



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 03:21 PM EDT

PDB ID : 7UMH / pdb_00007umh
EMDB ID : EMD-26601
Title : Energetic robustness to large scale structural dynamics in a photosynthetic supercomplex
Authors : Harris, D.; Toporik, H.; Schlau-Cohen, G.S.; Mazor, Y.
Deposited on : 2022-04-07
Resolution : 2.60 Å(reported)
Based on initial model : 6NWA

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

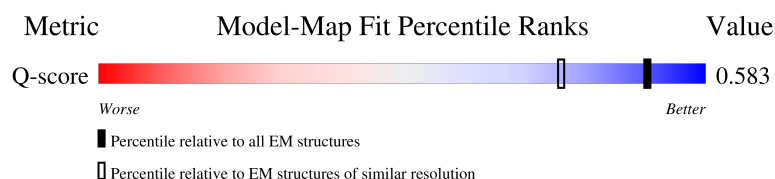
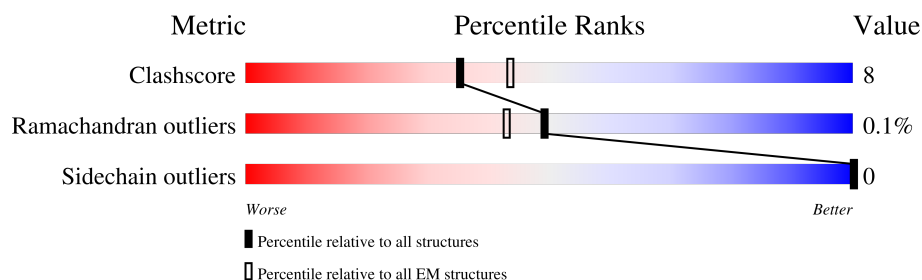
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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



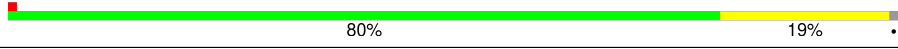
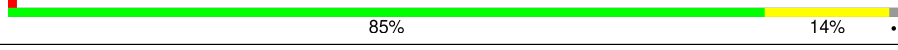
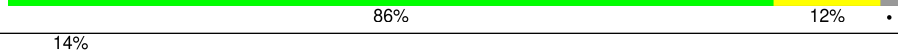
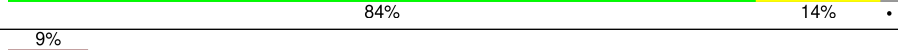
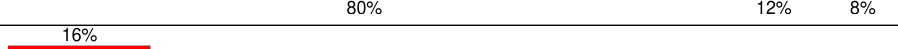
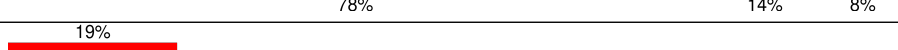
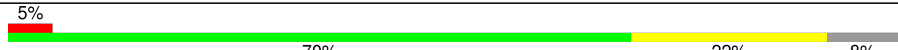
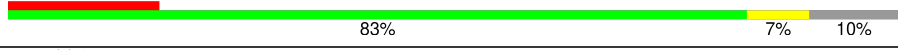
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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

Mol	Chain	Length	Quality of chain
1	A	751	
1	H	751	
1	a	751	
2	B	731	

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Mol	Chain	Length	Quality of chain
2	G	731	
2	b	731	
3	C	81	
3	N	81	
3	c	81	
4	D	141	
4	P	141	
4	d	141	
5	E	74	
5	O	74	
5	e	74	
6	F	165	
6	Q	165	
6	f	165	
7	I	40	
7	R	40	
7	i	40	
8	J	40	
8	S	40	
8	j	40	
9	K	86	
9	T	86	
9	k	86	
10	L	157	
10	U	157	

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Mol	Chain	Length	Quality of chain
10	l	157	
11	M	31	
11	V	31	
11	m	31	
12	W	342	
12	X	342	
12	Y	342	
12	Z	342	
12	g	342	
12	h	342	
12	n	342	
12	o	342	
12	p	342	
12	q	342	
12	r	342	
12	s	342	
12	t	342	
12	u	342	
12	v	342	
12	w	342	
12	x	342	
12	y	342	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 140516 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 I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	H	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	a	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		
2	G	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		
2	b	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	N	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		
4	d	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	68	Total	C	N	O		0	0
			537	337	95	105			
5	O	68	Total	C	N	O		0	0
			537	337	95	105			
5	e	68	Total	C	N	O		0	0
			537	337	95	105			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	Q	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	f	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	R	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	i	37	Total	C	N	O	S	0	0
			293	200	41	49	3		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			311	210	46	52	3		
8	S	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit Psak 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	77	Total	C	N	O	S	0	0
			538	353	89	92	4		
9	T	77	Total	C	N	O	S	0	0
			538	353	89	92	4		
9	k	77	Total	C	N	O	S	0	0
			538	353	89	92	4		

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		
10	U	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		
10	l	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	V	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is a protein called Iron stress-induced chlorophyll-binding protein.

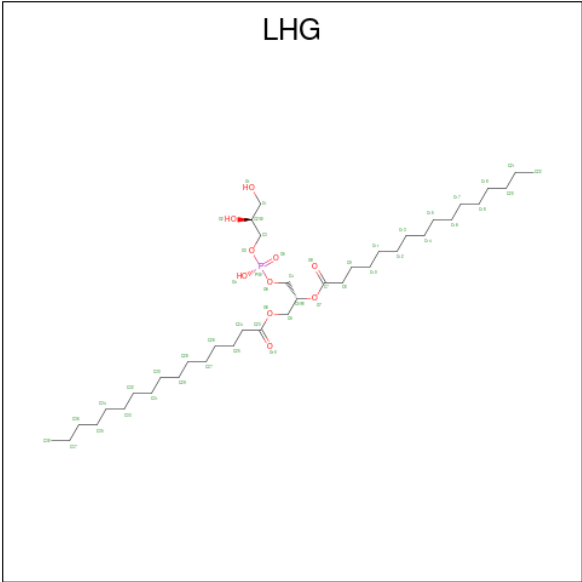
Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	X	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	Y	340	Total	C	N	O	S	0	0
			2622	1744	428	445	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	g	333	Total	C	N	O	S	0	0
			2573	1714	420	434	5		
12	h	330	Total	C	N	O	S	0	0
			2538	1692	412	429	5		
12	n	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	o	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	p	340	Total	C	N	O	S	0	0
			2622	1744	428	445	5		
12	q	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	r	332	Total	C	N	O	S	0	0
			2566	1709	419	433	5		
12	s	339	Total	C	N	O	S	0	0
			2617	1741	427	444	5		
12	t	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	u	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	v	330	Total	C	N	O	S	0	0
			2538	1692	412	429	5		
12	w	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	x	332	Total	C	N	O	S	0	0
			2566	1709	419	433	5		
12	y	330	Total	C	N	O	S	0	0
			2532	1689	409	429	5		

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



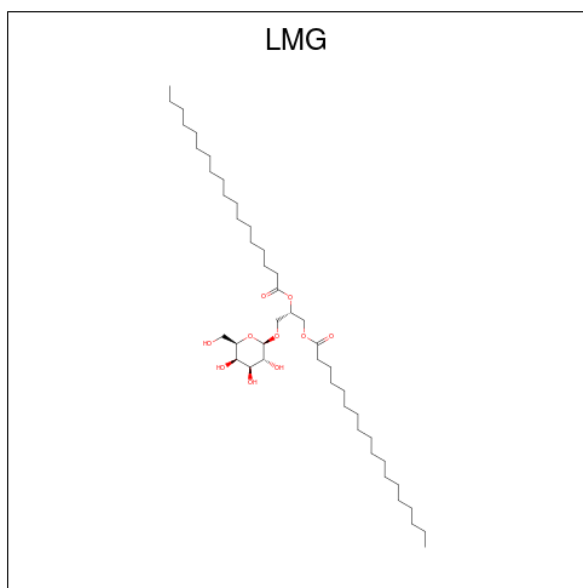
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			43	32	10	1	
13	A	1	Total	C	O	P	0
			26	15	10	1	
13	B	1	Total	C	O	P	0
			38	27	10	1	
13	G	1	Total	C	O	P	0
			38	27	10	1	
13	H	1	Total	C	O	P	0
			43	32	10	1	
13	H	1	Total	C	O	P	0
			26	15	10	1	
13	I	1	Total	C	O	P	0
			40	29	10	1	
13	R	1	Total	C	O	P	0
			40	29	10	1	
13	X	1	Total	C	O	P	0
			27	16	10	1	
13	Y	1	Total	C	O	P	0
			32	21	10	1	
13	a	1	Total	C	O	P	0
			43	32	10	1	
13	a	1	Total	C	O	P	0
			26	15	10	1	
13	b	1	Total	C	O	P	0
			38	27	10	1	
13	g	1	Total	C	O	P	0
			31	20	10	1	

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Mol	Chain	Residues	Atoms				AltConf
13	i	1	Total	C	O	P	0
			40	29	10	1	
13	o	1	Total	C	O	P	0
			27	16	10	1	
13	p	1	Total	C	O	P	0
			32	21	10	1	
13	r	1	Total	C	O	P	0
			31	20	10	1	
13	s	1	Total	C	O	P	0
			32	21	10	1	
13	u	1	Total	C	O	P	0
			27	16	10	1	
13	x	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



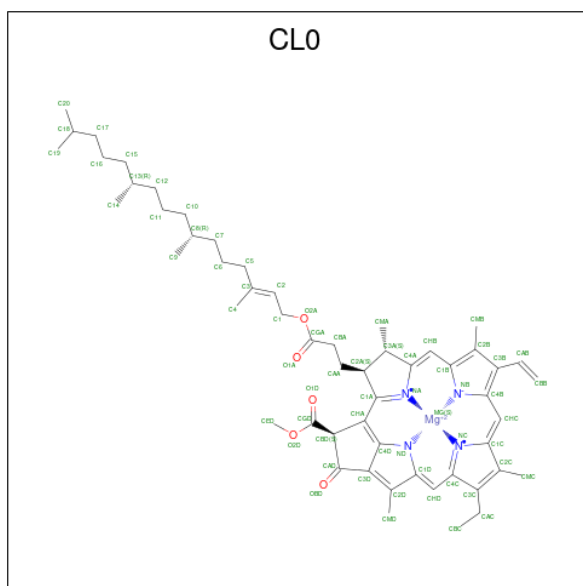
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O		0
			38	28	10		
14	A	1	Total	C	O		0
			46	36	10		
14	A	1	Total	C	O		0
			32	22	10		
14	B	1	Total	C	O		0
			43	33	10		

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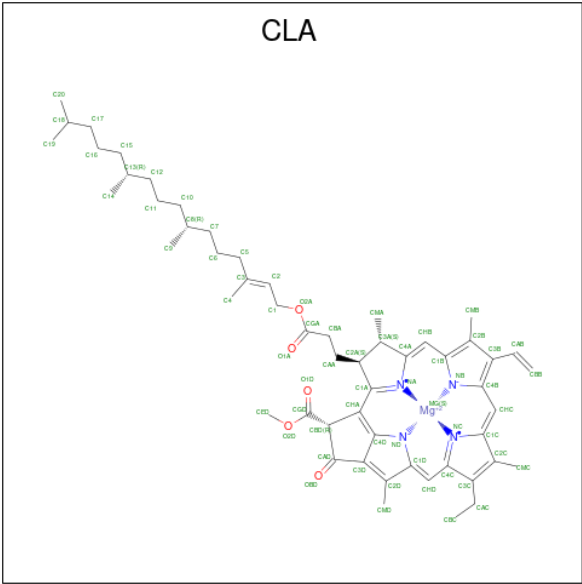
Mol	Chain	Residues	Atoms			AltConf
14	F	1	Total	C	O	0
			27	17	10	
14	G	1	Total	C	O	0
			43	33	10	
14	H	1	Total	C	O	0
			38	28	10	
14	H	1	Total	C	O	0
			46	36	10	
14	H	1	Total	C	O	0
			32	22	10	
14	Q	1	Total	C	O	0
			27	17	10	
14	a	1	Total	C	O	0
			38	28	10	
14	a	1	Total	C	O	0
			46	36	10	
14	a	1	Total	C	O	0
			32	22	10	
14	b	1	Total	C	O	0
			43	33	10	
14	f	1	Total	C	O	0
			27	17	10	

- Molecule 15 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
16	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	G	1	Total 62	C 52	Mg 1	N 4	O 5	0
16	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	H	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	J	1	Total 37	C 31	Mg 1	N 4	O 1	0
16	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	K	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	S	1	Total 37	C 31	Mg 1	N 4	O 1	0
16	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	T	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	U	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	U	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	W	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	W	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	Y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	b	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
16	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	f	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	j	1	Total 37	C 31	Mg 1	N 4	O 1	0
16	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	l	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	n	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	o	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	o	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	o	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	o	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	s	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	t	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	t	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	t	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	t	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	u	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	u	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	u	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	u	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	v	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	v	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	v	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	v	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	v	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	w	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	w	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	w	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	w	1	Total 50	C 40	Mg 1	N 4	O 5	0

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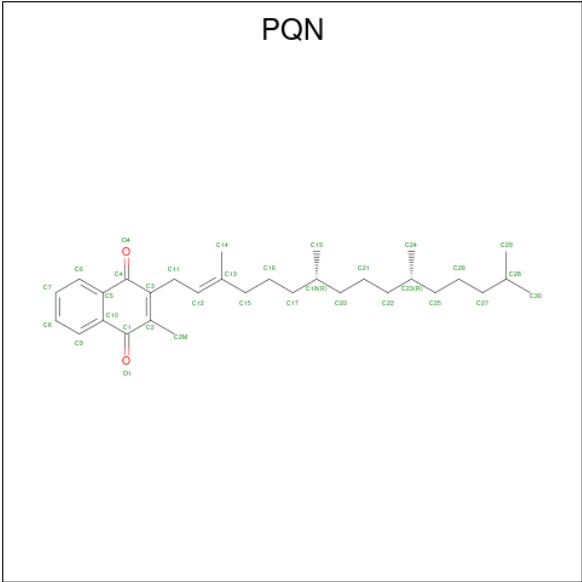
Mol	Chain	Residues	Atoms					AltConf
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	w	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	x	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	x	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	x	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	x	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	y	1	Total 46	C 36	Mg 1	N 4	O 5	0

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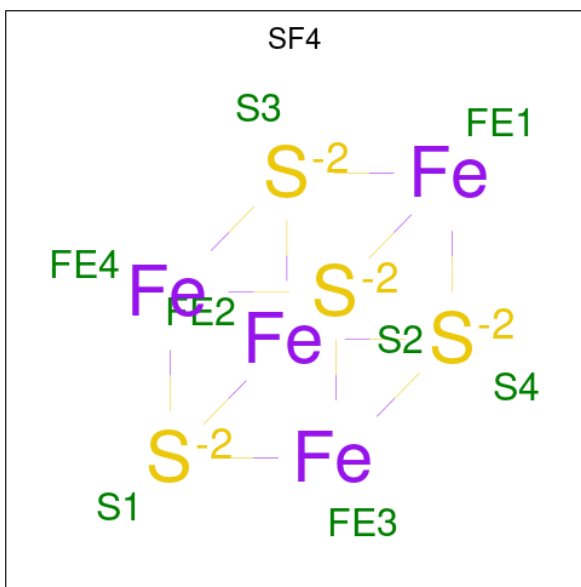
Mol	Chain	Residues	Atoms					AltConf
16	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 17 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



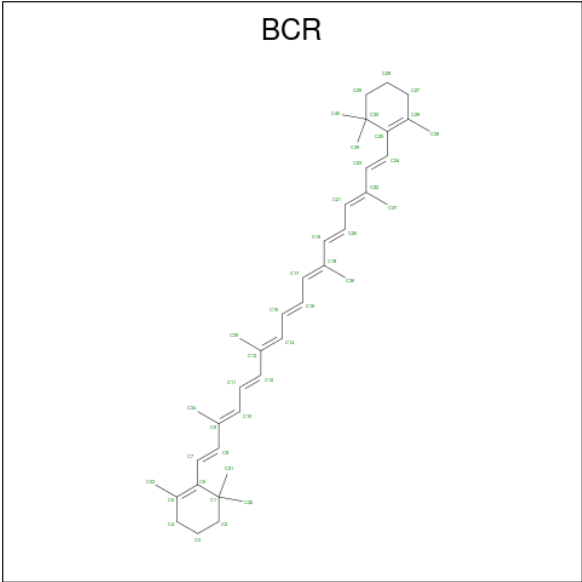
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			33	31	2	
17	B	1	Total	C	O	0
			33	31	2	
17	G	1	Total	C	O	0
			33	31	2	
17	H	1	Total	C	O	0
			33	31	2	
17	a	1	Total	C	O	0
			33	31	2	
17	b	1	Total	C	O	0
			33	31	2	

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	
18	H	1	Total	Fe	S	0
			8	4	4	
18	N	1	Total	Fe	S	0
			8	4	4	
18	N	1	Total	Fe	S	0
			8	4	4	
18	a	1	Total	Fe	S	0
			8	4	4	
18	c	1	Total	Fe	S	0
			8	4	4	
18	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 19 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			30	30	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	F	1	Total	C	0
			40	40	
19	G	1	Total	C	0
			40	40	
19	G	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
19	G	1	Total C 30 30	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	Q	1	Total C 40 40	0
19	R	1	Total C 40 40	0
19	S	1	Total C 40 40	0
19	S	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	S	1	Total C 40 40	0
19	T	1	Total C 40 40	0
19	T	1	Total C 40 40	0
19	U	1	Total C 40 40	0
19	U	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 30 30	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	f	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	i	1	Total C 40 40	0
19	j	1	Total C 40 40	0
19	j	1	Total C 40 40	0
19	j	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	k	1	Total C 40 40	0
19	k	1	Total C 40 40	0
19	l	1	Total C 40 40	0
19	l	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0

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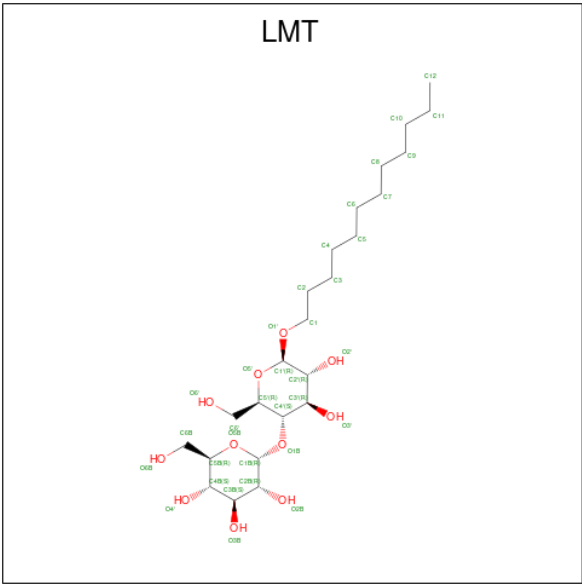
Mol	Chain	Residues	Atoms	AltConf
19	r	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	x	1	Total C 40 40	0
19	x	1	Total C 40 40	0
19	x	1	Total C 40 40	0

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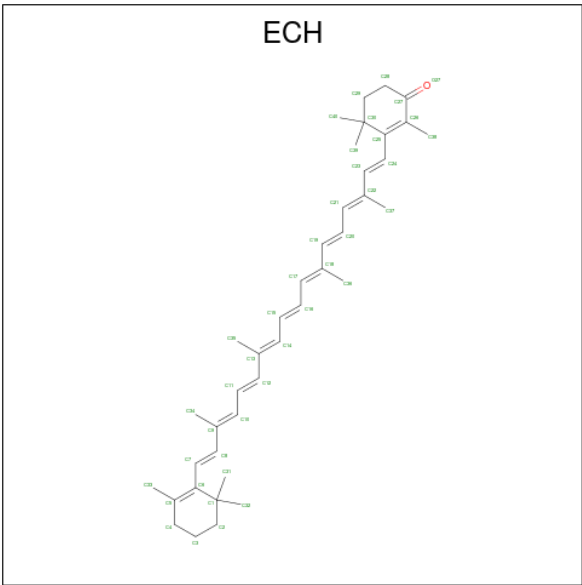
Mol	Chain	Residues	Atoms	AltConf
19	x	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0

- Molecule 20 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total C O 35 24 11	0
20	H	1	Total C O 35 24 11	0
20	L	1	Total C O 35 24 11	0
20	U	1	Total C O 35 24 11	0
20	a	1	Total C O 35 24 11	0
20	l	1	Total C O 35 24 11	0

- Molecule 21 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O) (labeled as "Ligand of Interest" by depositor).

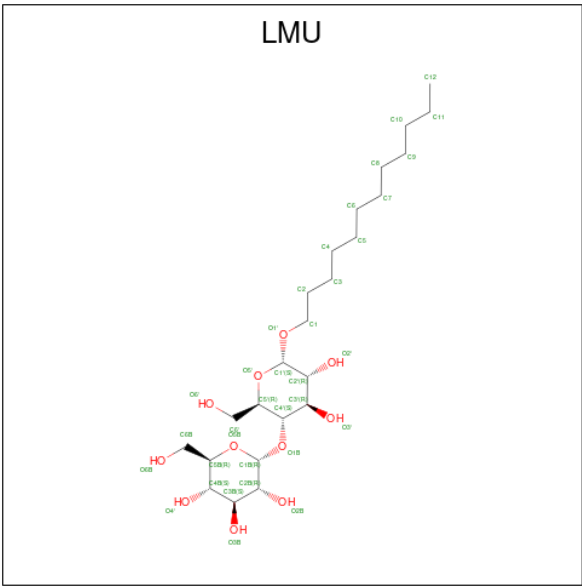


Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total	C	O	0
			41	40	1	
21	G	1	Total	C	O	0
			41	40	1	
21	I	1	Total	C	O	0
			41	40	1	
21	M	1	Total	C	O	0
			41	40	1	
21	R	1	Total	C	O	0
			41	40	1	
21	V	1	Total	C	O	0
			41	40	1	
21	b	1	Total	C	O	0
			41	40	1	
21	i	1	Total	C	O	0
			41	40	1	
21	m	1	Total	C	O	0
			41	40	1	

- Molecule 22 is CALCIUM ION (CCD ID: CA) (formula: Ca).

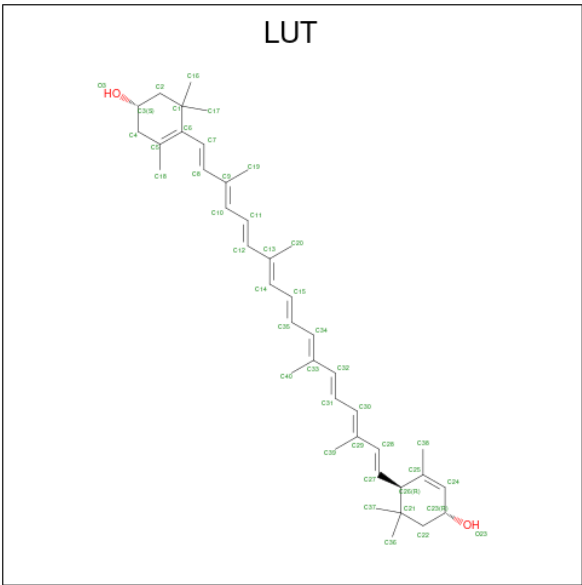
Mol	Chain	Residues	Atoms		AltConf
22	L	1	Total	Ca	0
			1	1	
22	U	1	Total	Ca	0
			1	1	
22	l	1	Total	Ca	0
			1	1	

- Molecule 23 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
23	Y	1	Total	C	O	0
			35	24	11	
23	Z	1	Total	C	O	0
			35	24	11	
23	g	1	Total	C	O	0
			35	24	11	
23	p	1	Total	C	O	0
			35	24	11	
23	q	1	Total	C	O	0
			35	24	11	
23	r	1	Total	C	O	0
			35	24	11	
23	s	1	Total	C	O	0
			35	24	11	
23	w	1	Total	C	O	0
			35	24	11	
23	x	1	Total	C	O	0
			35	24	11	

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
24	Z	1	Total	C	O	0
			42	40	2	
24	q	1	Total	C	O	0
			42	40	2	
24	w	1	Total	C	O	0
			42	40	2	

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	A	56	Total	O	0
			56	56	
25	B	52	Total	O	0
			52	52	
25	C	7	Total	O	0
			7	7	
25	D	3	Total	O	0
			3	3	
25	E	4	Total	O	0
			4	4	
25	F	3	Total	O	0
			3	3	
25	G	55	Total	O	0
			55	55	
25	H	52	Total	O	0
			52	52	
25	I	1	Total	O	0
			1	1	

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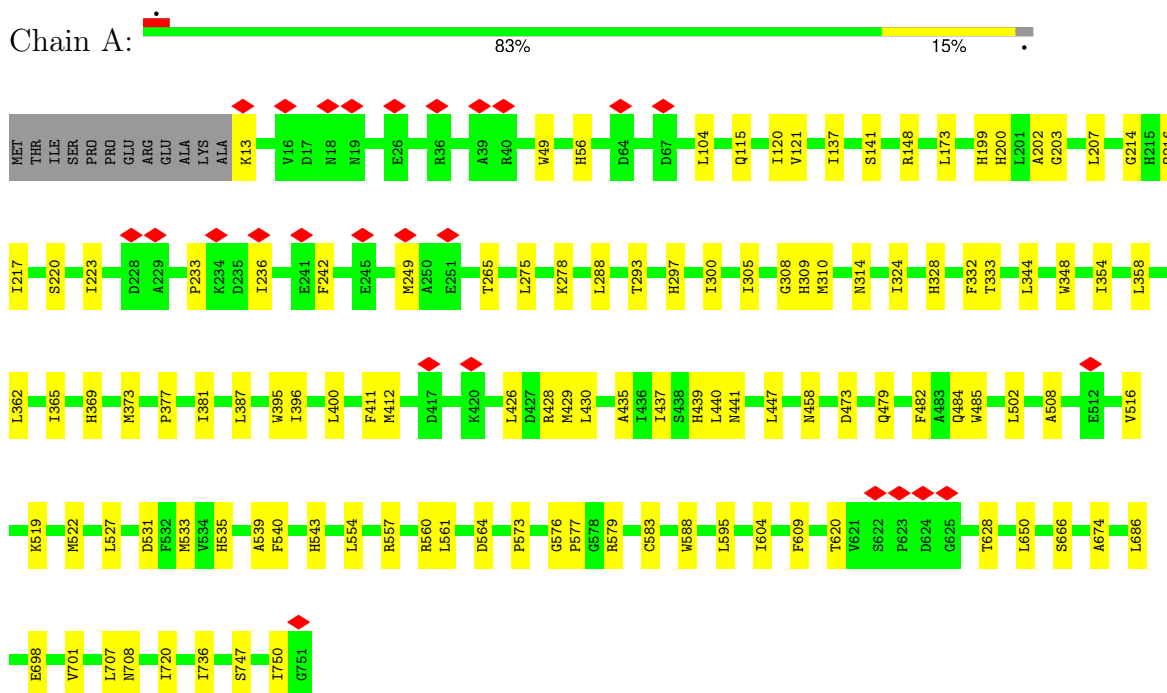
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Mol	Chain	Residues	Atoms		AltConf
25	J	1	Total 1	O 1	0
25	L	5	Total 5	O 5	0
25	N	13	Total 13	O 13	0
25	O	11	Total 11	O 11	0
25	P	6	Total 6	O 6	0
25	Q	4	Total 4	O 4	0
25	R	1	Total 1	O 1	0
25	S	3	Total 3	O 3	0
25	U	3	Total 3	O 3	0
25	a	57	Total 57	O 57	0
25	b	74	Total 74	O 74	0
25	c	17	Total 17	O 17	0
25	d	7	Total 7	O 7	0
25	e	10	Total 10	O 10	0
25	f	7	Total 7	O 7	0
25	i	1	Total 1	O 1	0
25	j	1	Total 1	O 1	0
25	k	1	Total 1	O 1	0
25	l	6	Total 6	O 6	0

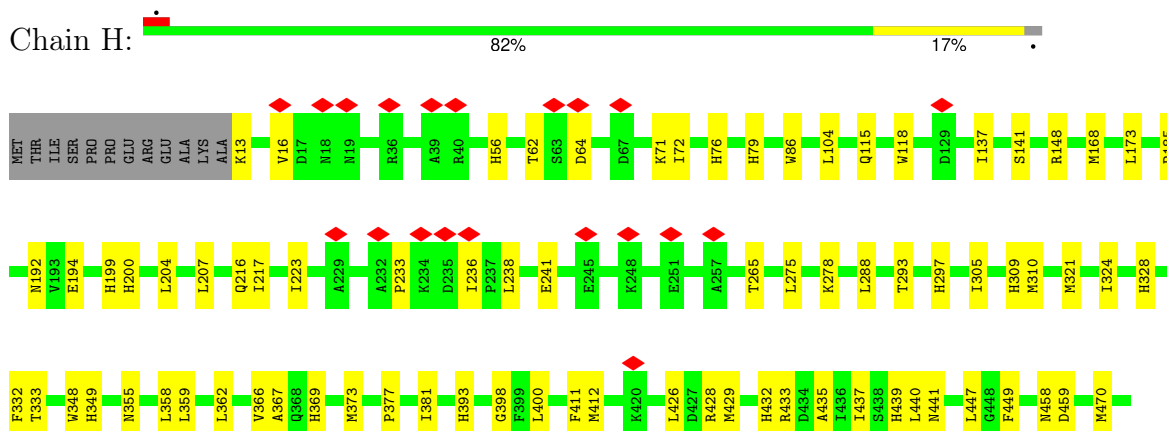
3 Residue-property plots

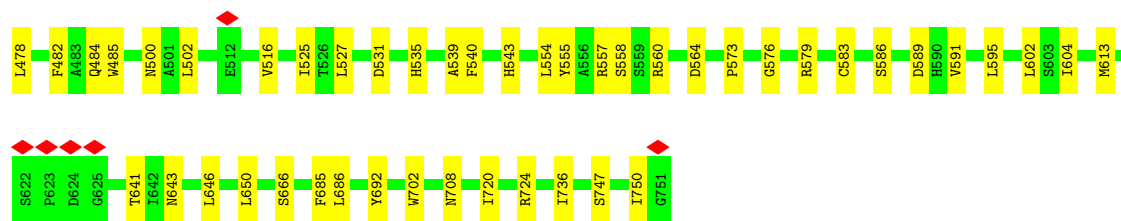
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

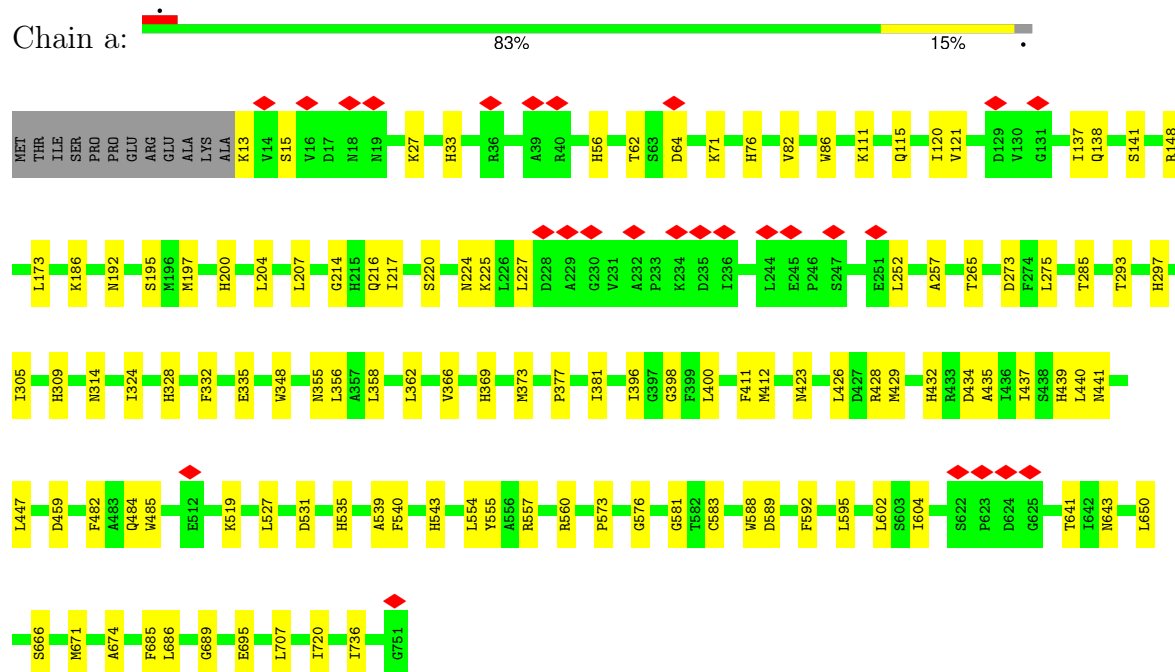


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

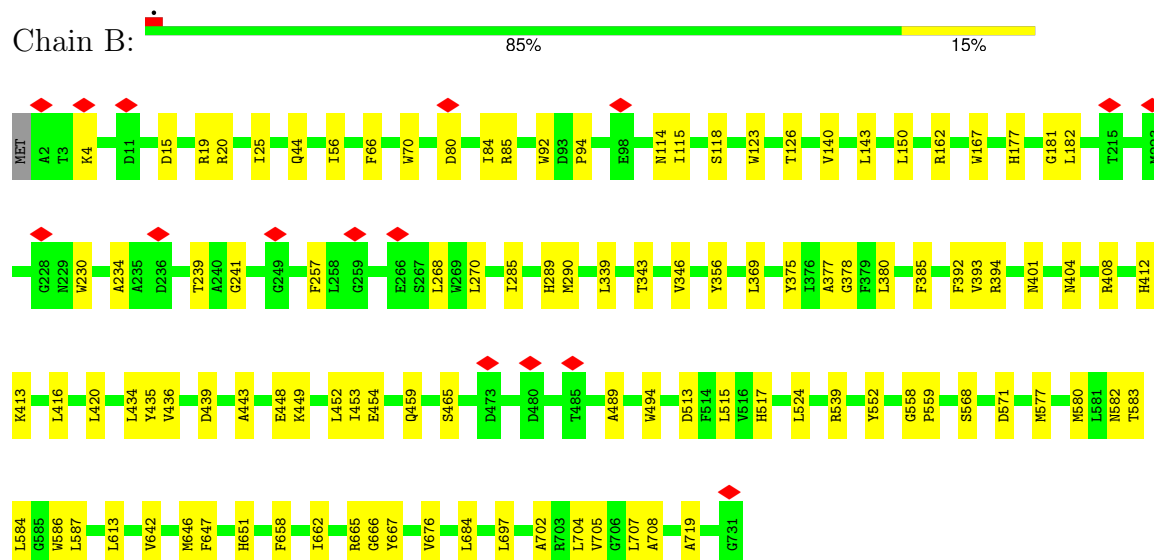




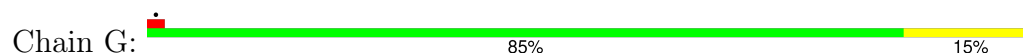
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

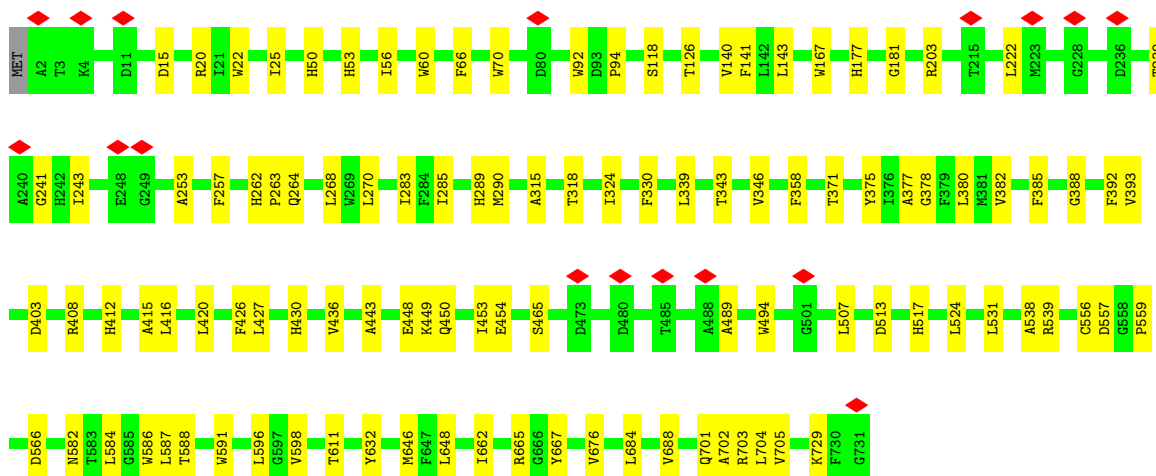


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

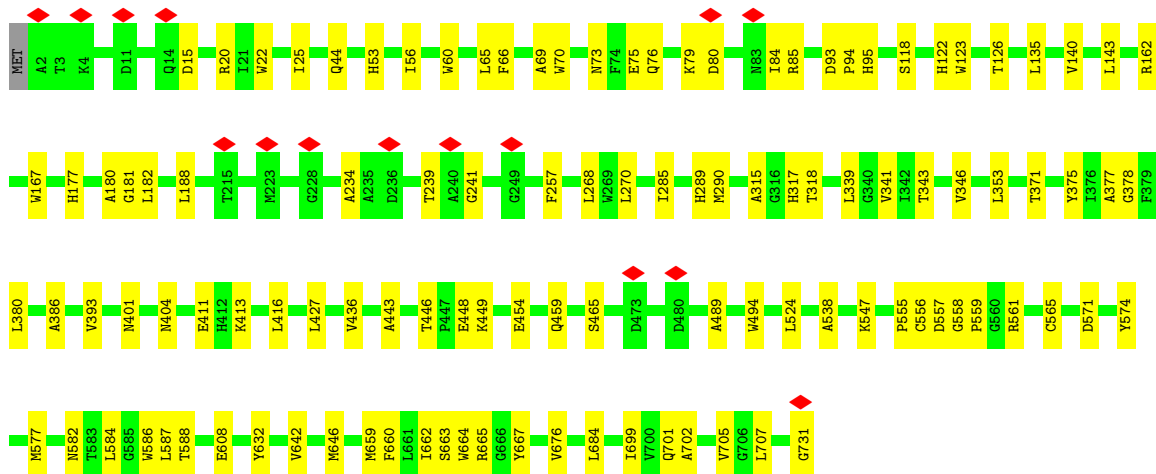
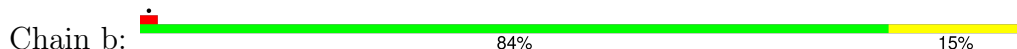


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

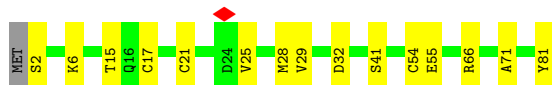
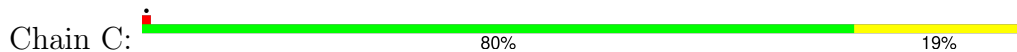




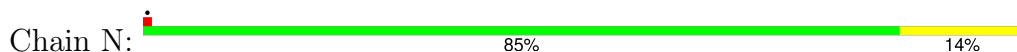
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 3: Photosystem I iron-sulfur center



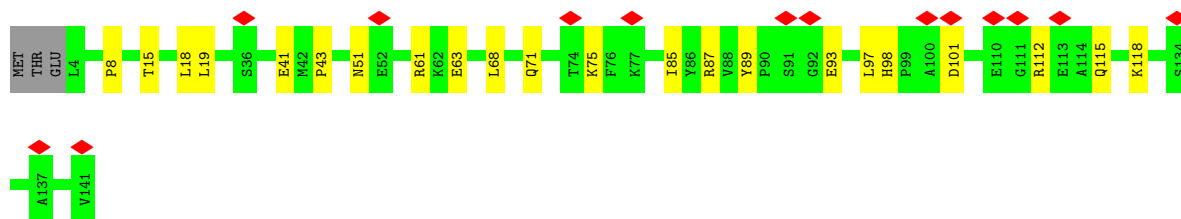
- Molecule 3: Photosystem I iron-sulfur center

Chain c: 



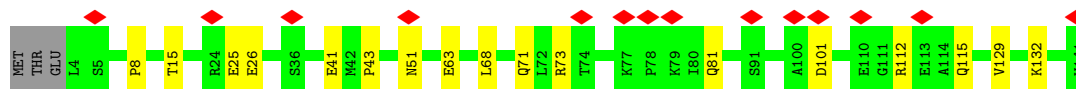
- Molecule 4: Photosystem I reaction center subunit II

Chain D: 



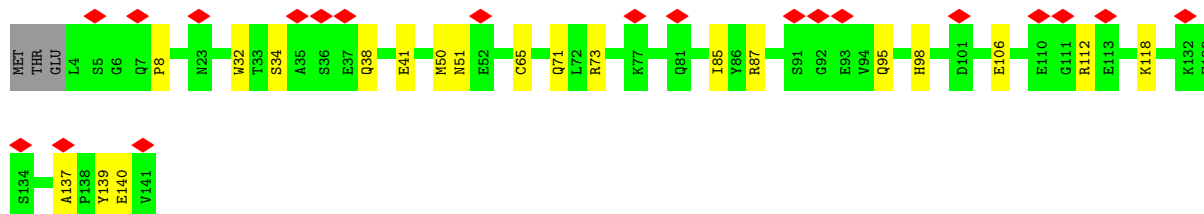
- Molecule 4: Photosystem I reaction center subunit II

Chain P: 



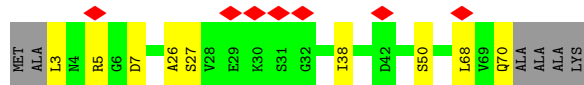
- Molecule 4: Photosystem I reaction center subunit II

Chain d: 



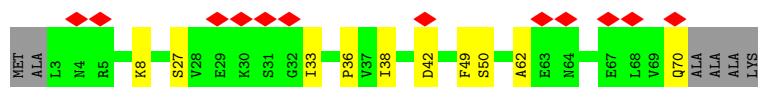
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 

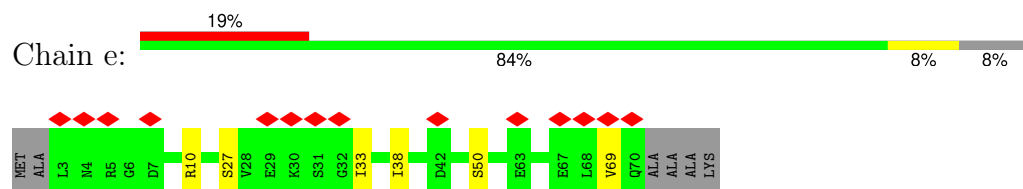


- Molecule 5: Photosystem I reaction center subunit IV

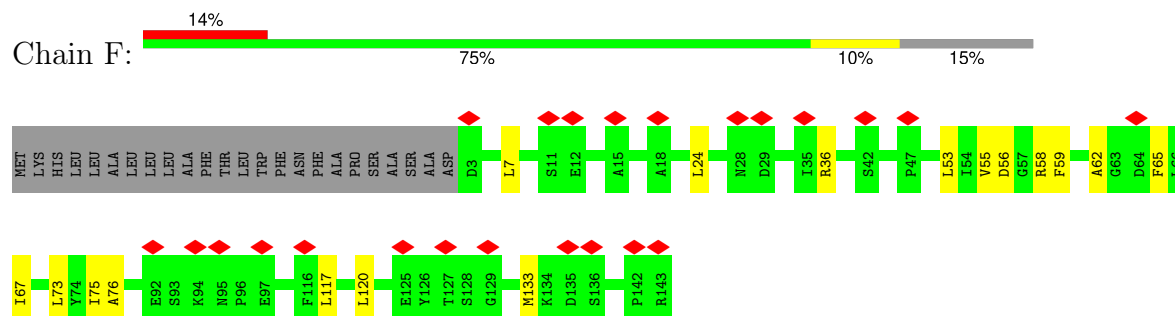
Chain O: 



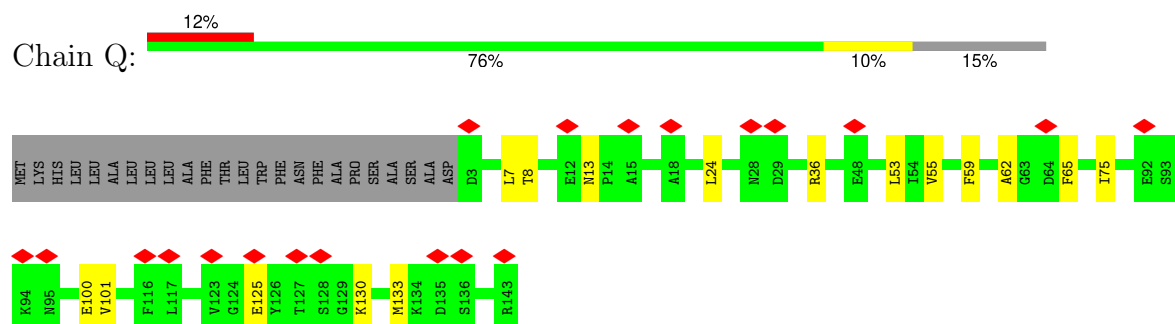
- Molecule 5: Photosystem I reaction center subunit IV



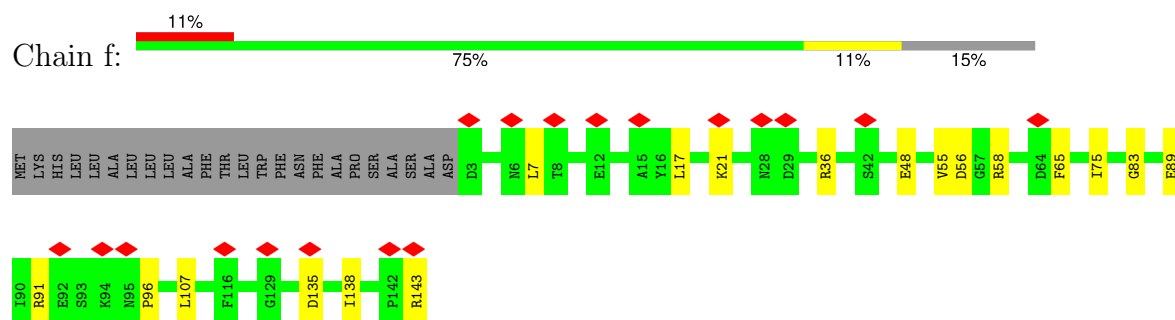
- Molecule 6: Photosystem I reaction center subunit III



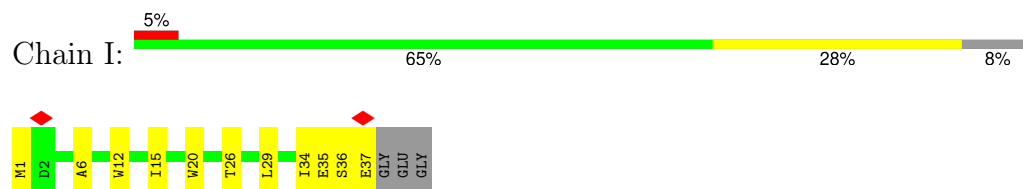
- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



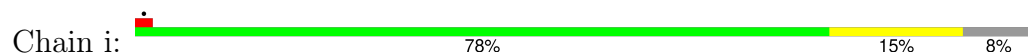
- Molecule 7: Photosystem I reaction center subunit VIII



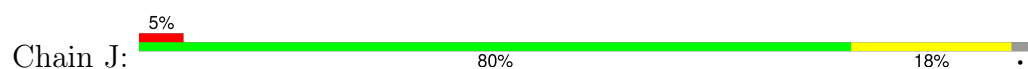
- Molecule 7: Photosystem I reaction center subunit VIII



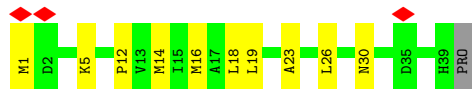
- Molecule 7: Photosystem I reaction center subunit VIII



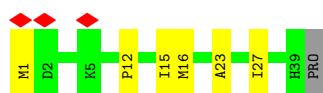
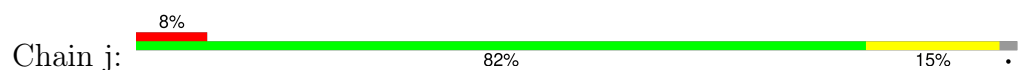
- Molecule 8: Photosystem I reaction center subunit IX



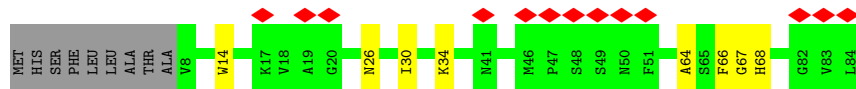
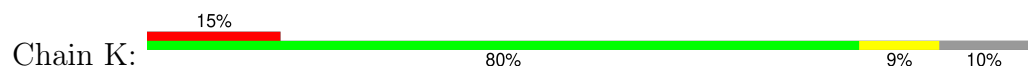
- Molecule 8: Photosystem I reaction center subunit IX



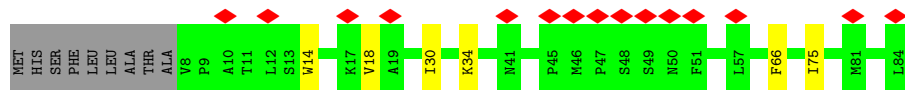
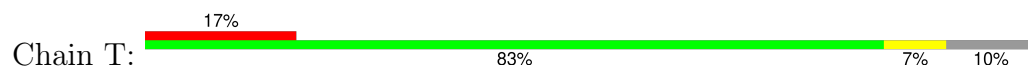
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit PsaK 1

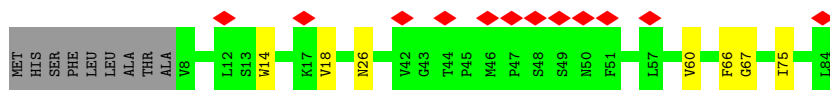


- Molecule 9: Photosystem I reaction center subunit PsaK 1



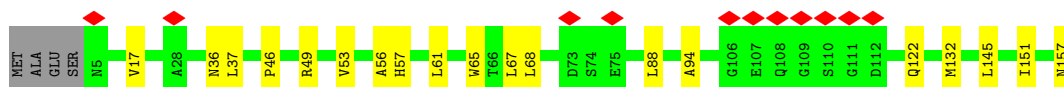
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain k: 



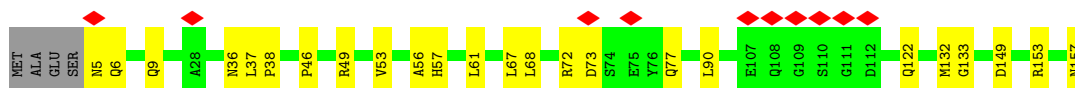
- Molecule 10: Photosystem I reaction center subunit XI

Chain L: 



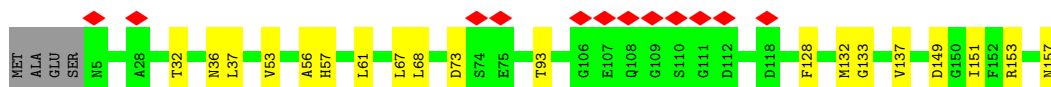
- Molecule 10: Photosystem I reaction center subunit XI

Chain U: 



- Molecule 10: Photosystem I reaction center subunit XI

Chain I: 

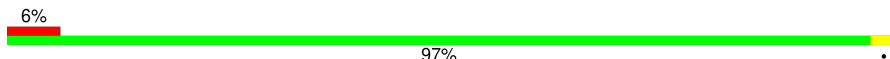


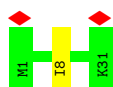
- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 

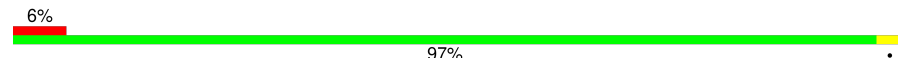


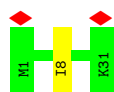
- Molecule 11: Photosystem I reaction center subunit XII

Chain V: 



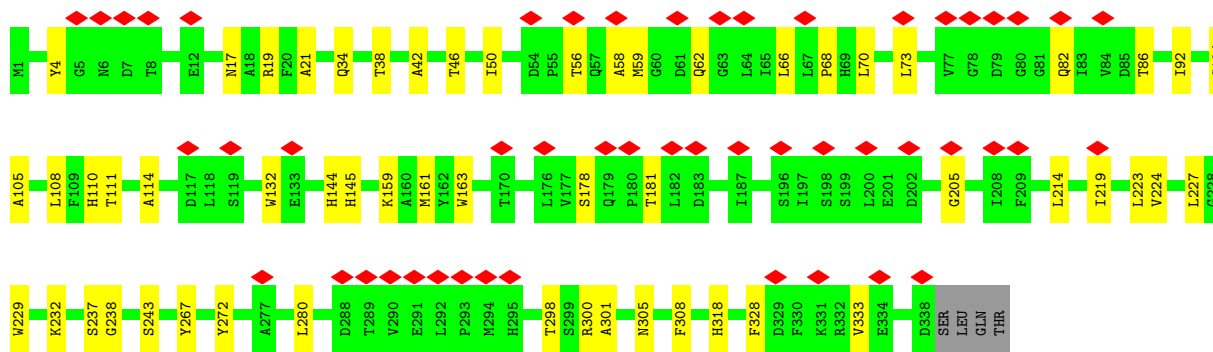
- Molecule 11: Photosystem I reaction center subunit XII

Chain m: 



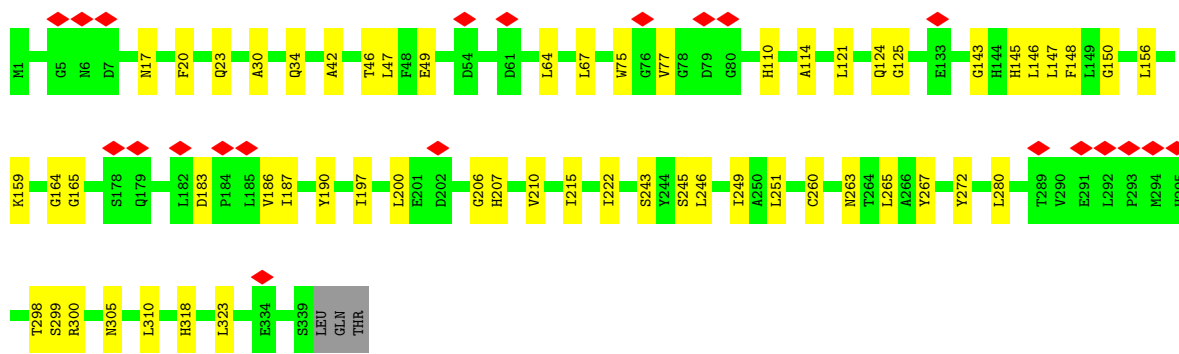
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain W: 15% 82% 16%



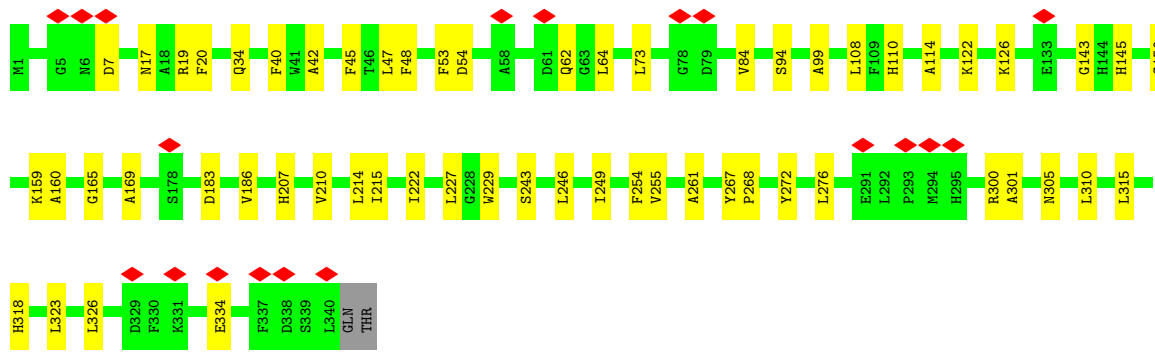
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain X: 6% 82% 17%



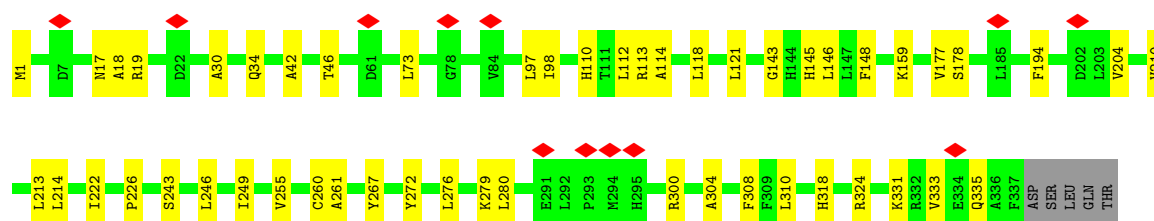
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Y: 6% 82% 17%



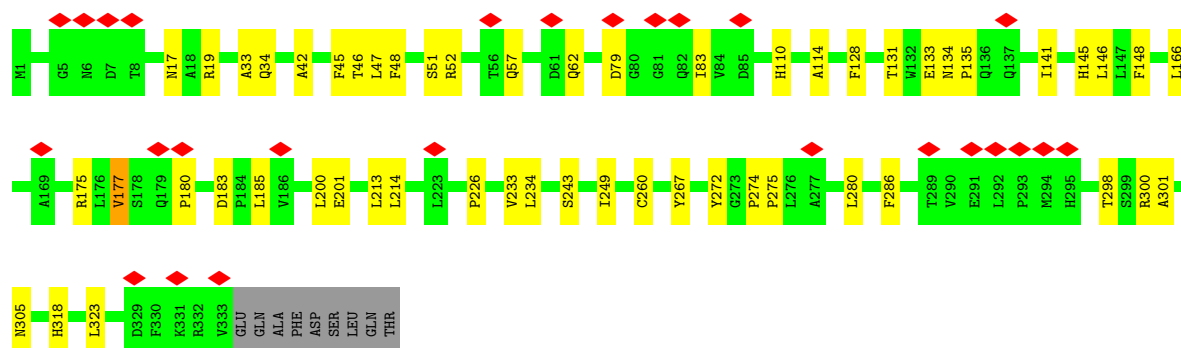
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Z:  84% 15%



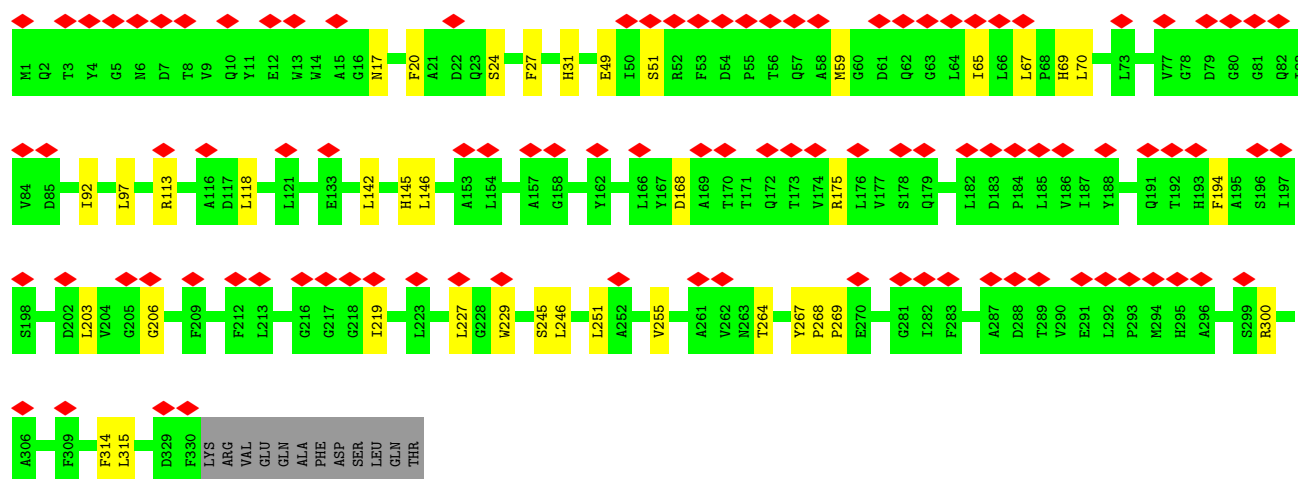
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain g:  8% 82% 15%



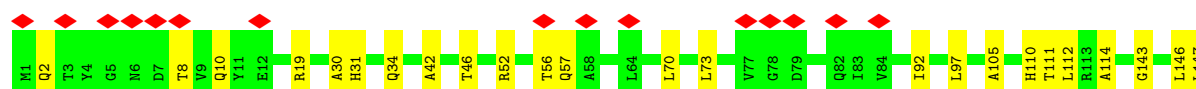
• Molecule 12: Iron stress-induced chlorophyll-binding protein

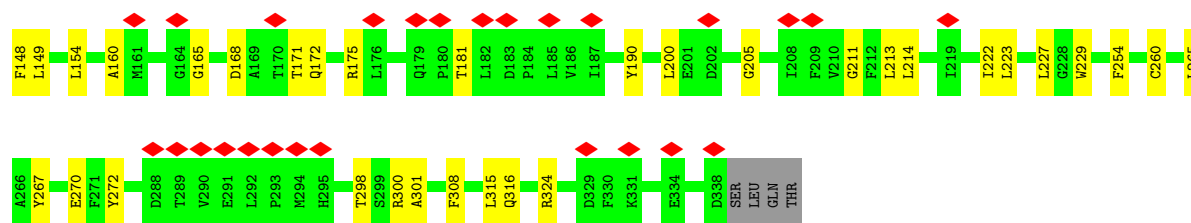
Chain h:  29% 85% 11%



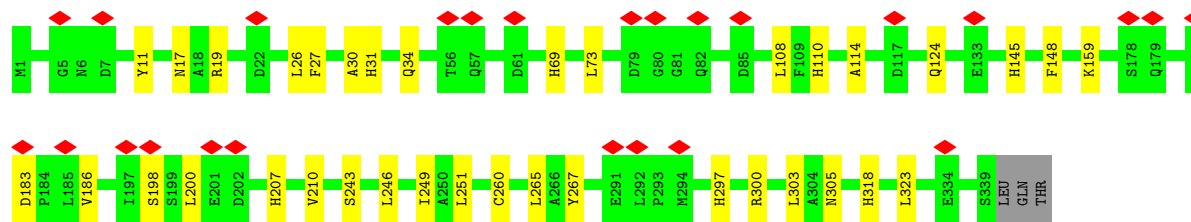
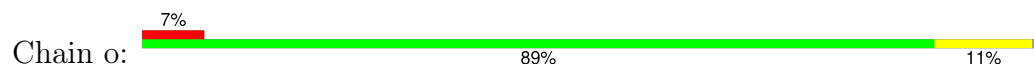
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain n:  12% 82% 17%

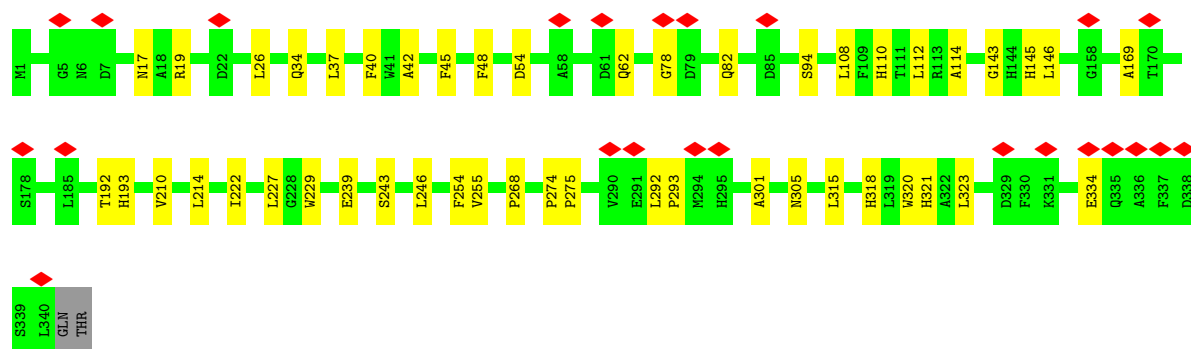
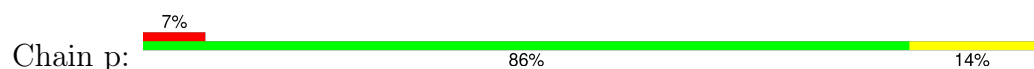




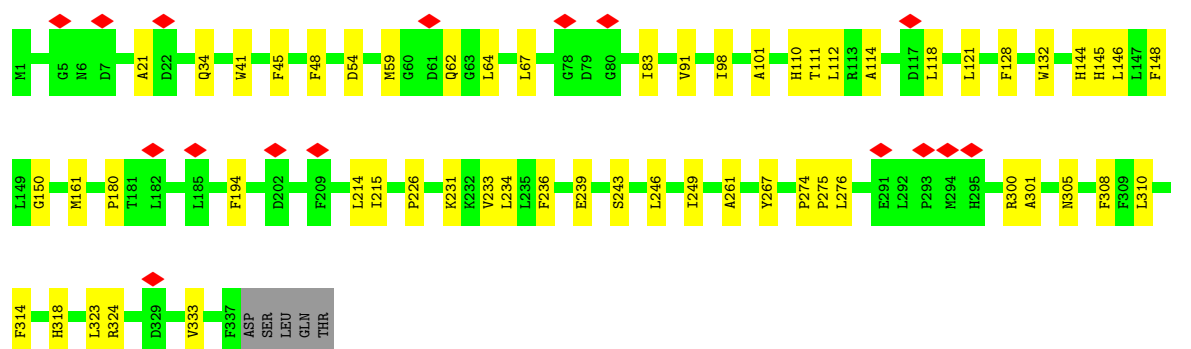
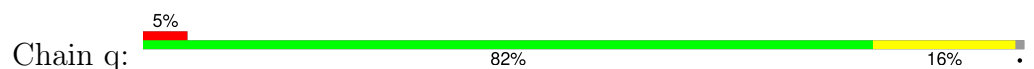
- Molecule 12: Iron stress-induced chlorophyll-binding protein



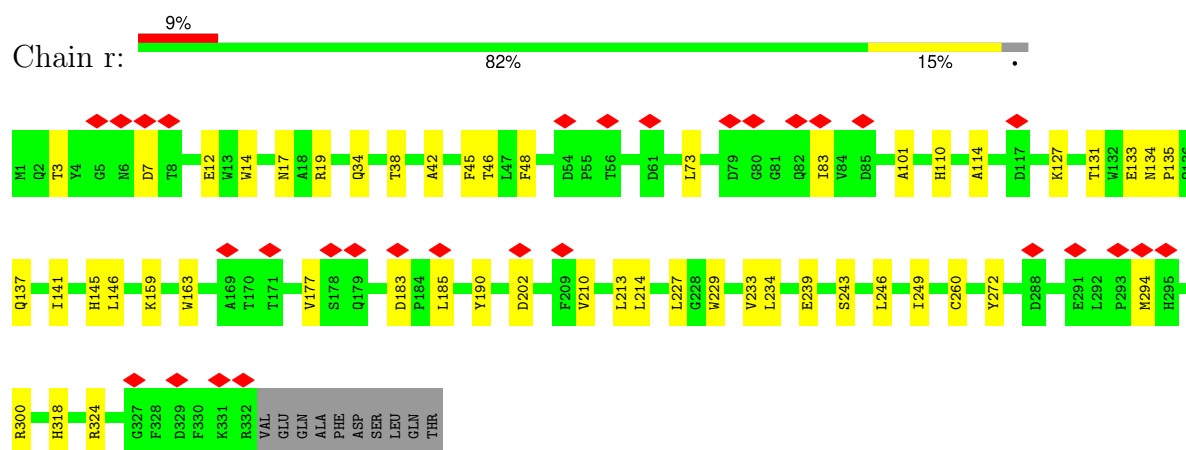
- Molecule 12: Iron stress-induced chlorophyll-binding protein



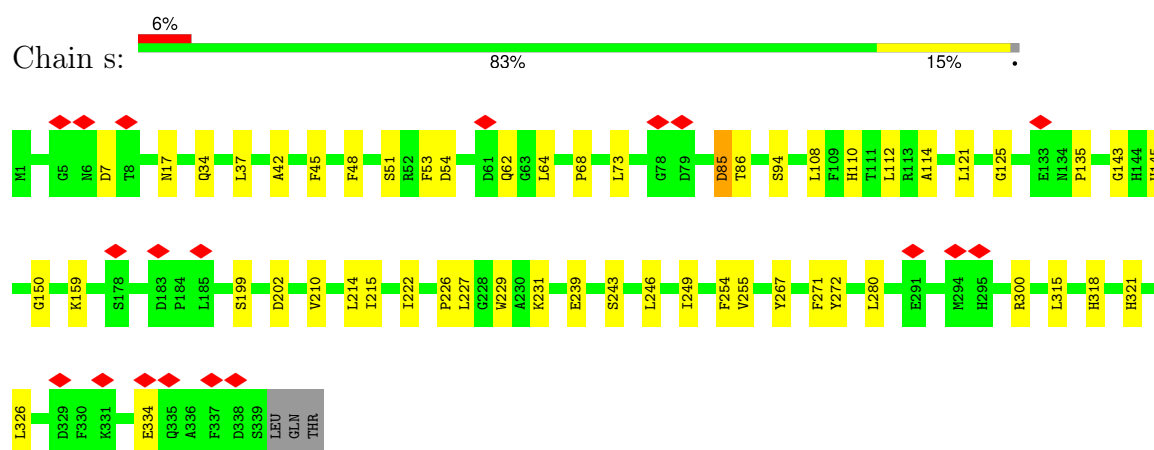
- Molecule 12: Iron stress-induced chlorophyll-binding protein



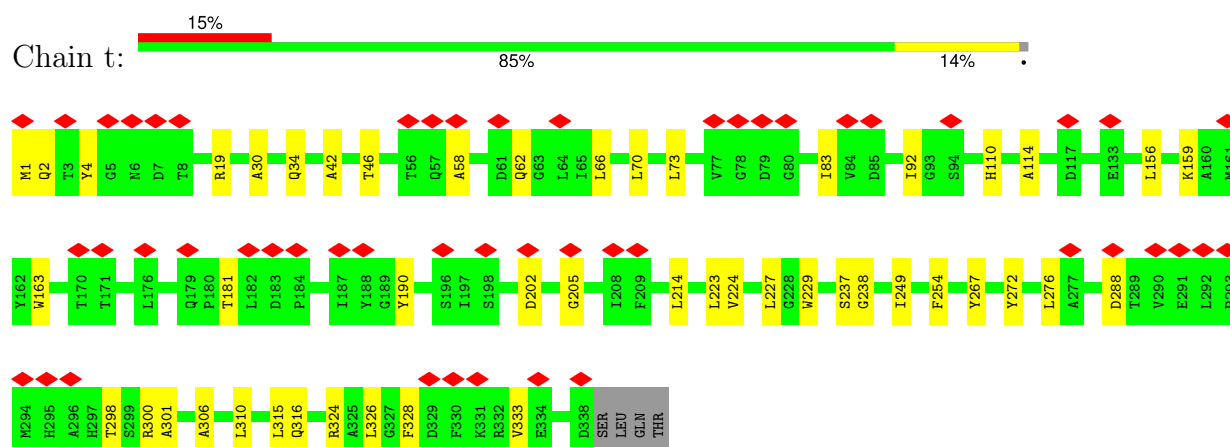
- Molecule 12: Iron stress-induced chlorophyll-binding protein



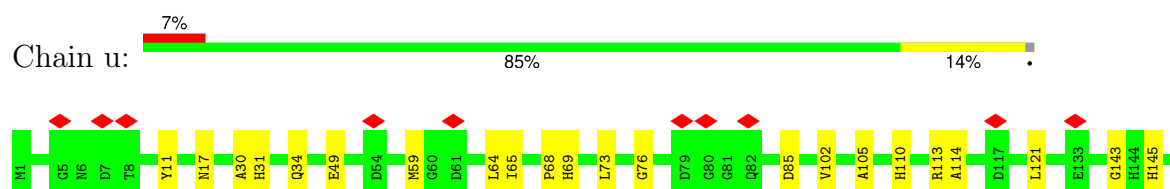
• Molecule 12: Iron stress-induced chlorophyll-binding protein

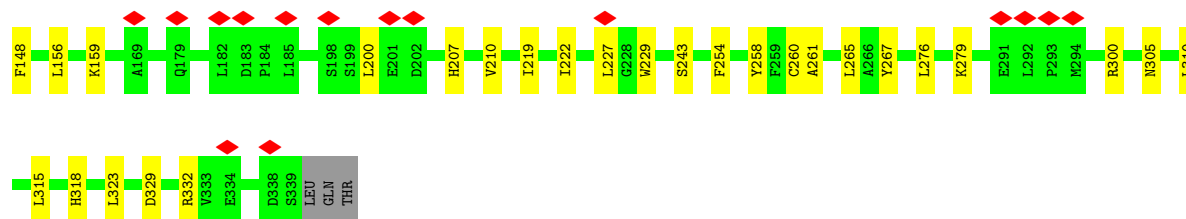


• Molecule 12: Iron stress-induced chlorophyll-binding protein

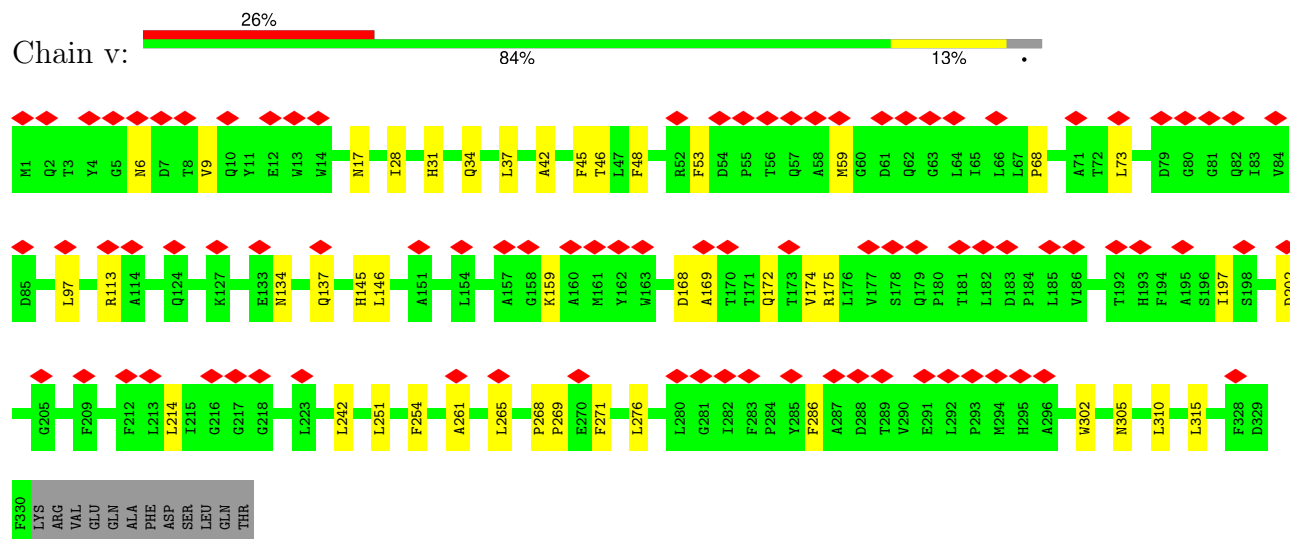


• Molecule 12: Iron stress-induced chlorophyll-binding protein

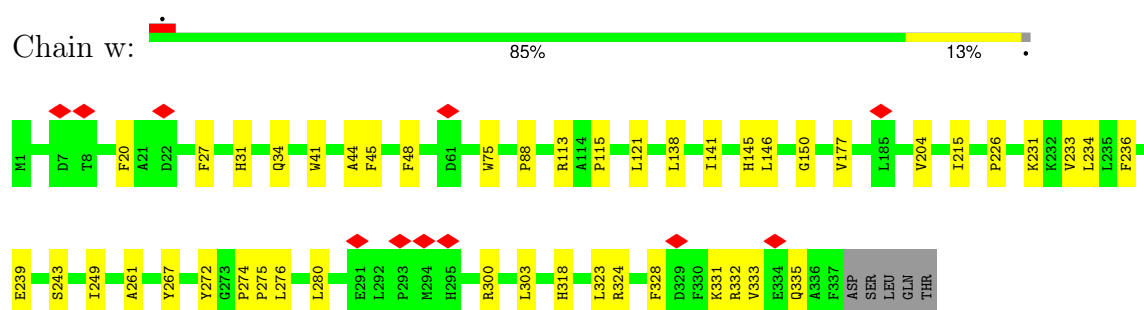




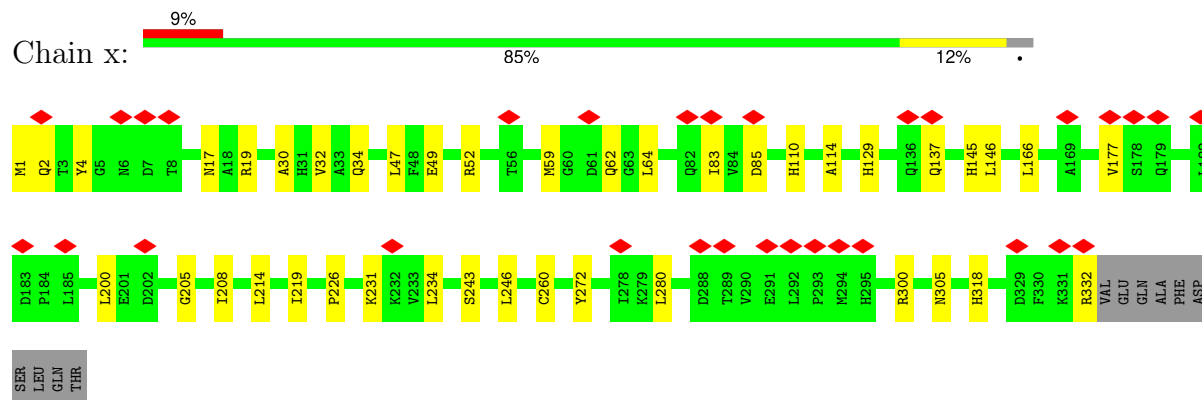
- Molecule 12: Iron stress-induced chlorophyll-binding protein



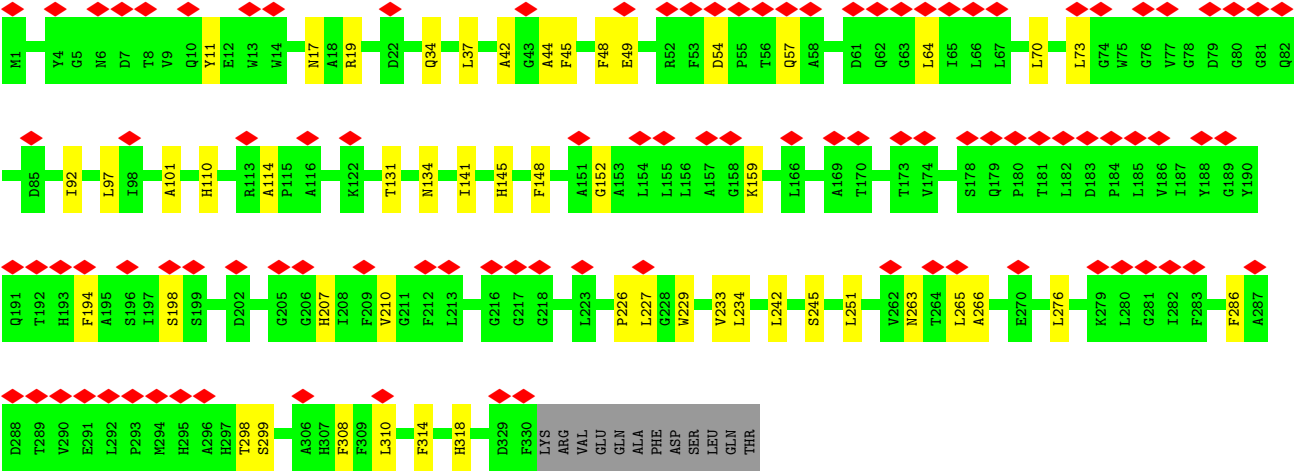
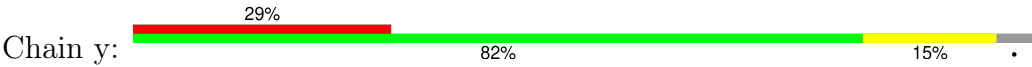
- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	70.466	Depositor
Minimum map value	-42.667	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	2.305	Depositor
Recommended contour level	9.2	Depositor
Map size ($\text{\AA}$)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LUT, SF4, BCR, LHG, CL0, LMU, CA, CLA, ECH, PQN, LMG, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/5985	0.43	0/8158
1	H	0.23	0/5985	0.44	0/8158
1	a	0.23	0/5985	0.45	0/8158
2	B	0.22	0/5986	0.44	0/8185
2	G	0.23	0/5986	0.45	0/8185
2	b	0.23	0/5986	0.45	0/8185
3	C	0.20	0/610	0.48	0/826
3	N	0.21	0/610	0.48	0/826
3	c	0.22	0/610	0.51	0/826
4	D	0.19	0/1102	0.44	0/1485
4	P	0.18	0/1102	0.38	0/1485
4	d	0.18	0/1102	0.40	0/1485
5	E	0.13	0/546	0.31	0/738
5	O	0.13	0/546	0.32	0/738
5	e	0.14	0/546	0.33	0/738
6	F	0.20	0/1130	0.43	0/1535
6	Q	0.22	0/1130	0.46	0/1535
6	f	0.21	0/1130	0.44	0/1535
7	I	0.27	0/304	0.55	0/416
7	R	0.30	0/304	0.57	0/416
7	i	0.31	0/304	0.61	0/416
8	J	0.20	0/319	0.45	0/431
8	S	0.22	0/319	0.47	0/431
8	j	0.30	0/319	0.48	0/431
9	K	0.15	0/549	0.36	0/745
9	T	0.16	0/549	0.43	0/745
9	k	0.16	0/549	0.44	0/745
10	L	0.20	0/1180	0.47	0/1603
10	U	0.21	0/1180	0.49	0/1603
10	l	0.21	0/1180	0.46	0/1603
11	M	0.19	0/241	0.38	0/326
11	V	0.22	0/241	0.45	0/326

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	m	0.24	0/241	0.50	0/326
12	W	0.18	0/2691	0.44	1/3678 (0.0%)
12	X	0.20	0/2712	0.47	0/3703
12	Y	0.21	0/2712	0.45	0/3704
12	Z	0.20	0/2693	0.44	1/3678 (0.0%)
12	g	0.19	0/2662	0.45	0/3636
12	h	0.17	0/2627	0.42	0/3592
12	n	0.16	0/2691	0.37	0/3678
12	o	0.20	0/2712	0.47	0/3703
12	p	0.20	0/2712	0.43	0/3704
12	q	0.18	0/2693	0.39	0/3678
12	r	0.20	0/2655	0.49	0/3626
12	s	0.20	0/2707	0.42	0/3697
12	t	0.17	0/2691	0.41	0/3678
12	u	0.20	0/2712	0.45	0/3703
12	v	0.16	0/2627	0.40	0/3592
12	w	0.19	0/2693	0.43	0/3678
12	x	0.18	0/2655	0.45	2/3626 (0.1%)
12	y	0.16	0/2621	0.40	0/3585
All	All	0.21	0/102122	0.44	4/139283 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
12	Y	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	x	85	ASP	CA-C-N	5.76	131.60	122.61
12	x	85	ASP	C-N-CA	5.76	131.60	122.61
12	W	308	PHE	N-CA-C	-5.49	106.25	113.12
12	Z	333	VAL	N-CA-C	-5.27	108.36	113.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	Y	84	VAL	Peptide
2	b	664	TRP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5787	0	5648	95	0
1	H	5787	0	5648	100	0
1	a	5787	0	5648	90	0
2	B	5775	0	5554	86	0
2	G	5775	0	5554	86	0
2	b	5775	0	5554	85	0
3	C	600	0	589	12	0
3	N	600	0	589	9	0
3	c	600	0	589	5	0
4	D	1078	0	1076	17	0
4	P	1078	0	1076	11	0
4	d	1078	0	1076	12	0
5	E	537	0	520	5	0
5	O	537	0	520	7	0
5	e	537	0	520	4	0
6	F	1100	0	1096	14	0
6	Q	1100	0	1096	12	0
6	f	1100	0	1096	13	0
7	I	293	0	292	10	0
7	R	293	0	292	8	0
7	i	293	0	292	4	0
8	J	311	0	321	7	0
8	S	311	0	321	10	0
8	j	311	0	321	6	0
9	K	538	0	565	6	0
9	T	538	0	565	5	0
9	k	538	0	565	5	0
10	L	1150	0	1122	19	0
10	U	1150	0	1122	23	0
10	l	1150	0	1122	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	238	0	260	2	0
11	V	238	0	260	1	0
11	m	238	0	260	1	0
12	W	2601	0	2532	39	0
12	X	2622	0	2567	47	0
12	Y	2622	0	2561	43	0
12	Z	2603	0	2550	38	0
12	g	2573	0	2526	39	0
12	h	2538	0	2476	32	0
12	n	2601	0	2532	47	0
12	o	2622	0	2567	32	0
12	p	2622	0	2561	34	0
12	q	2603	0	2550	44	0
12	r	2566	0	2517	36	0
12	s	2617	0	2559	38	0
12	t	2601	0	2532	34	0
12	u	2622	0	2567	38	0
12	v	2538	0	2476	33	0
12	w	2603	0	2550	37	0
12	x	2566	0	2517	29	0
12	y	2532	0	2465	35	0
13	A	69	0	78	2	0
13	B	38	0	49	1	0
13	G	38	0	49	1	0
13	H	69	0	78	2	0
13	I	40	0	50	2	0
13	R	40	0	50	2	0
13	X	27	0	24	1	0
13	Y	32	0	34	0	0
13	a	69	0	78	0	0
13	b	38	0	49	3	0
13	g	31	0	32	0	0
13	i	40	0	50	2	0
13	o	27	0	24	1	0
13	p	32	0	34	1	0
13	r	31	0	32	2	0
13	s	32	0	34	1	0
13	u	27	0	24	1	0
13	x	31	0	32	0	0
14	A	116	0	142	6	0
14	B	43	0	56	2	0
14	F	27	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	G	43	0	56	2	0
14	H	116	0	142	8	0
14	Q	27	0	24	1	0
14	a	116	0	142	3	0
14	b	43	0	56	0	0
14	f	27	0	24	1	0
15	A	65	0	72	3	0
15	H	65	0	72	4	0
15	a	65	0	72	4	0
16	A	2545	0	2497	100	0
16	B	2309	0	2201	99	0
16	F	91	0	66	1	0
16	G	2310	0	2204	89	0
16	H	2545	0	2497	105	0
16	J	82	0	58	1	0
16	K	145	0	115	3	0
16	L	185	0	190	11	0
16	Q	91	0	66	3	0
16	S	82	0	58	0	0
16	T	145	0	115	3	0
16	U	185	0	190	11	0
16	W	963	0	910	26	0
16	X	959	0	904	40	0
16	Y	973	0	936	33	0
16	Z	977	0	942	37	0
16	a	2540	0	2487	97	0
16	b	2310	0	2204	84	0
16	f	91	0	66	2	0
16	g	978	0	949	31	0
16	h	969	0	930	32	0
16	j	82	0	58	0	0
16	k	145	0	115	2	0
16	l	185	0	190	15	0
16	n	968	0	923	41	0
16	o	959	0	904	34	0
16	p	973	0	936	36	0
16	q	977	0	942	43	0
16	r	978	0	949	38	0
16	s	973	0	936	34	0
16	t	968	0	923	24	0
16	u	959	0	904	32	0
16	v	969	0	930	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	w	977	0	942	35	0
16	x	978	0	949	35	0
16	y	969	0	930	38	0
17	A	33	0	46	4	0
17	B	33	0	46	5	0
17	G	33	0	46	5	0
17	H	33	0	46	4	0
17	a	33	0	46	4	0
17	b	33	0	46	2	0
18	A	8	0	0	0	0
18	C	16	0	0	0	0
18	H	8	0	0	0	0
18	N	16	0	0	0	0
18	a	8	0	0	0	0
18	c	16	0	0	0	0
19	A	200	0	280	12	0
19	B	230	0	319	15	0
19	F	40	0	56	4	0
19	G	230	0	319	16	0
19	H	200	0	280	13	0
19	I	40	0	56	3	0
19	J	120	0	168	8	0
19	K	80	0	112	5	0
19	L	80	0	112	9	0
19	Q	40	0	56	2	0
19	R	40	0	56	0	0
19	S	120	0	168	9	0
19	T	80	0	112	3	0
19	U	80	0	112	13	0
19	W	120	0	168	6	0
19	X	160	0	224	11	0
19	Y	160	0	224	6	0
19	Z	120	0	168	4	0
19	a	200	0	280	15	0
19	b	230	0	319	15	0
19	f	40	0	56	4	0
19	g	160	0	224	12	0
19	h	120	0	168	9	0
19	i	40	0	56	5	0
19	j	120	0	168	7	0
19	k	80	0	112	4	0
19	l	80	0	112	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	n	120	0	168	9	0
19	o	160	0	224	5	0
19	p	160	0	224	10	0
19	q	120	0	168	13	0
19	r	160	0	224	7	0
19	s	160	0	224	11	0
19	t	120	0	168	5	0
19	u	160	0	224	8	0
19	v	120	0	168	7	0
19	w	120	0	168	8	0
19	x	160	0	224	9	0
19	y	120	0	168	11	0
20	A	35	0	46	1	0
20	H	35	0	46	1	0
20	L	35	0	46	3	0
20	U	35	0	46	2	0
20	a	35	0	45	1	0
20	l	35	0	46	3	0
21	B	41	0	54	3	0
21	G	41	0	54	2	0
21	I	41	0	54	2	0
21	M	41	0	54	2	0
21	R	41	0	54	2	0
21	V	41	0	54	4	0
21	b	41	0	54	2	0
21	i	41	0	54	1	0
21	m	41	0	54	2	0
22	L	1	0	0	0	0
22	U	1	0	0	0	0
22	l	1	0	0	0	0
23	Y	35	0	46	1	0
23	Z	35	0	46	0	0
23	g	35	0	46	1	0
23	p	35	0	46	1	0
23	q	35	0	46	2	0
23	r	35	0	46	3	0
23	s	35	0	46	0	0
23	w	35	0	46	0	0
23	x	35	0	46	2	0
24	Z	42	0	55	0	0
24	q	42	0	55	1	0
24	w	42	0	55	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	56	0	0	1	0
25	B	52	0	0	1	0
25	C	7	0	0	0	0
25	D	3	0	0	0	0
25	E	4	0	0	0	0
25	F	3	0	0	0	0
25	G	55	0	0	1	0
25	H	52	0	0	0	0
25	I	1	0	0	0	0
25	J	1	0	0	0	0
25	L	5	0	0	0	0
25	N	13	0	0	0	0
25	O	11	0	0	0	0
25	P	6	0	0	0	0
25	Q	4	0	0	0	0
25	R	1	0	0	0	0
25	S	3	0	0	0	0
25	U	3	0	0	0	0
25	a	57	0	0	0	0
25	b	74	0	0	1	0
25	c	17	0	0	0	0
25	d	7	0	0	0	0
25	e	10	0	0	0	0
25	f	7	0	0	0	0
25	i	1	0	0	0	0
25	j	1	0	0	0	0
25	k	1	0	0	0	0
25	l	6	0	0	0	0
All	All	140516	0	138986	2192	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2192 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)
1:A:440:LEU:HB2	16:A:1137:CLA:HBB1	1.61	0.81
16:b:1206:CLA:H3A	16:b:1207:CLA:HBB1	1.64	0.78
16:H:1107:CLA:HBB1	19:S:4012:BCR:HC7	1.67	0.77
16:B:1206:CLA:H3A	16:B:1207:CLA:HBB1	1.66	0.77
1:a:440:LEU:HB2	16:a:1137:CLA:HBB1	1.68	0.76

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	A	737/751 (98%)	712 (97%)	25 (3%)	0	100	100
1	H	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
1	a	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
2	B	728/731 (100%)	713 (98%)	15 (2%)	0	100	100
2	G	728/731 (100%)	712 (98%)	16 (2%)	0	100	100
2	b	728/731 (100%)	711 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	78 (100%)	0	0	100	100
3	N	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	c	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
4	P	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
4	d	136/141 (96%)	130 (96%)	6 (4%)	0	100	100
5	E	66/74 (89%)	65 (98%)	1 (2%)	0	100	100
5	O	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
5	e	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
6	F	139/165 (84%)	135 (97%)	4 (3%)	0	100	100
6	Q	139/165 (84%)	134 (96%)	5 (4%)	0	100	100
6	f	139/165 (84%)	134 (96%)	5 (4%)	0	100	100
7	I	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
7	R	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
7	i	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
8	J	37/40 (92%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S	37/40 (92%)	37 (100%)	0	0	100	100
8	j	37/40 (92%)	37 (100%)	0	0	100	100
9	K	75/86 (87%)	74 (99%)	1 (1%)	0	100	100
9	T	75/86 (87%)	74 (99%)	1 (1%)	0	100	100
9	k	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
10	L	151/157 (96%)	150 (99%)	1 (1%)	0	100	100
10	U	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
10	l	151/157 (96%)	147 (97%)	4 (3%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	29 (100%)	0	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	W	336/342 (98%)	317 (94%)	18 (5%)	1 (0%)	36	58
12	X	337/342 (98%)	318 (94%)	19 (6%)	0	100	100
12	Y	338/342 (99%)	320 (95%)	17 (5%)	1 (0%)	36	58
12	Z	335/342 (98%)	326 (97%)	8 (2%)	1 (0%)	36	58
12	g	331/342 (97%)	304 (92%)	25 (8%)	2 (1%)	21	42
12	h	328/342 (96%)	308 (94%)	20 (6%)	0	100	100
12	n	336/342 (98%)	322 (96%)	14 (4%)	0	100	100
12	o	337/342 (98%)	318 (94%)	17 (5%)	2 (1%)	21	42
12	p	338/342 (99%)	317 (94%)	21 (6%)	0	100	100
12	q	335/342 (98%)	326 (97%)	9 (3%)	0	100	100
12	r	330/342 (96%)	316 (96%)	12 (4%)	2 (1%)	21	42
12	s	337/342 (98%)	321 (95%)	14 (4%)	2 (1%)	21	42
12	t	336/342 (98%)	319 (95%)	16 (5%)	1 (0%)	36	58
12	u	337/342 (98%)	322 (96%)	14 (4%)	1 (0%)	36	58
12	v	328/342 (96%)	312 (95%)	15 (5%)	1 (0%)	36	58
12	w	335/342 (98%)	322 (96%)	13 (4%)	0	100	100
12	x	330/342 (96%)	311 (94%)	17 (5%)	2 (1%)	21	42
12	y	328/342 (96%)	307 (94%)	21 (6%)	0	100	100
All	All	12645/13047 (97%)	12150 (96%)	479 (4%)	16 (0%)	49	70

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	W	59	MET
12	v	174	VAL
12	s	85	ASP
12	o	11	TYR
12	s	7	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	593/603 (98%)	593 (100%)	0	100	100
1	H	593/603 (98%)	593 (100%)	0	100	100
1	a	593/603 (98%)	593 (100%)	0	100	100
2	B	582/583 (100%)	582 (100%)	0	100	100
2	G	582/583 (100%)	582 (100%)	0	100	100
2	b	582/583 (100%)	582 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
3	N	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	113/116 (97%)	113 (100%)	0	100	100
4	P	113/116 (97%)	113 (100%)	0	100	100
4	d	113/116 (97%)	113 (100%)	0	100	100
5	E	58/60 (97%)	58 (100%)	0	100	100
5	O	58/60 (97%)	58 (100%)	0	100	100
5	e	58/60 (97%)	58 (100%)	0	100	100
6	F	118/137 (86%)	118 (100%)	0	100	100
6	Q	118/137 (86%)	118 (100%)	0	100	100
6	f	118/137 (86%)	118 (100%)	0	100	100
7	I	31/32 (97%)	31 (100%)	0	100	100
7	R	31/32 (97%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	i	31/32 (97%)	31 (100%)	0	100	100
8	J	34/35 (97%)	34 (100%)	0	100	100
8	S	34/35 (97%)	34 (100%)	0	100	100
8	j	34/35 (97%)	34 (100%)	0	100	100
9	K	55/62 (89%)	55 (100%)	0	100	100
9	T	55/62 (89%)	55 (100%)	0	100	100
9	k	55/62 (89%)	55 (100%)	0	100	100
10	L	115/118 (98%)	115 (100%)	0	100	100
10	U	115/118 (98%)	115 (100%)	0	100	100
10	l	115/118 (98%)	115 (100%)	0	100	100
11	M	25/25 (100%)	25 (100%)	0	100	100
11	V	25/25 (100%)	25 (100%)	0	100	100
11	m	25/25 (100%)	25 (100%)	0	100	100
12	W	252/260 (97%)	252 (100%)	0	100	100
12	X	256/260 (98%)	256 (100%)	0	100	100
12	Y	255/260 (98%)	255 (100%)	0	100	100
12	Z	253/260 (97%)	253 (100%)	0	100	100
12	g	251/260 (96%)	251 (100%)	0	100	100
12	h	246/260 (95%)	246 (100%)	0	100	100
12	n	252/260 (97%)	252 (100%)	0	100	100
12	o	256/260 (98%)	256 (100%)	0	100	100
12	p	255/260 (98%)	255 (100%)	0	100	100
12	q	253/260 (97%)	253 (100%)	0	100	100
12	r	250/260 (96%)	250 (100%)	0	100	100
12	s	255/260 (98%)	255 (100%)	0	100	100
12	t	252/260 (97%)	252 (100%)	0	100	100
12	u	256/260 (98%)	256 (100%)	0	100	100
12	v	246/260 (95%)	246 (100%)	0	100	100
12	w	253/260 (97%)	253 (100%)	0	100	100
12	x	250/260 (96%)	250 (100%)	0	100	100
12	y	245/260 (94%)	245 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	9912/10200 (97%)	9912 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
12	r	124	GLN
12	x	6	ASN
12	s	129	HIS
12	u	179	GLN
12	y	17	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 798 ligands modelled in this entry, 3 are monoatomic - leaving 795 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	$\# Z > 2$
19	BCR	Z	603	-	41,41,41	0.84	0	56,56,56	1.17	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	LHG	I	103	-	39,39,48	0.68	2 (5%)	42,45,54	1.23	4 (9%)
16	CLA	j	1302	8	49,53,73	1.19	5 (10%)	58,89,113	1.18	6 (10%)
16	CLA	G	1213	2	59,63,73	1.08	5 (8%)	70,101,113	1.10	4 (5%)
16	CLA	G	1232	25	49,53,73	1.19	5 (10%)	58,89,113	1.29	6 (10%)
16	CLA	A	1136	1	69,73,73	0.98	4 (5%)	82,113,113	1.00	3 (3%)
14	LMG	Q	4017	-	27,27,55	1.07	1 (3%)	35,35,63	1.18	3 (8%)
16	CLA	B	1240	13	50,54,73	1.18	5 (10%)	59,90,113	1.21	4 (6%)
16	CLA	r	501	12	54,58,73	1.10	4 (7%)	64,95,113	1.21	6 (9%)
19	BCR	K	4005	-	41,41,41	0.86	0	56,56,56	1.28	6 (10%)
16	CLA	w	517	12	59,63,73	1.09	6 (10%)	70,101,113	1.07	3 (4%)
16	CLA	B	1235	2	66,70,73	1.03	5 (7%)	78,109,113	1.19	9 (11%)
16	CLA	v	508	12	59,63,73	1.07	5 (8%)	70,101,113	1.31	7 (10%)
16	CLA	p	515	12	69,73,73	0.98	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	H	1107	1	54,58,73	1.11	4 (7%)	64,95,113	1.07	6 (9%)
16	CLA	q	503	12	50,54,73	1.15	6 (12%)	59,90,113	1.26	5 (8%)
16	CLA	u	511	-	69,73,73	0.97	4 (5%)	82,113,113	1.10	4 (4%)
19	BCR	g	602	-	41,41,41	0.86	0	56,56,56	1.28	7 (12%)
19	BCR	T	4005	-	41,41,41	0.85	0	56,56,56	1.26	7 (12%)
16	CLA	b	1202	-	69,73,73	0.97	4 (5%)	82,113,113	0.97	3 (3%)
16	CLA	G	1240	13	50,54,73	1.18	5 (10%)	59,90,113	1.30	6 (10%)
16	CLA	h	506	12	64,68,73	1.05	6 (9%)	76,107,113	1.38	10 (13%)
16	CLA	n	508	12	59,63,73	1.07	5 (8%)	70,101,113	0.99	2 (2%)
16	CLA	G	1235	2	66,70,73	1.02	5 (7%)	78,109,113	1.19	10 (12%)
16	CLA	A	1132	1	69,73,73	0.99	6 (8%)	82,113,113	1.14	6 (7%)
16	CLA	A	1120	1	53,57,73	1.10	4 (7%)	61,93,113	1.12	5 (8%)
16	CLA	q	511	12	69,73,73	1.00	4 (5%)	82,113,113	1.05	3 (3%)
16	CLA	t	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	f	1301	25	49,53,73	1.17	4 (8%)	58,89,113	1.06	4 (6%)
16	CLA	t	502	12	54,58,73	1.14	6 (11%)	64,95,113	1.13	4 (6%)
16	CLA	q	509	12	69,73,73	1.01	5 (7%)	82,113,113	0.98	6 (7%)
19	BCR	J	4012	-	41,41,41	0.87	0	56,56,56	1.31	8 (14%)
23	LMU	s	606	-	36,36,36	0.83	0	47,47,47	1.27	4 (8%)
16	CLA	b	1210	2	69,73,73	1.02	5 (7%)	82,113,113	1.05	6 (7%)
18	SF4	a	3001	-	0,12,12	-	-	-	-	-
19	BCR	A	4007	-	41,41,41	0.91	1 (2%)	56,56,56	1.40	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	a	1137	1	51,55,73	1.13	4 (7%)	60,91,113	1.14	5 (8%)
16	CLA	Y	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.04	5 (7%)
14	LMG	H	4101	-	46,46,55	0.91	1 (2%)	54,54,63	1.23	4 (7%)
16	CLA	A	1115	1	58,62,73	1.06	6 (10%)	68,99,113	1.17	3 (4%)
16	CLA	A	1113	1	49,53,73	1.19	4 (8%)	58,89,113	1.06	2 (3%)
16	CLA	q	515	12	69,73,73	0.99	5 (7%)	82,113,113	1.20	7 (8%)
16	CLA	a	1120	1	53,57,73	1.08	4 (7%)	61,93,113	1.21	5 (8%)
16	CLA	x	516	-	50,54,73	1.14	4 (8%)	59,90,113	1.18	5 (8%)
16	CLA	B	1225	-	69,73,73	0.99	6 (8%)	82,113,113	1.01	4 (4%)
16	CLA	J	1303	8	41,45,73	1.24	5 (12%)	50,78,113	1.07	3 (6%)
16	CLA	W	506	12	64,68,73	1.03	3 (4%)	76,107,113	1.09	5 (6%)
23	LMU	p	606	-	36,36,36	0.83	0	47,47,47	1.33	5 (10%)
16	CLA	B	1218	-	59,63,73	1.07	4 (6%)	70,101,113	1.15	5 (7%)
16	CLA	B	1238	25	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	Y	509	12	64,68,73	1.04	4 (6%)	76,107,113	1.06	6 (7%)
16	CLA	B	1215	2	64,68,73	1.00	5 (7%)	76,107,113	1.11	3 (3%)
16	CLA	G	1205	2	69,73,73	0.99	5 (7%)	82,113,113	1.09	4 (4%)
16	CLA	p	517	12	59,63,73	1.07	4 (6%)	70,101,113	1.02	4 (5%)
16	CLA	B	1230	2	49,53,73	1.18	4 (8%)	58,89,113	1.11	4 (6%)
16	CLA	v	516	12	50,54,73	1.14	4 (8%)	59,90,113	0.99	3 (5%)
16	CLA	b	1231	25	49,53,73	1.18	4 (8%)	58,89,113	1.21	4 (6%)
16	CLA	A	1123	25	69,73,73	0.99	4 (5%)	82,113,113	1.07	4 (4%)
16	CLA	X	512	12	69,73,73	0.99	5 (7%)	82,113,113	1.00	5 (6%)
16	CLA	A	1117	1	69,73,73	0.99	5 (7%)	82,113,113	1.14	4 (4%)
19	BCR	f	4016	-	41,41,41	0.87	0	56,56,56	1.29	5 (8%)
16	CLA	a	1128	1	69,73,73	0.97	6 (8%)	82,113,113	1.10	6 (7%)
19	BCR	S	4015	-	41,41,41	0.87	0	56,56,56	1.20	8 (14%)
16	CLA	B	1234	2	54,58,73	1.13	6 (11%)	64,95,113	1.13	5 (7%)
16	CLA	q	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.03	3 (3%)
16	CLA	b	1229	2	62,66,73	1.06	4 (6%)	73,104,113	1.04	5 (6%)
16	CLA	x	515	12	69,73,73	0.98	4 (5%)	82,113,113	1.14	6 (7%)
16	CLA	a	1130	1	64,68,73	1.04	5 (7%)	76,107,113	1.01	6 (7%)
16	CLA	o	506	-	64,68,73	1.04	5 (7%)	76,107,113	1.06	4 (5%)
16	CLA	A	1135	1	55,59,73	1.13	7 (12%)	64,96,113	1.12	5 (7%)
21	ECH	I	4020	-	42,42,42	0.88	1 (2%)	55,58,58	1.90	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	1116	1	58,62,73	1.04	5 (8%)	68,99,113	1.20	7 (10%)
16	CLA	a	1013	-	69,73,73	0.99	6 (8%)	82,113,113	1.17	5 (6%)
19	BCR	v	604	-	41,41,41	0.86	0	56,56,56	1.28	8 (14%)
19	BCR	U	4019	-	41,41,41	0.86	0	56,56,56	1.49	8 (14%)
13	LHG	p	605	-	31,31,48	0.77	1 (3%)	34,37,54	1.29	4 (11%)
19	BCR	s	602	-	41,41,41	0.87	0	56,56,56	1.32	8 (14%)
16	CLA	v	510	-	69,73,73	1.02	4 (5%)	82,113,113	1.01	7 (8%)
19	BCR	l	4022	-	41,41,41	0.89	1 (2%)	56,56,56	1.41	8 (14%)
16	CLA	b	1209	2	49,53,73	1.17	4 (8%)	58,89,113	1.10	3 (5%)
16	CLA	b	1235	2	66,70,73	1.04	6 (9%)	78,109,113	1.15	8 (10%)
19	BCR	X	604	-	41,41,41	0.88	0	56,56,56	1.31	5 (8%)
19	BCR	o	602	-	41,41,41	0.88	0	56,56,56	1.37	7 (12%)
16	CLA	h	511	12	69,73,73	1.00	6 (8%)	82,113,113	1.08	8 (9%)
17	PQN	A	2001	-	34,34,34	0.37	0	43,45,45	1.08	2 (4%)
19	BCR	h	603	-	41,41,41	0.83	0	56,56,56	1.19	4 (7%)
16	CLA	o	510	-	64,68,73	1.04	4 (6%)	76,107,113	0.98	5 (6%)
16	CLA	h	503	-	50,54,73	1.18	5 (10%)	59,90,113	1.26	6 (10%)
16	CLA	G	1204	2	69,73,73	0.98	4 (5%)	82,113,113	0.98	3 (3%)
16	CLA	B	1221	25	69,73,73	0.99	4 (5%)	82,113,113	1.02	3 (3%)
19	BCR	g	601	-	41,41,41	0.88	0	56,56,56	1.44	9 (16%)
16	CLA	t	510	-	69,73,73	1.00	4 (5%)	82,113,113	0.99	5 (6%)
19	BCR	G	4014	-	41,41,41	0.90	1 (2%)	56,56,56	1.29	8 (14%)
16	CLA	h	501	12	50,54,73	1.17	5 (10%)	59,90,113	1.26	6 (10%)
16	CLA	y	509	12	69,73,73	1.00	4 (5%)	82,113,113	0.97	5 (6%)
16	CLA	y	508	12	59,63,73	1.08	4 (6%)	70,101,113	1.20	6 (8%)
16	CLA	W	507	12	69,73,73	1.01	4 (5%)	82,113,113	1.01	4 (4%)
16	CLA	W	511	12	69,73,73	1.01	5 (7%)	82,113,113	1.09	6 (7%)
16	CLA	a	1123	-	69,73,73	1.00	4 (5%)	82,113,113	1.01	4 (4%)
19	BCR	Y	604	-	41,41,41	0.86	0	56,56,56	1.16	6 (10%)
16	CLA	X	510	-	64,68,73	1.03	4 (6%)	76,107,113	0.97	4 (5%)
19	BCR	p	602	-	41,41,41	0.87	0	56,56,56	1.31	7 (12%)
16	CLA	b	1207	2	69,73,73	0.99	4 (5%)	82,113,113	1.17	4 (4%)
16	CLA	A	1119	25	69,73,73	1.00	4 (5%)	82,113,113	0.99	4 (4%)
16	CLA	Y	510	-	69,73,73	1.00	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	A	1103	-	69,73,73	0.97	4 (5%)	82,113,113	1.00	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	1106	1	69,73,73	0.98	4 (5%)	82,113,113	1.12	4 (4%)
16	CLA	H	1022	25	69,73,73	1.00	5 (7%)	82,113,113	1.15	8 (9%)
16	CLA	W	512	12	64,68,73	1.04	6 (9%)	76,107,113	1.08	4 (5%)
16	CLA	a	1110	1	58,62,73	1.04	4 (6%)	68,99,113	1.01	2 (2%)
16	CLA	y	510	-	69,73,73	1.01	4 (5%)	82,113,113	0.95	5 (6%)
16	CLA	K	4002	9	49,53,73	1.17	4 (8%)	58,89,113	1.02	2 (3%)
16	CLA	s	502	12	54,58,73	1.10	5 (9%)	64,95,113	1.09	3 (4%)
16	CLA	a	1104	1	69,73,73	1.00	6 (8%)	82,113,113	1.03	4 (4%)
19	BCR	x	603	-	41,41,41	0.85	0	56,56,56	1.26	6 (10%)
16	CLA	H	1125	1	69,73,73	0.98	4 (5%)	82,113,113	0.99	2 (2%)
16	CLA	a	1114	-	50,54,73	1.15	5 (10%)	59,90,113	1.31	5 (8%)
16	CLA	t	507	12	69,73,73	1.01	4 (5%)	82,113,113	0.98	3 (3%)
16	CLA	U	1501	10	64,68,73	1.03	5 (7%)	76,107,113	1.01	4 (5%)
19	BCR	r	601	-	41,41,41	0.86	1 (2%)	56,56,56	1.28	7 (12%)
19	BCR	s	604	-	41,41,41	0.87	0	56,56,56	1.22	5 (8%)
19	BCR	v	603	-	41,41,41	0.85	0	56,56,56	1.27	8 (14%)
24	LUT	q	601	-	42,43,43	0.77	0	51,60,60	1.51	9 (17%)
16	CLA	X	507	12	69,73,73	1.00	4 (5%)	82,113,113	0.95	4 (4%)
16	CLA	J	1302	8	49,53,73	1.19	5 (10%)	58,89,113	1.26	6 (10%)
16	CLA	G	1230	2	49,53,73	1.17	4 (8%)	58,89,113	1.03	2 (3%)
19	BCR	G	4010	-	41,41,41	0.94	0	56,56,56	1.39	9 (16%)
23	LMU	r	606	-	36,36,36	0.87	0	47,47,47	1.10	2 (4%)
16	CLA	g	503	-	50,54,73	1.15	4 (8%)	59,90,113	1.13	4 (6%)
18	SF4	N	102	-	0,12,12	-	-	-	-	-
19	BCR	s	601	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	g	506	12	64,68,73	1.01	4 (6%)	76,107,113	1.01	5 (6%)
16	CLA	G	1209	2	49,53,73	1.18	4 (8%)	58,89,113	1.17	4 (6%)
16	CLA	X	501	12	50,54,73	1.14	4 (8%)	59,90,113	1.11	5 (8%)
16	CLA	p	502	12	54,58,73	1.10	5 (9%)	64,95,113	1.07	4 (6%)
16	CLA	S	1303	8	41,45,73	1.25	5 (12%)	50,78,113	1.03	2 (4%)
14	LMG	A	4101	-	46,46,55	0.92	2 (4%)	54,54,63	1.23	4 (7%)
19	BCR	y	604	-	41,41,41	0.87	0	56,56,56	1.29	7 (12%)
19	BCR	B	4017	-	41,41,41	0.88	0	56,56,56	1.22	6 (10%)
13	LHG	b	4018	16	37,37,48	0.71	0	40,43,54	1.31	5 (12%)
16	CLA	H	1136	1	69,73,73	0.98	5 (7%)	82,113,113	0.99	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	o	513	-	50,54,73	1.16	4 (8%)	59,90,113	0.98	1 (1%)
13	LHG	A	849	-	42,42,48	0.69	1 (2%)	45,48,54	1.23	5 (11%)
16	CLA	G	1217	2	49,53,73	1.17	4 (8%)	58,89,113	1.04	2 (3%)
16	CLA	a	1237	25	69,73,73	0.99	4 (5%)	82,113,113	1.12	6 (7%)
16	CLA	B	1227	2	53,57,73	1.13	6 (11%)	61,93,113	1.13	4 (6%)
14	LMG	H	4201	-	32,32,55	0.98	1 (3%)	40,40,63	1.17	3 (7%)
16	CLA	n	510	-	69,73,73	1.01	3 (4%)	82,113,113	1.04	4 (4%)
16	CLA	W	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.22	5 (8%)
16	CLA	G	1234	2	54,58,73	1.13	6 (11%)	64,95,113	1.16	4 (6%)
16	CLA	G	1226	2	64,68,73	1.04	6 (9%)	76,107,113	1.10	5 (6%)
16	CLA	H	1117	1	69,73,73	0.99	5 (7%)	82,113,113	1.15	6 (7%)
16	CLA	S	1302	8	49,53,73	1.18	5 (10%)	58,89,113	1.11	5 (8%)
14	LMG	a	4201	-	32,32,55	0.98	1 (3%)	40,40,63	1.17	3 (7%)
16	CLA	Y	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.12	5 (7%)
16	CLA	a	1133	1	58,62,73	1.09	5 (8%)	68,99,113	1.10	5 (7%)
16	CLA	G	1221	25	69,73,73	1.00	4 (5%)	82,113,113	1.07	3 (3%)
16	CLA	o	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.06	4 (4%)
19	BCR	u	604	-	41,41,41	0.89	0	56,56,56	1.35	10 (17%)
19	BCR	Y	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	b	1226	2	64,68,73	1.04	6 (9%)	76,107,113	1.08	4 (5%)
16	CLA	o	509	12	64,68,73	1.03	4 (6%)	76,107,113	0.95	5 (6%)
16	CLA	t	516	-	50,54,73	1.16	4 (8%)	59,90,113	1.10	4 (6%)
14	LMG	G	848	-	43,43,55	0.86	0	51,51,63	1.27	7 (13%)
16	CLA	W	515	12	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	y	515	12	69,73,73	1.01	4 (5%)	82,113,113	1.14	8 (9%)
19	BCR	H	4008	-	41,41,41	0.90	1 (2%)	56,56,56	1.37	4 (7%)
19	BCR	p	601	-	41,41,41	0.87	0	56,56,56	1.32	8 (14%)
16	CLA	a	1111	1	59,63,73	1.09	5 (8%)	70,101,113	1.03	2 (2%)
16	CLA	u	504	12	64,68,73	1.06	6 (9%)	76,107,113	1.05	4 (5%)
14	LMG	A	4201	-	32,32,55	1.00	1 (3%)	40,40,63	1.18	3 (7%)
16	CLA	y	501	12	50,54,73	1.15	4 (8%)	59,90,113	1.27	7 (11%)
18	SF4	N	101	-	0,12,12	-	-	-	-	-
16	CLA	v	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.24	7 (11%)
16	CLA	n	501	12	54,58,73	1.12	4 (7%)	64,95,113	1.21	7 (10%)
16	CLA	G	1222	25	54,58,73	1.13	6 (11%)	64,95,113	1.15	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	L	1502	10	64,68,73	1.00	5 (7%)	76,107,113	1.12	4 (5%)
16	CLA	y	507	12	69,73,73	1.02	5 (7%)	82,113,113	0.96	4 (4%)
19	BCR	S	4012	-	41,41,41	0.88	0	56,56,56	1.28	7 (12%)
16	CLA	g	509	12	69,73,73	1.01	6 (8%)	82,113,113	1.09	5 (6%)
16	CLA	H	1114	-	50,54,73	1.13	5 (10%)	59,90,113	1.27	7 (11%)
16	CLA	o	505	12	69,73,73	0.99	4 (5%)	82,113,113	1.09	4 (4%)
19	BCR	s	603	-	41,41,41	0.86	0	56,56,56	1.18	6 (10%)
16	CLA	Z	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.03	6 (7%)
16	CLA	n	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.24	5 (8%)
19	BCR	A	4011	-	41,41,41	0.88	0	56,56,56	1.29	4 (7%)
19	BCR	o	603	-	41,41,41	0.87	0	56,56,56	1.31	8 (14%)
19	BCR	n	603	-	41,41,41	0.83	0	56,56,56	1.20	5 (8%)
16	CLA	Z	504	12	69,73,73	1.01	6 (8%)	82,113,113	1.09	6 (7%)
16	CLA	t	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.28	5 (8%)
16	CLA	b	1203	2	69,73,73	1.00	5 (7%)	82,113,113	1.08	6 (7%)
16	CLA	g	514	-	54,58,73	1.13	6 (11%)	64,95,113	1.08	5 (7%)
16	CLA	W	516	-	50,54,73	1.16	4 (8%)	59,90,113	1.12	4 (6%)
16	CLA	B	1207	2	69,73,73	0.99	5 (7%)	82,113,113	1.18	6 (7%)
16	CLA	X	505	12	69,73,73	1.00	5 (7%)	82,113,113	1.12	6 (7%)
19	BCR	v	601	-	41,41,41	0.83	0	56,56,56	1.30	7 (12%)
16	CLA	H	1140	1	69,73,73	0.97	5 (7%)	82,113,113	1.07	3 (3%)
16	CLA	X	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.16	4 (6%)
19	BCR	q	602	-	41,41,41	0.85	0	56,56,56	1.24	6 (10%)
16	CLA	X	504	12	64,68,73	1.06	6 (9%)	76,107,113	1.16	3 (3%)
16	CLA	q	517	12	59,63,73	1.08	5 (8%)	70,101,113	1.13	6 (8%)
16	CLA	Y	503	-	50,54,73	1.14	4 (8%)	59,90,113	1.19	5 (8%)
16	CLA	t	515	12	69,73,73	1.00	4 (5%)	82,113,113	1.15	5 (6%)
16	CLA	G	1207	2	69,73,73	1.00	4 (5%)	82,113,113	1.15	5 (6%)
19	BCR	p	603	-	41,41,41	0.86	0	56,56,56	1.21	5 (8%)
16	CLA	a	1140	1	69,73,73	0.97	5 (7%)	82,113,113	1.11	5 (6%)
16	CLA	p	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	W	517	12	59,63,73	1.09	5 (8%)	70,101,113	0.98	4 (5%)
16	CLA	H	1132	1	69,73,73	0.99	6 (8%)	82,113,113	1.11	5 (6%)
16	CLA	u	514	-	54,58,73	1.12	4 (7%)	64,95,113	1.20	6 (9%)
16	CLA	H	1120	1	53,57,73	1.09	4 (7%)	61,93,113	1.18	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMT	U	4101	-	36,36,36	1.16	6 (16%)	47,47,47	1.09	1 (2%)
13	LHG	a	849	-	42,42,48	0.71	1 (2%)	45,48,54	1.22	4 (8%)
18	SF4	A	3001	-	0,12,12	-	-	-		
20	LMT	a	4202	-	36,36,36	1.17	5 (13%)	47,47,47	0.93	0
16	CLA	w	506	-	64,68,73	1.03	5 (7%)	76,107,113	1.09	4 (5%)
16	CLA	a	1124	25	64,68,73	1.03	4 (6%)	76,107,113	0.99	2 (2%)
16	CLA	a	1131	1	69,73,73	1.01	6 (8%)	82,113,113	1.13	3 (3%)
16	CLA	G	1236	2	54,58,73	1.10	4 (7%)	64,95,113	1.14	3 (4%)
16	CLA	H	1104	1	69,73,73	1.00	6 (8%)	82,113,113	1.07	6 (7%)
14	LMG	F	4017	-	27,27,55	1.10	2 (7%)	35,35,63	1.16	3 (8%)
16	CLA	r	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.11	5 (7%)
16	CLA	b	1232	25	49,53,73	1.19	5 (10%)	58,89,113	1.35	4 (6%)
16	CLA	o	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	H	1115	1	58,62,73	1.06	4 (6%)	68,99,113	1.16	2 (2%)
19	BCR	q	604	-	41,41,41	0.87	0	56,56,56	1.26	6 (10%)
16	CLA	r	511	12	69,73,73	1.01	5 (7%)	82,113,113	0.89	2 (2%)
13	LHG	R	103	-	39,39,48	0.68	2 (5%)	42,45,54	1.24	4 (9%)
19	BCR	b	4005	-	41,41,41	0.85	0	56,56,56	1.15	5 (8%)
16	CLA	t	514	-	54,58,73	1.12	4 (7%)	64,95,113	1.12	5 (7%)
16	CLA	G	1216	25	51,55,73	1.13	5 (9%)	60,91,113	1.33	4 (6%)
16	CLA	g	511	12	69,73,73	0.99	5 (7%)	82,113,113	0.98	3 (3%)
16	CLA	v	514	-	54,58,73	1.13	4 (7%)	64,95,113	1.05	2 (3%)
16	CLA	n	504	12	64,68,73	1.04	4 (6%)	76,107,113	1.10	4 (5%)
19	BCR	g	603	-	41,41,41	0.84	0	56,56,56	1.21	6 (10%)
16	CLA	B	1223	2	69,73,73	0.98	4 (5%)	82,113,113	1.07	3 (3%)
20	LMT	L	4101	-	36,36,36	1.17	6 (16%)	47,47,47	1.15	3 (6%)
16	CLA	x	513	-	50,54,73	1.18	5 (10%)	59,90,113	1.03	2 (3%)
16	CLA	H	1801	13	50,54,73	1.13	4 (8%)	59,90,113	1.15	5 (8%)
19	BCR	q	603	-	41,41,41	0.84	0	56,56,56	1.16	5 (8%)
16	CLA	h	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.15	6 (8%)
16	CLA	g	517	12	59,63,73	1.09	4 (6%)	70,101,113	0.99	3 (4%)
16	CLA	y	505	12	69,73,73	1.02	5 (7%)	82,113,113	1.21	5 (6%)
16	CLA	X	509	12	64,68,73	1.05	5 (7%)	76,107,113	1.00	6 (7%)
16	CLA	H	1237	25	69,73,73	0.99	5 (7%)	82,113,113	1.08	6 (7%)
16	CLA	Y	501	12	54,58,73	1.10	4 (7%)	64,95,113	1.20	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	y	503	-	50,54,73	1.18	6 (12%)	59,90,113	1.21	6 (10%)
19	BCR	H	4003	-	41,41,41	0.86	0	56,56,56	1.22	4 (7%)
19	BCR	U	4022	-	41,41,41	0.88	0	56,56,56	1.32	6 (10%)
16	CLA	B	1232	-	49,53,73	1.18	5 (10%)	58,89,113	1.30	5 (8%)
16	CLA	x	501	-	54,58,73	1.12	5 (9%)	64,95,113	1.34	7 (10%)
16	CLA	Z	511	12	69,73,73	0.99	5 (7%)	82,113,113	1.08	4 (4%)
19	BCR	G	4004	-	41,41,41	0.83	0	56,56,56	1.25	6 (10%)
16	CLA	H	1102	1,16	60,64,73	1.05	4 (6%)	71,102,113	0.94	2 (2%)
14	LMG	b	848	-	43,43,55	0.86	1 (2%)	51,51,63	1.28	6 (11%)
16	CLA	h	505	12	69,73,73	1.02	5 (7%)	82,113,113	1.15	6 (7%)
14	LMG	H	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.23	4 (8%)
16	CLA	W	508	12	59,63,73	1.07	4 (6%)	70,101,113	0.96	3 (4%)
16	CLA	w	511	12	69,73,73	0.99	5 (7%)	82,113,113	1.04	5 (6%)
20	LMT	l	4101	-	36,36,36	1.16	6 (16%)	47,47,47	1.09	1 (2%)
19	BCR	Y	602	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
14	LMG	a	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.24	4 (8%)
13	LHG	u	605	-	26,26,48	0.83	0	29,32,54	1.27	2 (6%)
16	CLA	r	509	12	69,73,73	1.01	5 (7%)	82,113,113	1.03	5 (6%)
19	BCR	r	603	-	41,41,41	0.83	0	56,56,56	1.20	6 (10%)
16	CLA	G	1202	2	69,73,73	0.96	4 (5%)	82,113,113	0.99	5 (6%)
19	BCR	g	604	-	41,41,41	0.88	0	56,56,56	1.28	6 (10%)
19	BCR	w	603	-	41,41,41	0.85	0	56,56,56	1.17	6 (10%)
16	CLA	u	502	12	54,58,73	1.12	6 (11%)	64,95,113	1.12	3 (4%)
16	CLA	Z	509	12	69,73,73	1.00	5 (7%)	82,113,113	1.01	4 (4%)
16	CLA	H	1124	-	64,68,73	1.02	5 (7%)	76,107,113	0.98	3 (3%)
16	CLA	A	1110	1	58,62,73	1.05	4 (6%)	68,99,113	1.01	3 (4%)
16	CLA	h	502	12	54,58,73	1.13	5 (9%)	64,95,113	1.05	5 (7%)
16	CLA	y	516	12	50,54,73	1.17	5 (10%)	59,90,113	1.18	5 (8%)
16	CLA	Y	513	-	50,54,73	1.16	4 (8%)	59,90,113	1.08	5 (8%)
16	CLA	B	1204	2	69,73,73	0.97	4 (5%)	82,113,113	0.94	3 (3%)
16	CLA	H	1106	1	69,73,73	0.96	4 (5%)	82,113,113	1.11	4 (4%)
16	CLA	H	1122	1	63,67,73	1.06	5 (7%)	74,105,113	1.09	6 (8%)
14	LMG	A	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.23	4 (8%)
16	CLA	s	517	12	59,63,73	1.10	5 (8%)	70,101,113	1.09	5 (7%)
16	CLA	b	1211	2	69,73,73	0.98	5 (7%)	82,113,113	0.98	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	x	505	12	69,73,73	0.99	5 (7%)	82,113,113	1.23	6 (7%)
16	CLA	A	1140	1	69,73,73	0.98	5 (7%)	82,113,113	1.12	5 (6%)
19	BCR	h	604	-	41,41,41	0.86	0	56,56,56	1.25	6 (10%)
16	CLA	a	1117	1	69,73,73	0.98	5 (7%)	82,113,113	1.14	6 (7%)
16	CLA	v	505	12	69,73,73	1.02	5 (7%)	82,113,113	1.24	5 (6%)
13	LHG	G	4018	16	37,37,48	0.73	1 (2%)	40,43,54	1.32	5 (12%)
16	CLA	H	1129	1	50,54,73	1.13	5 (10%)	59,90,113	1.16	6 (10%)
16	CLA	o	502	12	54,58,73	1.11	6 (11%)	64,95,113	1.03	4 (6%)
16	CLA	s	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.22	5 (7%)
19	BCR	b	4014	-	41,41,41	0.91	0	56,56,56	1.45	8 (14%)
16	CLA	y	517	-	59,63,73	1.11	5 (8%)	70,101,113	1.26	6 (8%)
19	BCR	j	4013	-	41,41,41	0.86	0	56,56,56	1.26	7 (12%)
16	CLA	b	1213	2	59,63,73	1.08	6 (10%)	70,101,113	1.09	6 (8%)
16	CLA	A	1109	1,16	69,73,73	0.98	5 (7%)	82,113,113	1.13	5 (6%)
21	ECH	b	4006	-	42,42,42	0.85	2 (4%)	55,58,58	1.52	8 (14%)
16	CLA	n	517	12	59,63,73	1.08	5 (8%)	70,101,113	1.02	3 (4%)
16	CLA	Z	516	-	50,54,73	1.13	4 (8%)	59,90,113	1.07	4 (6%)
16	CLA	A	1122	1	63,67,73	1.05	5 (7%)	74,105,113	1.09	6 (8%)
16	CLA	b	1217	2	49,53,73	1.16	4 (8%)	58,89,113	1.20	5 (8%)
16	CLA	A	1801	13	50,54,73	1.14	4 (8%)	59,90,113	1.22	5 (8%)
23	LMU	Y	606	-	36,36,36	0.84	0	47,47,47	1.36	6 (12%)
16	CLA	Y	504	12	69,73,73	1.01	5 (7%)	82,113,113	0.99	3 (3%)
16	CLA	B	1239	2	69,73,73	0.95	3 (4%)	82,113,113	1.11	6 (7%)
19	BCR	W	604	-	41,41,41	0.86	0	56,56,56	1.37	9 (16%)
16	CLA	q	504	12	69,73,73	1.02	5 (7%)	82,113,113	1.11	4 (4%)
16	CLA	B	1222	25	54,58,73	1.13	5 (9%)	64,95,113	1.10	5 (7%)
16	CLA	b	1234	2	54,58,73	1.14	5 (9%)	64,95,113	1.13	8 (12%)
16	CLA	p	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.02	4 (5%)
16	CLA	x	504	12	69,73,73	1.01	4 (5%)	82,113,113	1.04	6 (7%)
16	CLA	Y	517	12	59,63,73	1.08	4 (6%)	70,101,113	1.05	3 (4%)
16	CLA	H	1126	1	69,73,73	0.99	4 (5%)	82,113,113	1.12	5 (6%)
16	CLA	y	513	-	50,54,73	1.16	4 (8%)	59,90,113	1.01	3 (5%)
13	LHG	H	849	-	42,42,48	0.68	0	45,48,54	1.21	4 (8%)
16	CLA	H	1139	25	64,68,73	1.03	5 (7%)	76,107,113	1.01	4 (5%)
16	CLA	u	517	12	59,63,73	1.09	4 (6%)	70,101,113	1.04	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	v	511	12	69,73,73	0.99	4 (5%)	82,113,113	1.08	4 (4%)
16	CLA	G	1223	2	69,73,73	0.98	4 (5%)	82,113,113	1.09	4 (4%)
19	BCR	B	4014	-	41,41,41	0.88	0	56,56,56	1.25	7 (12%)
16	CLA	b	1023	-	69,73,73	1.01	7 (10%)	82,113,113	1.12	5 (6%)
16	CLA	A	1121	1	55,59,73	1.11	5 (9%)	64,96,113	1.11	4 (6%)
16	CLA	B	1226	2	64,68,73	1.05	6 (9%)	76,107,113	1.05	3 (3%)
16	CLA	a	1127	1	69,73,73	1.00	6 (8%)	82,113,113	1.08	4 (4%)
16	CLA	h	513	-	50,54,73	1.17	4 (8%)	59,90,113	0.99	4 (6%)
16	CLA	G	1203	2	69,73,73	0.99	5 (7%)	82,113,113	1.14	6 (7%)
19	BCR	L	4022	-	41,41,41	0.86	0	56,56,56	1.30	6 (10%)
16	CLA	a	1115	1	58,62,73	1.07	5 (8%)	68,99,113	1.14	3 (4%)
16	CLA	B	1224	2	64,68,73	1.05	6 (9%)	76,107,113	1.07	4 (5%)
16	CLA	k	4004	-	59,63,73	1.07	4 (6%)	70,101,113	0.98	5 (7%)
16	CLA	n	509	12	64,68,73	1.04	4 (6%)	76,107,113	1.00	6 (7%)
19	BCR	t	604	-	41,41,41	0.83	0	56,56,56	1.23	4 (7%)
16	CLA	G	1212	2	49,53,73	1.19	5 (10%)	58,89,113	1.20	4 (6%)
16	CLA	Z	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.12	4 (4%)
17	PQN	b	2002	-	34,34,34	0.36	0	43,45,45	1.06	2 (4%)
16	CLA	s	506	12	64,68,73	1.02	6 (9%)	76,107,113	1.12	8 (10%)
16	CLA	A	1237	25	69,73,73	0.99	4 (5%)	82,113,113	1.10	6 (7%)
16	CLA	b	1239	2	69,73,73	0.97	3 (4%)	82,113,113	1.07	7 (8%)
16	CLA	b	1206	2	69,73,73	0.99	5 (7%)	82,113,113	0.94	2 (2%)
16	CLA	u	513	-	50,54,73	1.15	5 (10%)	59,90,113	1.03	3 (5%)
16	CLA	w	512	12	69,73,73	1.00	6 (8%)	82,113,113	1.11	5 (6%)
16	CLA	n	506	12	64,68,73	1.03	4 (6%)	76,107,113	1.08	5 (6%)
18	SF4	c	102	-	0,12,12	-	-	-	-	-
16	CLA	A	1126	1	69,73,73	0.98	5 (7%)	82,113,113	1.13	2 (2%)
19	BCR	b	4004	-	41,41,41	0.84	0	56,56,56	1.26	6 (10%)
16	CLA	A	1131	1	69,73,73	1.02	5 (7%)	82,113,113	1.16	5 (6%)
15	CL0	A	1011	1	69,73,73	1.01	6 (8%)	82,113,113	1.03	5 (6%)
16	CLA	v	517	-	59,63,73	1.11	5 (8%)	70,101,113	1.03	6 (8%)
16	CLA	a	1136	1	69,73,73	0.99	5 (7%)	82,113,113	1.00	3 (3%)
16	CLA	G	1012	25	59,63,73	1.13	6 (10%)	70,101,113	1.19	7 (10%)
16	CLA	W	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.24	5 (7%)
16	CLA	a	1132	1	69,73,73	0.99	6 (8%)	82,113,113	1.20	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	u	509	12	64,68,73	1.03	5 (7%)	76,107,113	1.07	6 (7%)
16	CLA	y	504	12	64,68,73	1.05	6 (9%)	76,107,113	1.19	8 (10%)
16	CLA	w	516	12	50,54,73	1.14	4 (8%)	59,90,113	1.01	4 (6%)
16	CLA	X	514	-	54,58,73	1.12	6 (11%)	64,95,113	1.30	6 (9%)
16	CLA	b	1218	-	59,63,73	1.07	4 (6%)	70,101,113	1.10	7 (10%)
16	CLA	A	1118	1	59,63,73	1.06	4 (6%)	70,101,113	1.00	3 (4%)
16	CLA	a	1135	1	55,59,73	1.14	7 (12%)	64,96,113	1.08	5 (7%)
16	CLA	t	505	12	69,73,73	1.00	5 (7%)	82,113,113	1.19	6 (7%)
16	CLA	p	506	12	64,68,73	1.01	4 (6%)	76,107,113	1.12	5 (6%)
19	BCR	H	4011	-	41,41,41	0.88	0	56,56,56	1.26	6 (10%)
16	CLA	X	513	-	50,54,73	1.14	4 (8%)	59,90,113	1.09	3 (5%)
16	CLA	B	1208	2	49,53,73	1.16	4 (8%)	58,89,113	1.16	6 (10%)
16	CLA	p	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.11	6 (7%)
16	CLA	b	1228	2	59,63,73	1.07	4 (6%)	70,101,113	1.07	5 (7%)
16	CLA	B	1231	25	49,53,73	1.19	4 (8%)	58,89,113	1.16	4 (6%)
16	CLA	o	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.10	4 (6%)
19	BCR	R	4018	-	41,41,41	0.85	0	56,56,56	1.20	7 (12%)
16	CLA	b	1214	2	59,63,73	1.06	5 (8%)	70,101,113	1.03	4 (5%)
19	BCR	t	603	-	41,41,41	0.84	0	56,56,56	1.18	4 (7%)
16	CLA	G	1239	2	69,73,73	0.96	3 (4%)	82,113,113	1.14	6 (7%)
16	CLA	B	1229	2	62,66,73	1.06	4 (6%)	73,104,113	1.05	5 (6%)
16	CLA	q	501	12	54,58,73	1.13	5 (9%)	64,95,113	1.19	6 (9%)
16	CLA	h	507	12	69,73,73	0.99	4 (5%)	82,113,113	1.11	5 (6%)
24	LUT	w	601	-	42,43,43	0.74	0	51,60,60	1.46	7 (13%)
16	CLA	T	4004	-	59,63,73	1.07	4 (6%)	70,101,113	1.13	4 (5%)
19	BCR	n	604	-	41,41,41	0.86	0	56,56,56	1.33	7 (12%)
19	BCR	j	4015	-	41,41,41	0.88	0	56,56,56	1.22	7 (12%)
16	CLA	Z	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.12	5 (7%)
19	BCR	X	603	-	41,41,41	0.85	0	56,56,56	1.15	4 (7%)
16	CLA	H	1128	1	69,73,73	0.98	5 (7%)	82,113,113	1.04	5 (6%)
19	BCR	S	4013	-	41,41,41	0.87	0	56,56,56	1.32	7 (12%)
19	BCR	t	601	-	41,41,41	0.83	0	56,56,56	1.18	6 (10%)
16	CLA	B	1236	2	54,58,73	1.11	6 (11%)	64,95,113	1.14	4 (6%)
16	CLA	G	1224	2	64,68,73	1.05	5 (7%)	76,107,113	1.12	4 (5%)
19	BCR	y	603	-	41,41,41	0.83	0	56,56,56	1.17	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LMG	B	848	-	43,43,55	0.87	1 (2%)	51,51,63	1.28	6 (11%)
16	CLA	K	4003	9	49,53,73	1.20	4 (8%)	58,89,113	1.14	4 (6%)
16	CLA	T	4002	9	49,53,73	1.17	4 (8%)	58,89,113	1.03	3 (5%)
16	CLA	Z	513	-	54,58,73	1.12	4 (7%)	64,95,113	1.07	5 (7%)
16	CLA	A	1124	25	64,68,73	1.03	4 (6%)	76,107,113	1.05	4 (5%)
21	ECH	G	4006	-	42,42,42	0.79	0	55,58,58	1.50	8 (14%)
16	CLA	A	1128	1	69,73,73	0.98	5 (7%)	82,113,113	1.08	4 (4%)
16	CLA	x	508	12	59,63,73	1.08	4 (6%)	70,101,113	0.99	3 (4%)
19	BCR	k	4001	-	41,41,41	0.86	0	56,56,56	1.30	6 (10%)
19	BCR	X	601	-	41,41,41	0.87	1 (2%)	56,56,56	1.33	6 (10%)
16	CLA	U	1503	-	69,73,73	1.00	4 (5%)	82,113,113	0.87	3 (3%)
18	SF4	H	3001	-	0,12,12	-	-	-	-	-
16	CLA	b	1215	2	64,68,73	1.00	4 (6%)	76,107,113	1.15	3 (3%)
19	BCR	F	4016	-	41,41,41	0.86	0	56,56,56	1.31	8 (14%)
19	BCR	J	4013	-	41,41,41	0.86	0	56,56,56	1.23	8 (14%)
16	CLA	h	509	12	69,73,73	1.02	6 (8%)	82,113,113	1.07	6 (7%)
16	CLA	x	507	12	69,73,73	1.00	5 (7%)	82,113,113	1.07	6 (7%)
13	LHG	x	605	-	30,30,48	0.78	1 (3%)	33,36,54	1.28	3 (9%)
16	CLA	g	505	12	69,73,73	0.99	5 (7%)	82,113,113	1.19	7 (8%)
16	CLA	B	1216	25	51,55,73	1.17	6 (11%)	60,91,113	1.15	4 (6%)
16	CLA	n	513	-	50,54,73	1.16	5 (10%)	59,90,113	1.05	4 (6%)
16	CLA	F	1302	6	50,54,73	1.17	5 (10%)	59,90,113	1.05	3 (5%)
16	CLA	W	504	12	64,68,73	1.05	5 (7%)	76,107,113	1.01	3 (3%)
16	CLA	b	1223	2	69,73,73	0.99	4 (5%)	82,113,113	1.09	1 (1%)
16	CLA	q	505	-	69,73,73	0.99	6 (8%)	82,113,113	1.16	8 (9%)
16	CLA	A	1108	1	49,53,73	1.18	5 (10%)	58,89,113	1.10	2 (3%)
16	CLA	G	1227	2	53,57,73	1.12	6 (11%)	61,93,113	1.15	5 (8%)
16	CLA	B	1023	-	69,73,73	1.01	7 (10%)	82,113,113	1.12	5 (6%)
19	BCR	Y	603	-	41,41,41	0.85	0	56,56,56	1.16	4 (7%)
19	BCR	G	4017	-	41,41,41	0.87	0	56,56,56	1.18	6 (10%)
16	CLA	A	1134	1	49,53,73	1.19	5 (10%)	58,89,113	1.09	2 (3%)
16	CLA	u	515	12	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	A	1139	25	64,68,73	1.03	5 (7%)	76,107,113	1.03	4 (5%)
16	CLA	a	1122	1	63,67,73	1.04	5 (7%)	74,105,113	1.10	4 (5%)
16	CLA	s	513	-	50,54,73	1.15	4 (8%)	59,90,113	1.16	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	W	505	12	69,73,73	1.00	4 (5%)	82,113,113	1.15	6 (7%)
16	CLA	a	1801	13	50,54,73	1.16	4 (8%)	59,90,113	1.20	4 (6%)
16	CLA	G	1211	2	69,73,73	0.98	4 (5%)	82,113,113	1.01	2 (2%)
16	CLA	o	511	-	69,73,73	0.98	4 (5%)	82,113,113	1.03	5 (6%)
16	CLA	a	1118	1	59,63,73	1.06	4 (6%)	70,101,113	0.96	2 (2%)
16	CLA	n	511	12	69,73,73	1.00	5 (7%)	82,113,113	1.05	5 (6%)
16	CLA	x	514	-	54,58,73	1.11	5 (9%)	64,95,113	1.10	5 (7%)
19	BCR	G	4005	-	41,41,41	0.85	0	56,56,56	1.14	4 (7%)
16	CLA	v	506	-	64,68,73	1.05	5 (7%)	76,107,113	1.33	7 (9%)
23	LMU	x	606	-	36,36,36	0.88	0	47,47,47	1.26	6 (12%)
16	CLA	o	504	12	64,68,73	1.05	5 (7%)	76,107,113	1.05	4 (5%)
16	CLA	x	517	12	59,63,73	1.09	4 (6%)	70,101,113	0.96	2 (2%)
19	BCR	k	4005	-	41,41,41	0.85	0	56,56,56	1.26	5 (8%)
16	CLA	A	1105	-	62,66,73	1.06	5 (8%)	73,104,113	1.00	4 (5%)
16	CLA	a	1103	1	69,73,73	0.97	4 (5%)	82,113,113	0.98	2 (2%)
16	CLA	G	1208	2	49,53,73	1.16	4 (8%)	58,89,113	1.22	6 (10%)
16	CLA	b	1222	25	54,58,73	1.14	5 (9%)	64,95,113	1.08	4 (6%)
16	CLA	A	1101	1	69,73,73	0.98	5 (7%)	82,113,113	1.04	7 (8%)
19	BCR	j	4012	-	41,41,41	0.88	0	56,56,56	1.29	7 (12%)
16	CLA	r	505	12	69,73,73	0.99	5 (7%)	82,113,113	1.17	4 (4%)
21	ECH	R	4020	-	42,42,42	0.99	3 (7%)	55,58,58	1.93	14 (25%)
16	CLA	w	515	12	69,73,73	0.99	5 (7%)	82,113,113	1.12	4 (4%)
16	CLA	H	1113	1	49,53,73	1.20	6 (12%)	58,89,113	1.18	3 (5%)
16	CLA	b	1238	25	69,73,73	0.98	4 (5%)	82,113,113	1.06	8 (9%)
16	CLA	r	504	12	69,73,73	1.01	4 (5%)	82,113,113	0.99	3 (3%)
19	BCR	i	4018	-	41,41,41	0.87	0	56,56,56	1.23	8 (14%)
19	BCR	n	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	Z	502	12	54,58,73	1.11	6 (11%)	64,95,113	1.11	5 (7%)
16	CLA	l	1502	10	64,68,73	1.00	5 (7%)	76,107,113	1.16	5 (6%)
16	CLA	s	504	12	69,73,73	0.99	4 (5%)	82,113,113	0.95	3 (3%)
19	BCR	G	4009	-	30,30,41	0.84	0	39,39,56	1.32	5 (12%)
19	BCR	T	4001	-	41,41,41	0.86	1 (2%)	56,56,56	1.26	6 (10%)
16	CLA	a	1126	1	69,73,73	0.99	5 (7%)	82,113,113	1.08	3 (3%)
19	BCR	y	601	-	41,41,41	0.83	0	56,56,56	1.24	6 (10%)
16	CLA	H	1110	1	58,62,73	1.05	4 (6%)	68,99,113	1.03	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	H	1135	1	55,59,73	1.12	4 (7%)	64,96,113	1.26	6 (9%)
16	CLA	s	516	-	50,54,73	1.15	4 (8%)	59,90,113	1.06	3 (5%)
16	CLA	p	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.16	6 (9%)
16	CLA	G	1229	2	62,66,73	1.05	4 (6%)	73,104,113	1.03	4 (5%)
16	CLA	y	514	-	54,58,73	1.13	6 (11%)	64,95,113	1.13	6 (9%)
16	CLA	p	509	12	64,68,73	1.05	4 (6%)	76,107,113	0.98	3 (3%)
16	CLA	U	1502	10	64,68,73	1.01	5 (7%)	76,107,113	1.14	5 (6%)
16	CLA	a	1106	1	69,73,73	0.97	4 (5%)	82,113,113	1.10	3 (3%)
16	CLA	A	1112	1	49,53,73	1.19	4 (8%)	58,89,113	1.07	4 (6%)
21	ECH	V	4021	-	42,42,42	0.84	1 (2%)	55,58,58	1.55	7 (12%)
16	CLA	v	513	-	50,54,73	1.17	4 (8%)	59,90,113	1.01	3 (5%)
16	CLA	g	502	12	54,58,73	1.10	5 (9%)	64,95,113	1.07	2 (3%)
20	LMT	H	4202	-	36,36,36	1.16	5 (13%)	47,47,47	0.91	0
13	LHG	B	4018	16	37,37,48	0.72	1 (2%)	40,43,54	1.32	5 (12%)
16	CLA	A	1130	1	64,68,73	1.03	5 (7%)	76,107,113	0.94	4 (5%)
16	CLA	a	1107	1	54,58,73	1.11	4 (7%)	64,95,113	1.14	3 (4%)
16	CLA	H	1109	1,16	69,73,73	0.98	4 (5%)	82,113,113	1.12	6 (7%)
16	CLA	v	501	12	50,54,73	1.17	5 (10%)	59,90,113	1.26	7 (11%)
16	CLA	H	1133	1	58,62,73	1.08	6 (10%)	68,99,113	1.28	6 (8%)
16	CLA	n	516	-	50,54,73	1.17	4 (8%)	59,90,113	0.99	3 (5%)
18	SF4	C	102	-	0,12,12	-	-	-	-	-
16	CLA	G	1201	2	58,62,73	1.08	4 (6%)	68,99,113	1.05	4 (5%)
16	CLA	a	1138	1	69,73,73	0.98	5 (7%)	82,113,113	1.04	7 (8%)
18	SF4	C	101	-	0,12,12	-	-	-	-	-
16	CLA	H	1105	-	62,66,73	1.05	5 (8%)	73,104,113	1.08	5 (6%)
16	CLA	w	505	-	69,73,73	0.99	4 (5%)	82,113,113	1.05	5 (6%)
16	CLA	p	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.18	5 (6%)
16	CLA	H	1119	25	69,73,73	0.98	5 (7%)	82,113,113	1.02	4 (4%)
16	CLA	q	513	-	54,58,73	1.12	4 (7%)	64,95,113	1.08	4 (6%)
19	BCR	w	602	-	41,41,41	0.86	0	56,56,56	1.26	7 (12%)
16	CLA	a	1108	1	49,53,73	1.17	5 (10%)	58,89,113	1.25	5 (8%)
19	BCR	B	4004	-	41,41,41	0.83	0	56,56,56	1.26	5 (8%)
16	CLA	H	1138	1	69,73,73	0.99	5 (7%)	82,113,113	1.07	4 (4%)
16	CLA	G	1206	2	69,73,73	0.98	5 (7%)	82,113,113	0.95	3 (3%)
19	BCR	a	4007	-	41,41,41	0.89	1 (2%)	56,56,56	1.30	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	T	4003	9	49,53,73	1.18	4 (8%)	58,89,113	1.05	3 (5%)
16	CLA	a	1134	1	49,53,73	1.16	4 (8%)	58,89,113	1.16	4 (6%)
16	CLA	o	515	12	69,73,73	0.98	4 (5%)	82,113,113	1.07	6 (7%)
16	CLA	o	517	12	59,63,73	1.08	4 (6%)	70,101,113	0.98	4 (5%)
16	CLA	t	517	12	59,63,73	1.09	5 (8%)	70,101,113	1.00	3 (4%)
19	BCR	J	4015	-	41,41,41	0.87	0	56,56,56	1.26	9 (16%)
16	CLA	G	1220	2	58,62,73	1.10	4 (6%)	68,99,113	1.09	5 (7%)
16	CLA	B	1219	-	49,53,73	1.21	6 (12%)	58,89,113	1.15	4 (6%)
16	CLA	F	1301	25	49,53,73	1.18	4 (8%)	58,89,113	1.13	3 (5%)
13	LHG	o	605	-	26,26,48	0.85	0	29,32,54	1.27	2 (6%)
16	CLA	Z	510	-	64,68,73	1.04	4 (6%)	76,107,113	1.04	3 (3%)
16	CLA	v	512	12	69,73,73	1.02	4 (5%)	82,113,113	1.08	7 (8%)
16	CLA	a	1113	1	49,53,73	1.21	7 (14%)	58,89,113	1.15	2 (3%)
16	CLA	u	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.03	4 (5%)
19	BCR	a	4011	-	41,41,41	0.89	0	56,56,56	1.26	5 (8%)
17	PQN	B	2002	-	34,34,34	0.36	0	43,45,45	1.04	2 (4%)
16	CLA	A	1127	1	69,73,73	0.99	6 (8%)	82,113,113	1.07	4 (4%)
16	CLA	H	1121	1	55,59,73	1.12	5 (9%)	64,96,113	1.14	4 (6%)
16	CLA	w	502	12	54,58,73	1.11	6 (11%)	64,95,113	1.17	5 (7%)
16	CLA	G	1219	-	49,53,73	1.21	5 (10%)	58,89,113	1.14	5 (8%)
16	CLA	B	1202	-	69,73,73	0.99	4 (5%)	82,113,113	0.92	2 (2%)
19	BCR	r	604	-	41,41,41	0.89	0	56,56,56	1.27	6 (10%)
16	CLA	B	1021	2	69,73,73	1.00	5 (7%)	82,113,113	1.14	6 (7%)
13	LHG	X	605	-	26,26,48	0.82	0	29,32,54	1.27	2 (6%)
16	CLA	l	1501	10	64,68,73	1.03	5 (7%)	76,107,113	0.99	4 (5%)
13	LHG	g	605	-	30,30,48	0.80	2 (6%)	33,36,54	1.26	3 (9%)
16	CLA	x	509	12	69,73,73	1.00	5 (7%)	82,113,113	1.08	6 (7%)
16	CLA	G	1214	2	59,63,73	1.06	6 (10%)	70,101,113	1.11	5 (7%)
16	CLA	B	1212	2	49,53,73	1.19	5 (10%)	58,89,113	1.14	4 (6%)
16	CLA	v	502	12	54,58,73	1.12	5 (9%)	64,95,113	1.06	5 (7%)
19	BCR	K	4001	-	41,41,41	0.86	0	56,56,56	1.31	7 (12%)
16	CLA	G	1021	2	69,73,73	0.99	5 (7%)	82,113,113	1.16	5 (6%)
19	BCR	b	4009	-	30,30,41	0.85	0	39,39,56	1.35	6 (15%)
16	CLA	g	512	12	69,73,73	1.00	5 (7%)	82,113,113	1.17	4 (4%)
16	CLA	w	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.14	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	p	504	12	69,73,73	1.00	4 (5%)	82,113,113	1.00	3 (3%)
13	LHG	Y	605	-	31,31,48	0.78	1 (3%)	34,37,54	1.29	4 (11%)
13	LHG	r	605	-	30,30,48	0.81	2 (6%)	33,36,54	1.28	3 (9%)
19	BCR	a	4002	-	41,41,41	0.85	0	56,56,56	1.18	5 (8%)
16	CLA	B	1220	2	57,61,73	1.11	4 (7%)	67,98,113	1.11	6 (8%)
13	LHG	A	851	16	25,25,48	0.87	1 (4%)	28,31,54	1.27	2 (7%)
16	CLA	p	514	-	54,58,73	1.13	5 (9%)	64,95,113	1.10	4 (6%)
16	CLA	X	511	-	69,73,73	0.98	4 (5%)	82,113,113	1.10	6 (7%)
16	CLA	G	1225	-	69,73,73	0.99	6 (8%)	82,113,113	1.14	4 (4%)
16	CLA	H	1118	1	59,63,73	1.07	4 (6%)	70,101,113	1.07	7 (10%)
16	CLA	g	516	-	50,54,73	1.15	4 (8%)	59,90,113	1.19	3 (5%)
16	CLA	r	508	12	59,63,73	1.08	4 (6%)	70,101,113	1.01	3 (4%)
19	BCR	Q	4016	-	41,41,41	0.86	0	56,56,56	1.28	7 (12%)
16	CLA	W	502	12	54,58,73	1.14	6 (11%)	64,95,113	1.16	5 (7%)
16	CLA	u	516	12	50,54,73	1.14	5 (10%)	59,90,113	1.15	4 (6%)
19	BCR	x	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
20	LMT	A	4202	-	36,36,36	1.16	5 (13%)	47,47,47	0.92	0
16	CLA	q	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.13	6 (7%)
16	CLA	a	1112	1	49,53,73	1.19	5 (10%)	58,89,113	1.00	3 (5%)
16	CLA	Z	503	12	50,54,73	1.15	6 (12%)	59,90,113	1.19	6 (10%)
16	CLA	Q	1302	6	50,54,73	1.16	5 (10%)	59,90,113	1.07	4 (6%)
16	CLA	s	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	v	504	12	64,68,73	1.04	5 (7%)	76,107,113	1.09	6 (7%)
16	CLA	x	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.11	6 (7%)
16	CLA	H	1103	-	69,73,73	0.99	4 (5%)	82,113,113	1.01	4 (4%)
16	CLA	y	511	12	69,73,73	1.00	4 (5%)	82,113,113	1.12	5 (6%)
21	ECH	M	4021	-	42,42,42	0.86	0	55,58,58	1.53	9 (16%)
13	LHG	s	605	-	31,31,48	0.79	1 (3%)	34,37,54	1.28	4 (11%)
23	LMU	w	605	-	36,36,36	0.84	0	47,47,47	1.10	4 (8%)
16	CLA	G	1228	2	59,63,73	1.07	4 (6%)	70,101,113	1.09	5 (7%)
16	CLA	q	506	-	64,68,73	1.03	4 (6%)	76,107,113	1.05	4 (5%)
19	BCR	u	602	-	41,41,41	0.88	0	56,56,56	1.36	6 (10%)
16	CLA	h	516	12	50,54,73	1.16	4 (8%)	59,90,113	1.12	4 (6%)
16	CLA	r	512	12	69,73,73	1.00	6 (8%)	82,113,113	1.20	4 (4%)
16	CLA	k	4003	9	49,53,73	1.20	4 (8%)	58,89,113	1.14	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	r	502	12	54,58,73	1.11	5 (9%)	64,95,113	1.07	3 (4%)
16	CLA	A	1138	1	69,73,73	0.99	4 (5%)	82,113,113	0.98	4 (4%)
16	CLA	n	514	-	54,58,73	1.11	6 (11%)	64,95,113	1.10	5 (7%)
23	LMU	Z	605	-	36,36,36	0.87	0	47,47,47	1.20	4 (8%)
16	CLA	b	1216	25	51,55,73	1.16	5 (9%)	60,91,113	1.46	8 (13%)
16	CLA	g	510	-	69,73,73	0.99	5 (7%)	82,113,113	1.11	5 (6%)
16	CLA	Y	511	12	69,73,73	0.98	4 (5%)	82,113,113	1.02	5 (6%)
21	ECH	i	4020	-	42,42,42	0.84	1 (2%)	55,58,58	1.84	10 (18%)
16	CLA	r	507	12	69,73,73	1.00	5 (7%)	82,113,113	0.95	3 (3%)
16	CLA	r	516	-	50,54,73	1.15	5 (10%)	59,90,113	1.13	4 (6%)
16	CLA	B	1203	2	69,73,73	0.99	5 (7%)	82,113,113	1.14	5 (6%)
16	CLA	Z	507	12	69,73,73	1.00	3 (4%)	82,113,113	1.08	5 (6%)
16	CLA	w	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.06	5 (7%)
15	CL0	H	1011	1	69,73,73	1.01	6 (8%)	82,113,113	1.04	5 (6%)
16	CLA	A	1133	1	58,62,73	1.08	6 (10%)	68,99,113	1.22	7 (10%)
16	CLA	b	1201	2	58,62,73	1.07	4 (6%)	68,99,113	1.15	5 (7%)
16	CLA	h	517	-	59,63,73	1.10	4 (6%)	70,101,113	0.99	5 (7%)
16	CLA	w	507	12	69,73,73	0.99	4 (5%)	82,113,113	0.92	3 (3%)
19	BCR	B	4010	-	41,41,41	0.91	0	56,56,56	1.35	8 (14%)
16	CLA	b	1204	2	69,73,73	0.97	4 (5%)	82,113,113	0.98	3 (3%)
21	ECH	m	4021	-	42,42,42	0.84	0	55,58,58	1.55	9 (16%)
16	CLA	X	515	12	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
19	BCR	o	604	-	41,41,41	0.88	0	56,56,56	1.31	10 (17%)
16	CLA	w	509	12	69,73,73	1.00	5 (7%)	82,113,113	1.02	5 (6%)
16	CLA	W	510	-	69,73,73	1.01	3 (4%)	82,113,113	1.01	5 (6%)
19	BCR	w	604	-	41,41,41	0.87	0	56,56,56	1.27	6 (10%)
16	CLA	w	510	-	64,68,73	1.04	3 (4%)	76,107,113	0.98	2 (2%)
16	CLA	n	502	12	54,58,73	1.12	6 (11%)	64,95,113	1.13	3 (4%)
16	CLA	B	1012	25	59,63,73	1.12	4 (6%)	70,101,113	1.11	6 (8%)
19	BCR	A	4003	-	41,41,41	0.85	0	56,56,56	1.29	7 (12%)
16	CLA	g	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.01	6 (7%)
16	CLA	W	513	-	50,54,73	1.16	5 (10%)	59,90,113	1.14	6 (10%)
19	BCR	A	4008	-	41,41,41	0.89	0	56,56,56	1.35	8 (14%)
16	CLA	g	513	-	50,54,73	1.18	4 (8%)	59,90,113	1.00	5 (8%)
16	CLA	B	1217	2	49,53,73	1.18	4 (8%)	58,89,113	1.11	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	t	506	12	64,68,73	1.04	5 (7%)	76,107,113	1.07	5 (6%)
16	CLA	A	1137	1	51,55,73	1.14	4 (7%)	60,91,113	1.09	6 (10%)
16	CLA	w	504	12	69,73,73	1.01	5 (7%)	82,113,113	1.02	5 (6%)
16	CLA	H	1108	1	49,53,73	1.17	5 (10%)	58,89,113	1.24	4 (6%)
16	CLA	s	509	12	64,68,73	1.04	4 (6%)	76,107,113	1.04	4 (5%)
16	CLA	s	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.15	7 (8%)
16	CLA	X	506	-	64,68,73	1.02	4 (6%)	76,107,113	1.24	4 (5%)
16	CLA	H	1134	1	49,53,73	1.18	4 (8%)	58,89,113	1.09	2 (3%)
16	CLA	s	510	-	69,73,73	1.01	4 (5%)	82,113,113	0.97	4 (4%)
19	BCR	b	4010	-	41,41,41	0.91	0	56,56,56	1.33	7 (12%)
16	CLA	f	1302	6	50,54,73	1.17	5 (10%)	59,90,113	1.07	4 (6%)
19	BCR	u	603	-	41,41,41	0.88	0	56,56,56	1.35	8 (14%)
16	CLA	n	505	12	69,73,73	1.00	6 (8%)	82,113,113	1.22	6 (7%)
16	CLA	s	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.15	6 (7%)
16	CLA	b	1227	2	53,57,73	1.11	6 (11%)	61,93,113	1.15	6 (9%)
16	CLA	Y	516	-	50,54,73	1.13	4 (8%)	59,90,113	1.11	4 (6%)
16	CLA	a	1102	1,16	60,64,73	1.06	5 (8%)	71,102,113	1.05	3 (4%)
16	CLA	L	1501	10	64,68,73	1.02	5 (7%)	76,107,113	0.98	5 (6%)
16	CLA	A	1107	1	54,58,73	1.12	4 (7%)	64,95,113	1.15	5 (7%)
19	BCR	B	4005	-	41,41,41	0.85	0	56,56,56	1.17	4 (7%)
16	CLA	Z	515	12	69,73,73	0.99	4 (5%)	82,113,113	1.16	5 (6%)
14	LMG	f	4017	-	27,27,55	1.10	2 (7%)	35,35,63	1.16	3 (8%)
16	CLA	W	509	12	64,68,73	1.04	4 (6%)	76,107,113	1.08	5 (6%)
18	SF4	c	101	-	0,12,12	-	-	-	-	-
19	BCR	I	4018	-	41,41,41	0.86	0	56,56,56	1.27	8 (14%)
16	CLA	Y	506	12	64,68,73	1.01	4 (6%)	76,107,113	1.12	5 (6%)
16	CLA	H	1101	1	69,73,73	0.98	4 (5%)	82,113,113	1.04	3 (3%)
16	CLA	a	1109	1,16	69,73,73	0.98	4 (5%)	82,113,113	1.16	6 (7%)
19	BCR	l	4019	-	41,41,41	0.88	0	56,56,56	1.44	8 (14%)
19	BCR	H	4002	-	41,41,41	0.85	0	56,56,56	1.19	5 (8%)
19	BCR	p	604	-	41,41,41	0.87	0	56,56,56	1.23	6 (10%)
16	CLA	r	513	-	50,54,73	1.18	4 (8%)	59,90,113	1.10	5 (8%)
16	CLA	B	1206	2	69,73,73	0.98	5 (7%)	82,113,113	0.94	4 (4%)
16	CLA	Y	515	12	69,73,73	0.98	4 (5%)	82,113,113	1.04	5 (6%)
16	CLA	a	1105	-	62,66,73	1.07	5 (8%)	73,104,113	1.03	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	BCR	L	4019	-	41,41,41	0.90	0	56,56,56	1.41	6 (10%)
16	CLA	a	1119	-	69,73,73	1.00	5 (7%)	82,113,113	0.98	4 (4%)
16	CLA	g	515	12	69,73,73	1.00	4 (5%)	82,113,113	1.16	6 (7%)
16	CLA	b	1221	25	69,73,73	1.00	5 (7%)	82,113,113	1.10	5 (6%)
16	CLA	t	513	-	50,54,73	1.17	5 (10%)	59,90,113	1.15	6 (10%)
19	BCR	W	603	-	41,41,41	0.85	0	56,56,56	1.21	3 (5%)
16	CLA	s	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.19	6 (9%)
19	BCR	B	4009	-	30,30,41	0.84	0	39,39,56	1.32	5 (12%)
16	CLA	B	1209	2	49,53,73	1.17	4 (8%)	58,89,113	1.10	3 (5%)
16	CLA	p	510	-	69,73,73	1.01	4 (5%)	82,113,113	1.01	3 (3%)
16	CLA	v	507	12	69,73,73	1.00	5 (7%)	82,113,113	1.08	6 (7%)
16	CLA	Z	517	12	59,63,73	1.09	5 (8%)	70,101,113	1.03	3 (4%)
19	BCR	W	601	-	41,41,41	0.86	0	56,56,56	1.27	8 (14%)
16	CLA	Y	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.18	8 (9%)
16	CLA	b	1205	2	69,73,73	0.98	4 (5%)	82,113,113	1.08	4 (4%)
16	CLA	r	517	12	59,63,73	1.09	4 (6%)	70,101,113	1.01	3 (4%)
16	CLA	t	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.22	5 (7%)
16	CLA	Q	1301	25	49,53,73	1.17	4 (8%)	58,89,113	1.13	4 (6%)
16	CLA	t	509	12	64,68,73	1.06	5 (7%)	76,107,113	1.15	6 (7%)
21	ECH	B	4006	-	42,42,42	0.74	0	55,58,58	1.53	11 (20%)
16	CLA	u	512	12	69,73,73	0.98	6 (8%)	82,113,113	1.02	2 (2%)
16	CLA	l	1503	-	69,73,73	1.00	4 (5%)	82,113,113	0.91	4 (4%)
16	CLA	t	511	12	69,73,73	1.00	4 (5%)	82,113,113	1.04	5 (6%)
13	LHG	a	851	16	25,25,48	0.88	2 (8%)	28,31,54	1.26	2 (7%)
16	CLA	H	1112	1	49,53,73	1.19	4 (8%)	58,89,113	0.99	3 (5%)
16	CLA	Z	514	-	54,58,73	1.12	4 (7%)	64,95,113	1.13	5 (7%)
16	CLA	q	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.15	5 (7%)
16	CLA	v	509	12	69,73,73	1.02	6 (8%)	82,113,113	1.06	7 (8%)
16	CLA	r	510	-	69,73,73	0.99	4 (5%)	82,113,113	1.00	4 (4%)
16	CLA	y	506	12	64,68,73	1.04	4 (6%)	76,107,113	1.40	9 (11%)
16	CLA	G	1218	-	59,63,73	1.08	4 (6%)	70,101,113	1.10	4 (5%)
16	CLA	b	1021	2	69,73,73	1.00	5 (7%)	82,113,113	1.12	6 (7%)
19	BCR	o	601	-	41,41,41	0.88	1 (2%)	56,56,56	1.37	8 (14%)
16	CLA	G	1215	2	64,68,73	1.00	4 (6%)	76,107,113	1.09	2 (2%)
16	CLA	Y	507	12	69,73,73	1.01	4 (5%)	82,113,113	1.01	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	BCR	a	4003	-	41,41,41	0.87	0	56,56,56	1.22	5 (8%)
16	CLA	h	512	12	69,73,73	1.03	6 (8%)	82,113,113	1.06	7 (8%)
16	CLA	b	1220	2	58,62,73	1.10	6 (10%)	68,99,113	1.11	5 (7%)
16	CLA	t	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.13	5 (6%)
16	CLA	b	1240	13	50,54,73	1.15	4 (8%)	59,90,113	1.16	2 (3%)
16	CLA	A	1111	1	59,63,73	1.08	6 (10%)	70,101,113	1.20	5 (7%)
16	CLA	B	1211	2	69,73,73	0.98	6 (8%)	82,113,113	1.02	5 (6%)
16	CLA	A	1022	25	69,73,73	1.01	5 (7%)	82,113,113	1.08	9 (10%)
16	CLA	H	1130	1	64,68,73	1.03	5 (7%)	76,107,113	1.01	7 (9%)
16	CLA	h	504	-	64,68,73	1.05	5 (7%)	76,107,113	1.24	7 (9%)
16	CLA	b	1230	2	49,53,73	1.18	5 (10%)	58,89,113	1.15	4 (6%)
16	CLA	b	1212	2	49,53,73	1.19	5 (10%)	58,89,113	1.19	4 (6%)
16	CLA	x	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.16	4 (6%)
16	CLA	q	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.17	5 (7%)
19	BCR	u	601	-	41,41,41	0.91	1 (2%)	56,56,56	1.38	9 (16%)
16	CLA	b	1236	2	54,58,73	1.12	5 (9%)	64,95,113	1.14	6 (9%)
19	BCR	x	602	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	Z	506	-	64,68,73	1.02	3 (4%)	76,107,113	1.03	2 (2%)
16	CLA	u	510	-	64,68,73	1.04	4 (6%)	76,107,113	0.95	5 (6%)
16	CLA	o	501	12	50,54,73	1.14	4 (8%)	59,90,113	1.13	4 (6%)
16	CLA	w	503	12	50,54,73	1.16	6 (12%)	59,90,113	1.18	5 (8%)
16	CLA	s	507	12	69,73,73	1.01	4 (5%)	82,113,113	1.01	5 (6%)
16	CLA	X	516	12	50,54,73	1.13	5 (10%)	59,90,113	1.09	3 (5%)
16	CLA	x	511	12	69,73,73	1.00	6 (8%)	82,113,113	0.94	2 (2%)
16	CLA	B	1210	2	69,73,73	1.01	5 (7%)	82,113,113	1.09	6 (7%)
16	CLA	q	502	12	54,58,73	1.13	6 (11%)	64,95,113	1.04	3 (4%)
16	CLA	q	516	-	50,54,73	1.14	5 (10%)	59,90,113	0.99	2 (3%)
16	CLA	A	1129	1	50,54,73	1.12	4 (8%)	59,90,113	1.15	5 (8%)
16	CLA	h	515	12	69,73,73	1.01	4 (5%)	82,113,113	1.24	9 (10%)
19	BCR	Z	602	-	41,41,41	0.87	0	56,56,56	1.36	8 (14%)
19	BCR	A	4002	-	41,41,41	0.84	0	56,56,56	1.15	3 (5%)
23	LMU	q	605	-	36,36,36	0.83	0	47,47,47	1.13	4 (8%)
16	CLA	w	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.07	5 (7%)
16	CLA	X	502	12	54,58,73	1.11	6 (11%)	64,95,113	1.04	3 (4%)
17	PQN	G	2002	-	34,34,34	0.38	0	43,45,45	1.04	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	r	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.13	4 (6%)
16	CLA	H	1111	1	59,63,73	1.09	4 (6%)	70,101,113	1.03	2 (2%)
16	CLA	r	506	12	64,68,73	1.01	3 (4%)	76,107,113	1.07	7 (9%)
16	CLA	s	511	12	69,73,73	0.98	5 (7%)	82,113,113	1.01	4 (4%)
16	CLA	K	4004	-	59,63,73	1.07	4 (6%)	70,101,113	1.10	4 (5%)
16	CLA	s	503	-	50,54,73	1.16	6 (12%)	59,90,113	1.25	5 (8%)
19	BCR	X	602	-	41,41,41	0.88	0	56,56,56	1.36	7 (12%)
16	CLA	H	1127	1	69,73,73	1.00	6 (8%)	82,113,113	1.11	5 (6%)
16	CLA	p	513	-	50,54,73	1.14	5 (10%)	59,90,113	1.04	4 (6%)
16	CLA	n	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.03	4 (4%)
16	CLA	a	1129	1	50,54,73	1.11	5 (10%)	59,90,113	1.13	5 (8%)
19	BCR	r	602	-	41,41,41	0.86	0	56,56,56	1.24	4 (7%)
23	LMU	g	606	-	36,36,36	0.86	0	47,47,47	1.32	5 (10%)
16	CLA	t	504	12	64,68,73	1.04	4 (6%)	76,107,113	1.02	3 (3%)
16	CLA	L	1503	25	69,73,73	0.99	4 (5%)	82,113,113	0.92	3 (3%)
16	CLA	A	1104	1	69,73,73	0.99	5 (7%)	82,113,113	0.98	6 (7%)
16	CLA	s	515	12	69,73,73	0.98	4 (5%)	82,113,113	1.02	6 (7%)
16	CLA	g	501	12	54,58,73	1.11	4 (7%)	64,95,113	1.08	5 (7%)
13	LHG	H	851	16	25,25,48	0.88	1 (4%)	28,31,54	1.27	2 (7%)
16	CLA	x	502	12	54,58,73	1.13	6 (11%)	64,95,113	1.12	3 (4%)
16	CLA	b	1012	25	59,63,73	1.13	4 (6%)	70,101,113	1.20	8 (11%)
16	CLA	H	1013	-	69,73,73	1.01	7 (10%)	82,113,113	1.20	9 (10%)
16	CLA	u	501	12	50,54,73	1.14	4 (8%)	59,90,113	0.99	3 (5%)
16	CLA	p	511	12	69,73,73	0.98	4 (5%)	82,113,113	1.05	5 (6%)
16	CLA	A	1125	1	69,73,73	0.98	4 (5%)	82,113,113	0.97	3 (3%)
16	CLA	r	515	12	69,73,73	1.00	4 (5%)	82,113,113	1.12	6 (7%)
16	CLA	B	1201	2	58,62,73	1.07	4 (6%)	68,99,113	1.04	4 (5%)
19	BCR	x	604	-	41,41,41	0.88	0	56,56,56	1.29	6 (10%)
16	CLA	j	1303	8	41,45,73	1.24	5 (12%)	50,78,113	1.10	3 (6%)
16	CLA	v	515	12	69,73,73	1.02	4 (5%)	82,113,113	1.18	7 (8%)
13	LHG	i	103	-	39,39,48	0.69	2 (5%)	42,45,54	1.24	5 (11%)
15	CL0	a	1011	1	69,73,73	1.00	6 (8%)	82,113,113	0.98	5 (6%)
16	CLA	b	1224	2	64,68,73	1.05	6 (9%)	76,107,113	1.20	4 (5%)
16	CLA	o	516	12	50,54,73	1.14	5 (10%)	59,90,113	1.05	2 (3%)
16	CLA	Y	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.06	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	y	512	12	69,73,73	1.00	5 (7%)	82,113,113	1.01	6 (7%)
16	CLA	B	1213	2	59,63,73	1.07	6 (10%)	70,101,113	1.08	4 (5%)
16	CLA	a	1139	25	59,63,73	1.07	5 (8%)	70,101,113	1.00	5 (7%)
17	PQN	H	2001	-	34,34,34	0.38	0	43,45,45	1.06	2 (4%)
16	CLA	G	1231	25	49,53,73	1.19	4 (8%)	58,89,113	1.13	4 (6%)
16	CLA	p	503	-	50,54,73	1.14	6 (12%)	59,90,113	1.17	6 (10%)
16	CLA	x	506	12	64,68,73	1.02	6 (9%)	76,107,113	1.12	4 (5%)
16	CLA	H	1131	1	69,73,73	1.01	4 (5%)	82,113,113	1.11	4 (4%)
19	BCR	h	601	-	41,41,41	0.84	0	56,56,56	1.28	7 (12%)
16	CLA	A	1102	1,16	60,64,73	1.06	4 (6%)	71,102,113	0.95	3 (4%)
16	CLA	x	510	-	69,73,73	0.99	5 (7%)	82,113,113	1.05	4 (4%)
16	CLA	o	514	-	54,58,73	1.12	6 (11%)	64,95,113	1.35	4 (6%)
16	CLA	H	1123	-	69,73,73	1.00	4 (5%)	82,113,113	0.96	3 (3%)
16	CLA	b	1225	-	69,73,73	0.99	6 (8%)	82,113,113	1.02	5 (6%)
16	CLA	y	502	12	54,58,73	1.13	5 (9%)	64,95,113	1.01	4 (6%)
16	CLA	b	1219	-	49,53,73	1.21	5 (10%)	58,89,113	1.21	5 (8%)
19	BCR	Z	604	-	41,41,41	0.87	0	56,56,56	1.24	6 (10%)
19	BCR	b	4017	-	41,41,41	0.87	0	56,56,56	1.16	4 (7%)
19	BCR	H	4007	-	41,41,41	0.91	1 (2%)	56,56,56	1.30	7 (12%)
16	CLA	B	1214	2	59,63,73	1.06	4 (6%)	70,101,113	1.19	4 (5%)
16	CLA	G	1238	25	69,73,73	0.98	4 (5%)	82,113,113	1.04	6 (7%)
16	CLA	g	508	12	59,63,73	1.07	4 (6%)	70,101,113	0.98	3 (4%)
16	CLA	X	517	12	59,63,73	1.07	4 (6%)	70,101,113	1.00	5 (7%)
16	CLA	o	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.16	5 (6%)
24	LUT	Z	601	-	42,43,43	0.81	1 (2%)	51,60,60	1.48	6 (11%)
16	CLA	n	512	12	69,73,73	1.00	6 (8%)	82,113,113	1.08	4 (4%)
16	CLA	a	1101	1	69,73,73	0.98	4 (5%)	82,113,113	1.06	4 (4%)
16	CLA	u	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.05	6 (7%)
16	CLA	a	1125	1	69,73,73	0.97	5 (7%)	82,113,113	1.06	3 (3%)
16	CLA	H	1116	1	58,62,73	1.05	5 (8%)	68,99,113	1.08	5 (7%)
16	CLA	Y	502	12	54,58,73	1.11	4 (7%)	64,95,113	1.03	4 (6%)
16	CLA	q	510	-	64,68,73	1.03	4 (6%)	76,107,113	0.96	3 (3%)
16	CLA	b	1208	2	49,53,73	1.16	5 (10%)	58,89,113	1.19	6 (10%)
16	CLA	w	513	-	54,58,73	1.13	4 (7%)	64,95,113	1.15	6 (9%)
16	CLA	G	1210	2	69,73,73	1.00	5 (7%)	82,113,113	1.05	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	X	508	12	59,63,73	1.07	4 (6%)	70,101,113	0.97	4 (5%)
16	CLA	p	516	-	50,54,73	1.14	4 (8%)	59,90,113	1.07	3 (5%)
16	CLA	a	1121	1	55,59,73	1.12	5 (9%)	64,96,113	1.11	5 (7%)
16	CLA	a	1116	1	58,62,73	1.07	5 (8%)	68,99,113	1.02	4 (5%)
14	LMG	a	4101	-	46,46,55	0.90	2 (4%)	54,54,63	1.22	4 (7%)
16	CLA	H	1137	1	51,55,73	1.12	5 (9%)	60,91,113	1.11	5 (8%)
16	CLA	h	510	-	69,73,73	1.01	5 (7%)	82,113,113	1.00	6 (7%)
16	CLA	B	1205	2	69,73,73	0.99	4 (5%)	82,113,113	1.06	3 (3%)
16	CLA	W	514	-	54,58,73	1.11	5 (9%)	64,95,113	1.11	4 (6%)
16	CLA	u	505	12	69,73,73	0.99	4 (5%)	82,113,113	1.08	5 (6%)
16	CLA	k	4002	9	49,53,73	1.17	4 (8%)	58,89,113	1.12	4 (6%)
16	CLA	g	504	12	69,73,73	1.01	4 (5%)	82,113,113	1.01	6 (7%)
16	CLA	u	503	-	50,54,73	1.15	4 (8%)	59,90,113	1.06	3 (5%)
16	CLA	u	506	-	64,68,73	1.08	6 (9%)	76,107,113	1.64	12 (15%)
16	CLA	A	1114	-	50,54,73	1.12	4 (8%)	59,90,113	1.23	4 (6%)
16	CLA	h	514	-	54,58,73	1.13	4 (7%)	64,95,113	1.14	7 (10%)
16	CLA	Z	501	12	54,58,73	1.11	5 (9%)	64,95,113	1.18	7 (10%)
16	CLA	G	1023	-	69,73,73	1.02	8 (11%)	82,113,113	1.13	8 (9%)
16	CLA	A	1013	-	69,73,73	0.99	6 (8%)	82,113,113	1.20	10 (12%)
17	PQN	a	2001	-	34,34,34	0.39	0	43,45,45	1.06	2 (4%)
16	CLA	a	1022	-	69,73,73	1.01	5 (7%)	82,113,113	1.04	6 (7%)
19	BCR	a	4008	-	41,41,41	0.91	1 (2%)	56,56,56	1.35	6 (10%)
16	CLA	n	515	12	69,73,73	1.00	4 (5%)	82,113,113	1.07	5 (6%)
16	CLA	B	1228	2	59,63,73	1.08	4 (6%)	70,101,113	1.09	4 (5%)

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
19	BCR	Z	603	-	-	8/29/63/63	0/2/2/2
13	LHG	I	103	-	-	20/44/44/53	-
16	CLA	j	1302	8	-	7/15/91/115	-
16	CLA	G	1213	2	-	8/27/103/115	-
16	CLA	G	1232	25	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	1136	1	-	7/39/115/115	-
14	LMG	Q	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	B	1240	13	-	6/17/93/115	-
16	CLA	r	501	12	-	6/21/97/115	-
19	BCR	K	4005	-	-	9/29/63/63	0/2/2/2
16	CLA	w	517	12	-	8/27/103/115	-
16	CLA	B	1235	2	-	11/36/112/115	-
16	CLA	v	508	12	-	13/27/103/115	-
16	CLA	p	515	12	-	14/39/115/115	-
16	CLA	H	1107	1	-	5/21/97/115	-
16	CLA	q	503	12	-	9/17/93/115	-
16	CLA	u	511	-	-	8/39/115/115	-
19	BCR	g	602	-	-	14/29/63/63	0/2/2/2
19	BCR	T	4005	-	-	9/29/63/63	0/2/2/2
16	CLA	b	1202	-	-	16/39/115/115	-
16	CLA	G	1240	13	-	5/17/93/115	-
16	CLA	h	506	12	-	11/33/109/115	-
16	CLA	n	508	12	-	9/27/103/115	-
16	CLA	G	1235	2	-	11/36/112/115	-
16	CLA	A	1132	1	-	15/39/115/115	-
16	CLA	A	1120	1	-	7/20/96/115	-
16	CLA	q	511	12	-	5/39/115/115	-
16	CLA	t	508	12	-	9/27/103/115	-
16	CLA	f	1301	25	-	4/15/91/115	-
16	CLA	t	502	12	-	10/21/97/115	-
16	CLA	q	509	12	-	12/39/115/115	-
19	BCR	J	4012	-	-	12/29/63/63	0/2/2/2
23	LMU	s	606	-	-	6/21/61/61	0/2/2/2
16	CLA	b	1210	2	-	12/39/115/115	-
18	SF4	a	3001	-	-	-	0/6/5/5
19	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	a	1137	1	-	6/18/94/115	-
16	CLA	Y	508	12	-	13/27/103/115	-
14	LMG	H	4101	-	-	23/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	1115	1	-	8/26/102/115	-
16	CLA	A	1113	1	-	7/15/91/115	-
16	CLA	q	515	12	-	12/39/115/115	-
16	CLA	a	1120	1	-	8/20/96/115	-
16	CLA	x	516	-	-	5/17/93/115	-
16	CLA	B	1225	-	-	11/39/115/115	-
16	CLA	J	1303	8	-	2/4/76/115	-
16	CLA	W	506	12	-	11/33/109/115	-
23	LMU	p	606	-	-	9/21/61/61	0/2/2/2
16	CLA	B	1218	-	-	9/27/103/115	-
16	CLA	B	1238	25	-	9/39/115/115	-
16	CLA	Y	509	12	-	15/33/109/115	-
16	CLA	B	1215	2	-	7/33/109/115	-
16	CLA	G	1205	2	-	10/39/115/115	-
16	CLA	p	517	12	-	10/27/103/115	-
16	CLA	B	1230	2	-	7/15/91/115	-
16	CLA	v	516	12	-	6/17/93/115	-
16	CLA	b	1231	25	-	8/15/91/115	-
16	CLA	A	1123	25	-	8/39/115/115	-
16	CLA	X	512	12	-	11/39/115/115	-
16	CLA	A	1117	1	-	7/39/115/115	-
19	BCR	f	4016	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1128	1	-	18/39/115/115	-
19	BCR	S	4015	-	-	10/29/63/63	0/2/2/2
16	CLA	B	1234	2	-	5/21/97/115	-
16	CLA	q	512	12	-	15/39/115/115	-
16	CLA	b	1229	2	-	9/31/107/115	-
16	CLA	x	515	12	-	10/39/115/115	-
16	CLA	a	1130	1	-	10/33/109/115	-
16	CLA	o	506	-	-	16/33/109/115	-
16	CLA	A	1135	1	-	3/23/99/115	-
21	ECH	I	4020	-	-	11/29/66/66	0/2/2/2
16	CLA	A	1116	1	-	12/26/102/115	-
16	CLA	a	1013	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	v	604	-	-	12/29/63/63	0/2/2/2
19	BCR	U	4019	-	-	10/29/63/63	0/2/2/2
13	LHG	p	605	-	-	13/36/36/53	-
19	BCR	s	602	-	-	11/29/63/63	0/2/2/2
16	CLA	v	510	-	-	6/39/115/115	-
19	BCR	l	4022	-	-	18/29/63/63	0/2/2/2
16	CLA	b	1209	2	-	5/15/91/115	-
16	CLA	b	1235	2	-	14/36/112/115	-
19	BCR	X	604	-	-	19/29/63/63	0/2/2/2
19	BCR	o	602	-	-	14/29/63/63	0/2/2/2
16	CLA	h	511	12	-	15/39/115/115	-
17	PQN	A	2001	-	-	3/23/43/43	0/2/2/2
19	BCR	h	603	-	-	11/29/63/63	0/2/2/2
16	CLA	o	510	-	-	5/33/109/115	-
16	CLA	h	503	-	-	5/17/93/115	-
16	CLA	G	1204	2	-	9/39/115/115	-
16	CLA	B	1221	25	-	15/39/115/115	-
19	BCR	g	601	-	-	17/29/63/63	0/2/2/2
16	CLA	t	510	-	-	9/39/115/115	-
19	BCR	G	4014	-	-	16/29/63/63	0/2/2/2
16	CLA	h	501	12	-	9/17/93/115	-
16	CLA	y	509	12	-	19/39/115/115	-
16	CLA	y	508	12	-	10/27/103/115	-
16	CLA	W	507	12	-	12/39/115/115	-
16	CLA	W	511	12	-	9/39/115/115	-
16	CLA	a	1123	-	-	13/39/115/115	-
19	BCR	Y	604	-	-	14/29/63/63	0/2/2/2
16	CLA	X	510	-	-	8/33/109/115	-
19	BCR	p	602	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1207	2	-	14/39/115/115	-
16	CLA	A	1119	25	-	5/39/115/115	-
16	CLA	Y	510	-	-	11/39/115/115	-
16	CLA	A	1103	-	-	10/39/115/115	-
16	CLA	A	1106	1	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1022	25	-	10/39/115/115	-
16	CLA	W	512	12	-	18/33/109/115	-
16	CLA	a	1110	1	-	9/26/102/115	-
16	CLA	y	510	-	-	6/39/115/115	-
16	CLA	K	4002	9	-	4/15/91/115	-
16	CLA	s	502	12	-	6/21/97/115	-
16	CLA	a	1104	1	-	18/39/115/115	-
19	BCR	x	603	-	-	14/29/63/63	0/2/2/2
16	CLA	H	1125	1	-	11/39/115/115	-
16	CLA	a	1114	-	-	10/17/93/115	-
16	CLA	t	507	12	-	11/39/115/115	-
16	CLA	U	1501	10	-	13/33/109/115	-
19	BCR	r	601	-	-	15/29/63/63	0/2/2/2
19	BCR	s	604	-	-	16/29/63/63	0/2/2/2
19	BCR	v	603	-	-	12/29/63/63	0/2/2/2
24	LUT	q	601	-	-	7/29/67/67	0/2/2/2
16	CLA	X	507	12	-	10/39/115/115	-
16	CLA	J	1302	8	-	6/15/91/115	-
16	CLA	G	1230	2	-	8/15/91/115	-
19	BCR	G	4010	-	-	17/29/63/63	0/2/2/2
23	LMU	r	606	-	-	6/21/61/61	0/2/2/2
16	CLA	g	503	-	-	9/17/93/115	-
18	SF4	N	102	-	-	-	0/6/5/5
19	BCR	s	601	-	-	12/29/63/63	0/2/2/2
16	CLA	g	506	12	-	11/33/109/115	-
16	CLA	G	1209	2	-	5/15/91/115	-
16	CLA	X	501	12	-	9/17/93/115	-
16	CLA	p	502	12	-	5/21/97/115	-
16	CLA	S	1303	8	-	2/4/76/115	-
14	LMG	A	4101	-	-	24/41/61/70	0/1/1/1
19	BCR	y	604	-	-	11/29/63/63	0/2/2/2
19	BCR	B	4017	-	-	11/29/63/63	0/2/2/2
13	LHG	b	4018	16	-	16/42/42/53	-
16	CLA	H	1136	1	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	o	513	-	-	5/17/93/115	-
13	LHG	A	849	-	-	19/47/47/53	-
16	CLA	G	1217	2	-	9/15/91/115	-
16	CLA	a	1237	25	-	13/39/115/115	-
16	CLA	B	1227	2	-	11/20/96/115	-
14	LMG	H	4201	-	-	10/27/47/70	0/1/1/1
16	CLA	n	510	-	-	14/39/115/115	-
16	CLA	W	503	-	-	10/17/93/115	-
16	CLA	G	1234	2	-	3/21/97/115	-
16	CLA	G	1226	2	-	17/33/109/115	-
16	CLA	H	1117	1	-	9/39/115/115	-
16	CLA	S	1302	8	-	7/15/91/115	-
14	LMG	a	4201	-	-	11/27/47/70	0/1/1/1
16	CLA	Y	514	-	-	7/21/97/115	-
16	CLA	a	1133	1	-	8/26/102/115	-
16	CLA	G	1221	25	-	18/39/115/115	-
16	CLA	o	507	12	-	13/39/115/115	-
19	BCR	u	604	-	-	17/29/63/63	0/2/2/2
19	BCR	Y	601	-	-	12/29/63/63	0/2/2/2
16	CLA	b	1226	2	-	16/33/109/115	-
16	CLA	o	509	12	-	11/33/109/115	-
16	CLA	t	516	-	-	9/17/93/115	-
14	LMG	G	848	-	-	18/38/58/70	0/1/1/1
16	CLA	W	515	12	-	16/39/115/115	-
16	CLA	y	515	12	-	15/39/115/115	-
19	BCR	H	4008	-	-	13/29/63/63	0/2/2/2
19	BCR	p	601	-	-	9/29/63/63	0/2/2/2
16	CLA	a	1111	1	-	8/27/103/115	-
16	CLA	u	504	12	-	18/33/109/115	-
14	LMG	A	4201	-	-	13/27/47/70	0/1/1/1
16	CLA	y	501	12	-	8/17/93/115	-
18	SF4	N	101	-	-	-	0/6/5/5
16	CLA	v	503	-	-	7/17/93/115	-
16	CLA	n	501	12	-	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1222	25	-	8/21/97/115	-
16	CLA	L	1502	10	-	9/33/109/115	-
16	CLA	y	507	12	-	13/39/115/115	-
19	BCR	S	4012	-	-	10/29/63/63	0/2/2/2
16	CLA	g	509	12	-	8/39/115/115	-
16	CLA	H	1114	-	-	9/17/93/115	-
16	CLA	o	505	12	-	16/39/115/115	-
19	BCR	s	603	-	-	7/29/63/63	0/2/2/2
16	CLA	Z	505	-	-	14/39/115/115	-
16	CLA	n	503	-	-	8/17/93/115	-
19	BCR	A	4011	-	-	17/29/63/63	0/2/2/2
19	BCR	o	603	-	-	9/29/63/63	0/2/2/2
19	BCR	n	603	-	-	12/29/63/63	0/2/2/2
16	CLA	Z	504	12	-	14/39/115/115	-
16	CLA	t	503	-	-	7/17/93/115	-
16	CLA	b	1203	2	-	16/39/115/115	-
16	CLA	g	514	-	-	7/21/97/115	-
16	CLA	W	516	-	-	7/17/93/115	-
16	CLA	B	1207	2	-	18/39/115/115	-
16	CLA	X	505	12	-	12/39/115/115	-
19	BCR	v	601	-	-	11/29/63/63	0/2/2/2
16	CLA	H	1140	1	-	15/39/115/115	-
16	CLA	X	503	-	-	11/17/93/115	-
19	BCR	q	602	-	-	12/29/63/63	0/2/2/2
16	CLA	X	504	12	-	16/33/109/115	-
16	CLA	q	517	12	-	11/27/103/115	-
16	CLA	Y	503	-	-	7/17/93/115	-
16	CLA	t	515	12	-	15/39/115/115	-
16	CLA	G	1207	2	-	14/39/115/115	-
19	BCR	p	603	-	-	7/29/63/63	0/2/2/2
16	CLA	a	1140	1	-	13/39/115/115	-
16	CLA	p	507	12	-	9/39/115/115	-
16	CLA	W	517	12	-	10/27/103/115	-
16	CLA	H	1132	1	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	u	514	-	-	6/21/97/115	-
16	CLA	H	1120	1	-	9/20/96/115	-
20	LMT	U	4101	-	-	8/21/61/61	0/2/2/2
13	LHG	a	849	-	-	17/47/47/53	-
18	SF4	A	3001	-	-	-	0/6/5/5
20	LMT	a	4202	-	-	8/21/61/61	0/2/2/2
16	CLA	w	506	-	-	7/33/109/115	-
16	CLA	a	1124	25	-	7/33/109/115	-
16	CLA	a	1131	1	-	13/39/115/115	-
16	CLA	G	1236	2	-	7/21/97/115	-
16	CLA	H	1104	1	-	17/39/115/115	-
14	LMG	F	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	r	514	-	-	10/21/97/115	-
16	CLA	b	1232	25	-	8/15/91/115	-
16	CLA	o	508	12	-	14/27/103/115	-
16	CLA	H	1115	1	-	10/26/102/115	-
19	BCR	q	604	-	-	16/29/63/63	0/2/2/2
16	CLA	r	511	12	-	6/39/115/115	-
13	LHG	R	103	-	-	23/44/44/53	-
19	BCR	b	4005	-	-	12/29/63/63	0/2/2/2
16	CLA	t	514	-	-	8/21/97/115	-
16	CLA	G	1216	25	-	4/18/94/115	-
16	CLA	g	511	12	-	9/39/115/115	-
16	CLA	v	514	-	-	7/21/97/115	-
16	CLA	n	504	12	-	5/33/109/115	-
19	BCR	g	603	-	-	15/29/63/63	0/2/2/2
16	CLA	B	1223	2	-	11/39/115/115	-
20	LMT	L	4101	-	-	9/21/61/61	0/2/2/2
16	CLA	x	513	-	-	10/17/93/115	-
16	CLA	H	1801	13	-	5/17/93/115	-
19	BCR	q	603	-	-	6/29/63/63	0/2/2/2
16	CLA	h	508	12	-	12/27/103/115	-
16	CLA	g	517	12	-	10/27/103/115	-
16	CLA	y	505	12	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	X	509	12	-	13/33/109/115	-
16	CLA	H	1237	25	-	11/39/115/115	-
16	CLA	Y	501	12	-	6/21/97/115	-
16	CLA	y	503	-	-	4/17/93/115	-
19	BCR	H	4003	-	-	10/29/63/63	0/2/2/2
19	BCR	U	4022	-	-	16/29/63/63	0/2/2/2
16	CLA	B	1232	-	-	8/15/91/115	-
16	CLA	x	501	-	-	6/21/97/115	-
16	CLA	Z	511	12	-	4/39/115/115	-
19	BCR	G	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	H	1102	1,16	-	5/29/105/115	-
14	LMG	b	848	-	-	19/38/58/70	0/1/1/1
16	CLA	h	505	12	-	6/39/115/115	-
14	LMG	H	852	-	-	6/33/53/70	0/1/1/1
16	CLA	W	508	12	-	9/27/103/115	-
16	CLA	w	511	12	-	9/39/115/115	-
20	LMT	l	4101	-	-	7/21/61/61	0/2/2/2
19	BCR	Y	602	-	-	10/29/63/63	0/2/2/2
14	LMG	a	852	-	-	10/33/53/70	0/1/1/1
13	LHG	u	605	-	-	12/31/31/53	-
16	CLA	r	509	12	-	10/39/115/115	-
19	BCR	r	603	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1202	2	-	18/39/115/115	-
19	BCR	g	604	-	-	16/29/63/63	0/2/2/2
19	BCR	w	603	-	-	13/29/63/63	0/2/2/2
16	CLA	u	502	12	-	7/21/97/115	-
16	CLA	Z	509	12	-	16/39/115/115	-
16	CLA	H	1124	-	-	6/33/109/115	-
16	CLA	A	1110	1	-	10/26/102/115	-
16	CLA	h	502	12	-	7/21/97/115	-
16	CLA	y	516	12	-	7/17/93/115	-
16	CLA	Y	513	-	-	10/17/93/115	-
16	CLA	B	1204	2	-	9/39/115/115	-
16	CLA	H	1106	1	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1122	1	-	9/32/108/115	-
14	LMG	A	852	-	-	10/33/53/70	0/1/1/1
16	CLA	s	517	12	-	9/27/103/115	-
16	CLA	b	1211	2	-	13/39/115/115	-
16	CLA	x	505	12	-	10/39/115/115	-
16	CLA	A	1140	1	-	12/39/115/115	-
19	BCR	h	604	-	-	13/29/63/63	0/2/2/2
16	CLA	a	1117	1	-	10/39/115/115	-
16	CLA	v	505	12	-	13/39/115/115	-
13	LHG	G	4018	16	-	12/42/42/53	-
16	CLA	H	1129	1	-	6/17/93/115	-
16	CLA	o	502	12	-	8/21/97/115	-
16	CLA	s	514	-	-	7/21/97/115	-
19	BCR	b	4014	-	-	15/29/63/63	0/2/2/2
16	CLA	y	517	-	-	15/27/103/115	-
19	BCR	j	4013	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1213	2	-	6/27/103/115	-
16	CLA	A	1109	1,16	-	9/39/115/115	-
21	ECH	b	4006	-	-	9/29/66/66	0/2/2/2
16	CLA	n	517	12	-	11/27/103/115	-
16	CLA	Z	516	-	-	11/17/93/115	-
16	CLA	A	1122	1	-	9/32/108/115	-
16	CLA	b	1217	2	-	3/15/91/115	-
16	CLA	A	1801	13	-	9/17/93/115	-
23	LMU	Y	606	-	-	6/21/61/61	0/2/2/2
16	CLA	Y	504	12	-	16/39/115/115	-
16	CLA	B	1239	2	-	14/39/115/115	-
19	BCR	W	604	-	-	10/29/63/63	0/2/2/2
16	CLA	q	504	12	-	14/39/115/115	-
16	CLA	B	1222	25	-	8/21/97/115	-
16	CLA	b	1234	2	-	4/21/97/115	-
16	CLA	p	508	12	-	10/27/103/115	-
16	CLA	x	504	12	-	21/39/115/115	-
16	CLA	Y	517	12	-	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1126	1	-	12/39/115/115	-
16	CLA	y	513	-	-	7/17/93/115	-
13	LHG	H	849	-	-	17/47/47/53	-
16	CLA	H	1139	25	-	13/33/109/115	-
16	CLA	u	517	12	-	8/27/103/115	-
16	CLA	v	511	12	-	11/39/115/115	-
16	CLA	G	1223	2	-	6/39/115/115	-
19	BCR	B	4014	-	-	16/29/63/63	0/2/2/2
16	CLA	b	1023	-	-	12/39/115/115	-
16	CLA	A	1121	1	-	8/23/99/115	-
16	CLA	B	1226	2	-	13/33/109/115	-
16	CLA	a	1127	1	-	4/39/115/115	-
16	CLA	h	513	-	-	6/17/93/115	-
16	CLA	G	1203	2	-	16/39/115/115	-
19	BCR	L	4022	-	-	14/29/63/63	0/2/2/2
16	CLA	a	1115	1	-	8/26/102/115	-
16	CLA	B	1224	2	-	10/33/109/115	-
16	CLA	k	4004	-	-	6/27/103/115	-
16	CLA	n	509	12	-	9/33/109/115	-
19	BCR	t	604	-	-	14/29/63/63	0/2/2/2
16	CLA	G	1212	2	-	8/15/91/115	-
16	CLA	Z	512	12	-	14/39/115/115	-
17	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
16	CLA	s	506	12	-	11/33/109/115	-
16	CLA	A	1237	25	-	11/39/115/115	-
16	CLA	b	1239	2	-	14/39/115/115	-
16	CLA	b	1206	2	-	15/39/115/115	-
16	CLA	u	513	-	-	7/17/93/115	-
16	CLA	w	512	12	-	11/39/115/115	-
16	CLA	n	506	12	-	8/33/109/115	-
18	SF4	c	102	-	-	-	0/6/5/5
16	CLA	A	1126	1	-	11/39/115/115	-
19	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	A	1131	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CL0	A	1011	1	-	8/39/115/115	-
16	CLA	v	517	-	-	15/27/103/115	-
16	CLA	a	1136	1	-	11/39/115/115	-
16	CLA	G	1012	25	-	7/27/103/115	-
16	CLA	W	501	12	-	8/21/97/115	-
16	CLA	a	1132	1	-	14/39/115/115	-
16	CLA	u	509	12	-	8/33/109/115	-
16	CLA	y	504	12	-	12/33/109/115	-
16	CLA	w	516	12	-	10/17/93/115	-
16	CLA	X	514	-	-	4/21/97/115	-
16	CLA	b	1218	-	-	9/27/103/115	-
16	CLA	A	1118	1	-	11/27/103/115	-
16	CLA	a	1135	1	-	3/23/99/115	-
16	CLA	t	505	12	-	11/39/115/115	-
16	CLA	p	506	12	-	15/33/109/115	-
19	BCR	H	4011	-	-	16/29/63/63	0/2/2/2
16	CLA	X	513	-	-	9/17/93/115	-
16	CLA	B	1208	2	-	6/15/91/115	-
16	CLA	p	505	-	-	14/39/115/115	-
16	CLA	b	1228	2	-	12/27/103/115	-
16	CLA	B	1231	25	-	9/15/91/115	-
16	CLA	o	503	-	-	5/17/93/115	-
19	BCR	R	4018	-	-	13/29/63/63	0/2/2/2
16	CLA	b	1214	2	-	7/27/103/115	-
19	BCR	t	603	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1239	2	-	15/39/115/115	-
16	CLA	B	1229	2	-	9/31/107/115	-
16	CLA	q	501	12	-	7/21/97/115	-
16	CLA	h	507	12	-	15/39/115/115	-
24	LUT	w	601	-	-	7/29/67/67	0/2/2/2
16	CLA	T	4004	-	-	4/27/103/115	-
19	BCR	n	604	-	-	13/29/63/63	0/2/2/2
19	BCR	j	4015	-	-	14/29/63/63	0/2/2/2
16	CLA	Z	508	12	-	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	X	603	-	-	12/29/63/63	0/2/2/2
16	CLA	H	1128	1	-	17/39/115/115	-
19	BCR	S	4013	-	-	10/29/63/63	0/2/2/2
19	BCR	t	601	-	-	14/29/63/63	0/2/2/2
16	CLA	B	1236	2	-	11/21/97/115	-
16	CLA	G	1224	2	-	12/33/109/115	-
19	BCR	y	603	-	-	11/29/63/63	0/2/2/2
14	LMG	B	848	-	-	18/38/58/70	0/1/1/1
16	CLA	K	4003	9	-	8/15/91/115	-
16	CLA	T	4002	9	-	7/15/91/115	-
16	CLA	Z	513	-	-	8/21/97/115	-
16	CLA	A	1124	25	-	7/33/109/115	-
21	ECH	G	4006	-	-	10/29/66/66	0/2/2/2
16	CLA	A	1128	1	-	20/39/115/115	-
16	CLA	x	508	12	-	12/27/103/115	-
19	BCR	k	4001	-	-	12/29/63/63	0/2/2/2
19	BCR	X	601	-	-	10/29/63/63	0/2/2/2
16	CLA	U	1503	-	-	9/39/115/115	-
18	SF4	H	3001	-	-	-	0/6/5/5
16	CLA	b	1215	2	-	6/33/109/115	-
19	BCR	F	4016	-	-	9/29/63/63	0/2/2/2
19	BCR	J	4013	-	-	9/29/63/63	0/2/2/2
16	CLA	h	509	12	-	18/39/115/115	-
16	CLA	x	507	12	-	10/39/115/115	-
13	LHG	x	605	-	-	20/35/35/53	-
16	CLA	g	505	12	-	11/39/115/115	-
16	CLA	B	1216	25	-	5/18/94/115	-
16	CLA	n	513	-	-	9/17/93/115	-
16	CLA	F	1302	6	-	8/17/93/115	-
16	CLA	W	504	12	-	6/33/109/115	-
16	CLA	b	1223	2	-	11/39/115/115	-
16	CLA	q	505	-	-	13/39/115/115	-
16	CLA	A	1108	1	-	3/15/91/115	-
16	CLA	G	1227	2	-	9/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	1023	-	-	9/39/115/115	-
19	BCR	Y	603	-	-	8/29/63/63	0/2/2/2
19	BCR	G	4017	-	-	13/29/63/63	0/2/2/2
16	CLA	A	1134	1	-	6/15/91/115	-
16	CLA	u	515	12	-	17/39/115/115	-
16	CLA	A	1139	25	-	15/33/109/115	-
16	CLA	a	1122	1	-	10/32/108/115	-
16	CLA	s	513	-	-	9/17/93/115	-
16	CLA	W	505	12	-	20/39/115/115	-
16	CLA	a	1801	13	-	7/17/93/115	-
16	CLA	G	1211	2	-	22/39/115/115	-
16	CLA	o	511	-	-	10/39/115/115	-
16	CLA	a	1118	1	-	11/27/103/115	-
16	CLA	n	511	12	-	7/39/115/115	-
16	CLA	x	514	-	-	7/21/97/115	-
19	BCR	G	4005	-	-	11/29/63/63	0/2/2/2
16	CLA	v	506	-	-	5/33/109/115	-
23	LMU	x	606	-	-	14/21/61/61	0/2/2/2
16	CLA	o	504	12	-	10/33/109/115	-
16	CLA	x	517	12	-	9/27/103/115	-
19	BCR	k	4005	-	-	7/29/63/63	0/2/2/2
16	CLA	A	1105	-	-	9/31/107/115	-
16	CLA	a	1103	1	-	12/39/115/115	-
16	CLA	G	1208	2	-	8/15/91/115	-
16	CLA	b	1222	25	-	8/21/97/115	-
16	CLA	A	1101	1	-	15/39/115/115	-
19	BCR	j	4012	-	-	9/29/63/63	0/2/2/2
16	CLA	r	505	12	-	13/39/115/115	-
21	ECH	R	4020	-	-	11/29/66/66	0/2/2/2
16	CLA	w	515	12	-	13/39/115/115	-
16	CLA	H	1113	1	-	1/15/91/115	-
16	CLA	b	1238	25	-	18/39/115/115	-
16	CLA	r	504	12	-	17/39/115/115	-
19	BCR	i	4018	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	n	601	-	-	12/29/63/63	0/2/2/2
16	CLA	Z	502	12	-	7/21/97/115	-
16	CLA	l	1502	10	-	9/33/109/115	-
16	CLA	s	504	12	-	16/39/115/115	-
19	BCR	G	4009	-	-	7/24/41/63	0/1/1/2
19	BCR	T	4001	-	-	12/29/63/63	0/2/2/2
16	CLA	a	1126	1	-	11/39/115/115	-
19	BCR	y	601	-	-	15/29/63/63	0/2/2/2
16	CLA	H	1110	1	-	9/26/102/115	-
16	CLA	H	1135	1	-	4/23/99/115	-
16	CLA	s	516	-	-	10/17/93/115	-
16	CLA	p	501	12	-	7/21/97/115	-
16	CLA	G	1229	2	-	10/31/107/115	-
16	CLA	y	514	-	-	8/21/97/115	-
16	CLA	p	509	12	-	20/33/109/115	-
16	CLA	U	1502	10	-	9/33/109/115	-
16	CLA	a	1106	1	-	17/39/115/115	-
16	CLA	A	1112	1	-	4/15/91/115	-
21	ECH	V	4021	-	-	14/29/66/66	0/2/2/2
16	CLA	v	513	-	-	4/17/93/115	-
16	CLA	g	502	12	-	6/21/97/115	-
20	LMT	H	4202	-	-	8/21/61/61	0/2/2/2
13	LHG	B	4018	16	-	17/42/42/53	-
16	CLA	A	1130	1	-	10/33/109/115	-
16	CLA	a	1107	1	-	8/21/97/115	-
16	CLA	H	1109	1,16	-	11/39/115/115	-
16	CLA	v	501	12	-	6/17/93/115	-
16	CLA	H	1133	1	-	10/26/102/115	-
16	CLA	n	516	-	-	8/17/93/115	-
18	SF4	C	102	-	-	-	0/6/5/5
16	CLA	G	1201	2	-	4/26/102/115	-
16	CLA	a	1138	1	-	15/39/115/115	-
18	SF4	C	101	-	-	-	0/6/5/5
16	CLA	H	1105	-	-	9/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	w	505	-	-	9/39/115/115	-
16	CLA	p	512	12	-	10/39/115/115	-
16	CLA	H	1119	25	-	12/39/115/115	-
16	CLA	q	513	-	-	8/21/97/115	-
19	BCR	w	602	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1108	1	-	7/15/91/115	-
19	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	H	1138	1	-	11/39/115/115	-
16	CLA	G	1206	2	-	12/39/115/115	-
19	BCR	a	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	T	4003	9	-	9/15/91/115	-
16	CLA	a	1134	1	-	6/15/91/115	-
16	CLA	o	515	12	-	16/39/115/115	-
16	CLA	o	517	12	-	11/27/103/115	-
16	CLA	t	517	12	-	8/27/103/115	-
19	BCR	J	4015	-	-	7/29/63/63	0/2/2/2
16	CLA	G	1220	2	-	15/26/102/115	-
16	CLA	B	1219	-	-	4/15/91/115	-
16	CLA	F	1301	25	-	3/15/91/115	-
13	LHG	o	605	-	-	12/31/31/53	-
16	CLA	Z	510	-	-	11/33/109/115	-
16	CLA	v	512	12	-	12/39/115/115	-
16	CLA	a	1113	1	-	3/15/91/115	-
16	CLA	u	508	12	-	12/27/103/115	-
19	BCR	a	4011	-	-	16/29/63/63	0/2/2/2
17	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
16	CLA	A	1127	1	-	5/39/115/115	-
16	CLA	H	1121	1	-	8/23/99/115	-
16	CLA	w	502	12	-	8/21/97/115	-
16	CLA	G	1219	-	-	6/15/91/115	-
16	CLA	B	1202	-	-	16/39/115/115	-
19	BCR	r	604	-	-	15/29/63/63	0/2/2/2
16	CLA	B	1021	2	-	13/39/115/115	-
13	LHG	X	605	-	-	12/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	l	1501	10	-	15/33/109/115	-
13	LHG	g	605	-	-	16/35/35/53	-
16	CLA	x	509	12	-	14/39/115/115	-
16	CLA	G	1214	2	-	13/27/103/115	-
16	CLA	B	1212	2	-	6/15/91/115	-
16	CLA	v	502	12	-	6/21/97/115	-
19	BCR	K	4001	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1021	2	-	14/39/115/115	-
19	BCR	b	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	g	512	12	-	10/39/115/115	-
16	CLA	w	501	12	-	10/21/97/115	-
16	CLA	p	504	12	-	16/39/115/115	-
13	LHG	Y	605	-	-	16/36/36/53	-
13	LHG	r	605	-	-	17/35/35/53	-
19	BCR	a	4002	-	-	12/29/63/63	0/2/2/2
16	CLA	B	1220	2	-	12/25/101/115	-
13	LHG	A	851	16	-	7/30/30/53	-
16	CLA	p	514	-	-	8/21/97/115	-
16	CLA	X	511	-	-	10/39/115/115	-
16	CLA	G	1225	-	-	11/39/115/115	-
16	CLA	H	1118	1	-	13/27/103/115	-
16	CLA	g	516	-	-	5/17/93/115	-
16	CLA	r	508	12	-	9/27/103/115	-
19	BCR	Q	4016	-	-	11/29/63/63	0/2/2/2
16	CLA	W	502	12	-	10/21/97/115	-
16	CLA	u	516	12	-	9/17/93/115	-
19	BCR	x	601	-	-	11/29/63/63	0/2/2/2
20	LMT	A	4202	-	-	7/21/61/61	0/2/2/2
16	CLA	q	507	12	-	12/39/115/115	-
16	CLA	a	1112	1	-	6/15/91/115	-
16	CLA	Z	503	12	-	9/17/93/115	-
16	CLA	Q	1302	6	-	6/17/93/115	-
16	CLA	s	508	12	-	10/27/103/115	-
16	CLA	v	504	12	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	x	512	12	-	9/39/115/115	-
16	CLA	H	1103	-	-	12/39/115/115	-
16	CLA	y	511	12	-	11/39/115/115	-
21	ECH	M	4021	-	-	15/29/66/66	0/2/2/2
13	LHG	s	605	-	-	12/36/36/53	-
23	LMU	w	605	-	-	5/21/61/61	0/2/2/2
16	CLA	G	1228	2	-	15/27/103/115	-
16	CLA	q	506	-	-	12/33/109/115	-
19	BCR	u	602	-	-	13/29/63/63	0/2/2/2
16	CLA	h	516	12	-	8/17/93/115	-
16	CLA	r	512	12	-	11/39/115/115	-
16	CLA	k	4003	9	-	5/15/91/115	-
16	CLA	r	502	12	-	6/21/97/115	-
16	CLA	A	1138	1	-	12/39/115/115	-
16	CLA	n	514	-	-	7/21/97/115	-
23	LMU	Z	605	-	-	5/21/61/61	0/2/2/2
16	CLA	b	1216	25	-	2/18/94/115	-
16	CLA	g	510	-	-	12/39/115/115	-
16	CLA	Y	511	12	-	14/39/115/115	-
21	ECH	i	4020	-	-	12/29/66/66	0/2/2/2
16	CLA	r	507	12	-	11/39/115/115	-
16	CLA	r	516	-	-	5/17/93/115	-
16	CLA	B	1203	2	-	15/39/115/115	-
16	CLA	Z	507	12	-	15/39/115/115	-
16	CLA	w	508	12	-	8/27/103/115	-
15	CL0	H	1011	1	-	6/39/115/115	-
16	CLA	A	1133	1	-	11/26/102/115	-
16	CLA	b	1201	2	-	4/26/102/115	-
16	CLA	h	517	-	-	10/27/103/115	-
16	CLA	w	507	12	-	10/39/115/115	-
19	BCR	B	4010	-	-	16/29/63/63	0/2/2/2
16	CLA	b	1204	2	-	13/39/115/115	-
21	ECH	m	4021	-	-	14/29/66/66	0/2/2/2
16	CLA	X	515	12	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	o	604	-	-	18/29/63/63	0/2/2/2
16	CLA	w	509	12	-	12/39/115/115	-
16	CLA	W	510	-	-	14/39/115/115	-
19	BCR	w	604	-	-	17/29/63/63	0/2/2/2
16	CLA	w	510	-	-	10/33/109/115	-
16	CLA	n	502	12	-	7/21/97/115	-
16	CLA	B	1012	25	-	11/27/103/115	-
19	BCR	A	4003	-	-	9/29/63/63	0/2/2/2
16	CLA	g	507	12	-	9/39/115/115	-
16	CLA	W	513	-	-	10/17/93/115	-
19	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
16	CLA	g	513	-	-	11/17/93/115	-
16	CLA	B	1217	2	-	7/15/91/115	-
16	CLA	t	506	12	-	13/33/109/115	-
16	CLA	A	1137	1	-	7/18/94/115	-
16	CLA	w	504	12	-	12/39/115/115	-
16	CLA	H	1108	1	-	5/15/91/115	-
16	CLA	s	509	12	-	15/33/109/115	-
16	CLA	s	505	-	-	13/39/115/115	-
16	CLA	X	506	-	-	13/33/109/115	-
16	CLA	H	1134	1	-	4/15/91/115	-
16	CLA	s	510	-	-	9/39/115/115	-
19	BCR	b	4010	-	-	15/29/63/63	0/2/2/2
16	CLA	f	1302	6	-	8/17/93/115	-
19	BCR	u	603	-	-	9/29/63/63	0/2/2/2
16	CLA	n	505	12	-	22/39/115/115	-
16	CLA	s	512	12	-	8/39/115/115	-
16	CLA	b	1227	2	-	6/20/96/115	-
16	CLA	Y	516	-	-	11/17/93/115	-
16	CLA	a	1102	1,16	-	7/29/105/115	-
16	CLA	L	1501	10	-	13/33/109/115	-
16	CLA	A	1107	1	-	6/21/97/115	-
19	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
16	CLA	Z	515	12	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMG	f	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	W	509	12	-	5/33/109/115	-
18	SF4	c	101	-	-	-	0/6/5/5
19	BCR	I	4018	-	-	11/29/63/63	0/2/2/2
16	CLA	Y	506	12	-	14/33/109/115	-
16	CLA	H	1101	1	-	17/39/115/115	-
16	CLA	a	1109	1,16	-	9/39/115/115	-
19	BCR	l	4019	-	-	12/29/63/63	0/2/2/2
19	BCR	H	4002	-	-	11/29/63/63	0/2/2/2
19	BCR	p	604	-	-	15/29/63/63	0/2/2/2
16	CLA	r	513	-	-	13/17/93/115	-
16	CLA	B	1206	2	-	17/39/115/115	-
16	CLA	Y	515	12	-	8/39/115/115	-
16	CLA	a	1105	-	-	7/31/107/115	-
19	BCR	L	4019	-	-	13/29/63/63	0/2/2/2
16	CLA	a	1119	-	-	8/39/115/115	-
16	CLA	g	515	12	-	9/39/115/115	-
16	CLA	b	1221	25	-	19/39/115/115	-
16	CLA	t	513	-	-	8/17/93/115	-
19	BCR	W	603	-	-	13/29/63/63	0/2/2/2
16	CLA	s	501	12	-	9/21/97/115	-
19	BCR	B	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	B	1209	2	-	7/15/91/115	-
16	CLA	p	510	-	-	11/39/115/115	-
16	CLA	v	507	12	-	9/39/115/115	-
16	CLA	Z	517	12	-	6/27/103/115	-
19	BCR	W	601	-	-	16/29/63/63	0/2/2/2
16	CLA	Y	512	12	-	9/39/115/115	-
16	CLA	b	1205	2	-	12/39/115/115	-
16	CLA	r	517	12	-	12/27/103/115	-
16	CLA	t	501	12	-	7/21/97/115	-
16	CLA	Q	1301	25	-	2/15/91/115	-
16	CLA	t	509	12	-	6/33/109/115	-
21	ECH	B	4006	-	-	10/29/66/66	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	u	512	12	-	11/39/115/115	-
16	CLA	l	1503	-	-	12/39/115/115	-
16	CLA	t	511	12	-	9/39/115/115	-
13	LHG	a	851	16	-	9/30/30/53	-
16	CLA	H	1112	1	-	2/15/91/115	-
16	CLA	Z	514	-	-	9/21/97/115	-
16	CLA	q	508	12	-	10/27/103/115	-
16	CLA	v	509	12	-	16/39/115/115	-
16	CLA	r	510	-	-	12/39/115/115	-
16	CLA	y	506	12	-	9/33/109/115	-
16	CLA	G	1218	-	-	14/27/103/115	-
16	CLA	b	1021	2	-	17/39/115/115	-
19	BCR	o	601	-	-	8/29/63/63	0/2/2/2
16	CLA	G	1215	2	-	8/33/109/115	-
16	CLA	Y	507	12	-	10/39/115/115	-
19	BCR	a	4003	-	-	12/29/63/63	0/2/2/2
16	CLA	h	512	12	-	16/39/115/115	-
16	CLA	b	1220	2	-	13/26/102/115	-
16	CLA	t	512	12	-	11/39/115/115	-
16	CLA	b	1240	13	-	5/17/93/115	-
16	CLA	A	1111	1	-	7/27/103/115	-
16	CLA	B	1211	2	-	17/39/115/115	-
16	CLA	A	1022	25	-	10/39/115/115	-
16	CLA	H	1130	1	-	10/33/109/115	-
16	CLA	h	504	-	-	14/33/109/115	-
16	CLA	b	1230	2	-	7/15/91/115	-
16	CLA	b	1212	2	-	4/15/91/115	-
16	CLA	x	503	-	-	8/17/93/115	-
16	CLA	q	514	-	-	10/21/97/115	-
19	BCR	u	601	-	-	8/29/63/63	0/2/2/2
16	CLA	b	1236	2	-	7/21/97/115	-
19	BCR	x	602	-	-	17/29/63/63	0/2/2/2
16	CLA	Z	506	-	-	8/33/109/115	-
16	CLA	u	510	-	-	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	o	501	12	-	9/17/93/115	-
16	CLA	w	503	12	-	8/17/93/115	-
16	CLA	s	507	12	-	11/39/115/115	-
16	CLA	X	516	12	-	8/17/93/115	-
16	CLA	x	511	12	-	7/39/115/115	-
16	CLA	B	1210	2	-	14/39/115/115	-
16	CLA	q	502	12	-	7/21/97/115	-
16	CLA	q	516	-	-	11/17/93/115	-
16	CLA	A	1129	1	-	6/17/93/115	-
16	CLA	h	515	12	-	17/39/115/115	-
19	BCR	Z	602	-	-	11/29/63/63	0/2/2/2
19	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
23	LMU	q	605	-	-	5/21/61/61	0/2/2/2
16	CLA	w	514	-	-	8/21/97/115	-
16	CLA	X	502	12	-	6/21/97/115	-
17	PQN	G	2002	-	-	10/23/43/43	0/2/2/2
16	CLA	r	503	-	-	9/17/93/115	-
16	CLA	H	1111	1	-	8/27/103/115	-
16	CLA	r	506	12	-	12/33/109/115	-
16	CLA	s	511	12	-	14/39/115/115	-
16	CLA	K	4004	-	-	5/27/103/115	-
16	CLA	s	503	-	-	10/17/93/115	-
19	BCR	X	602	-	-	17/29/63/63	0/2/2/2
16	CLA	H	1127	1	-	7/39/115/115	-
16	CLA	p	513	-	-	8/17/93/115	-
16	CLA	n	507	12	-	11/39/115/115	-
16	CLA	a	1129	1	-	3/17/93/115	-
19	BCR	r	602	-	-	16/29/63/63	0/2/2/2
23	LMU	g	606	-	-	5/21/61/61	0/2/2/2
16	CLA	t	504	12	-	6/33/109/115	-
16	CLA	L	1503	25	-	11/39/115/115	-
16	CLA	A	1104	1	-	19/39/115/115	-
16	CLA	s	515	12	-	12/39/115/115	-
16	CLA	g	501	12	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LHG	H	851	16	-	7/30/30/53	-
16	CLA	x	502	12	-	5/21/97/115	-
16	CLA	b	1012	25	-	10/27/103/115	-
16	CLA	H	1013	-	-	13/39/115/115	-
16	CLA	u	501	12	-	6/17/93/115	-
16	CLA	p	511	12	-	15/39/115/115	-
16	CLA	A	1125	1	-	11/39/115/115	-
16	CLA	r	515	12	-	12/39/115/115	-
16	CLA	B	1201	2	-	4/26/102/115	-
19	BCR	x	604	-	-	12/29/63/63	0/2/2/2
16	CLA	j	1303	8	-	2/4/76/115	-
16	CLA	v	515	12	-	17/39/115/115	-
13	LHG	i	103	-	-	22/44/44/53	-
15	CL0	a	1011	1	-	7/39/115/115	-
16	CLA	b	1224	2	-	9/33/109/115	-
16	CLA	o	516	12	-	11/17/93/115	-
16	CLA	Y	505	-	-	15/39/115/115	-
16	CLA	y	512	12	-	12/39/115/115	-
16	CLA	B	1213	2	-	8/27/103/115	-
16	CLA	a	1139	25	-	6/27/103/115	-
17	PQN	H	2001	-	-	3/23/43/43	0/2/2/2
16	CLA	G	1231	25	-	5/15/91/115	-
16	CLA	p	503	-	-	6/17/93/115	-
16	CLA	x	506	12	-	14/33/109/115	-
16	CLA	H	1131	1	-	10/39/115/115	-
19	BCR	h	601	-	-	14/29/63/63	0/2/2/2
16	CLA	A	1102	1,16	-	6/29/105/115	-
16	CLA	x	510	-	-	13/39/115/115	-
16	CLA	o	514	-	-	8/21/97/115	-
16	CLA	H	1123	-	-	10/39/115/115	-
16	CLA	b	1225	-	-	12/39/115/115	-
16	CLA	y	502	12	-	5/21/97/115	-
16	CLA	b	1219	-	-	6/15/91/115	-
19	BCR	Z	604	-	-	19/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	b	4017	-	-	12/29/63/63	0/2/2/2
19	BCR	H	4007	-	-	8/29/63/63	0/2/2/2
16	CLA	B	1214	2	-	10/27/103/115	-
16	CLA	G	1238	25	-	11/39/115/115	-
16	CLA	g	508	12	-	7/27/103/115	-
16	CLA	X	517	12	-	7/27/103/115	-
16	CLA	o	512	12	-	8/39/115/115	-
24	LUT	Z	601	-	-	7/29/67/67	0/2/2/2
16	CLA	n	512	12	-	19/39/115/115	-
16	CLA	a	1101	1	-	19/39/115/115	-
16	CLA	u	507	12	-	12/39/115/115	-
16	CLA	a	1125	1	-	10/39/115/115	-
16	CLA	H	1116	1	-	10/26/102/115	-
16	CLA	Y	502	12	-	6/21/97/115	-
16	CLA	q	510	-	-	10/33/109/115	-
16	CLA	b	1208	2	-	8/15/91/115	-
16	CLA	w	513	-	-	8/21/97/115	-
16	CLA	G	1210	2	-	16/39/115/115	-
16	CLA	X	508	12	-	15/27/103/115	-
16	CLA	p	516	-	-	9/17/93/115	-
16	CLA	a	1121	1	-	6/23/99/115	-
16	CLA	a	1116	1	-	9/26/102/115	-
14	LMG	a	4101	-	-	21/41/61/70	0/1/1/1
16	CLA	H	1137	1	-	6/18/94/115	-
16	CLA	h	510	-	-	9/39/115/115	-
16	CLA	B	1205	2	-	10/39/115/115	-
16	CLA	W	514	-	-	8/21/97/115	-
16	CLA	u	505	12	-	14/39/115/115	-
16	CLA	k	4002	9	-	7/15/91/115	-
16	CLA	g	504	12	-	22/39/115/115	-
16	CLA	u	503	-	-	9/17/93/115	-
16	CLA	u	506	-	-	11/33/109/115	-
16	CLA	A	1114	-	-	9/17/93/115	-
16	CLA	h	514	-	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	Z	501	12	-	7/21/97/115	-
16	CLA	G	1023	-	-	8/39/115/115	-
16	CLA	A	1013	-	-	14/39/115/115	-
17	PQN	a	2001	-	-	5/23/43/43	0/2/2/2
16	CLA	a	1022	-	-	8/39/115/115	-
19	BCR	a	4008	-	-	10/29/63/63	0/2/2/2
16	CLA	n	515	12	-	15/39/115/115	-
16	CLA	B	1228	2	-	14/27/103/115	-

The worst 5 of 2891 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1012	CLA	C1D-ND	3.66	1.42	1.37
16	G	1218	CLA	C1D-ND	3.63	1.42	1.37
16	n	510	CLA	C1D-ND	3.61	1.42	1.37
16	g	504	CLA	C1D-ND	3.56	1.42	1.37
16	p	510	CLA	C1D-ND	3.56	1.42	1.37

The worst 5 of 3850 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	u	506	CLA	C4A-NA-C1A	8.41	110.52	106.68
21	i	4020	ECH	C8-C9-C10	6.94	129.93	119.01
16	x	505	CLA	C4A-NA-C1A	6.63	109.70	106.68
16	v	505	CLA	C4A-NA-C1A	6.59	109.69	106.68
16	b	1216	CLA	C4A-NA-C1A	6.57	109.68	106.68

There are no chirality outliers.

5 of 8156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	849	LHG	O1-C1-C2-O2
13	A	849	LHG	O1-C1-C2-C3
13	A	849	LHG	C3-O3-P-O5
13	A	851	LHG	C3-O3-P-O5
13	B	4018	LHG	O1-C1-C2-O2

There are no ring outliers.

673 monomers are involved in 1441 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Z	603	BCR	1	0
13	I	103	LHG	2	0
16	G	1213	CLA	2	0
16	G	1232	CLA	1	0
16	A	1136	CLA	3	0
14	Q	4017	LMG	1	0
16	B	1240	CLA	4	0
19	K	4005	BCR	2	0
16	w	517	CLA	1	0
16	B	1235	CLA	3	0
16	p	515	CLA	6	0
16	H	1107	CLA	3	0
16	q	503	CLA	2	0
16	u	511	CLA	3	0
19	g	602	BCR	4	0
16	b	1202	CLA	2	0
16	G	1240	CLA	2	0
16	h	506	CLA	1	0
16	n	508	CLA	4	0
16	G	1235	CLA	2	0
16	A	1132	CLA	3	0
16	A	1120	CLA	2	0
16	q	511	CLA	3	0
16	t	508	CLA	2	0
16	f	1301	CLA	2	0
16	t	502	CLA	1	0
16	q	509	CLA	4	0
19	J	4012	BCR	5	0
16	b	1210	CLA	5	0
19	A	4007	BCR	1	0
16	a	1137	CLA	4	0
16	Y	508	CLA	1	0
14	H	4101	LMG	6	0
16	A	1113	CLA	1	0
16	q	515	CLA	4	0
16	a	1120	CLA	2	0
16	x	516	CLA	2	0
16	B	1225	CLA	8	0
16	J	1303	CLA	1	0
16	W	506	CLA	3	0
23	p	606	LMU	1	0
16	B	1218	CLA	1	0
16	B	1238	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	509	CLA	5	0
16	B	1215	CLA	3	0
16	G	1205	CLA	5	0
16	p	517	CLA	2	0
16	B	1230	CLA	3	0
16	v	516	CLA	3	0
16	b	1231	CLA	1	0
16	A	1123	CLA	4	0
16	X	512	CLA	3	0
16	A	1117	CLA	7	0
19	f	4016	BCR	4	0
16	a	1128	CLA	5	0
19	S	4015	BCR	2	0
16	B	1234	CLA	1	0
16	q	512	CLA	3	0
16	b	1229	CLA	4	0
16	x	515	CLA	4	0
16	a	1130	CLA	2	0
16	o	506	CLA	3	0
16	A	1135	CLA	2	0
21	I	4020	ECH	2	0
16	A	1116	CLA	4	0
16	a	1013	CLA	2	0
19	v	604	BCR	3	0
19	U	4019	BCR	1	0
13	p	605	LHG	1	0
19	s	602	BCR	1	0
16	v	510	CLA	5	0
19	l	4022	BCR	6	0
16	b	1209	CLA	1	0
16	b	1235	CLA	3	0
19	X	604	BCR	4	0
19	o	602	BCR	1	0
16	h	511	CLA	6	0
17	A	2001	PQN	4	0
19	h	603	BCR	5	0
16	o	510	CLA	4	0
16	G	1204	CLA	5	0
16	B	1221	CLA	2	0
19	g	601	BCR	2	0
16	t	510	CLA	3	0
19	G	4014	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	h	501	CLA	1	0
16	y	509	CLA	8	0
16	y	508	CLA	5	0
16	W	507	CLA	5	0
16	W	511	CLA	2	0
16	a	1123	CLA	6	0
16	X	510	CLA	6	0
19	p	602	BCR	3	0
16	b	1207	CLA	6	0
16	A	1119	CLA	5	0
16	Y	510	CLA	5	0
16	A	1103	CLA	3	0
16	A	1106	CLA	2	0
16	H	1022	CLA	2	0
16	W	512	CLA	2	0
16	a	1110	CLA	3	0
16	y	510	CLA	5	0
16	s	502	CLA	2	0
16	a	1104	CLA	4	0
19	x	603	BCR	2	0
16	H	1125	CLA	2	0
16	a	1114	CLA	1	0
16	t	507	CLA	1	0
16	U	1501	CLA	4	0
19	r	601	BCR	2	0
19	s	604	BCR	3	0
19	v	603	BCR	3	0
24	q	601	LUT	1	0
16	X	507	CLA	1	0
16	G	1230	CLA	2	0
19	G	4010	BCR	3	0
23	r	606	LMU	3	0
16	g	503	CLA	1	0
19	s	601	BCR	2	0
16	g	506	CLA	2	0
16	X	501	CLA	2	0
16	p	502	CLA	1	0
14	A	4101	LMG	5	0
19	y	604	BCR	5	0
19	B	4017	BCR	2	0
13	b	4018	LHG	3	0
16	H	1136	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	o	513	CLA	1	0
16	a	1237	CLA	2	0
16	B	1227	CLA	1	0
14	H	4201	LMG	1	0
16	n	510	CLA	6	0
16	G	1234	CLA	2	0
16	G	1226	CLA	4	0
16	H	1117	CLA	4	0
16	a	1133	CLA	2	0
16	G	1221	CLA	8	0
19	Y	601	BCR	2	0
16	b	1226	CLA	5	0
16	o	509	CLA	5	0
14	G	848	LMG	2	0
16	W	515	CLA	1	0
16	y	515	CLA	5	0
19	H	4008	BCR	4	0
19	p	601	BCR	2	0
16	a	1111	CLA	4	0
16	u	504	CLA	3	0
14	A	4201	LMG	1	0
16	n	501	CLA	3	0
16	G	1222	CLA	3	0
16	L	1502	CLA	3	0
16	y	507	CLA	2	0
19	S	4012	BCR	4	0
16	g	509	CLA	3	0
16	o	505	CLA	7	0
19	s	603	BCR	5	0
16	Z	505	CLA	7	0
16	n	503	CLA	1	0
19	A	4011	BCR	4	0
19	o	603	BCR	2	0
19	n	603	BCR	1	0
16	Z	504	CLA	2	0
16	b	1203	CLA	7	0
16	B	1207	CLA	6	0
16	X	505	CLA	4	0
19	v	601	BCR	1	0
16	H	1140	CLA	4	0
16	X	503	CLA	2	0
19	q	602	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	X	504	CLA	4	0
16	q	517	CLA	3	0
16	t	515	CLA	4	0
16	G	1207	CLA	5	0
19	p	603	BCR	4	0
16	a	1140	CLA	3	0
16	p	507	CLA	2	0
16	W	517	CLA	1	0
16	H	1132	CLA	1	0
16	u	514	CLA	1	0
16	H	1120	CLA	2	0
20	U	4101	LMT	2	0
20	a	4202	LMT	1	0
16	w	506	CLA	3	0
16	a	1124	CLA	7	0
16	a	1131	CLA	3	0
16	G	1236	CLA	5	0
16	H	1104	CLA	5	0
16	o	508	CLA	4	0
19	q	604	BCR	5	0
16	r	511	CLA	3	0
13	R	103	LHG	2	0
19	b	4005	BCR	4	0
16	G	1216	CLA	2	0
16	g	511	CLA	1	0
16	v	514	CLA	2	0
16	n	504	CLA	5	0
19	g	603	BCR	3	0
16	B	1223	CLA	2	0
20	L	4101	LMT	3	0
16	H	1801	CLA	3	0
19	q	603	BCR	4	0
16	h	508	CLA	2	0
16	g	517	CLA	1	0
16	y	505	CLA	3	0
16	X	509	CLA	6	0
16	H	1237	CLA	3	0
19	H	4003	BCR	2	0
19	U	4022	BCR	12	0
16	x	501	CLA	1	0
16	Z	511	CLA	2	0
19	G	4004	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	h	505	CLA	2	0
14	H	852	LMG	2	0
16	w	511	CLA	1	0
20	l	4101	LMT	3	0
19	Y	602	BCR	2	0
14	a	852	LMG	2	0
13	u	605	LHG	1	0
16	r	509	CLA	6	0
19	r	603	BCR	3	0
16	G	1202	CLA	6	0
19	g	604	BCR	4	0
19	w	603	BCR	3	0
16	u	502	CLA	2	0
16	Z	509	CLA	5	0
16	H	1124	CLA	4	0
16	A	1110	CLA	1	0
16	y	516	CLA	1	0
16	B	1204	CLA	5	0
16	H	1106	CLA	2	0
16	H	1122	CLA	3	0
14	A	852	LMG	1	0
16	s	517	CLA	2	0
16	b	1211	CLA	2	0
16	x	505	CLA	3	0
16	A	1140	CLA	2	0
19	h	604	BCR	3	0
16	a	1117	CLA	4	0
16	v	505	CLA	5	0
13	G	4018	LHG	1	0
16	H	1129	CLA	3	0
16	o	502	CLA	3	0
19	b	4014	BCR	7	0
16	y	517	CLA	3	0
19	j	4013	BCR	2	0
16	b	1213	CLA	1	0
16	A	1109	CLA	1	0
21	b	4006	ECH	2	0
16	n	517	CLA	1	0
16	Z	516	CLA	4	0
16	A	1122	CLA	3	0
16	A	1801	CLA	2	0
23	Y	606	LMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	504	CLA	4	0
16	B	1239	CLA	3	0
19	W	604	BCR	1	0
16	q	504	CLA	3	0
16	B	1222	CLA	3	0
16	b	1234	CLA	1	0
16	p	508	CLA	2	0
16	x	504	CLA	2	0
16	Y	517	CLA	2	0
16	H	1126	CLA	5	0
16	y	513	CLA	1	0
16	H	1139	CLA	7	0
16	u	517	CLA	1	0
16	v	511	CLA	5	0
16	G	1223	CLA	2	0
19	B	4014	BCR	6	0
16	b	1023	CLA	3	0
16	A	1121	CLA	1	0
16	B	1226	CLA	2	0
16	a	1127	CLA	1	0
16	G	1203	CLA	4	0
19	L	4022	BCR	6	0
16	a	1115	CLA	1	0
16	B	1224	CLA	2	0
16	n	509	CLA	5	0
16	Z	512	CLA	2	0
17	b	2002	PQN	2	0
16	s	506	CLA	4	0
16	A	1237	CLA	3	0
16	b	1239	CLA	5	0
16	b	1206	CLA	4	0
16	w	512	CLA	1	0
16	n	506	CLA	4	0
16	A	1126	CLA	8	0
19	b	4004	BCR	1	0
16	A	1131	CLA	2	0
15	A	1011	CL0	3	0
16	a	1136	CLA	2	0
16	G	1012	CLA	2	0
16	W	501	CLA	2	0
16	a	1132	CLA	2	0
16	u	509	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	y	504	CLA	2	0
16	w	516	CLA	1	0
16	X	514	CLA	1	0
16	b	1218	CLA	1	0
16	A	1118	CLA	1	0
16	a	1135	CLA	3	0
16	t	505	CLA	3	0
16	p	506	CLA	2	0
19	H	4011	BCR	3	0
16	X	513	CLA	2	0
16	B	1208	CLA	2	0
16	p	505	CLA	7	0
16	b	1228	CLA	1	0
16	B	1231	CLA	2	0
16	o	503	CLA	1	0
16	b	1214	CLA	2	0
19	t	603	BCR	2	0
16	G	1239	CLA	5	0
16	B	1229	CLA	2	0
16	h	507	CLA	4	0
19	n	604	BCR	4	0
19	j	4015	BCR	2	0
16	Z	508	CLA	1	0
19	X	603	BCR	2	0
16	H	1128	CLA	5	0
19	S	4013	BCR	3	0
19	t	601	BCR	3	0
16	B	1236	CLA	3	0
16	G	1224	CLA	2	0
19	y	603	BCR	5	0
14	B	848	LMG	2	0
16	K	4003	CLA	2	0
16	T	4002	CLA	1	0
16	A	1124	CLA	6	0
21	G	4006	ECH	2	0
16	A	1128	CLA	5	0
16	x	508	CLA	1	0
19	k	4001	BCR	4	0
19	X	601	BCR	3	0
16	U	1503	CLA	4	0
16	b	1215	CLA	3	0
19	F	4016	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	J	4013	BCR	1	0
16	h	509	CLA	4	0
16	x	507	CLA	6	0
16	g	505	CLA	6	0
16	W	504	CLA	5	0
16	b	1223	CLA	1	0
16	q	505	CLA	4	0
16	A	1108	CLA	1	0
16	G	1227	CLA	2	0
16	B	1023	CLA	5	0
19	Y	603	BCR	2	0
19	G	4017	BCR	3	0
16	A	1134	CLA	1	0
16	u	515	CLA	2	0
16	A	1139	CLA	5	0
16	a	1122	CLA	5	0
16	s	513	CLA	1	0
16	W	505	CLA	2	0
16	a	1801	CLA	1	0
16	G	1211	CLA	3	0
16	o	511	CLA	1	0
16	a	1118	CLA	1	0
16	n	511	CLA	5	0
16	x	514	CLA	1	0
19	G	4005	BCR	2	0
16	v	506	CLA	3	0
23	x	606	LMU	2	0
16	o	504	CLA	2	0
16	x	517	CLA	1	0
16	A	1105	CLA	1	0
16	a	1103	CLA	5	0
16	G	1208	CLA	1	0
16	b	1222	CLA	2	0
16	A	1101	CLA	5	0
19	j	4012	BCR	3	0
16	r	505	CLA	7	0
21	R	4020	ECH	2	0
16	w	515	CLA	4	0
16	b	1238	CLA	2	0
16	r	504	CLA	2	0
19	i	4018	BCR	5	0
19	n	601	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Z	502	CLA	2	0
16	l	1502	CLA	2	0
16	s	504	CLA	6	0
19	G	4009	BCR	1	0
19	T	4001	BCR	3	0
16	a	1126	CLA	4	0
19	y	601	BCR	1	0
16	H	1110	CLA	2	0
16	H	1135	CLA	1	0
16	s	516	CLA	1	0
16	p	509	CLA	3	0
16	U	1502	CLA	3	0
16	a	1106	CLA	2	0
16	A	1112	CLA	1	0
21	V	4021	ECH	4	0
16	g	502	CLA	2	0
20	H	4202	LMT	1	0
13	B	4018	LHG	1	0
16	A	1130	CLA	4	0
16	a	1107	CLA	2	0
16	H	1109	CLA	2	0
16	H	1133	CLA	1	0
16	n	516	CLA	2	0
16	G	1201	CLA	2	0
16	a	1138	CLA	1	0
16	H	1105	CLA	3	0
16	w	505	CLA	3	0
16	p	512	CLA	2	0
16	H	1119	CLA	9	0
16	q	513	CLA	2	0
19	w	602	BCR	3	0
16	a	1108	CLA	1	0
16	H	1138	CLA	4	0
16	G	1206	CLA	3	0
19	a	4007	BCR	1	0
16	T	4003	CLA	2	0
16	o	515	CLA	1	0
16	o	517	CLA	3	0
19	J	4015	BCR	2	0
16	G	1220	CLA	3	0
16	B	1219	CLA	1	0
16	F	1301	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	o	605	LHG	1	0
16	Z	510	CLA	6	0
16	v	512	CLA	4	0
16	a	1113	CLA	1	0
16	u	508	CLA	2	0
19	a	4011	BCR	4	0
17	B	2002	PQN	5	0
16	A	1127	CLA	4	0
16	H	1121	CLA	1	0
16	w	502	CLA	1	0
16	G	1219	CLA	1	0
16	B	1202	CLA	4	0
16	B	1021	CLA	4	0
13	X	605	LHG	1	0
16	l	1501	CLA	7	0
16	x	509	CLA	3	0
16	G	1214	CLA	2	0
16	v	502	CLA	3	0
19	K	4001	BCR	3	0
16	G	1021	CLA	2	0
16	g	512	CLA	2	0
16	p	504	CLA	7	0
13	r	605	LHG	2	0
19	a	4002	BCR	4	0
16	B	1220	CLA	3	0
13	A	851	LHG	2	0
16	X	511	CLA	1	0
16	G	1225	CLA	4	0
16	H	1118	CLA	2	0
16	g	516	CLA	2	0
16	r	508	CLA	2	0
19	Q	4016	BCR	2	0
16	W	502	CLA	4	0
19	x	601	BCR	5	0
20	A	4202	LMT	1	0
16	q	507	CLA	6	0
16	a	1112	CLA	1	0
16	Z	503	CLA	2	0
16	Q	1302	CLA	1	0
16	s	508	CLA	2	0
16	v	504	CLA	4	0
16	x	512	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	H	1103	CLA	8	0
16	y	511	CLA	6	0
21	M	4021	ECH	2	0
13	s	605	LHG	1	0
16	G	1228	CLA	2	0
16	q	506	CLA	4	0
19	u	602	BCR	2	0
16	h	516	CLA	2	0
16	r	512	CLA	3	0
16	k	4003	CLA	1	0
16	r	502	CLA	1	0
16	A	1138	CLA	3	0
16	n	514	CLA	1	0
16	b	1216	CLA	2	0
16	g	510	CLA	4	0
16	Y	511	CLA	3	0
21	i	4020	ECH	1	0
16	r	507	CLA	6	0
16	r	516	CLA	3	0
16	B	1203	CLA	7	0
16	Z	507	CLA	6	0
16	w	508	CLA	2	0
15	H	1011	CL0	4	0
16	b	1201	CLA	2	0
16	w	507	CLA	6	0
19	B	4010	BCR	2	0
16	b	1204	CLA	4	0
21	m	4021	ECH	2	0
16	X	515	CLA	3	0
19	o	604	BCR	1	0
16	w	509	CLA	6	0
16	W	510	CLA	4	0
19	w	604	BCR	2	0
16	w	510	CLA	5	0
16	n	502	CLA	3	0
16	B	1012	CLA	4	0
19	A	4003	BCR	2	0
16	g	507	CLA	4	0
19	A	4008	BCR	3	0
16	g	513	CLA	1	0
16	t	506	CLA	3	0
16	A	1137	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	w	504	CLA	3	0
16	H	1108	CLA	1	0
16	s	509	CLA	4	0
16	s	505	CLA	6	0
16	X	506	CLA	2	0
16	H	1134	CLA	3	0
16	s	510	CLA	5	0
19	b	4010	BCR	2	0
19	u	603	BCR	2	0
16	n	505	CLA	3	0
16	s	512	CLA	3	0
16	b	1227	CLA	1	0
16	Y	516	CLA	1	0
16	a	1102	CLA	5	0
16	L	1501	CLA	3	0
16	A	1107	CLA	4	0
19	B	4005	BCR	3	0
16	Z	515	CLA	3	0
14	f	4017	LMG	1	0
16	W	509	CLA	2	0
19	I	4018	BCR	3	0
16	Y	506	CLA	5	0
16	H	1101	CLA	5	0
16	a	1109	CLA	2	0
19	l	4019	BCR	4	0
19	H	4002	BCR	3	0
19	p	604	BCR	1	0
16	r	513	CLA	1	0
16	B	1206	CLA	7	0
16	Y	515	CLA	3	0
16	a	1105	CLA	4	0
19	L	4019	BCR	3	0
16	a	1119	CLA	6	0
16	g	515	CLA	3	0
16	b	1221	CLA	6	0
19	B	4009	BCR	2	0
16	p	510	CLA	7	0
16	v	507	CLA	5	0
16	Z	517	CLA	1	0
19	W	601	BCR	5	0
16	Y	512	CLA	3	0
16	b	1205	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	1301	CLA	2	0
16	t	509	CLA	3	0
21	B	4006	ECH	3	0
16	u	512	CLA	2	0
16	l	1503	CLA	6	0
16	t	511	CLA	2	0
16	H	1112	CLA	1	0
16	q	508	CLA	3	0
16	v	509	CLA	7	0
16	r	510	CLA	6	0
16	y	506	CLA	2	0
16	G	1218	CLA	2	0
16	b	1021	CLA	2	0
19	o	601	BCR	1	0
16	G	1215	CLA	2	0
16	Y	507	CLA	5	0
19	a	4003	BCR	4	0
16	h	512	CLA	3	0
16	b	1220	CLA	3	0
16	t	512	CLA	3	0
16	b	1240	CLA	2	0
16	A	1111	CLA	3	0
16	B	1211	CLA	3	0
16	A	1022	CLA	4	0
16	H	1130	CLA	1	0
16	h	504	CLA	2	0
16	b	1230	CLA	1	0
16	x	503	CLA	2	0
19	u	601	BCR	4	0
16	b	1236	CLA	1	0
19	x	602	BCR	1	0
16	Z	506	CLA	3	0
16	u	510	CLA	3	0
16	o	501	CLA	1	0
16	w	503	CLA	3	0
16	s	507	CLA	5	0
16	x	511	CLA	6	0
16	B	1210	CLA	7	0
16	q	502	CLA	4	0
16	q	516	CLA	2	0
16	A	1129	CLA	1	0
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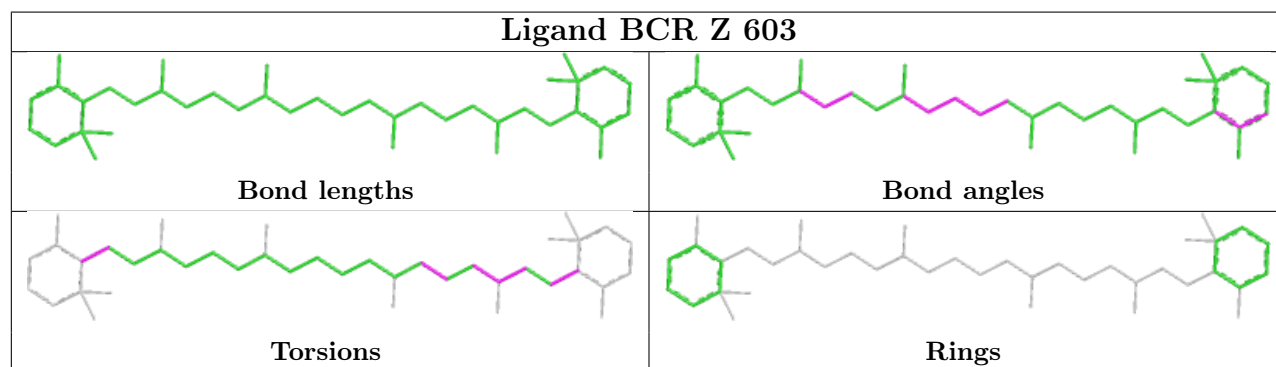
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Z	602	BCR	2	0
19	A	4002	BCR	3	0
23	q	605	LMU	2	0
16	X	502	CLA	3	0
17	G	2002	PQN	5	0
16	H	1111	CLA	3	0
16	r	506	CLA	2	0
16	K	4004	CLA	1	0
19	X	602	BCR	3	0
16	H	1127	CLA	1	0
16	p	513	CLA	1	0
16	n	507	CLA	6	0
16	a	1129	CLA	2	0
19	r	602	BCR	2	0
23	g	606	LMU	1	0
16	t	504	CLA	2	0
16	L	1503	CLA	5	0
16	A	1104	CLA	4	0
16	s	515	CLA	2	0
13	H	851	LHG	2	0
16	b	1012	CLA	3	0
16	H	1013	CLA	3	0
16	u	501	CLA	1	0
16	p	511	CLA	1	0
16	A	1125	CLA	1	0
16	r	515	CLA	4	0
16	B	1201	CLA	3	0
19	x	604	BCR	1	0
16	v	515	CLA	1	0
13	i	103	LHG	2	0
15	a	1011	CL0	4	0
16	b	1224	CLA	2	0
16	Y	505	CLA	4	0
16	y	512	CLA	4	0
16	B	1213	CLA	3	0
17	H	2001	PQN	4	0
16	G	1231	CLA	1	0
16	p	503	CLA	1	0
16	x	506	CLA	2	0
16	H	1131	CLA	5	0
19	h	601	BCR	1	0
16	A	1102	CLA	2	0

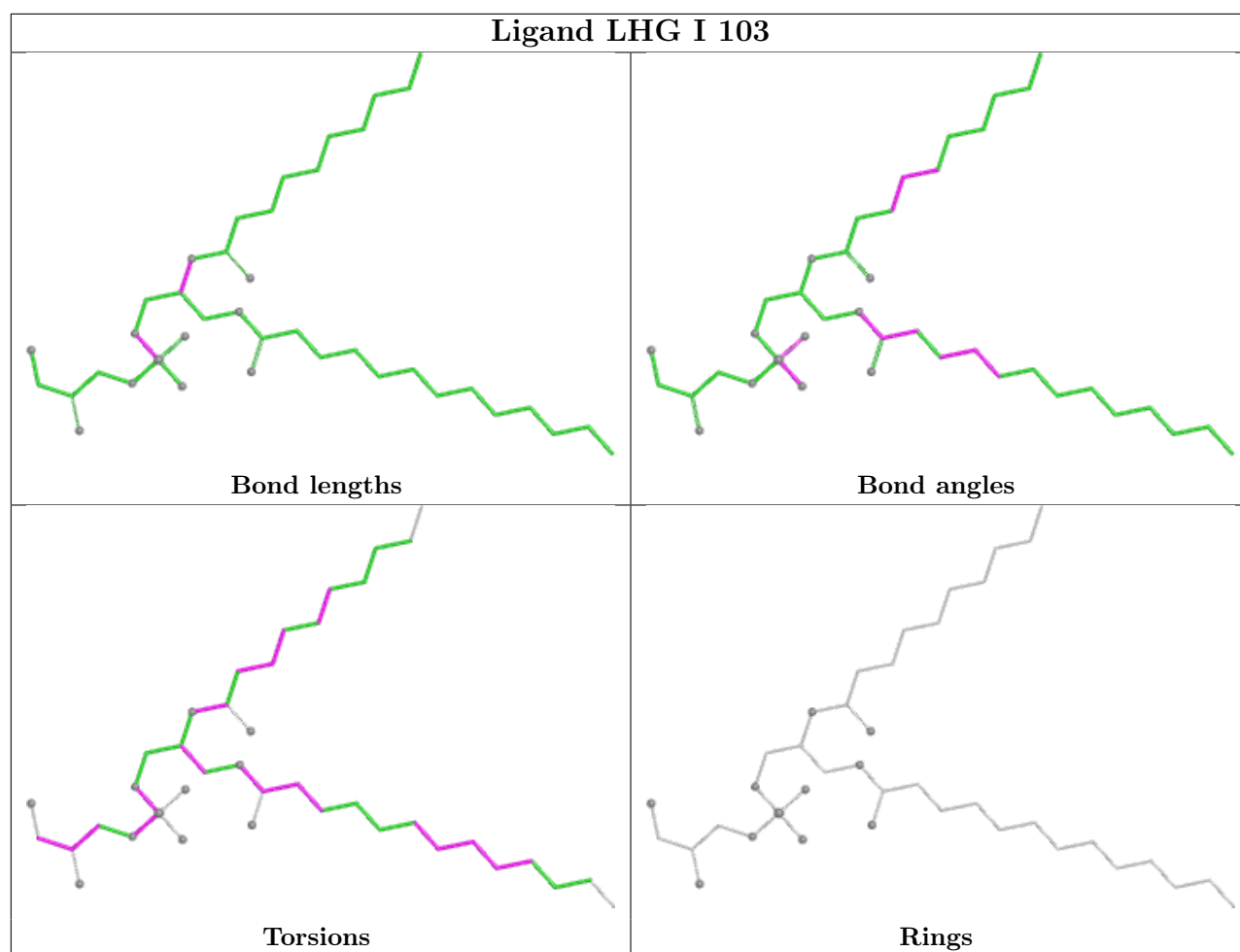
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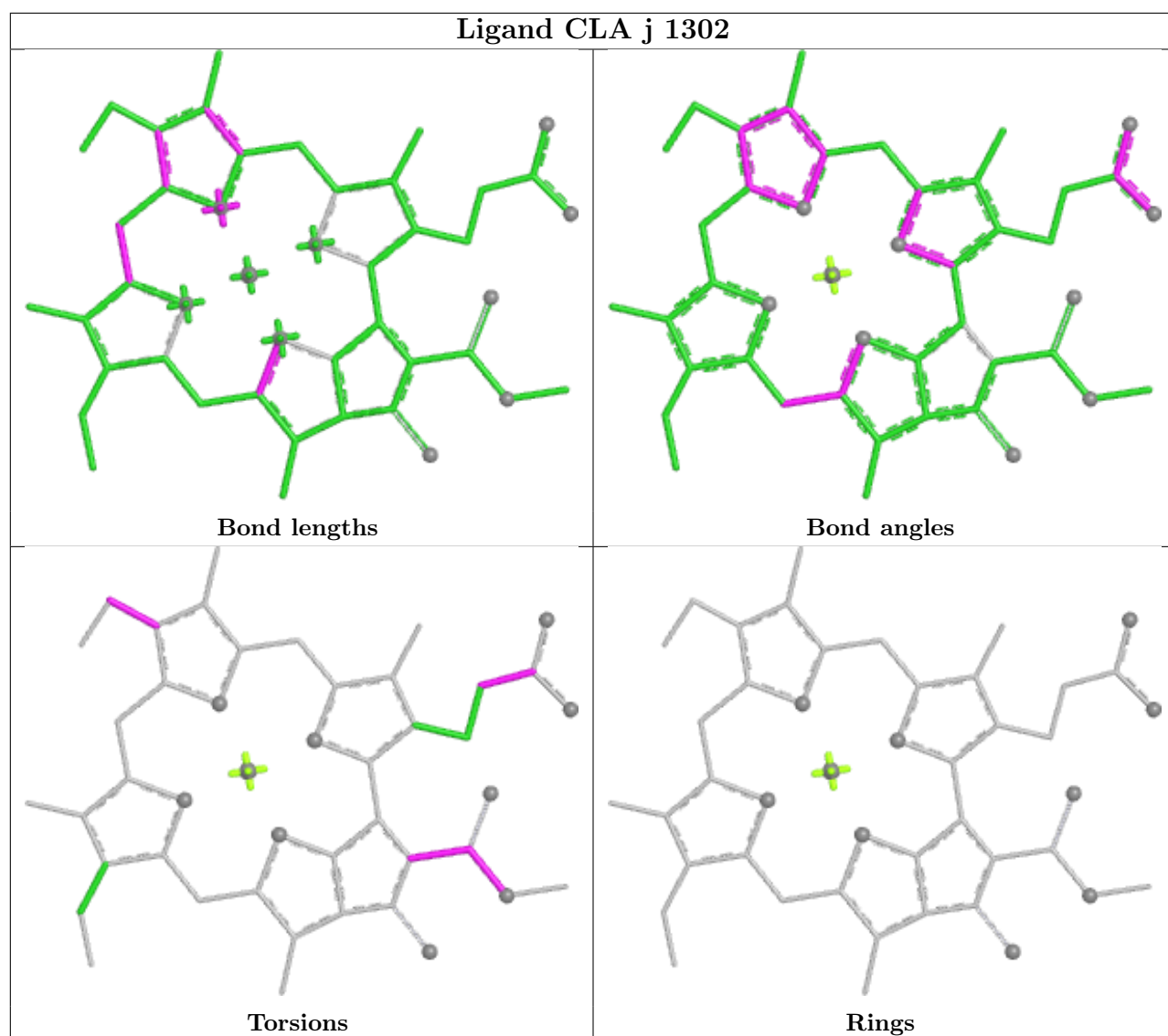
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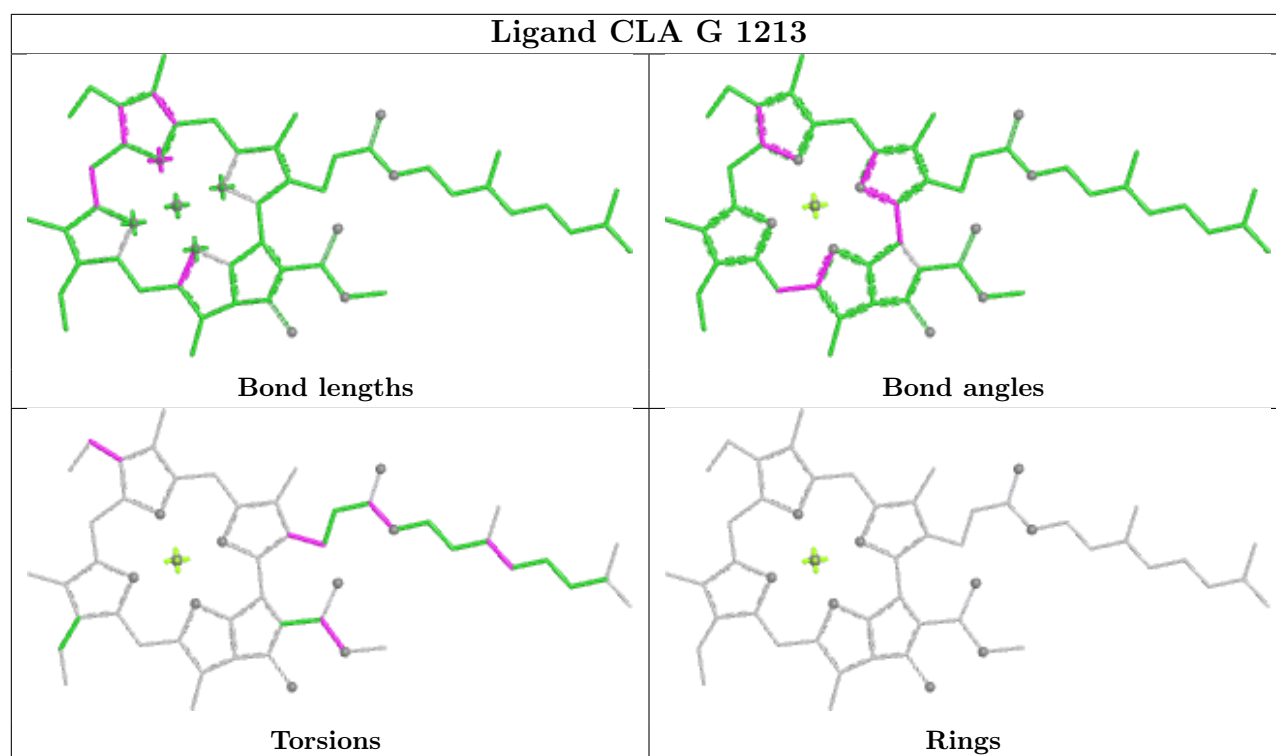
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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16	o	514	CLA	1	0
16	H	1123	CLA	2	0
16	b	1225	CLA	5	0
16	y	502	CLA	2	0
16	b	1219	CLA	1	0
19	Z	604	BCR	1	0
19	b	4017	BCR	1	0
19	H	4007	BCR	1	0
16	B	1214	CLA	4	0
16	G	1238	CLA	2	0
16	g	508	CLA	3	0
16	X	517	CLA	1	0
16	o	512	CLA	3	0
16	n	512	CLA	1	0
16	a	1101	CLA	5	0
16	u	507	CLA	1	0
16	a	1125	CLA	1	0
16	H	1116	CLA	3	0
16	q	510	CLA	7	0
16	b	1208	CLA	2	0
16	w	513	CLA	1	0
16	G	1210	CLA	6	0
16	X	508	CLA	2	0
16	p	516	CLA	1	0
16	a	1116	CLA	4	0
14	a	4101	LMG	1	0
16	H	1137	CLA	5	0
16	h	510	CLA	6	0
16	B	1205	CLA	4	0
16	u	505	CLA	3	0
16	k	4002	CLA	1	0
16	g	504	CLA	2	0
16	u	503	CLA	2	0
16	u	506	CLA	5	0
16	G	1023	CLA	3	0
16	A	1013	CLA	1	0
17	a	2001	PQN	4	0
16	a	1022	CLA	3	0
19	a	4008	BCR	3	0
16	n	515	CLA	2	0
16	B	1228	CLA	1	0

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

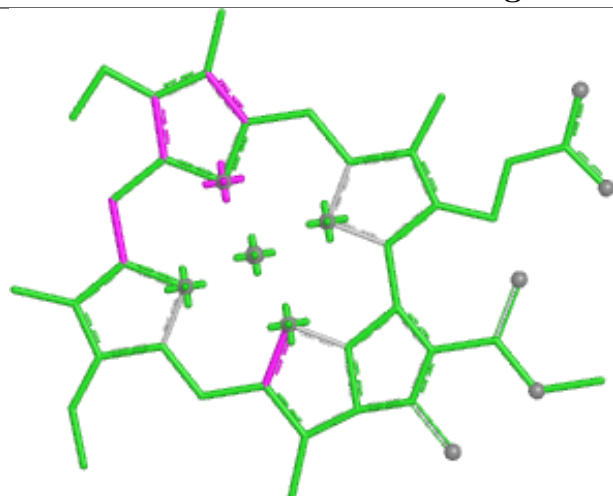




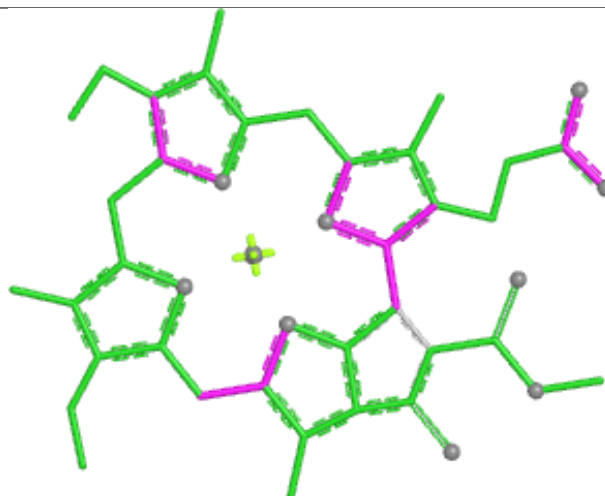




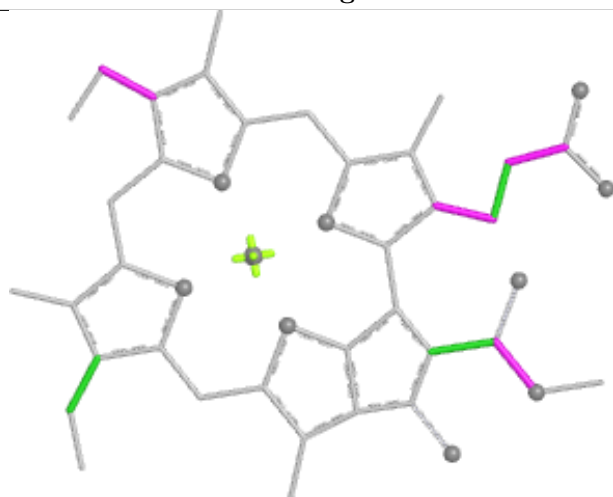
Ligand CLA G 1232



Bond lengths



Bond angles

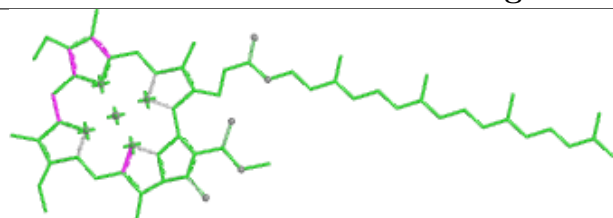


Torsions

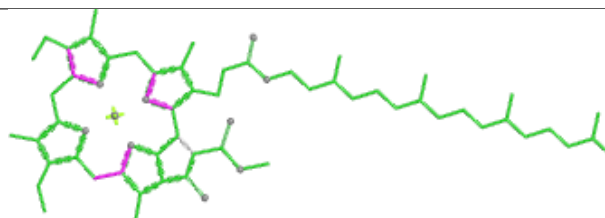


Rings

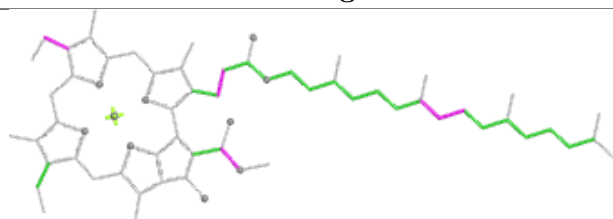
Ligand CLA A 1136



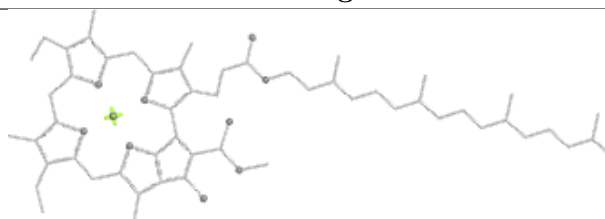
Bond lengths



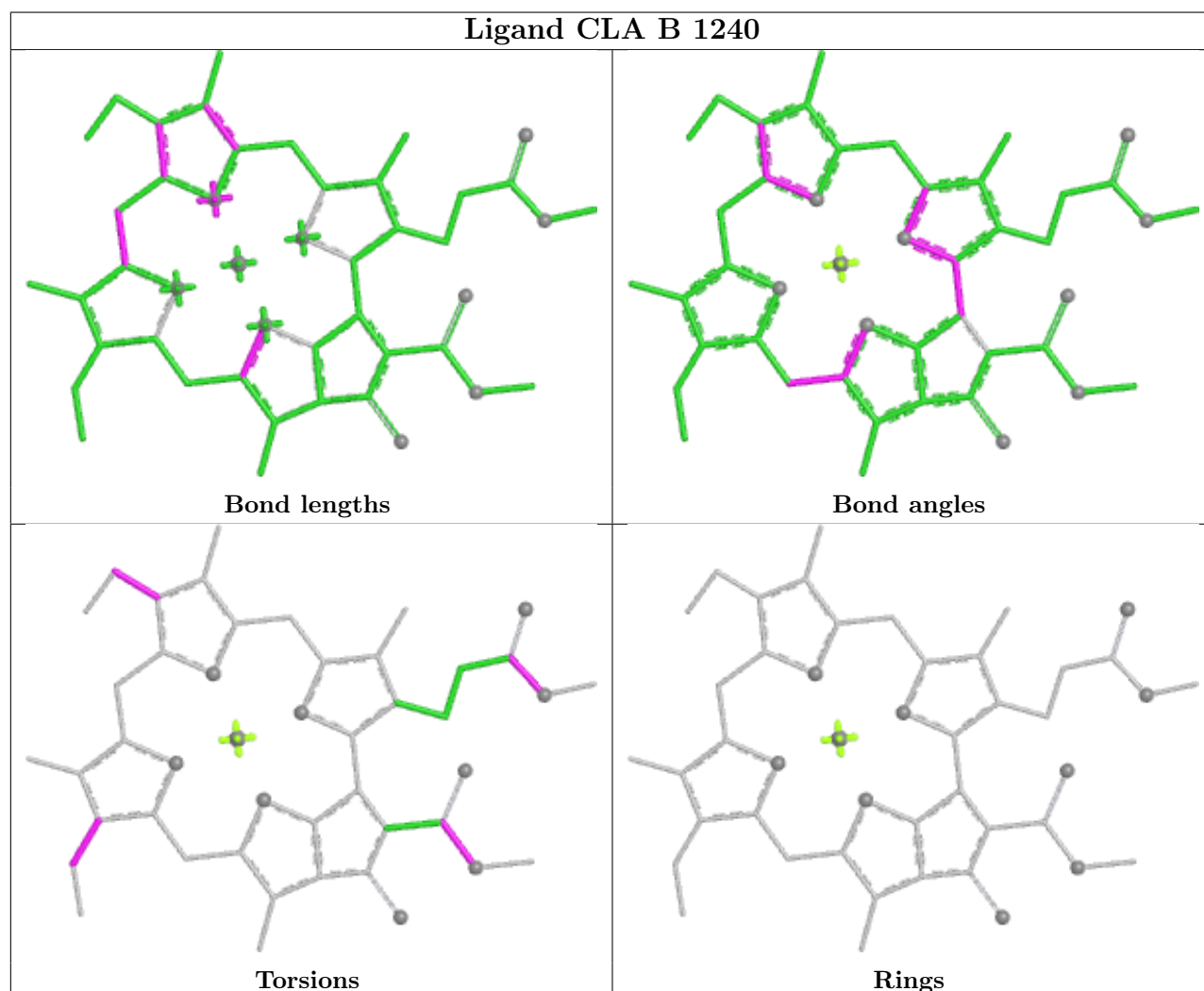
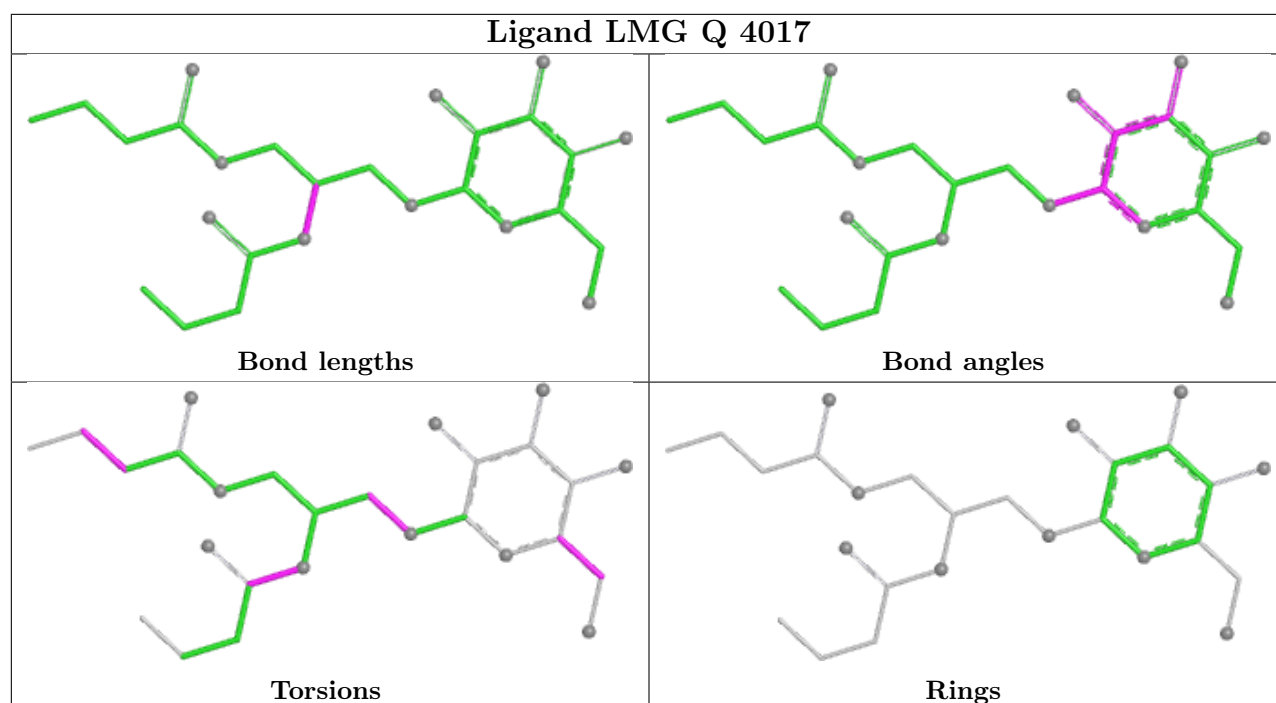
Bond angles

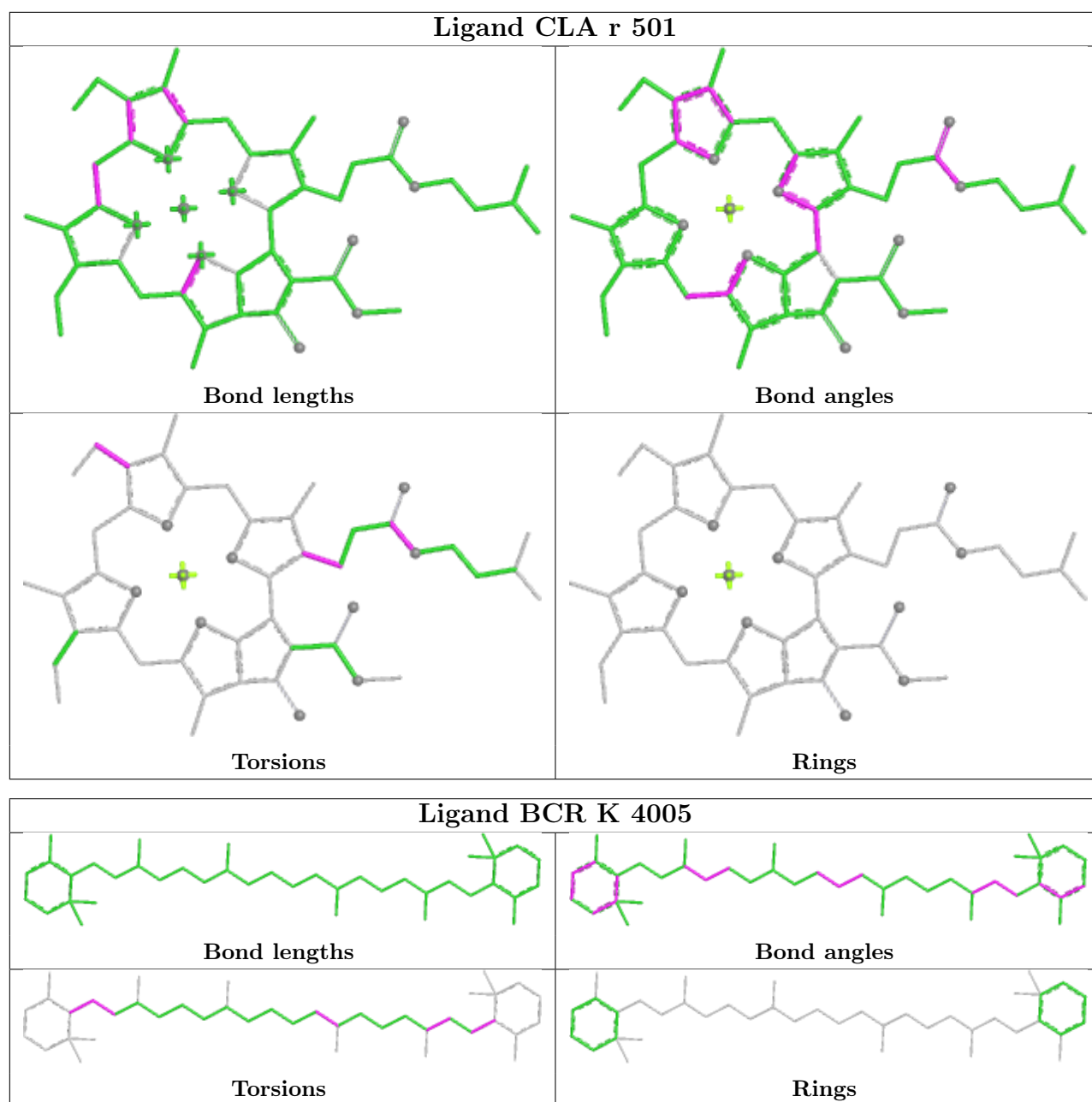


Torsions

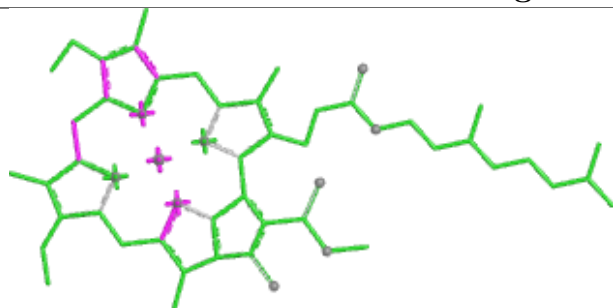


Rings

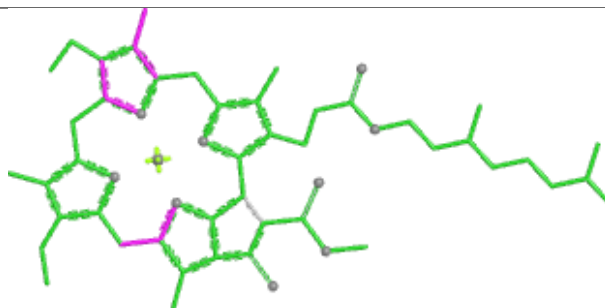




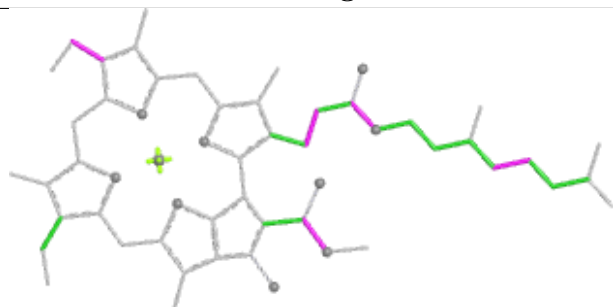
Ligand CLA w 517



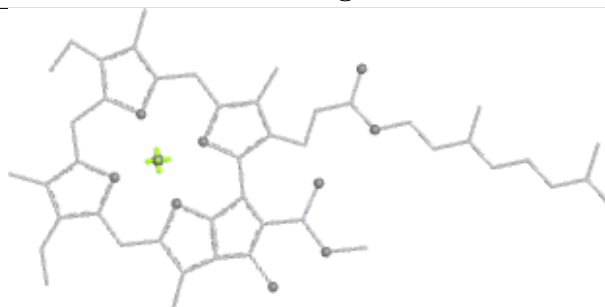
Bond lengths



Bond angles

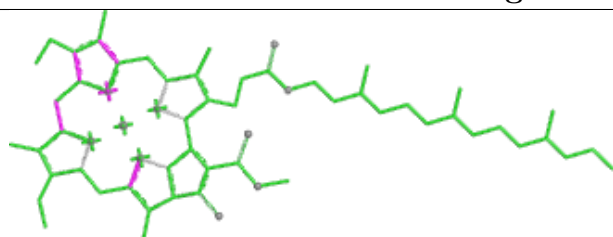


Torsions

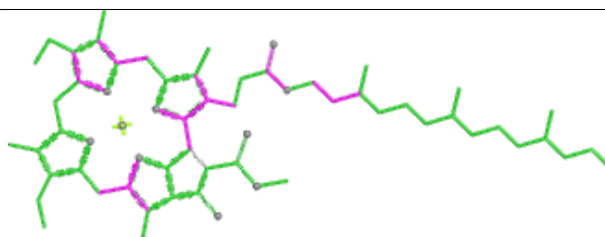


Rings

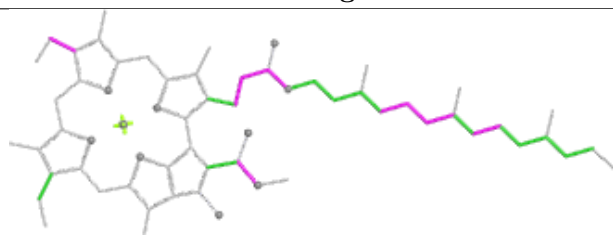
Ligand CLA B 1235



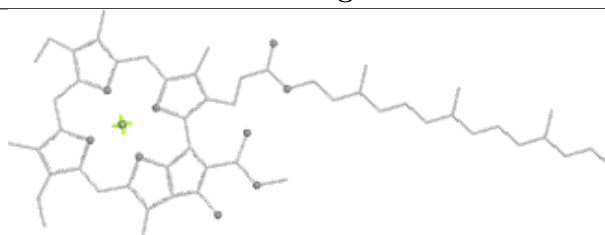
Bond lengths



Bond angles

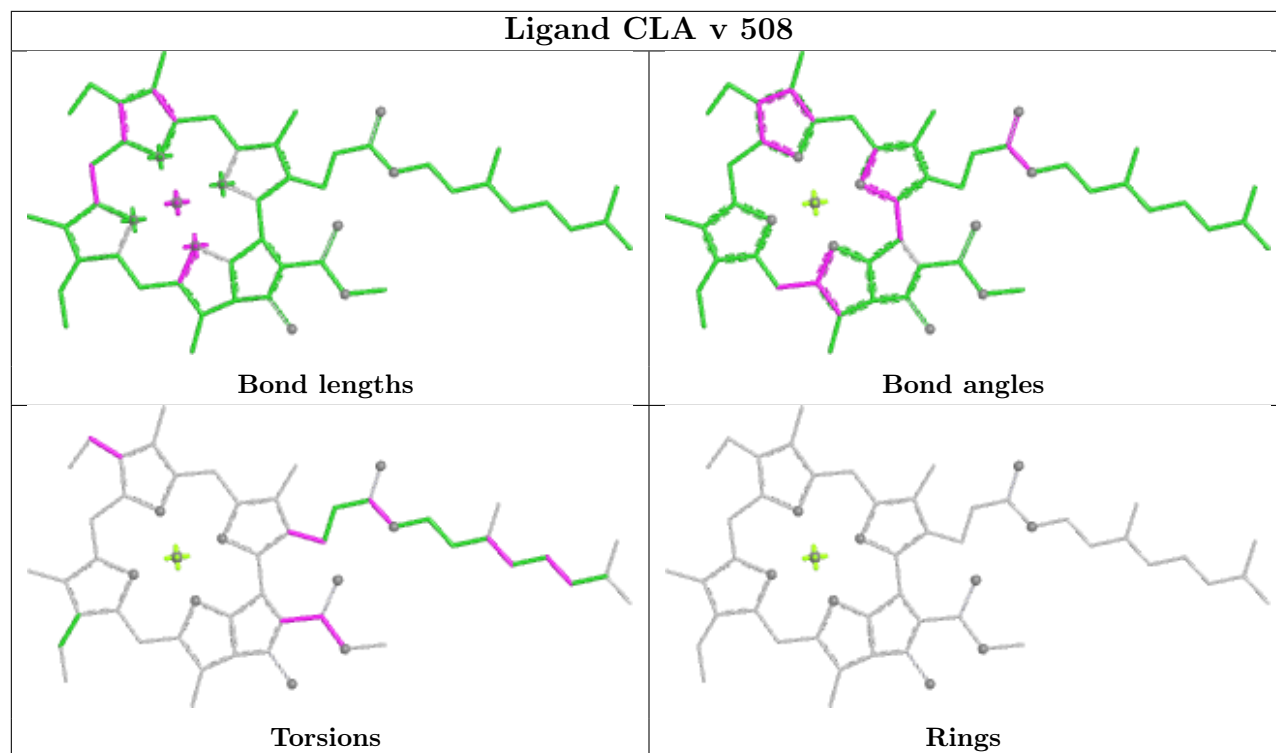


Torsions

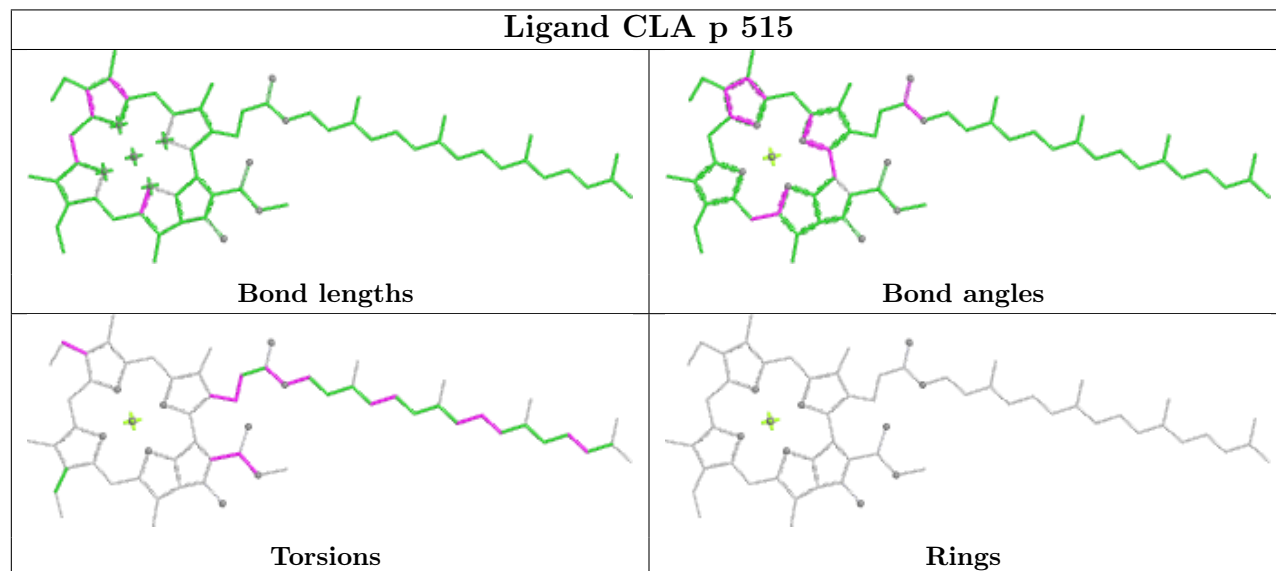


Rings

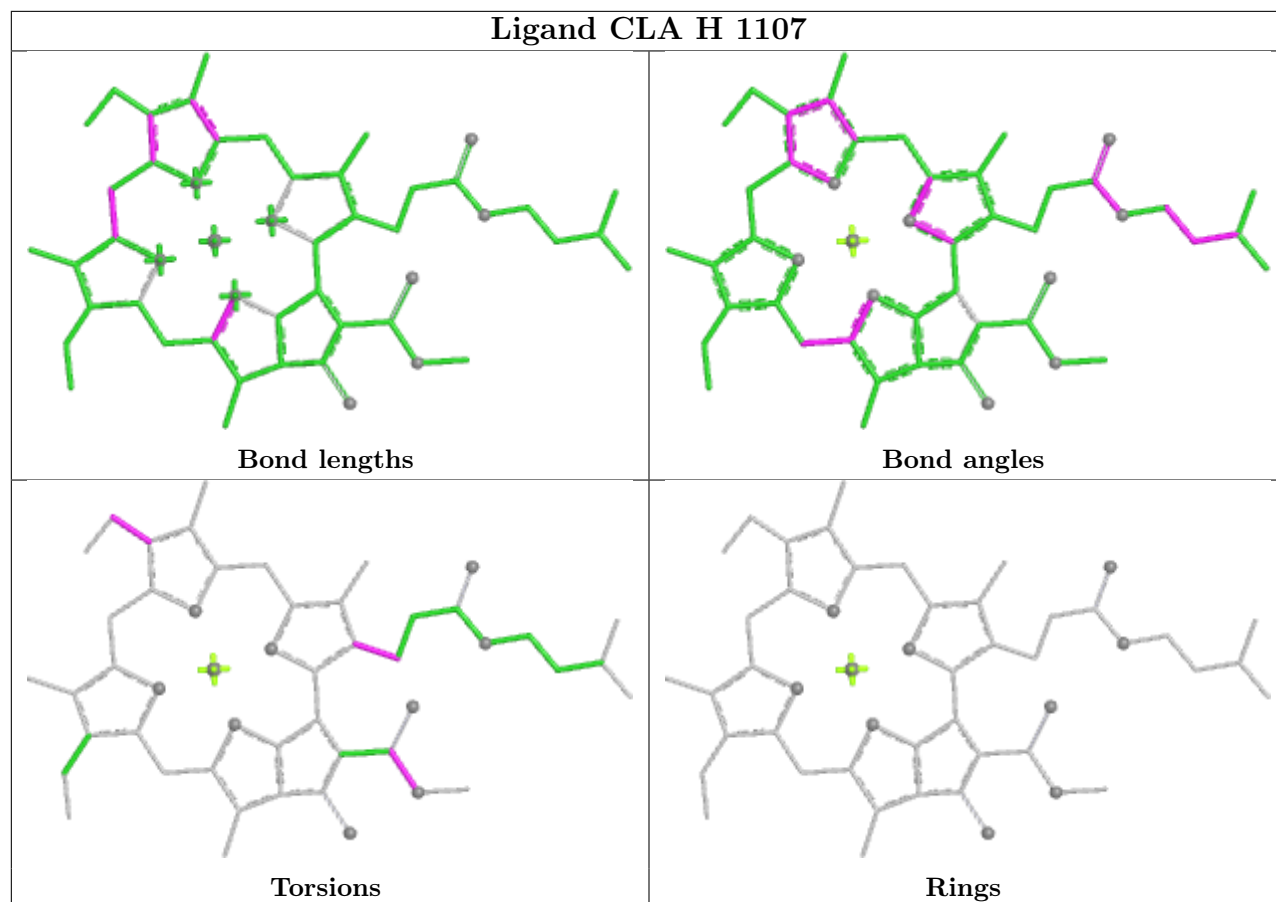
Ligand CLA v 508



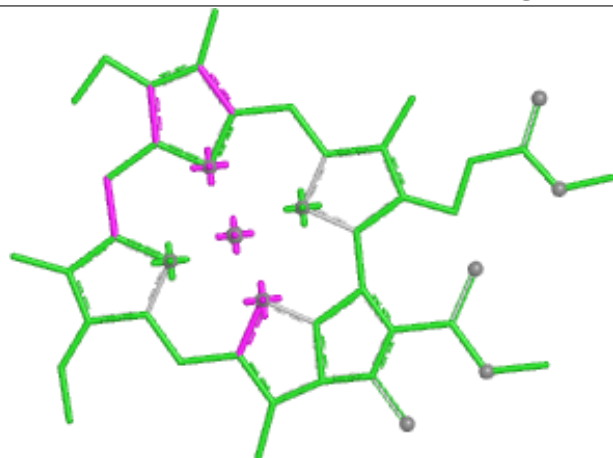
Ligand CLA p 515



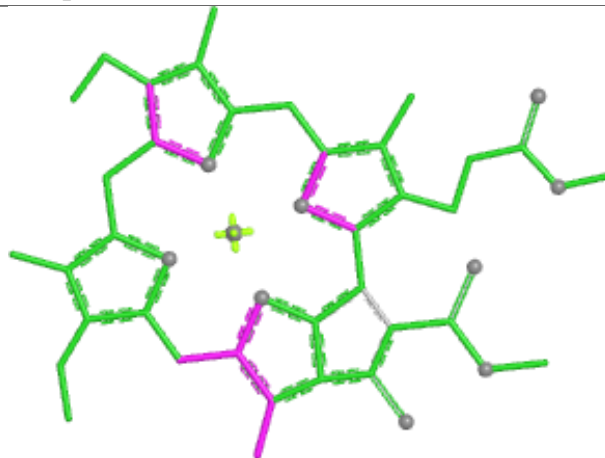
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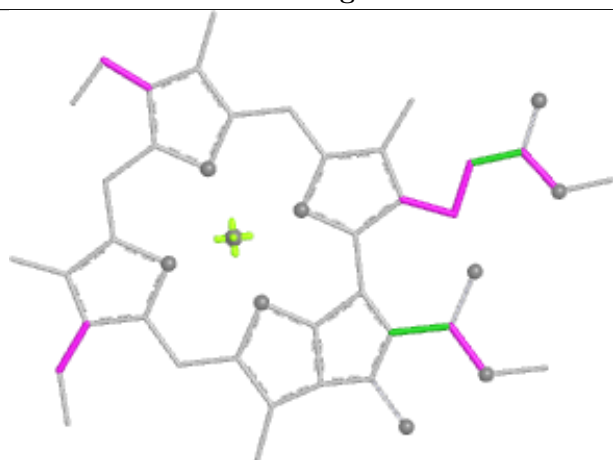
Ligand CLA q 503



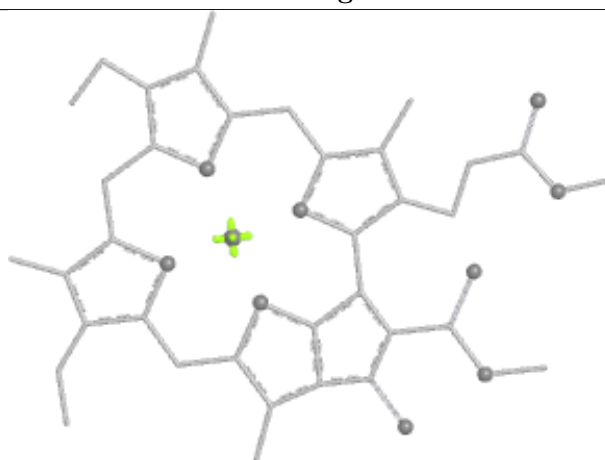
Bond lengths



Bond angles

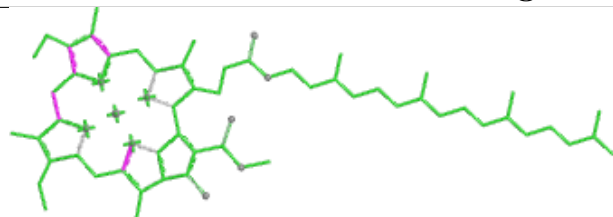


Torsions

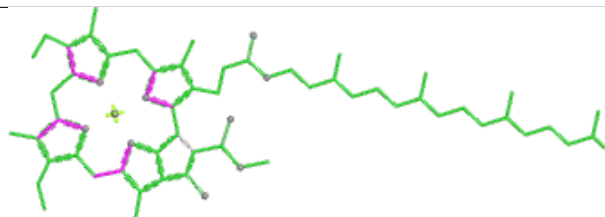


Rings

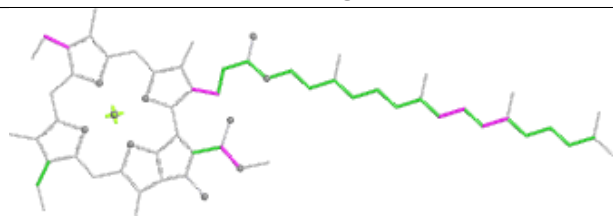
Ligand CLA u 511



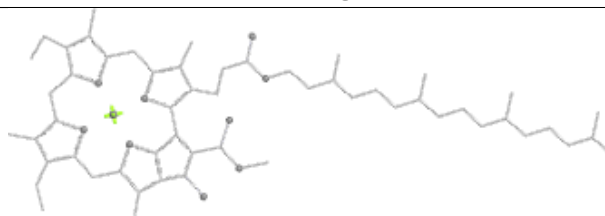
Bond lengths



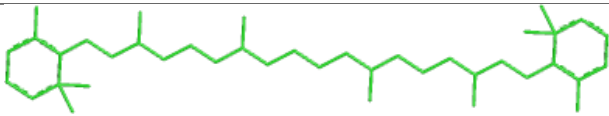
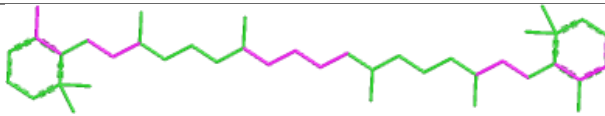
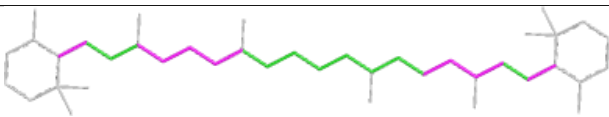
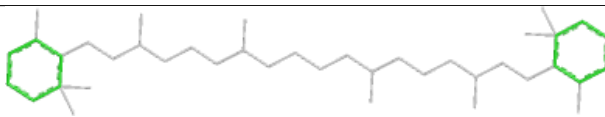
Bond angles

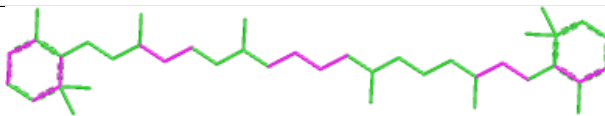
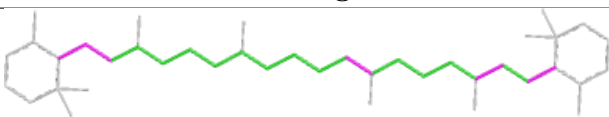
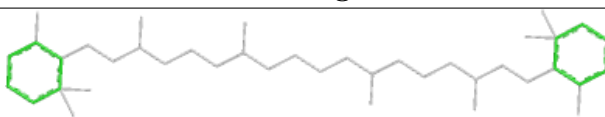


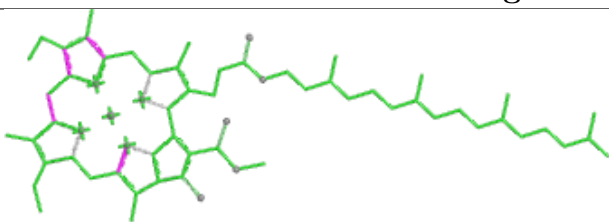
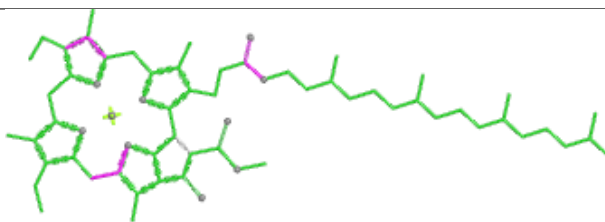
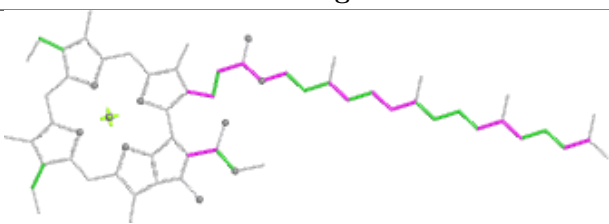
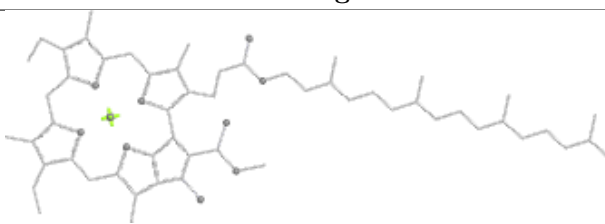
Torsions



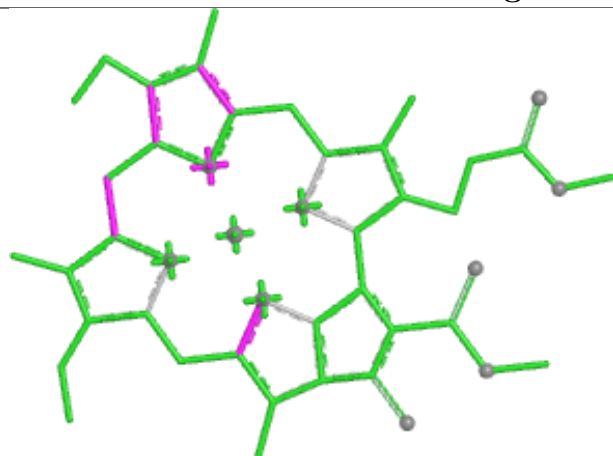
Rings

Ligand BCR g 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

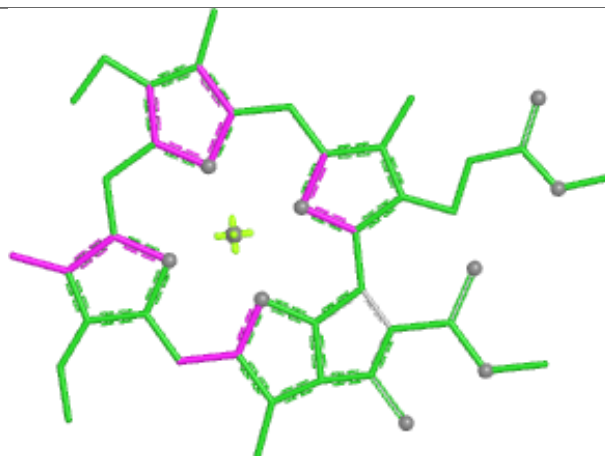
Ligand BCR T 4005	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1202	
	
Bond lengths	Bond angles
	
Torsions	Rings

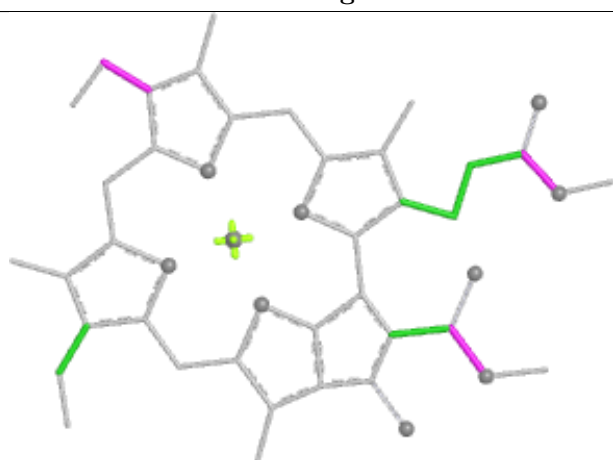
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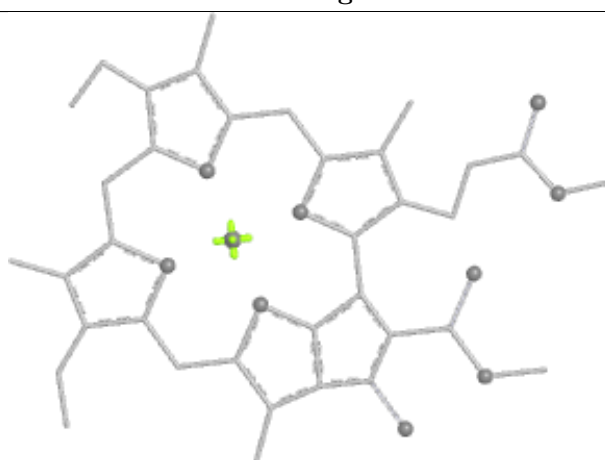
Bond lengths



Bond angles

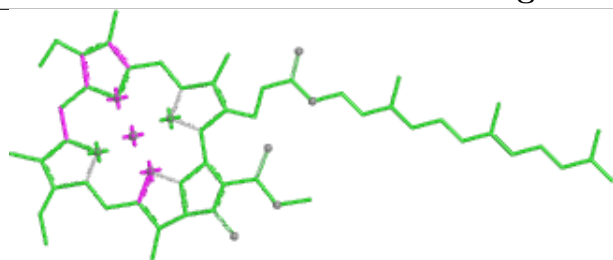


Torsions

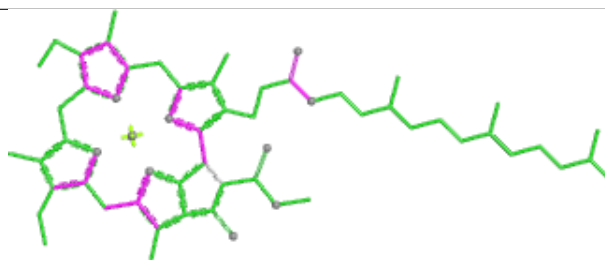


Rings

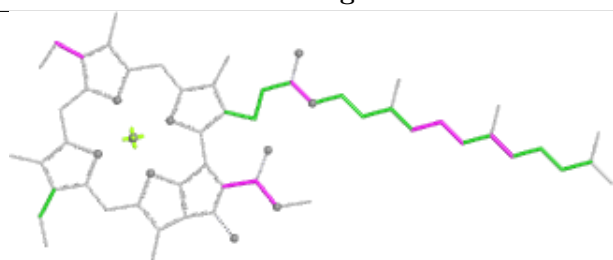
Ligand CLA h 506



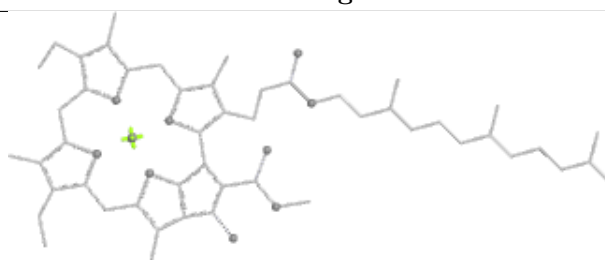
Bond lengths



Bond angles

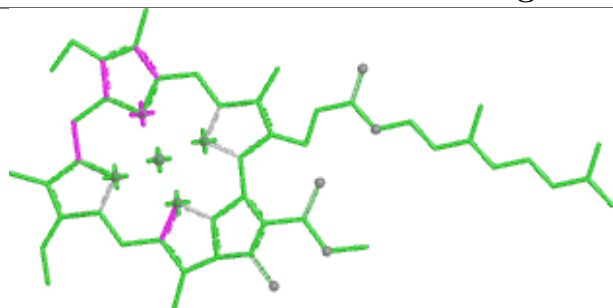


Torsions

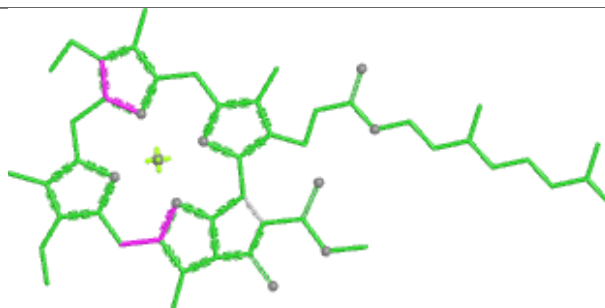


Rings

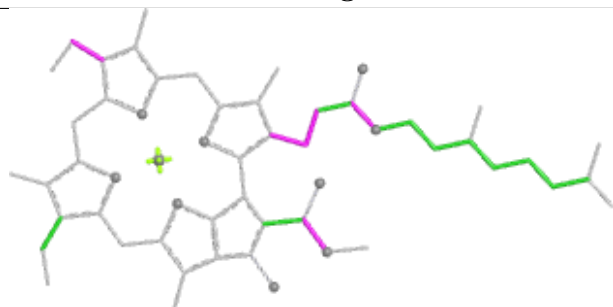
Ligand CLA n 508



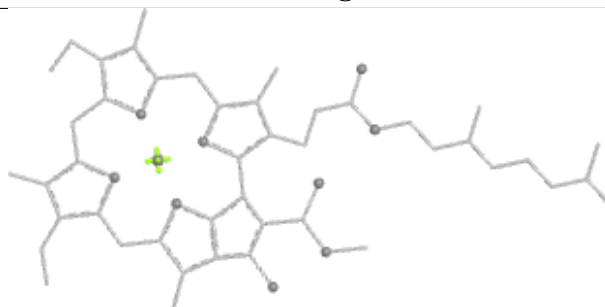
Bond lengths



Bond angles

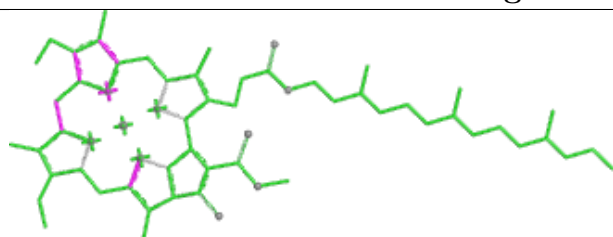


Torsions

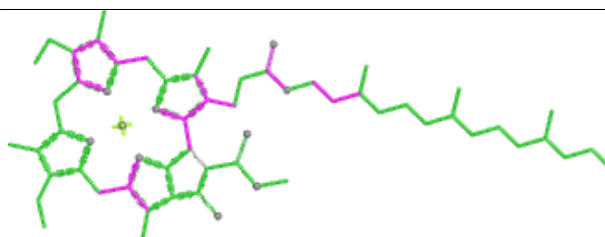


Rings

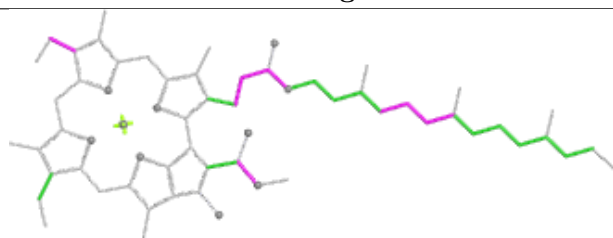
Ligand CLA G 1235



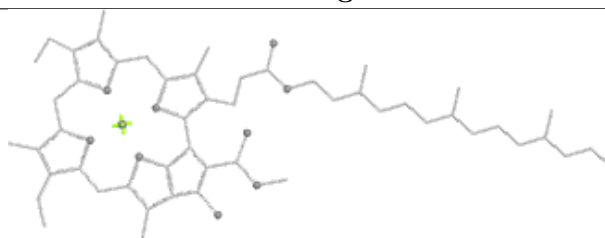
Bond lengths



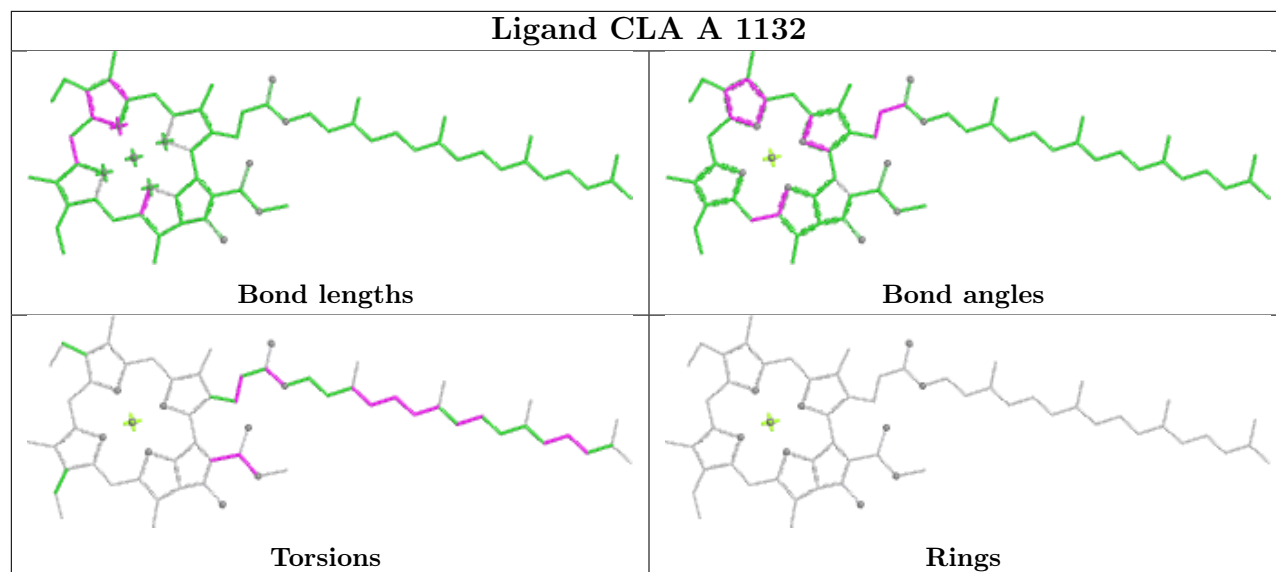
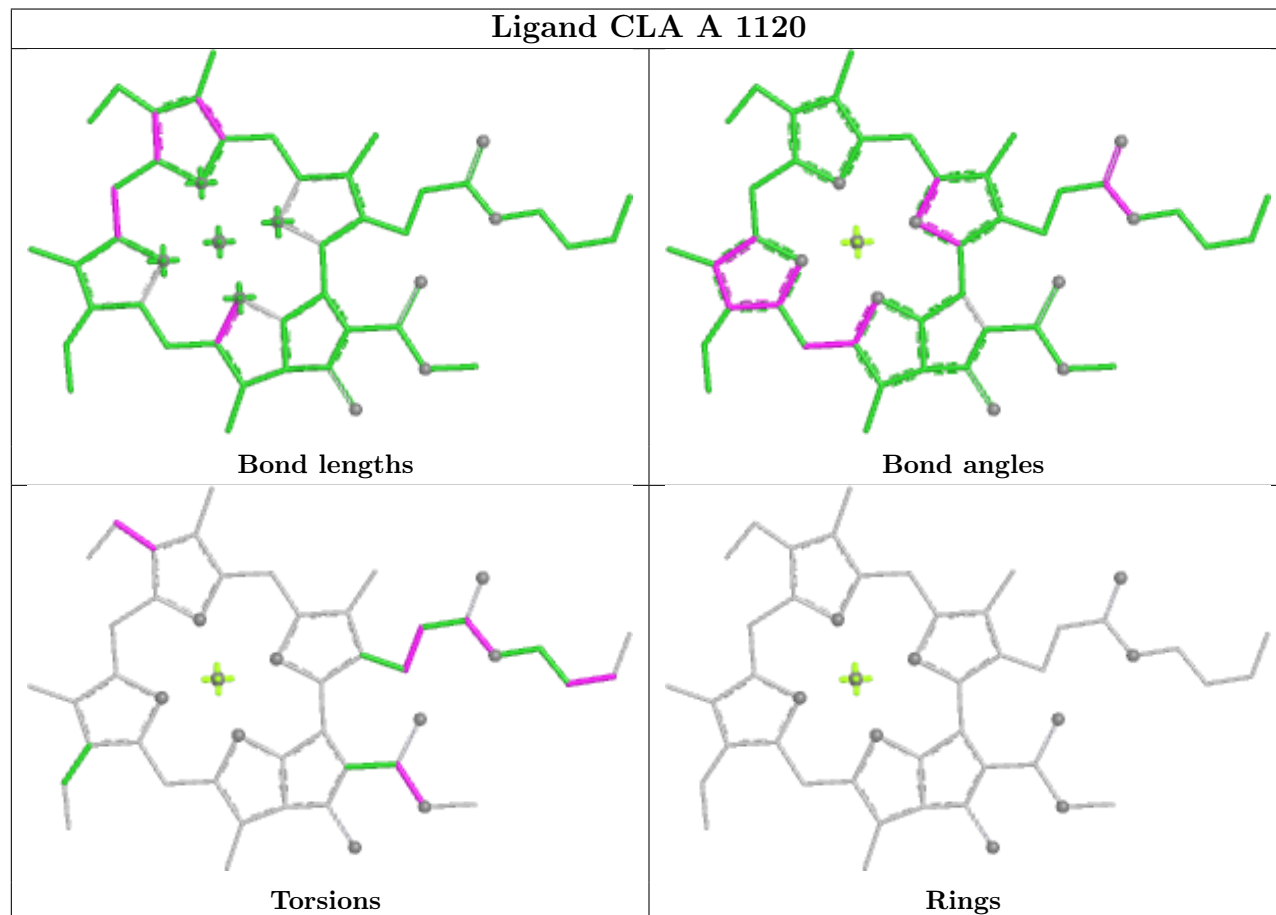
Bond angles

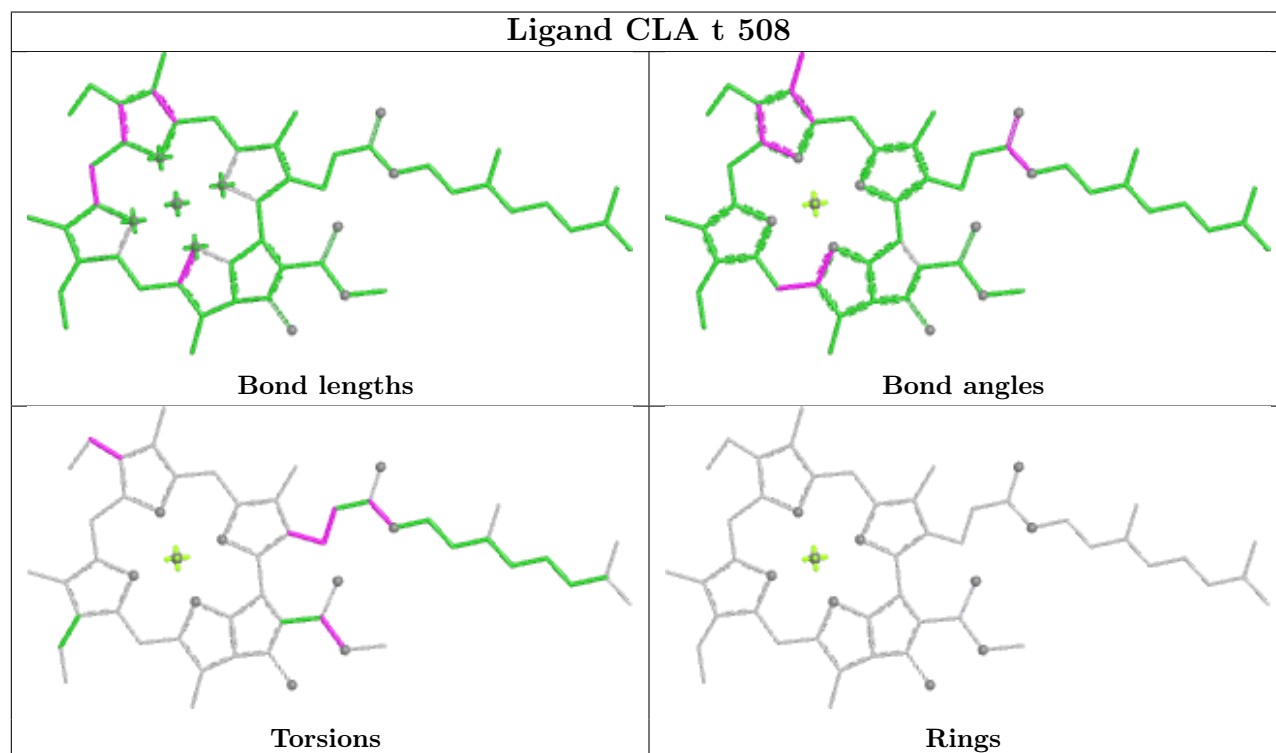
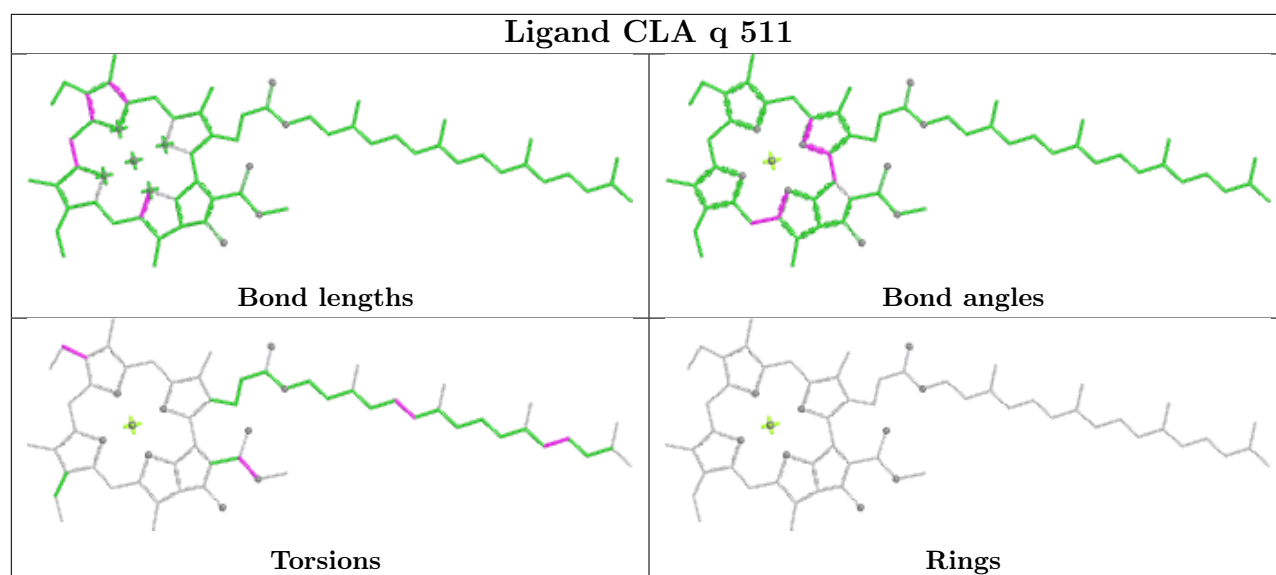


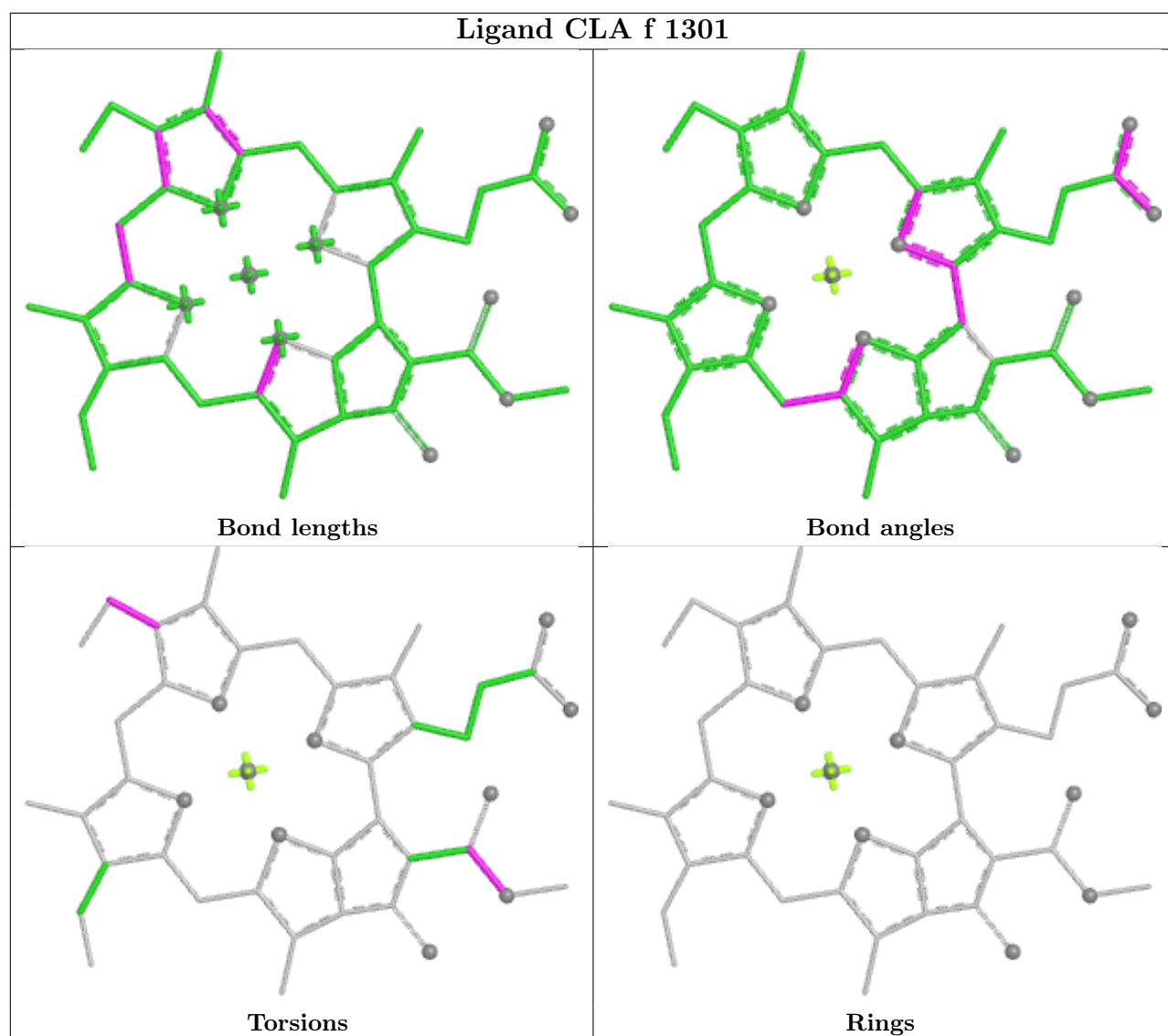
Torsions



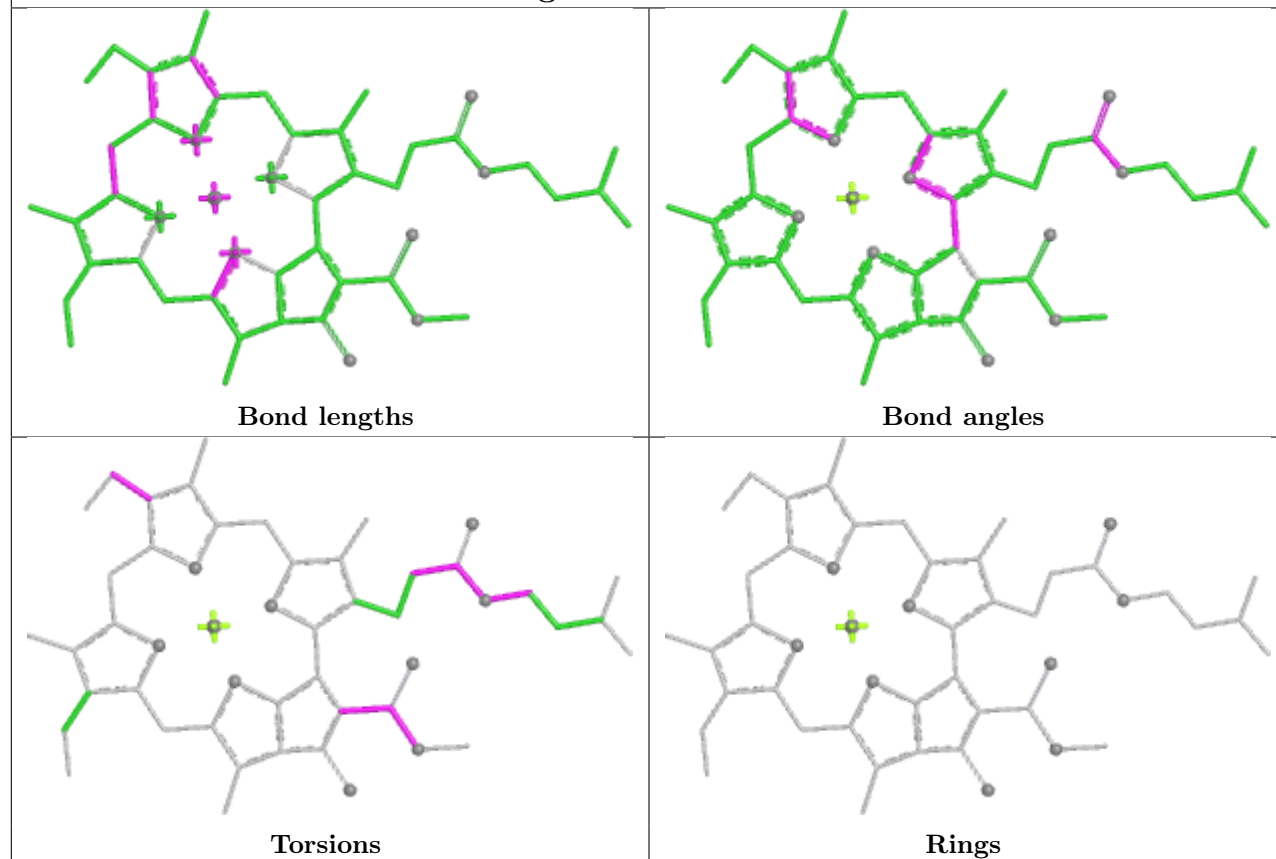
Rings

Ligand CLA A 1132**Ligand CLA A 1120**

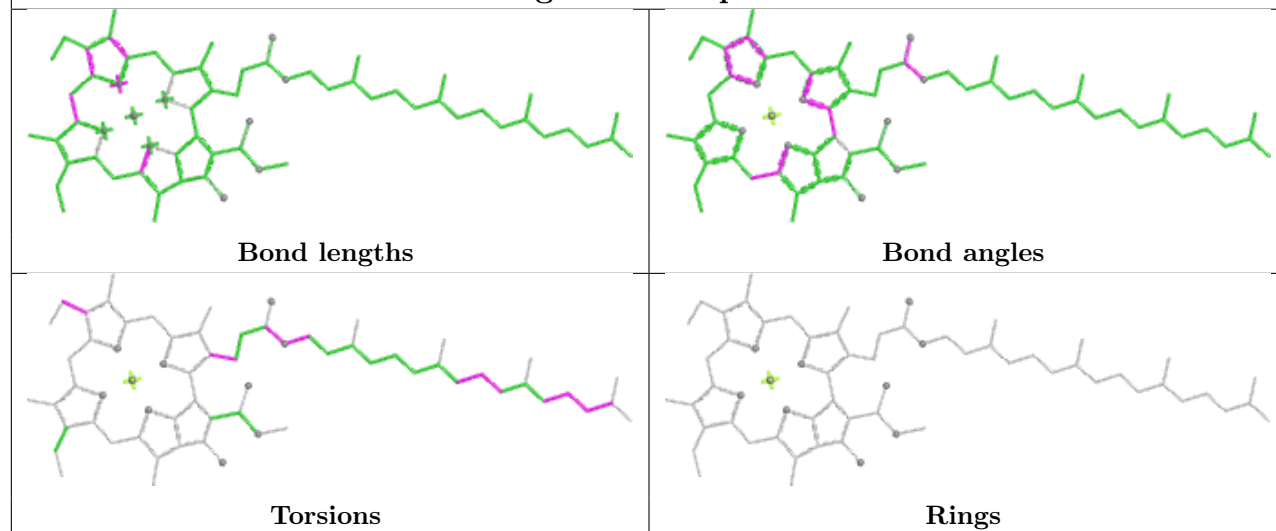


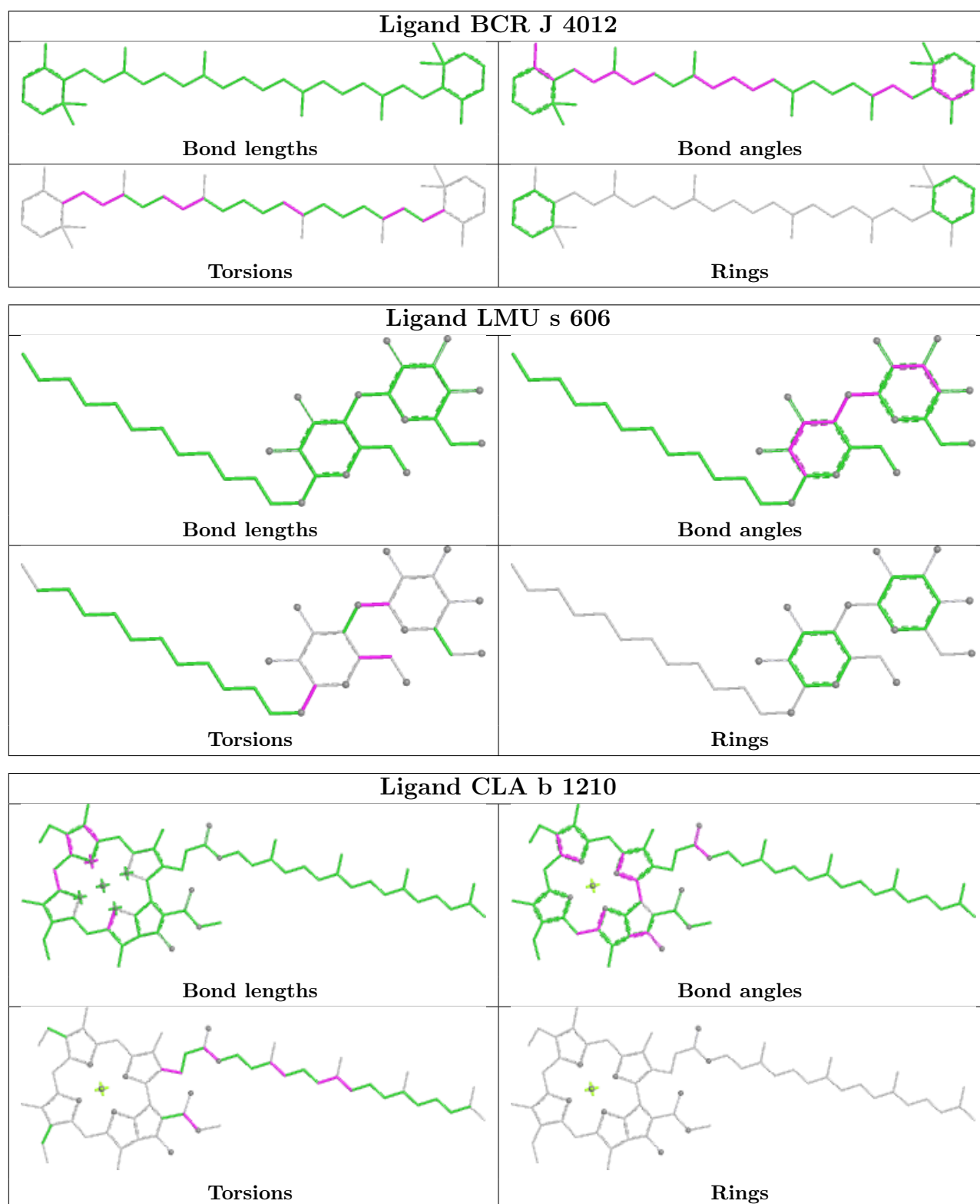


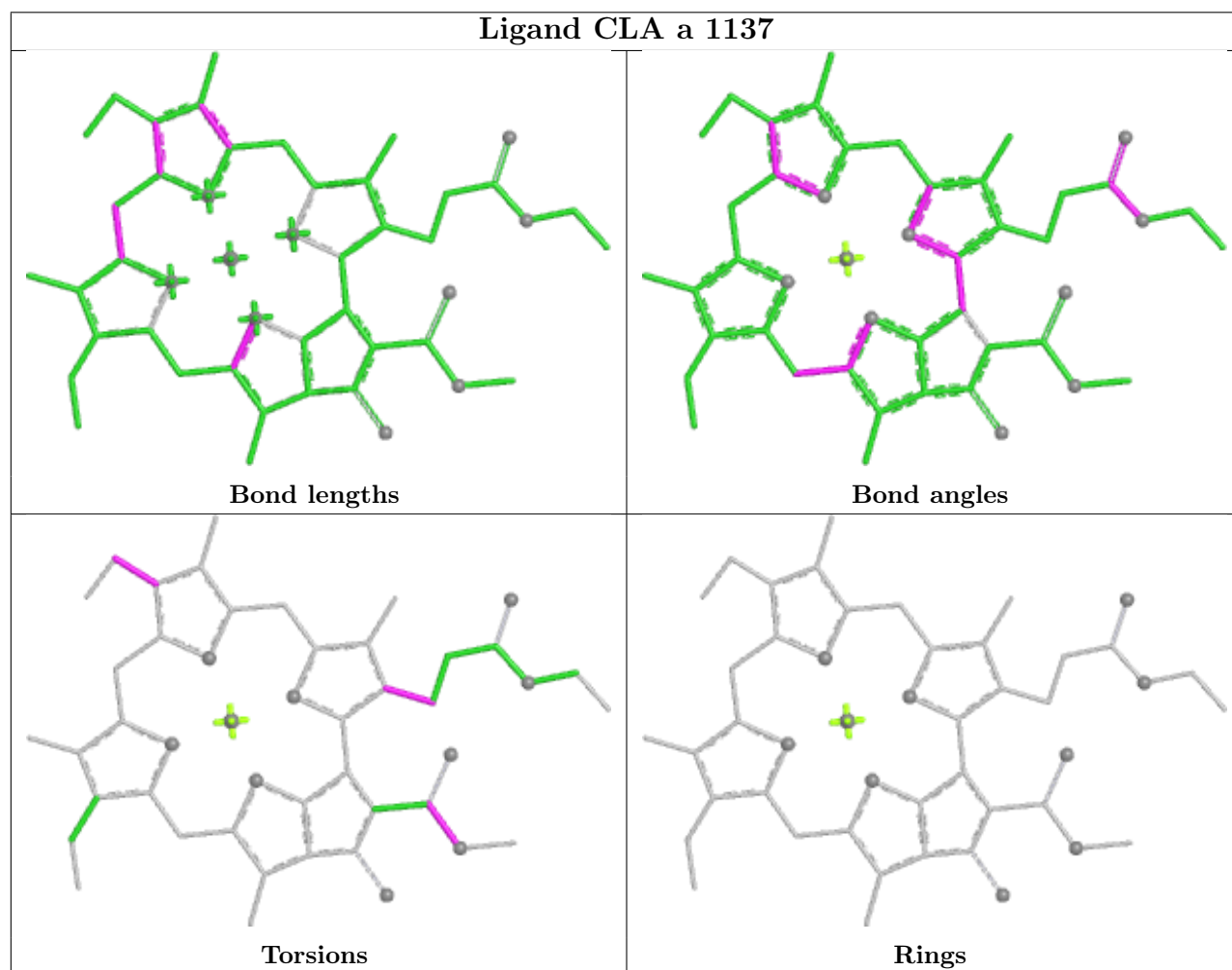
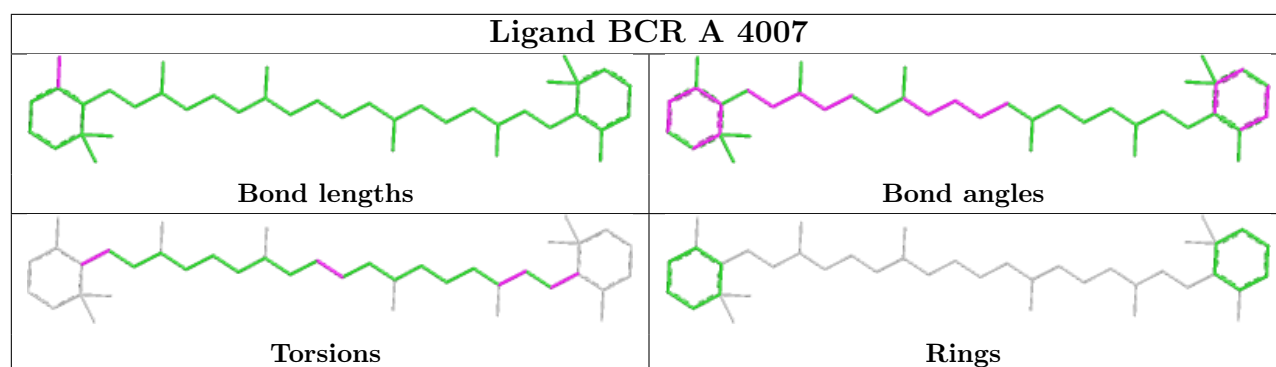
Ligand CLA t 502

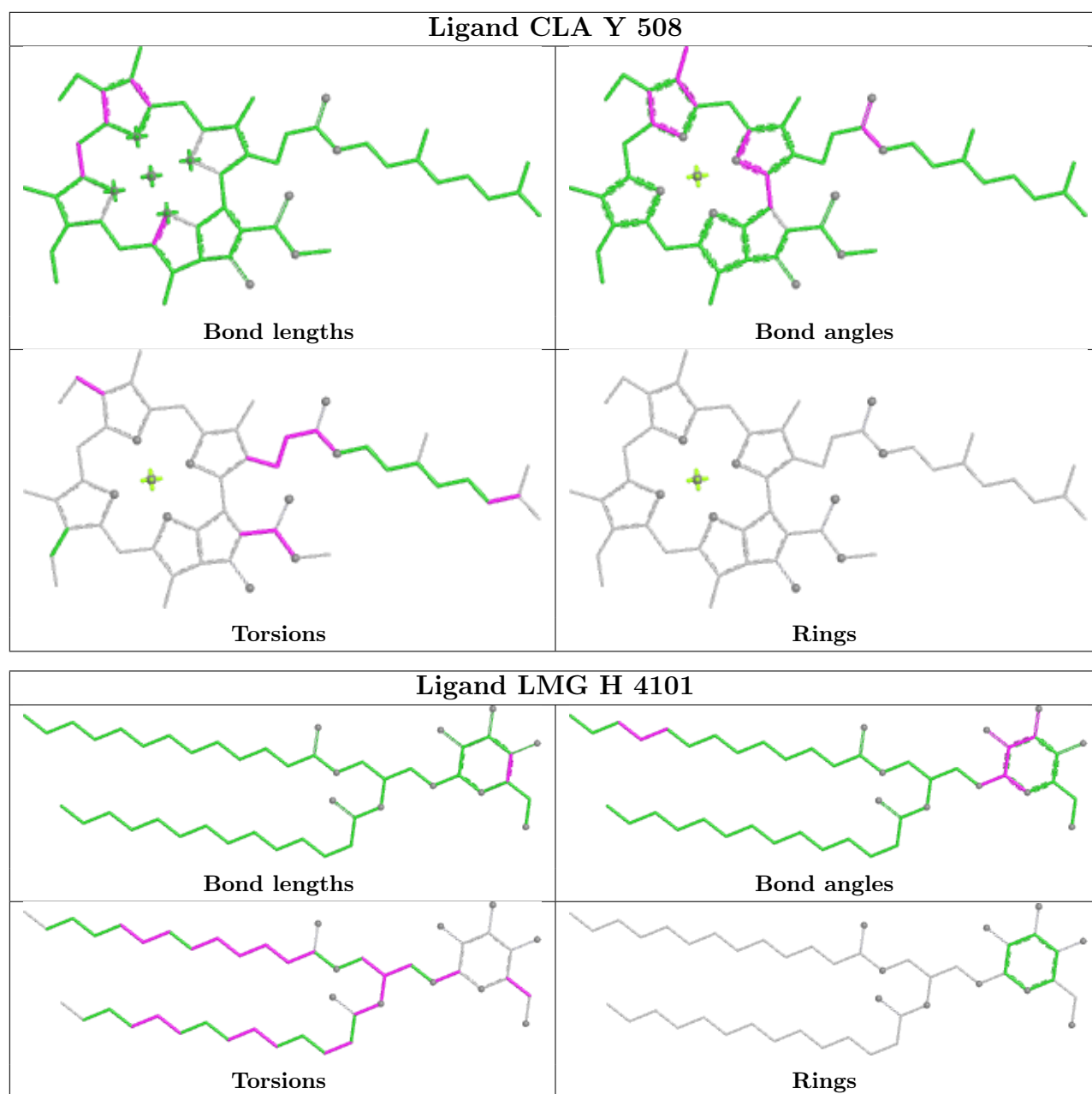


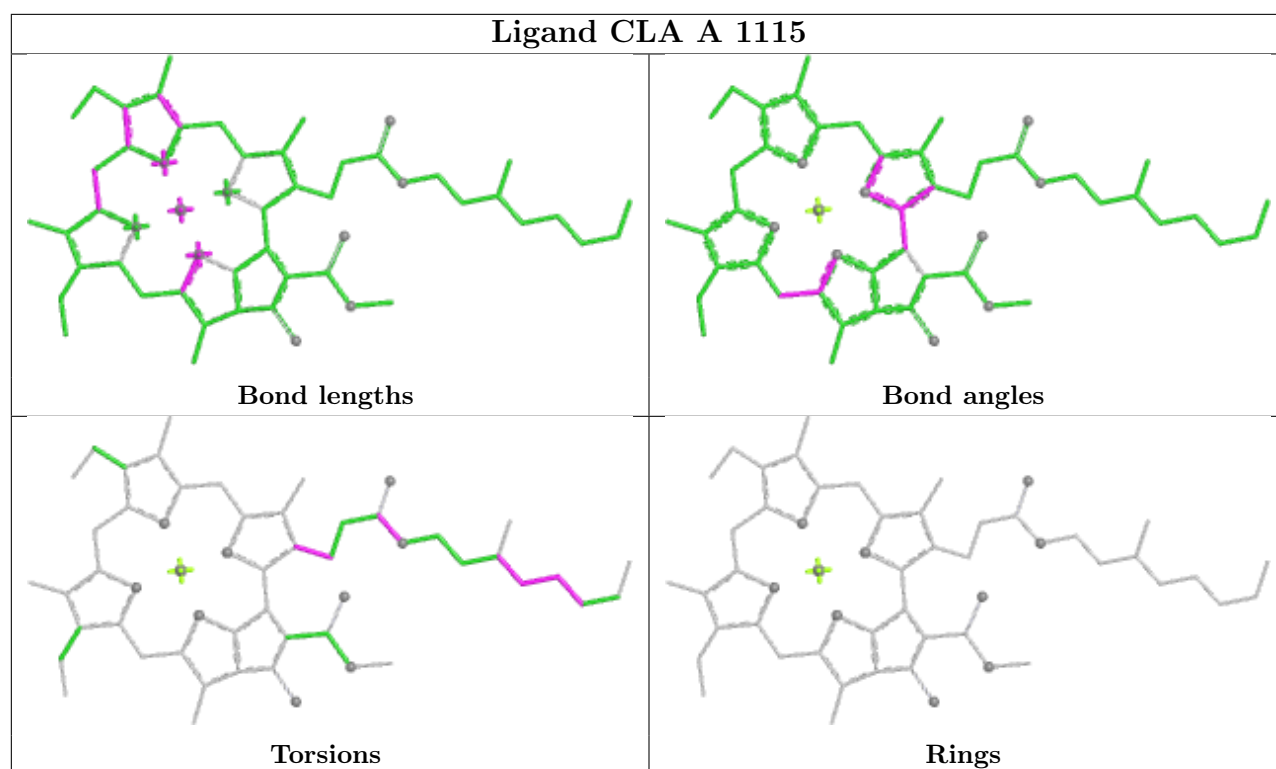
Ligand CLA q 509



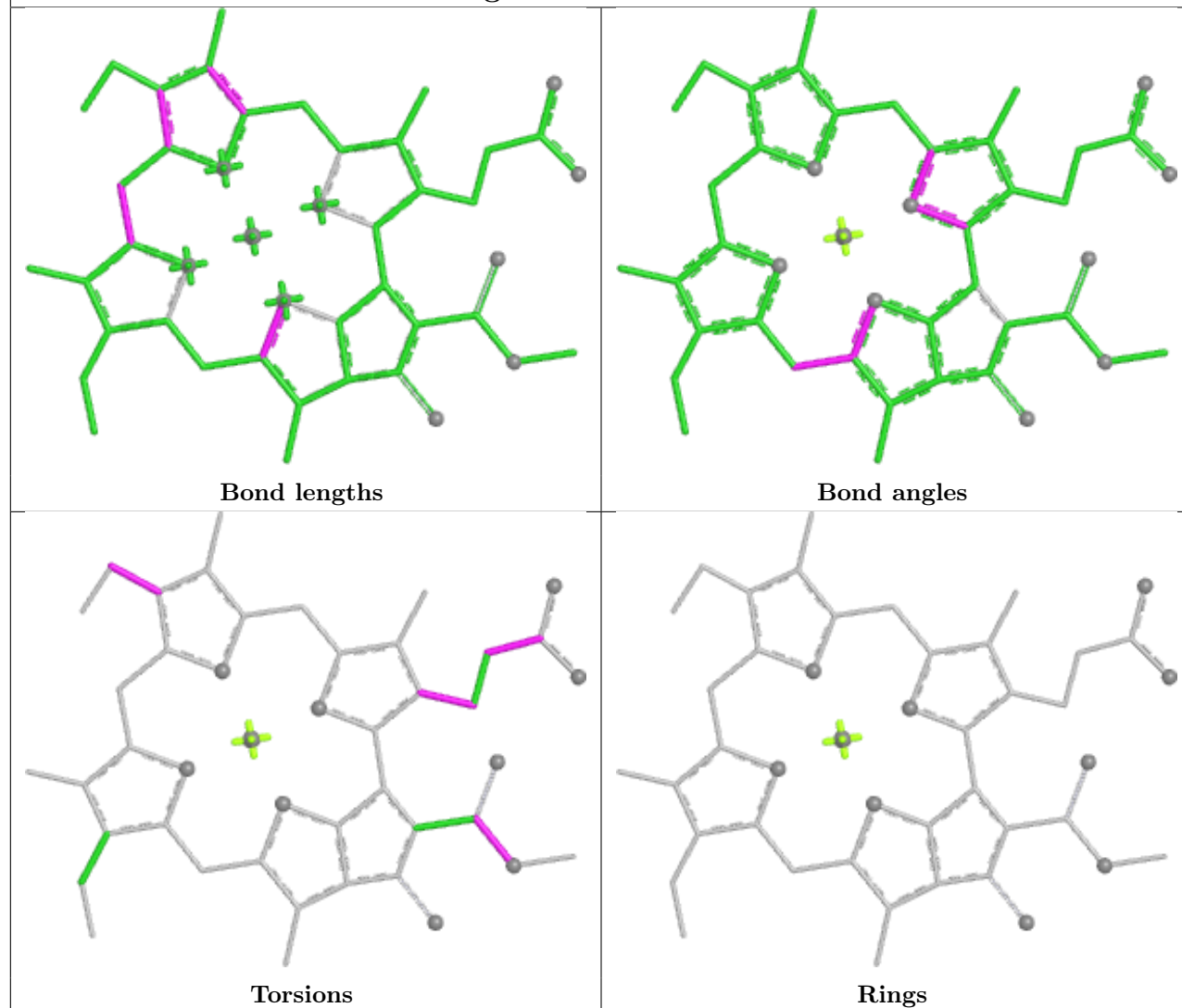




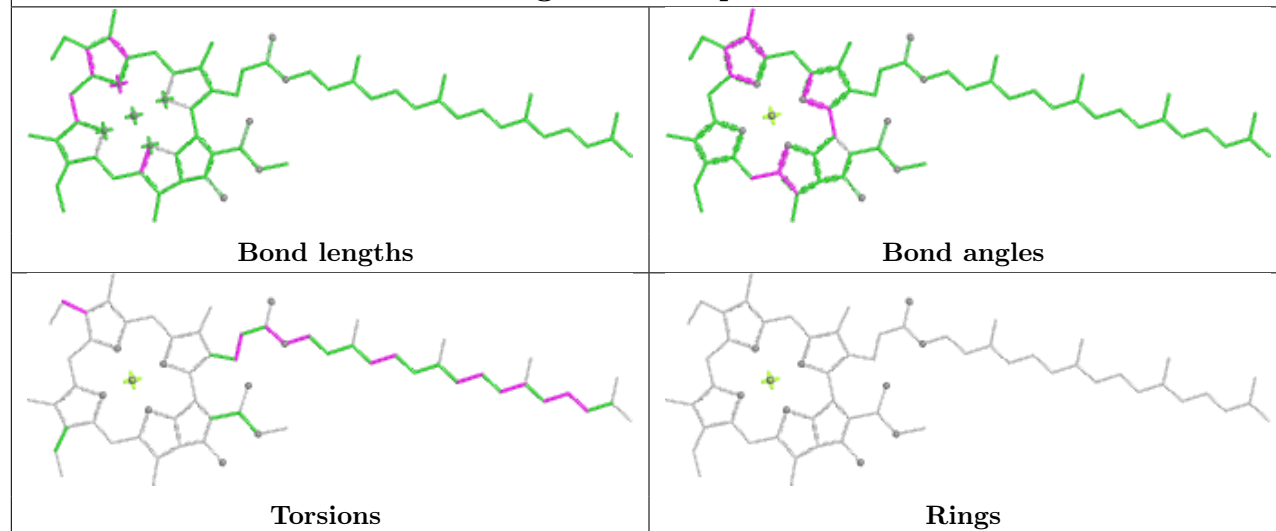


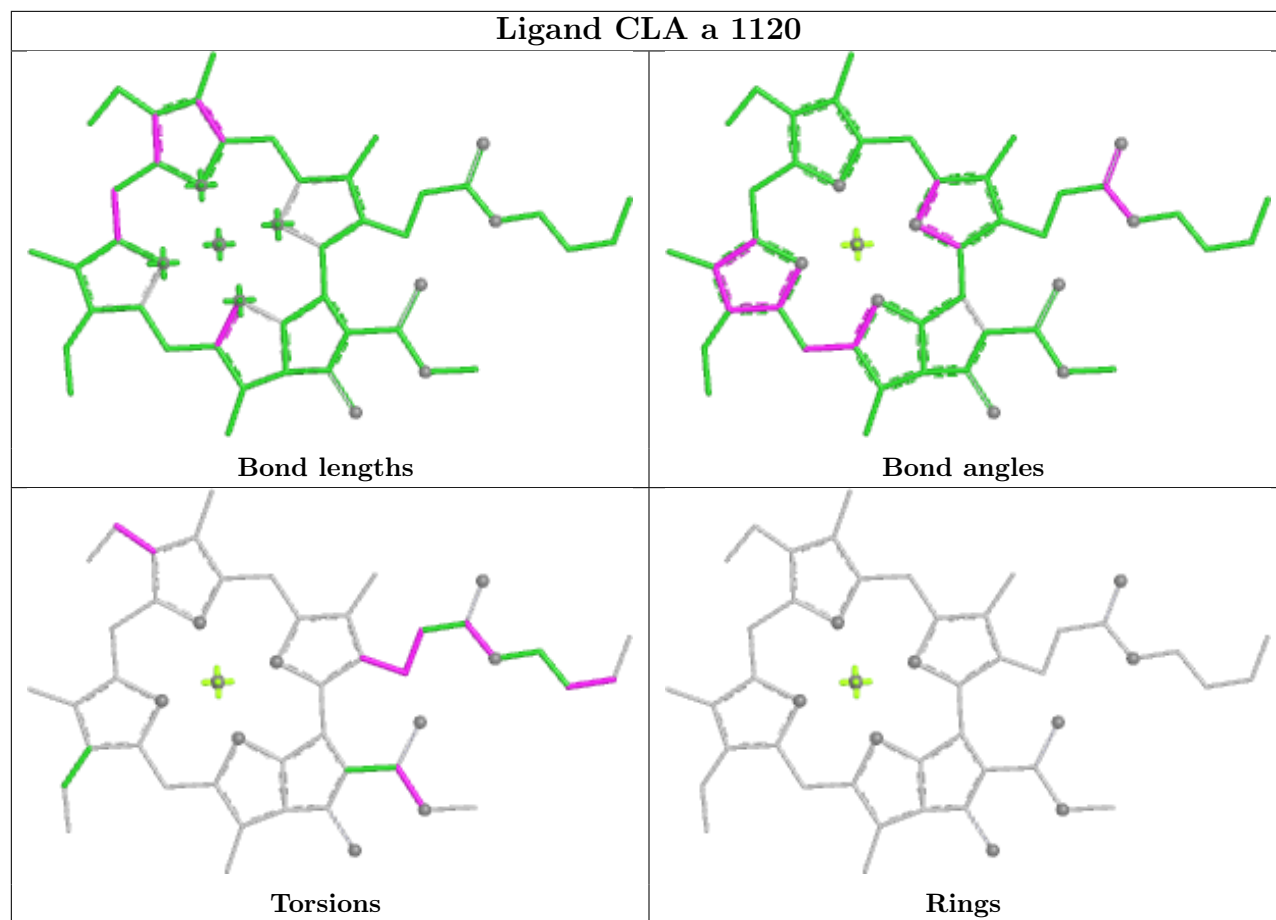


Ligand CLA A 1113

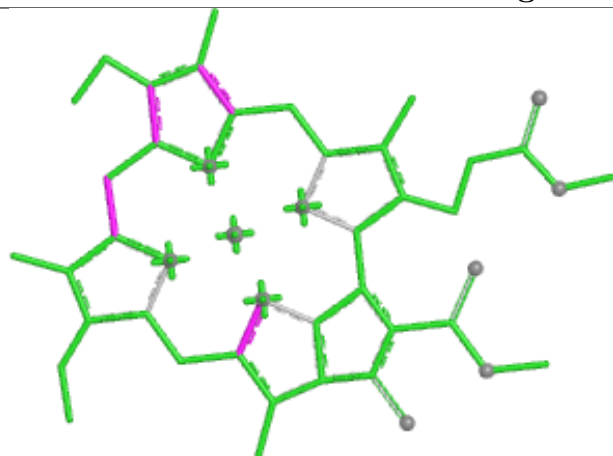


Ligand CLA q 515

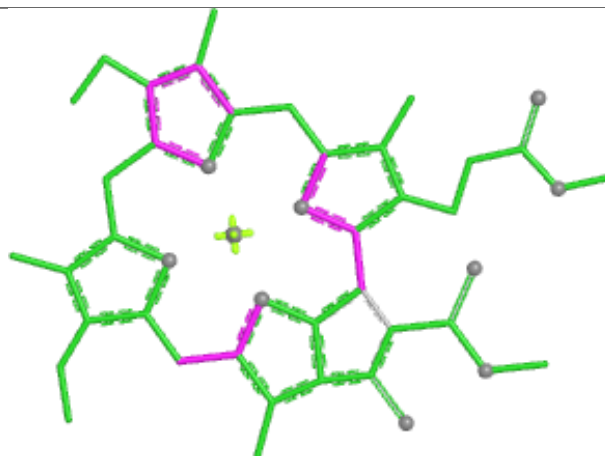




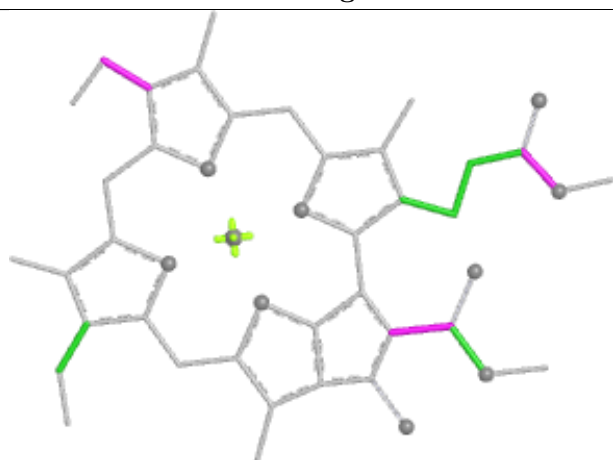
Ligand CLA x 516



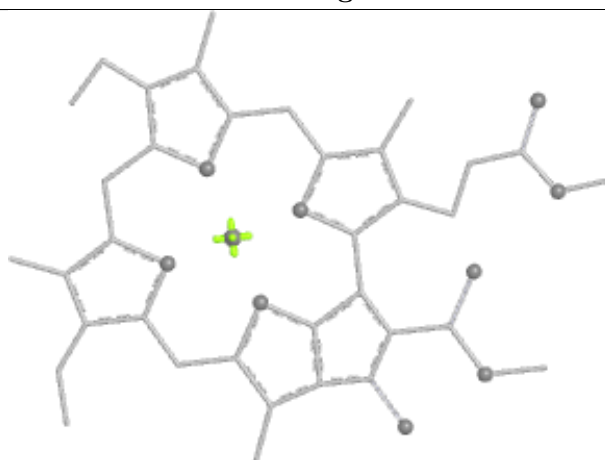
Bond lengths



Bond angles

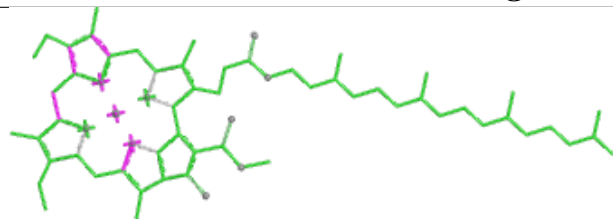


Torsions

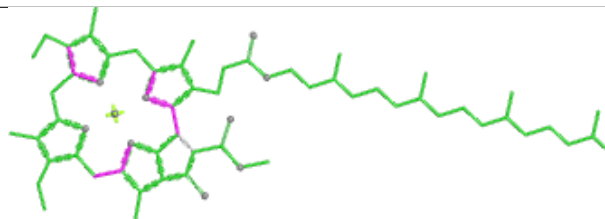


Rings

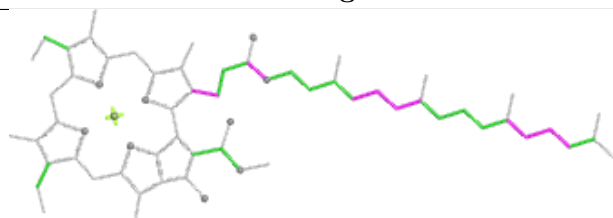
Ligand CLA B 1225



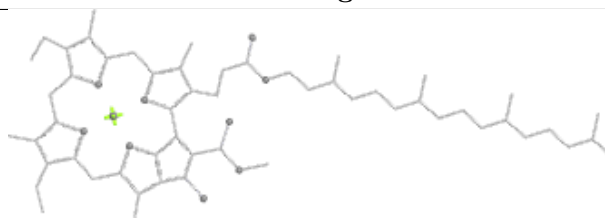
Bond lengths



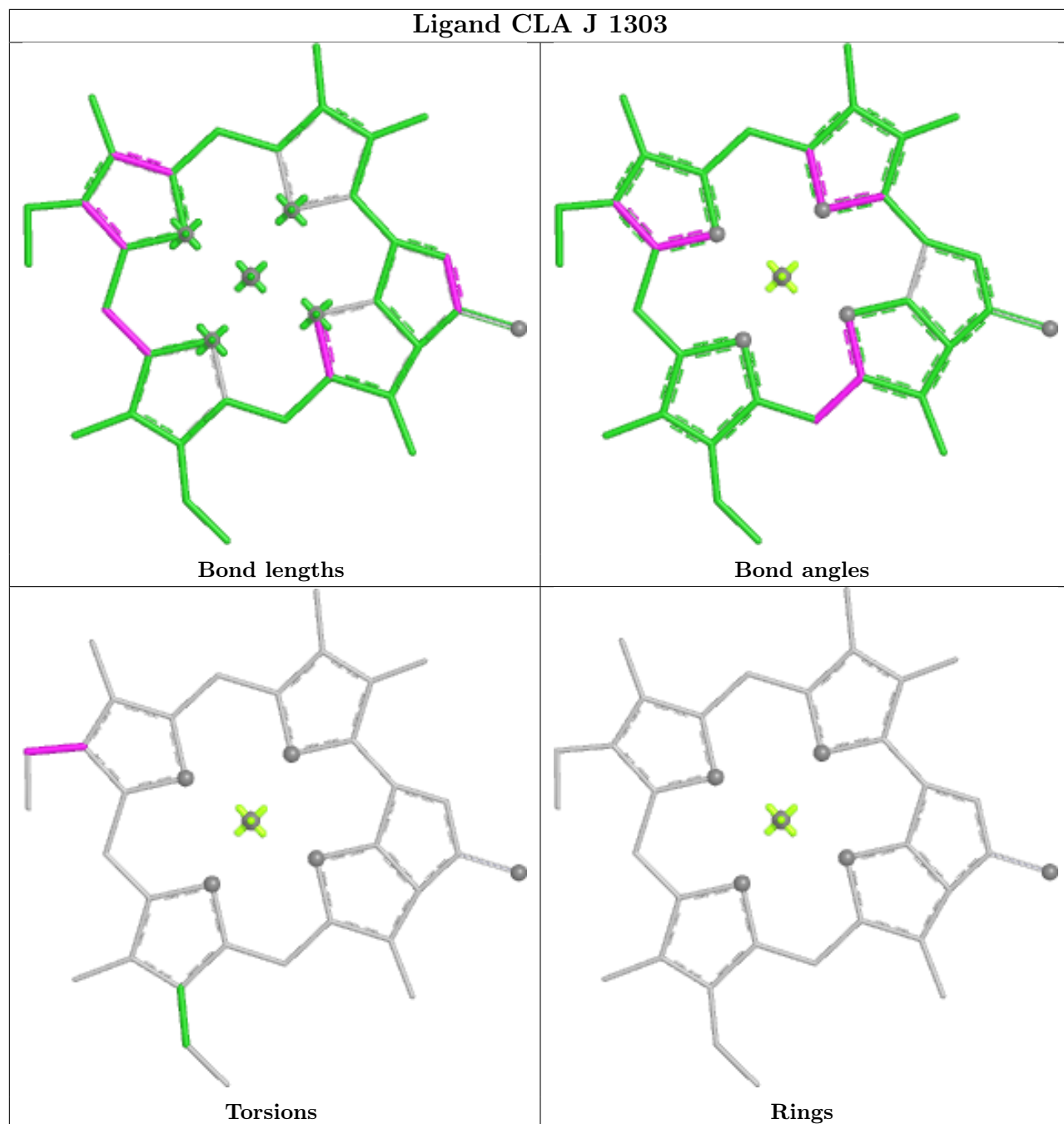
Bond angles

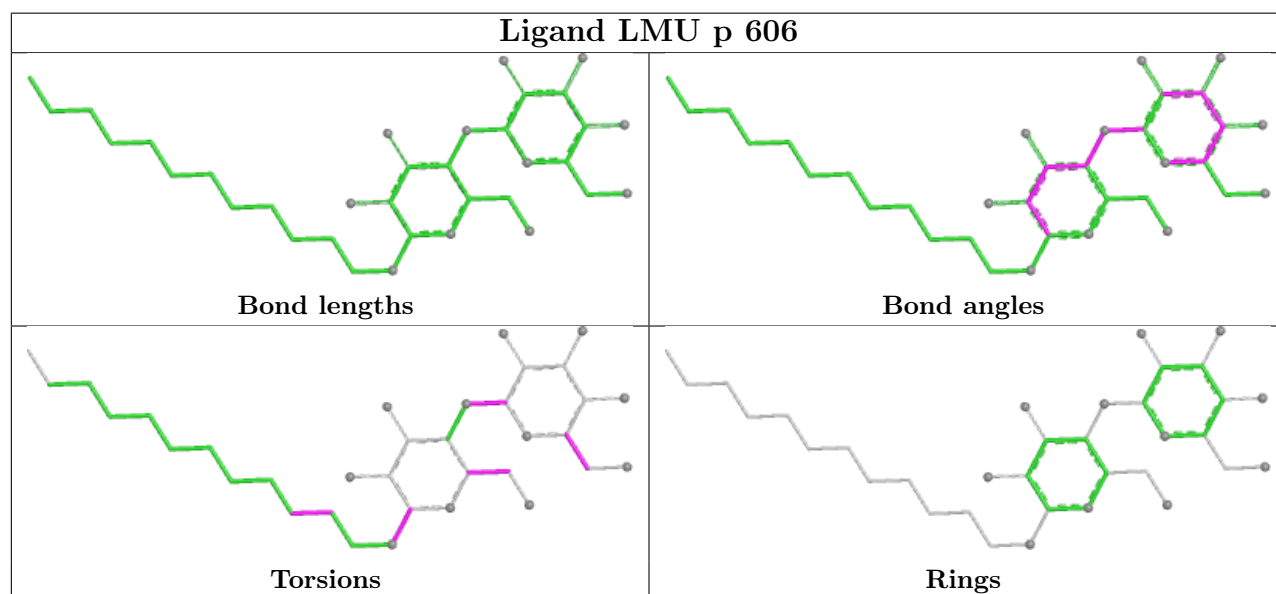
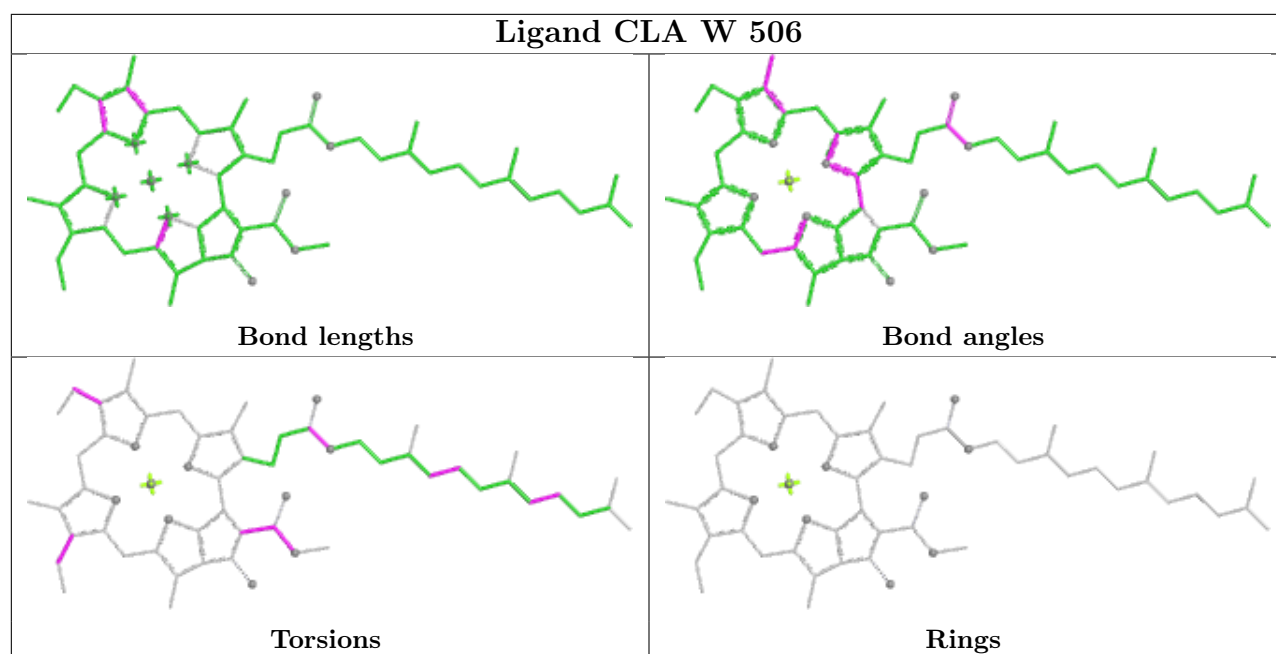


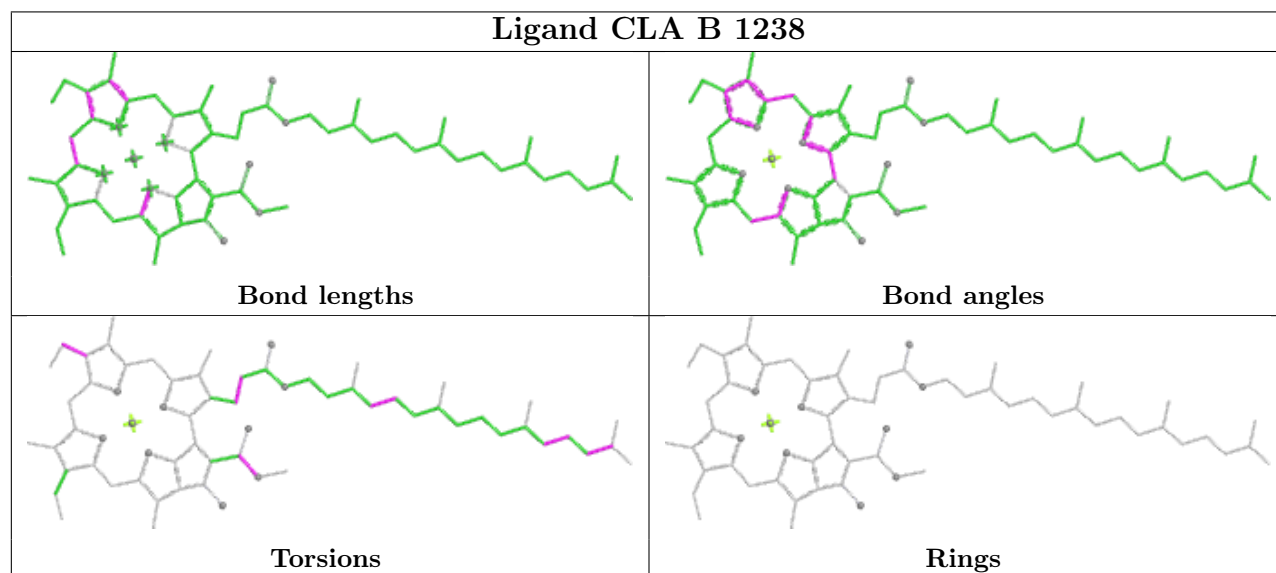
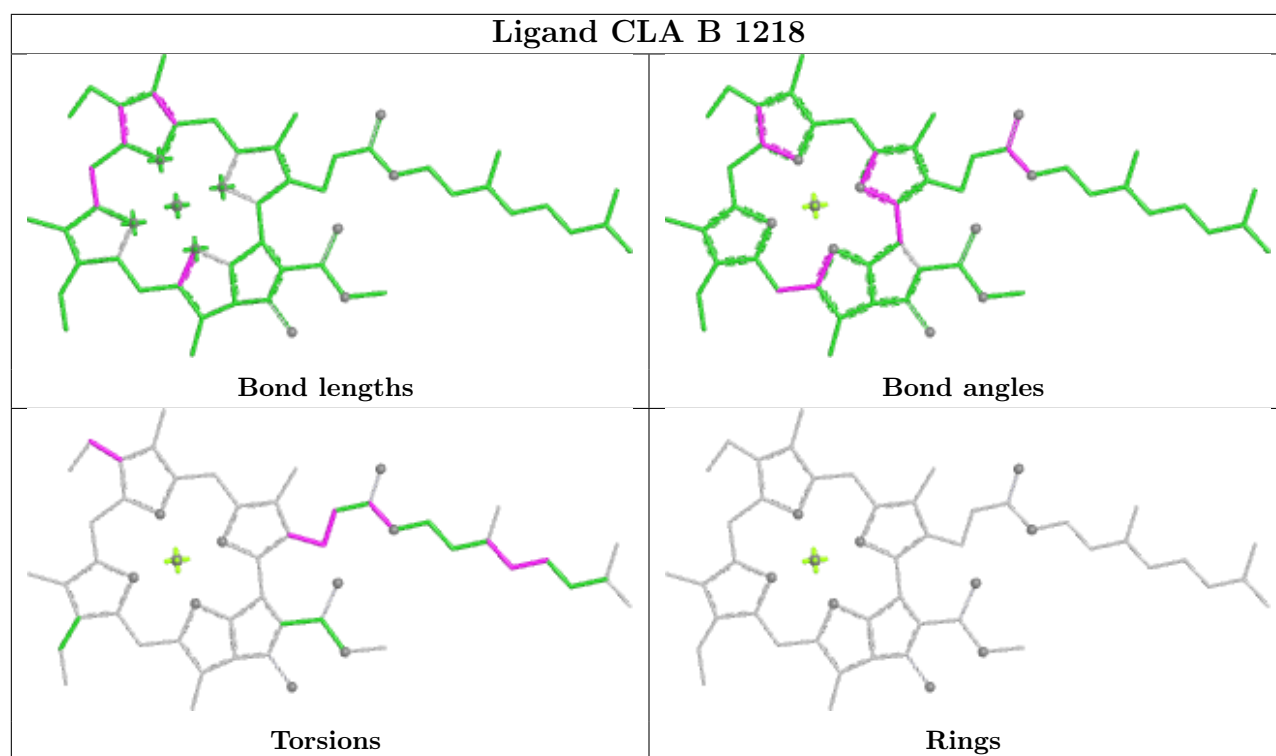
Torsions

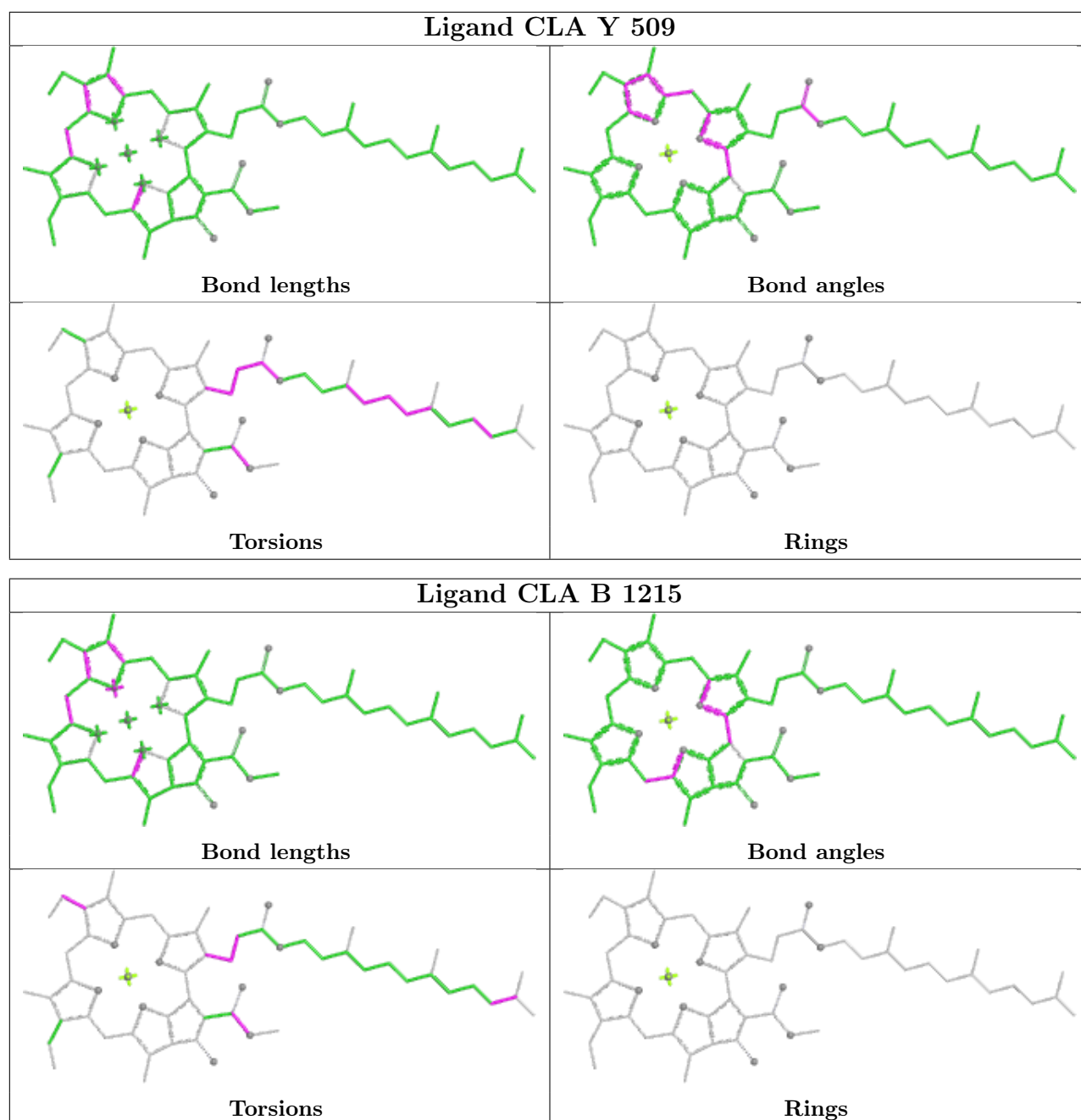


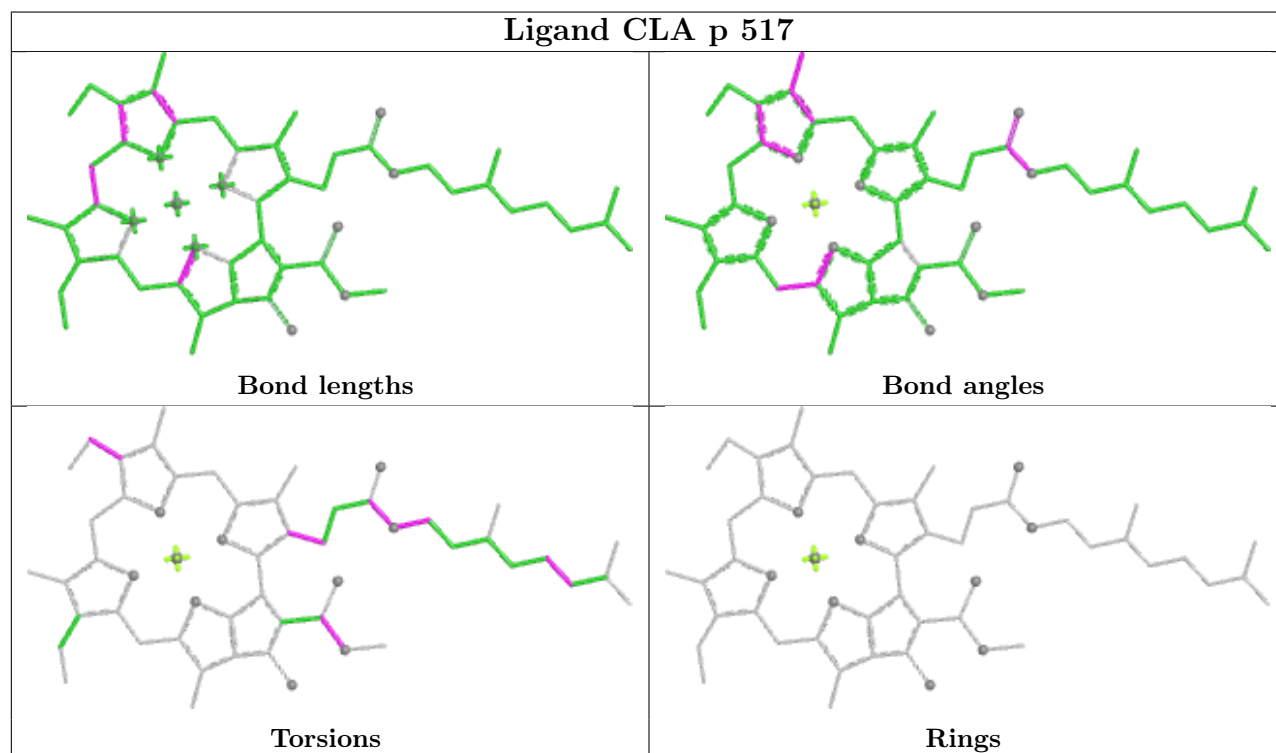
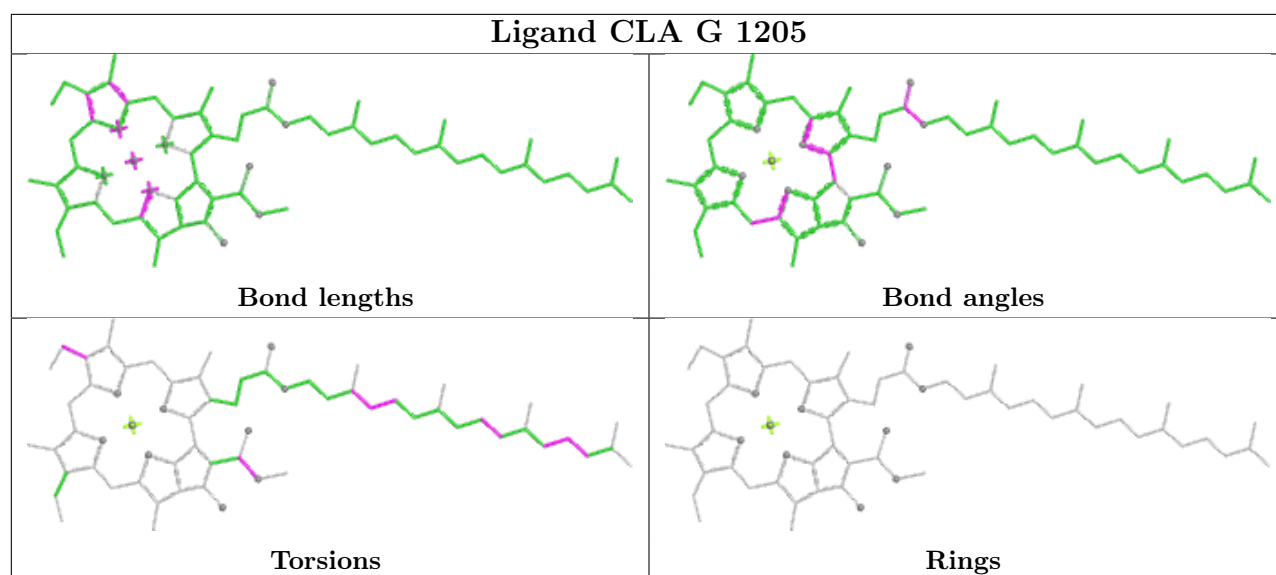
Rings



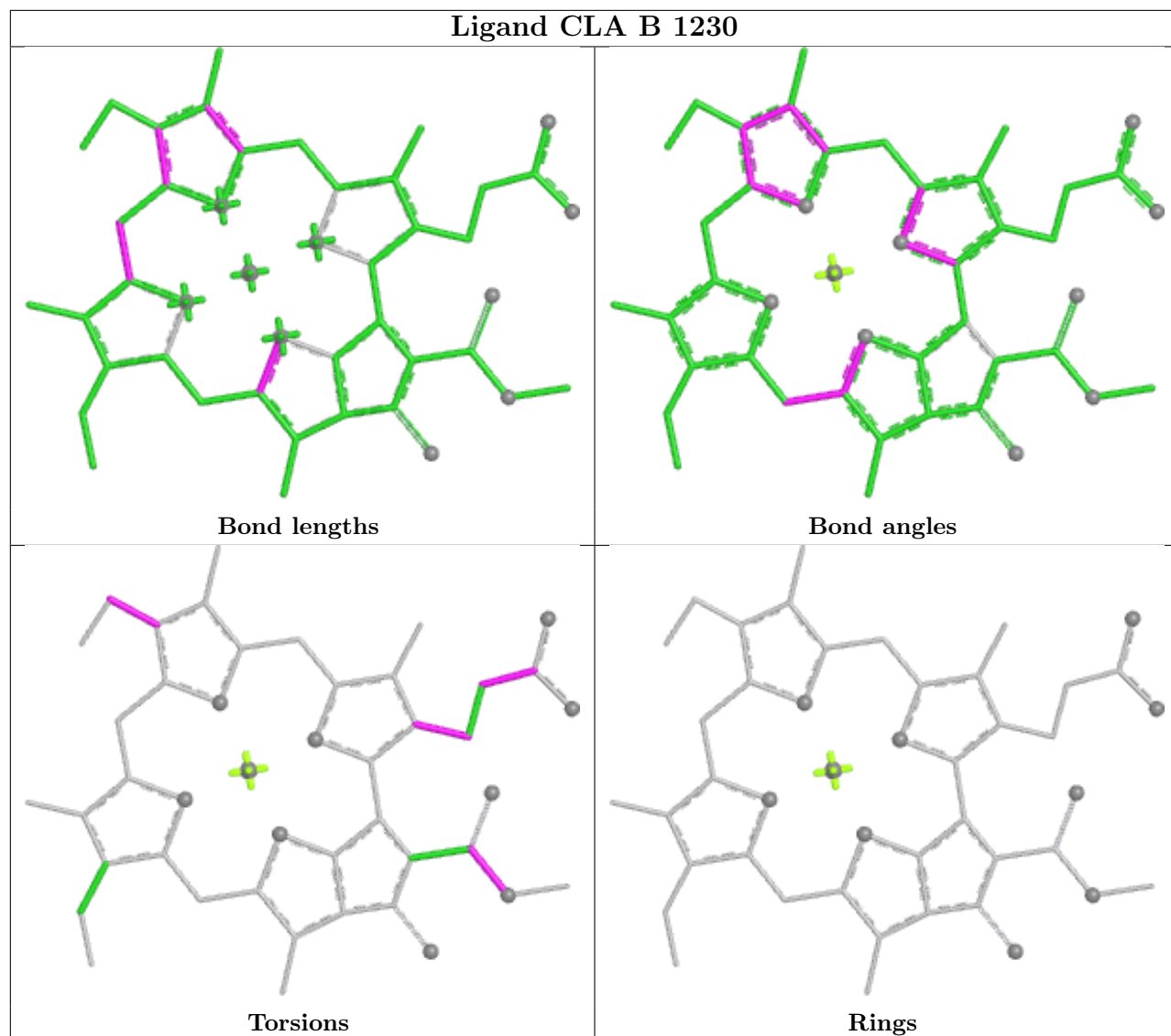




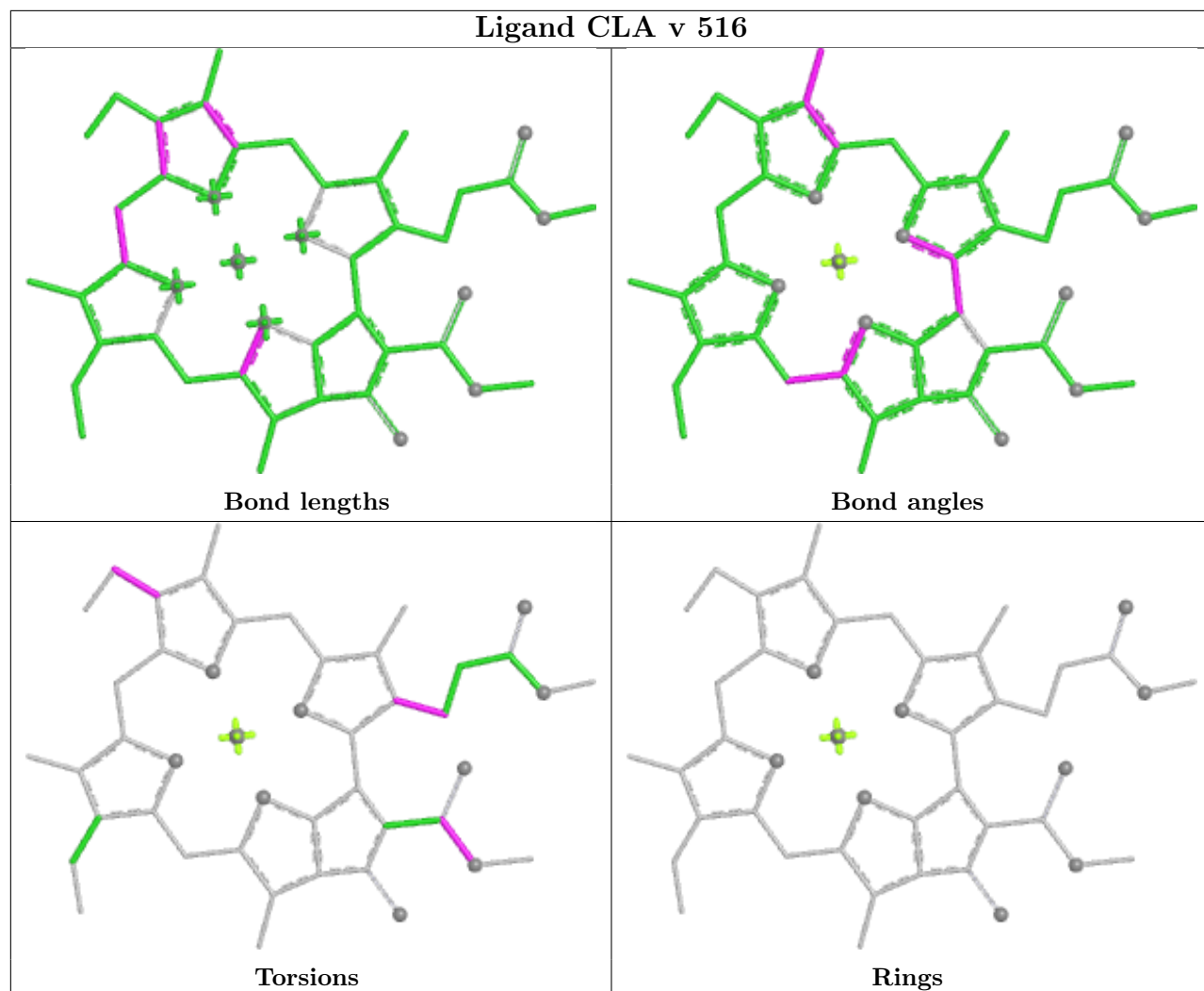


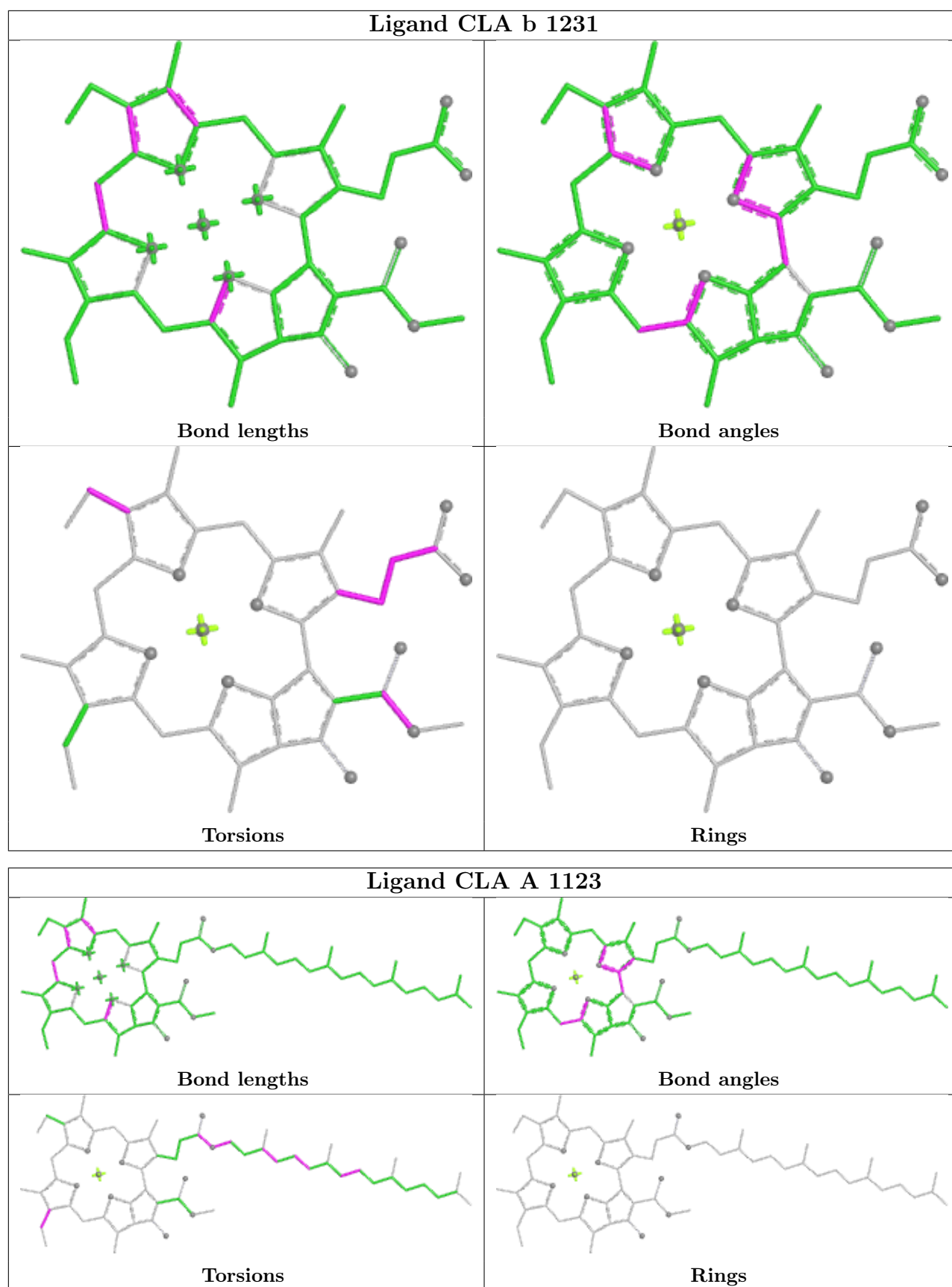


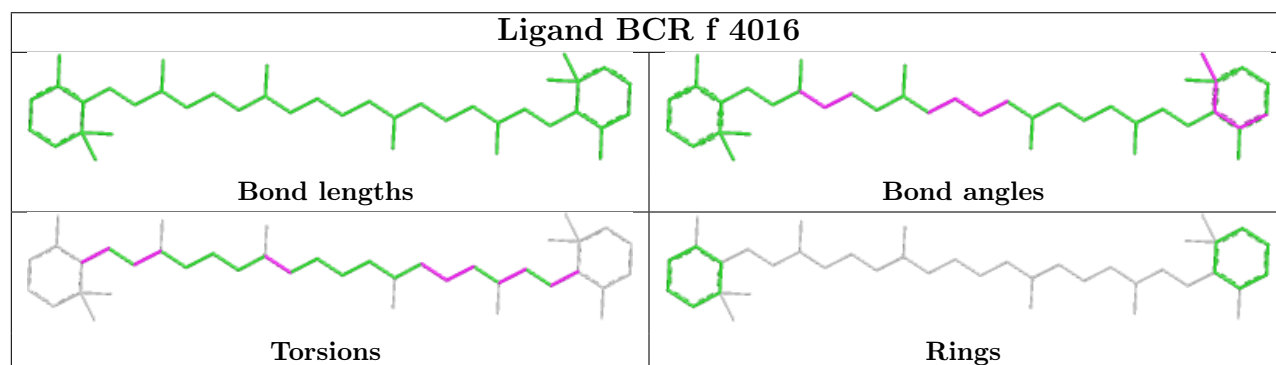
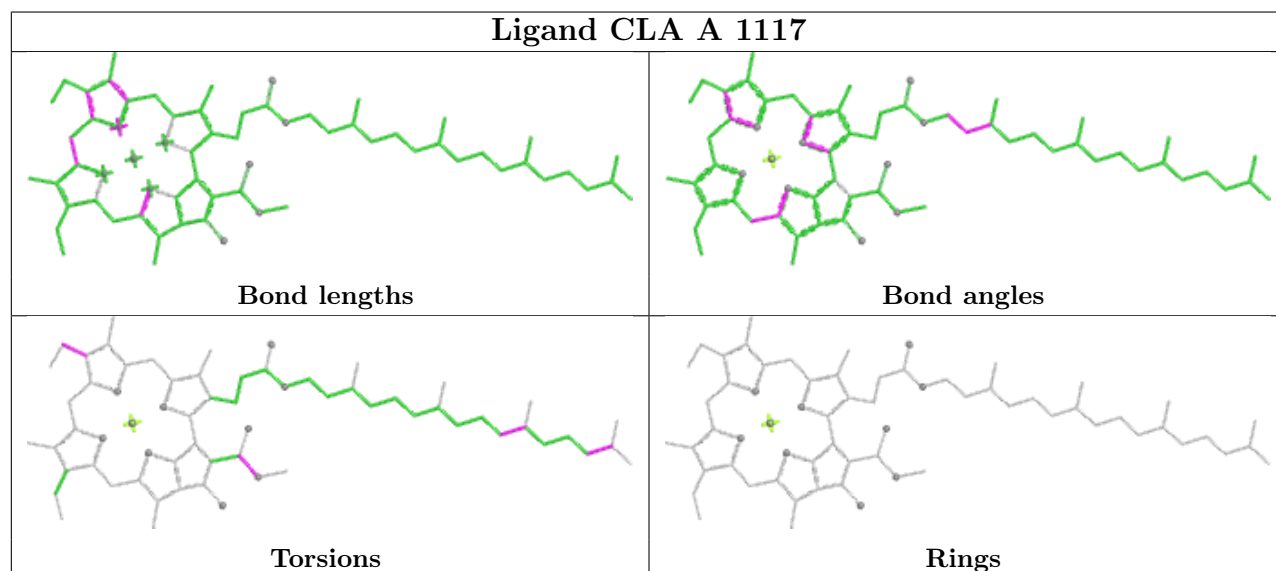
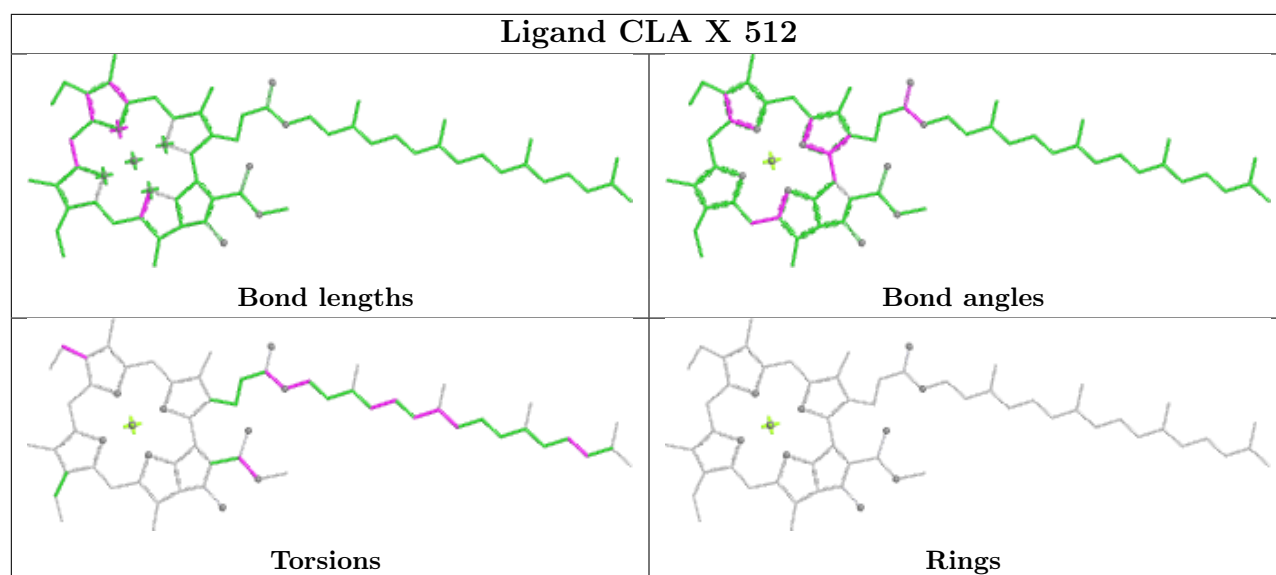
Ligand CLA B 1230

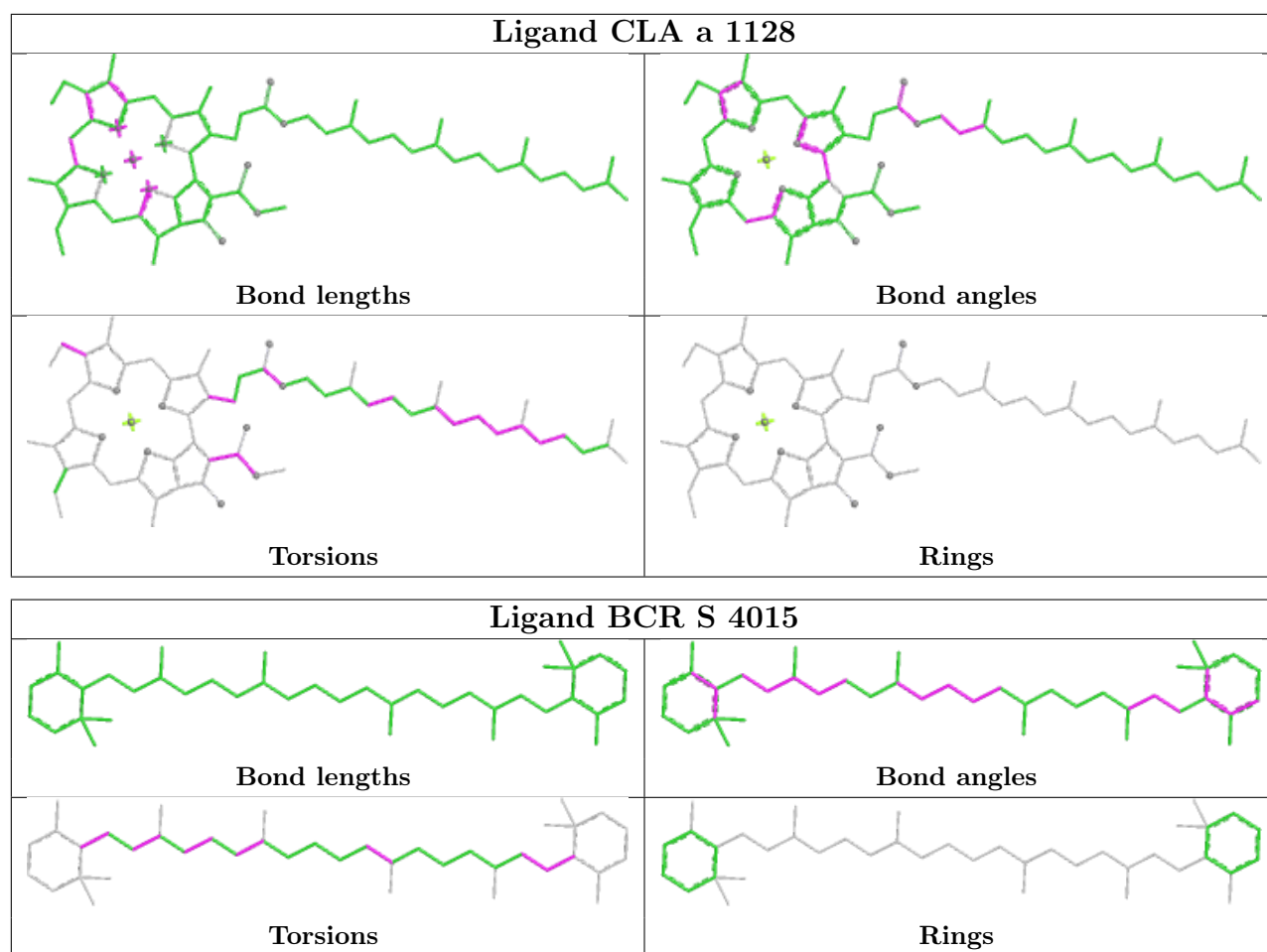


Ligand CLA v 516

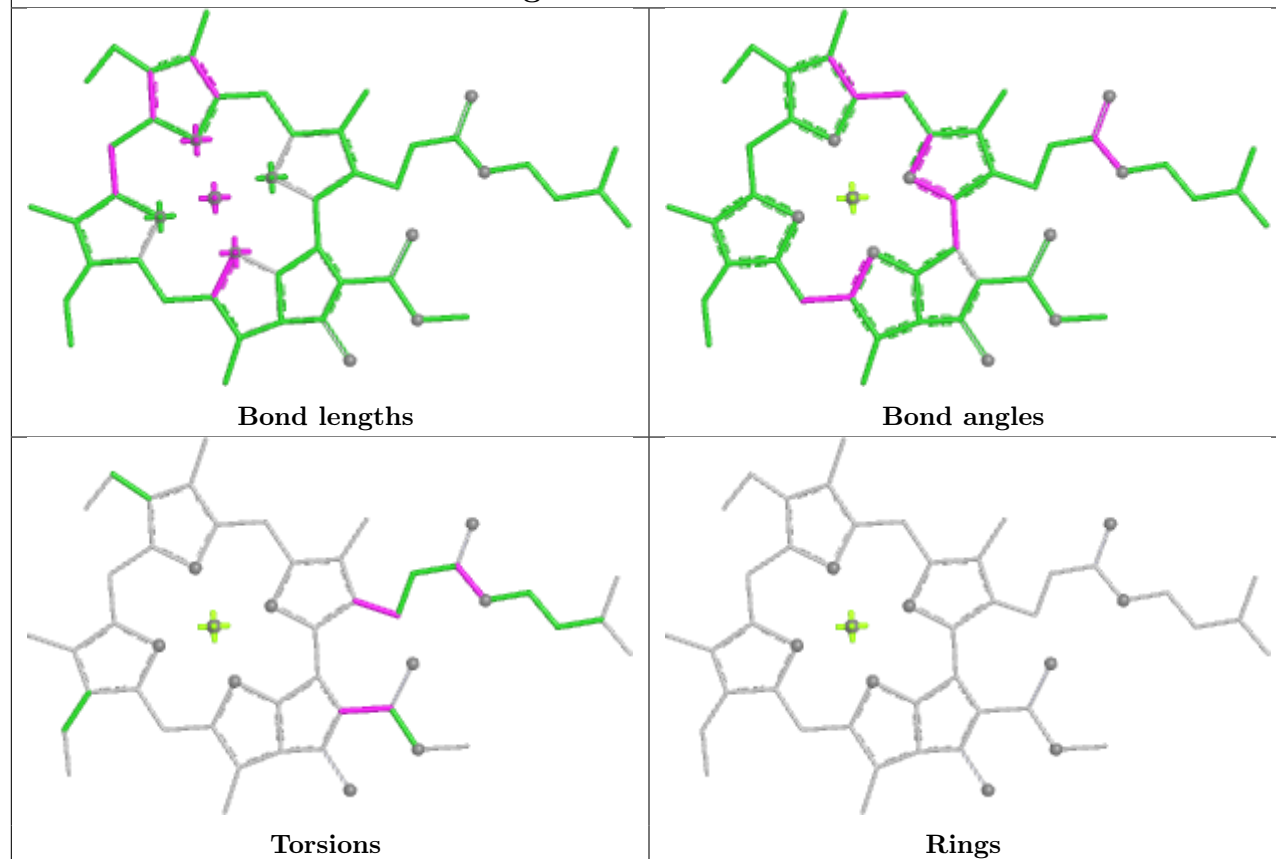




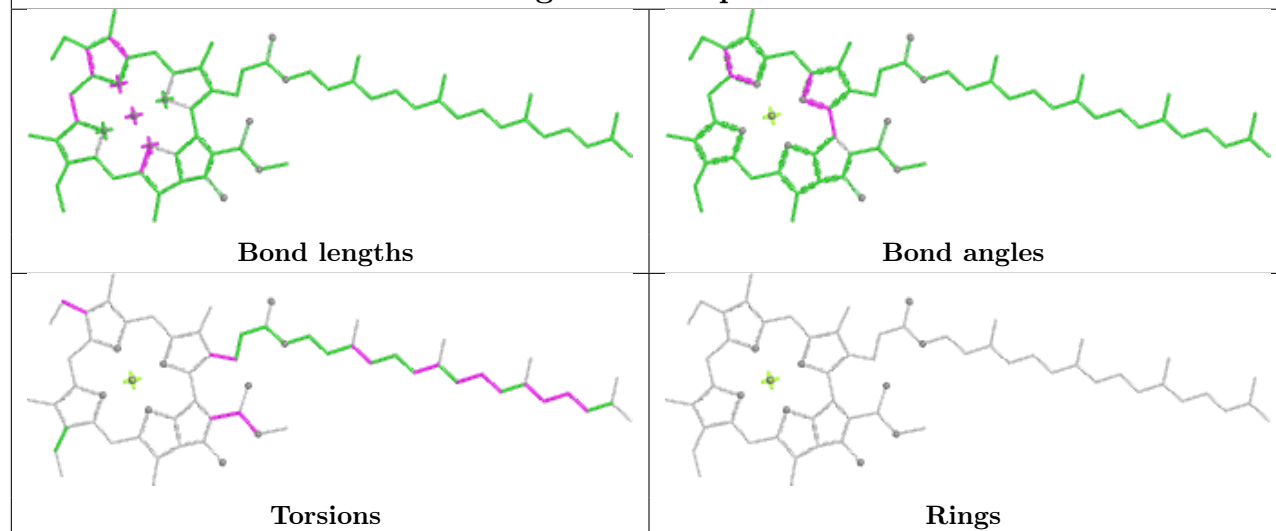


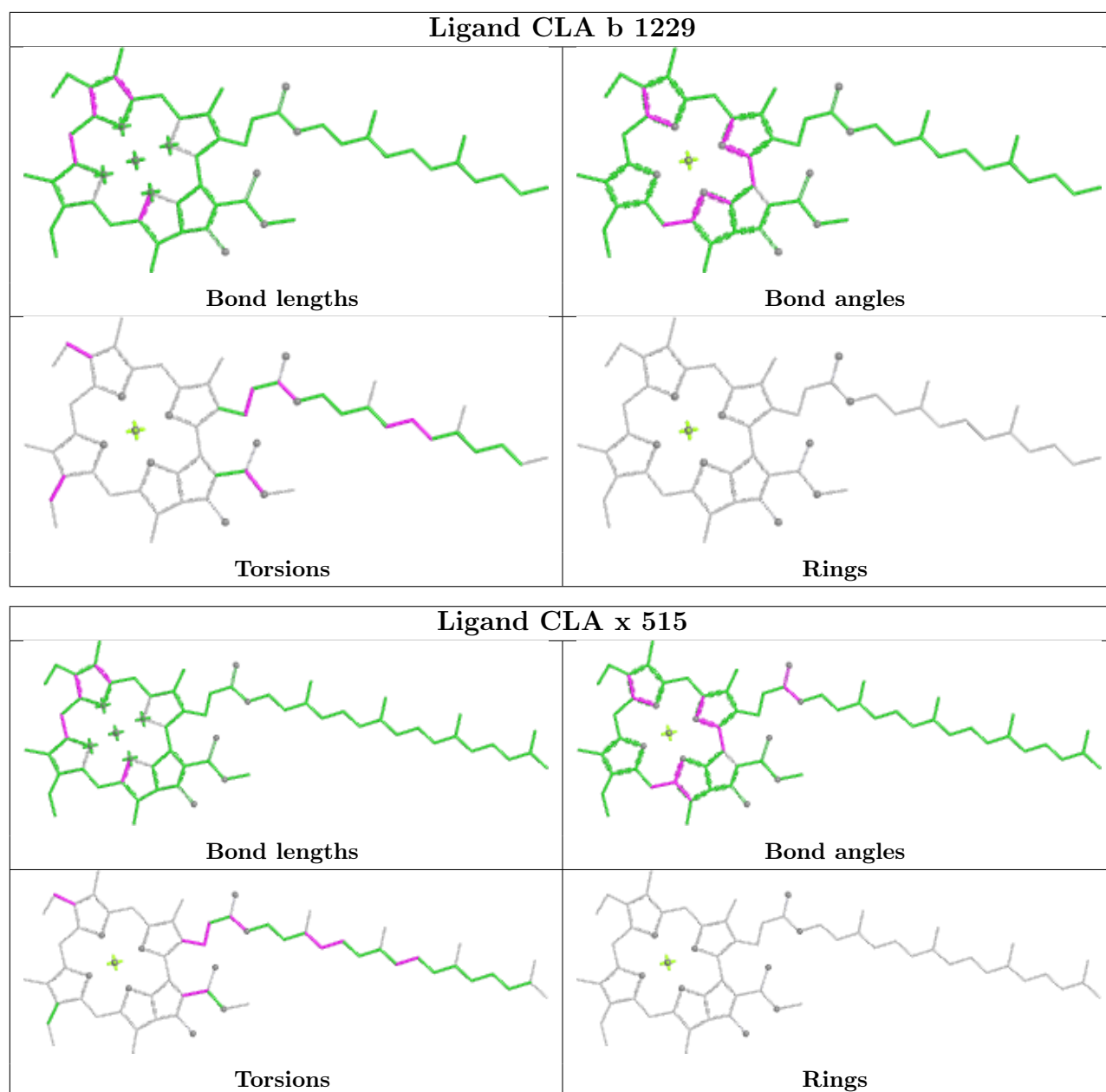


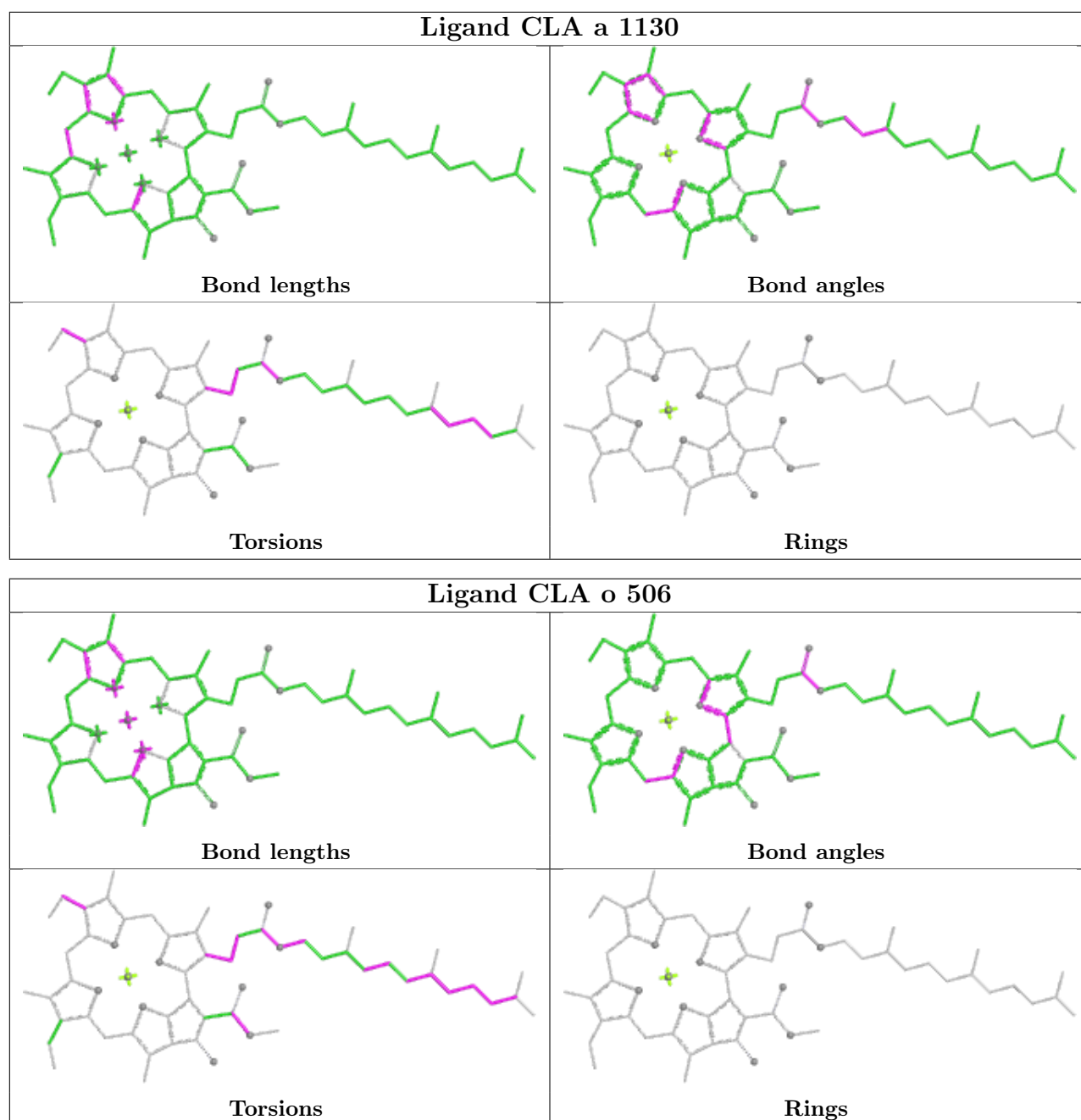
Ligand CLA B 1234



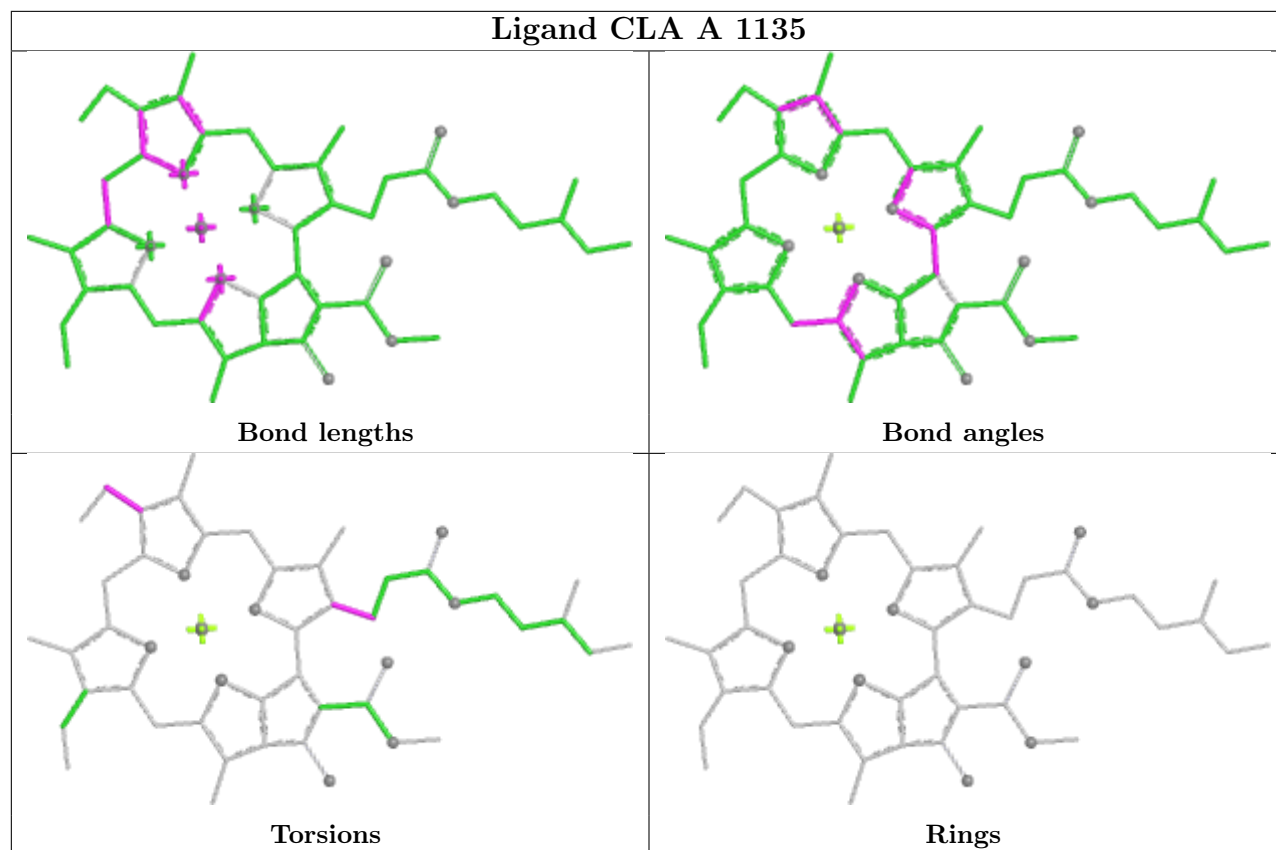
Ligand CLA q 512



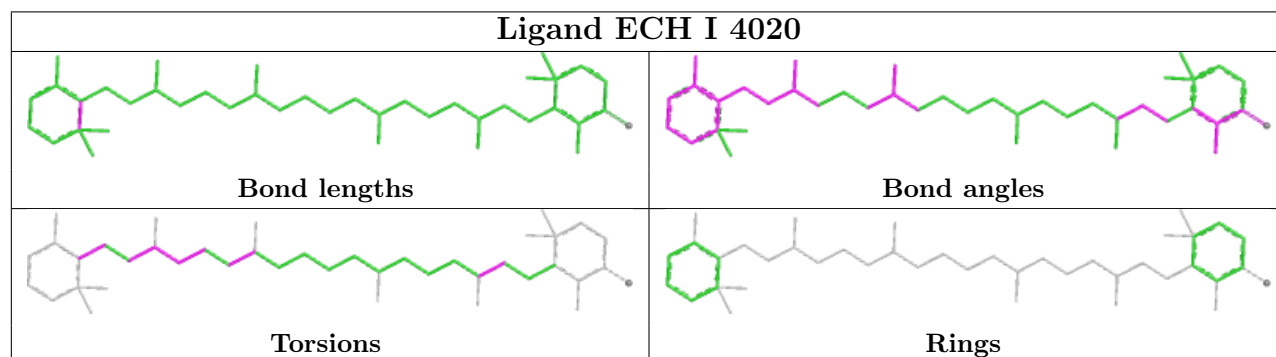


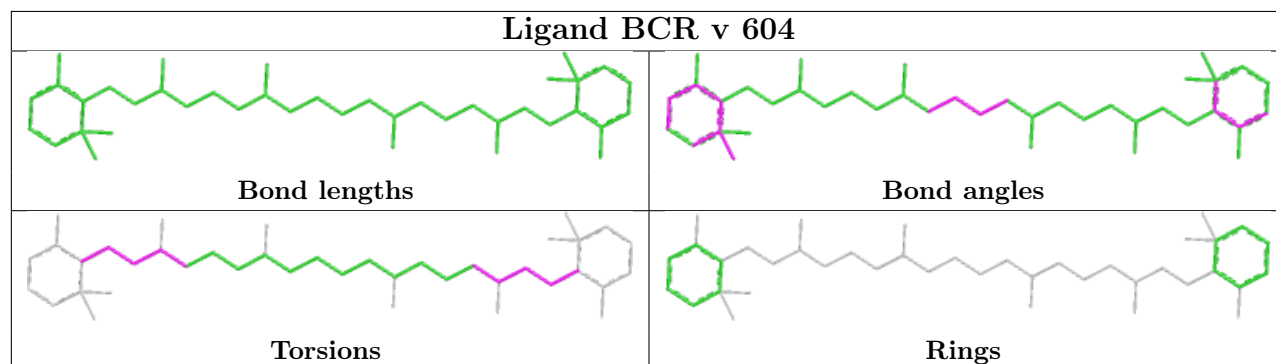
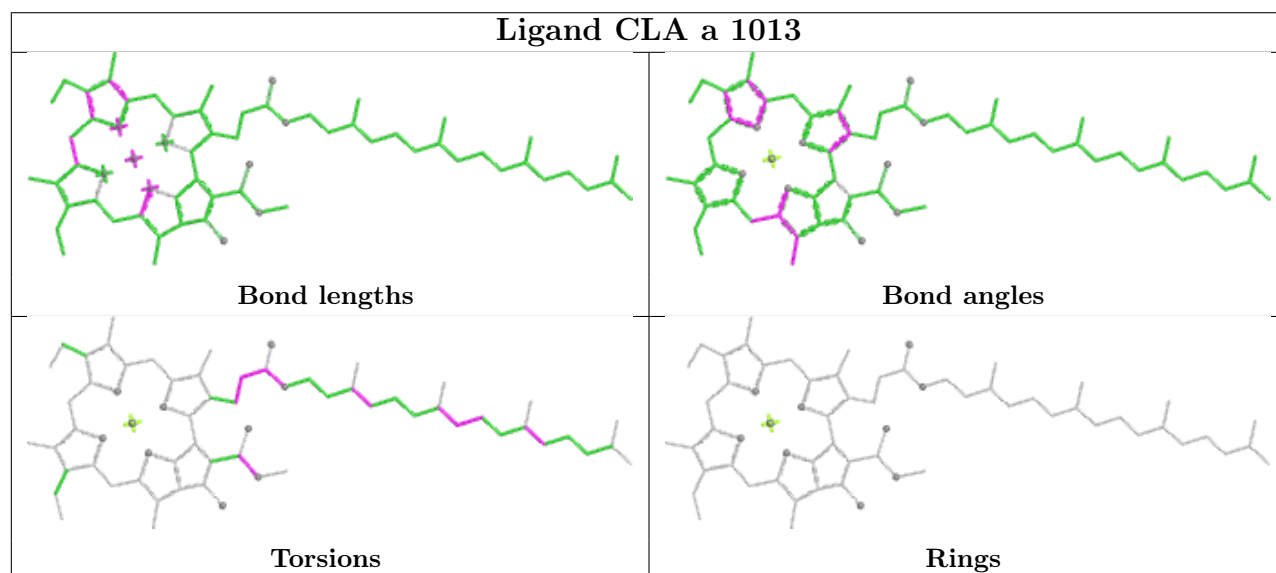
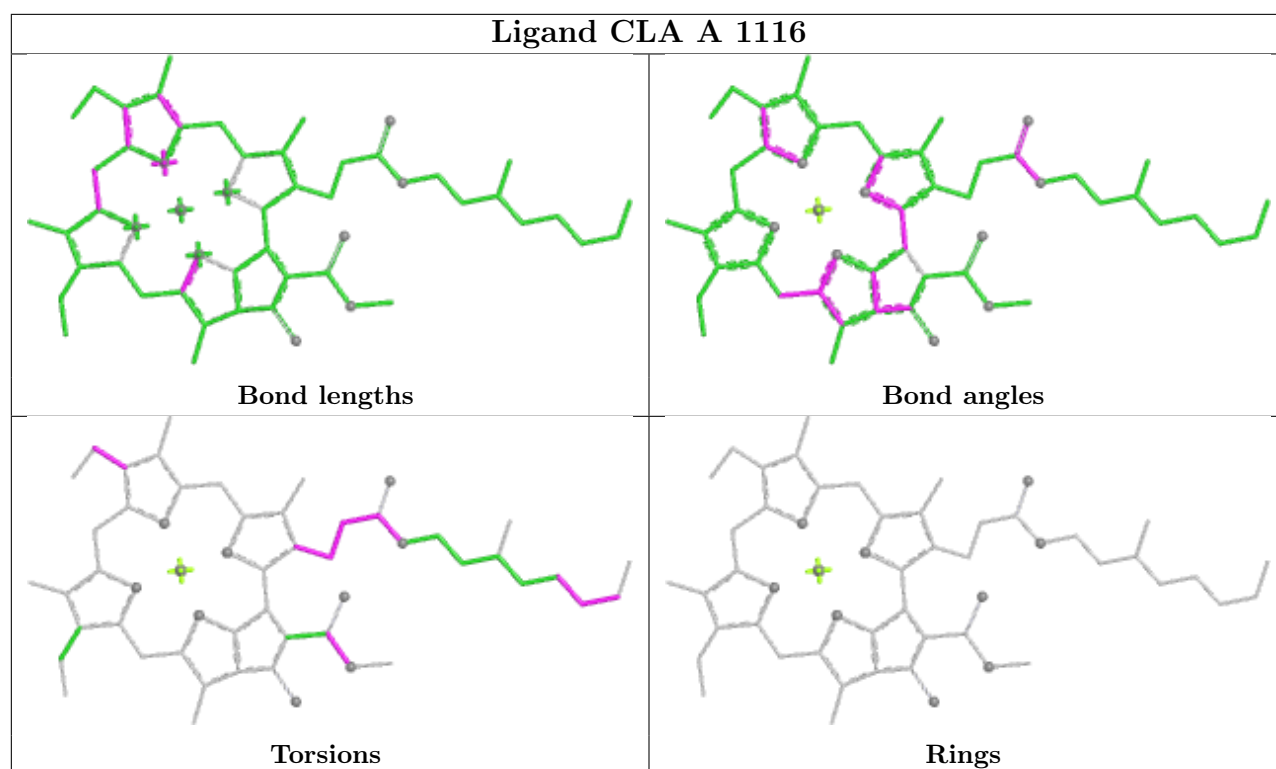


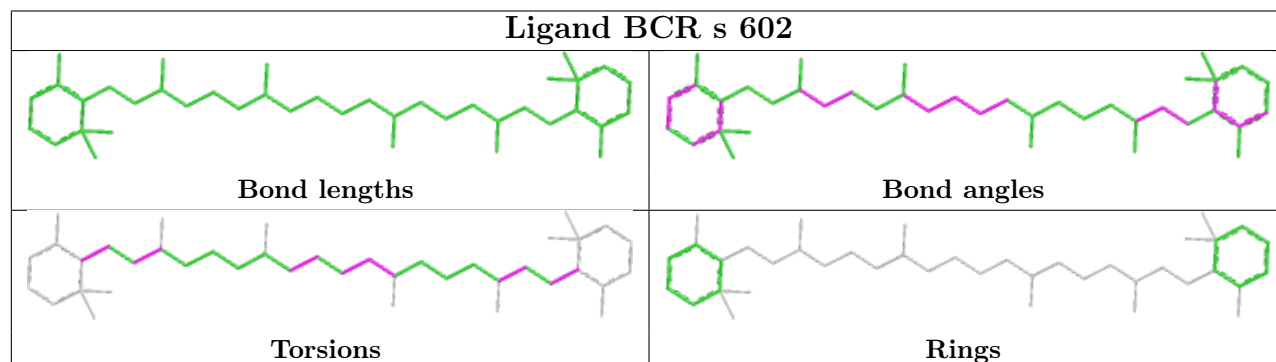
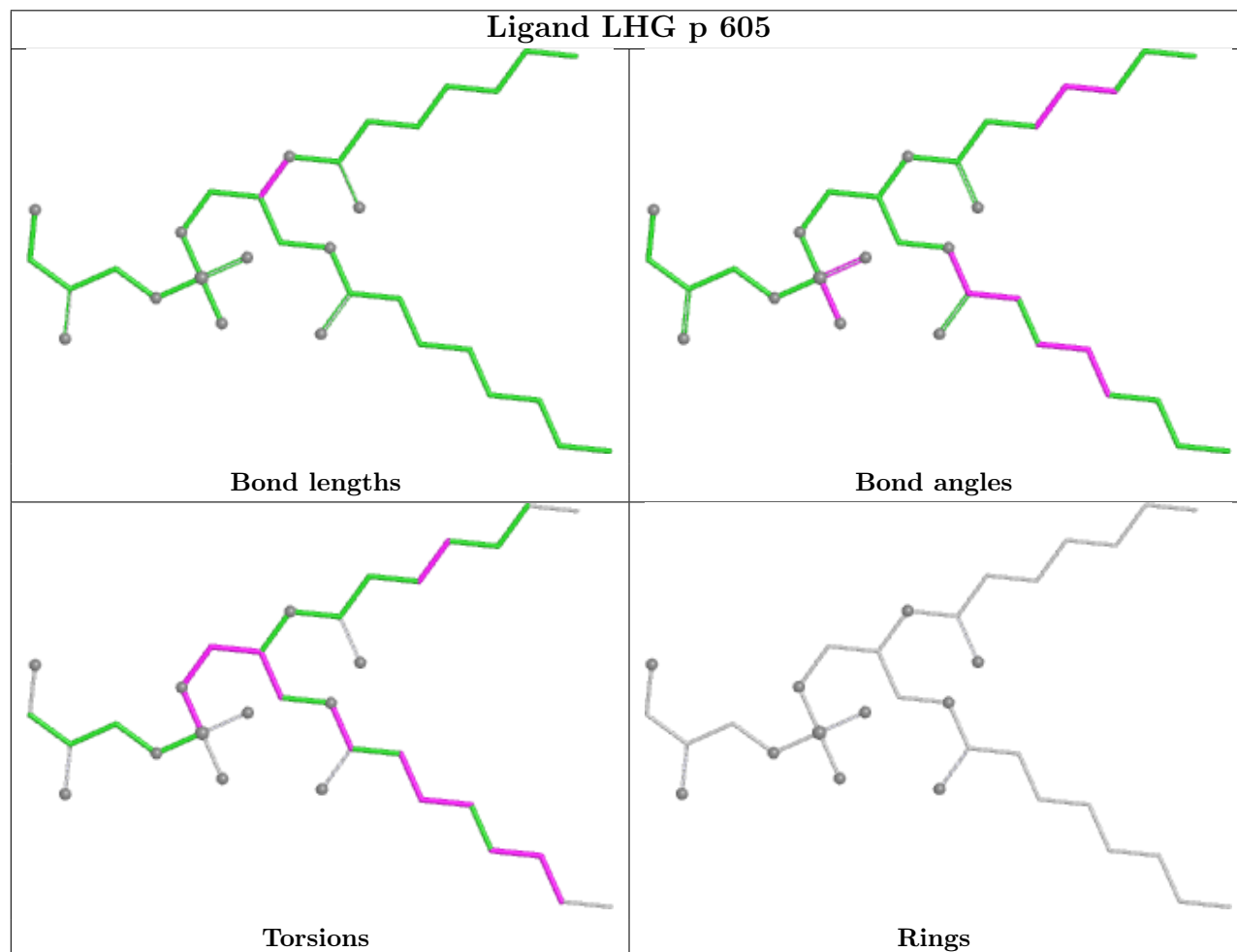
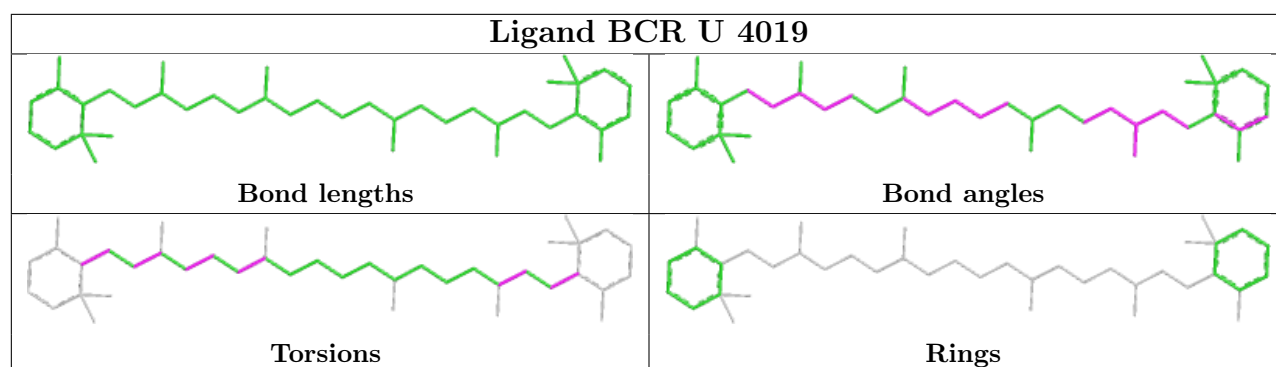
Ligand CLA A 1135

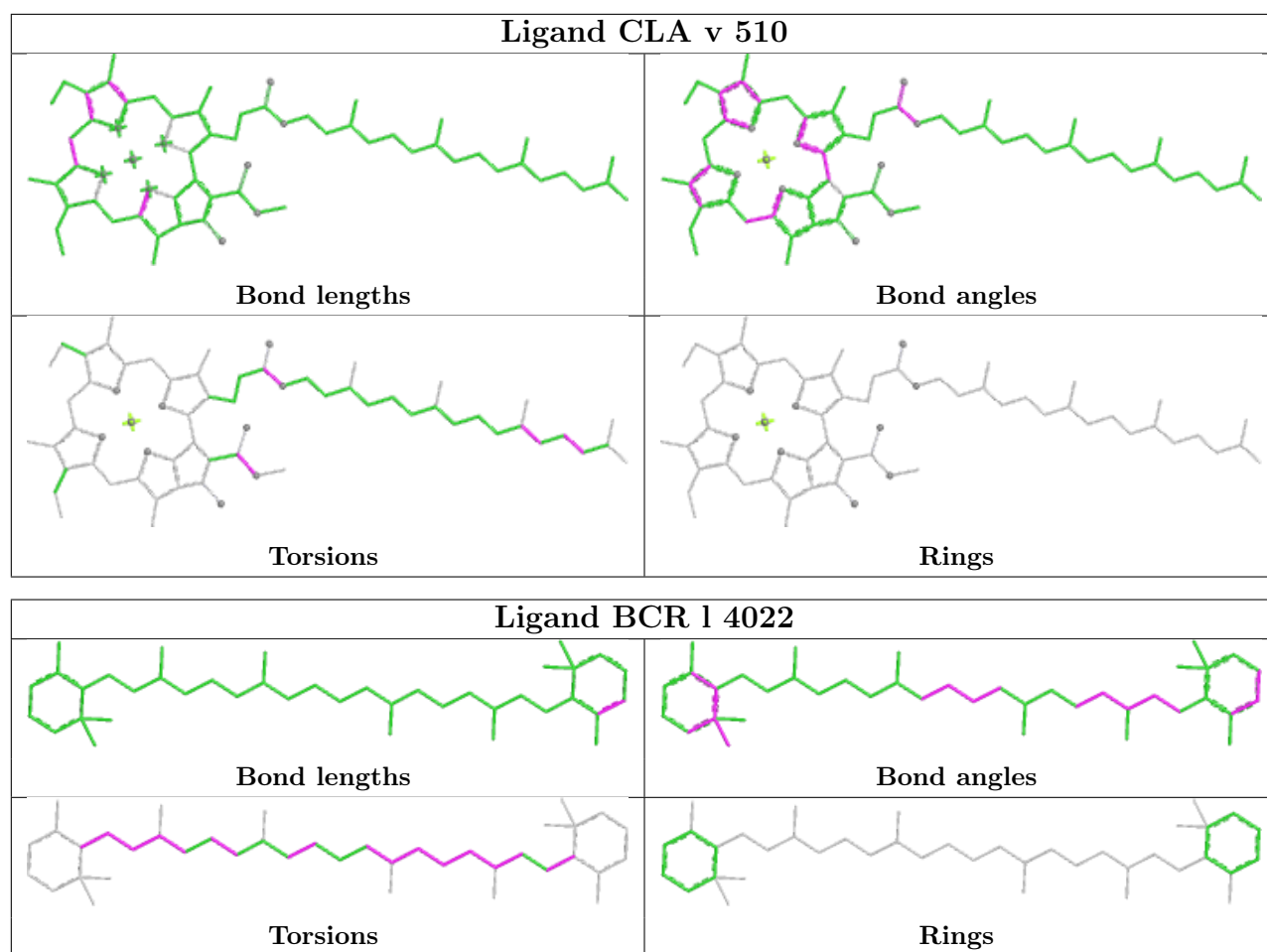


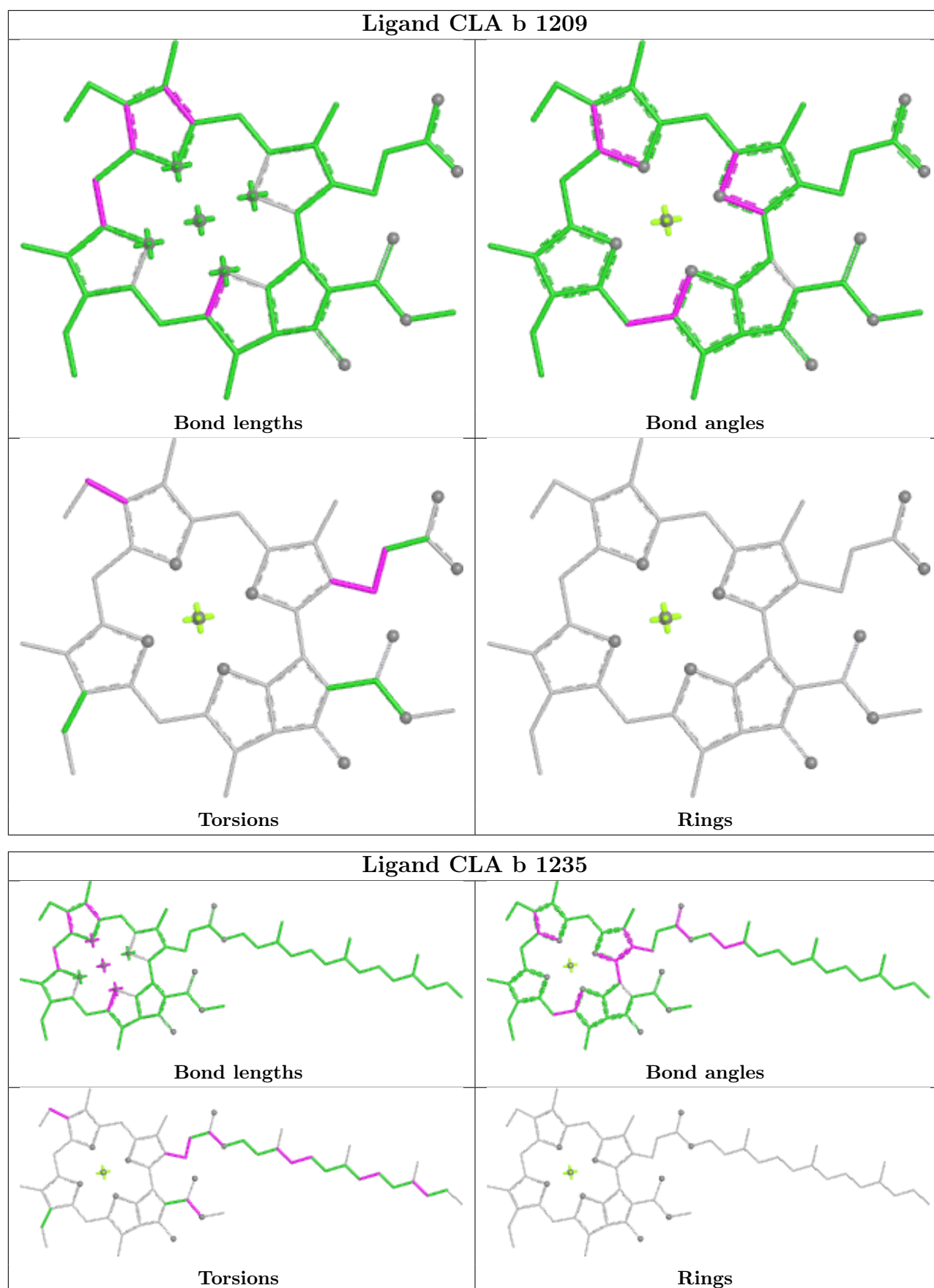
Ligand ECH I 4020

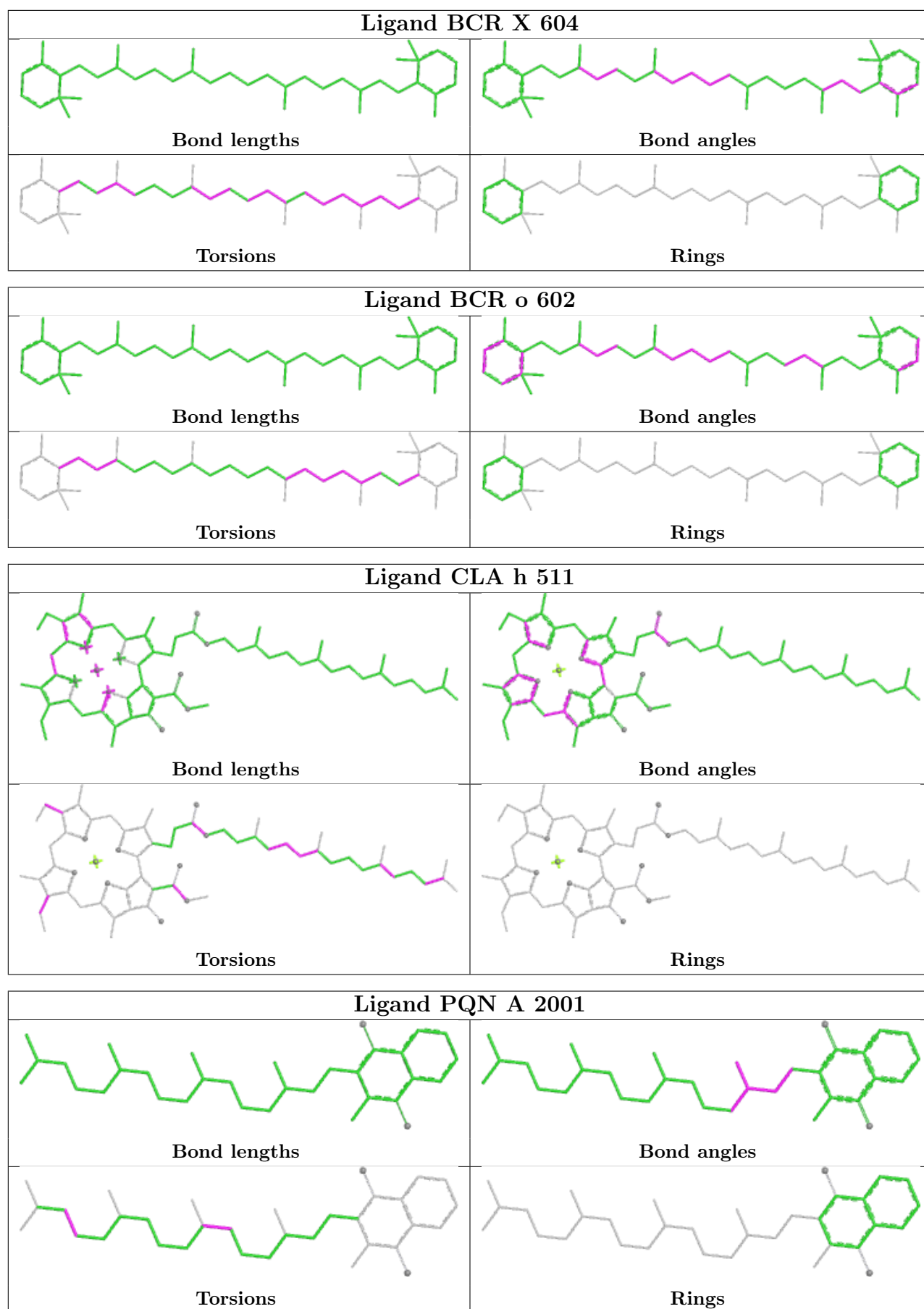


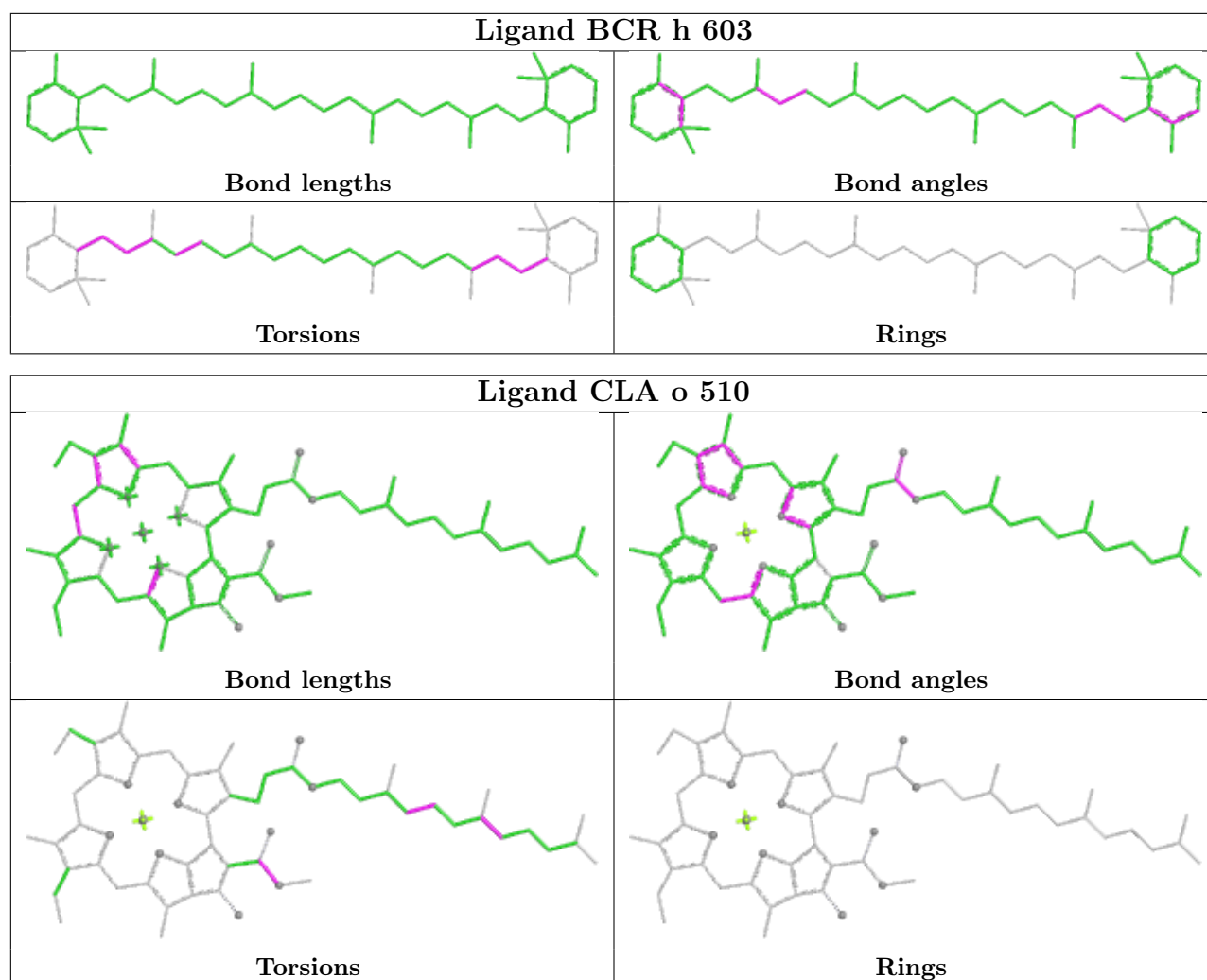




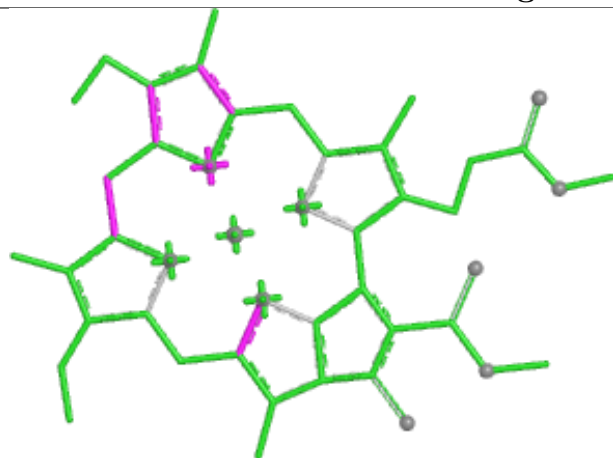




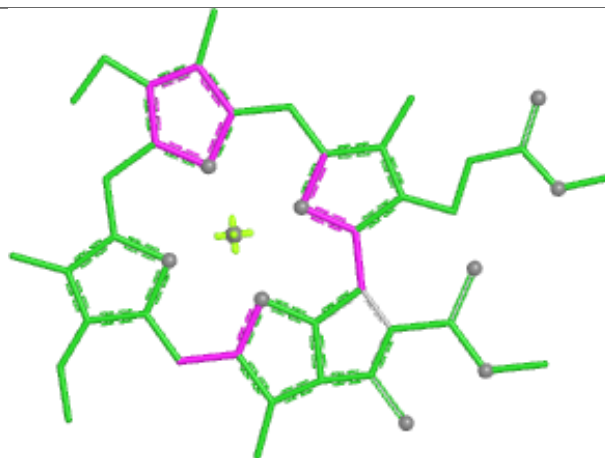




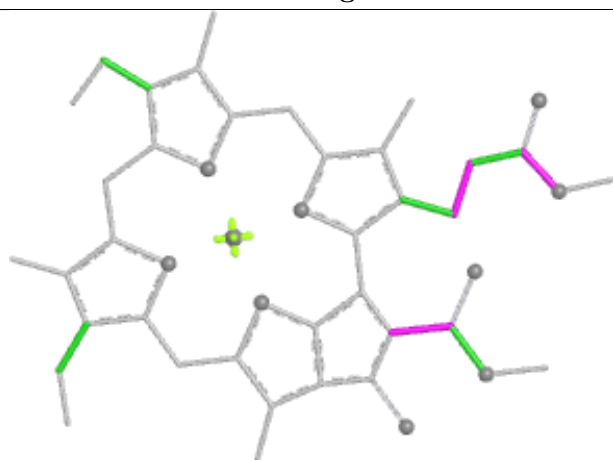
Ligand CLA h 503



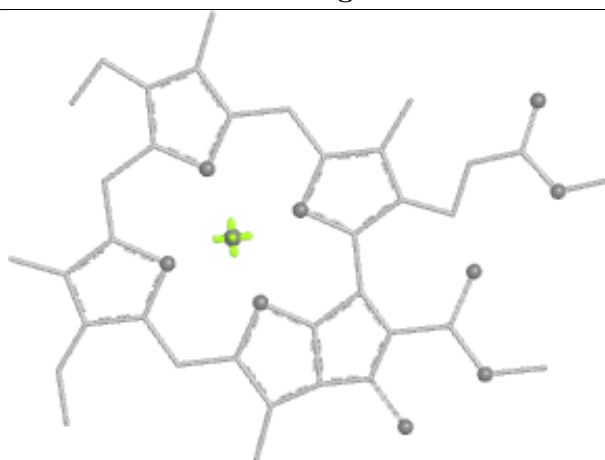
Bond lengths



Bond angles

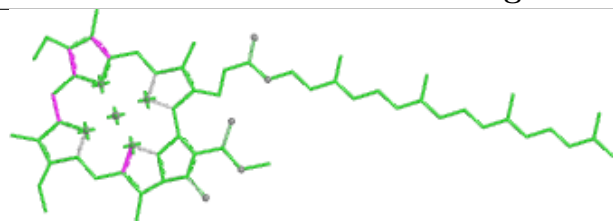


Torsions

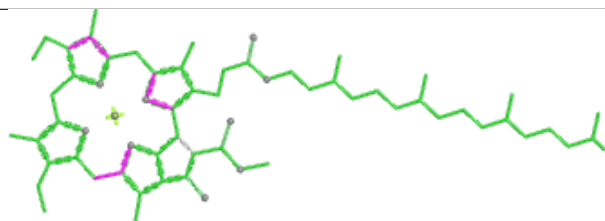


Rings

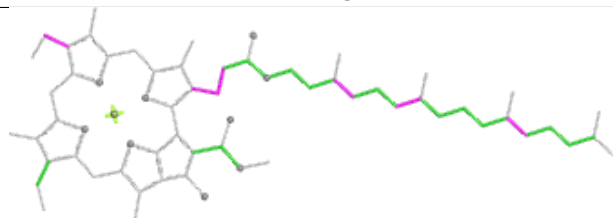
Ligand CLA G 1204



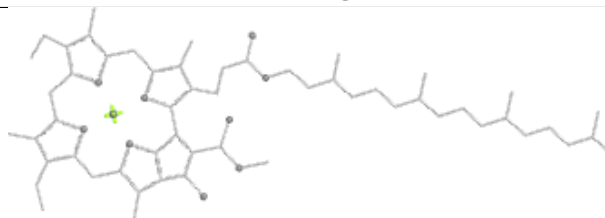
Bond lengths



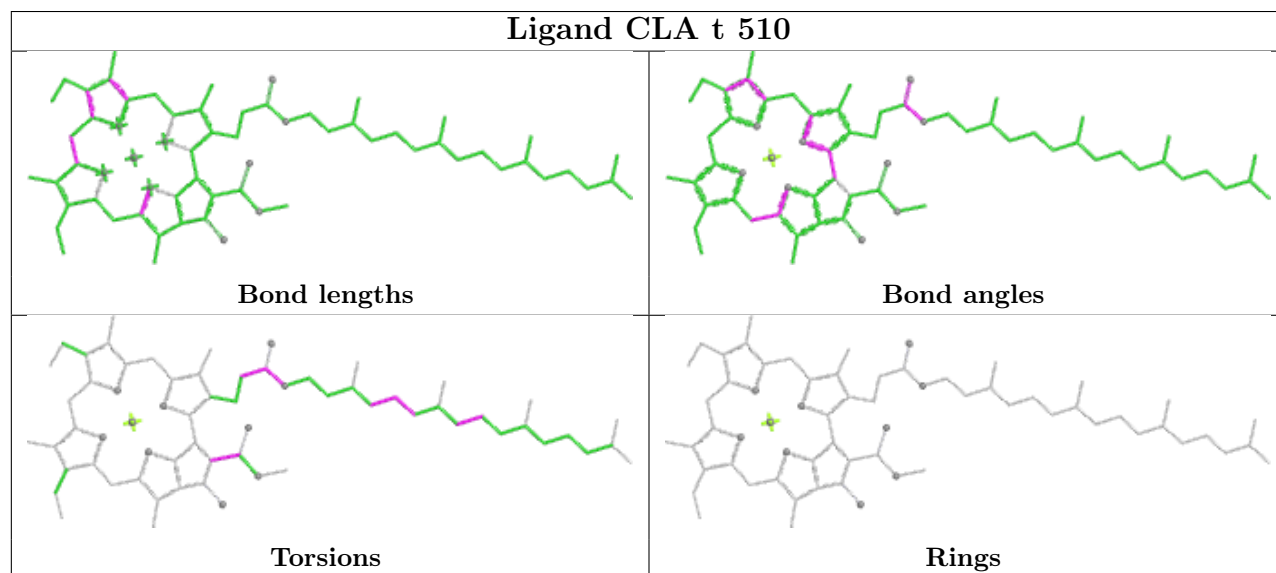
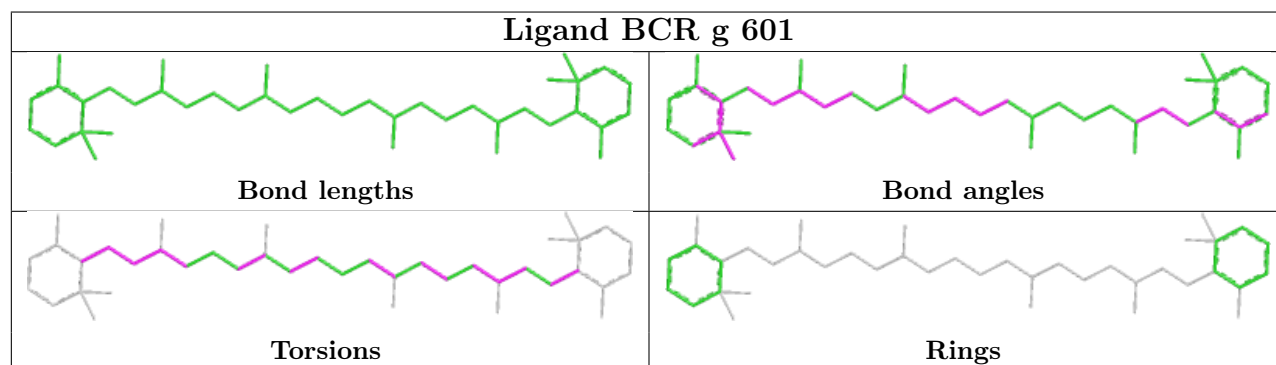
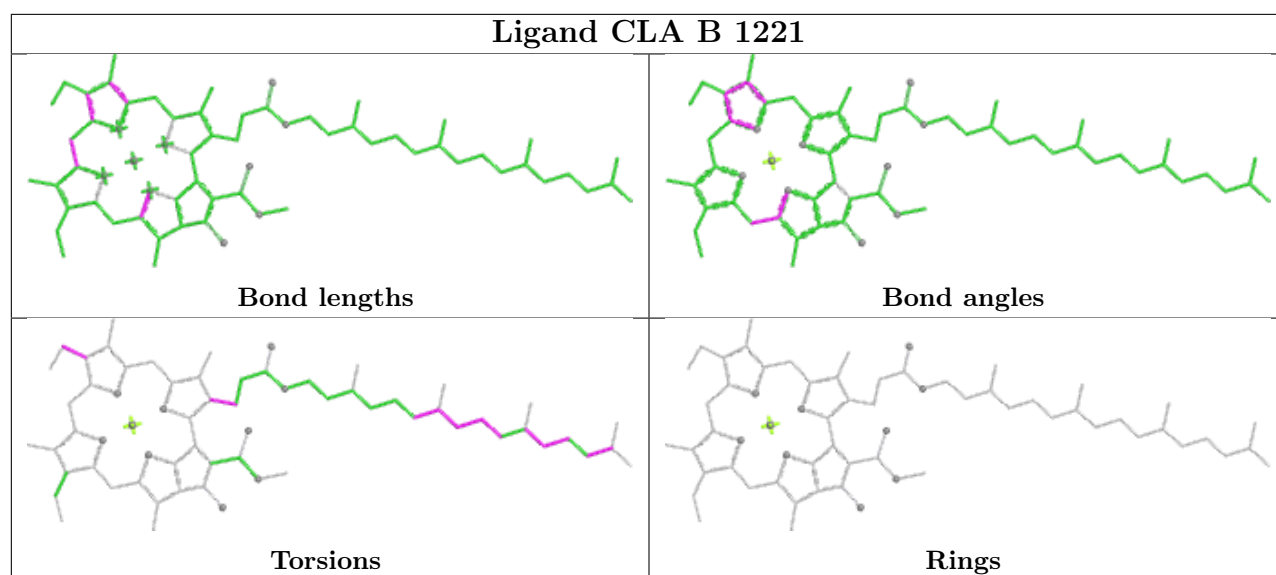
Bond angles

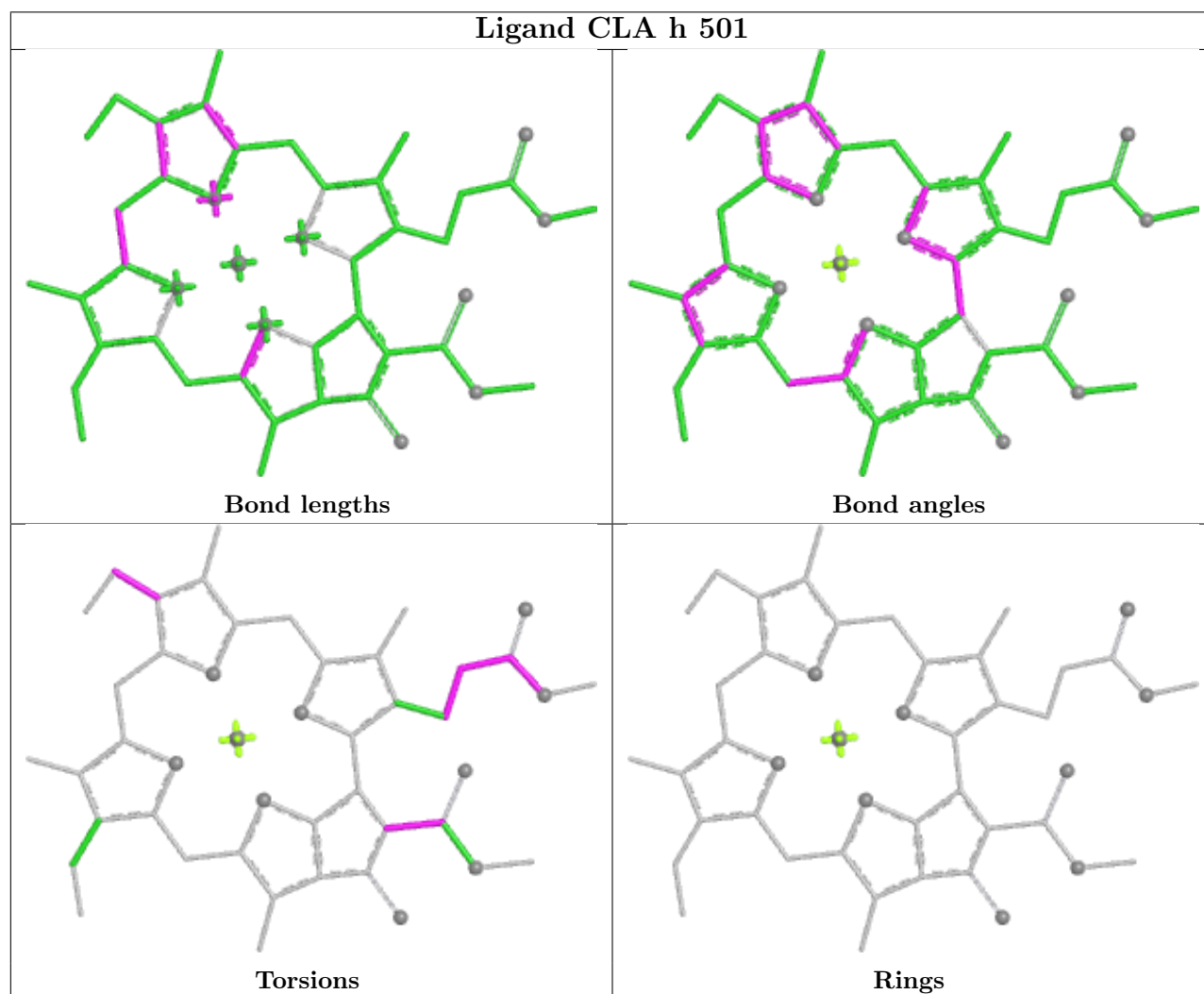
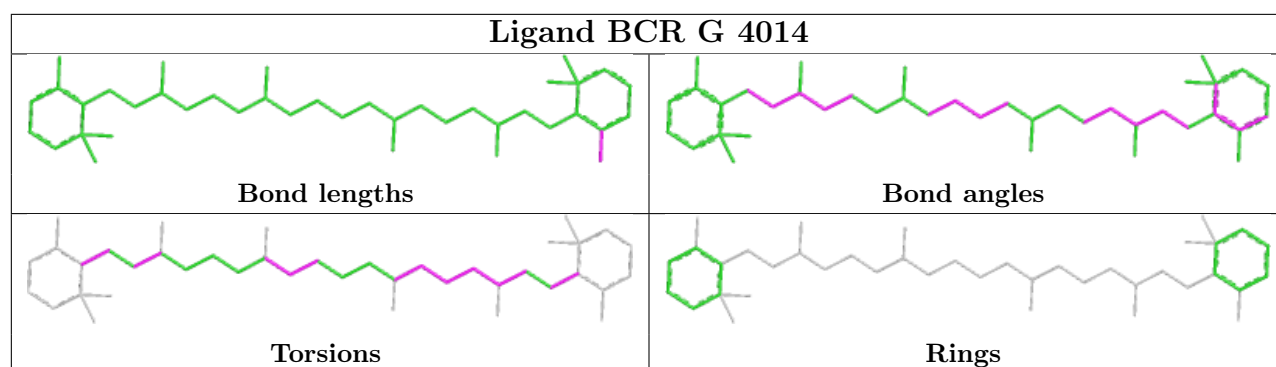


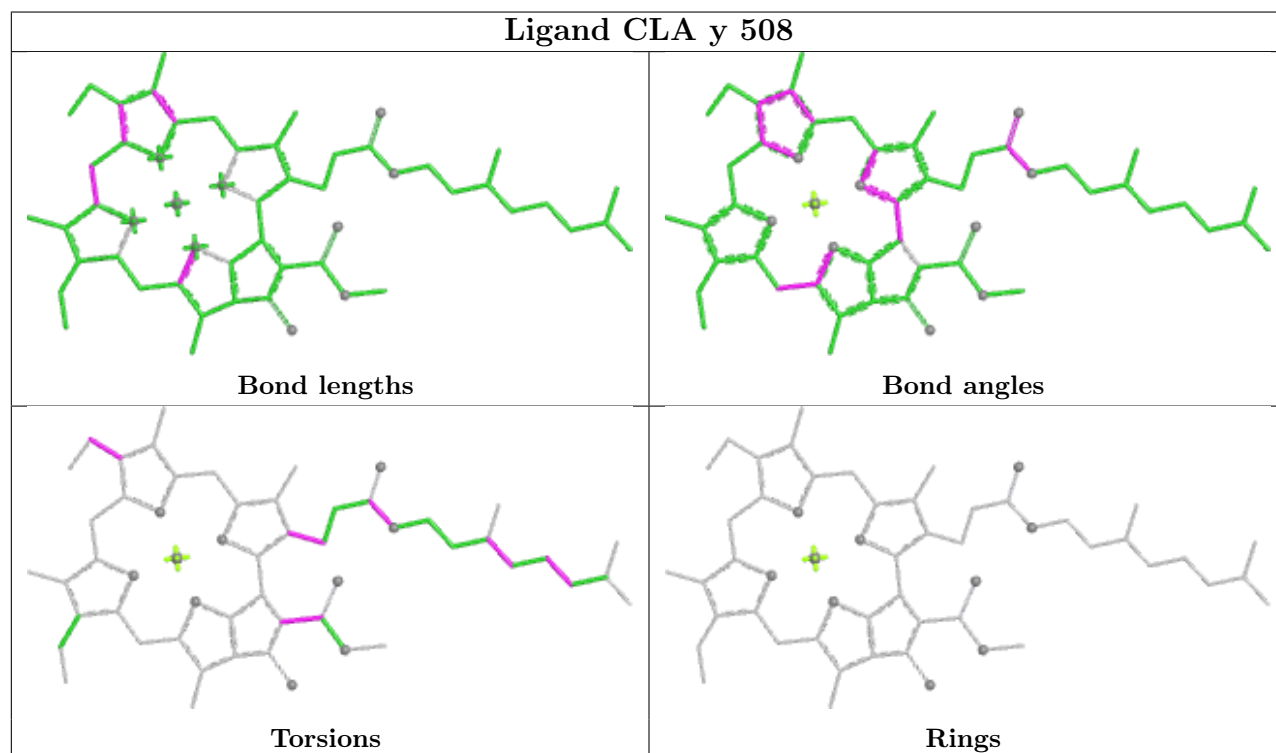
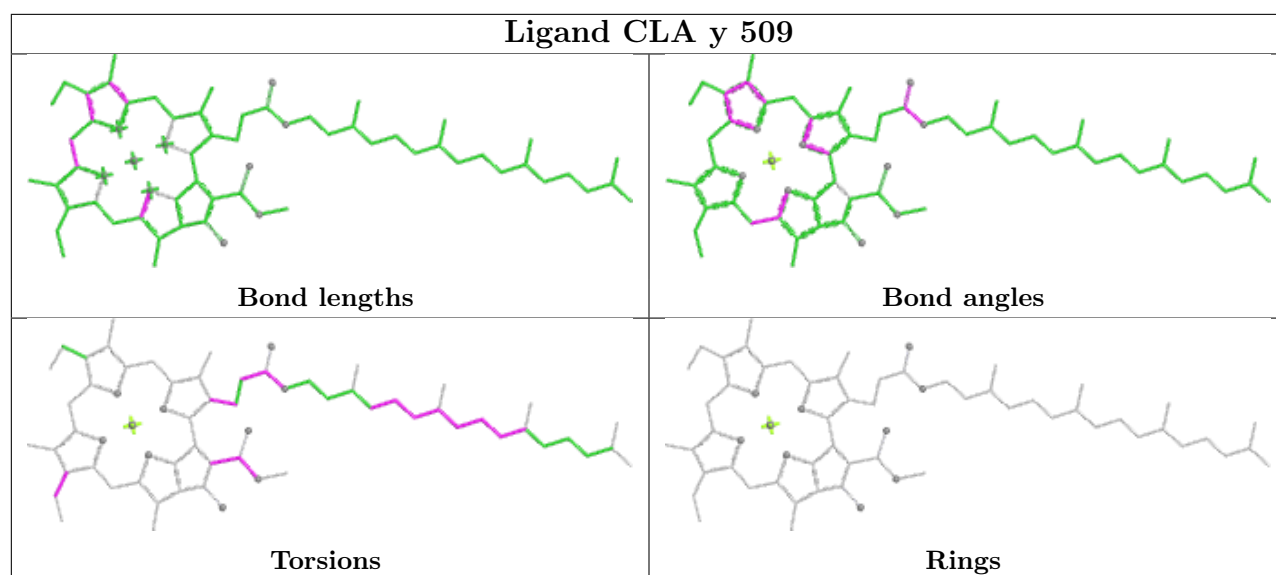
Torsions

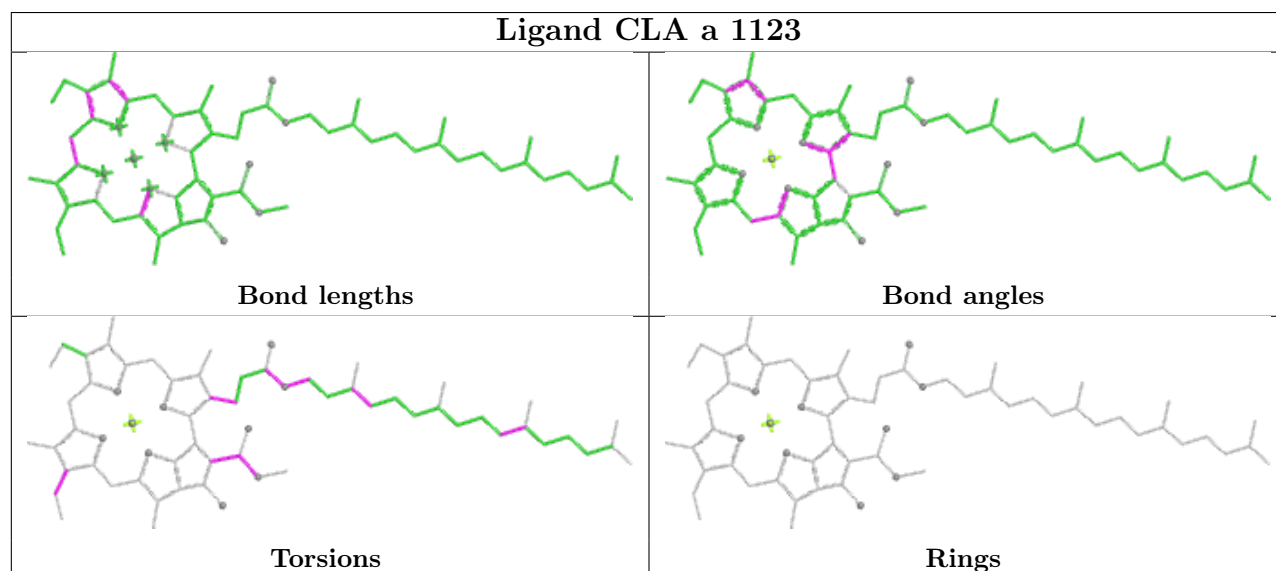
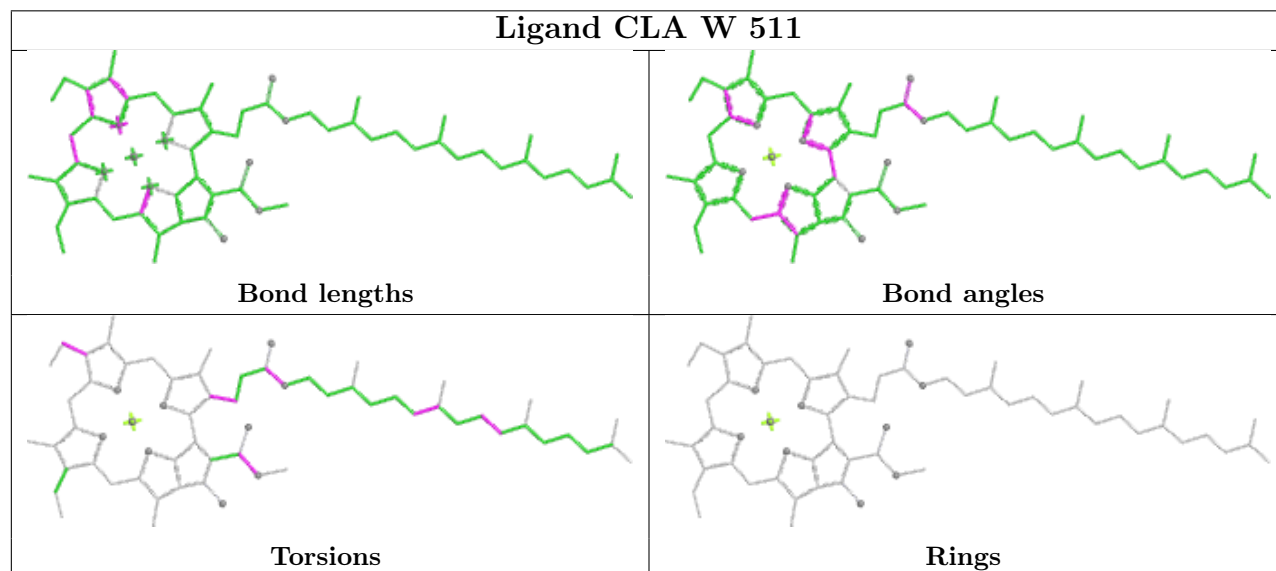
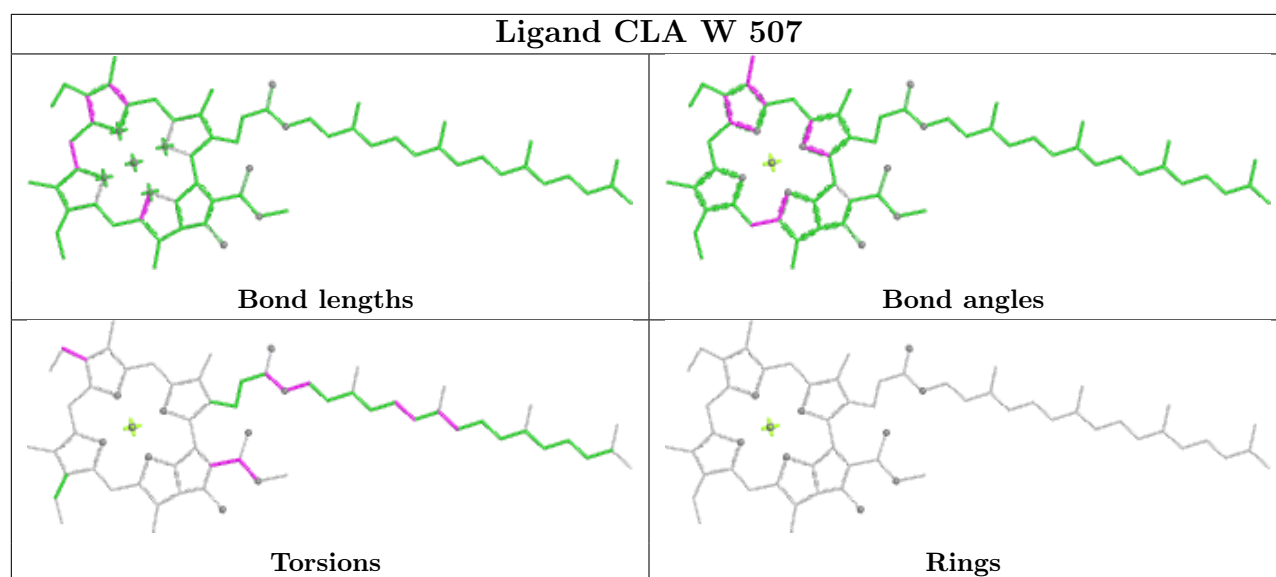


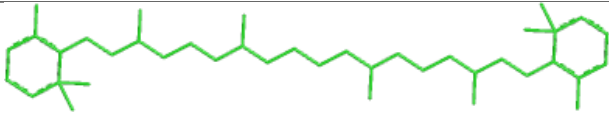
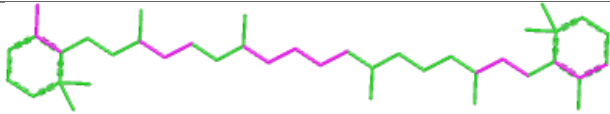
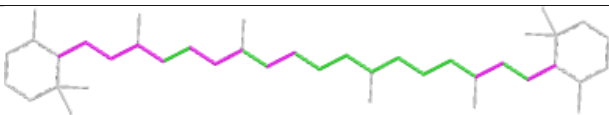
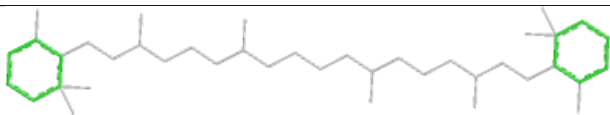
Rings

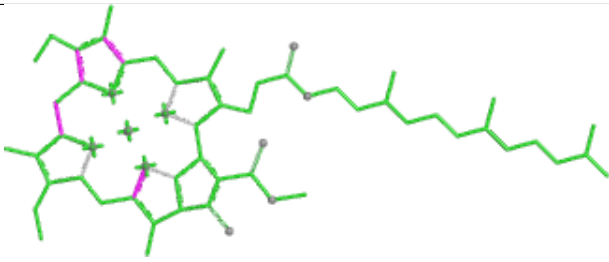
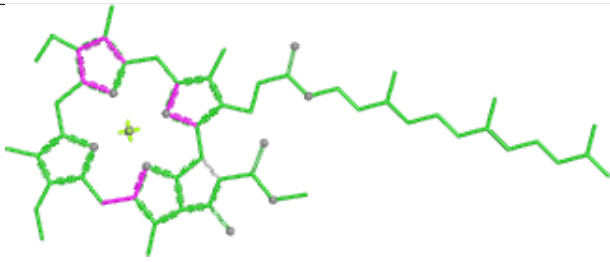
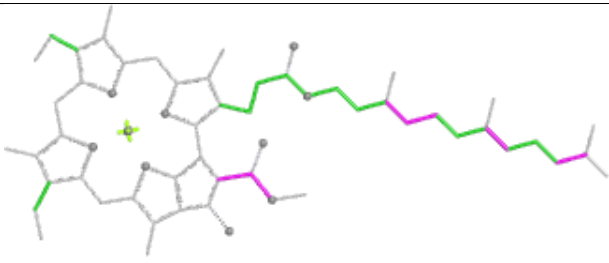
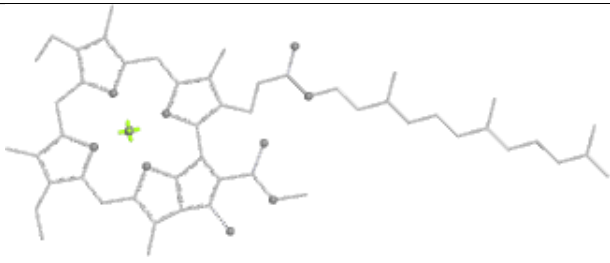


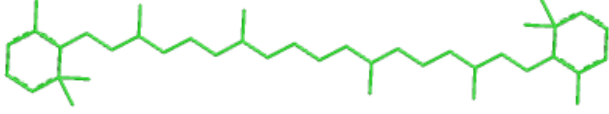
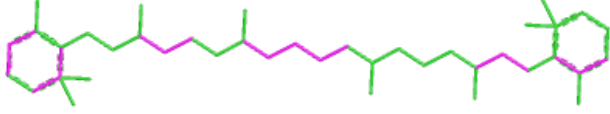
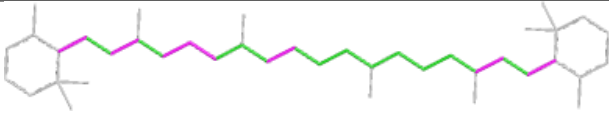
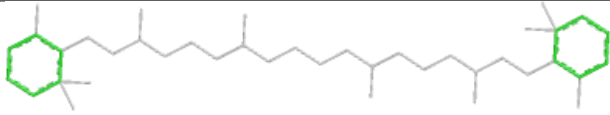


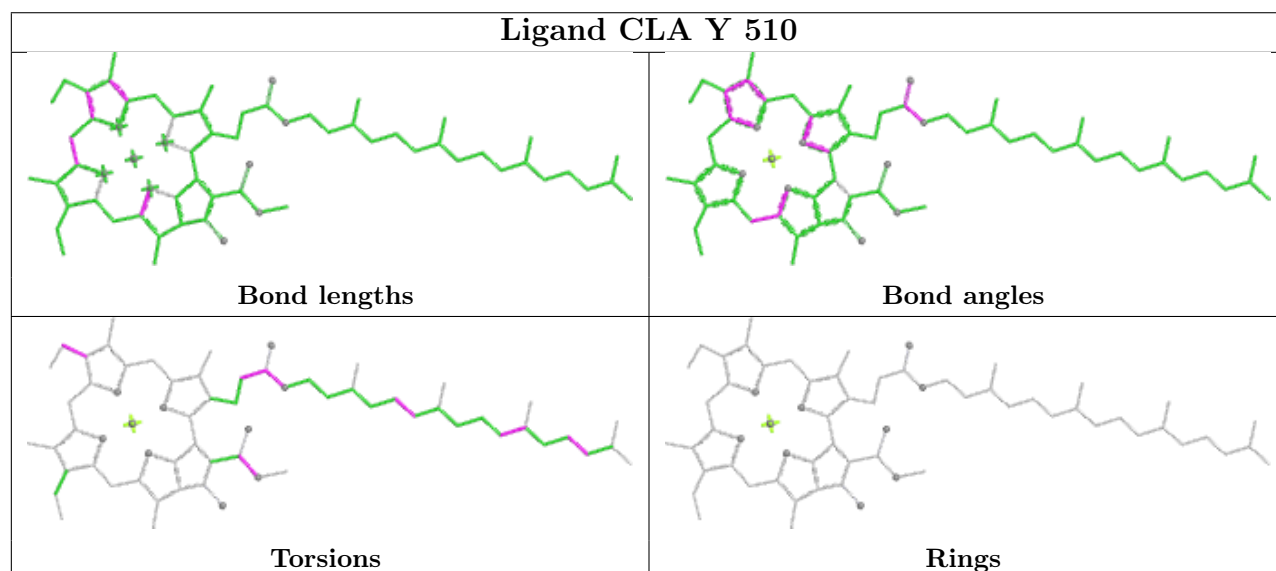
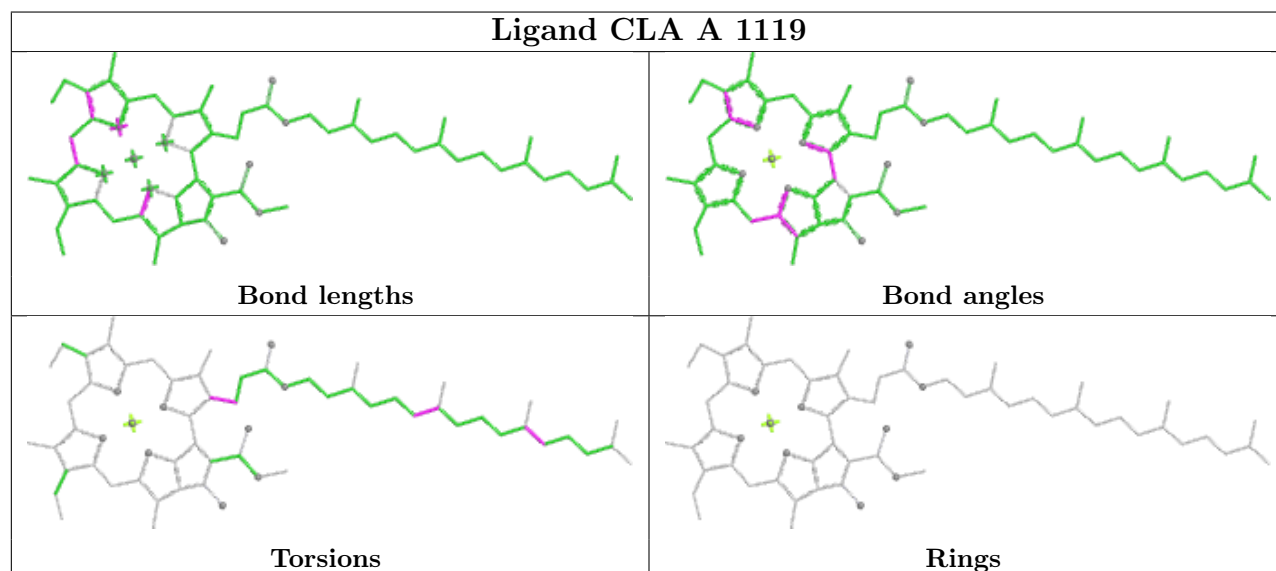
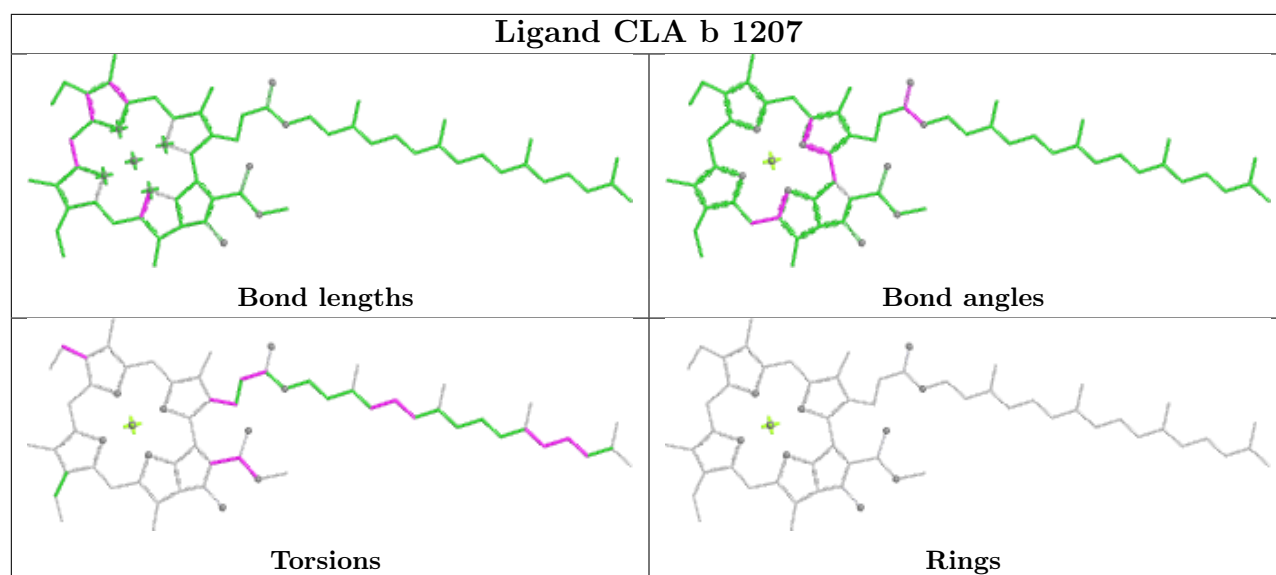


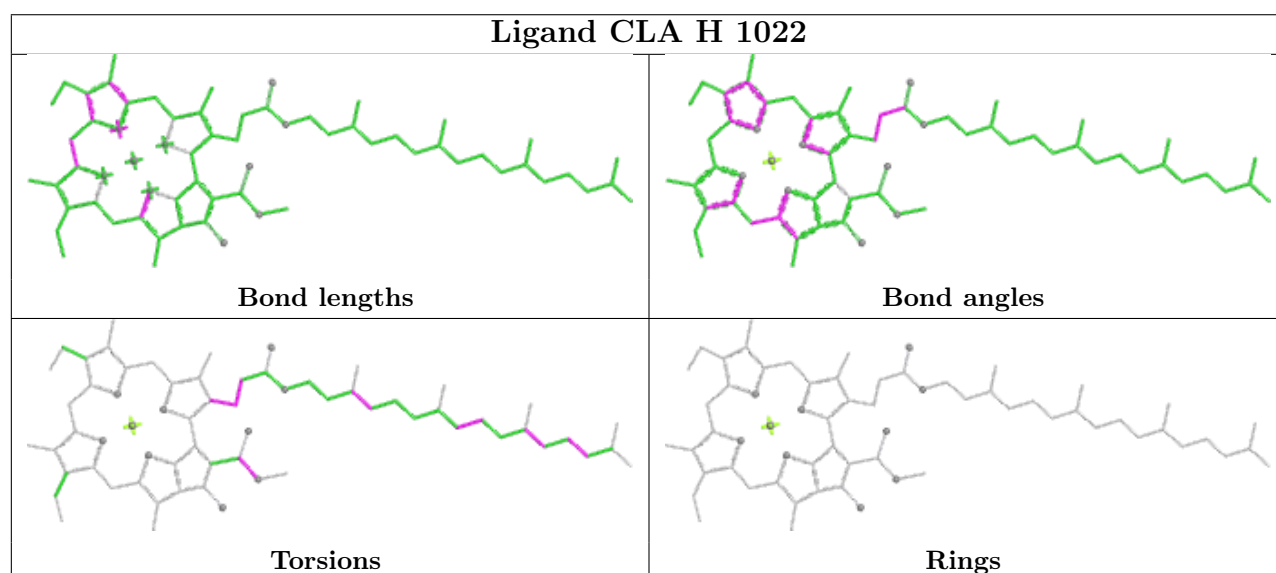
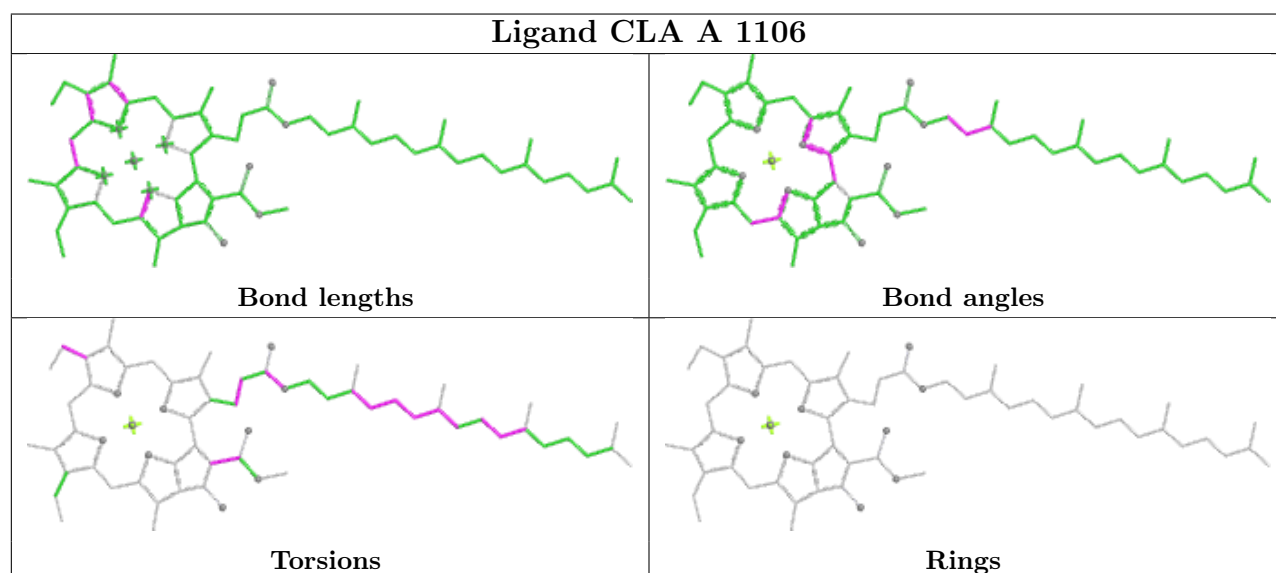
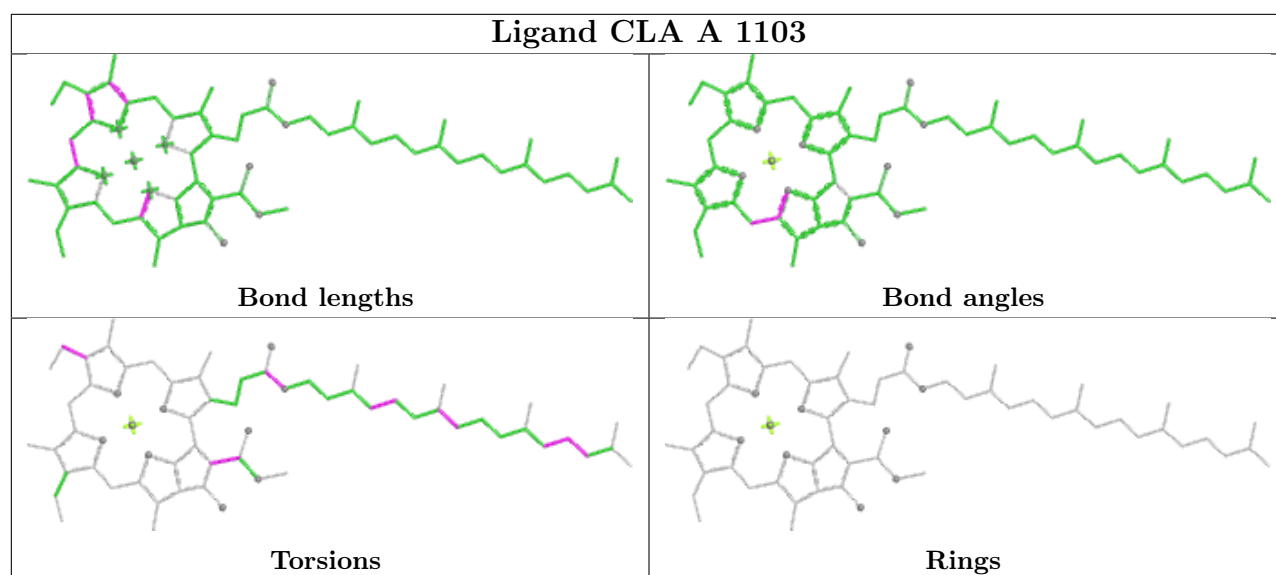


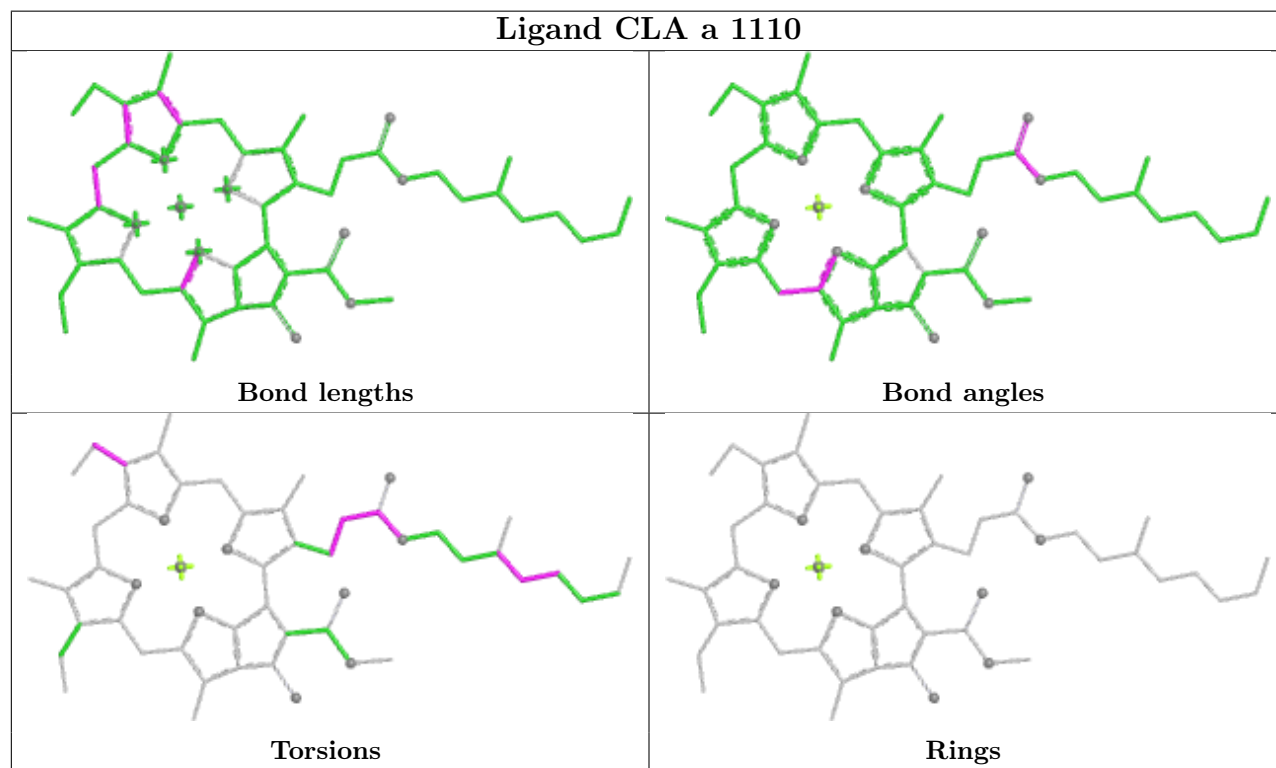
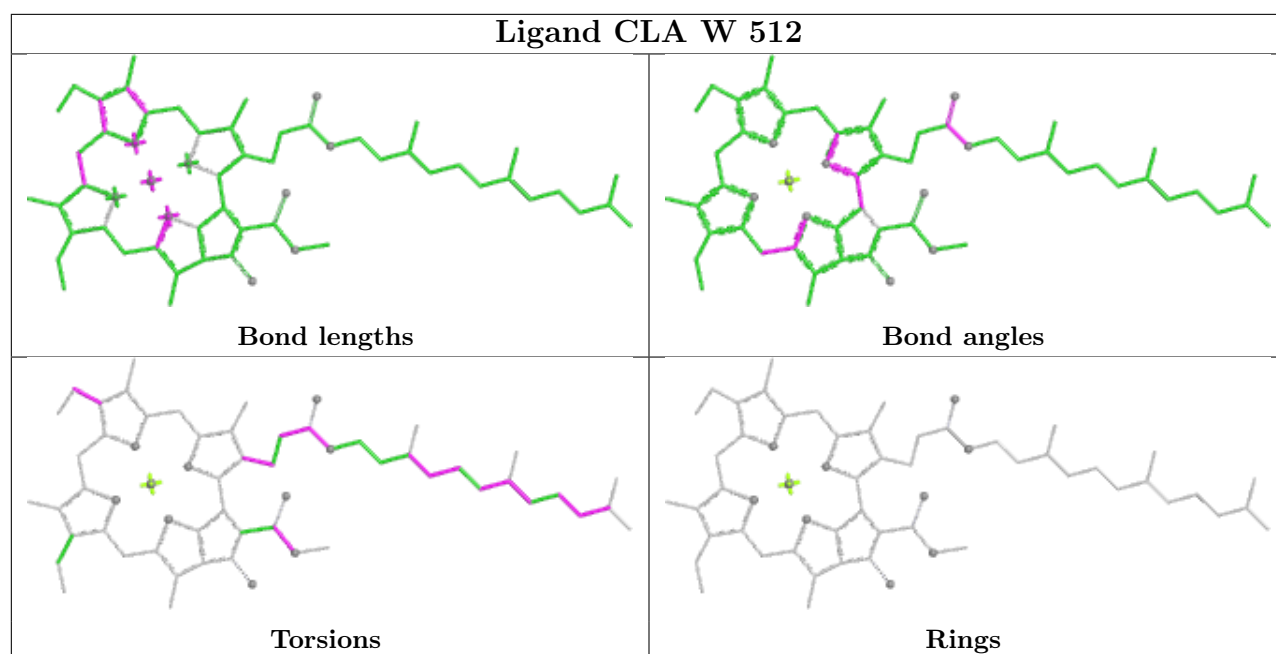
Ligand BCR Y 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

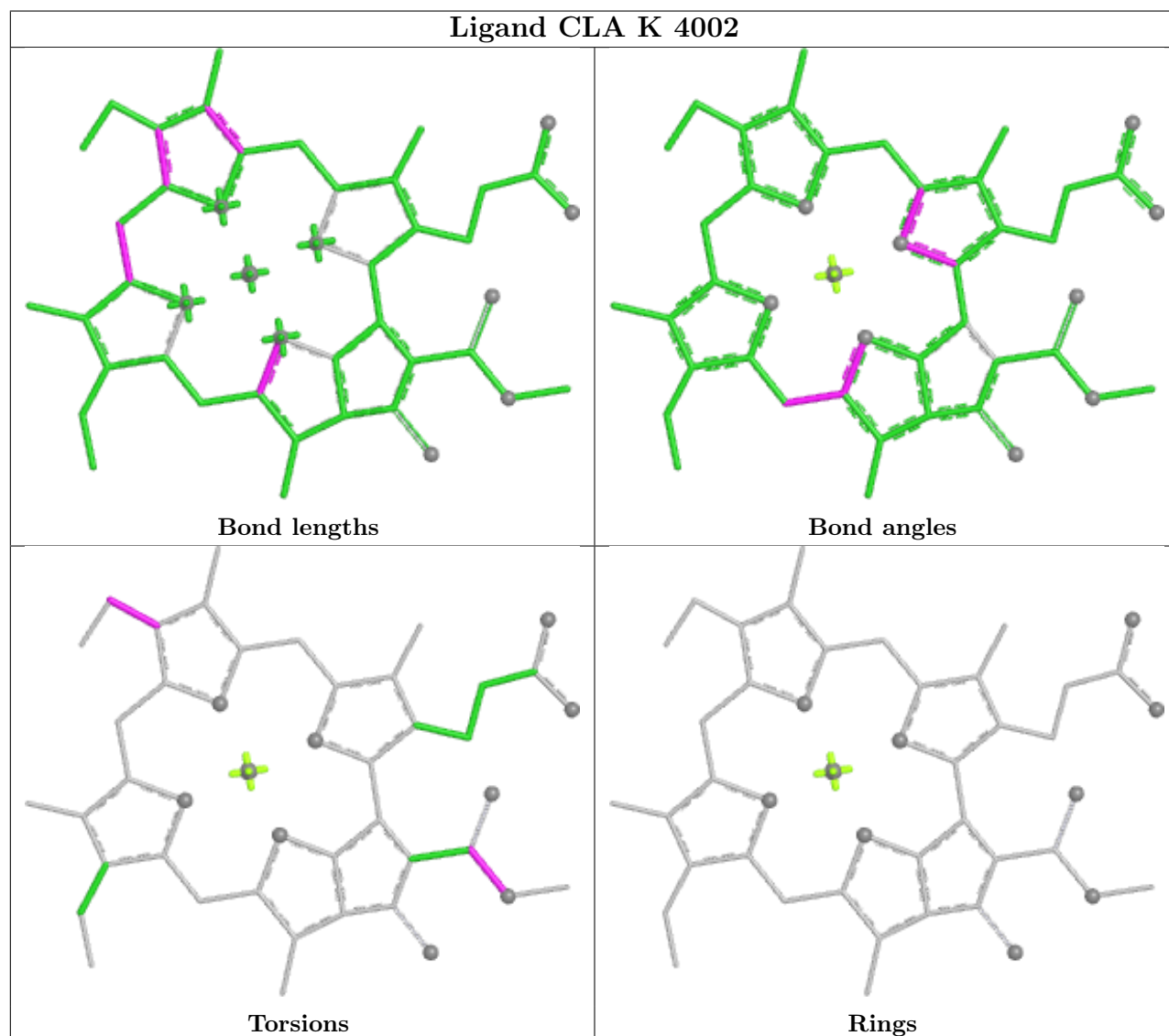
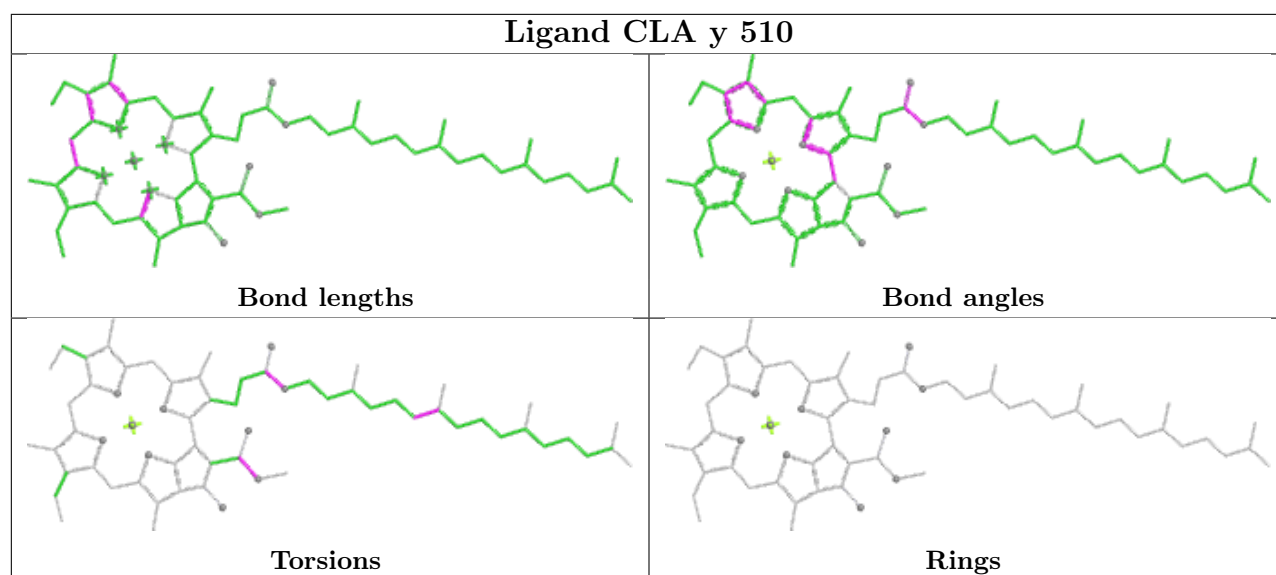
Ligand CLA X 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR p 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

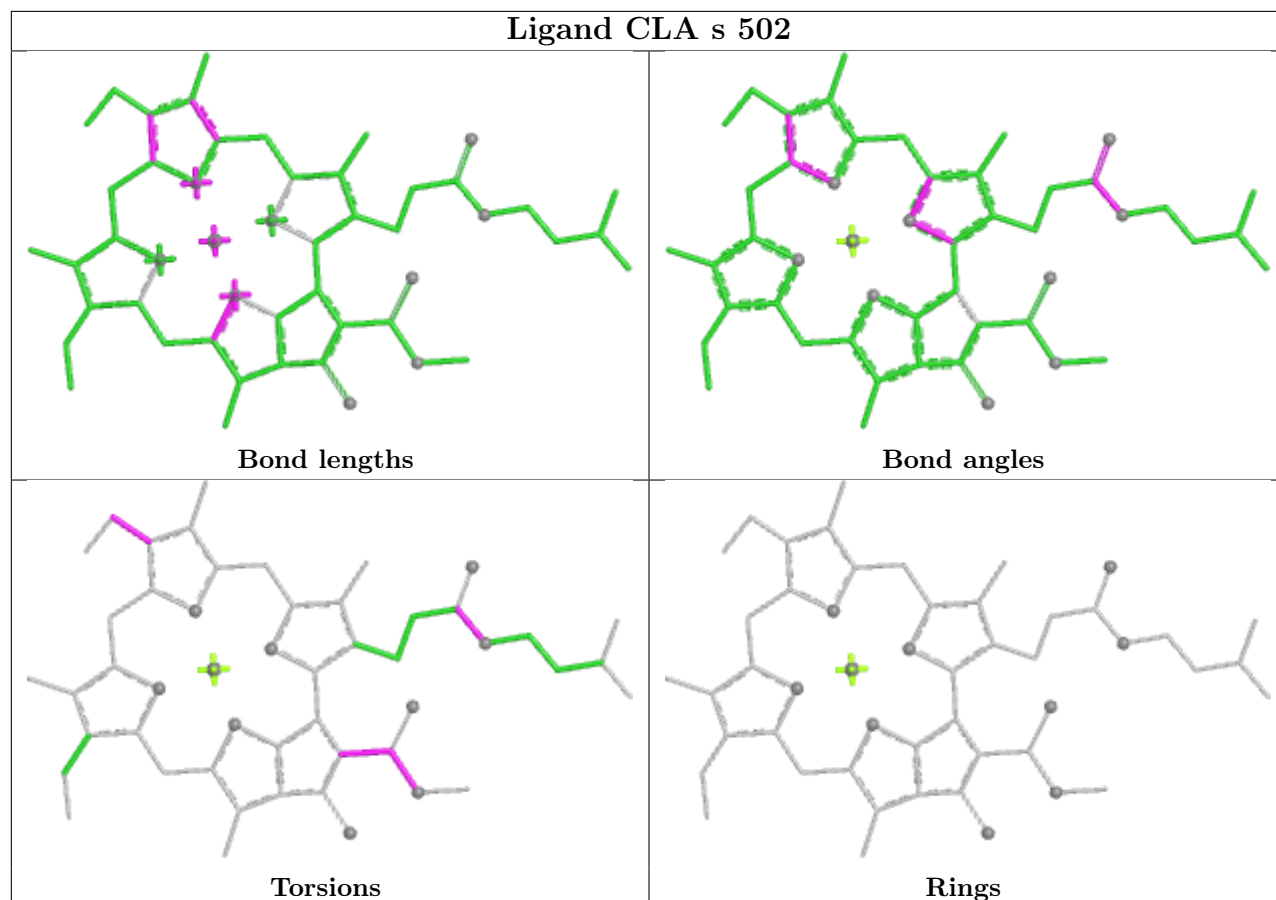




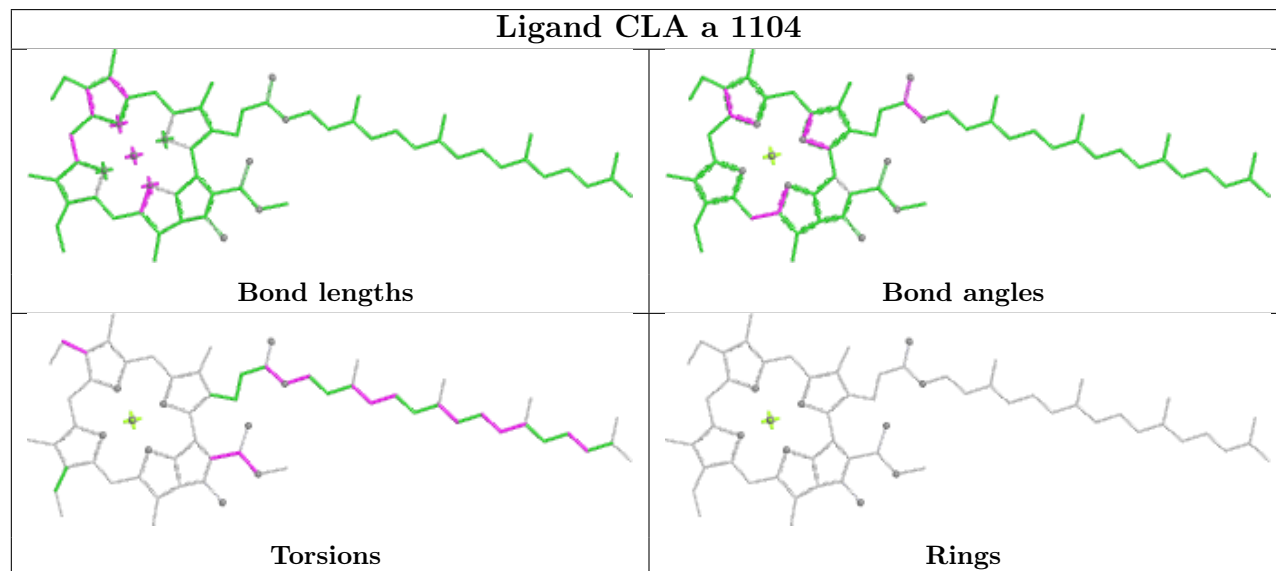


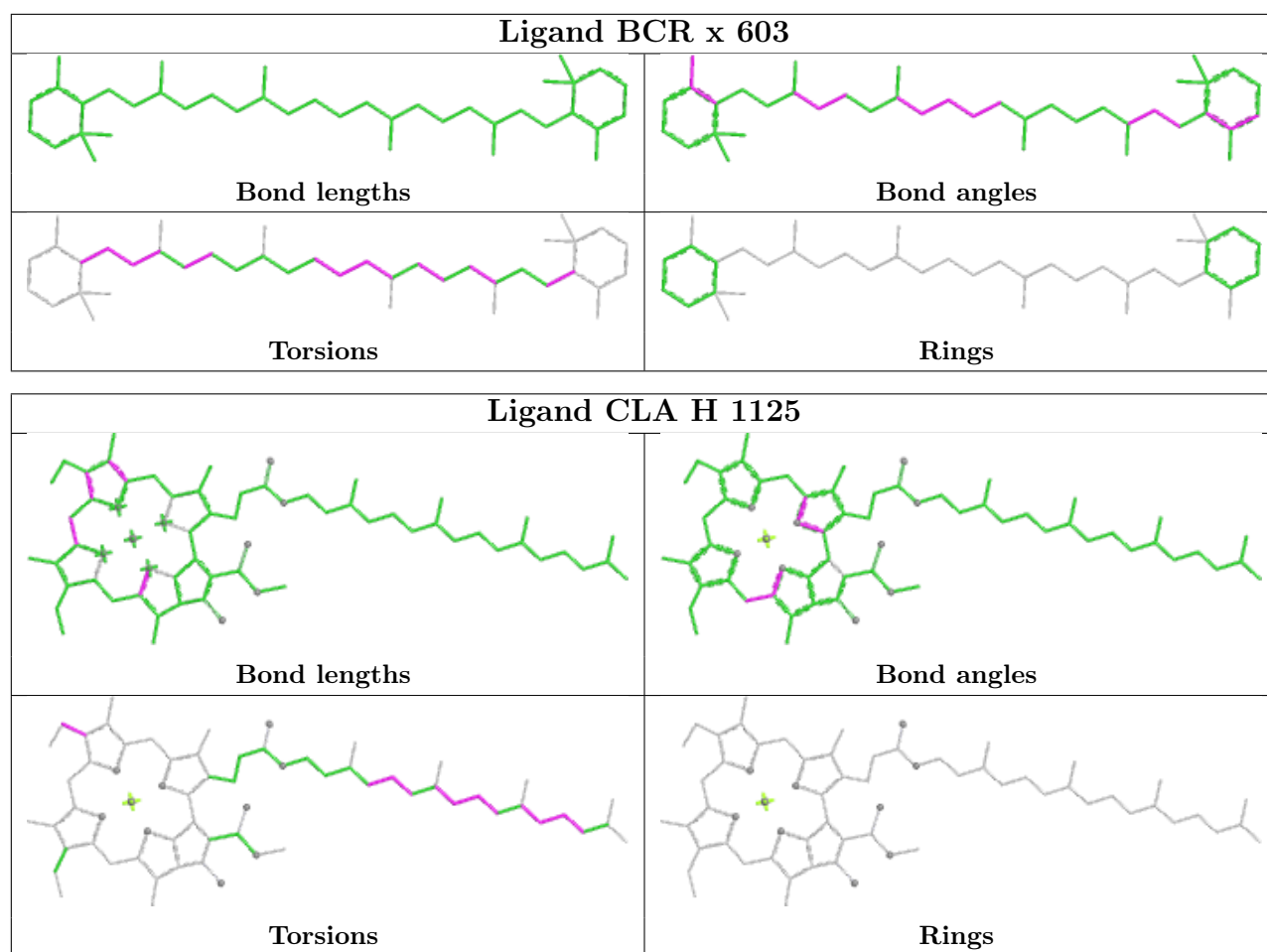


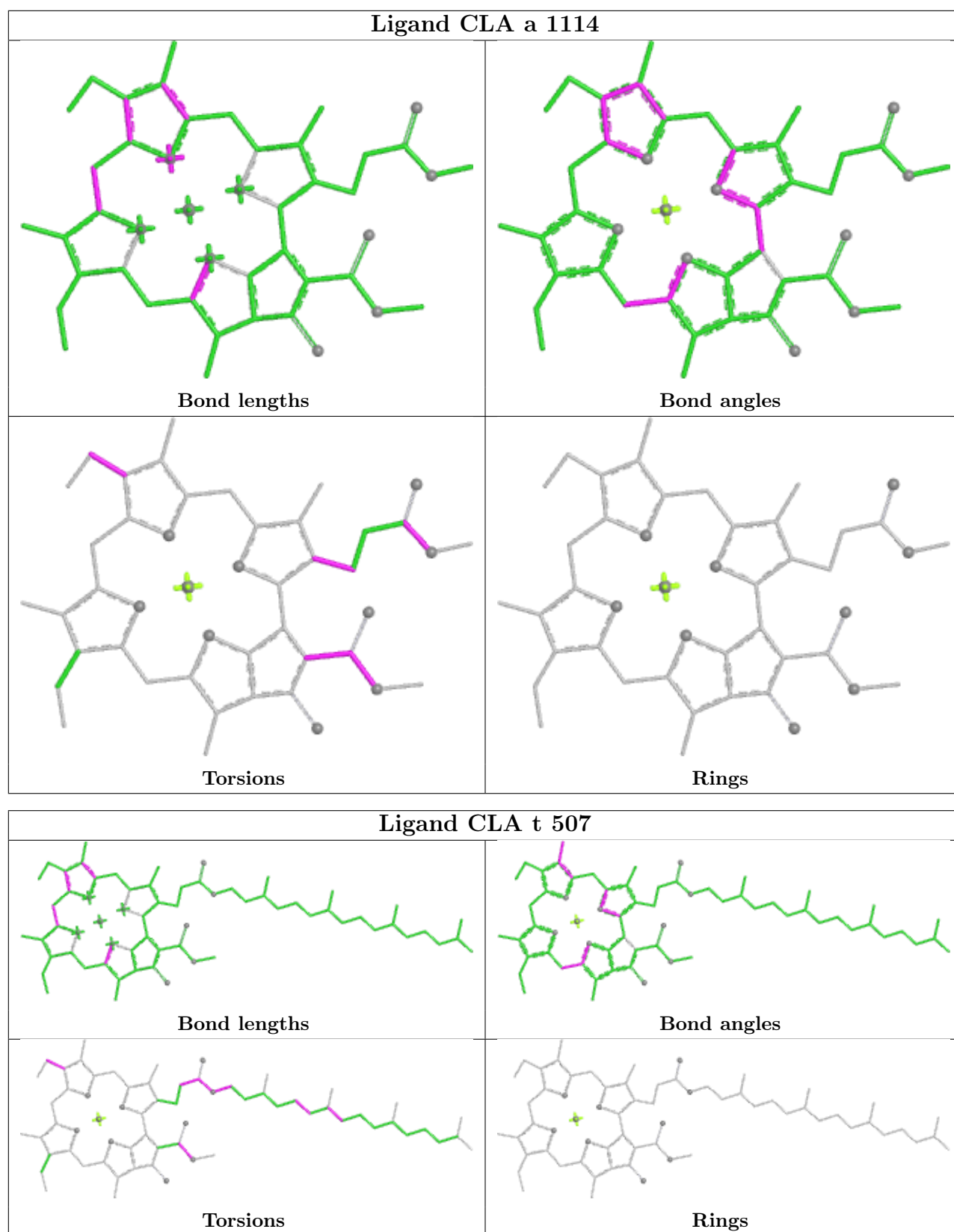
Ligand CLA s 502

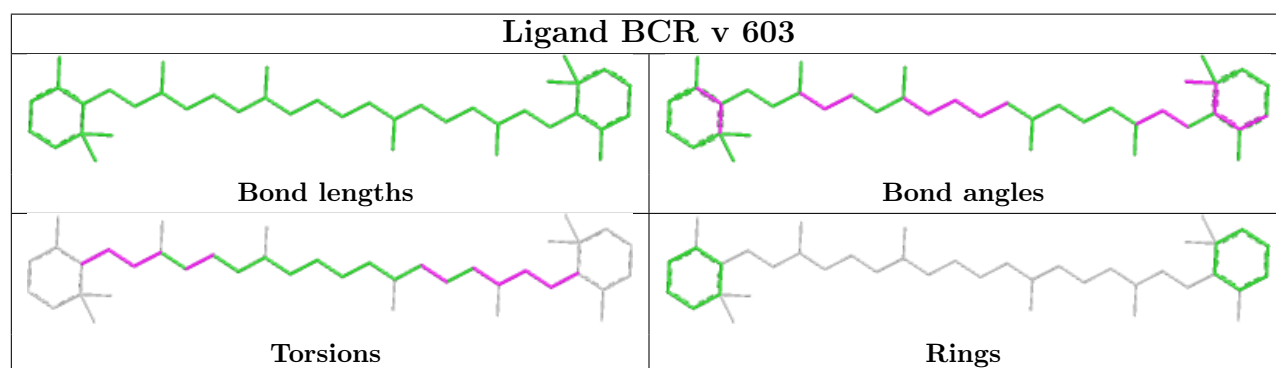
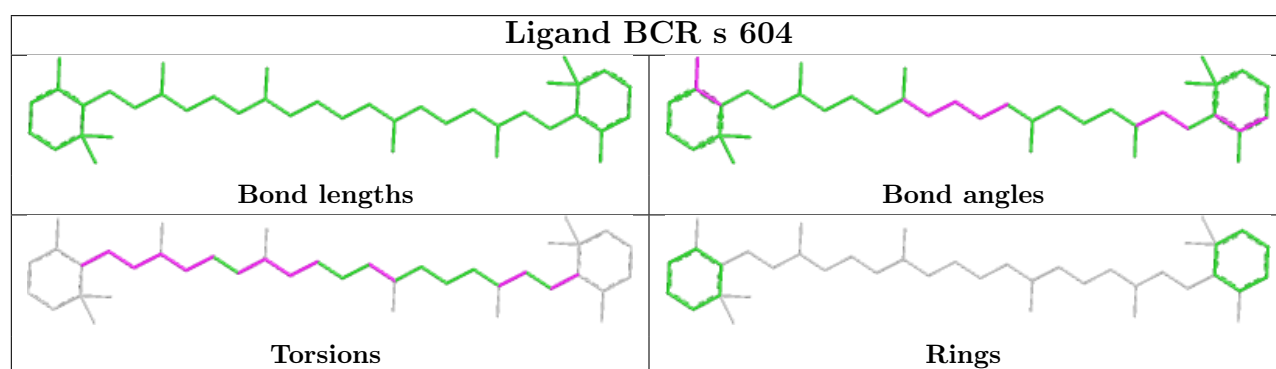
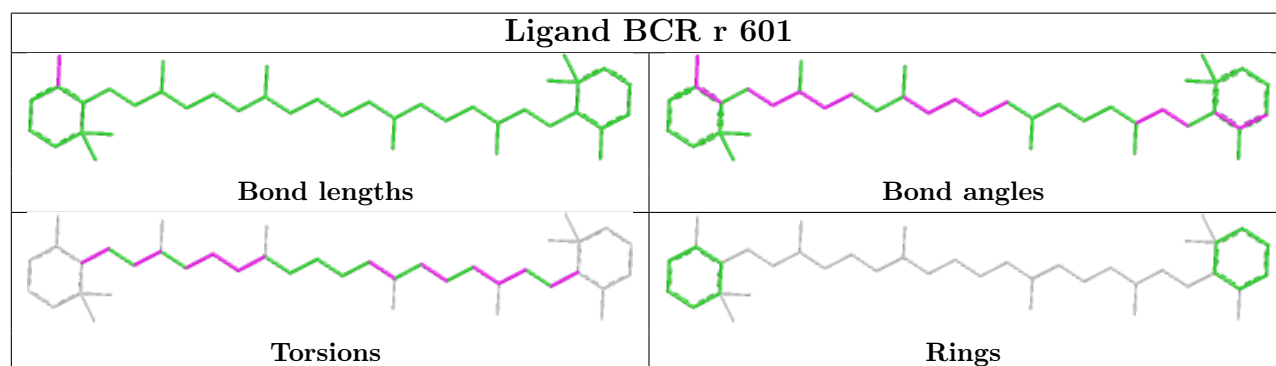
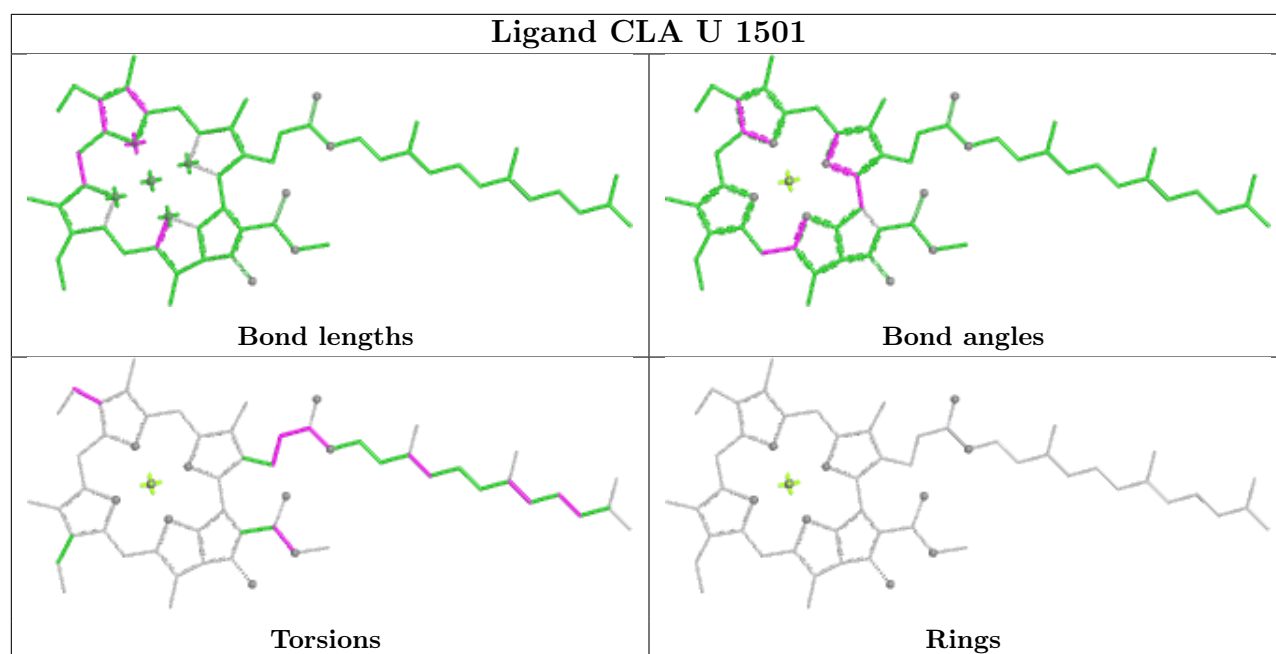


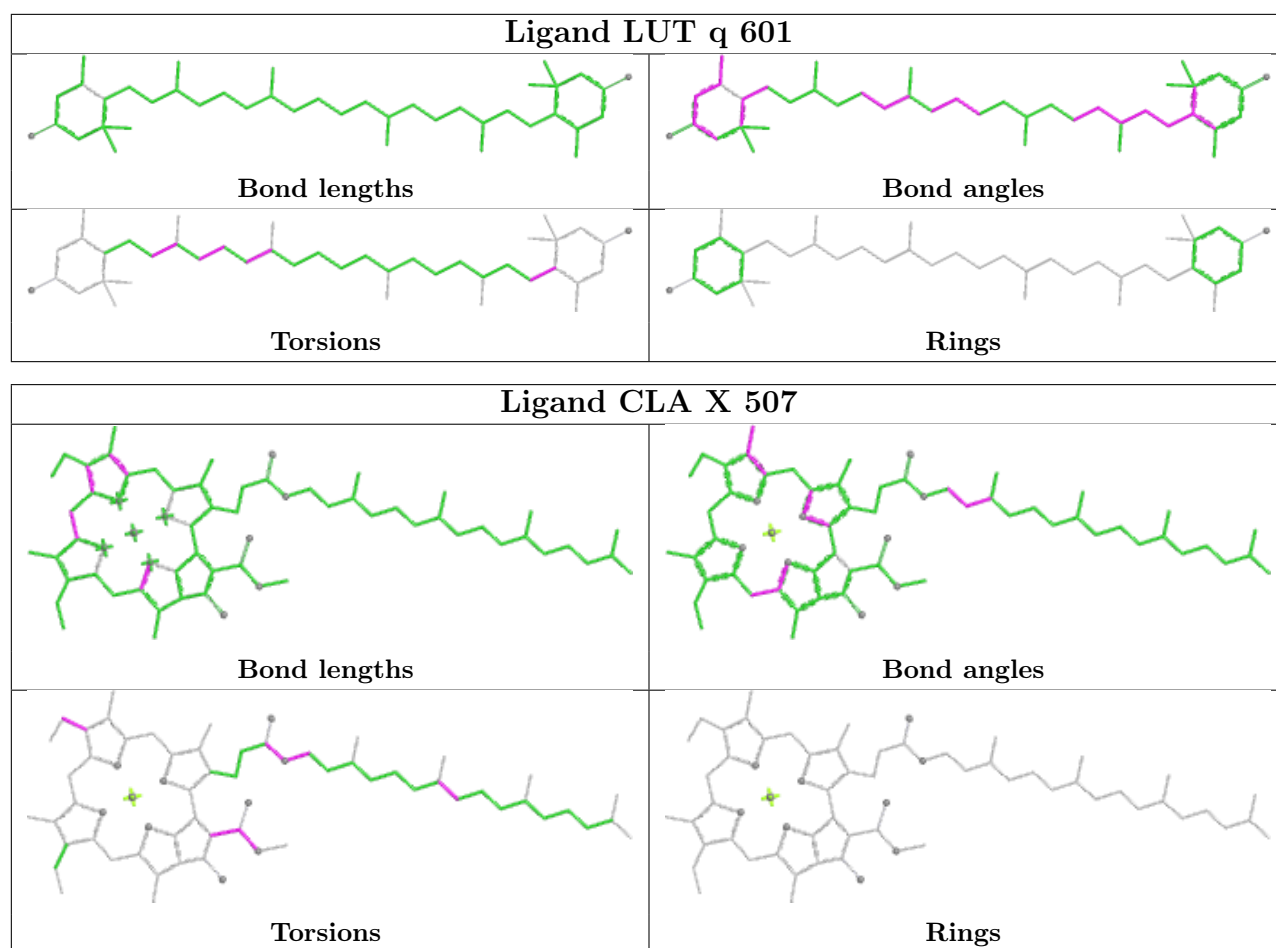
Ligand CLA a 1104

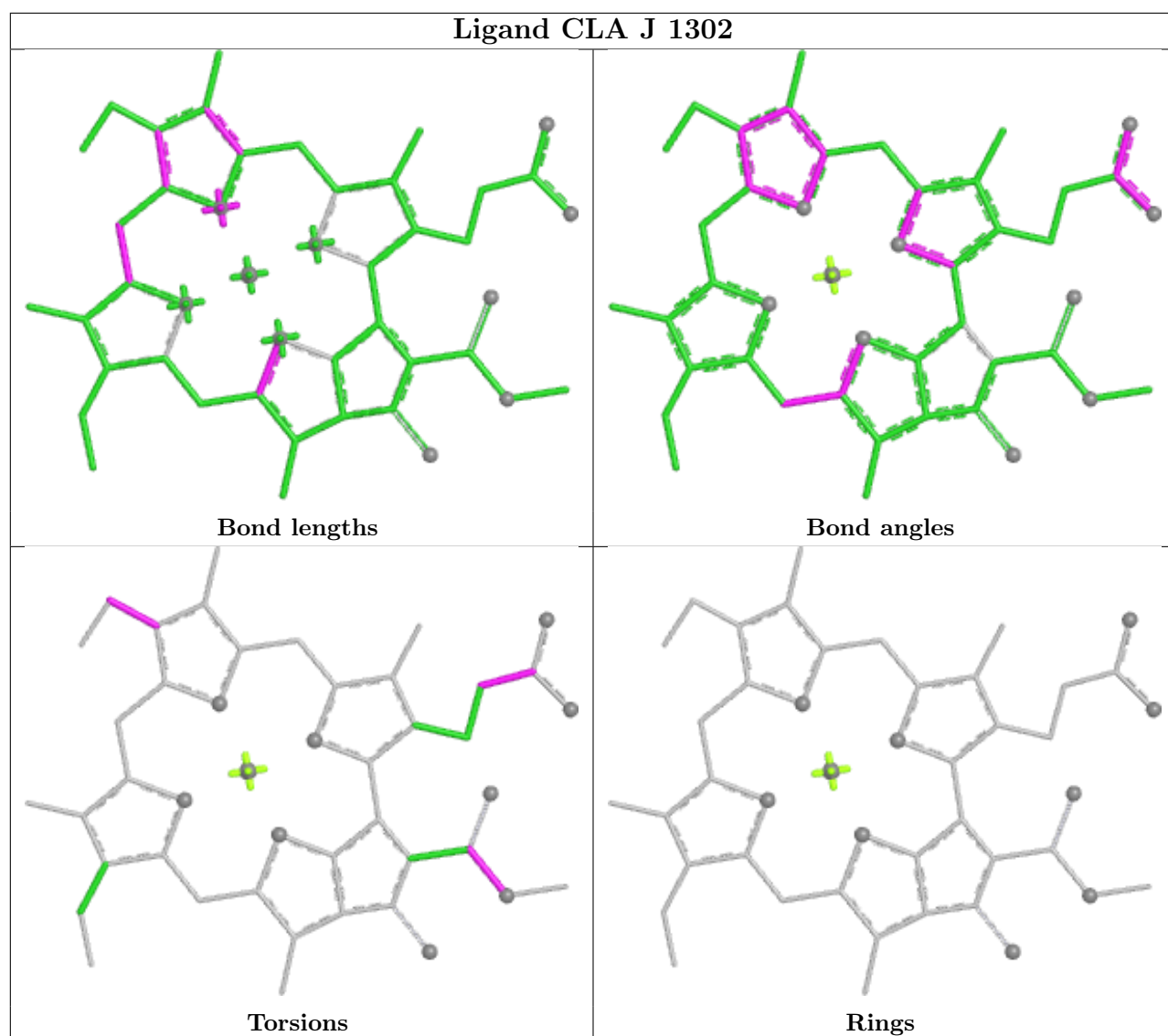




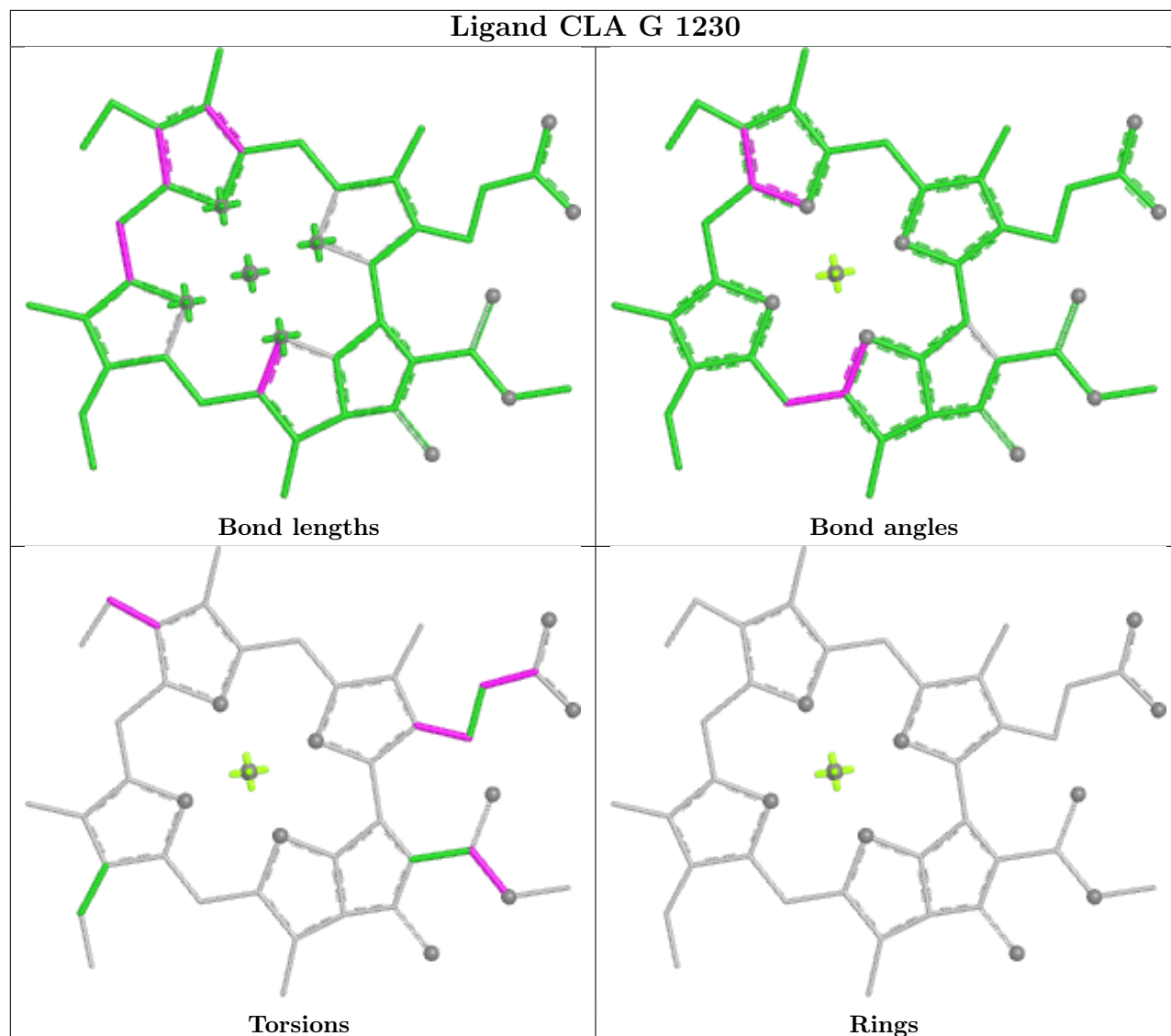




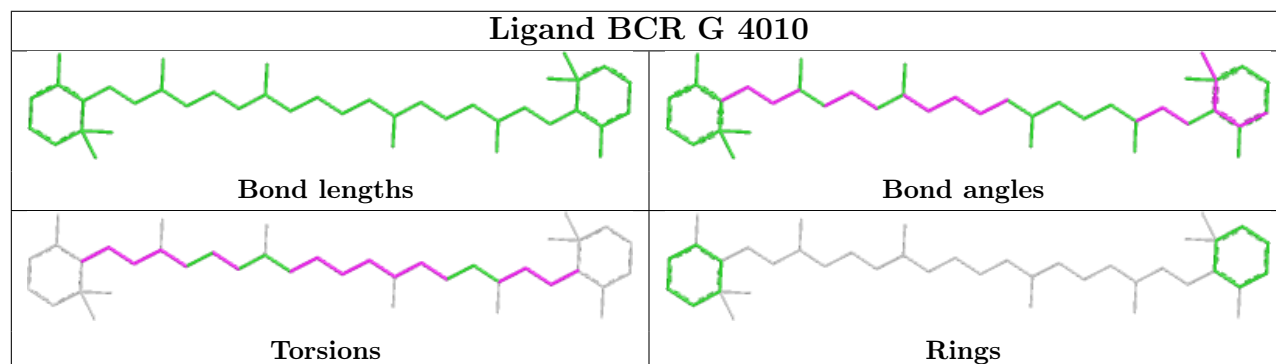


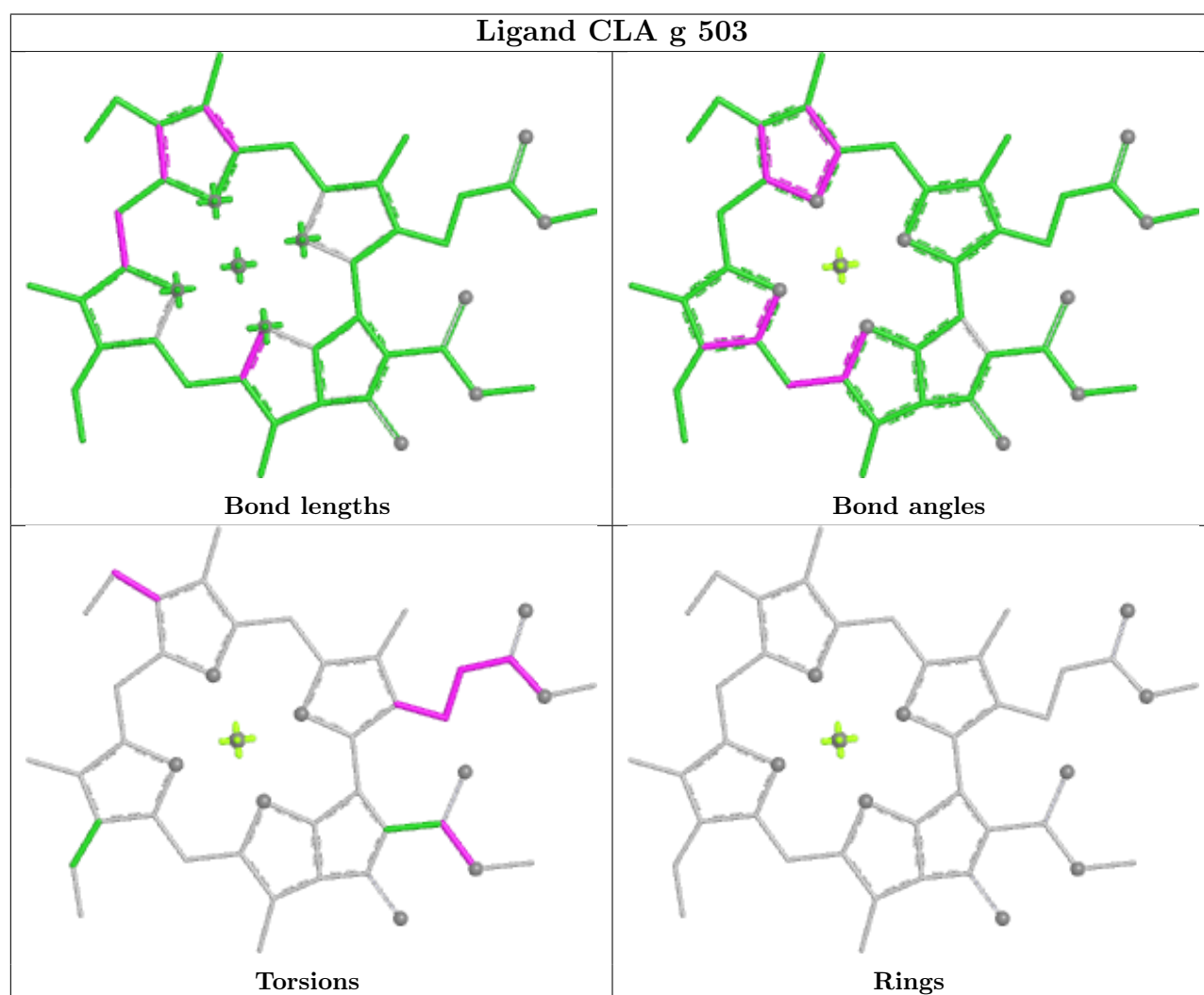
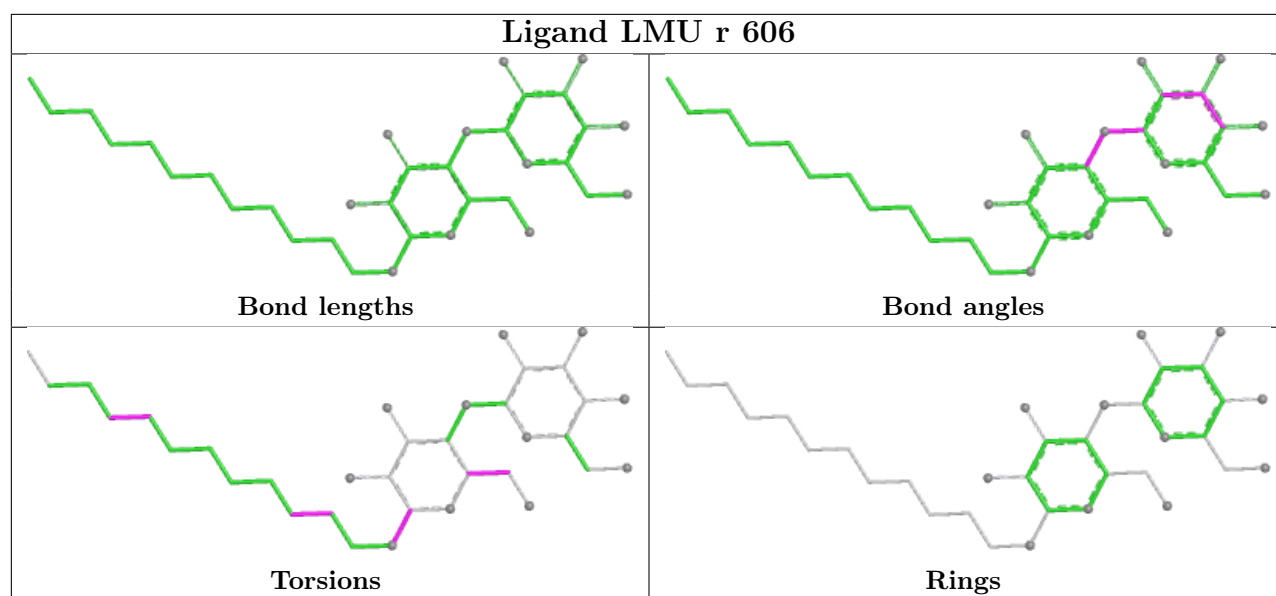


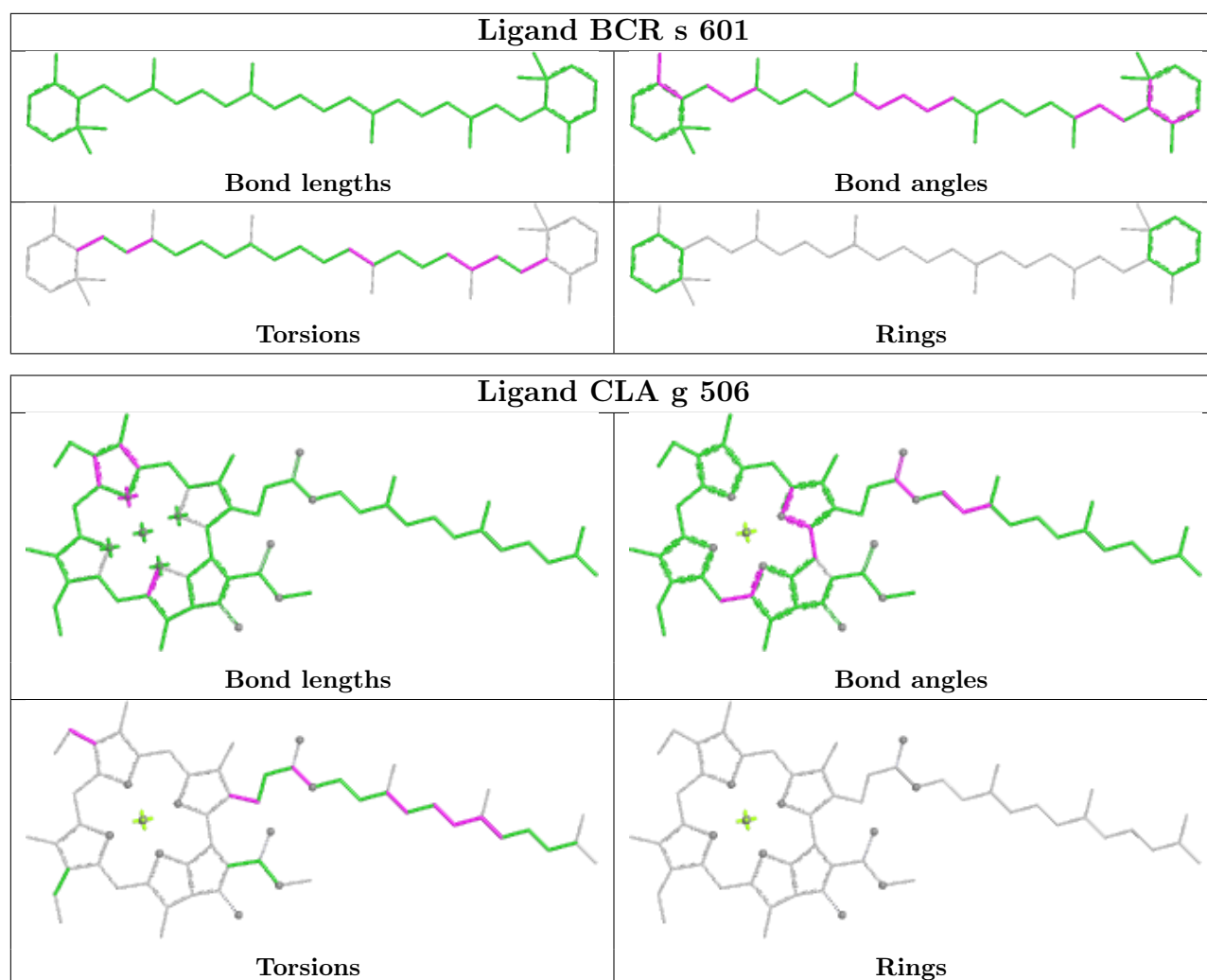
Ligand CLA G 1230



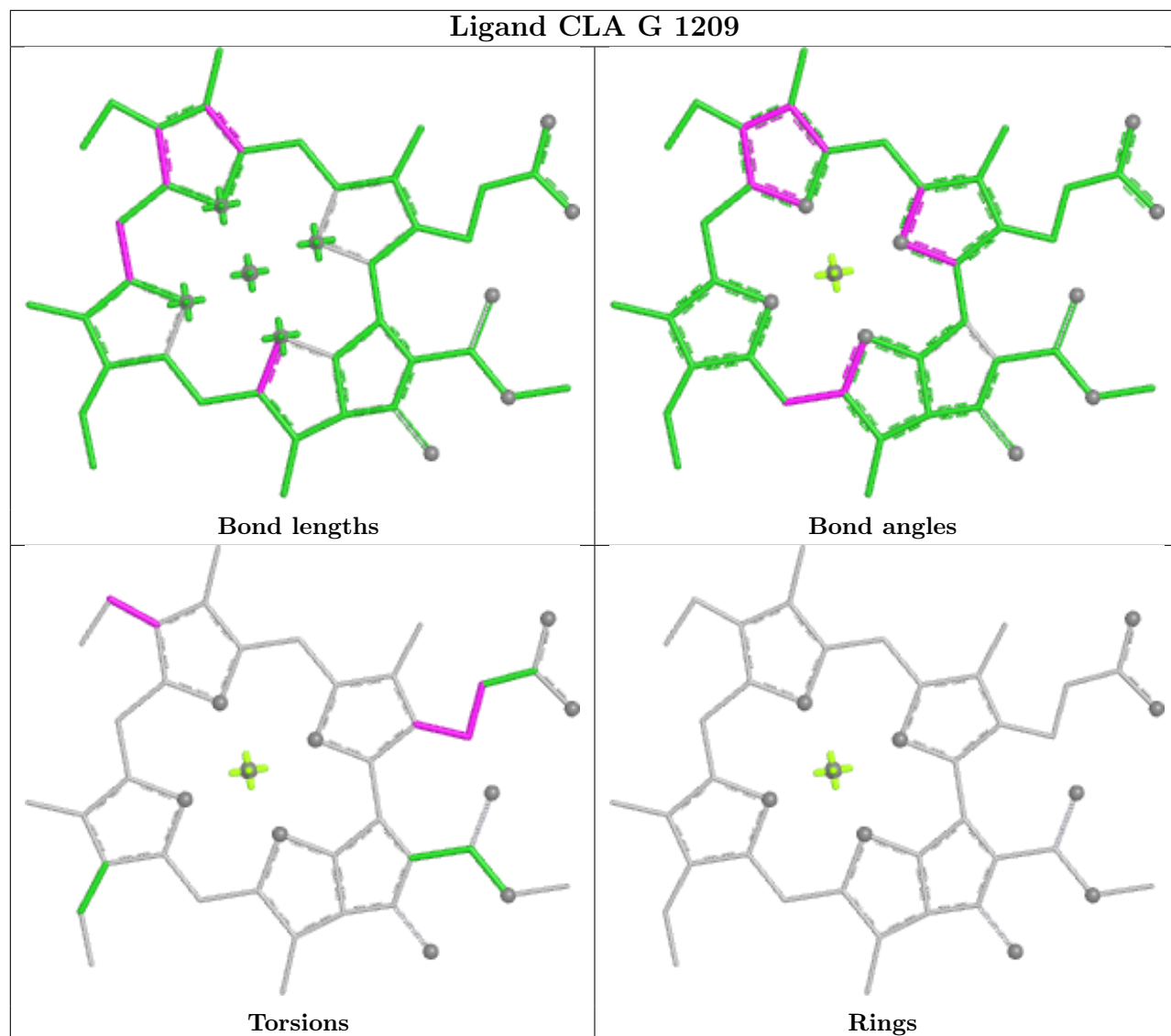
Ligand BCR G 4010

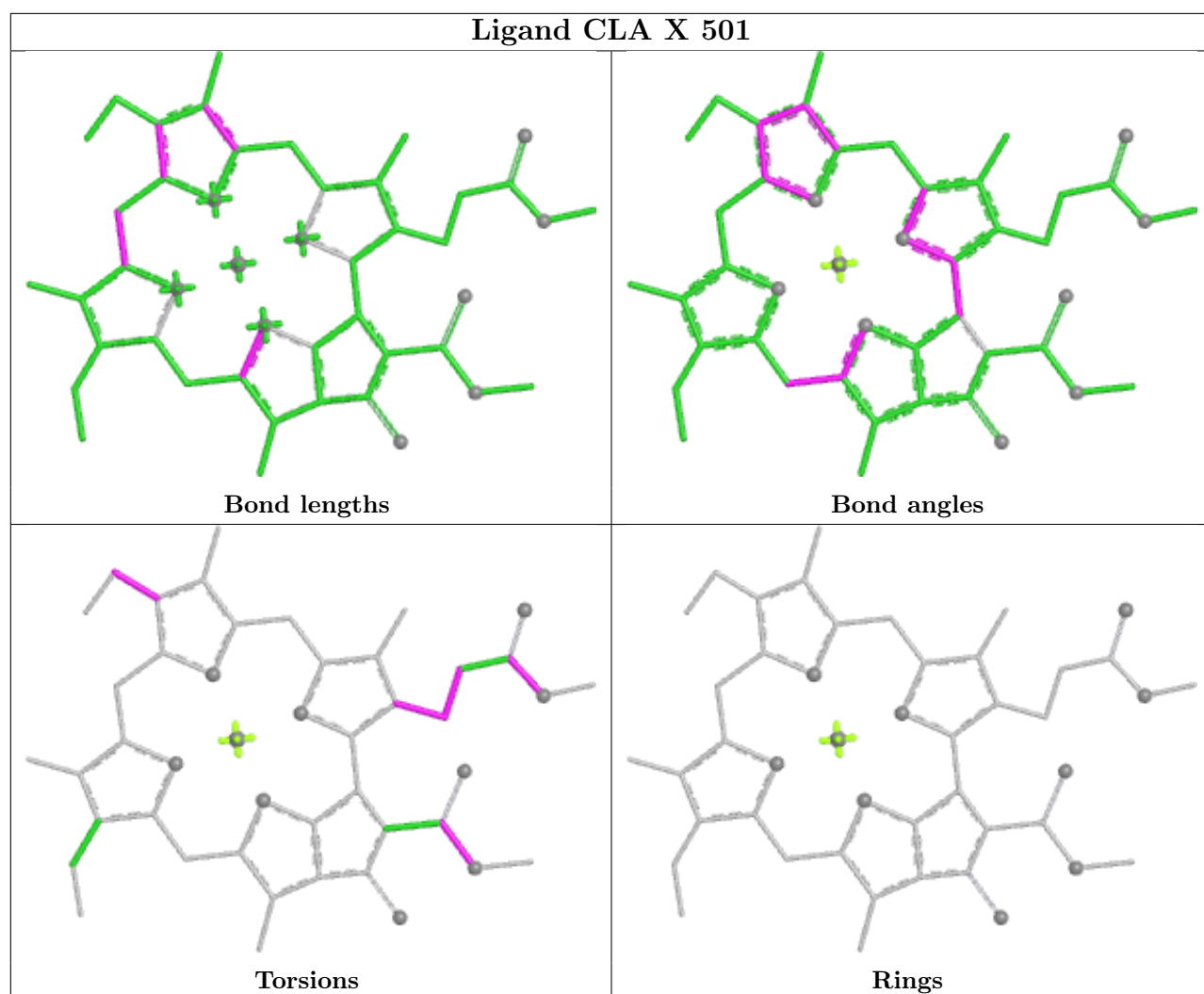




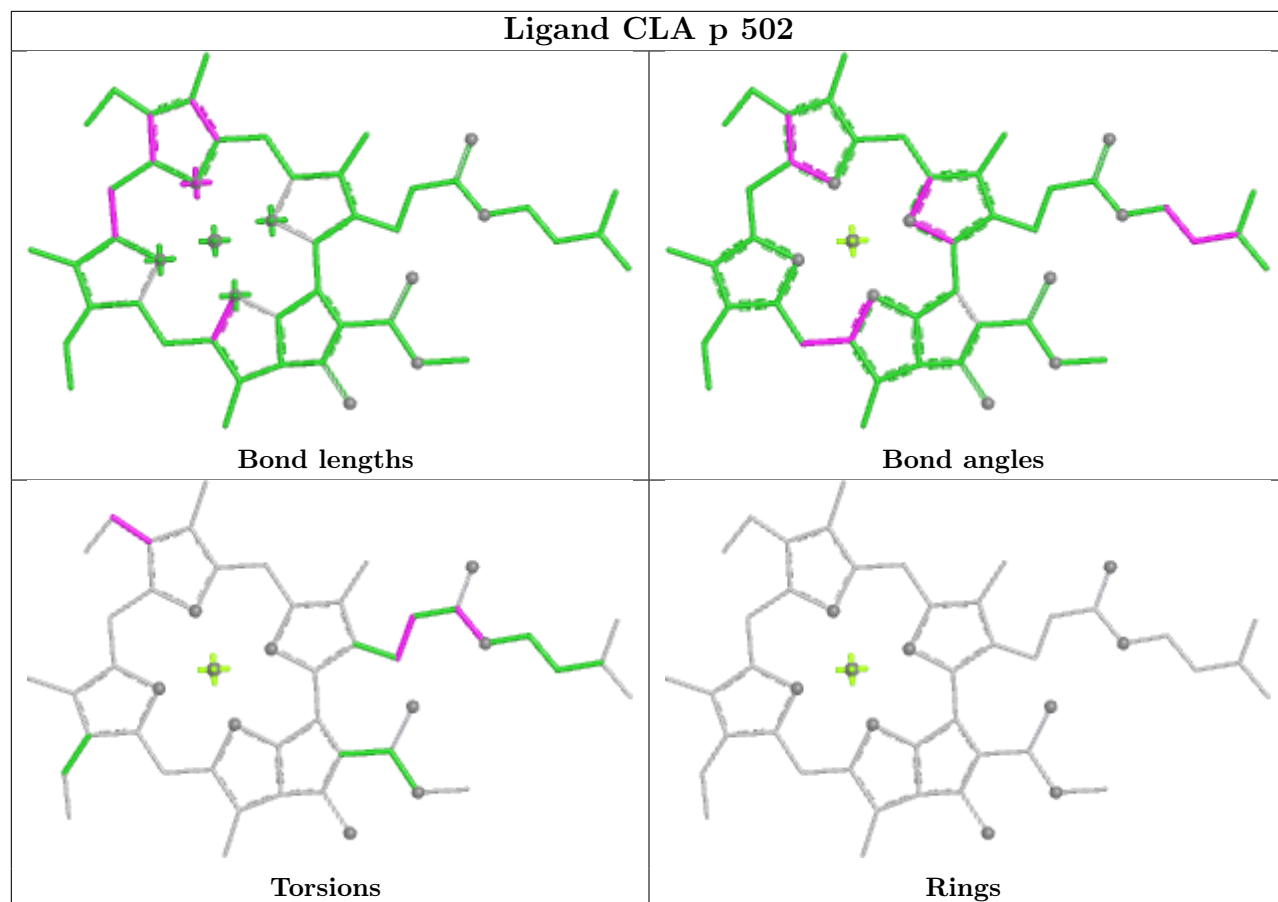


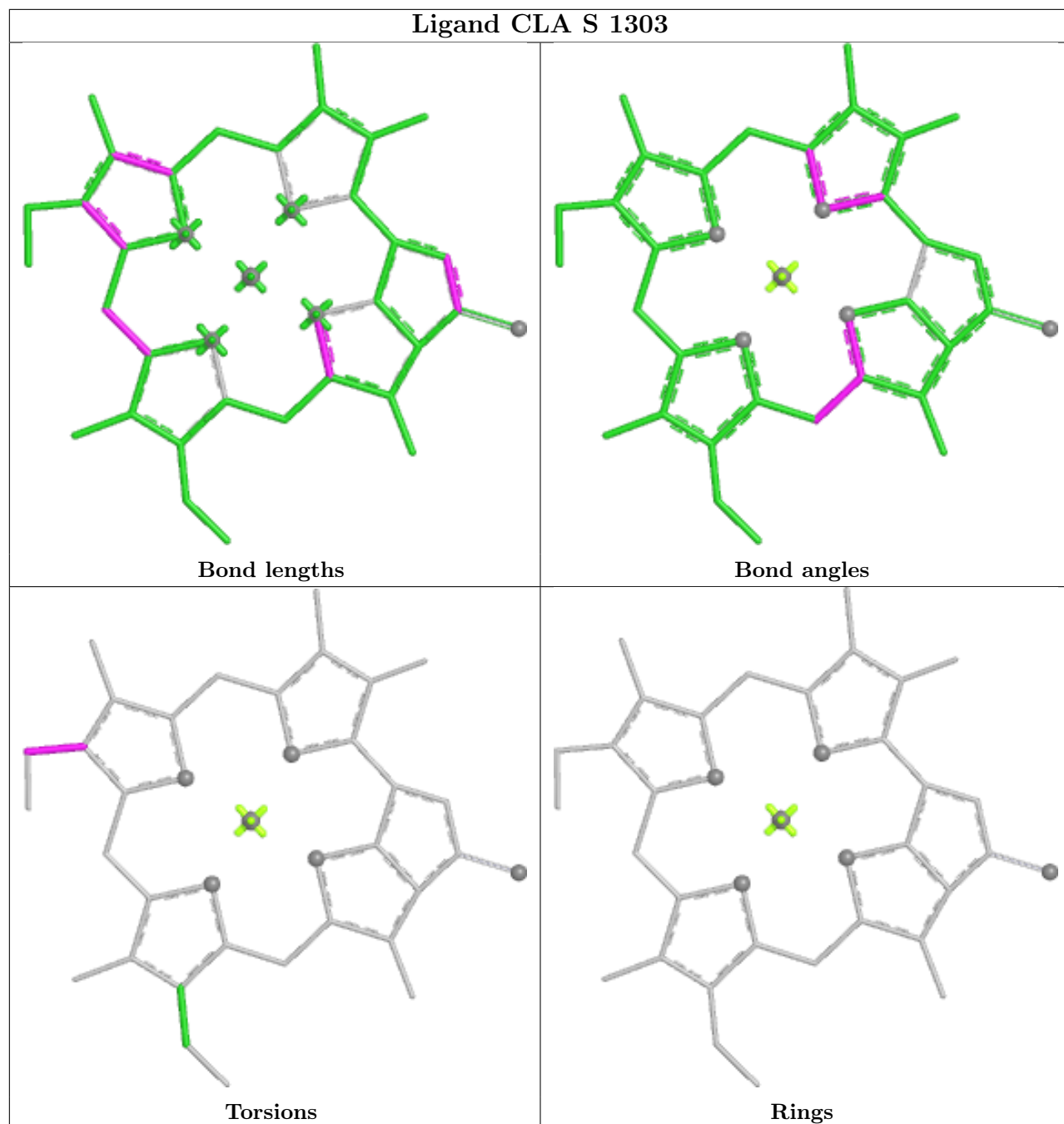
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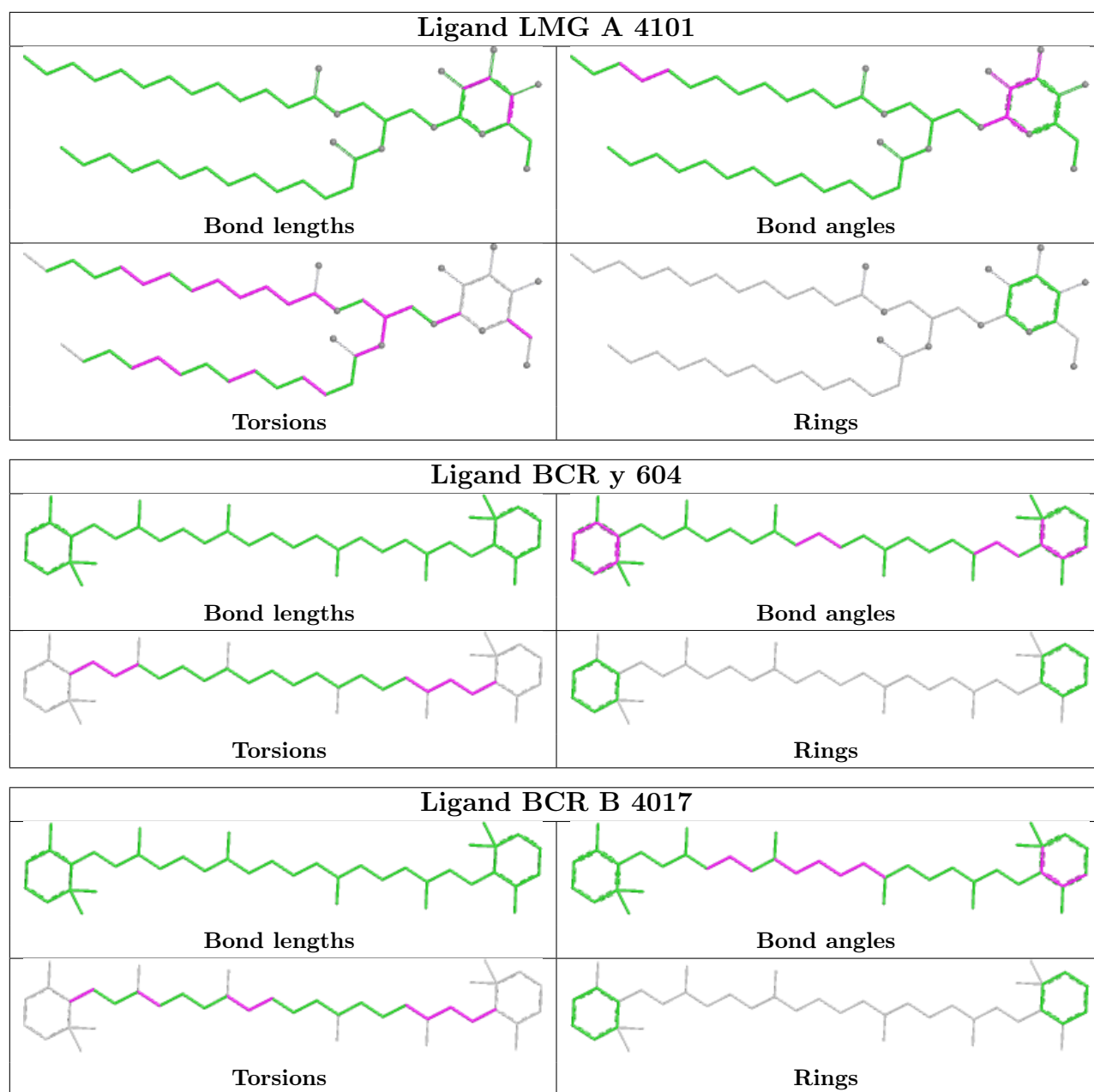


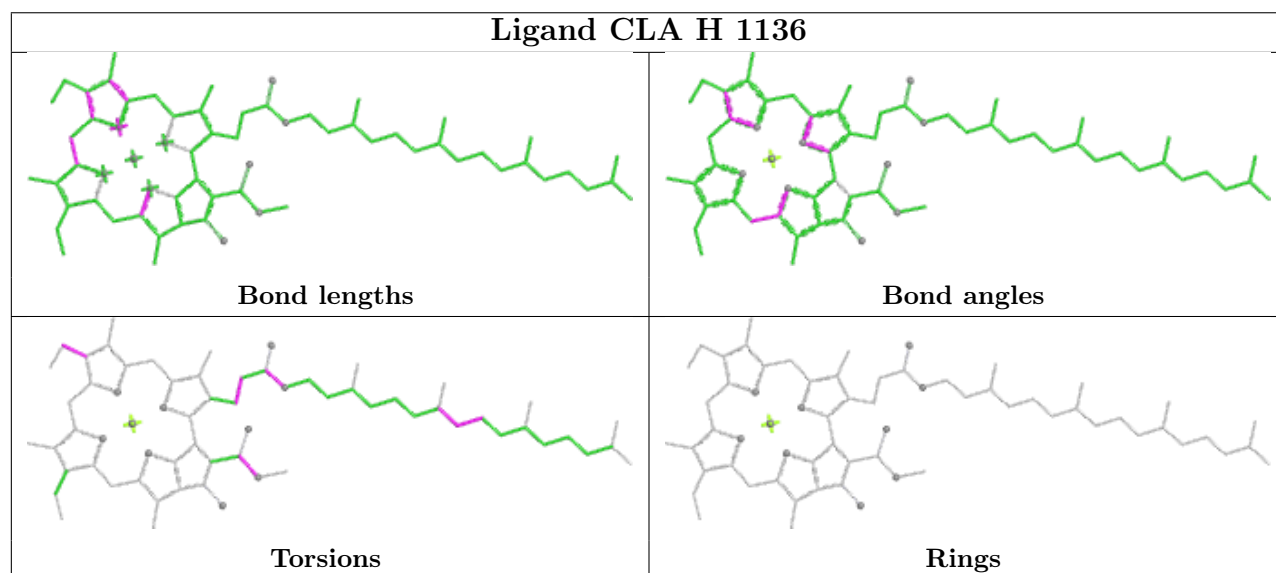
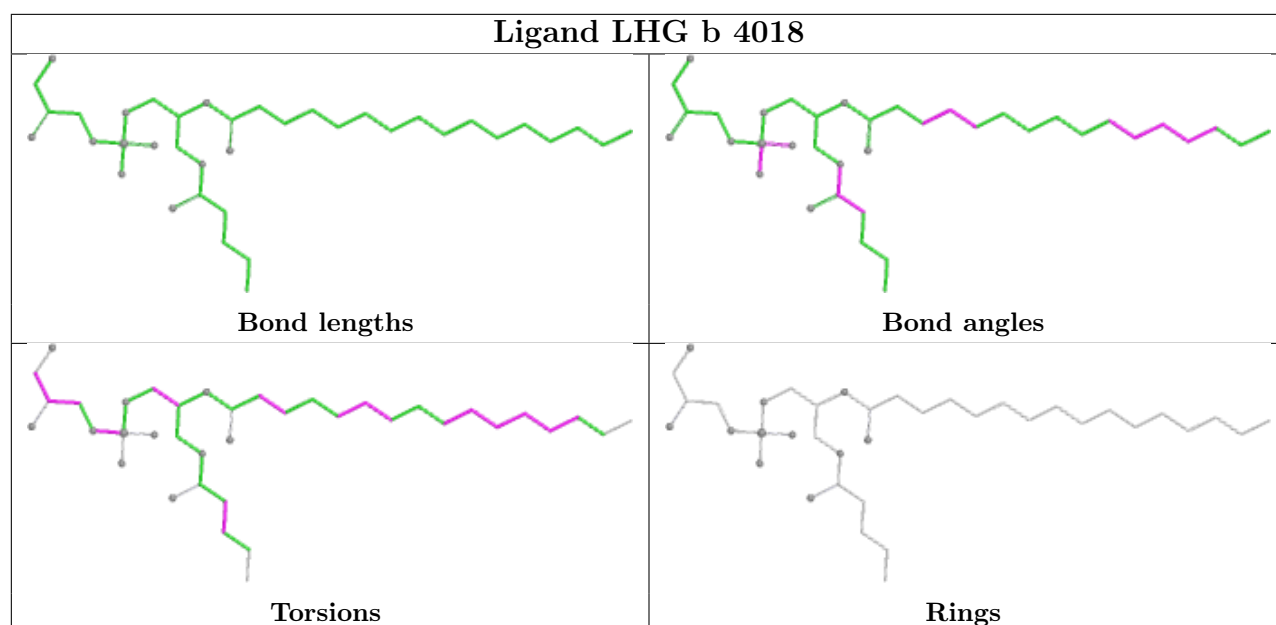


Ligand CLA p 502

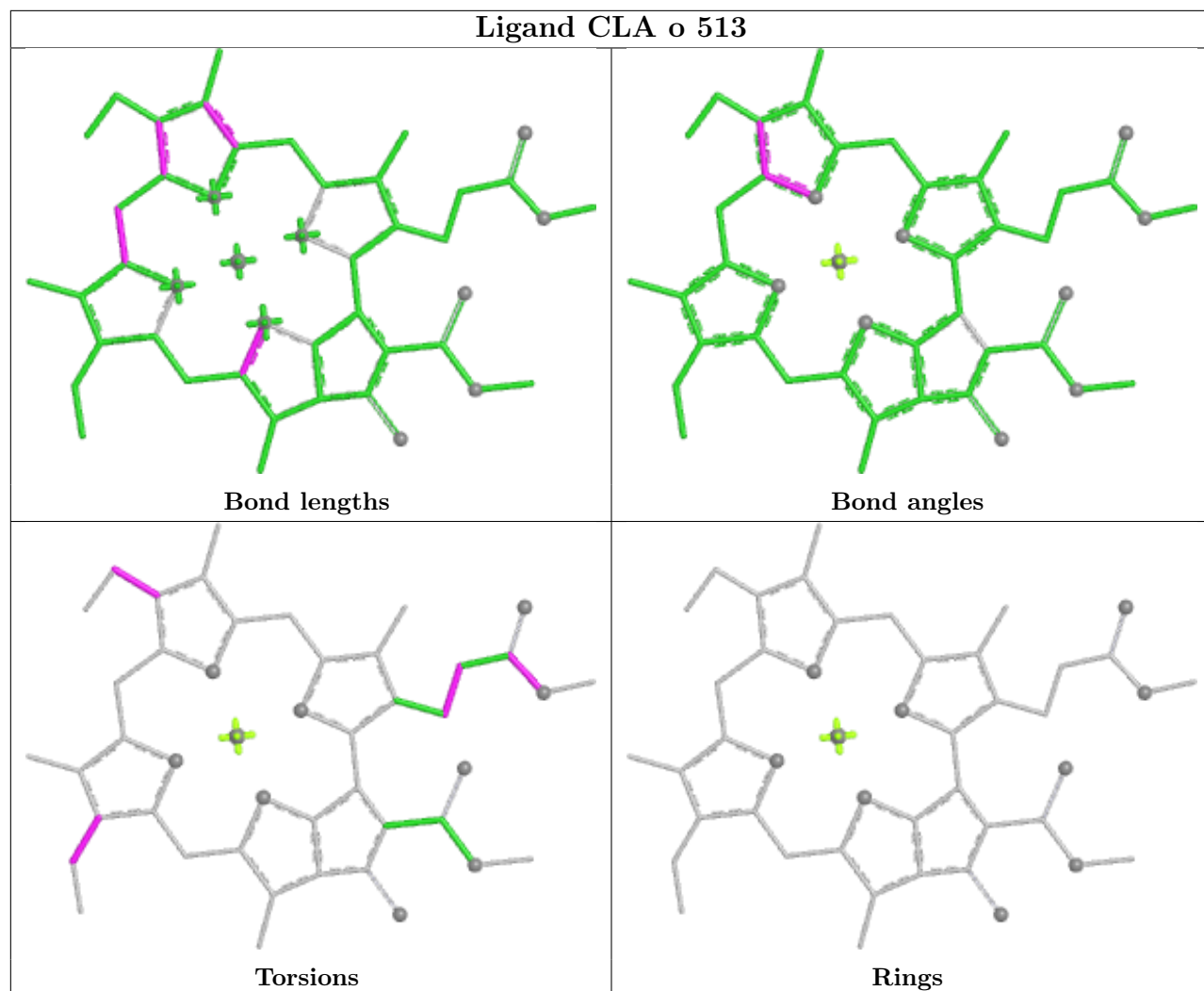


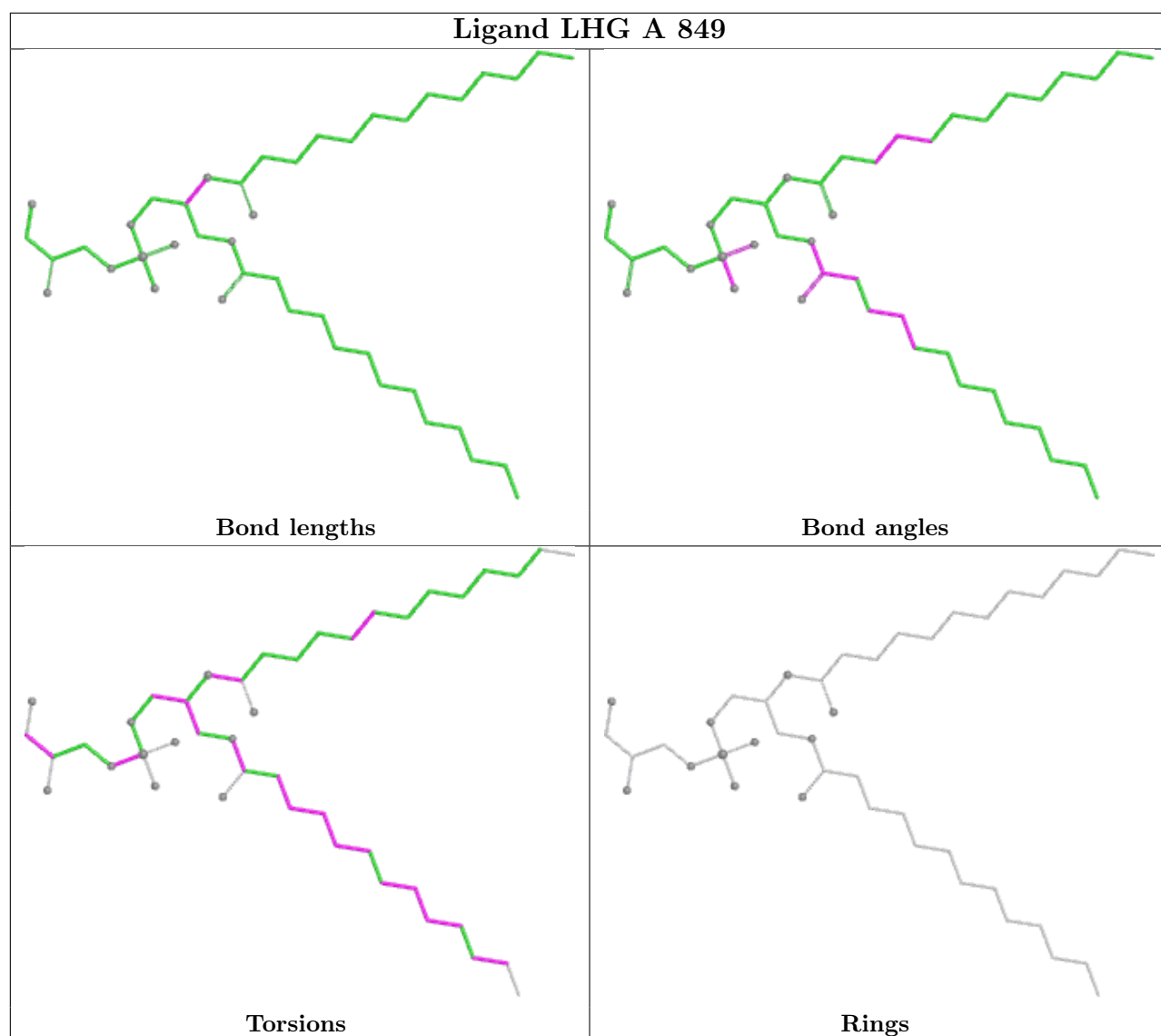




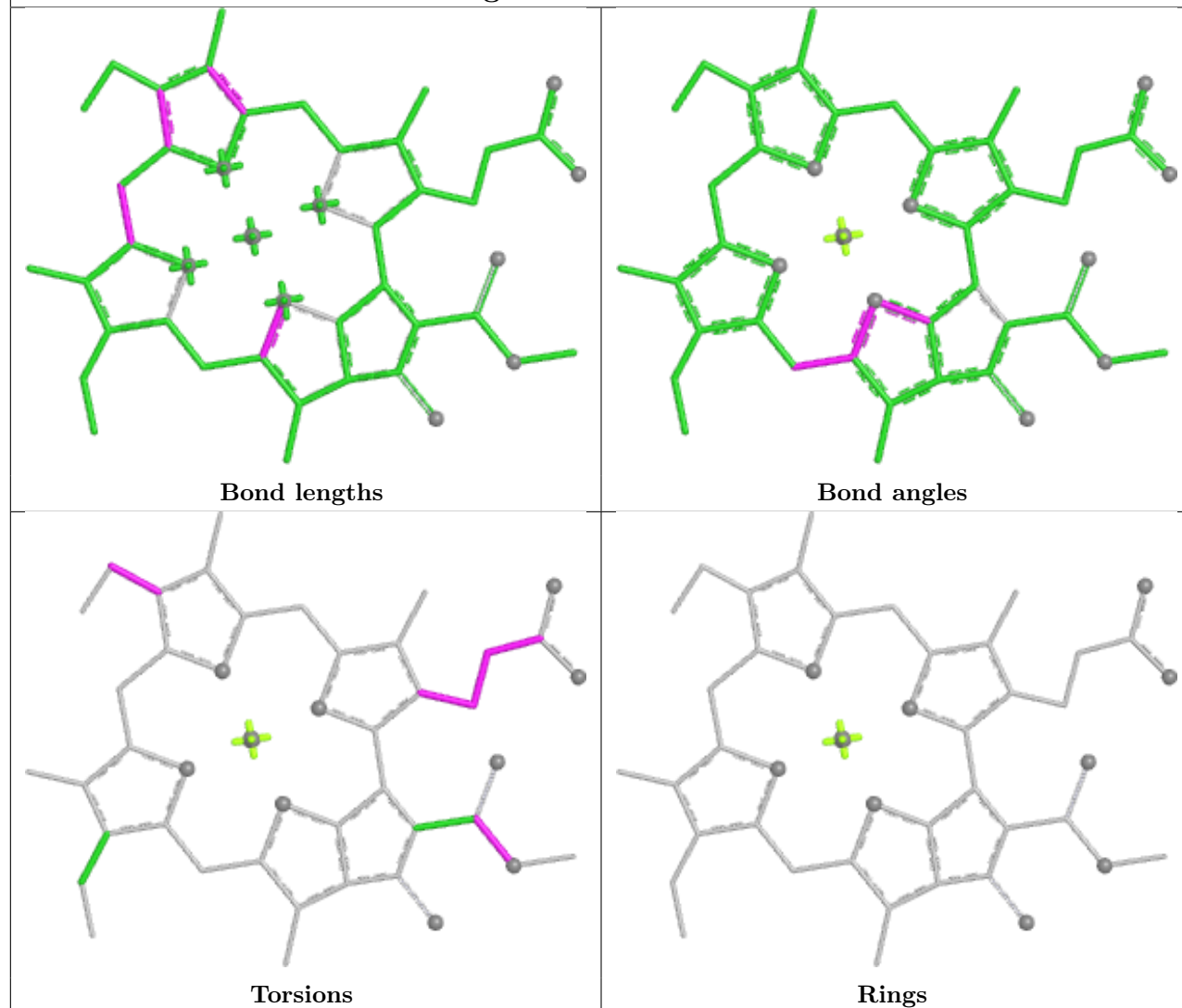


Ligand CLA o 513

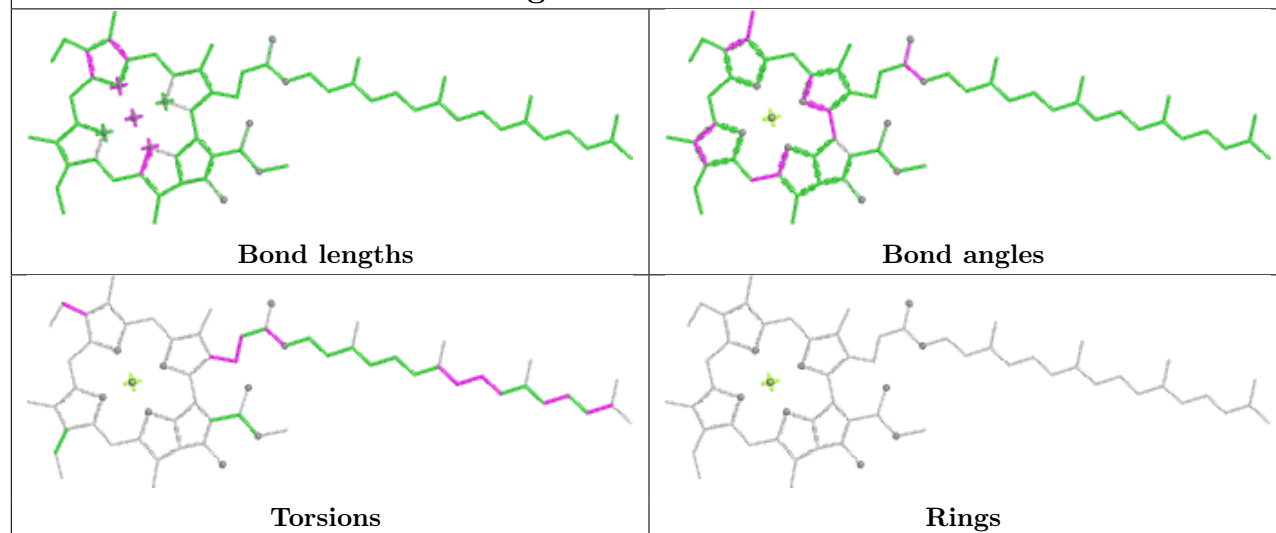




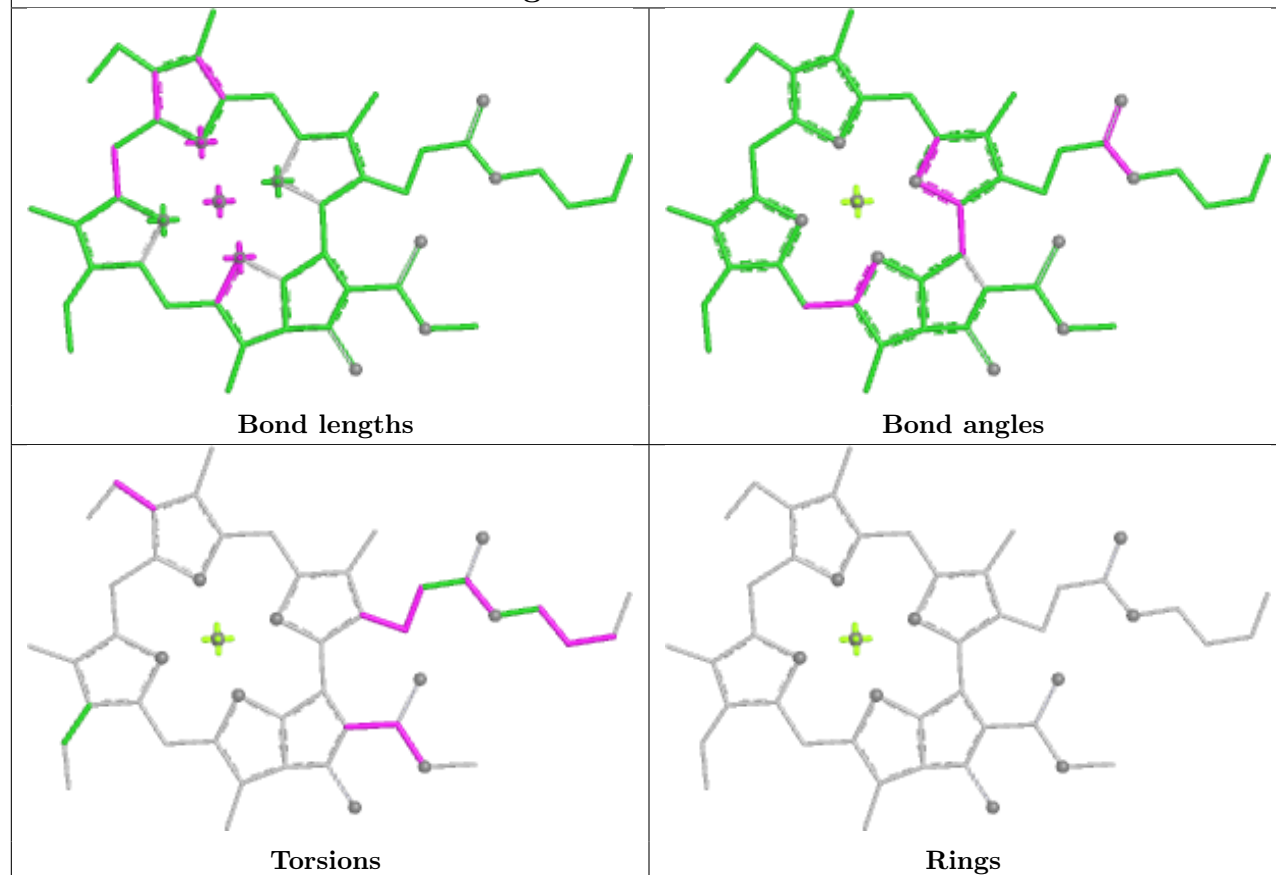
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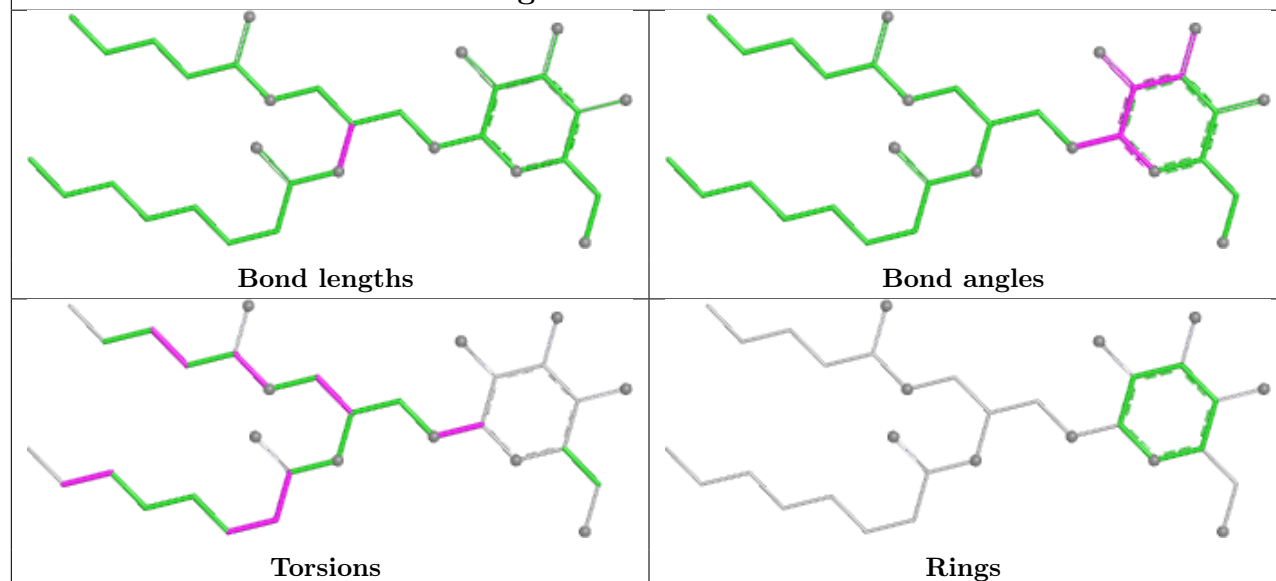
Ligand CLA a 1237



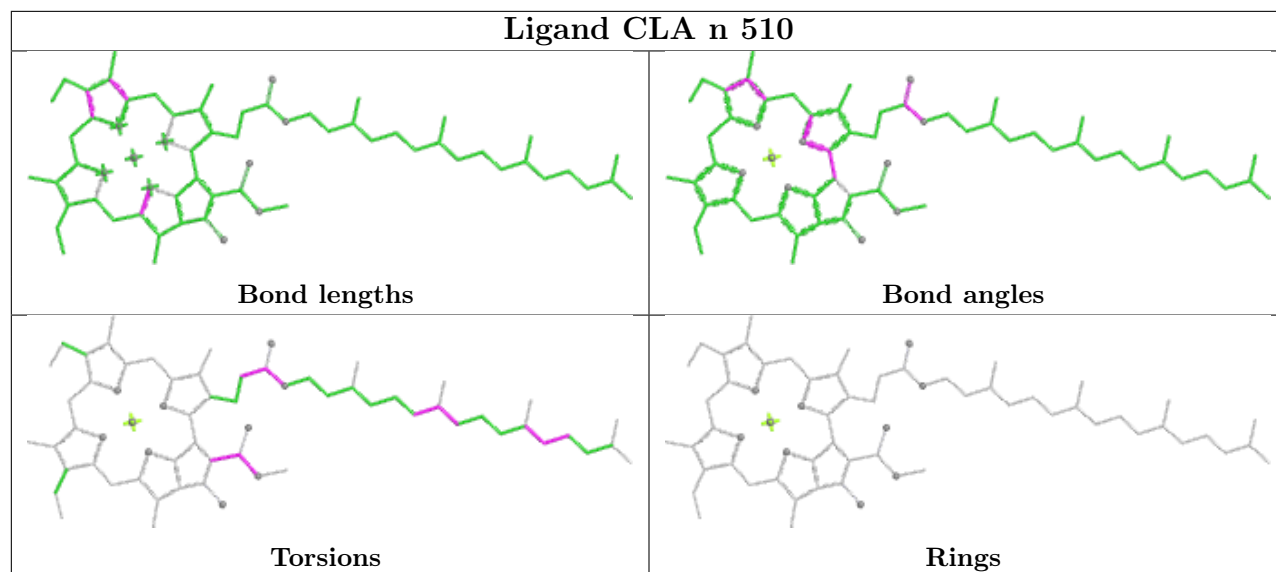
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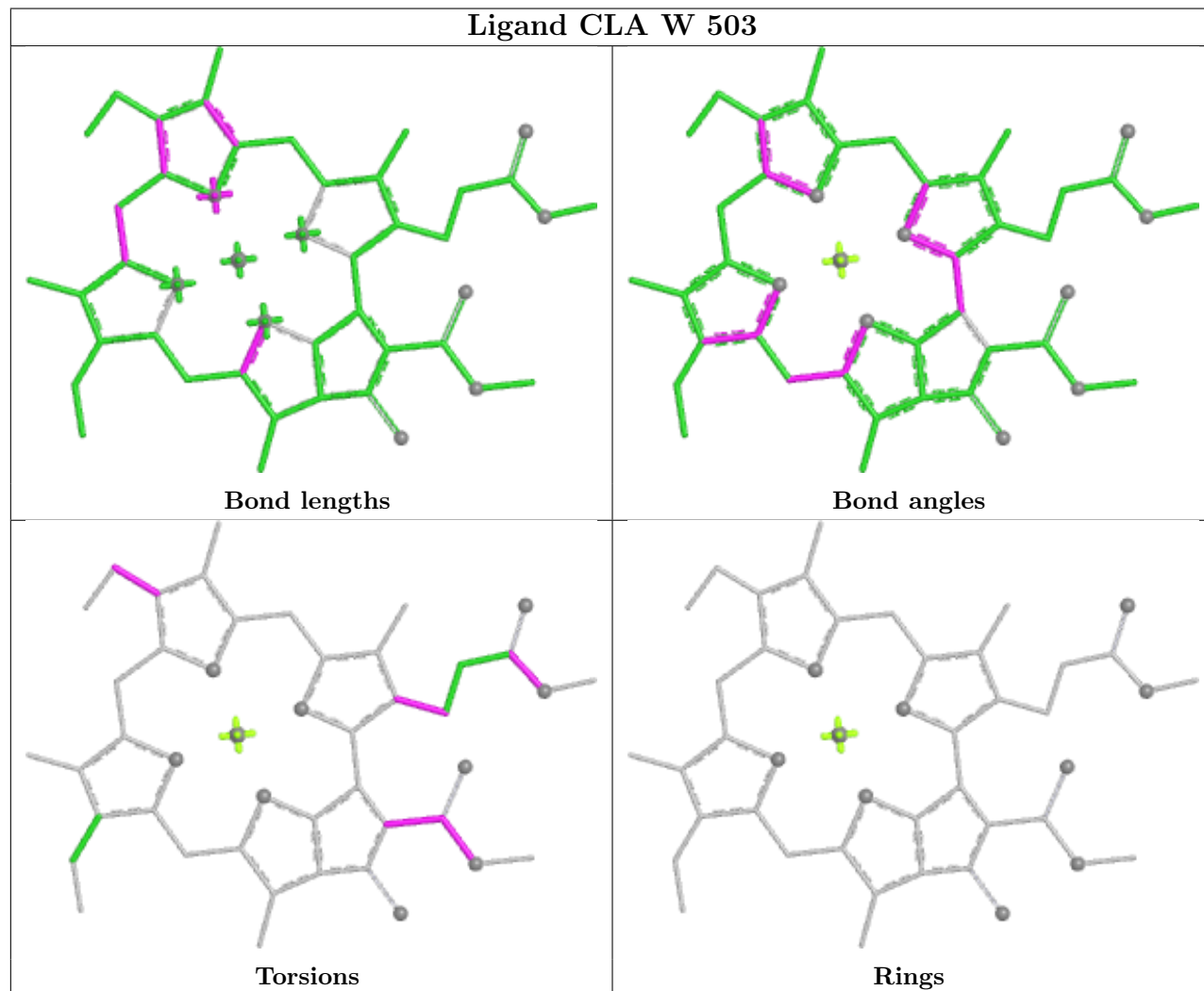
Ligand LMG H 4201



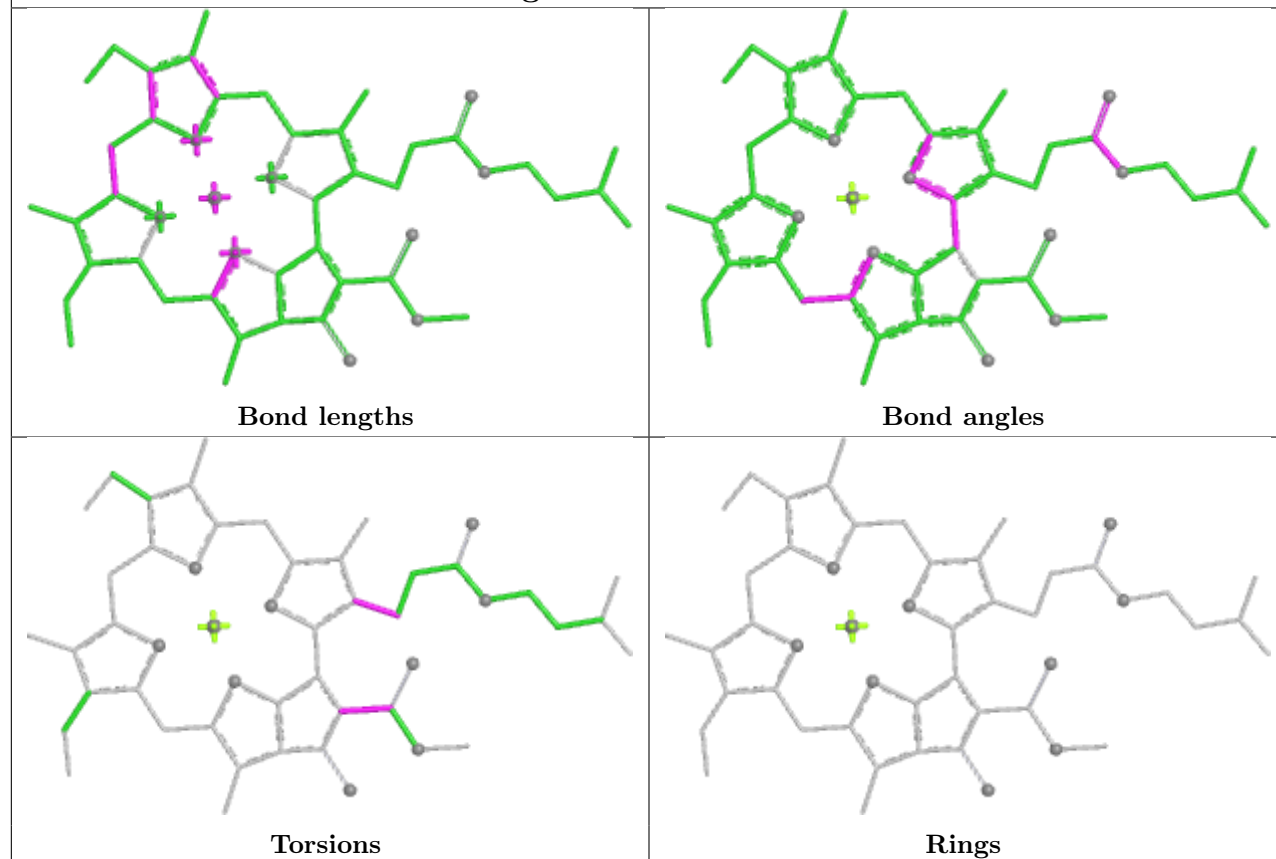
Ligand CLA n 510



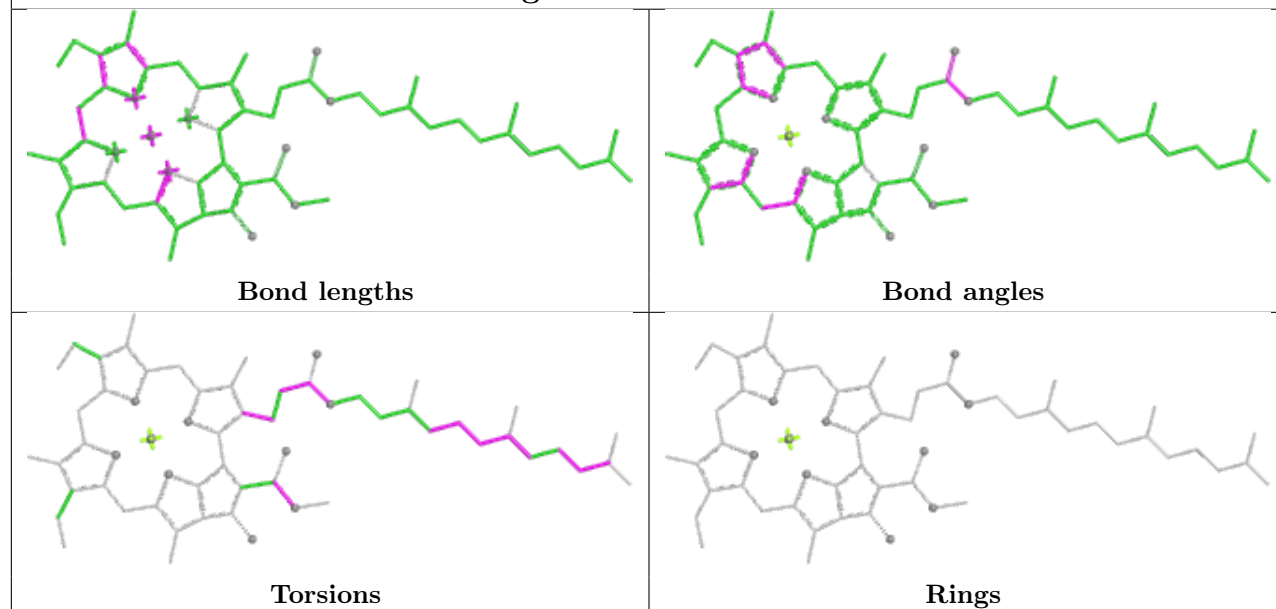
Ligand CLA W 503



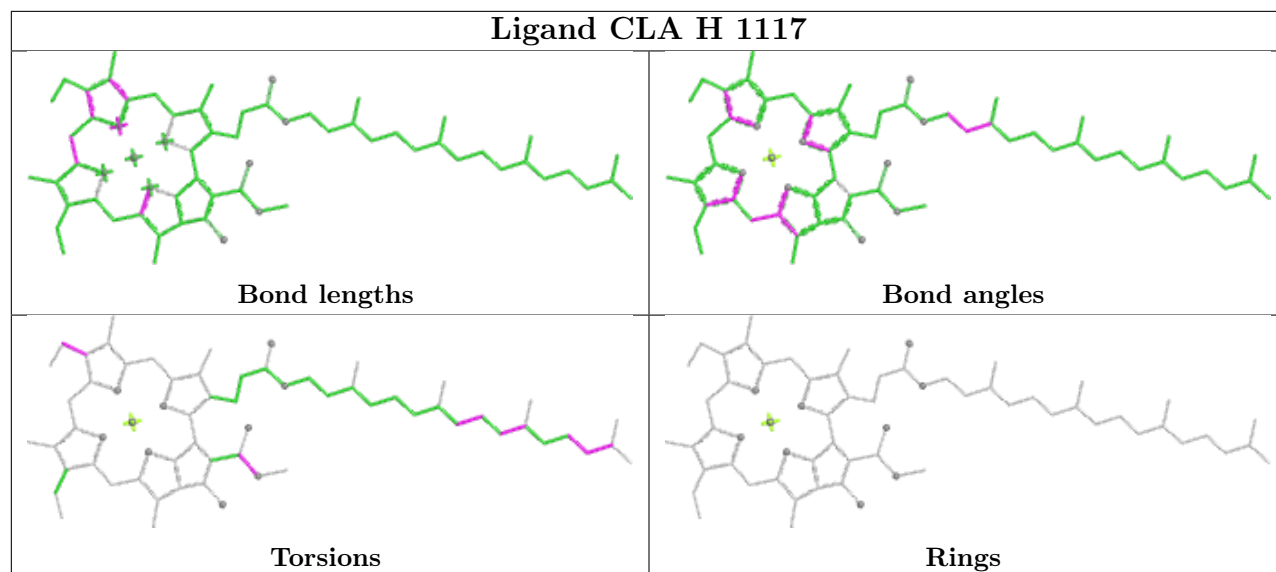
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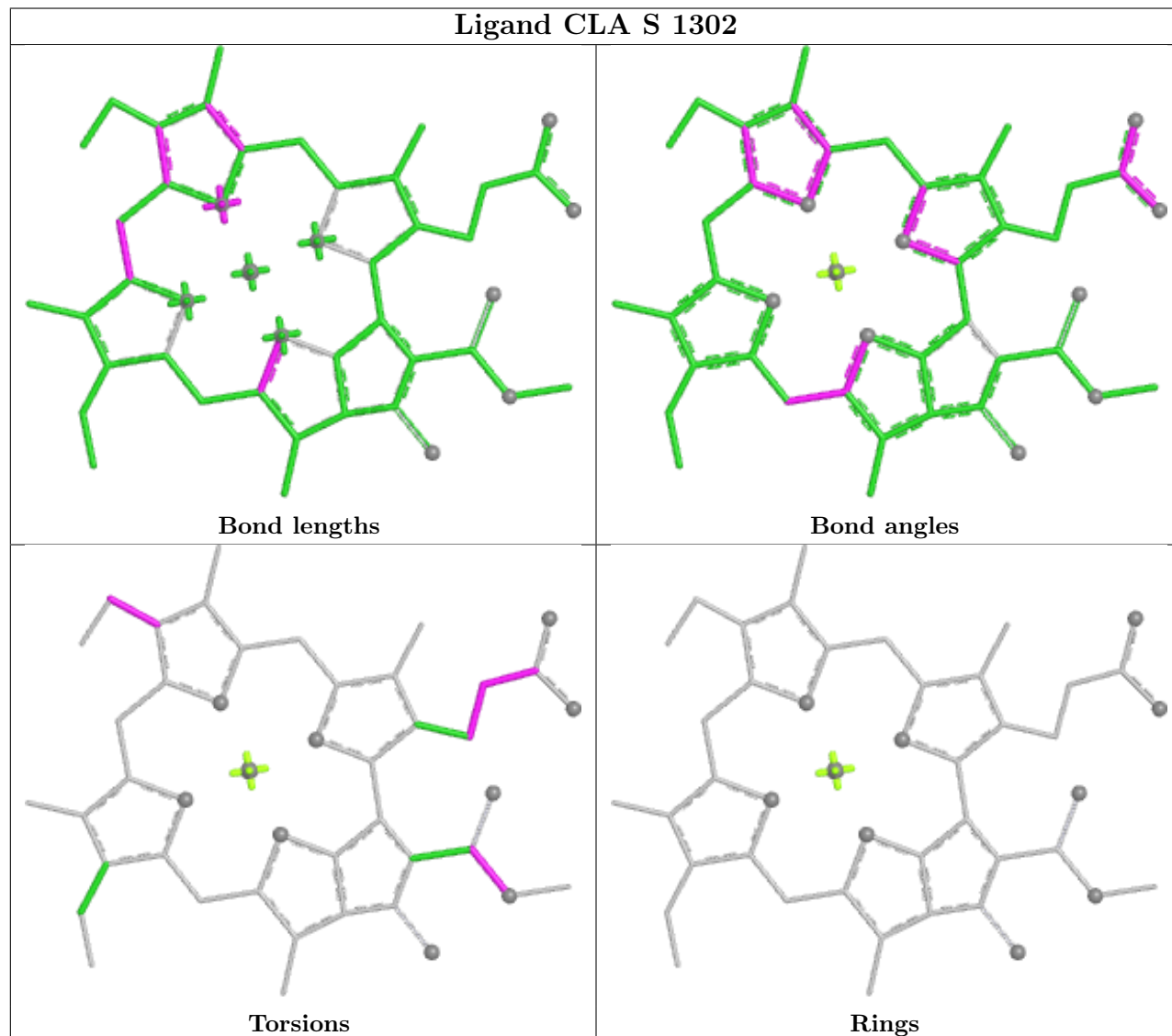
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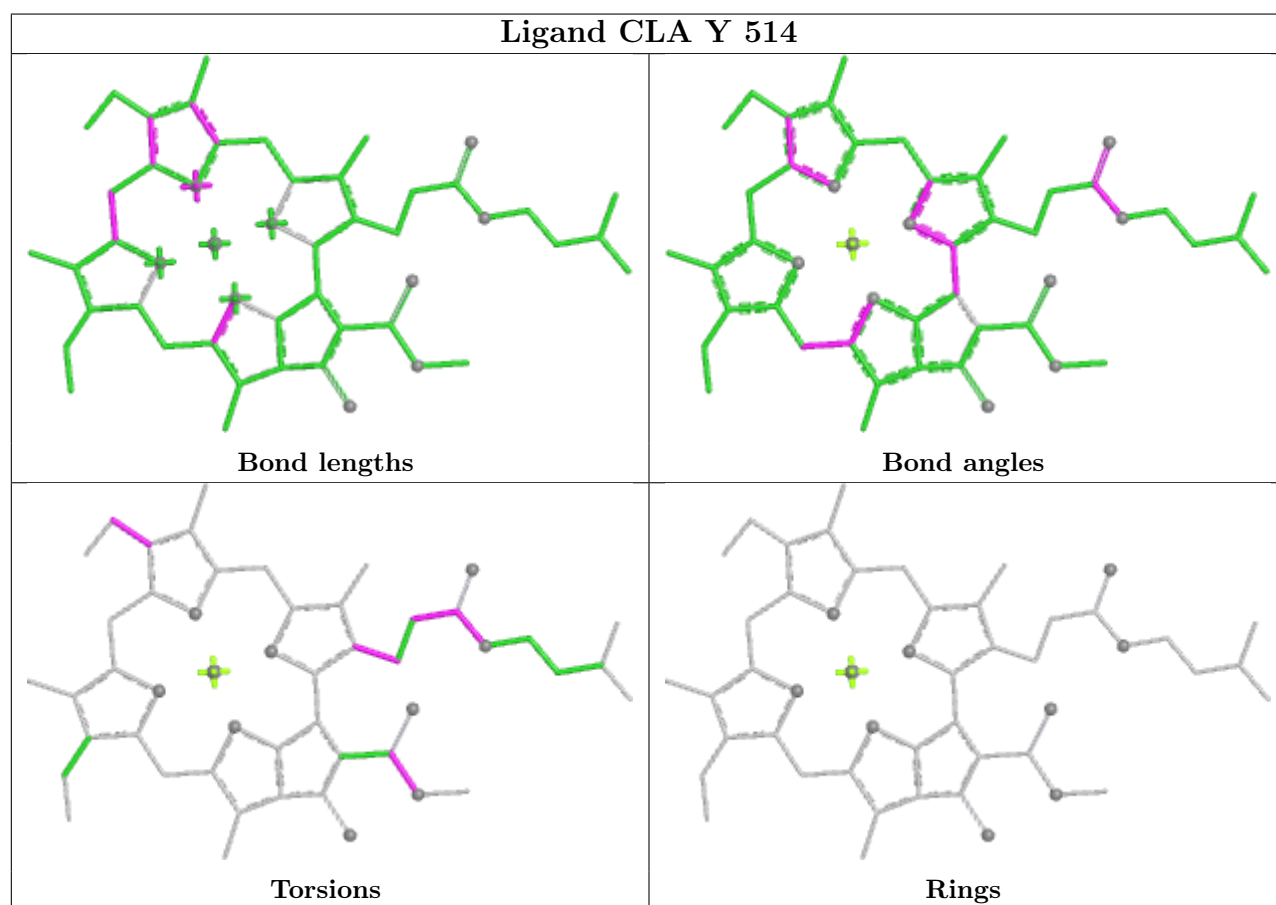
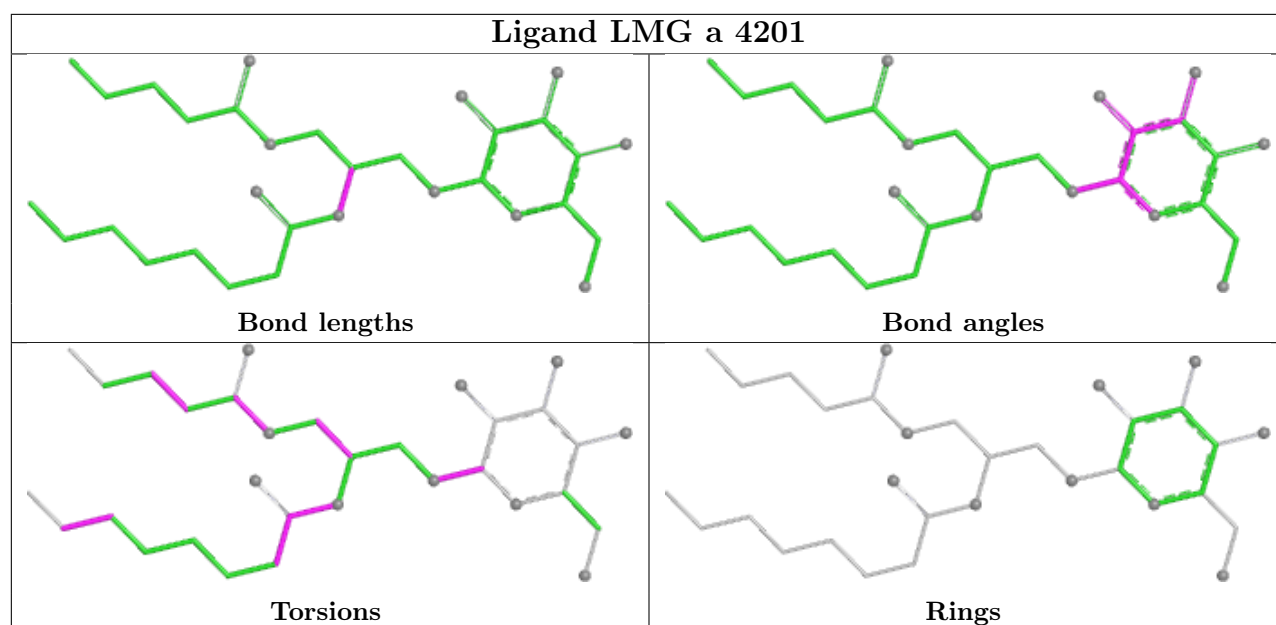


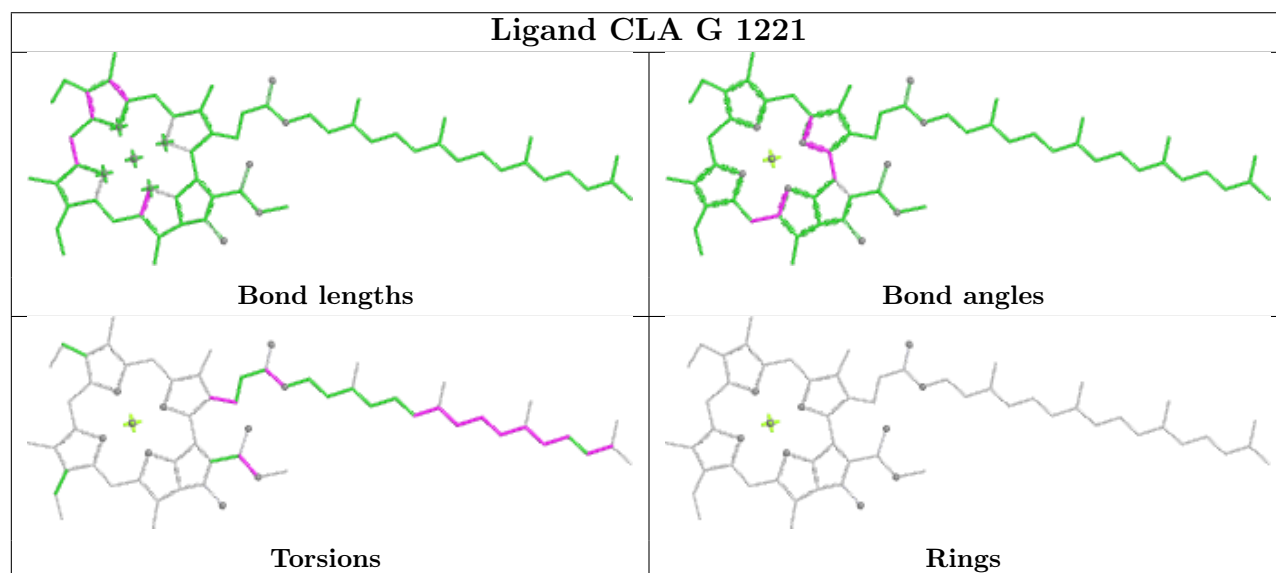
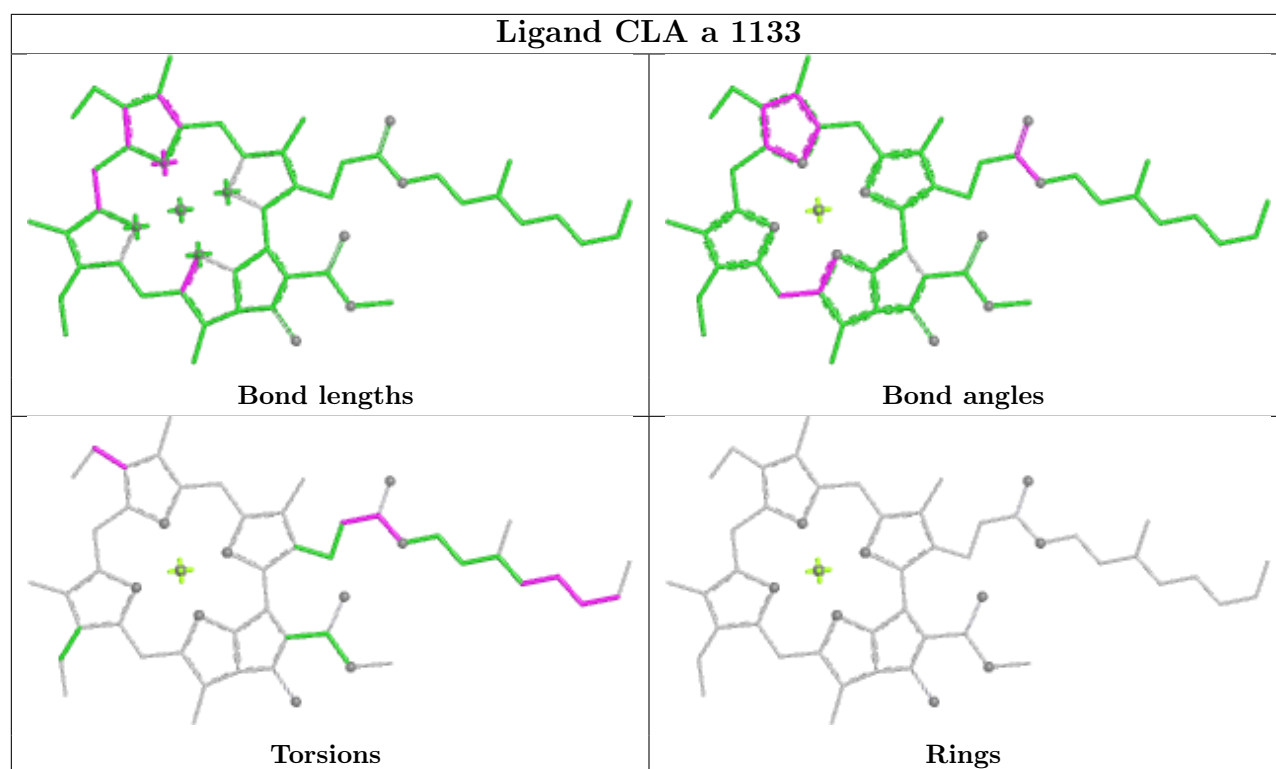
Ligand CLA H 1117

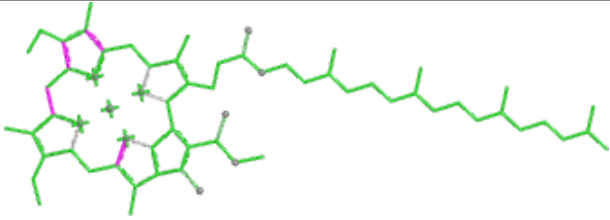
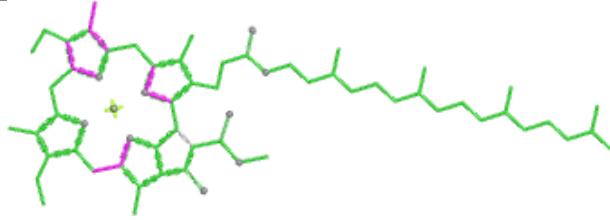
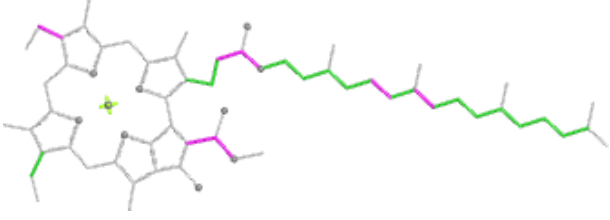
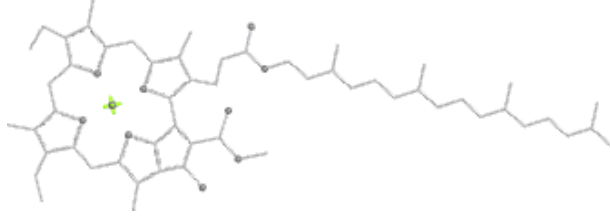
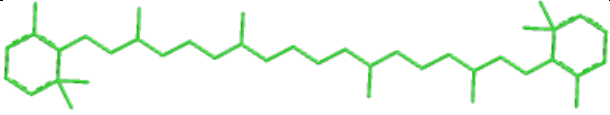
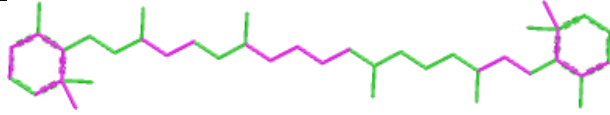
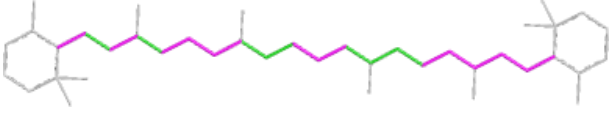
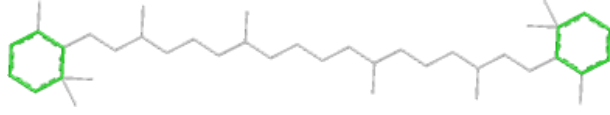
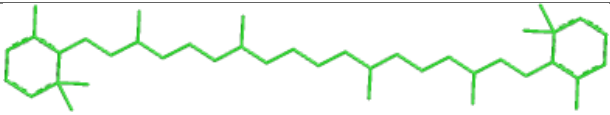
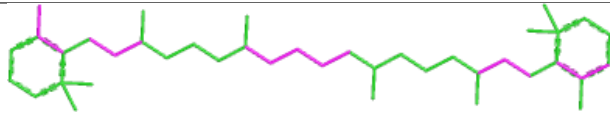
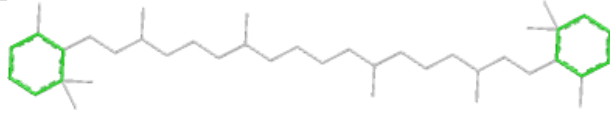


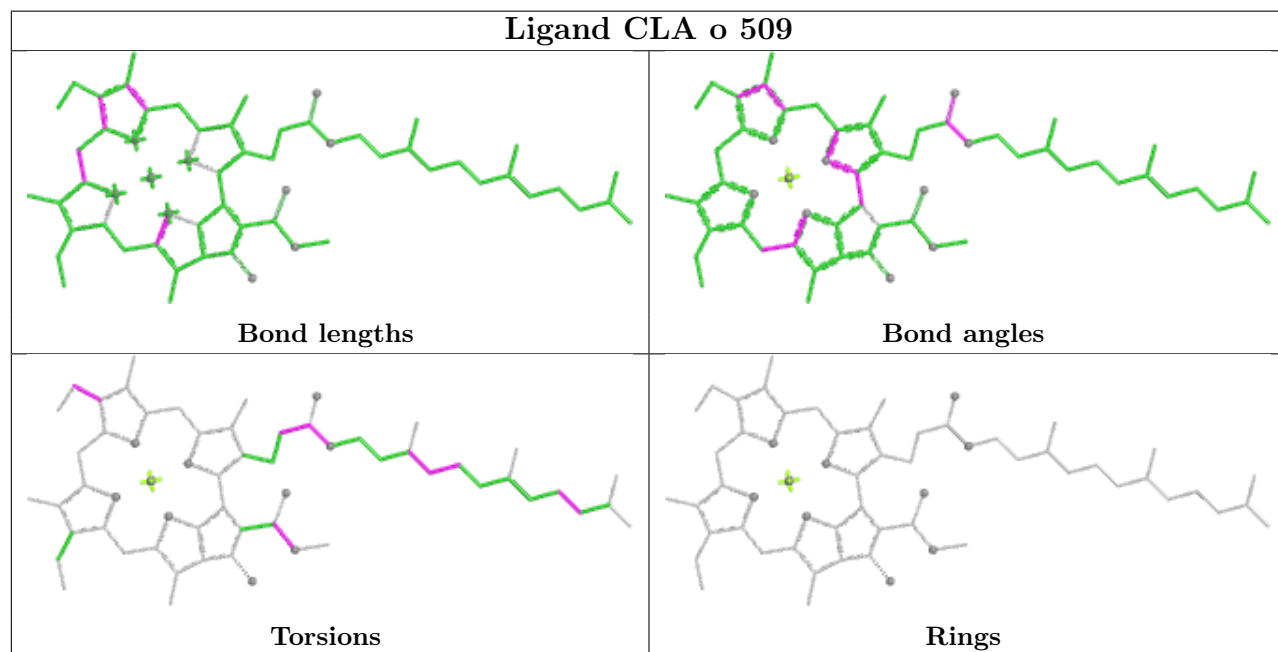
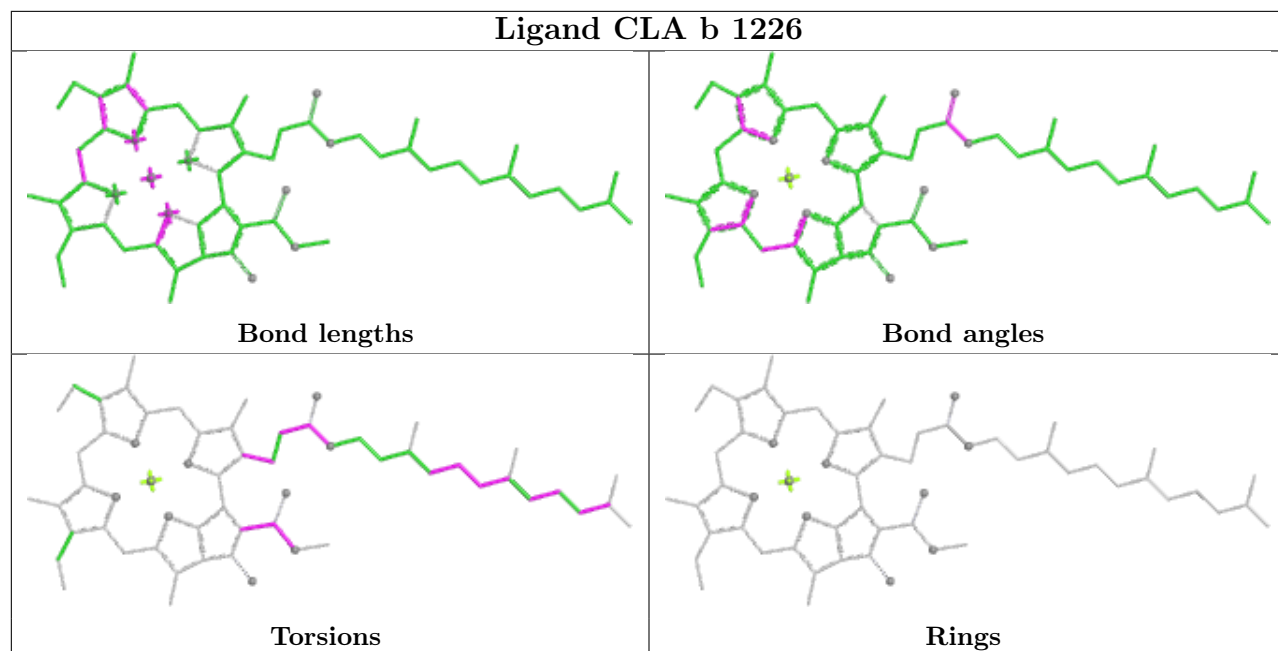
Ligand CLA S 1302



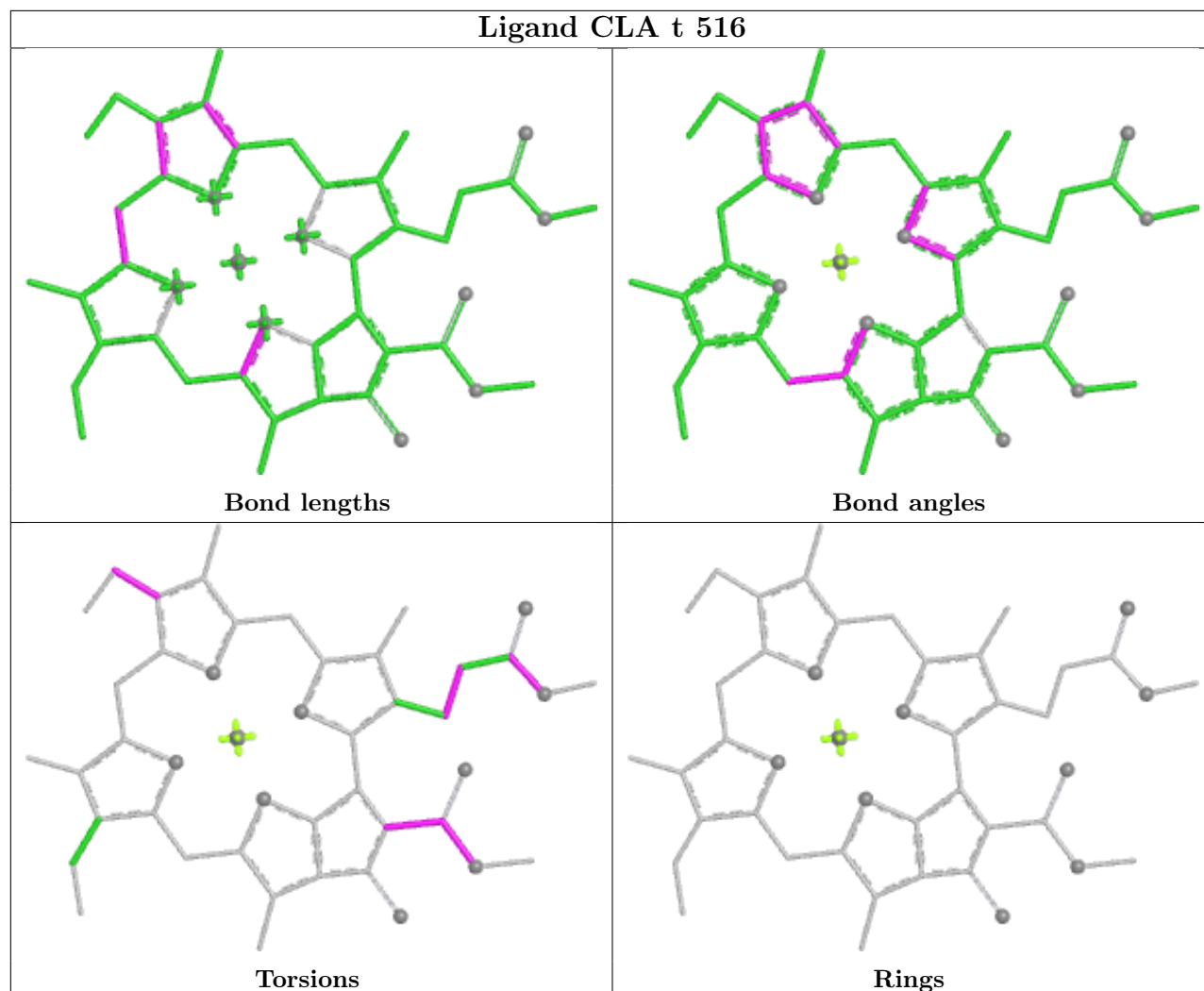




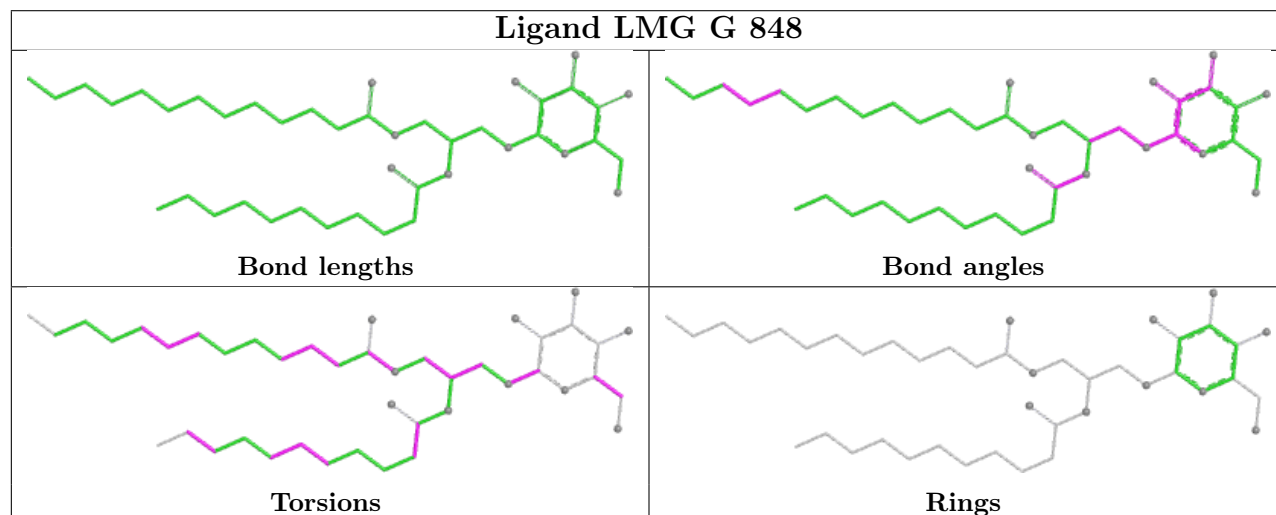
Ligand CLA o 507	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR u 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Y 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

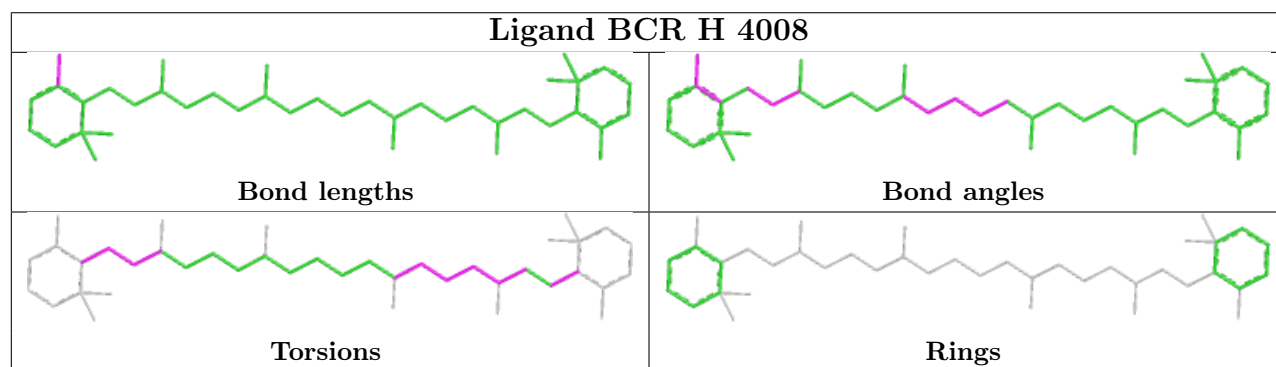
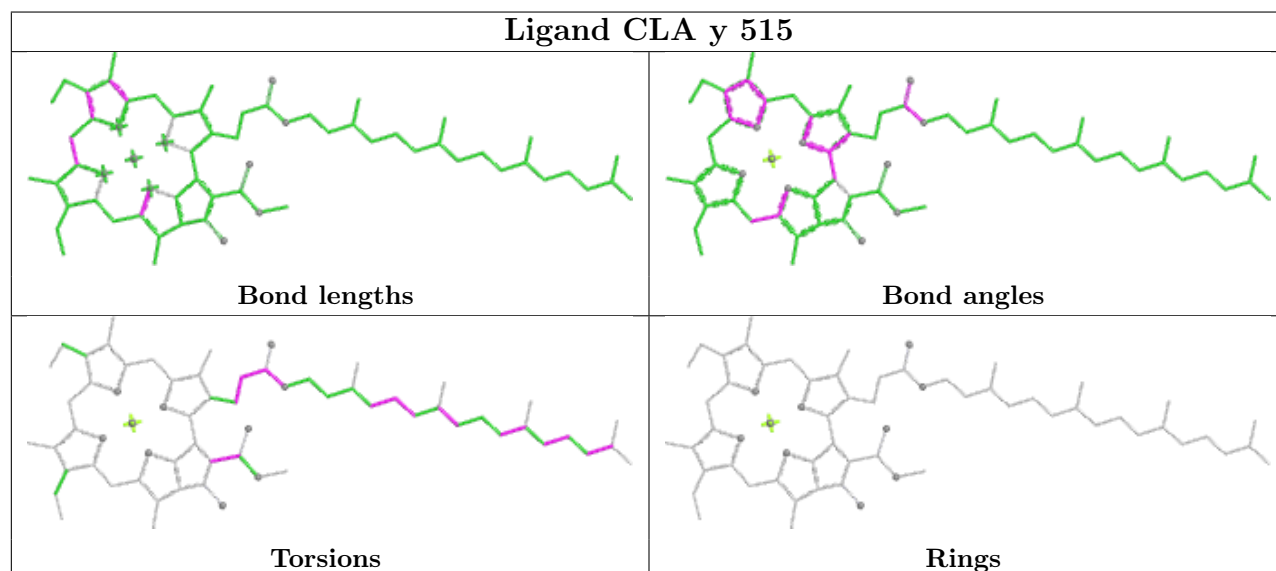
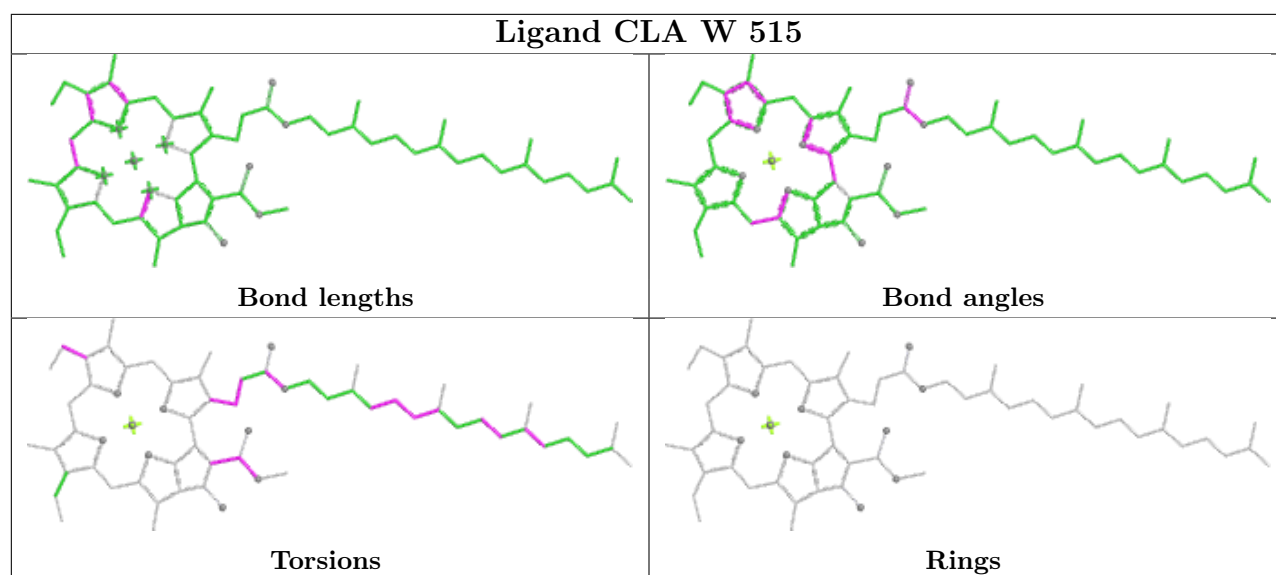


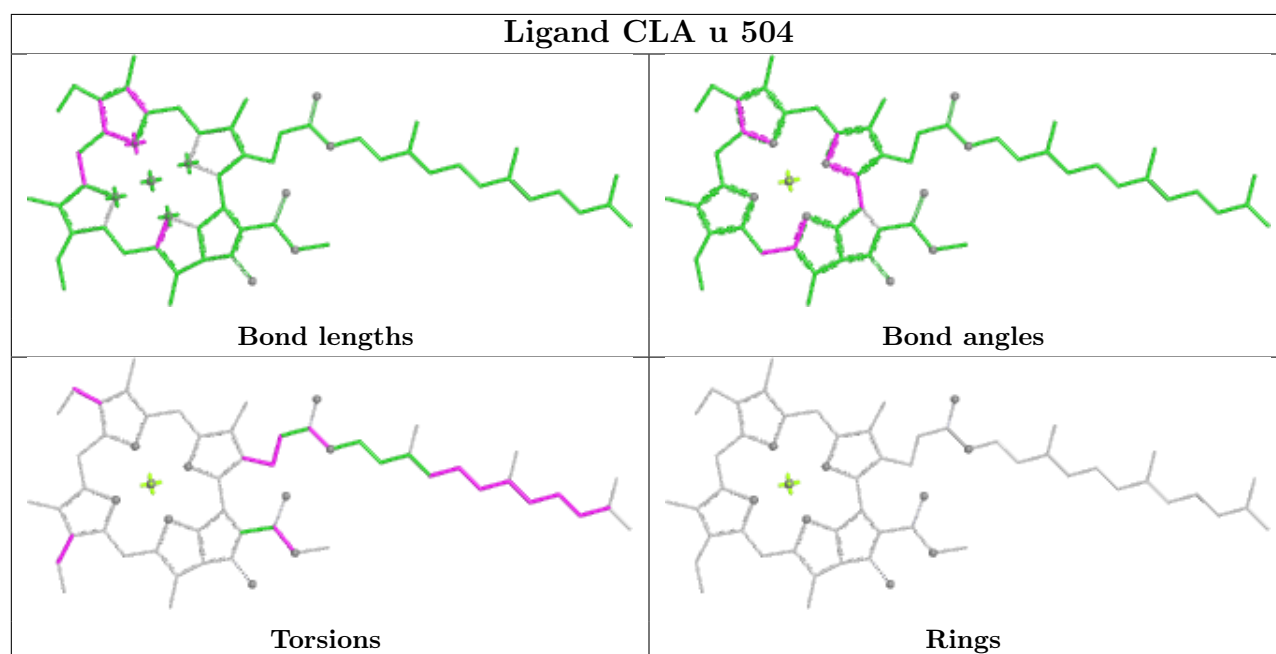
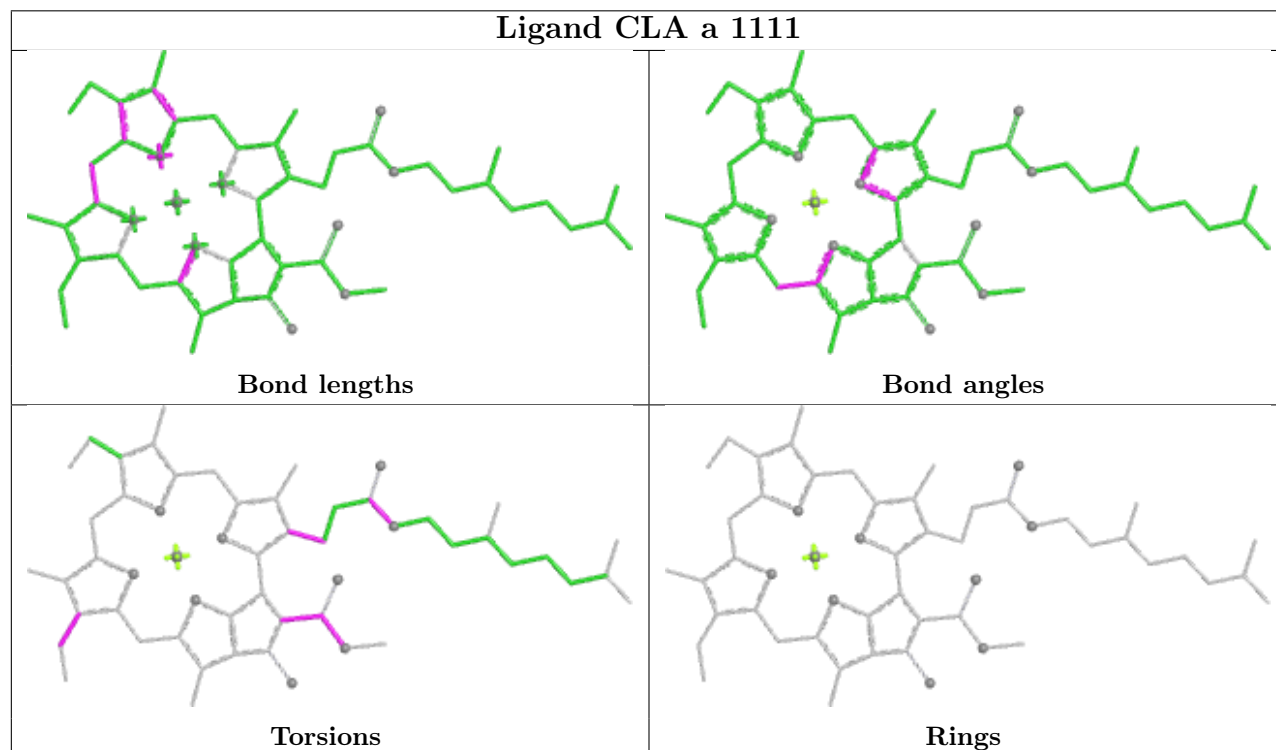
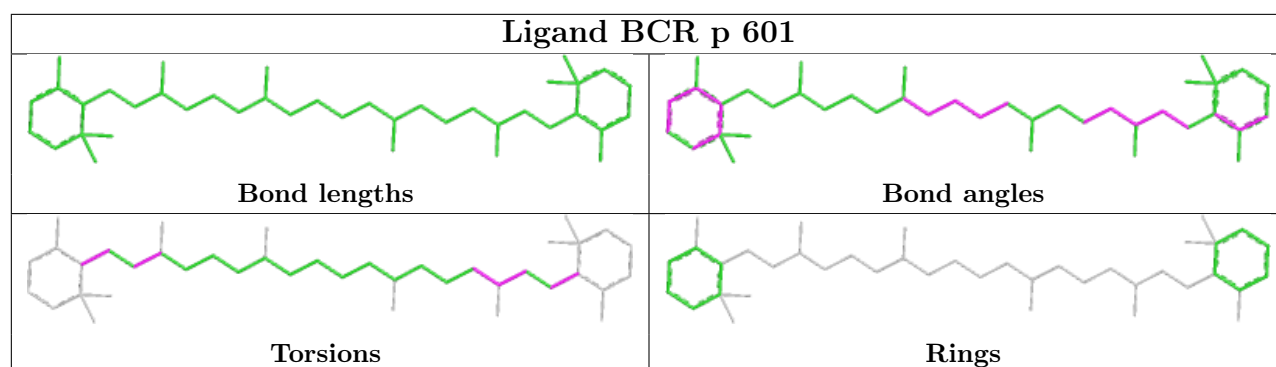
Ligand CLA t 516

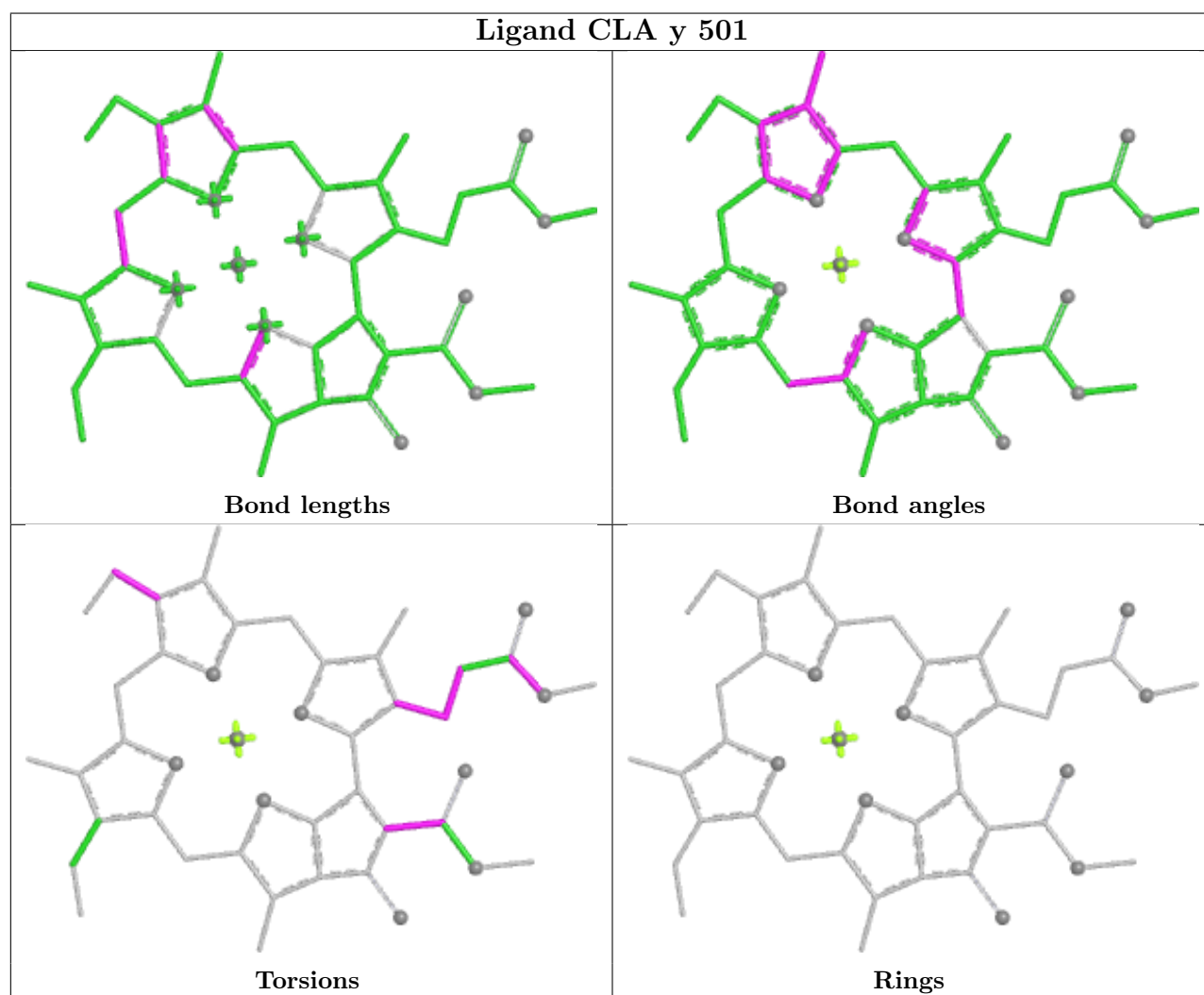
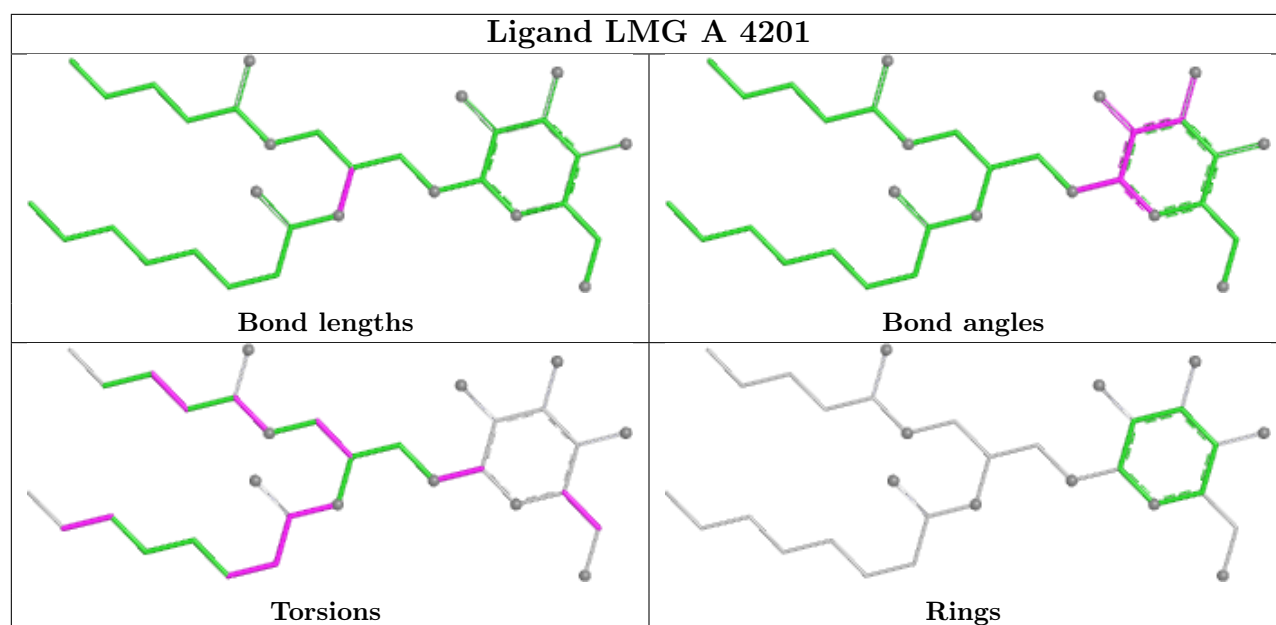


Ligand LMG G 848

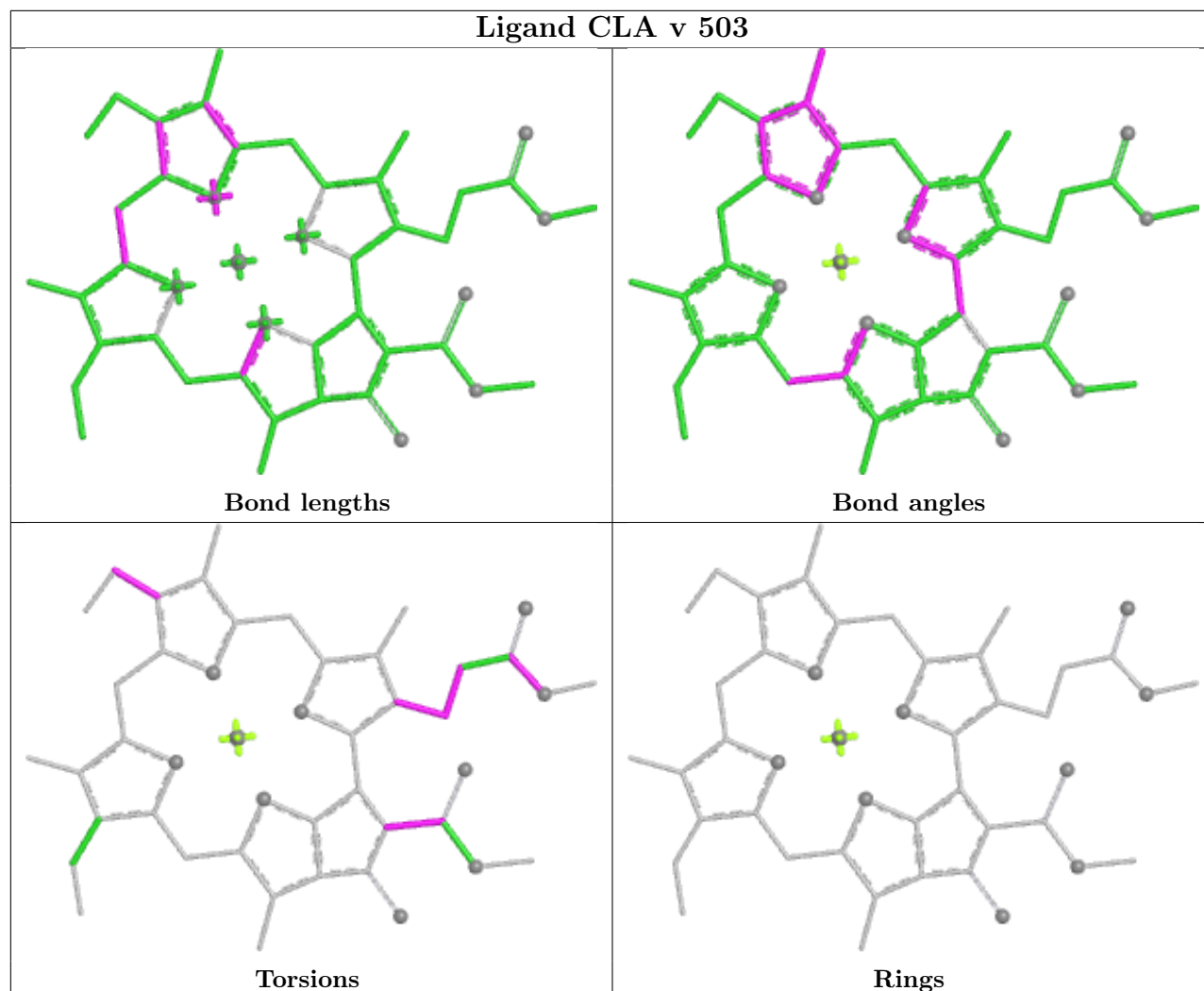


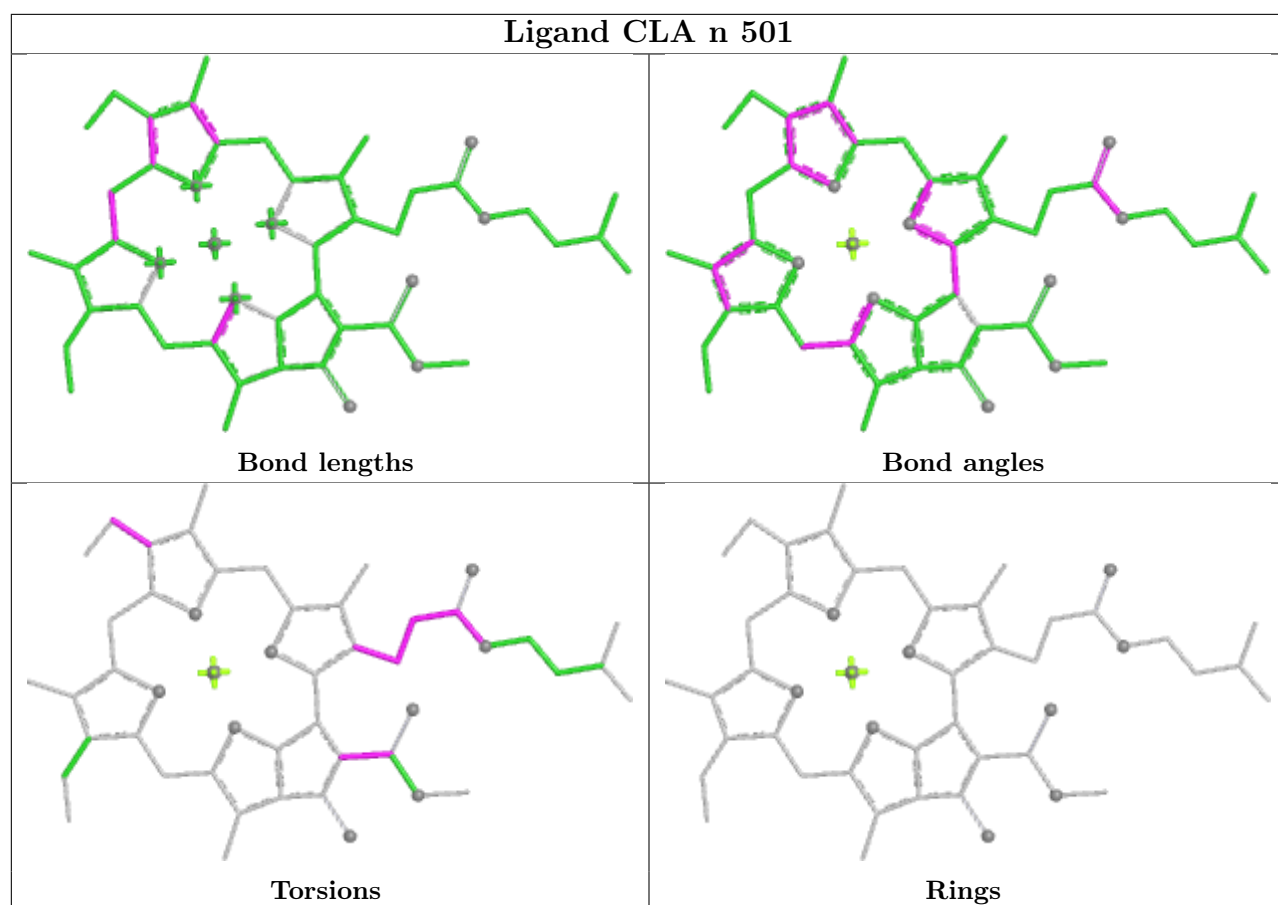




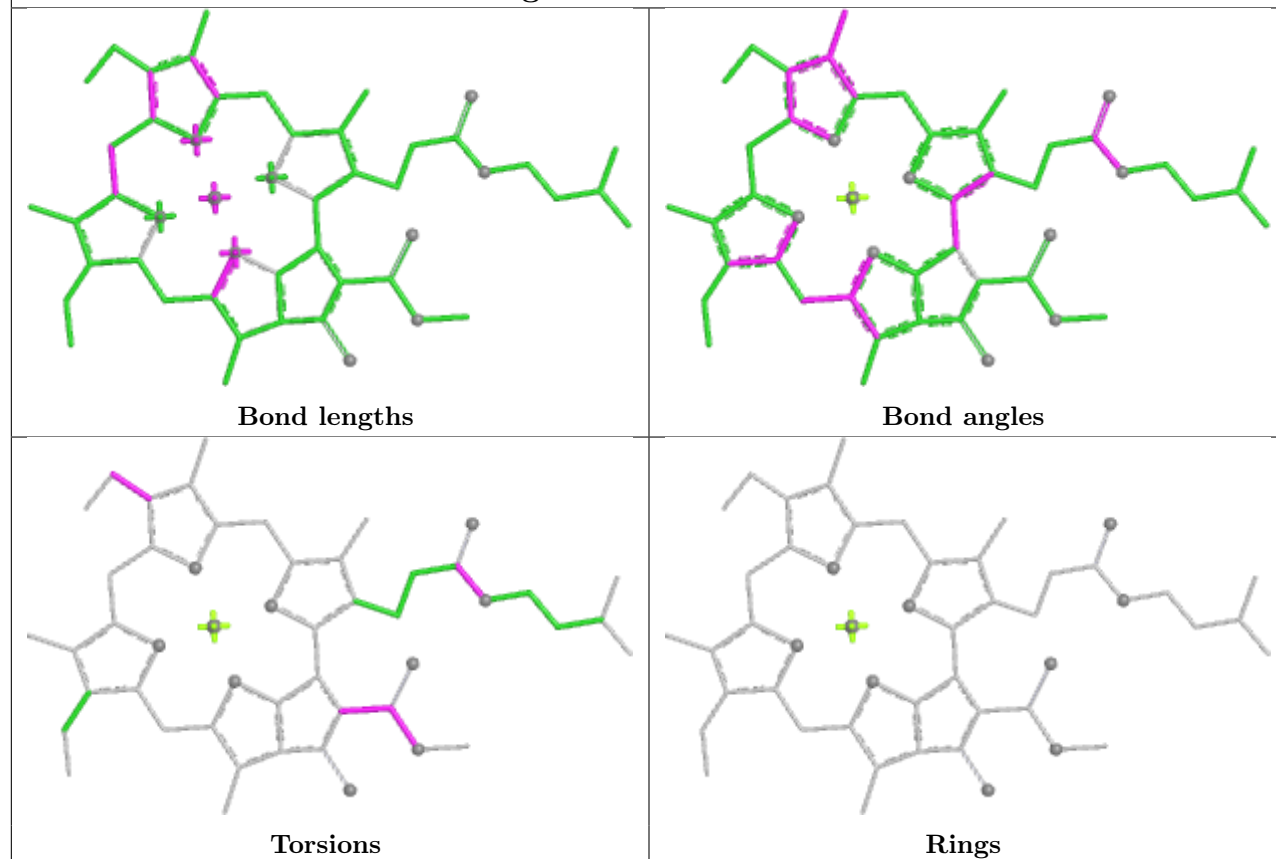


Ligand CLA v 503

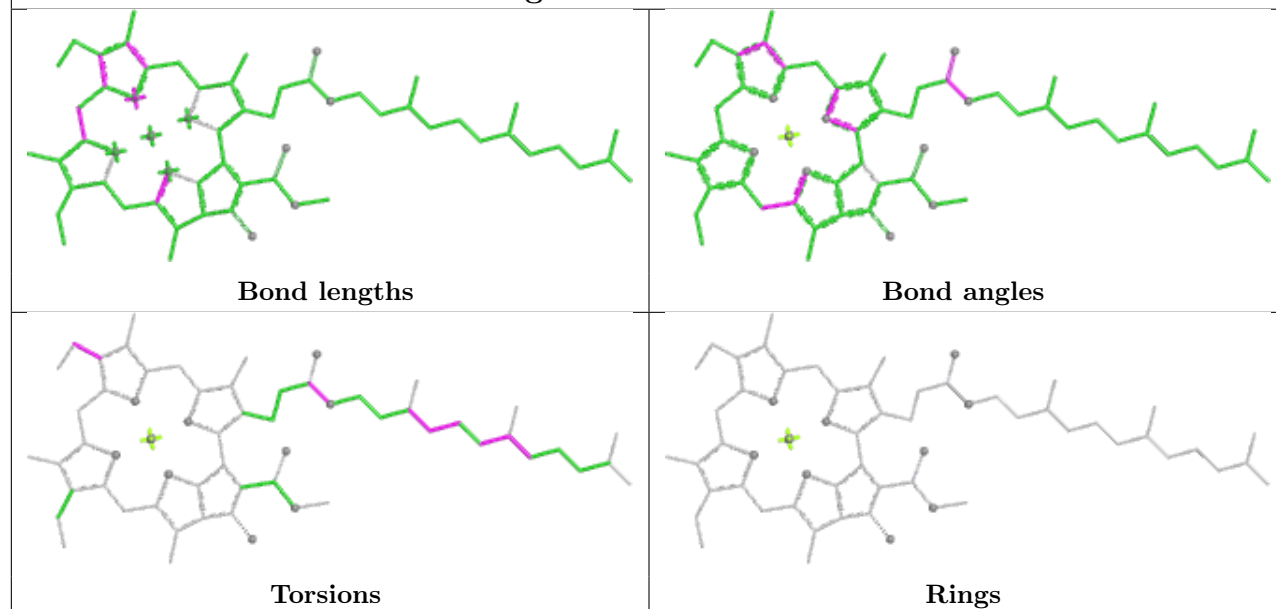


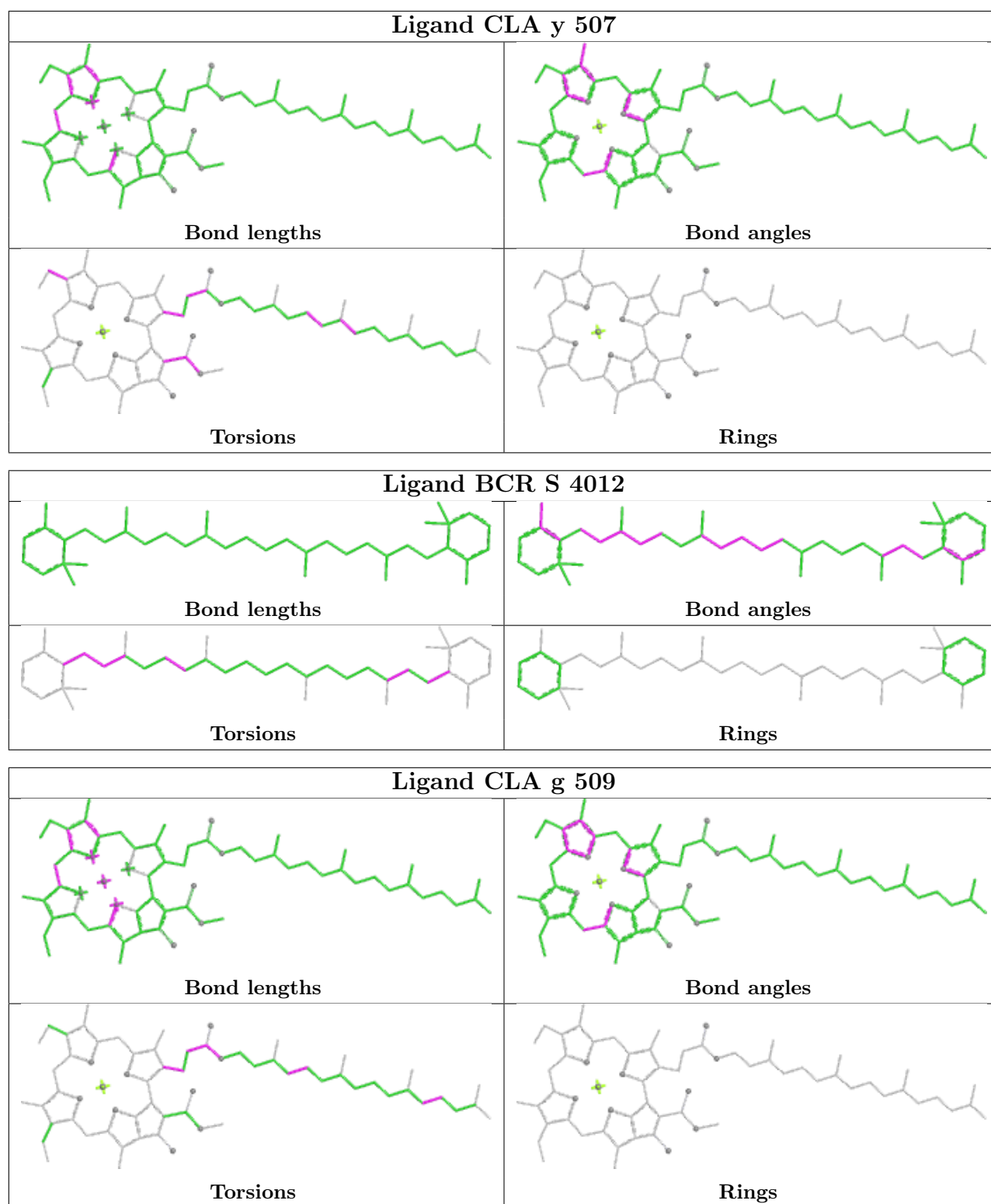


Ligand CLA G 1222

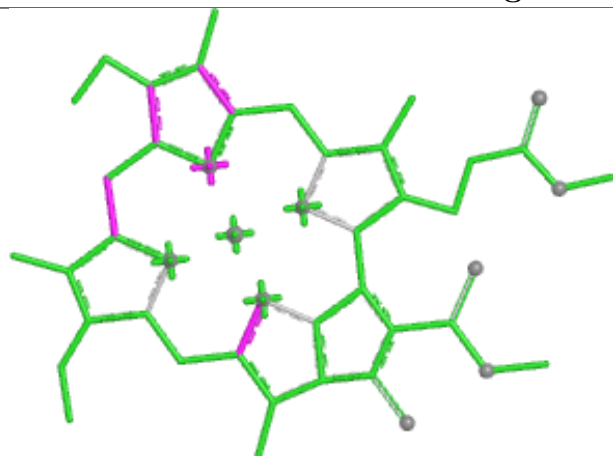


Ligand CLA L 1502

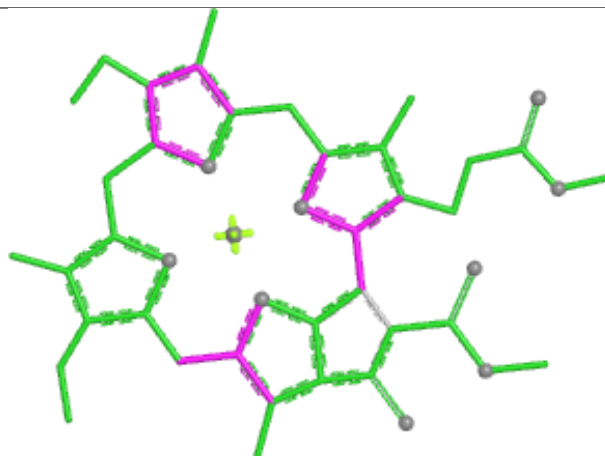




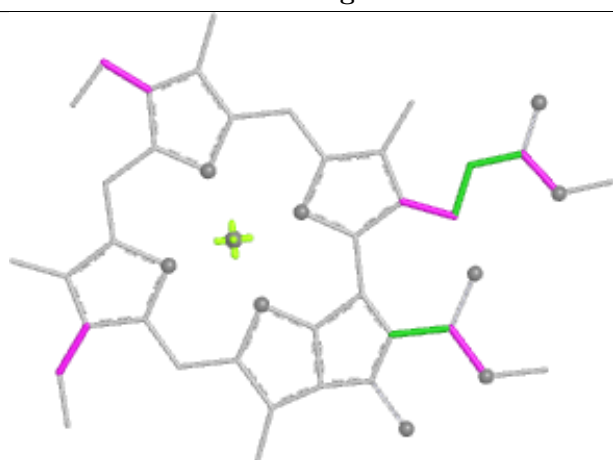
Ligand CLA H 1114



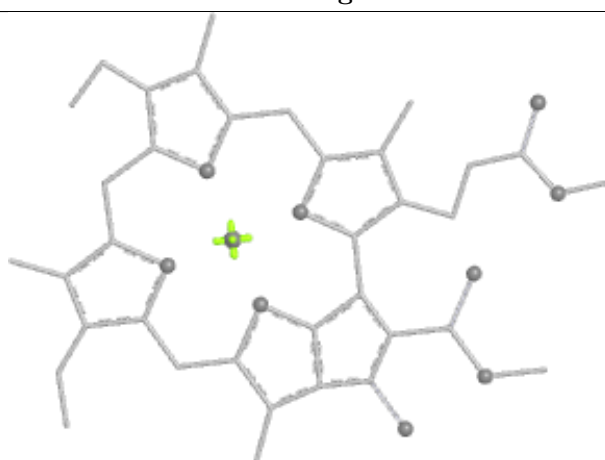
Bond lengths



Bond angles

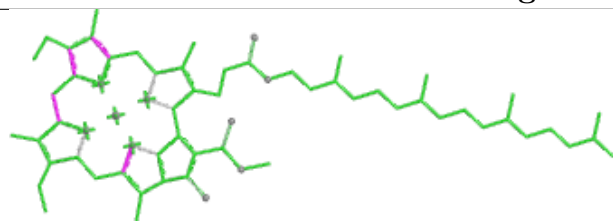


Torsions

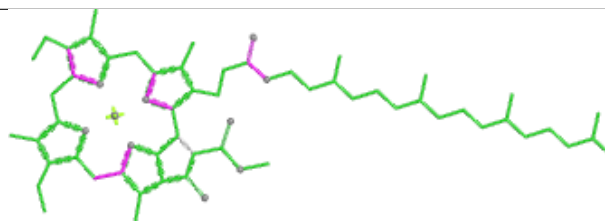


Rings

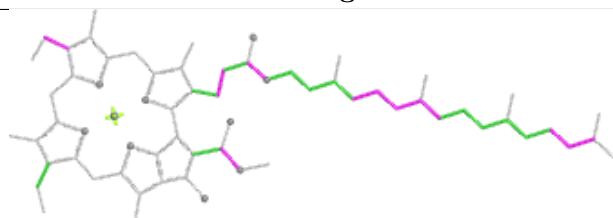
Ligand CLA o 505



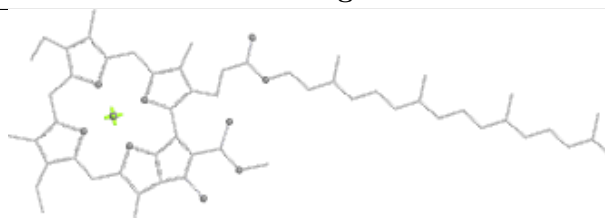
Bond lengths



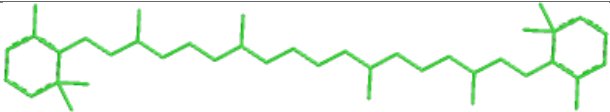
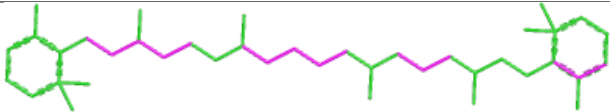
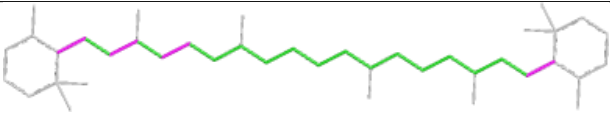
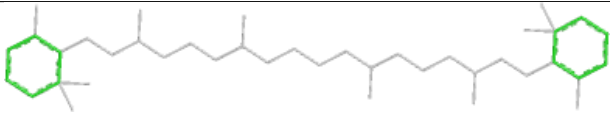
Bond angles

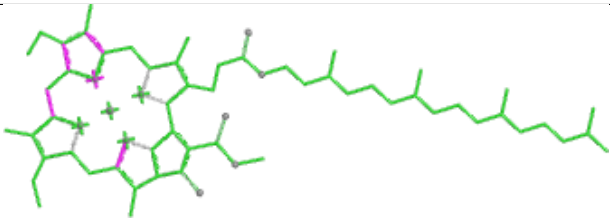
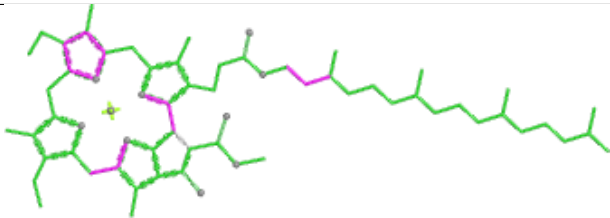
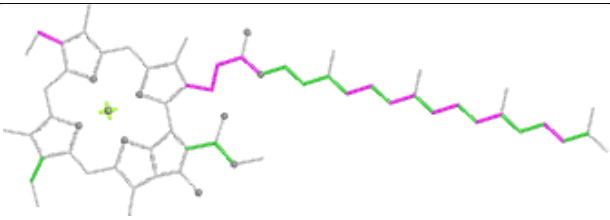
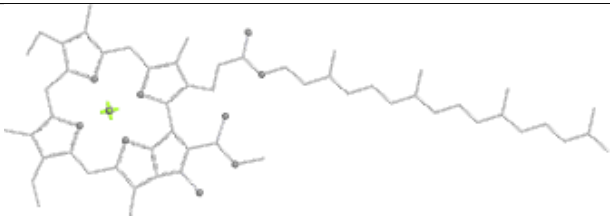


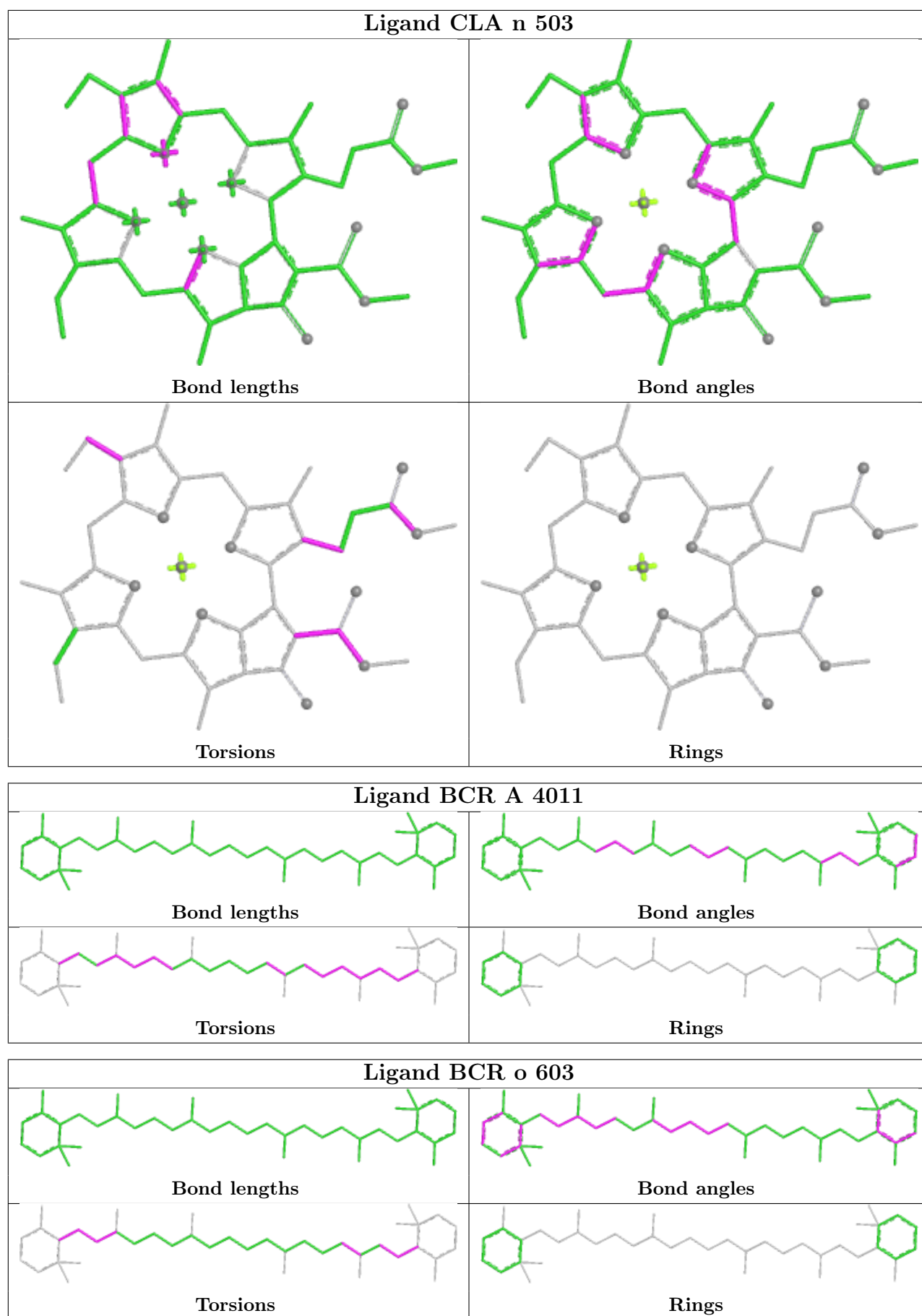
Torsions

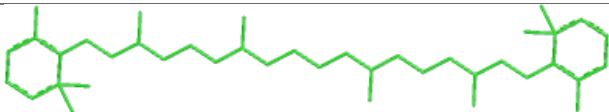
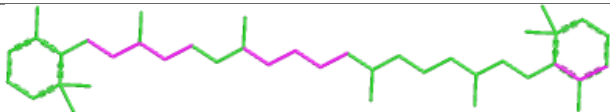
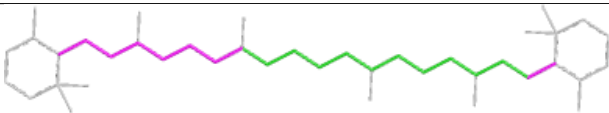
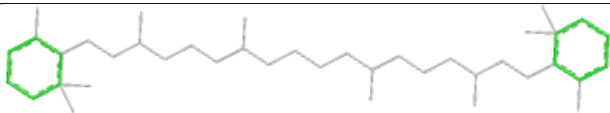


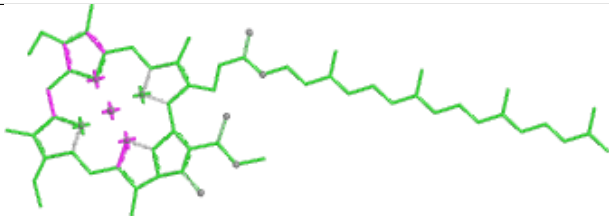
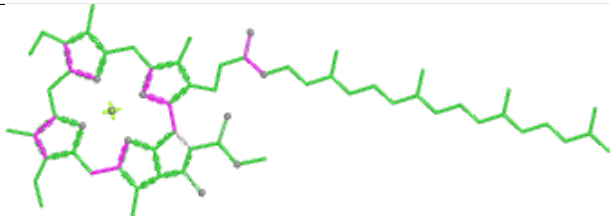
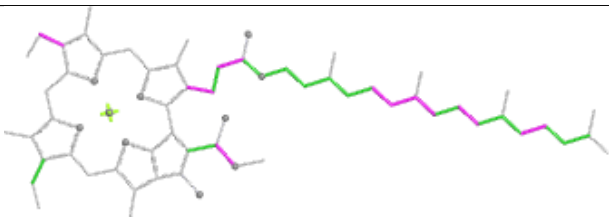
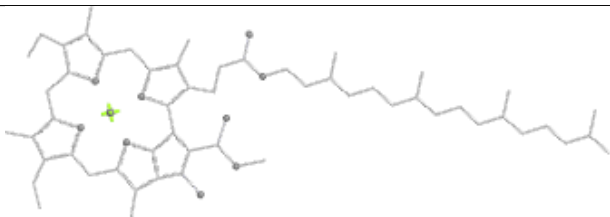
Rings

Ligand BCR s 603			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

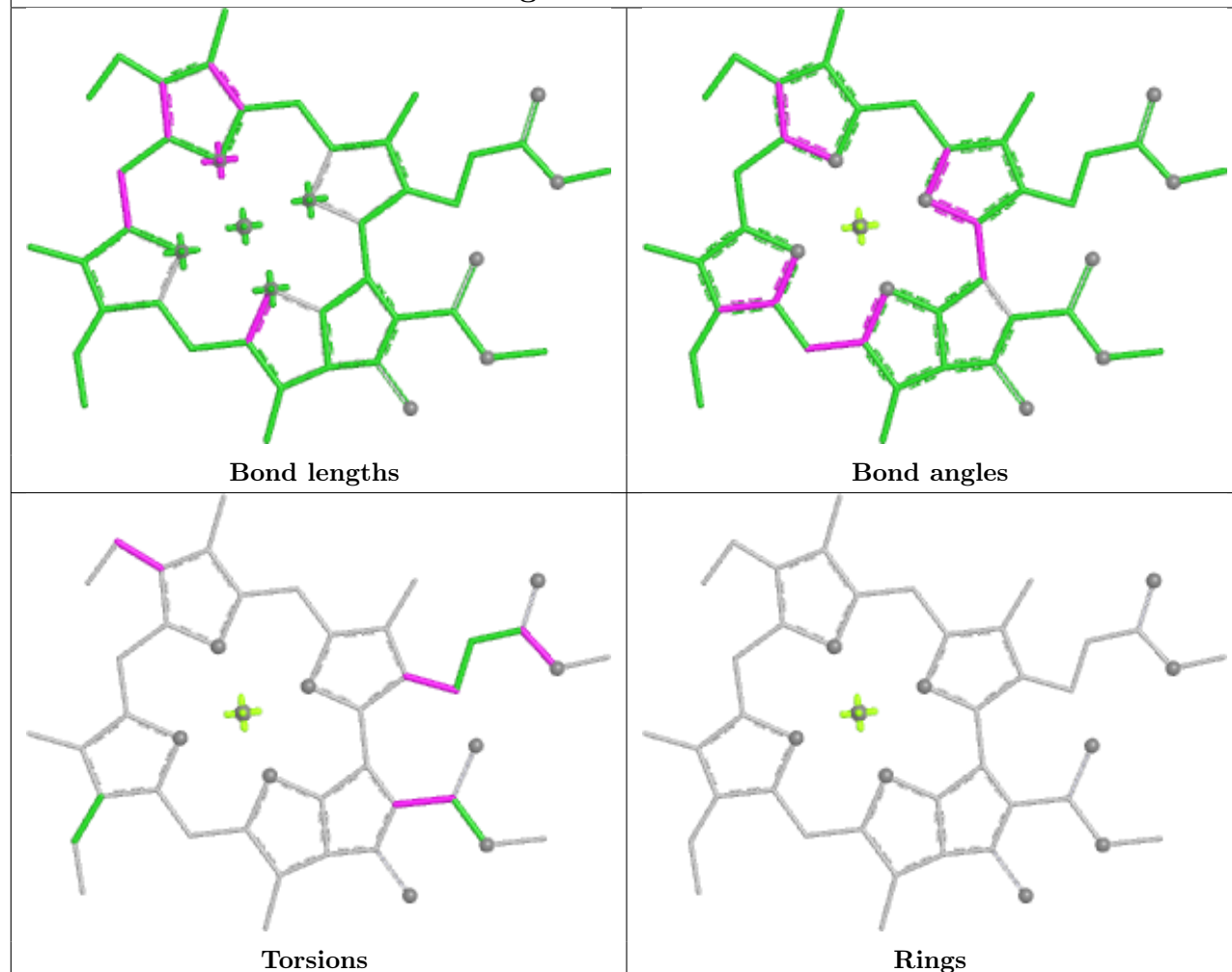
Ligand CLA Z 505			
			
Bond lengths	Bond angles		
			
Torsions	Rings		



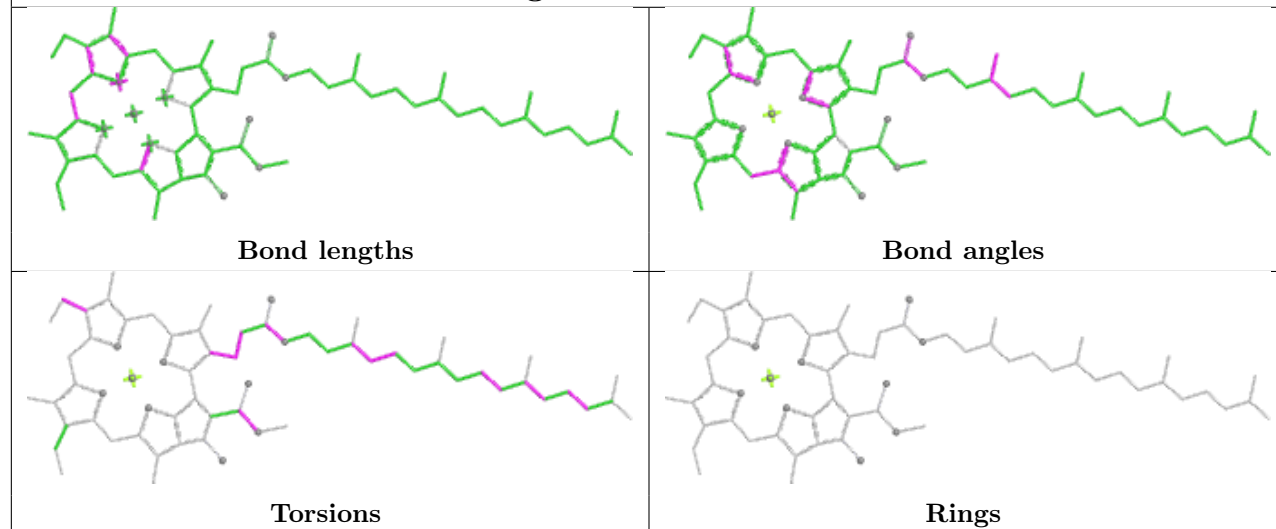
Ligand BCR n 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

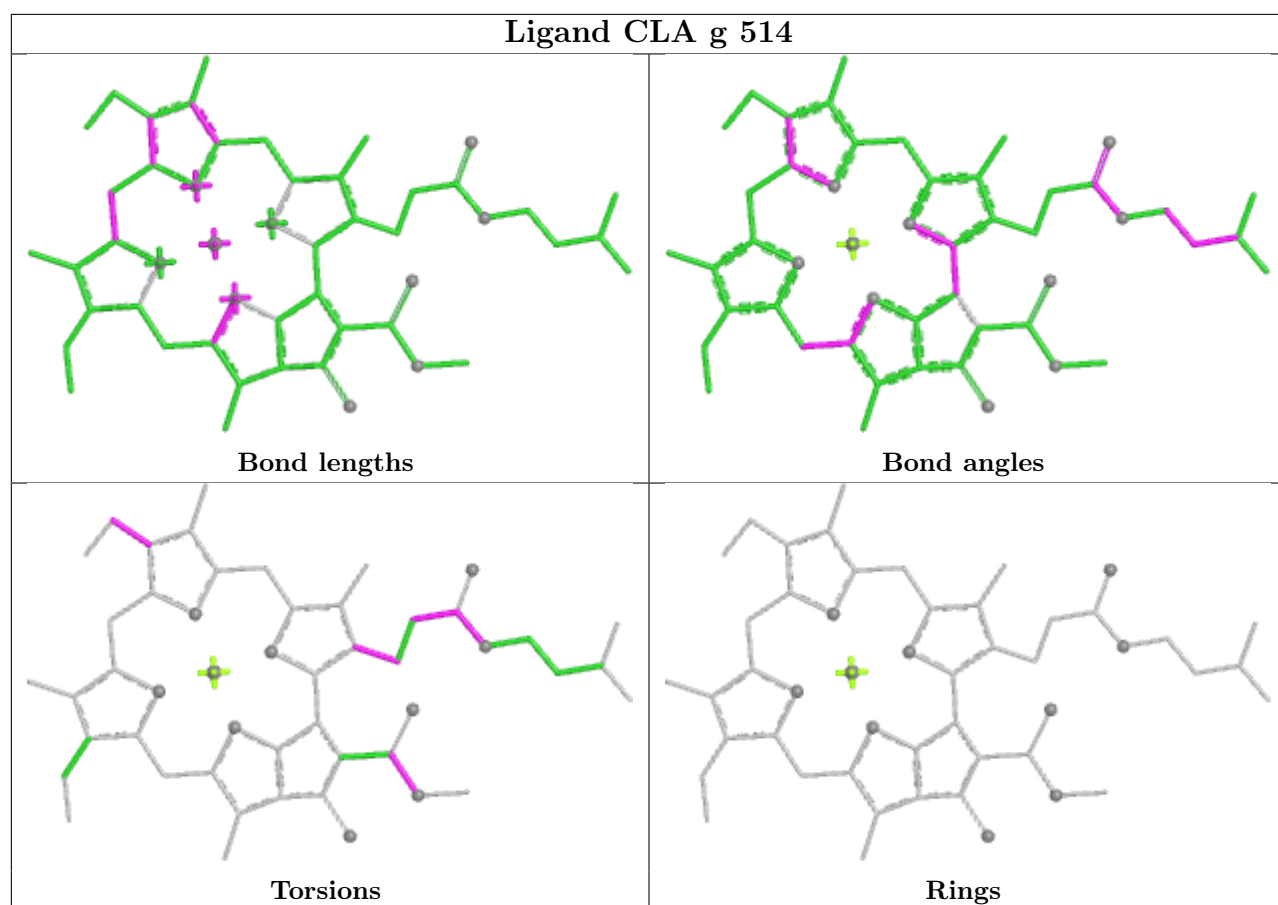
Ligand CLA Z 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

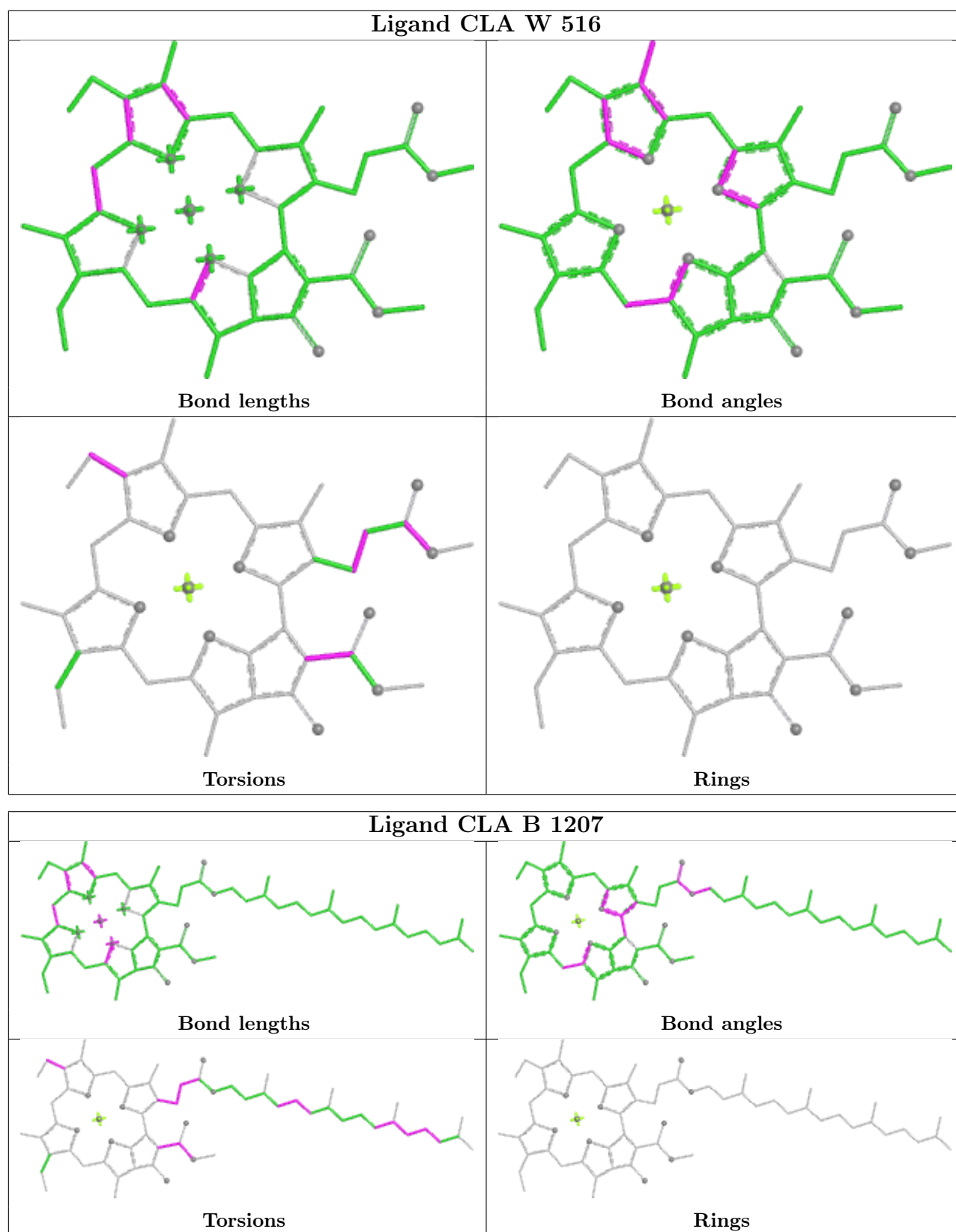
Ligand CLA t 503

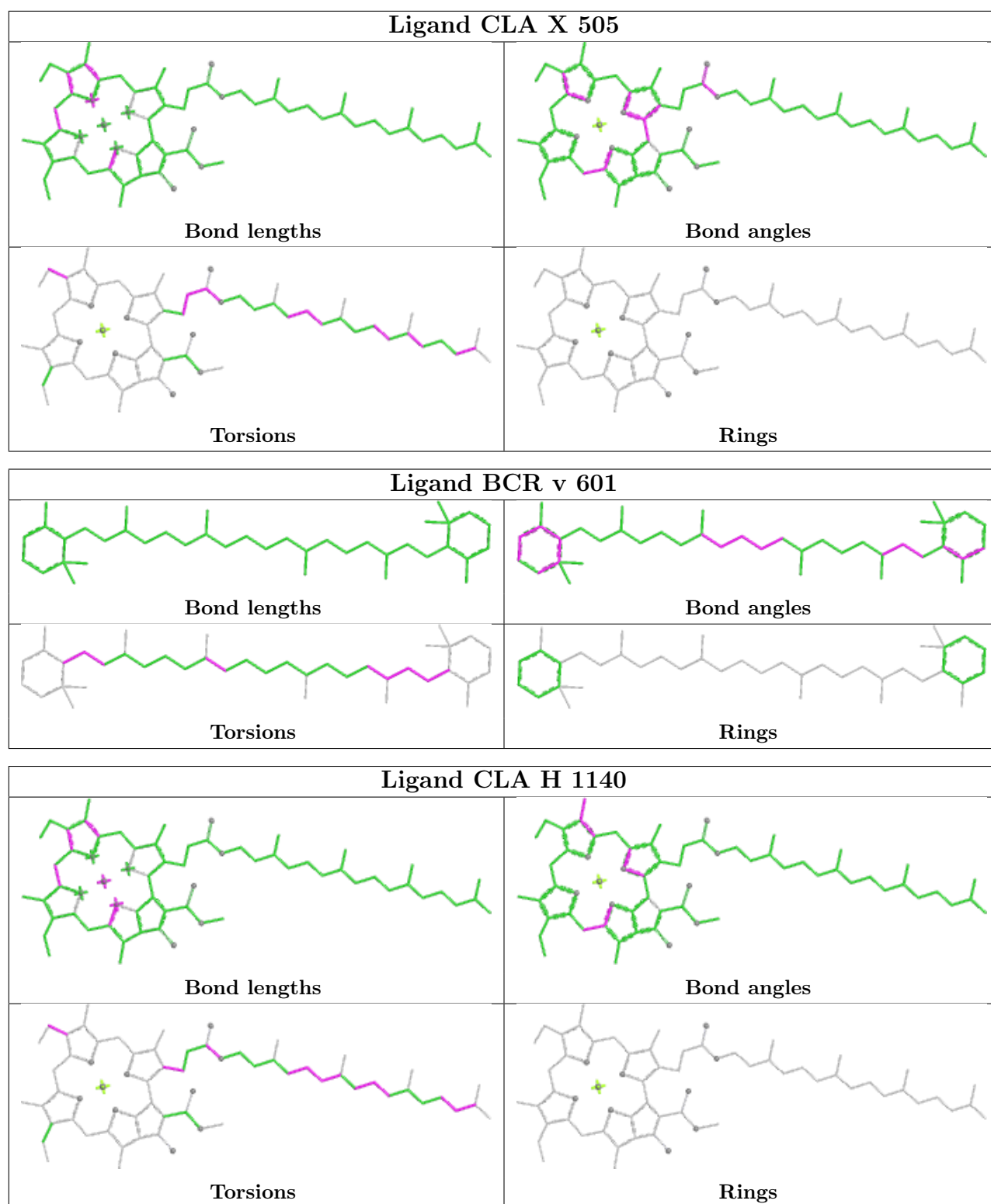


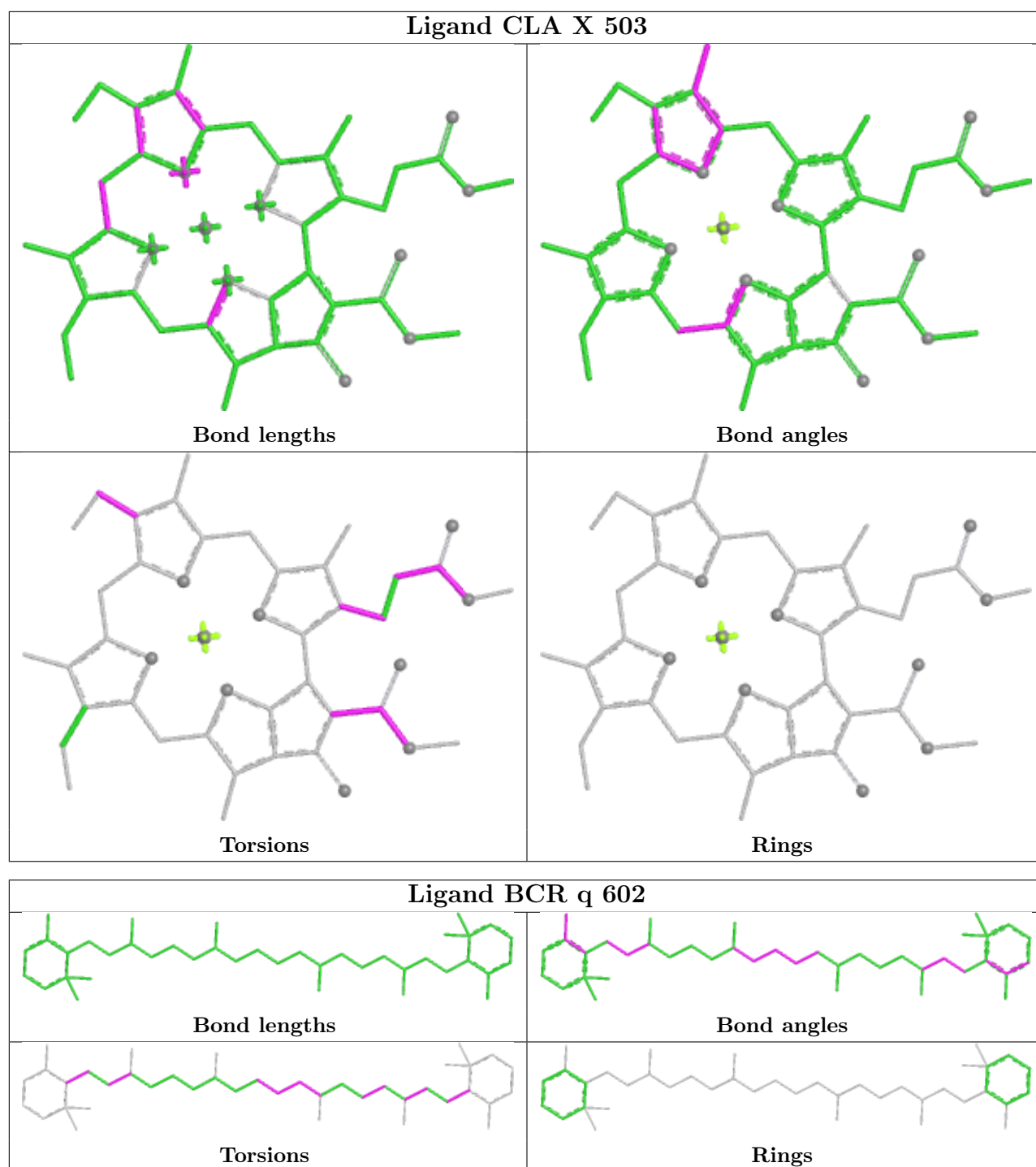
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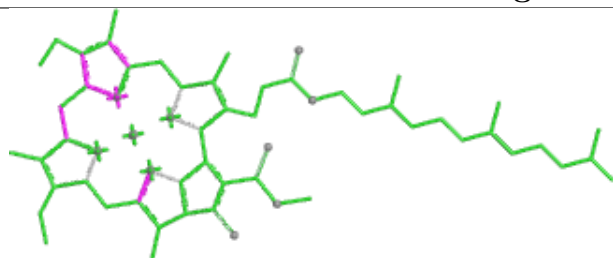




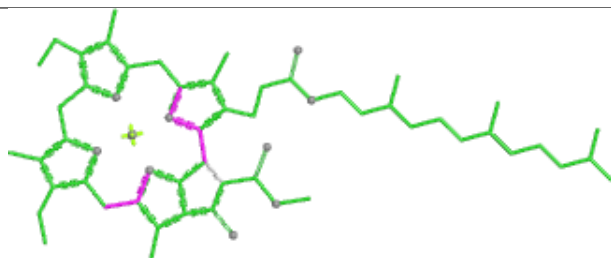




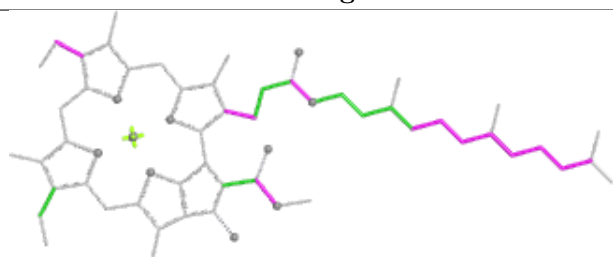
Ligand CLA X 504



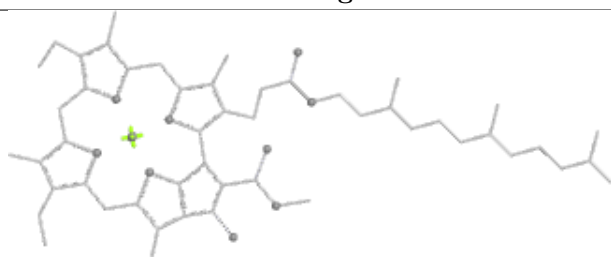
Bond lengths



Bond angles

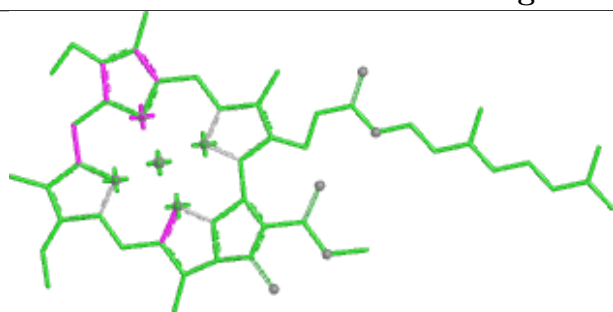


Torsions

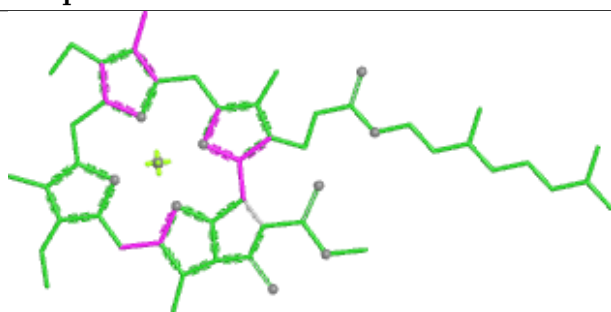


Rings

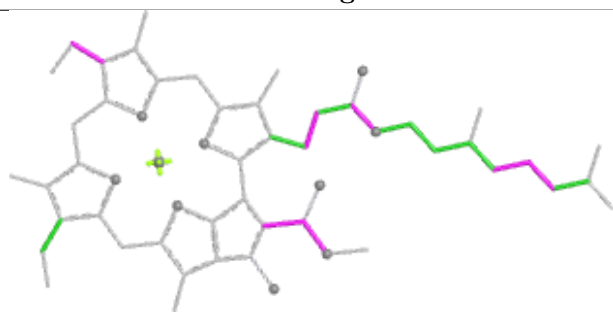
Ligand CLA q 517



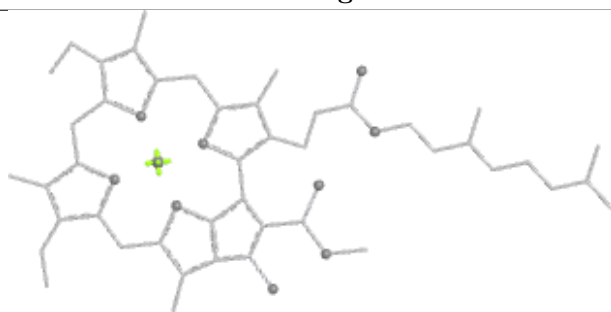
Bond lengths



Bond angles

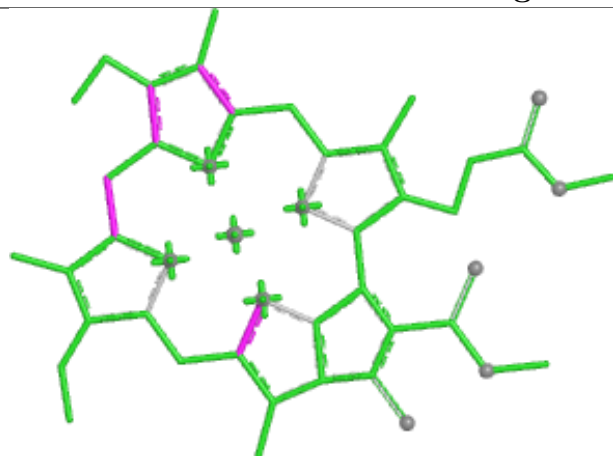


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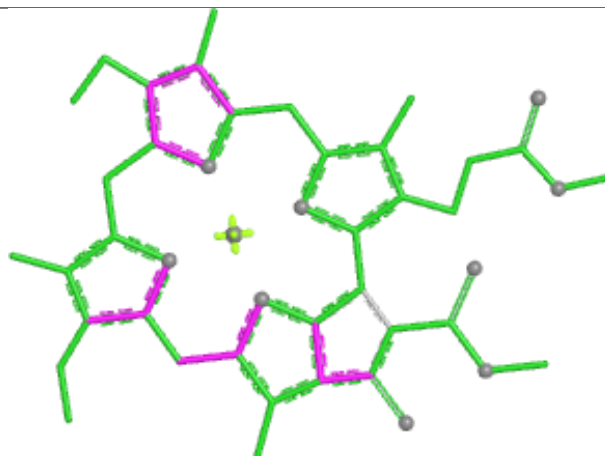


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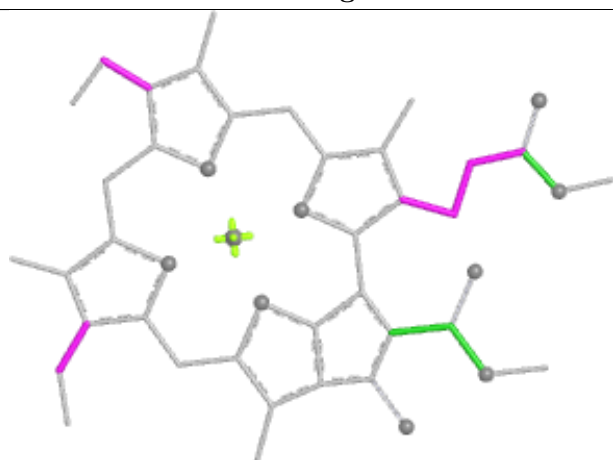
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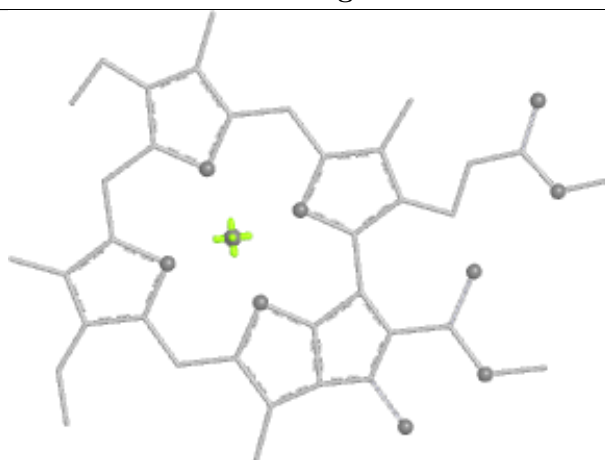
Bond lengths



Bond angles

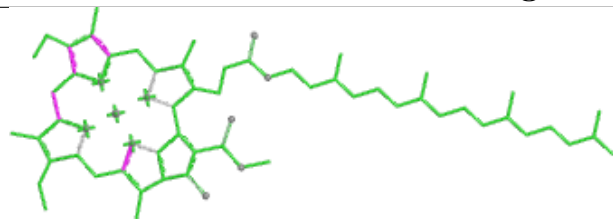


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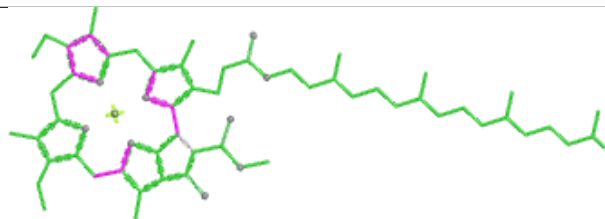


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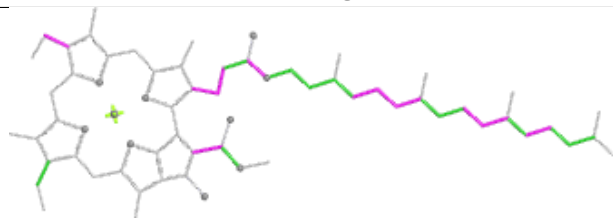
Ligand CLA t 515



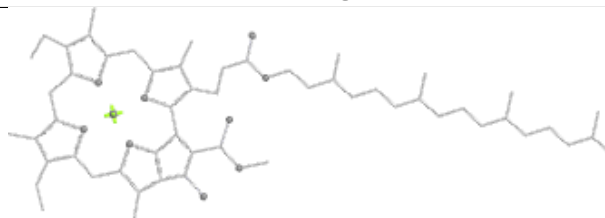
Bond lengths



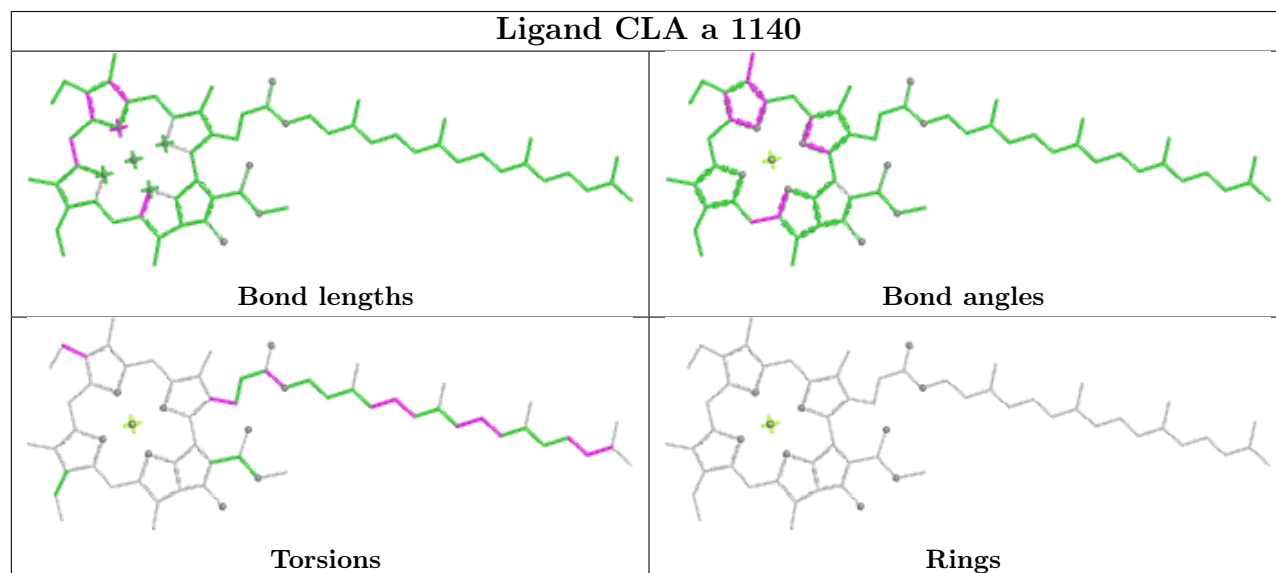
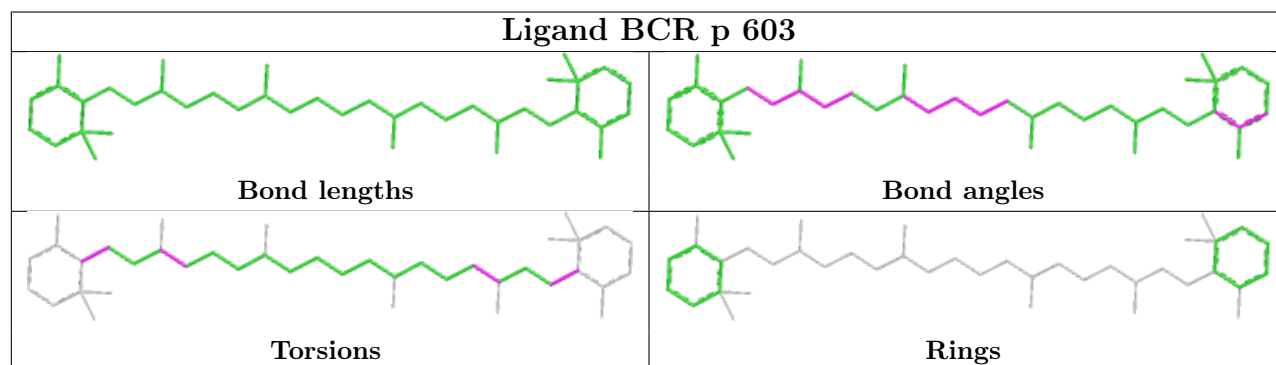
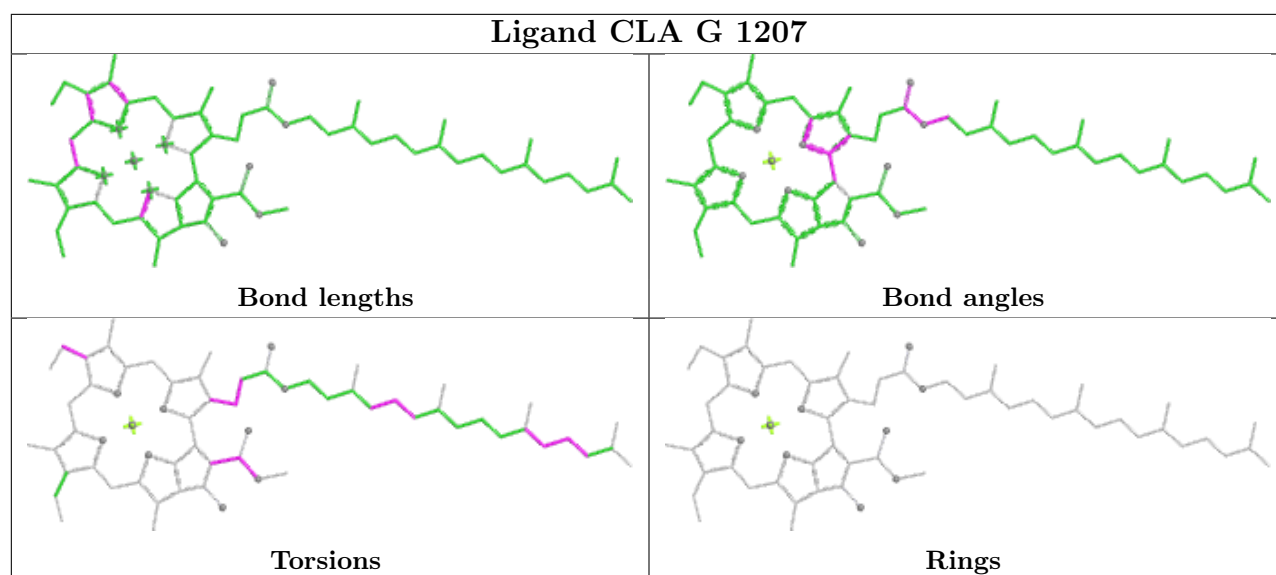
Bond angles

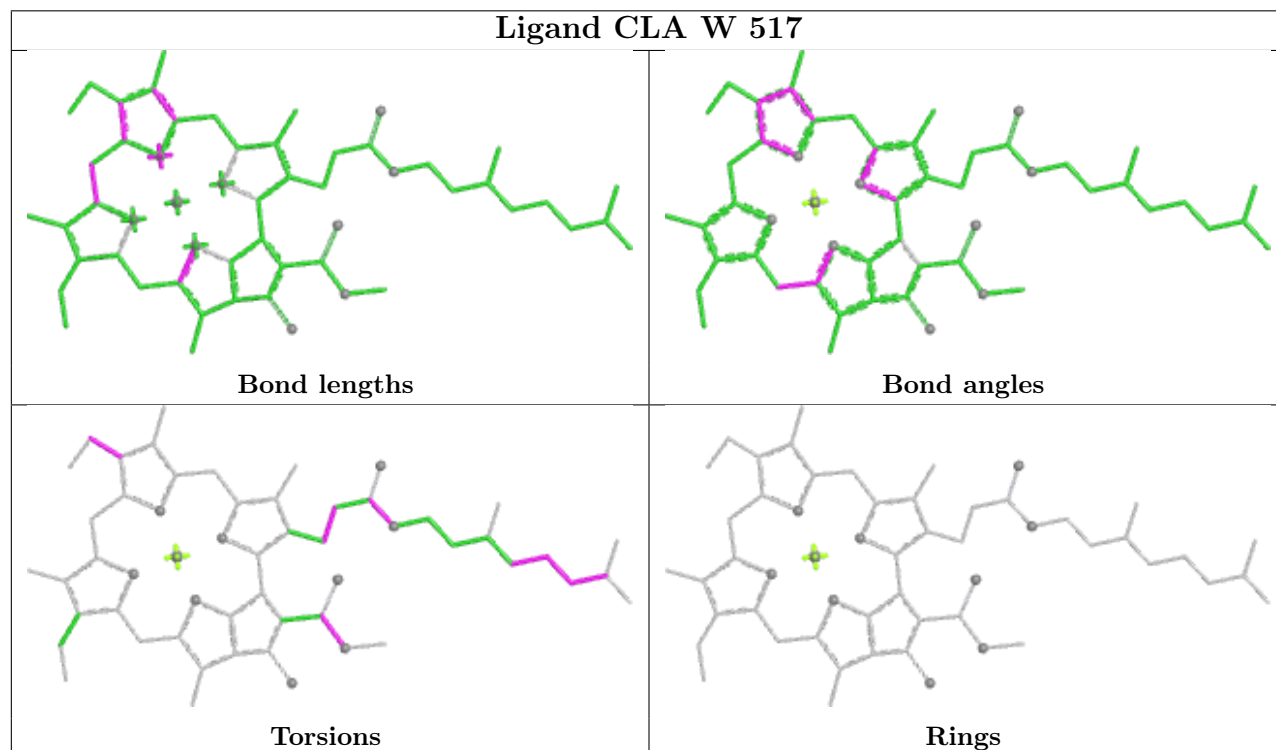
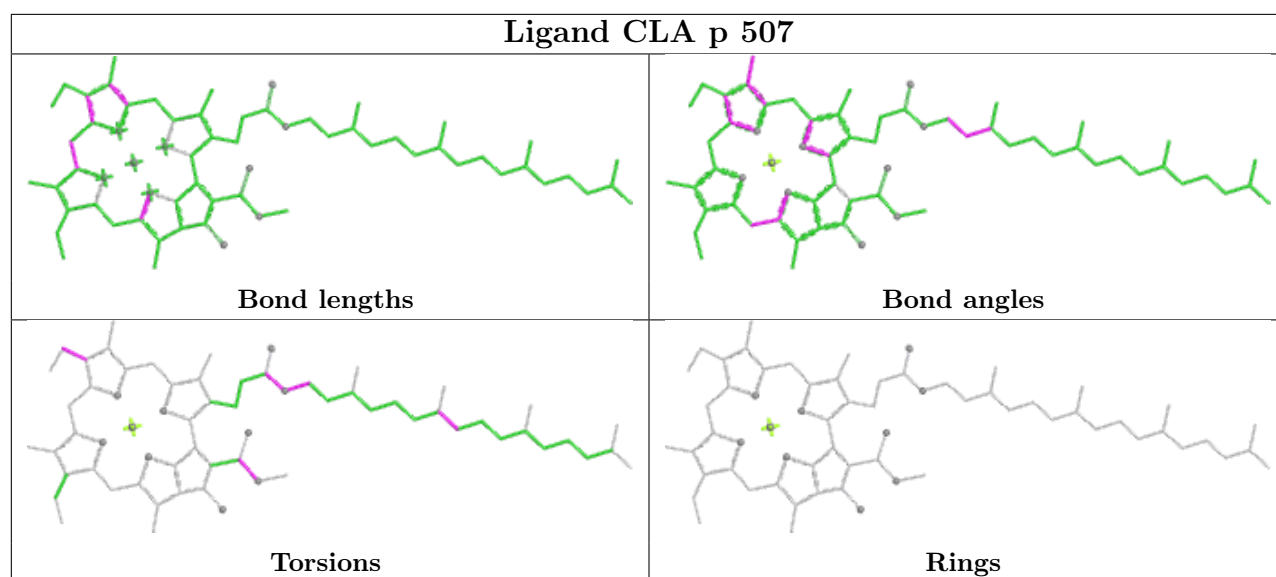


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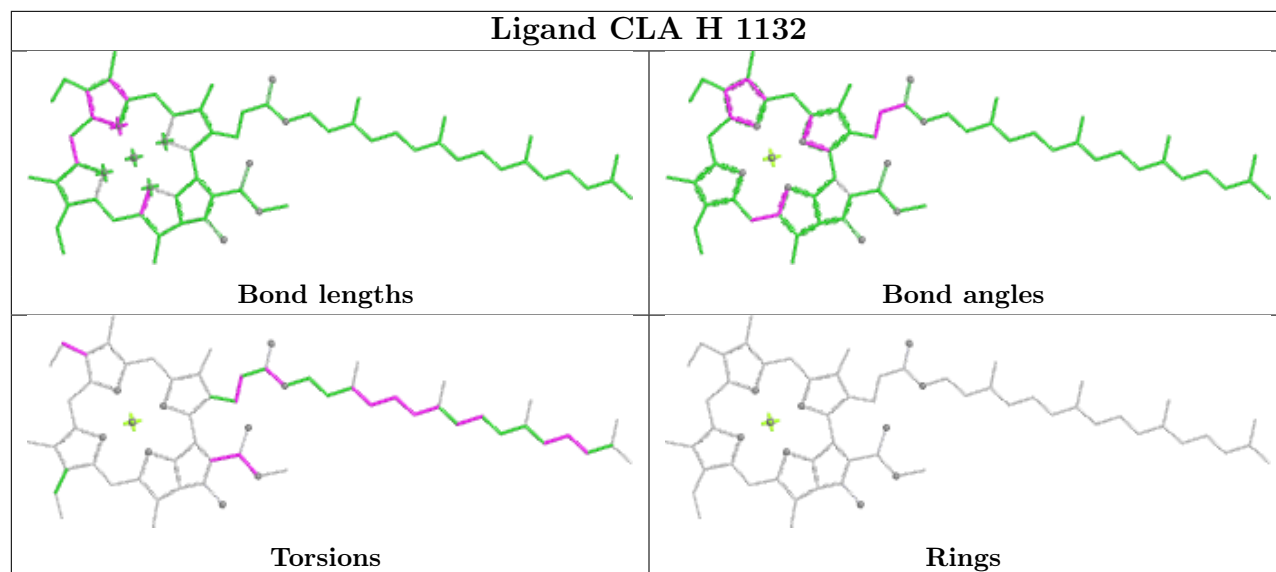


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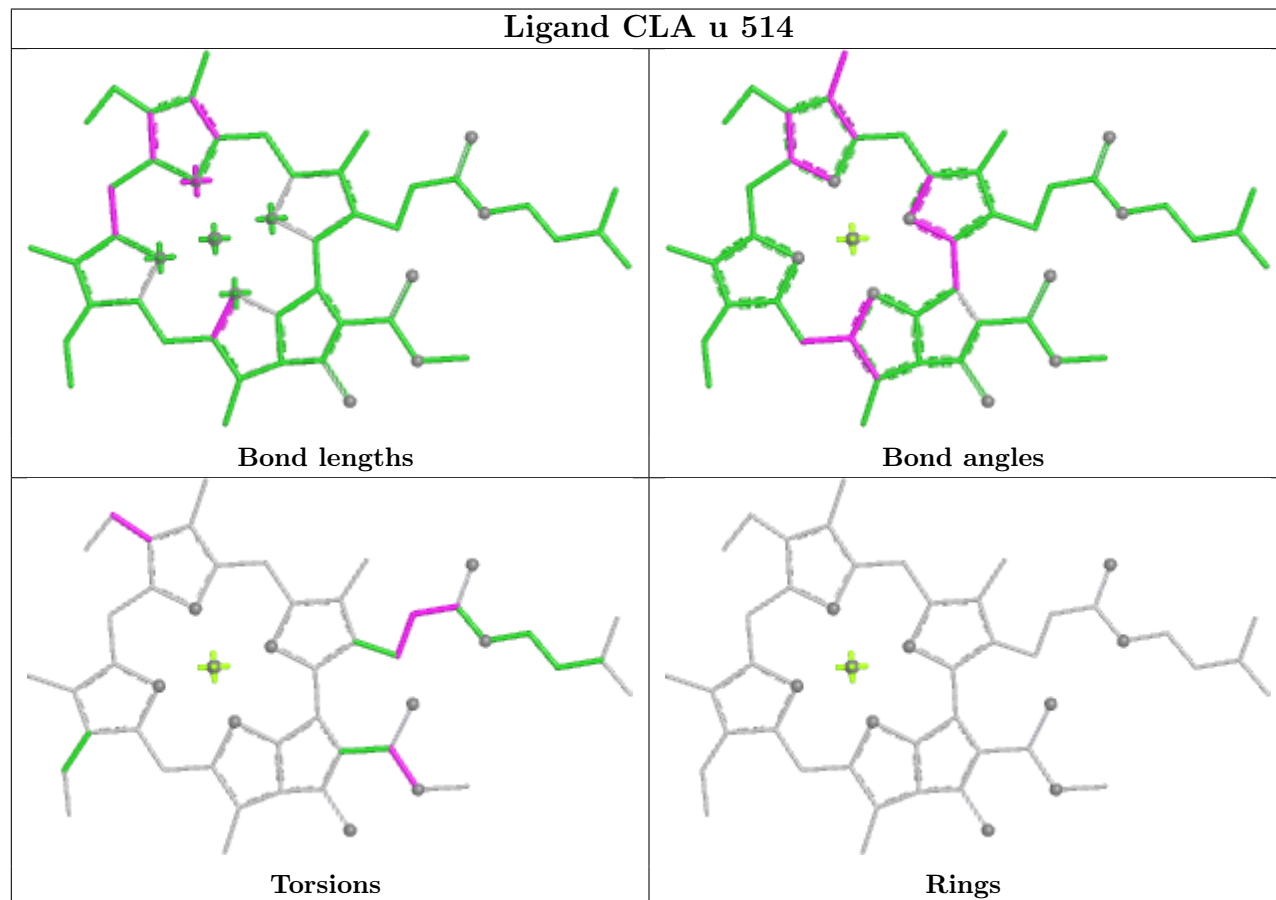




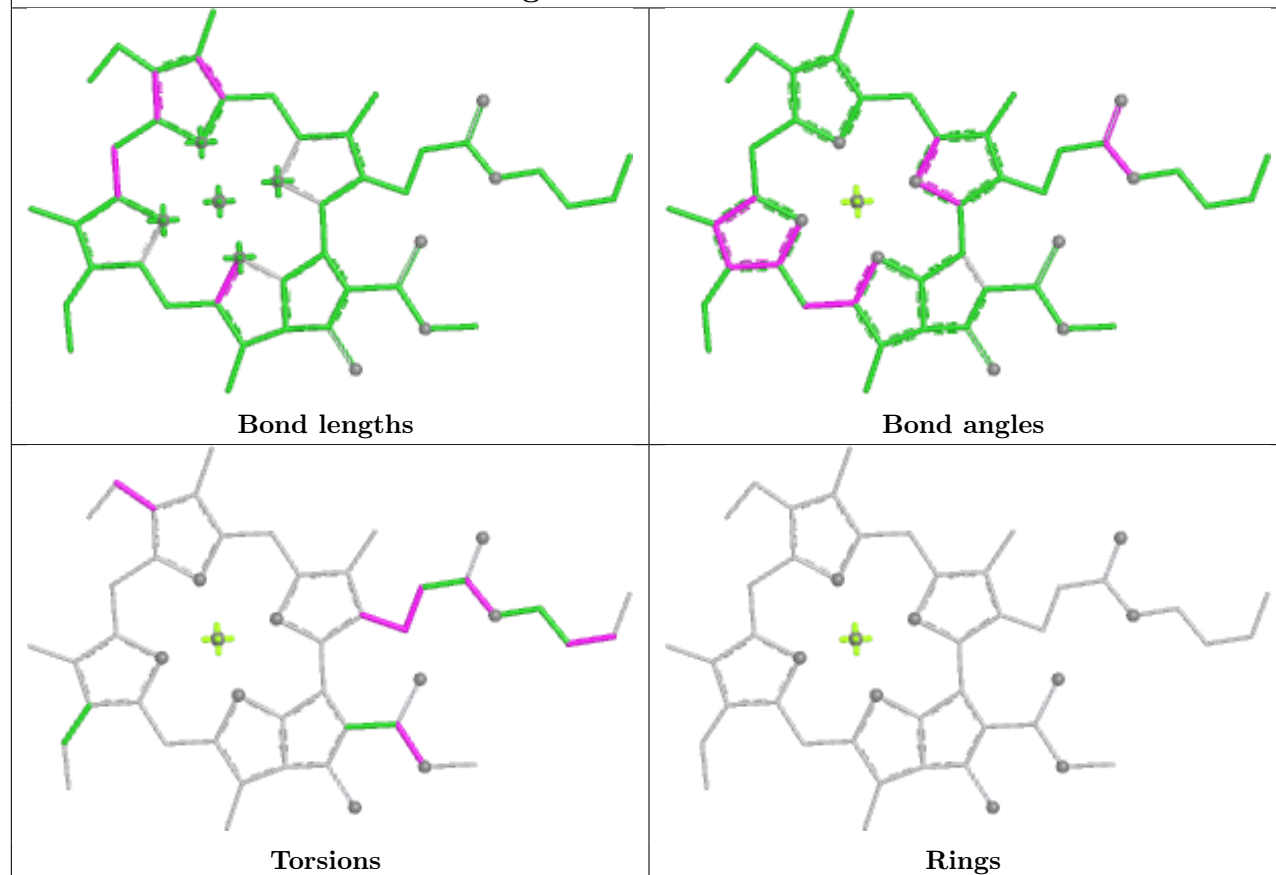
Ligand CLA H 1132



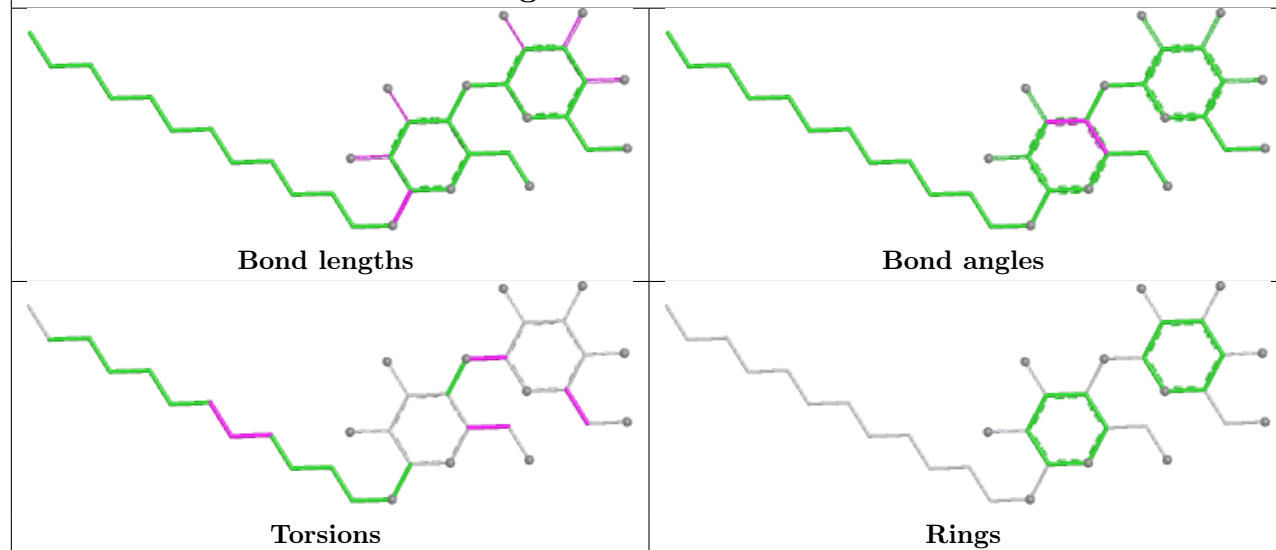
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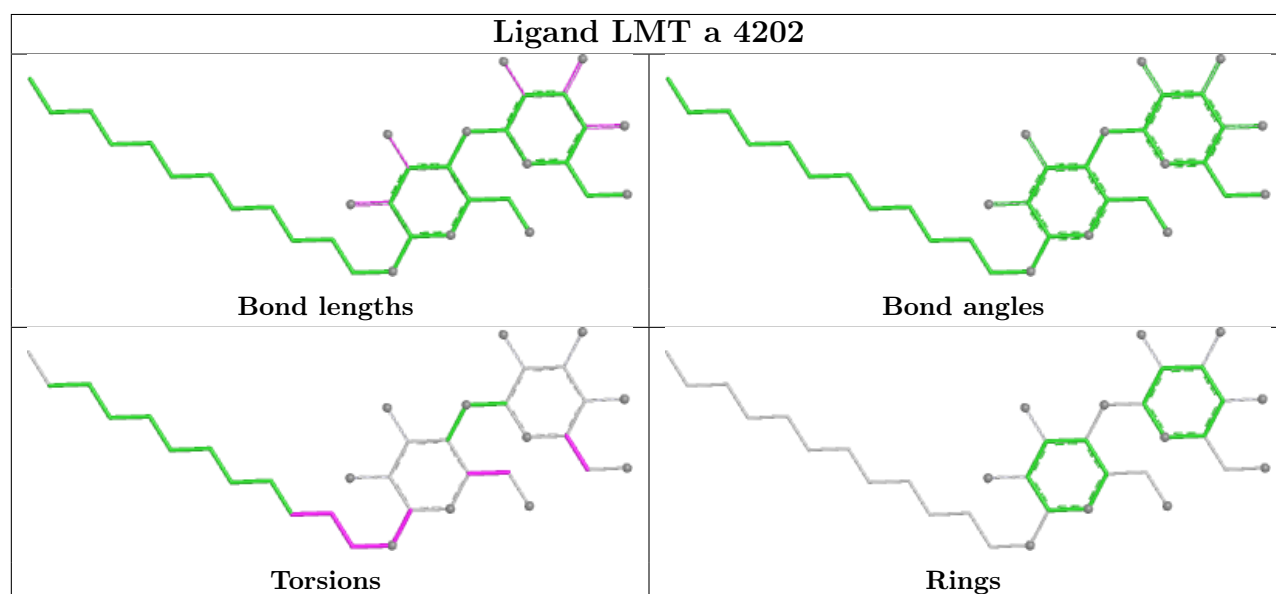
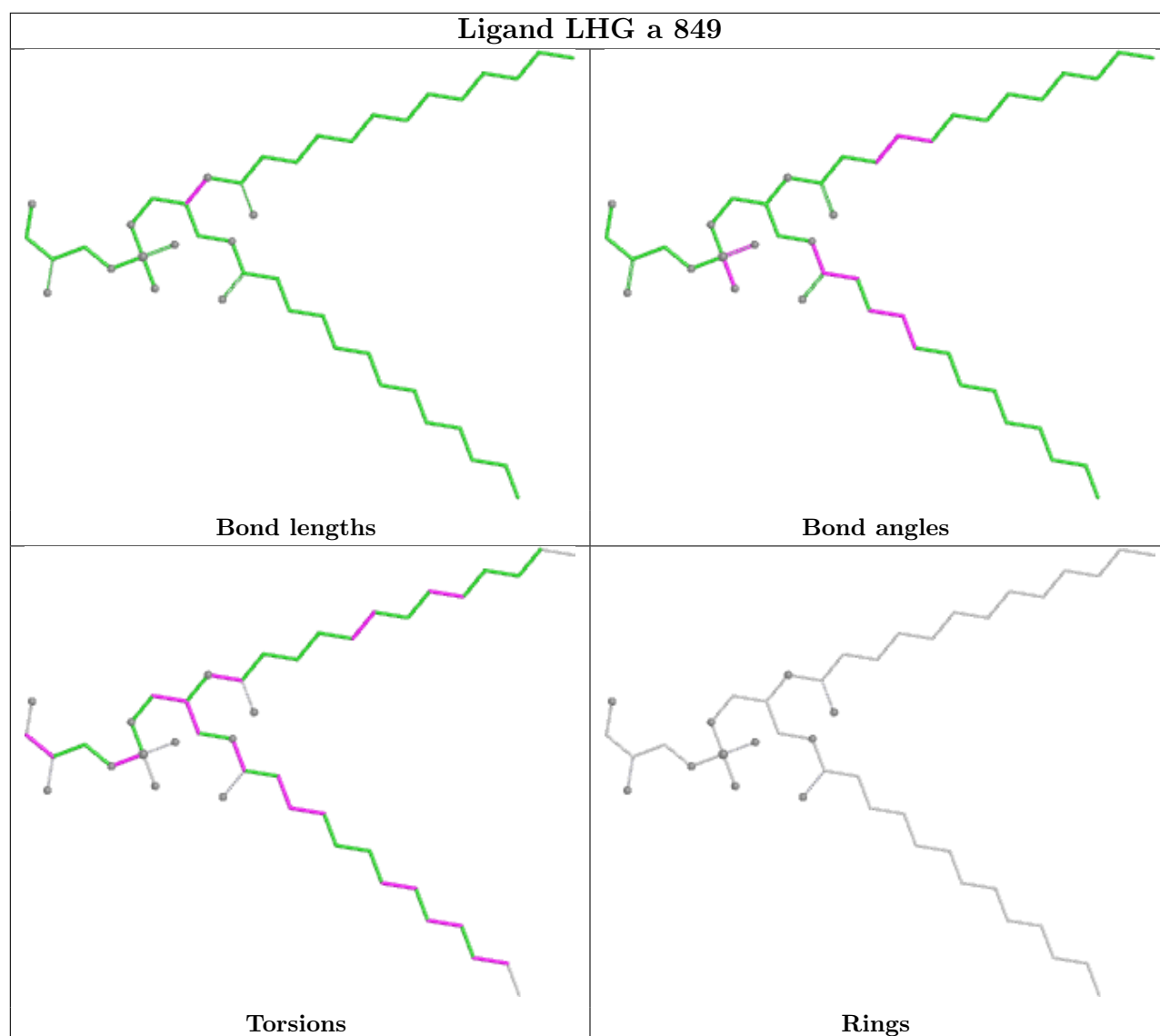


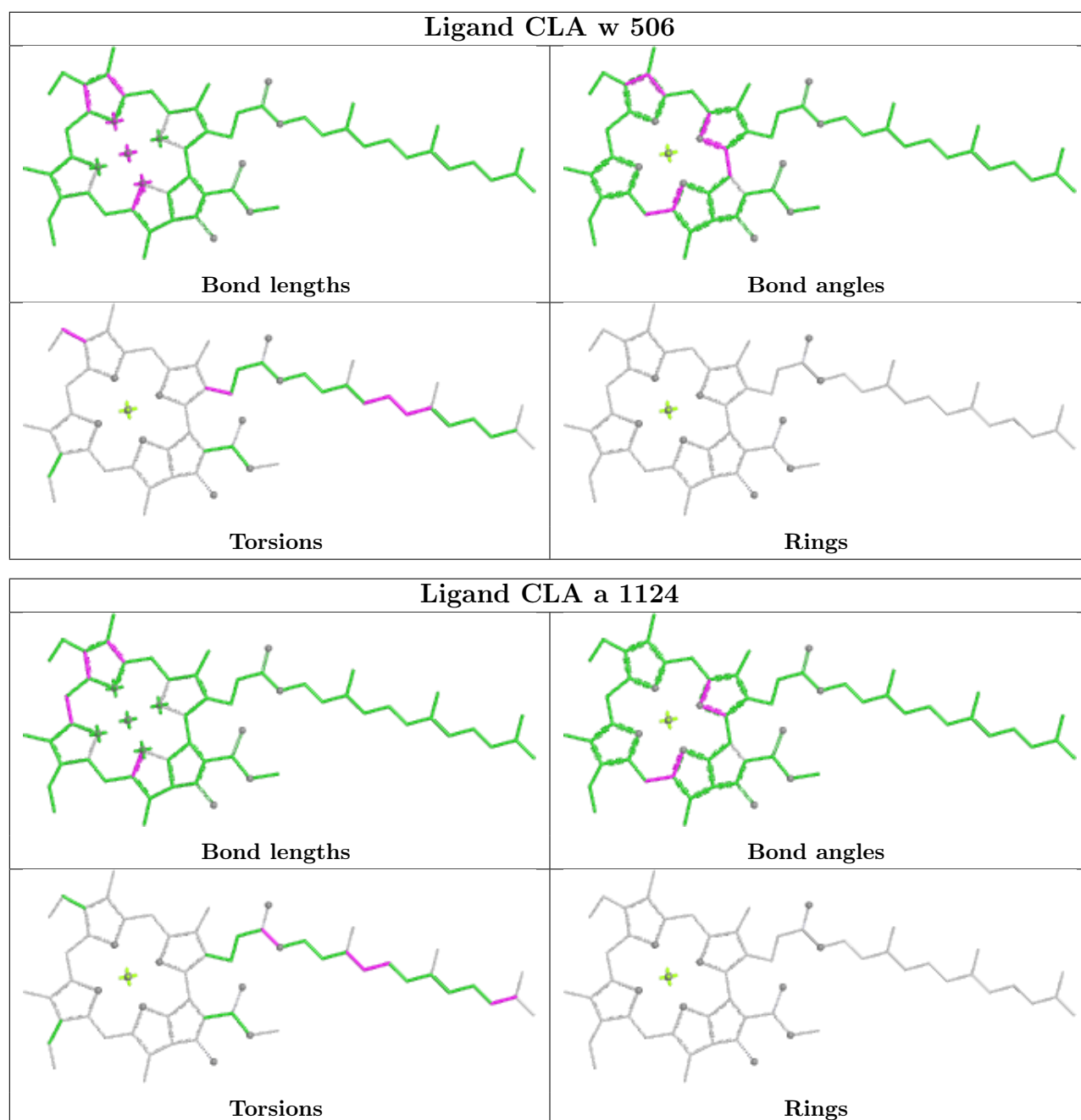
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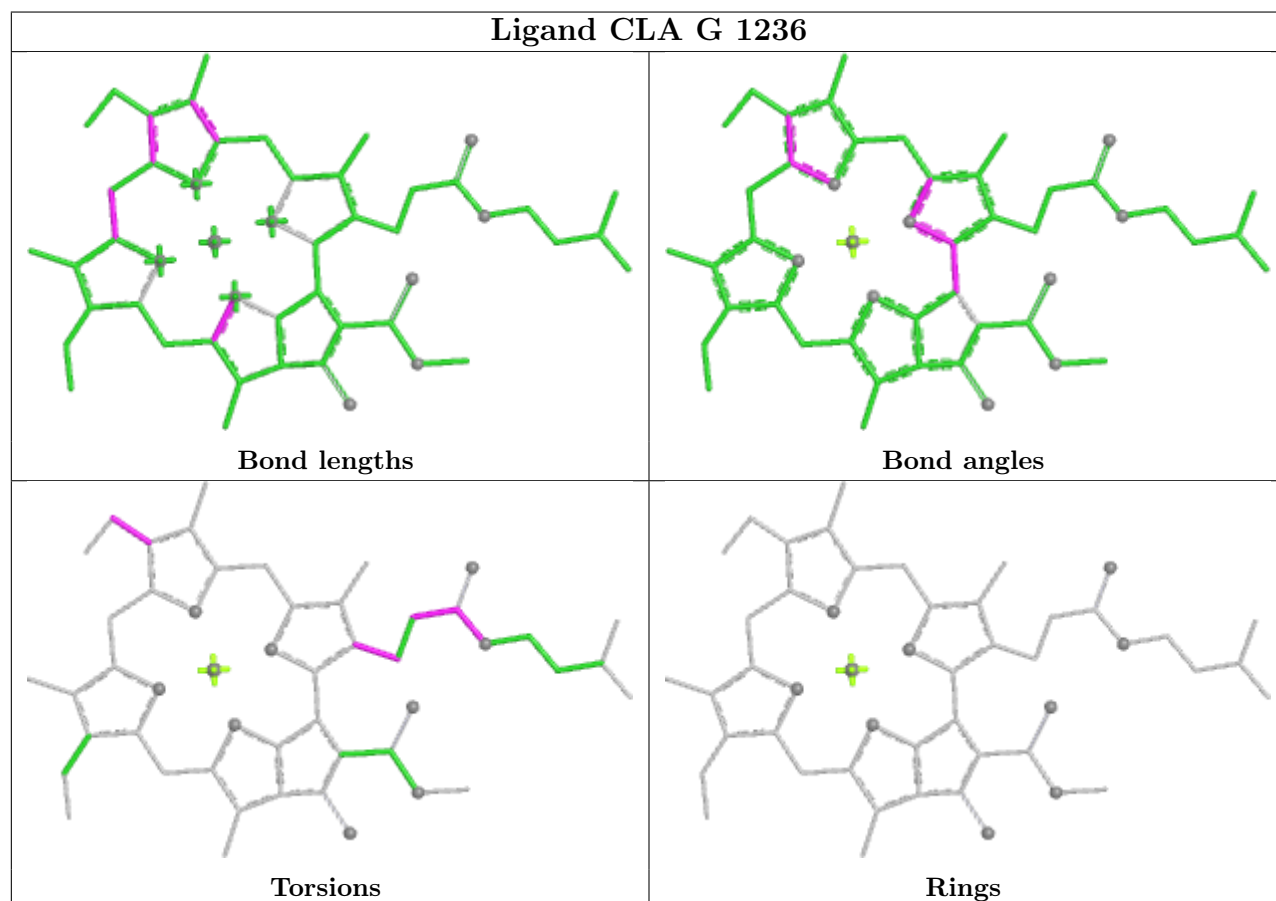
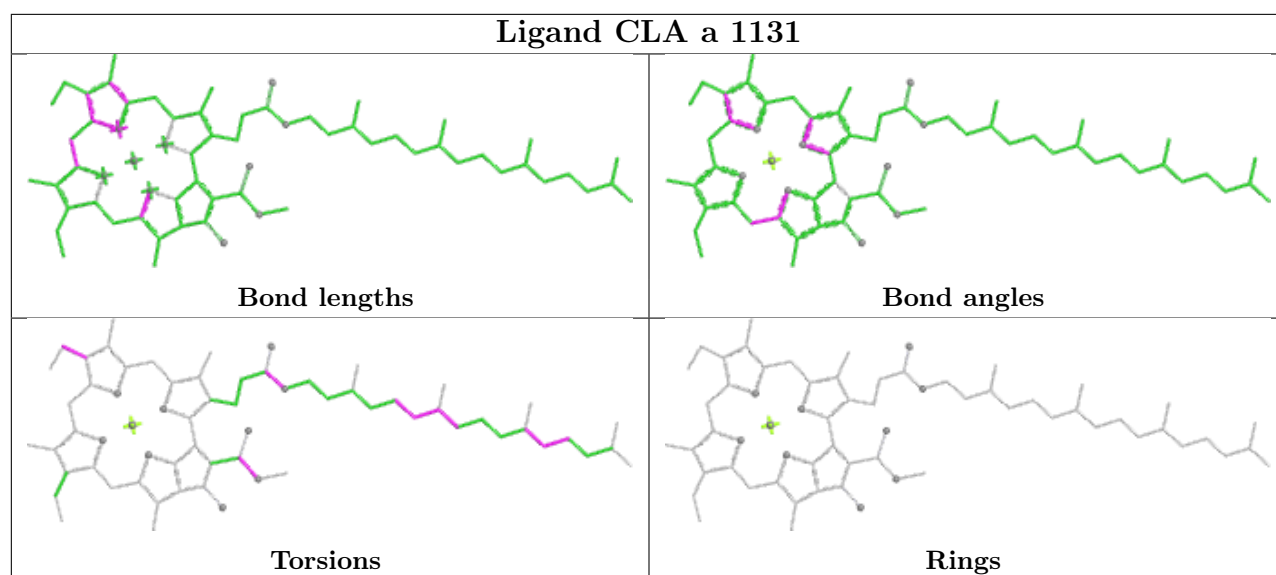


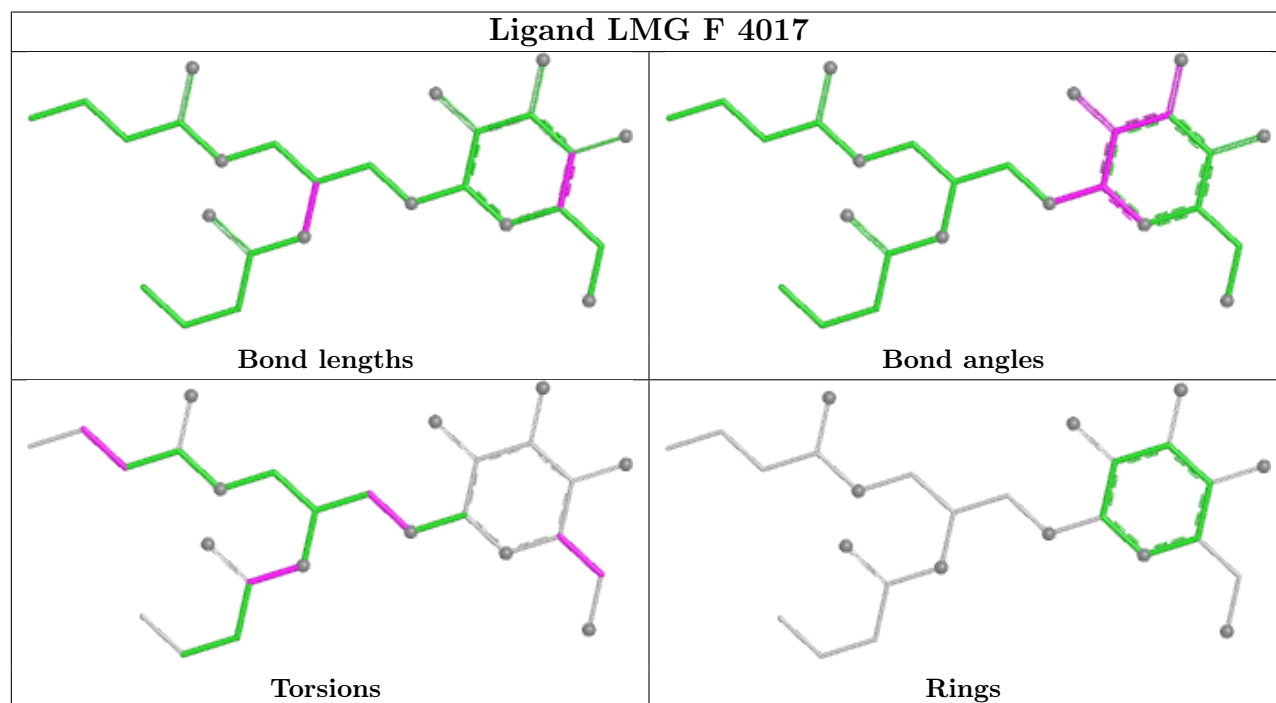
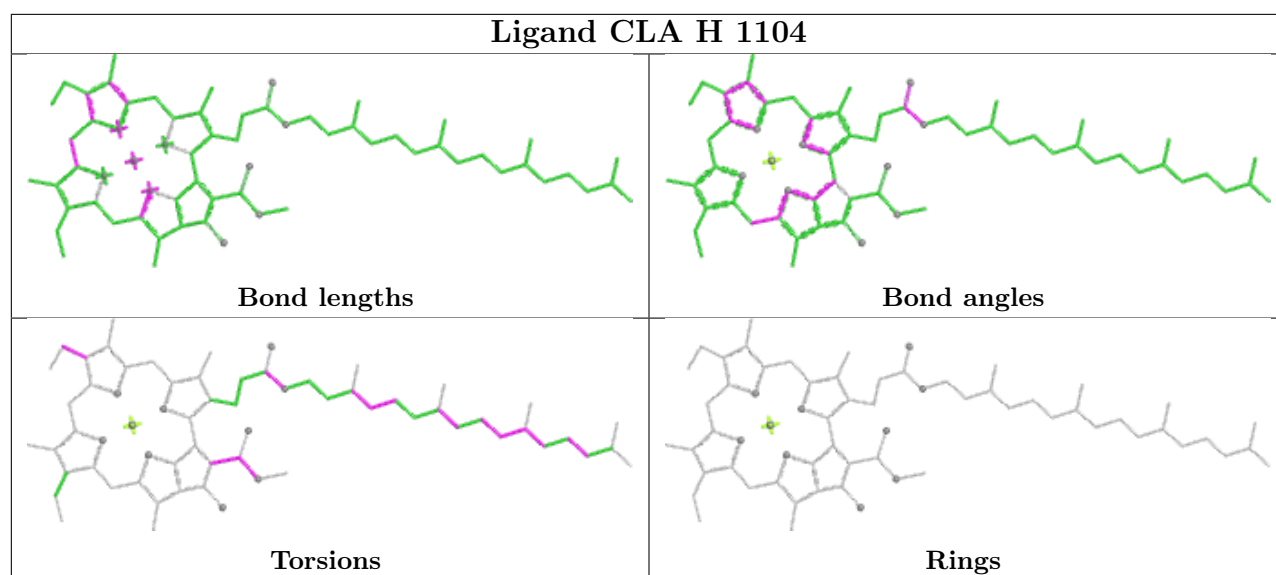
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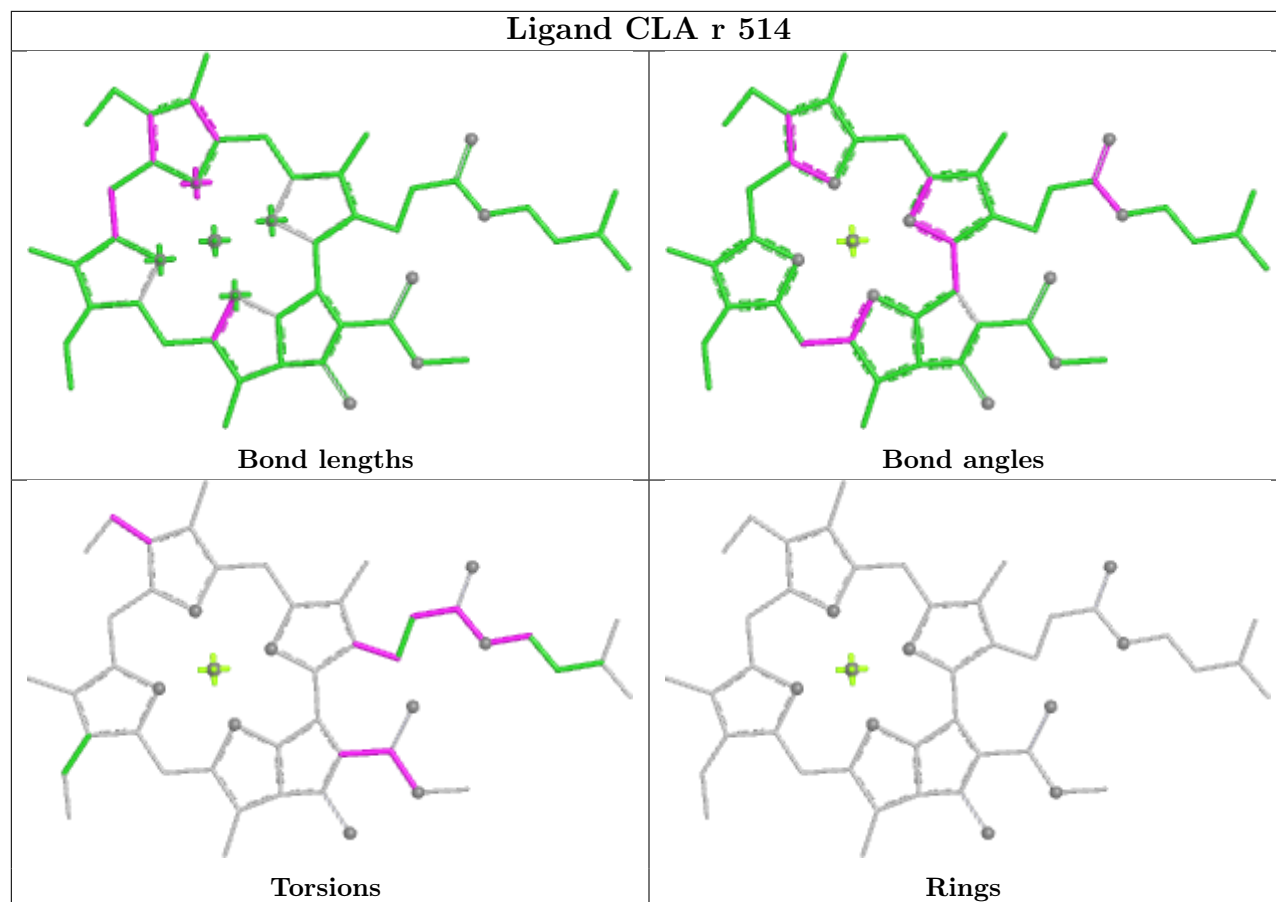


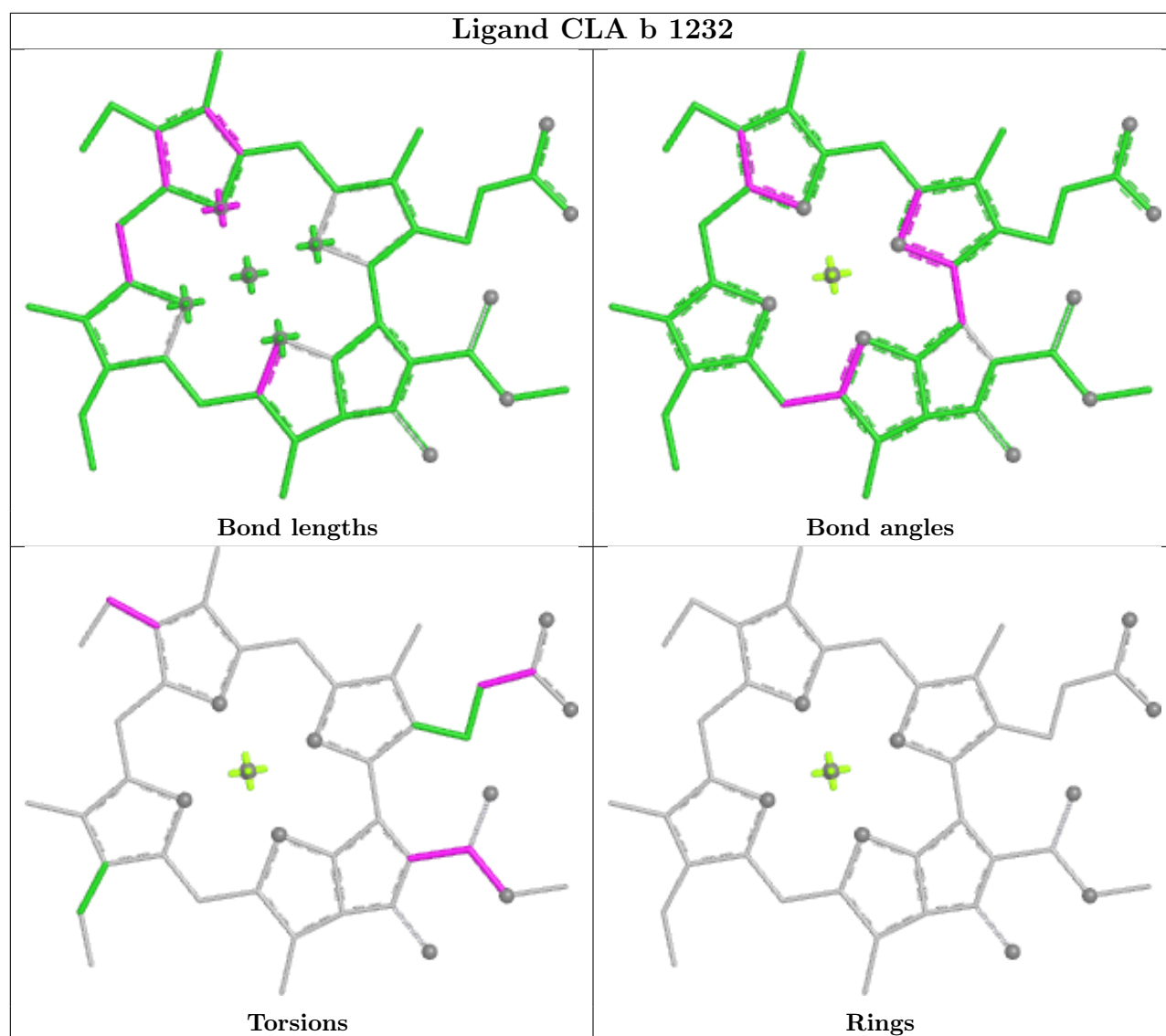




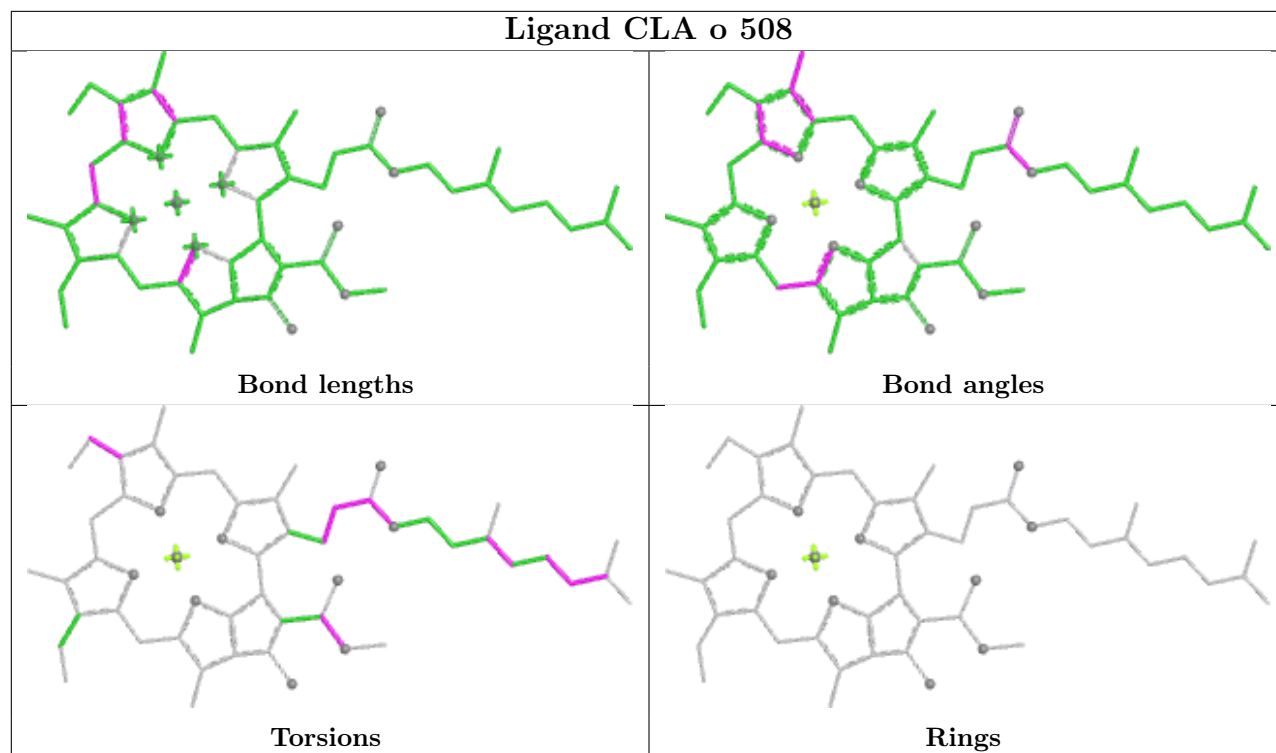


Ligand CLA r 514

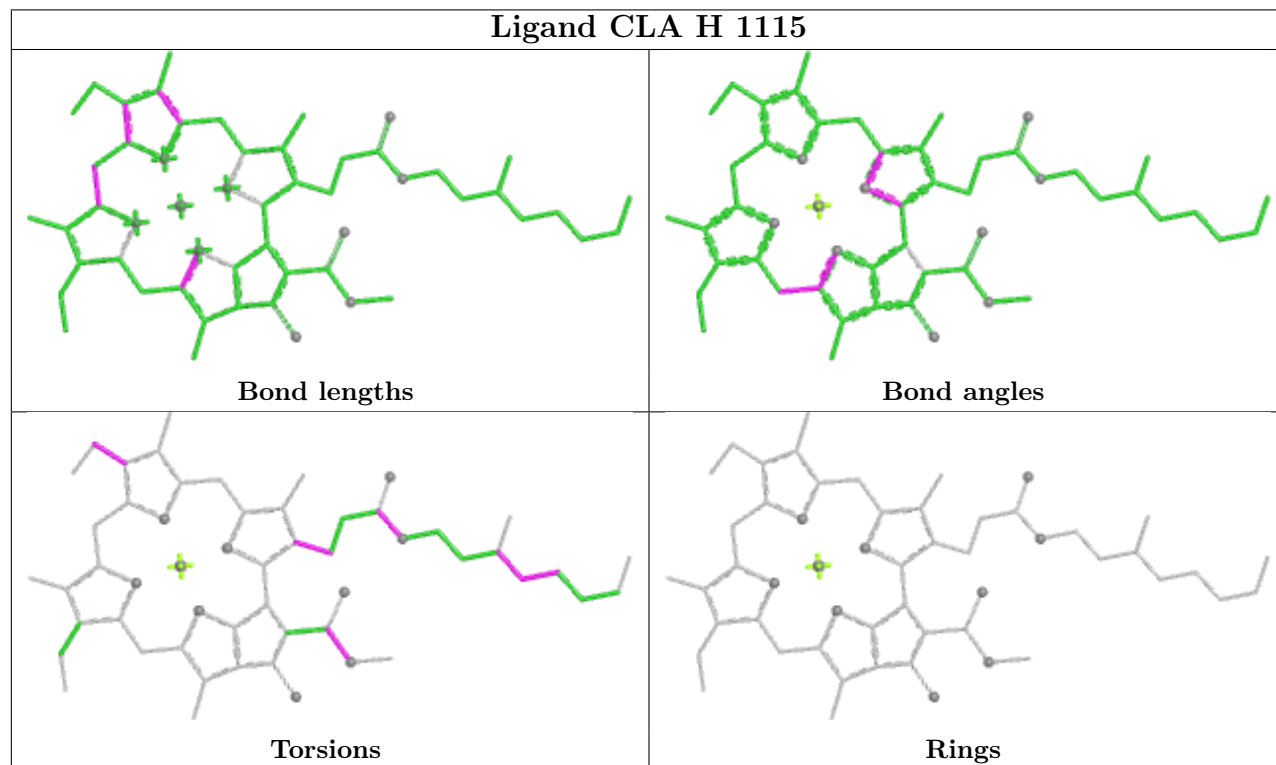


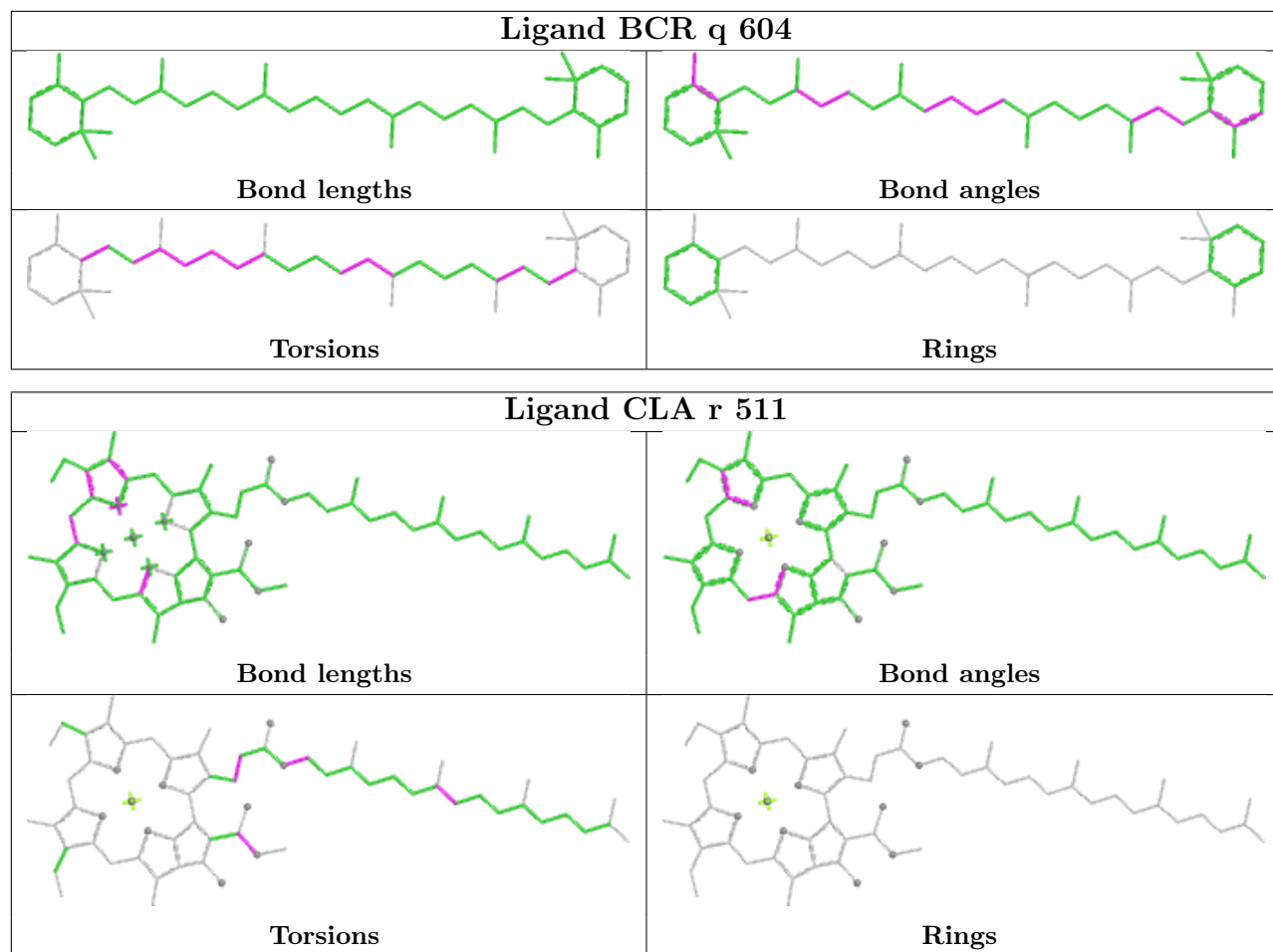


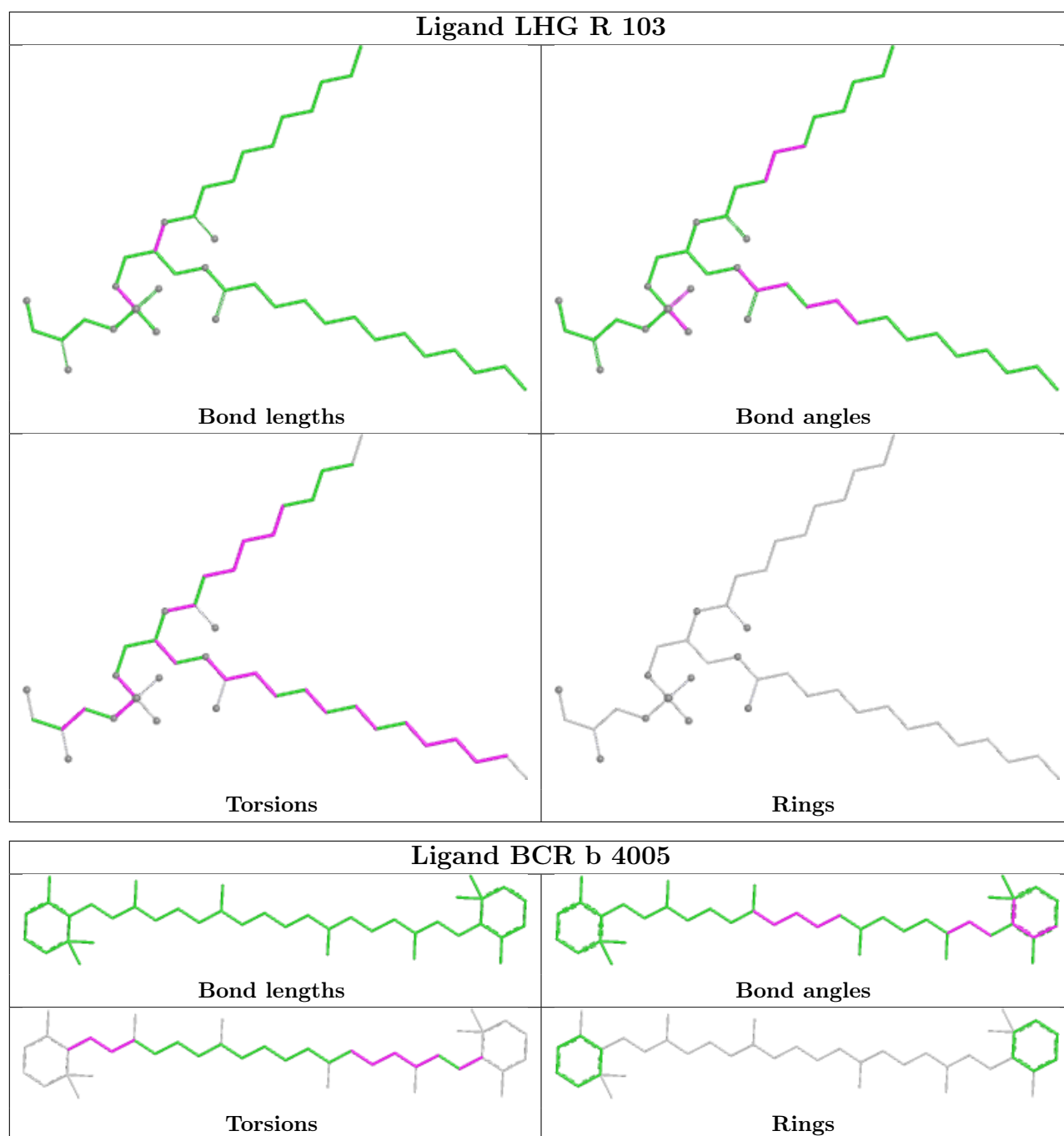
Ligand CLA o 508



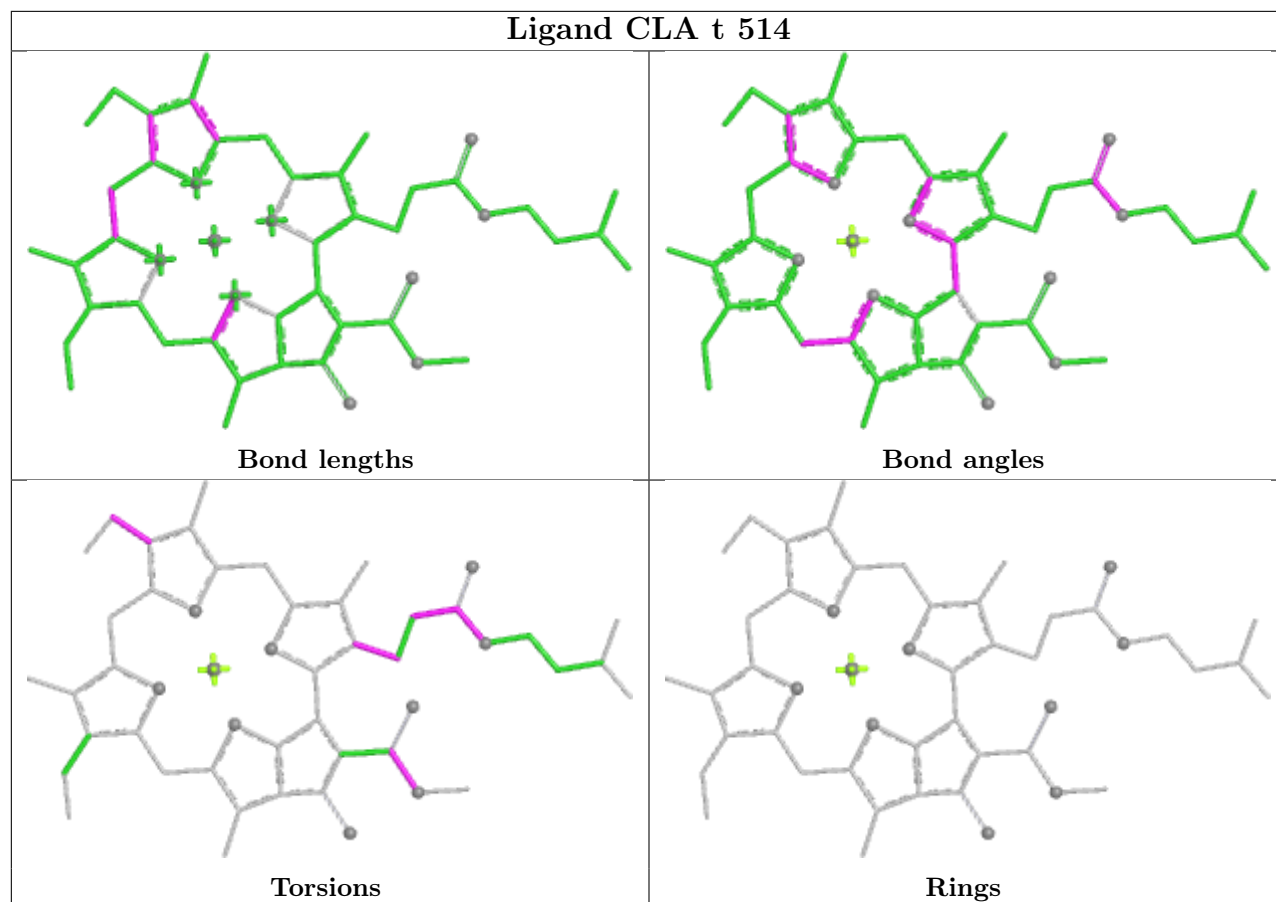
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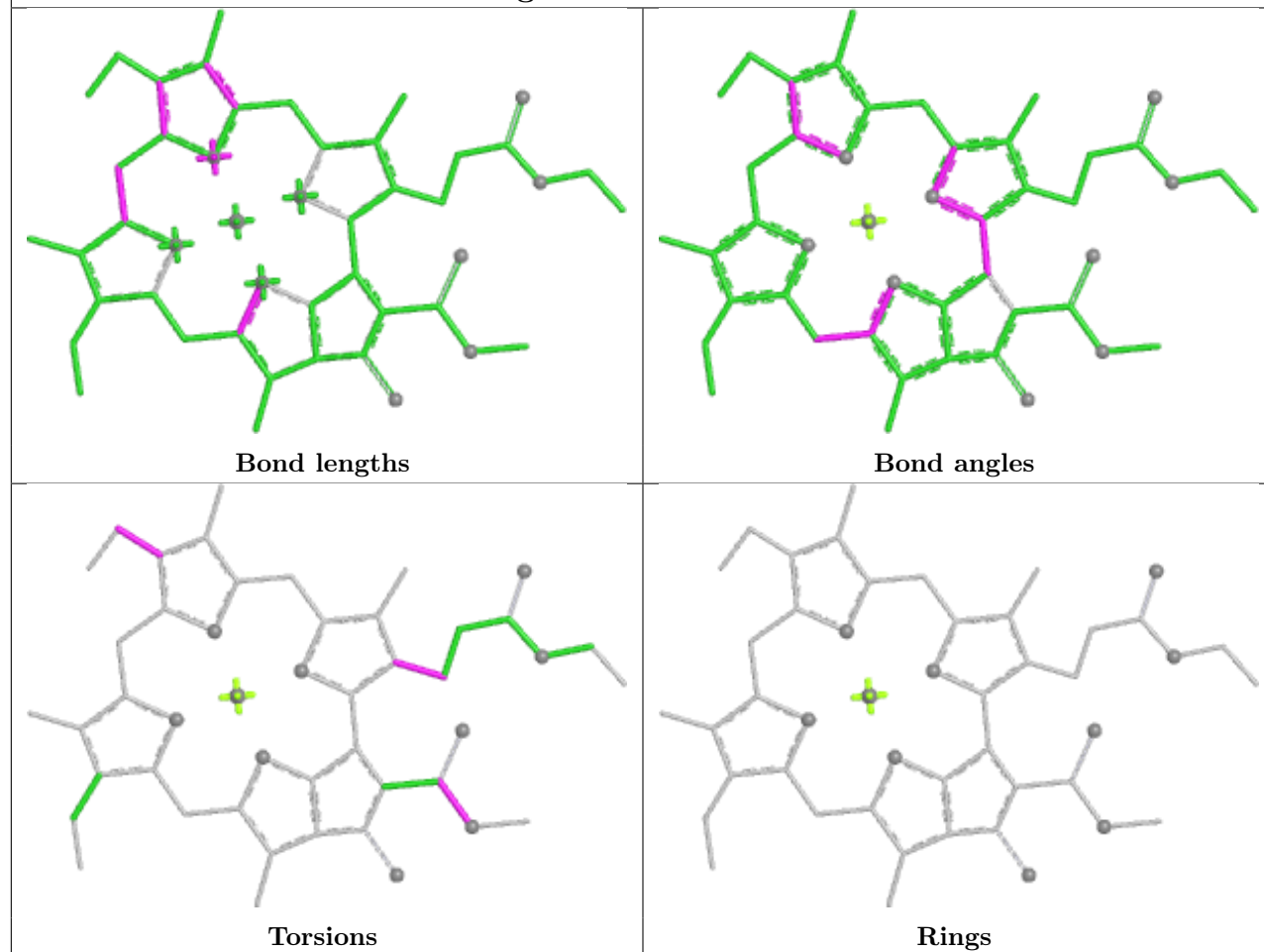




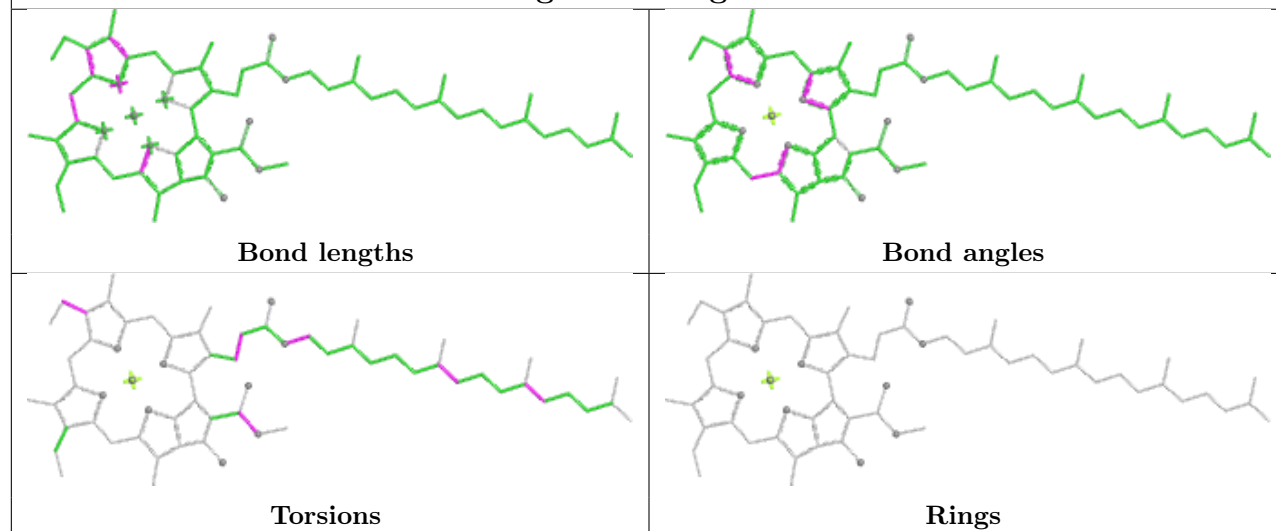
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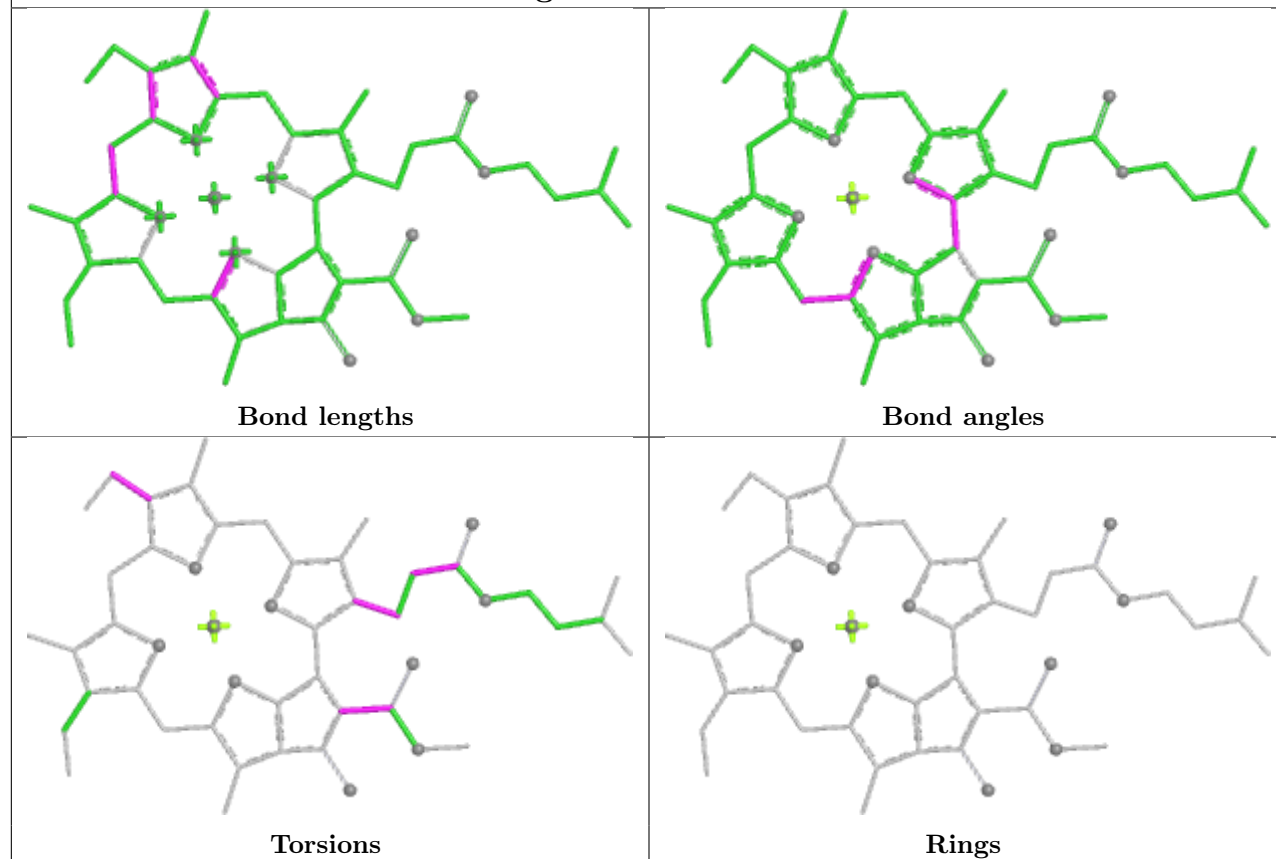
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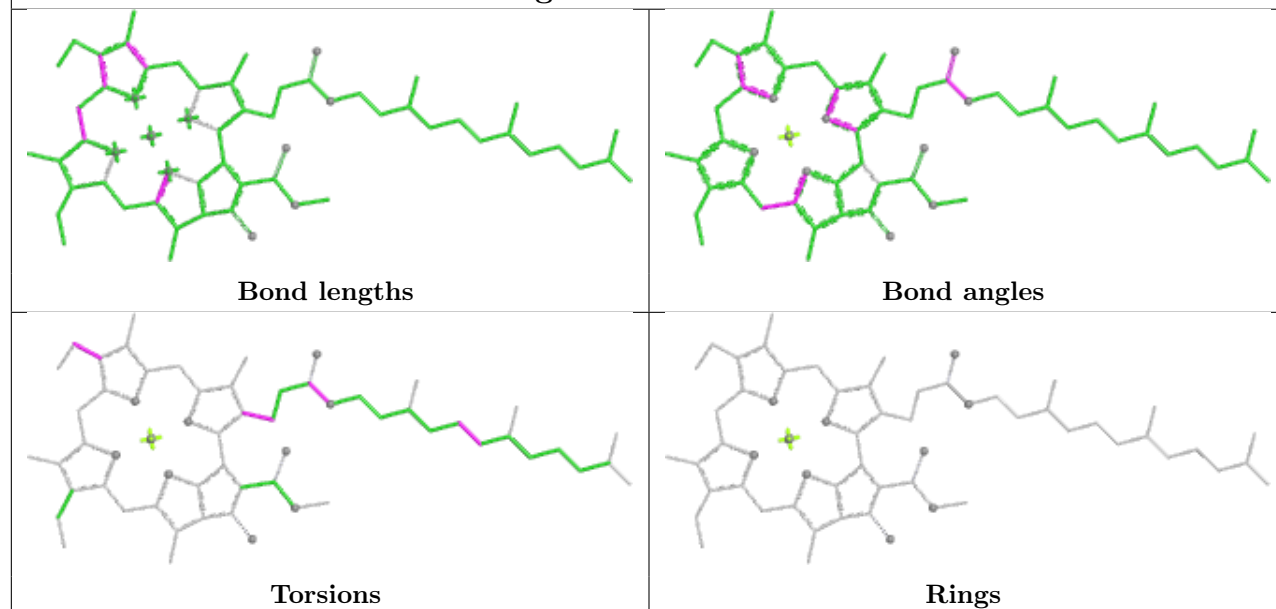
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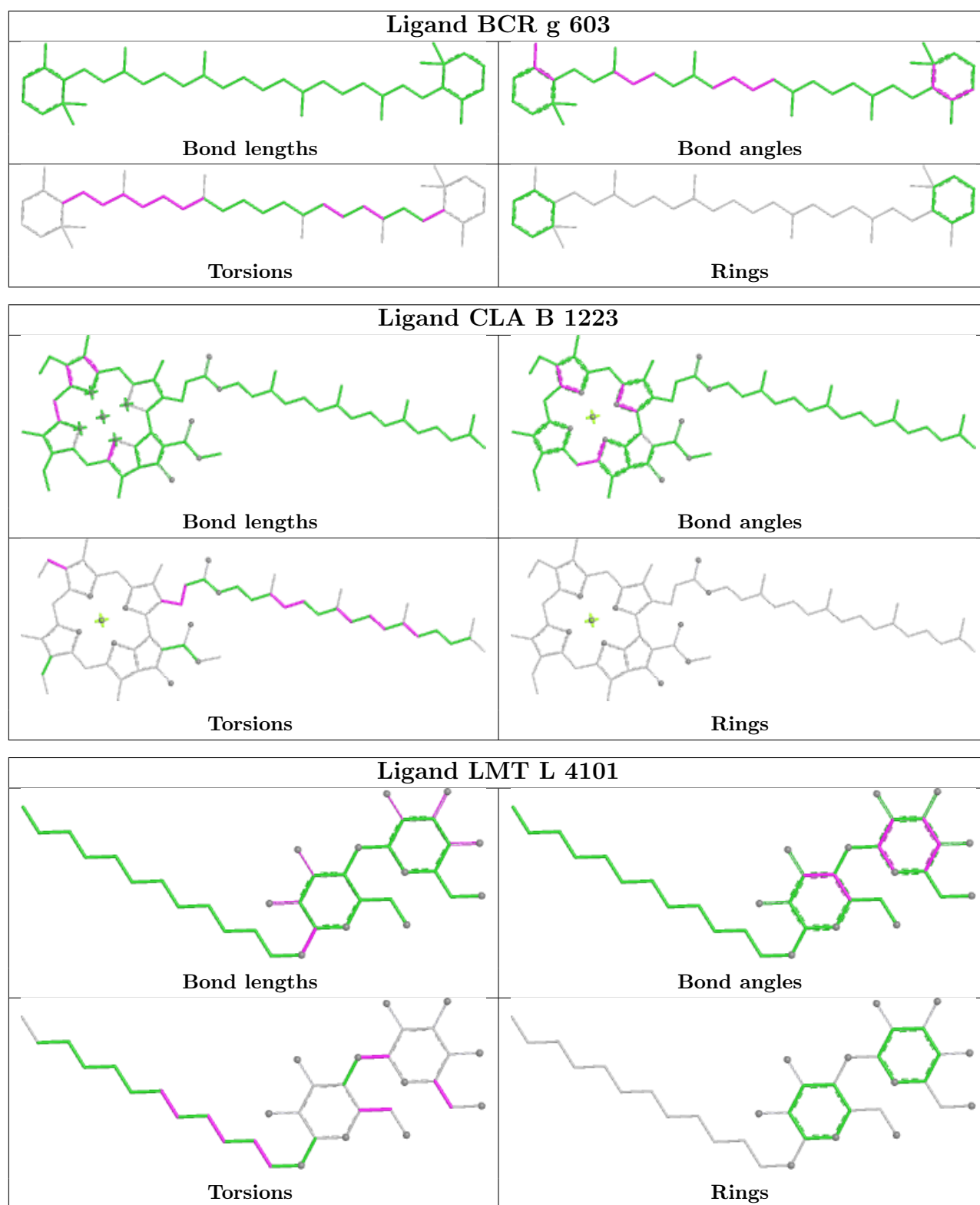


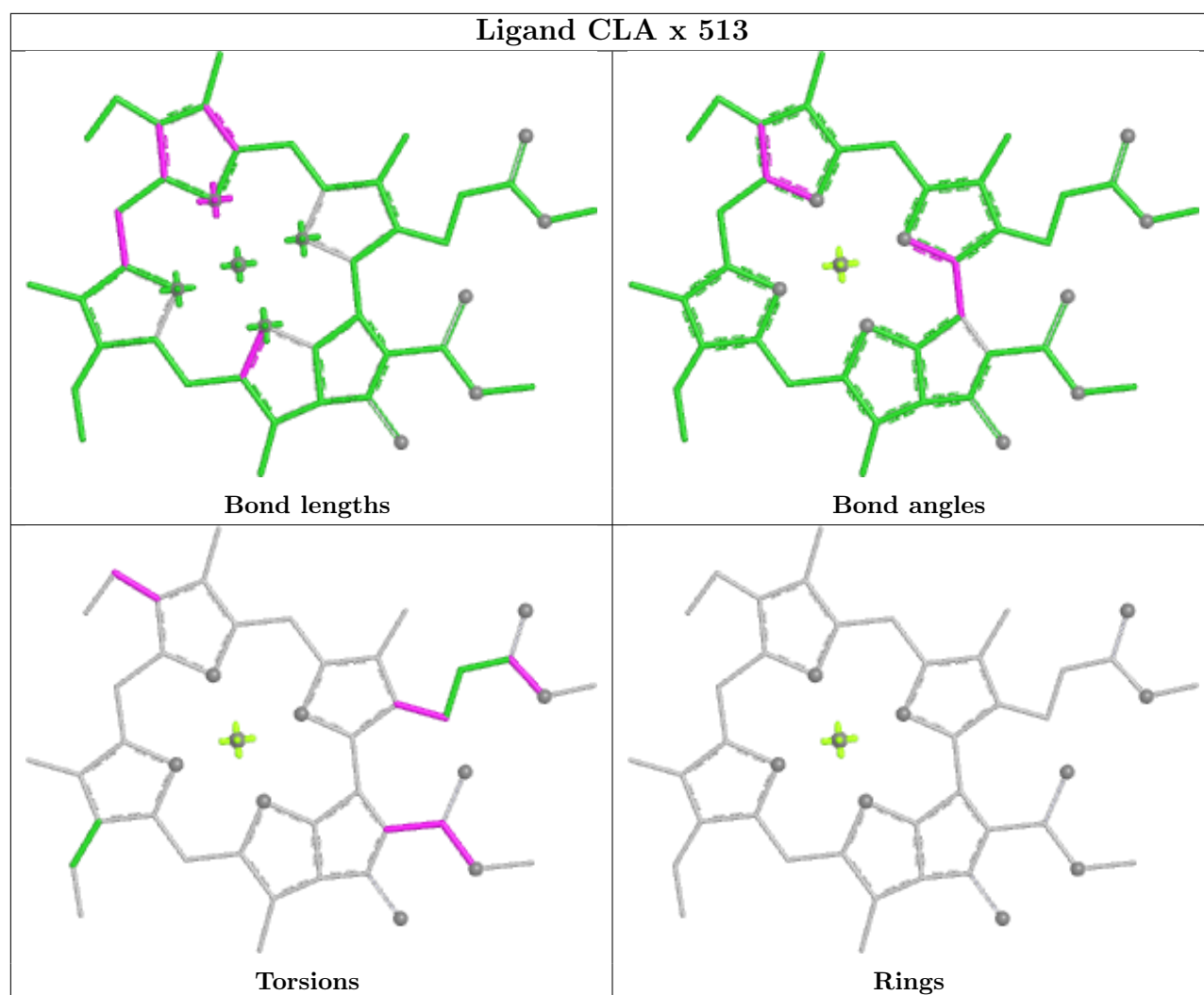
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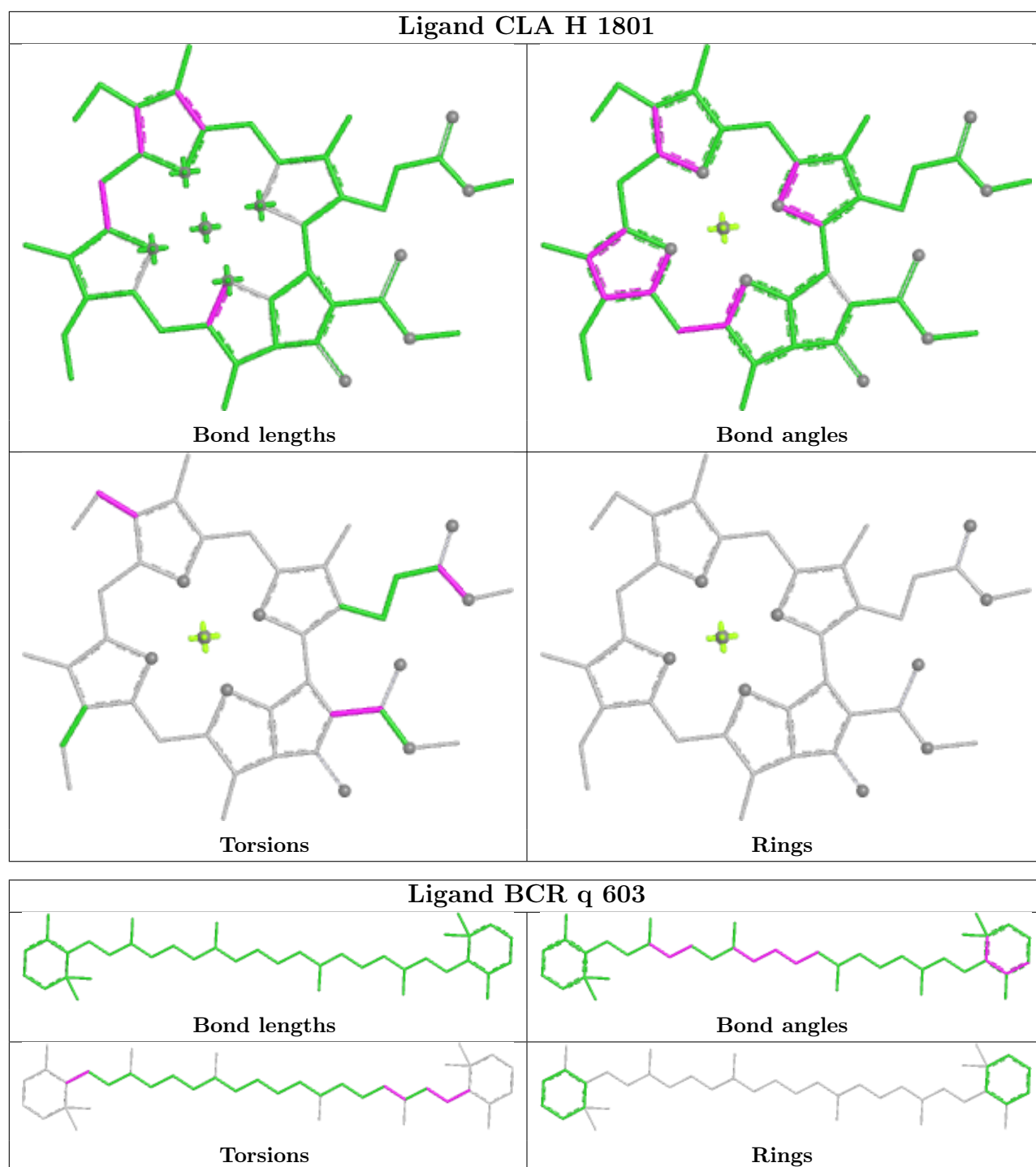


Ligand CLA n 504

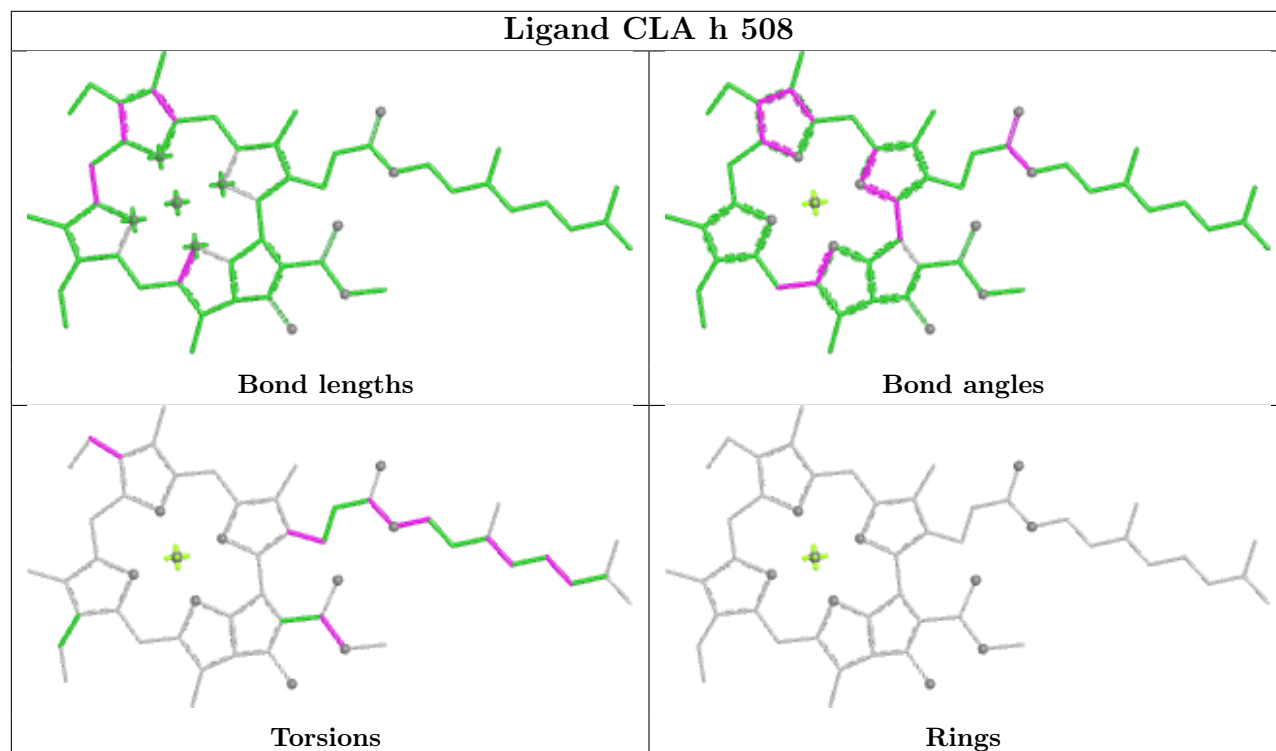




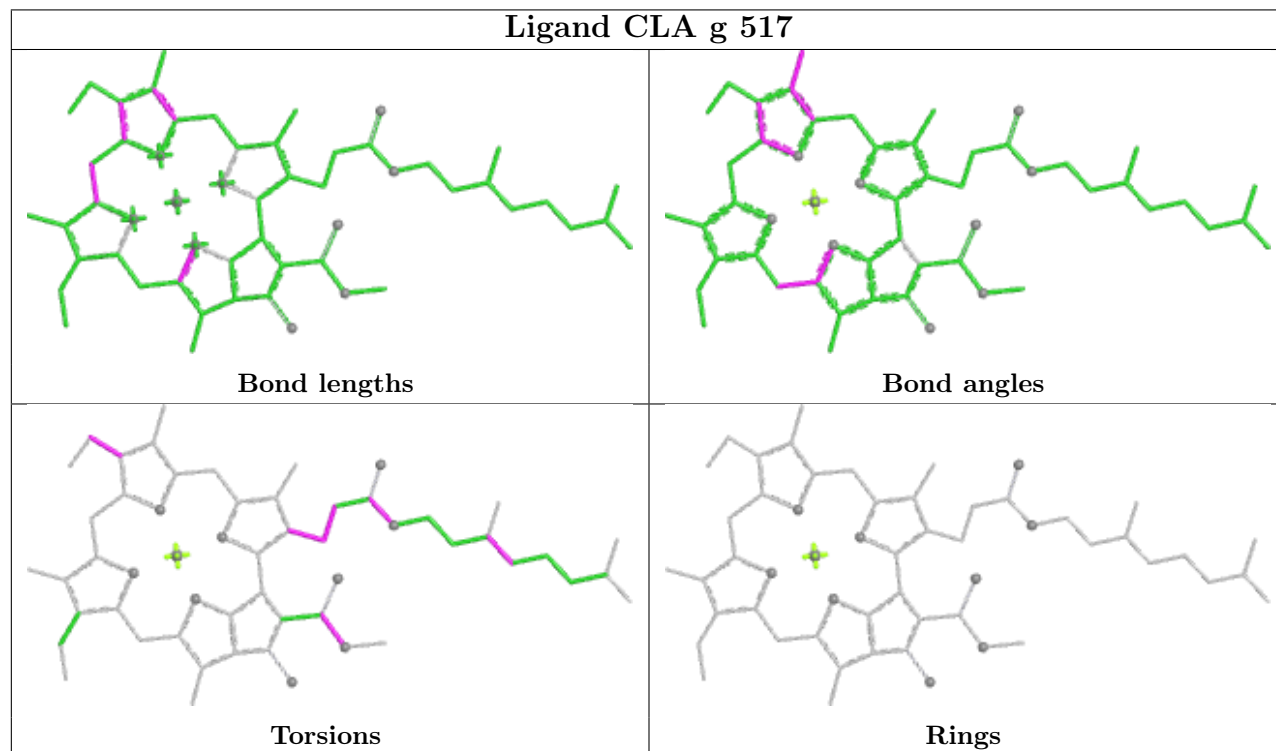


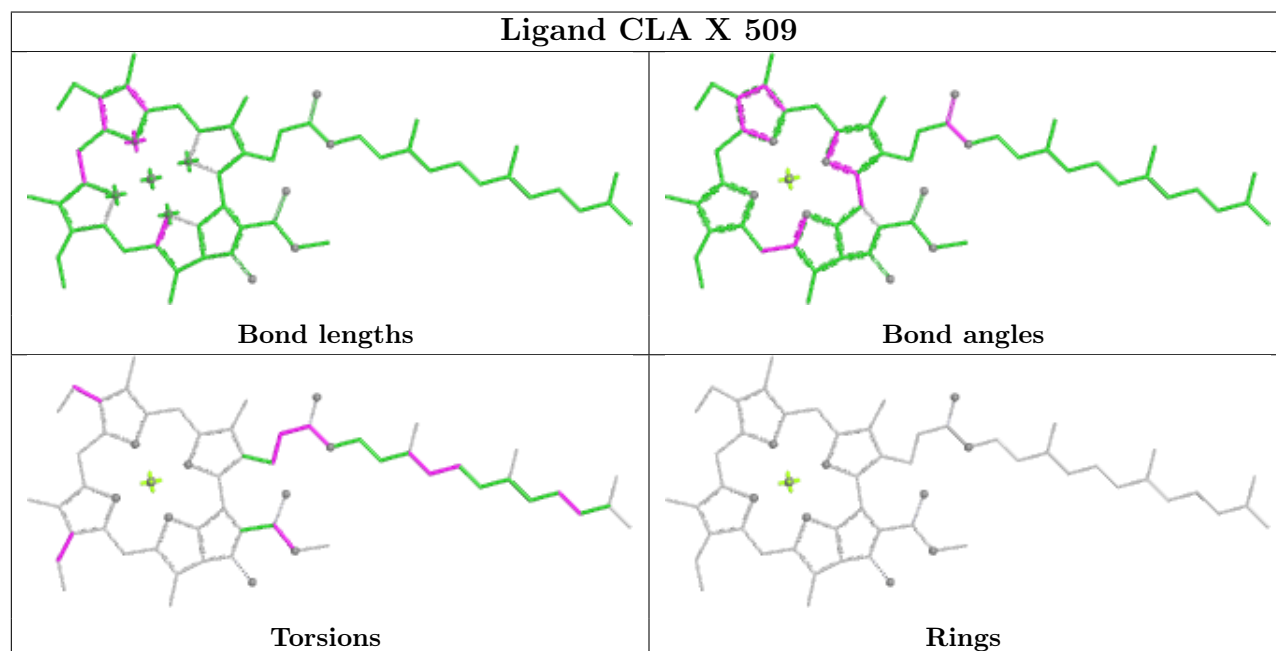
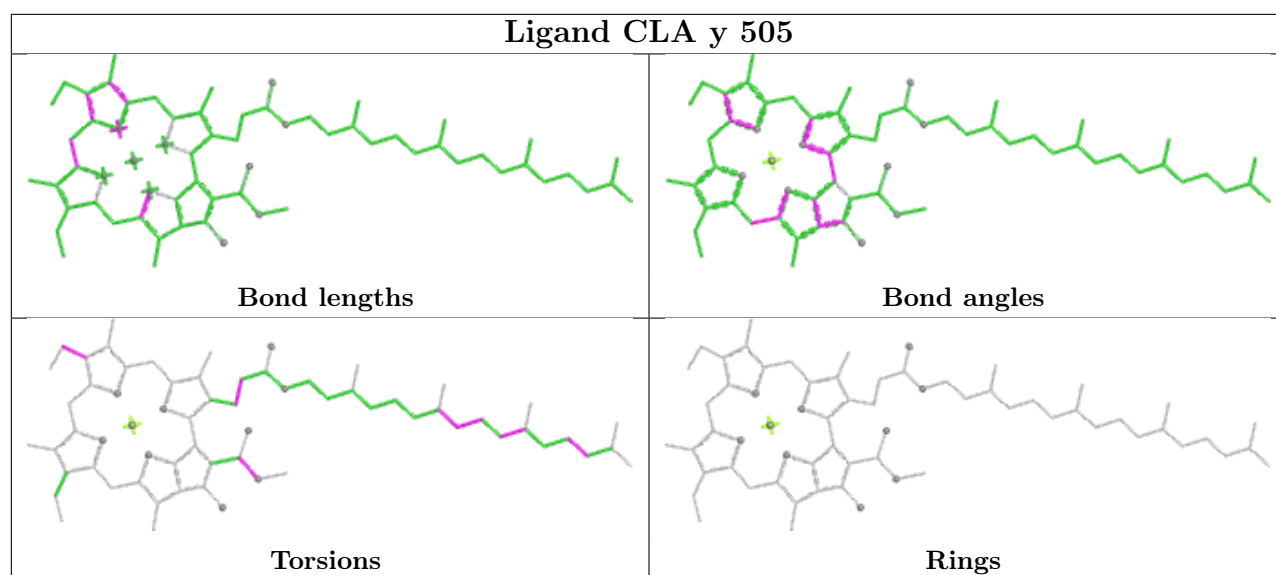


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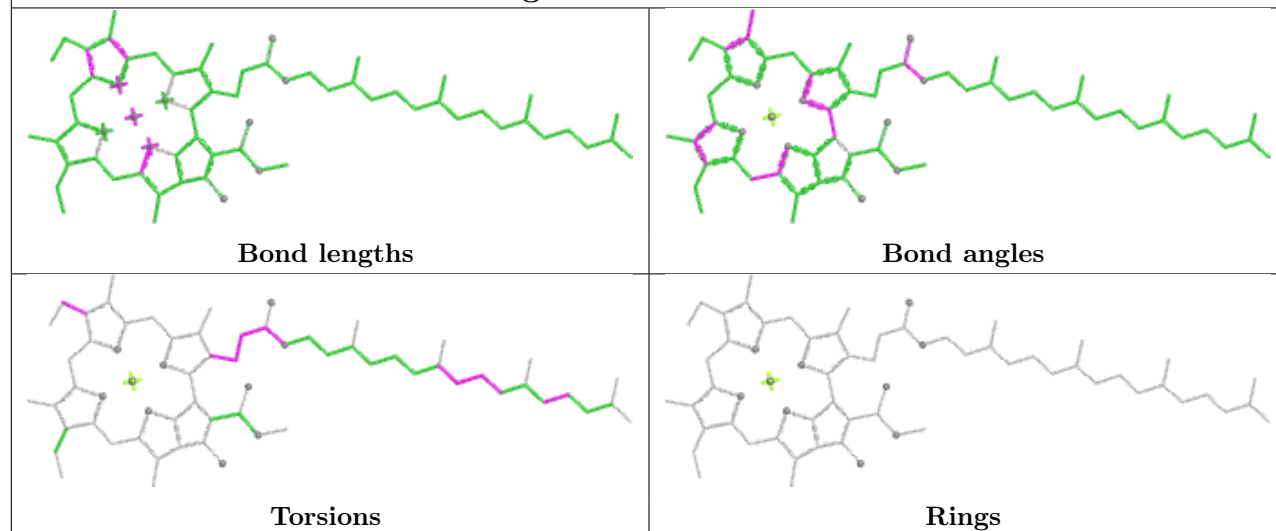


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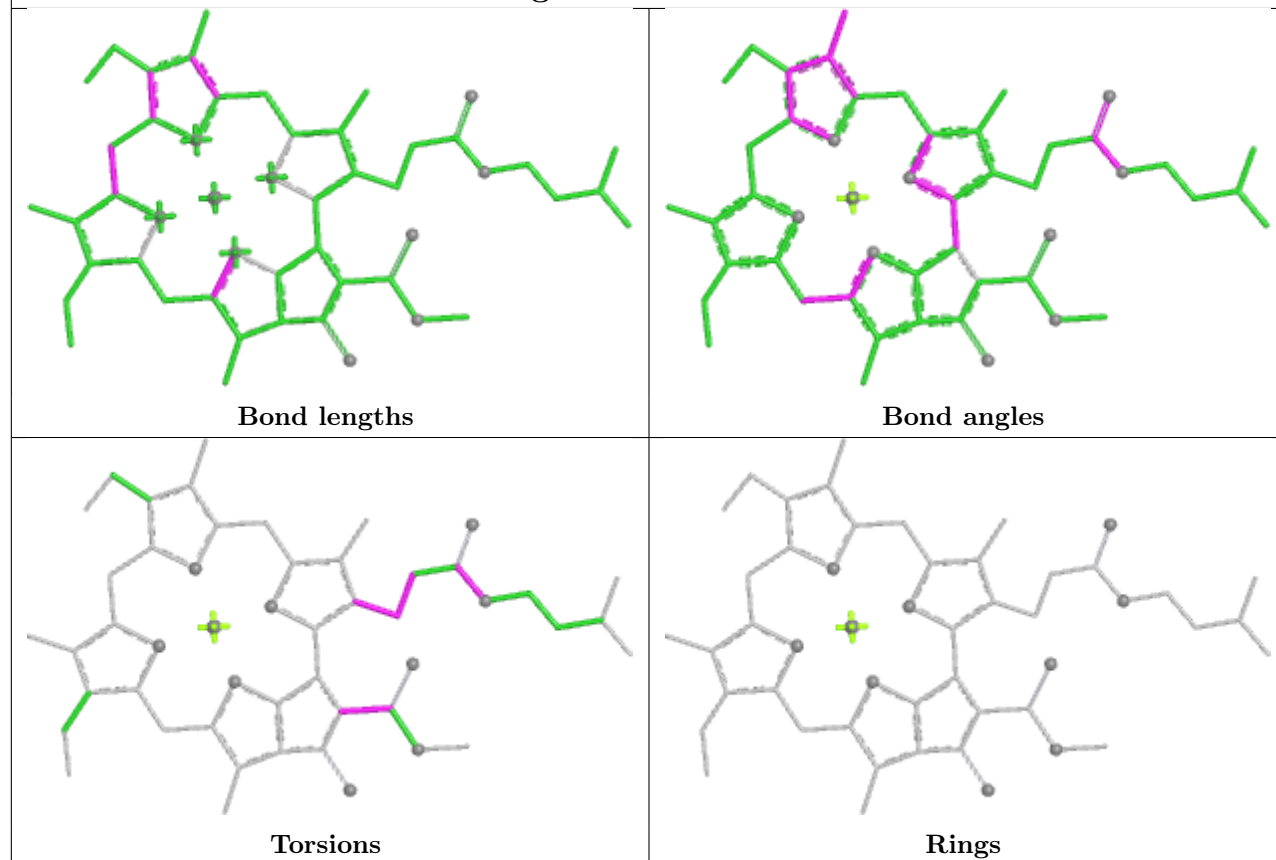


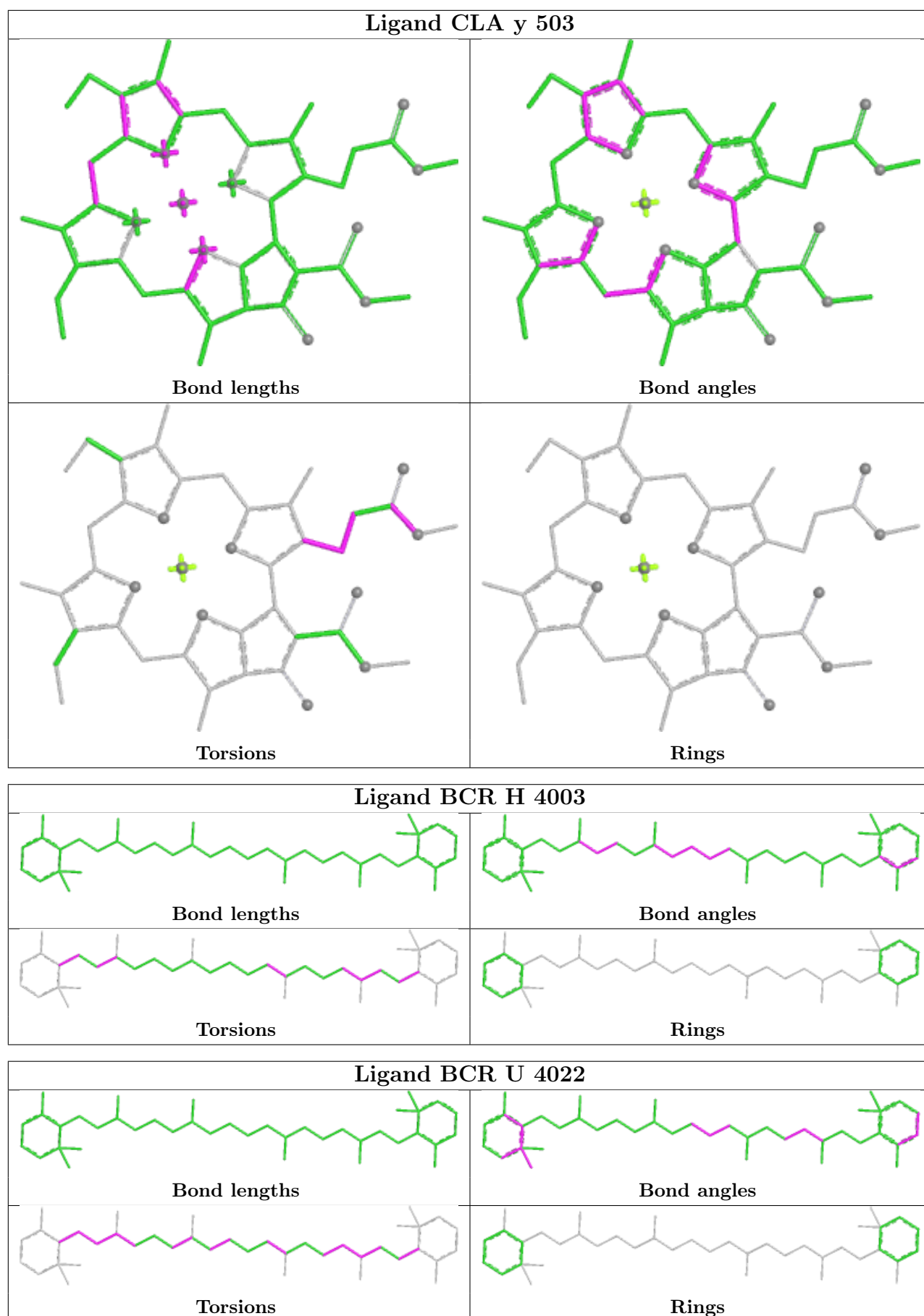


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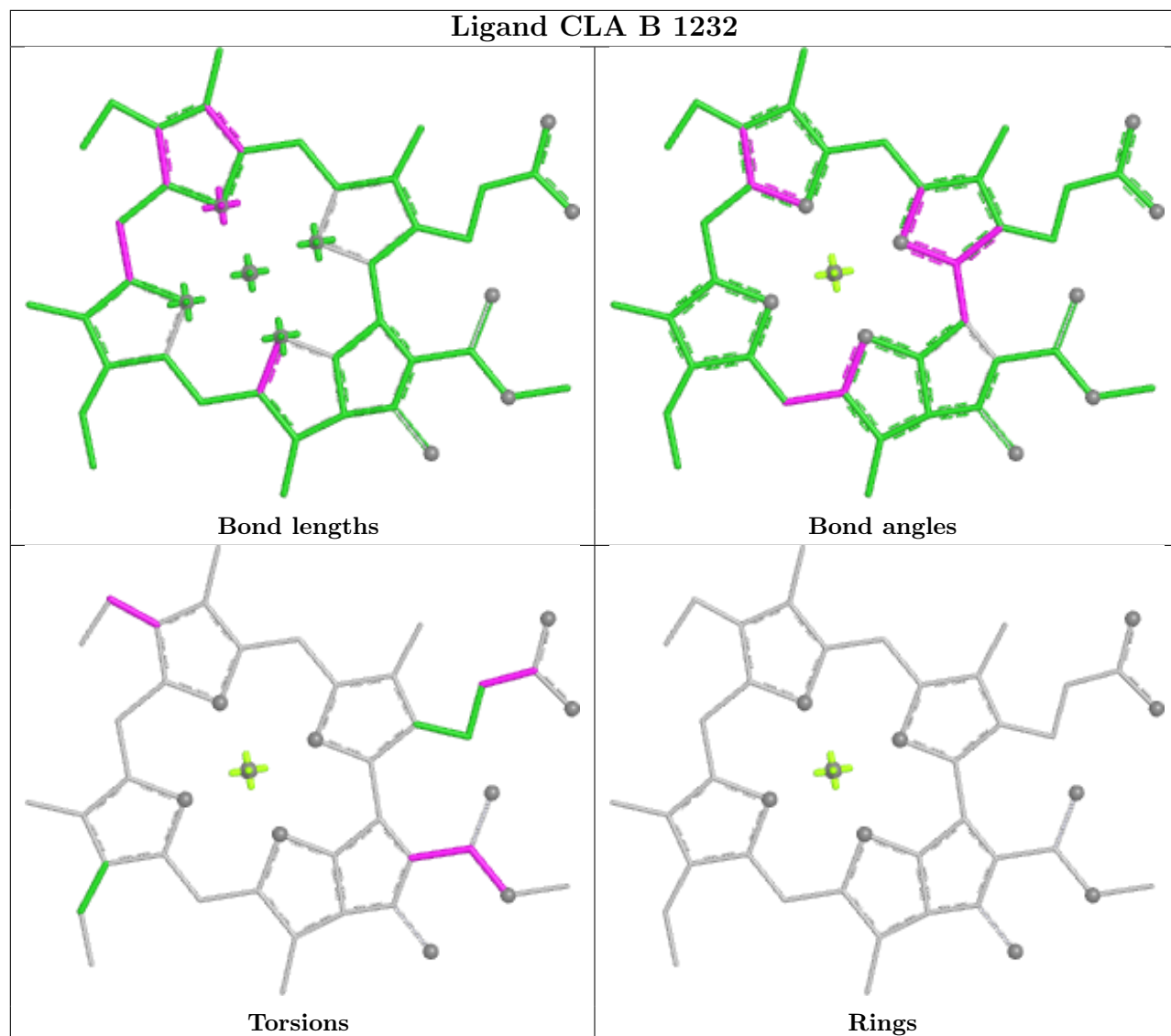


Ligand CLA Y 501

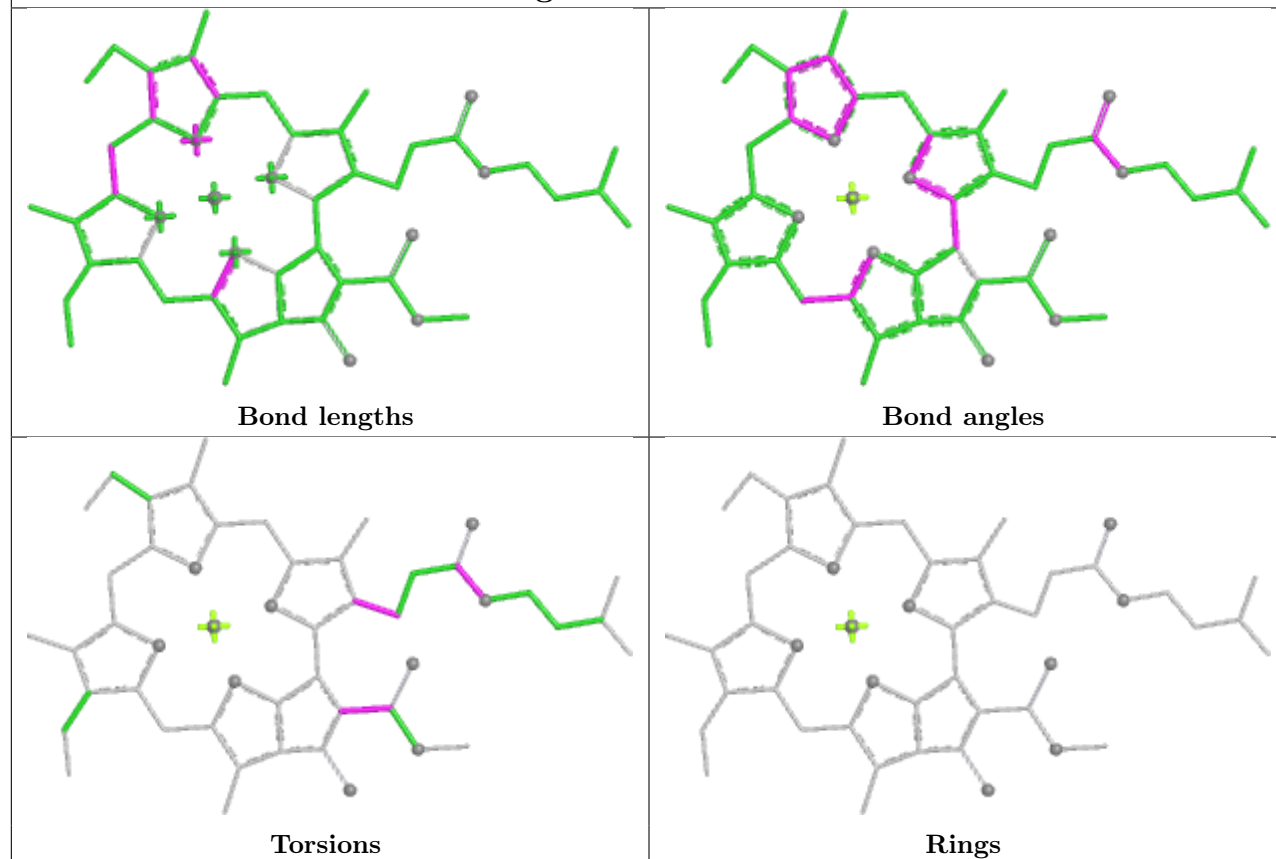




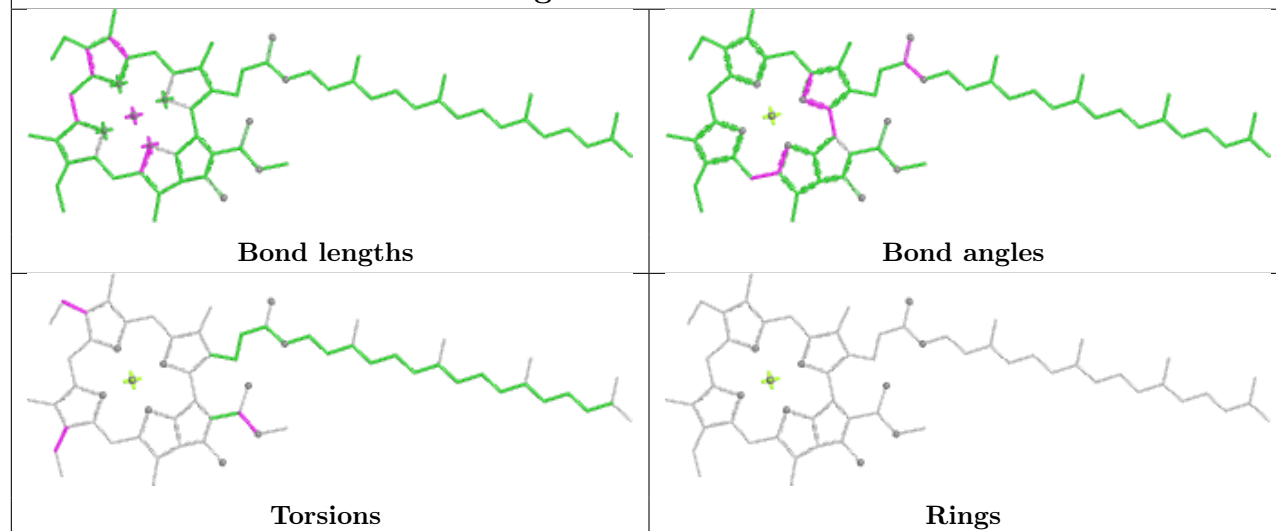
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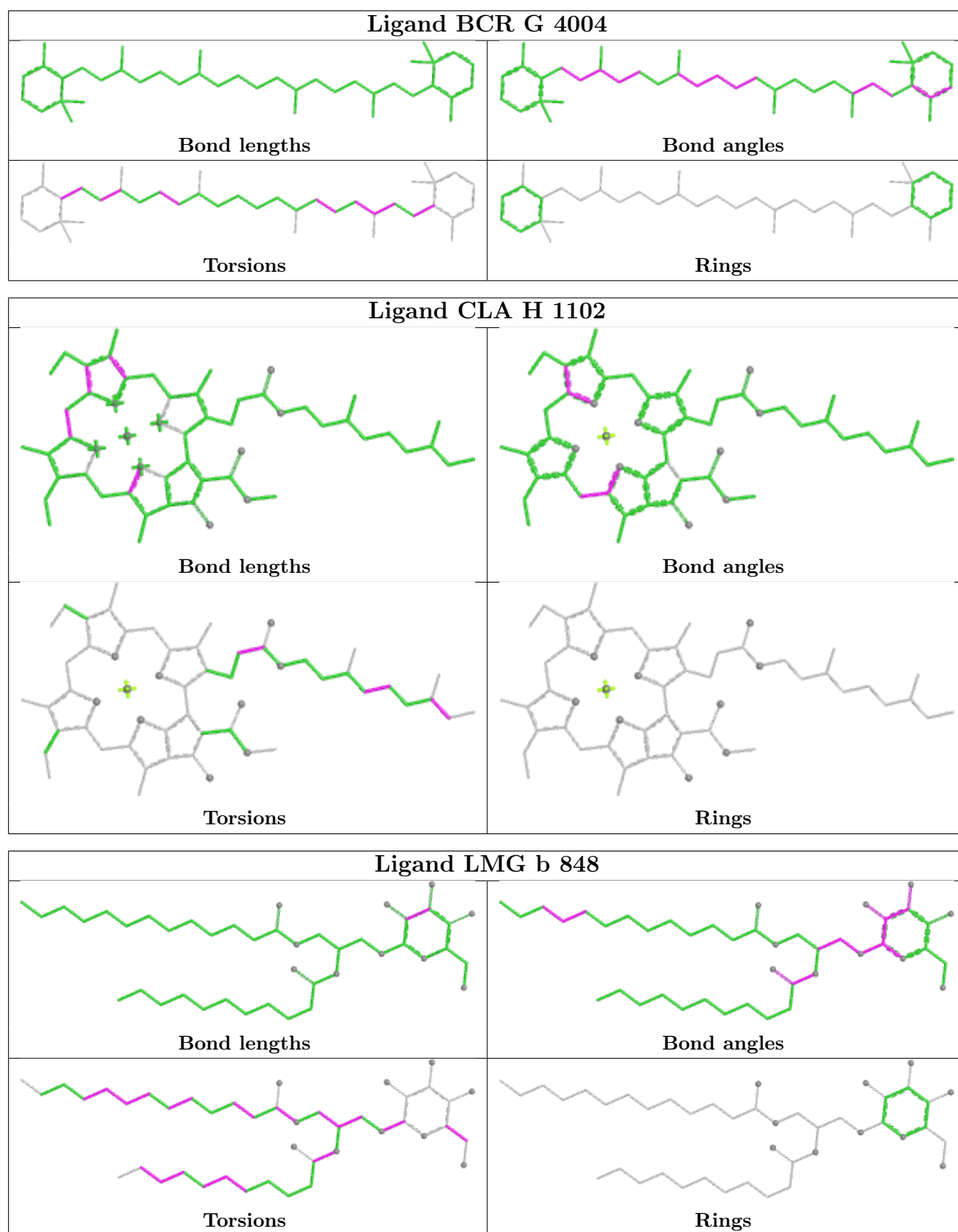


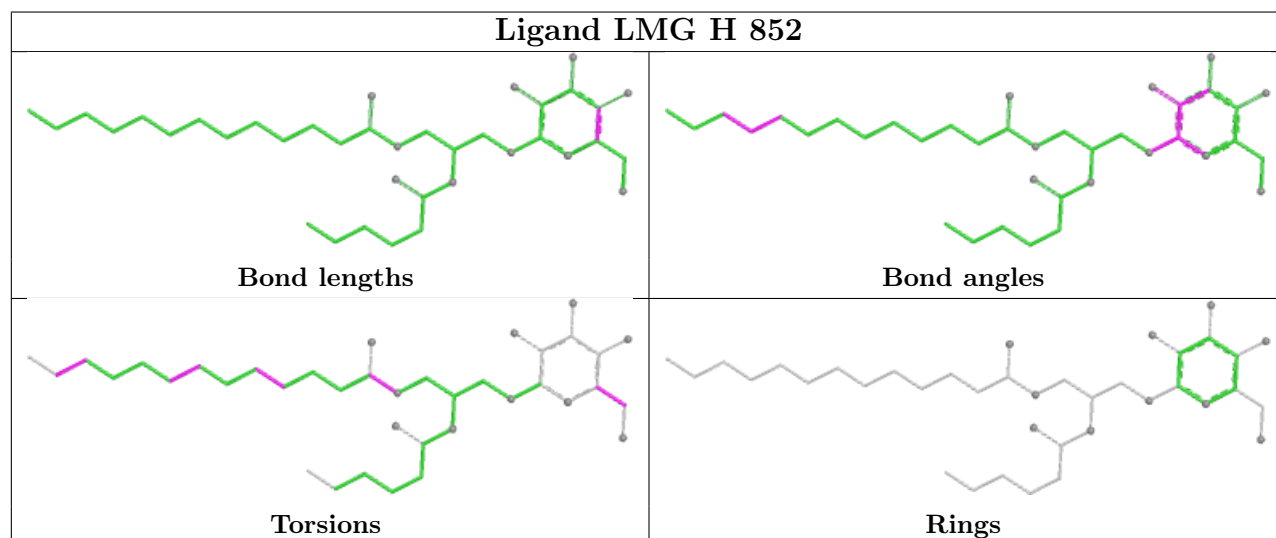
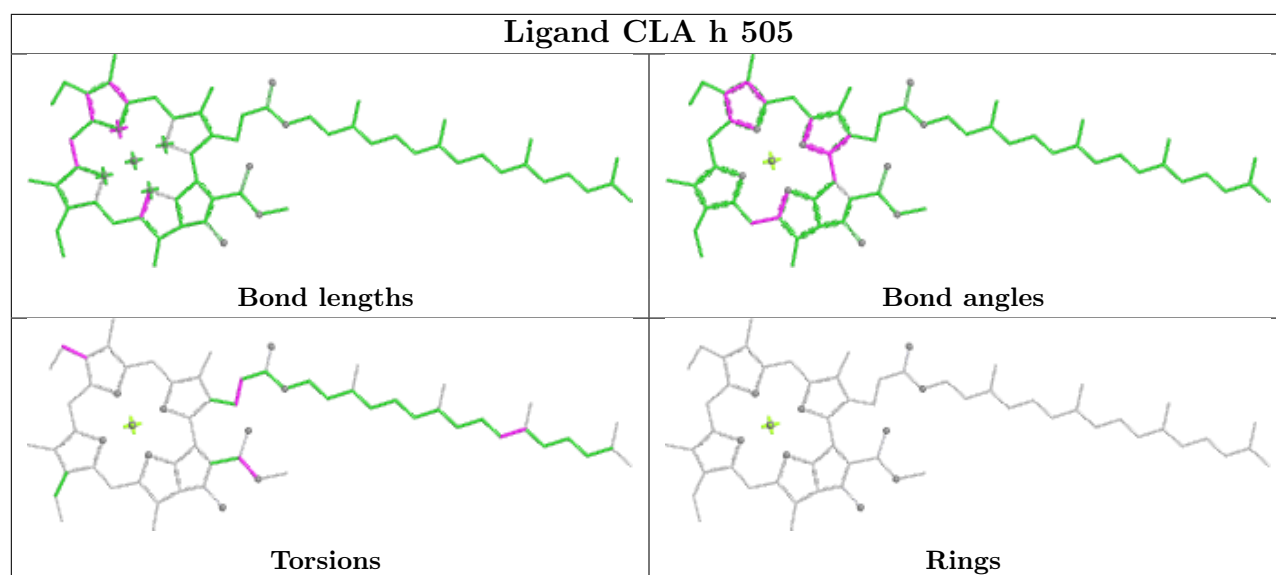
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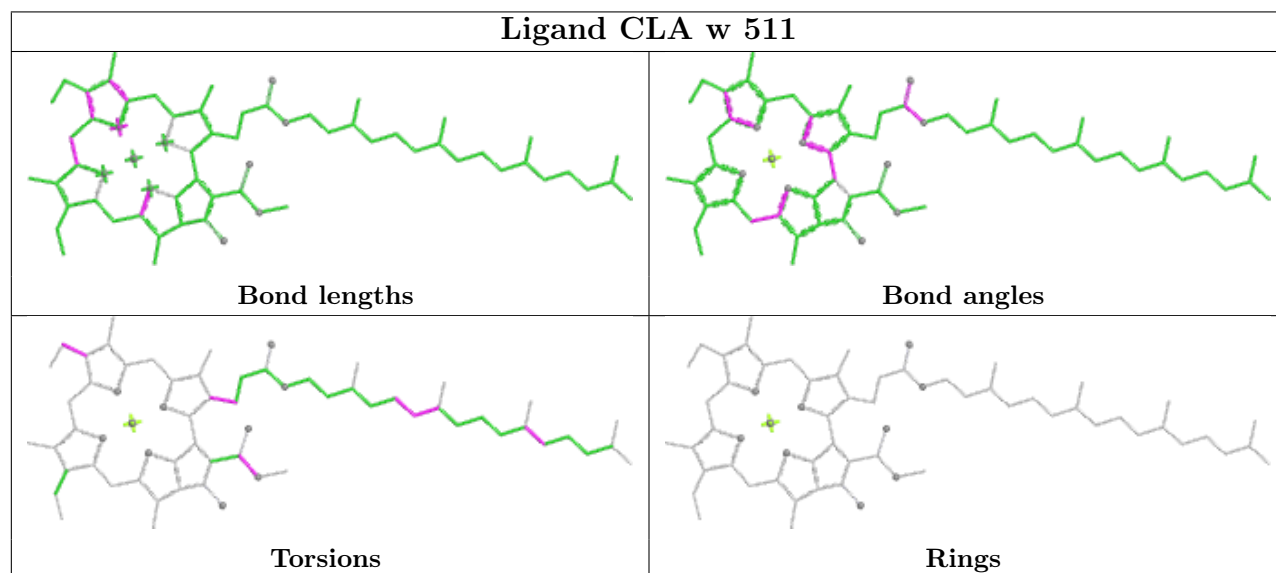
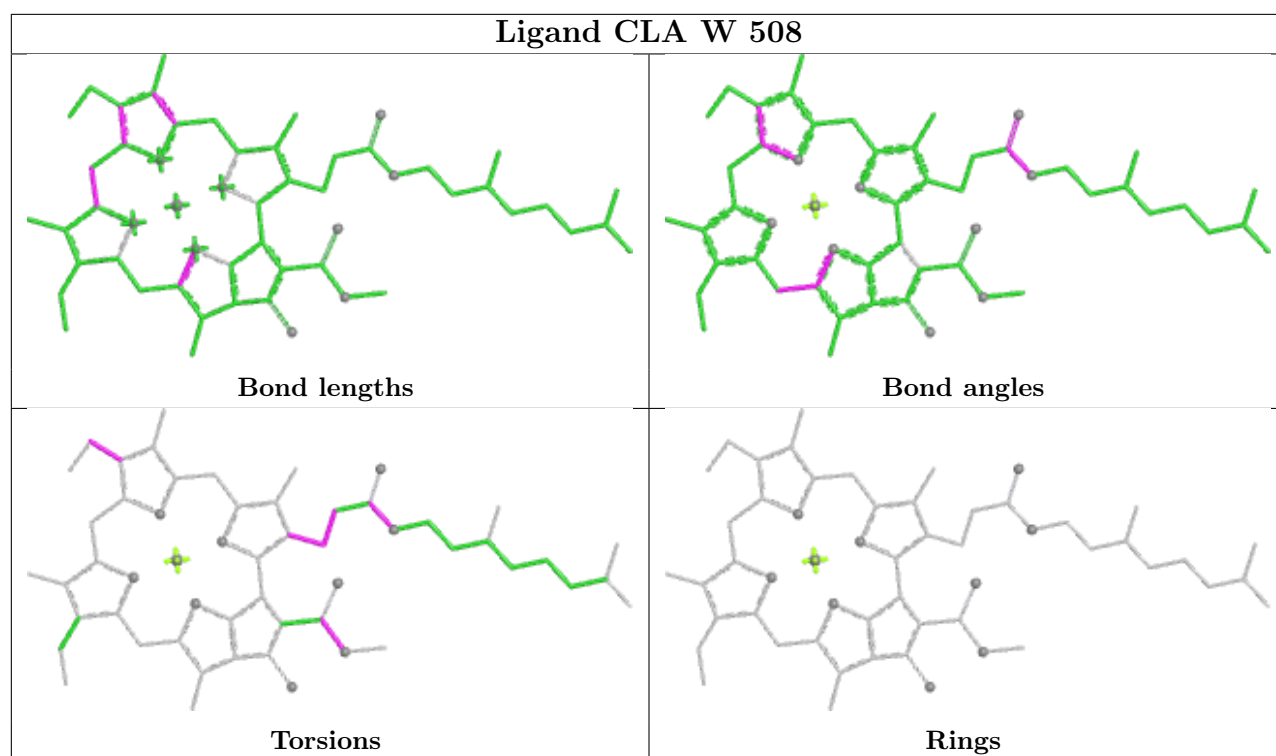


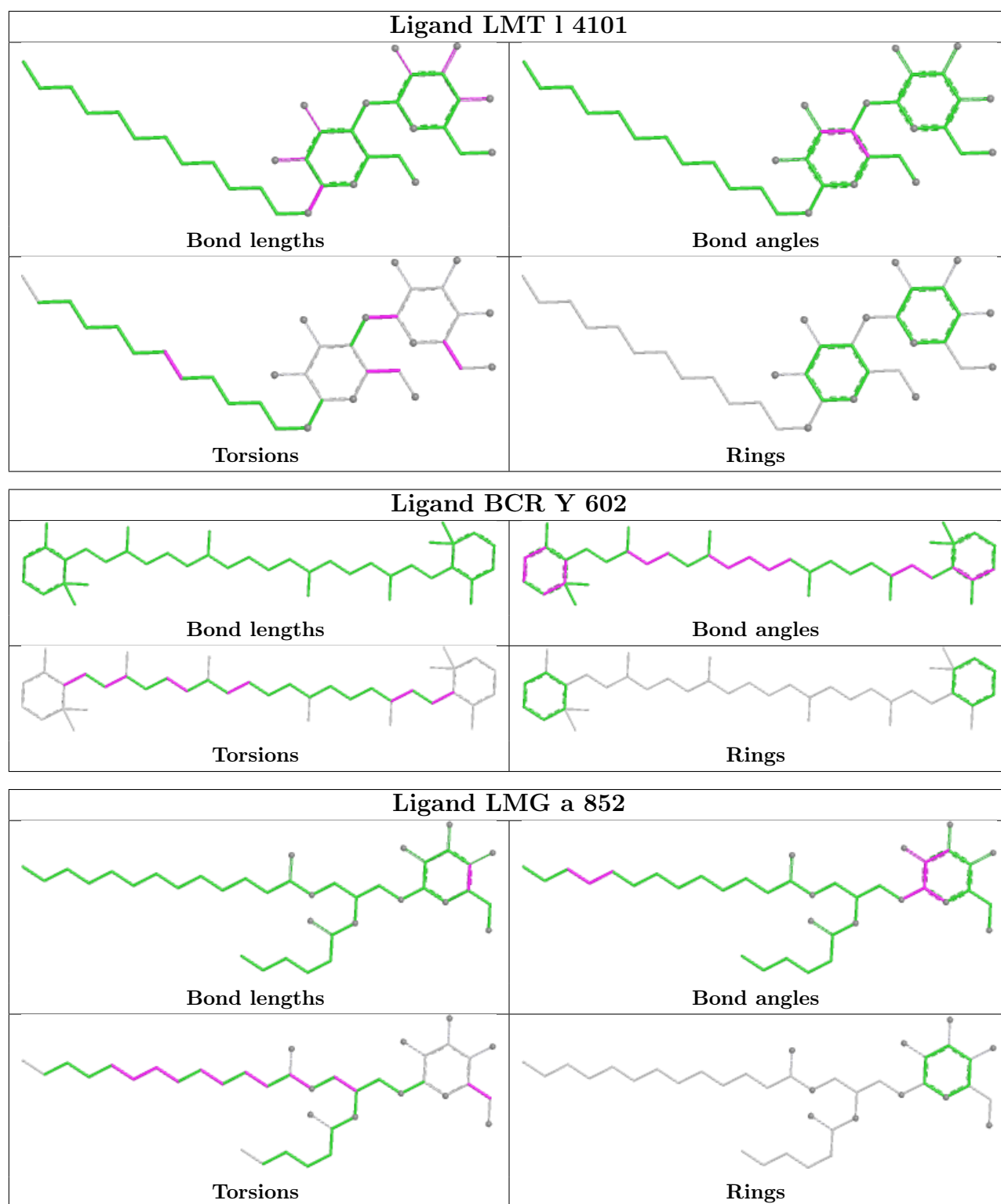
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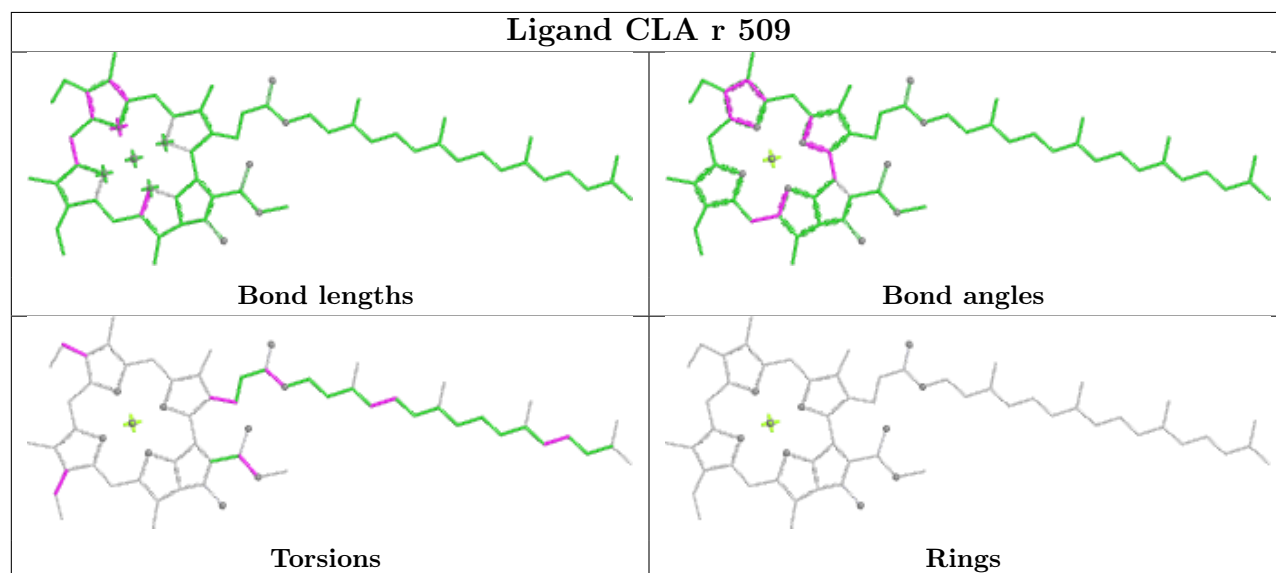
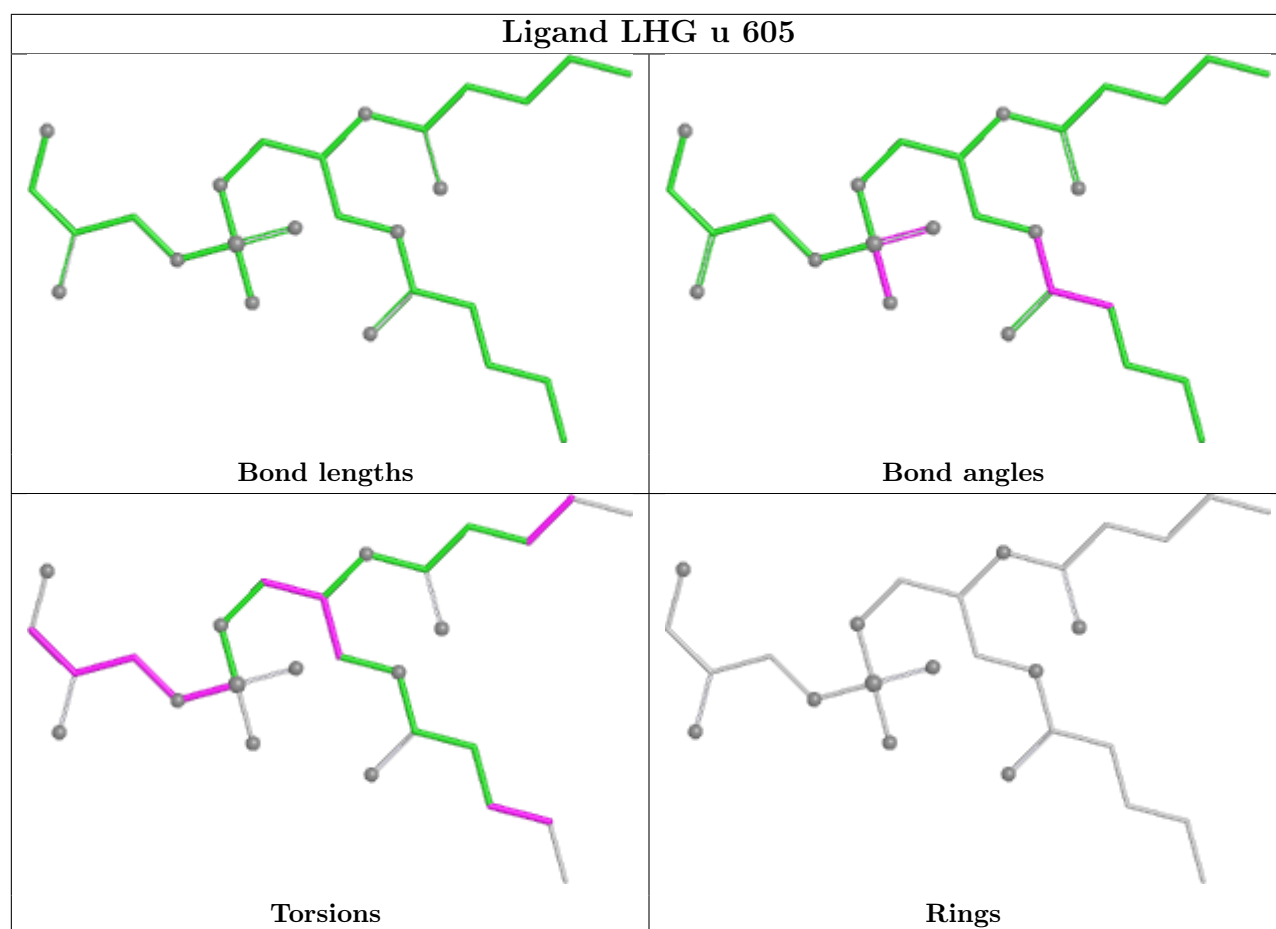


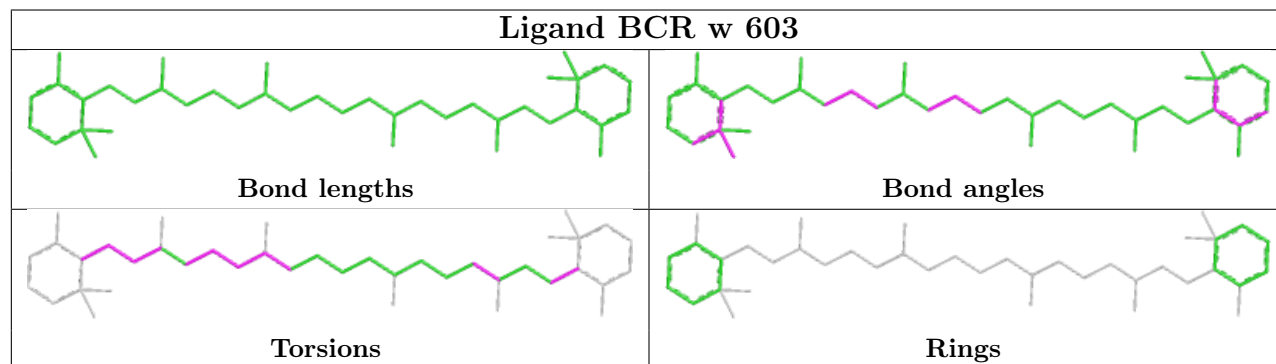
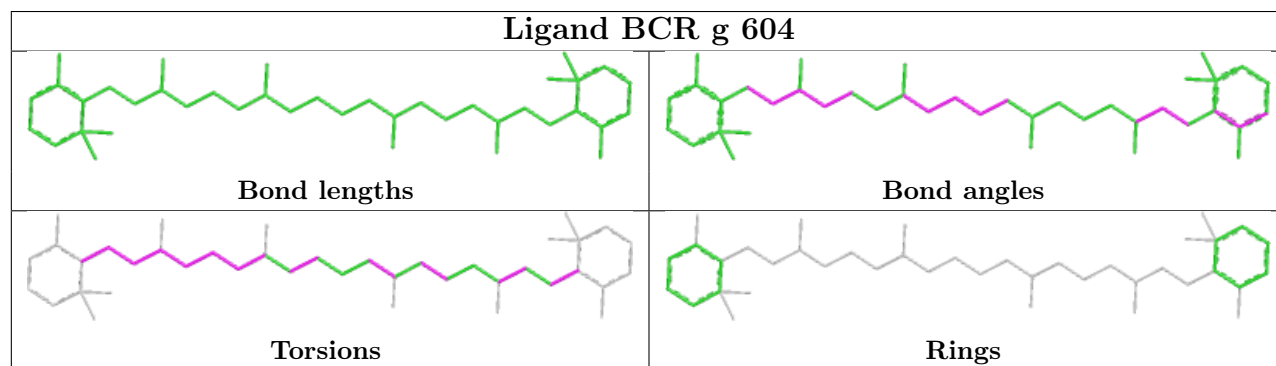
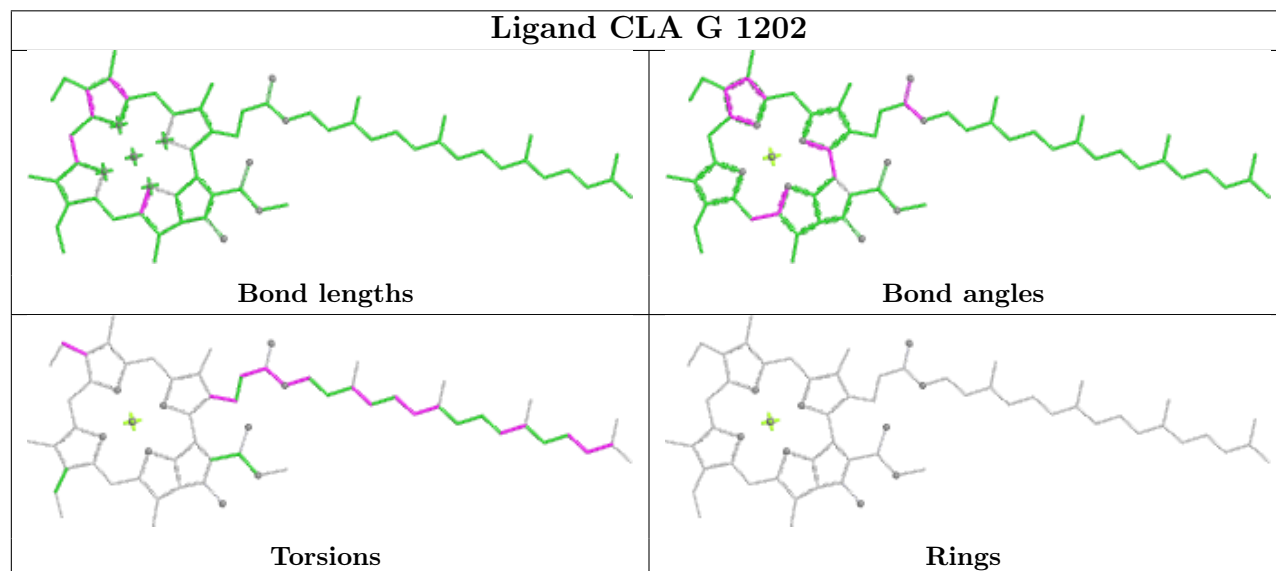
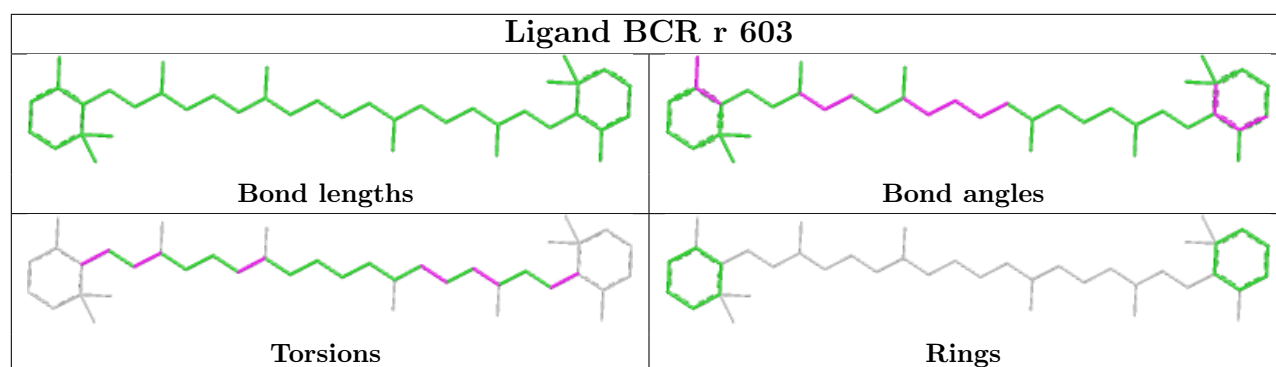




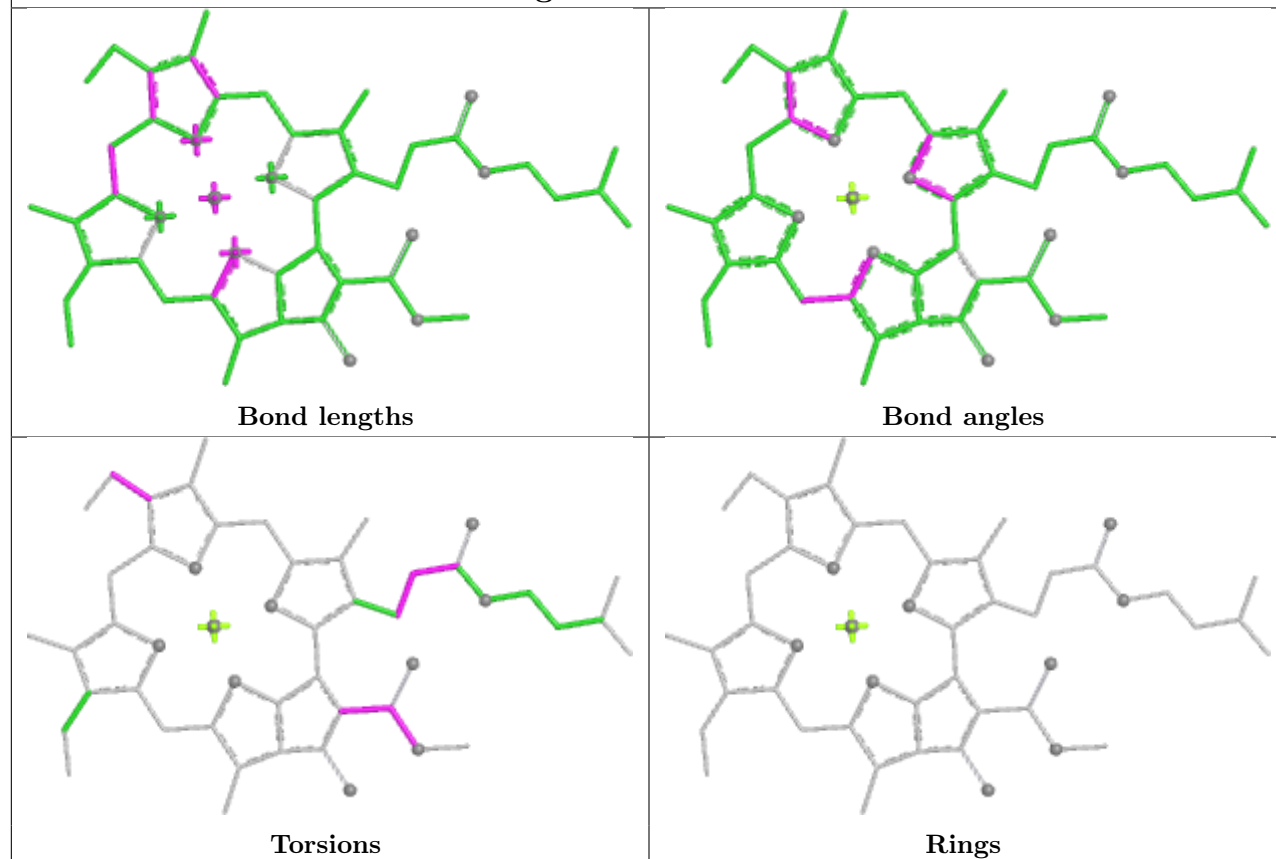




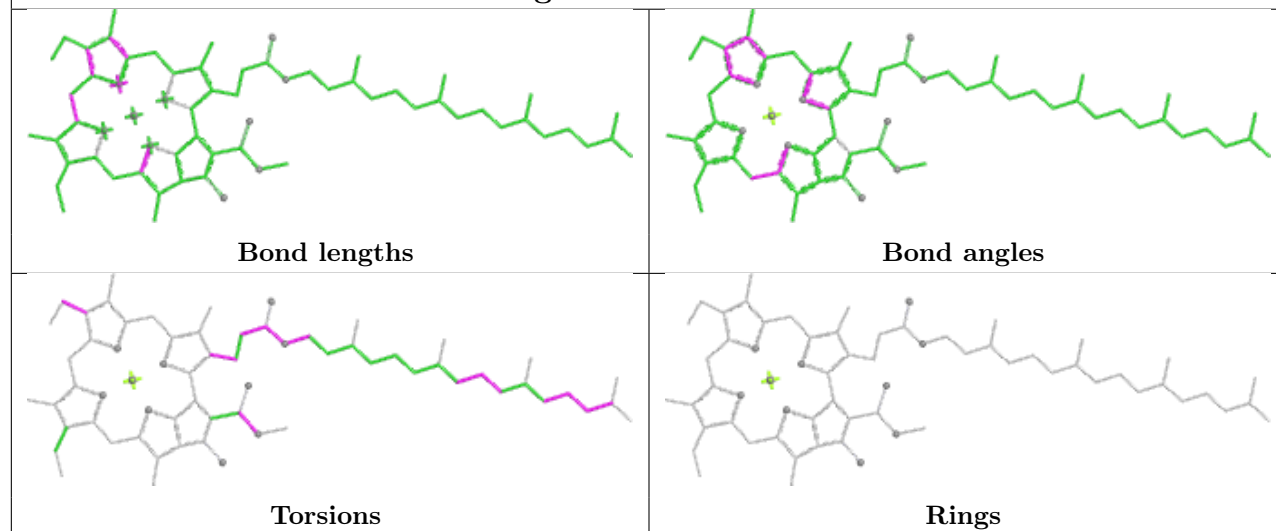


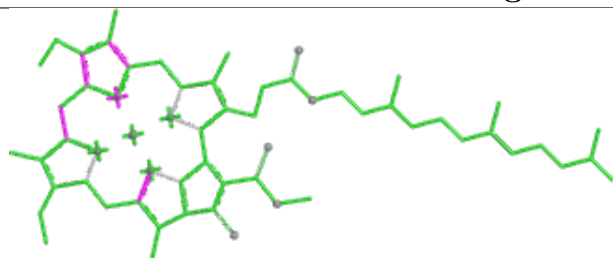
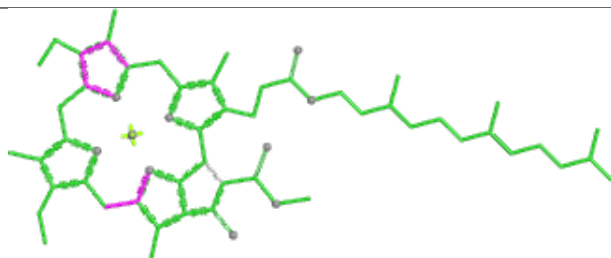
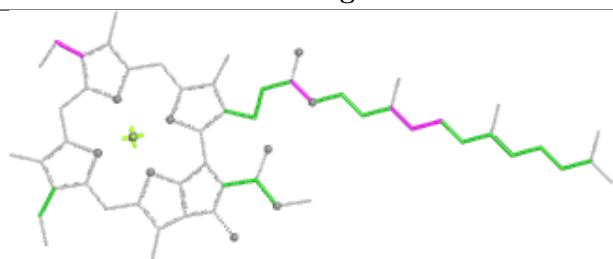
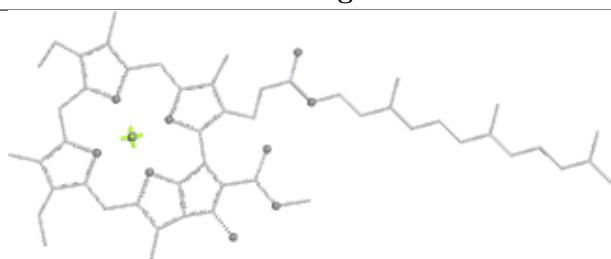
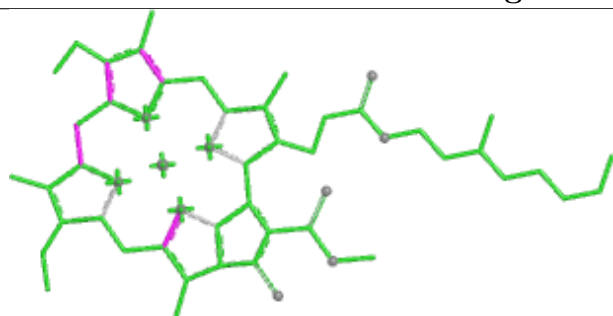
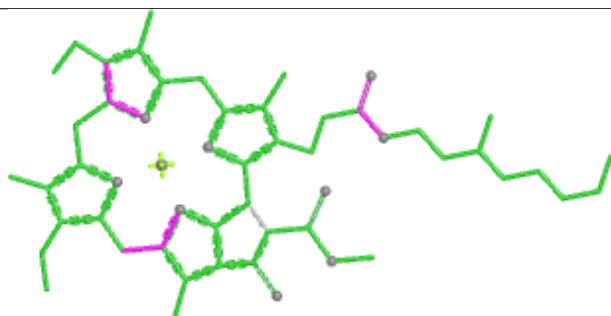
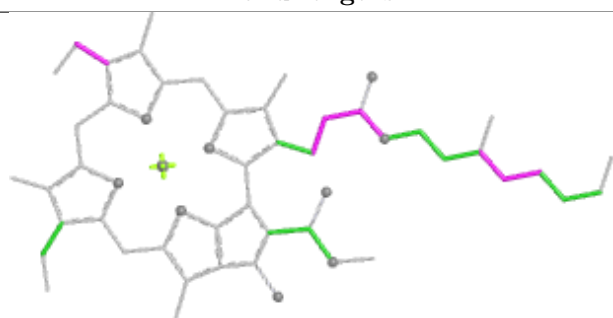
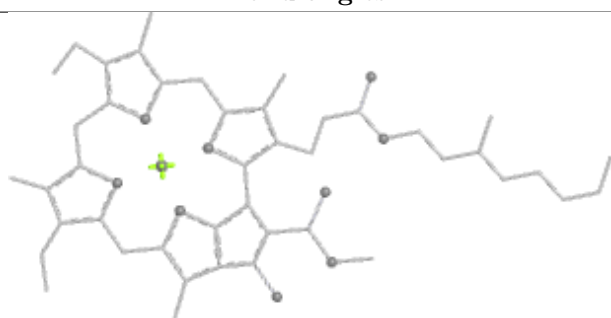


Ligand CLA u 502

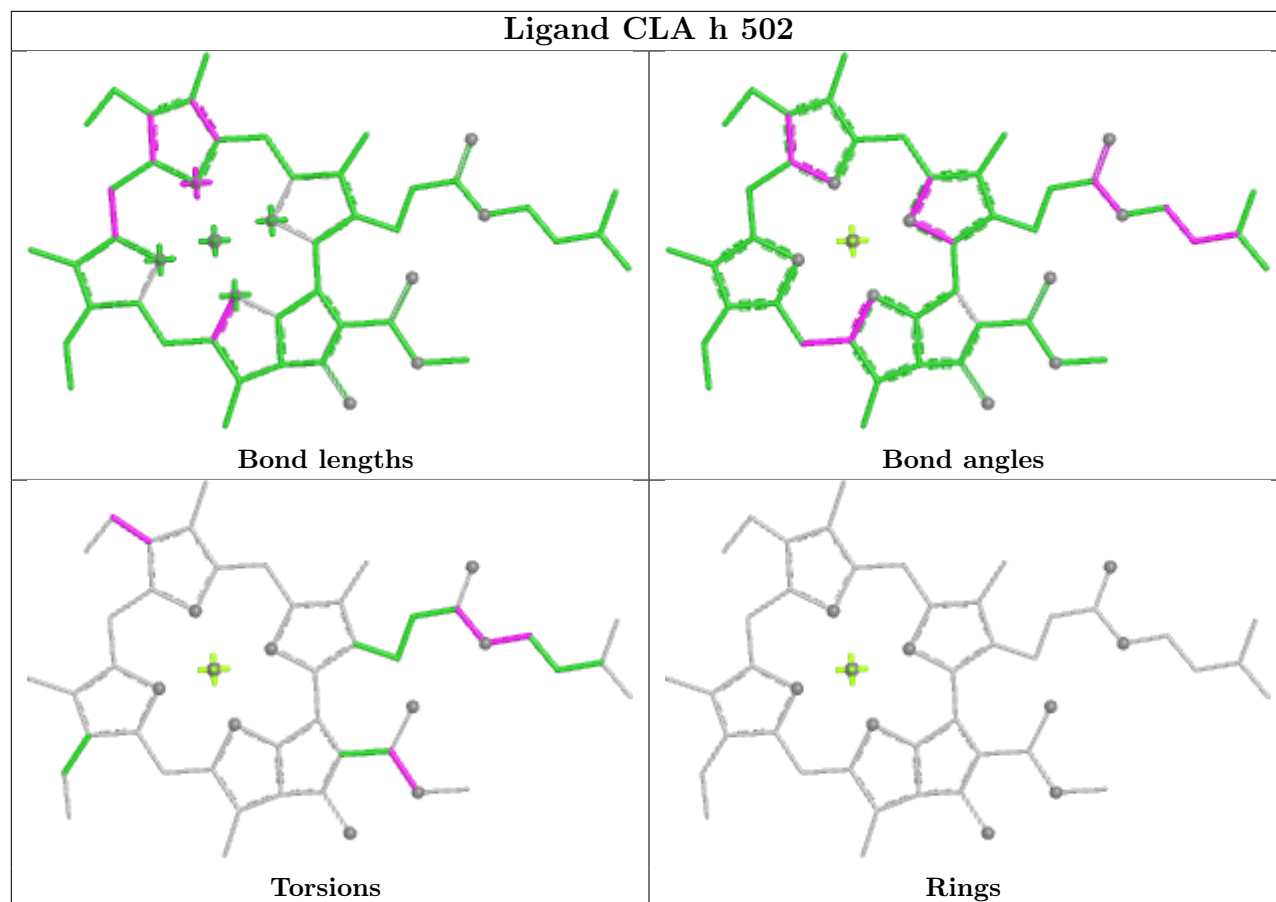


Ligand CLA Z 509

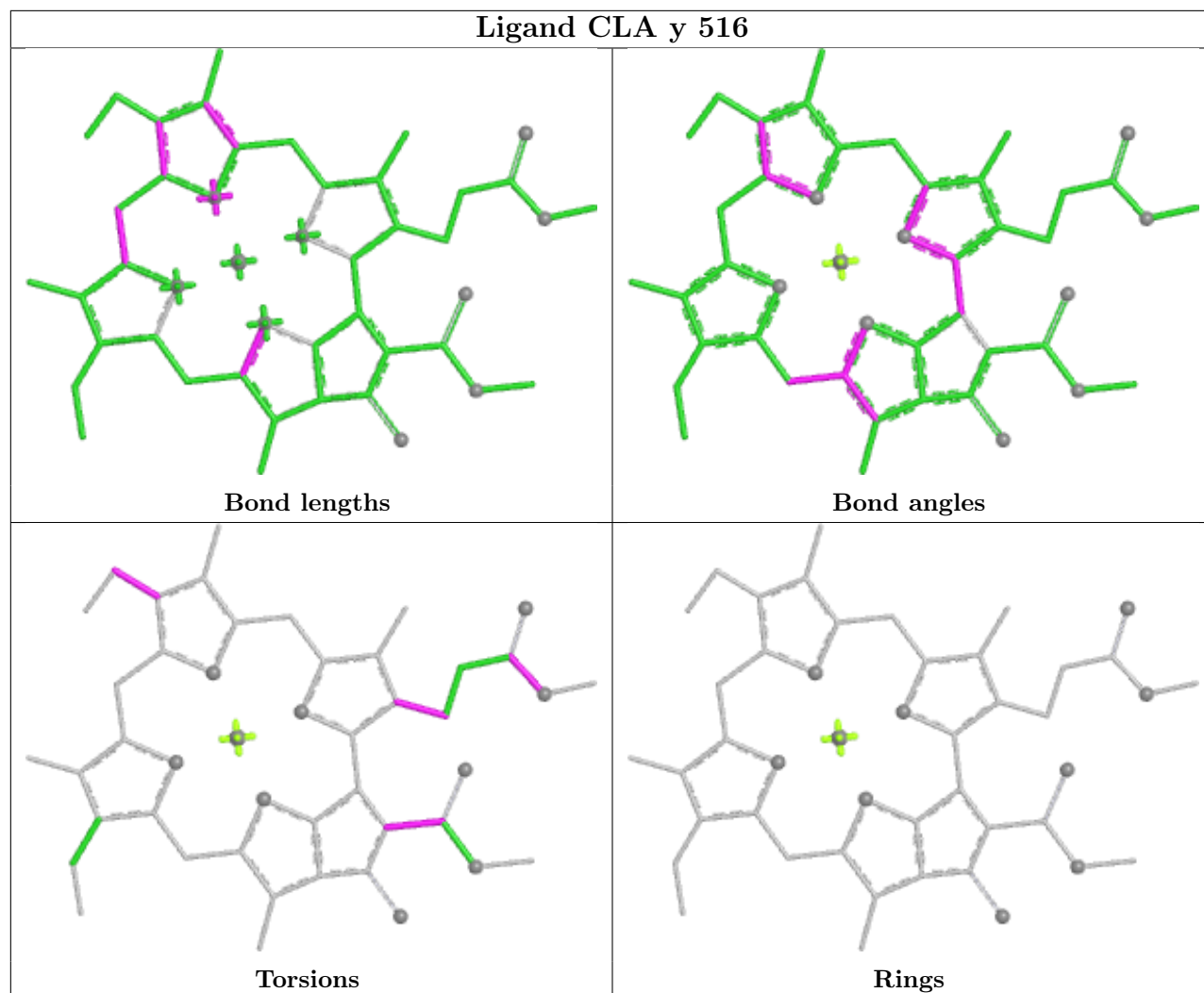


Ligand CLA H 1124**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 1110****Bond lengths****Bond angles****Torsions****Rings**

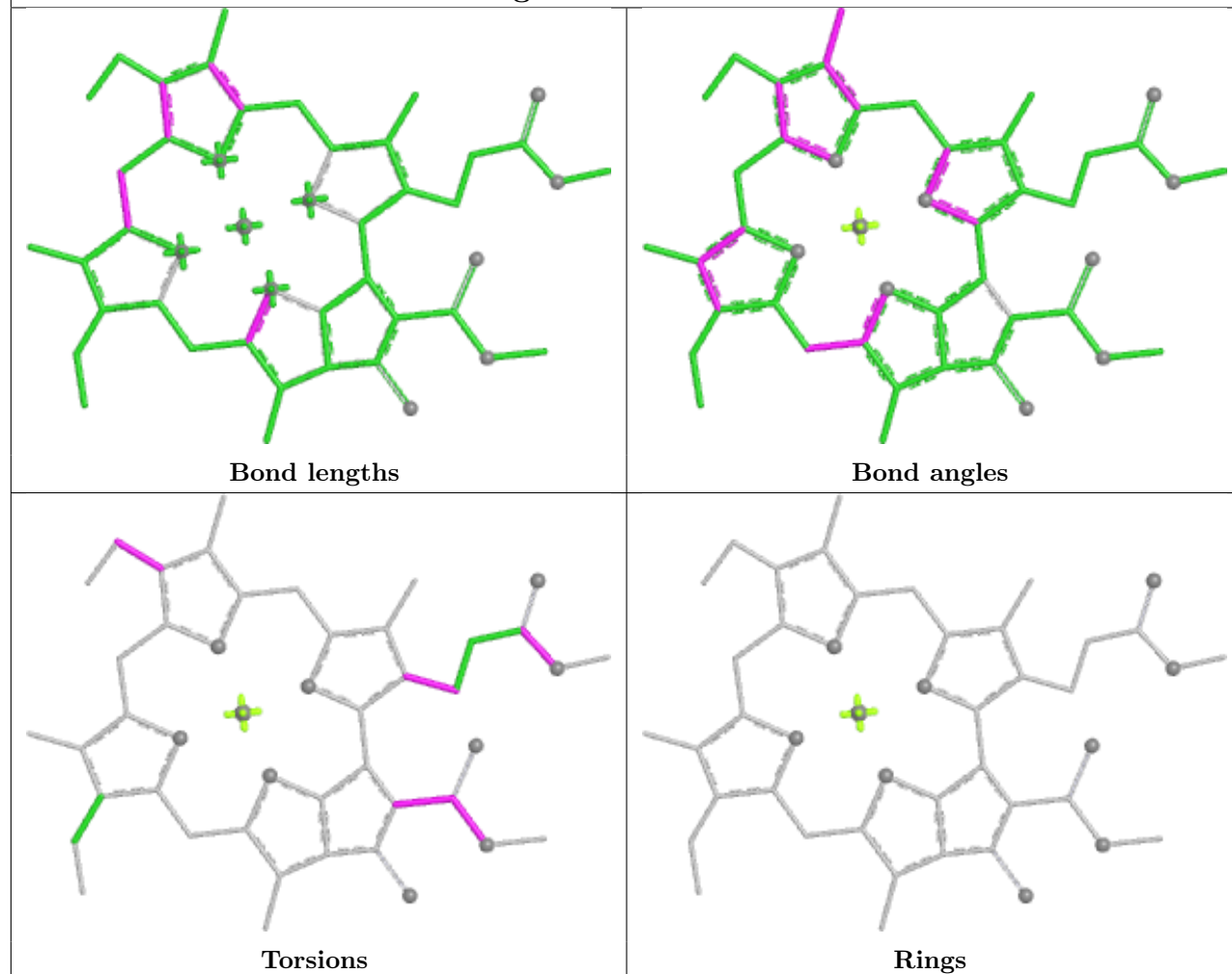
Ligand CLA h 502



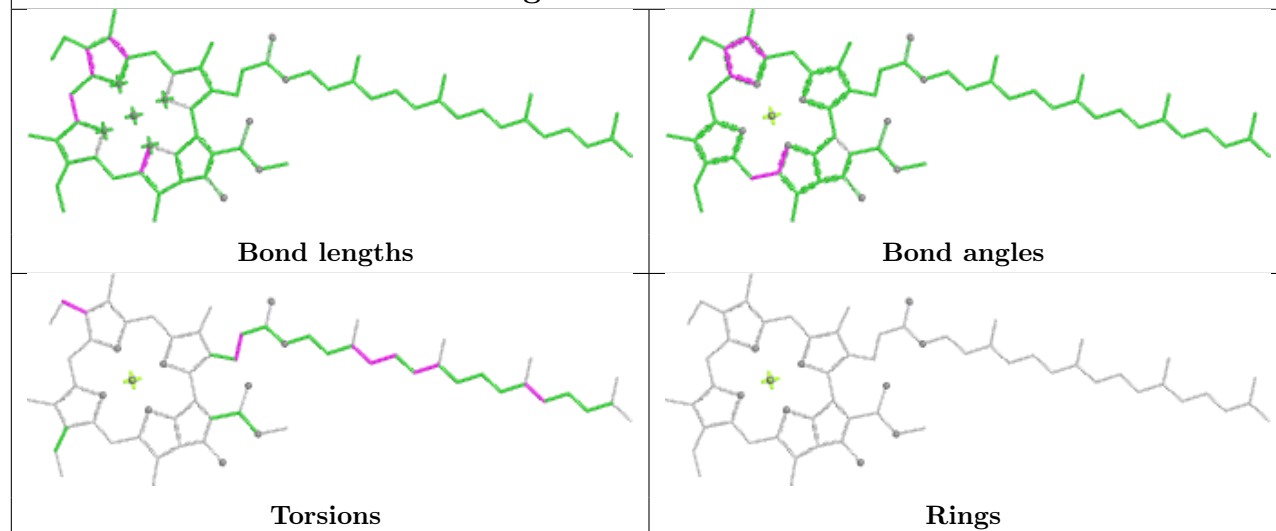
Ligand CLA y 516

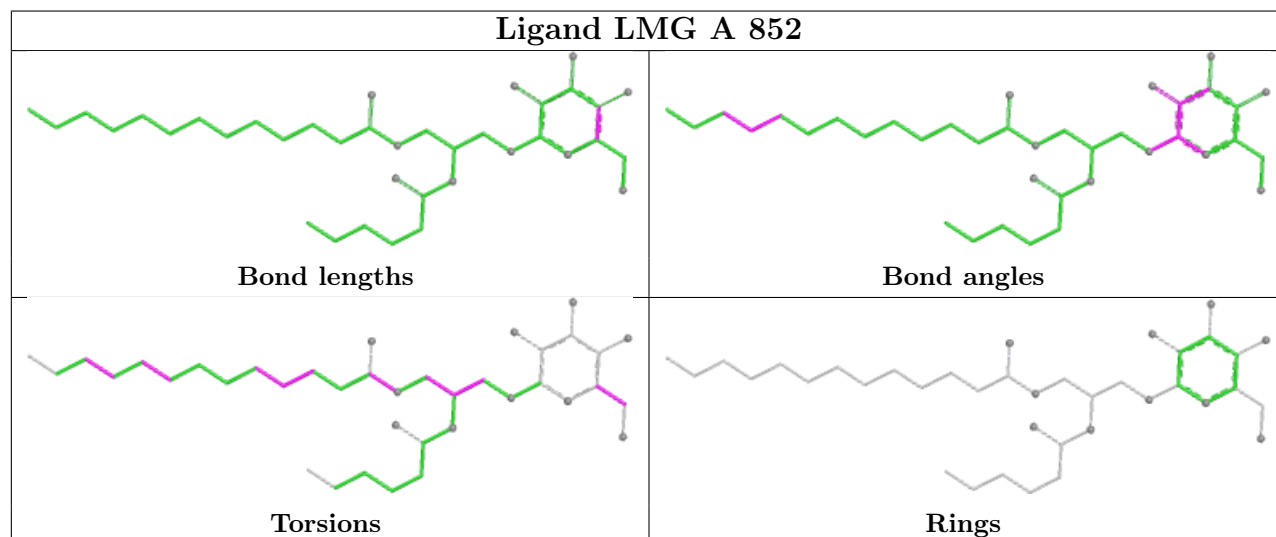
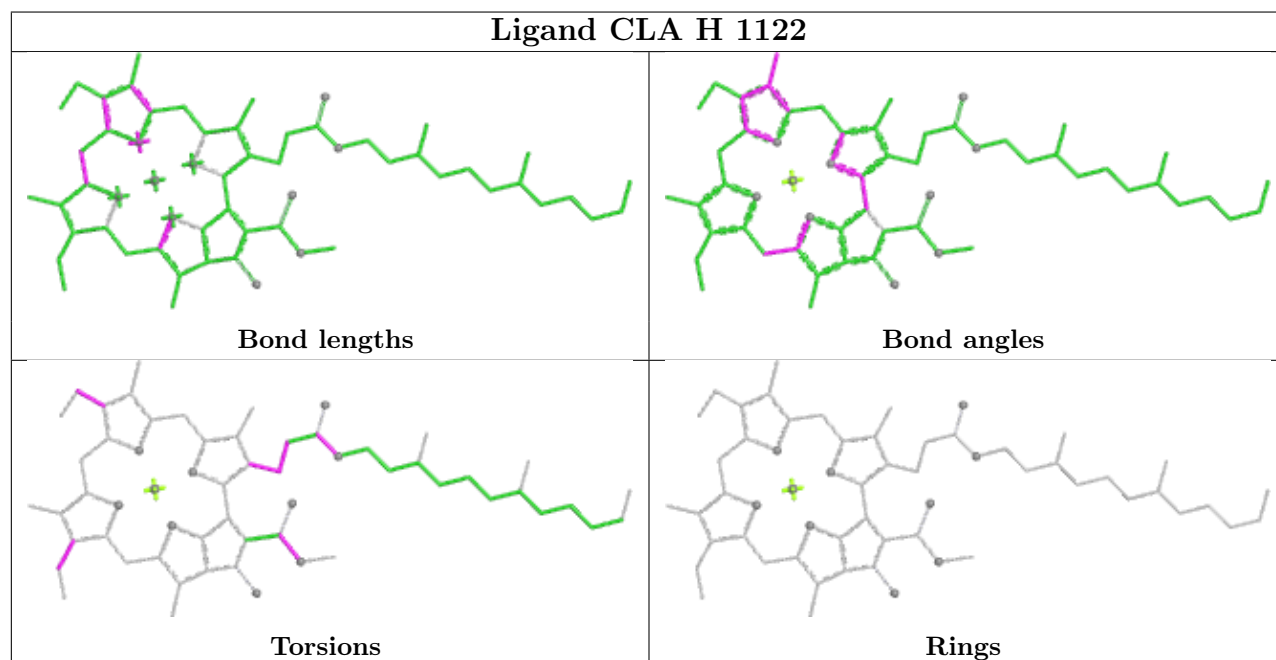
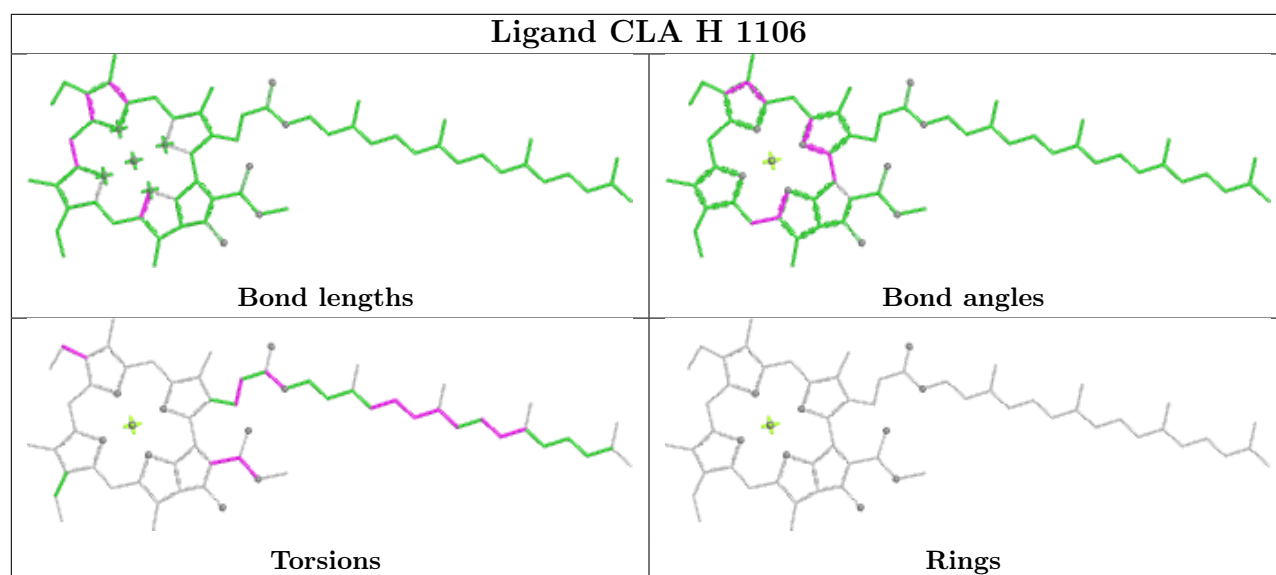


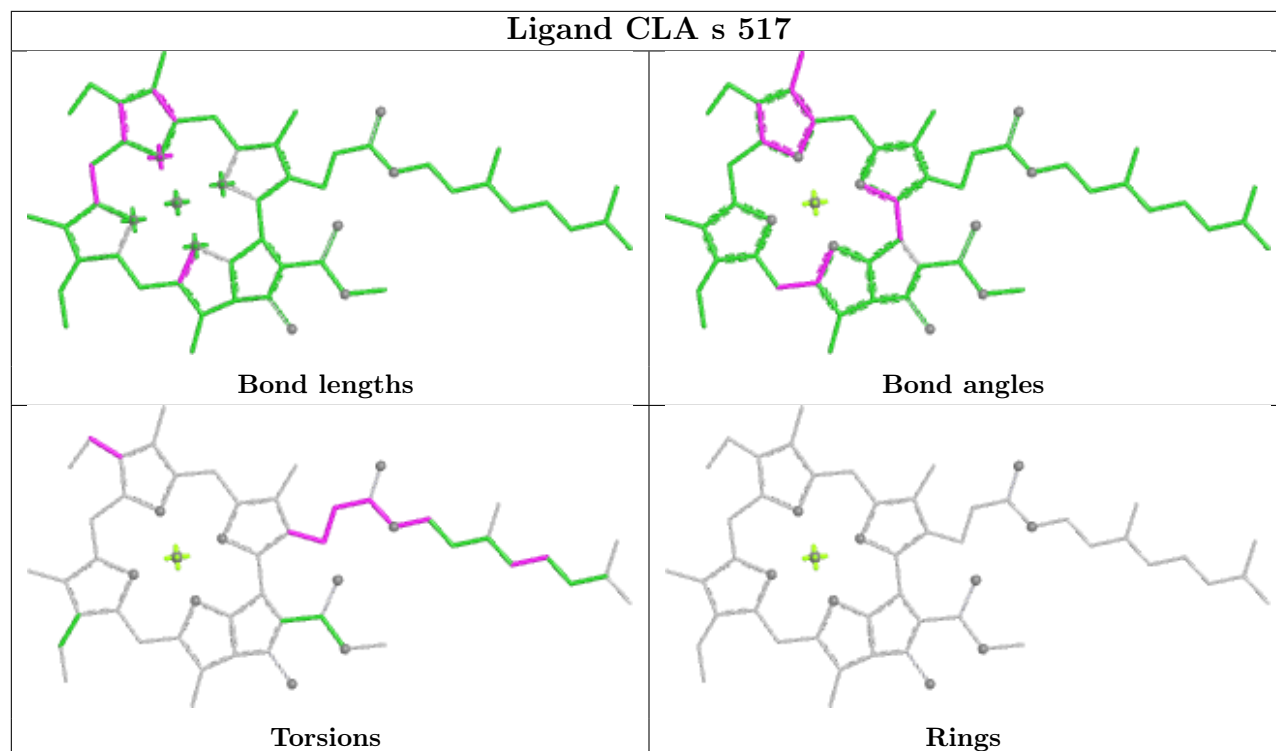
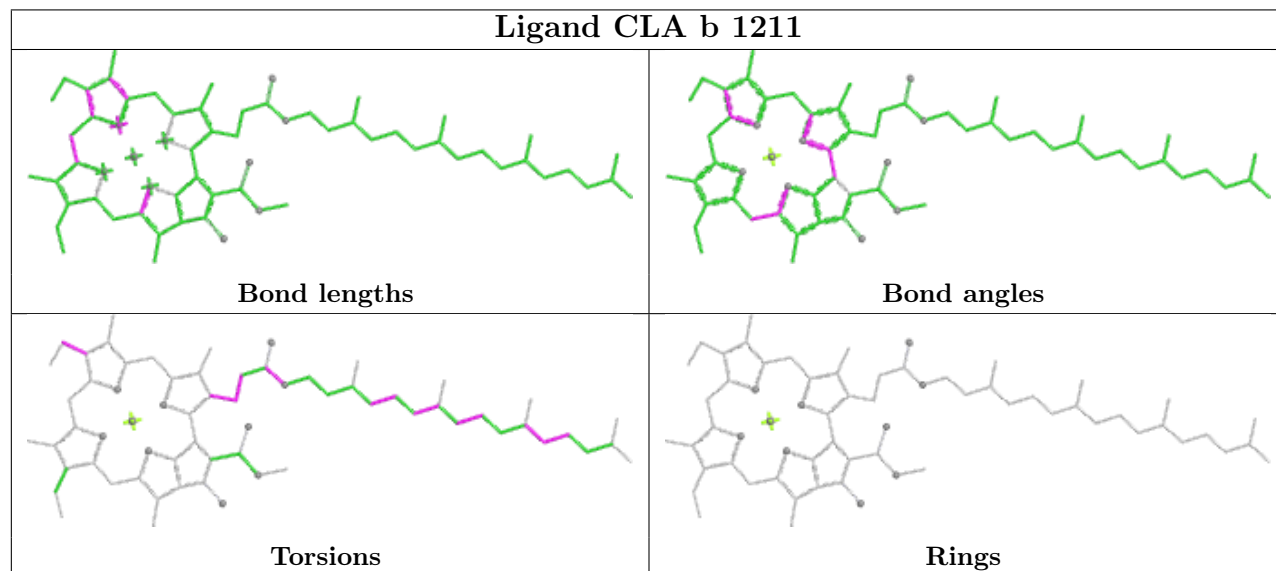
Ligand CLA Y 513

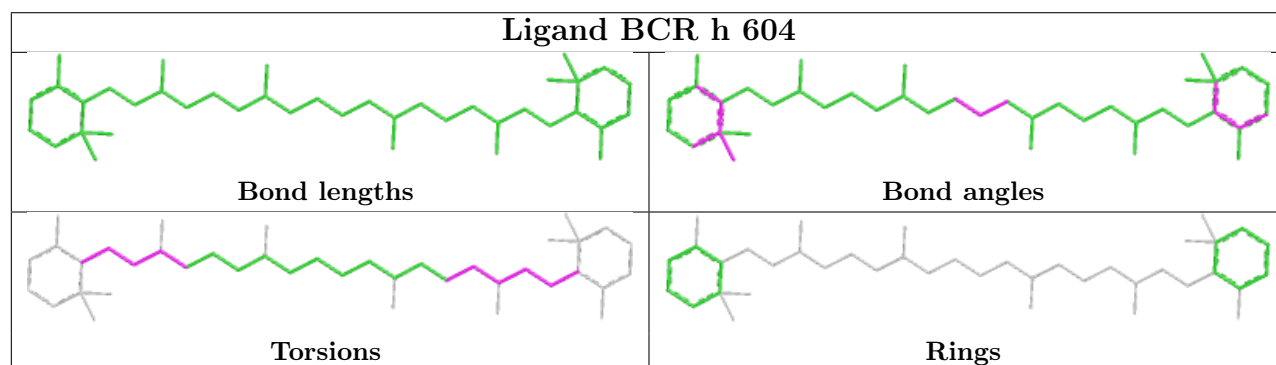
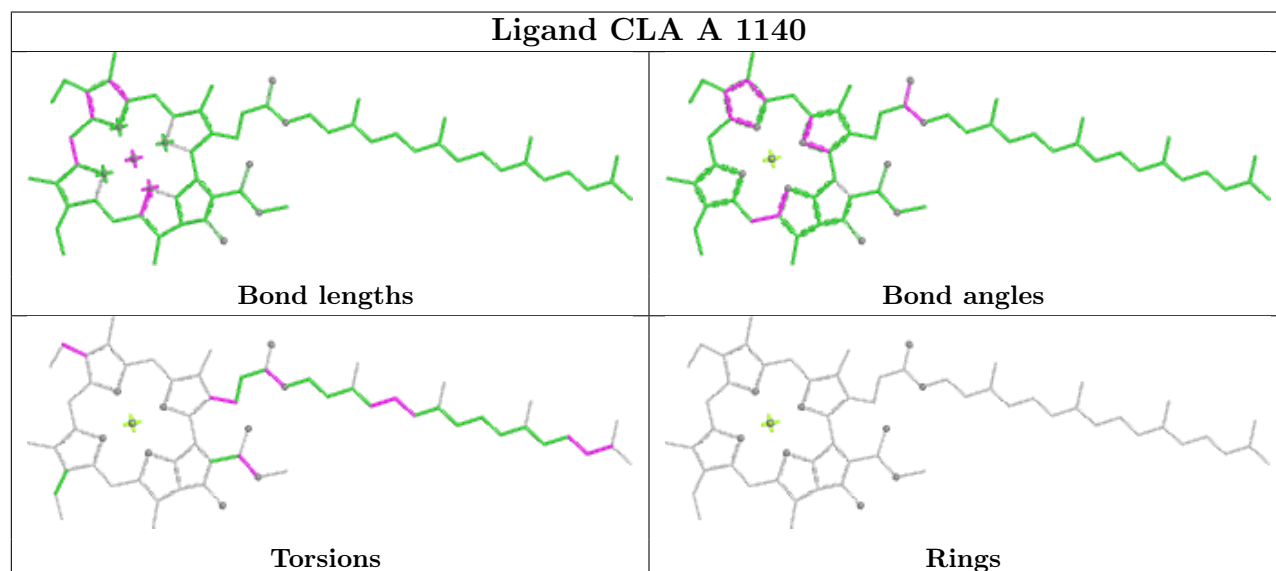
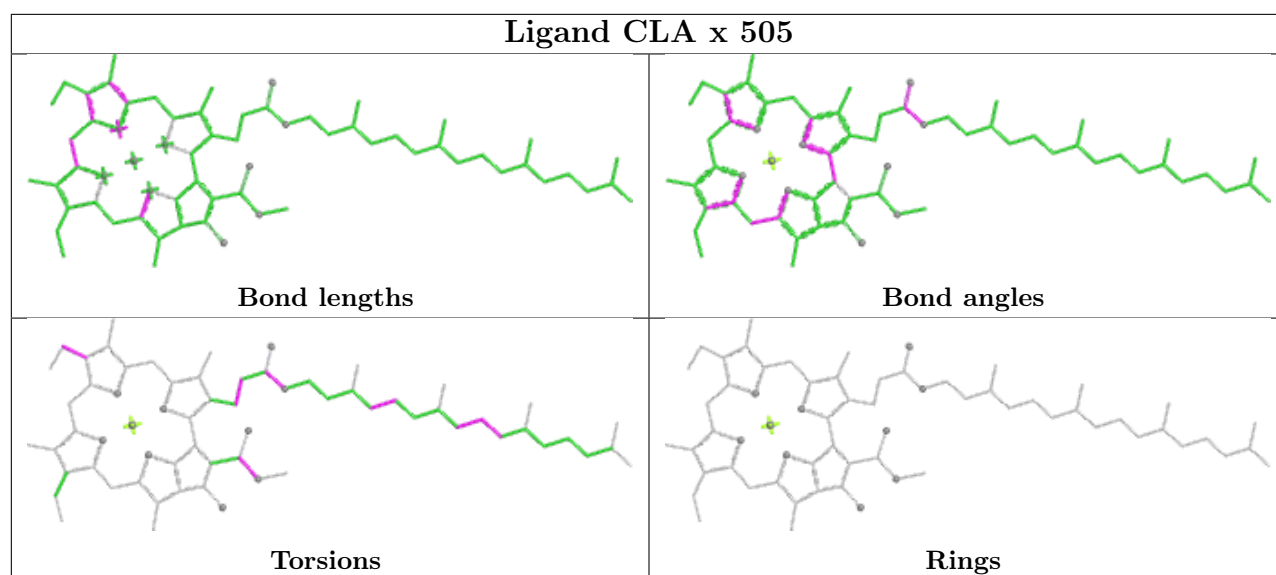


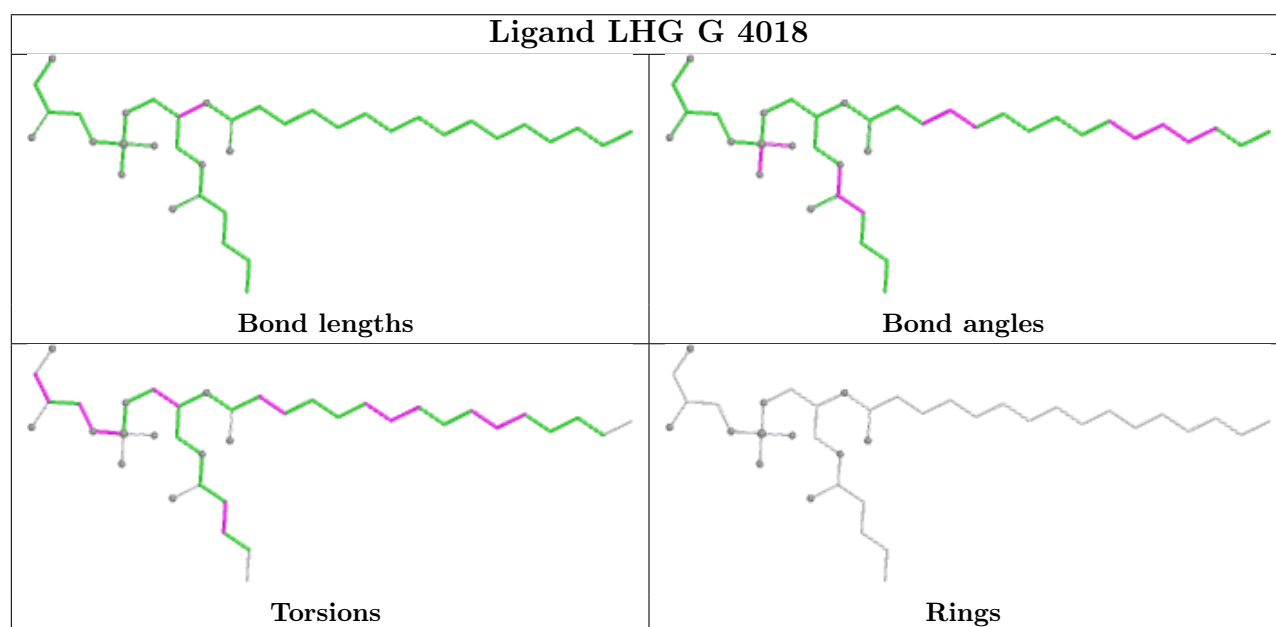
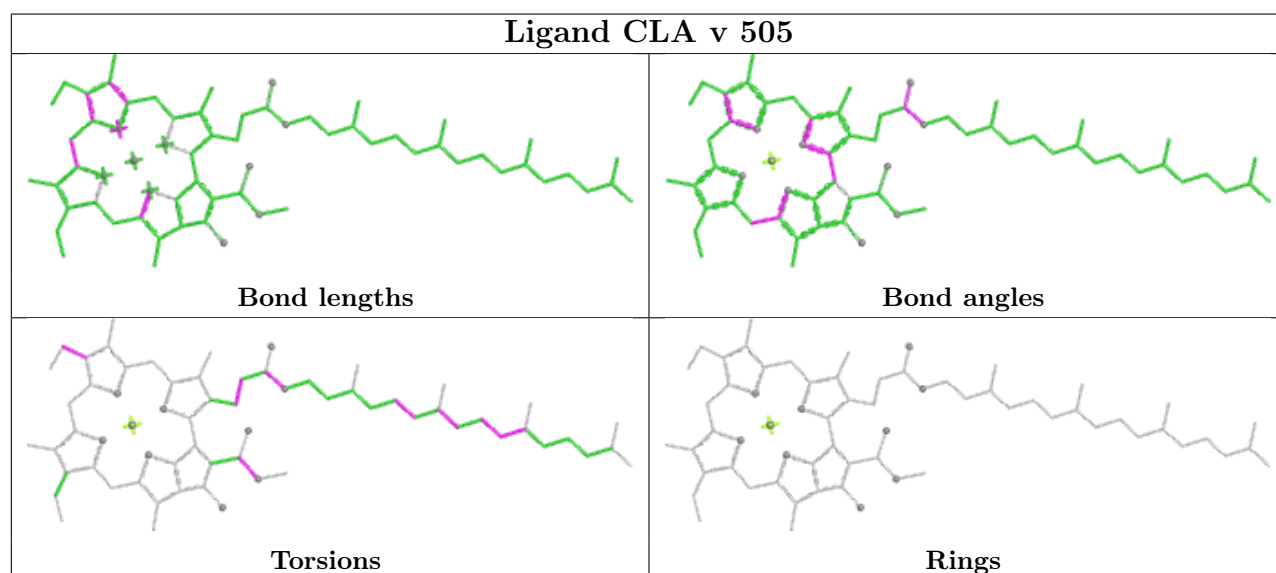
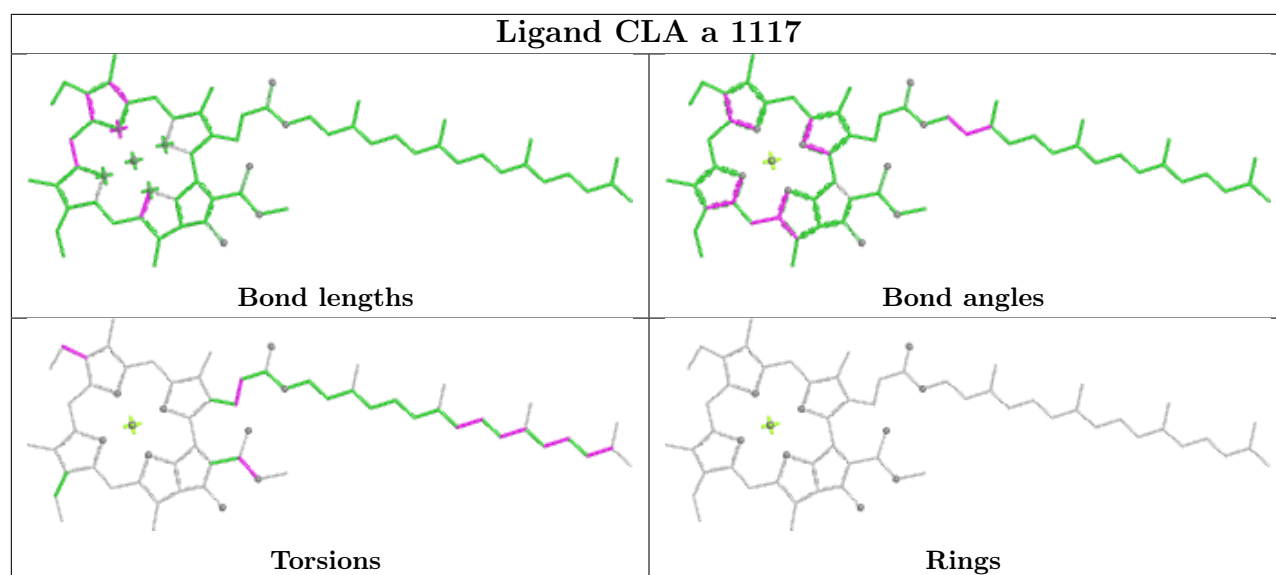
Ligand CLA B 1204



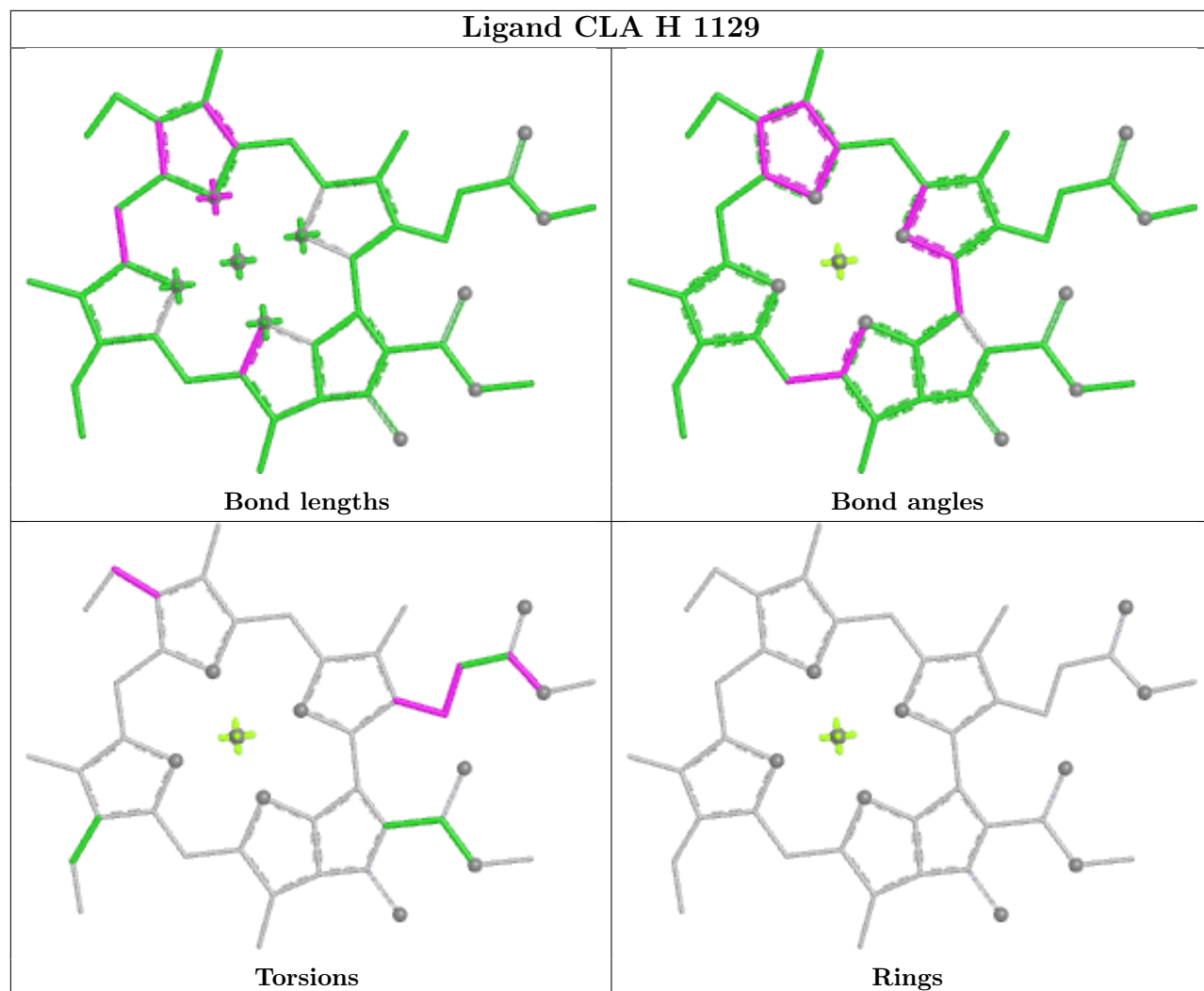


Ligand CLA s 517**Ligand CLA b 1211**

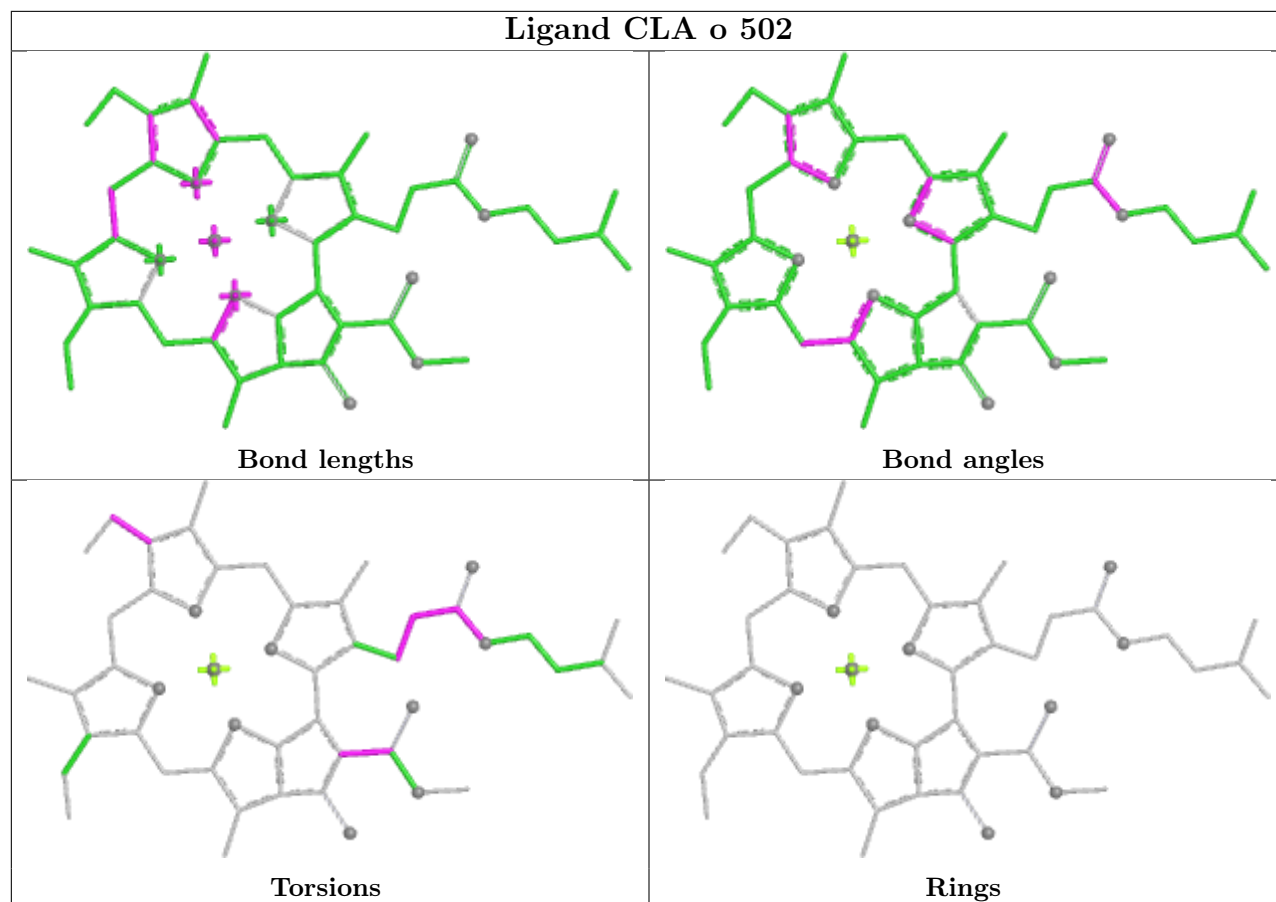




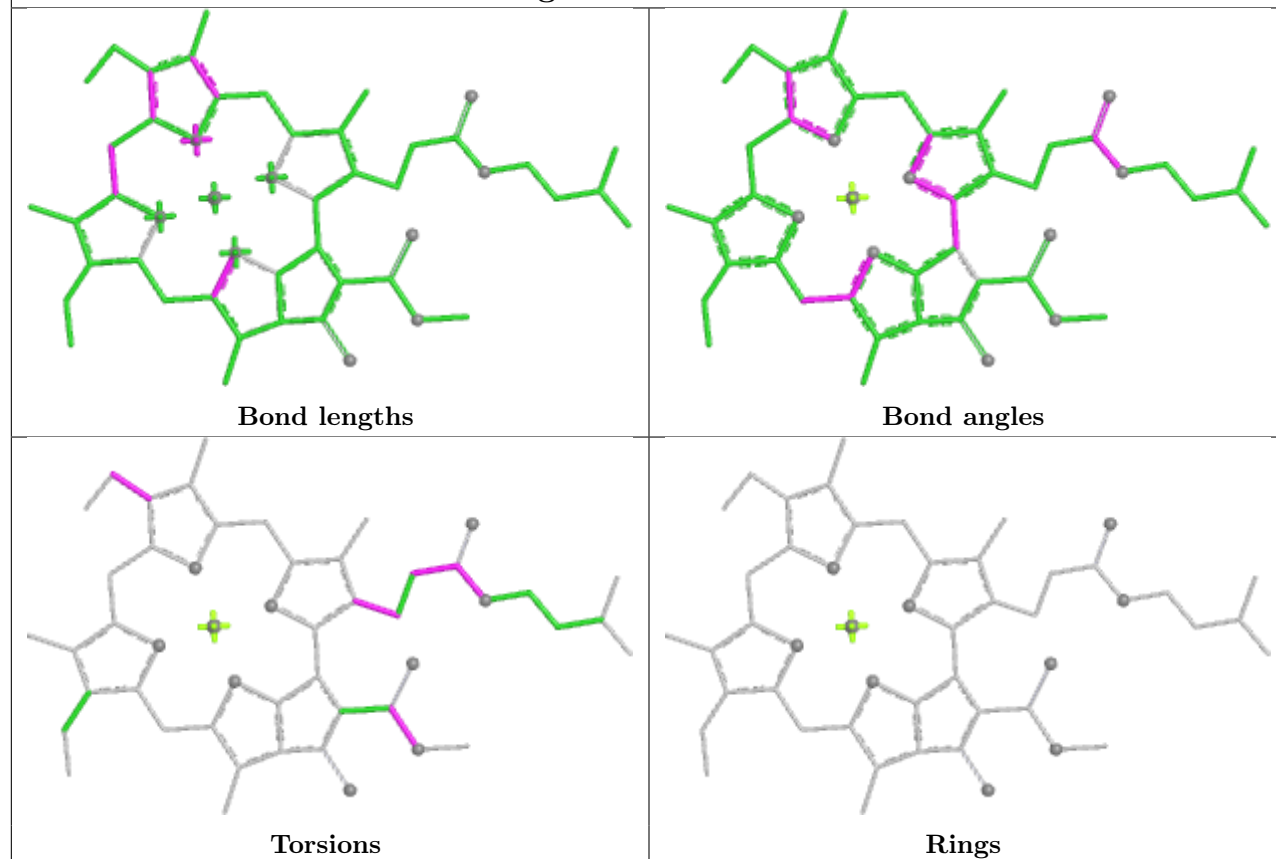
Ligand CLA H 1129



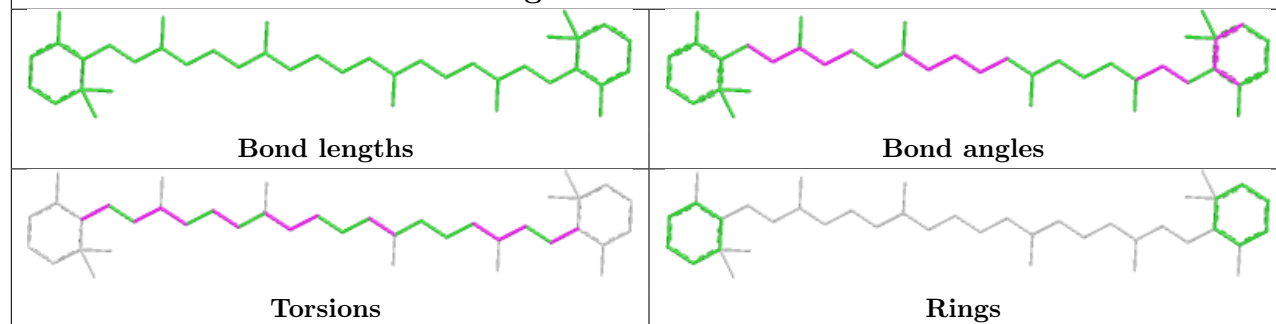
Ligand CLA o 502

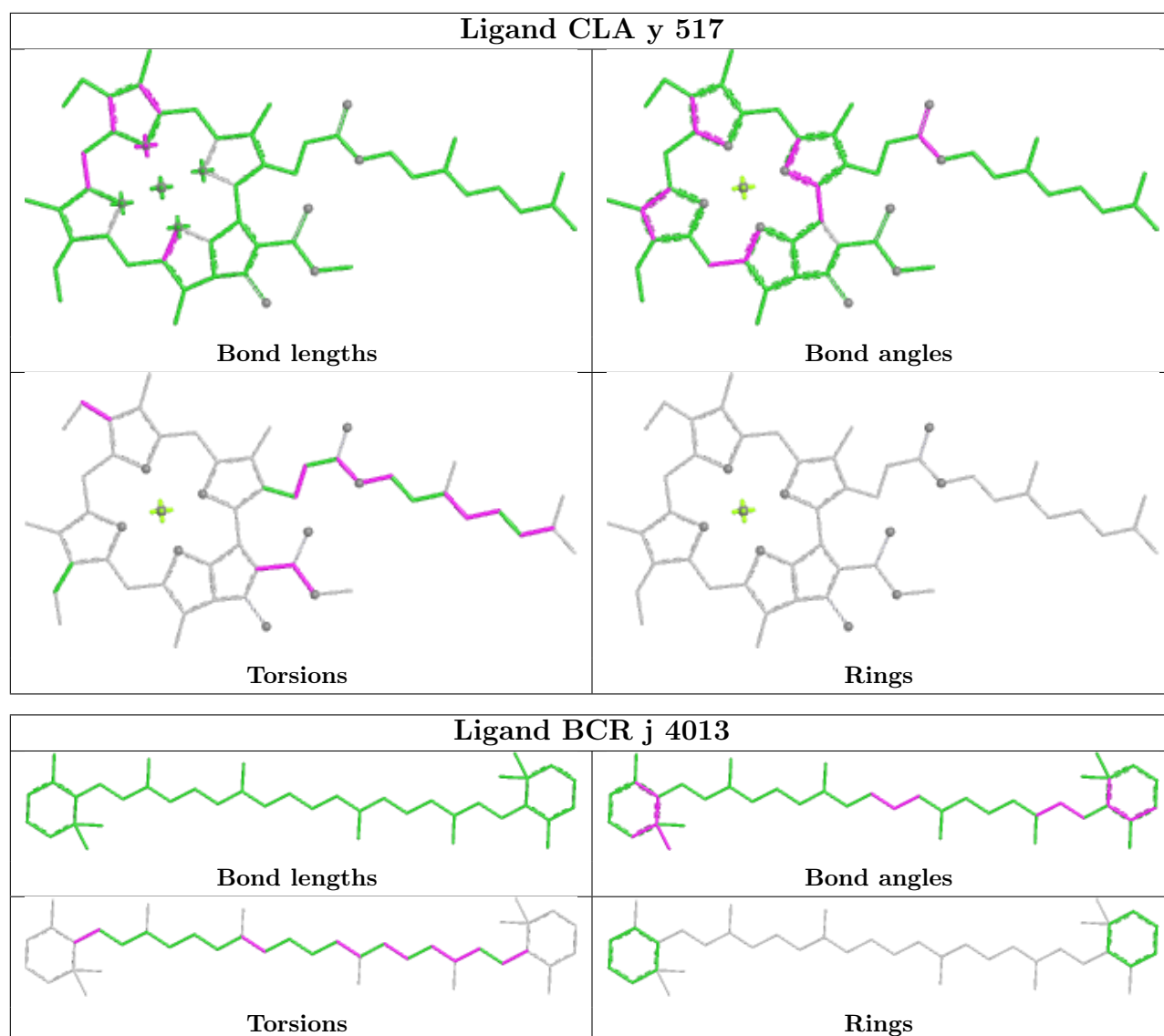


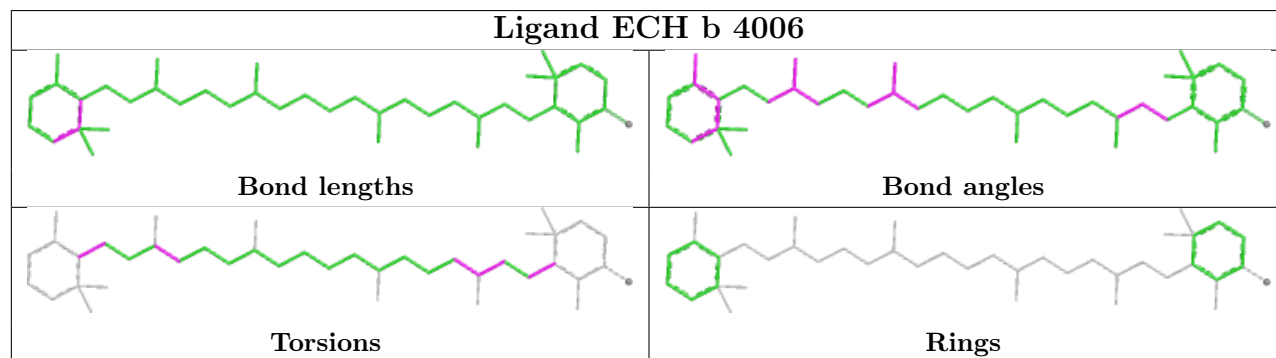
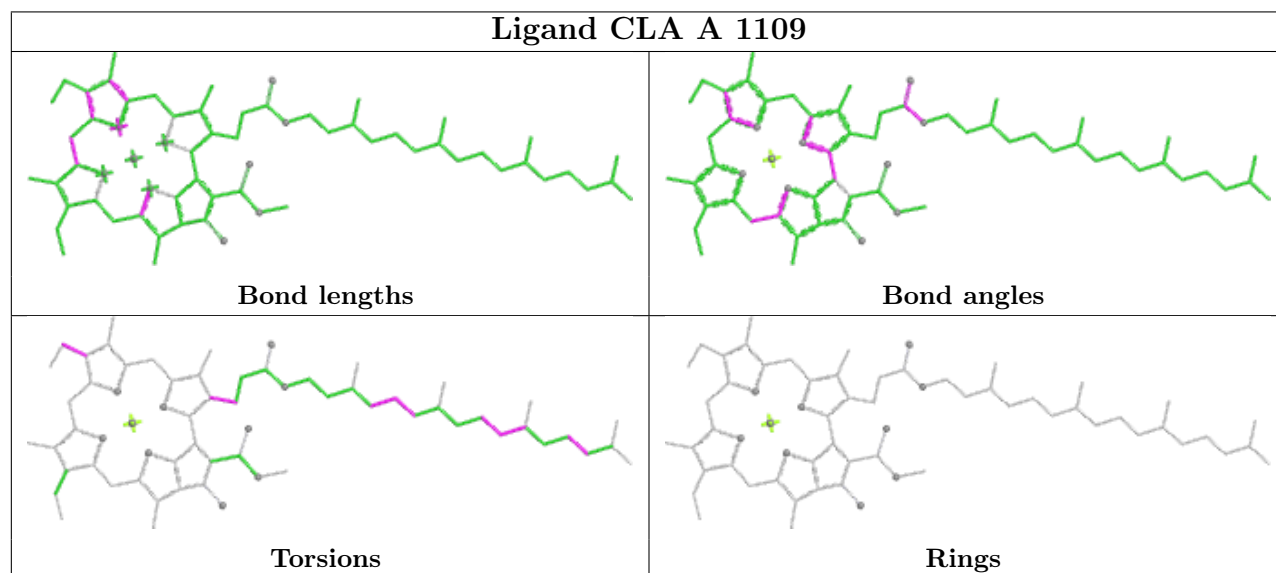
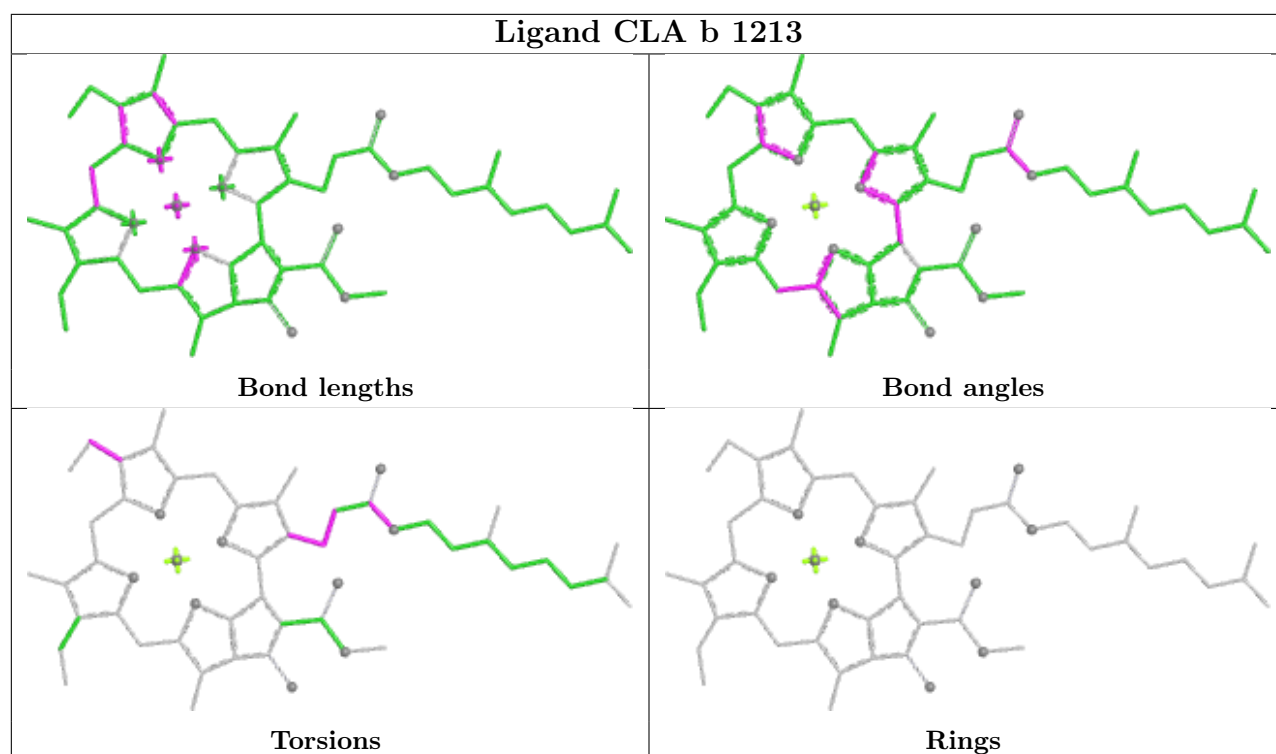
Ligand CLA s 514

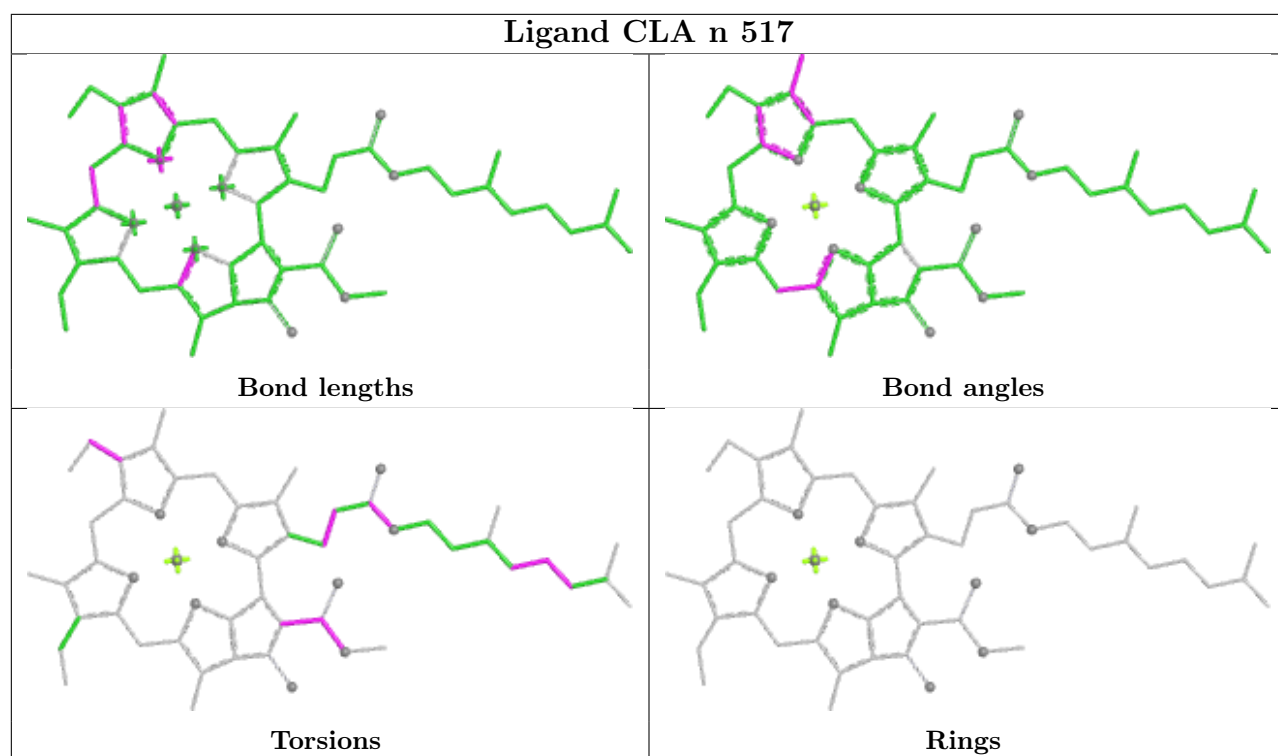


Ligand BCR b 4014

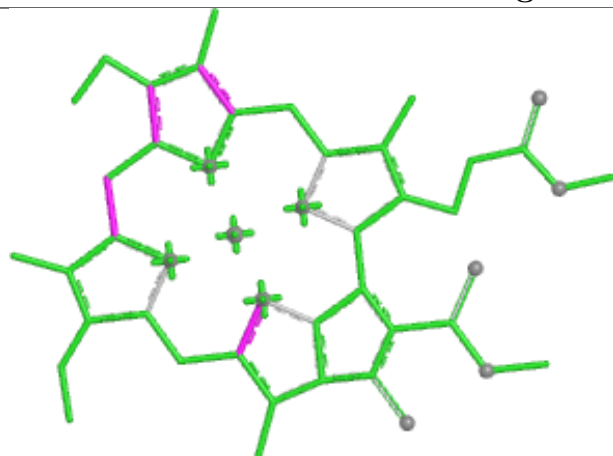




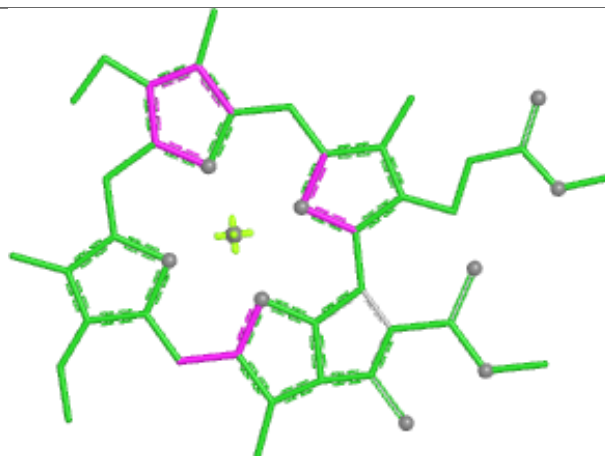




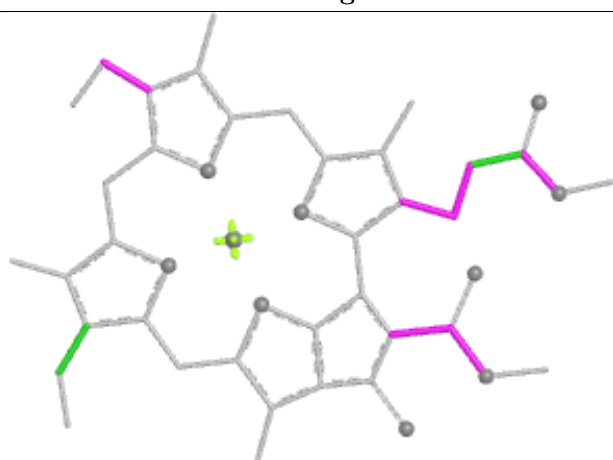
Ligand CLA Z 516



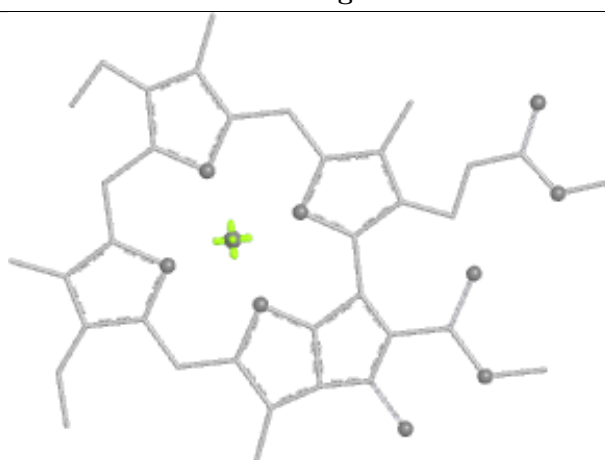
Bond lengths



Bond angles

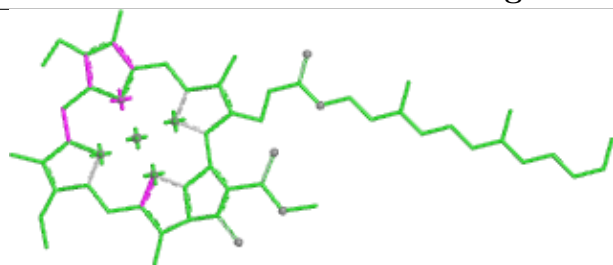


Torsions

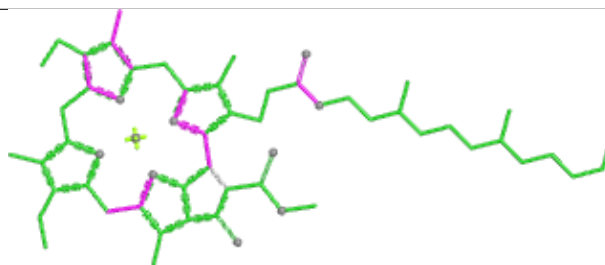


Rings

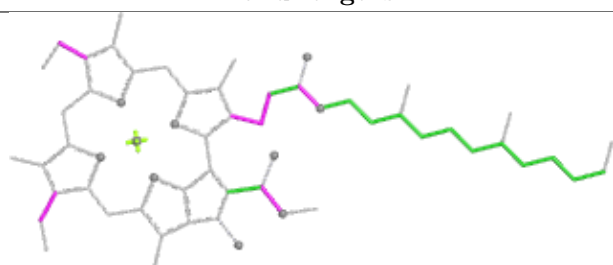
Ligand CLA A 1122



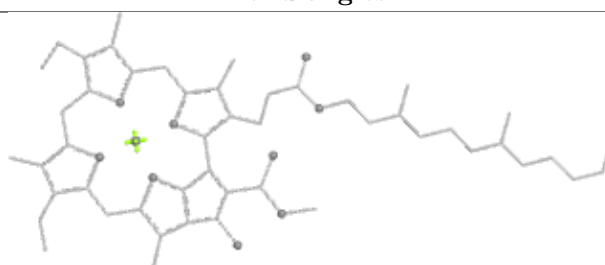
Bond lengths



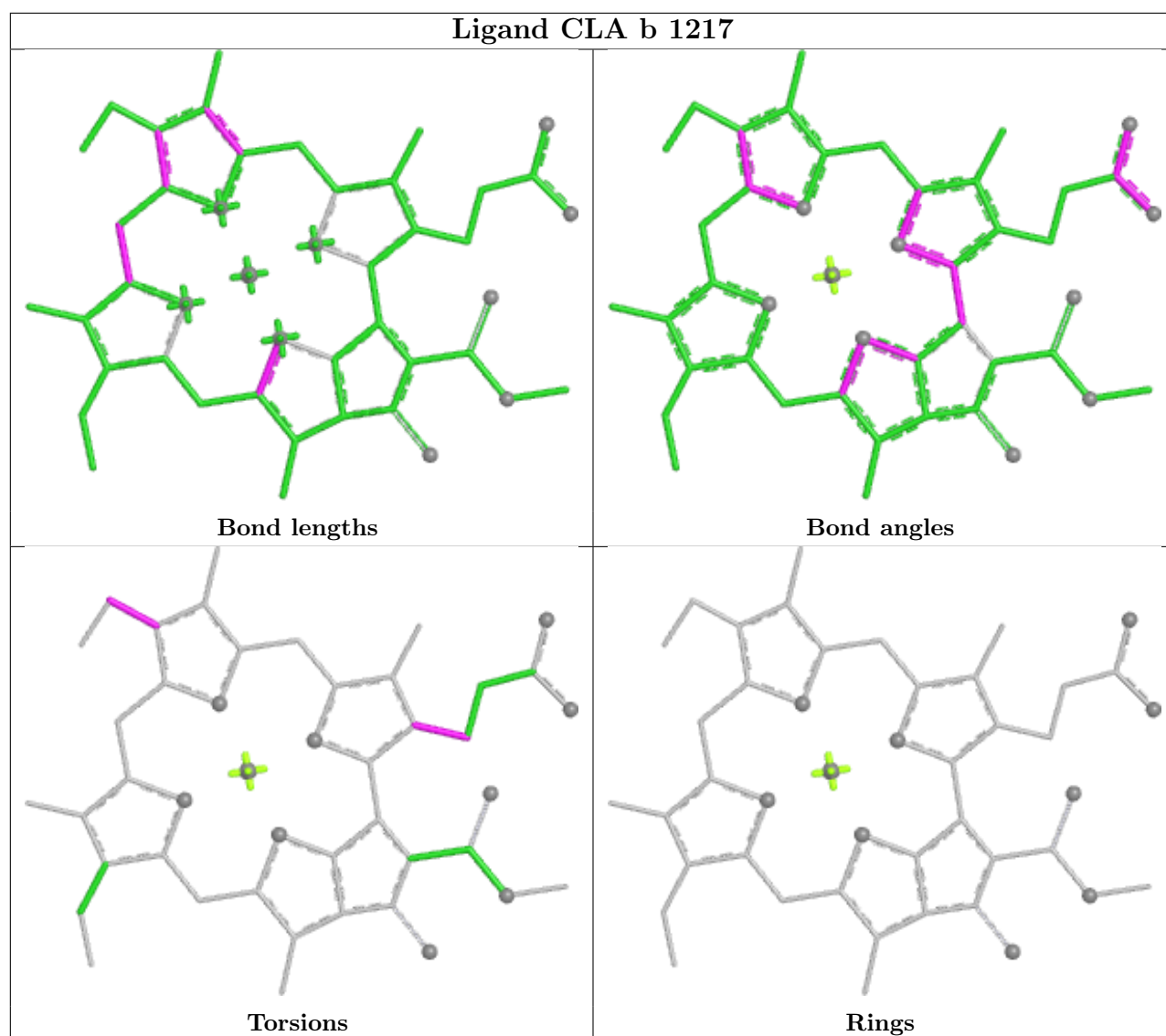
Bond angles



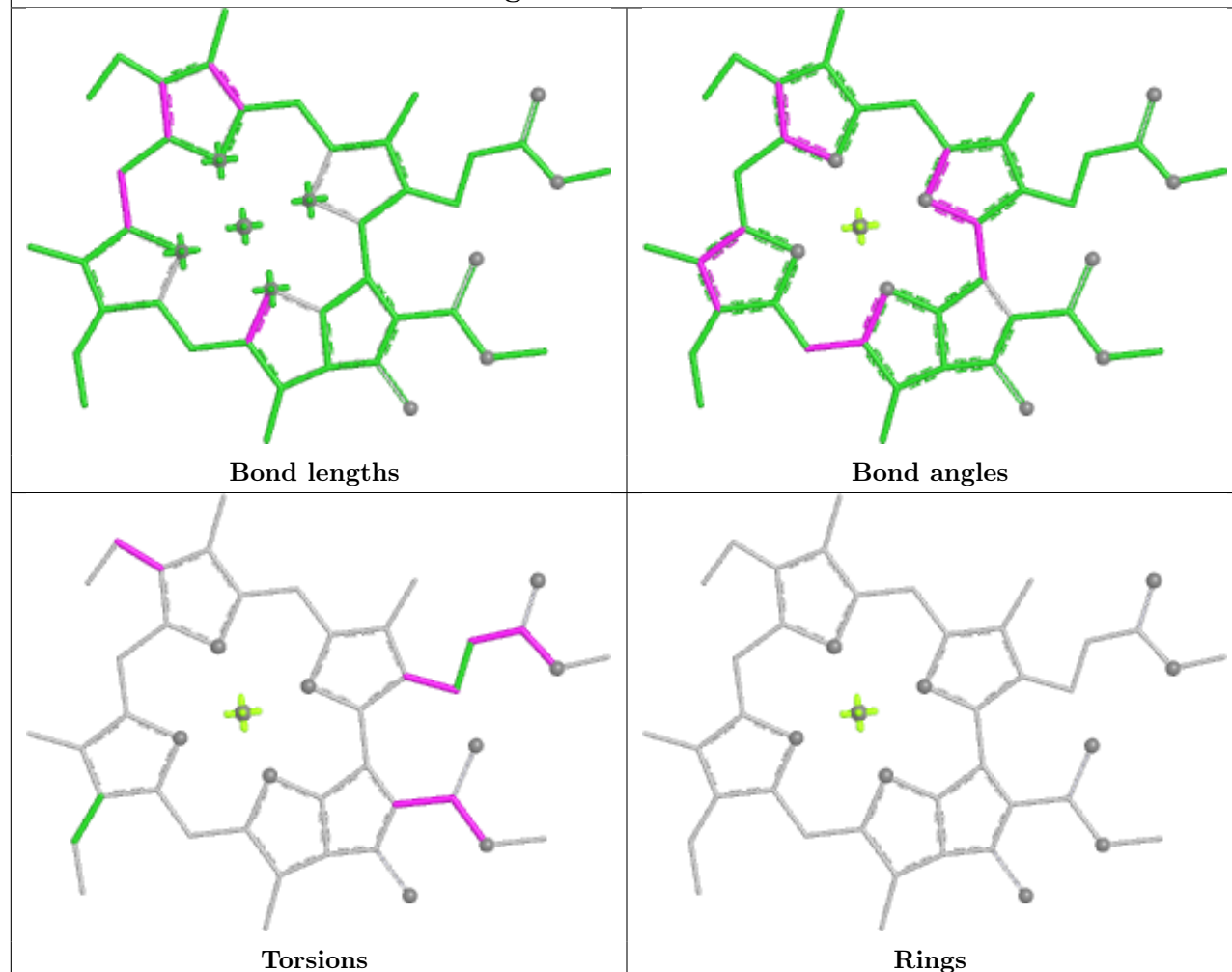
Torsions



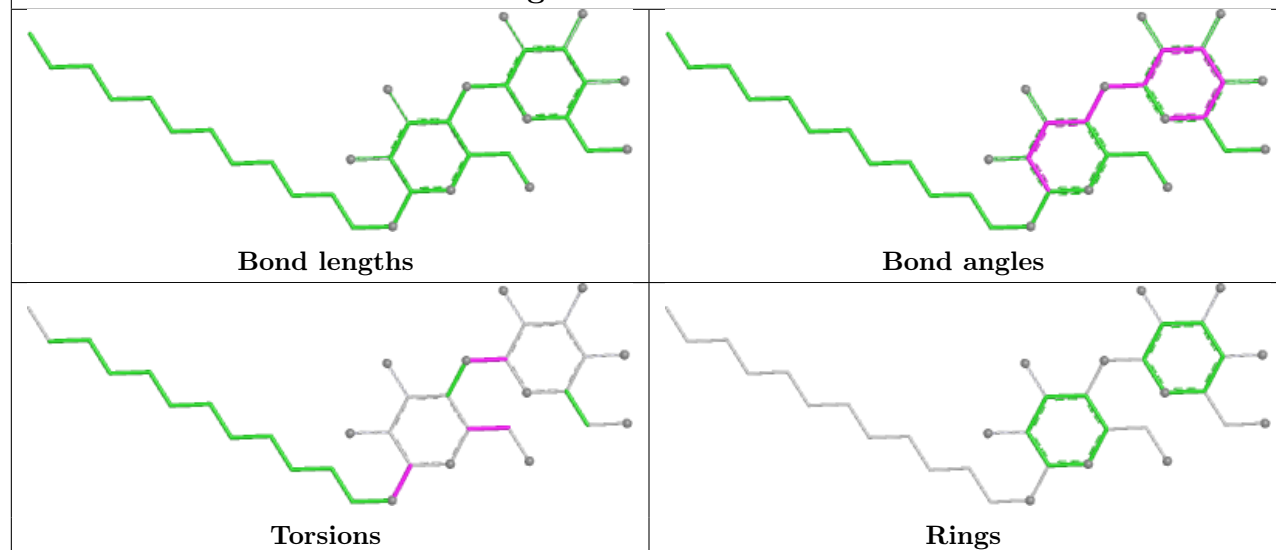
Rings

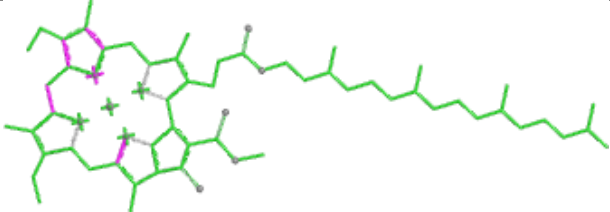
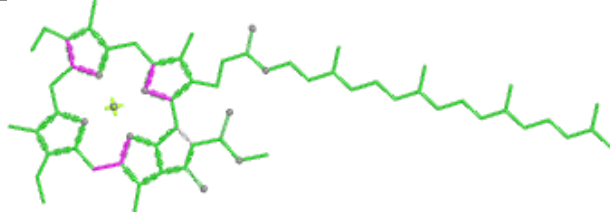
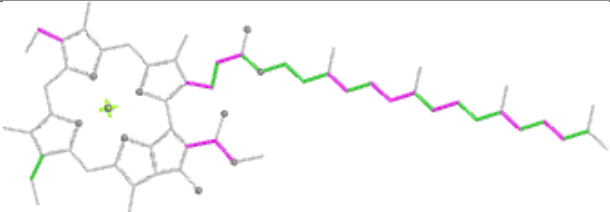
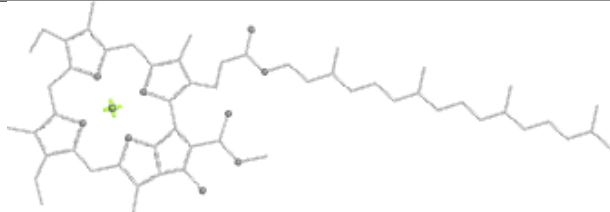
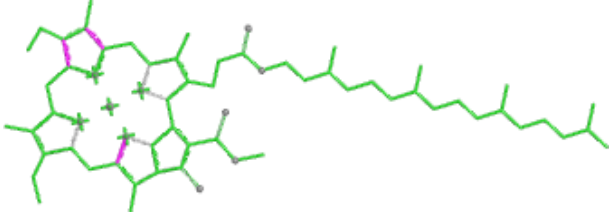
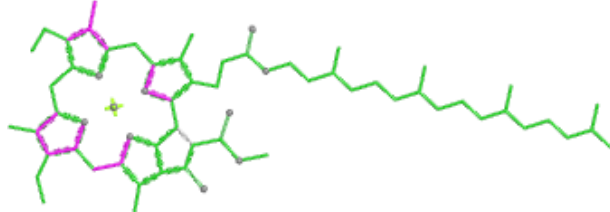
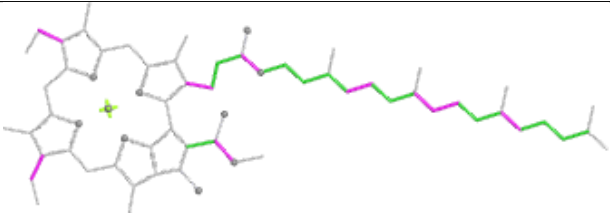
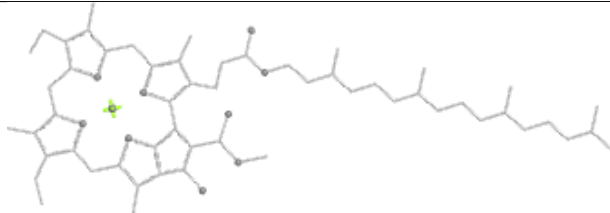
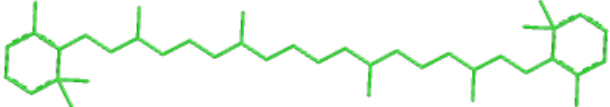
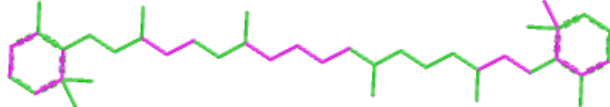
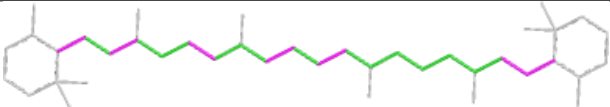
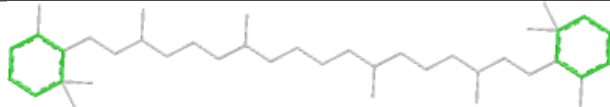


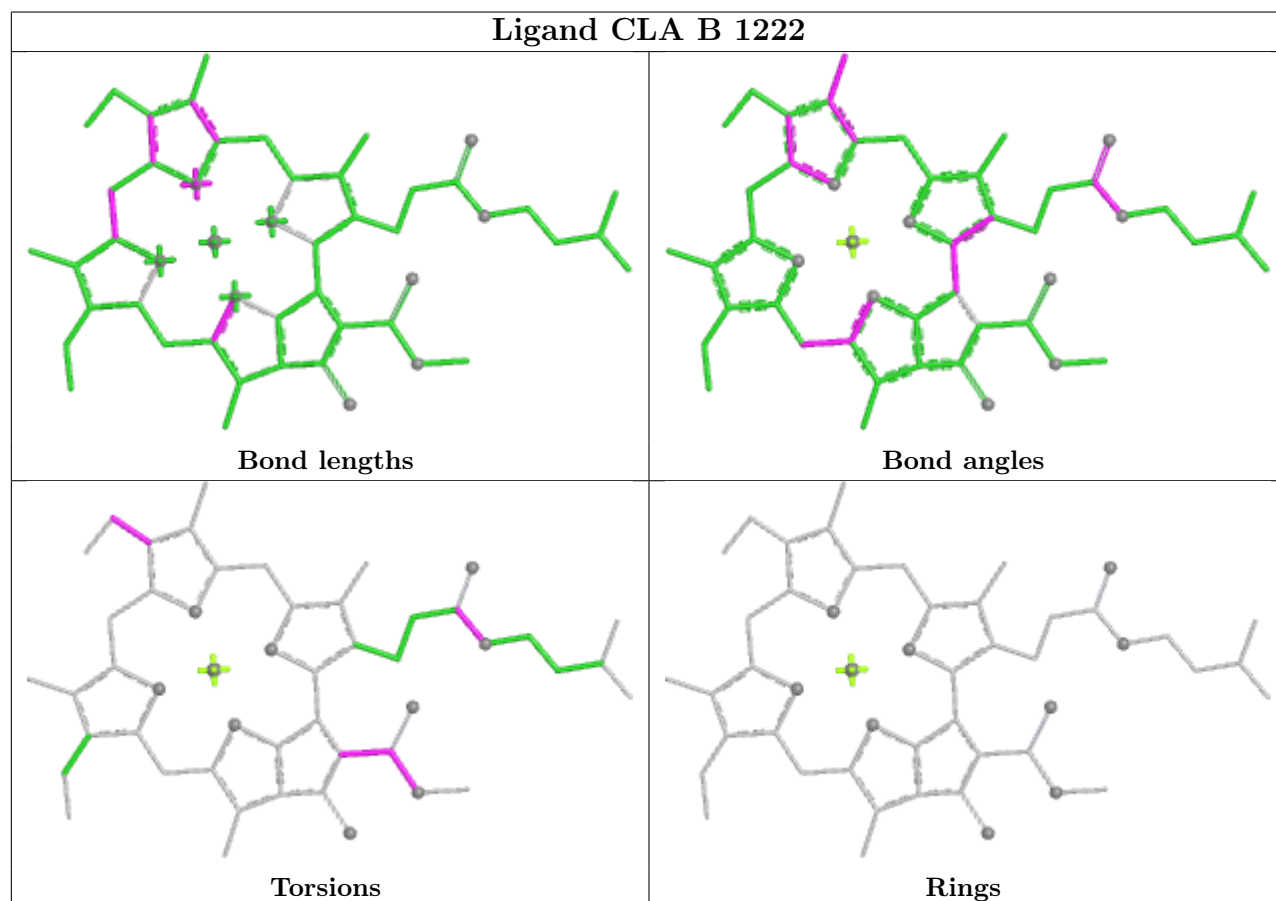
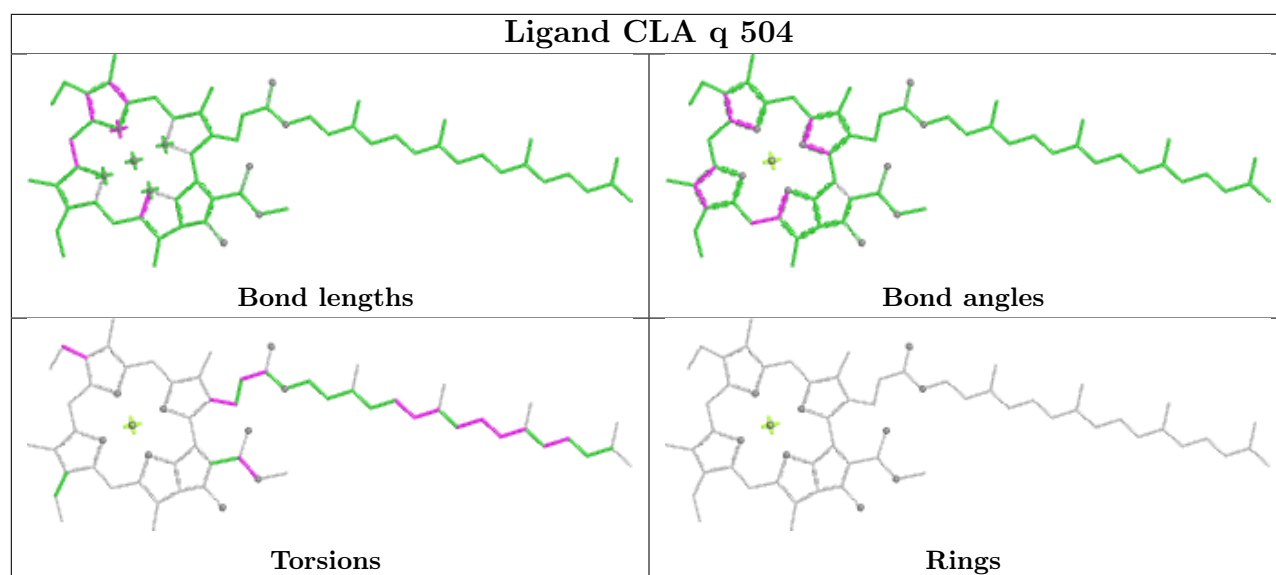
Ligand CLA A 1801

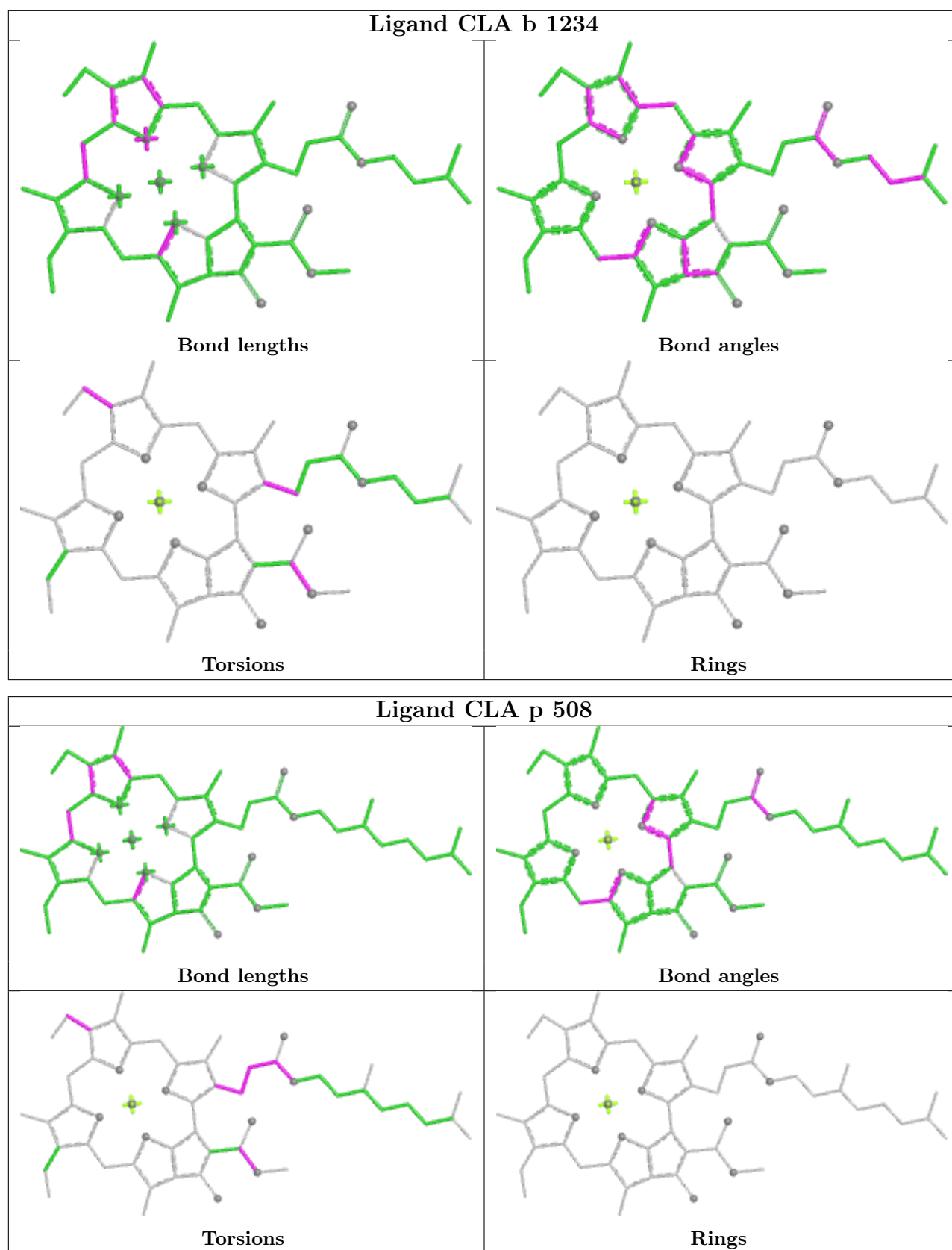


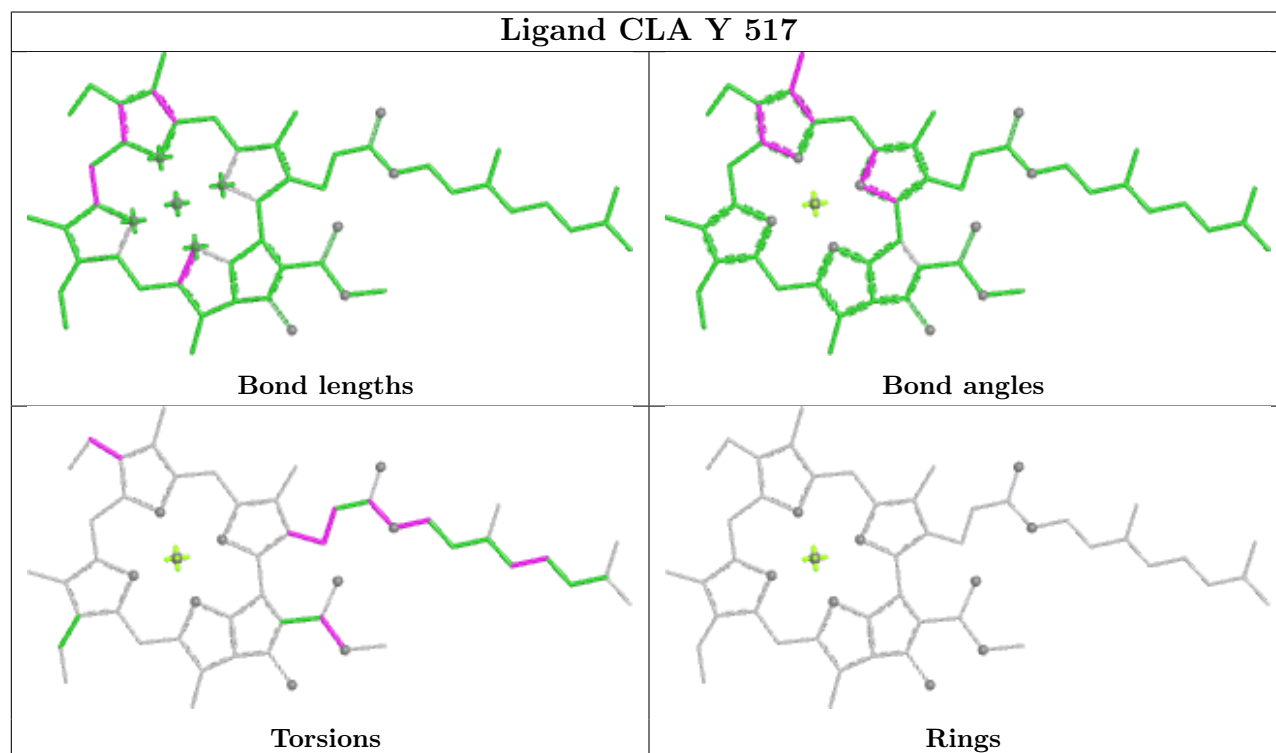
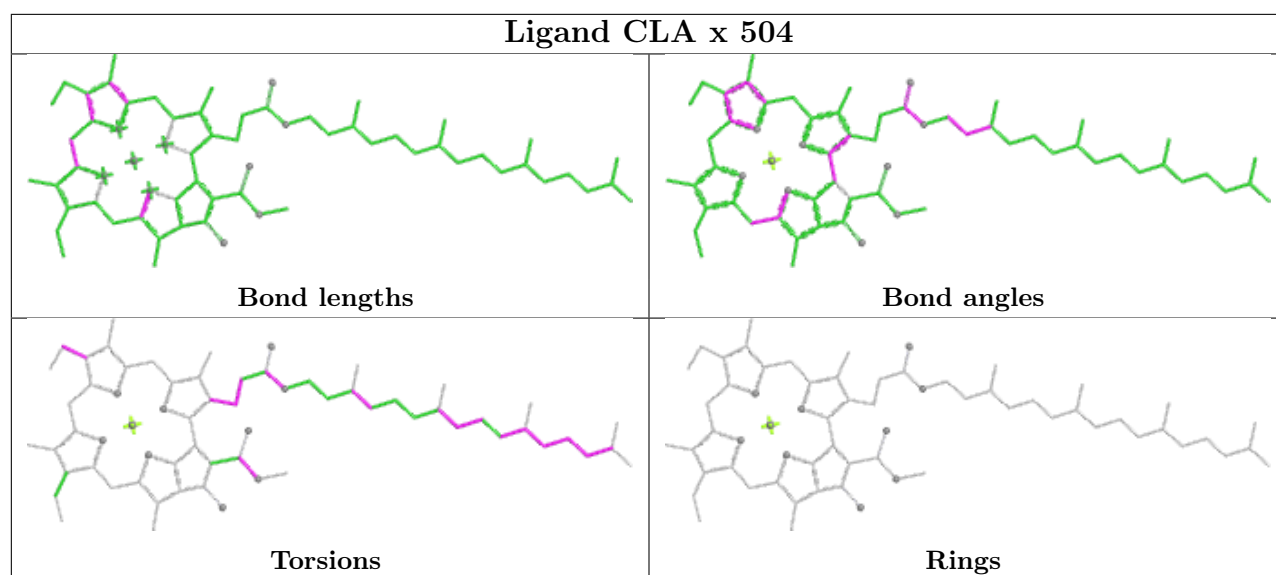
Ligand LMU Y 606



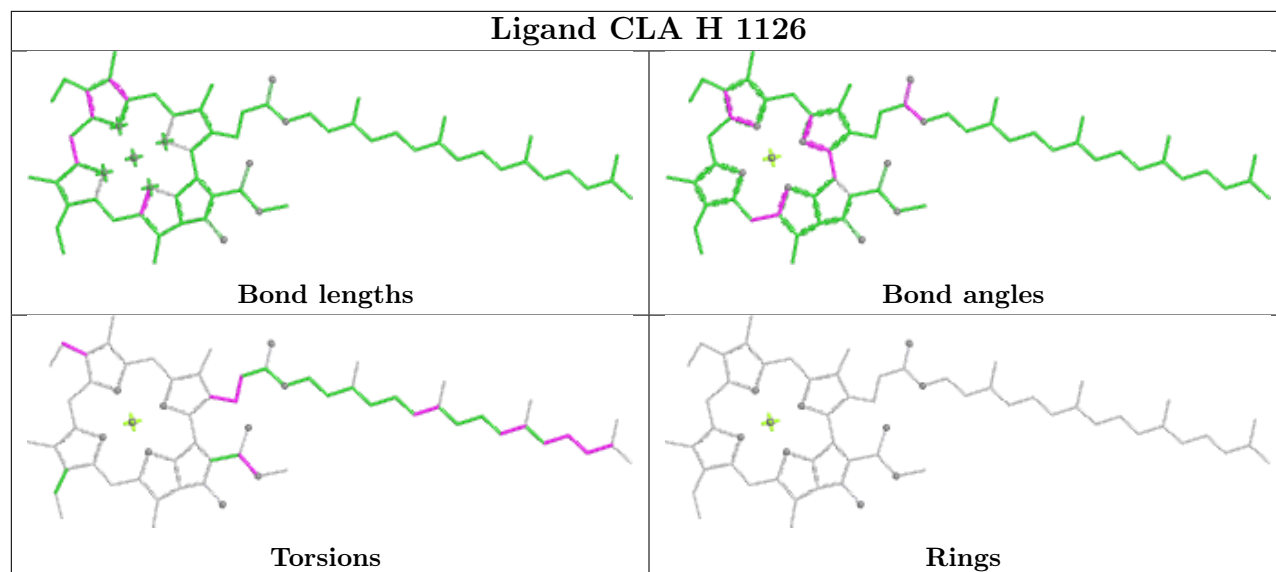
Ligand CLA Y 504	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 1239	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR W 604	
 Bond lengths	 Bond angles
 Torsions	 Rings



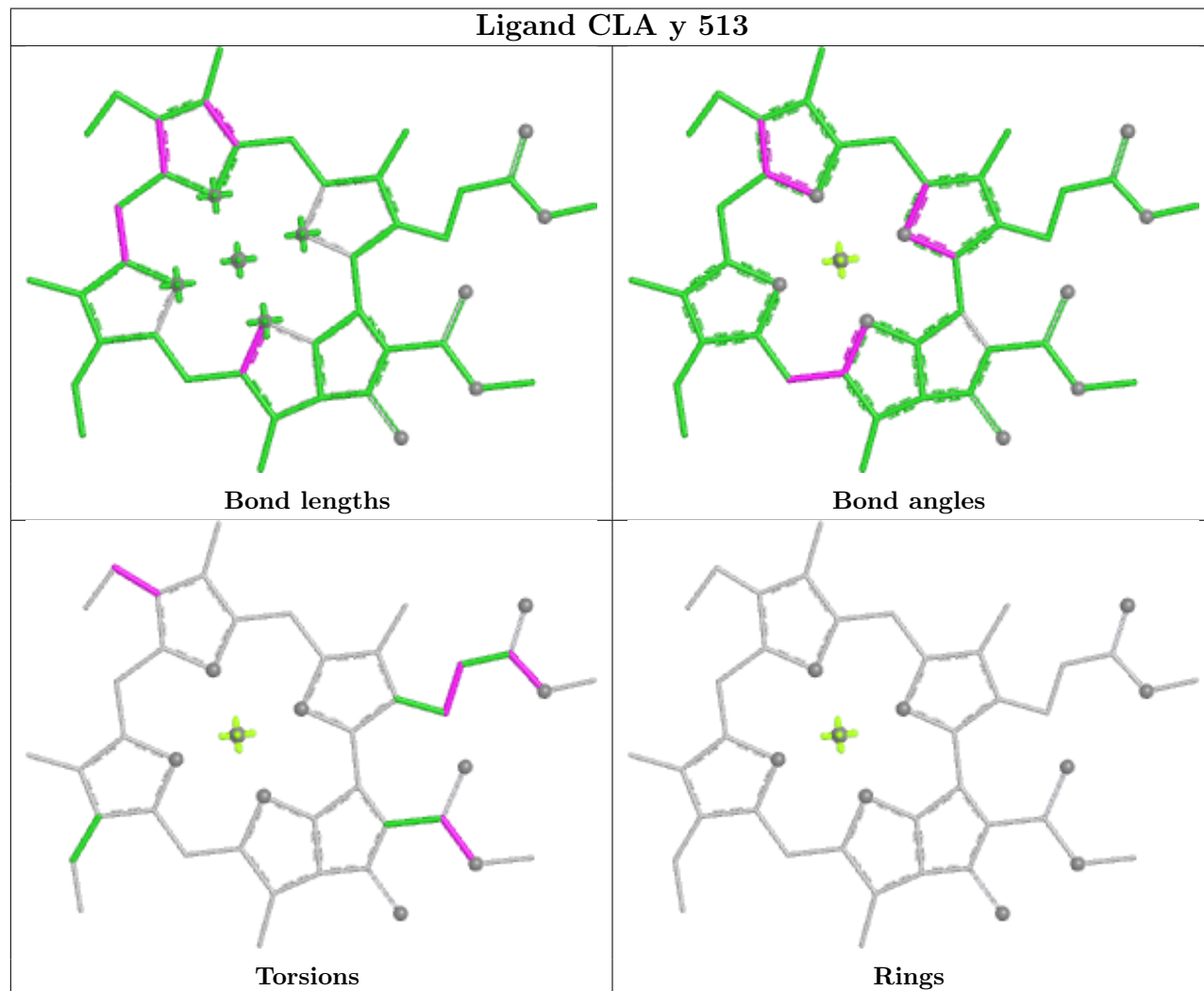


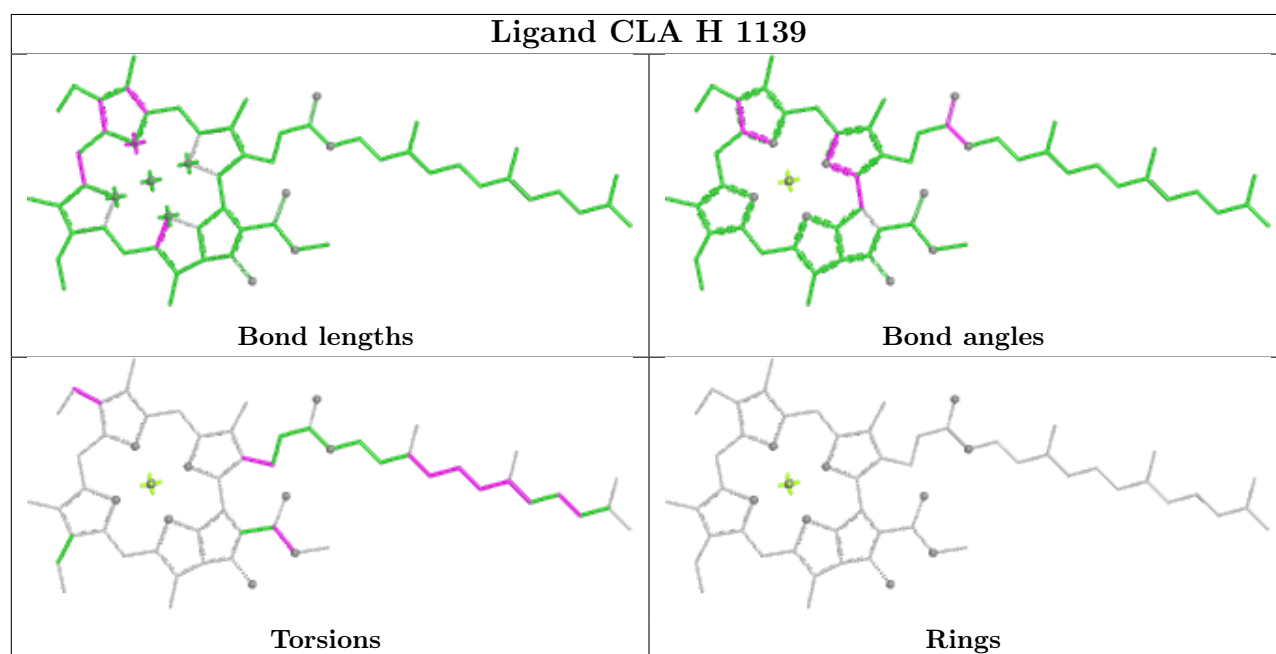
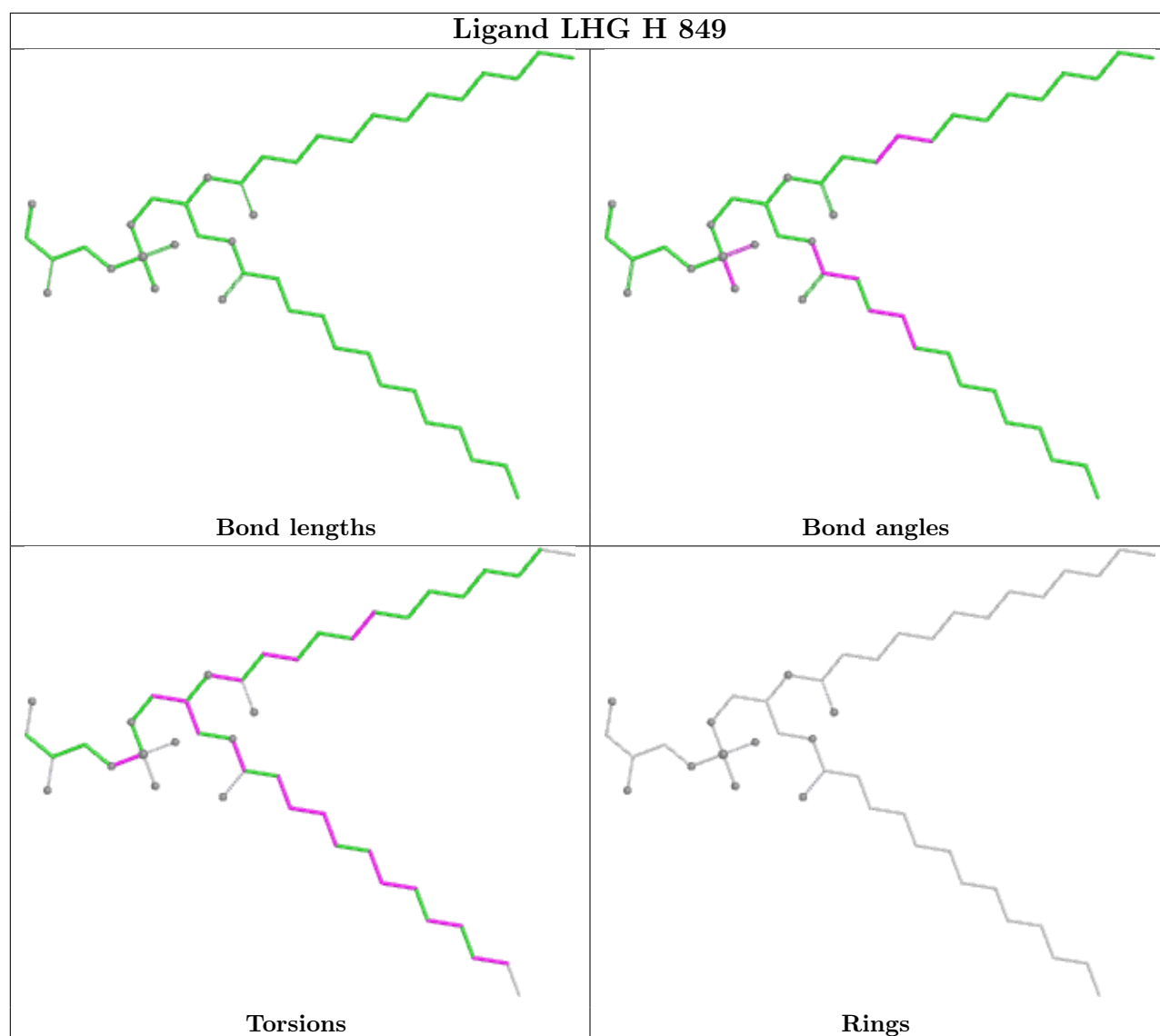


Ligand CLA H 1126

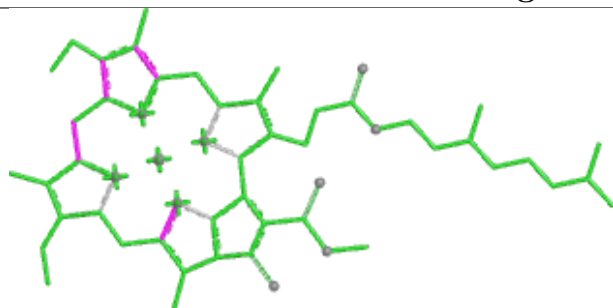


Ligand CLA y 513

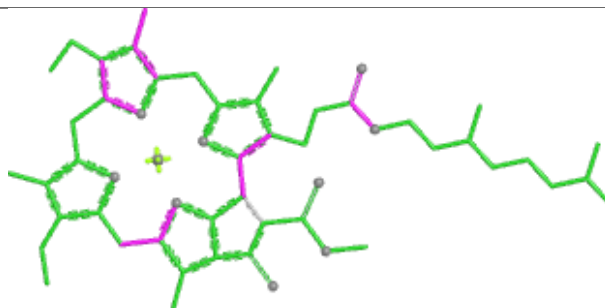




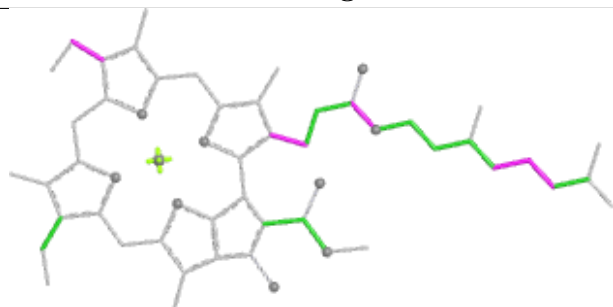
Ligand CLA u 517



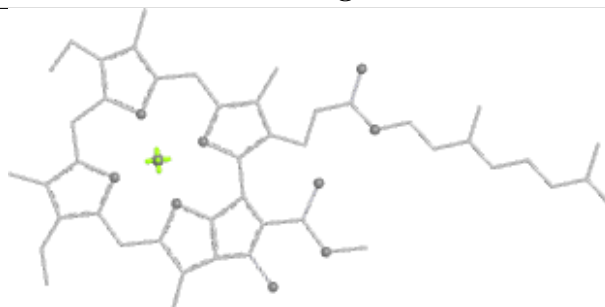
Bond lengths



Bond angles

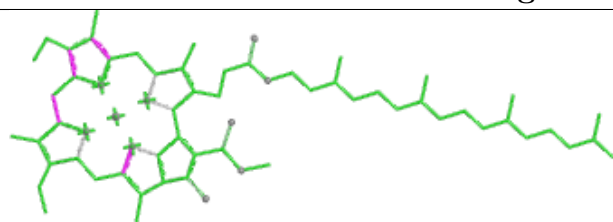


Torsions

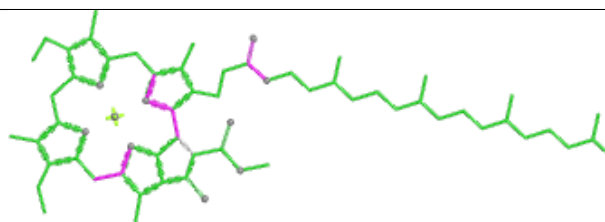


Rings

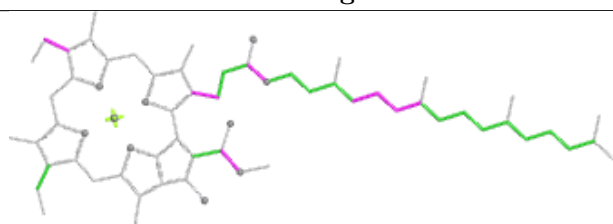
Ligand CLA v 511



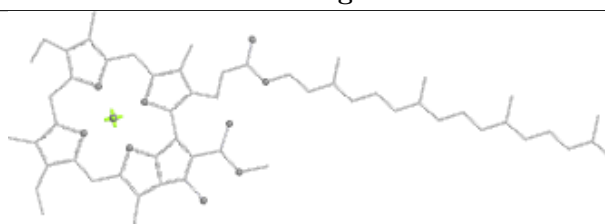
Bond lengths



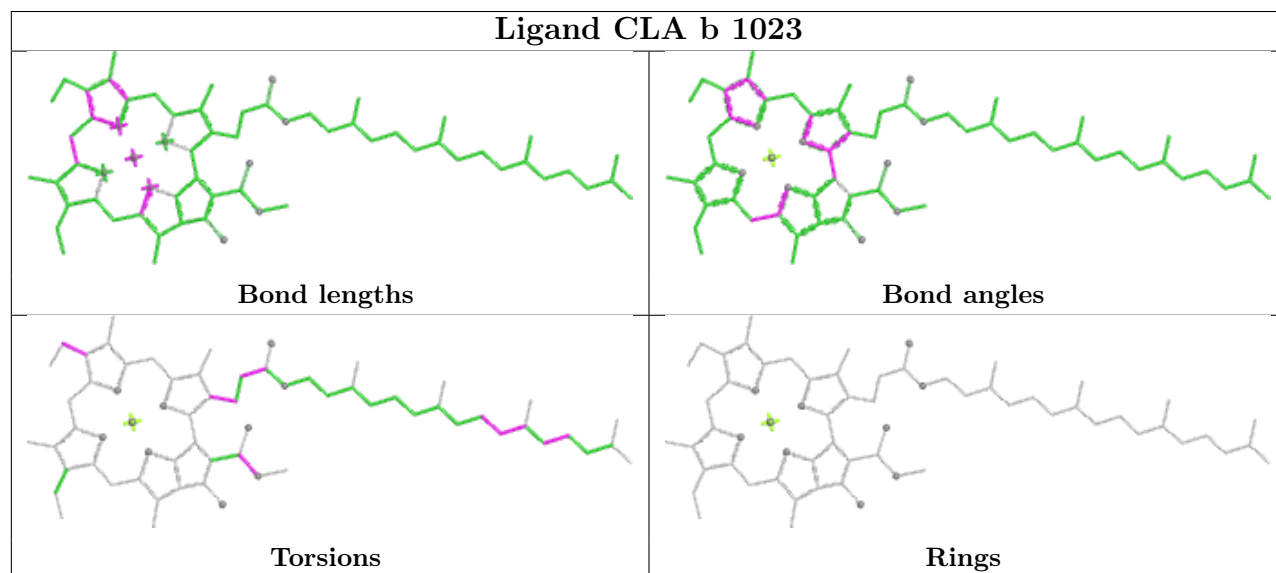
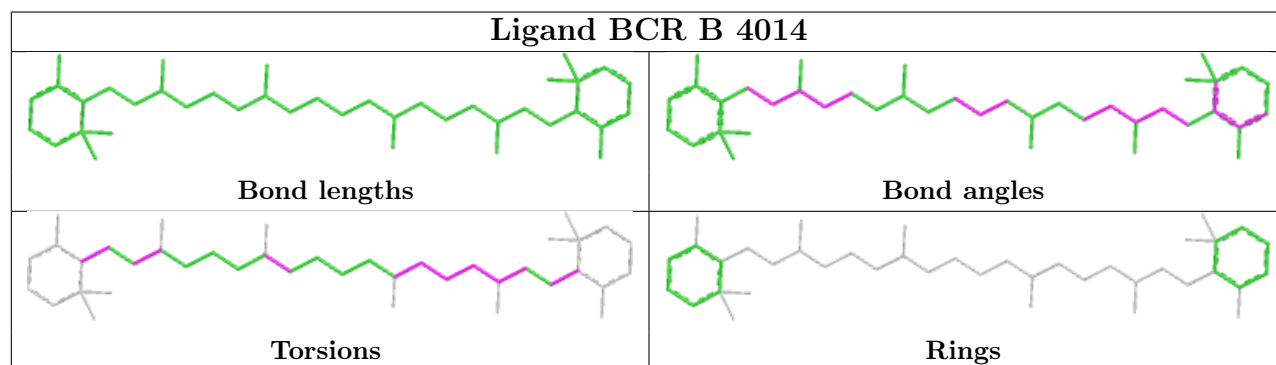
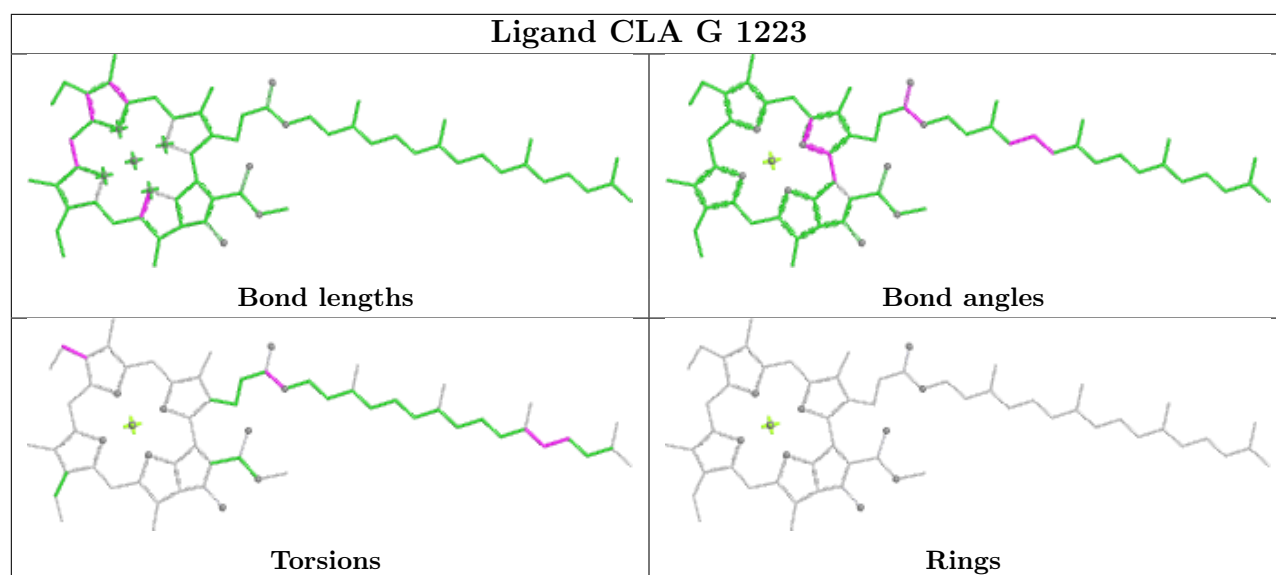
Bond angles



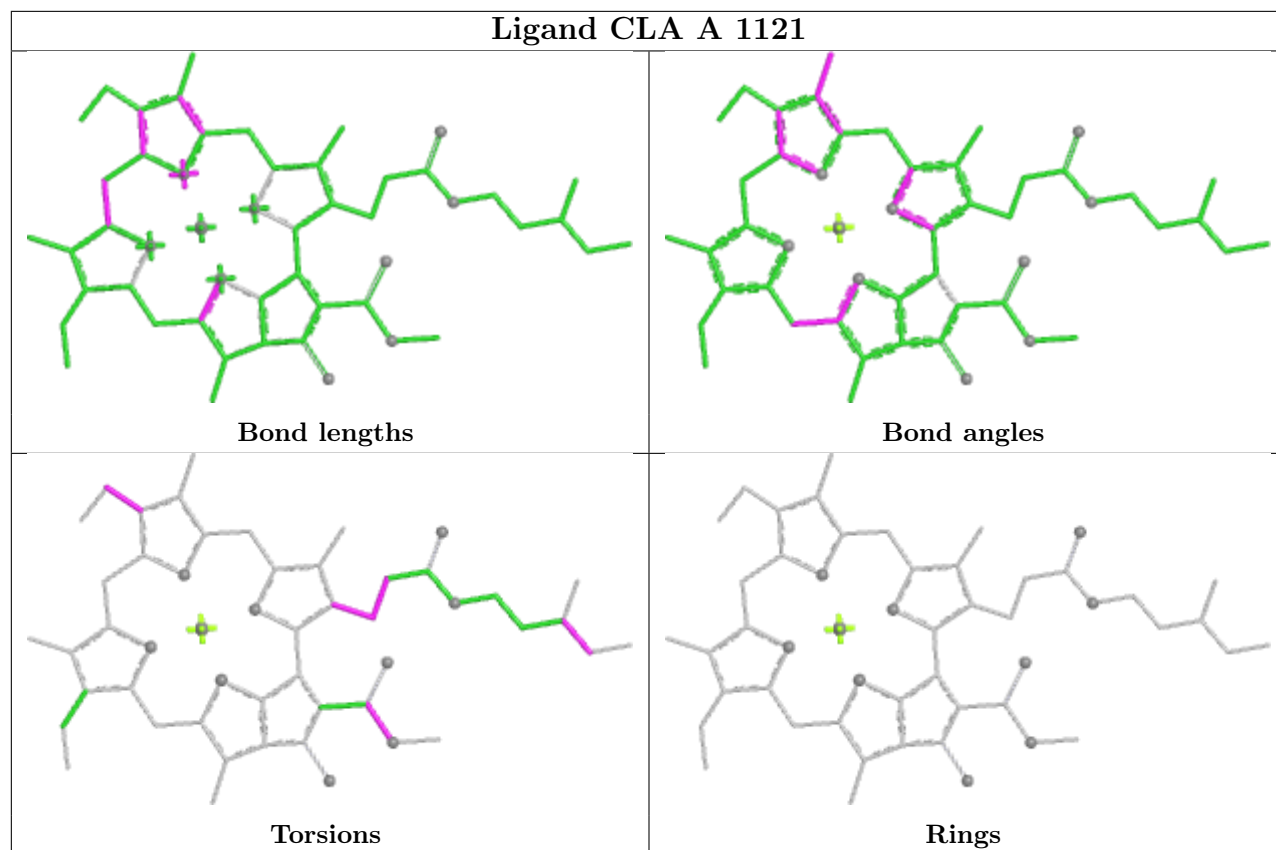
Torsions



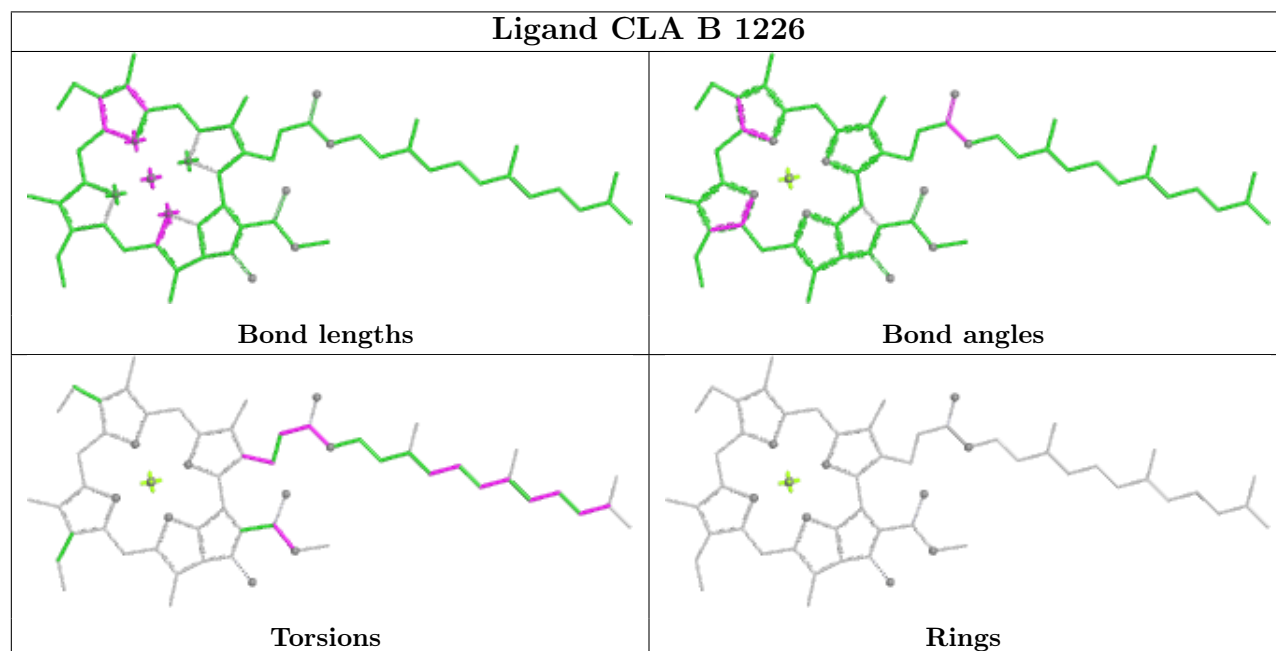
Rings

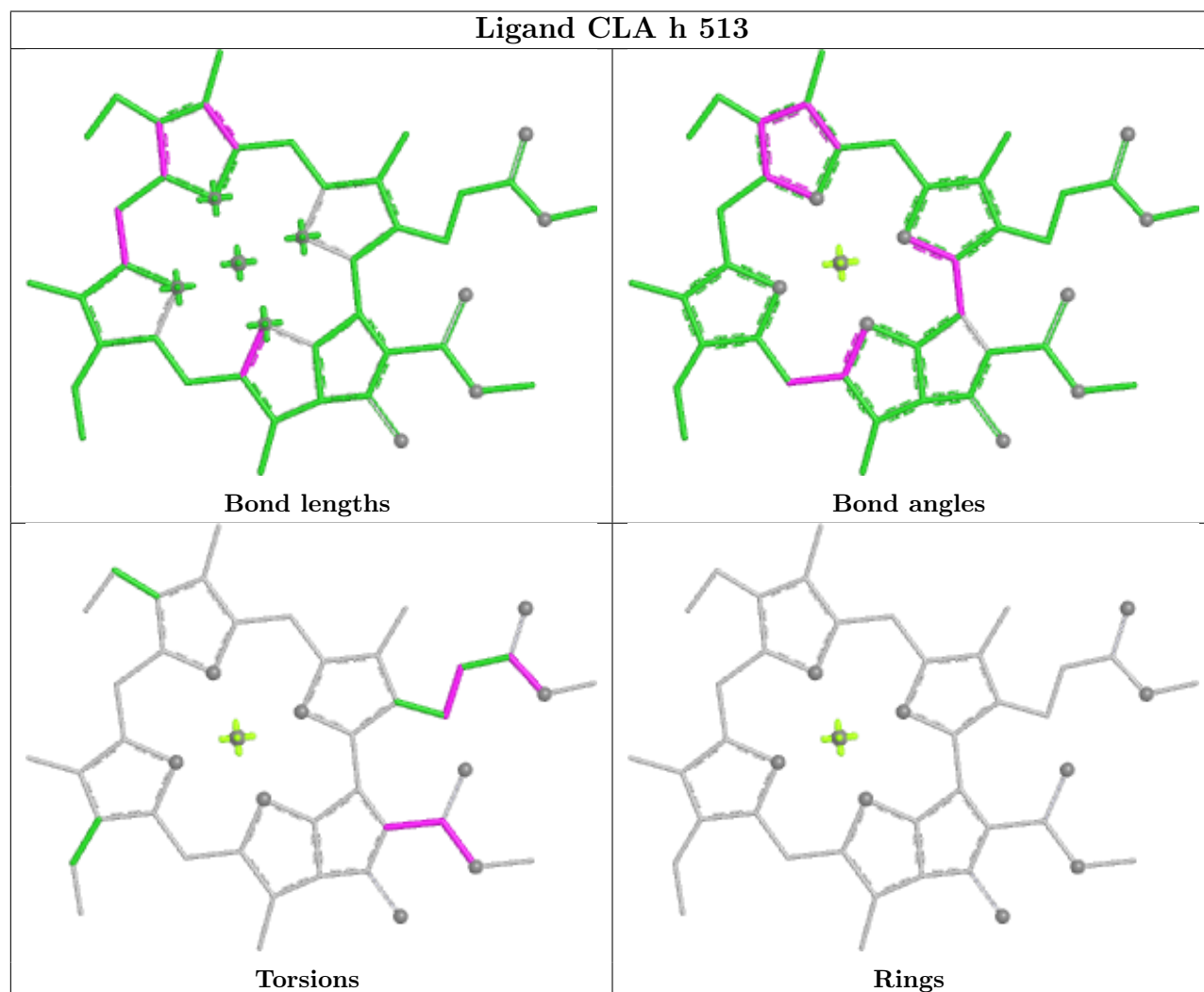
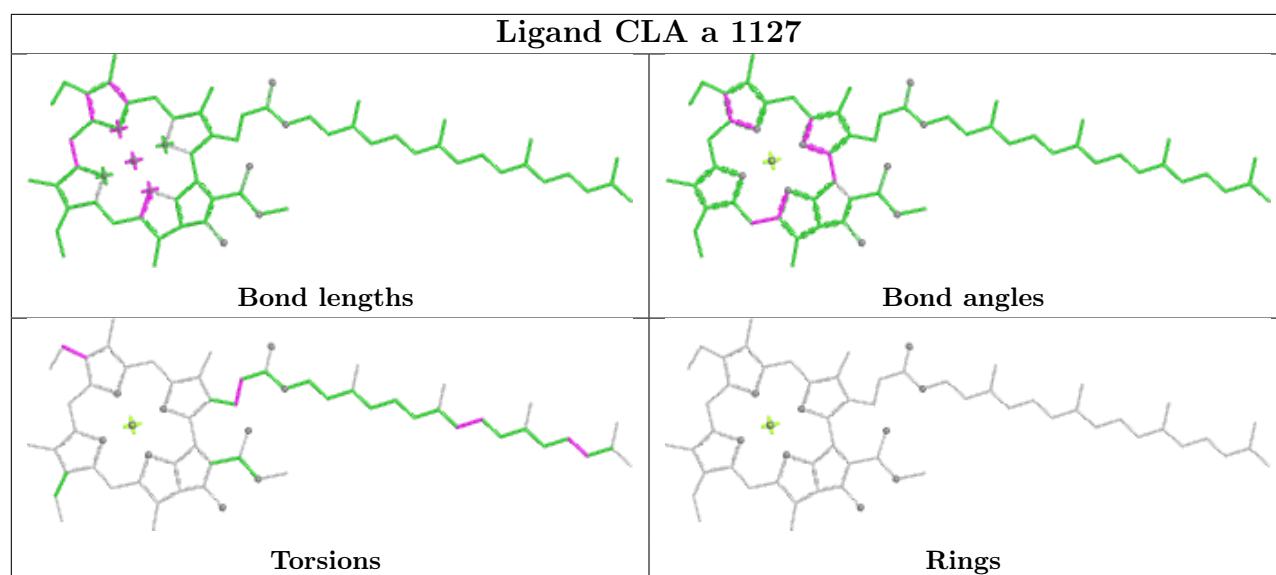


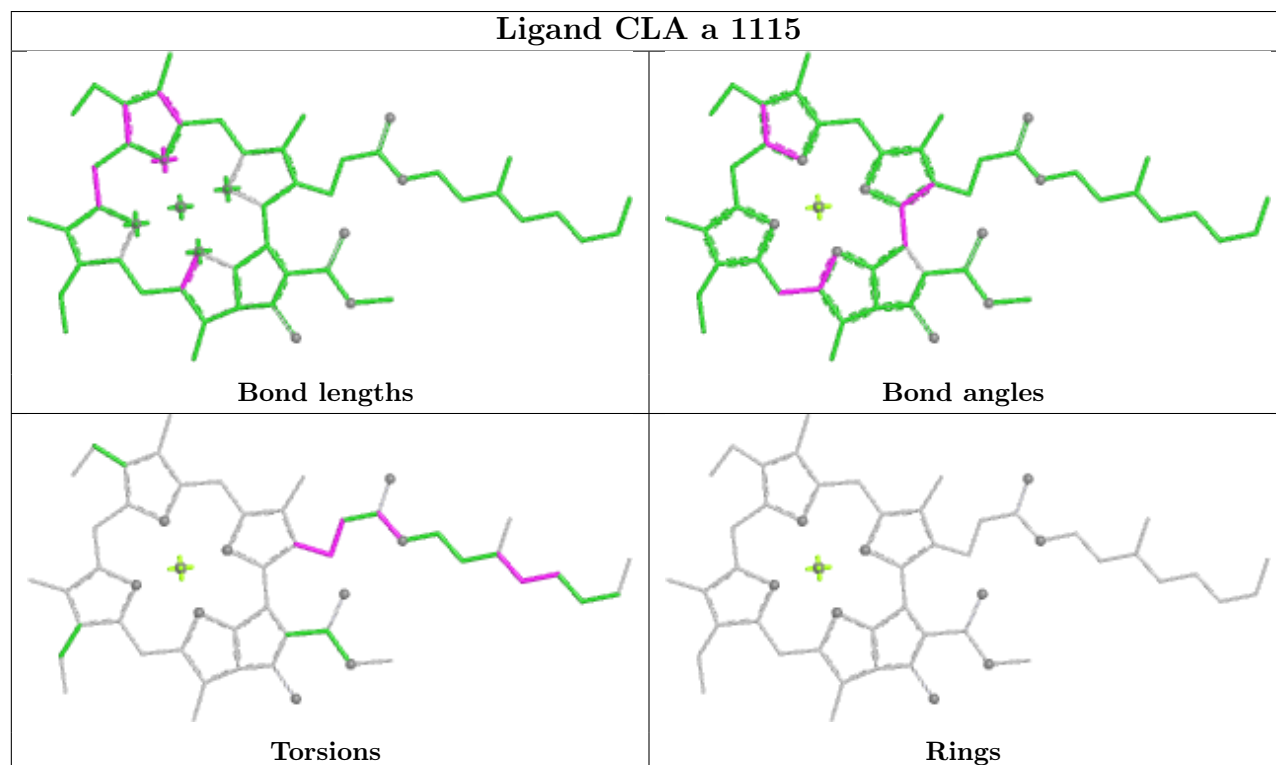
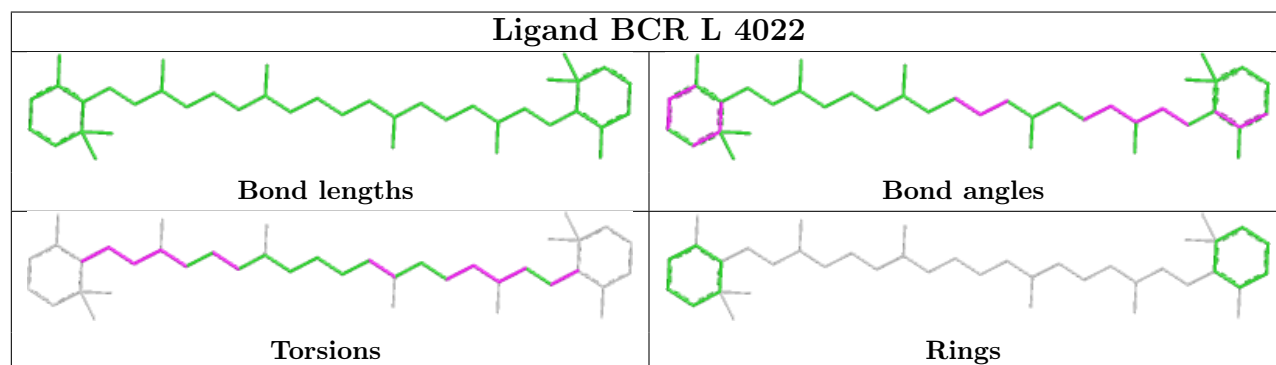
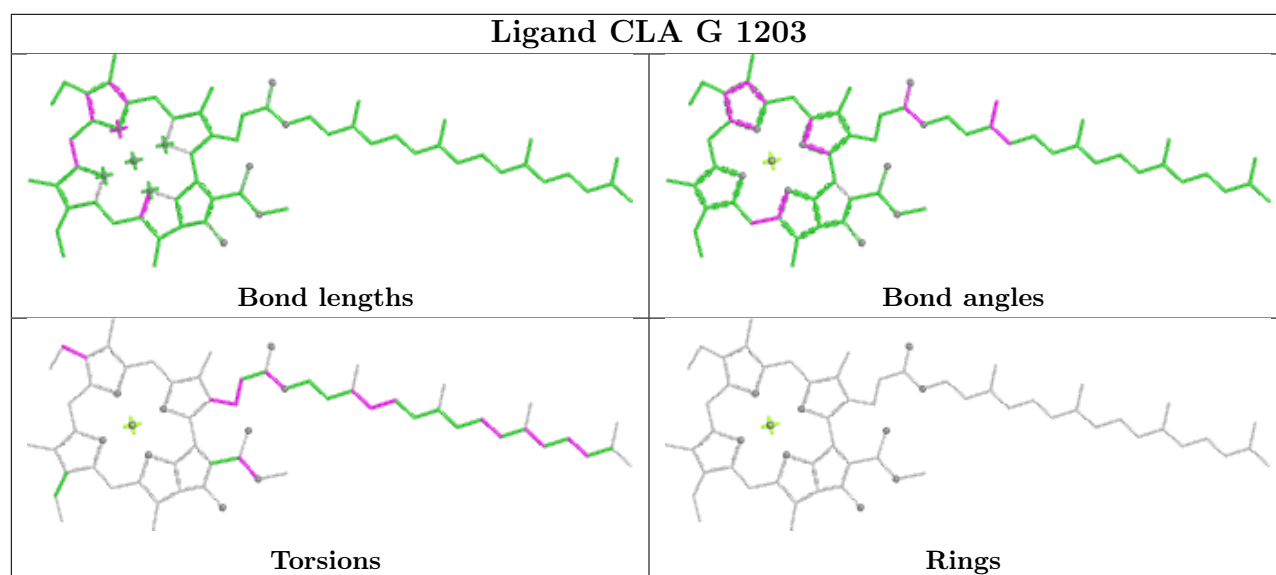
Ligand CLA A 1121

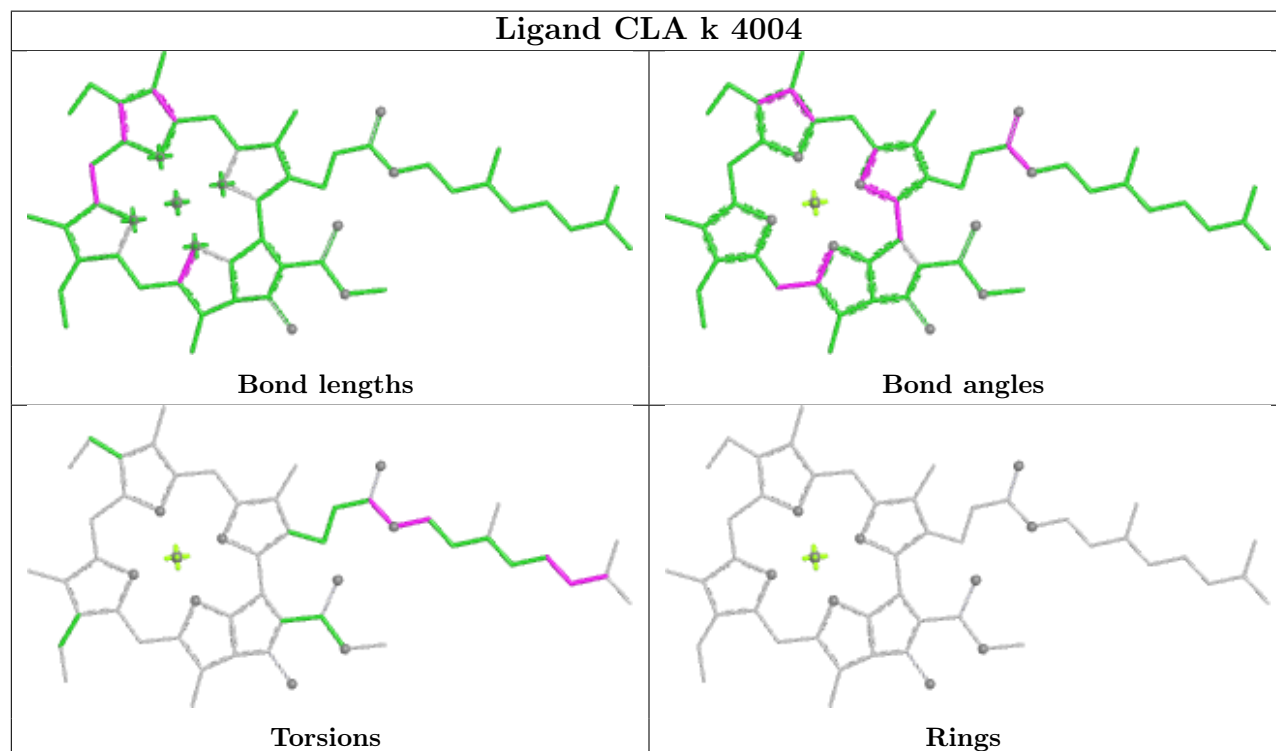
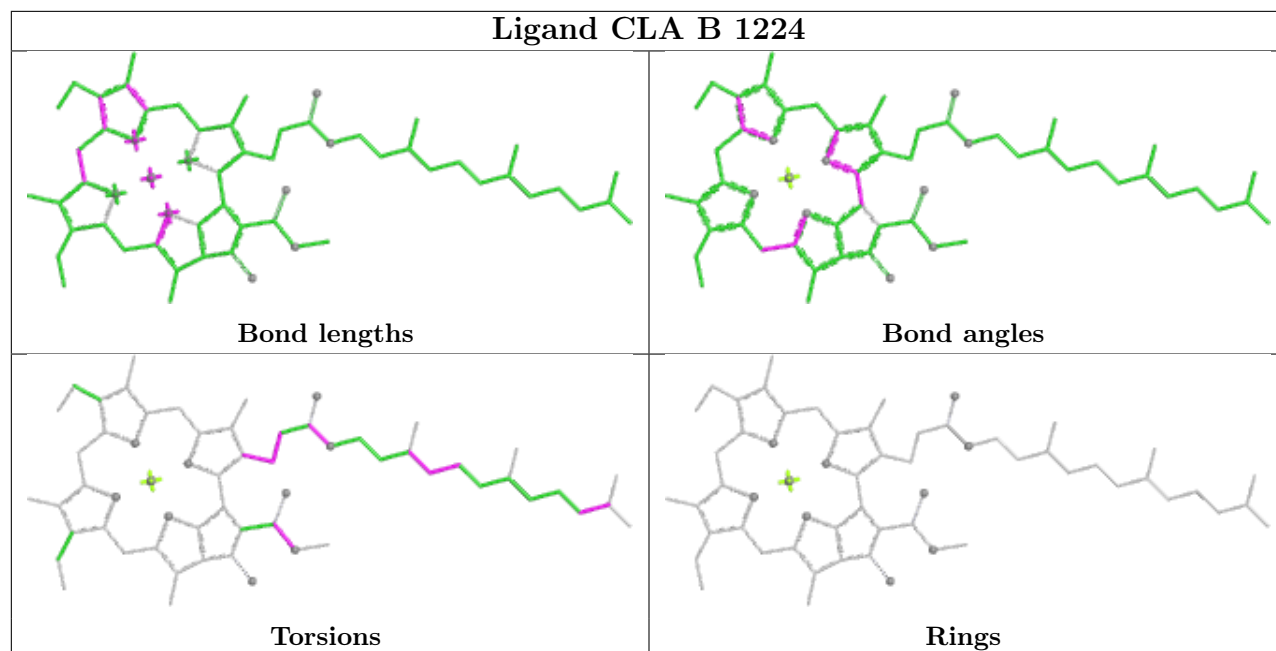


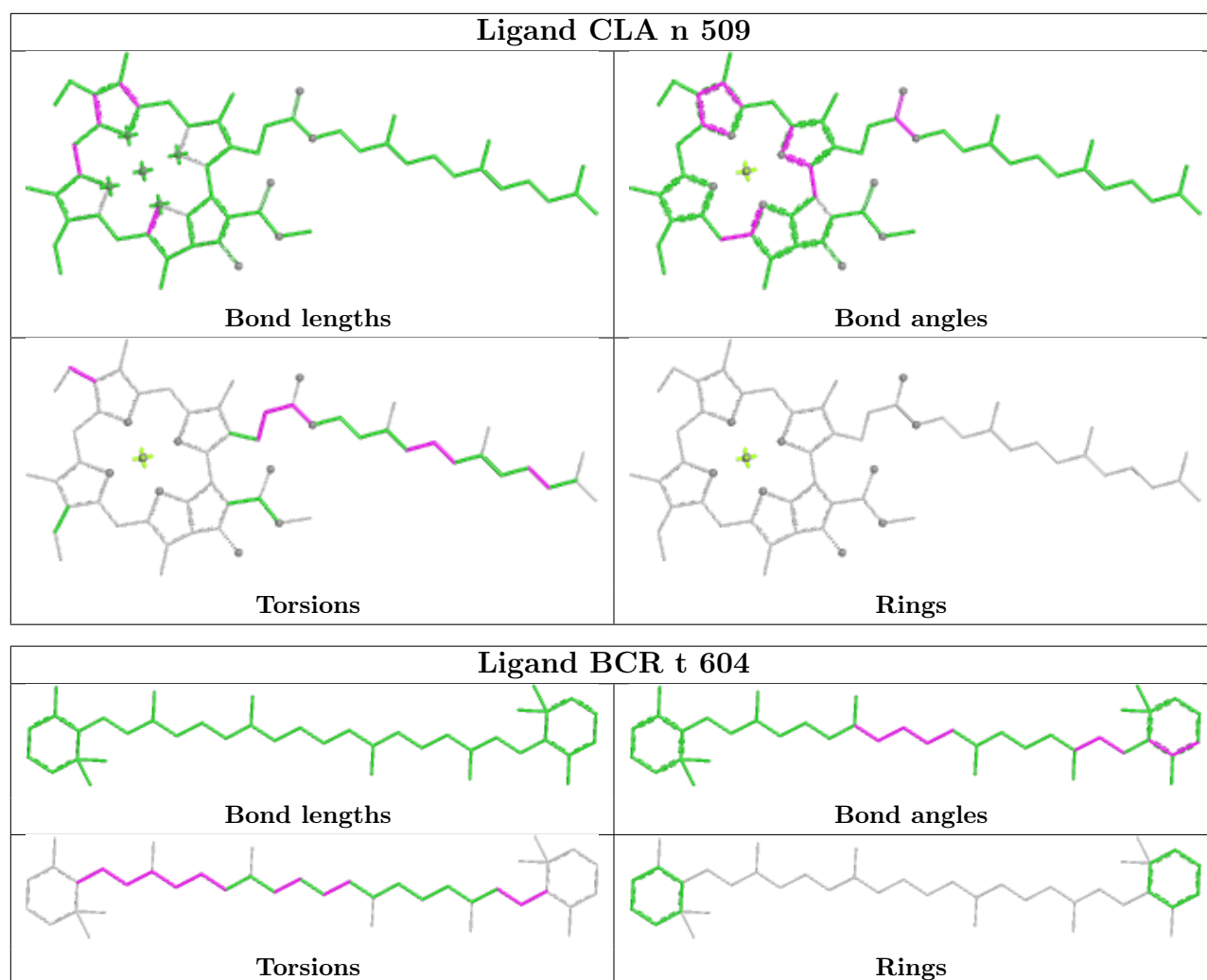
Ligand CLA B 1226



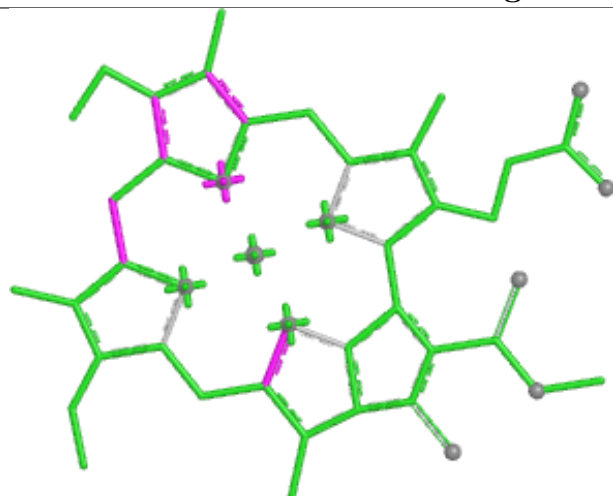




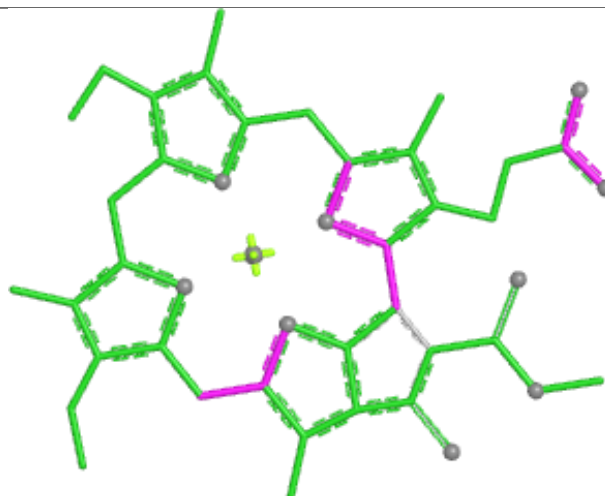




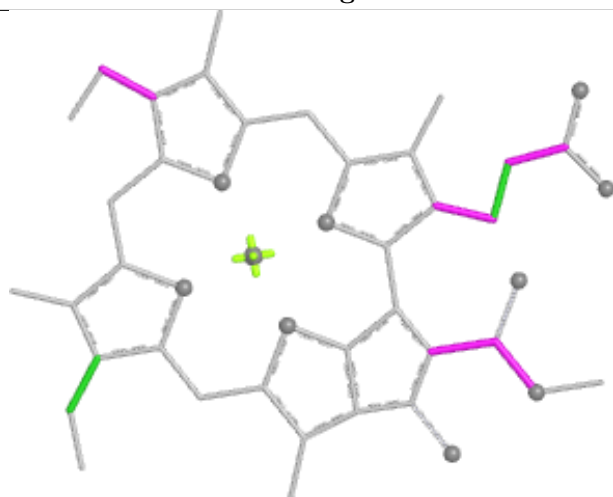
Ligand CLA G 1212



Bond lengths



Bond angles

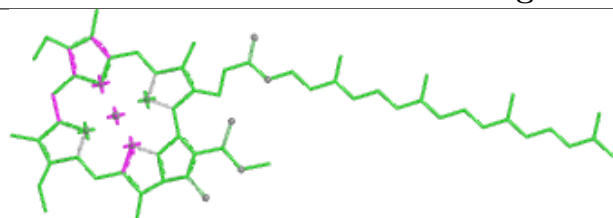


Torsions

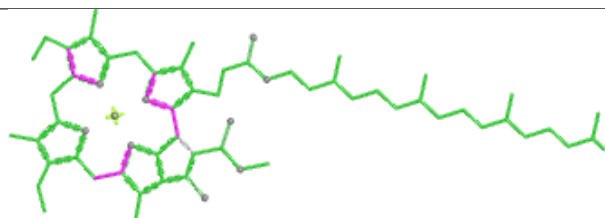


Rings

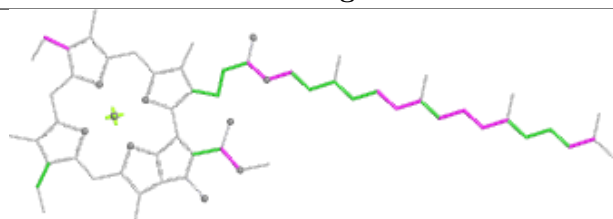
Ligand CLA Z 512



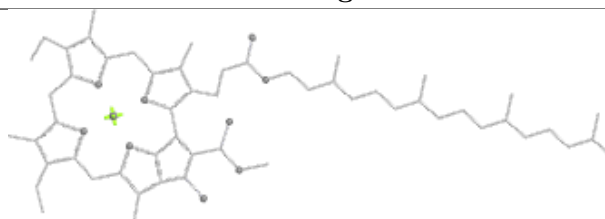
Bond lengths



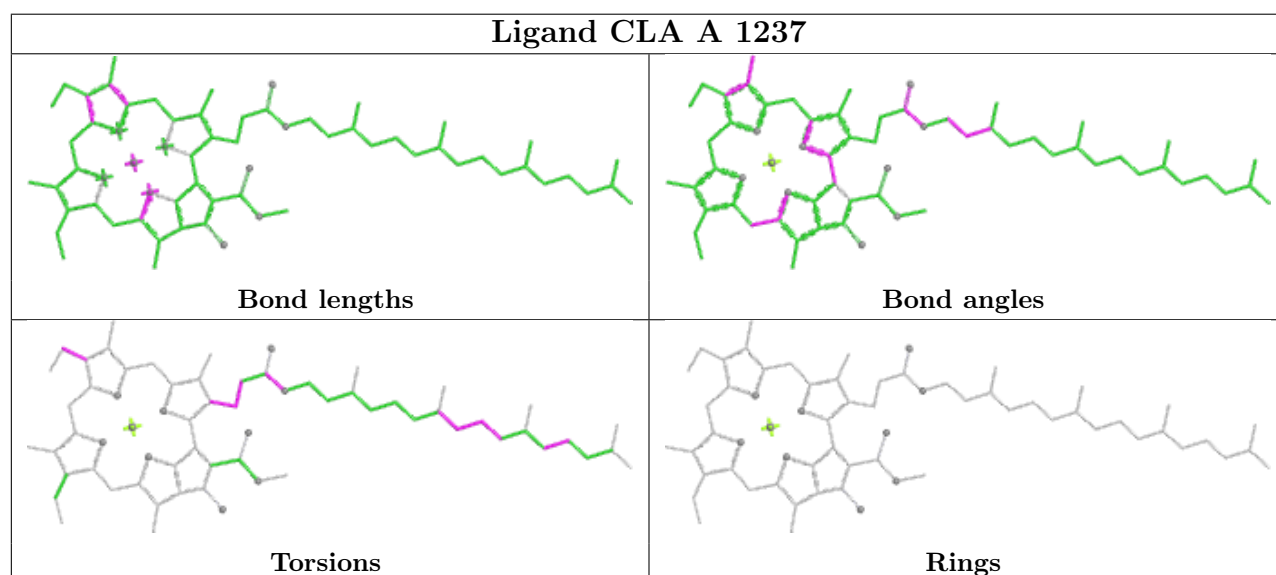
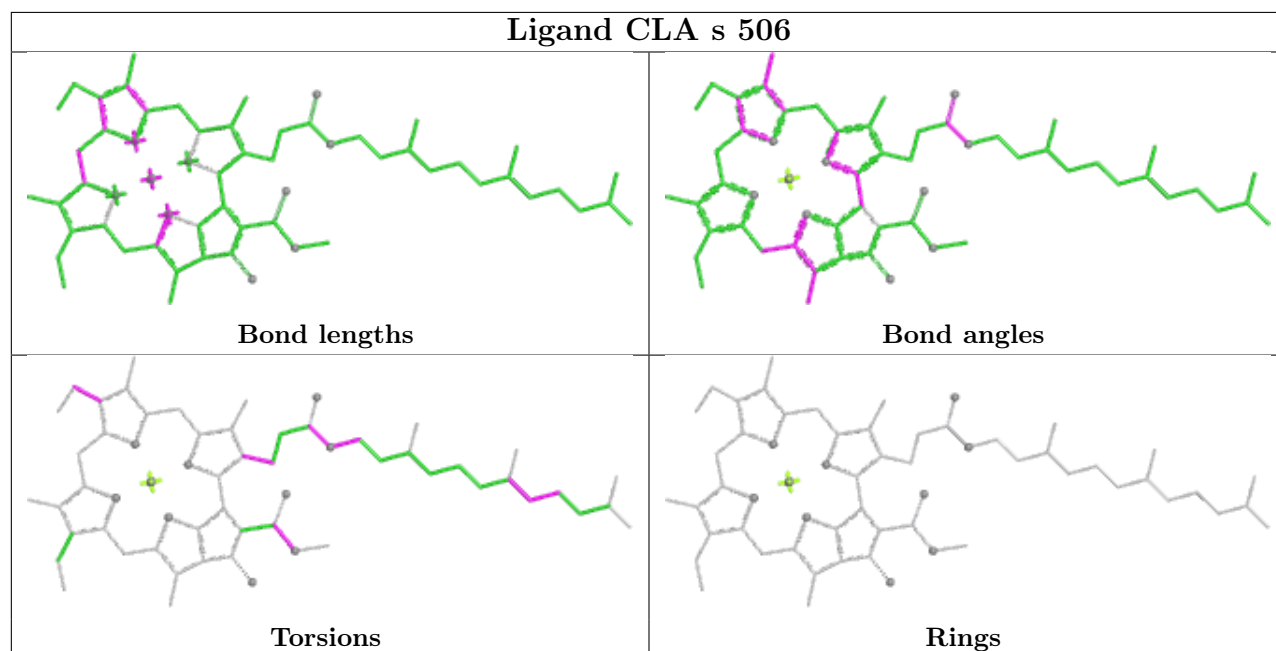
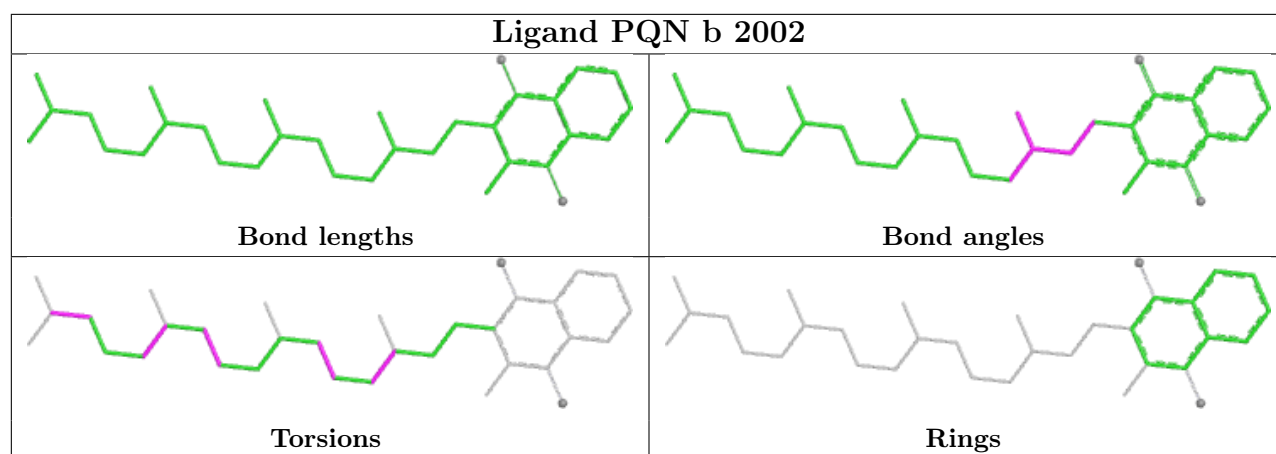
Bond angles

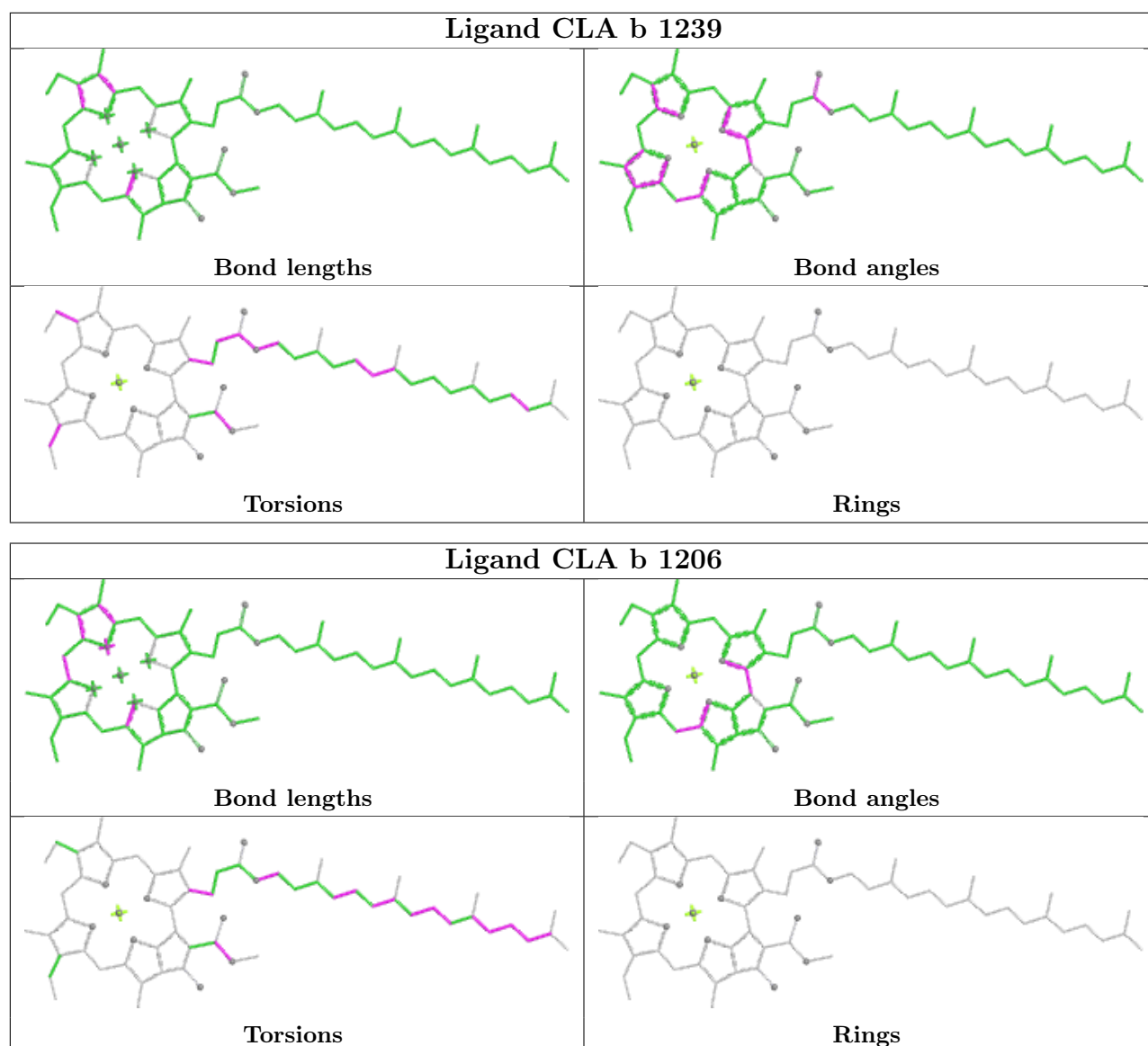


Torsions

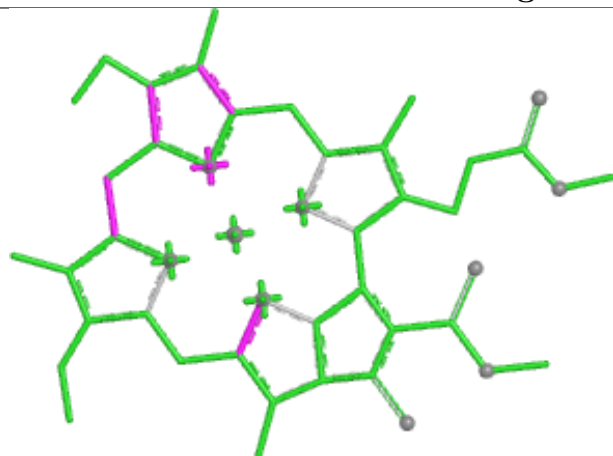


Rings

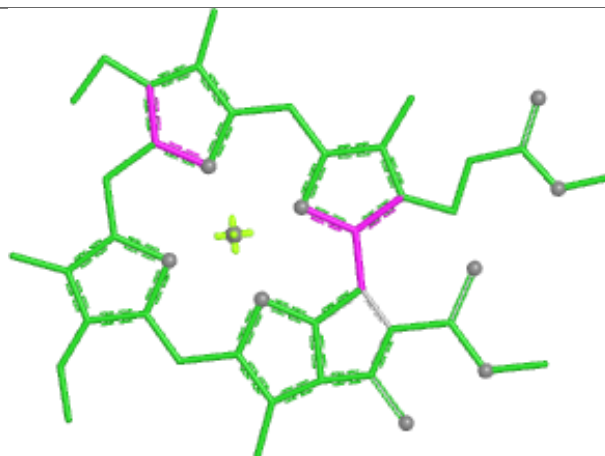




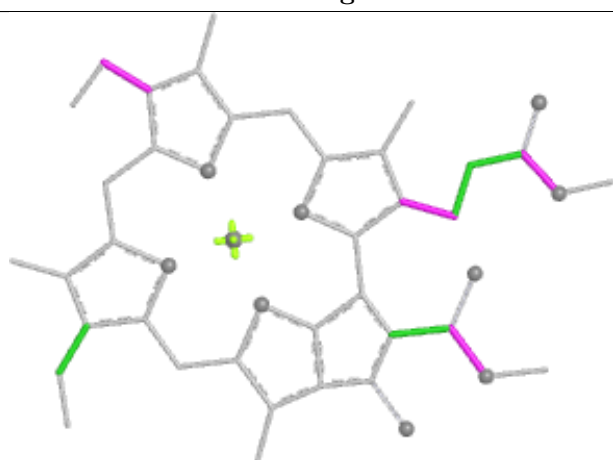
Ligand CLA u 513



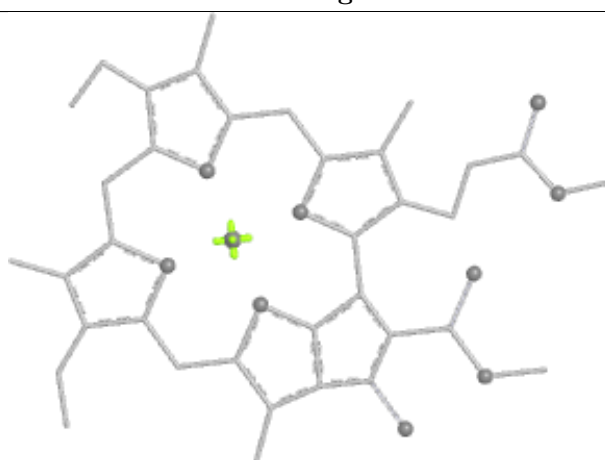
Bond lengths



Bond angles

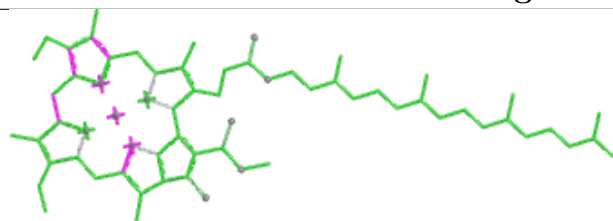


Torsions

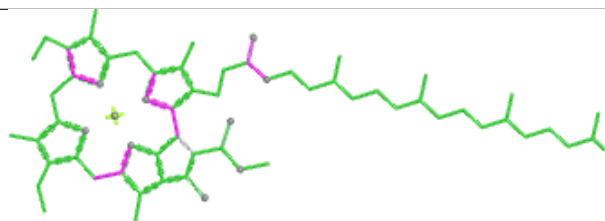


Rings

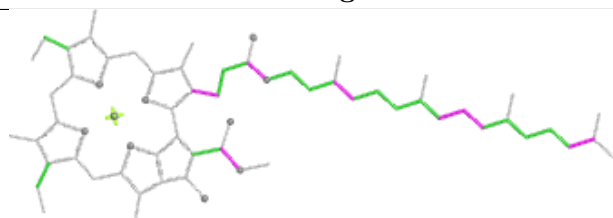
Ligand CLA w 512



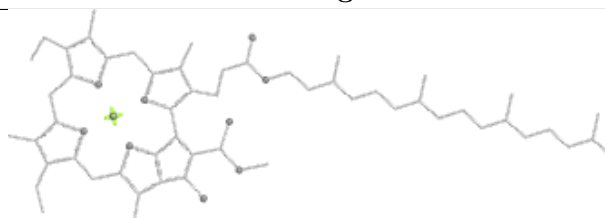
Bond lengths



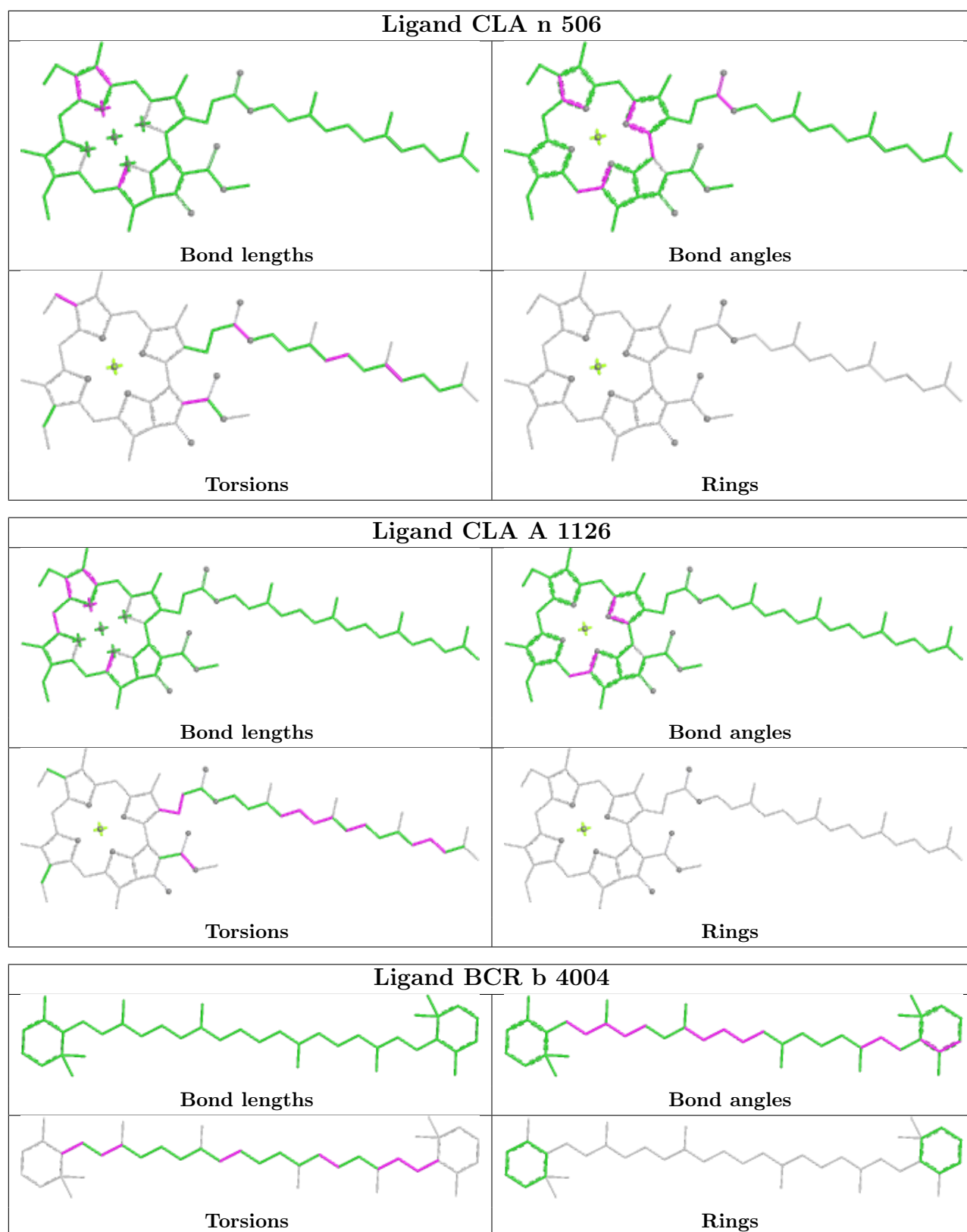
Bond angles

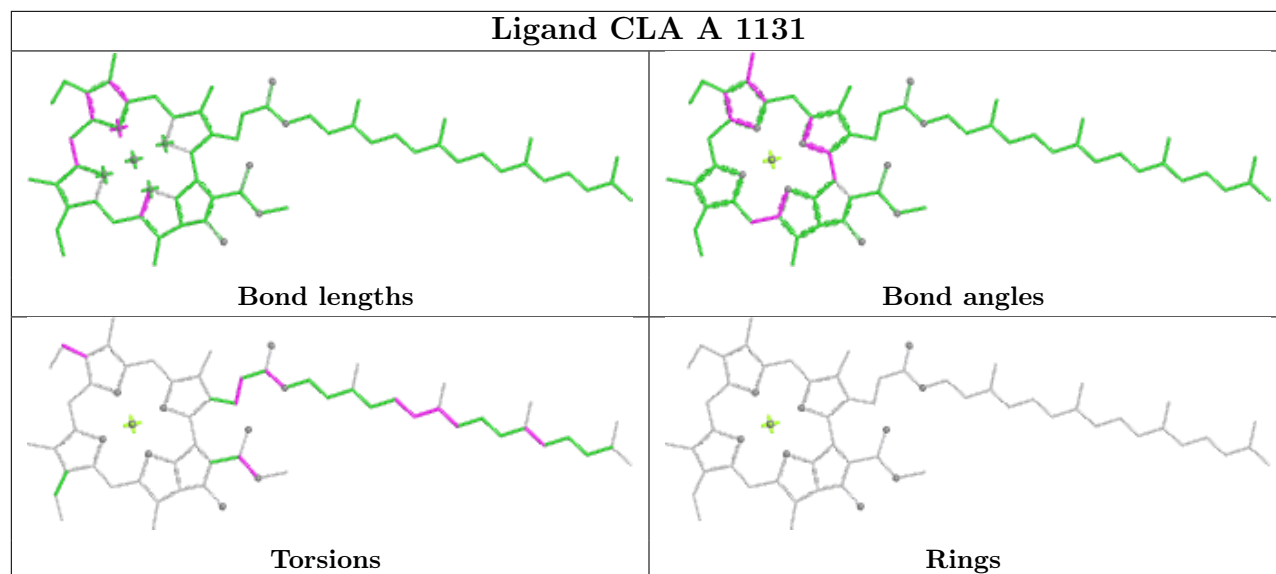
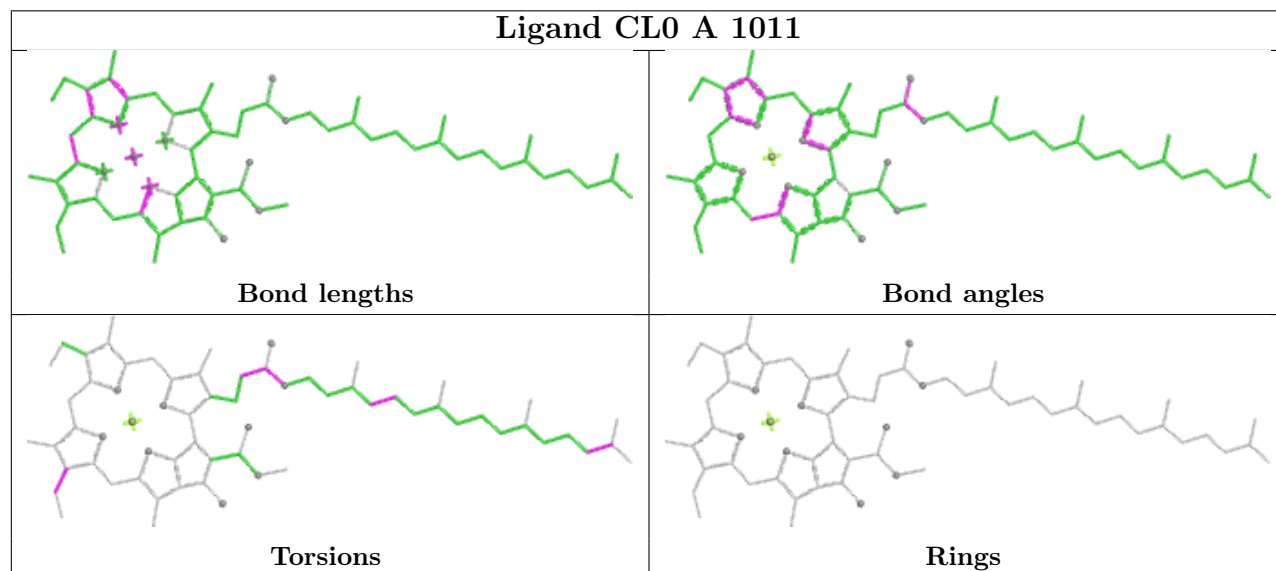


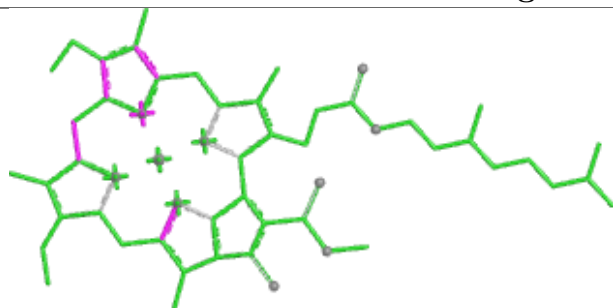
Torsions



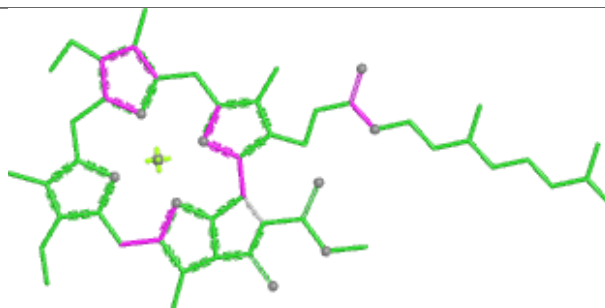
Rings



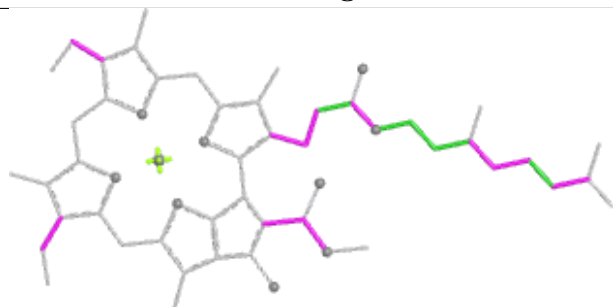
Ligand CLA A 1131**Ligand CL0 A 1011**

Ligand CLA v 517

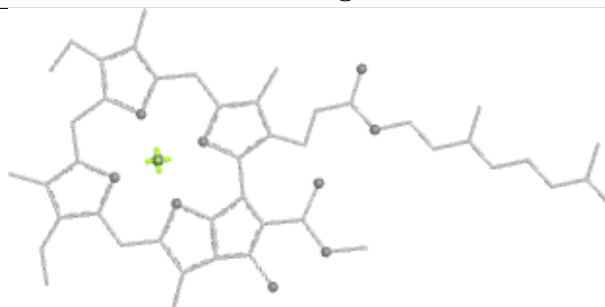
Bond lengths



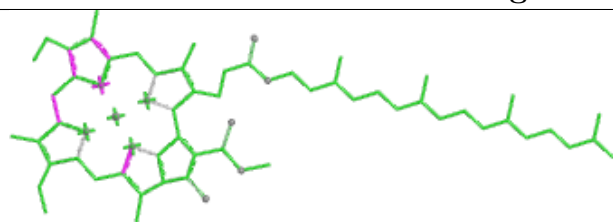
Bond angles



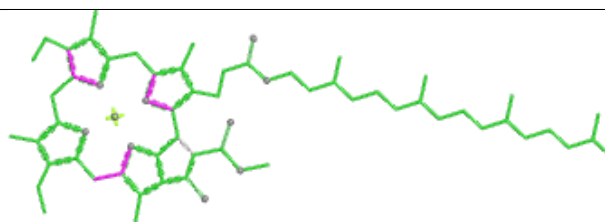
Torsions



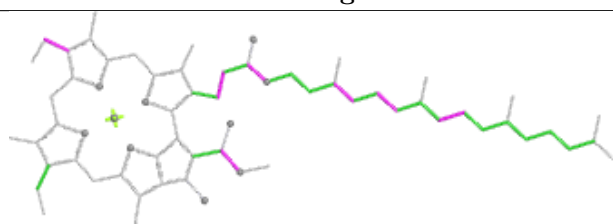
Rings

Ligand CLA a 1136

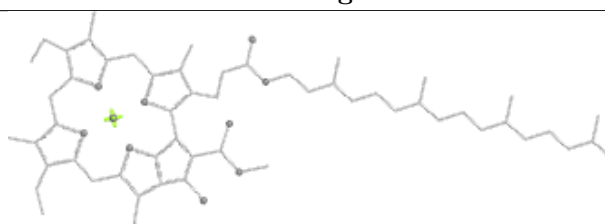
Bond lengths



Bond angles

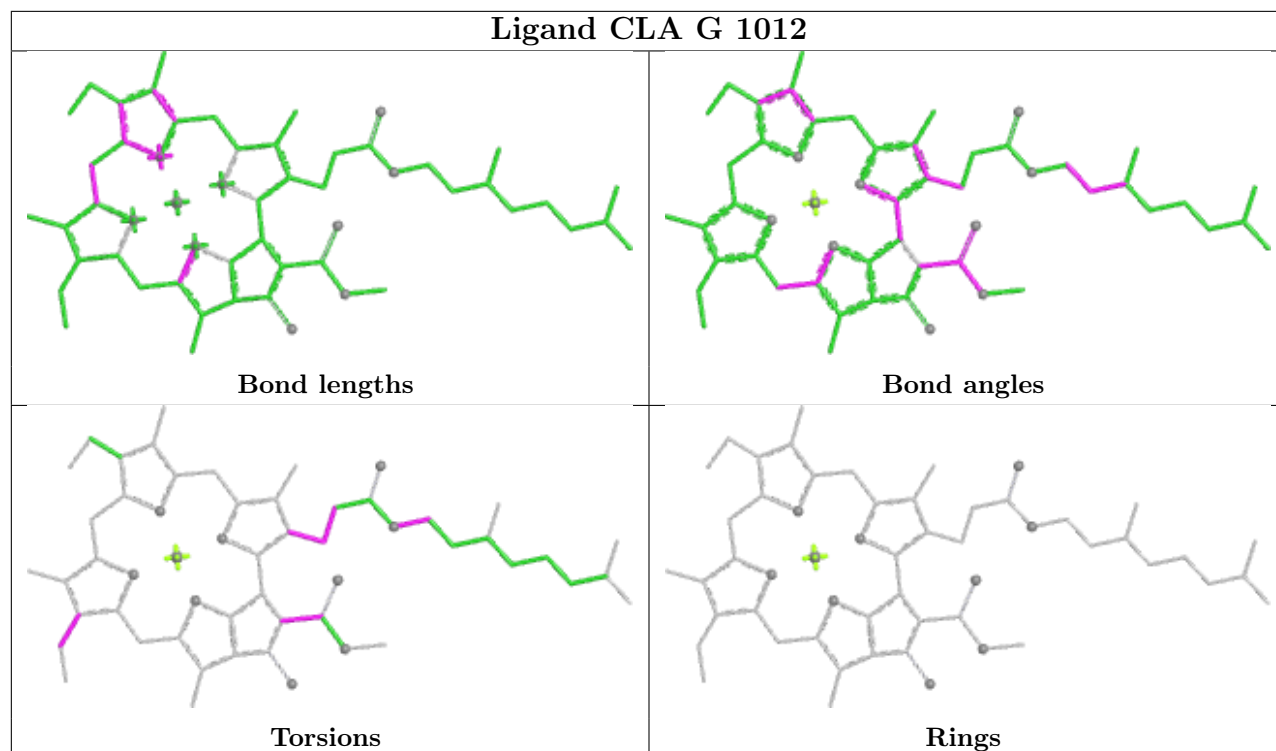


Torsions

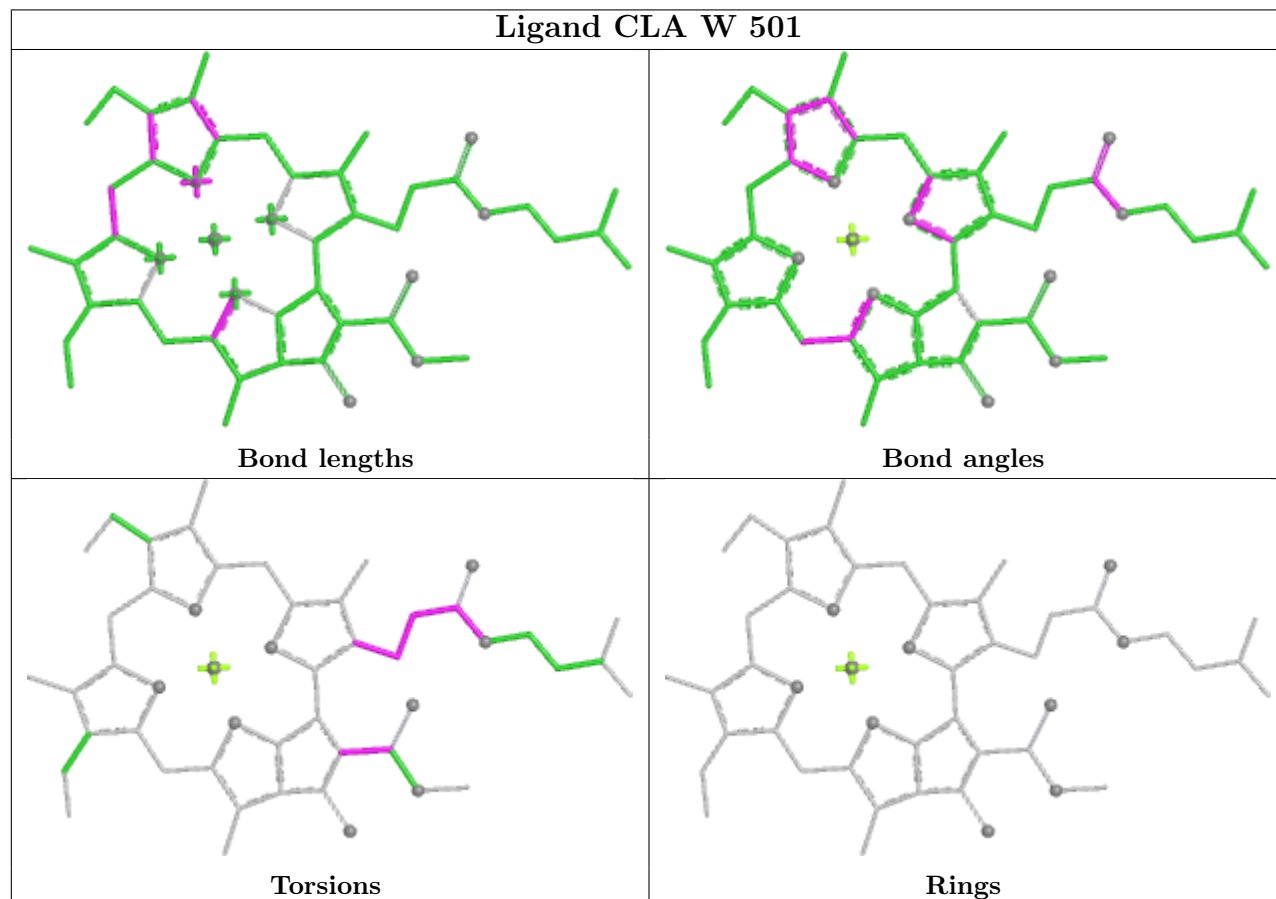


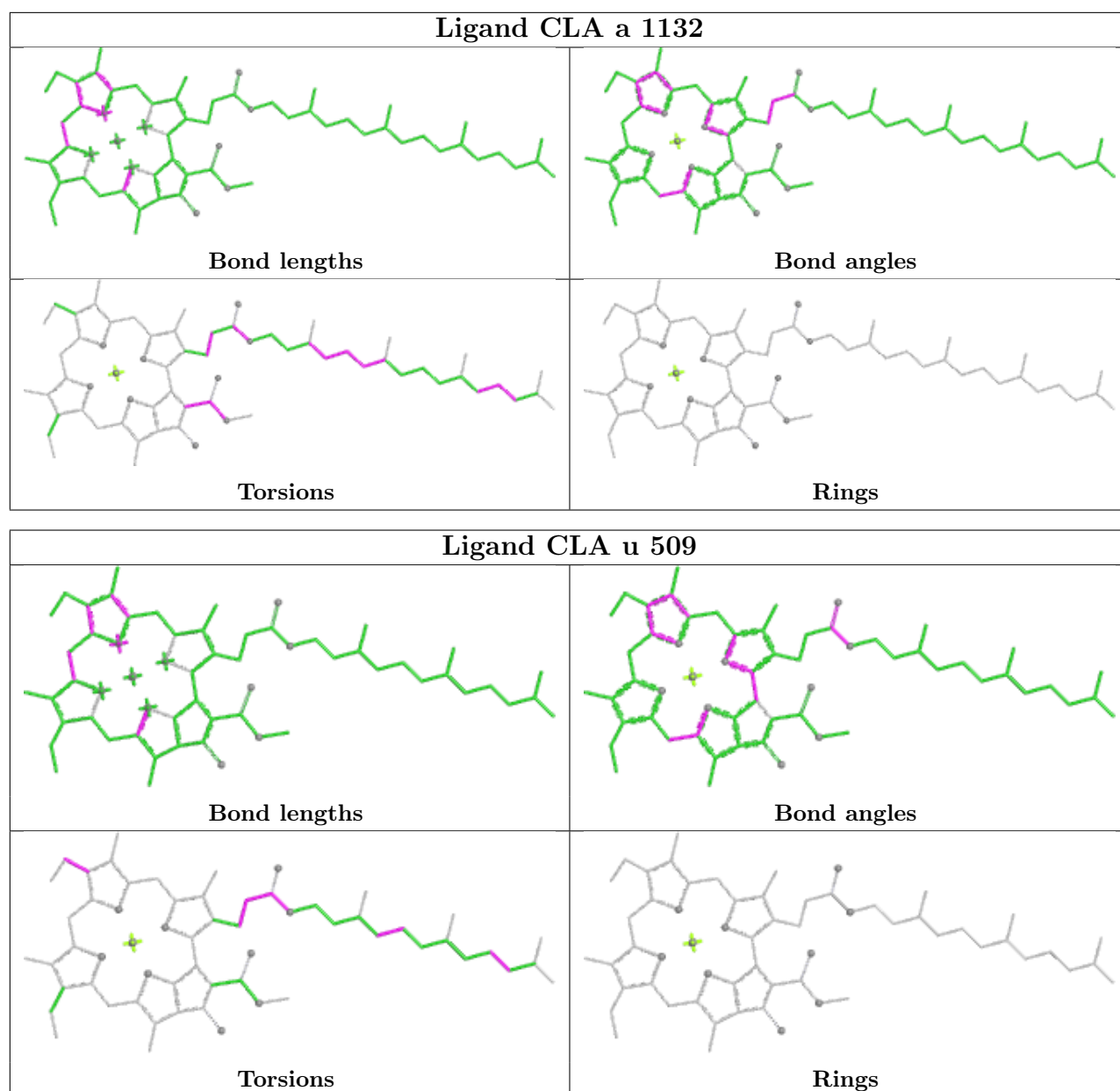
Rings

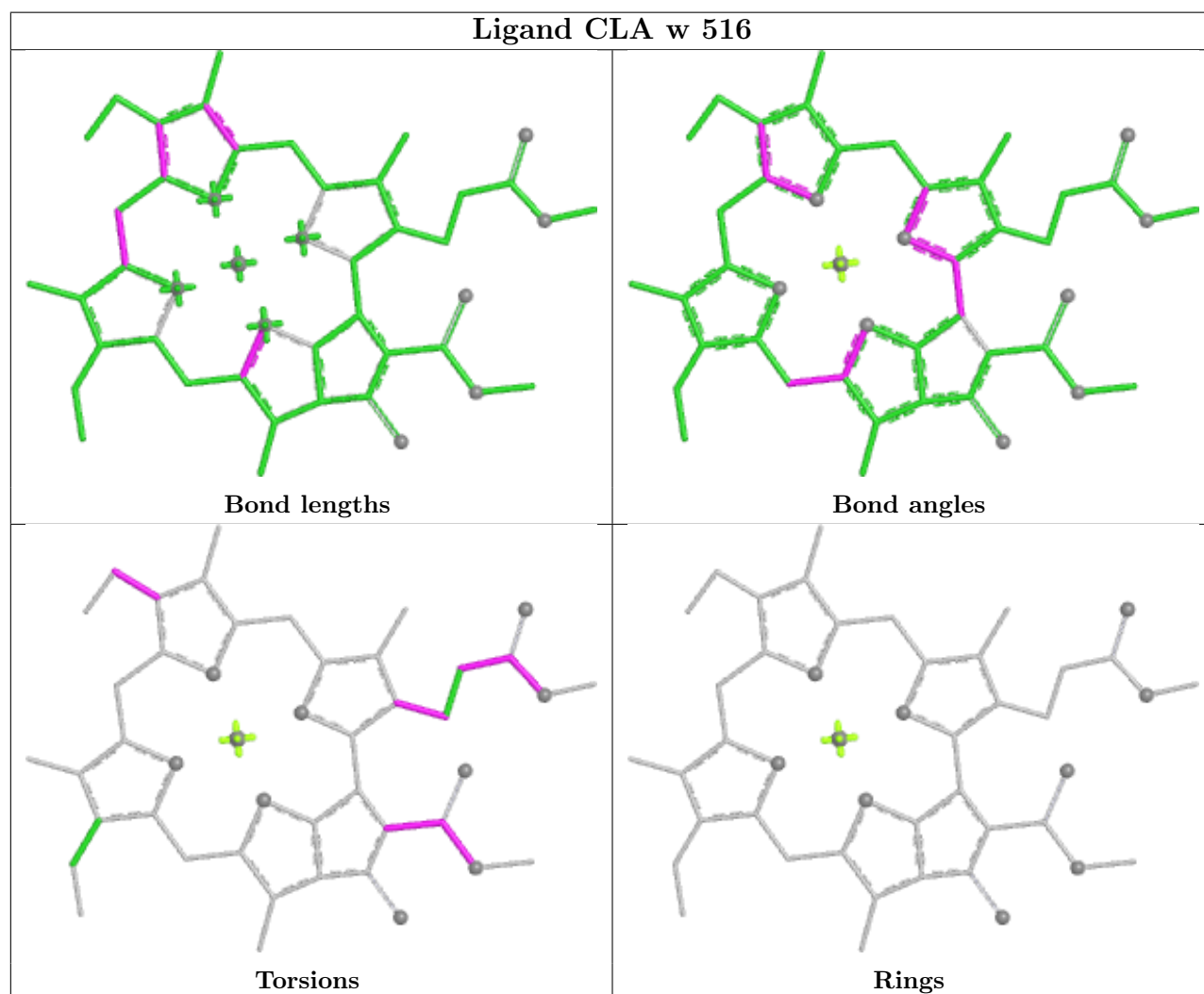
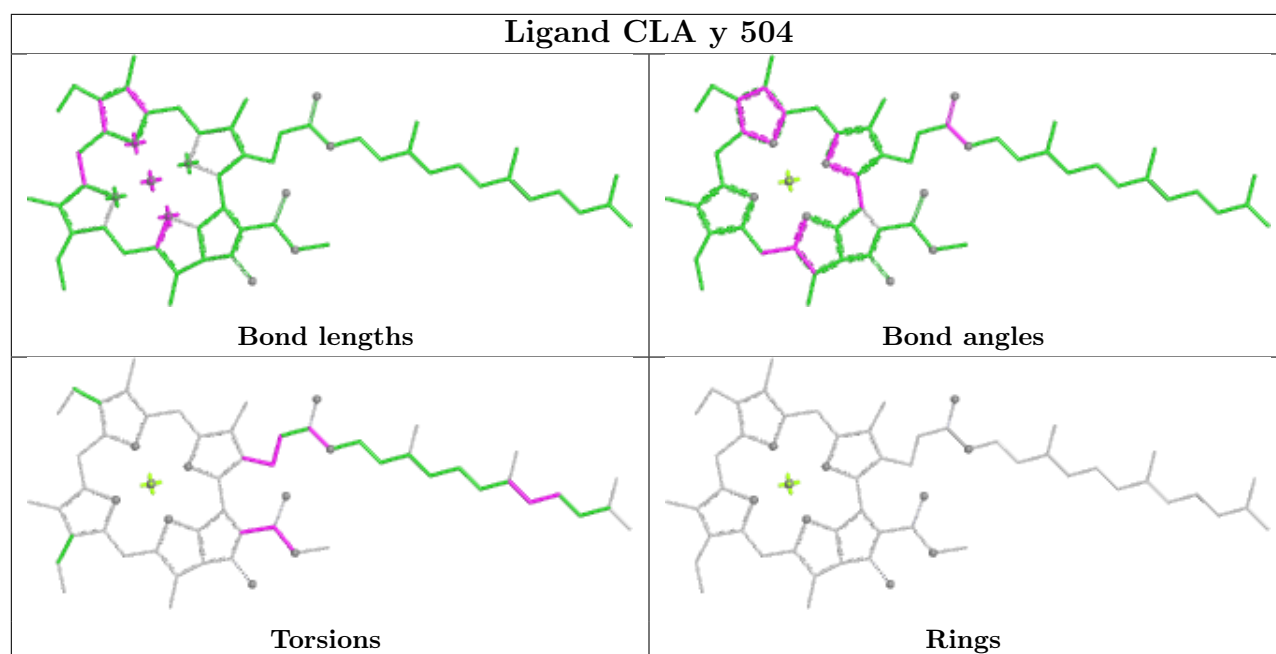
Ligand CLA G 1012



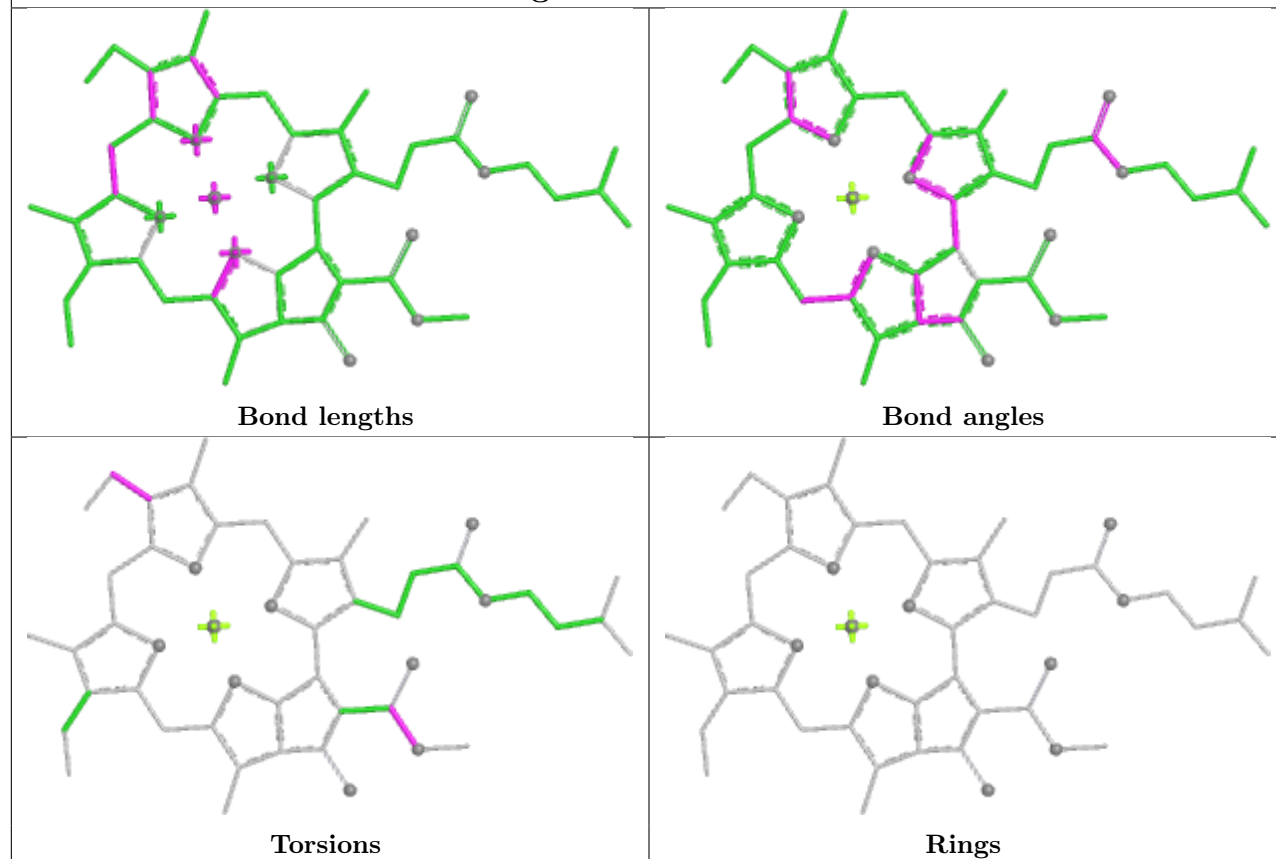
Ligand CLA W 501



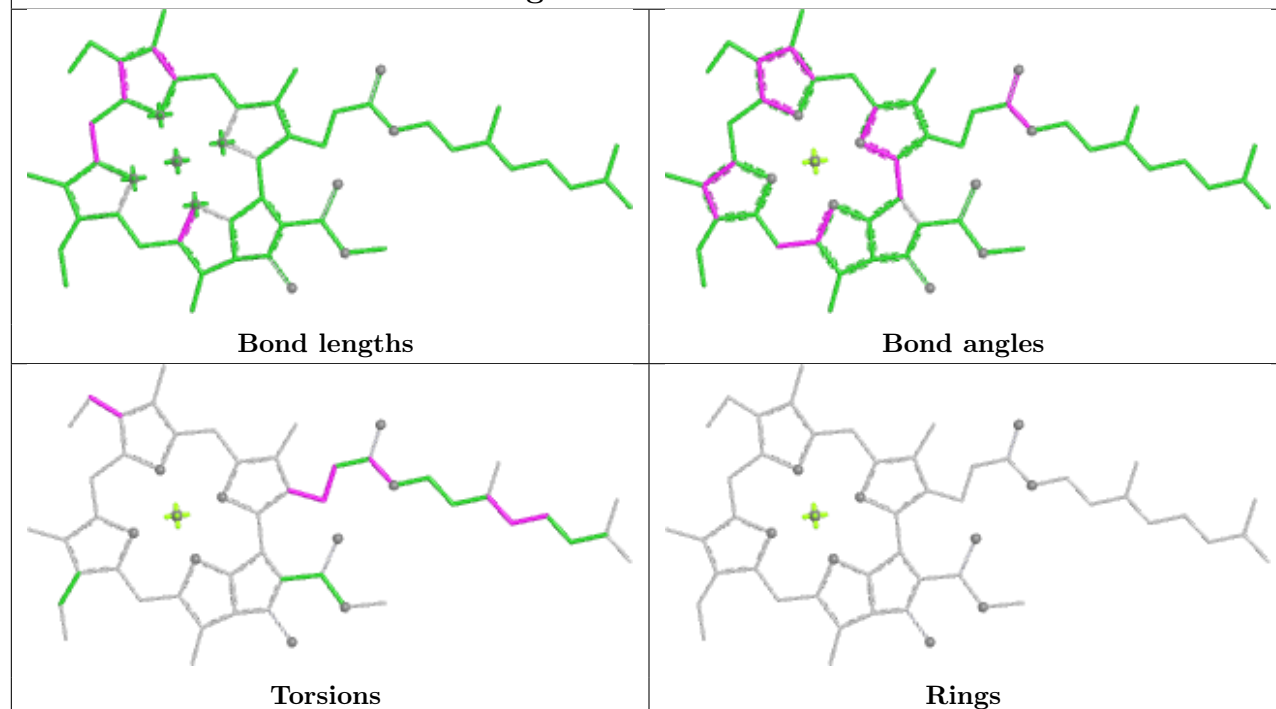




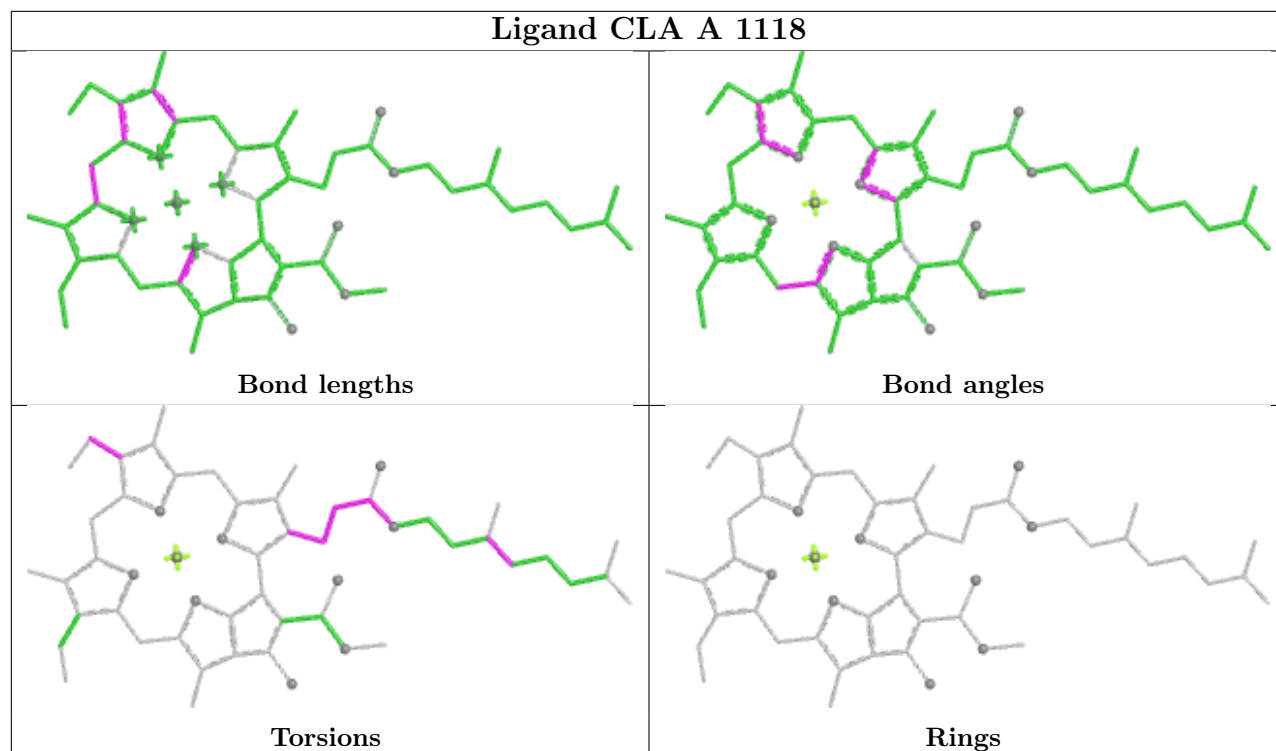
Ligand CLA X 514



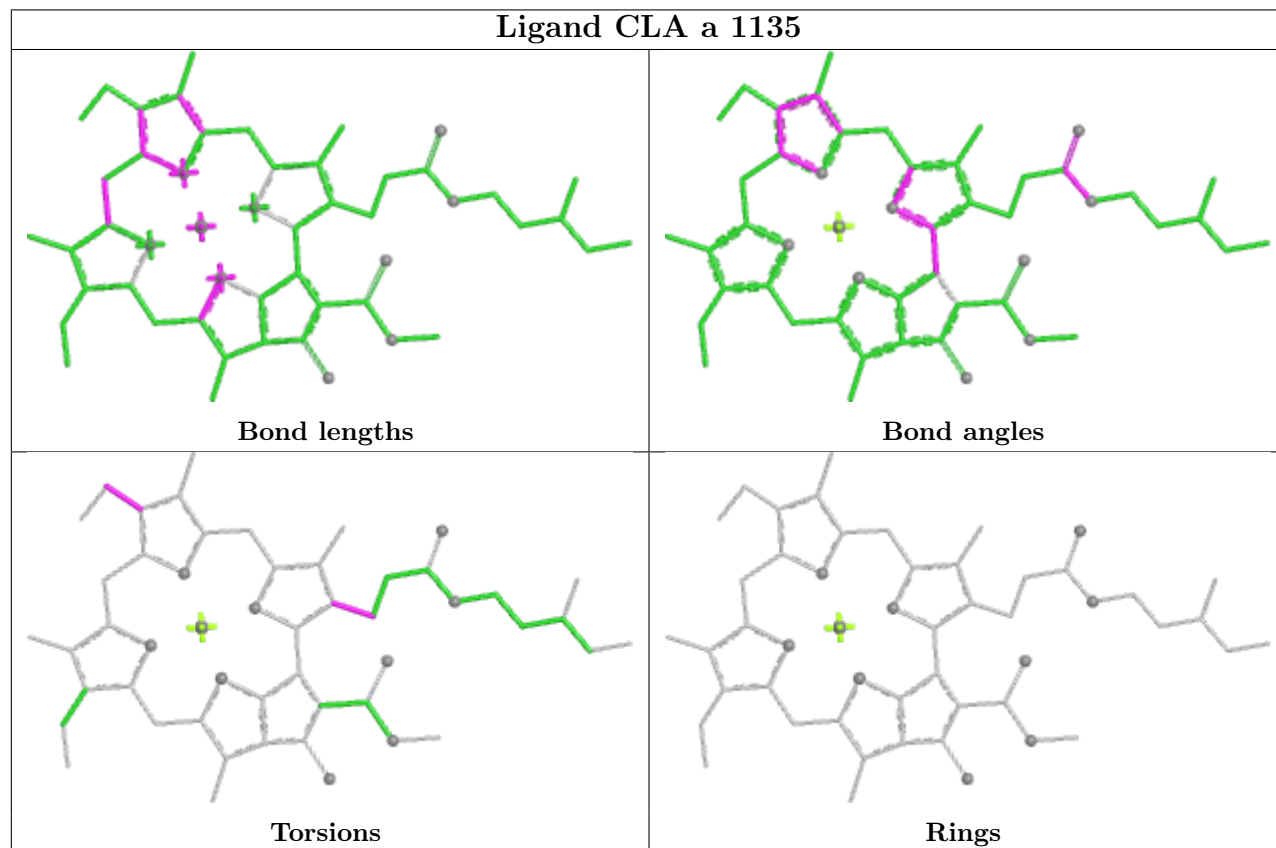
Ligand CLA b 1218

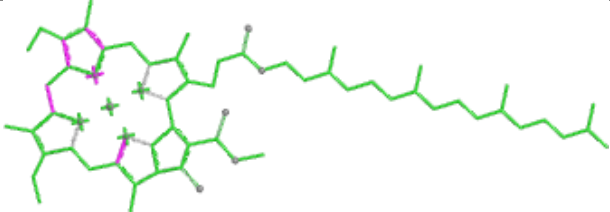
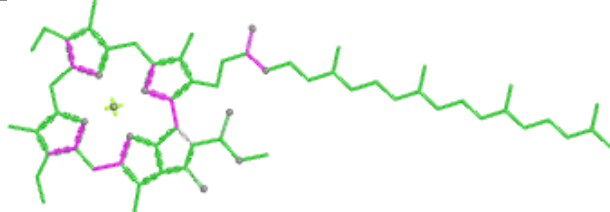
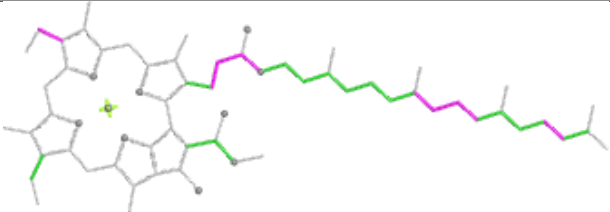
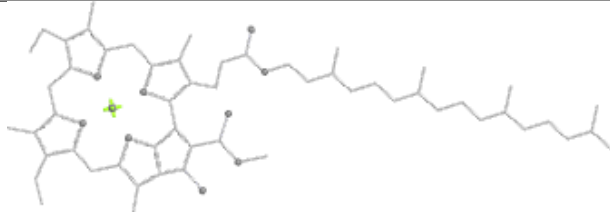
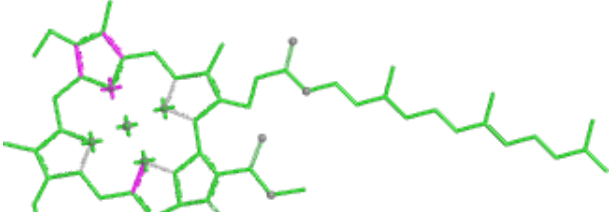
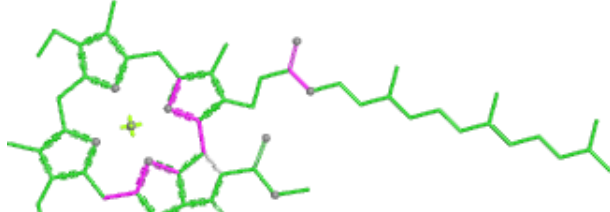
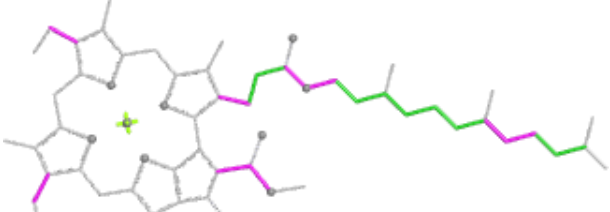
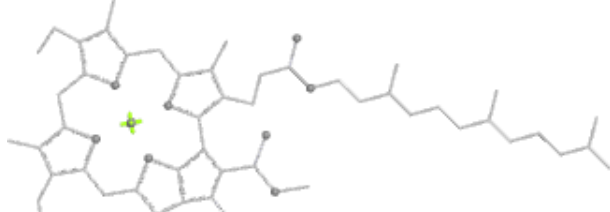
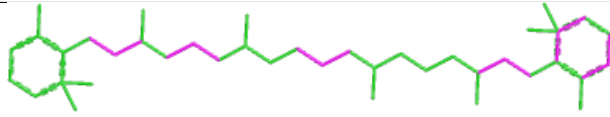
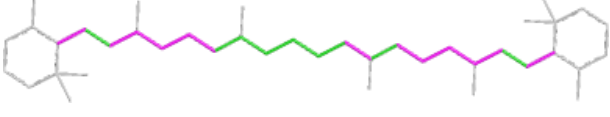
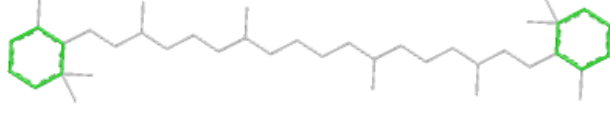


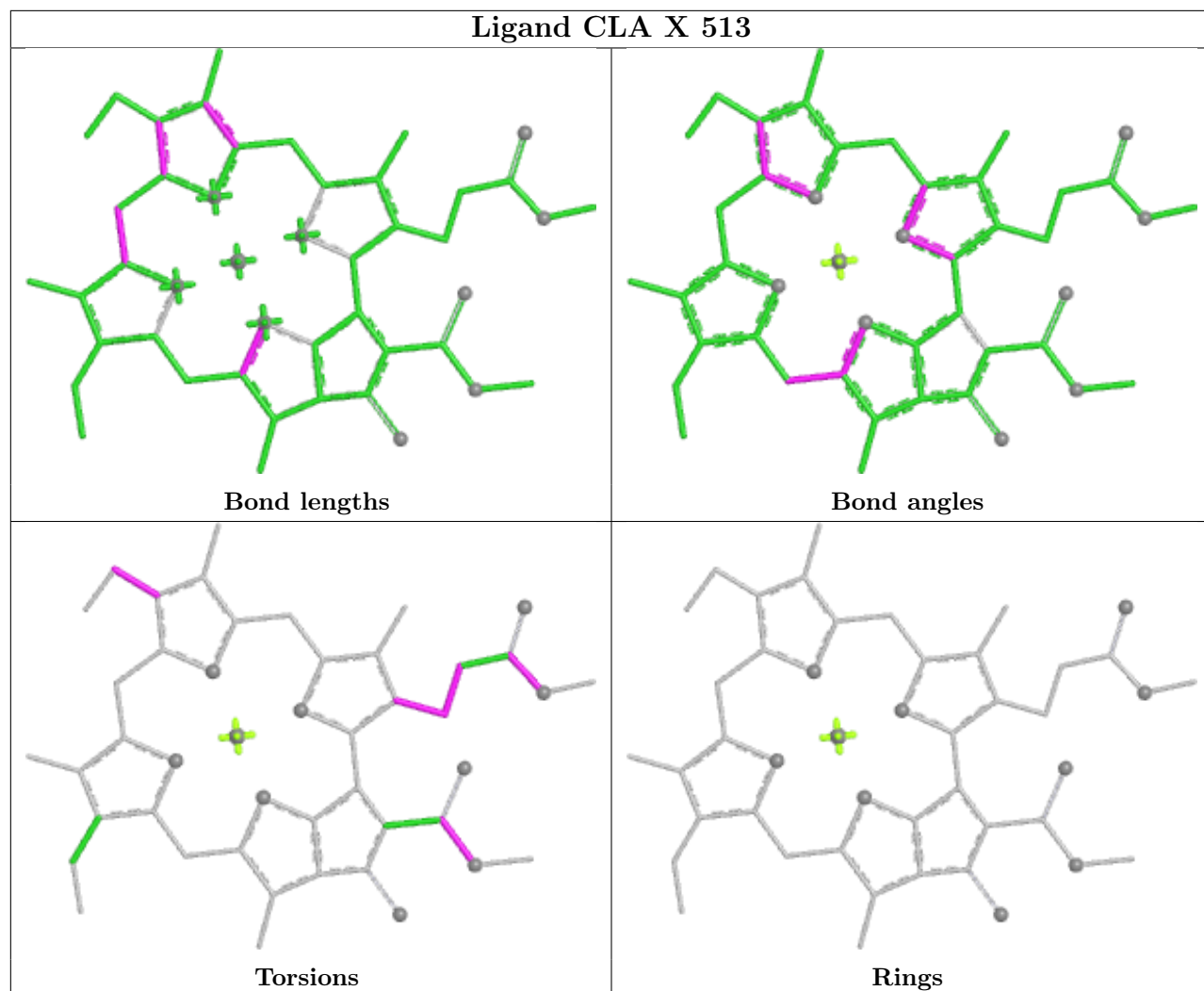
Ligand CLA A 1118



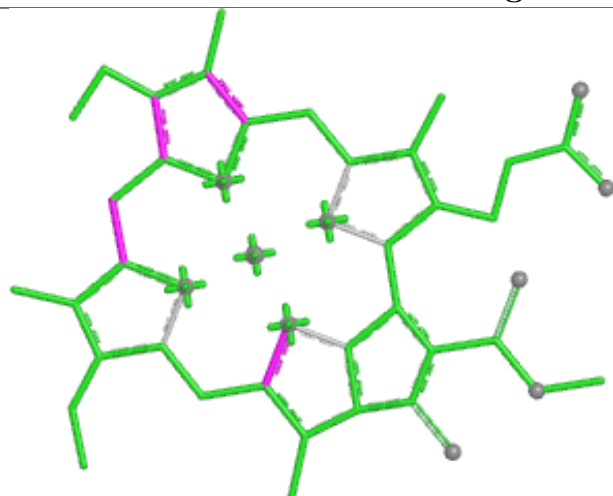
Ligand CLA a 1135



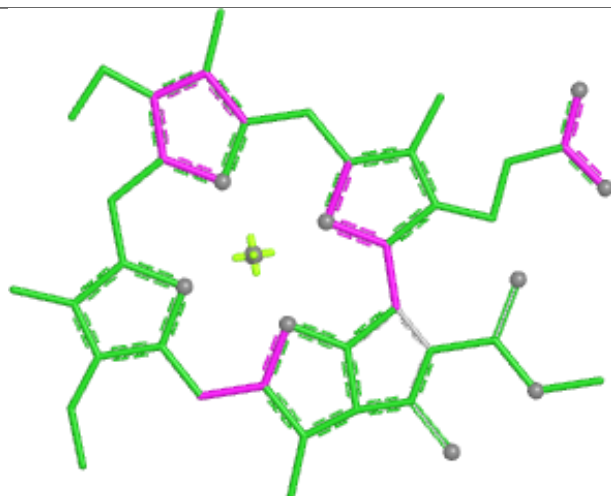
Ligand CLA t 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA p 506	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 4011	
 Bond lengths	 Bond angles
 Torsions	 Rings



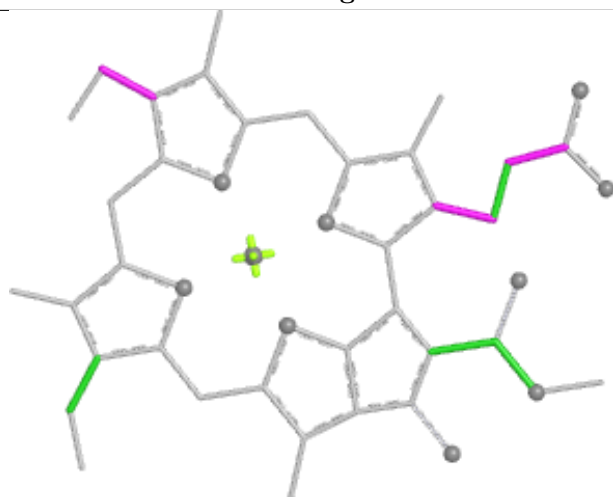
Ligand CLA B 1208



Bond lengths



Bond angles

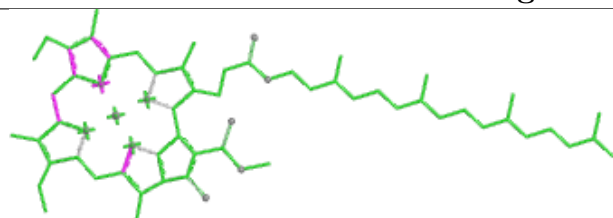


Torsions

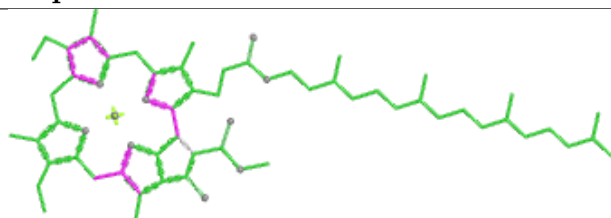


Rings

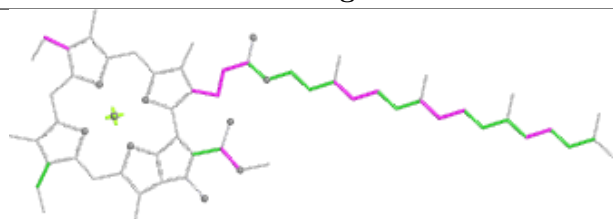
Ligand CLA p 505



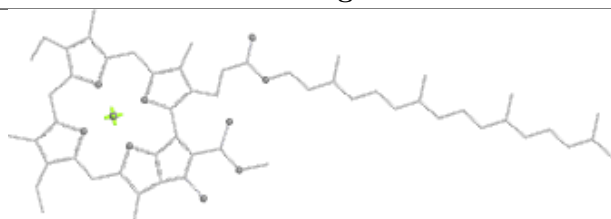
Bond lengths



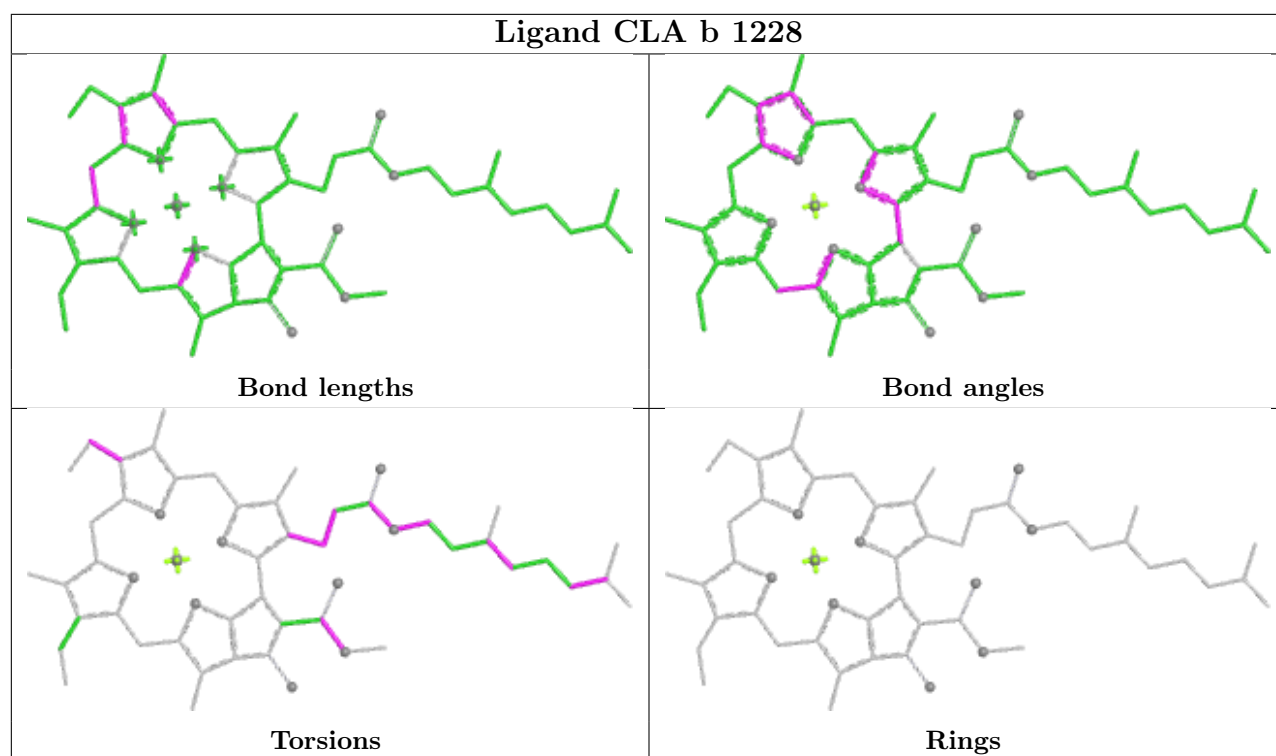
Bond angles



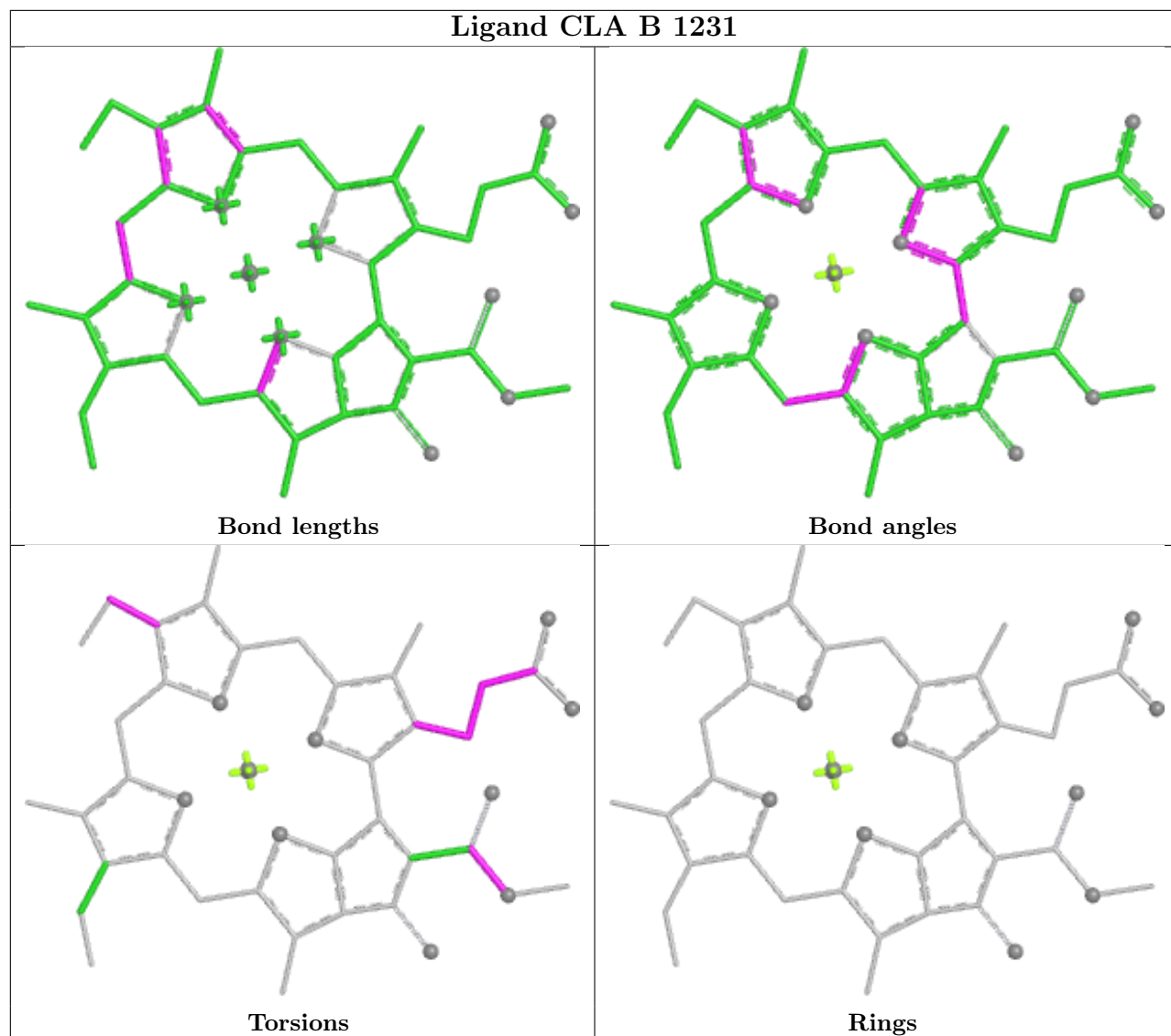
Torsions



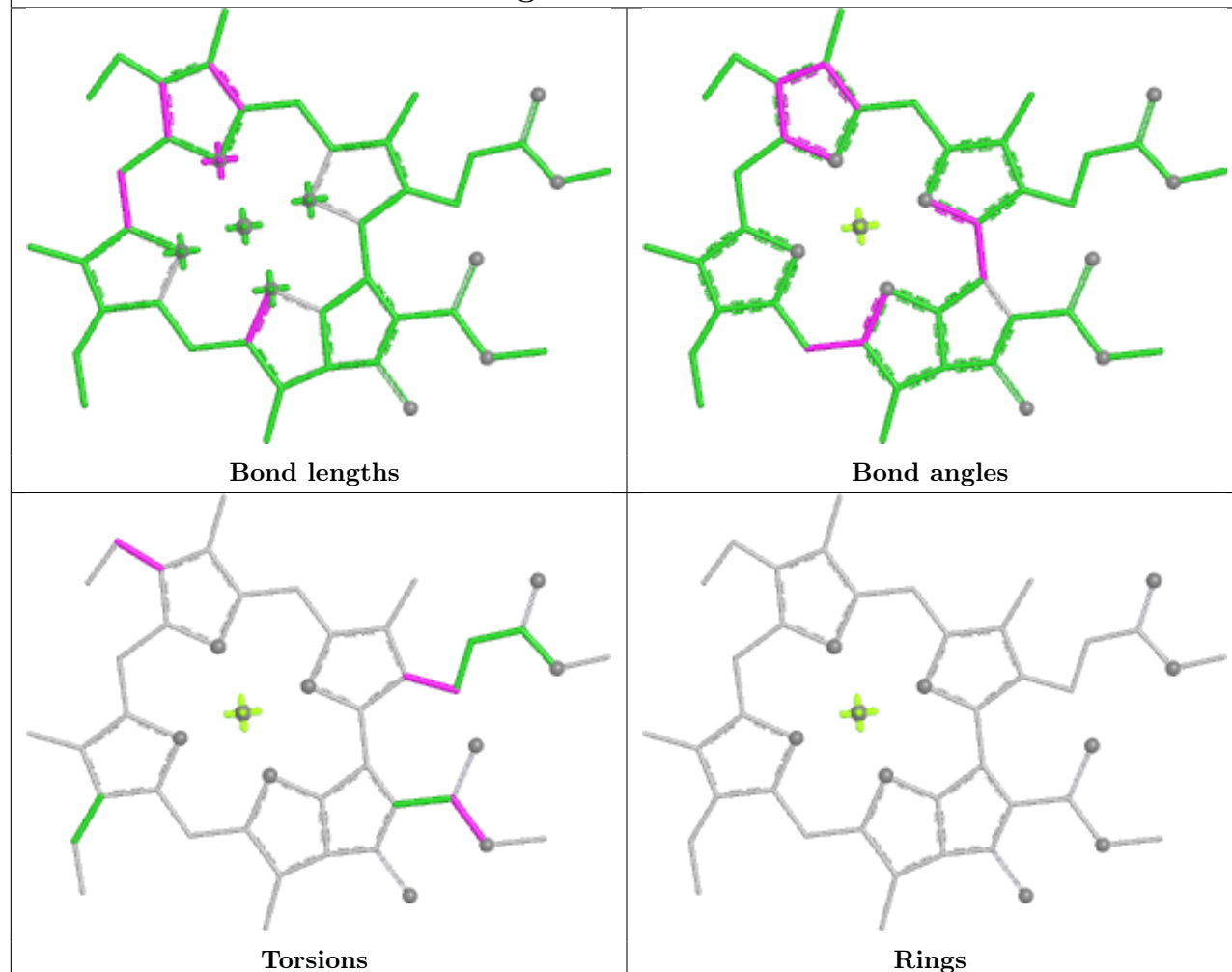
Rings



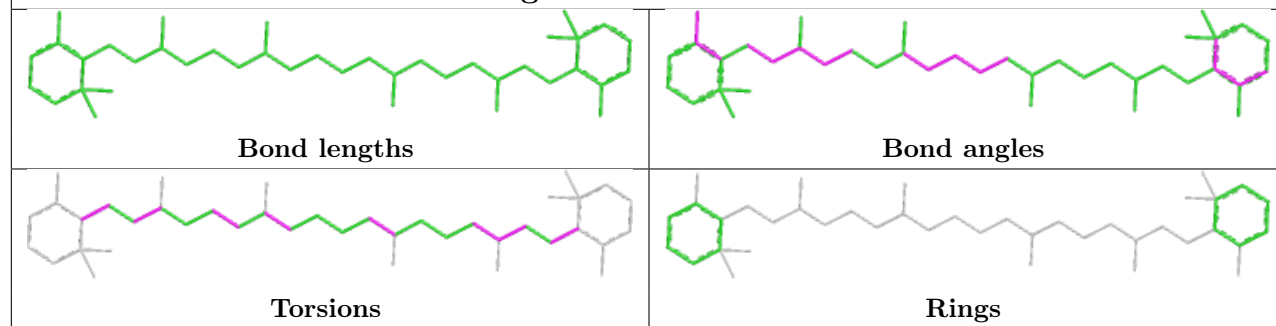
Ligand CLA B 1231

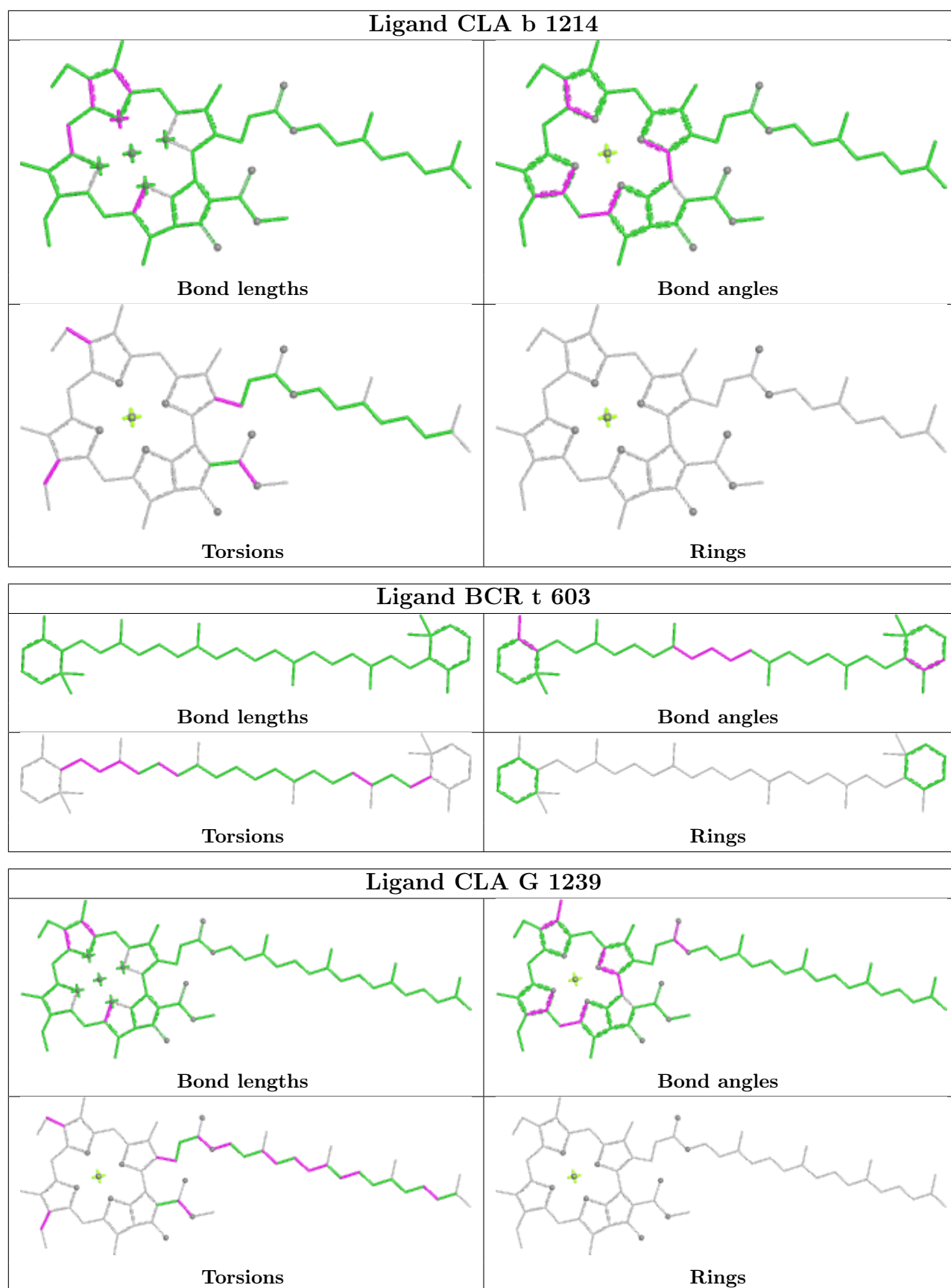


Ligand CLA o 503

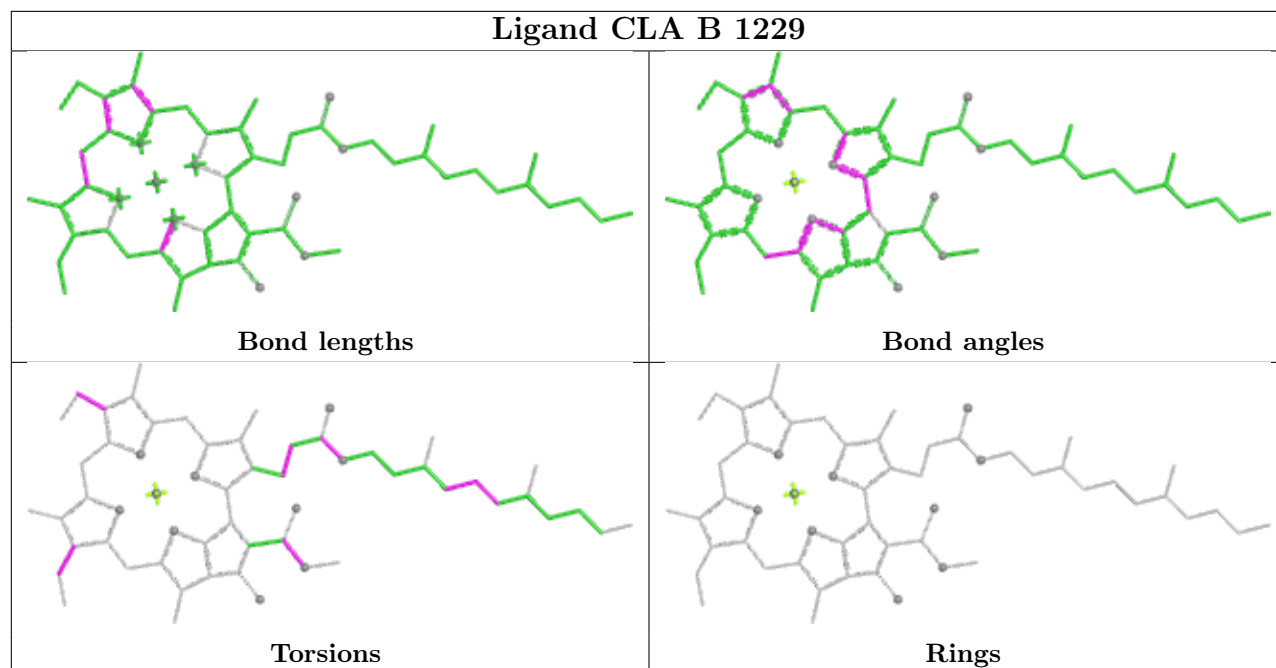


Ligand BCR R 4018

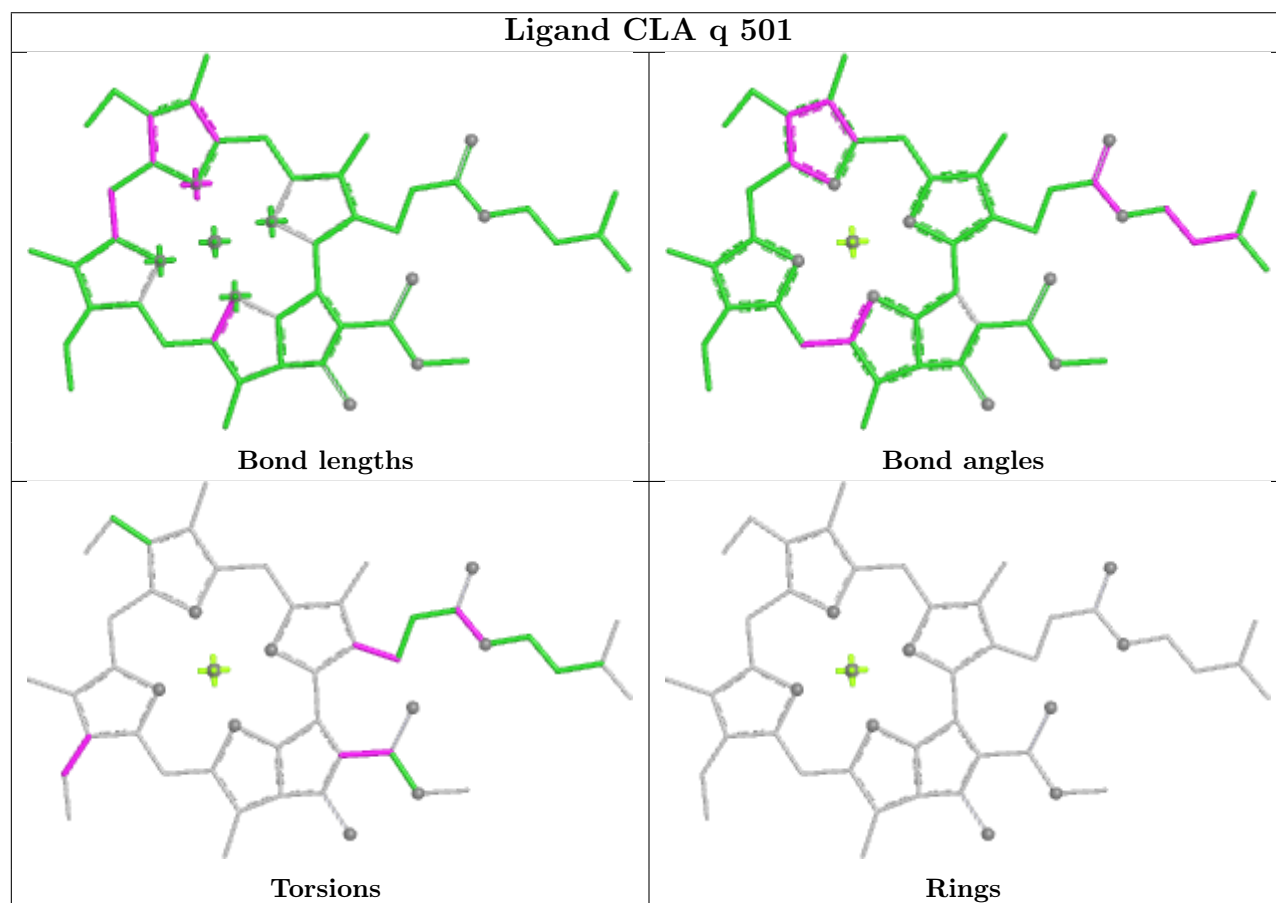


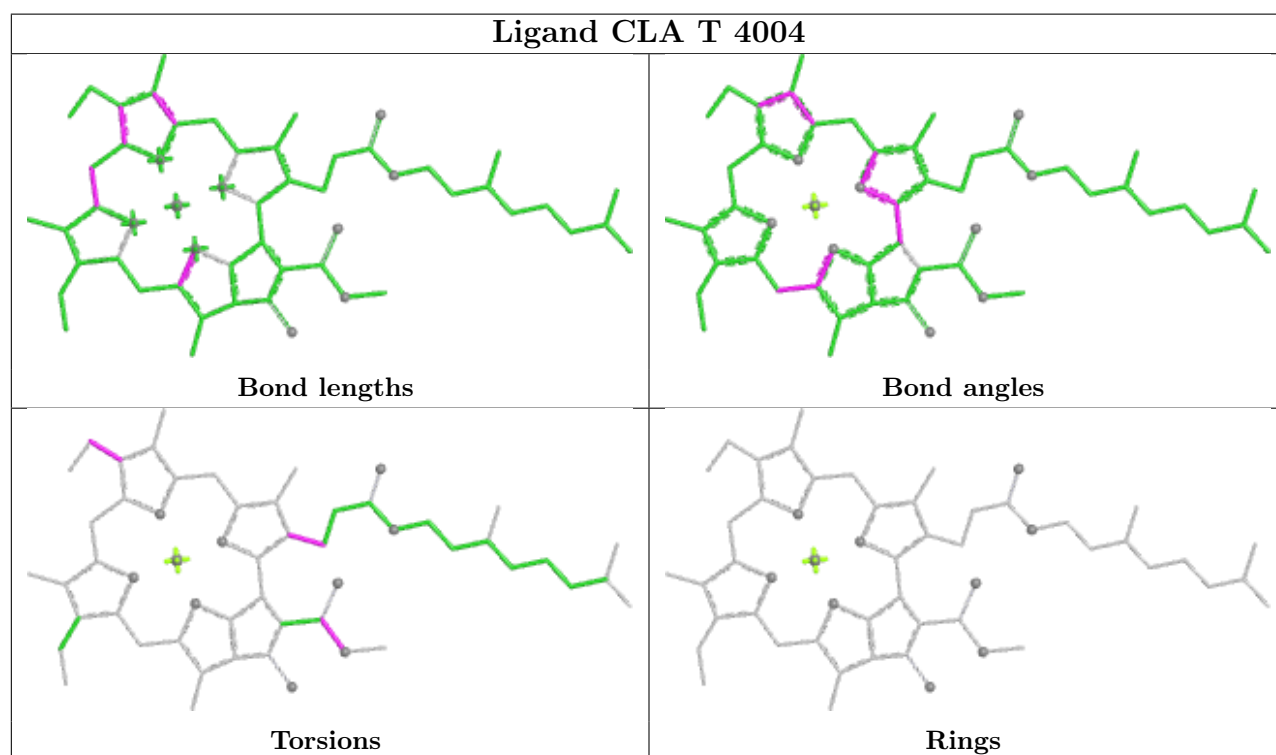
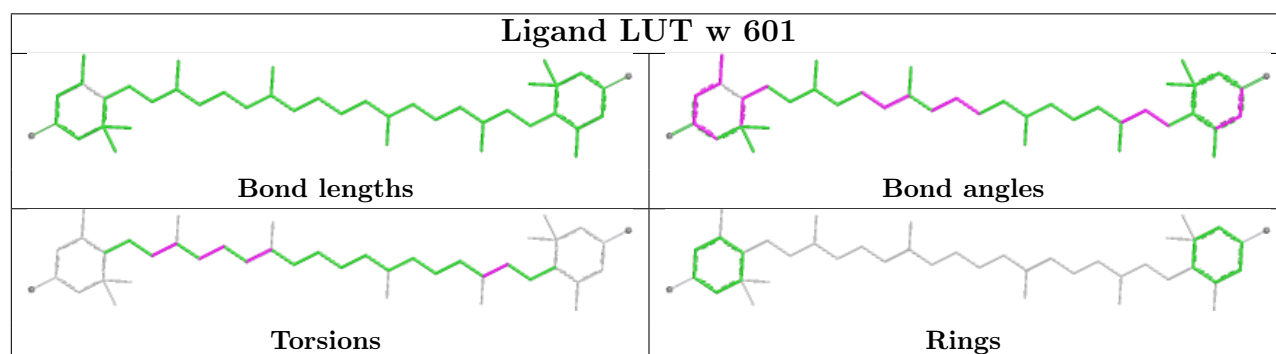
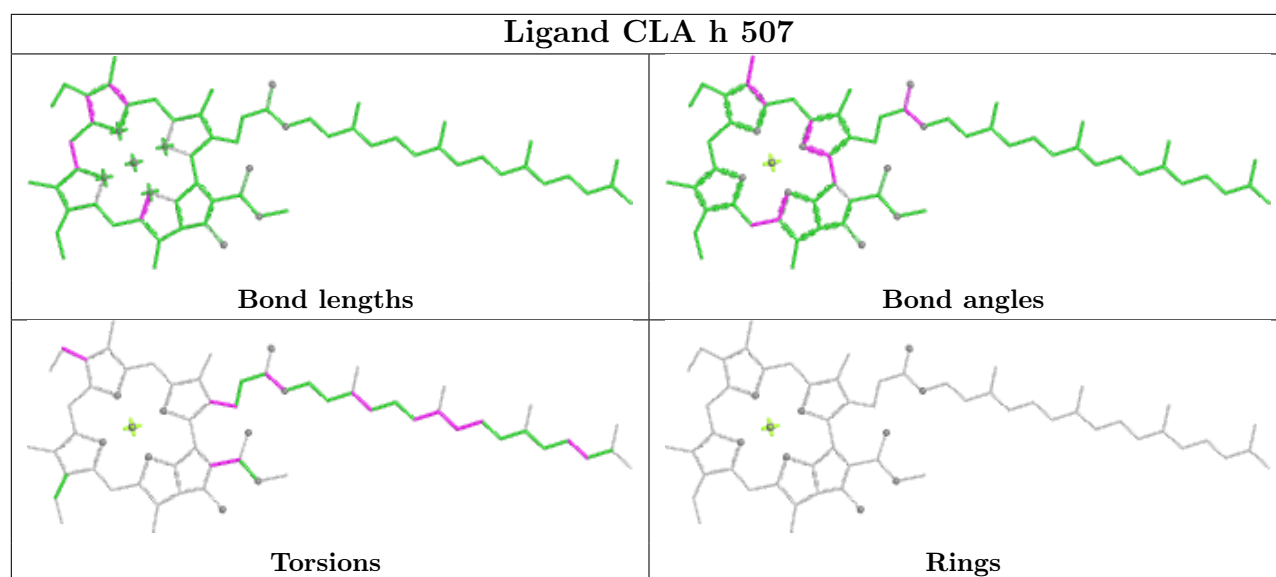


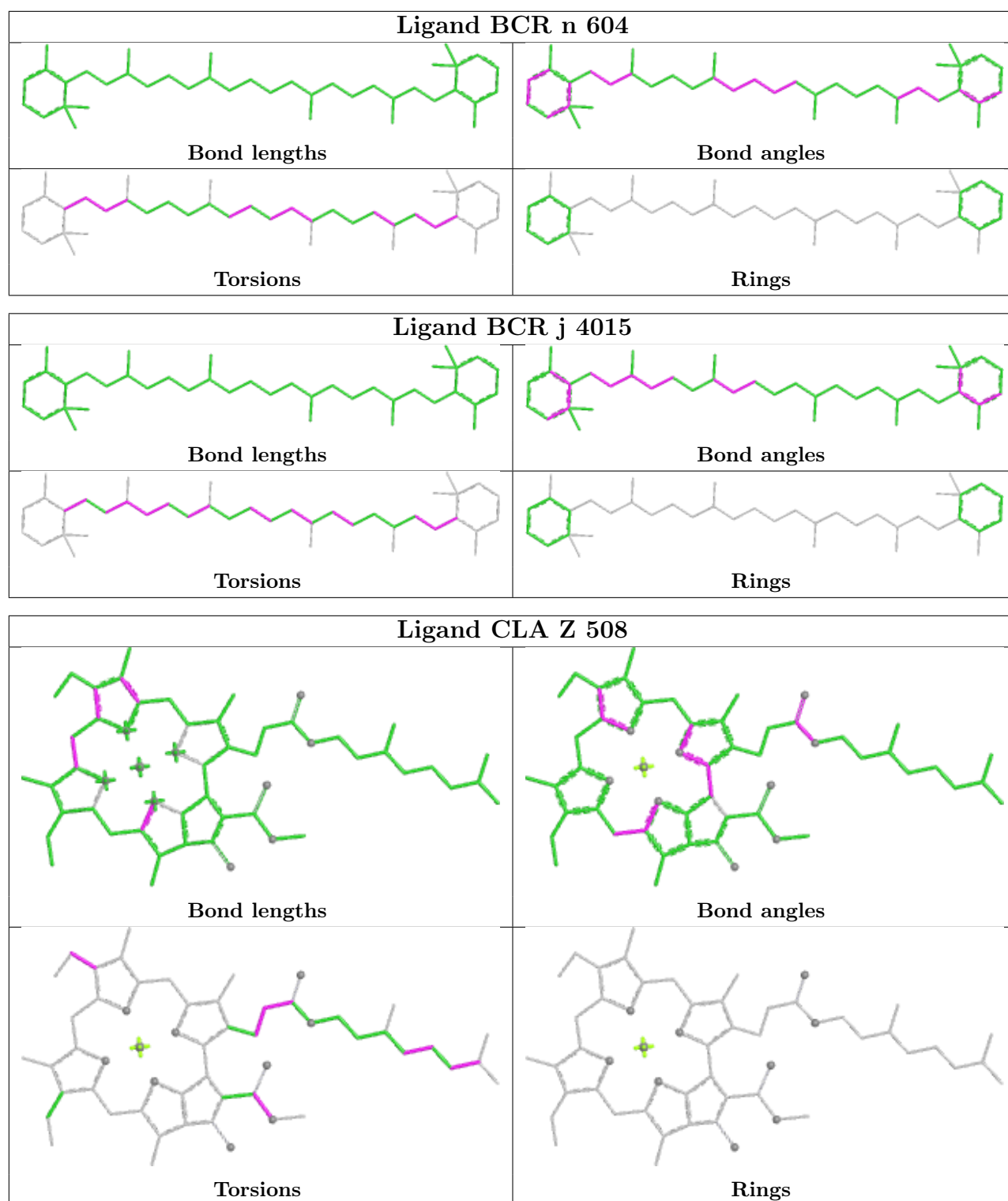
Ligand CLA B 1229

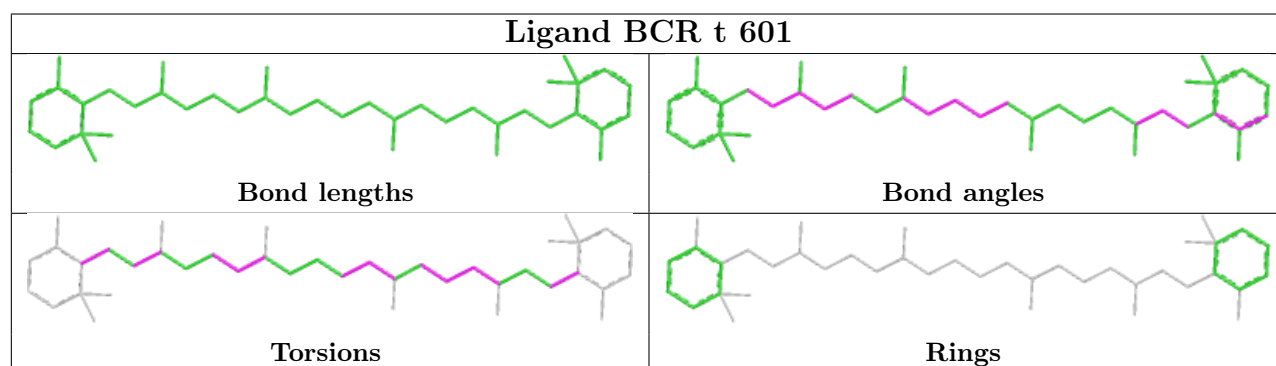
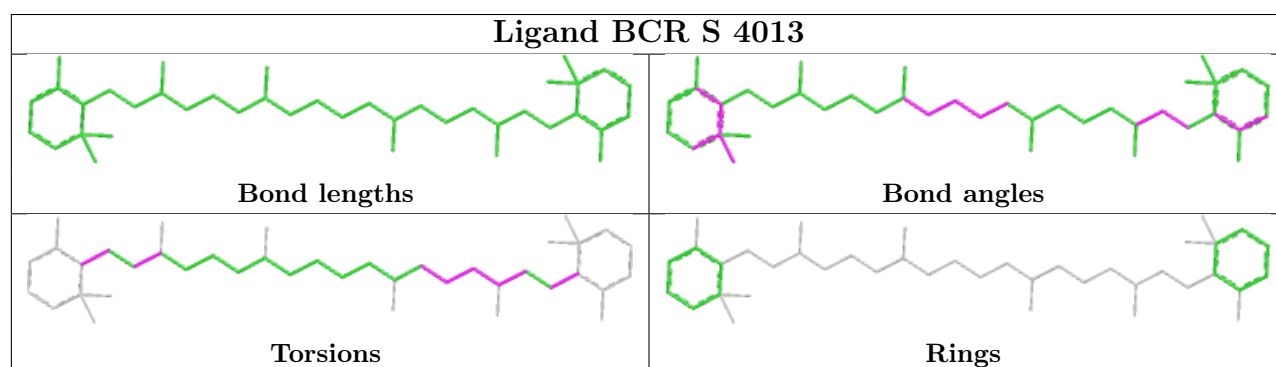
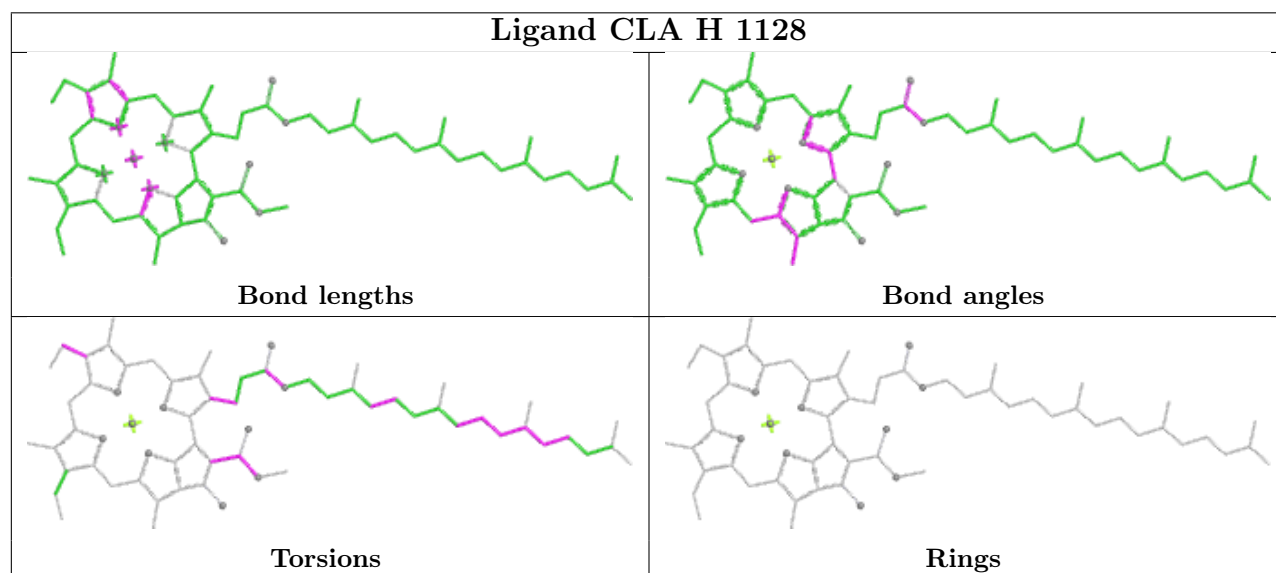
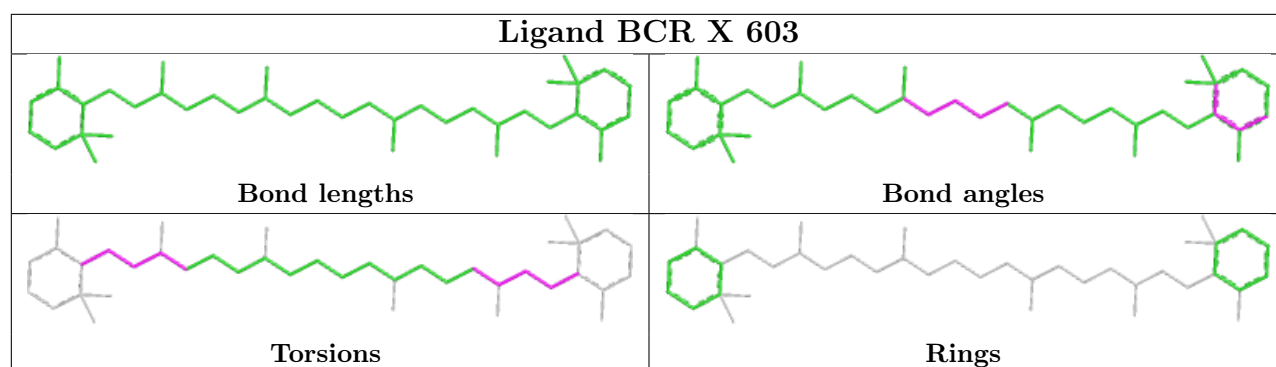


Ligand CLA q 501

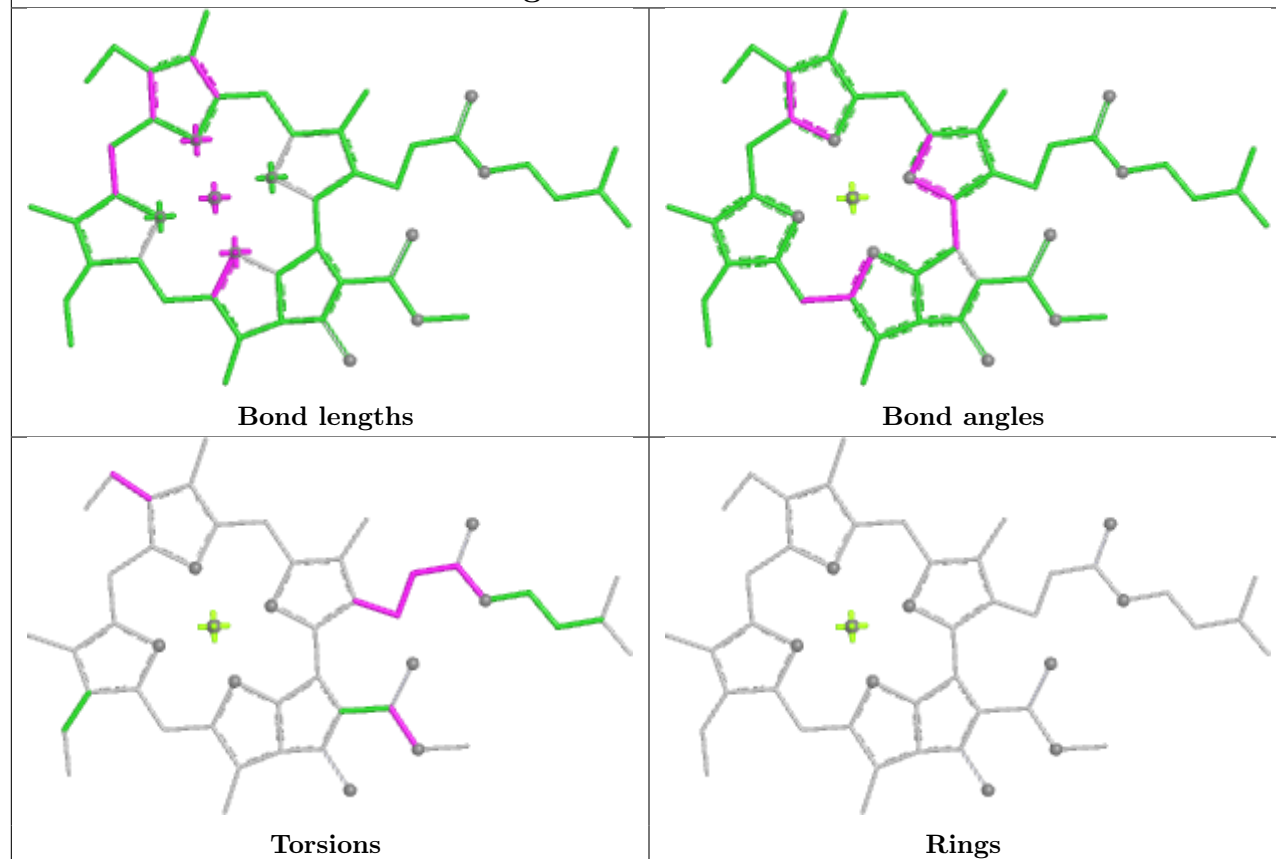




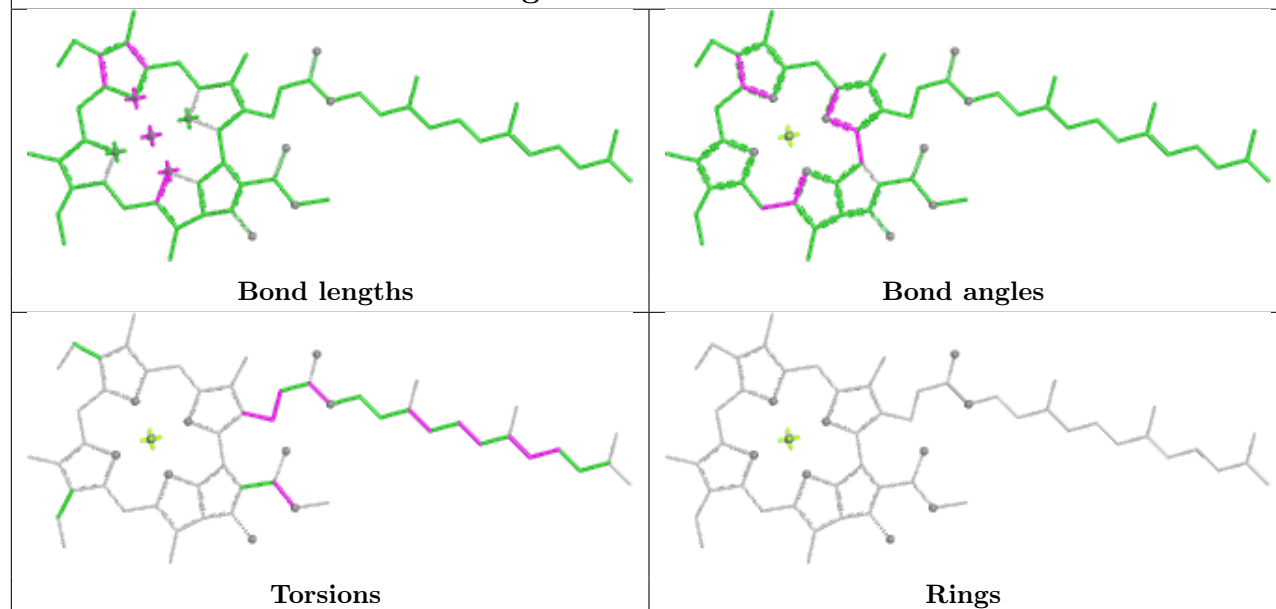


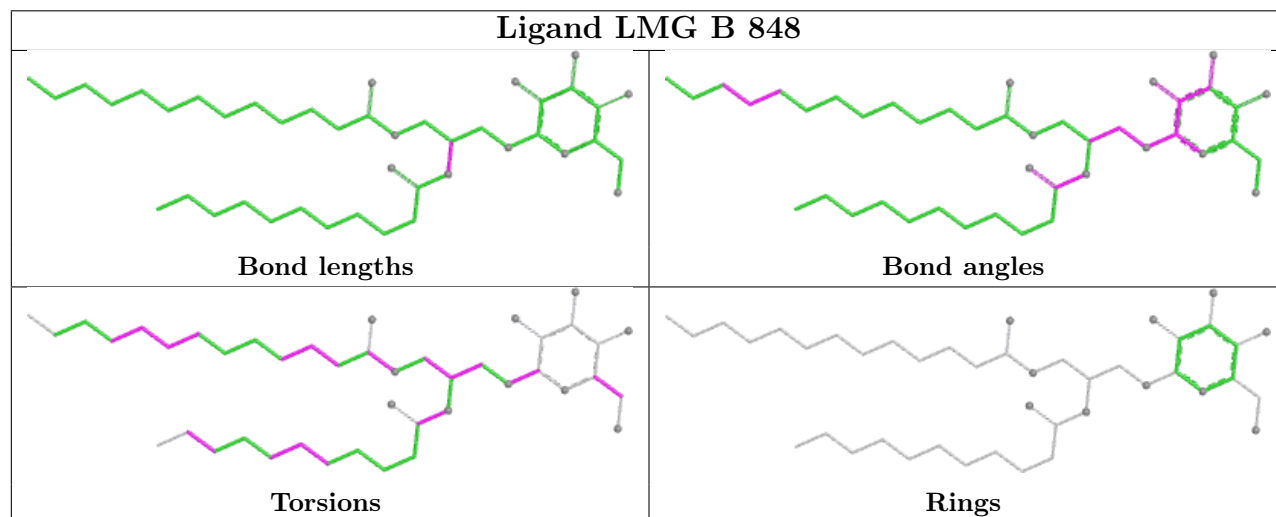
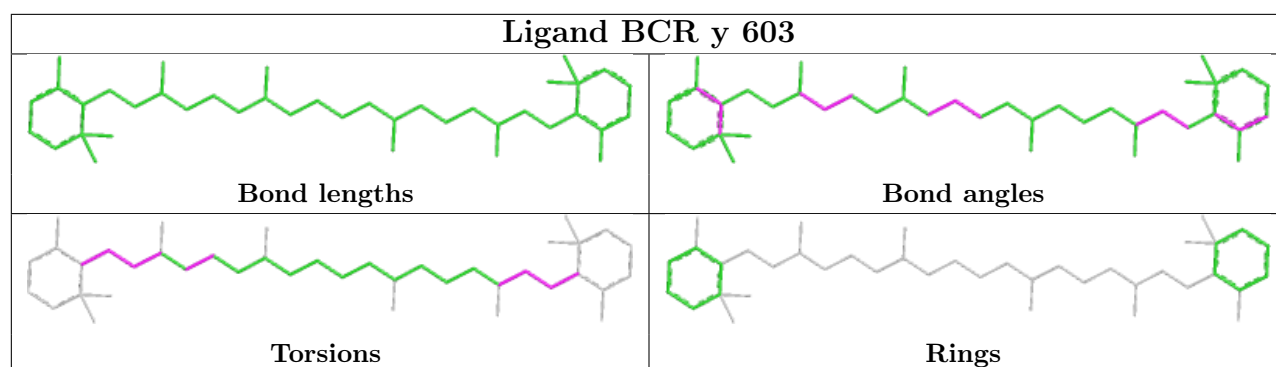


Ligand CLA B 1236

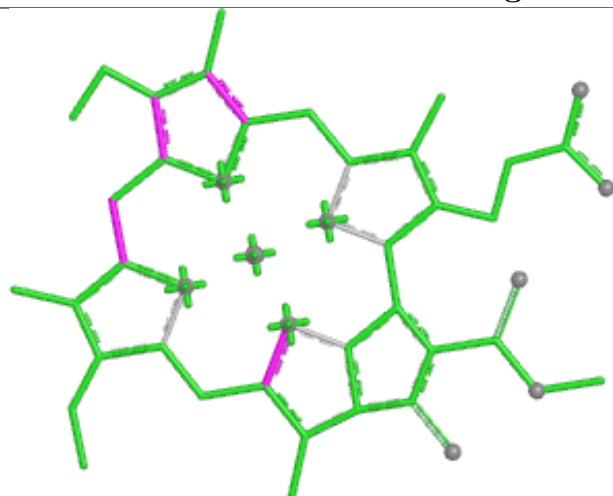


Ligand CLA G 1224

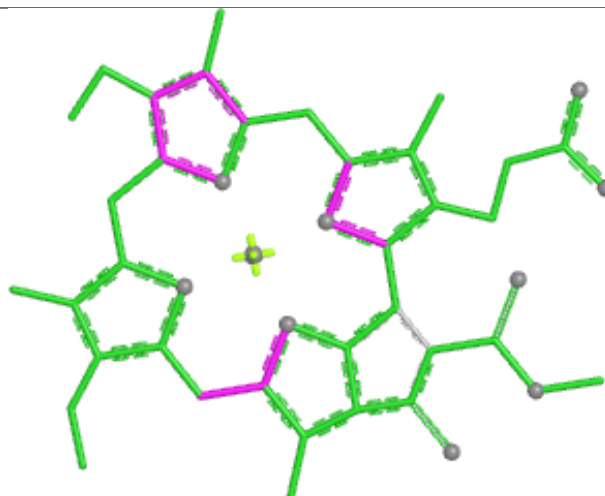




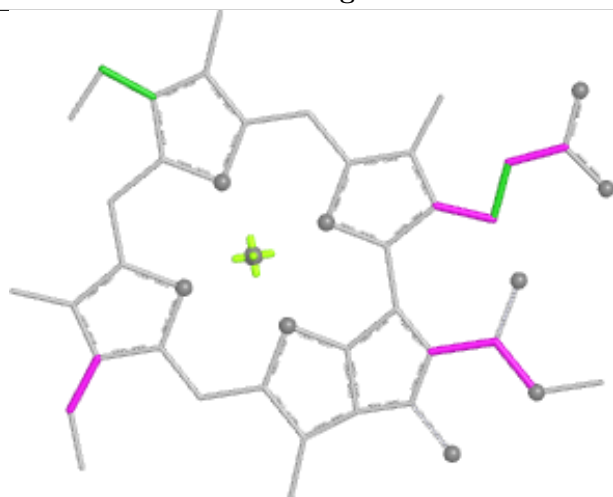
Ligand CLA K 4003



Bond lengths



Bond angles

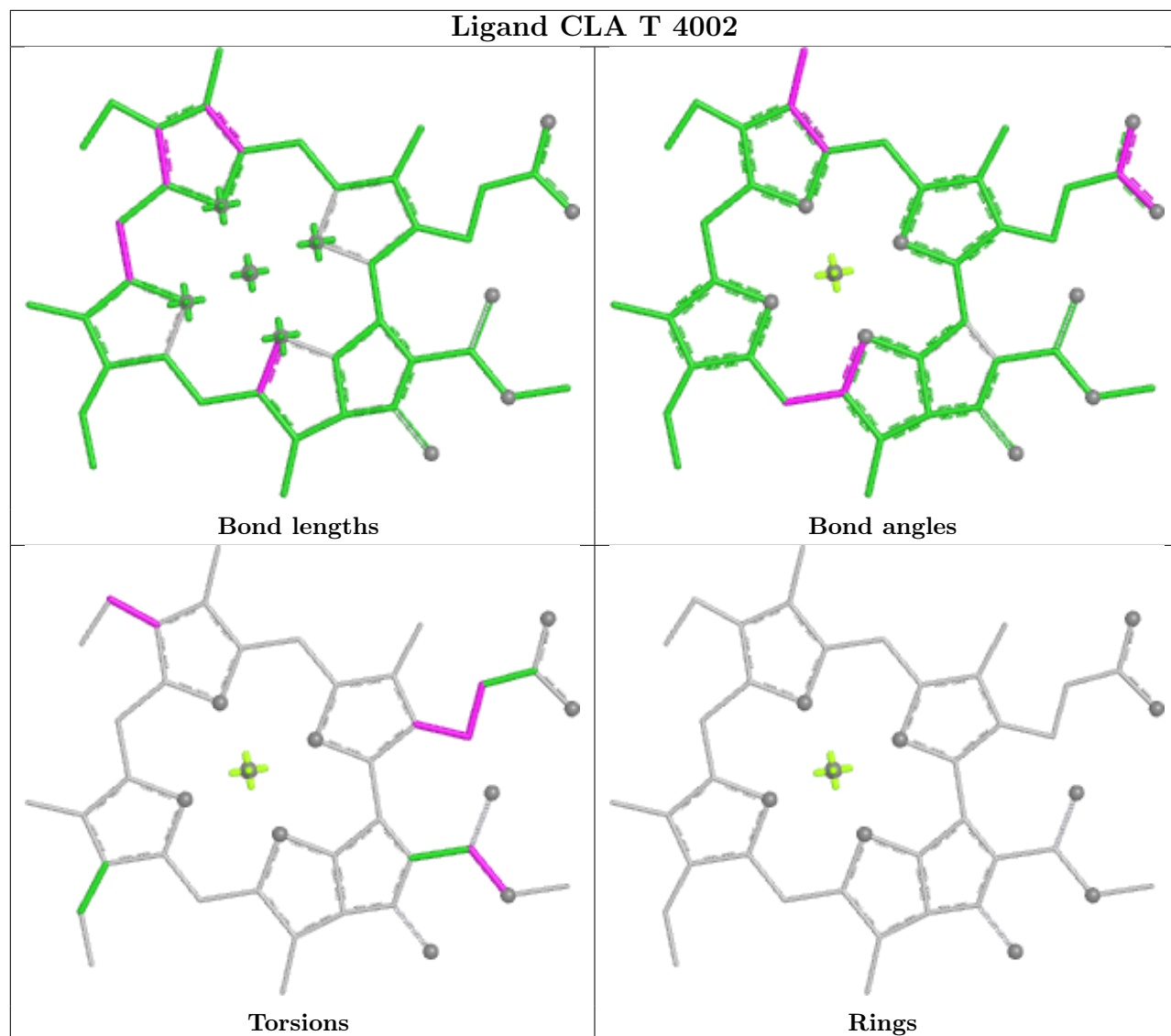


Torsions

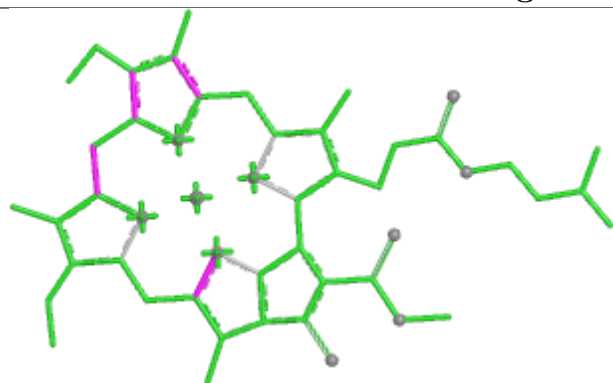


Rings

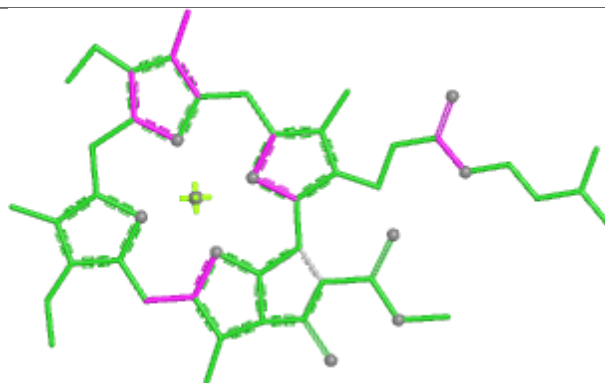
Ligand CLA T 4002



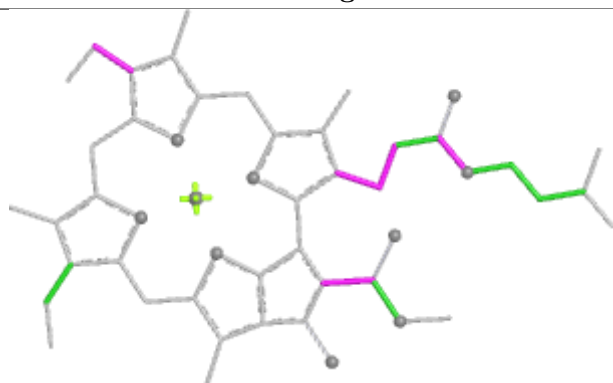
Ligand CLA Z 513



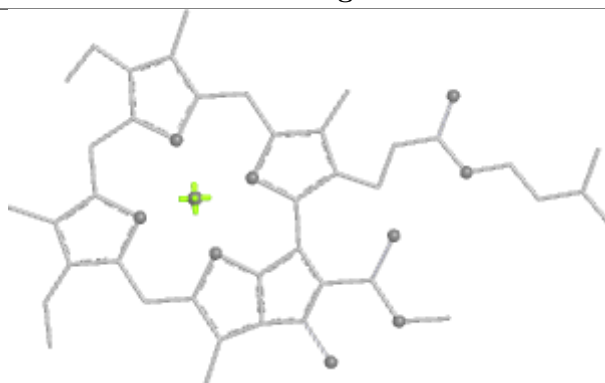
Bond lengths



Bond angles

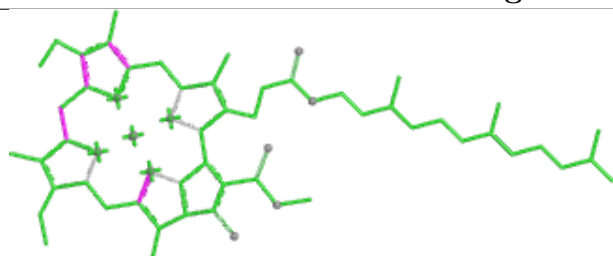


Torsions

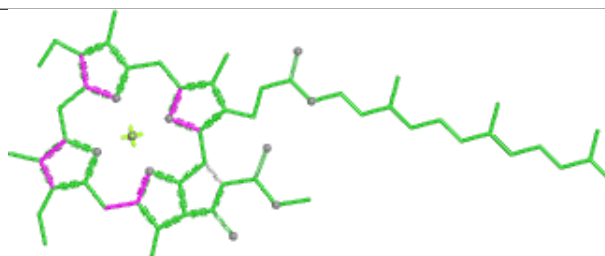


Rings

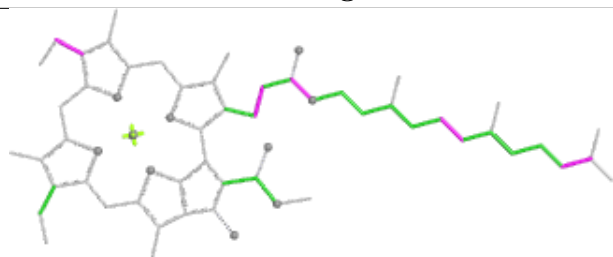
Ligand CLA A 1124



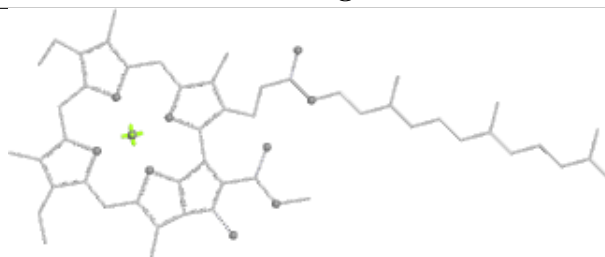
Bond lengths



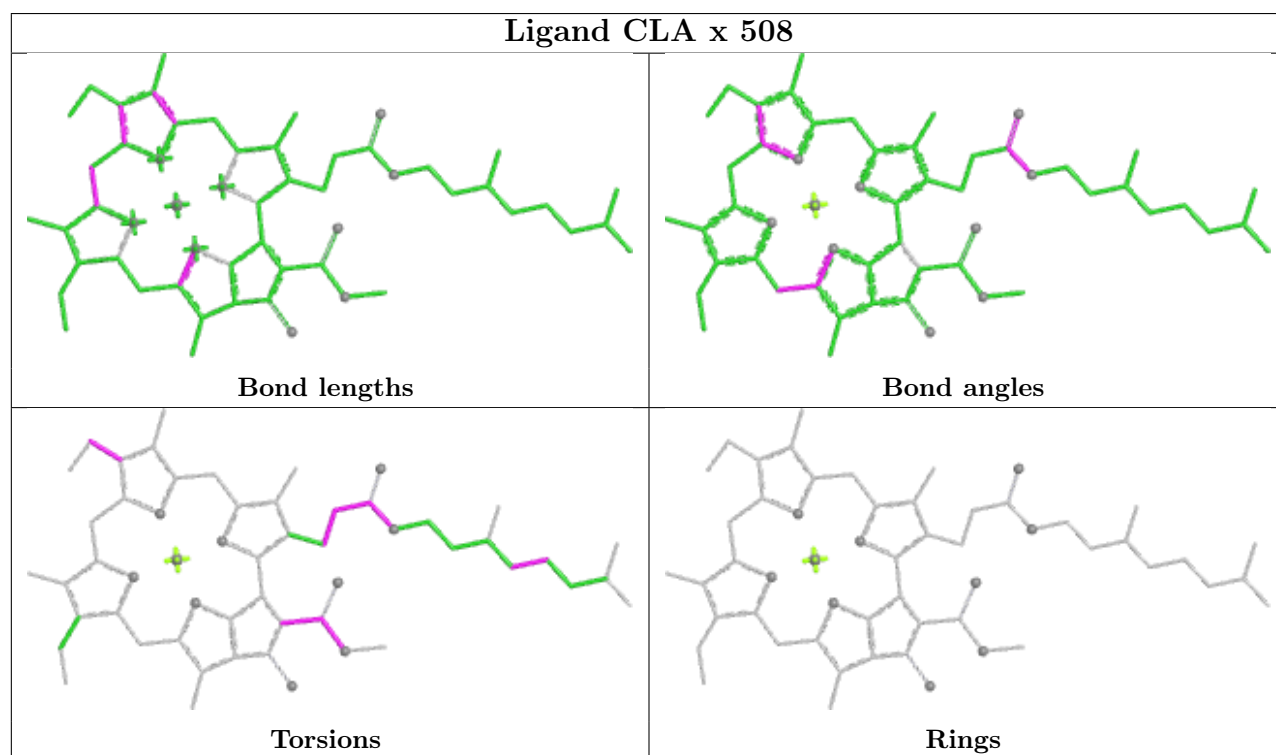
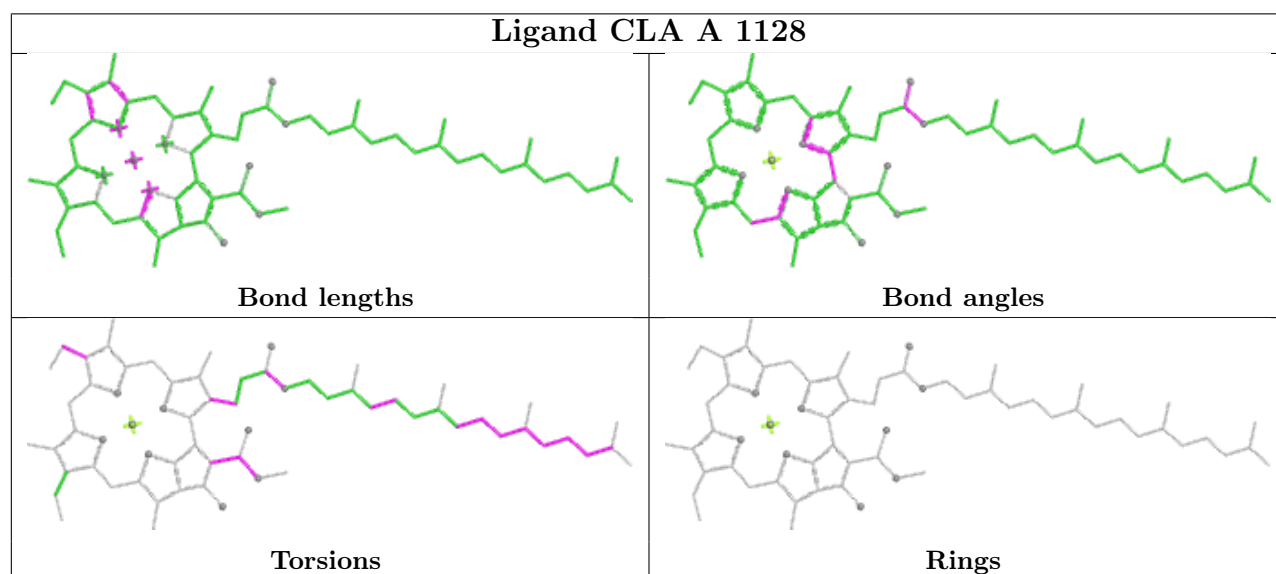
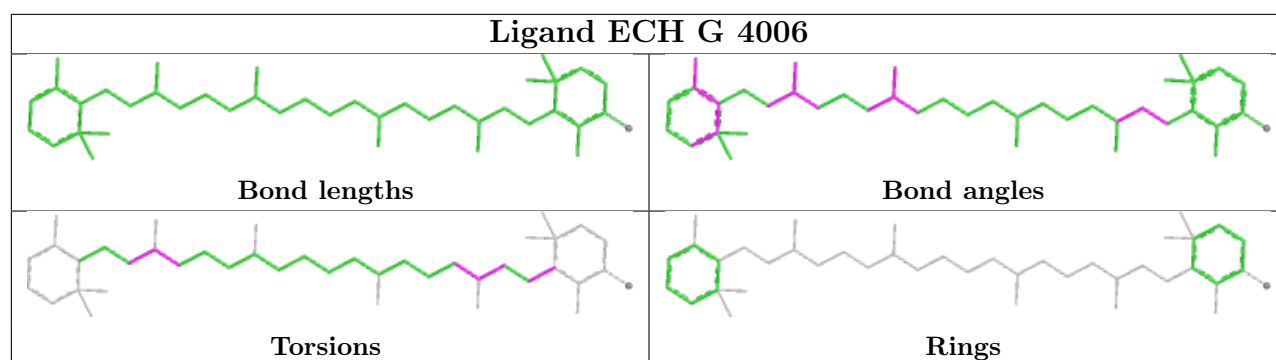
Bond angles

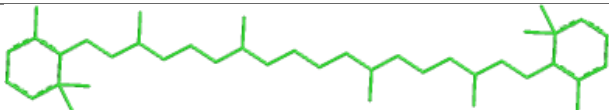
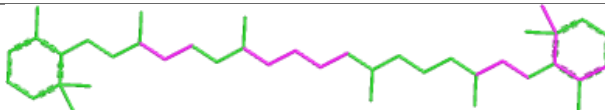
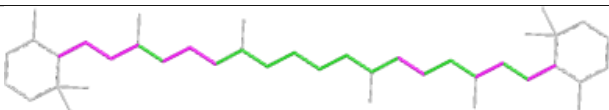
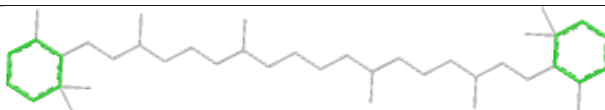


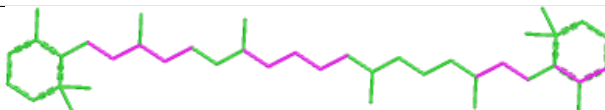
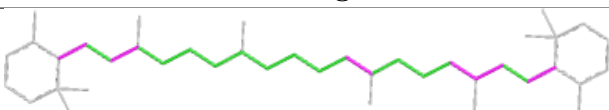
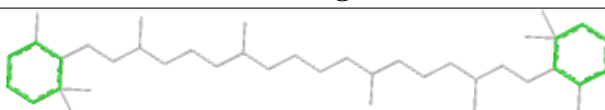
Torsions

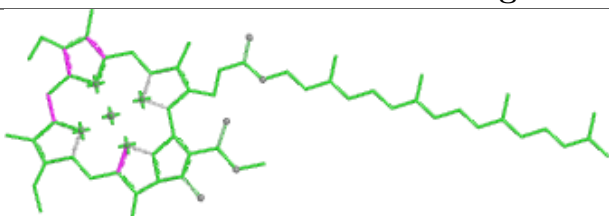
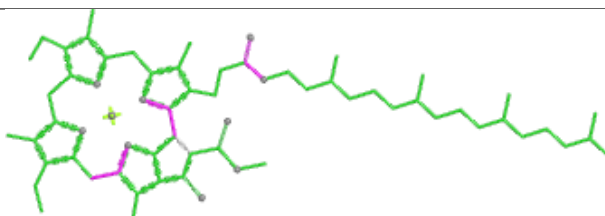
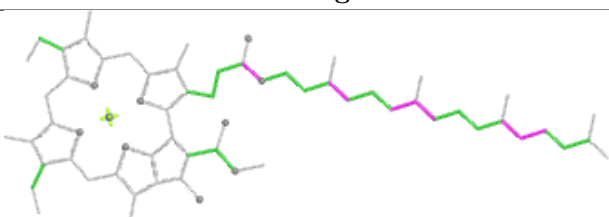
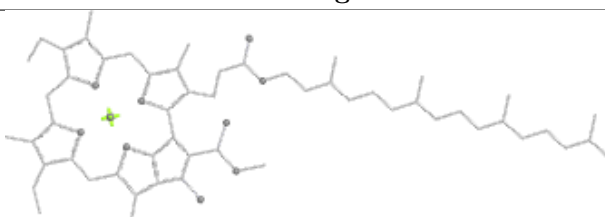


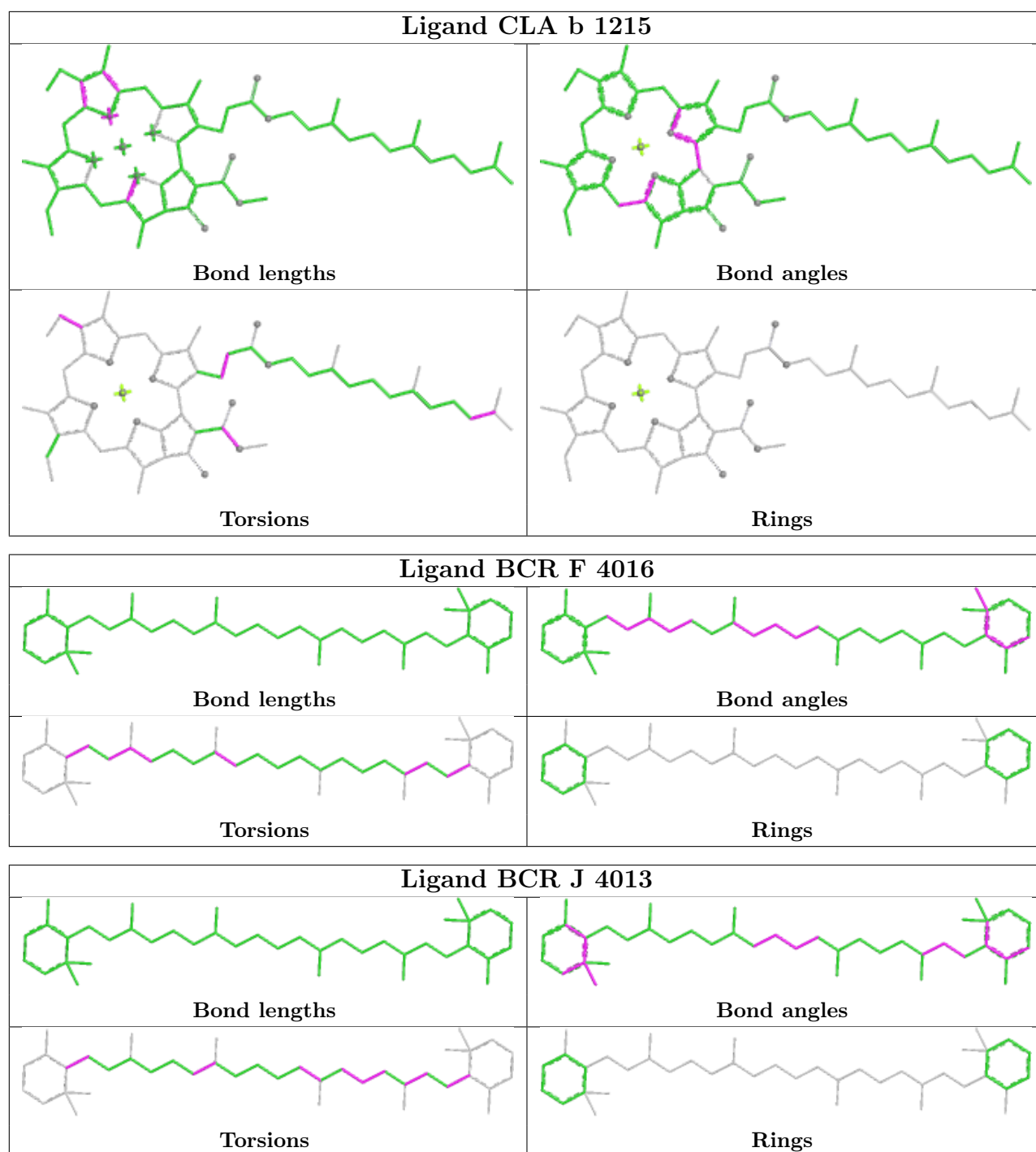
Rings

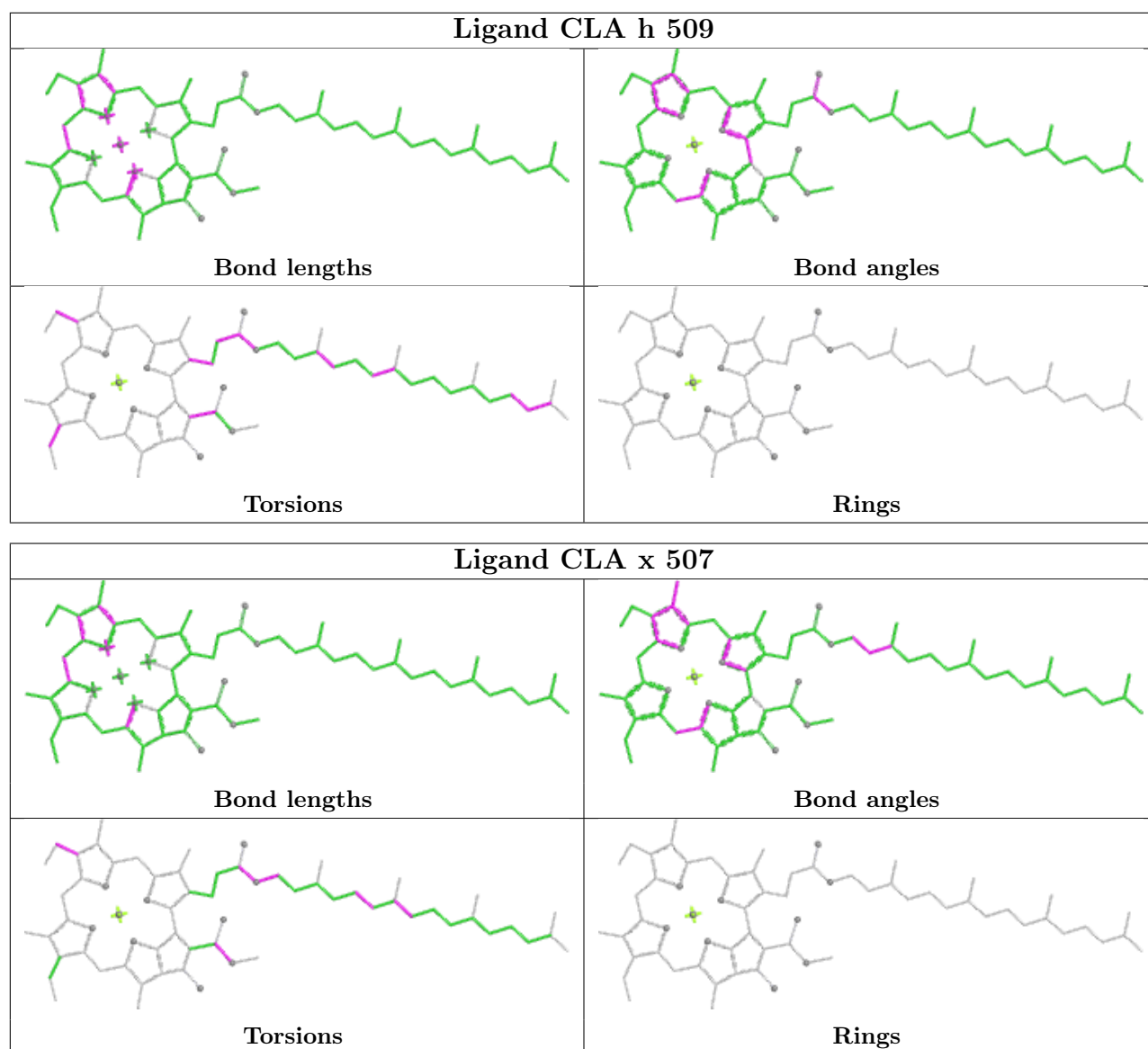


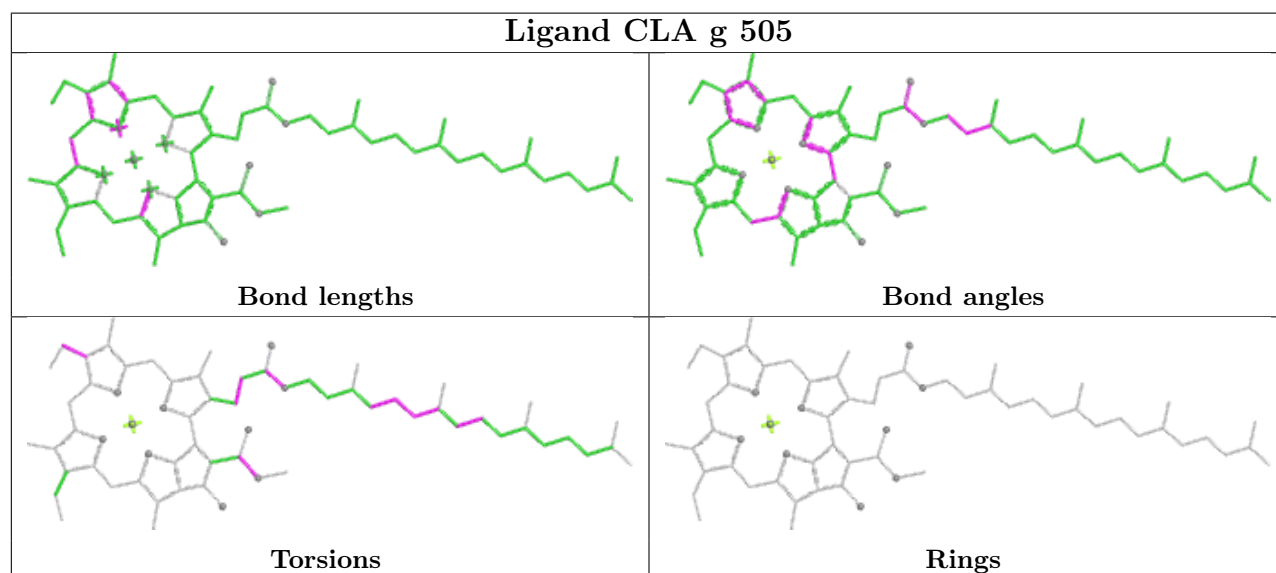
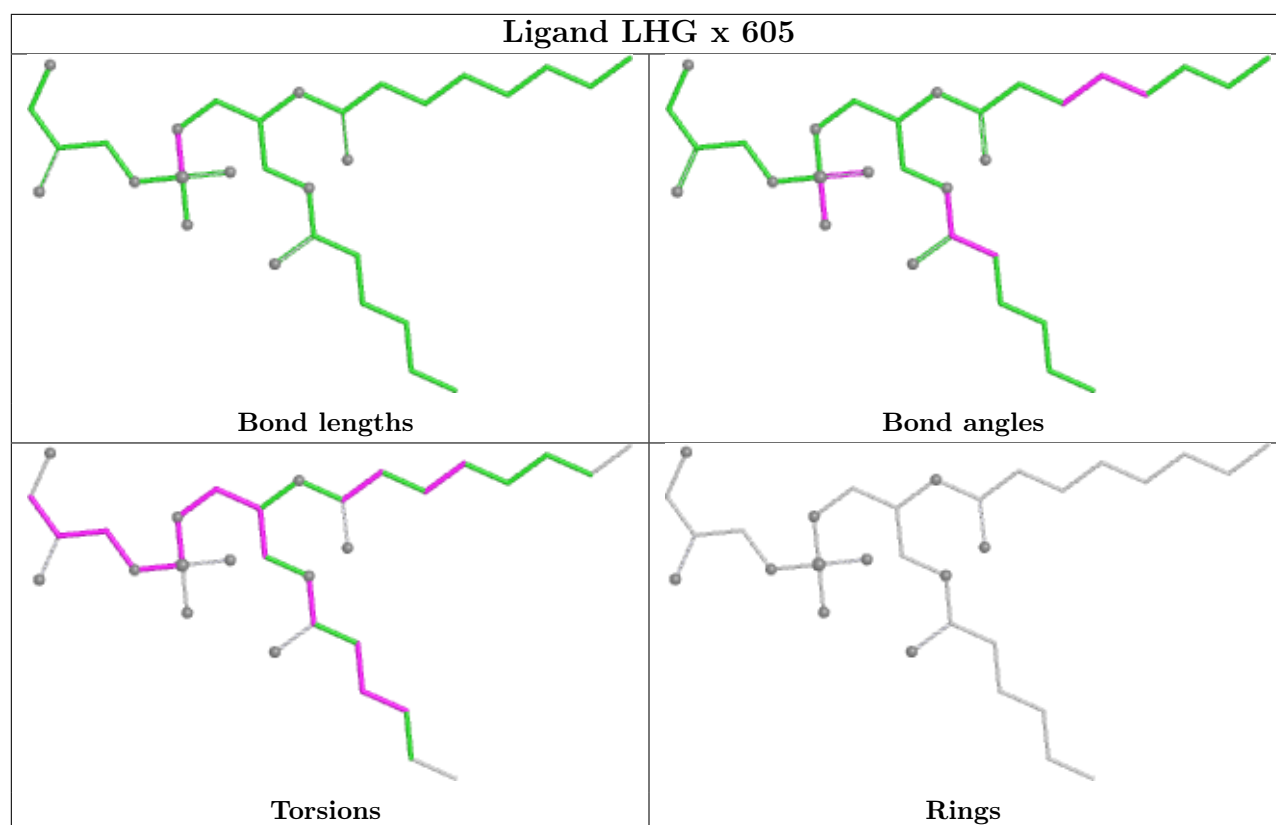
Ligand BCR k 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR X 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

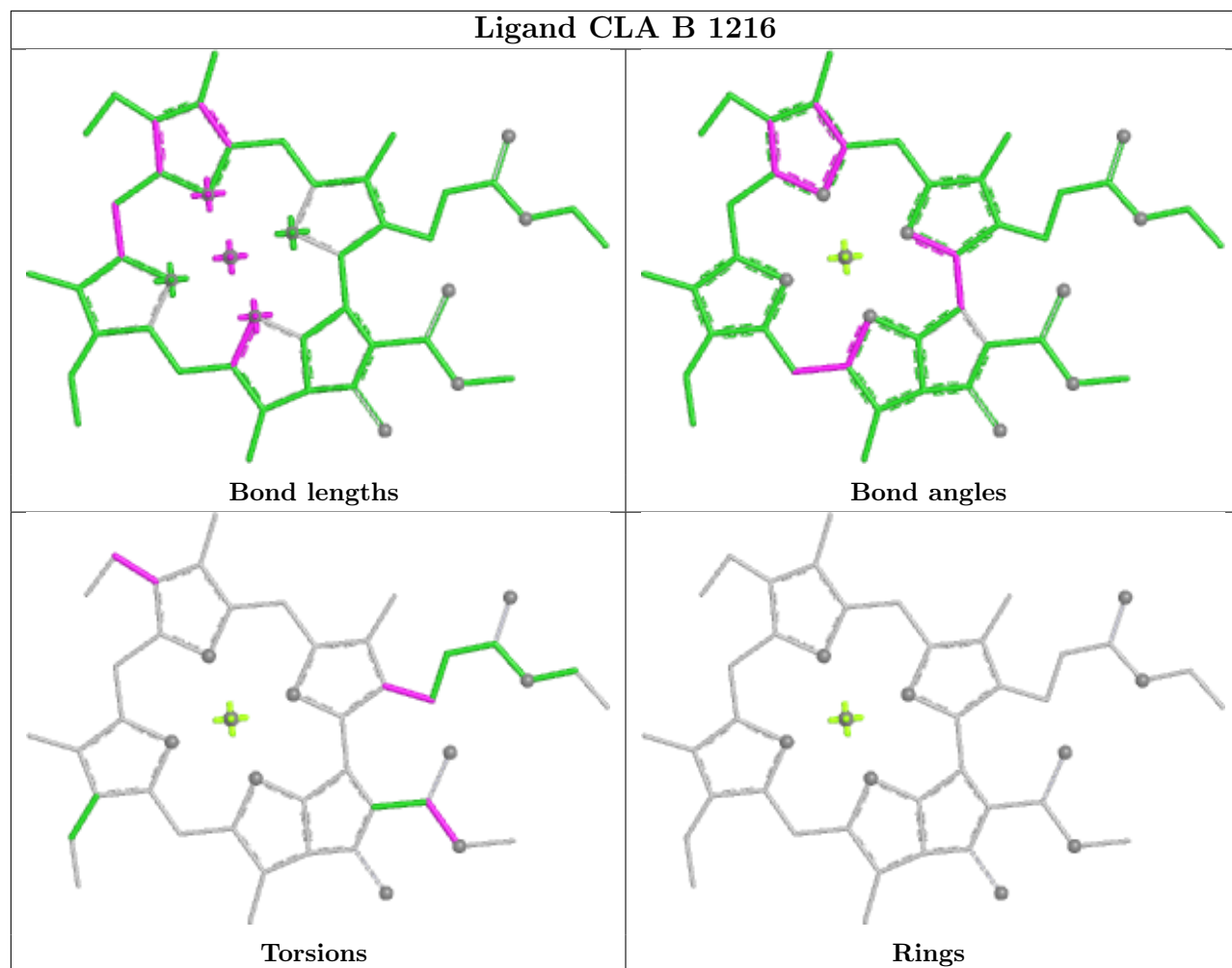
Ligand CLA U 1503	
	
Bond lengths	Bond angles
	
Torsions	Rings



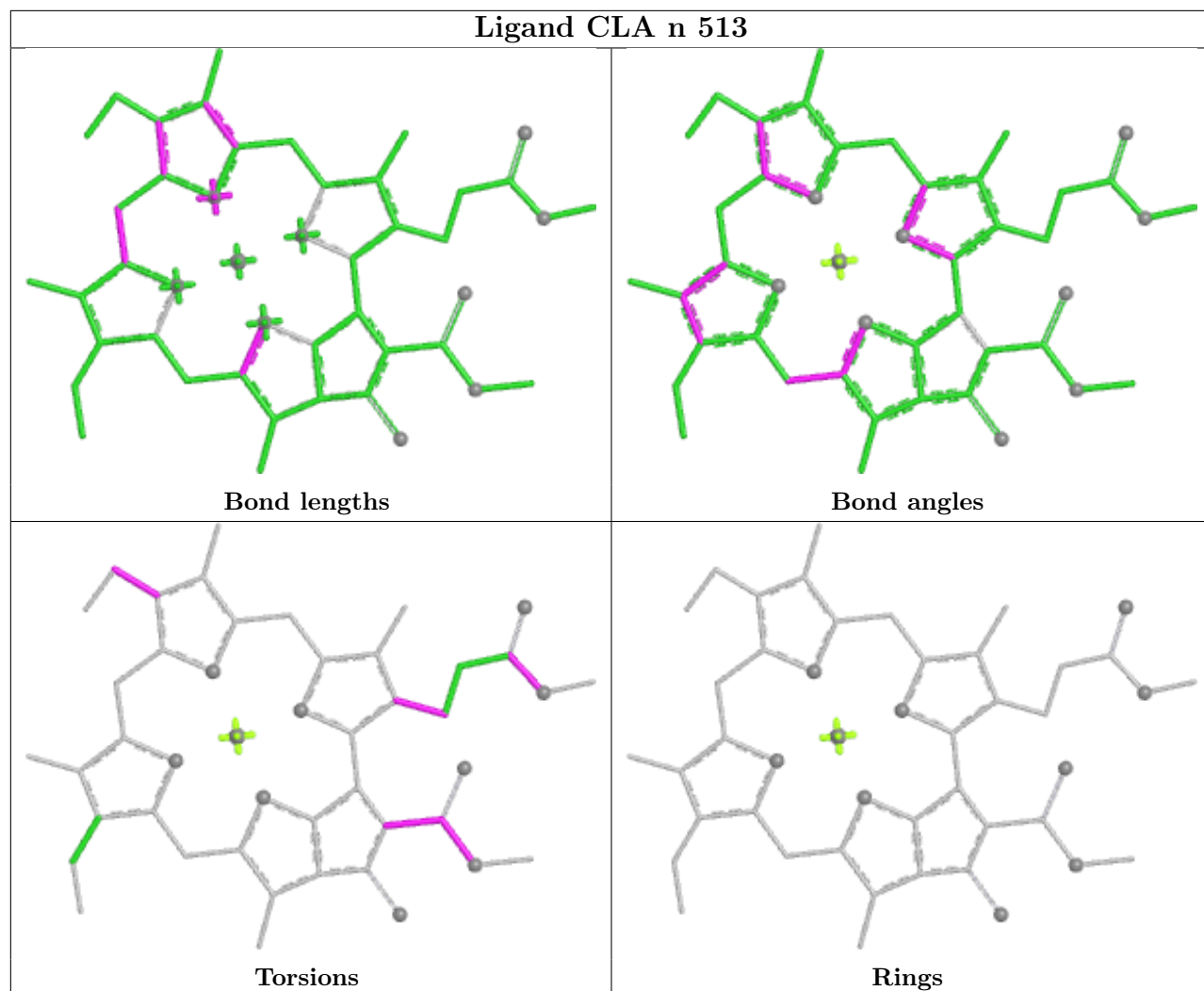




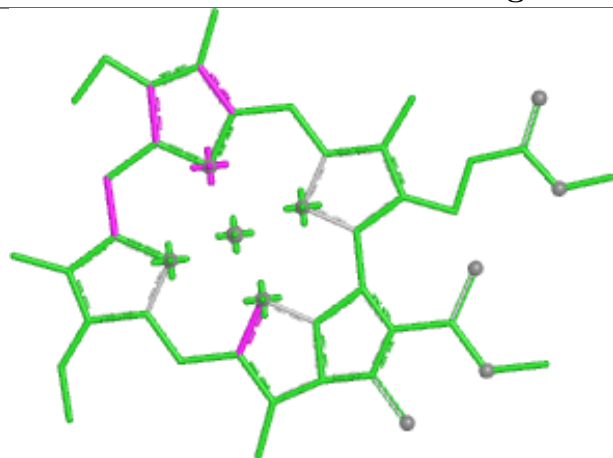
Ligand CLA B 1216



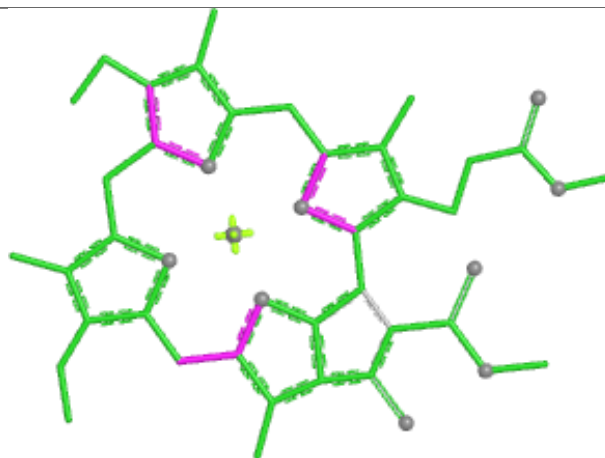
Ligand CLA n 513



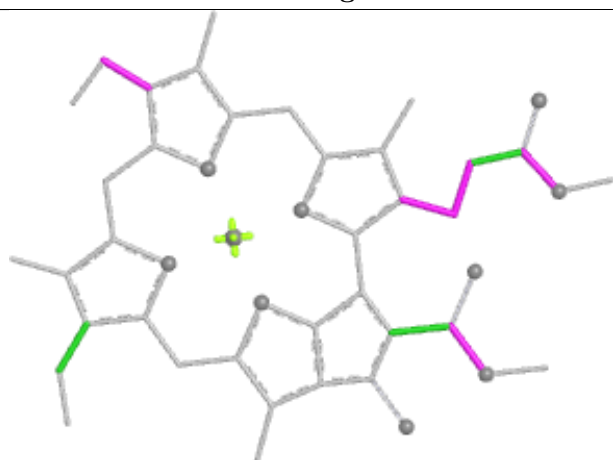
Ligand CLA F 1302



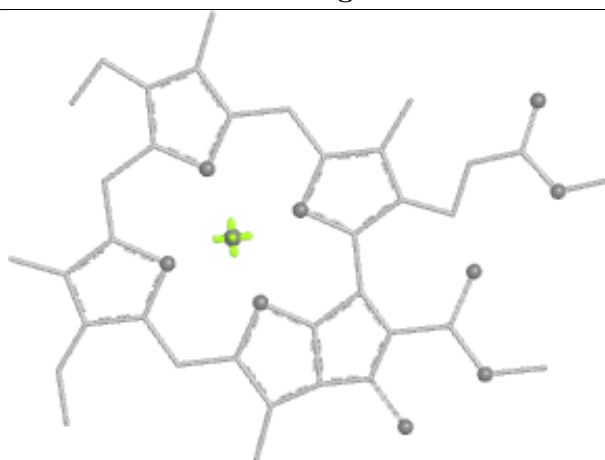
Bond lengths



Bond angles

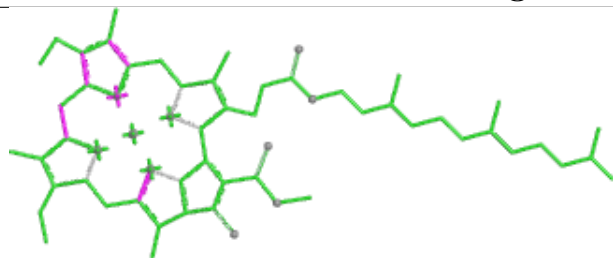


Torsions

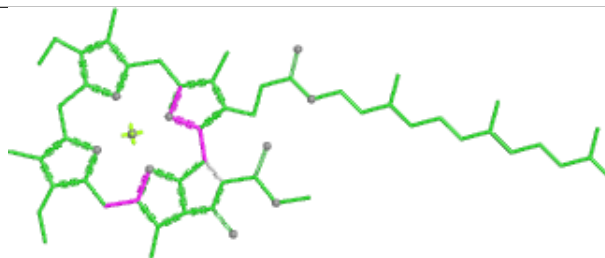


Rings

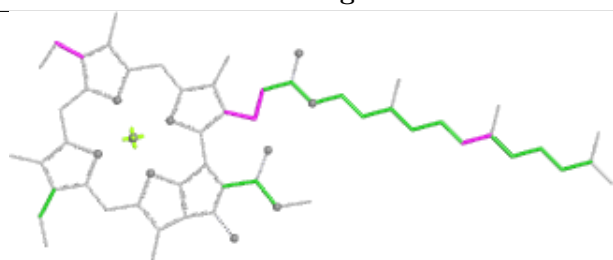
Ligand CLA W 504



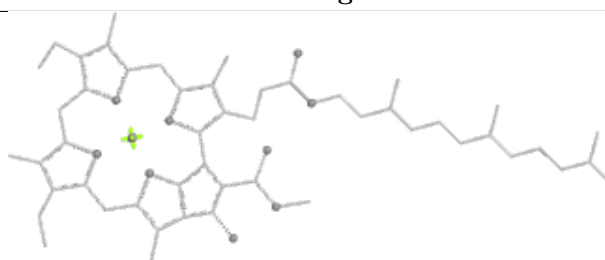
Bond lengths



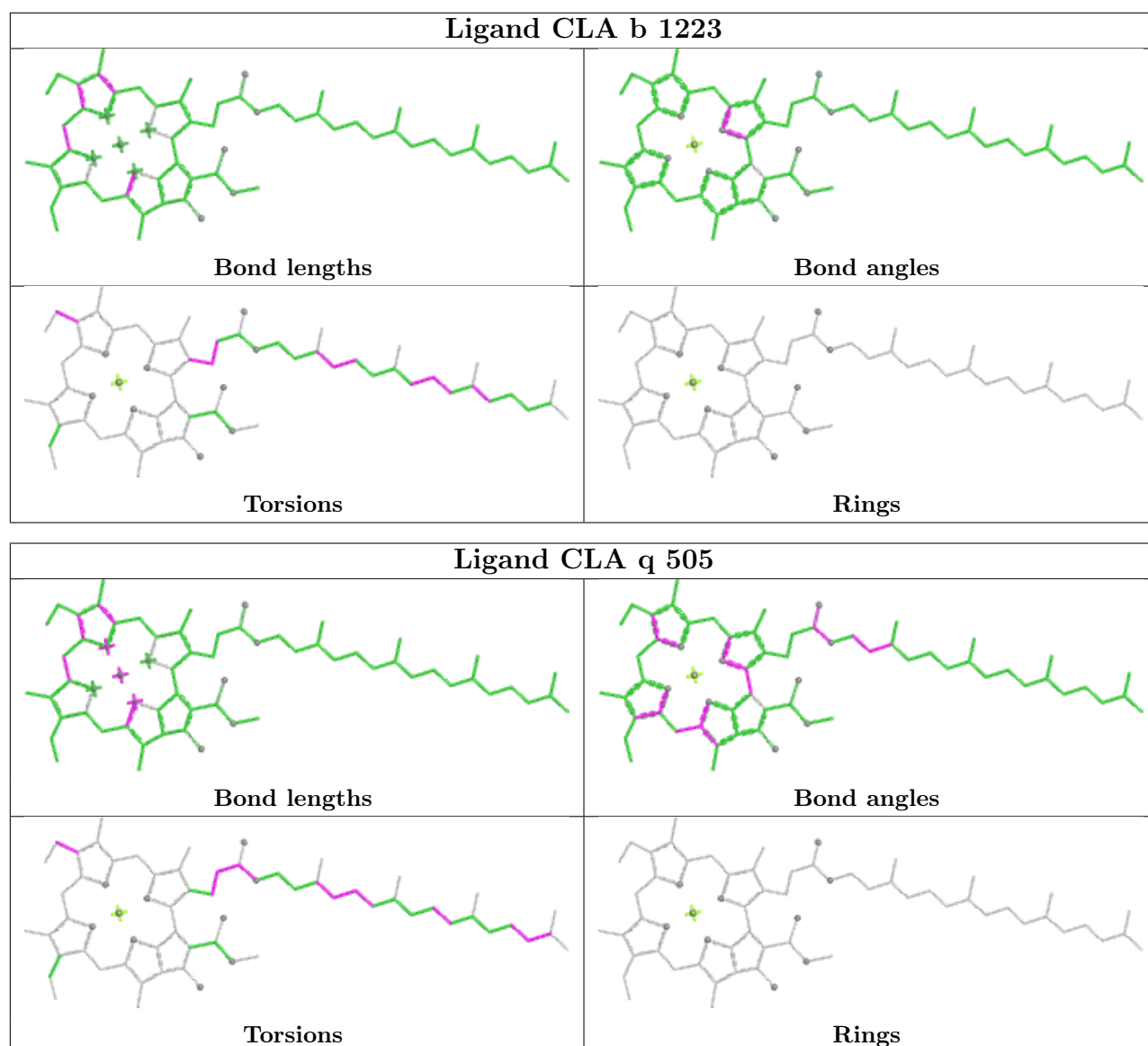
Bond angles



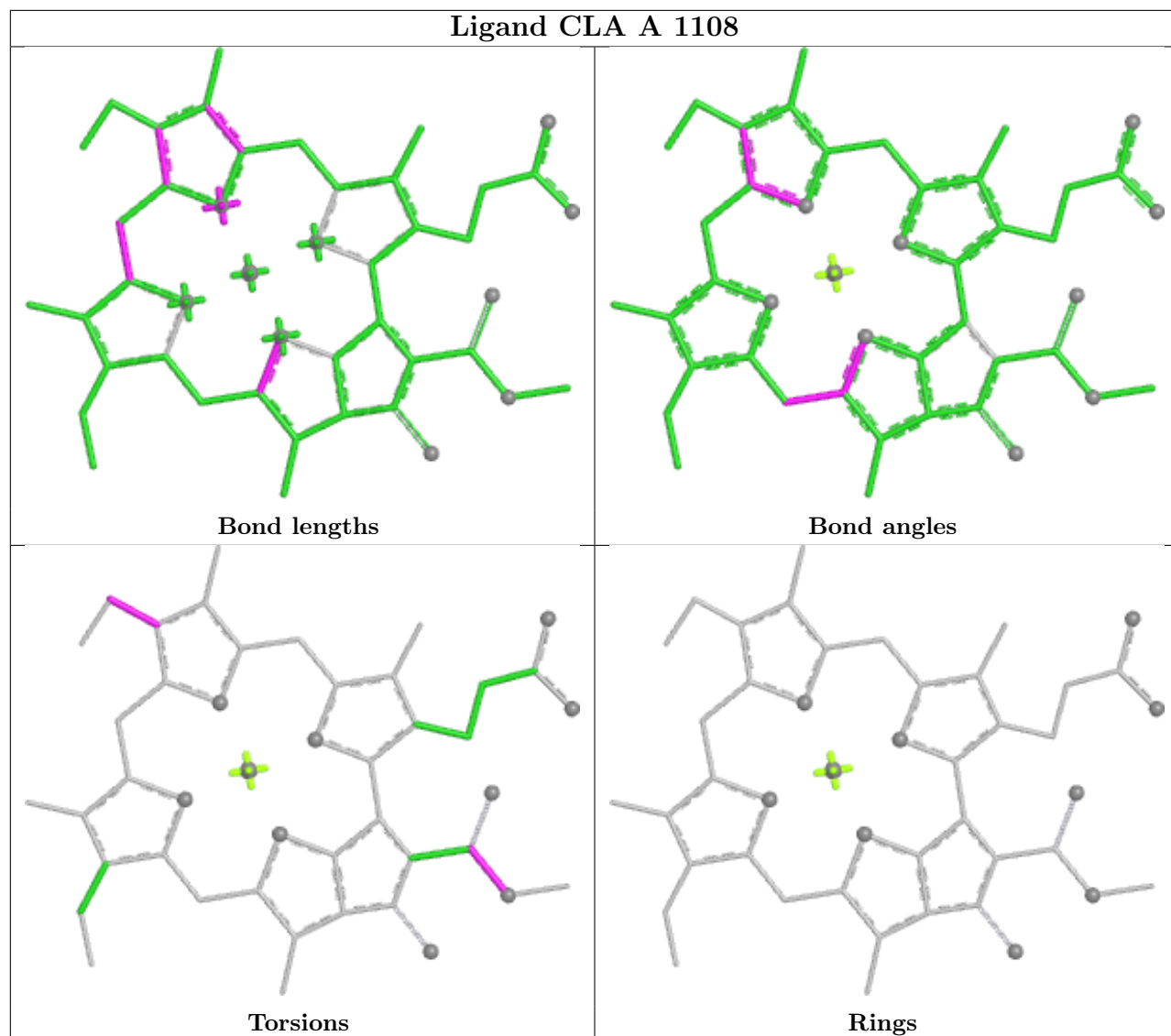
Torsions



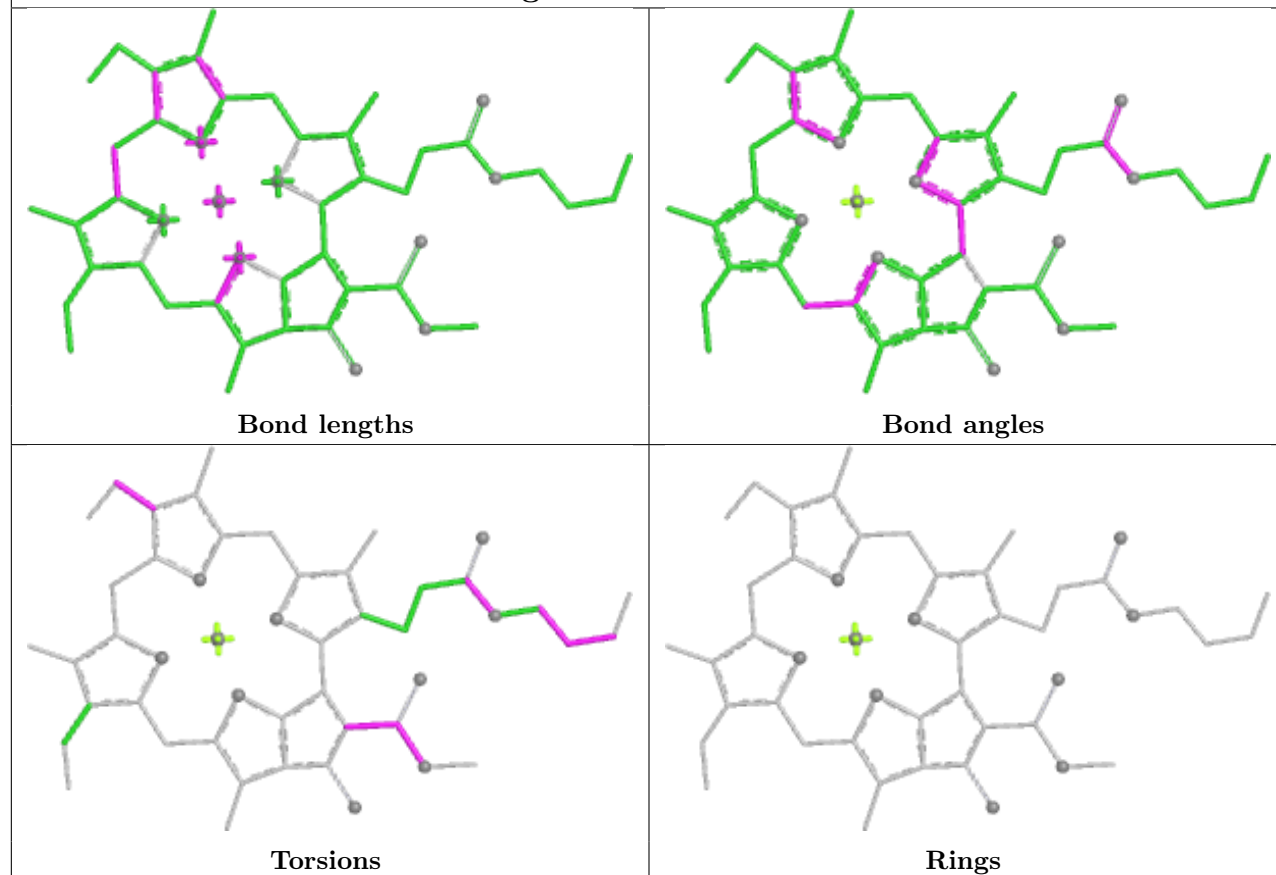
Rings



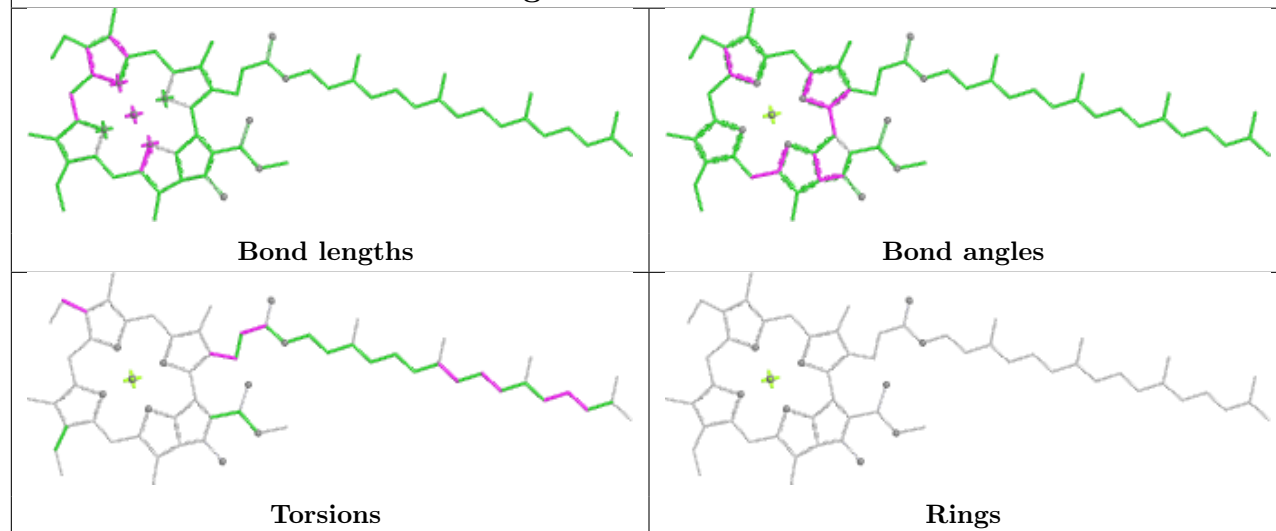
Ligand CLA A 1108

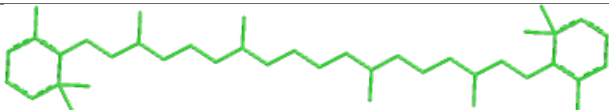
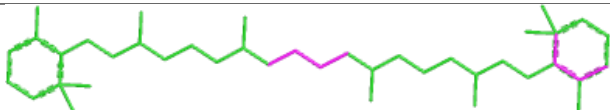
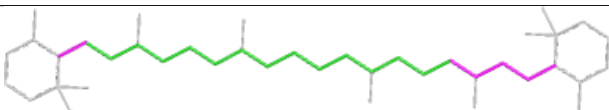
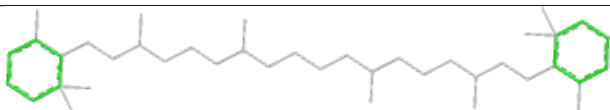


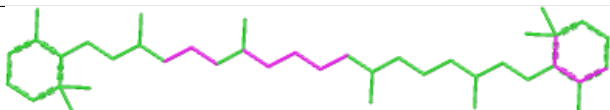
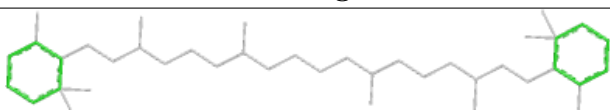
Ligand CLA G 1227



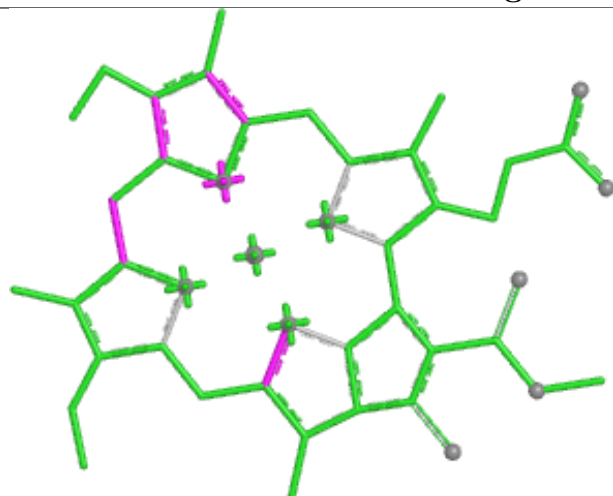
Ligand CLA B 1023



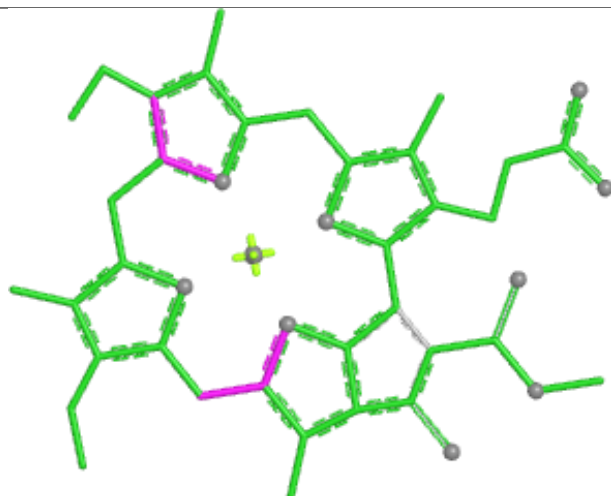
Ligand BCR Y 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR G 4017	
	
Bond lengths	Bond angles
	
Torsions	Rings

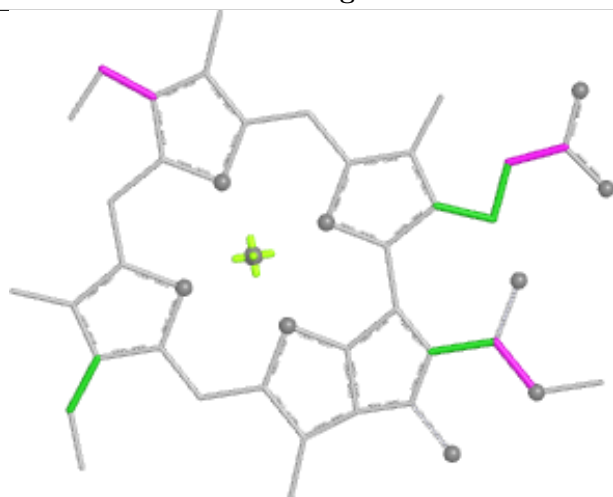
Ligand CLA A 1134



Bond lengths



Bond angles

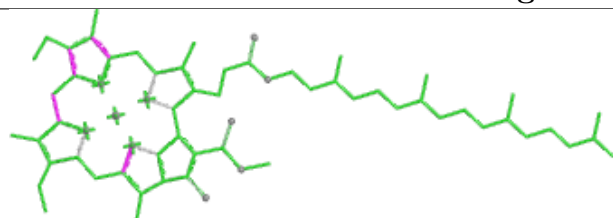


Torsions

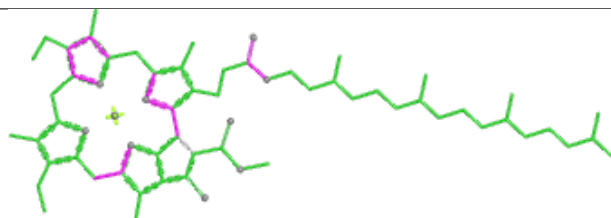


Rings

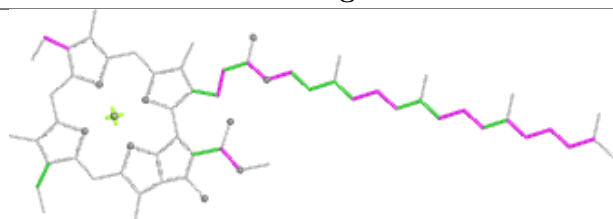
Ligand CLA u 515



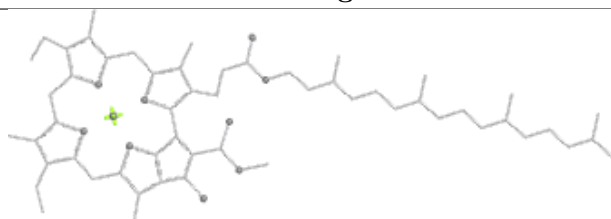
Bond lengths



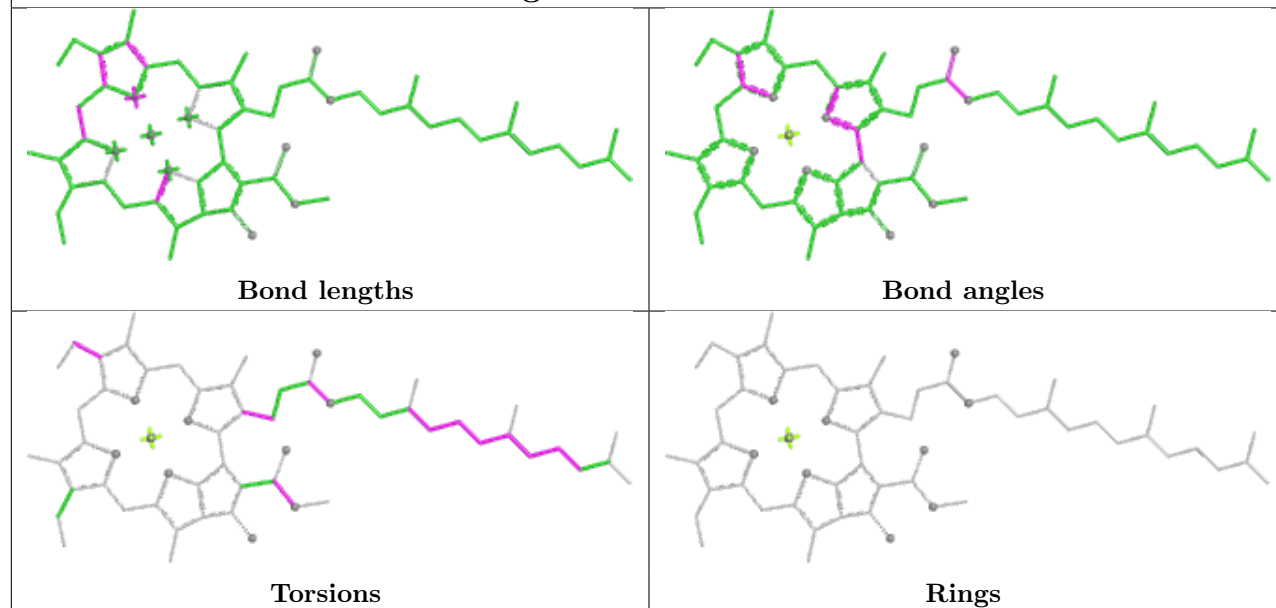
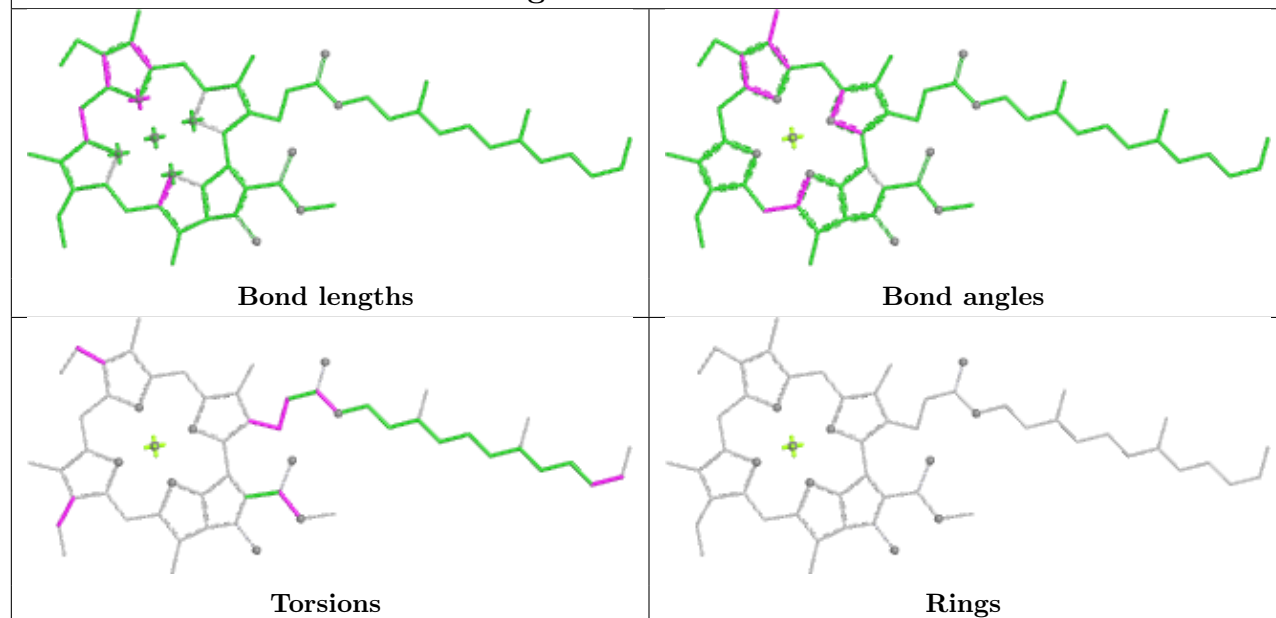
Bond angles



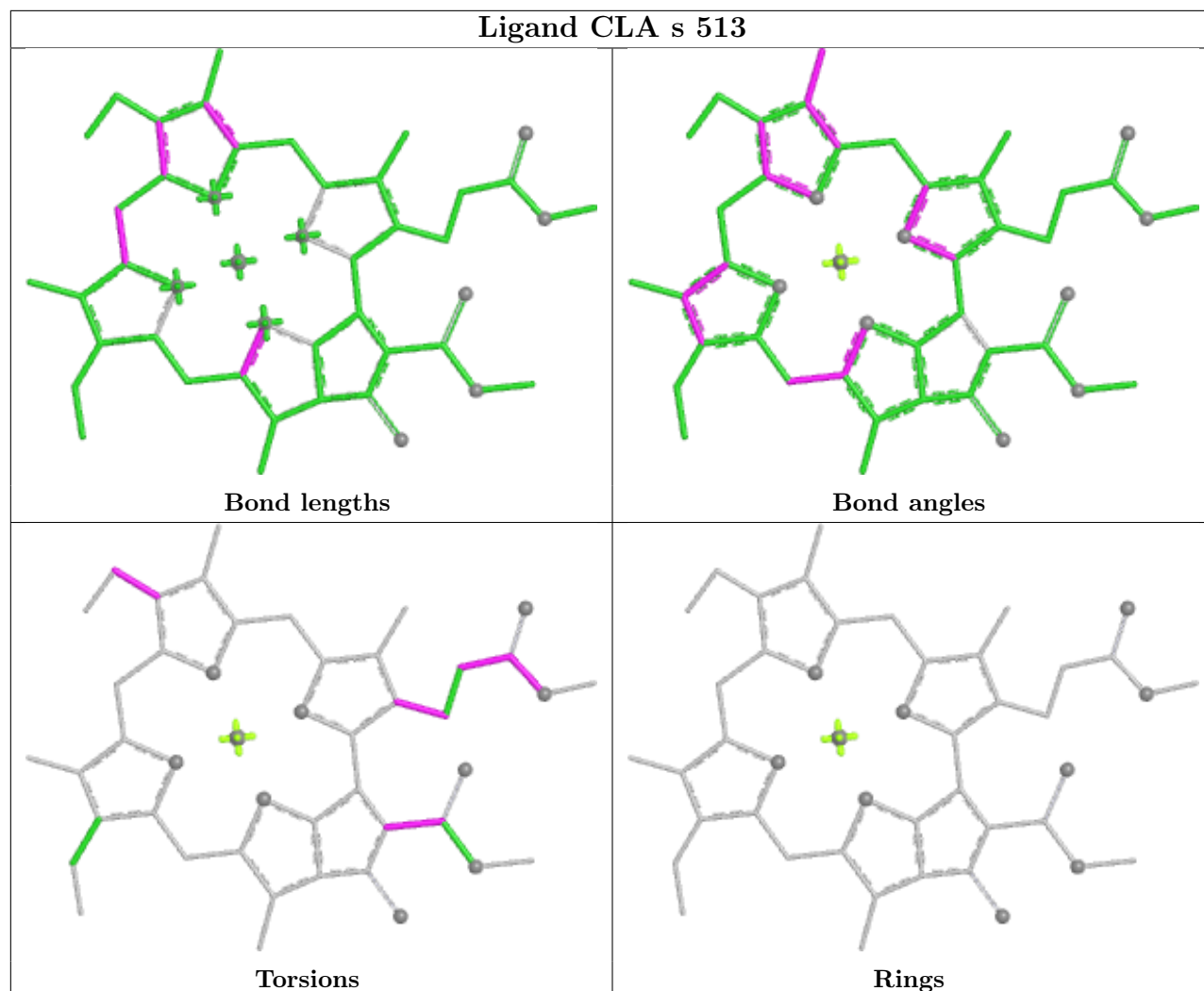
Torsions



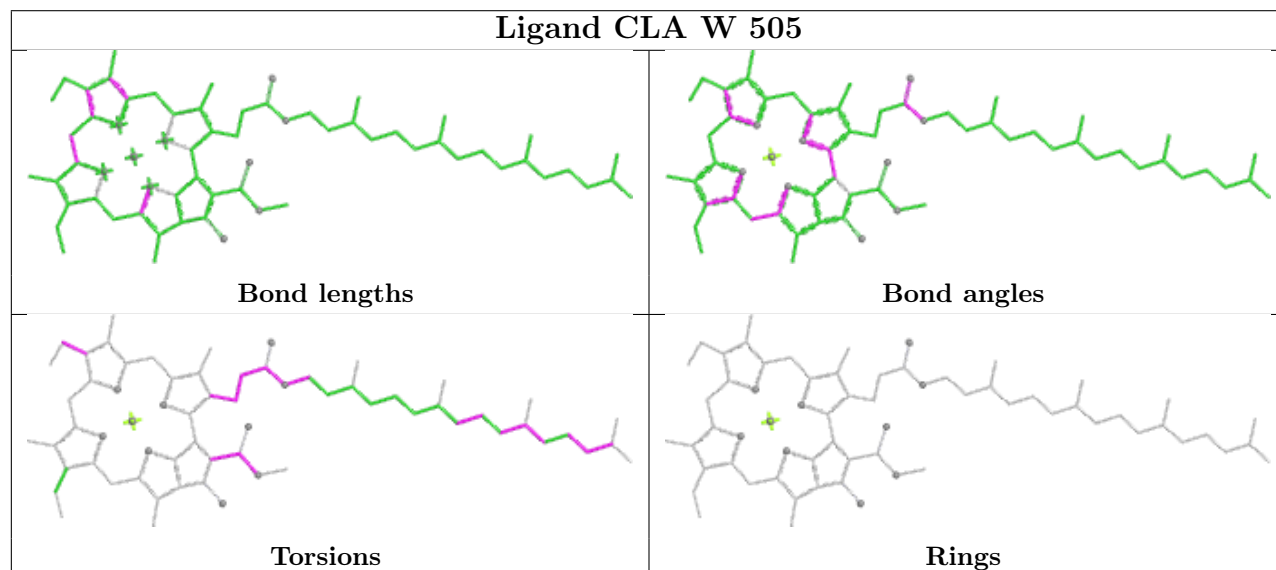
Rings

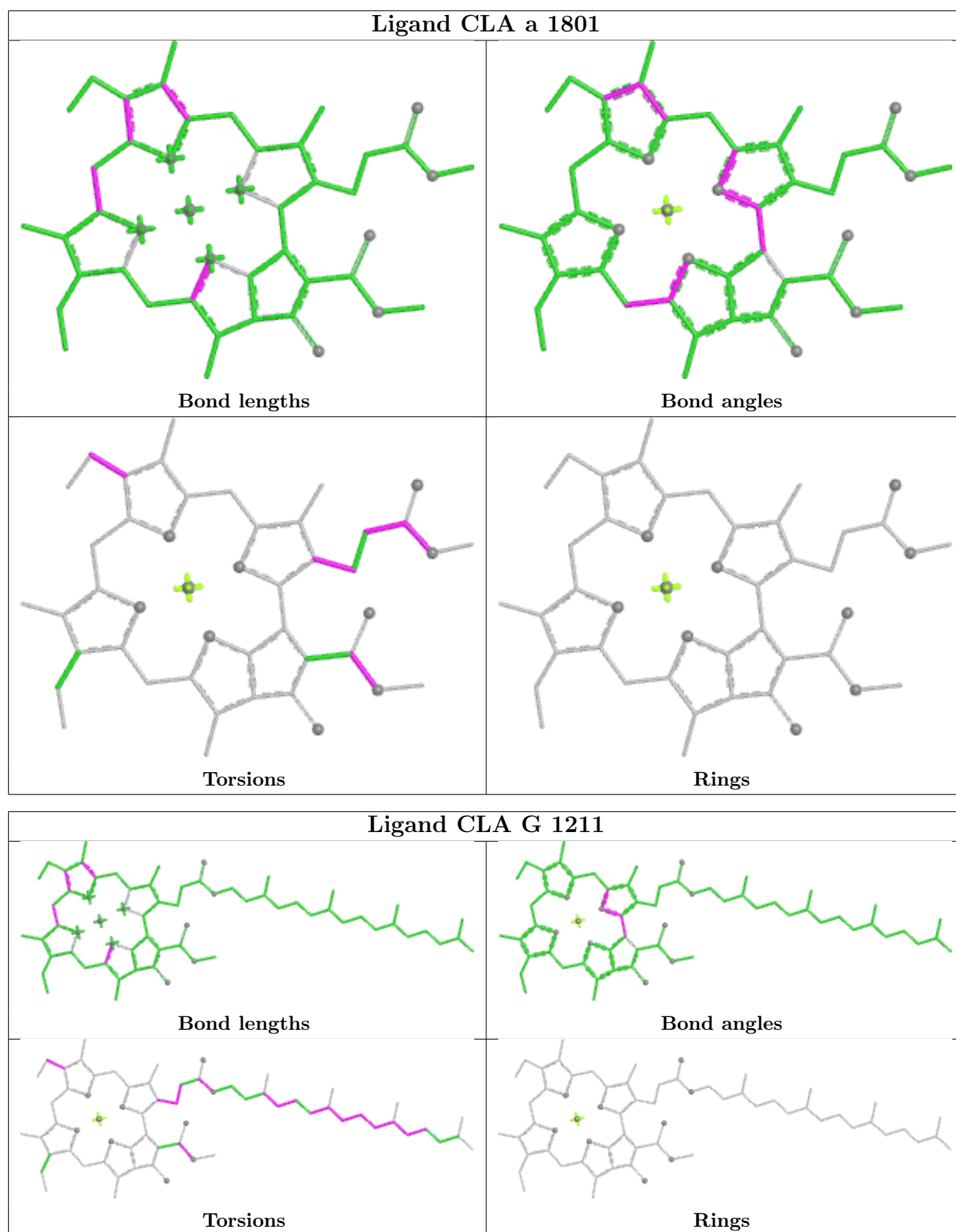
Ligand CLA A 1139**Ligand CLA a 1122**

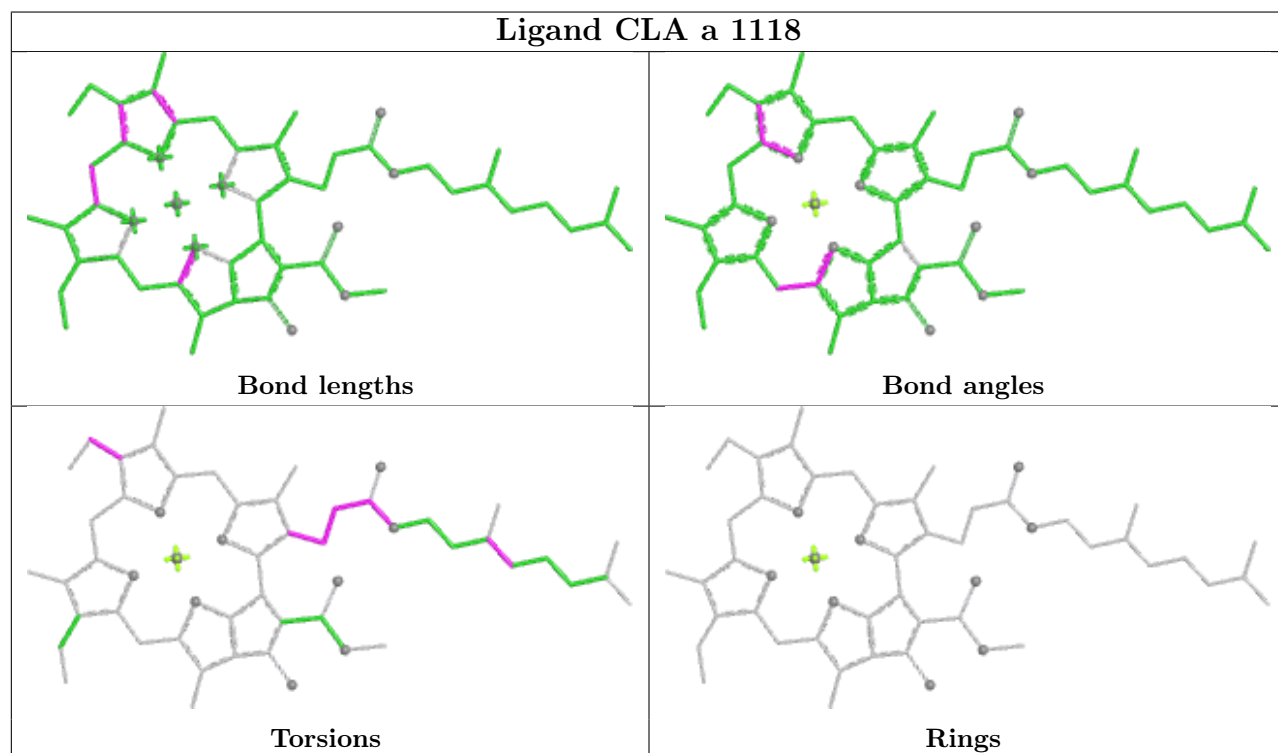
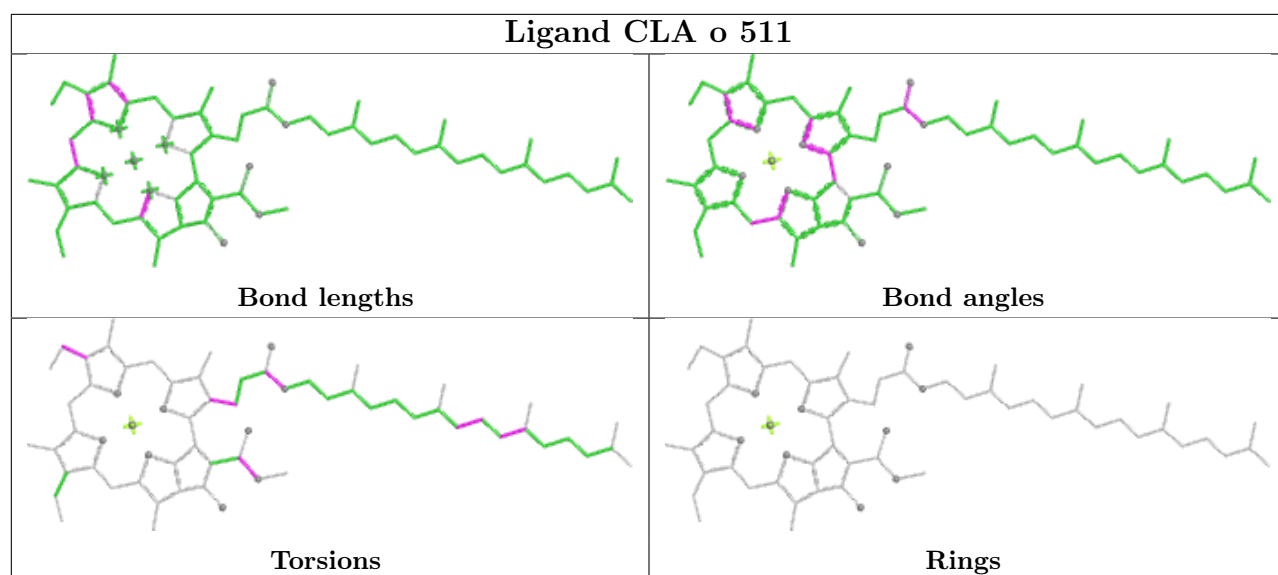
Ligand CLA s 513

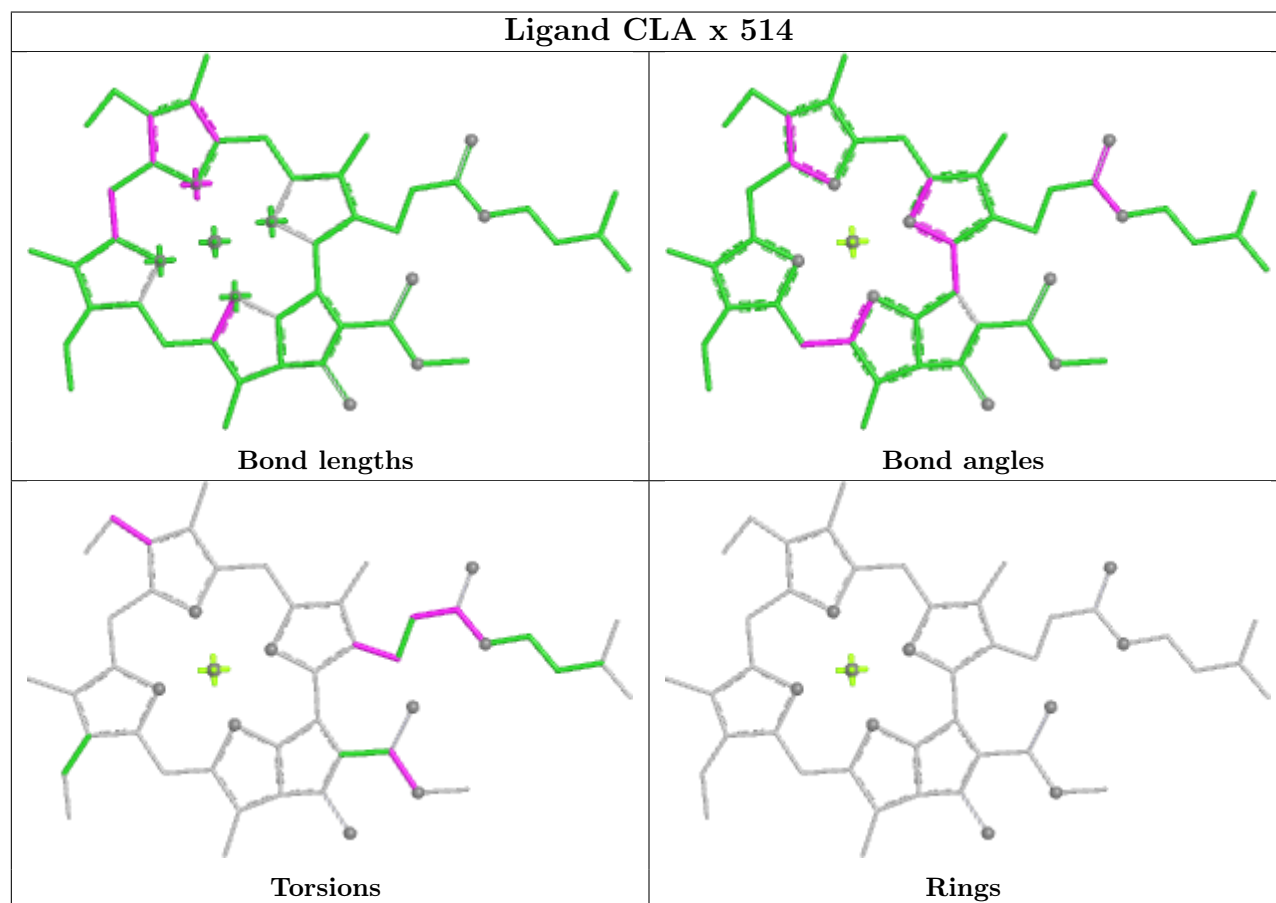
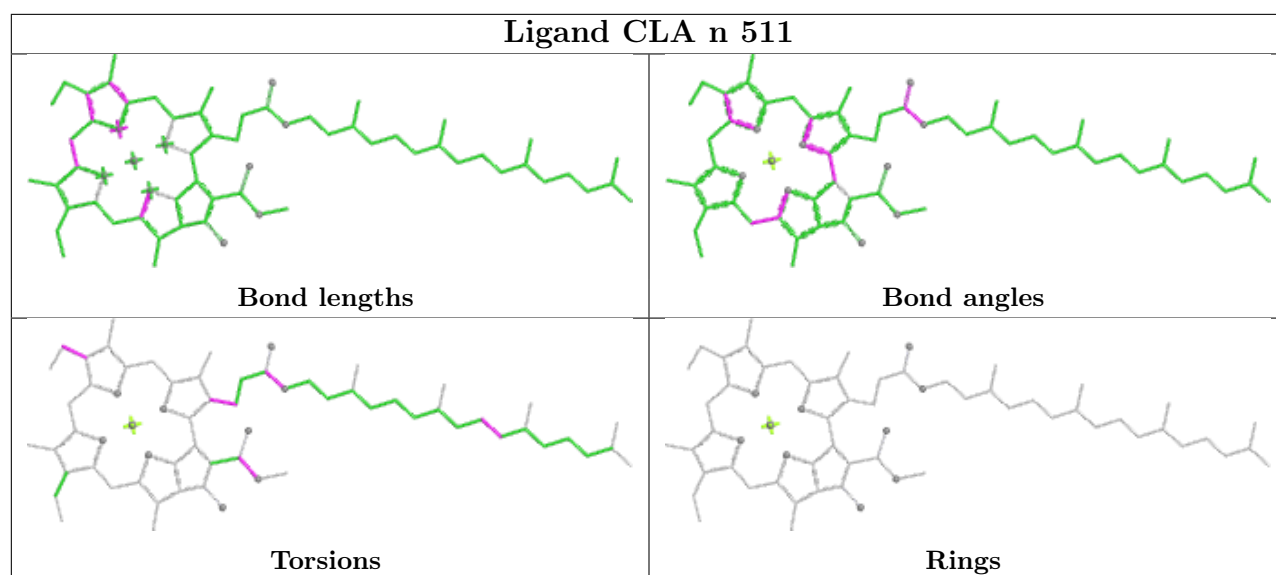


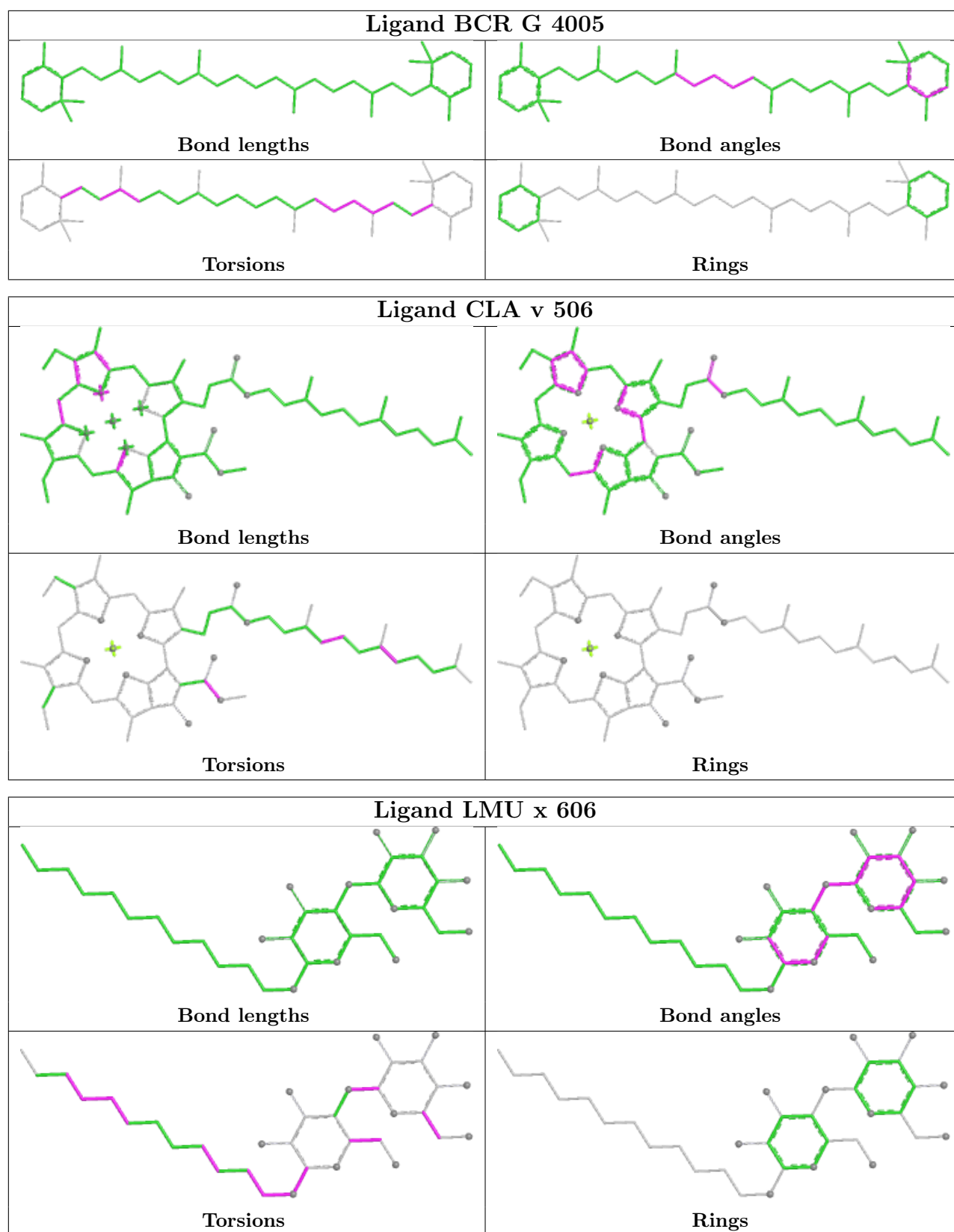
Ligand CLA W 505

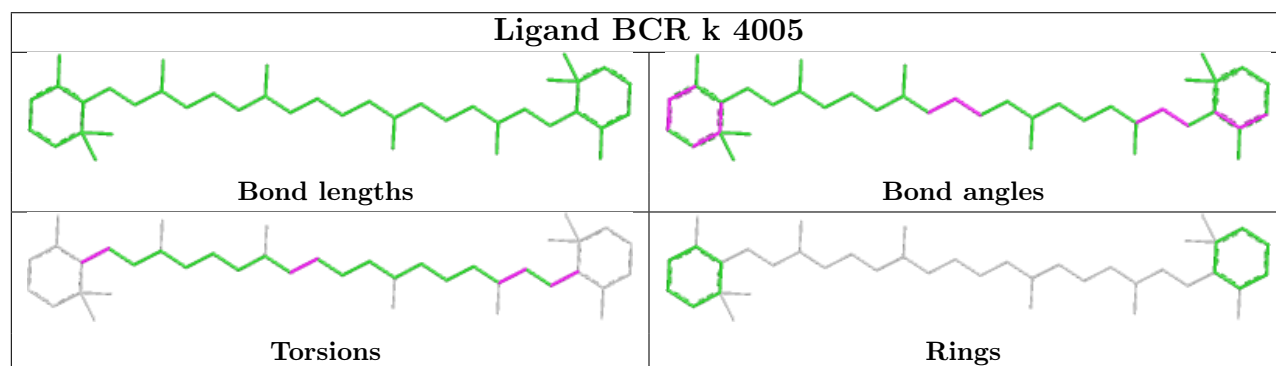
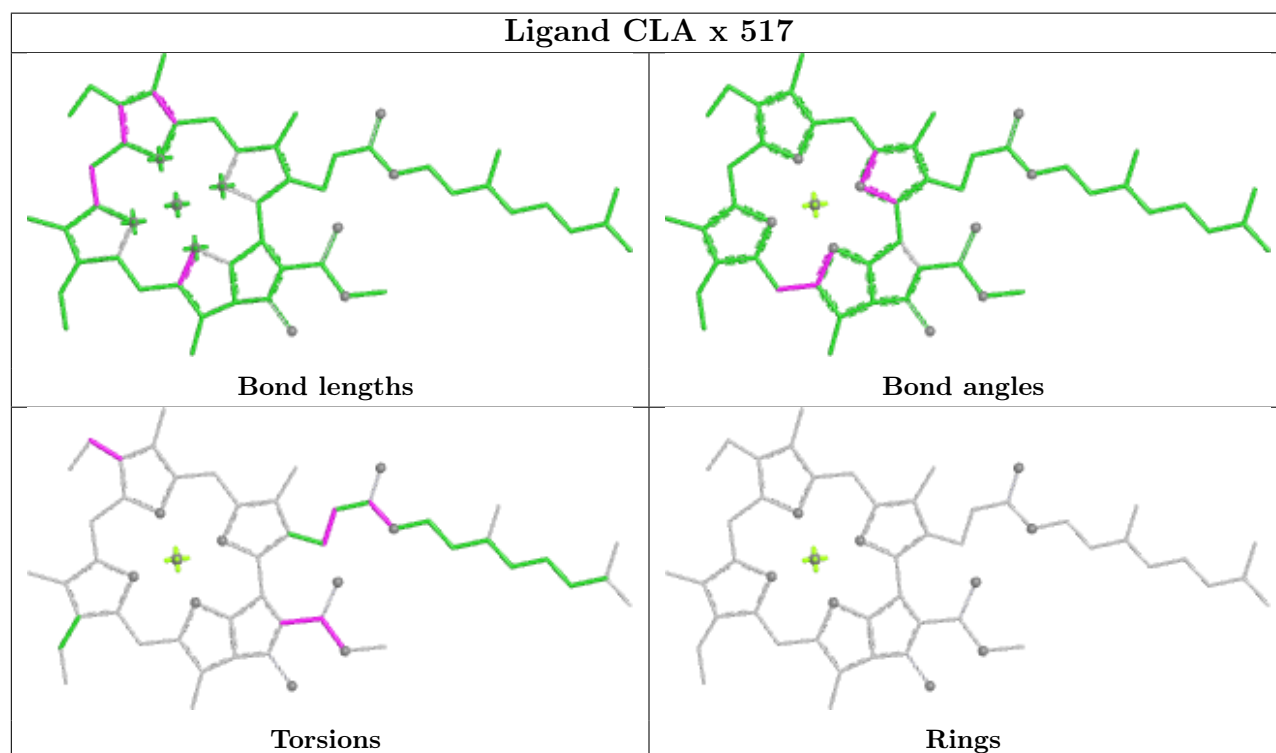
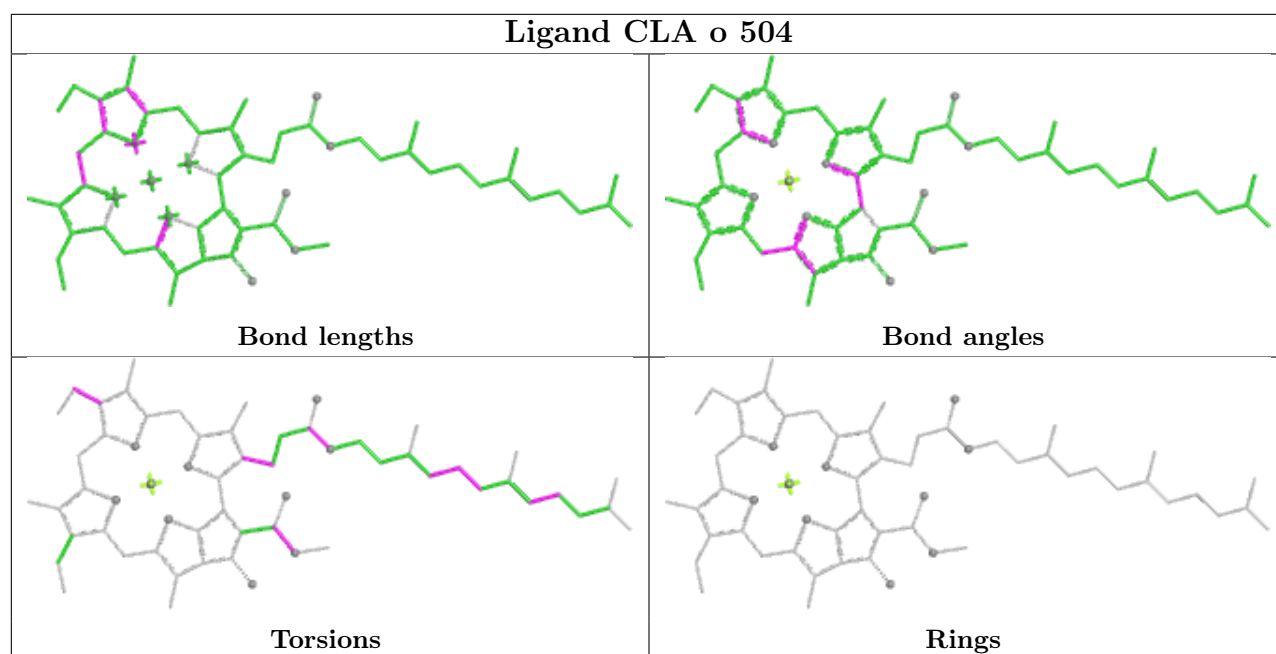


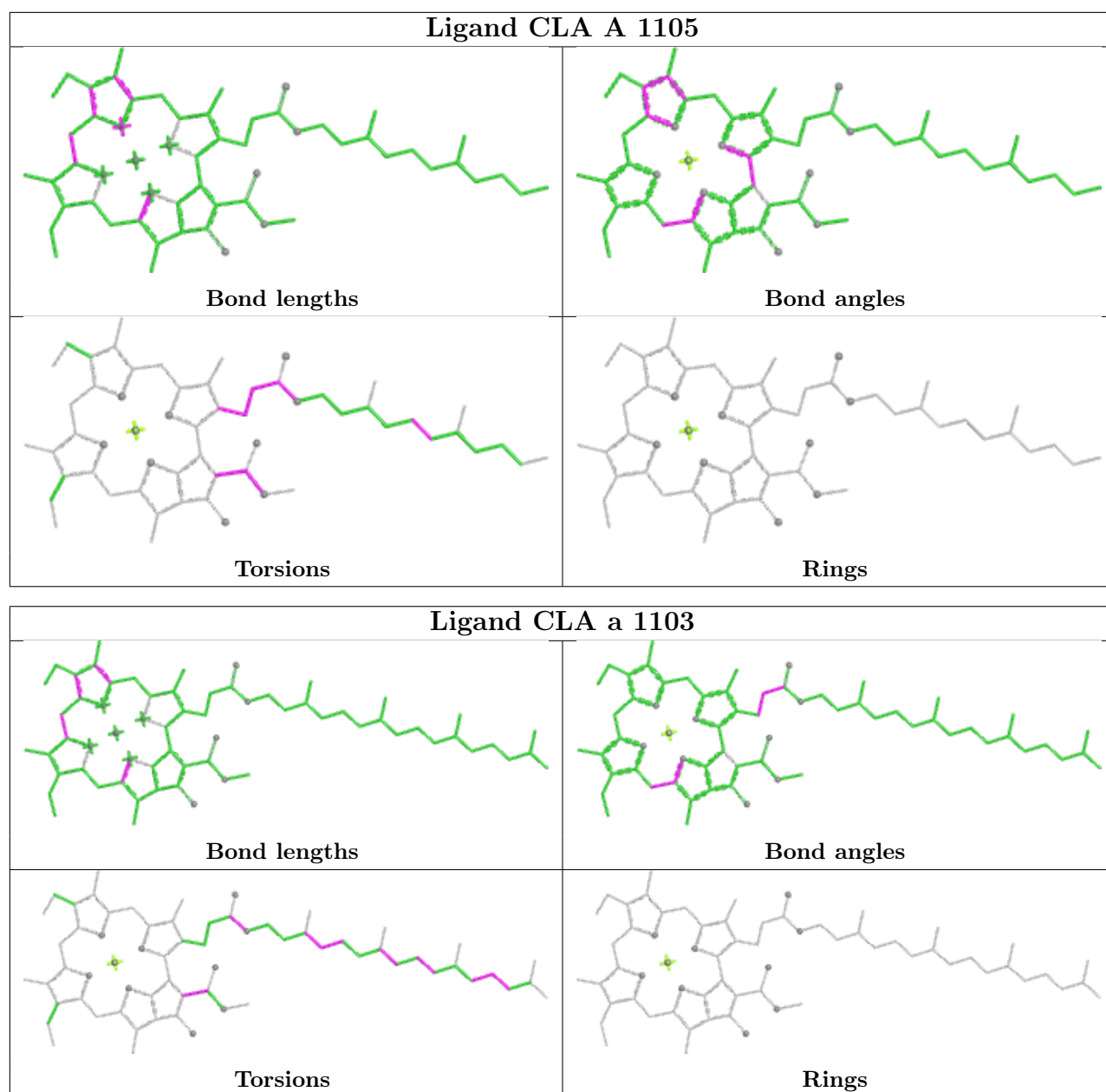




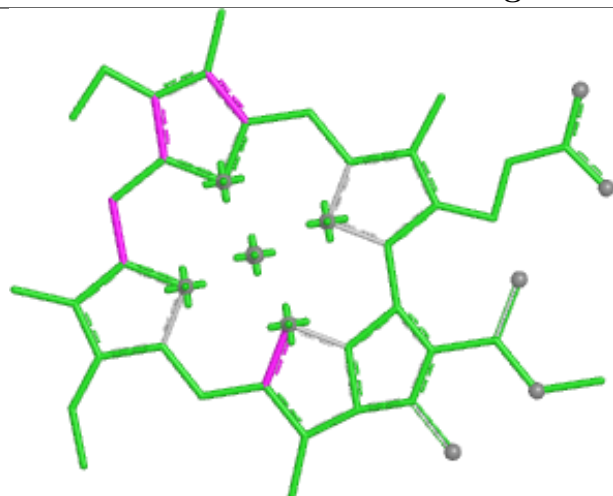




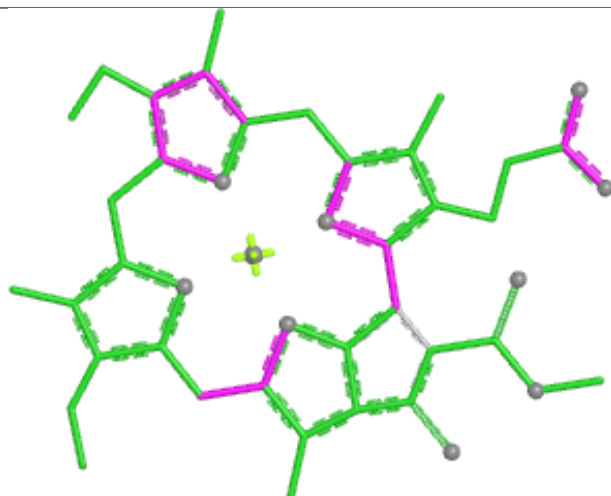




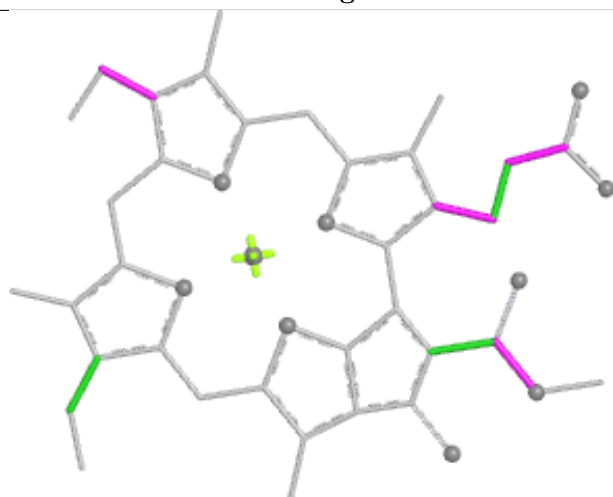
Ligand CLA G 1208



Bond lengths



Bond angles

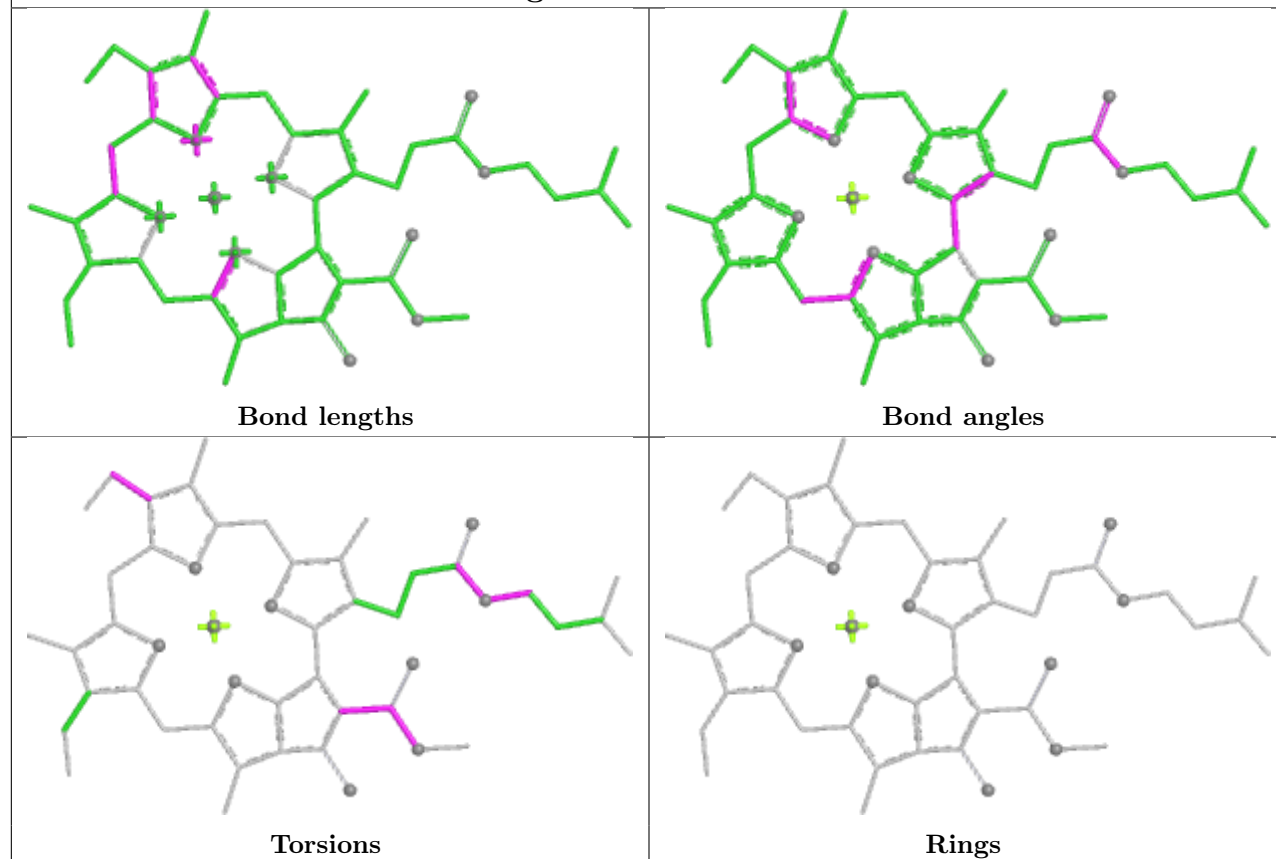


Torsions

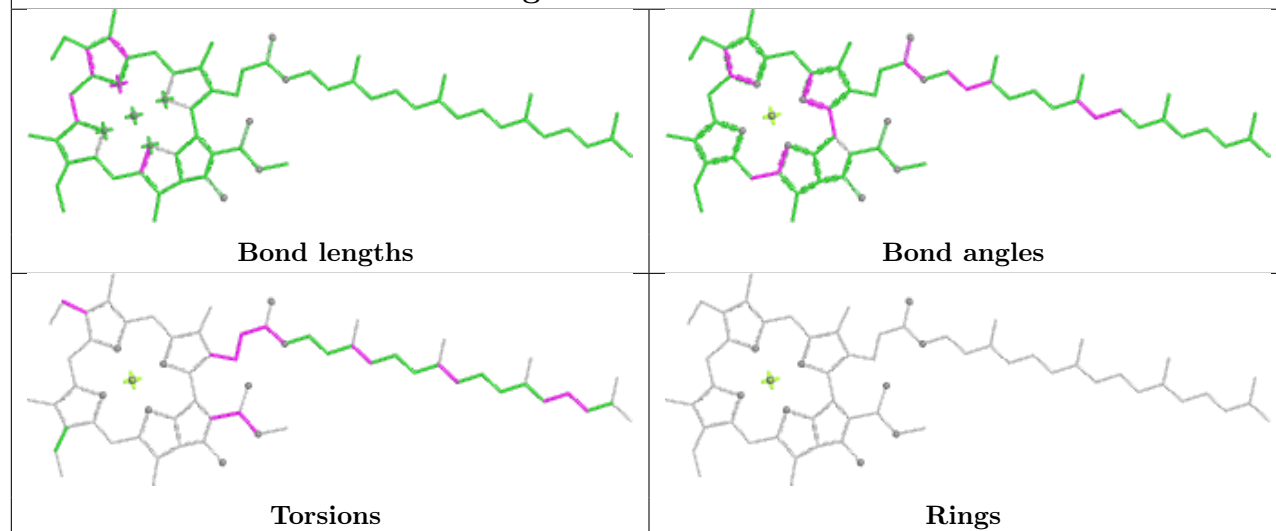


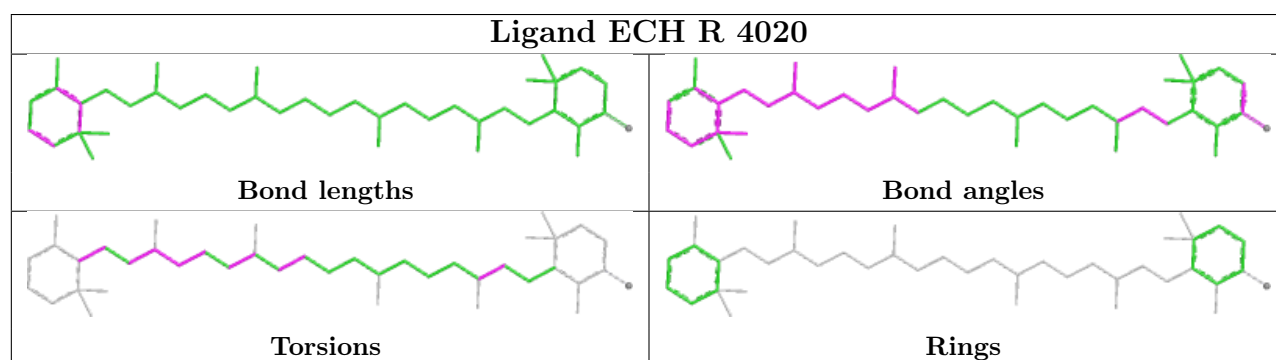
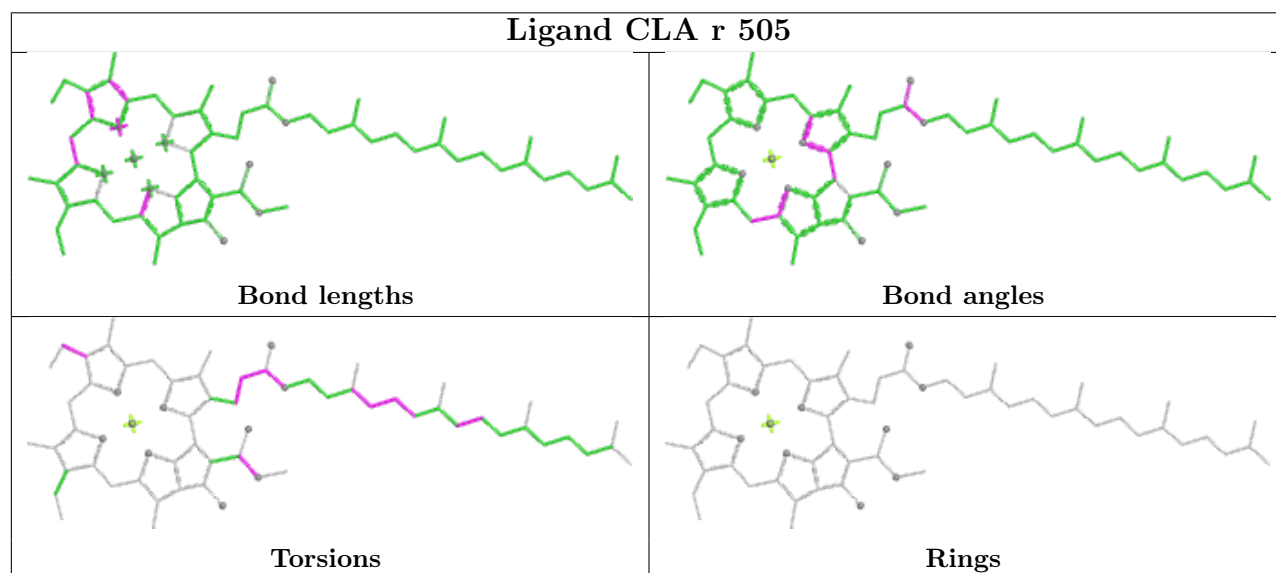
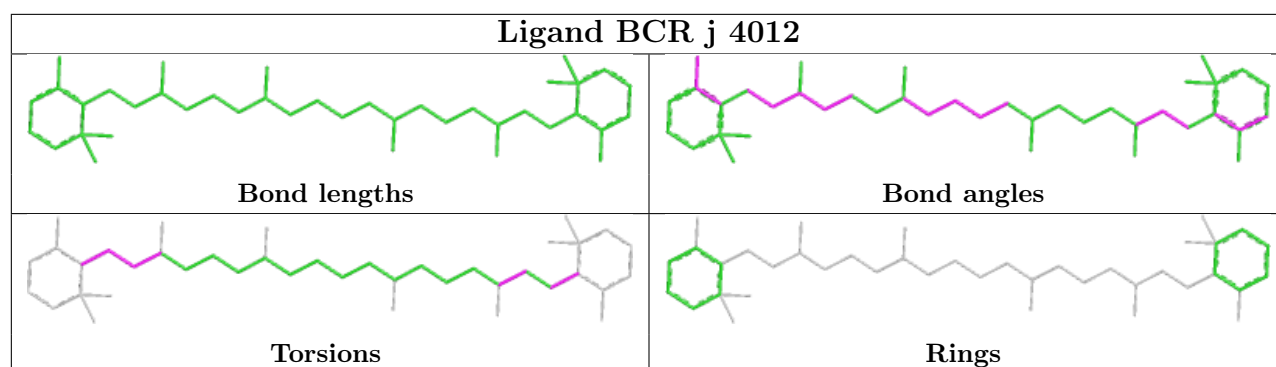
Rings

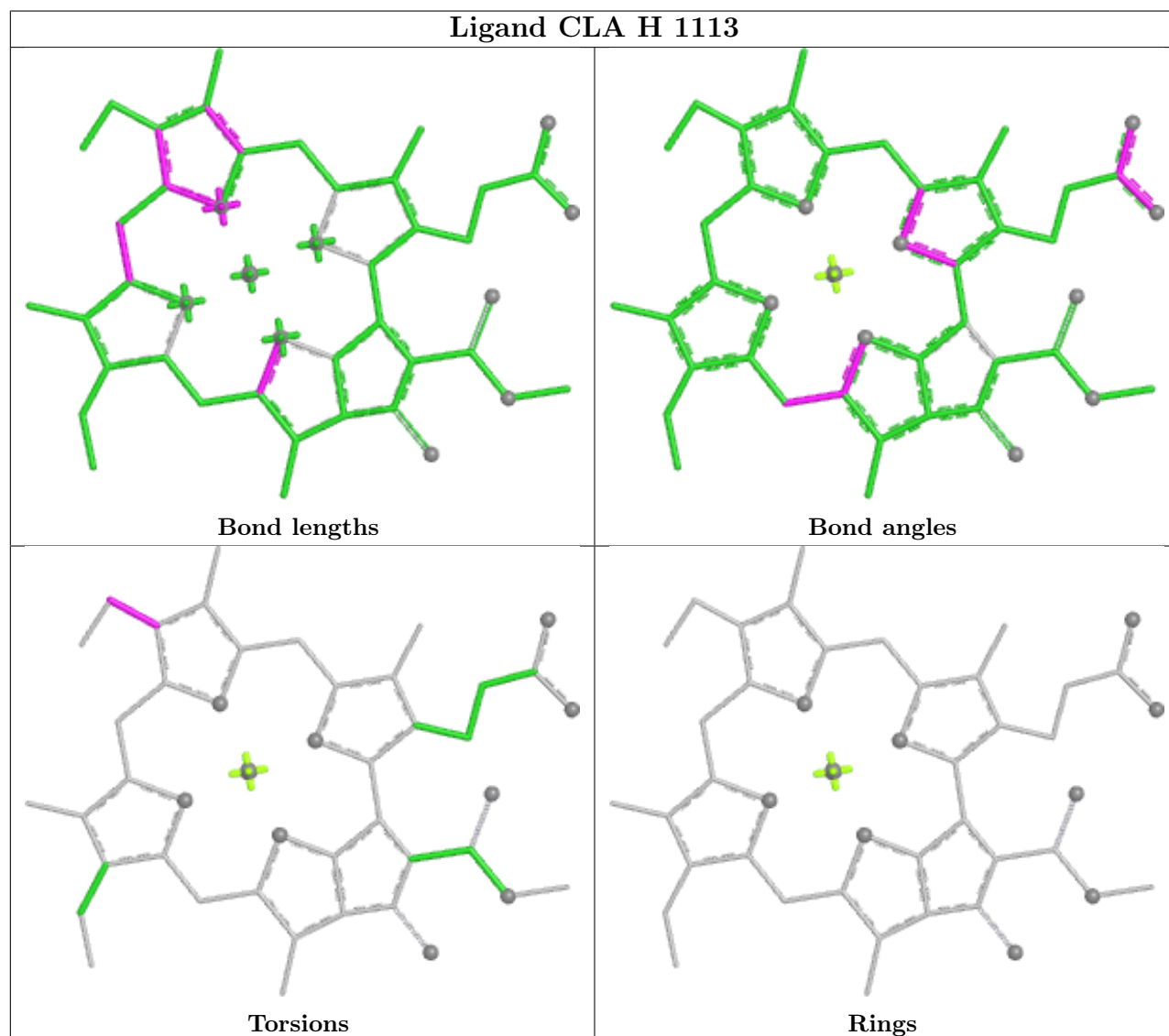
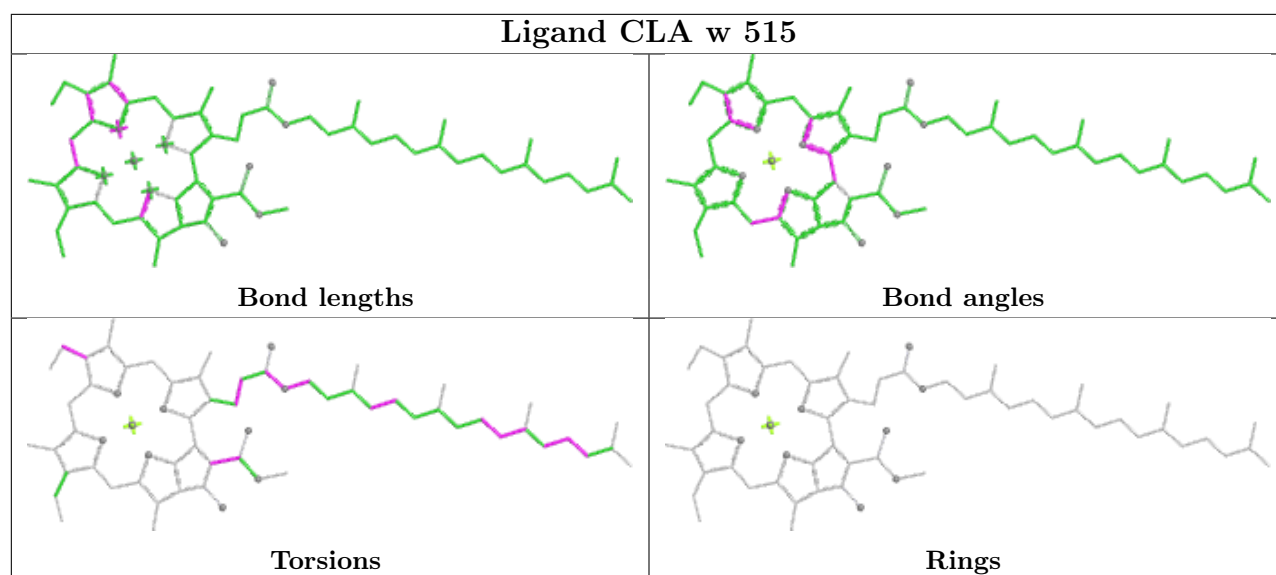
Ligand CLA b 1222

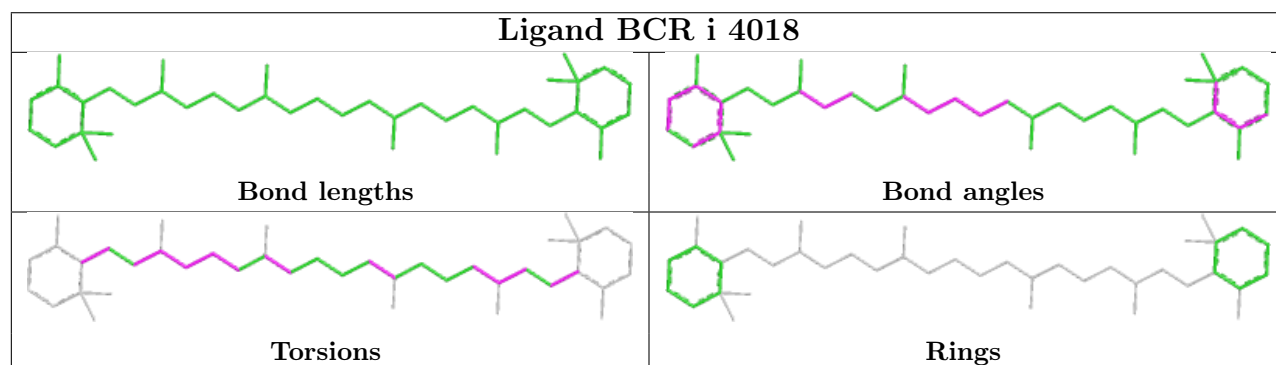
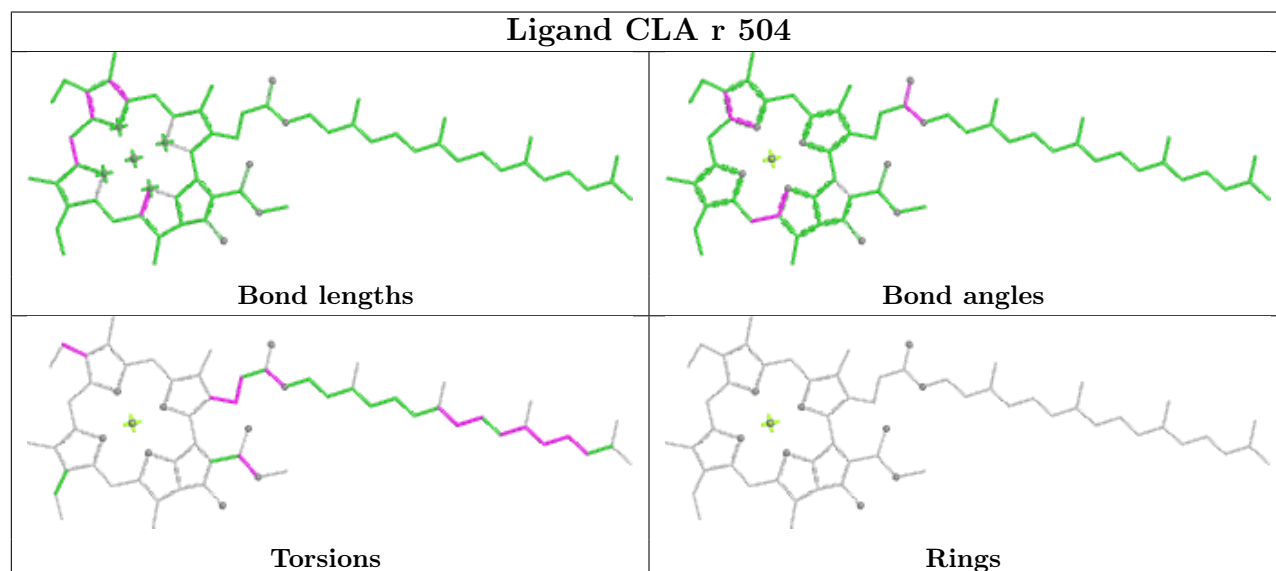
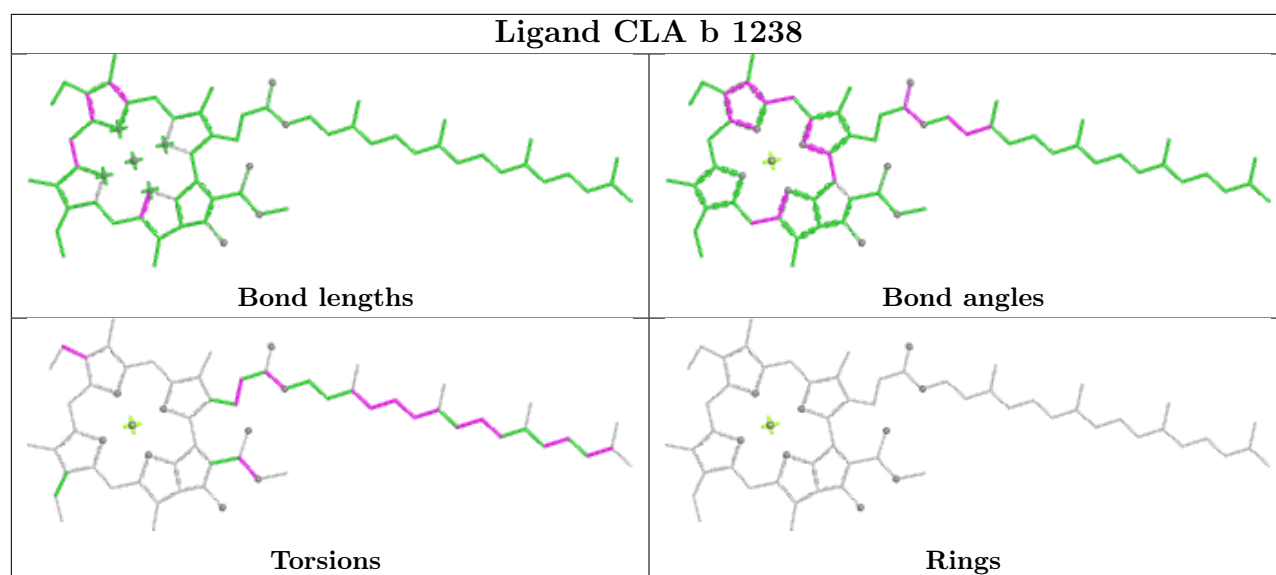


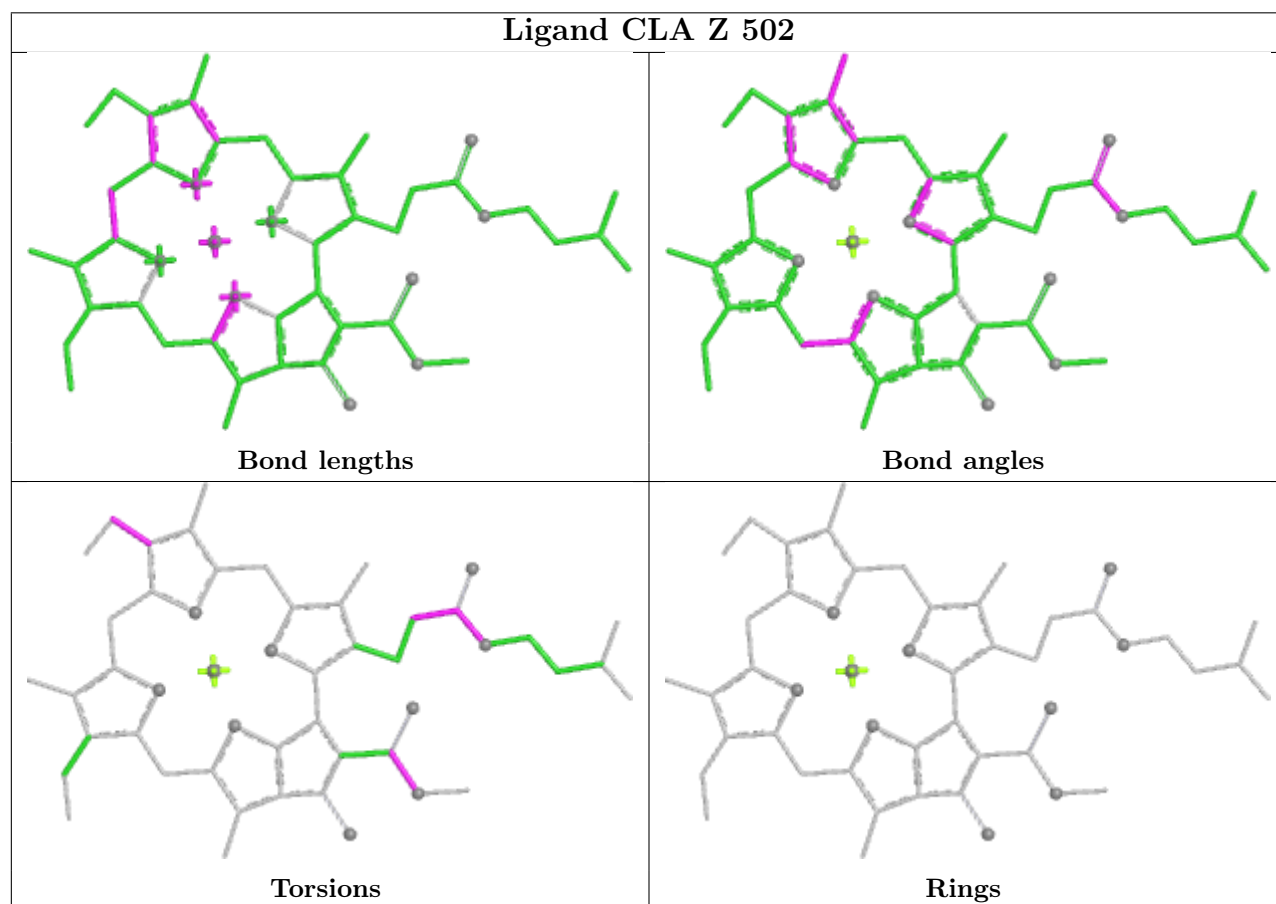
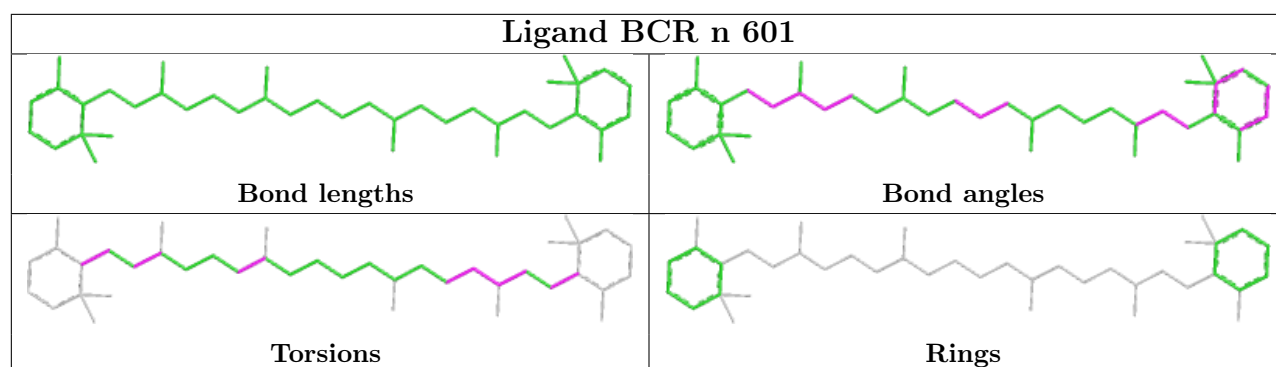
Ligand CLA A 1101

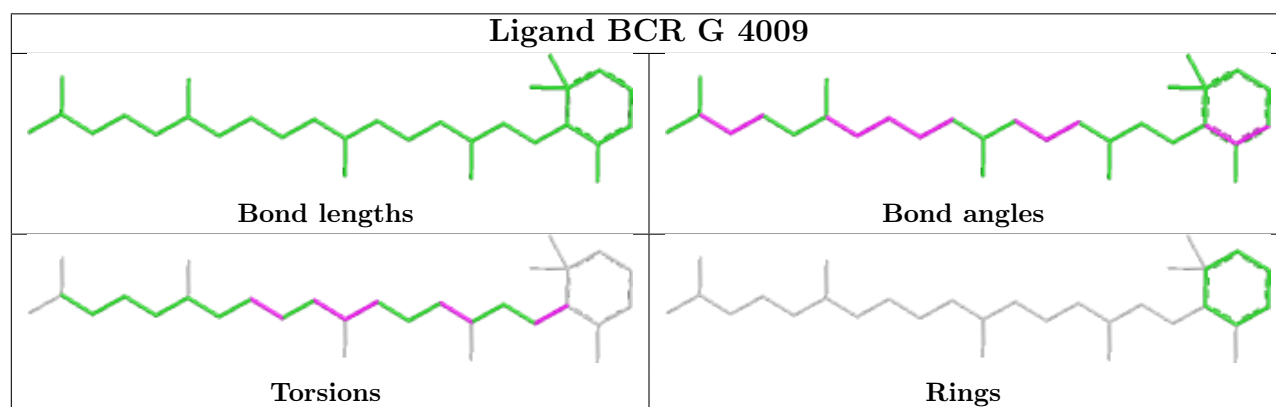
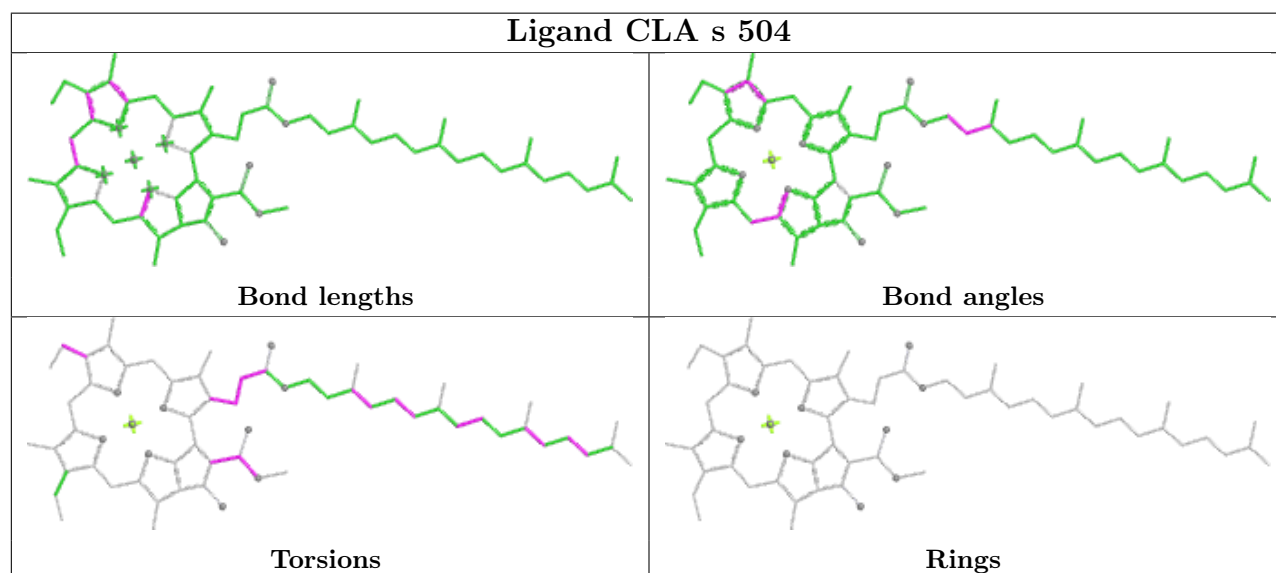
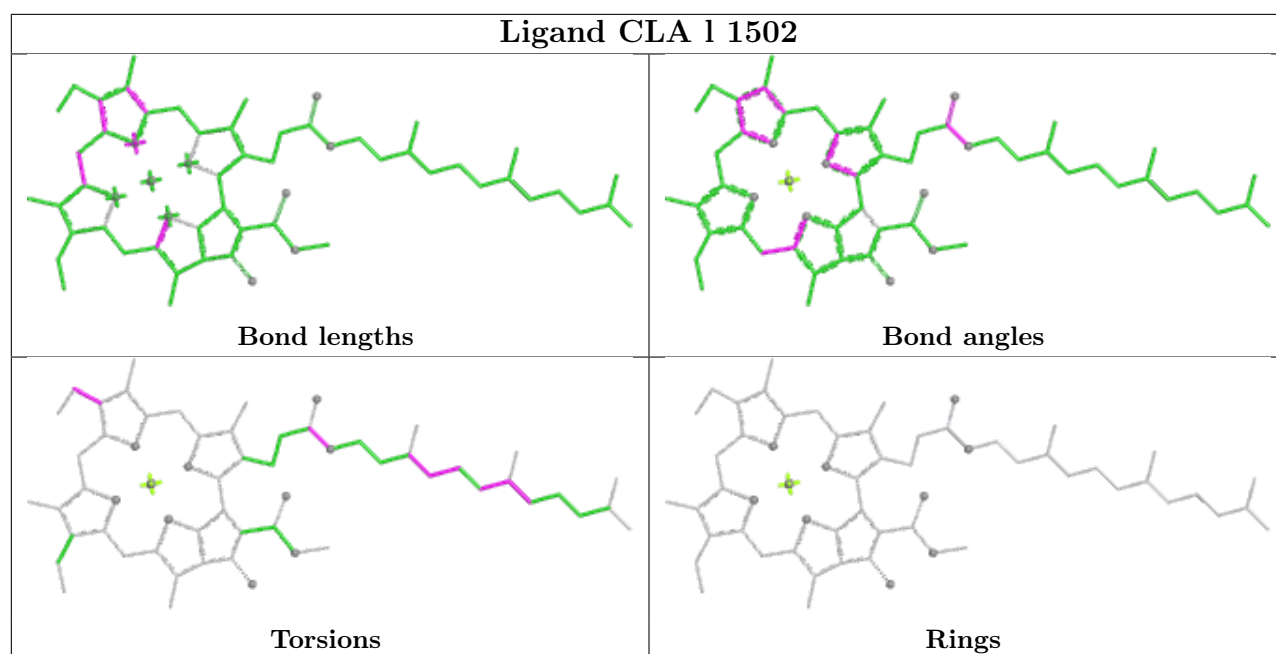


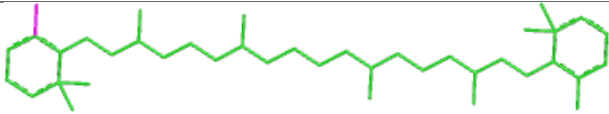
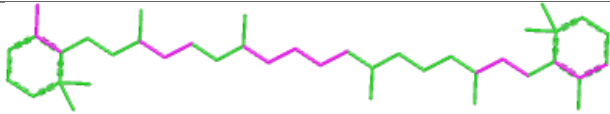
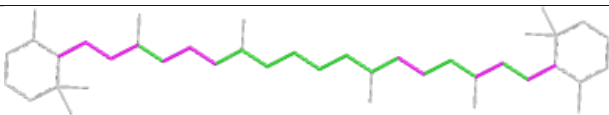
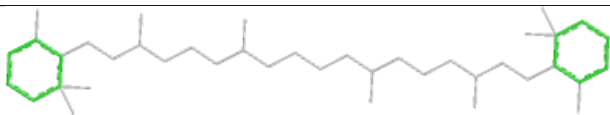


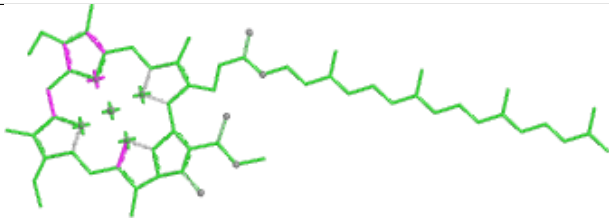
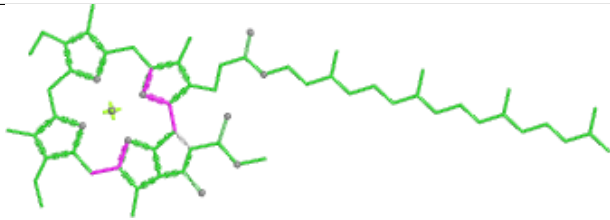
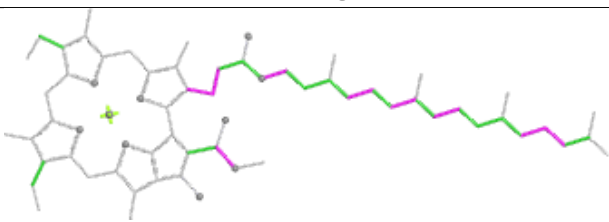
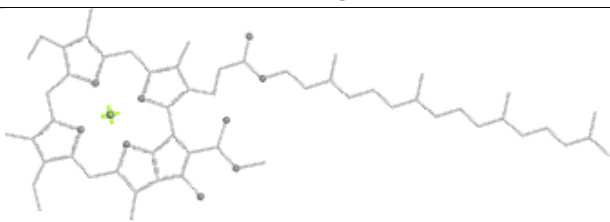


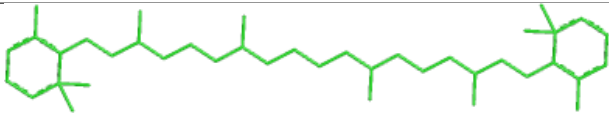
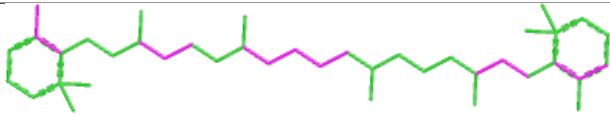
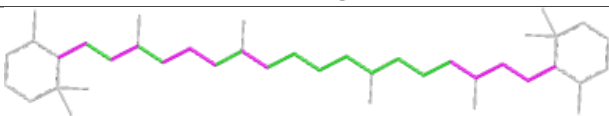
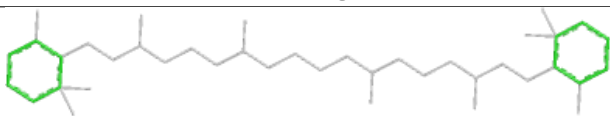




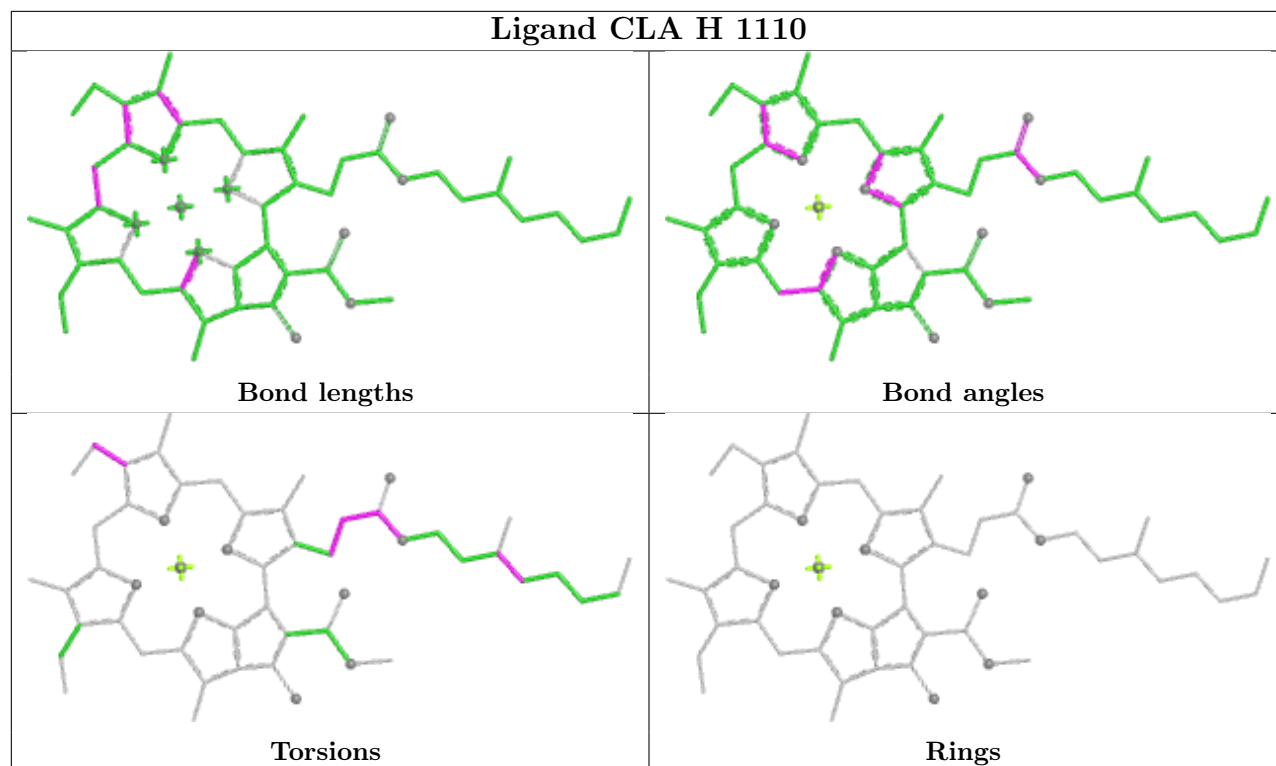


Ligand BCR T 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

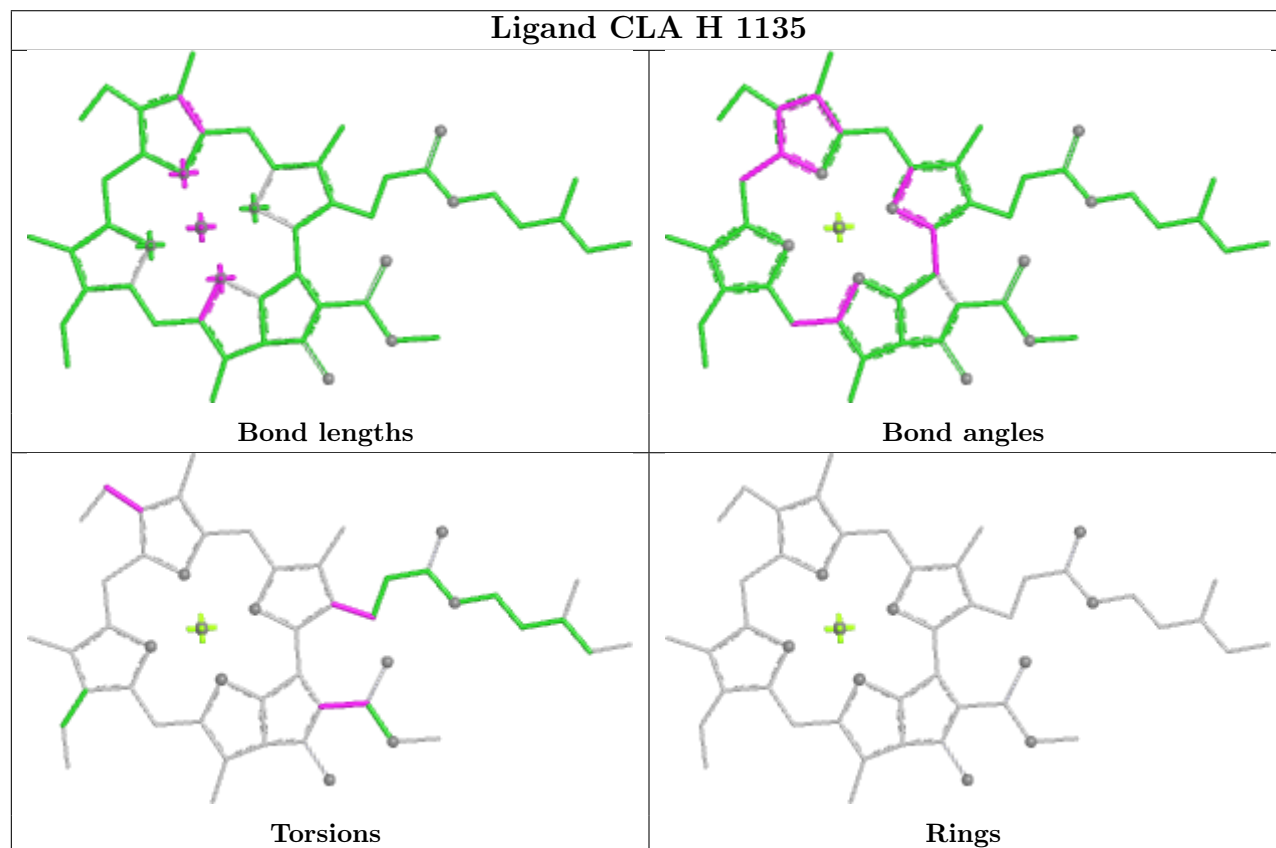
Ligand CLA a 1126	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR y 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

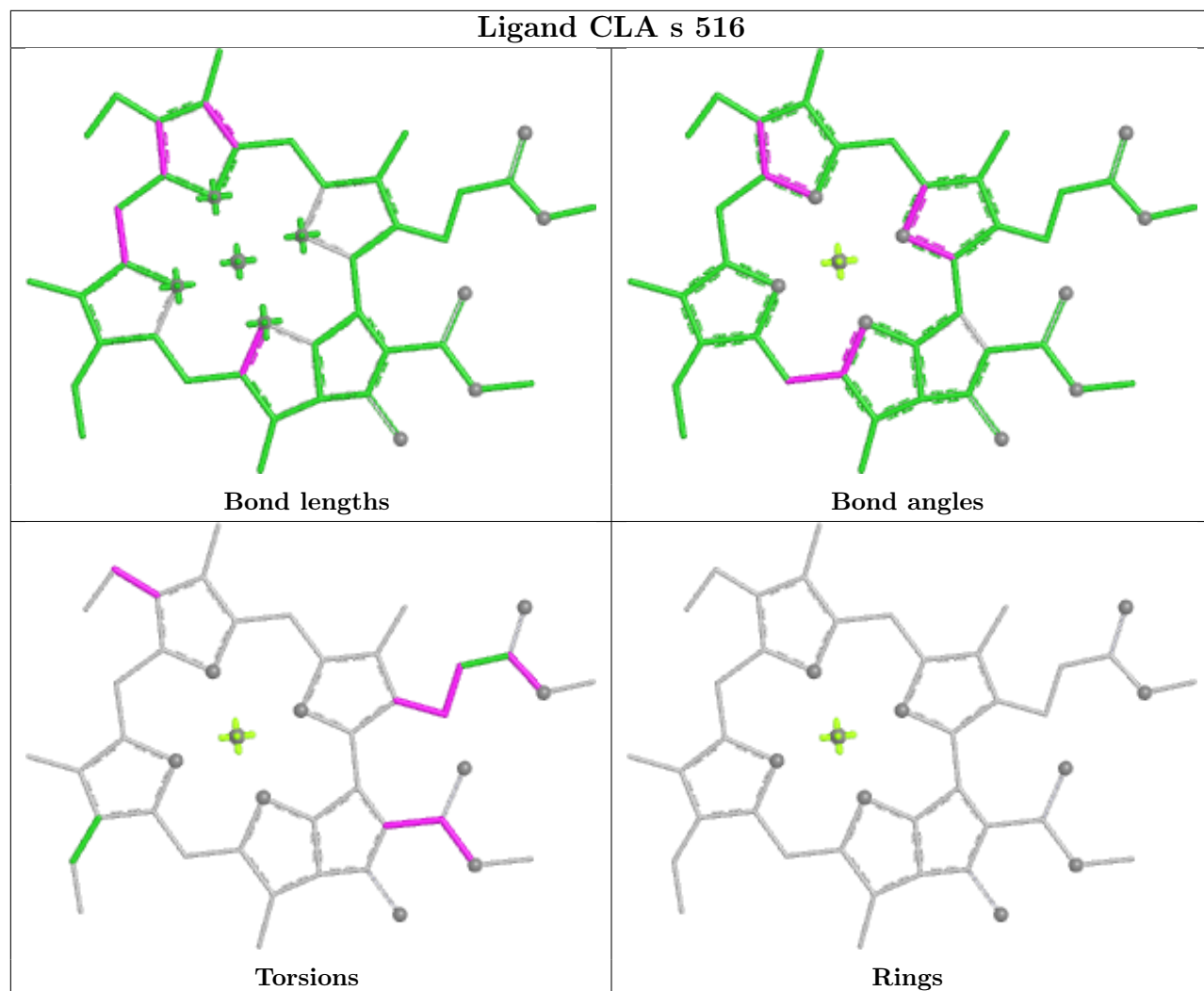
Ligand CLA H 1110



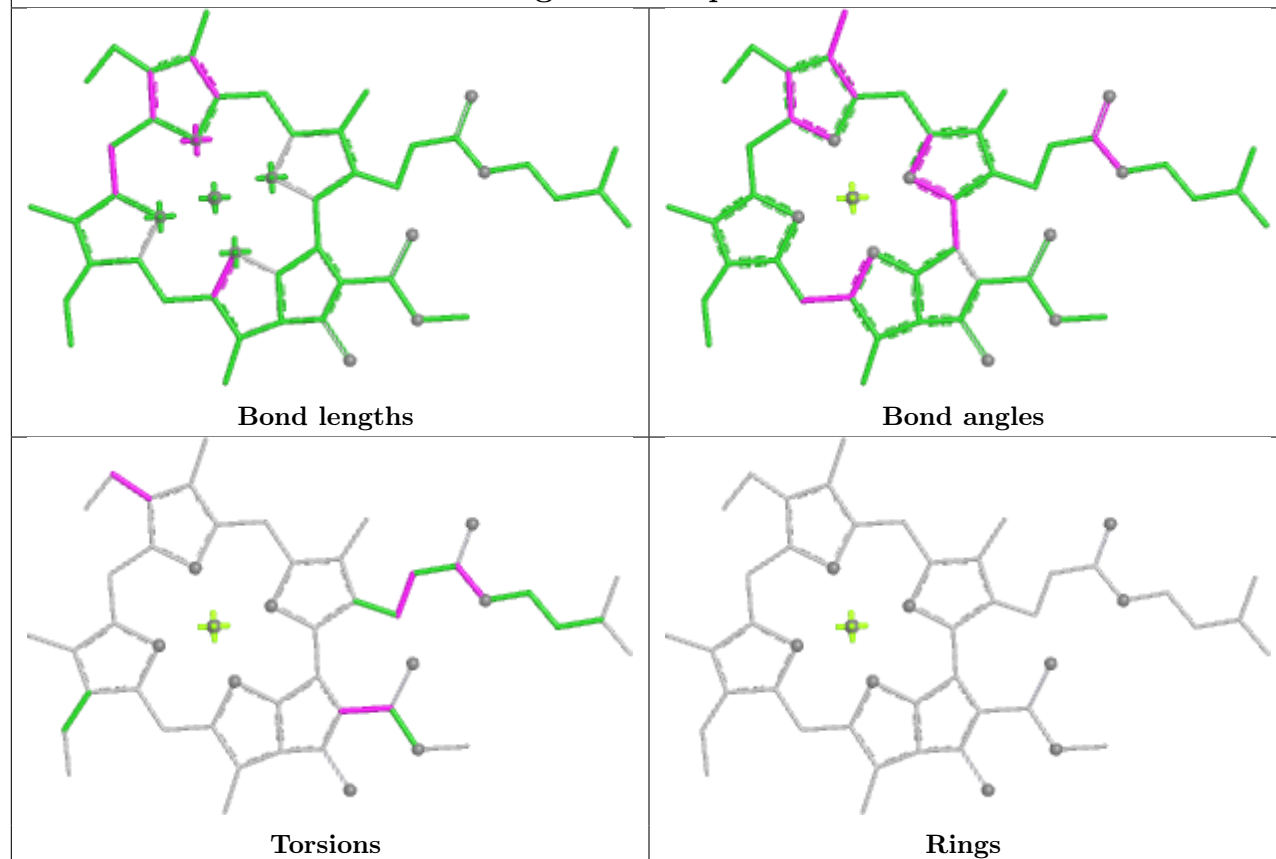
Ligand CLA H 1135



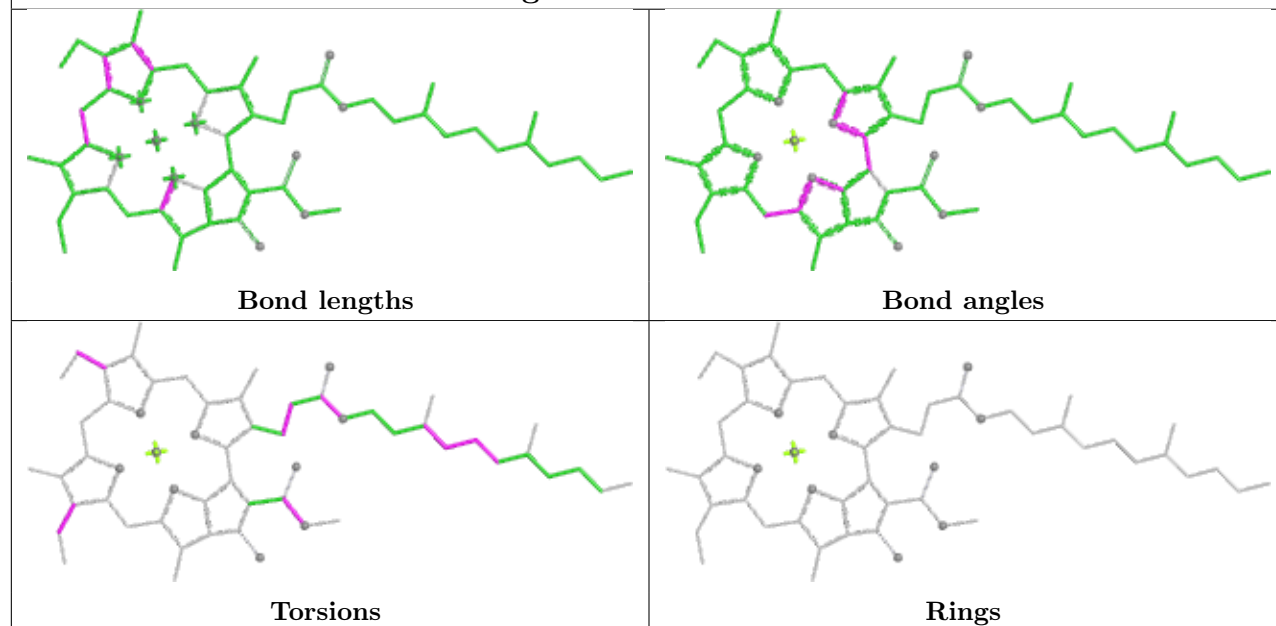
Ligand CLA s 516



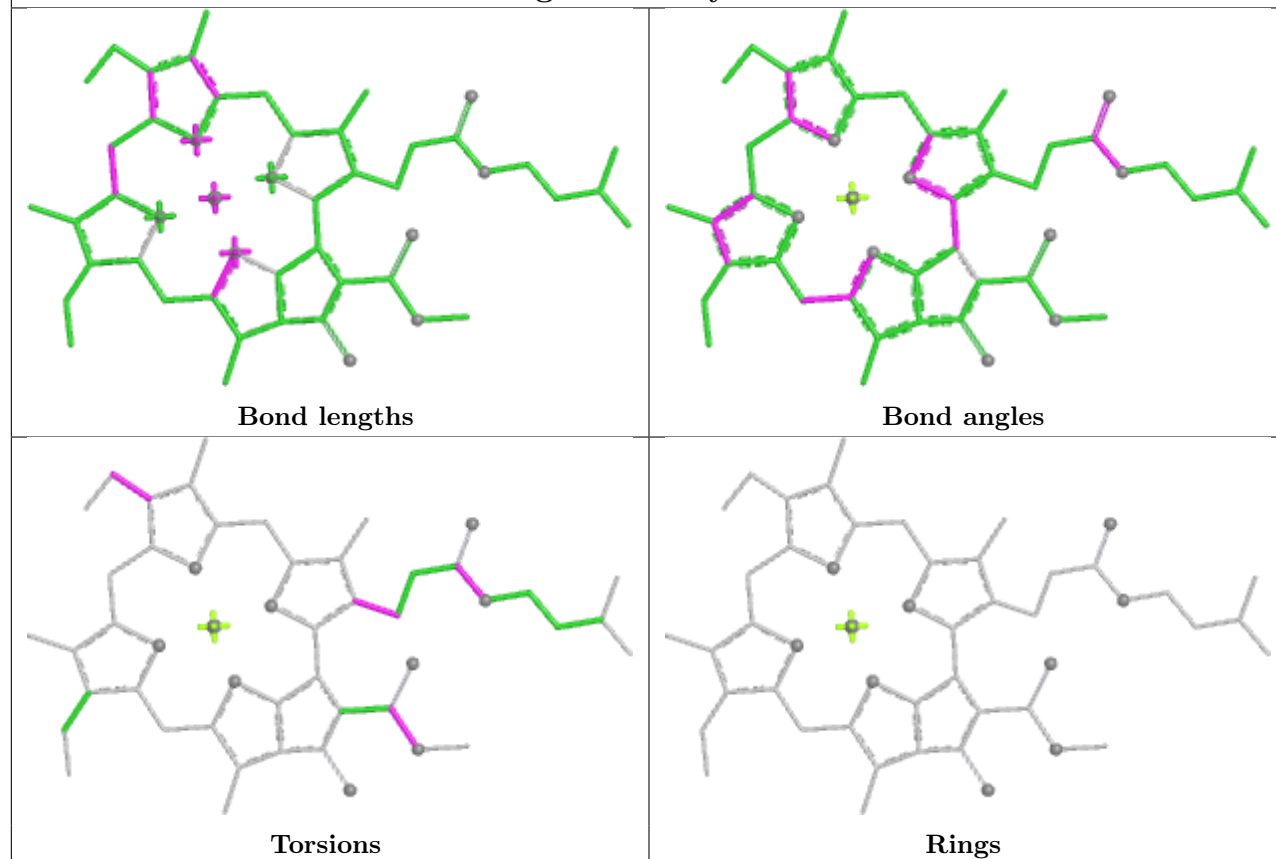
Ligand CLA p 501



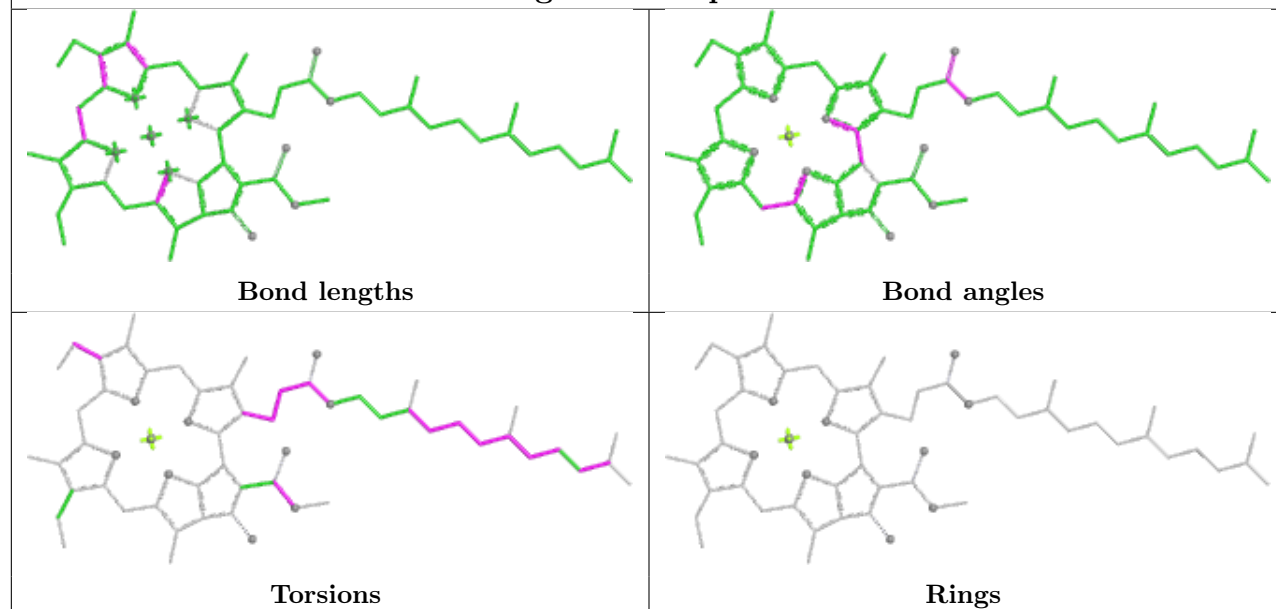
Ligand CLA G 1229

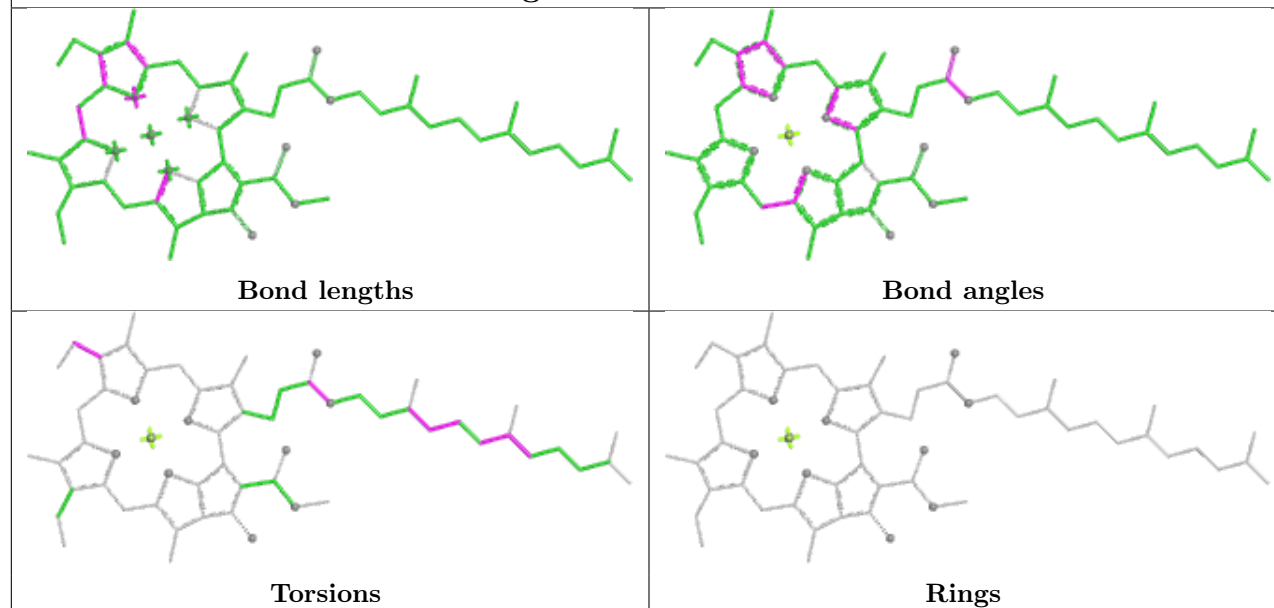
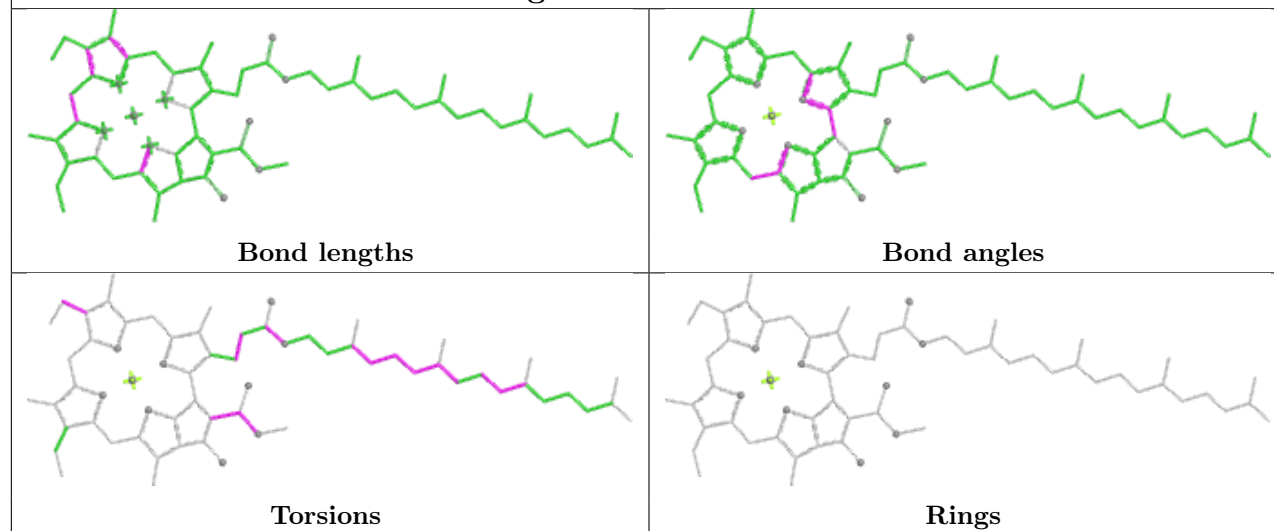


Ligand CLA y 514

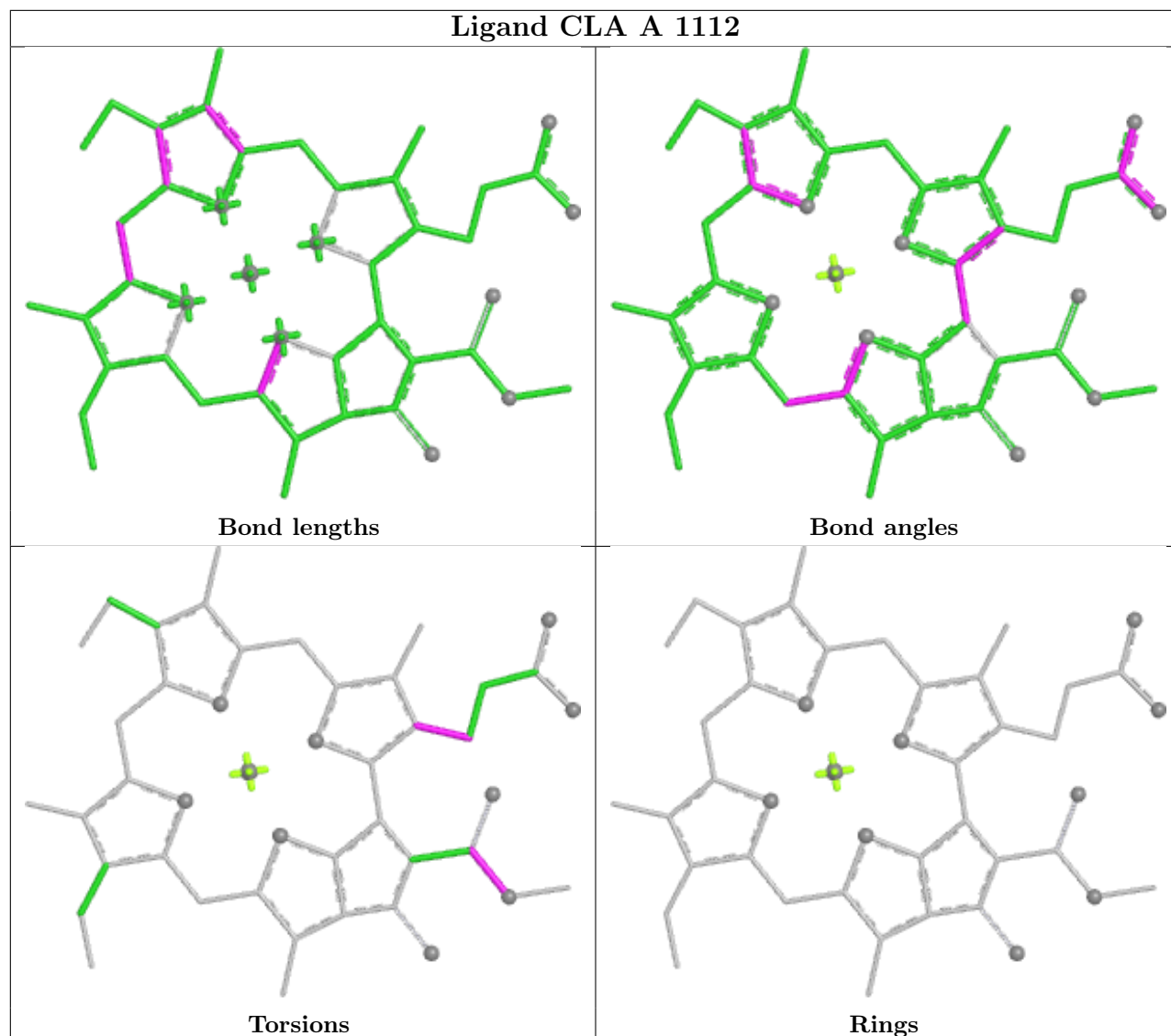


Ligand CLA p 509

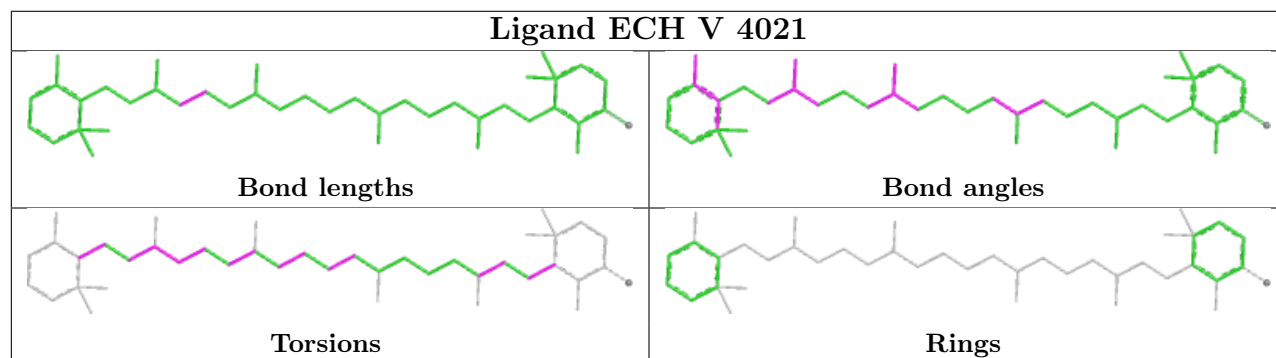


Ligand CLA U 1502**Ligand CLA a 1106**

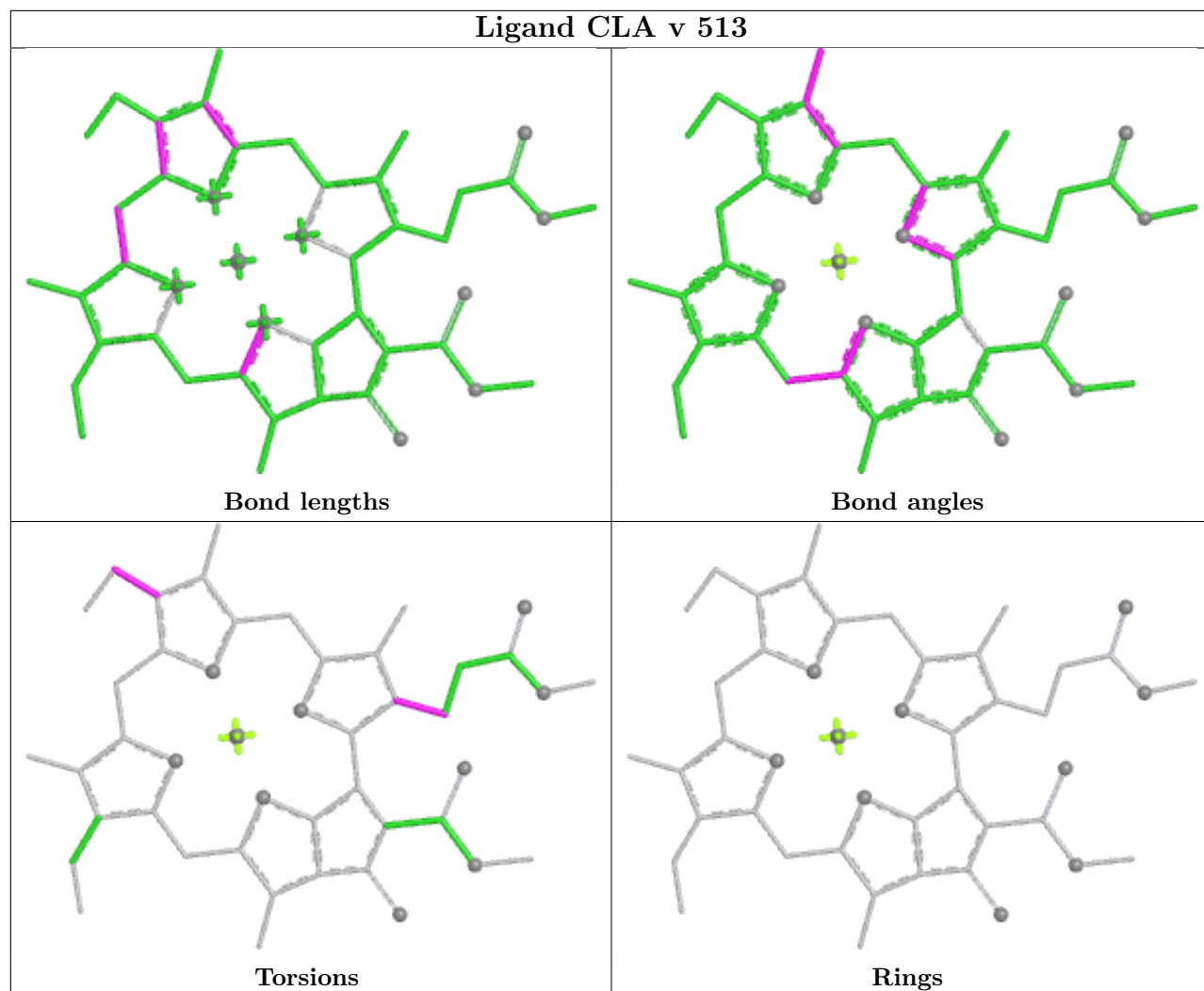
Ligand CLA A 1112



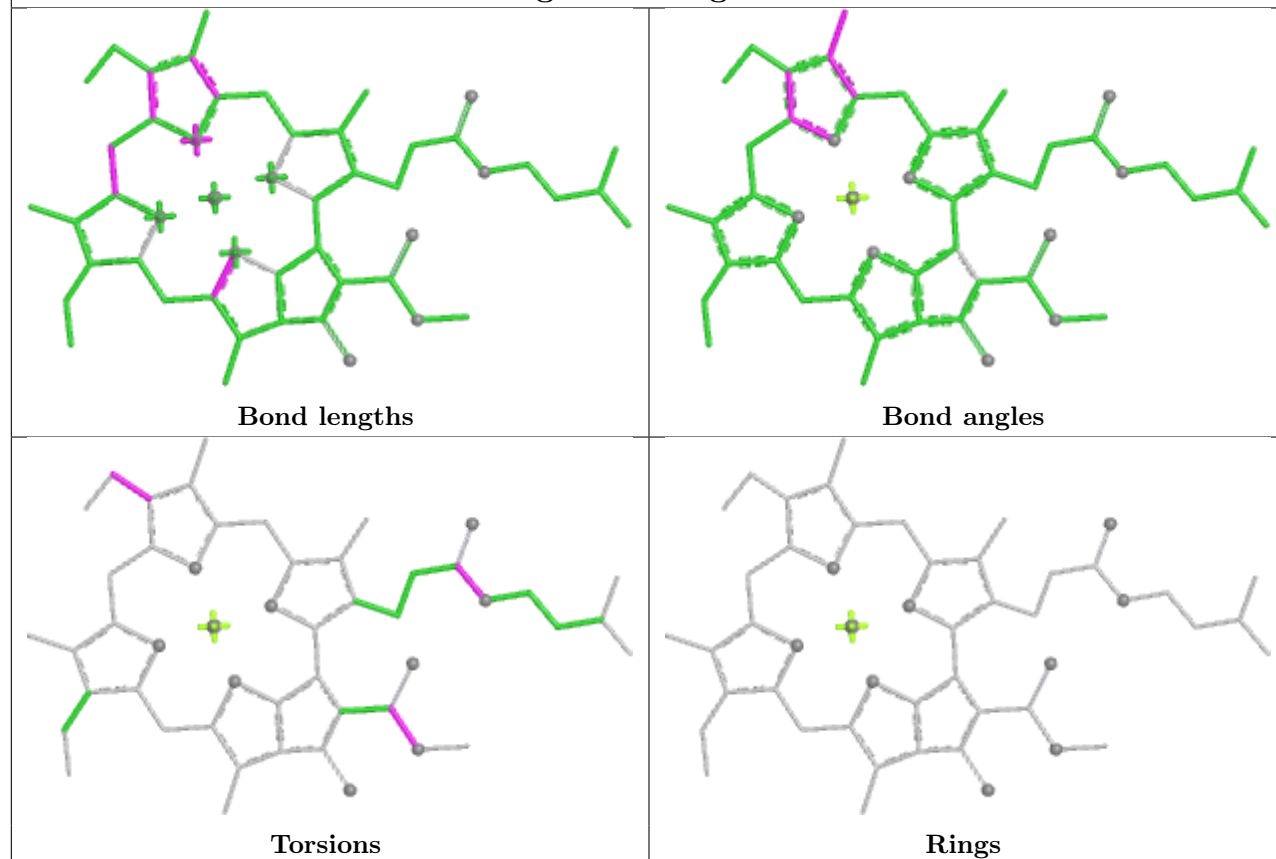
Ligand ECH V 4021



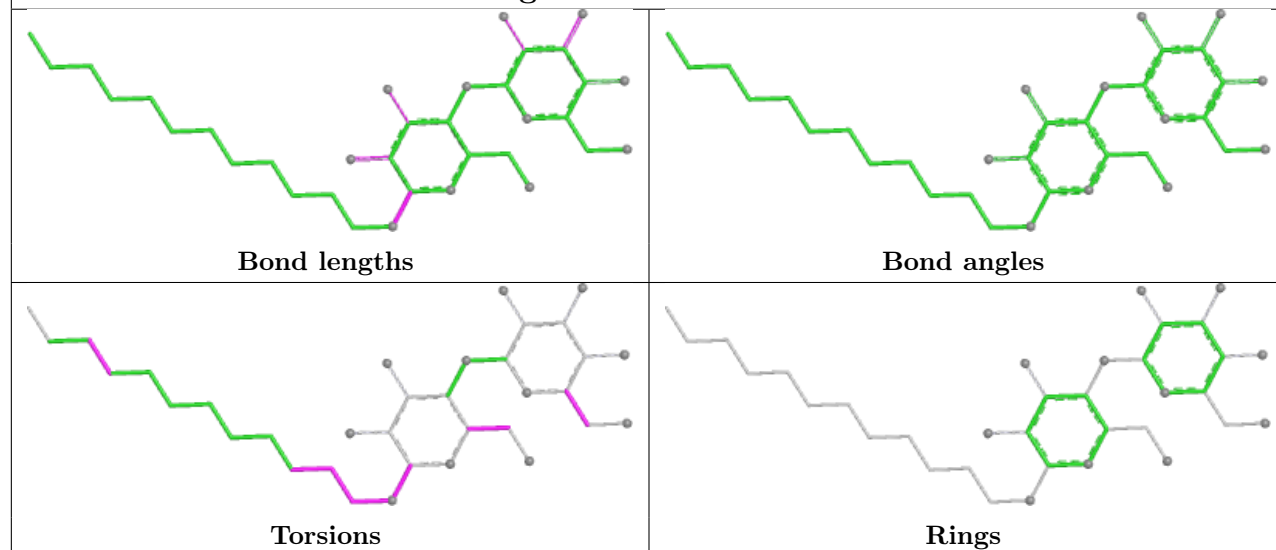
Ligand CLA v 513

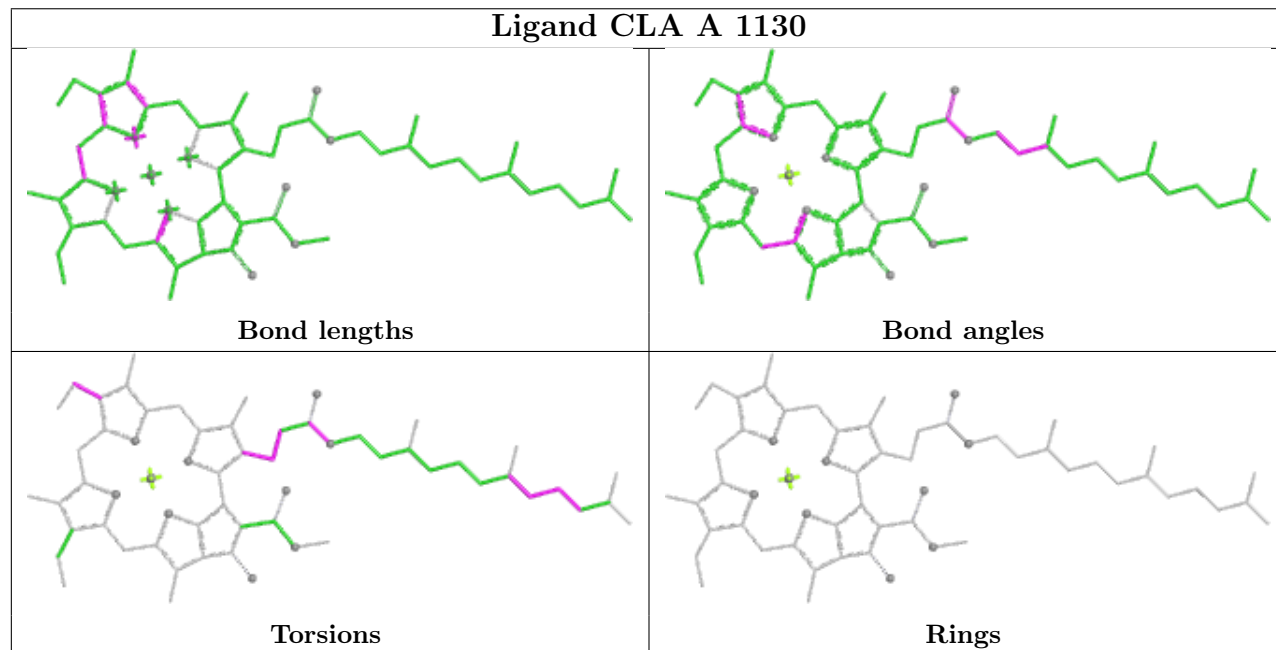
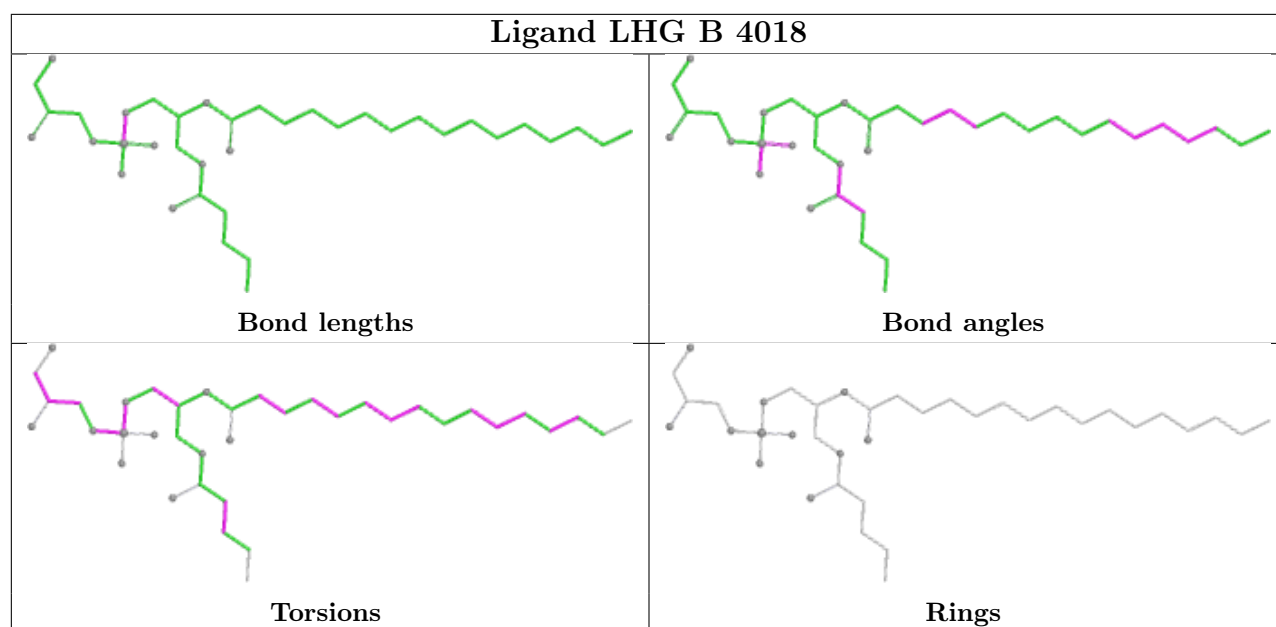


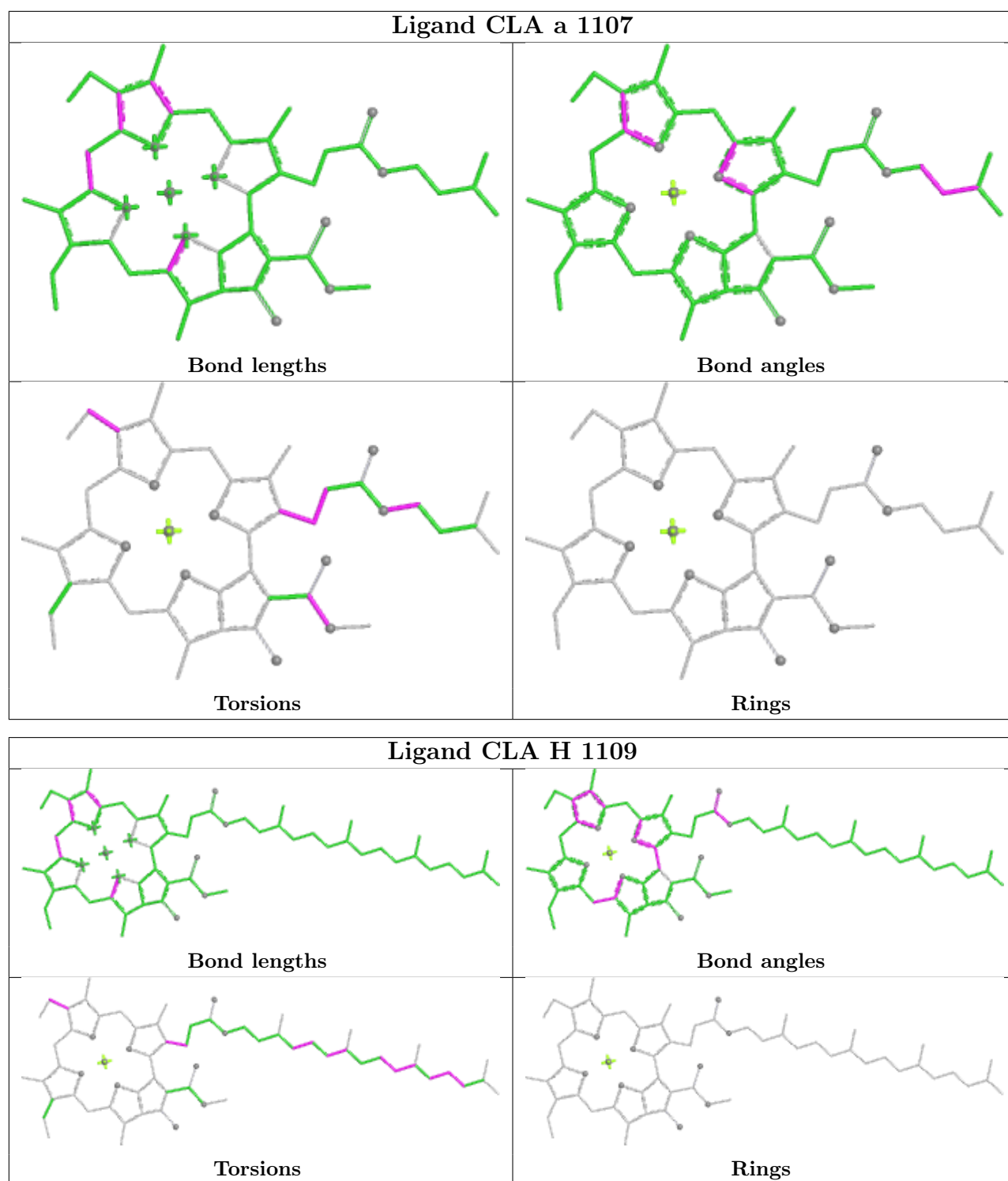
Ligand CLA g 502



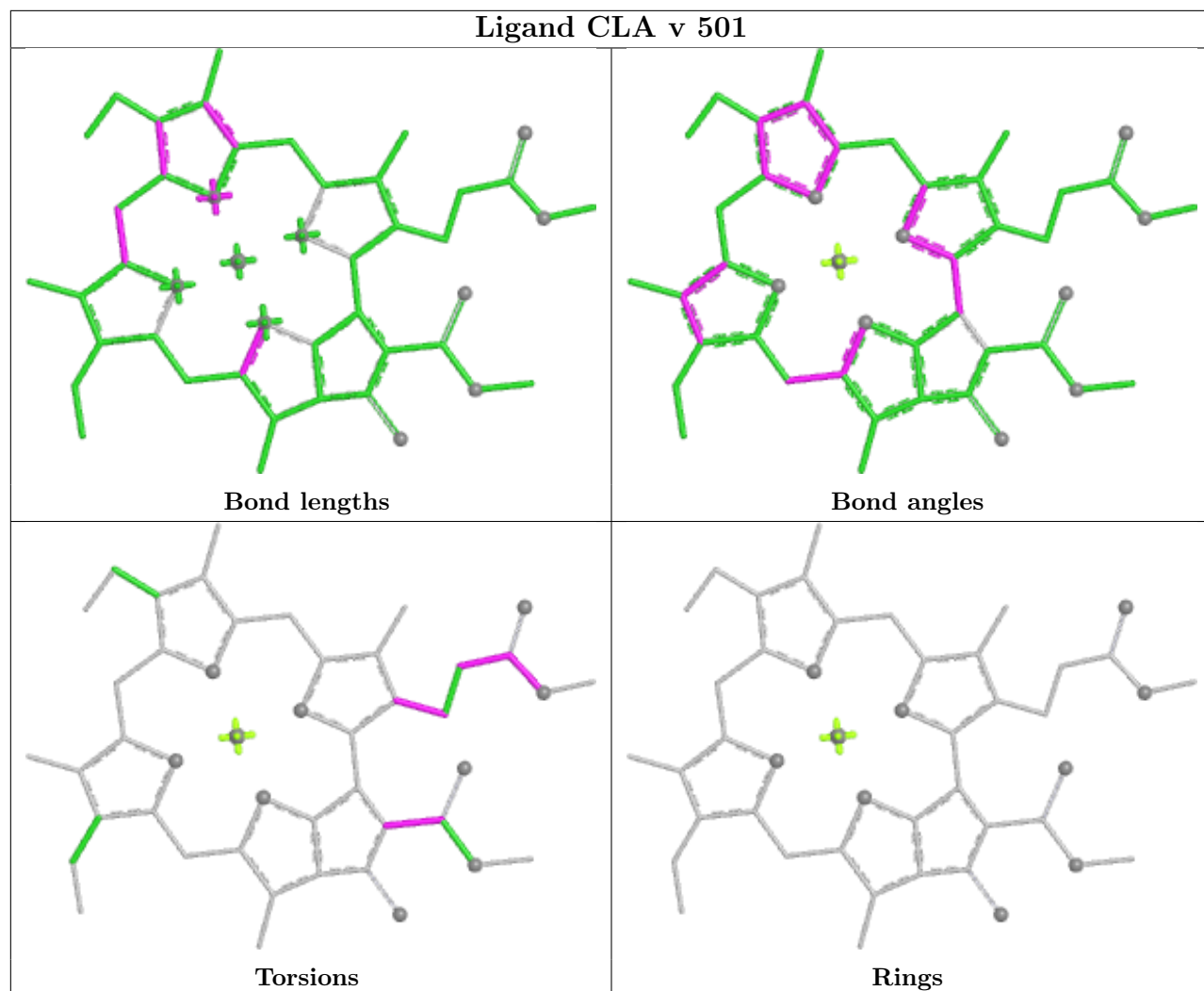
Ligand LMT H 4202

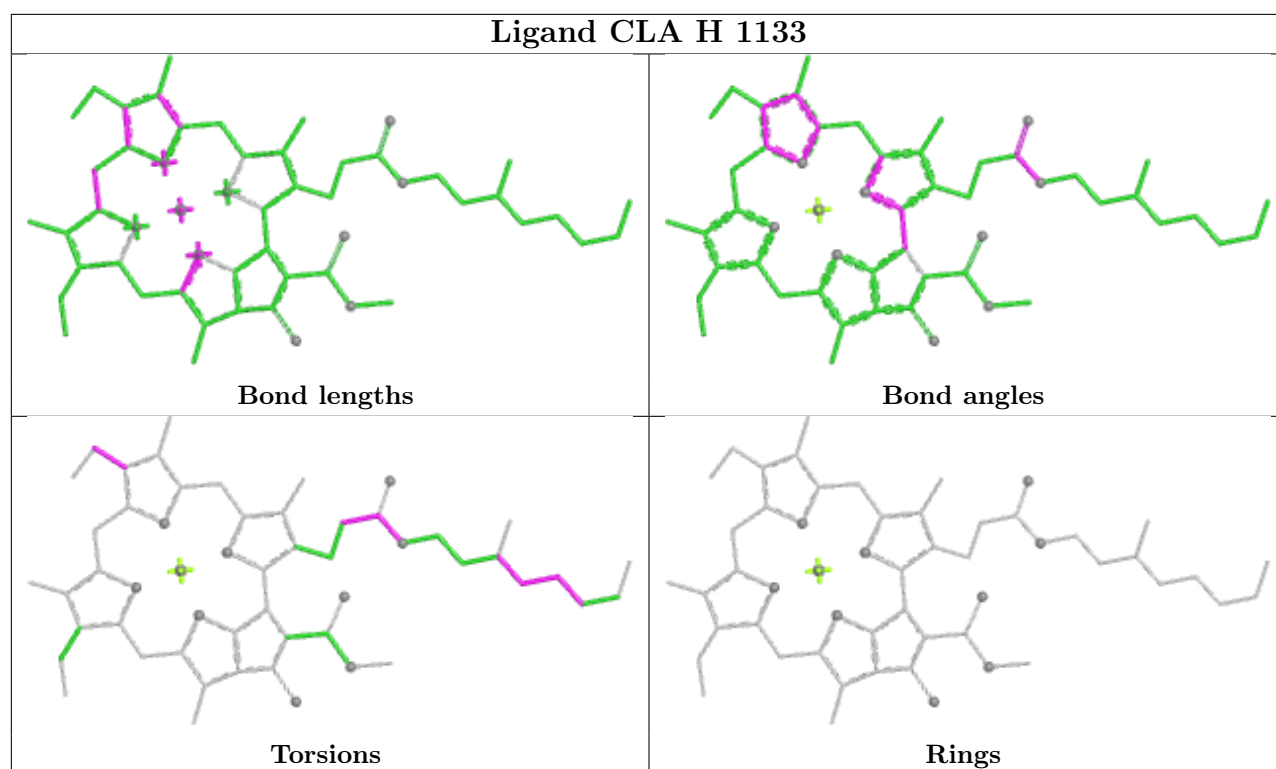




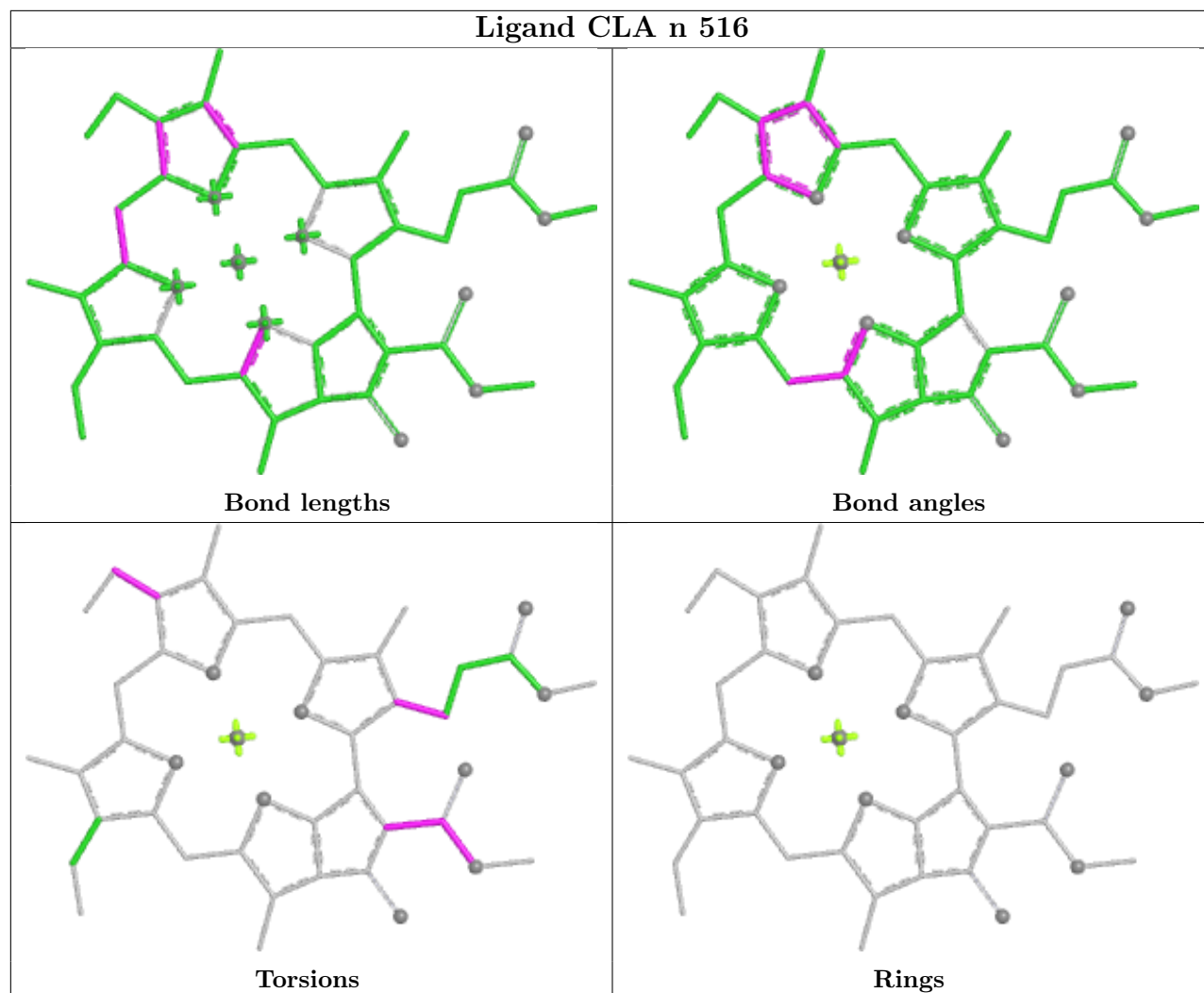


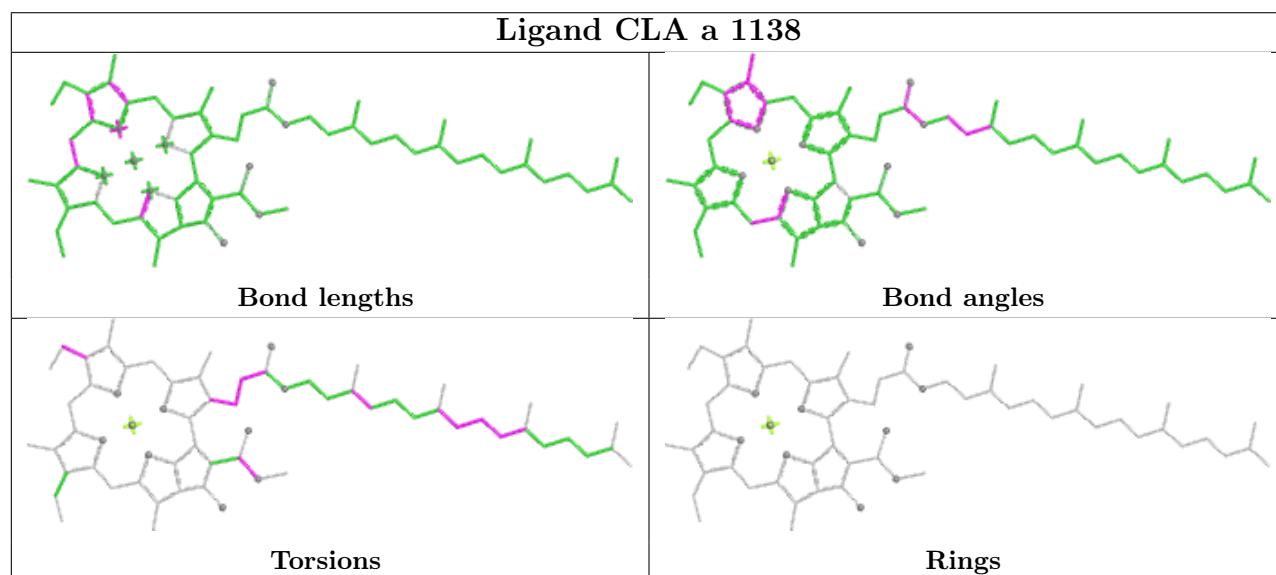
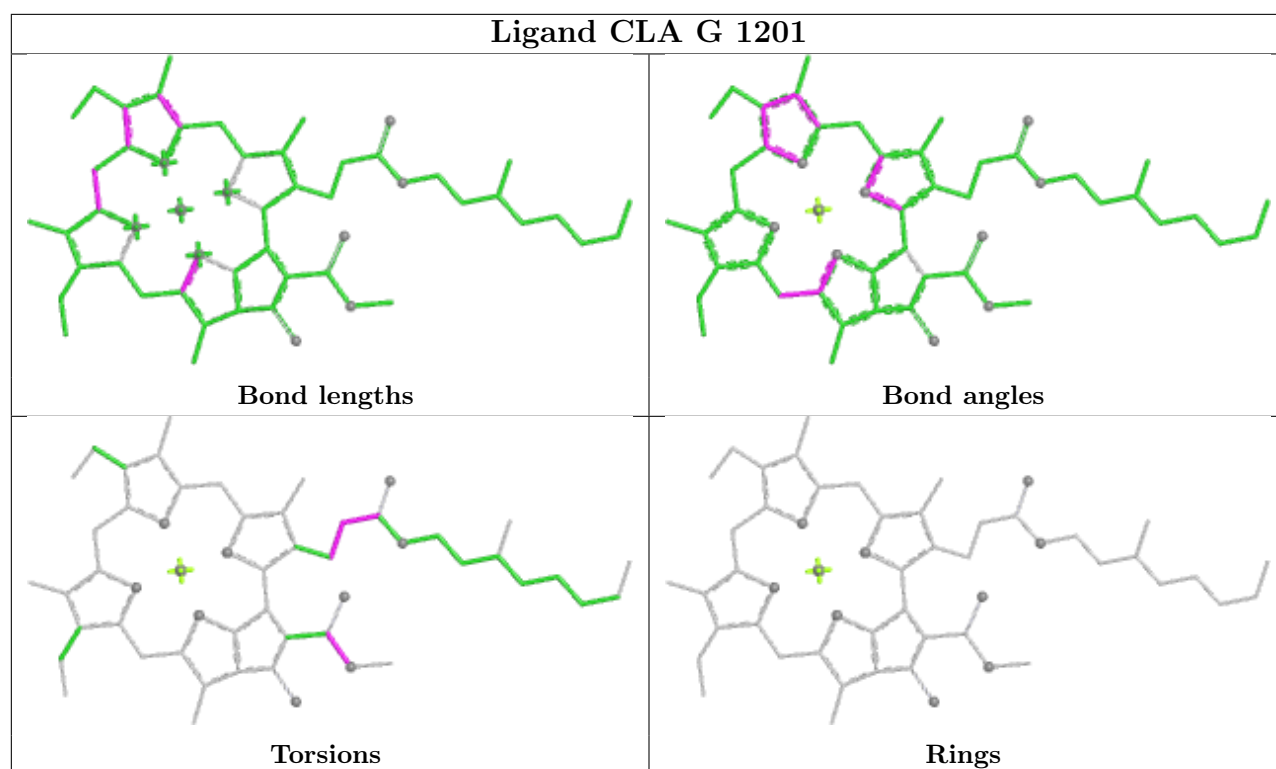
Ligand CLA v 501

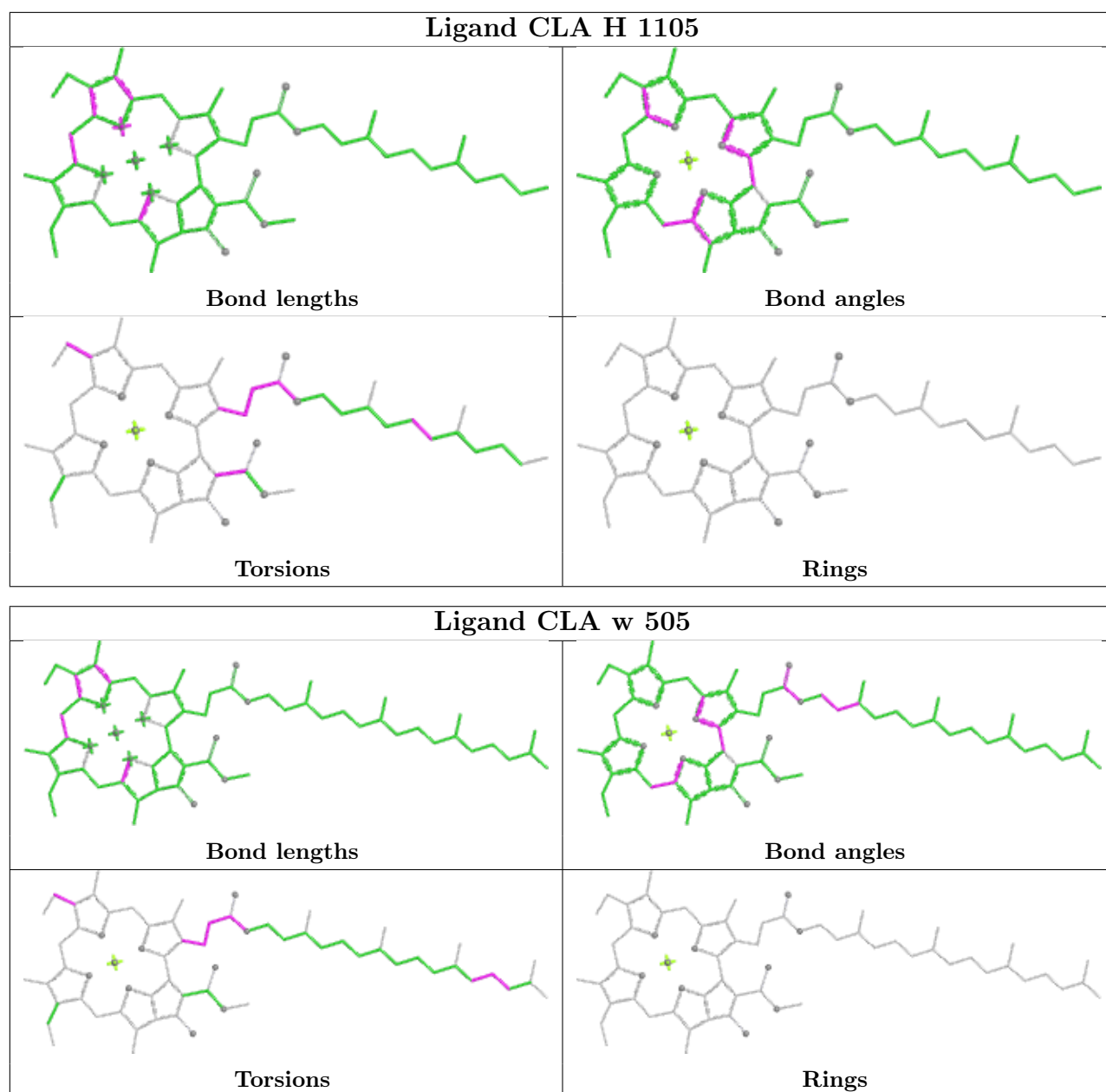


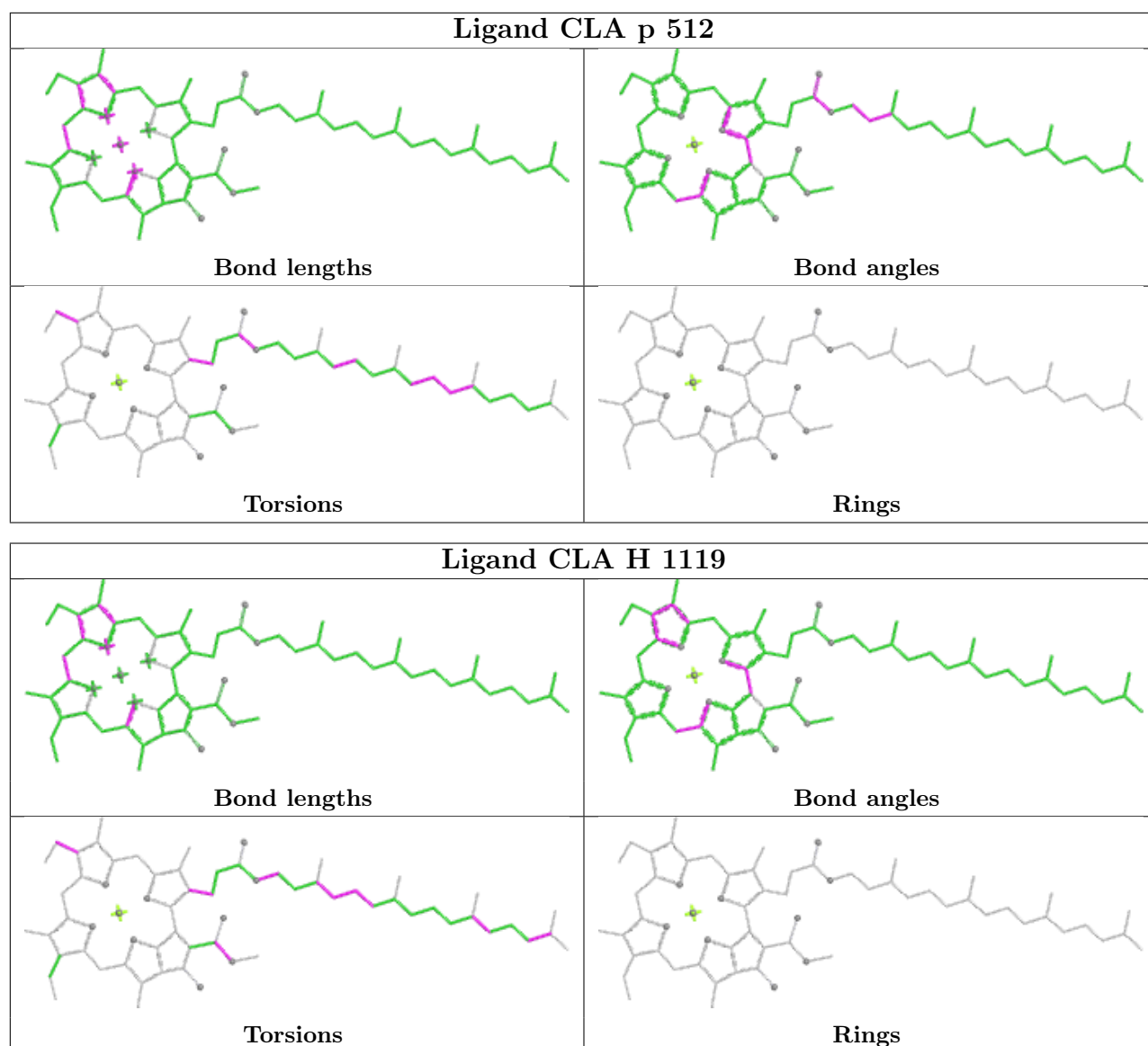


Ligand CLA n 516

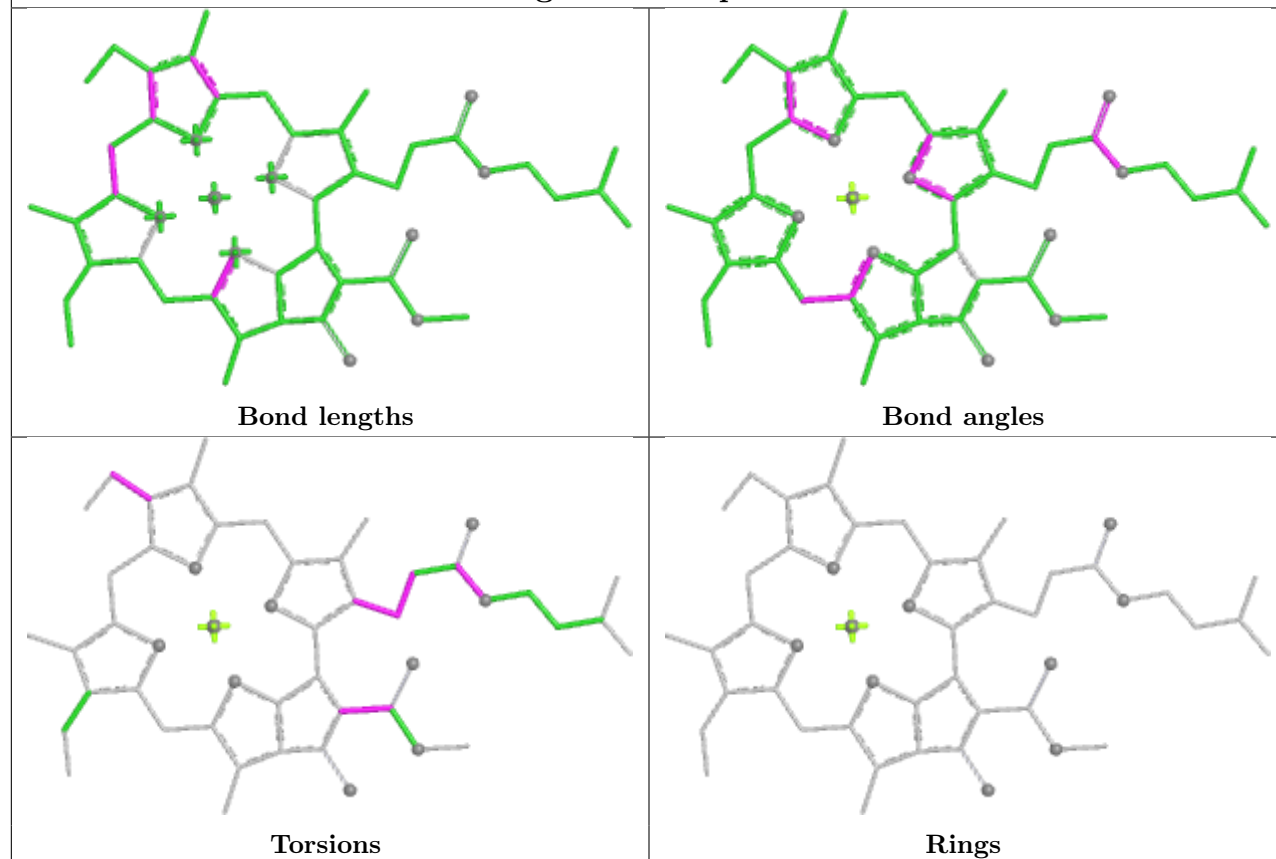




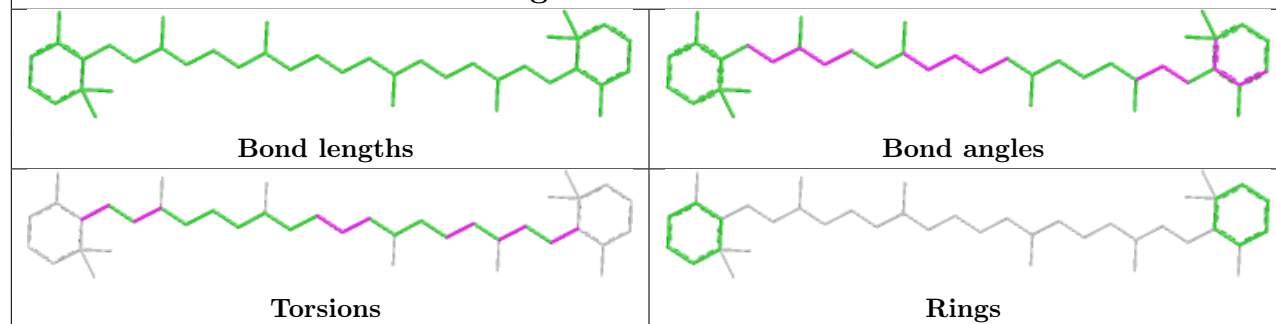


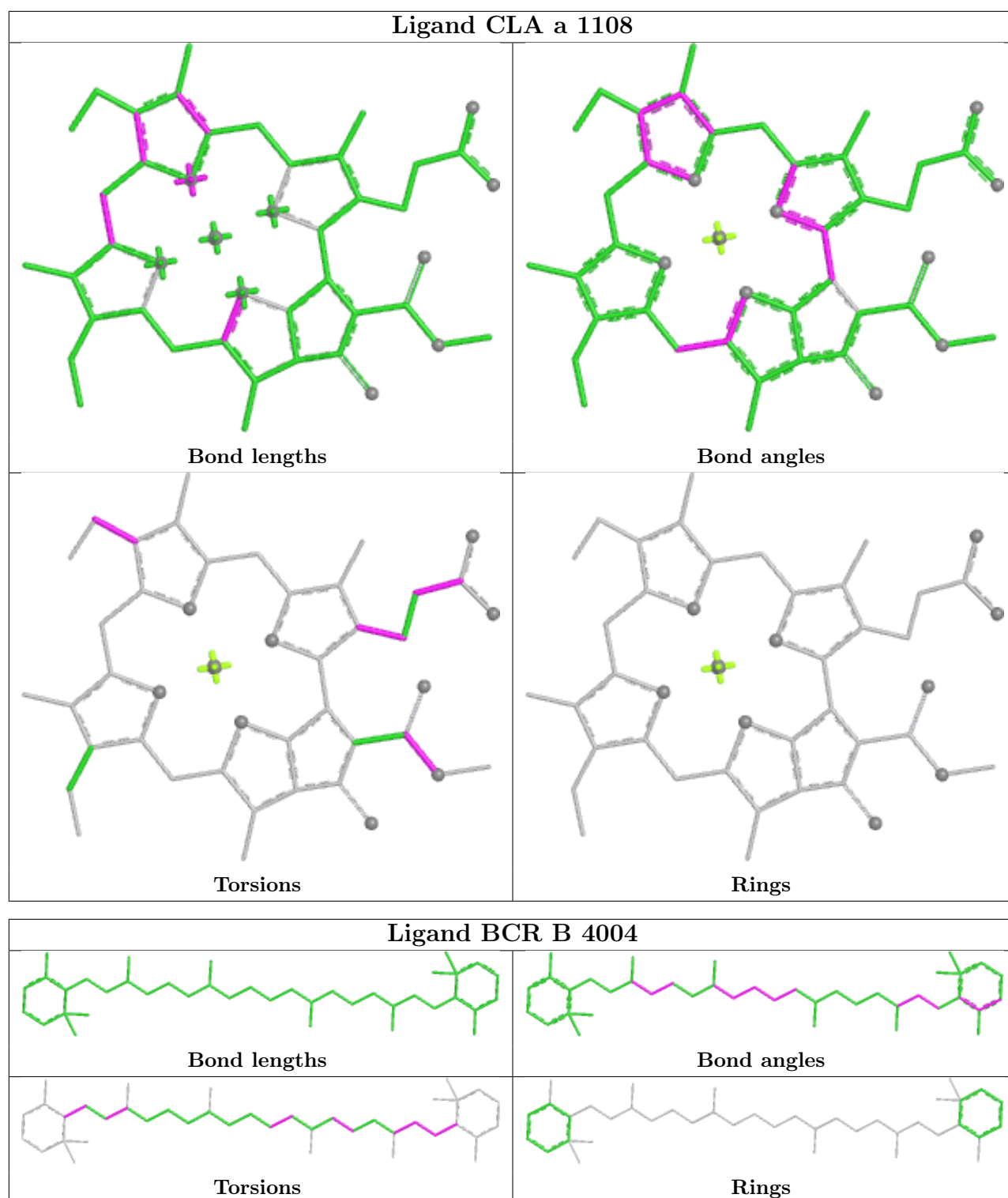


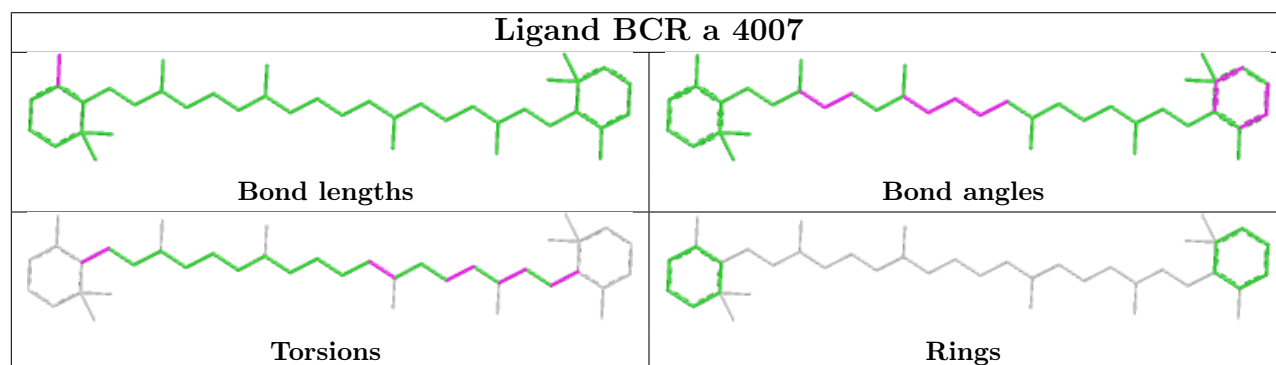
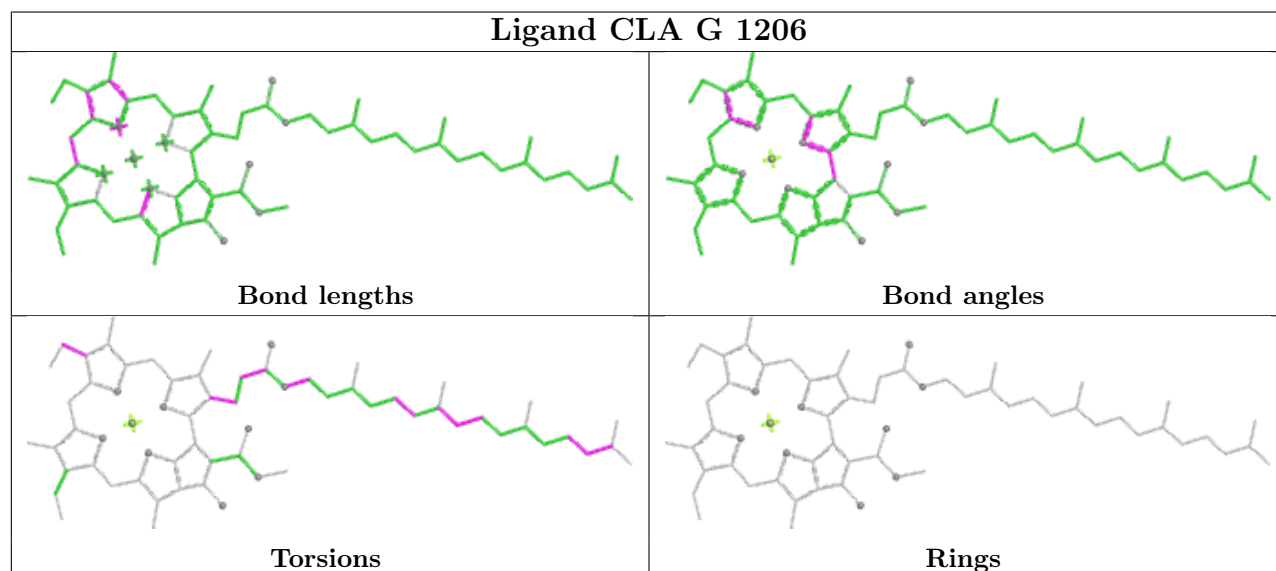
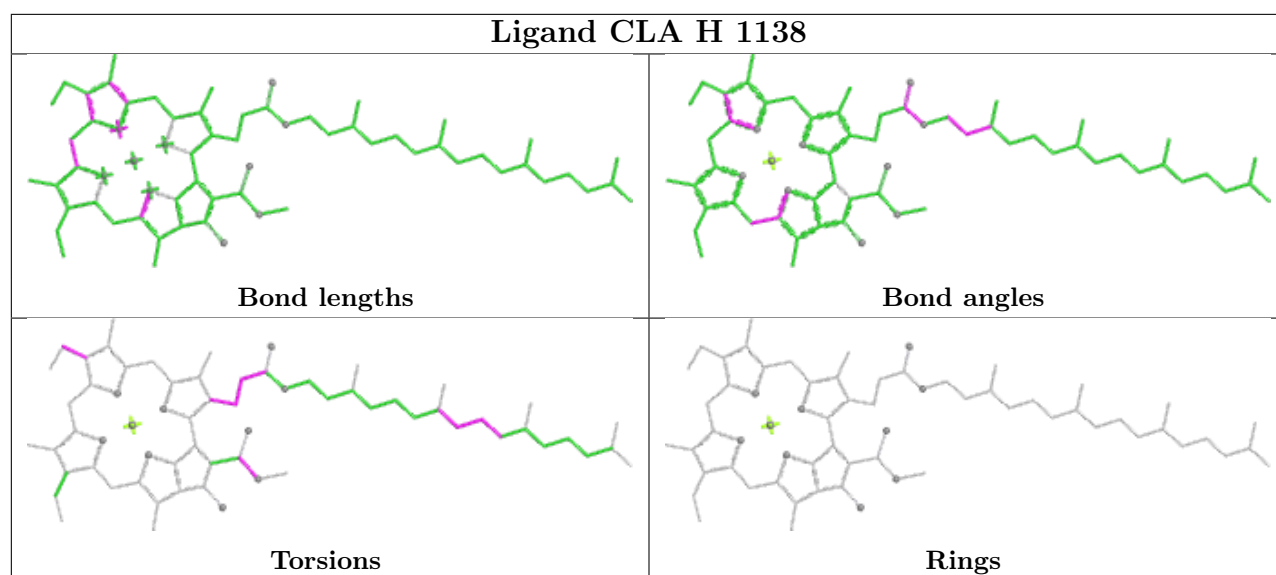
Ligand CLA q 513



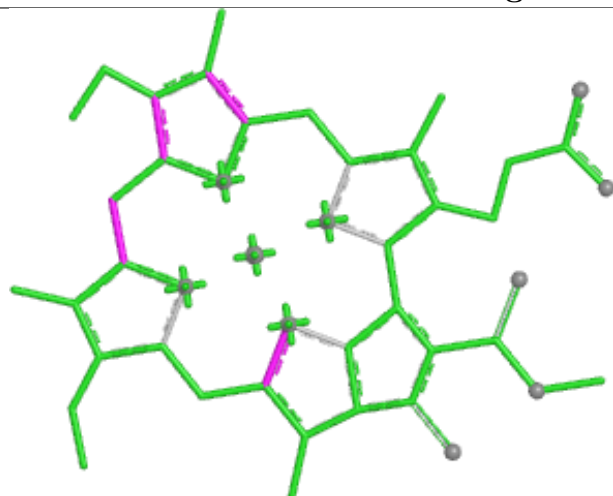
Ligand BCR w 602



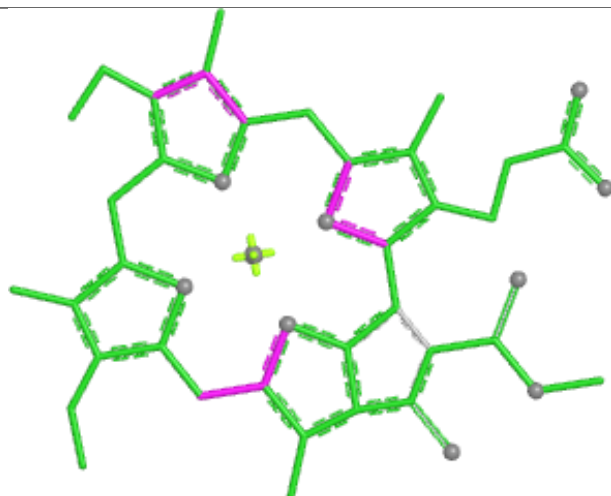




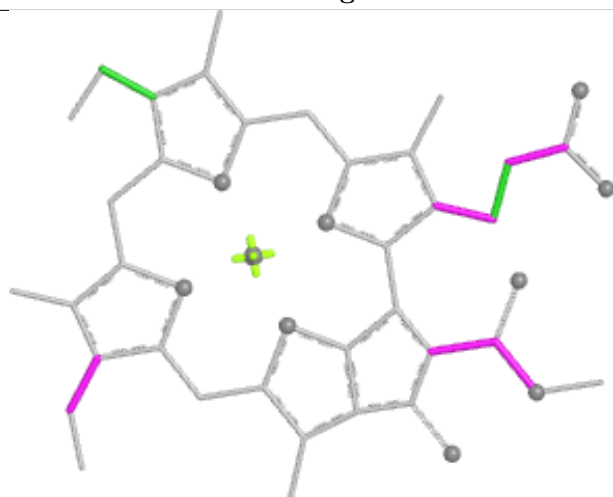
Ligand CLA T 4003



Bond lengths



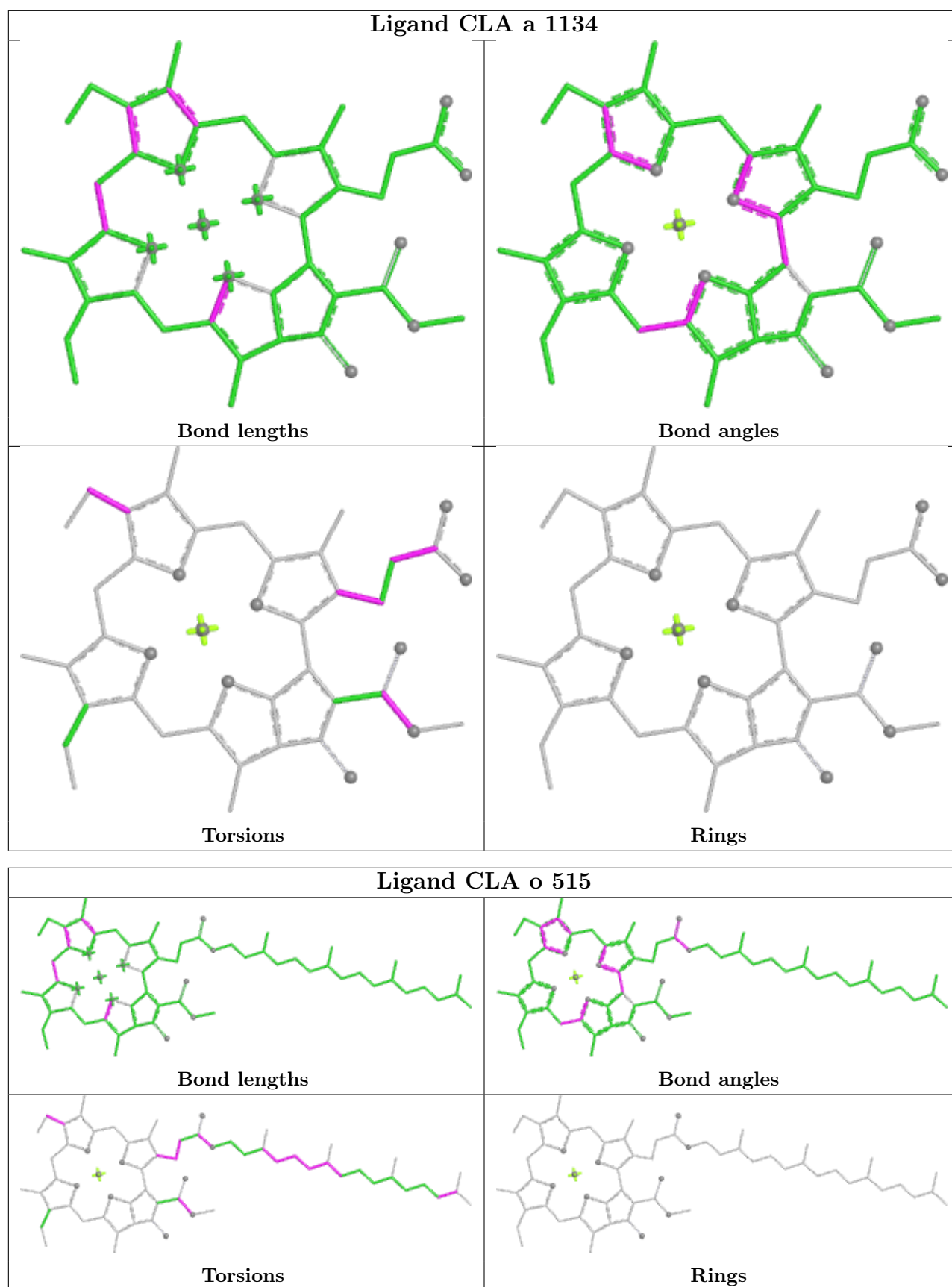
Bond angles



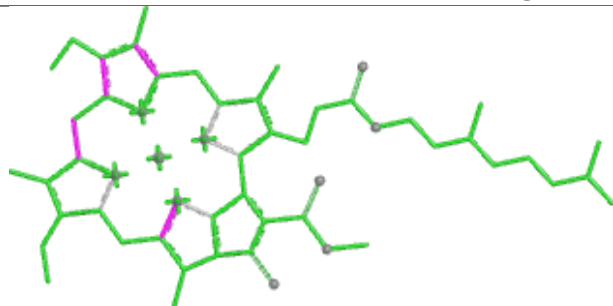
Torsions



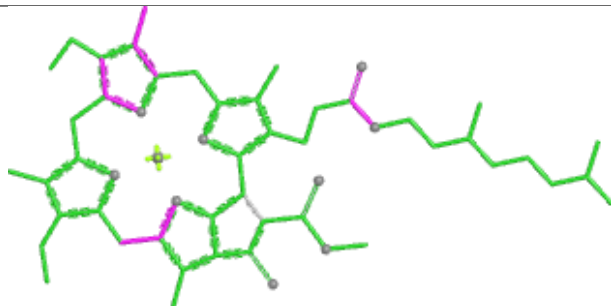
Rings



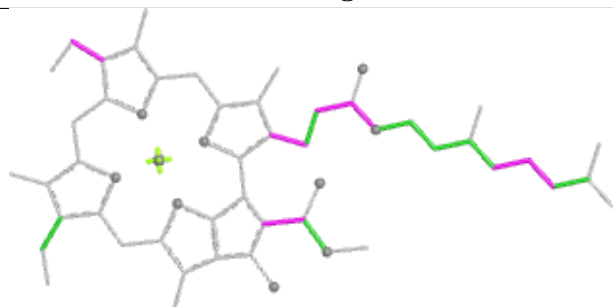
Ligand CLA o 517



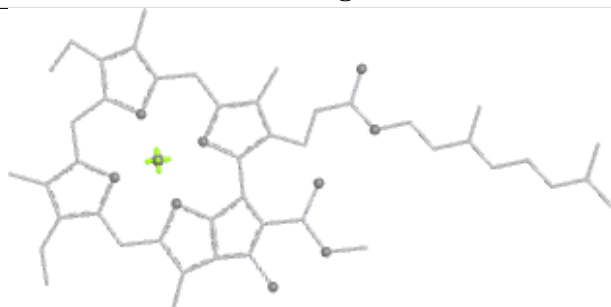
Bond lengths



Bond angles

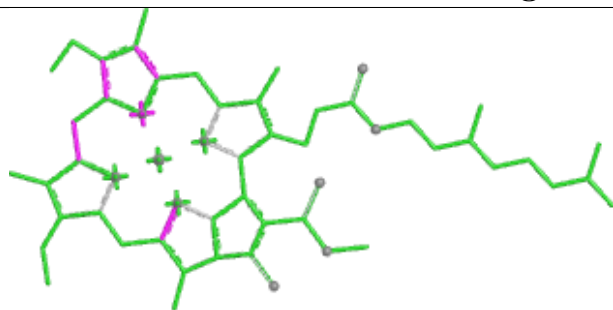


Torsions

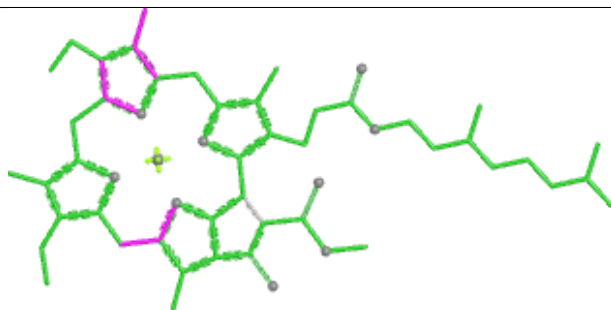


Rings

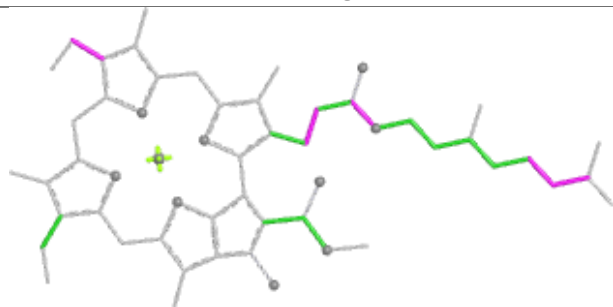
Ligand CLA t 517



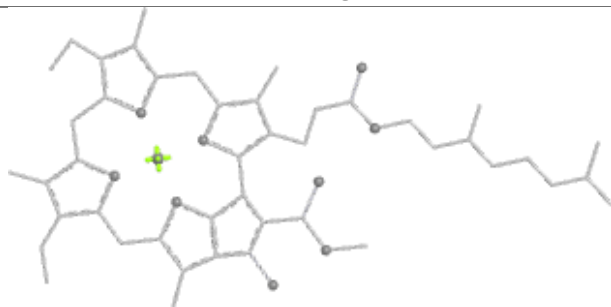
Bond lengths



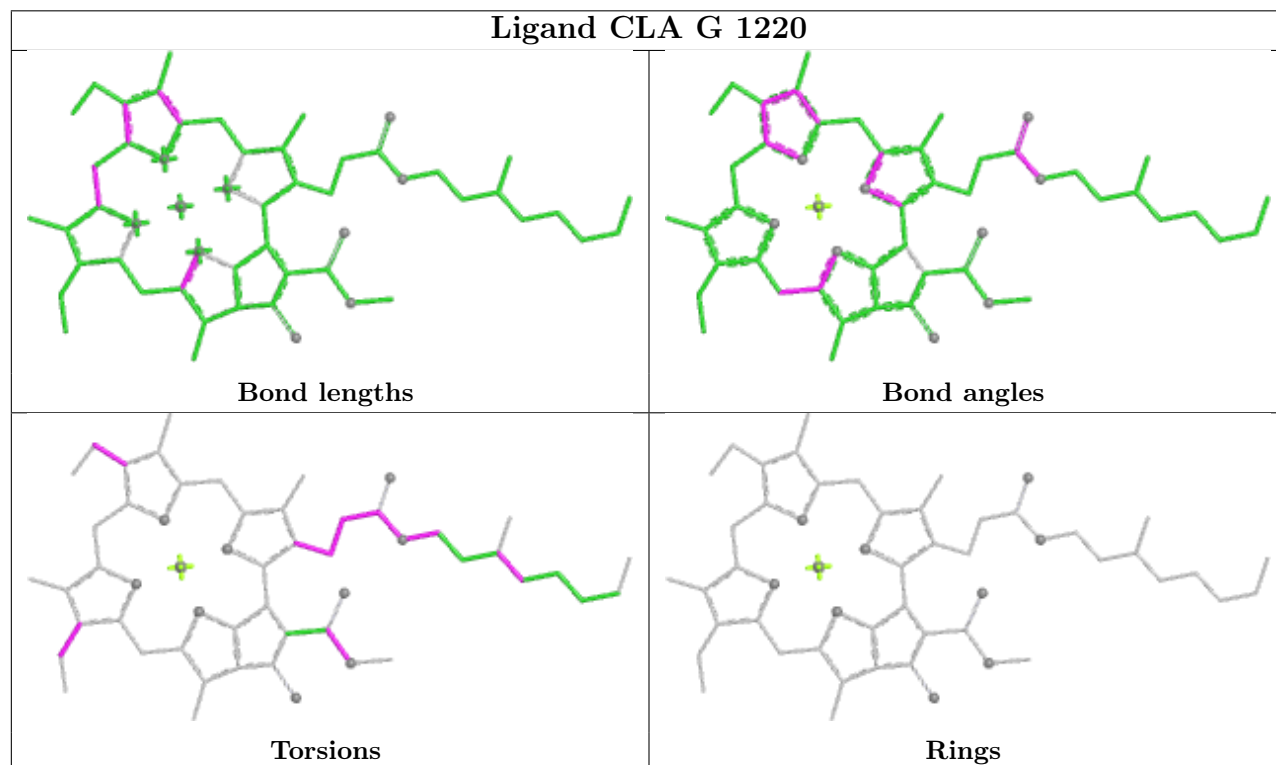
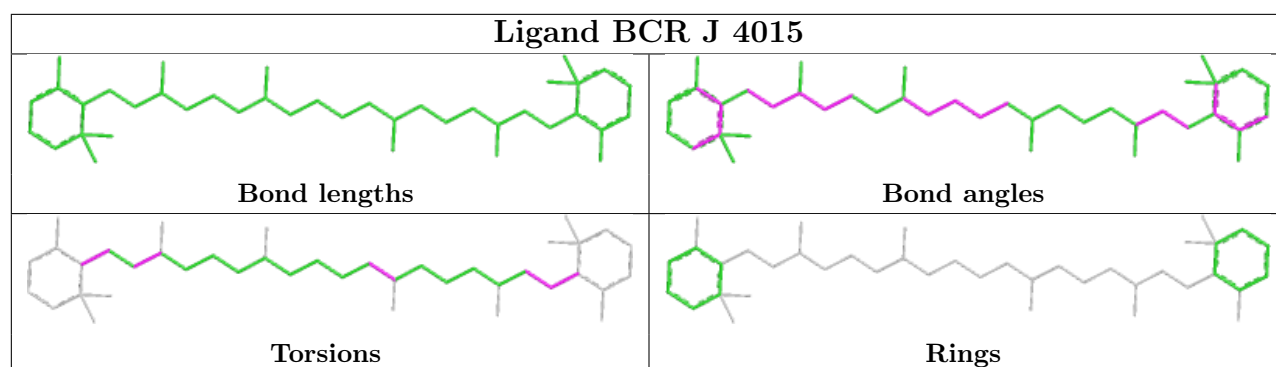
Bond angles



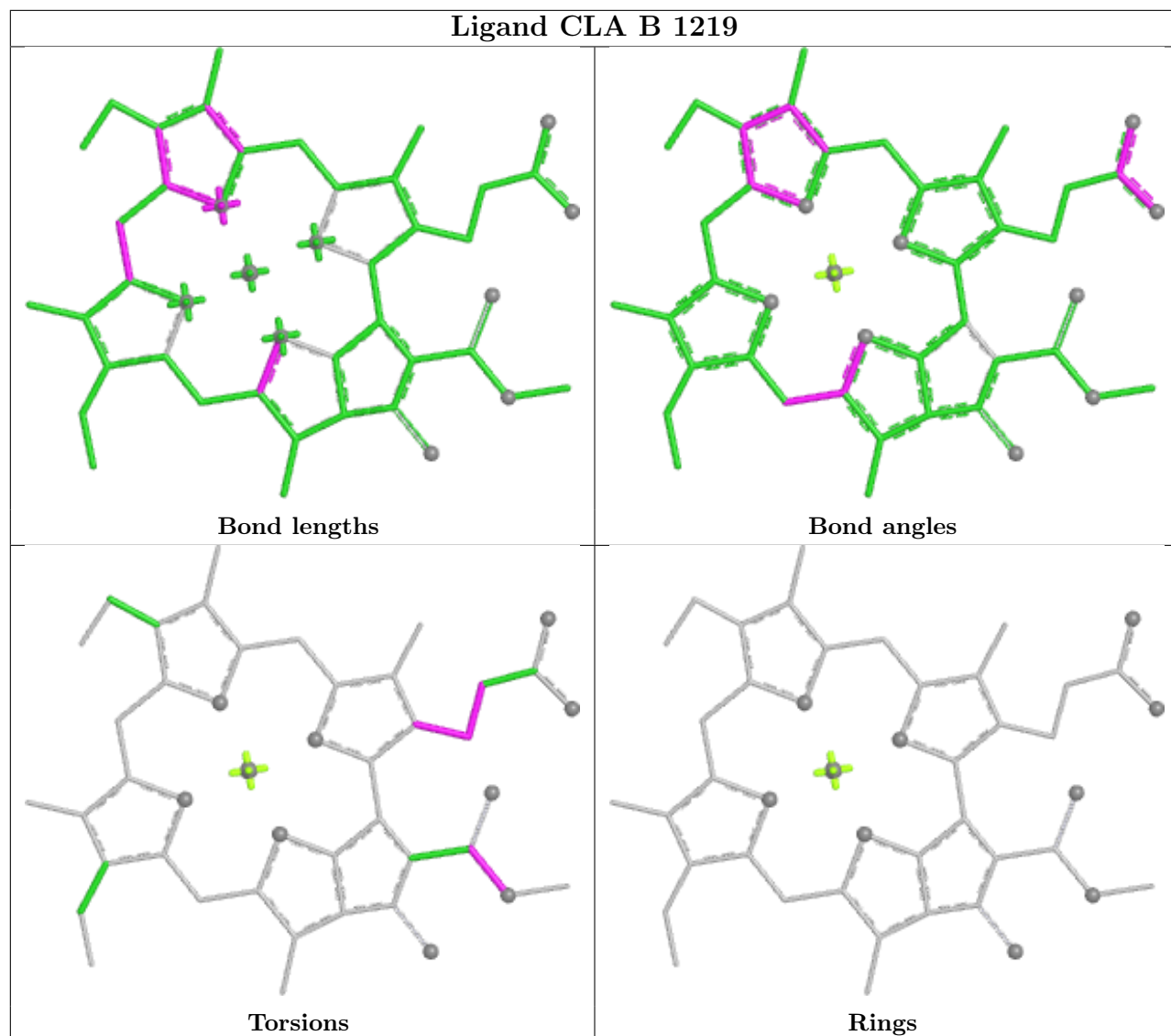
Torsions



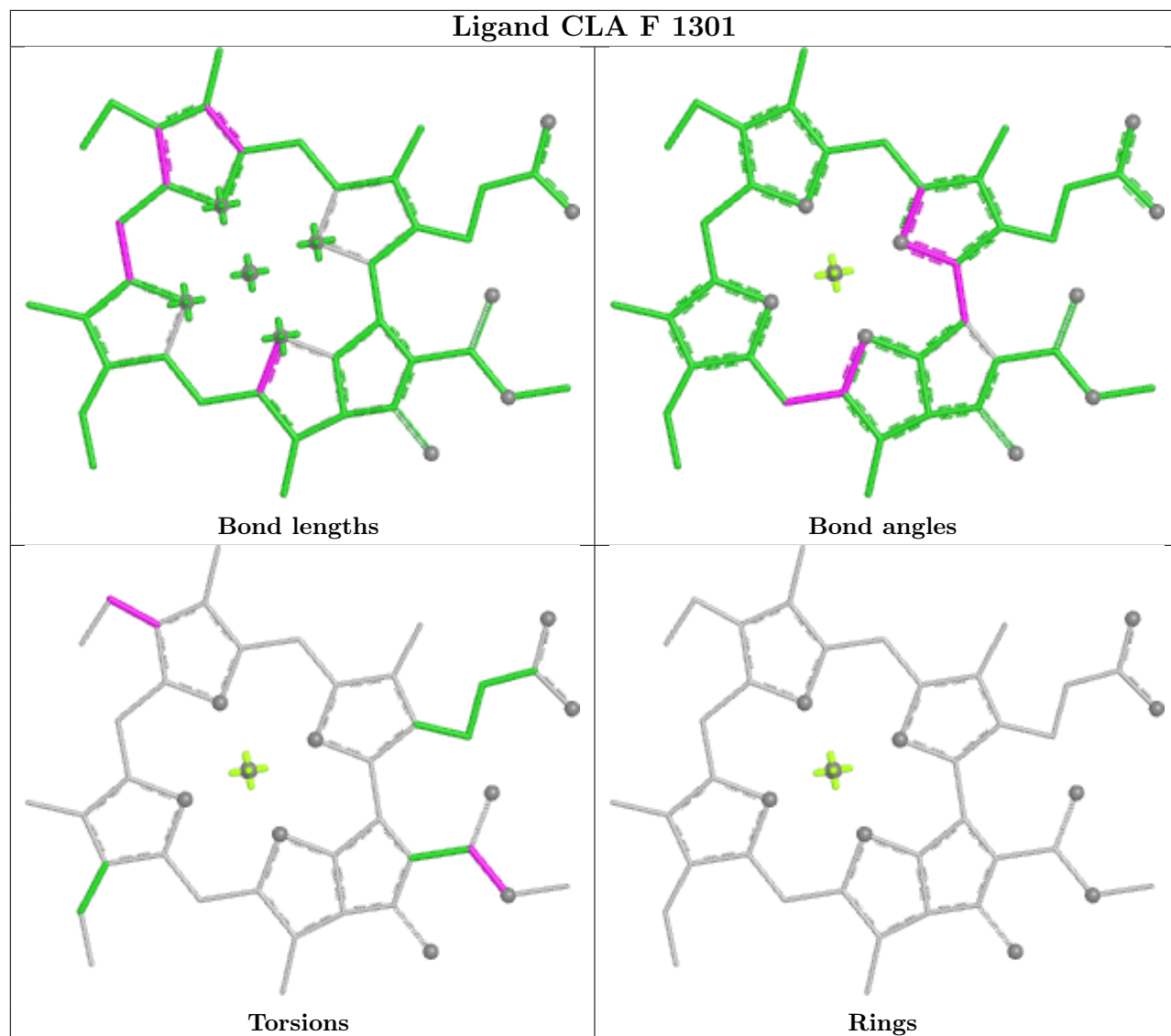
Rings

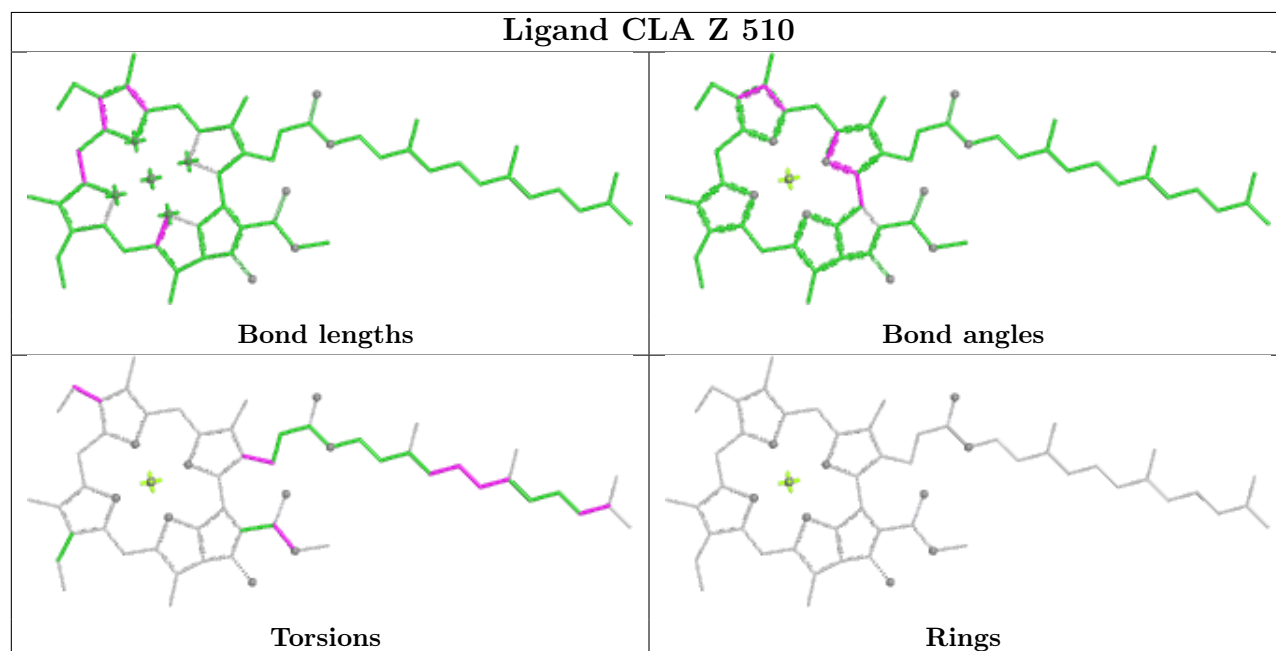
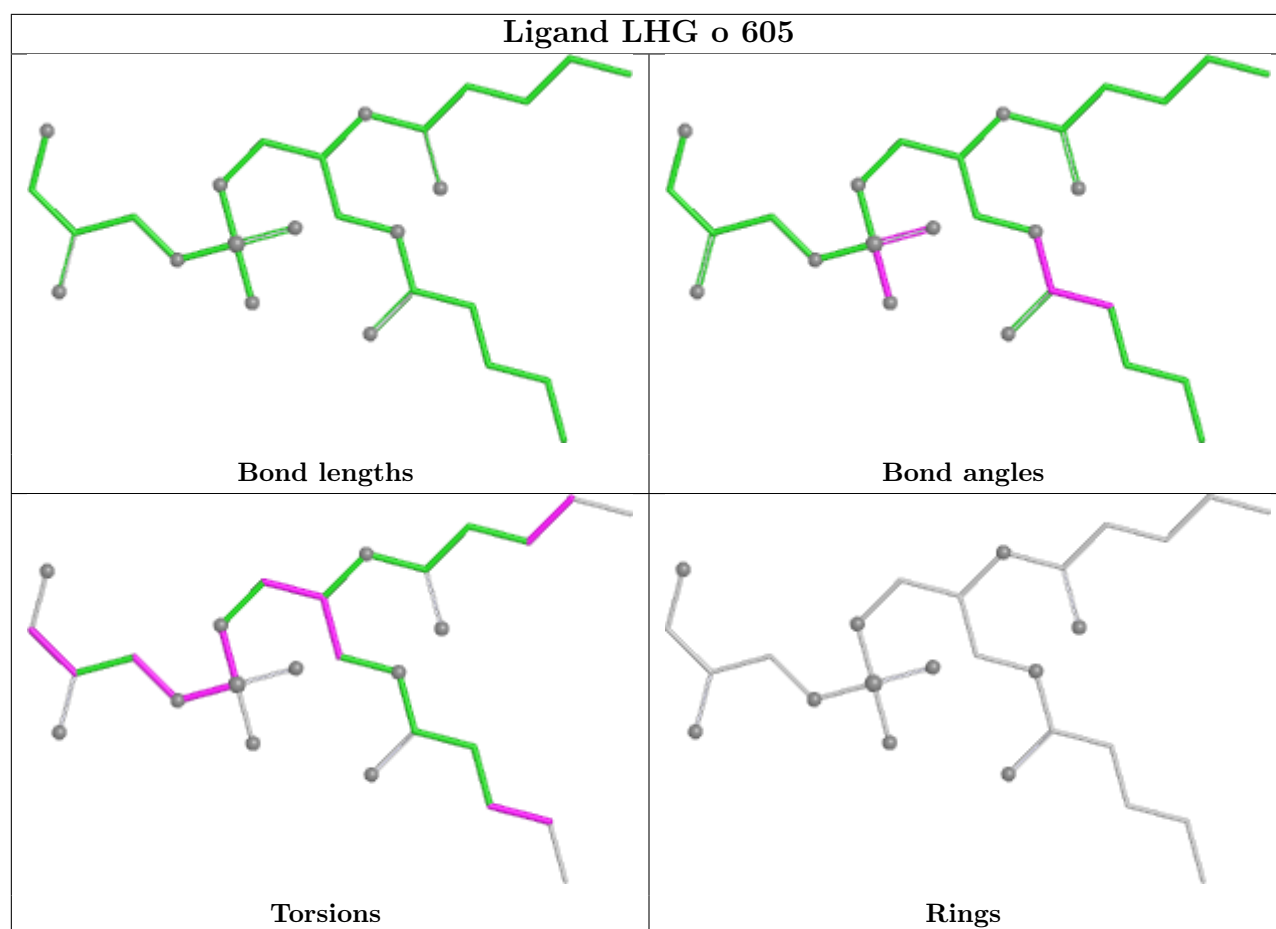


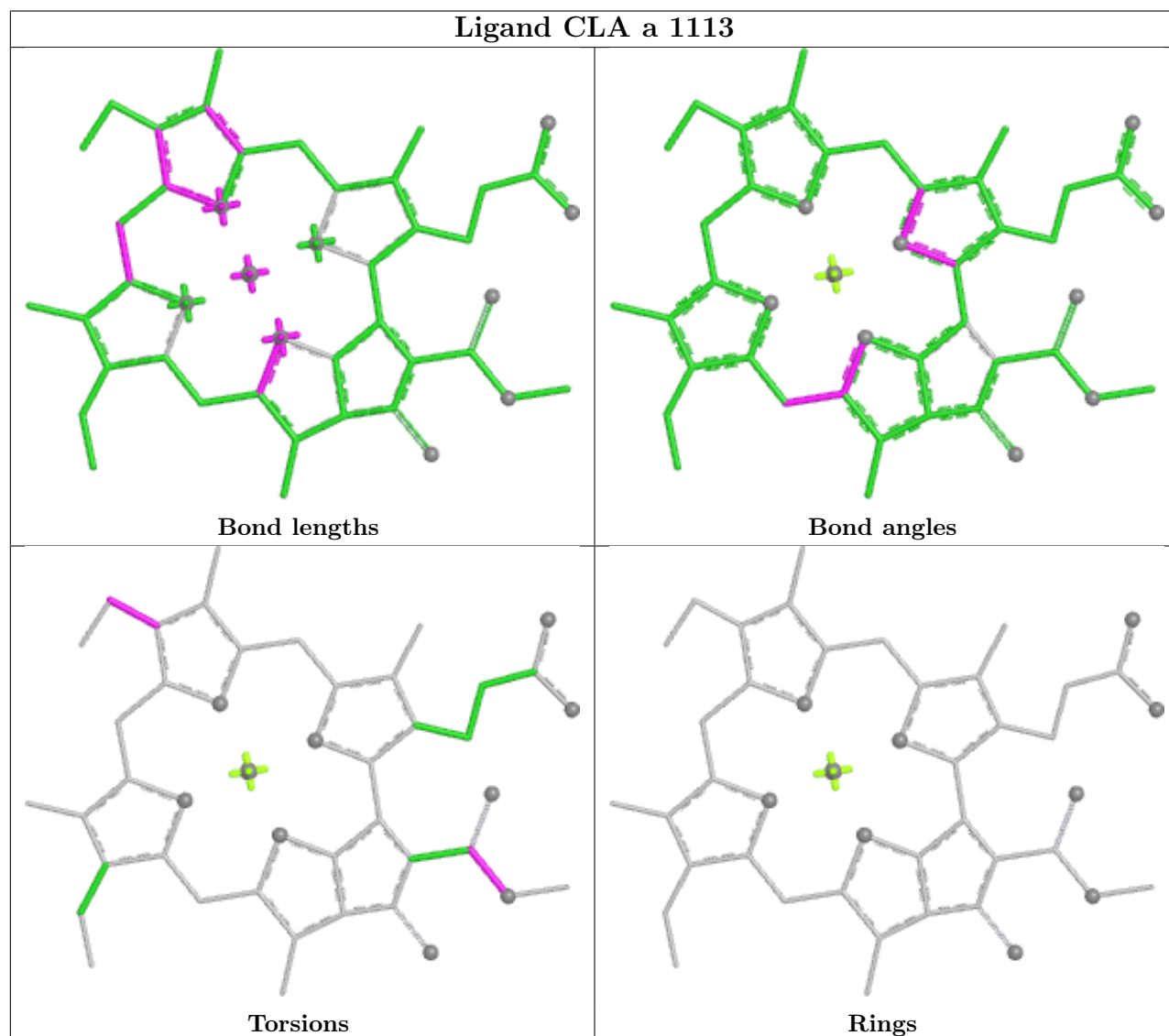
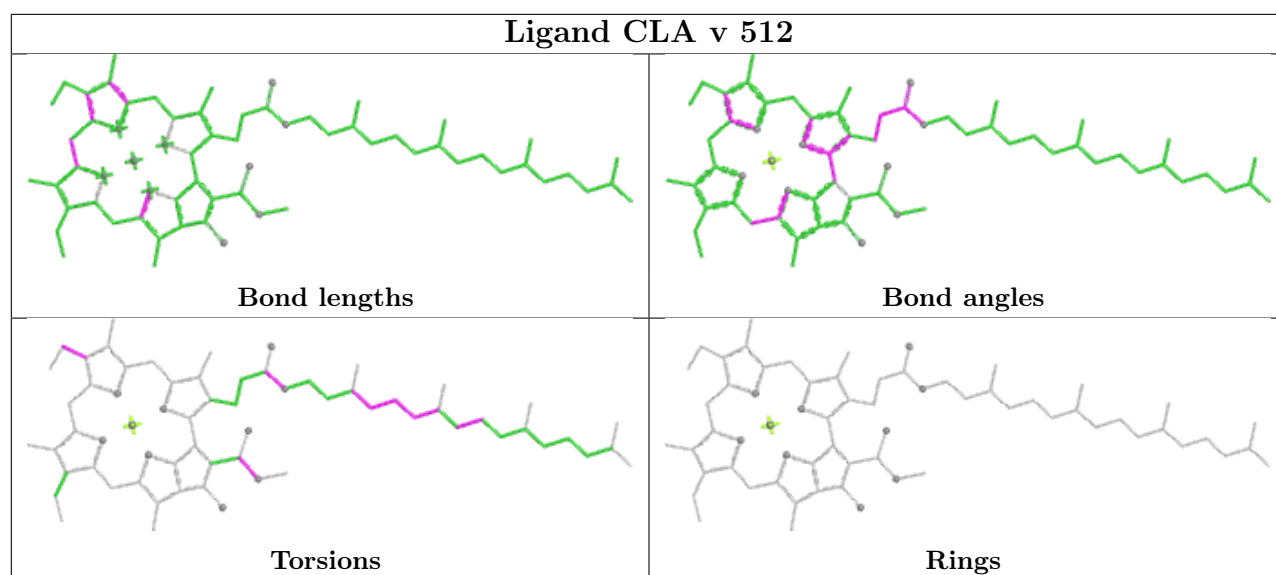
Ligand CLA B 1219

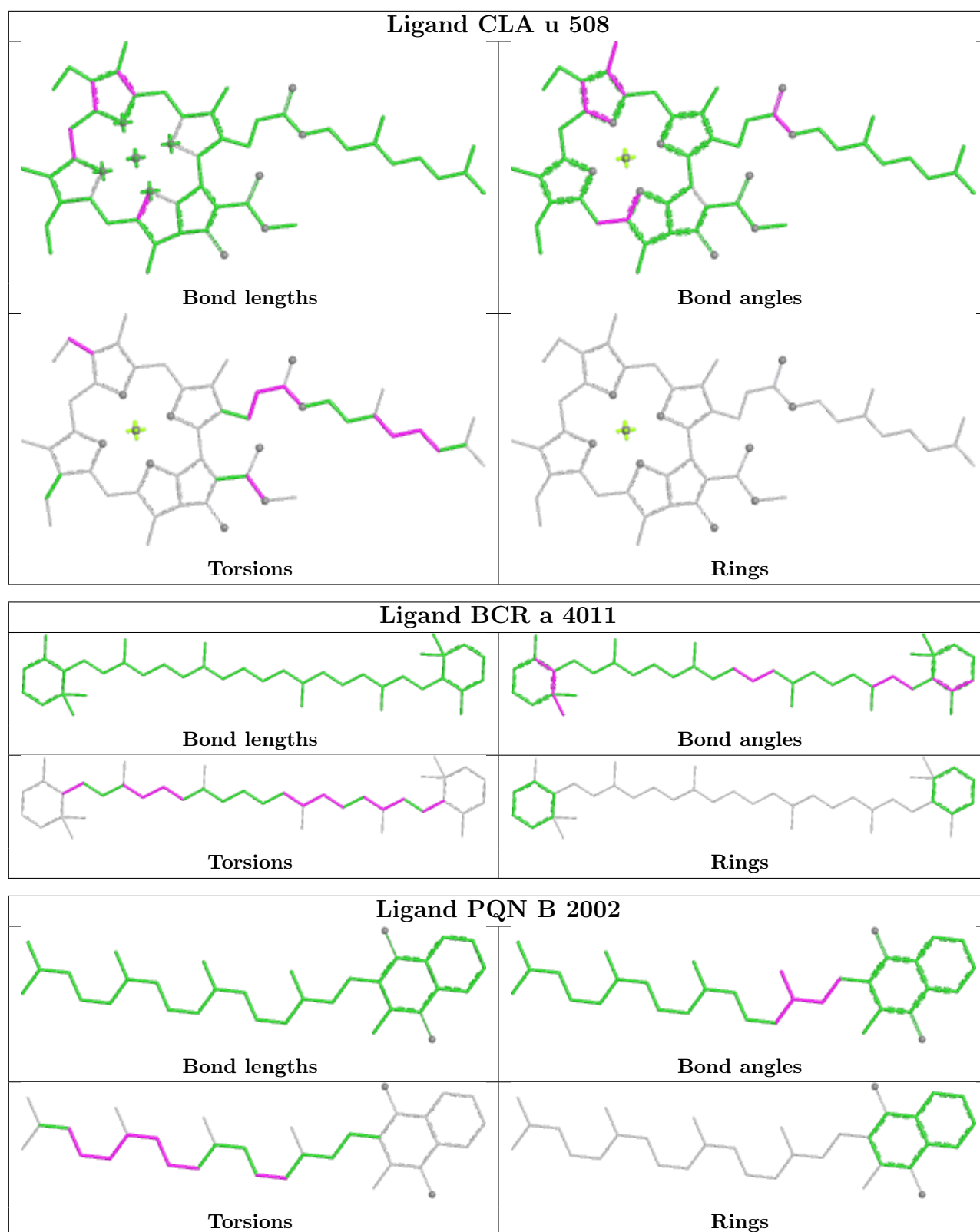


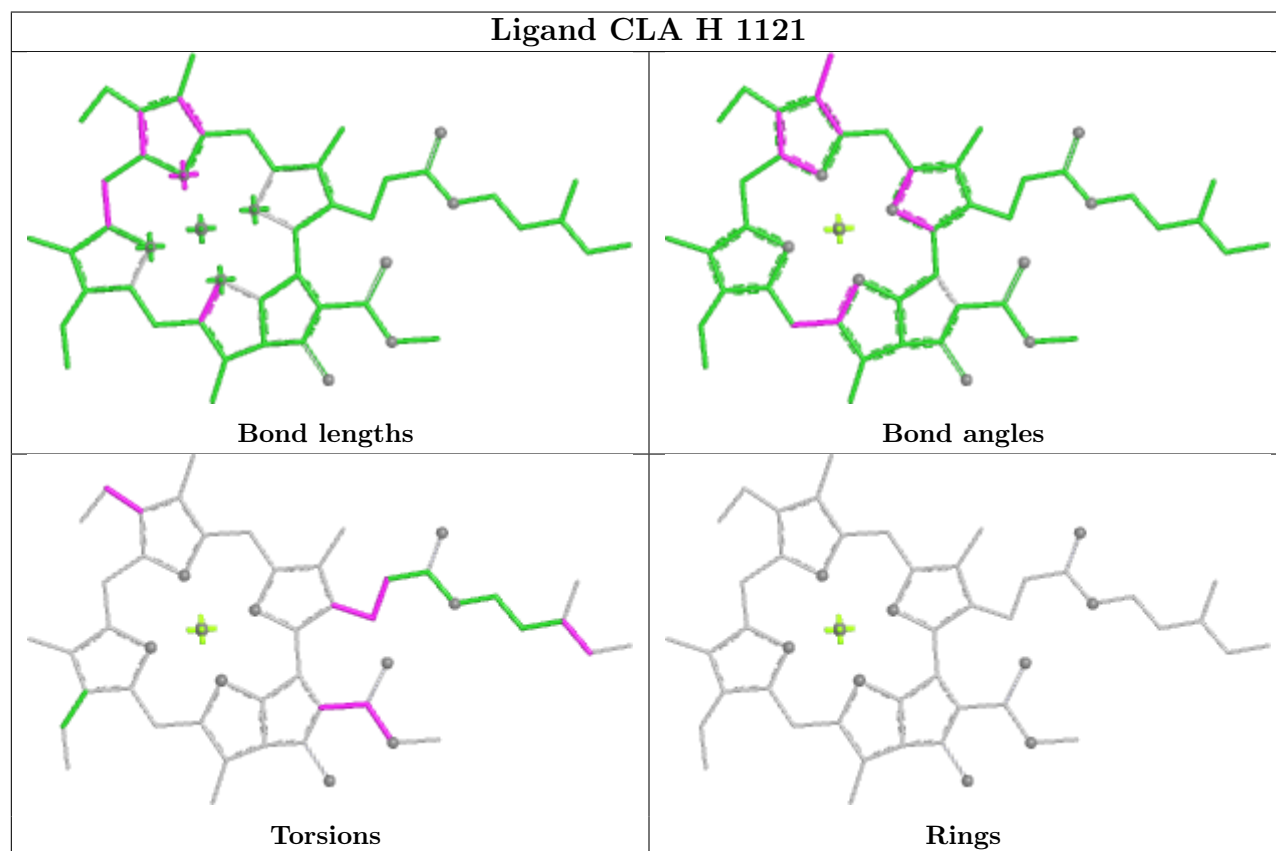
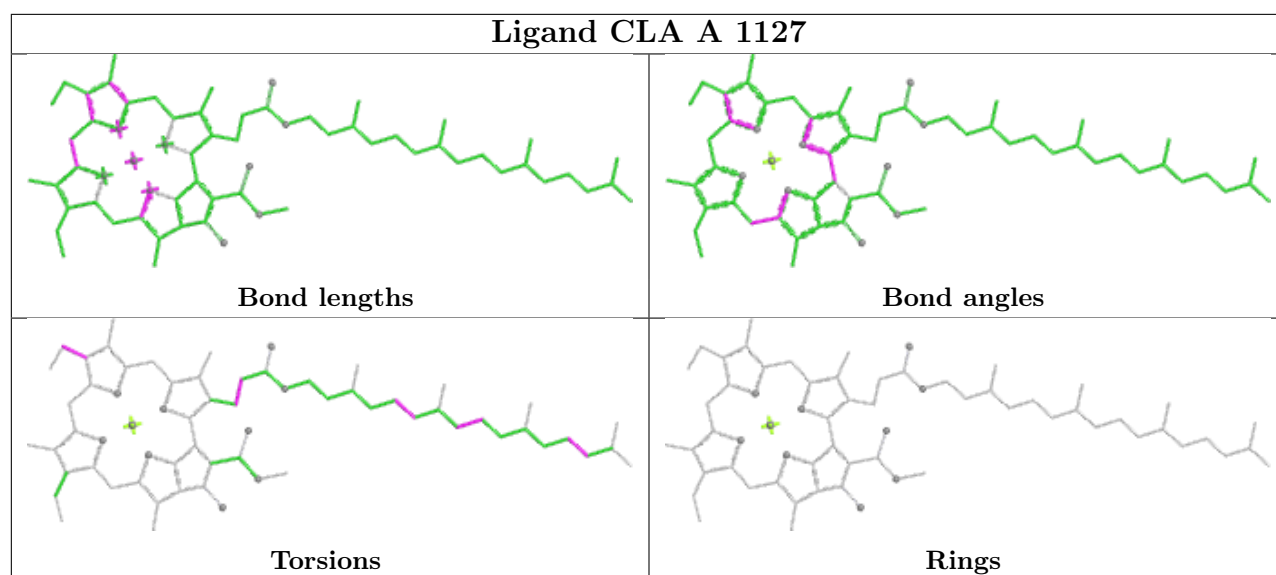
Ligand CLA F 1301

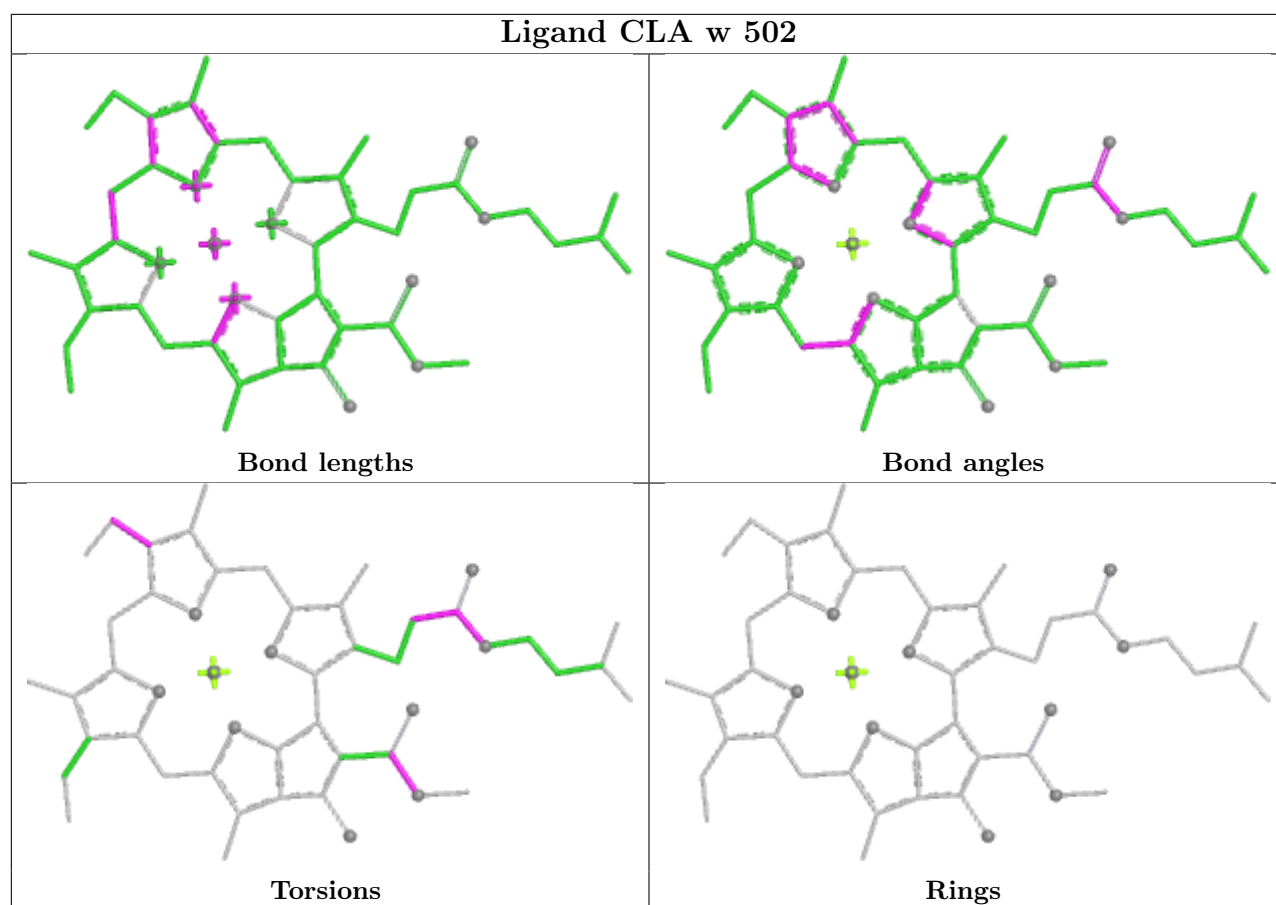




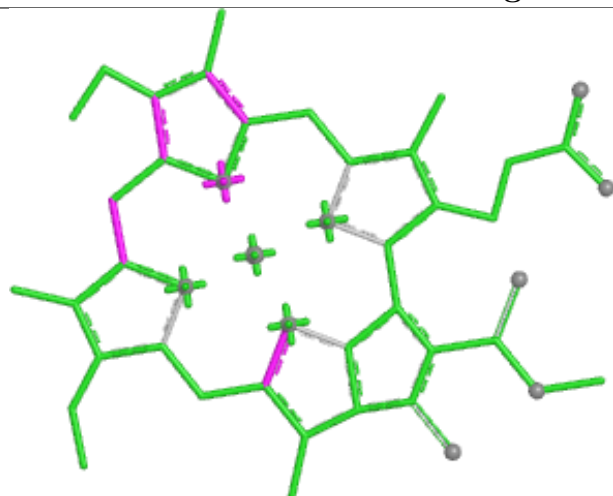




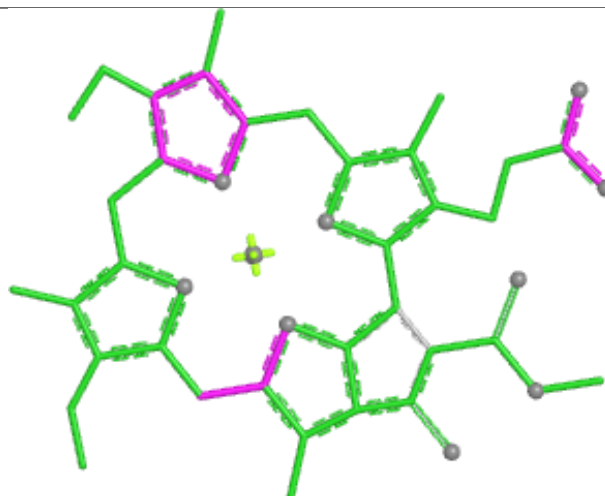




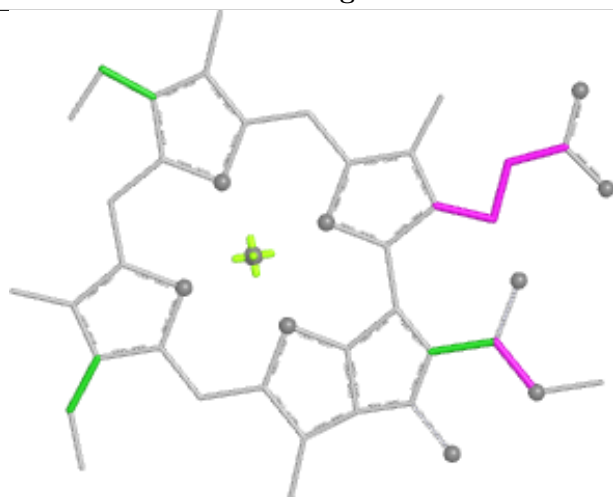
Ligand CLA G 1219



Bond lengths



Bond angles

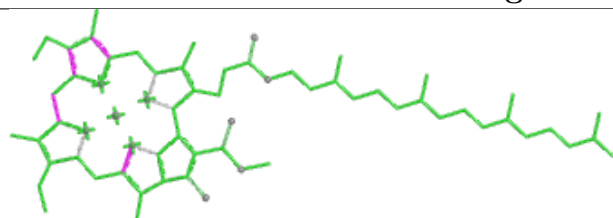


Torsions

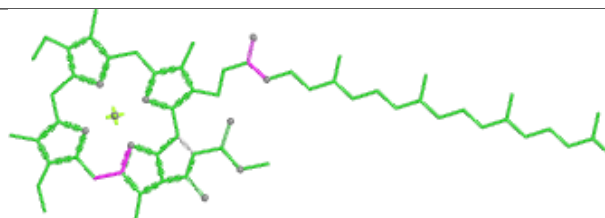


Rings

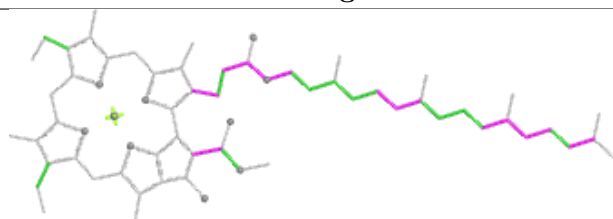
Ligand CLA B 1202



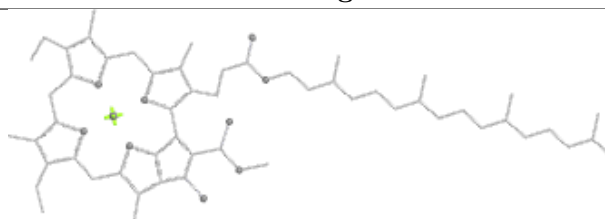
Bond lengths



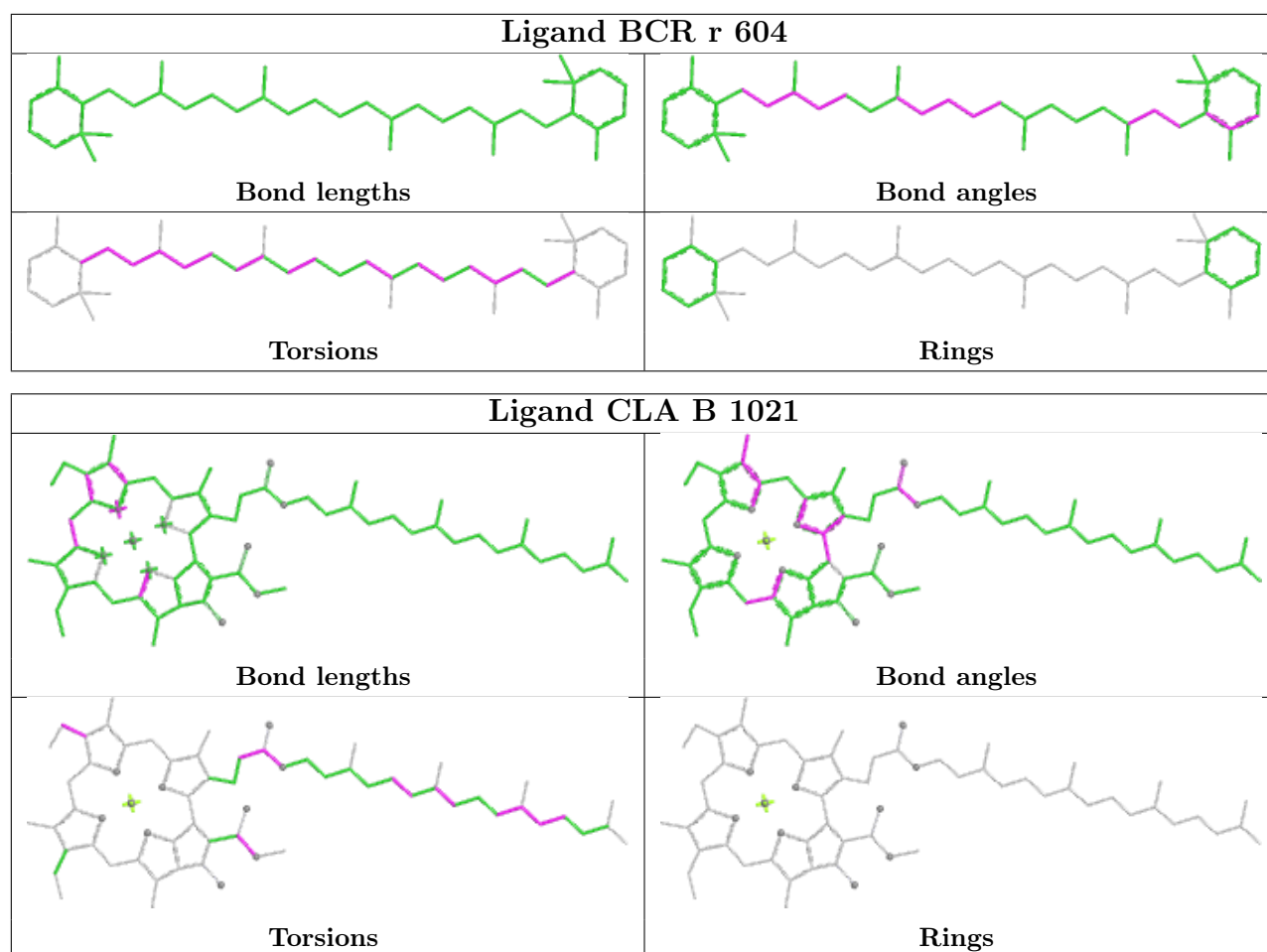
Bond angles

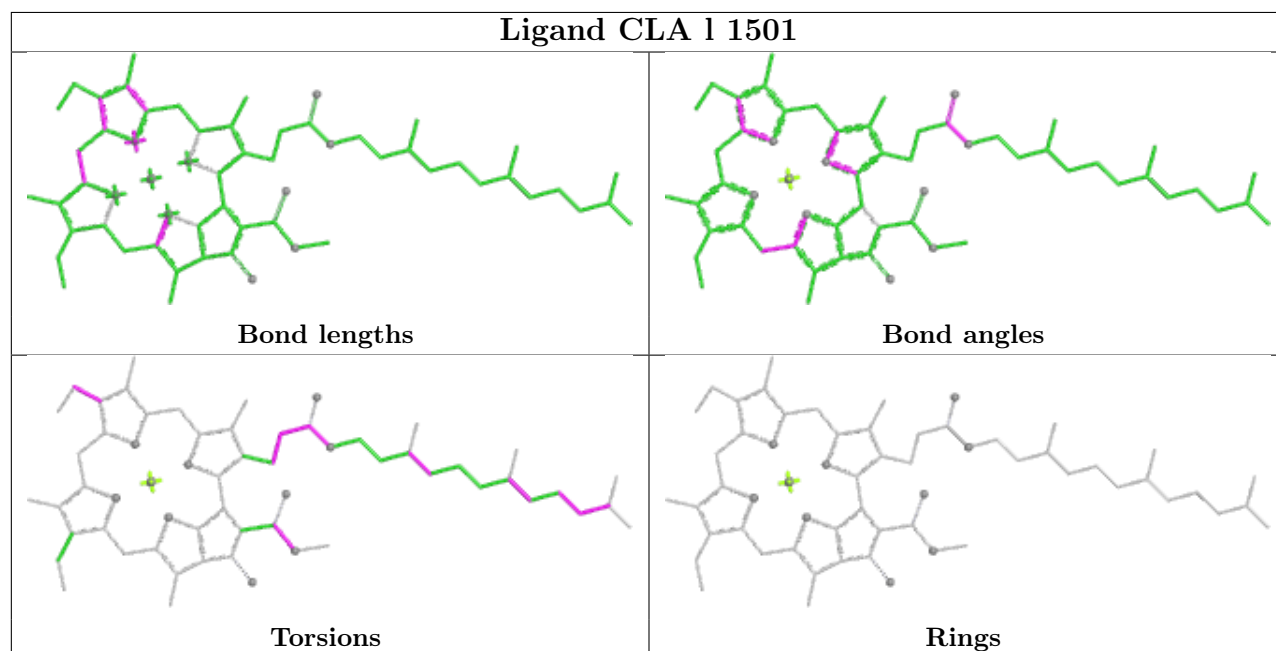
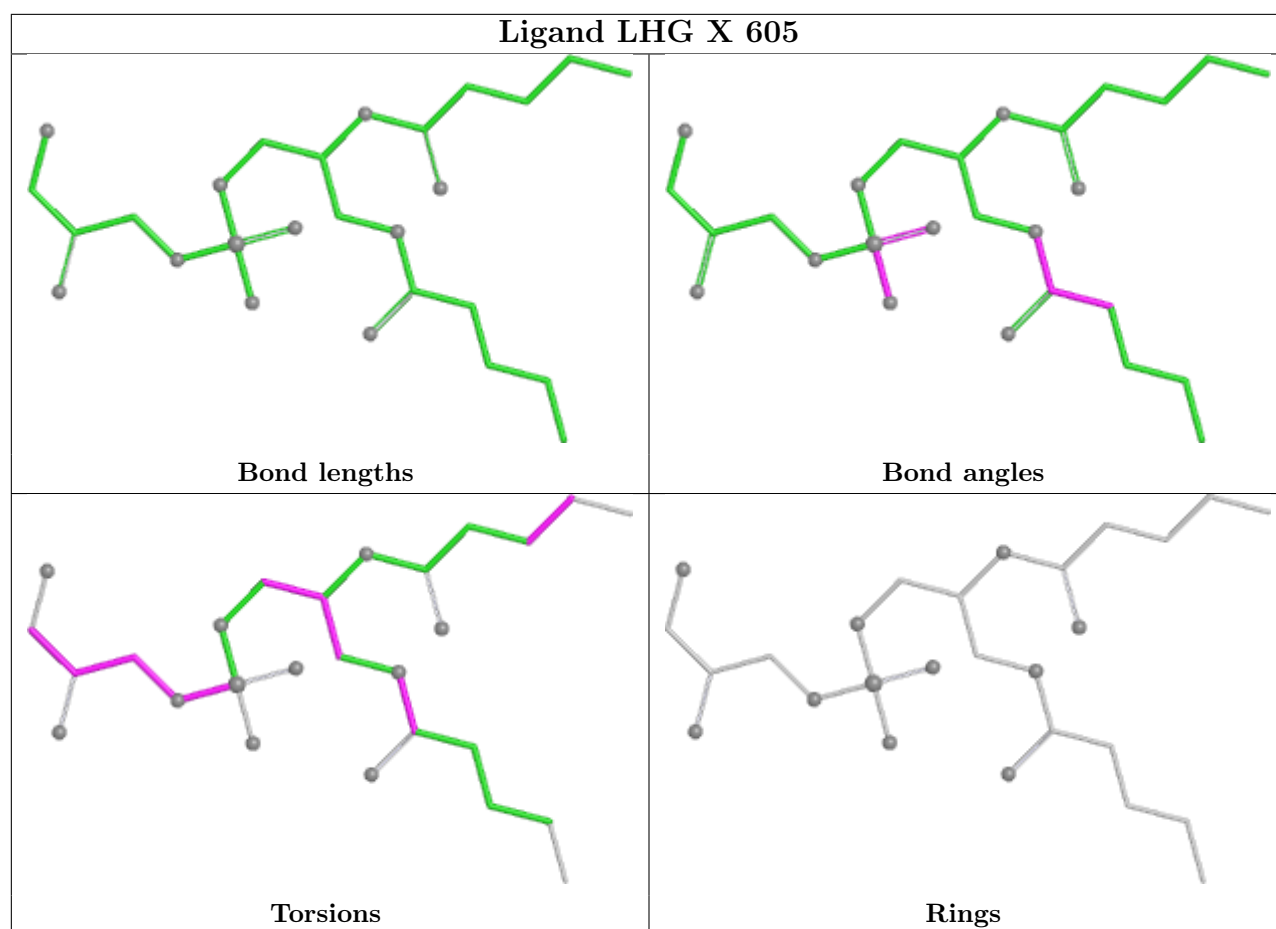


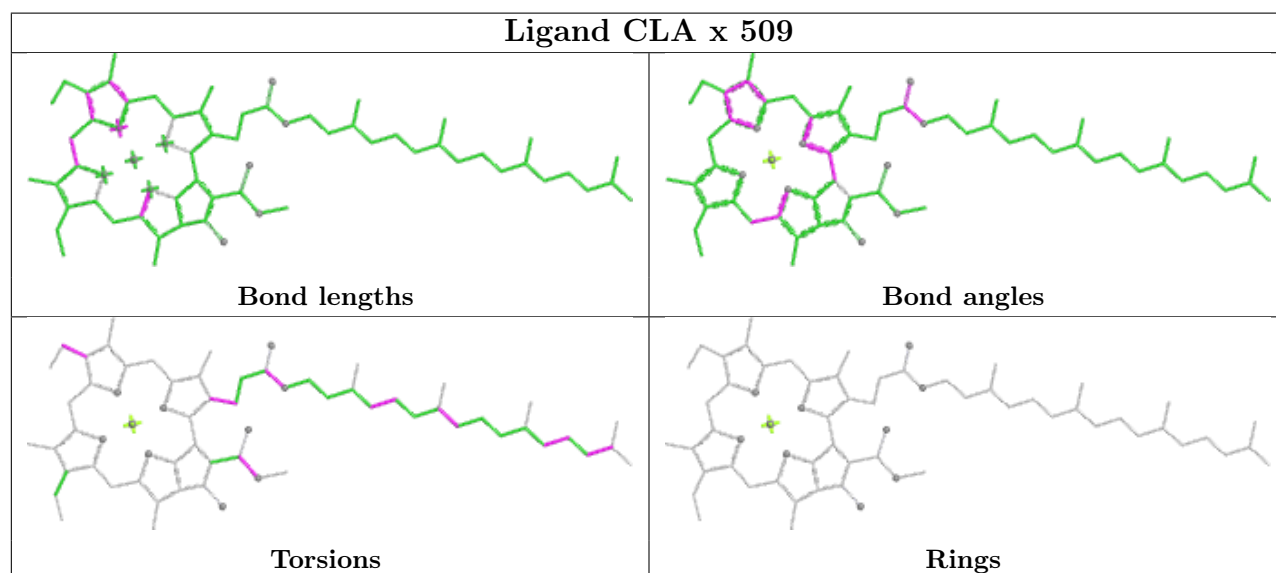
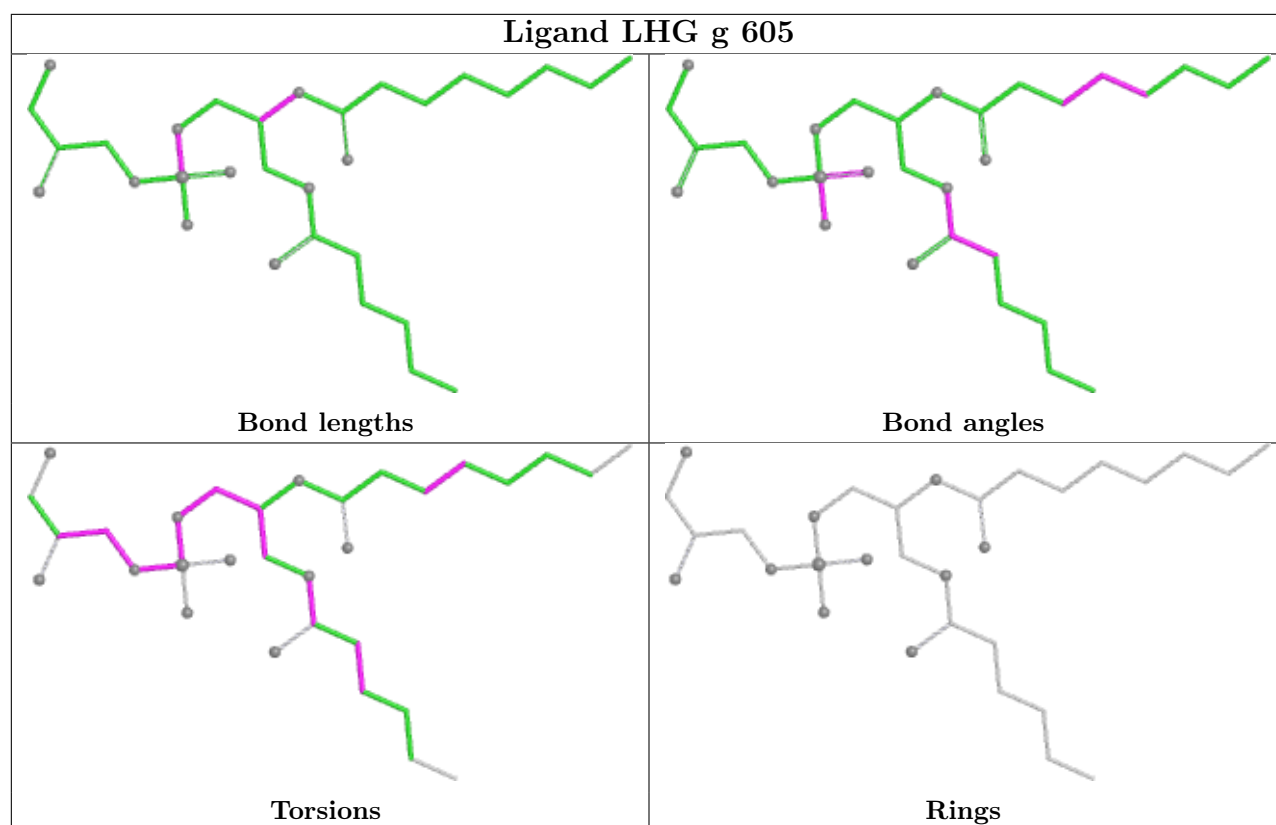
Torsions

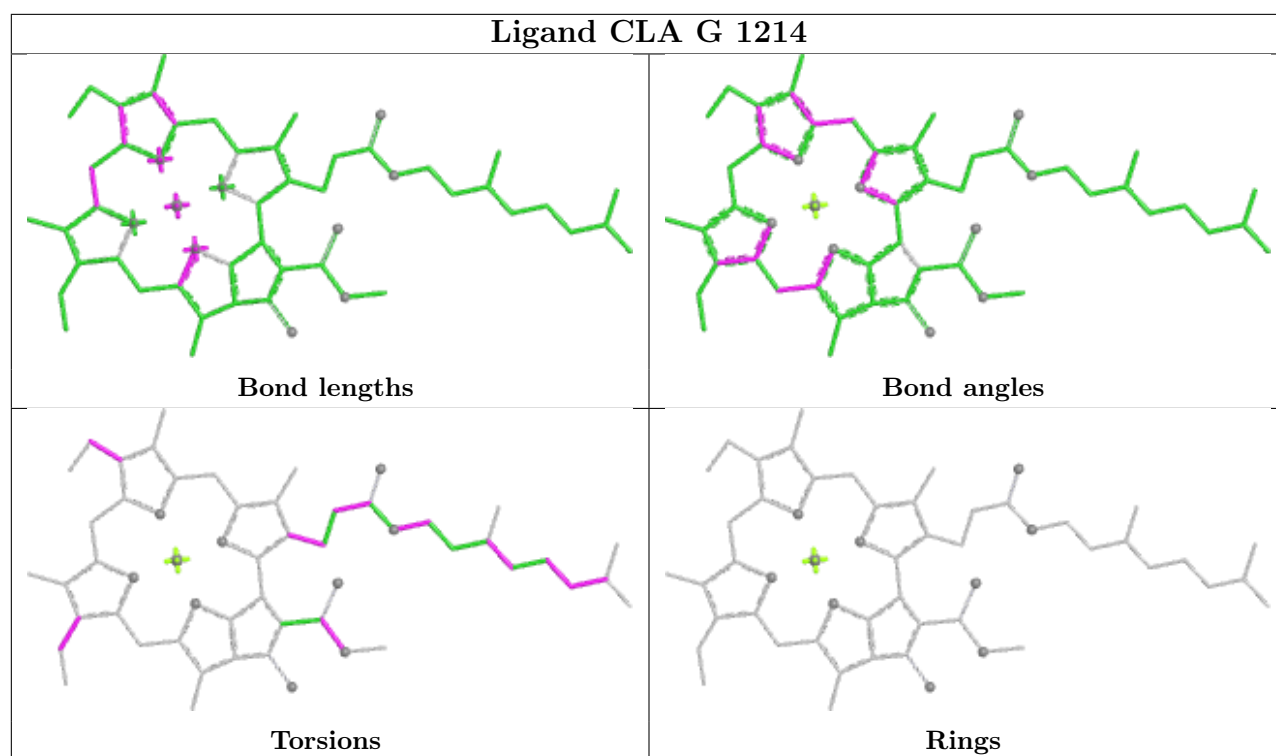


Rings

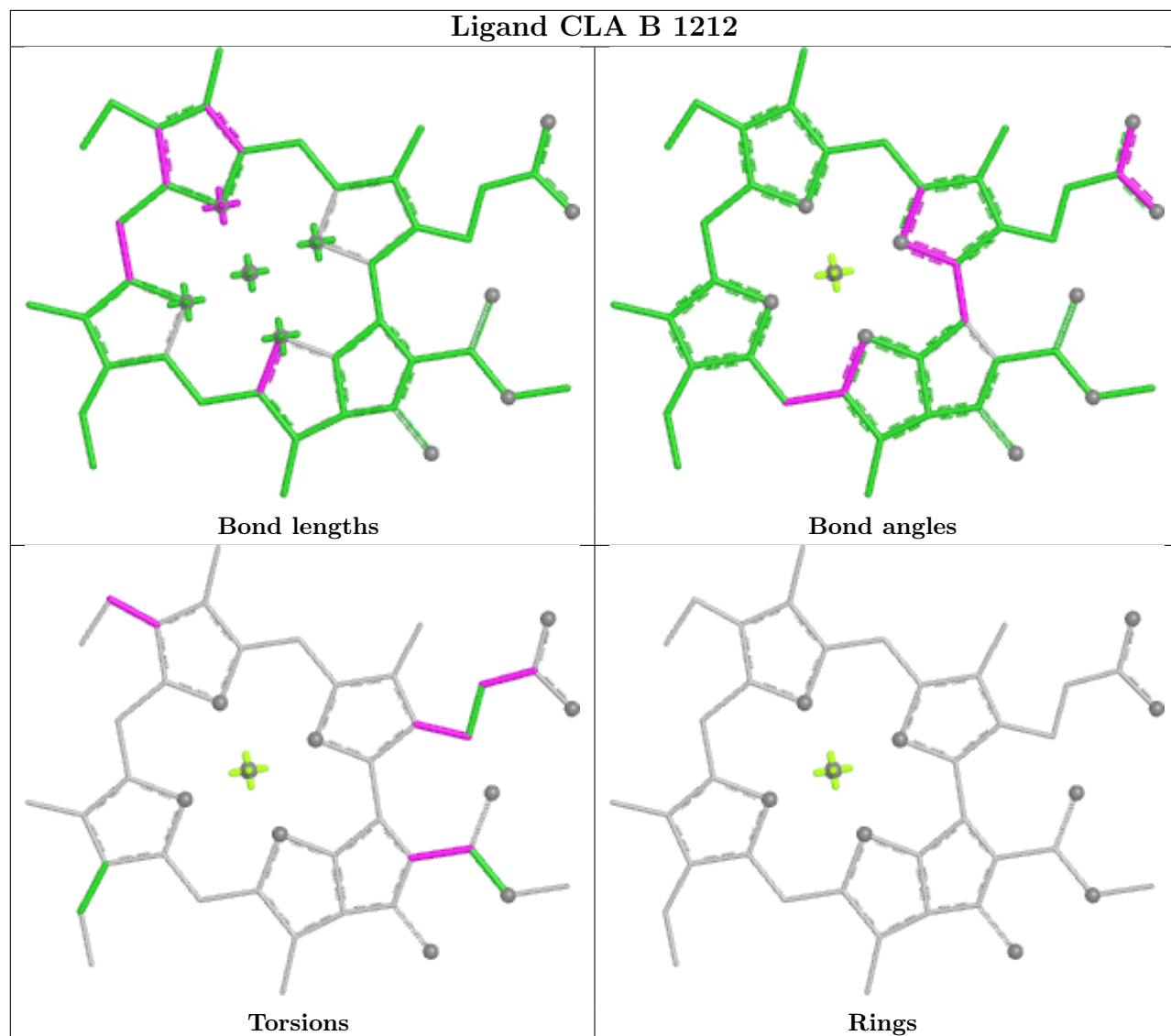


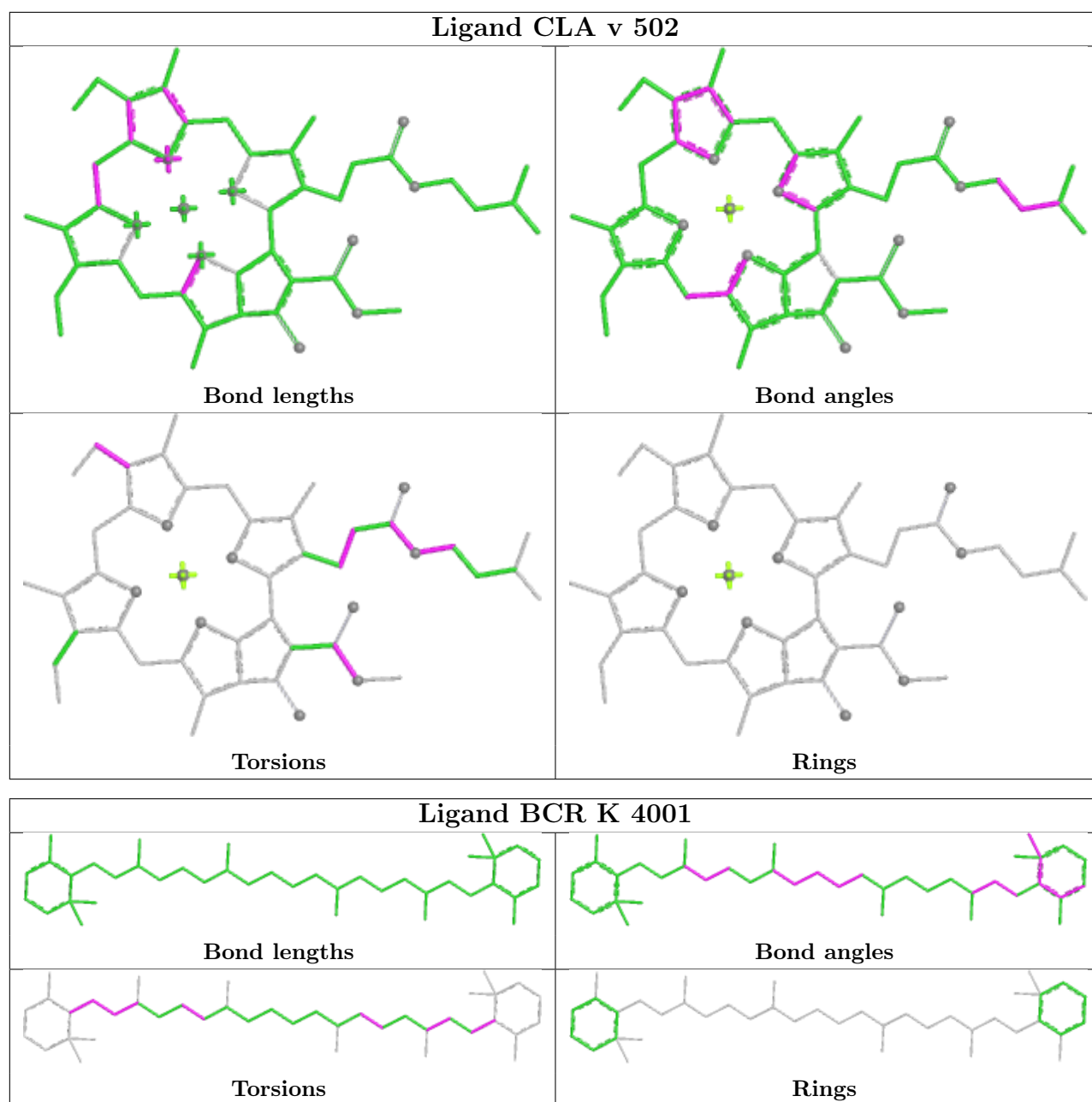


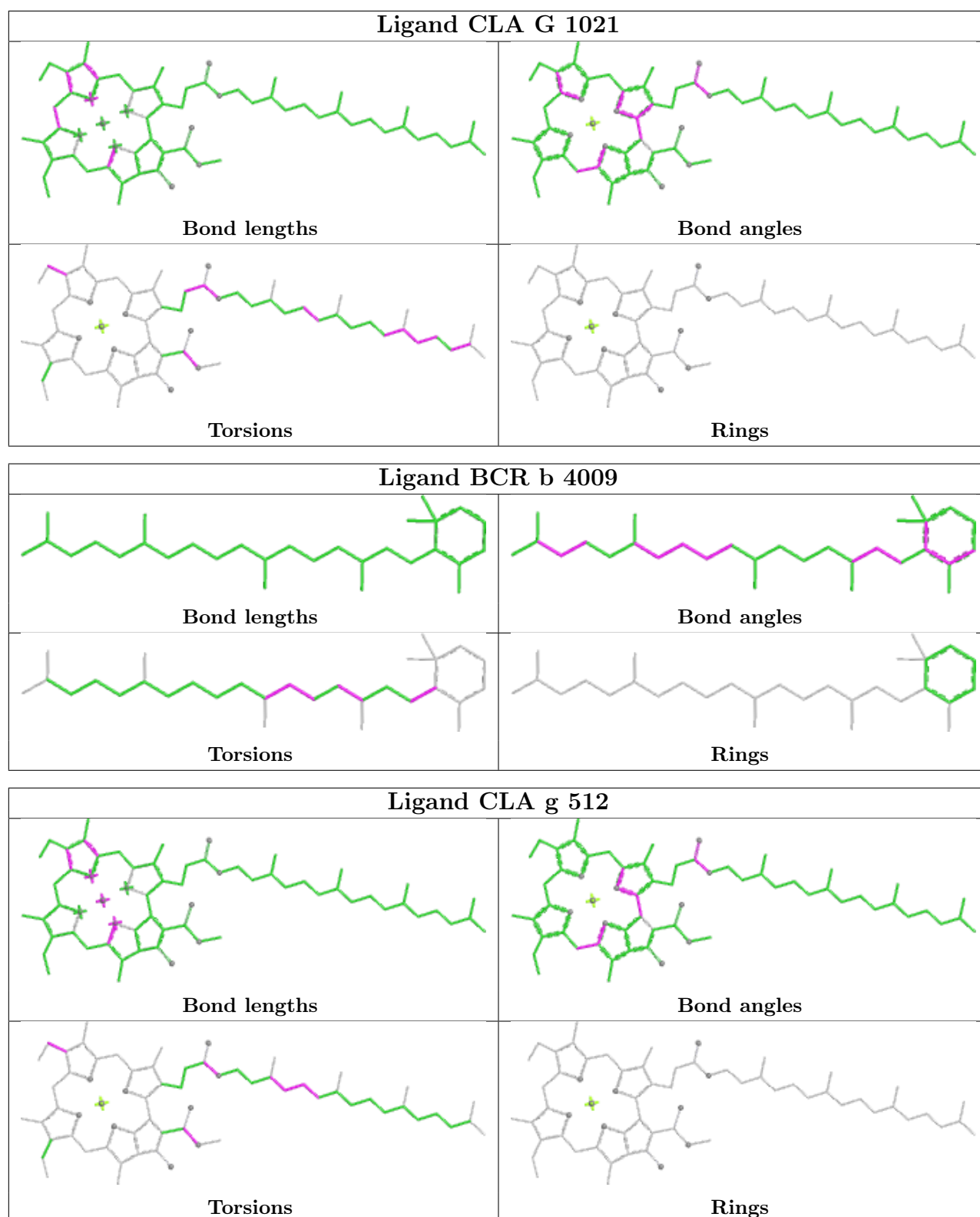


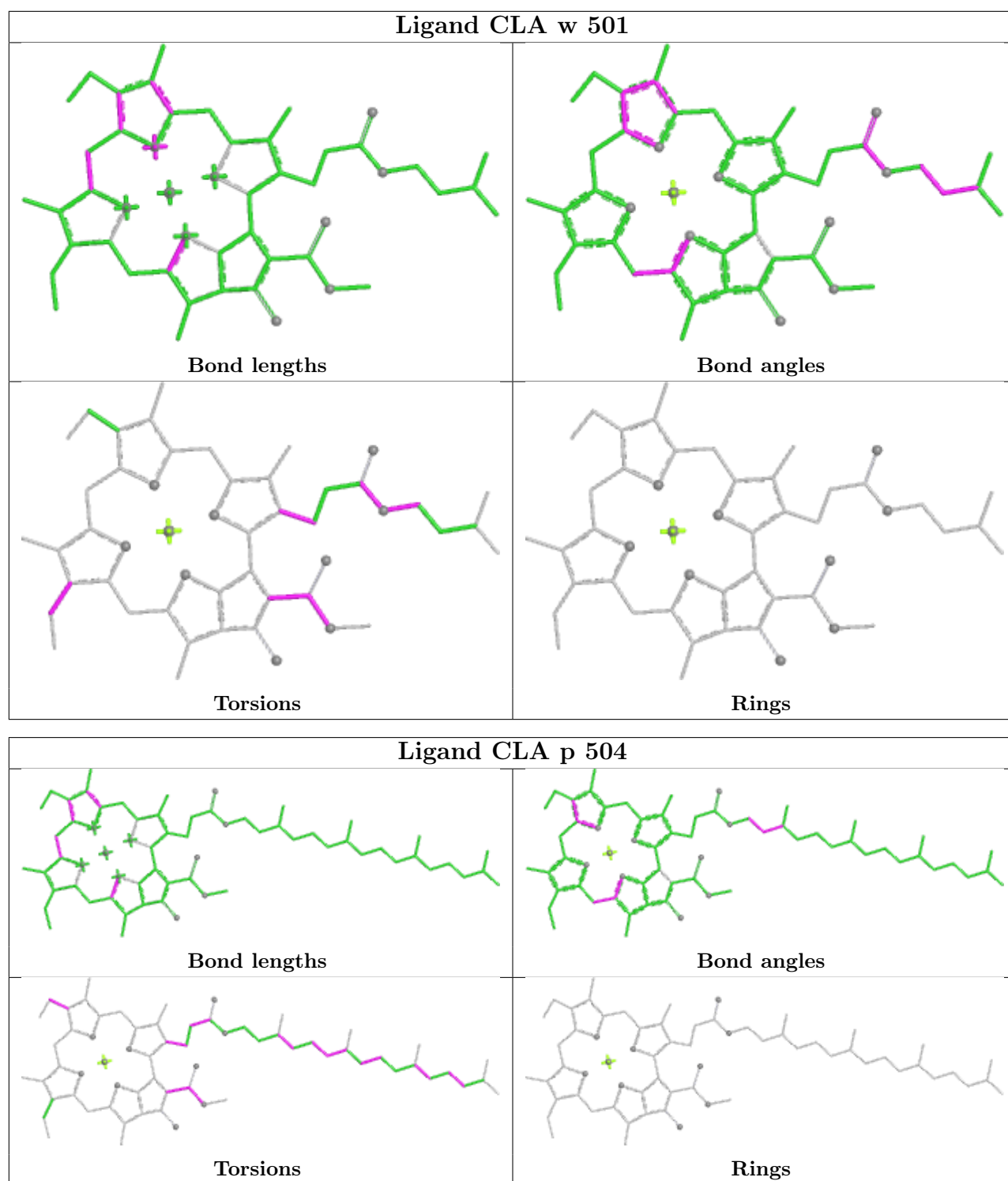


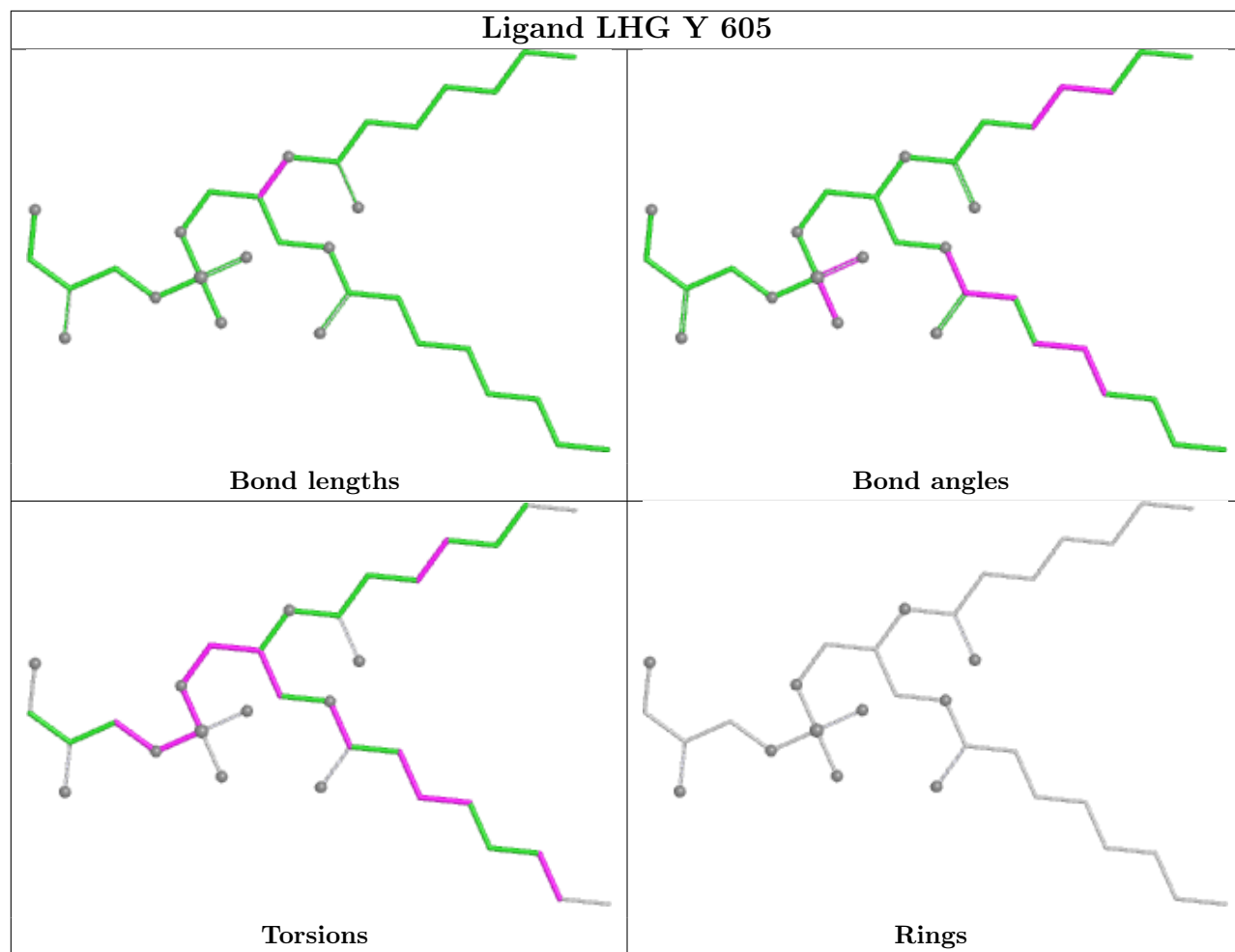
Ligand CLA B 1212

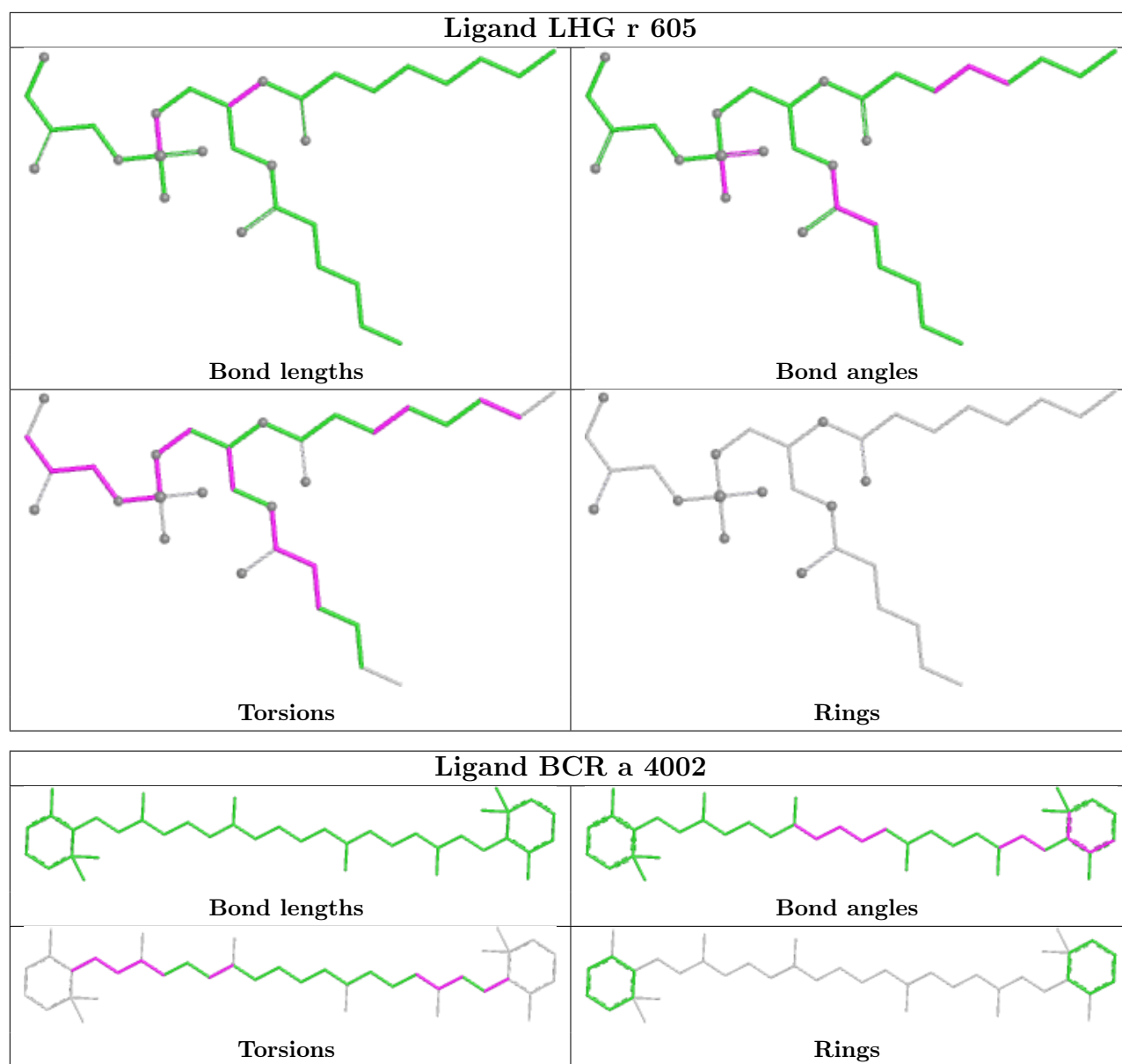


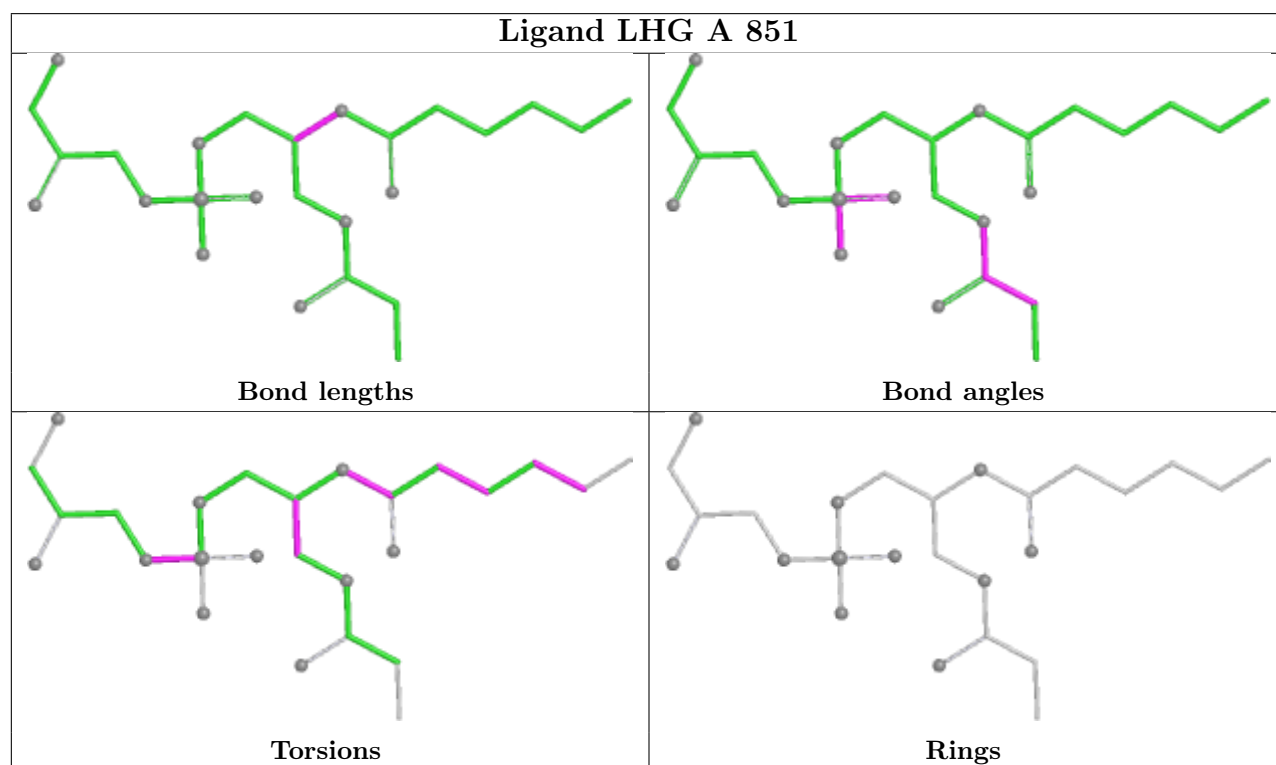
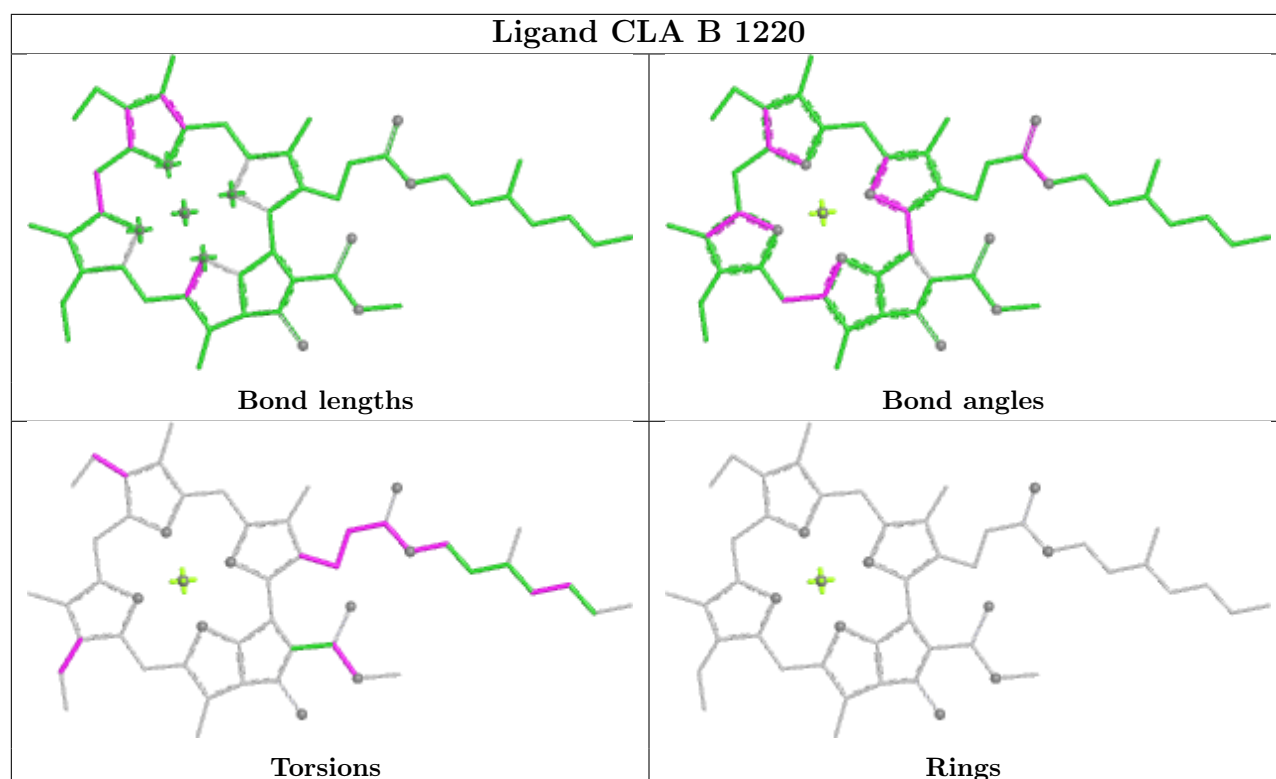




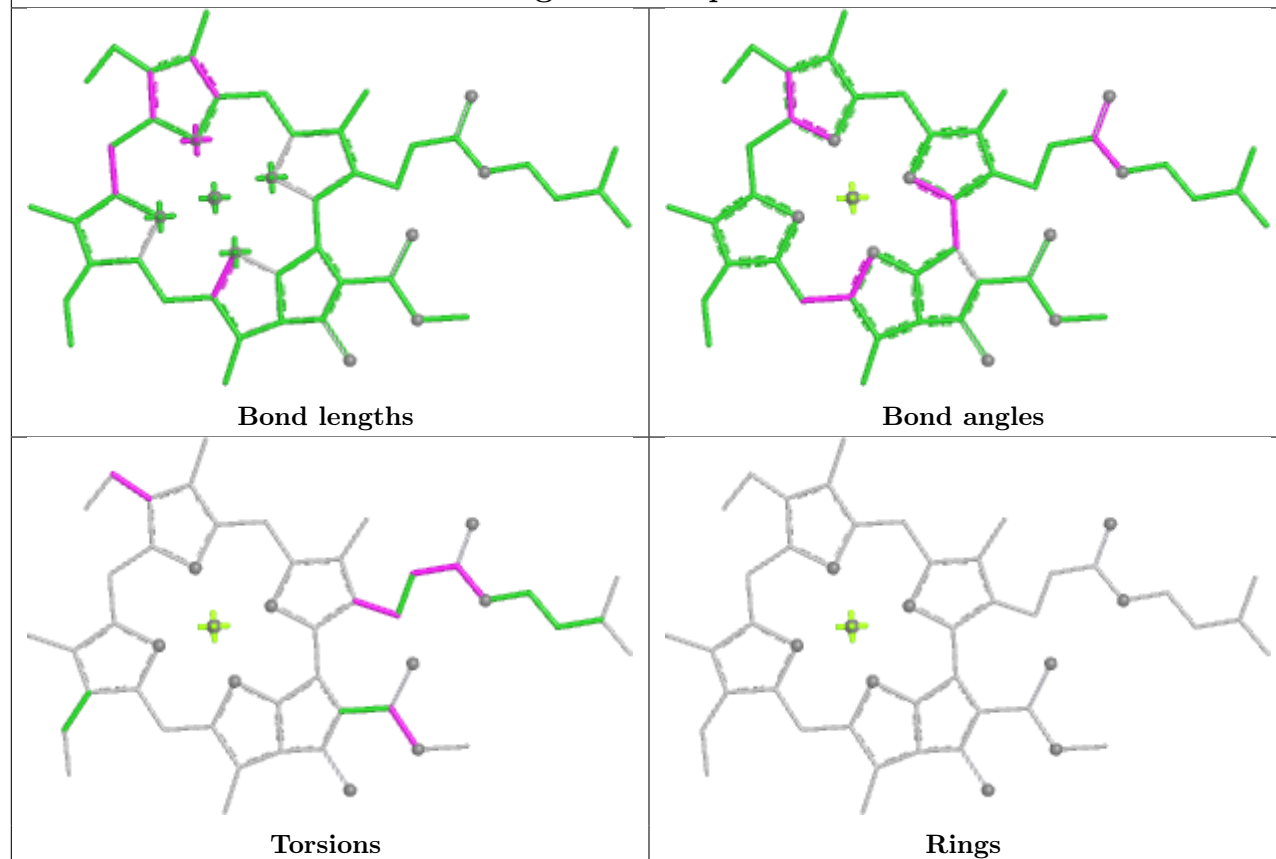




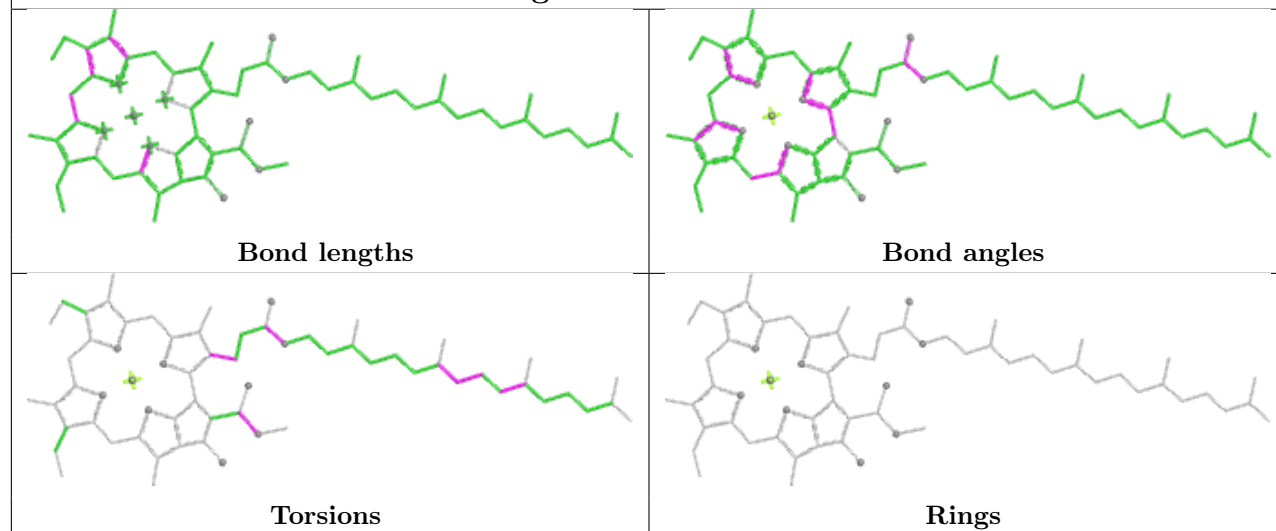


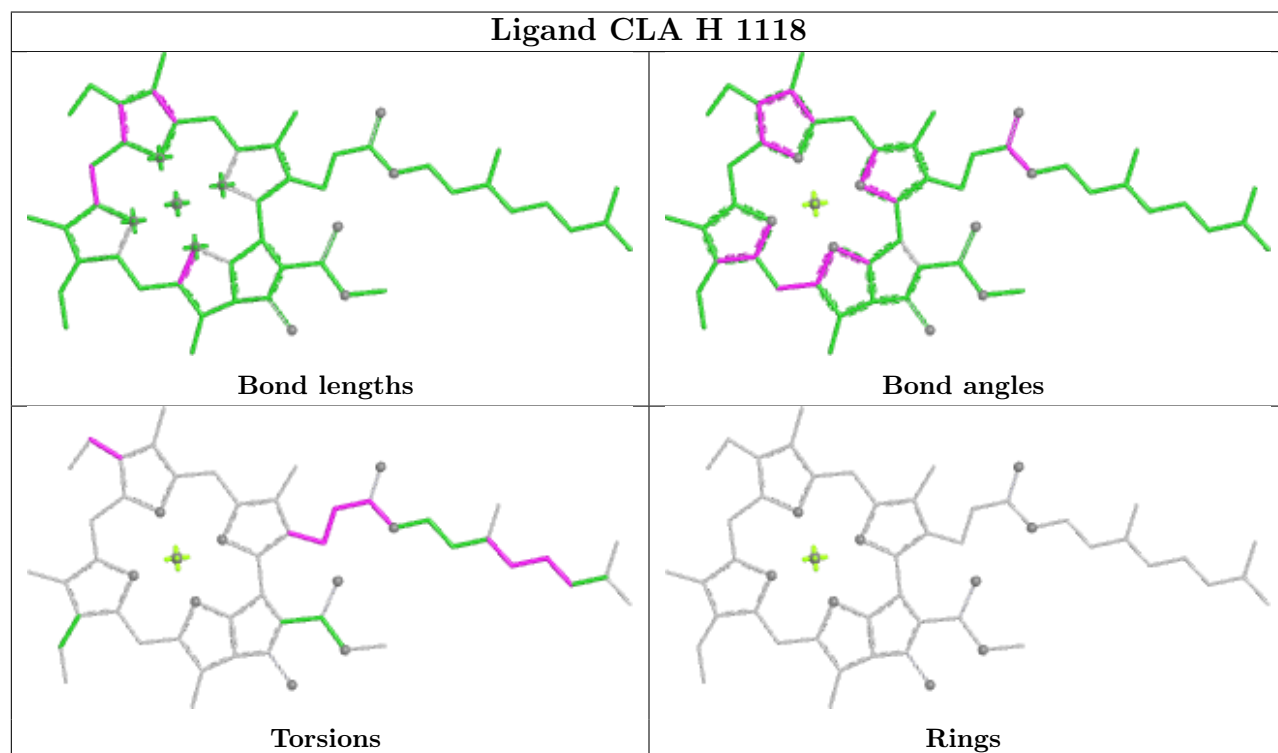
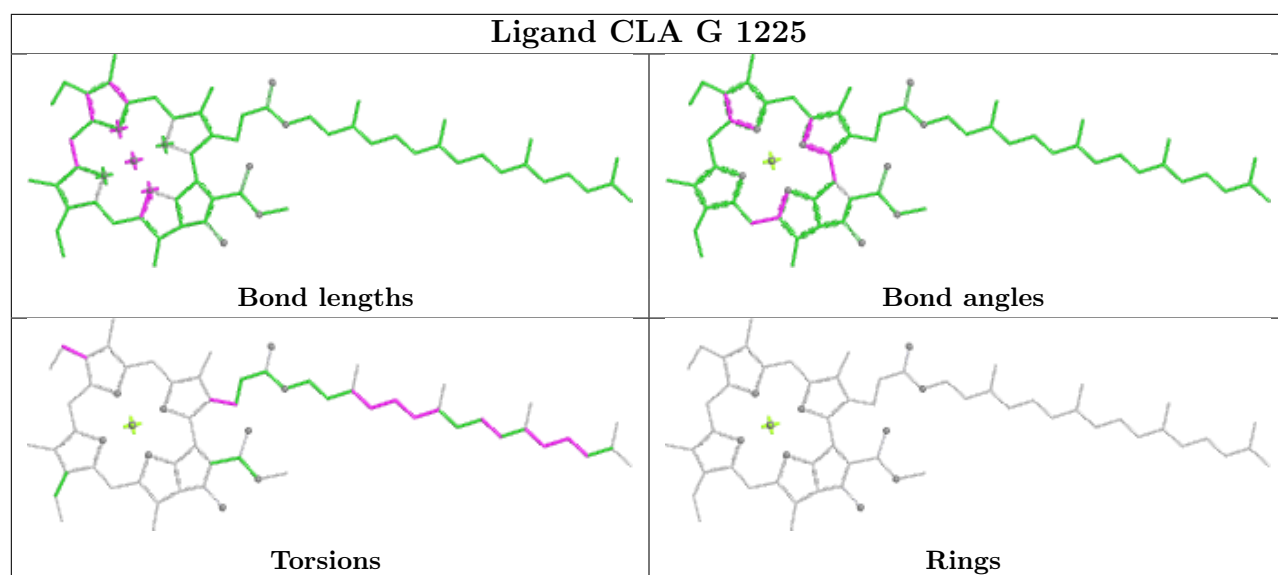


Ligand CLA p 514

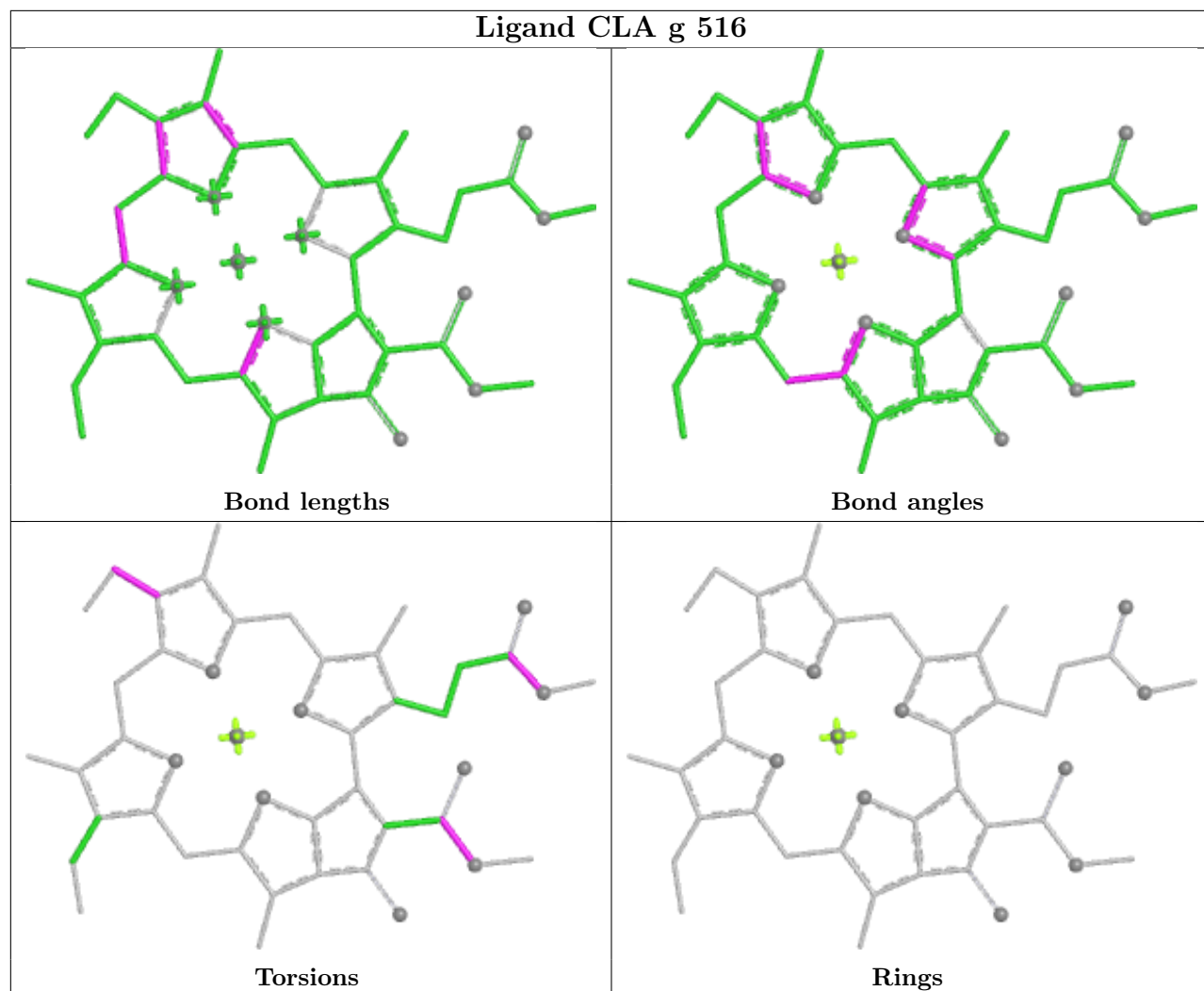


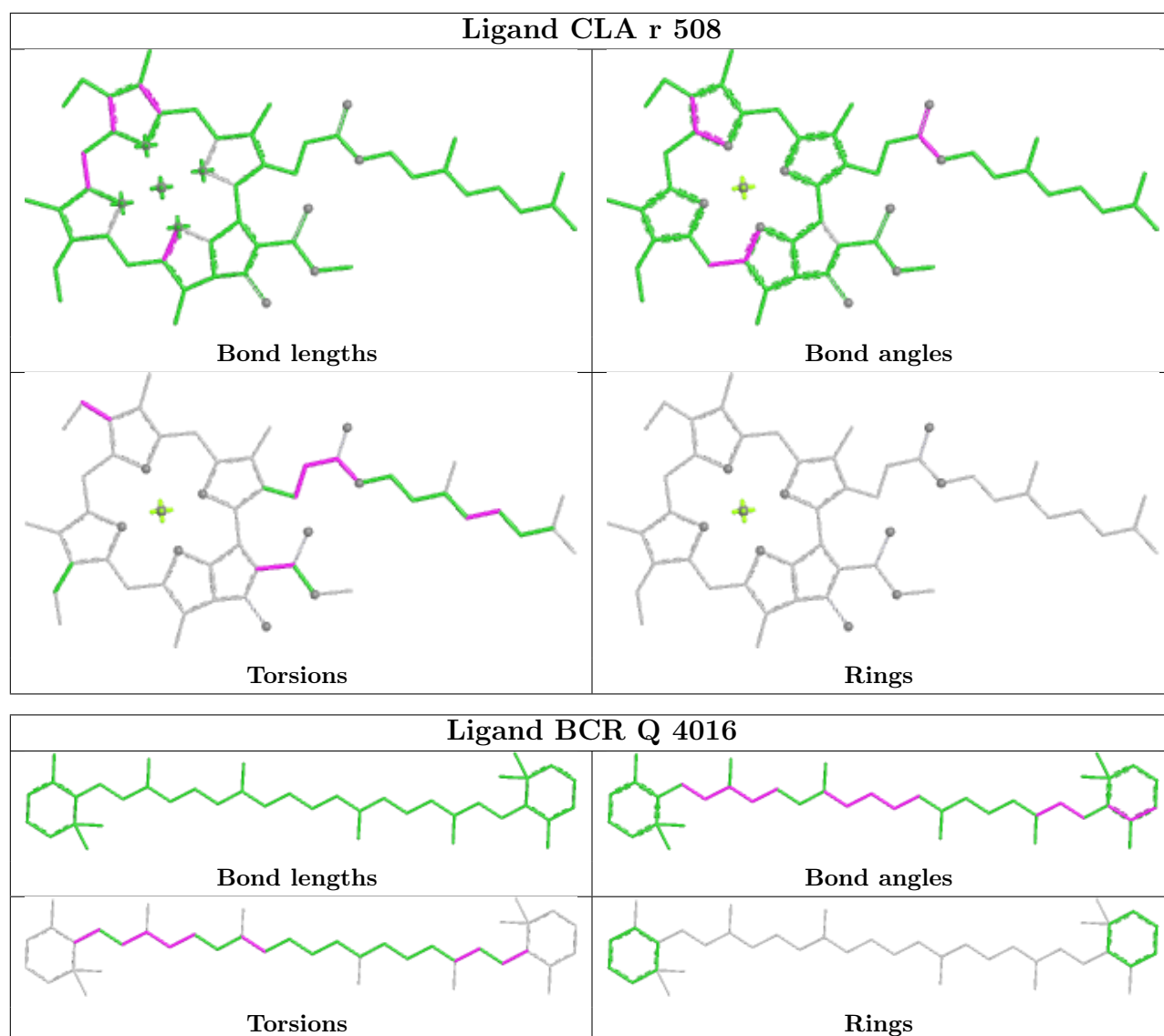
Ligand CLA X 511

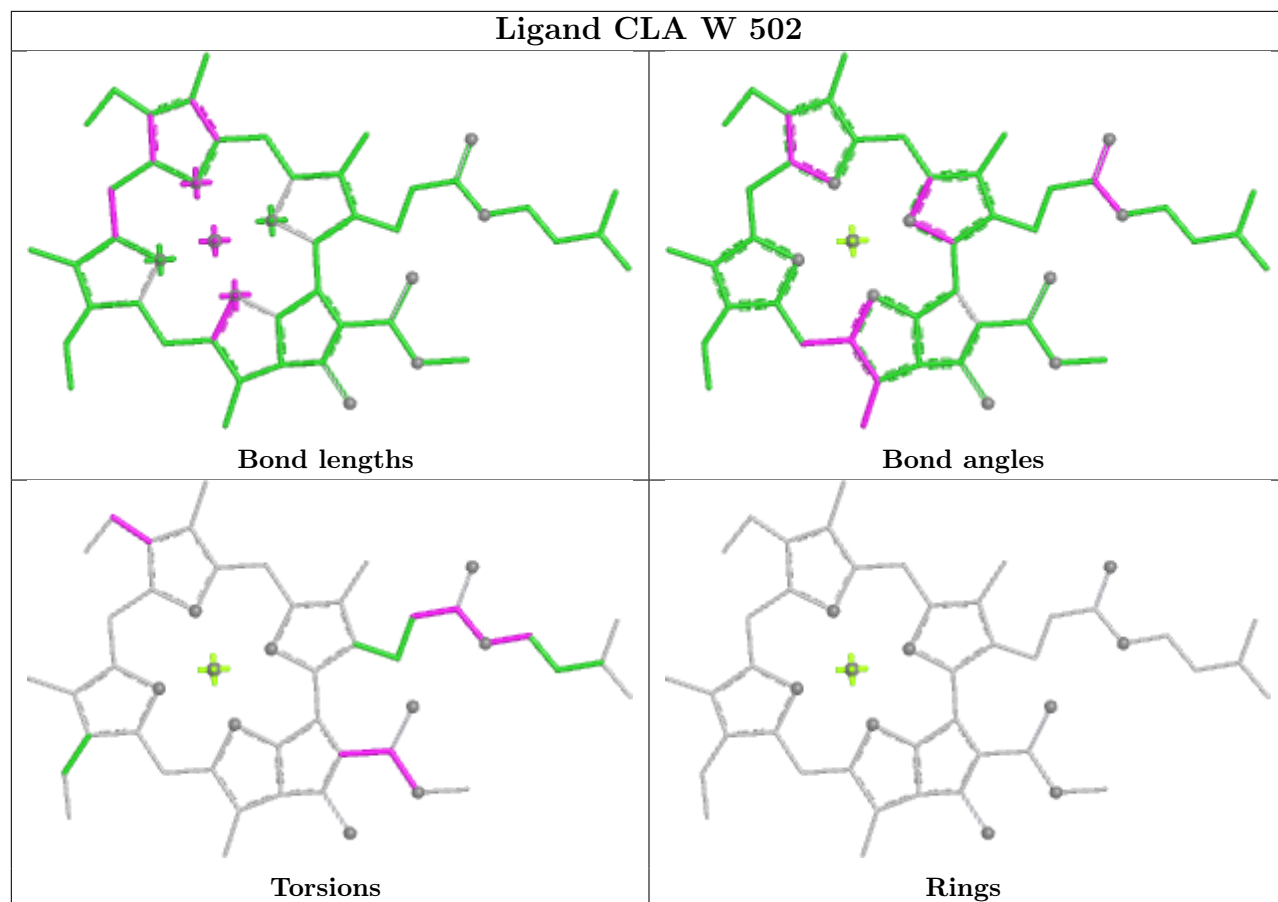


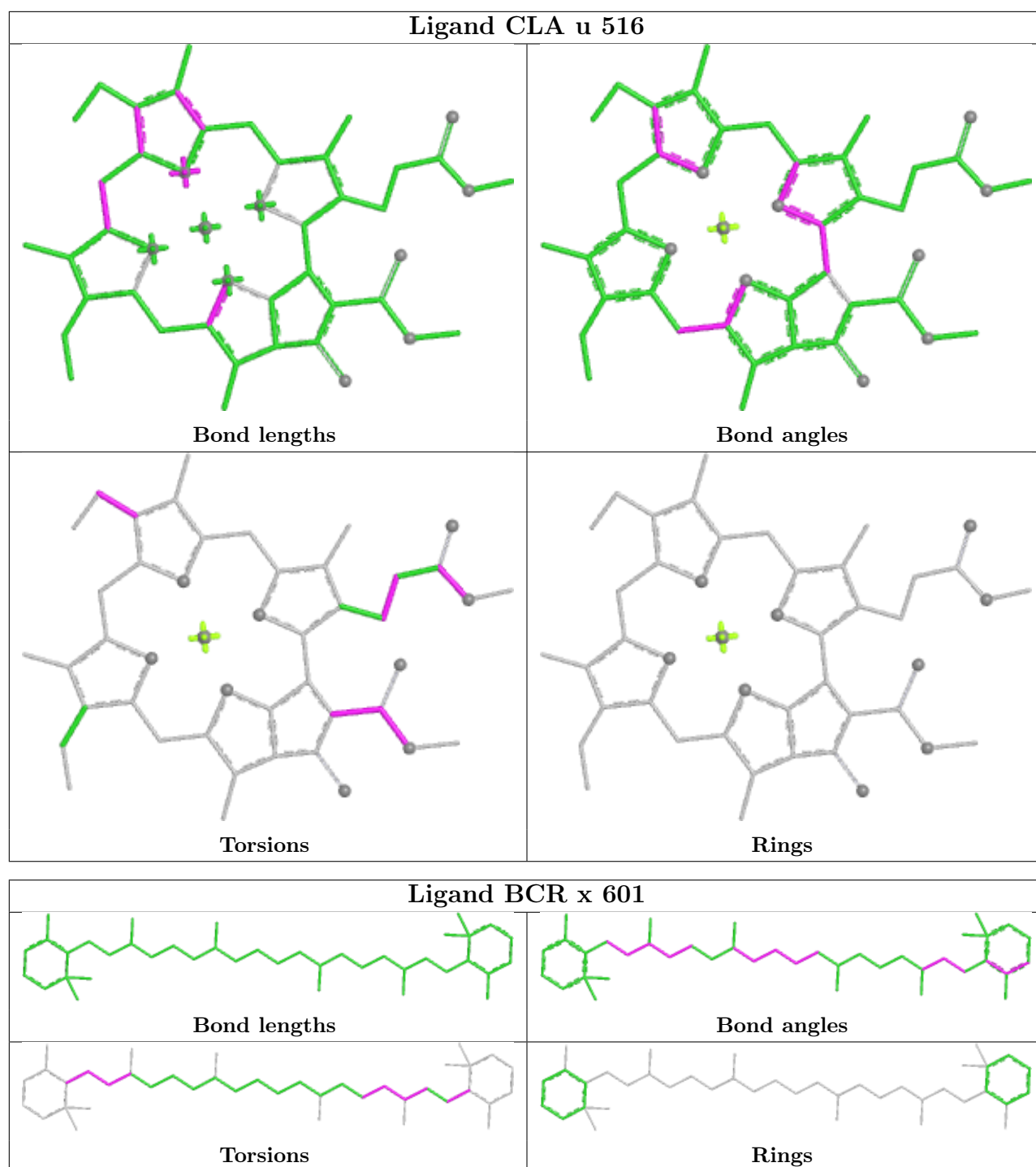


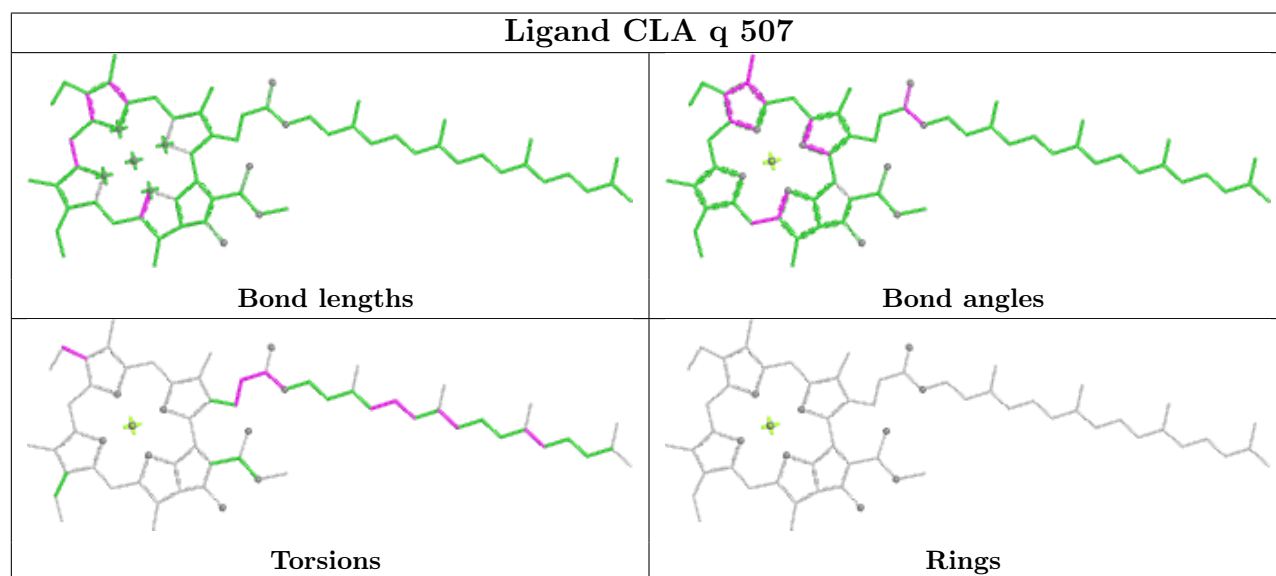
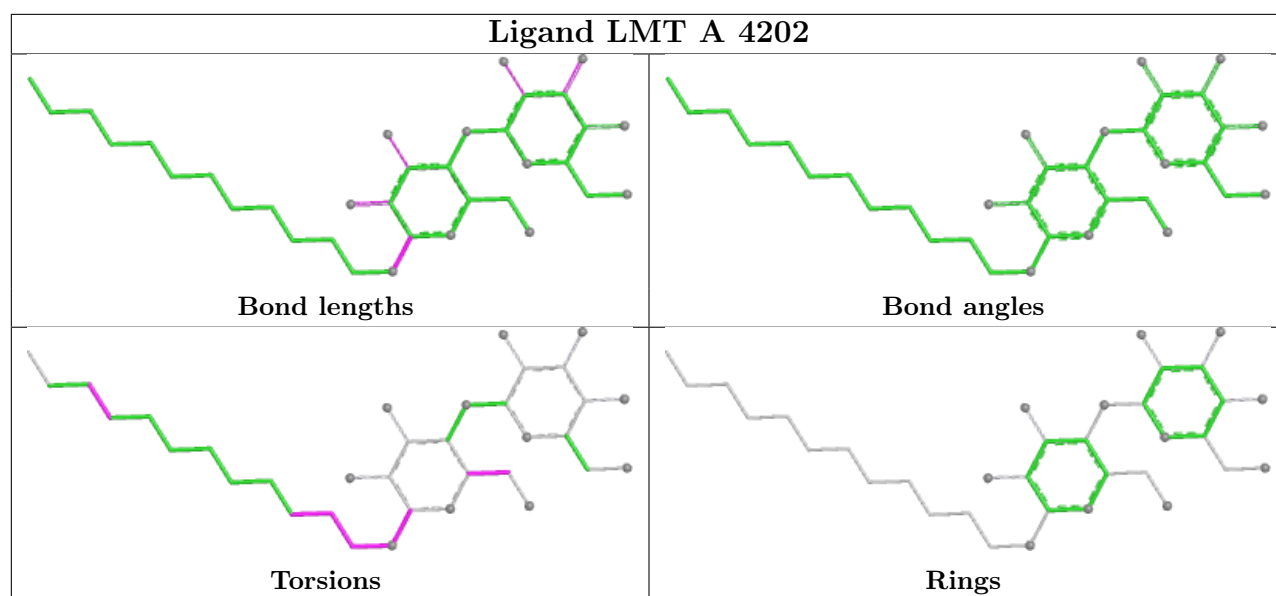
Ligand CLA g 516

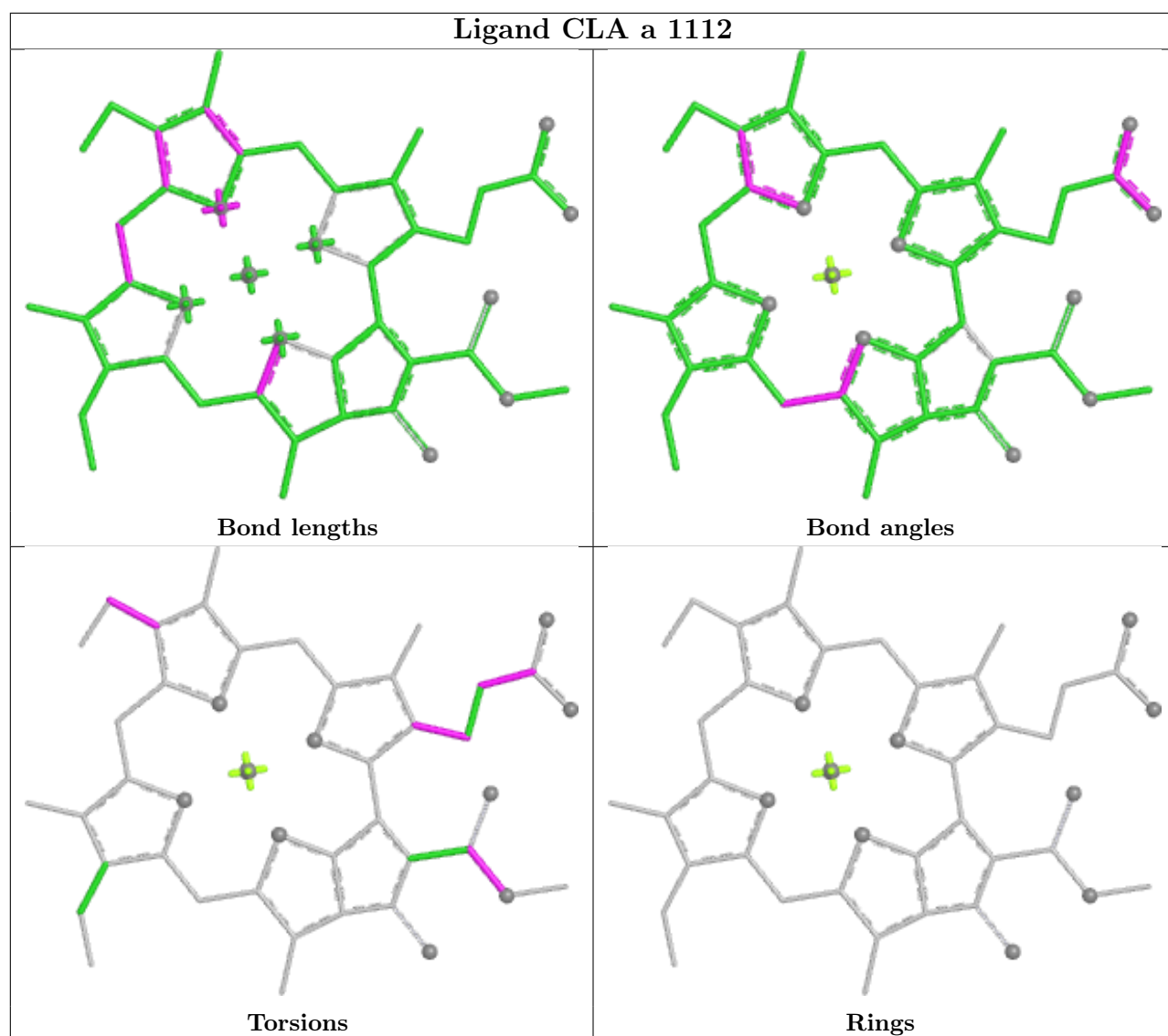




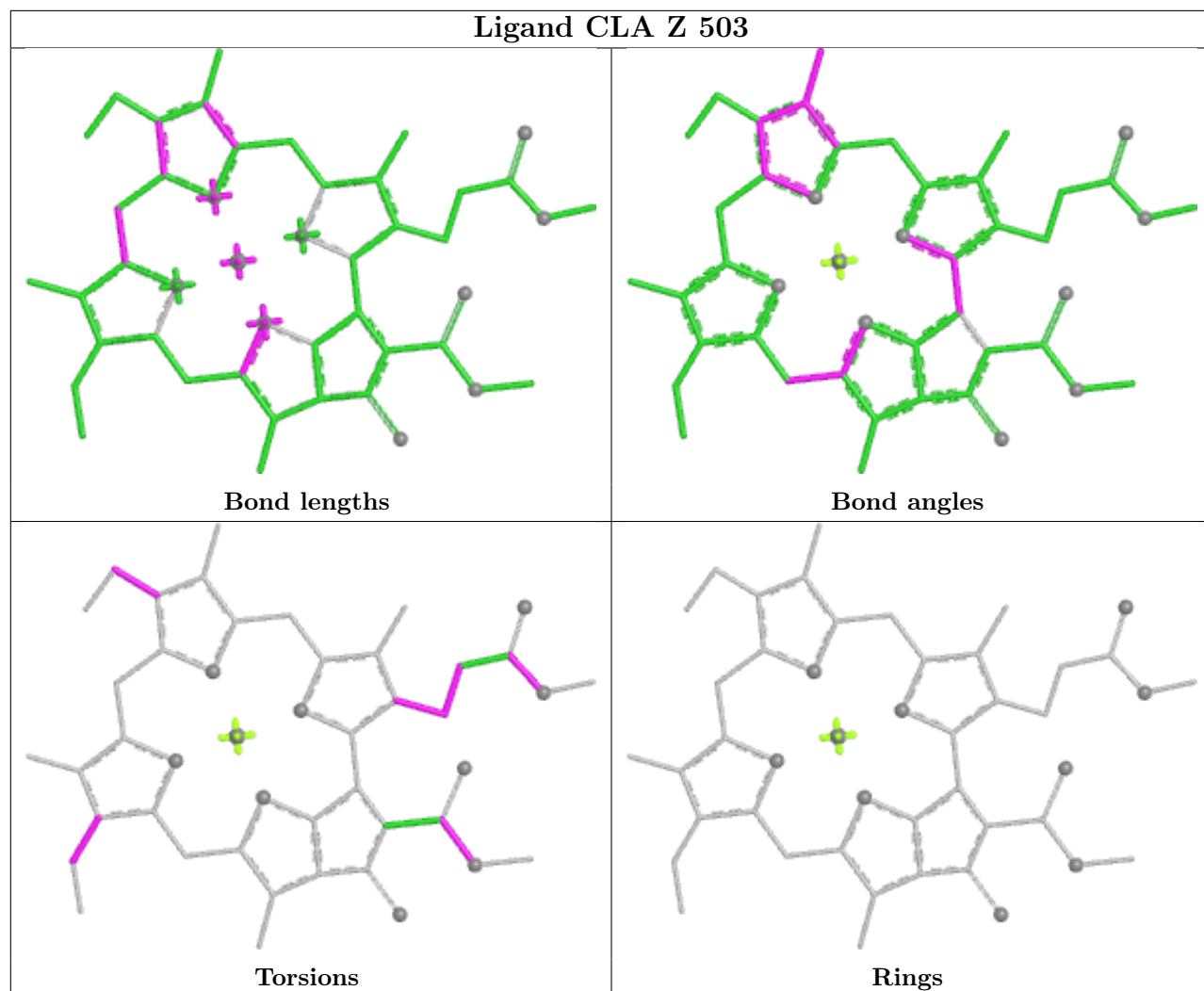


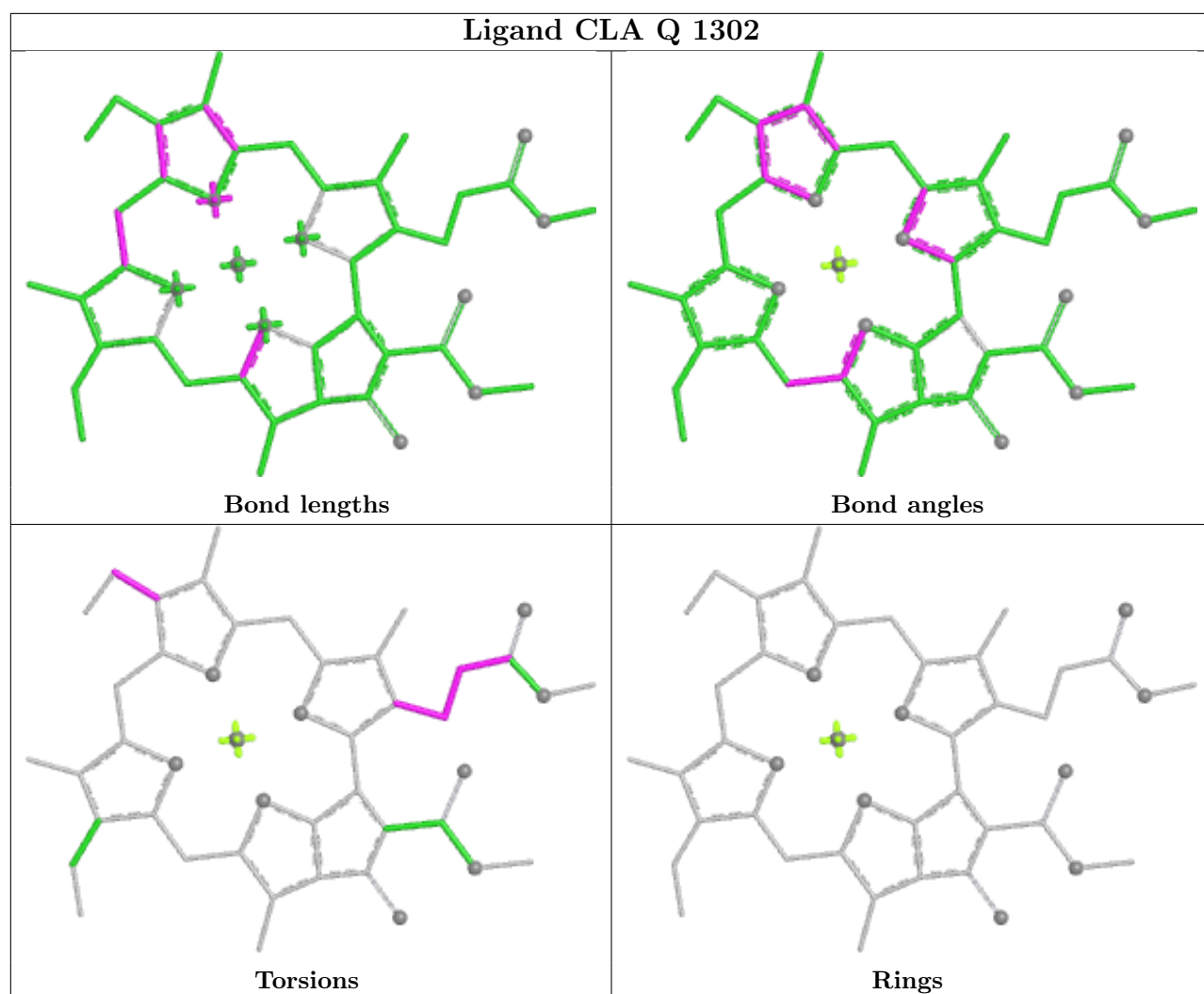




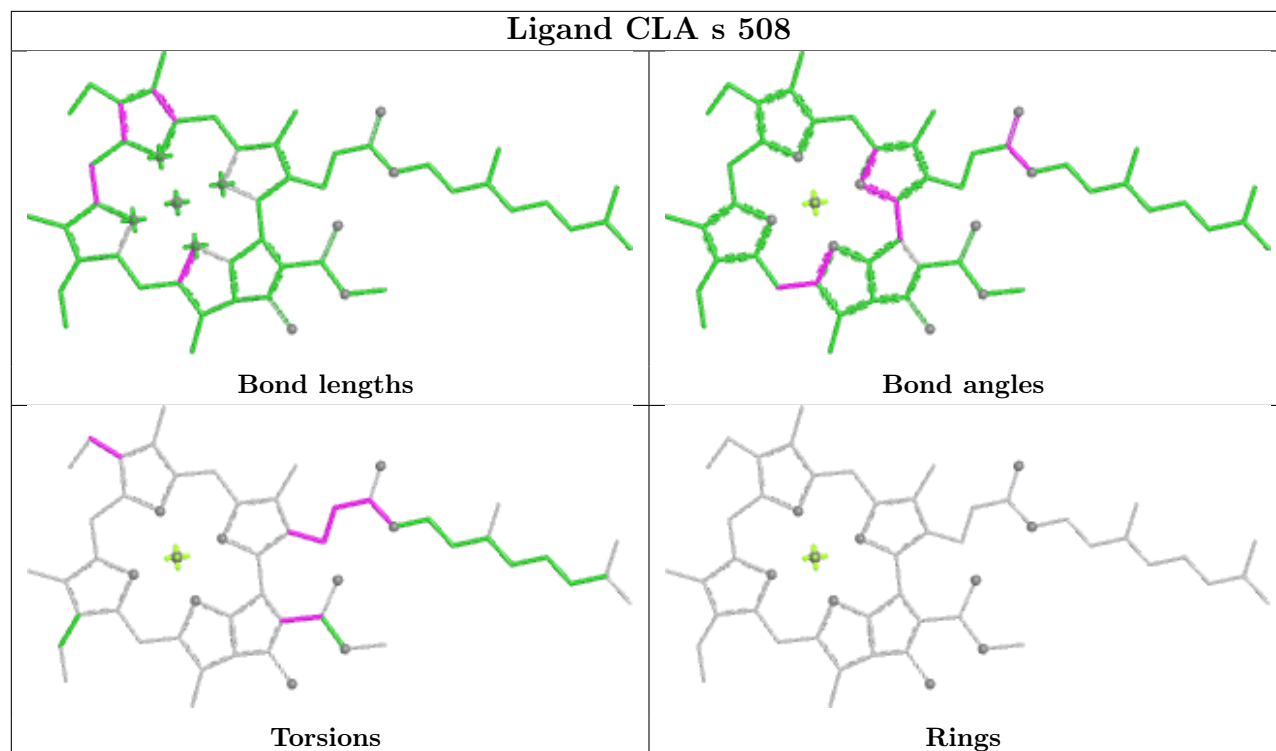


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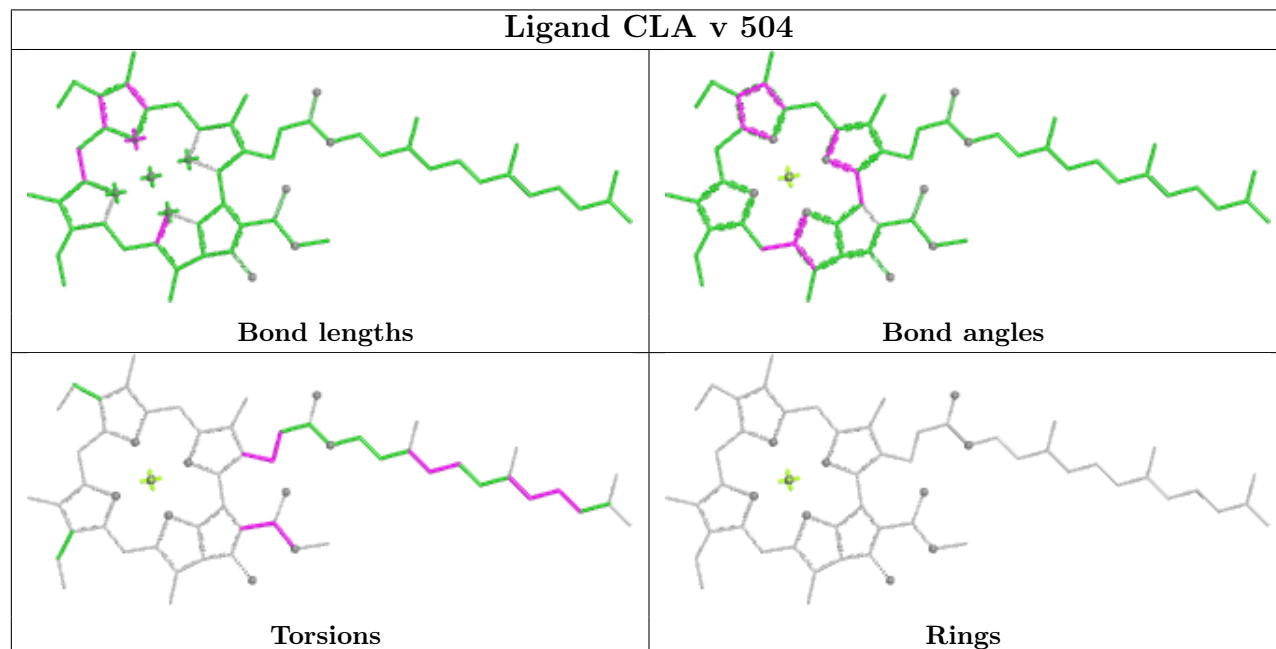


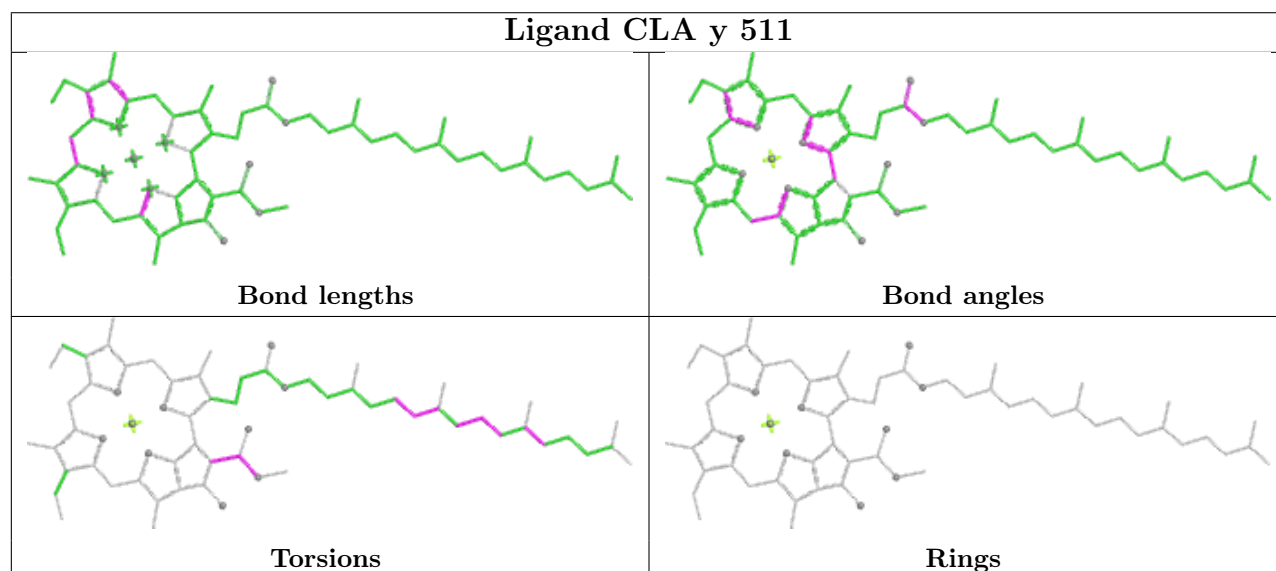
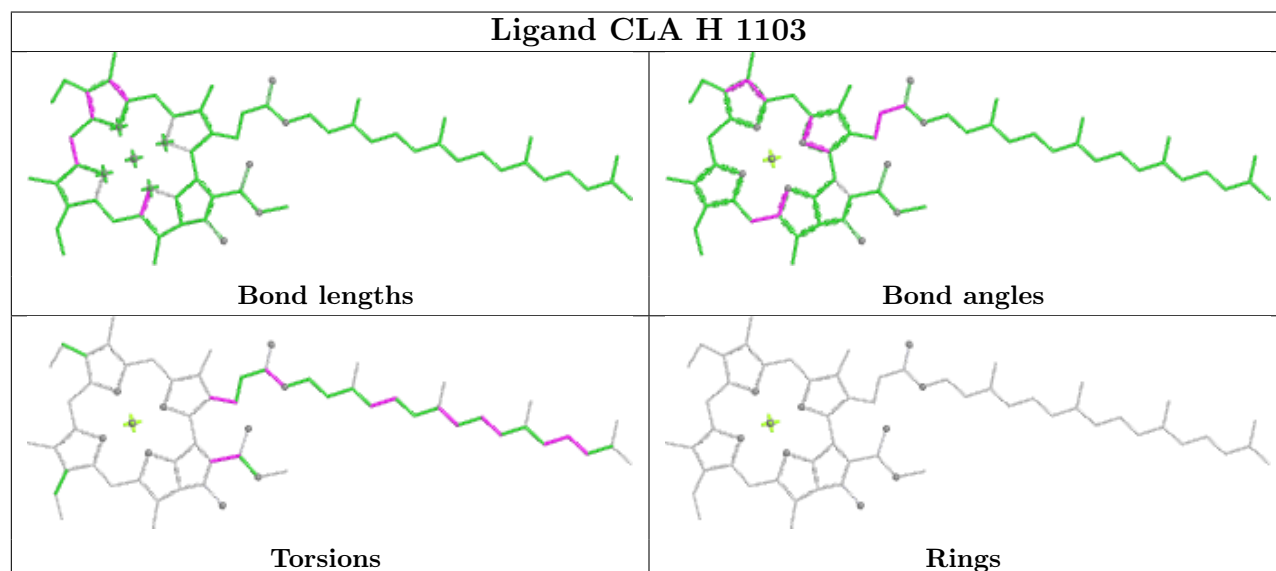
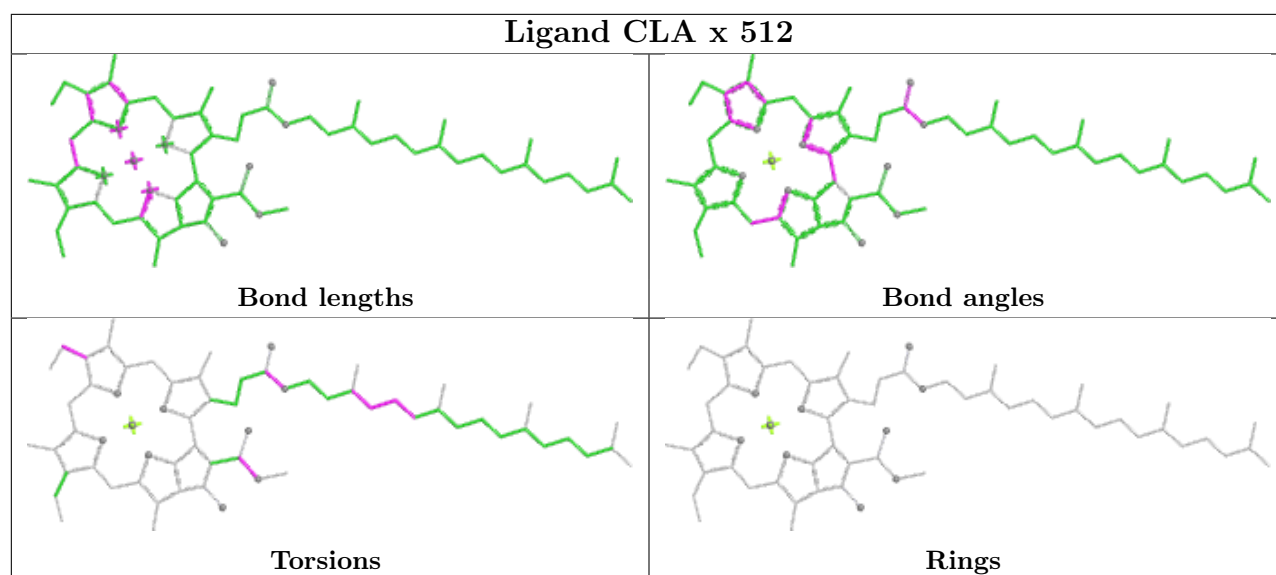


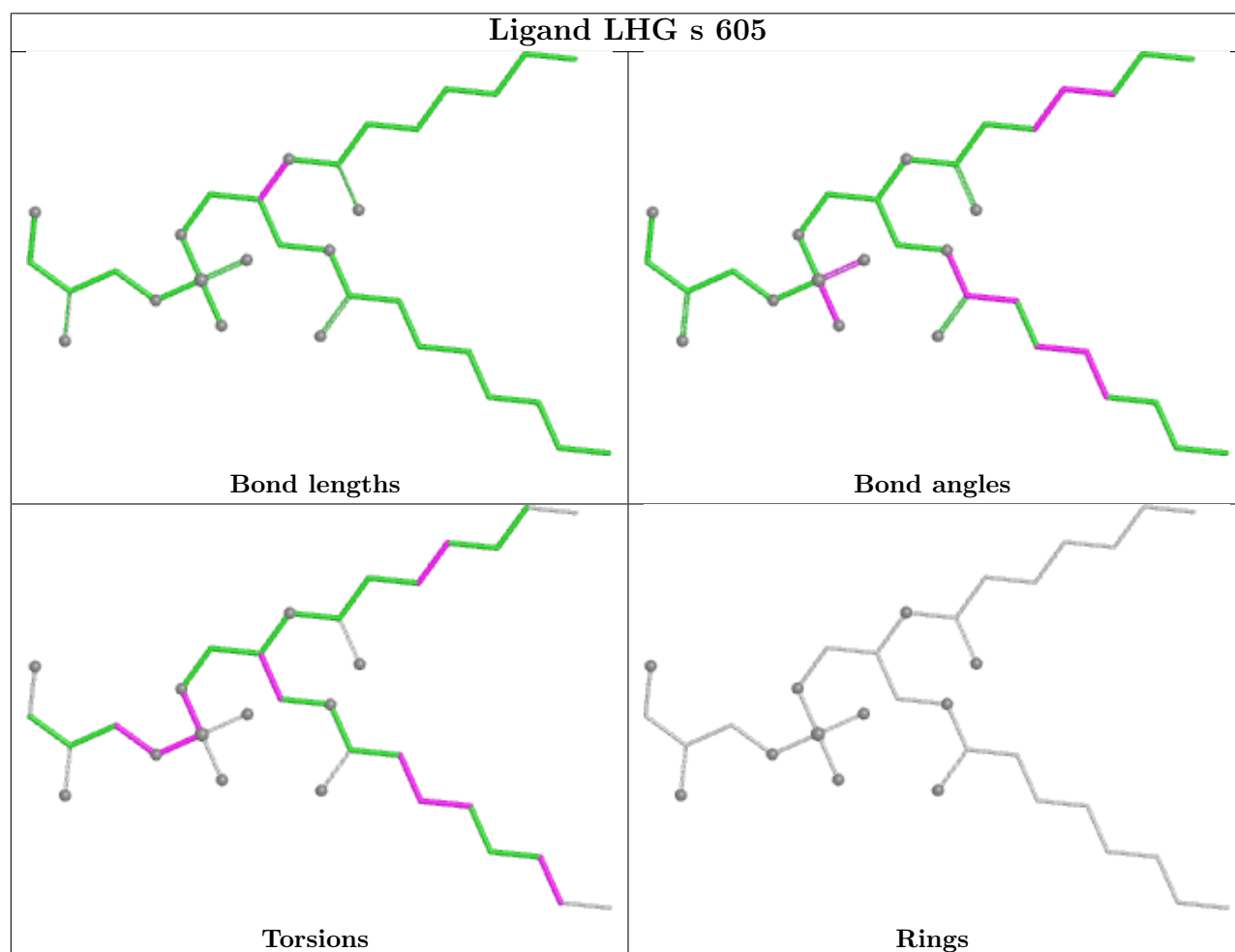
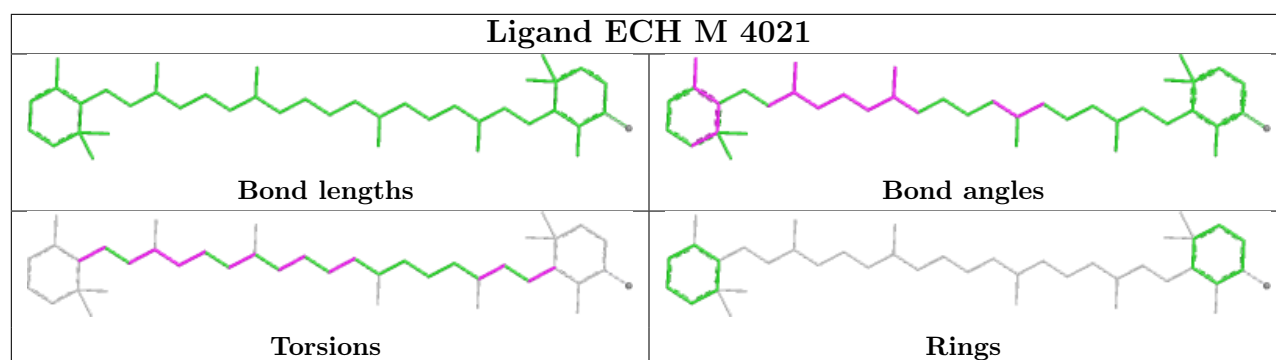
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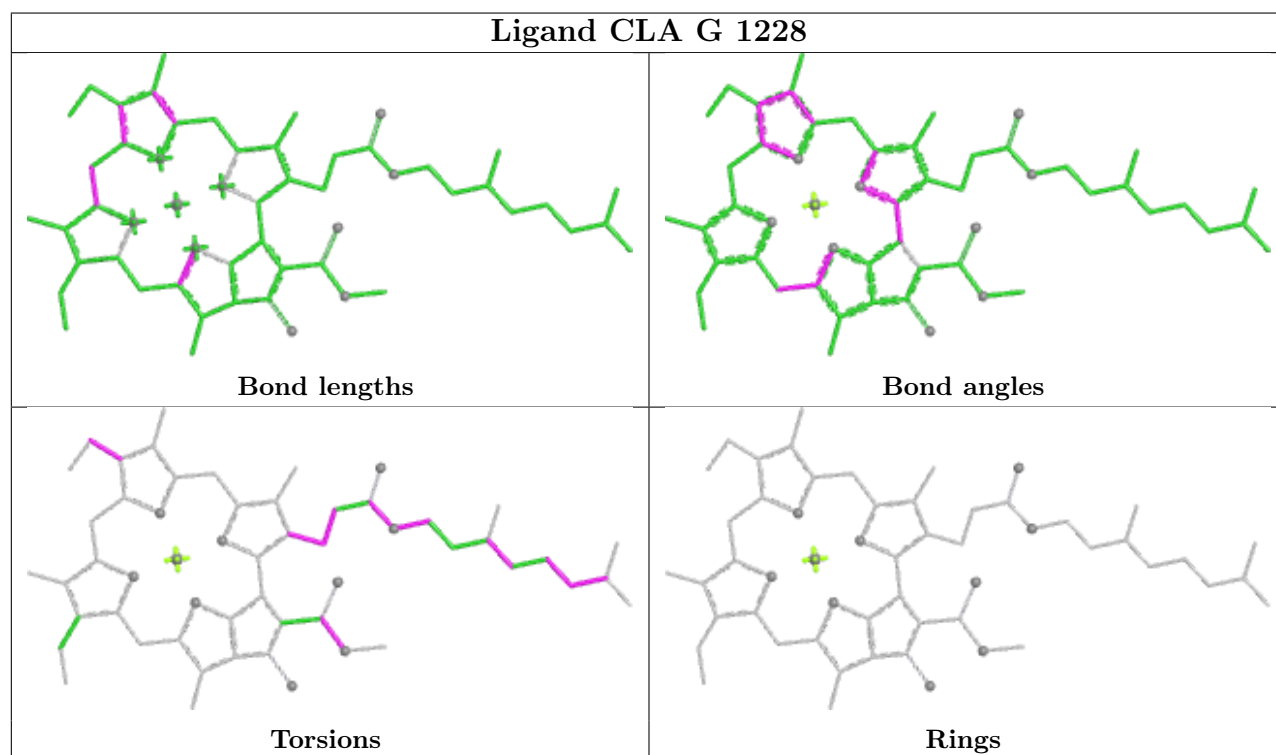
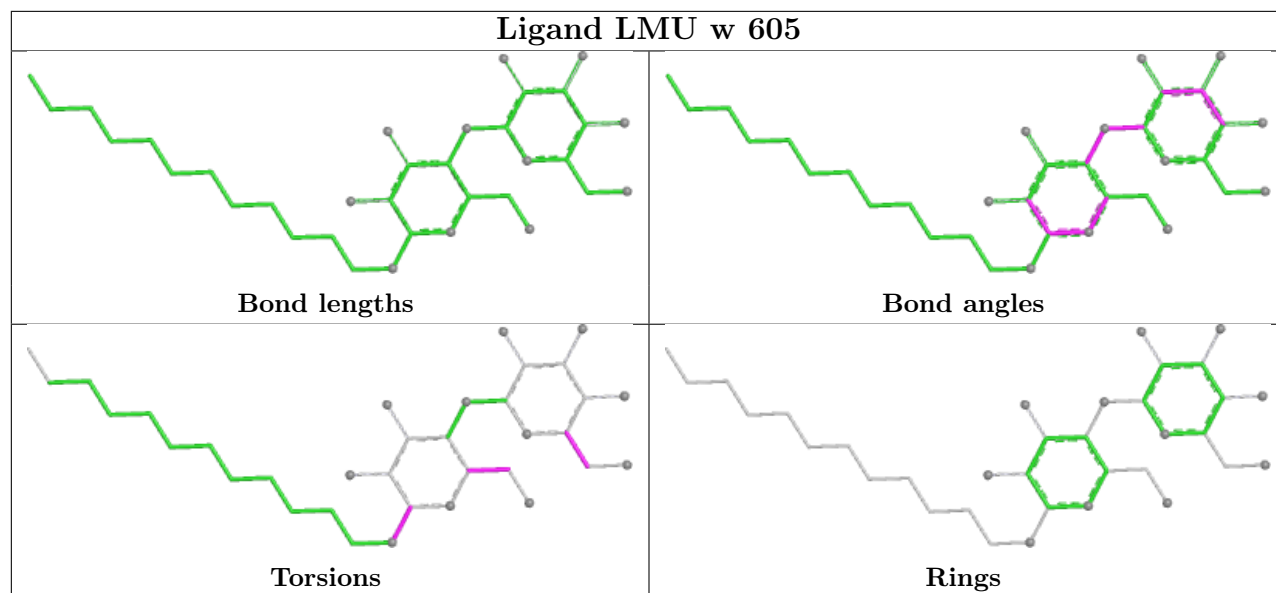


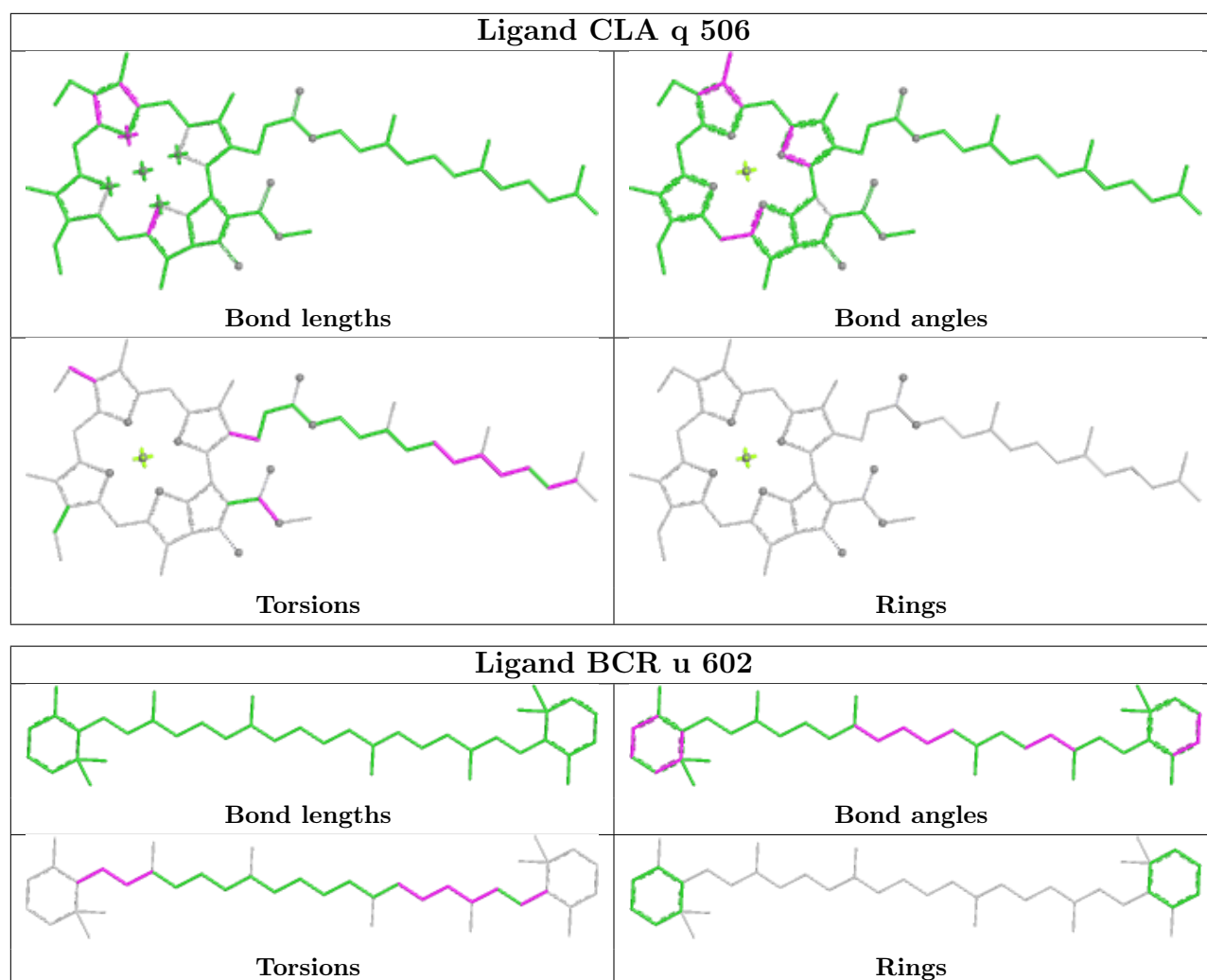
Ligand CLA v 504



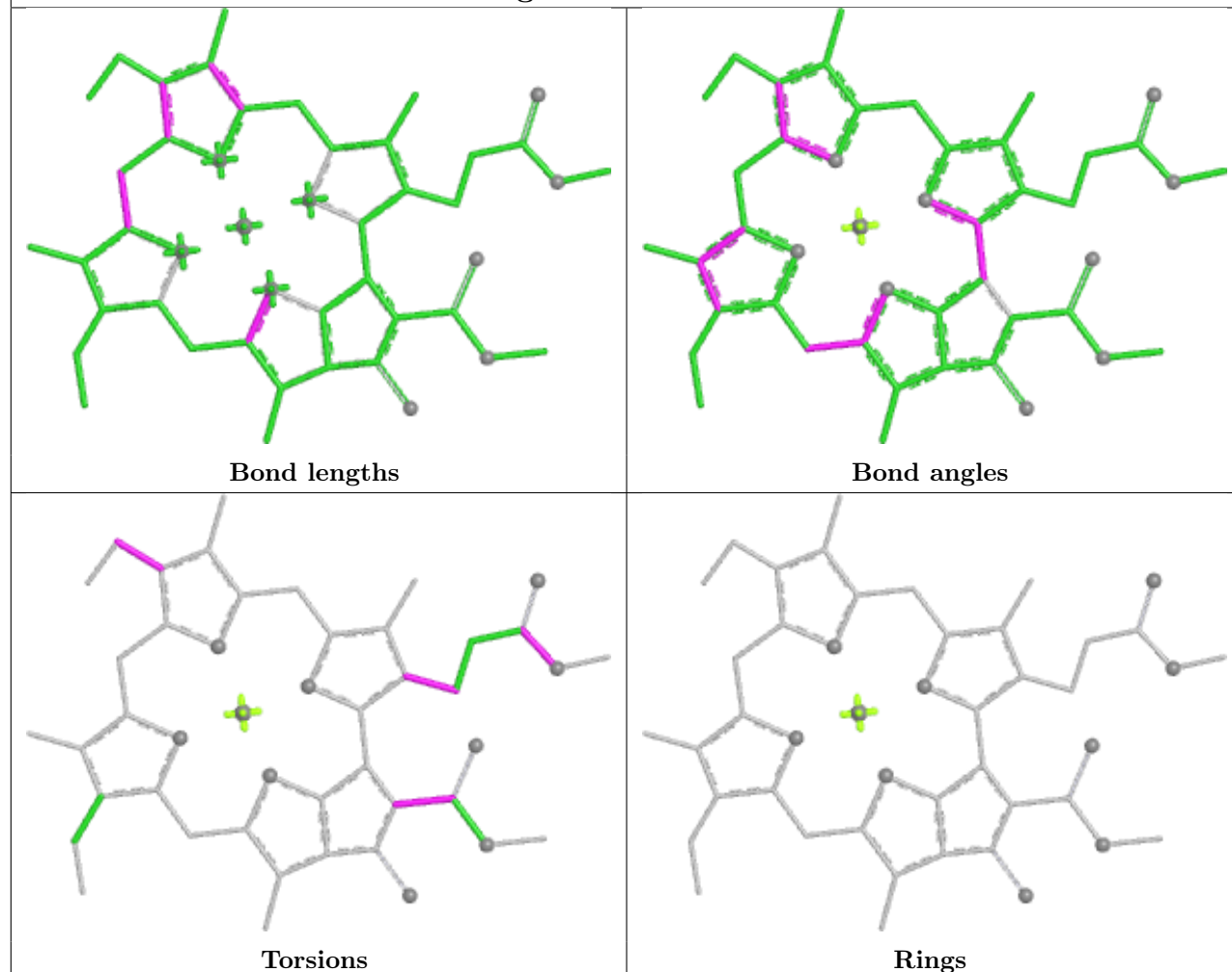




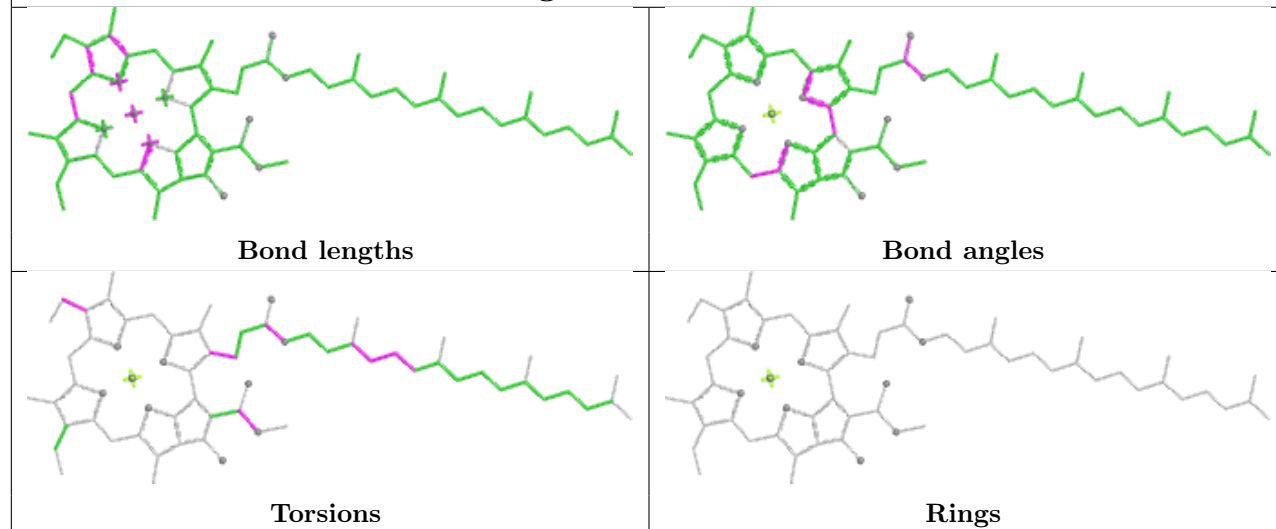


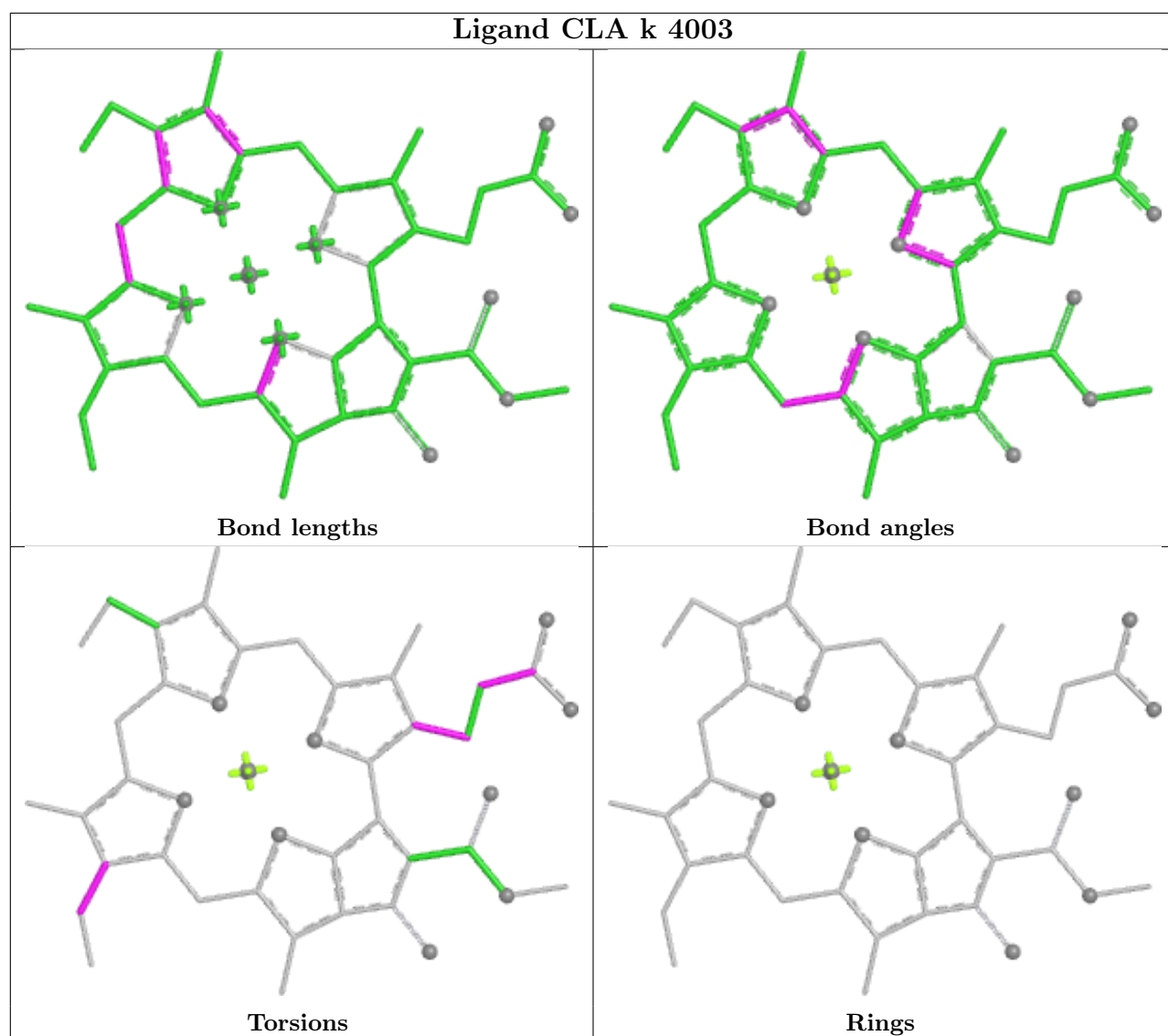


Ligand CLA h 516

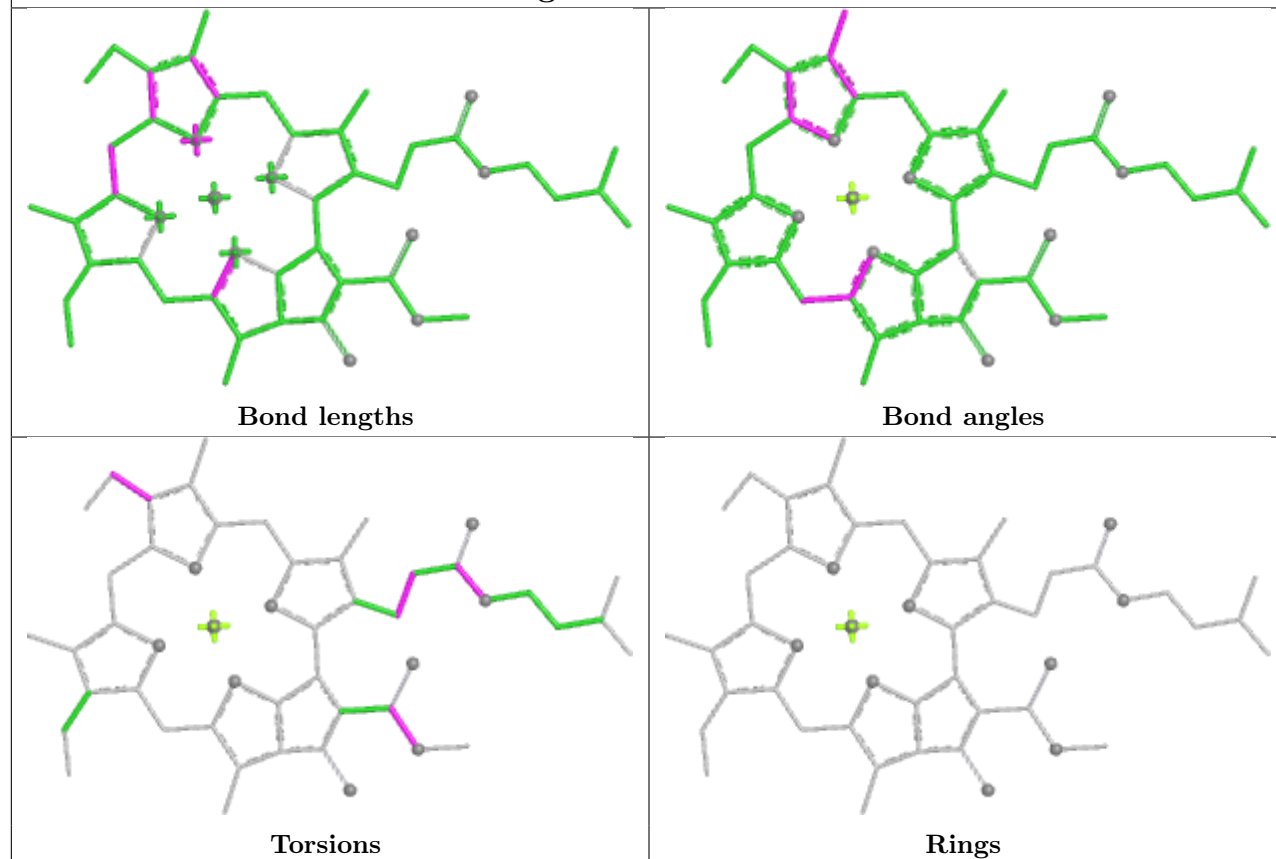


Ligand CLA r 512

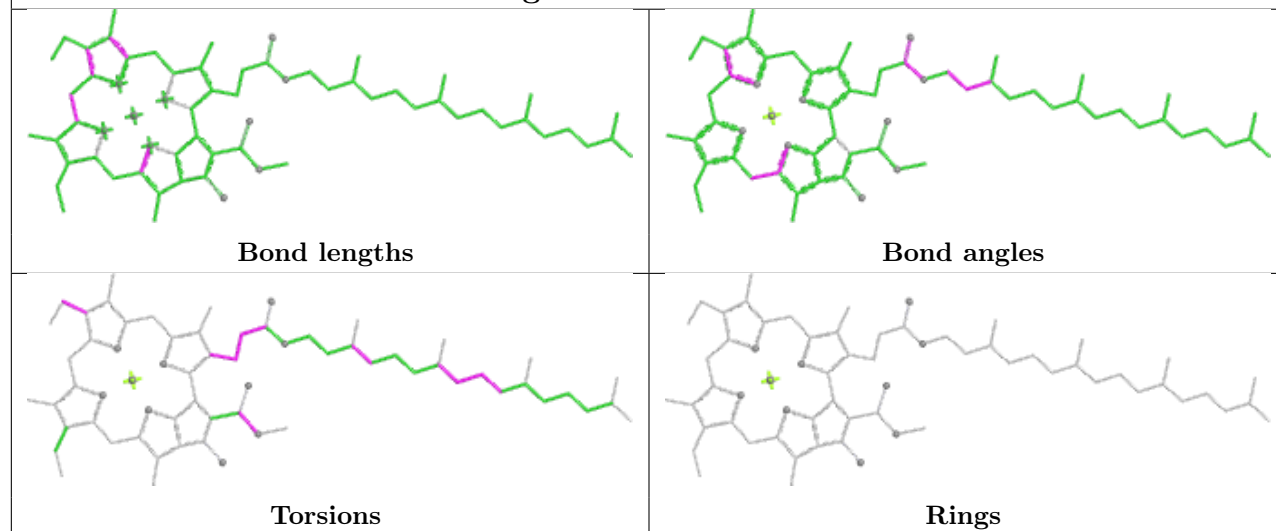




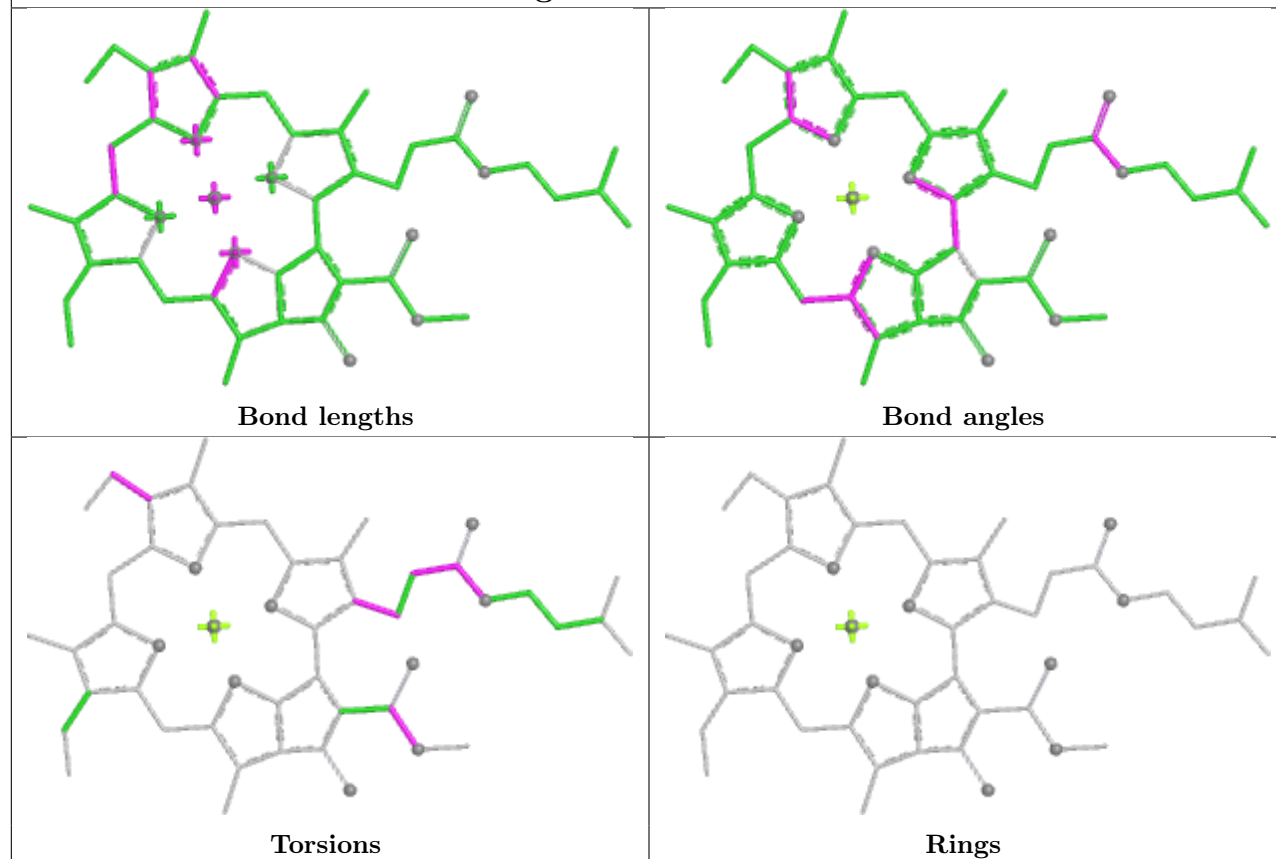
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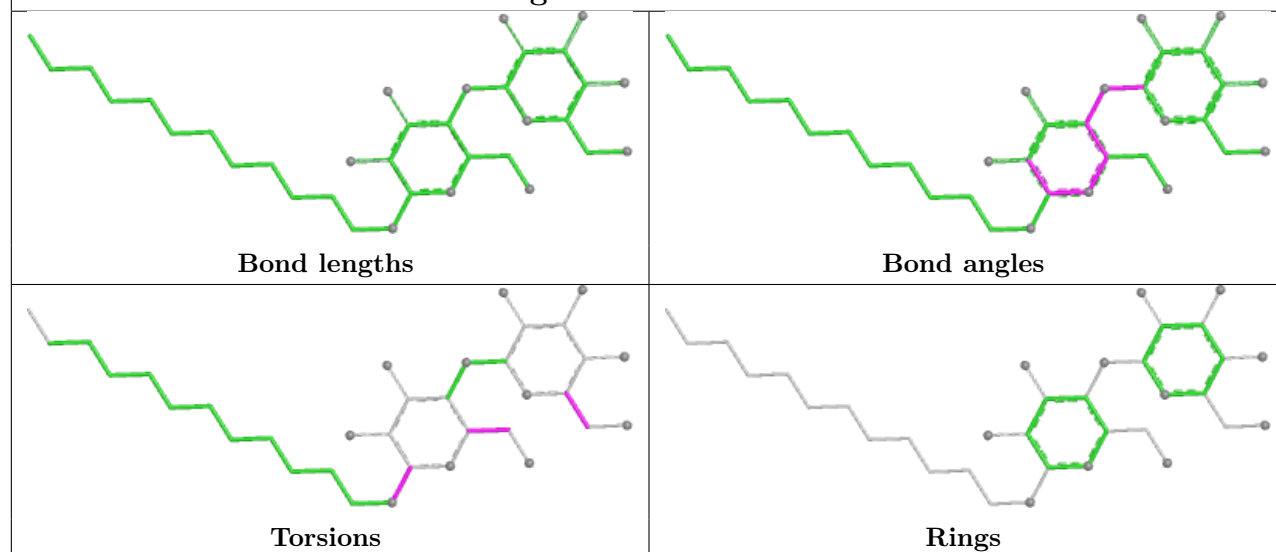
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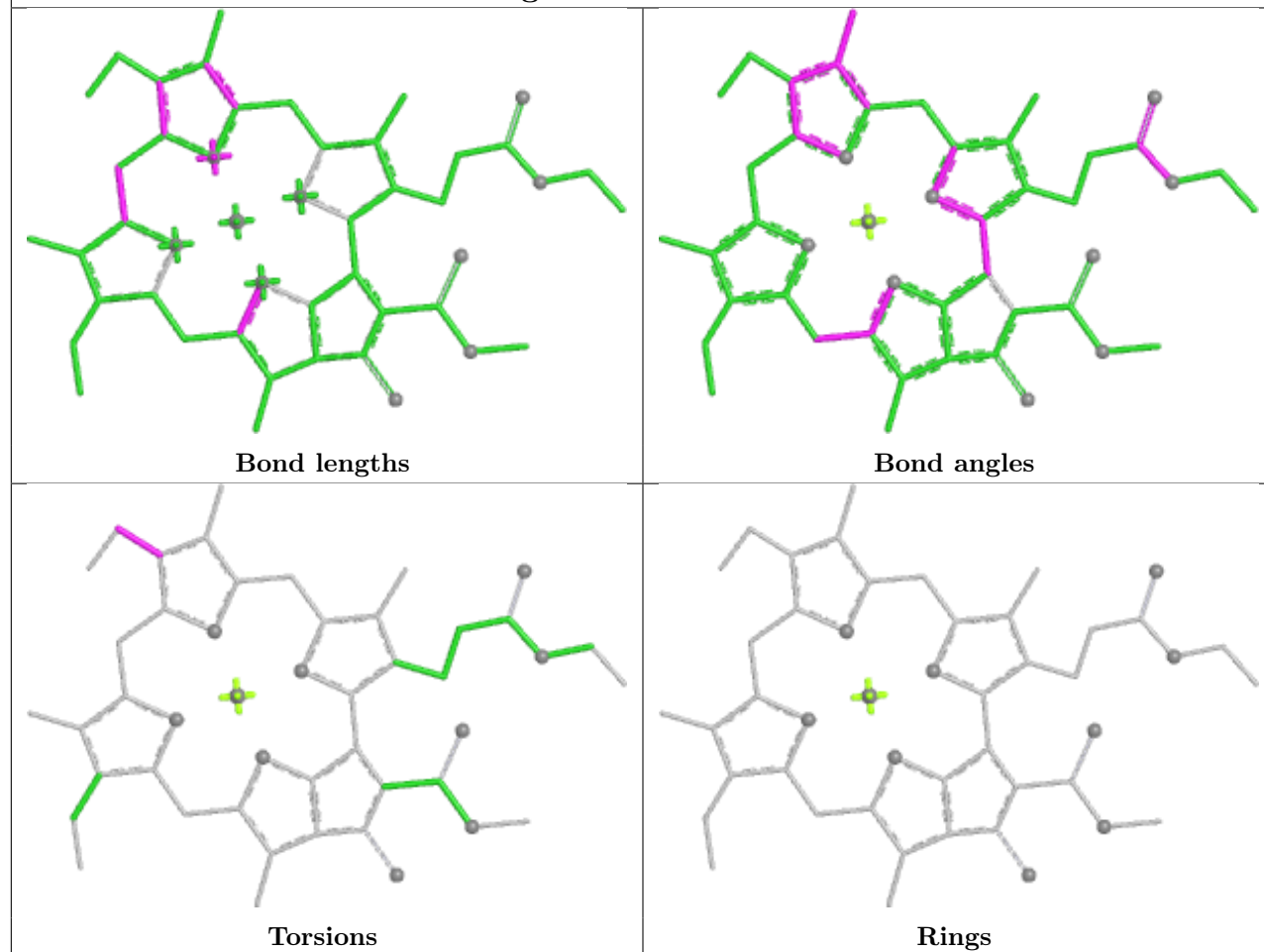
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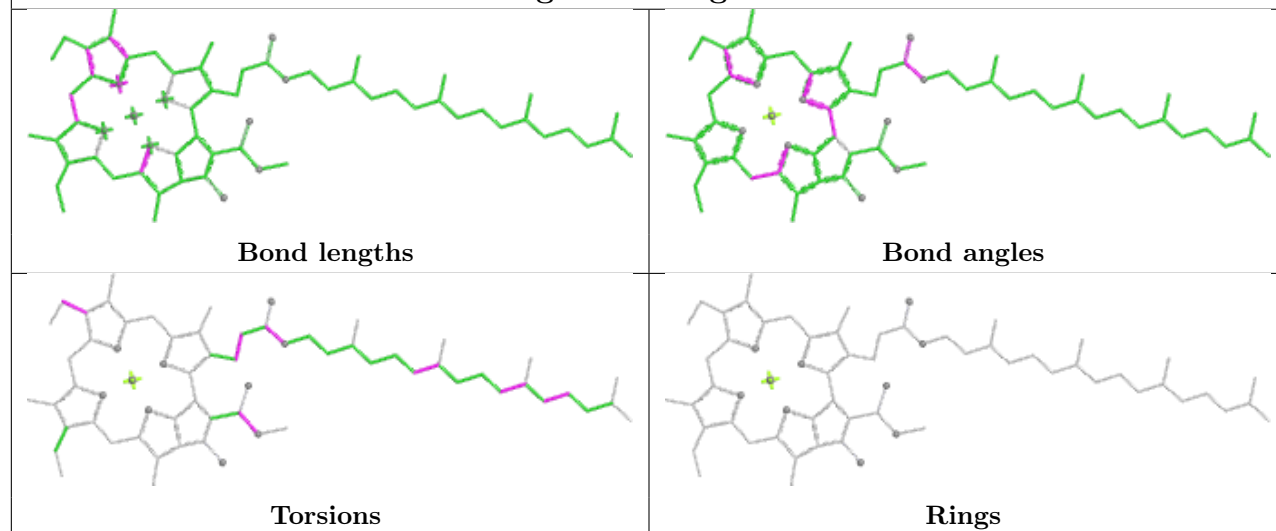
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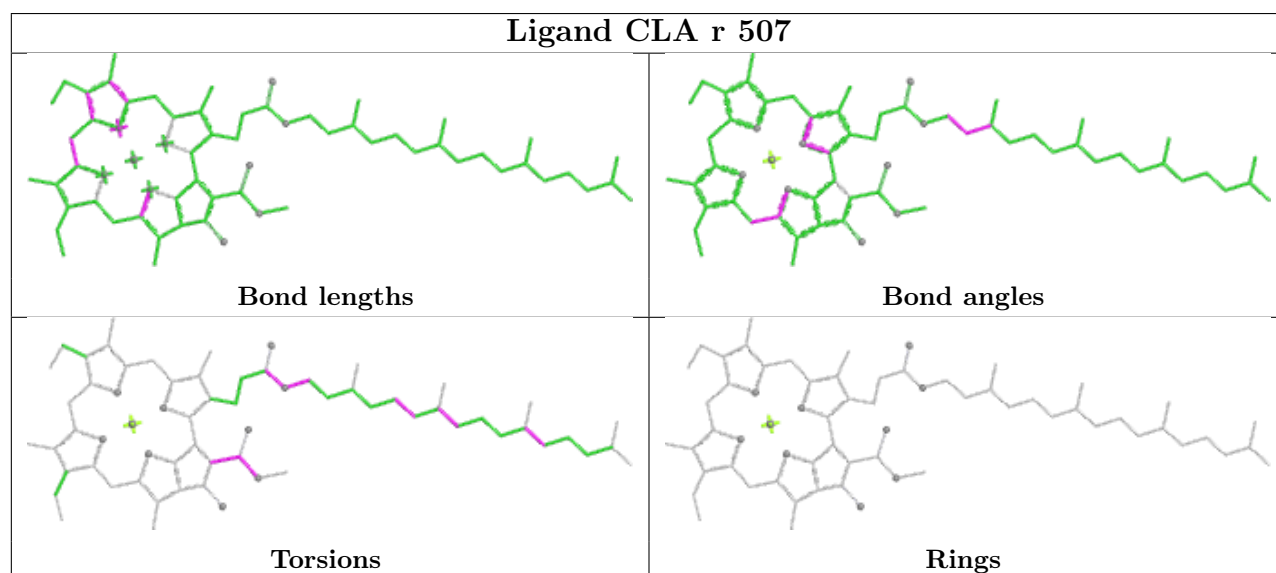
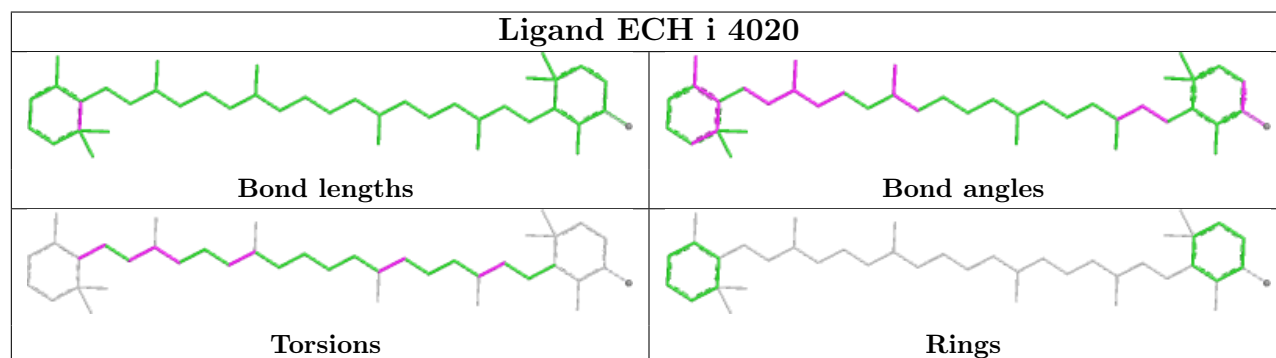
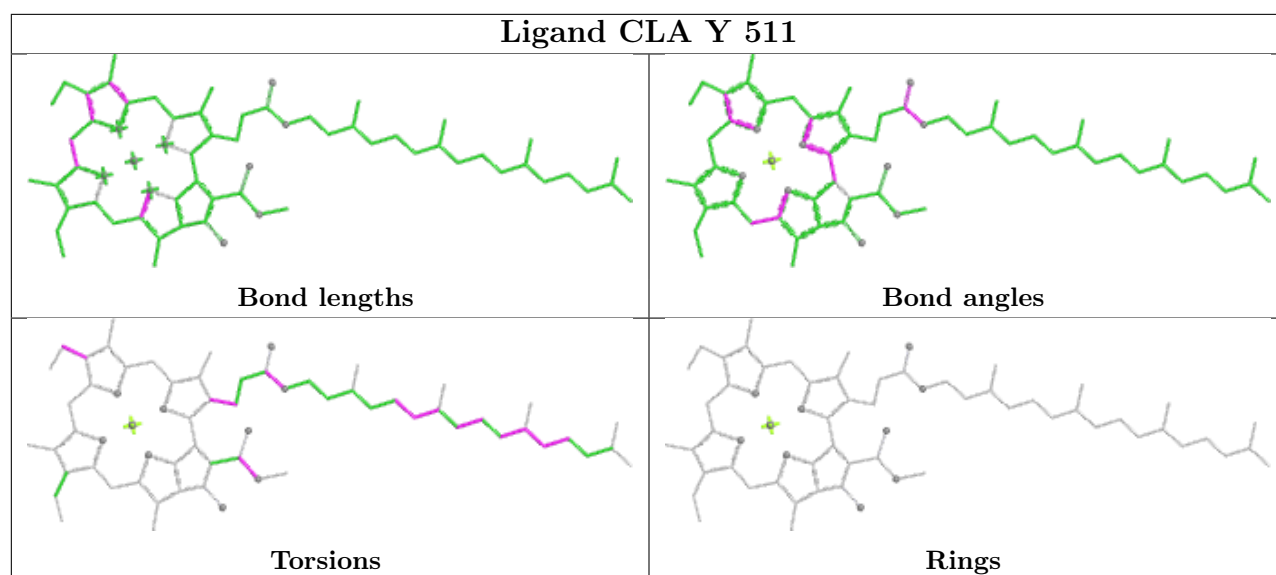


Ligand CLA b 1216

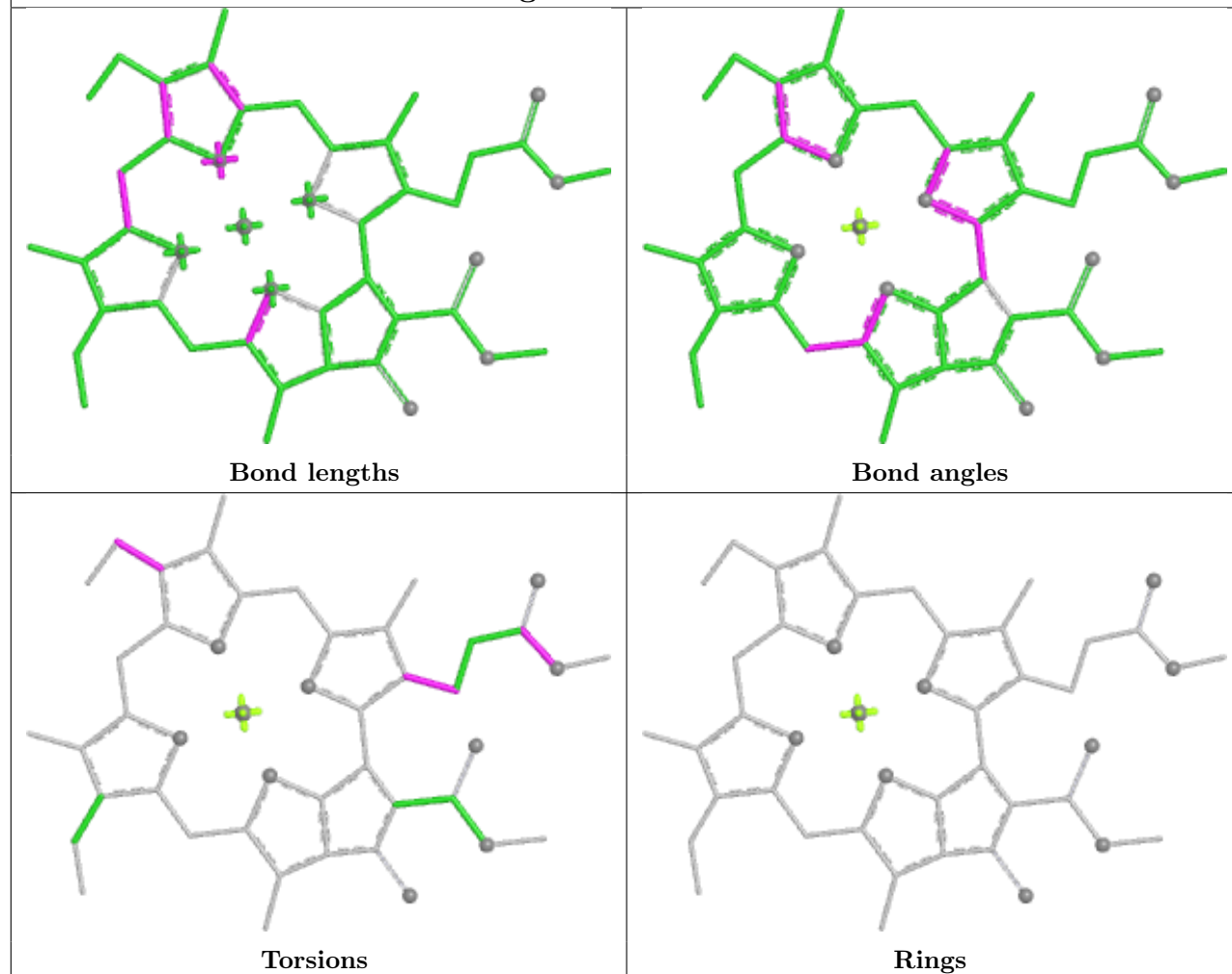


Ligand CLA g 510

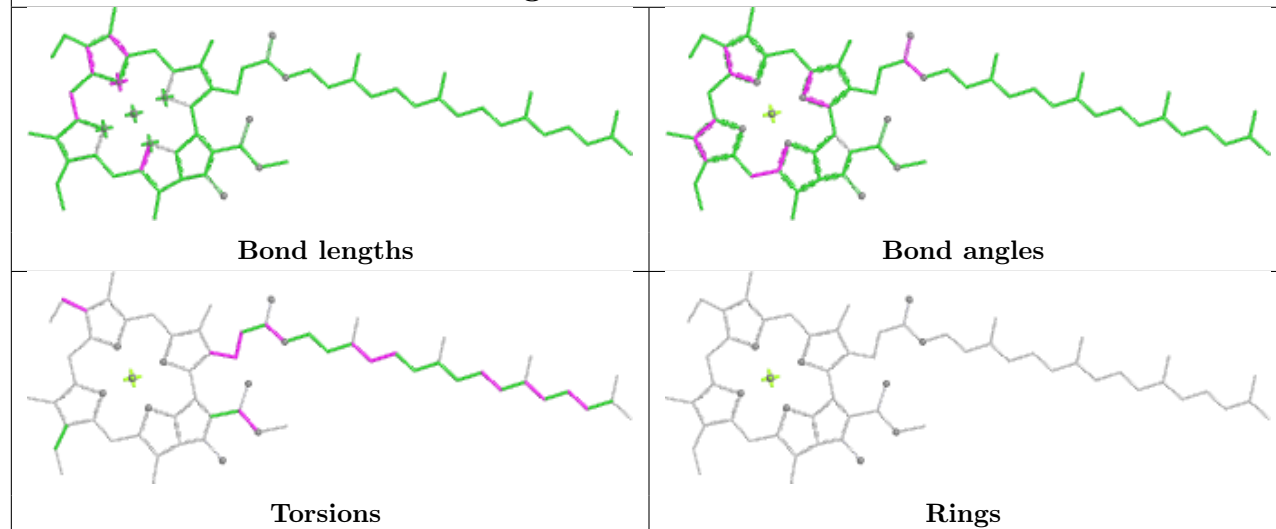


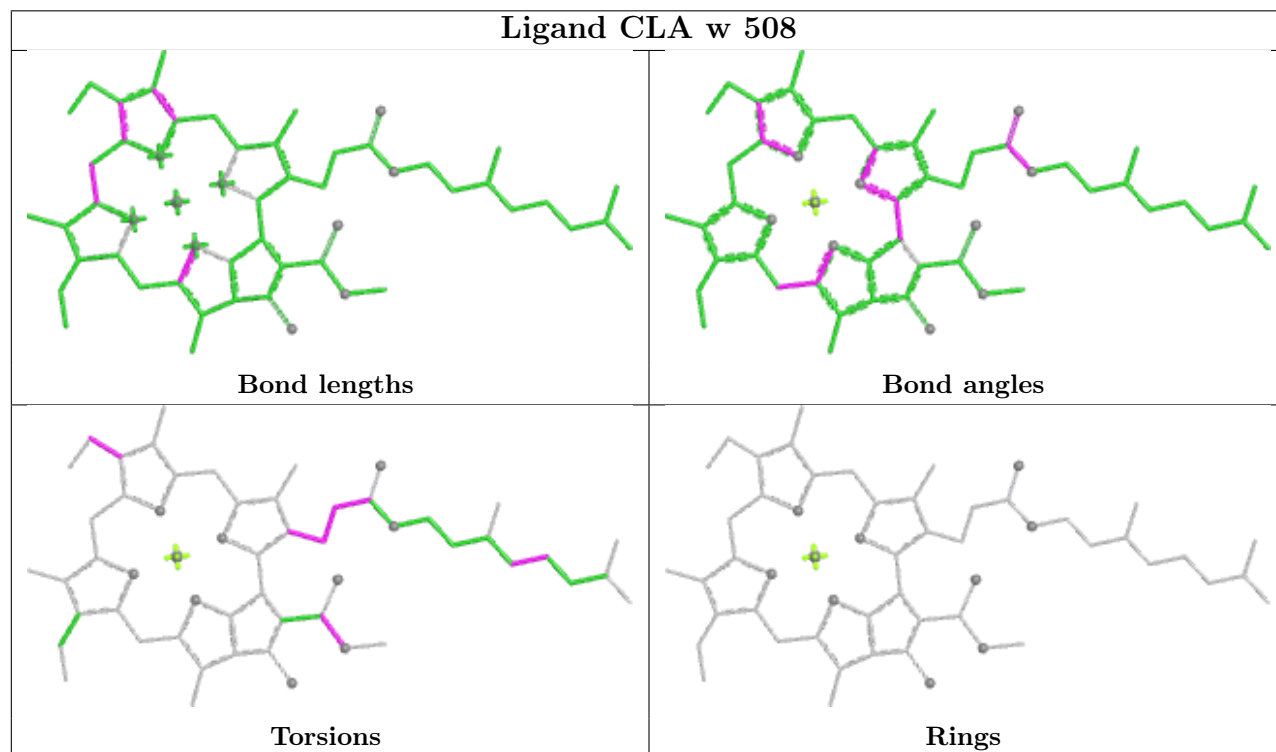
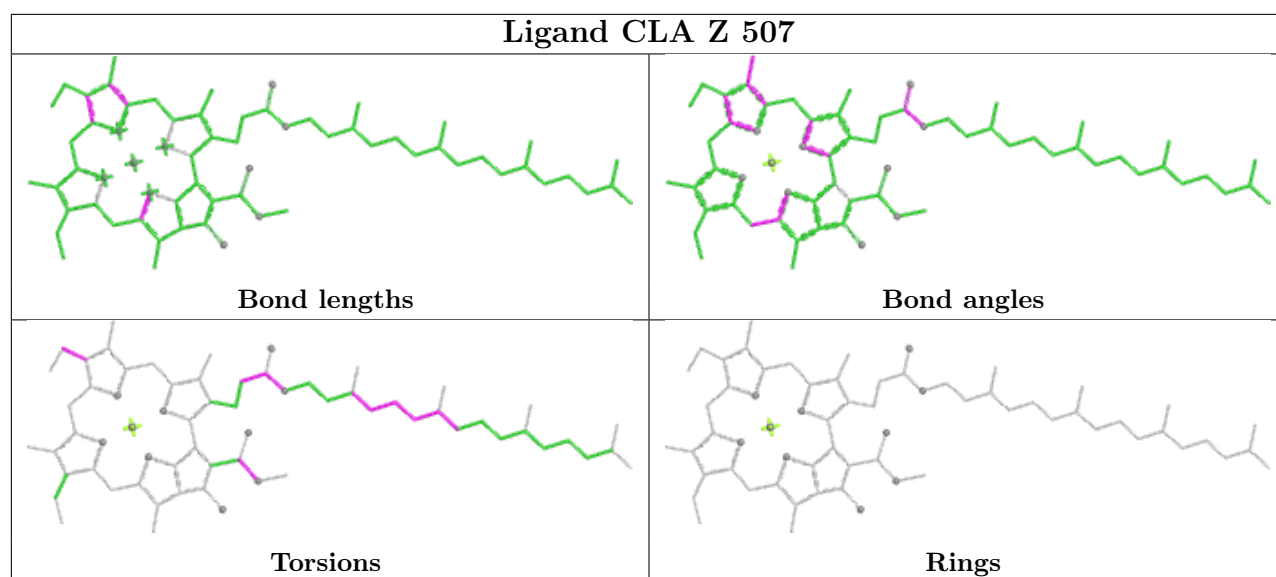


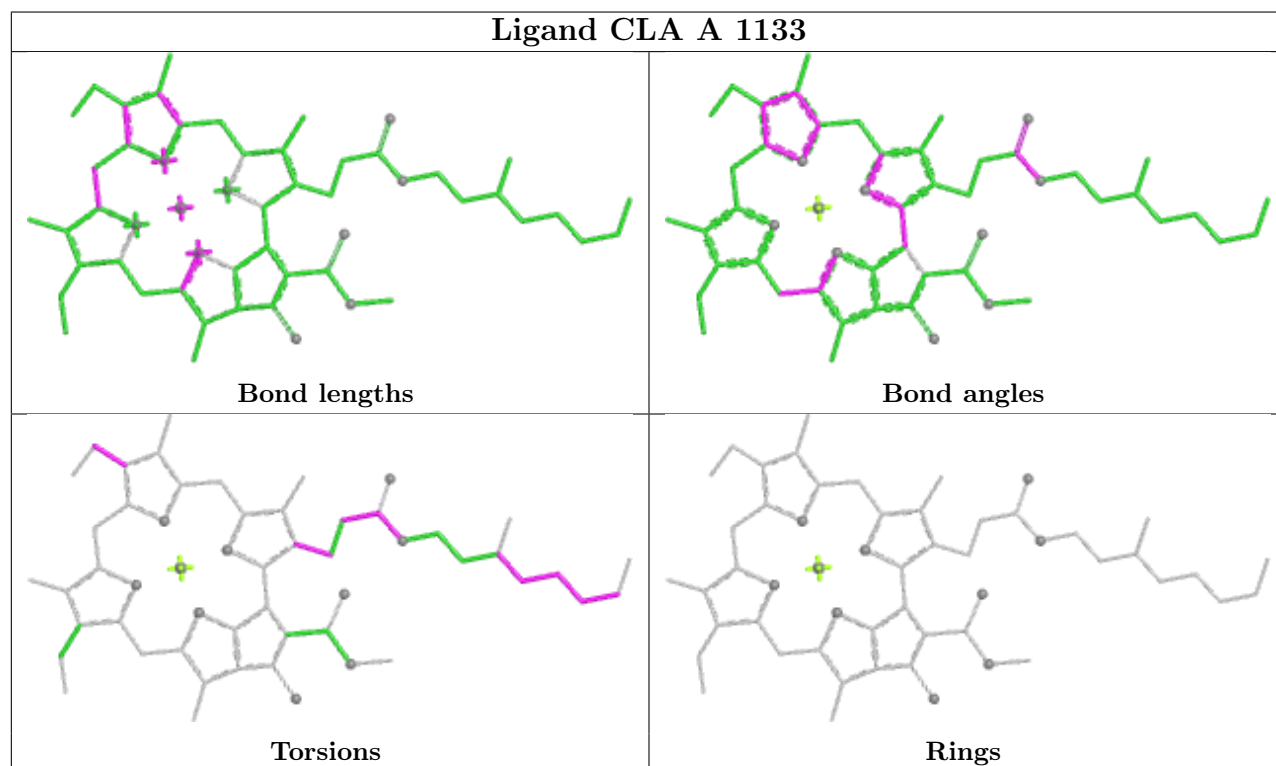
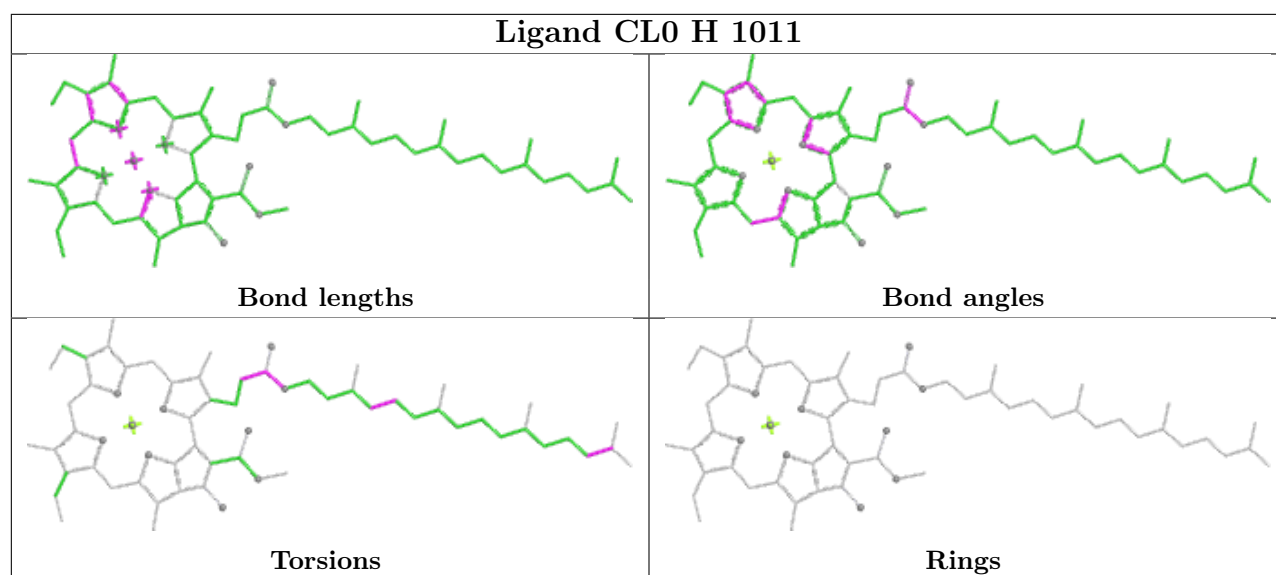
Ligand CLA r 516

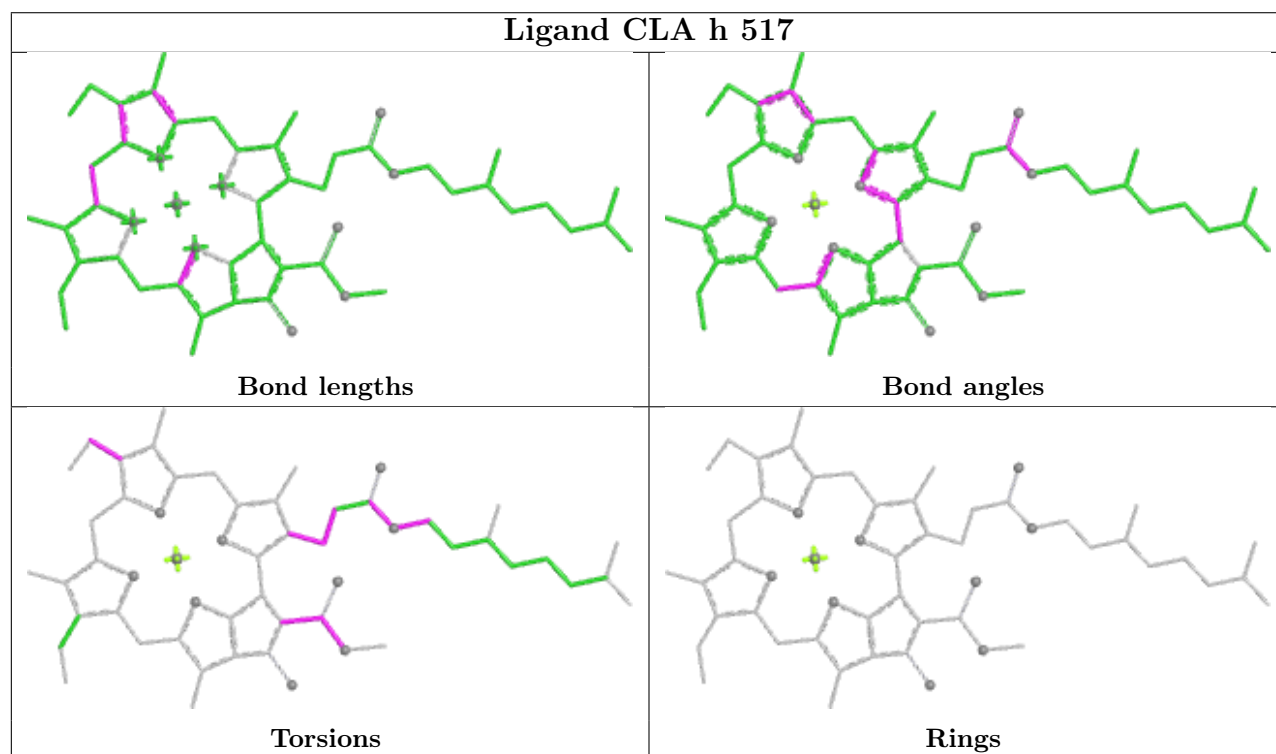
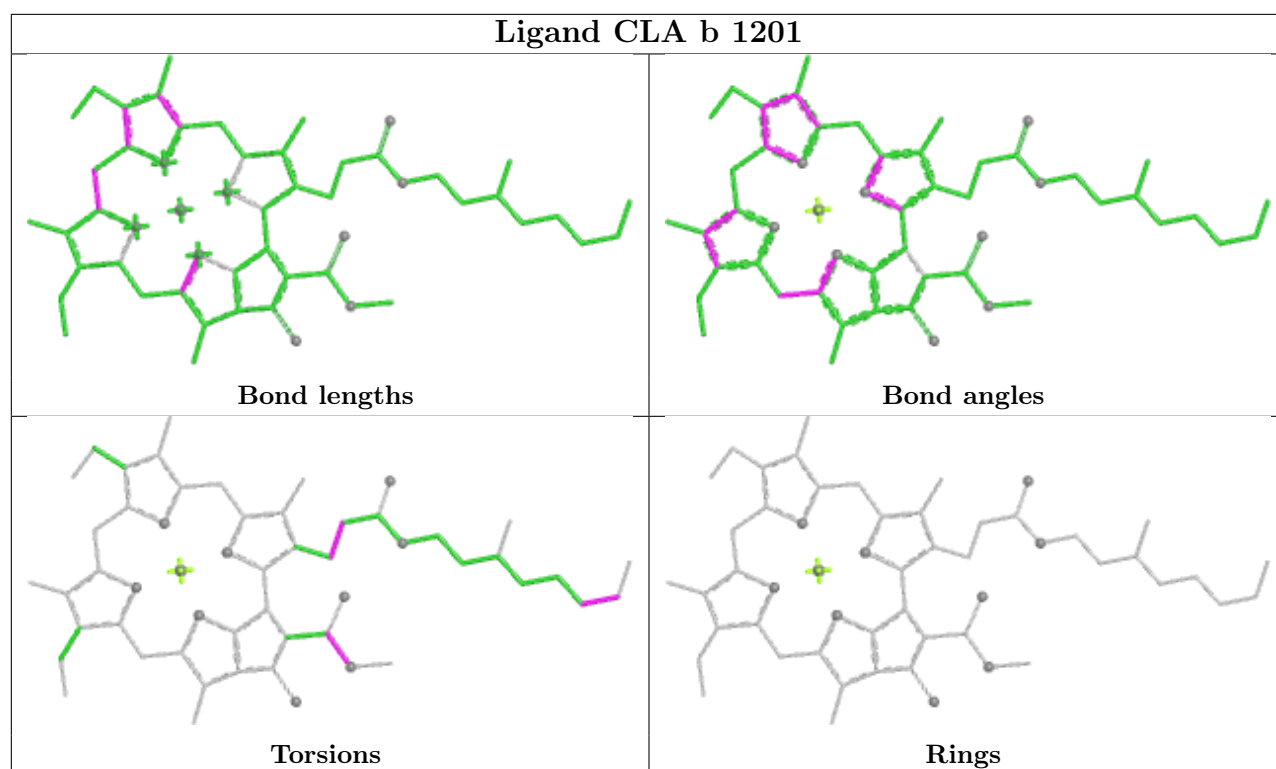


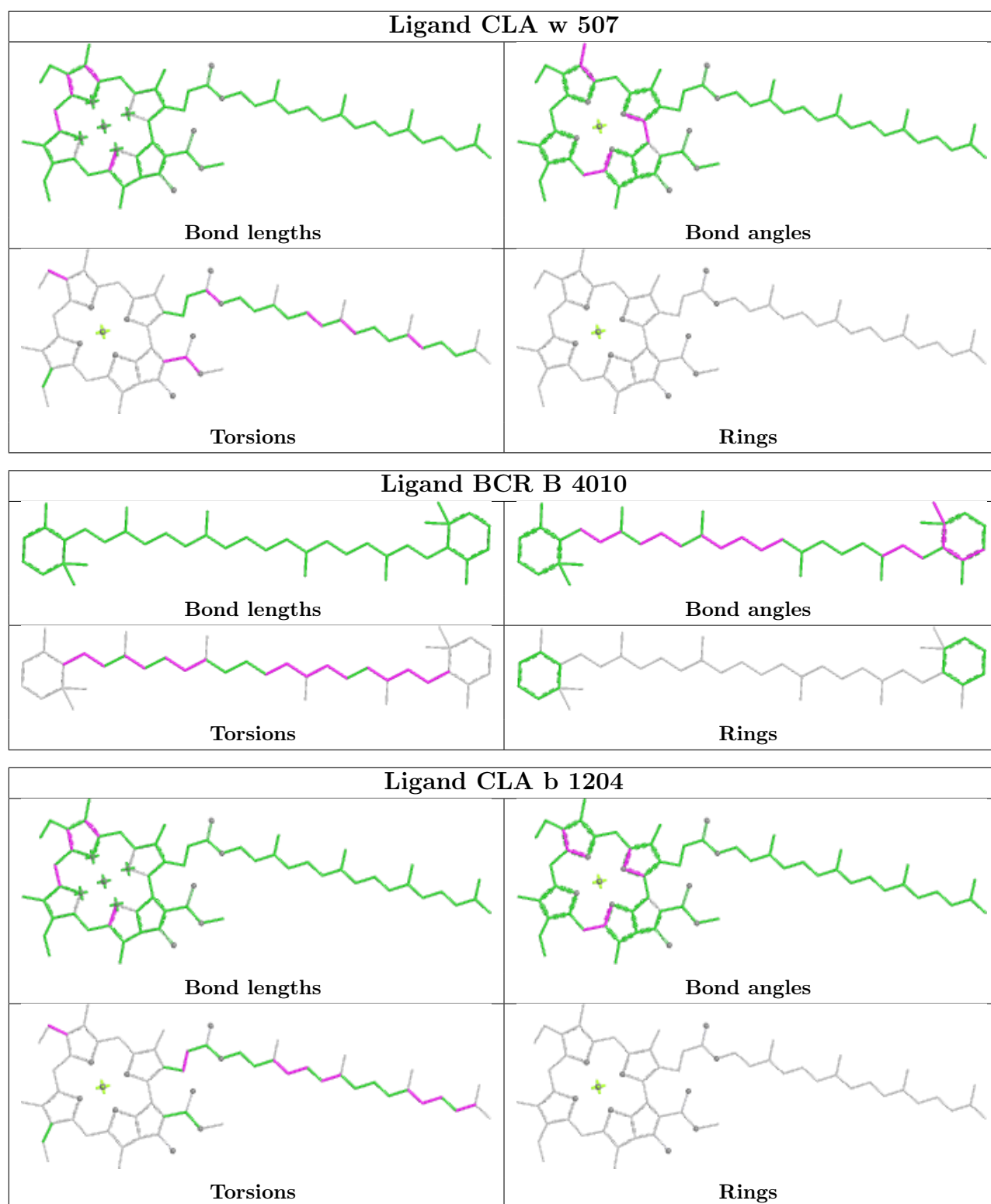
Ligand CLA B 1203

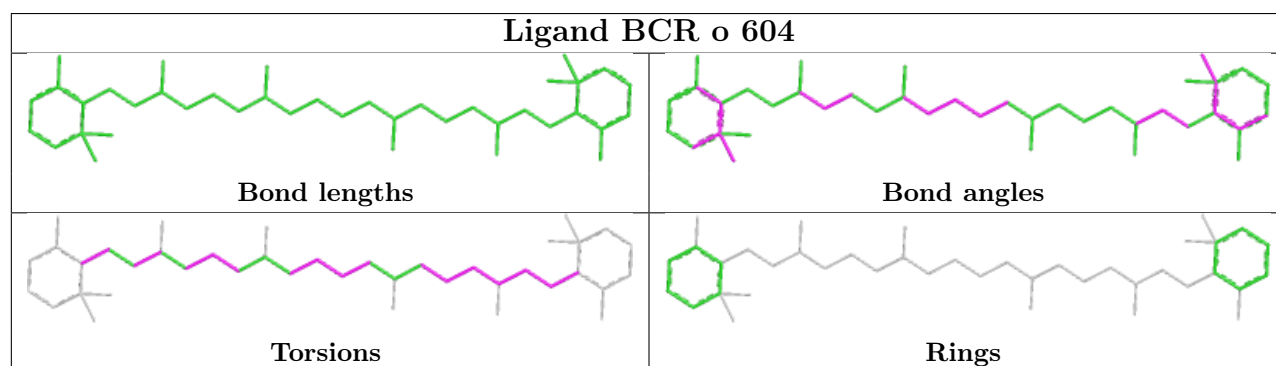
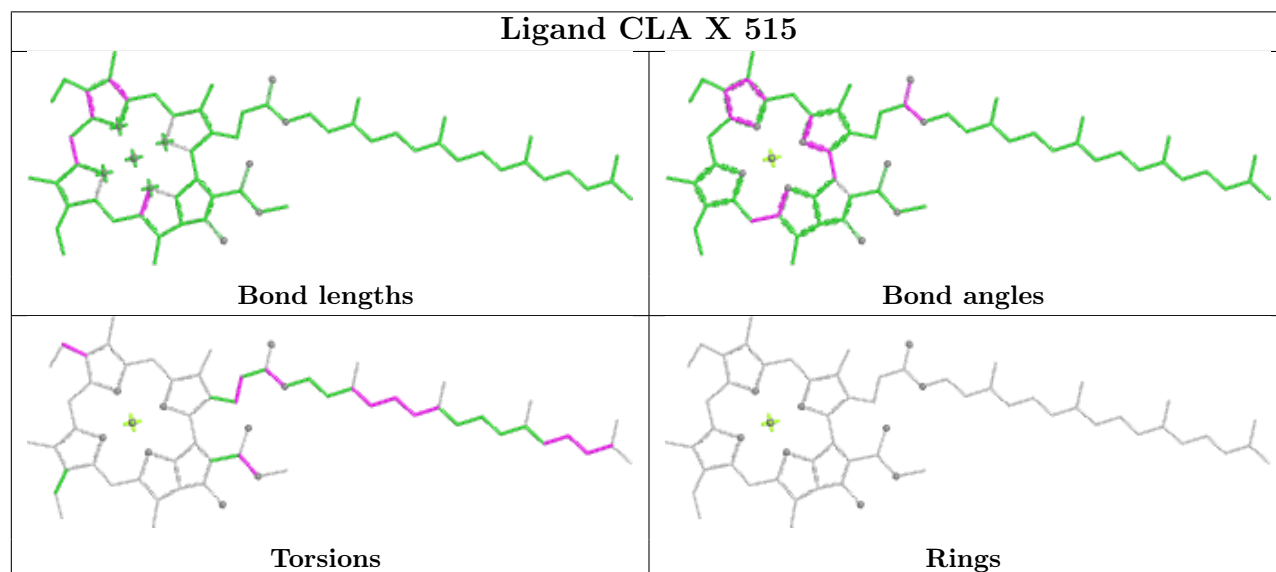
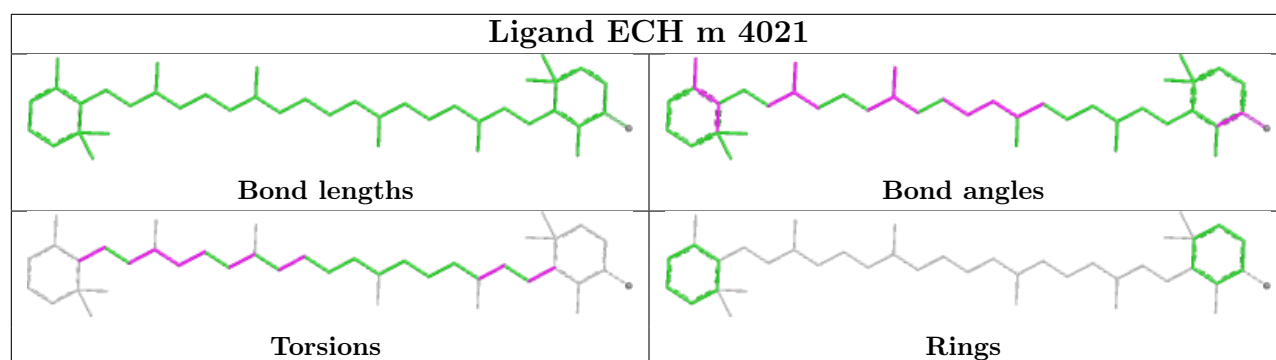


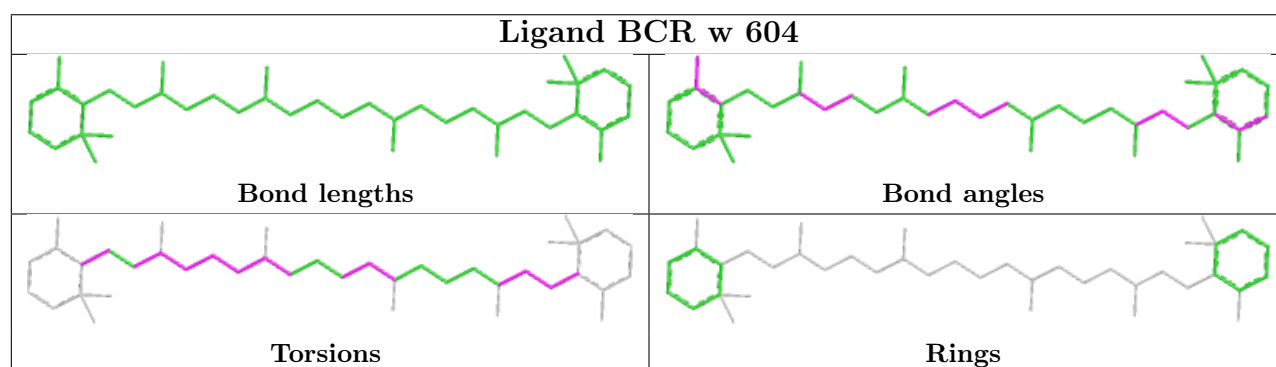
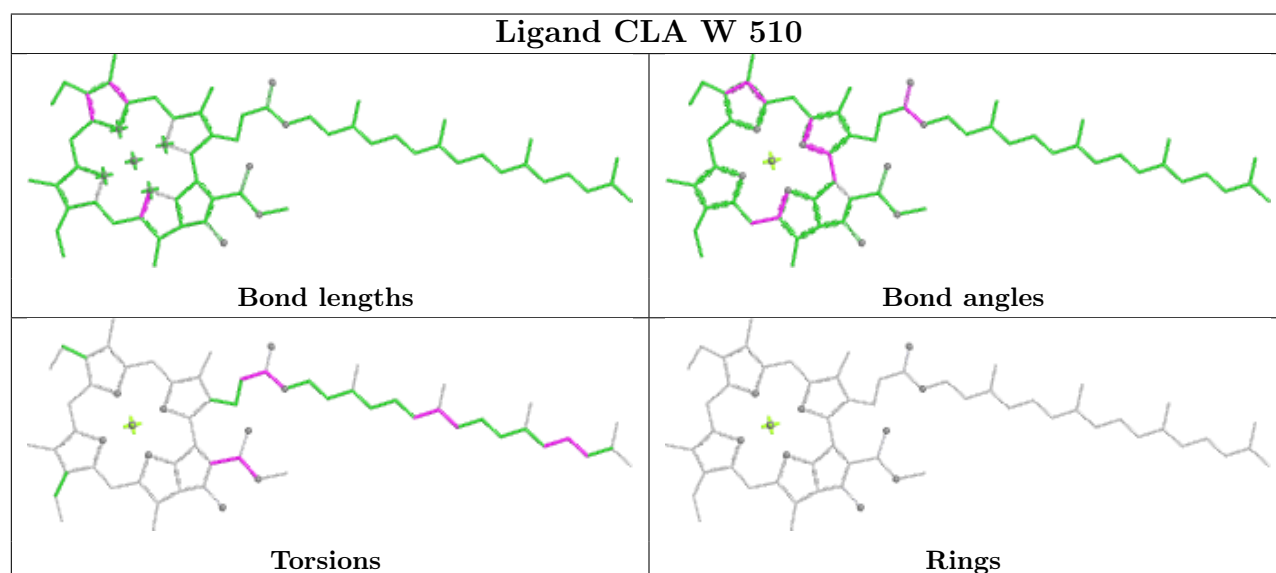
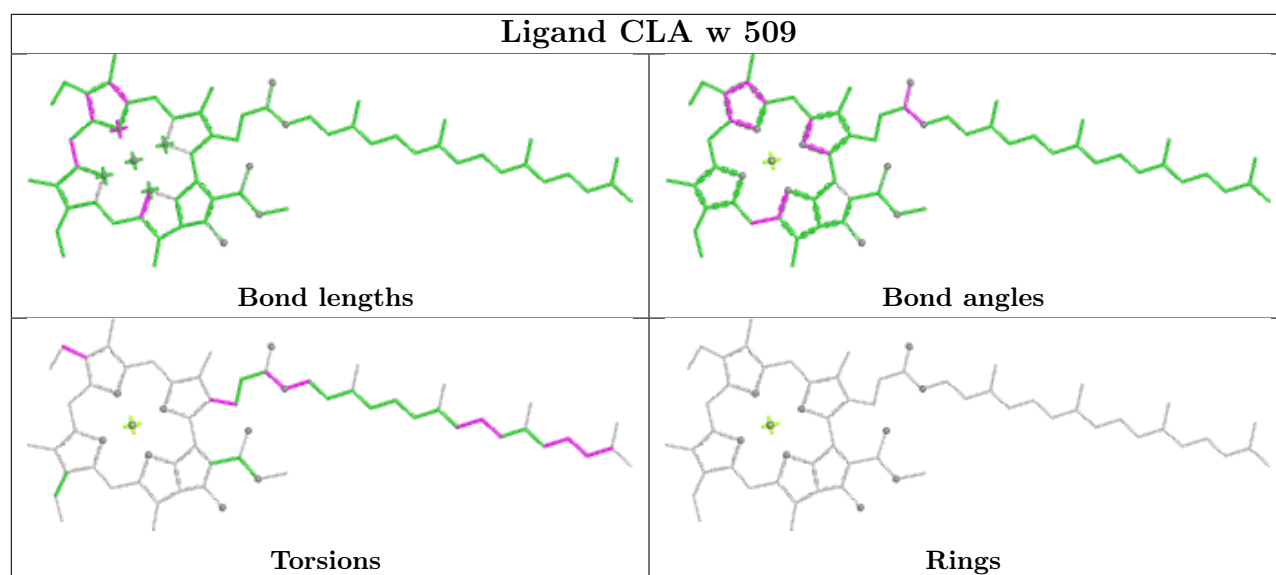


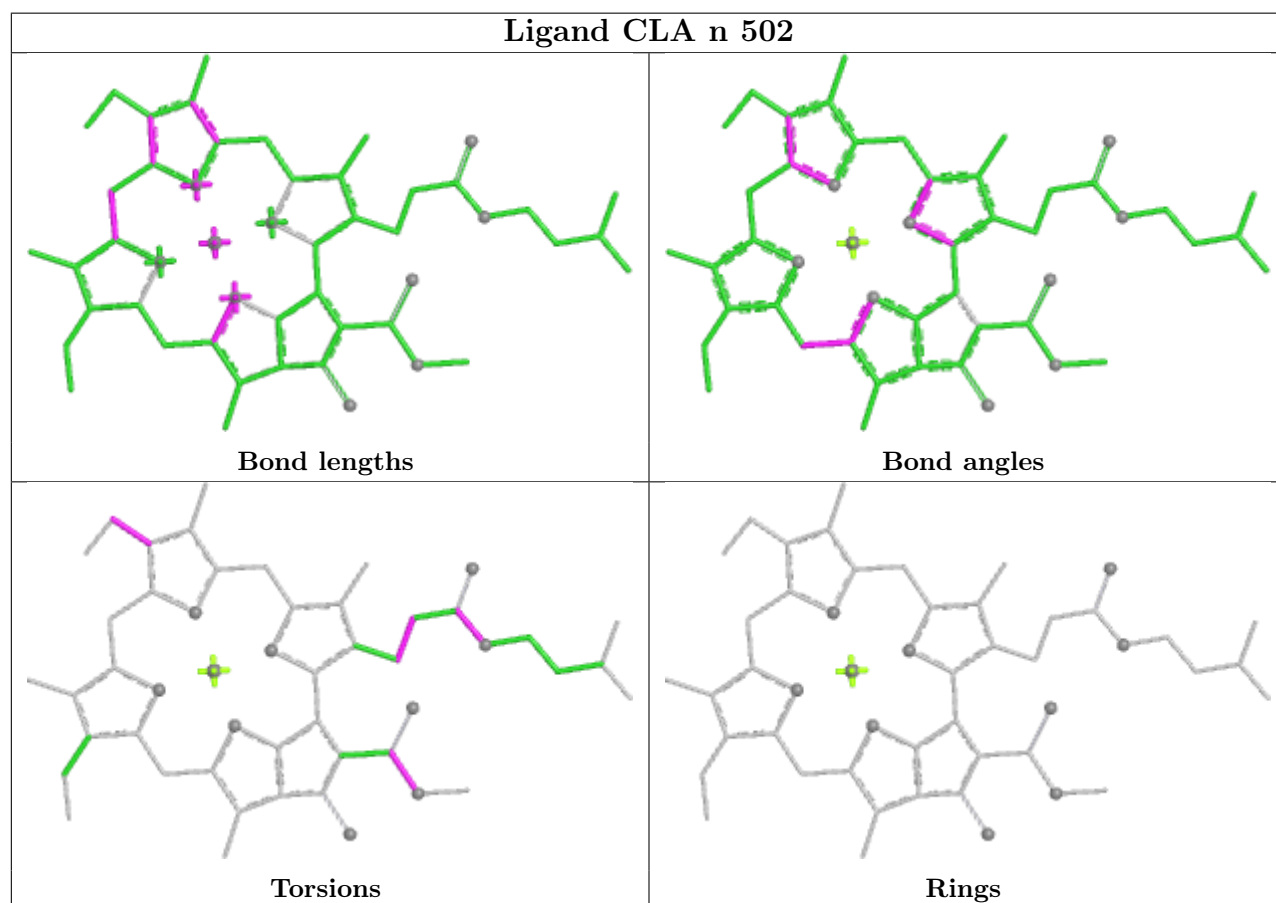
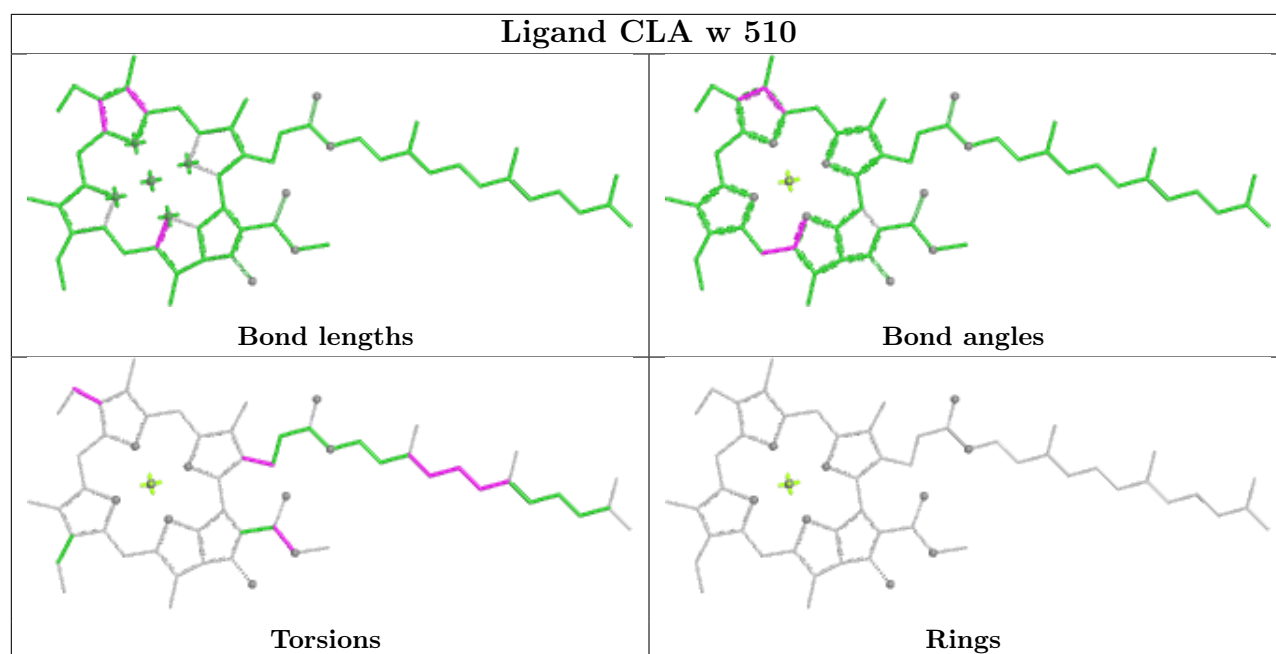


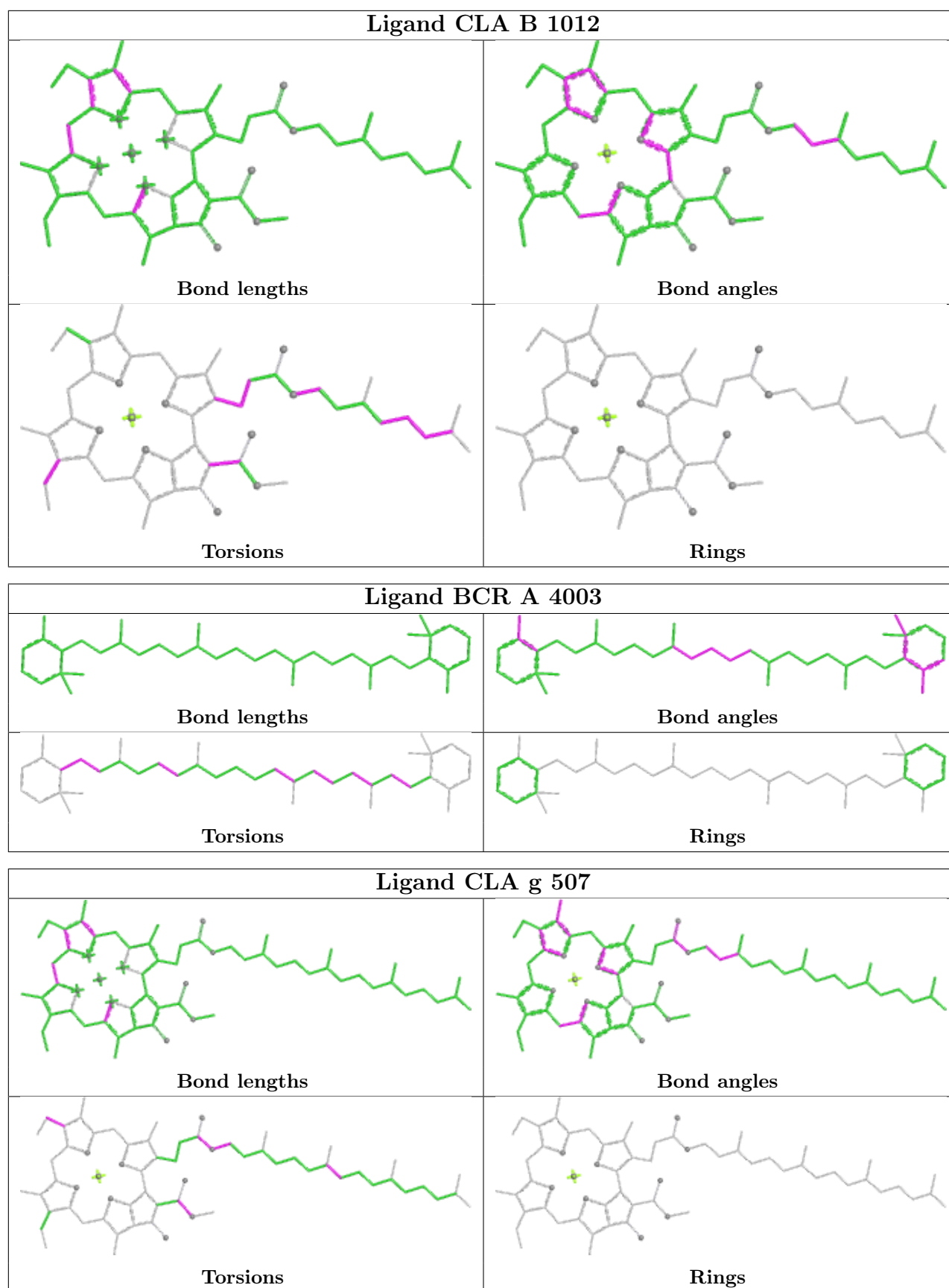


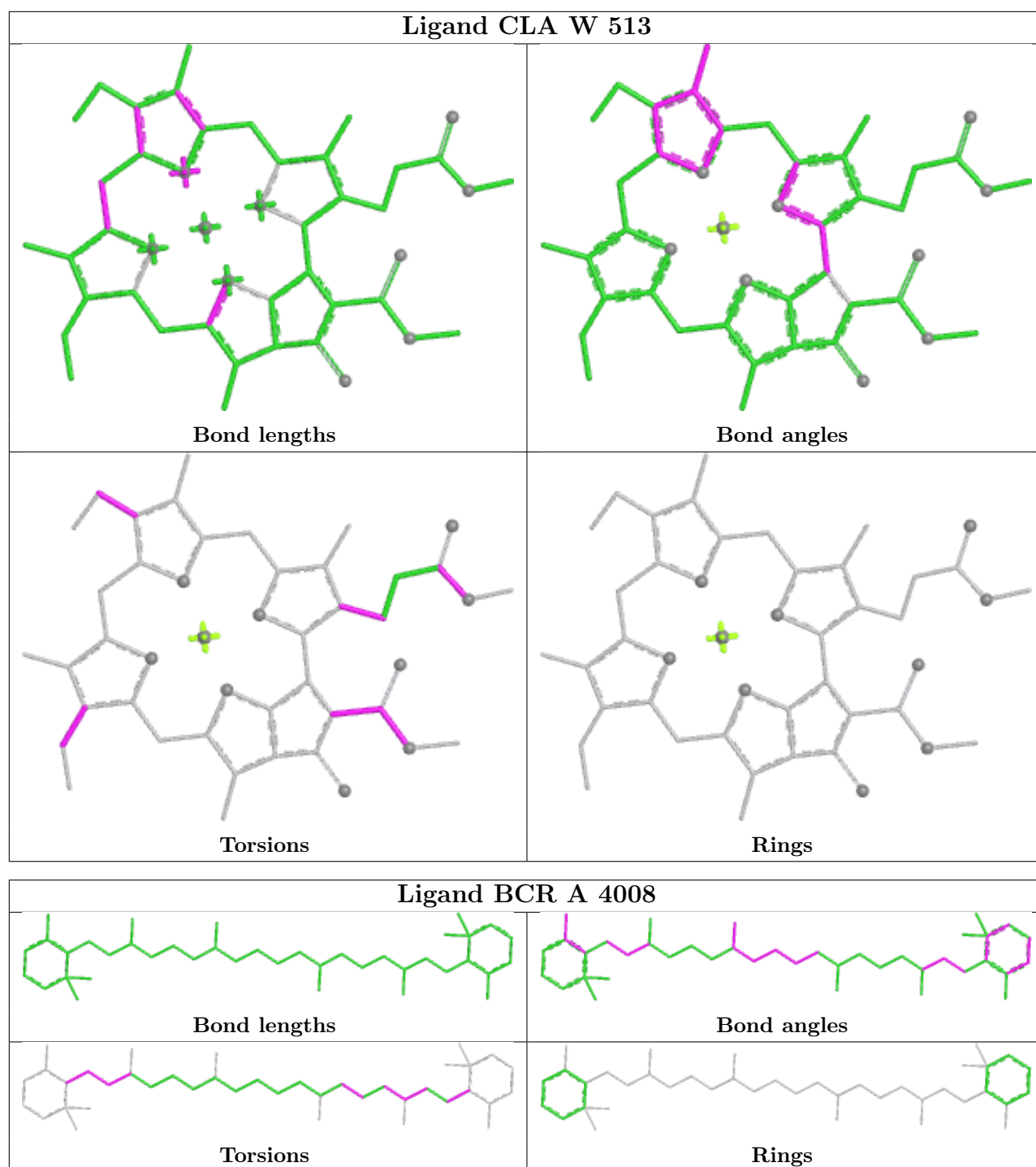




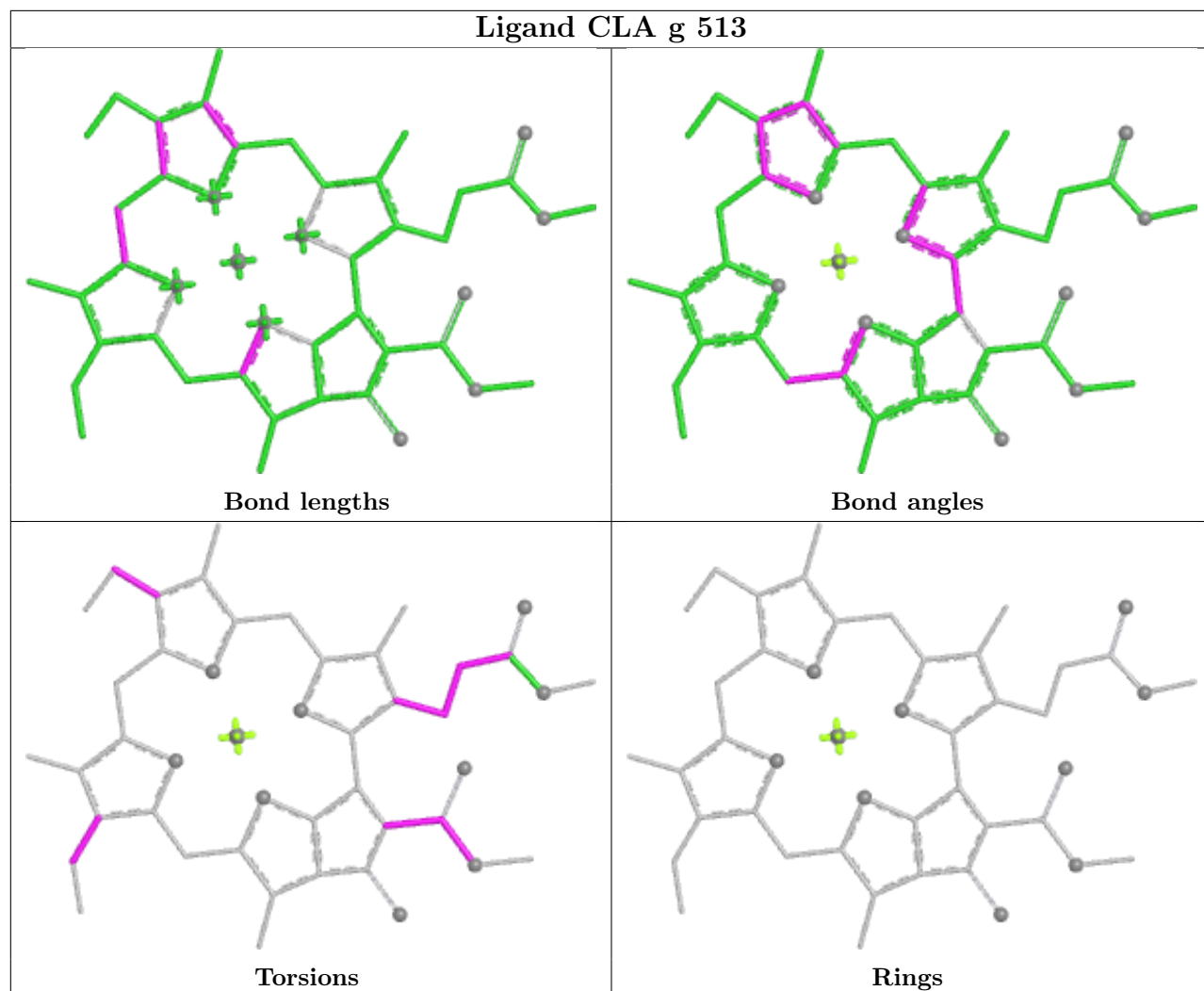




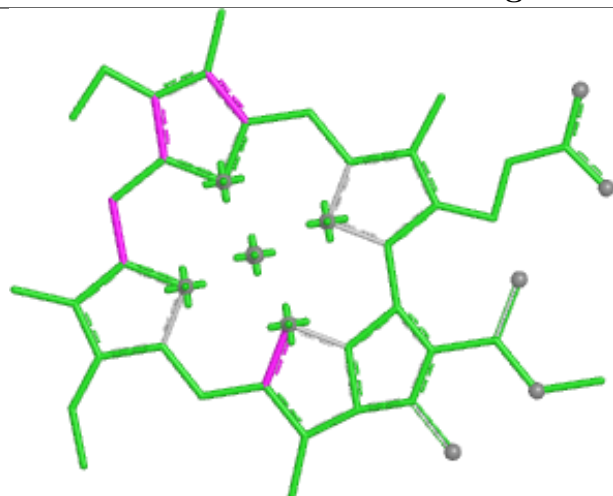




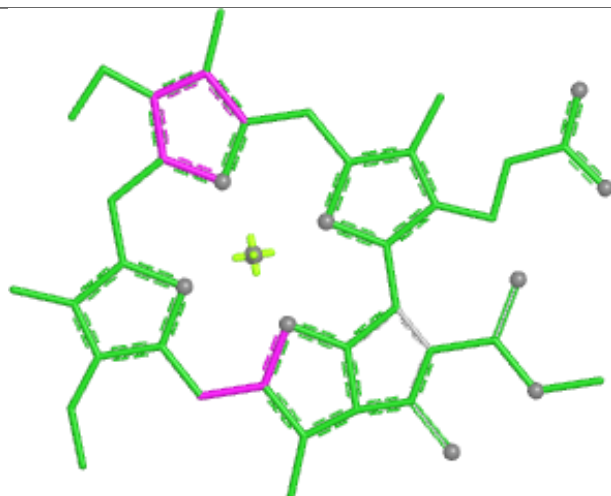
Ligand CLA g 513



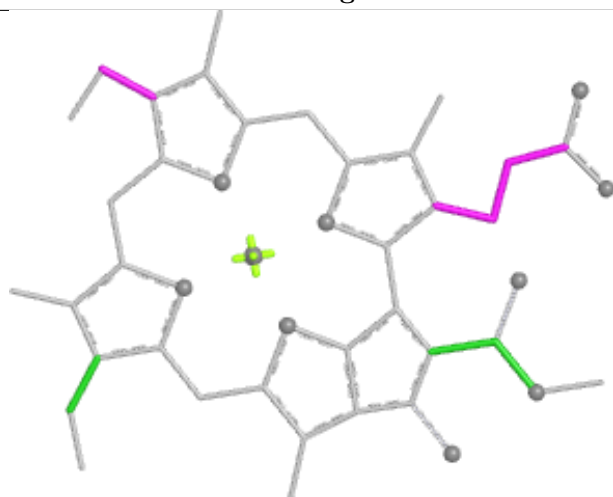
Ligand CLA B 1217



Bond lengths



Bond angles

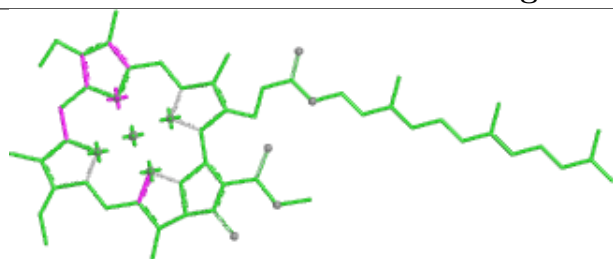


Torsions

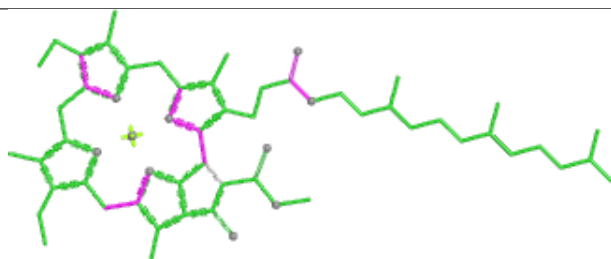


Rings

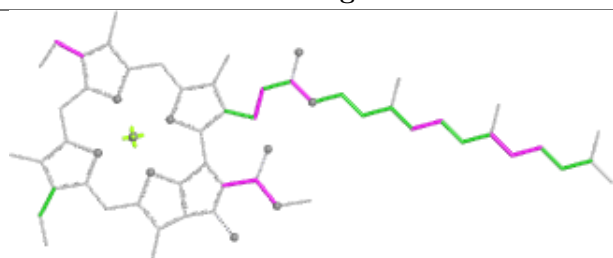
Ligand CLA t 506



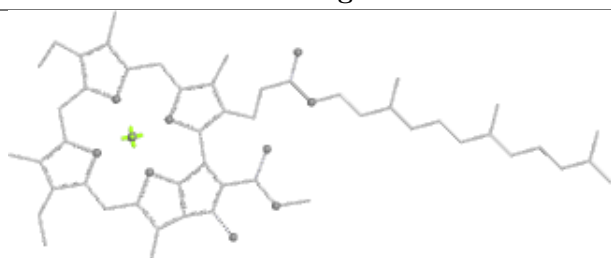
Bond lengths



Bond angles

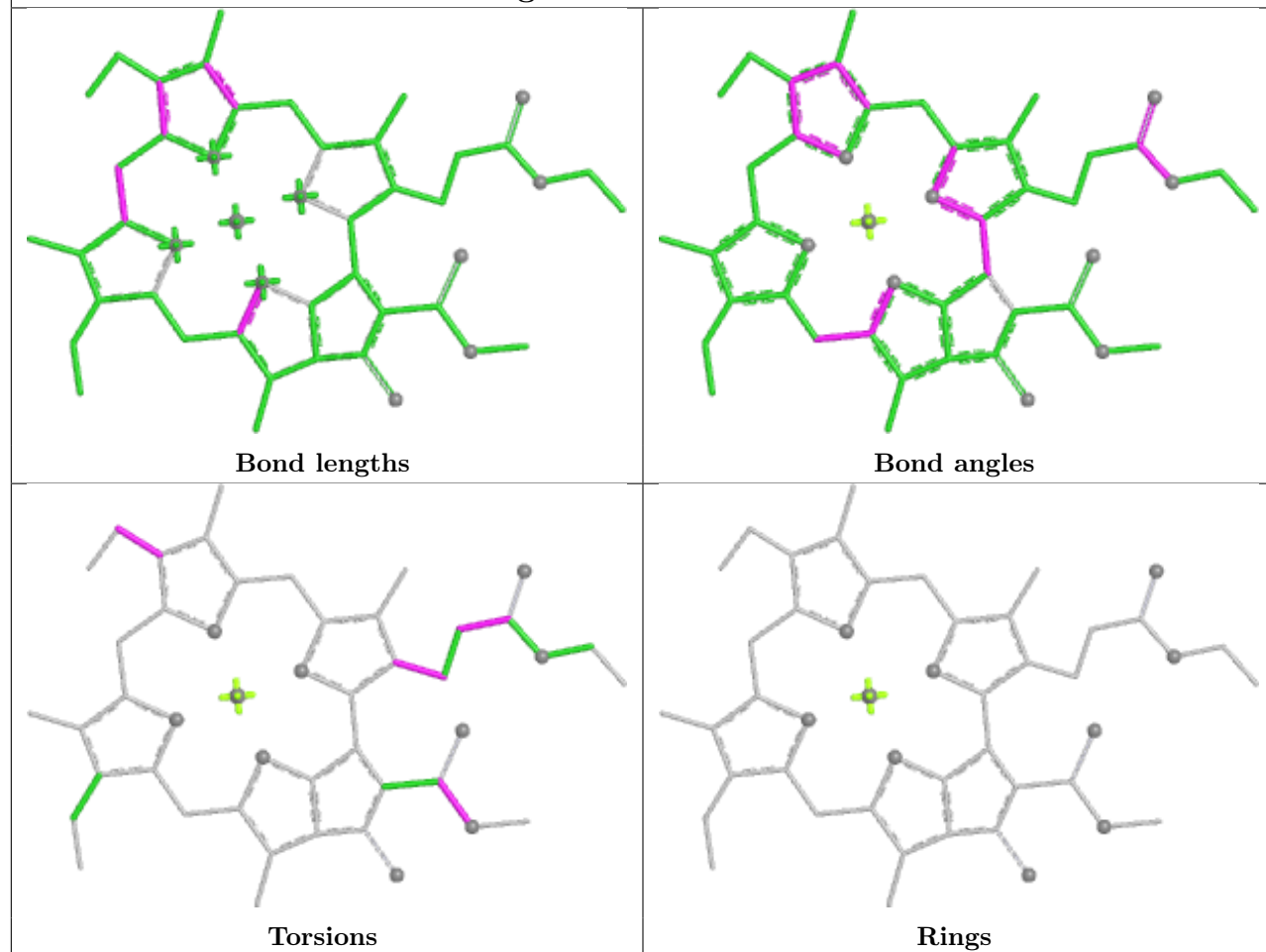


Torsions

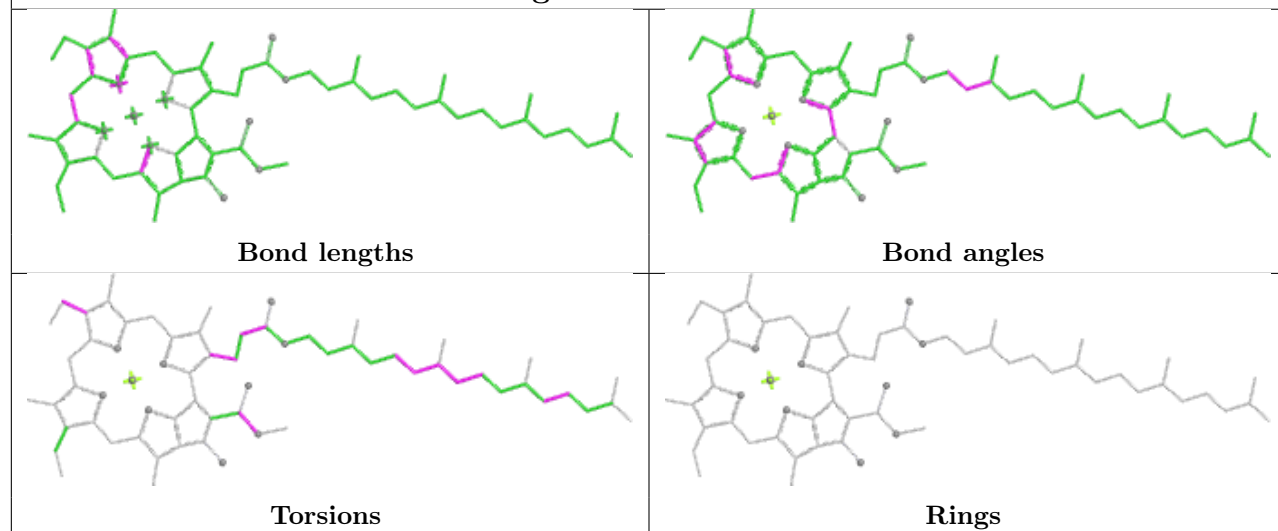


Rings

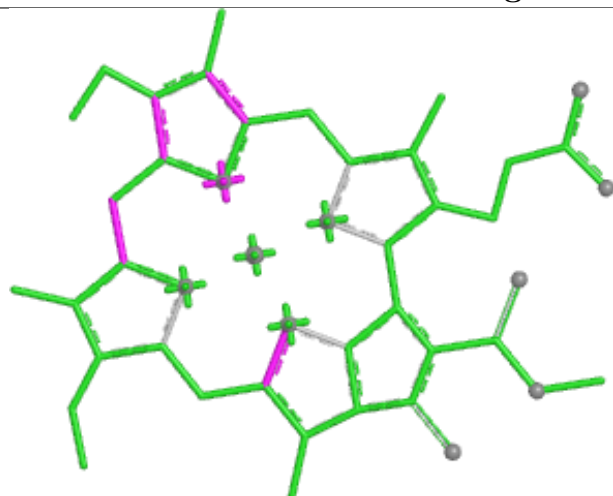
Ligand CLA A 1137



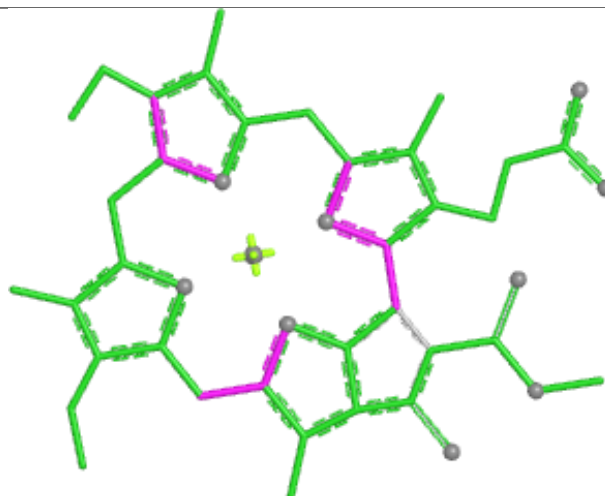
Ligand CLA w 504



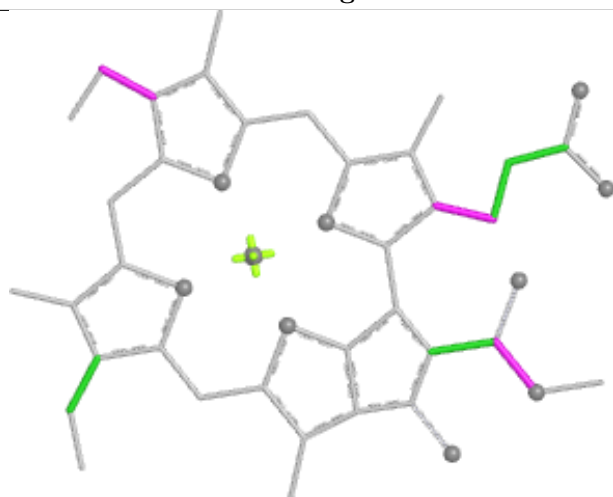
Ligand CLA H 1108



Bond lengths



Bond angles

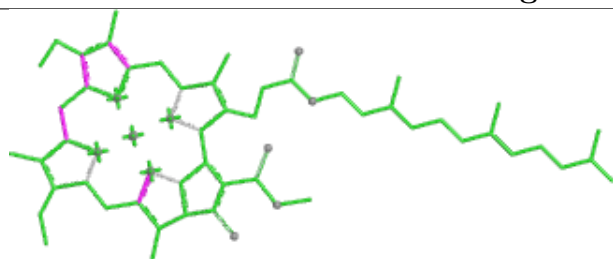


Torsions

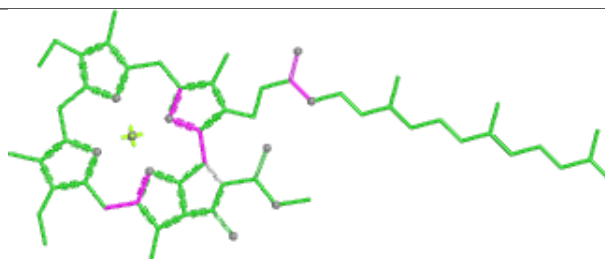


Rings

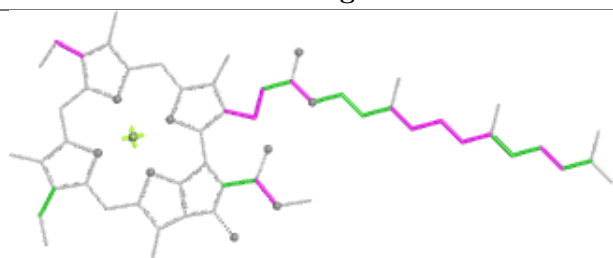
Ligand CLA s 509



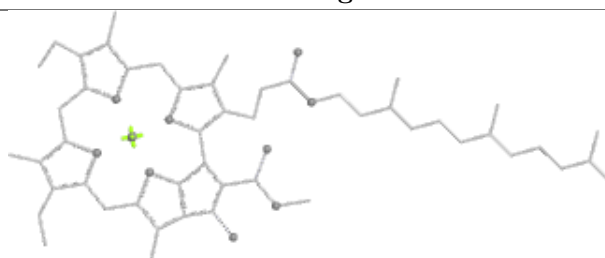
Bond lengths



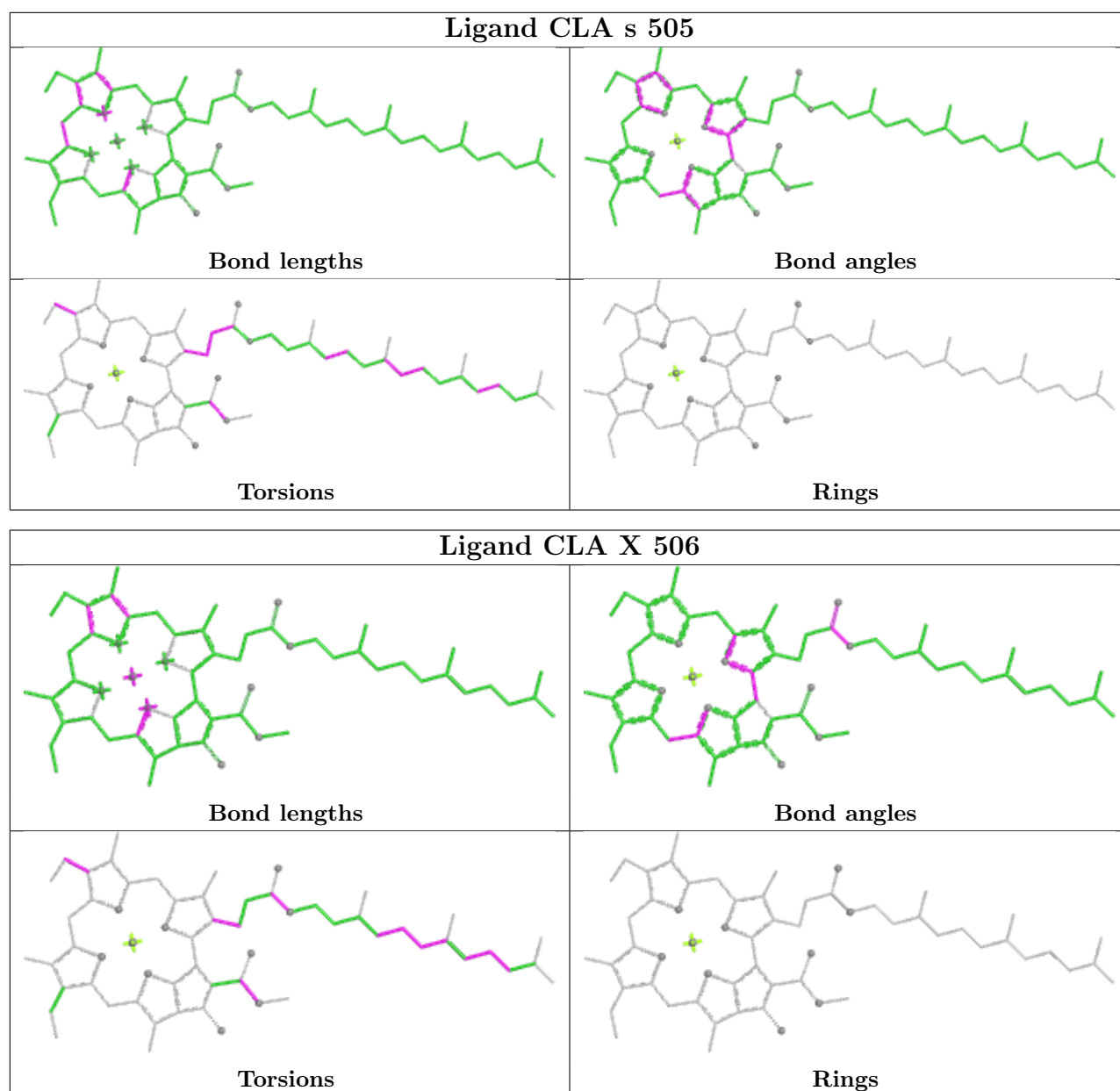
Bond angles



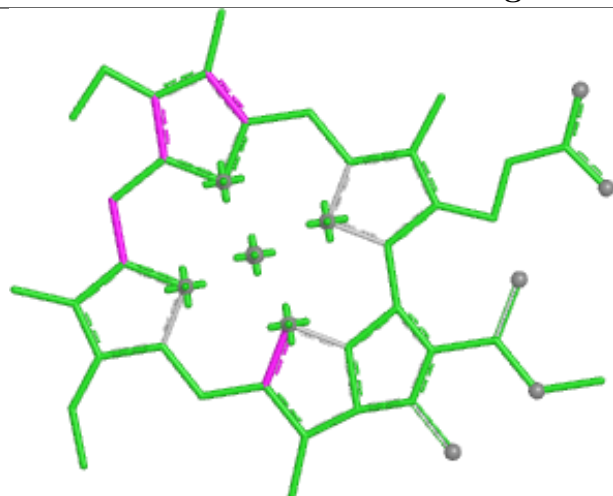
Torsions



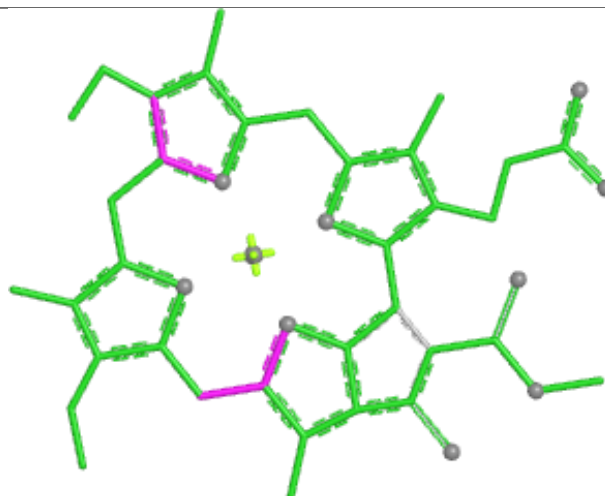
Rings



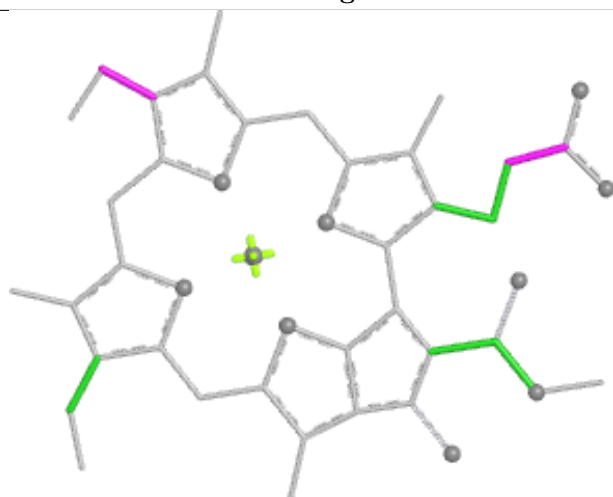
Ligand CLA H 1134



Bond lengths



Bond angles

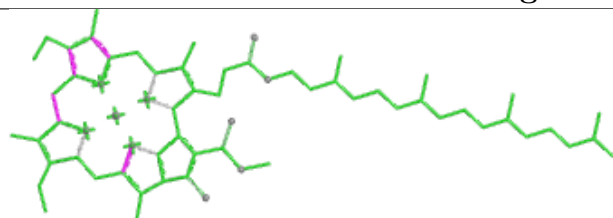


Torsions

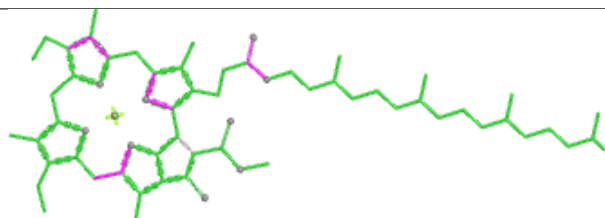


Rings

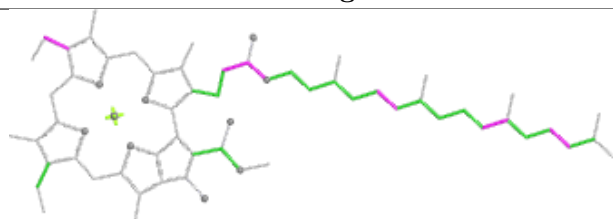
Ligand CLA s 510



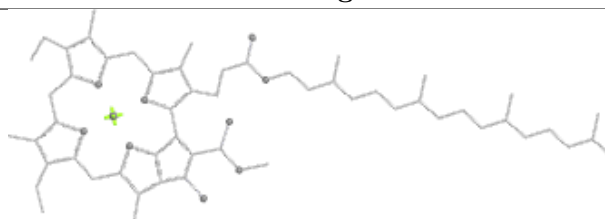
Bond lengths



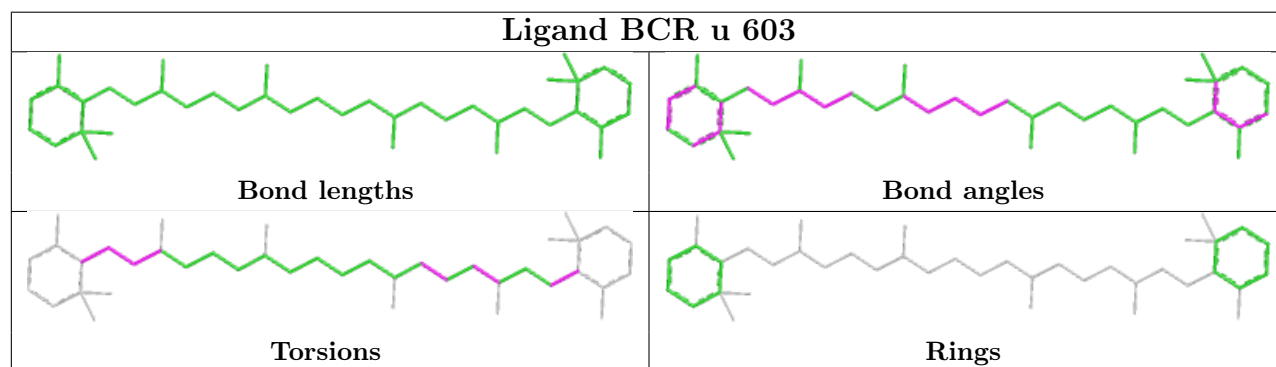
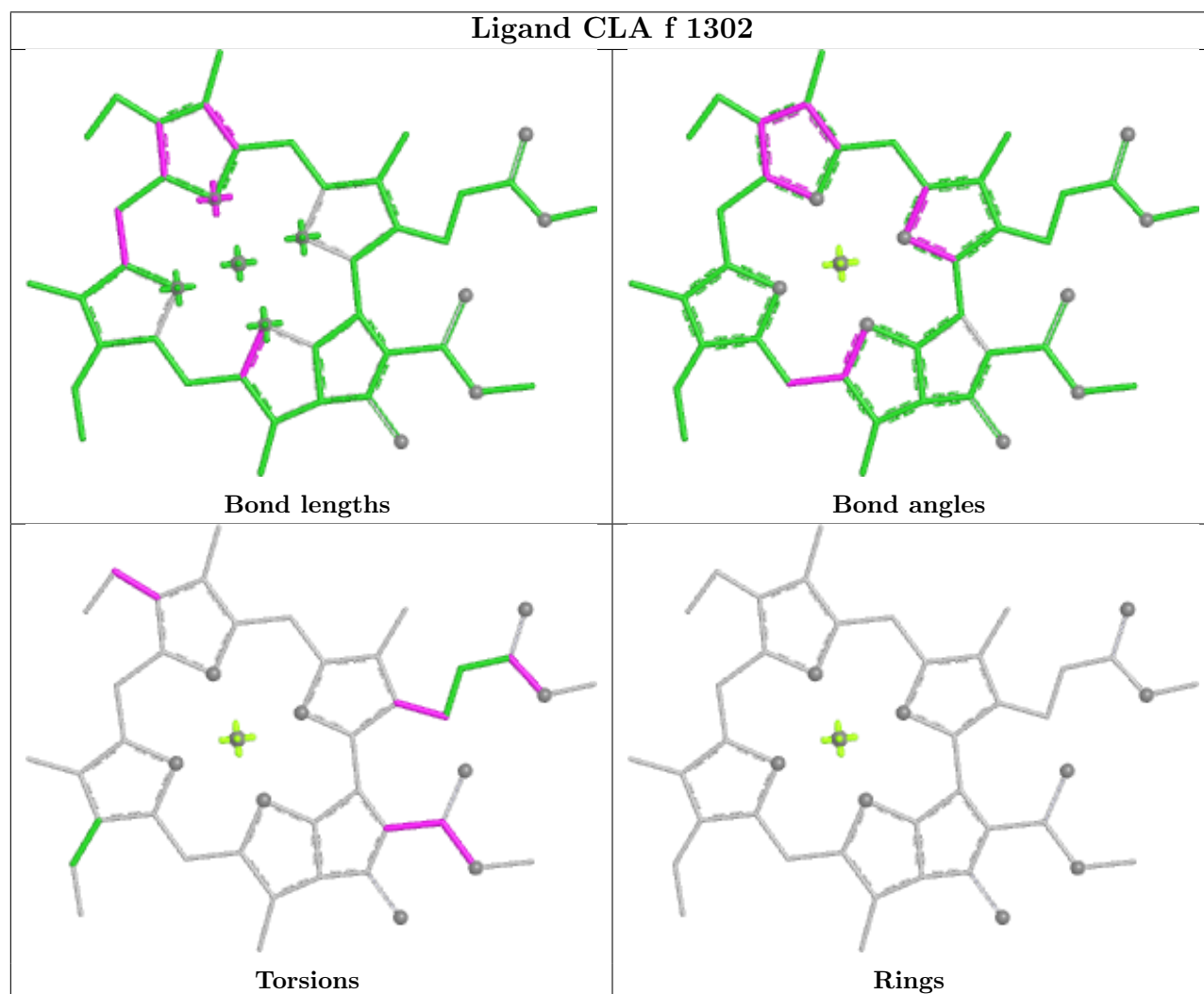
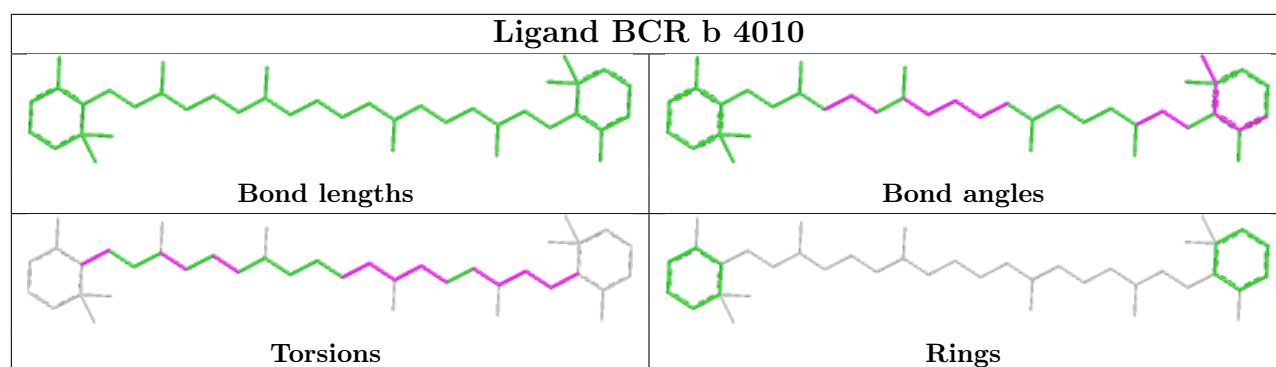
Bond angles

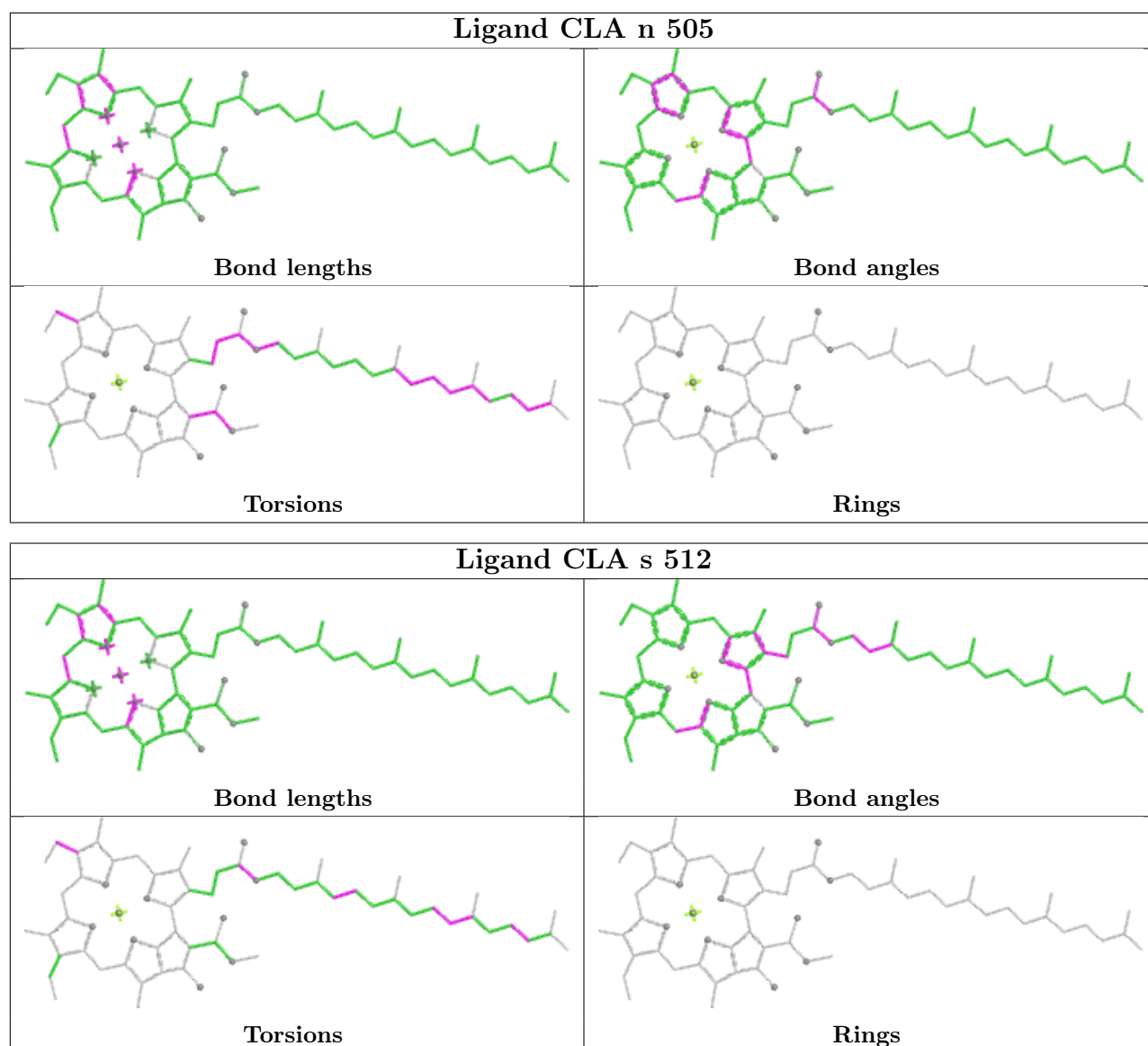


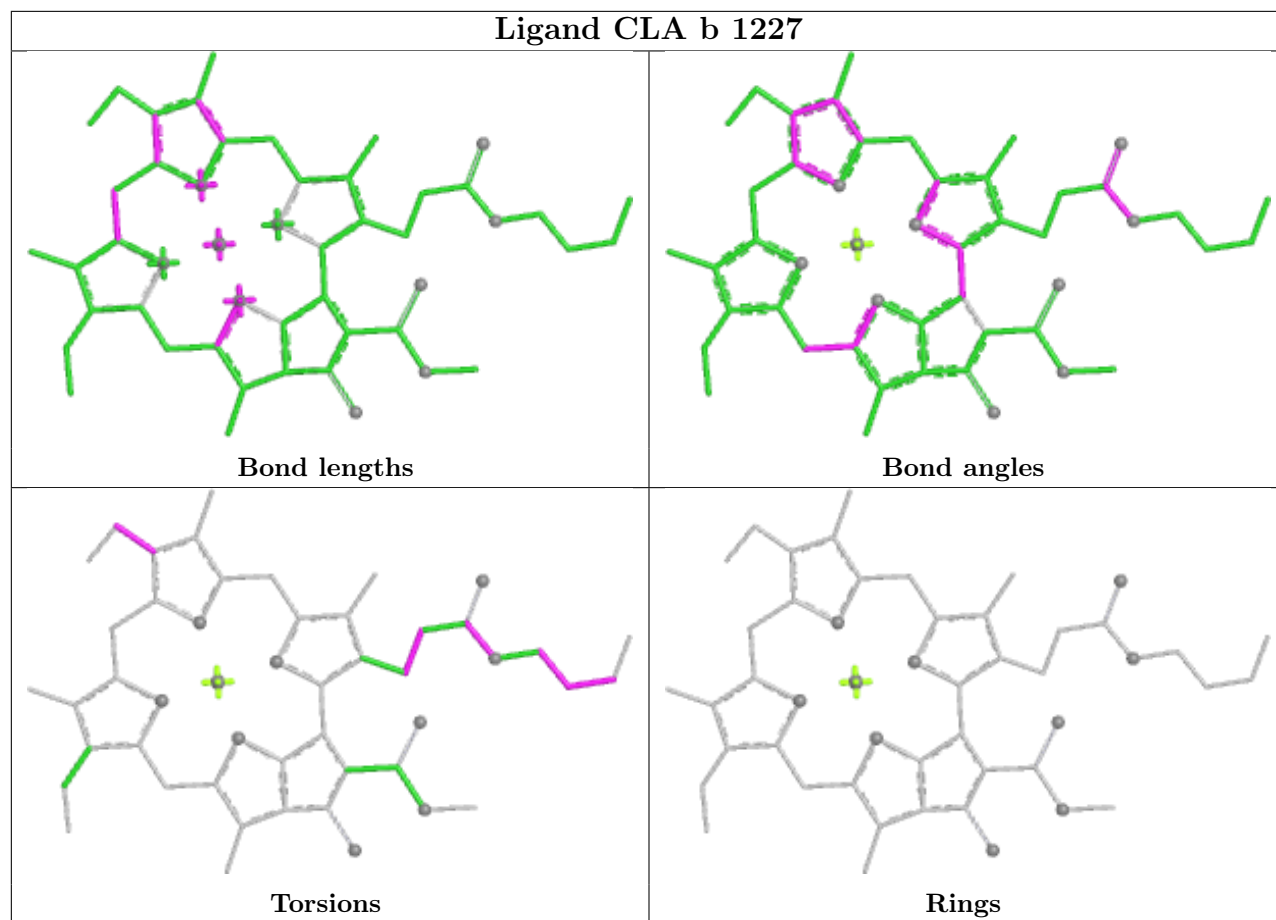
Torsions



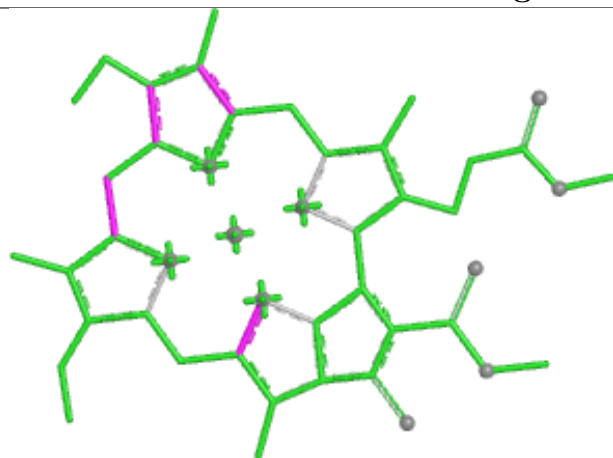
Rings



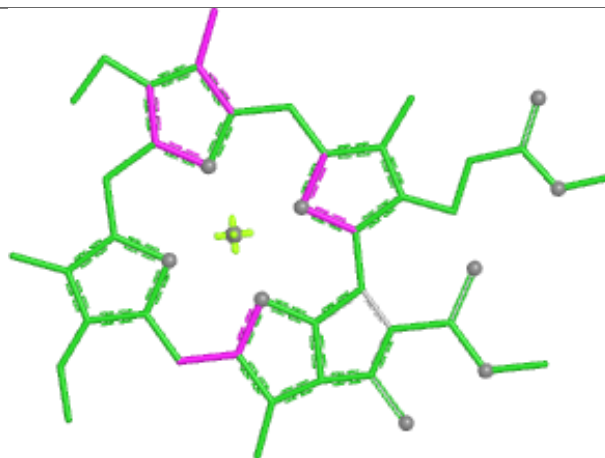




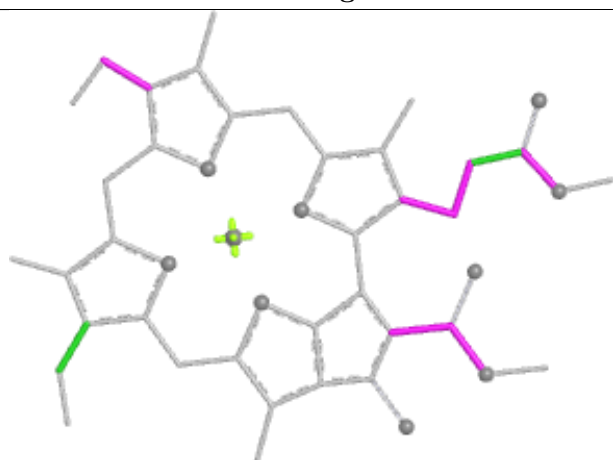
Ligand CLA Y 516



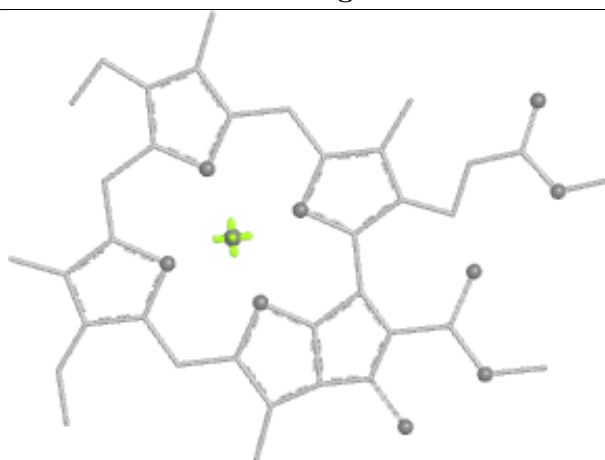
Bond lengths



Bond angles

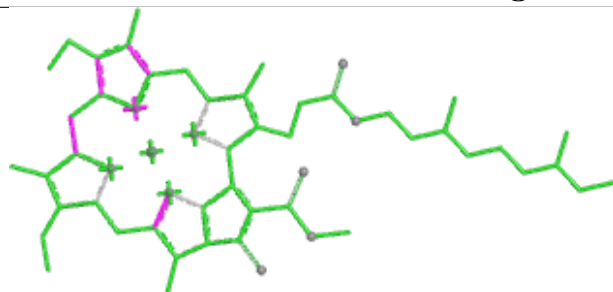


Torsions

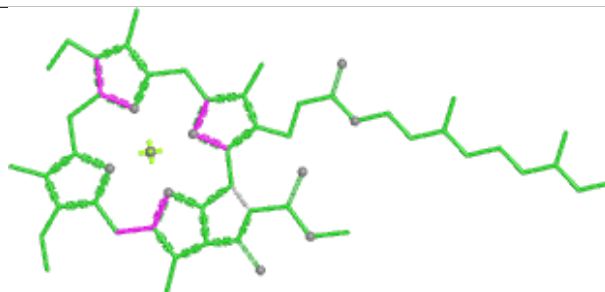


Rings

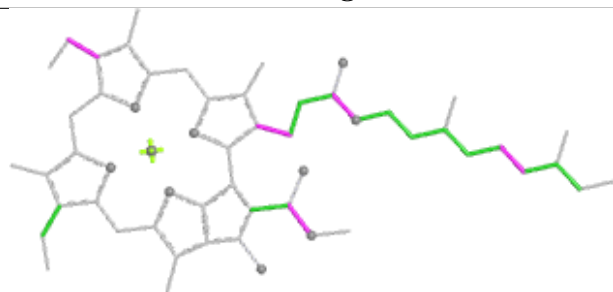
Ligand CLA a 1102



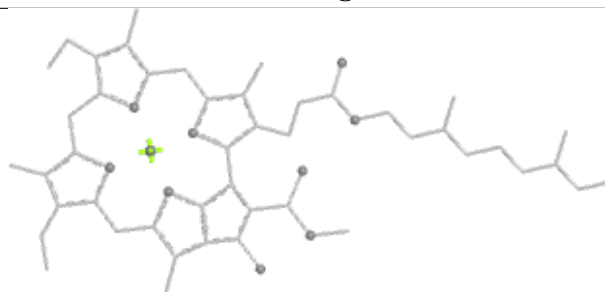
Bond lengths



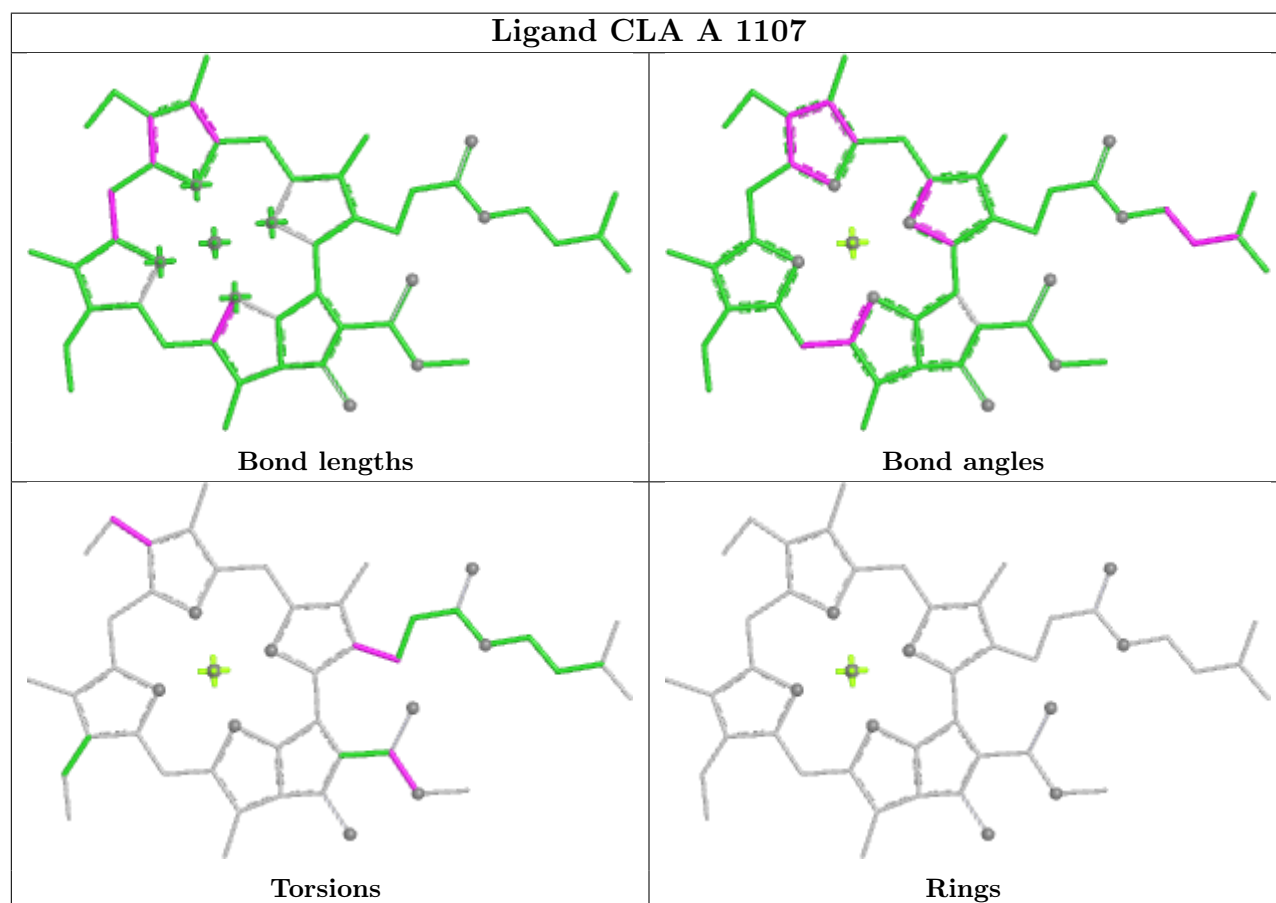
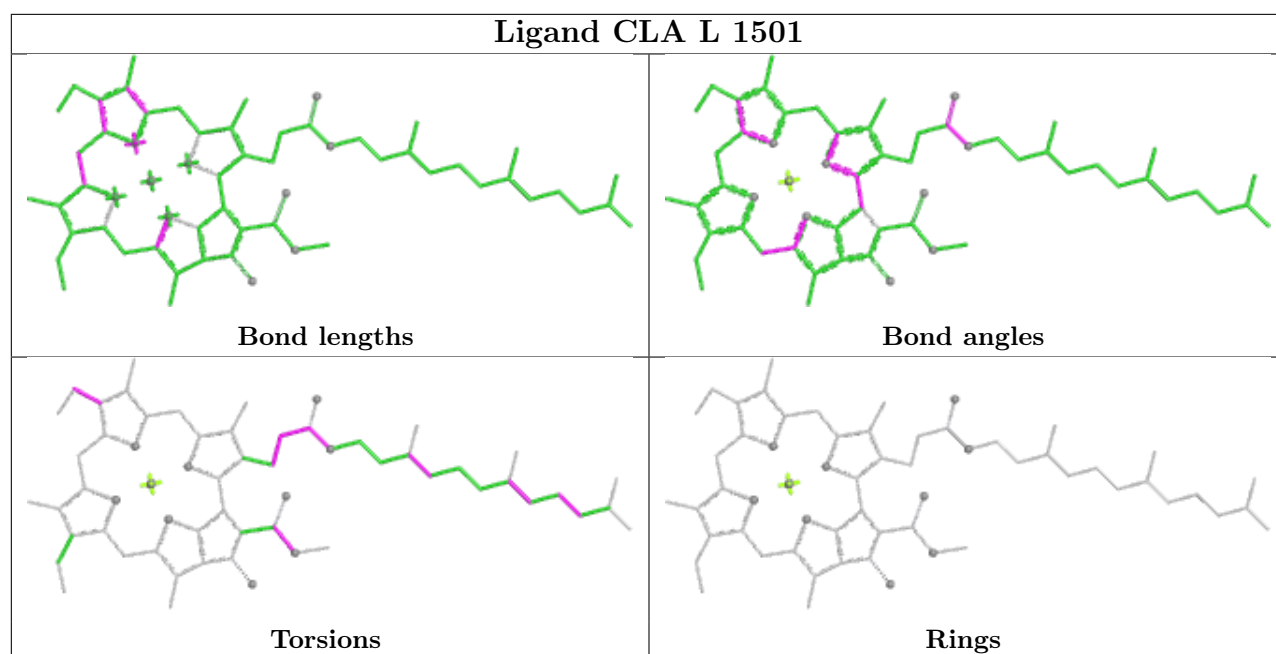
Bond angles

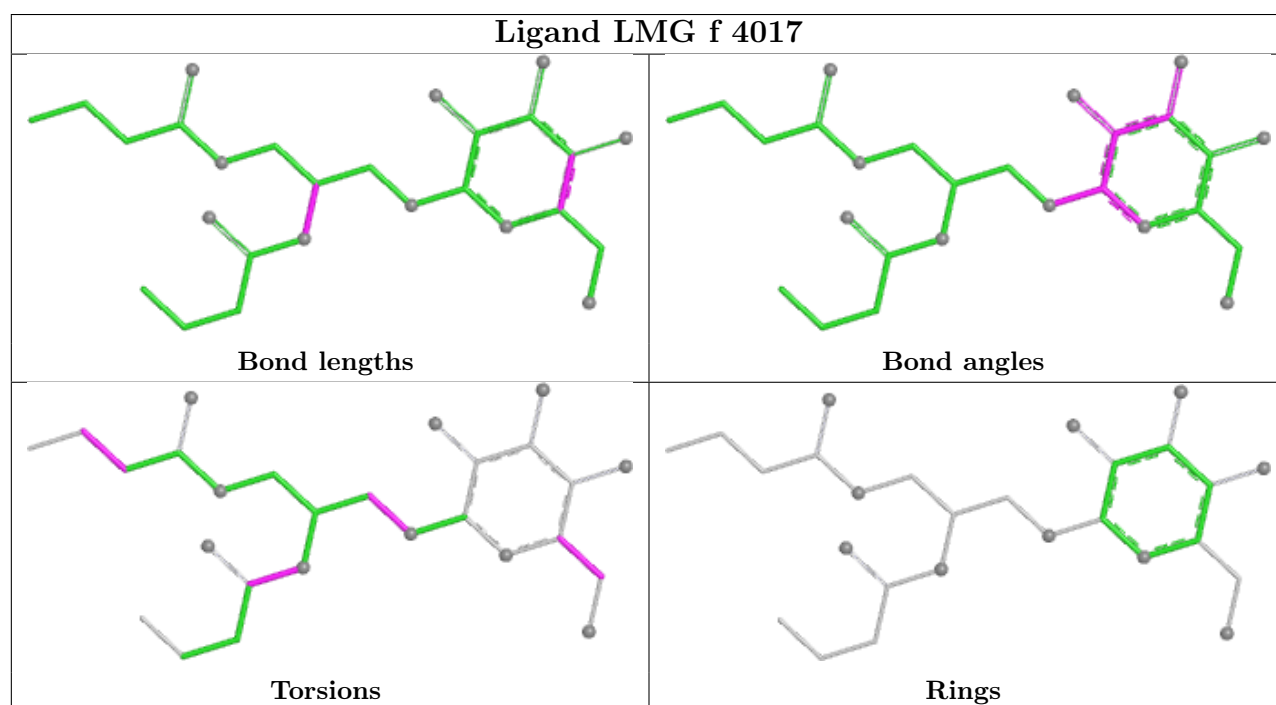
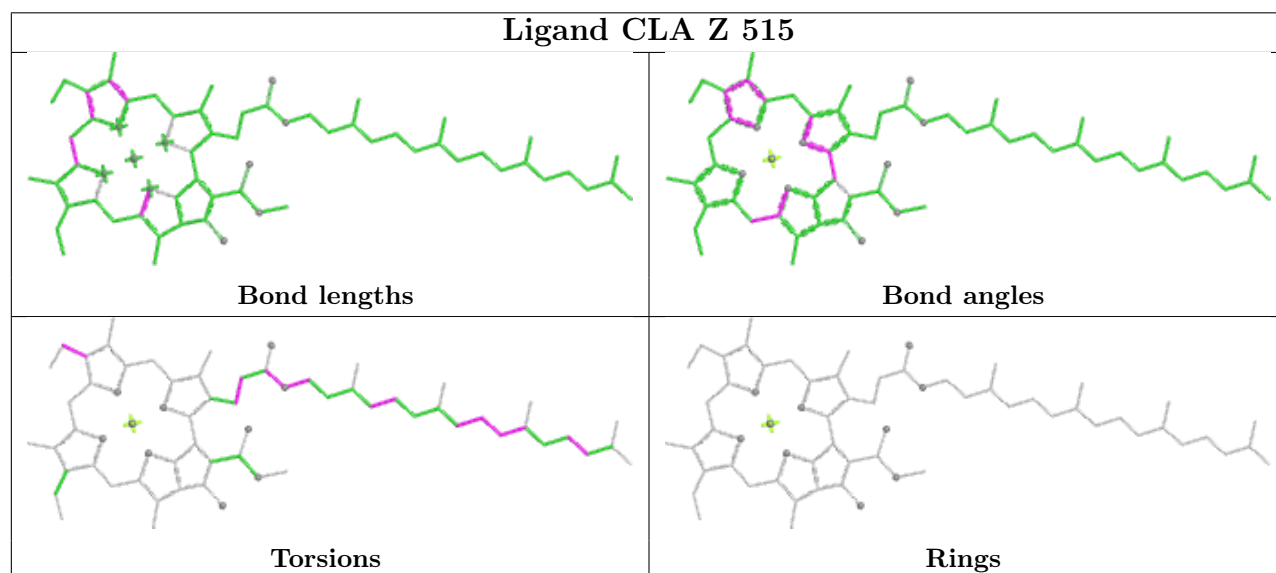
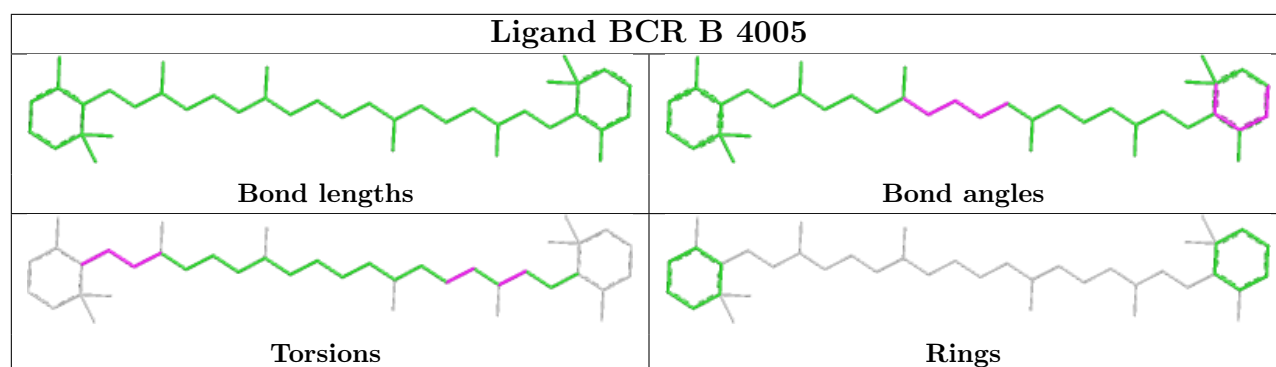


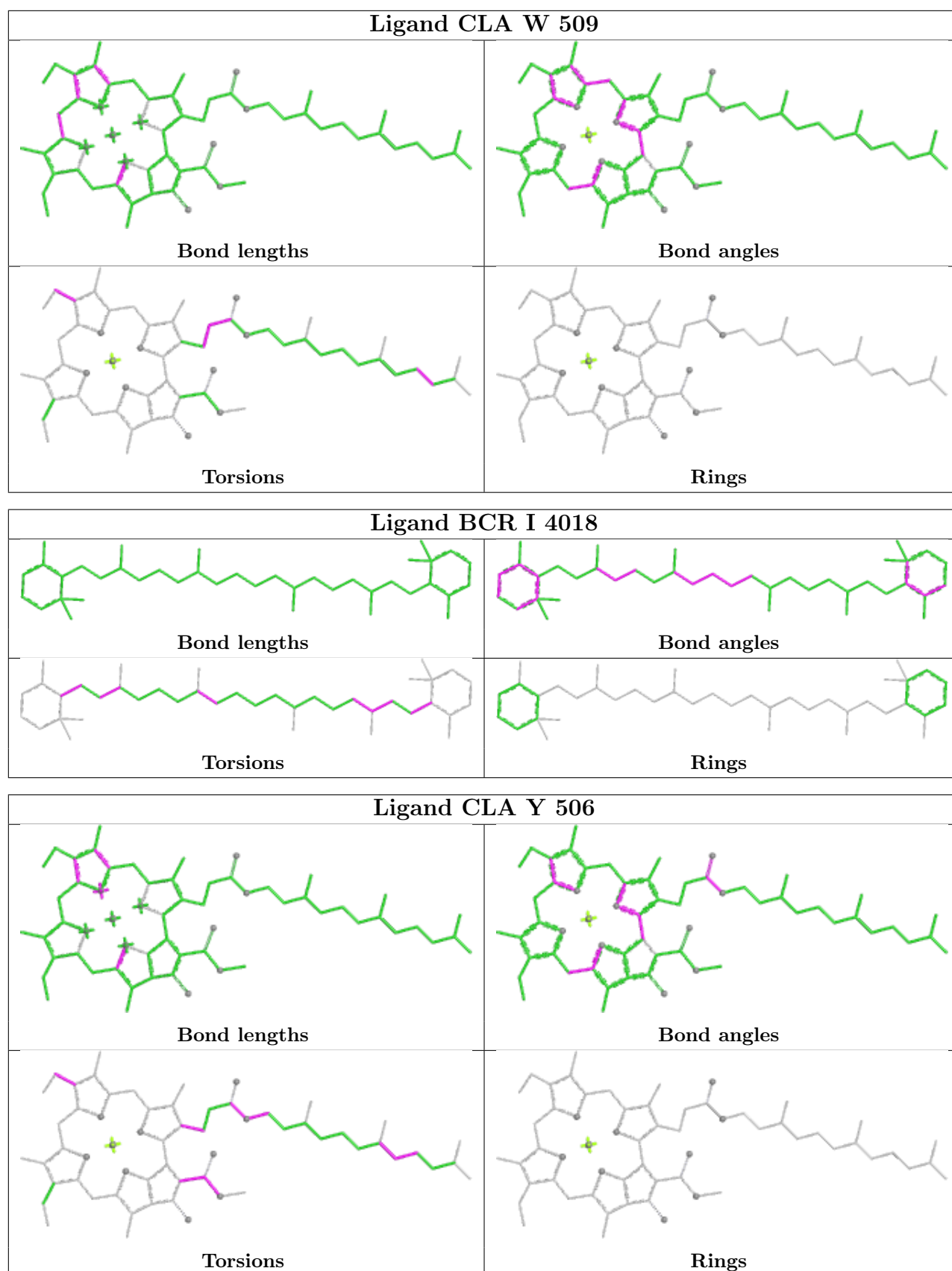
Torsions

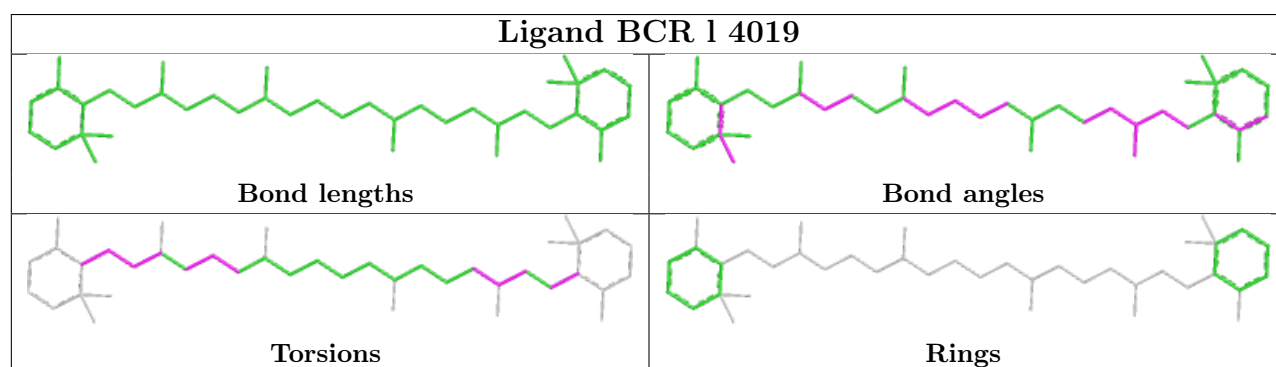
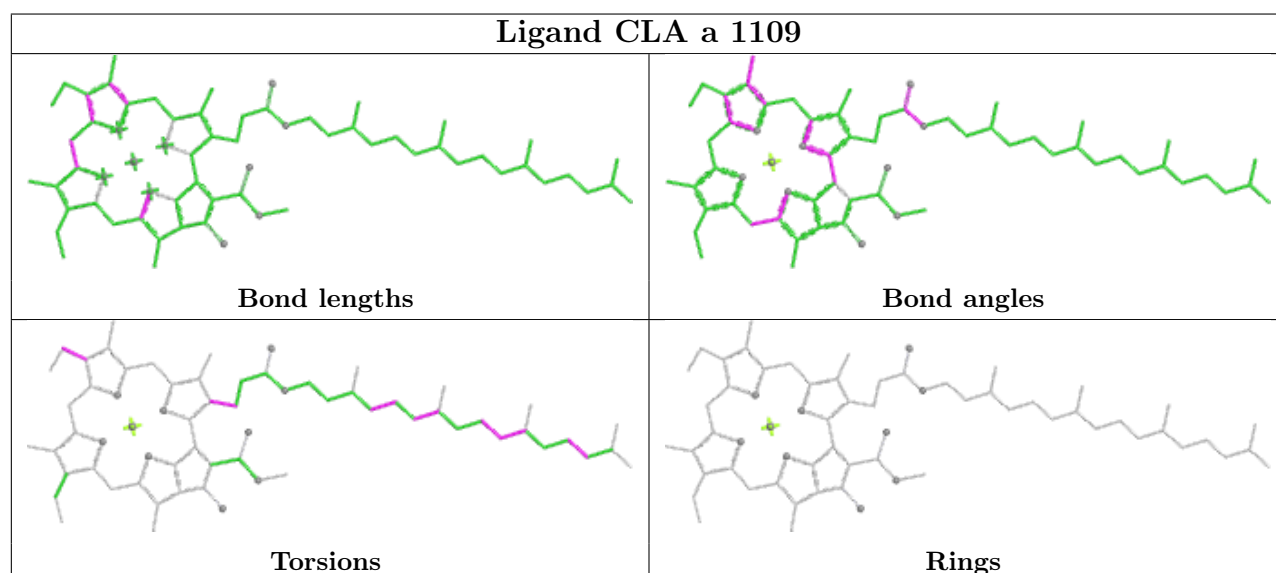
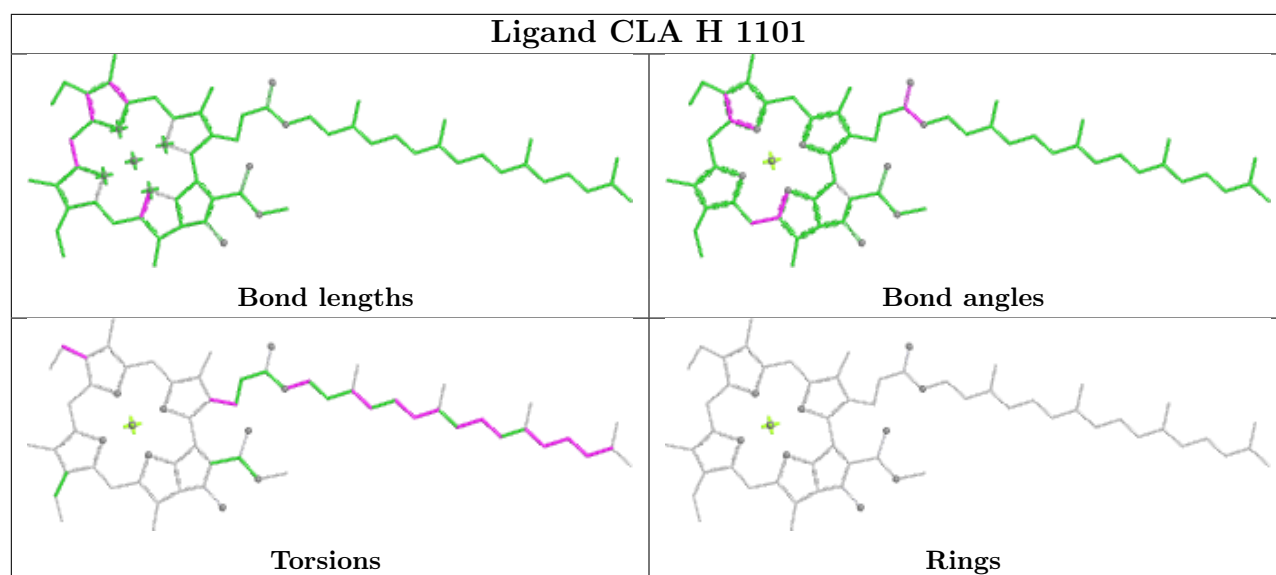


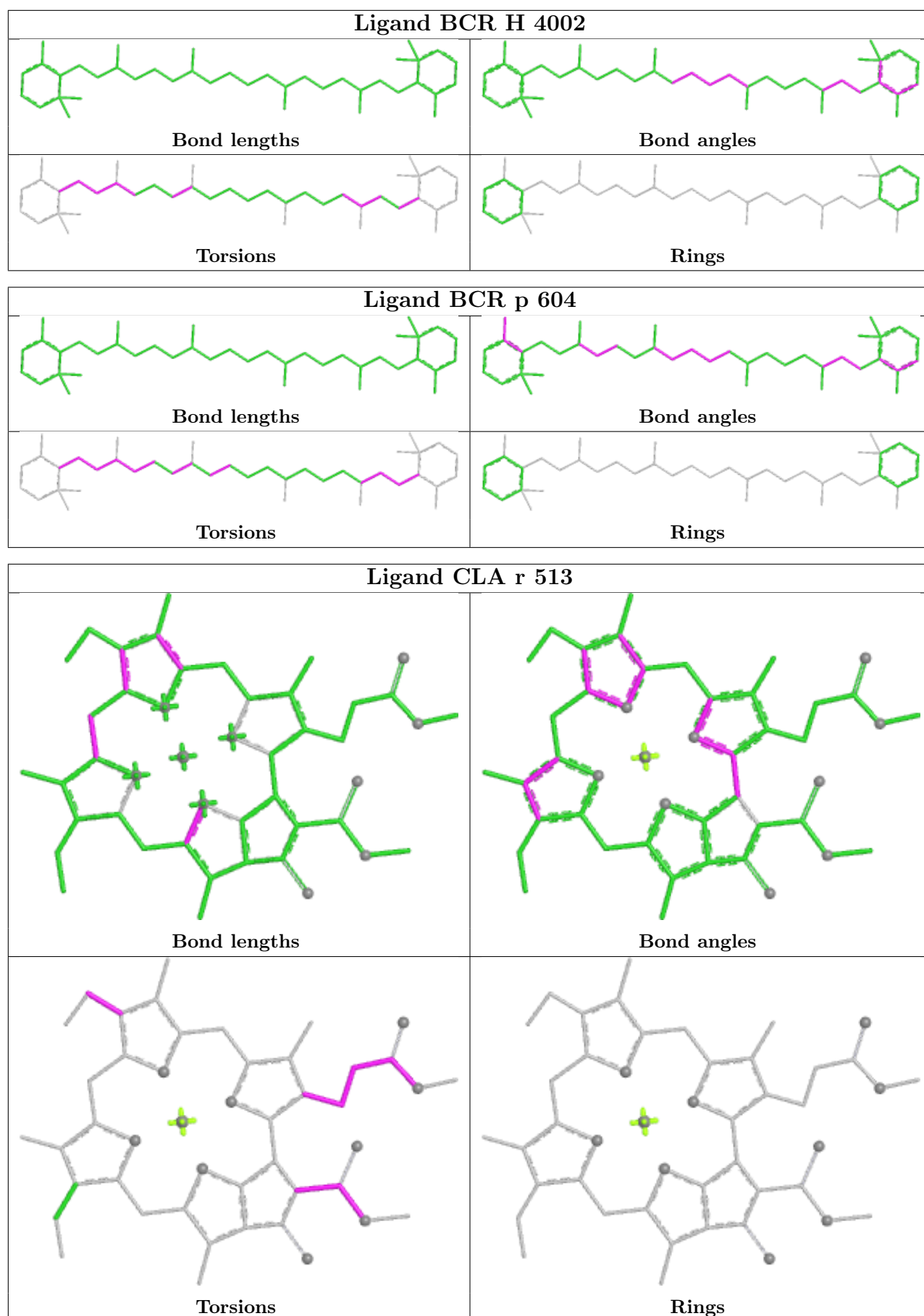
Rings

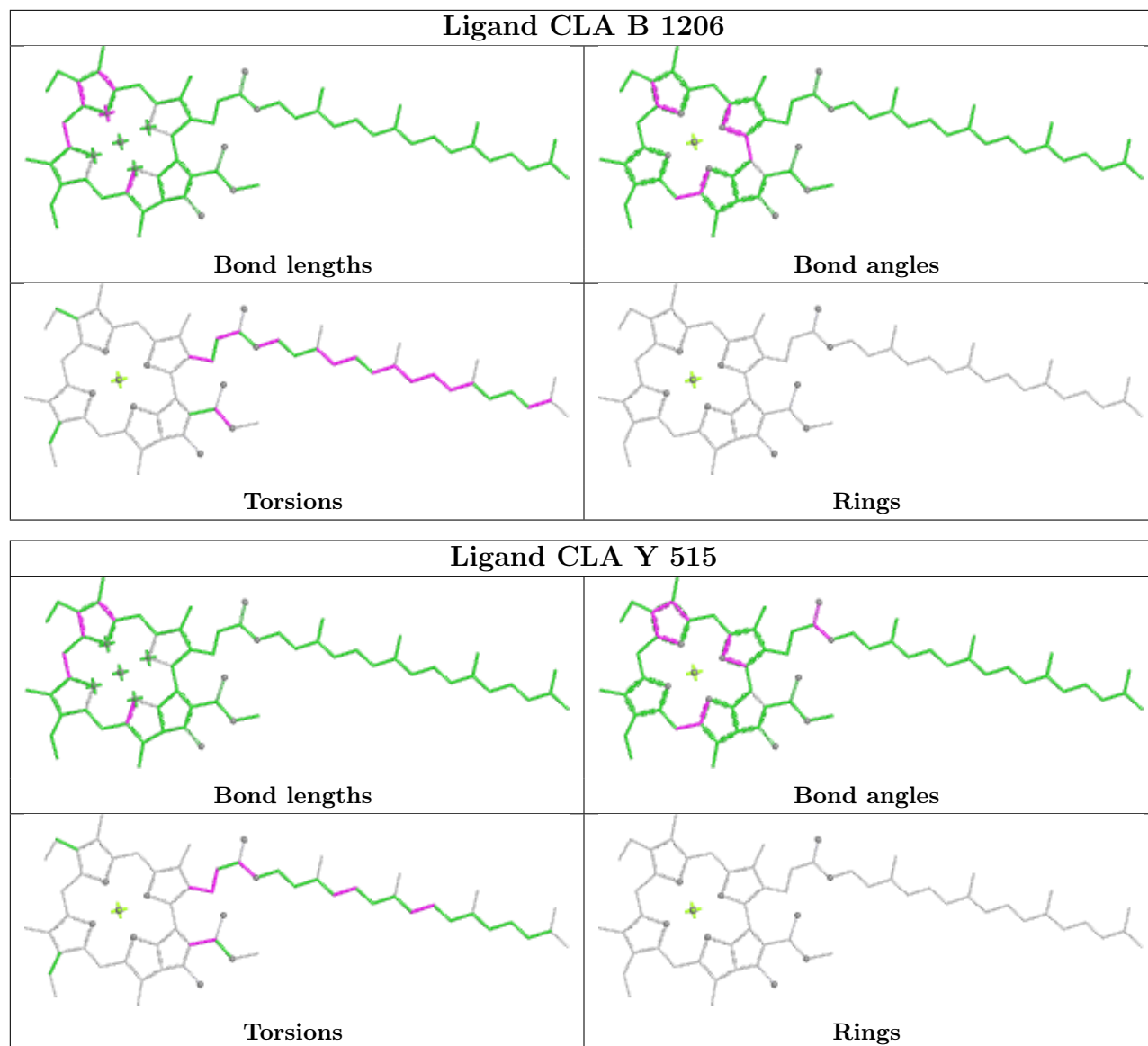


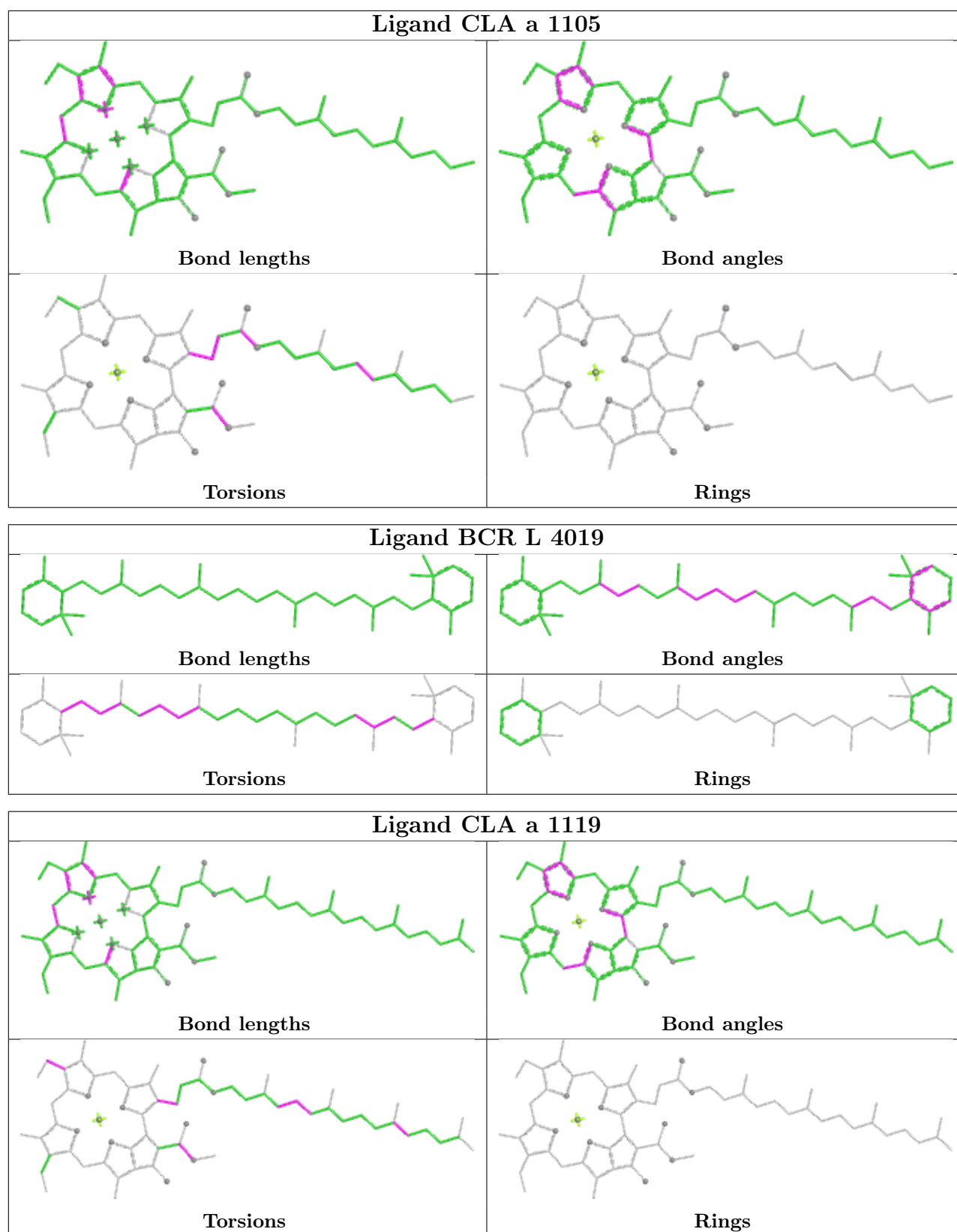


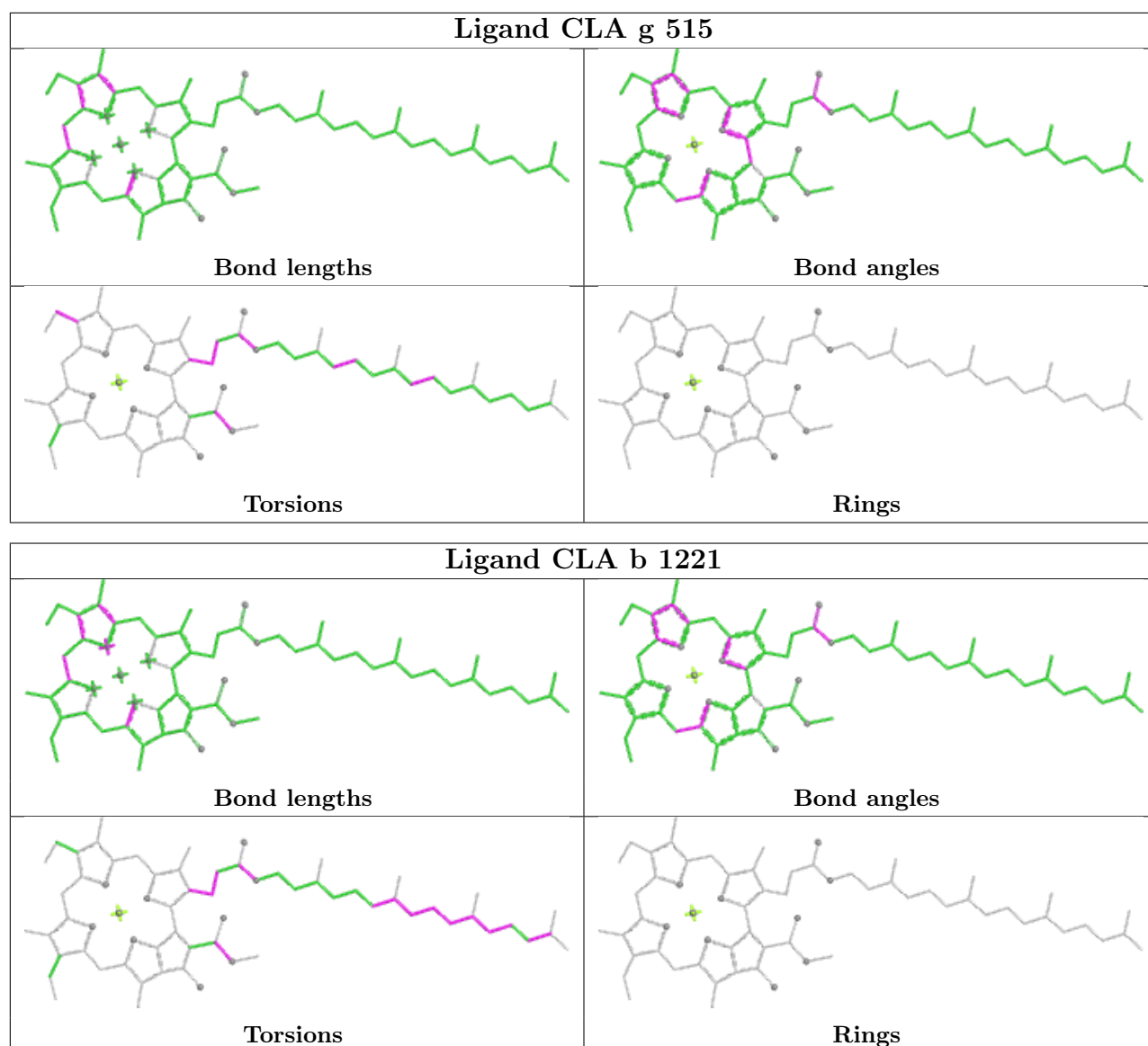




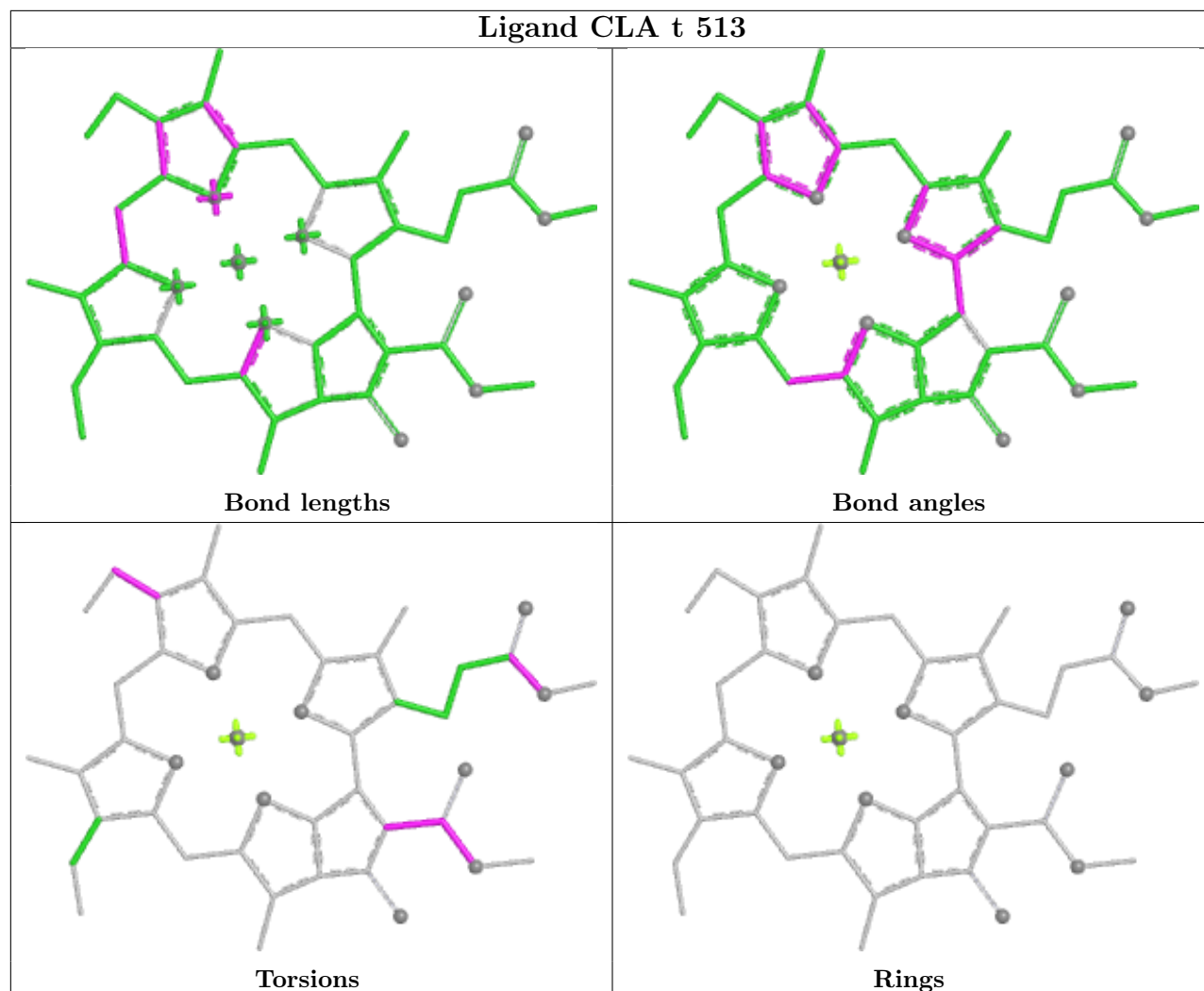




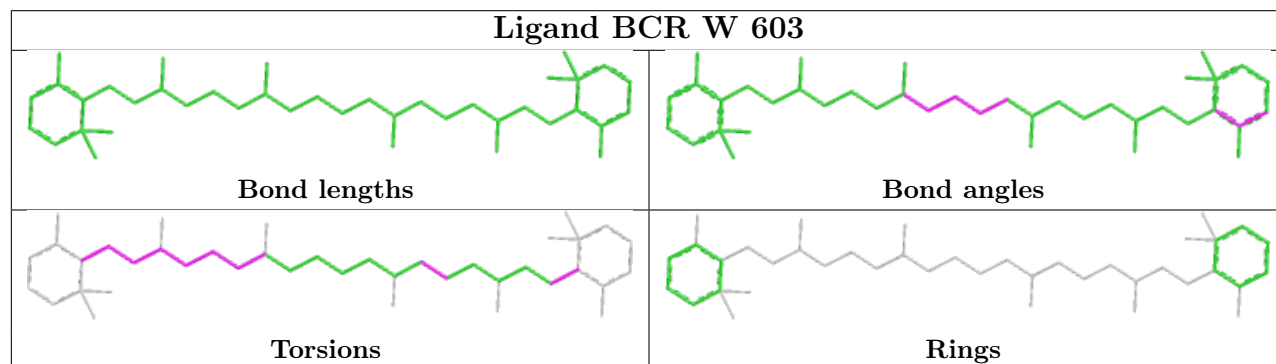


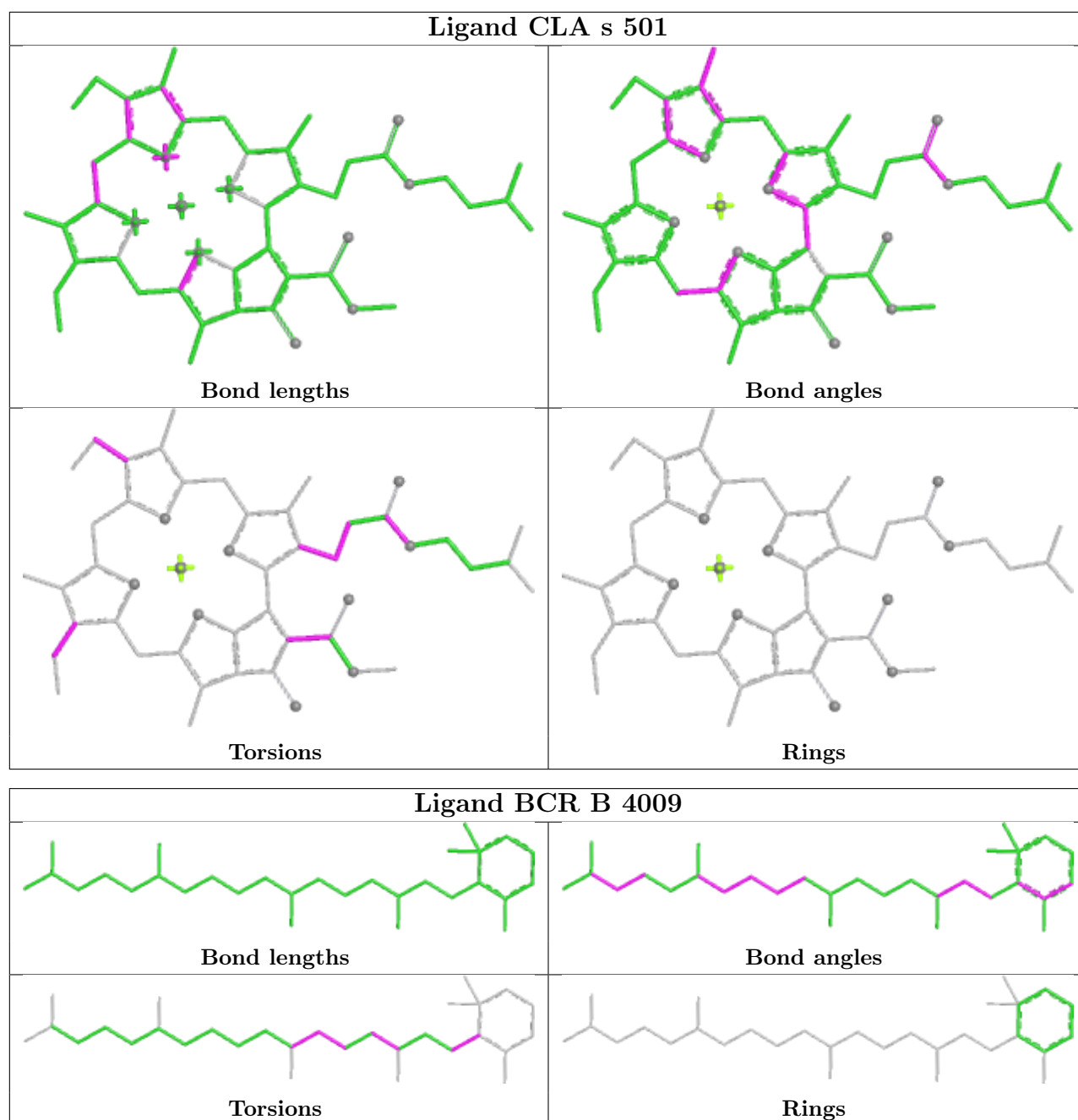


Ligand CLA t 513

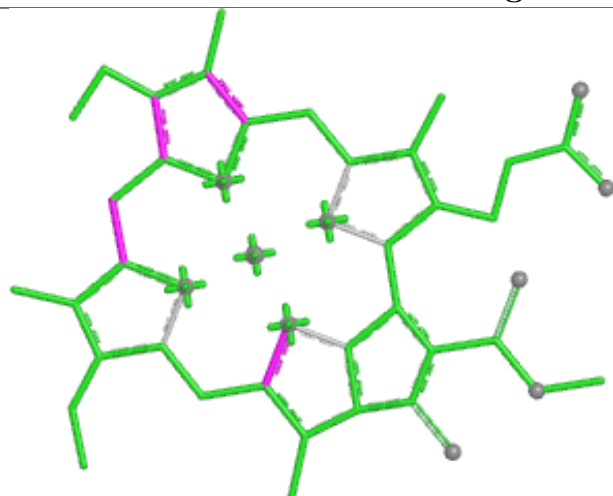


Ligand BCR W 603

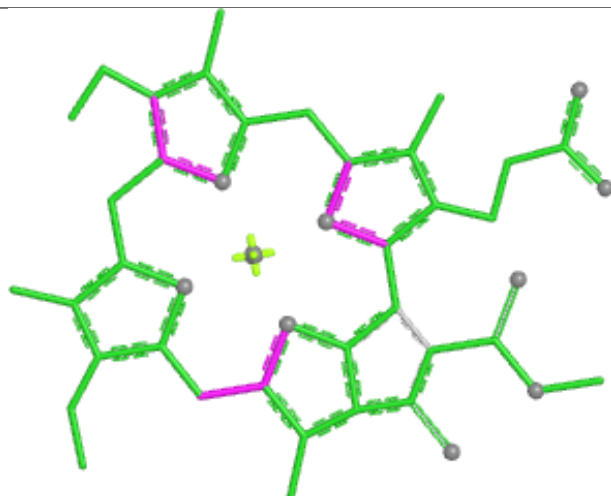




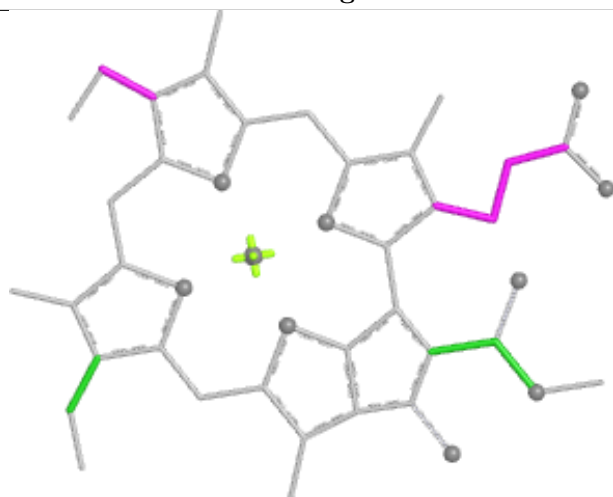
Ligand CLA B 1209



Bond lengths



Bond angles

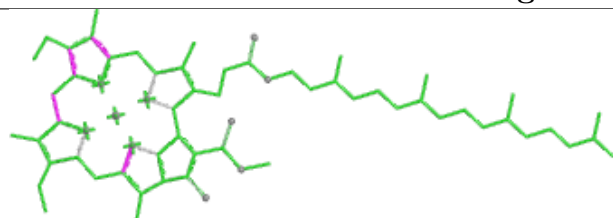


Torsions

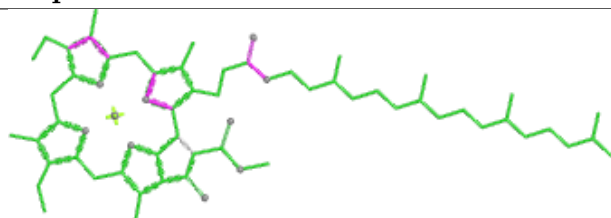


Rings

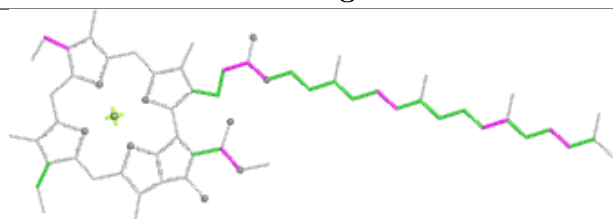
Ligand CLA p 510



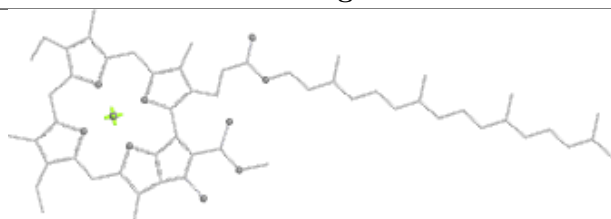
Bond lengths



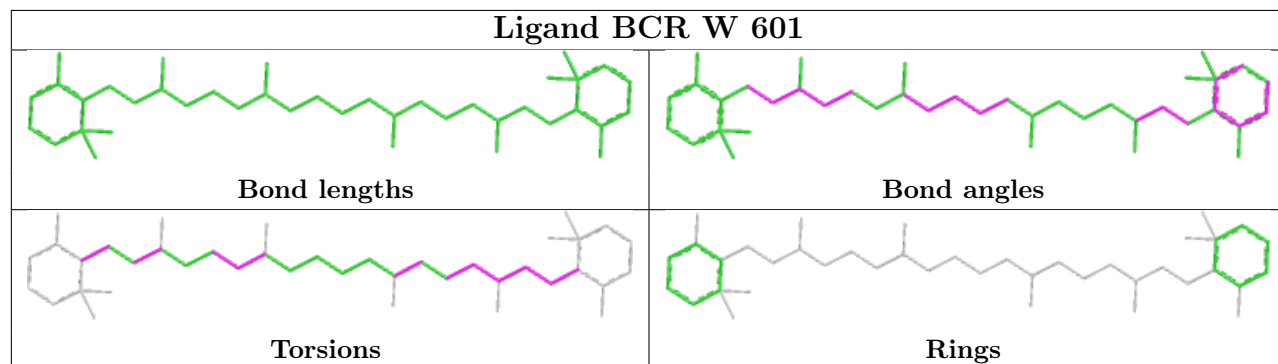
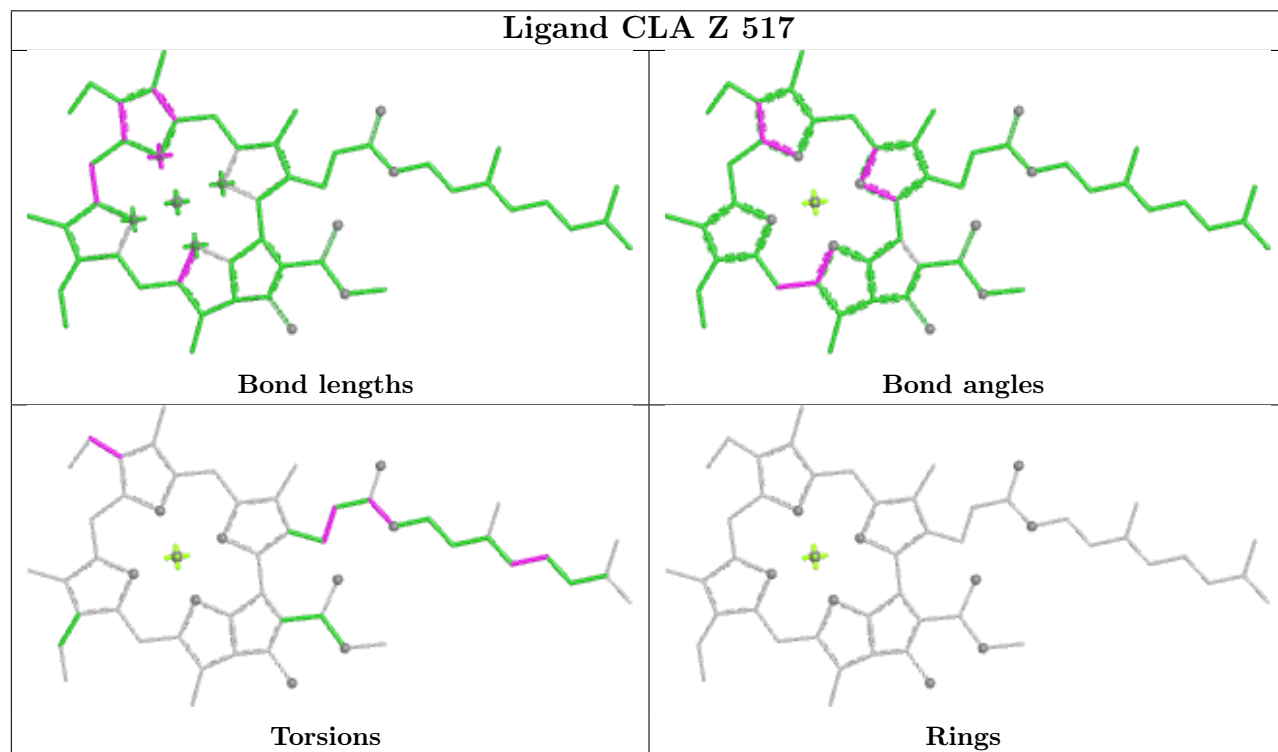
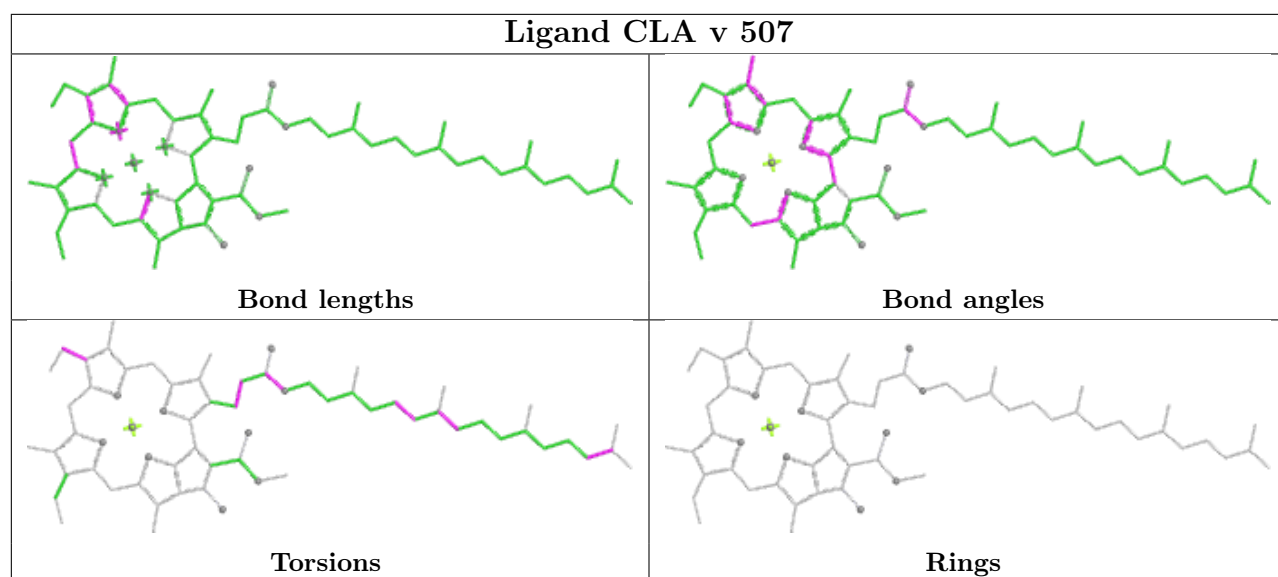
Bond angles

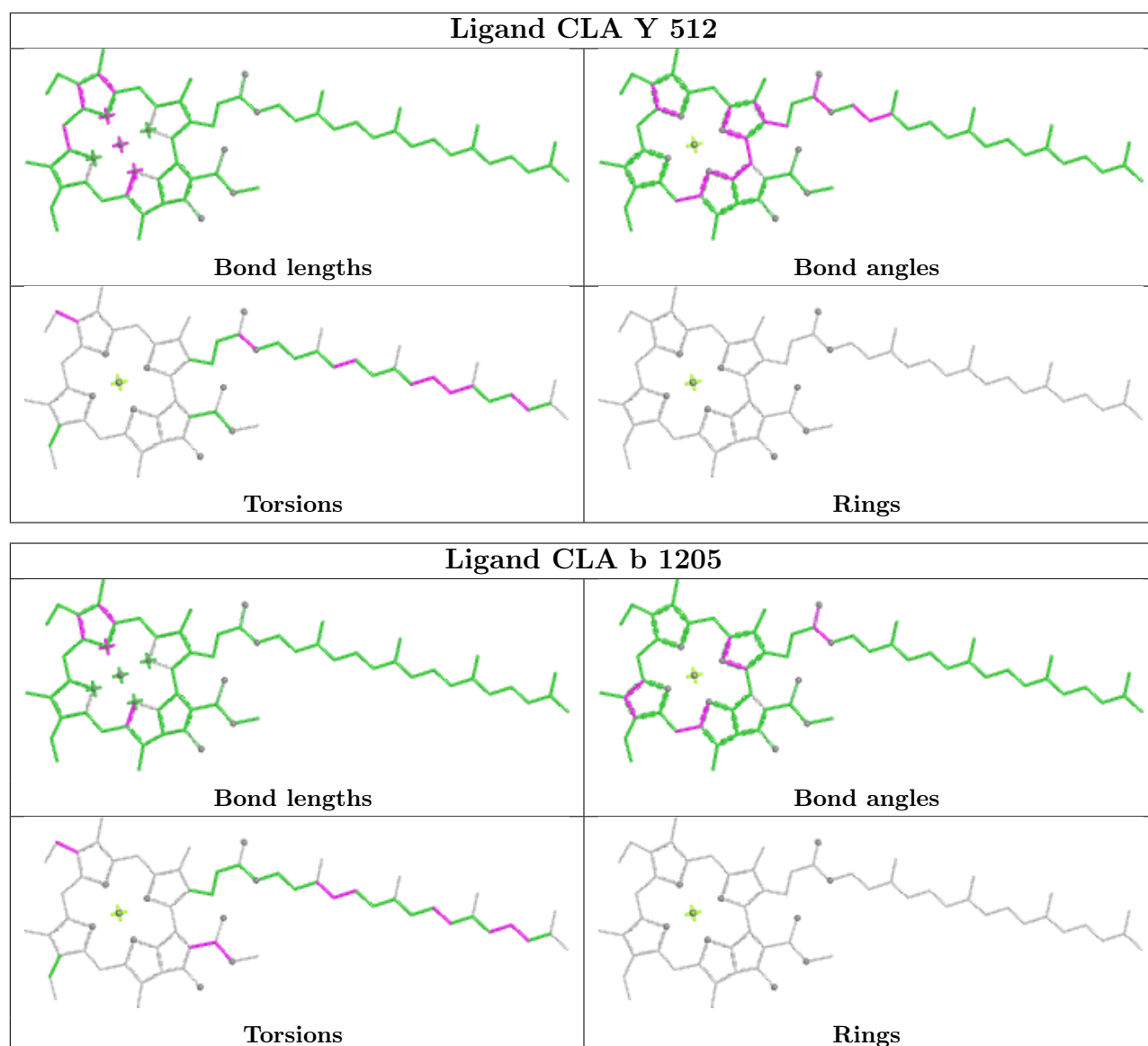


Torsions

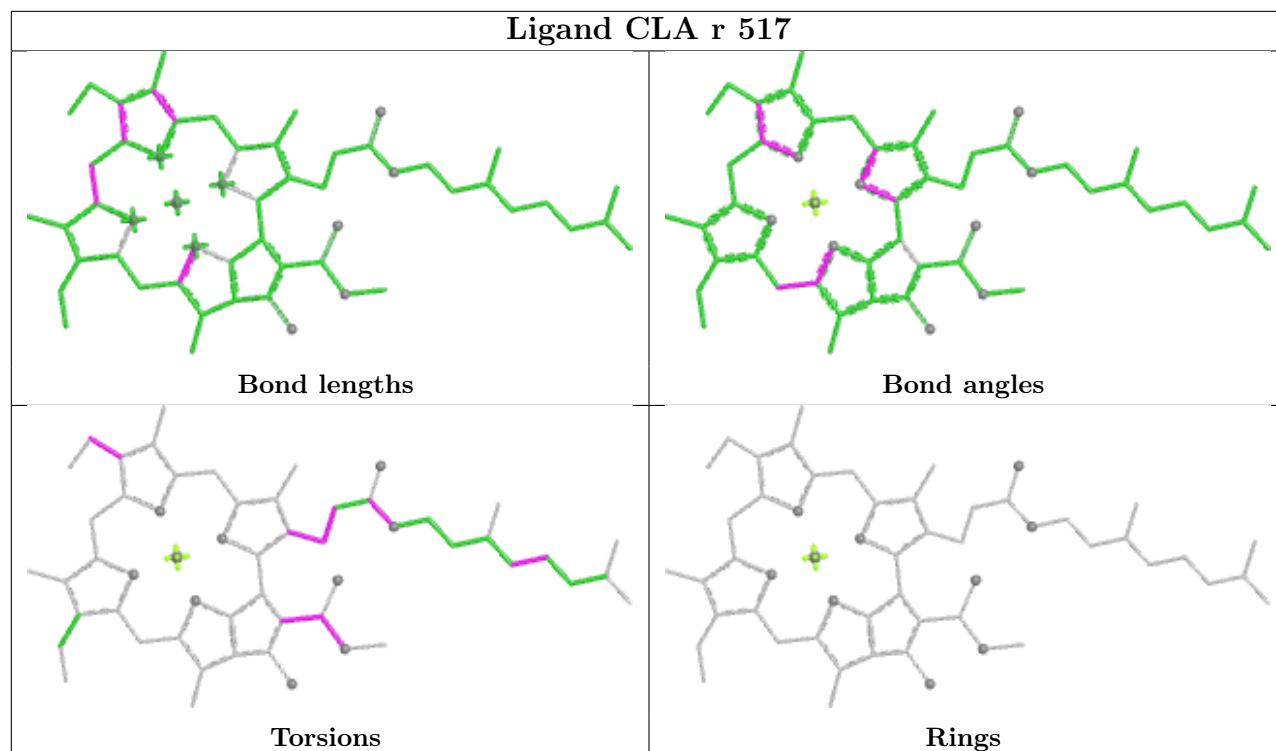


Rings

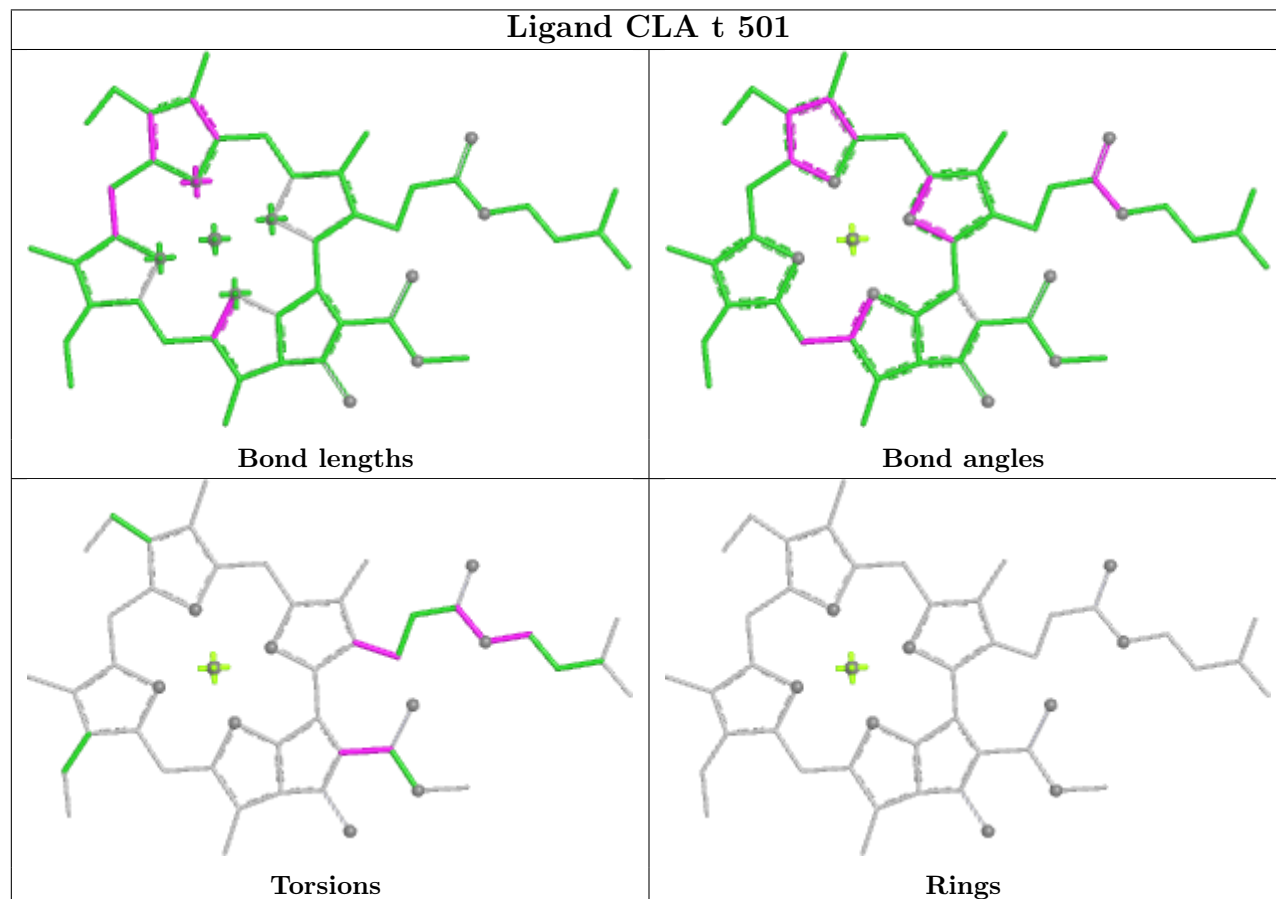




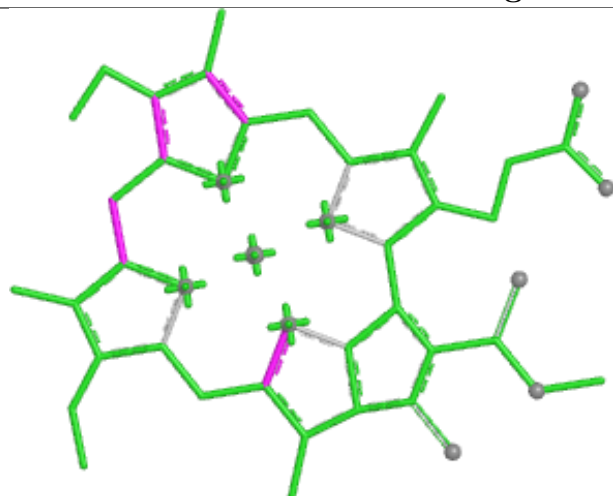
Ligand CLA r 517



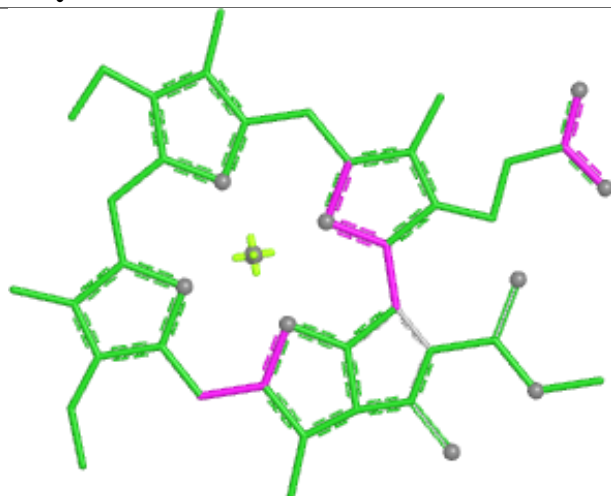
Ligand CLA t 501



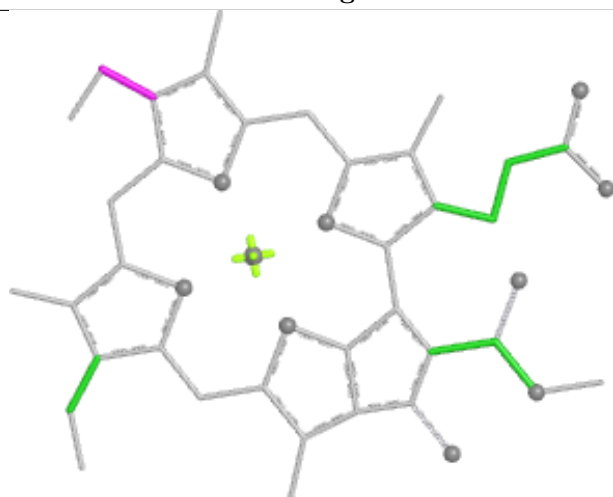
Ligand CLA Q 1301



Bond lengths



Bond angles

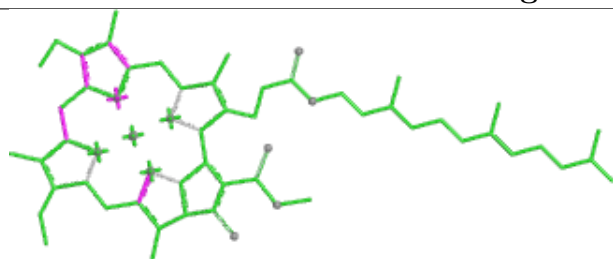


Torsions

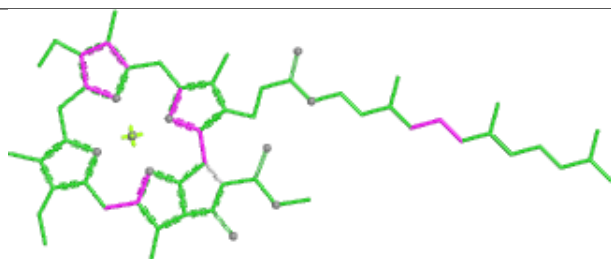


Rings

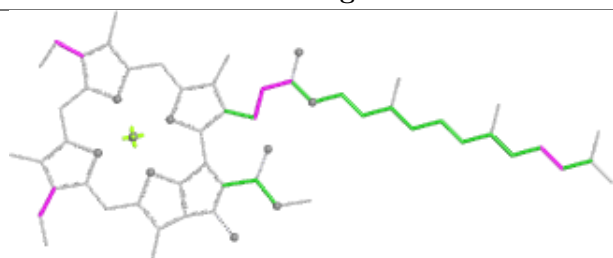
Ligand CLA t 509



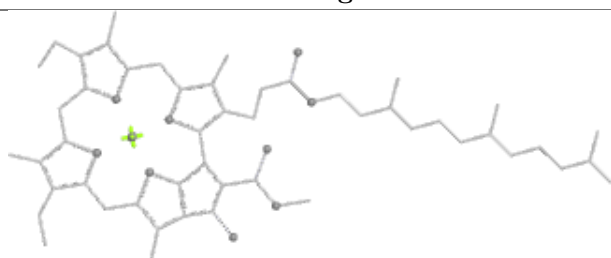
Bond lengths



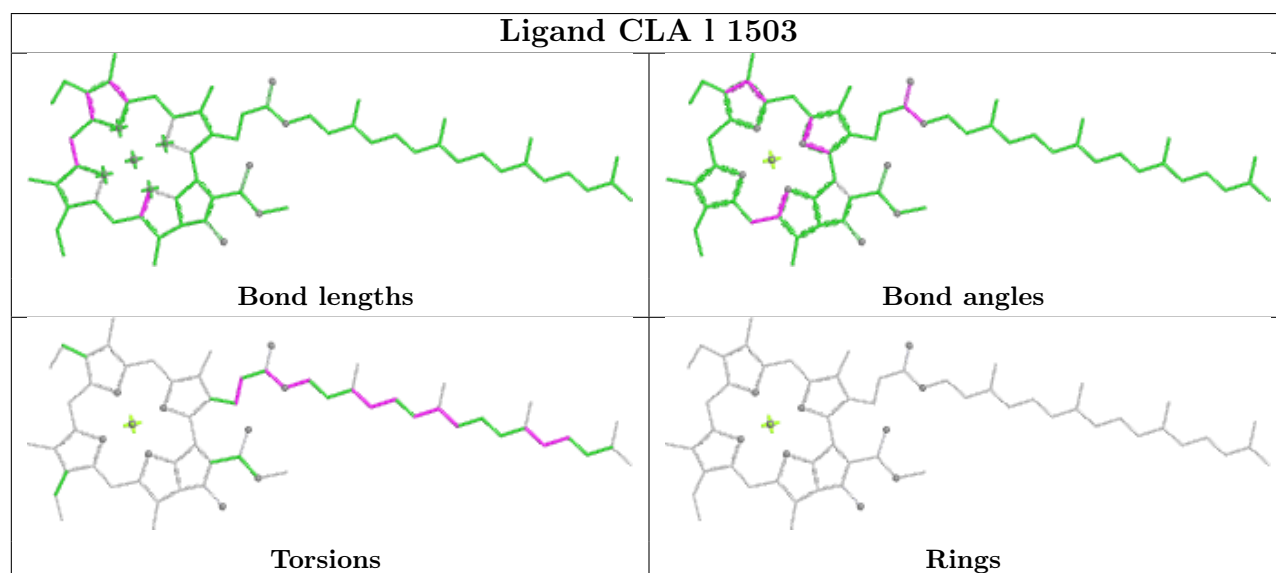
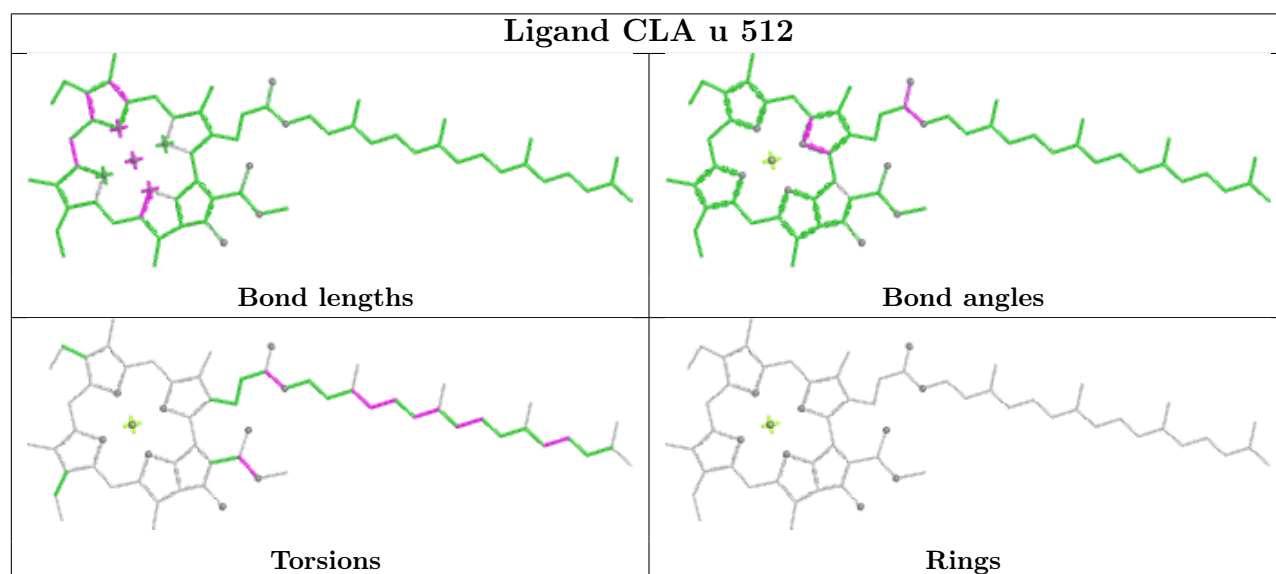
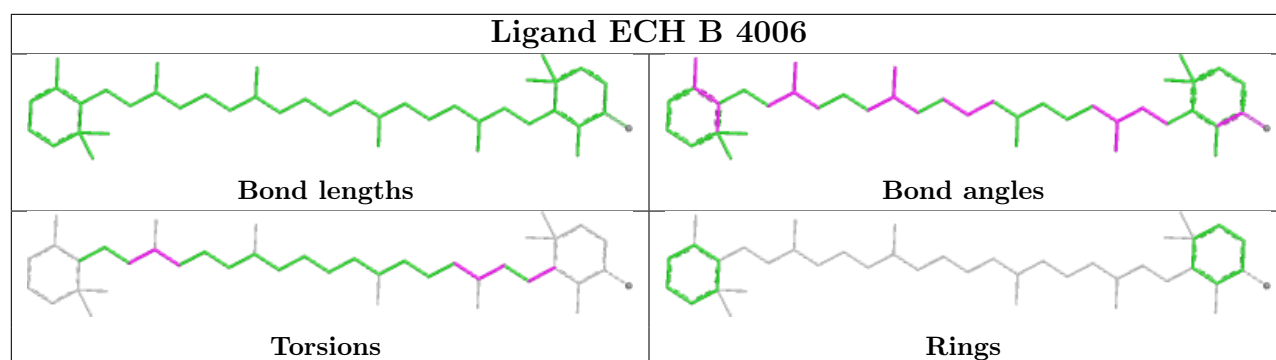
Bond angles



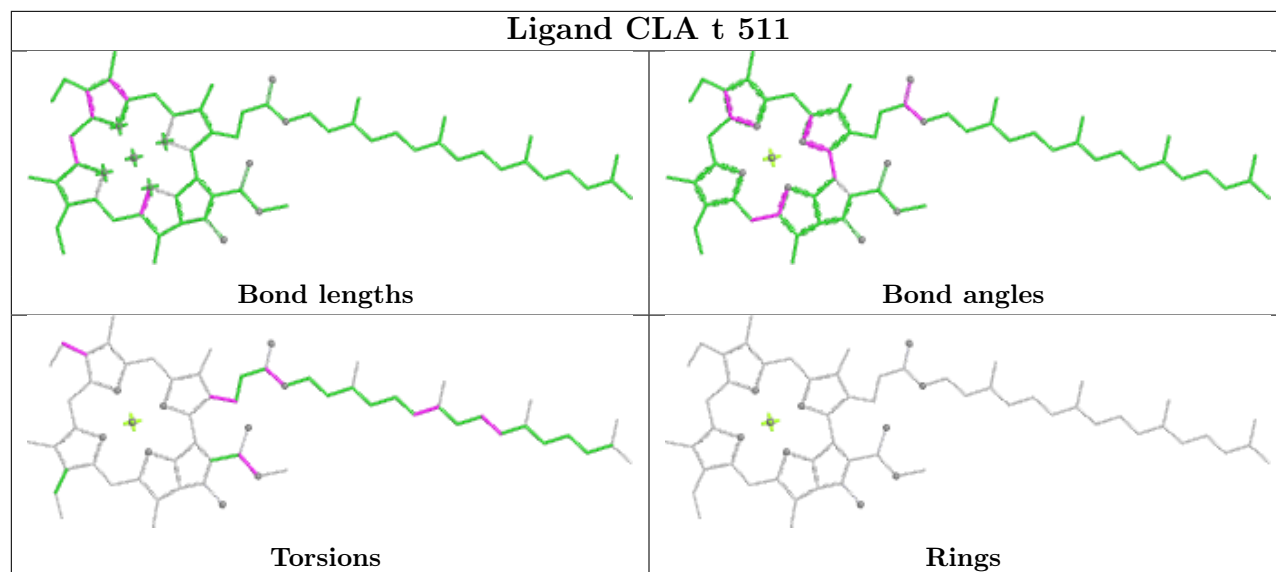
Torsions



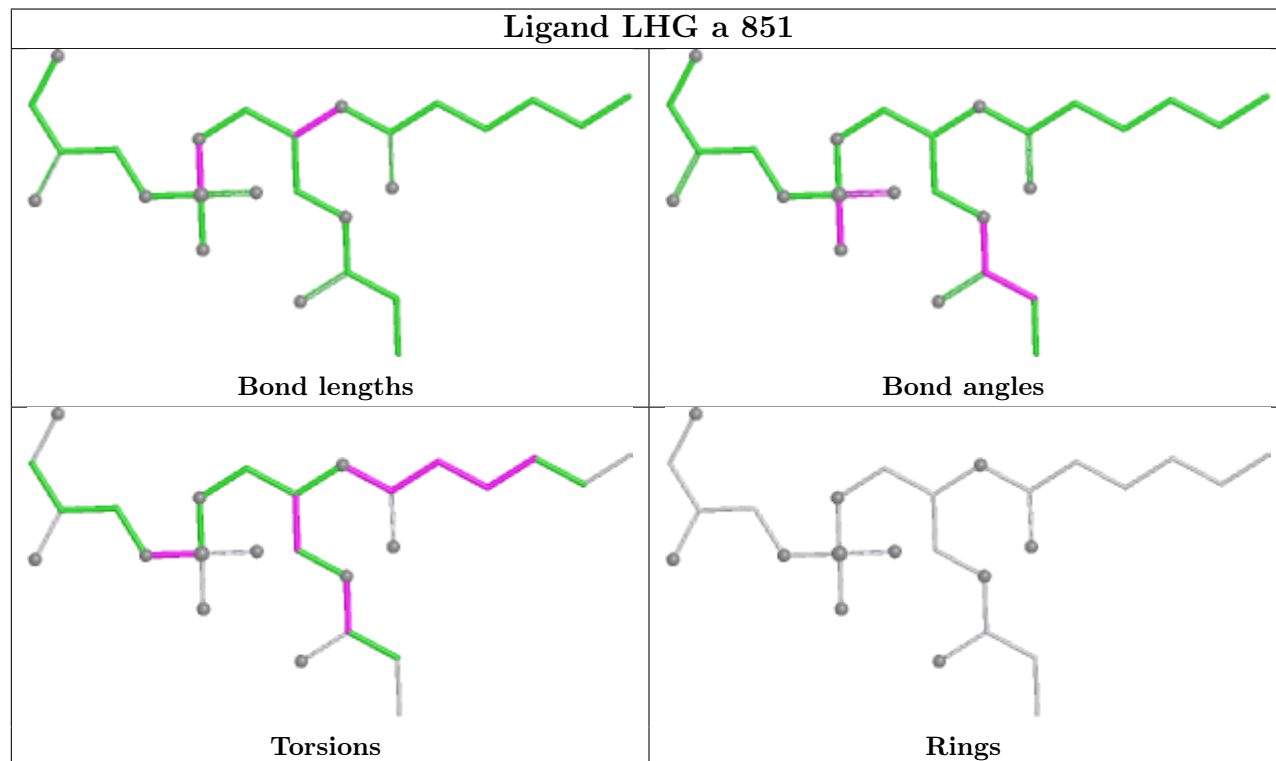
Rings



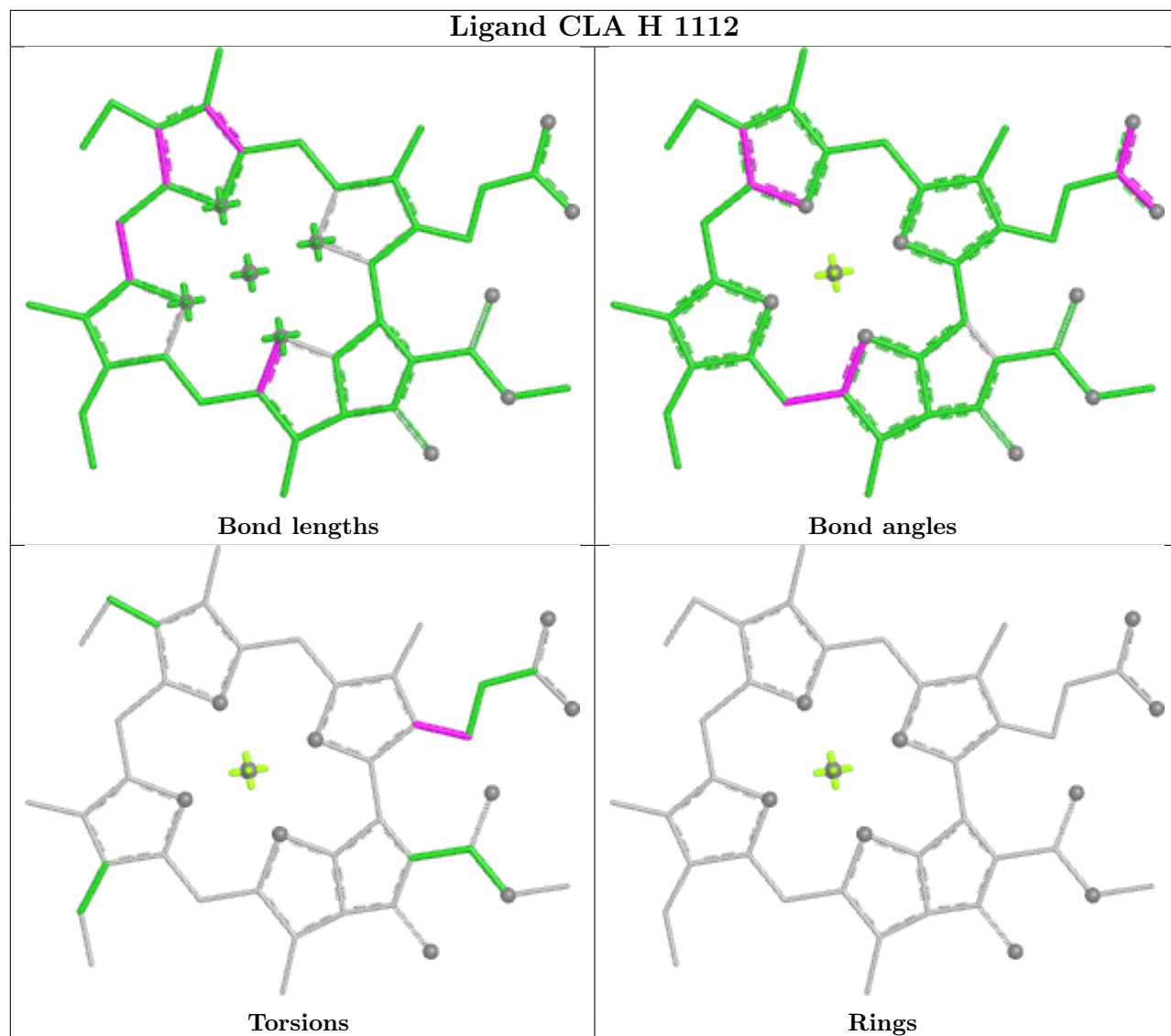
Ligand CLA t 511



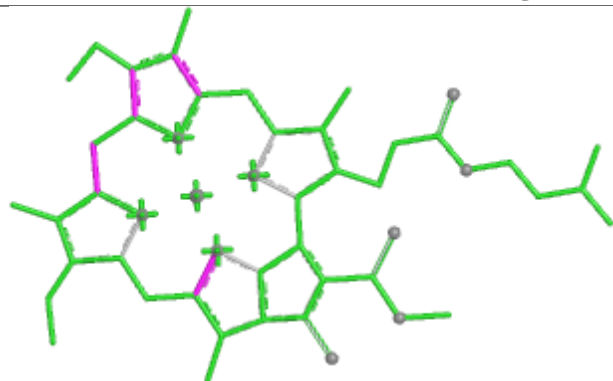
Ligand LHG a 851



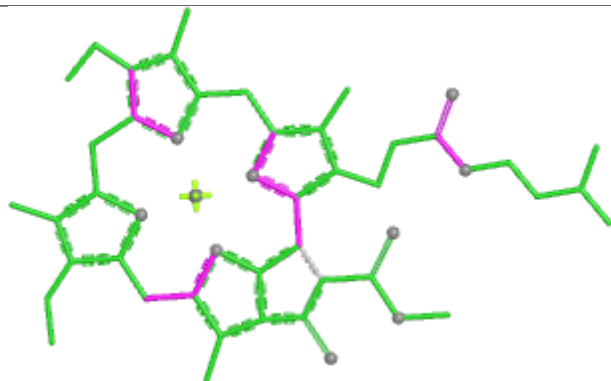
Ligand CLA H 1112



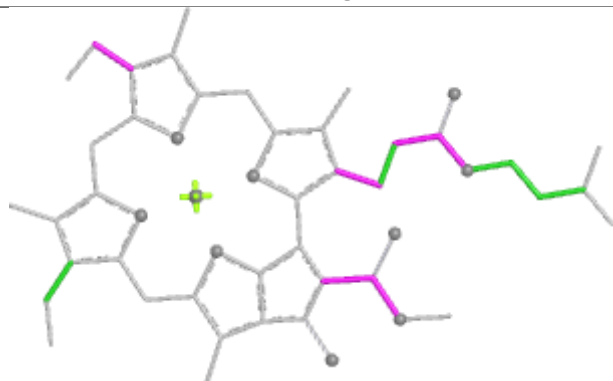
Ligand CLA Z 514



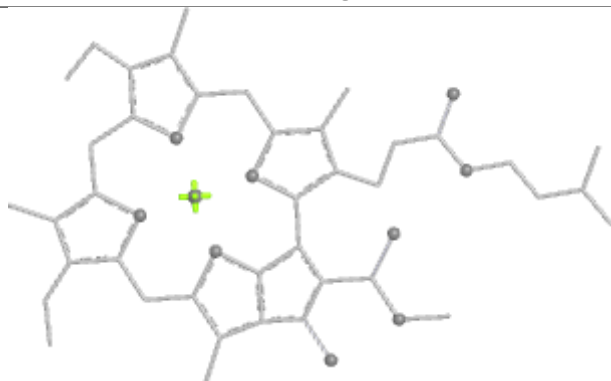
Bond lengths



Bond angles

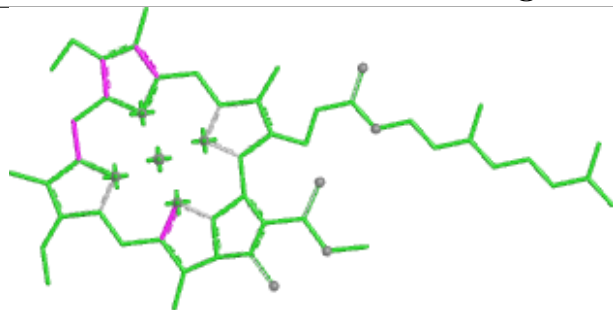


Torsions

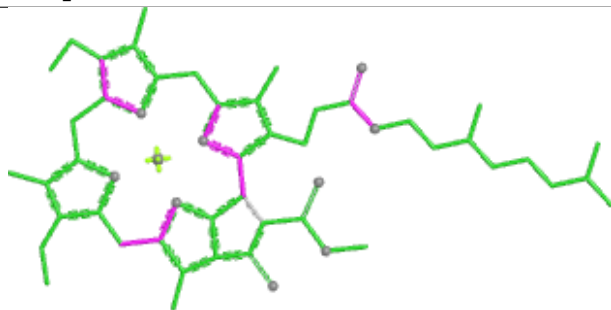


Rings

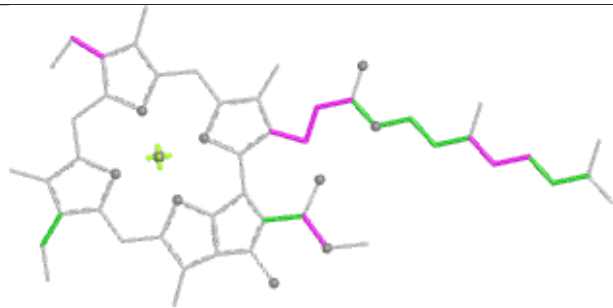
Ligand CLA q 508



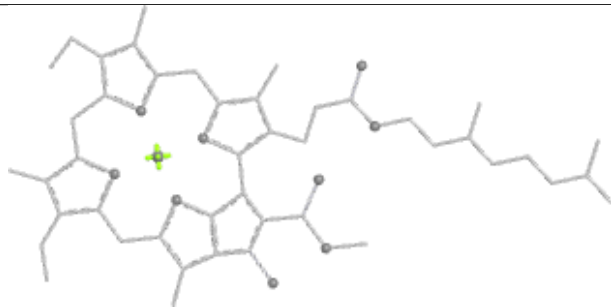
Bond lengths



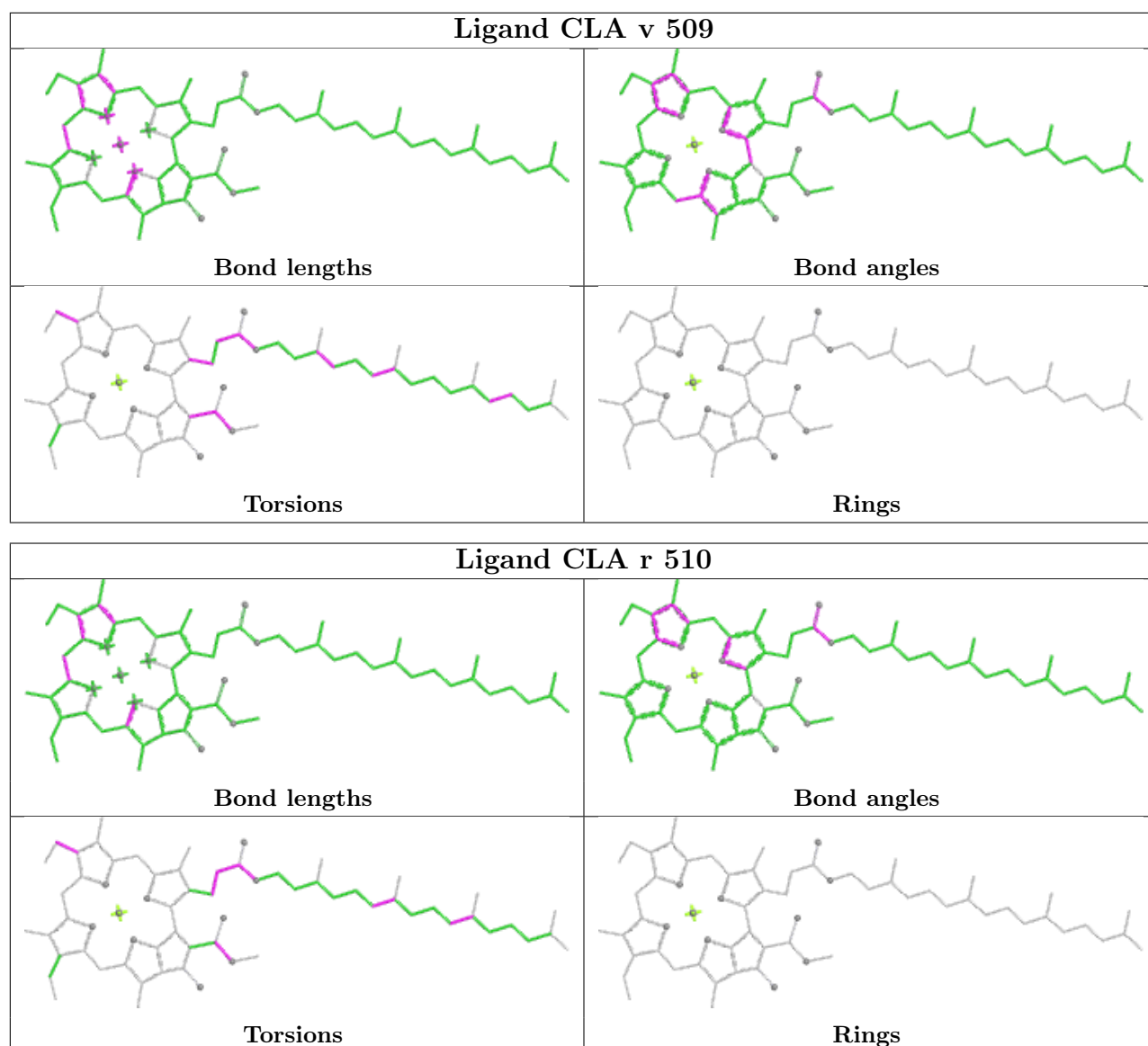
Bond angles

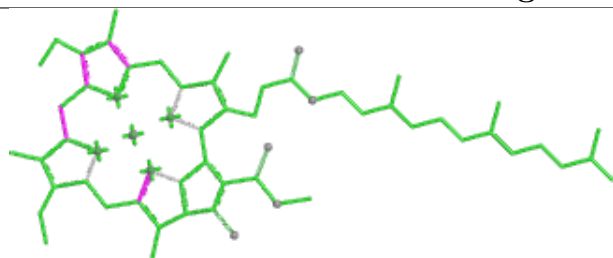
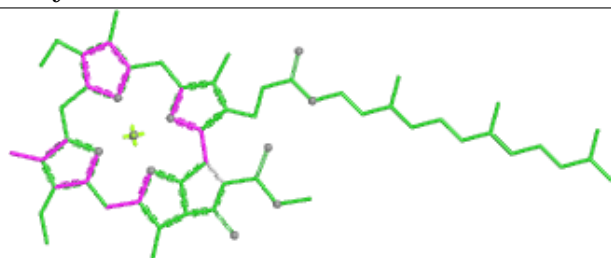
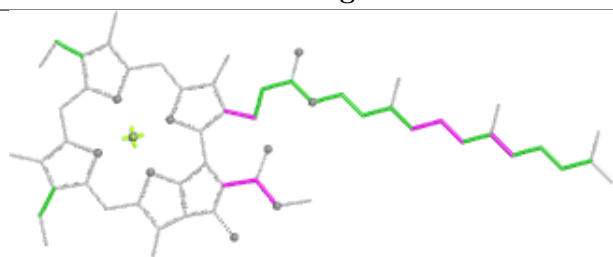
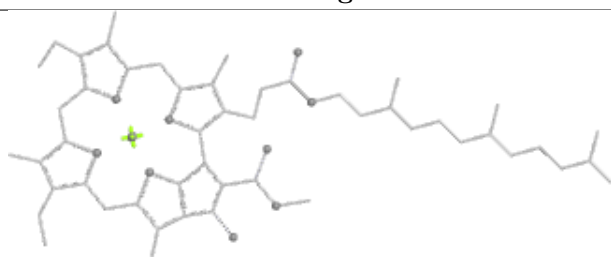
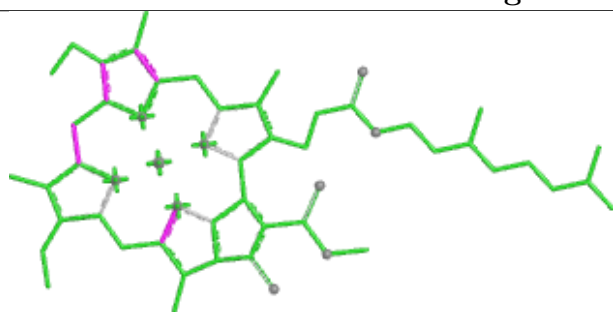
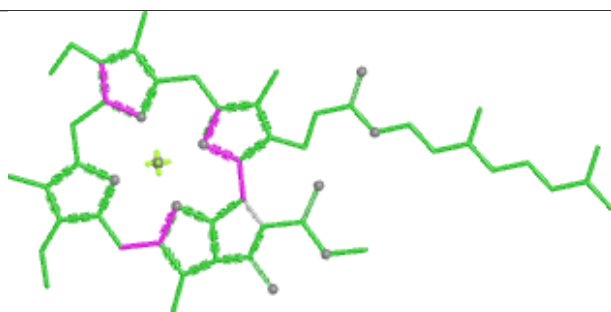
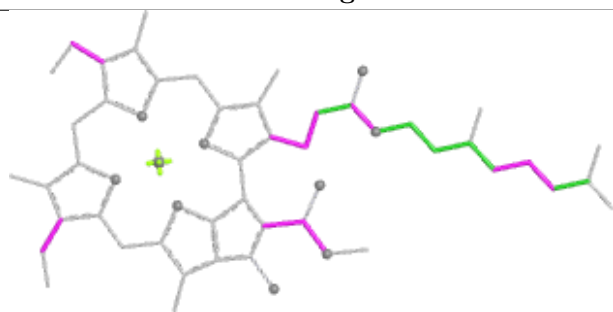
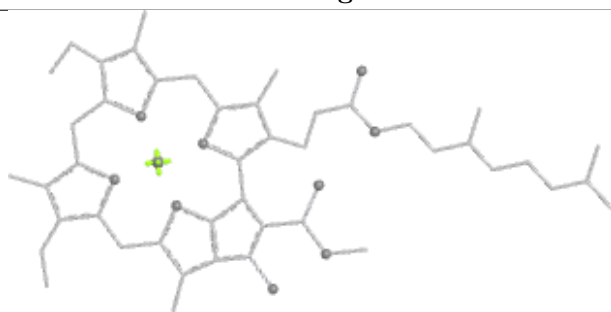


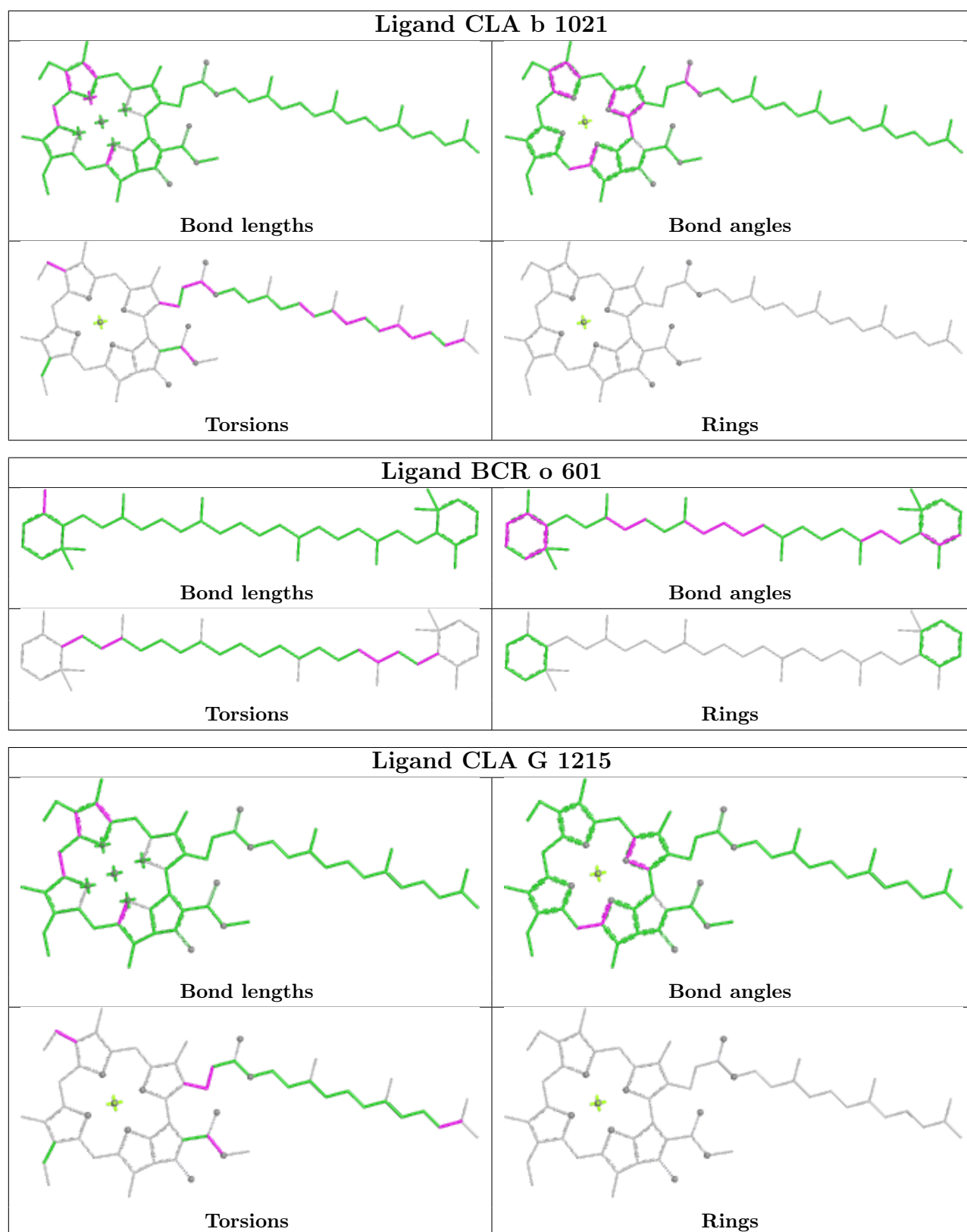
Torsions

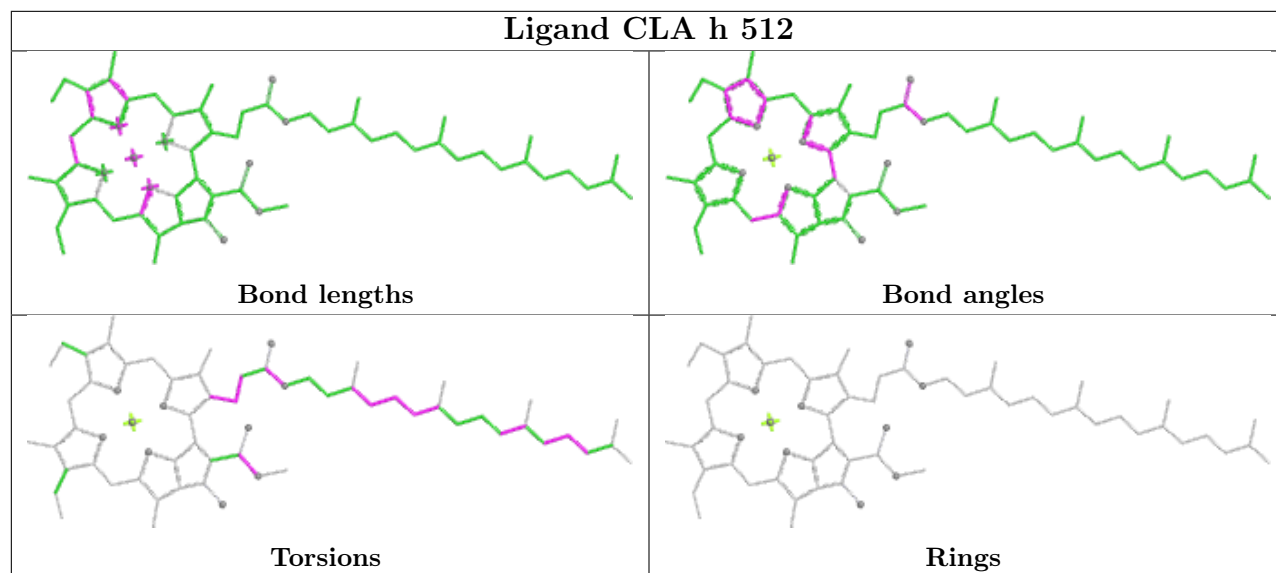
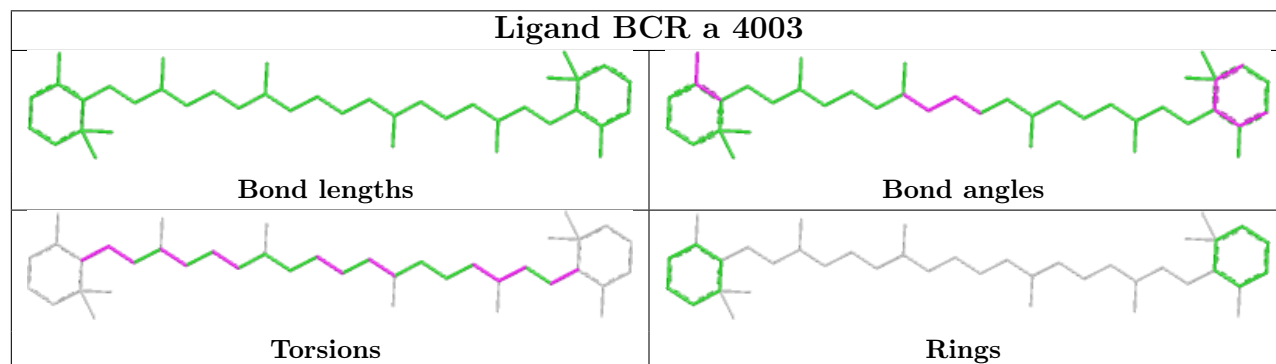
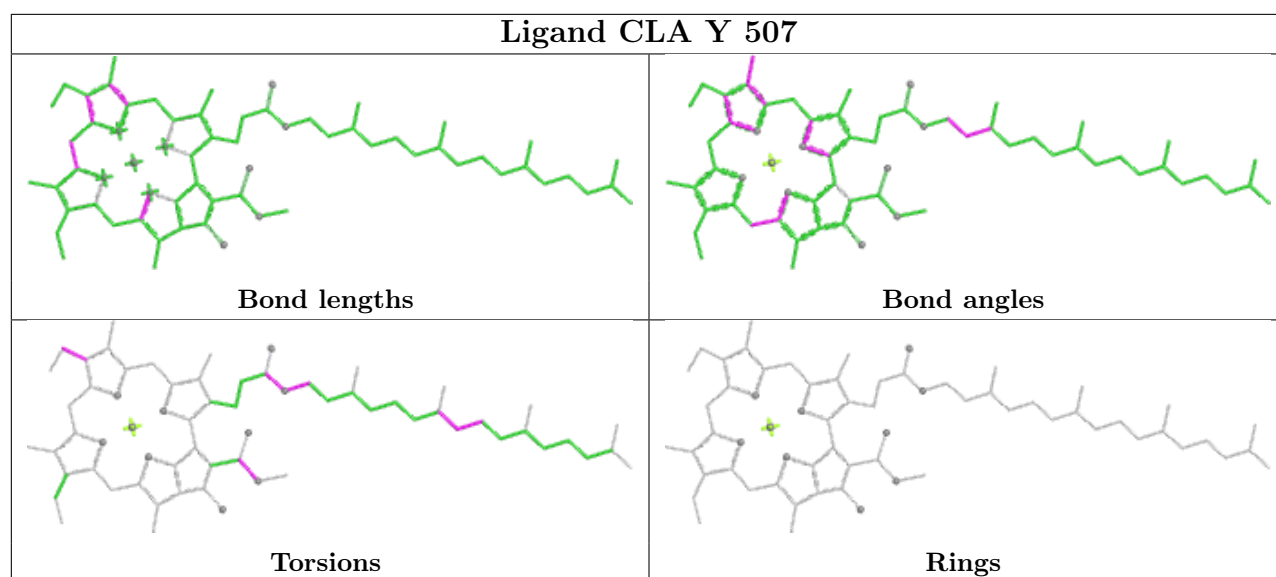


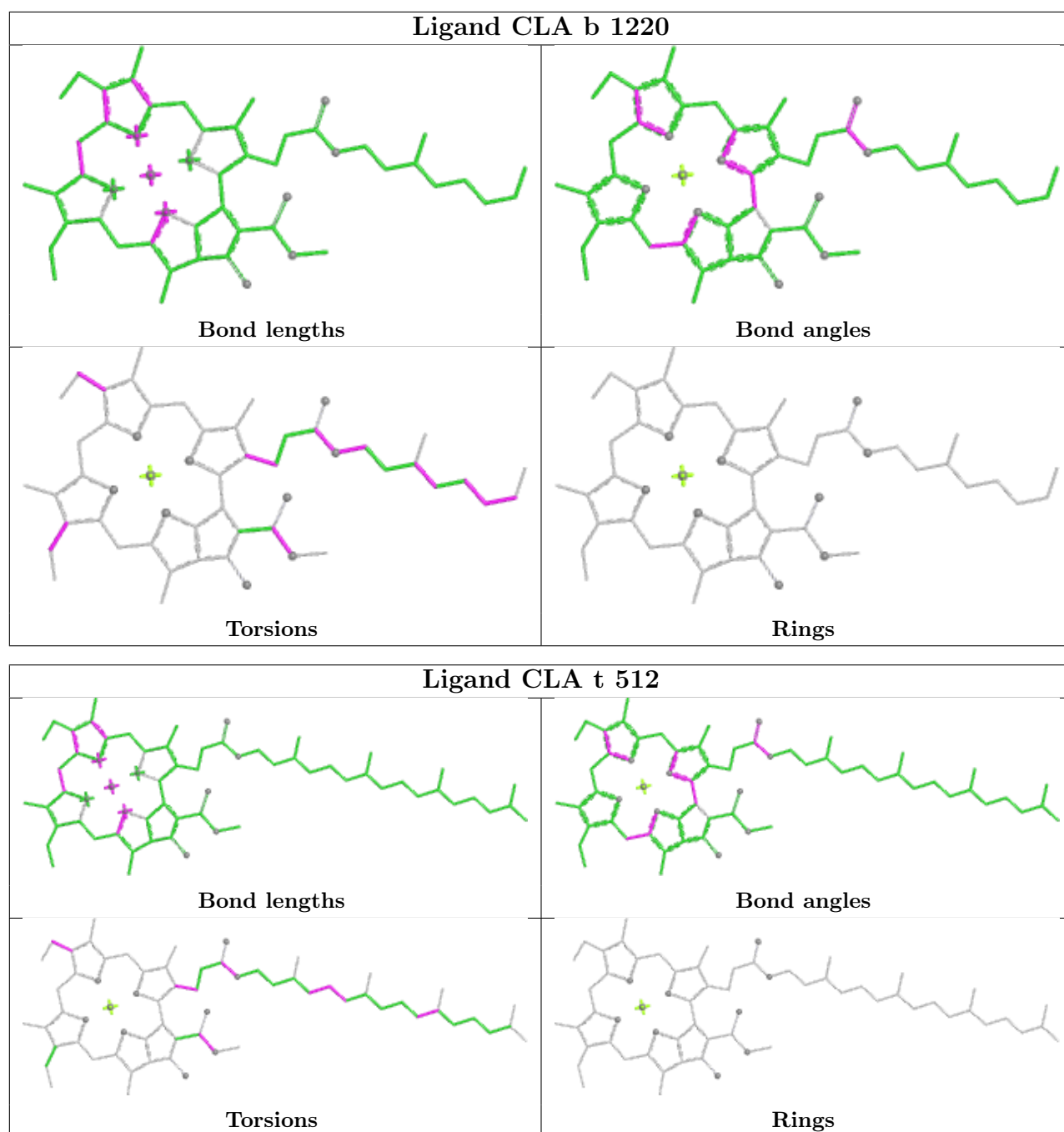
Rings

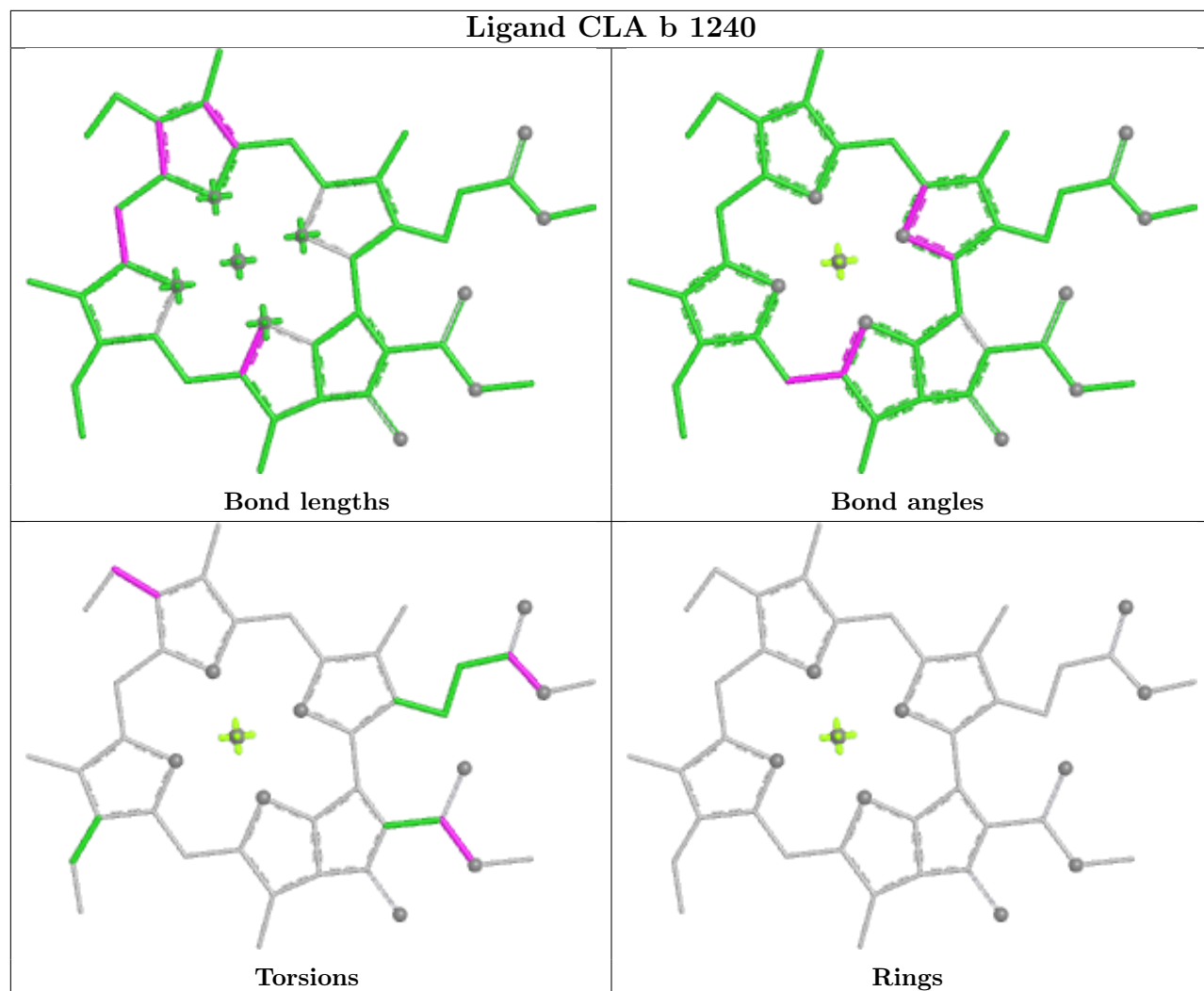


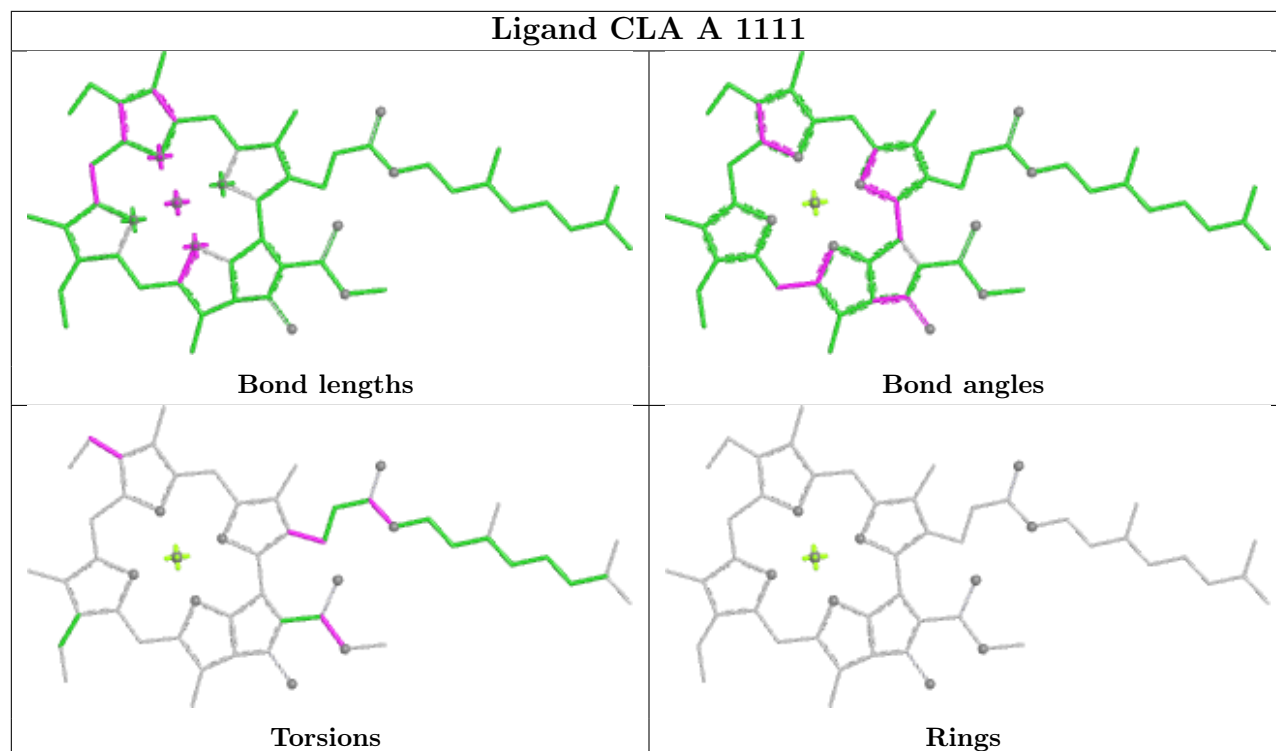
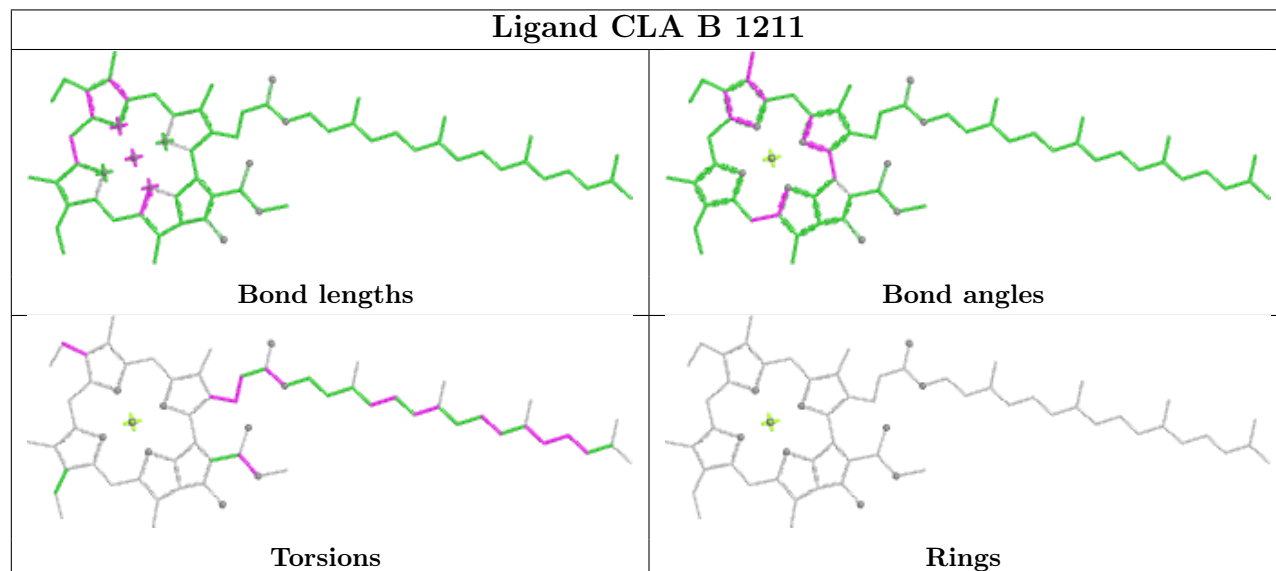
Ligand CLA y 506**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA G 1218****Bond lengths****Bond angles****Torsions****Rings**

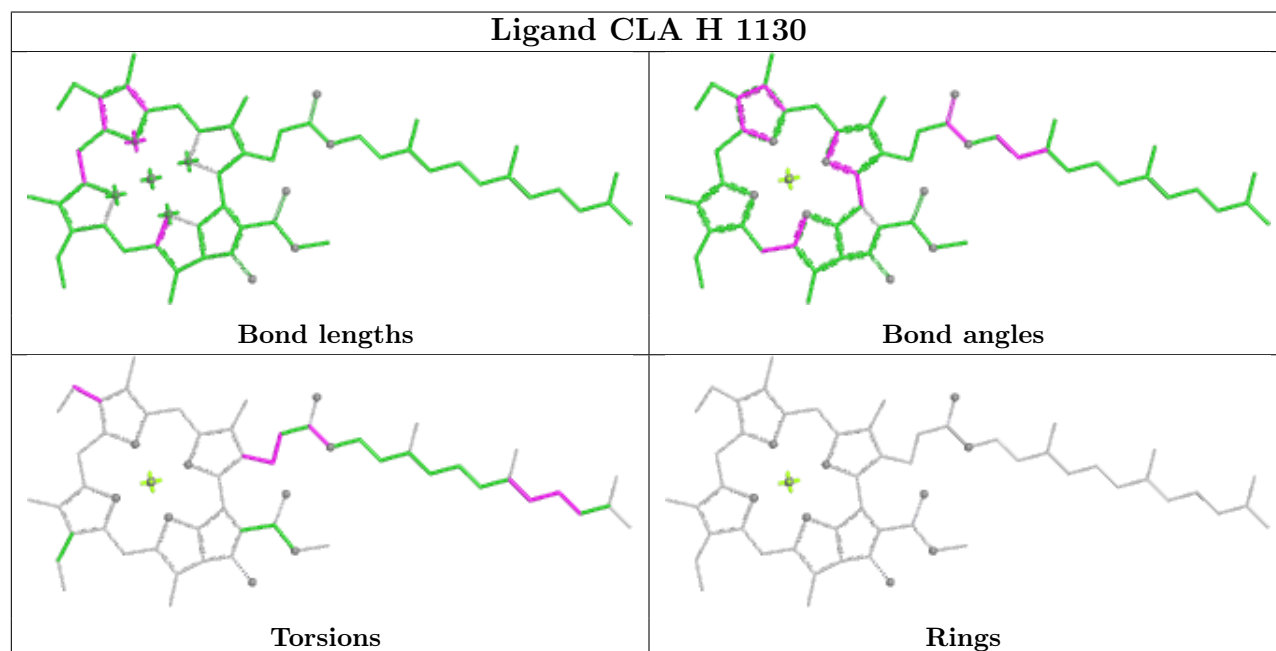
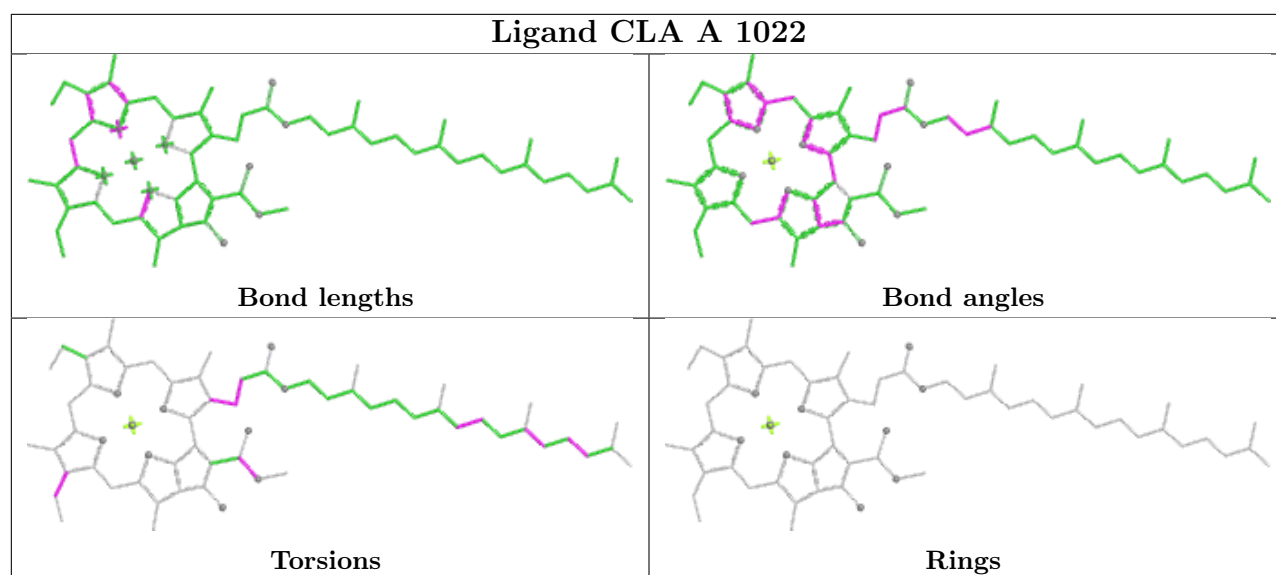




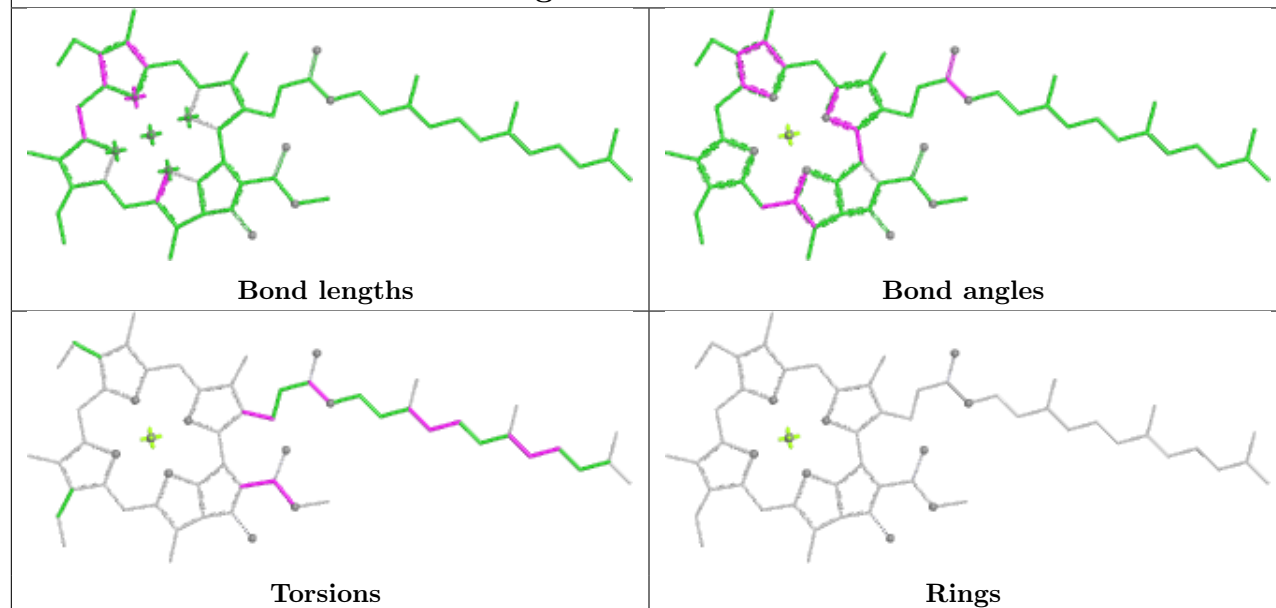




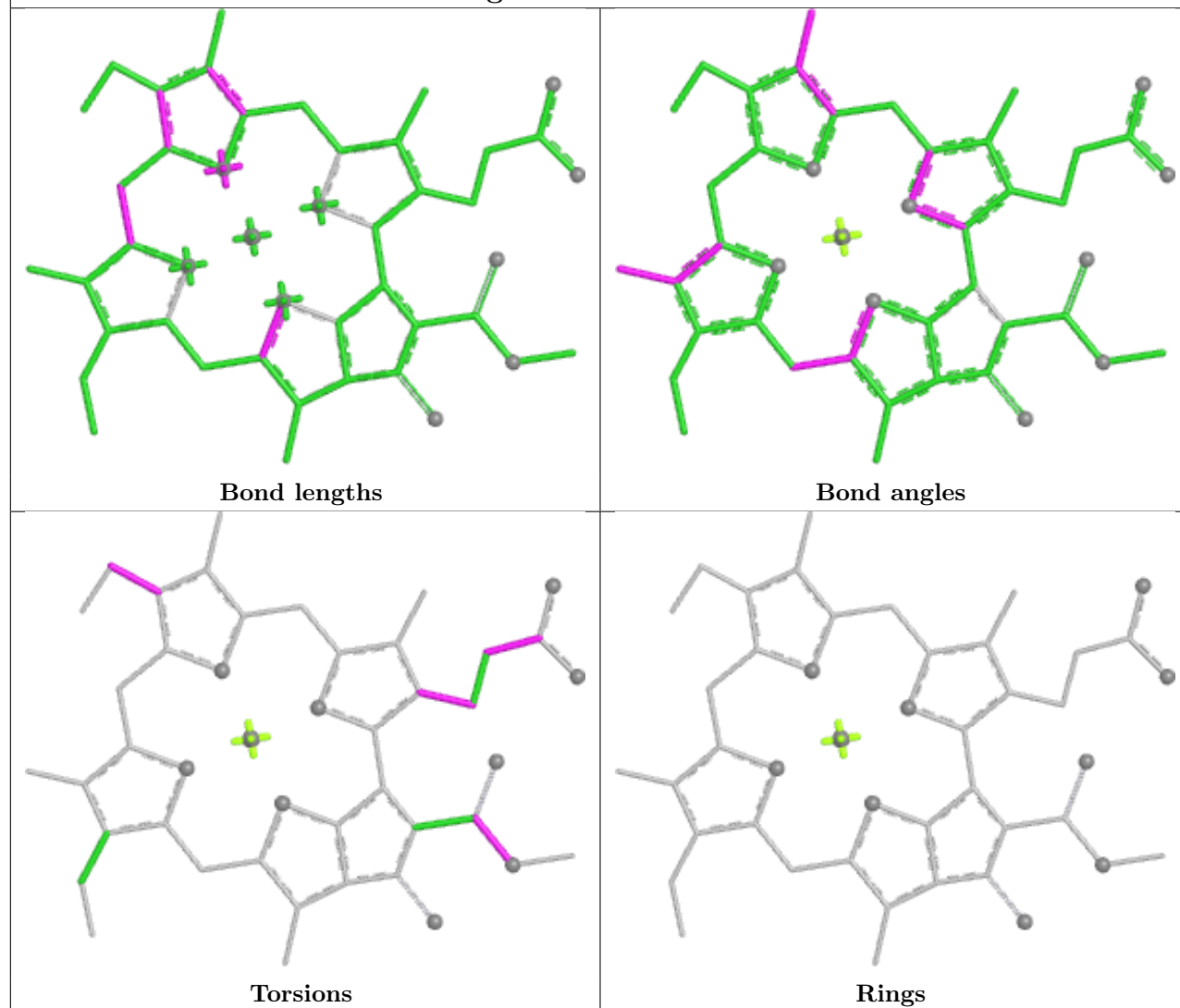
Ligand CLA A 1111**Ligand CLA B 1211**

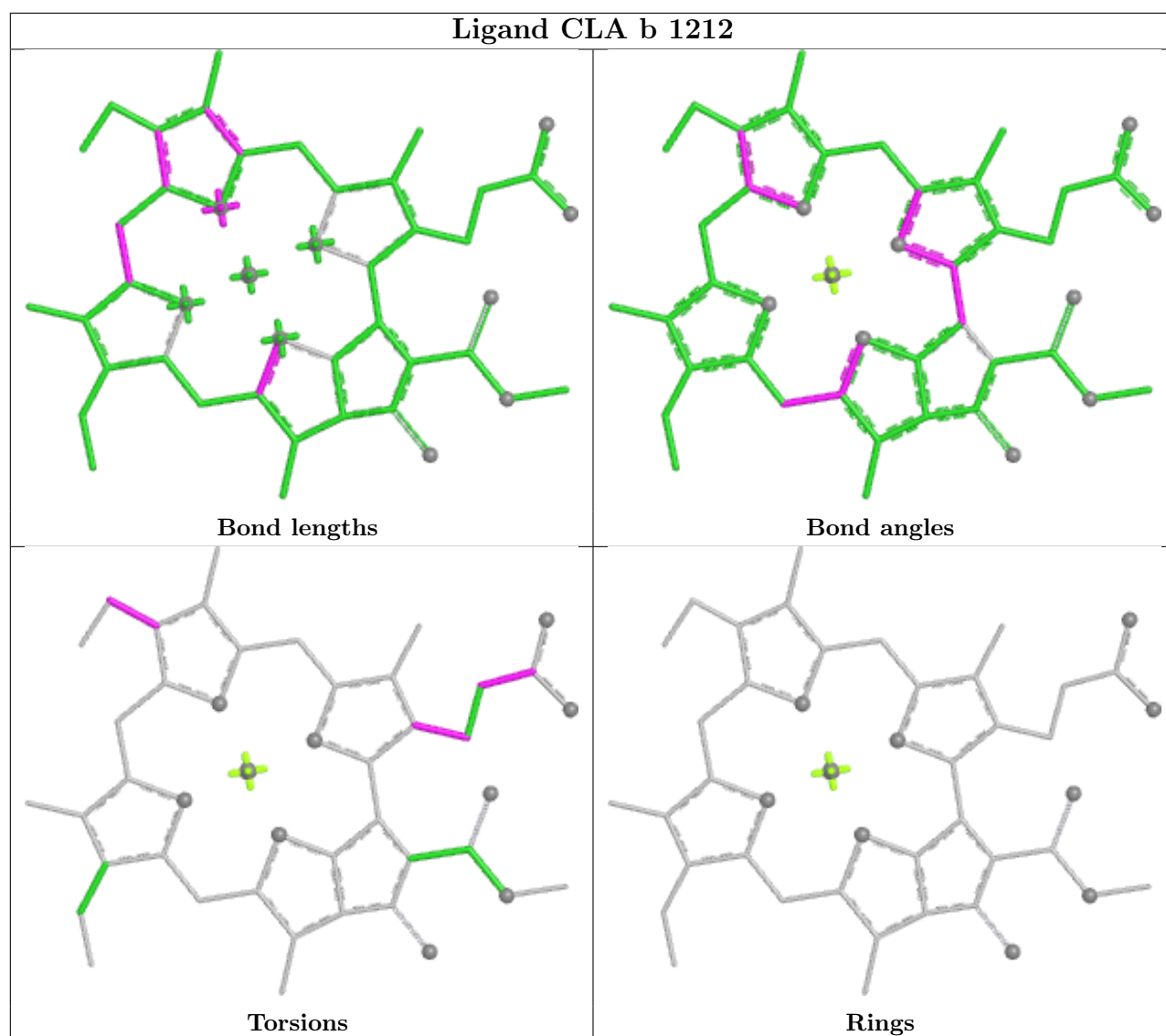


Ligand CLA h 504

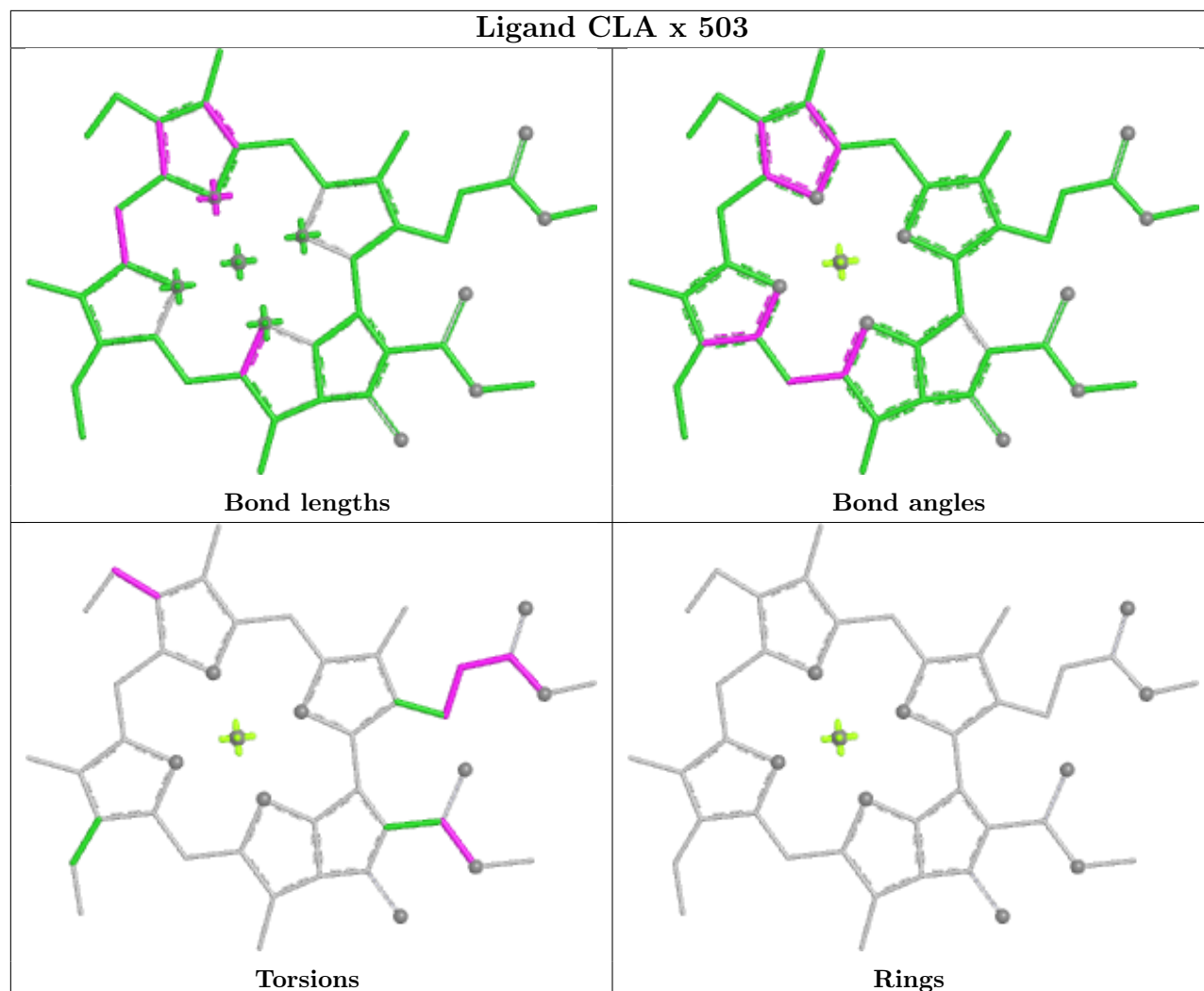


Ligand CLA b 1230

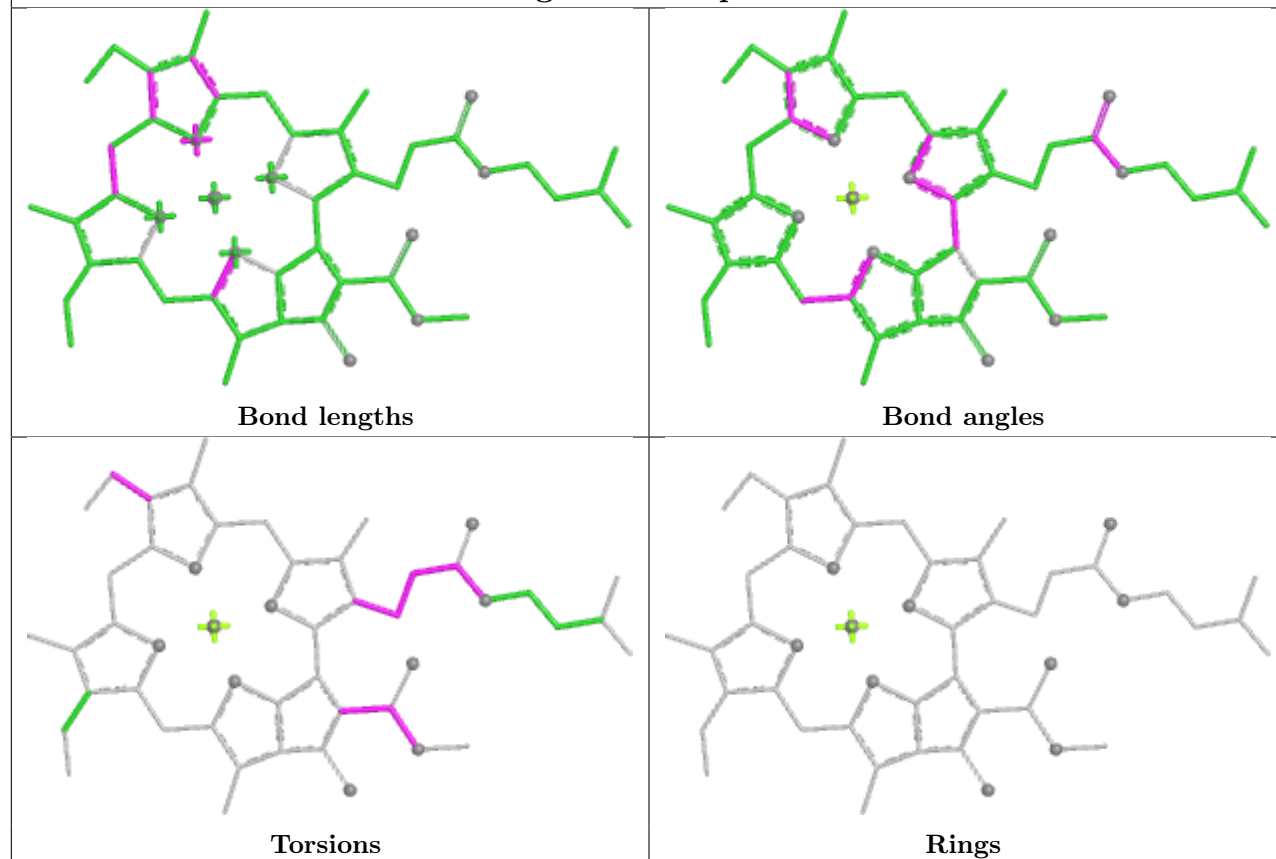




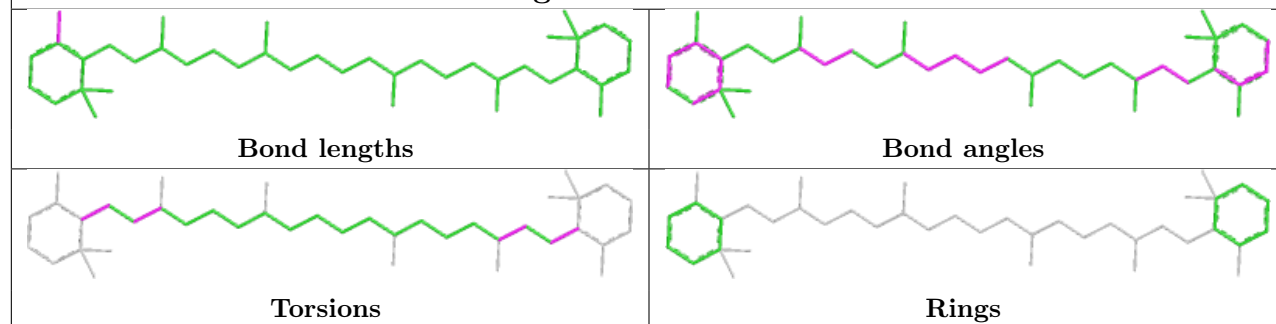
Ligand CLA x 503

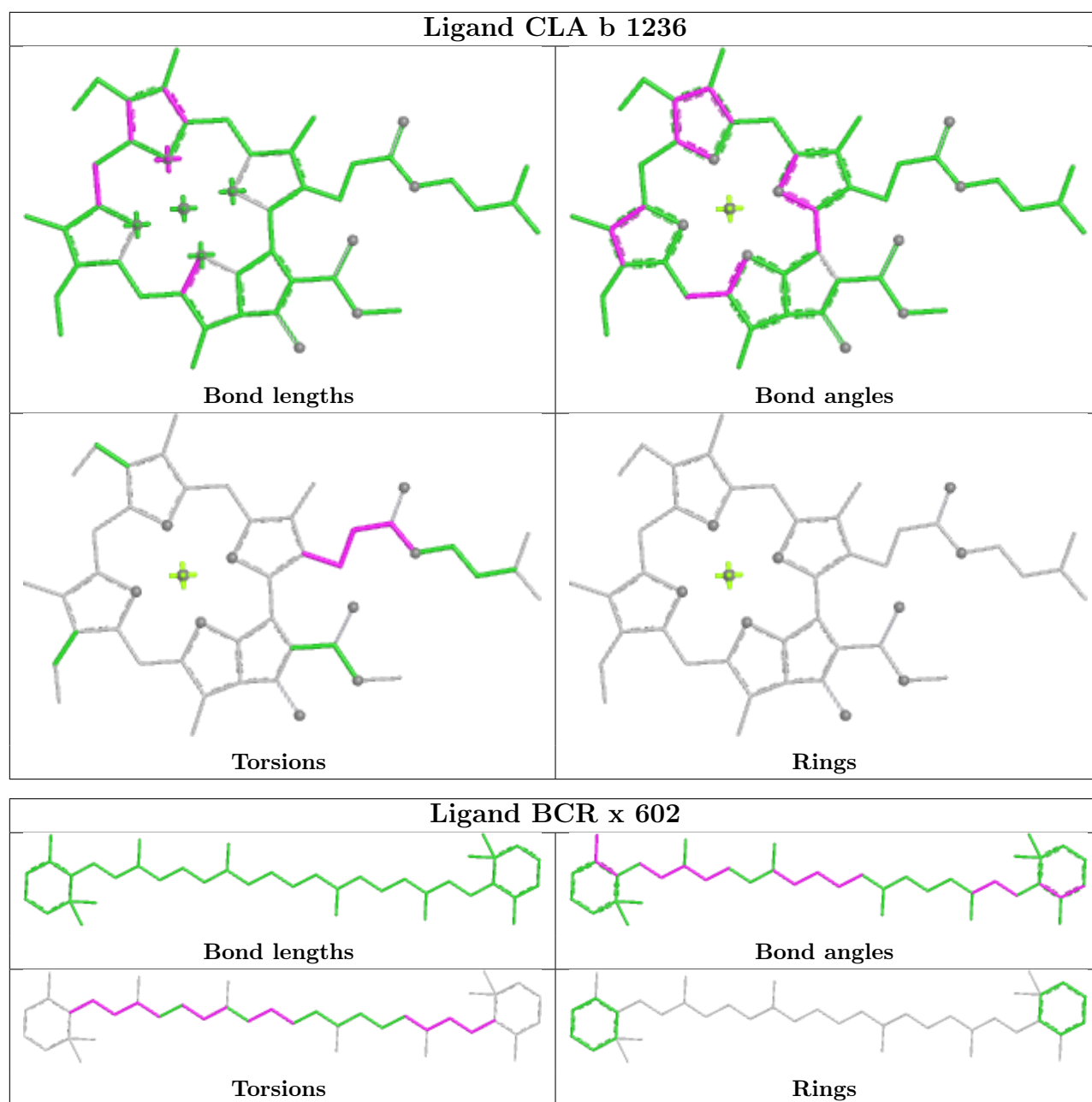


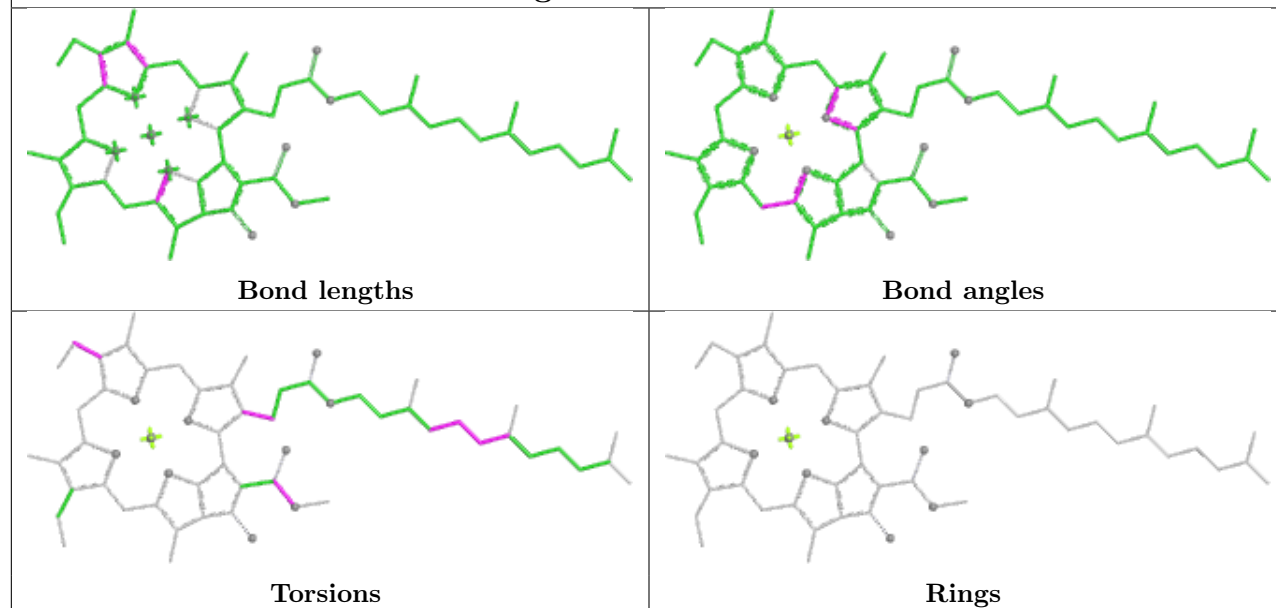
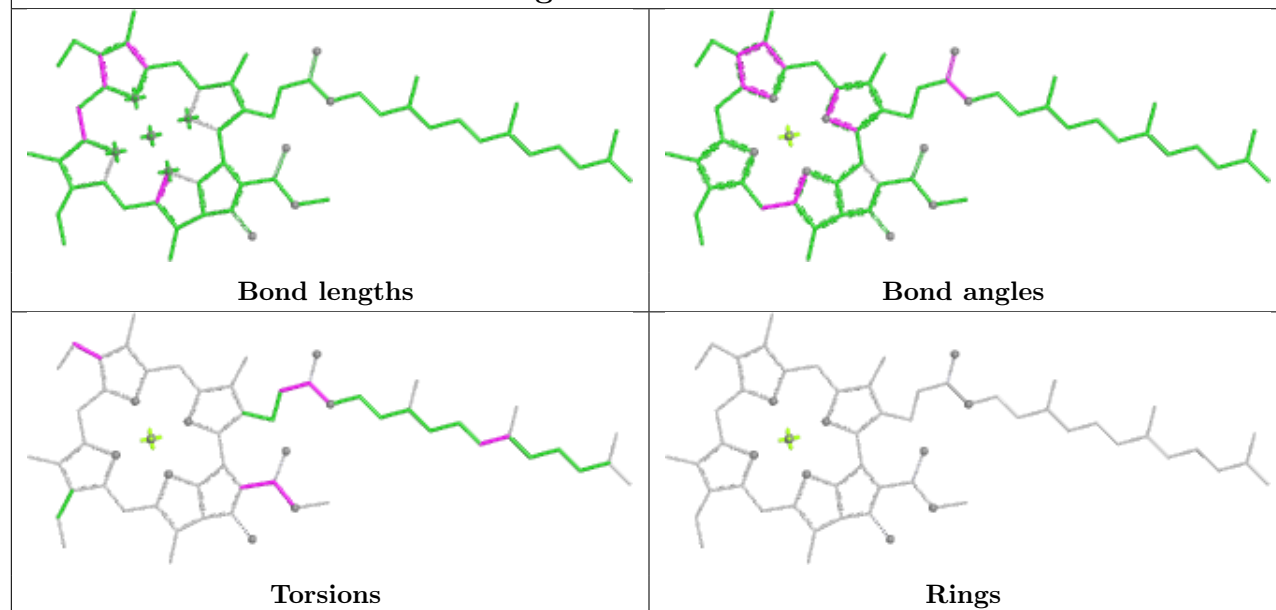
Ligand CLA q 514



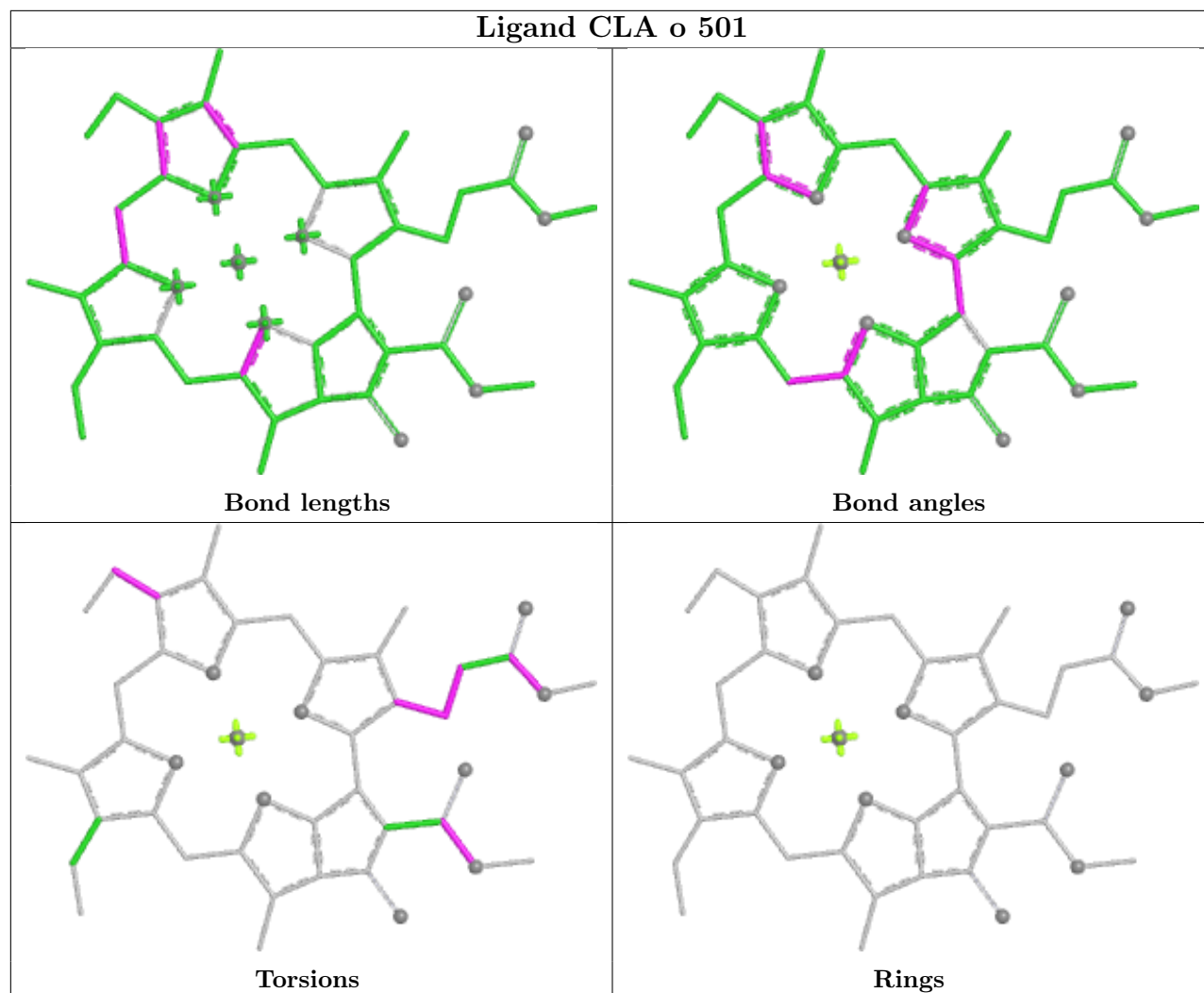
Ligand BCR u 601



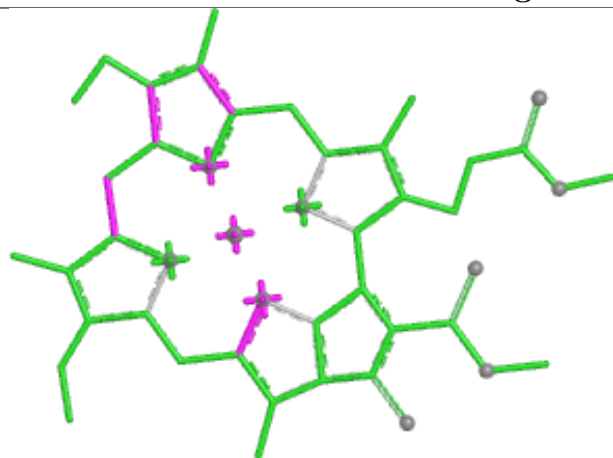


Ligand CLA Z 506**Ligand CLA u 510**

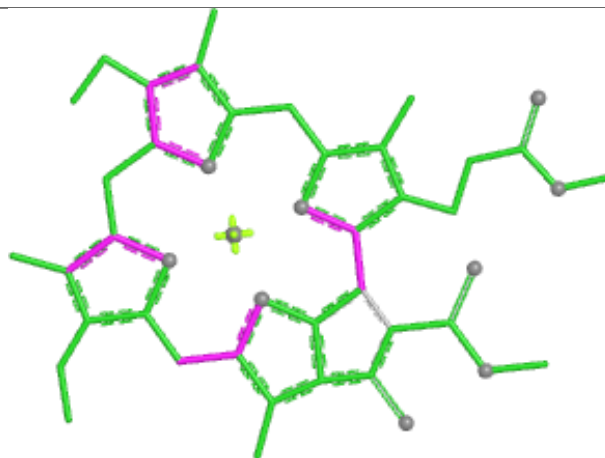
Ligand CLA o 501



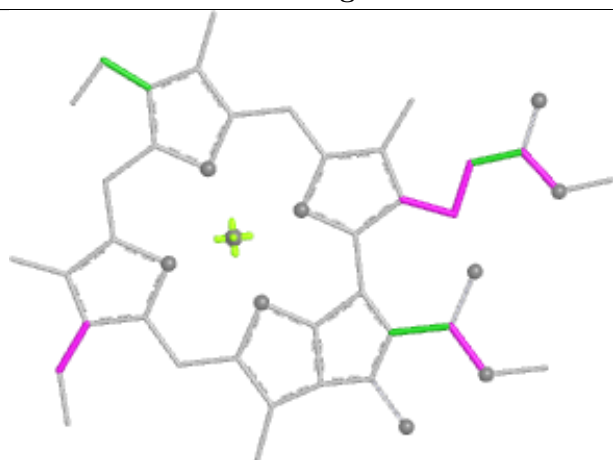
Ligand CLA w 503



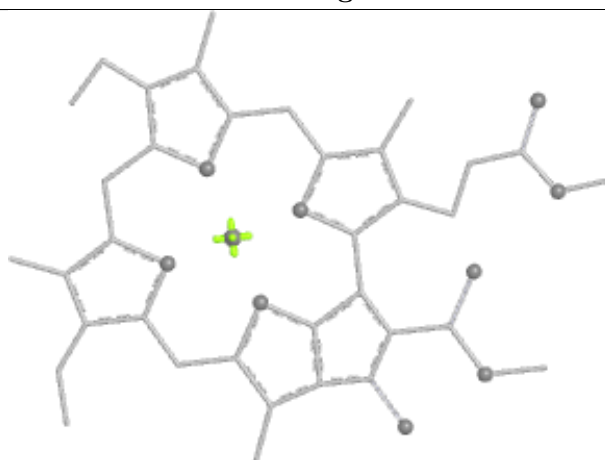
Bond lengths



Bond angles

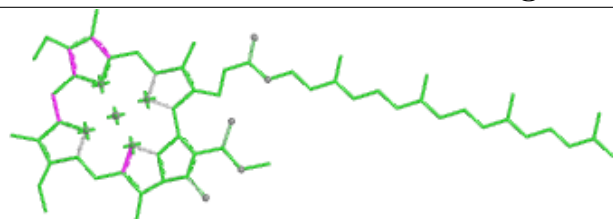


Torsions

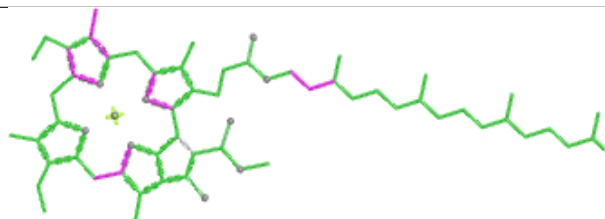


Rings

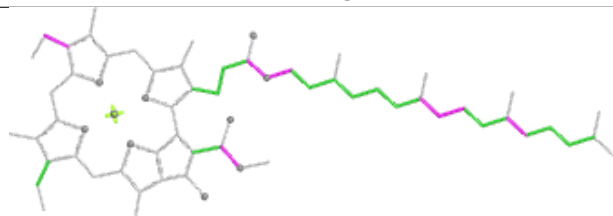
Ligand CLA s 507



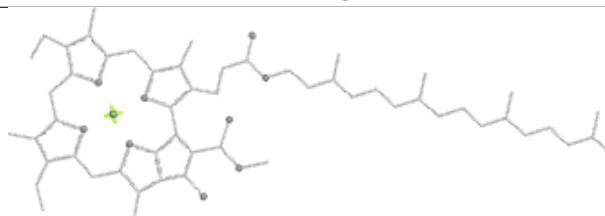
Bond lengths



Bond angles

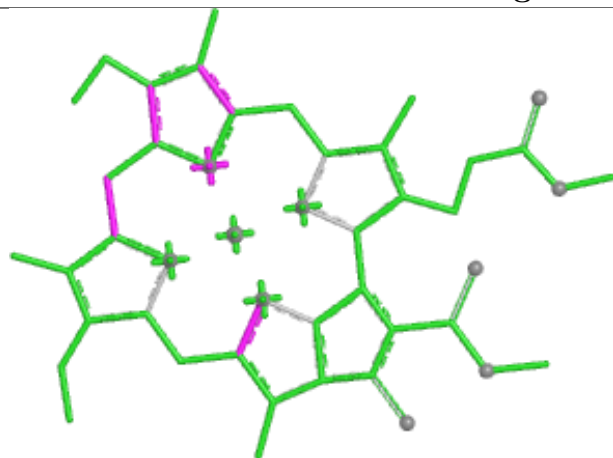


Torsions

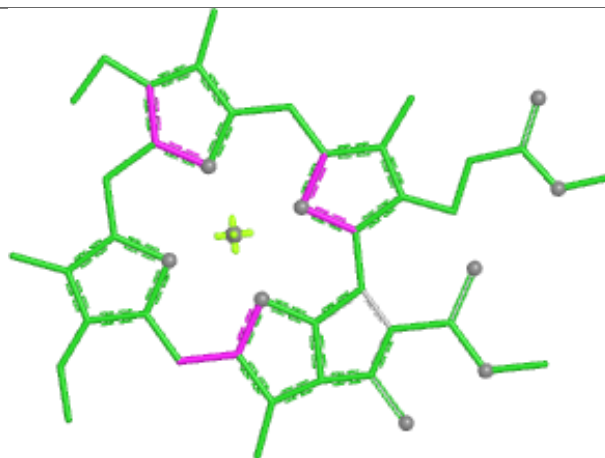


Rings

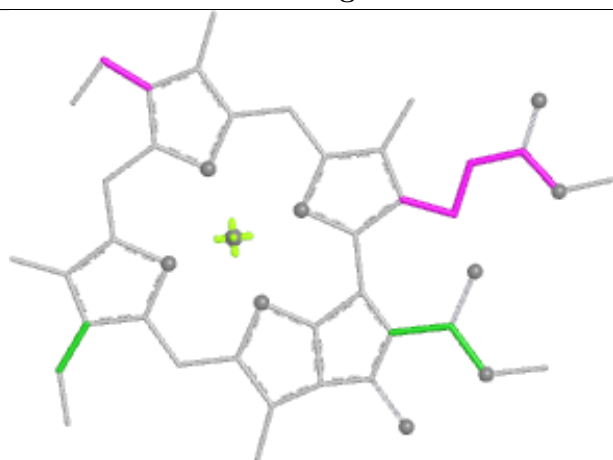
Ligand CLA X 516



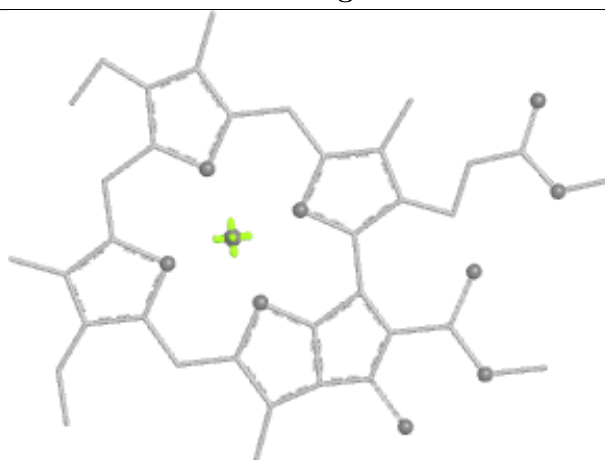
Bond lengths



Bond angles

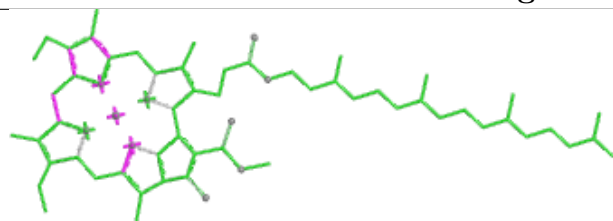


Torsions

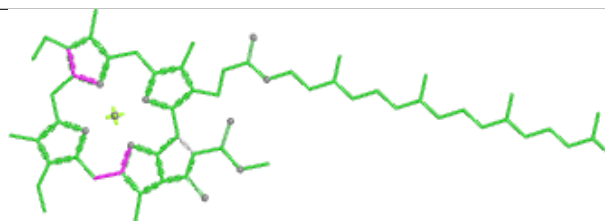


Rings

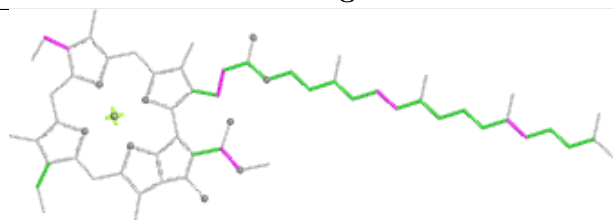
Ligand CLA x 511



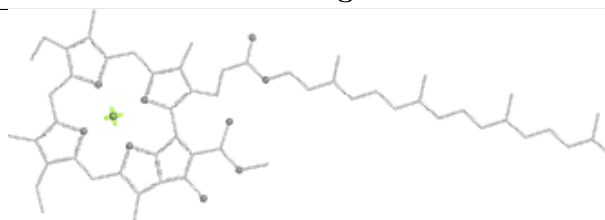
Bond lengths



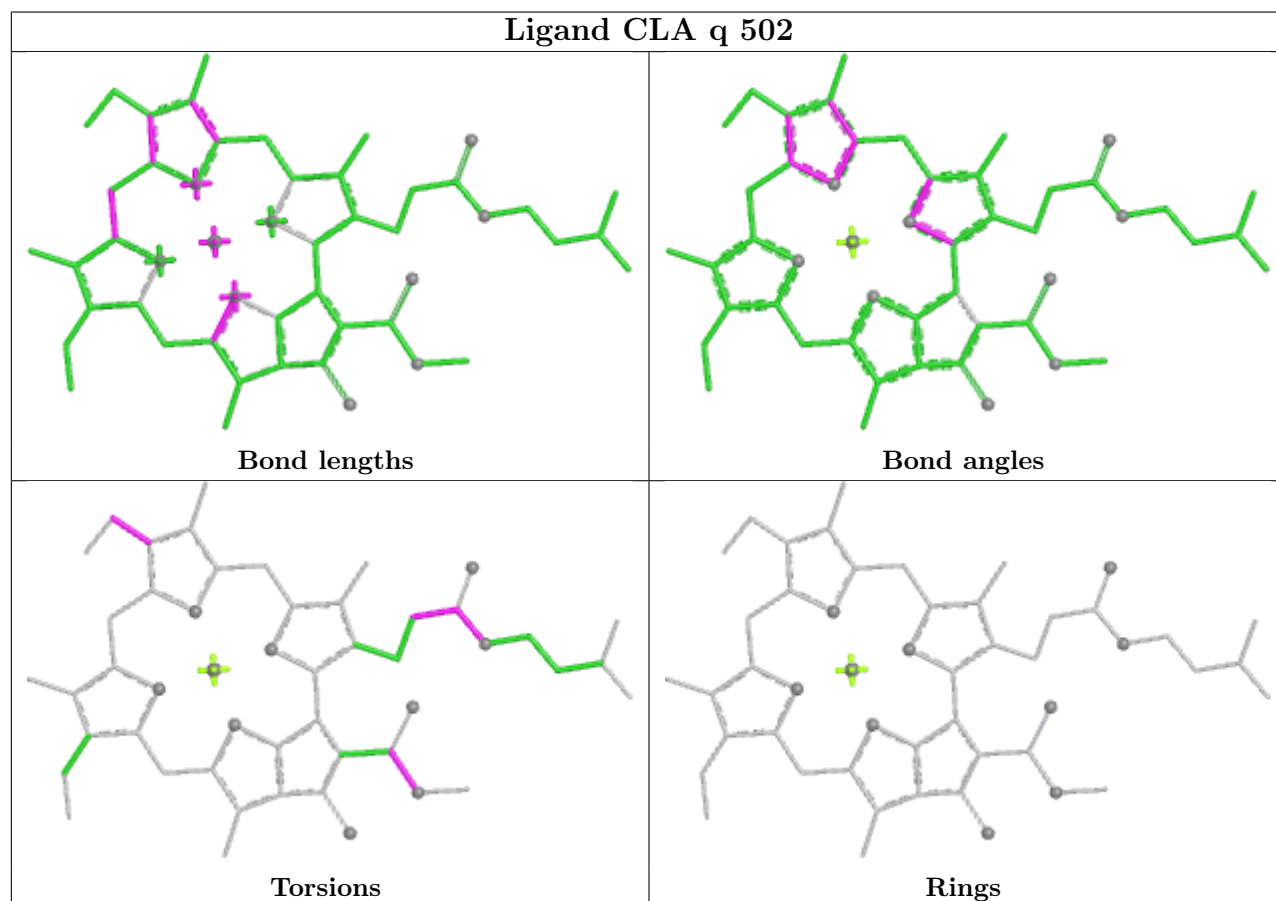
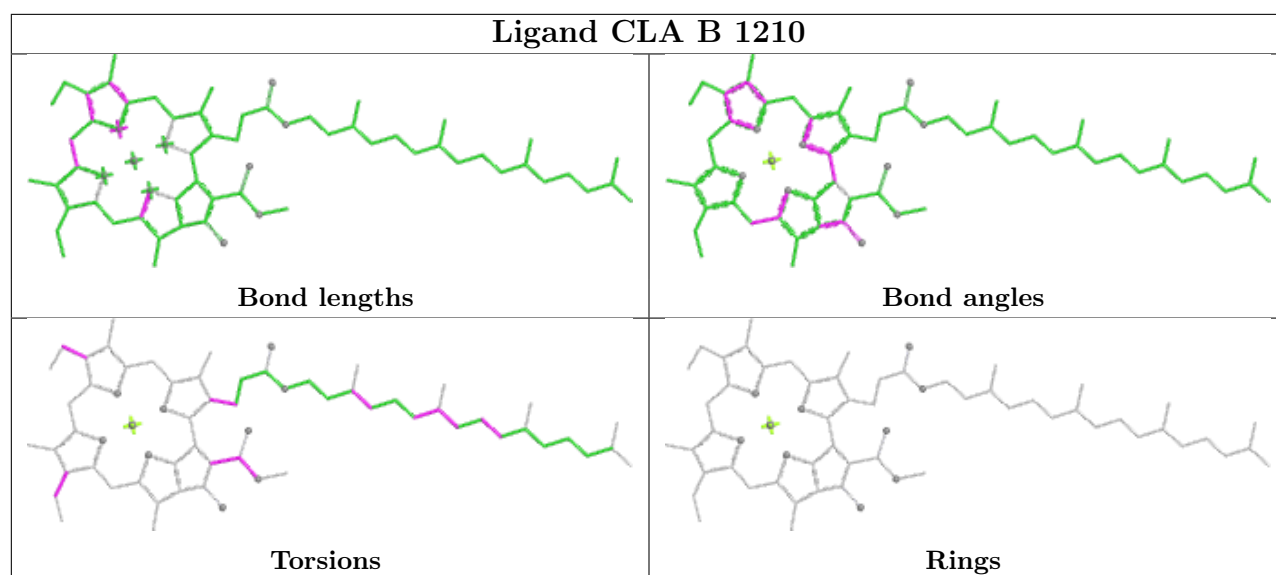
Bond angles



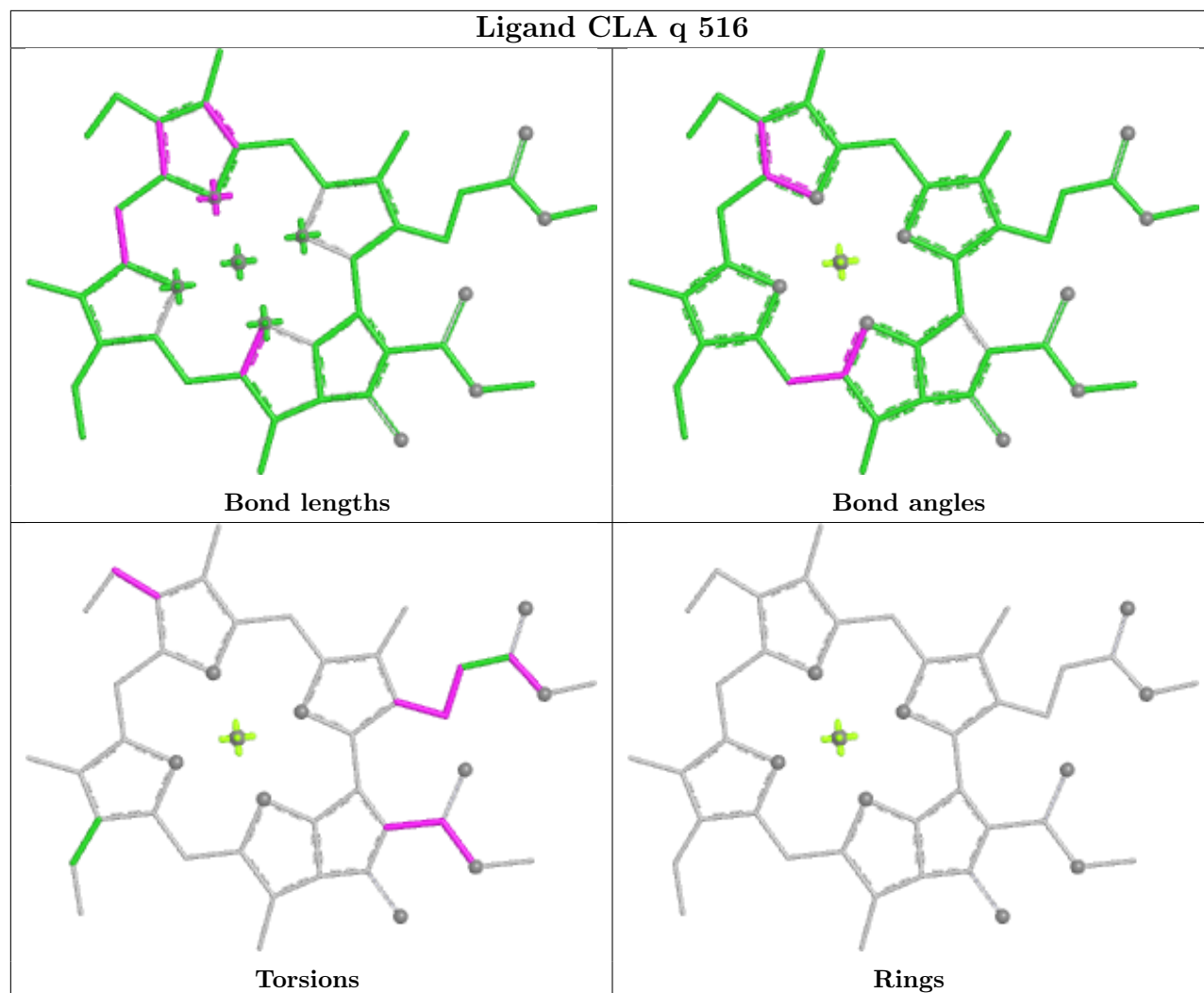
Torsions



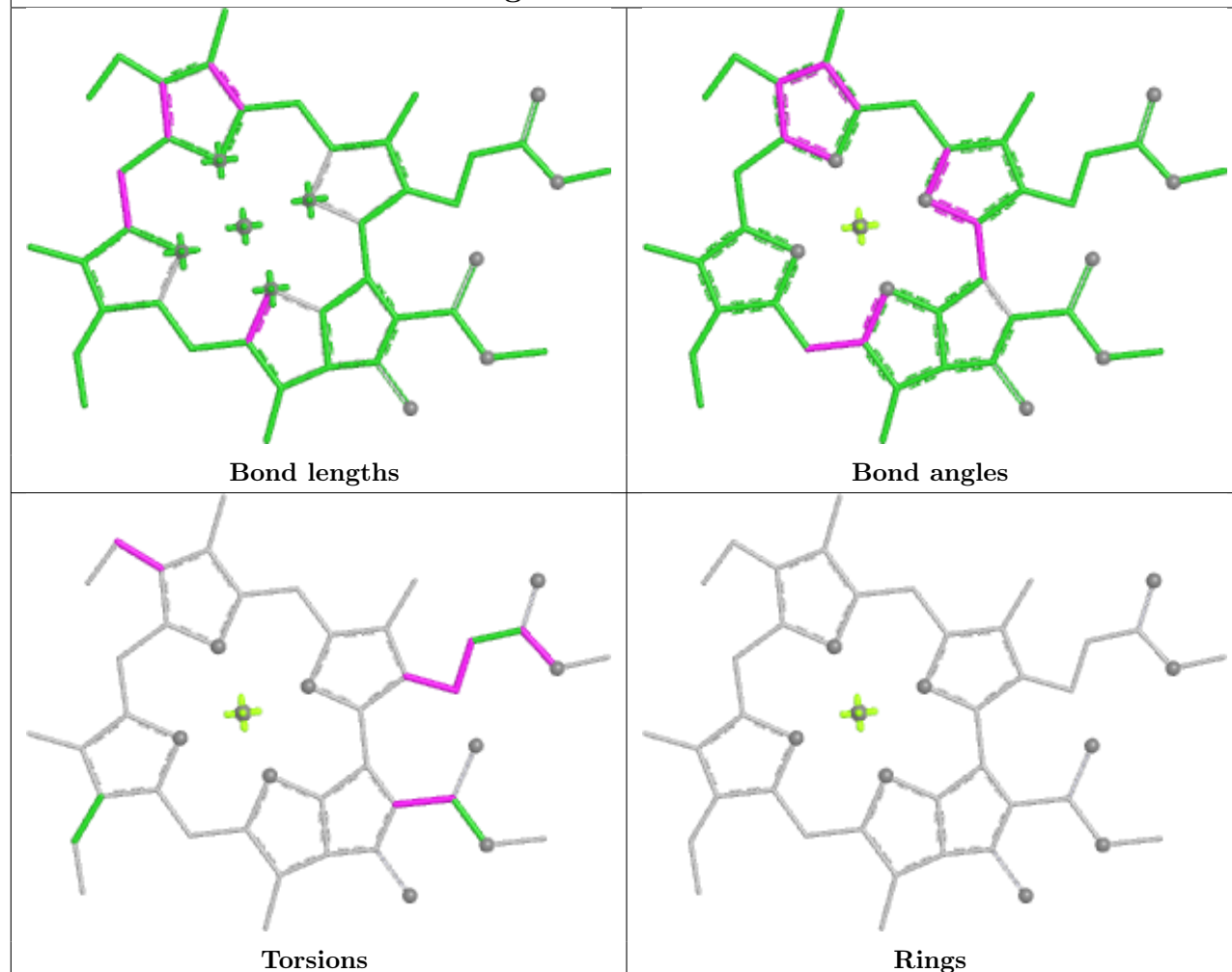
Rings



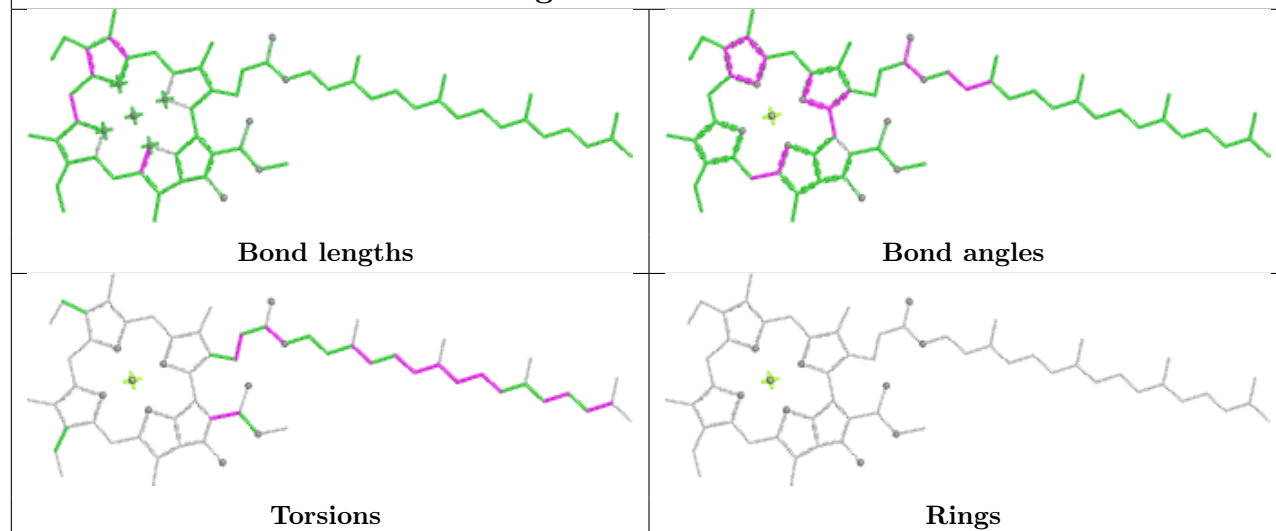
Ligand CLA q 516

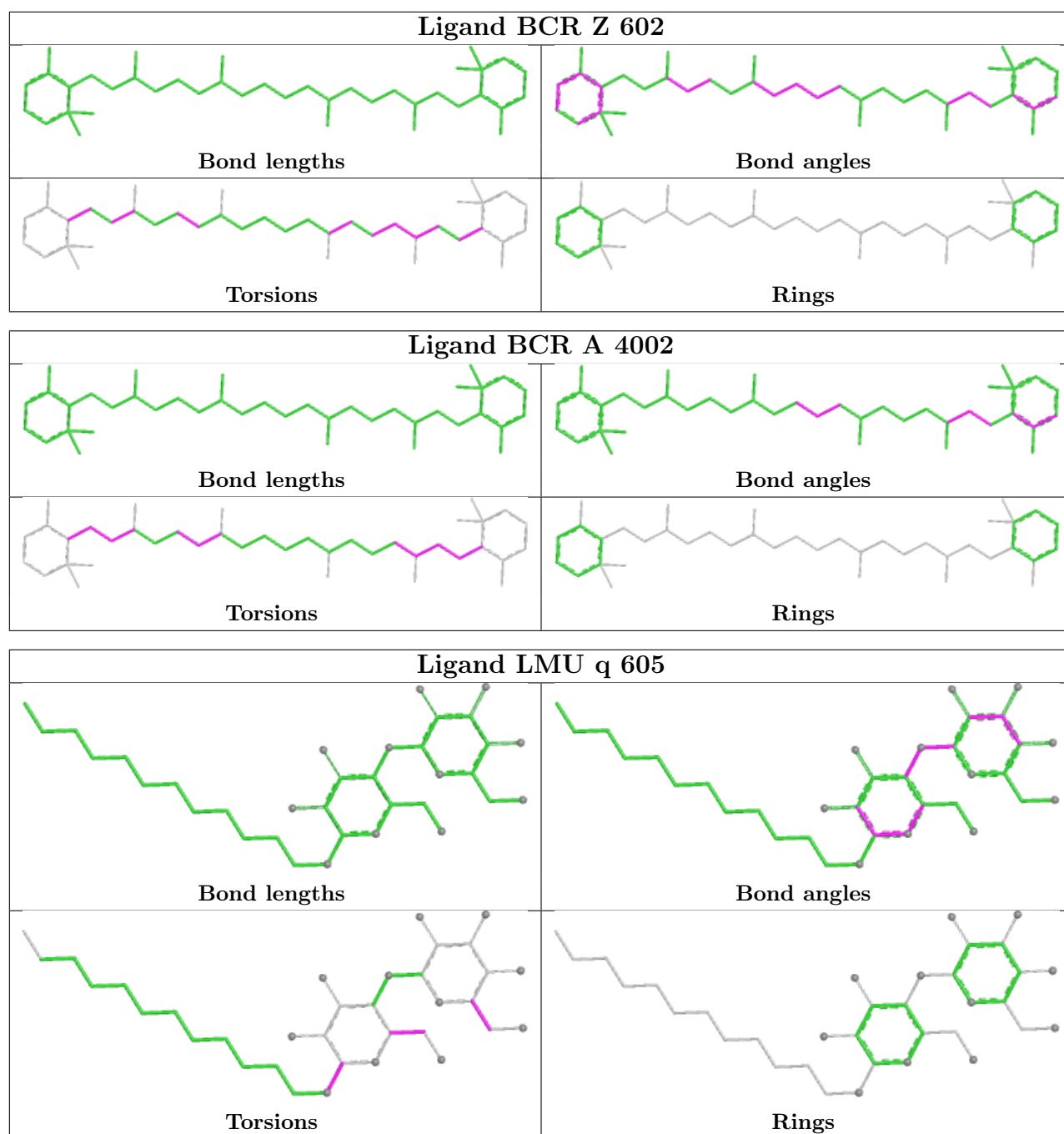


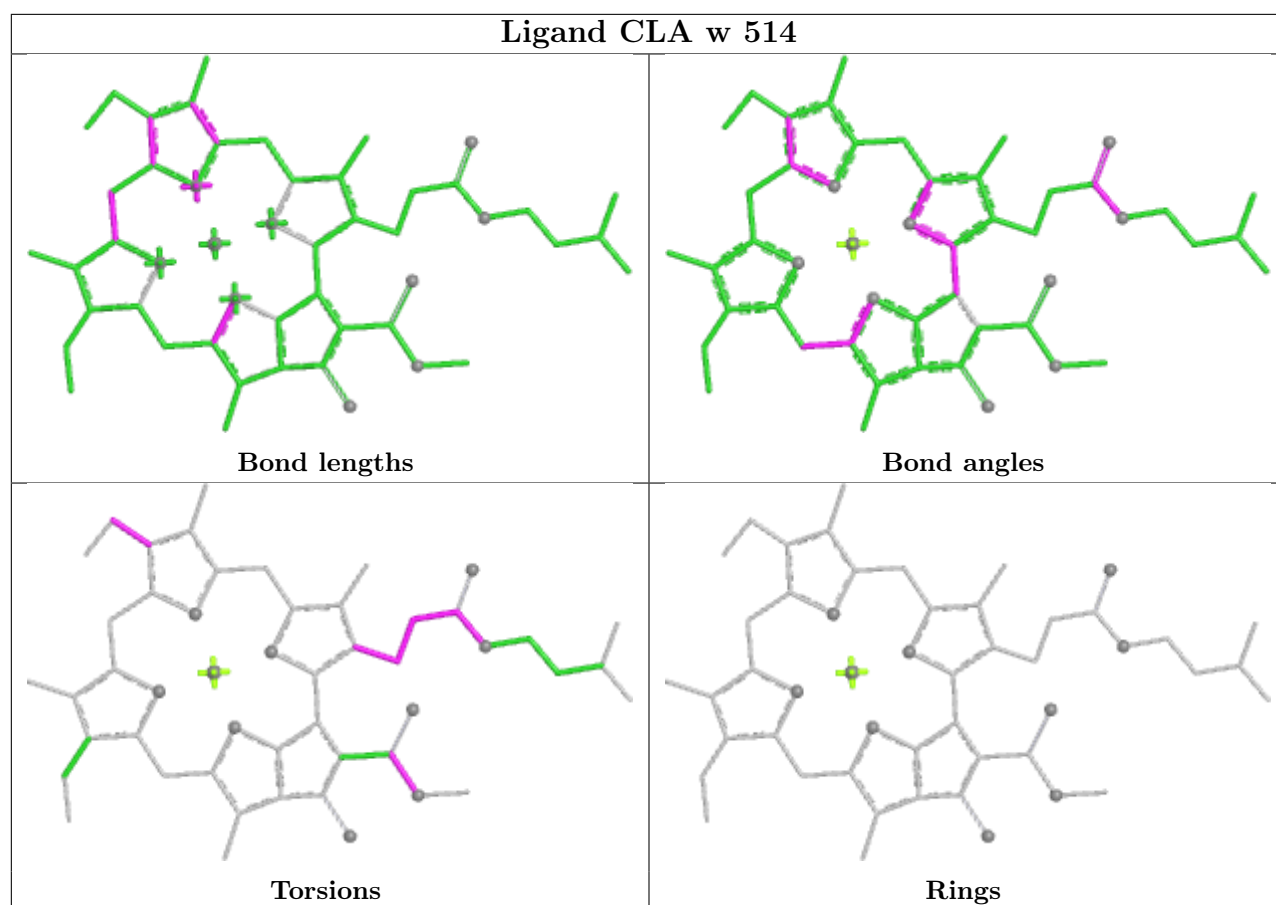
Ligand CLA A 1129

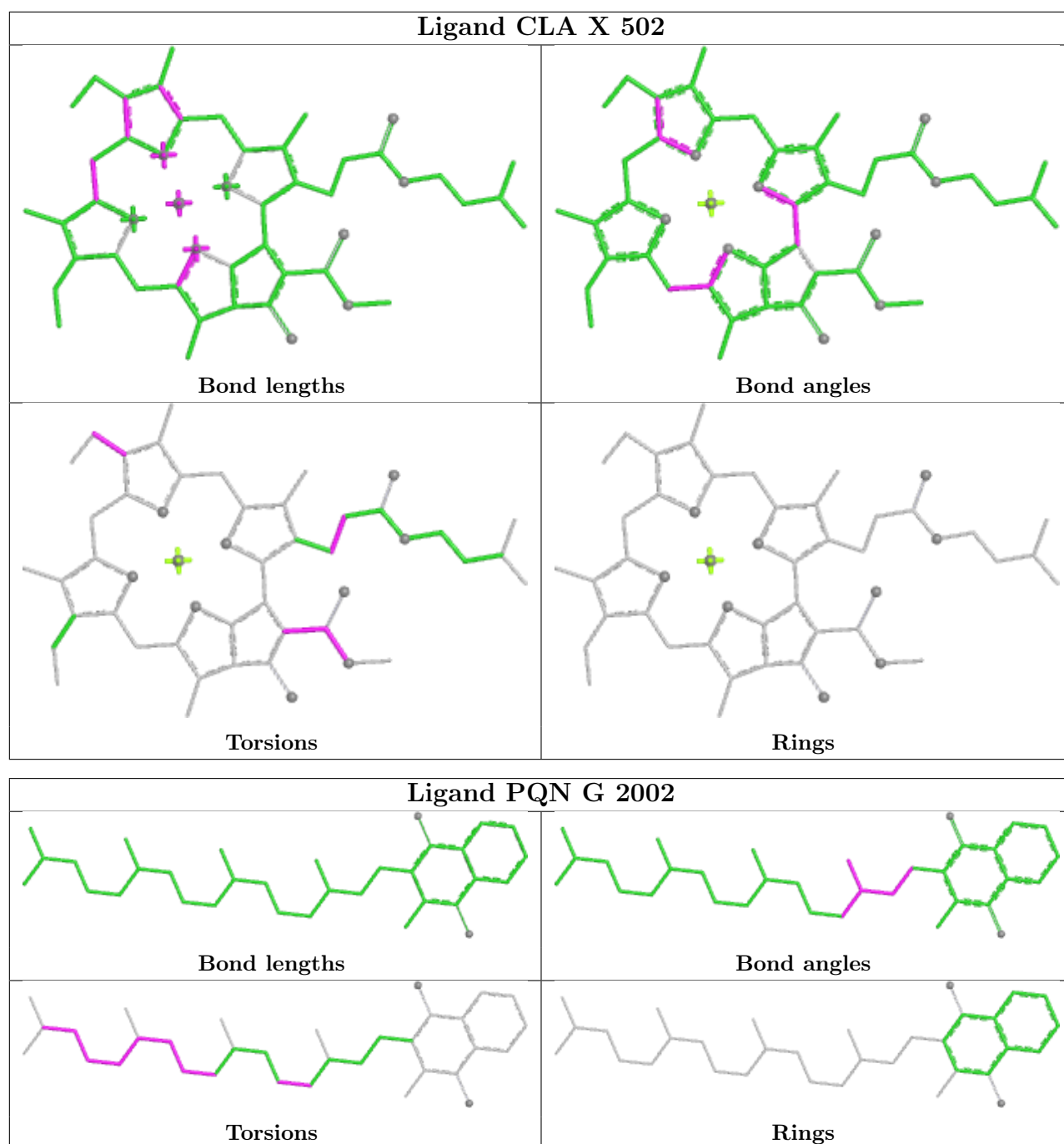


Ligand CLA h 515

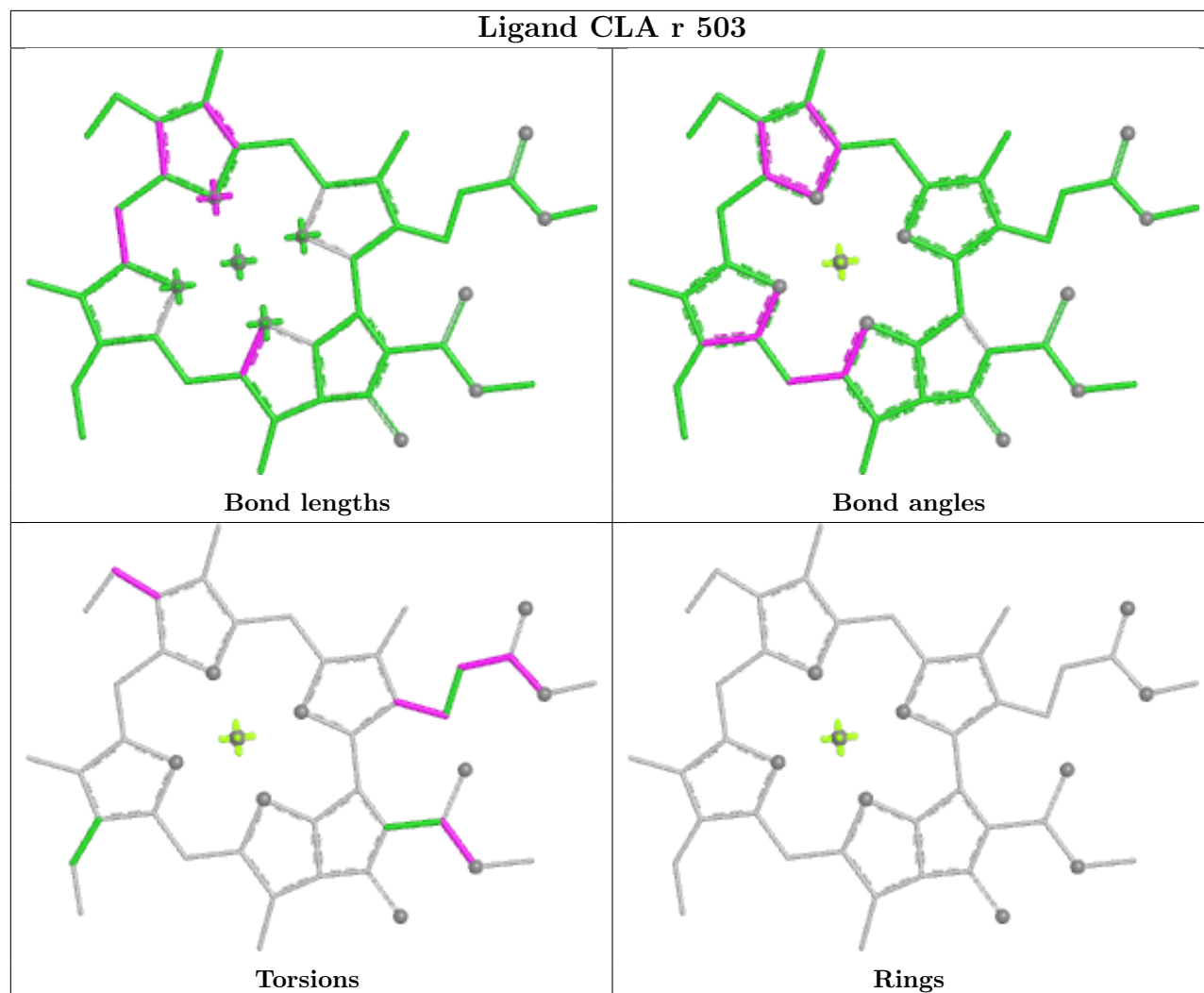




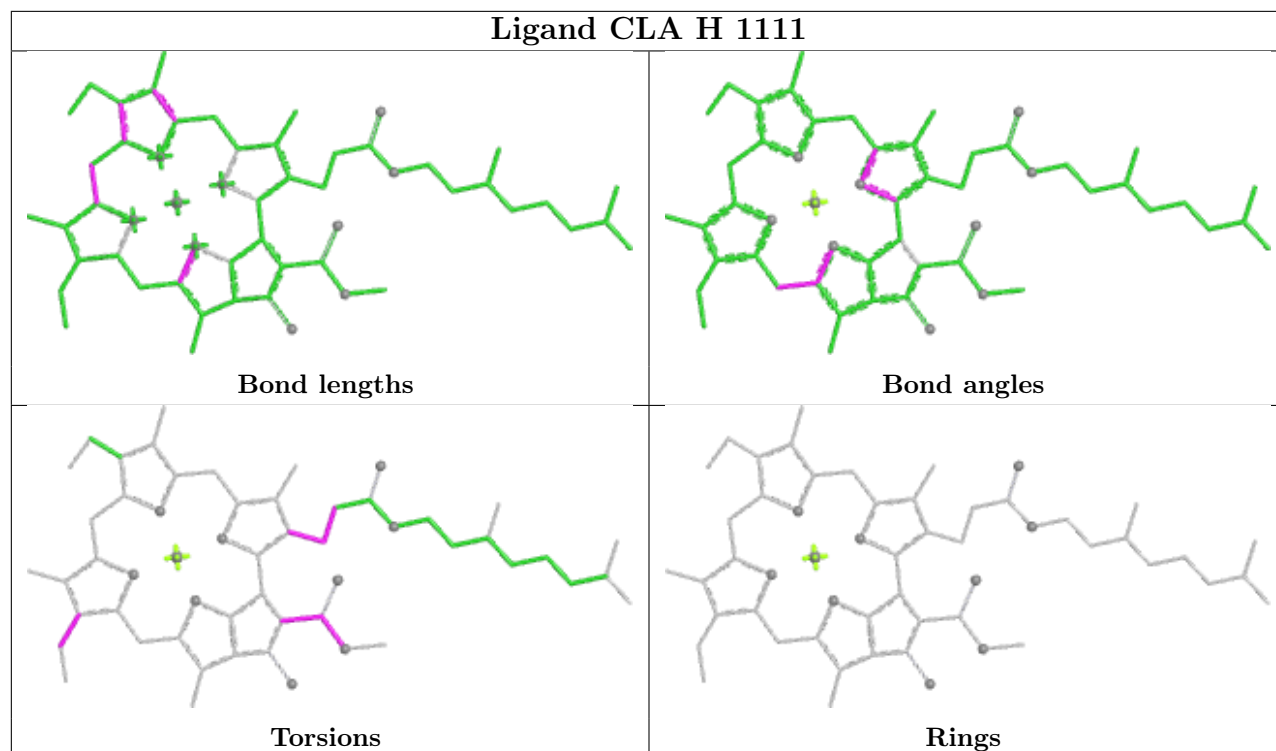




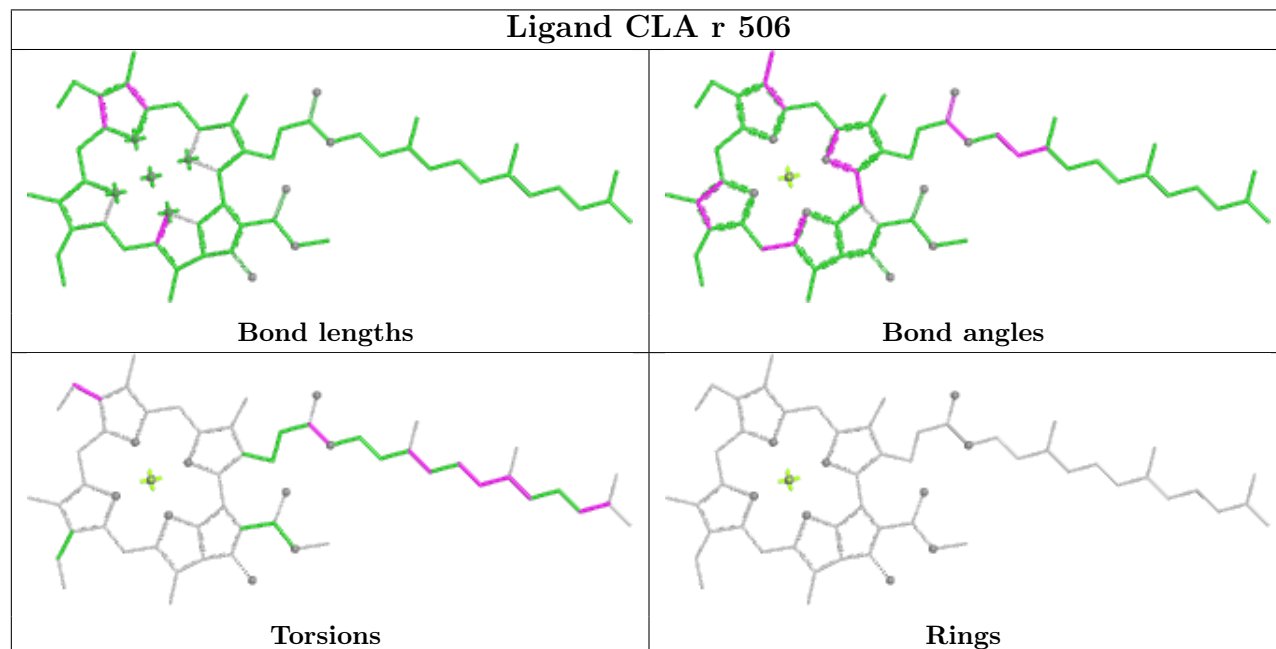
Ligand CLA r 503

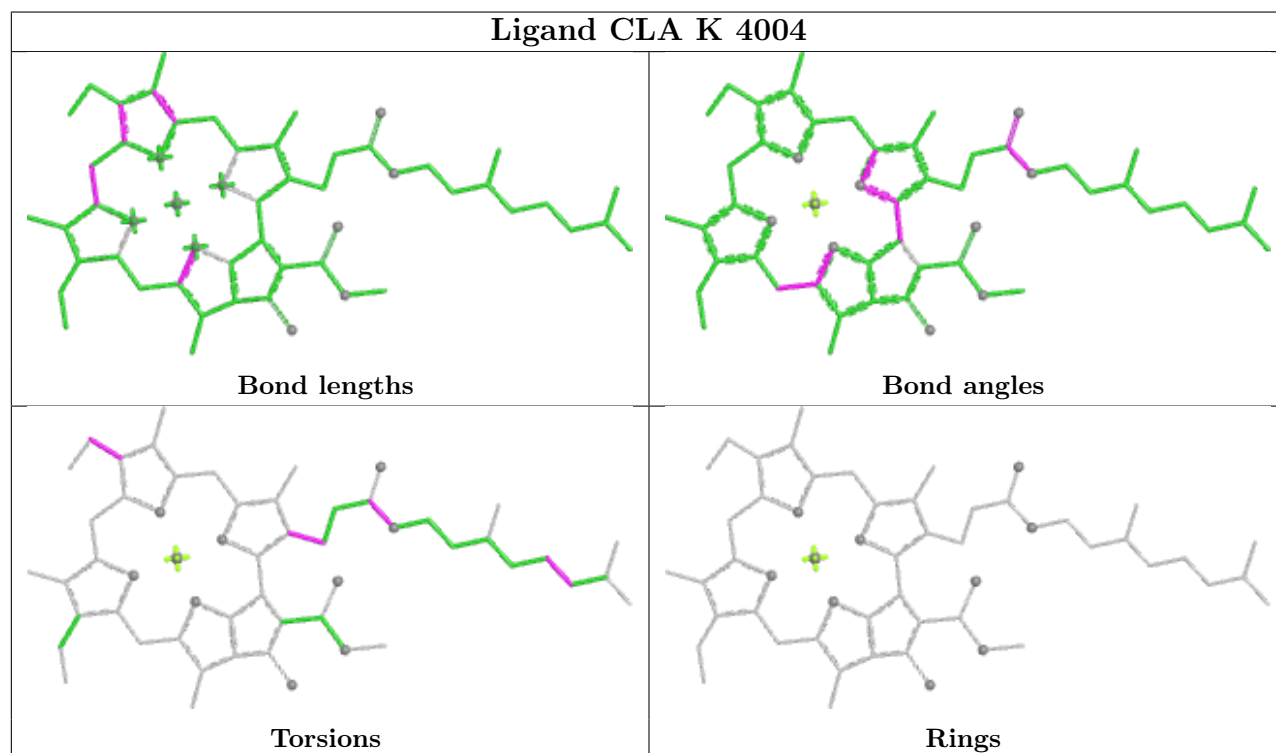
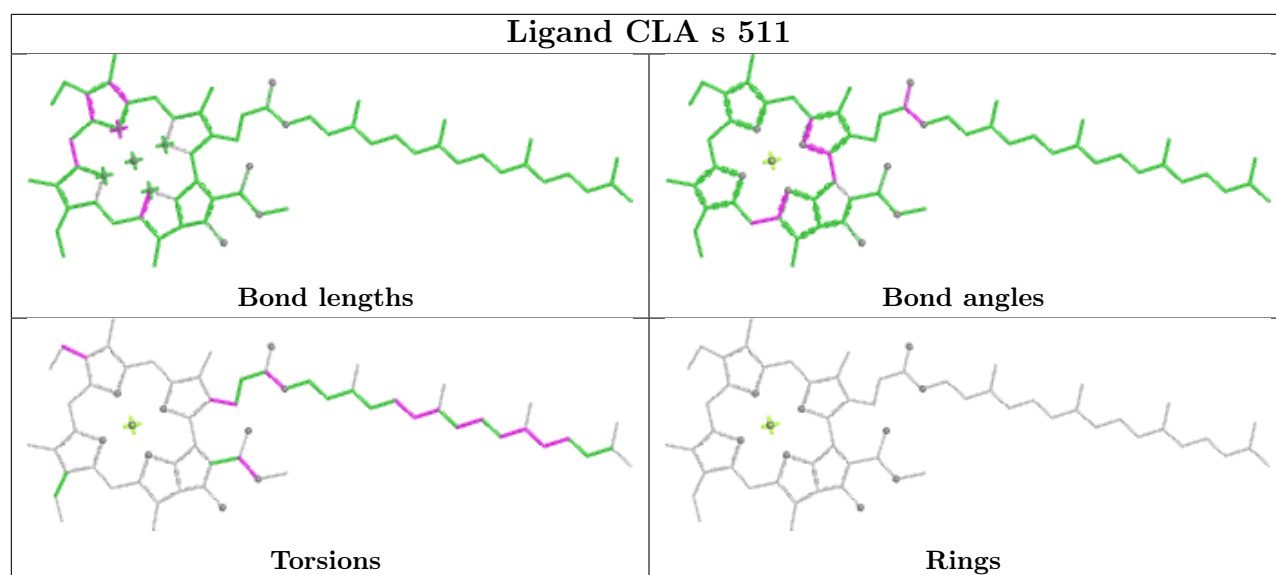


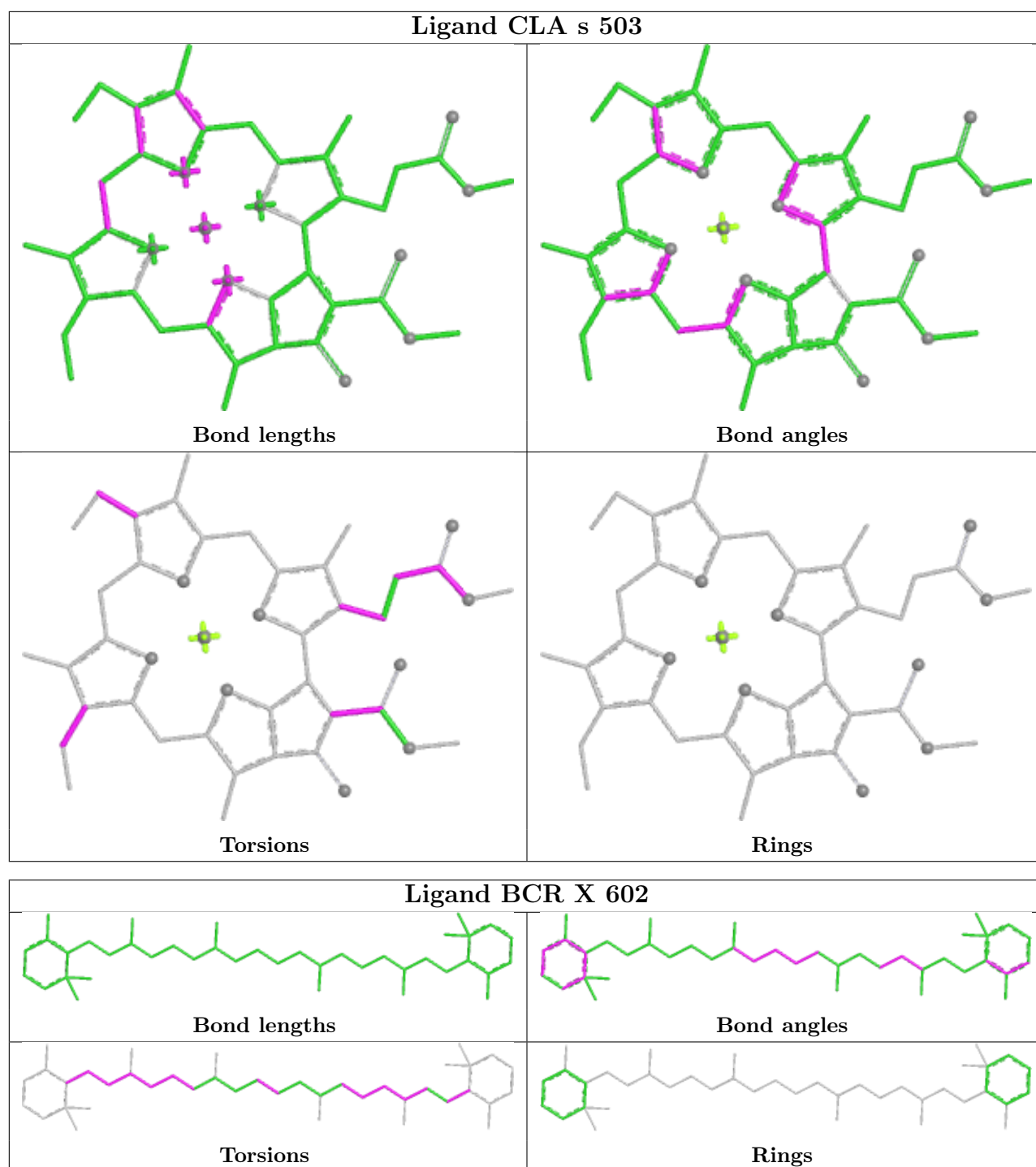
Ligand CLA H 1111



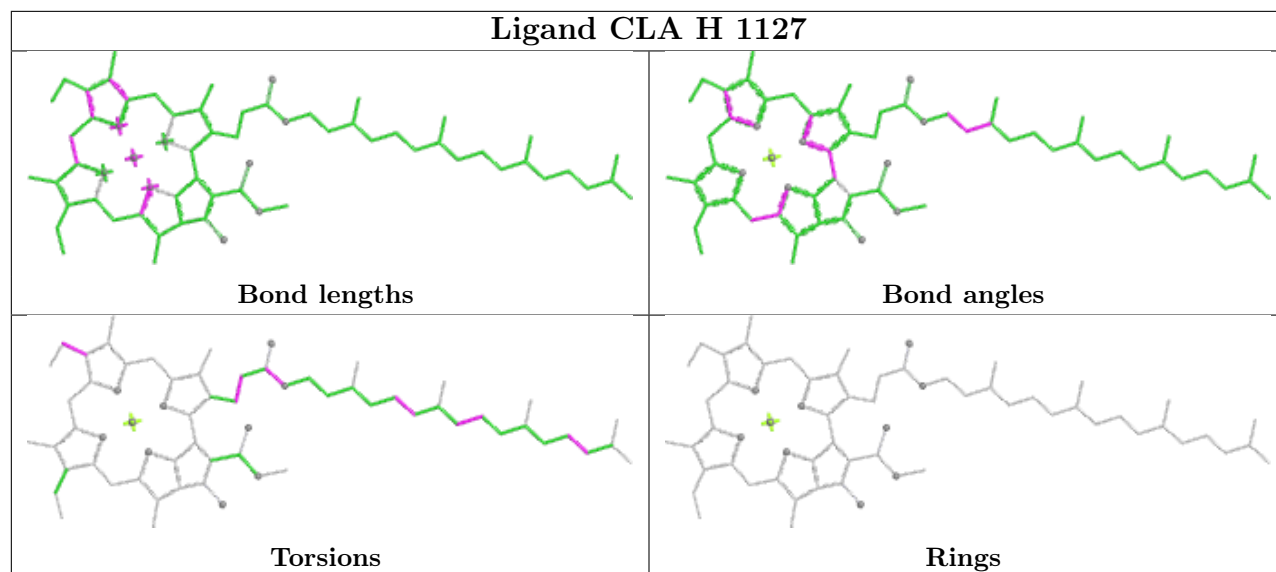
Ligand CLA r 506



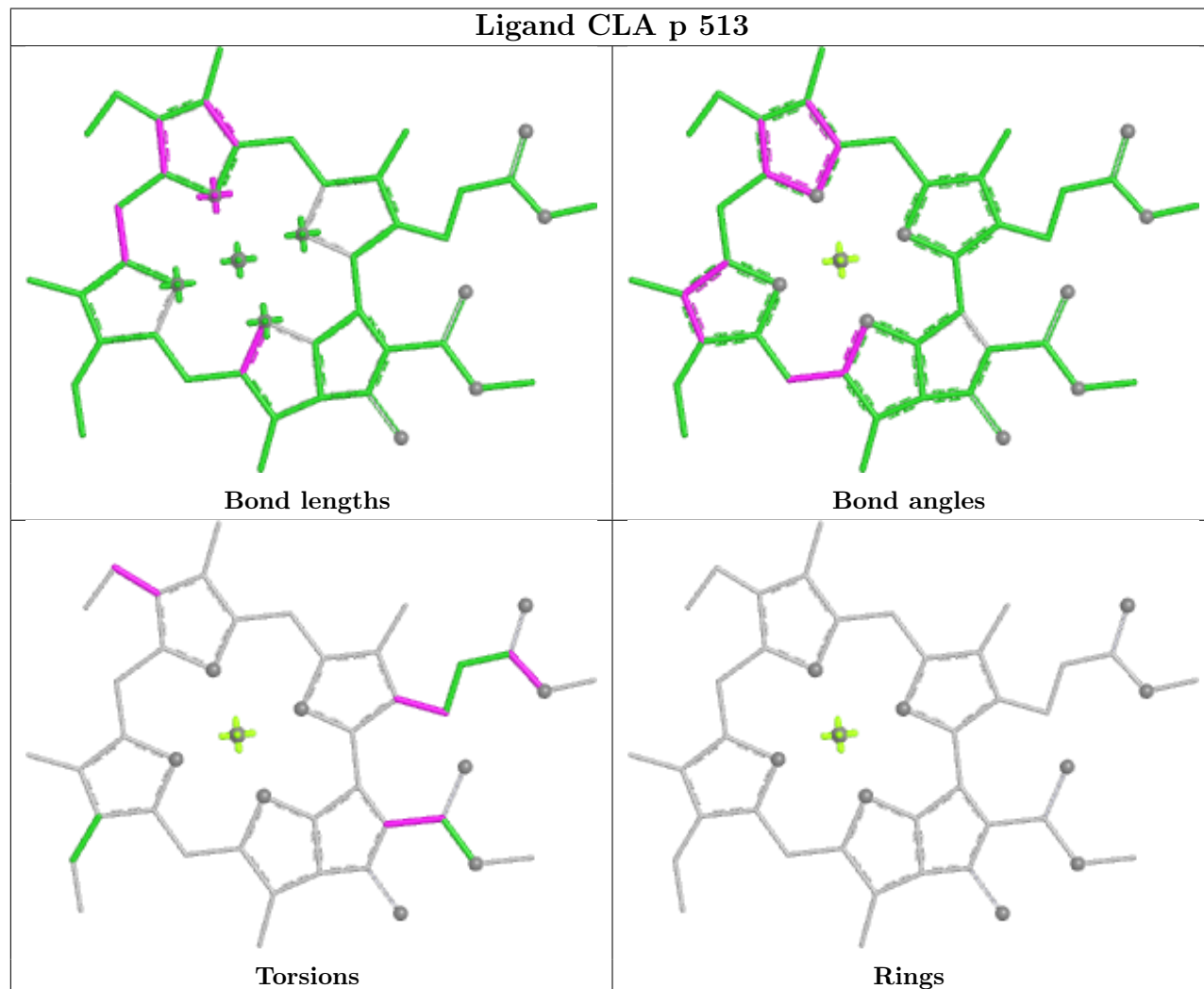




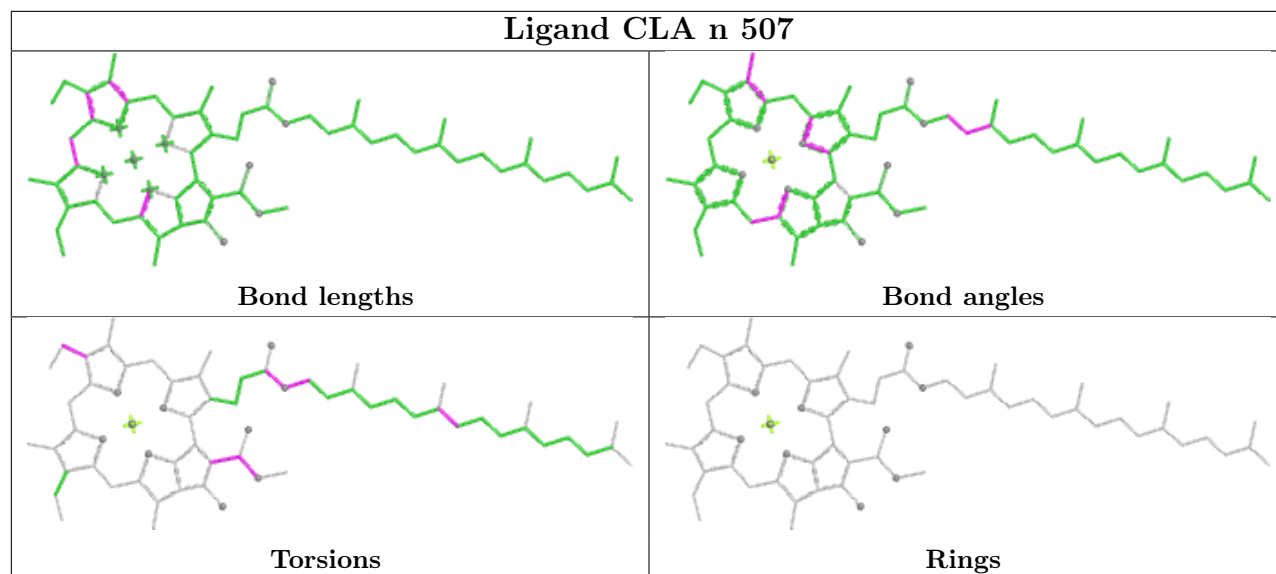
Ligand CLA H 1127



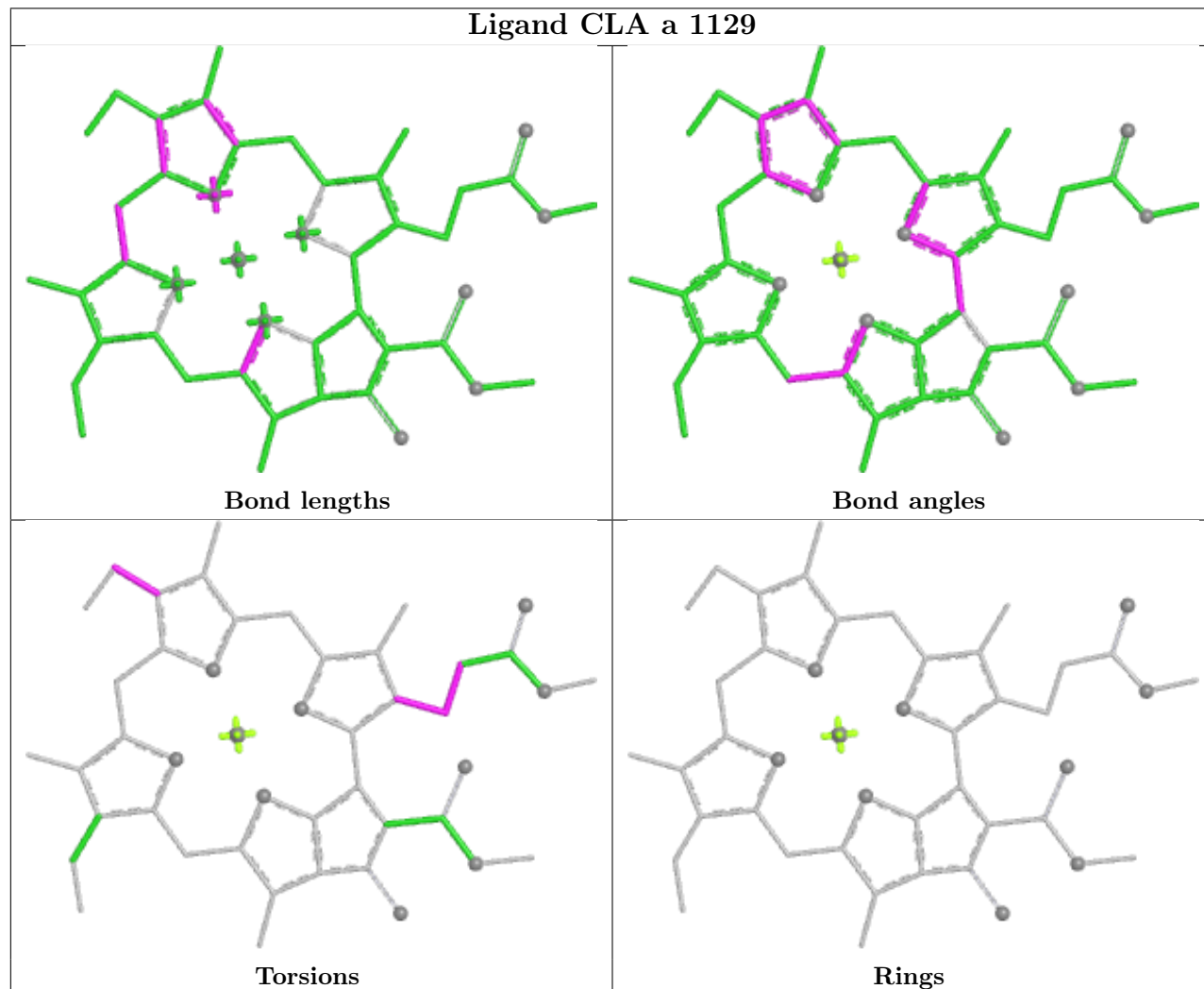
Ligand CLA p 513

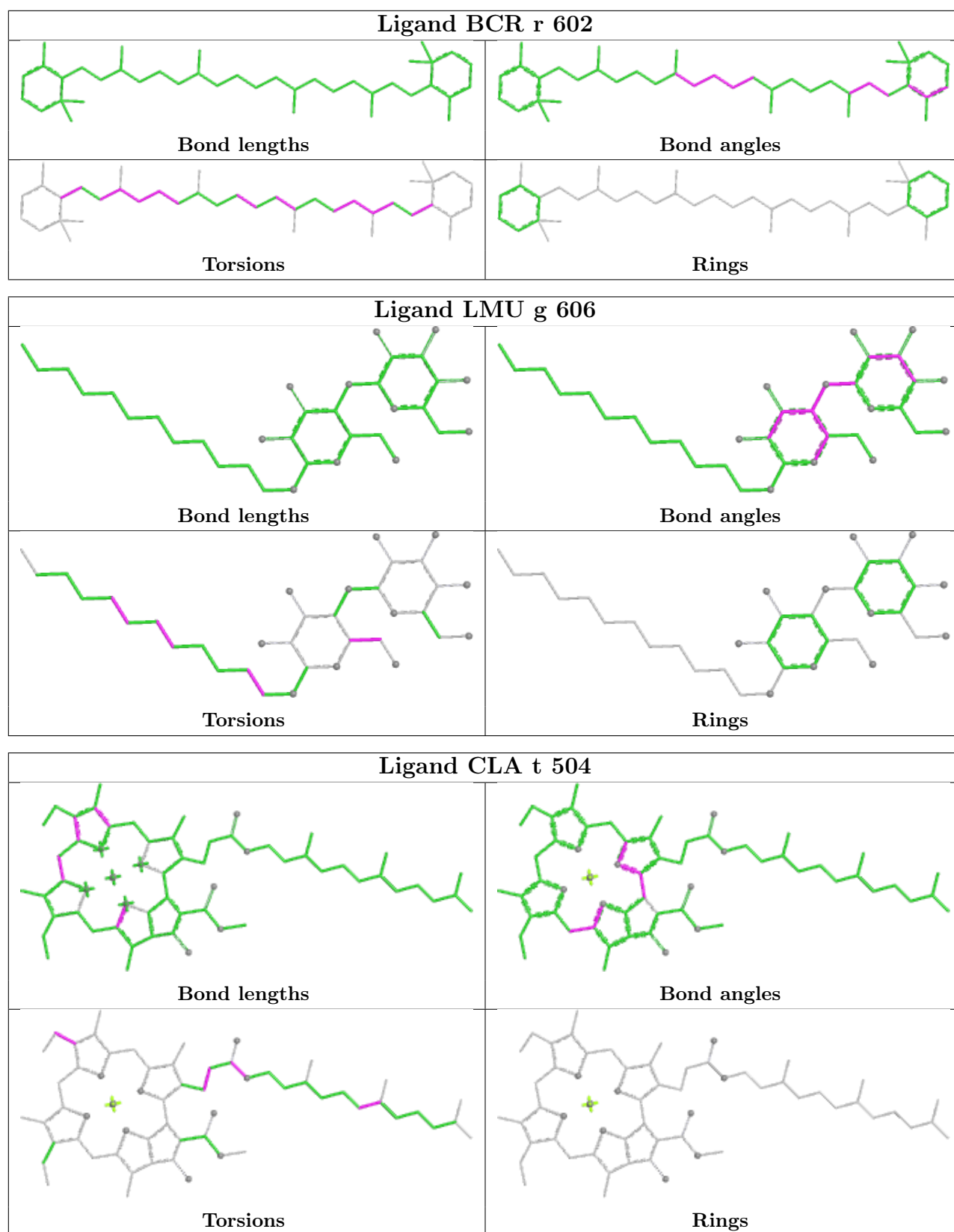


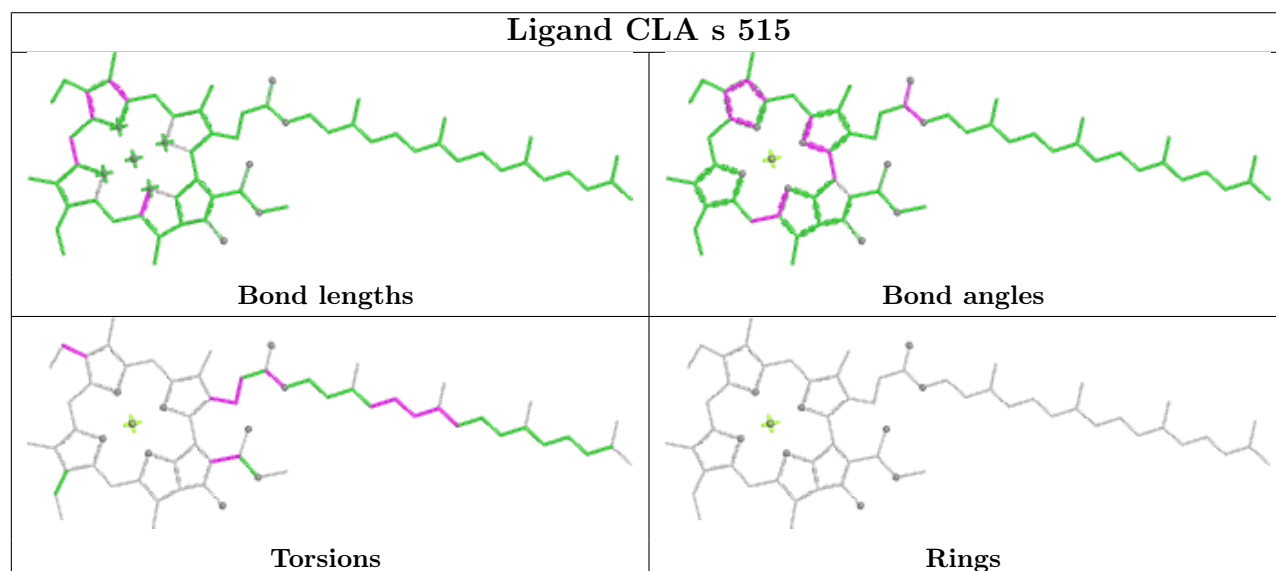
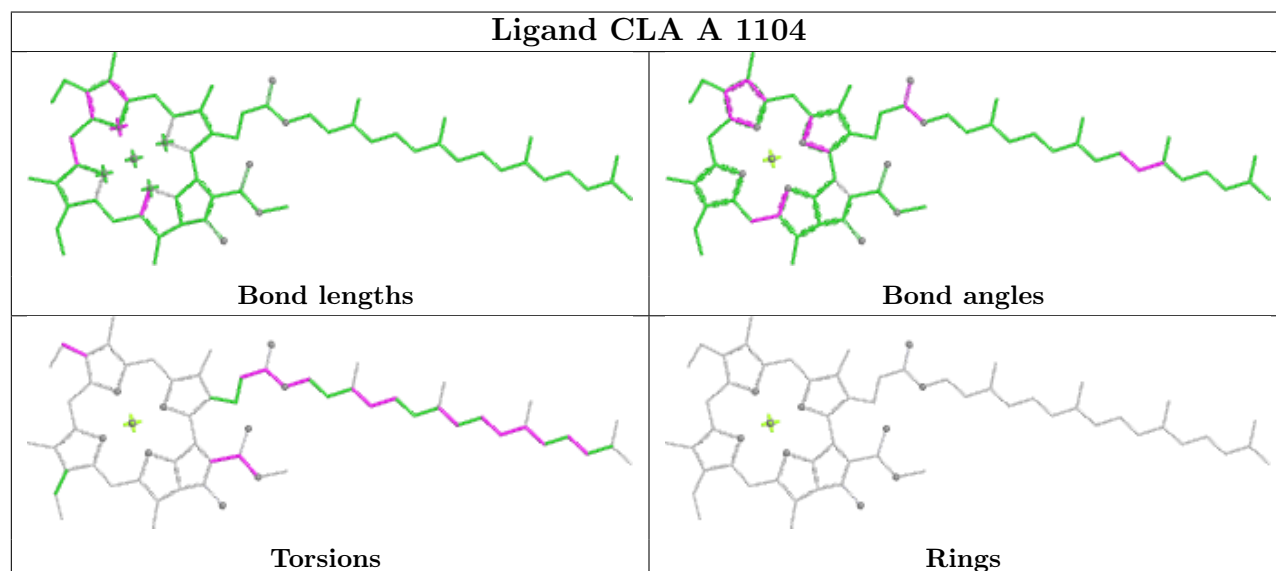
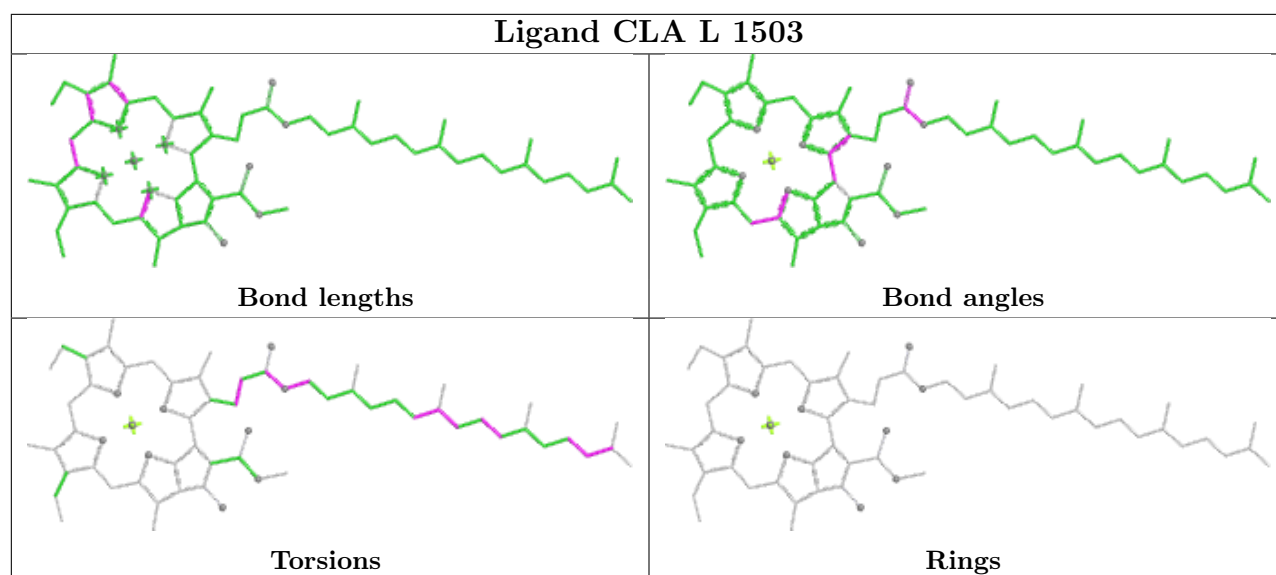
Ligand CLA n 507



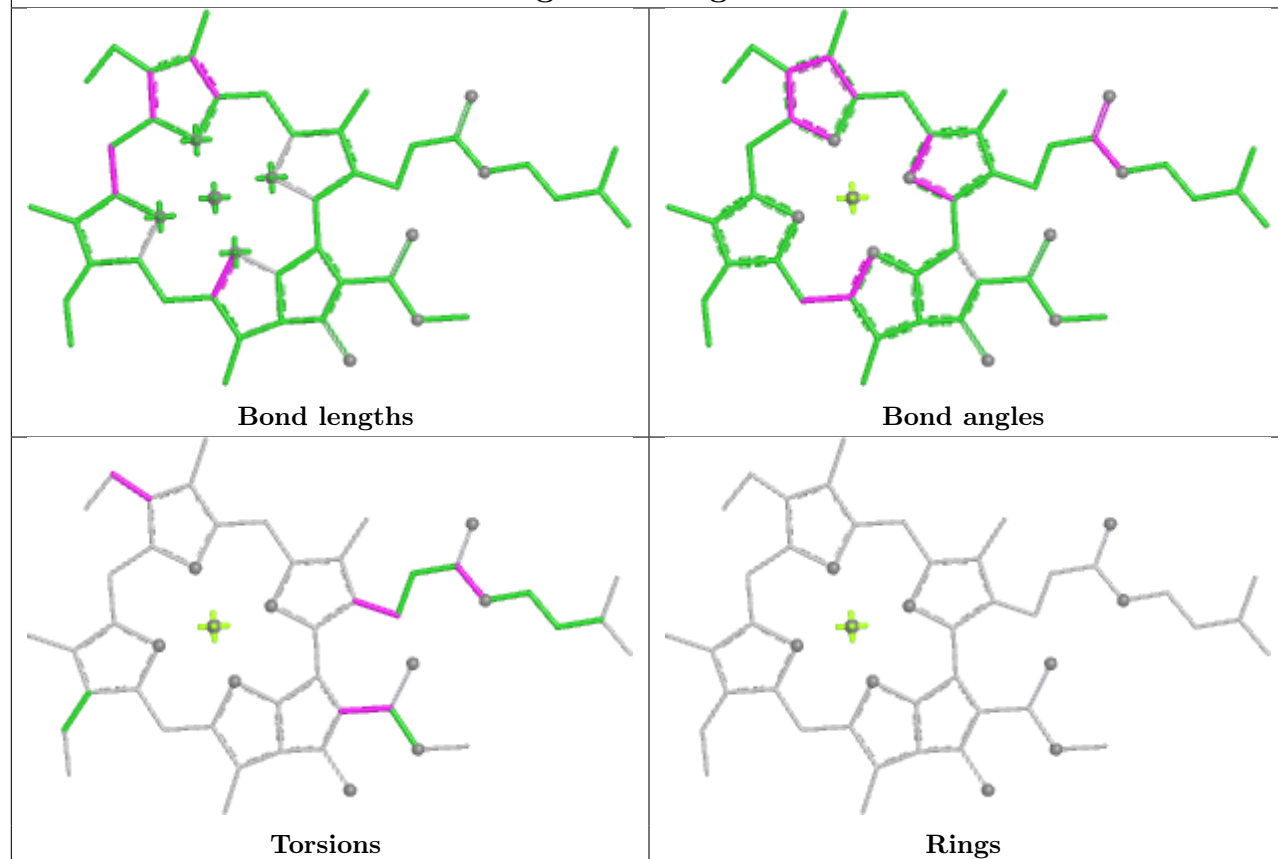
Ligand CLA a 1129



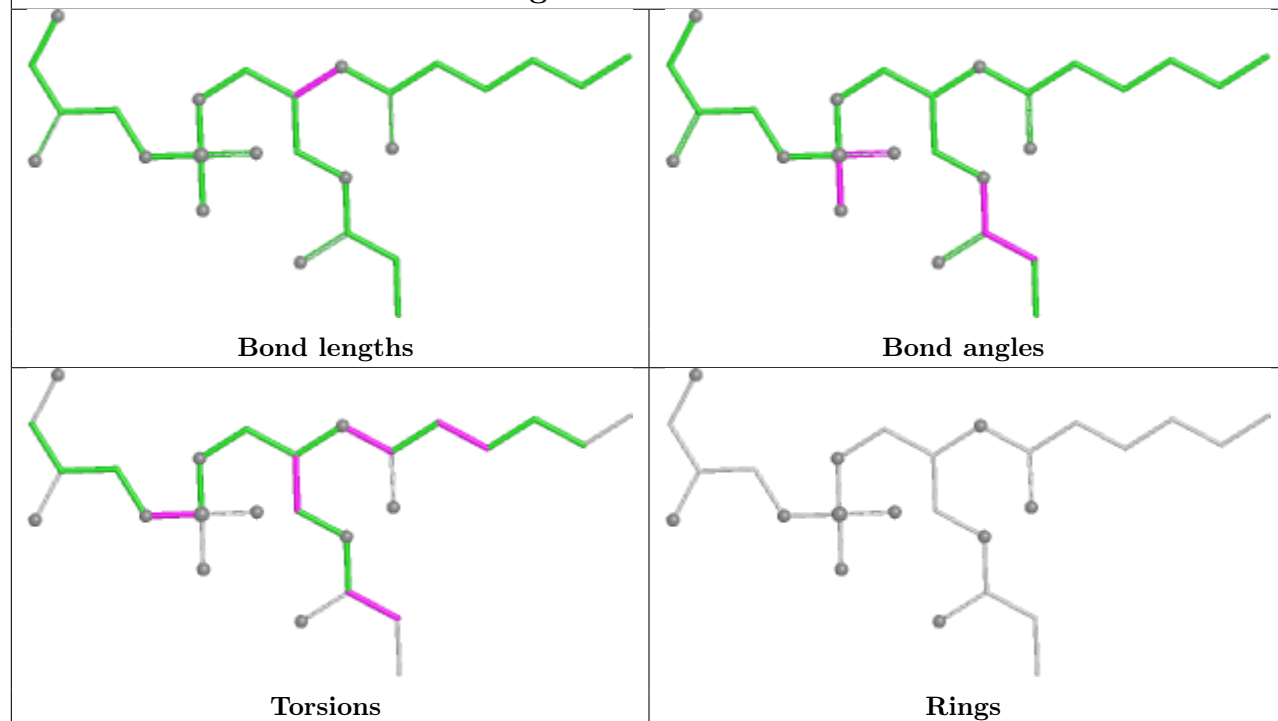




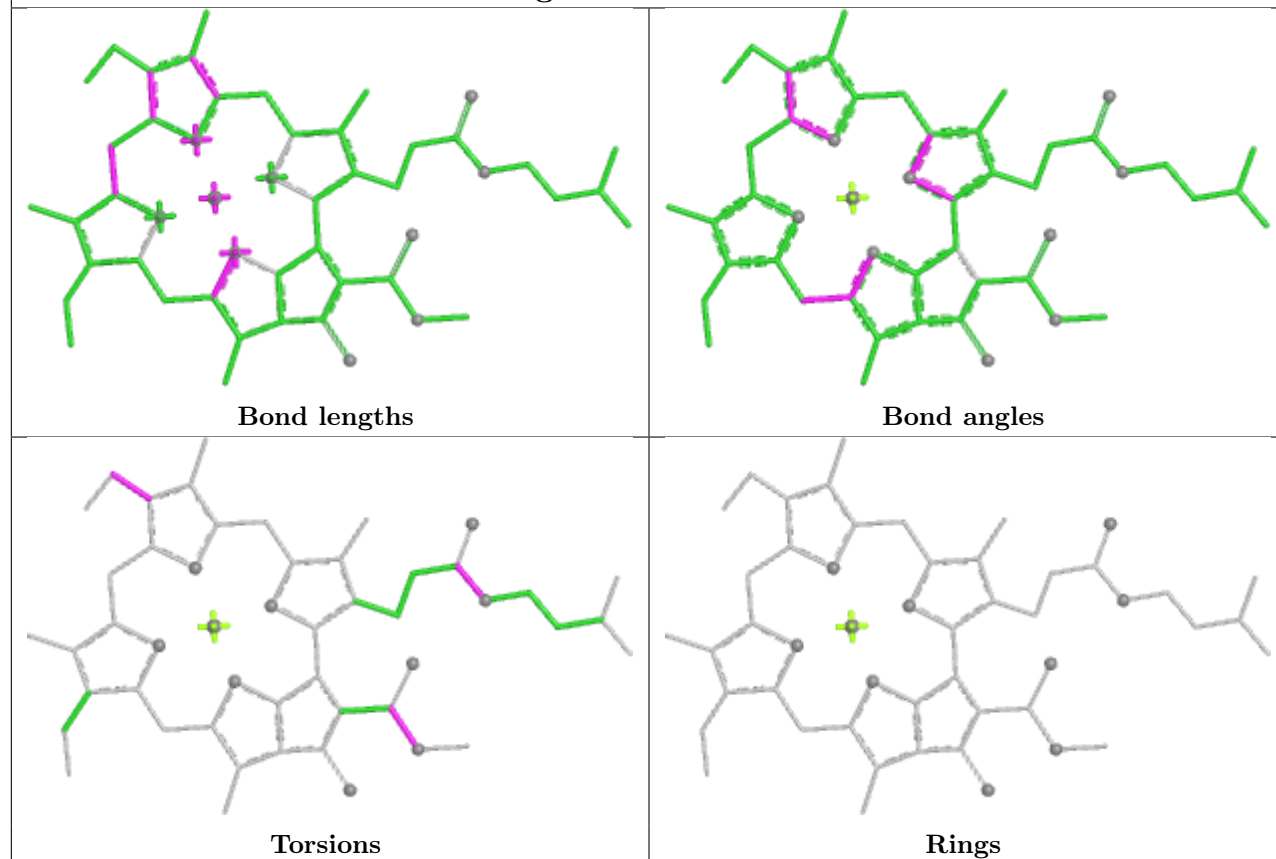
Ligand CLA g 501



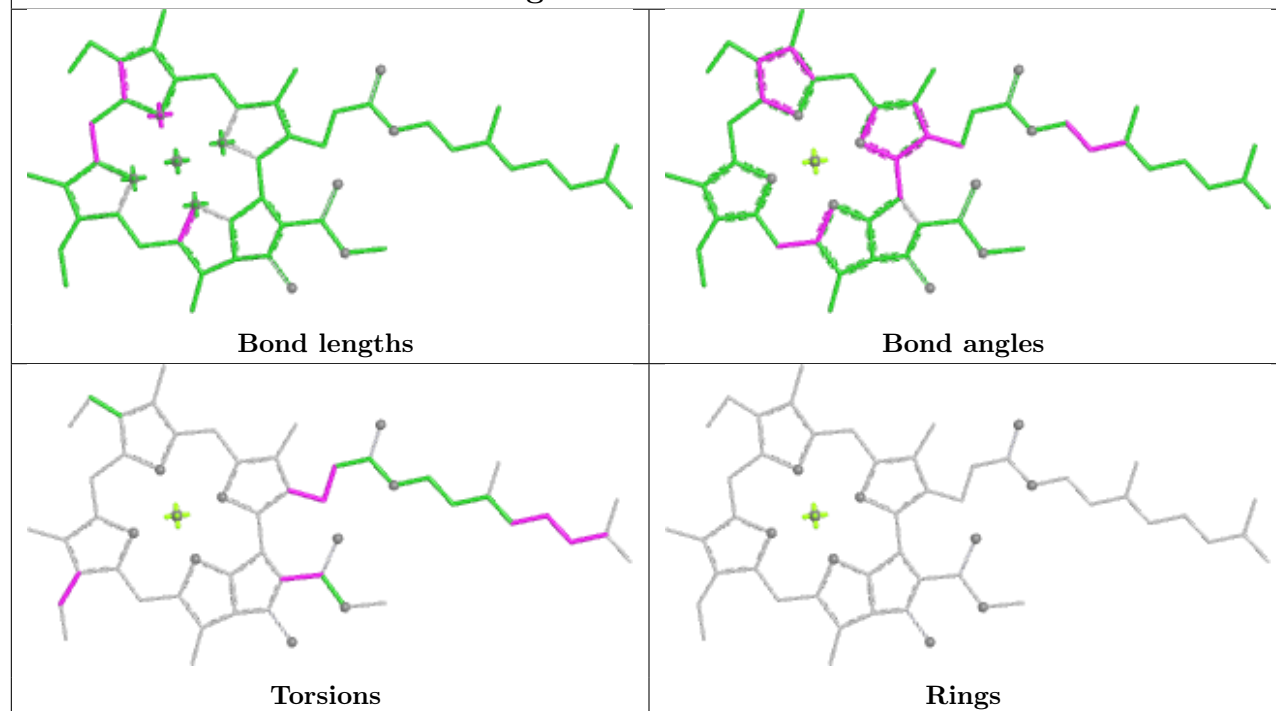
Ligand LHG H 851



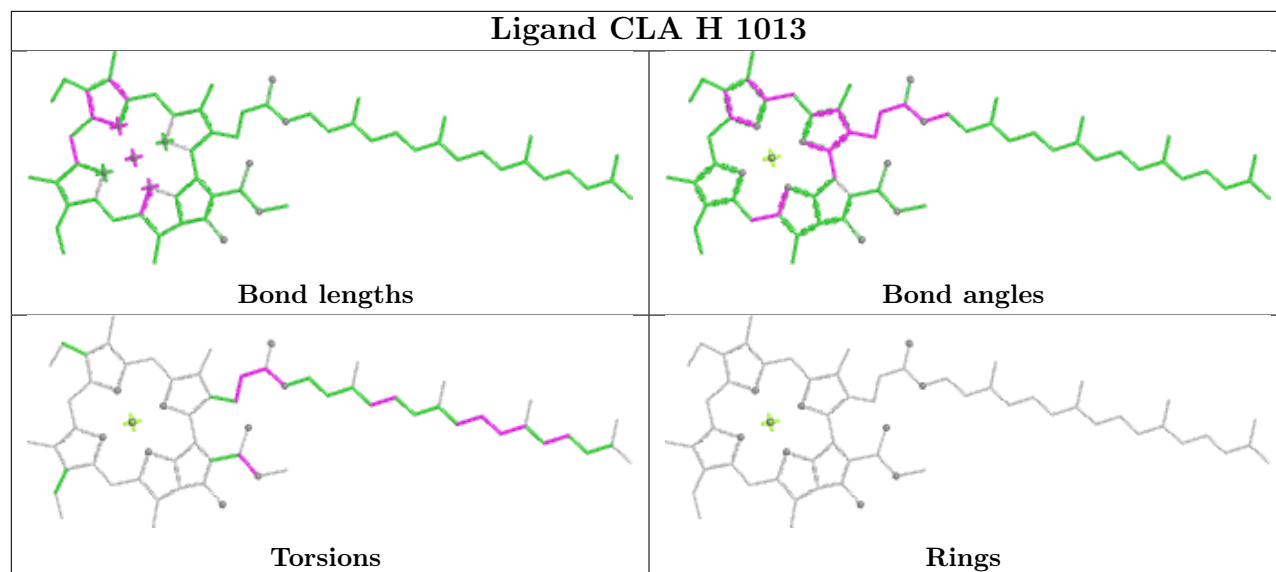
Ligand CLA x 502



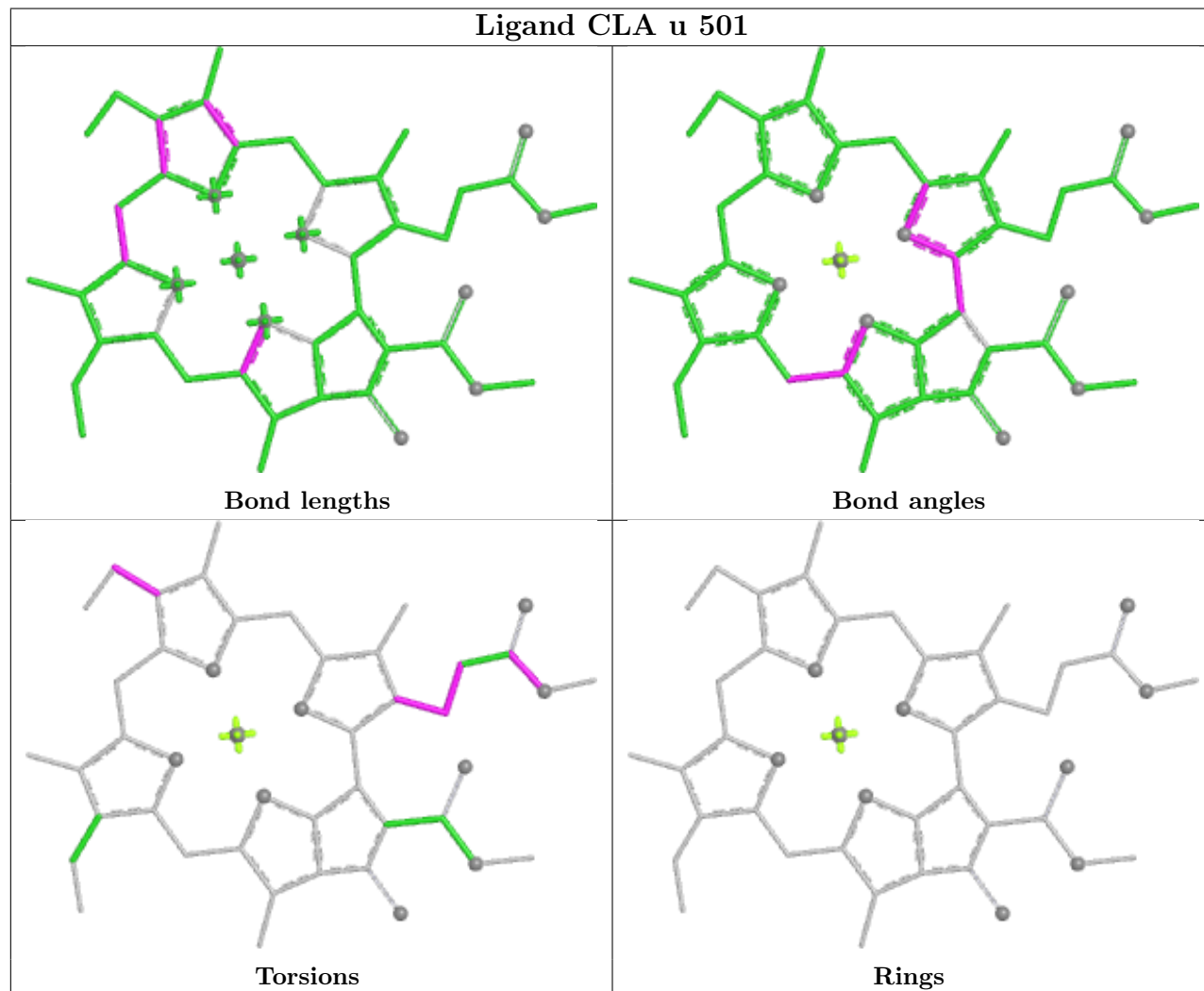
Ligand CLA b 1012

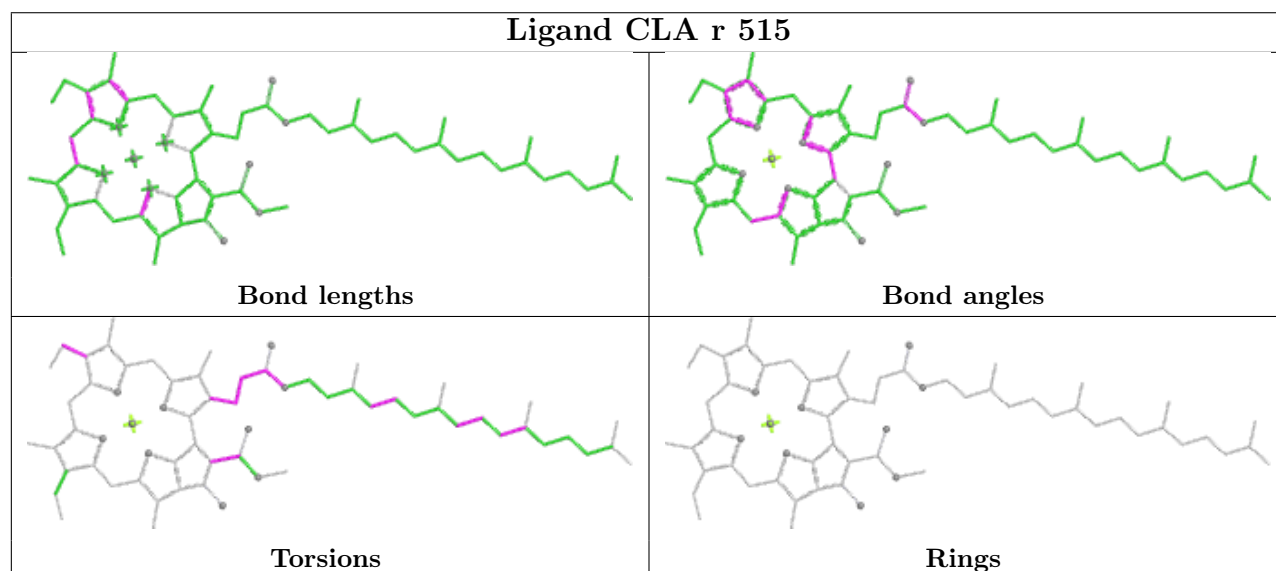
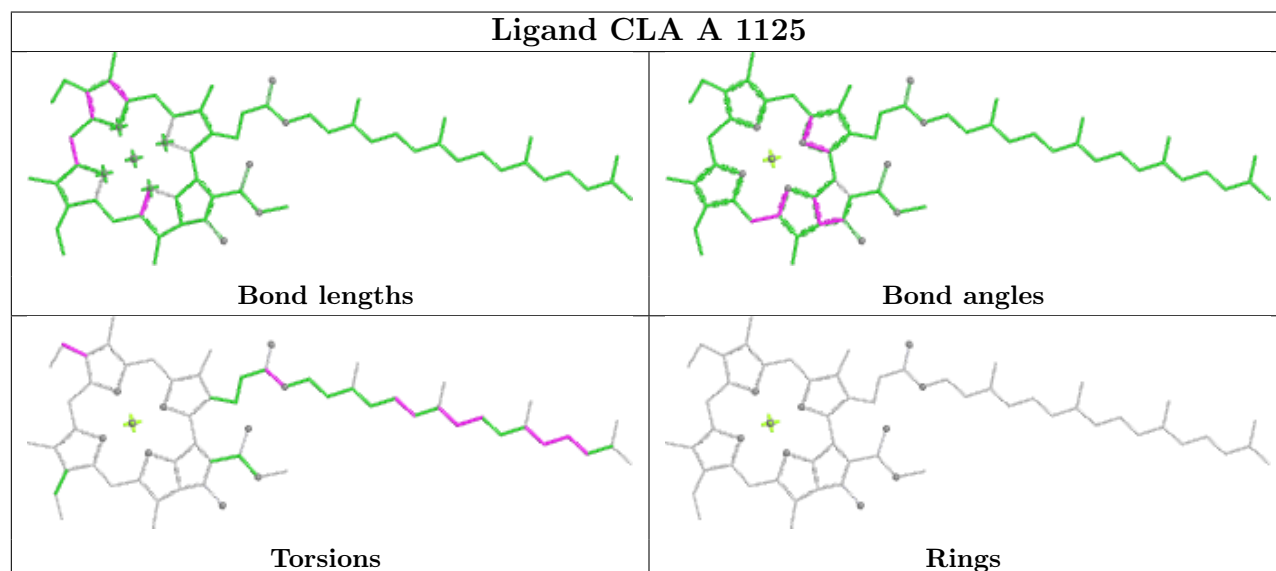
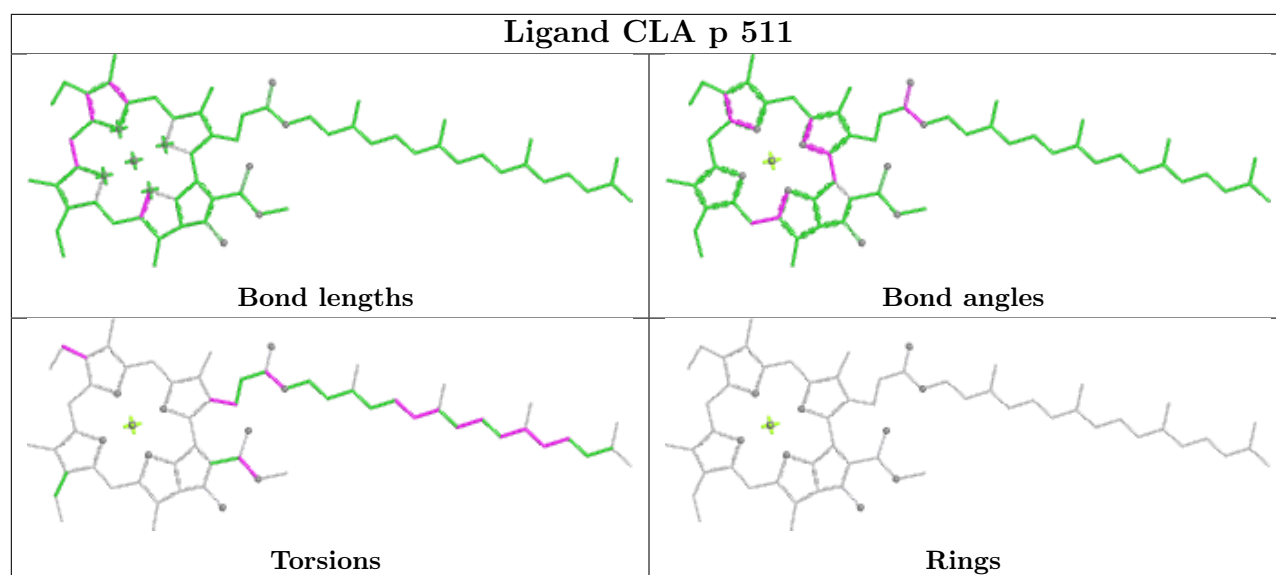


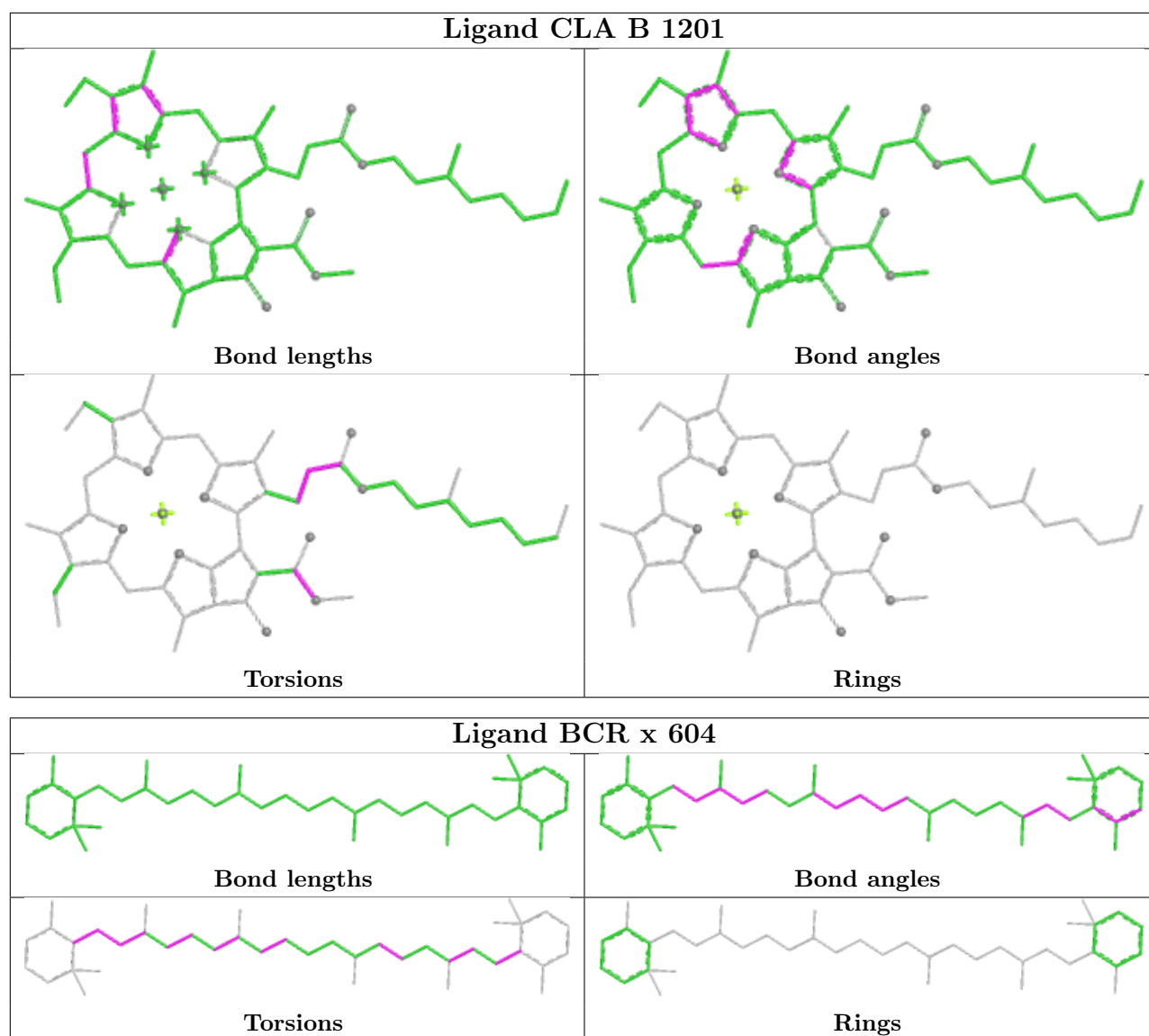
Ligand CLA H 1013



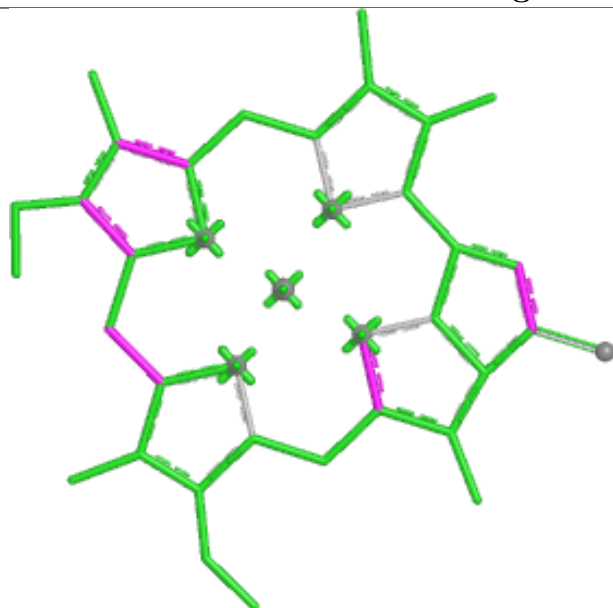
Ligand CLA u 501



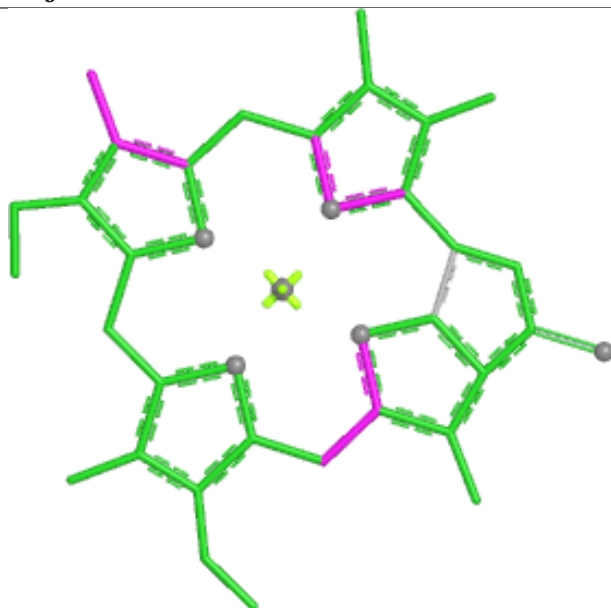




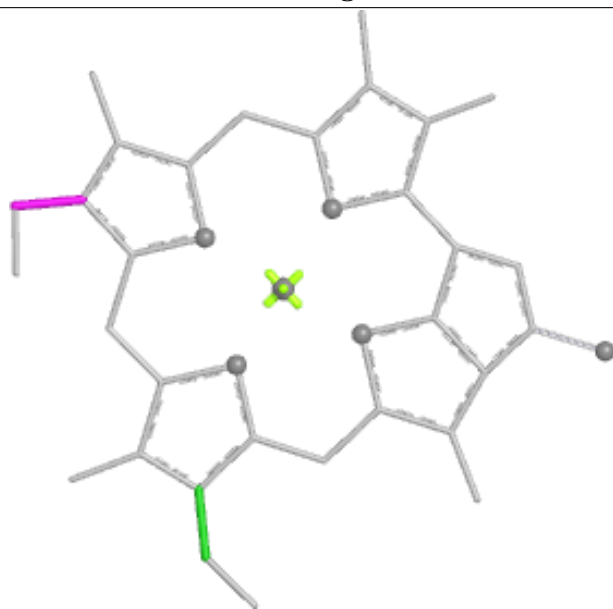
Ligand CLA j 1303



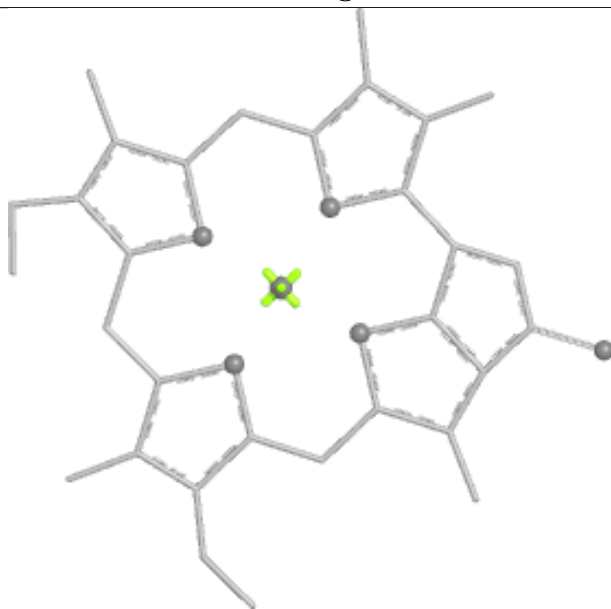
Bond lengths



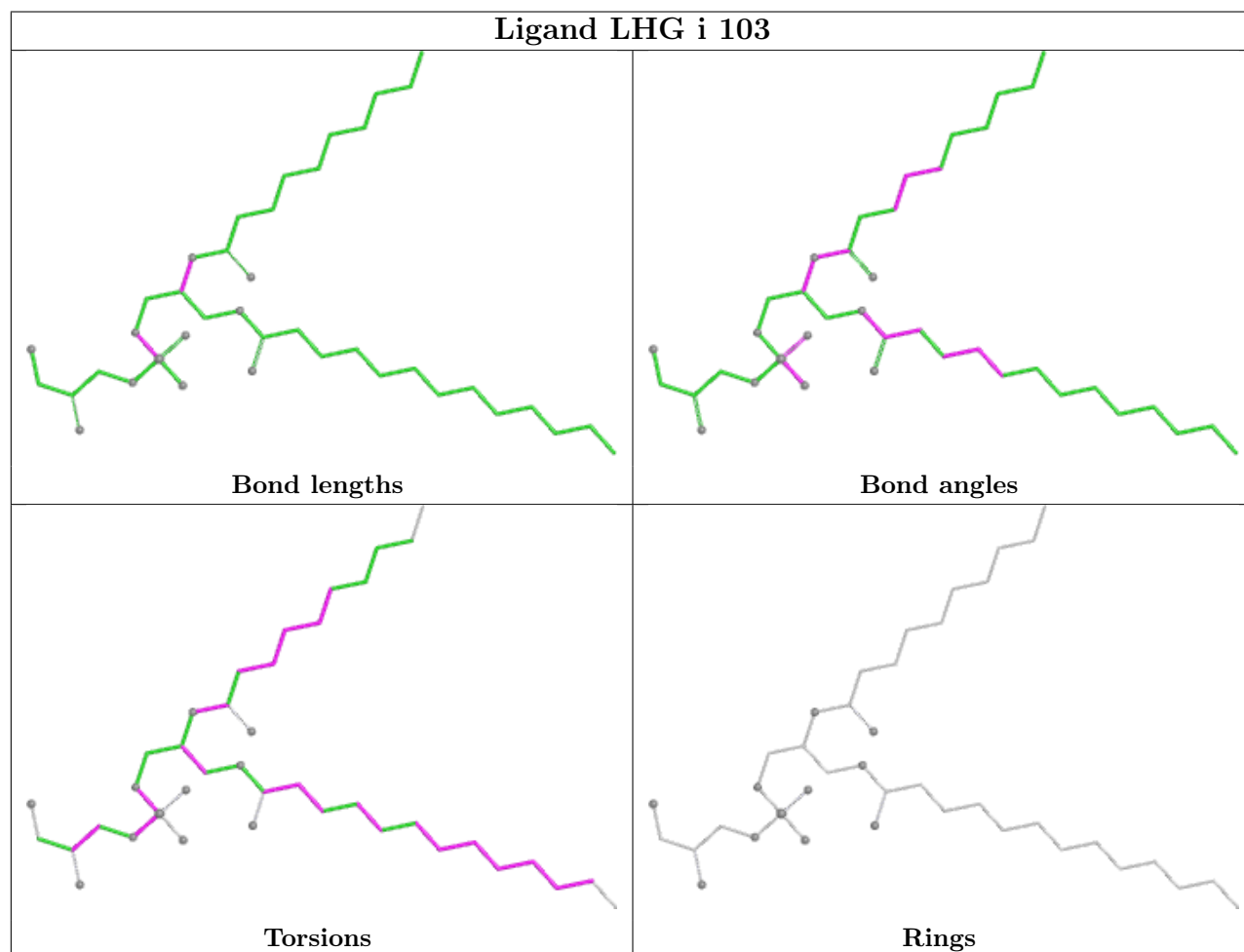
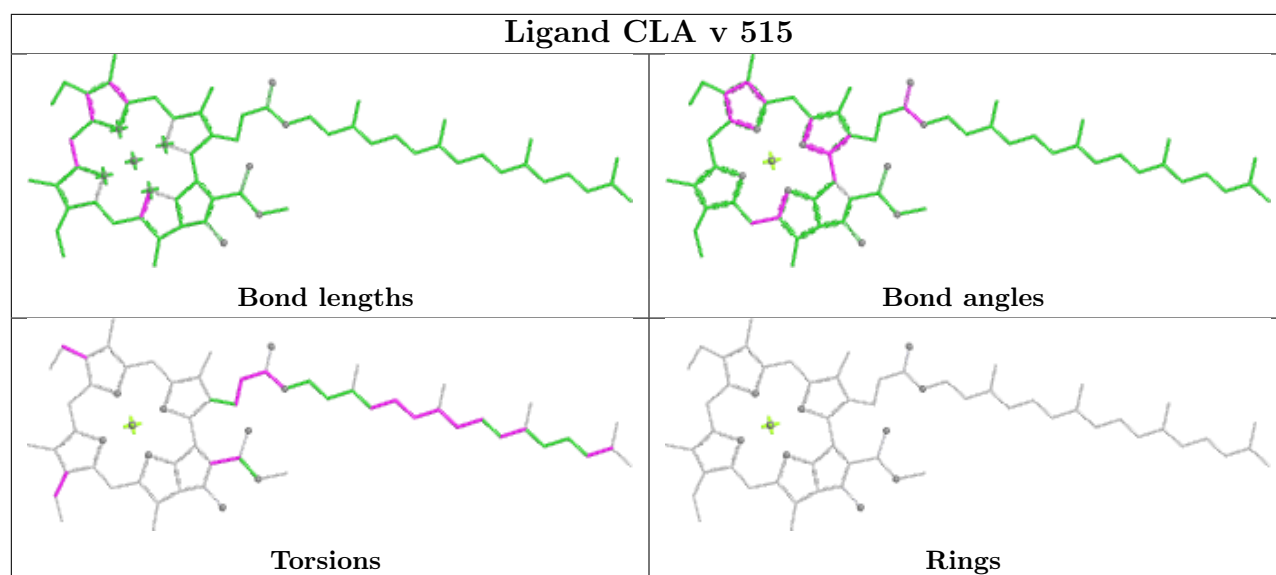
Bond angles

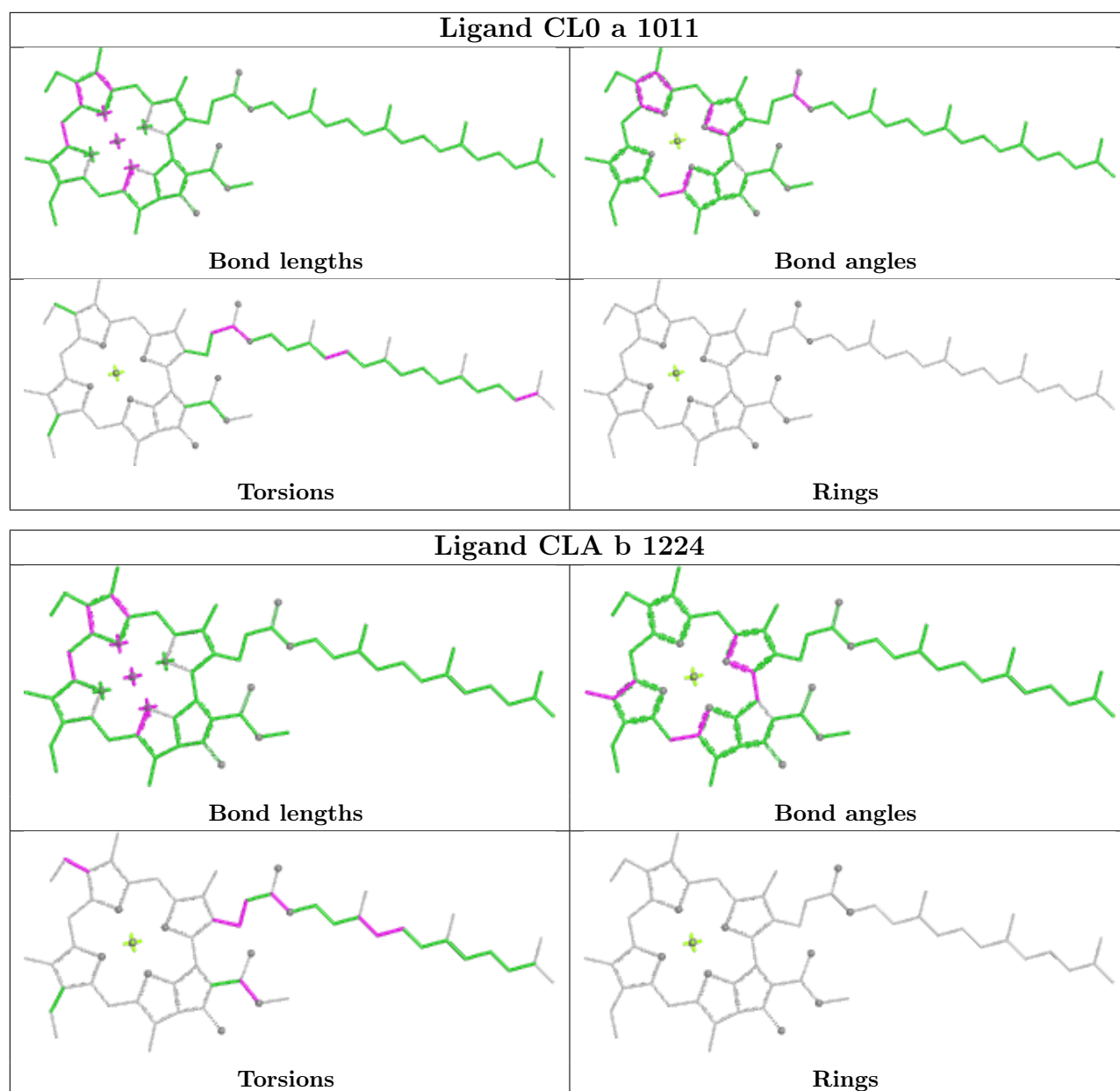


Torsions

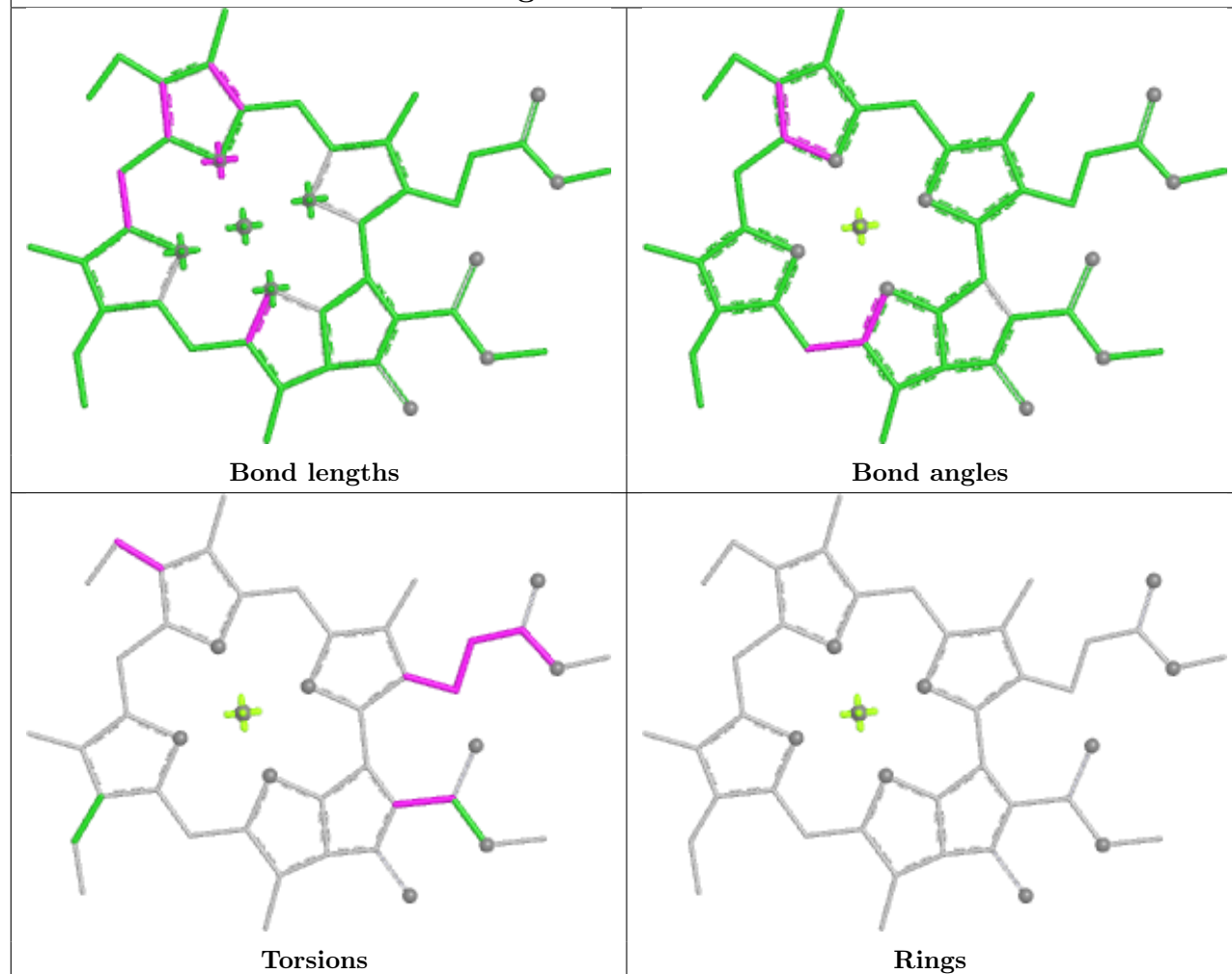


Rings

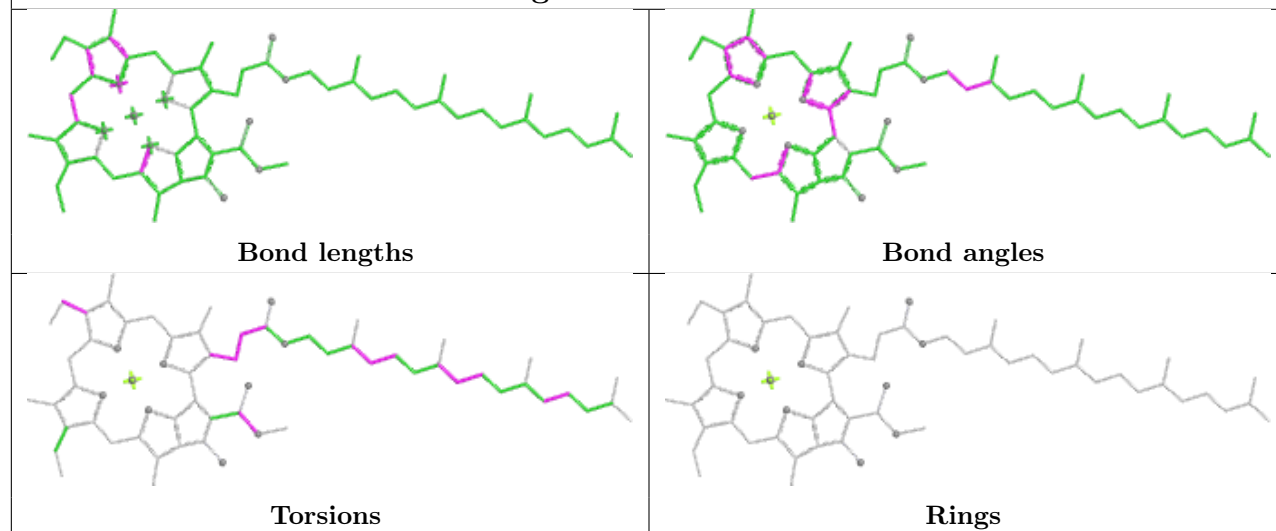


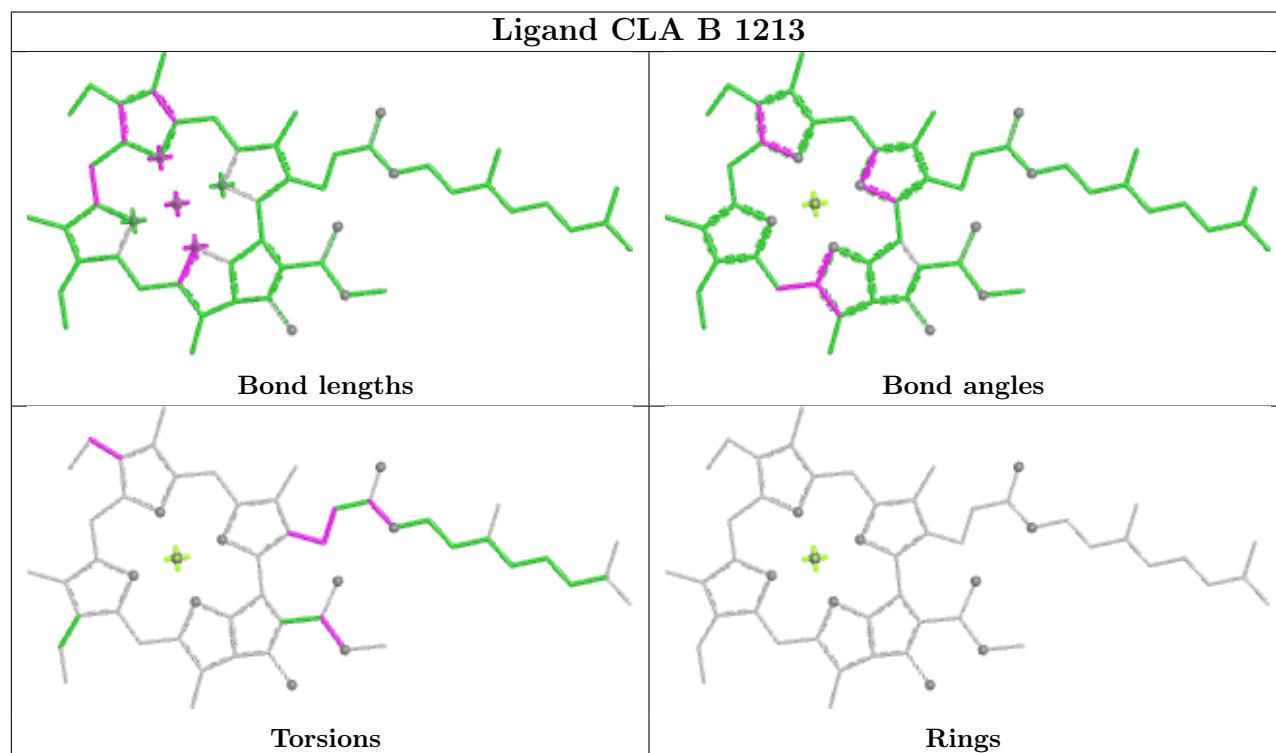
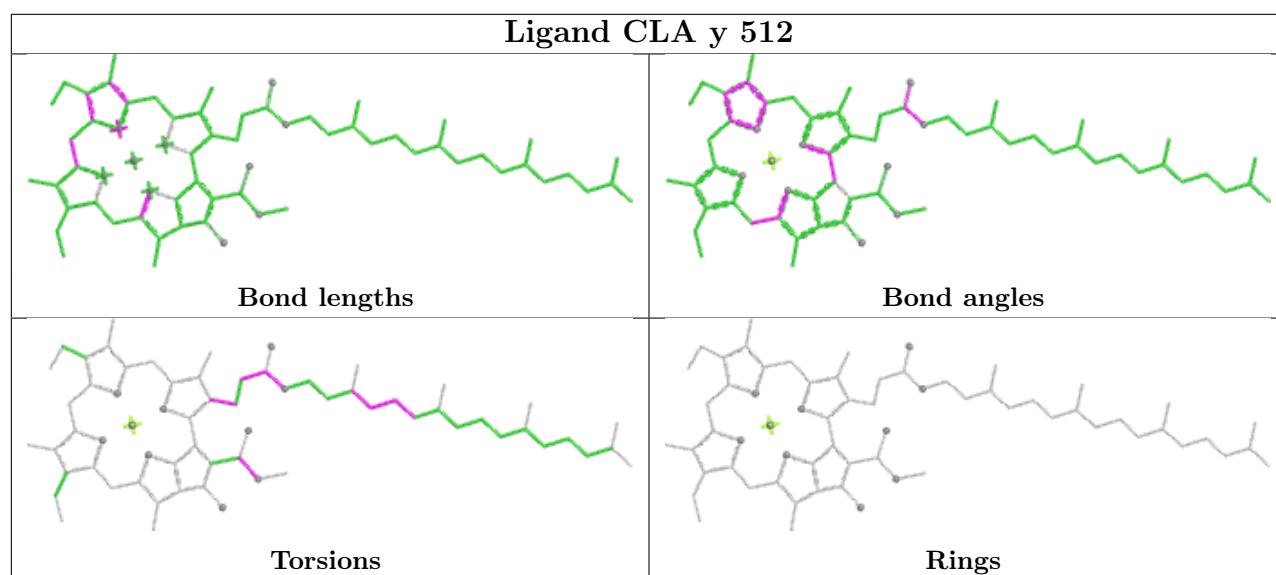


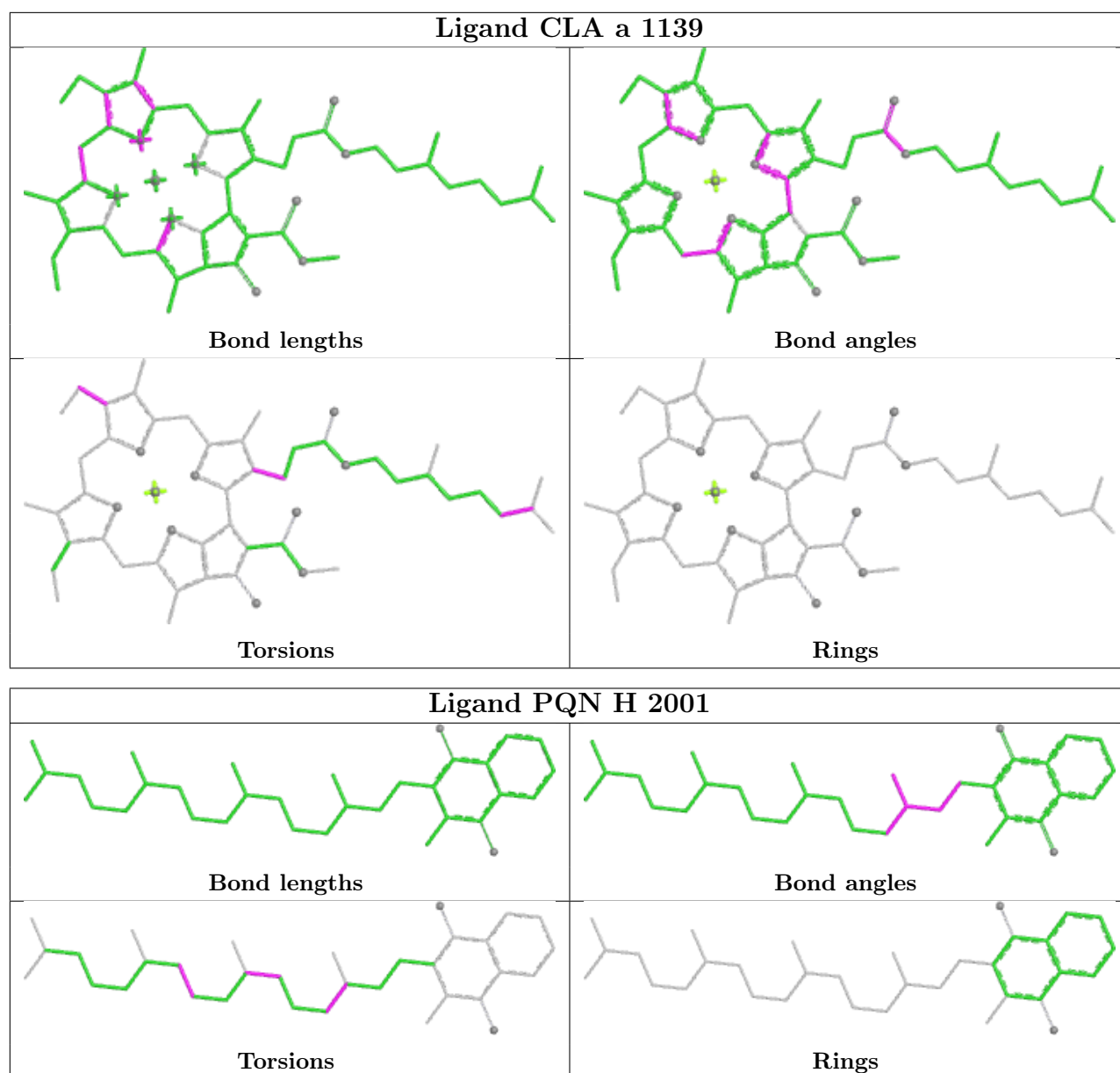
Ligand CLA o 516



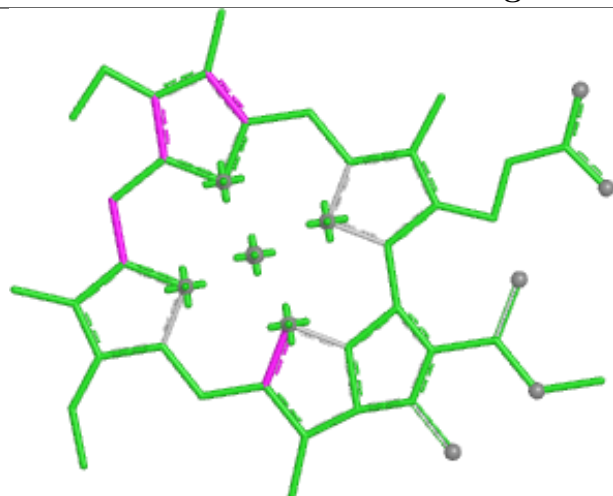
Ligand CLA Y 505



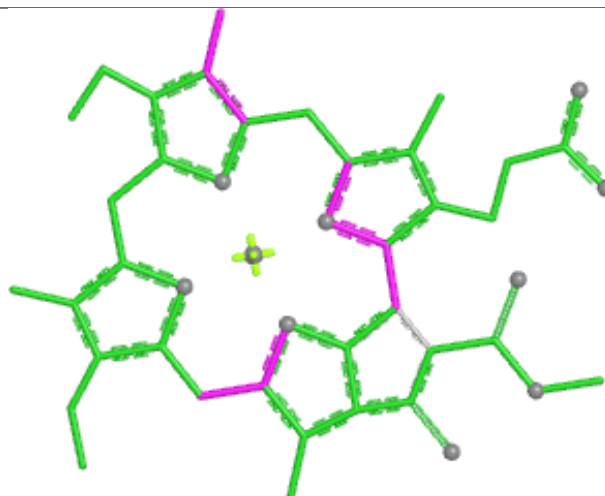




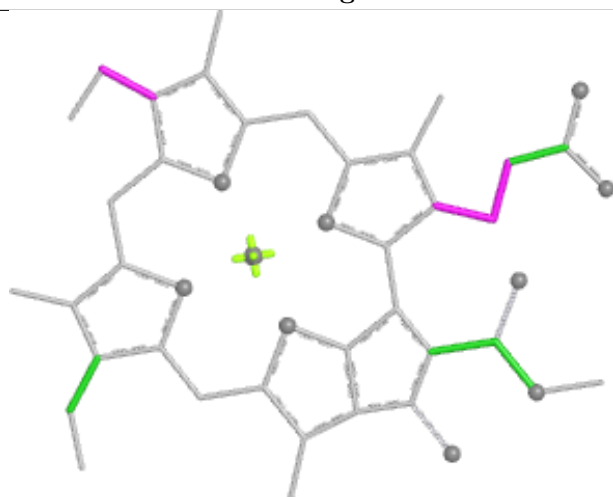
Ligand CLA G 1231



Bond lengths



Bond angles

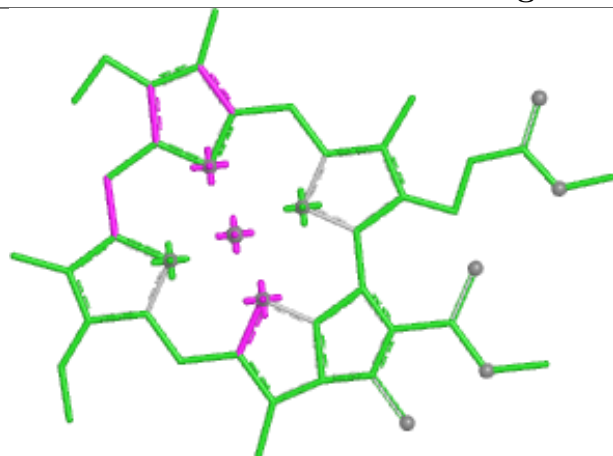


Torsions

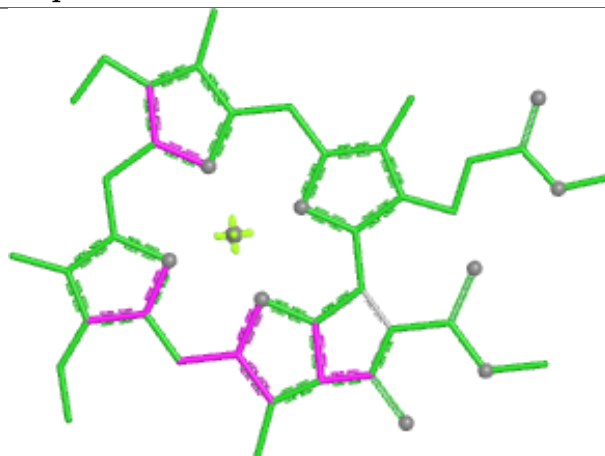


Rings

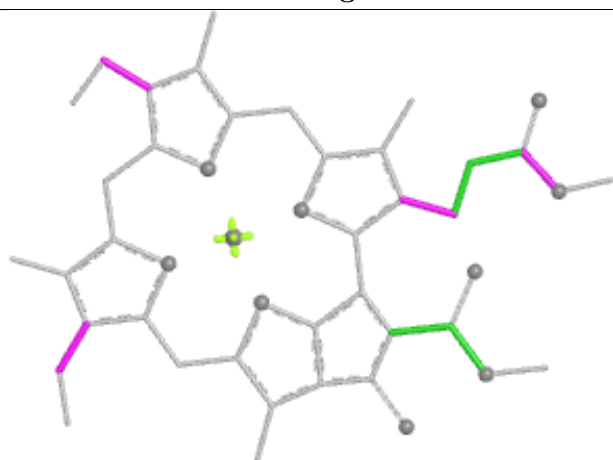
Ligand CLA p 503



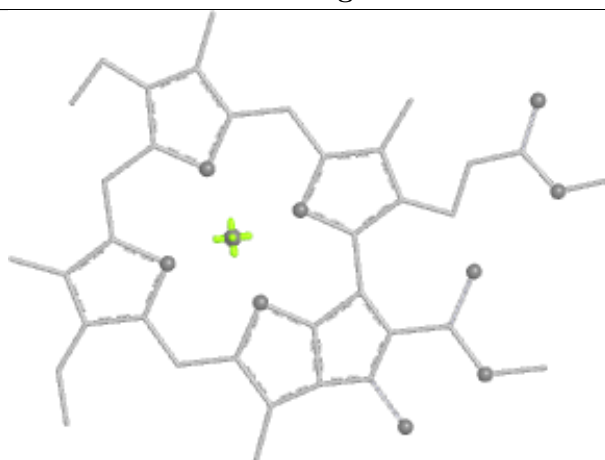
Bond lengths



Bond angles

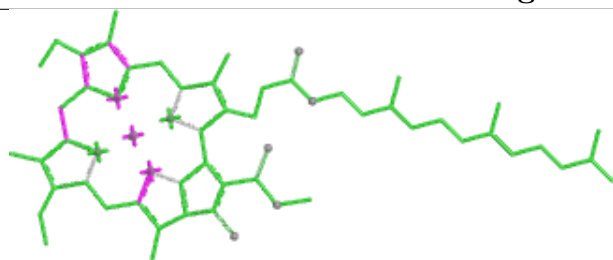


Torsions

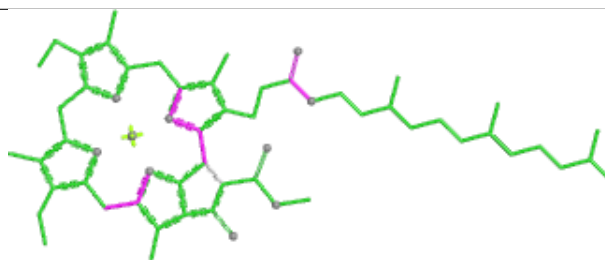


Rings

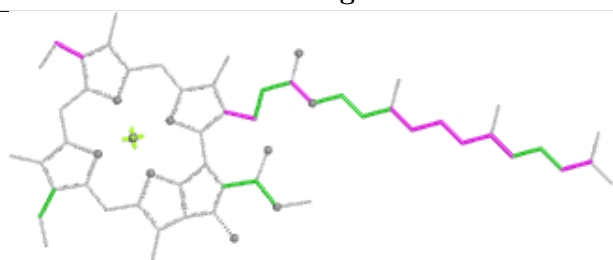
Ligand CLA x 506



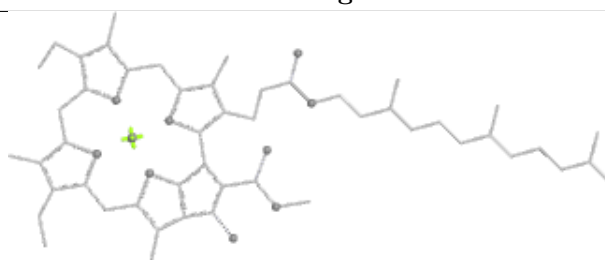
Bond lengths



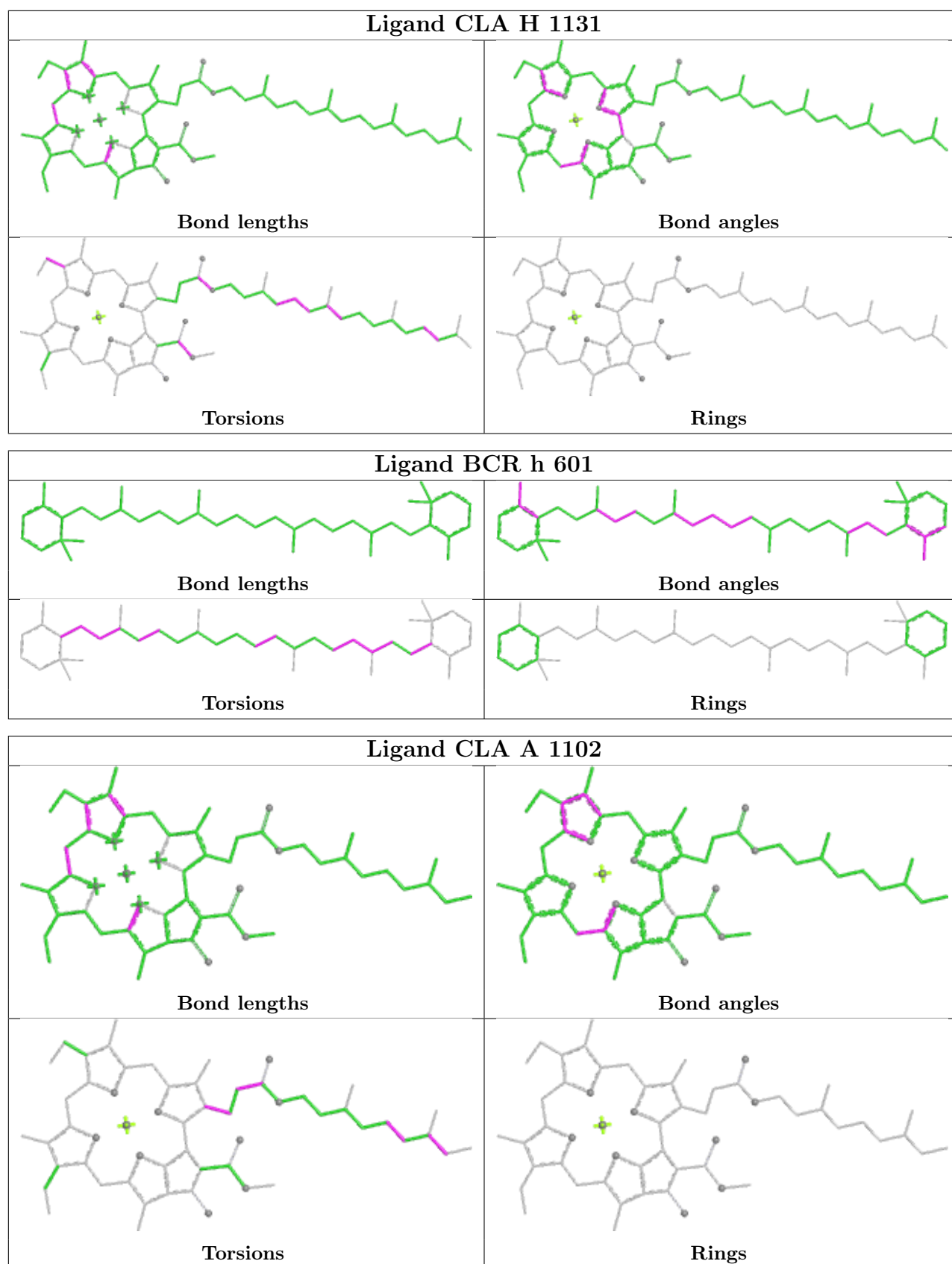
Bond angles

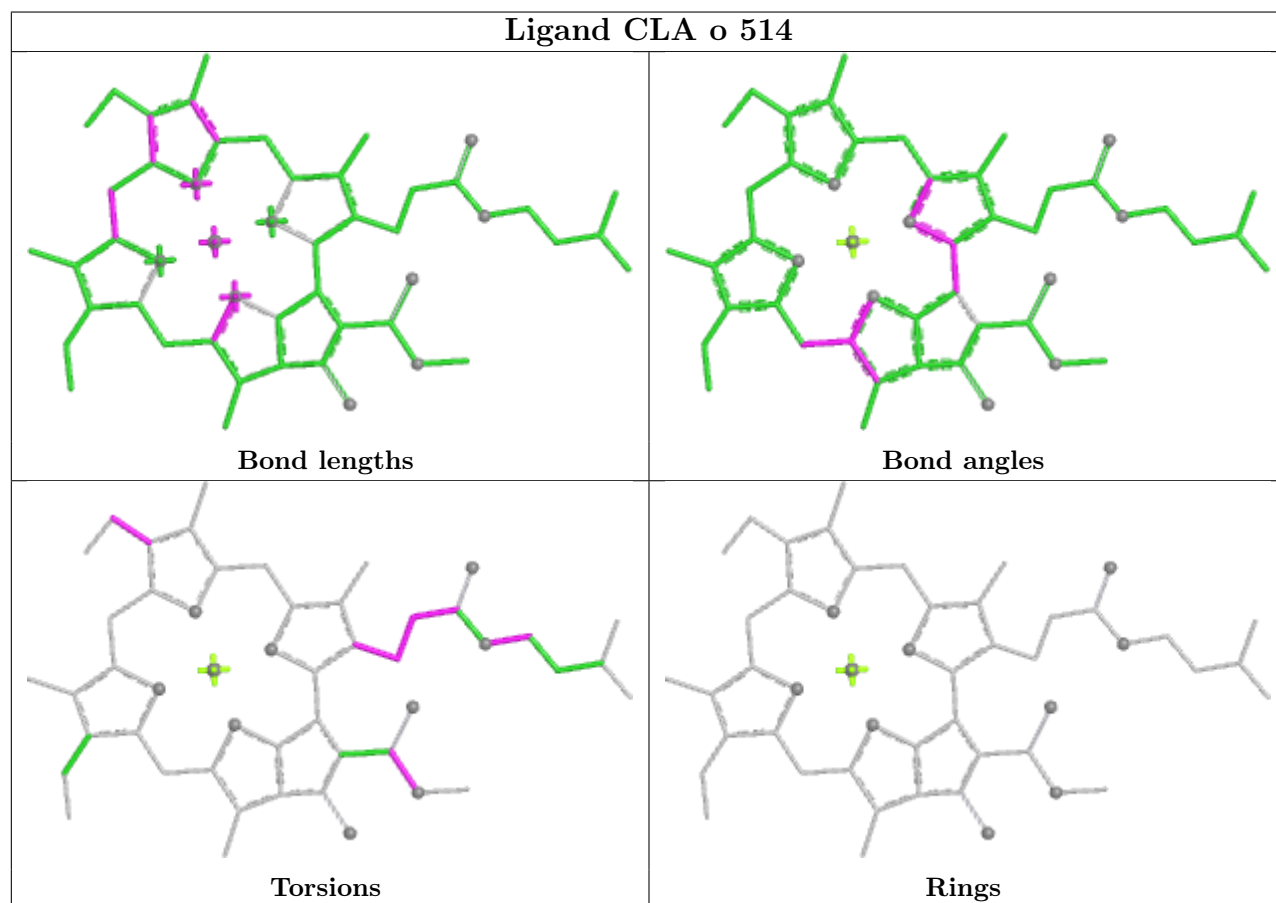
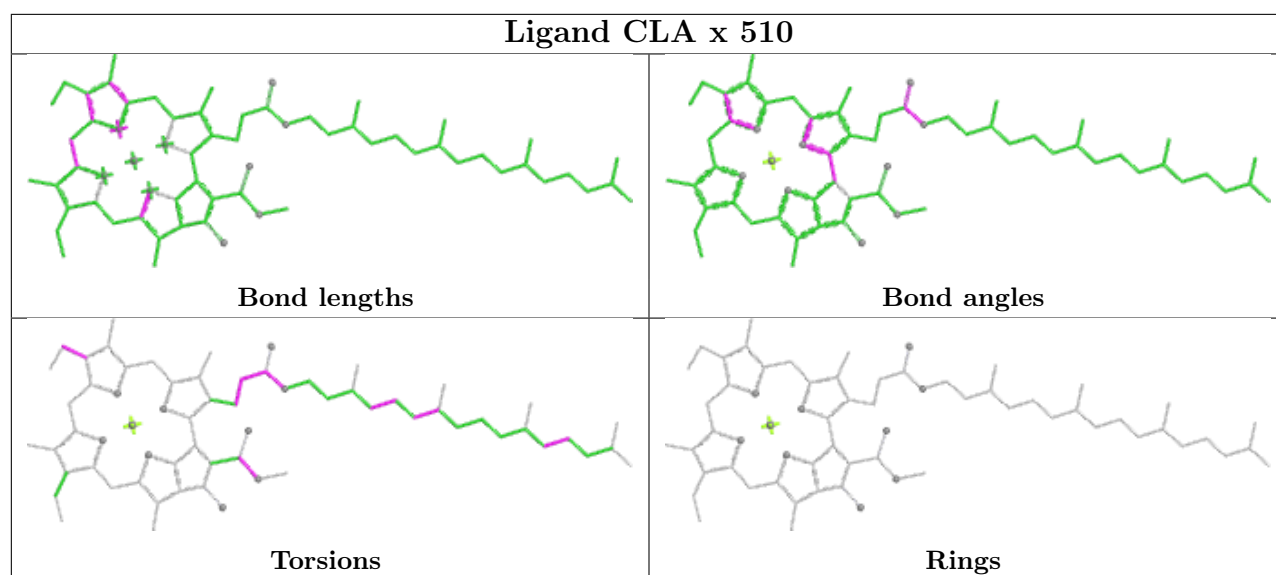


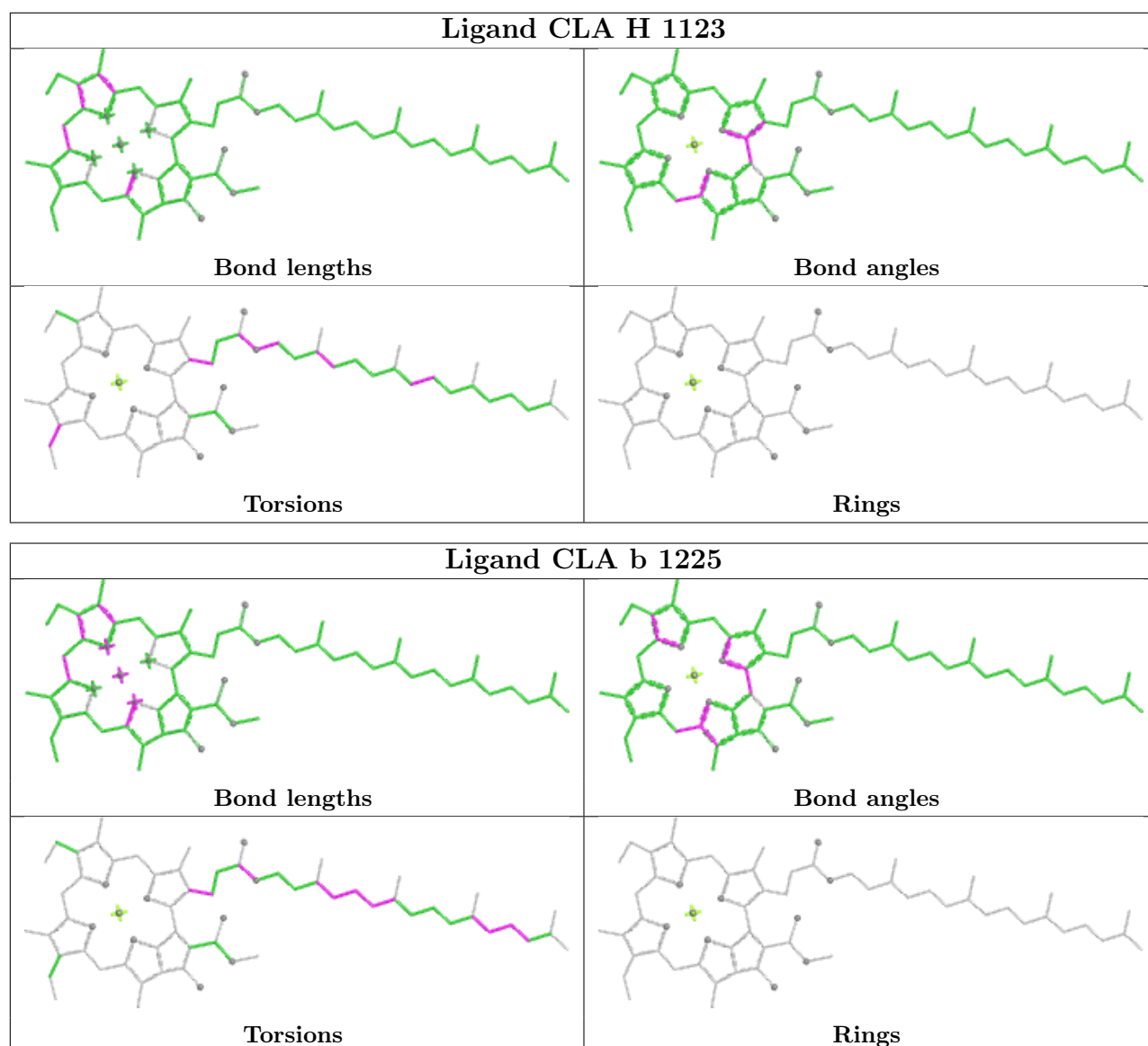
Torsions

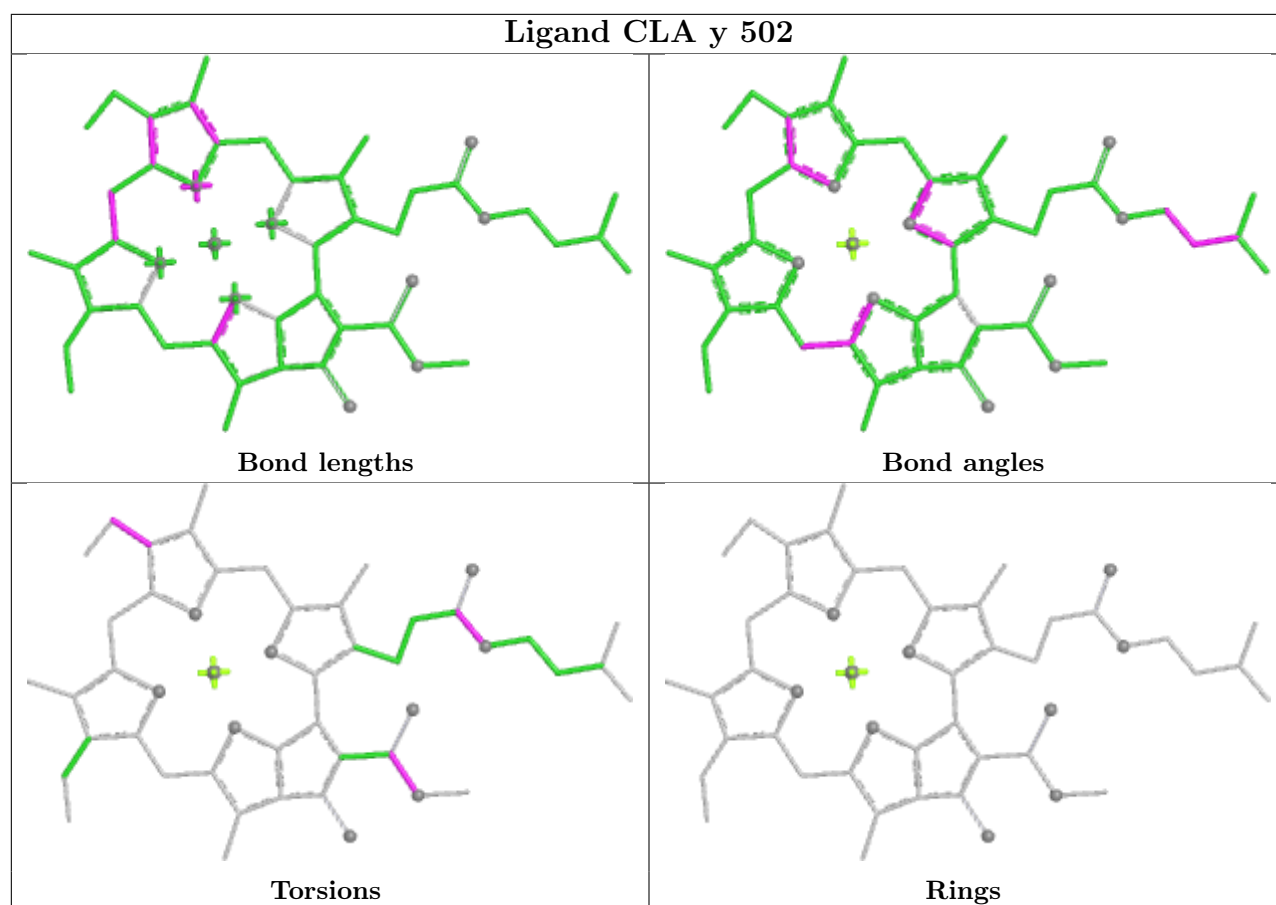


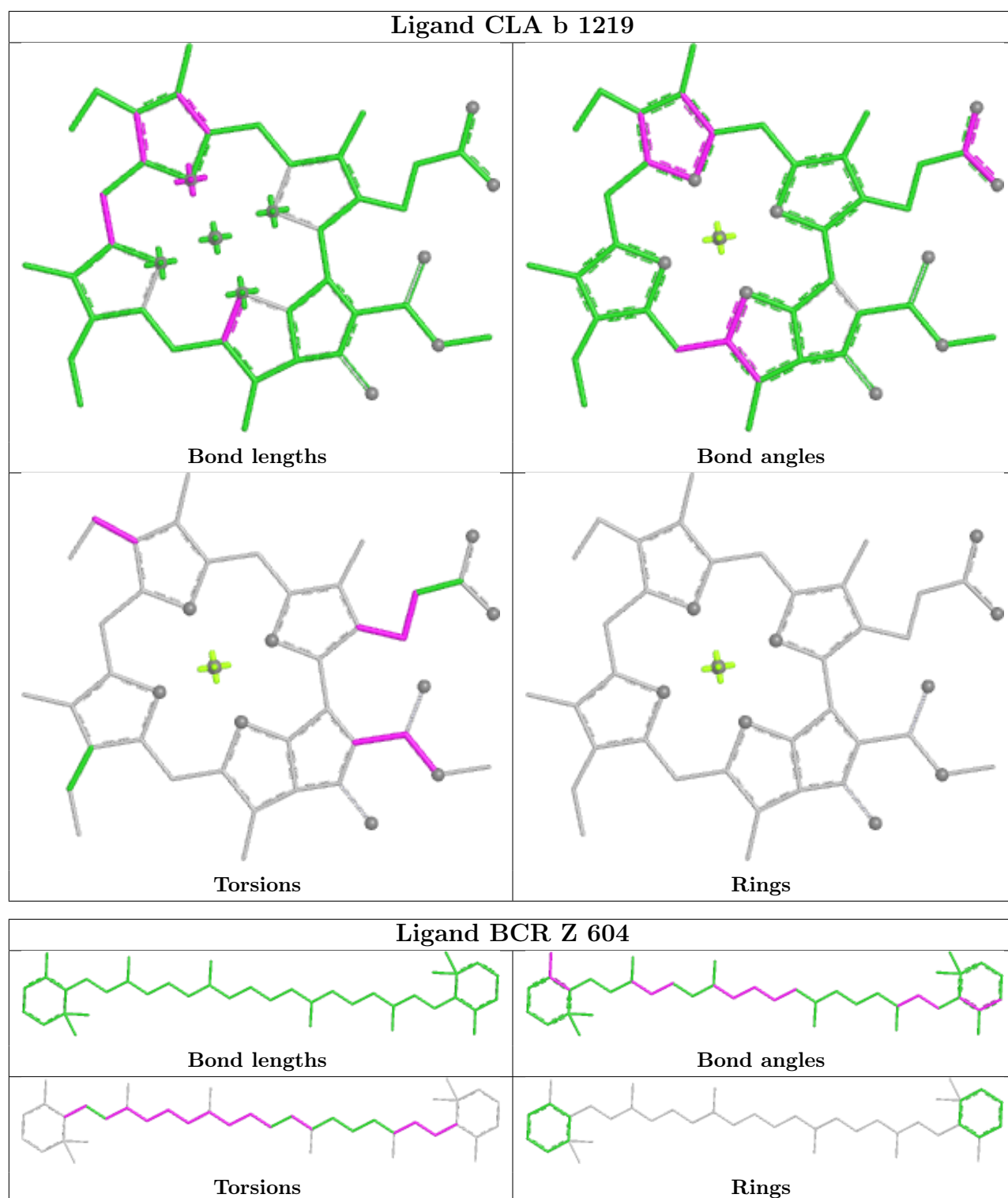
Rings

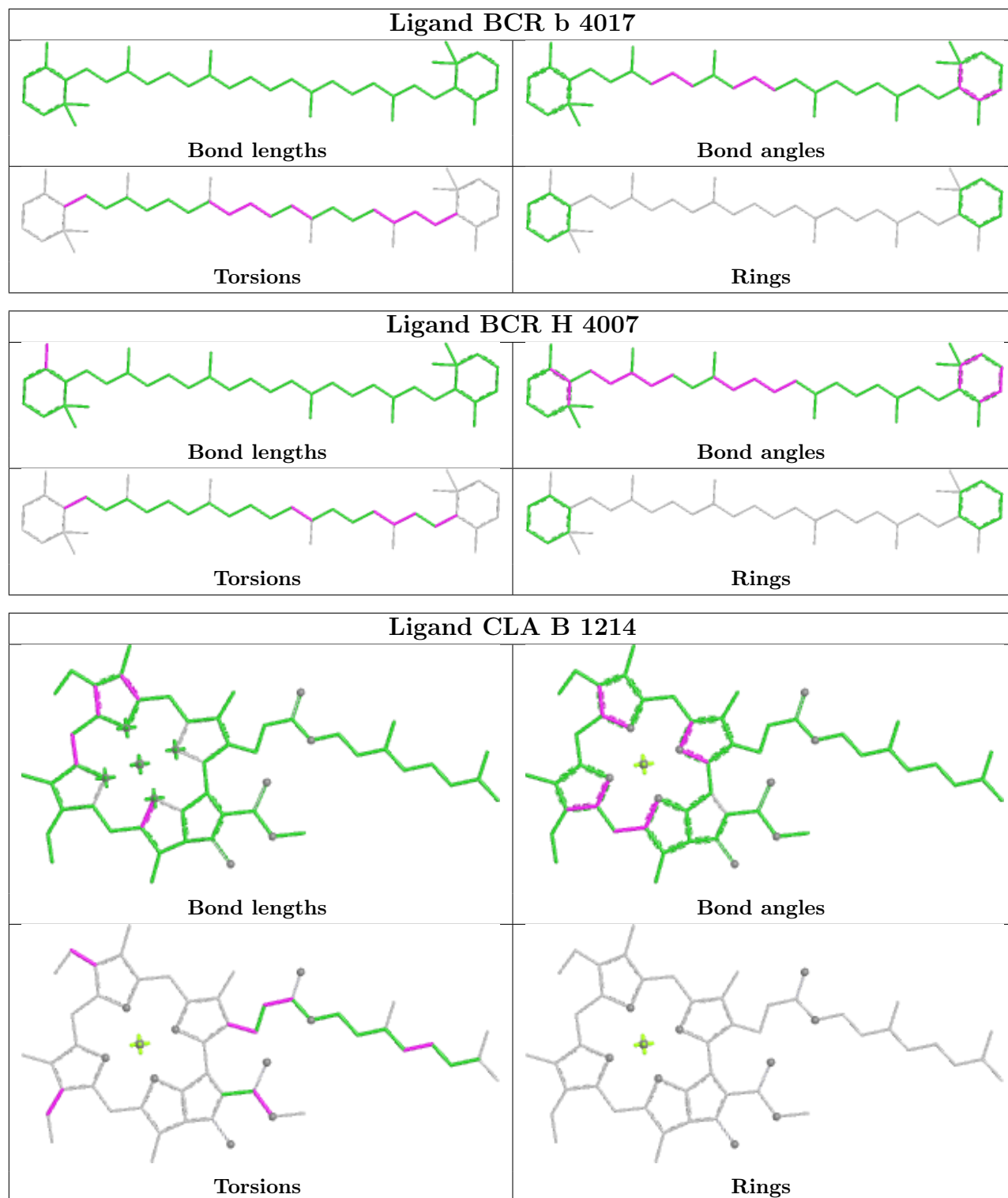


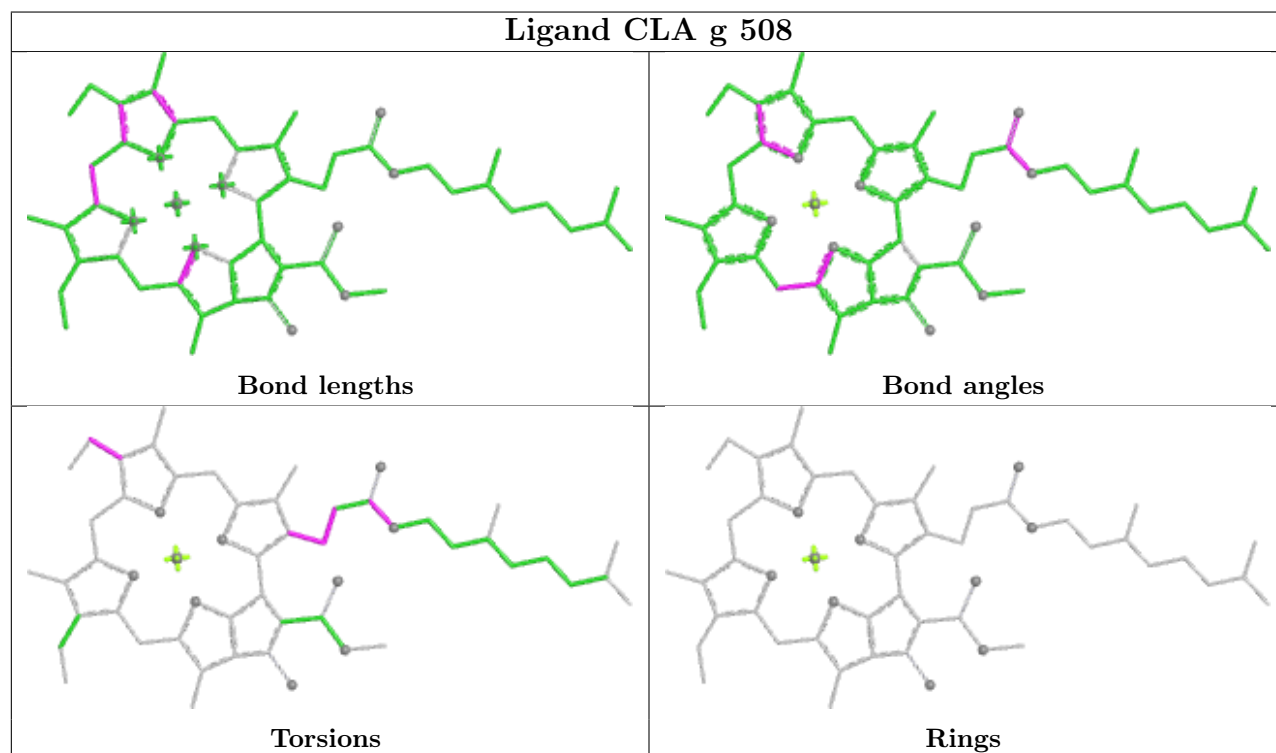
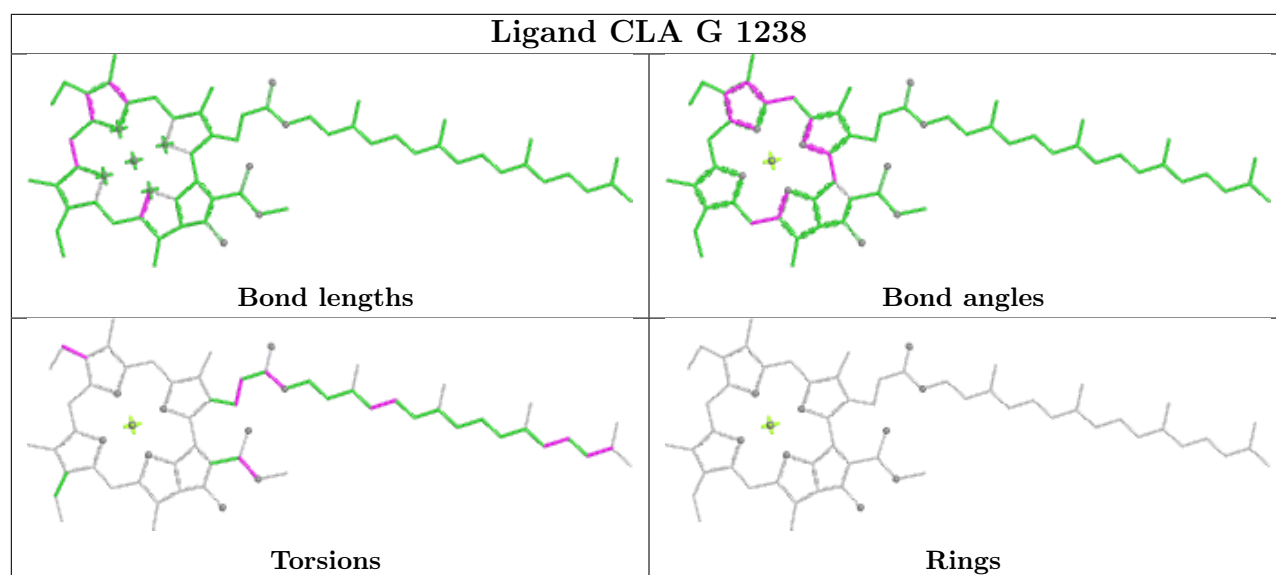


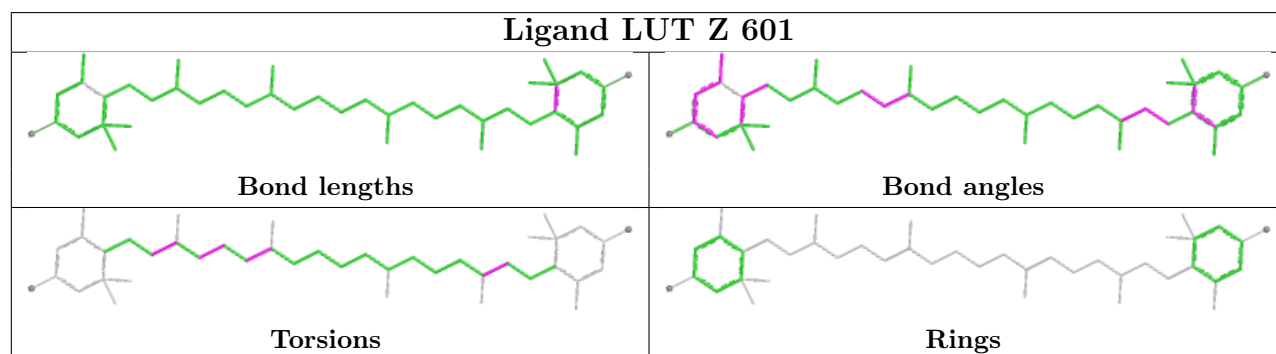
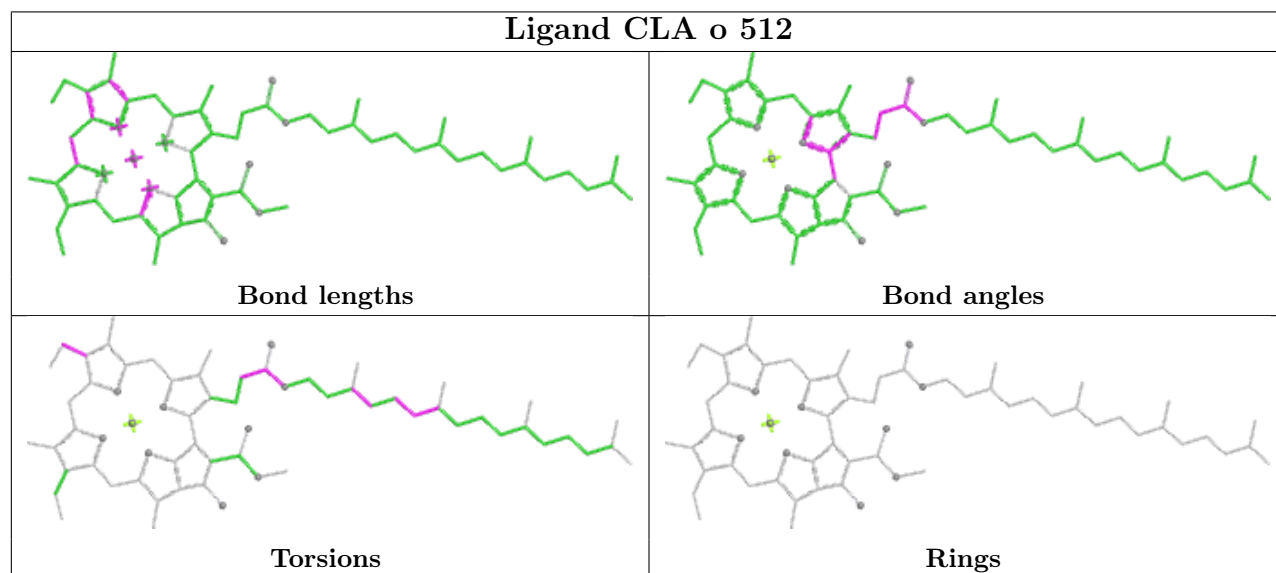
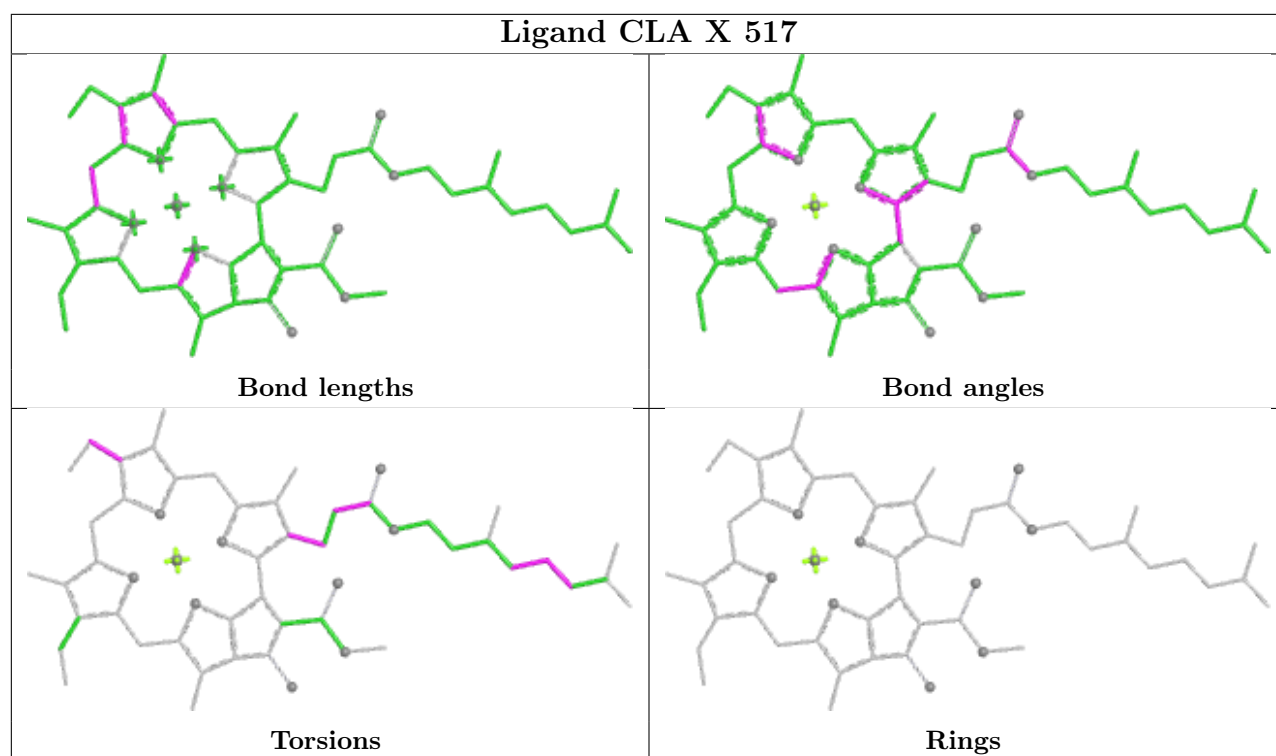


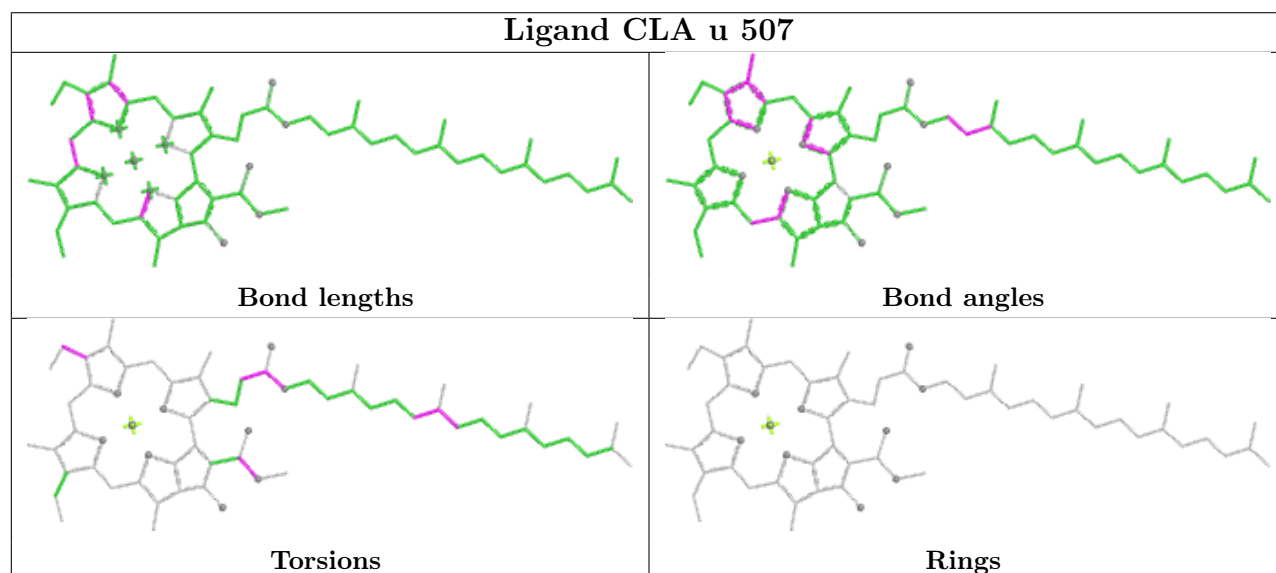
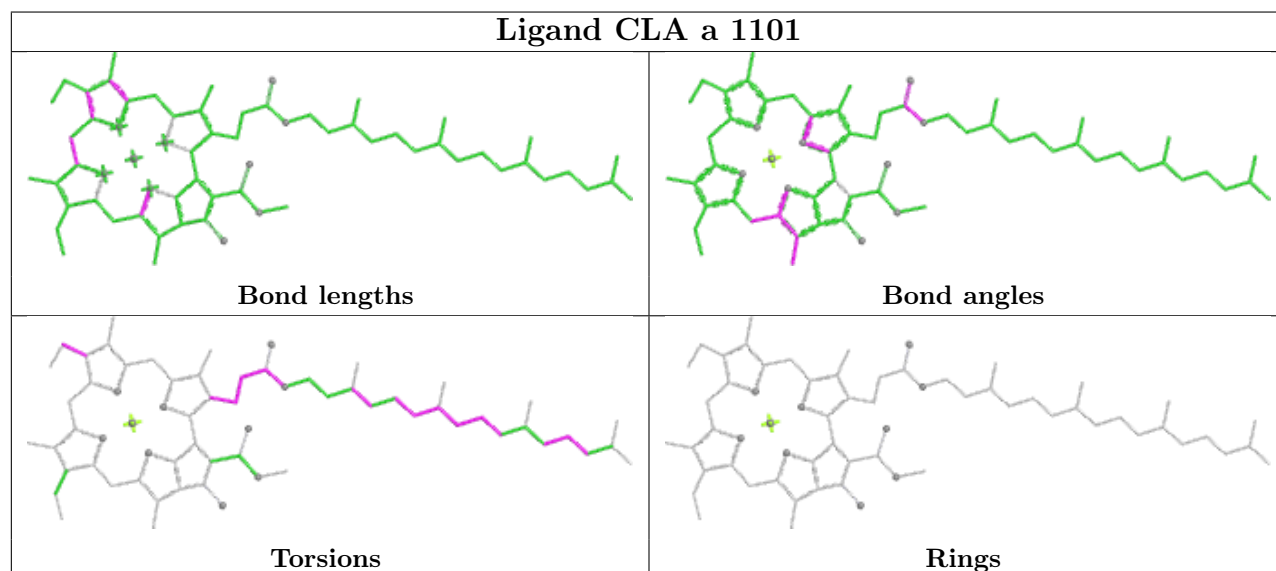
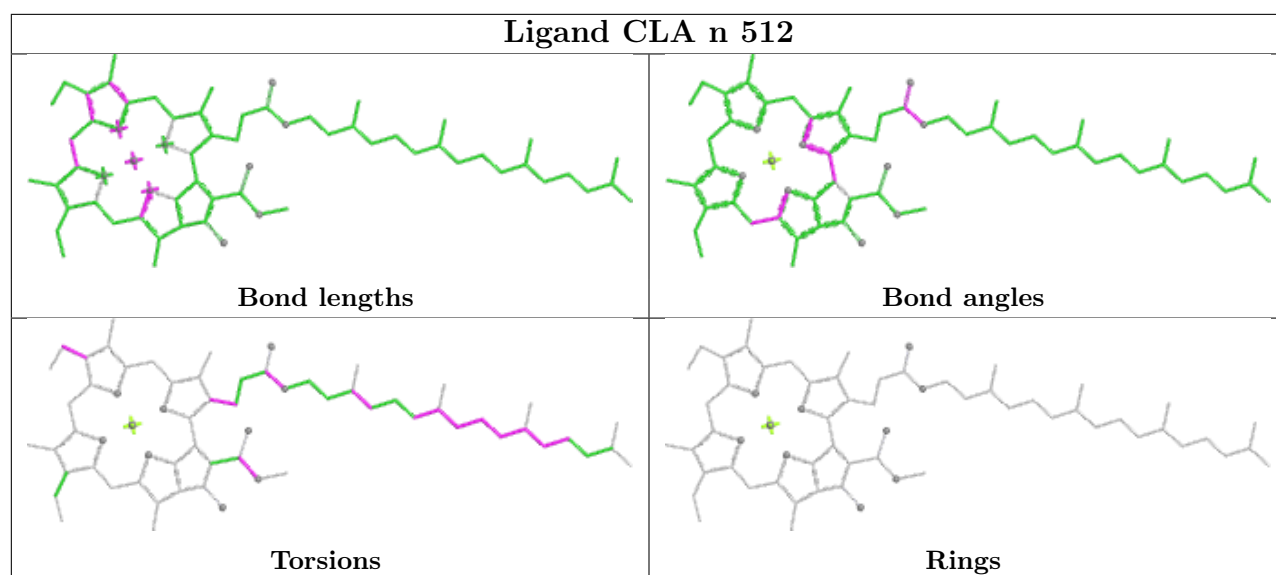


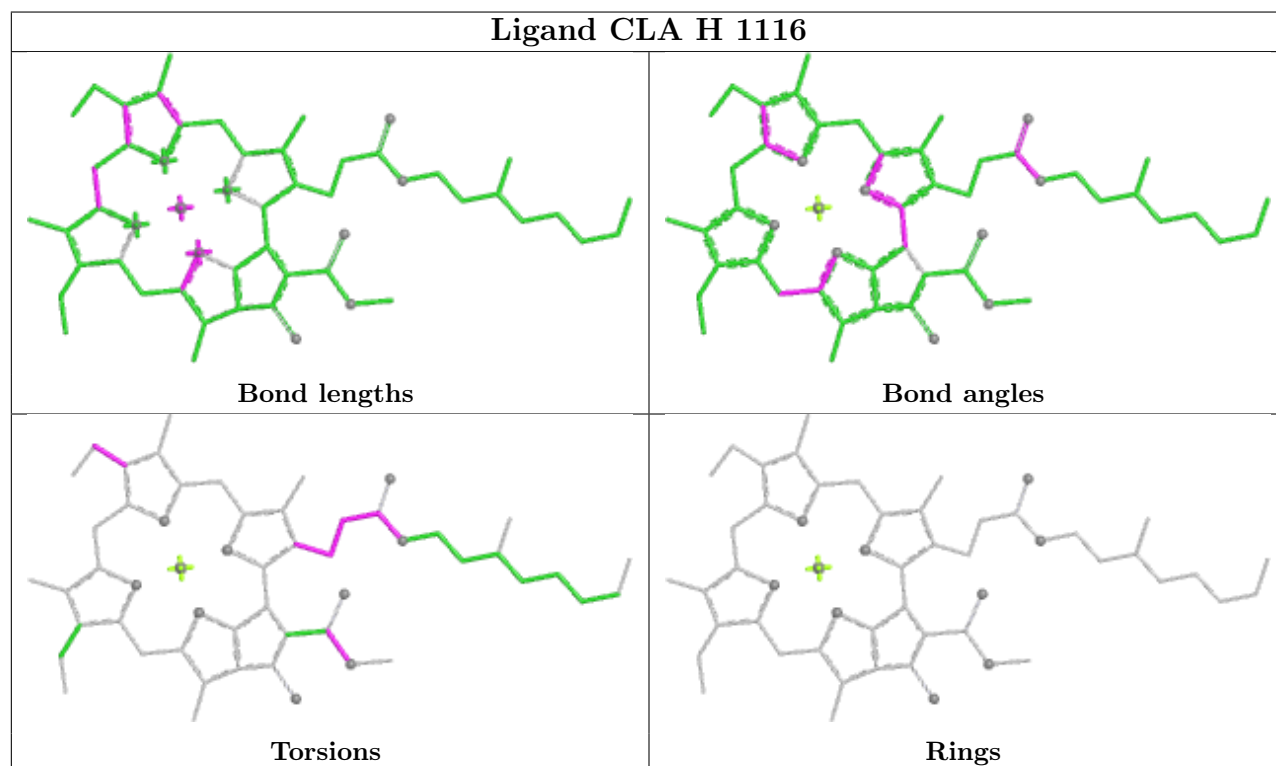
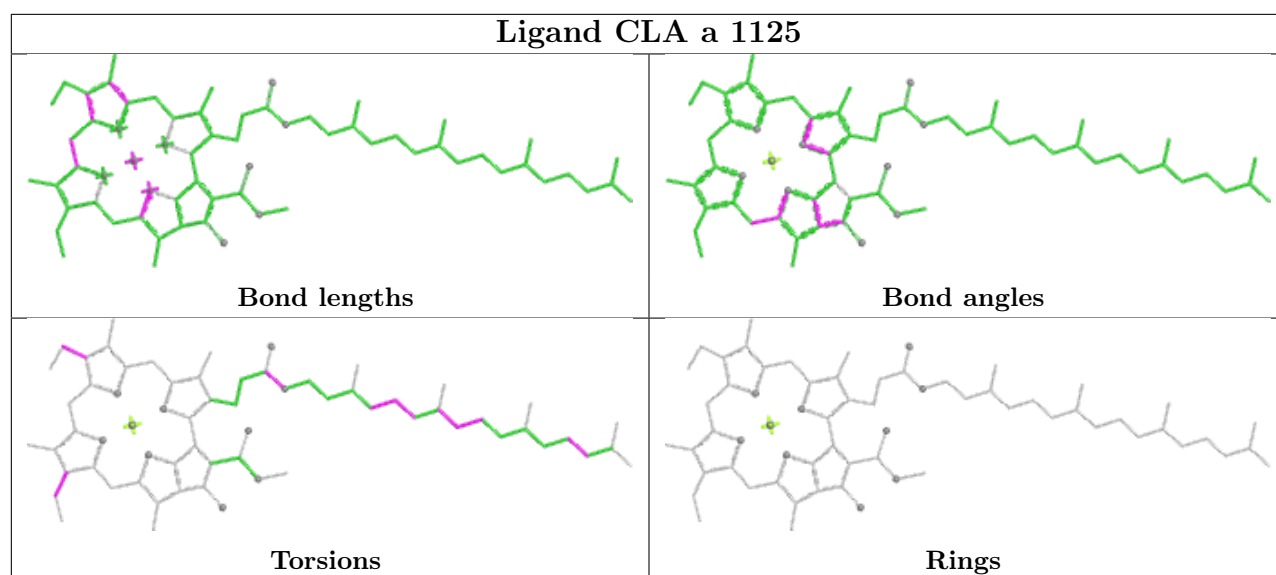




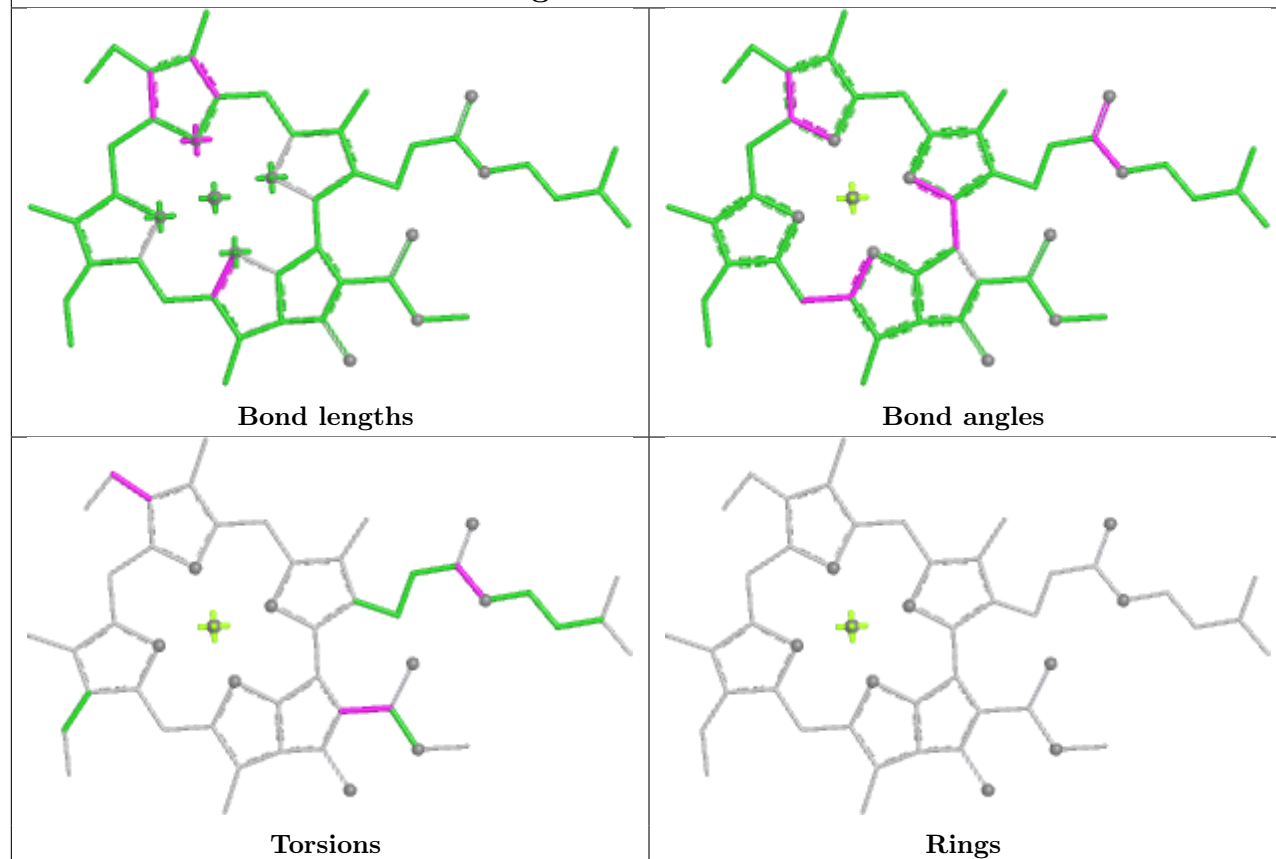




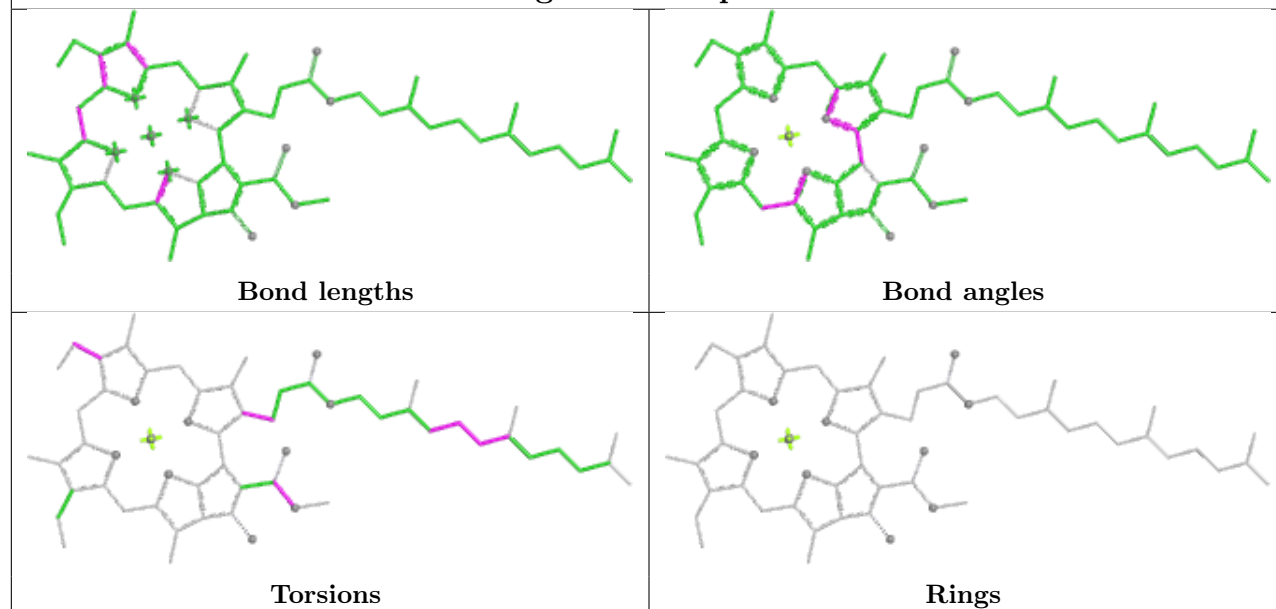


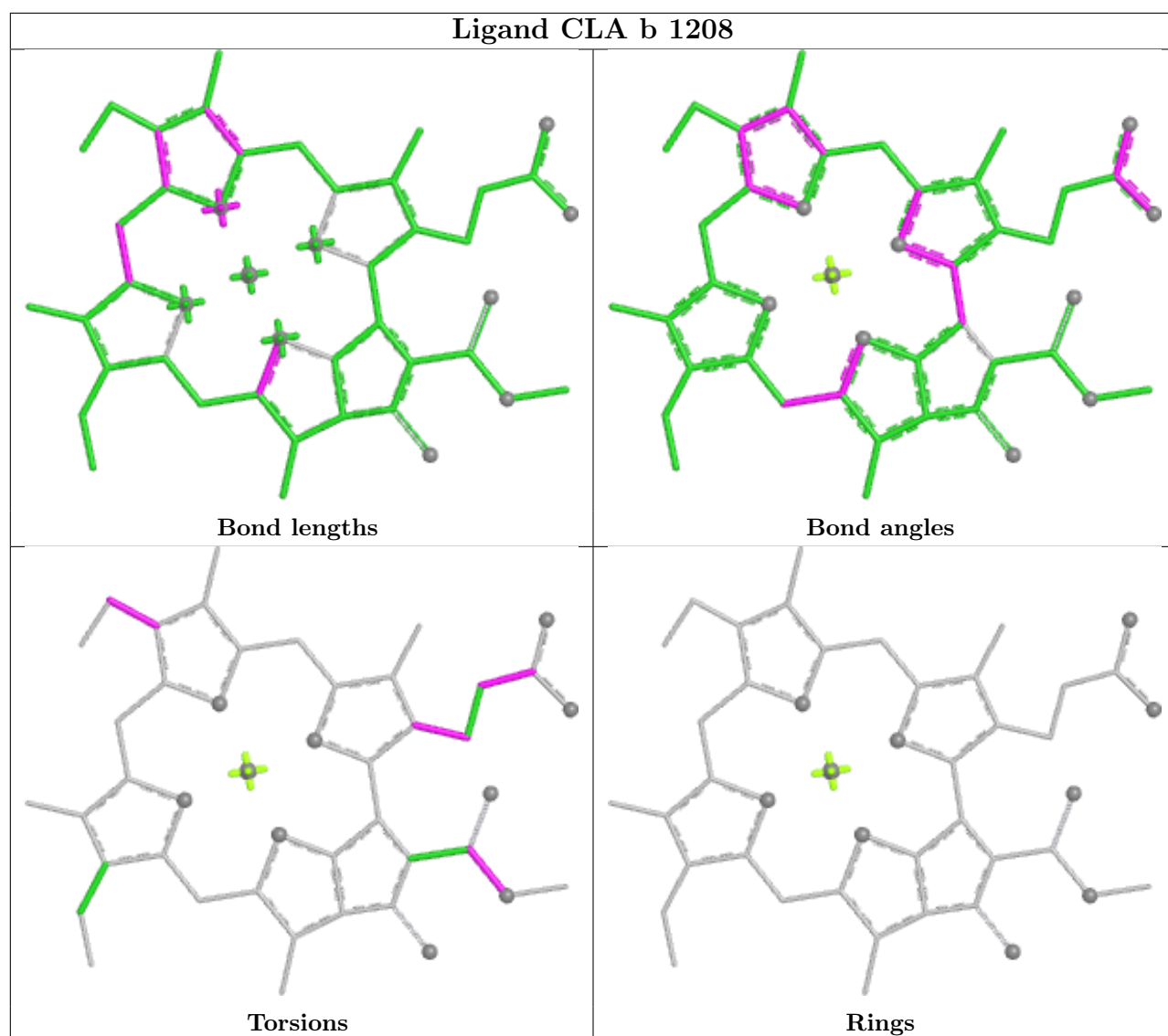


Ligand CLA Y 502

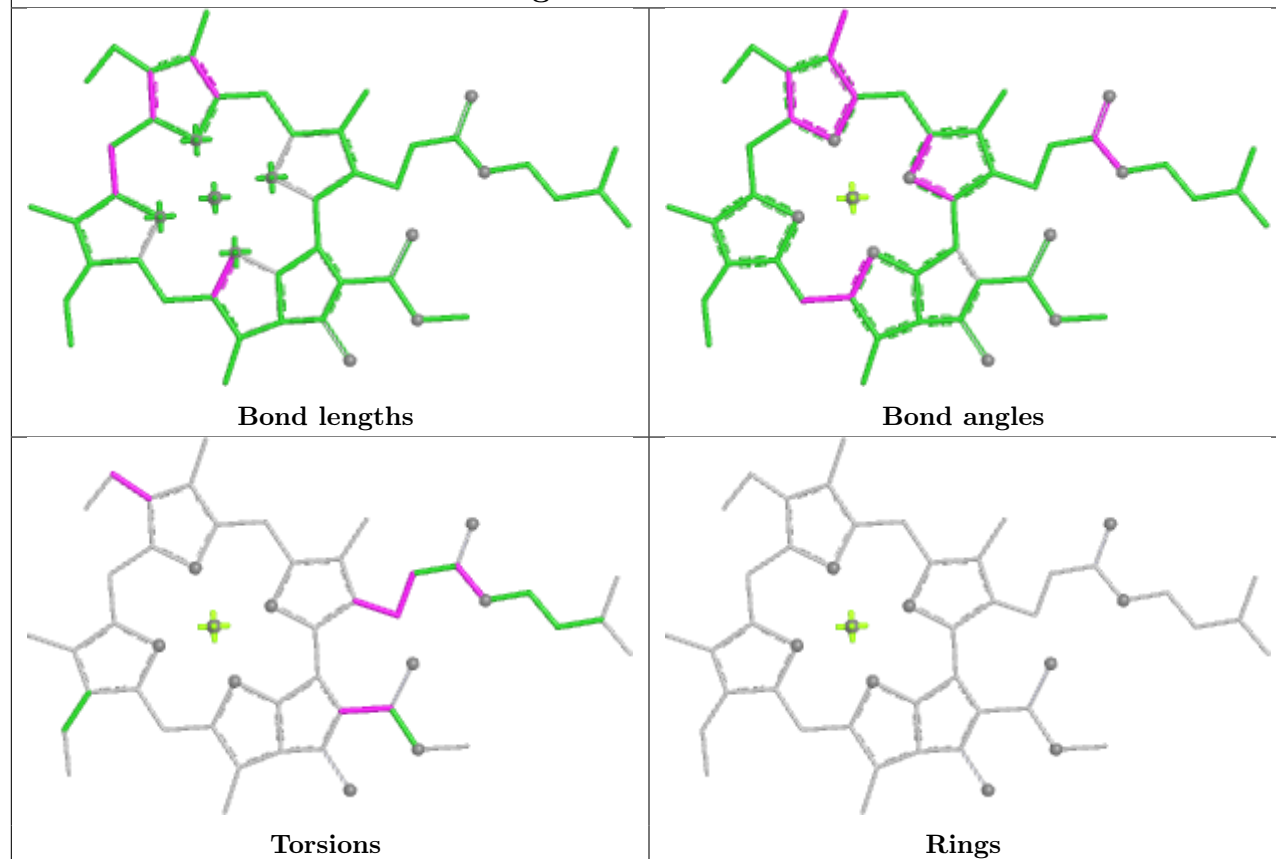


Ligand CLA q 510

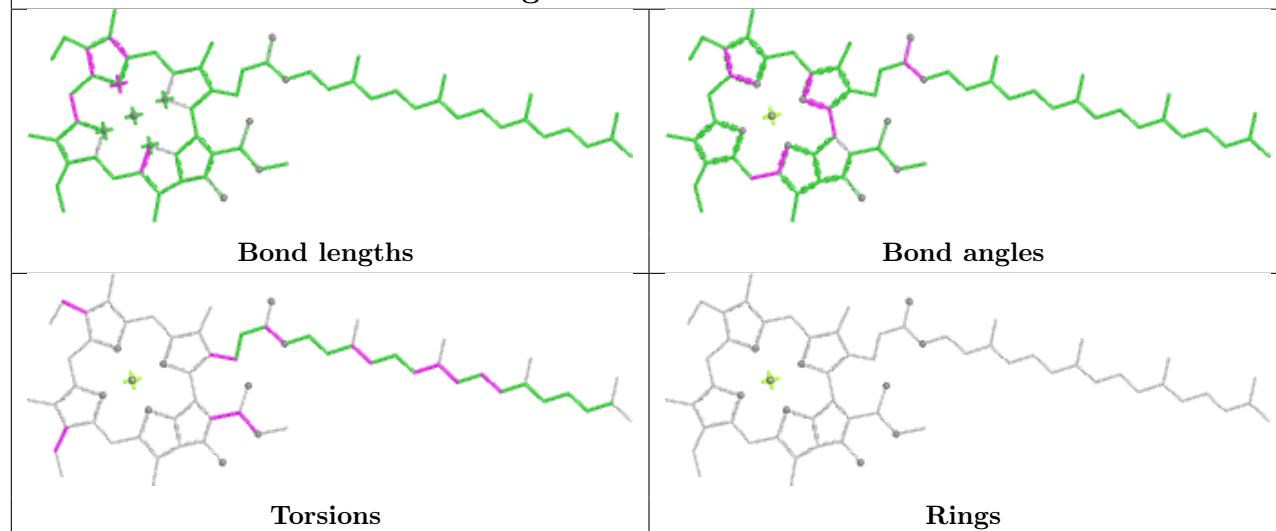


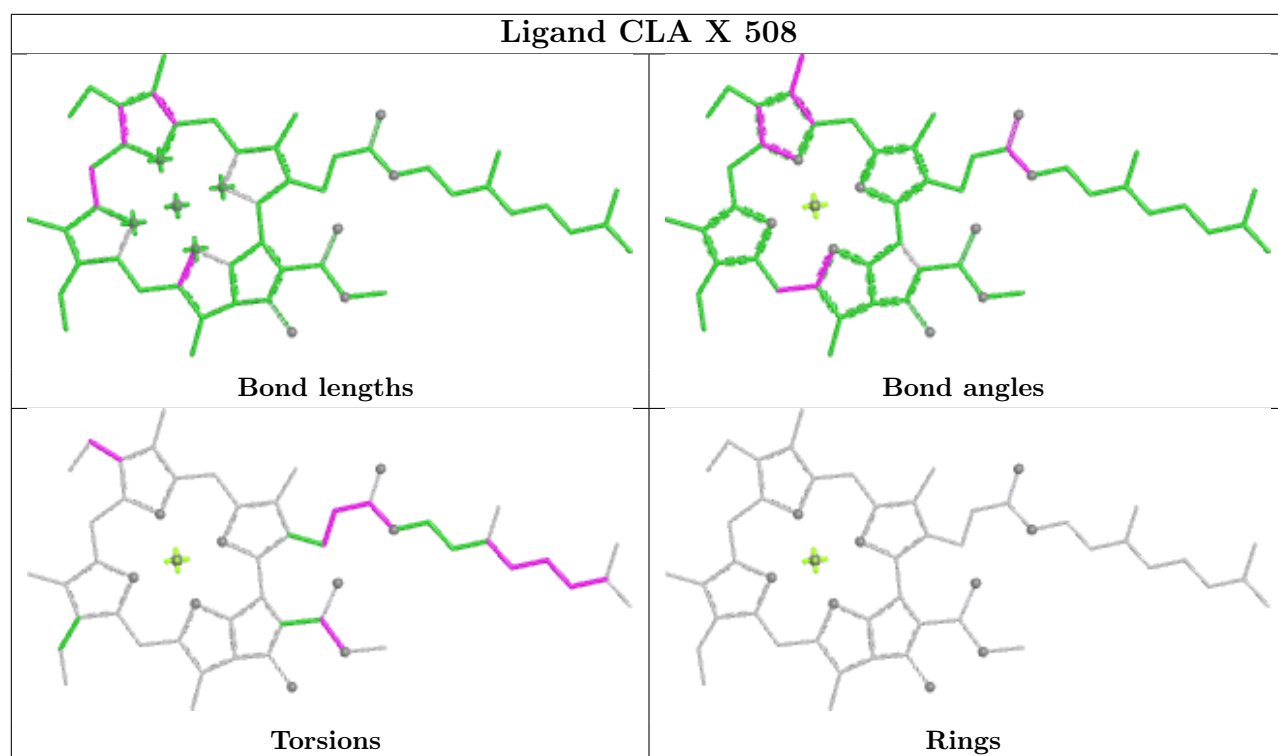


Ligand CLA w 513

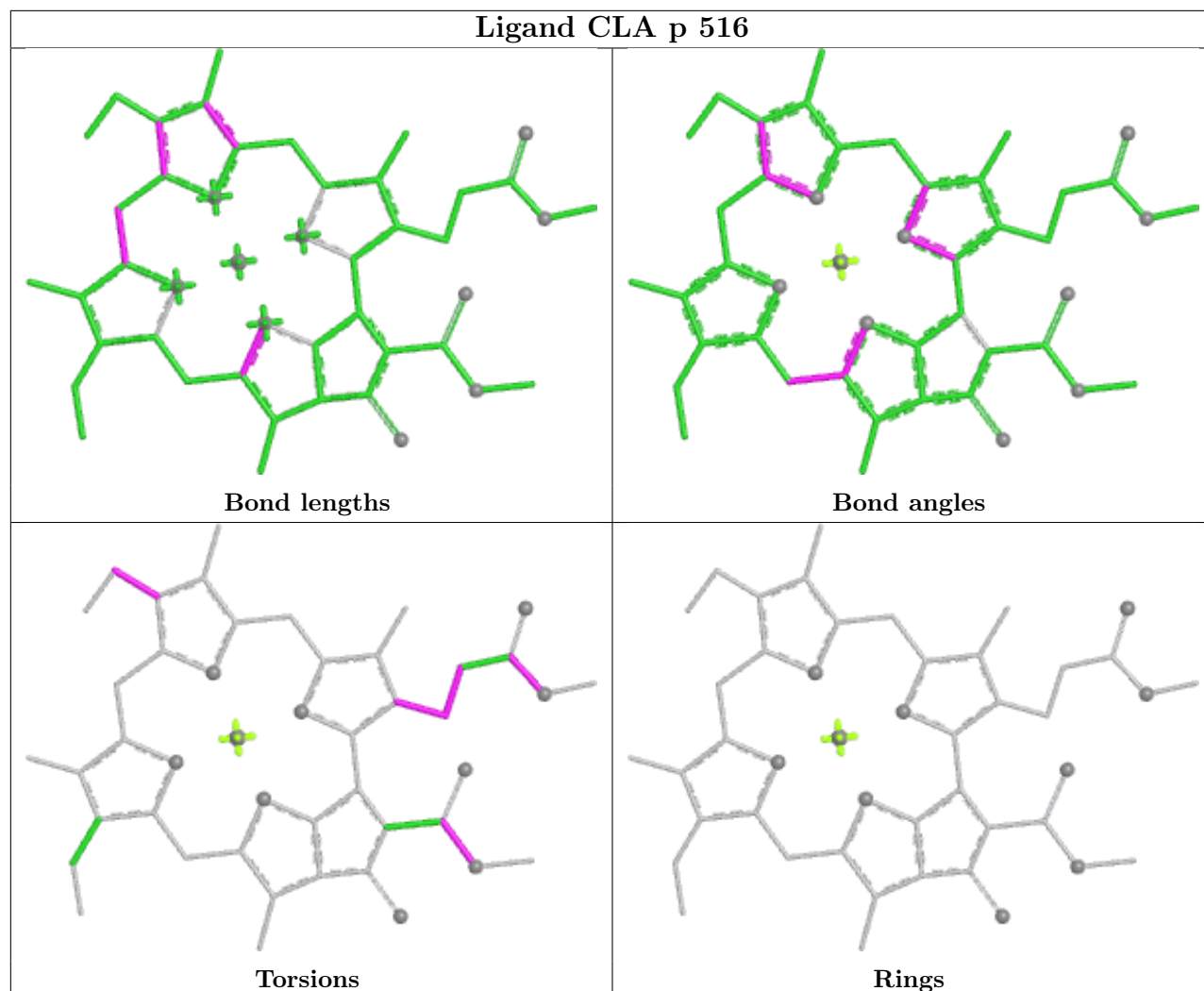


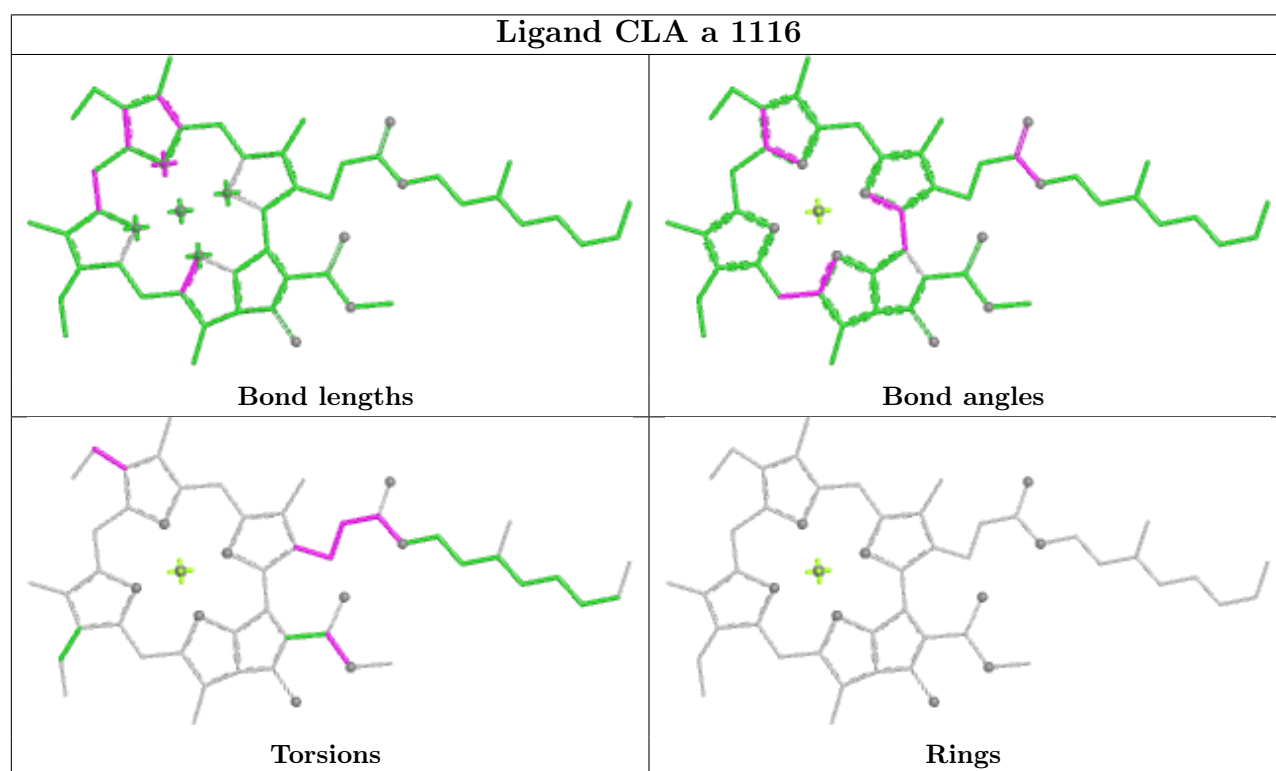
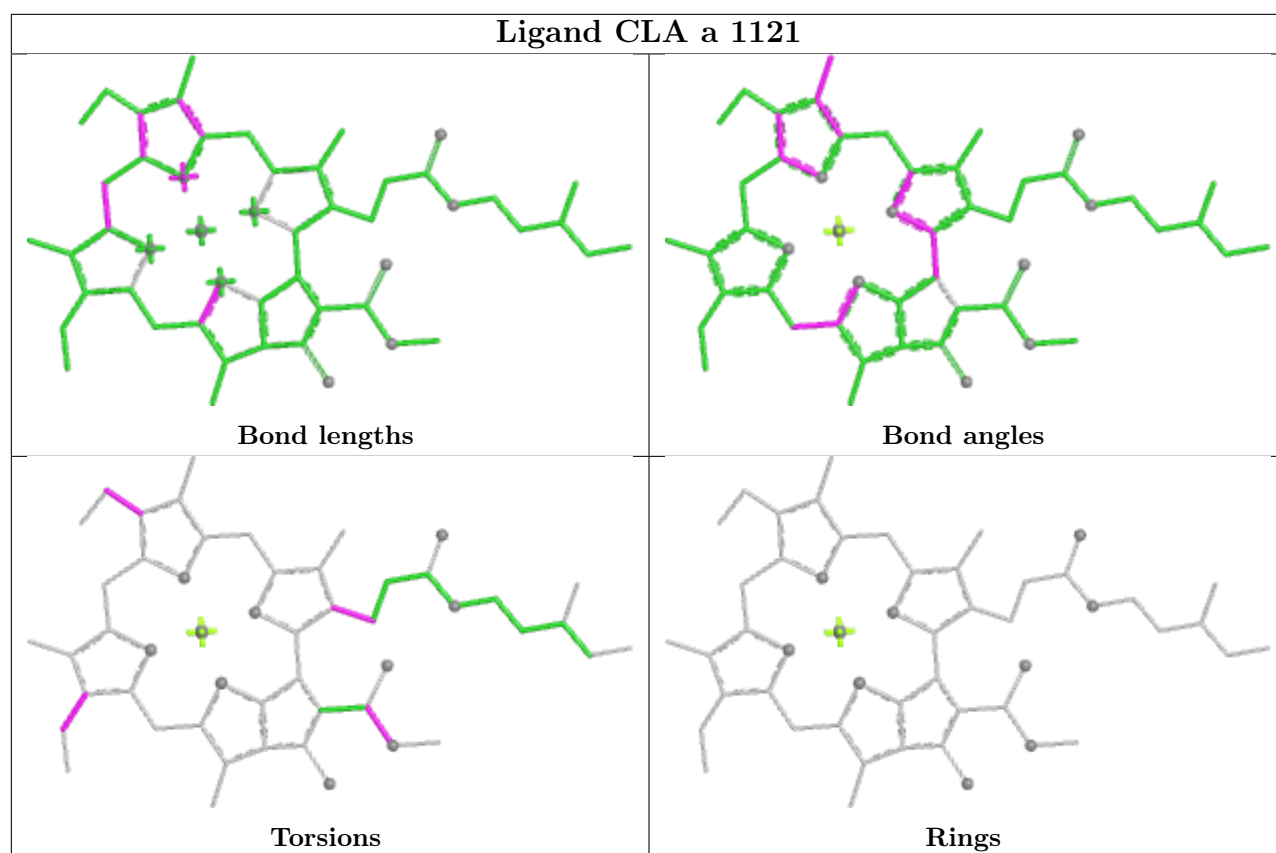
Ligand CLA G 1210

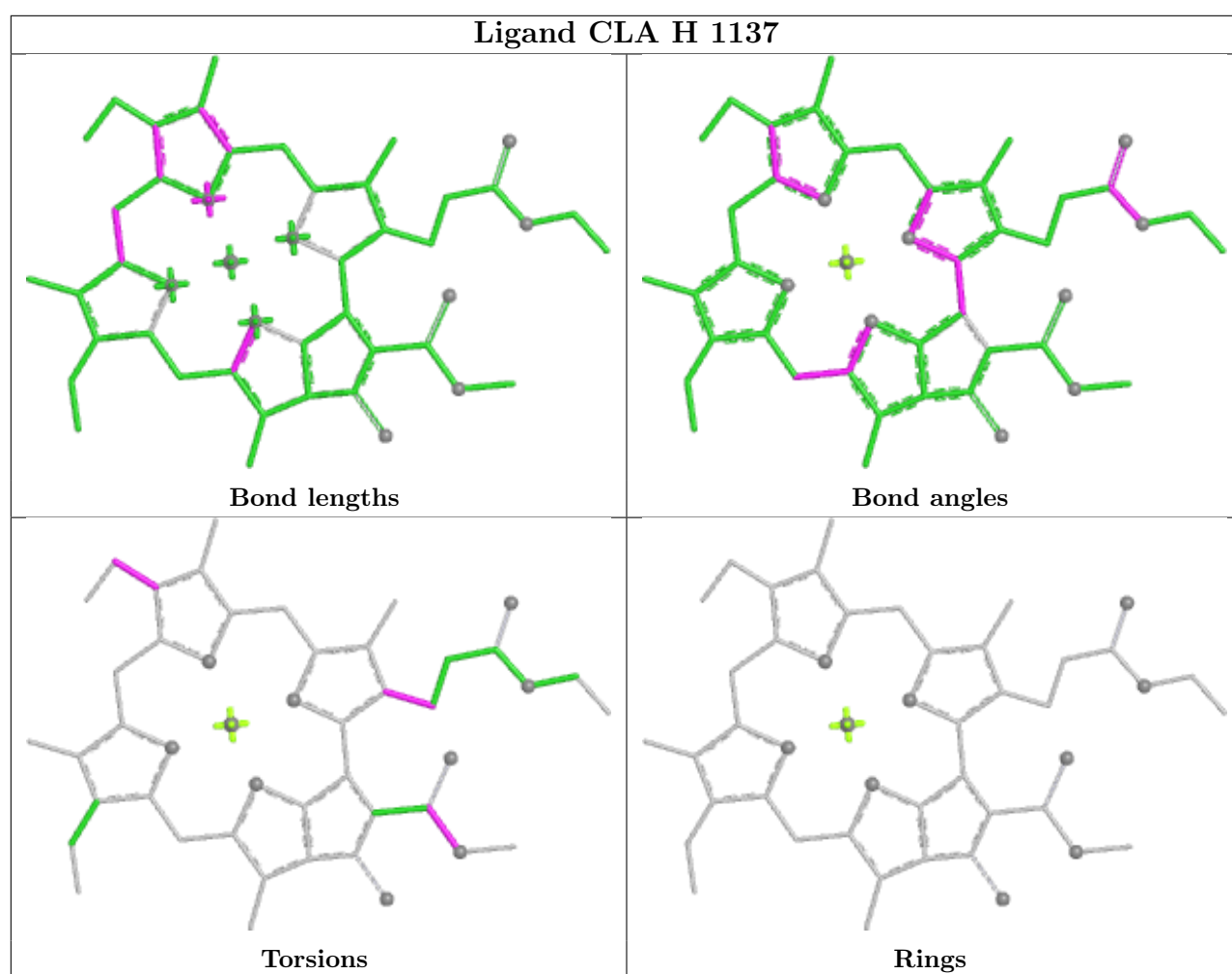
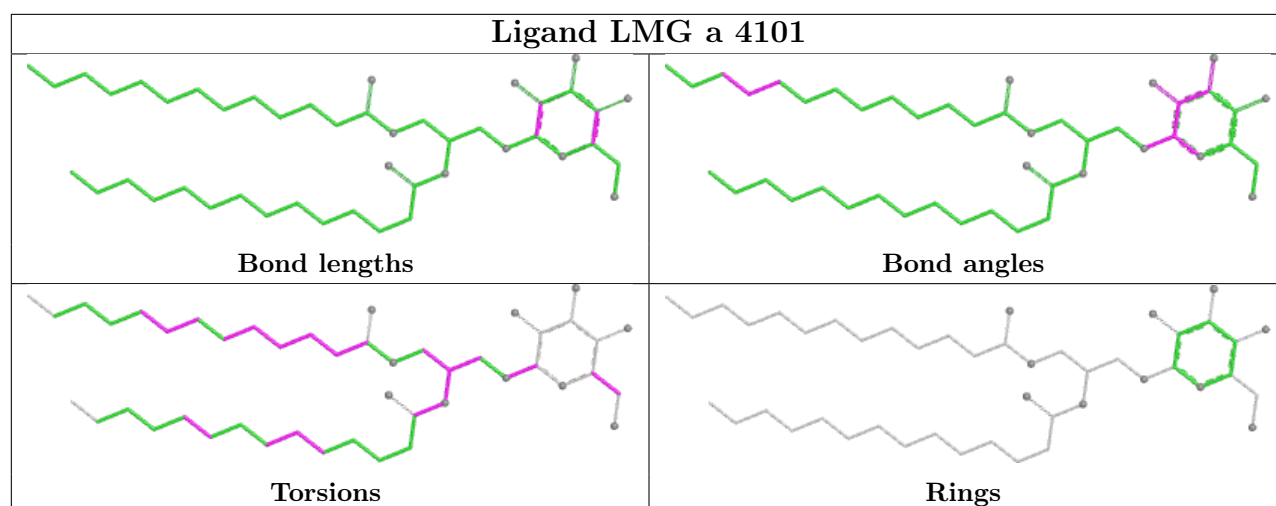


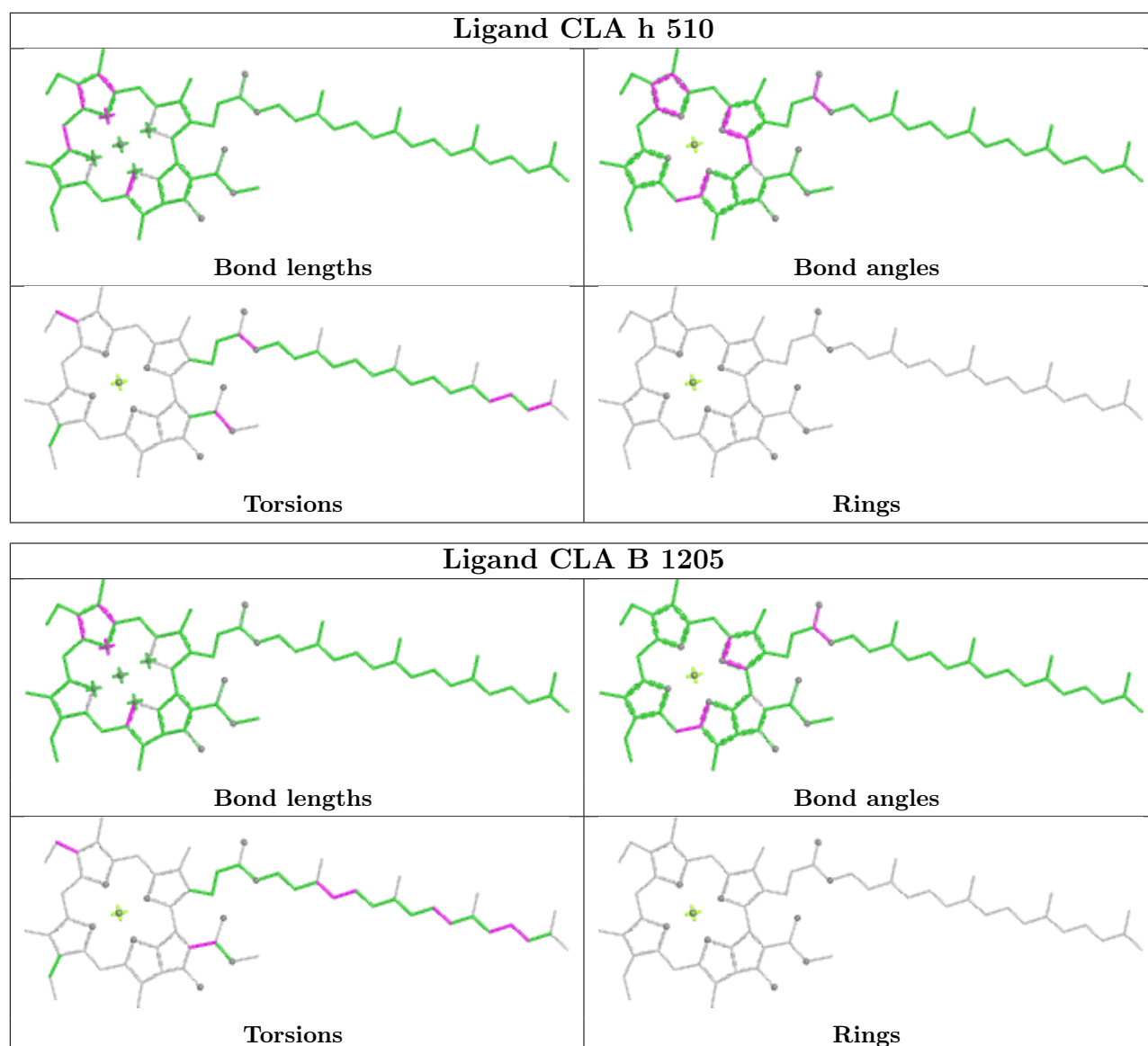


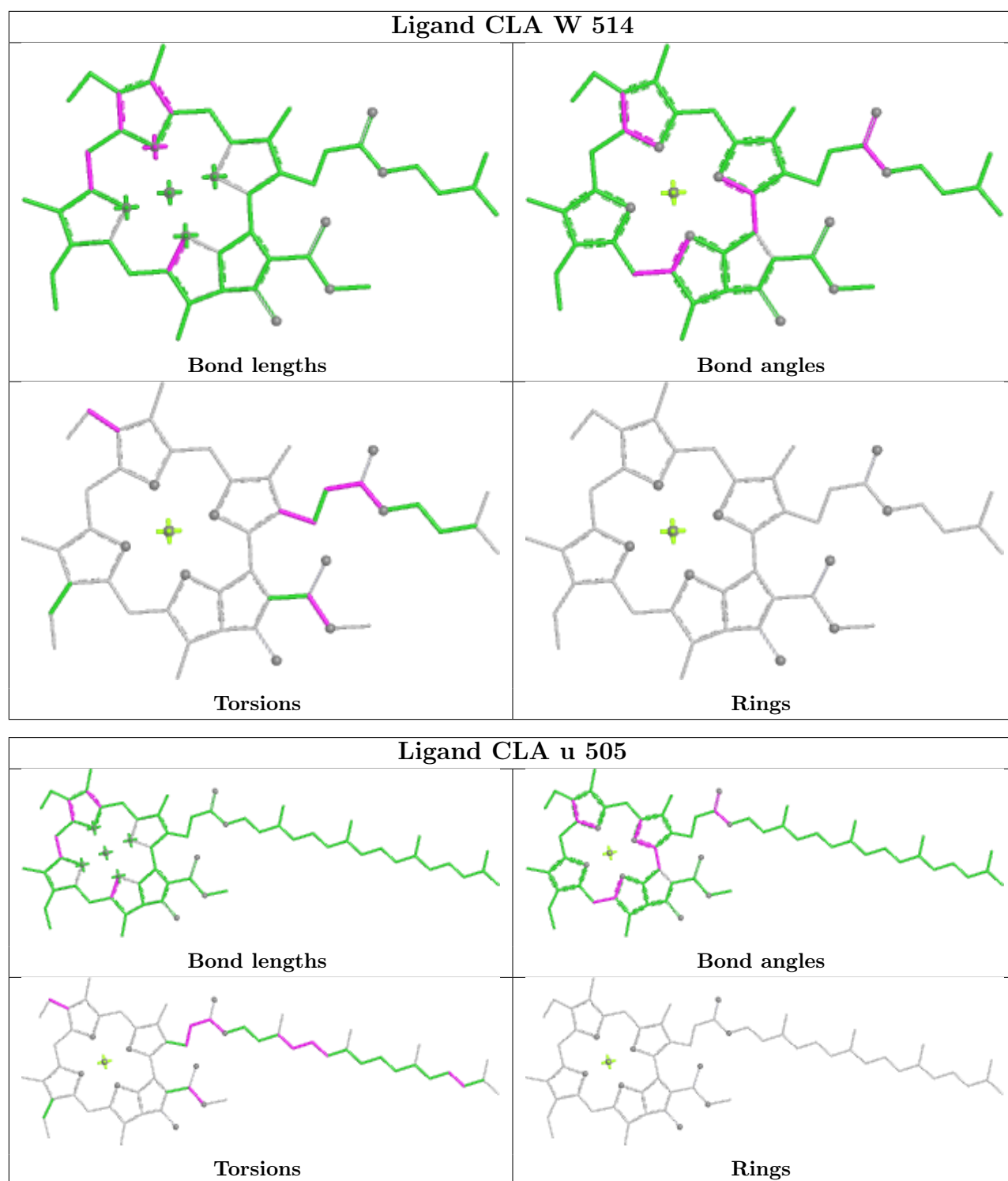
Ligand CLA p 516

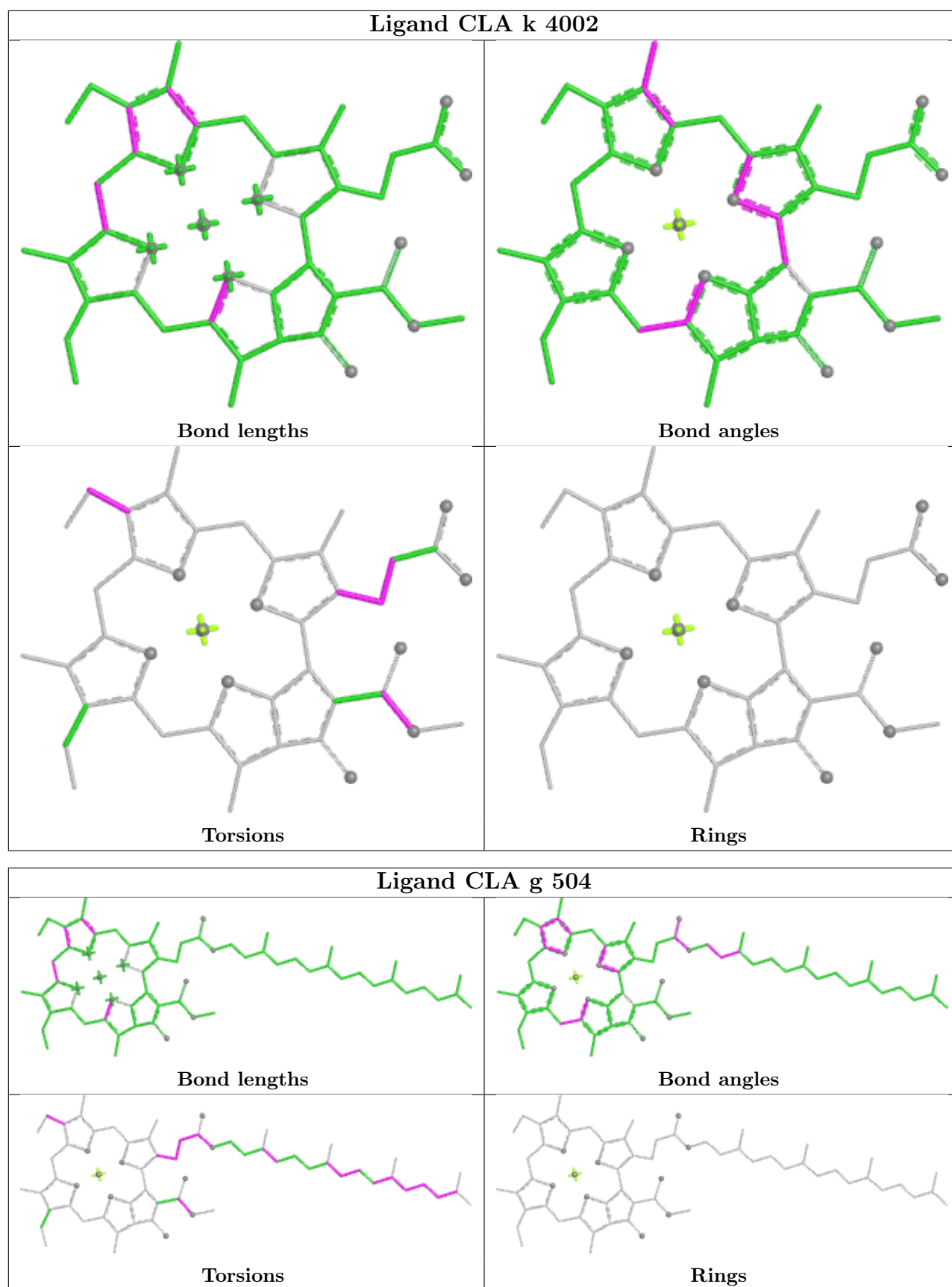




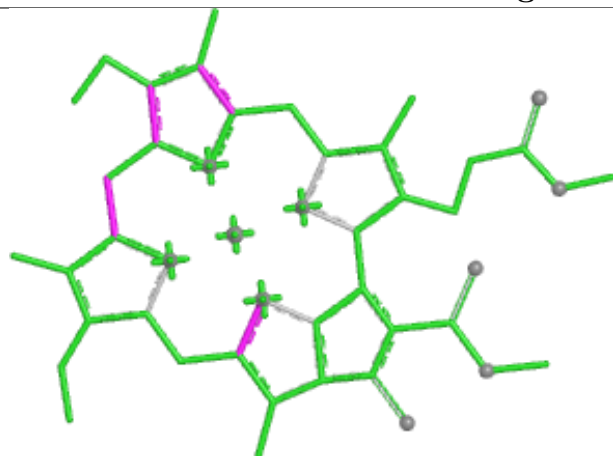




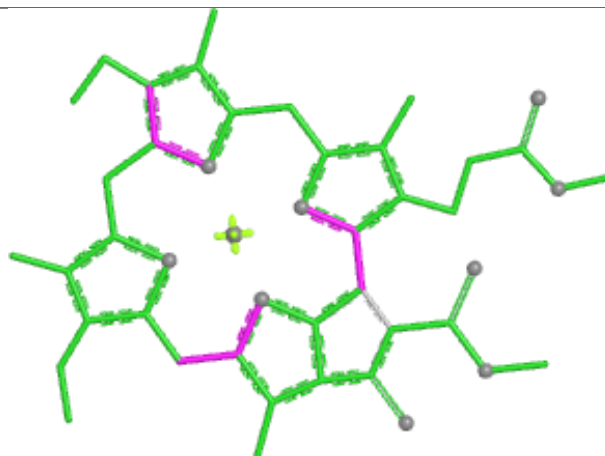




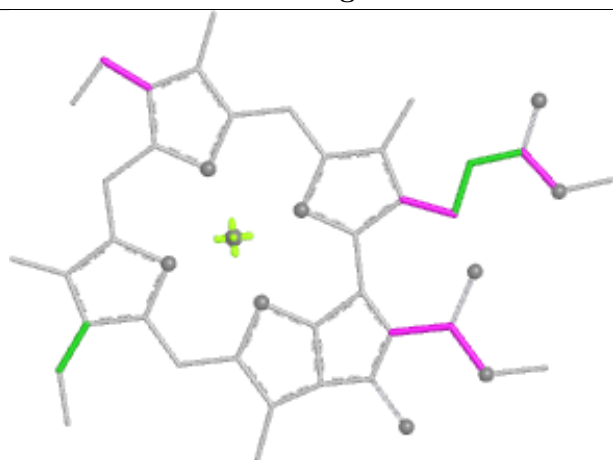
Ligand CLA u 503



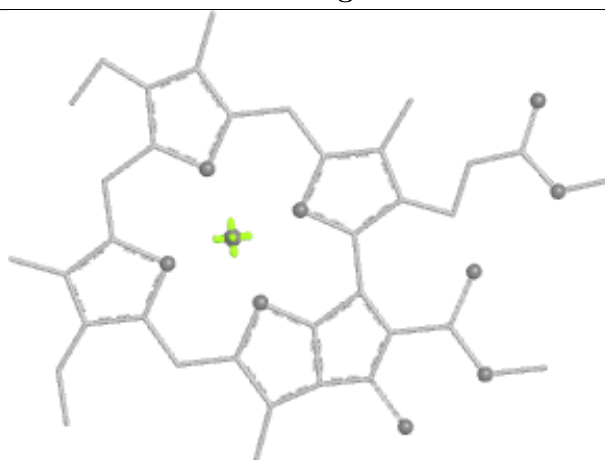
Bond lengths



Bond angles

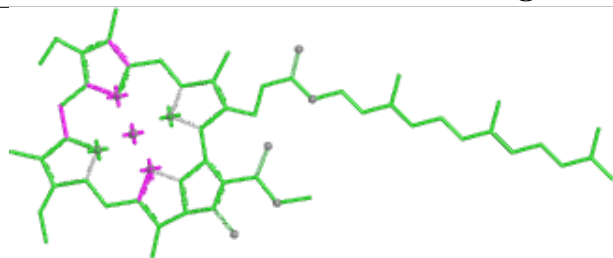


Torsions

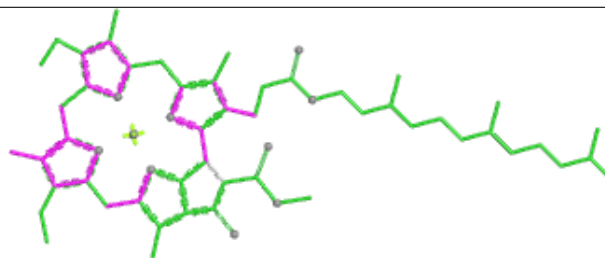


Rings

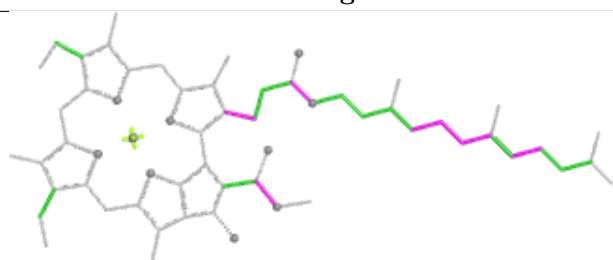
Ligand CLA u 506



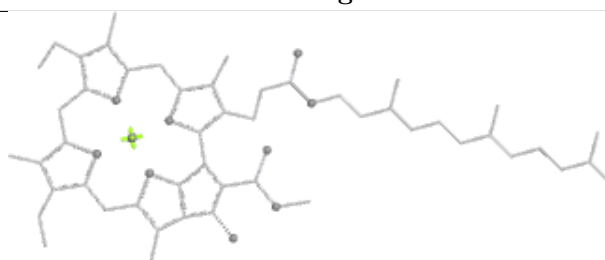
Bond lengths



Bond angles

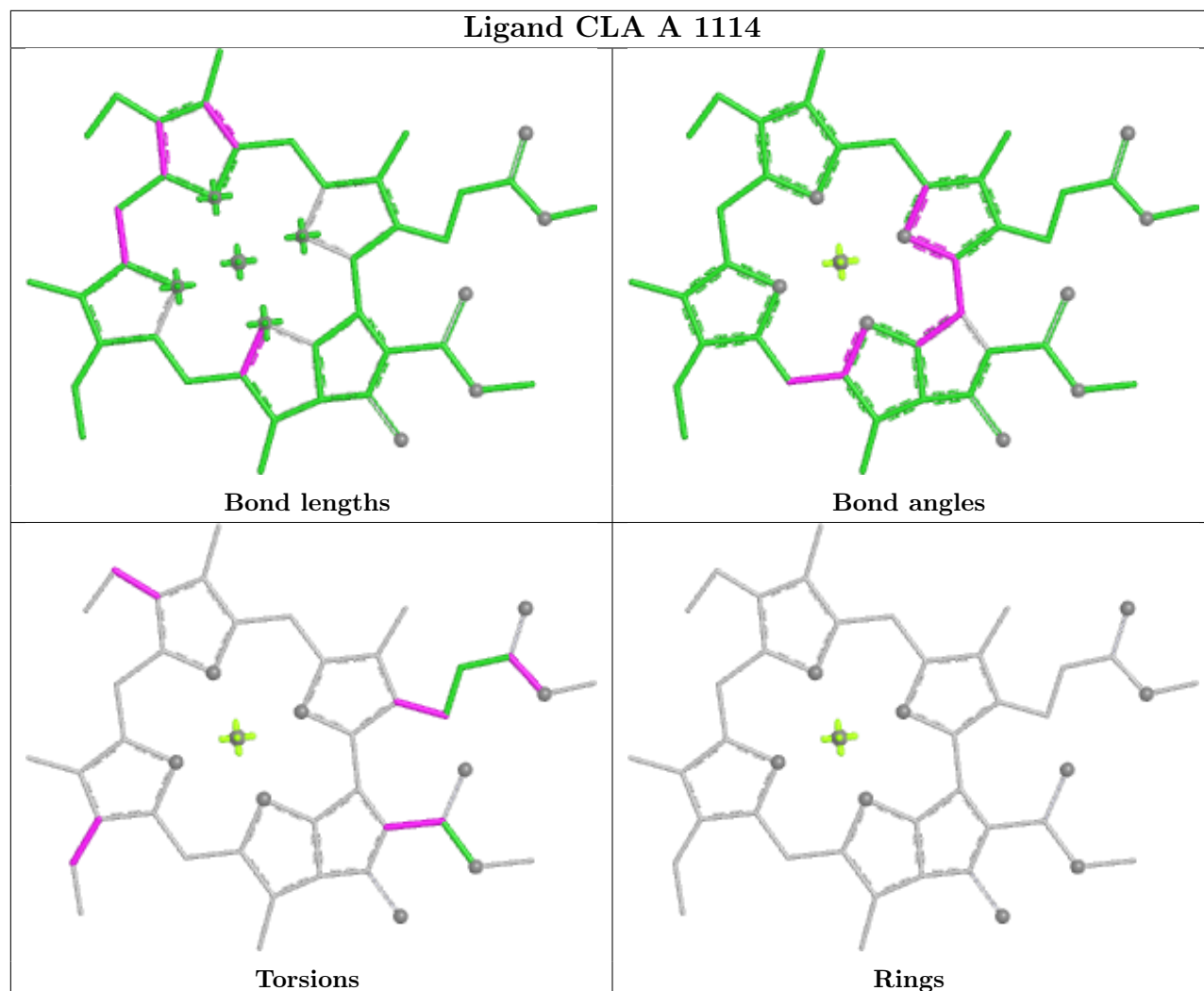


Torsions

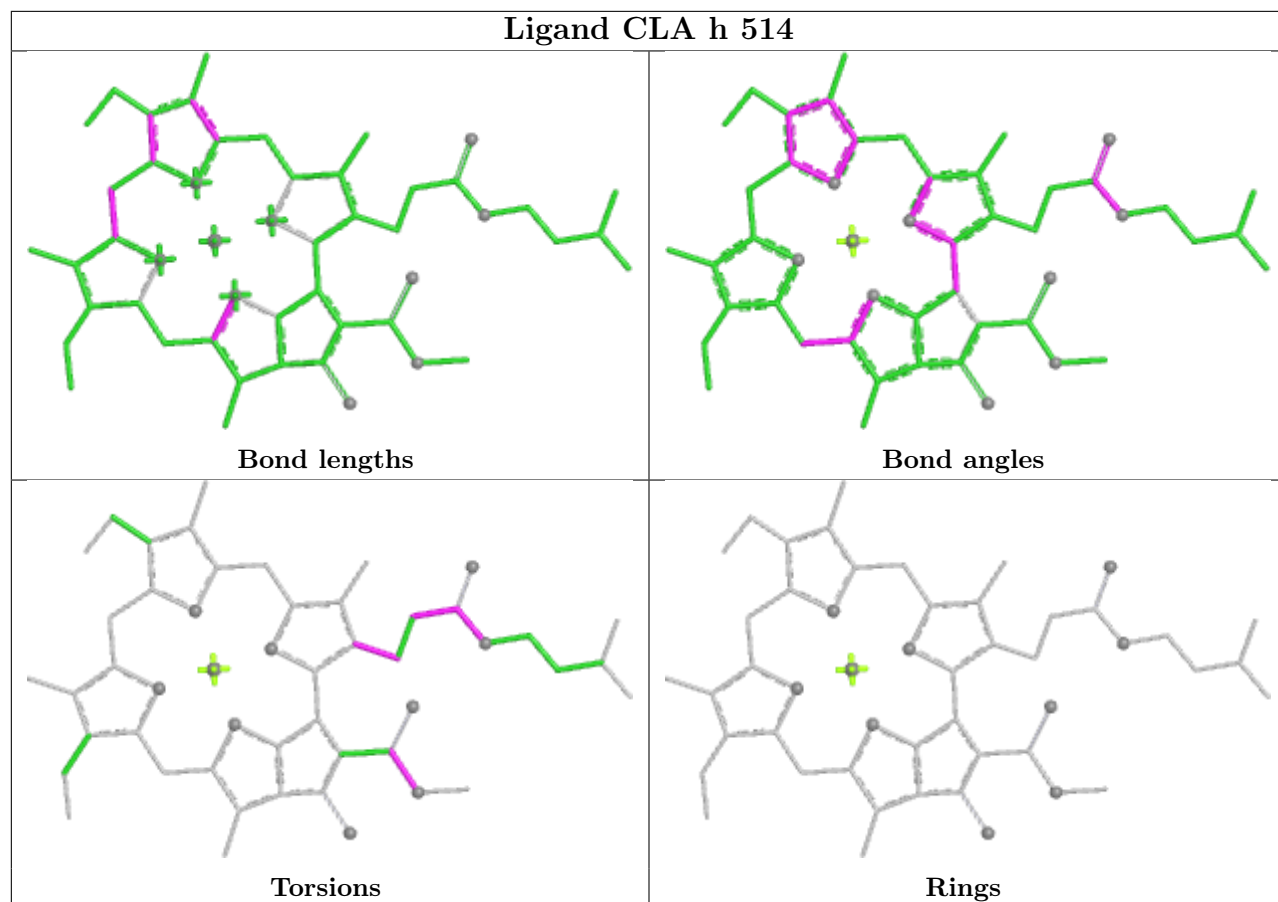


Rings

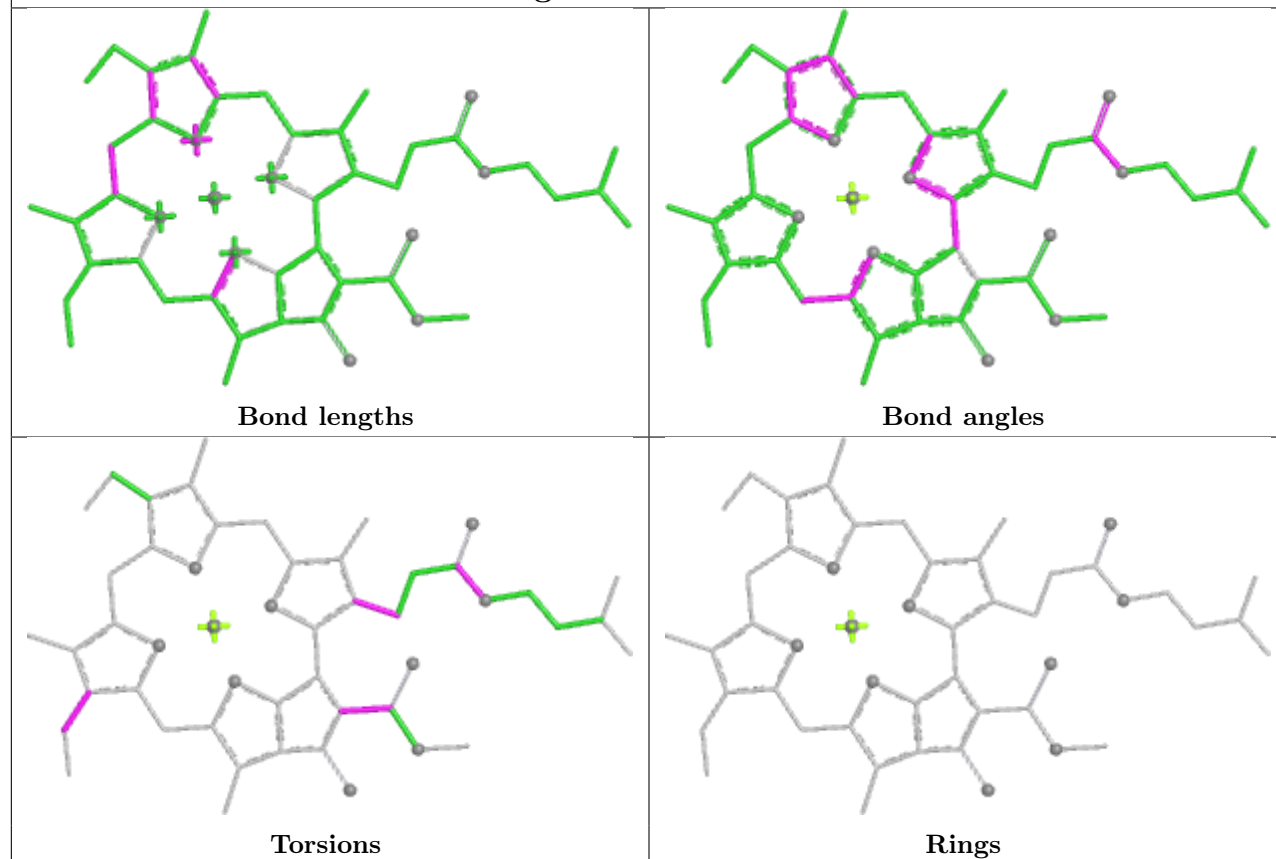
Ligand CLA A 1114



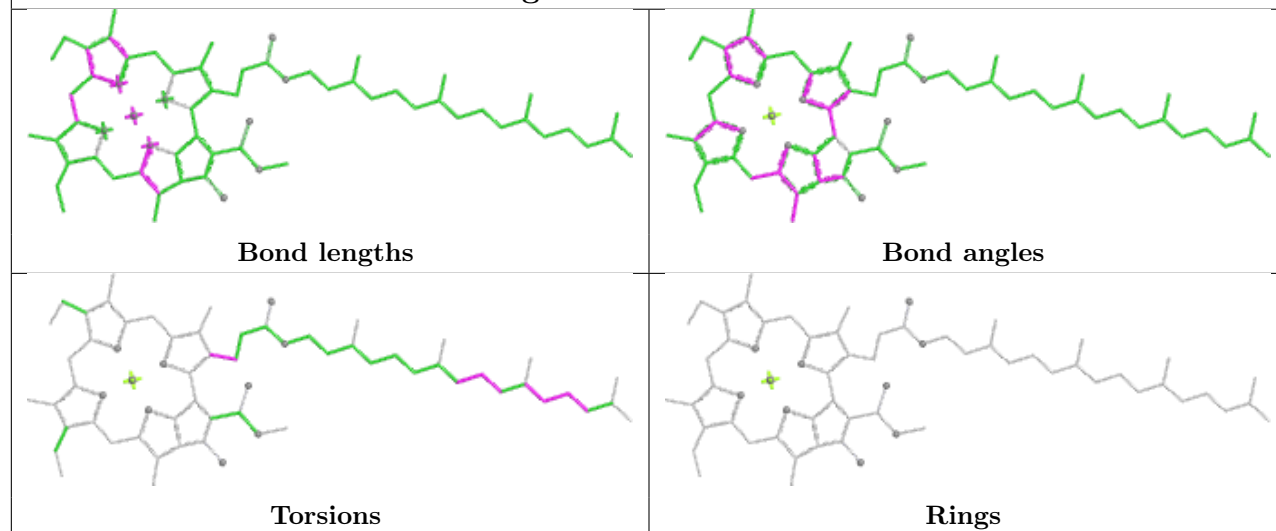
Ligand CLA h 514

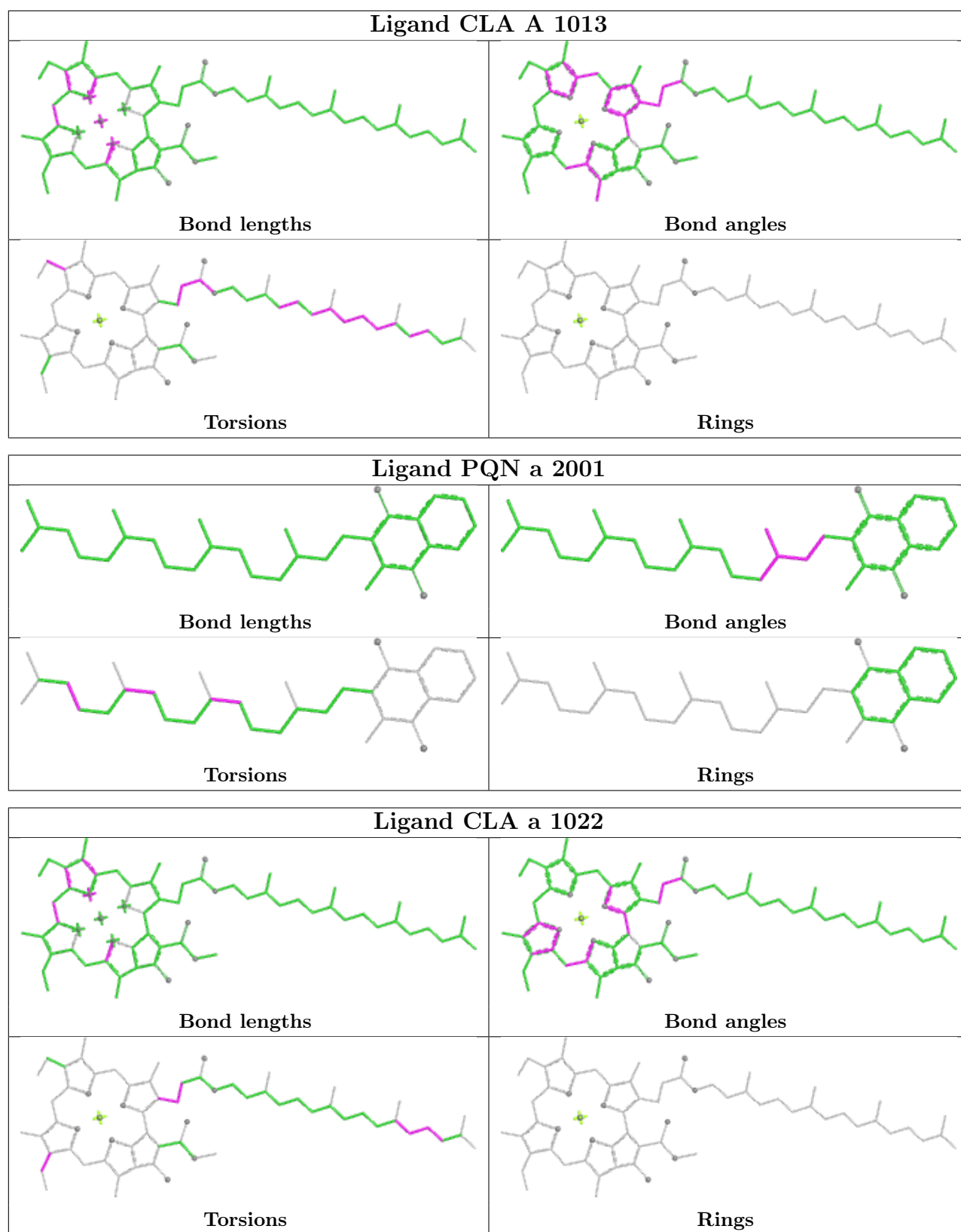


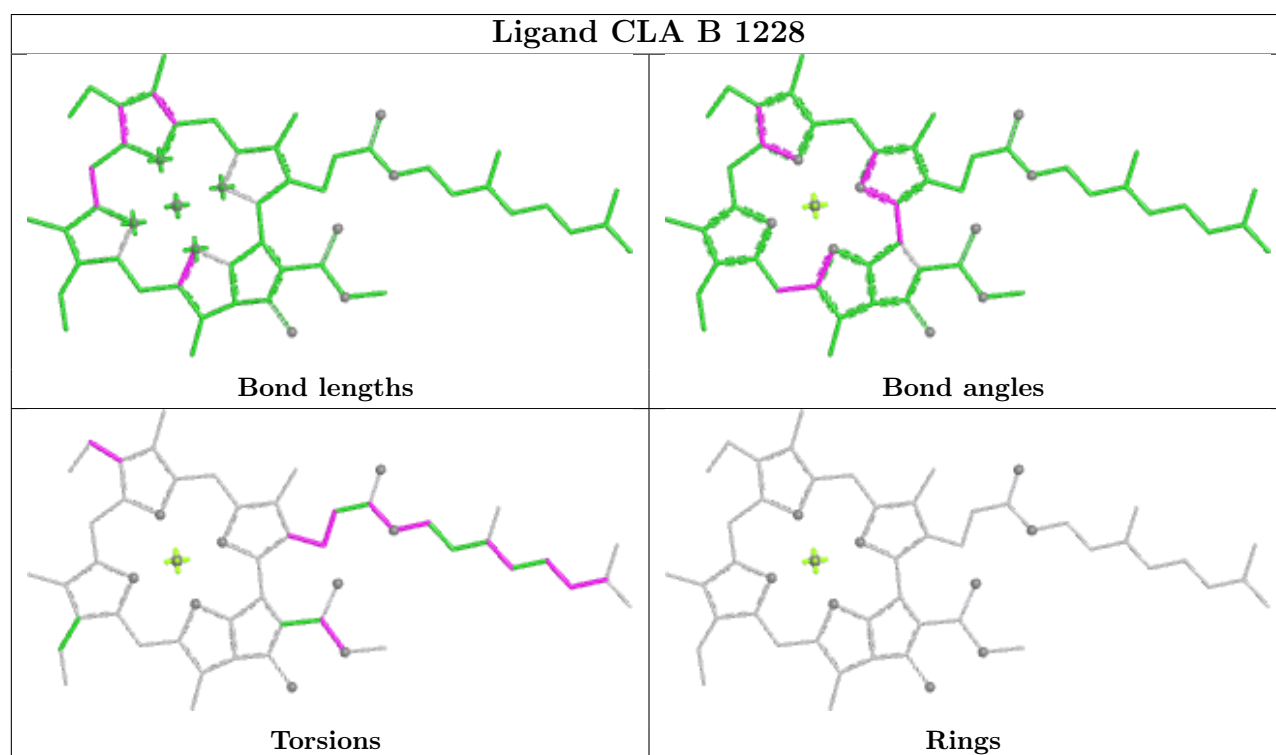
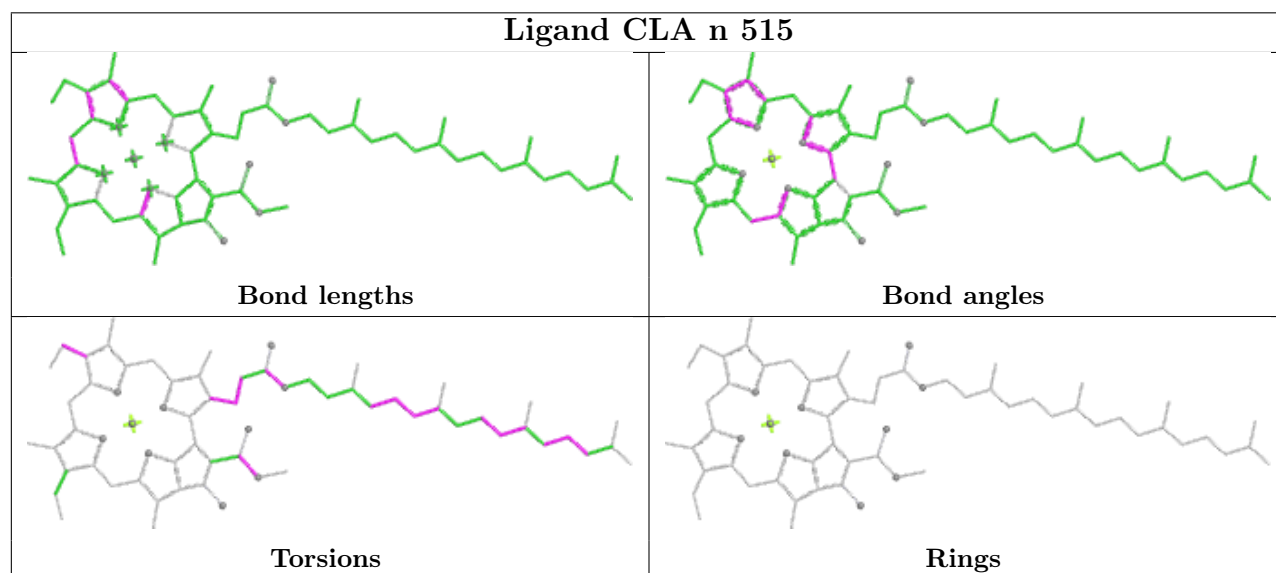
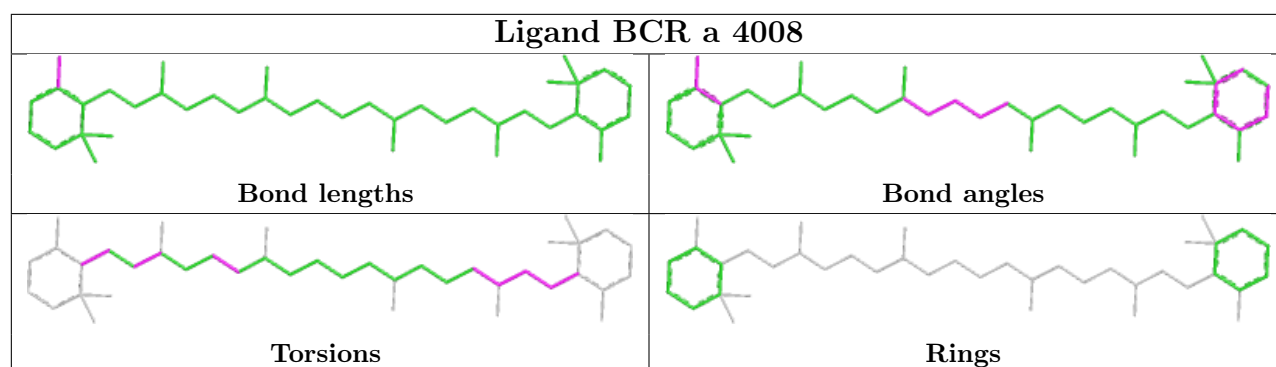
Ligand CLA Z 501



Ligand CLA G 1023







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.

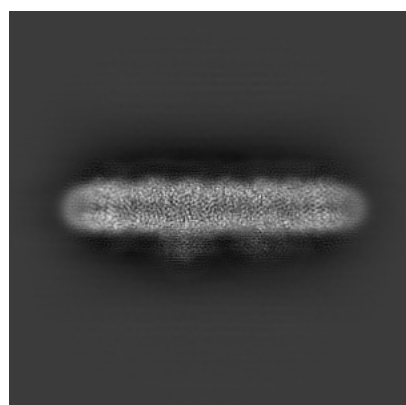
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26601. These allow visual inspection of the internal detail of the map and identification of artifacts.

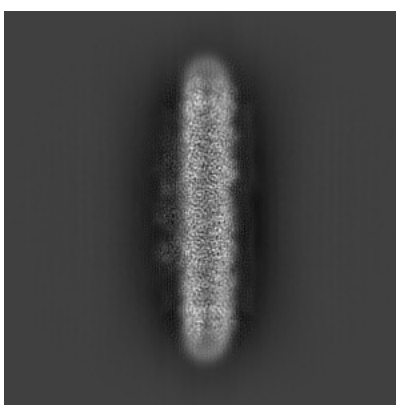
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

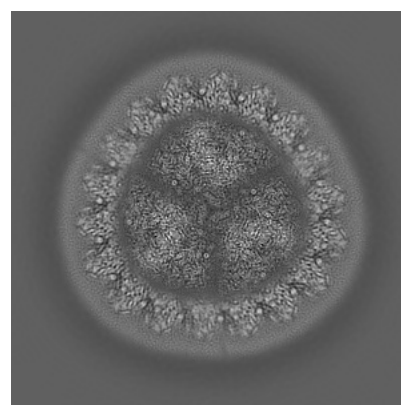
6.1.1 Primary map



X



Y

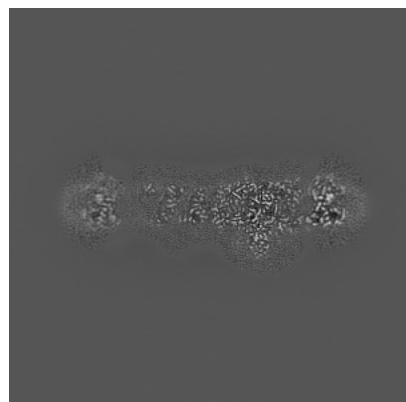


Z

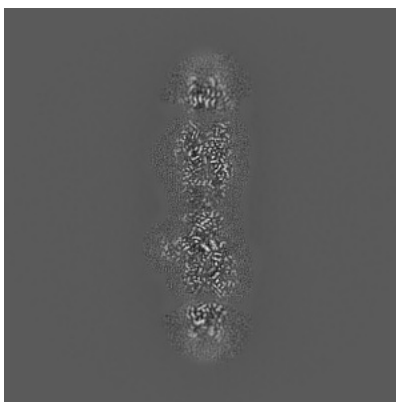
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

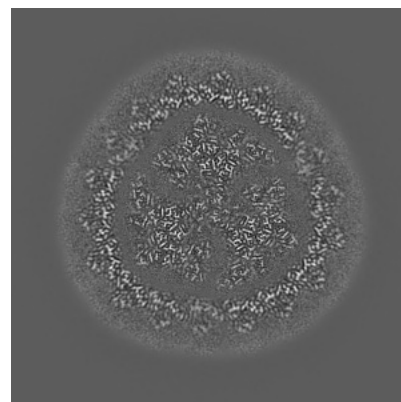
6.2.1 Primary map



X Index: 200



Y Index: 200

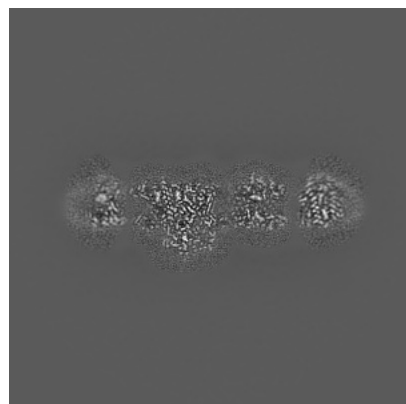


Z Index: 200

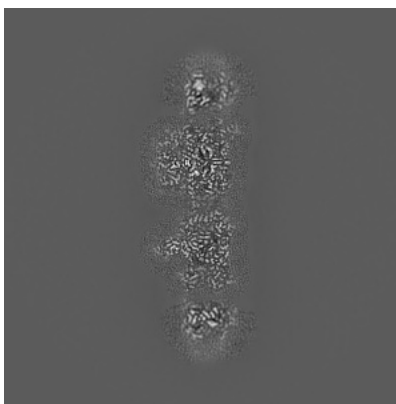
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

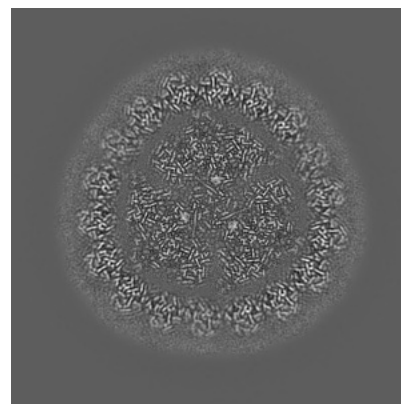
6.3.1 Primary map



X Index: 160



Y Index: 177

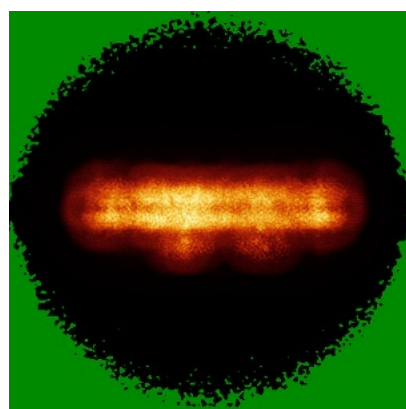


Z Index: 193

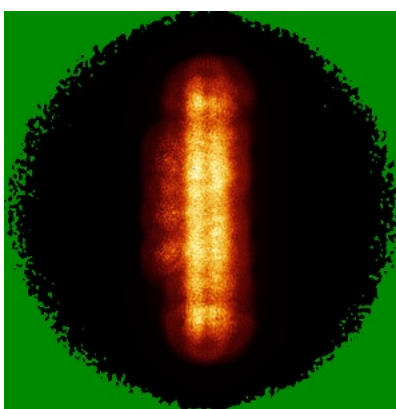
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

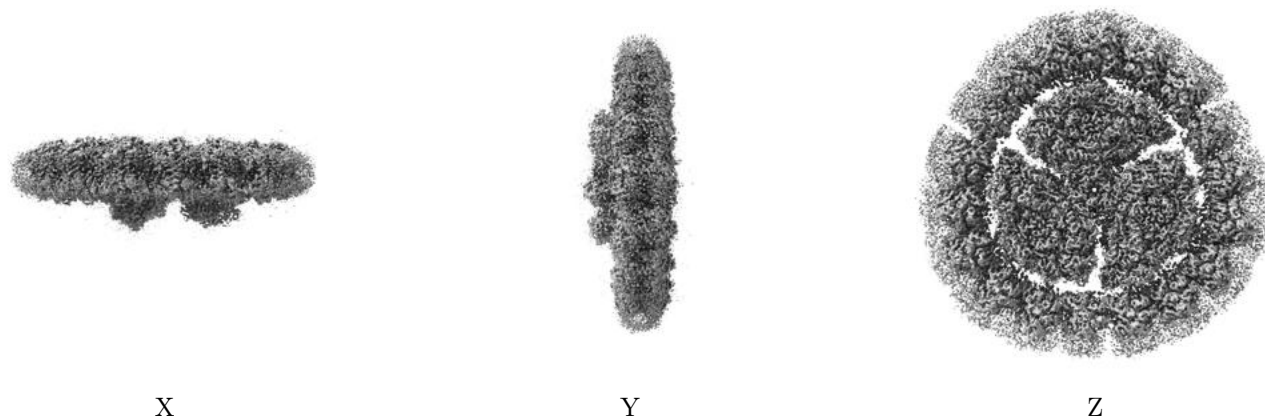


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 9.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

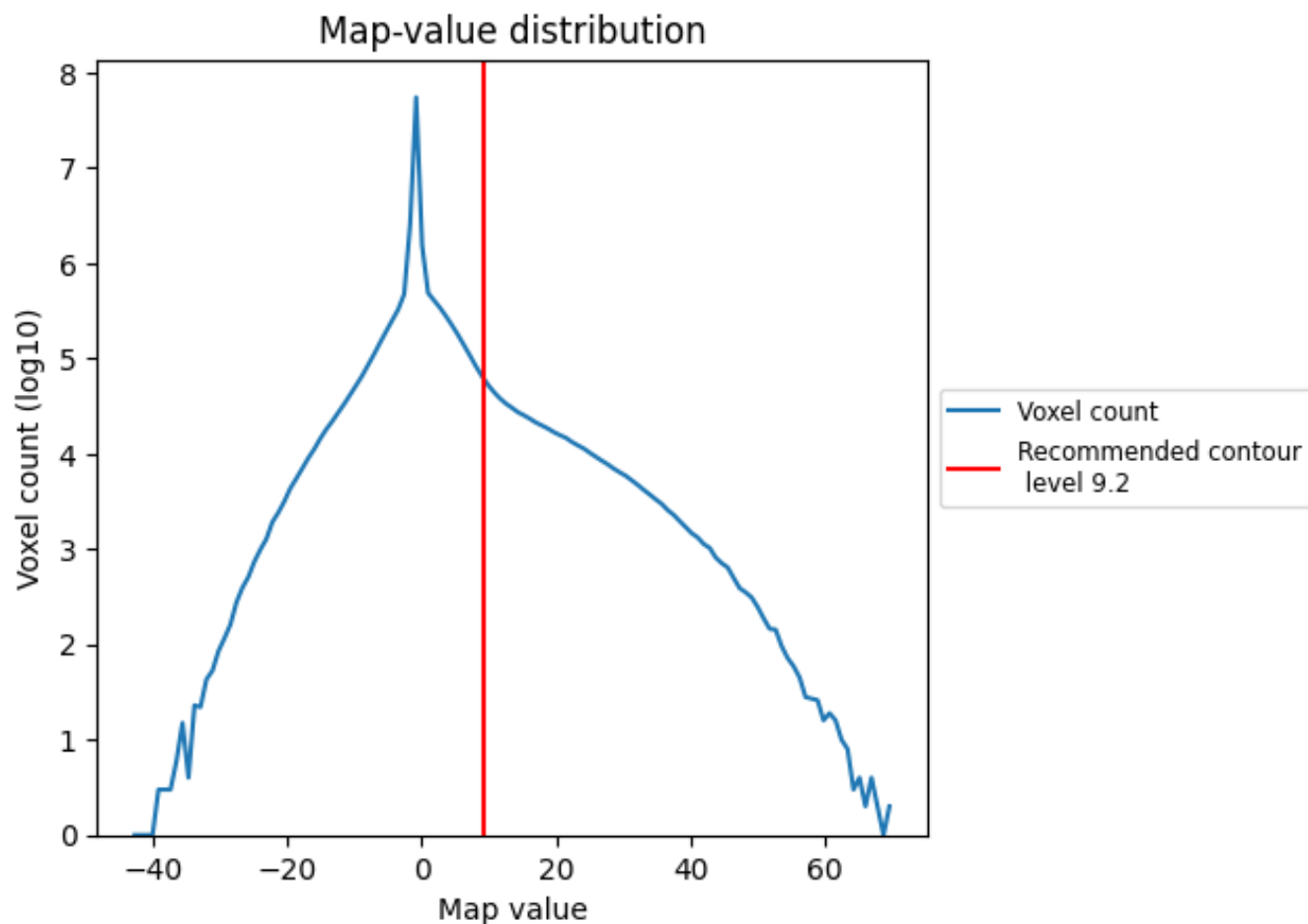
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

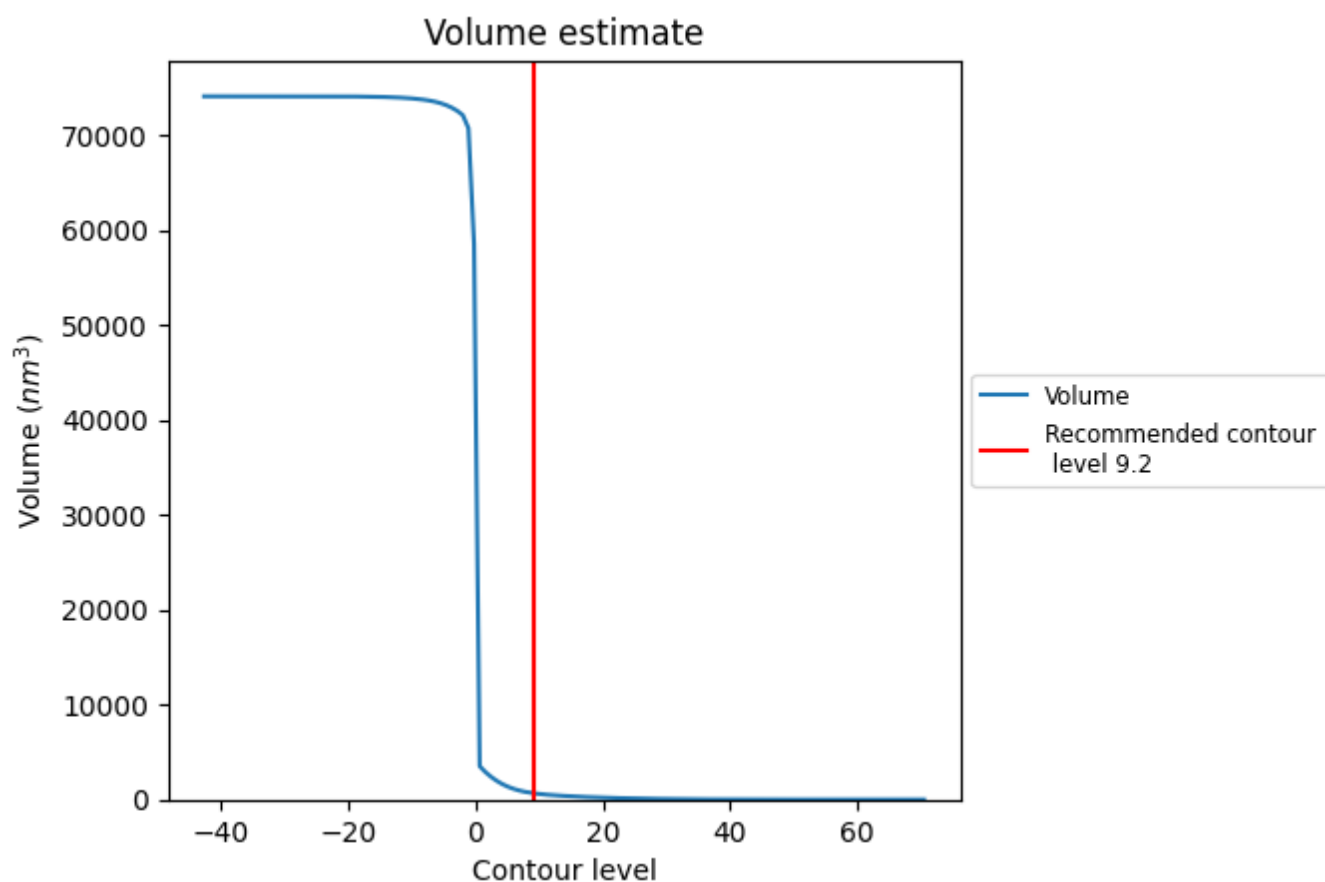
This section contains the results of statistical analysis of the map.

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.

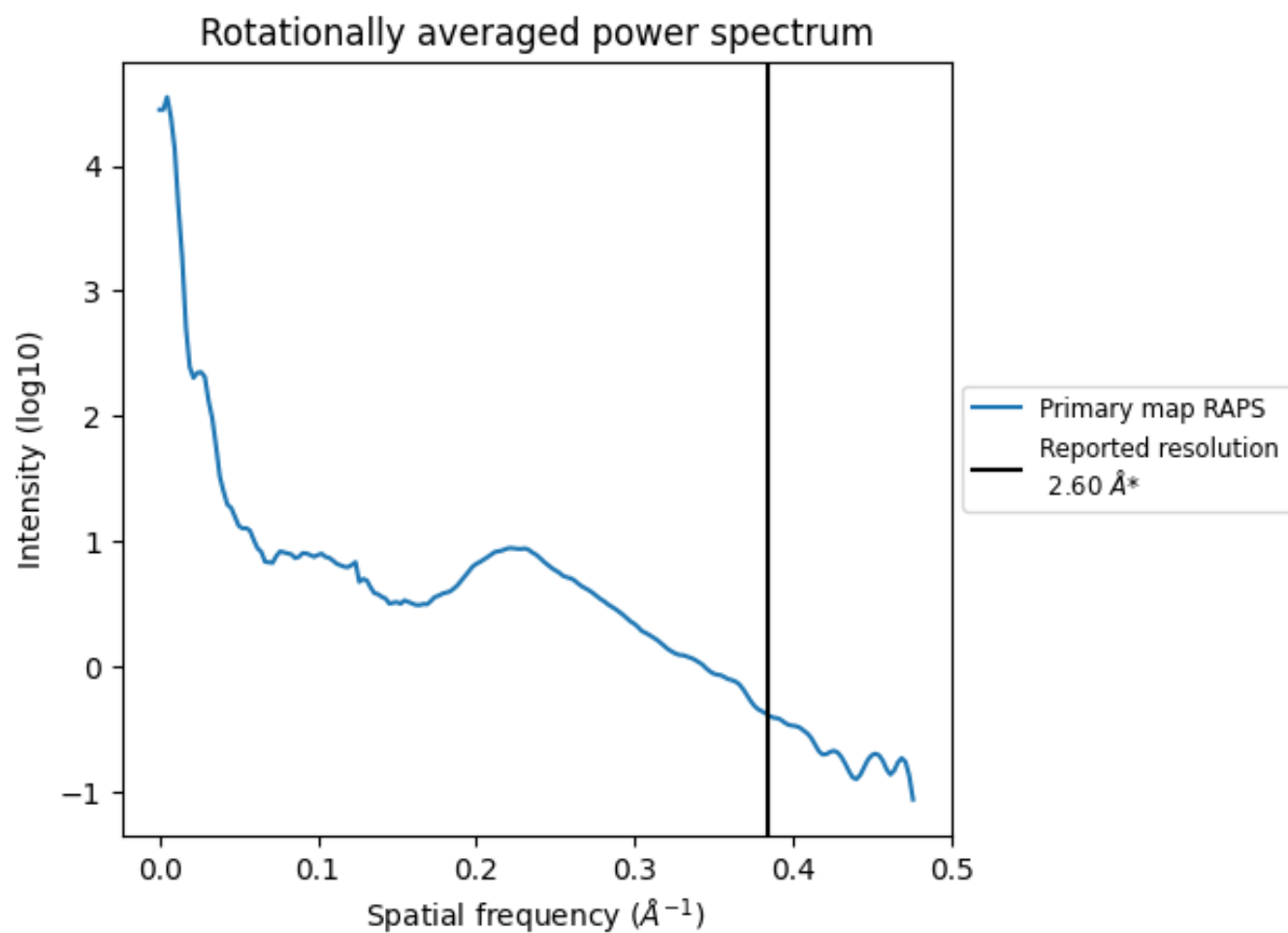
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 657 nm³; this corresponds to an approximate mass of 594 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

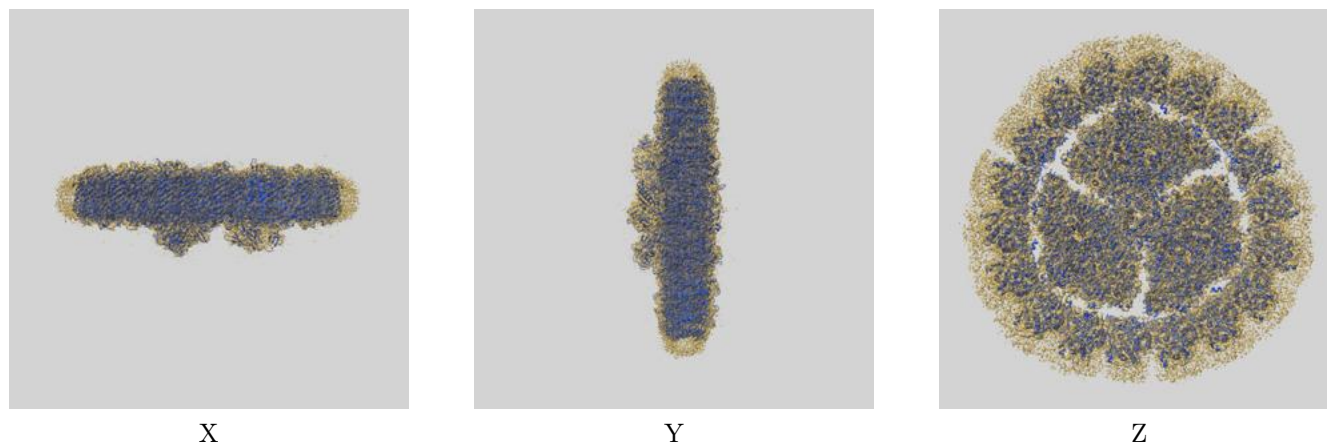
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

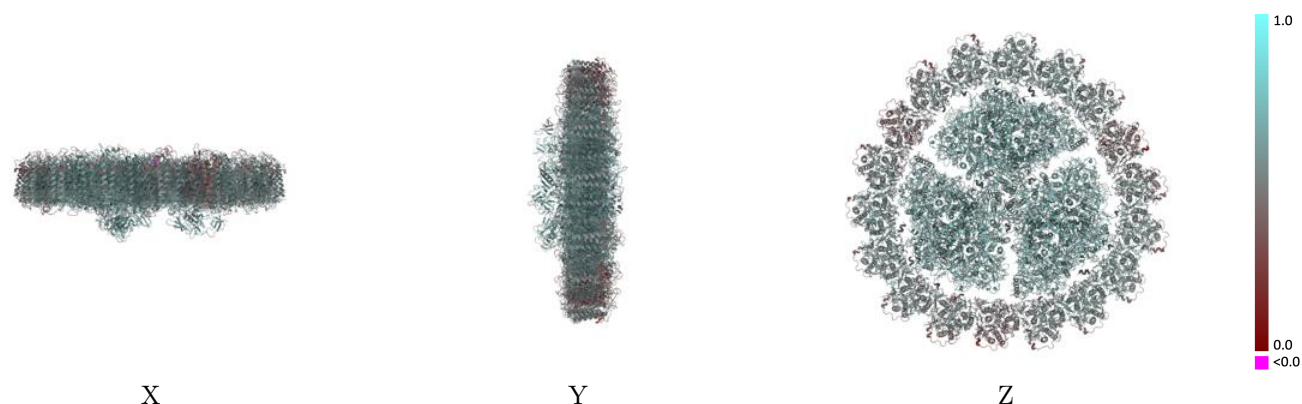
This section contains information regarding the fit between EMDB map EMD-26601 and PDB model 7UMH. Per-residue inclusion information can be found in [section 3](#) on [page 54](#).

9.1 Map-model overlay [i](#)



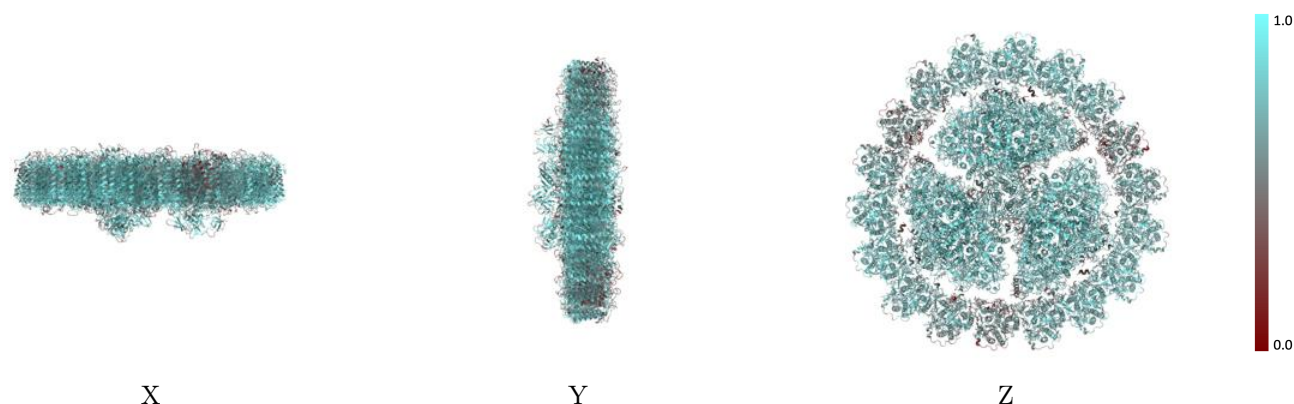
The images above show the 3D surface view of the map at the recommended contour level 9.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



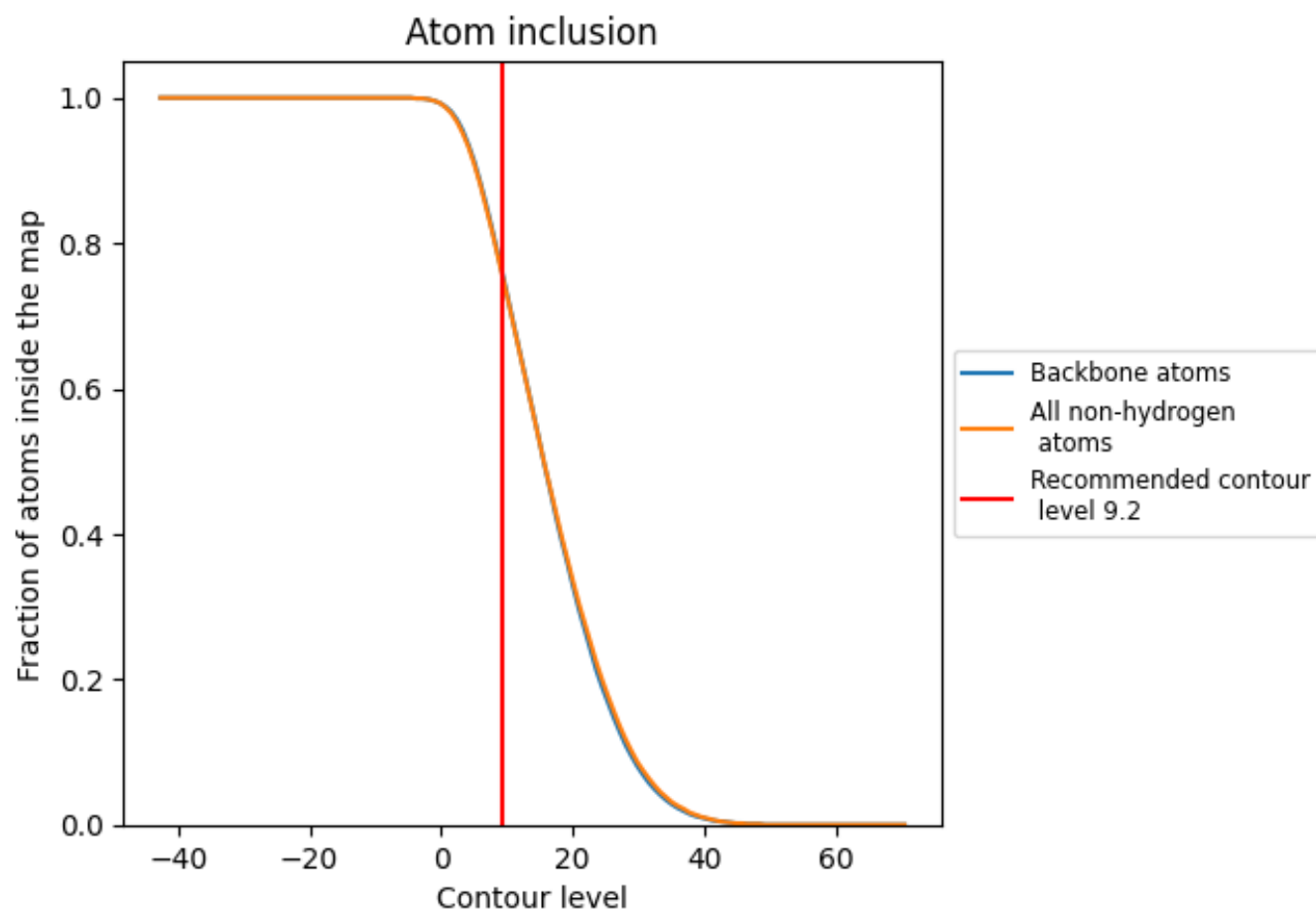
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (9.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.5830
A	 0.8500	 0.6590
B	 0.8530	 0.6580
C	 0.8720	 0.6440
D	 0.7320	 0.6010
E	 0.7110	 0.5910
F	 0.6610	 0.6030
G	 0.8570	 0.6580
H	 0.8550	 0.6590
I	 0.7320	 0.6300
J	 0.7310	 0.6300
K	 0.5930	 0.5910
L	 0.7710	 0.6360
M	 0.7140	 0.6350
N	 0.8740	 0.6450
O	 0.6800	 0.5860
P	 0.7240	 0.6040
Q	 0.6700	 0.6070
R	 0.7320	 0.6350
S	 0.7270	 0.6340
T	 0.6090	 0.5850
U	 0.7720	 0.6400
V	 0.6770	 0.6170
W	 0.6650	 0.5000
X	 0.7490	 0.5360
Y	 0.7840	 0.5560
Z	 0.7720	 0.5460
a	 0.8490	 0.6620
b	 0.8570	 0.6610
c	 0.8700	 0.6500
d	 0.7210	 0.6020
e	 0.6720	 0.5800
f	 0.6720	 0.6070
g	 0.7050	 0.5260
h	 0.5270	 0.4200



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Chain	Atom inclusion	Q-score
i	 0.7370	 0.6290
j	 0.7590	 0.6360
k	 0.6030	 0.5890
l	 0.7650	 0.6350
m	 0.7140	 0.6350
n	 0.6720	 0.5010
o	 0.7400	 0.5370
p	 0.7770	 0.5570
q	 0.7590	 0.5430
r	 0.6990	 0.5170
s	 0.7750	 0.5550
t	 0.6620	 0.4980
u	 0.7400	 0.5300
v	 0.5460	 0.4350
w	 0.7620	 0.5450
x	 0.6830	 0.5150
y	 0.5320	 0.4260