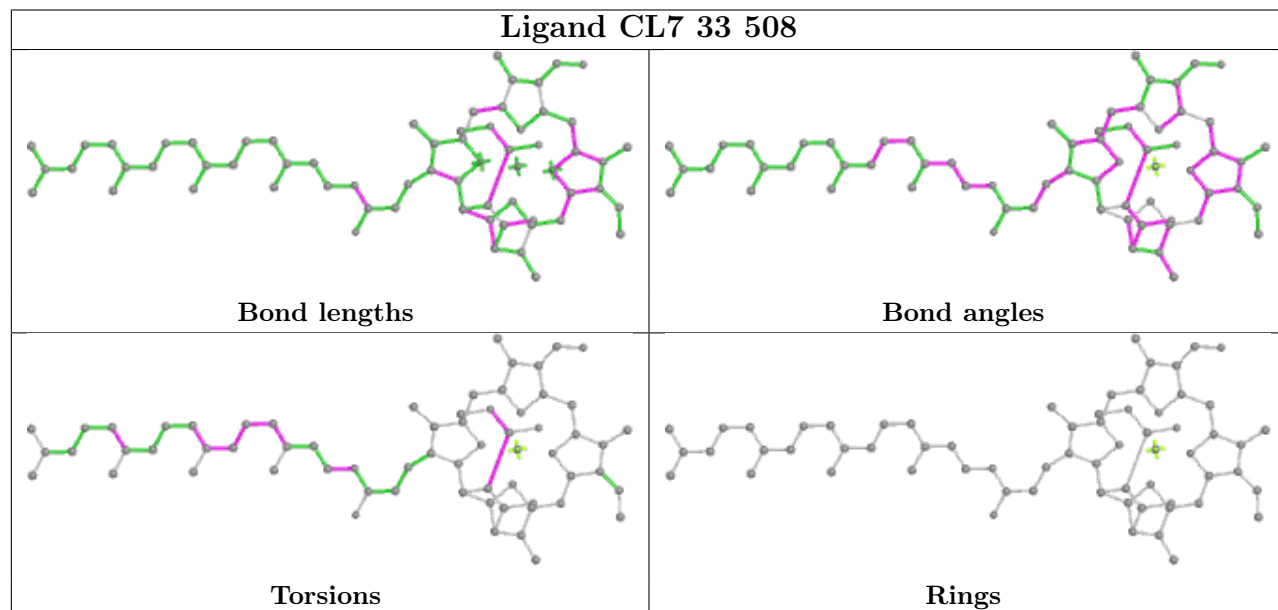
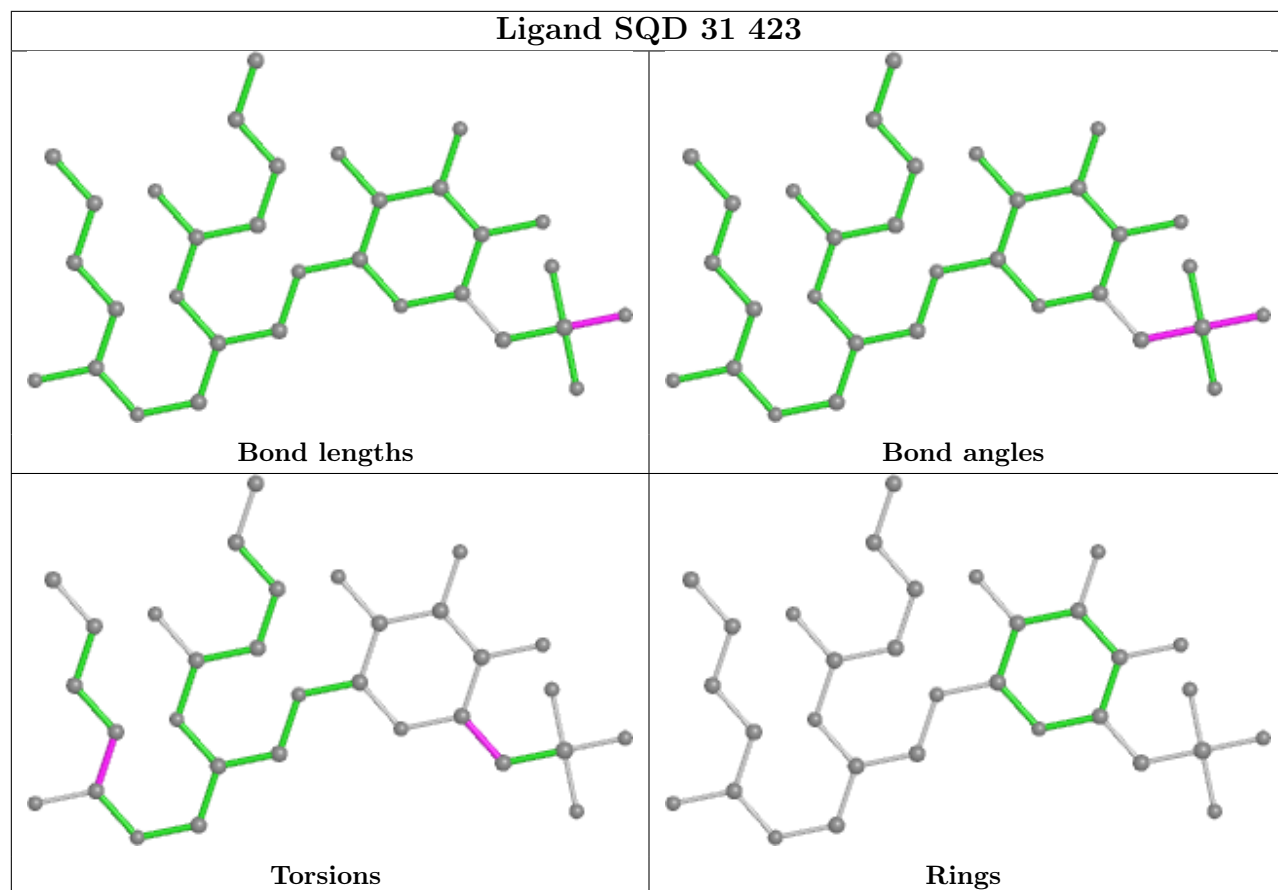


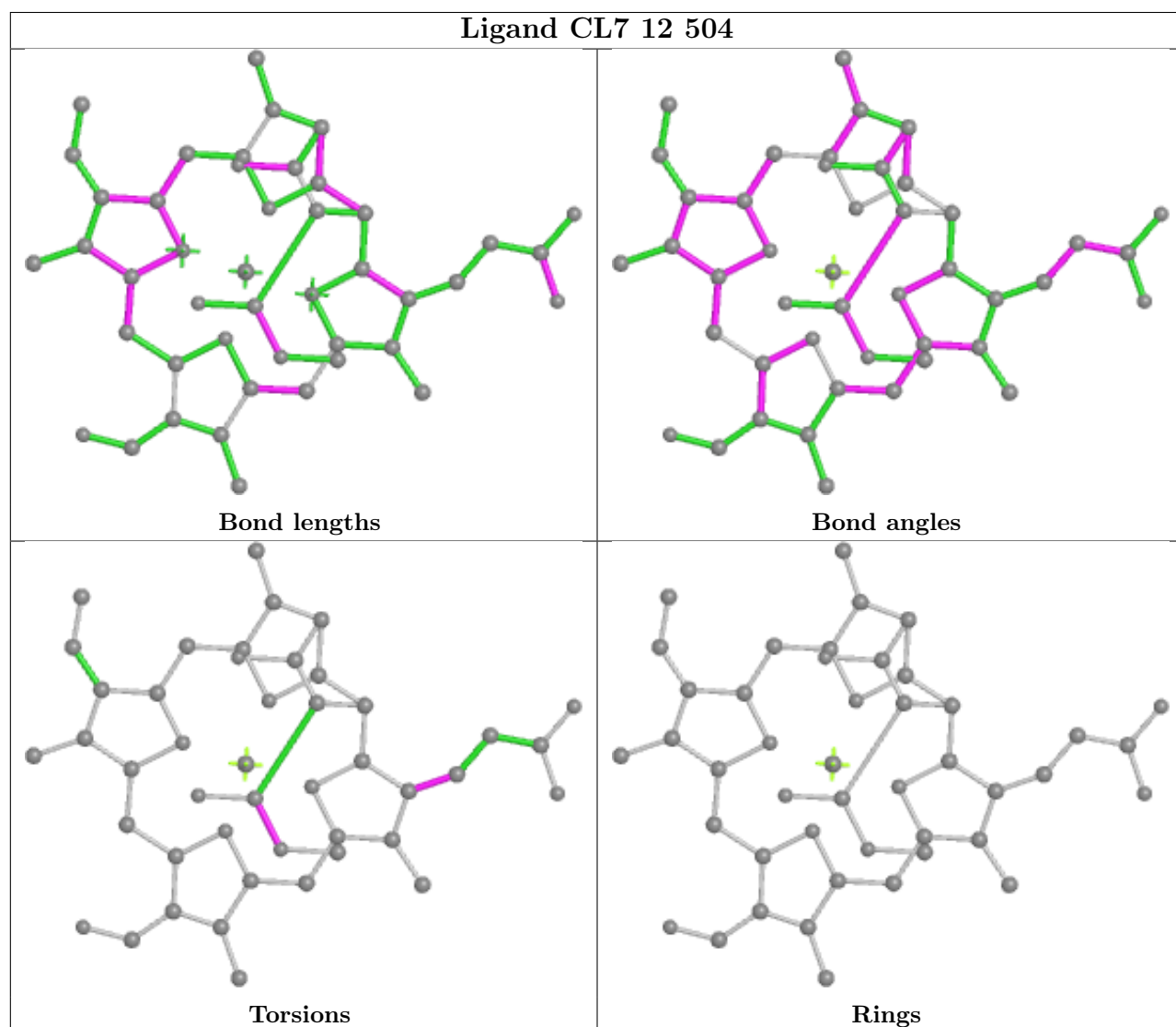
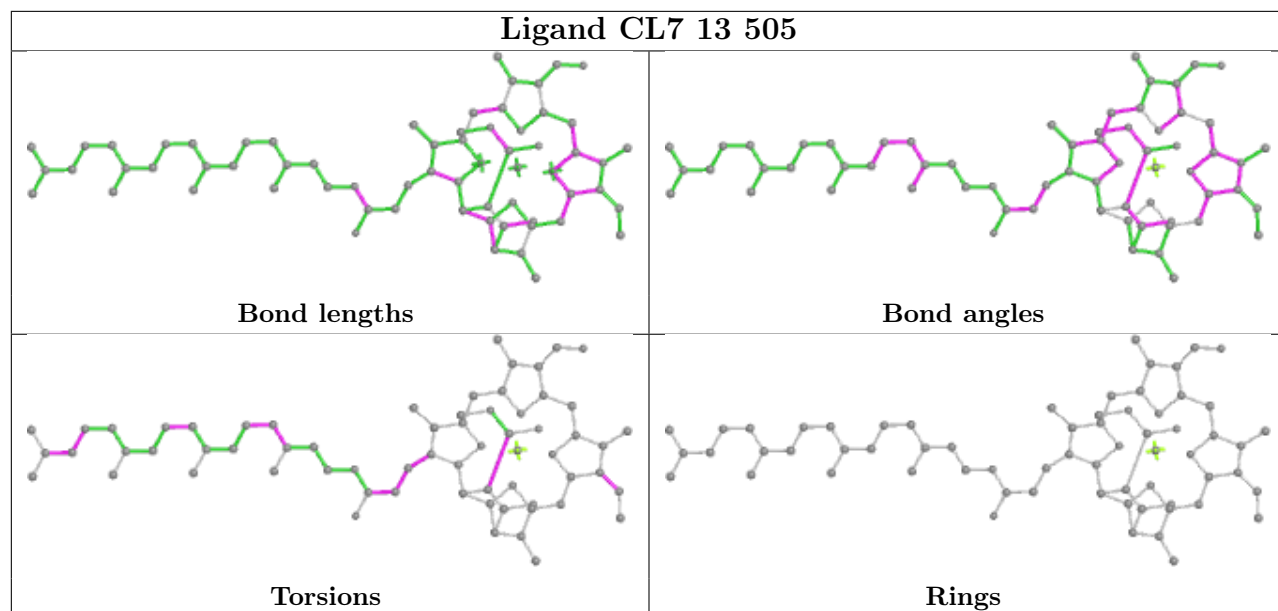


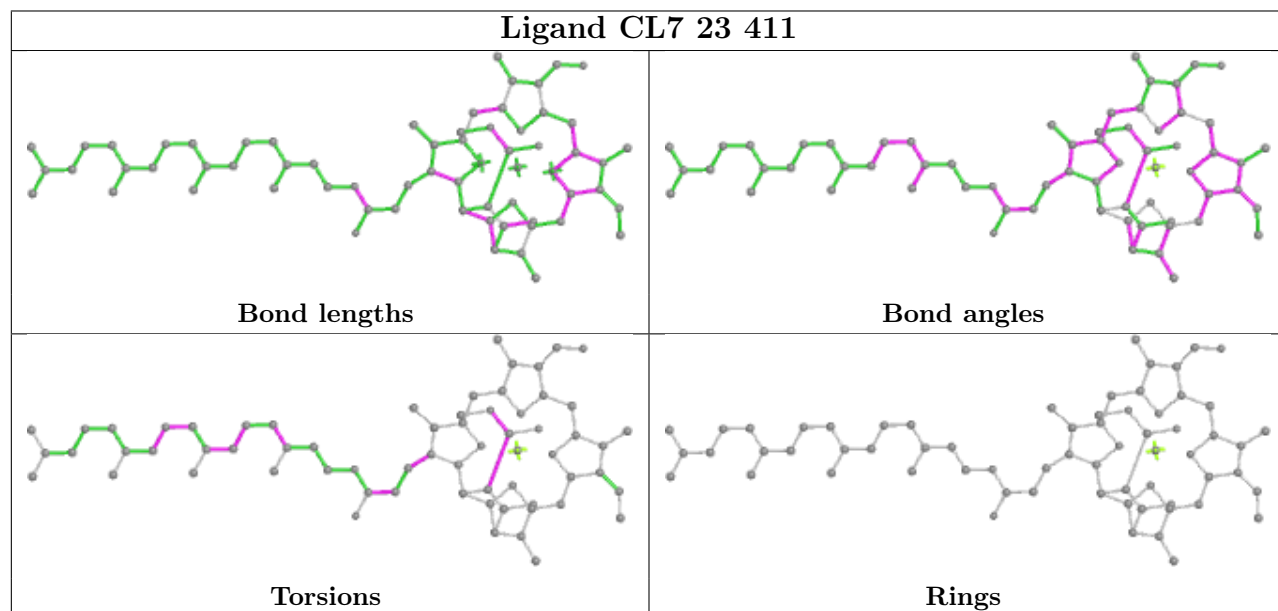
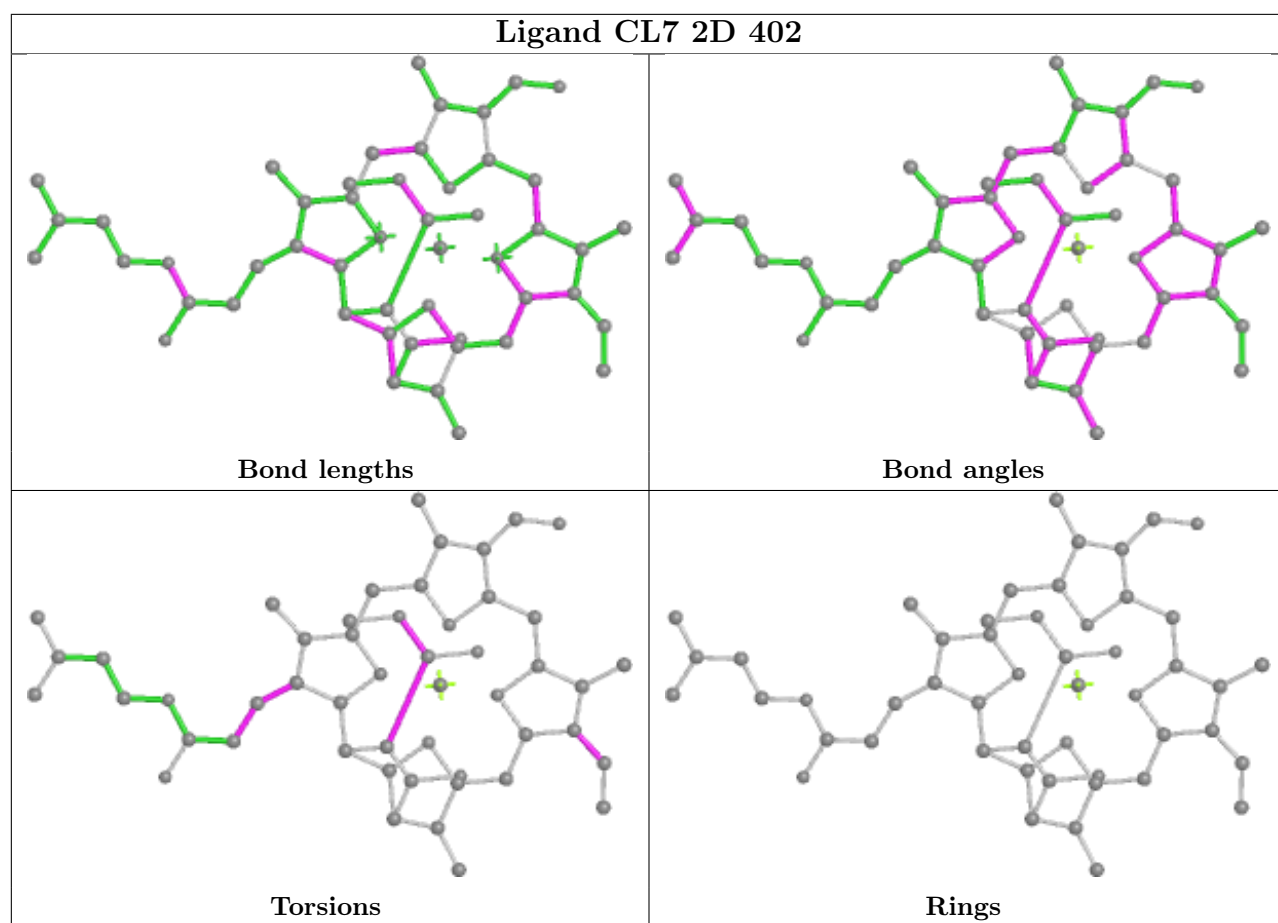


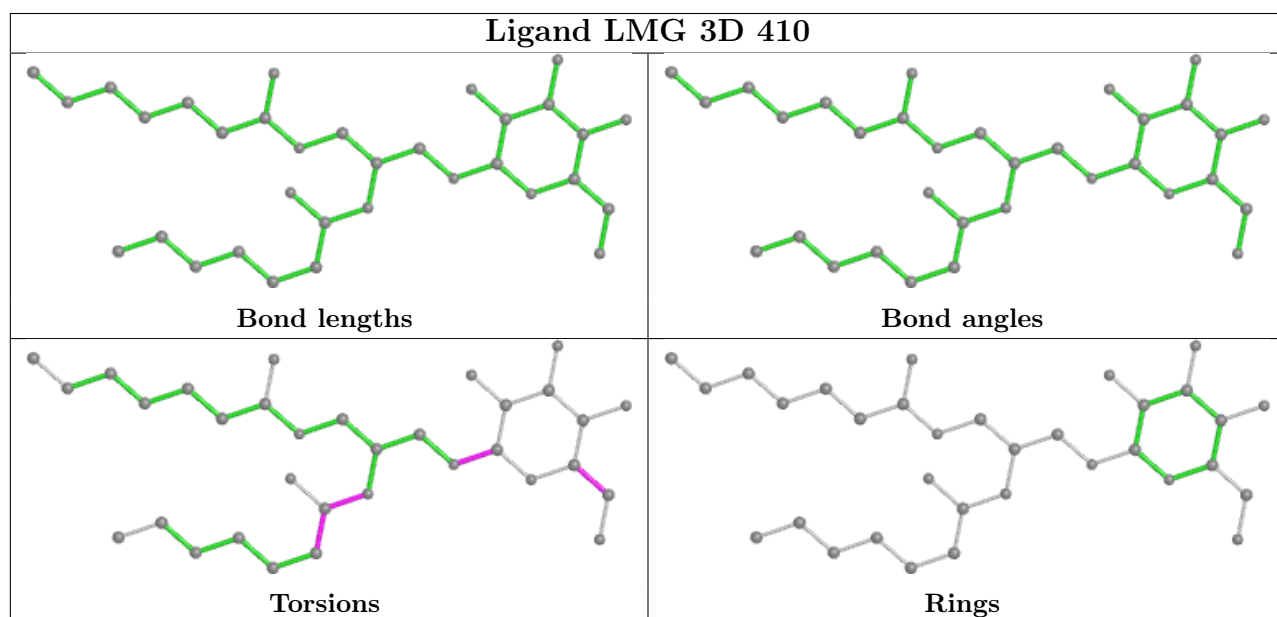
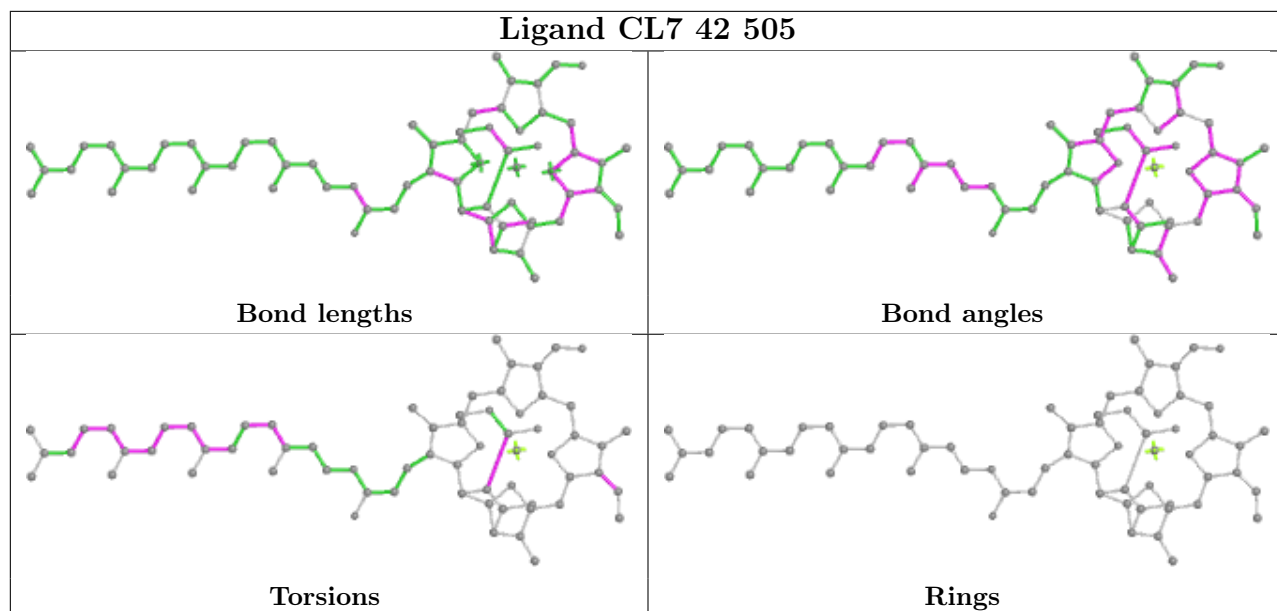


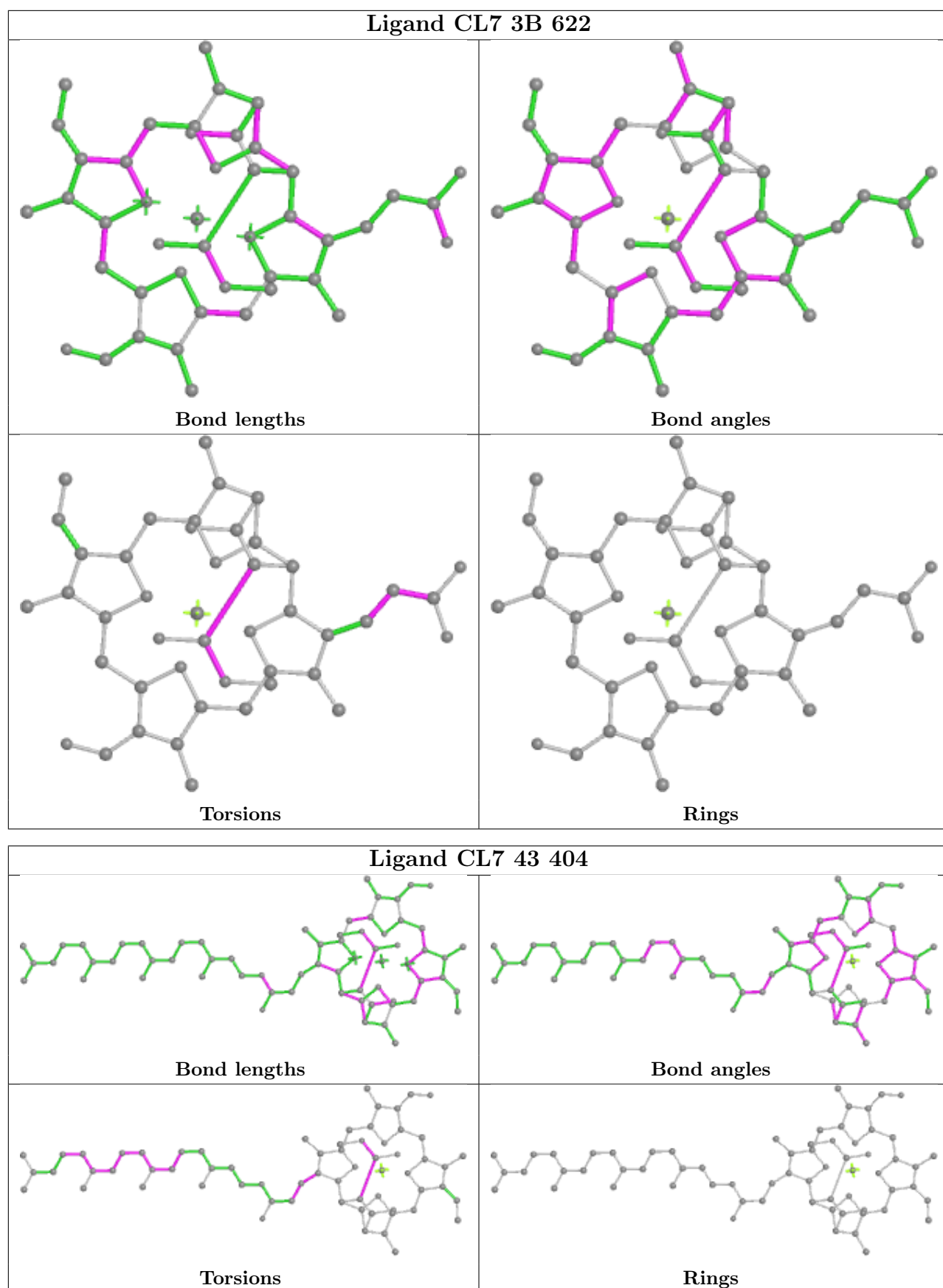


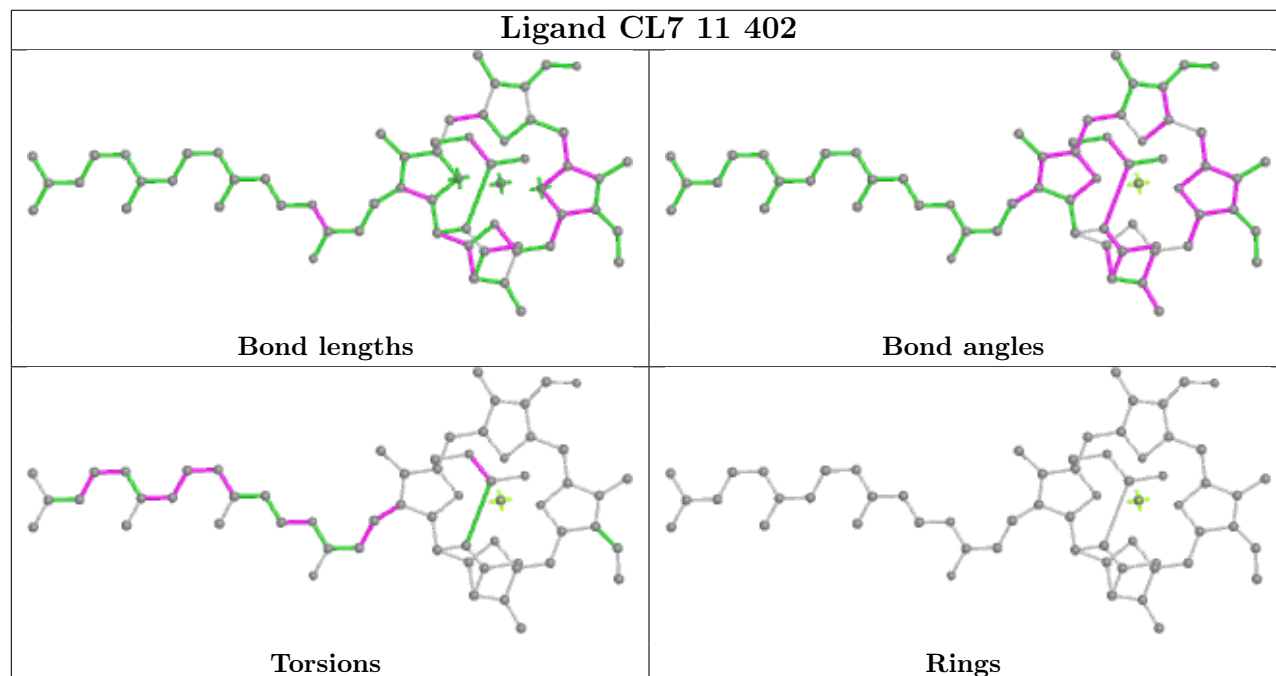
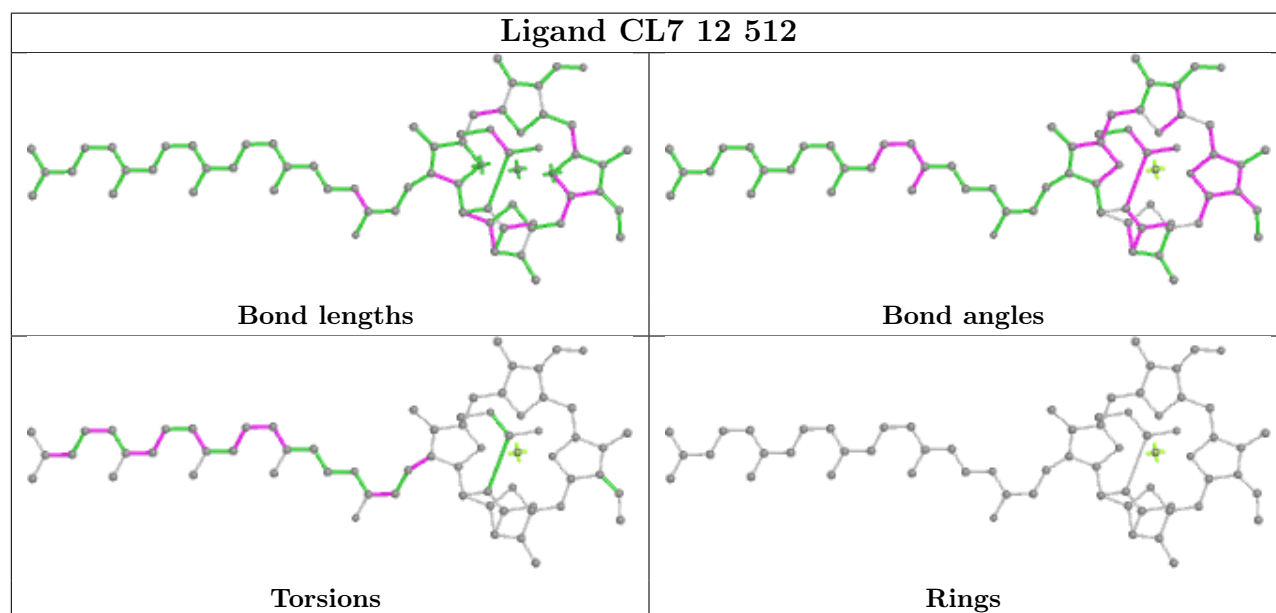
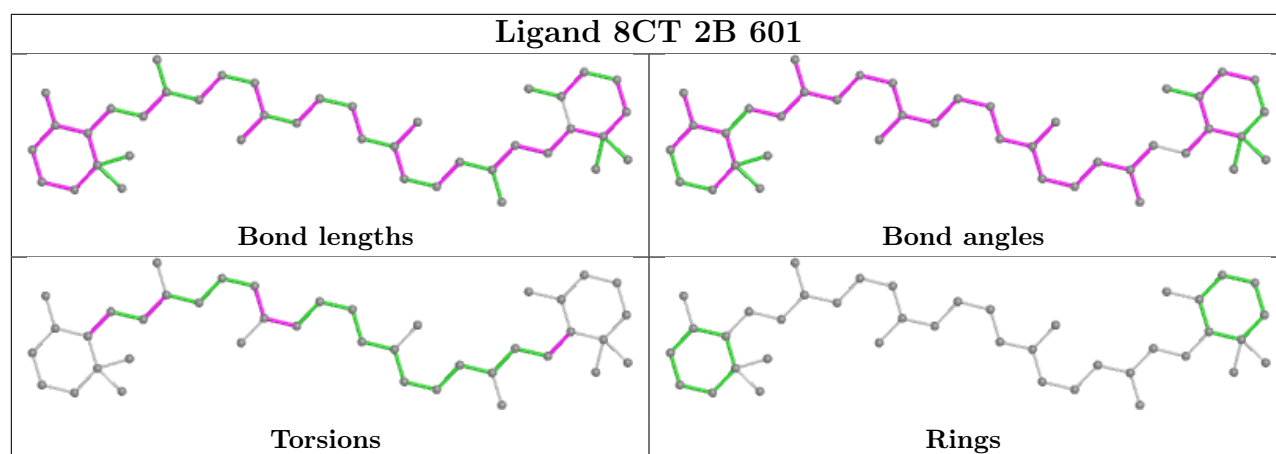


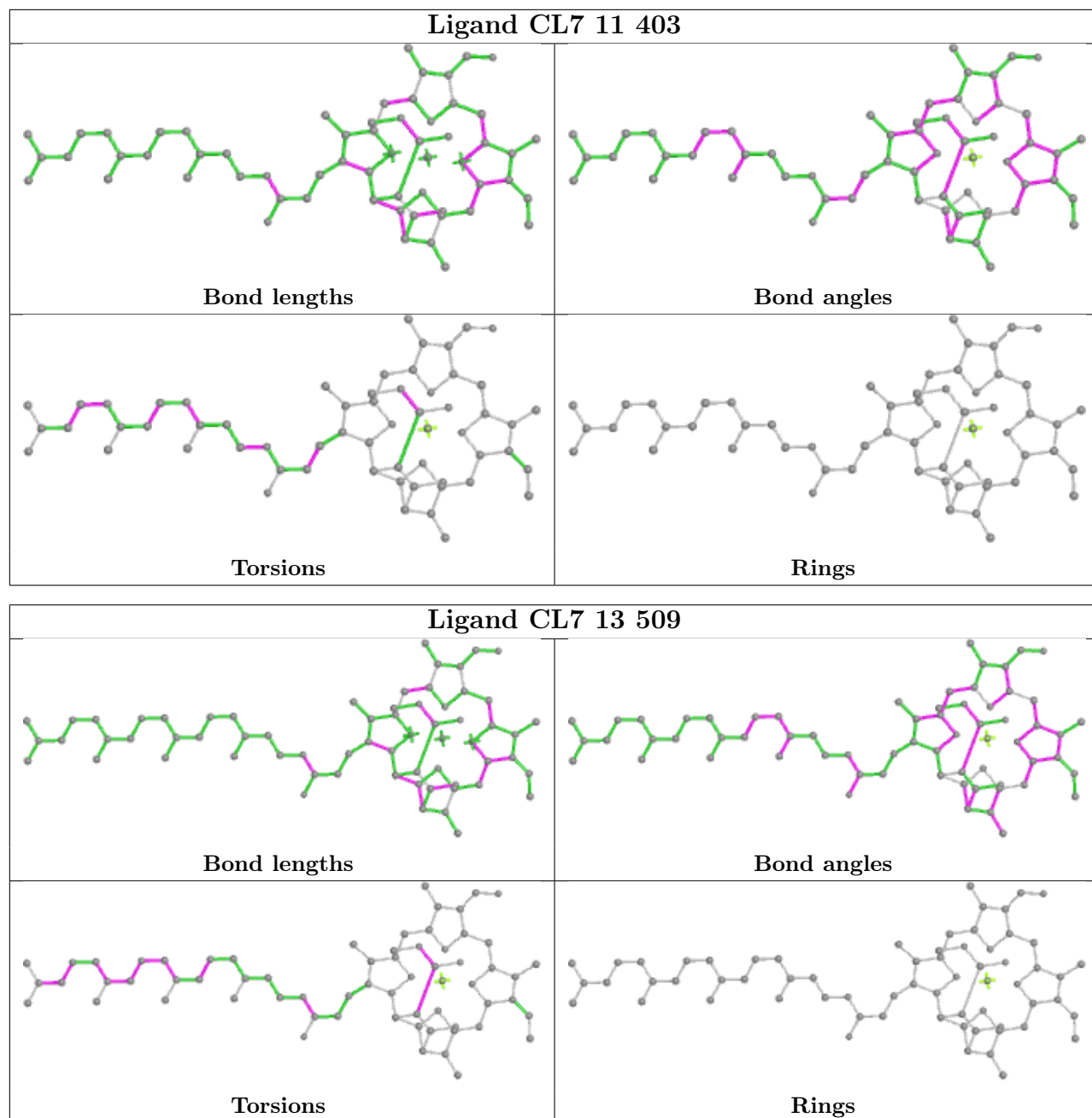


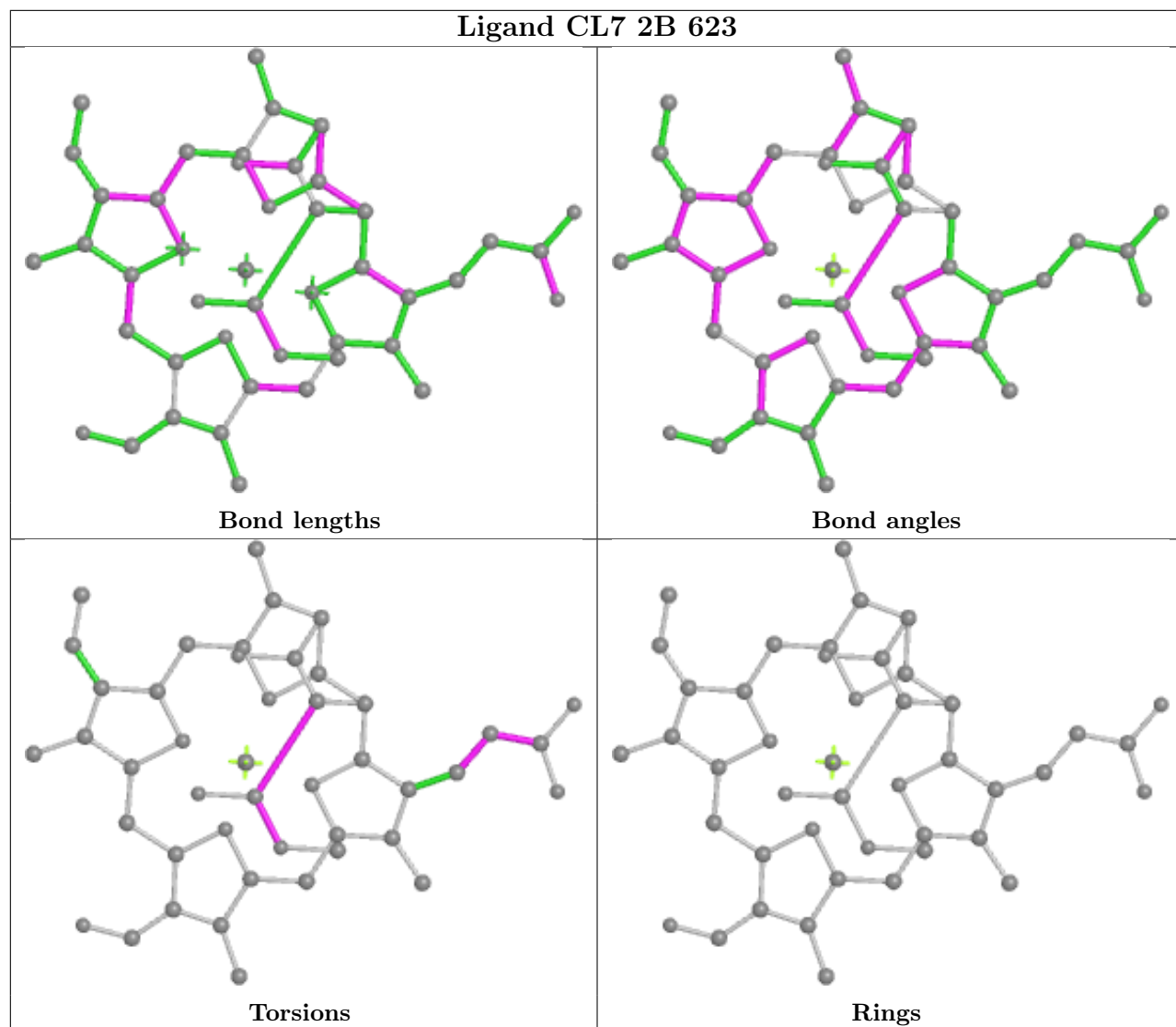


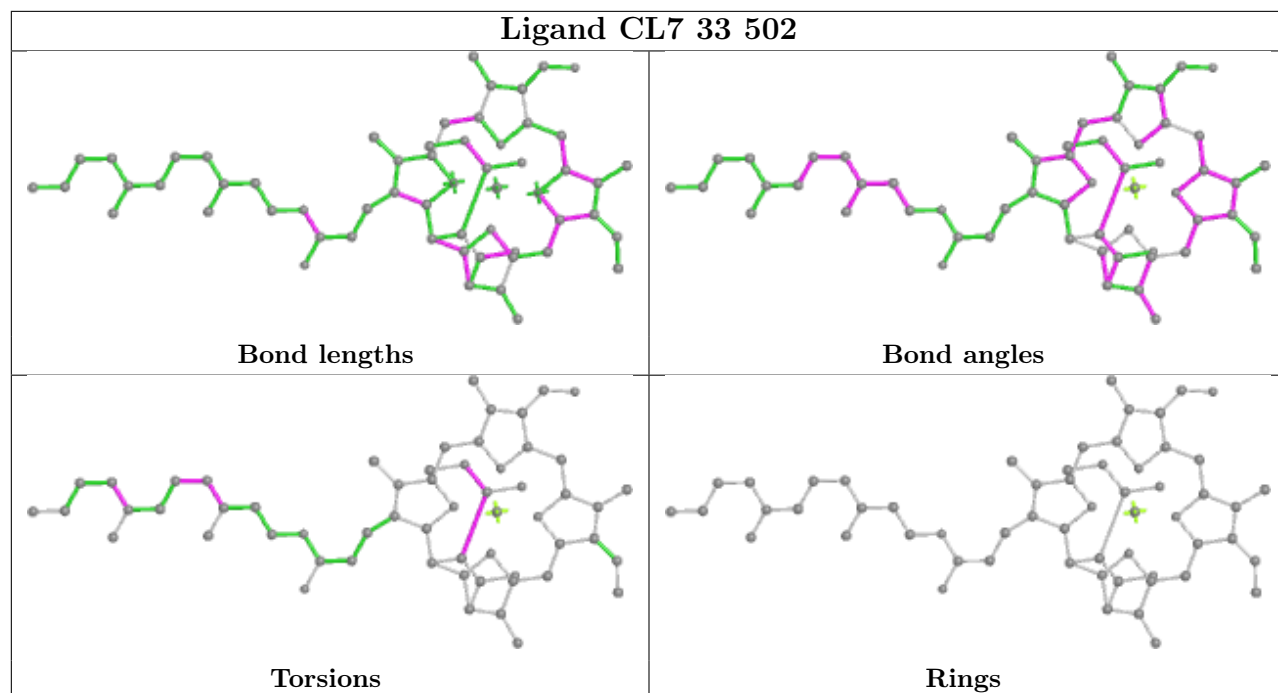


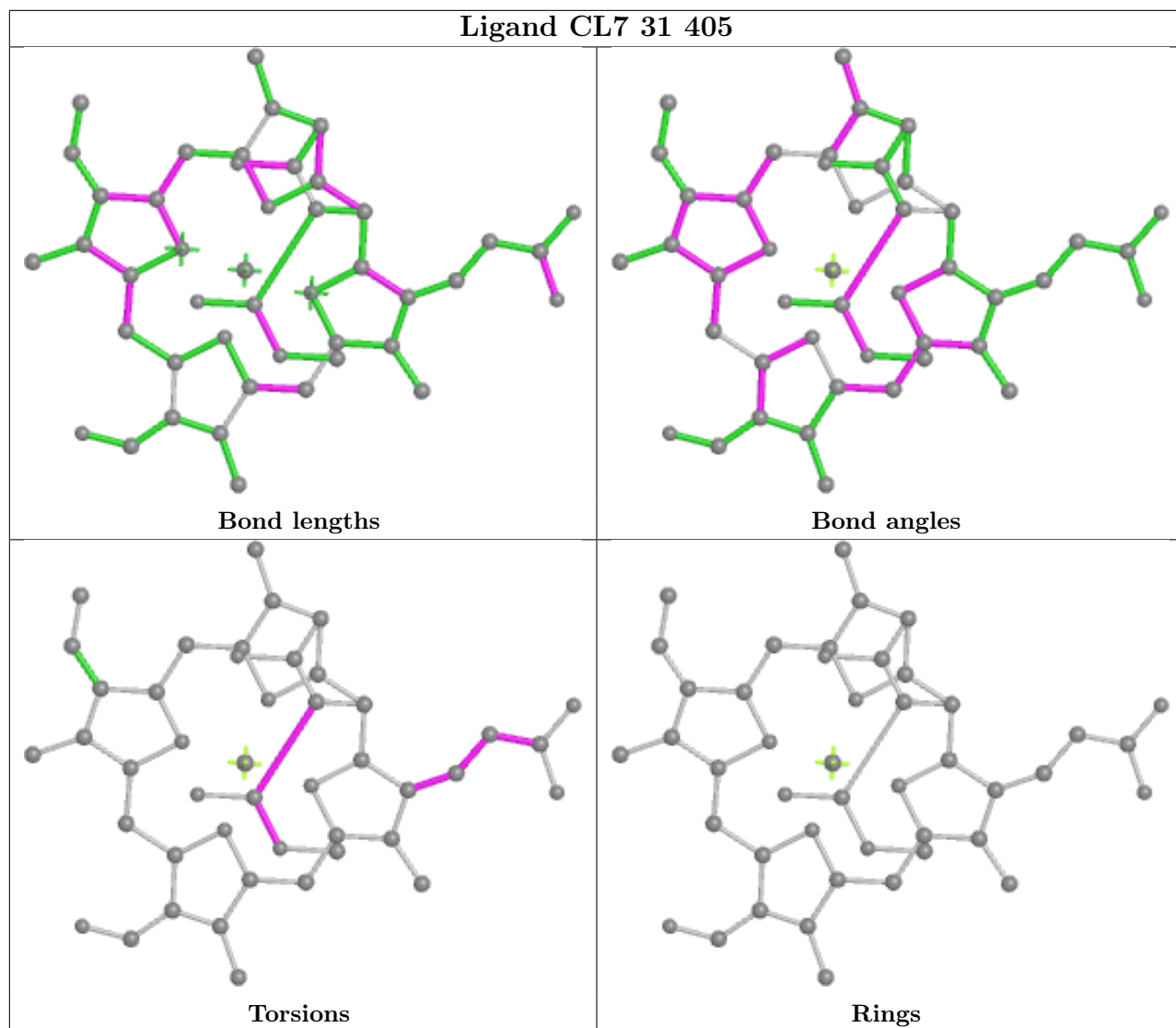


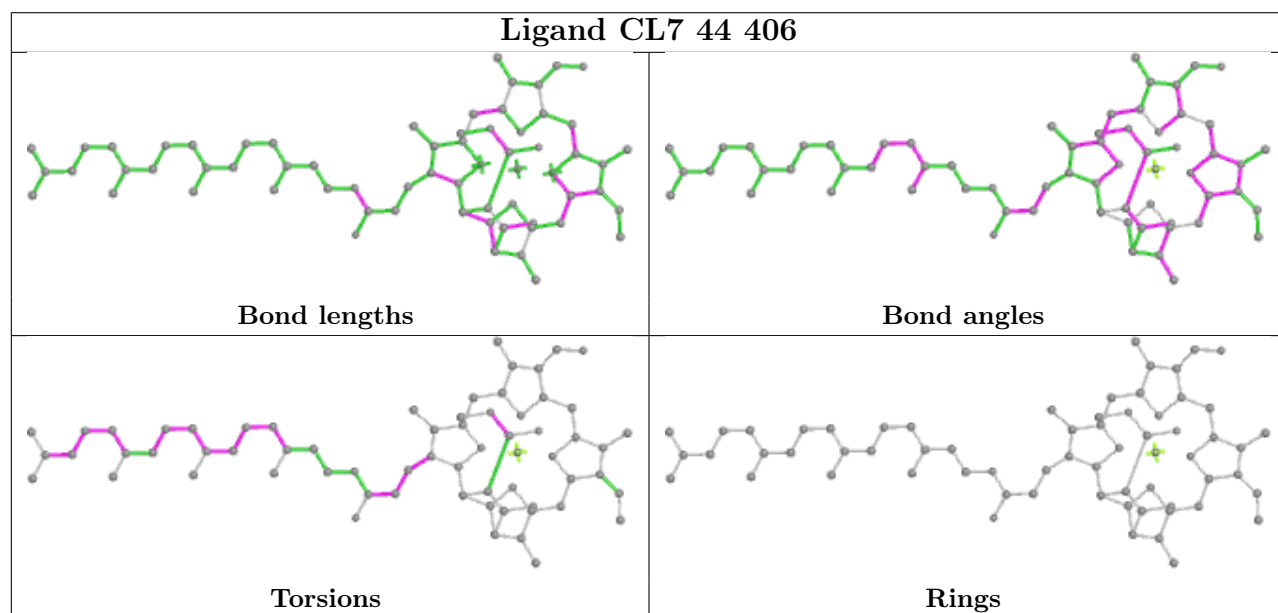
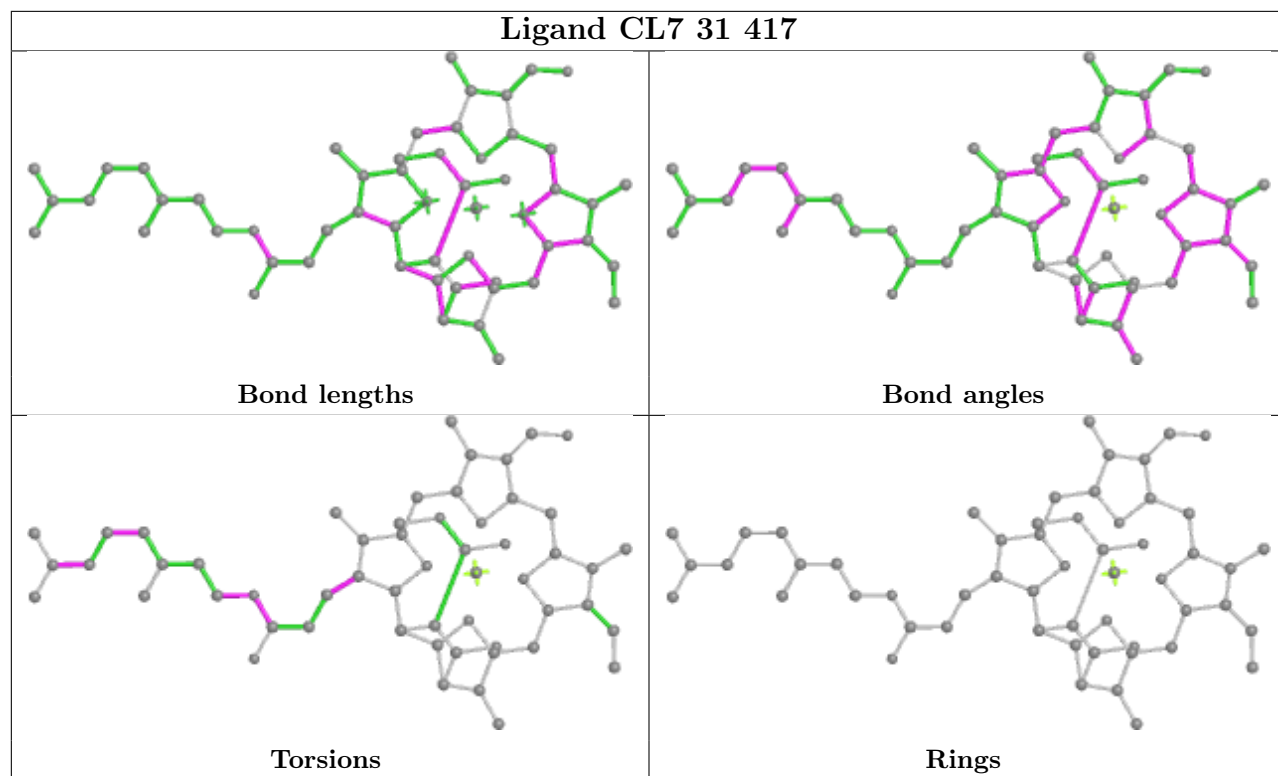


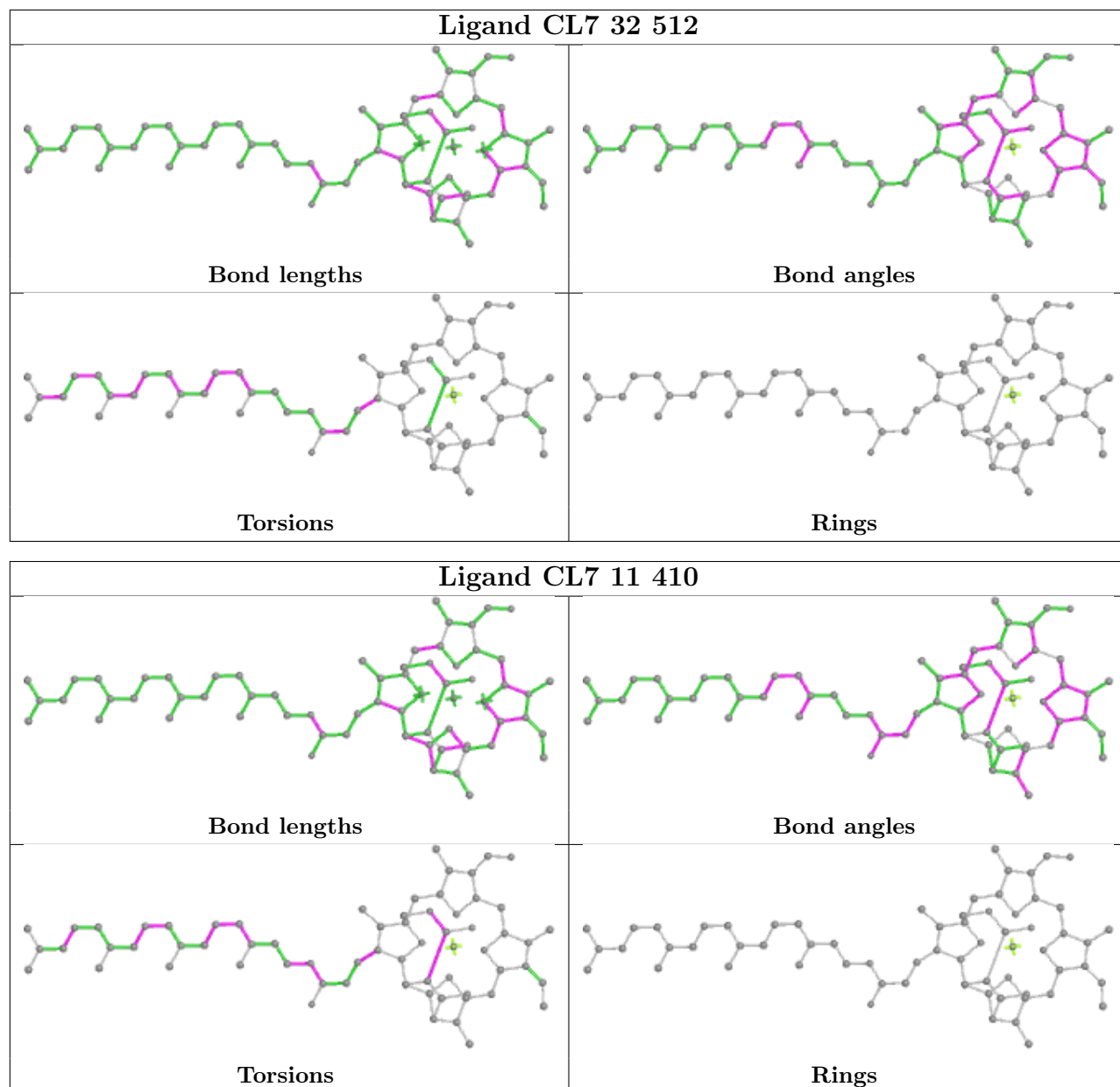


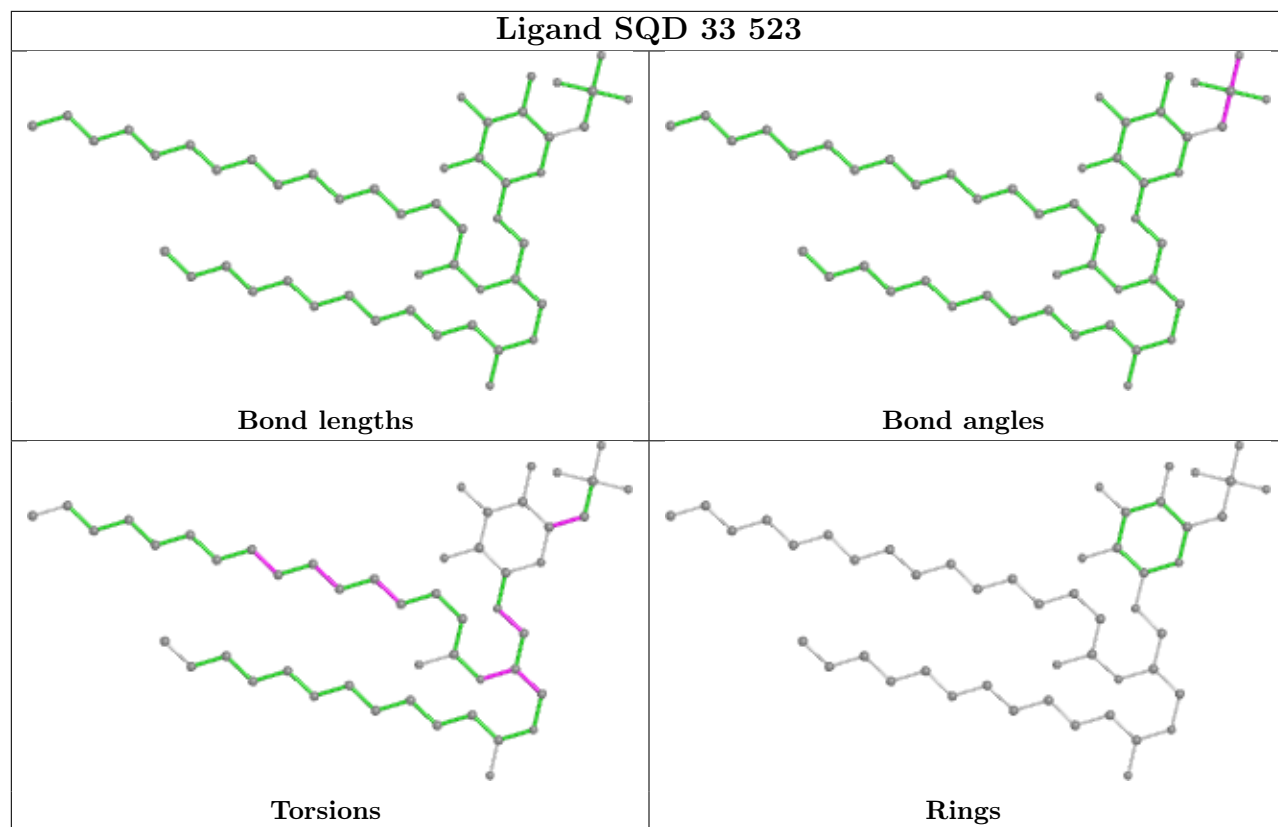


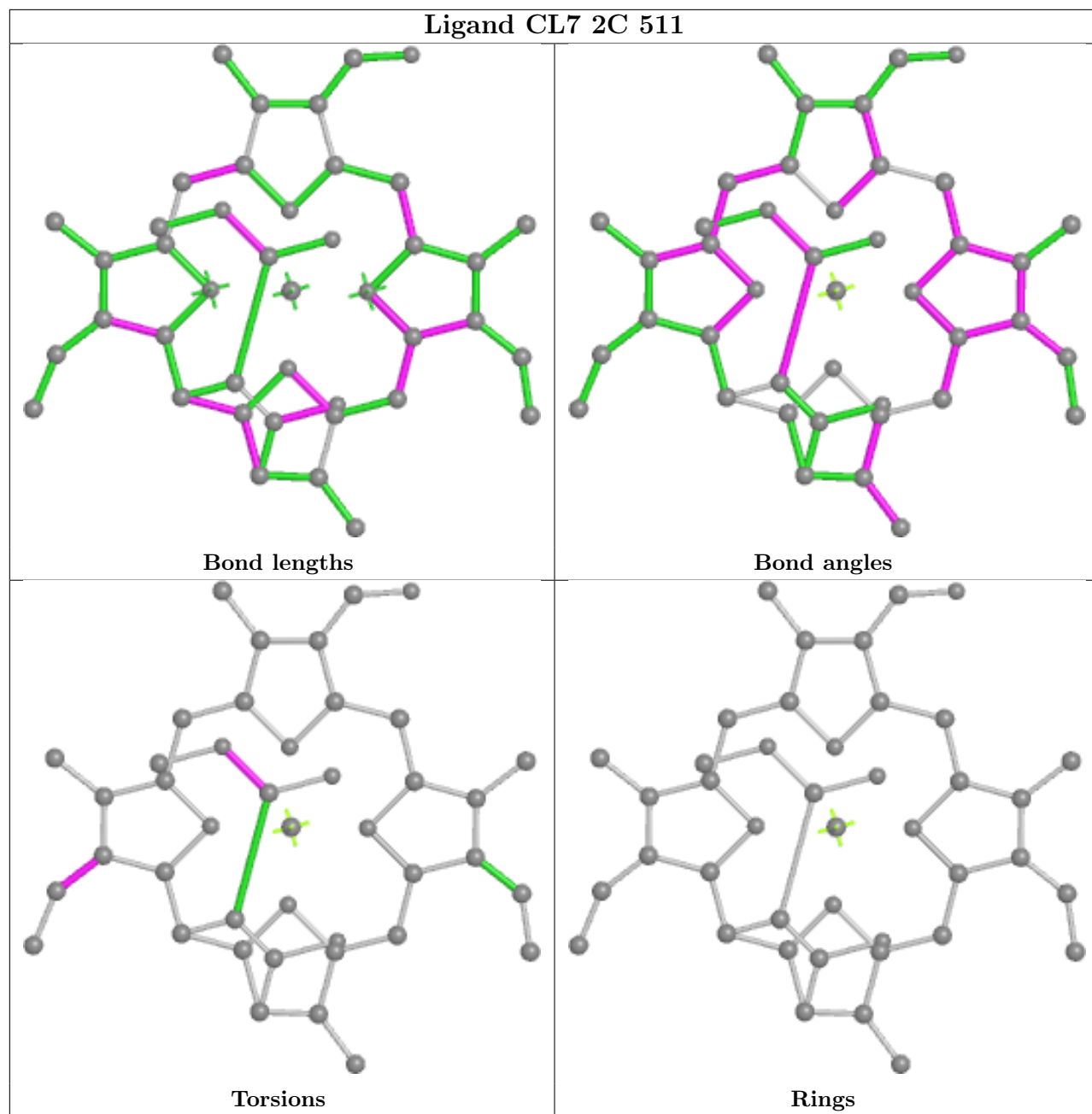


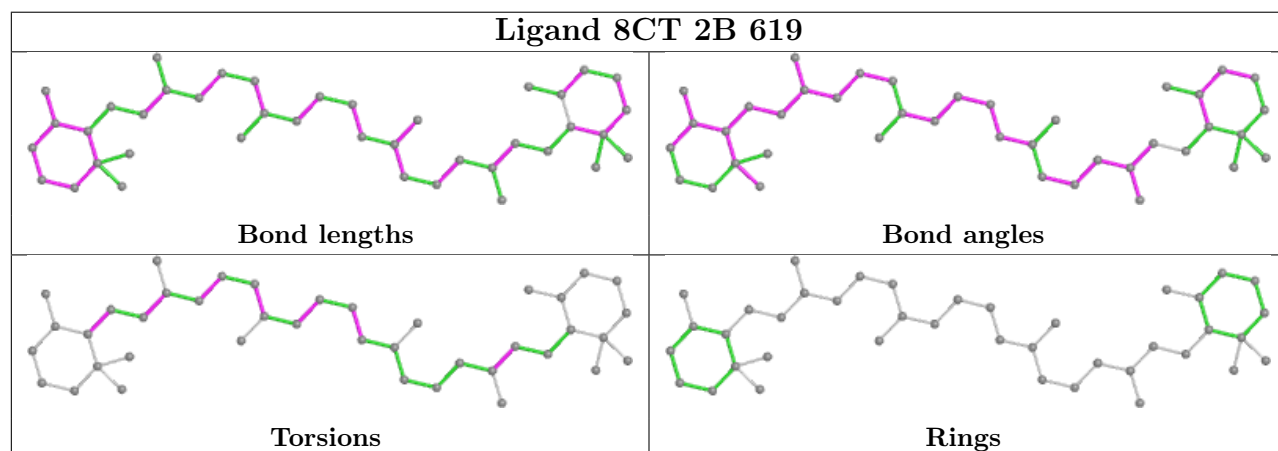
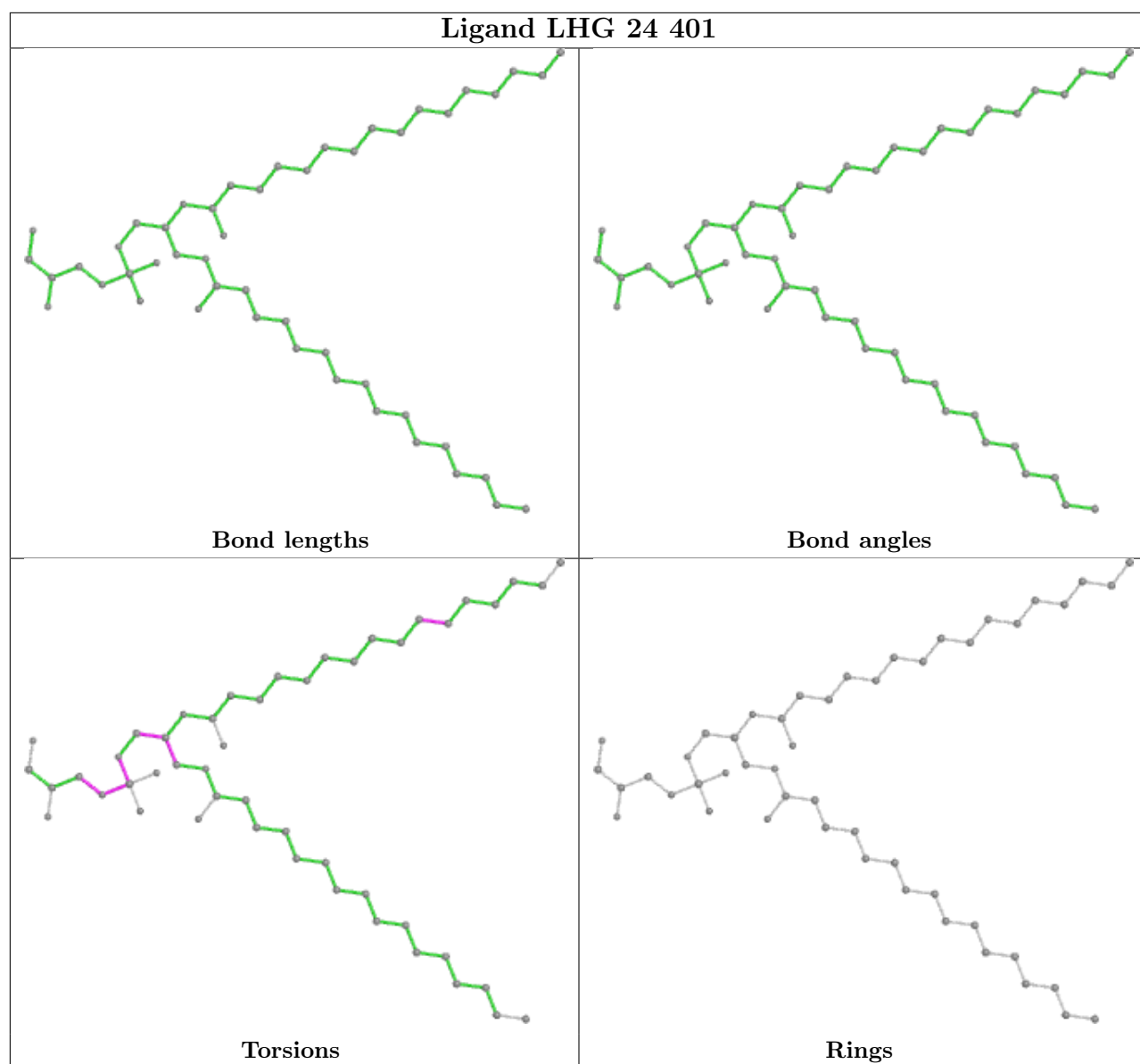


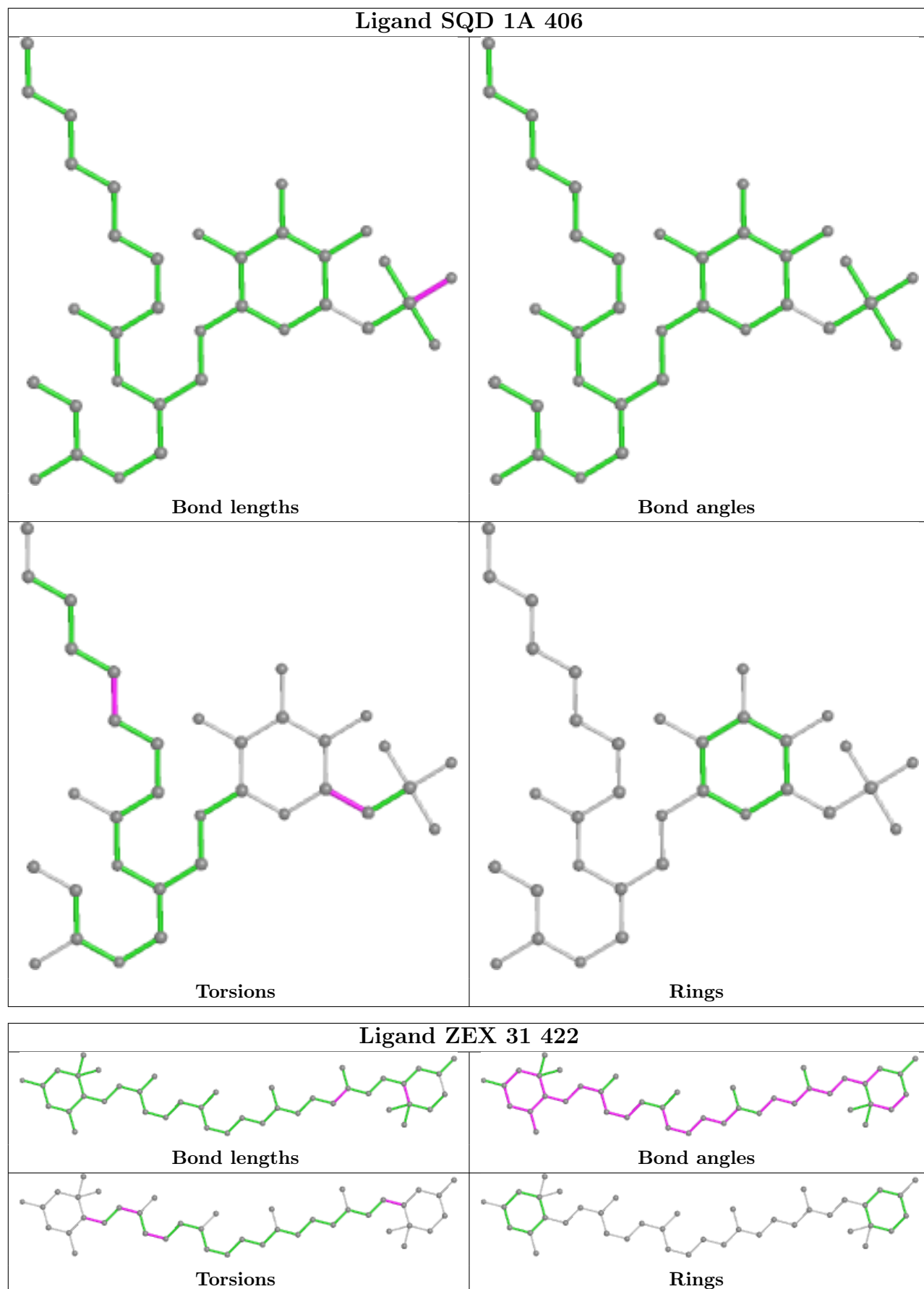


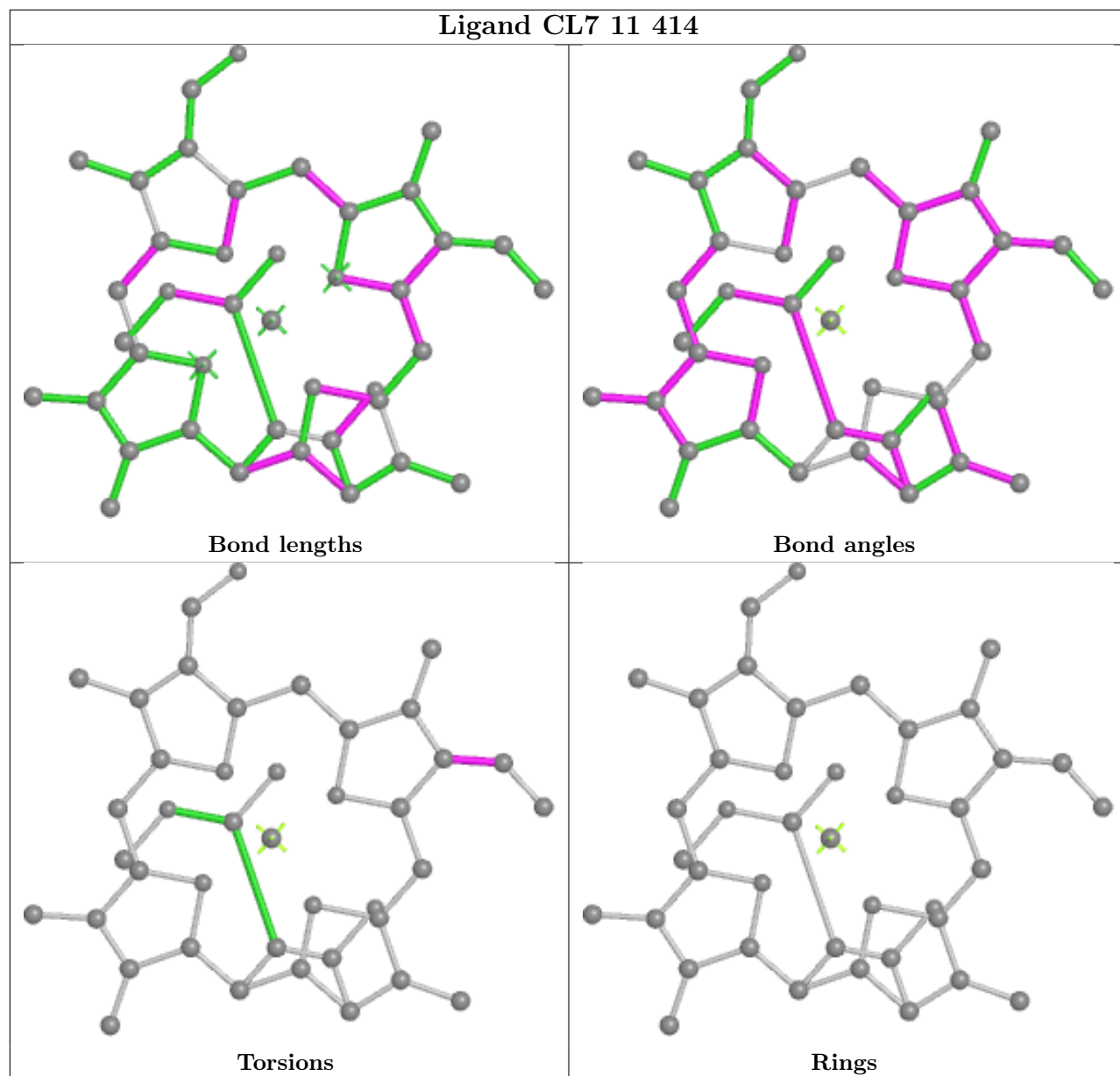


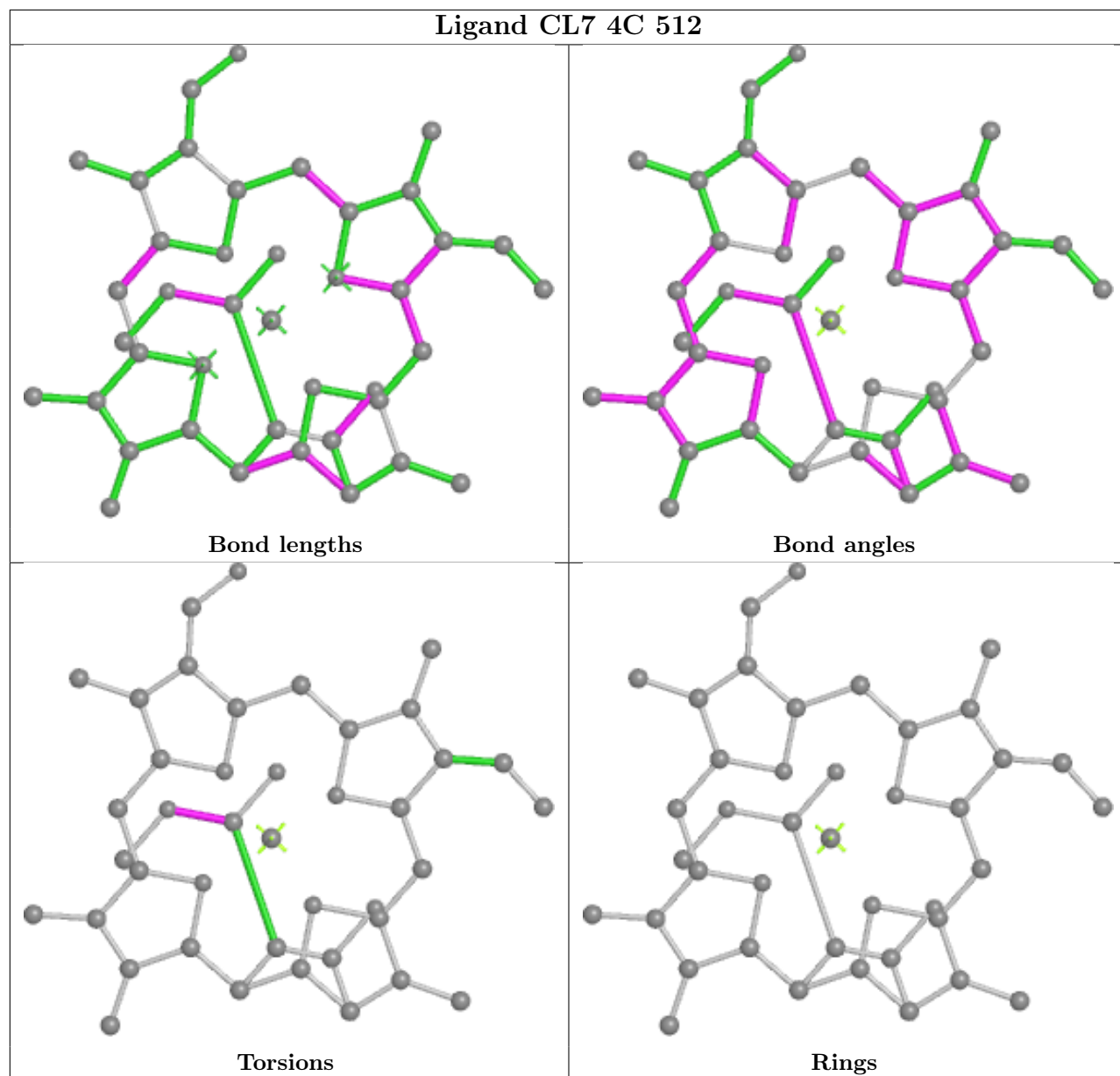


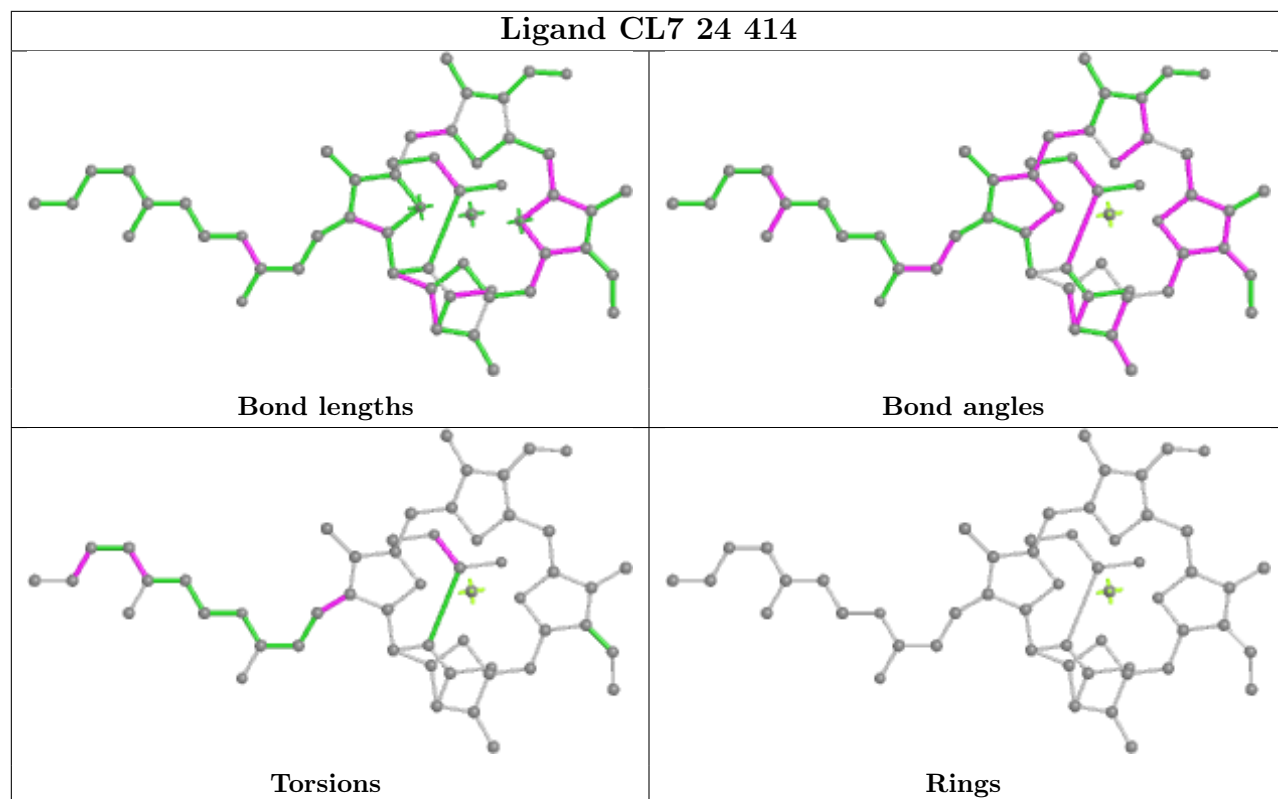


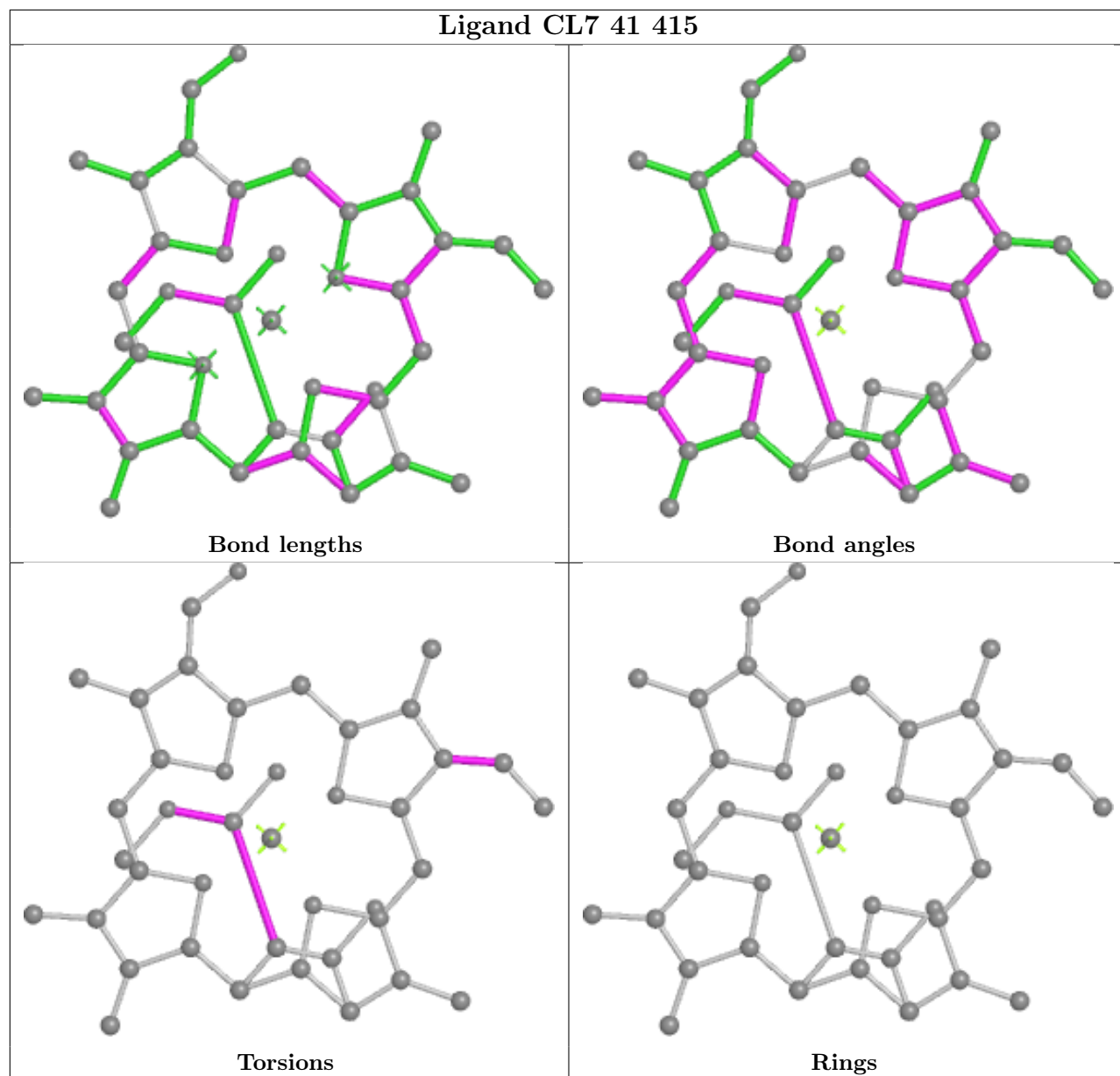


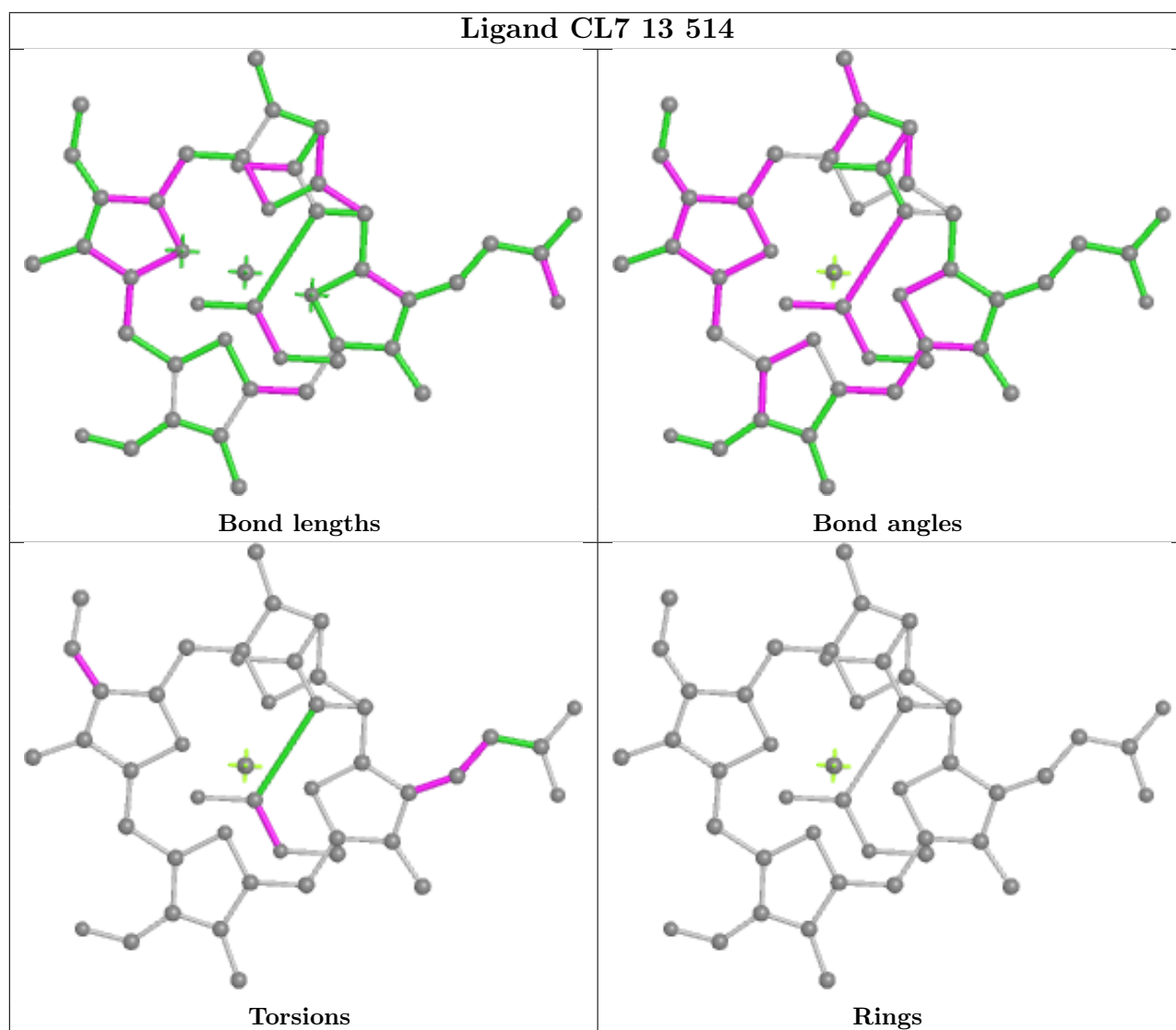
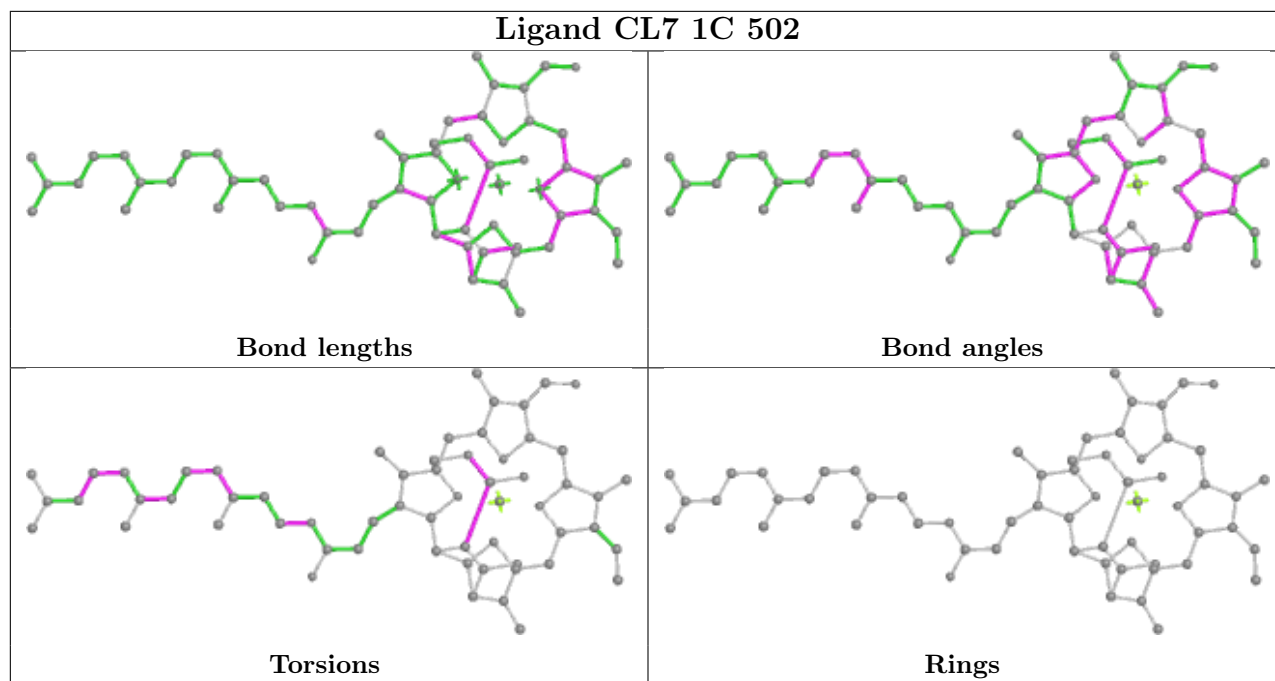


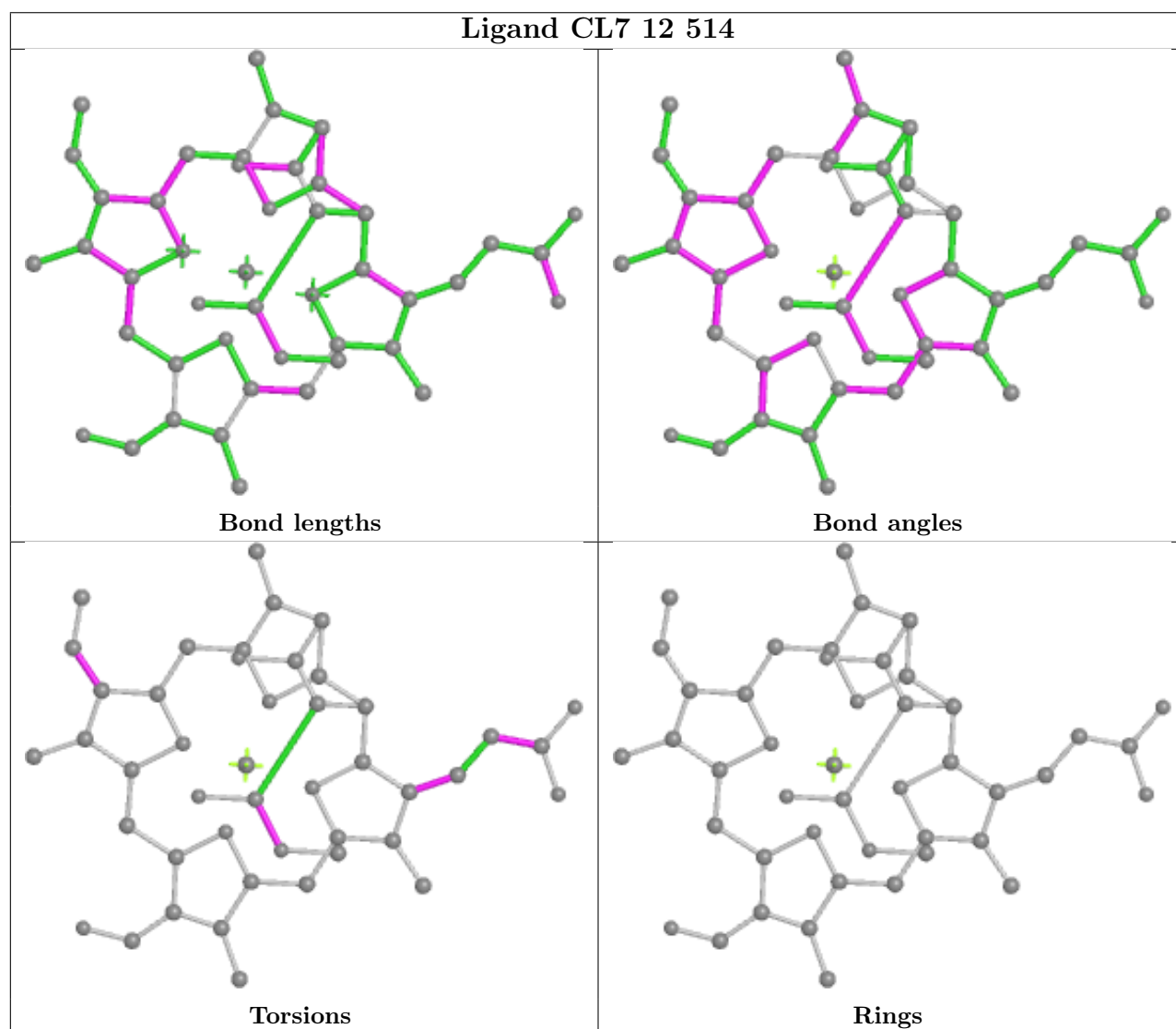
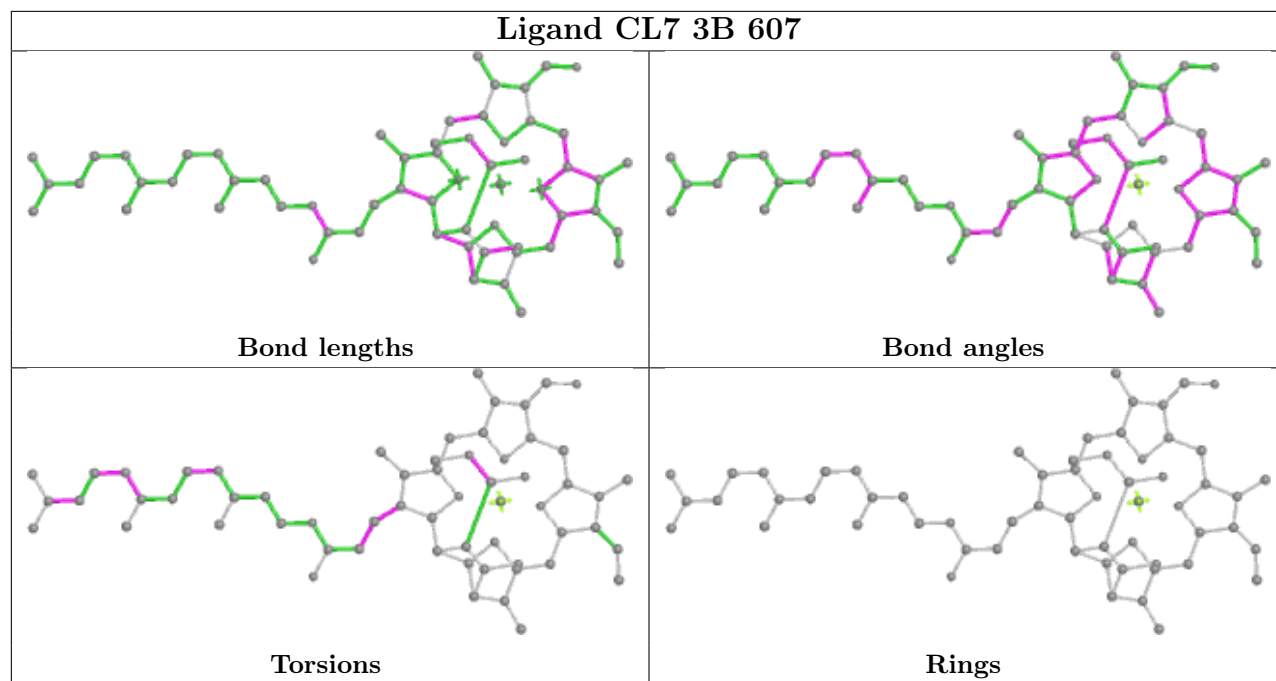


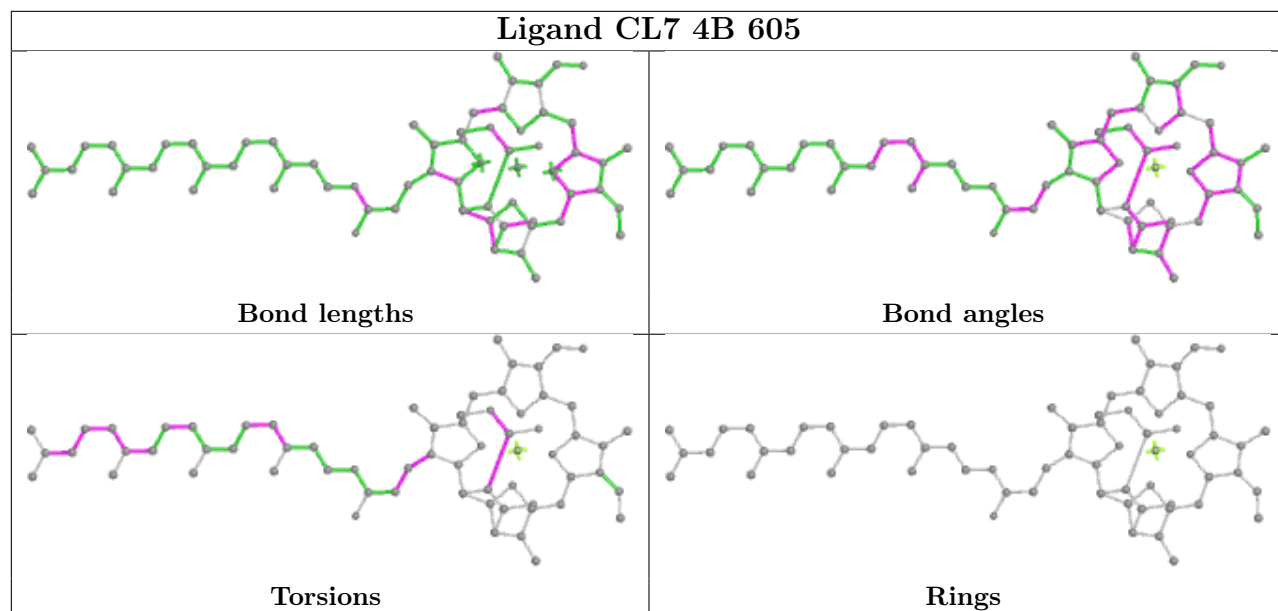


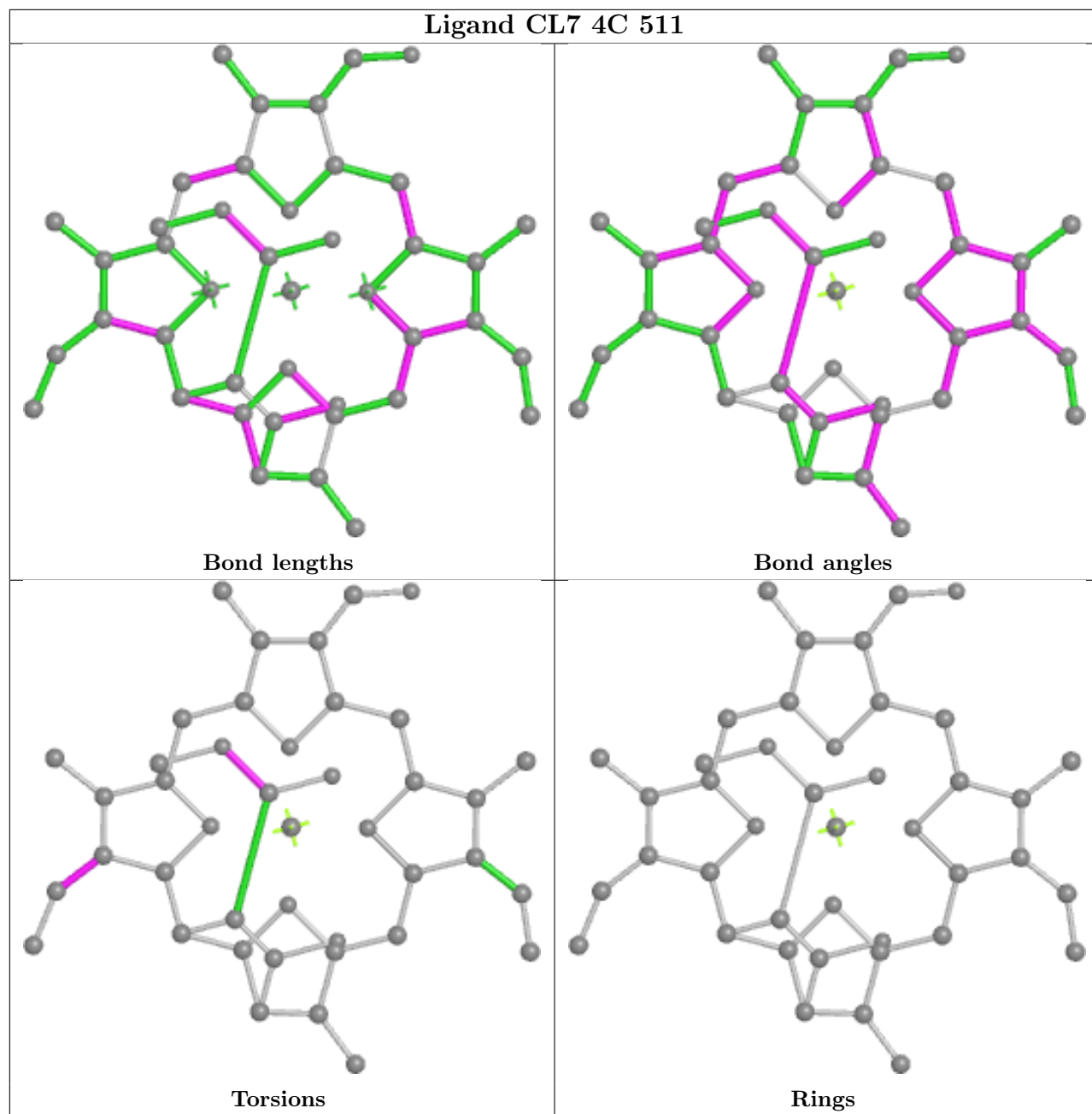


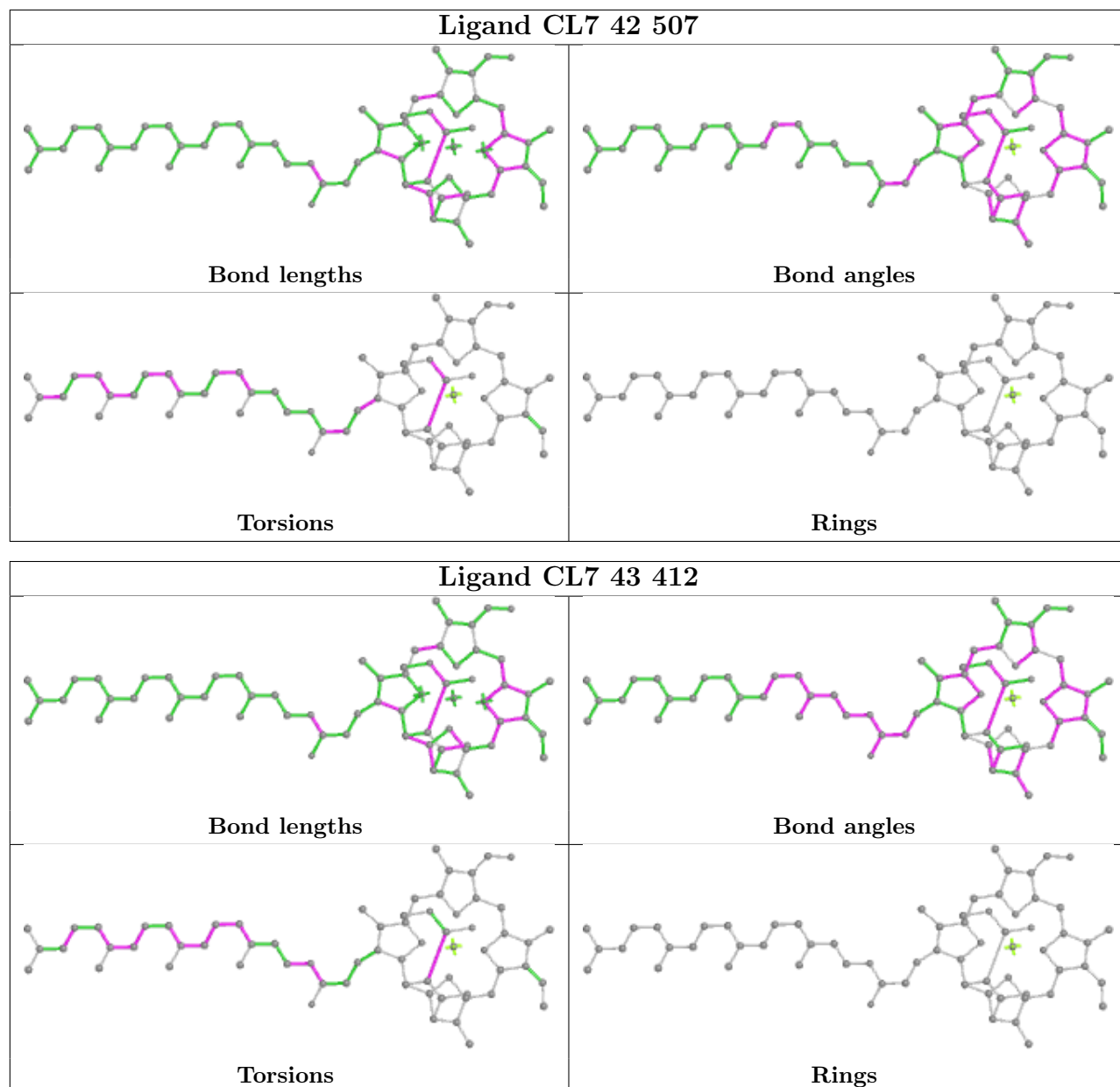


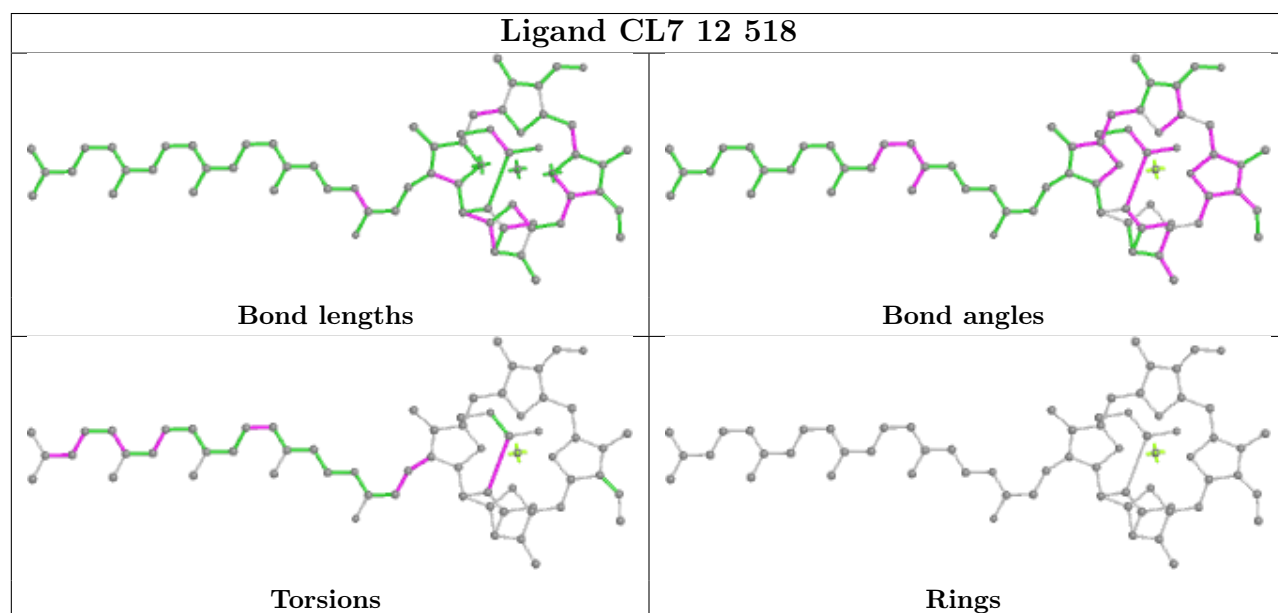
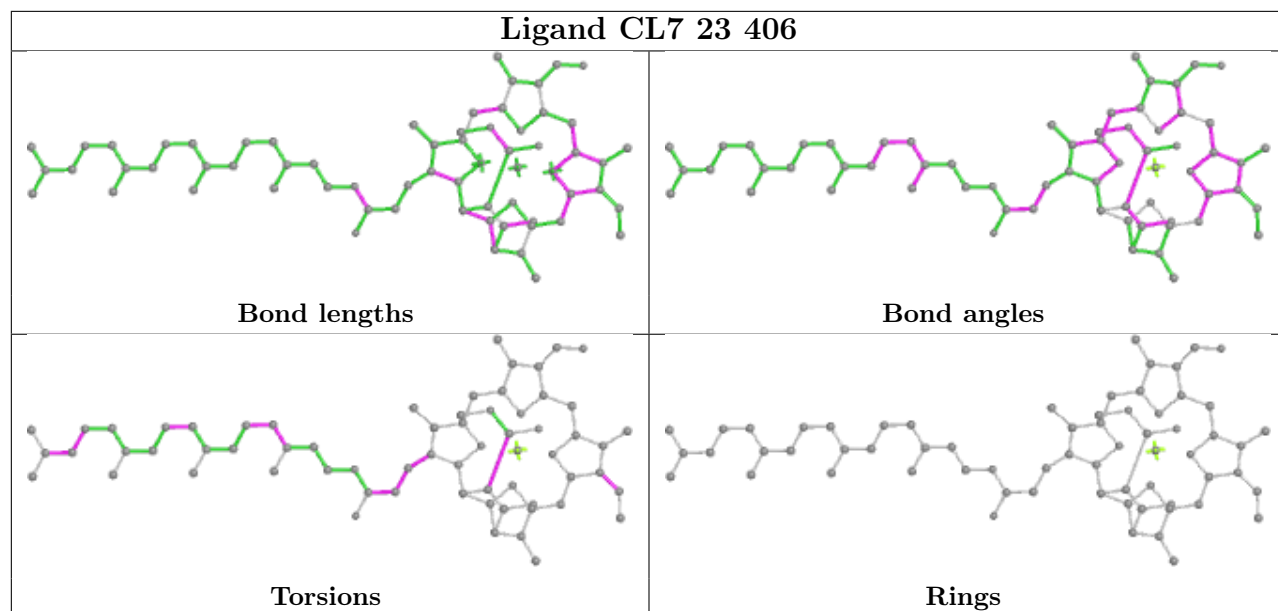


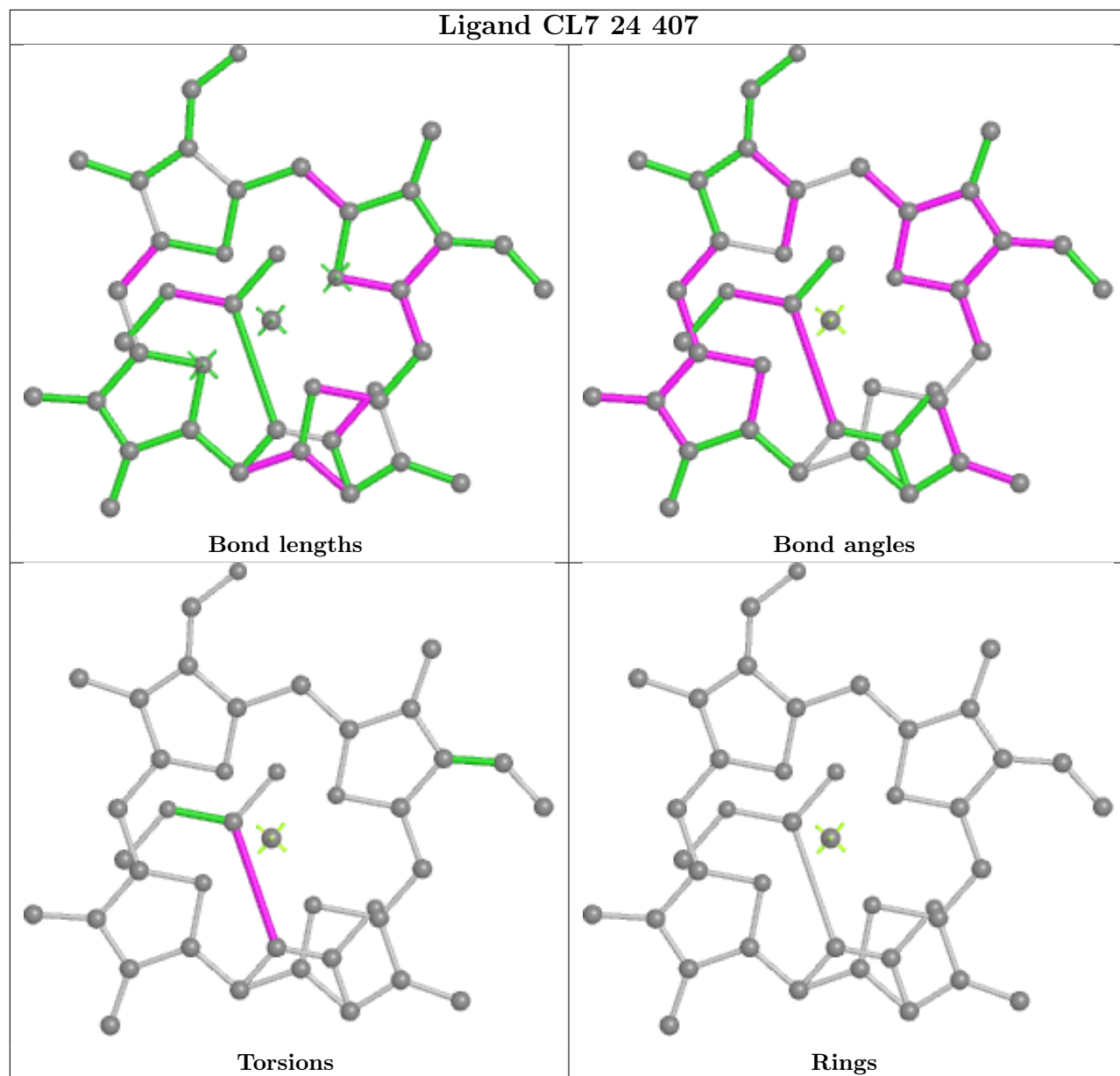


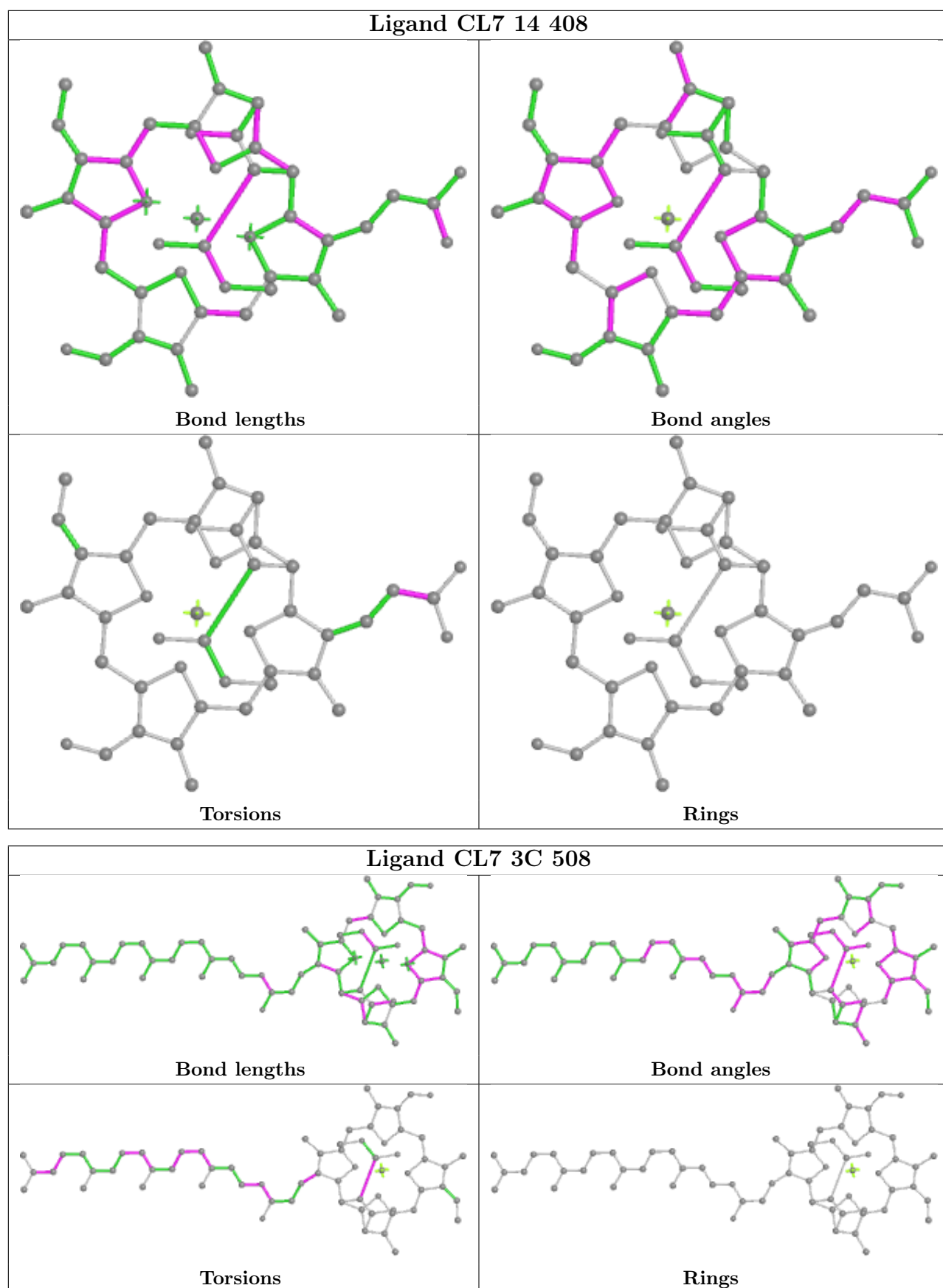


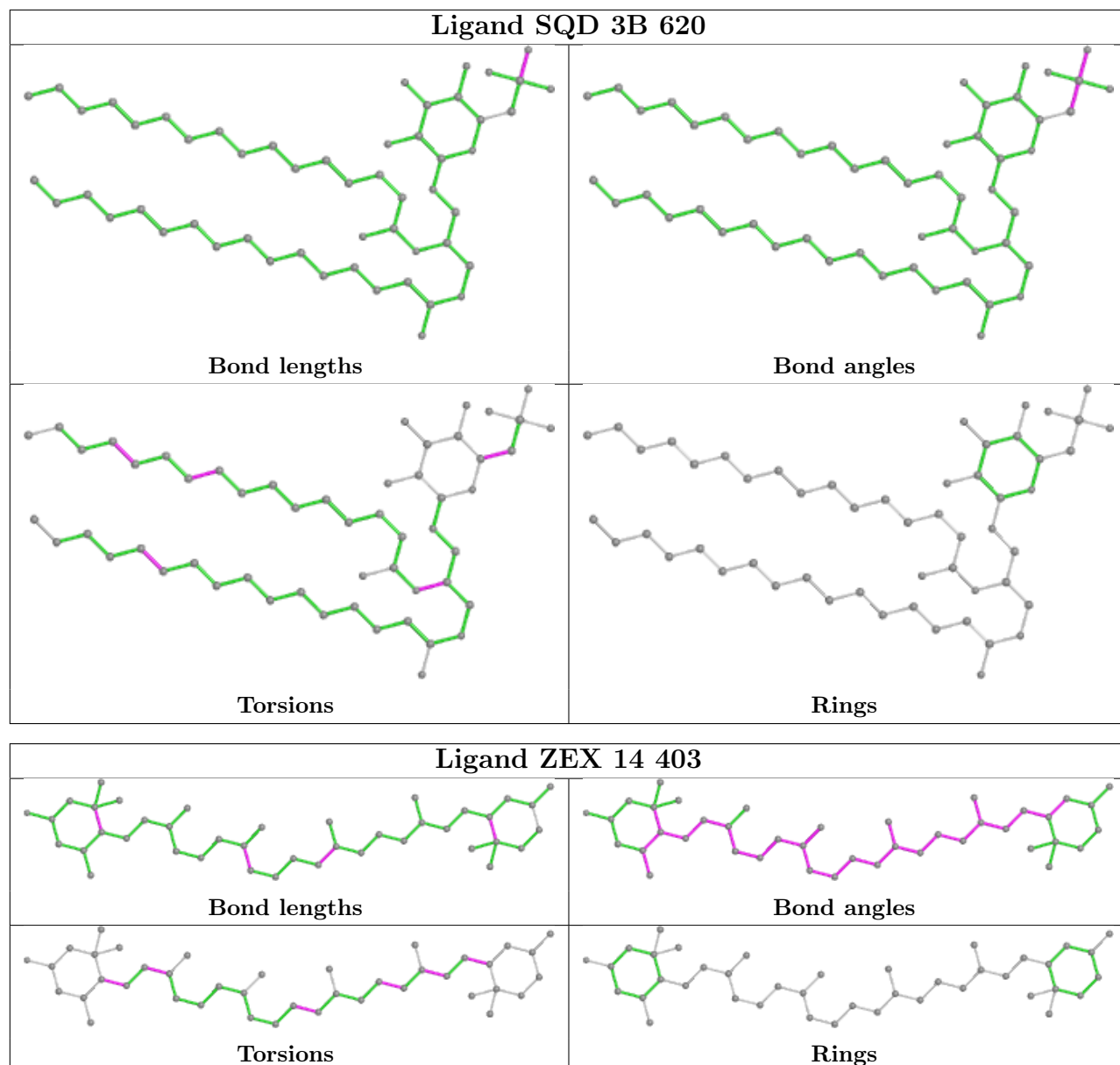


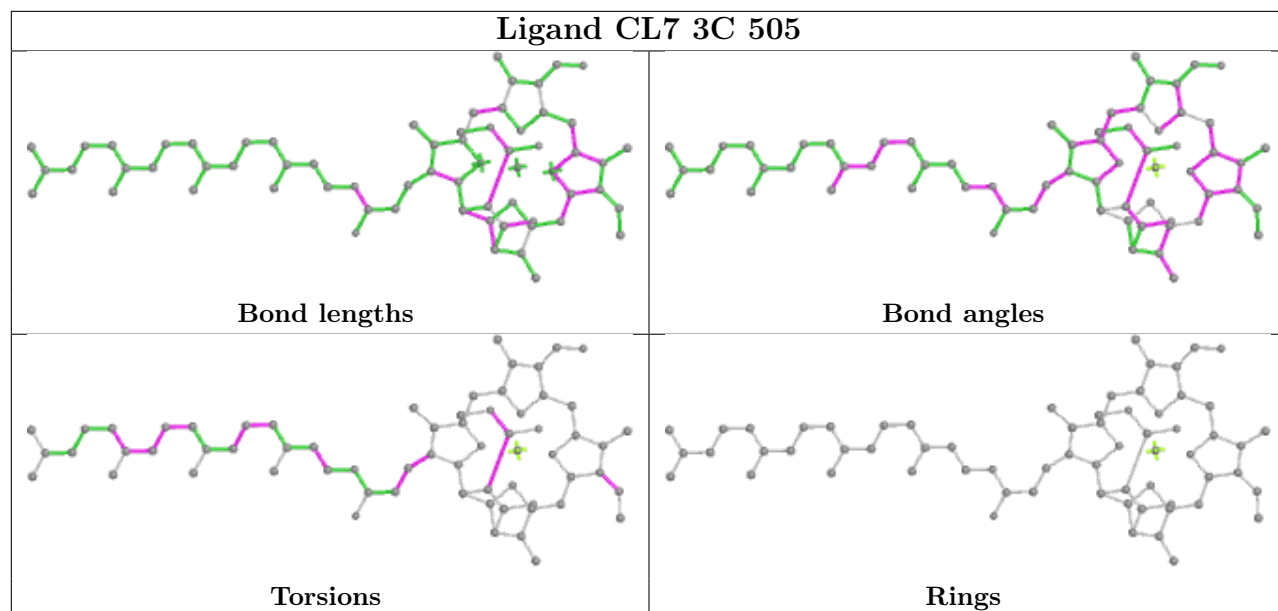


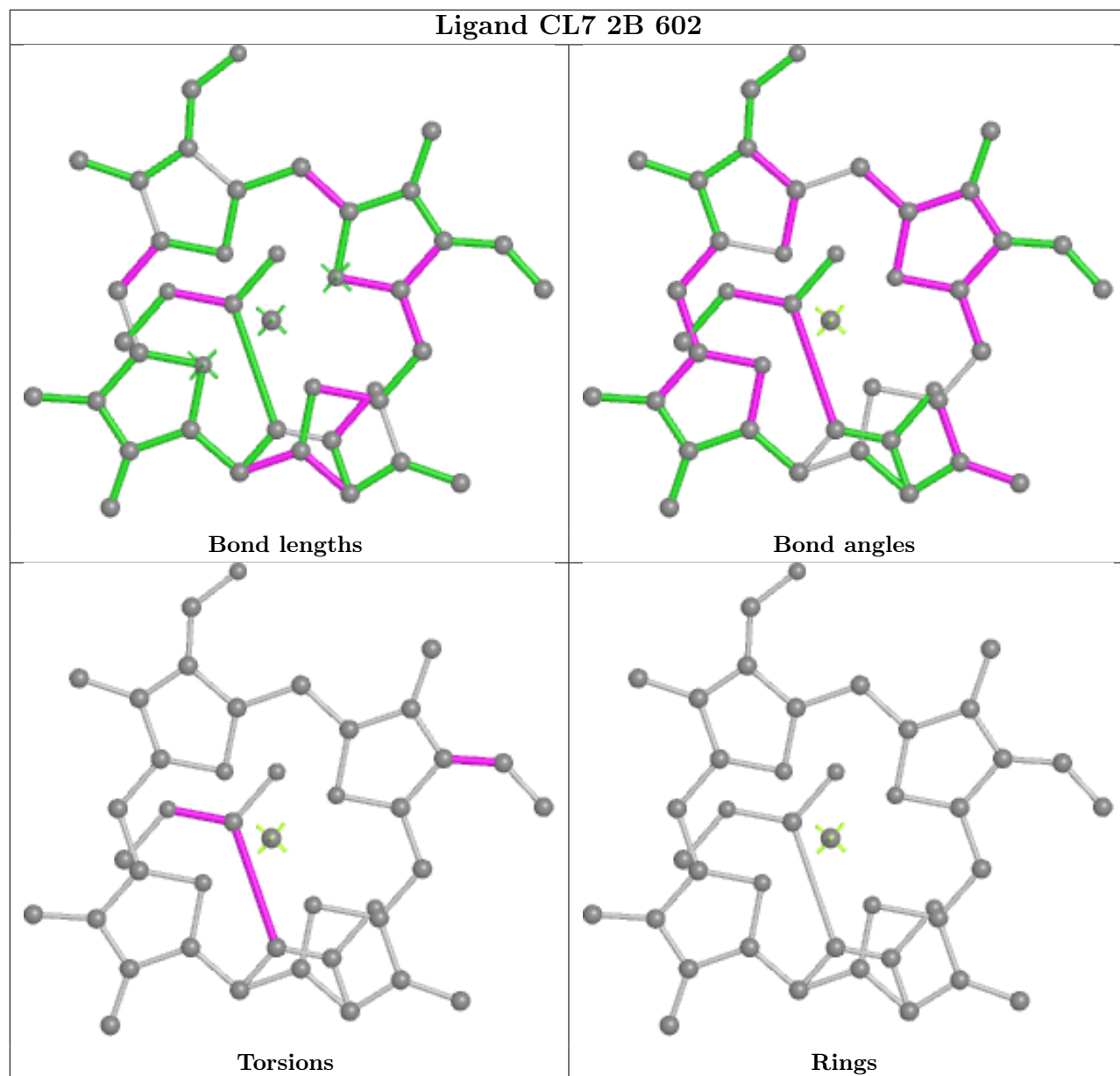


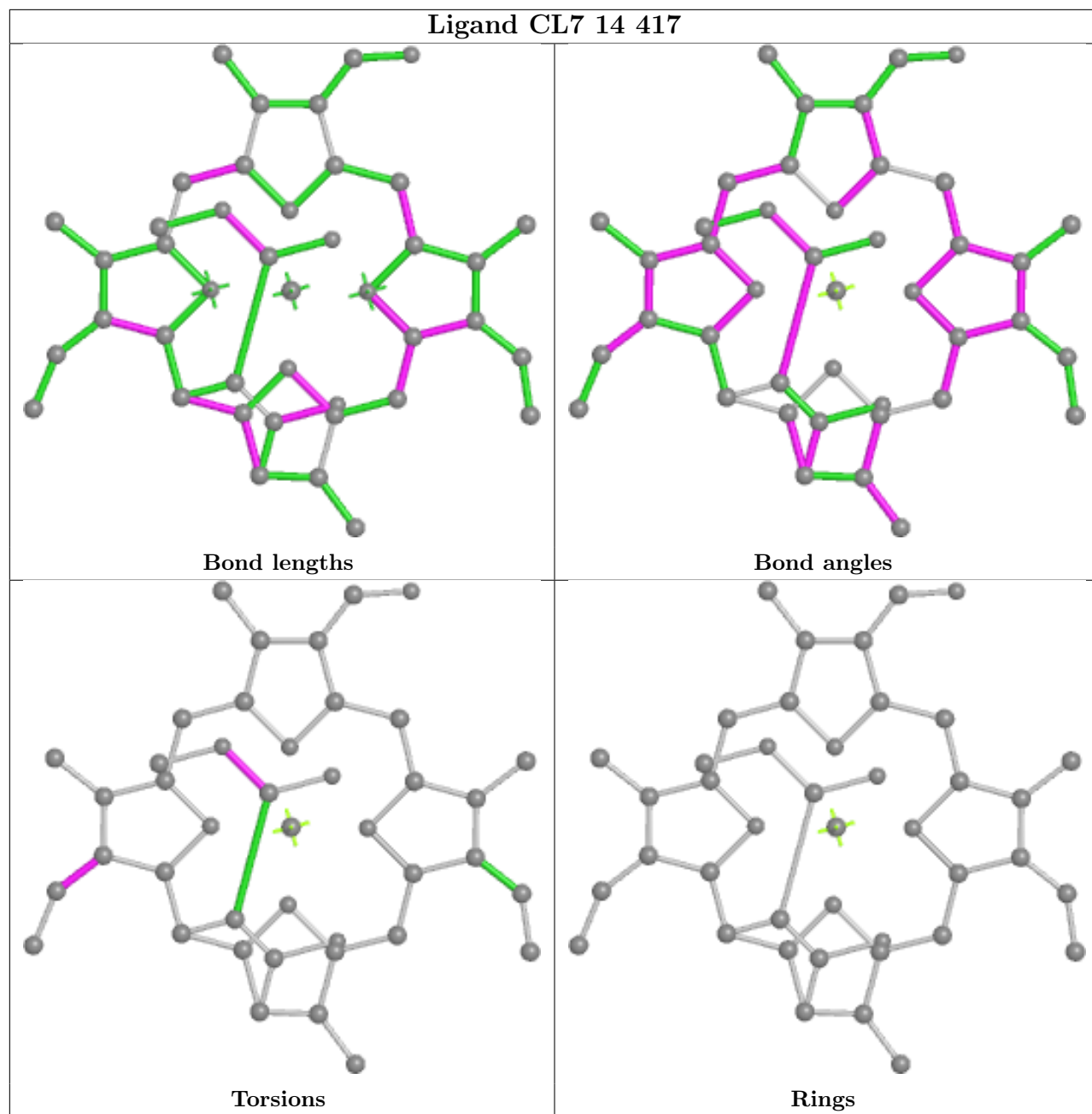


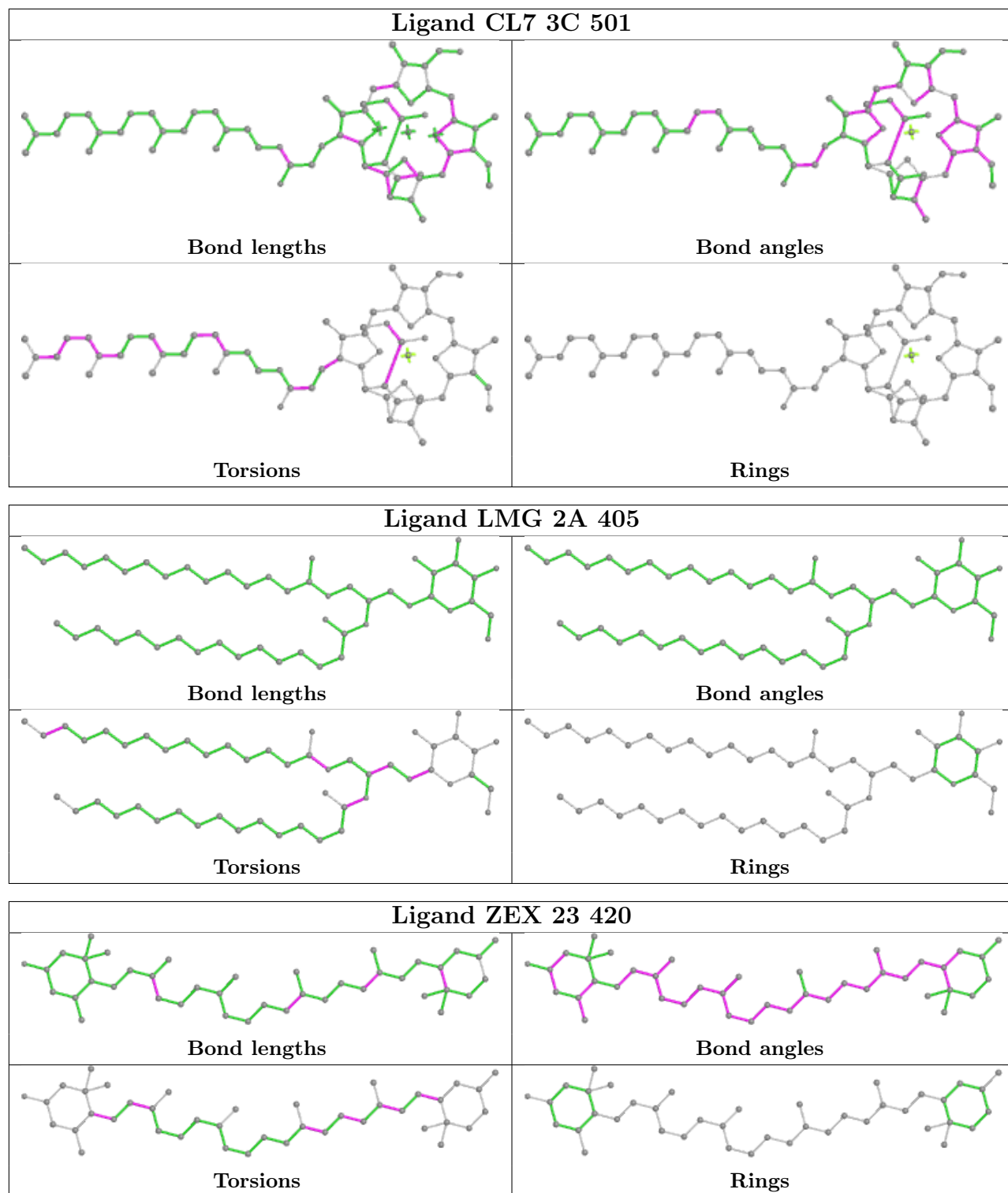


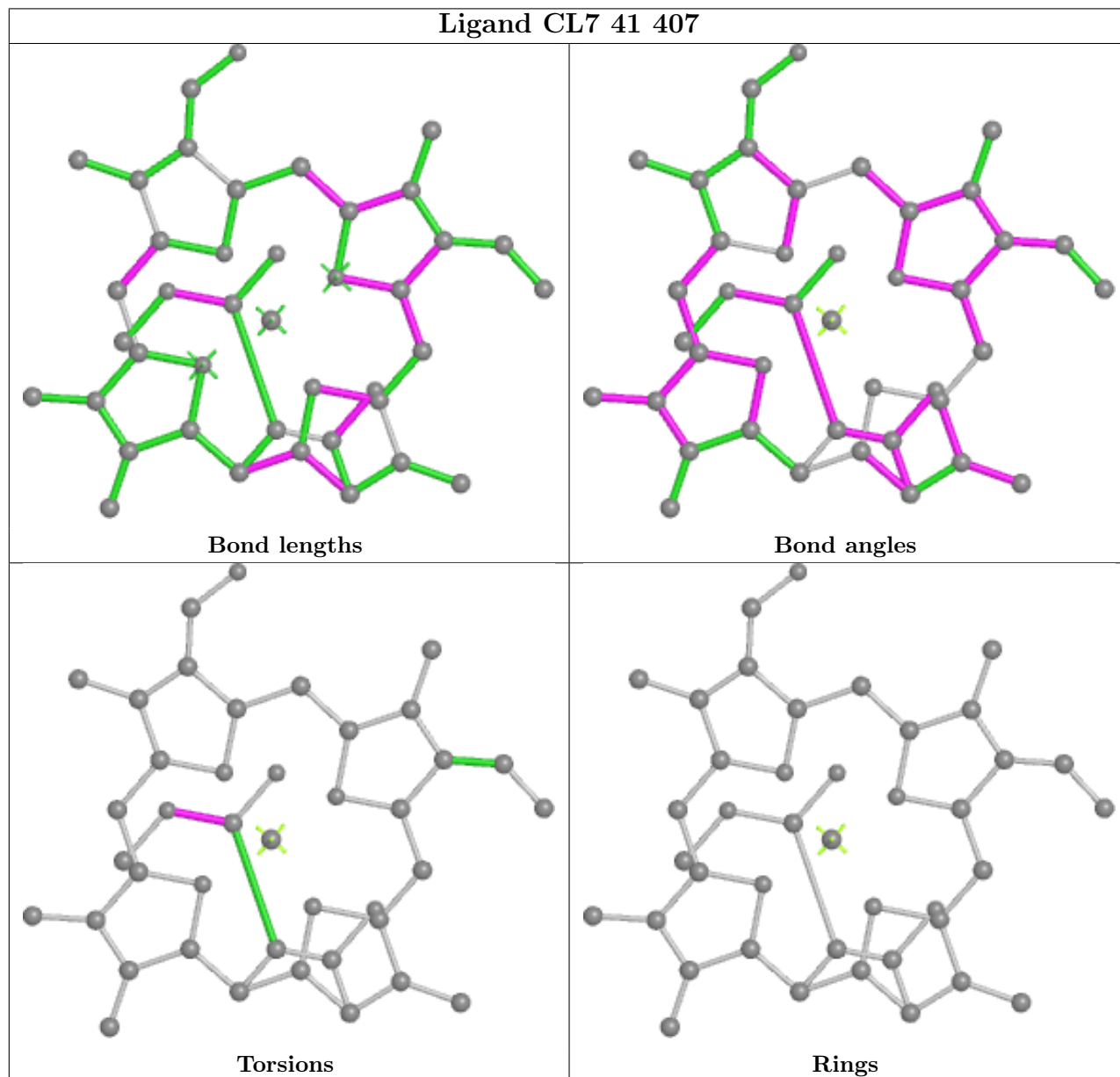
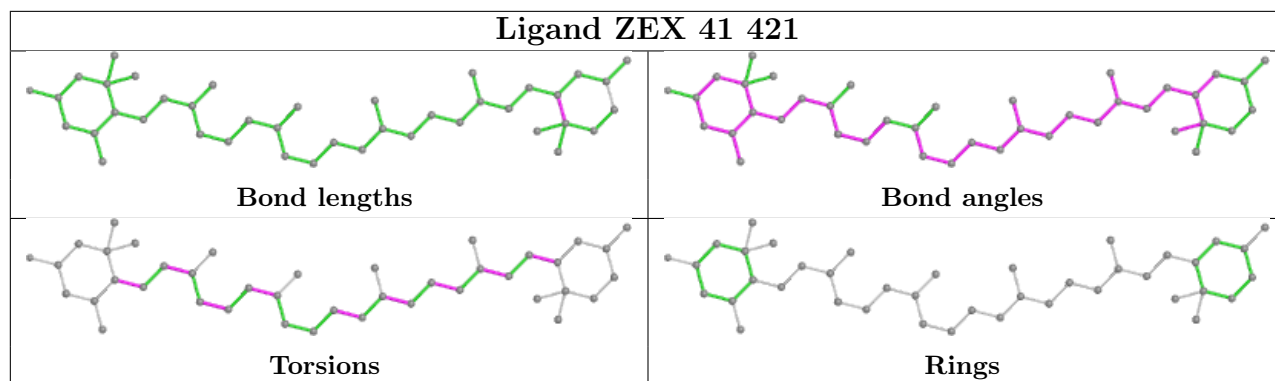


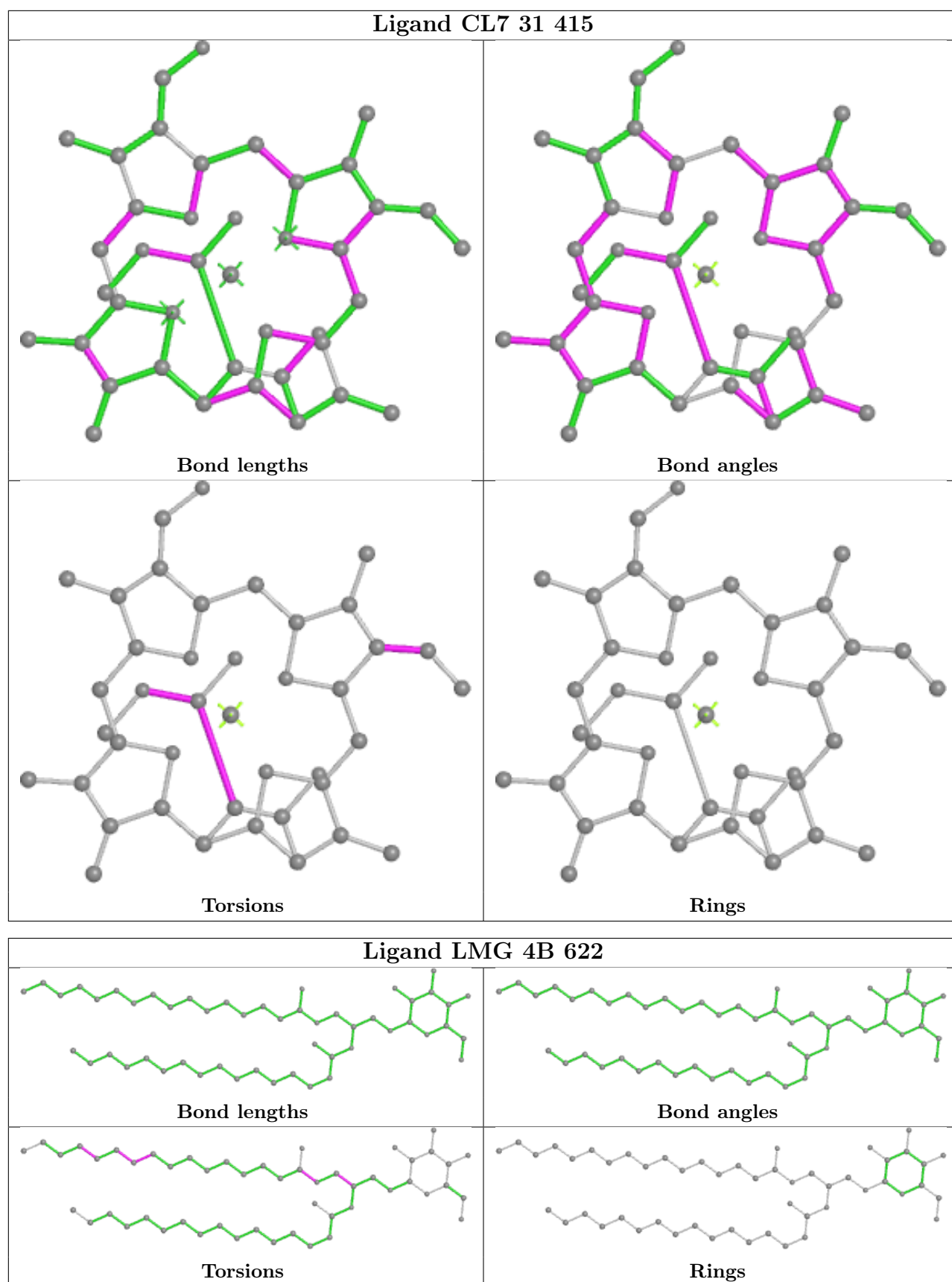


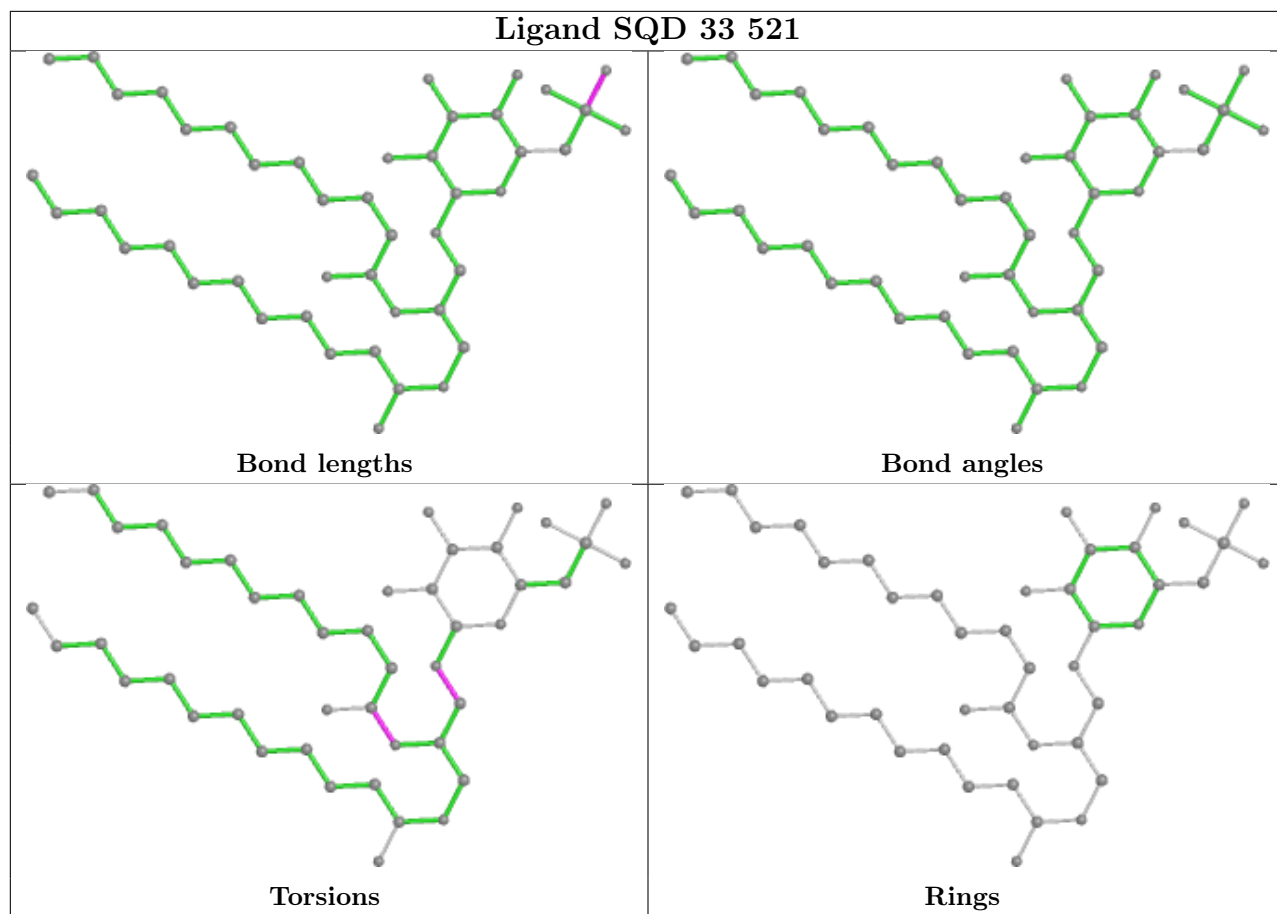


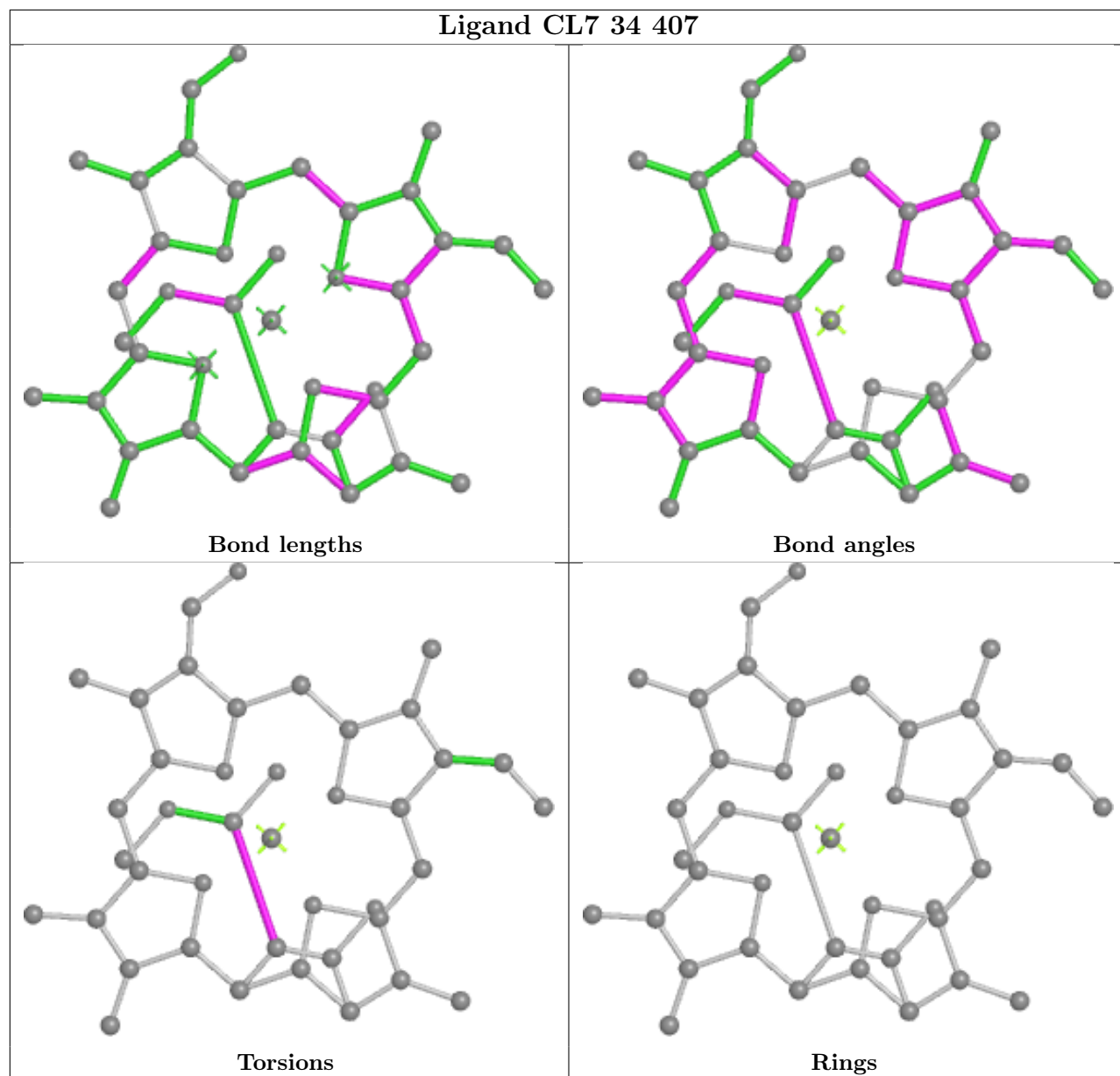


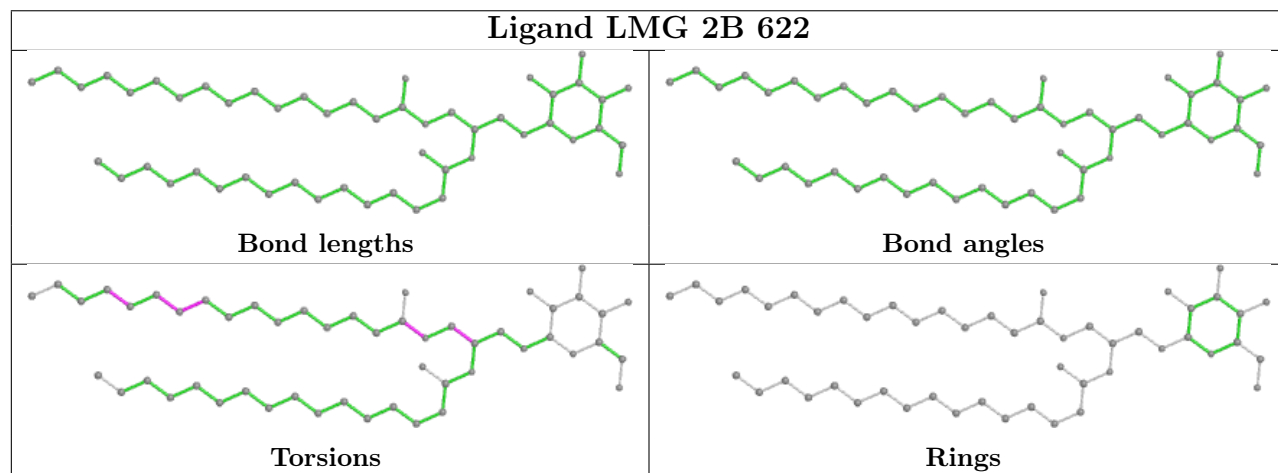
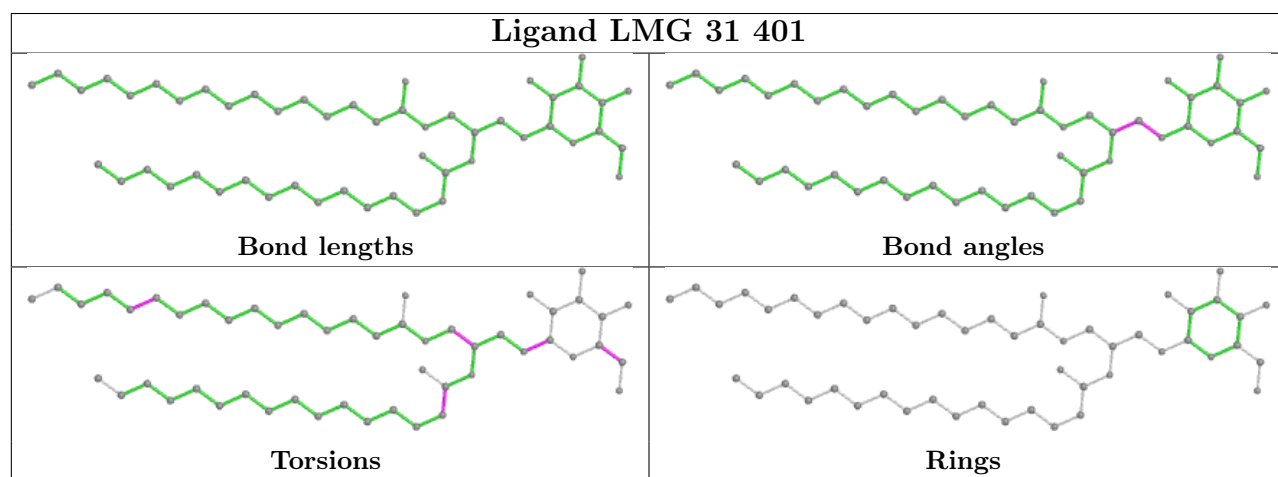
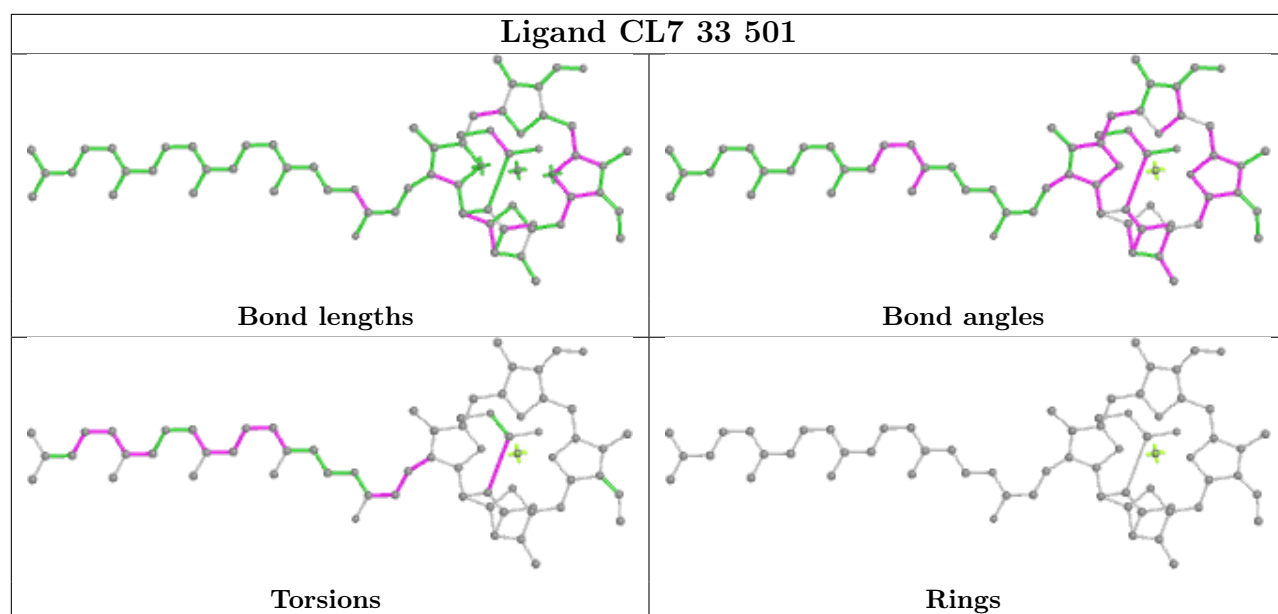


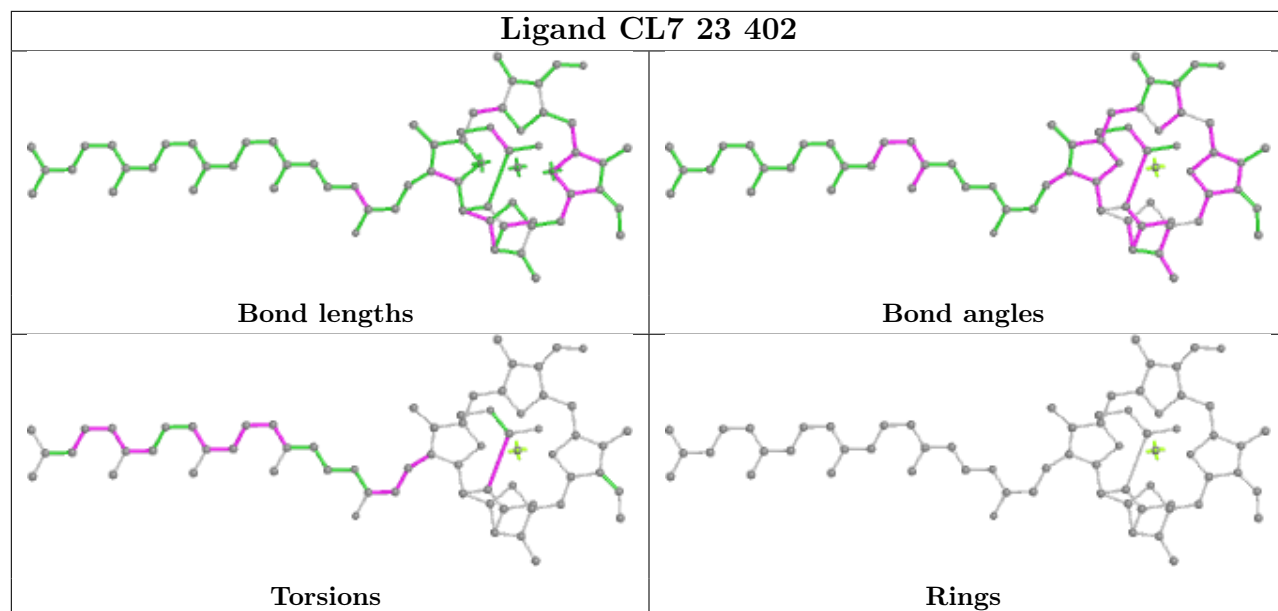


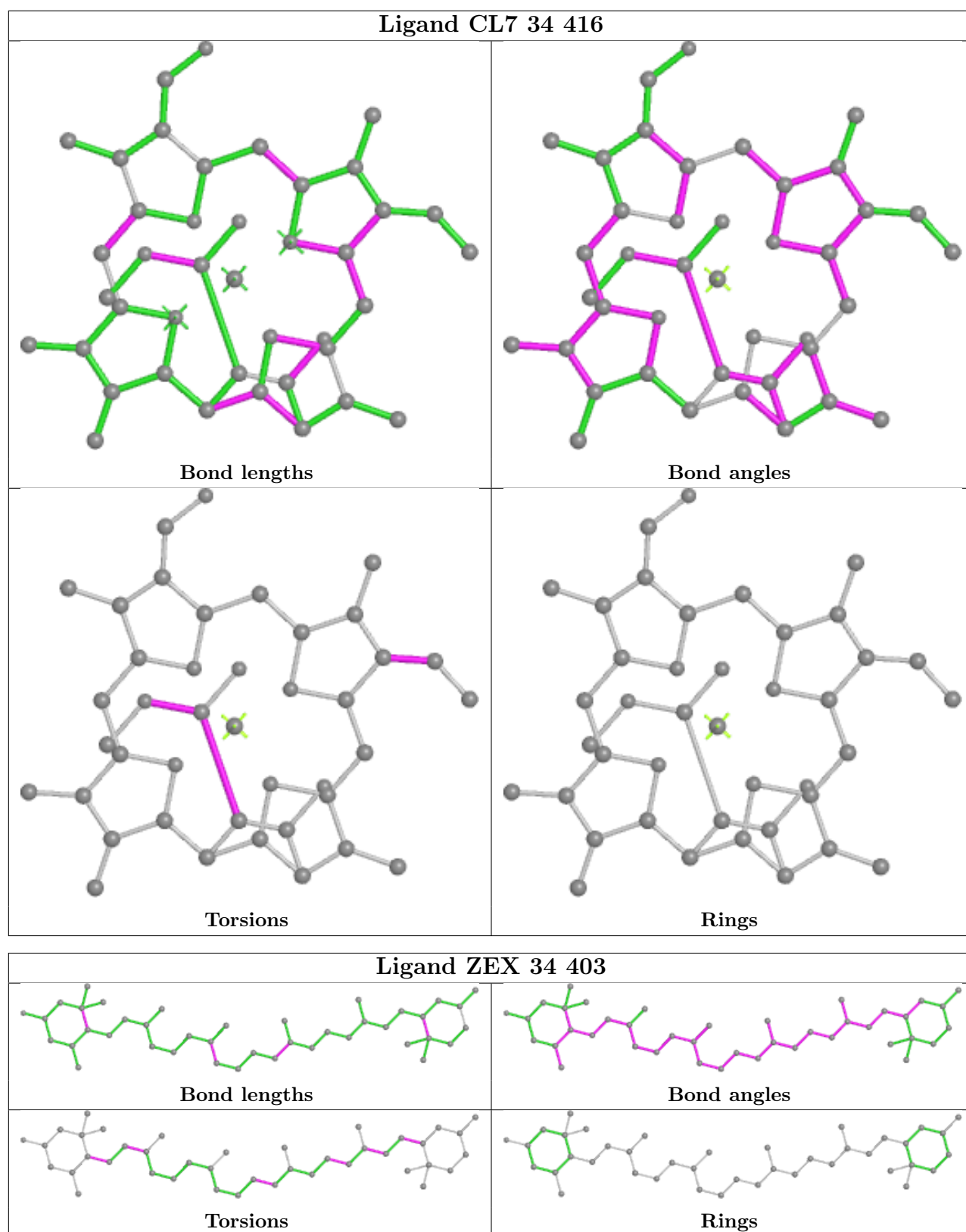


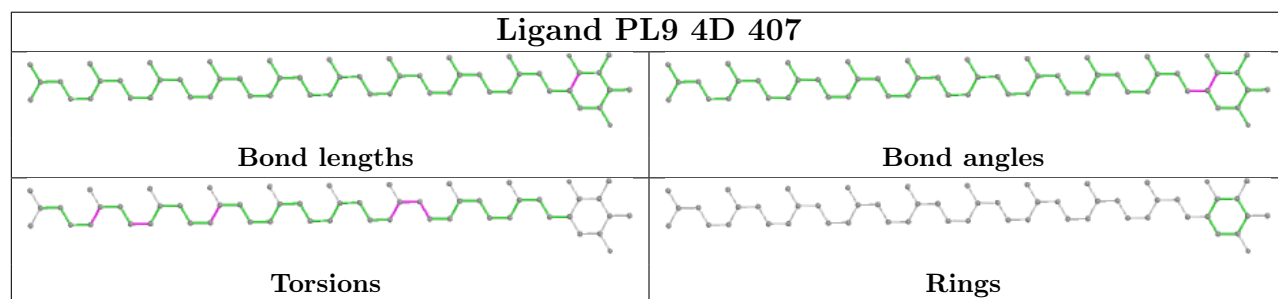
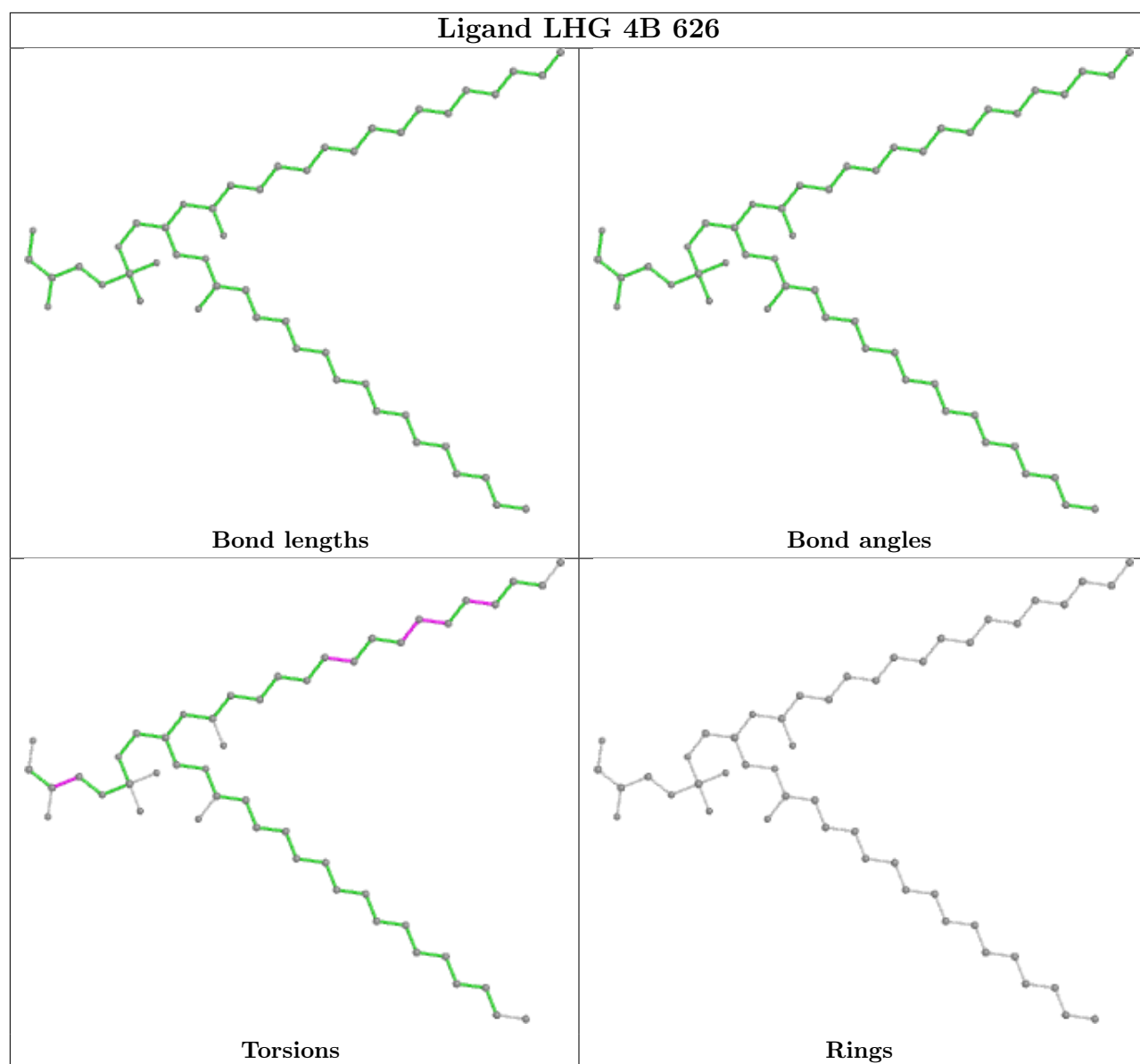


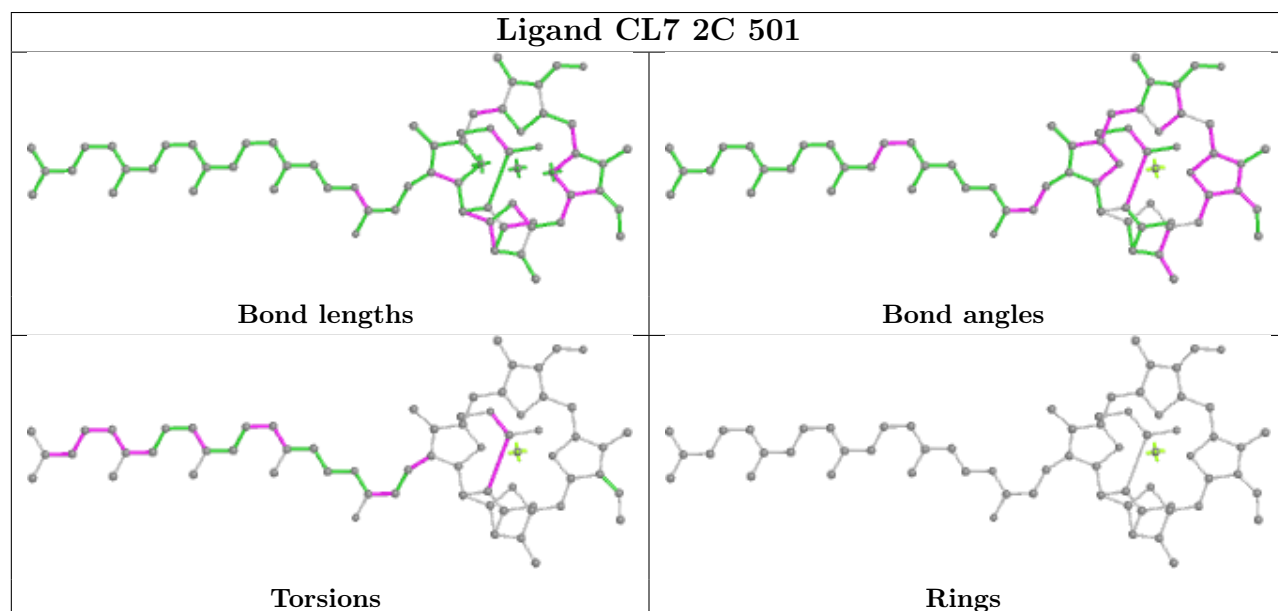
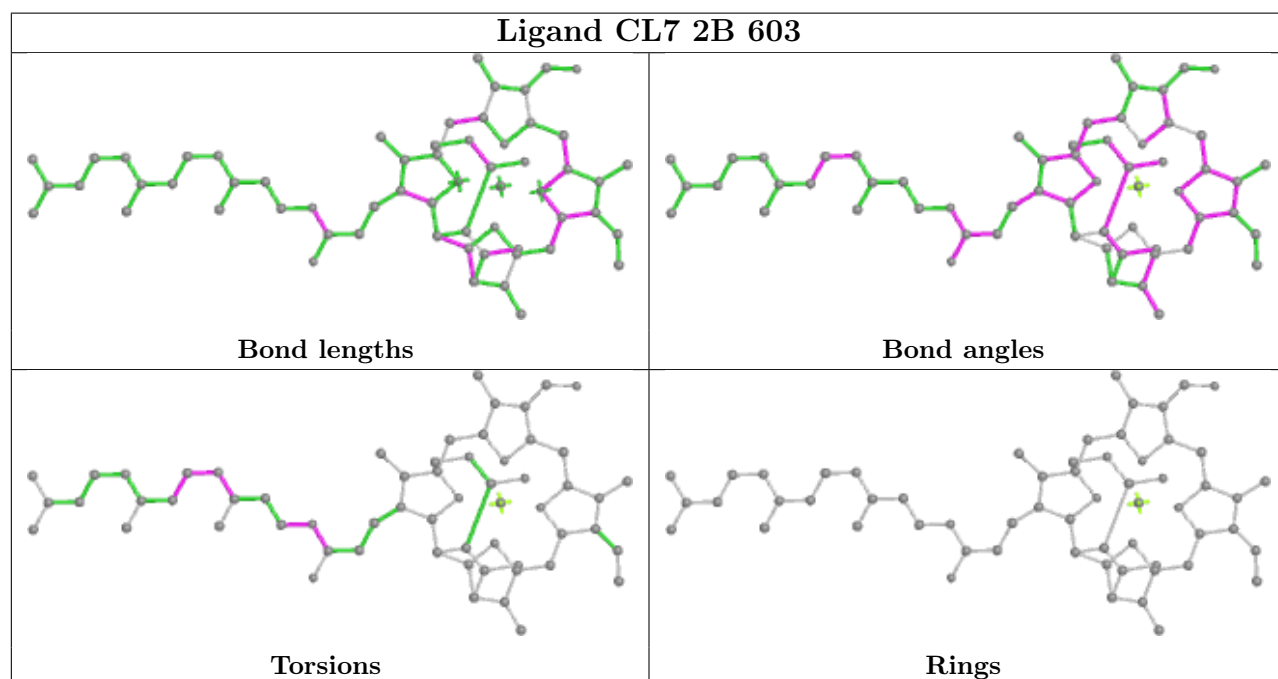
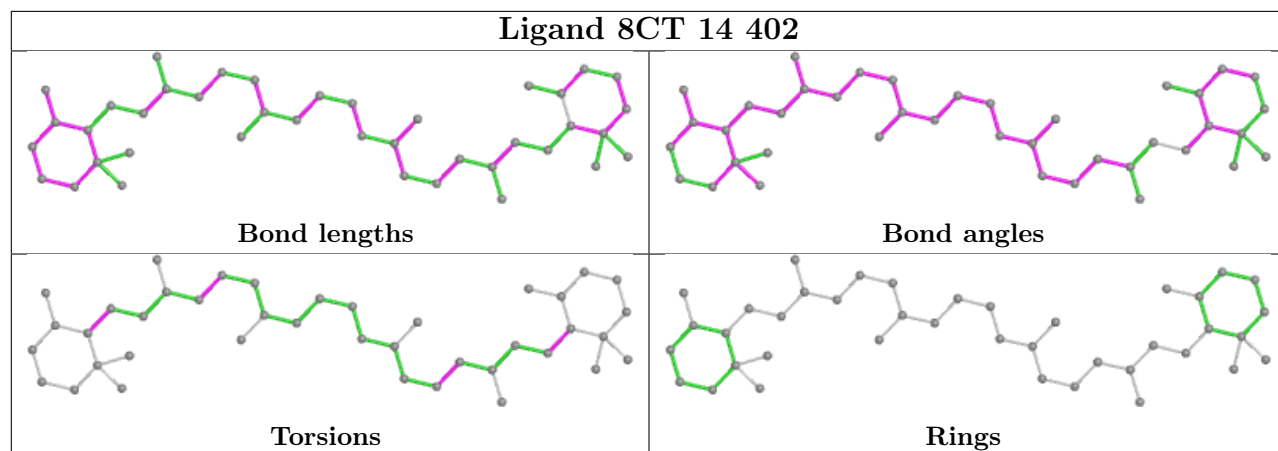


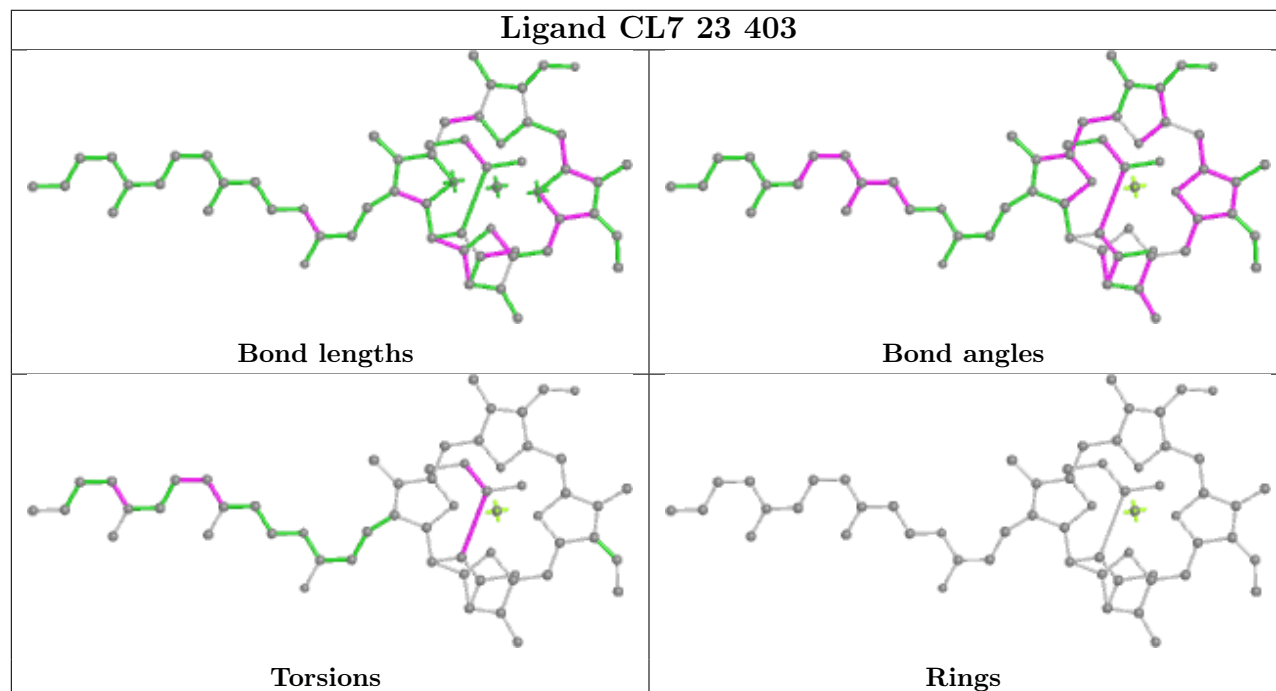
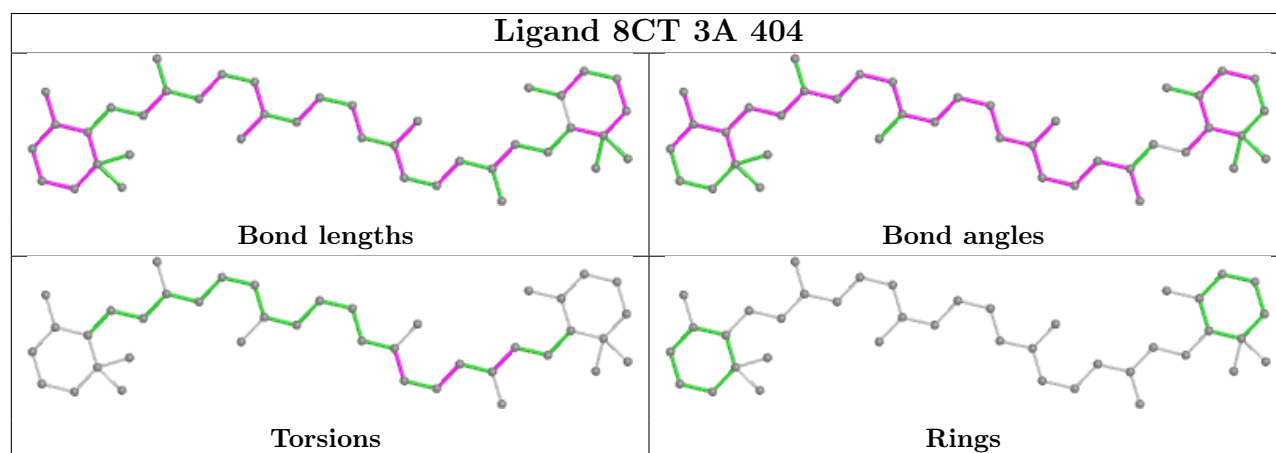
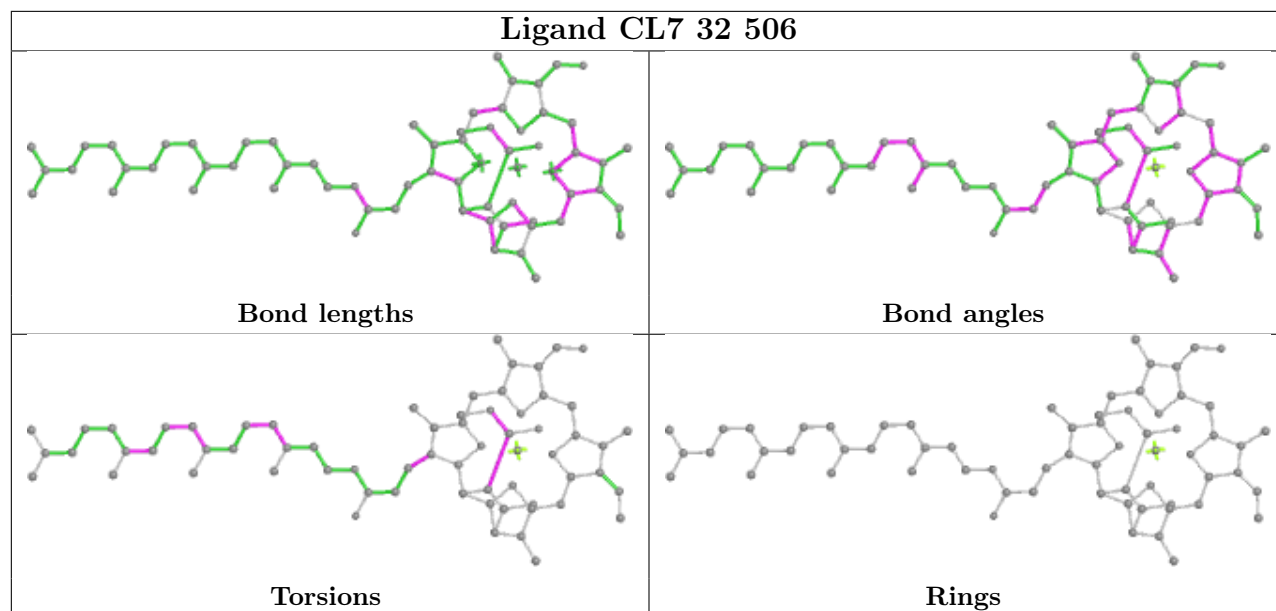


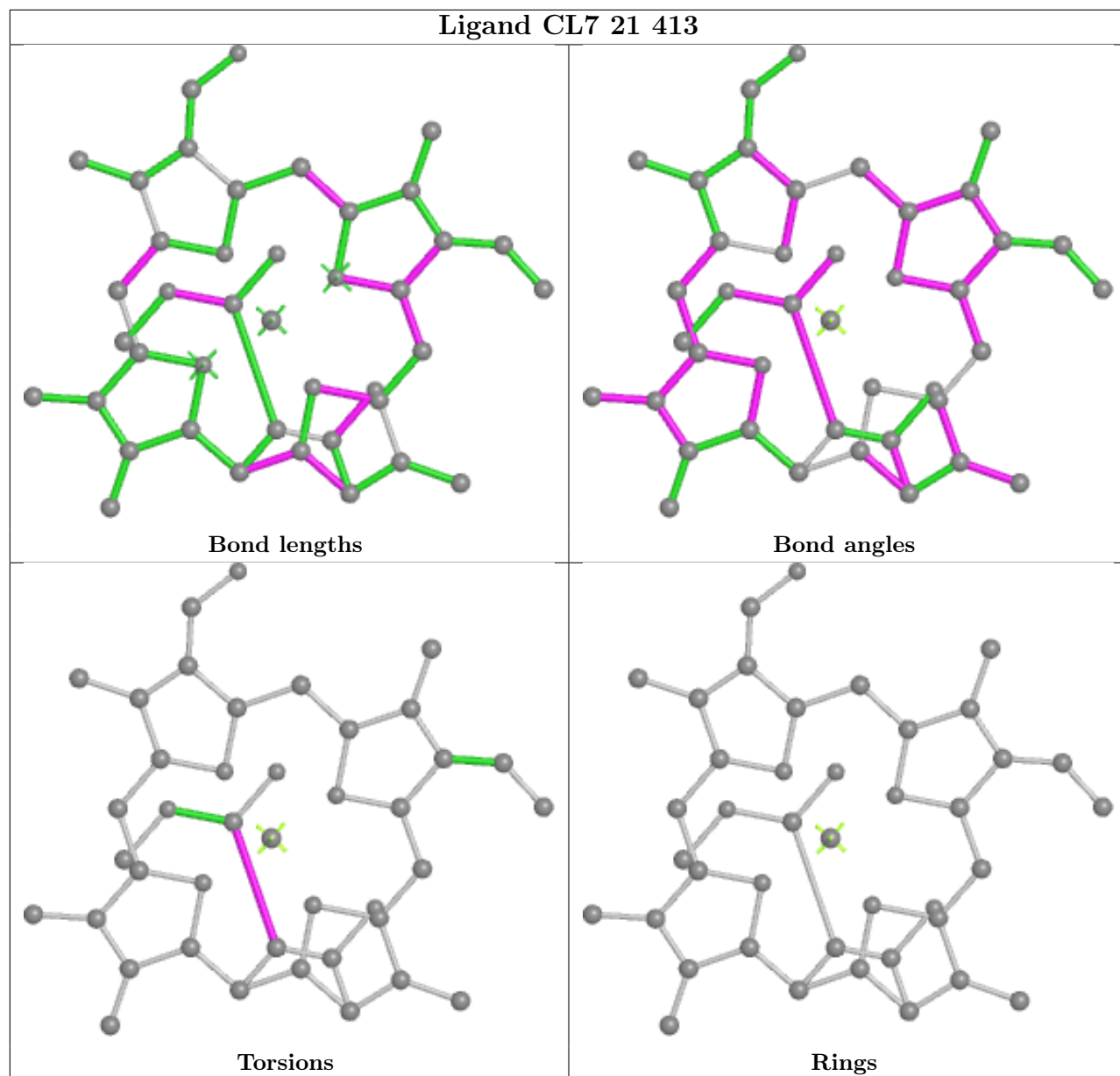


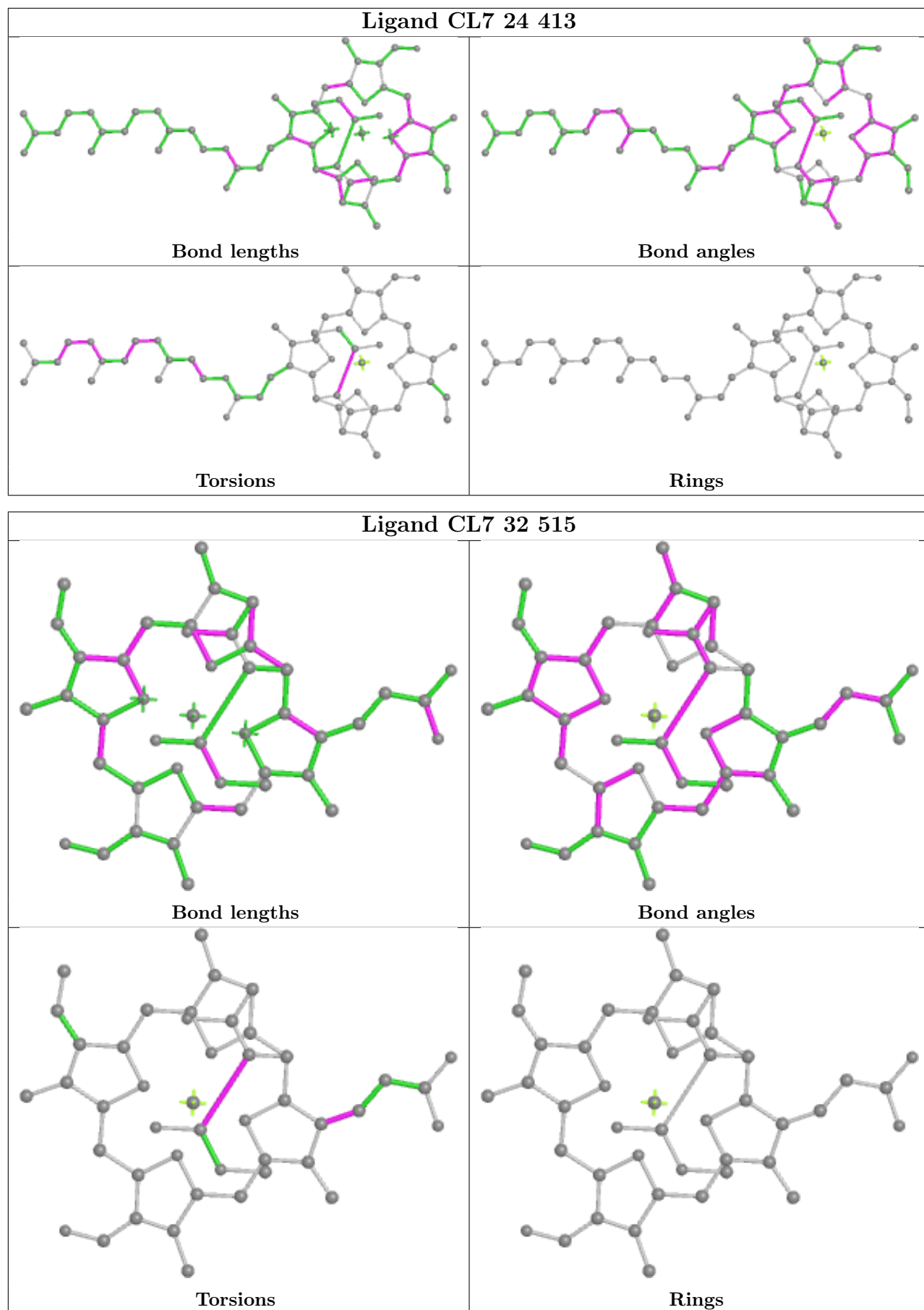


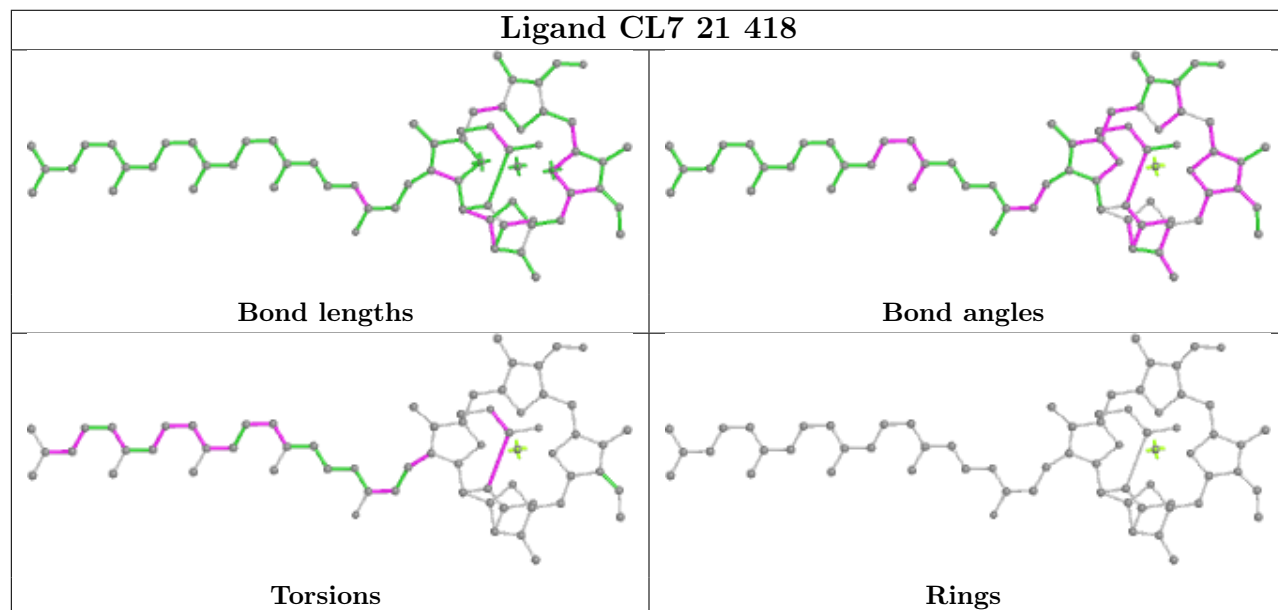
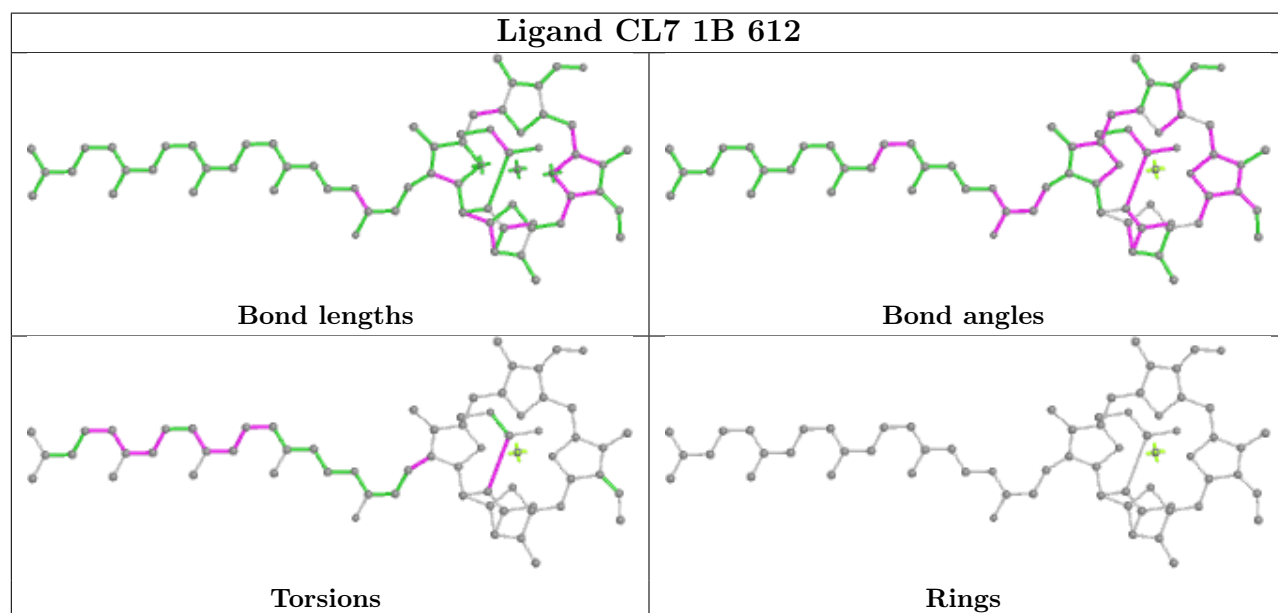
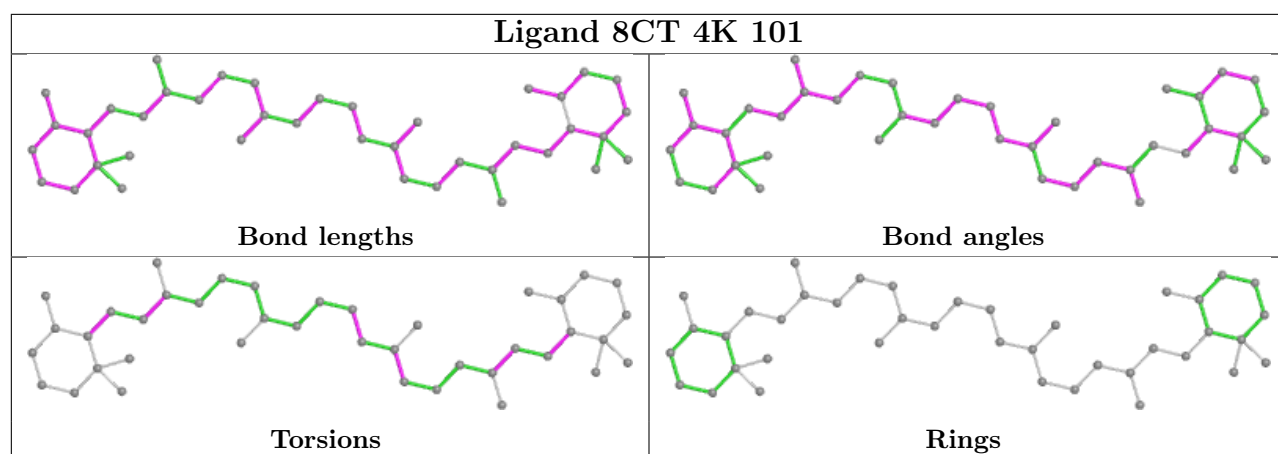


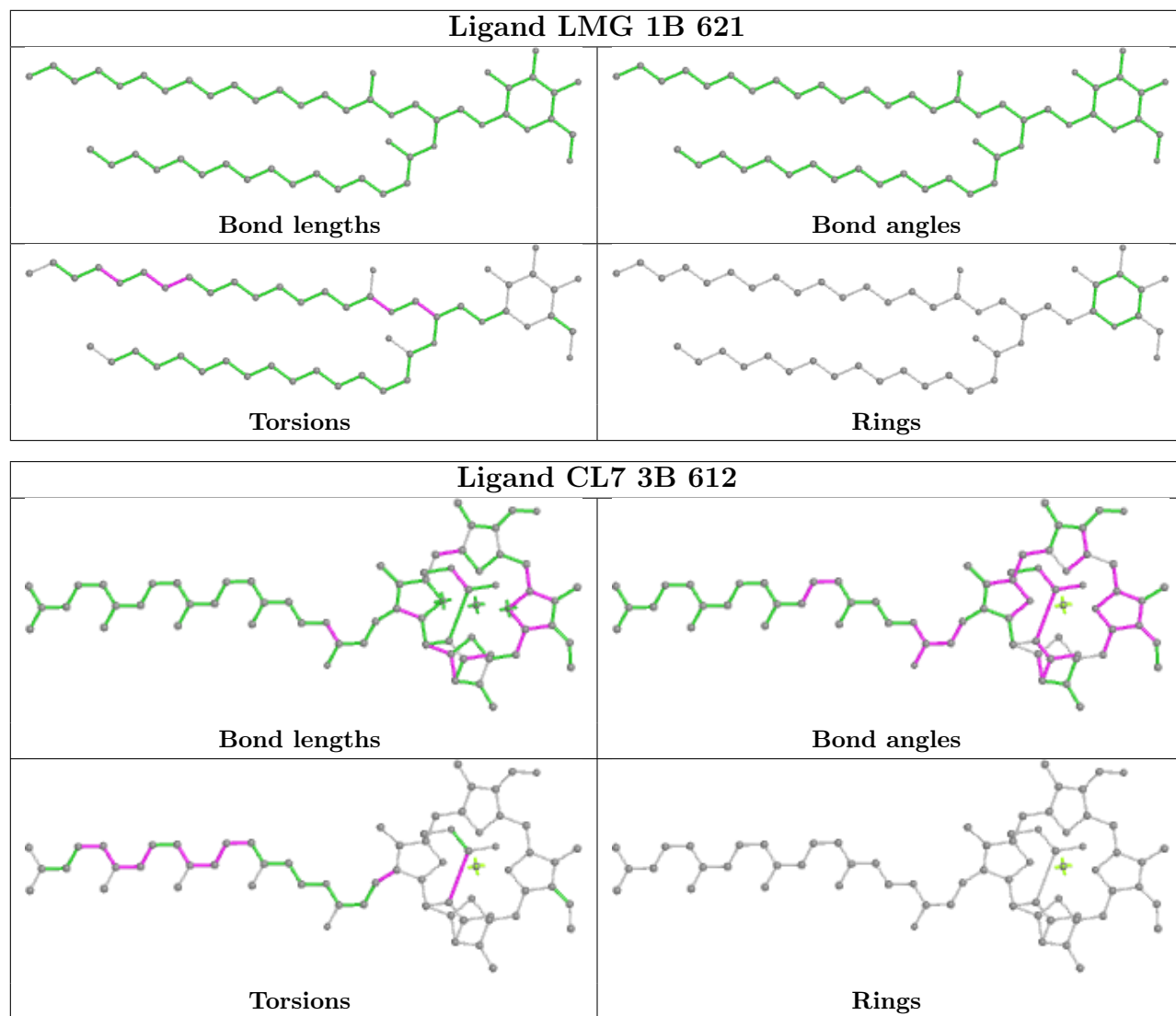


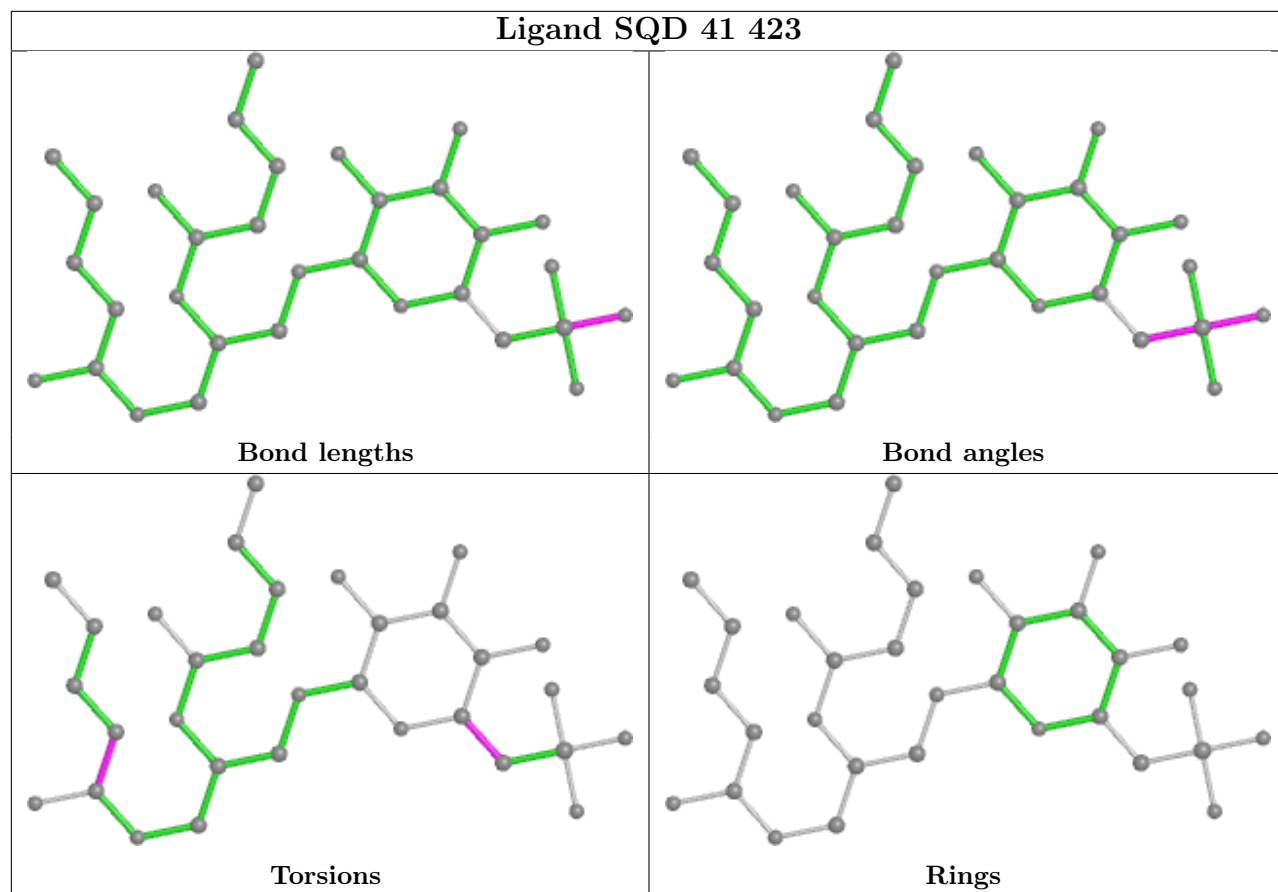


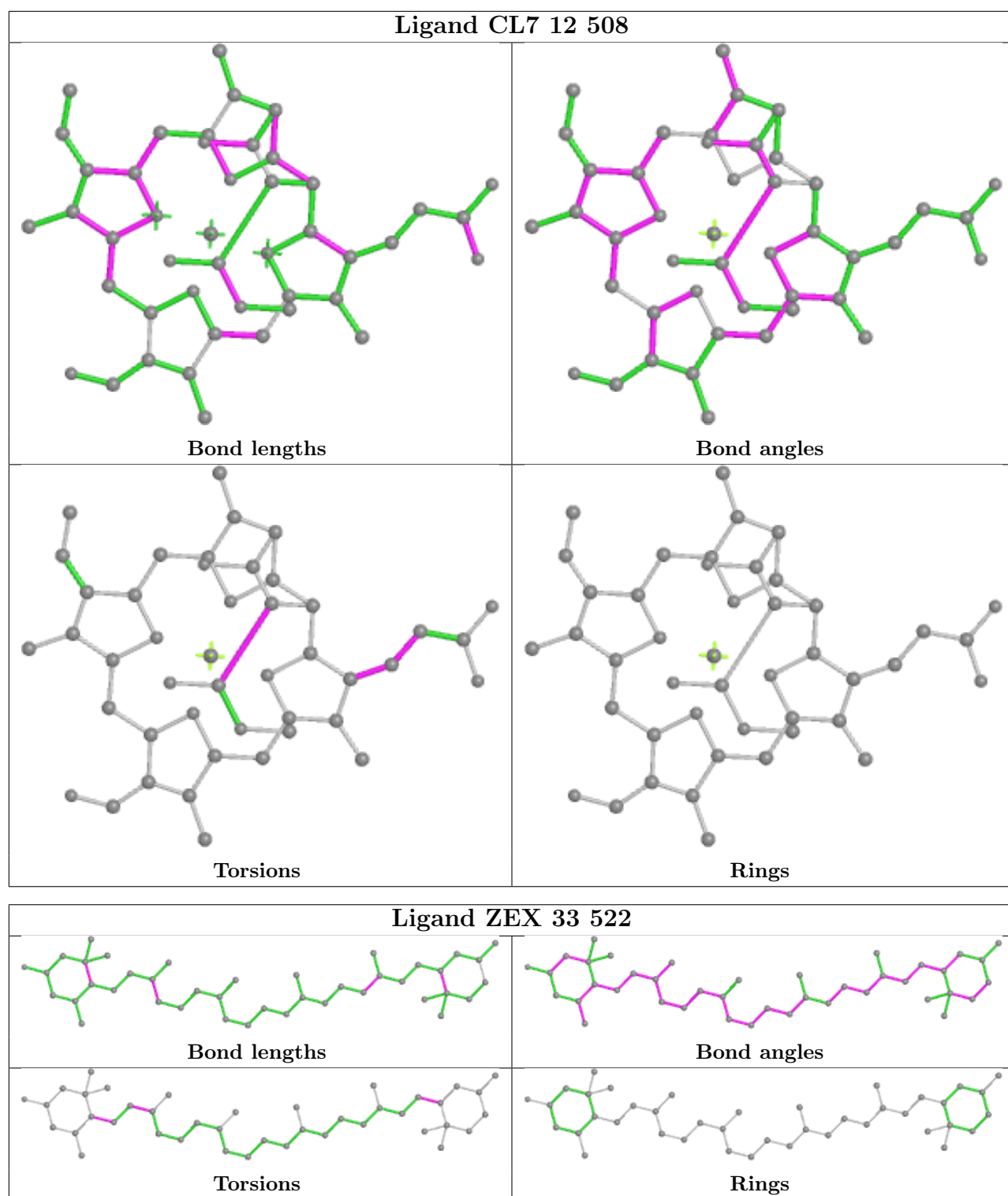


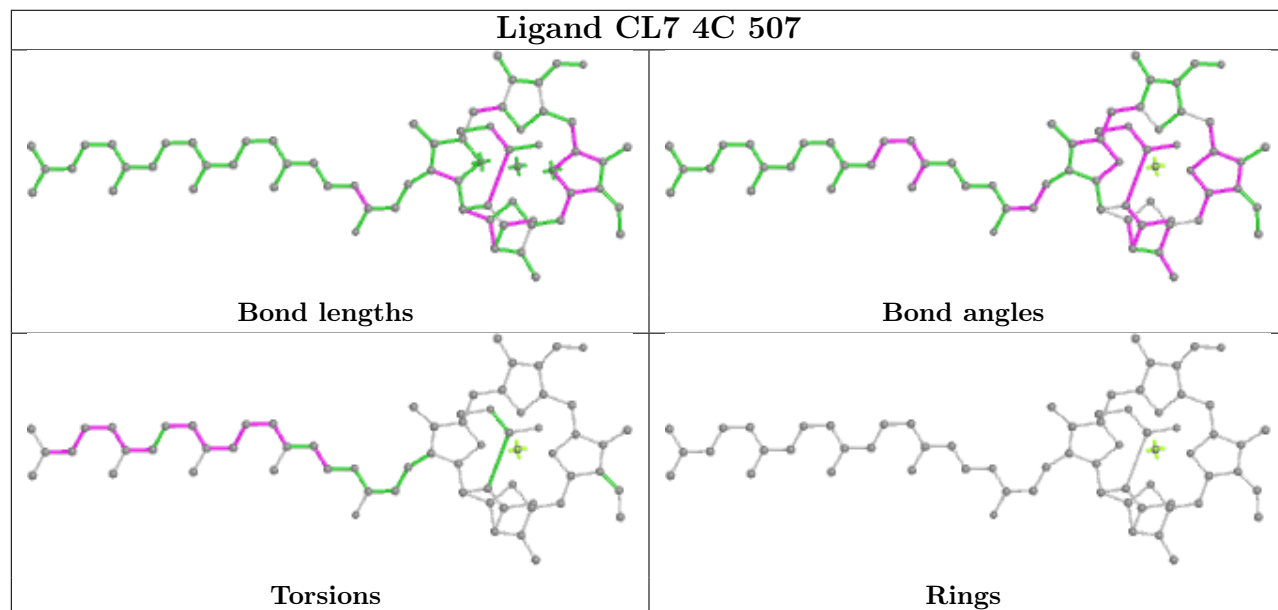
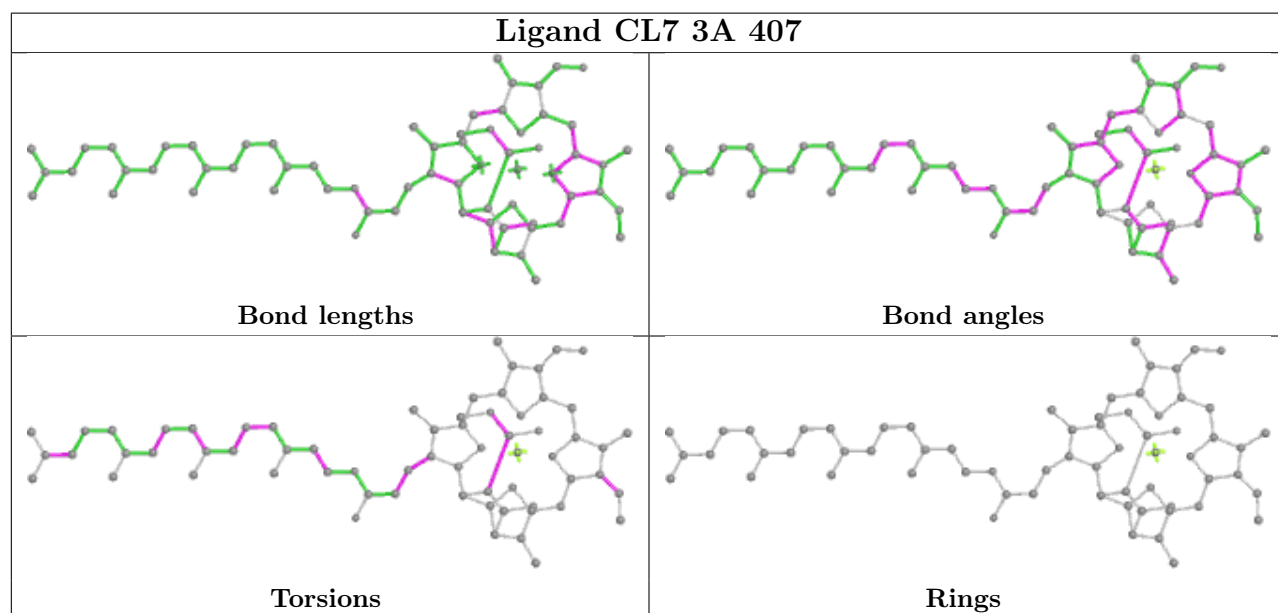
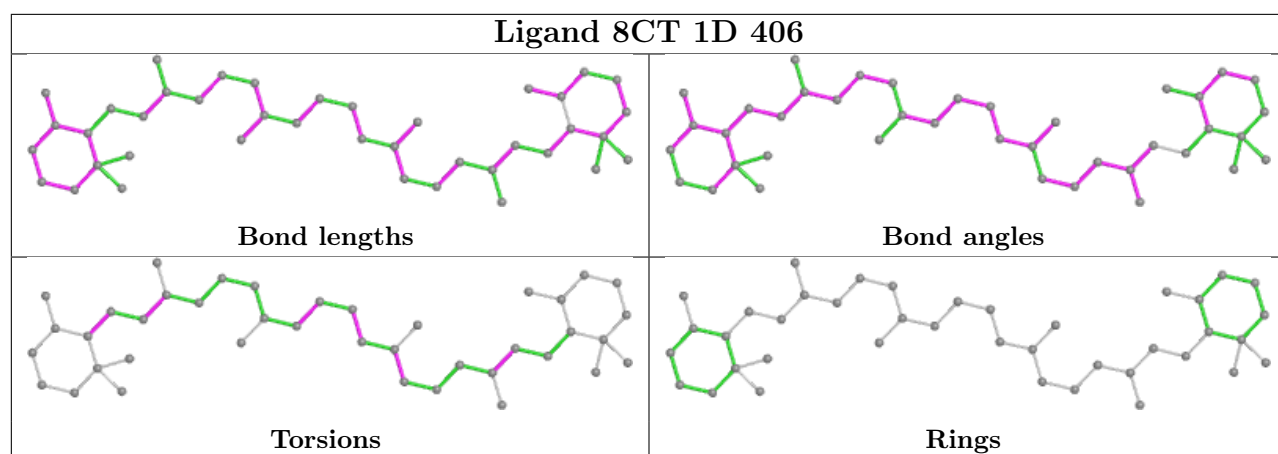


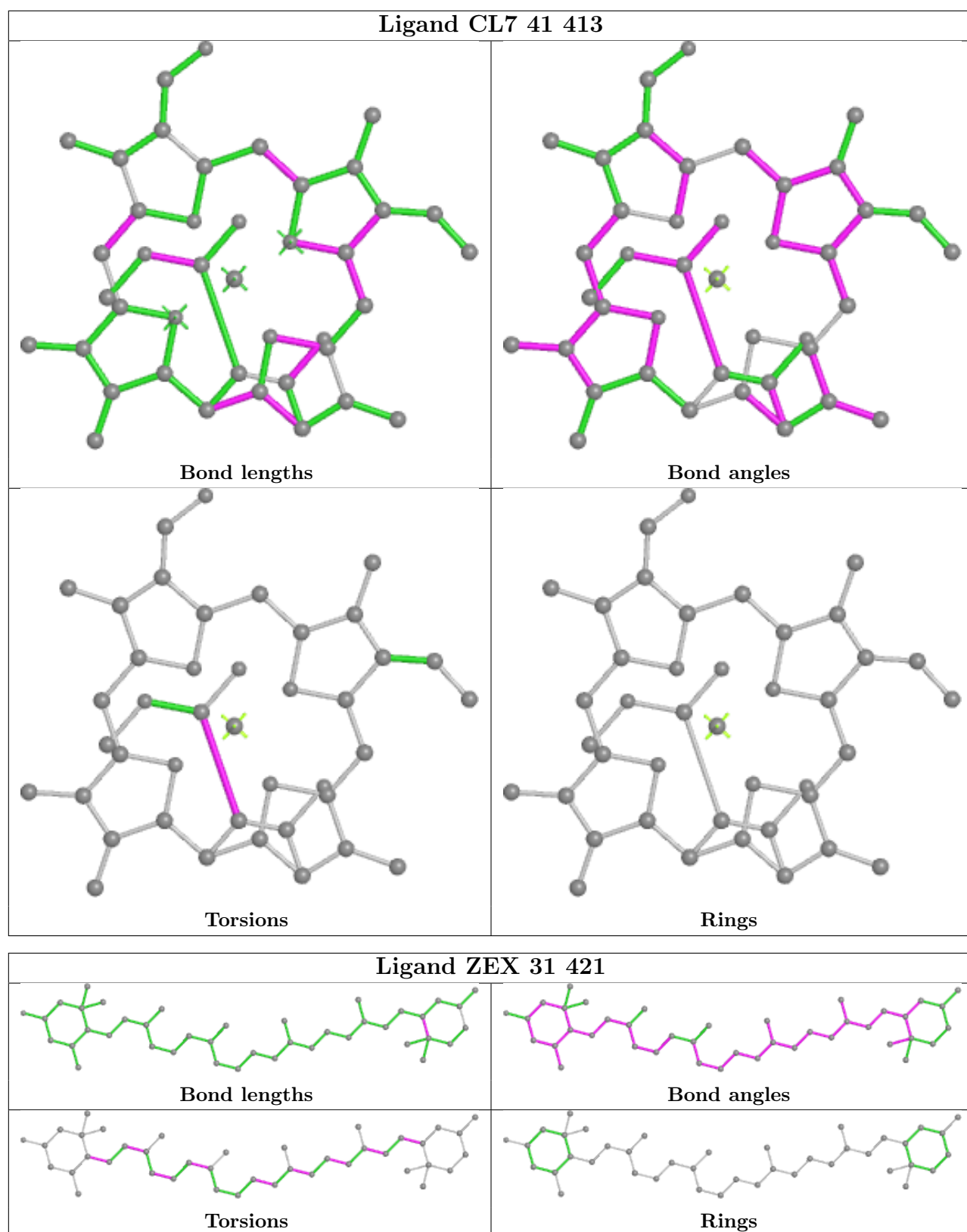


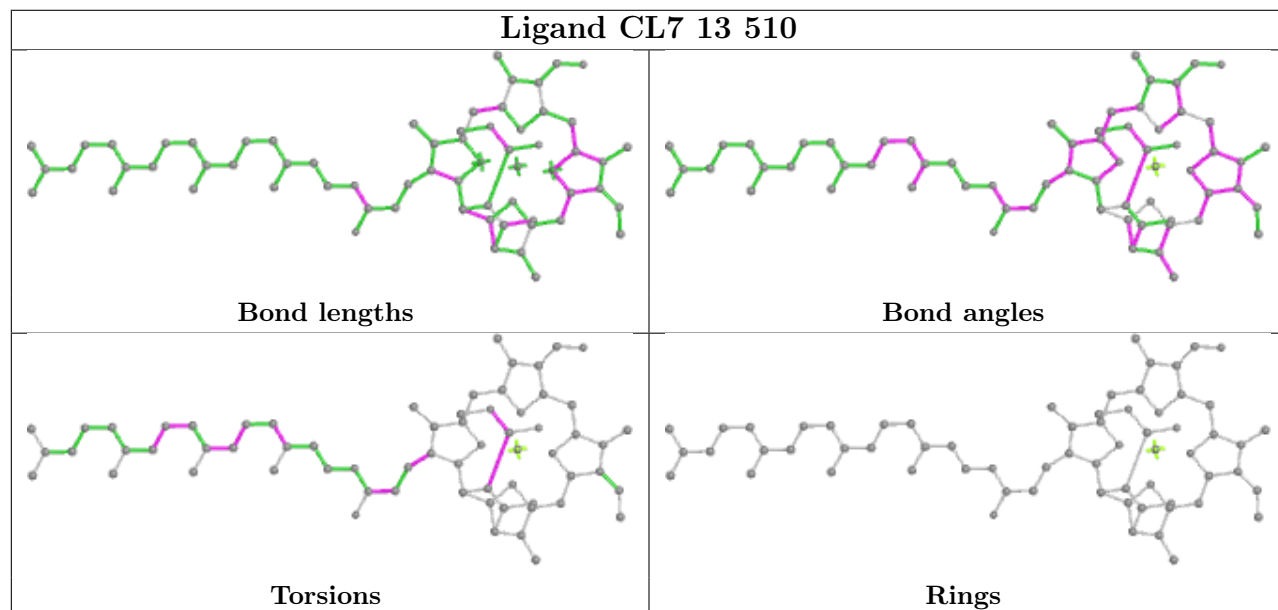
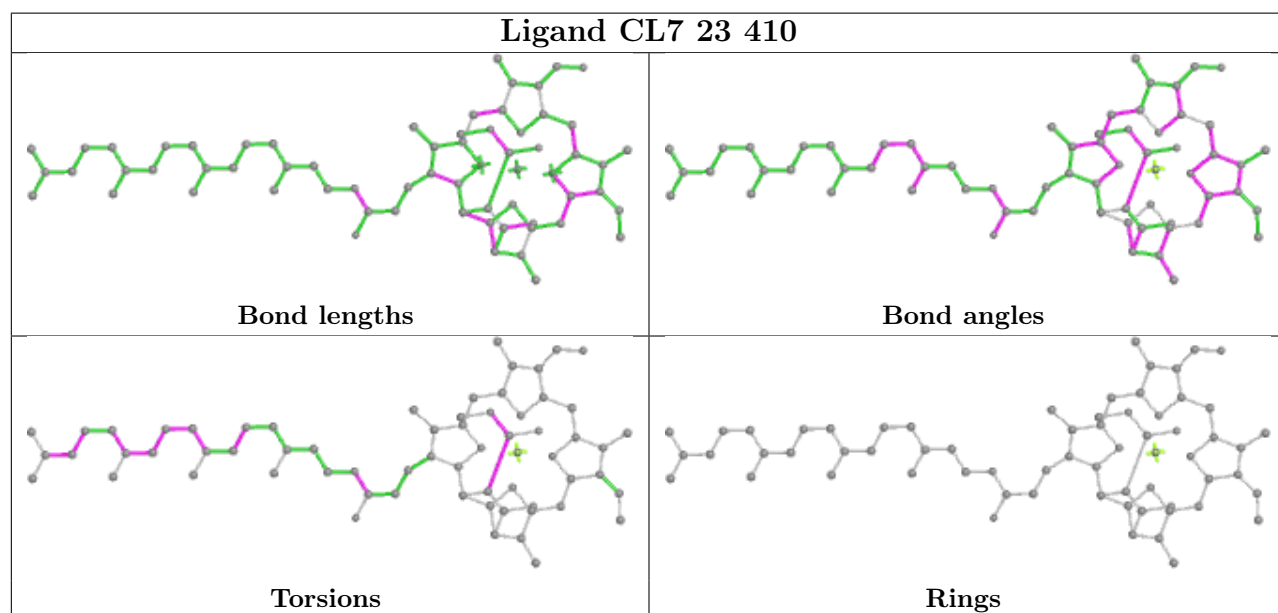
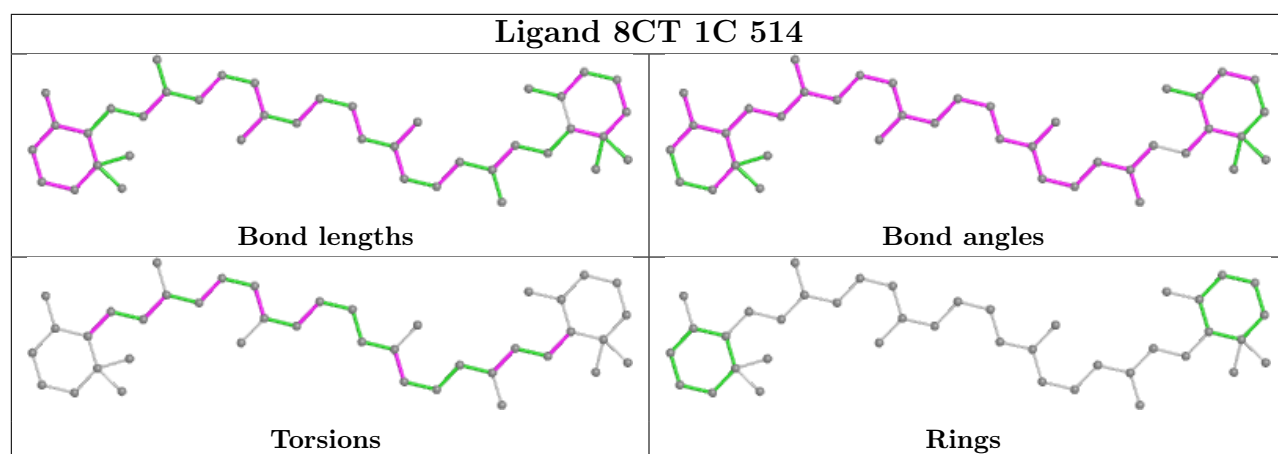


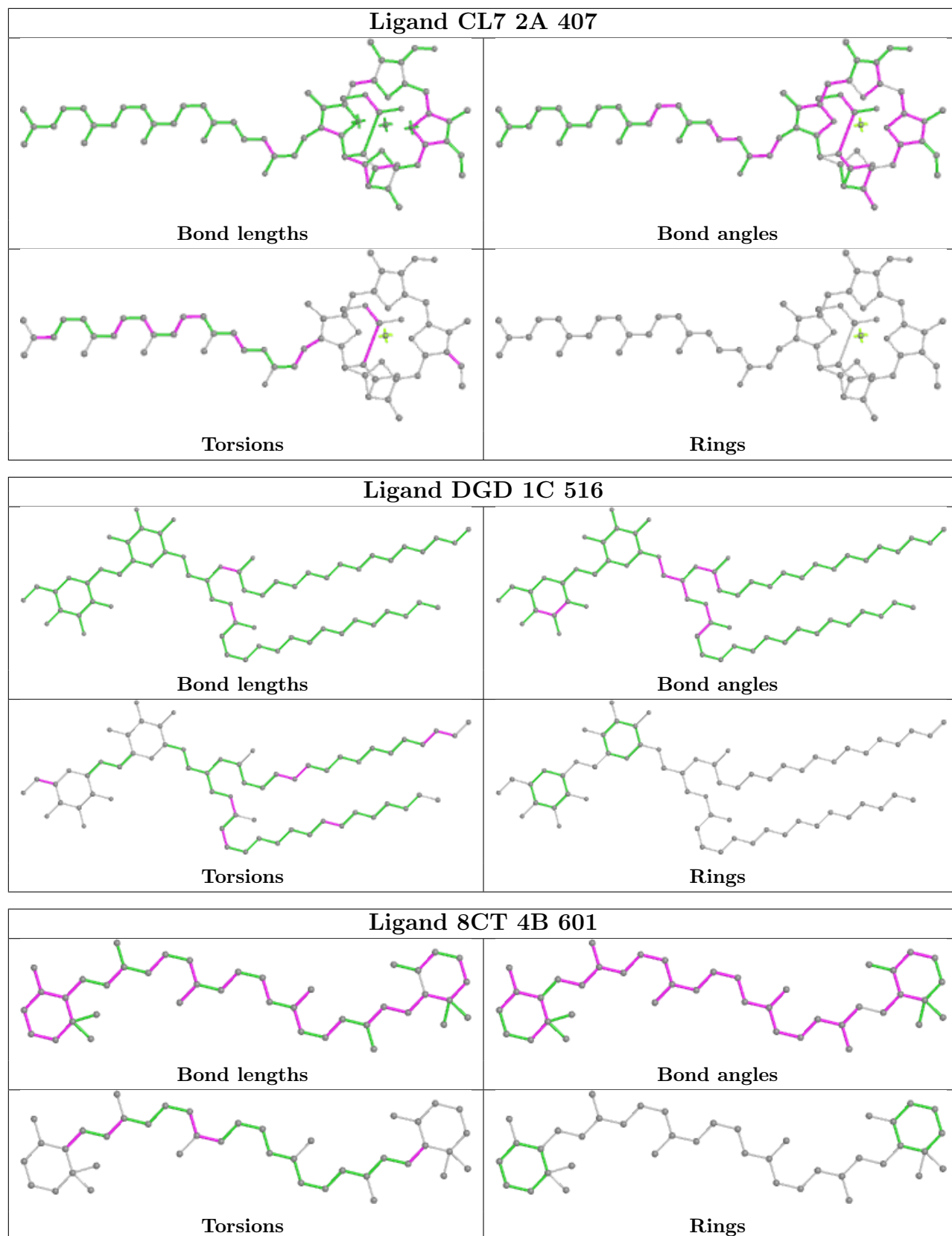


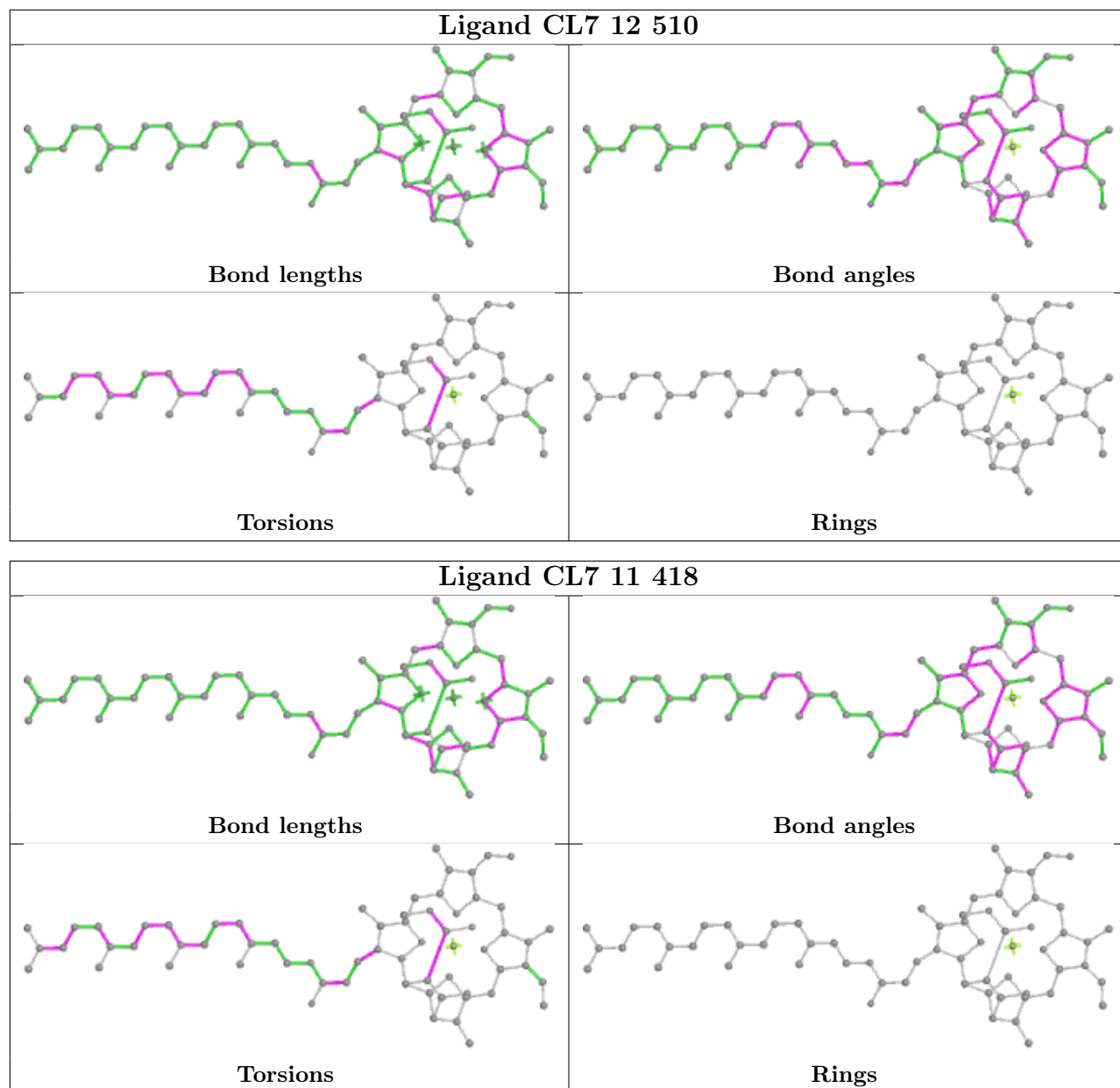


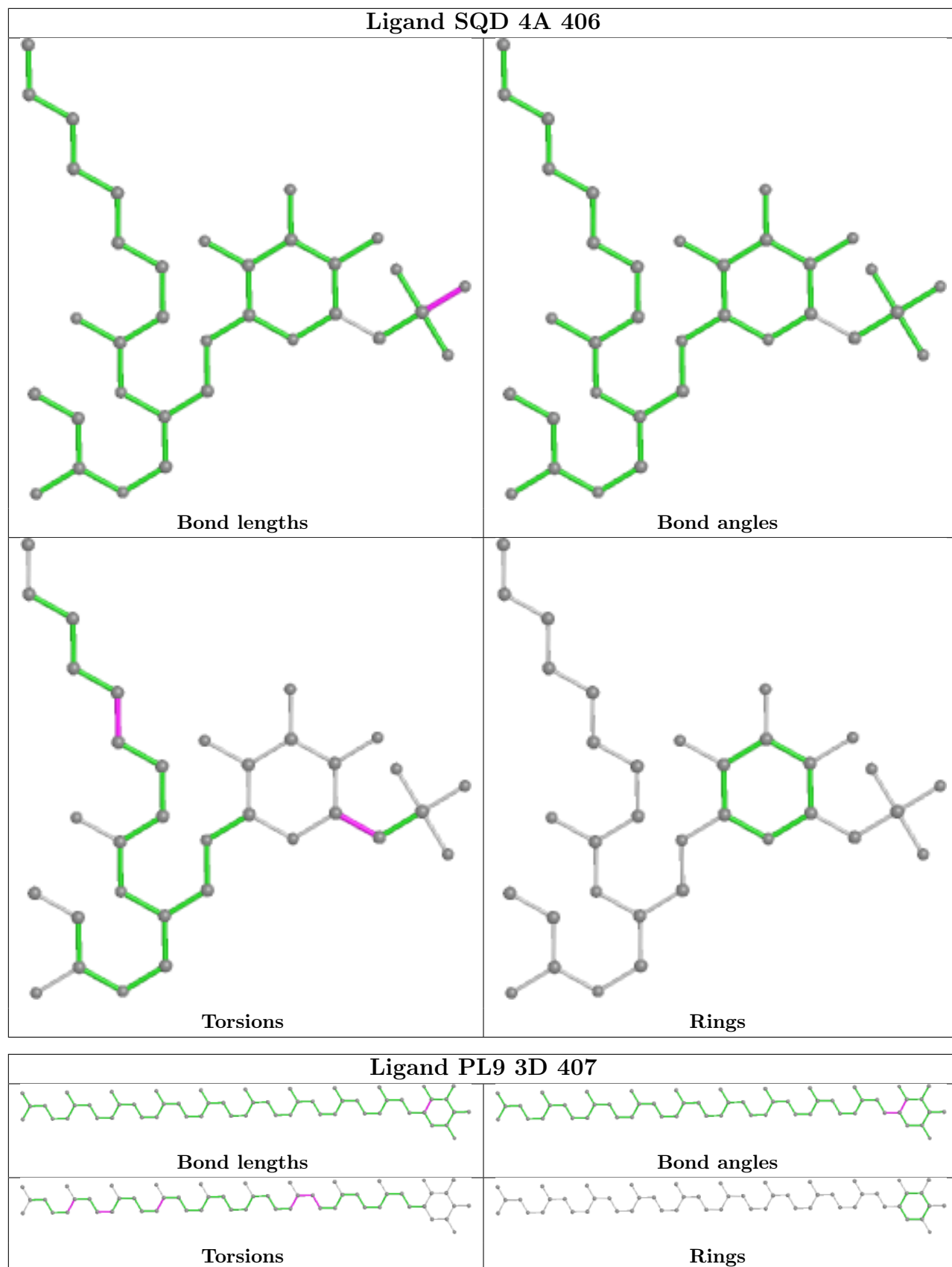


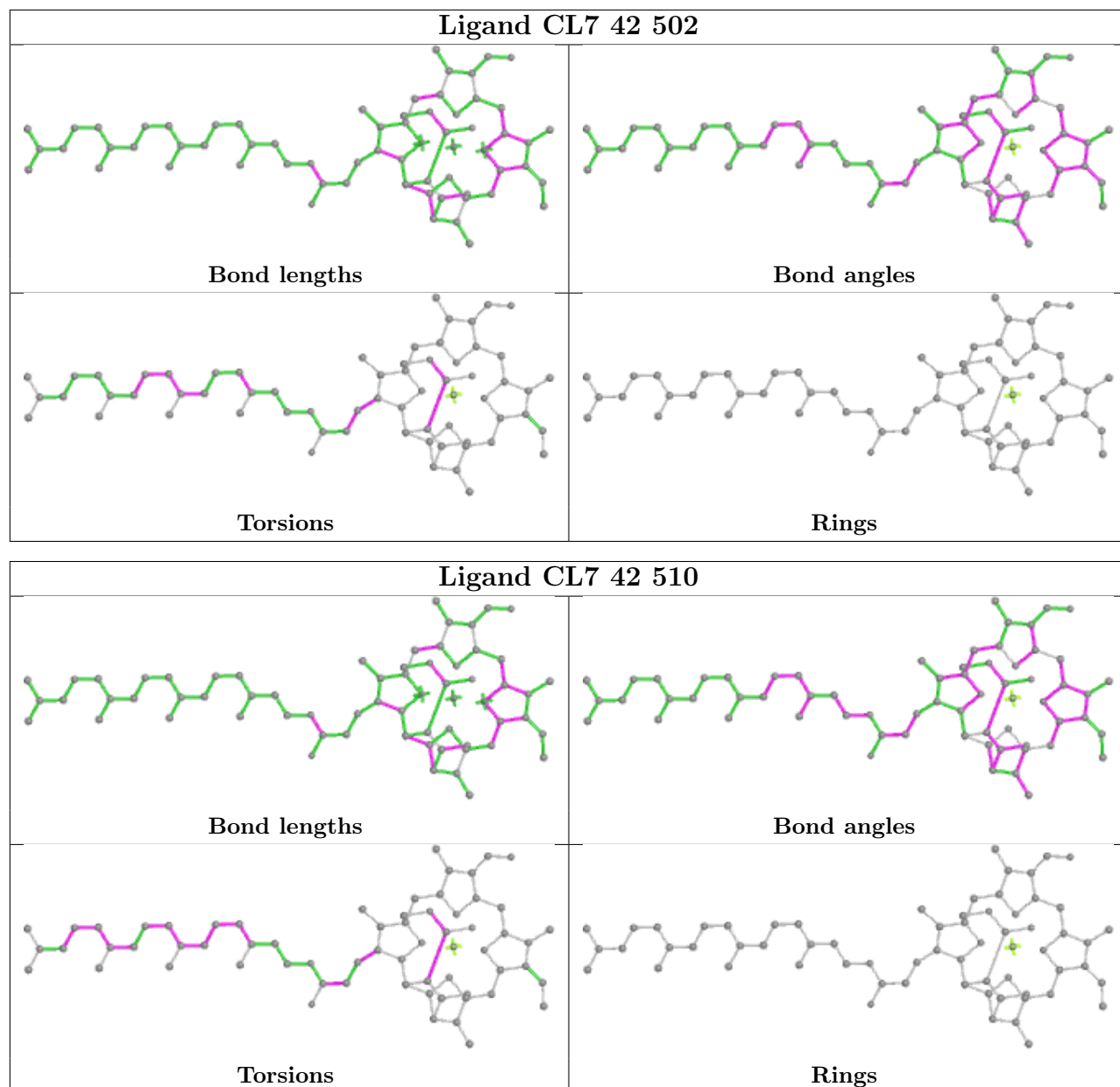


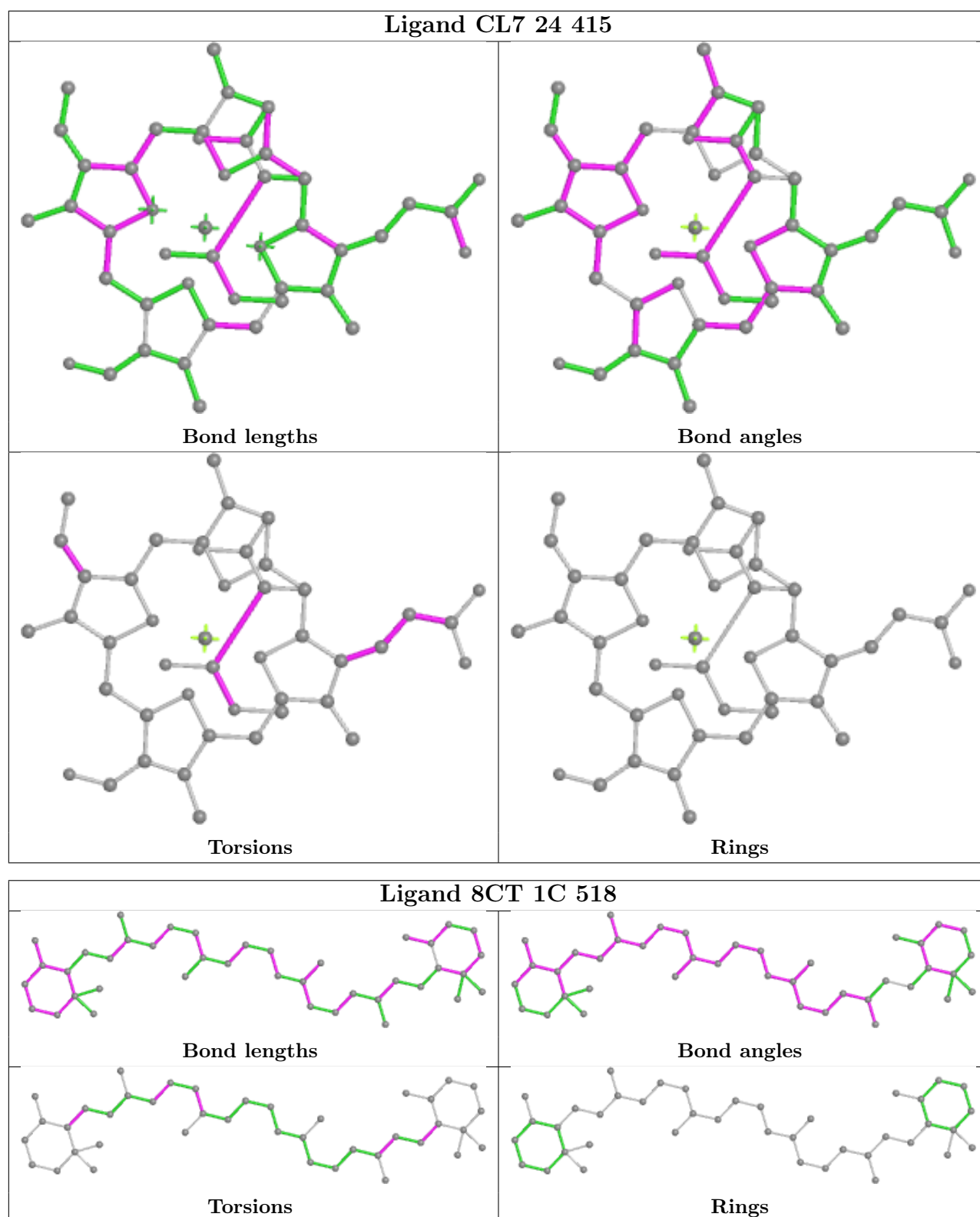


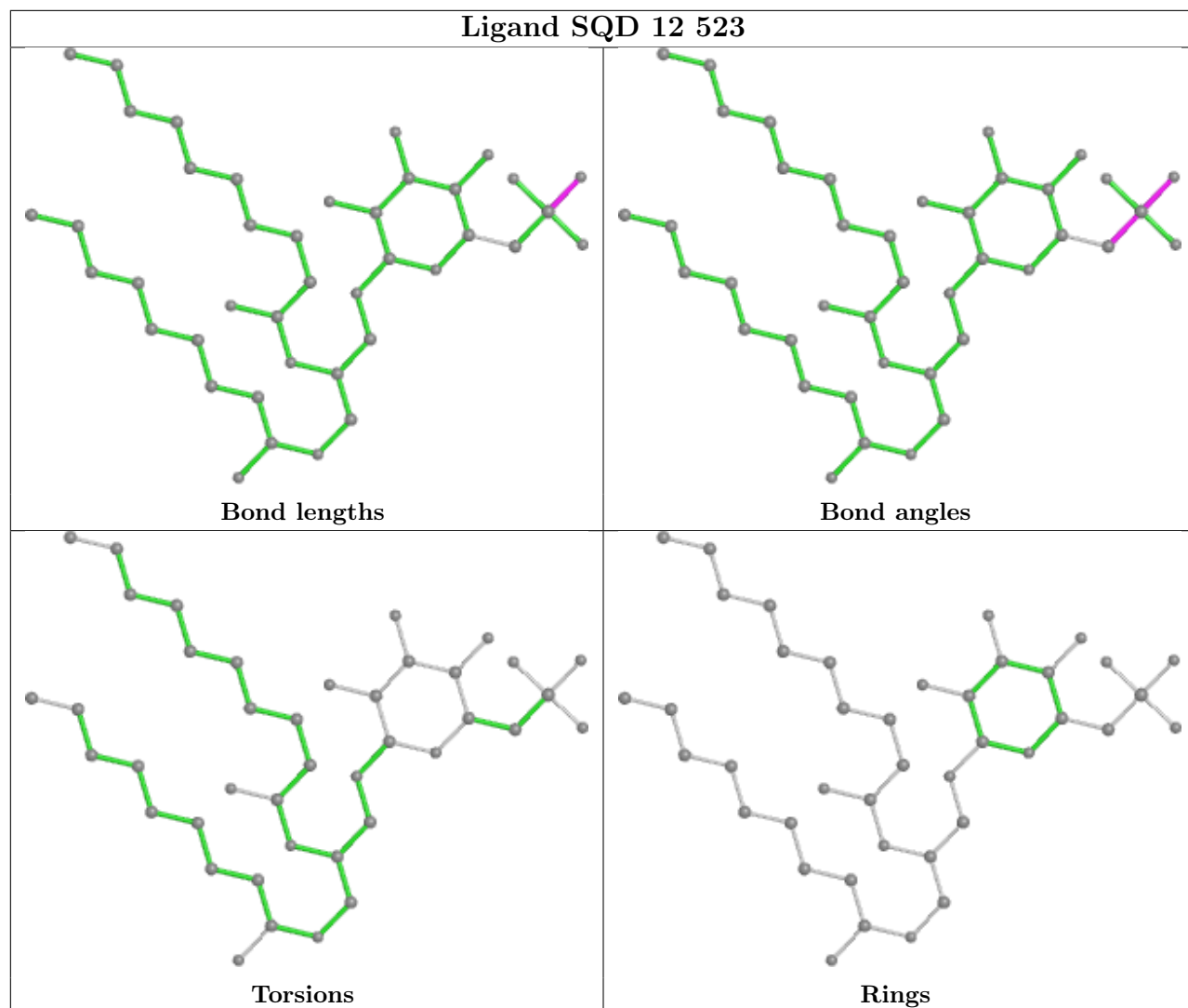


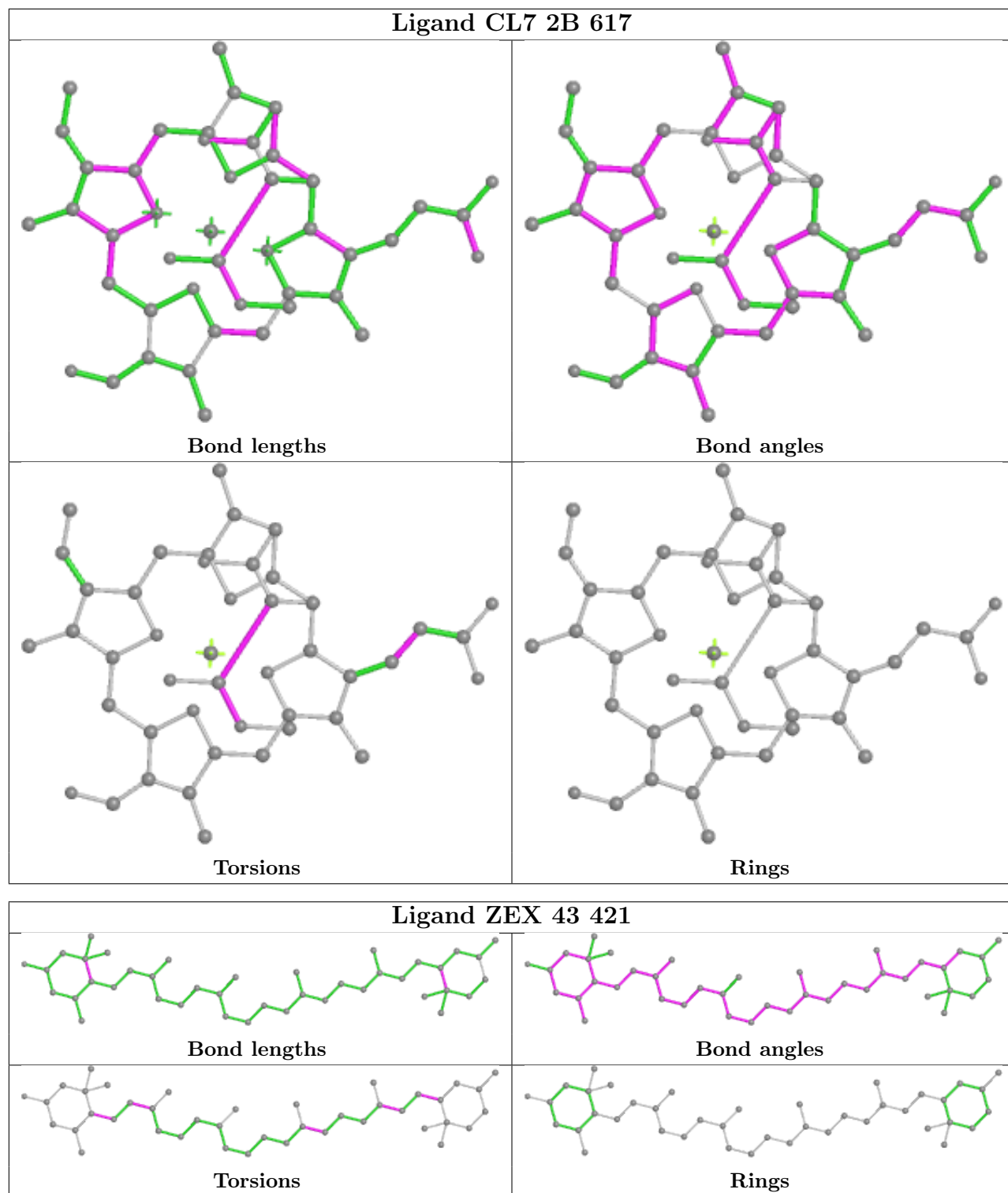


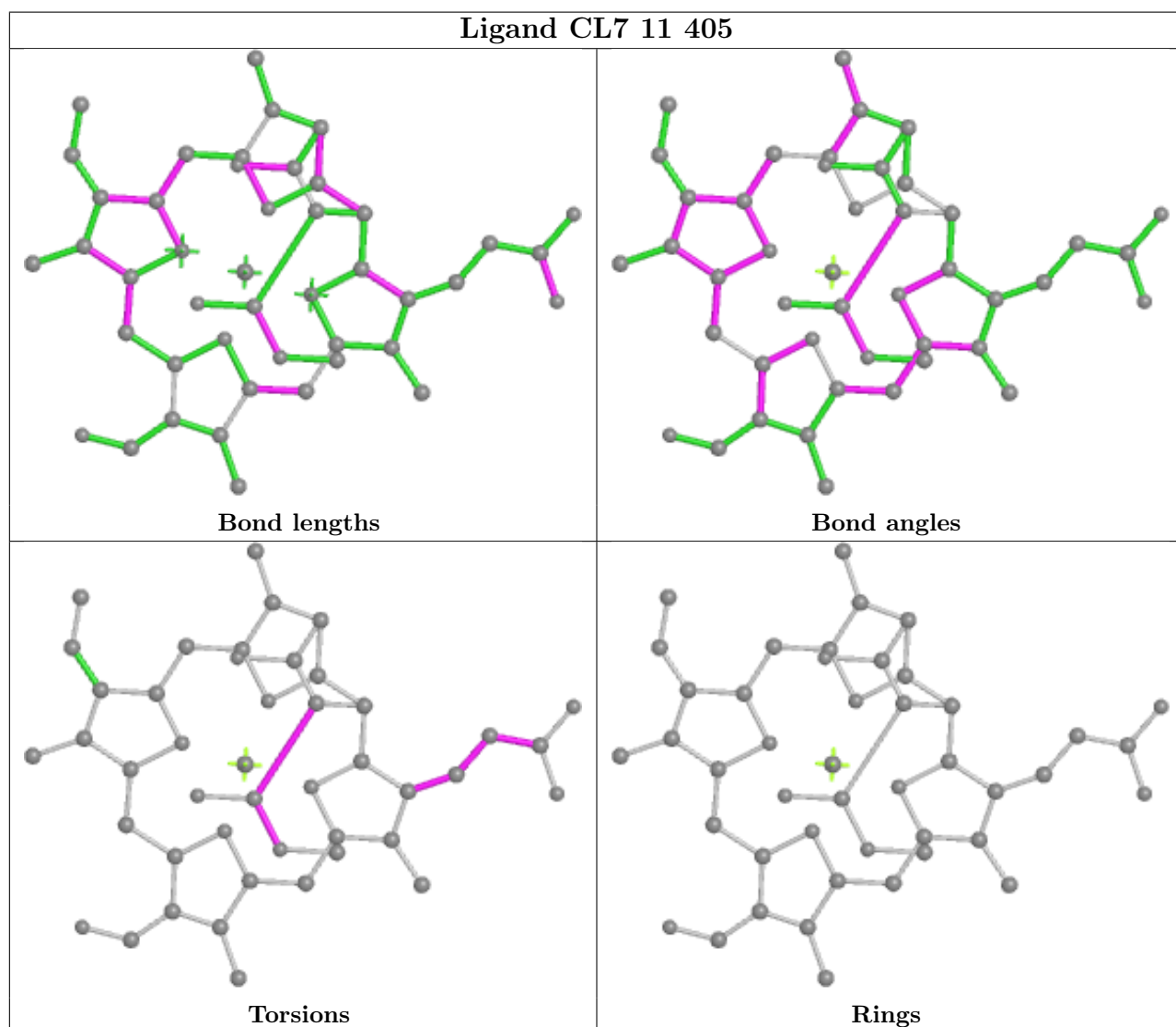
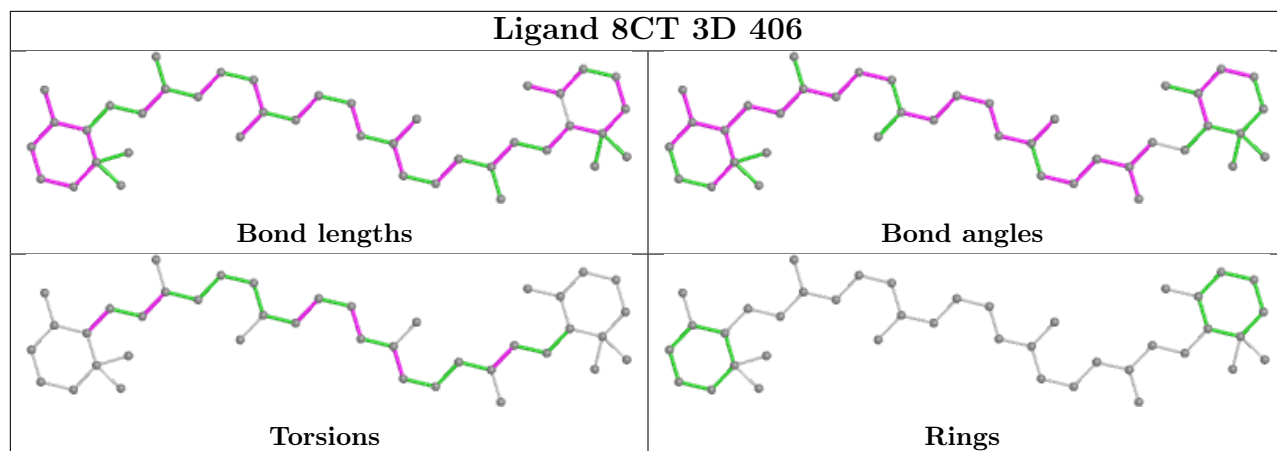


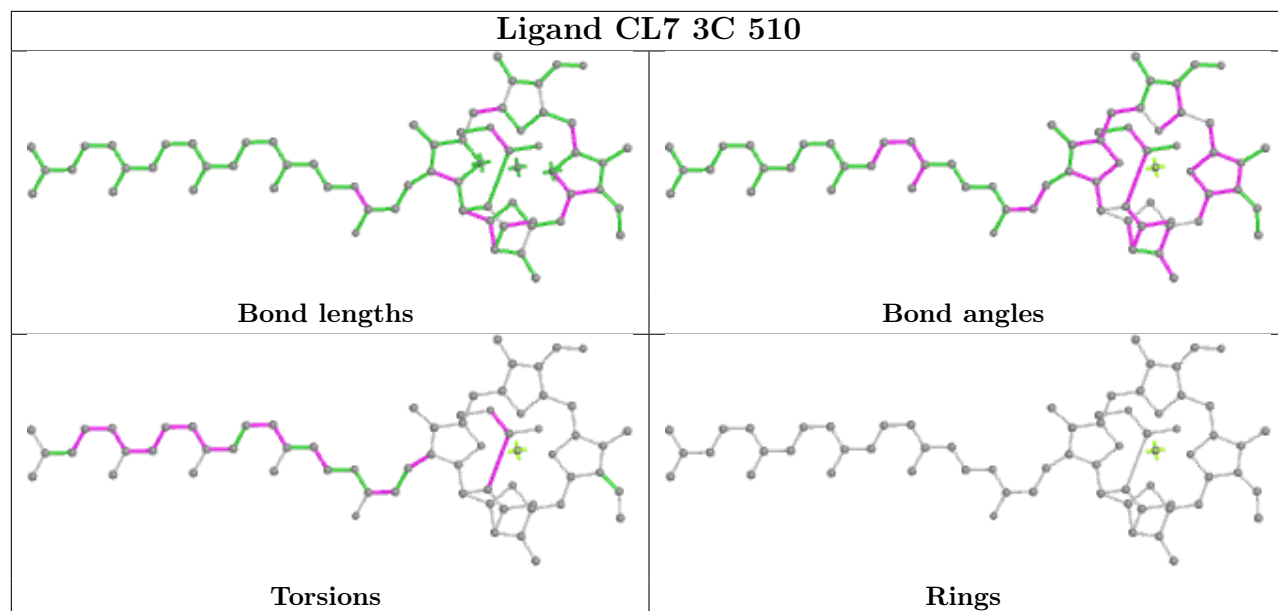


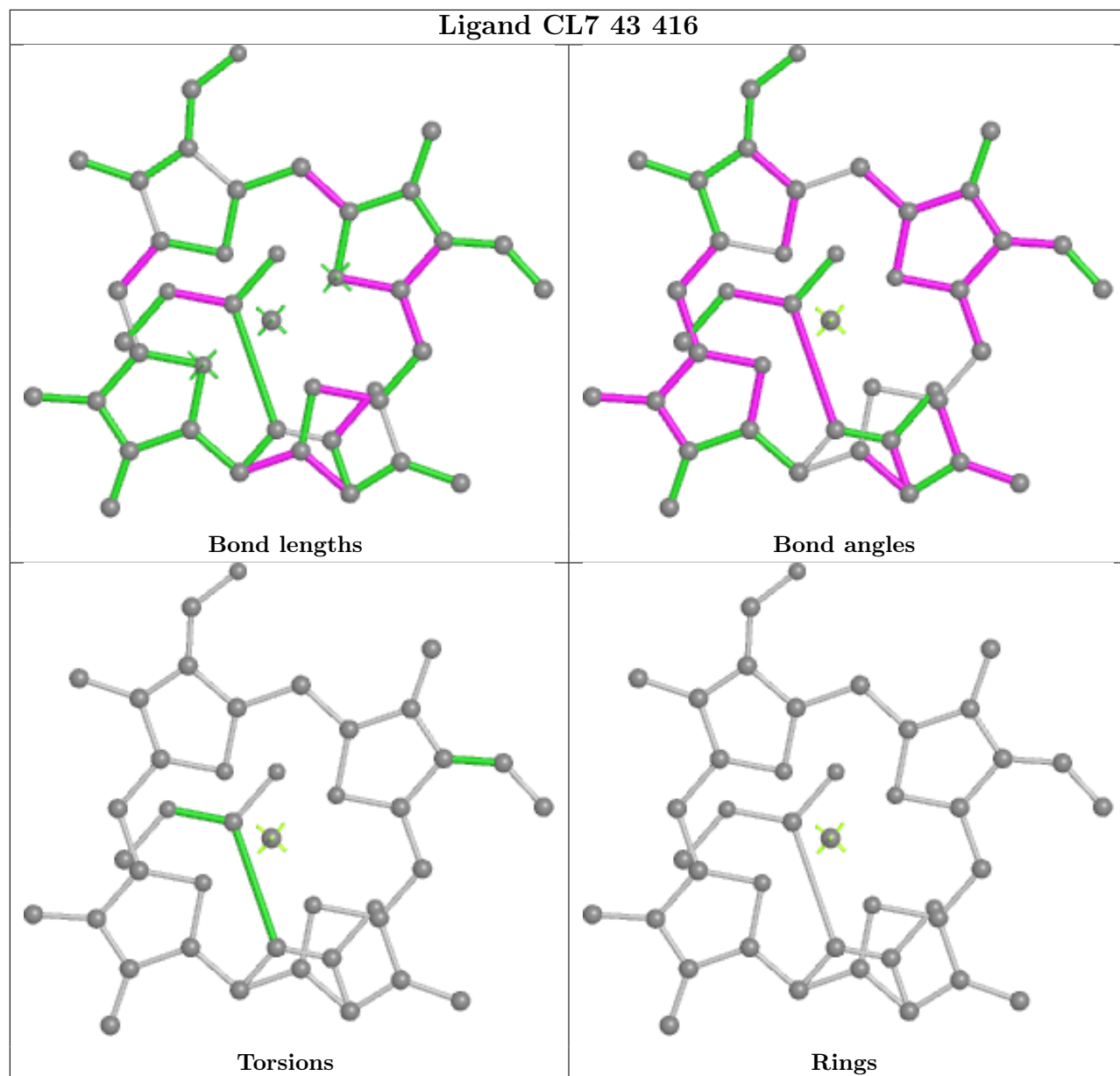


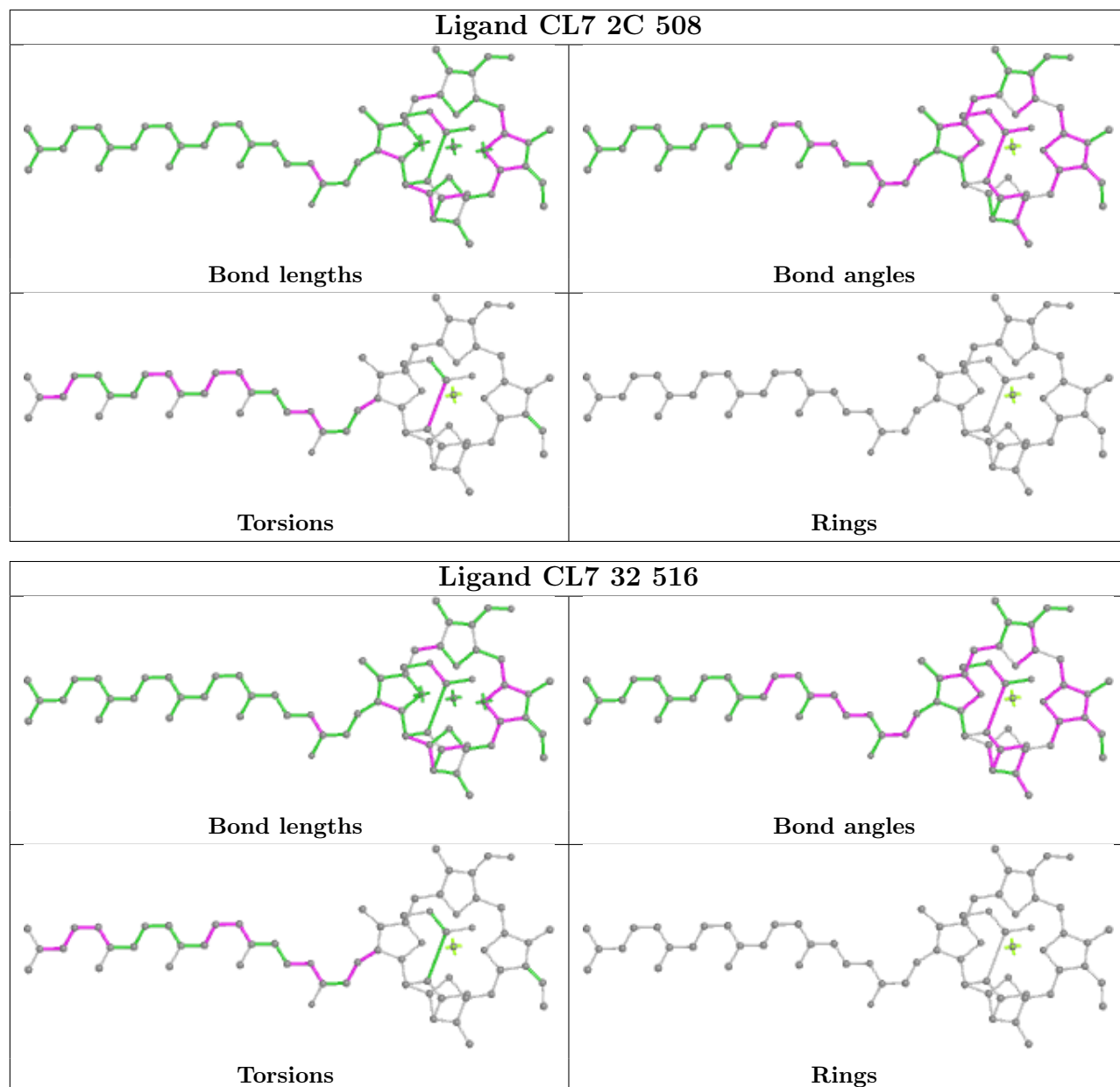




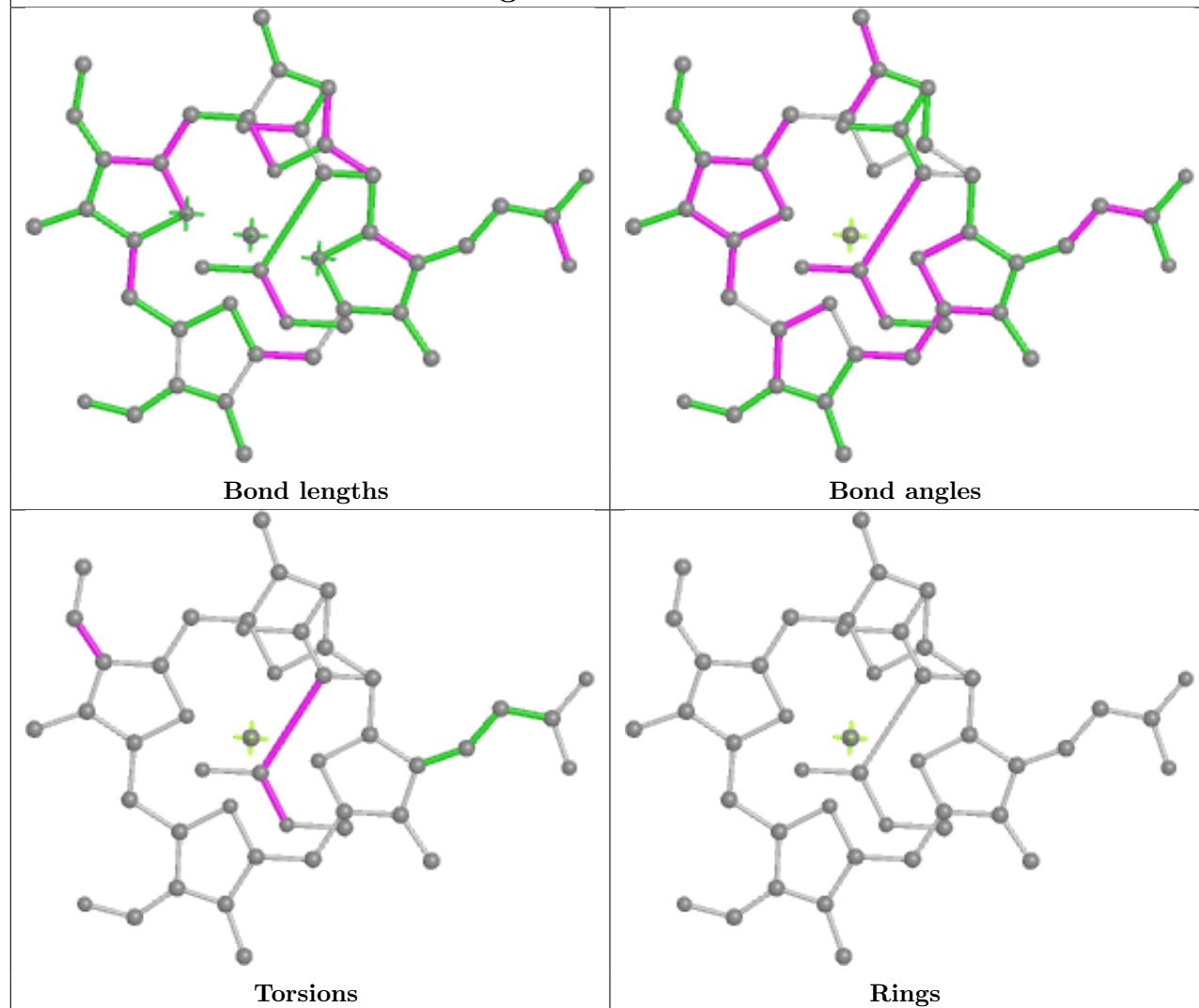




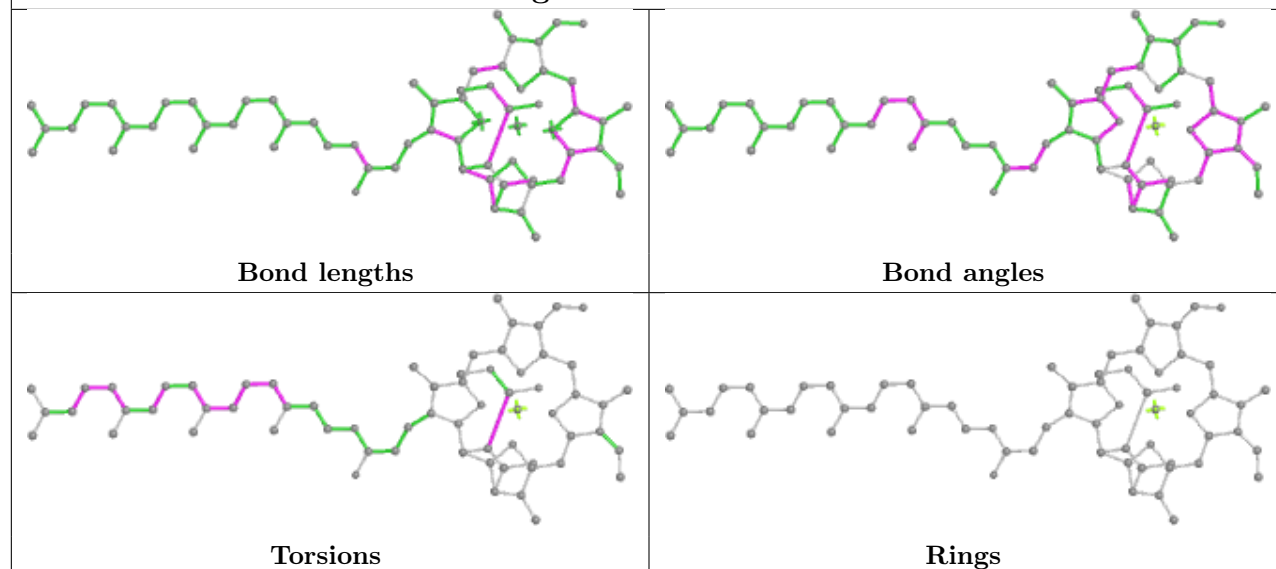


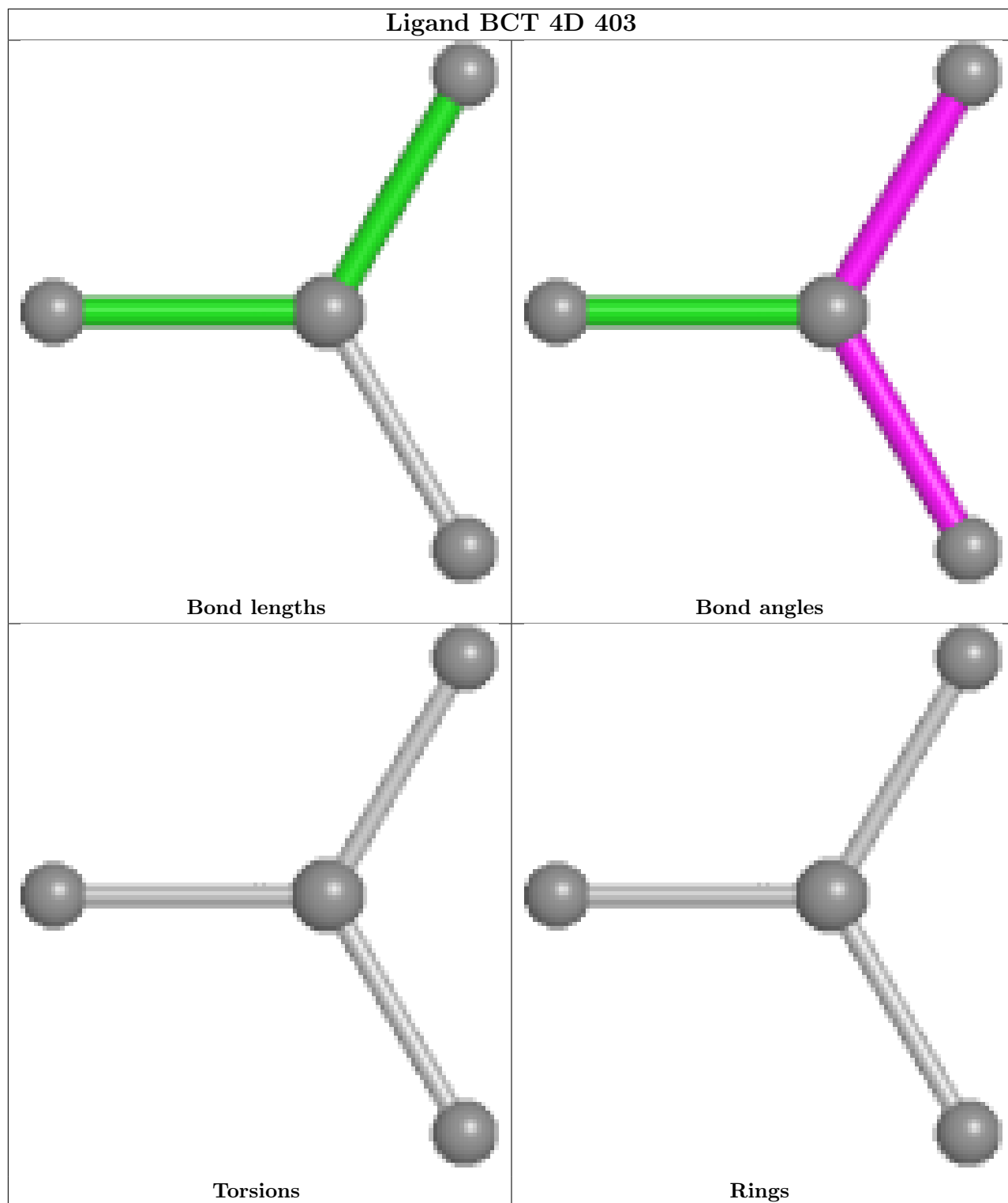


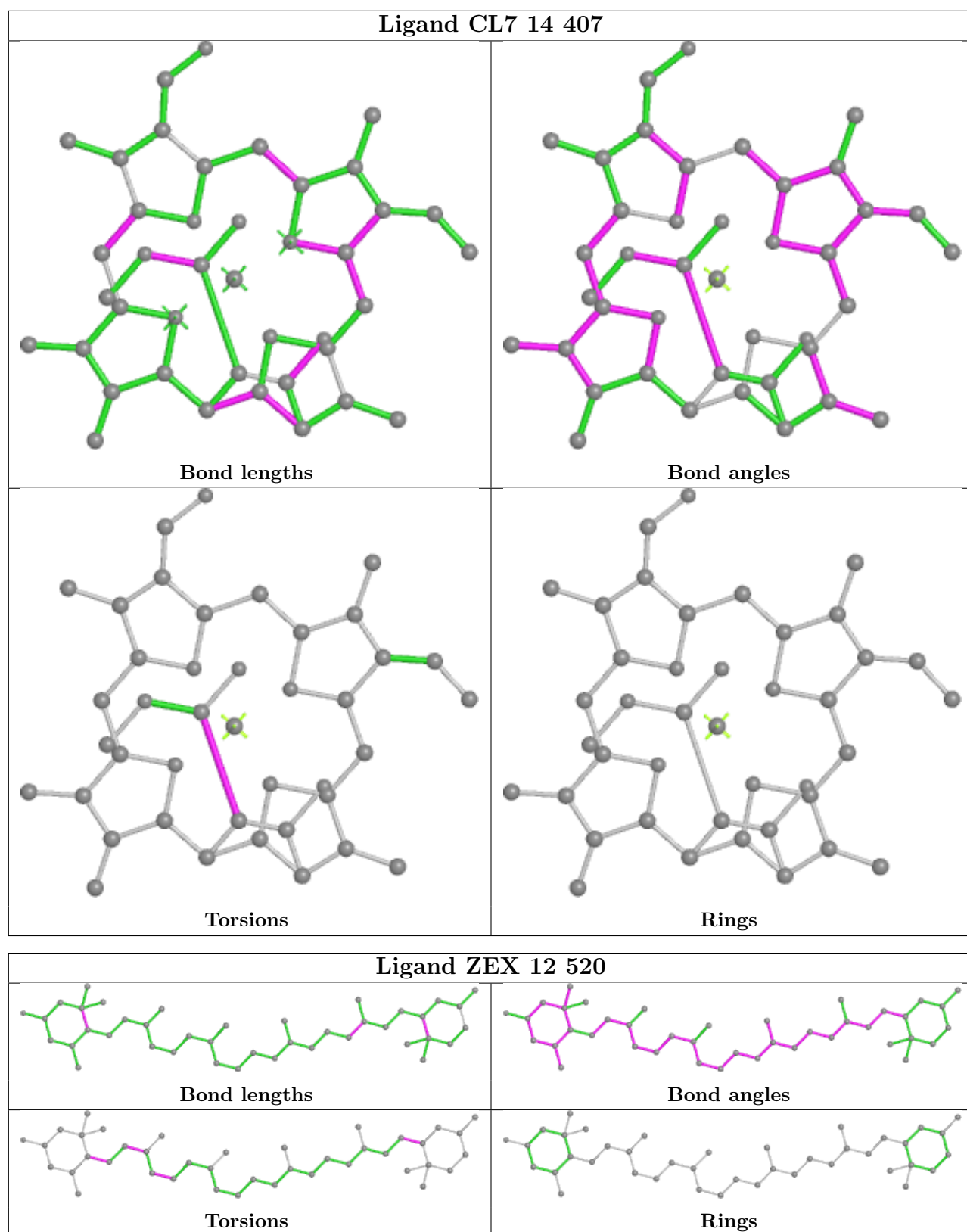
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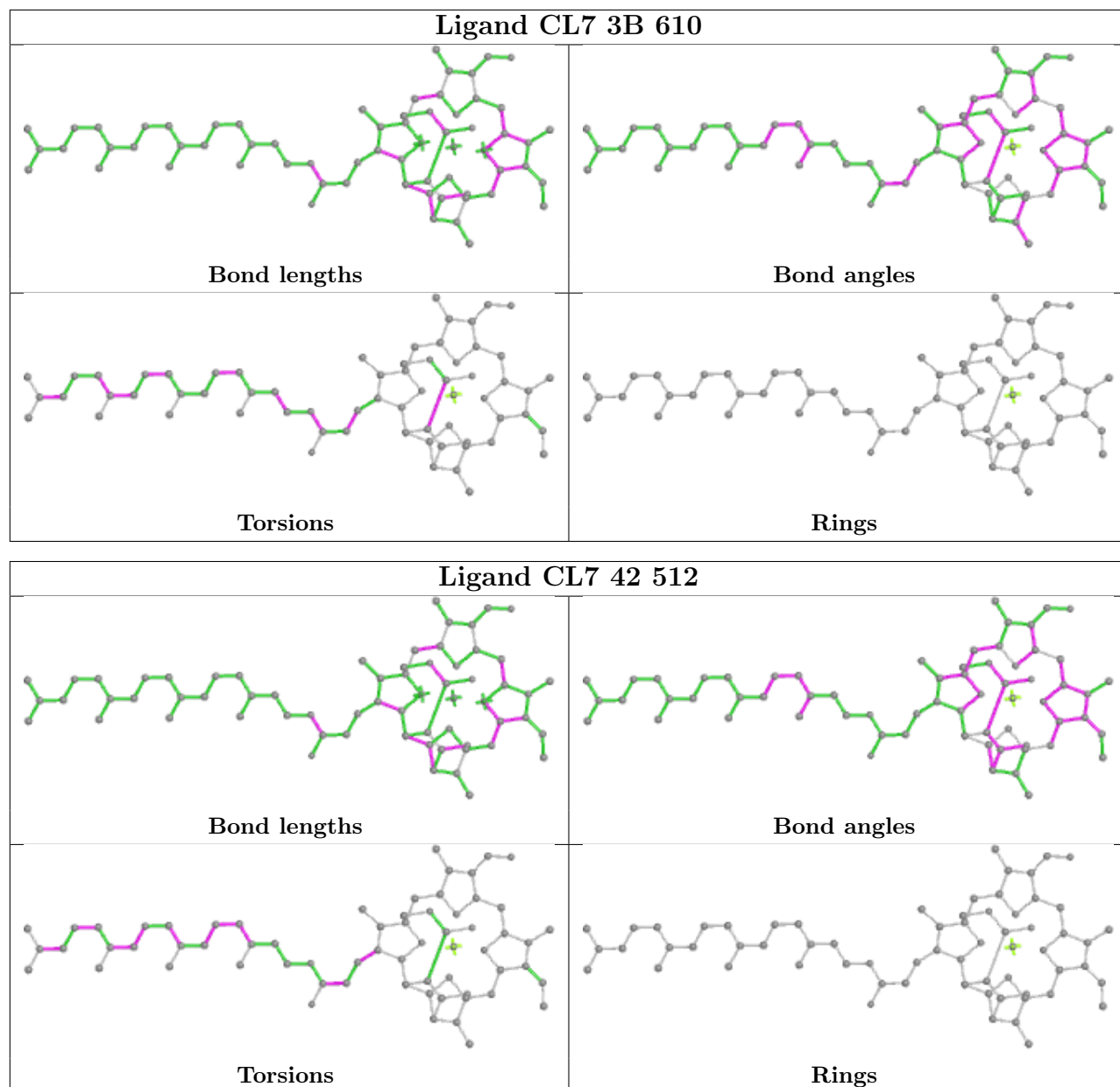


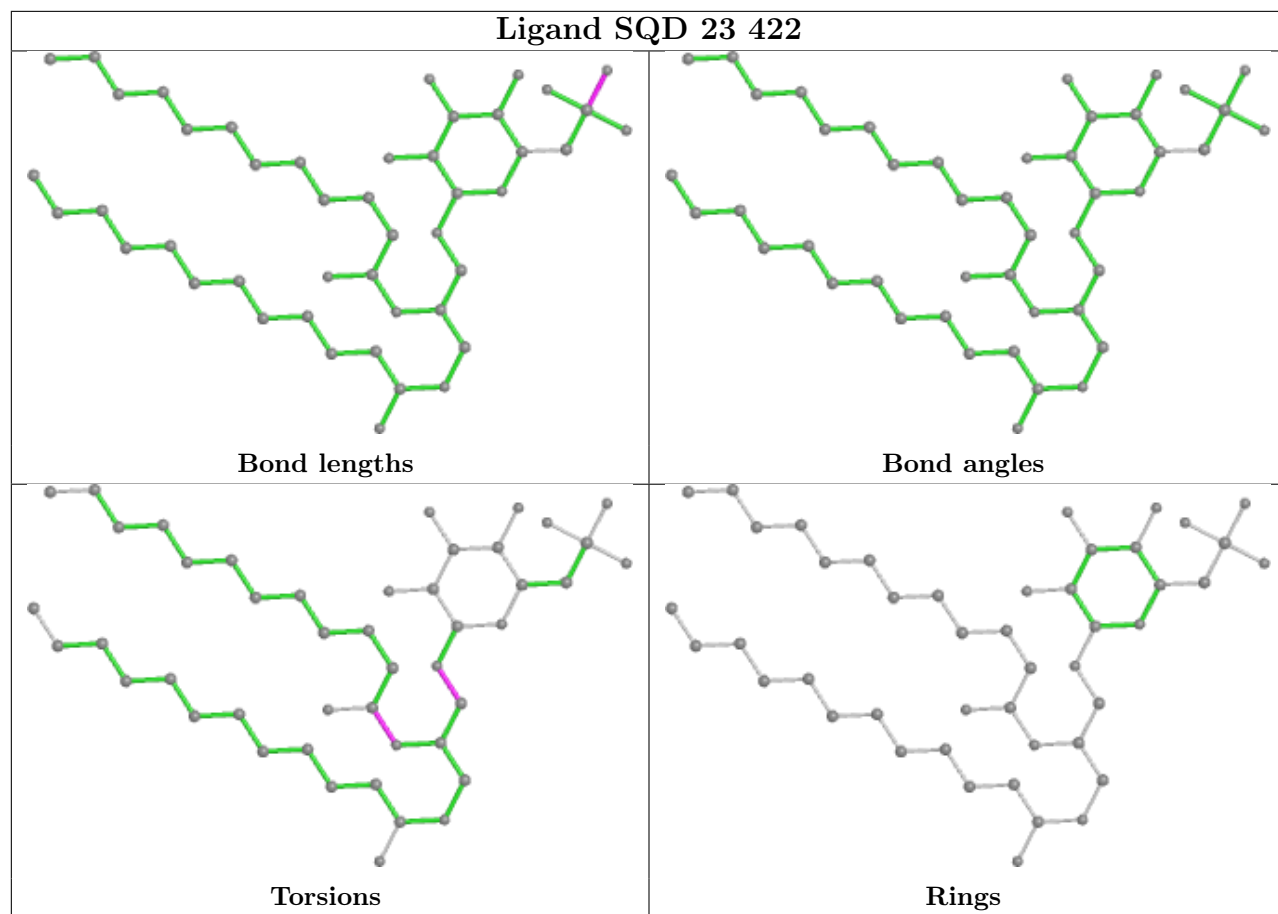
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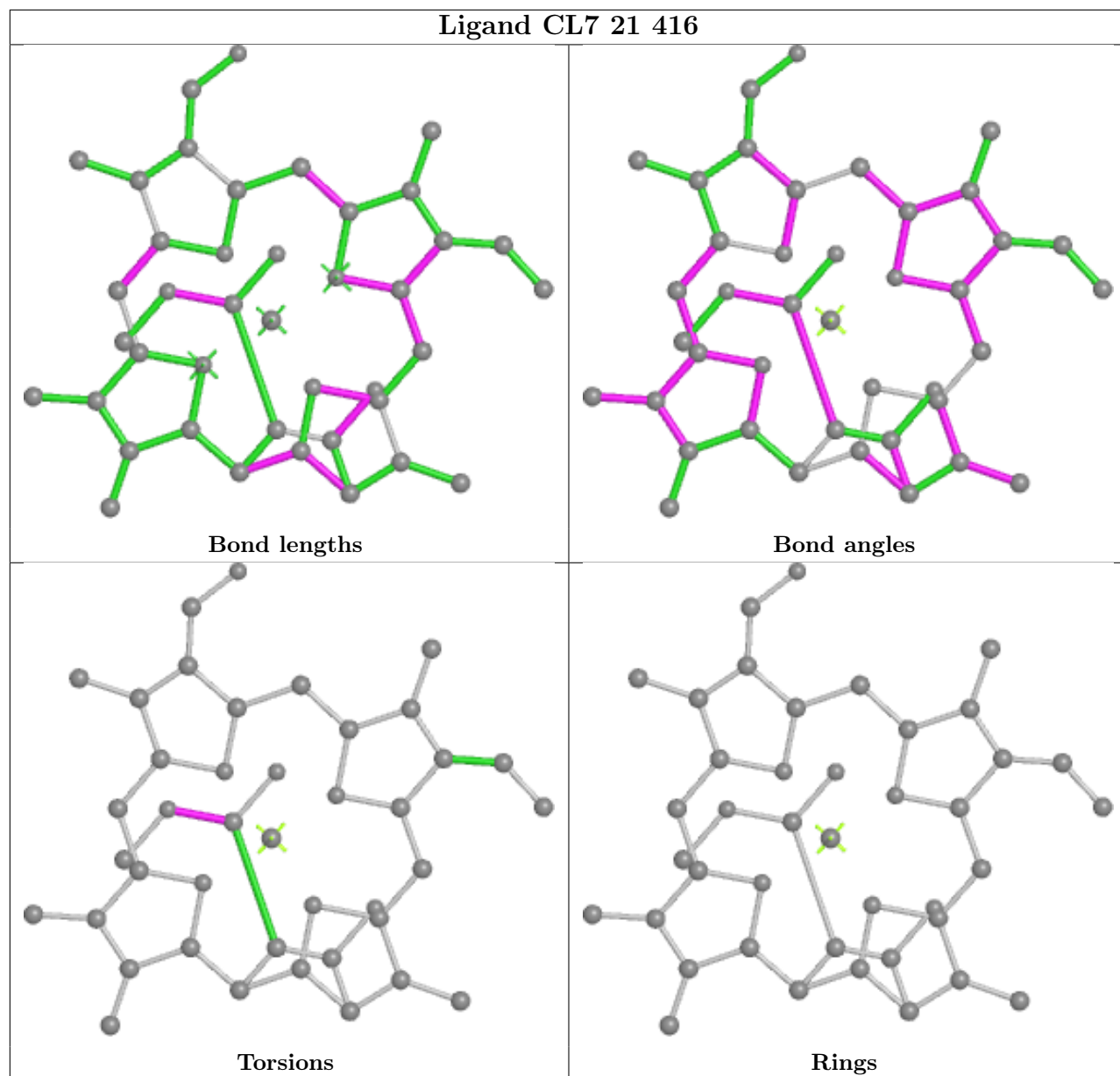


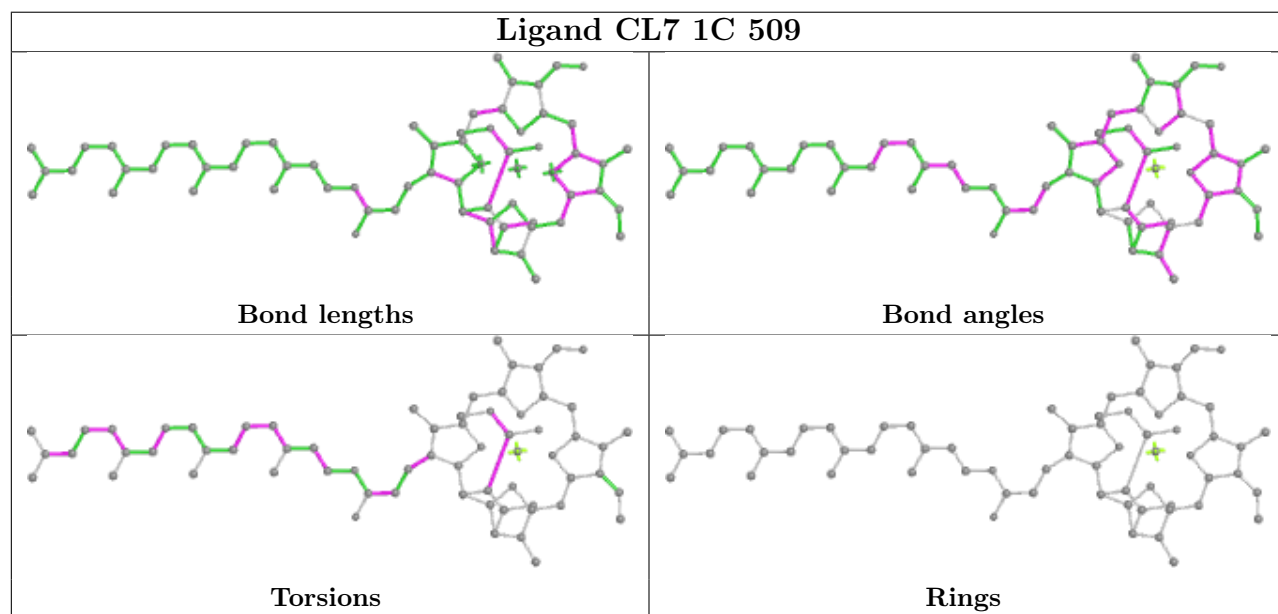
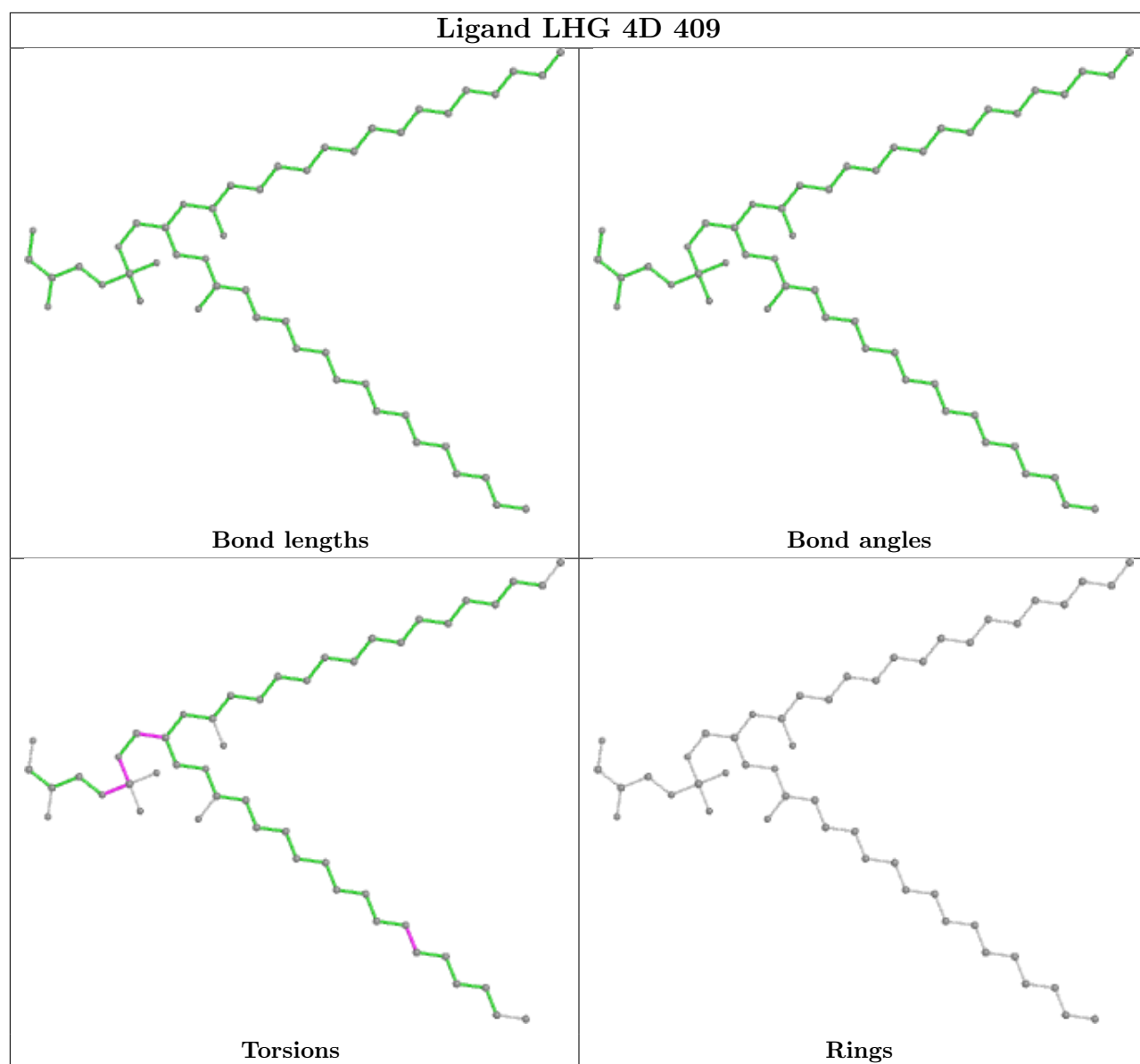


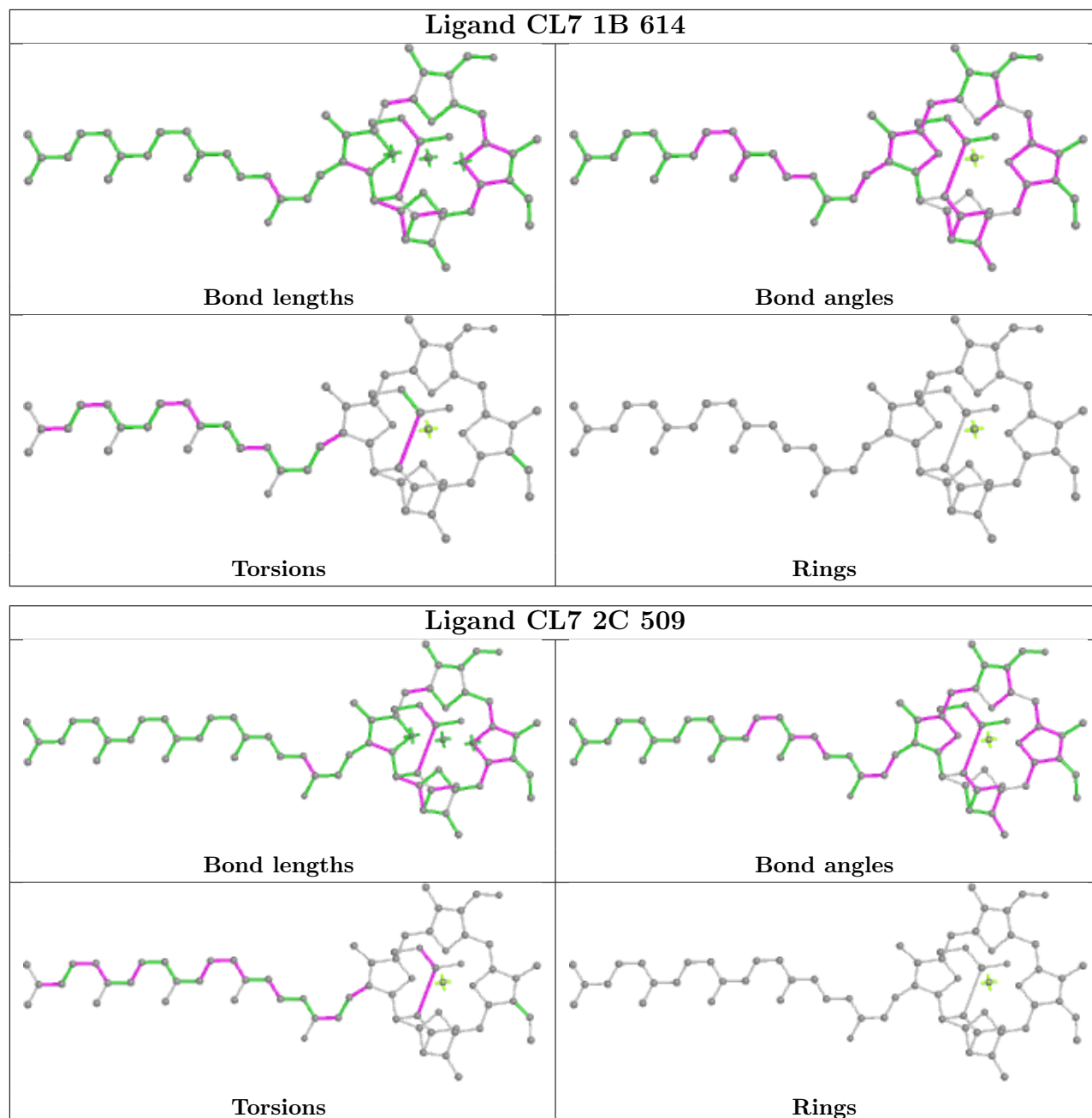


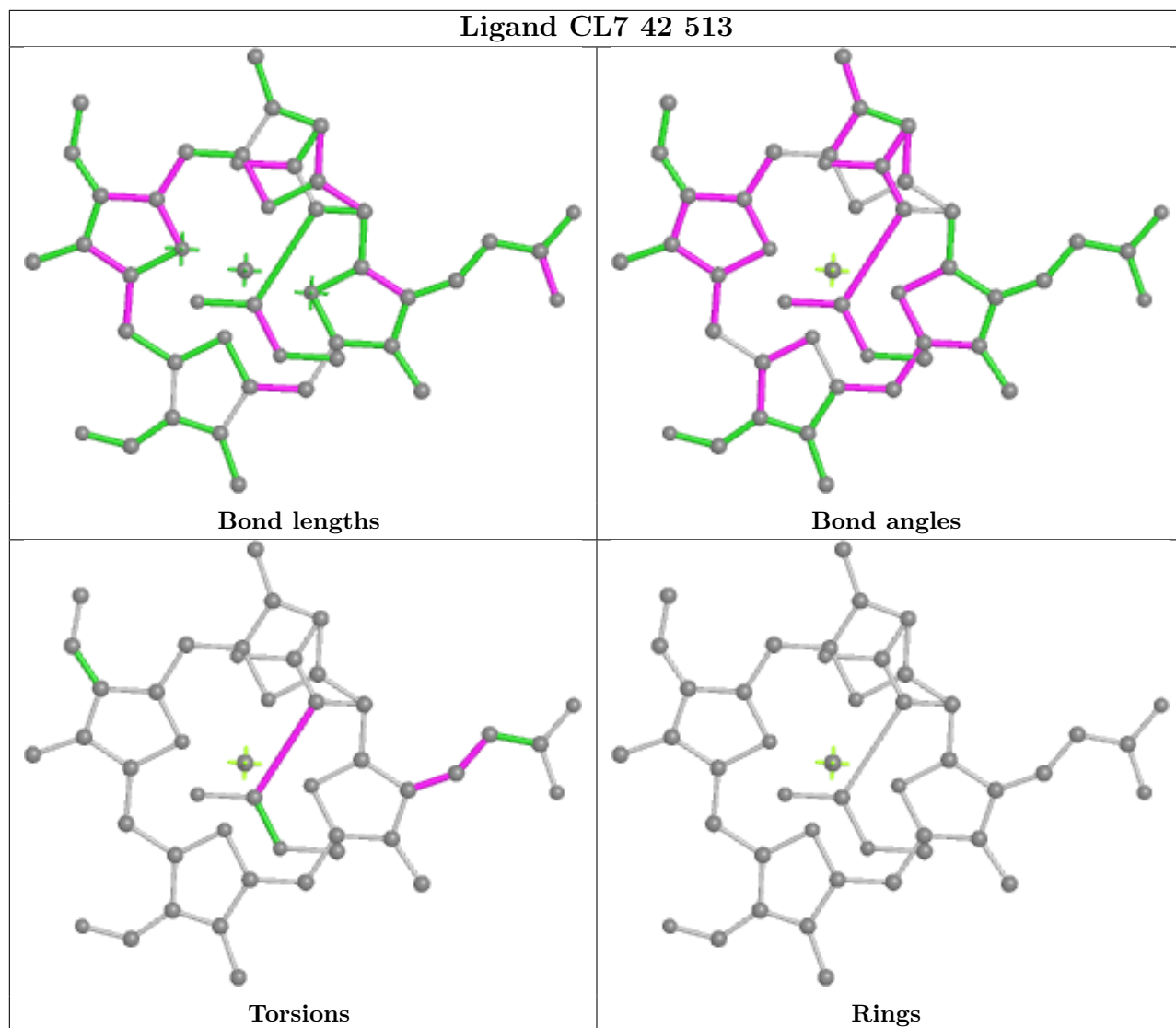


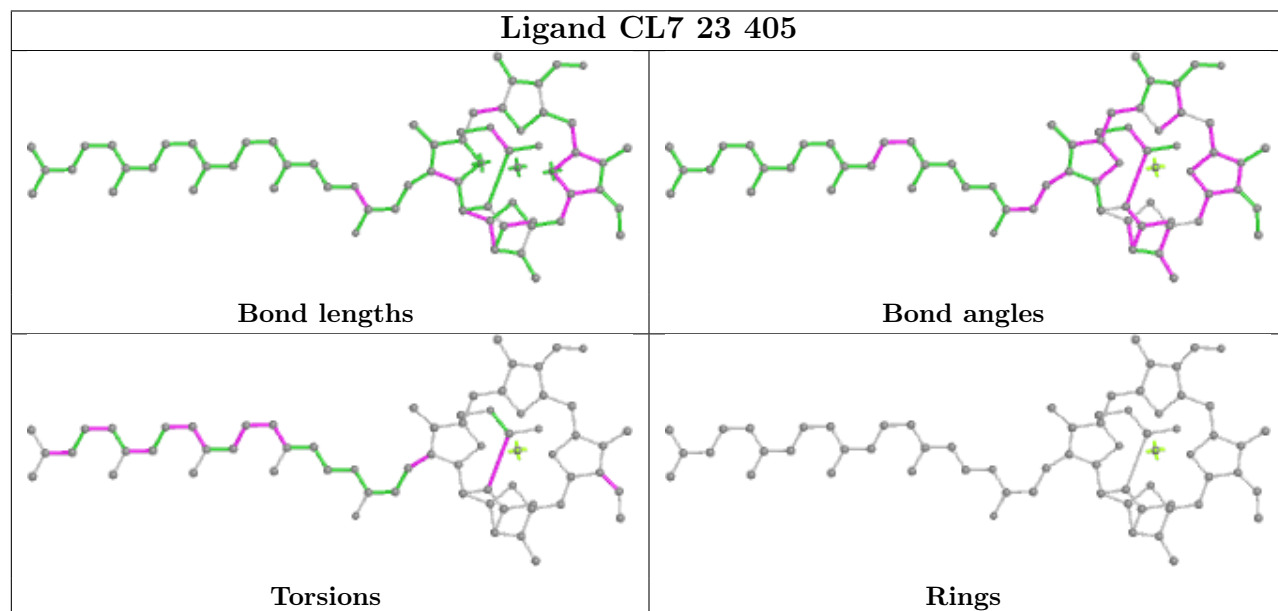
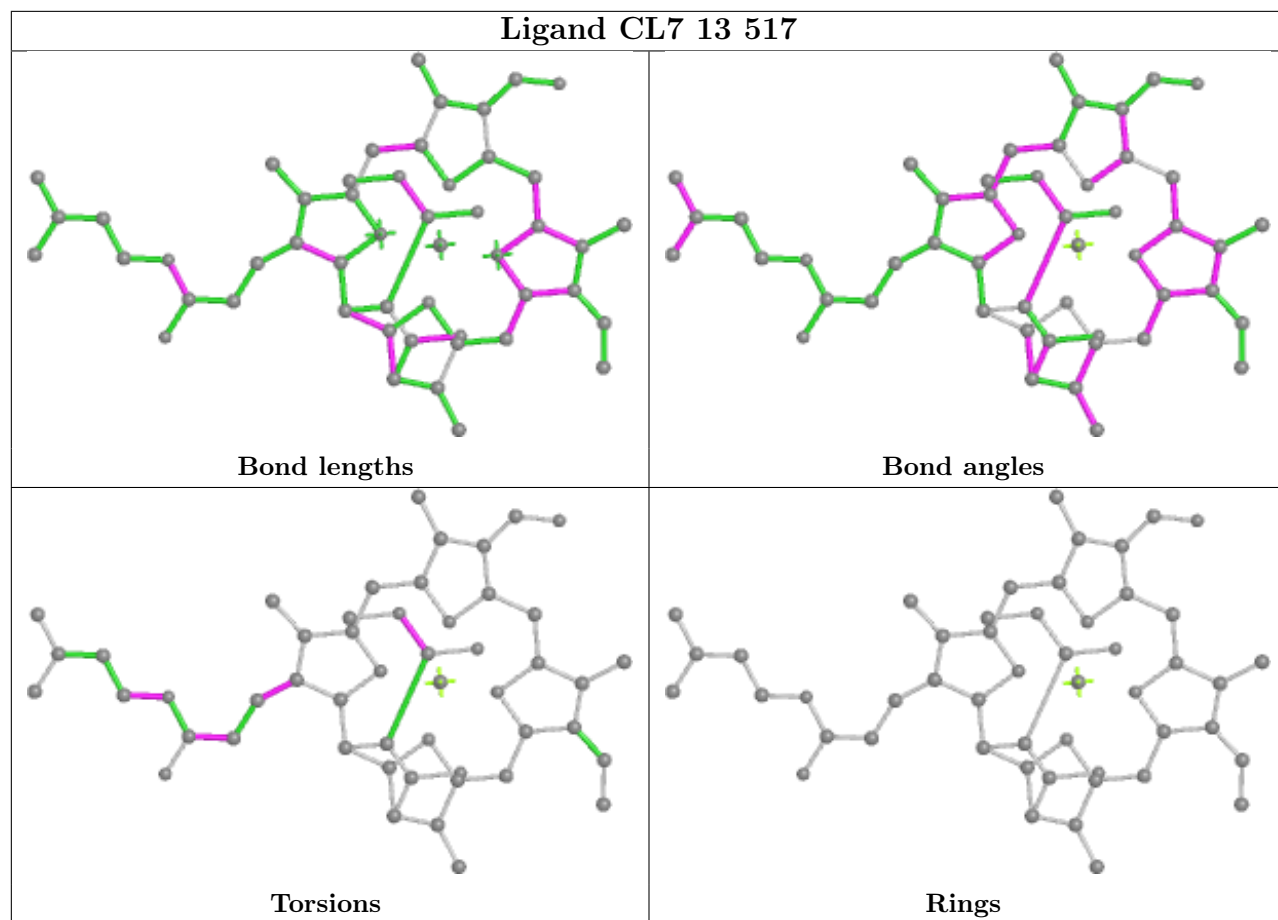


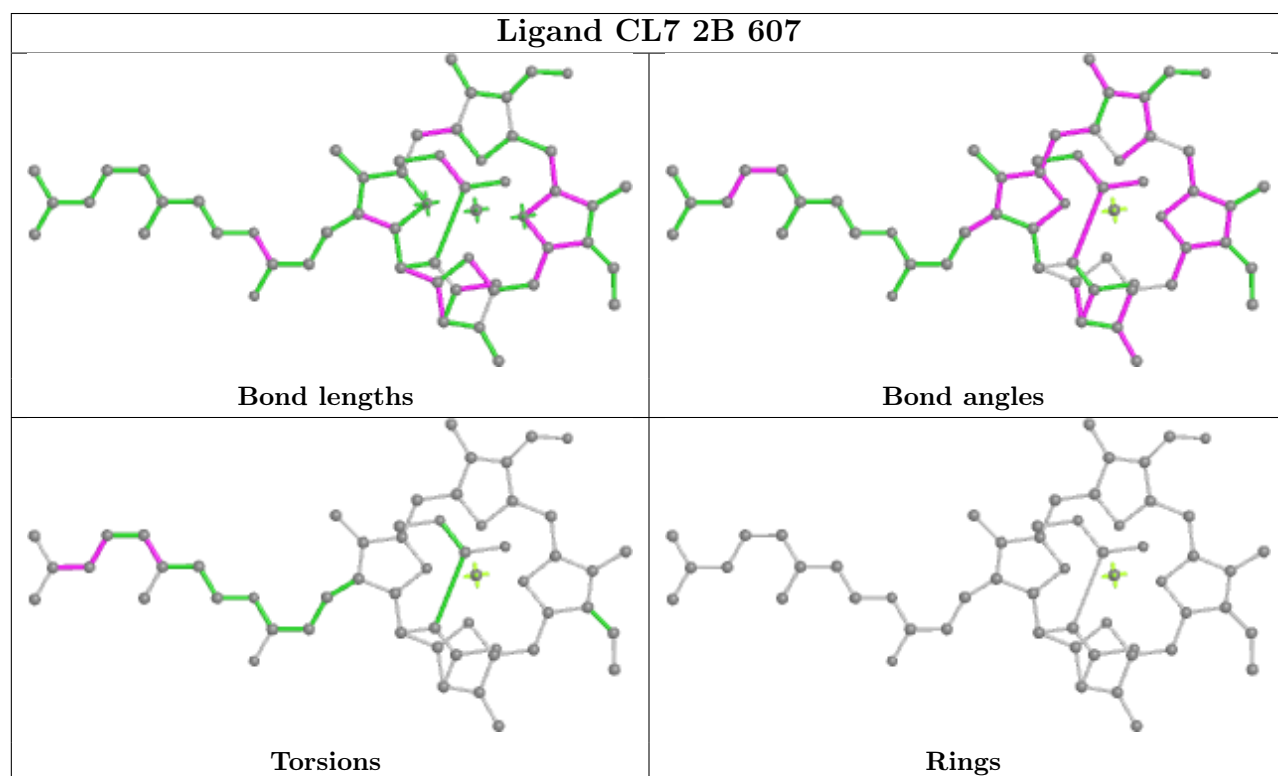
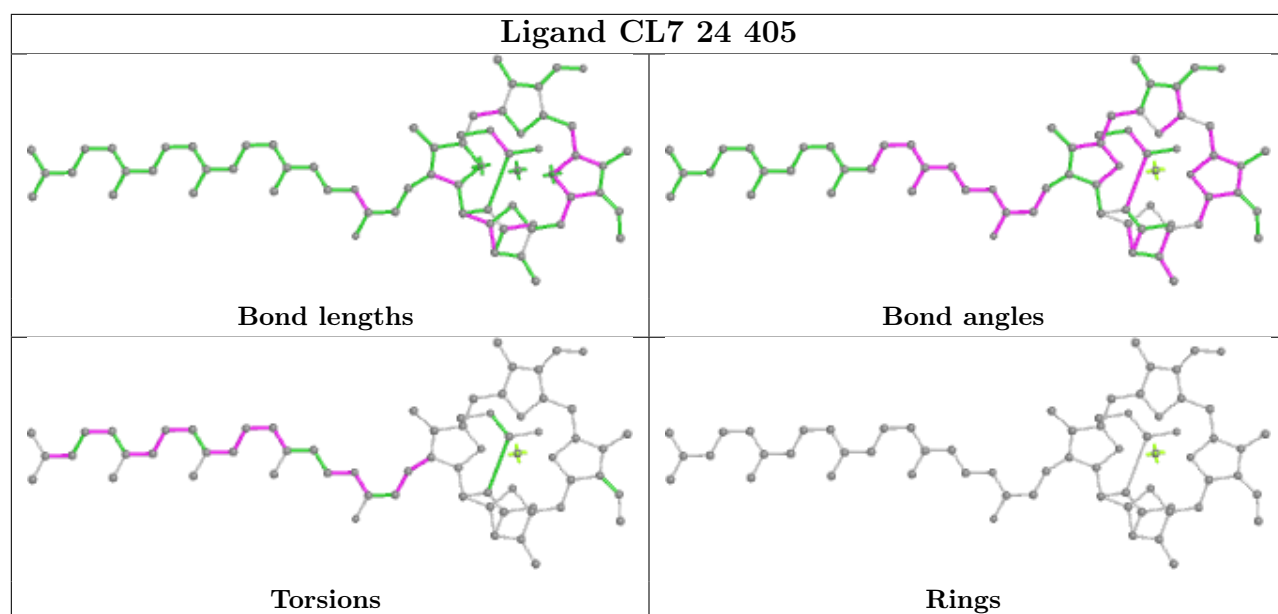


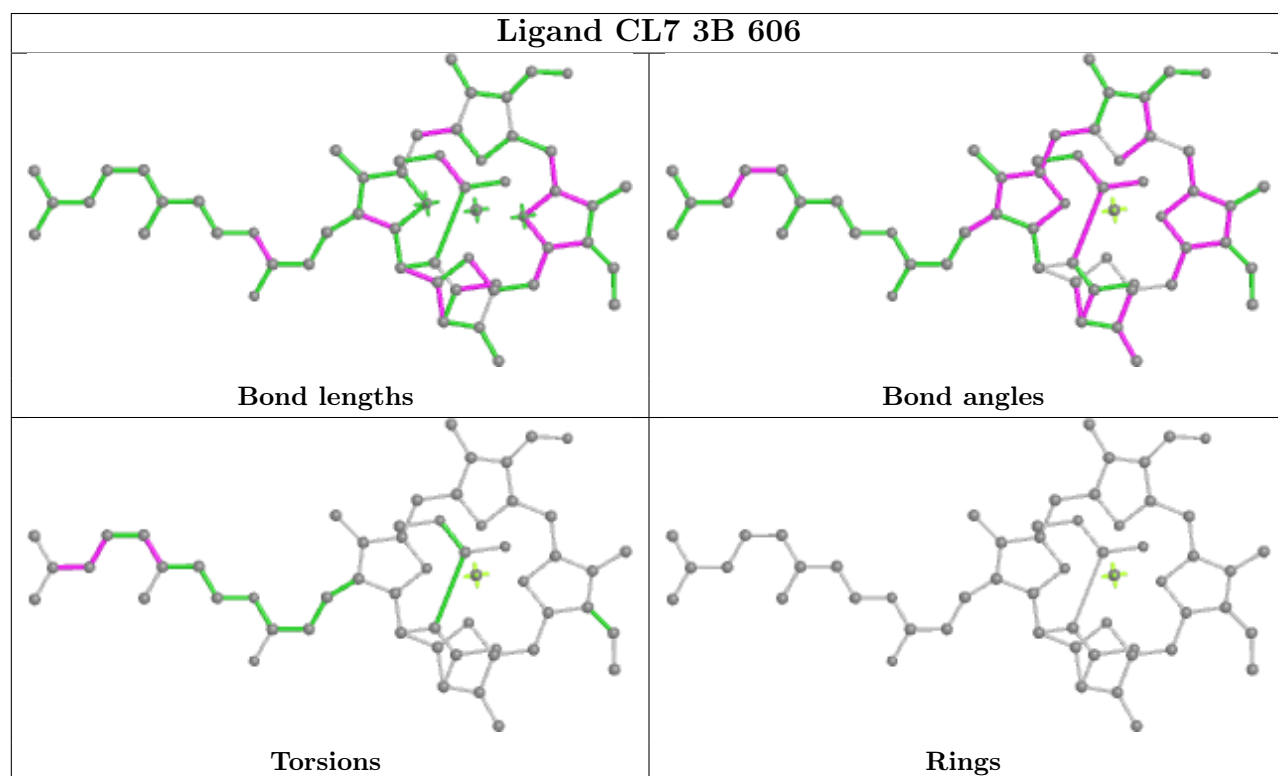
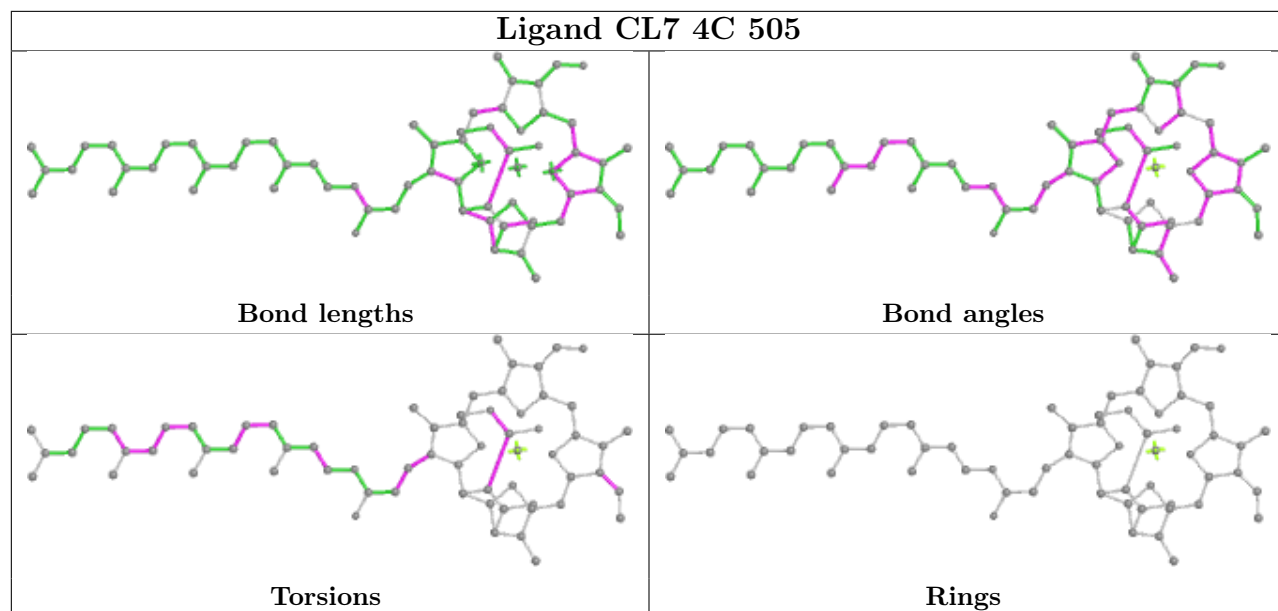


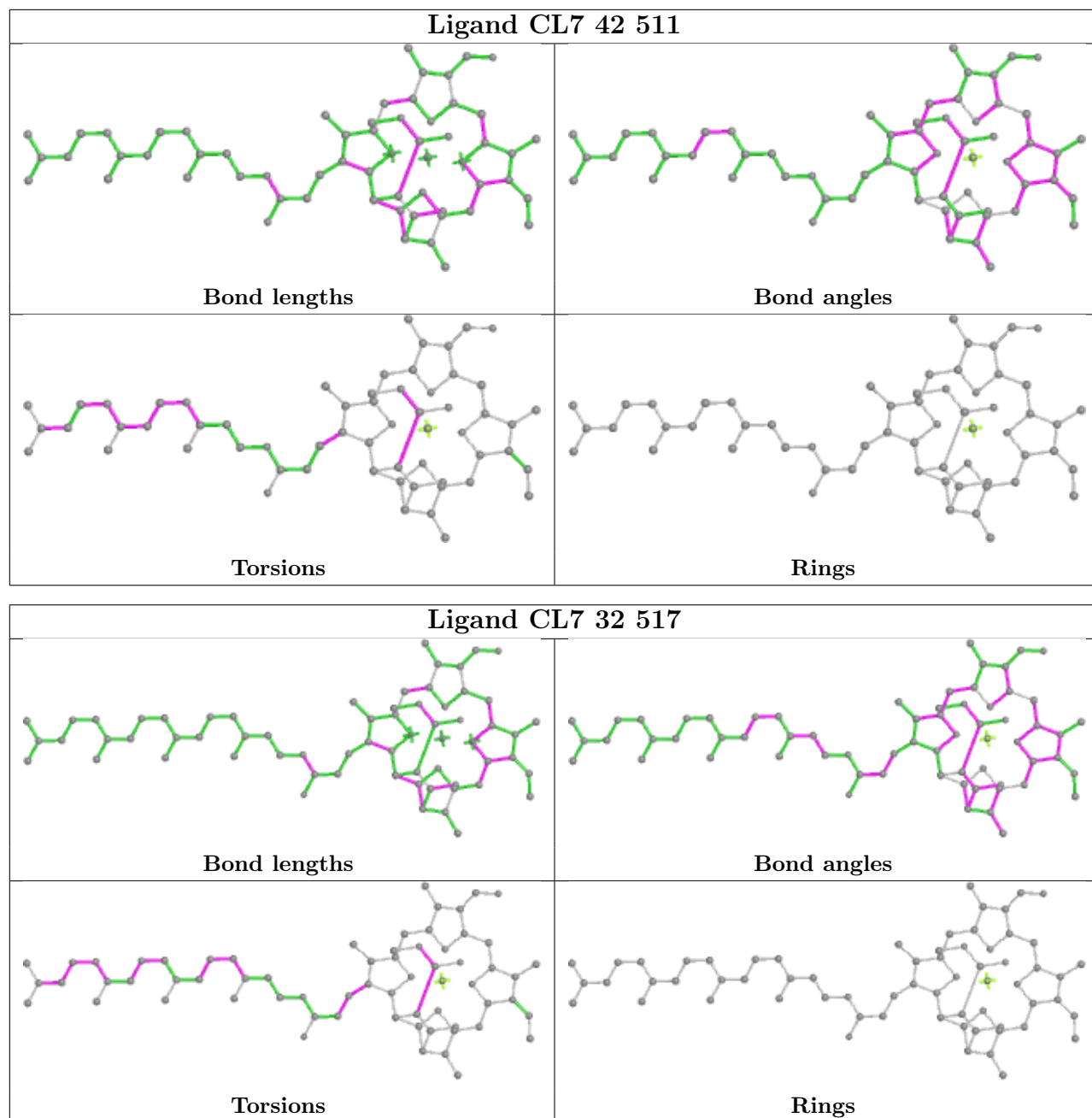


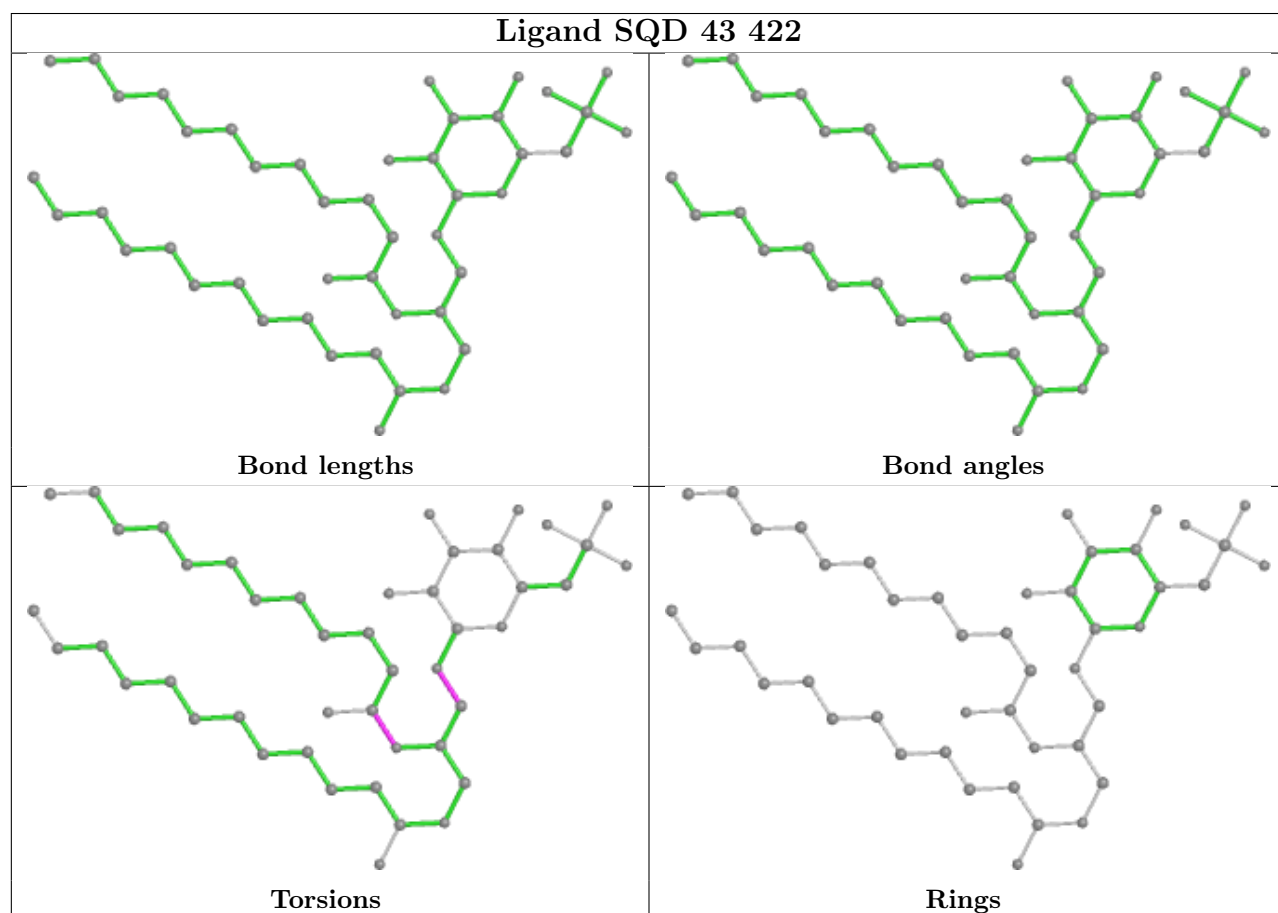
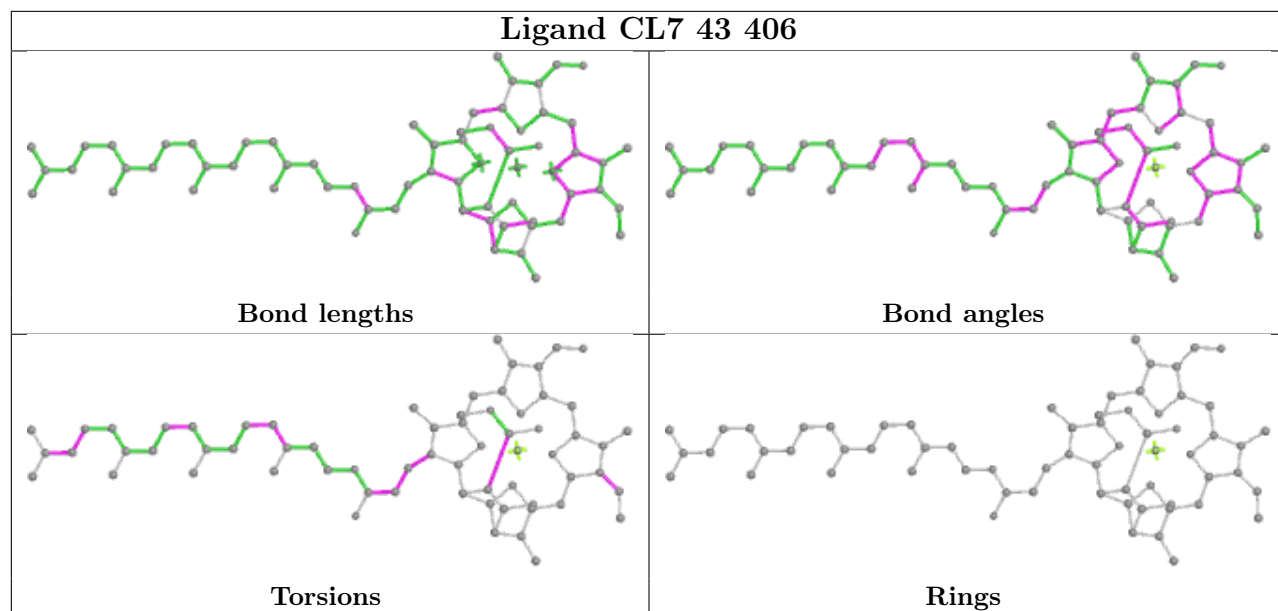


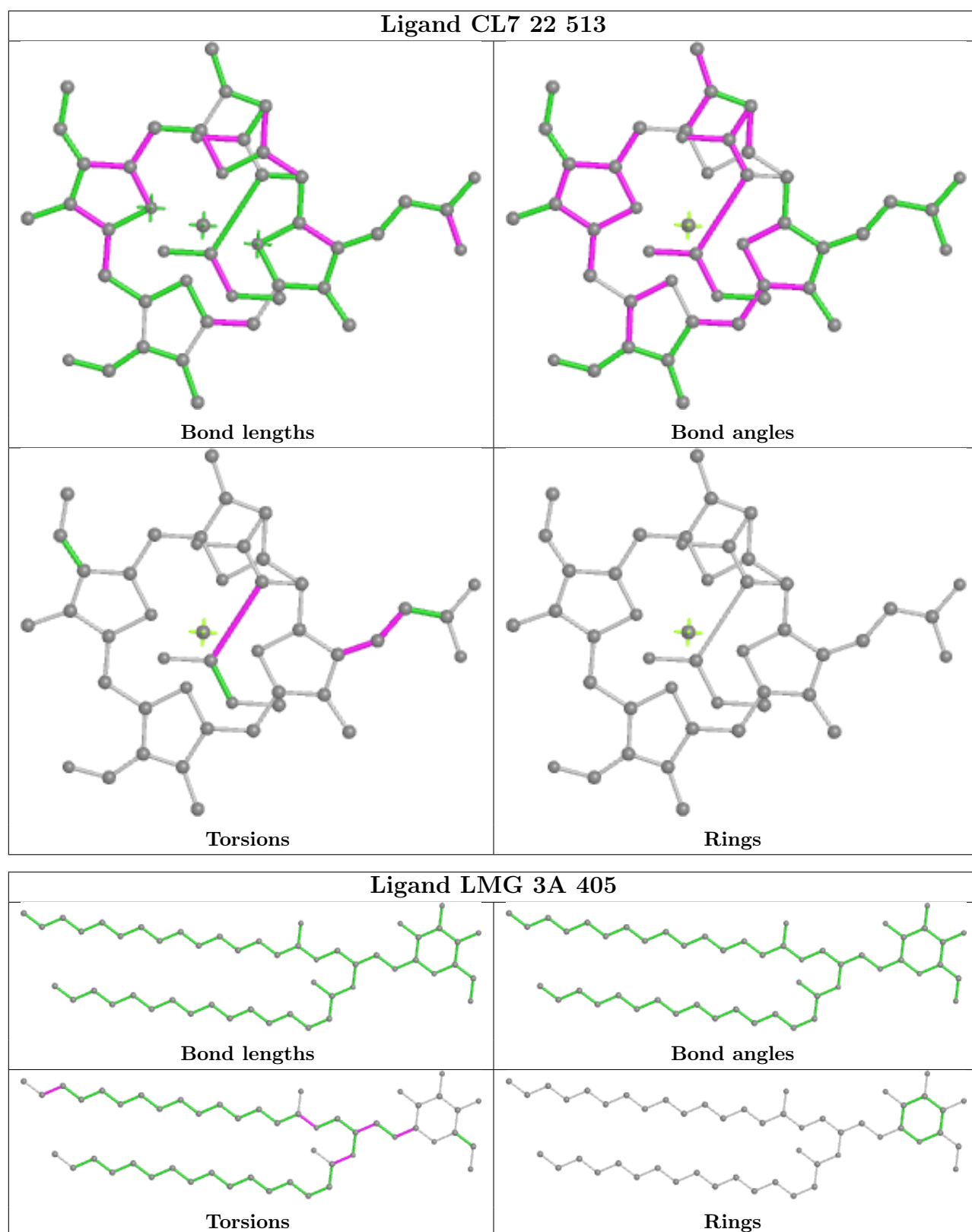


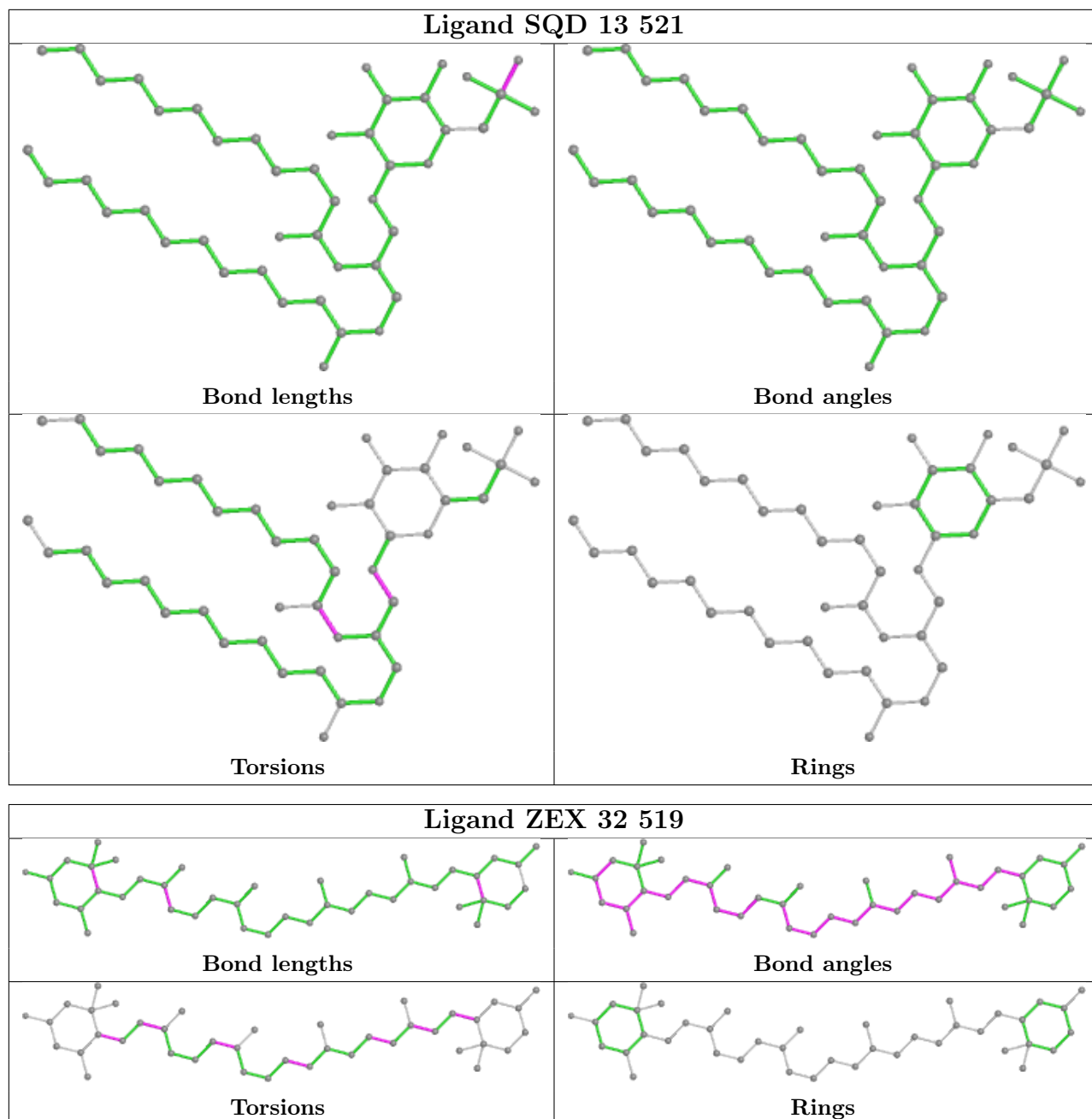


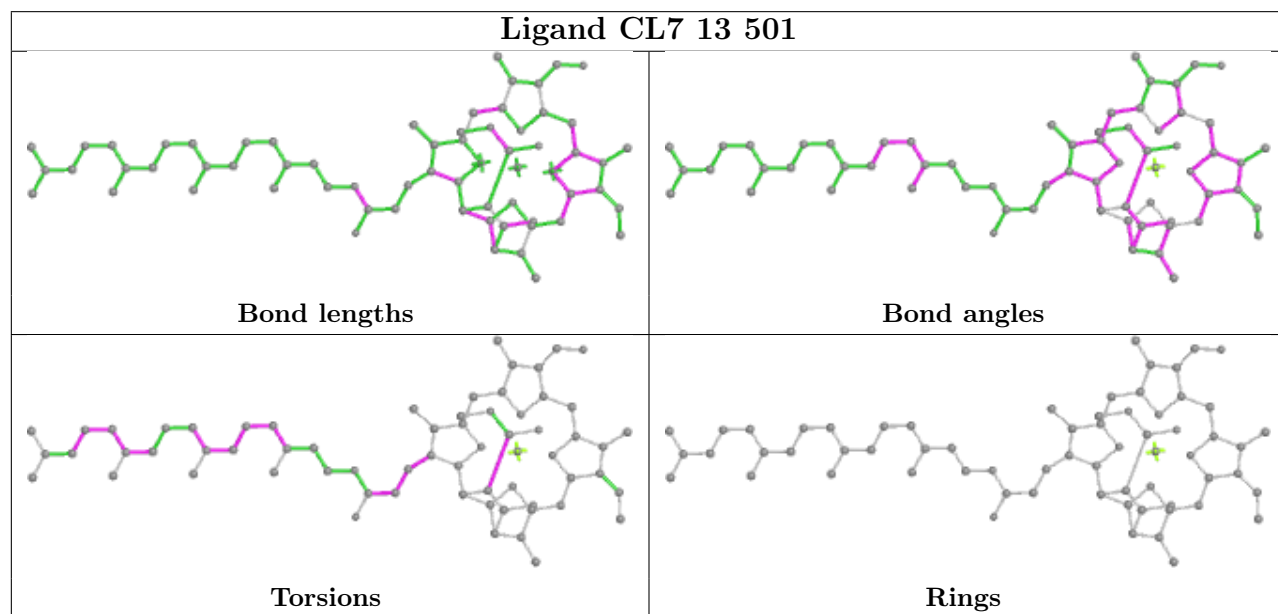
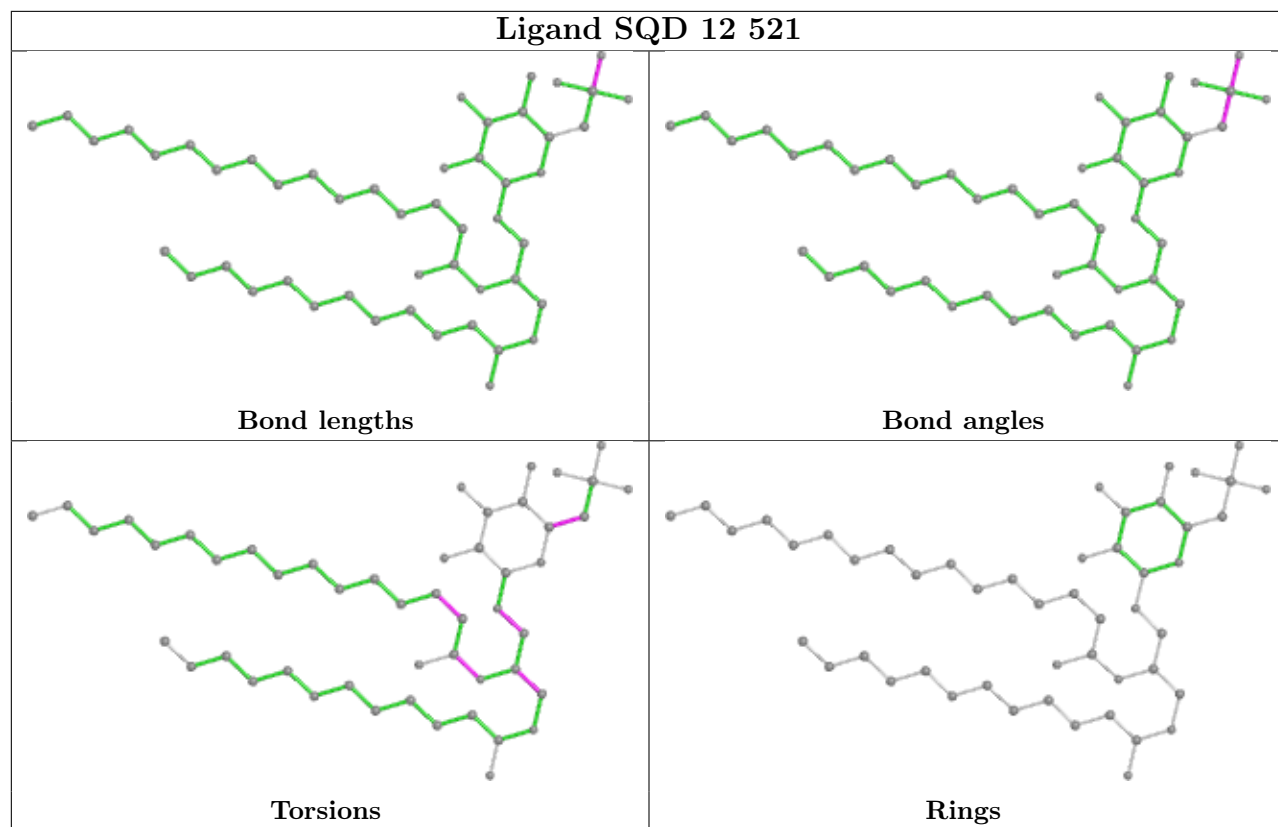


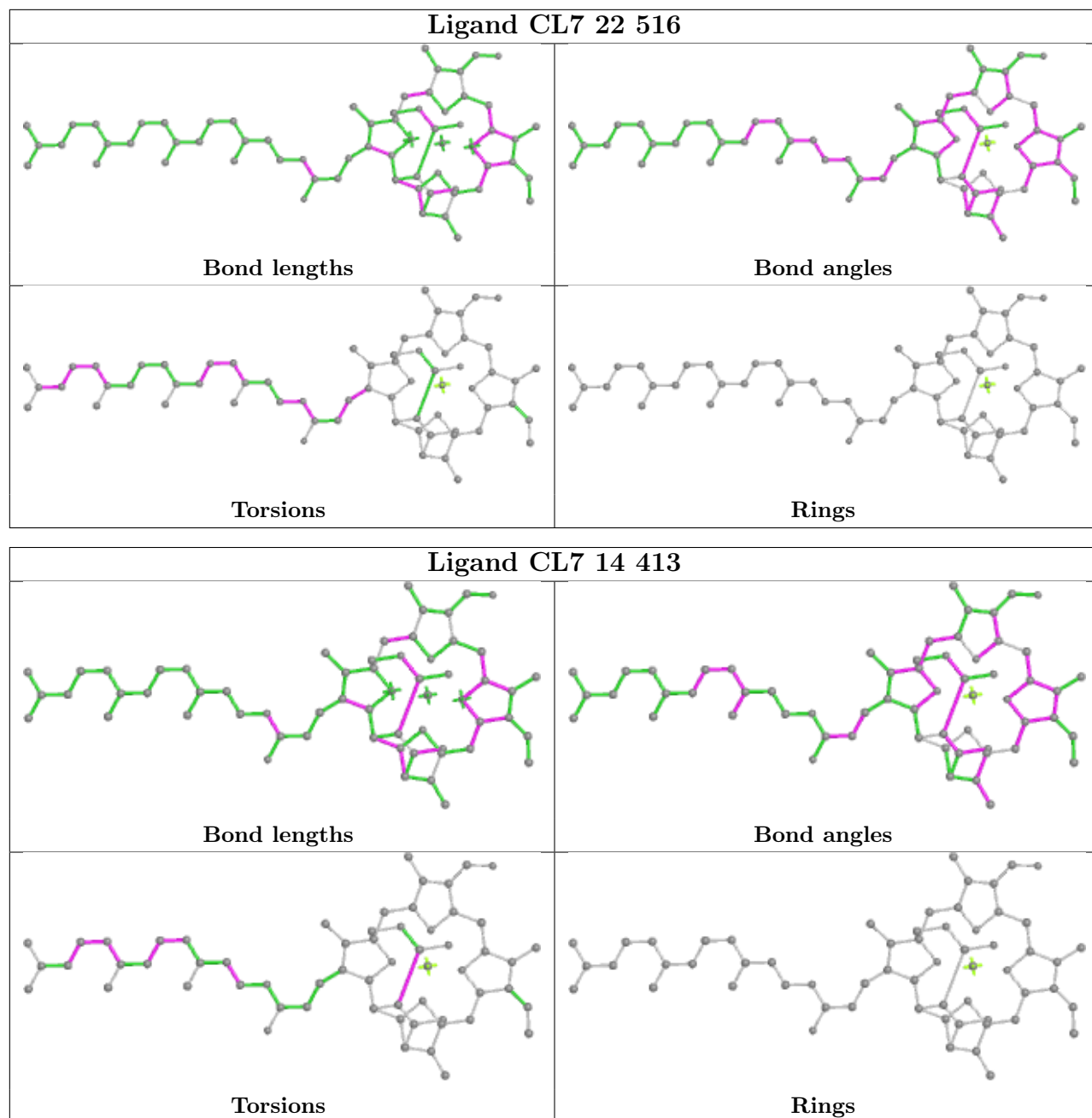


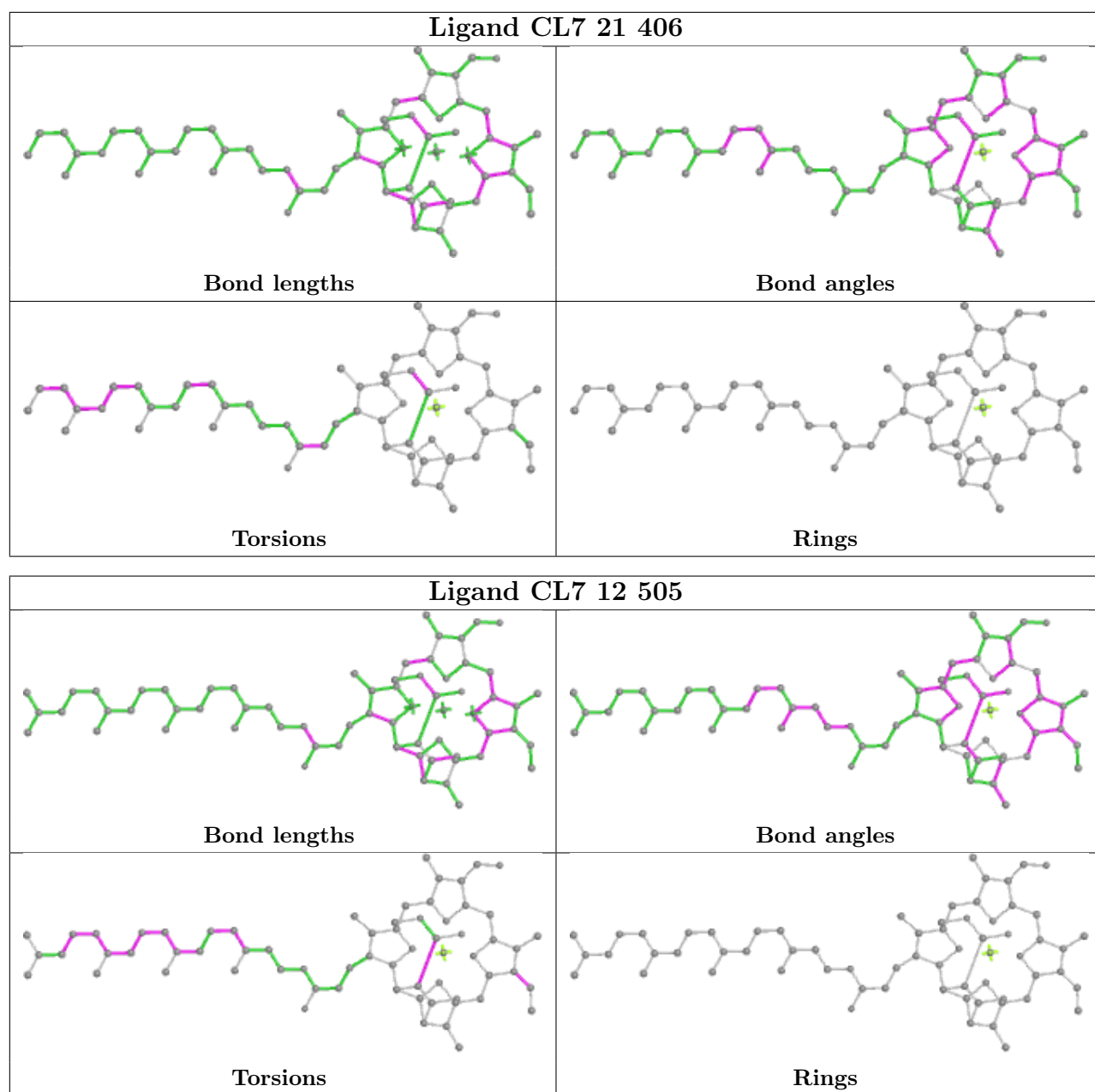


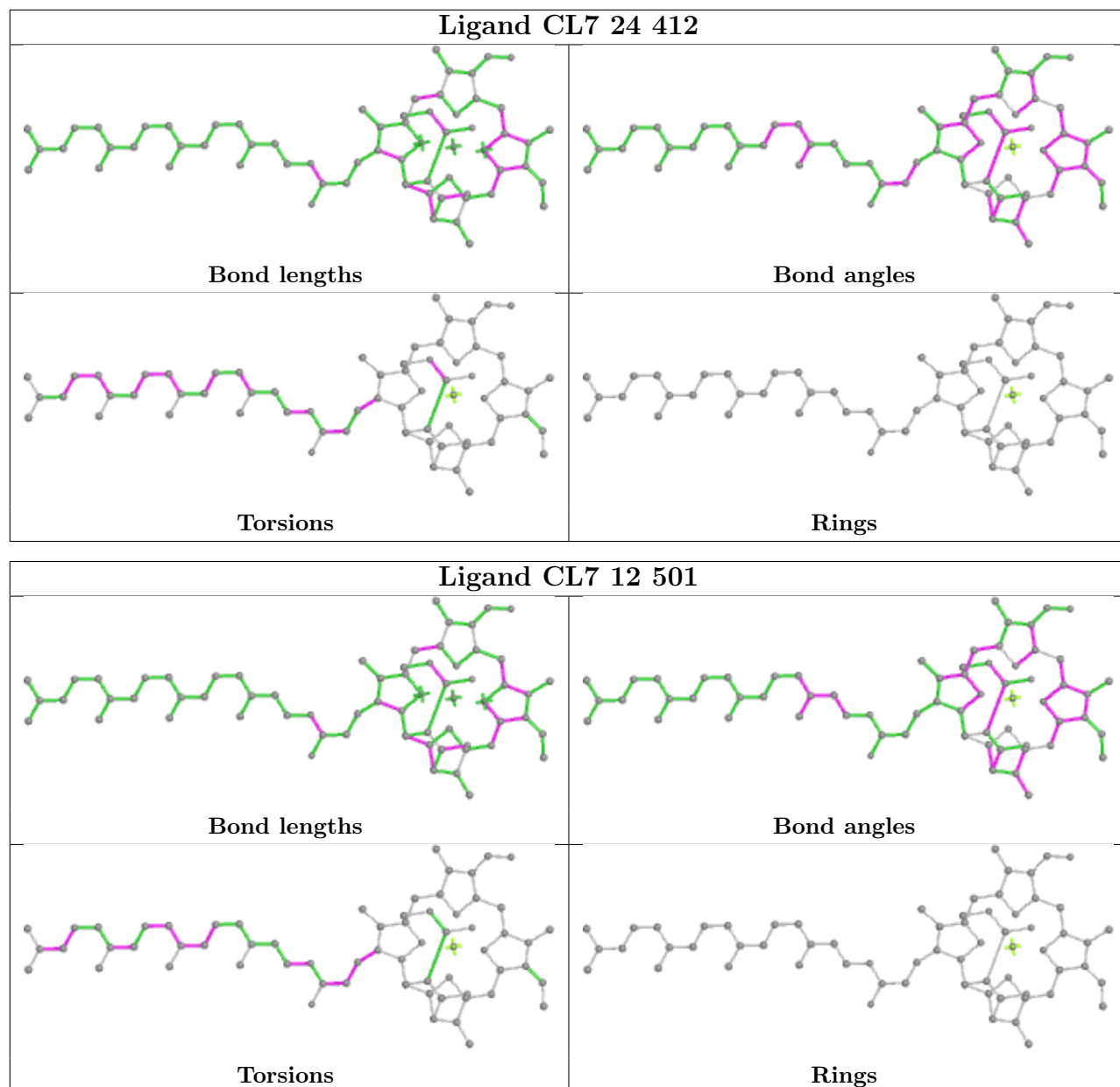


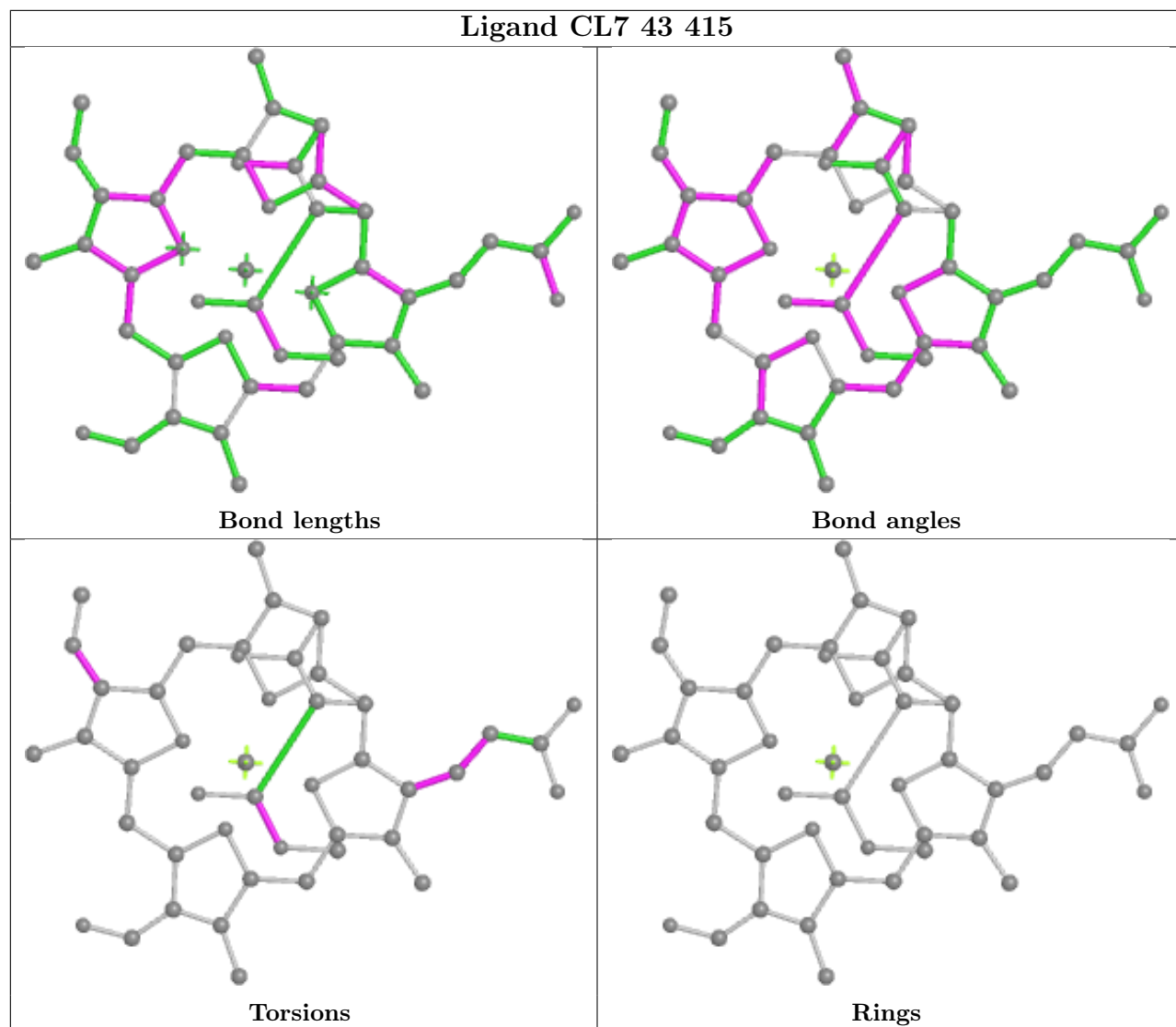


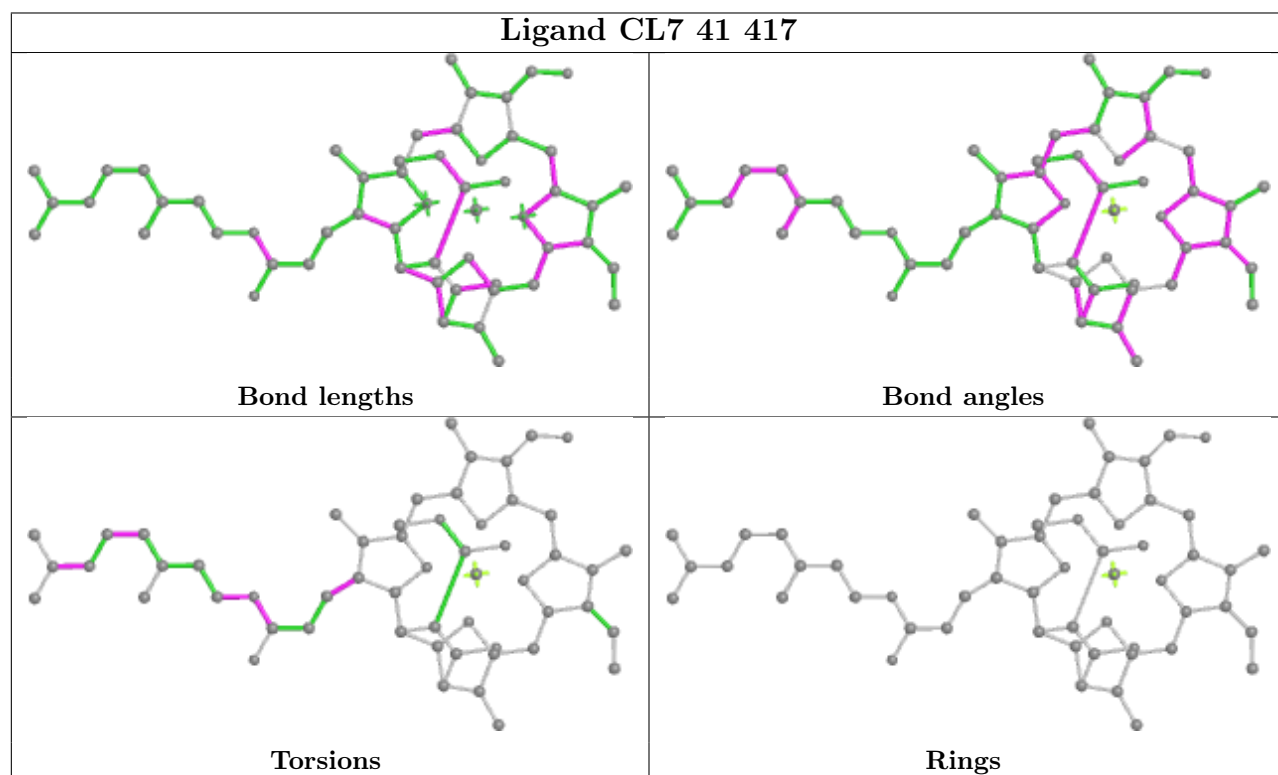
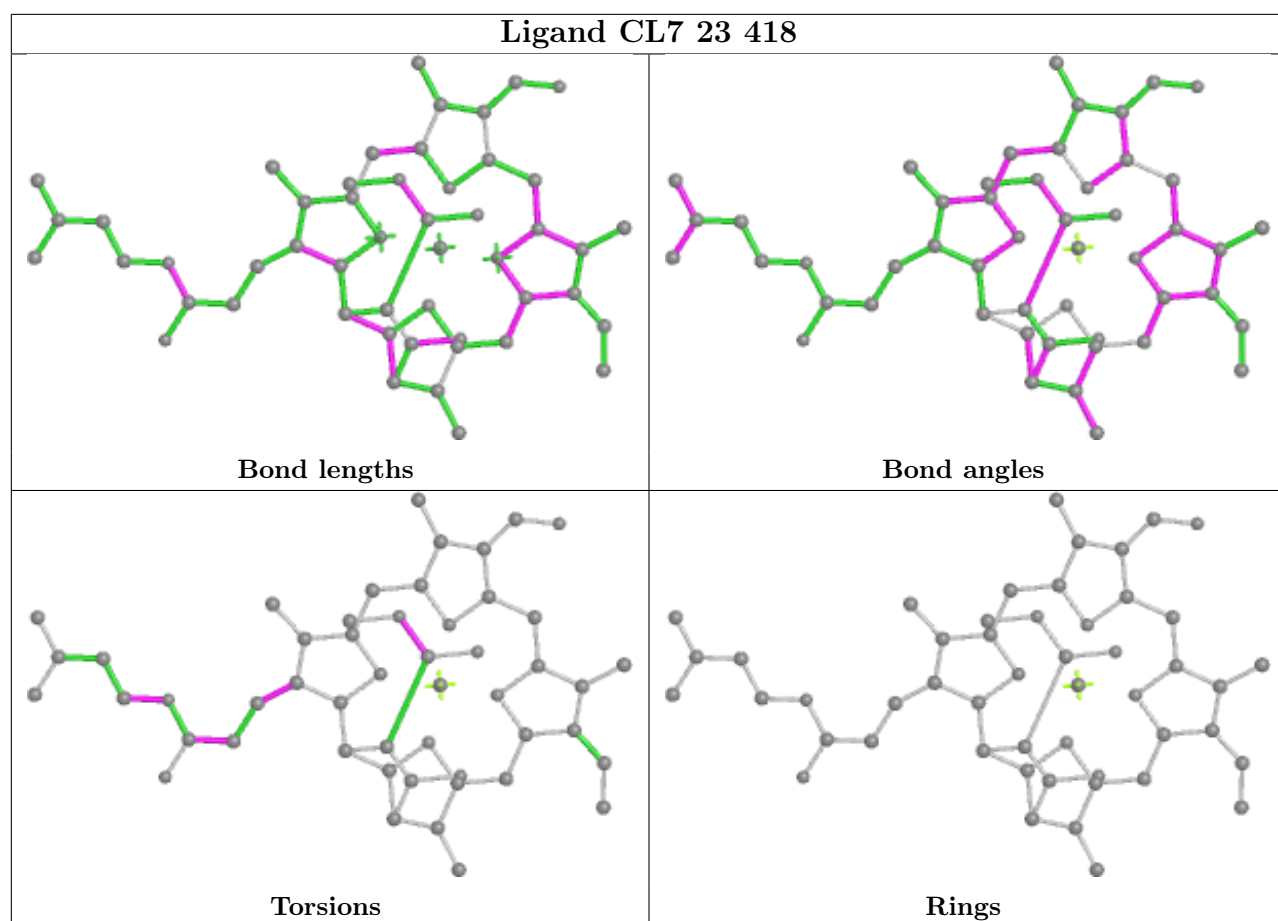


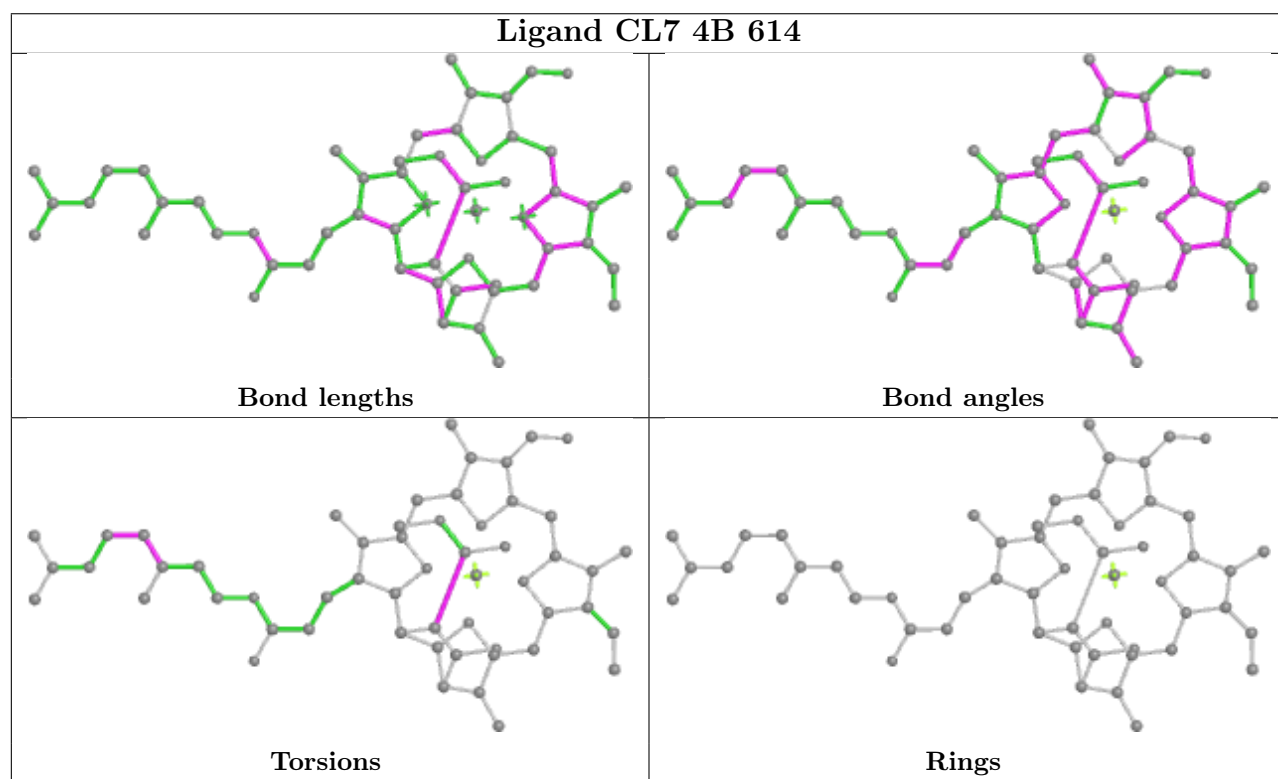
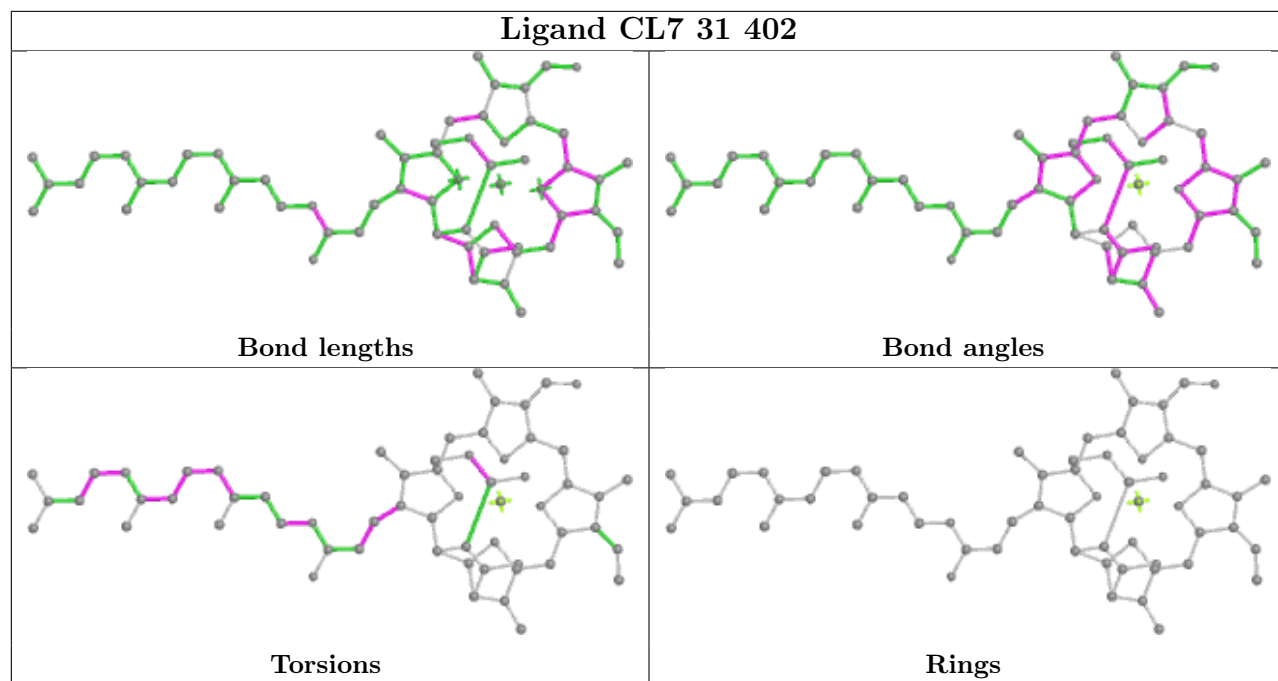


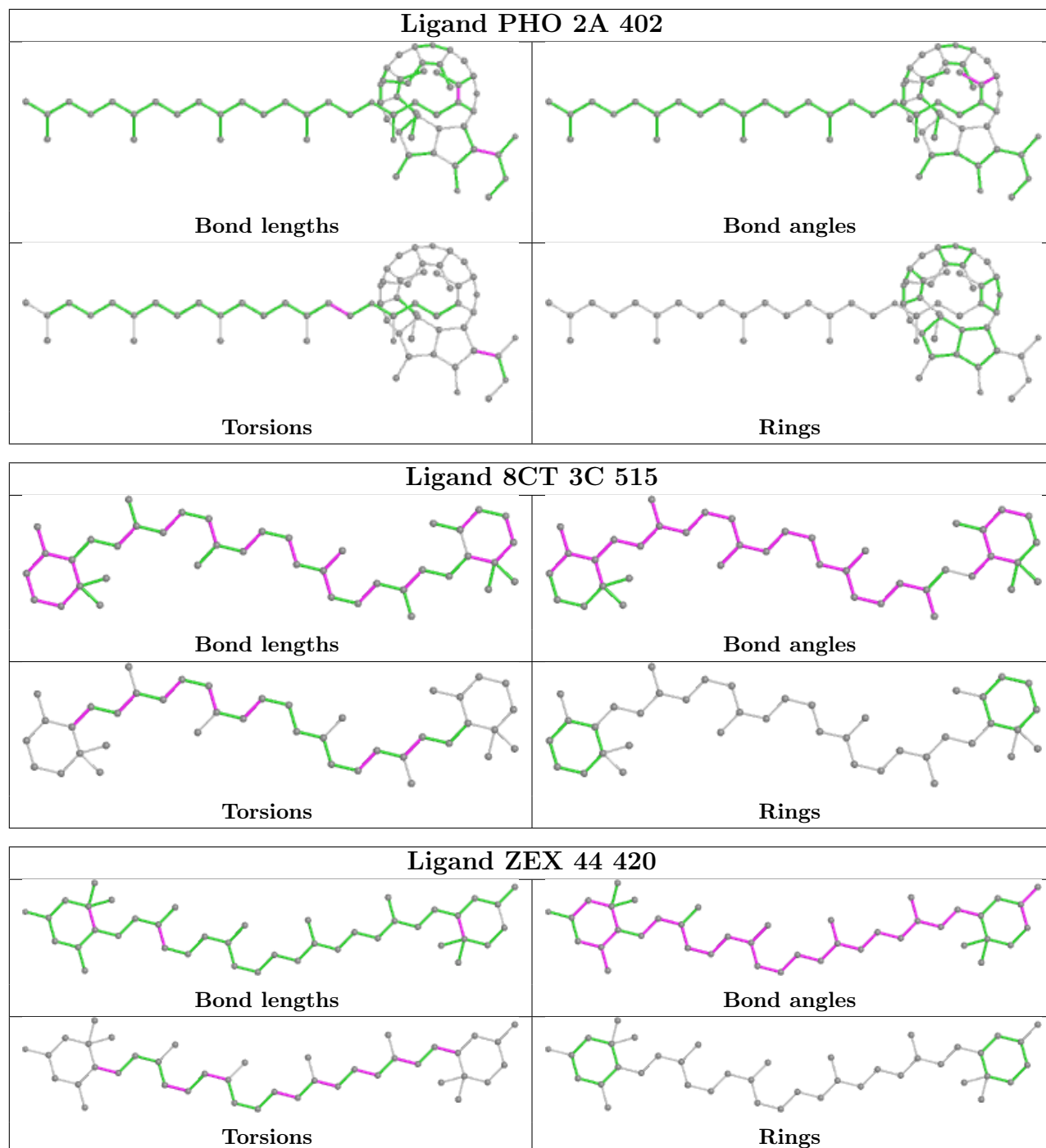


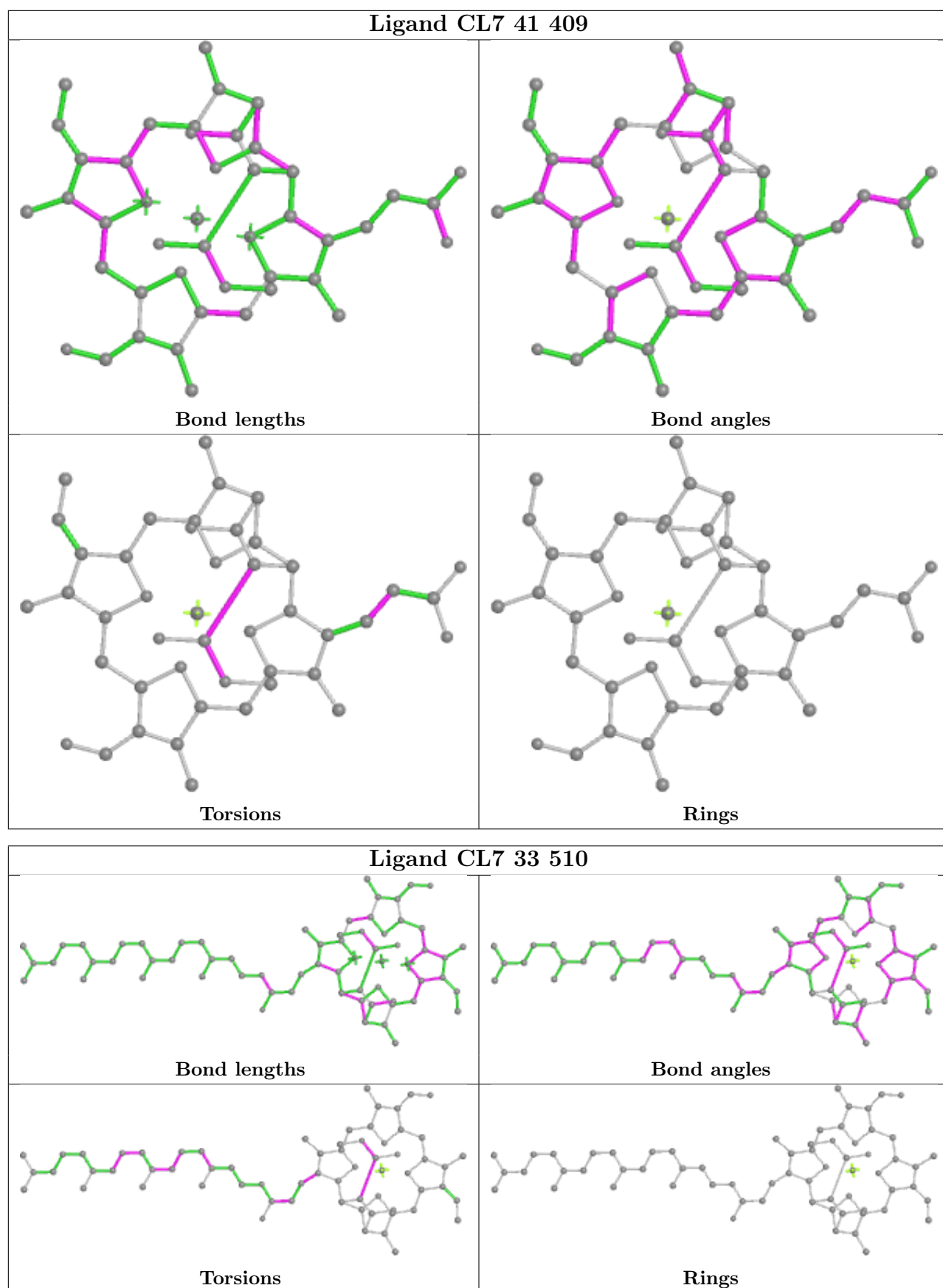


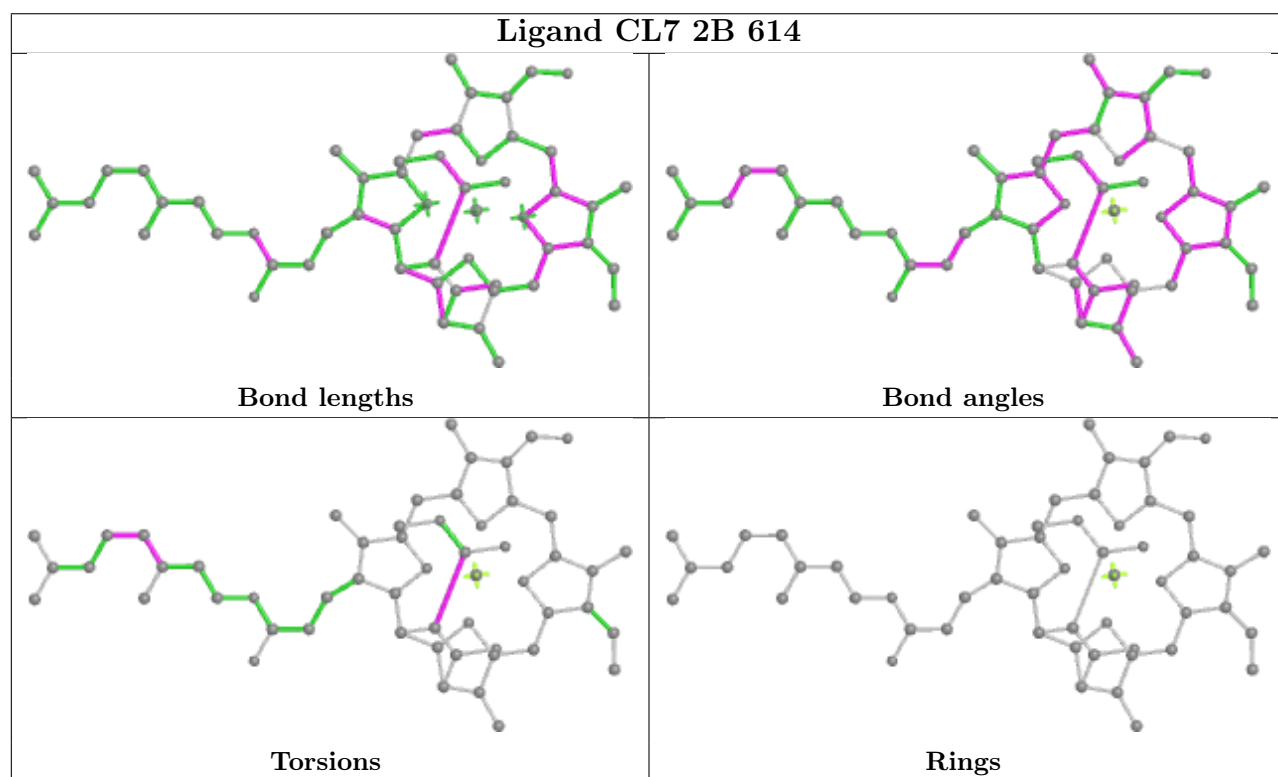
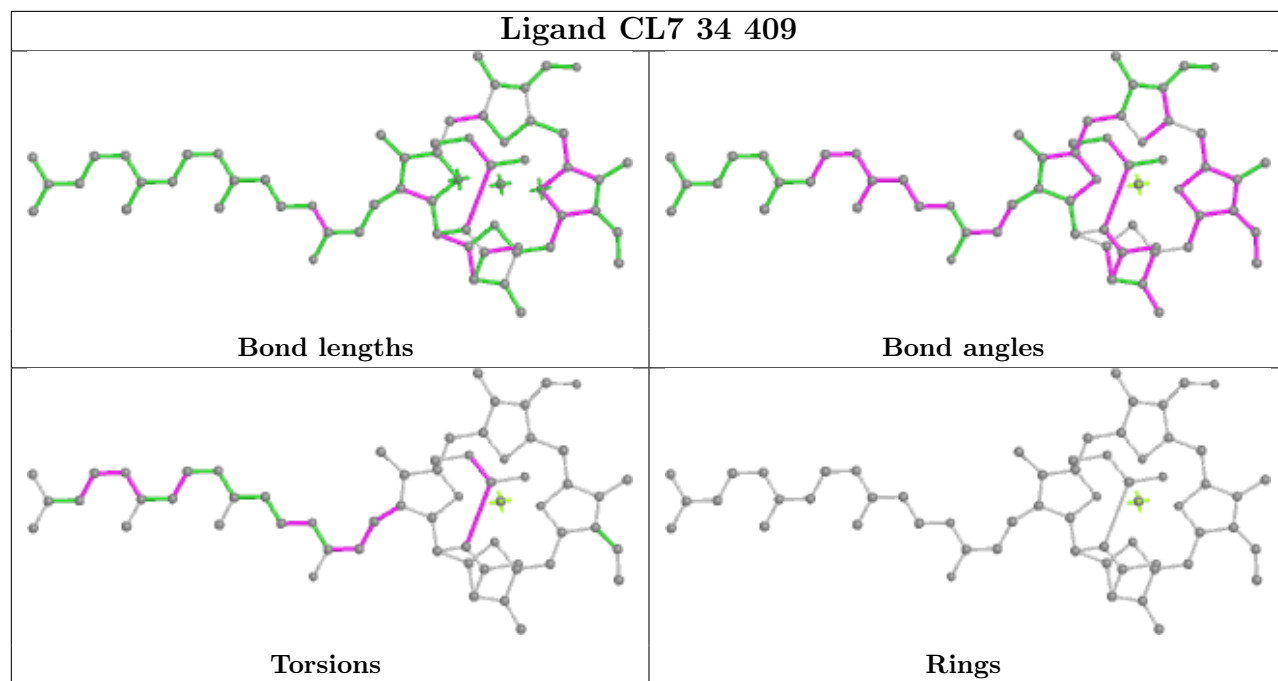


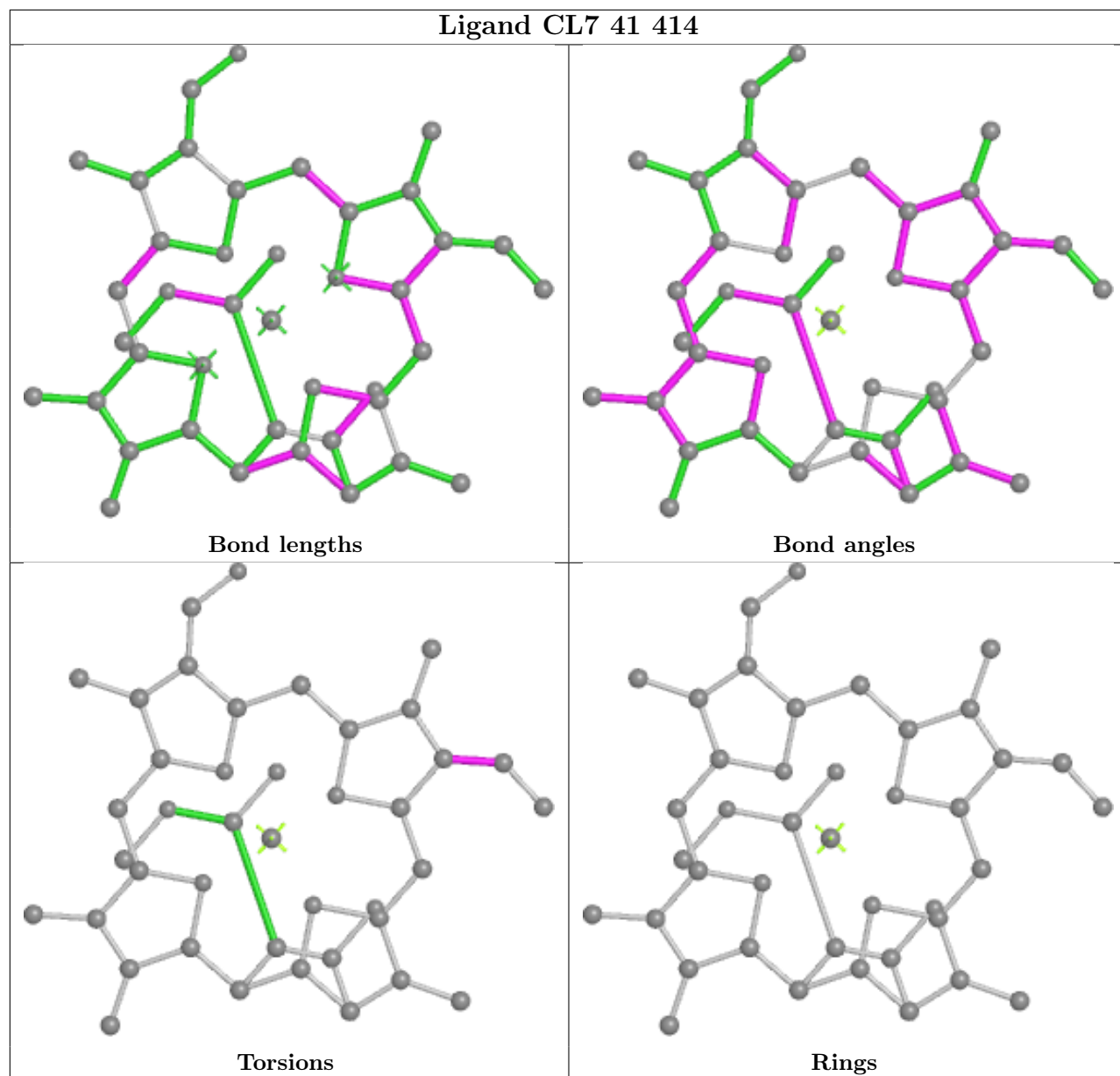


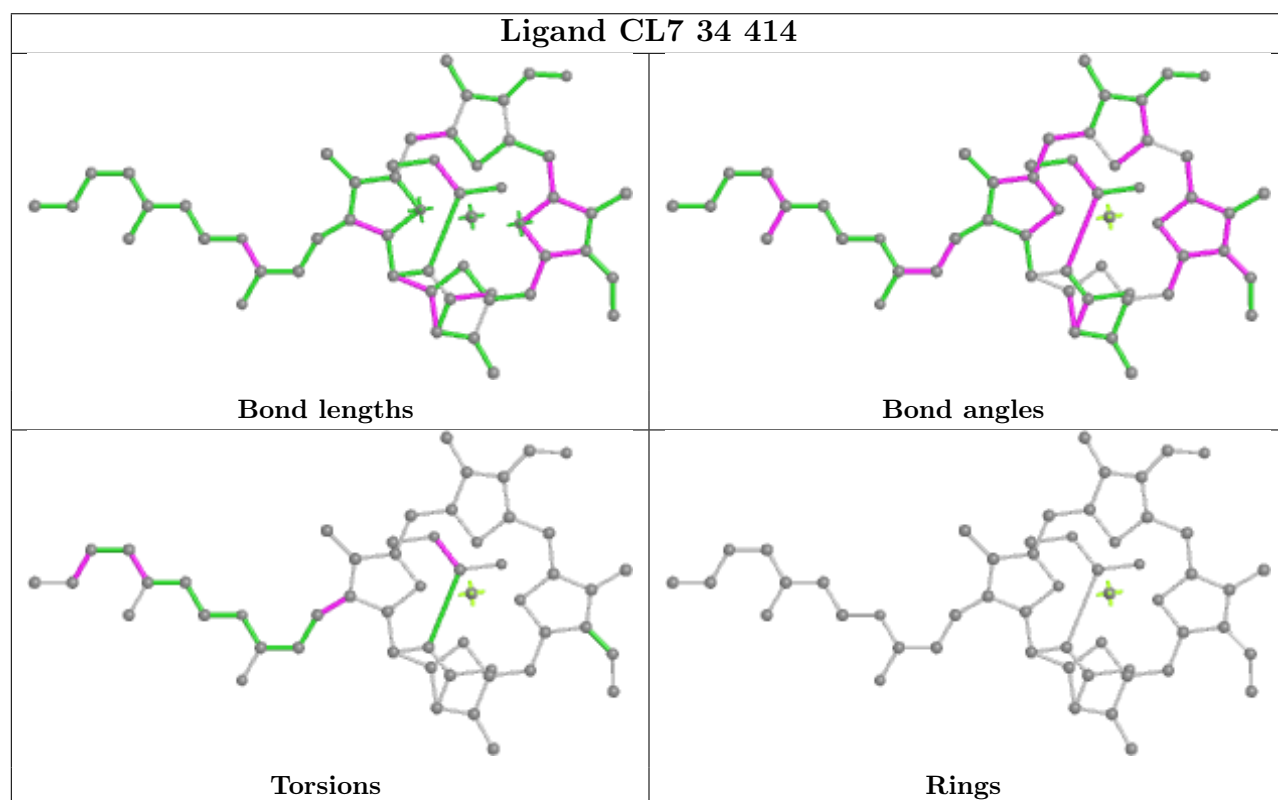
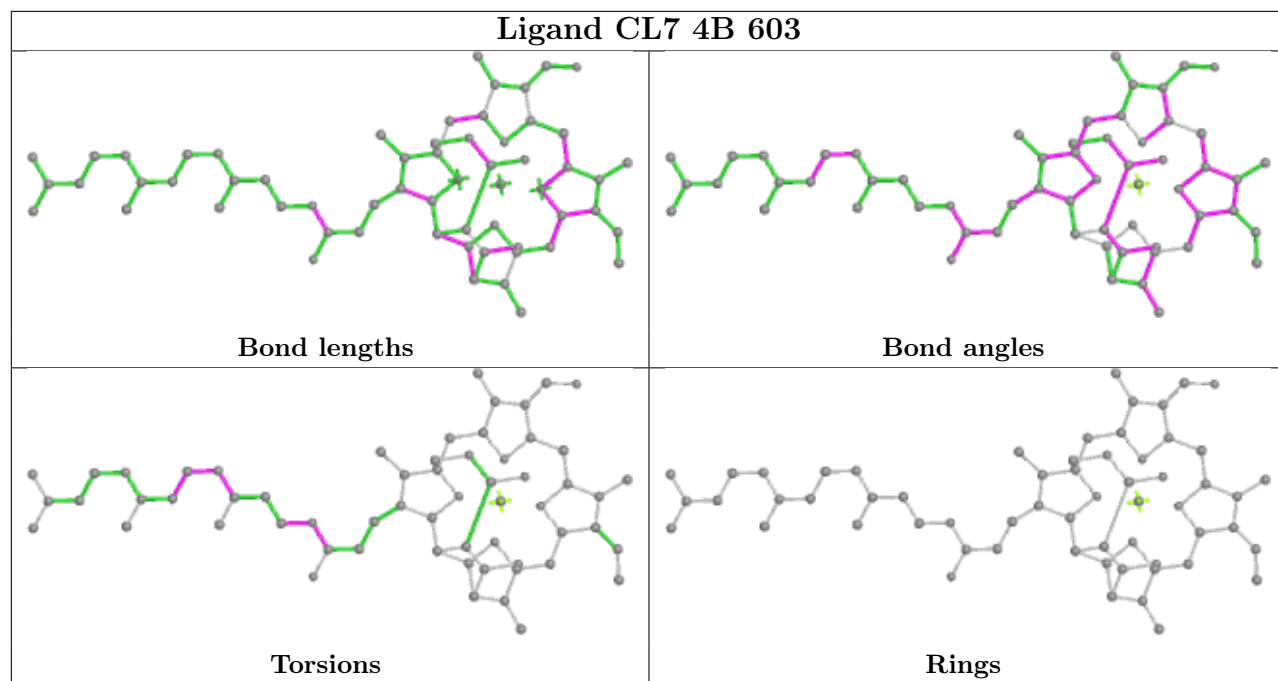


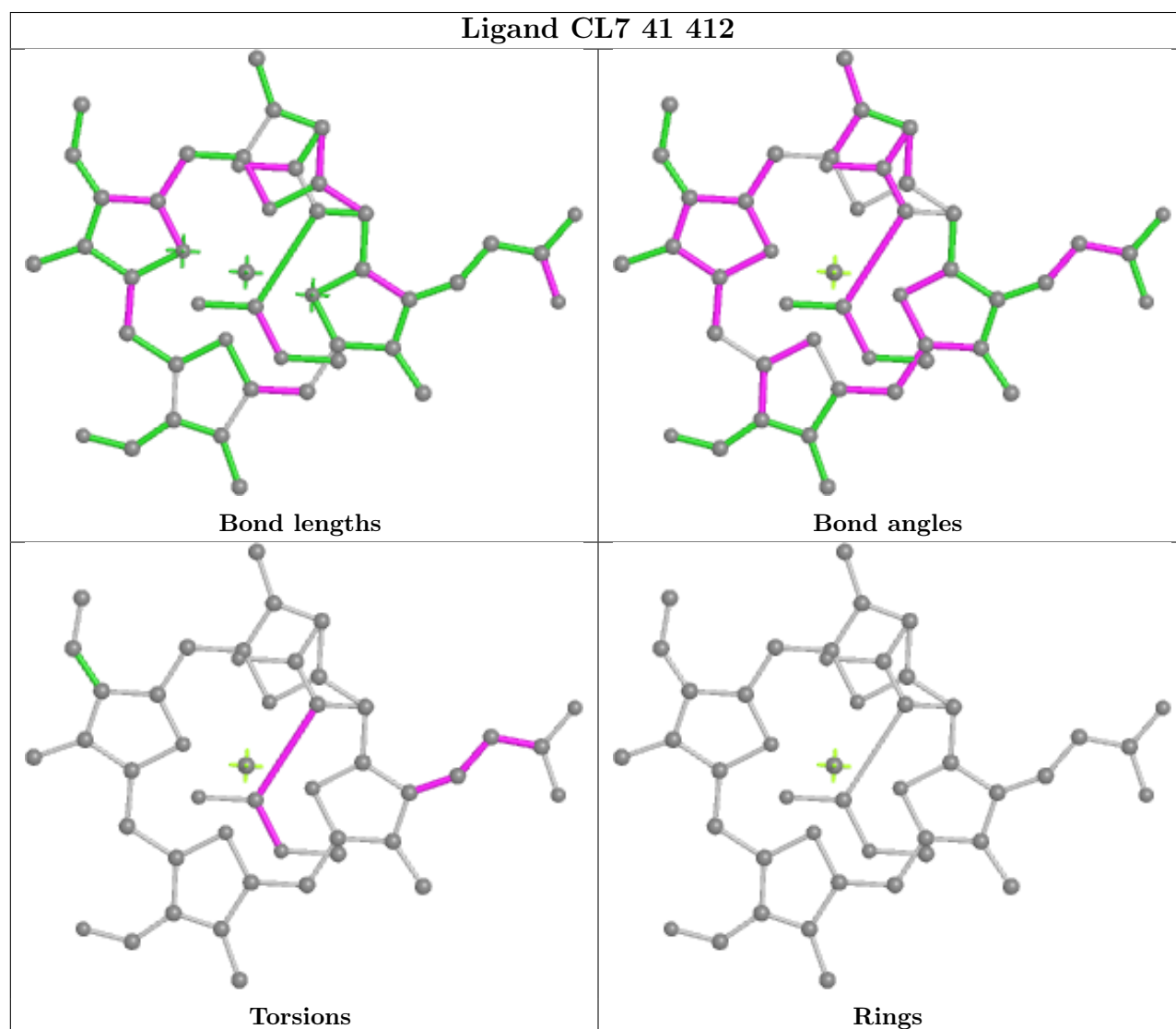
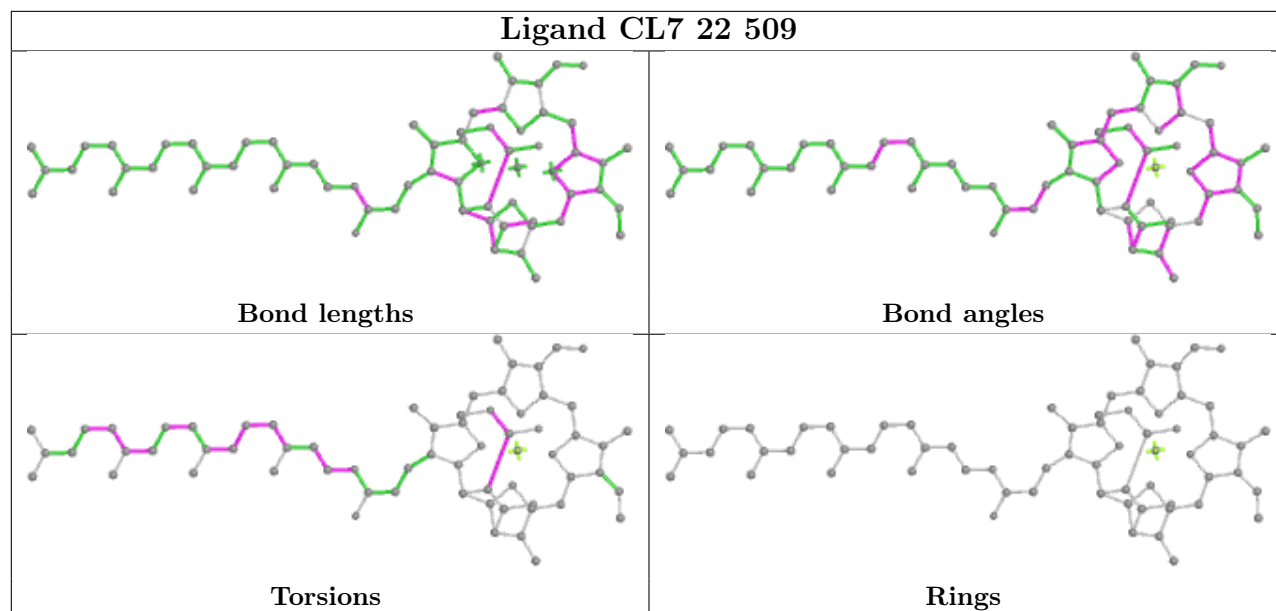


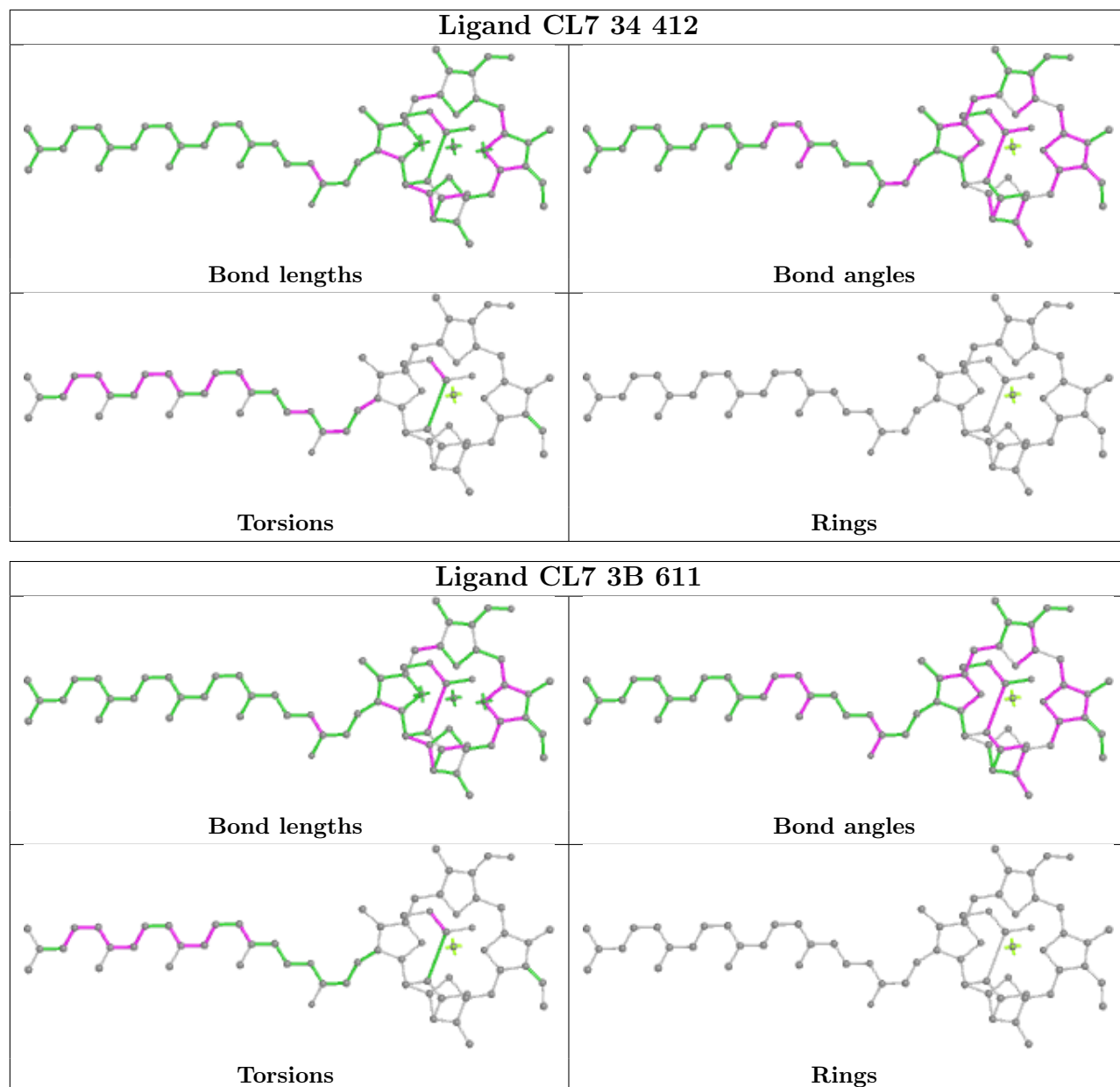


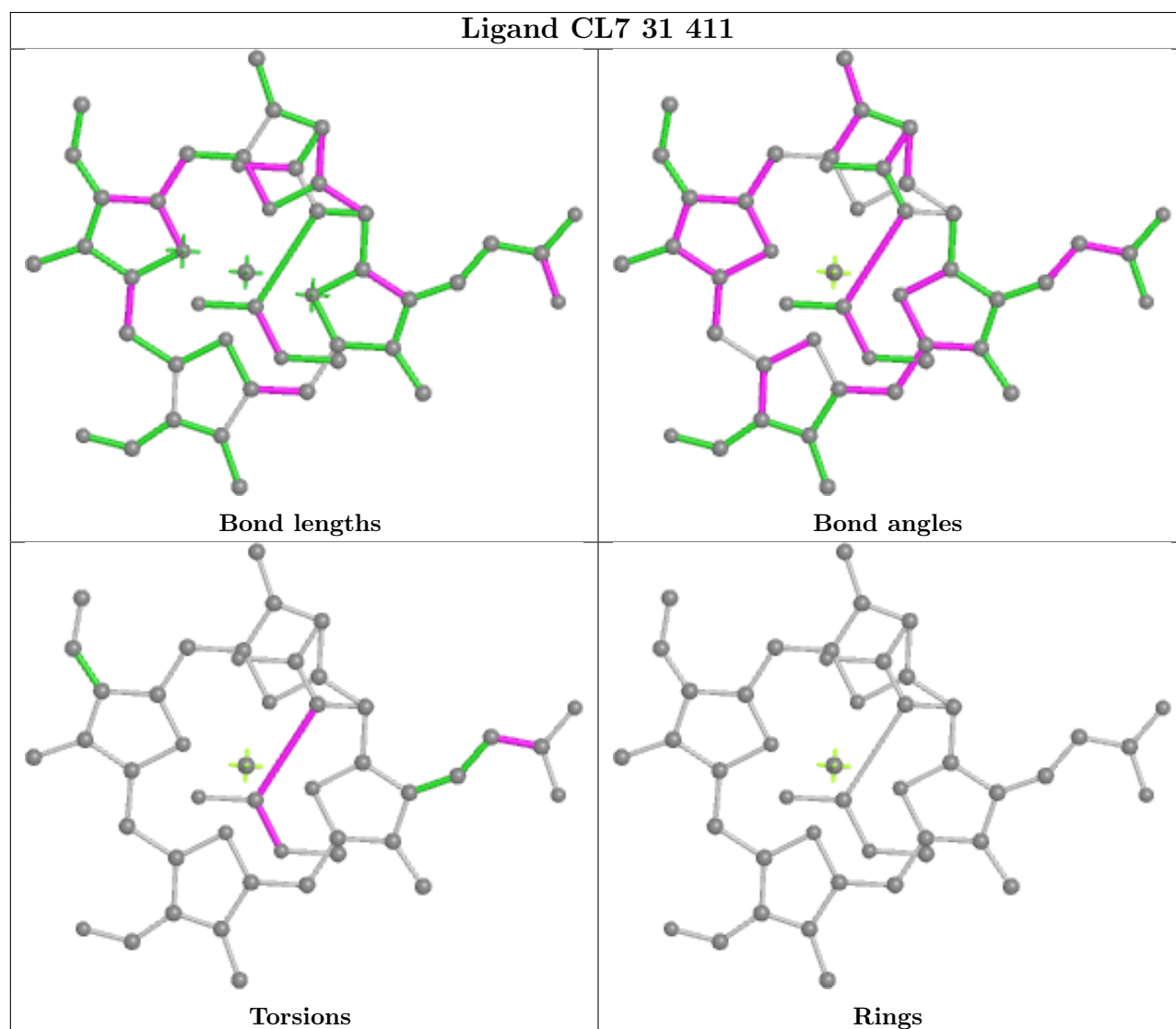
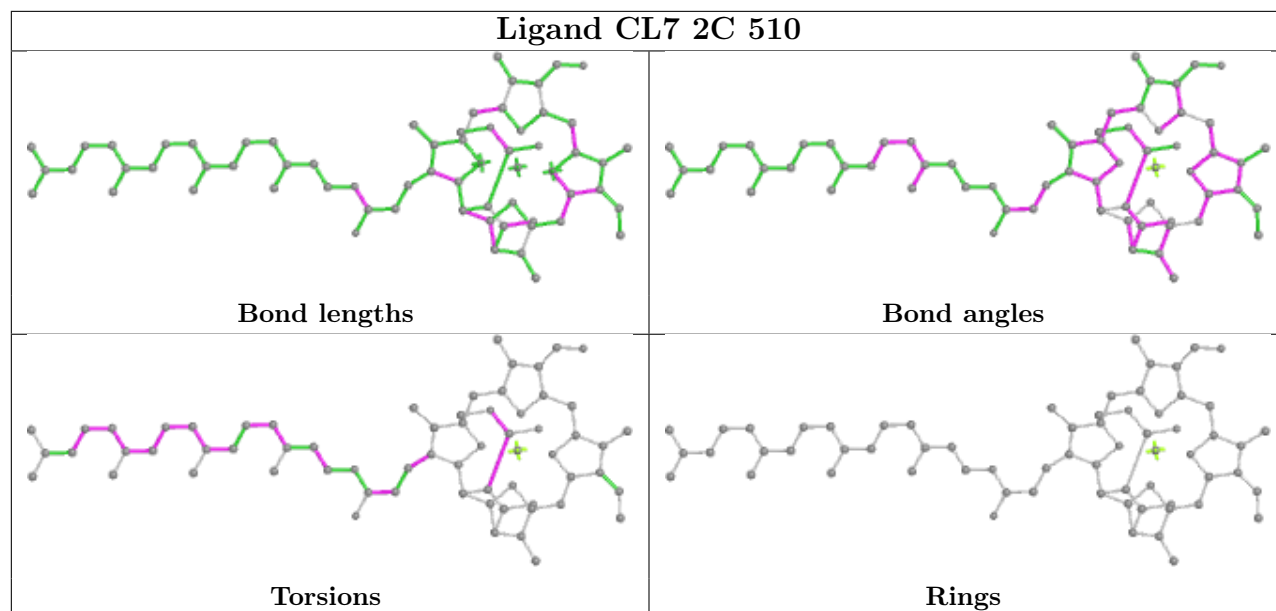


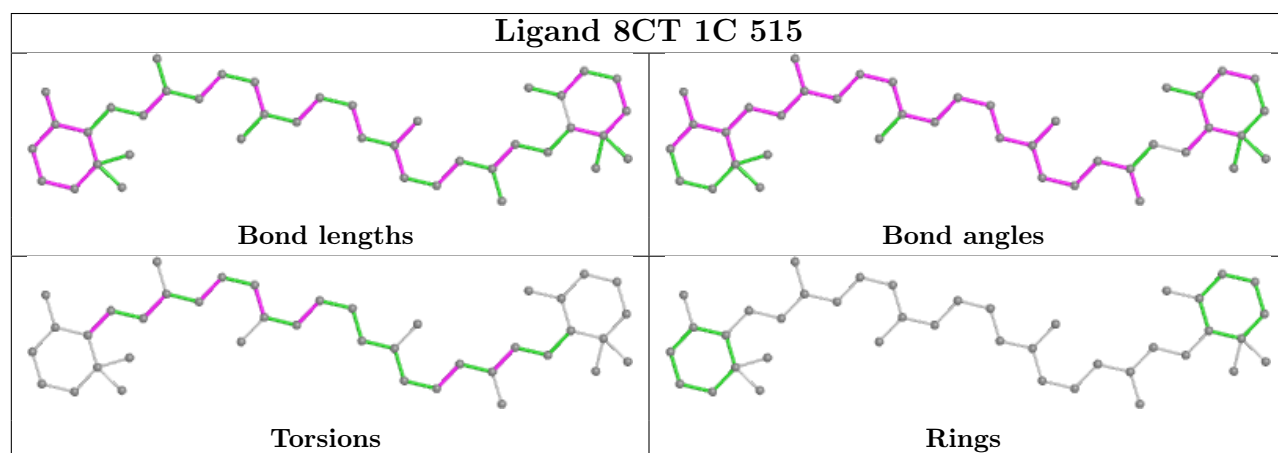
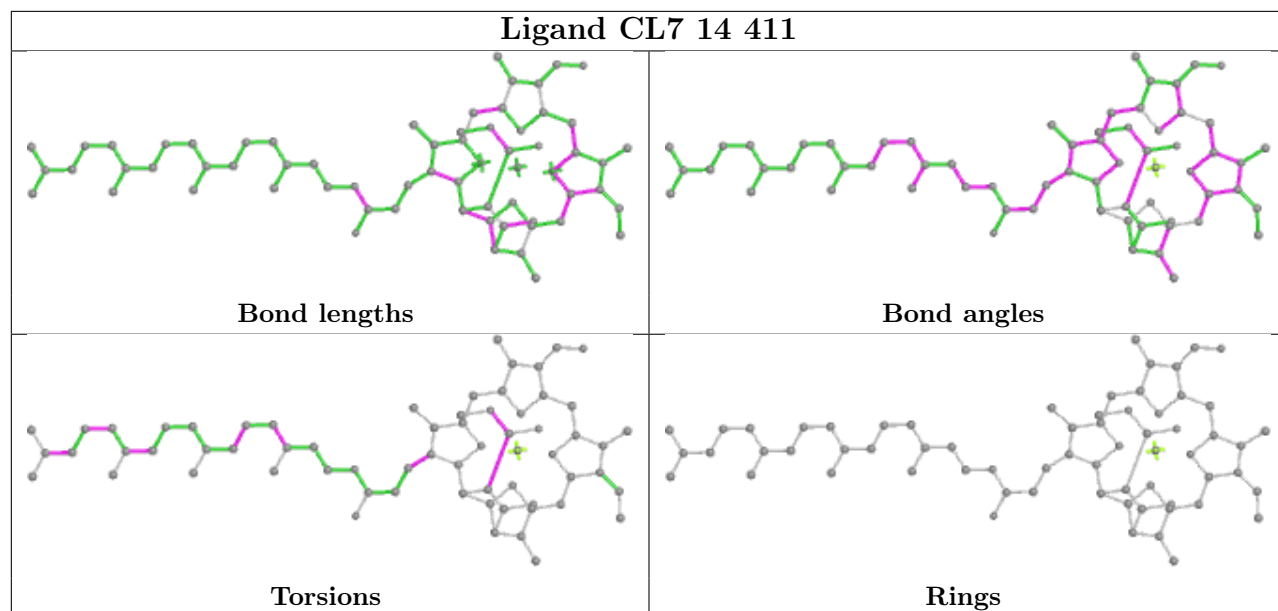


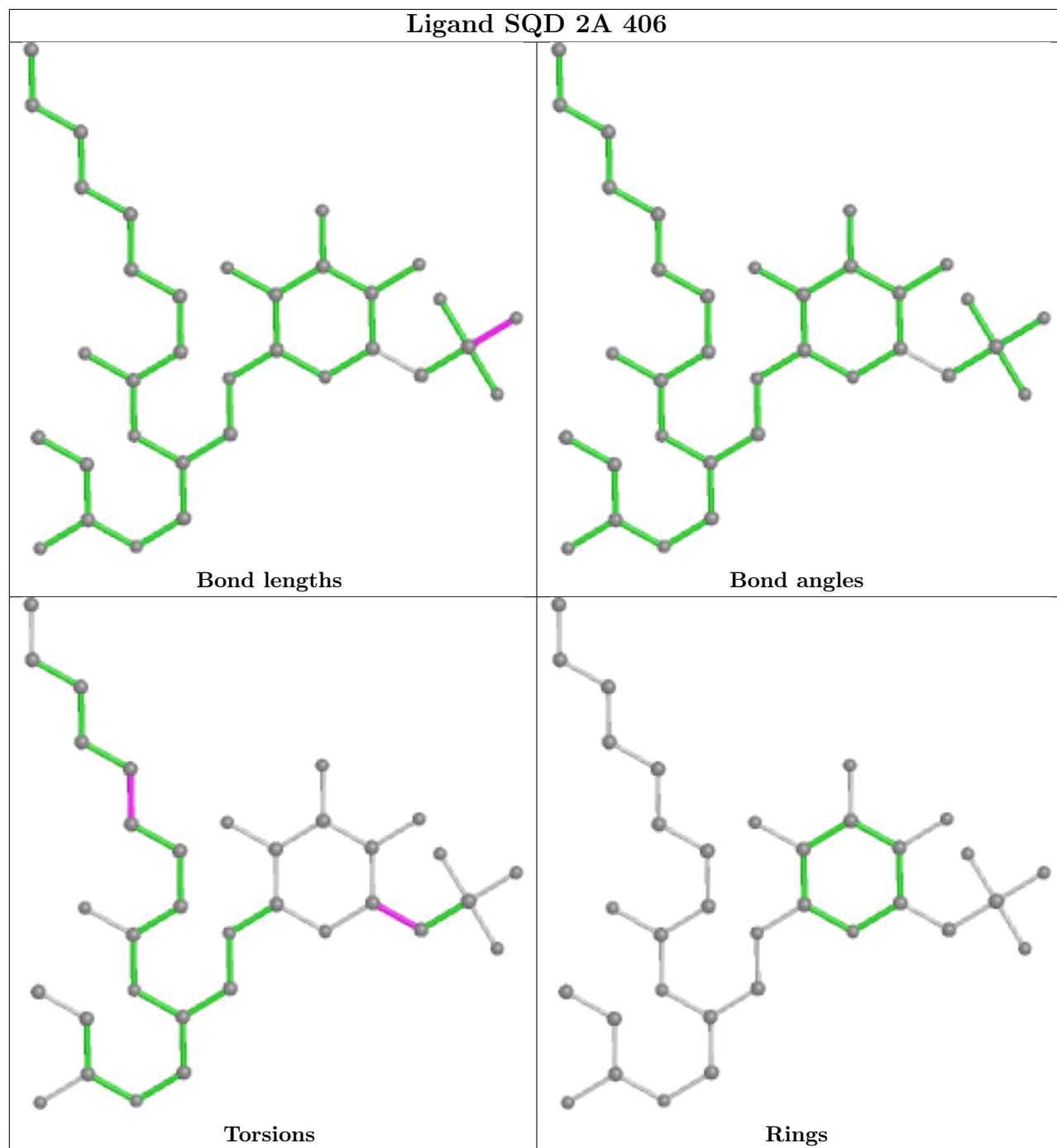


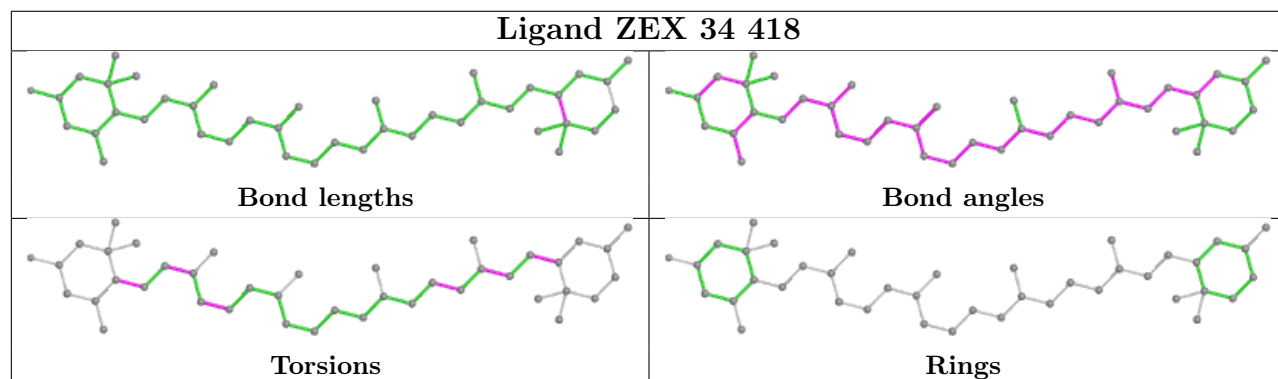
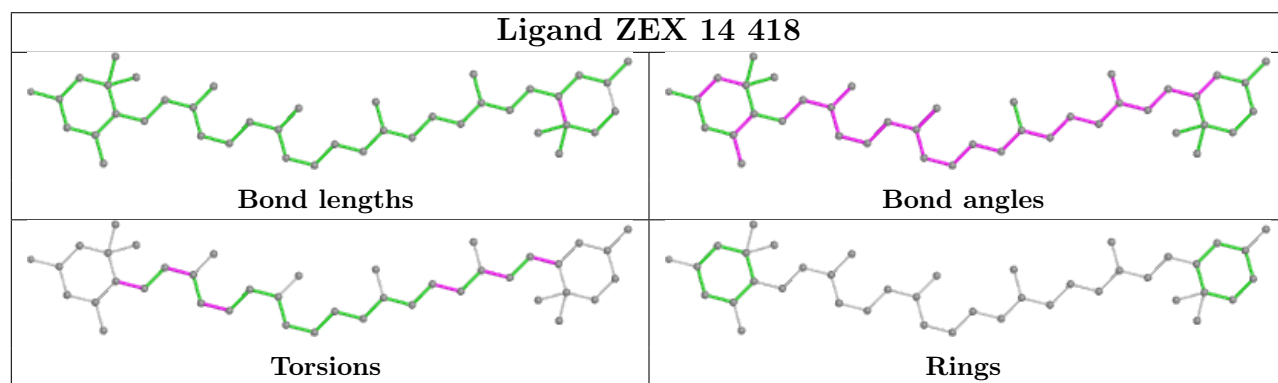
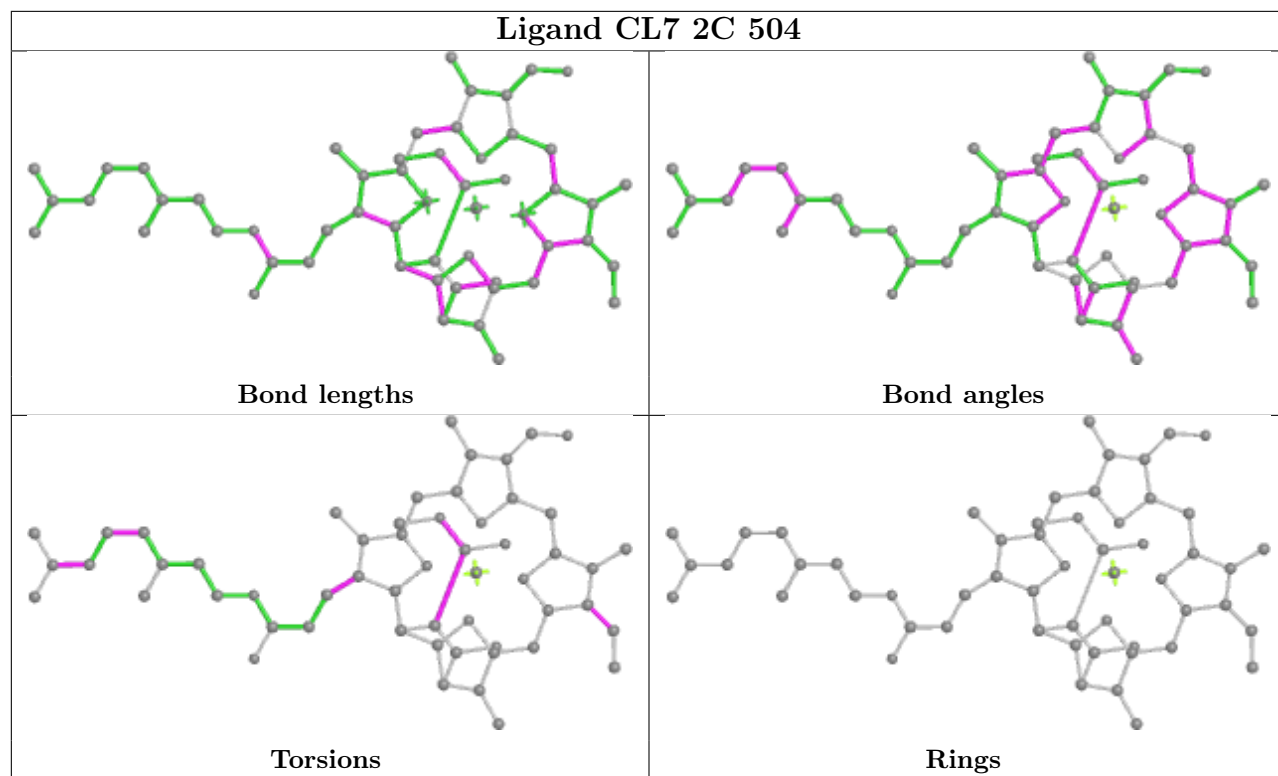


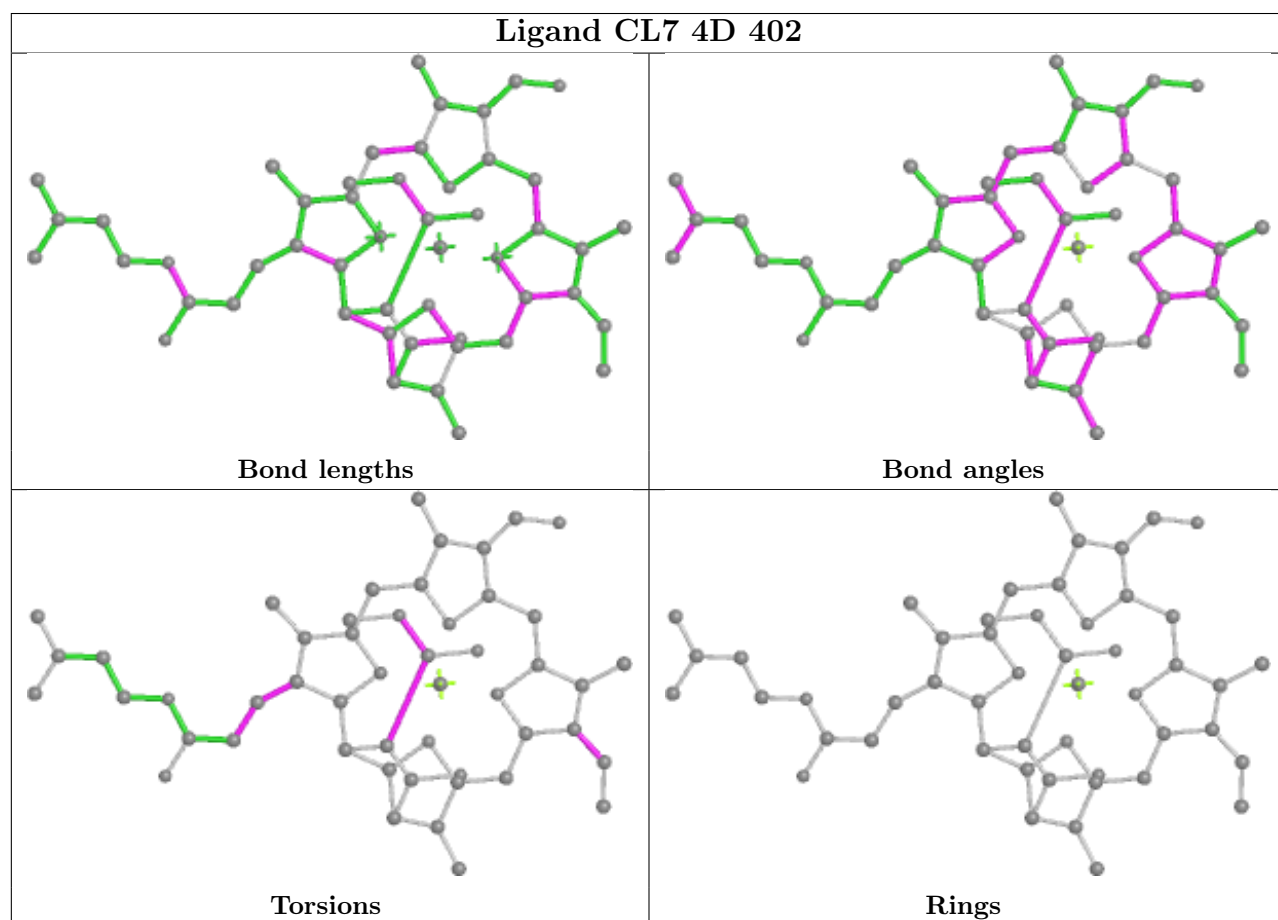
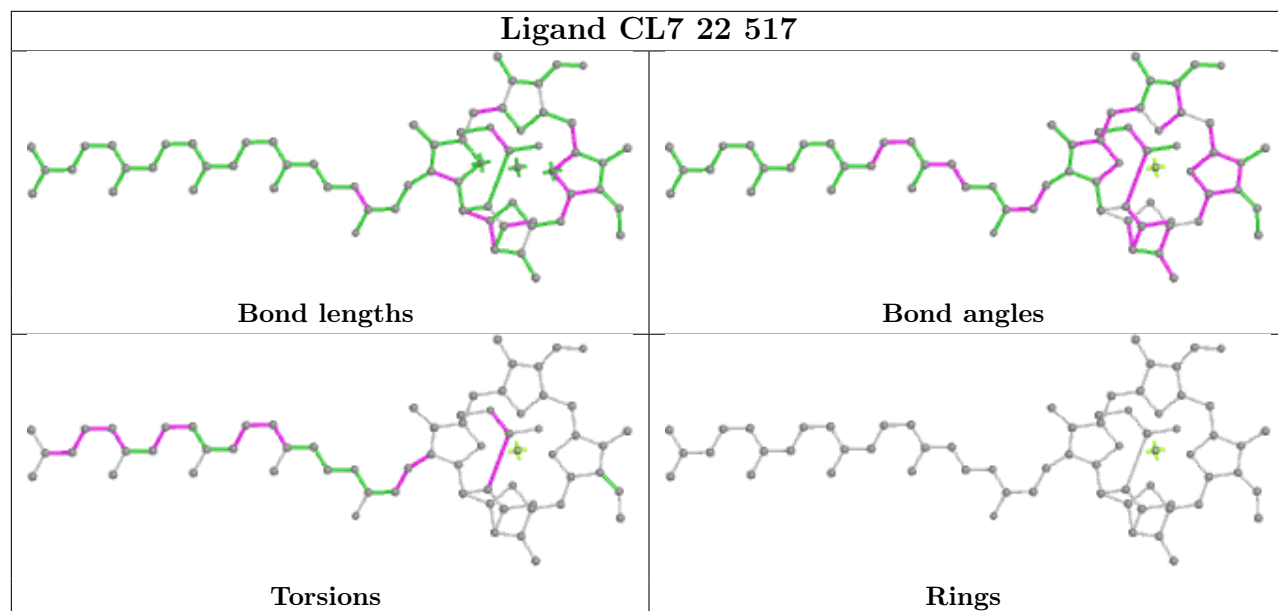


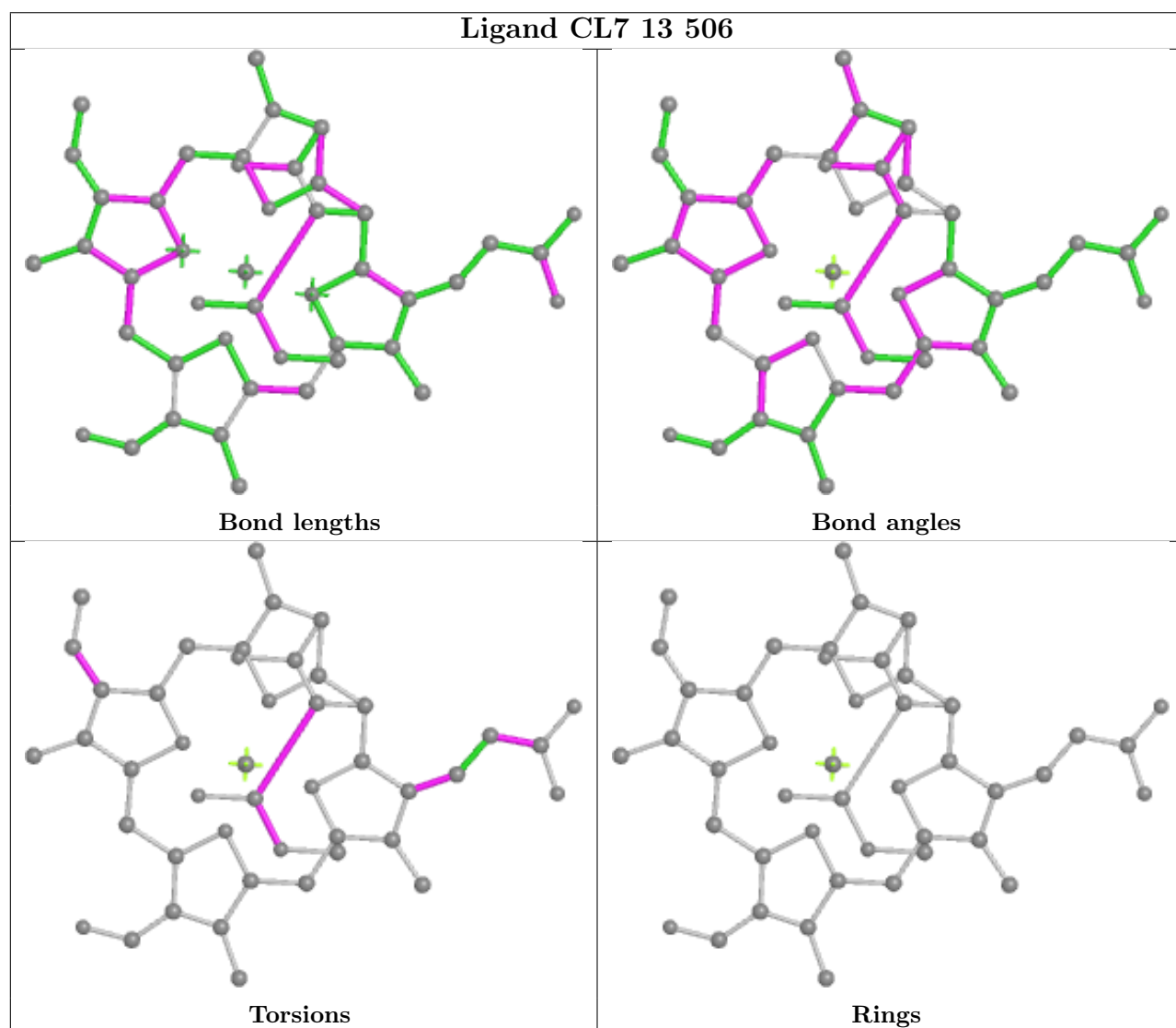
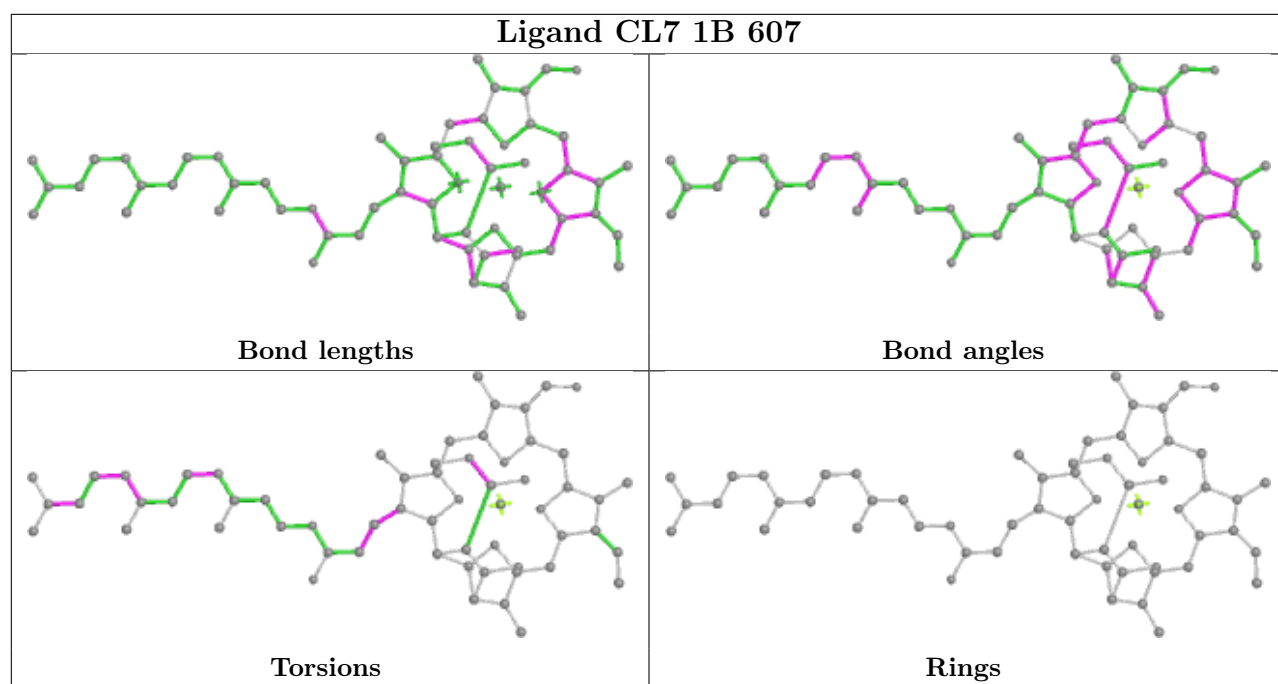


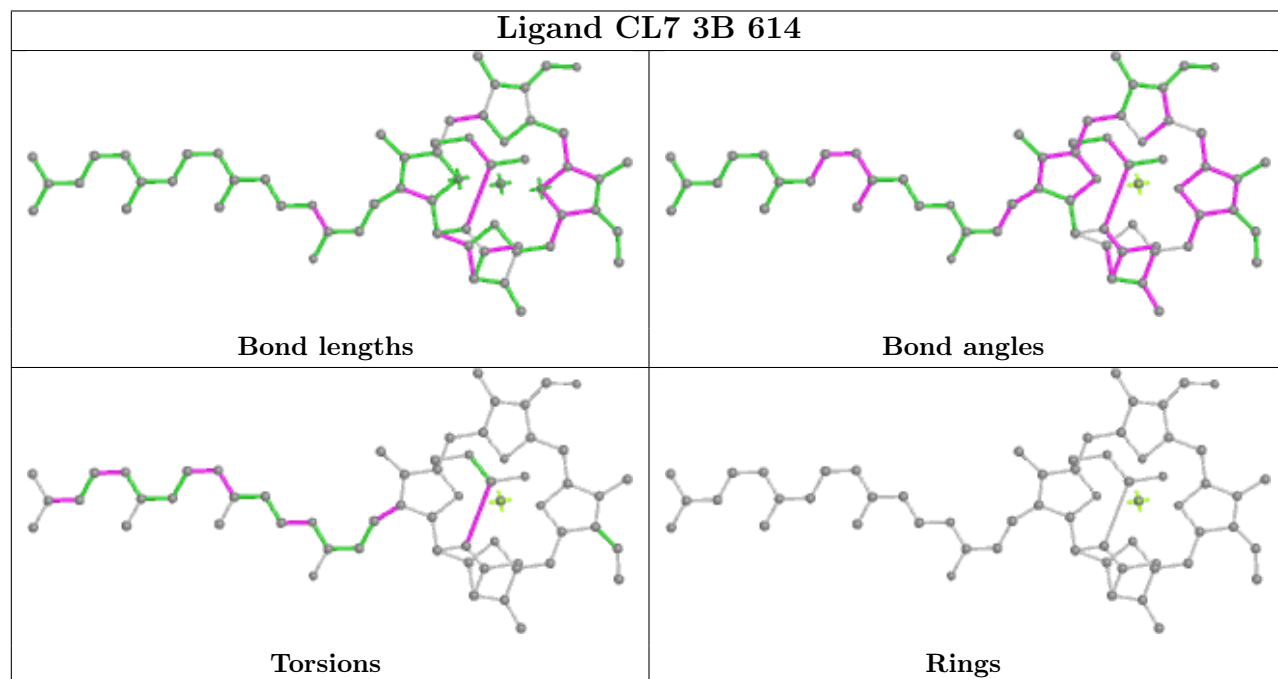
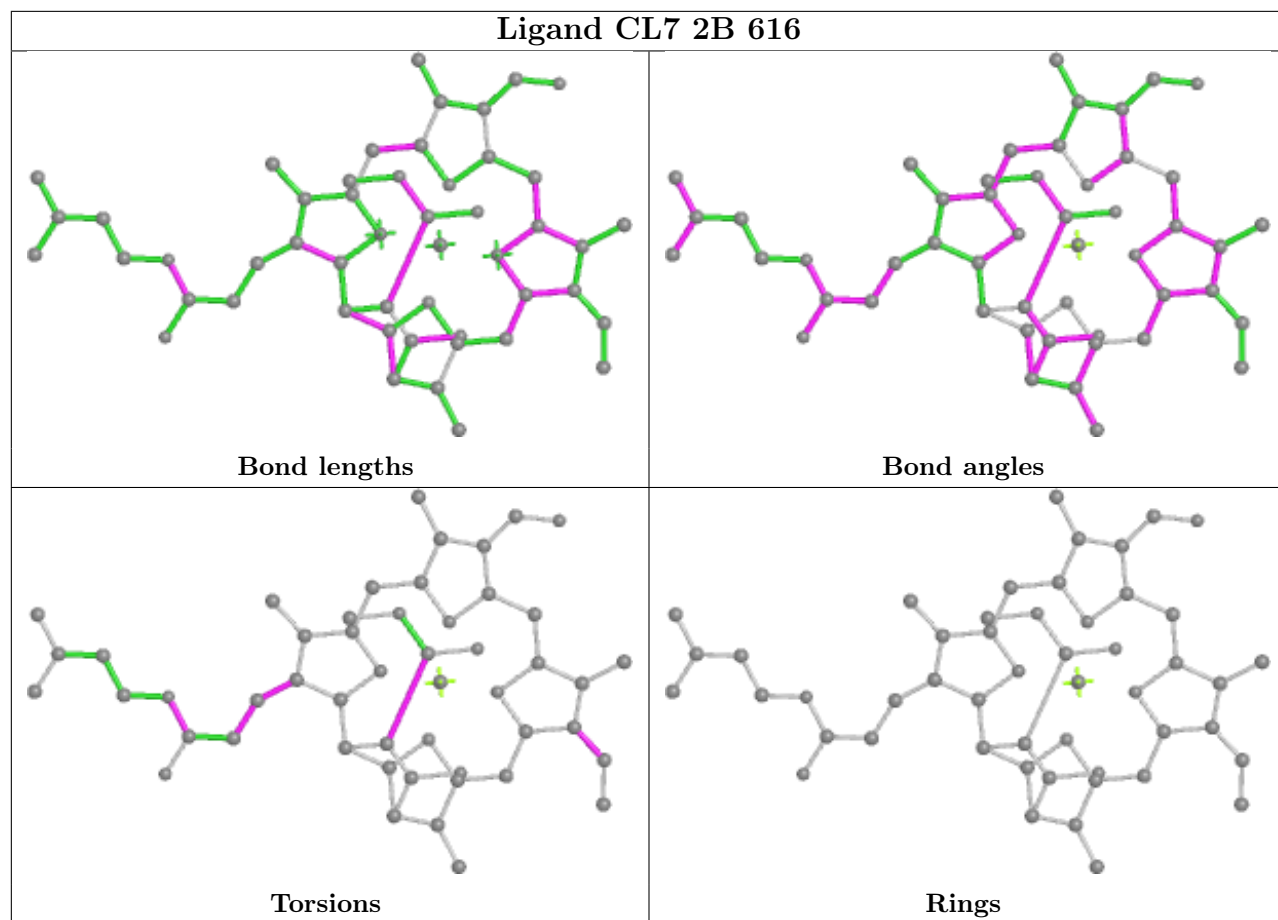


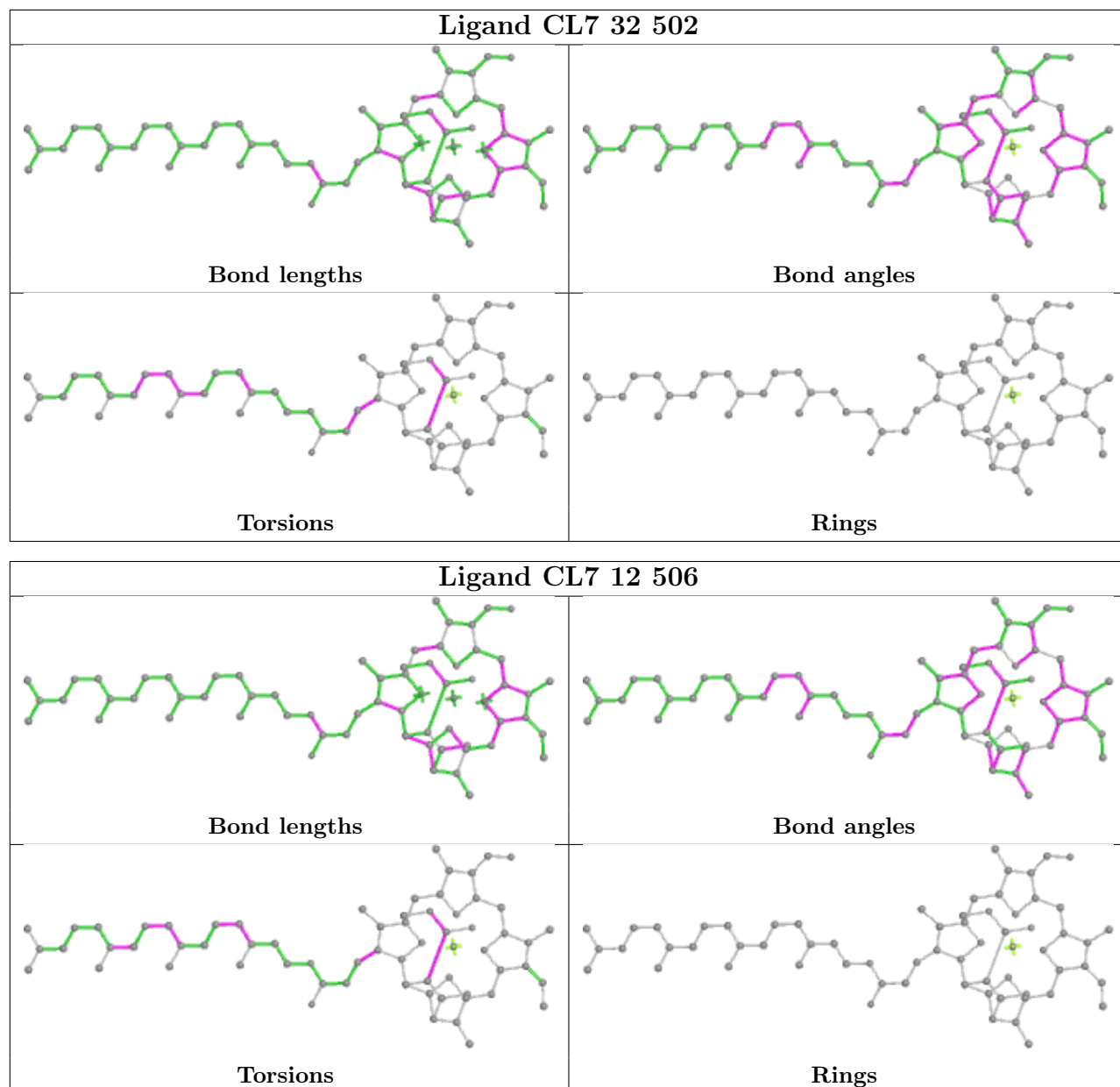


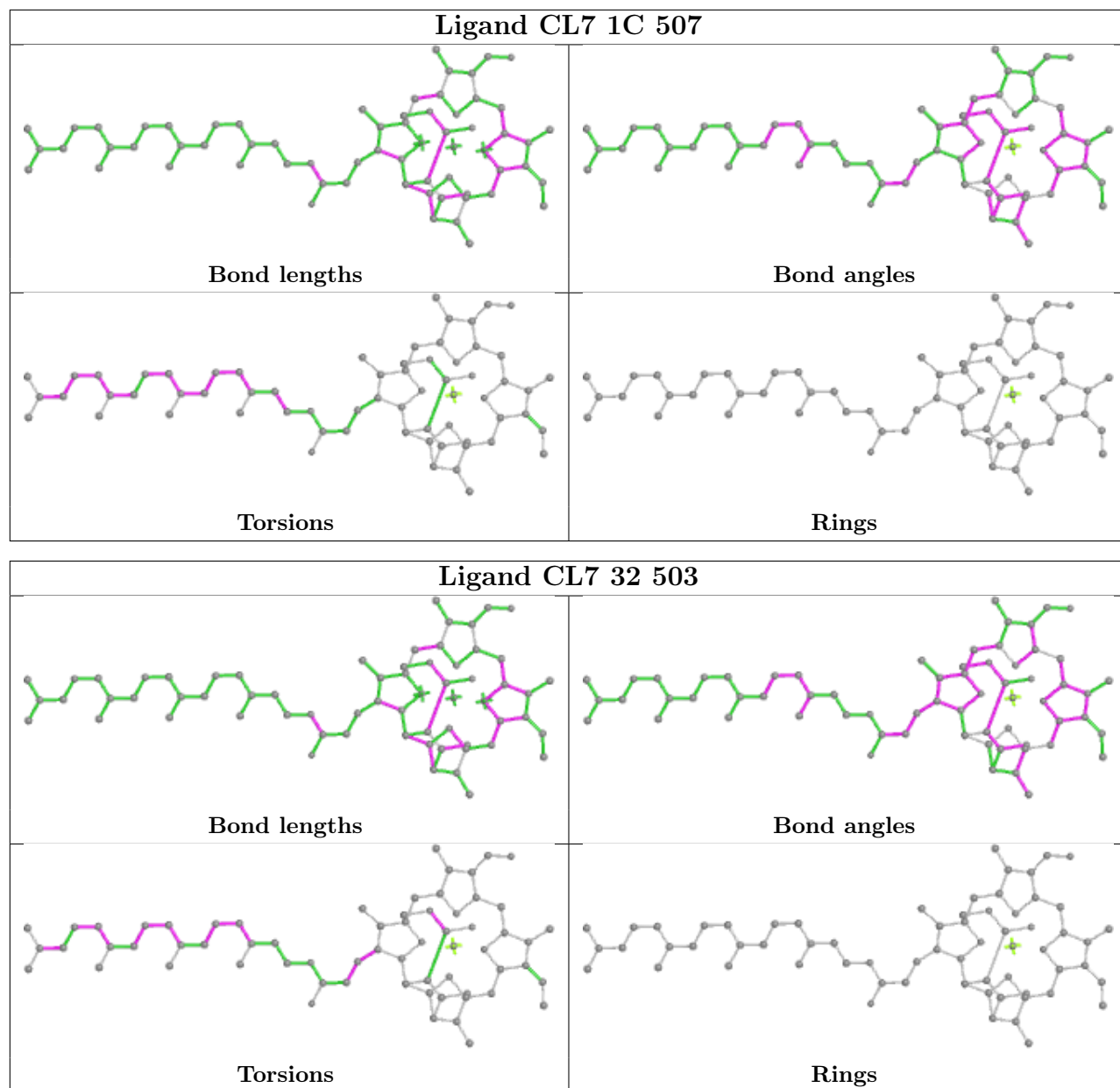


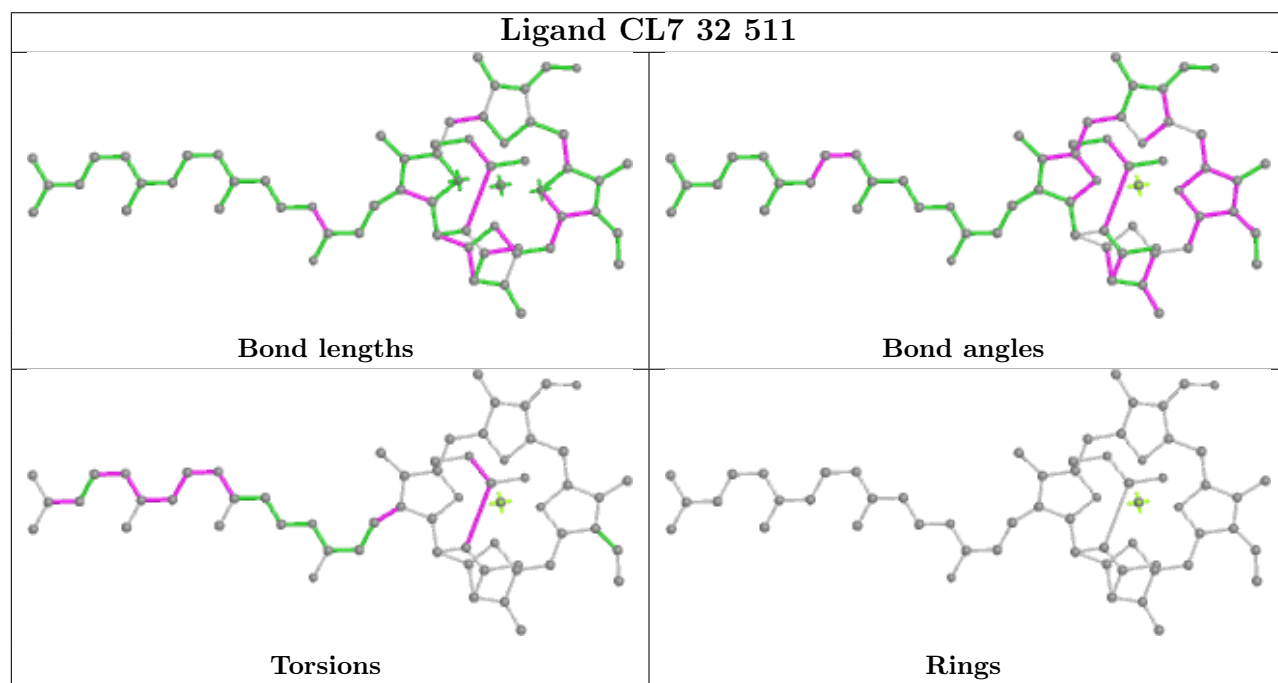
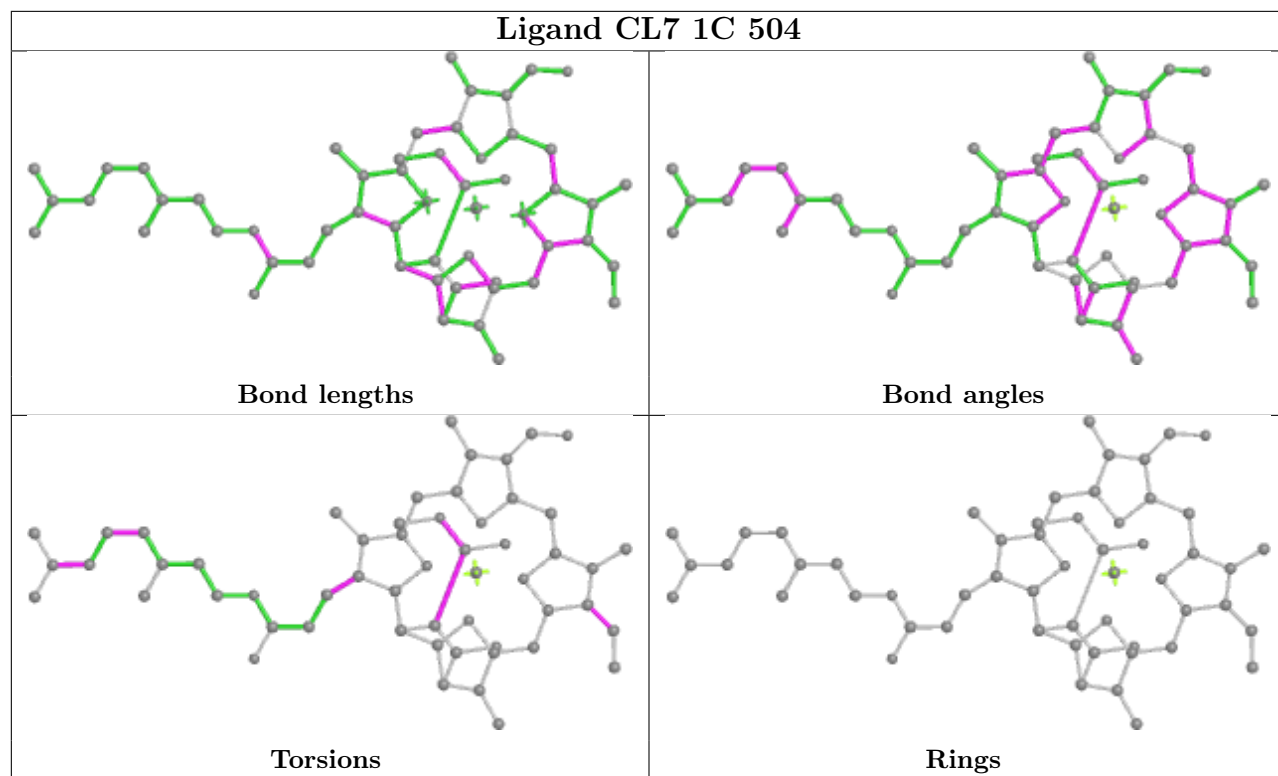


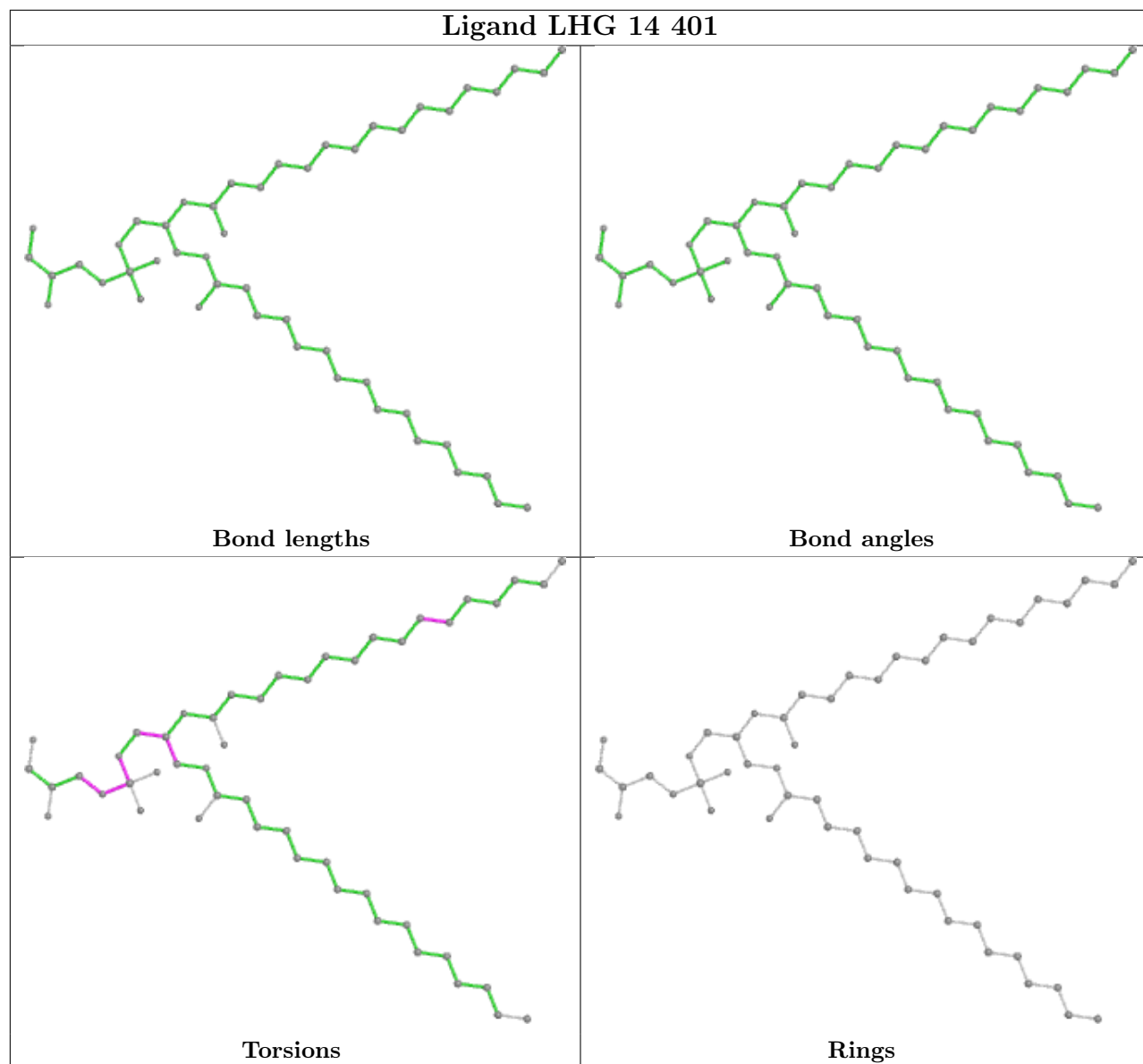


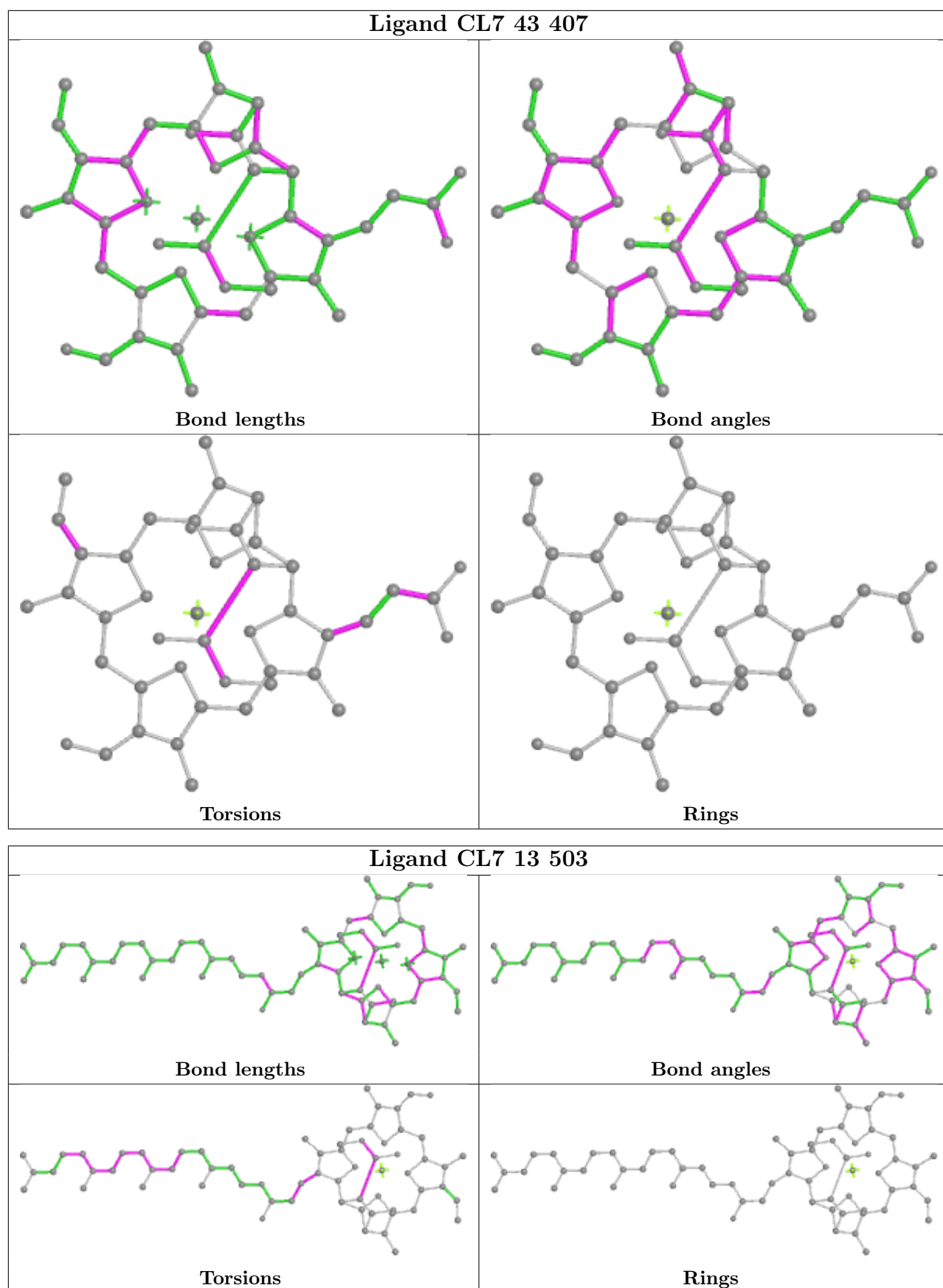


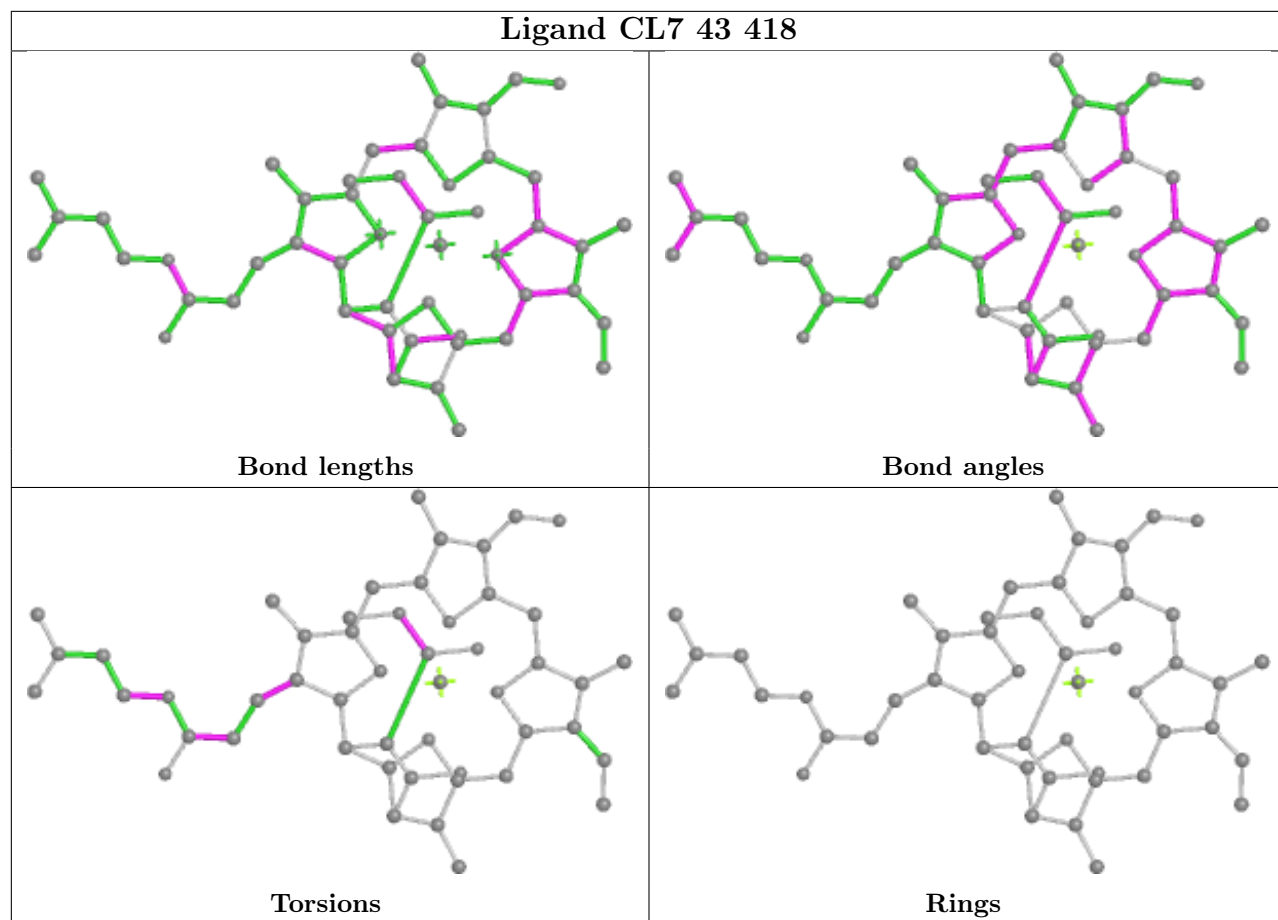


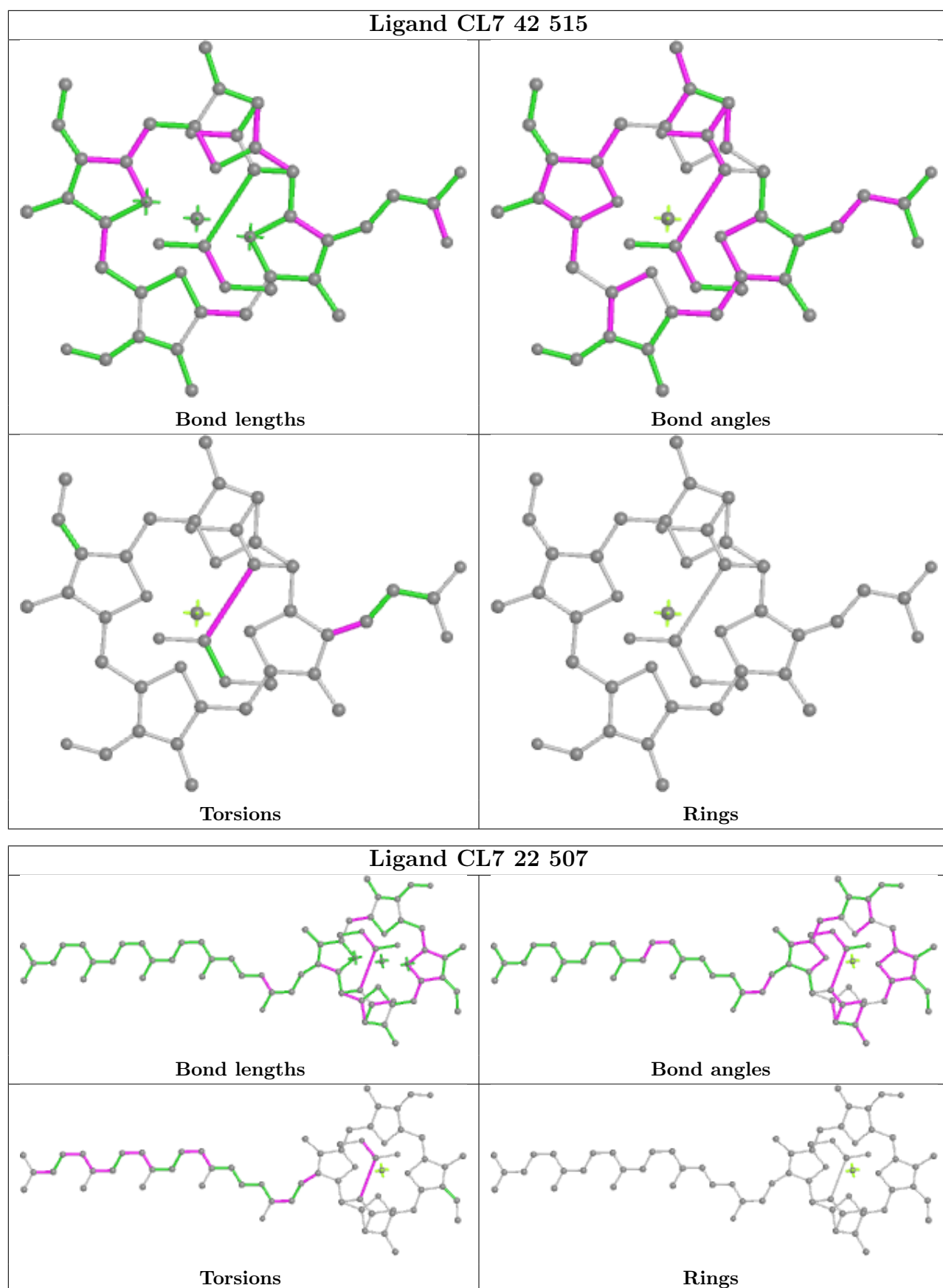


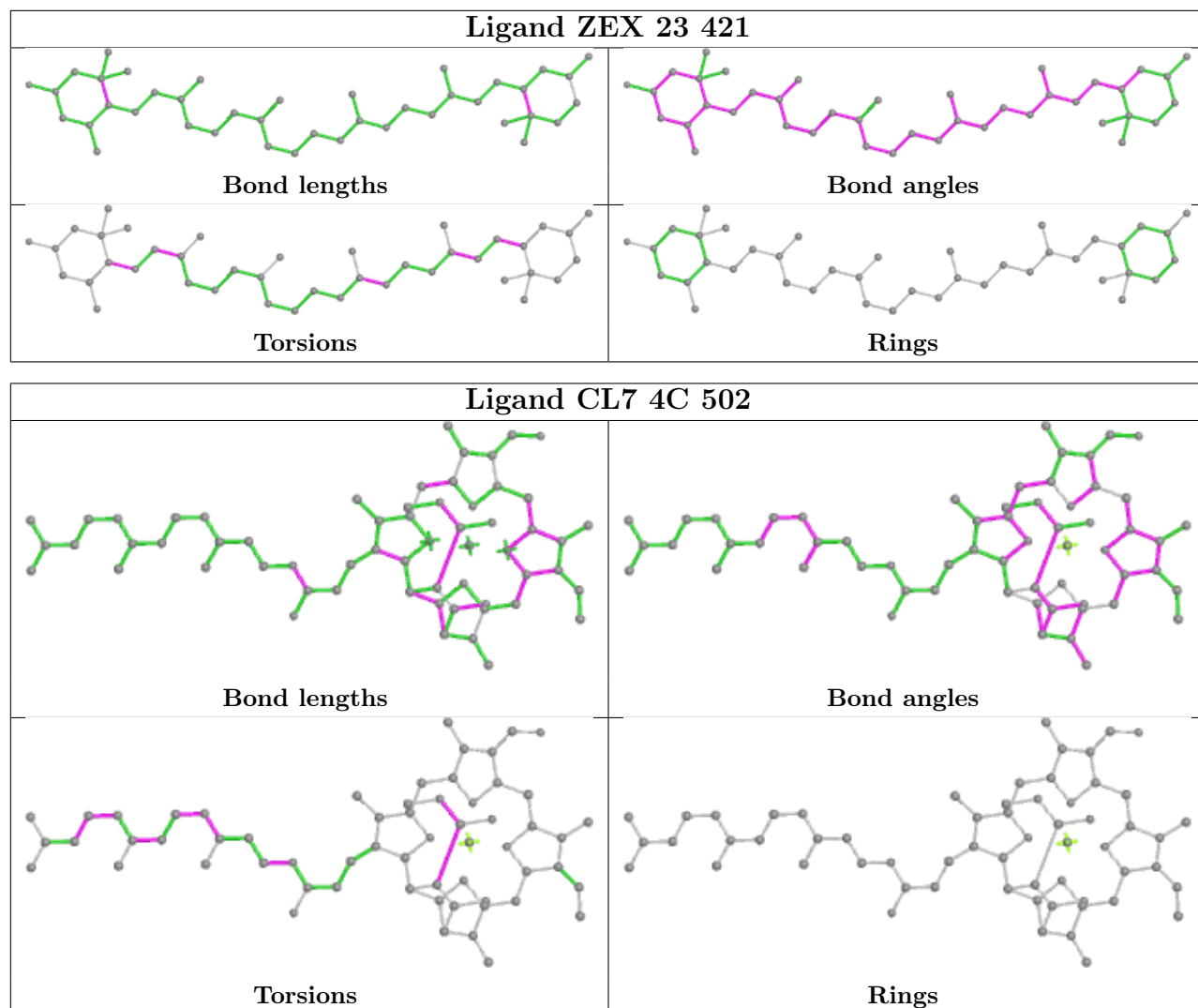


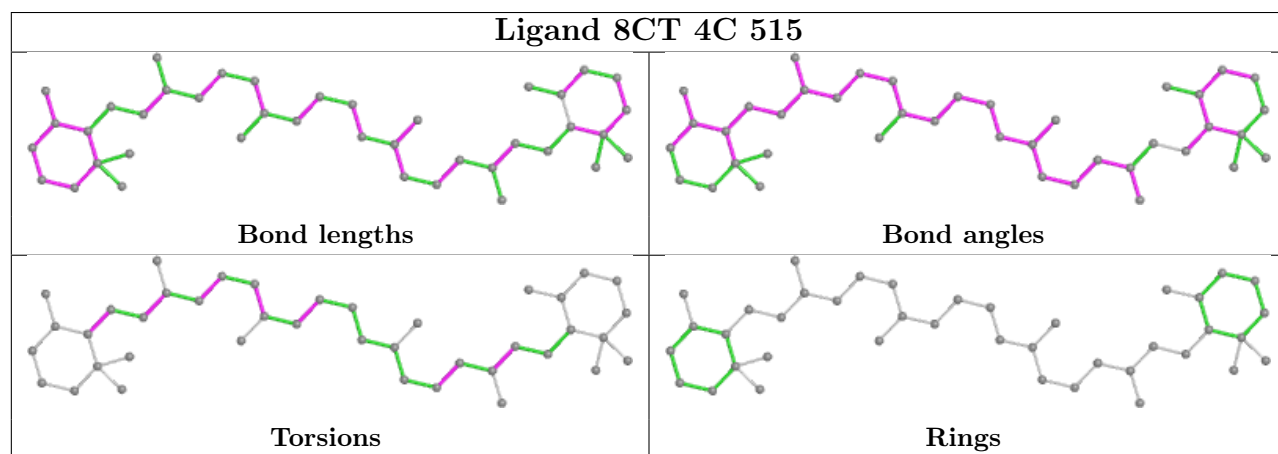
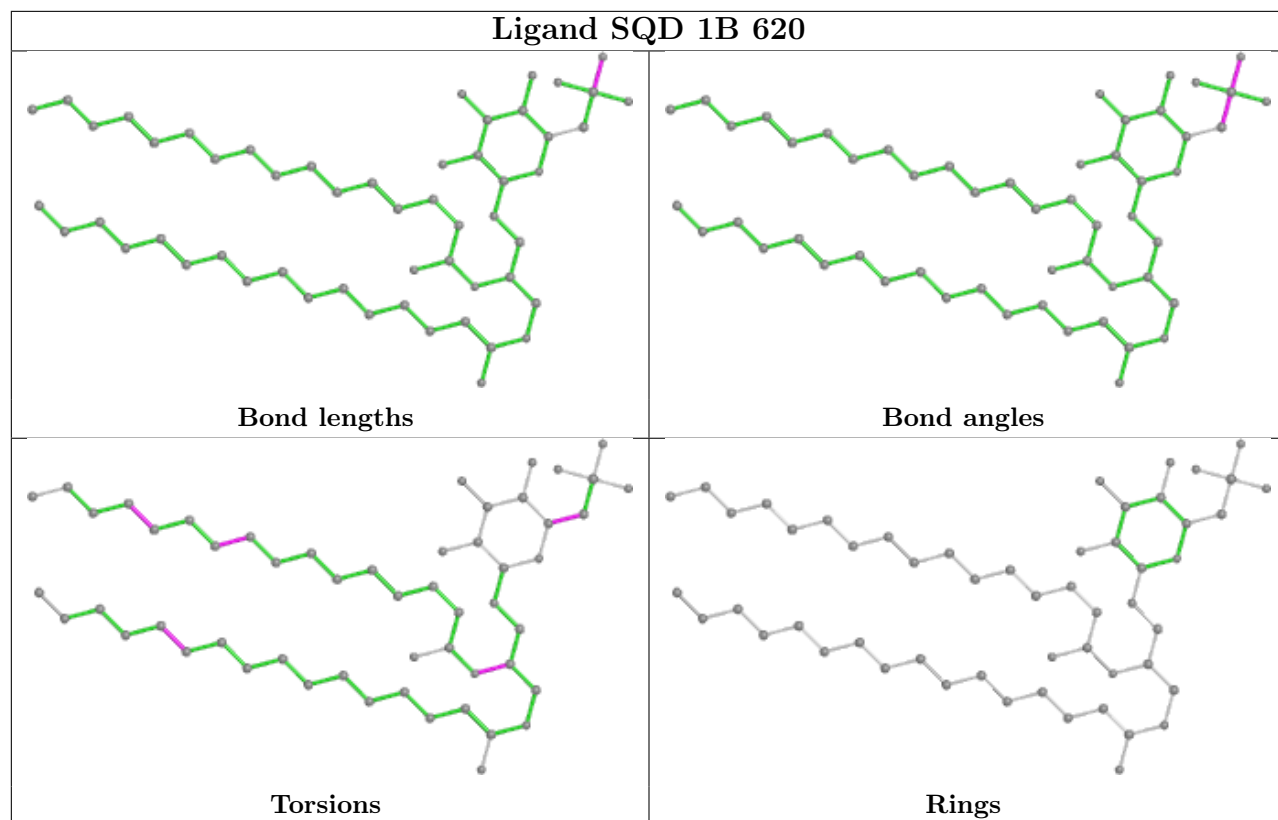


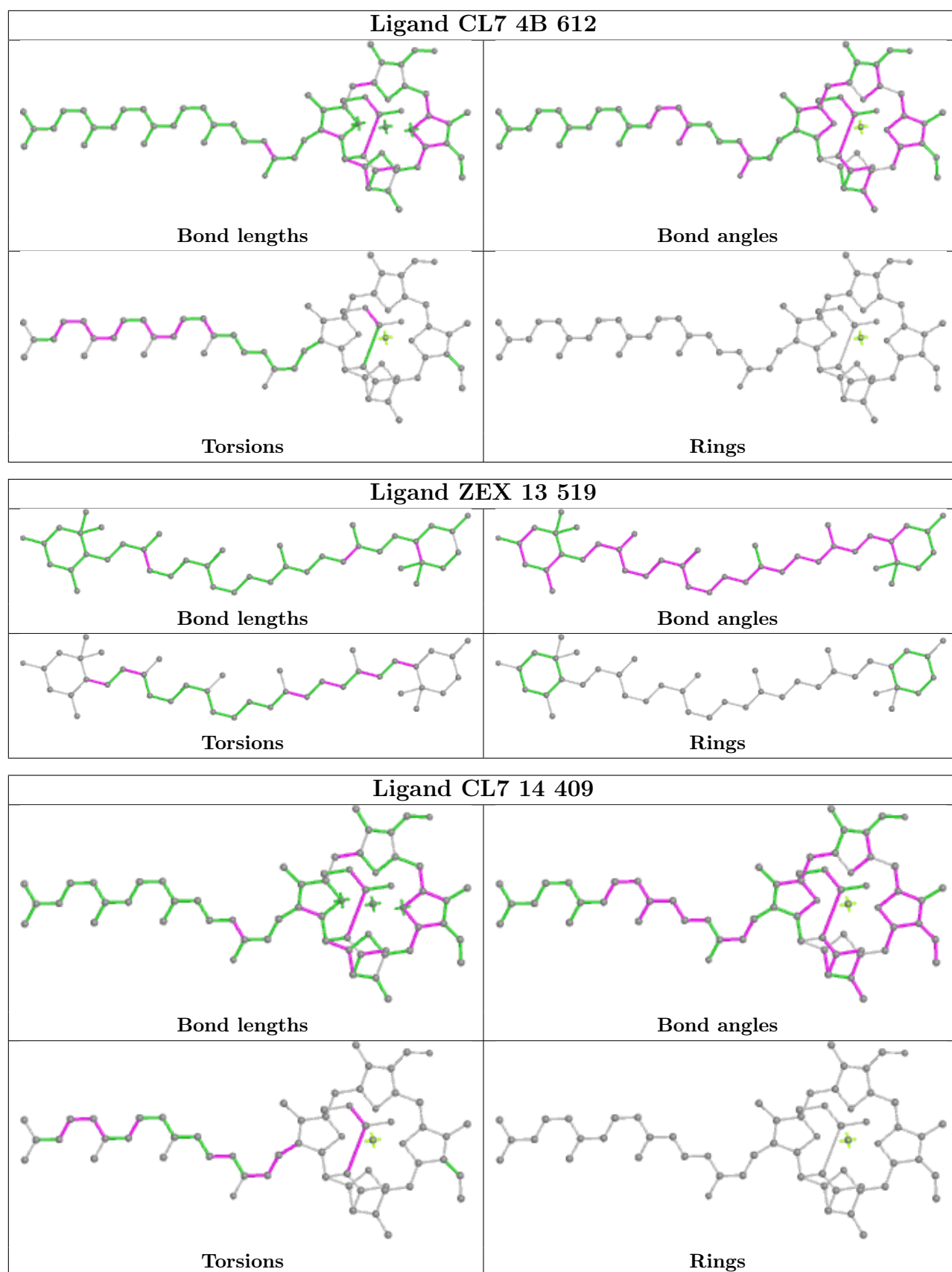


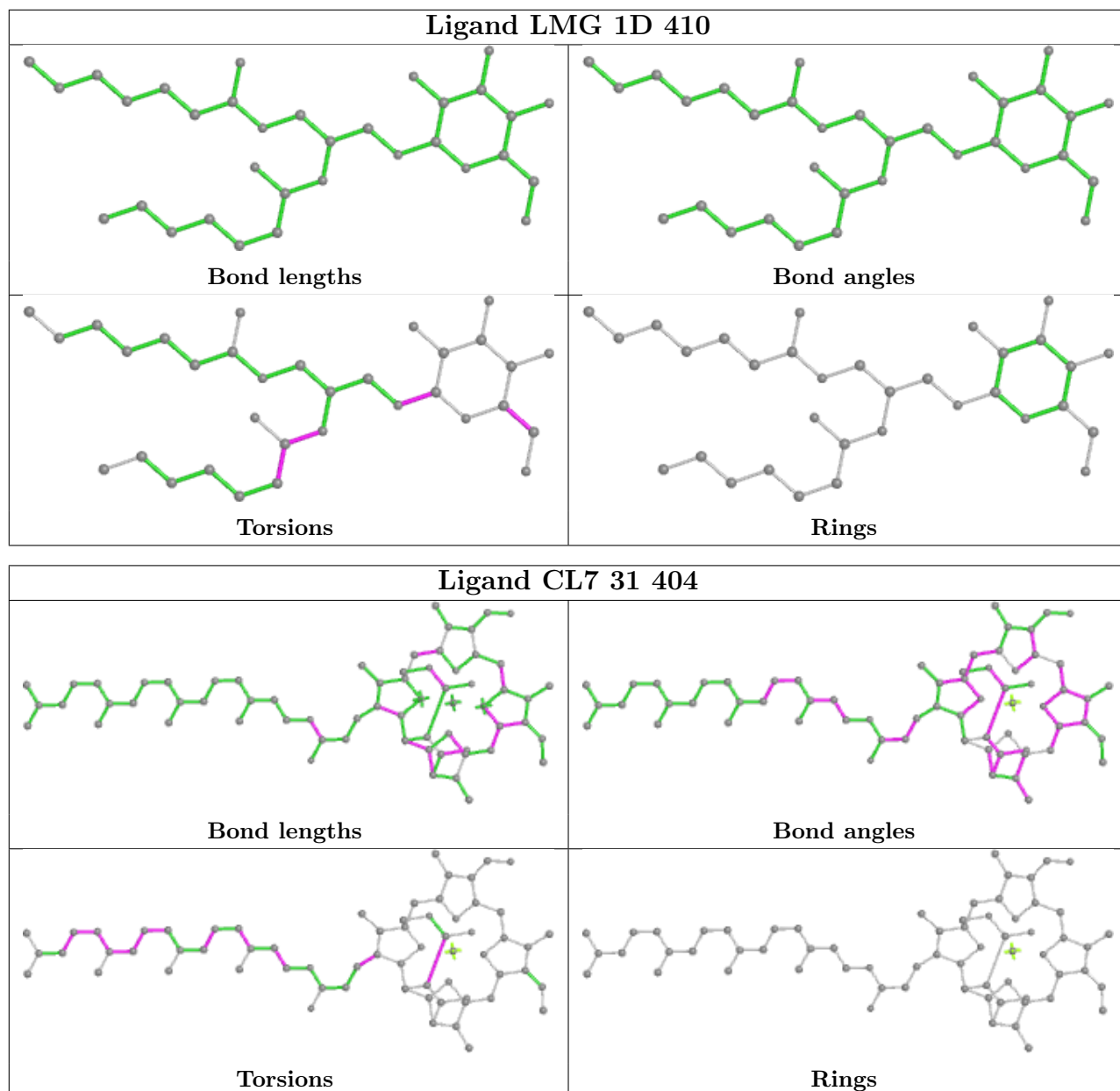


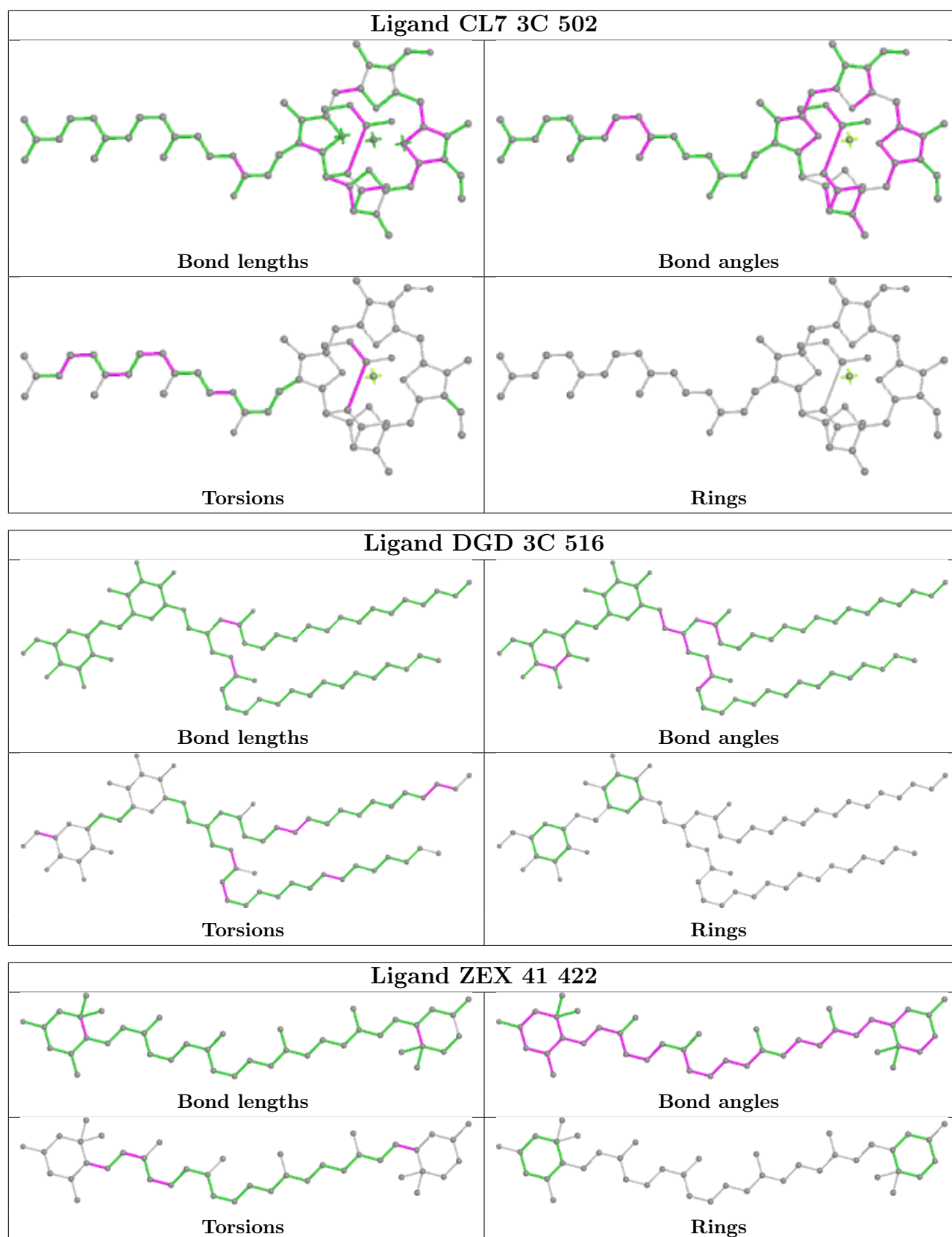


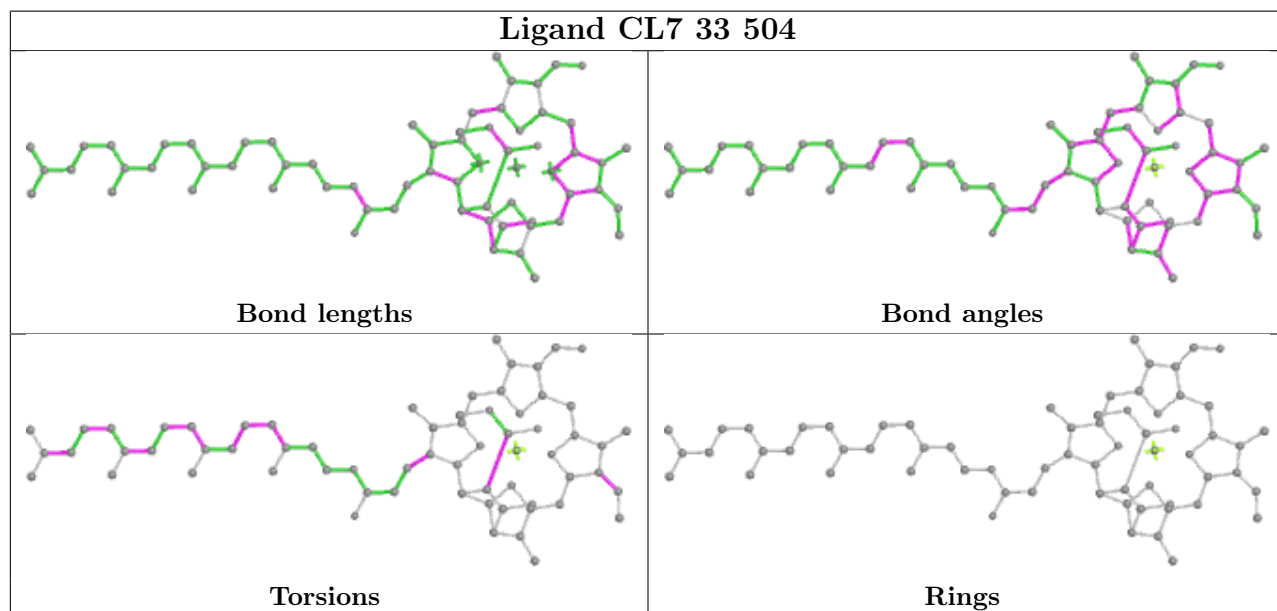
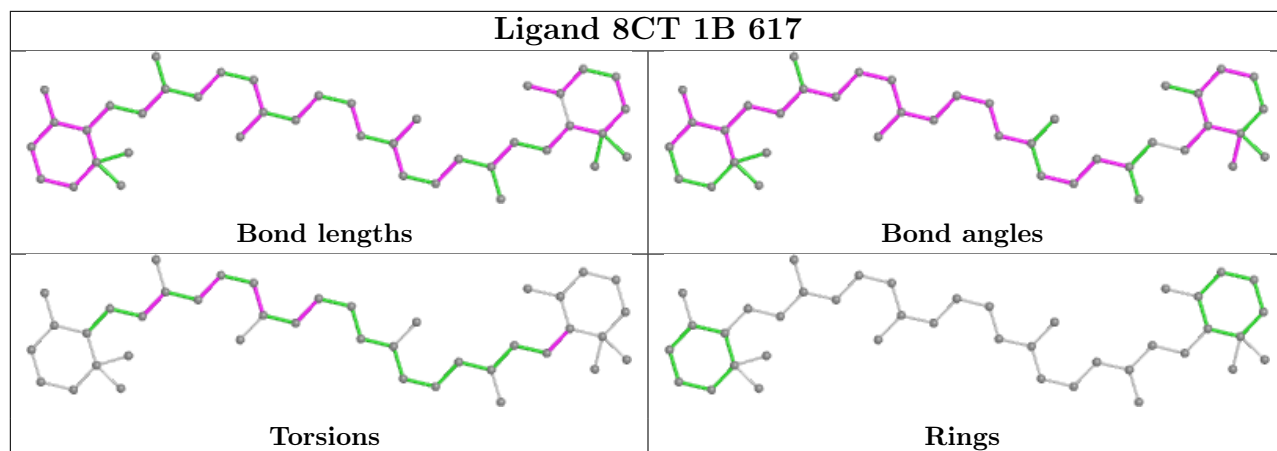


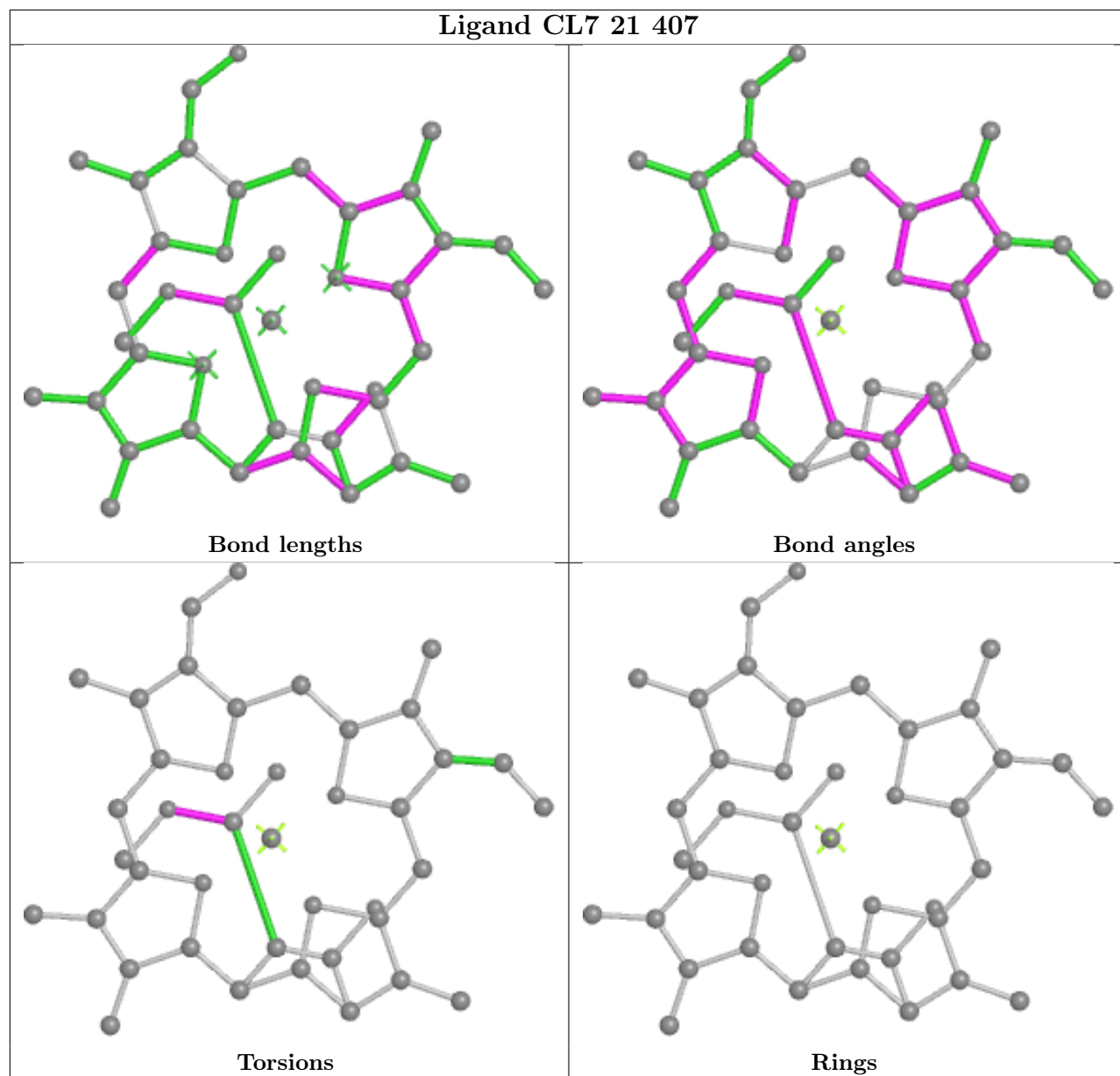


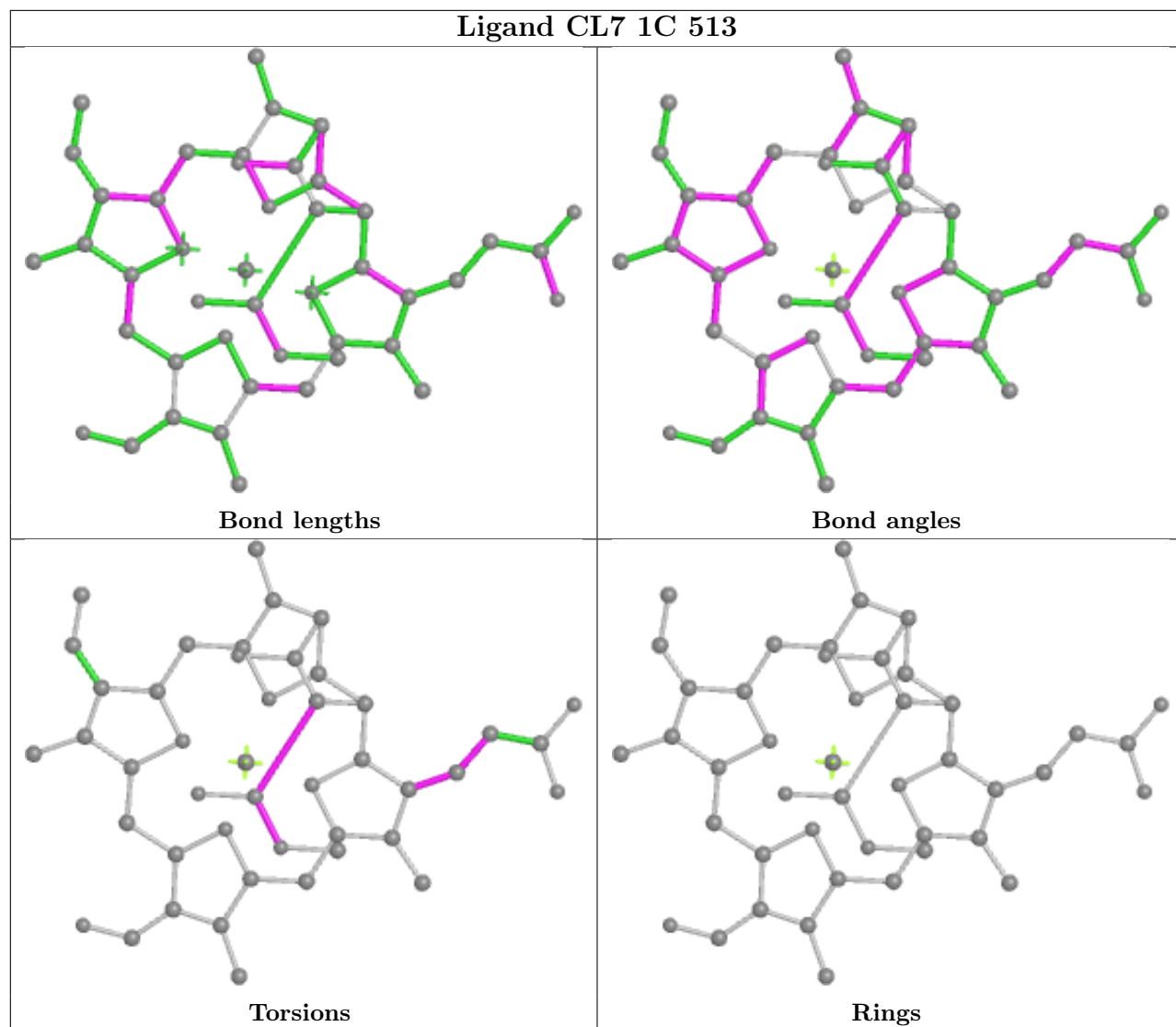


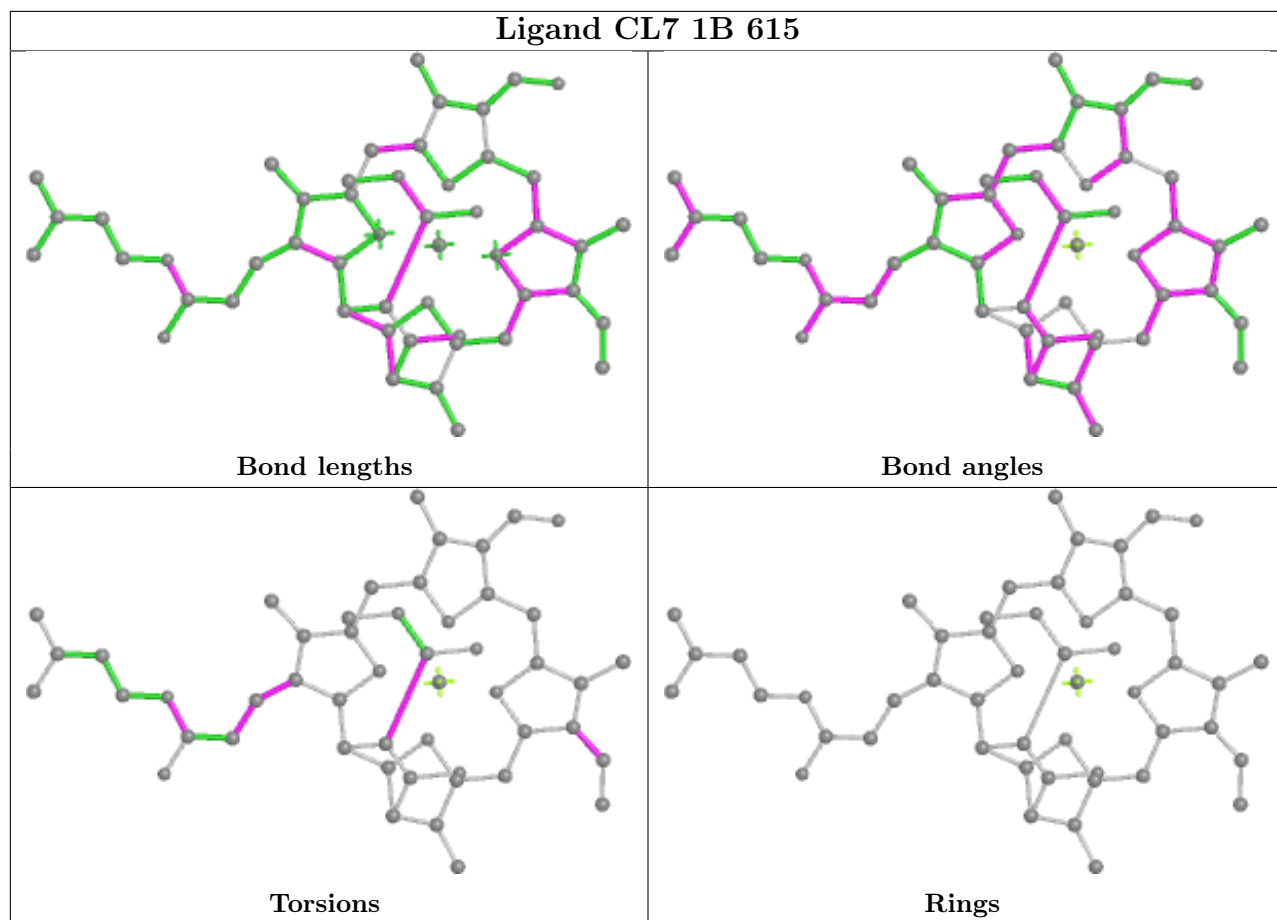


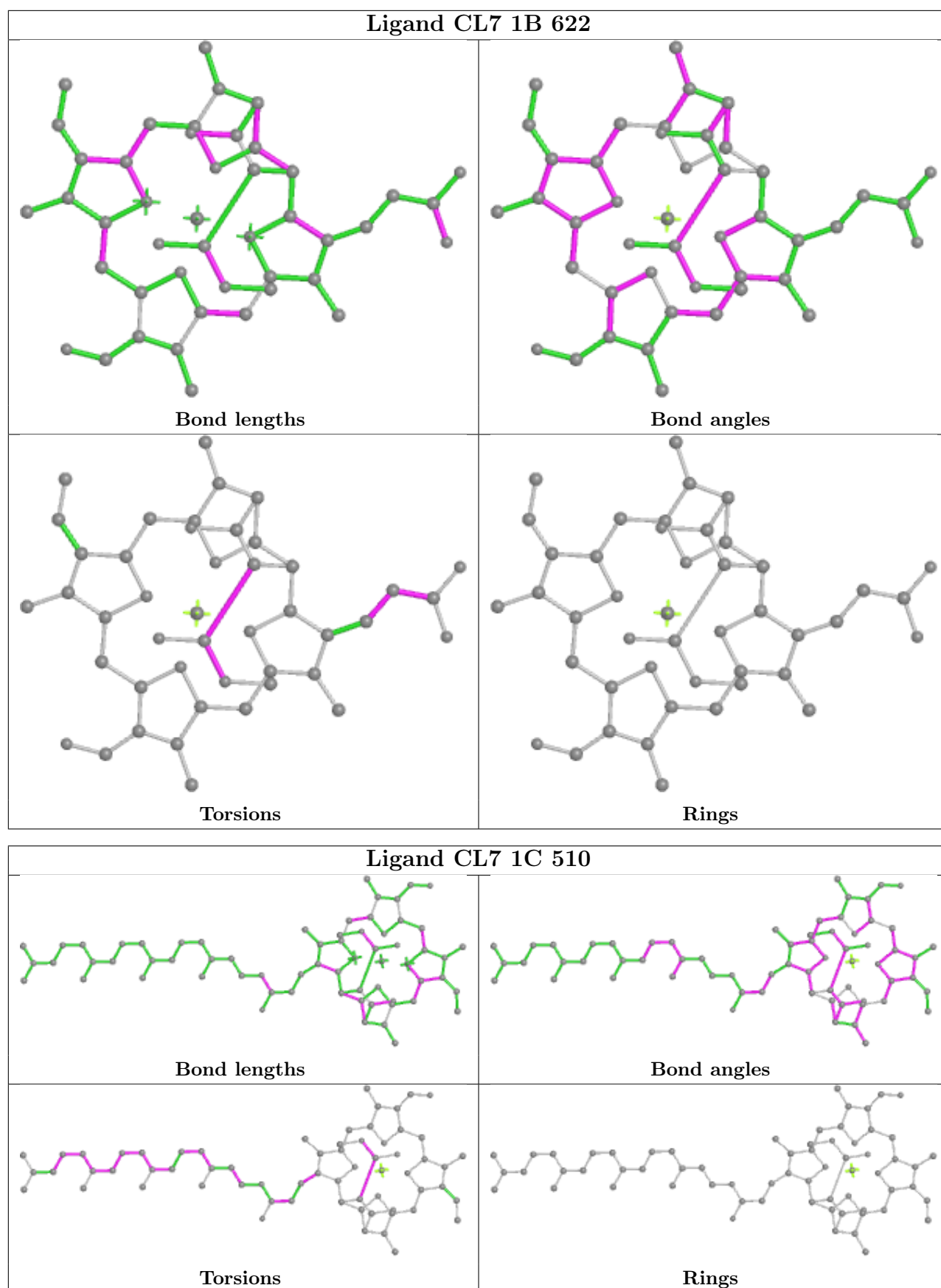


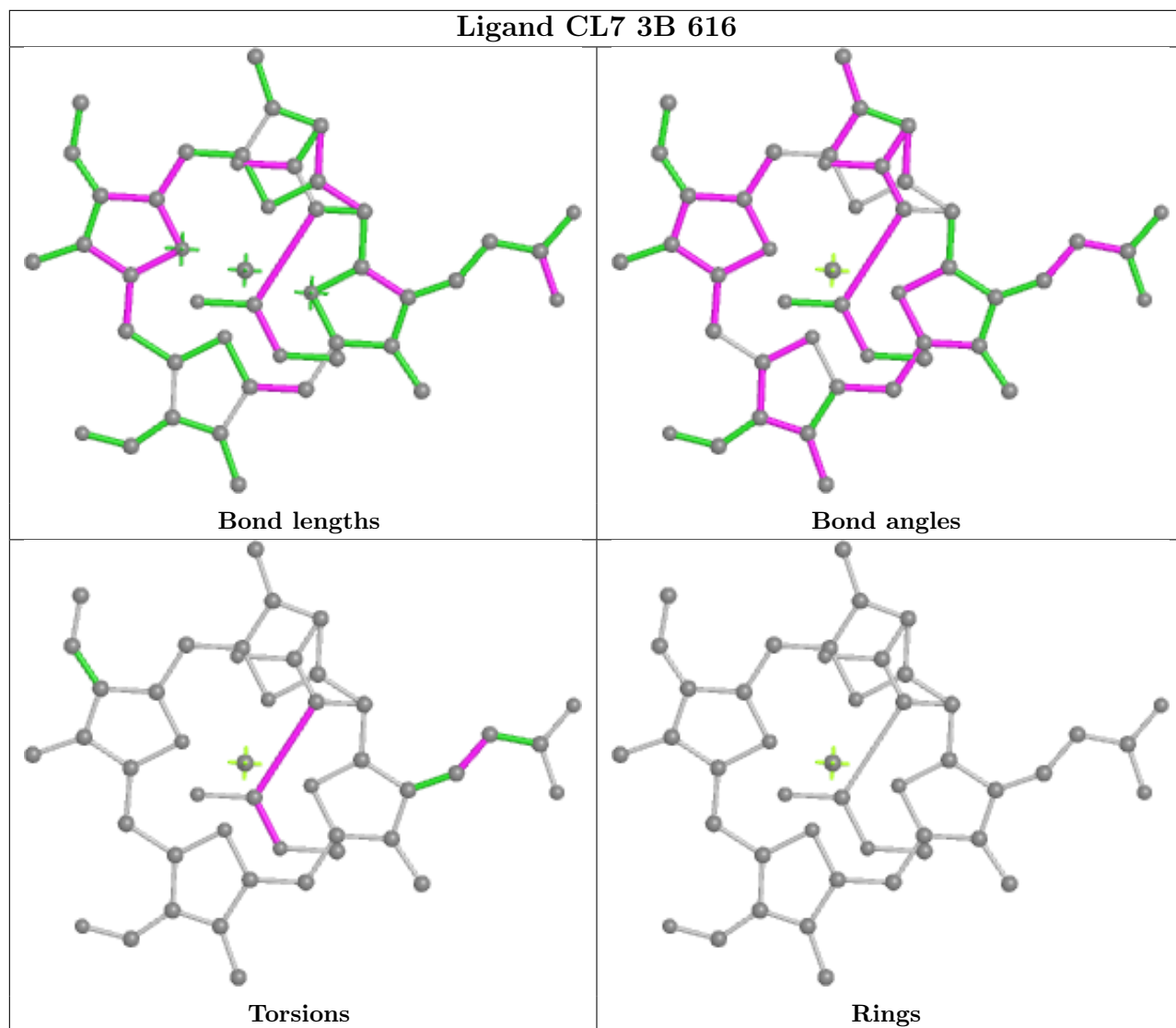


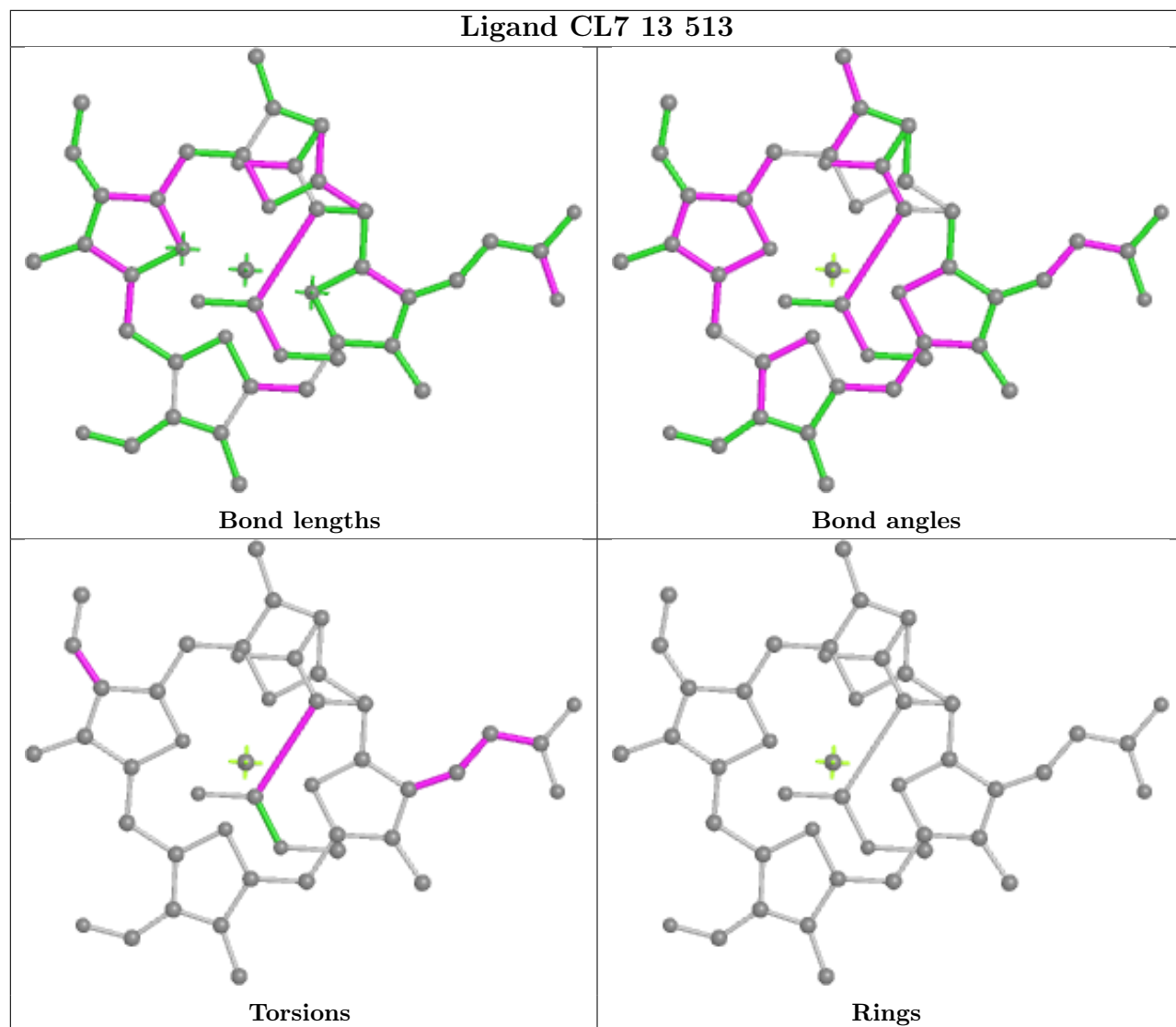


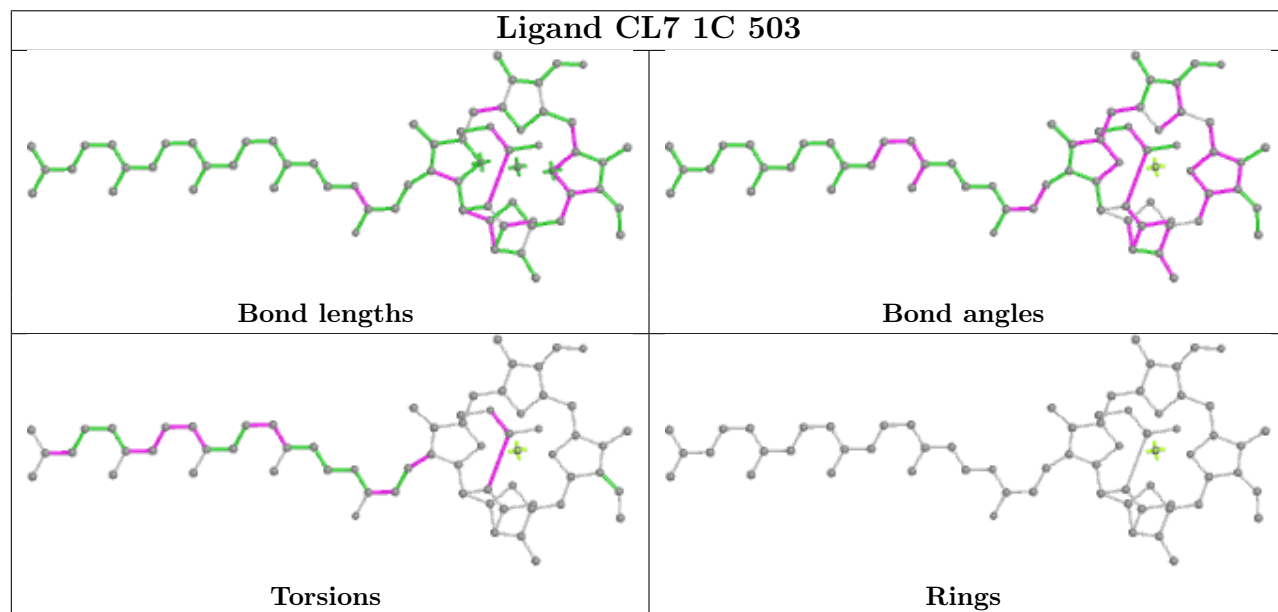
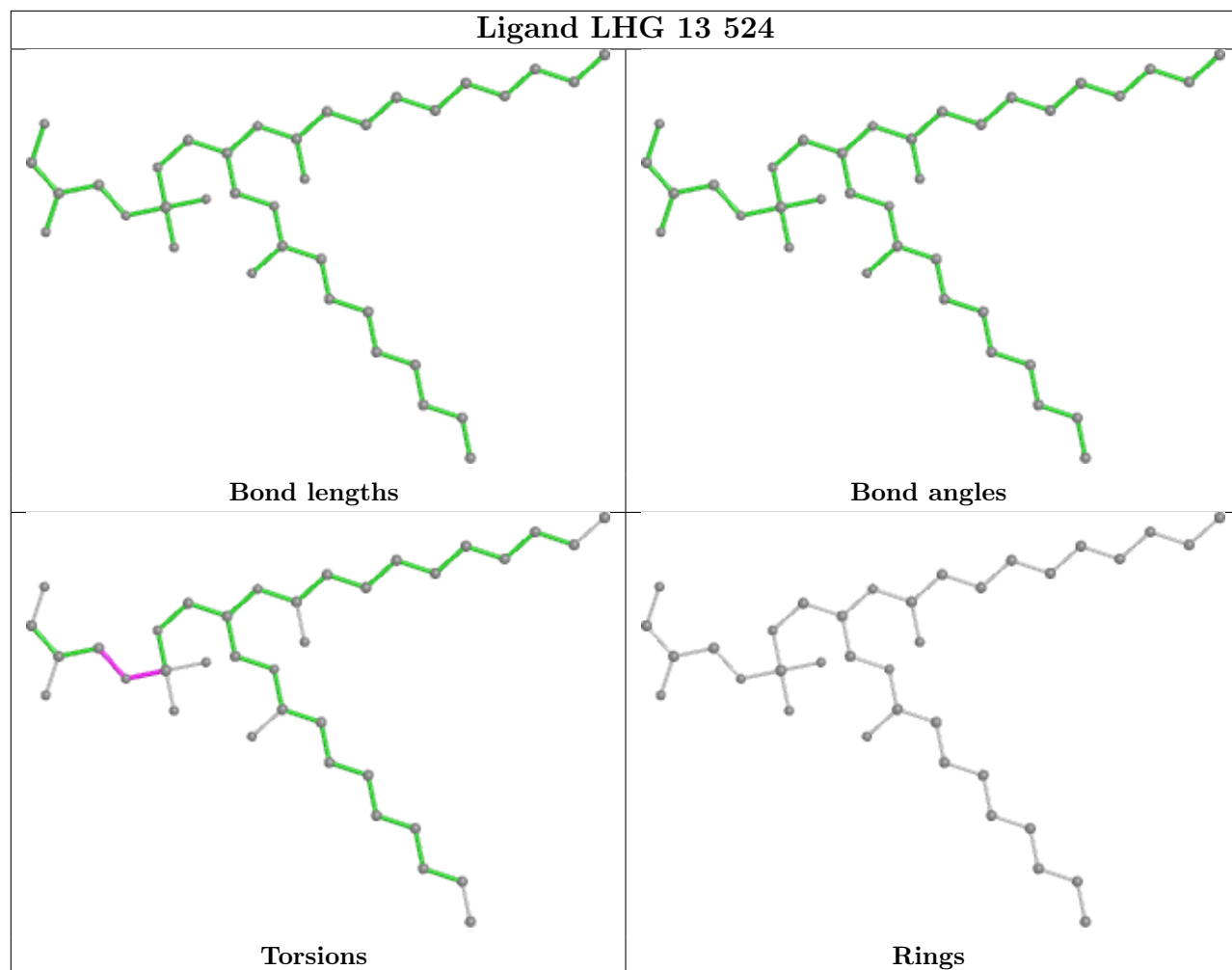


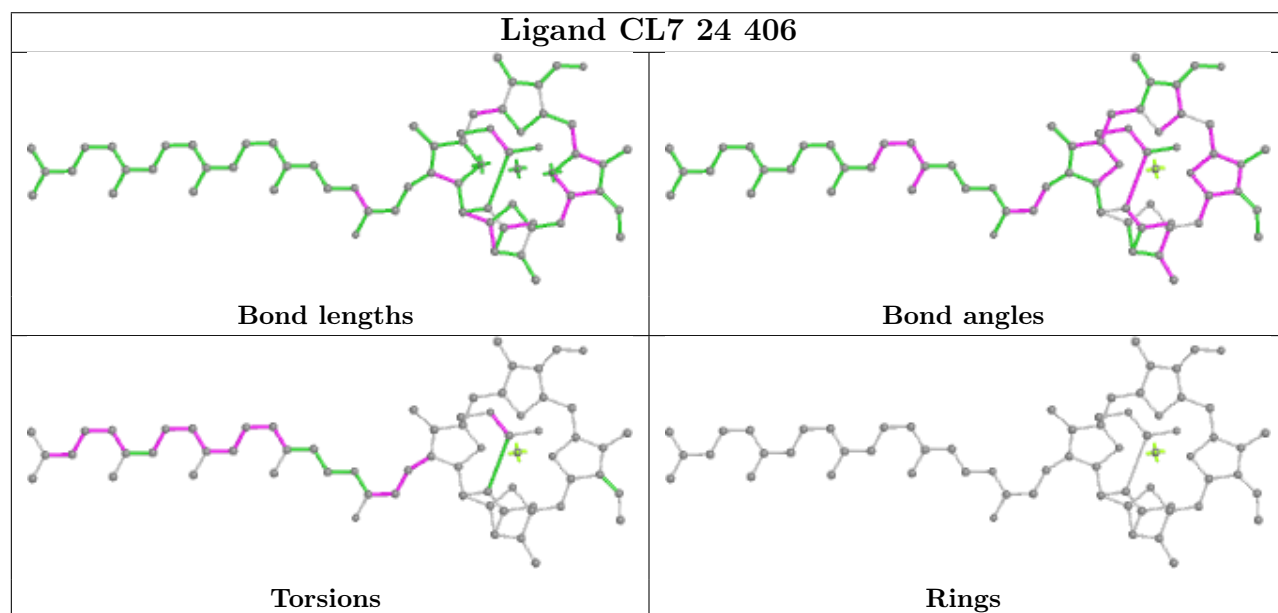
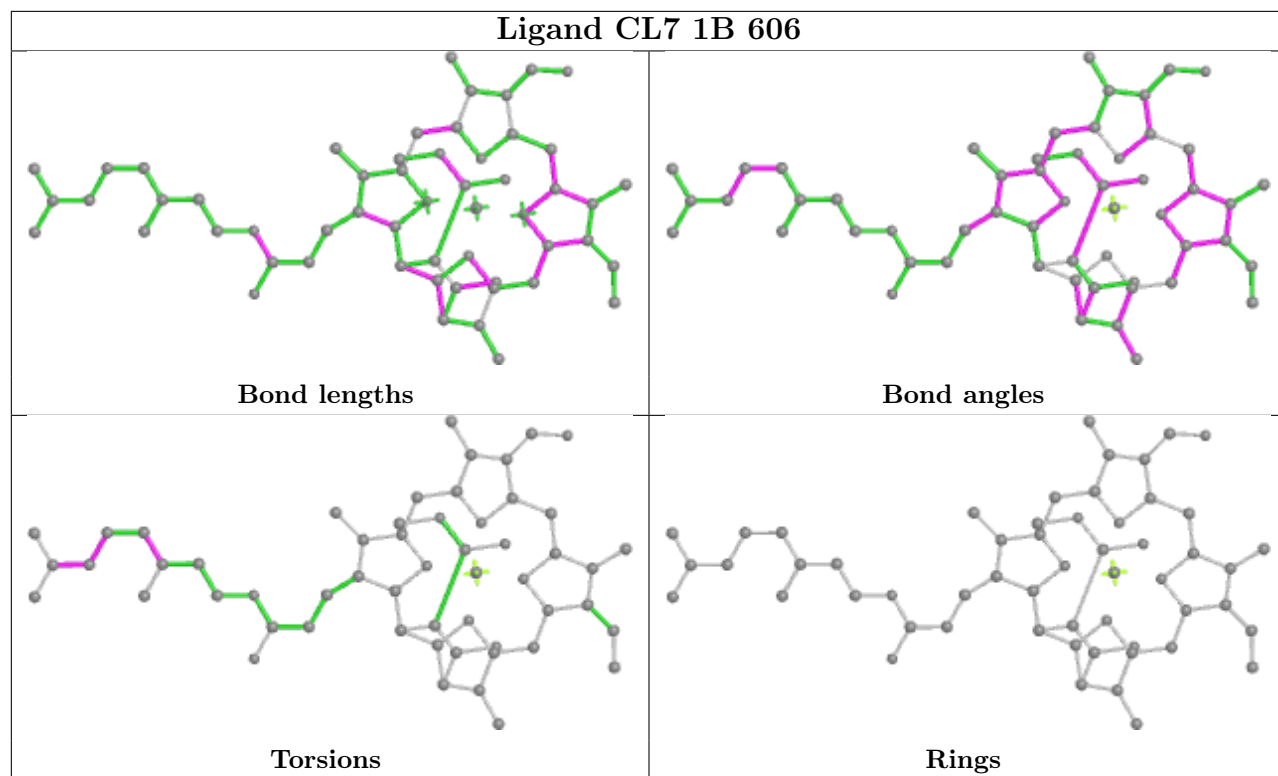


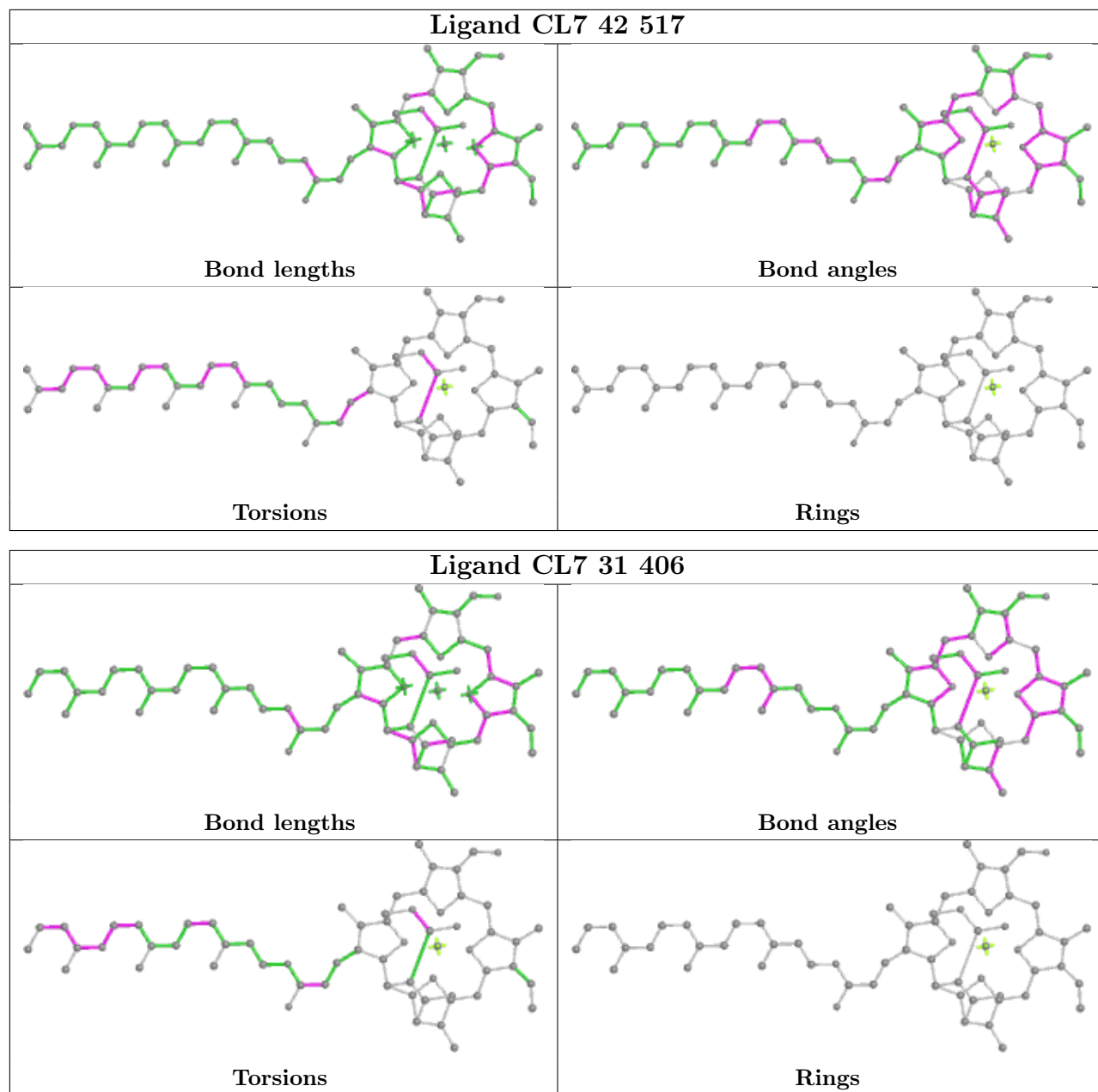


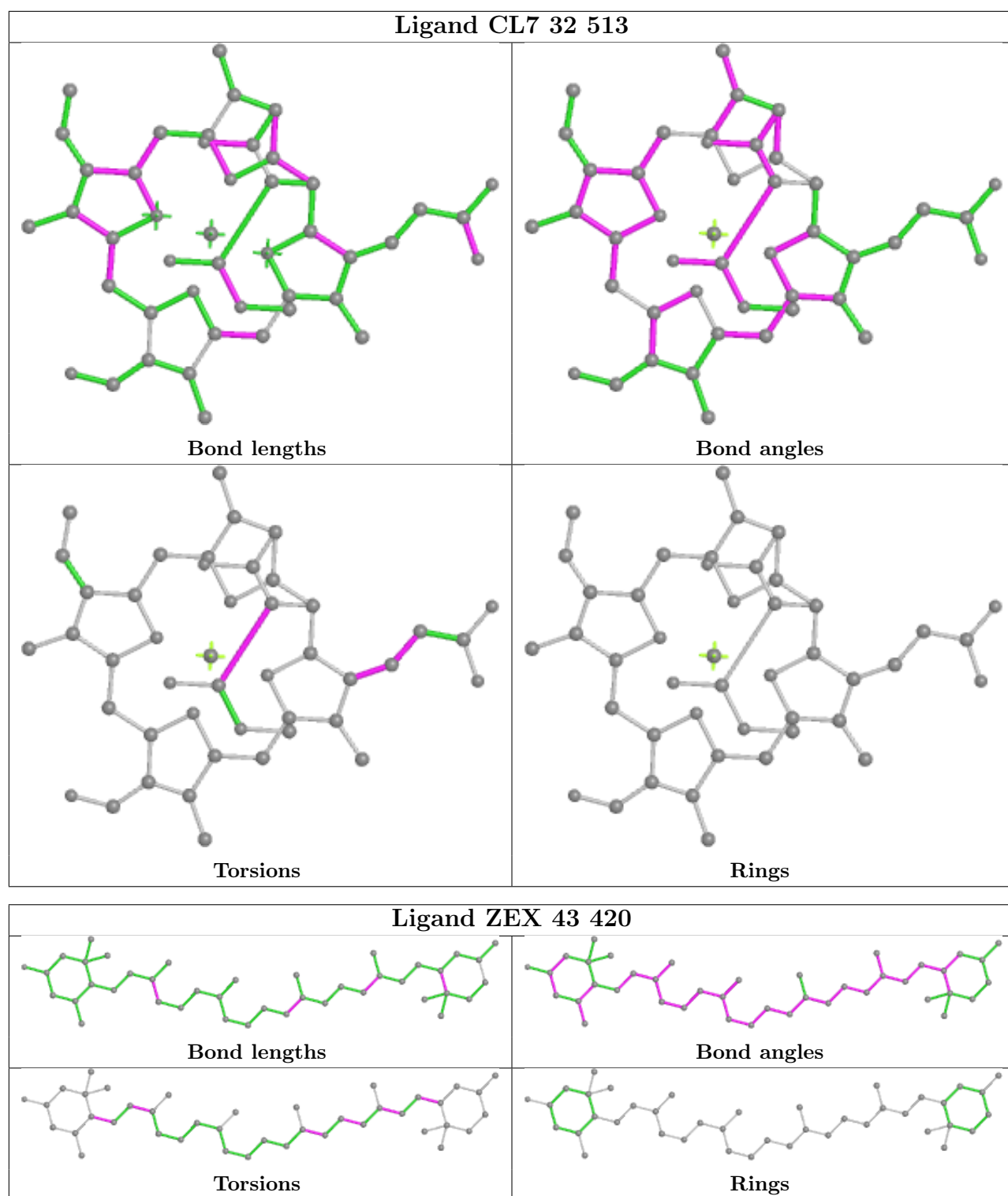


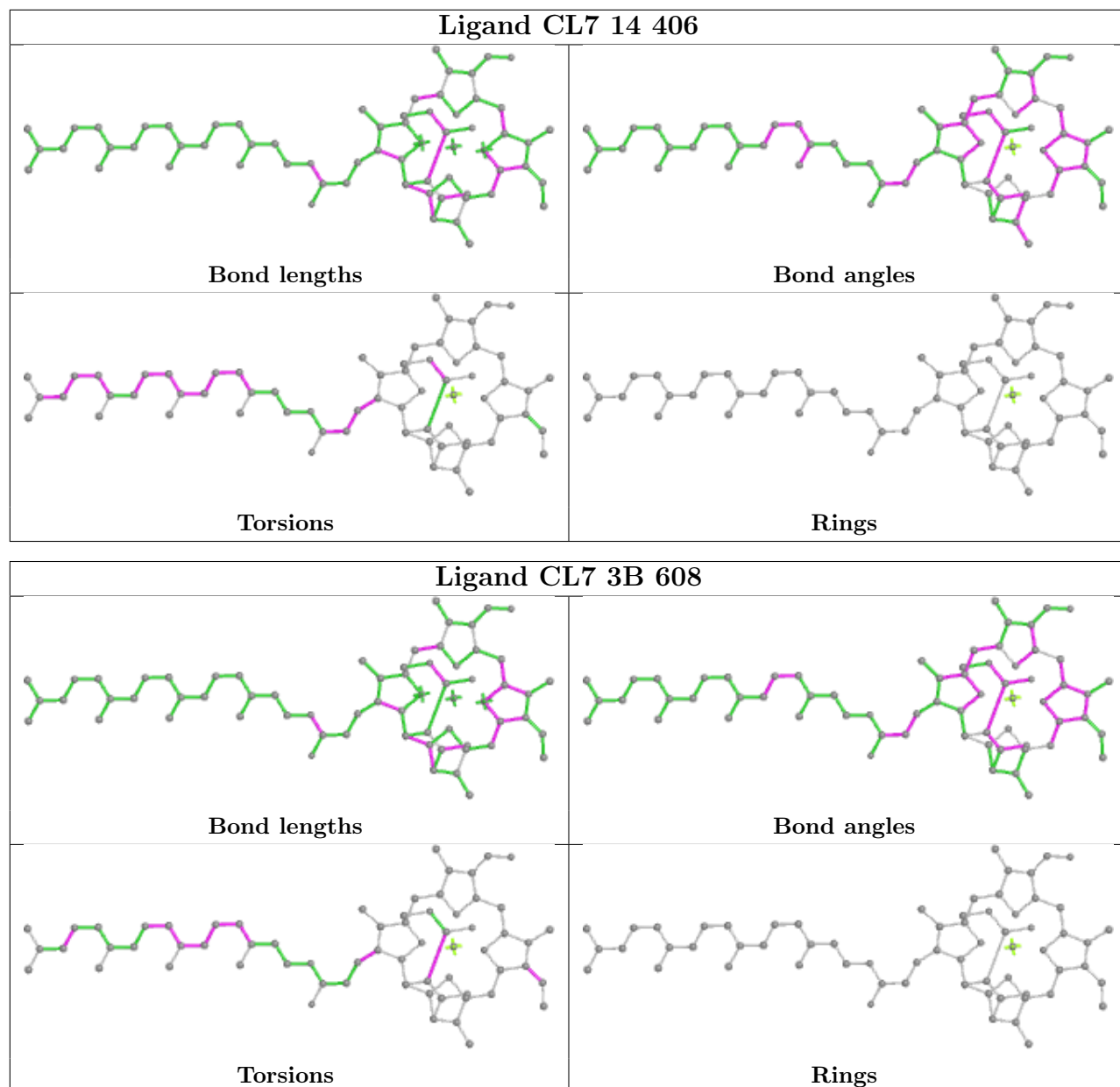


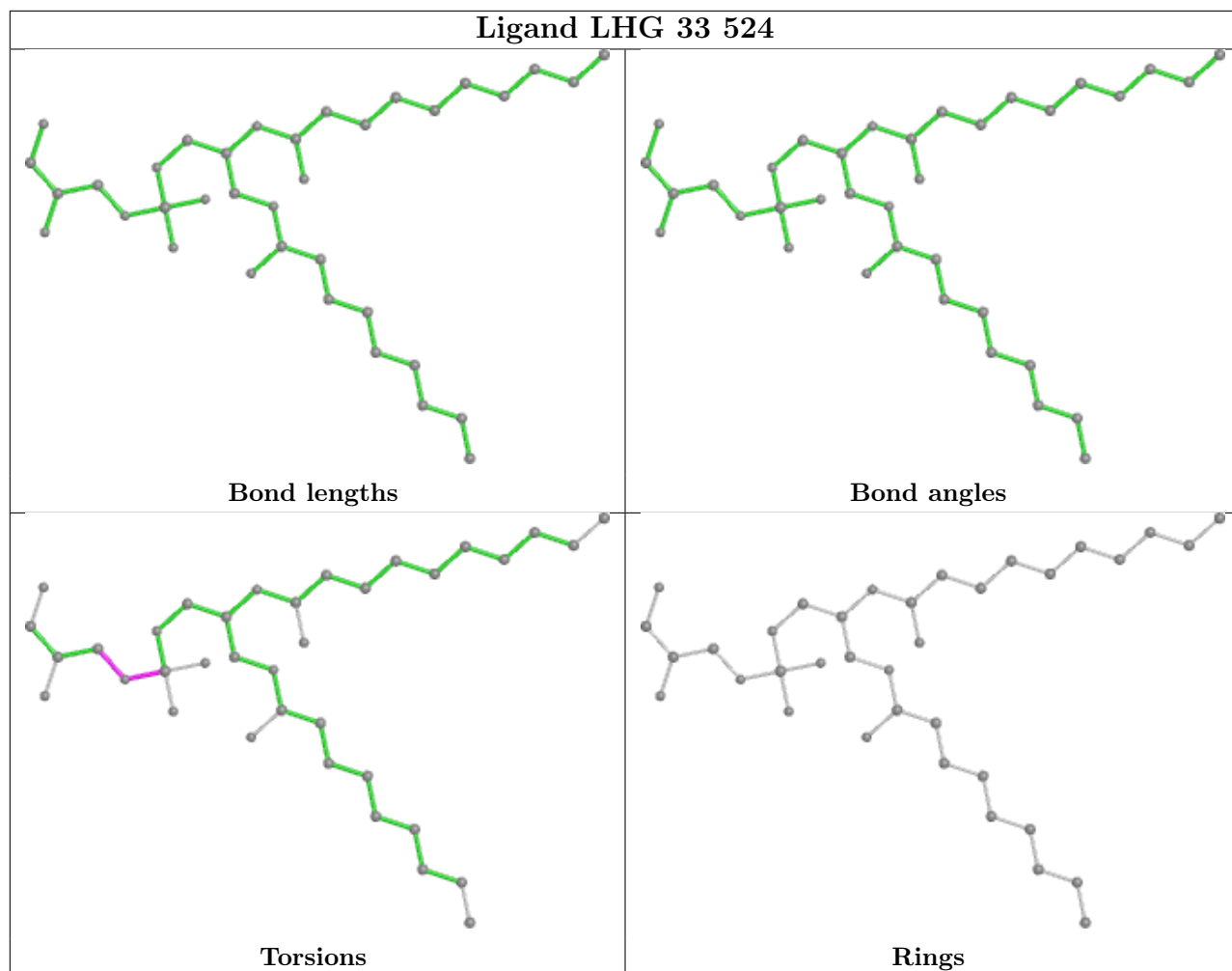


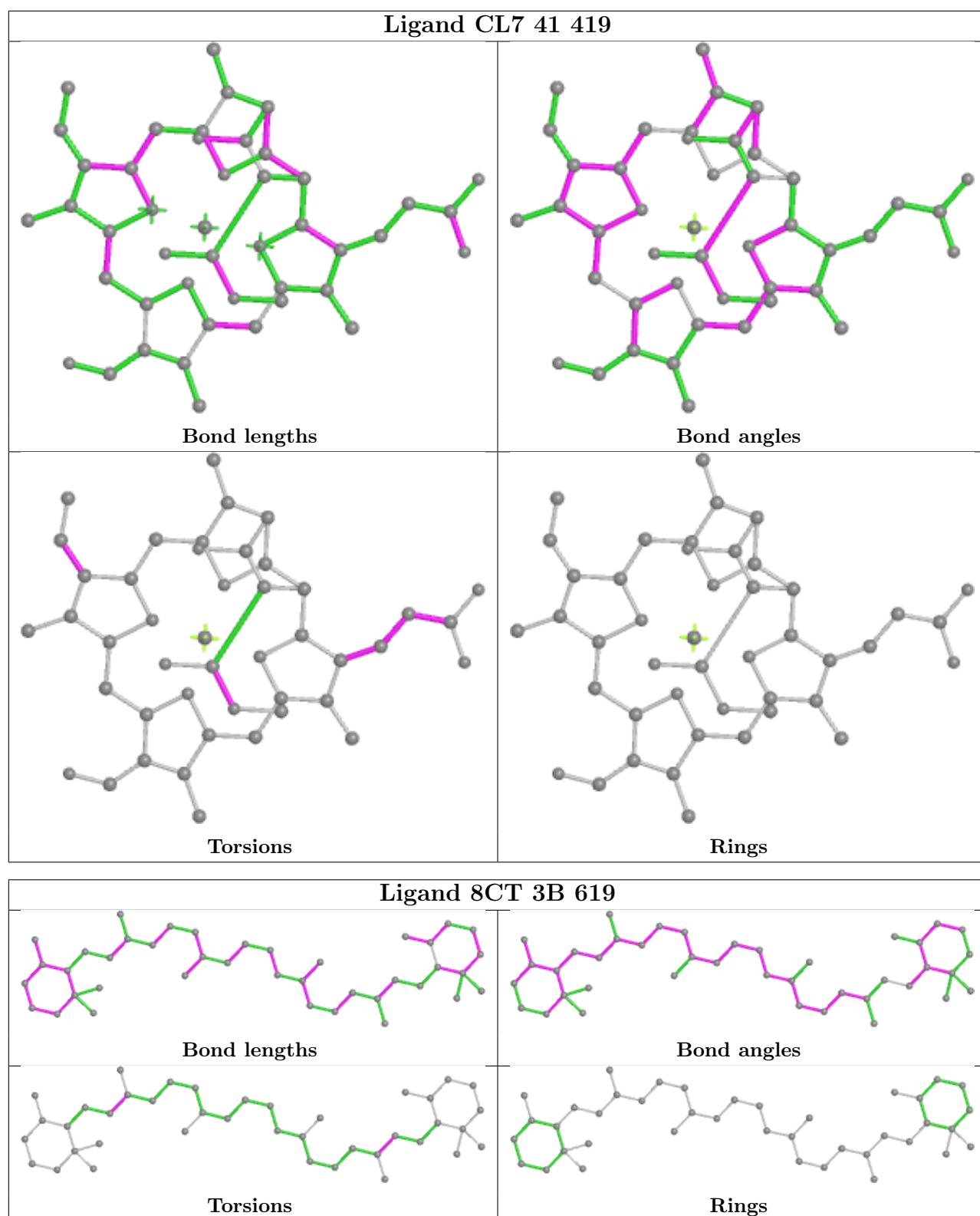


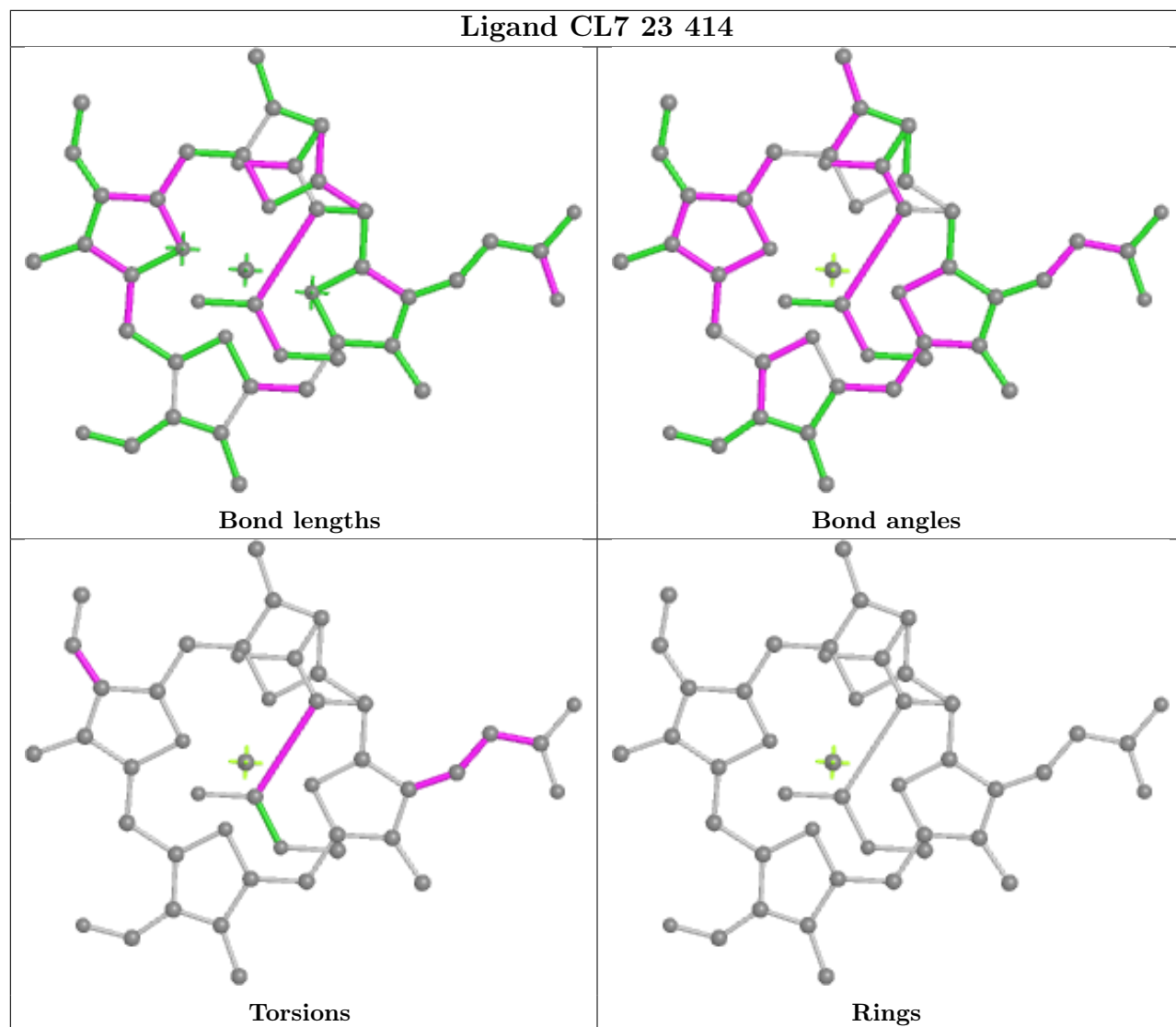


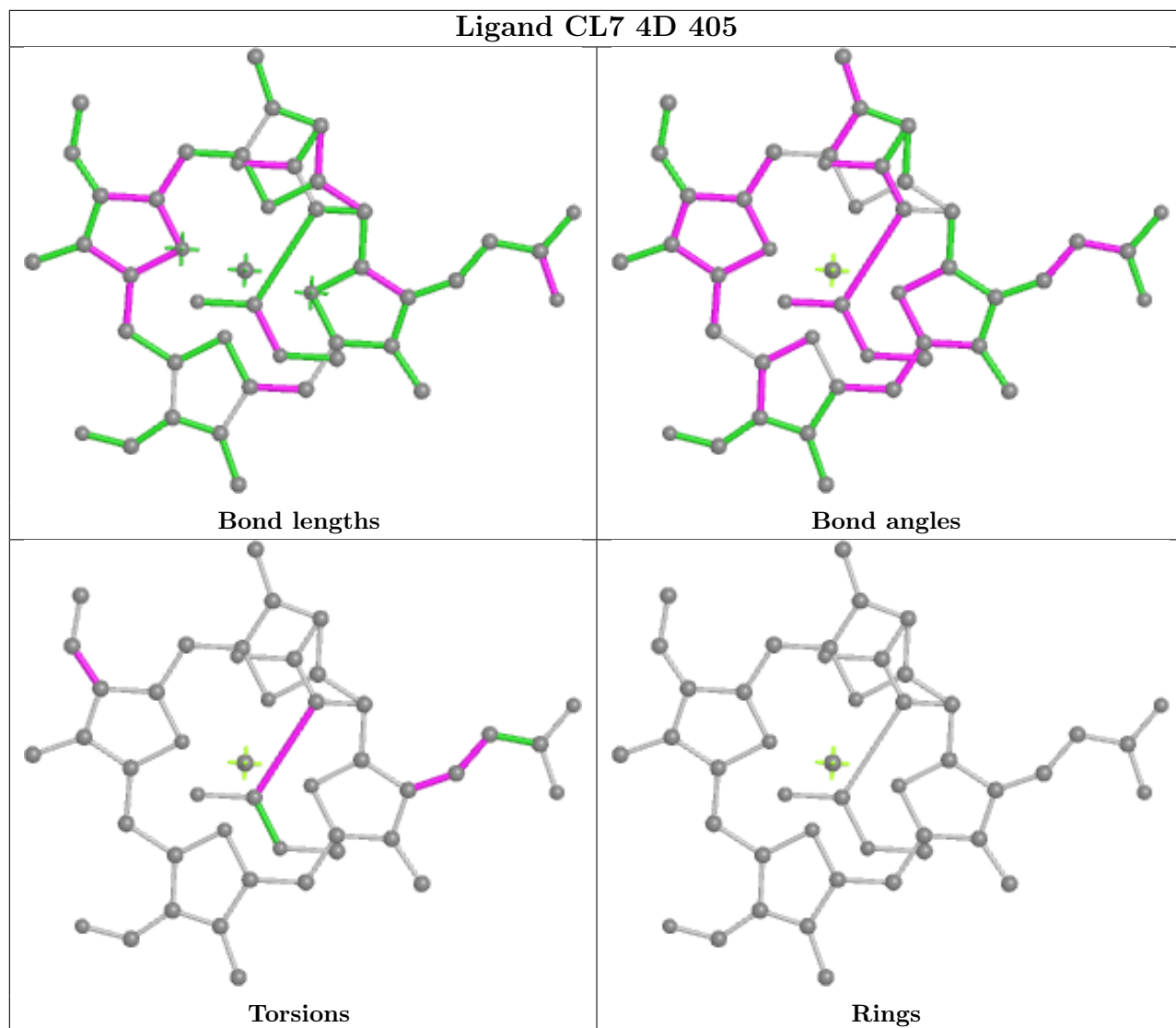


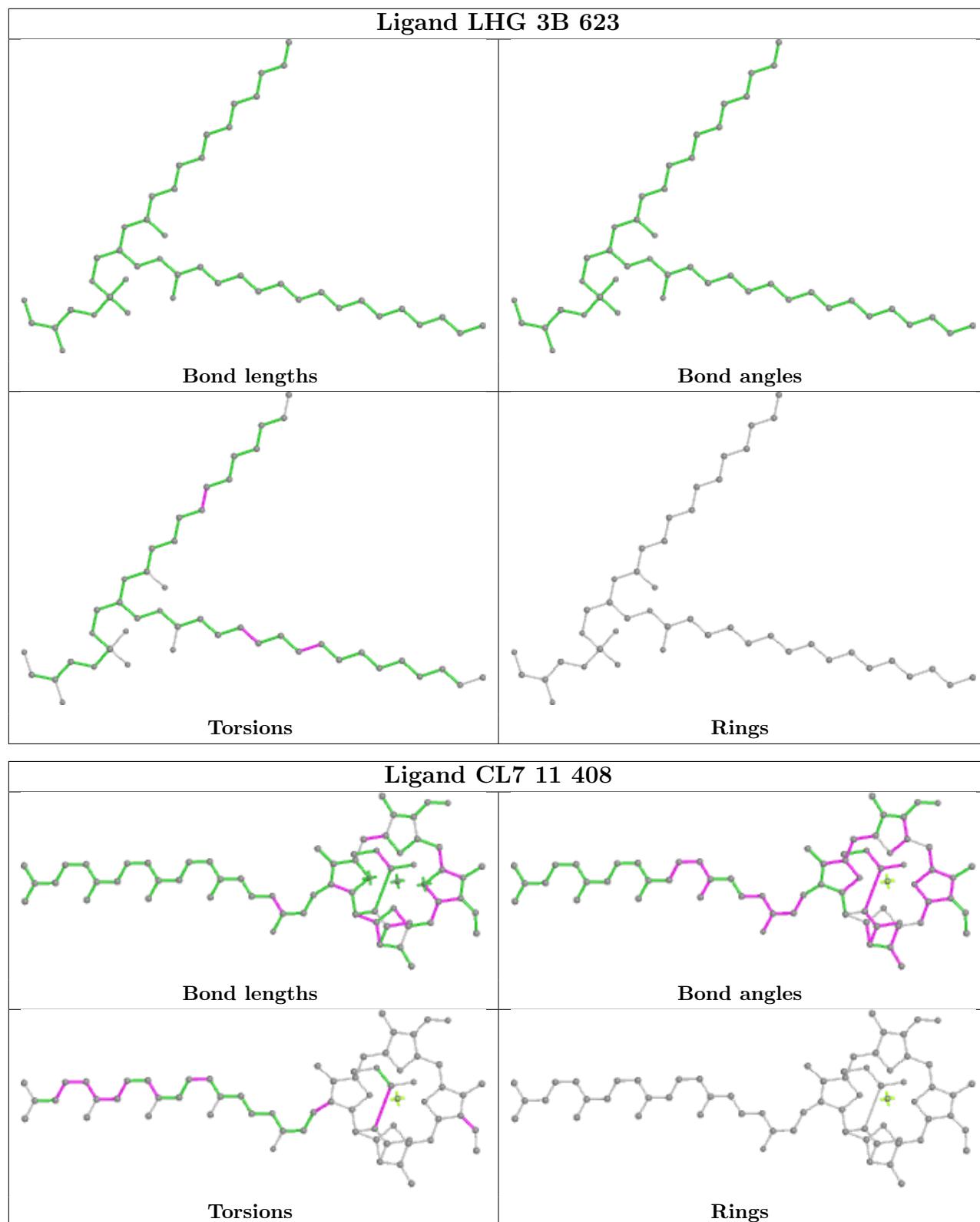


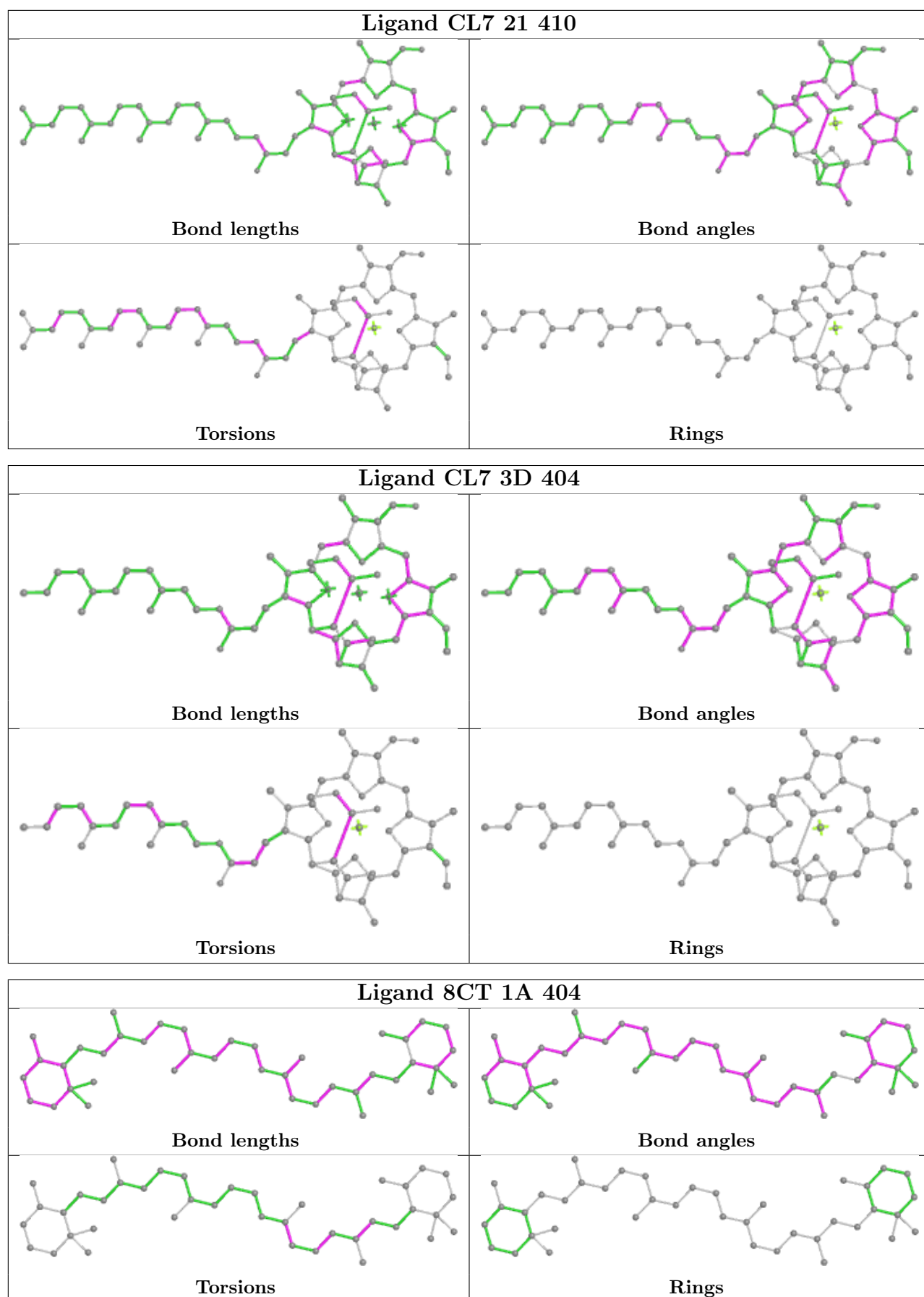


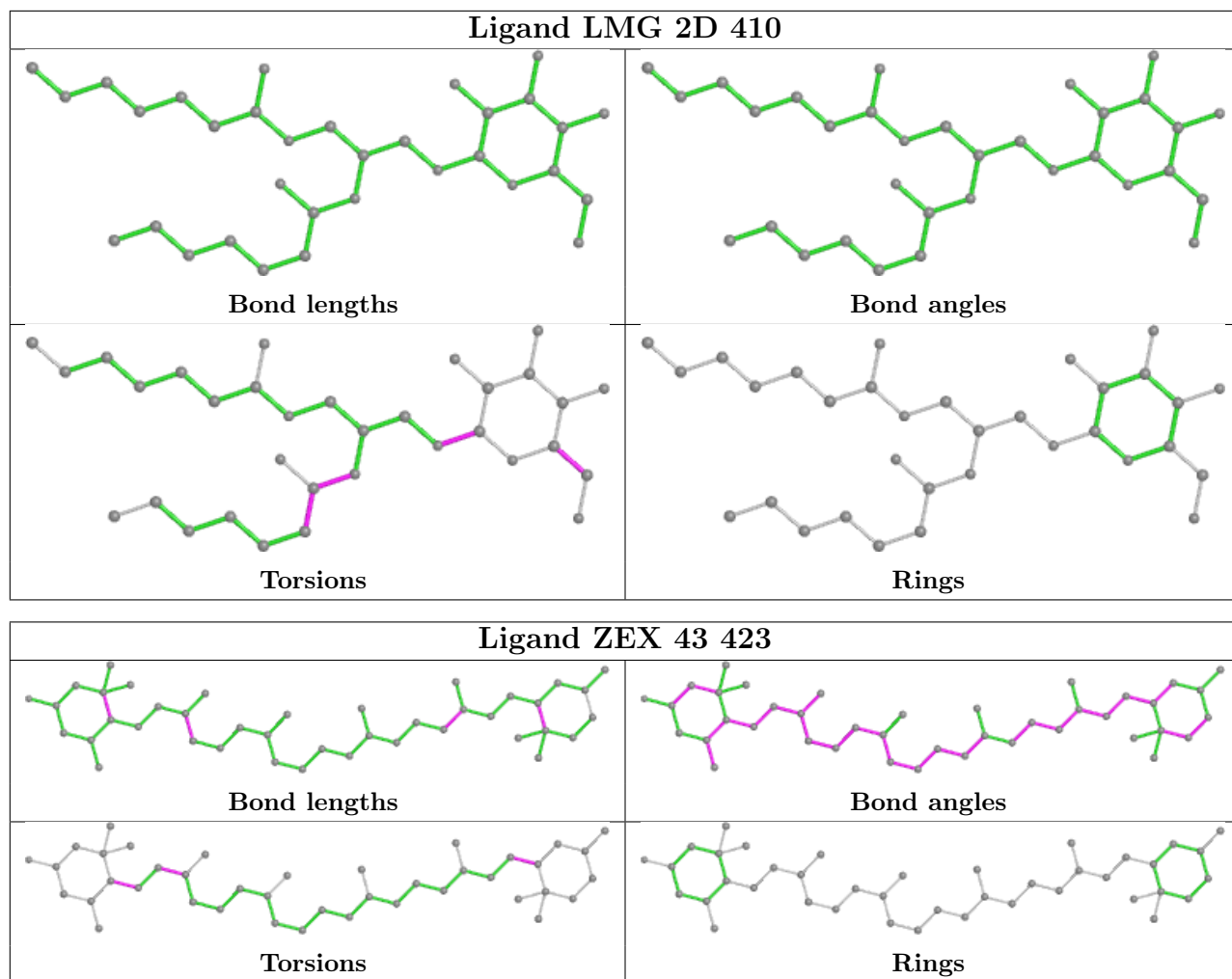


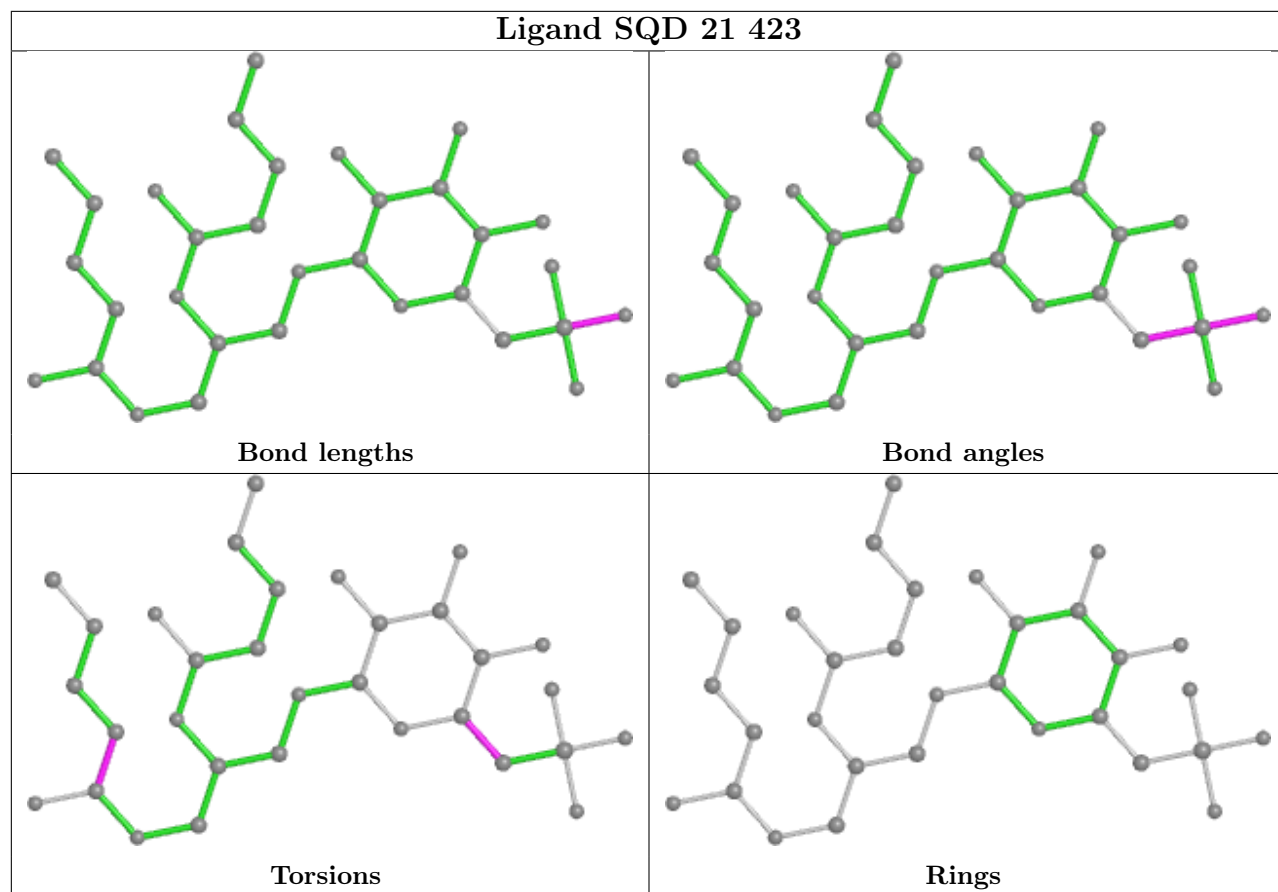


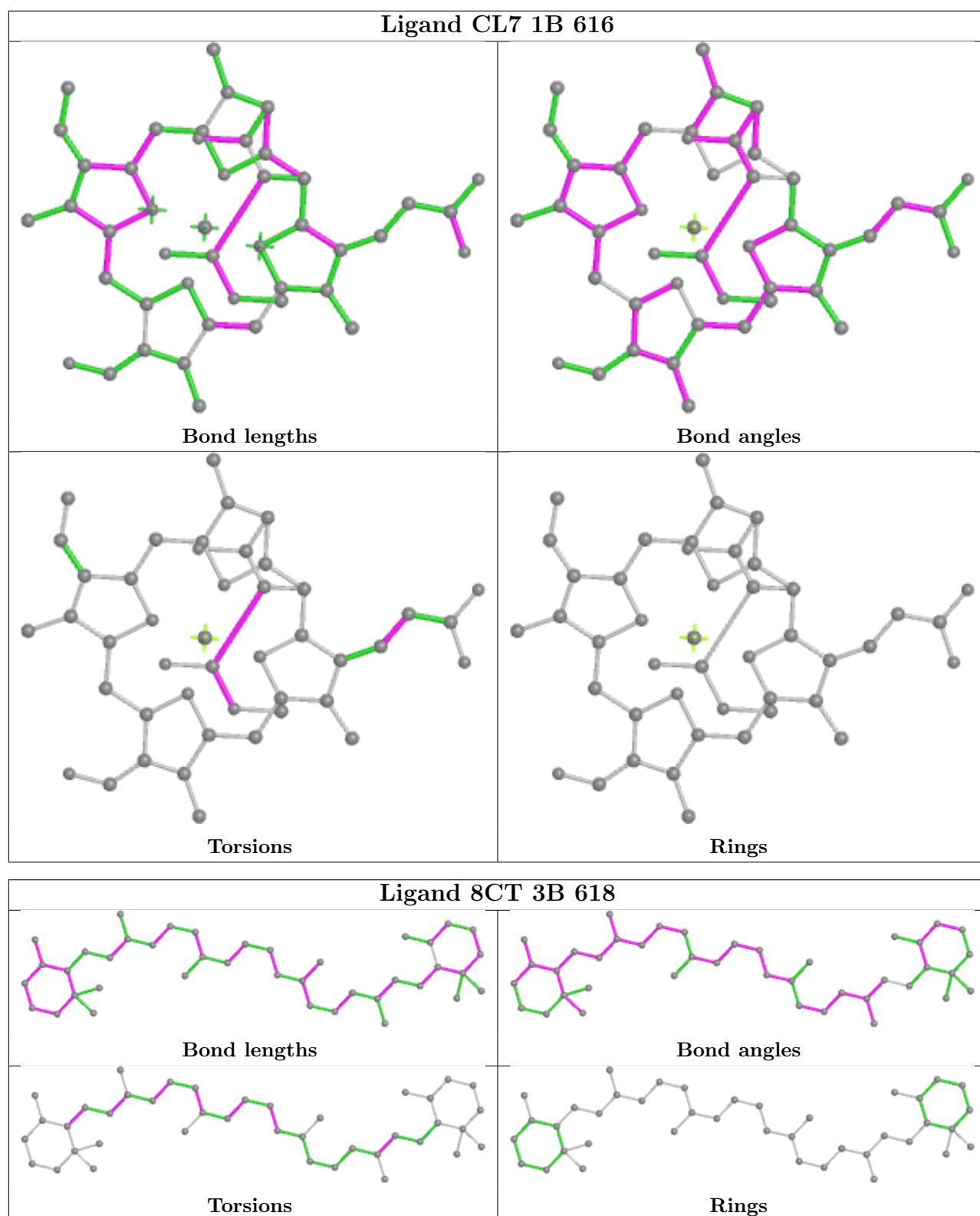


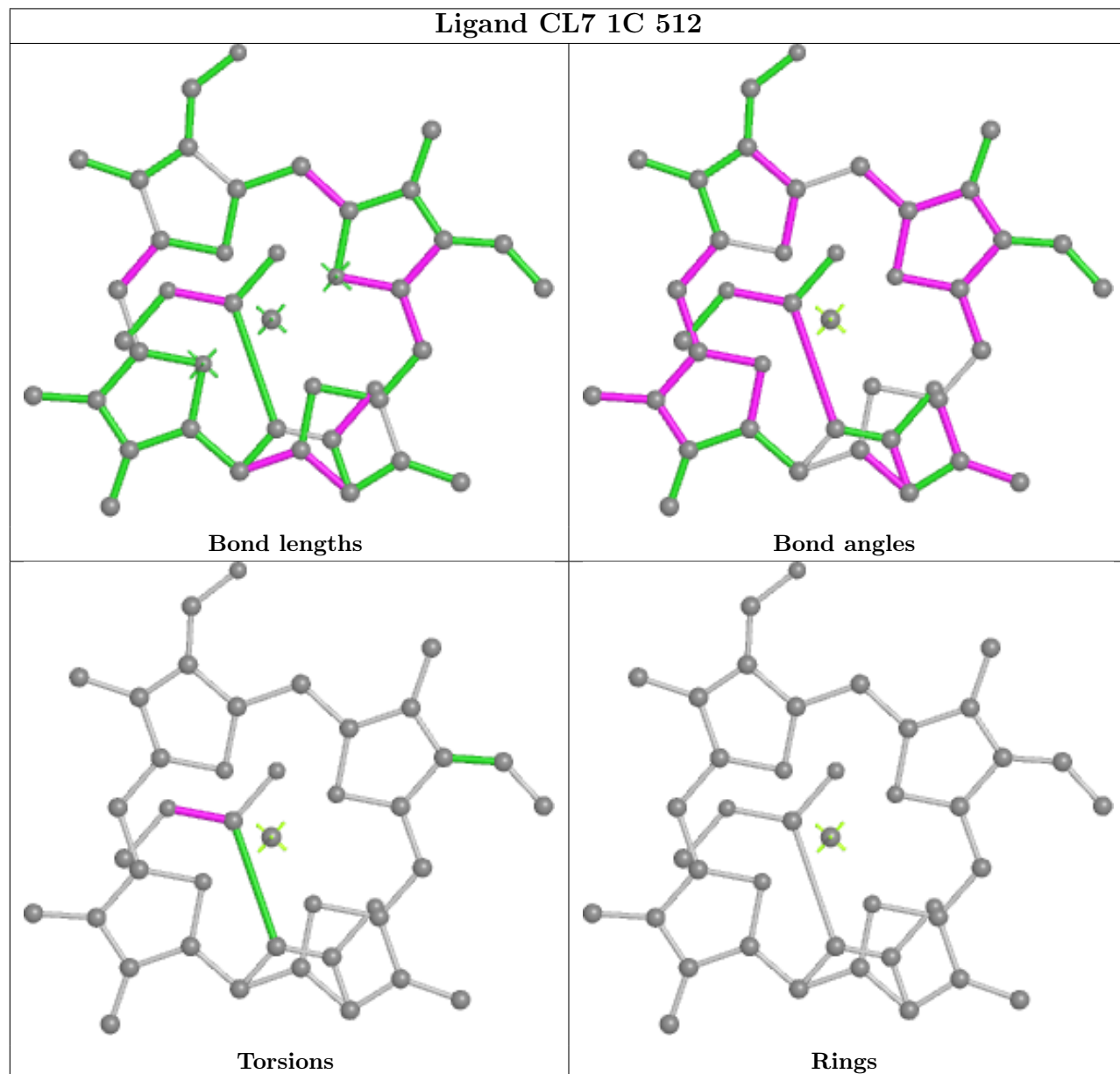
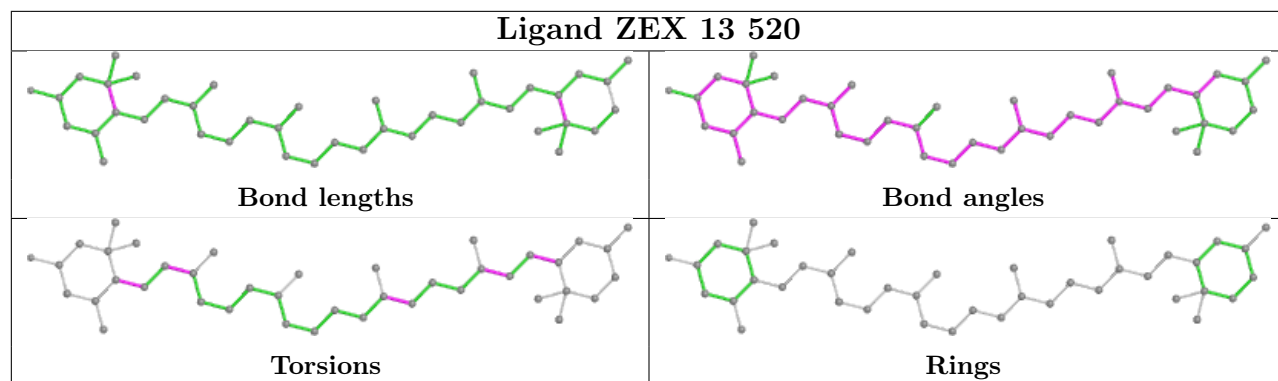


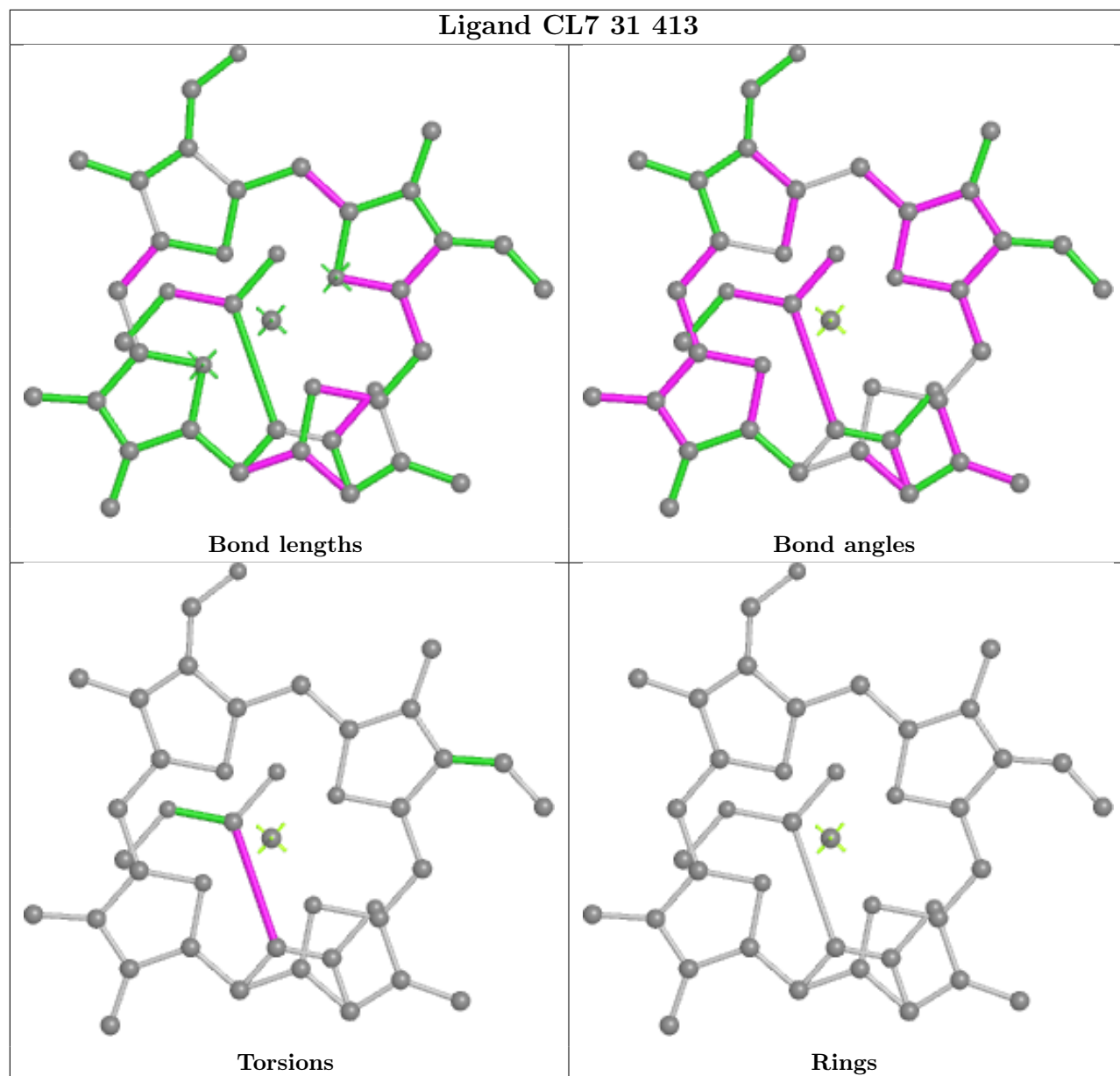


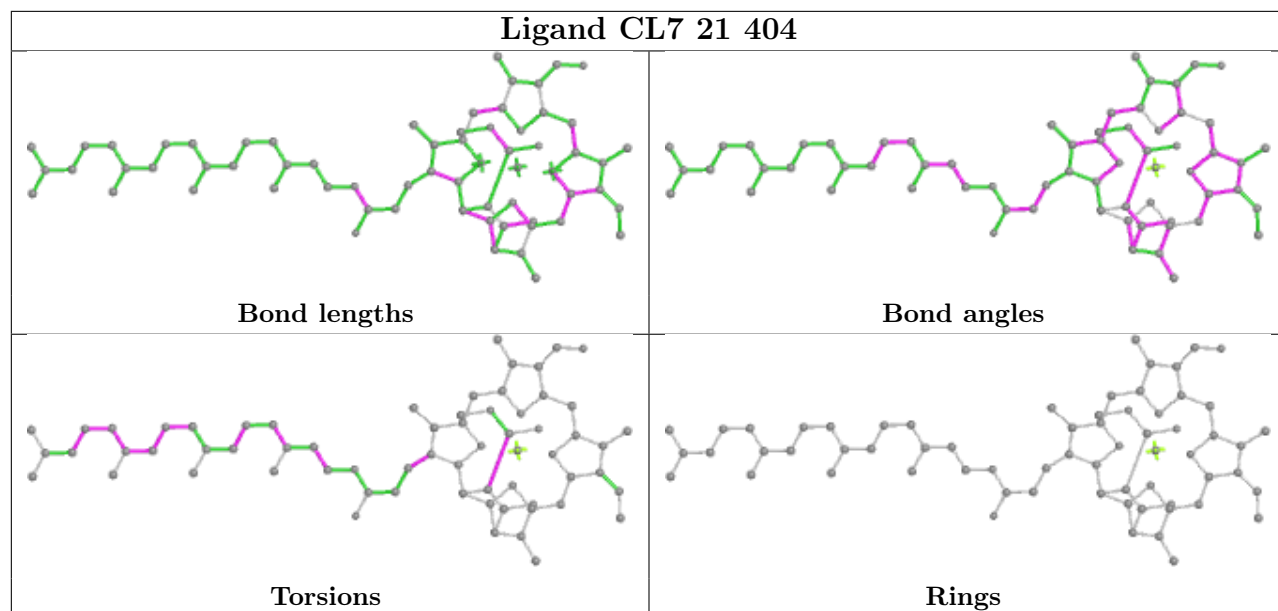


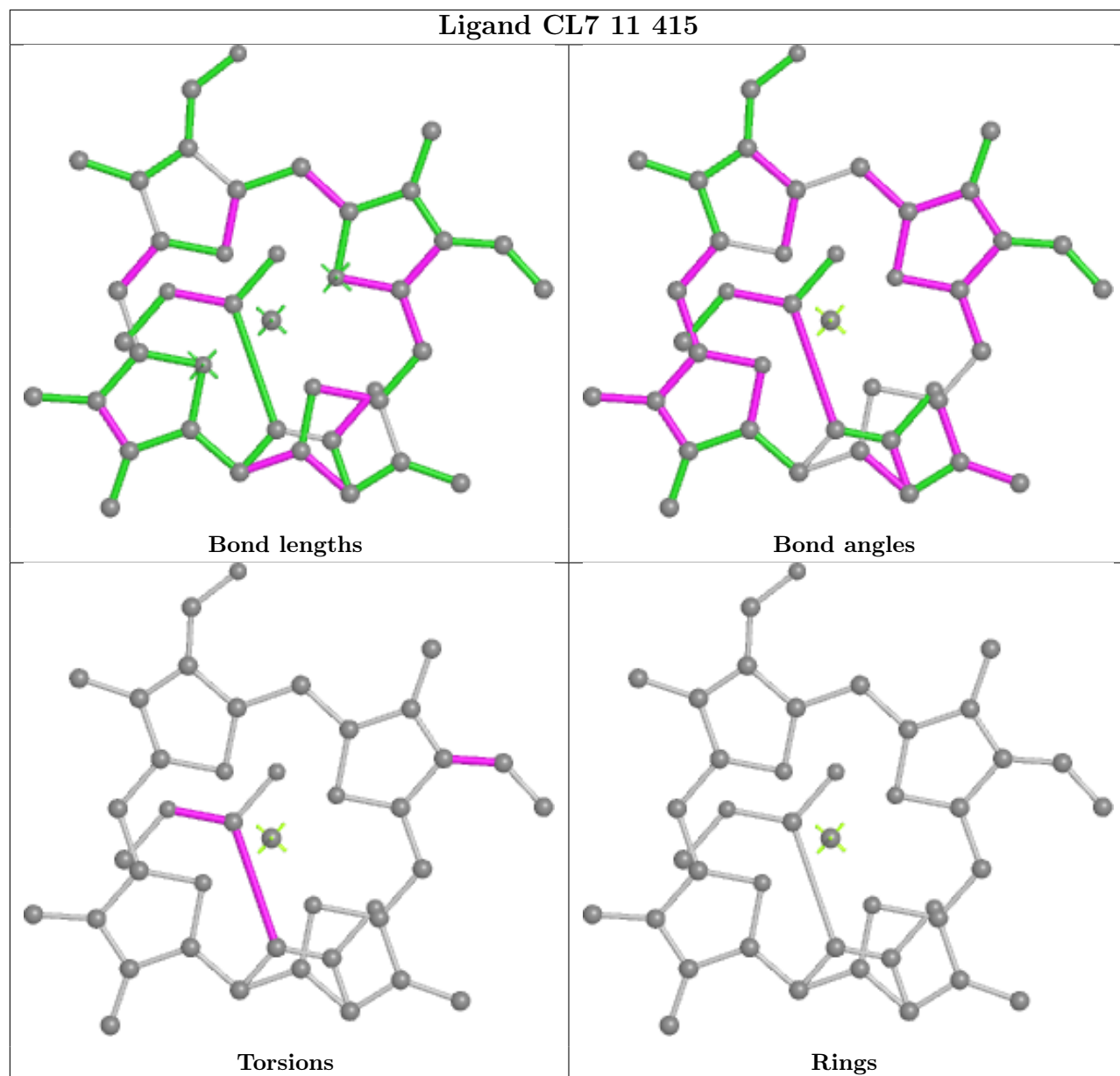


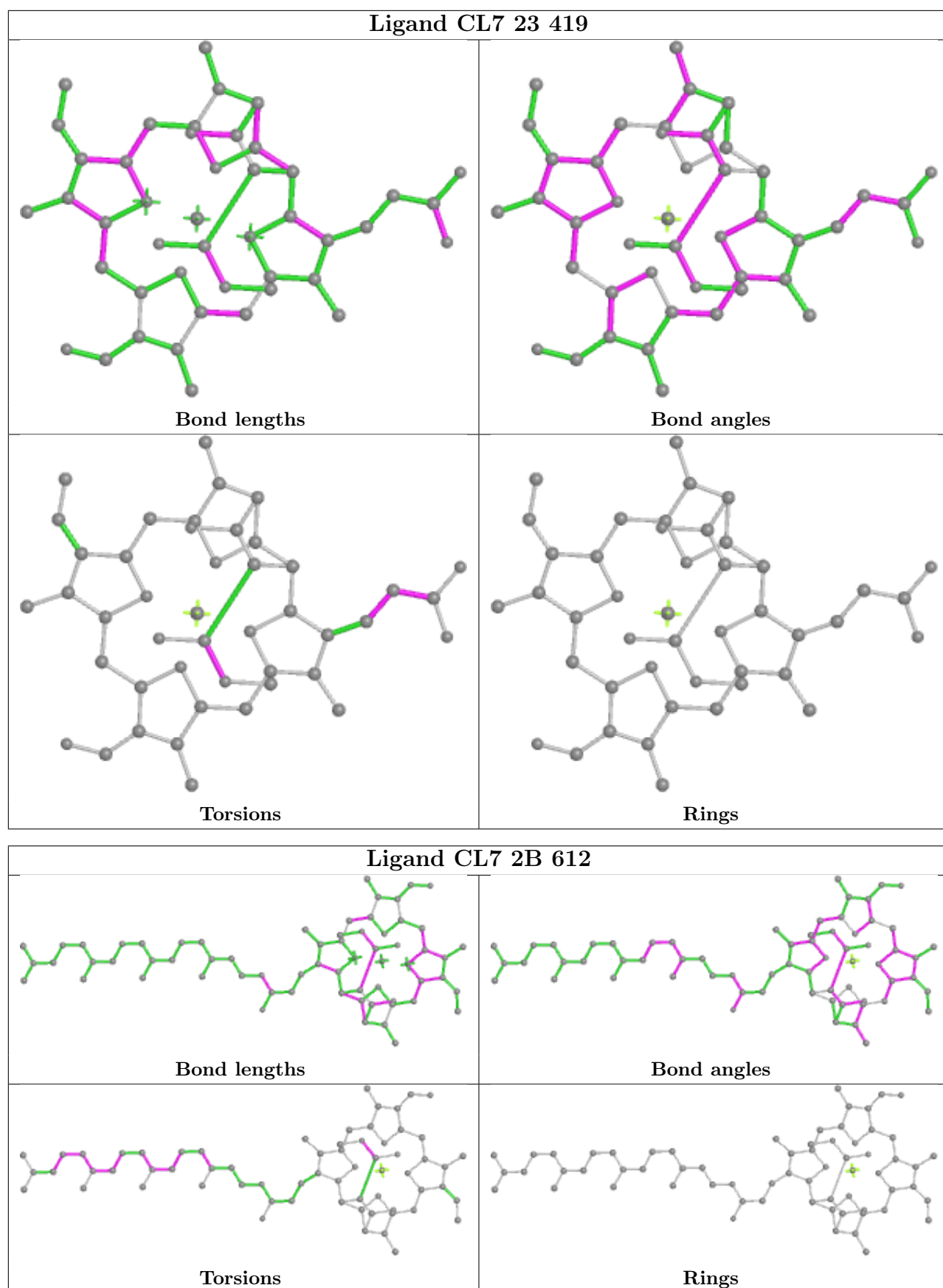


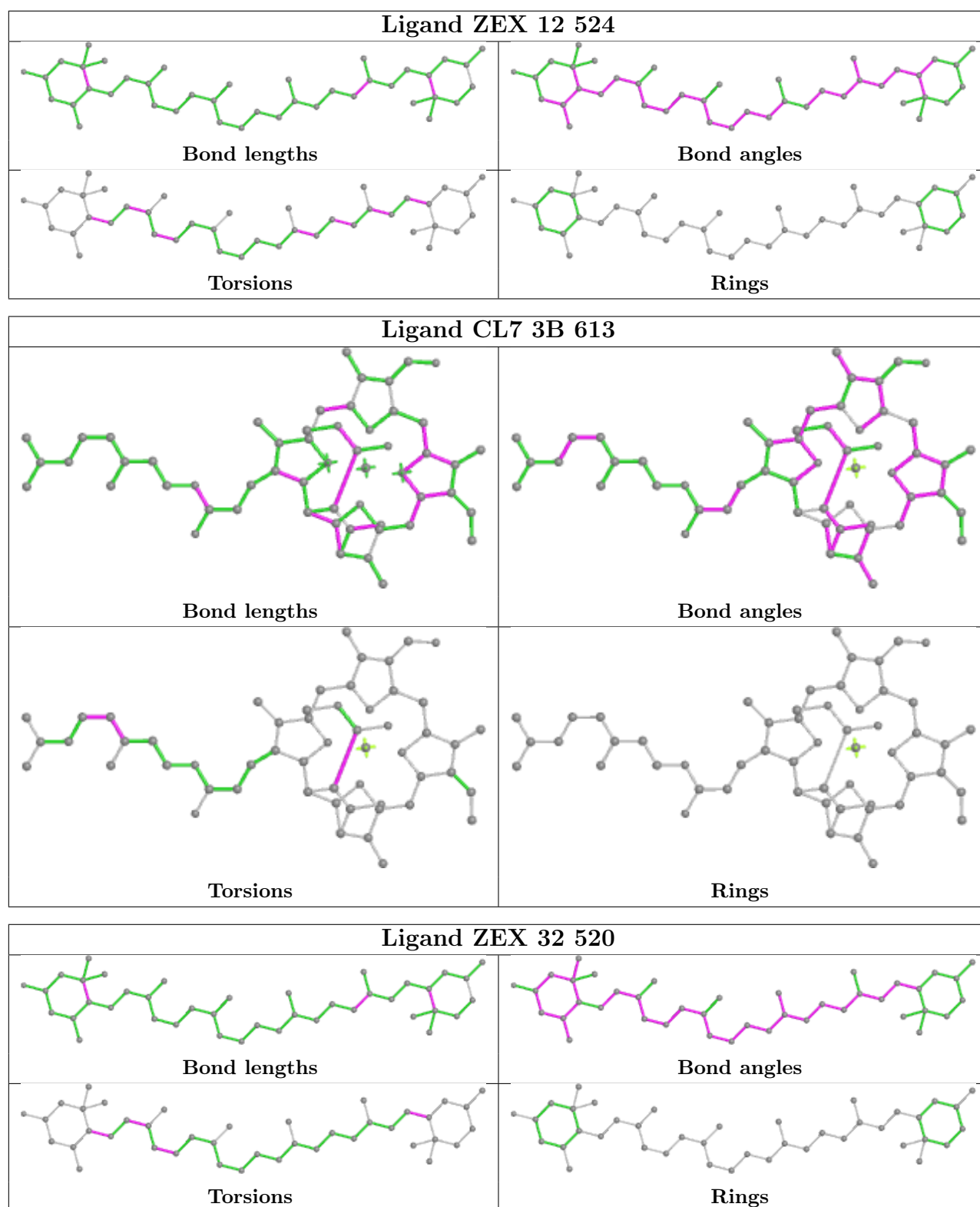


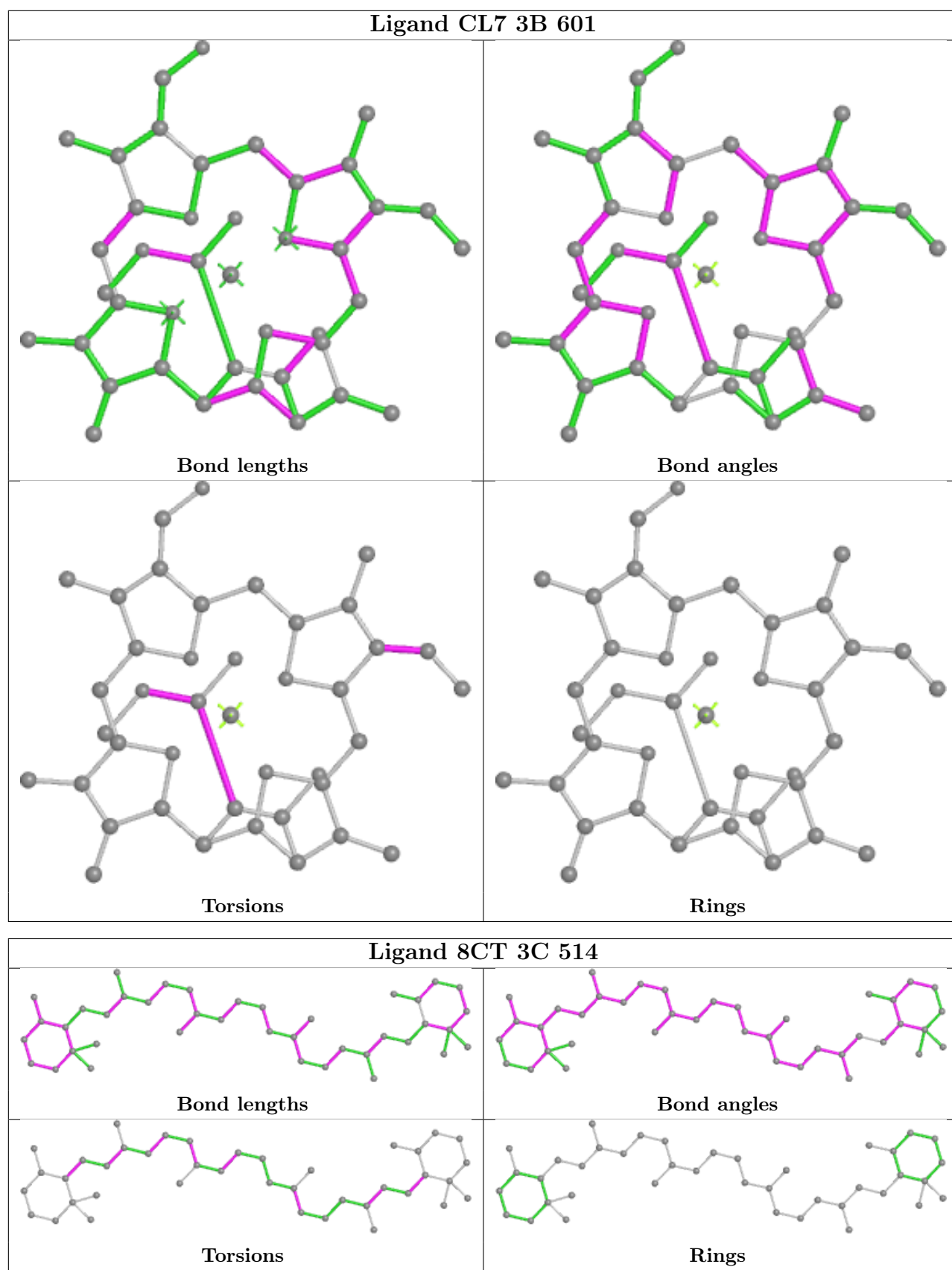


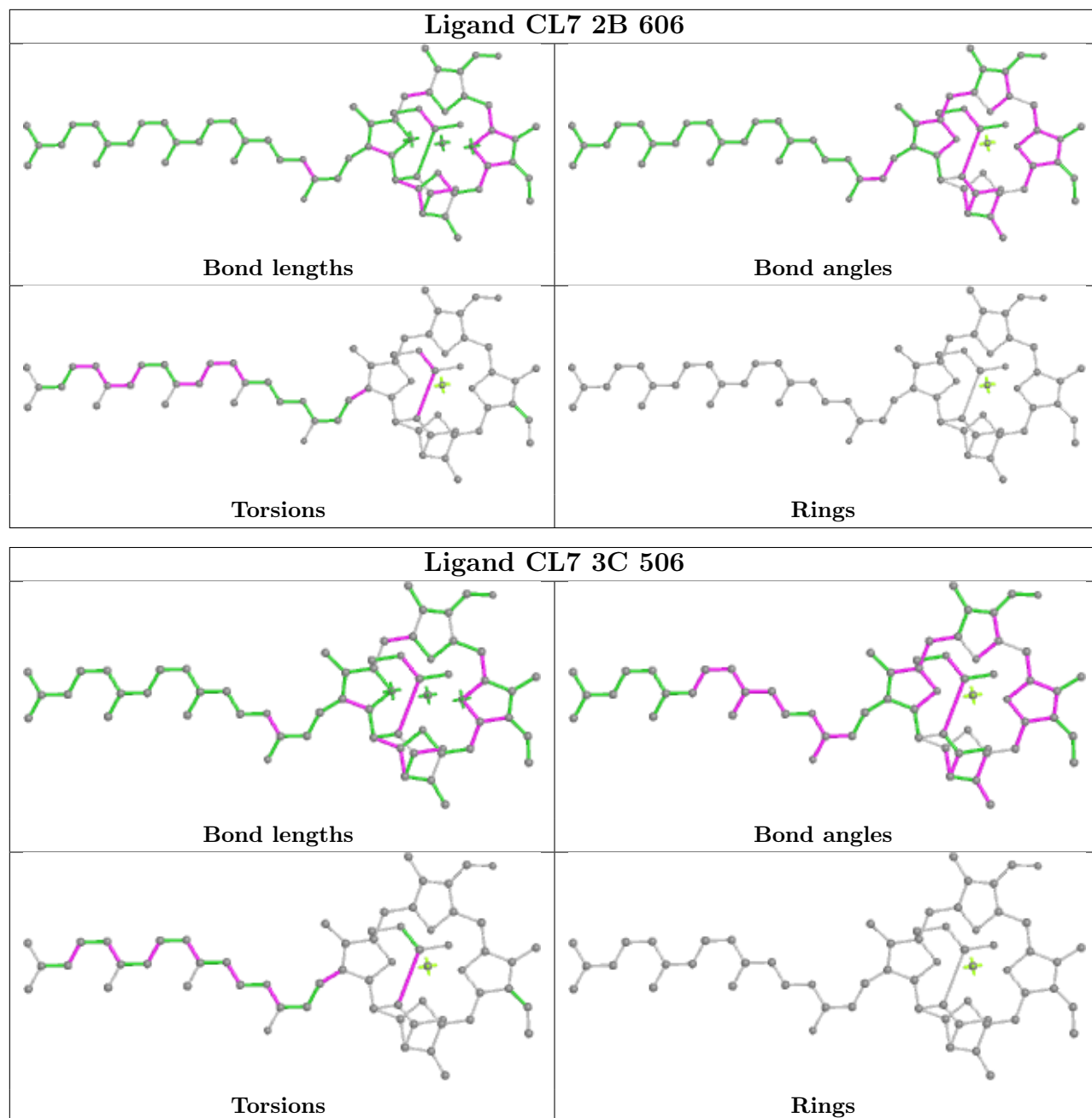


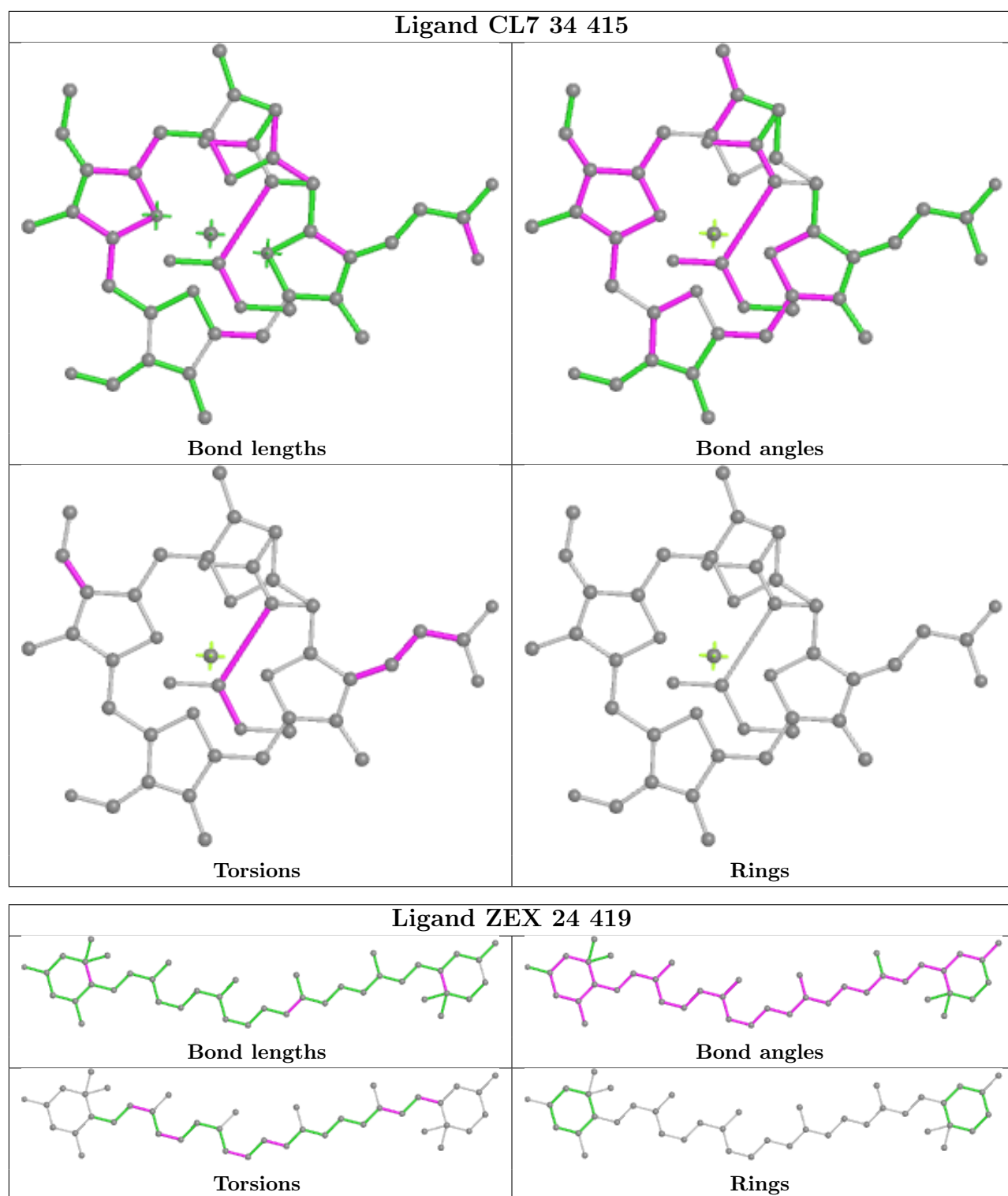


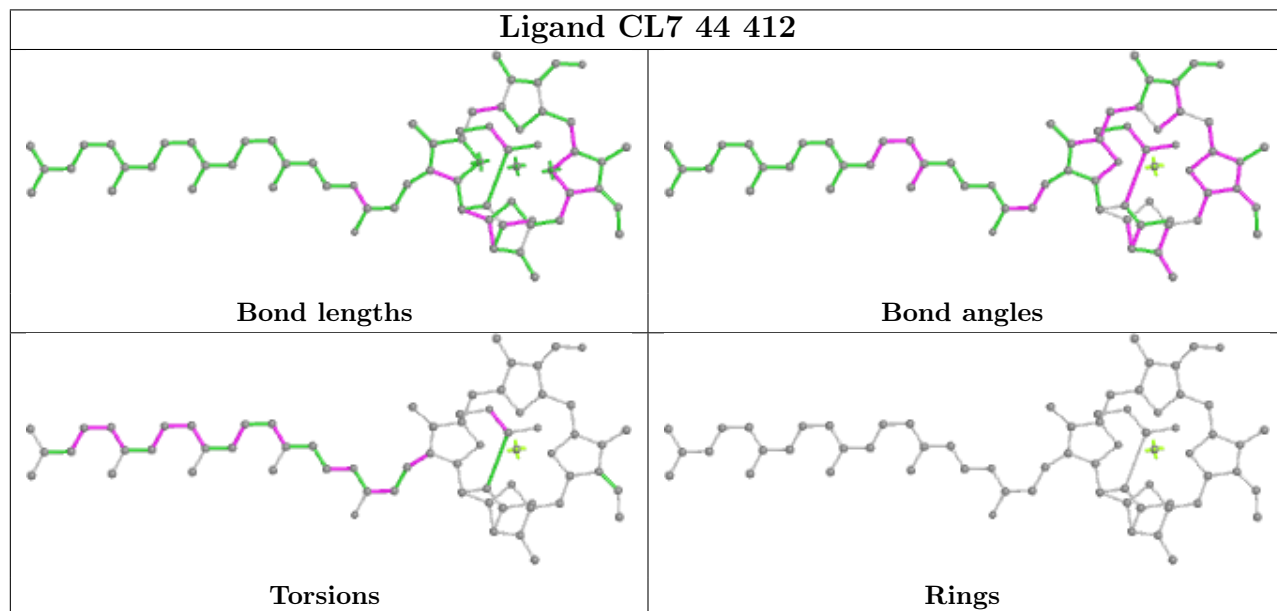
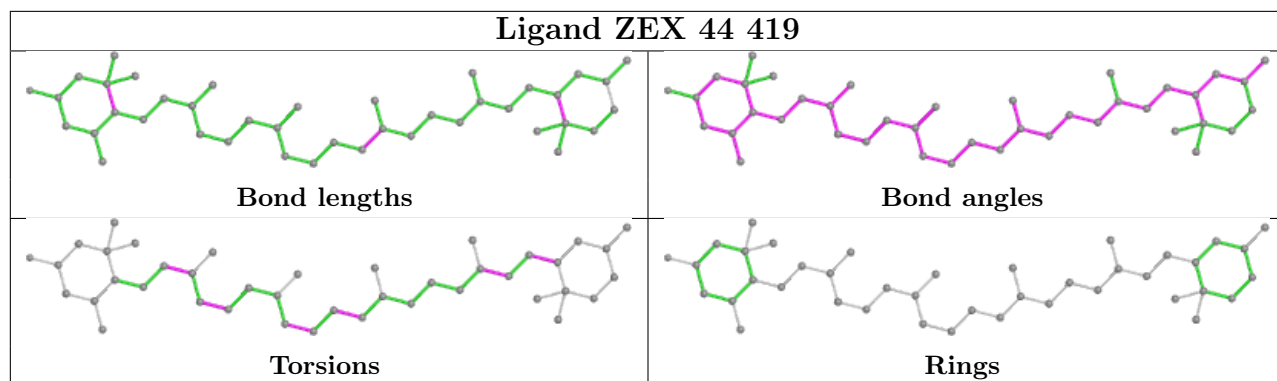


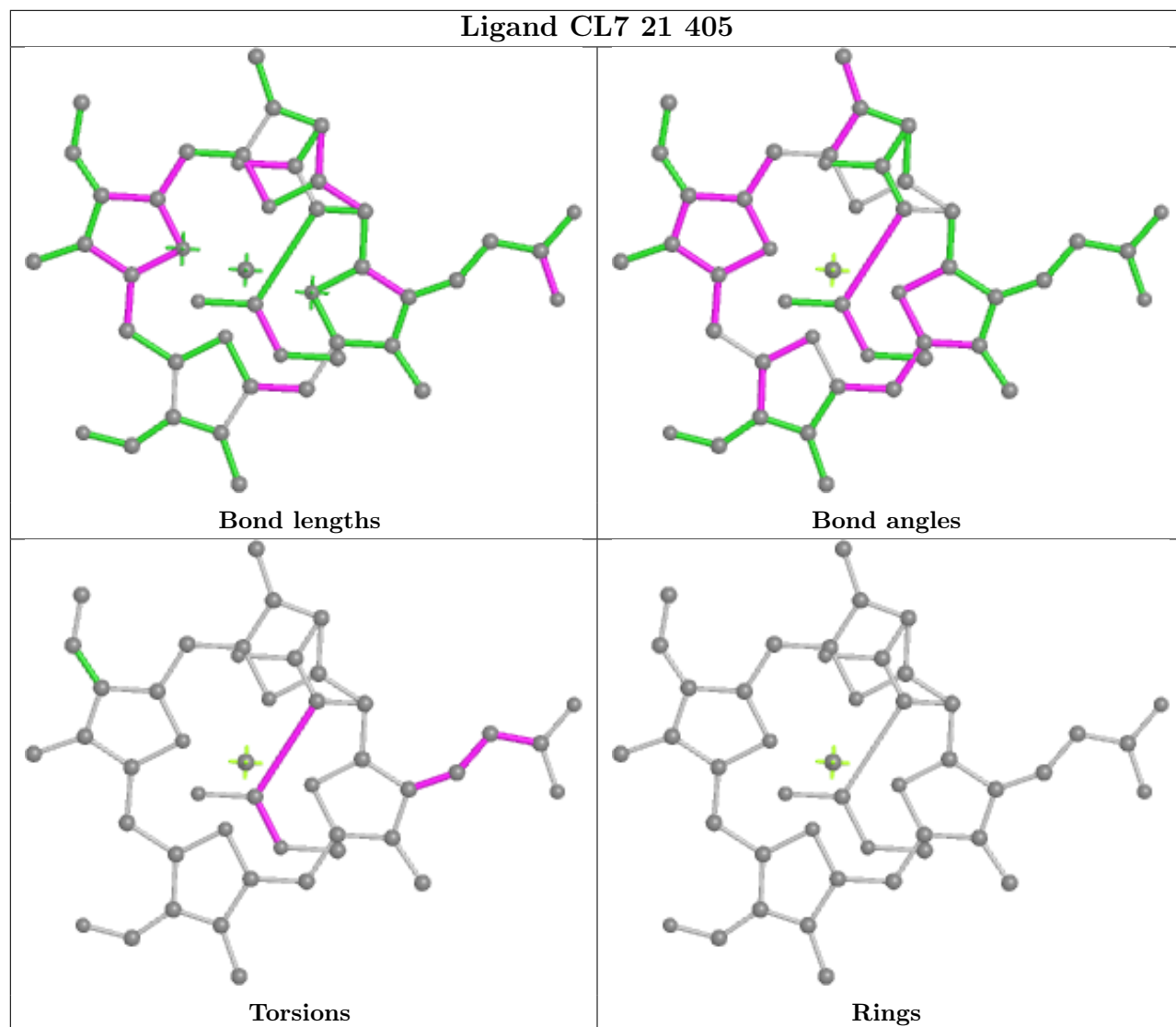


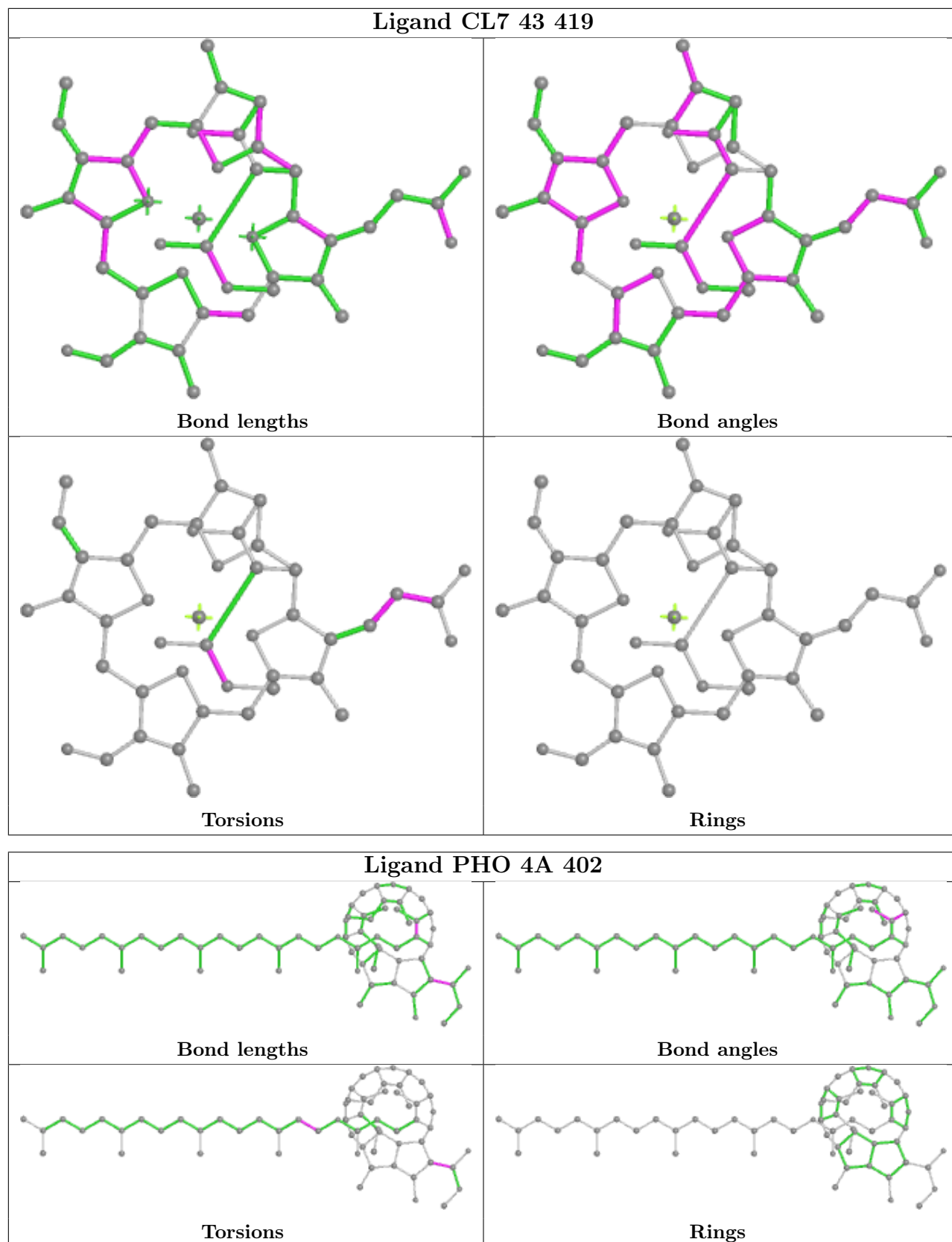


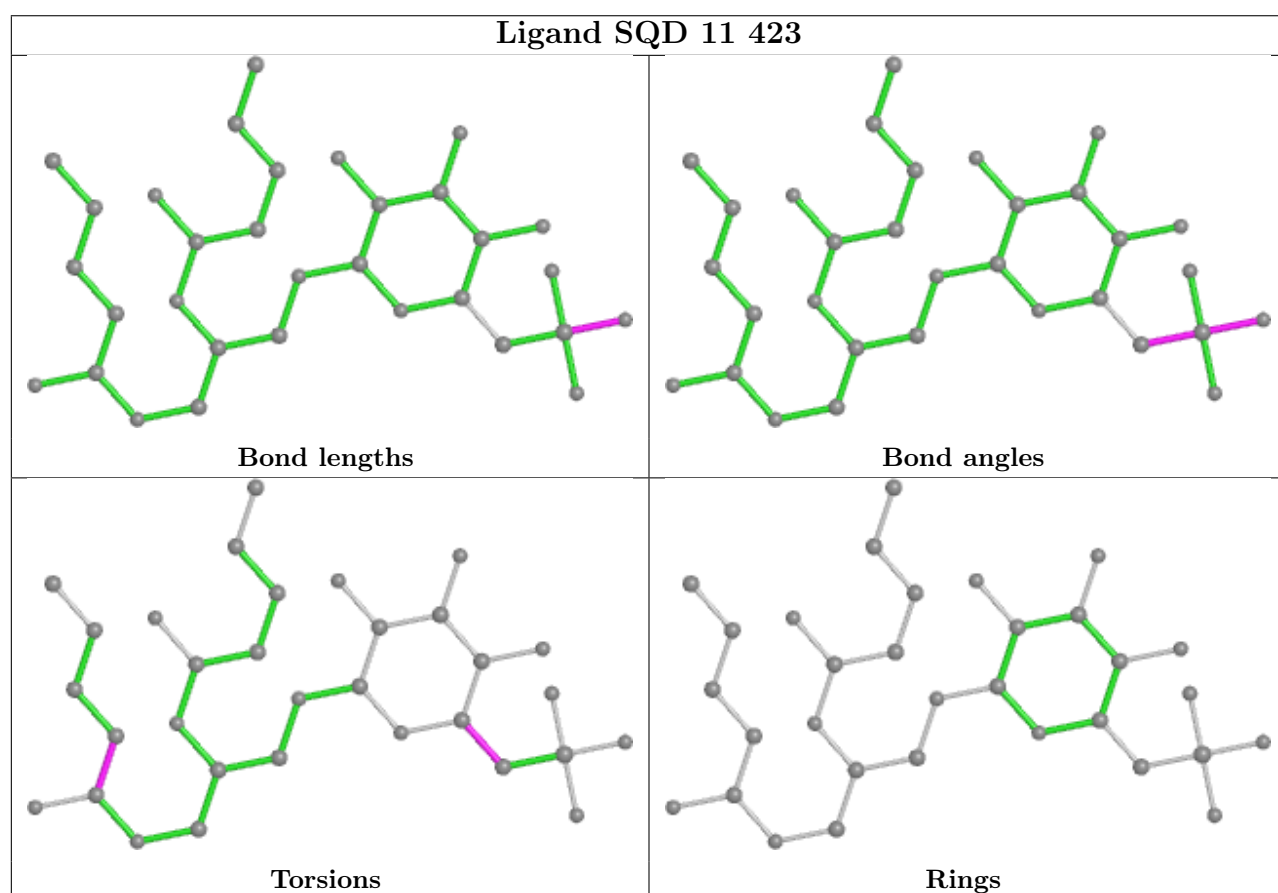
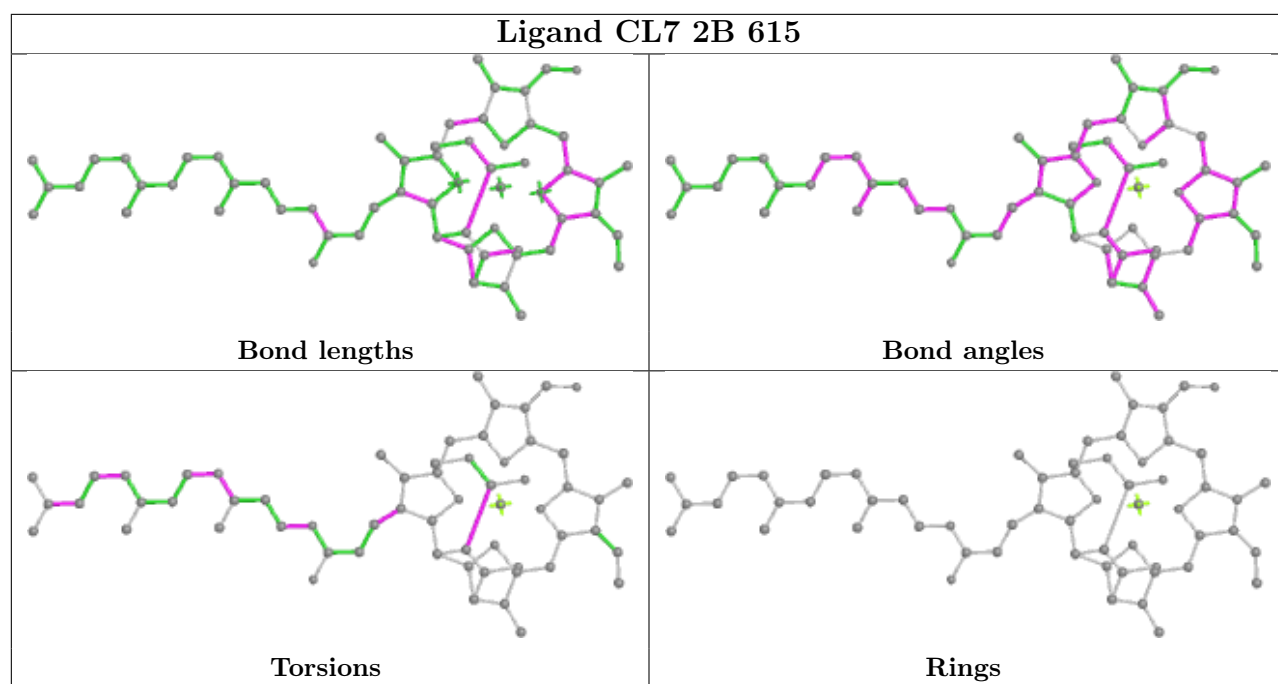


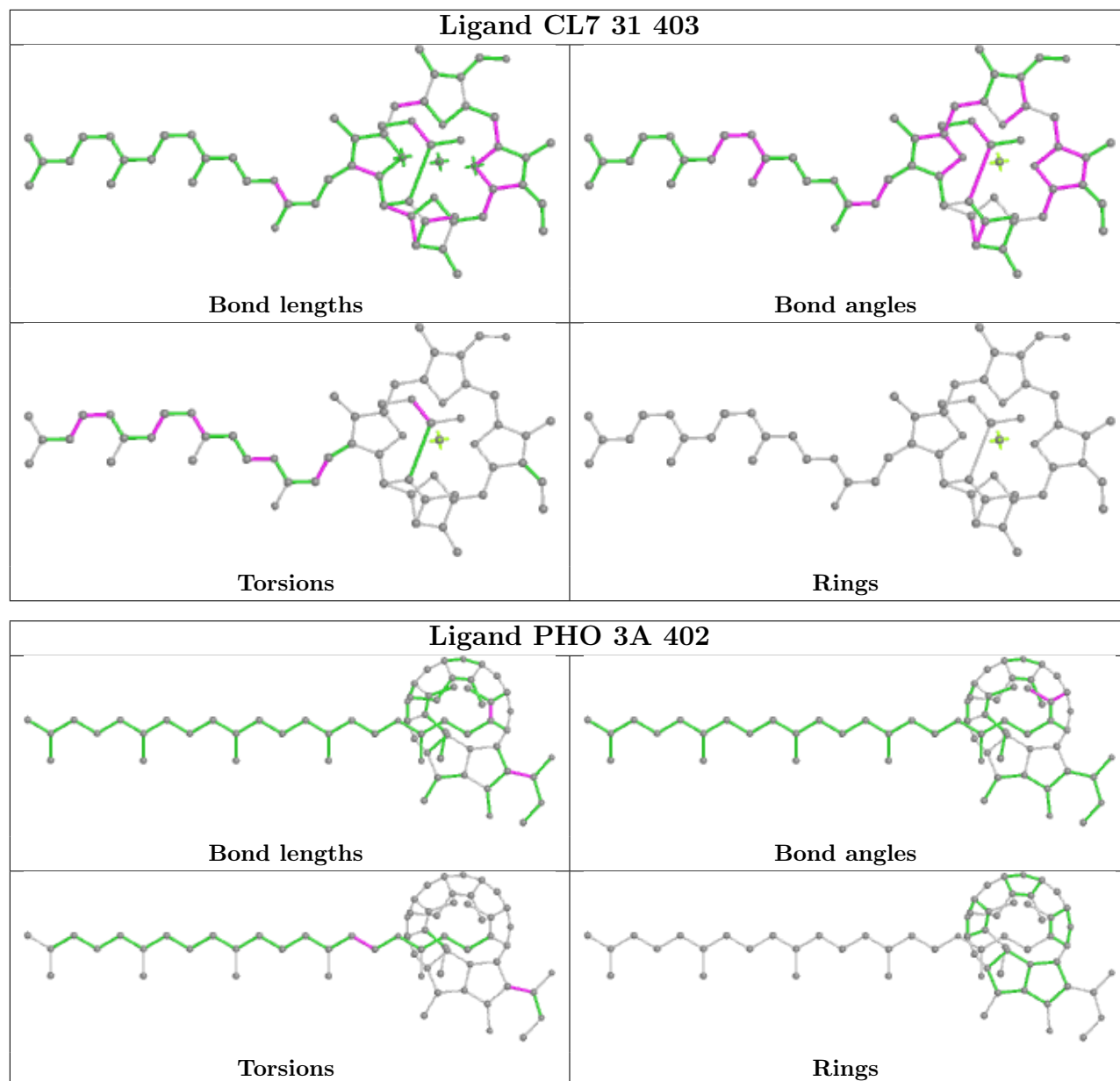


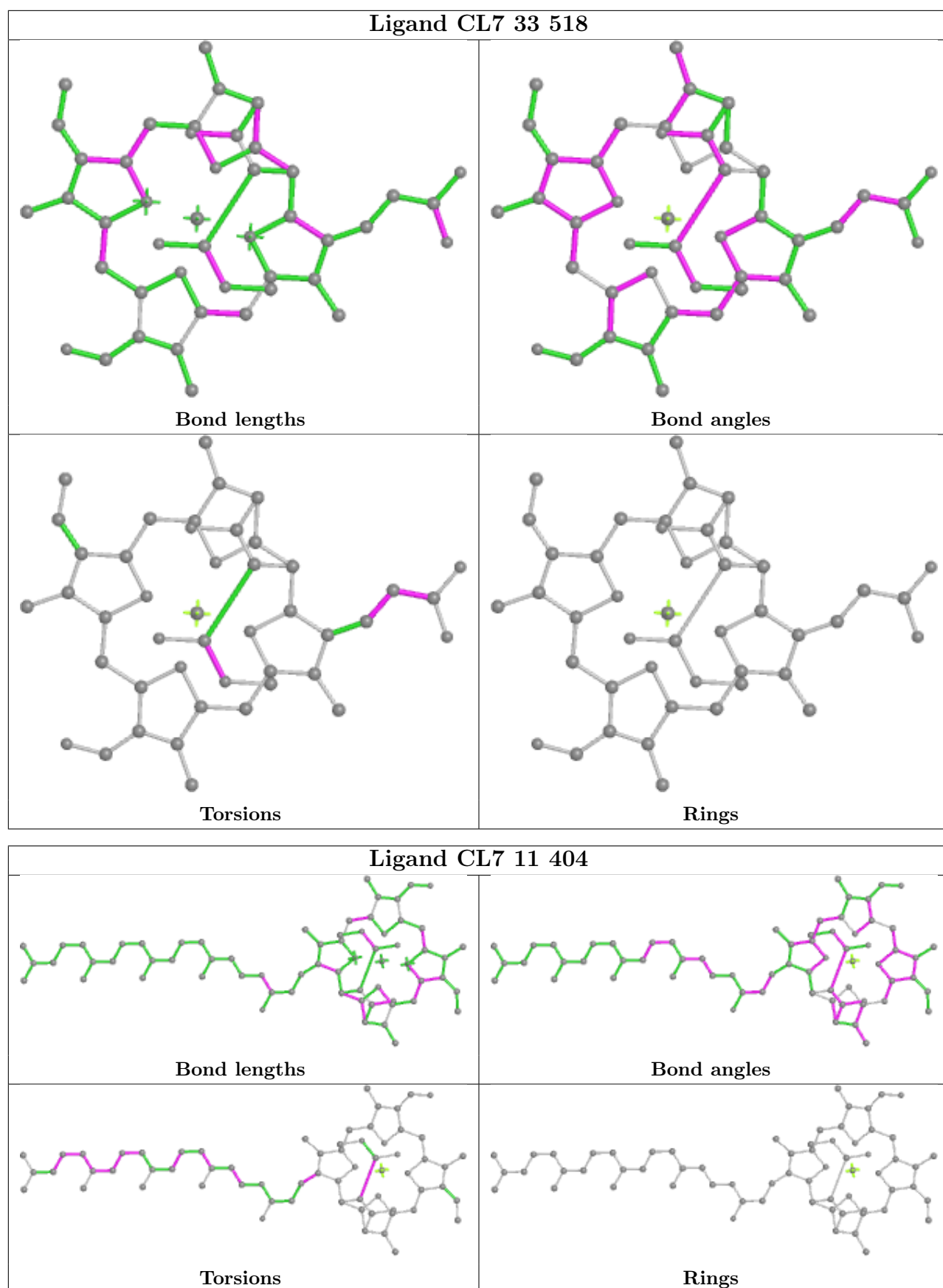


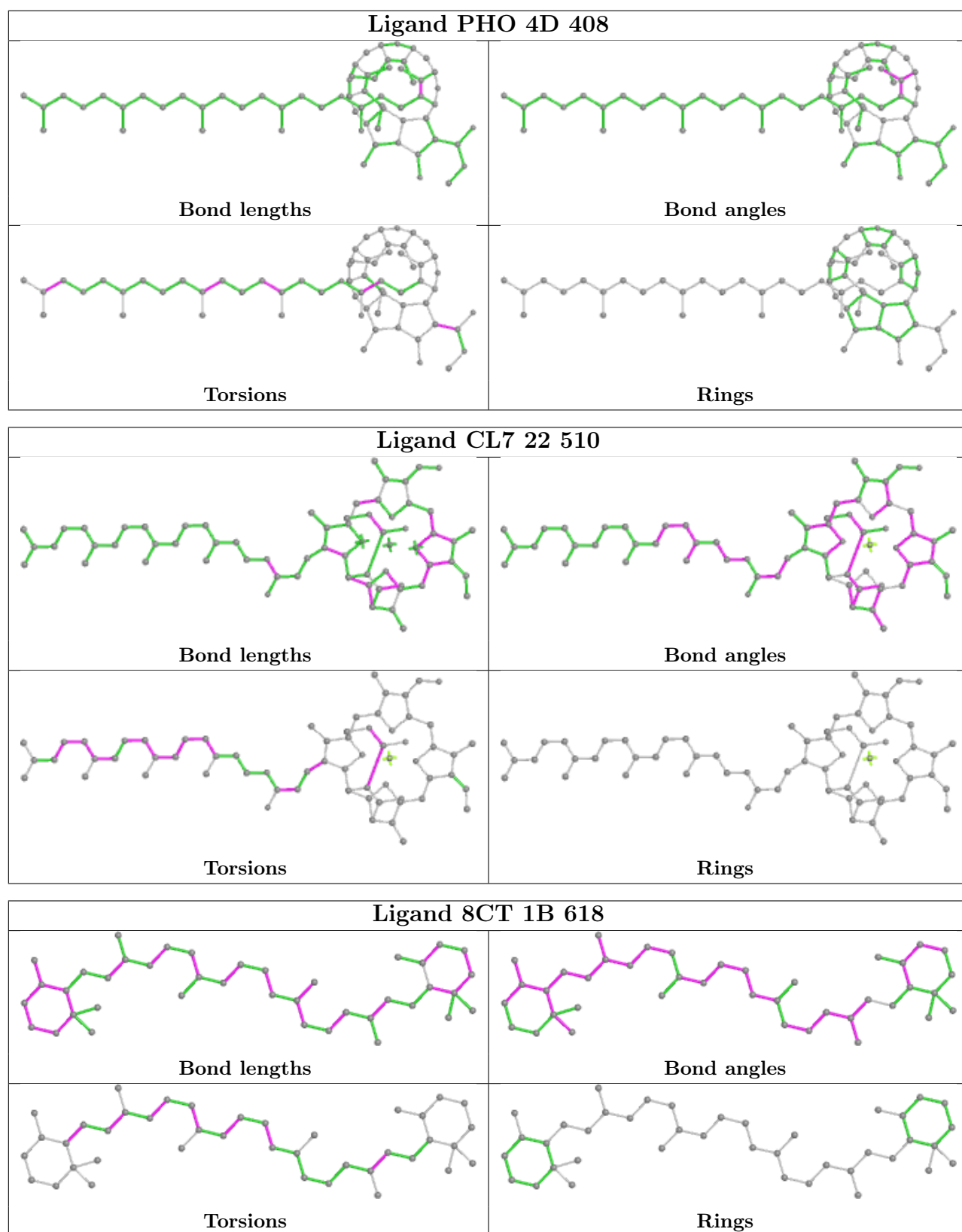


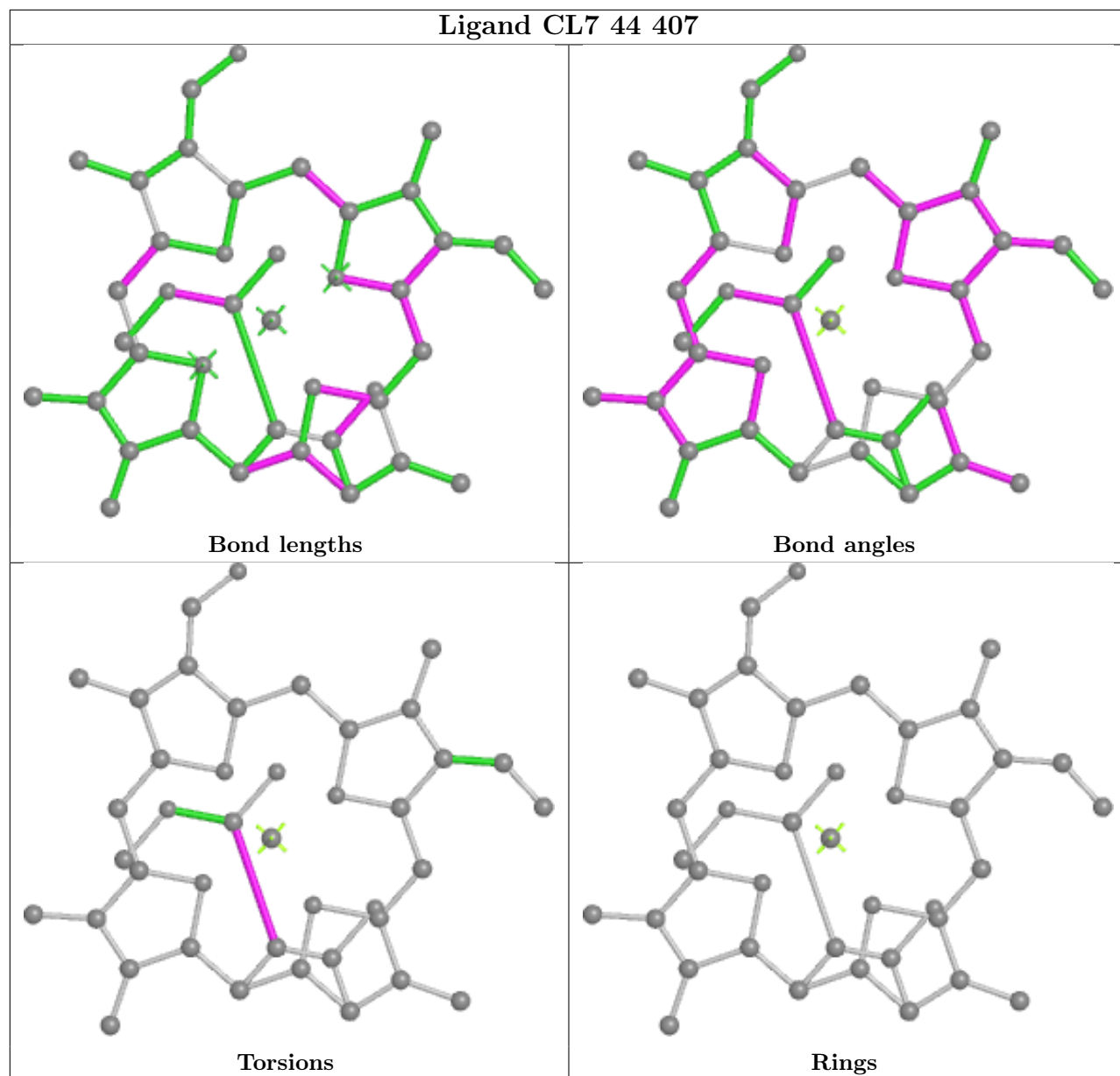


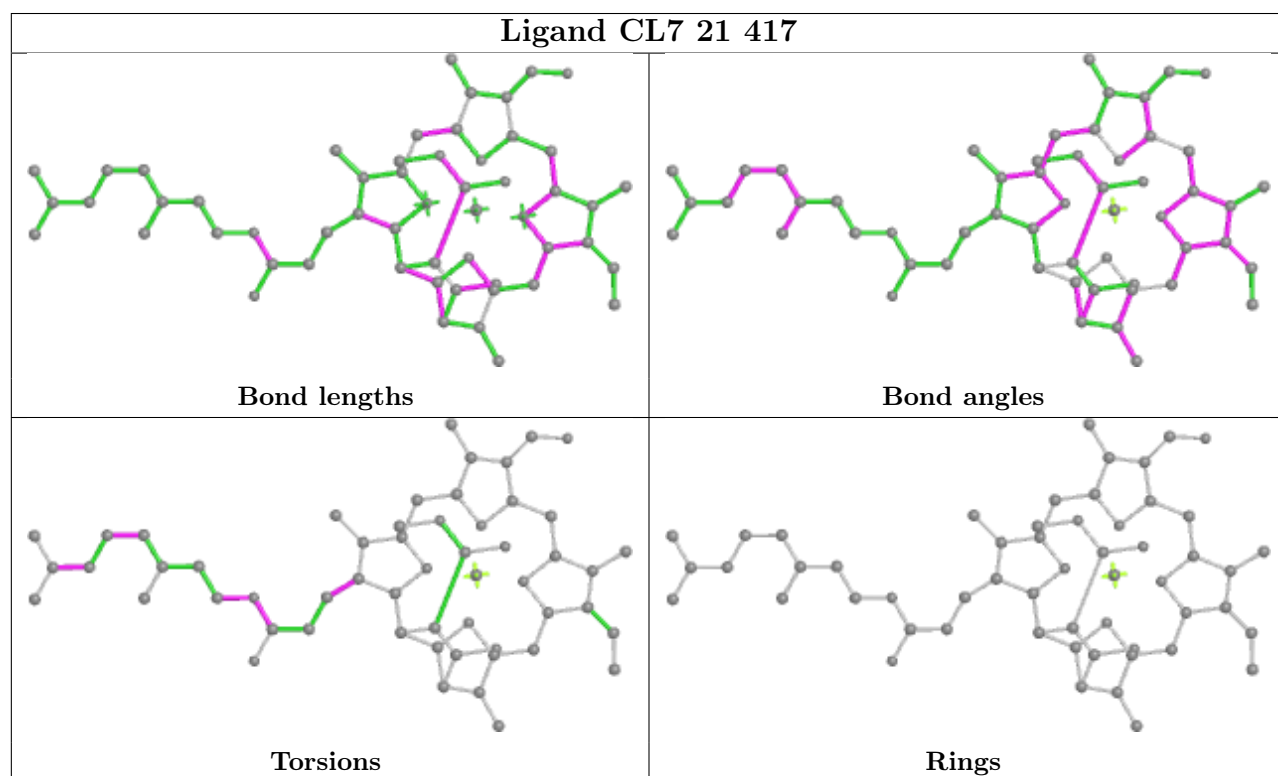
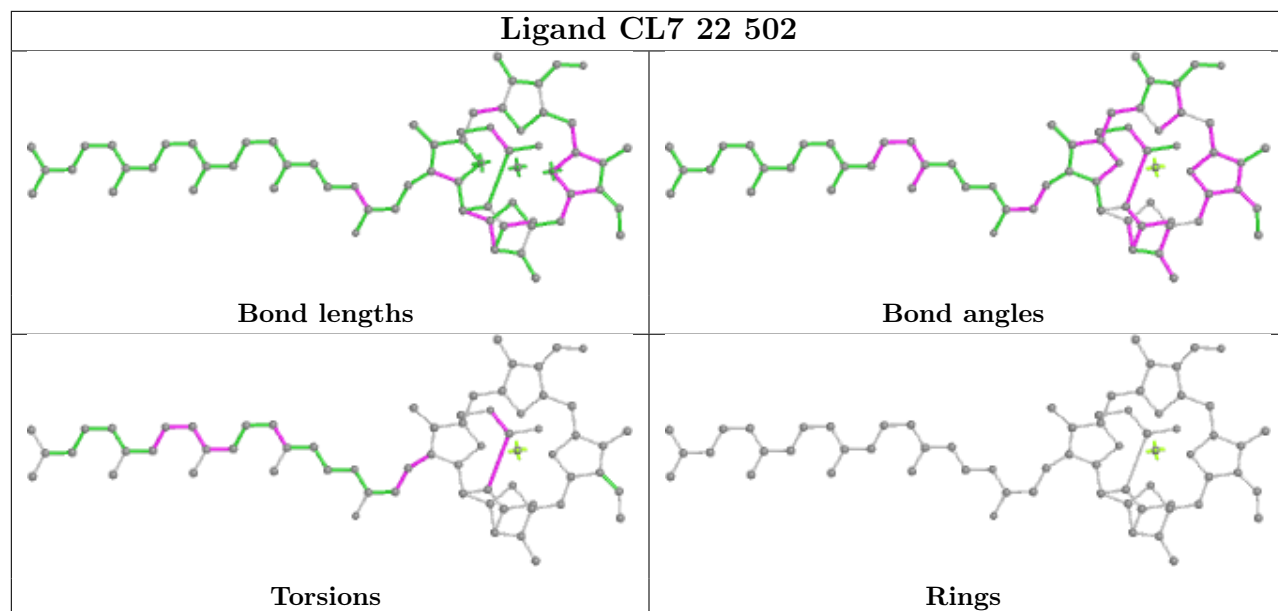


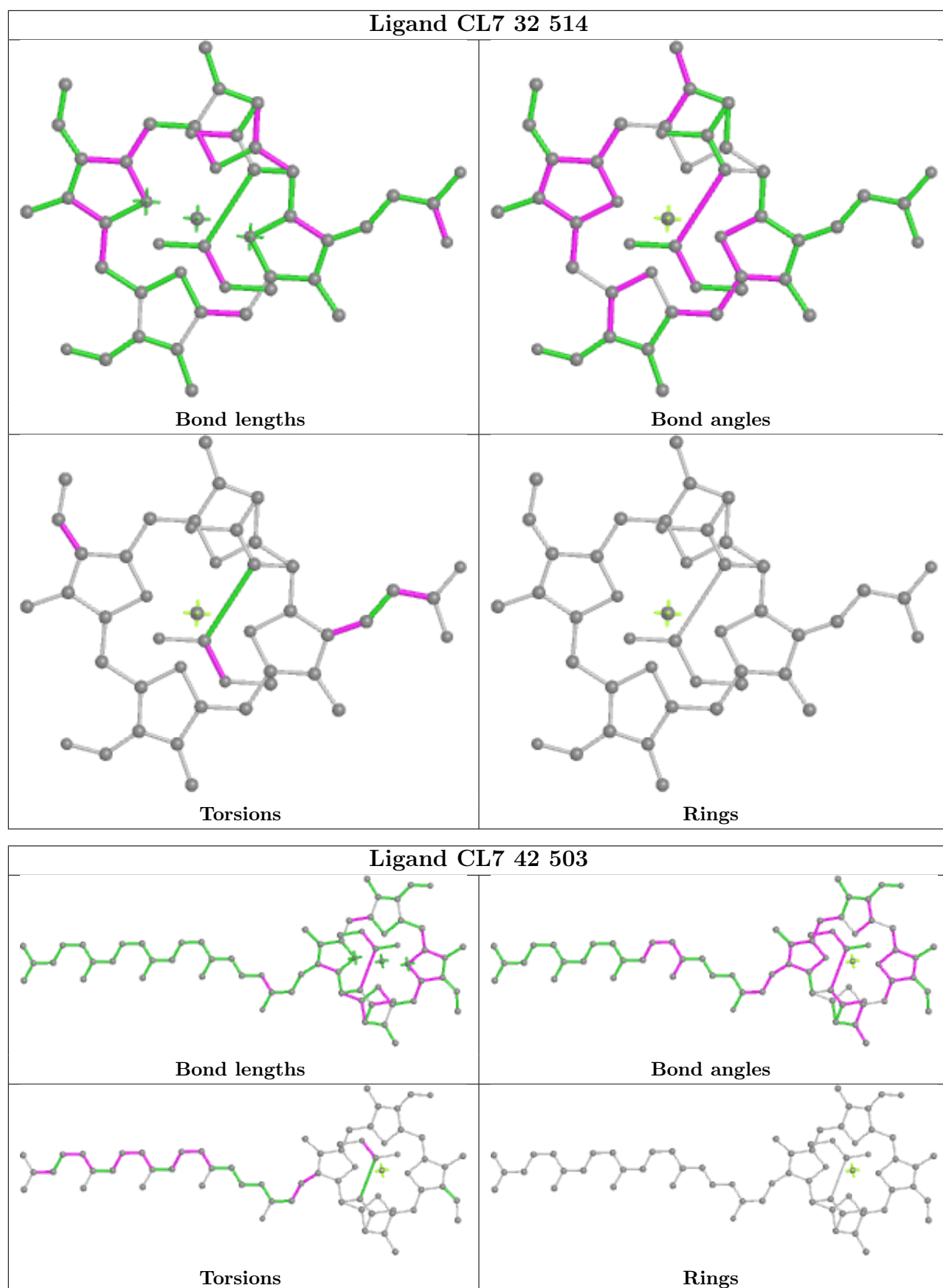


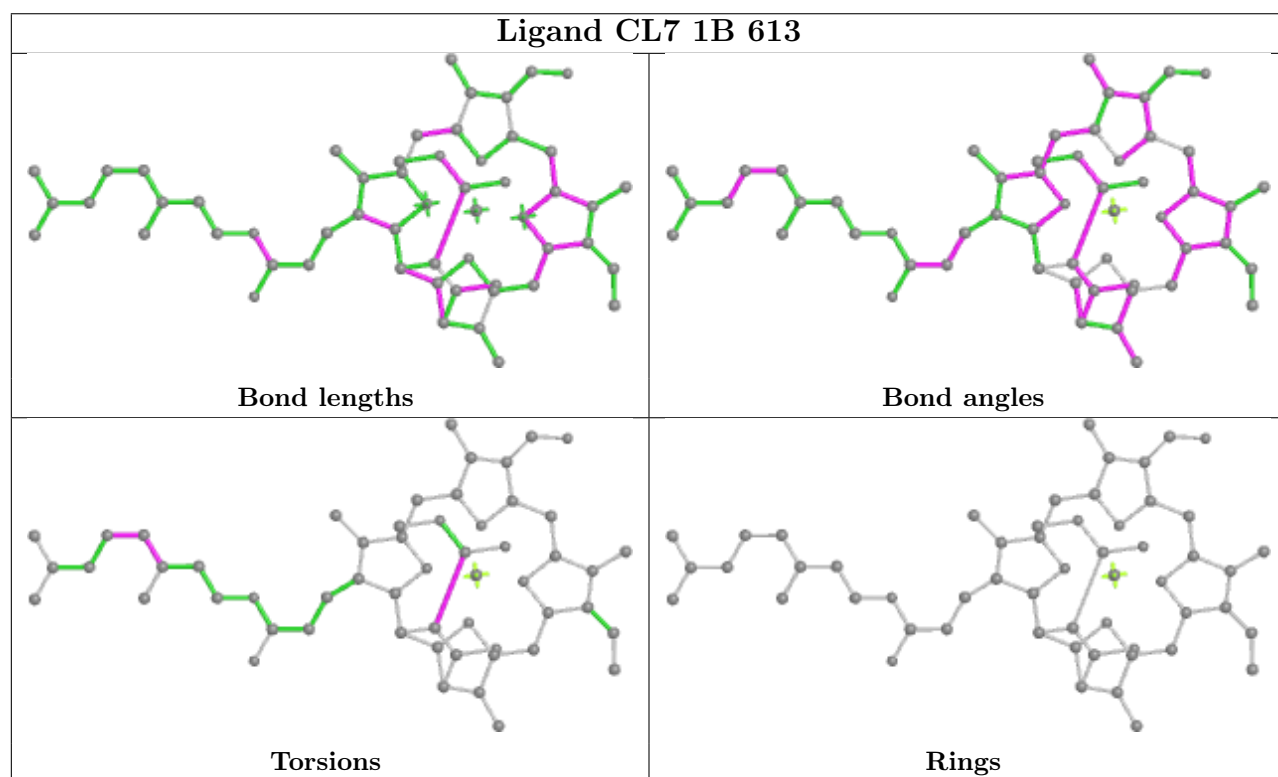
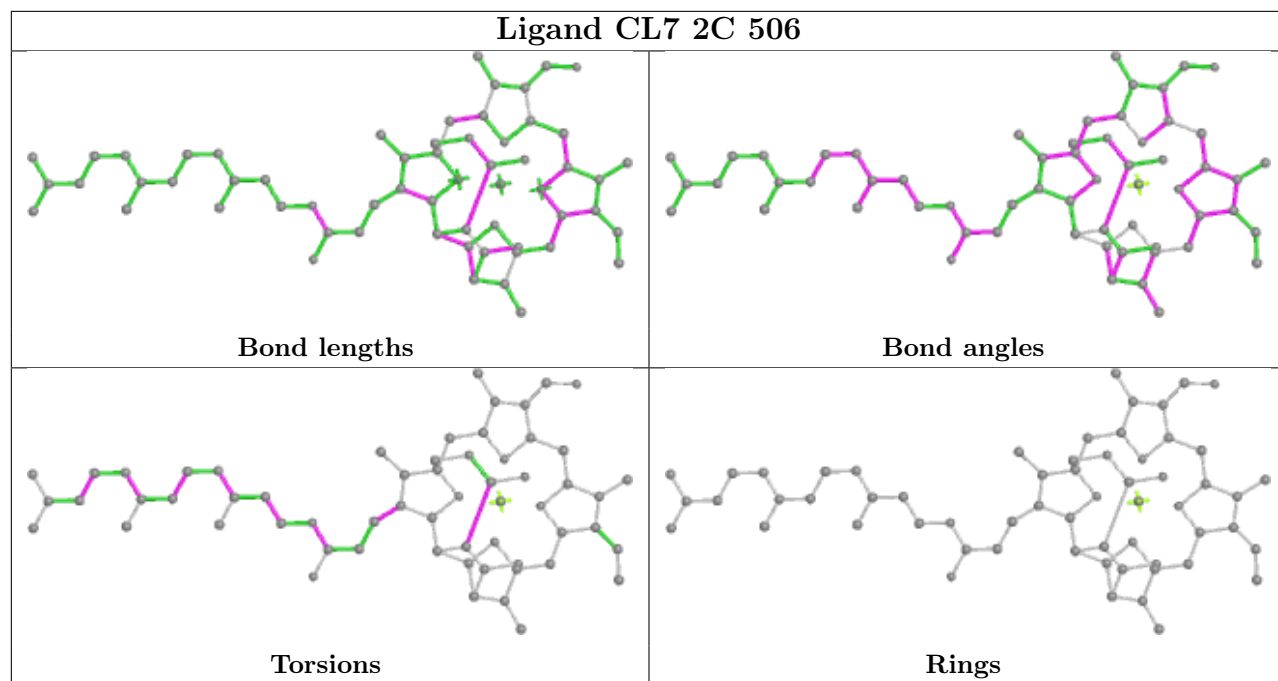


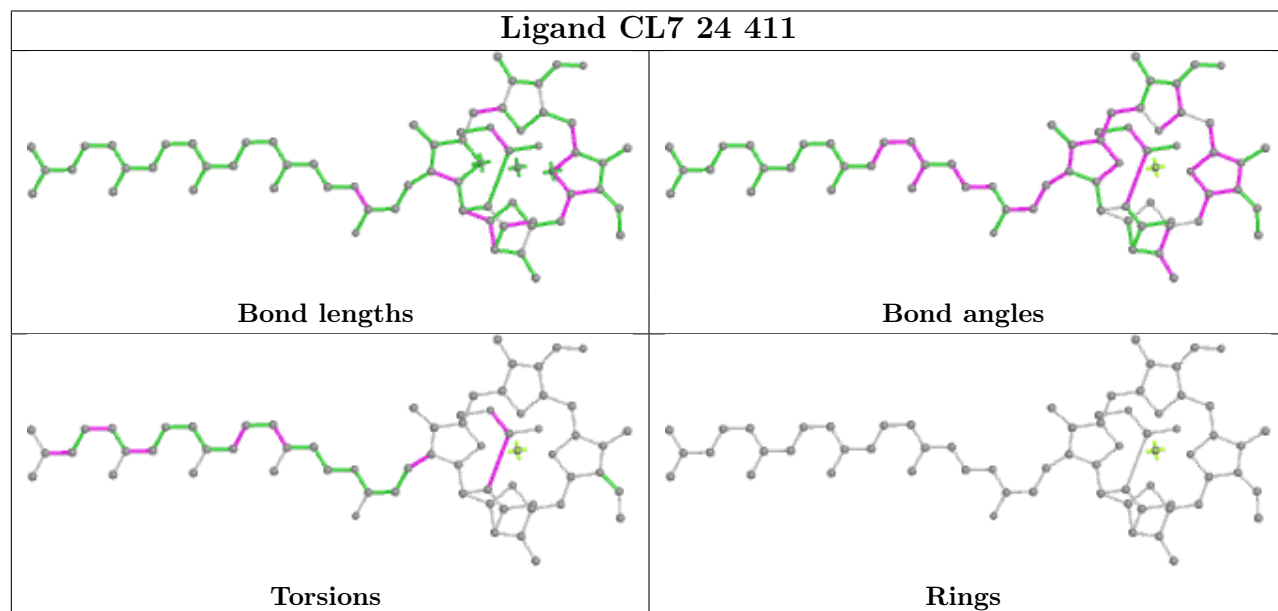
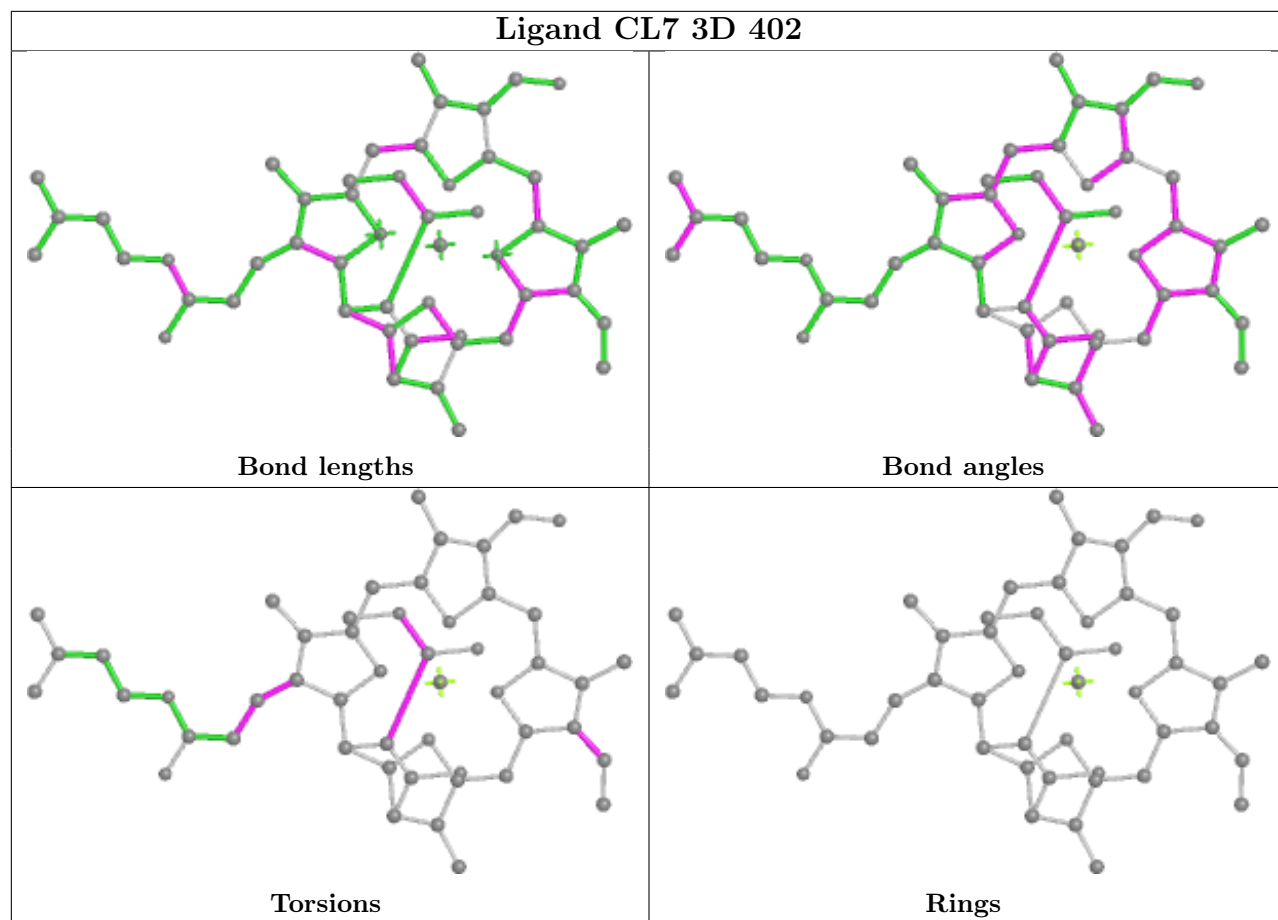


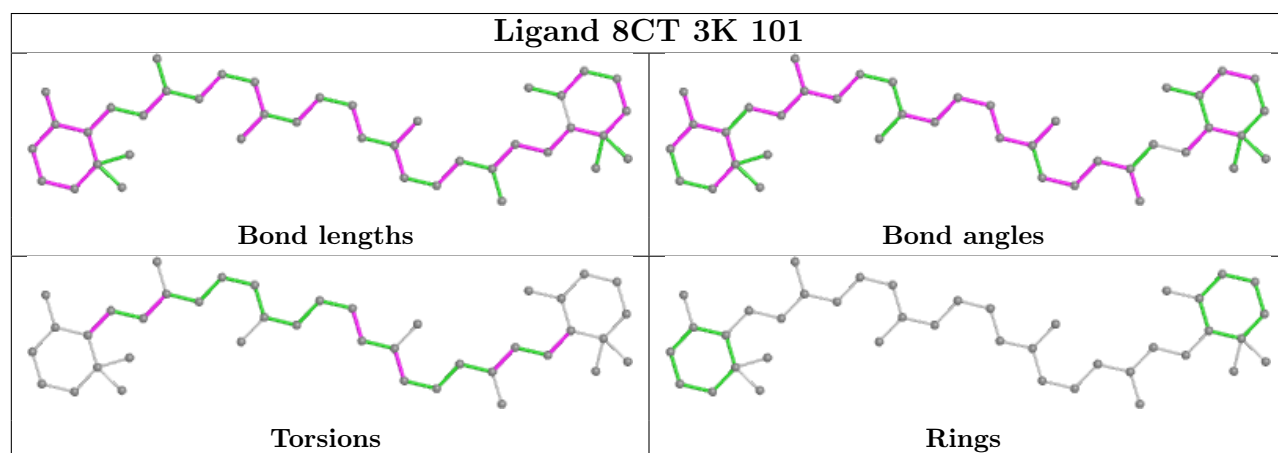
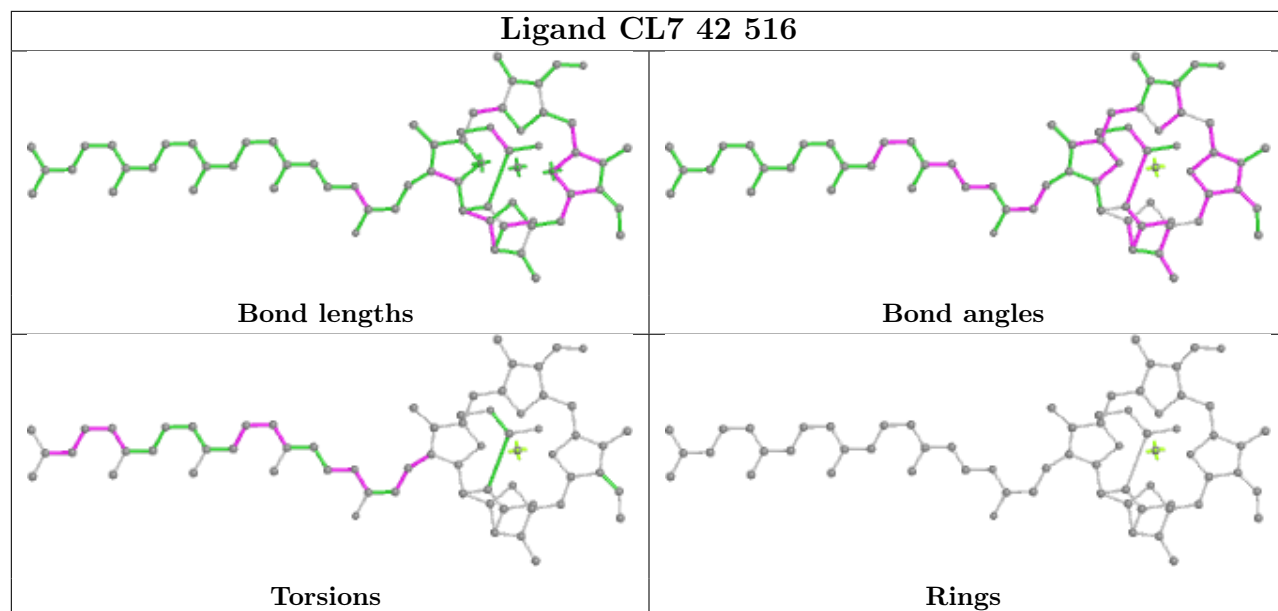


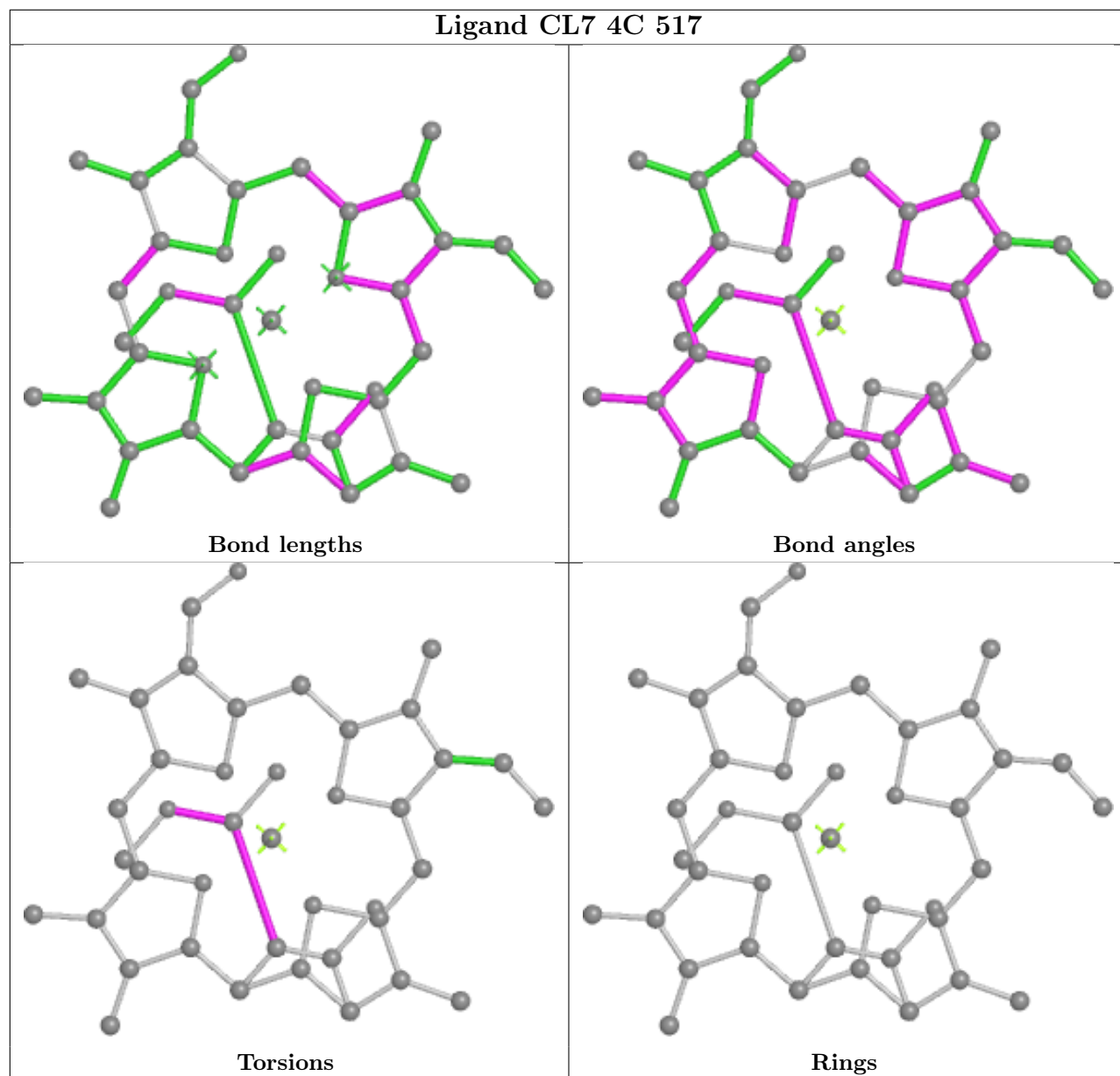


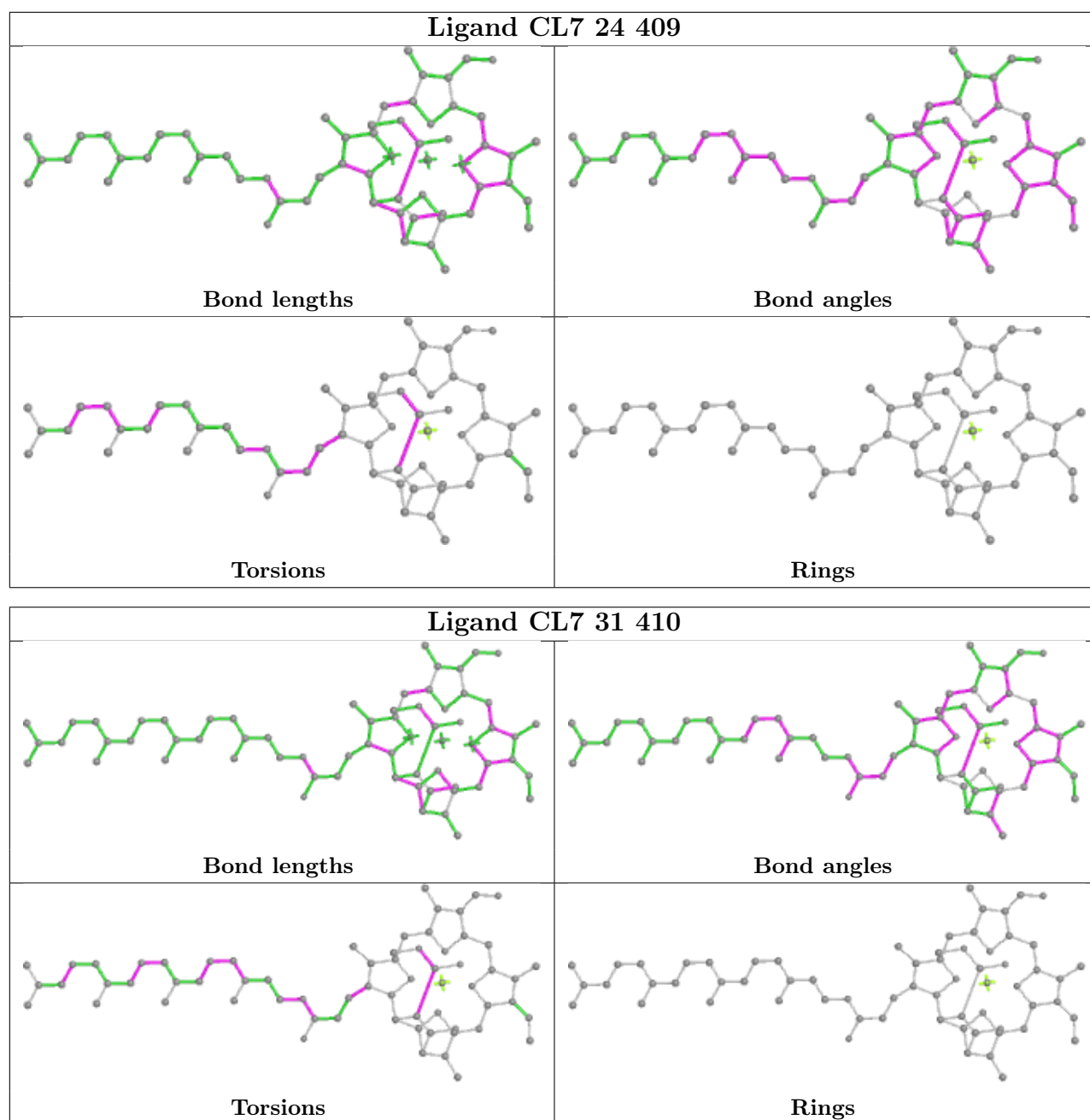


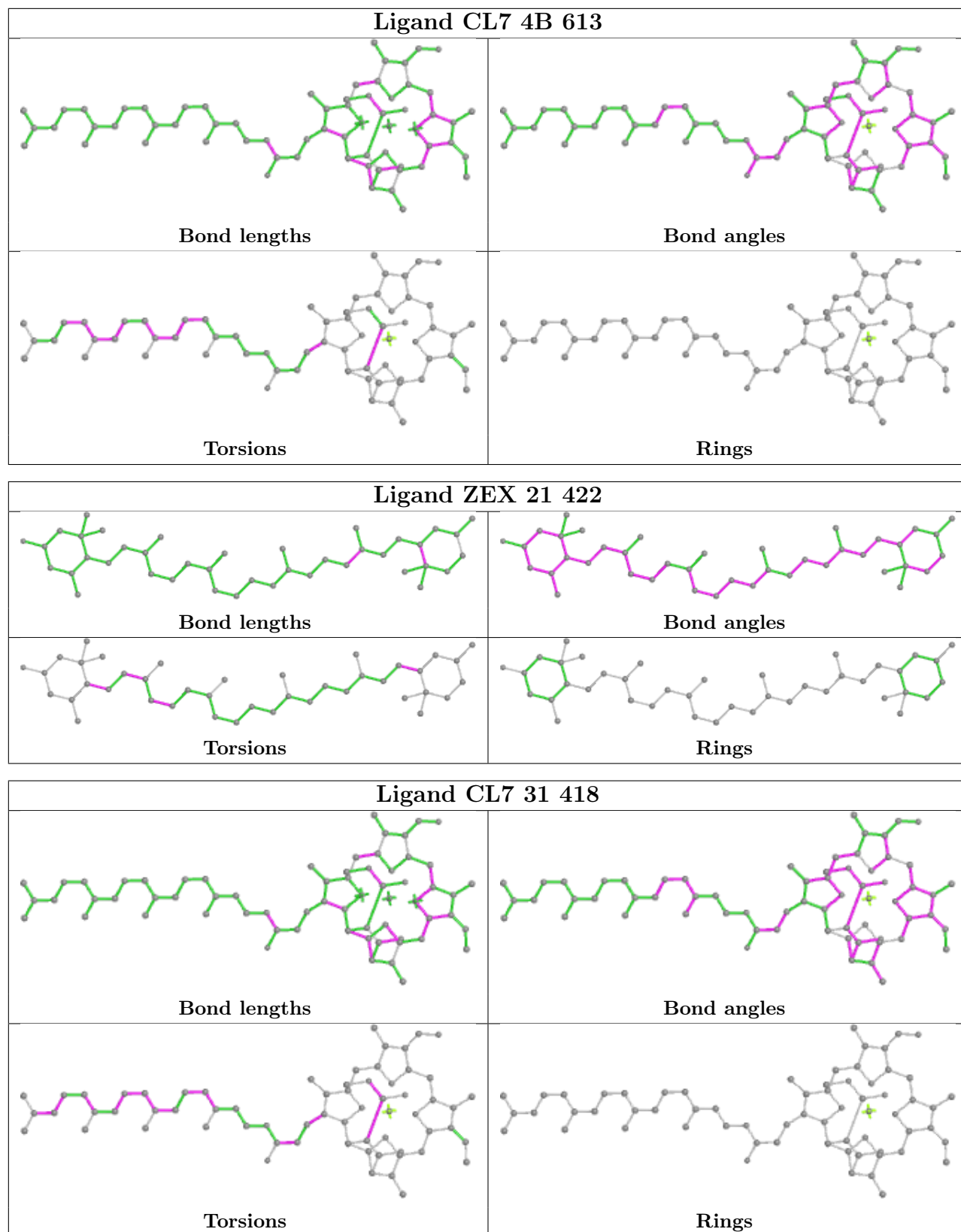


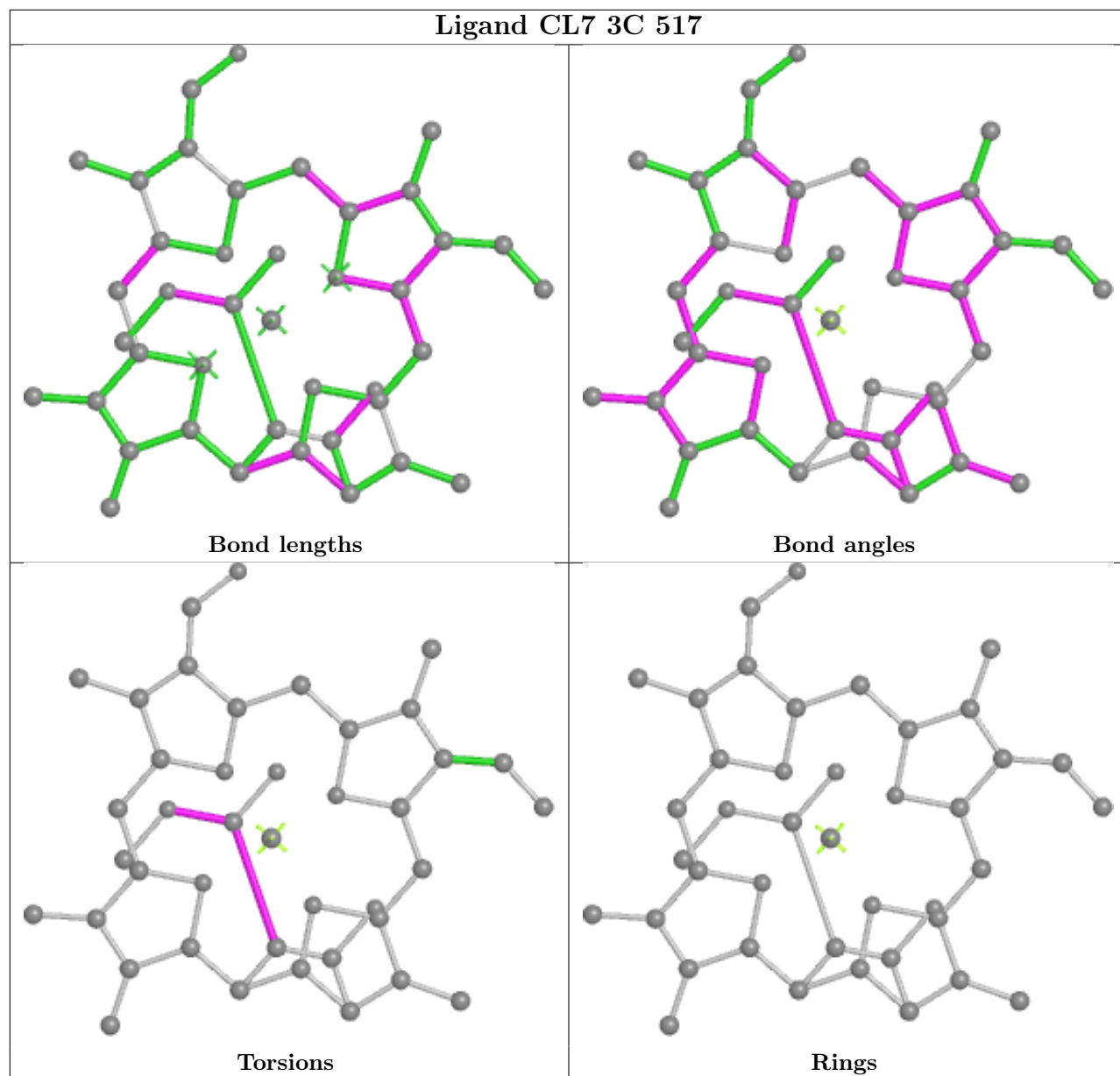


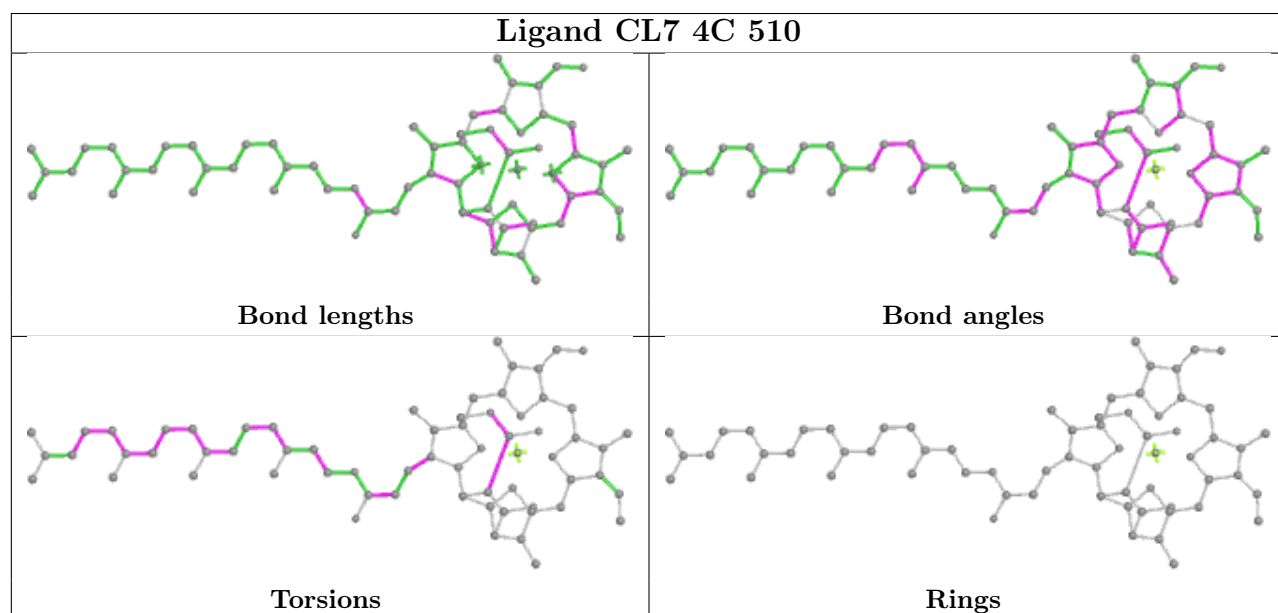
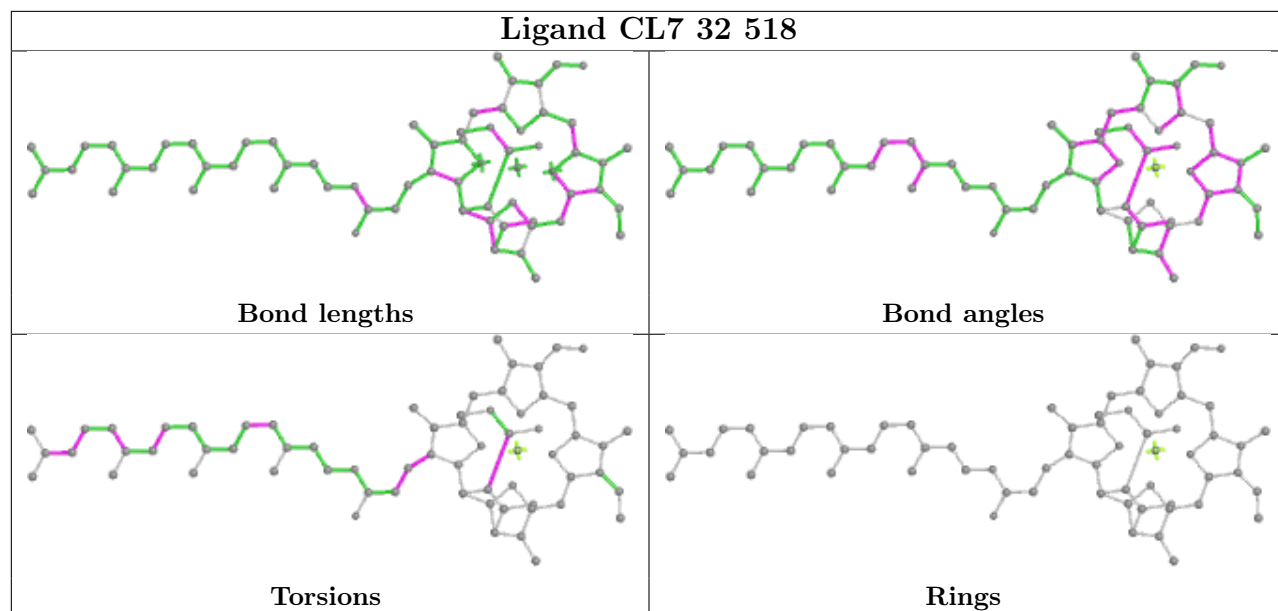


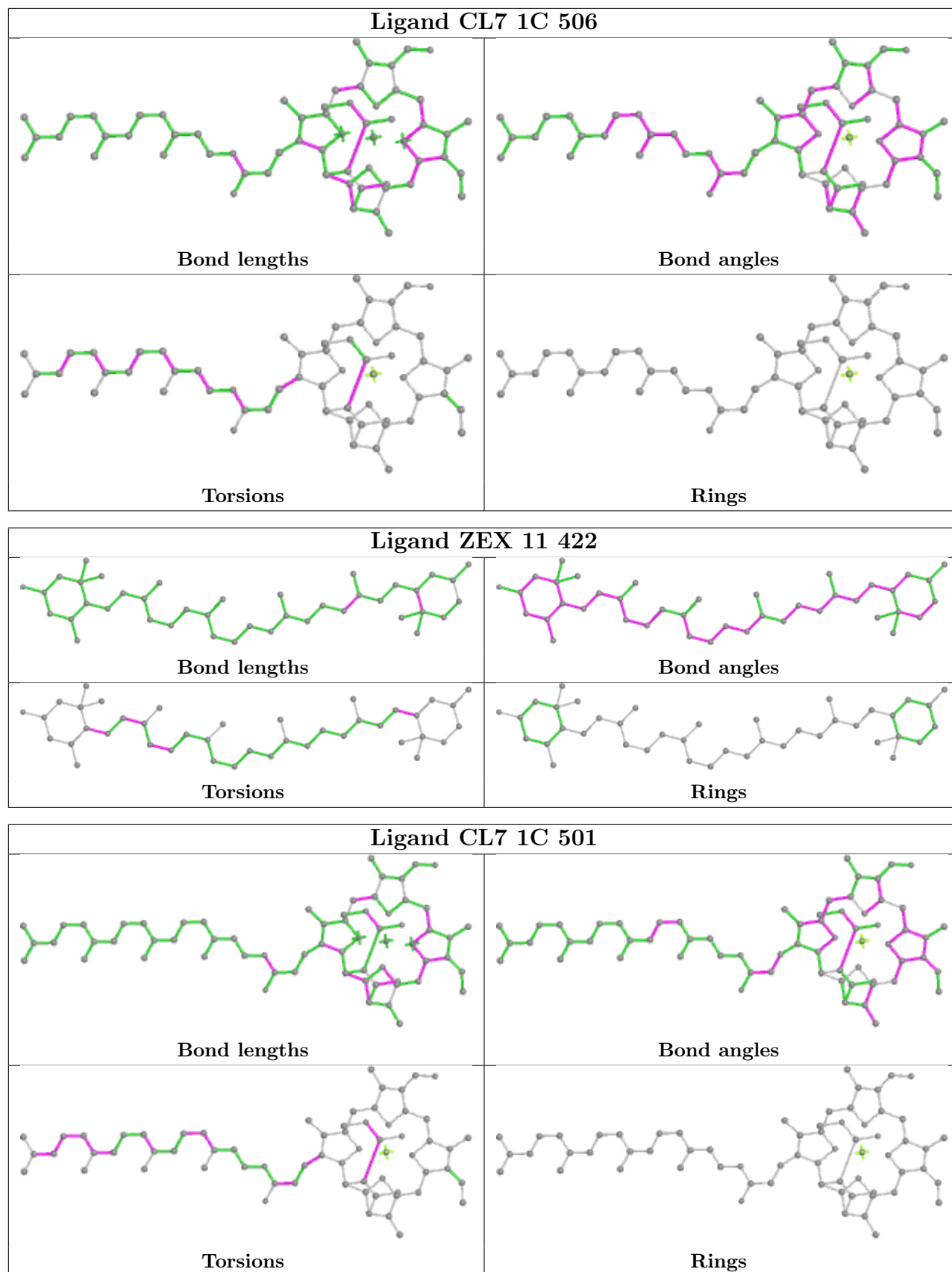


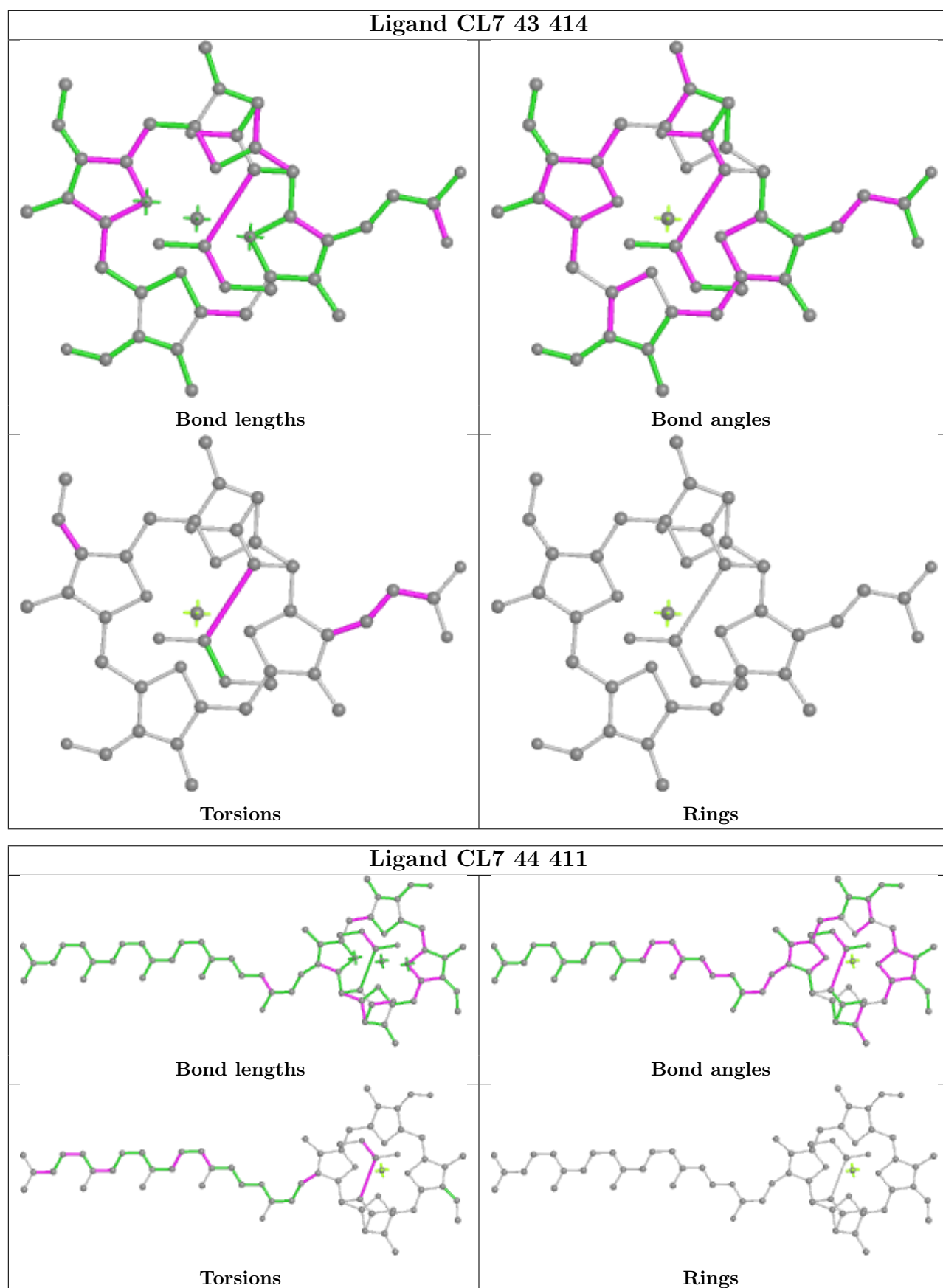


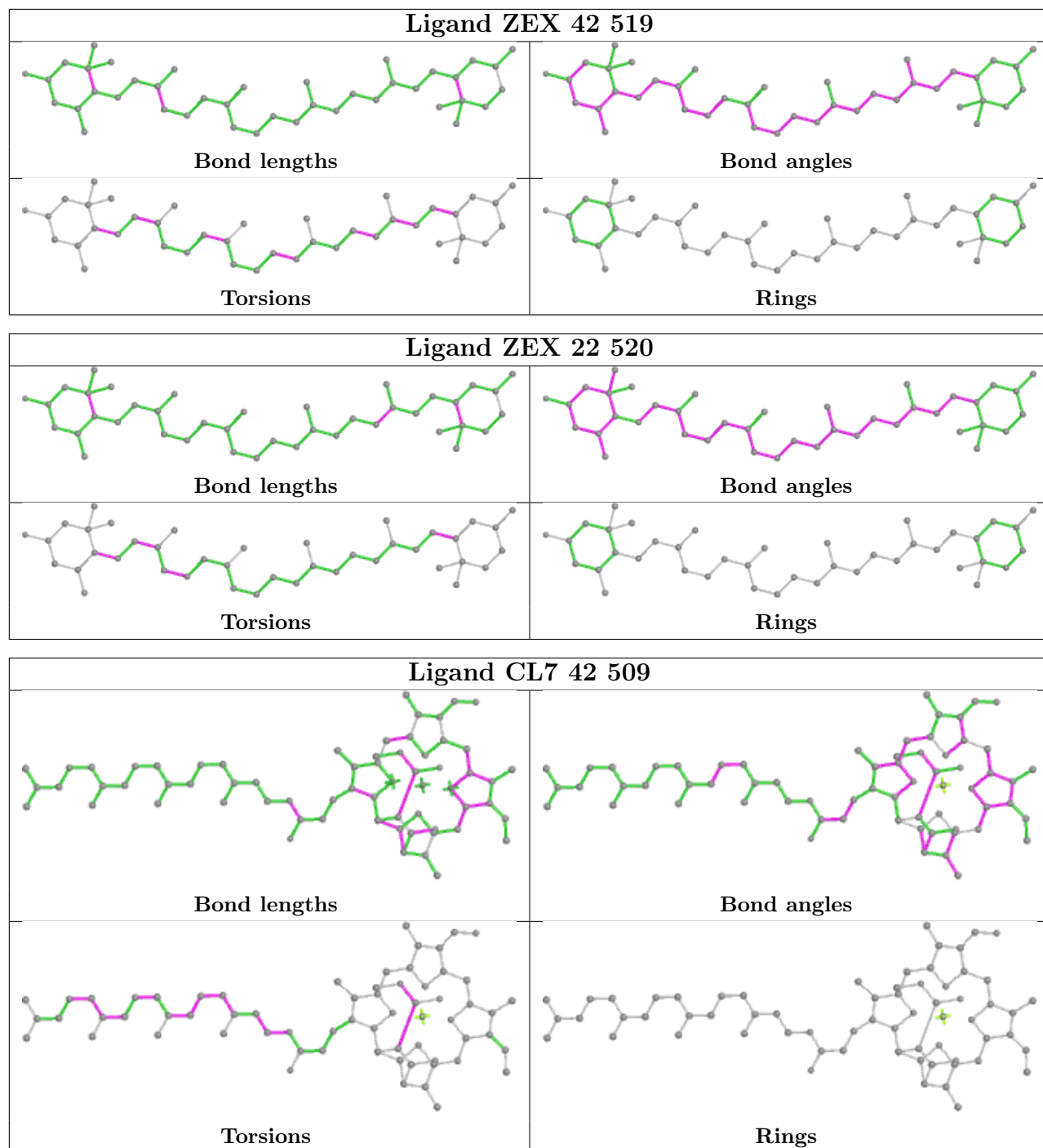


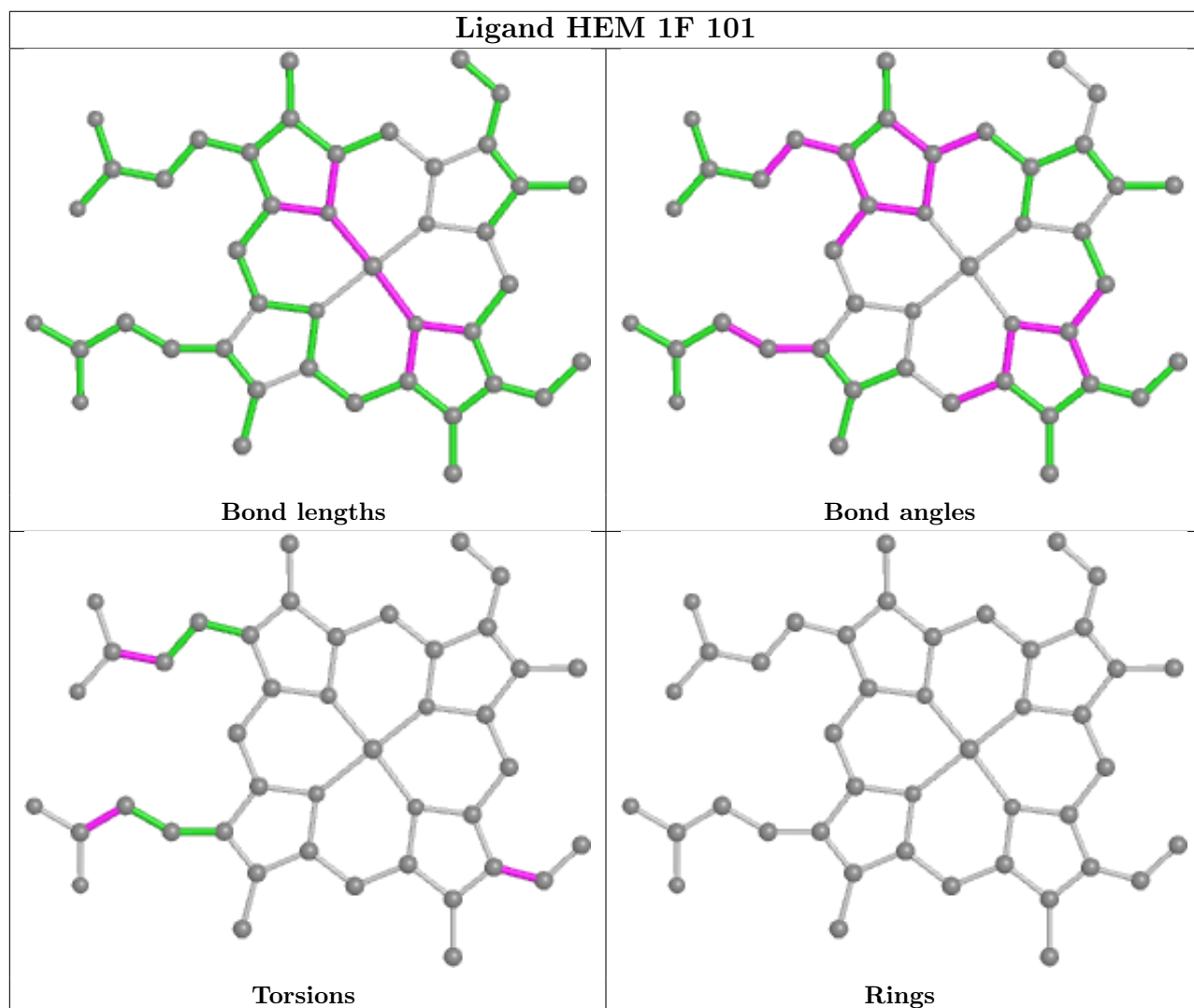
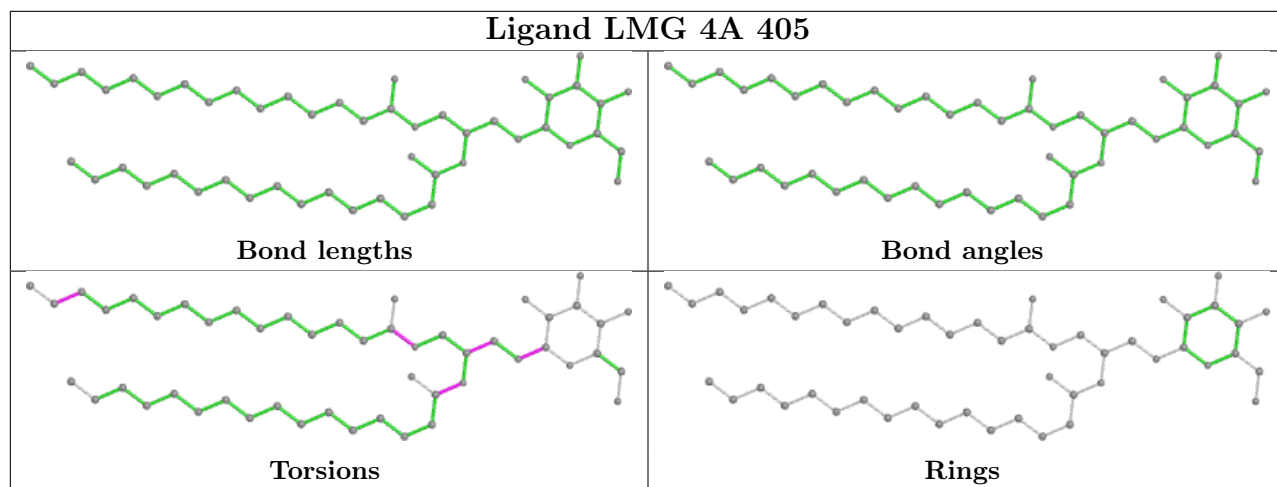


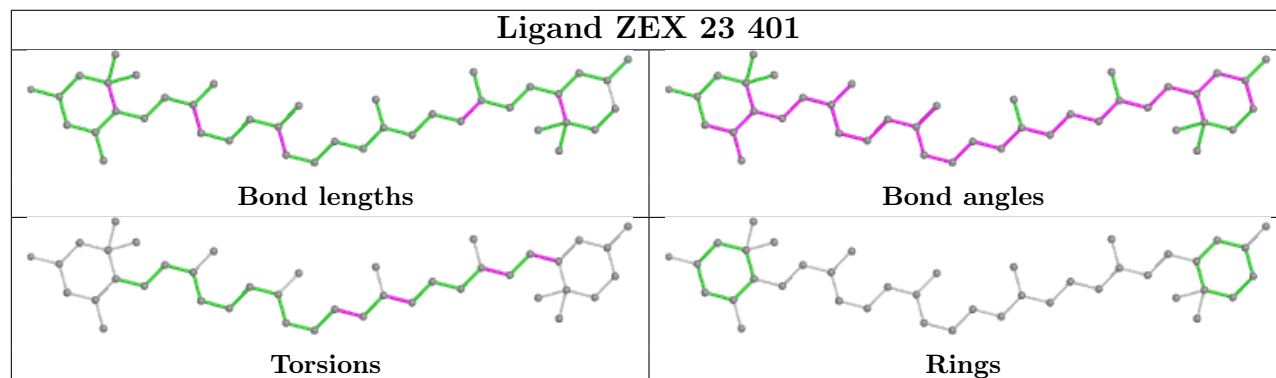
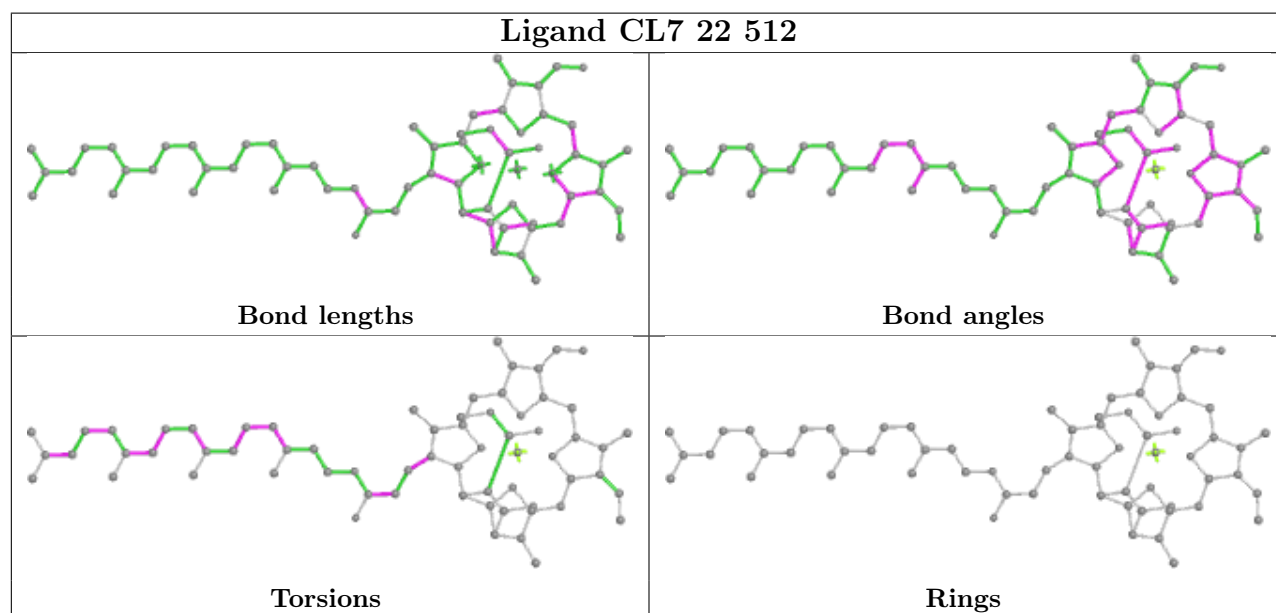
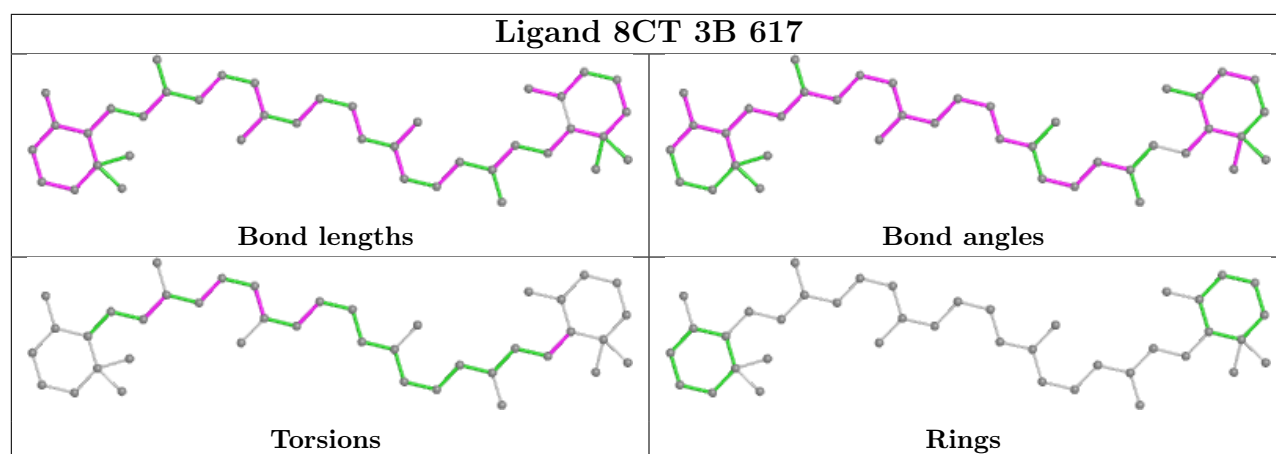


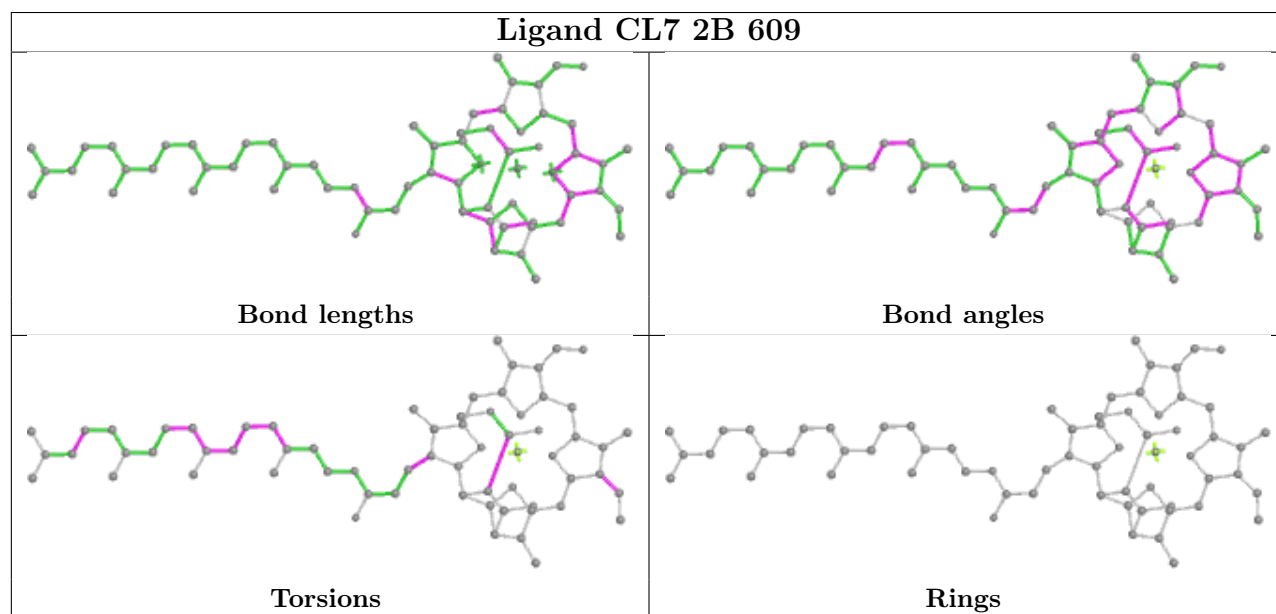
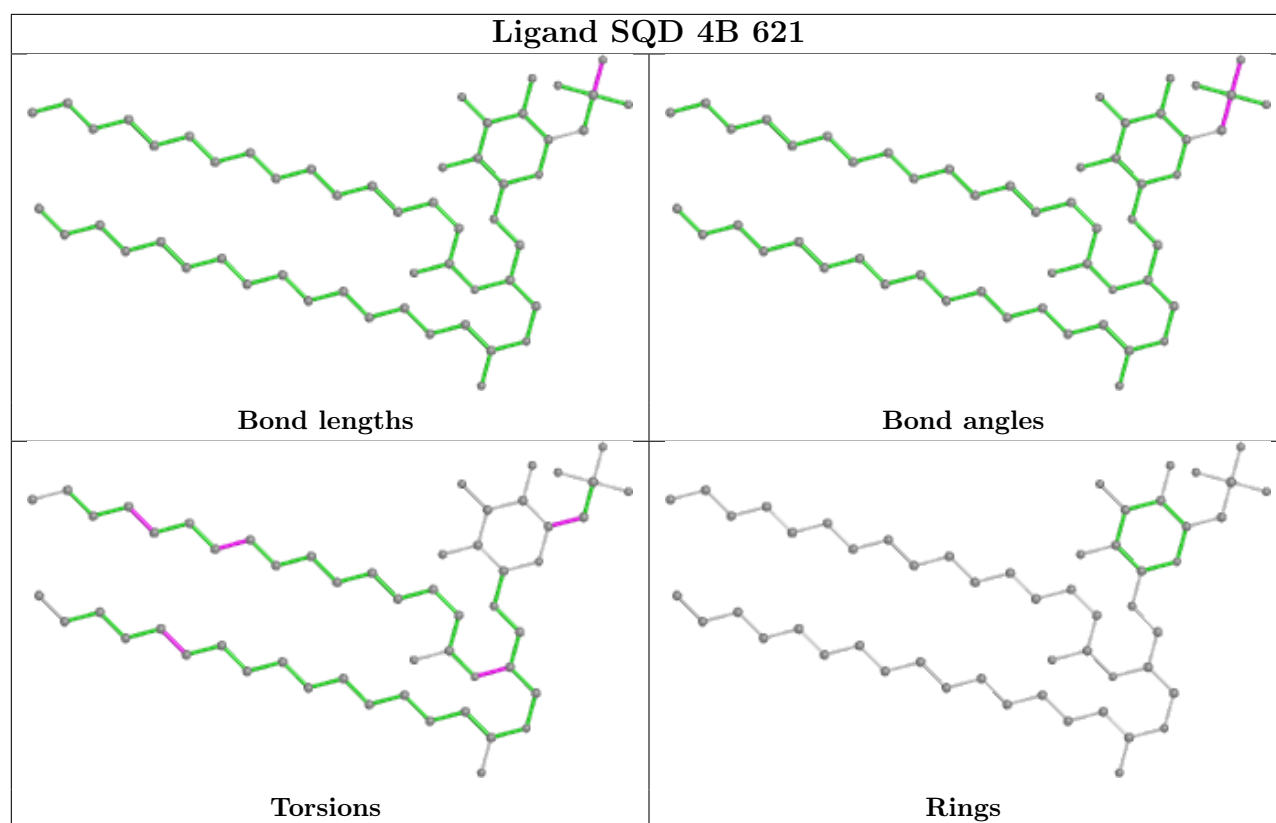


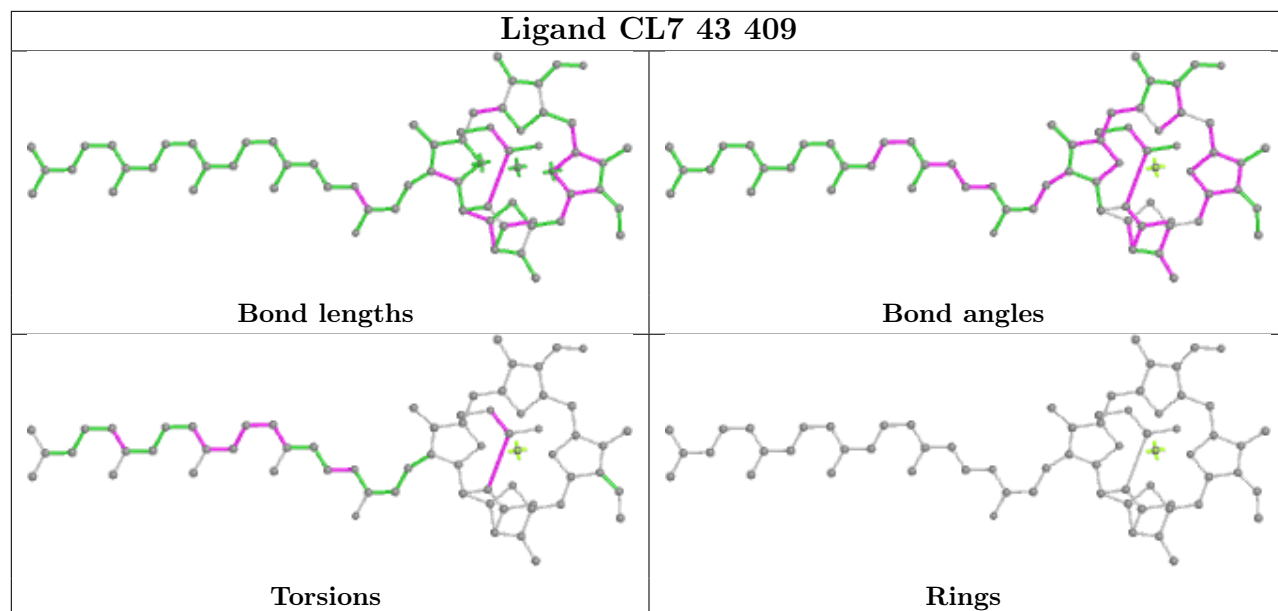


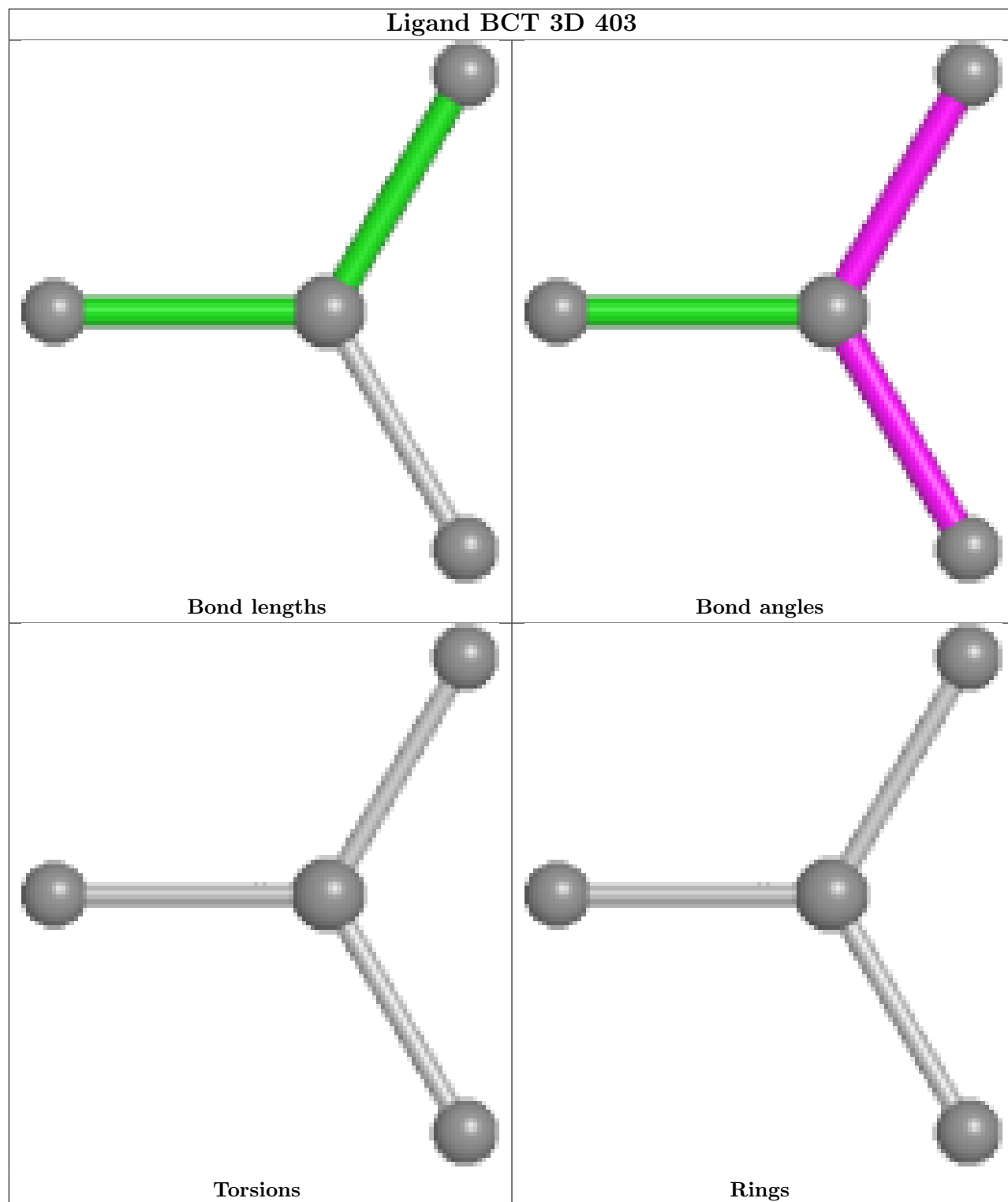


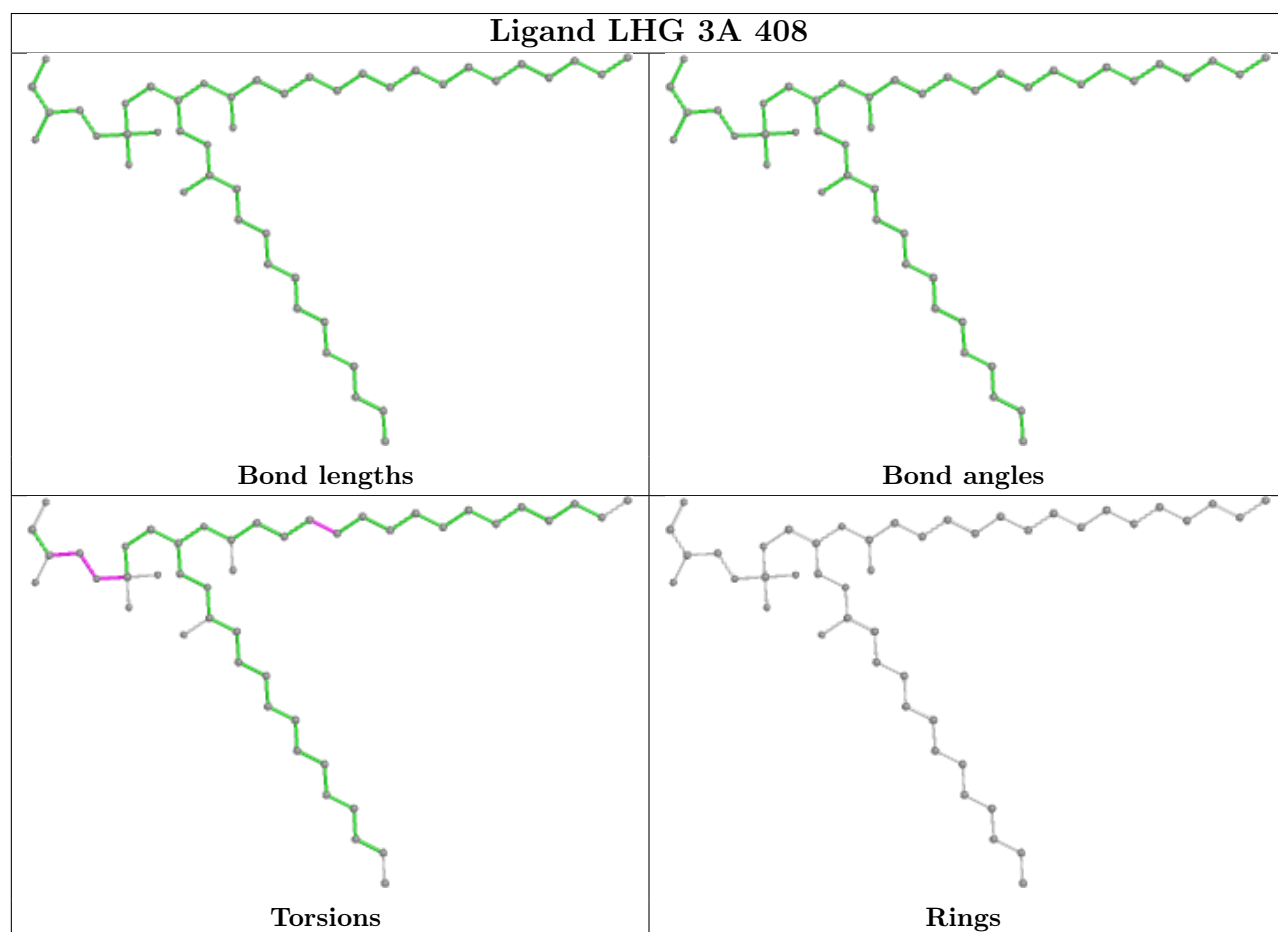
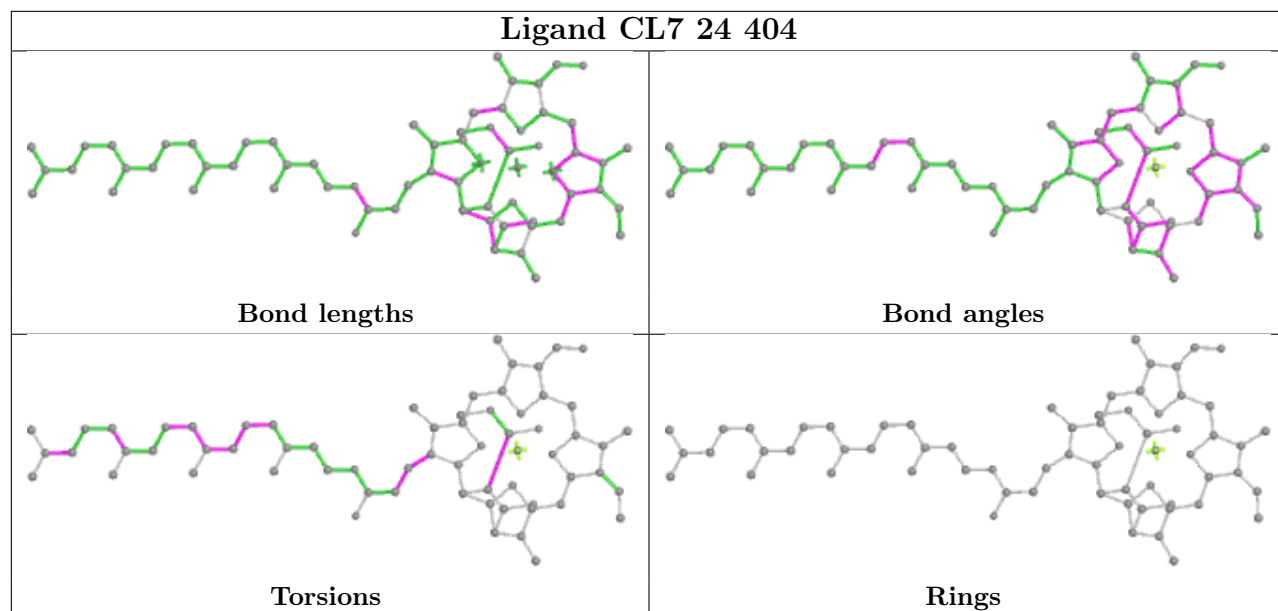


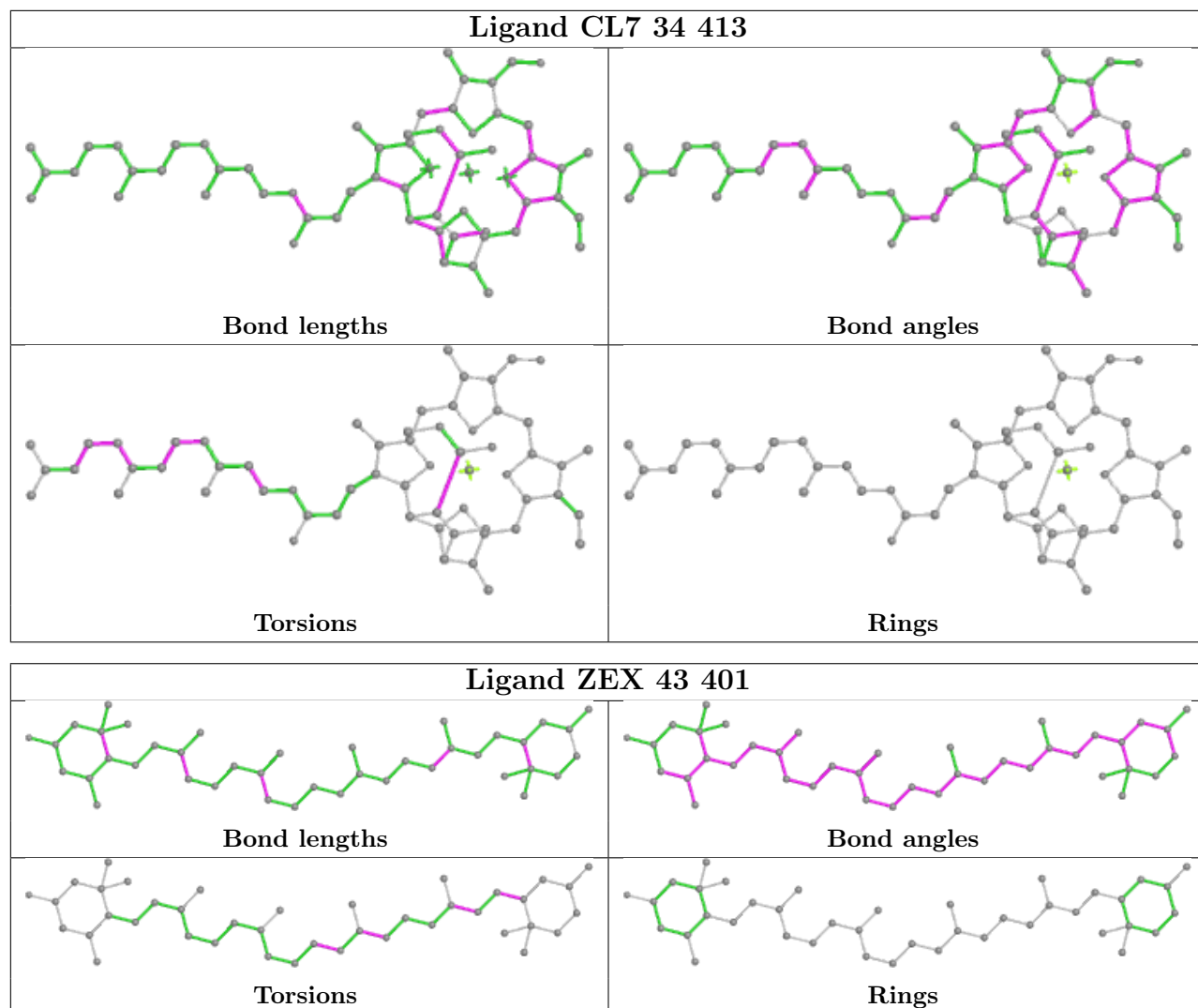


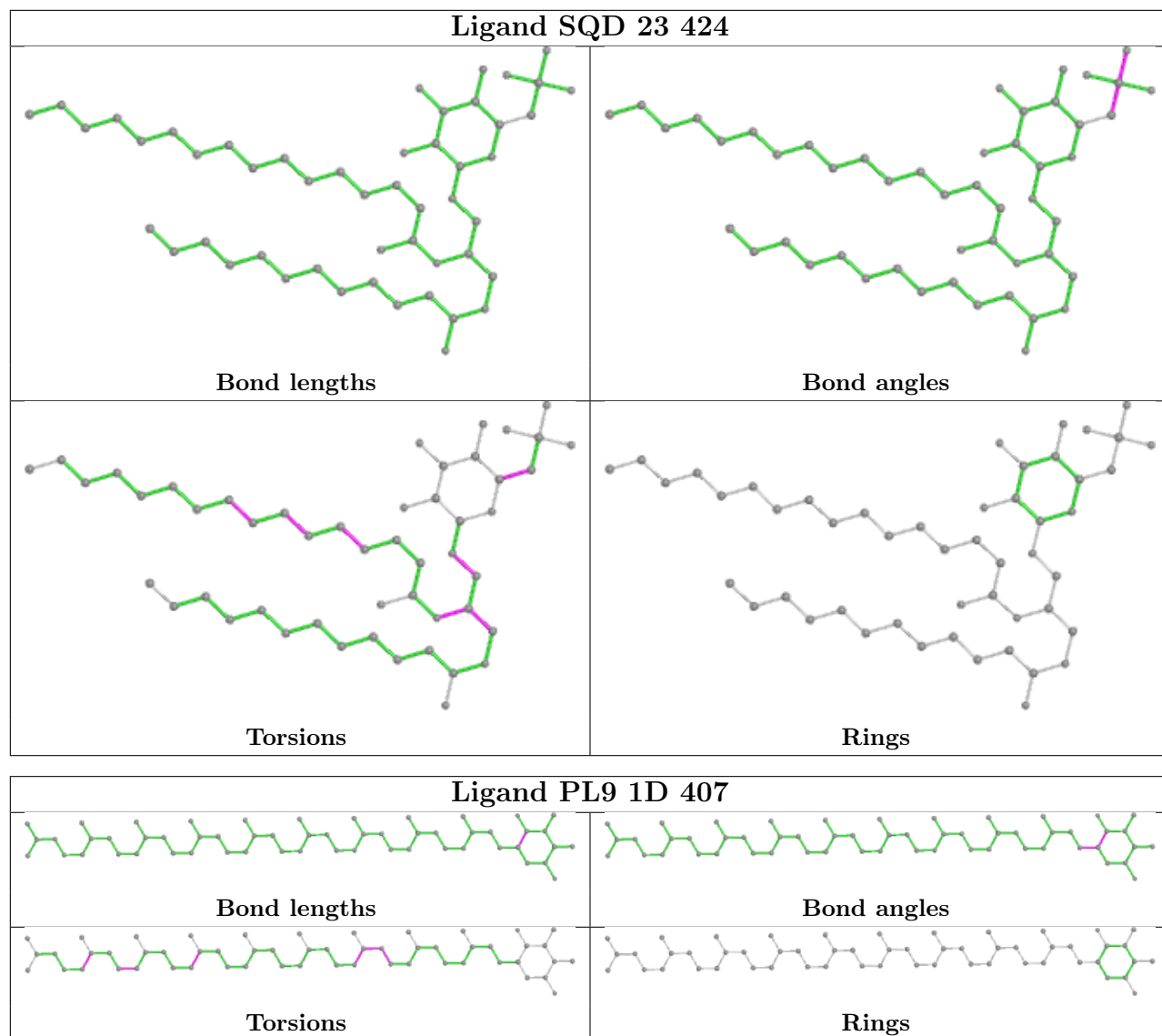


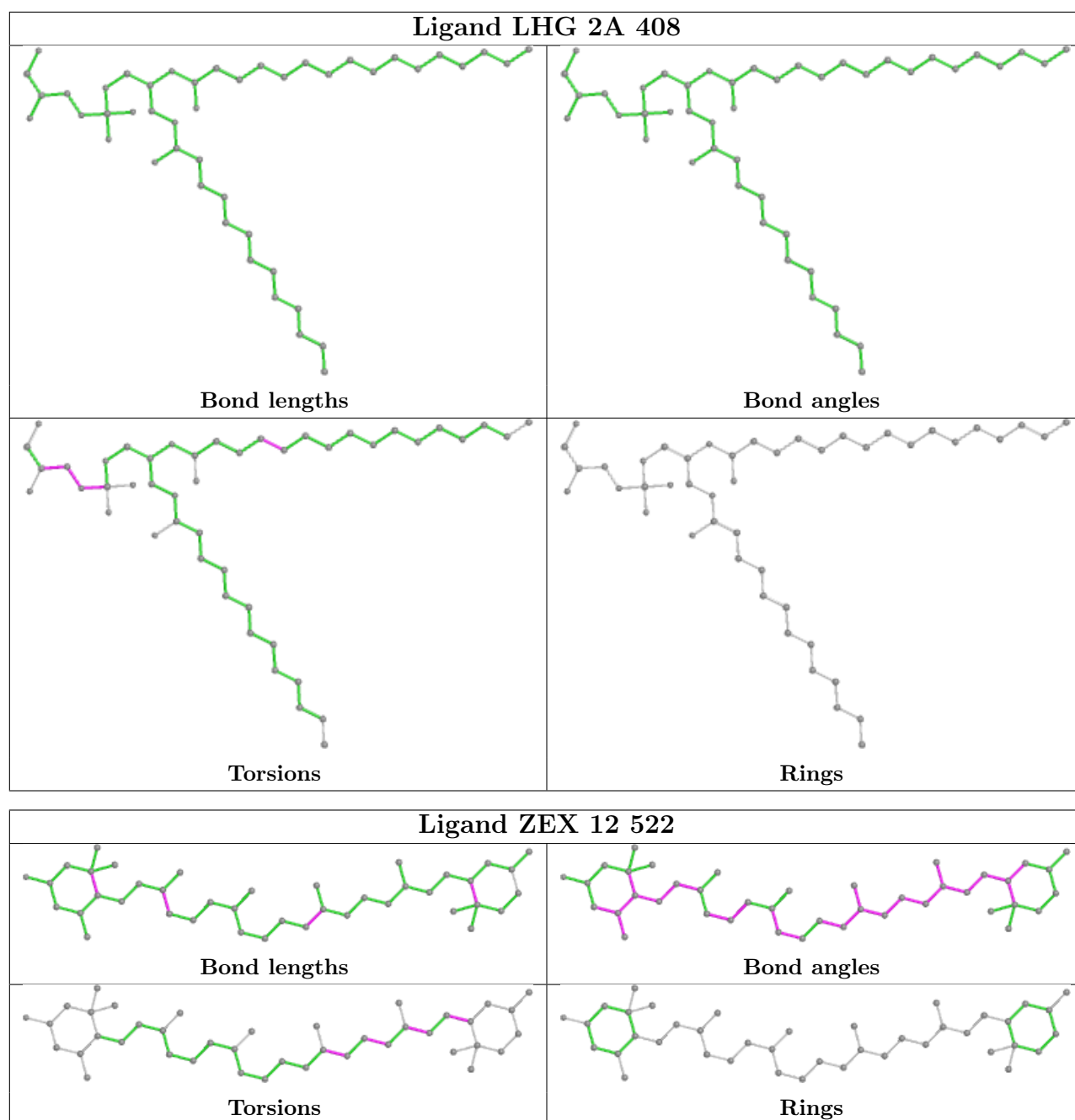












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

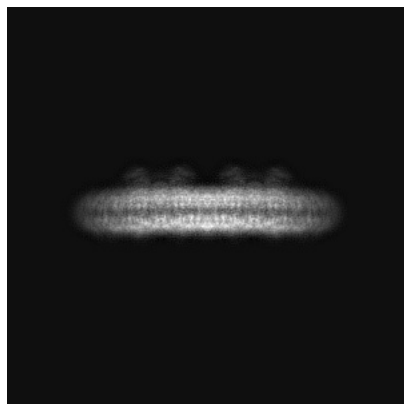
6 Map visualisation [i](#)

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.

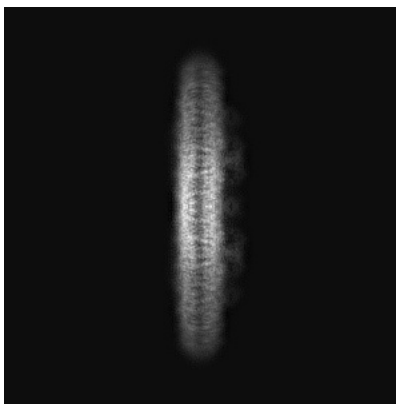
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

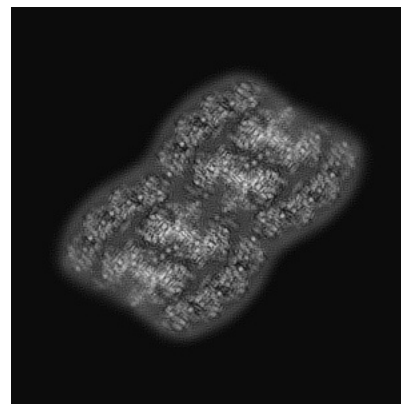
6.1.1 Primary map



X

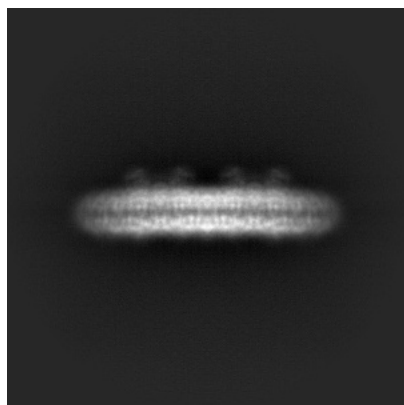


Y

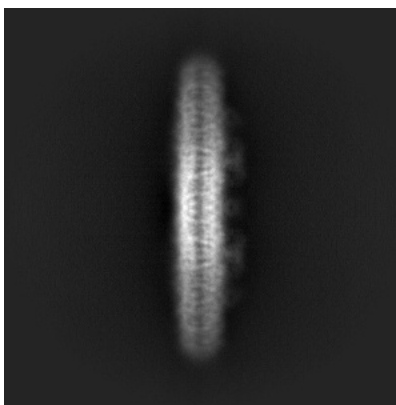


Z

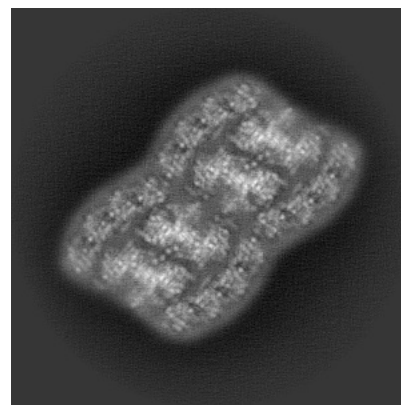
6.1.2 Raw map



X



Y

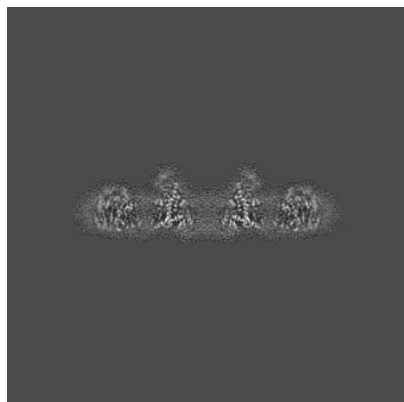


Z

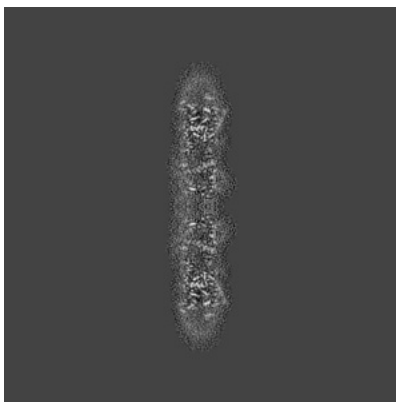
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

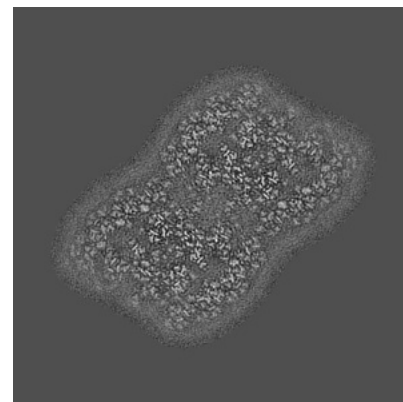
6.2.1 Primary map



X Index: 240

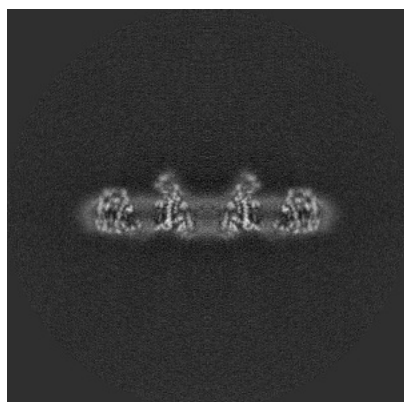


Y Index: 240

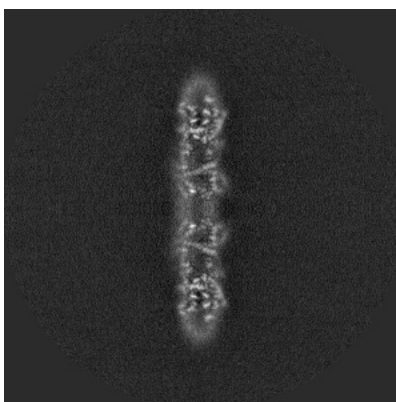


Z Index: 240

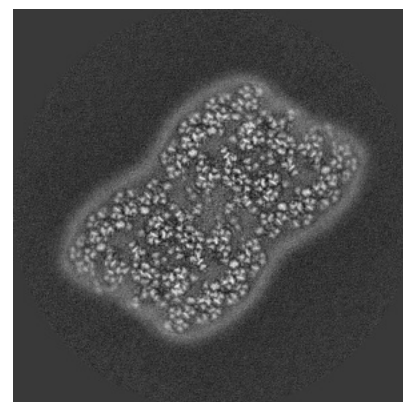
6.2.2 Raw map



X Index: 240



Y Index: 240

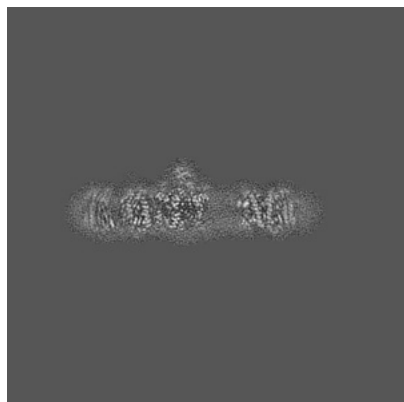


Z Index: 240

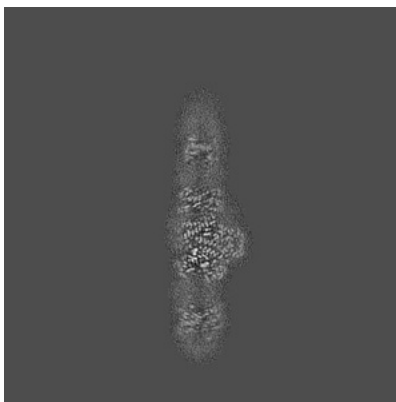
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

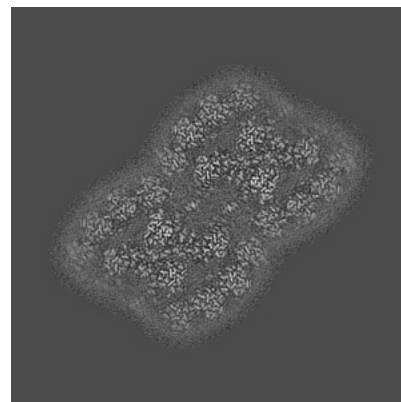
6.3.1 Primary map



X Index: 204

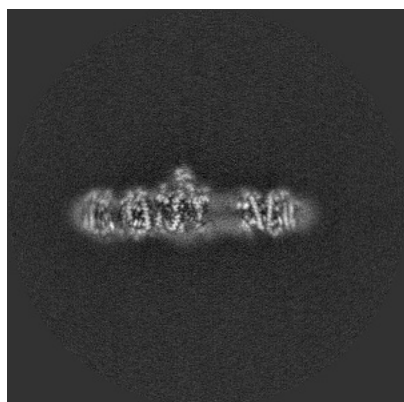


Y Index: 208

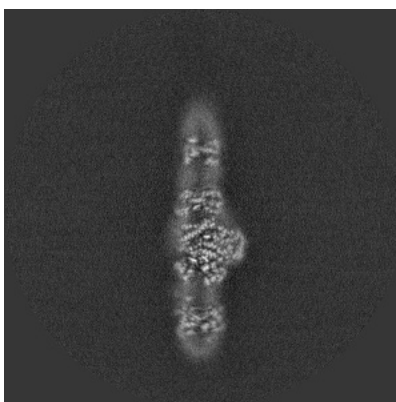


Z Index: 225

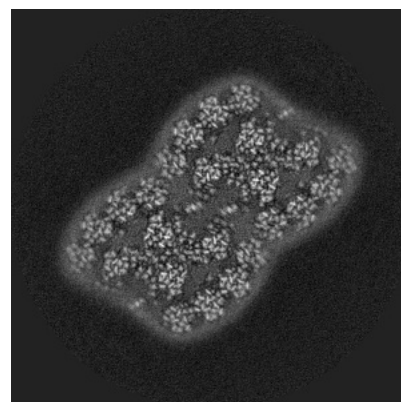
6.3.2 Raw map



X Index: 204



Y Index: 209

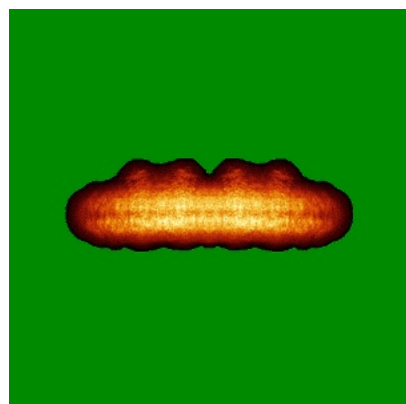


Z Index: 224

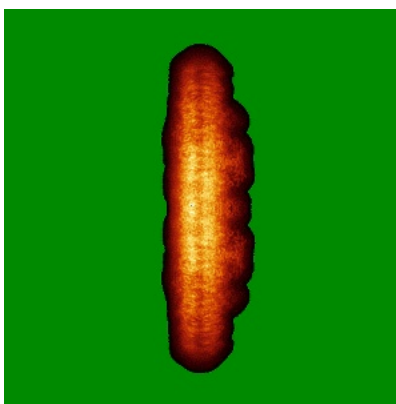
The images above show the largest variance slices of the map in three orthogonal directions.

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

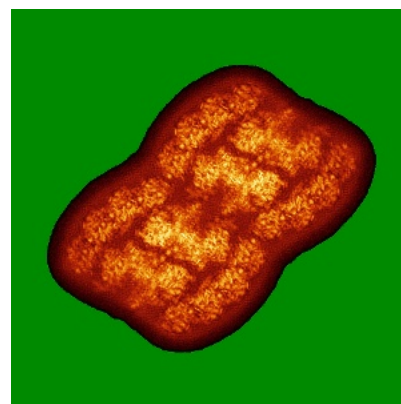
6.4.1 Primary map



X

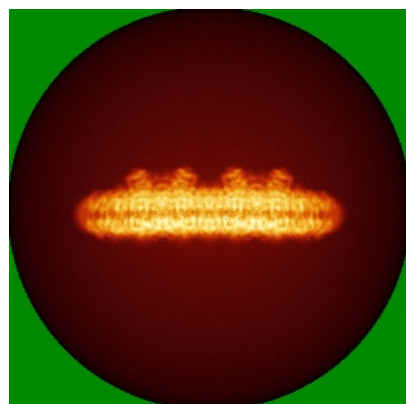


Y

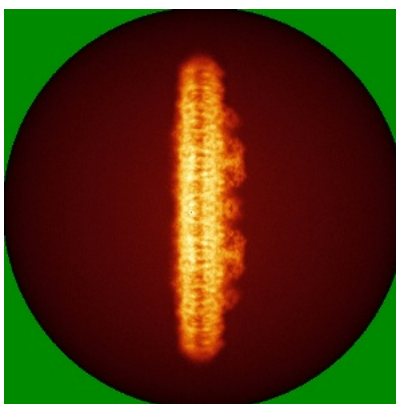


Z

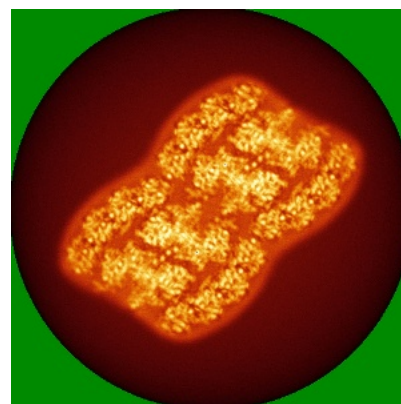
6.4.2 Raw map



X



Y

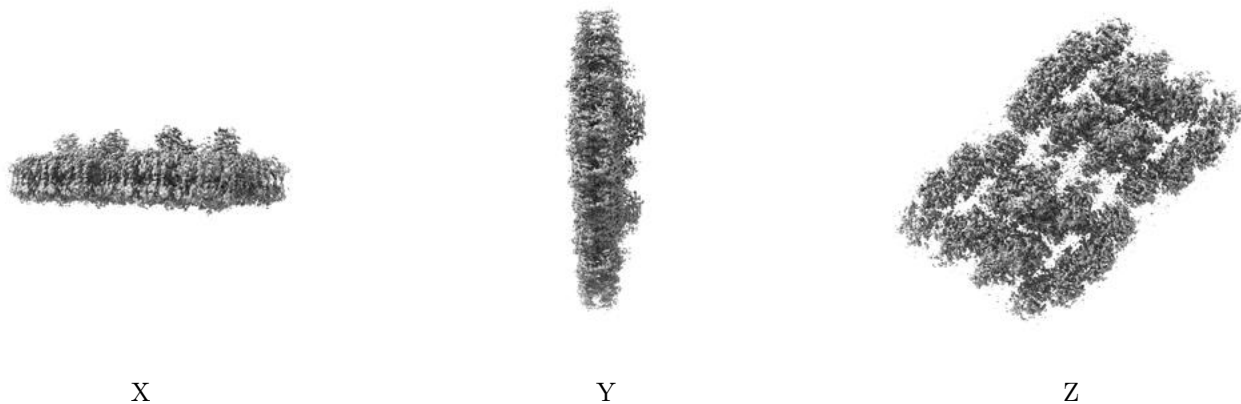


Z

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.

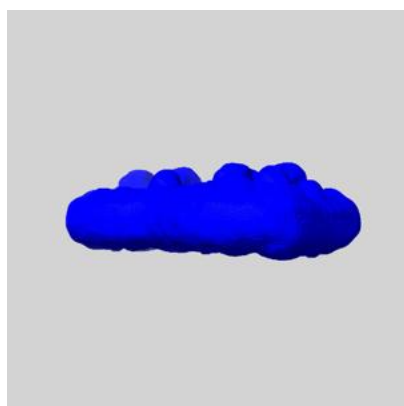
6.6 Mask visualisation [i](#)

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

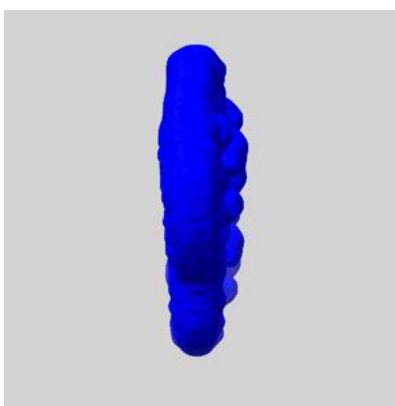
A mask typically either:

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

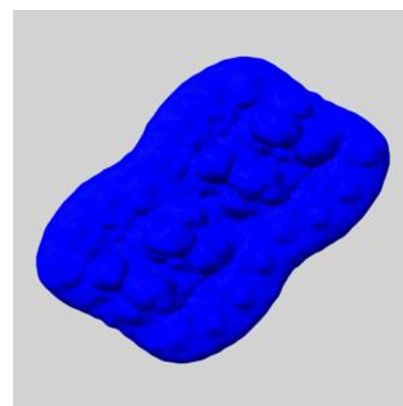
6.6.1 emd_33933_msk_1.map [i](#)



X



Y

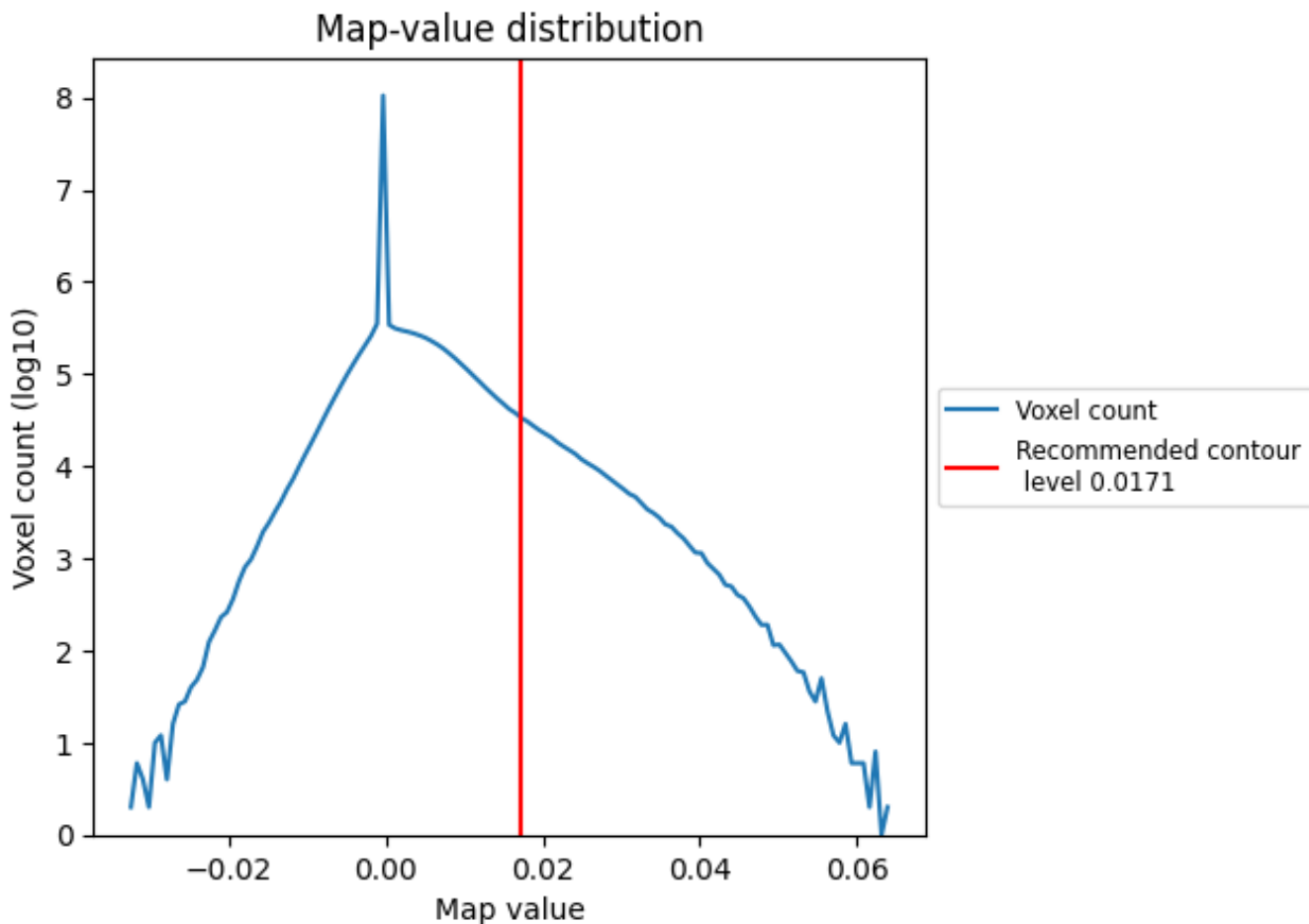


Z

7 Map analysis [i](#)

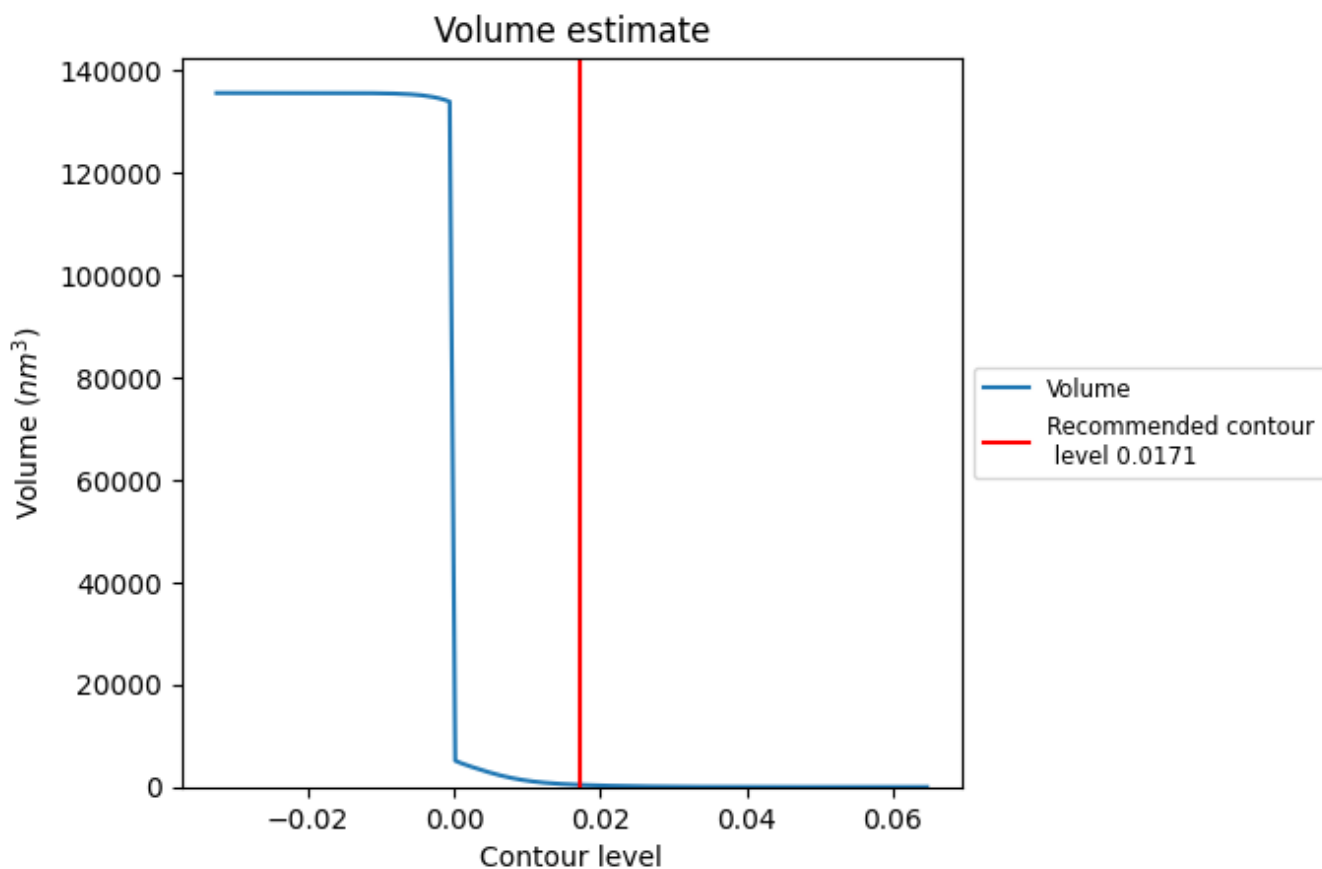
This section contains the results of statistical analysis of the map.

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.

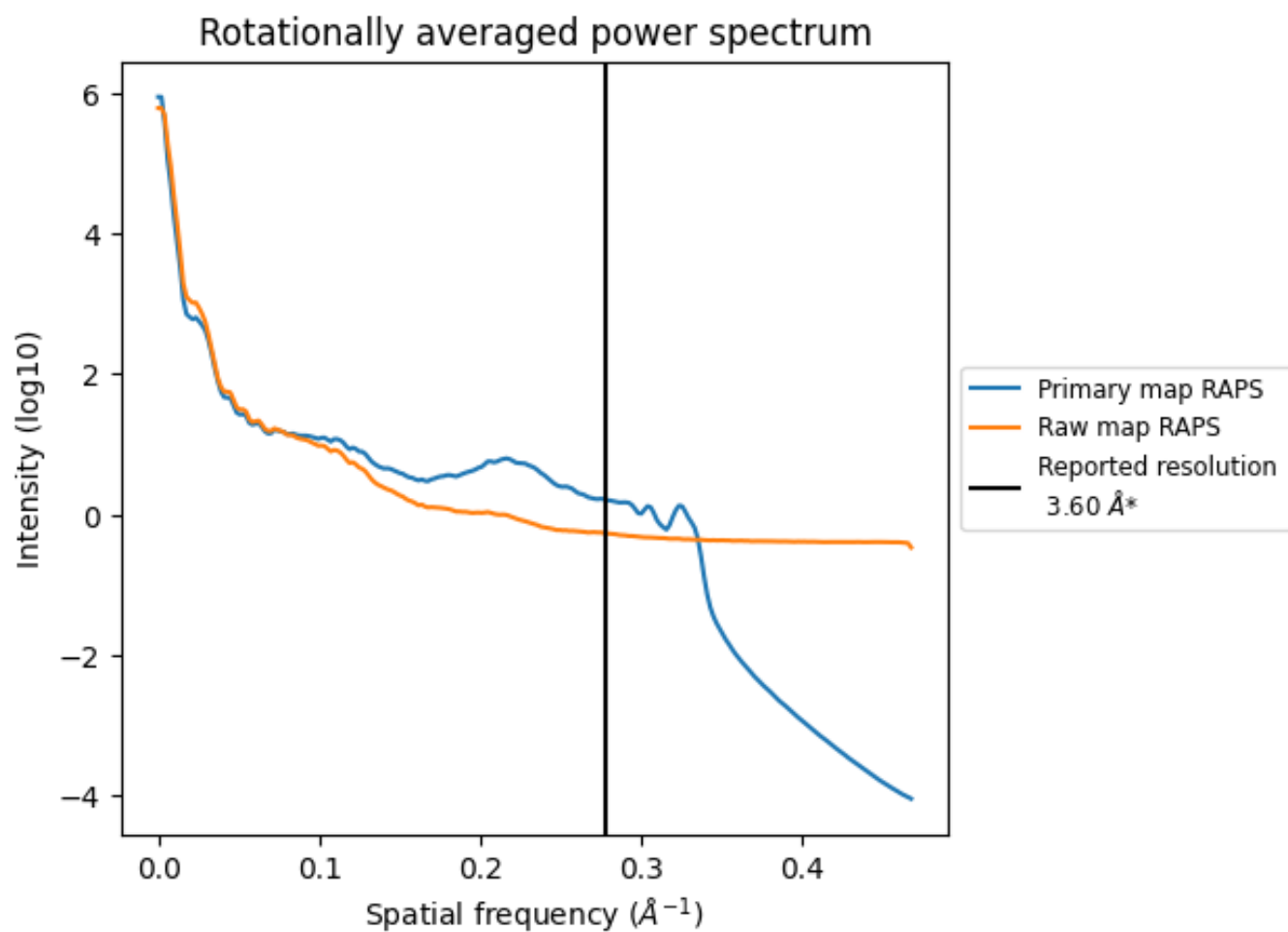
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 416 nm³; this corresponds to an approximate mass of 376 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

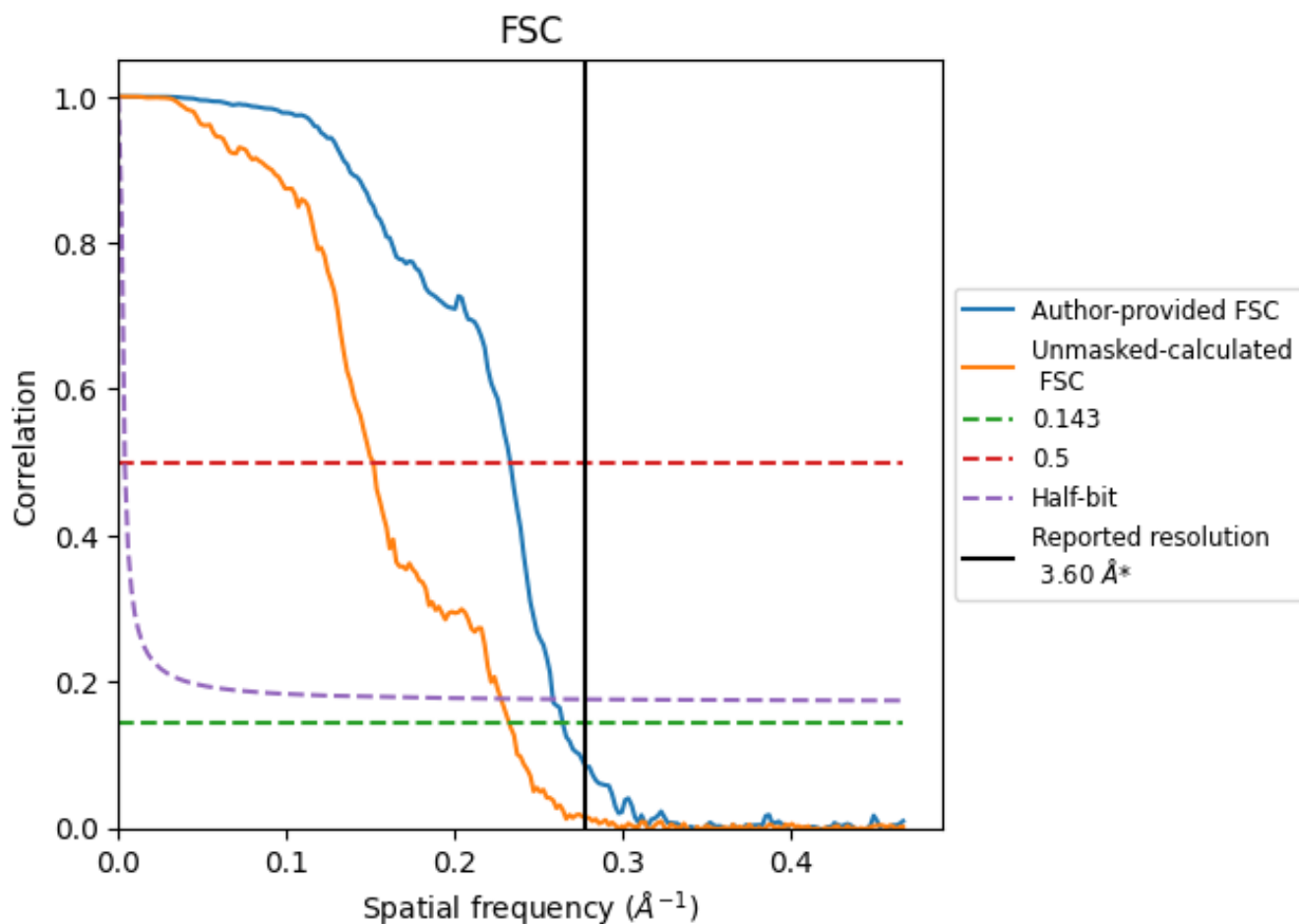


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [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 Å⁻¹

8.2 Resolution estimates [i](#)

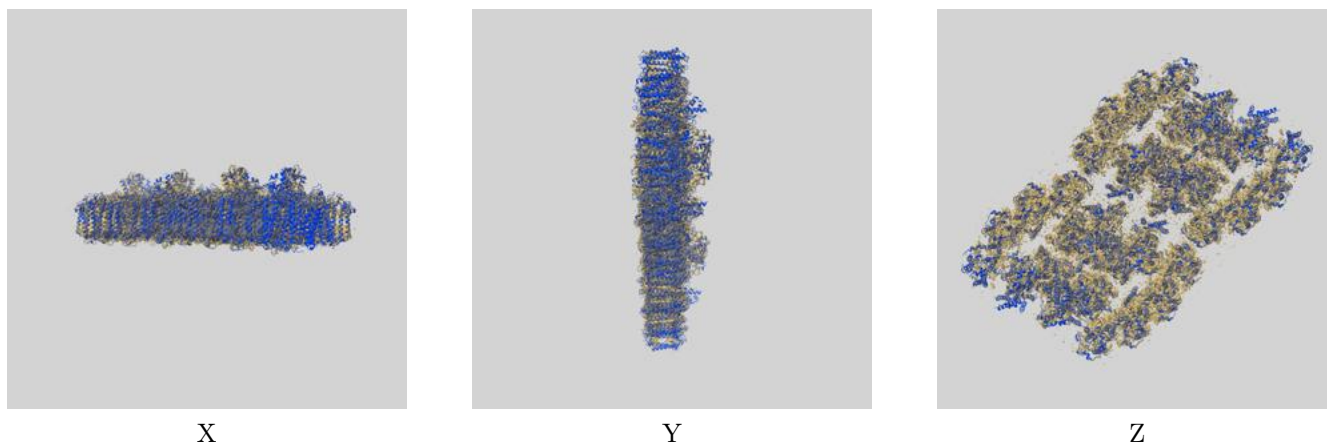
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.78	4.28	3.87
Unmasked-calculated*	4.30	6.59	4.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

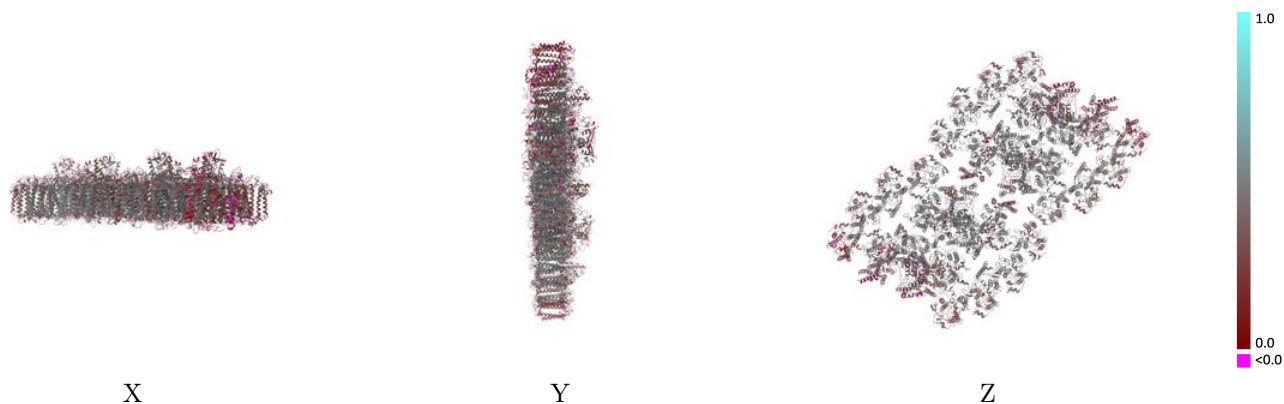
This section contains information regarding the fit between EMDB map EMD-33933 and PDB model 7YMM. Per-residue inclusion information can be found in section 3 on page 59.

9.1 Map-model overlay [i](#)



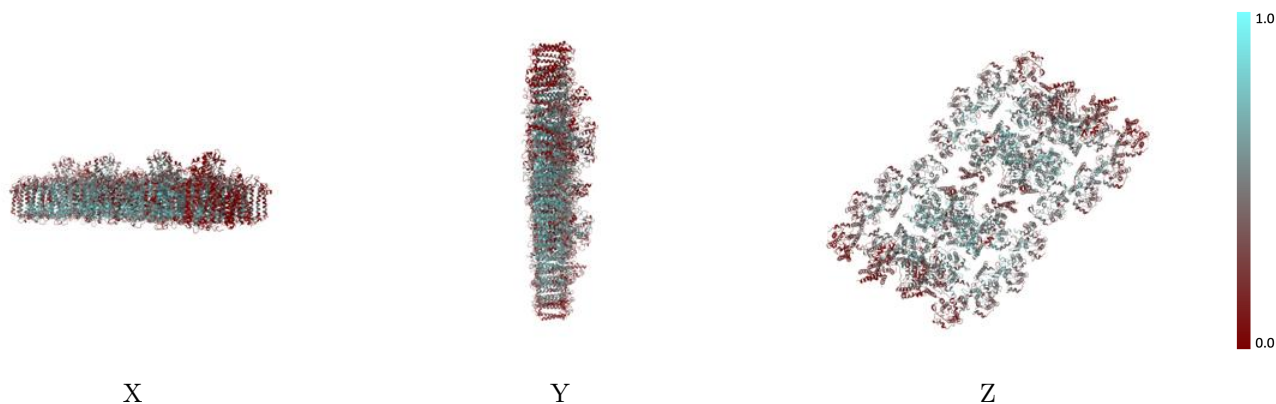
The images above show the 3D surface view of the map at the recommended contour level 0.0171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



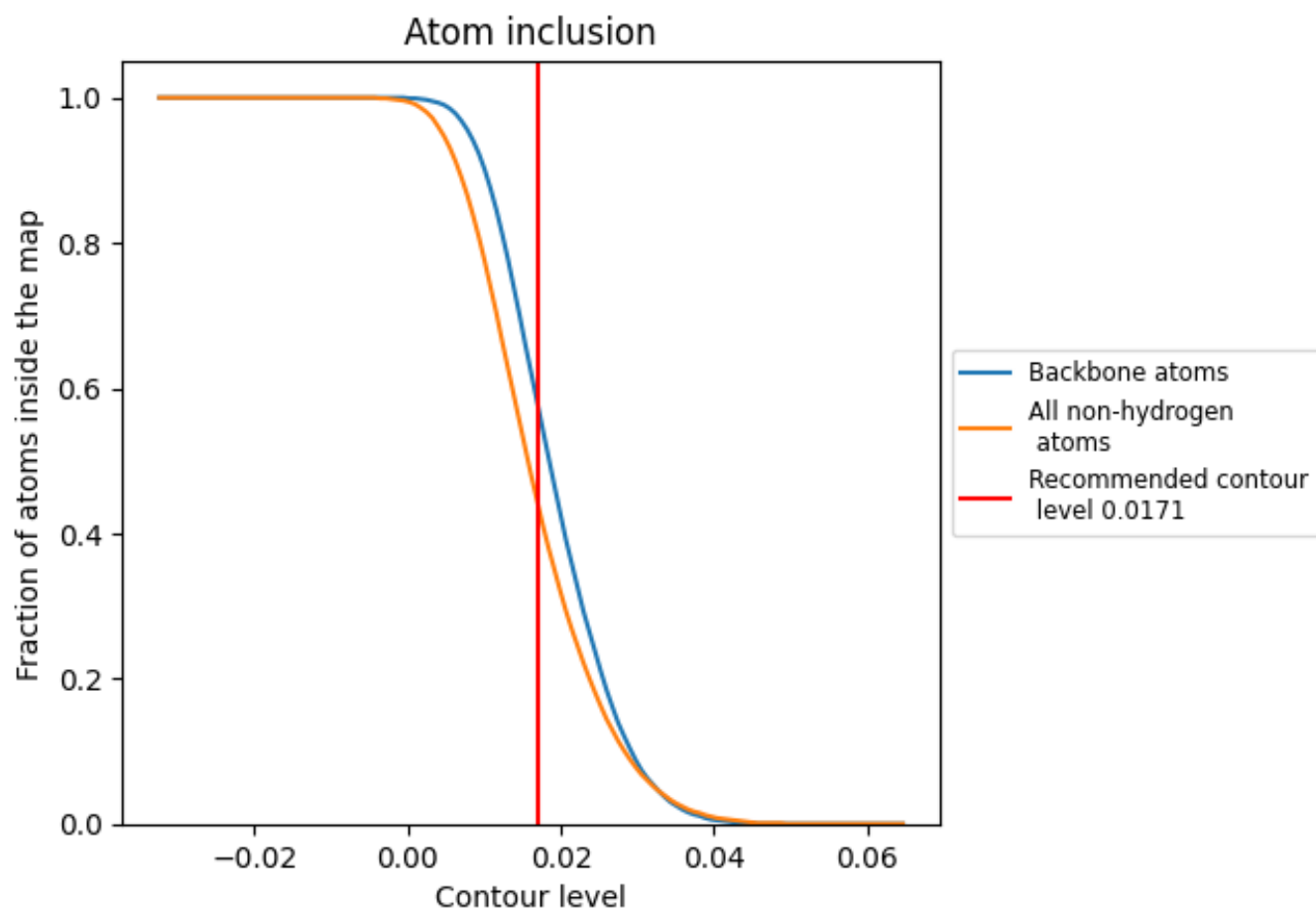
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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