



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 07:00 AM UTC

PDB ID : 6JLU / pdb_00006jlu
EMDB ID : EMD-9839
Title : Structure of PSII-FCP supercomplex from a centric diatom *Chaetoceros gracilis* at 3.02 angstrom resolution
Authors : Pi, X.; Zhao, S.; Wang, W.; Kuang, T.; Sui, S.; Shen, J.
Deposited on : 2019-03-06
Resolution : 3.02 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

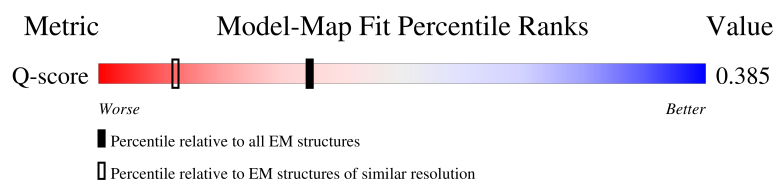
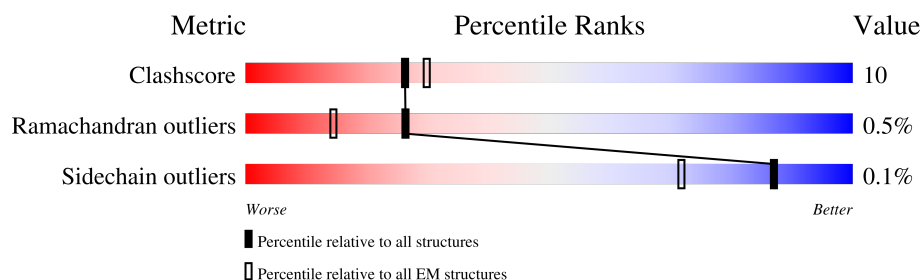
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.02 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.



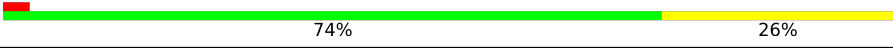
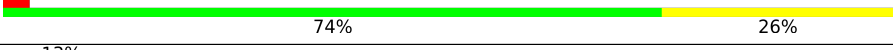
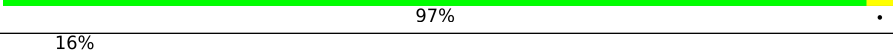
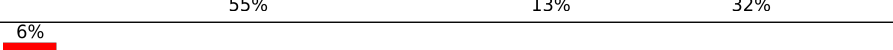
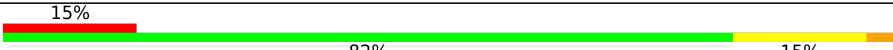
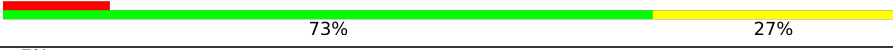
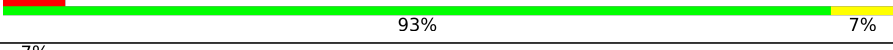
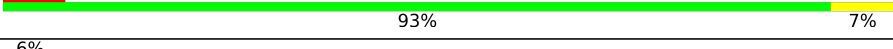
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13913 (2.52 - 3.52)

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	359	
1	a	359	
2	B	509	
2	b	509	

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Mol	Chain	Length	Quality of chain
3	C	450	
3	c	450	
4	D	341	
4	d	341	
5	E	79	
5	e	79	
6	F	32	
6	f	32	
7	G	179	
7	g	179	
8	H	65	
8	h	65	
9	I	34	
9	i	34	
10	J	34	
10	j	34	
11	K	37	
11	k	37	
12	L	38	
12	l	38	
13	M	41	
13	m	41	
14	N	30	
14	n	30	
15	O	249	

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Mol	Chain	Length	Quality of chain
15	o	249	
16	P	226	
16	p	226	
17	Q	211	
17	q	211	
18	R	73	
18	r	73	
19	T	31	
19	t	31	
20	U	93	
20	u	93	
21	V	137	
21	v	137	
22	W	51	
22	w	51	
23	X	35	
23	x	35	
24	Y	33	
24	y	33	
25	Z	61	
25	z	61	
26	0	178	
26	10	178	
27	1	172	
27	11	172	

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Mol	Chain	Length	Quality of chain
27	12	172	
27	13	172	
27	14	172	
27	15	172	
27	16	172	
27	17	172	
27	18	172	
27	2	172	
27	3	172	
27	4	172	
27	5	172	
27	6	172	
27	7	172	
27	8	172	
28	19	166	
28	9	166	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	0	307	X	-	-	-
31	CLA	0	308	X	-	-	-
31	CLA	0	311	X	-	-	-
31	CLA	0	312	X	-	-	-
31	CLA	0	313	X	-	-	-
31	CLA	0	316	X	-	-	-
31	CLA	1	307	X	-	-	-
31	CLA	1	310	X	-	-	-
31	CLA	1	312	X	-	-	-
31	CLA	1	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	1	316	X	-	-	-
31	CLA	1	321	X	-	-	-
31	CLA	10	307	X	-	-	-
31	CLA	10	308	X	-	-	-
31	CLA	10	311	X	-	-	-
31	CLA	10	312	X	-	-	-
31	CLA	10	313	X	-	-	-
31	CLA	10	314	X	-	-	-
31	CLA	10	316	X	-	-	-
31	CLA	10	317	X	-	-	-
31	CLA	11	307	X	-	-	-
31	CLA	11	308	X	-	-	-
31	CLA	11	310	X	-	-	-
31	CLA	11	312	X	-	-	-
31	CLA	11	313	X	-	-	-
31	CLA	11	315	X	-	-	-
31	CLA	11	316	X	-	-	-
31	CLA	12	307	X	-	-	-
31	CLA	12	308	X	-	-	-
31	CLA	12	310	X	-	-	-
31	CLA	12	312	X	-	-	-
31	CLA	12	316	X	-	-	-
31	CLA	13	307	X	-	-	-
31	CLA	13	308	X	-	-	-
31	CLA	13	310	X	-	-	-
31	CLA	13	312	X	-	-	-
31	CLA	14	306	X	-	-	-
31	CLA	14	307	X	-	-	-
31	CLA	14	309	X	-	-	-
31	CLA	14	311	X	-	-	-
31	CLA	14	312	X	-	-	-
31	CLA	14	314	X	-	-	-
31	CLA	14	315	X	-	-	-
31	CLA	15	306	X	-	-	-
31	CLA	15	307	X	-	-	-
31	CLA	15	309	X	-	-	-
31	CLA	15	311	X	-	-	-
31	CLA	15	313	X	-	-	-
31	CLA	16	307	X	-	-	-
31	CLA	16	308	X	-	-	-
31	CLA	16	310	X	-	-	-
31	CLA	16	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	16	313	X	-	-	-
31	CLA	16	315	X	-	-	-
31	CLA	17	307	X	-	-	-
31	CLA	17	310	X	-	-	-
31	CLA	17	312	X	-	-	-
31	CLA	17	313	X	-	-	-
31	CLA	17	315	X	-	-	-
31	CLA	18	306	X	-	-	-
31	CLA	18	307	X	-	-	-
31	CLA	18	309	X	-	-	-
31	CLA	18	312	X	-	-	-
31	CLA	18	314	X	-	-	-
31	CLA	19	307	X	-	-	-
31	CLA	19	308	X	-	-	-
31	CLA	19	310	X	-	-	-
31	CLA	19	311	X	-	-	-
31	CLA	19	312	X	-	-	-
31	CLA	19	313	X	-	-	-
31	CLA	19	315	X	-	-	-
31	CLA	2	306	X	-	-	-
31	CLA	2	307	X	-	-	-
31	CLA	2	309	X	-	-	-
31	CLA	3	307	X	-	-	-
31	CLA	3	308	X	-	-	-
31	CLA	3	310	X	-	-	-
31	CLA	3	313	X	-	-	-
31	CLA	3	315	X	-	-	-
31	CLA	4	307	X	-	-	-
31	CLA	4	309	X	-	-	-
31	CLA	4	311	X	-	-	-
31	CLA	4	312	X	-	-	-
31	CLA	4	314	X	-	-	-
31	CLA	4	315	X	-	-	-
31	CLA	5	306	X	-	-	-
31	CLA	5	307	X	-	-	-
31	CLA	5	309	X	-	-	-
31	CLA	5	311	X	-	-	-
31	CLA	5	314	X	-	-	-
31	CLA	6	308	X	-	-	-
31	CLA	6	309	X	-	-	-
31	CLA	6	311	X	-	-	-
31	CLA	6	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	6	314	X	-	-	-
31	CLA	6	316	X	-	-	-
31	CLA	7	307	X	-	-	-
31	CLA	7	310	X	-	-	-
31	CLA	7	312	X	-	-	-
31	CLA	7	313	X	-	-	-
31	CLA	7	315	X	-	-	-
31	CLA	8	307	X	-	-	-
31	CLA	8	308	X	-	-	-
31	CLA	8	310	X	-	-	-
31	CLA	8	313	X	-	-	-
31	CLA	8	315	X	-	-	-
31	CLA	9	307	X	-	-	-
31	CLA	9	308	X	-	-	-
31	CLA	9	310	X	-	-	-
31	CLA	9	311	X	-	-	-
31	CLA	9	312	X	-	-	-
31	CLA	9	313	X	-	-	-
31	CLA	9	315	X	-	-	-
31	CLA	A	403	X	-	-	-
31	CLA	A	404	X	-	-	-
31	CLA	A	406	X	-	-	-
31	CLA	B	601	X	-	-	-
31	CLA	B	602	X	-	-	-
31	CLA	B	603	X	-	-	-
31	CLA	B	604	X	-	-	-
31	CLA	B	605	X	-	-	-
31	CLA	B	606	X	-	-	-
31	CLA	B	607	X	-	-	-
31	CLA	B	608	X	-	-	-
31	CLA	B	611	X	-	-	-
31	CLA	B	612	X	-	-	-
31	CLA	B	613	X	-	-	-
31	CLA	B	614	X	-	-	-
31	CLA	B	615	X	-	-	-
31	CLA	B	616	X	-	-	-
31	CLA	C	502	X	-	-	-
31	CLA	C	503	X	-	-	-
31	CLA	C	504	X	-	-	-
31	CLA	C	505	X	-	-	-
31	CLA	C	506	X	-	-	-
31	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	C	508	X	-	-	-
31	CLA	C	509	X	-	-	-
31	CLA	C	510	X	-	-	-
31	CLA	C	511	X	-	-	-
31	CLA	C	512	X	-	-	-
31	CLA	C	513	X	-	-	-
31	CLA	C	514	X	-	-	-
31	CLA	D	402	X	-	-	-
31	CLA	D	405	X	-	-	-
31	CLA	D	406	X	-	-	-
31	CLA	P	601	X	-	-	-
31	CLA	P	602	X	-	-	-
31	CLA	P	603	X	-	-	-
31	CLA	P	604	X	-	-	-
31	CLA	P	605	X	-	-	-
31	CLA	P	606	X	-	-	-
31	CLA	P	607	X	-	-	-
31	CLA	P	608	X	-	-	-
31	CLA	P	610	X	-	-	-
31	CLA	R	101	X	-	-	-
31	CLA	W	202	X	-	-	-
31	CLA	Z	101	X	-	-	-
31	CLA	a	403	X	-	-	-
31	CLA	a	404	X	-	-	-
31	CLA	a	406	X	-	-	-
31	CLA	b	602	X	-	-	-
31	CLA	b	603	X	-	-	-
31	CLA	b	604	X	-	-	-
31	CLA	b	605	X	-	-	-
31	CLA	b	606	X	-	-	-
31	CLA	b	607	X	-	-	-
31	CLA	b	608	X	-	-	-
31	CLA	b	609	X	-	-	-
31	CLA	b	612	X	-	-	-
31	CLA	b	613	X	-	-	-
31	CLA	b	614	X	-	-	-
31	CLA	b	615	X	-	-	-
31	CLA	b	616	X	-	-	-
31	CLA	b	617	X	-	-	-
31	CLA	c	502	X	-	-	-
31	CLA	c	503	X	-	-	-
31	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	c	505	X	-	-	-
31	CLA	c	506	X	-	-	-
31	CLA	c	507	X	-	-	-
31	CLA	c	508	X	-	-	-
31	CLA	c	509	X	-	-	-
31	CLA	c	510	X	-	-	-
31	CLA	c	511	X	-	-	-
31	CLA	c	512	X	-	-	-
31	CLA	c	513	X	-	-	-
31	CLA	c	514	X	-	-	-
31	CLA	d	402	X	-	-	-
31	CLA	d	405	X	-	-	-
31	CLA	d	406	X	-	-	-
31	CLA	p	601	X	-	-	-
31	CLA	p	602	X	-	-	-
31	CLA	p	603	X	-	-	-
31	CLA	p	604	X	-	-	-
31	CLA	p	605	X	-	-	-
31	CLA	p	606	X	-	-	-
31	CLA	p	607	X	-	-	-
31	CLA	p	608	X	-	-	-
31	CLA	p	610	X	-	-	-
31	CLA	r	101	X	-	-	-
31	CLA	w	203	X	-	-	-
31	CLA	z	101	X	-	-	-
31	CLA	z	103	X	-	-	-

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 102777 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 PsbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2617	1711	429	462	15		
1	a	334	Total	C	N	O	S	0	0
			2617	1711	429	462	15		

- Molecule 2 is a protein called PsbB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	503	Total	C	N	O	S	0	0
			3960	2588	669	690	13		
2	b	503	Total	C	N	O	S	0	0
			3960	2588	669	690	13		

- Molecule 3 is a protein called PsbC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3496	2290	583	609	14		
3	c	450	Total	C	N	O	S	0	0
			3496	2290	583	609	14		

- Molecule 4 is a protein called PsbD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2696	1781	441	464	10		
4	d	341	Total	C	N	O	S	0	0
			2696	1781	441	464	10		

- Molecule 5 is a protein called PsbE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	79	Total	C	N	O	0	0
			642	415	106	121		
5	e	79	Total	C	N	O	0	0
			642	415	106	121		

- Molecule 6 is a protein called PsbF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	32	Total	C	N	O	S	0	0
			259	178	43	37	1		
6	f	32	Total	C	N	O	S	0	0
			259	178	43	37	1		

- Molecule 7 is a protein called Psb31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	122	Total	C	N	O	S	0	0
			922	580	167	174	1		
7	g	122	Total	C	N	O	S	0	0
			922	580	167	174	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total	C	N	O	S	0	0
			506	335	82	87	2		
8	h	65	Total	C	N	O	S	0	0
			506	335	82	87	2		

- Molecule 9 is a protein called PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			278	188	43	46	1		
9	i	34	Total	C	N	O	S	0	0
			278	188	43	46	1		

- Molecule 10 is a protein called PsbJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	34	Total	C	N	O	0	0
			247	167	38	42		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	34	Total	C	N	O	0	0
			247	167	38	42		

- Molecule 11 is a protein called PsbK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			300	210	44	45	1		
11	k	37	Total	C	N	O	S	0	0
			300	210	44	45	1		

- Molecule 12 is a protein called PsbL.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	37	Total	C	N	O	0	0
			301	203	47	51		
12	l	37	Total	C	N	O	0	0
			301	203	47	51		

- Molecule 13 is a protein called PsbM.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	41	Total	C	N	O	0	0
			308	203	50	55		
13	m	41	Total	C	N	O	0	0
			308	203	50	55		

- Molecule 14 is a protein called Psb34.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	30	Total	C	N	O	0	0
			150	90	30	30		
14	n	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 15 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	249	Total	C	N	O	S	0	0
			1881	1188	310	375	8		
15	o	249	Total	C	N	O	S	0	0
			1881	1188	310	375	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	185	SER	ASN	conflict	UNP B6ZHE8
O	336	GLU	ASP	conflict	UNP B6ZHE8
o	185	SER	ASN	conflict	UNP B6ZHE8
o	336	GLU	ASP	conflict	UNP B6ZHE8

- Molecule 16 is a protein called FCP-D.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	226	Total	C	N	O	S	0	0
			1745	1129	290	321	5		
16	p	226	Total	C	N	O	S	0	0
			1745	1129	290	321	5		

- Molecule 17 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	147	Total	C	N	O	S	0	0
			1143	725	188	229	1		
17	q	147	Total	C	N	O	S	0	0
			1143	725	188	229	1		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	30	VAL	ILE	conflict	UNP B6ZHE9
Q	34	ALA	GLY	conflict	UNP B6ZHE9
Q	70	ILE	VAL	conflict	UNP B6ZHE9
Q	110	SER	ASN	conflict	UNP B6ZHE9
Q	133	GLY	ALA	conflict	UNP B6ZHE9
q	30	VAL	ILE	conflict	UNP B6ZHE9
q	34	ALA	GLY	conflict	UNP B6ZHE9
q	70	ILE	VAL	conflict	UNP B6ZHE9
q	110	SER	ASN	conflict	UNP B6ZHE9
q	133	GLY	ALA	conflict	UNP B6ZHE9

- Molecule 18 is a protein called PsbG.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			365	219	73	73		

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Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	73	Total	C	N	O	0	0
			365	219	73	73		

- Molecule 19 is a protein called PsbT.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	30	Total	C	N	O	S	0	0
			250	174	36	38	2		
19	t	30	Total	C	N	O	S	0	0
			250	174	36	38	2		

- Molecule 20 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	93	Total	C	N	O	S	0	0
			711	454	119	136	2		
20	u	93	Total	C	N	O	S	0	0
			711	454	119	136	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	33	ILE	VAL	conflict	UNP B6ZHF0
U	60	SER	ALA	conflict	UNP B6ZHF0
u	33	ILE	VAL	conflict	UNP B6ZHF0
u	60	SER	ALA	conflict	UNP B6ZHF0

- Molecule 21 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	137	Total	C	N	O	S	0	0
			1043	652	182	205	4		
21	v	137	Total	C	N	O	S	0	0
			1043	652	182	205	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	70	ASN	SER	conflict	UNP B6ZHF4
v	70	ASN	SER	conflict	UNP B6ZHF4

- Molecule 22 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	51	Total	C	N	O	S	0	0
			394	247	73	71	3		
22	w	51	Total	C	N	O	S	0	0
			394	247	73	71	3		

- Molecule 23 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	35	Total	C	N	O	S	0	0
			244	159	40	44	1		
23	x	35	Total	C	N	O	S	0	0
			244	159	40	44	1		

- Molecule 24 is a protein called PsbY.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	33	Total	C	N	O	S	0	0
			256	168	47	41			
24	y	33	Total	C	N	O	S	0	0
			256	168	47	41			

- Molecule 25 is a protein called PsbZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	61	Total	C	N	O	S	0	0
			452	301	68	82	1		
25	z	61	Total	C	N	O	S	0	0
			452	301	68	82	1		

- Molecule 26 is a protein called FCP-E.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	178	Total	C	N	O	S	0	0
			1291	827	219	241	4		
26	10	178	Total	C	N	O	S	0	0
			1291	827	219	241	4		

- Molecule 27 is a protein called FCP-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		

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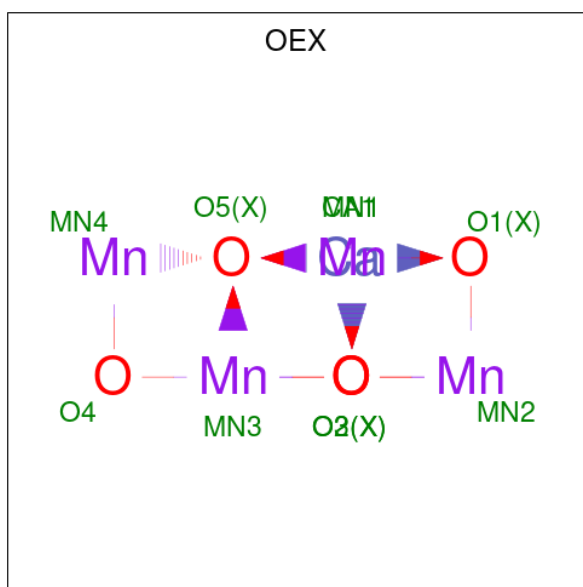
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Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		
27	3	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		
27	4	172	Total	C	N	O	S	0	0
			1313	855	212	241	5		
27	5	172	Total	C	N	O	S	0	0
			1280	826	207	242	5		
27	6	172	Total	C	N	O	S	0	0
			1335	871	216	243	5		
27	7	172	Total	C	N	O	S	0	0
			1335	871	216	243	5		
27	8	172	Total	C	N	O	S	0	0
			1291	832	211	243	5		
27	11	172	Total	C	N	O	S	0	0
			1335	871	216	243	5		
27	12	172	Total	C	N	O	S	0	0
			1328	866	215	243	4		
27	13	172	Total	C	N	O	S	0	0
			1332	869	215	243	5		
27	14	172	Total	C	N	O	S	0	0
			1313	855	212	241	5		
27	15	172	Total	C	N	O	S	0	0
			1280	826	207	242	5		
27	16	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		
27	17	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		
27	18	172	Total	C	N	O	S	0	0
			1304	841	215	243	5		

- Molecule 28 is a protein called FCP-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	9	166	Total	C	N	O	S	0	0
			1286	829	212	241	4		
28	19	166	Total	C	N	O	S	0	0
			1286	829	212	241	4		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

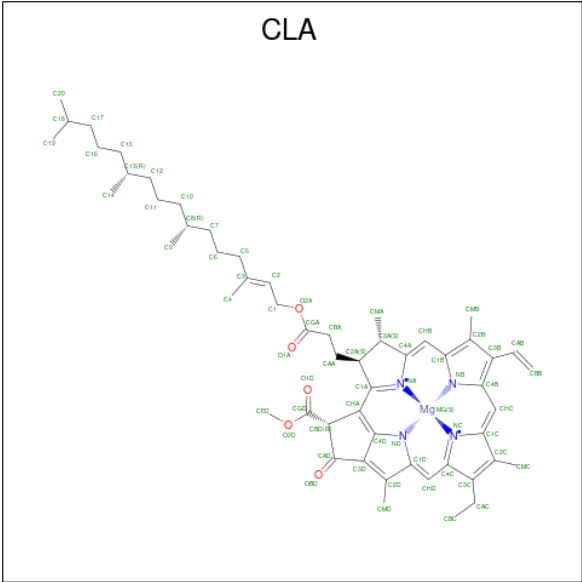


Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	P	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	P	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	P	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	P	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	P	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	R	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Z	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	p	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	p	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	p	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	p	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	p	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	p	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	r	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	z	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	z	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	0	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	0	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	0	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	0	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	0	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	0	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	0	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	1	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	3	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
31	3	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 44	C 35	Mg 1	N 4	O 4	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	5	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	6	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
31	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	6	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	9	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	10	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	10	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	10	1	Total 59	C 49	Mg 1	N 4	O 5	0
31	10	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	10	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	10	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	10	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	10	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	10	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	11	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	11	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	11	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	11	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	11	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	12	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	12	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	12	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	12	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	12	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	12	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	13	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	13	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	13	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	13	1	Total 44	C 35	Mg 1	N 4	O 4	0
31	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	14	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	14	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	14	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	14	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	14	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	15	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	15	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	15	1	Total 45	C 35	Mg 1	N 4	O 5	0

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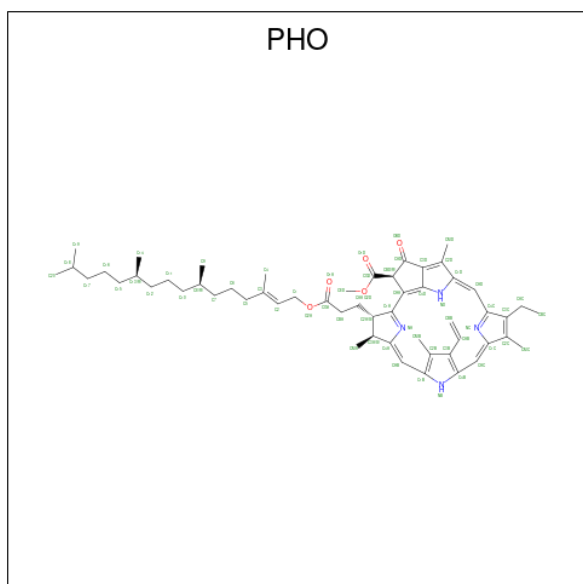
Mol	Chain	Residues	Atoms					AltConf
31	15	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	15	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	16	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	16	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	16	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	16	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	16	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	17	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	17	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	17	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	17	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	17	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	18	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	18	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	18	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	18	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	18	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	18	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	19	1	Total 61	C 51	Mg 1	N 4	O 5	0

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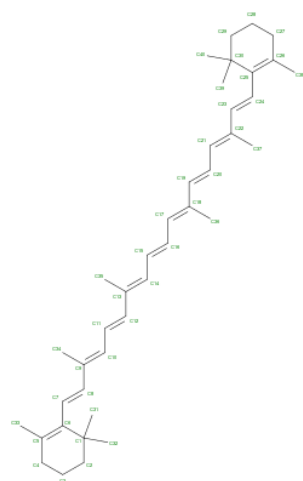
Mol	Chain	Residues	Atoms					AltConf
31	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	19	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	19	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).

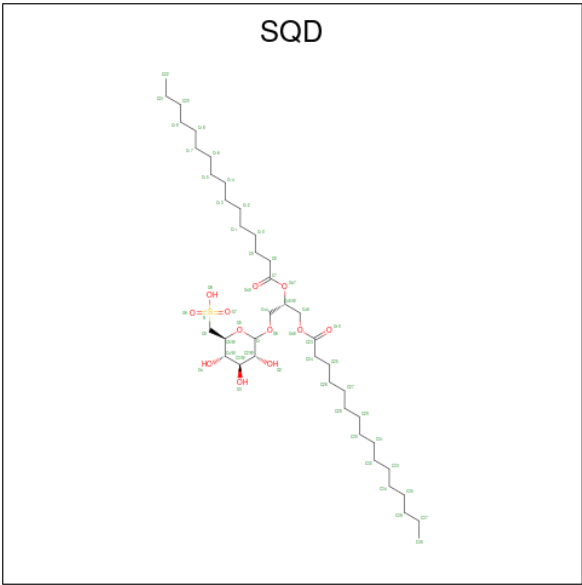


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Mol	Chain	Residues	Atoms		AltConf
33	c	1	Total	C	0
			40	40	
33	c	1	Total	C	0
			40	40	
33	c	1	Total	C	0
			40	40	
33	f	1	Total	C	0
			40	40	
33	h	1	Total	C	0
			40	40	
33	y	1	Total	C	0
			40	40	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



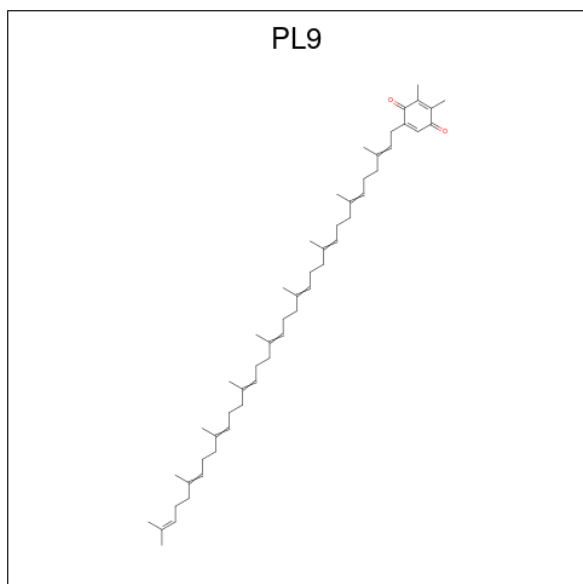
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	S	0
			54	41	12	1	
34	A	1	Total	C	O	S	0
			40	27	12	1	
34	B	1	Total	C	O	S	0
			54	41	12	1	
34	L	1	Total	C	O	S	0
			54	41	12	1	
34	a	1	Total	C	O	S	0
			54	41	12	1	

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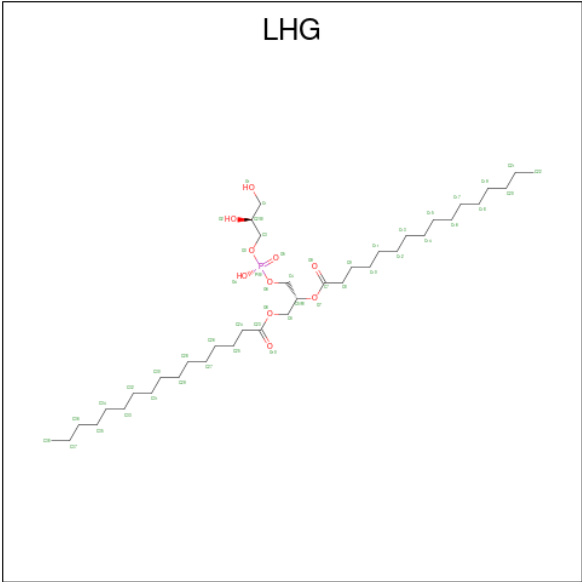
Mol	Chain	Residues	Atoms				AltConf
34	b	1	Total	C	O	S	0
			54	41	12	1	
34	i	1	Total	C	O	S	0
			40	27	12	1	
34	l	1	Total	C	O	S	0
			54	41	12	1	
34	8	1	Total	C	O	S	0
			41	28	12	1	
34	10	1	Total	C	O	S	0
			41	28	12	1	

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



Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O		0
			33	31	2		
35	D	1	Total	C	O		0
			55	53	2		
35	a	1	Total	C	O		0
			33	31	2		
35	d	1	Total	C	O		0
			55	53	2		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



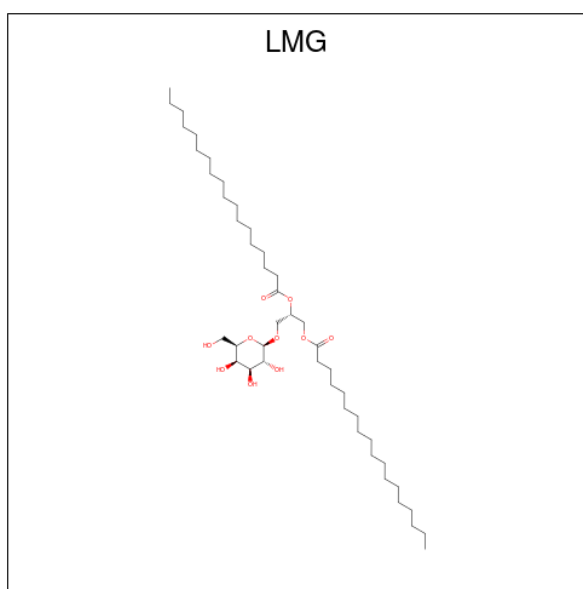
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	P	0
			37	26	10	1	
36	B	1	Total	C	O	P	0
			43	32	10	1	
36	C	1	Total	C	O	P	0
			40	29	10	1	
36	D	1	Total	C	O	P	0
			49	38	10	1	
36	L	1	Total	C	O	P	0
			49	38	10	1	
36	P	1	Total	C	O	P	0
			27	16	10	1	
36	Z	1	Total	C	O	P	0
			25	14	10	1	
36	a	1	Total	C	O	P	0
			37	26	10	1	
36	b	1	Total	C	O	P	0
			43	32	10	1	
36	d	1	Total	C	O	P	0
			49	38	10	1	
36	l	1	Total	C	O	P	0
			49	38	10	1	
36	p	1	Total	C	O	P	0
			27	16	10	1	
36	w	1	Total	C	O	P	0
			40	29	10	1	
36	z	1	Total	C	O	P	0
			25	14	10	1	

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Mol	Chain	Residues	Atoms				AltConf
36	4	1	Total	C	O	P	0
			35	24	10	1	
36	5	1	Total	C	O	P	0
			25	14	10	1	
36	8	1	Total	C	O	P	0
			39	28	10	1	
36	8	1	Total	C	O	P	0
			31	20	10	1	
36	14	1	Total	C	O	P	0
			35	24	10	1	
36	15	1	Total	C	O	P	0
			25	14	10	1	
36	18	1	Total	C	O	P	0
			39	28	10	1	
36	18	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			51	41	10	
37	C	1	Total	C	O	0
			51	41	10	
37	D	1	Total	C	O	0
			40	30	10	

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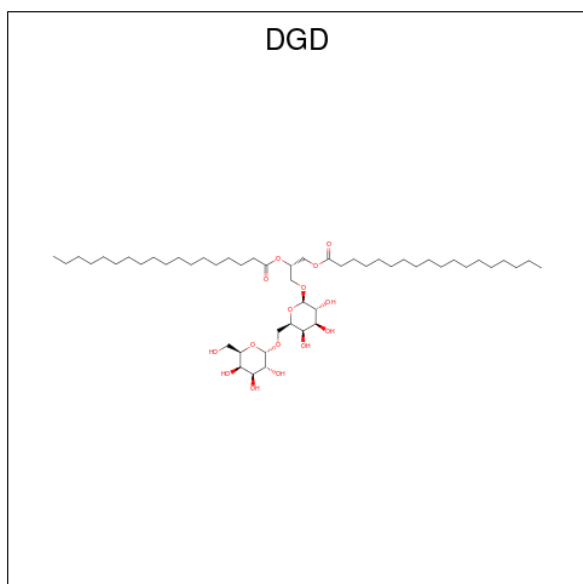
Mol	Chain	Residues	Atoms			AltConf
37	D	1	Total 37	C 27	O 10	0
37	F	1	Total 46	C 36	O 10	0
37	J	1	Total 50	C 40	O 10	0
37	K	1	Total 46	C 36	O 10	0
37	M	1	Total 40	C 30	O 10	0
37	N	1	Total 28	C 18	O 10	0
37	P	1	Total 31	C 21	O 10	0
37	W	1	Total 48	C 38	O 10	0
37	Z	1	Total 31	C 21	O 10	0
37	b	1	Total 51	C 41	O 10	0
37	c	1	Total 51	C 41	O 10	0
37	c	1	Total 31	C 21	O 10	0
37	d	1	Total 40	C 30	O 10	0
37	d	1	Total 37	C 27	O 10	0
37	f	1	Total 46	C 36	O 10	0
37	j	1	Total 50	C 40	O 10	0
37	k	1	Total 46	C 36	O 10	0
37	m	1	Total 40	C 30	O 10	0
37	n	1	Total 28	C 18	O 10	0
37	p	1	Total 31	C 21	O 10	0
37	w	1	Total 48	C 38	O 10	0

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Mol	Chain	Residues	Atoms			AltConf
37	0	1	Total	C	O	0
			31	21	10	
37	1	1	Total	C	O	0
			36	26	10	
37	1	1	Total	C	O	0
			45	35	10	
37	4	1	Total	C	O	0
			49	39	10	
37	5	1	Total	C	O	0
			37	27	10	
37	5	1	Total	C	O	0
			36	26	10	
37	10	1	Total	C	O	0
			31	21	10	
37	11	1	Total	C	O	0
			36	26	10	
37	11	1	Total	C	O	0
			45	35	10	
37	14	1	Total	C	O	0
			49	39	10	
37	15	1	Total	C	O	0
			37	27	10	
37	15	1	Total	C	O	0
			36	26	10	

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

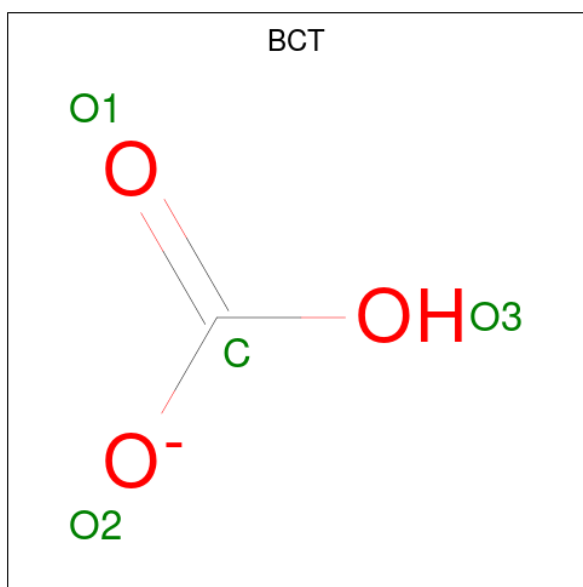


Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			54	39	15	
38	C	1	Total	C	O	0
			55	40	15	
38	C	1	Total	C	O	0
			62	47	15	
38	C	1	Total	C	O	0
			62	47	15	
38	H	1	Total	C	O	0
			62	47	15	
38	W	1	Total	C	O	0
			56	41	15	
38	b	1	Total	C	O	0
			55	40	15	
38	c	1	Total	C	O	0
			55	40	15	
38	c	1	Total	C	O	0
			62	47	15	
38	c	1	Total	C	O	0
			62	47	15	
38	h	1	Total	C	O	0
			62	47	15	
38	w	1	Total	C	O	0
			56	41	15	
38	1	1	Total	C	O	0
			54	39	15	
38	11	1	Total	C	O	0
			60	45	15	

- Molecule 39 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

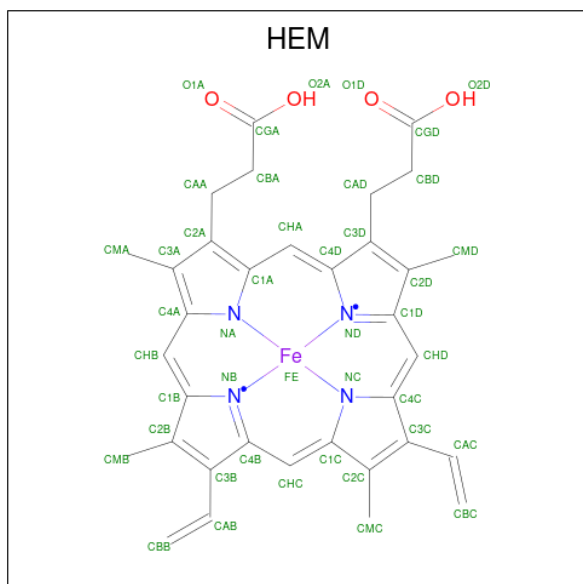
Mol	Chain	Residues	Atoms		AltConf
39	C	1	Total	Cl	0
			1	1	
39	c	1	Total	Cl	0
			1	1	

- Molecule 40 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			4	1	3	
40	d	1	Total	C	O	0
			4	1	3	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



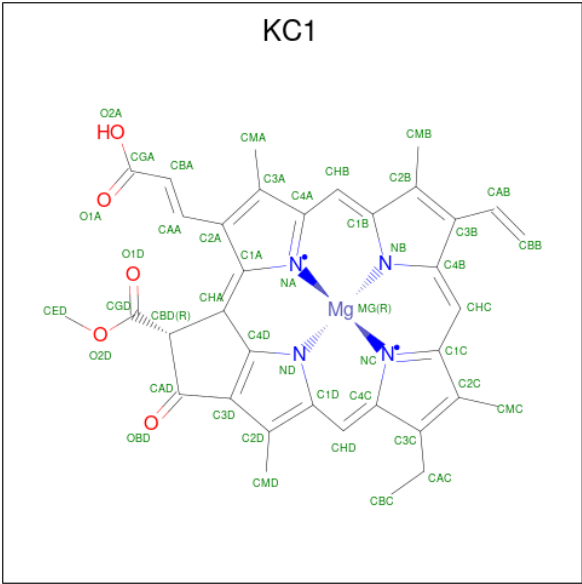
Mol	Chain	Residues	Atoms					AltConf
41	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
41	V	1	Total 43	C 34	Fe 1	N 4	O 4	0
41	e	1	Total 43	C 34	Fe 1	N 4	O 4	0
41	v	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 42 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



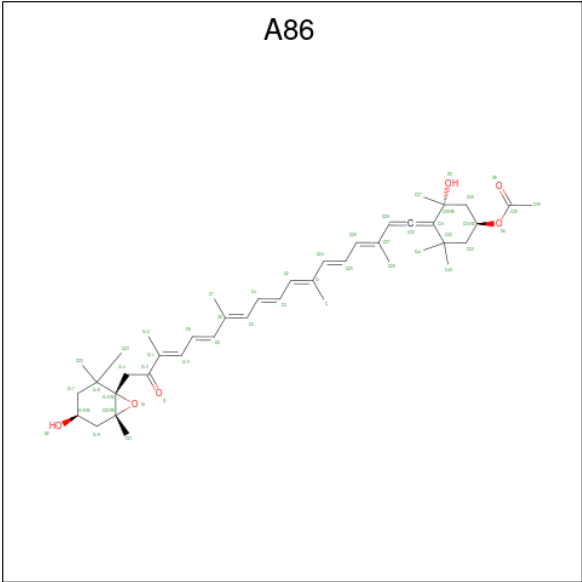
Mol	Chain	Residues	Atoms					AltConf
42	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
42	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
42	19	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 43 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆).



Mol	Chain	Residues	Atoms			AltConf
43	P	1	Total	C	O	0
			48	42	6	
43	P	1	Total	C	O	0
			48	42	6	
43	p	1	Total	C	O	0
			48	42	6	
43	p	1	Total	C	O	0
			48	42	6	
43	0	1	Total	C	O	0
			48	42	6	
43	0	1	Total	C	O	0
			48	42	6	
43	0	1	Total	C	O	0
			48	42	6	
43	0	1	Total	C	O	0
			48	42	6	
43	0	1	Total	C	O	0
			48	42	6	
43	1	1	Total	C	O	0
			48	42	6	
43	1	1	Total	C	O	0
			48	42	6	
43	1	1	Total	C	O	0
			48	42	6	
43	1	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
43	1	1	Total	C	O	0
			48	42	6	
43	1	1	Total	C	O	0
			48	42	6	
43	1	1	Total	C	O	0
			48	42	6	
43	2	1	Total	C	O	0
			48	42	6	
43	2	1	Total	C	O	0
			48	42	6	
43	2	1	Total	C	O	0
			48	42	6	
43	2	1	Total	C	O	0
			48	42	6	
43	2	1	Total	C	O	0
			48	42	6	
43	3	1	Total	C	O	0
			48	42	6	
43	3	1	Total	C	O	0
			48	42	6	
43	3	1	Total	C	O	0
			48	42	6	
43	3	1	Total	C	O	0
			48	42	6	
43	3	1	Total	C	O	0
			48	42	6	
43	3	1	Total	C	O	0
			48	42	6	
43	4	1	Total	C	O	0
			48	42	6	
43	4	1	Total	C	O	0
			48	42	6	
43	4	1	Total	C	O	0
			48	42	6	
43	4	1	Total	C	O	0
			48	42	6	
43	4	1	Total	C	O	0
			48	42	6	
43	4	1	Total	C	O	0
			48	42	6	
43	5	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
43	5	1	Total	C	O	0
			48	42	6	
43	5	1	Total	C	O	0
			48	42	6	
43	5	1	Total	C	O	0
			48	42	6	
43	5	1	Total	C	O	0
			48	42	6	
43	5	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	8	1	Total	C	O	0
			48	42	6	
43	8	1	Total	C	O	0
			48	42	6	
43	8	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
43	8	1	Total	C	O	0
			48	42	6	
43	8	1	Total	C	O	0
			48	42	6	
43	9	1	Total	C	O	0
			48	42	6	
43	9	1	Total	C	O	0
			48	42	6	
43	9	1	Total	C	O	0
			48	42	6	
43	9	1	Total	C	O	0
			48	42	6	
43	9	1	Total	C	O	0
			48	42	6	
43	10	1	Total	C	O	0
			48	42	6	
43	10	1	Total	C	O	0
			48	42	6	
43	10	1	Total	C	O	0
			48	42	6	
43	10	1	Total	C	O	0
			48	42	6	
43	10	1	Total	C	O	0
			48	42	6	
43	10	1	Total	C	O	0
			48	42	6	
43	10	1	Total	C	O	0
			48	42	6	
43	11	1	Total	C	O	0
			48	42	6	
43	11	1	Total	C	O	0
			48	42	6	
43	11	1	Total	C	O	0
			48	42	6	
43	11	1	Total	C	O	0
			48	42	6	
43	11	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
43	11	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	14	1	Total	C	O	0
			48	42	6	
43	14	1	Total	C	O	0
			48	42	6	
43	14	1	Total	C	O	0
			48	42	6	
43	14	1	Total	C	O	0
			48	42	6	
43	14	1	Total	C	O	0
			48	42	6	
43	15	1	Total	C	O	0
			48	42	6	
43	15	1	Total	C	O	0
			48	42	6	
43	15	1	Total	C	O	0
			48	42	6	

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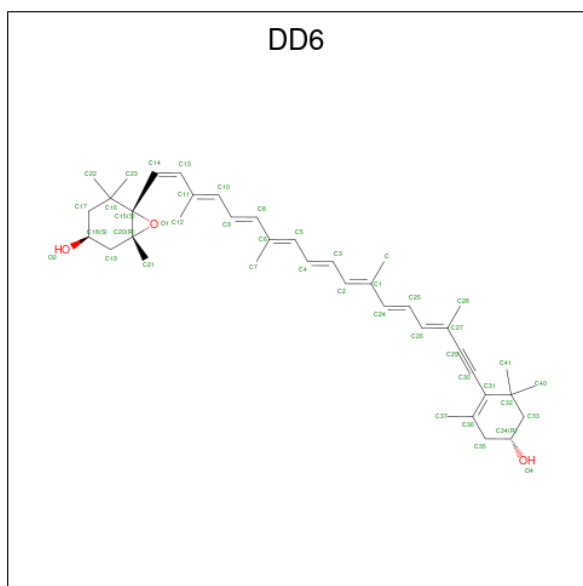
Mol	Chain	Residues	Atoms			AltConf
43	15	1	Total	C	O	0
			48	42	6	
43	15	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	18	1	Total	C	O	0
			48	42	6	
43	18	1	Total	C	O	0
			48	42	6	
43	18	1	Total	C	O	0
			48	42	6	
43	18	1	Total	C	O	0
			48	42	6	
43	18	1	Total	C	O	0
			48	42	6	
43	19	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
43	19	1	Total	C	O	0
			48	42	6	
43	19	1	Total	C	O	0
			48	42	6	
43	19	1	Total	C	O	0
			48	42	6	
43	19	1	Total	C	O	0
			48	42	6	
43	19	1	Total	C	O	0
			48	42	6	

- Molecule 44 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$).



Mol	Chain	Residues	Atoms			AltConf
44	P	1	Total	C	O	0
			43	40	3	
44	p	1	Total	C	O	0
			43	40	3	

- Molecule 45 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).



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Mol	Chain	Residues	Atoms					AltConf
45	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	18	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
45	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 46 is water.

Mol	Chain	Residues	Atoms		AltConf
46	Z	1	Total	O	0
			1	1	

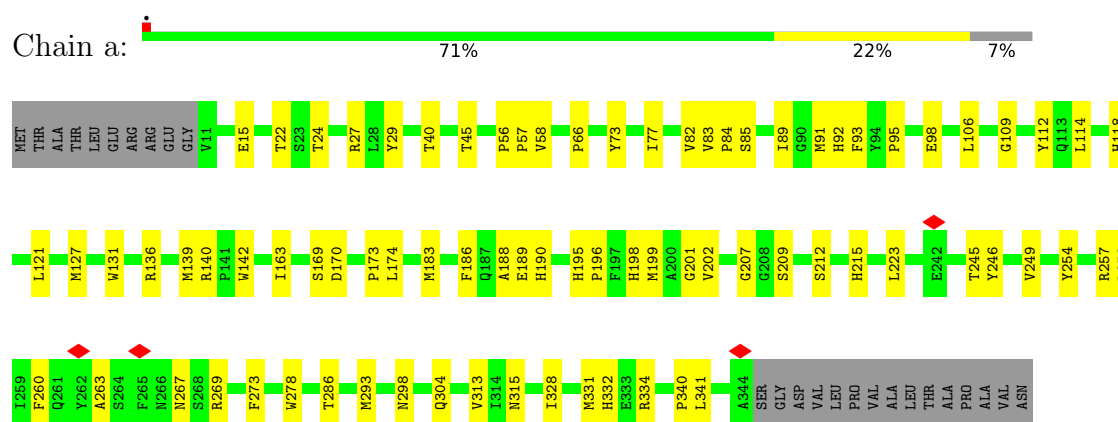
3 Residue-property plots

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.

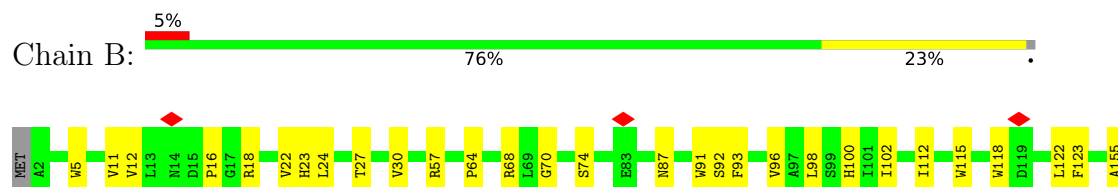
• Molecule 1: PsbA

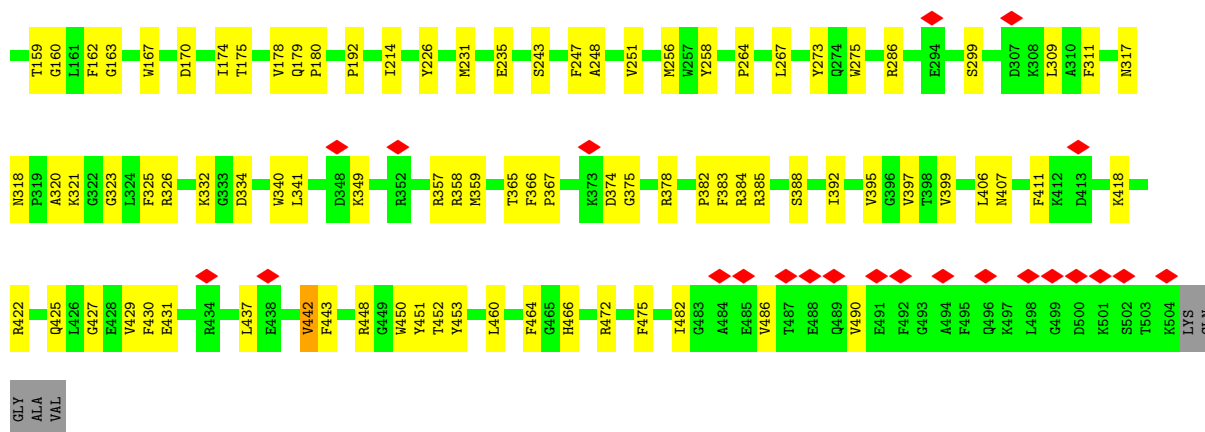


• Molecule 1: PsbA

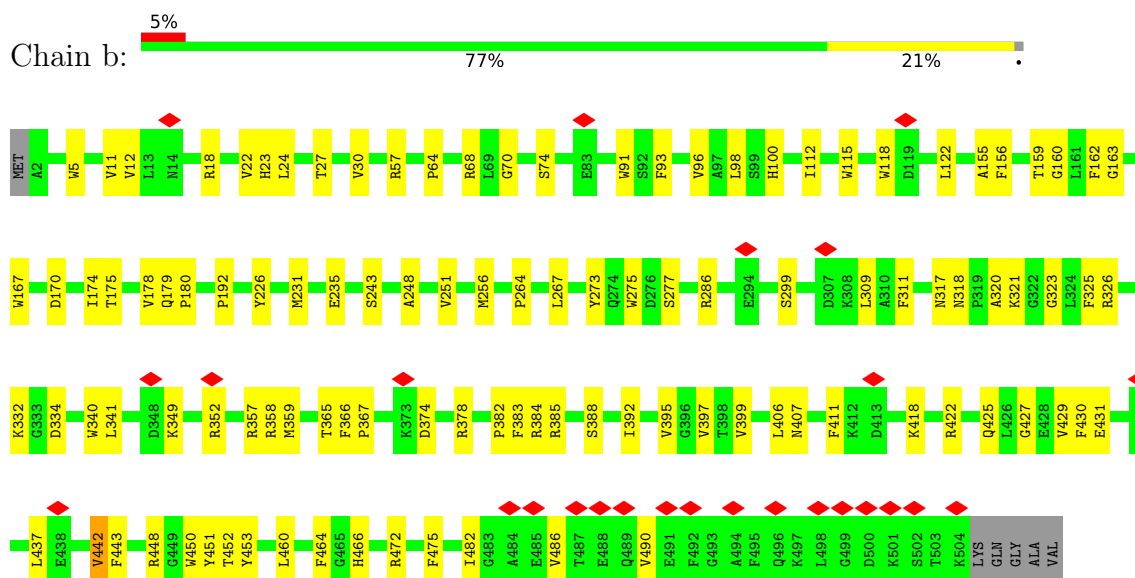


• Molecule 2: PsbB

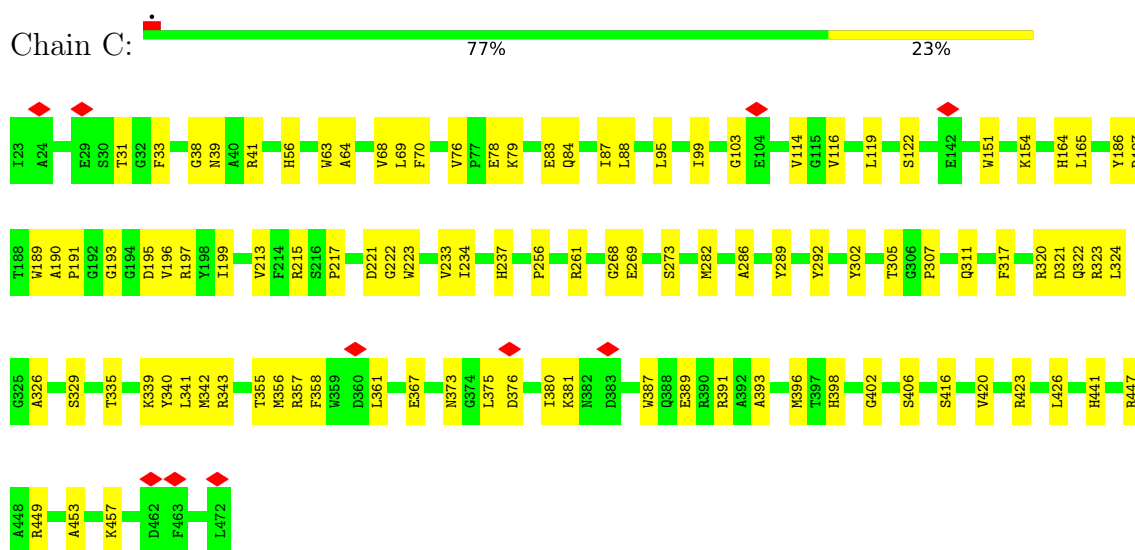




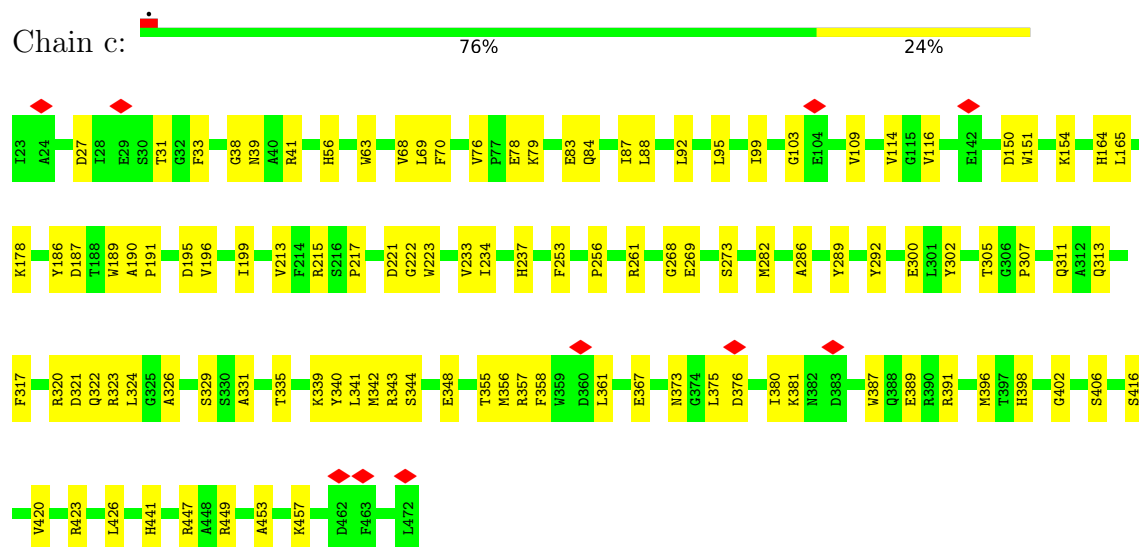
• Molecule 2: PsbB



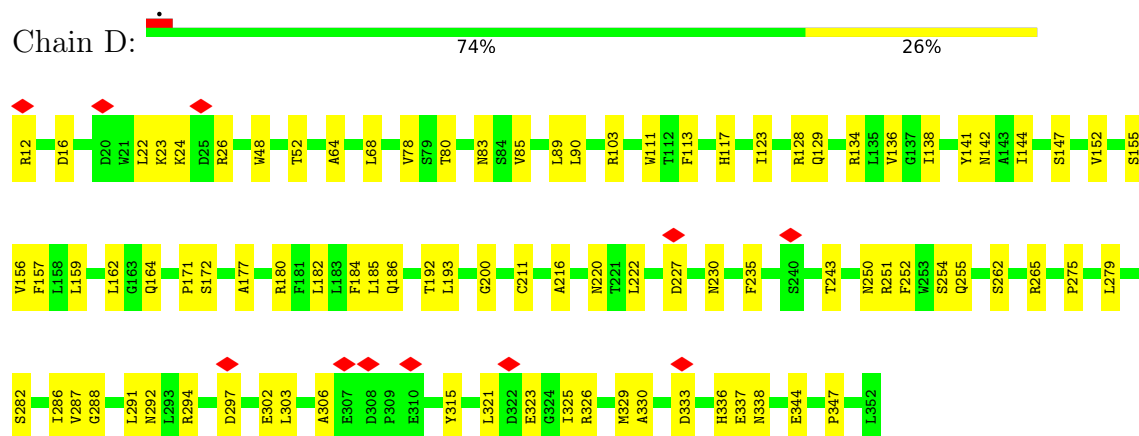
• Molecule 3: PsbC



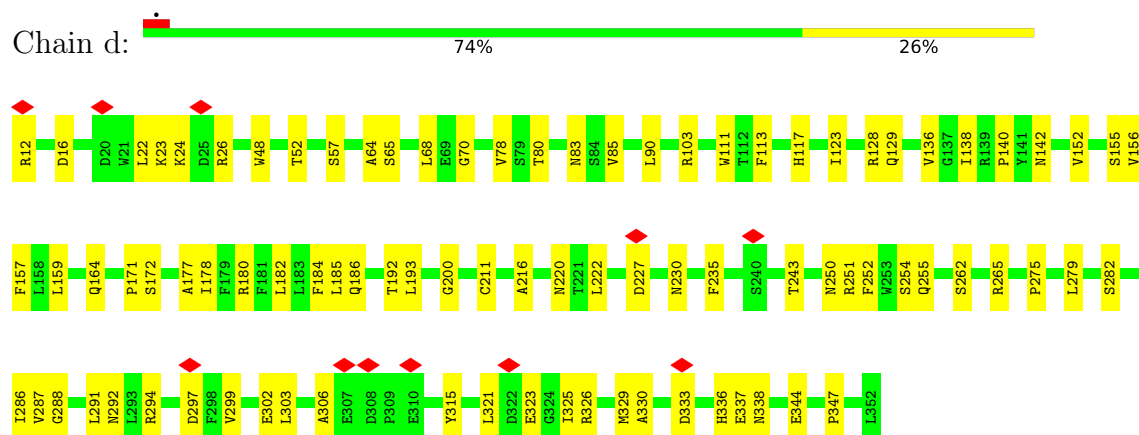
• Molecule 3: PsbC



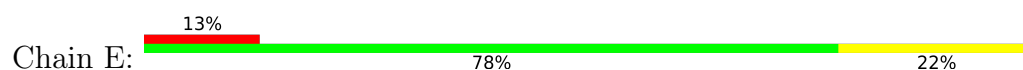
• Molecule 4: PsbD

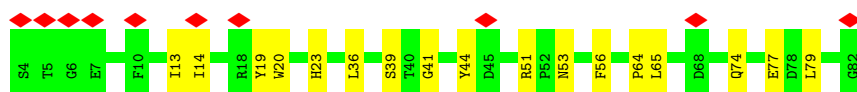


• Molecule 4: PsbD

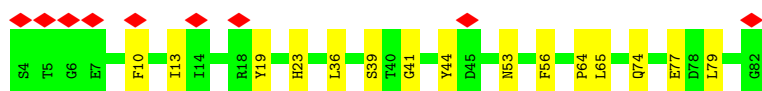
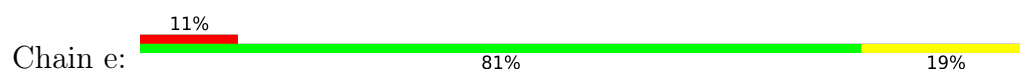


• Molecule 5: PsbE

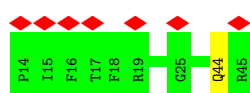




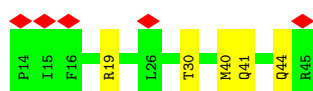
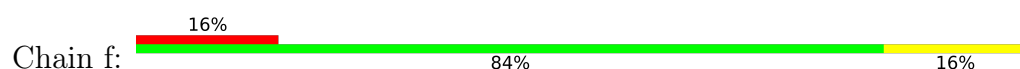
• Molecule 5: PsbE



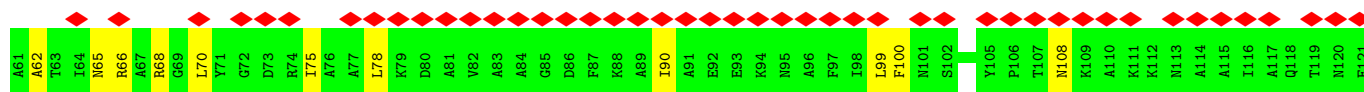
• Molecule 6: PsbF



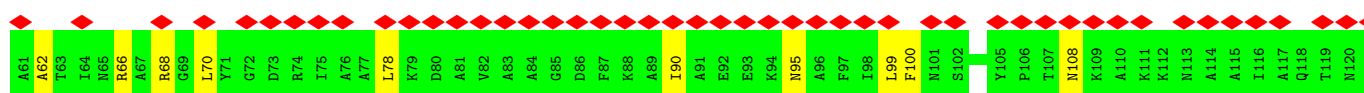
• Molecule 6: PsbF



• Molecule 7: Psb31

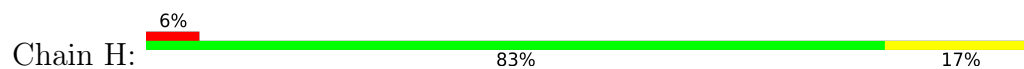


• Molecule 7: Psb31

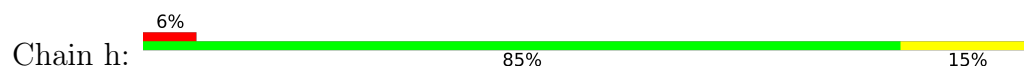




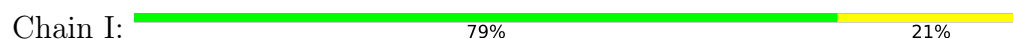
- Molecule 8: Photosystem II reaction center protein H



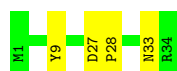
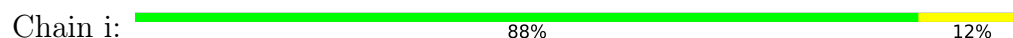
- Molecule 8: Photosystem II reaction center protein H



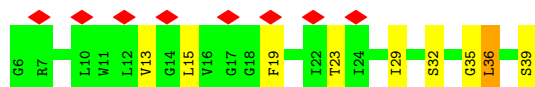
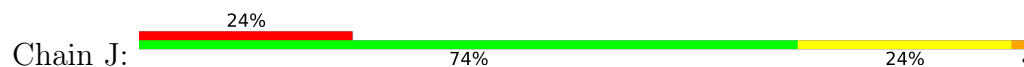
- Molecule 9: PsbI



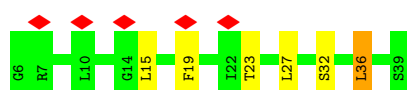
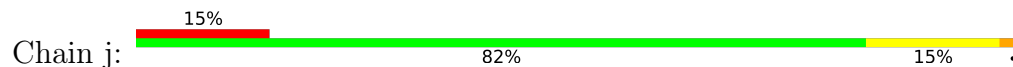
- Molecule 9: PsbI



- Molecule 10: PsbJ



- Molecule 10: PsbJ

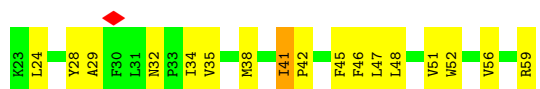


- Molecule 11: PsbK





- Molecule 11: PsbK



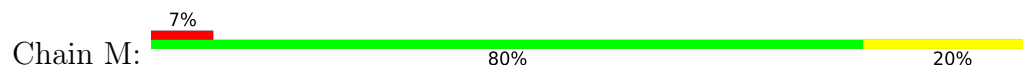
- Molecule 12: PsbL



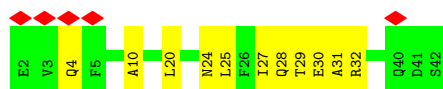
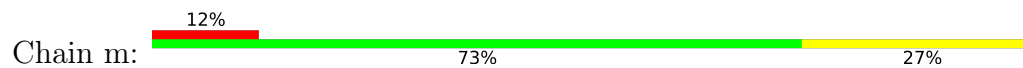
- Molecule 12: PsbL



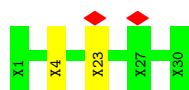
- Molecule 13: PsbM



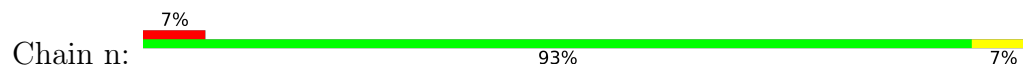
- Molecule 13: PsbM

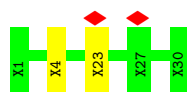


- Molecule 14: Psb34

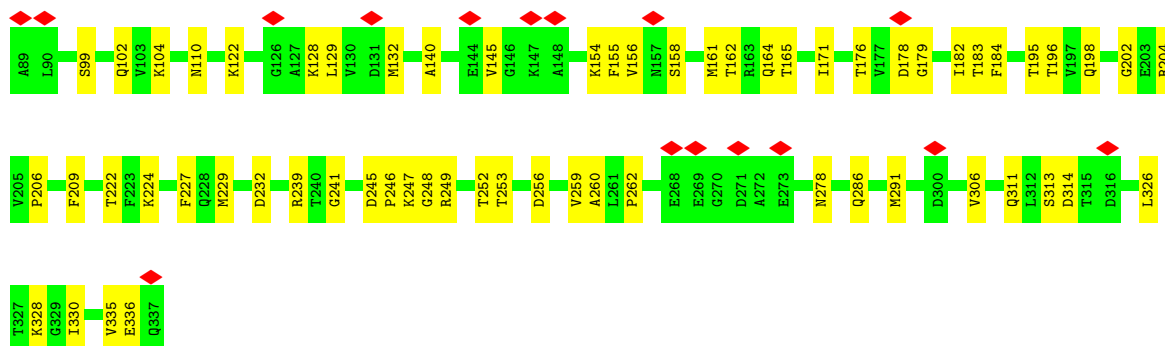
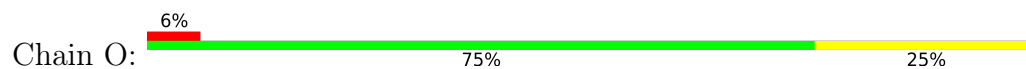


- Molecule 14: Psb34

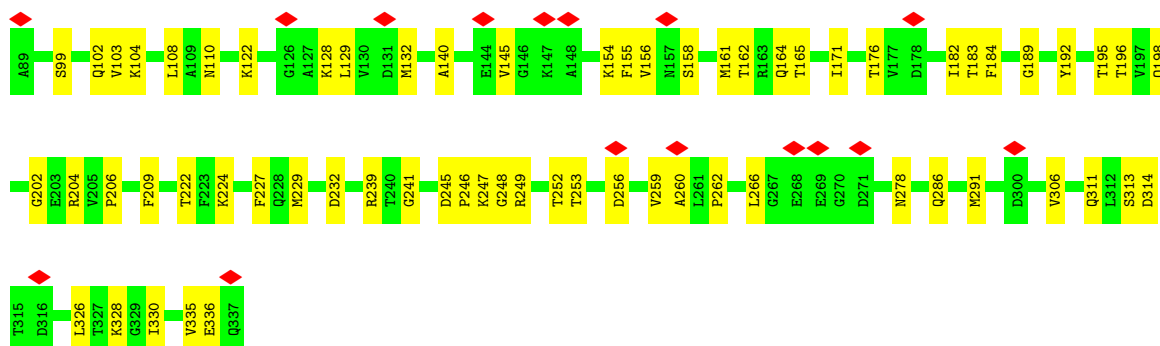
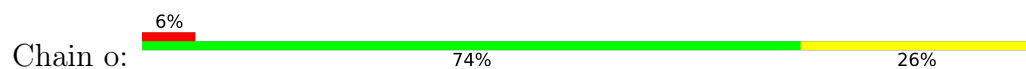




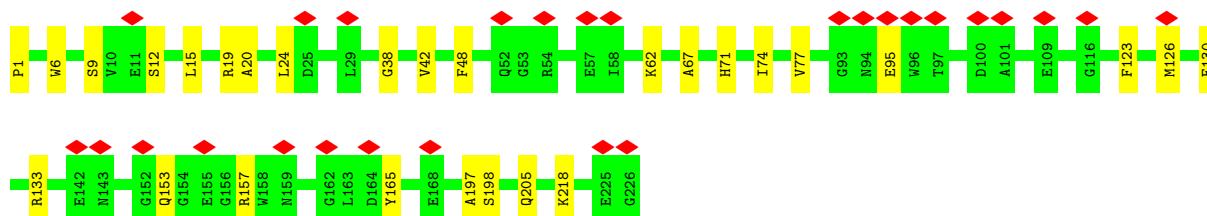
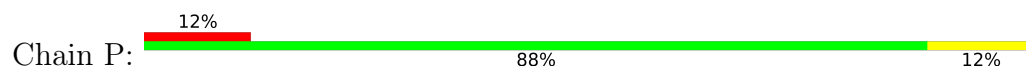
- Molecule 15: Extrinsic protein in photosystem II



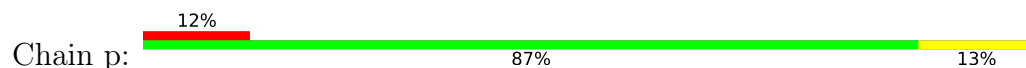
- Molecule 15: Extrinsic protein in photosystem II

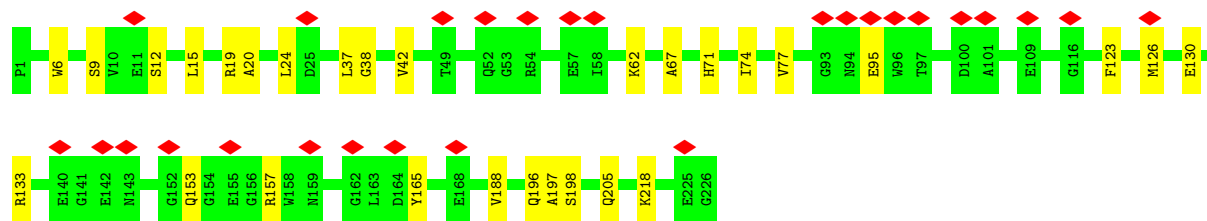


- Molecule 16: FCP-D

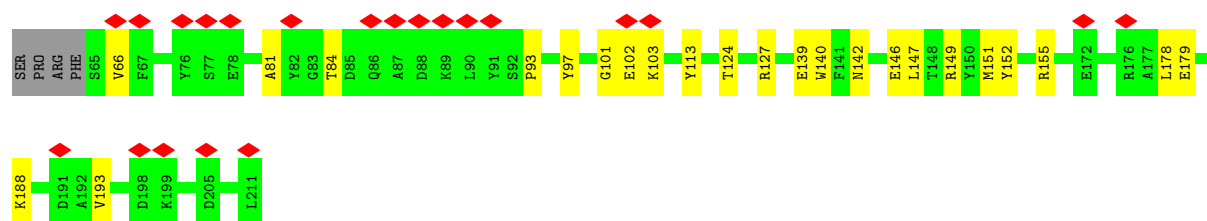


- Molecule 16: FCP-D

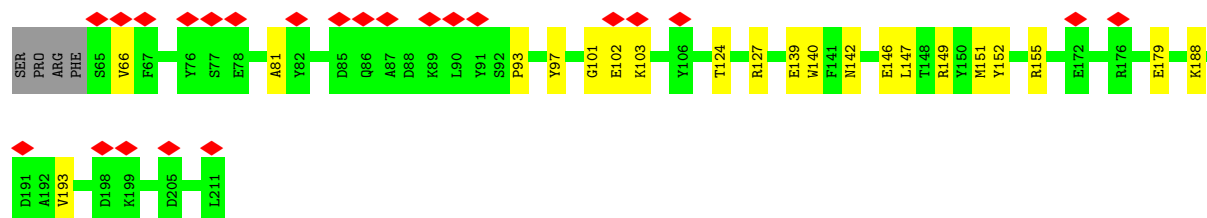




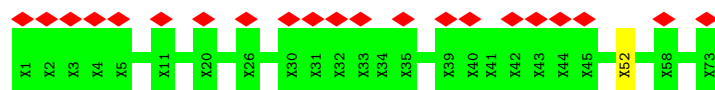
• Molecule 17: Extrinsic protein in photosystem II



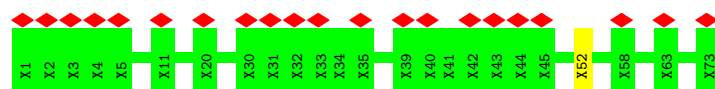
• Molecule 17: Extrinsic protein in photosystem II



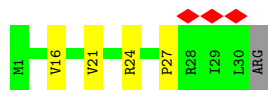
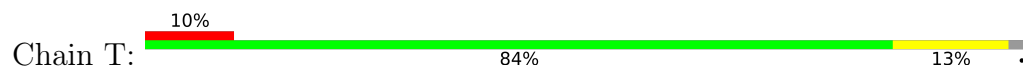
• Molecule 18: PsbG



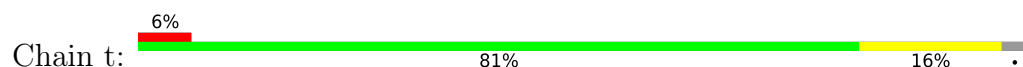
• Molecule 18: PsbG



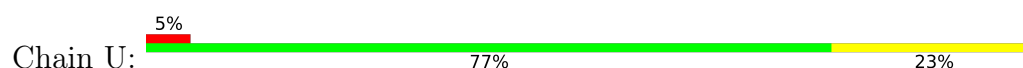
- Molecule 19: PsbT



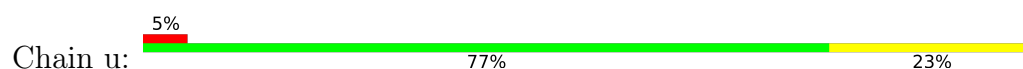
- Molecule 19: PsbT



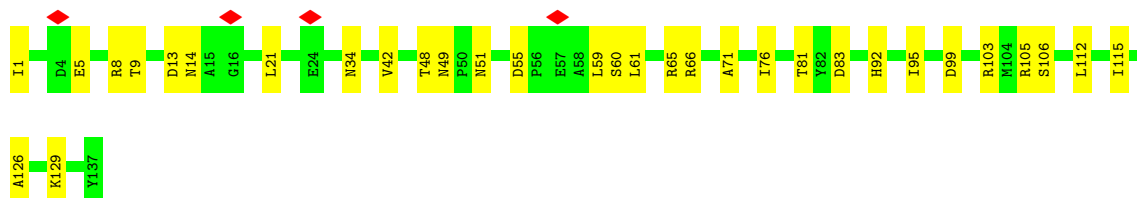
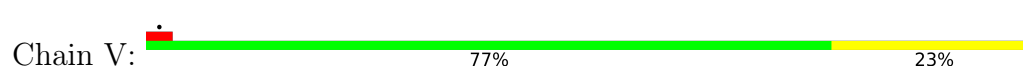
- Molecule 20: Extrinsic protein in photosystem II



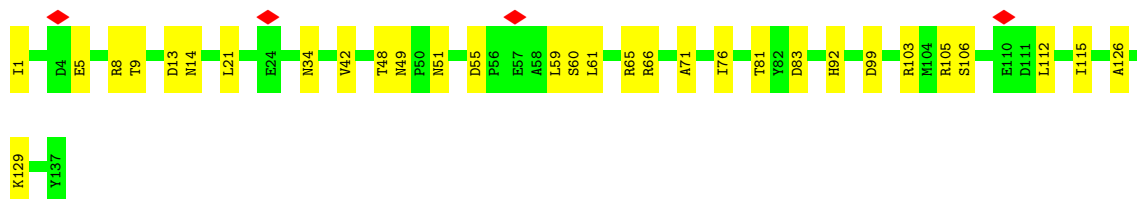
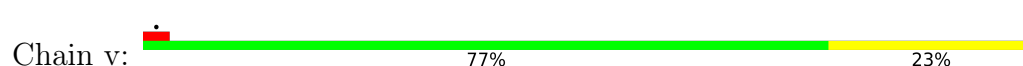
- Molecule 20: Extrinsic protein in photosystem II



- Molecule 21: Cytochrome c-550



- Molecule 21: Cytochrome c-550



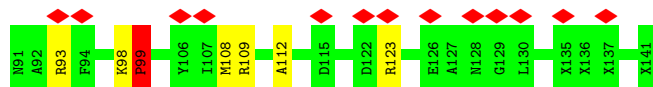
- Molecule 22: PsbW

Chain W: 



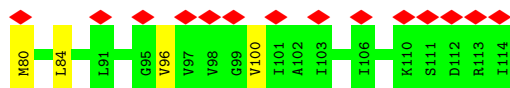
- Molecule 22: PsbW

Chain w: 



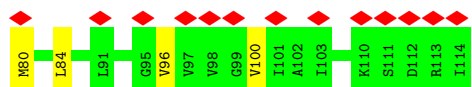
- Molecule 23: Photosystem II reaction center X protein

Chain X: 



- Molecule 23: Photosystem II reaction center X protein

Chain x: 



- Molecule 24: PsbY

Chain Y: 



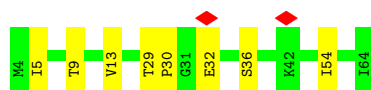
- Molecule 24: PsbY

Chain y: 

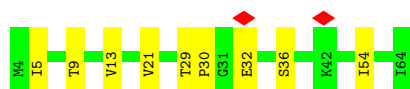
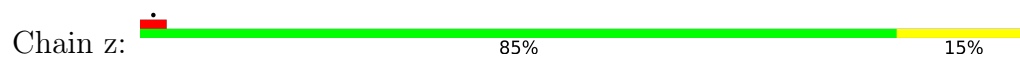


- Molecule 25: PsbZ

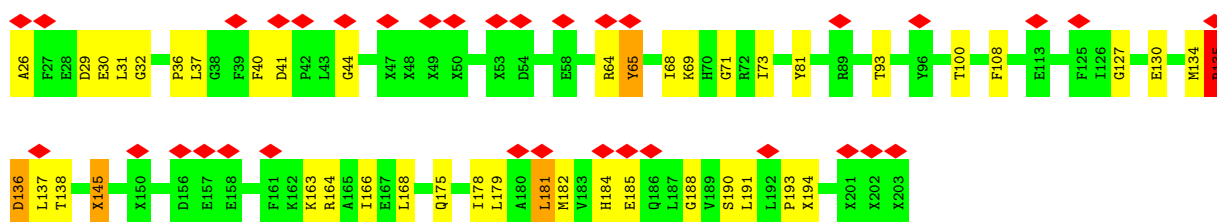
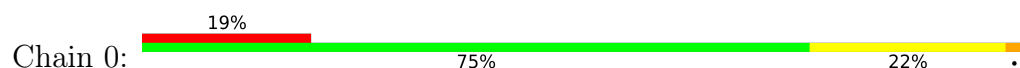
Chain Z: 



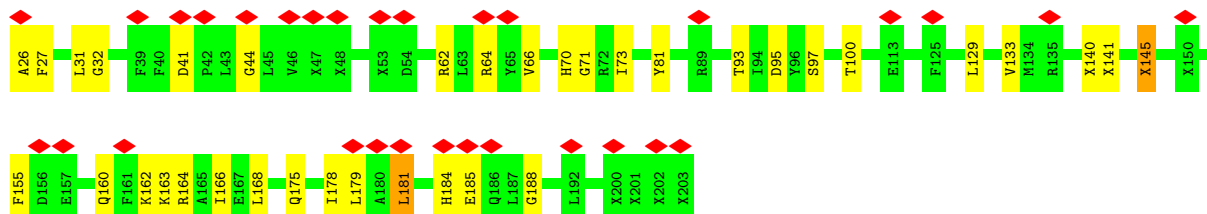
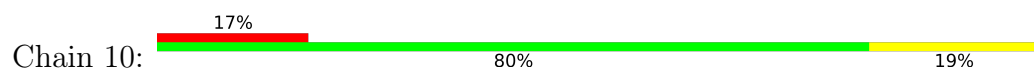
• Molecule 25: PsbZ



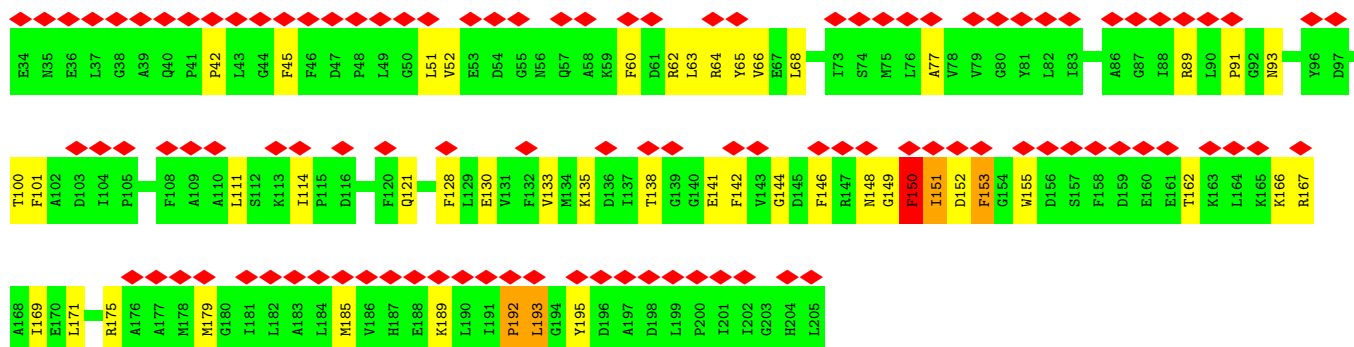
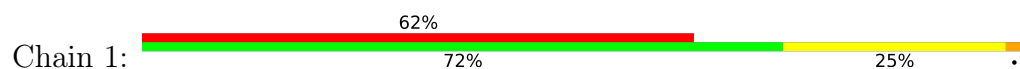
• Molecule 26: FCP-E



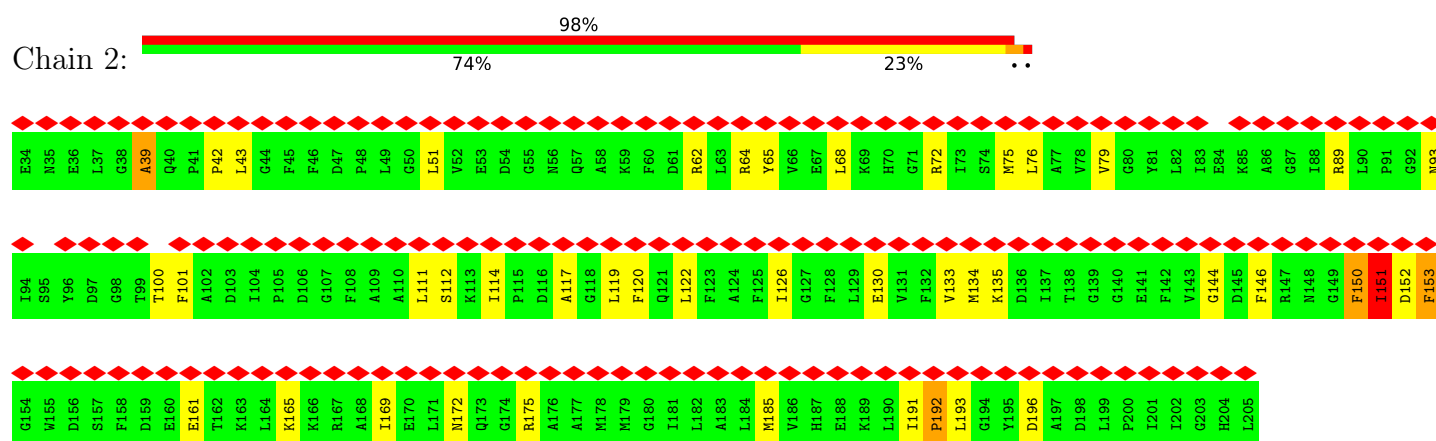
• Molecule 26: FCP-E



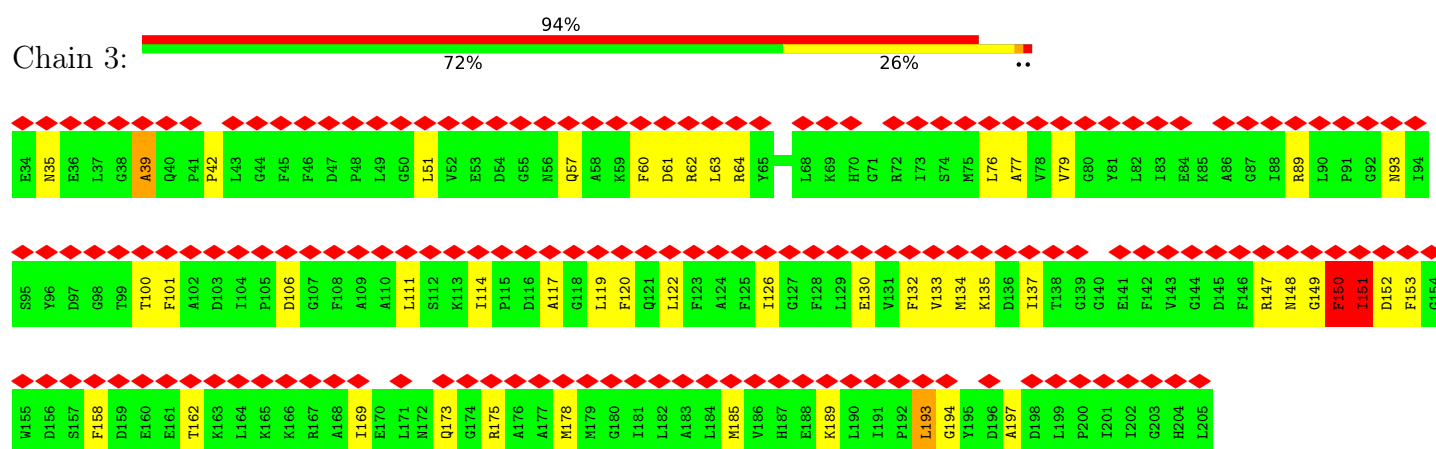
• Molecule 27: FCP-A



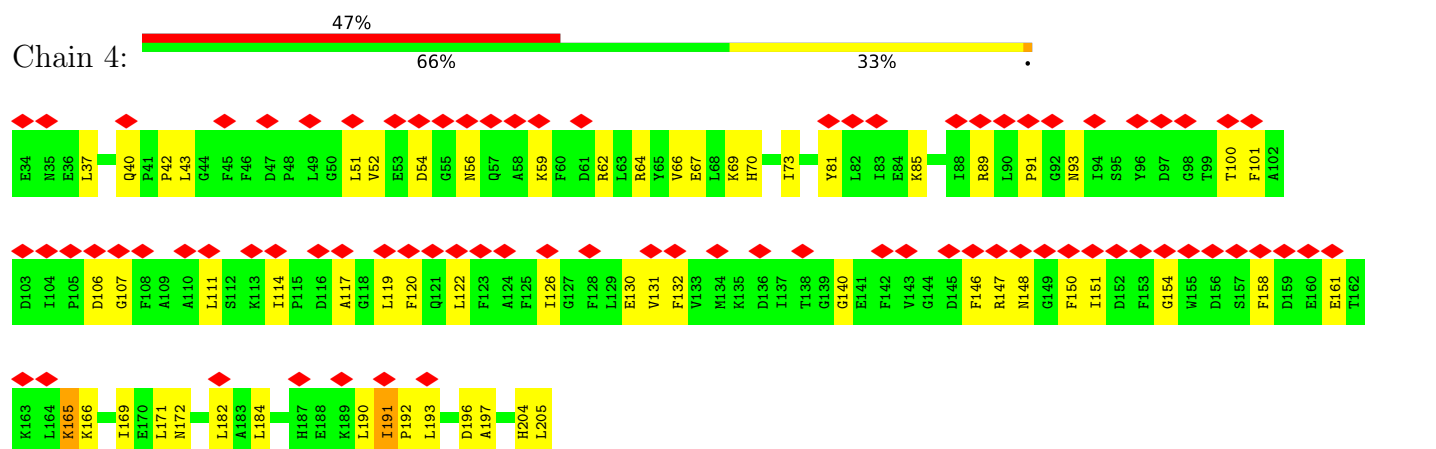
• Molecule 27: FCP-A



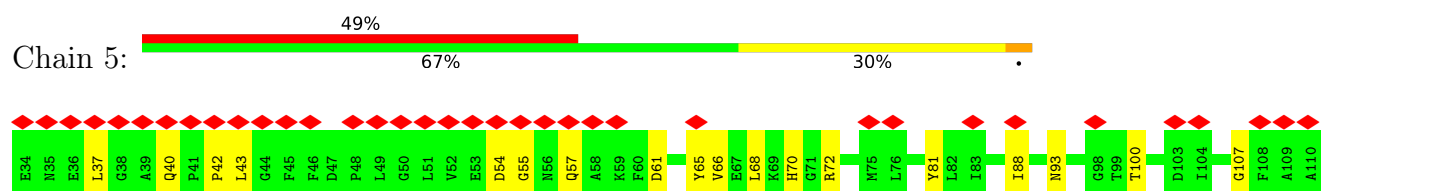
• Molecule 27: FCP-A

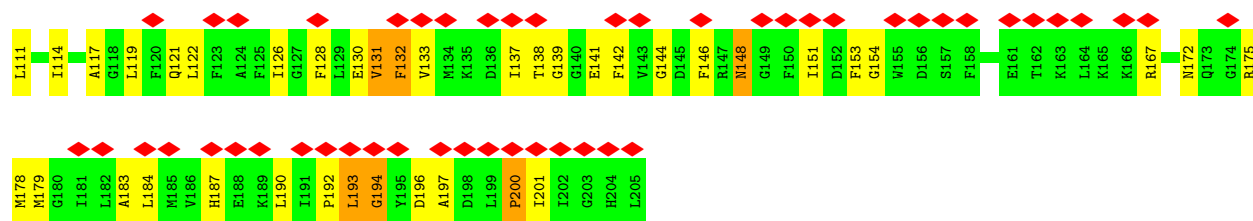


• Molecule 27: FCP-A

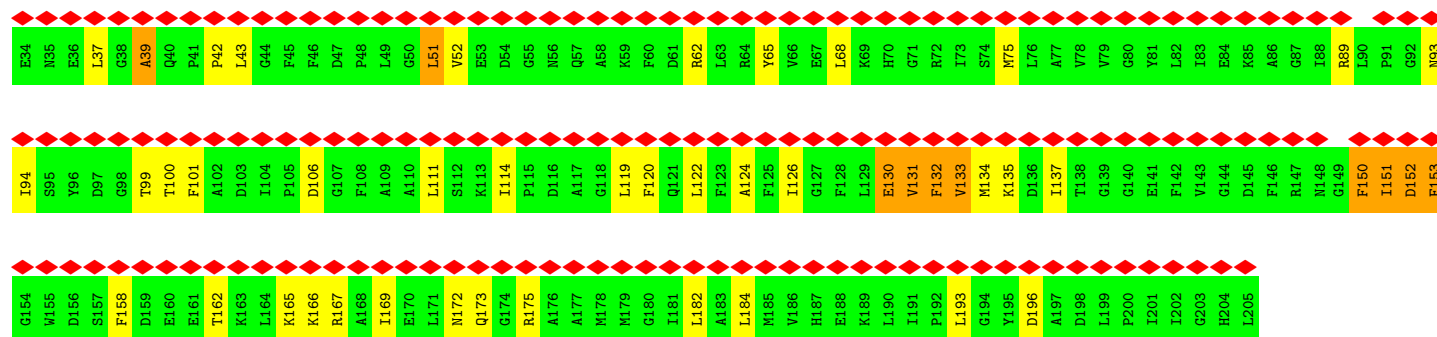


• Molecule 27: FCP-A

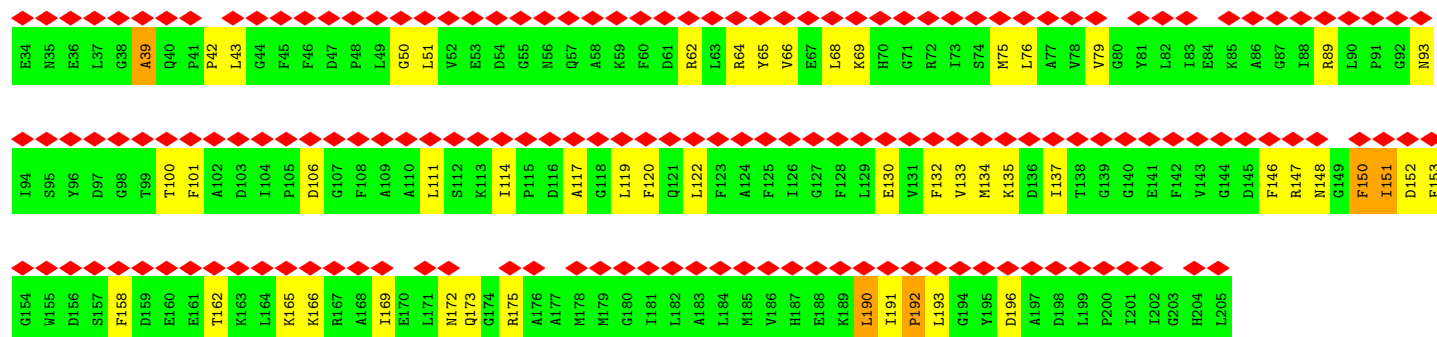




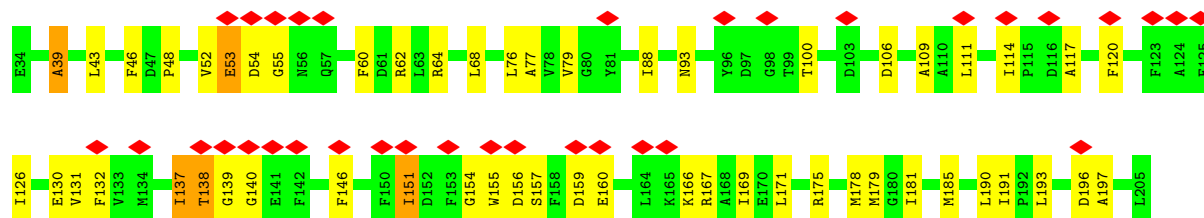
• Molecule 27: FCP-A



• Molecule 27: FCP-A

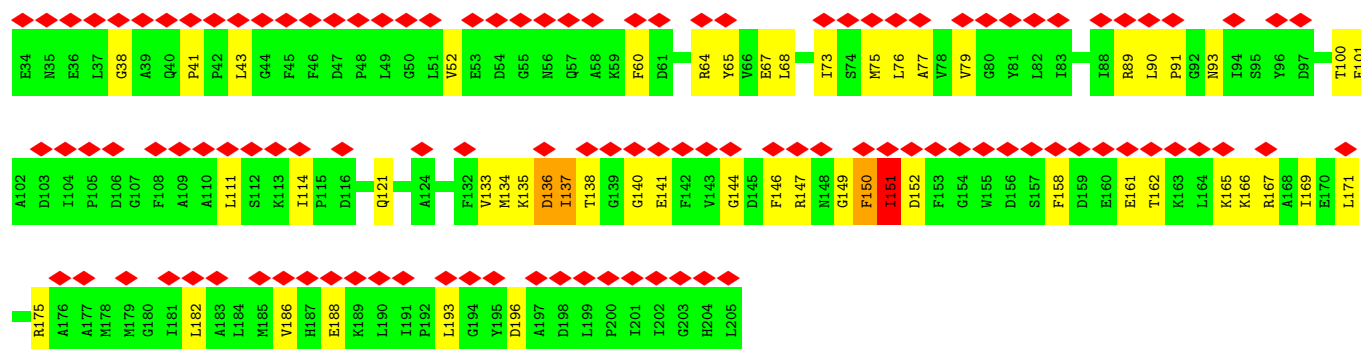


• Molecule 27: FCP-A

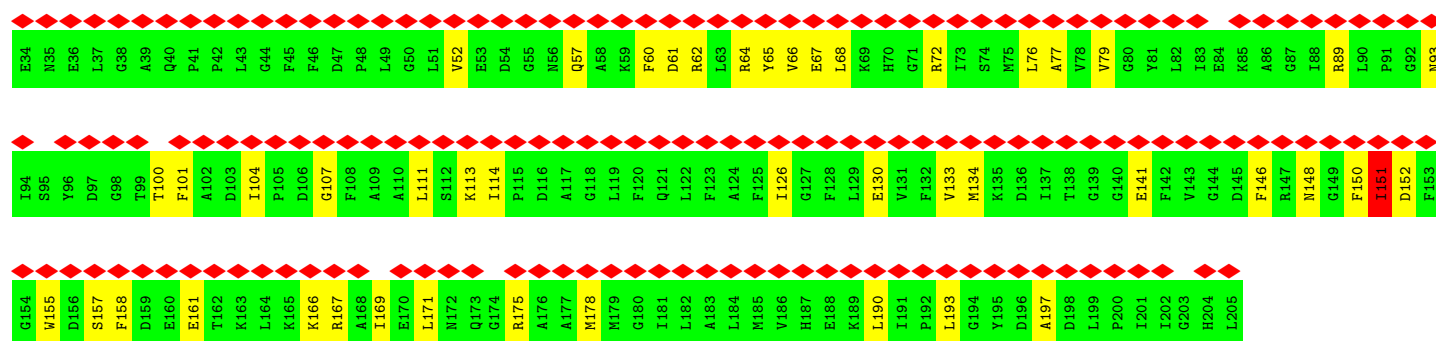


• Molecule 27: FCP-A

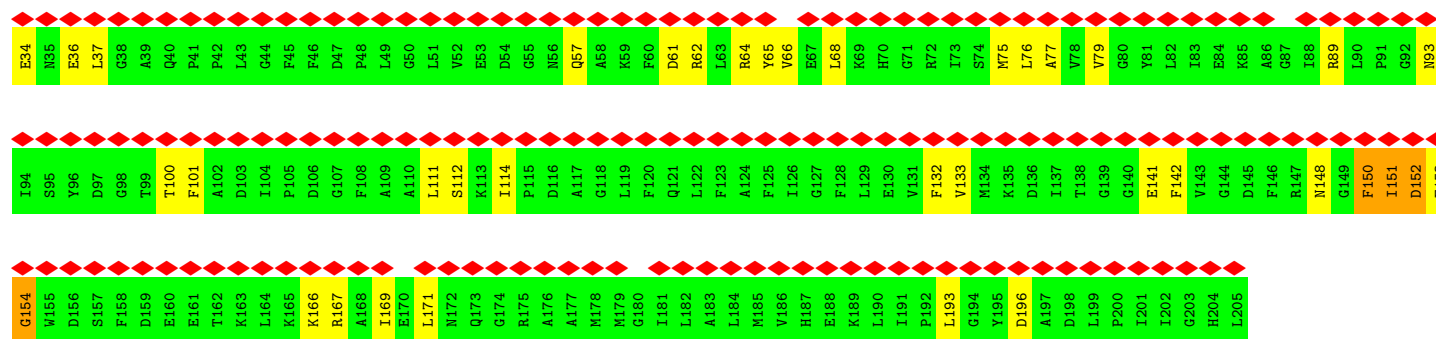
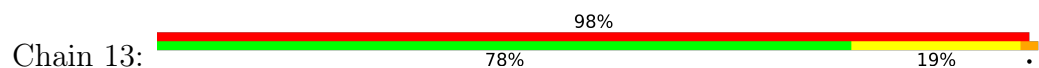




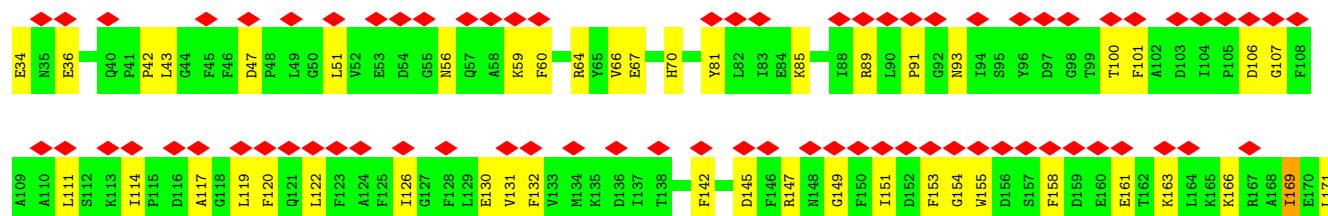
• Molecule 27: FCP-A

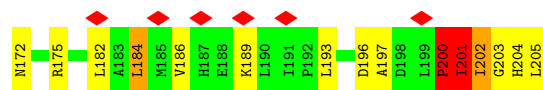


• Molecule 27: FCP-A

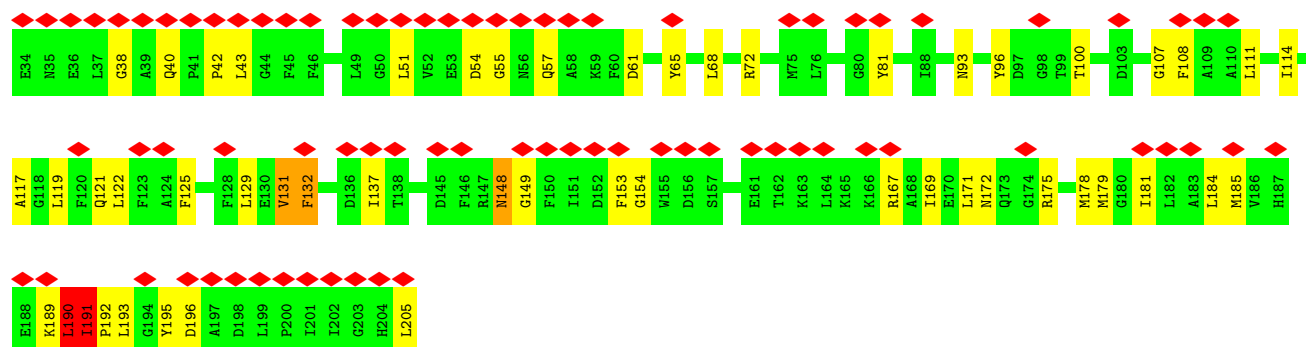


• Molecule 27: FCP-A

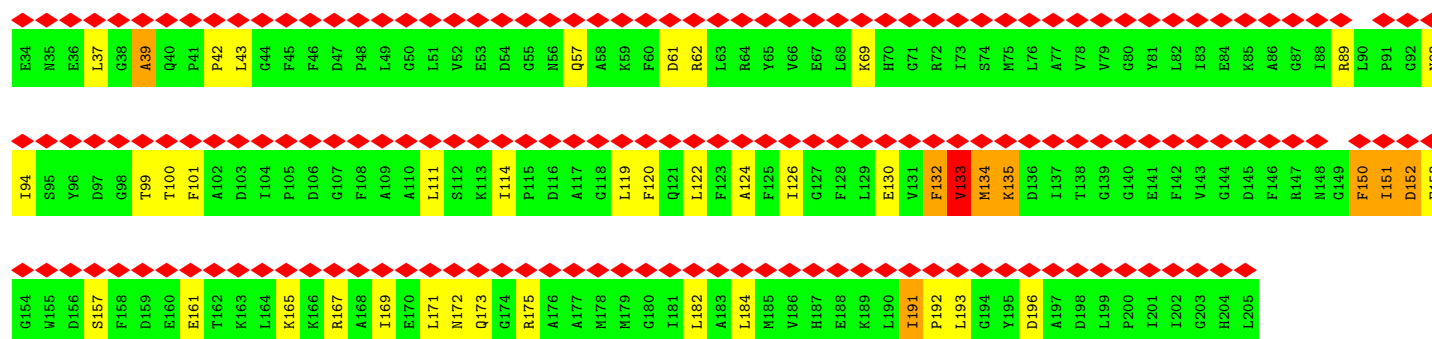
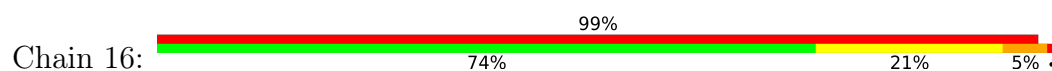




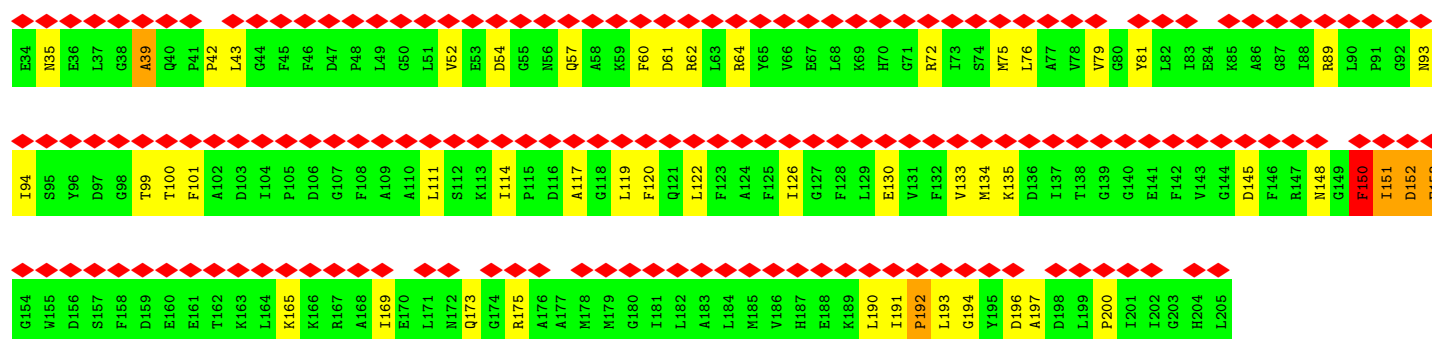
• Molecule 27: FCP-A



• Molecule 27: FCP-A

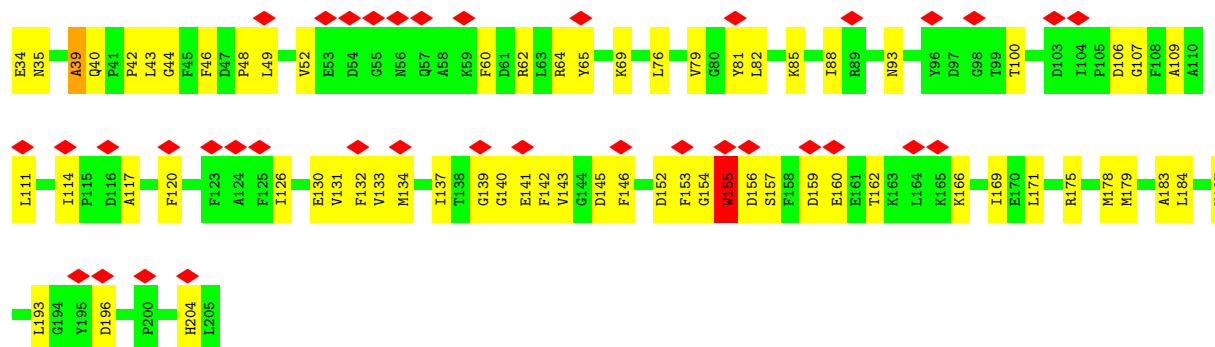


• Molecule 27: FCP-A

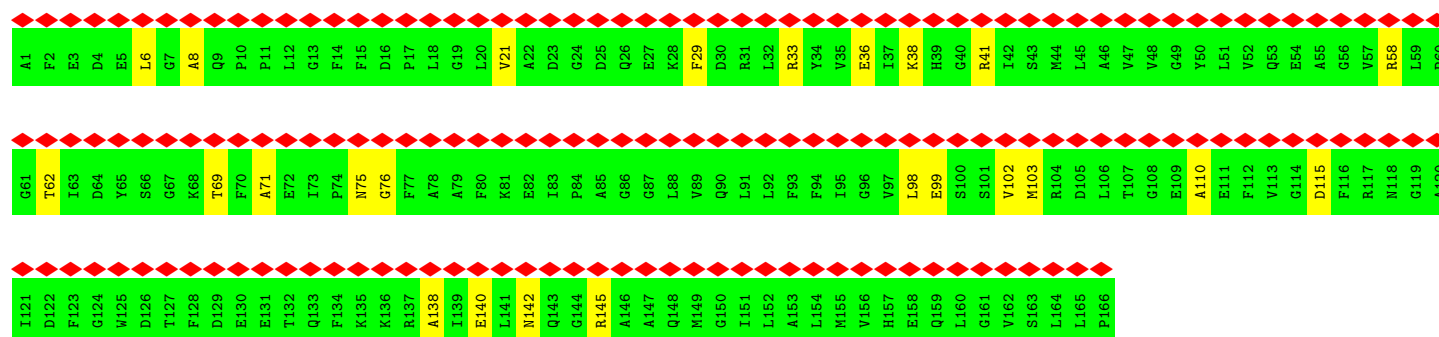
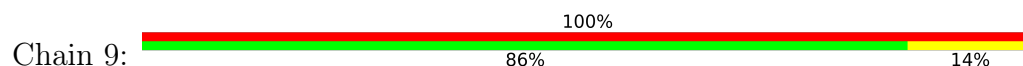


• Molecule 27: FCP-A

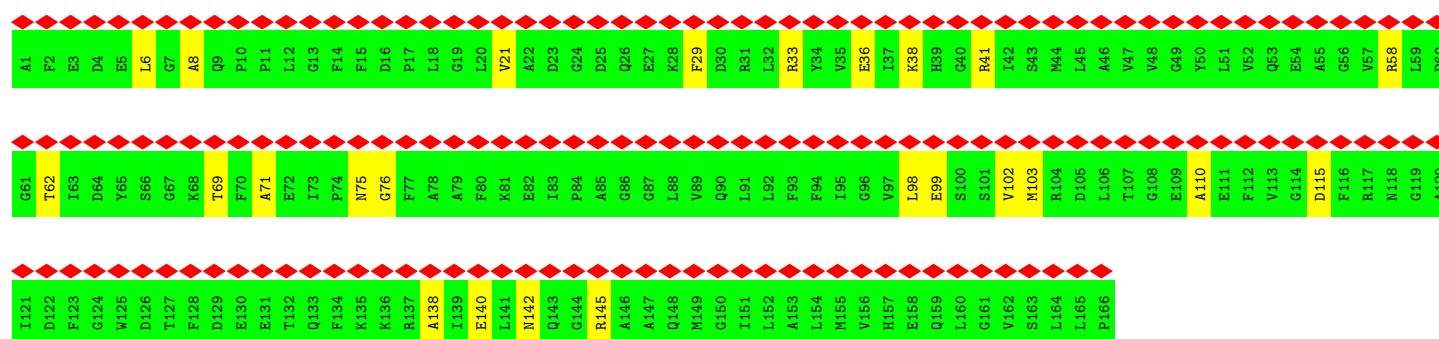
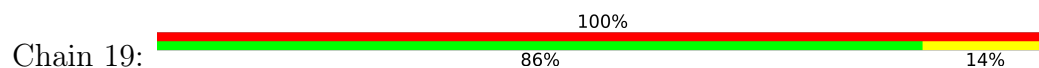




• Molecule 28: FCP-F



• Molecule 28: FCP-F



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	42033	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	444.2236, 444.2236, 444.2236	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, BCT, HEM, DD6, DGD, KC2, BCR, CL, LMG, SQD, PL9, LHG, OEX, KC1, PHO, FE2, A86

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	0.62	0/2700	0.70	0/3681
1	a	0.62	0/2700	0.70	0/3681
2	B	0.61	0/4092	0.71	0/5562
2	b	0.61	0/4092	0.71	0/5562
3	C	0.60	0/3613	0.74	5/4926 (0.1%)
3	c	0.60	0/3613	0.74	7/4926 (0.1%)
4	D	0.63	0/2788	0.72	2/3803 (0.1%)
4	d	0.63	0/2788	0.72	2/3803 (0.1%)
5	E	0.42	0/660	0.61	0/899
5	e	0.42	0/660	0.61	0/899
6	F	0.48	0/268	0.85	0/363
6	f	0.47	0/268	0.85	0/363
7	G	0.36	0/936	0.65	0/1261
7	g	0.36	0/936	0.65	0/1261
8	H	0.47	0/516	0.78	0/704
8	h	0.47	0/516	0.78	0/704
9	I	0.61	0/285	0.76	0/386
9	i	0.61	0/285	0.76	0/386
10	J	0.46	0/253	0.77	0/344
10	j	0.46	0/253	0.77	0/344
11	K	0.56	0/311	0.89	2/427 (0.5%)
11	k	0.56	0/311	0.89	2/427 (0.5%)
12	L	0.59	0/310	0.66	0/423
12	l	0.59	0/310	0.66	0/423
13	M	0.54	0/313	0.65	0/422
13	m	0.54	0/313	0.65	0/422
15	O	0.46	0/1911	0.75	0/2576
15	o	0.46	0/1911	0.75	0/2576
16	P	0.46	0/1795	0.75	0/2441
16	p	0.46	0/1795	0.75	0/2441
17	Q	0.40	0/1164	0.71	0/1569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	q	0.40	0/1164	0.71	0/1569
19	T	0.46	0/256	0.69	0/346
19	t	0.46	0/256	0.69	0/346
20	U	0.41	0/726	0.74	1/986 (0.1%)
20	u	0.41	0/726	0.74	1/986 (0.1%)
21	V	0.45	0/1062	0.66	0/1444
21	v	0.45	0/1062	0.66	0/1444
22	W	0.60	0/368	1.05	1/491 (0.2%)
22	w	0.60	0/368	1.05	1/491 (0.2%)
23	X	0.25	0/244	0.62	0/330
23	x	0.25	0/244	0.62	0/330
24	Y	0.56	0/259	0.99	0/353
24	y	0.56	0/259	0.99	0/353
25	Z	0.41	0/460	0.61	0/633
25	z	0.41	0/460	0.61	0/633
26	0	0.62	0/1151	0.97	6/1550 (0.4%)
26	10	0.56	0/1151	0.81	1/1550 (0.1%)
27	1	0.56	0/1371	1.03	8/1849 (0.4%)
27	11	0.59	0/1365	1.02	4/1841 (0.2%)
27	12	0.53	0/1358	0.92	3/1834 (0.2%)
27	13	0.49	0/1362	0.91	3/1838 (0.2%)
27	14	0.60	0/1342	1.06	7/1813 (0.4%)
27	15	0.65	0/1306	1.20	11/1769 (0.6%)
27	16	0.49	0/1371	1.10	10/1849 (0.5%)
27	17	0.48	0/1371	1.00	4/1849 (0.2%)
27	18	0.66	0/1330	1.11	7/1797 (0.4%)
27	2	0.55	0/1371	1.02	6/1849 (0.3%)
27	3	0.49	0/1371	1.03	5/1849 (0.3%)
27	4	0.61	0/1342	1.05	4/1813 (0.2%)
27	5	0.63	1/1306 (0.1%)	1.04	4/1769 (0.2%)
27	6	0.52	0/1365	1.06	6/1841 (0.3%)
27	7	0.53	0/1365	1.07	2/1841 (0.1%)
27	8	0.65	0/1316	1.15	2/1781 (0.1%)
28	19	0.32	0/1313	0.54	0/1771
28	9	0.32	0/1313	0.54	0/1771
All	All	0.55	1/77120 (0.0%)	0.83	117/104564 (0.1%)

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
2	b	0	1
3	C	0	2
3	c	0	2
13	M	0	1
13	m	0	1
14	N	0	1
14	n	0	1
16	P	0	1
16	p	0	1
22	W	0	2
22	w	0	2
24	Y	0	1
24	y	0	1
26	0	0	2
26	10	0	2
27	1	0	4
27	11	0	2
27	12	0	2
27	13	0	4
27	14	0	6
27	15	0	9
27	16	0	5
27	17	0	4
27	18	0	3
27	2	0	4
27	3	0	5
27	4	0	2
27	5	0	7
27	6	0	8
27	7	0	5
27	8	0	5
All	All	0	97

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	132	PHE	CD1-CE1	-6.18	1.20	1.38

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	191	ILE	CG1-CB-CG2	-8.83	84.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	12	152	ASP	N-CA-C	8.53	123.73	113.16
27	14	200	PRO	CA-C-N	8.01	136.40	121.97
27	14	200	PRO	C-N-CA	8.01	136.40	121.97
4	D	138	ILE	CA-C-N	7.53	130.86	120.39

There are no chirality outliers.

5 of 97 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	442	VAL	Peptide
3	C	222	GLY	Peptide
3	C	376	ASP	Peptide
13	M	4	GLN	Peptide
14	N	23	UNK	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	2617	0	2517	79	0
1	a	2617	0	2517	75	0
2	B	3960	0	3838	95	0
2	b	3960	0	3838	92	0
3	C	3496	0	3402	80	0
3	c	3496	0	3402	86	0
4	D	2696	0	2593	76	0
4	d	2696	0	2595	81	0
5	E	642	0	623	17	0
5	e	642	0	623	16	0
6	F	259	0	267	2	0
6	f	259	0	267	7	0
7	G	922	0	924	22	0
7	g	922	0	924	22	0
8	H	506	0	532	12	0
8	h	506	0	532	11	0
9	I	278	0	293	9	0
9	i	278	0	293	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	247	0	256	10	0
10	j	247	0	256	7	0
11	K	300	0	311	13	0
11	k	300	0	311	13	0
12	L	301	0	301	13	0
12	l	301	0	301	16	0
13	M	308	0	315	7	0
13	m	308	0	315	9	0
14	N	150	0	32	1	0
14	n	150	0	32	1	0
15	O	1881	0	1881	45	0
15	o	1881	0	1881	45	0
16	P	1745	0	1691	21	0
16	p	1745	0	1691	21	0
17	Q	1143	0	1130	24	0
17	q	1143	0	1130	17	0
18	R	365	0	80	1	0
18	r	365	0	80	1	0
19	T	250	0	268	4	0
19	t	250	0	268	6	0
20	U	711	0	713	16	0
20	u	711	0	713	15	0
21	V	1043	0	1044	24	0
21	v	1043	0	1044	23	0
22	W	394	0	346	8	0
22	w	394	0	346	6	0
23	X	244	0	274	2	0
23	x	244	0	274	2	0
24	Y	256	0	280	11	0
24	y	256	0	280	10	0
25	Z	452	0	479	7	0
25	z	452	0	479	8	0
26	0	1291	0	1165	31	0
26	10	1291	0	1166	35	0
27	1	1340	0	1332	49	0
27	11	1335	0	1325	49	0
27	12	1328	0	1309	42	0
27	13	1332	0	1318	24	0
27	14	1313	0	1294	43	0
27	15	1280	0	1222	33	0
27	16	1340	0	1330	29	0
27	17	1340	0	1330	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	18	1304	0	1281	46	0
27	2	1340	0	1330	43	0
27	3	1340	0	1330	36	0
27	4	1313	0	1294	47	0
27	5	1280	0	1223	44	0
27	6	1335	0	1325	32	0
27	7	1335	0	1325	37	0
27	8	1291	0	1259	44	0
28	19	1286	0	1267	17	0
28	9	1286	0	1267	17	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	1	0	0	0	0
30	a	1	0	0	0	0
31	0	394	0	313	7	0
31	1	413	0	369	24	0
31	10	442	0	349	8	0
31	11	351	0	304	15	0
31	12	330	0	267	8	0
31	13	345	0	303	10	0
31	14	374	0	345	10	0
31	15	295	0	249	15	0
31	16	280	0	231	8	0
31	17	265	0	194	7	0
31	18	307	0	255	12	0
31	19	408	0	407	9	0
31	2	330	0	265	17	0
31	3	345	0	303	13	0
31	4	313	0	284	8	0
31	5	295	0	249	12	0
31	6	280	0	231	12	0
31	7	265	0	194	12	0
31	8	307	0	256	11	0
31	9	408	0	408	7	0
31	A	174	0	170	9	0
31	B	1040	0	1152	42	0
31	C	829	0	900	32	0
31	D	195	0	216	14	0
31	P	447	0	382	10	0
31	R	47	0	35	1	0
31	W	65	0	72	3	0
31	Z	51	0	41	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	a	174	0	170	9	0
31	b	1040	0	1152	44	0
31	c	829	0	900	37	0
31	d	195	0	216	14	0
31	p	447	0	382	10	0
31	r	47	0	35	0	0
31	w	65	0	72	3	0
31	z	99	0	77	3	0
32	A	64	0	74	4	0
32	D	64	0	74	2	0
32	a	64	0	74	4	0
32	d	64	0	74	3	0
33	A	40	0	56	3	0
33	B	120	0	168	10	0
33	C	120	0	168	3	0
33	F	40	0	56	2	0
33	H	40	0	56	3	0
33	Y	40	0	56	6	0
33	a	40	0	56	2	0
33	b	120	0	168	7	0
33	c	120	0	168	5	0
33	f	40	0	56	3	0
33	h	40	0	56	4	0
33	y	40	0	56	5	0
34	10	41	0	45	1	0
34	8	41	0	45	2	0
34	A	94	0	118	5	0
34	B	54	0	77	7	0
34	L	54	0	77	4	0
34	a	54	0	74	3	0
34	b	54	0	76	9	0
34	i	40	0	44	2	0
34	l	54	0	77	6	0
35	A	33	0	42	1	0
35	D	55	0	80	4	0
35	a	33	0	42	2	0
35	d	55	0	80	5	0
36	14	35	0	43	2	0
36	15	25	0	20	0	0
36	18	70	0	80	4	0
36	4	35	0	43	3	0
36	5	25	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	8	70	0	80	2	0
36	A	37	0	44	1	0
36	B	43	0	59	1	0
36	C	40	0	50	1	0
36	D	49	0	74	5	0
36	L	49	0	74	5	0
36	P	27	0	24	1	0
36	Z	25	0	20	0	0
36	a	37	0	44	1	0
36	b	43	0	59	0	0
36	d	49	0	74	5	0
36	l	49	0	74	5	0
36	p	27	0	24	1	0
36	w	40	0	50	1	0
36	z	25	0	20	0	0
37	0	31	0	32	2	0
37	1	81	0	102	4	0
37	10	31	0	32	2	0
37	11	81	0	102	5	0
37	14	49	0	68	5	0
37	15	73	0	86	4	0
37	4	49	0	68	5	0
37	5	73	0	86	5	0
37	B	51	0	72	3	0
37	C	51	0	72	3	0
37	D	77	0	93	1	0
37	F	46	0	61	4	0
37	J	50	0	73	6	0
37	K	46	0	62	6	0
37	M	40	0	50	6	0
37	N	28	0	25	1	0
37	P	31	0	32	1	0
37	W	48	0	66	3	0
37	Z	31	0	32	0	0
37	b	51	0	72	2	0
37	c	82	0	104	2	0
37	d	77	0	93	3	0
37	f	46	0	61	5	0
37	j	50	0	73	4	0
37	k	46	0	62	4	0
37	m	40	0	50	3	0
37	n	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	p	31	0	32	2	0
37	w	48	0	66	4	0
38	1	54	0	66	2	0
38	11	60	0	81	2	0
38	B	54	0	66	6	0
38	C	179	0	228	8	0
38	H	62	0	82	4	0
38	W	56	0	70	0	0
38	b	55	0	68	12	0
38	c	179	0	229	6	0
38	h	62	0	82	4	0
38	w	56	0	70	0	0
39	C	1	0	0	0	0
39	c	1	0	0	0	0
40	D	4	0	1	1	0
40	d	4	0	1	1	0
41	E	43	0	30	2	0
41	V	43	0	30	4	0
41	e	43	0	30	2	0
41	v	43	0	30	3	0
42	0	45	0	0	0	0
42	1	45	0	0	0	0
42	10	45	0	0	0	0
42	11	45	0	0	0	0
42	12	45	0	0	0	0
42	13	45	0	0	0	0
42	14	45	0	0	0	0
42	15	45	0	0	0	0
42	16	45	0	0	0	0
42	17	45	0	0	0	0
42	18	45	0	0	0	0
42	19	45	0	0	0	0
42	2	45	0	0	0	0
42	3	45	0	0	0	0
42	4	45	0	0	1	0
42	5	45	0	0	0	0
42	6	45	0	0	0	0
42	7	45	0	0	0	0
42	8	45	0	0	1	0
42	9	45	0	0	0	0
42	P	45	0	0	0	0
42	p	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	0	288	0	0	1	0
43	1	336	0	0	2	0
43	10	336	0	0	1	0
43	11	336	0	0	1	0
43	12	288	0	0	0	0
43	13	288	0	0	2	0
43	14	240	0	0	6	0
43	15	240	0	0	4	0
43	16	288	0	0	1	0
43	17	336	0	0	2	0
43	18	240	0	0	10	0
43	19	288	0	0	2	0
43	2	240	0	0	0	0
43	3	288	0	0	0	0
43	4	288	0	0	3	0
43	5	288	0	0	5	0
43	6	336	0	0	1	0
43	7	288	0	0	1	0
43	8	240	0	0	0	0
43	9	288	0	0	2	0
43	P	96	0	0	1	0
43	p	96	0	0	1	0
44	P	43	0	0	1	0
44	p	43	0	0	3	0
45	0	45	0	0	0	0
45	1	90	0	0	0	0
45	10	45	0	0	1	0
45	11	90	0	0	0	0
45	12	90	0	0	0	0
45	13	90	0	0	0	0
45	14	90	0	0	0	0
45	15	90	0	0	1	0
45	16	90	0	0	1	0
45	17	90	0	0	1	0
45	18	90	0	0	1	0
45	19	45	0	0	1	0
45	2	90	0	0	1	0
45	3	90	0	0	1	0
45	4	90	0	0	1	0
45	5	90	0	0	1	0
45	6	90	0	0	1	0
45	7	90	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	8	90	0	0	1	0
45	9	45	0	0	1	0
46	Z	1	0	0	0	0
All	All	102777	0	92507	1968	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 10.

The worst 5 of 1968 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)
27:1:153:PHE:CZ	27:2:151:ILE:CG2	1.77	1.65
26:10:155:PHE:CZ	26:10:163:LYS:HE3	1.51	1.43
27:11:150:PHE:CD2	27:12:151:ILE:CD1	2.01	1.42
27:11:150:PHE:CE2	27:12:151:ILE:HD11	1.53	1.41
27:1:153:PHE:HZ	27:2:151:ILE:CG2	1.16	1.35

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	332/359 (92%)	321 (97%)	11 (3%)	0	100	100
1	a	332/359 (92%)	321 (97%)	11 (3%)	0	100	100
2	B	501/509 (98%)	479 (96%)	22 (4%)	0	100	100
2	b	501/509 (98%)	479 (96%)	22 (4%)	0	100	100
3	C	448/450 (100%)	420 (94%)	28 (6%)	0	100	100
3	c	448/450 (100%)	420 (94%)	28 (6%)	0	100	100
4	D	339/341 (99%)	322 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	339/341 (99%)	321 (95%)	18 (5%)	0	100	100
5	E	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
5	e	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
6	F	30/32 (94%)	27 (90%)	3 (10%)	0	100	100
6	f	30/32 (94%)	27 (90%)	3 (10%)	0	100	100
7	G	120/179 (67%)	114 (95%)	6 (5%)	0	100	100
7	g	120/179 (67%)	114 (95%)	6 (5%)	0	100	100
8	H	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
8	h	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
9	I	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
9	i	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
10	J	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
10	j	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	35/38 (92%)	31 (89%)	4 (11%)	0	100	100
12	l	35/38 (92%)	31 (89%)	4 (11%)	0	100	100
13	M	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
13	m	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
15	O	247/249 (99%)	217 (88%)	29 (12%)	1 (0%)	30	63
15	o	247/249 (99%)	217 (88%)	29 (12%)	1 (0%)	30	63
16	P	224/226 (99%)	195 (87%)	28 (12%)	1 (0%)	30	63
16	p	224/226 (99%)	196 (88%)	27 (12%)	1 (0%)	30	63
17	Q	145/211 (69%)	127 (88%)	18 (12%)	0	100	100
17	q	145/211 (69%)	127 (88%)	18 (12%)	0	100	100
19	T	28/31 (90%)	28 (100%)	0	0	100	100
19	t	28/31 (90%)	28 (100%)	0	0	100	100
20	U	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
20	u	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
21	V	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
21	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	W	43/51 (84%)	36 (84%)	7 (16%)	0	100	100
22	w	43/51 (84%)	36 (84%)	7 (16%)	0	100	100
23	X	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
23	x	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
24	Y	31/33 (94%)	27 (87%)	3 (10%)	1 (3%)	3	17
24	y	31/33 (94%)	27 (87%)	3 (10%)	1 (3%)	3	17
25	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
25	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
26	0	145/178 (82%)	128 (88%)	15 (10%)	2 (1%)	9	34
26	10	145/178 (82%)	130 (90%)	15 (10%)	0	100	100
27	1	170/172 (99%)	141 (83%)	27 (16%)	2 (1%)	10	38
27	11	170/172 (99%)	146 (86%)	22 (13%)	2 (1%)	10	38
27	12	170/172 (99%)	146 (86%)	23 (14%)	1 (1%)	21	54
27	13	170/172 (99%)	150 (88%)	18 (11%)	2 (1%)	10	38
27	14	170/172 (99%)	148 (87%)	19 (11%)	3 (2%)	6	29
27	15	170/172 (99%)	140 (82%)	29 (17%)	1 (1%)	21	54
27	16	170/172 (99%)	146 (86%)	21 (12%)	3 (2%)	6	29
27	17	170/172 (99%)	146 (86%)	18 (11%)	6 (4%)	3	15
27	18	170/172 (99%)	142 (84%)	25 (15%)	3 (2%)	6	29
27	2	170/172 (99%)	147 (86%)	19 (11%)	4 (2%)	4	23
27	3	170/172 (99%)	145 (85%)	23 (14%)	2 (1%)	10	38
27	4	170/172 (99%)	149 (88%)	21 (12%)	0	100	100
27	5	170/172 (99%)	140 (82%)	29 (17%)	1 (1%)	21	54
27	6	170/172 (99%)	143 (84%)	24 (14%)	3 (2%)	6	29
27	7	170/172 (99%)	142 (84%)	24 (14%)	4 (2%)	4	23
27	8	170/172 (99%)	136 (80%)	32 (19%)	2 (1%)	10	38
28	19	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
28	9	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
All	All	9576/10090 (95%)	8700 (91%)	829 (9%)	47 (0%)	26	59

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	1	151	ILE
27	1	193	LEU
27	2	151	ILE
27	3	151	ILE
27	6	151	ILE

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	272/291 (94%)	272 (100%)	0	100	100
1	a	272/291 (94%)	272 (100%)	0	100	100
2	B	401/405 (99%)	401 (100%)	0	100	100
2	b	401/405 (99%)	401 (100%)	0	100	100
3	C	355/355 (100%)	355 (100%)	0	100	100
3	c	355/355 (100%)	355 (100%)	0	100	100
4	D	273/273 (100%)	273 (100%)	0	100	100
4	d	273/273 (100%)	273 (100%)	0	100	100
5	E	72/72 (100%)	72 (100%)	0	100	100
5	e	72/72 (100%)	72 (100%)	0	100	100
6	F	26/26 (100%)	26 (100%)	0	100	100
6	f	26/26 (100%)	26 (100%)	0	100	100
7	G	88/128 (69%)	88 (100%)	0	100	100
7	g	88/128 (69%)	88 (100%)	0	100	100
8	H	54/54 (100%)	54 (100%)	0	100	100
8	h	54/54 (100%)	54 (100%)	0	100	100
9	I	33/33 (100%)	33 (100%)	0	100	100
9	i	33/33 (100%)	33 (100%)	0	100	100
10	J	26/26 (100%)	25 (96%)	1 (4%)	29	62
10	j	26/26 (100%)	25 (96%)	1 (4%)	29	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	32/32 (100%)	31 (97%)	1 (3%)	35	67
11	k	32/32 (100%)	31 (97%)	1 (3%)	35	67
12	L	33/34 (97%)	33 (100%)	0	100	100
12	l	33/34 (97%)	33 (100%)	0	100	100
13	M	30/30 (100%)	30 (100%)	0	100	100
13	m	30/30 (100%)	30 (100%)	0	100	100
15	O	201/201 (100%)	200 (100%)	1 (0%)	81	88
15	o	201/201 (100%)	200 (100%)	1 (0%)	81	88
16	P	174/174 (100%)	174 (100%)	0	100	100
16	p	174/174 (100%)	174 (100%)	0	100	100
17	Q	118/158 (75%)	118 (100%)	0	100	100
17	q	118/158 (75%)	118 (100%)	0	100	100
19	T	27/28 (96%)	27 (100%)	0	100	100
19	t	27/28 (96%)	27 (100%)	0	100	100
20	U	77/78 (99%)	77 (100%)	0	100	100
20	u	77/78 (99%)	77 (100%)	0	100	100
21	V	114/115 (99%)	114 (100%)	0	100	100
21	v	114/115 (99%)	114 (100%)	0	100	100
22	W	35/35 (100%)	35 (100%)	0	100	100
22	w	35/35 (100%)	35 (100%)	0	100	100
23	X	27/27 (100%)	27 (100%)	0	100	100
23	x	27/27 (100%)	27 (100%)	0	100	100
24	Y	26/26 (100%)	26 (100%)	0	100	100
24	y	26/26 (100%)	26 (100%)	0	100	100
25	Z	49/49 (100%)	49 (100%)	0	100	100
25	z	49/49 (100%)	49 (100%)	0	100	100
26	0	118/118 (100%)	118 (100%)	0	100	100
26	10	118/118 (100%)	118 (100%)	0	100	100
27	1	137/137 (100%)	137 (100%)	0	100	100
27	11	136/137 (99%)	136 (100%)	0	100	100
27	12	134/137 (98%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	13	135/137 (98%)	135 (100%)	0	100	100
27	14	132/137 (96%)	131 (99%)	1 (1%)	73	85
27	15	124/137 (90%)	124 (100%)	0	100	100
27	16	137/137 (100%)	137 (100%)	0	100	100
27	17	137/137 (100%)	137 (100%)	0	100	100
27	18	131/137 (96%)	131 (100%)	0	100	100
27	2	137/137 (100%)	136 (99%)	1 (1%)	76	85
27	3	137/137 (100%)	137 (100%)	0	100	100
27	4	132/137 (96%)	132 (100%)	0	100	100
27	5	124/137 (90%)	124 (100%)	0	100	100
27	6	136/137 (99%)	136 (100%)	0	100	100
27	7	136/137 (99%)	136 (100%)	0	100	100
27	8	128/137 (93%)	128 (100%)	0	100	100
28	19	131/131 (100%)	131 (100%)	0	100	100
28	9	131/131 (100%)	131 (100%)	0	100	100
All	All	7717/7990 (97%)	7709 (100%)	8 (0%)	87	92

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	14	169	ILE
27	2	192	PRO
11	k	41	ILE
10	j	36	LEU
15	o	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
27	8	70	HIS
28	9	26	GLN
27	16	173	GLN
20	U	98	ASN
20	U	53	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 536 ligands modelled in this entry, 4 are monoatomic - leaving 532 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	$\# Z > 2$
31	CLA	0	314	-	51,55,73	1.37	10 (19%)	60,91,113	1.53	13 (21%)
42	KC1	1	314	-	49,53,53	2.75	19 (38%)	61,89,89	4.06	34 (55%)
31	CLA	C	503	31	69,73,73	1.40	11 (15%)	82,113,113	2.37	21 (25%)
31	CLA	7	307	-	45,49,73	1.43	6 (13%)	54,84,113	2.03	17 (31%)
31	CLA	10	309	-	63,67,73	1.18	8 (12%)	74,105,113	1.45	9 (12%)
31	CLA	19	307	-	65,69,73	1.20	6 (9%)	77,108,113	1.46	8 (10%)
31	CLA	P	603	-	54,58,73	1.31	10 (18%)	64,95,113	1.55	10 (15%)
43	A86	10	303	-	47,50,50	1.67	8 (17%)	51,76,76	3.37	25 (49%)
31	CLA	11	313	-	69,73,73	1.26	8 (11%)	82,113,113	1.52	11 (13%)
42	KC1	0	315	-	49,53,53	2.63	21 (42%)	61,89,89	5.13	36 (59%)
33	BCR	y	101	-	41,41,41	1.36	4 (9%)	56,56,56	1.60	13 (23%)
45	KC2	13	309	-	49,53,53	2.87	21 (42%)	60,89,89	3.66	31 (51%)
31	CLA	18	312	-	59,63,73	1.37	11 (18%)	70,101,113	1.71	15 (21%)
31	CLA	B	613	-	69,73,73	1.19	9 (13%)	82,113,113	1.25	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	3	315	-	47,52,73	1.40	7 (14%)	55,87,113	1.50	6 (10%)
43	A86	9	304	-	47,50,50	1.89	7 (14%)	51,76,76	4.68	20 (39%)
45	KC2	13	311	-	49,53,53	2.99	23 (46%)	60,89,89	4.01	32 (53%)
32	PHO	a	405	-	58,69,69	2.03	10 (17%)	55,99,99	1.73	10 (18%)
33	BCR	b	618	-	41,41,41	1.21	2 (4%)	56,56,56	1.40	11 (19%)
36	LHG	a	410	-	36,36,48	0.77	1 (2%)	39,42,54	1.27	4 (10%)
31	CLA	14	309	-	69,73,73	1.12	8 (11%)	82,113,113	1.43	7 (8%)
31	CLA	9	315	-	45,49,73	1.41	8 (17%)	54,84,113	1.56	8 (14%)
37	LMG	k	101	-	46,46,55	1.08	4 (8%)	54,54,63	1.45	8 (14%)
31	CLA	2	306	-	46,50,73	1.40	6 (13%)	53,85,113	2.09	13 (24%)
43	A86	7	302	-	47,50,50	1.94	8 (17%)	51,76,76	4.32	26 (50%)
31	CLA	b	612	-	69,73,73	1.35	9 (13%)	82,113,113	1.76	12 (14%)
45	KC2	12	309	-	49,53,53	2.84	18 (36%)	60,89,89	3.92	35 (58%)
31	CLA	4	307	-	69,73,73	1.14	10 (14%)	82,113,113	1.35	9 (10%)
45	KC2	14	310	-	49,53,53	2.86	21 (42%)	60,89,89	3.89	34 (56%)
31	CLA	10	307	-	52,56,73	1.41	8 (15%)	61,92,113	1.73	14 (22%)
31	CLA	3	316	-	69,73,73	1.20	8 (11%)	82,113,113	2.07	19 (23%)
31	CLA	3	312	-	49,53,73	1.43	8 (16%)	58,89,113	1.55	9 (15%)
31	CLA	C	509	-	69,73,73	1.28	10 (14%)	82,113,113	1.76	14 (17%)
29	OEX	a	401	3,1	0,15,15	-	-	-	-	-
31	CLA	7	315	-	45,49,73	1.40	7 (15%)	54,84,113	1.58	6 (11%)
43	A86	15	302	-	47,50,50	1.63	7 (14%)	51,76,76	4.19	28 (54%)
31	CLA	19	308	-	69,73,73	1.15	8 (11%)	82,113,113	1.41	10 (12%)
45	KC2	8	309	-	49,53,53	2.79	21 (42%)	60,89,89	3.85	33 (55%)
31	CLA	1	313	-	69,73,73	1.26	9 (13%)	82,113,113	1.43	13 (15%)
43	A86	5	318	42	47,50,50	1.41	6 (12%)	51,76,76	3.21	21 (41%)
42	KC1	P	609	-	49,53,53	2.63	19 (38%)	61,89,89	3.83	36 (59%)
35	PL9	D	407	-	55,55,55	2.04	15 (27%)	68,69,69	1.35	10 (14%)
34	SQD	a	408	38	52,54,54	0.96	6 (11%)	62,65,65	1.52	11 (17%)
43	A86	5	301	31	47,50,50	1.50	6 (12%)	51,76,76	4.04	25 (49%)
31	CLA	a	403	-	69,73,73	1.23	8 (11%)	82,113,113	1.41	12 (14%)
36	LHG	C	521	-	39,39,48	0.68	1 (2%)	42,45,54	1.25	4 (9%)
45	KC2	16	311	-	49,53,53	2.89	22 (44%)	60,89,89	4.27	35 (58%)
31	CLA	5	306	-	46,50,73	1.41	7 (15%)	53,85,113	1.71	11 (20%)
36	LHG	18	316	-	30,30,48	0.84	1 (3%)	33,36,54	1.26	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	A86	6	307	-	47,50,50	1.83	8 (17%)	51,76,76	4.13	26 (50%)
43	A86	8	305	-	47,50,50	2.06	9 (19%)	51,76,76	4.81	27 (52%)
45	KC2	2	308	-	49,53,53	2.96	22 (44%)	60,89,89	3.91	29 (48%)
43	A86	12	306	-	47,50,50	1.64	7 (14%)	51,76,76	3.63	25 (49%)
43	A86	p	611	-	47,50,50	2.30	9 (19%)	51,76,76	6.10	27 (52%)
31	CLA	0	313	-	46,50,73	1.46	8 (17%)	53,85,113	2.09	11 (20%)
31	CLA	P	610	-	45,49,73	1.37	10 (22%)	54,84,113	1.67	9 (16%)
31	CLA	9	313	-	69,73,73	1.11	7 (10%)	82,113,113	1.93	15 (18%)
43	A86	19	303	-	47,50,50	1.48	6 (12%)	51,76,76	2.99	23 (45%)
31	CLA	12	315	-	45,49,73	1.40	7 (15%)	54,84,113	1.56	6 (11%)
31	CLA	b	611	-	69,73,73	1.18	10 (14%)	82,113,113	1.40	9 (10%)
36	LHG	p	615	-	26,26,48	0.88	1 (3%)	29,32,54	1.36	3 (10%)
31	CLA	9	310	-	69,73,73	1.16	6 (8%)	82,113,113	1.38	7 (8%)
38	DGD	C	519	-	63,63,67	1.12	8 (12%)	77,77,81	1.52	16 (20%)
43	A86	8	304	-	47,50,50	1.74	8 (17%)	51,76,76	3.11	25 (49%)
37	LMG	W	201	-	48,48,55	0.97	5 (10%)	56,56,63	1.41	9 (16%)
43	A86	13	305	-	47,50,50	1.50	6 (12%)	51,76,76	2.66	20 (39%)
31	CLA	2	312	-	52,56,73	1.65	10 (19%)	61,92,113	1.95	14 (22%)
31	CLA	1	321	-	65,69,73	1.24	9 (13%)	77,108,113	2.07	21 (27%)
31	CLA	10	314	-	51,55,73	1.40	10 (19%)	60,91,113	1.61	12 (20%)
42	KC1	13	314	-	49,53,53	2.78	19 (38%)	61,89,89	4.52	37 (60%)
43	A86	17	316	-	47,50,50	1.94	8 (17%)	51,76,76	6.32	32 (62%)
38	DGD	B	621	-	55,55,67	1.33	6 (10%)	69,69,81	1.73	15 (21%)
37	LMG	Z	102	-	31,31,55	1.15	3 (9%)	39,39,63	1.21	3 (7%)
31	CLA	13	316	-	69,73,73	1.14	7 (10%)	82,113,113	1.43	10 (12%)
45	KC2	5	308	-	49,53,53	2.88	23 (46%)	60,89,89	4.16	38 (63%)
31	CLA	D	402	-	69,73,73	1.15	9 (13%)	82,113,113	1.50	10 (12%)
31	CLA	0	307	-	52,56,73	1.37	10 (19%)	61,92,113	1.57	12 (19%)
36	LHG	L	101	-	48,48,48	0.81	3 (6%)	51,54,54	1.31	7 (13%)
43	A86	13	306	43	47,50,50	1.91	5 (10%)	51,76,76	5.05	23 (45%)
36	LHG	Z	103	-	24,24,48	0.95	0	27,30,54	1.34	3 (11%)
43	A86	4	302	-	47,50,50	1.72	6 (12%)	51,76,76	3.79	29 (56%)
31	CLA	C	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.55	8 (9%)
37	LMG	B	620	-	51,51,55	0.90	4 (7%)	59,59,63	1.51	11 (18%)
43	A86	18	304	-	47,50,50	1.98	9 (19%)	51,76,76	4.49	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	A86	0	301	-	47,50,50	1.97	7 (14%)	51,76,76	4.76	28 (54%)
41	HEM	v	201	21	50,50,50	1.42	6 (12%)	67,82,82	1.60	16 (23%)
31	CLA	14	312	-	55,59,73	1.49	10 (18%)	64,96,113	1.79	16 (25%)
43	A86	1	306	-	47,50,50	1.84	9 (19%)	51,76,76	4.36	25 (49%)
43	A86	9	302	-	47,50,50	1.51	6 (12%)	51,76,76	2.87	19 (37%)
31	CLA	C	508	-	69,73,73	1.15	9 (13%)	82,113,113	1.46	9 (10%)
31	CLA	15	312	-	51,55,73	1.53	11 (21%)	60,91,113	1.72	13 (21%)
31	CLA	8	313	-	59,63,73	1.44	11 (18%)	70,101,113	1.74	18 (25%)
31	CLA	0	308	-	54,58,73	1.33	9 (16%)	64,95,113	1.56	10 (15%)
43	A86	0	303	-	47,50,50	1.72	8 (17%)	51,76,76	3.41	26 (50%)
31	CLA	1	312	-	50,54,73	1.42	11 (22%)	59,90,113	1.57	9 (15%)
31	CLA	3	310	-	45,49,73	1.38	6 (13%)	54,84,113	1.66	8 (14%)
43	A86	3	304	-	47,50,50	1.75	8 (17%)	51,76,76	2.71	21 (41%)
31	CLA	8	310	-	56,60,73	1.25	10 (17%)	65,97,113	1.62	8 (12%)
31	CLA	4	314	-	47,51,73	1.38	9 (19%)	55,86,113	1.57	6 (10%)
42	KC1	16	314	-	49,53,53	2.88	20 (40%)	61,89,89	5.31	37 (60%)
43	A86	11	302	-	47,50,50	2.03	9 (19%)	51,76,76	5.97	31 (60%)
45	KC2	19	309	-	49,53,53	2.87	22 (44%)	60,89,89	4.36	36 (60%)
31	CLA	c	504	31	69,73,73	1.18	10 (14%)	82,113,113	1.50	15 (18%)
43	A86	4	303	-	47,50,50	1.92	9 (19%)	51,76,76	3.38	17 (33%)
43	A86	16	306	31	47,50,50	1.76	5 (10%)	51,76,76	4.13	24 (47%)
43	A86	2	302	-	47,50,50	2.13	7 (14%)	51,76,76	5.17	25 (49%)
42	KC1	4	313	-	49,53,53	2.63	18 (36%)	61,89,89	4.63	36 (59%)
29	OEX	A	401	3,1	0,15,15	-	-	-	-	-
43	A86	0	305	-	47,50,50	1.56	6 (12%)	51,76,76	3.30	24 (47%)
43	A86	16	304	-	47,50,50	1.48	6 (12%)	51,76,76	3.62	26 (50%)
43	A86	1	304	31	47,50,50	1.60	6 (12%)	51,76,76	2.53	18 (35%)
42	KC1	11	314	-	49,53,53	2.72	21 (42%)	61,89,89	4.17	36 (59%)
31	CLA	p	610	-	45,49,73	1.37	10 (22%)	54,84,113	1.66	10 (18%)
31	CLA	B	607	-	69,73,73	1.18	8 (11%)	82,113,113	1.36	6 (7%)
31	CLA	1	315	-	45,49,73	1.44	8 (17%)	54,84,113	1.52	3 (5%)
31	CLA	p	608	-	55,59,73	1.31	8 (14%)	64,96,113	1.52	5 (7%)
34	SQD	A	408	38	52,54,54	0.97	6 (11%)	62,65,65	1.52	11 (17%)
40	BCT	D	401	30	3,3,3	1.23	0	2,3,3	3.98	1 (50%)
33	BCR	C	516	-	41,41,41	1.26	5 (12%)	56,56,56	1.37	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	12	312	-	49,53,73	1.37	8 (16%)	58,89,113	1.65	9 (15%)
31	CLA	c	508	-	69,73,73	1.15	9 (13%)	82,113,113	1.47	9 (10%)
31	CLA	B	606	-	69,73,73	1.21	8 (11%)	82,113,113	1.92	19 (23%)
31	CLA	C	502	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	11 (13%)
43	A86	11	306	-	47,50,50	2.23	10 (21%)	51,76,76	5.19	22 (43%)
32	PHO	D	403	-	58,69,69	2.03	10 (17%)	55,99,99	1.78	12 (21%)
31	CLA	16	308	-	69,73,73	1.14	10 (14%)	82,113,113	1.49	8 (9%)
42	KC1	10	315	-	49,53,53	2.67	19 (38%)	61,89,89	5.06	40 (65%)
31	CLA	13	308	-	47,51,73	1.39	10 (21%)	55,86,113	1.62	10 (18%)
43	A86	15	301	31	47,50,50	1.60	8 (17%)	51,76,76	4.40	26 (50%)
43	A86	3	303	-	47,50,50	1.92	6 (12%)	51,76,76	5.02	28 (54%)
45	KC2	8	311	-	49,53,53	2.79	20 (40%)	60,89,89	4.65	36 (60%)
43	A86	2	301	-	47,50,50	1.62	6 (12%)	51,76,76	3.74	25 (49%)
31	CLA	17	313	-	54,58,73	1.56	9 (16%)	64,95,113	1.83	16 (25%)
31	CLA	3	313	-	69,73,73	1.34	10 (14%)	82,113,113	1.52	11 (13%)
31	CLA	b	617	-	69,73,73	1.20	9 (13%)	82,113,113	1.51	12 (14%)
31	CLA	2	309	-	47,51,73	1.36	6 (12%)	55,86,113	1.59	6 (10%)
31	CLA	16	315	-	47,51,73	1.40	6 (12%)	55,86,113	1.54	7 (12%)
33	BCR	a	407	-	41,41,41	1.25	4 (9%)	56,56,56	1.24	6 (10%)
31	CLA	B	615	-	69,73,73	1.18	8 (11%)	82,113,113	1.52	8 (9%)
35	PL9	A	409	-	33,33,55	1.29	5 (15%)	41,42,69	1.48	8 (19%)
37	LMG	10	319	-	31,31,55	1.39	4 (12%)	39,39,63	1.33	5 (12%)
45	KC2	15	310	27	49,53,53	2.77	22 (44%)	60,89,89	4.09	32 (53%)
31	CLA	18	309	-	56,60,73	1.25	10 (17%)	65,97,113	1.65	9 (13%)
43	A86	18	303	-	47,50,50	1.77	7 (14%)	51,76,76	2.77	19 (37%)
31	CLA	b	609	-	69,73,73	1.17	9 (13%)	82,113,113	1.35	7 (8%)
36	LHG	b	623	-	42,42,48	0.75	1 (2%)	45,48,54	1.23	4 (8%)
43	A86	5	302	-	47,50,50	1.66	7 (14%)	51,76,76	2.79	24 (47%)
31	CLA	D	405	-	69,73,73	1.27	11 (15%)	82,113,113	1.61	11 (13%)
31	CLA	p	606	-	47,51,73	2.01	9 (19%)	55,86,113	3.93	28 (50%)
31	CLA	C	507	-	69,73,73	1.20	9 (13%)	82,113,113	1.42	8 (9%)
31	CLA	1	310	-	54,58,73	1.26	7 (12%)	64,95,113	1.59	8 (12%)
31	CLA	5	309	-	59,63,73	1.22	8 (13%)	70,101,113	1.61	11 (15%)
34	SQD	b	601	38	52,54,54	0.90	3 (5%)	62,65,65	1.68	12 (19%)
31	CLA	B	610	-	69,73,73	1.18	10 (14%)	82,113,113	1.40	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	6	308	-	46,50,73	1.40	7 (15%)	53,85,113	1.99	10 (18%)
31	CLA	B	611	-	69,73,73	1.35	9 (13%)	82,113,113	1.76	12 (14%)
31	CLA	b	606	-	69,73,73	1.21	9 (13%)	82,113,113	1.53	9 (10%)
31	CLA	B	612	-	69,73,73	1.18	8 (11%)	82,113,113	1.59	12 (14%)
38	DGD	c	520	34	63,63,67	1.18	9 (14%)	77,77,81	1.57	14 (18%)
31	CLA	7	308	-	45,49,73	1.44	10 (22%)	54,84,113	1.65	11 (20%)
31	CLA	b	615	-	69,73,73	1.15	10 (14%)	82,113,113	1.49	10 (12%)
31	CLA	16	313	-	46,50,73	1.76	12 (26%)	53,85,113	2.26	17 (32%)
43	A86	4	305	-	47,50,50	1.52	7 (14%)	51,76,76	5.17	23 (45%)
33	BCR	b	620	-	41,41,41	1.23	3 (7%)	56,56,56	1.30	9 (16%)
45	KC2	14	308	-	49,53,53	2.85	19 (38%)	60,89,89	4.31	32 (53%)
43	A86	P	613	31	47,50,50	1.61	6 (12%)	51,76,76	3.58	28 (54%)
37	LMG	0	317	-	31,31,55	1.34	2 (6%)	39,39,63	1.40	6 (15%)
31	CLA	16	307	-	46,50,73	1.42	6 (13%)	53,85,113	1.99	9 (16%)
33	BCR	Y	101	-	41,41,41	1.36	4 (9%)	56,56,56	1.60	12 (21%)
43	A86	9	305	-	47,50,50	2.04	9 (19%)	51,76,76	5.11	24 (47%)
31	CLA	15	311	27	49,53,73	1.54	10 (20%)	58,89,113	2.03	18 (31%)
43	A86	10	304	-	47,50,50	1.87	8 (17%)	51,76,76	4.92	26 (50%)
43	A86	13	304	-	47,50,50	2.14	10 (21%)	51,76,76	5.30	27 (52%)
43	A86	14	304	-	47,50,50	1.37	6 (12%)	51,76,76	4.13	24 (47%)
31	CLA	12	316	-	50,54,73	1.39	6 (12%)	59,90,113	1.51	6 (10%)
31	CLA	13	315	-	47,52,73	1.44	8 (17%)	55,87,113	1.39	5 (9%)
31	CLA	P	605	-	45,49,73	1.40	8 (17%)	54,84,113	1.63	10 (18%)
43	A86	1	302	-	47,50,50	1.50	5 (10%)	51,76,76	4.94	31 (60%)
42	KC1	19	314	-	49,53,53	2.81	21 (42%)	61,89,89	4.11	37 (60%)
31	CLA	P	607	43	47,51,73	1.37	10 (21%)	55,86,113	1.70	10 (18%)
43	A86	7	305	-	47,50,50	1.74	6 (12%)	51,76,76	3.85	24 (47%)
43	A86	7	304	-	47,50,50	1.85	7 (14%)	51,76,76	5.78	31 (60%)
43	A86	12	301	-	47,50,50	2.03	7 (14%)	51,76,76	5.11	25 (49%)
31	CLA	15	313	-	45,49,73	1.45	8 (17%)	54,84,113	1.61	9 (16%)
43	A86	8	303	-	47,50,50	1.86	8 (17%)	51,76,76	3.81	26 (50%)
43	A86	6	306	31	47,50,50	1.77	5 (10%)	51,76,76	3.71	22 (43%)
43	A86	19	306	-	47,50,50	1.54	6 (12%)	51,76,76	2.59	15 (29%)
31	CLA	8	315	-	47,51,73	1.36	9 (19%)	55,86,113	1.57	6 (10%)
43	A86	2	305	31	47,50,50	1.76	6 (12%)	51,76,76	3.79	24 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	b	608	-	69,73,73	1.19	8 (11%)	82,113,113	1.36	6 (7%)
31	CLA	a	404	-	53,57,73	1.30	8 (15%)	61,93,113	1.58	10 (16%)
45	KC2	4	310	-	49,53,53	2.86	21 (42%)	60,89,89	3.93	34 (56%)
31	CLA	10	308	-	54,58,73	1.33	9 (16%)	64,95,113	1.57	8 (12%)
31	CLA	R	101	-	51,55,73	1.33	9 (17%)	60,91,113	1.49	7 (11%)
31	CLA	C	513	-	69,73,73	1.14	8 (11%)	82,113,113	1.39	9 (10%)
37	LMG	4	316	-	49,49,55	0.82	2 (4%)	57,57,63	1.47	13 (22%)
31	CLA	c	514	-	53,57,73	1.28	10 (18%)	61,93,113	1.55	8 (13%)
42	KC1	15	317	-	49,53,53	2.78	19 (38%)	61,89,89	4.36	38 (62%)
37	LMG	15	314	-	37,37,55	0.97	3 (8%)	45,45,63	1.13	2 (4%)
31	CLA	W	202	-	69,73,73	1.16	9 (13%)	82,113,113	1.51	12 (14%)
37	LMG	11	317	-	45,45,55	0.95	2 (4%)	53,53,63	1.25	5 (9%)
37	LMG	P	614	-	31,31,55	0.93	1 (3%)	39,39,63	1.71	9 (23%)
45	KC2	2	310	-	49,53,53	2.87	20 (40%)	60,89,89	4.44	36 (60%)
38	DGD	11	318	-	61,61,67	0.92	3 (4%)	75,75,81	1.32	10 (13%)
31	CLA	13	313	-	69,73,73	1.32	11 (15%)	82,113,113	1.52	14 (17%)
37	LMG	c	522	-	31,31,55	1.15	4 (12%)	39,39,63	1.21	3 (7%)
43	A86	10	302	-	47,50,50	1.60	6 (12%)	51,76,76	3.02	22 (43%)
43	A86	p	613	31	47,50,50	1.61	6 (12%)	51,76,76	3.58	28 (54%)
31	CLA	c	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.54	8 (9%)
44	DD6	p	612	-	40,45,45	1.80	6 (15%)	51,67,67	3.62	21 (41%)
38	DGD	C	518	-	56,56,67	1.23	10 (17%)	70,70,81	1.68	16 (22%)
31	CLA	6	316	-	47,51,73	1.40	6 (12%)	55,86,113	1.54	7 (12%)
33	BCR	h	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.39	7 (12%)
36	LHG	4	317	-	34,34,48	0.77	1 (2%)	37,40,54	1.27	3 (8%)
31	CLA	2	307	-	69,73,73	1.16	9 (13%)	82,113,113	1.57	9 (10%)
31	CLA	10	317	-	52,56,73	1.36	10 (19%)	61,92,113	1.54	9 (14%)
32	PHO	d	403	-	58,69,69	2.03	10 (17%)	55,99,99	1.79	12 (21%)
31	CLA	c	505	-	69,73,73	1.14	10 (14%)	82,113,113	1.58	9 (10%)
31	CLA	9	308	-	69,73,73	1.15	8 (11%)	82,113,113	1.38	10 (12%)
43	A86	11	320	-	47,50,50	1.50	6 (12%)	51,76,76	3.47	23 (45%)
37	LMG	f	102	-	46,46,55	0.96	1 (2%)	54,54,63	1.49	8 (14%)
31	CLA	A	406	-	64,68,73	1.18	9 (14%)	76,107,113	1.41	7 (9%)
36	LHG	8	316	-	38,38,48	0.71	2 (5%)	41,44,54	1.31	4 (9%)
37	LMG	1	317	-	45,45,55	0.98	3 (6%)	53,53,63	1.22	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LMG	m	101	-	40,40,55	0.95	1 (2%)	48,48,63	1.35	4 (8%)
43	A86	5	305	-	47,50,50	1.68	8 (17%)	51,76,76	3.28	22 (43%)
43	A86	1	303	-	47,50,50	1.96	8 (17%)	51,76,76	4.94	28 (54%)
43	A86	17	301	-	47,50,50	1.64	9 (19%)	51,76,76	4.52	23 (45%)
31	CLA	13	312	-	49,53,73	1.40	7 (14%)	58,89,113	1.55	6 (10%)
31	CLA	p	605	-	45,49,73	1.40	8 (17%)	54,84,113	1.64	10 (18%)
31	CLA	b	605	-	69,73,73	1.39	11 (15%)	82,113,113	2.30	21 (25%)
33	BCR	H	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.38	7 (12%)
43	A86	0	306	-	47,50,50	1.73	9 (19%)	51,76,76	2.90	18 (35%)
35	PL9	d	407	-	55,55,55	2.04	15 (27%)	68,69,69	1.35	10 (14%)
31	CLA	15	307	-	69,73,73	1.16	10 (14%)	82,113,113	1.28	8 (9%)
31	CLA	p	604	-	52,56,73	1.31	10 (19%)	61,92,113	1.58	9 (14%)
31	CLA	18	314	-	47,51,73	1.35	10 (21%)	55,86,113	1.66	7 (12%)
36	LHG	14	317	-	34,34,48	0.73	1 (2%)	37,40,54	1.29	4 (10%)
36	LHG	8	317	-	30,30,48	0.79	1 (3%)	33,36,54	1.29	2 (6%)
43	A86	19	301	-	47,50,50	1.96	7 (14%)	51,76,76	5.00	29 (56%)
45	KC2	17	309	-	49,53,53	2.94	22 (44%)	60,89,89	3.88	30 (50%)
43	A86	14	302	43	47,50,50	1.67	7 (14%)	51,76,76	2.36	16 (31%)
31	CLA	c	509	-	69,73,73	1.27	10 (14%)	82,113,113	1.76	14 (17%)
43	A86	3	306	-	47,50,50	1.58	5 (10%)	51,76,76	4.57	23 (45%)
45	KC2	5	310	27	49,53,53	2.78	22 (44%)	60,89,89	3.93	34 (56%)
45	KC2	3	311	-	49,53,53	2.88	20 (40%)	60,89,89	4.24	35 (58%)
38	DGD	w	204	-	57,57,67	1.15	7 (12%)	71,71,81	1.48	10 (14%)
31	CLA	17	307	-	45,49,73	1.43	6 (13%)	54,84,113	2.01	14 (25%)
31	CLA	0	312	34,26	50,54,73	1.39	8 (16%)	59,90,113	1.79	11 (18%)
31	CLA	A	403	-	69,73,73	1.23	7 (10%)	82,113,113	1.41	12 (14%)
43	A86	19	304	-	47,50,50	1.90	6 (12%)	51,76,76	4.84	22 (43%)
45	KC2	7	311	27	49,53,53	2.85	19 (38%)	60,89,89	4.25	35 (58%)
37	LMG	d	409	-	37,37,55	0.90	2 (5%)	45,45,63	1.37	6 (13%)
43	A86	4	301	-	47,50,50	1.54	6 (12%)	51,76,76	3.64	20 (39%)
43	A86	11	304	31	47,50,50	1.54	6 (12%)	51,76,76	2.62	22 (43%)
31	CLA	19	312	43	69,73,73	1.19	8 (11%)	82,113,113	1.37	11 (13%)
31	CLA	8	308	-	65,69,73	1.24	10 (15%)	77,108,113	1.57	9 (11%)
32	PHO	A	405	-	58,69,69	2.03	10 (17%)	55,99,99	1.73	10 (18%)
33	BCR	C	515	-	41,41,41	1.22	4 (9%)	56,56,56	1.43	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	A86	15	304	-	47,50,50	1.64	7 (14%)	51,76,76	4.51	28 (54%)
43	A86	8	302	-	47,50,50	1.78	8 (17%)	51,76,76	4.50	34 (66%)
43	A86	1	305	-	47,50,50	1.84	8 (17%)	51,76,76	4.06	32 (62%)
36	LHG	5	317	-	24,24,48	0.77	0	27,30,54	1.30	2 (7%)
31	CLA	13	307	-	46,50,73	1.41	7 (15%)	53,85,113	1.72	8 (15%)
31	CLA	12	313	-	52,56,73	1.49	8 (15%)	61,92,113	1.60	12 (19%)
31	CLA	D	406	-	69,73,73	1.13	9 (13%)	82,113,113	1.37	6 (7%)
31	CLA	17	308	-	45,49,73	1.43	10 (22%)	54,84,113	1.63	9 (16%)
31	CLA	C	504	31	69,73,73	1.18	10 (14%)	82,113,113	1.50	15 (18%)
37	LMG	11	301	-	36,36,55	1.16	4 (11%)	44,44,63	1.45	7 (15%)
31	CLA	3	308	-	47,51,73	1.38	9 (19%)	55,86,113	1.68	8 (14%)
31	CLA	14	314	-	47,51,73	1.39	9 (19%)	55,86,113	1.60	6 (10%)
43	A86	4	304	-	47,50,50	1.43	6 (12%)	51,76,76	2.94	21 (41%)
31	CLA	1	316	43	46,50,73	1.42	7 (15%)	53,85,113	1.49	5 (9%)
42	KC1	18	313	31	49,53,53	2.70	20 (40%)	61,89,89	5.06	35 (57%)
31	CLA	6	311	-	45,49,73	1.36	5 (11%)	54,84,113	1.68	8 (14%)
31	CLA	19	311	43	50,54,73	1.37	7 (14%)	59,90,113	1.80	7 (11%)
45	KC2	3	309	-	49,53,53	2.93	23 (46%)	60,89,89	4.12	35 (58%)
43	A86	15	305	-	47,50,50	1.65	7 (14%)	51,76,76	4.48	22 (43%)
31	CLA	16	310	-	45,49,73	1.37	5 (11%)	54,84,113	1.68	8 (14%)
41	HEM	E	101	5,6	50,50,50	1.49	6 (12%)	67,82,82	1.05	4 (5%)
34	SQD	10	320	31	39,41,54	1.12	5 (12%)	49,52,65	1.66	10 (20%)
31	CLA	0	309	-	63,67,73	1.19	10 (15%)	74,105,113	1.47	10 (13%)
37	LMG	F	102	-	46,46,55	0.96	1 (2%)	54,54,63	1.49	8 (14%)
33	BCR	A	407	-	41,41,41	1.25	4 (9%)	56,56,56	1.24	6 (10%)
43	A86	6	302	-	47,50,50	1.61	7 (14%)	51,76,76	3.22	24 (47%)
43	A86	19	302	-	47,50,50	1.61	6 (12%)	51,76,76	5.11	23 (45%)
31	CLA	c	506	-	69,73,73	1.14	11 (15%)	82,113,113	1.48	8 (9%)
31	CLA	d	402	-	69,73,73	1.15	8 (11%)	82,113,113	1.50	10 (12%)
37	LMG	N	101	-	28,28,55	1.09	3 (10%)	36,36,63	1.32	6 (16%)
37	LMG	D	404	-	40,40,55	1.10	4 (10%)	48,48,63	1.54	8 (16%)
31	CLA	C	506	-	69,73,73	1.14	11 (15%)	82,113,113	1.48	8 (9%)
31	CLA	8	307	42	54,58,73	1.33	9 (16%)	64,95,113	1.79	13 (20%)
31	CLA	19	315	-	45,49,73	1.41	7 (15%)	54,84,113	1.57	7 (12%)
43	A86	18	302	-	47,50,50	1.60	6 (12%)	51,76,76	2.64	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	A86	17	305	-	47,50,50	2.05	12 (25%)	51,76,76	5.69	23 (45%)
31	CLA	11	312	27	50,54,73	1.40	10 (20%)	59,90,113	1.60	8 (13%)
31	CLA	B	609	-	69,73,73	1.13	9 (13%)	82,113,113	1.35	8 (9%)
31	CLA	2	314	-	45,49,73	1.42	8 (17%)	54,84,113	1.61	8 (14%)
31	CLA	14	311	-	50,54,73	1.36	8 (16%)	59,90,113	1.65	9 (15%)
43	A86	P	611	-	47,50,50	2.30	9 (19%)	51,76,76	6.10	28 (54%)
43	A86	16	303	43	47,50,50	1.82	9 (19%)	51,76,76	5.34	26 (50%)
31	CLA	A	404	-	53,57,73	1.30	8 (15%)	61,93,113	1.57	10 (16%)
43	A86	2	304	-	47,50,50	2.15	9 (19%)	51,76,76	5.73	26 (50%)
43	A86	3	302	-	47,50,50	1.58	7 (14%)	51,76,76	3.22	24 (47%)
42	KC1	2	313	-	49,53,53	2.76	18 (36%)	61,89,89	4.30	33 (54%)
31	CLA	2	315	43	50,54,73	1.49	9 (18%)	59,90,113	2.50	17 (28%)
31	CLA	4	315	-	47,51,73	1.38	10 (21%)	55,86,113	1.80	8 (14%)
38	DGD	b	622	34	56,56,67	1.29	7 (12%)	70,70,81	1.61	14 (20%)
37	LMG	5	316	-	36,36,55	1.23	4 (11%)	44,44,63	1.77	8 (18%)
38	DGD	h	102	-	63,63,67	0.99	5 (7%)	77,77,81	1.41	8 (10%)
43	A86	13	303	-	47,50,50	1.48	5 (10%)	51,76,76	2.80	17 (33%)
43	A86	7	303	-	47,50,50	1.46	6 (12%)	51,76,76	2.60	12 (23%)
31	CLA	b	613	-	69,73,73	1.17	8 (11%)	82,113,113	1.59	12 (14%)
42	KC1	7	314	-	49,53,53	2.80	19 (38%)	61,89,89	3.86	35 (57%)
43	A86	10	301	-	47,50,50	1.99	7 (14%)	51,76,76	4.78	27 (52%)
31	CLA	b	610	-	69,73,73	1.13	9 (13%)	82,113,113	1.36	8 (9%)
31	CLA	a	406	-	64,68,73	1.17	9 (14%)	76,107,113	1.40	7 (9%)
43	A86	18	301	-	47,50,50	2.16	7 (14%)	51,76,76	5.46	25 (49%)
31	CLA	6	314	-	46,50,73	1.64	9 (19%)	53,85,113	1.88	14 (26%)
33	BCR	B	617	-	41,41,41	1.22	2 (4%)	56,56,56	1.40	11 (19%)
31	CLA	11	315	-	45,49,73	1.45	9 (20%)	54,84,113	1.85	11 (20%)
43	A86	7	306	-	47,50,50	1.66	7 (14%)	51,76,76	4.08	23 (45%)
31	CLA	B	605	-	69,73,73	1.22	9 (13%)	82,113,113	1.53	8 (9%)
37	LMG	d	404	-	40,40,55	1.06	4 (10%)	48,48,63	1.57	7 (14%)
42	KC1	17	314	-	49,53,53	2.75	19 (38%)	61,89,89	4.96	35 (57%)
45	KC2	12	311	-	49,53,53	2.86	21 (42%)	60,89,89	4.35	33 (55%)
31	CLA	b	604	-	69,73,73	1.20	8 (11%)	82,113,113	1.52	11 (13%)
31	CLA	0	316	-	50,54,73	1.34	9 (18%)	59,90,113	1.49	8 (13%)
43	A86	12	304	-	47,50,50	1.95	8 (17%)	51,76,76	4.83	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	BCT	d	401	30	3,3,3	1.23	0	2,3,3	3.97	1 (50%)
31	CLA	P	601	16	69,73,73	1.16	10 (14%)	82,113,113	1.30	7 (8%)
31	CLA	6	309	-	69,73,73	1.15	10 (14%)	82,113,113	1.47	7 (8%)
43	A86	3	301	-	47,50,50	1.81	8 (17%)	51,76,76	4.06	26 (50%)
31	CLA	c	507	-	69,73,73	1.19	9 (13%)	82,113,113	1.43	8 (9%)
43	A86	6	301	43	47,50,50	1.46	6 (12%)	51,76,76	3.75	27 (52%)
37	LMG	p	614	-	31,31,55	0.95	1 (3%)	39,39,63	1.70	9 (23%)
31	CLA	B	608	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	7 (8%)
31	CLA	p	603	-	54,58,73	1.31	10 (18%)	64,95,113	1.55	10 (15%)
37	LMG	j	101	-	50,50,55	0.96	3 (6%)	58,58,63	1.32	4 (6%)
31	CLA	c	513	-	69,73,73	1.14	8 (11%)	82,113,113	1.39	9 (10%)
45	KC2	6	310	-	49,53,53	2.91	20 (40%)	60,89,89	3.84	31 (51%)
43	A86	17	303	-	47,50,50	1.73	8 (17%)	51,76,76	4.18	22 (43%)
33	BCR	B	619	-	41,41,41	1.23	4 (9%)	56,56,56	1.30	9 (16%)
33	BCR	C	517	-	41,41,41	1.21	3 (7%)	56,56,56	1.36	7 (12%)
31	CLA	18	307	-	65,69,73	1.27	10 (15%)	77,108,113	1.59	13 (16%)
43	A86	10	306	-	47,50,50	1.62	6 (12%)	51,76,76	2.69	19 (37%)
34	SQD	i	101	-	38,40,54	1.10	6 (15%)	48,51,65	1.94	13 (27%)
43	A86	13	301	-	47,50,50	1.65	7 (14%)	51,76,76	3.42	24 (47%)
31	CLA	P	606	-	47,51,73	2.01	9 (19%)	55,86,113	3.93	28 (50%)
31	CLA	17	310	-	49,53,73	1.37	8 (16%)	58,89,113	1.59	7 (12%)
31	CLA	4	312	27	55,59,73	1.46	10 (18%)	64,96,113	2.06	17 (26%)
31	CLA	c	511	-	69,73,73	1.18	11 (15%)	82,113,113	1.40	7 (8%)
37	LMG	C	522	-	51,51,55	0.88	2 (3%)	59,59,63	1.24	4 (6%)
43	A86	14	301	-	47,50,50	1.53	8 (17%)	51,76,76	3.20	22 (43%)
45	KC2	17	311	27	49,53,53	2.87	20 (40%)	60,89,89	4.14	36 (60%)
31	CLA	9	307	-	65,69,73	1.20	6 (9%)	77,108,113	1.46	7 (9%)
45	KC2	1	311	-	49,53,53	2.74	19 (38%)	60,89,89	3.98	36 (60%)
31	CLA	3	307	-	46,50,73	1.39	6 (13%)	53,85,113	1.91	10 (18%)
36	LHG	w	202	-	39,39,48	0.68	1 (2%)	42,45,54	1.24	4 (9%)
37	LMG	M	101	-	40,40,55	0.88	1 (2%)	48,48,63	1.32	5 (10%)
42	KC1	3	314	-	49,53,53	2.78	19 (38%)	61,89,89	5.04	34 (55%)
42	KC1	5	313	-	49,53,53	2.78	19 (38%)	61,89,89	5.13	40 (65%)
42	KC1	p	609	-	49,53,53	2.63	19 (38%)	61,89,89	3.82	37 (60%)
33	BCR	f	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.43	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	A86	1	320	-	47,50,50	1.48	6 (12%)	51,76,76	3.35	25 (49%)
31	CLA	11	316	43	45,49,73	1.45	8 (17%)	54,84,113	1.53	6 (11%)
31	CLA	C	505	-	69,73,73	1.14	10 (14%)	82,113,113	1.57	9 (10%)
31	CLA	p	602	-	69,73,73	1.17	10 (14%)	82,113,113	1.37	8 (9%)
31	CLA	w	203	-	69,73,73	1.16	9 (13%)	82,113,113	1.51	12 (14%)
31	CLA	Z	101	-	55,59,73	1.29	10 (18%)	64,96,113	1.44	6 (9%)
31	CLA	8	312	-	50,54,73	1.40	9 (18%)	59,90,113	1.61	12 (20%)
34	SQD	B	623	-	52,54,54	0.91	4 (7%)	62,65,65	1.68	12 (19%)
43	A86	4	306	-	47,50,50	1.59	6 (12%)	51,76,76	3.94	24 (47%)
33	BCR	c	517	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	7 (12%)
45	KC2	4	308	-	49,53,53	2.85	21 (42%)	60,89,89	4.29	33 (55%)
31	CLA	C	512	3	69,73,73	1.23	8 (11%)	82,113,113	1.53	10 (12%)
43	A86	14	303	-	47,50,50	1.40	6 (12%)	51,76,76	2.94	19 (37%)
31	CLA	19	310	-	69,73,73	1.17	6 (8%)	82,113,113	1.38	7 (8%)
31	CLA	p	601	16	69,73,73	1.16	10 (14%)	82,113,113	1.30	7 (8%)
31	CLA	P	602	-	69,73,73	1.17	10 (14%)	82,113,113	1.36	8 (9%)
31	CLA	P	608	-	55,59,73	1.30	8 (14%)	64,96,113	1.50	5 (7%)
31	CLA	10	313	26	46,50,73	1.44	9 (19%)	53,85,113	1.89	8 (15%)
43	A86	6	305	43	47,50,50	2.20	11 (23%)	51,76,76	5.40	30 (58%)
43	A86	13	302	-	47,50,50	1.94	6 (12%)	51,76,76	5.08	27 (52%)
36	LHG	d	408	-	48,48,48	0.68	1 (2%)	51,54,54	1.30	7 (13%)
45	KC2	0	310	-	49,53,53	2.71	21 (42%)	60,89,89	3.93	33 (55%)
31	CLA	z	101	-	55,59,73	1.29	10 (18%)	64,96,113	1.45	6 (9%)
31	CLA	0	311	-	59,63,73	1.22	11 (18%)	70,101,113	1.48	9 (12%)
43	A86	10	305	-	47,50,50	1.56	6 (12%)	51,76,76	3.26	25 (49%)
36	LHG	P	615	-	26,26,48	0.89	1 (3%)	29,32,54	1.36	3 (10%)
43	A86	14	305	-	47,50,50	1.55	7 (14%)	51,76,76	4.31	28 (54%)
43	A86	18	305	-	47,50,50	1.80	7 (14%)	51,76,76	2.94	18 (35%)
43	A86	5	303	-	47,50,50	1.67	7 (14%)	51,76,76	4.43	23 (45%)
43	A86	1	319	-	47,50,50	1.85	6 (12%)	51,76,76	5.19	28 (54%)
31	CLA	5	314	-	45,49,73	1.43	6 (13%)	54,84,113	1.52	6 (11%)
31	CLA	16	312	-	51,55,73	1.40	10 (19%)	60,91,113	1.40	6 (10%)
43	A86	3	305	-	47,50,50	2.11	10 (21%)	51,76,76	5.64	29 (56%)
31	CLA	7	313	-	54,58,73	1.52	10 (18%)	64,95,113	1.82	14 (21%)
31	CLA	19	313	-	69,73,73	1.12	6 (8%)	82,113,113	1.97	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	6	313	-	51,55,73	1.38	10 (19%)	60,91,113	1.43	7 (11%)
35	PL9	a	409	-	33,33,55	1.29	5 (15%)	41,42,69	1.47	7 (17%)
31	CLA	10	316	-	50,54,73	1.34	9 (18%)	59,90,113	1.49	7 (11%)
31	CLA	c	503	31	69,73,73	1.39	11 (15%)	82,113,113	2.37	21 (25%)
43	A86	5	304	-	47,50,50	1.63	7 (14%)	51,76,76	3.82	28 (54%)
31	CLA	14	315	-	47,51,73	1.37	10 (21%)	55,86,113	1.94	9 (16%)
33	BCR	B	618	-	41,41,41	1.10	2 (4%)	56,56,56	1.48	9 (16%)
37	LMG	K	101	-	46,46,55	1.08	4 (8%)	54,54,63	1.45	8 (14%)
43	A86	0	304	-	47,50,50	1.87	9 (19%)	51,76,76	5.02	26 (50%)
31	CLA	5	312	-	51,55,73	1.42	8 (15%)	60,91,113	1.60	11 (18%)
43	A86	11	303	-	47,50,50	1.89	6 (12%)	51,76,76	4.73	29 (56%)
41	HEM	V	201	21	50,50,50	1.42	5 (10%)	67,82,82	1.60	16 (23%)
45	KC2	11	311	-	49,53,53	2.76	19 (38%)	60,89,89	3.97	36 (60%)
31	CLA	z	103	-	52,56,73	1.37	10 (19%)	61,92,113	1.55	10 (16%)
43	A86	10	318	-	47,50,50	1.67	9 (19%)	51,76,76	3.55	23 (45%)
45	KC2	16	309	-	49,53,53	2.90	21 (42%)	60,89,89	3.86	30 (50%)
31	CLA	c	512	3	69,73,73	1.23	8 (11%)	82,113,113	1.54	10 (12%)
36	LHG	A	410	-	36,36,48	0.77	1 (2%)	39,42,54	1.27	4 (10%)
45	KC2	18	310	27	49,53,53	2.79	20 (40%)	60,89,89	4.69	34 (56%)
31	CLA	18	311	-	50,54,73	1.43	9 (18%)	59,90,113	1.65	10 (16%)
31	CLA	12	308	-	69,73,73	1.17	10 (14%)	82,113,113	1.51	12 (14%)
31	CLA	B	604	-	69,73,73	1.39	12 (17%)	82,113,113	2.29	21 (25%)
43	A86	0	302	-	47,50,50	1.62	8 (17%)	51,76,76	3.57	23 (45%)
45	KC2	6	312	27	49,53,53	2.88	22 (44%)	60,89,89	4.29	35 (58%)
45	KC2	10	310	-	49,53,53	2.70	21 (42%)	60,89,89	3.91	34 (56%)
31	CLA	B	601	-	69,73,73	1.15	9 (13%)	82,113,113	1.42	8 (9%)
31	CLA	b	603	-	69,73,73	1.21	10 (14%)	82,113,113	1.46	13 (15%)
36	LHG	B	622	-	42,42,48	0.76	1 (2%)	45,48,54	1.23	4 (8%)
31	CLA	B	616	-	69,73,73	1.20	9 (13%)	82,113,113	1.50	12 (14%)
37	LMG	b	621	-	51,51,55	0.90	4 (7%)	59,59,63	1.50	11 (18%)
31	CLA	17	315	-	45,49,73	1.40	7 (15%)	54,84,113	1.56	6 (11%)
31	CLA	5	307	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	10 (12%)
31	CLA	12	307	-	46,50,73	1.44	8 (17%)	53,85,113	1.91	17 (32%)
42	KC1	14	313	27	49,53,53	2.65	21 (42%)	61,89,89	4.94	38 (62%)
42	KC1	9	314	-	49,53,53	2.82	20 (40%)	61,89,89	4.11	34 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	A86	16	302	-	47,50,50	1.67	8 (17%)	51,76,76	3.19	24 (47%)
43	A86	12	302	-	47,50,50	1.92	7 (14%)	51,76,76	4.92	30 (58%)
31	CLA	c	502	-	69,73,73	1.18	9 (13%)	82,113,113	1.45	10 (12%)
43	A86	15	303	-	47,50,50	1.74	7 (14%)	51,76,76	4.29	22 (43%)
36	LHG	z	102	-	24,24,48	0.95	0	27,30,54	1.34	3 (11%)
43	A86	16	301	43	47,50,50	1.46	6 (12%)	51,76,76	3.60	24 (47%)
38	DGD	W	203	-	57,57,67	1.15	7 (12%)	71,71,81	1.48	10 (14%)
31	CLA	7	312	-	51,55,73	1.40	9 (17%)	60,91,113	1.39	6 (10%)
31	CLA	7	310	-	49,53,73	1.35	8 (16%)	58,89,113	1.59	7 (12%)
41	HEM	e	101	5,6	50,50,50	1.50	6 (12%)	67,82,82	1.06	4 (5%)
36	LHG	D	408	-	48,48,48	0.68	1 (2%)	51,54,54	1.30	7 (13%)
43	A86	11	319	-	47,50,50	1.49	6 (12%)	51,76,76	3.51	21 (41%)
34	SQD	l	101	-	52,54,54	0.94	3 (5%)	62,65,65	1.45	11 (17%)
43	A86	2	303	-	47,50,50	1.57	7 (14%)	51,76,76	3.27	25 (49%)
42	KC1	6	315	-	49,53,53	2.83	20 (40%)	61,89,89	5.47	38 (62%)
43	A86	17	306	-	47,50,50	1.75	5 (10%)	51,76,76	3.79	23 (45%)
31	CLA	b	602	-	69,73,73	1.15	9 (13%)	82,113,113	1.43	7 (8%)
31	CLA	d	405	-	69,73,73	1.27	11 (15%)	82,113,113	1.61	11 (13%)
31	CLA	P	604	-	52,56,73	1.31	10 (19%)	61,92,113	1.57	10 (16%)
31	CLA	B	614	-	69,73,73	1.16	10 (14%)	82,113,113	1.48	10 (12%)
31	CLA	1	308	-	69,73,73	1.17	8 (11%)	82,113,113	1.40	8 (9%)
38	DGD	c	519	-	63,63,67	1.12	9 (14%)	77,77,81	1.52	16 (20%)
31	CLA	4	309	-	69,73,73	1.13	8 (11%)	82,113,113	1.44	7 (8%)
43	A86	17	304	-	47,50,50	1.51	6 (12%)	51,76,76	2.67	12 (23%)
31	CLA	B	602	-	69,73,73	1.20	10 (14%)	82,113,113	1.47	13 (15%)
31	CLA	1	307	-	47,51,73	1.36	8 (17%)	55,86,113	1.85	15 (27%)
31	CLA	9	311	43	50,54,73	1.36	7 (14%)	59,90,113	1.85	8 (13%)
31	CLA	b	614	-	69,73,73	1.18	9 (13%)	82,113,113	1.26	7 (8%)
31	CLA	10	311	-	59,63,73	1.22	11 (18%)	70,101,113	1.50	9 (12%)
37	LMG	5	315	-	37,37,55	0.98	3 (8%)	45,45,63	1.17	2 (4%)
37	LMG	c	521	-	51,51,55	0.89	2 (3%)	59,59,63	1.24	4 (6%)
34	SQD	A	411	-	38,40,54	1.10	6 (15%)	48,51,65	1.95	13 (27%)
36	LHG	l	102	-	48,48,48	0.81	3 (6%)	51,54,54	1.31	7 (13%)
33	BCR	c	516	-	41,41,41	1.26	5 (12%)	56,56,56	1.36	9 (16%)
43	A86	12	305	-	47,50,50	1.59	6 (12%)	51,76,76	2.71	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LMG	14	316	-	49,49,55	0.78	0	57,57,63	1.42	11 (19%)
37	LMG	D	409	-	37,37,55	0.90	2 (5%)	45,45,63	1.37	6 (13%)
37	LMG	15	315	-	36,36,55	1.21	4 (11%)	44,44,63	1.75	9 (20%)
43	A86	12	303	-	47,50,50	1.49	4 (8%)	51,76,76	3.69	23 (45%)
43	A86	17	302	-	47,50,50	2.00	11 (23%)	51,76,76	3.37	24 (47%)
33	BCR	F	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.43	10 (17%)
42	KC1	8	314	43,31	49,53,53	2.58	19 (38%)	61,89,89	5.60	35 (57%)
31	CLA	10	312	34,26	50,54,73	1.37	8 (16%)	59,90,113	1.77	10 (16%)
31	CLA	B	603	-	69,73,73	1.20	9 (13%)	82,113,113	1.53	12 (14%)
31	CLA	11	310	-	54,58,73	1.27	7 (12%)	64,95,113	1.55	7 (10%)
31	CLA	13	310	-	45,49,73	1.38	7 (15%)	54,84,113	1.60	7 (12%)
43	A86	7	301	-	47,50,50	1.56	7 (14%)	51,76,76	3.46	23 (45%)
43	A86	8	306	-	47,50,50	1.64	8 (17%)	51,76,76	3.62	23 (45%)
33	BCR	c	515	-	41,41,41	1.23	3 (7%)	56,56,56	1.43	8 (14%)
34	SQD	8	301	31	39,41,54	1.12	5 (12%)	49,52,65	1.71	12 (24%)
36	LHG	15	316	-	24,24,48	0.79	0	27,30,54	1.28	2 (7%)
31	CLA	p	607	43	47,51,73	1.37	10 (21%)	55,86,113	1.69	10 (18%)
31	CLA	4	311	-	50,54,73	1.33	8 (16%)	59,90,113	1.58	7 (11%)
31	CLA	11	308	-	69,73,73	1.15	9 (13%)	82,113,113	1.52	15 (18%)
45	KC2	11	309	-	49,53,53	2.77	21 (42%)	60,89,89	4.23	33 (55%)
31	CLA	b	607	-	69,73,73	1.21	9 (13%)	82,113,113	1.91	17 (20%)
31	CLA	r	101	-	51,55,73	1.34	9 (17%)	60,91,113	1.50	6 (10%)
42	KC1	12	314	-	49,53,53	2.73	19 (38%)	61,89,89	3.88	34 (55%)
43	A86	6	303	-	47,50,50	1.83	7 (14%)	51,76,76	4.39	27 (52%)
31	CLA	18	306	42	54,58,73	1.30	10 (18%)	64,95,113	1.74	12 (18%)
31	CLA	5	311	-	49,53,73	1.42	9 (18%)	58,89,113	1.84	11 (18%)
38	DGD	C	520	34	63,63,67	1.18	9 (14%)	77,77,81	1.58	14 (18%)
38	DGD	1	318	-	55,55,67	1.03	3 (5%)	69,69,81	1.36	9 (13%)
31	CLA	15	306	-	46,50,73	1.41	6 (13%)	53,85,113	1.75	10 (18%)
43	A86	19	305	-	47,50,50	2.02	8 (17%)	51,76,76	5.09	23 (45%)
31	CLA	11	307	-	47,51,73	1.42	8 (17%)	55,86,113	2.17	19 (34%)
31	CLA	d	406	-	69,73,73	1.13	10 (14%)	82,113,113	1.38	6 (7%)
43	A86	6	304	-	47,50,50	1.56	6 (12%)	51,76,76	3.17	23 (45%)
43	A86	9	301	-	47,50,50	1.87	5 (10%)	51,76,76	5.81	25 (49%)
37	LMG	J	101	-	50,50,55	0.96	3 (6%)	58,58,63	1.32	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	C	511	-	69,73,73	1.18	10 (14%)	82,113,113	1.39	7 (8%)
43	A86	11	305	-	47,50,50	1.72	7 (14%)	51,76,76	3.88	33 (64%)
33	BCR	b	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.48	10 (17%)
43	A86	9	303	-	47,50,50	1.47	6 (12%)	51,76,76	2.87	22 (43%)
45	KC2	15	308	-	49,53,53	2.90	21 (42%)	60,89,89	4.34	38 (63%)
44	DD6	P	612	-	40,45,45	1.65	3 (7%)	51,67,67	2.13	12 (23%)
31	CLA	2	311	-	49,53,73	1.42	10 (20%)	58,89,113	1.49	7 (12%)
31	CLA	12	310	-	47,51,73	1.36	7 (14%)	55,86,113	1.54	7 (12%)
45	KC2	9	309	-	49,53,53	2.86	20 (40%)	60,89,89	4.29	36 (60%)
37	LMG	w	201	-	48,48,55	0.97	5 (10%)	56,56,63	1.41	9 (16%)
43	A86	16	305	43	47,50,50	2.15	10 (21%)	51,76,76	5.43	29 (56%)
43	A86	9	306	-	47,50,50	1.73	10 (21%)	51,76,76	2.62	18 (35%)
37	LMG	n	701	-	28,28,55	1.08	3 (10%)	36,36,63	1.33	6 (16%)
36	LHG	18	315	-	38,38,48	0.70	1 (2%)	41,44,54	1.30	4 (9%)
31	CLA	9	312	43	69,73,73	1.19	8 (11%)	82,113,113	1.39	12 (14%)
31	CLA	15	309	-	59,63,73	1.22	8 (13%)	70,101,113	1.61	10 (14%)
45	KC2	1	309	-	49,53,53	2.84	21 (42%)	60,89,89	3.79	30 (50%)
31	CLA	14	306	-	65,69,73	1.36	11 (16%)	77,108,113	2.18	21 (27%)
31	CLA	17	312	-	51,55,73	1.39	10 (19%)	60,91,113	1.39	6 (10%)
31	CLA	14	307	-	69,73,73	1.14	10 (14%)	82,113,113	1.31	9 (10%)
45	KC2	7	309	-	49,53,53	2.93	22 (44%)	60,89,89	3.90	31 (51%)
45	KC2	18	308	-	49,53,53	2.81	22 (44%)	60,89,89	3.88	34 (56%)
31	CLA	C	514	-	53,57,73	1.28	10 (18%)	61,93,113	1.56	8 (13%)
34	SQD	L	102	-	52,54,54	0.94	3 (5%)	62,65,65	1.46	11 (17%)
38	DGD	H	102	-	63,63,67	0.99	4 (6%)	77,77,81	1.41	8 (10%)
38	DGD	c	518	-	56,56,67	1.23	10 (17%)	70,70,81	1.68	16 (22%)
31	CLA	b	616	-	69,73,73	1.20	9 (13%)	82,113,113	1.54	7 (8%)
37	LMG	1	301	-	36,36,55	1.16	4 (11%)	44,44,63	1.45	7 (15%)

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
31	CLA	0	314	-	-	7/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	KC1	1	314	-	-	6/15/71/71	-
31	CLA	C	503	31	1/1/15/20	13/39/115/115	-
31	CLA	7	307	-	1/1/10/20	3/10/86/115	-
31	CLA	10	309	-	-	13/32/108/115	-
31	CLA	19	307	-	1/1/14/20	8/35/111/115	-
31	CLA	P	603	-	1/1/12/20	7/21/97/115	-
43	A86	10	303	-	-	7/34/90/90	0/3/3/3
31	CLA	11	313	-	1/1/15/20	14/39/115/115	-
42	KC1	0	315	-	-	4/15/71/71	-
33	BCR	y	101	-	-	11/29/63/63	0/2/2/2
45	KC2	13	309	-	-	10/15/71/71	-
31	CLA	18	312	-	1/1/13/20	10/27/103/115	-
31	CLA	B	613	-	1/1/15/20	9/39/115/115	-
31	CLA	3	315	-	1/1/10/20	5/14/90/115	-
43	A86	9	304	-	-	7/34/90/90	0/3/3/3
45	KC2	13	311	-	-	7/15/71/71	-
32	PHO	a	405	-	-	13/37/103/103	0/5/6/6
33	BCR	b	618	-	-	11/29/63/63	0/2/2/2
36	LHG	a	410	-	-	16/41/41/53	-
31	CLA	14	309	-	1/1/15/20	18/39/115/115	-
31	CLA	9	315	-	1/1/10/20	2/10/86/115	-
37	LMG	k	101	-	-	23/41/61/70	0/1/1/1
31	CLA	2	306	-	1/1/10/20	5/12/88/115	-
43	A86	7	302	-	-	10/34/90/90	0/3/3/3
31	CLA	b	612	-	1/1/15/20	12/39/115/115	-
45	KC2	12	309	-	-	6/15/71/71	-
31	CLA	4	307	-	1/1/15/20	15/39/115/115	-
45	KC2	14	310	-	-	6/15/71/71	-
31	CLA	10	307	-	1/1/11/20	9/19/95/115	-
31	CLA	3	316	-	-	17/39/115/115	-
31	CLA	3	312	-	-	6/15/91/115	-
31	CLA	C	509	-	1/1/15/20	9/39/115/115	-
31	CLA	7	315	-	1/1/10/20	6/10/86/115	-
43	A86	15	302	-	-	9/34/90/90	1/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	19	308	-	1/1/15/20	14/39/115/115	-
45	KC2	8	309	-	-	10/15/71/71	-
31	CLA	1	313	-	1/1/15/20	14/39/115/115	-
43	A86	5	318	42	-	9/34/90/90	0/3/3/3
42	KC1	P	609	-	-	8/15/71/71	-
35	PL9	D	407	-	-	9/53/73/73	0/1/1/1
34	SQD	a	408	38	-	24/49/69/69	0/1/1/1
43	A86	5	301	31	-	6/34/90/90	0/3/3/3
31	CLA	a	403	-	1/1/15/20	10/39/115/115	-
36	LHG	C	521	-	-	19/44/44/53	-
45	KC2	16	311	-	-	6/15/71/71	-
31	CLA	5	306	-	1/1/10/20	3/12/88/115	-
36	LHG	18	316	-	-	22/34/34/53	-
43	A86	6	307	-	-	12/34/90/90	0/3/3/3
43	A86	8	305	-	-	8/34/90/90	0/3/3/3
45	KC2	2	308	-	-	10/15/71/71	-
43	A86	12	306	-	-	9/34/90/90	0/3/3/3
43	A86	p	611	-	-	7/34/90/90	1/3/3/3
31	CLA	0	313	-	1/1/10/20	2/12/88/115	-
31	CLA	P	610	-	1/1/10/20	2/10/86/115	-
31	CLA	9	313	-	1/1/15/20	11/39/115/115	-
43	A86	19	303	-	-	7/34/90/90	0/3/3/3
31	CLA	12	315	-	-	1/10/86/115	-
31	CLA	b	611	-	-	10/39/115/115	-
36	LHG	p	615	-	-	14/31/31/53	-
31	CLA	9	310	-	1/1/15/20	13/39/115/115	-
38	DGD	C	519	-	-	28/51/91/95	0/2/2/2
43	A86	8	304	-	-	9/34/90/90	0/3/3/3
37	LMG	W	201	-	-	24/43/63/70	0/1/1/1
43	A86	13	305	-	-	9/34/90/90	0/3/3/3
31	CLA	2	312	-	-	10/19/95/115	-
31	CLA	1	321	-	1/1/14/20	11/35/111/115	-
31	CLA	10	314	-	1/1/11/20	4/18/94/115	-
42	KC1	13	314	-	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	17	316	-	-	9/34/90/90	0/3/3/3
38	DGD	B	621	-	-	31/43/83/95	0/2/2/2
37	LMG	Z	102	-	-	10/26/46/70	0/1/1/1
31	CLA	13	316	-	-	16/39/115/115	-
45	KC2	5	308	-	-	6/15/71/71	-
31	CLA	D	402	-	1/1/15/20	7/39/115/115	-
31	CLA	0	307	-	1/1/11/20	6/19/95/115	-
36	LHG	L	101	-	-	22/53/53/53	-
43	A86	13	306	43	-	10/34/90/90	0/3/3/3
36	LHG	Z	103	-	-	16/29/29/53	-
43	A86	4	302	-	-	6/34/90/90	0/3/3/3
31	CLA	C	510	-	1/1/15/20	7/39/115/115	-
37	LMG	B	620	-	-	26/46/66/70	0/1/1/1
43	A86	18	304	-	-	7/34/90/90	0/3/3/3
43	A86	0	301	-	-	8/34/90/90	0/3/3/3
41	HEM	v	201	21	-	7/14/54/54	-
31	CLA	14	312	-	1/1/12/20	10/23/99/115	-
43	A86	1	306	-	-	8/34/90/90	0/3/3/3
43	A86	9	302	-	-	6/34/90/90	0/3/3/3
31	CLA	C	508	-	1/1/15/20	16/39/115/115	-
31	CLA	15	312	-	-	6/18/94/115	-
31	CLA	8	313	-	1/1/13/20	12/27/103/115	-
31	CLA	0	308	-	1/1/12/20	8/21/97/115	-
43	A86	0	303	-	-	7/34/90/90	0/3/3/3
31	CLA	1	312	-	1/1/11/20	6/17/93/115	-
31	CLA	3	310	-	1/1/10/20	2/10/86/115	-
43	A86	3	304	-	-	6/34/90/90	0/3/3/3
31	CLA	8	310	-	1/1/12/20	6/24/100/115	-
31	CLA	4	314	-	1/1/10/20	7/13/89/115	-
42	KC1	16	314	-	-	1/15/71/71	-
43	A86	11	302	-	-	5/34/90/90	0/3/3/3
45	KC2	19	309	-	-	4/15/71/71	-
31	CLA	c	504	31	1/1/15/20	23/39/115/115	-
43	A86	4	303	-	-	11/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	16	306	31	-	8/34/90/90	0/3/3/3
43	A86	2	302	-	-	10/34/90/90	0/3/3/3
42	KC1	4	313	-	-	9/15/71/71	-
43	A86	0	305	-	-	9/34/90/90	0/3/3/3
43	A86	16	304	-	-	7/34/90/90	0/3/3/3
43	A86	1	304	31	-	7/34/90/90	0/3/3/3
42	KC1	11	314	-	-	8/15/71/71	-
31	CLA	p	610	-	1/1/10/20	2/10/86/115	-
31	CLA	B	607	-	1/1/15/20	14/39/115/115	-
31	CLA	1	315	-	-	4/10/86/115	-
31	CLA	p	608	-	1/1/12/20	7/23/99/115	-
34	SQD	A	408	38	-	24/49/69/69	0/1/1/1
33	BCR	C	516	-	-	9/29/63/63	0/2/2/2
31	CLA	12	312	-	1/1/11/20	6/15/91/115	-
31	CLA	c	508	-	1/1/15/20	16/39/115/115	-
31	CLA	B	606	-	1/1/15/20	12/39/115/115	-
31	CLA	C	502	-	1/1/15/20	12/39/115/115	-
43	A86	11	306	-	-	9/34/90/90	0/3/3/3
32	PHO	D	403	-	-	5/37/103/103	0/5/6/6
31	CLA	16	308	-	1/1/15/20	15/39/115/115	-
42	KC1	10	315	-	-	4/15/71/71	-
31	CLA	13	308	-	1/1/10/20	2/13/89/115	-
43	A86	15	301	31	-	6/34/90/90	0/3/3/3
43	A86	3	303	-	-	9/34/90/90	0/3/3/3
45	KC2	8	311	-	-	6/15/71/71	-
43	A86	2	301	-	-	10/34/90/90	0/3/3/3
31	CLA	17	313	-	1/1/12/20	6/21/97/115	-
31	CLA	3	313	-	1/1/15/20	19/39/115/115	-
31	CLA	b	617	-	1/1/15/20	13/39/115/115	-
31	CLA	2	309	-	1/1/10/20	5/13/89/115	-
31	CLA	16	315	-	1/1/10/20	4/13/89/115	-
33	BCR	a	407	-	-	8/29/63/63	0/2/2/2
31	CLA	B	615	-	1/1/15/20	7/39/115/115	-
35	PL9	A	409	-	-	16/27/47/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	10	319	-	-	9/26/46/70	0/1/1/1
45	KC2	15	310	27	-	7/15/71/71	-
31	CLA	18	309	-	1/1/12/20	6/24/100/115	-
43	A86	18	303	-	-	12/34/90/90	0/3/3/3
31	CLA	b	609	-	1/1/15/20	16/39/115/115	-
36	LHG	b	623	-	-	14/47/47/53	-
43	A86	5	302	-	-	9/34/90/90	0/3/3/3
31	CLA	D	405	-	1/1/15/20	12/39/115/115	-
31	CLA	p	606	-	1/1/10/20	7/13/89/115	-
31	CLA	C	507	-	1/1/15/20	14/39/115/115	-
31	CLA	1	310	-	1/1/12/20	4/21/97/115	-
31	CLA	5	309	-	1/1/13/20	9/27/103/115	-
34	SQD	b	601	38	-	26/49/69/69	0/1/1/1
31	CLA	6	308	-	1/1/10/20	7/12/88/115	-
31	CLA	B	610	-	-	10/39/115/115	-
31	CLA	B	611	-	1/1/15/20	12/39/115/115	-
31	CLA	b	606	-	1/1/15/20	12/39/115/115	-
31	CLA	B	612	-	1/1/15/20	13/39/115/115	-
38	DGD	c	520	34	-	32/51/91/95	0/2/2/2
31	CLA	7	308	-	-	3/10/86/115	-
31	CLA	b	615	-	1/1/15/20	18/39/115/115	-
31	CLA	16	313	-	1/1/10/20	5/12/88/115	-
43	A86	4	305	-	-	8/34/90/90	0/3/3/3
33	BCR	b	620	-	-	11/29/63/63	0/2/2/2
45	KC2	14	308	-	-	7/15/71/71	-
43	A86	P	613	31	-	7/34/90/90	1/3/3/3
37	LMG	0	317	-	-	8/26/46/70	0/1/1/1
31	CLA	16	307	-	1/1/10/20	4/12/88/115	-
33	BCR	Y	101	-	-	11/29/63/63	0/2/2/2
43	A86	9	305	-	-	8/34/90/90	0/3/3/3
31	CLA	15	311	27	1/1/11/20	5/15/91/115	-
43	A86	10	304	-	-	6/34/90/90	0/3/3/3
43	A86	13	304	-	-	7/34/90/90	0/3/3/3
43	A86	14	304	-	-	7/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	12	316	-	1/1/11/20	5/17/93/115	-
31	CLA	13	315	-	-	2/14/90/115	-
31	CLA	P	605	-	1/1/10/20	5/10/86/115	-
43	A86	1	302	-	-	7/34/90/90	0/3/3/3
42	KC1	19	314	-	-	5/15/71/71	-
31	CLA	P	607	43	1/1/10/20	6/13/89/115	-
43	A86	7	305	-	-	8/34/90/90	0/3/3/3
43	A86	7	304	-	-	9/34/90/90	0/3/3/3
43	A86	12	301	-	-	8/34/90/90	0/3/3/3
31	CLA	15	313	-	1/1/10/20	0/10/86/115	-
43	A86	8	303	-	-	8/34/90/90	0/3/3/3
43	A86	6	306	31	-	8/34/90/90	0/3/3/3
43	A86	19	306	-	-	8/34/90/90	0/3/3/3
31	CLA	8	315	-	1/1/10/20	4/13/89/115	-
43	A86	2	305	31	-	7/34/90/90	0/3/3/3
31	CLA	b	608	-	1/1/15/20	14/39/115/115	-
31	CLA	a	404	-	1/1/11/20	5/20/96/115	-
45	KC2	4	310	-	-	7/15/71/71	-
31	CLA	10	308	-	1/1/12/20	7/21/97/115	-
31	CLA	R	101	-	1/1/11/20	6/18/94/115	-
31	CLA	C	513	-	1/1/15/20	16/39/115/115	-
37	LMG	4	316	-	-	24/44/64/70	0/1/1/1
31	CLA	c	514	-	1/1/11/20	4/20/96/115	-
42	KC1	15	317	-	-	0/15/71/71	-
37	LMG	15	314	-	-	17/32/52/70	0/1/1/1
31	CLA	W	202	-	1/1/15/20	15/39/115/115	-
37	LMG	11	317	-	-	24/40/60/70	0/1/1/1
37	LMG	P	614	-	-	11/26/46/70	0/1/1/1
45	KC2	2	310	-	-	8/15/71/71	-
38	DGD	11	318	-	-	31/49/89/95	0/2/2/2
31	CLA	13	313	-	-	16/39/115/115	-
37	LMG	c	522	-	-	10/26/46/70	0/1/1/1
43	A86	10	302	-	-	8/34/90/90	0/3/3/3
43	A86	p	613	31	-	7/34/90/90	1/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	510	-	1/1/15/20	7/39/115/115	-
44	DD6	p	612	-	-	9/26/80/80	0/3/3/3
38	DGD	C	518	-	-	22/44/84/95	0/2/2/2
31	CLA	6	316	-	1/1/10/20	4/13/89/115	-
33	BCR	h	101	-	-	10/29/63/63	0/2/2/2
36	LHG	4	317	-	-	17/38/38/53	-
31	CLA	2	307	-	1/1/15/20	17/39/115/115	-
31	CLA	10	317	-	1/1/11/20	6/19/95/115	-
32	PHO	d	403	-	-	5/37/103/103	0/5/6/6
31	CLA	c	505	-	1/1/15/20	9/39/115/115	-
31	CLA	9	308	-	1/1/15/20	15/39/115/115	-
43	A86	11	320	-	-	8/34/90/90	0/3/3/3
37	LMG	f	102	-	-	14/41/61/70	0/1/1/1
31	CLA	A	406	-	1/1/14/20	4/33/109/115	-
36	LHG	8	316	-	-	23/43/43/53	-
37	LMG	1	317	-	-	26/40/60/70	0/1/1/1
37	LMG	m	101	-	-	19/35/55/70	0/1/1/1
43	A86	5	305	-	-	6/34/90/90	0/3/3/3
43	A86	1	303	-	-	8/34/90/90	0/3/3/3
43	A86	17	301	-	-	10/34/90/90	0/3/3/3
31	CLA	13	312	-	1/1/11/20	6/15/91/115	-
31	CLA	p	605	-	1/1/10/20	5/10/86/115	-
31	CLA	b	605	-	1/1/15/20	13/39/115/115	-
33	BCR	H	101	-	-	10/29/63/63	0/2/2/2
43	A86	0	306	-	-	8/34/90/90	0/3/3/3
35	PL9	d	407	-	-	9/53/73/73	0/1/1/1
31	CLA	15	307	-	1/1/15/20	17/39/115/115	-
31	CLA	p	604	-	1/1/11/20	6/19/95/115	-
31	CLA	18	314	-	1/1/10/20	9/13/89/115	-
36	LHG	14	317	-	-	21/38/38/53	-
36	LHG	8	317	-	-	20/34/34/53	-
43	A86	19	301	-	-	9/34/90/90	0/3/3/3
45	KC2	17	309	-	-	10/15/71/71	-
43	A86	14	302	43	-	7/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	509	-	1/1/15/20	9/39/115/115	-
43	A86	3	306	-	-	8/34/90/90	0/3/3/3
45	KC2	5	310	27	-	7/15/71/71	-
45	KC2	3	311	-	-	6/15/71/71	-
38	DGD	w	204	-	-	29/45/85/95	0/2/2/2
31	CLA	17	307	-	1/1/10/20	3/10/86/115	-
31	CLA	0	312	34,26	1/1/11/20	5/17/93/115	-
31	CLA	A	403	-	1/1/15/20	10/39/115/115	-
43	A86	19	304	-	-	7/34/90/90	0/3/3/3
45	KC2	7	311	27	-	6/15/71/71	-
37	LMG	d	409	-	-	17/32/52/70	0/1/1/1
43	A86	4	301	-	-	9/34/90/90	0/3/3/3
43	A86	11	304	31	-	8/34/90/90	0/3/3/3
31	CLA	19	312	43	1/1/15/20	8/39/115/115	-
31	CLA	8	308	-	1/1/14/20	9/35/111/115	-
32	PHO	A	405	-	-	13/37/103/103	0/5/6/6
33	BCR	C	515	-	-	11/29/63/63	0/2/2/2
43	A86	15	304	-	-	11/34/90/90	1/3/3/3
43	A86	8	302	-	-	11/34/90/90	0/3/3/3
43	A86	1	305	-	-	10/34/90/90	0/3/3/3
36	LHG	5	317	-	-	14/29/29/53	-
31	CLA	13	307	-	1/1/10/20	3/12/88/115	-
31	CLA	12	313	-	-	9/19/95/115	-
31	CLA	D	406	-	1/1/15/20	12/39/115/115	-
31	CLA	17	308	-	-	3/10/86/115	-
31	CLA	C	504	31	1/1/15/20	23/39/115/115	-
37	LMG	11	301	-	-	14/31/51/70	0/1/1/1
31	CLA	3	308	-	1/1/10/20	4/13/89/115	-
31	CLA	14	314	-	1/1/10/20	7/13/89/115	-
43	A86	4	304	-	-	9/34/90/90	0/3/3/3
31	CLA	1	316	43	1/1/10/20	5/12/88/115	-
42	KC1	18	313	31	-	3/15/71/71	-
31	CLA	6	311	-	1/1/10/20	3/10/86/115	-
31	CLA	19	311	43	1/1/11/20	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	KC2	3	309	-	-	10/15/71/71	-
43	A86	15	305	-	-	6/34/90/90	0/3/3/3
31	CLA	16	310	-	1/1/10/20	3/10/86/115	-
41	HEM	E	101	5,6	-	4/14/54/54	-
34	SQD	10	320	31	-	22/36/56/69	0/1/1/1
31	CLA	0	309	-	-	12/32/108/115	-
37	LMG	F	102	-	-	14/41/61/70	0/1/1/1
33	BCR	A	407	-	-	8/29/63/63	0/2/2/2
43	A86	6	302	-	-	9/34/90/90	0/3/3/3
43	A86	19	302	-	-	8/34/90/90	0/3/3/3
31	CLA	c	506	-	1/1/15/20	11/39/115/115	-
31	CLA	d	402	-	1/1/15/20	7/39/115/115	-
37	LMG	N	101	-	-	5/23/43/70	0/1/1/1
37	LMG	D	404	-	-	22/35/55/70	0/1/1/1
31	CLA	C	506	-	1/1/15/20	11/39/115/115	-
31	CLA	8	307	42	1/1/12/20	5/21/97/115	-
31	CLA	19	315	-	1/1/10/20	3/10/86/115	-
43	A86	18	302	-	-	9/34/90/90	0/3/3/3
43	A86	17	305	-	-	8/34/90/90	0/3/3/3
31	CLA	11	312	27	1/1/11/20	6/17/93/115	-
31	CLA	B	609	-	-	10/39/115/115	-
31	CLA	2	314	-	-	6/10/86/115	-
31	CLA	14	311	-	1/1/11/20	10/17/93/115	-
43	A86	P	611	-	-	7/34/90/90	1/3/3/3
43	A86	16	303	43	-	8/34/90/90	0/3/3/3
31	CLA	A	404	-	1/1/11/20	5/20/96/115	-
43	A86	2	304	-	-	6/34/90/90	1/3/3/3
43	A86	3	302	-	-	8/34/90/90	0/3/3/3
42	KC1	2	313	-	-	4/15/71/71	-
31	CLA	2	315	43	-	7/17/93/115	-
31	CLA	4	315	-	1/1/10/20	9/13/89/115	-
38	DGD	b	622	34	-	30/44/84/95	0/2/2/2
37	LMG	5	316	-	-	17/31/51/70	0/1/1/1
38	DGD	h	102	-	-	29/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	13	303	-	-	6/34/90/90	0/3/3/3
43	A86	7	303	-	-	8/34/90/90	0/3/3/3
31	CLA	b	613	-	1/1/15/20	13/39/115/115	-
42	KC1	7	314	-	-	2/15/71/71	-
43	A86	10	301	-	-	7/34/90/90	0/3/3/3
31	CLA	b	610	-	-	10/39/115/115	-
31	CLA	a	406	-	1/1/14/20	4/33/109/115	-
43	A86	18	301	-	-	5/34/90/90	0/3/3/3
31	CLA	6	314	-	1/1/10/20	5/12/88/115	-
33	BCR	B	617	-	-	11/29/63/63	0/2/2/2
31	CLA	11	315	-	1/1/10/20	4/10/86/115	-
43	A86	7	306	-	-	7/34/90/90	0/3/3/3
31	CLA	B	605	-	1/1/15/20	12/39/115/115	-
37	LMG	d	404	-	-	17/35/55/70	0/1/1/1
42	KC1	17	314	-	-	3/15/71/71	-
45	KC2	12	311	-	-	8/15/71/71	-
31	CLA	b	604	-	1/1/15/20	16/39/115/115	-
31	CLA	0	316	-	1/1/11/20	7/17/93/115	-
43	A86	12	304	-	-	7/34/90/90	0/3/3/3
31	CLA	P	601	16	1/1/15/20	21/39/115/115	-
31	CLA	6	309	-	1/1/15/20	15/39/115/115	-
43	A86	3	301	-	-	9/34/90/90	0/3/3/3
31	CLA	c	507	-	1/1/15/20	14/39/115/115	-
43	A86	6	301	43	-	9/34/90/90	0/3/3/3
37	LMG	p	614	-	-	11/26/46/70	0/1/1/1
31	CLA	B	608	-	1/1/15/20	16/39/115/115	-
31	CLA	p	603	-	1/1/12/20	7/21/97/115	-
37	LMG	j	101	-	-	29/45/65/70	0/1/1/1
31	CLA	c	513	-	1/1/15/20	16/39/115/115	-
45	KC2	6	310	-	-	10/15/71/71	-
43	A86	17	303	-	-	9/34/90/90	0/3/3/3
33	BCR	B	619	-	-	11/29/63/63	0/2/2/2
33	BCR	C	517	-	-	10/29/63/63	0/2/2/2
31	CLA	18	307	-	1/1/14/20	10/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	10	306	-	-	8/34/90/90	0/3/3/3
34	SQD	i	101	-	-	21/35/55/69	0/1/1/1
43	A86	13	301	-	-	7/34/90/90	0/3/3/3
31	CLA	P	606	-	1/1/10/20	7/13/89/115	-
31	CLA	17	310	-	1/1/11/20	5/15/91/115	-
31	CLA	4	312	27	1/1/12/20	11/23/99/115	-
31	CLA	c	511	-	1/1/15/20	18/39/115/115	-
37	LMG	C	522	-	-	24/46/66/70	0/1/1/1
43	A86	14	301	-	-	13/34/90/90	0/3/3/3
45	KC2	17	311	27	-	6/15/71/71	-
31	CLA	9	307	-	1/1/14/20	8/35/111/115	-
45	KC2	1	311	-	-	4/15/71/71	-
31	CLA	3	307	-	1/1/10/20	3/12/88/115	-
36	LHG	w	202	-	-	19/44/44/53	-
37	LMG	M	101	-	-	18/35/55/70	0/1/1/1
42	KC1	3	314	-	-	1/15/71/71	-
42	KC1	5	313	-	-	3/15/71/71	-
42	KC1	p	609	-	-	8/15/71/71	-
33	BCR	f	101	-	-	19/29/63/63	0/2/2/2
43	A86	1	320	-	-	7/34/90/90	0/3/3/3
31	CLA	11	316	43	1/1/10/20	0/10/86/115	-
31	CLA	C	505	-	1/1/15/20	9/39/115/115	-
31	CLA	p	602	-	1/1/15/20	12/39/115/115	-
31	CLA	w	203	-	1/1/15/20	15/39/115/115	-
31	CLA	Z	101	-	1/1/12/20	7/23/99/115	-
31	CLA	8	312	-	-	9/17/93/115	-
34	SQD	B	623	-	-	26/49/69/69	0/1/1/1
43	A86	4	306	-	-	8/34/90/90	1/3/3/3
33	BCR	c	517	-	-	10/29/63/63	0/2/2/2
45	KC2	4	308	-	-	4/15/71/71	-
31	CLA	C	512	3	1/1/15/20	8/39/115/115	-
43	A86	14	303	-	-	9/34/90/90	0/3/3/3
31	CLA	19	310	-	1/1/15/20	13/39/115/115	-
31	CLA	p	601	16	1/1/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	P	602	-	1/1/15/20	12/39/115/115	-
31	CLA	P	608	-	1/1/12/20	7/23/99/115	-
31	CLA	10	313	26	1/1/10/20	4/12/88/115	-
43	A86	6	305	43	-	8/34/90/90	0/3/3/3
43	A86	13	302	-	-	8/34/90/90	0/3/3/3
36	LHG	d	408	-	-	29/53/53/53	-
45	KC2	0	310	-	-	8/15/71/71	-
31	CLA	z	101	-	1/1/12/20	7/23/99/115	-
31	CLA	0	311	-	1/1/13/20	6/27/103/115	-
43	A86	10	305	-	-	9/34/90/90	0/3/3/3
36	LHG	P	615	-	-	14/31/31/53	-
43	A86	14	305	-	-	6/34/90/90	1/3/3/3
43	A86	18	305	-	-	11/34/90/90	0/3/3/3
43	A86	5	303	-	-	8/34/90/90	0/3/3/3
43	A86	1	319	-	-	7/34/90/90	0/3/3/3
31	CLA	5	314	-	1/1/10/20	0/10/86/115	-
31	CLA	16	312	-	1/1/11/20	8/18/94/115	-
43	A86	3	305	-	-	10/34/90/90	0/3/3/3
31	CLA	7	313	-	1/1/12/20	7/21/97/115	-
31	CLA	19	313	-	1/1/15/20	13/39/115/115	-
31	CLA	6	313	-	1/1/11/20	7/18/94/115	-
35	PL9	a	409	-	-	16/27/47/73	0/1/1/1
31	CLA	10	316	-	1/1/11/20	6/17/93/115	-
31	CLA	c	503	31	1/1/15/20	13/39/115/115	-
43	A86	5	304	-	-	11/34/90/90	0/3/3/3
31	CLA	14	315	-	1/1/10/20	8/13/89/115	-
33	BCR	B	618	-	-	9/29/63/63	0/2/2/2
37	LMG	K	101	-	-	23/41/61/70	0/1/1/1
43	A86	0	304	-	-	6/34/90/90	0/3/3/3
31	CLA	5	312	-	-	6/18/94/115	-
43	A86	11	303	-	-	9/34/90/90	0/3/3/3
41	HEM	V	201	21	-	7/14/54/54	-
45	KC2	11	311	-	-	4/15/71/71	-
31	CLA	z	103	-	1/1/11/20	4/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	10	318	-	-	8/34/90/90	0/3/3/3
45	KC2	16	309	-	-	10/15/71/71	-
31	CLA	c	512	3	1/1/15/20	8/39/115/115	-
36	LHG	A	410	-	-	16/41/41/53	-
45	KC2	18	310	27	-	8/15/71/71	-
31	CLA	18	311	-	-	7/17/93/115	-
31	CLA	12	308	-	1/1/15/20	16/39/115/115	-
31	CLA	B	604	-	1/1/15/20	13/39/115/115	-
43	A86	0	302	-	-	8/34/90/90	0/3/3/3
45	KC2	6	312	27	-	6/15/71/71	-
45	KC2	10	310	-	-	8/15/71/71	-
31	CLA	B	601	-	1/1/15/20	19/39/115/115	-
31	CLA	b	603	-	1/1/15/20	14/39/115/115	-
36	LHG	B	622	-	-	14/47/47/53	-
31	CLA	B	616	-	1/1/15/20	14/39/115/115	-
37	LMG	b	621	-	-	26/46/66/70	0/1/1/1
31	CLA	17	315	-	1/1/10/20	6/10/86/115	-
31	CLA	5	307	-	1/1/15/20	13/39/115/115	-
31	CLA	12	307	-	1/1/10/20	2/12/88/115	-
42	KC1	14	313	27	-	9/15/71/71	-
42	KC1	9	314	-	-	5/15/71/71	-
43	A86	16	302	-	-	9/34/90/90	0/3/3/3
43	A86	12	302	-	-	7/34/90/90	0/3/3/3
31	CLA	c	502	-	1/1/15/20	12/39/115/115	-
43	A86	15	303	-	-	8/34/90/90	0/3/3/3
36	LHG	z	102	-	-	16/29/29/53	-
43	A86	16	301	43	-	10/34/90/90	0/3/3/3
38	DGD	W	203	-	-	29/45/85/95	0/2/2/2
31	CLA	7	312	-	1/1/11/20	11/18/94/115	-
31	CLA	7	310	-	1/1/11/20	5/15/91/115	-
41	HEM	e	101	5,6	-	4/14/54/54	-
36	LHG	D	408	-	-	29/53/53/53	-
43	A86	11	319	-	-	6/34/90/90	0/3/3/3
34	SQD	l	101	-	-	25/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	2	303	-	-	7/34/90/90	0/3/3/3
42	KC1	6	315	-	-	1/15/71/71	-
43	A86	17	306	-	-	8/34/90/90	0/3/3/3
31	CLA	b	602	-	1/1/15/20	19/39/115/115	-
31	CLA	d	405	-	1/1/15/20	12/39/115/115	-
31	CLA	P	604	-	1/1/11/20	5/19/95/115	-
31	CLA	B	614	-	1/1/15/20	18/39/115/115	-
31	CLA	1	308	-	-	13/39/115/115	-
38	DGD	c	519	-	-	28/51/91/95	0/2/2/2
31	CLA	4	309	-	1/1/15/20	17/39/115/115	-
43	A86	17	304	-	-	8/34/90/90	0/3/3/3
31	CLA	B	602	-	1/1/15/20	14/39/115/115	-
31	CLA	1	307	-	1/1/10/20	2/13/89/115	-
31	CLA	9	311	43	1/1/11/20	8/17/93/115	-
31	CLA	b	614	-	1/1/15/20	8/39/115/115	-
31	CLA	10	311	-	1/1/13/20	6/27/103/115	-
37	LMG	5	315	-	-	16/32/52/70	0/1/1/1
37	LMG	c	521	-	-	24/46/66/70	0/1/1/1
34	SQD	A	411	-	-	22/35/55/69	0/1/1/1
36	LHG	l	102	-	-	22/53/53/53	-
33	BCR	c	516	-	-	9/29/63/63	0/2/2/2
43	A86	12	305	-	-	8/34/90/90	0/3/3/3
37	LMG	14	316	-	-	24/44/64/70	0/1/1/1
37	LMG	D	409	-	-	17/32/52/70	0/1/1/1
37	LMG	15	315	-	-	18/31/51/70	0/1/1/1
43	A86	12	303	-	-	7/34/90/90	0/3/3/3
43	A86	17	302	-	-	6/34/90/90	0/3/3/3
33	BCR	F	101	-	-	19/29/63/63	0/2/2/2
42	KC1	8	314	43,31	-	2/15/71/71	-
31	CLA	10	312	34,26	1/1/11/20	5/17/93/115	-
31	CLA	B	603	-	1/1/15/20	17/39/115/115	-
31	CLA	11	310	-	1/1/12/20	5/21/97/115	-
31	CLA	13	310	-	1/1/10/20	4/10/86/115	-
43	A86	7	301	-	-	5/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	8	306	-	-	8/34/90/90	0/3/3/3
33	BCR	c	515	-	-	11/29/63/63	0/2/2/2
34	SQD	8	301	31	-	21/36/56/69	0/1/1/1
36	LHG	15	316	-	-	14/29/29/53	-
31	CLA	p	607	43	1/1/10/20	5/13/89/115	-
31	CLA	4	311	-	1/1/11/20	8/17/93/115	-
31	CLA	11	308	-	1/1/15/20	19/39/115/115	-
45	KC2	11	309	-	-	10/15/71/71	-
31	CLA	b	607	-	1/1/15/20	12/39/115/115	-
31	CLA	r	101	-	1/1/11/20	6/18/94/115	-
42	KC1	12	314	-	-	3/15/71/71	-
43	A86	6	303	-	-	9/34/90/90	0/3/3/3
31	CLA	18	306	42	1/1/12/20	7/21/97/115	-
31	CLA	5	311	-	1/1/11/20	3/15/91/115	-
38	DGD	C	520	34	-	32/51/91/95	0/2/2/2
38	DGD	1	318	-	-	27/43/83/95	0/2/2/2
31	CLA	15	306	-	1/1/10/20	4/12/88/115	-
43	A86	19	305	-	-	9/34/90/90	0/3/3/3
31	CLA	11	307	-	1/1/10/20	4/13/89/115	-
31	CLA	d	406	-	1/1/15/20	12/39/115/115	-
43	A86	6	304	-	-	7/34/90/90	0/3/3/3
43	A86	9	301	-	-	9/34/90/90	0/3/3/3
37	LMG	J	101	-	-	29/45/65/70	0/1/1/1
31	CLA	C	511	-	1/1/15/20	18/39/115/115	-
43	A86	11	305	-	-	9/34/90/90	0/3/3/3
33	BCR	b	619	-	-	9/29/63/63	0/2/2/2
43	A86	9	303	-	-	8/34/90/90	0/3/3/3
45	KC2	15	308	-	-	6/15/71/71	-
44	DD6	P	612	-	-	7/26/80/80	0/3/3/3
31	CLA	12	310	-	1/1/10/20	6/13/89/115	-
31	CLA	2	311	-	-	6/15/91/115	-
45	KC2	9	309	-	-	5/15/71/71	-
37	LMG	w	201	-	-	24/43/63/70	0/1/1/1
43	A86	16	305	43	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	9	306	-	-	8/34/90/90	0/3/3/3
37	LMG	n	701	-	-	6/23/43/70	0/1/1/1
36	LHG	18	315	-	-	21/43/43/53	-
31	CLA	9	312	43	1/1/15/20	6/39/115/115	-
31	CLA	15	309	-	1/1/13/20	10/27/103/115	-
45	KC2	1	309	-	-	9/15/71/71	-
31	CLA	14	306	-	1/1/14/20	11/35/111/115	-
31	CLA	17	312	-	1/1/11/20	7/18/94/115	-
31	CLA	14	307	-	1/1/15/20	15/39/115/115	-
45	KC2	7	309	-	-	10/15/71/71	-
45	KC2	18	308	-	-	10/15/71/71	-
31	CLA	C	514	-	1/1/11/20	4/20/96/115	-
34	SQD	L	102	-	-	22/49/69/69	0/1/1/1
38	DGD	H	102	-	-	29/51/91/95	0/2/2/2
38	DGD	c	518	-	-	22/44/84/95	0/2/2/2
31	CLA	b	616	-	1/1/15/20	7/39/115/115	-
37	LMG	1	301	-	-	14/31/51/70	0/1/1/1

The worst 5 of 4536 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	18	301	A86	C20-C15	10.22	1.61	1.48
43	2	302	A86	C20-C15	9.64	1.60	1.48
43	12	301	A86	C20-C15	9.49	1.60	1.48
43	2	304	A86	C20-C15	9.40	1.60	1.48
43	9	301	A86	C20-C15	9.17	1.60	1.48

The worst 5 of 8283 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	17	316	A86	C29-C30-C31	-26.83	146.00	177.66
43	16	303	A86	O1-C20-C19	-26.45	88.70	113.49
43	4	305	A86	C29-C30-C31	-25.48	147.59	177.66
42	8	314	KC1	CMD-C2D-C1D	-23.93	88.98	125.42
43	9	301	A86	C29-C30-C31	-23.57	149.85	177.66

5 of 204 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	A	403	CLA	ND
31	A	404	CLA	ND
31	A	406	CLA	ND
31	B	601	CLA	ND
31	B	602	CLA	ND

5 of 5457 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	A	403	CLA	CBD-CGD-O2D-CED
31	B	601	CLA	C1A-C2A-CAA-CBA
31	B	601	CLA	C3A-C2A-CAA-CBA
31	B	601	CLA	CAD-CBD-CGD-O1D
31	B	601	CLA	CAD-CBD-CGD-O2D

5 of 9 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	14	305	A86	C31-C32-C33-C34-C35-C36
43	p	613	A86	C31-C32-C33-C34-C35-C36
43	P	613	A86	C31-C32-C33-C34-C35-C36
43	2	304	A86	C31-C32-C33-C34-C35-C36
43	4	306	A86	C31-C32-C33-C34-C35-C36

332 monomers are involved in 729 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	0	314	CLA	1	0
31	C	503	CLA	6	0
31	7	307	CLA	4	0
31	19	307	CLA	1	0
31	11	313	CLA	4	0
33	y	101	BCR	5	0
31	18	312	CLA	1	0
32	a	405	PHO	4	0
33	b	618	BCR	2	0
36	a	410	LHG	1	0
31	14	309	CLA	1	0
37	k	101	LMG	4	0
31	2	306	CLA	5	0
31	b	612	CLA	3	0
31	3	316	CLA	2	0
31	C	509	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	19	308	CLA	4	0
45	8	309	KC2	1	0
31	1	313	CLA	8	0
35	D	407	PL9	4	0
34	a	408	SQD	3	0
43	5	301	A86	1	0
31	a	403	CLA	6	0
36	C	521	LHG	1	0
31	5	306	CLA	3	0
36	18	316	LHG	3	0
45	2	308	KC2	1	0
31	0	313	CLA	1	0
31	b	611	CLA	2	0
36	p	615	LHG	1	0
31	9	310	CLA	2	0
38	C	519	DGD	5	0
37	W	201	LMG	3	0
31	2	312	CLA	3	0
31	1	321	CLA	3	0
31	10	314	CLA	1	0
38	B	621	DGD	6	0
31	13	316	CLA	3	0
45	5	308	KC2	1	0
31	D	402	CLA	4	0
36	L	101	LHG	5	0
43	13	306	A86	1	0
31	C	510	CLA	2	0
37	B	620	LMG	3	0
43	0	301	A86	1	0
41	v	201	HEM	3	0
31	14	312	CLA	3	0
43	1	306	A86	1	0
31	C	508	CLA	1	0
31	15	312	CLA	4	0
31	0	308	CLA	3	0
31	1	312	CLA	1	0
31	3	310	CLA	1	0
31	8	310	CLA	1	0
31	4	314	CLA	1	0
43	11	302	A86	1	0
45	19	309	KC2	1	0
31	c	504	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	4	303	A86	2	0
42	4	313	KC1	1	0
31	B	607	CLA	4	0
31	1	315	CLA	1	0
34	A	408	SQD	3	0
40	D	401	BCT	1	0
33	C	516	BCR	2	0
31	12	312	CLA	1	0
31	c	508	CLA	1	0
31	B	606	CLA	5	0
31	C	502	CLA	4	0
32	D	403	PHO	2	0
31	16	308	CLA	1	0
43	15	301	A86	1	0
31	17	313	CLA	2	0
31	3	313	CLA	5	0
31	b	617	CLA	3	0
31	2	309	CLA	2	0
31	16	315	CLA	1	0
33	a	407	BCR	2	0
31	B	615	CLA	5	0
35	A	409	PL9	1	0
37	10	319	LMG	2	0
31	18	309	CLA	3	0
43	18	303	A86	5	0
31	b	609	CLA	2	0
43	5	302	A86	1	0
31	D	405	CLA	7	0
31	p	606	CLA	4	0
31	C	507	CLA	3	0
31	1	310	CLA	2	0
31	5	309	CLA	1	0
34	b	601	SQD	9	0
31	B	610	CLA	3	0
31	6	308	CLA	5	0
31	B	611	CLA	3	0
31	b	606	CLA	2	0
31	B	612	CLA	2	0
38	c	520	DGD	2	0
31	7	308	CLA	2	0
31	b	615	CLA	4	0
31	16	313	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	b	620	BCR	3	0
43	P	613	A86	1	0
37	0	317	LMG	2	0
31	16	307	CLA	2	0
33	Y	101	BCR	6	0
43	9	305	A86	2	0
31	15	311	CLA	2	0
31	b	608	CLA	5	0
31	a	404	CLA	2	0
31	10	308	CLA	2	0
31	R	101	CLA	1	0
37	4	316	LMG	5	0
31	W	202	CLA	3	0
37	11	317	LMG	4	0
37	P	614	LMG	1	0
38	11	318	DGD	2	0
31	13	313	CLA	2	0
43	p	613	A86	1	0
31	c	510	CLA	3	0
44	p	612	DD6	3	0
38	C	518	DGD	1	0
31	6	316	CLA	1	0
33	h	101	BCR	4	0
36	4	317	LHG	3	0
31	2	307	CLA	3	0
31	10	317	CLA	3	0
32	d	403	PHO	3	0
31	c	505	CLA	6	0
31	9	308	CLA	3	0
37	f	102	LMG	5	0
31	A	406	CLA	1	0
36	8	316	LHG	1	0
37	1	317	LMG	2	0
37	m	101	LMG	3	0
43	5	305	A86	1	0
43	1	303	A86	1	0
31	13	312	CLA	2	0
31	b	605	CLA	4	0
33	H	101	BCR	3	0
35	d	407	PL9	5	0
31	15	307	CLA	4	0
31	p	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	14	317	LHG	2	0
36	8	317	LHG	1	0
45	17	309	KC2	1	0
43	14	302	A86	1	0
31	c	509	CLA	3	0
31	17	307	CLA	3	0
31	A	403	CLA	6	0
37	d	409	LMG	2	0
31	19	312	CLA	2	0
31	8	308	CLA	4	0
32	A	405	PHO	4	0
33	C	515	BCR	1	0
43	15	304	A86	1	0
31	13	307	CLA	1	0
31	12	313	CLA	1	0
31	D	406	CLA	3	0
31	17	308	CLA	2	0
31	C	504	CLA	7	0
37	11	301	LMG	1	0
31	3	308	CLA	2	0
31	14	314	CLA	1	0
43	4	304	A86	1	0
31	1	316	CLA	1	0
31	6	311	CLA	1	0
45	3	309	KC2	1	0
43	15	305	A86	1	0
31	16	310	CLA	1	0
41	E	101	HEM	2	0
34	10	320	SQD	1	0
31	0	309	CLA	1	0
37	F	102	LMG	4	0
33	A	407	BCR	3	0
31	c	506	CLA	2	0
31	d	402	CLA	5	0
37	N	101	LMG	1	0
31	C	506	CLA	1	0
31	8	307	CLA	2	0
43	18	302	A86	1	0
31	11	312	CLA	2	0
31	B	609	CLA	2	0
31	14	311	CLA	1	0
43	16	303	A86	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	404	CLA	2	0
31	2	315	CLA	4	0
38	b	622	DGD	12	0
37	5	316	LMG	3	0
38	h	102	DGD	4	0
31	b	613	CLA	2	0
43	10	301	A86	1	0
31	b	610	CLA	1	0
31	a	406	CLA	1	0
31	6	314	CLA	2	0
33	B	617	BCR	5	0
31	11	315	CLA	2	0
31	B	605	CLA	1	0
37	d	404	LMG	2	0
31	b	604	CLA	3	0
40	d	401	BCT	1	0
31	P	601	CLA	3	0
31	6	309	CLA	2	0
31	c	507	CLA	3	0
37	p	614	LMG	2	0
31	B	608	CLA	1	0
37	j	101	LMG	4	0
45	6	310	KC2	1	0
43	17	303	A86	1	0
33	B	619	BCR	2	0
31	18	307	CLA	2	0
34	i	101	SQD	2	0
43	13	301	A86	1	0
31	P	606	CLA	4	0
31	4	312	CLA	5	0
31	c	511	CLA	3	0
37	C	522	LMG	3	0
43	14	301	A86	4	0
31	9	307	CLA	1	0
31	3	307	CLA	3	0
36	w	202	LHG	1	0
37	M	101	LMG	6	0
33	f	101	BCR	3	0
31	11	316	CLA	1	0
31	C	505	CLA	4	0
31	p	602	CLA	4	0
31	w	203	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	Z	101	CLA	1	0
31	8	312	CLA	4	0
34	B	623	SQD	7	0
33	c	517	BCR	3	0
45	4	308	KC2	1	0
31	C	512	CLA	2	0
43	14	303	A86	1	0
31	19	310	CLA	1	0
31	p	601	CLA	1	0
31	P	602	CLA	2	0
31	10	313	CLA	2	0
36	d	408	LHG	5	0
31	z	101	CLA	2	0
31	0	311	CLA	1	0
36	P	615	LHG	1	0
43	18	305	A86	4	0
43	5	303	A86	1	0
31	5	314	CLA	1	0
31	7	313	CLA	4	0
31	19	313	CLA	1	0
31	6	313	CLA	1	0
35	a	409	PL9	2	0
31	c	503	CLA	6	0
43	5	304	A86	1	0
33	B	618	BCR	3	0
37	K	101	LMG	6	0
31	5	312	CLA	3	0
41	V	201	HEM	4	0
31	z	103	CLA	1	0
45	16	309	KC2	1	0
31	c	512	CLA	2	0
36	A	410	LHG	1	0
31	18	311	CLA	3	0
31	12	308	CLA	1	0
31	B	604	CLA	3	0
45	10	310	KC2	1	0
31	B	601	CLA	1	0
31	b	603	CLA	6	0
36	B	622	LHG	1	0
31	B	616	CLA	2	0
37	b	621	LMG	2	0
31	5	307	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	12	307	CLA	2	0
31	c	502	CLA	4	0
43	15	303	A86	1	0
31	7	312	CLA	2	0
41	e	101	HEM	2	0
36	D	408	LHG	5	0
34	l	101	SQD	6	0
31	b	602	CLA	2	0
31	d	405	CLA	8	0
31	P	604	CLA	1	0
31	B	614	CLA	4	0
31	1	308	CLA	7	0
38	c	519	DGD	3	0
31	4	309	CLA	1	0
31	B	602	CLA	7	0
31	1	307	CLA	1	0
37	5	315	LMG	2	0
37	c	521	LMG	2	0
34	A	411	SQD	2	0
36	l	102	LHG	5	0
33	c	516	BCR	1	0
37	14	316	LMG	5	0
37	D	409	LMG	1	0
37	15	315	LMG	4	0
43	17	302	A86	1	0
33	F	101	BCR	2	0
42	8	314	KC1	1	0
31	B	603	CLA	3	0
31	11	310	CLA	2	0
31	13	310	CLA	2	0
43	7	301	A86	1	0
33	c	515	BCR	1	0
34	8	301	SQD	2	0
31	4	311	CLA	1	0
31	11	308	CLA	2	0
31	b	607	CLA	4	0
43	6	303	A86	1	0
31	18	306	CLA	3	0
31	5	311	CLA	2	0
38	C	520	DGD	2	0
38	1	318	DGD	2	0
31	15	306	CLA	5	0

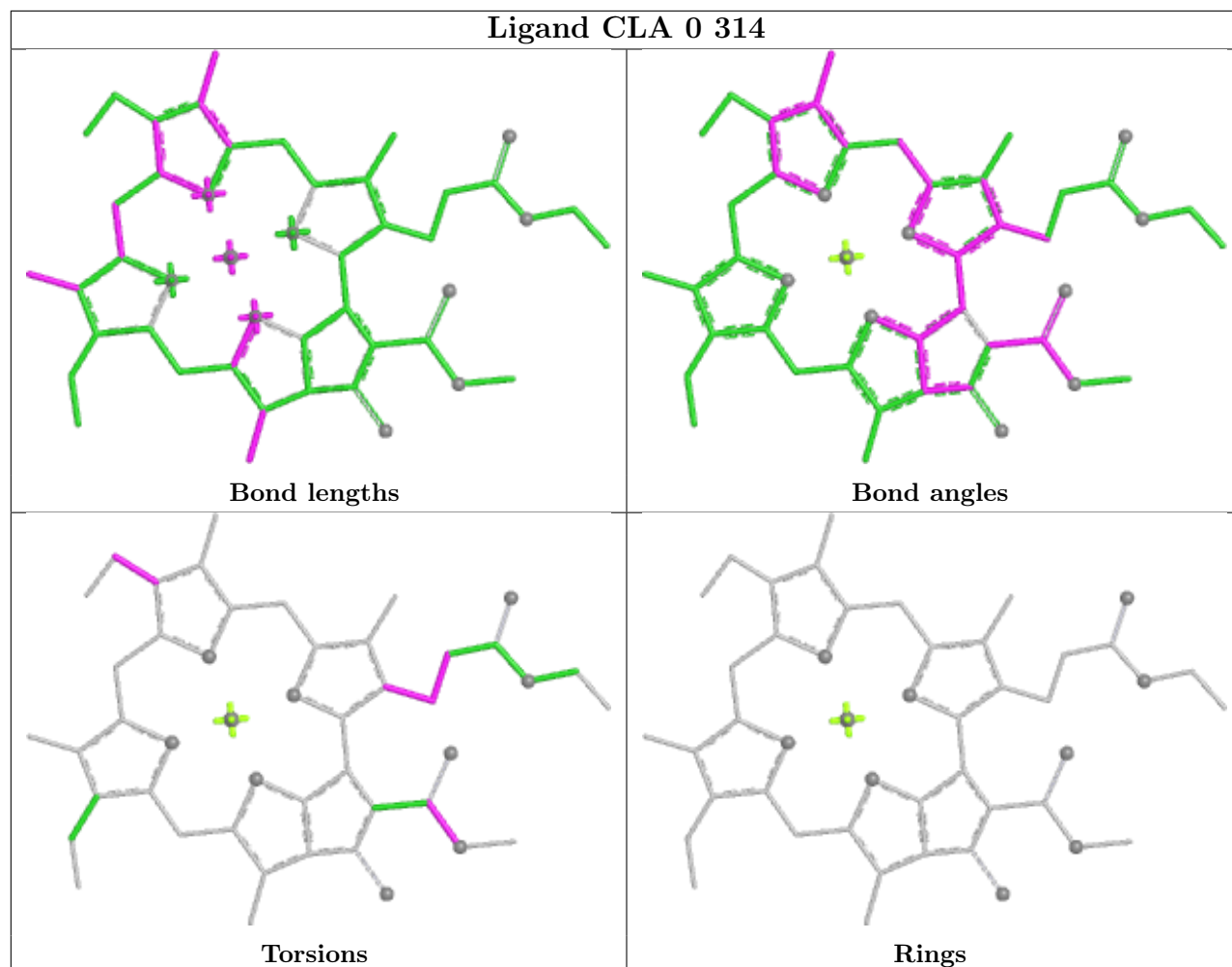
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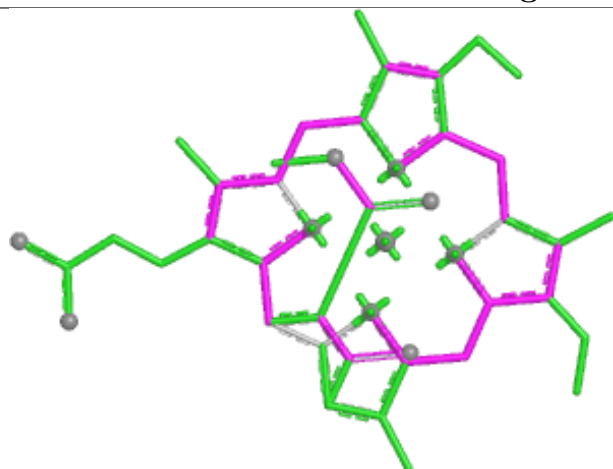
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	19	305	A86	2	0
31	11	307	CLA	2	0
31	d	406	CLA	1	0
37	J	101	LMG	6	0
31	C	511	CLA	3	0
33	b	619	BCR	2	0
45	15	308	KC2	1	0
44	P	612	DD6	1	0
31	12	310	CLA	3	0
45	9	309	KC2	1	0
37	w	201	LMG	4	0
37	n	701	LMG	1	0
36	18	315	LHG	1	0
31	9	312	CLA	1	0
31	14	306	CLA	4	0
45	7	309	KC2	1	0
45	18	308	KC2	1	0
34	L	102	SQD	4	0
38	H	102	DGD	4	0
38	c	518	DGD	1	0
31	b	616	CLA	5	0
37	1	301	LMG	2	0

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

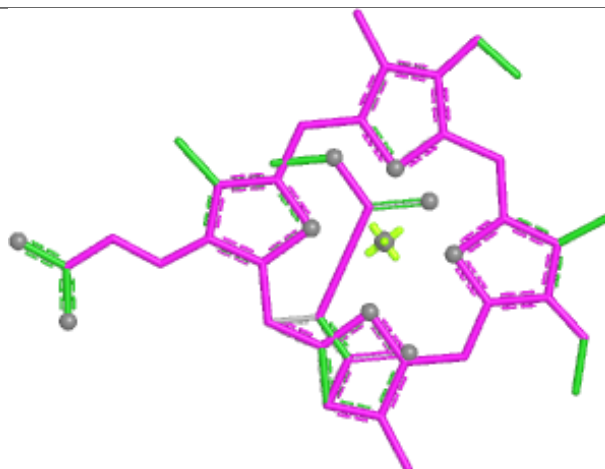
Ligand CLA 0 314



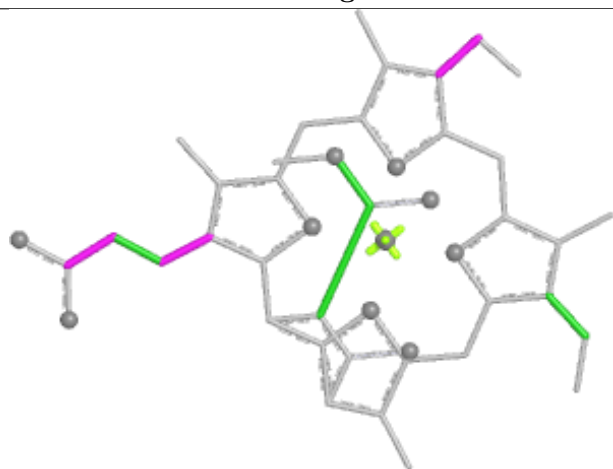
Ligand KC1 1 314



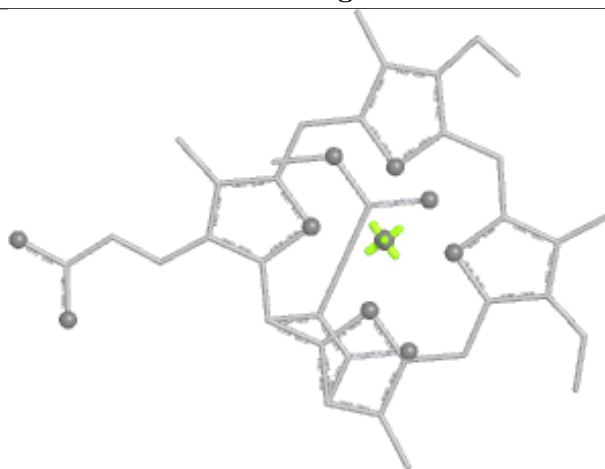
Bond lengths



Bond angles

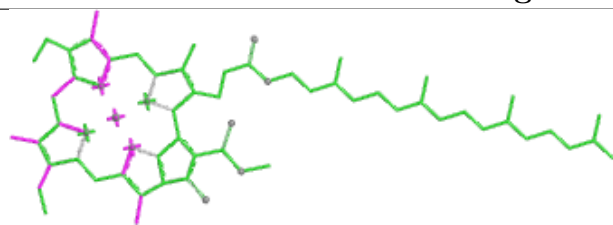


Torsions

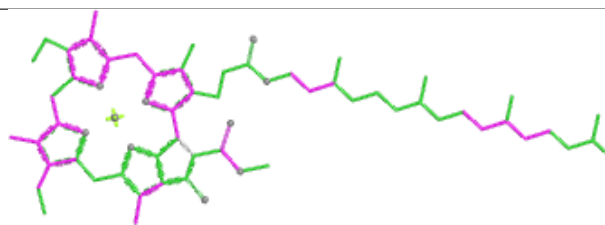


Rings

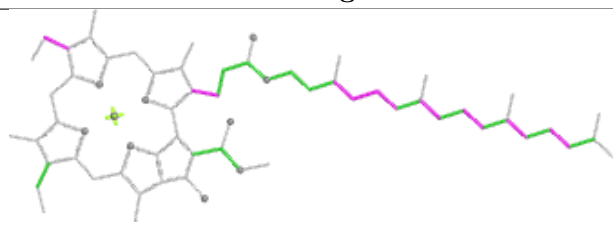
Ligand CLA C 503



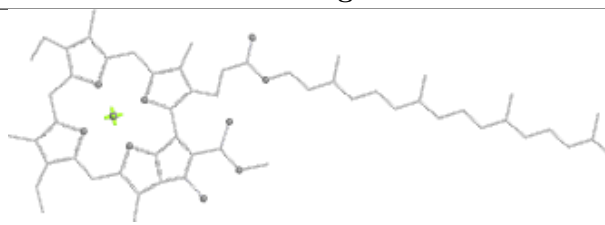
Bond lengths



Bond angles

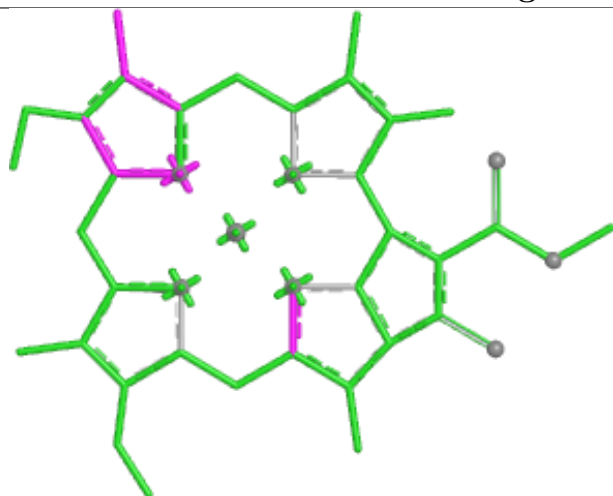


Torsions

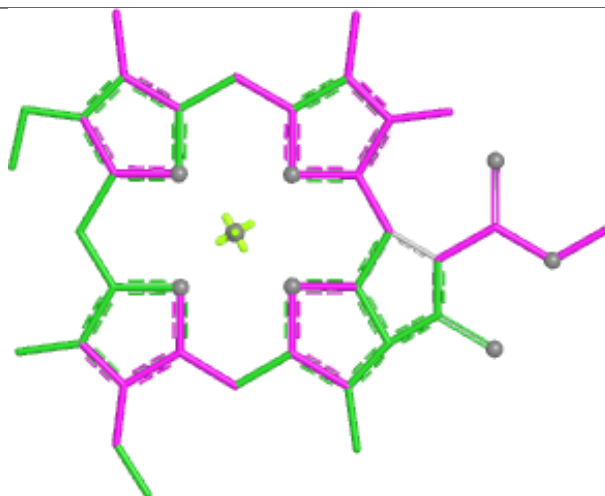


Rings

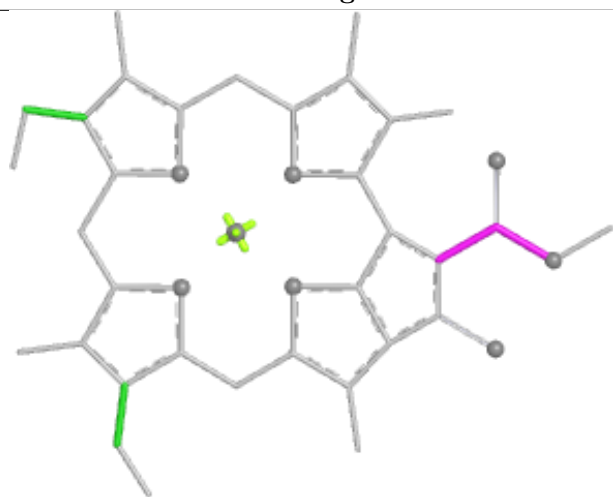
Ligand CLA 7 307



Bond lengths



Bond angles

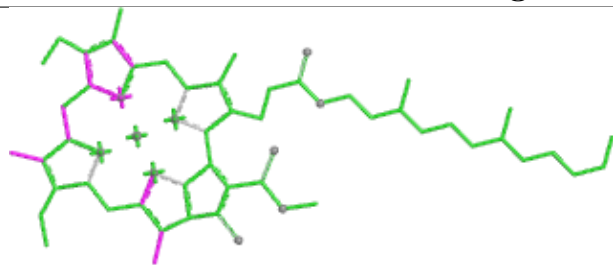


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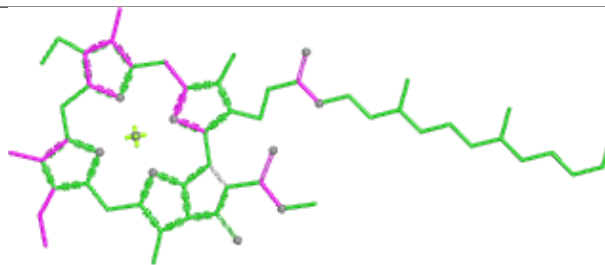


Rings

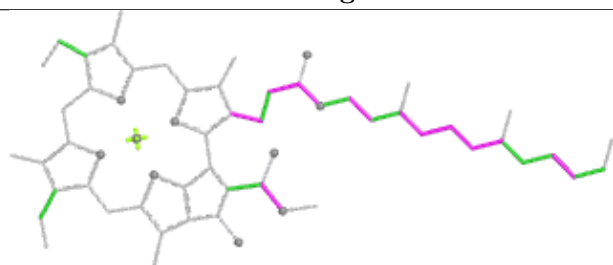
Ligand CLA 10 309



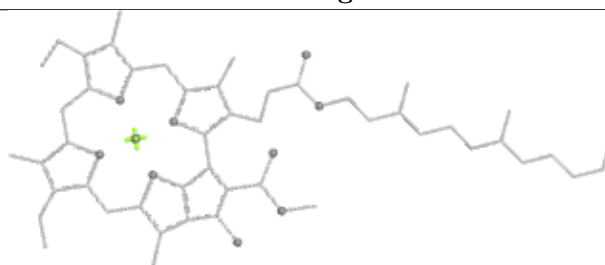
Bond lengths



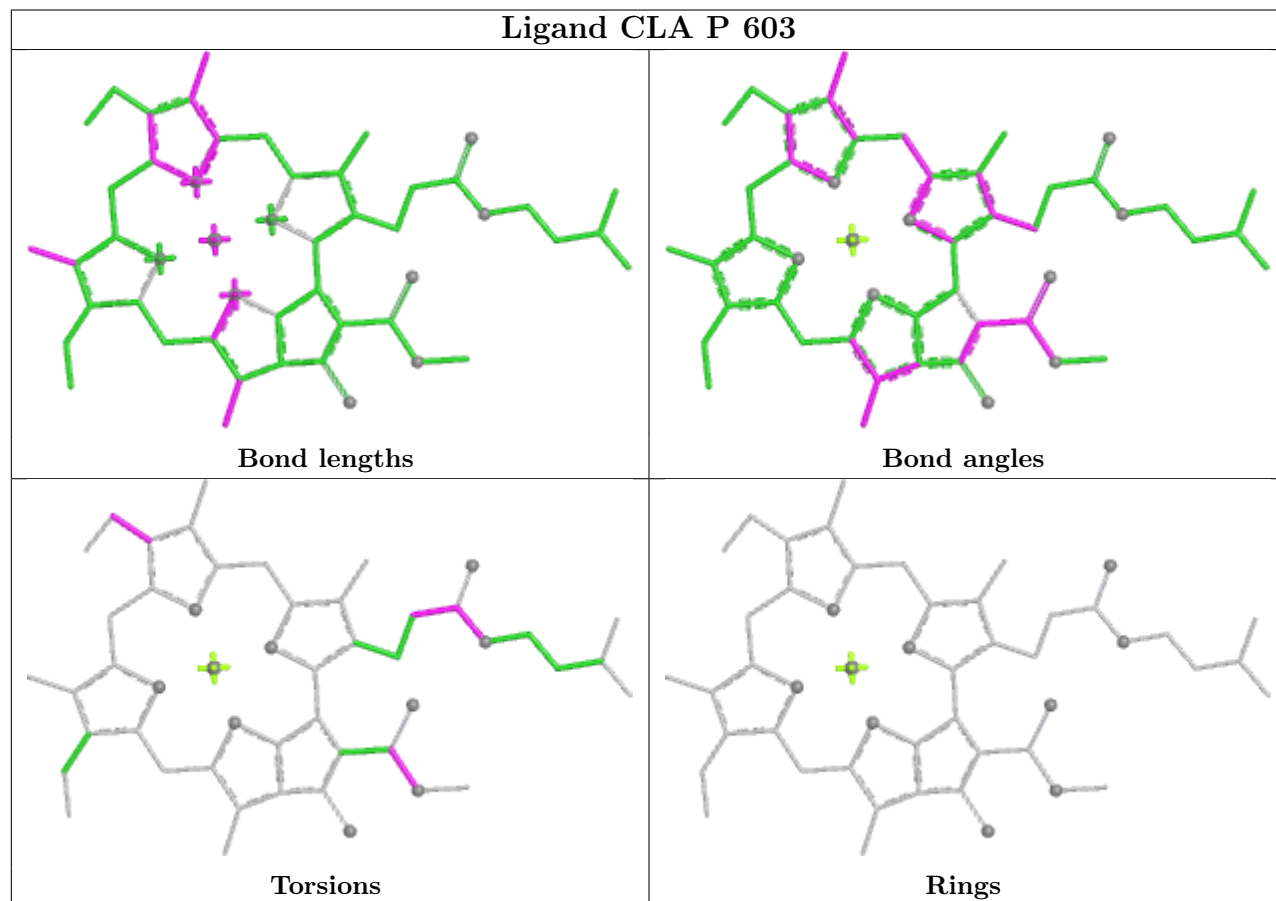
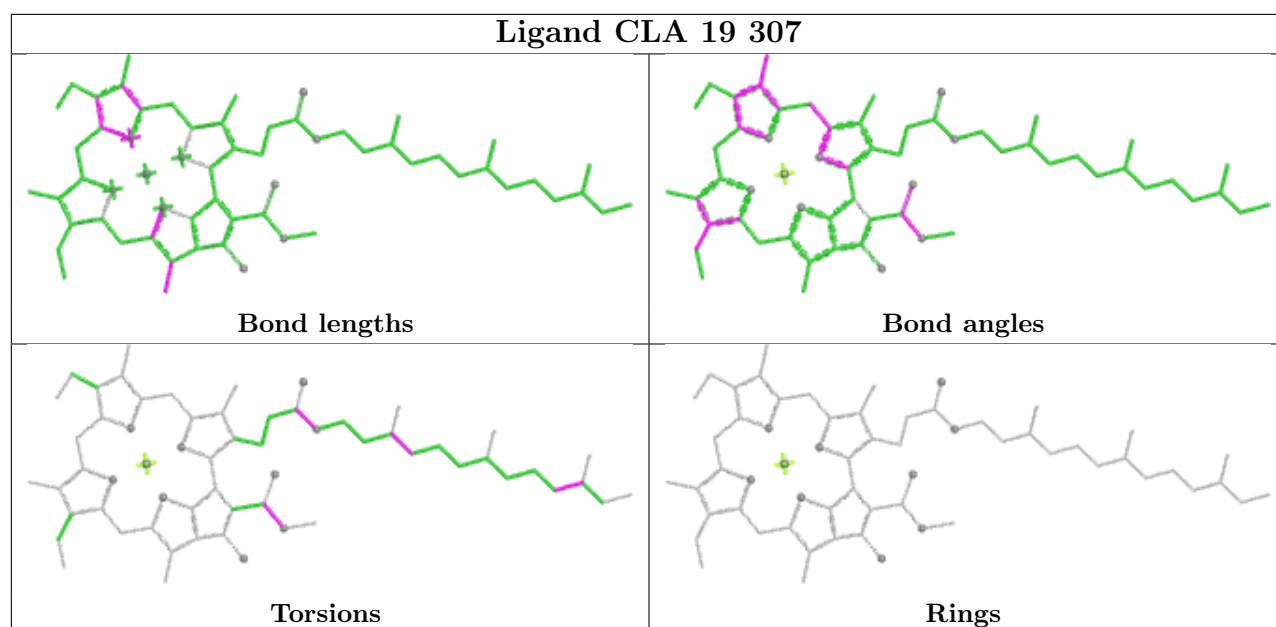
Bond angles

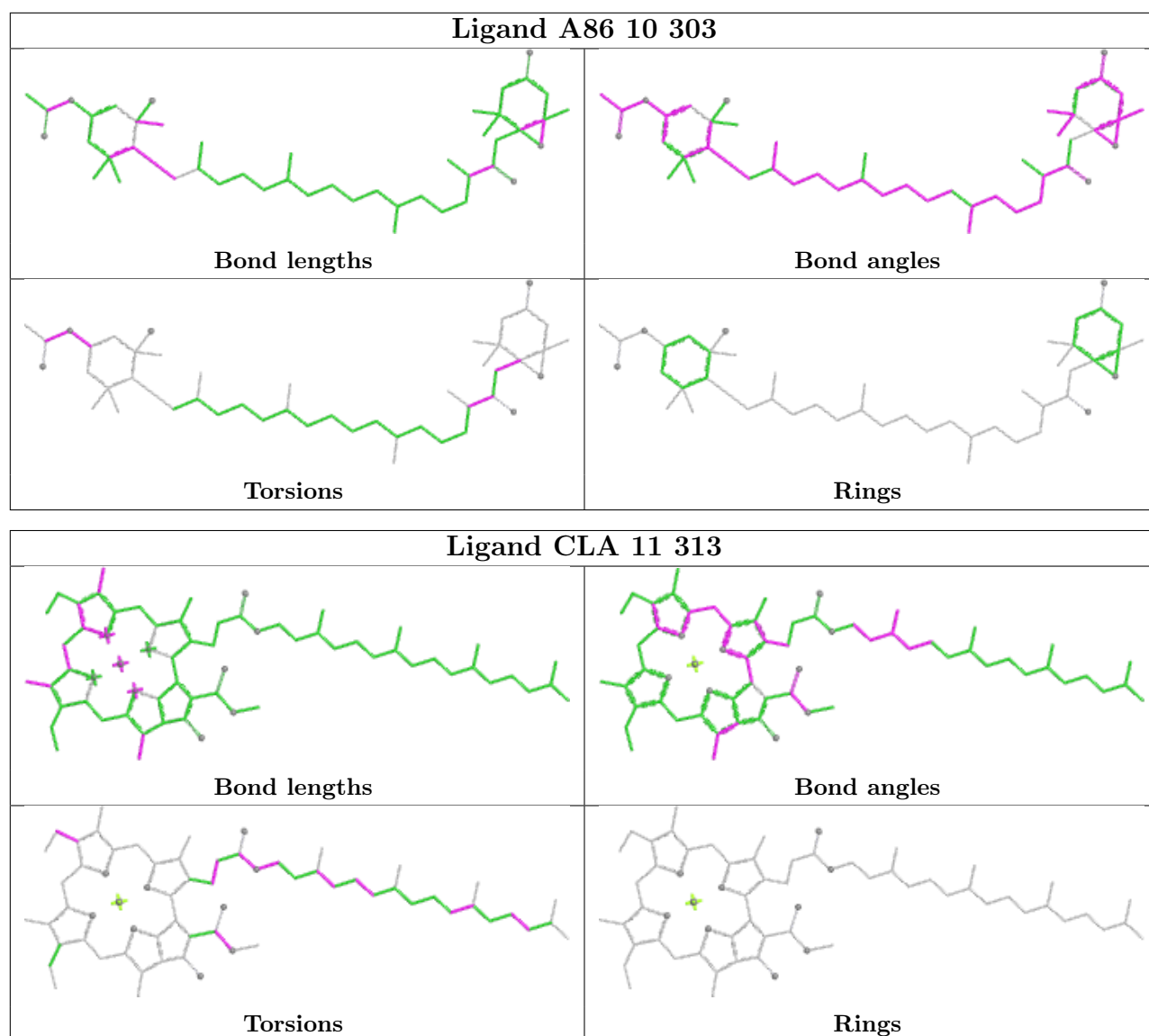


Torsions

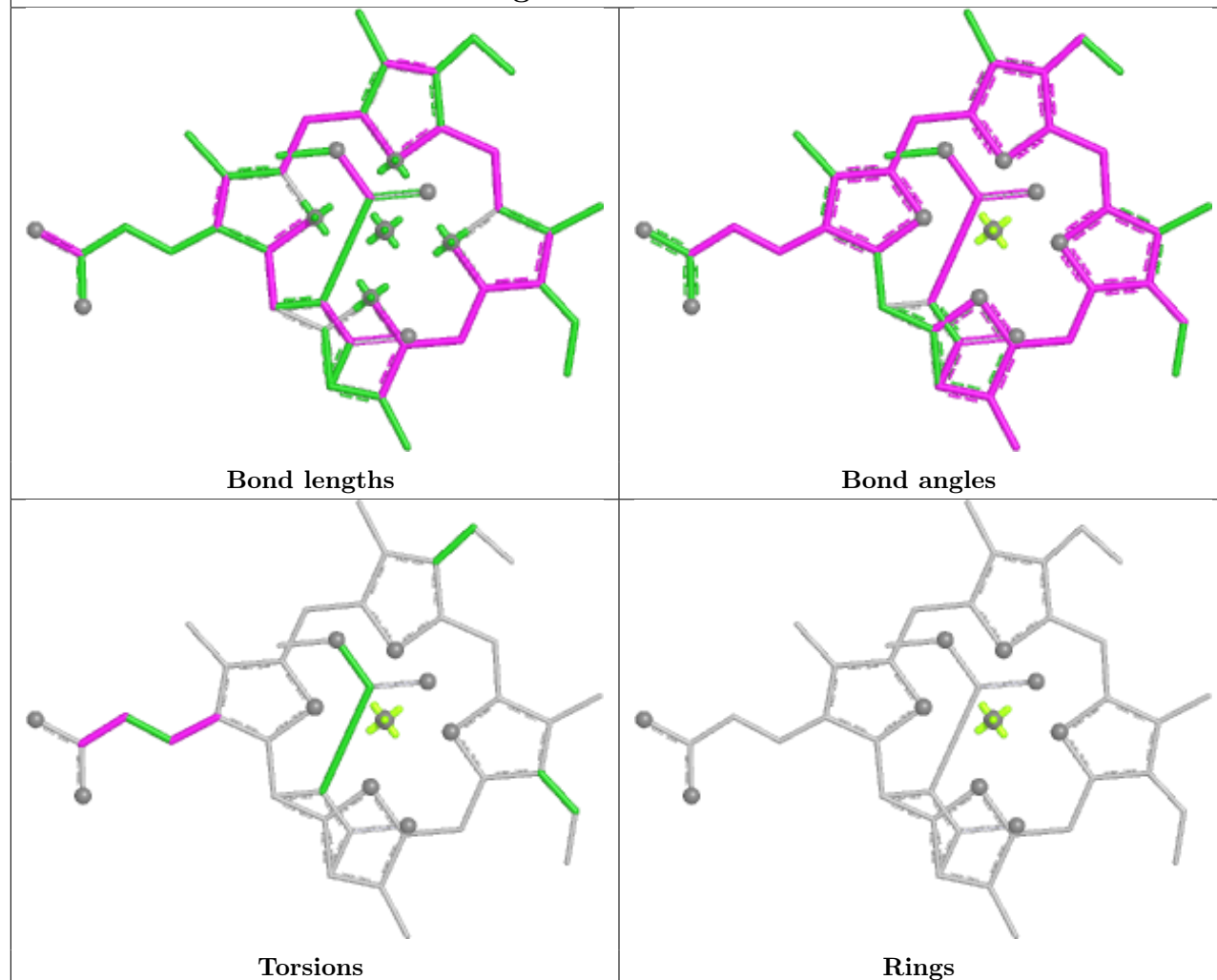


Rings

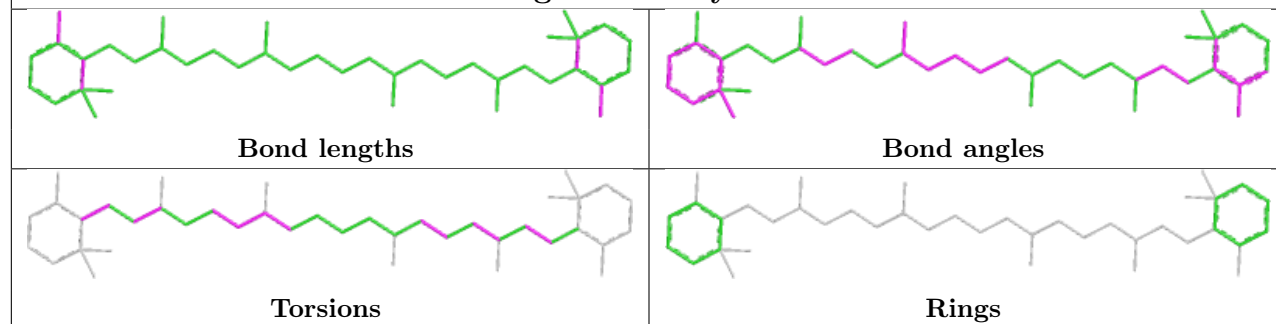


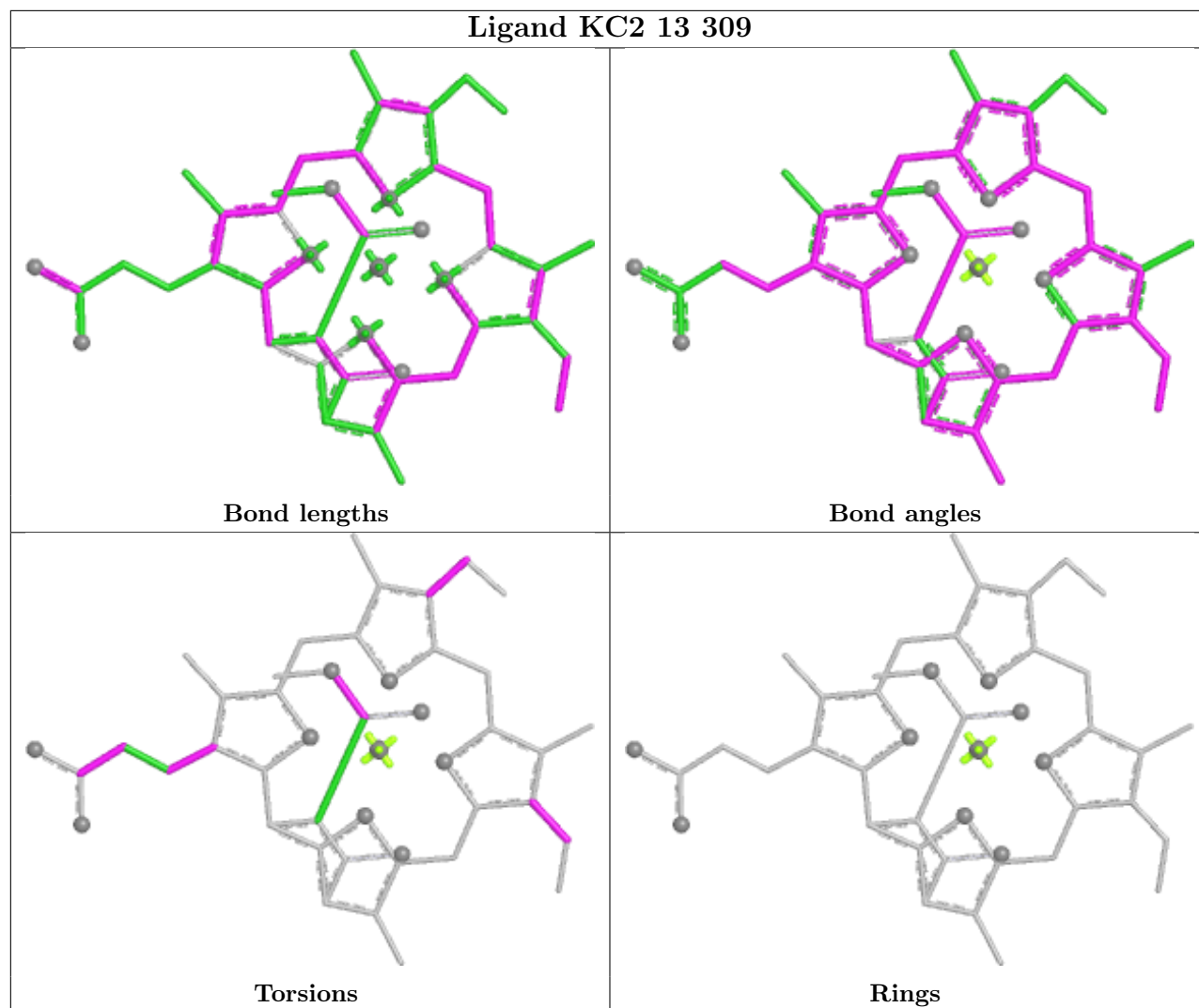


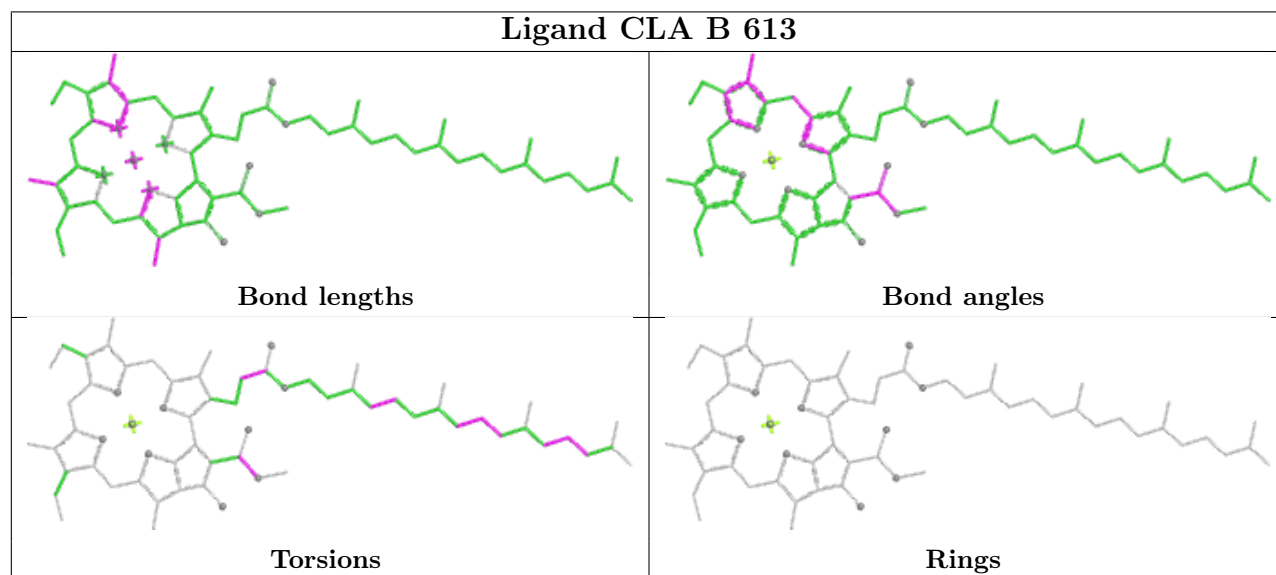
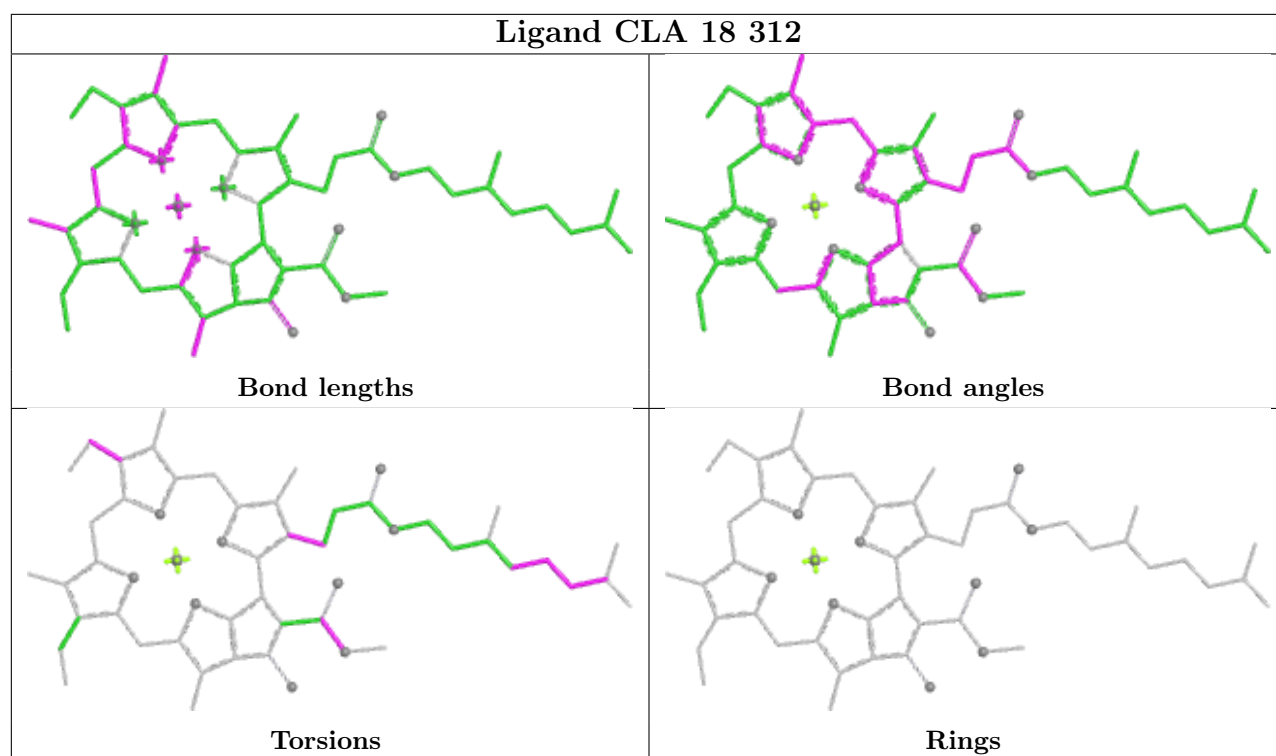
Ligand KC1 0 315



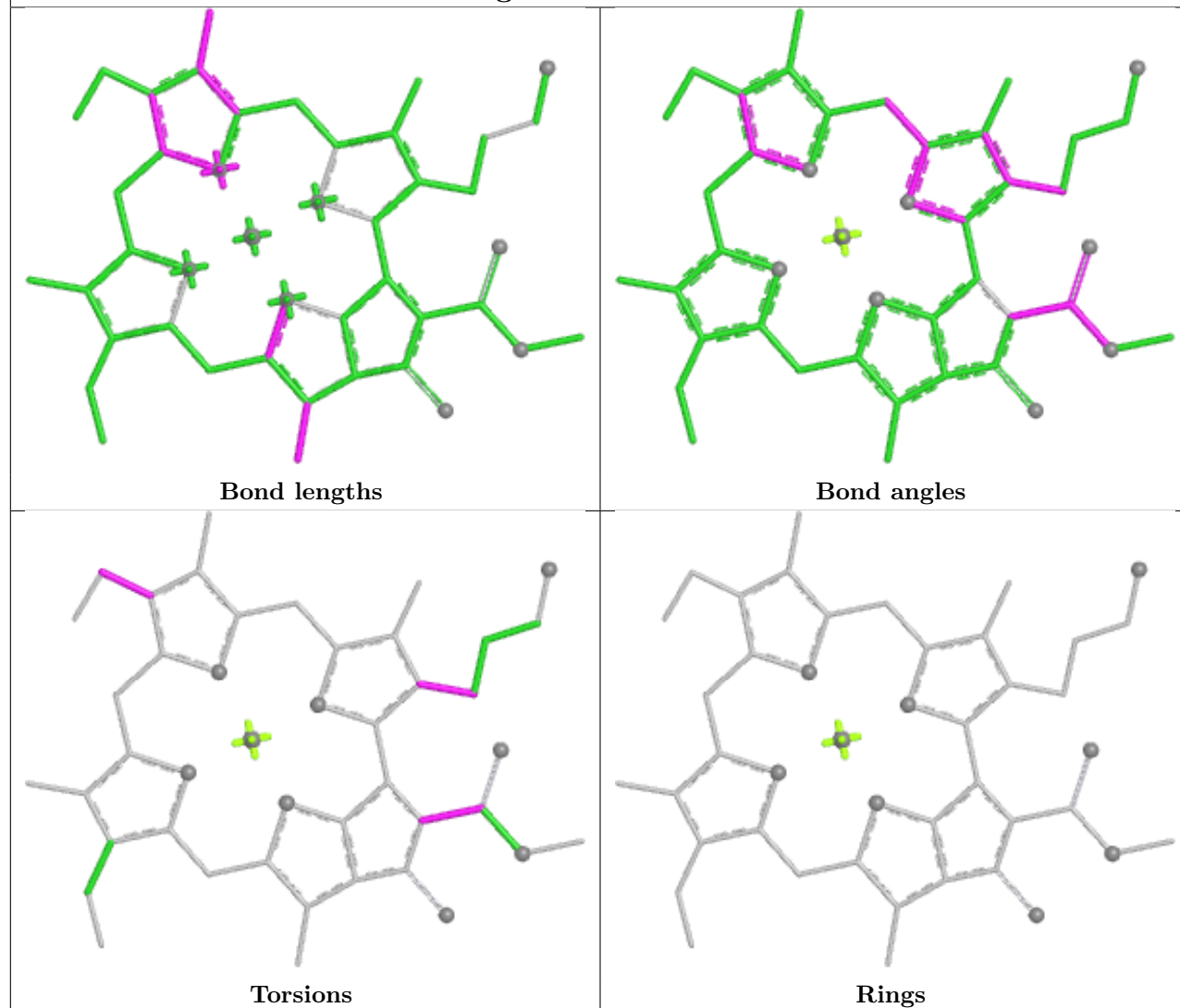
Ligand BCR y 101



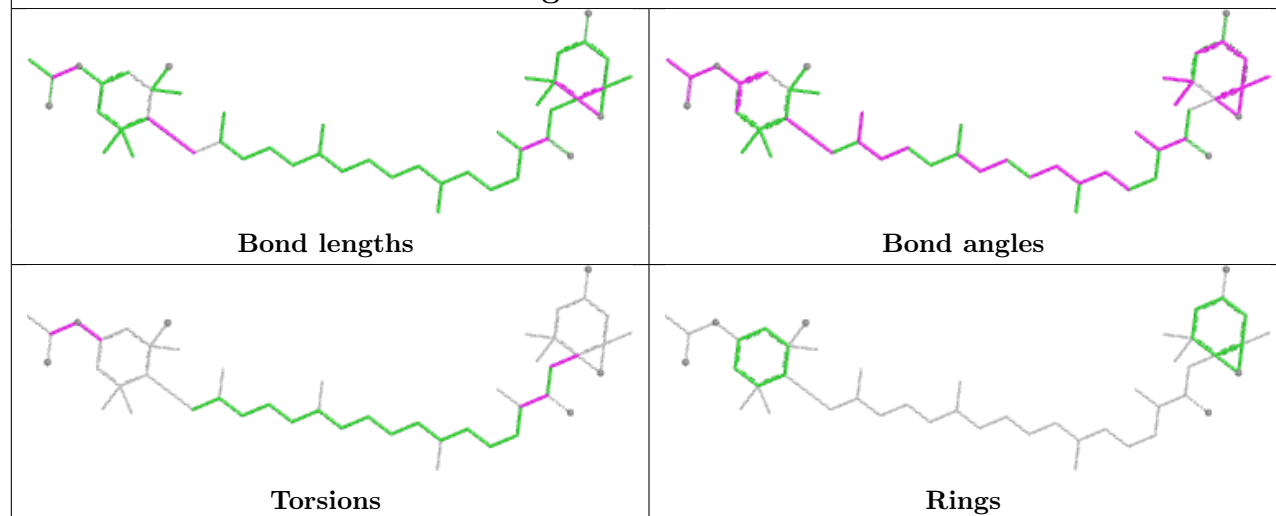


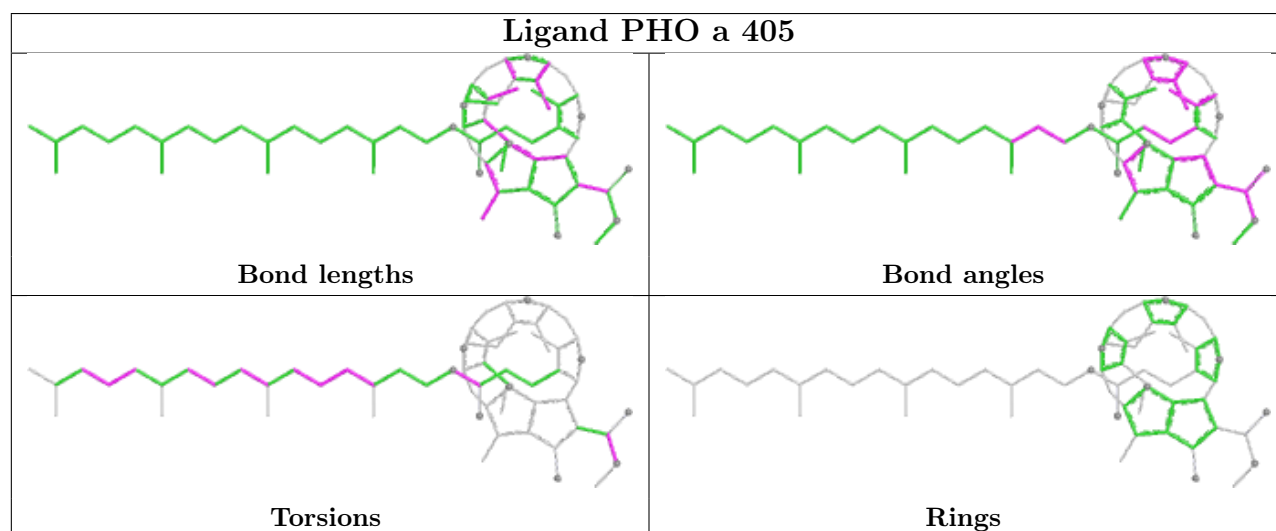
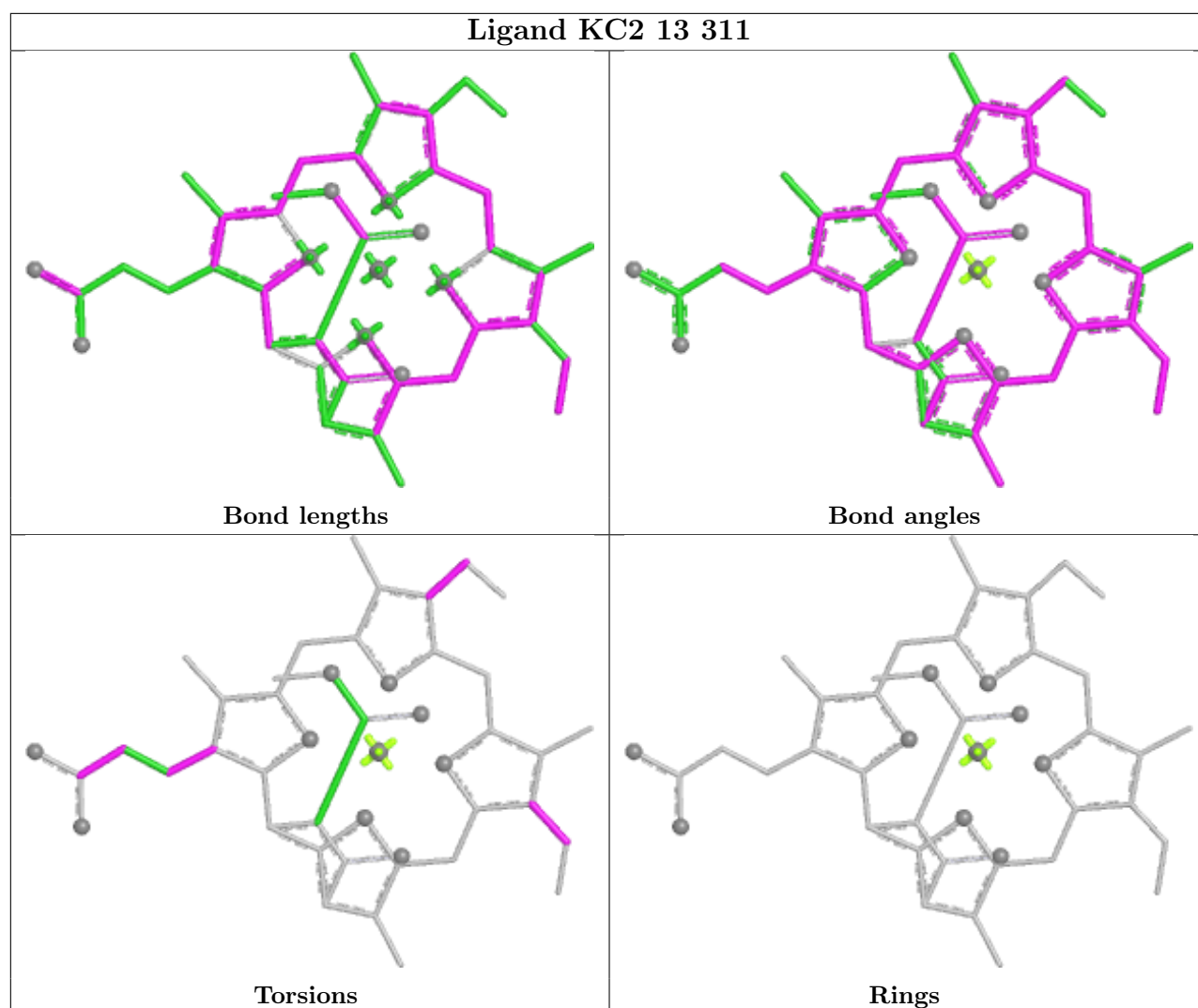


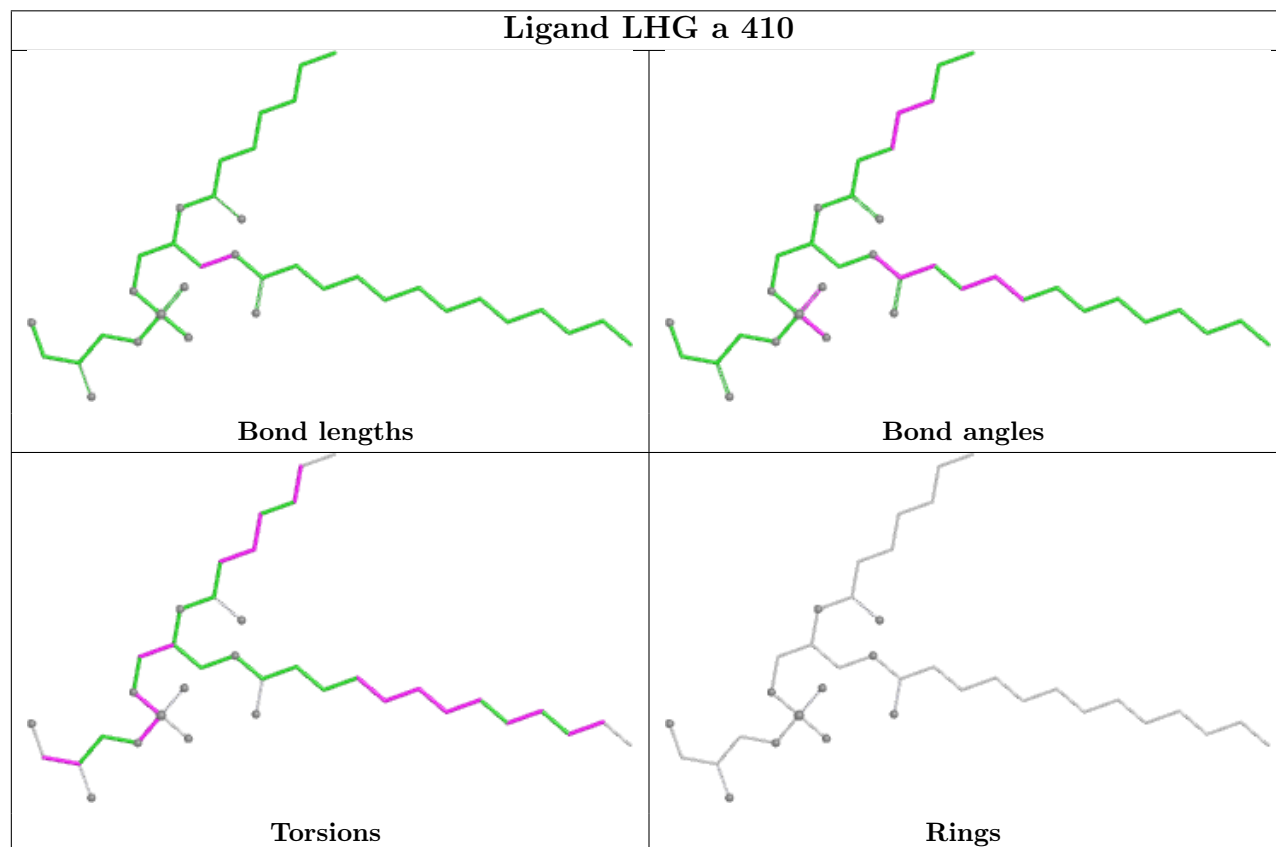
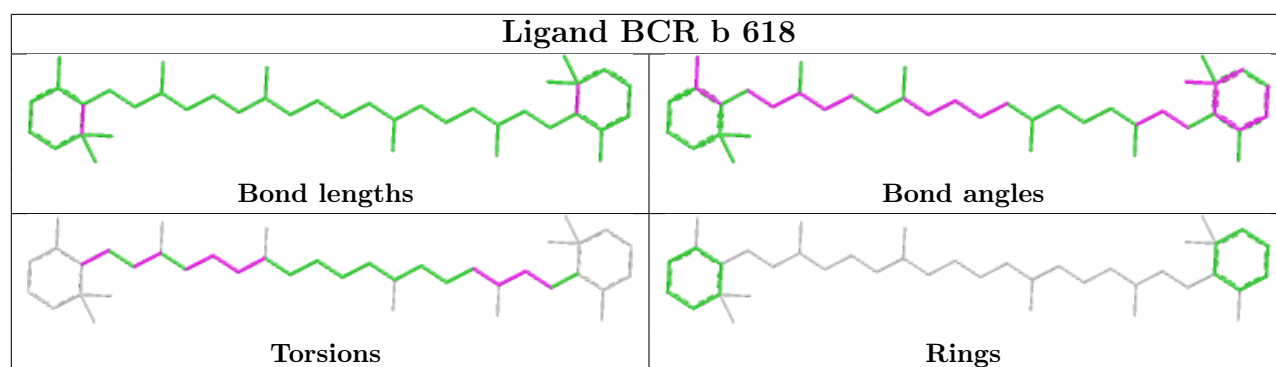
Ligand CLA 3 315

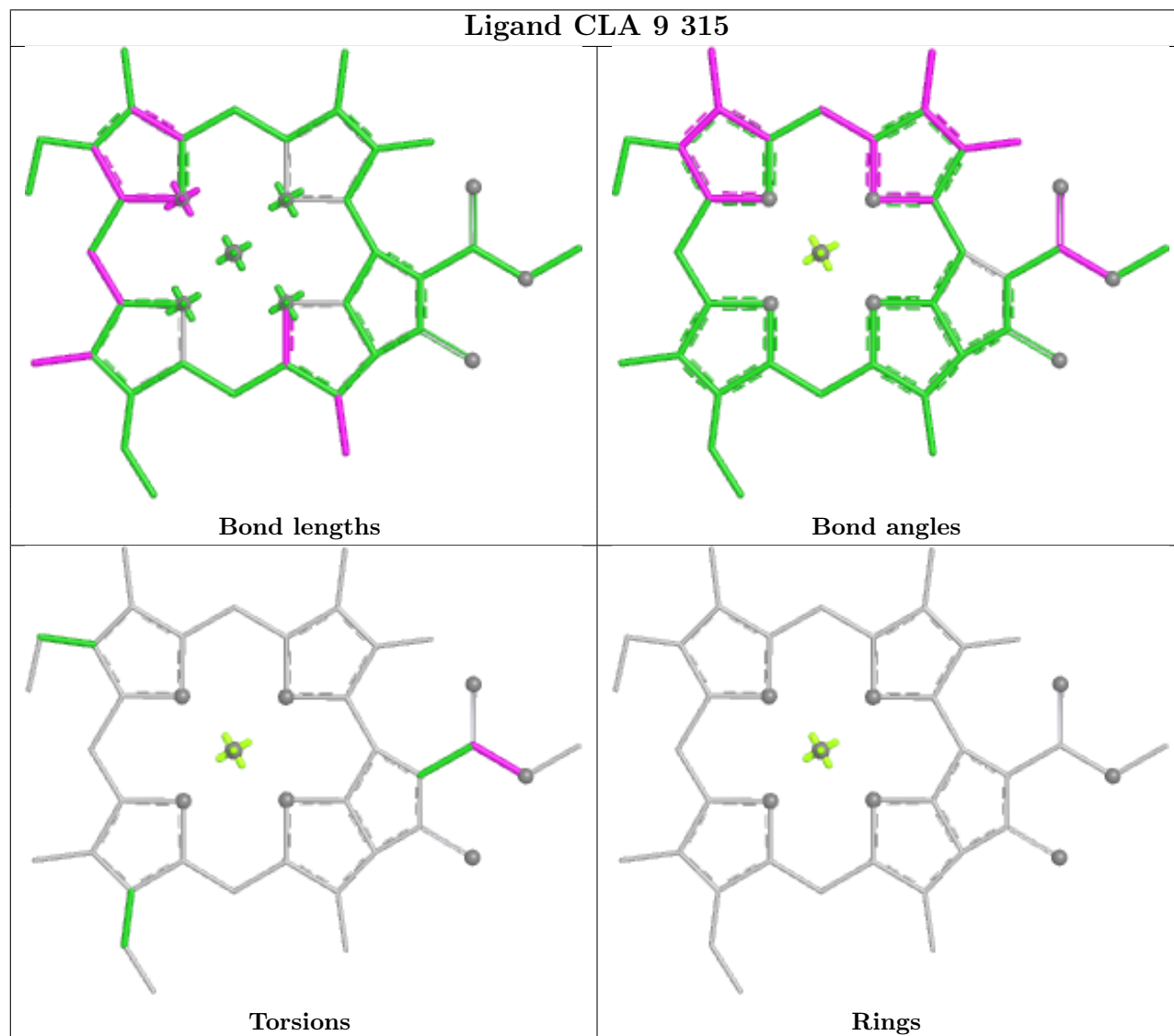
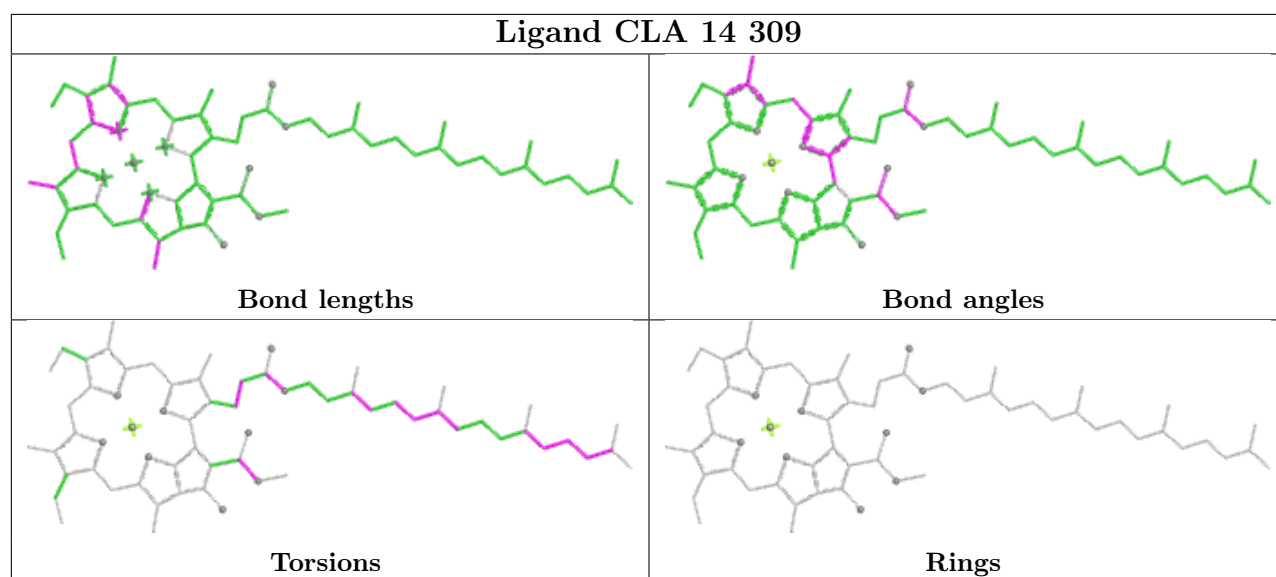


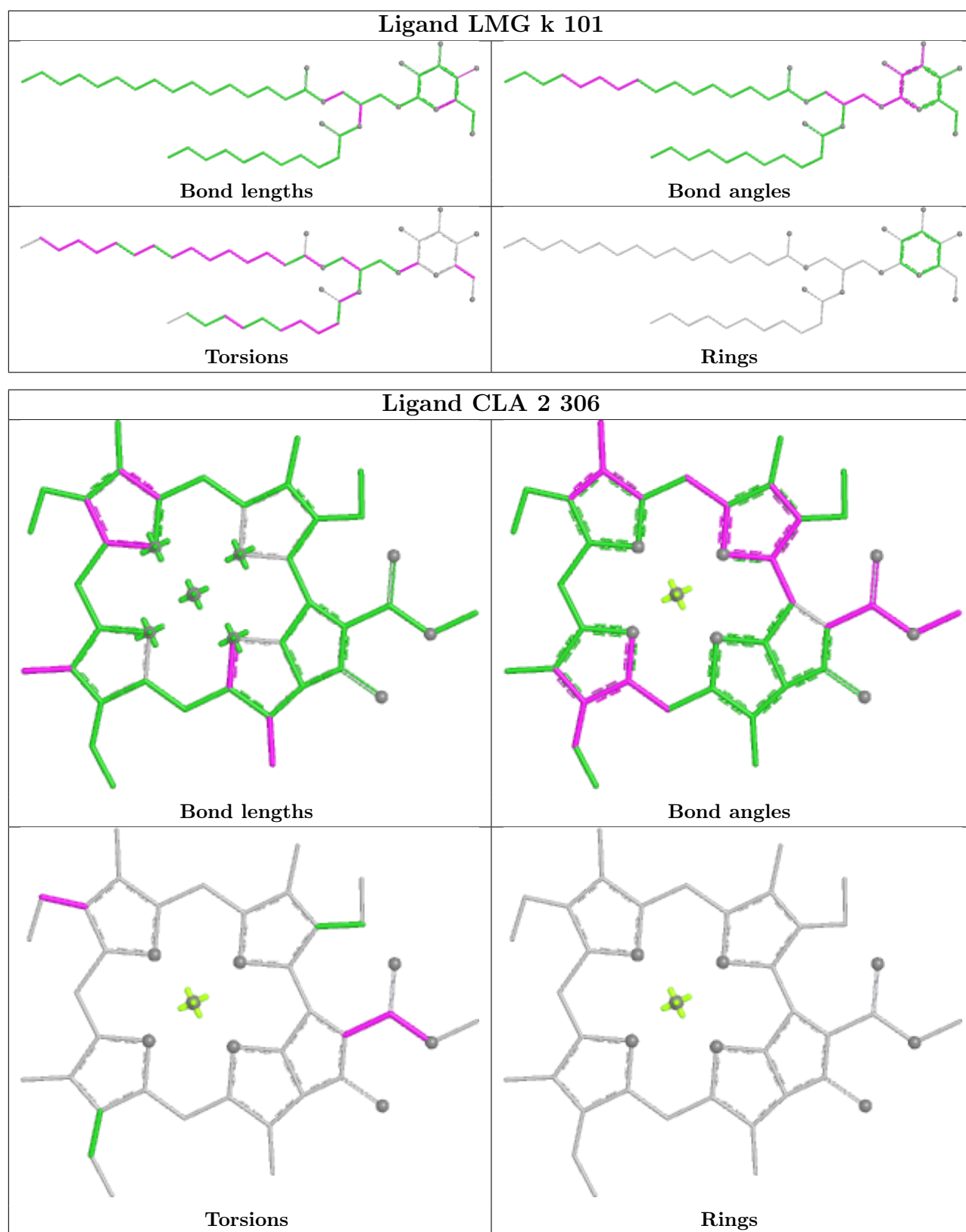
Ligand A86 9 304

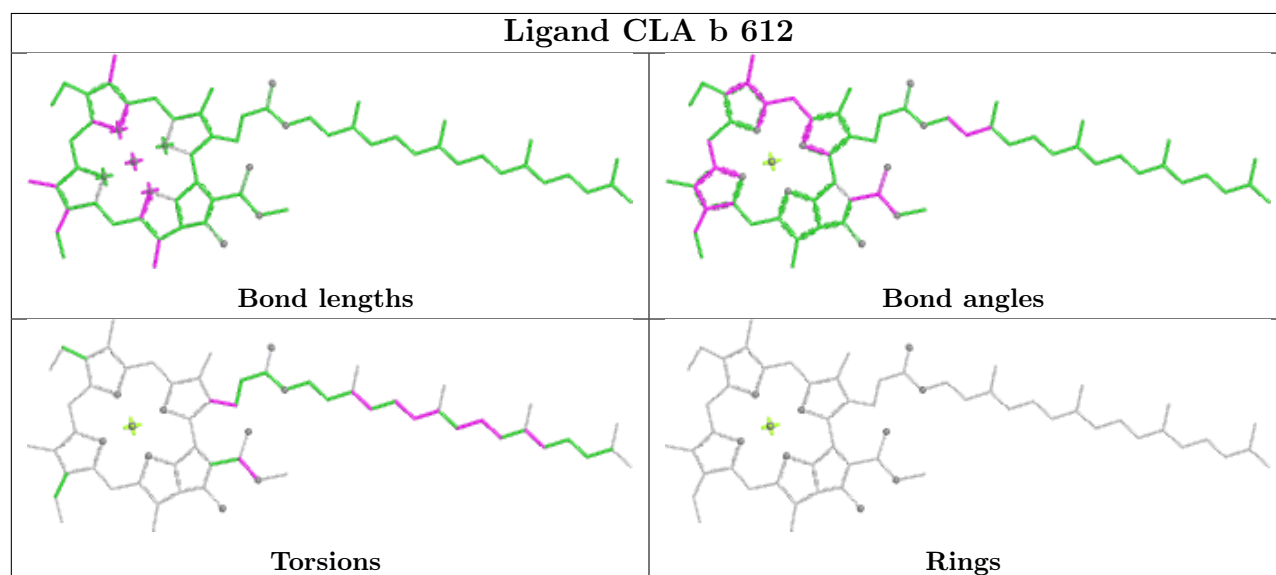
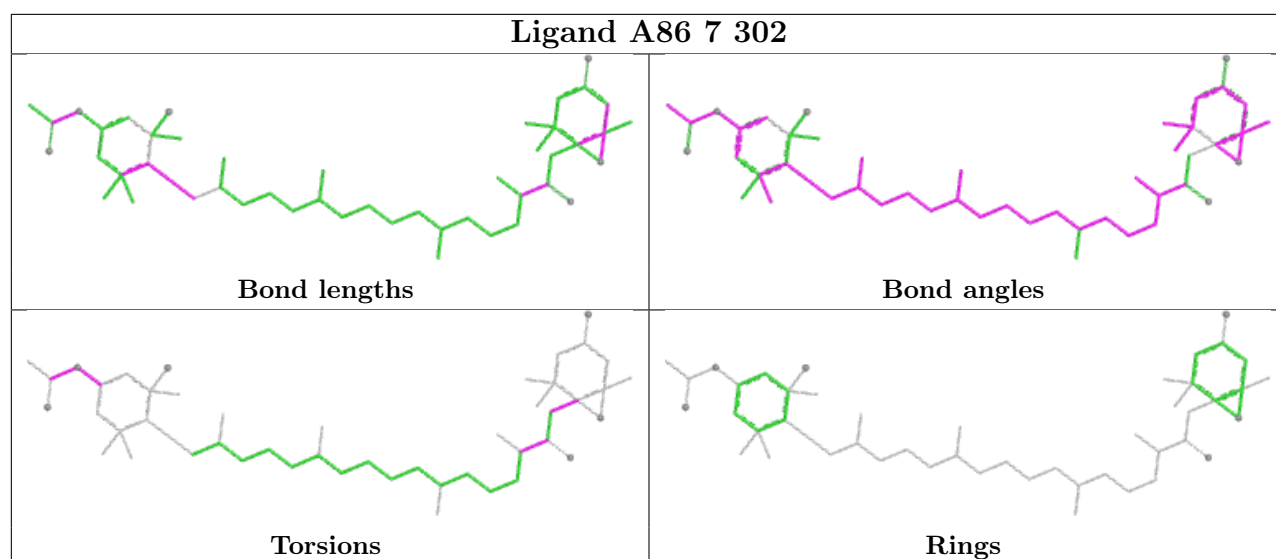


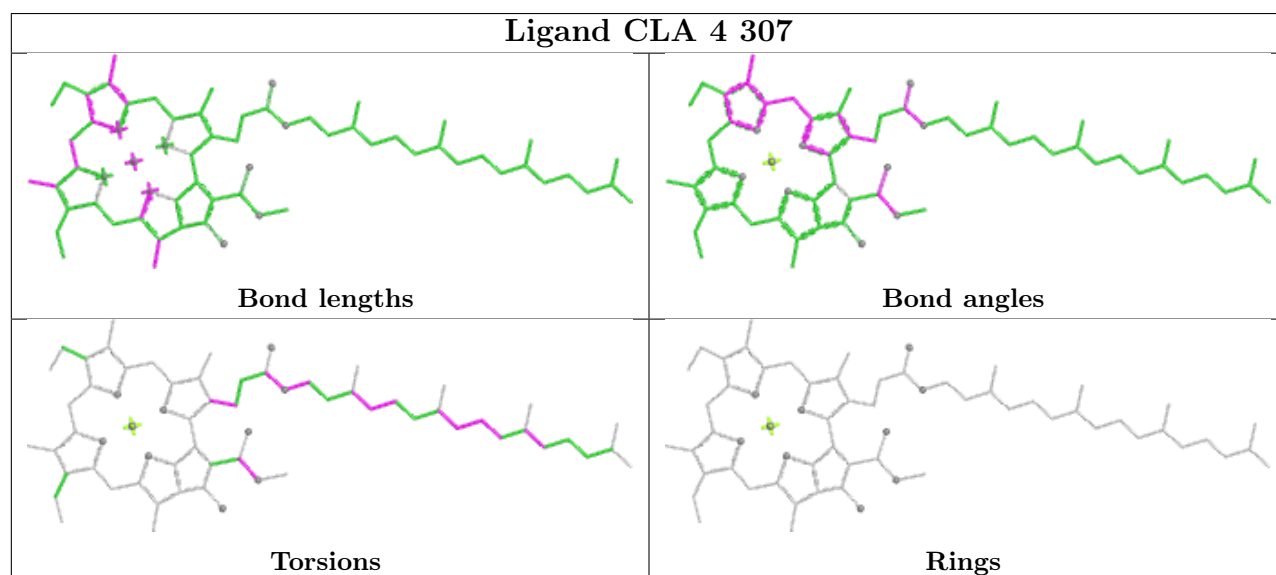
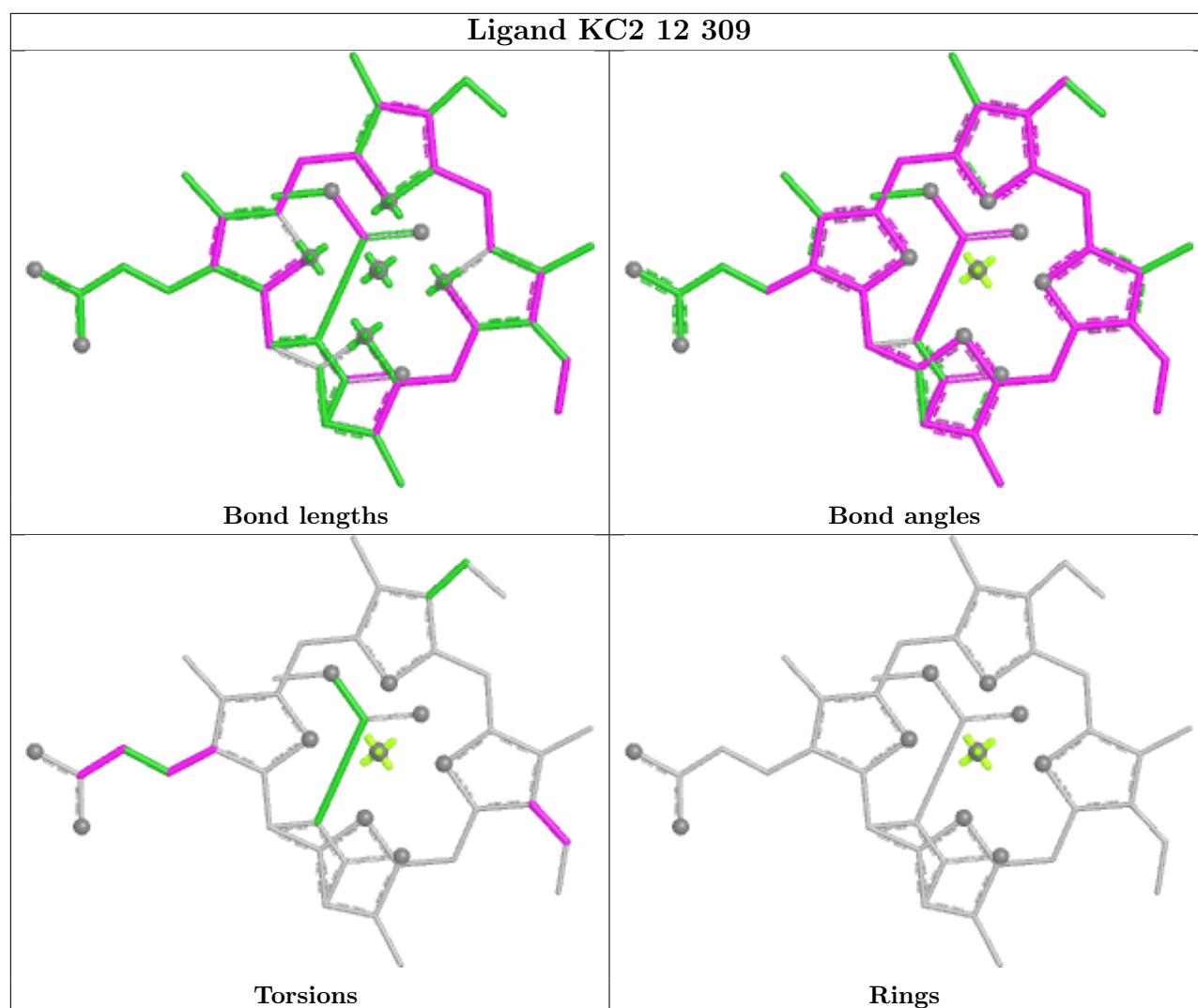


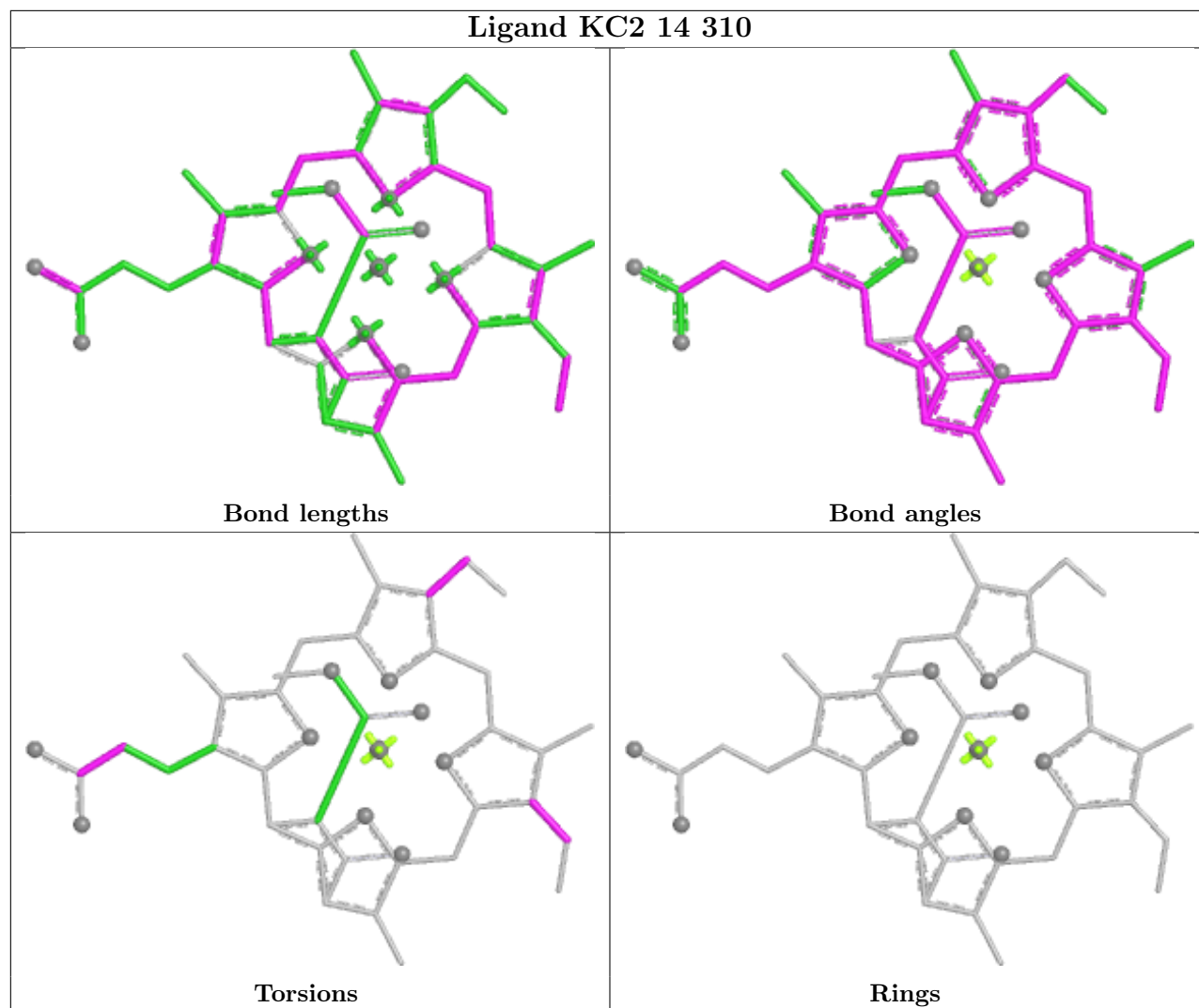


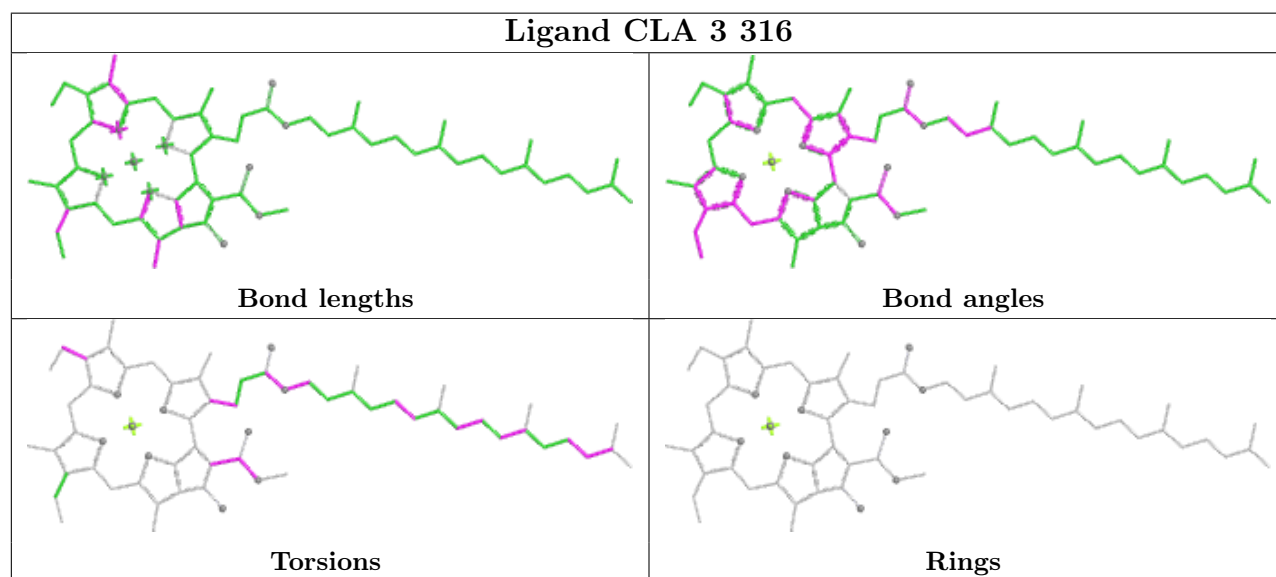
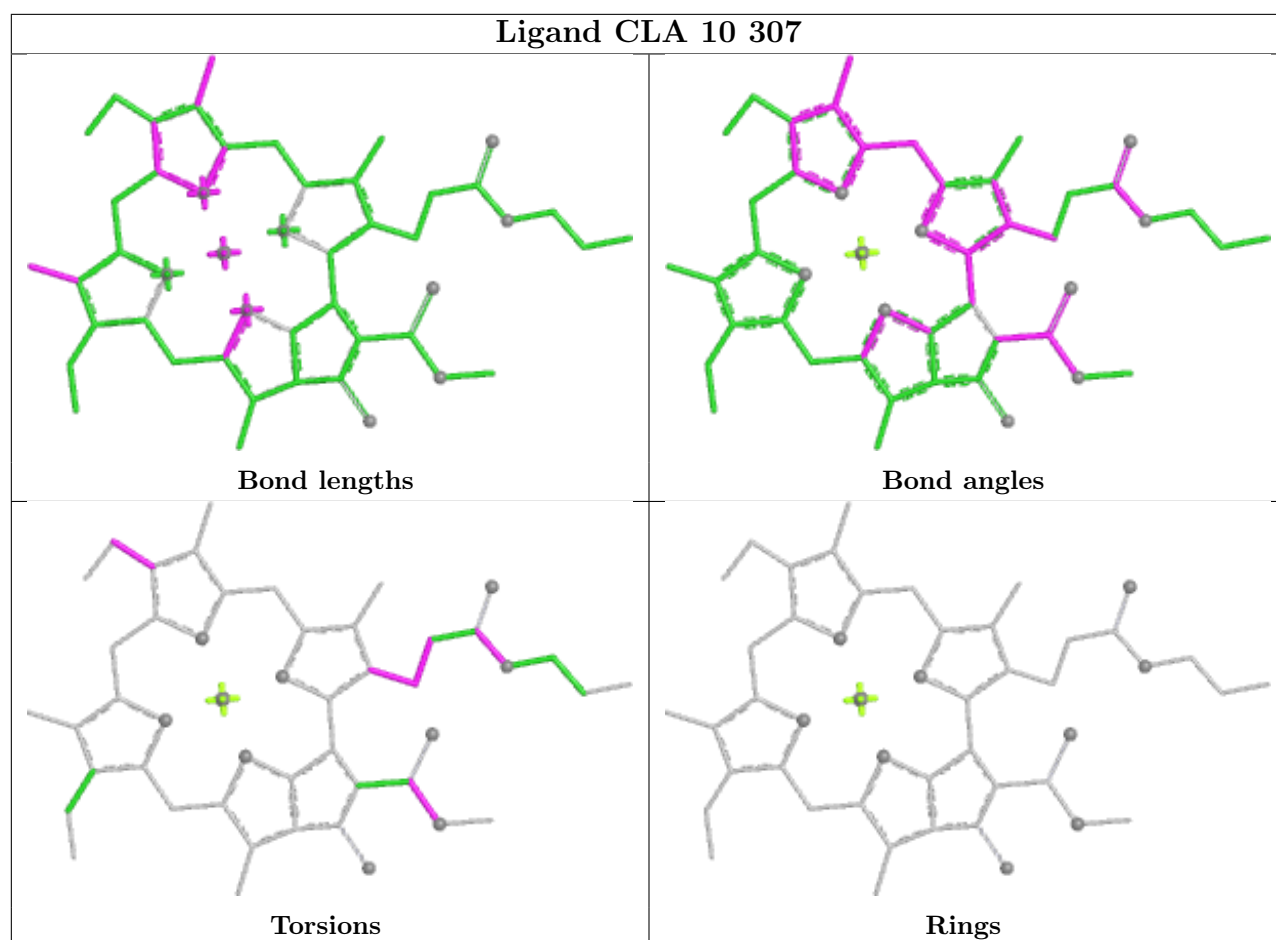




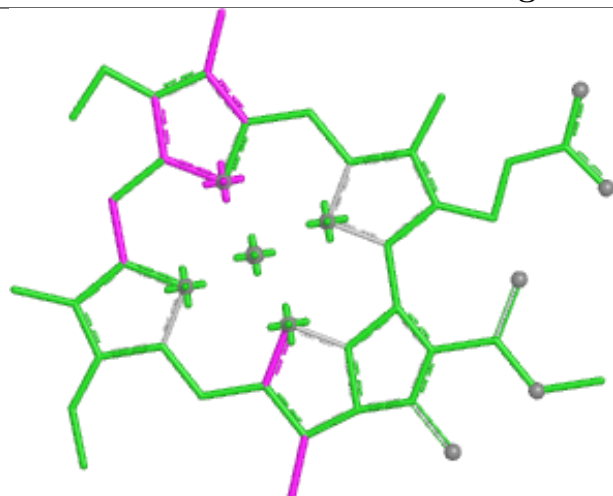




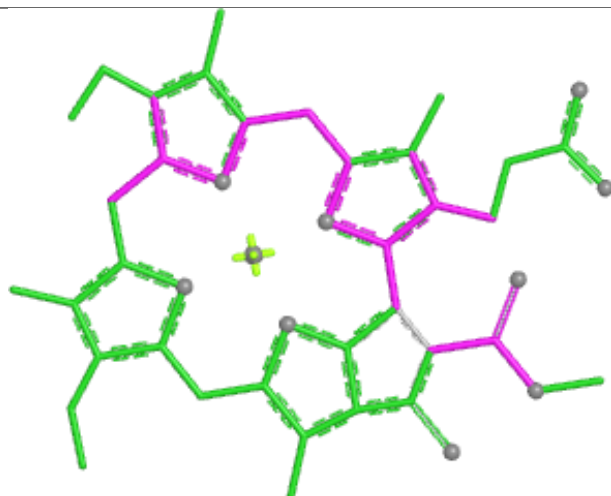




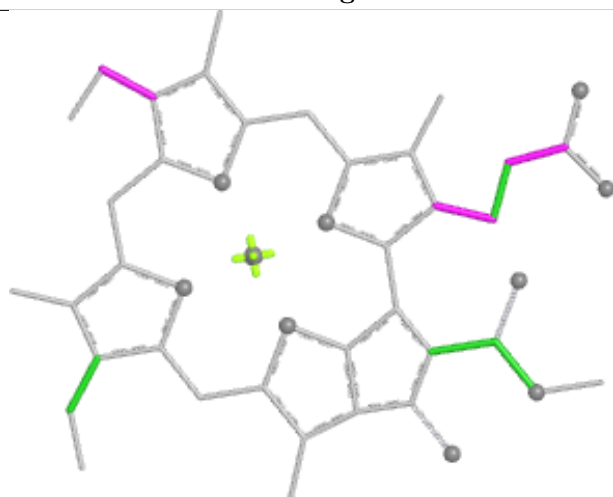
Ligand CLA 3 312



Bond lengths



Bond angles

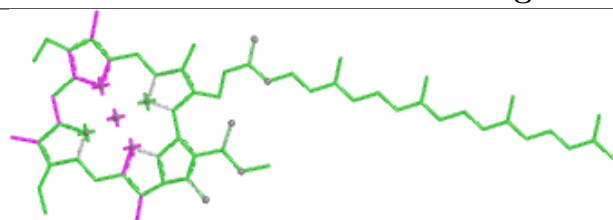


Torsions

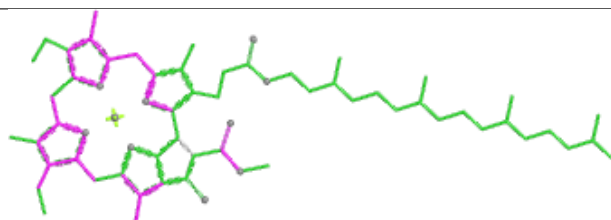


Rings

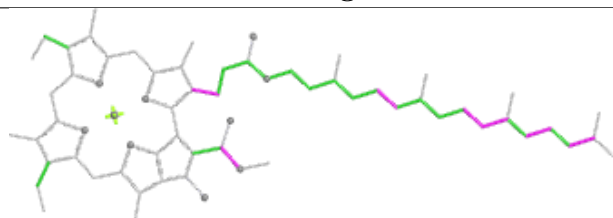
Ligand CLA C 509



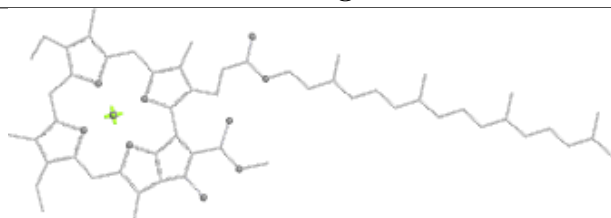
Bond lengths



Bond angles

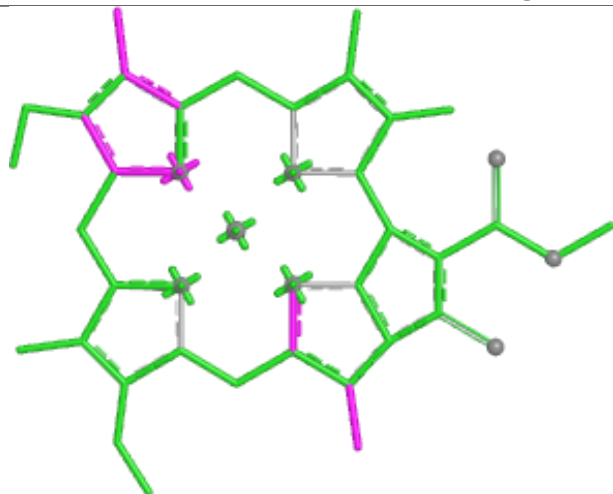


Torsions

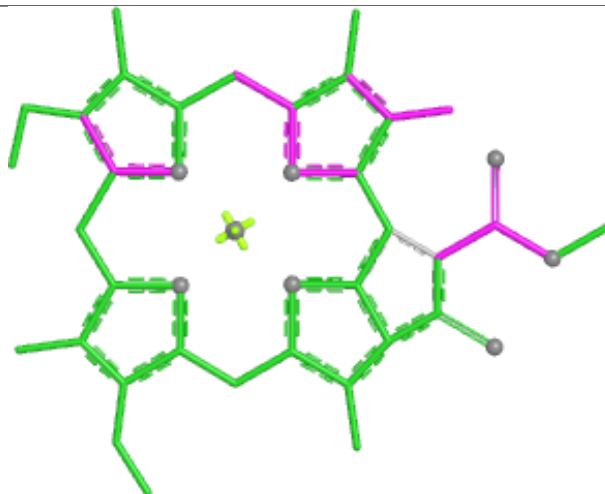


Rings

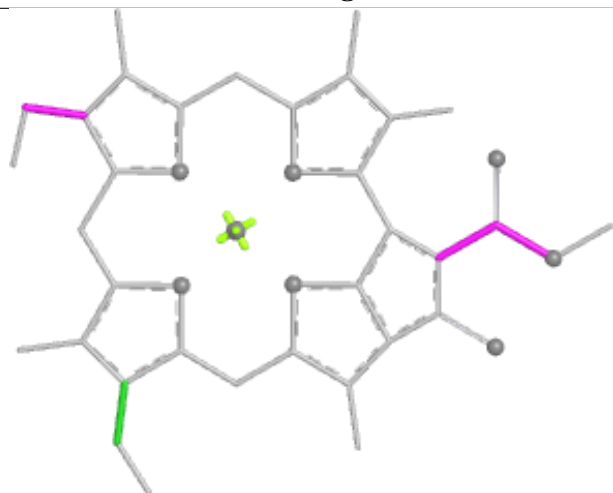
Ligand CLA 7 315



Bond lengths



Bond angles

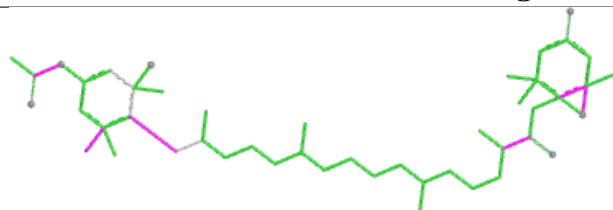


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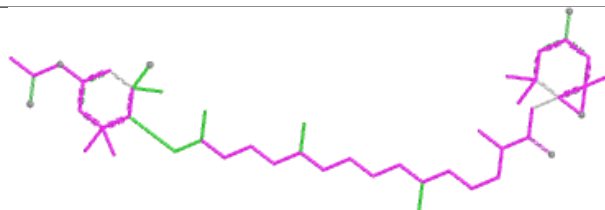


Rings

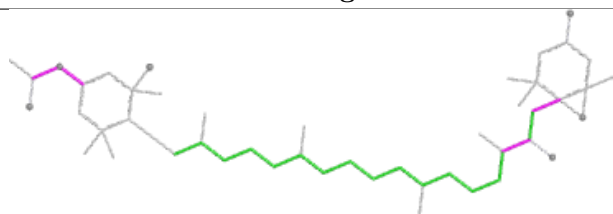
Ligand A86 15 302



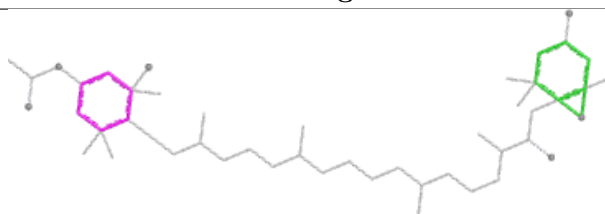
Bond lengths



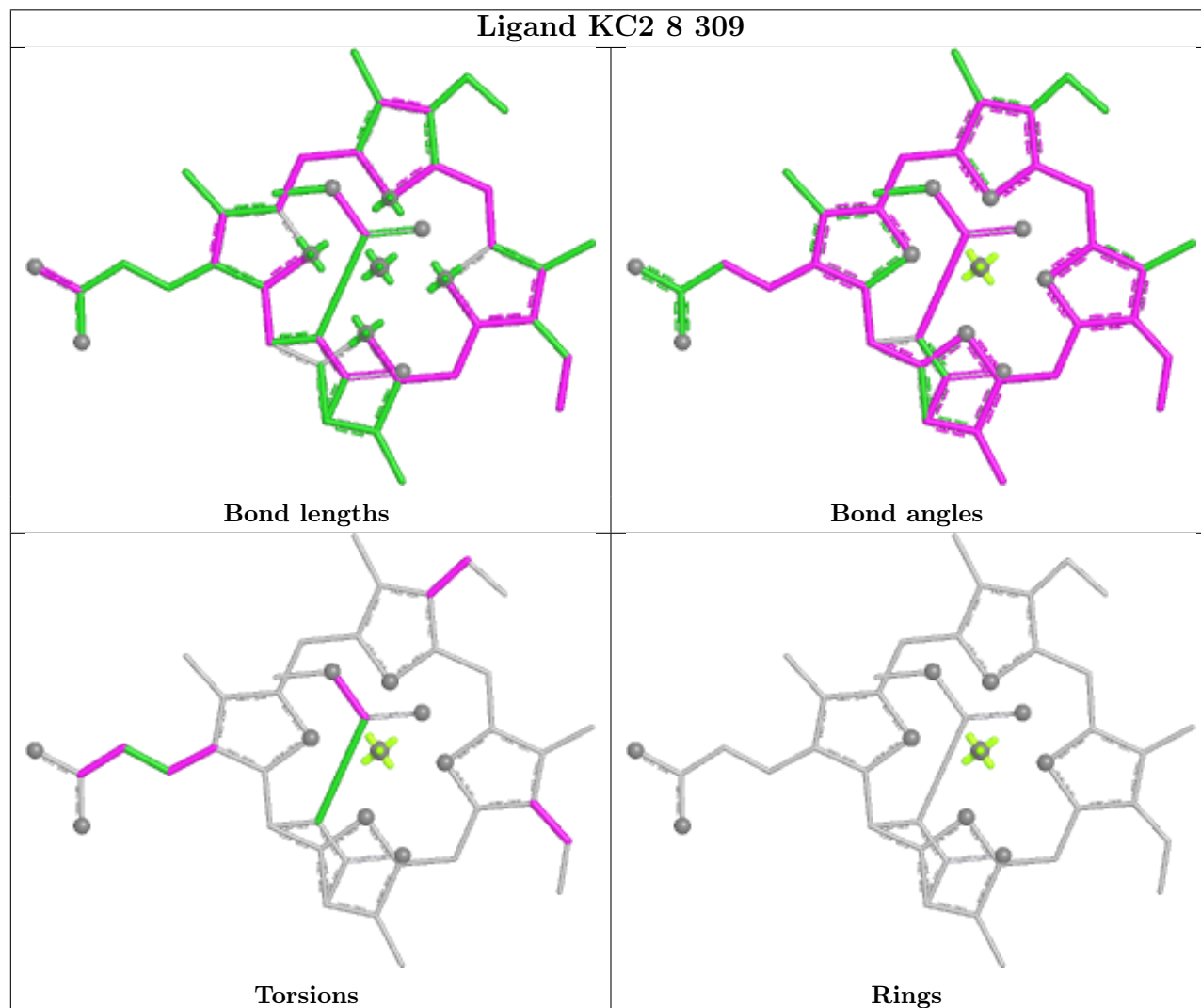
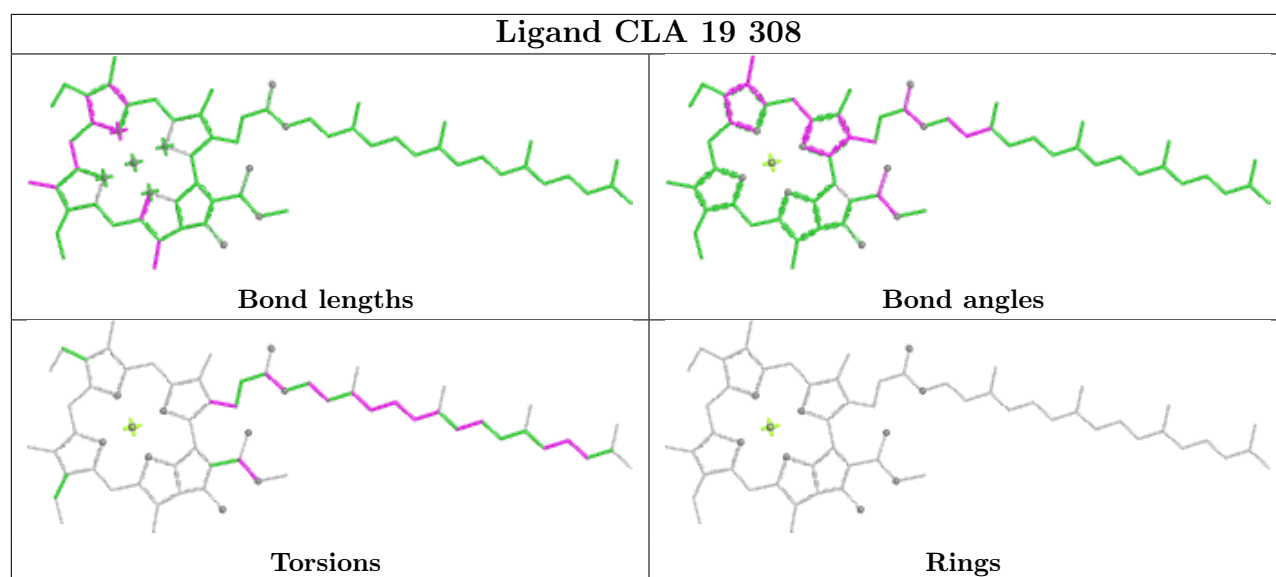
Bond angles

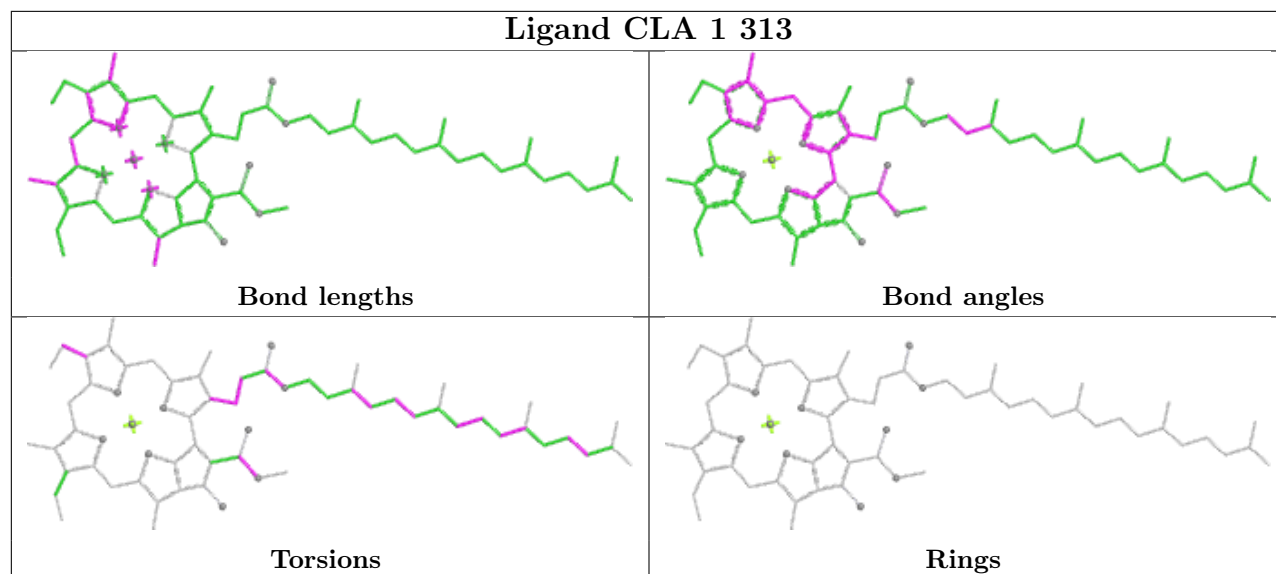
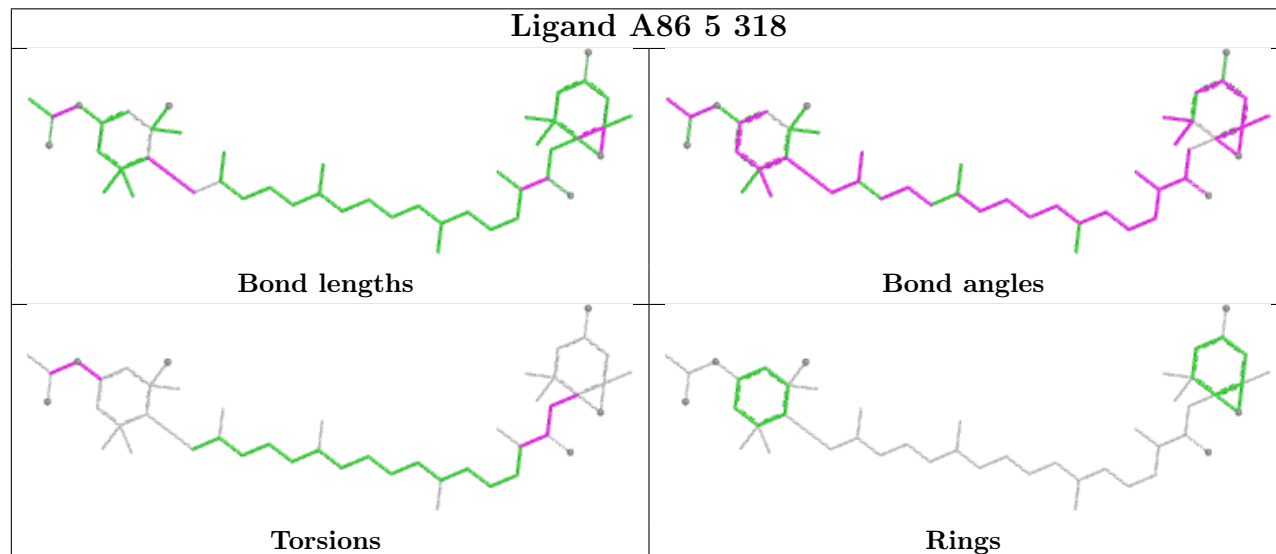


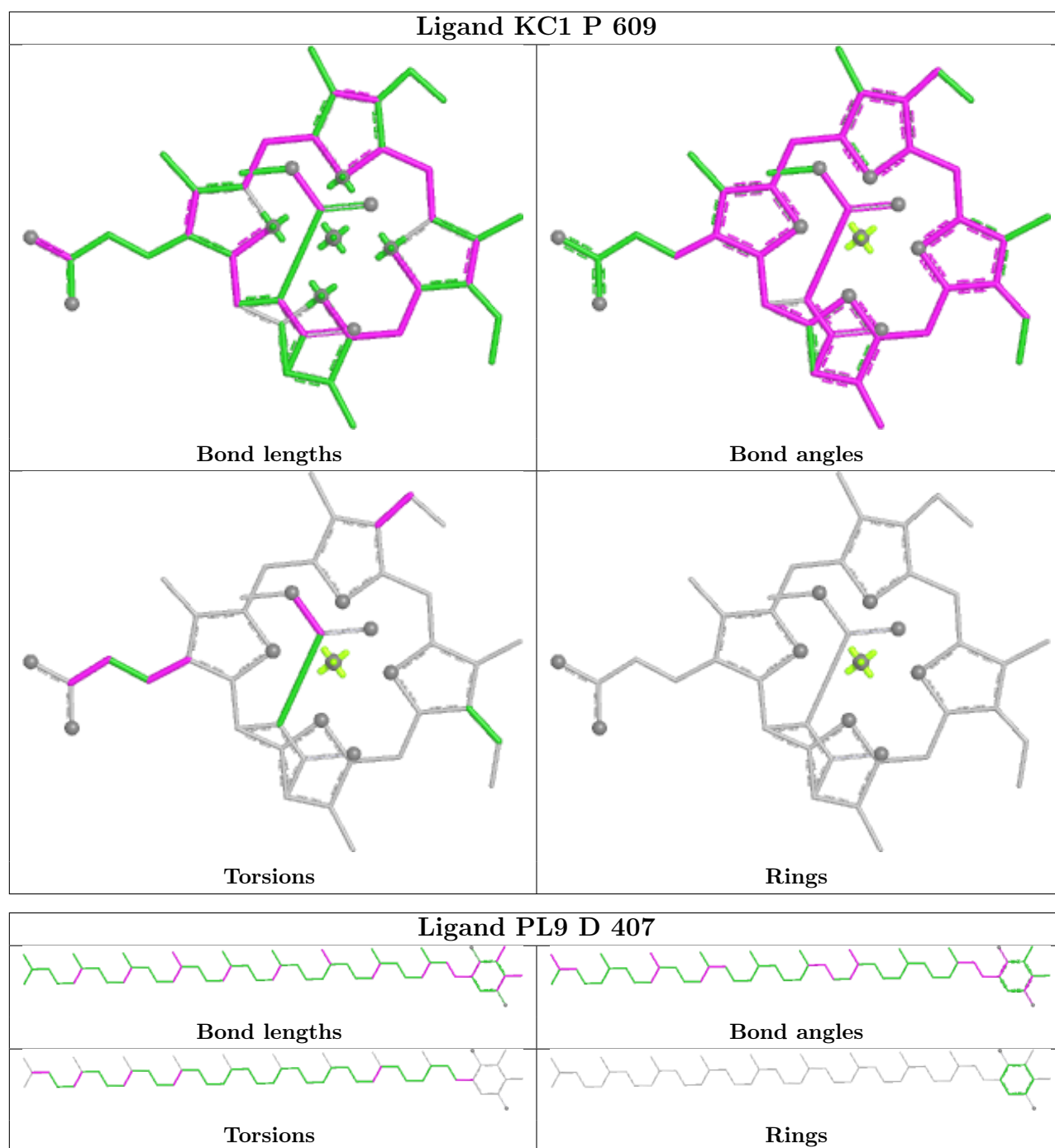
Torsions

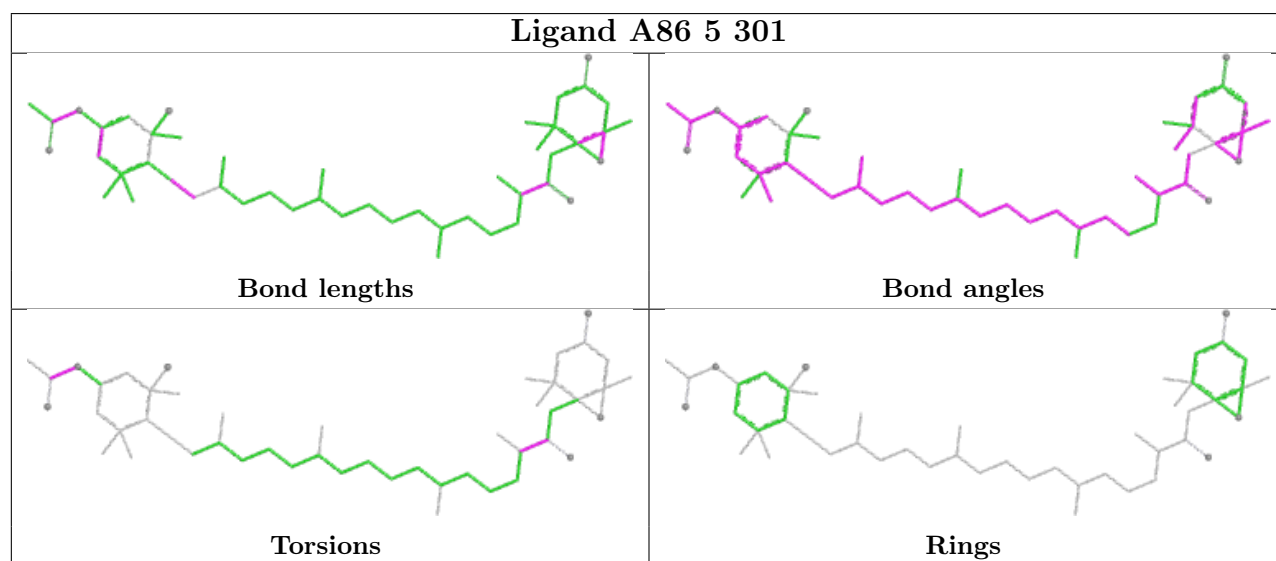
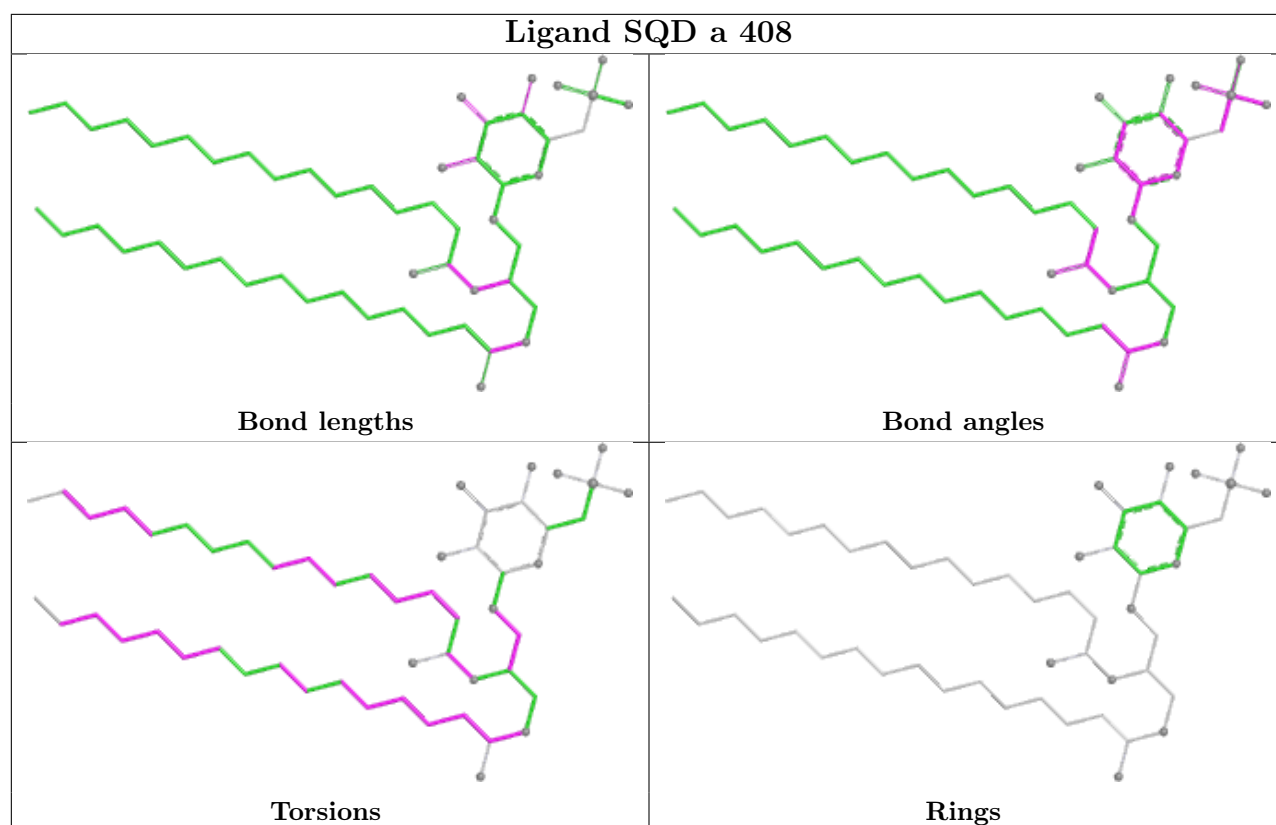


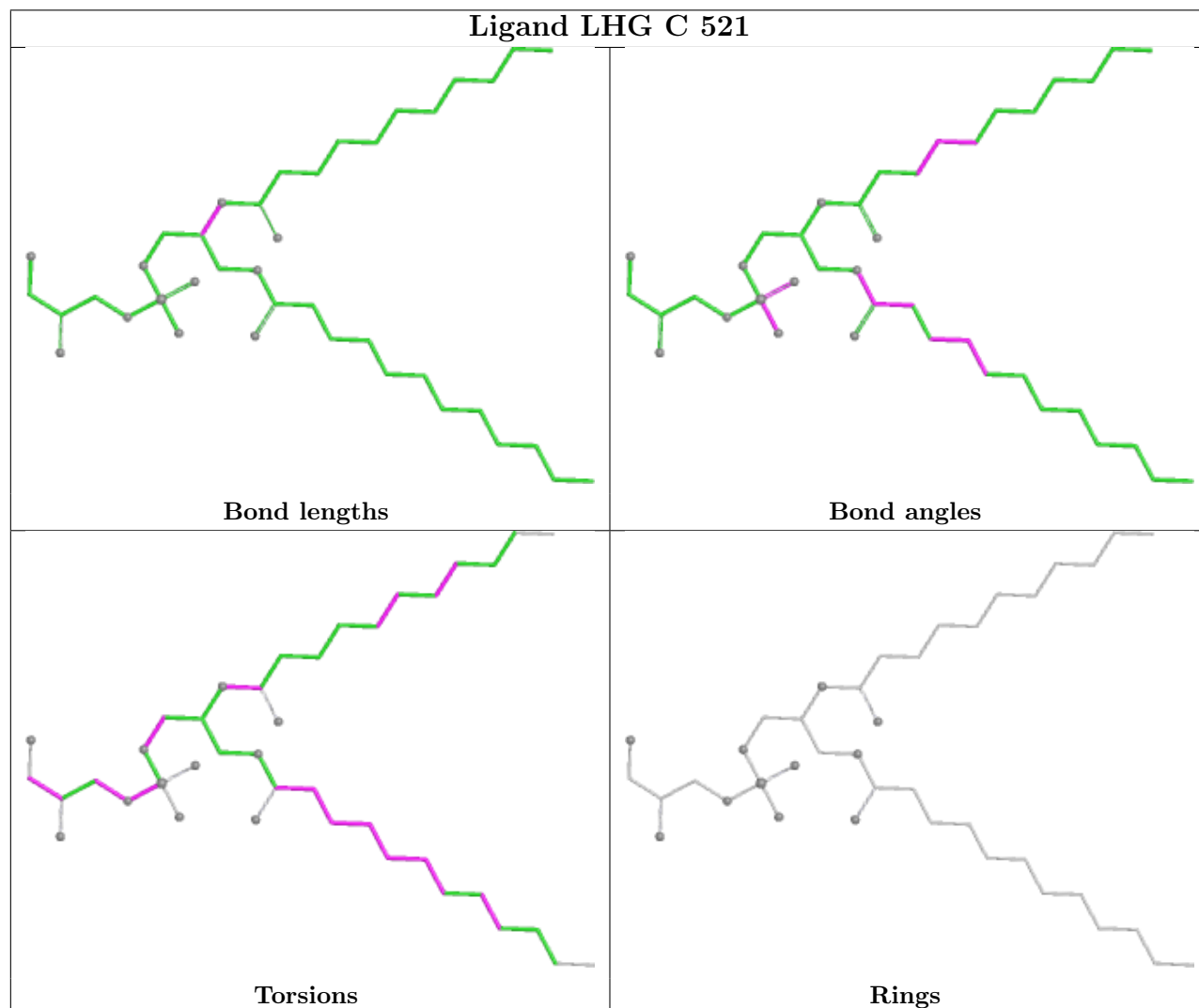
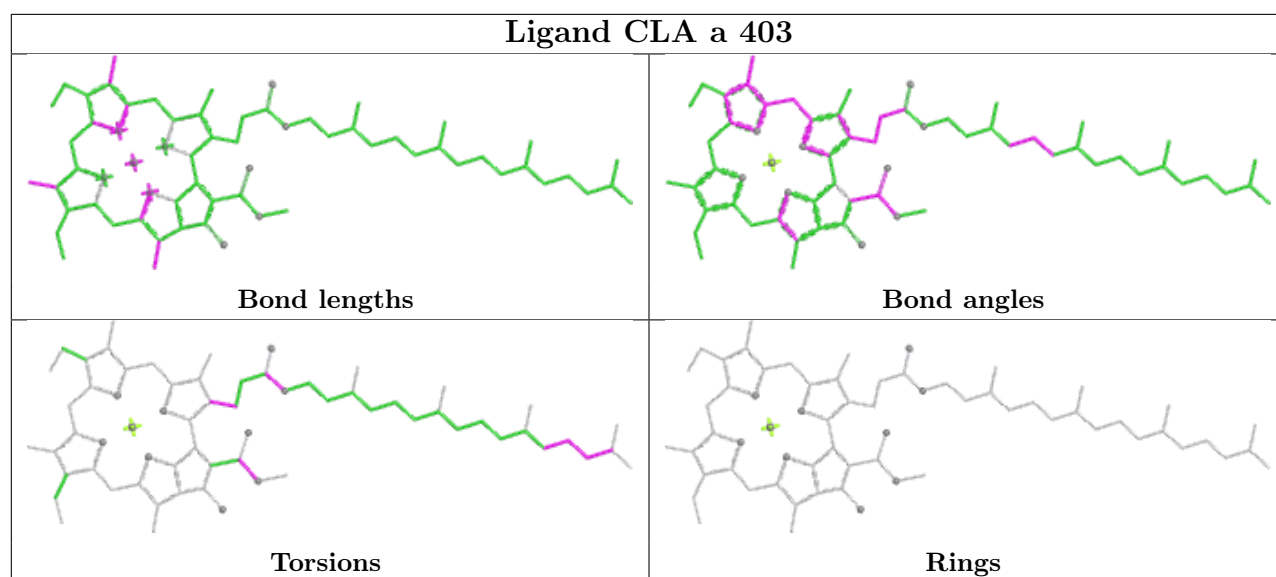
Rings

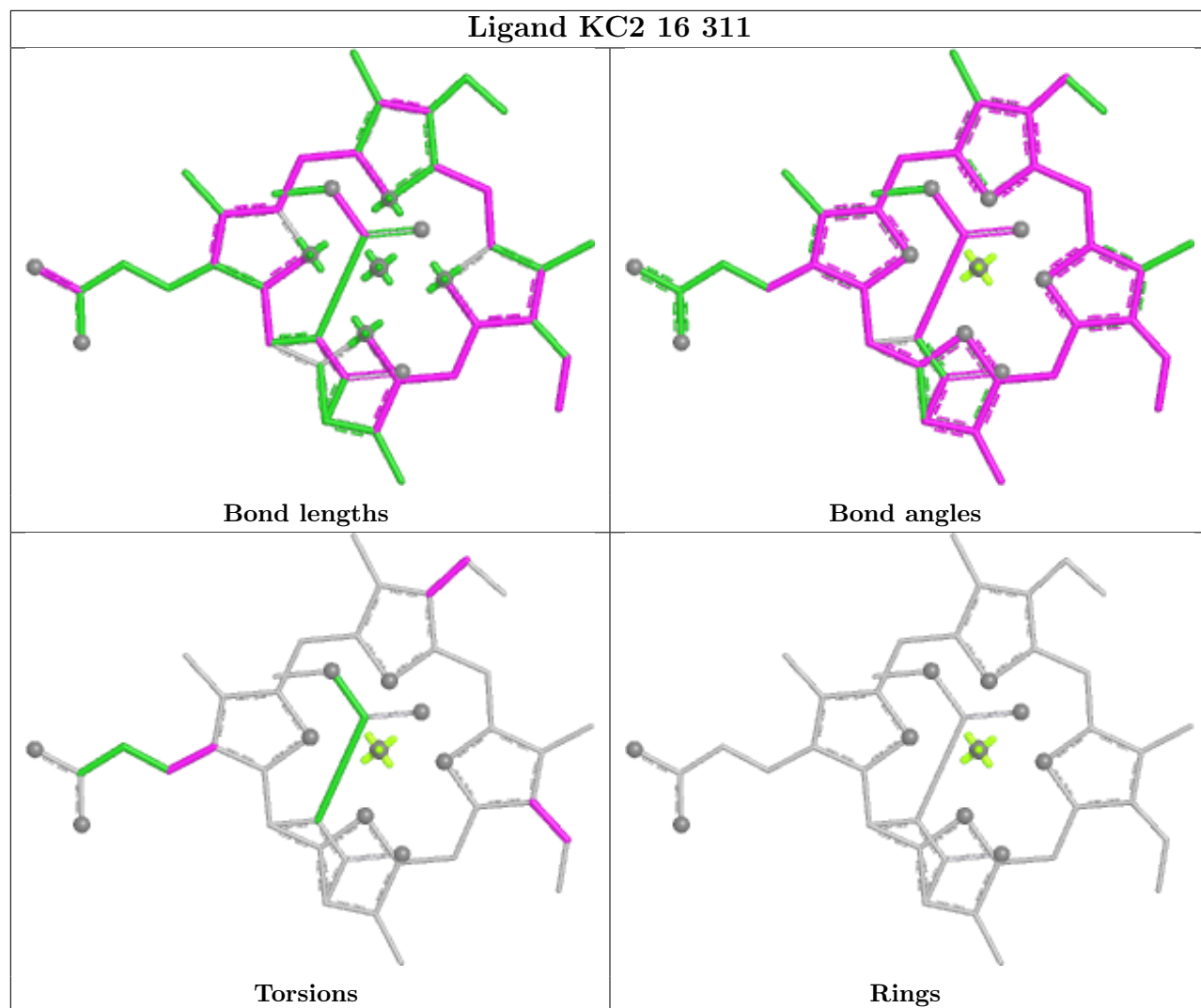


Ligand CLA 1 313**Ligand A86 5 318**

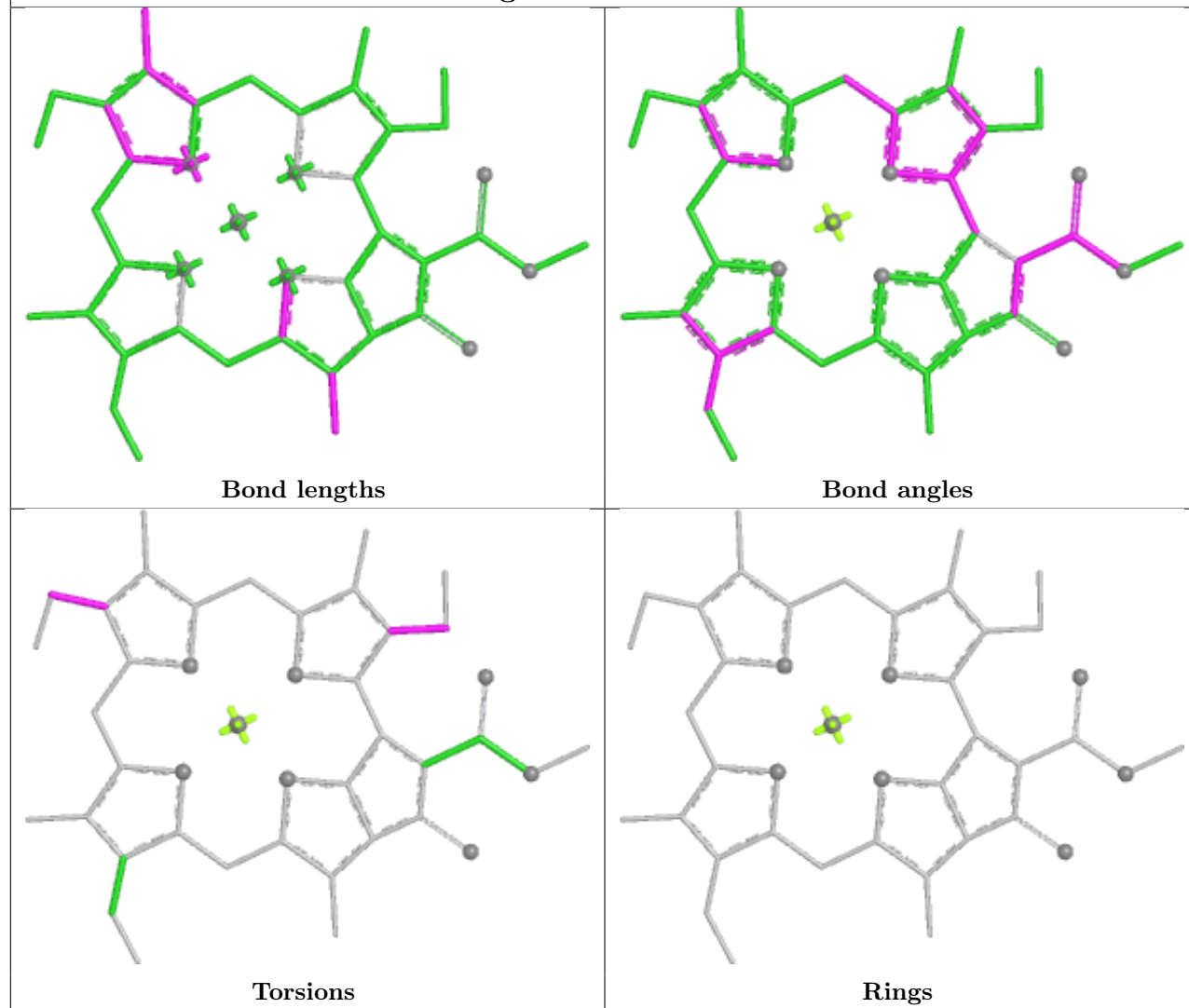




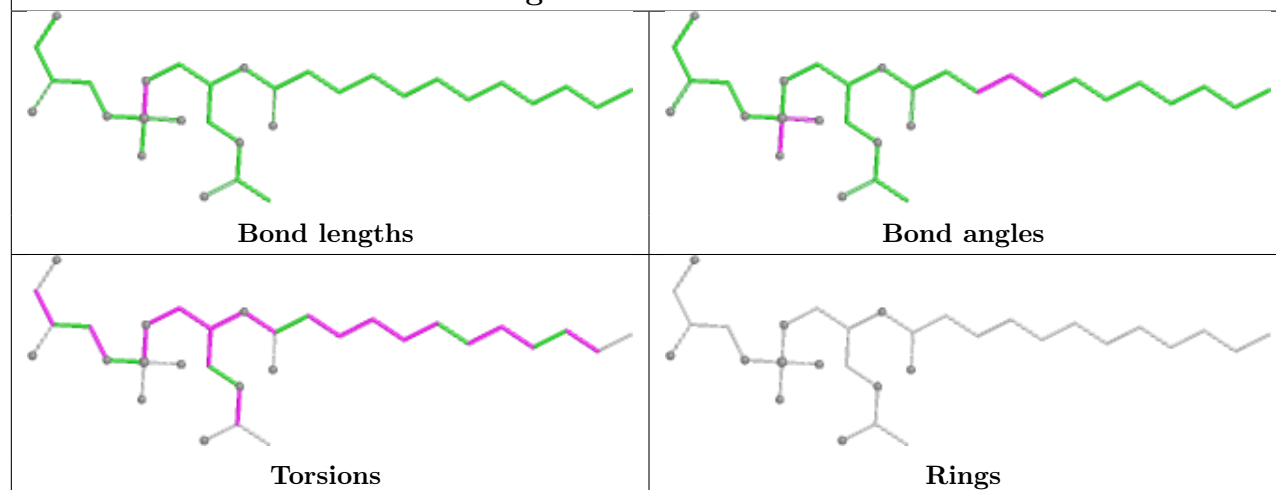


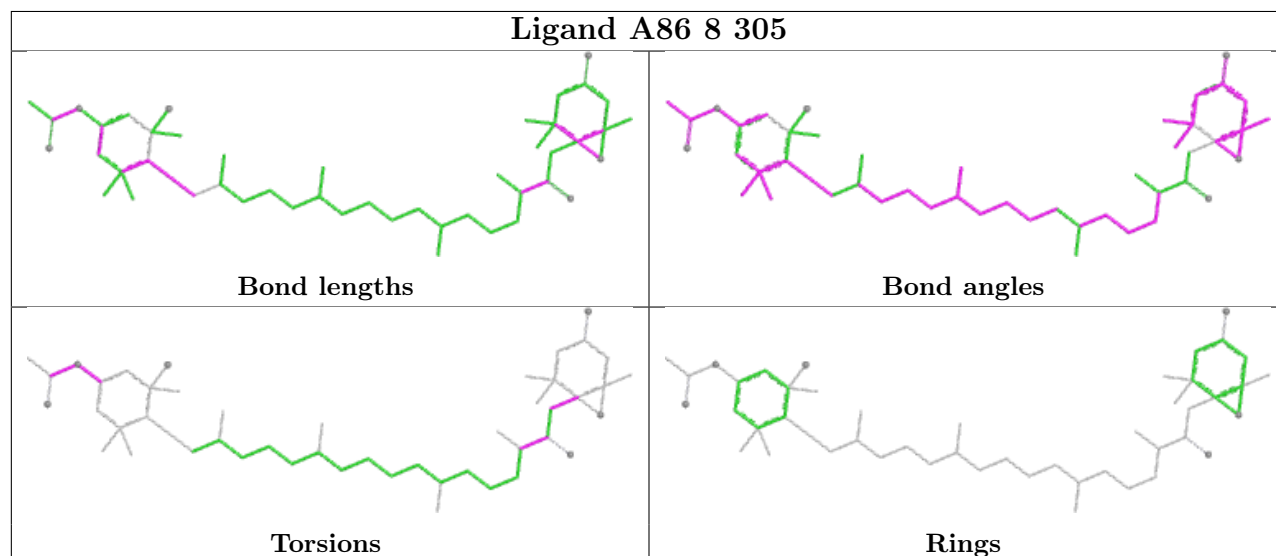
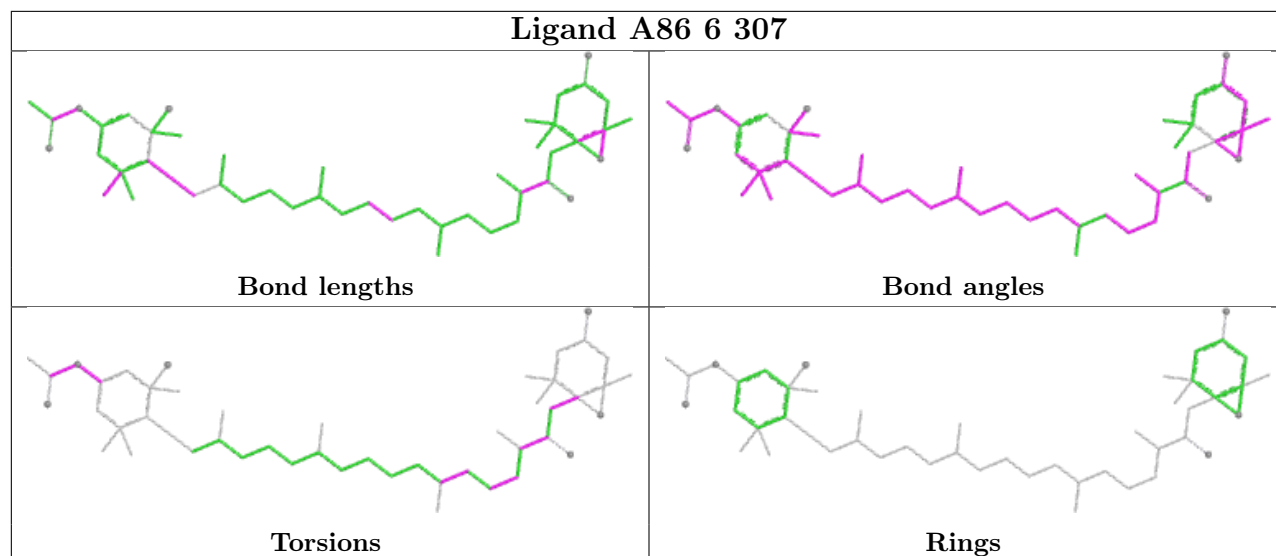


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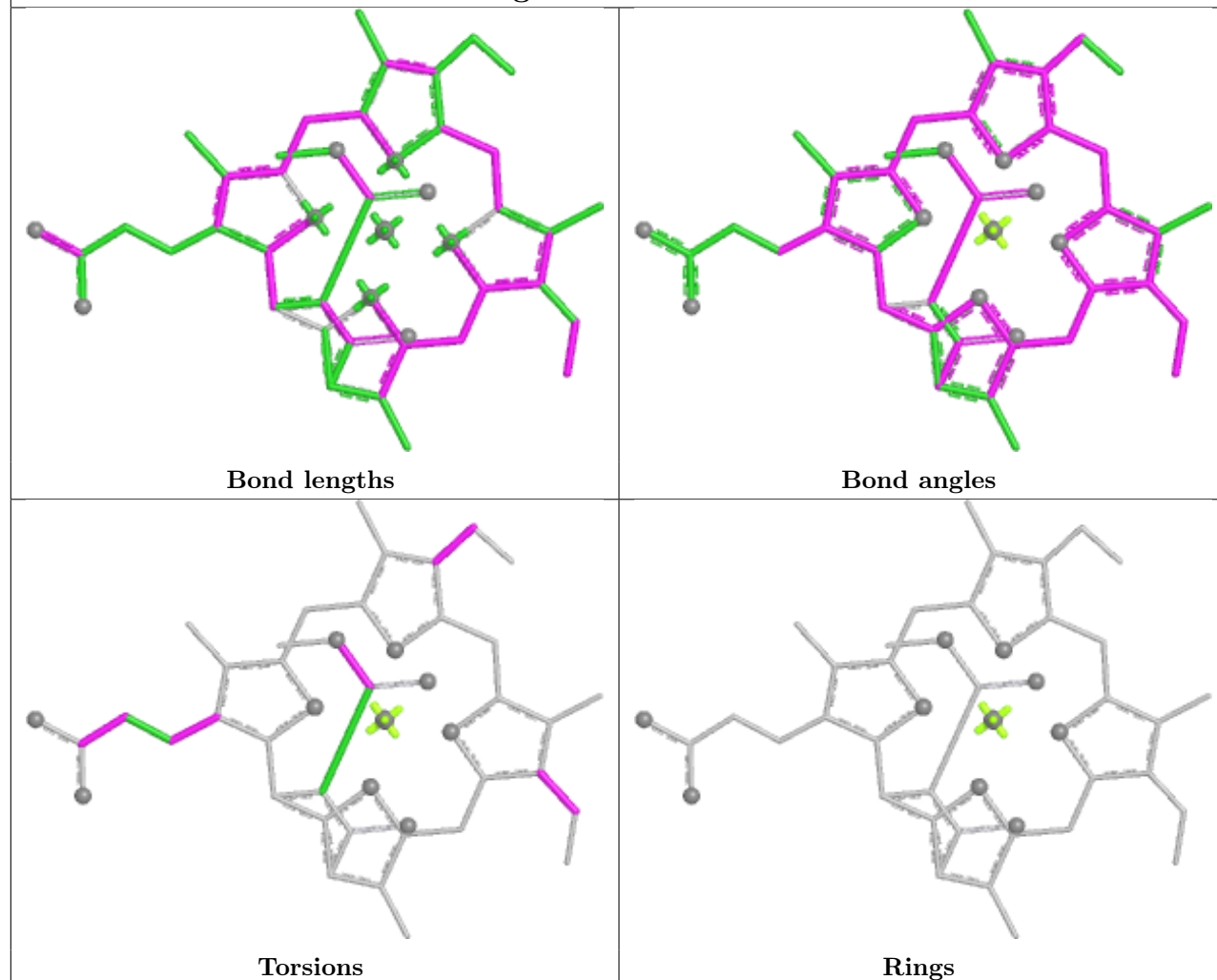


Ligand LHG 18 316

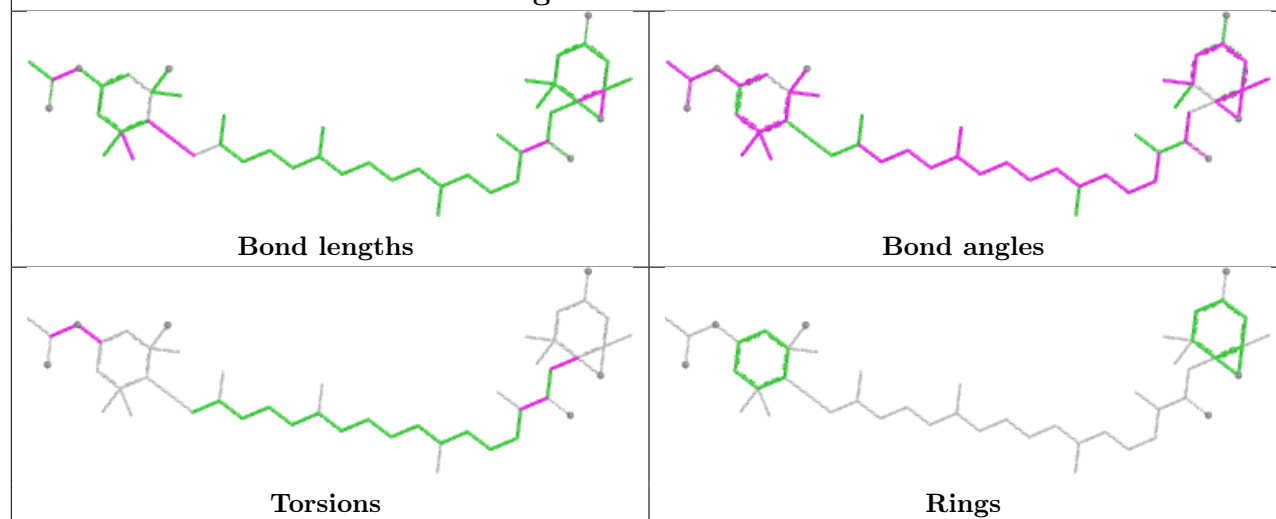


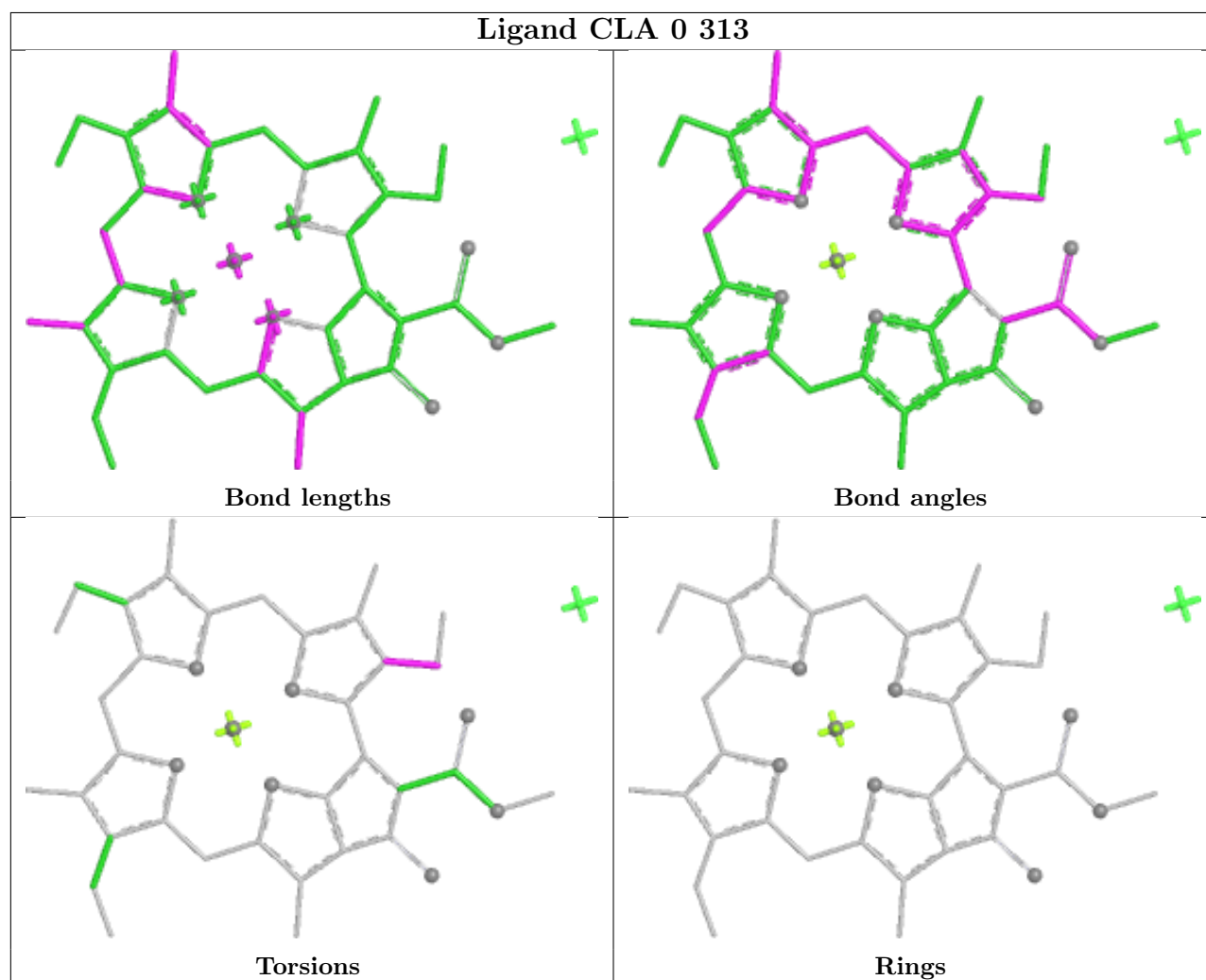
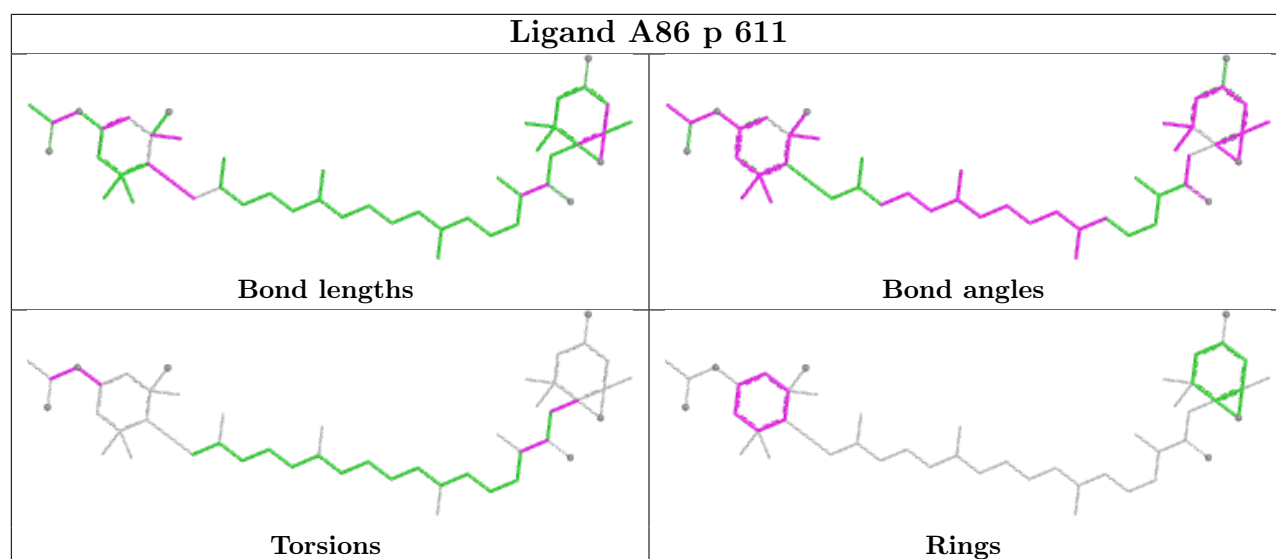


Ligand KC2 2 308

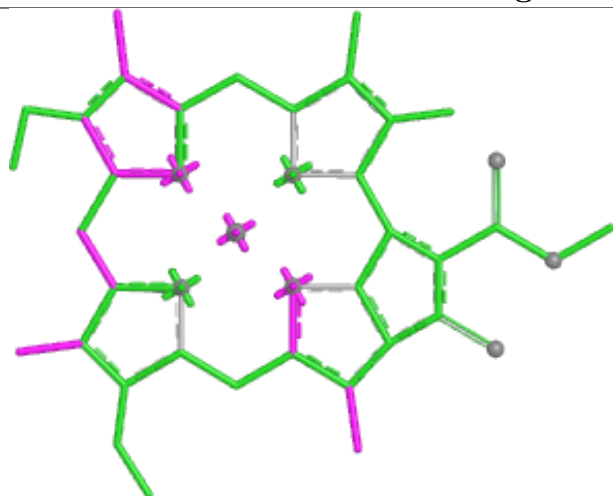


Ligand A86 12 306

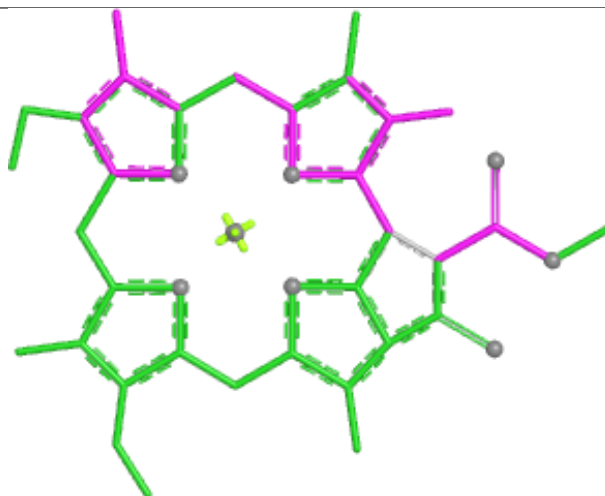




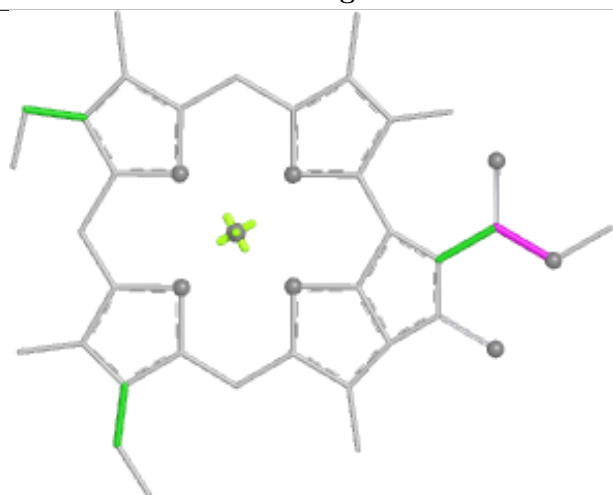
Ligand CLA P 610



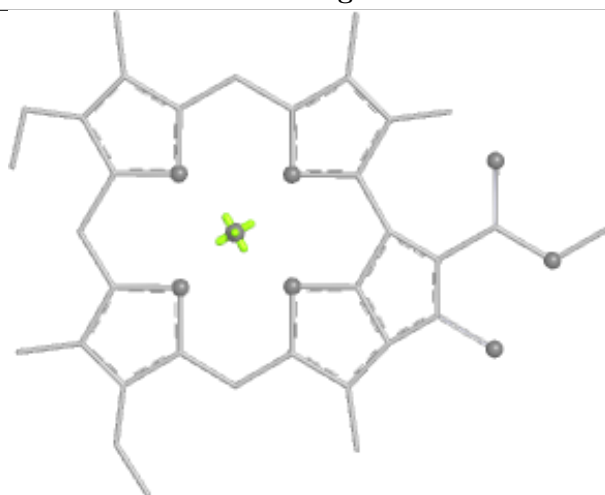
Bond lengths



Bond angles

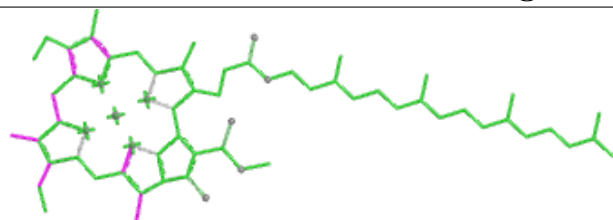


Torsions

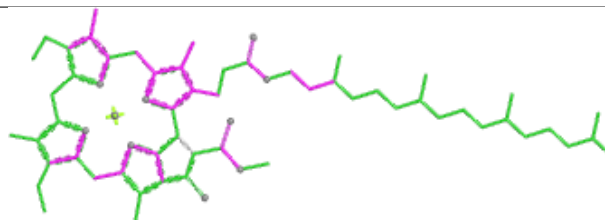


Rings

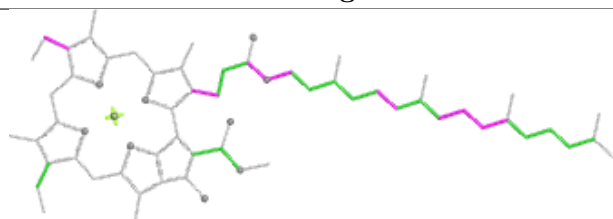
Ligand CLA 9 313



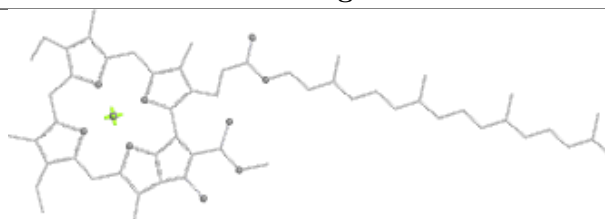
Bond lengths



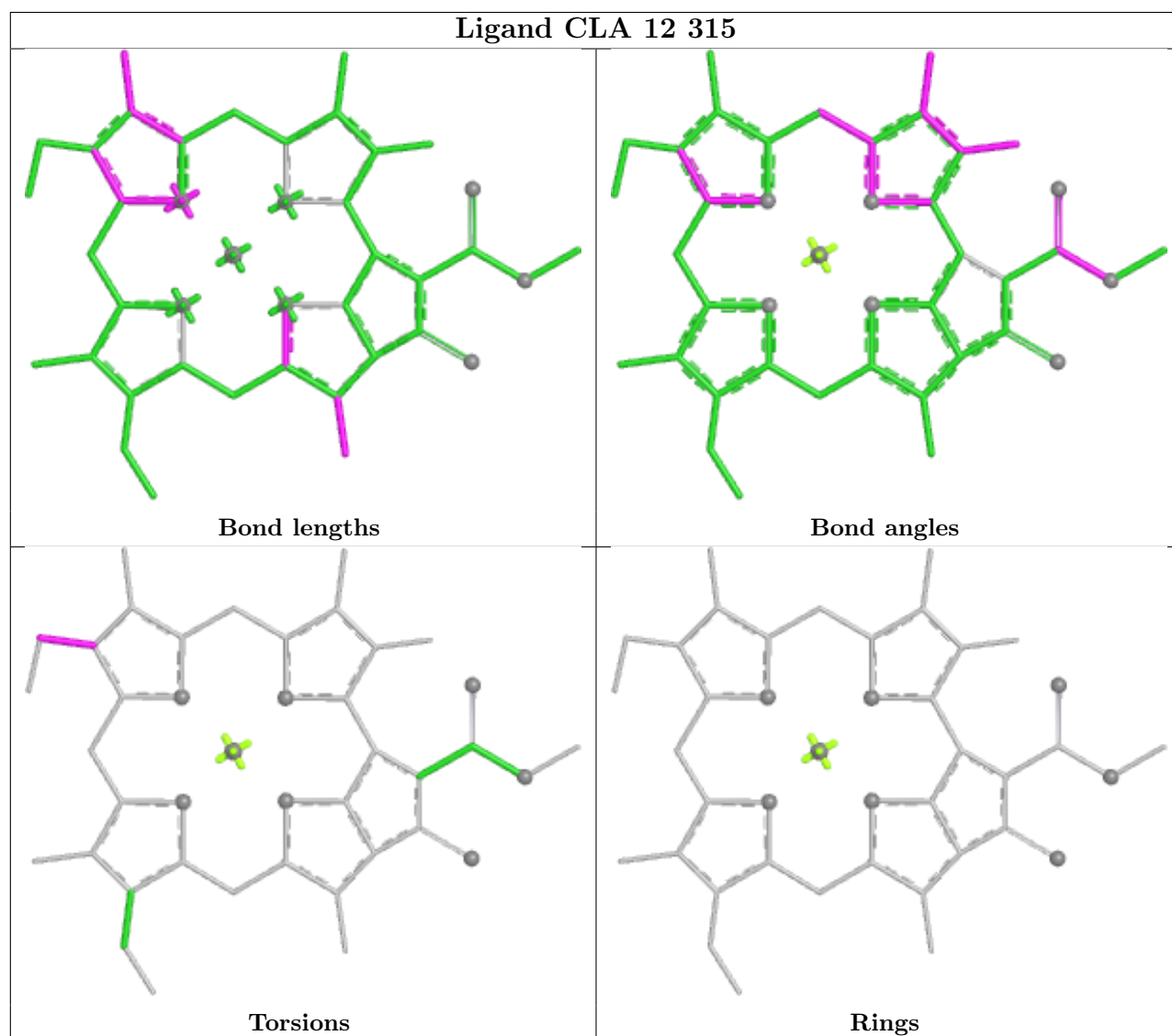
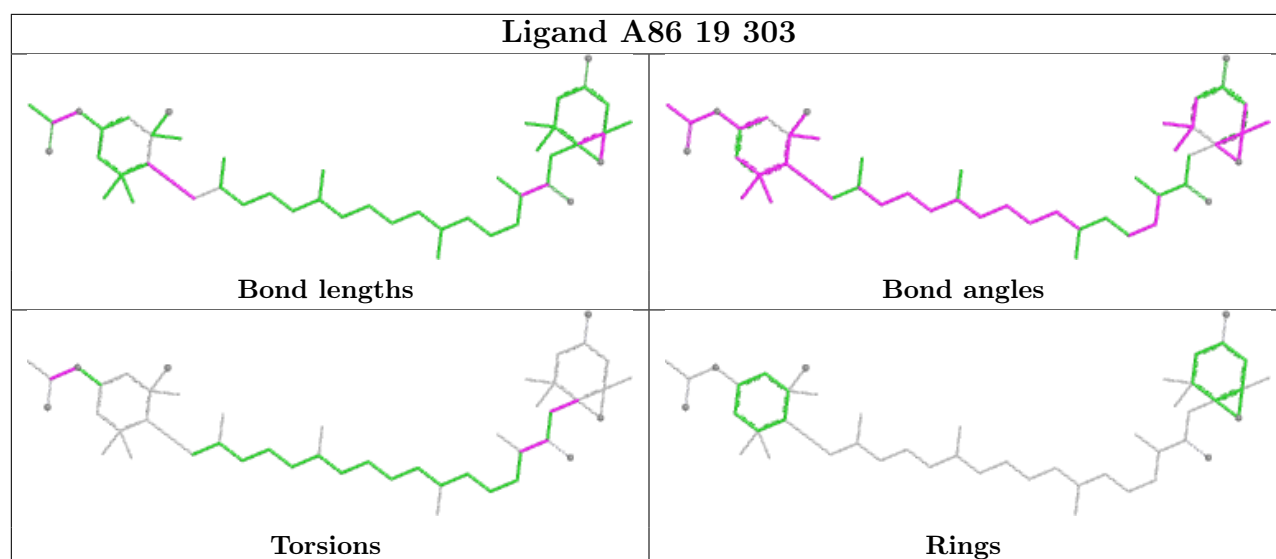
Bond angles



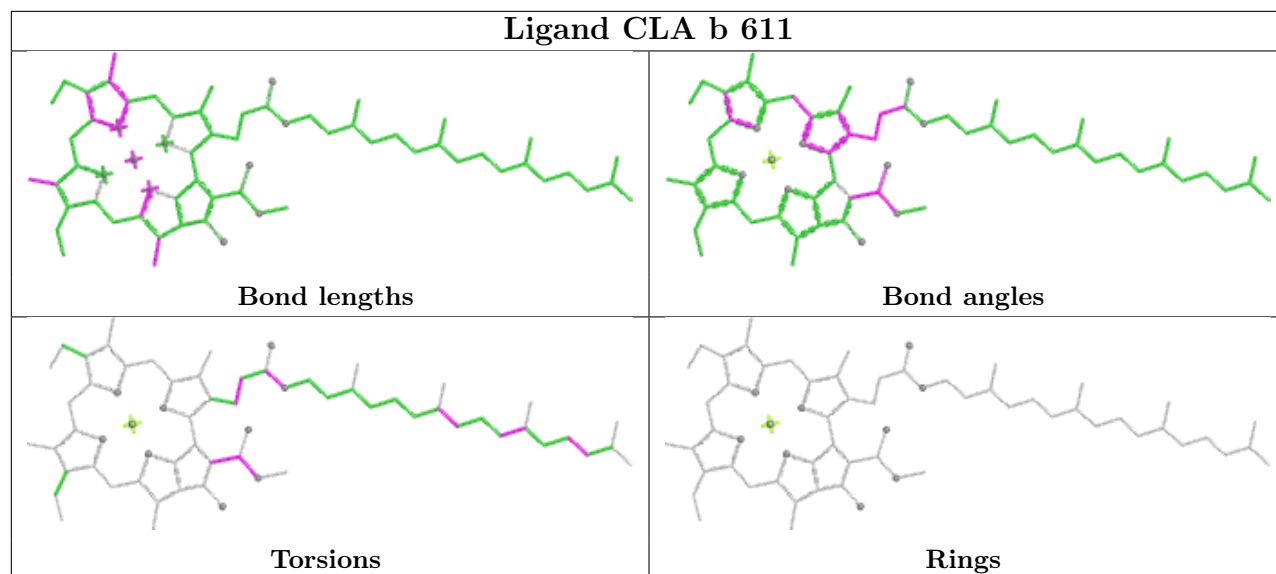
Torsions



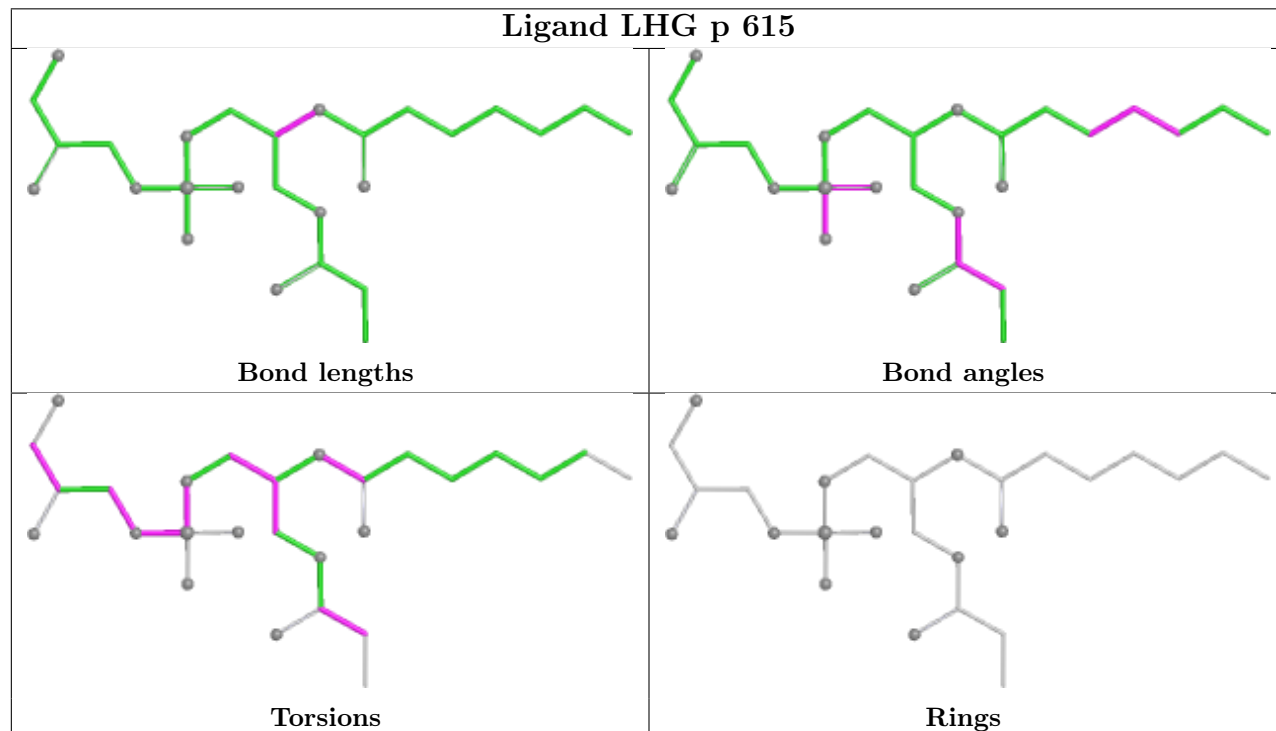
Rings

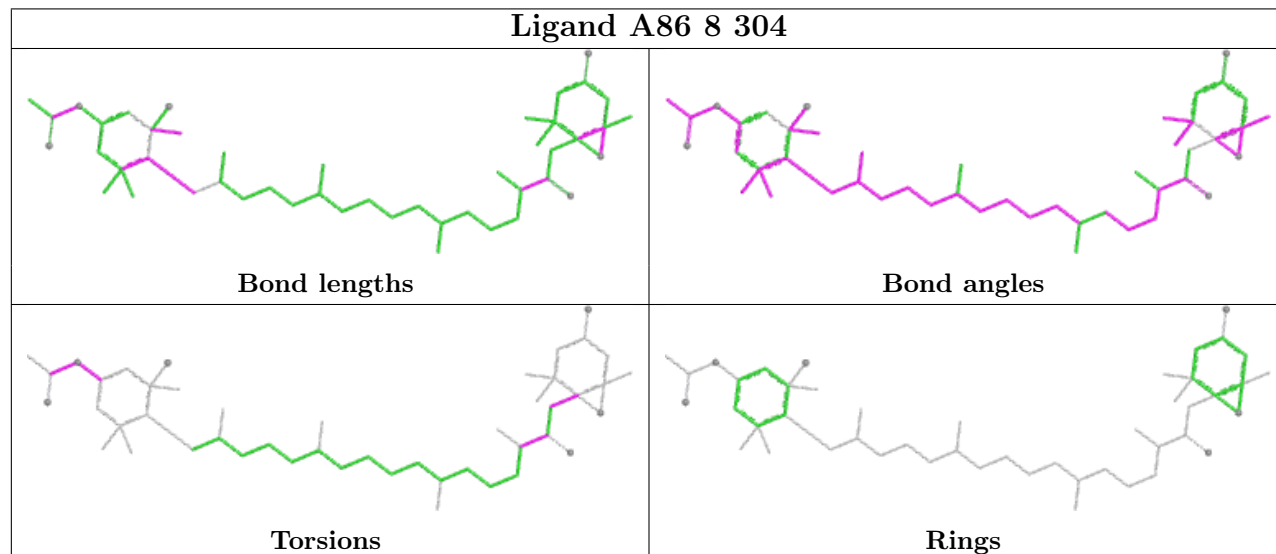
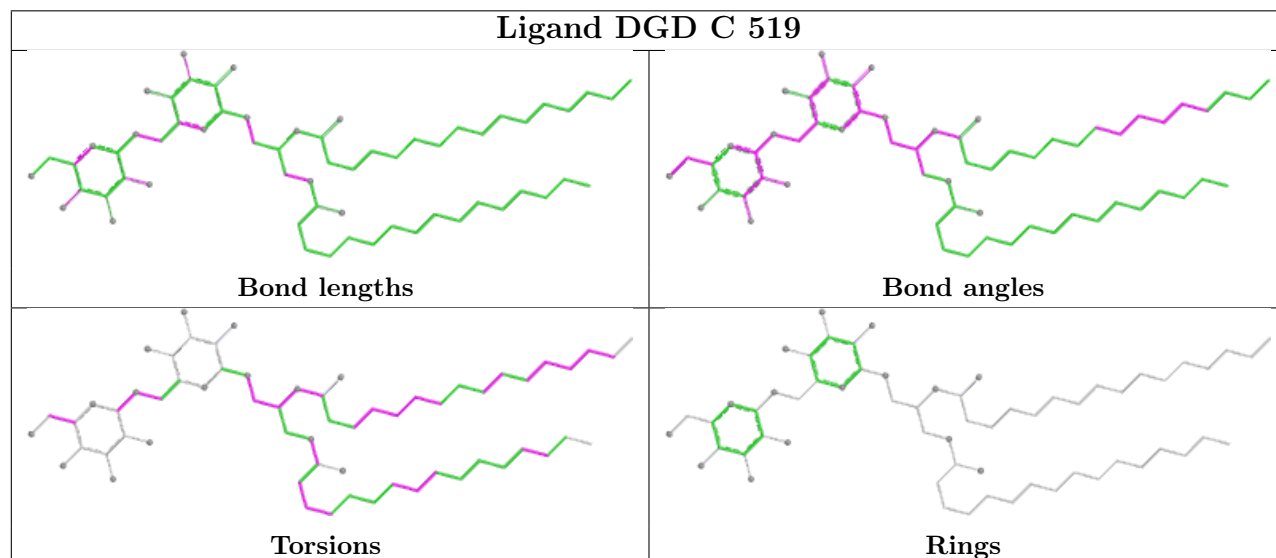
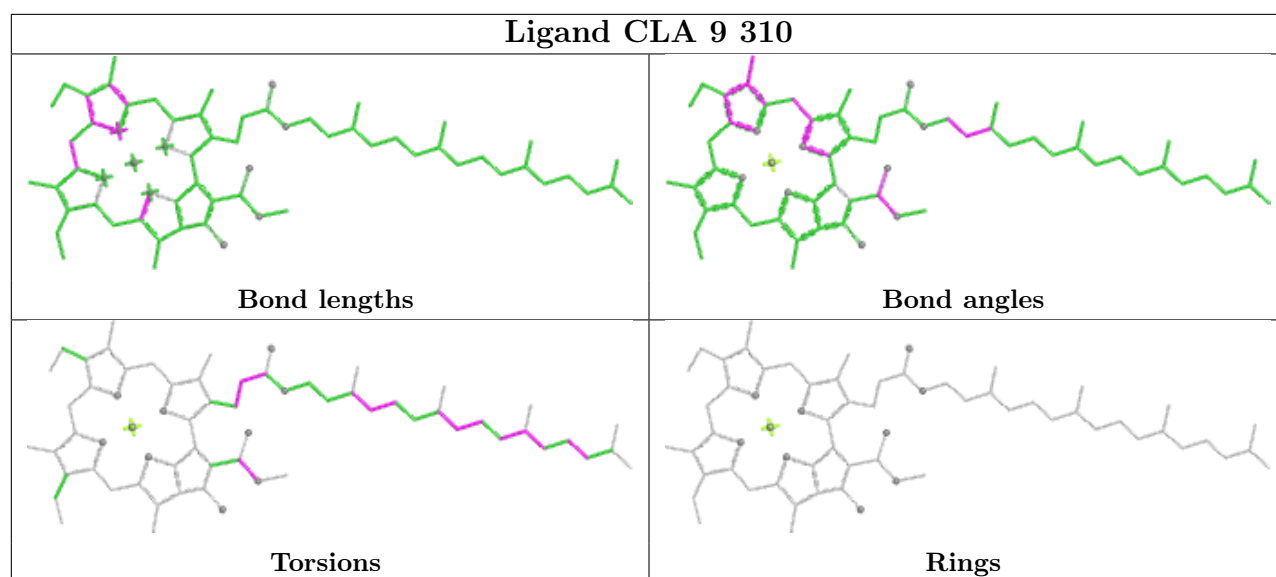


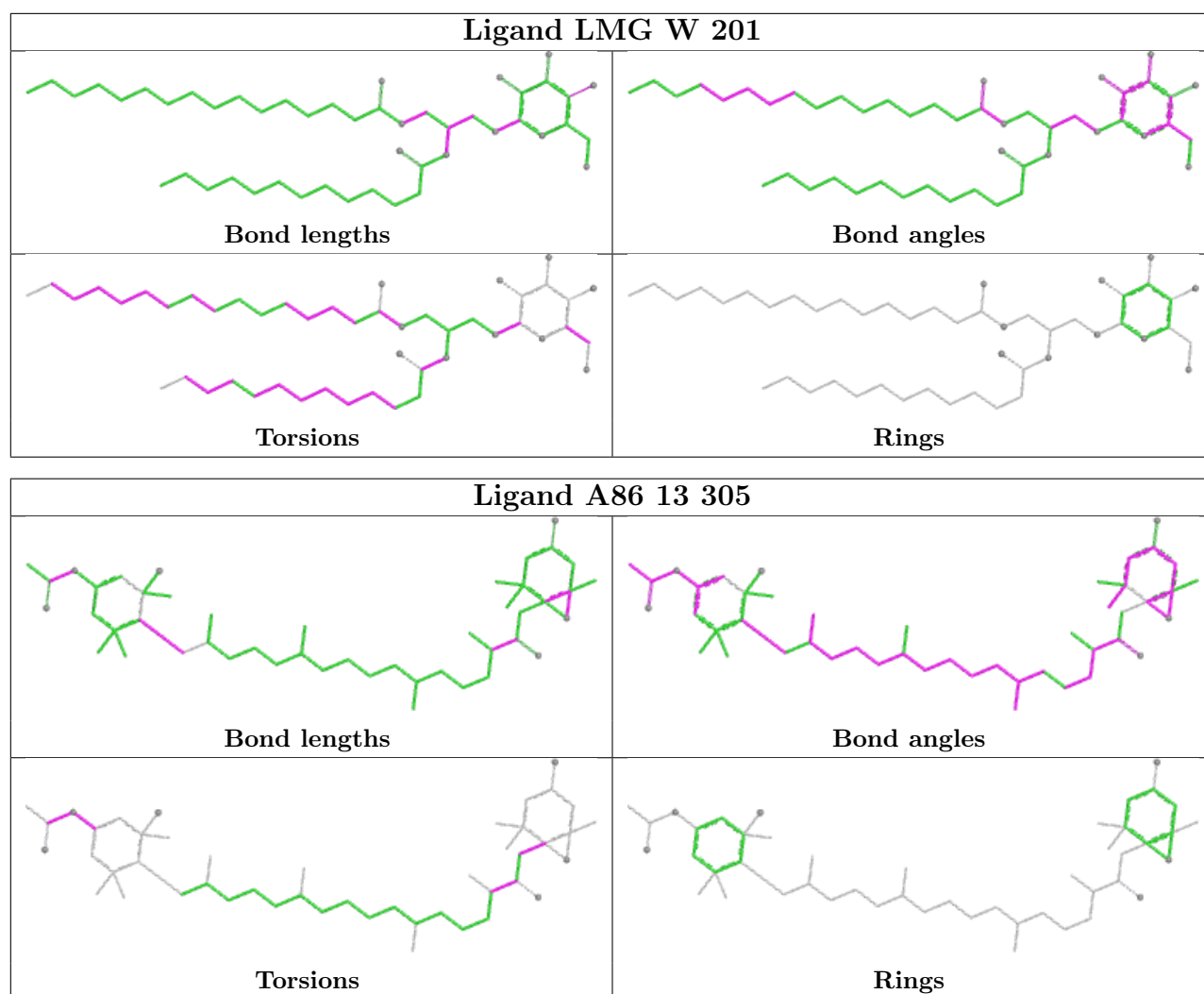
Ligand CLA b 611



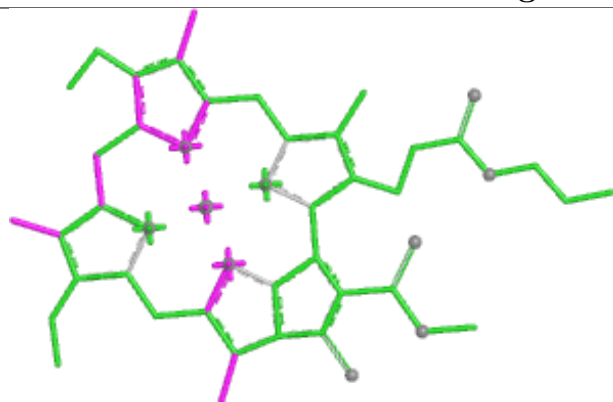
Ligand LHG p 615



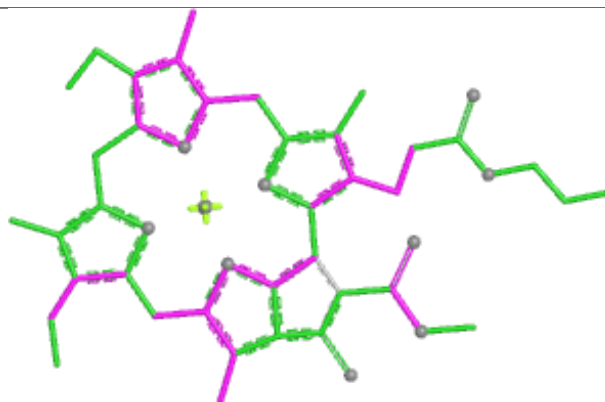




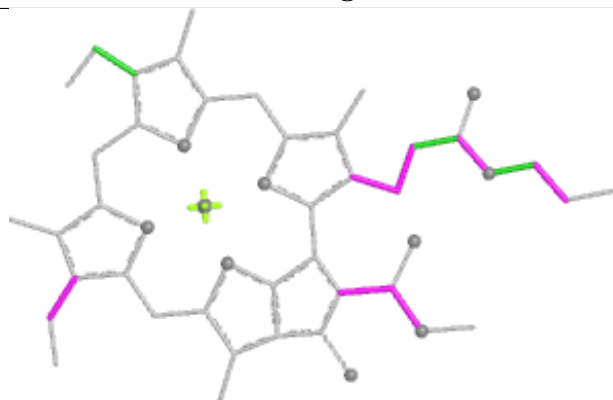
Ligand CLA 2 312



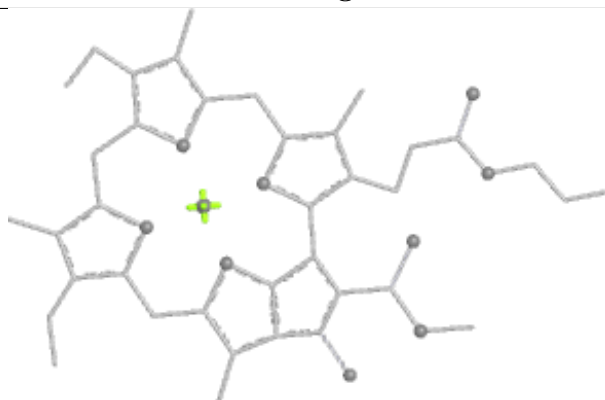
Bond lengths



Bond angles

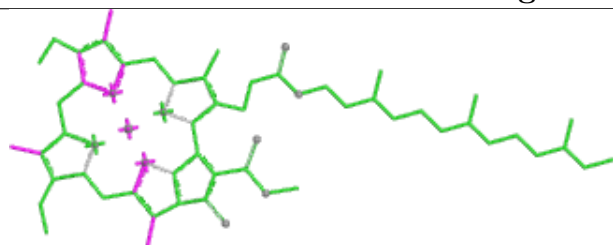


Torsions

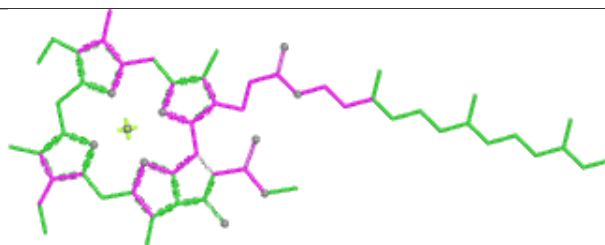


Rings

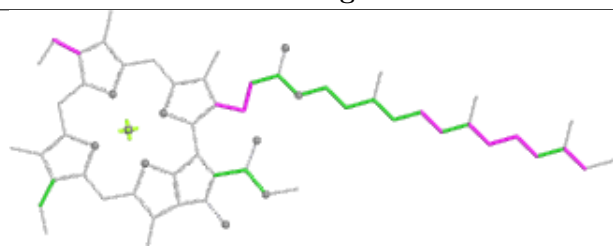
Ligand CLA 1 321



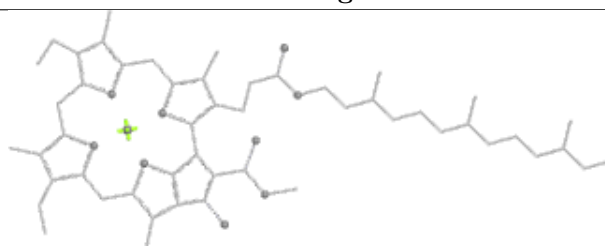
Bond lengths



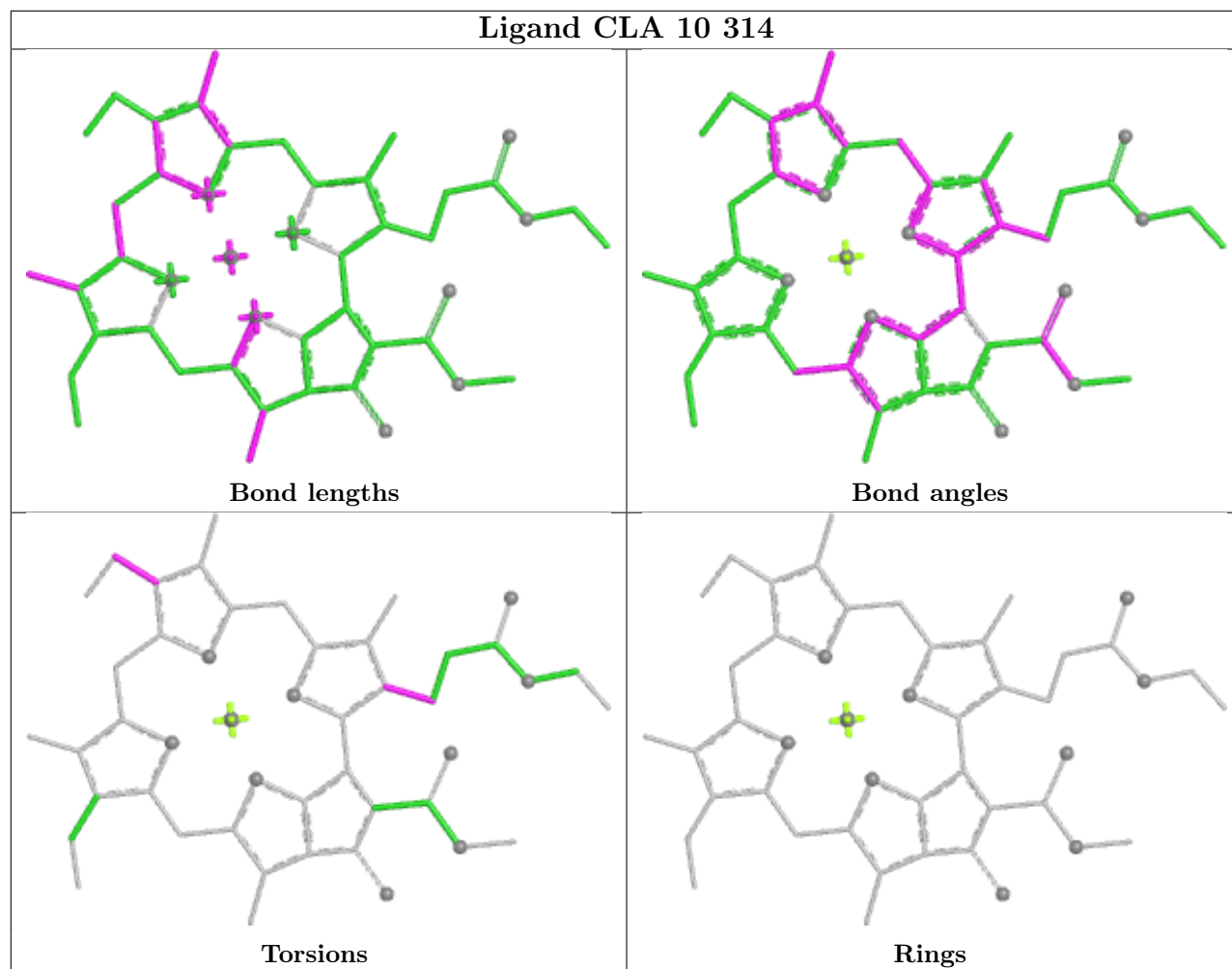
Bond angles

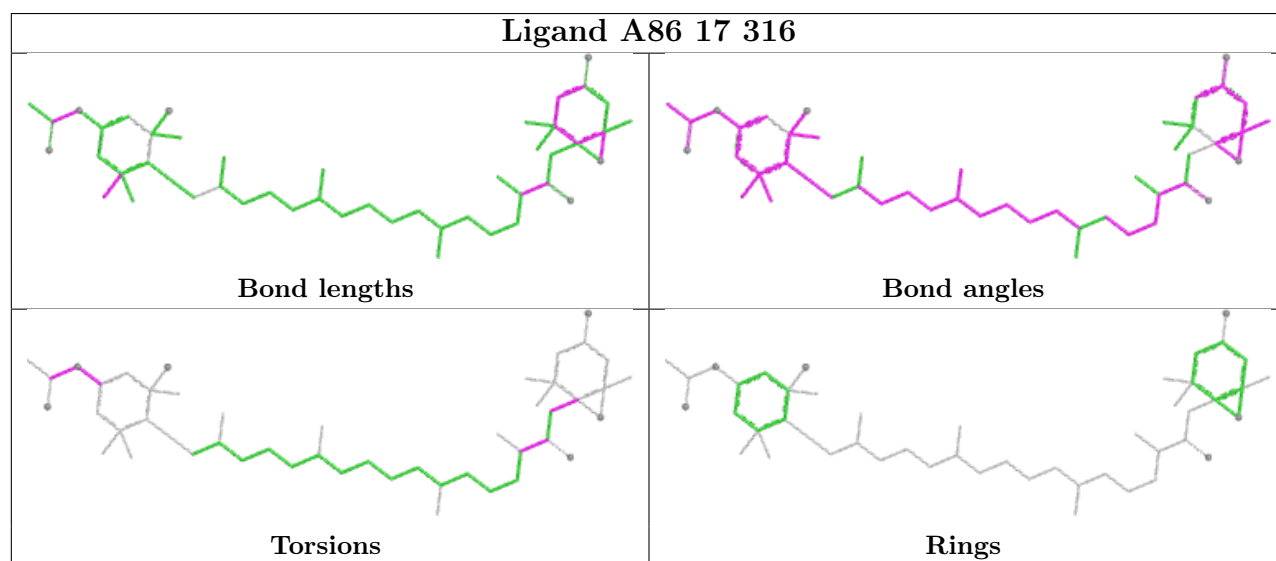
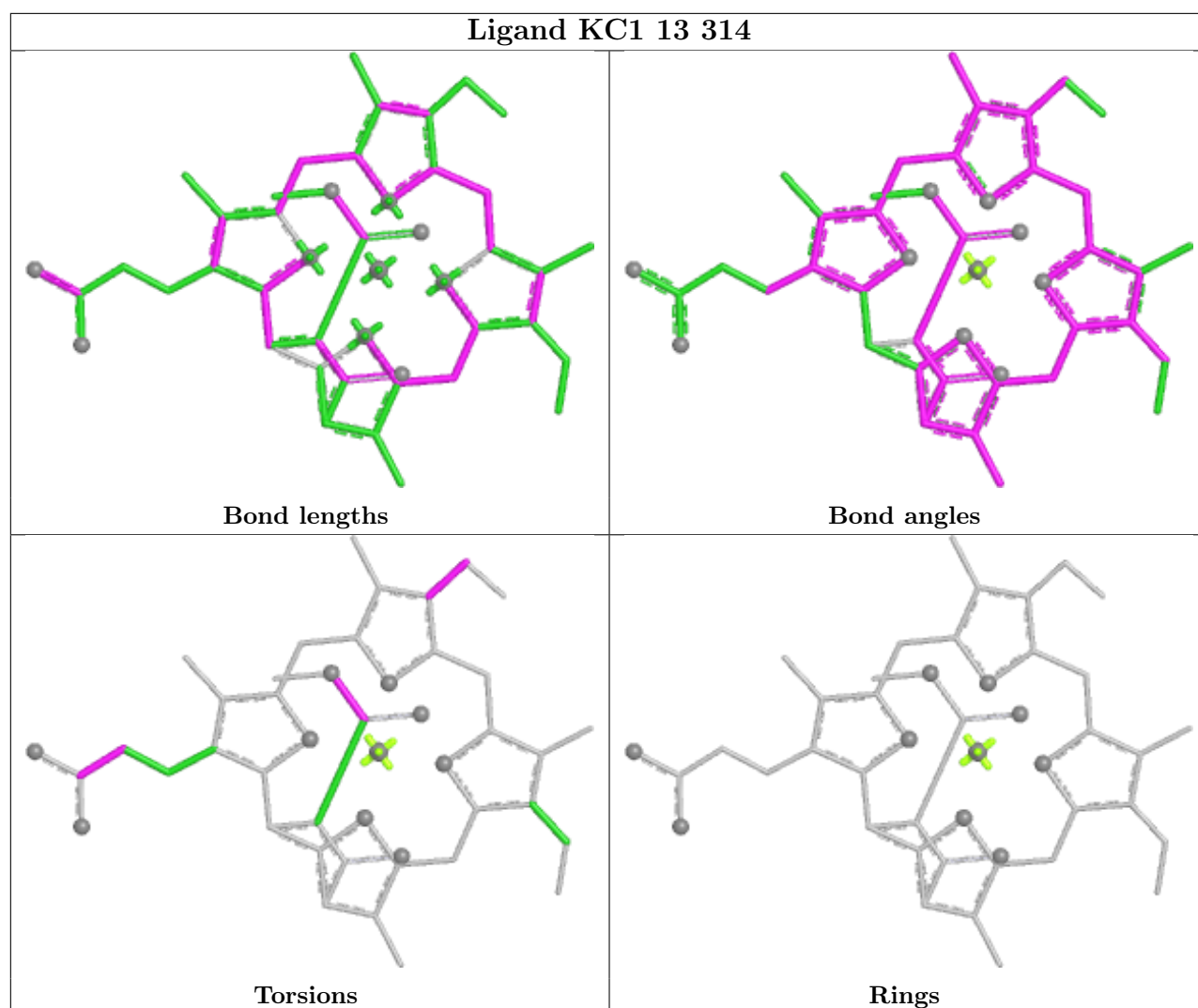


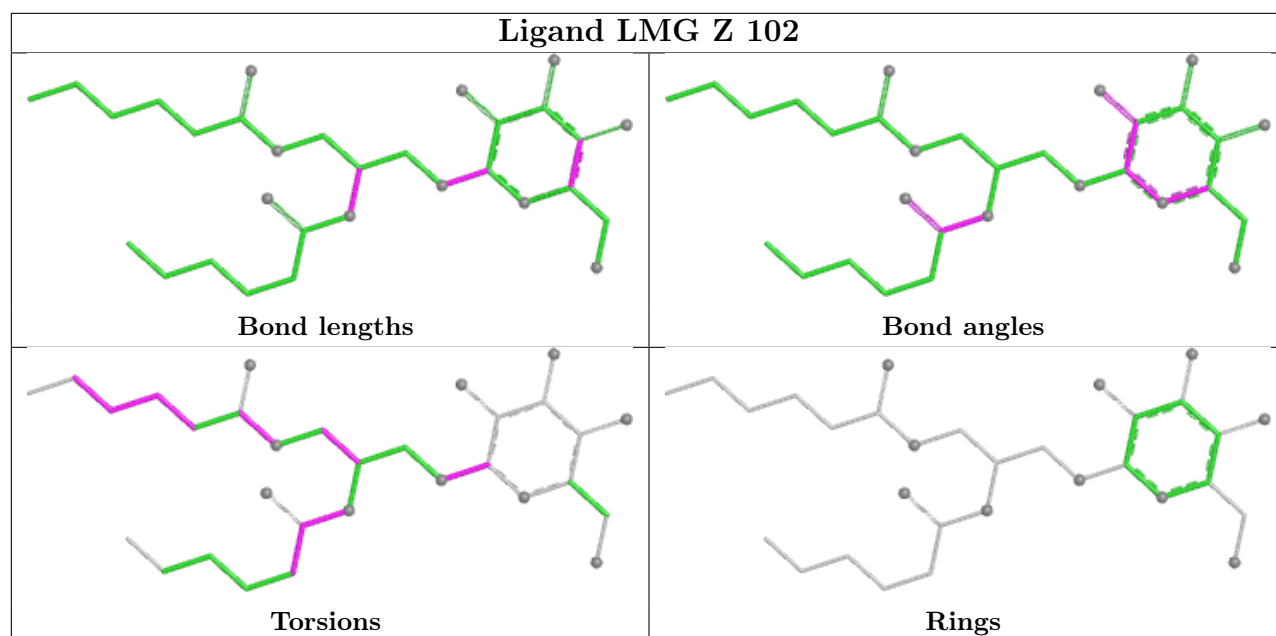
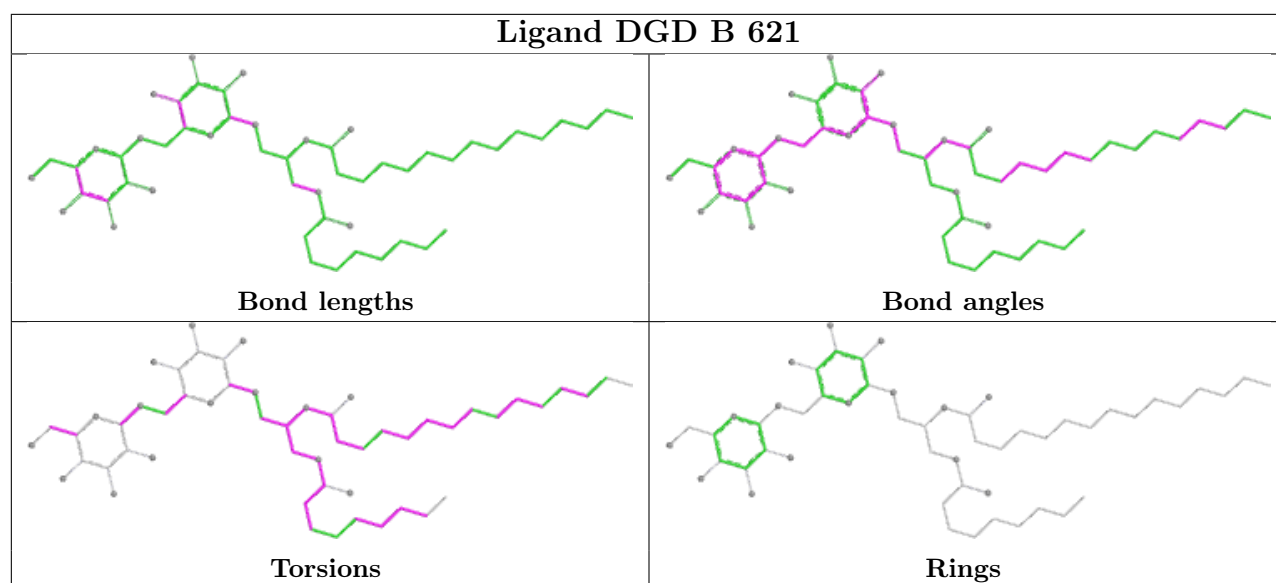
Torsions

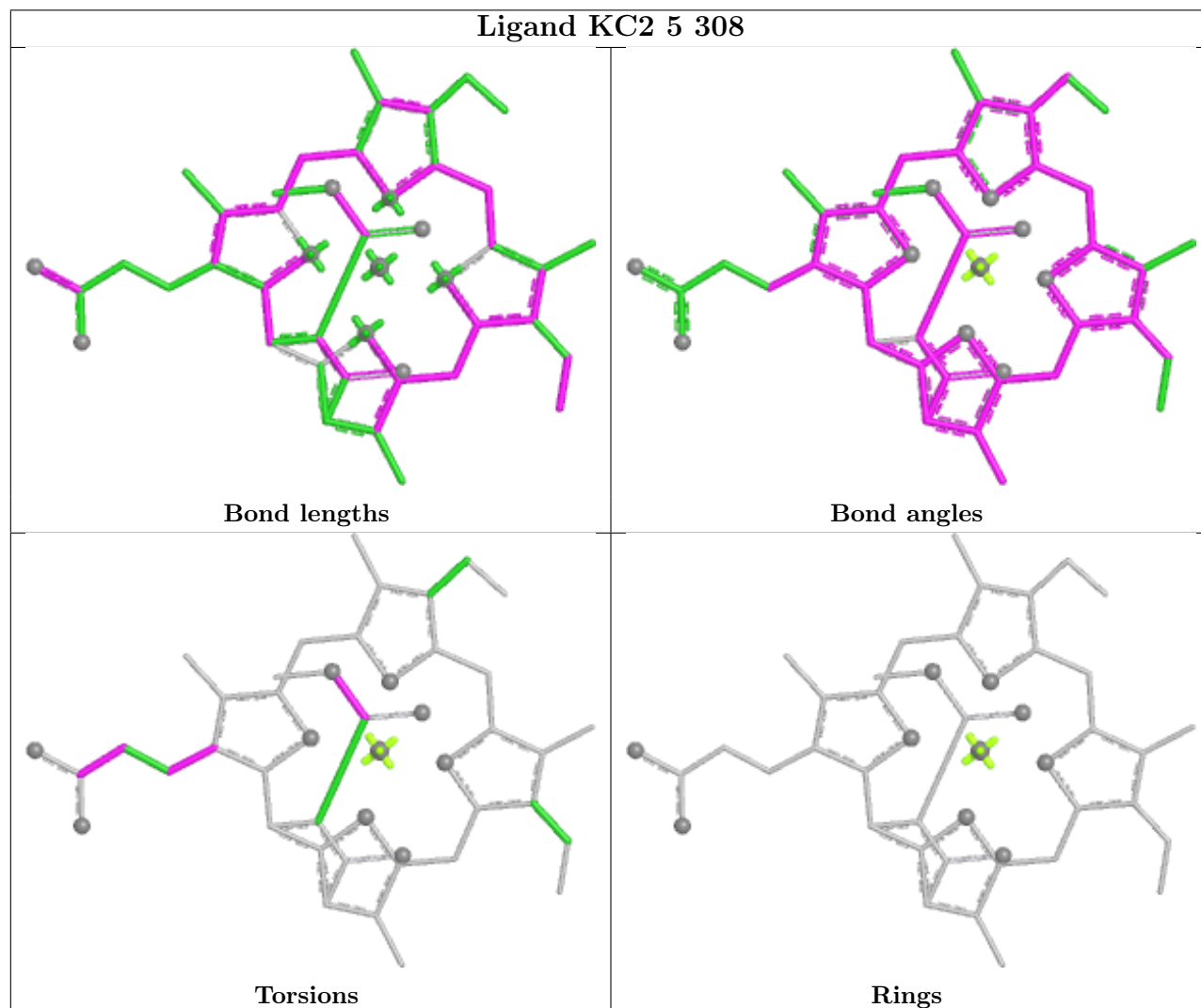
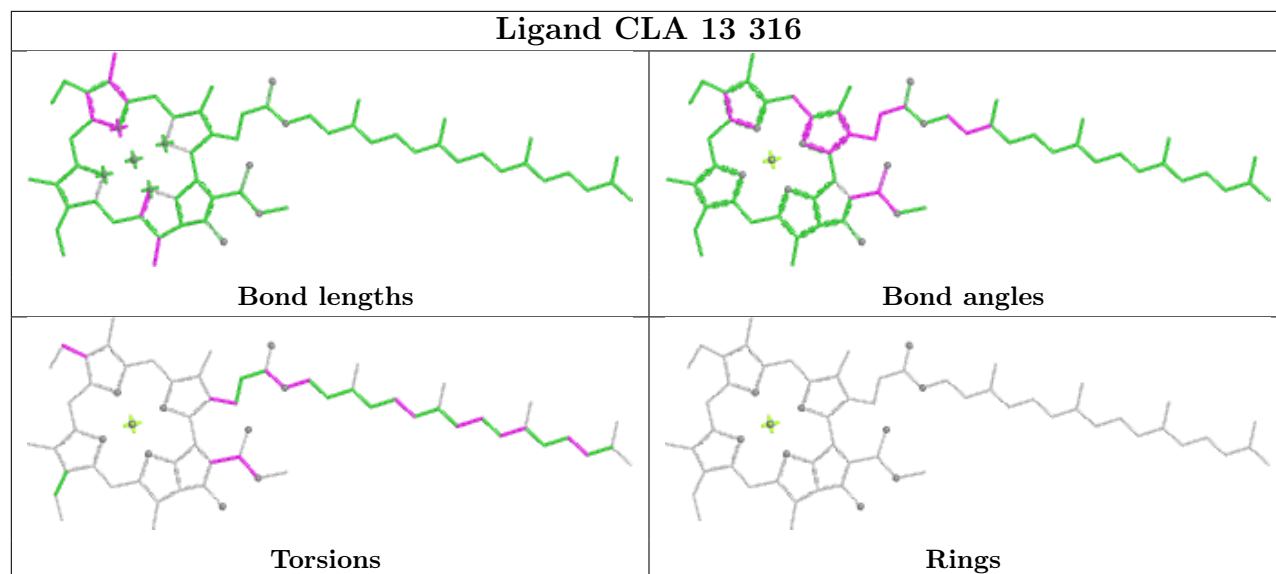


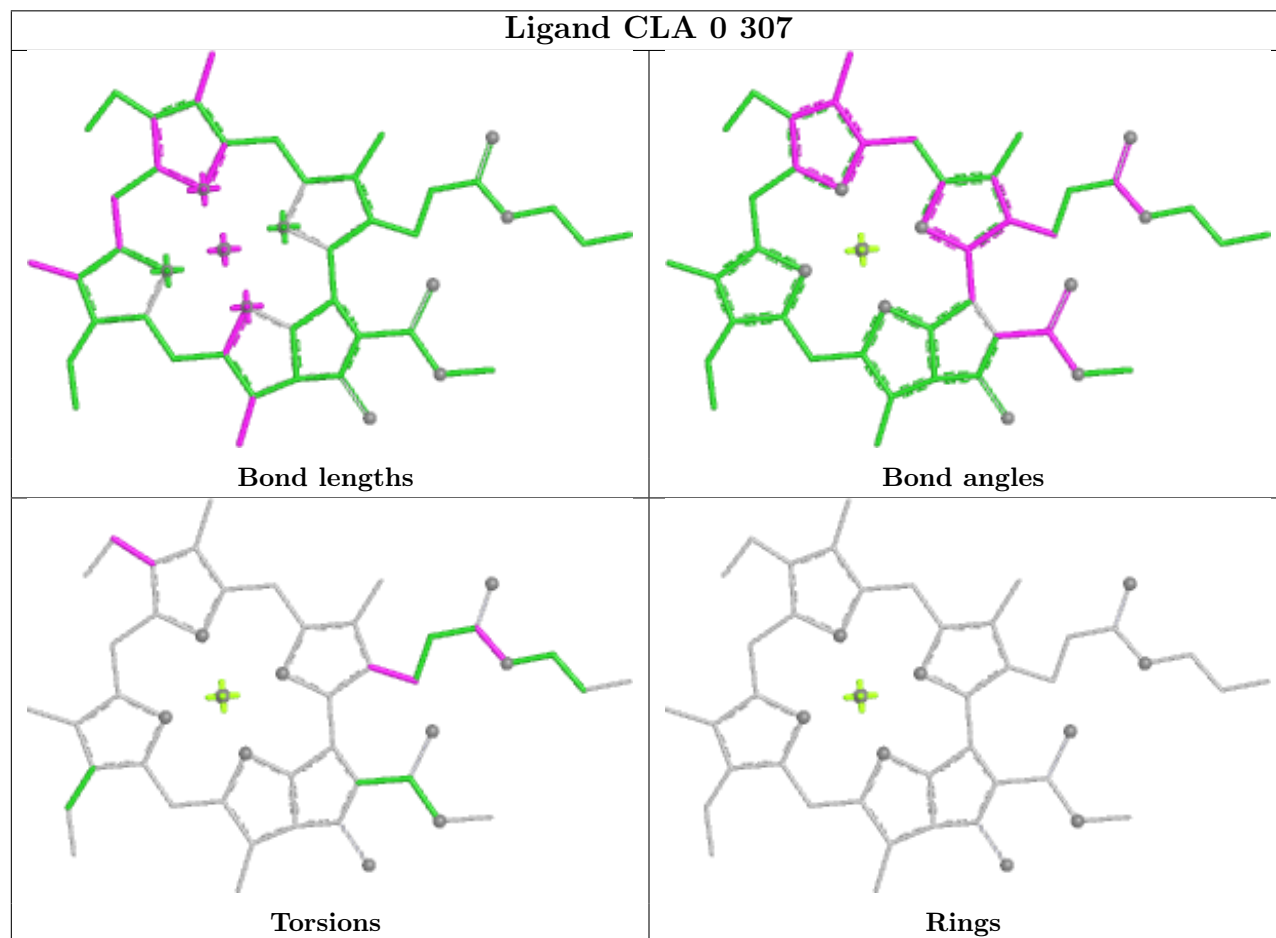
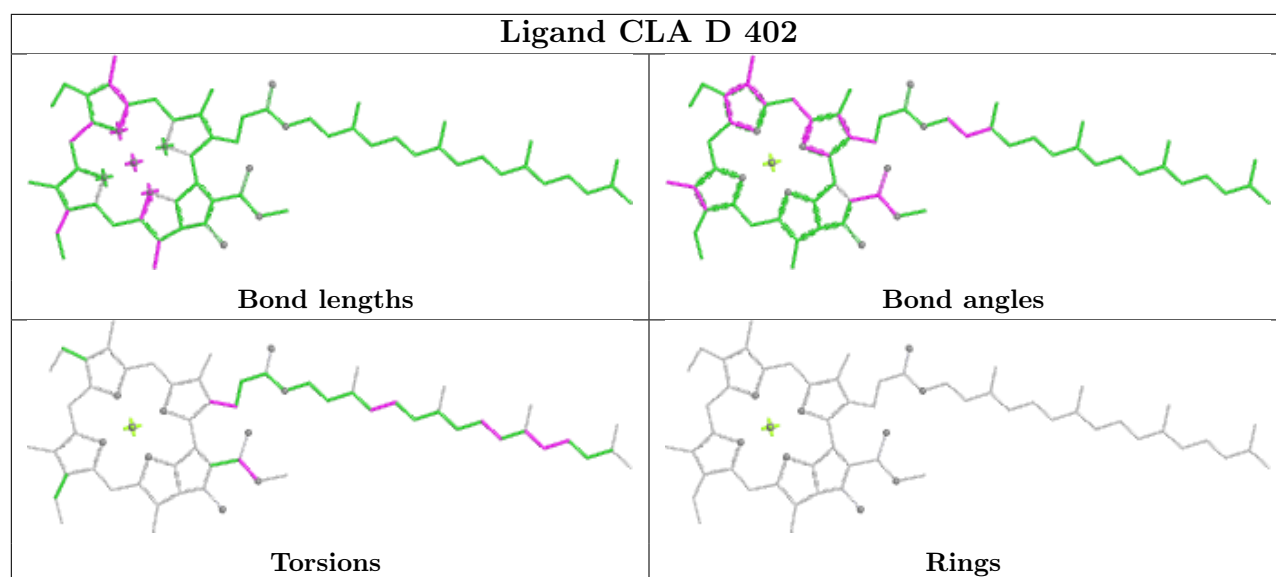
Rings

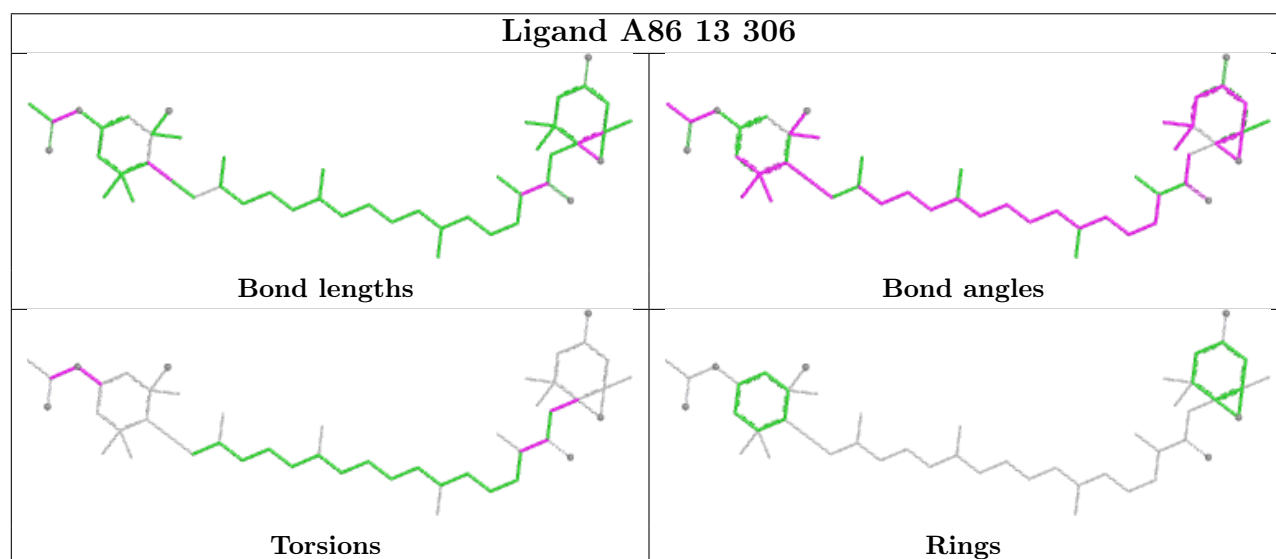
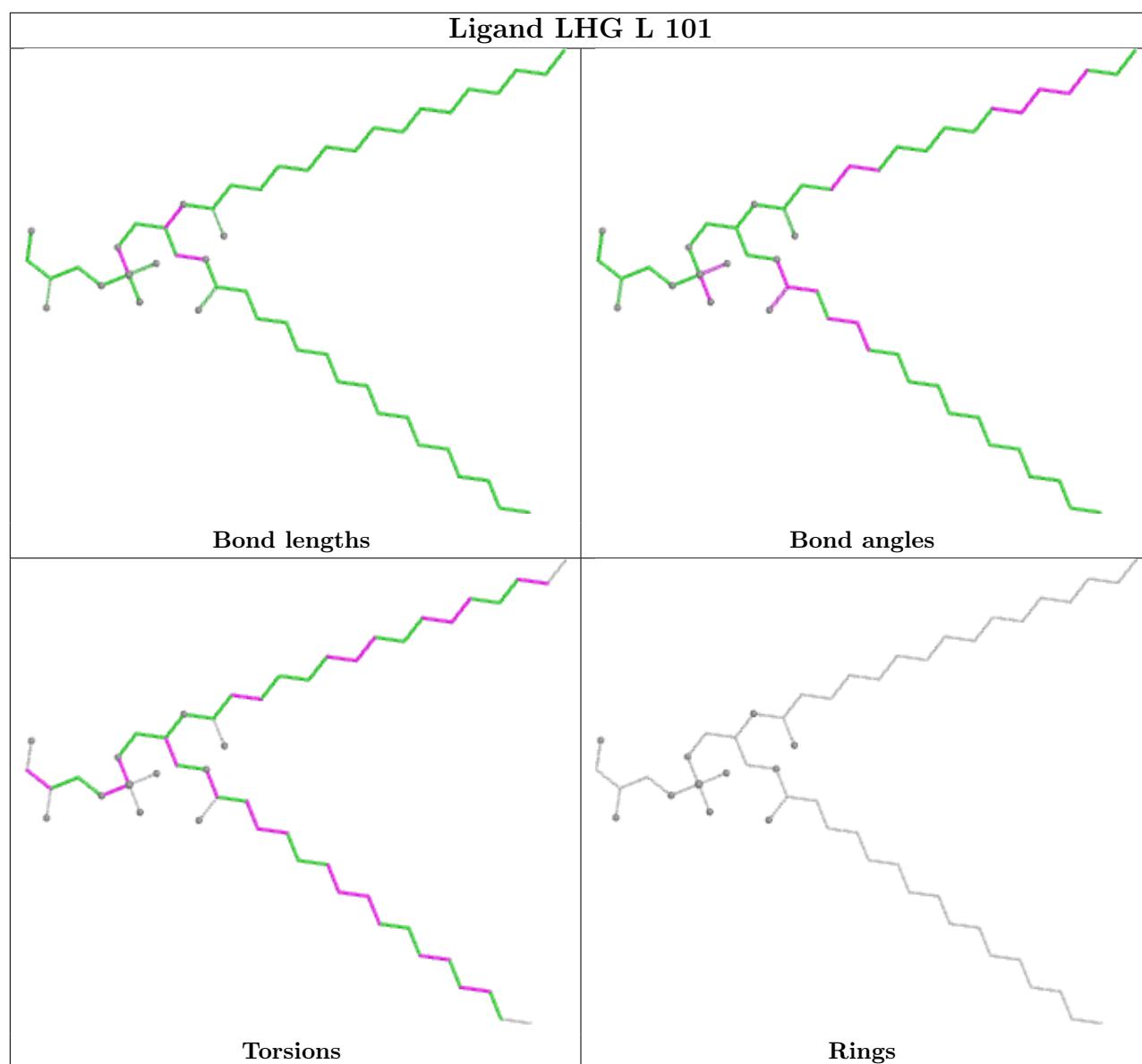


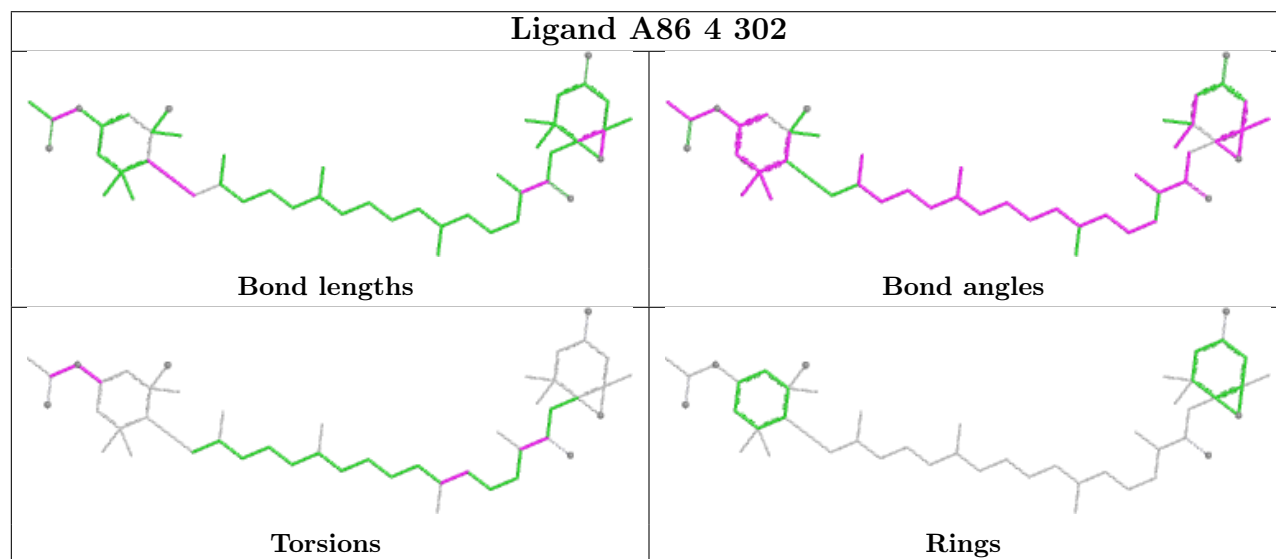
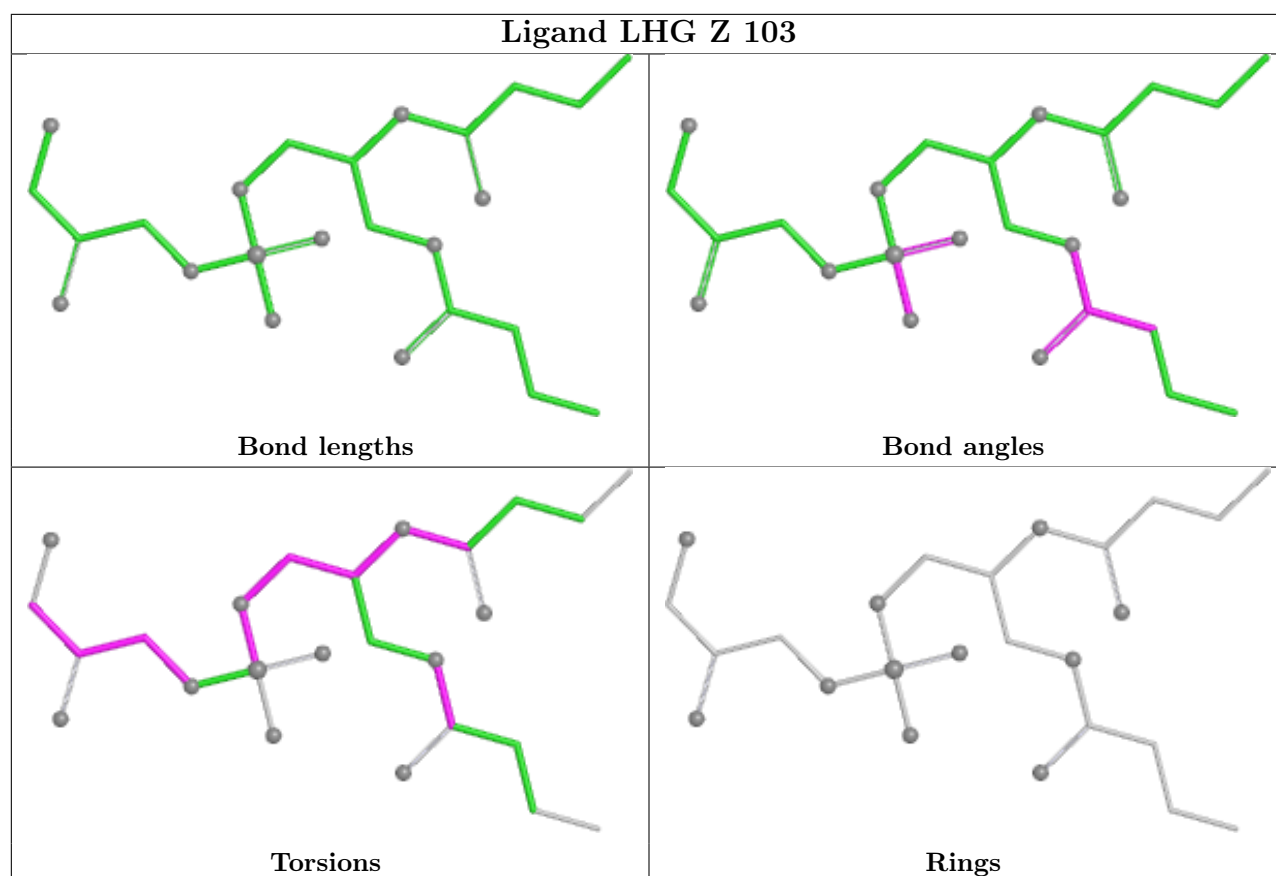


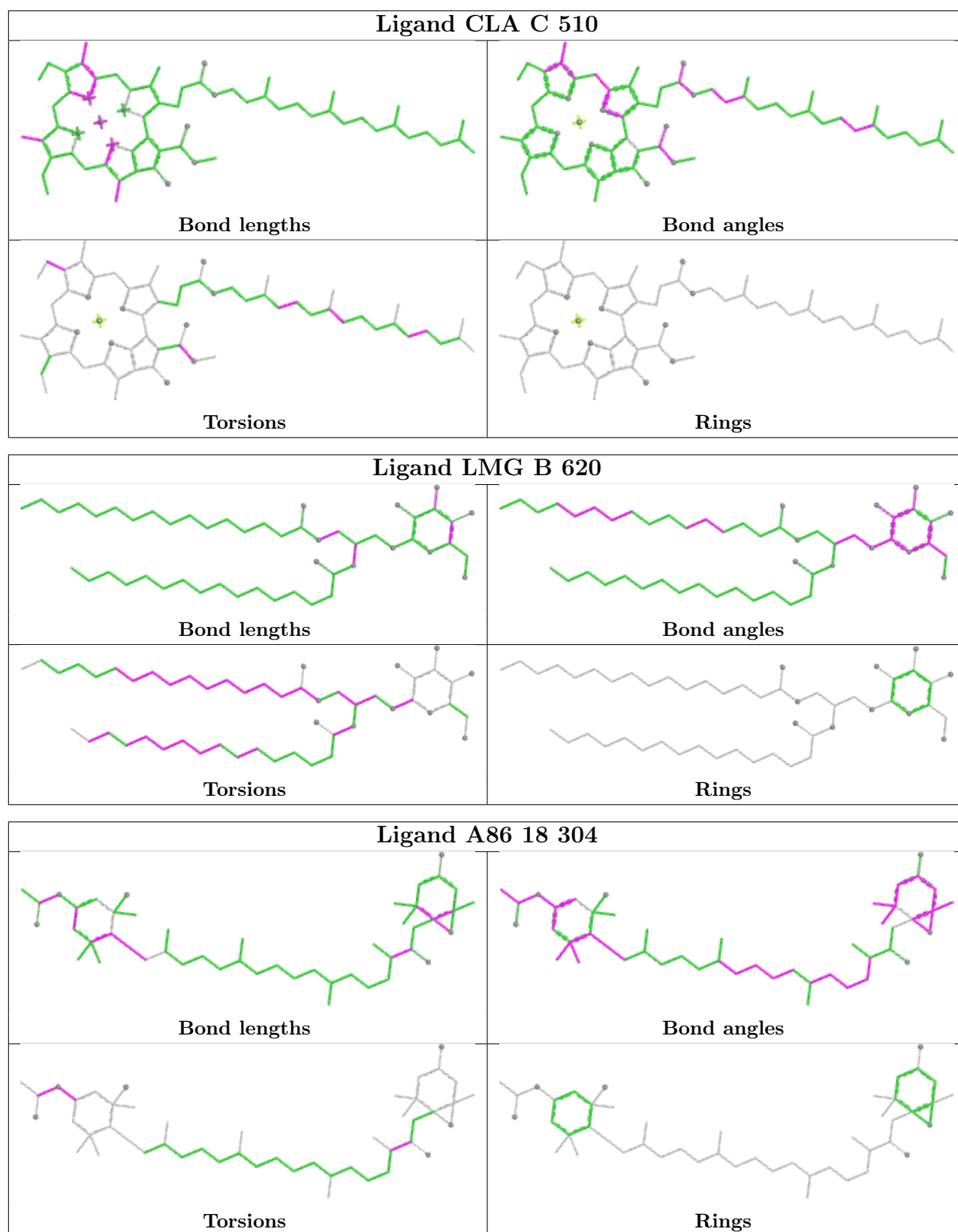


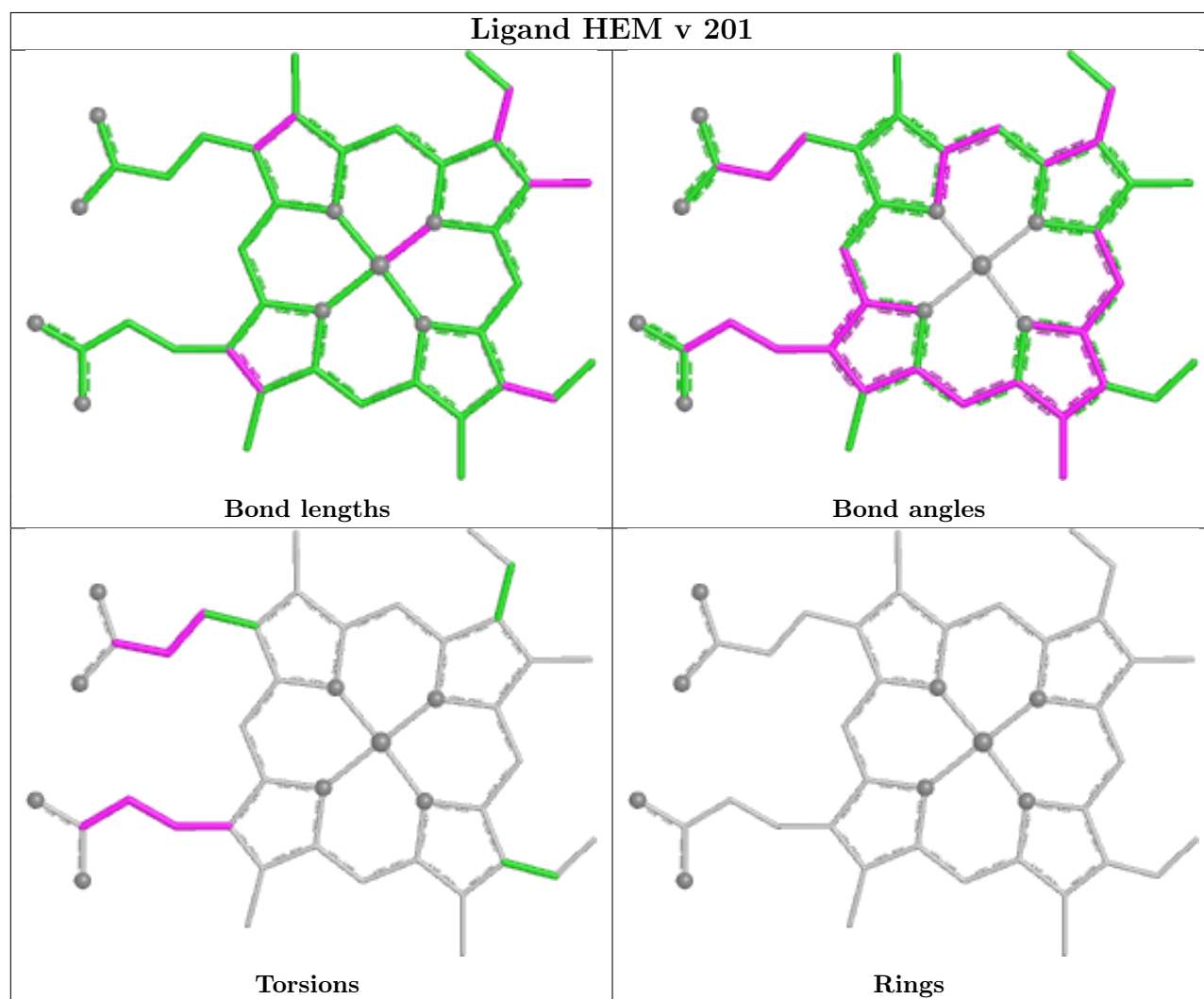
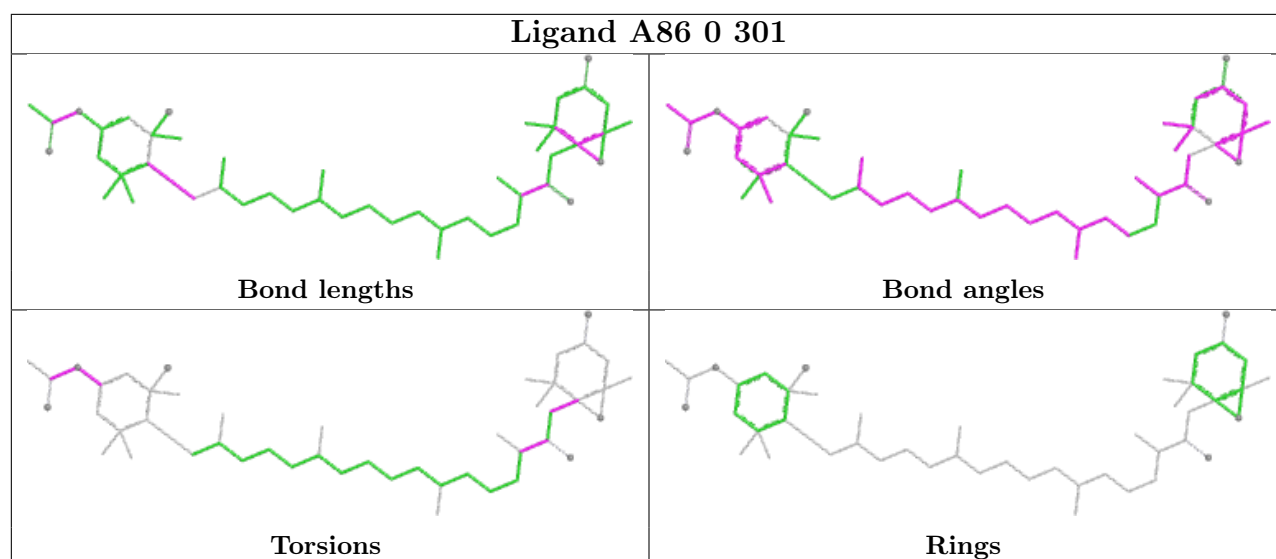


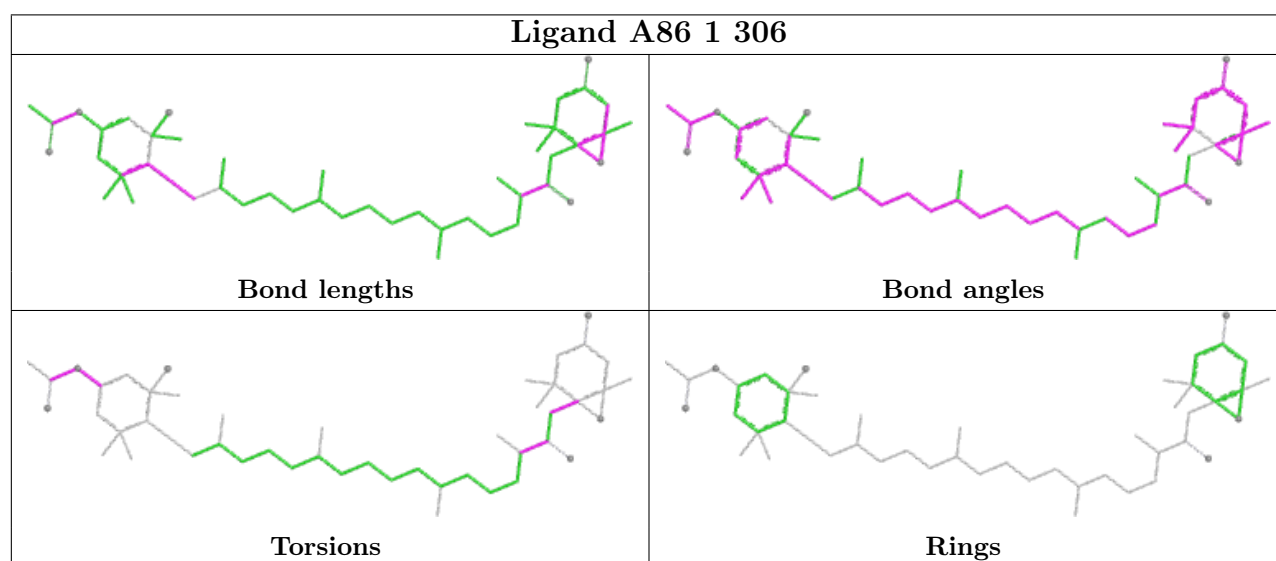
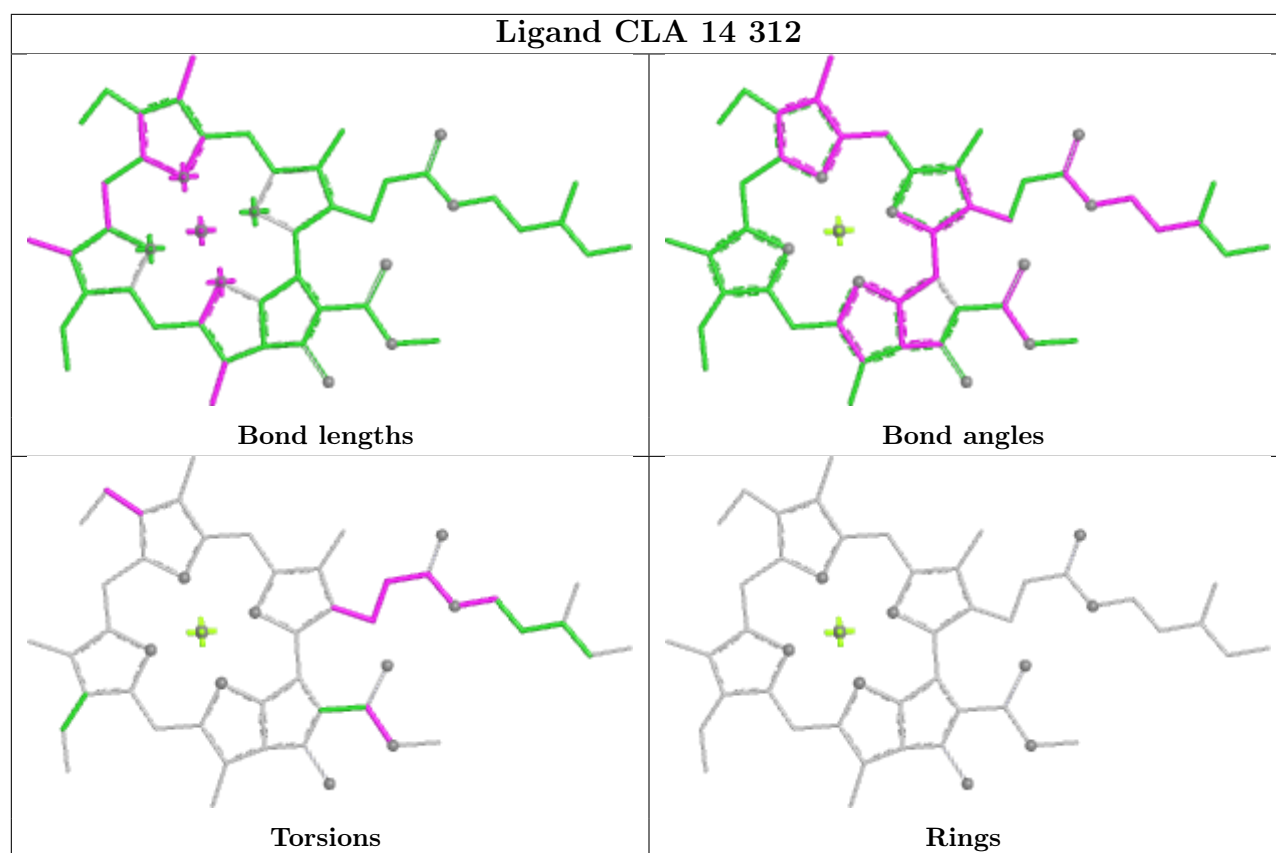


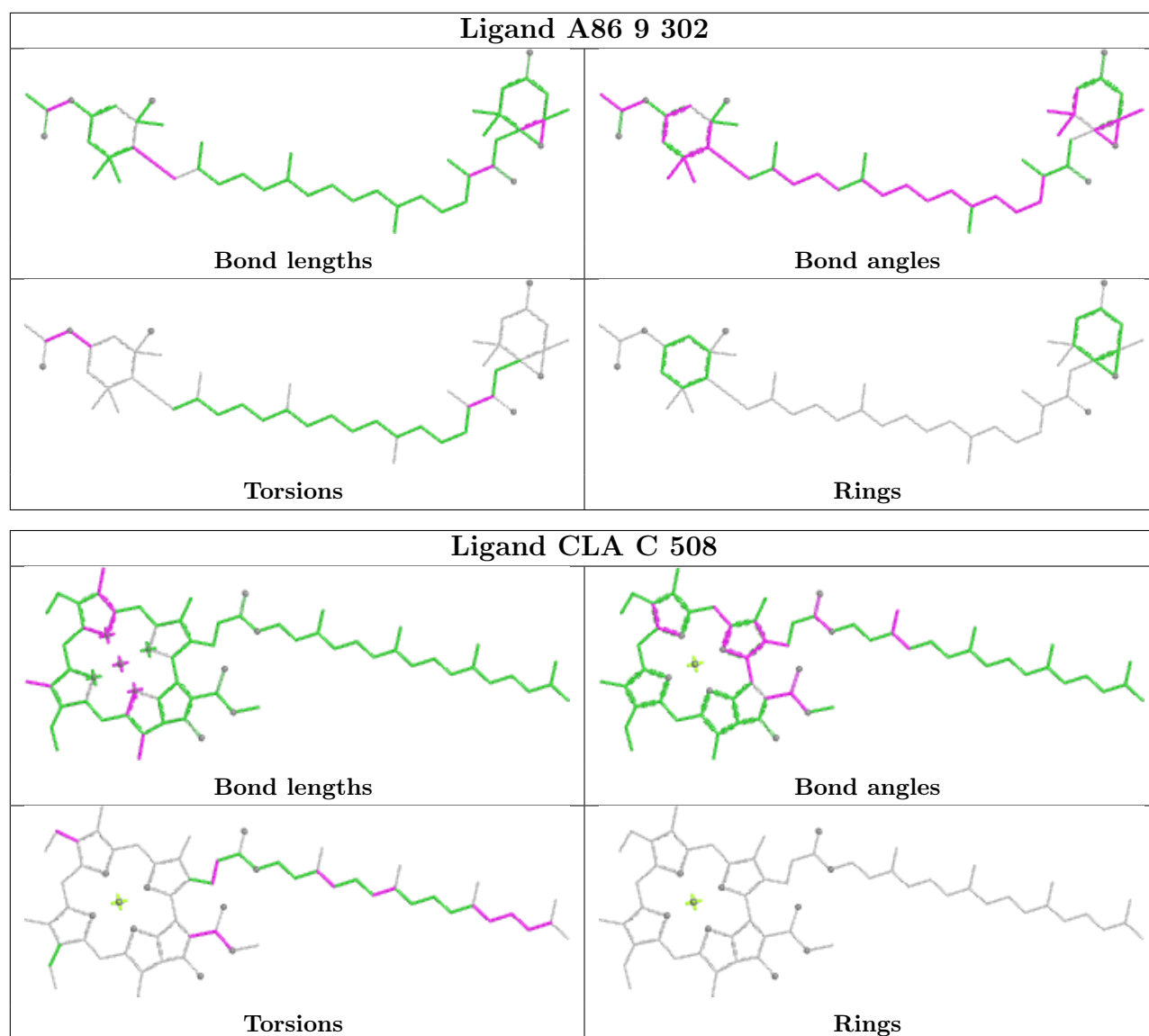




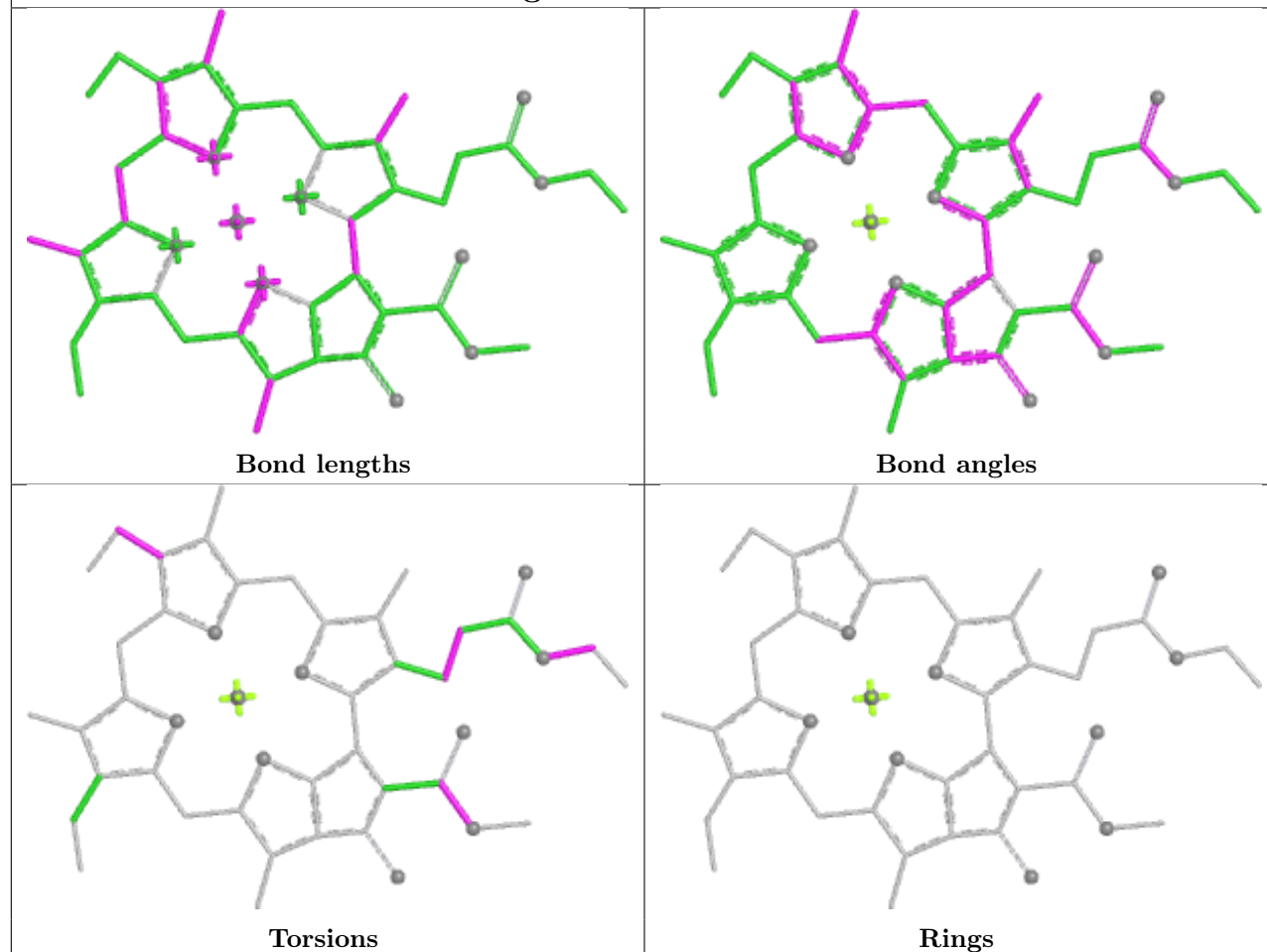




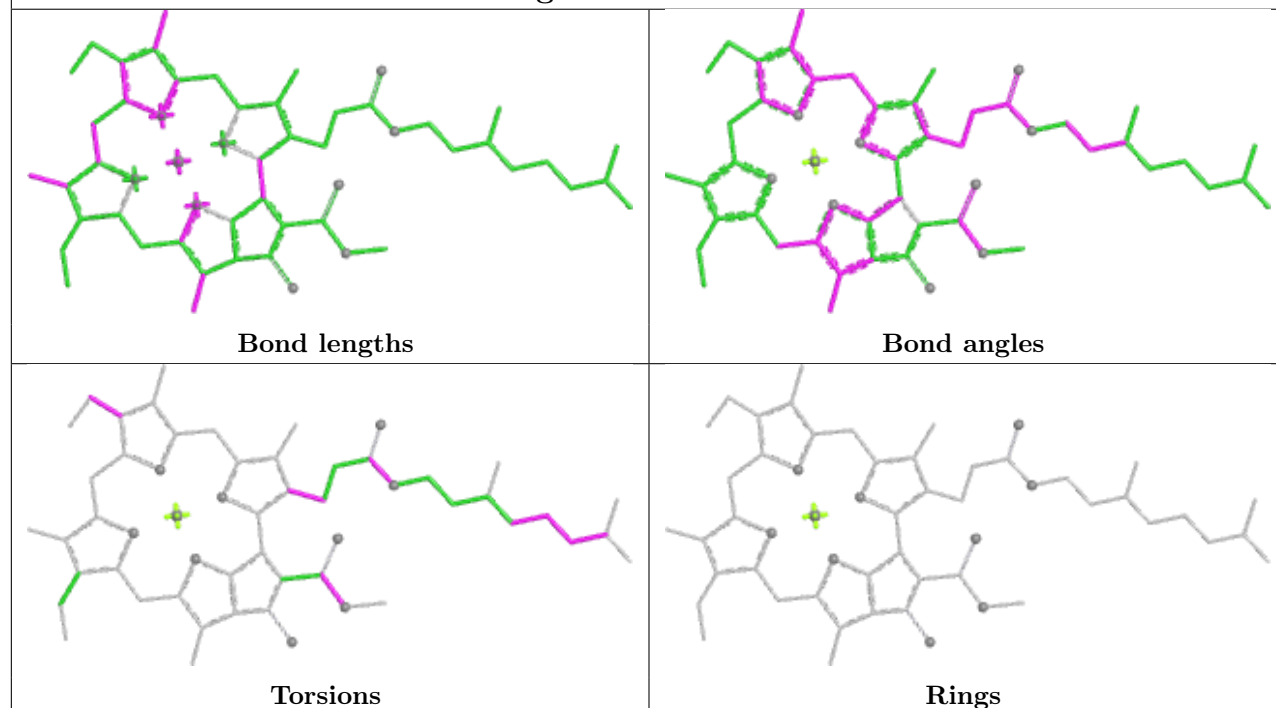




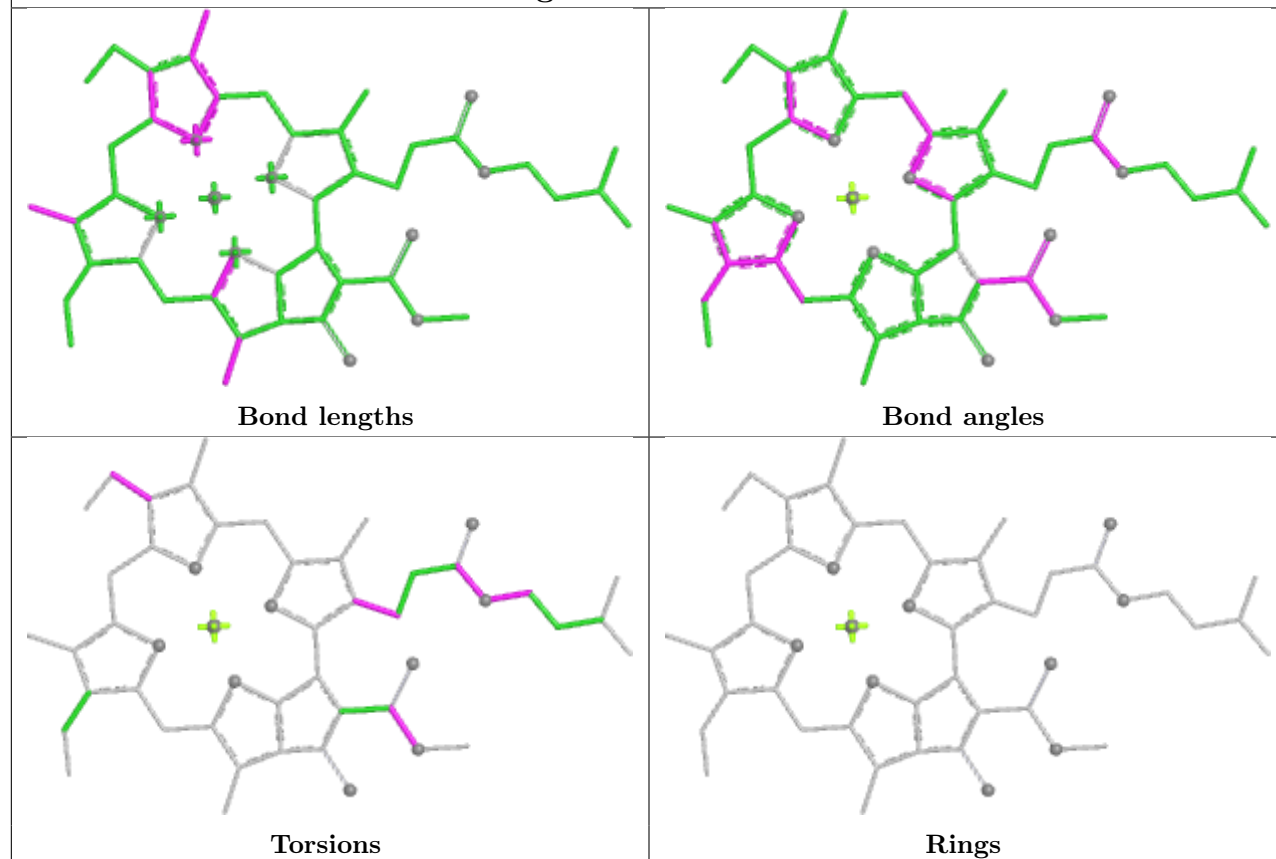
Ligand CLA 15 312



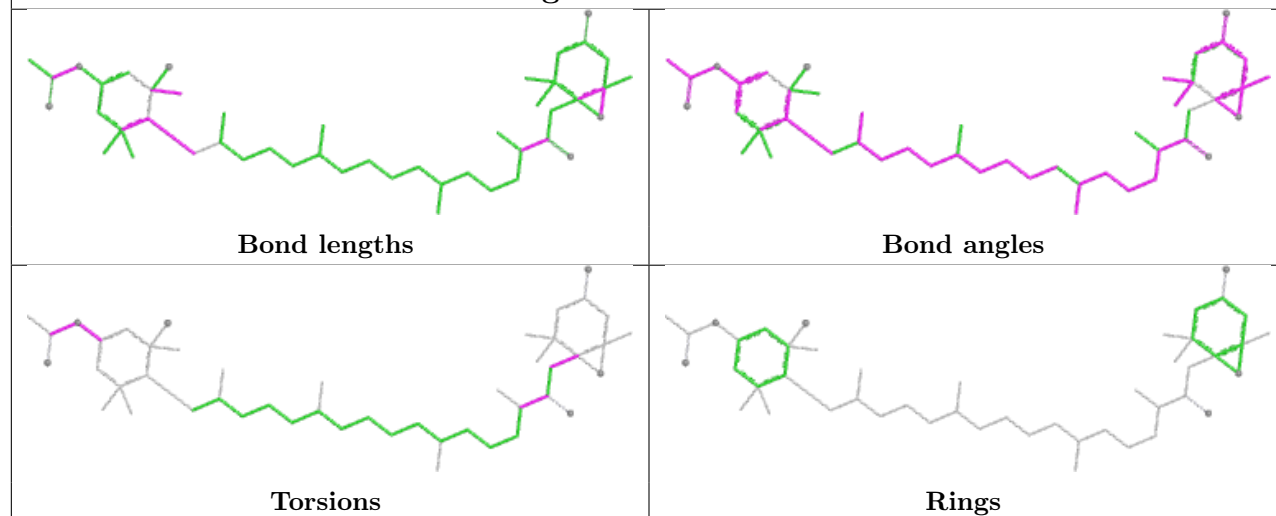
Ligand CLA 8 313



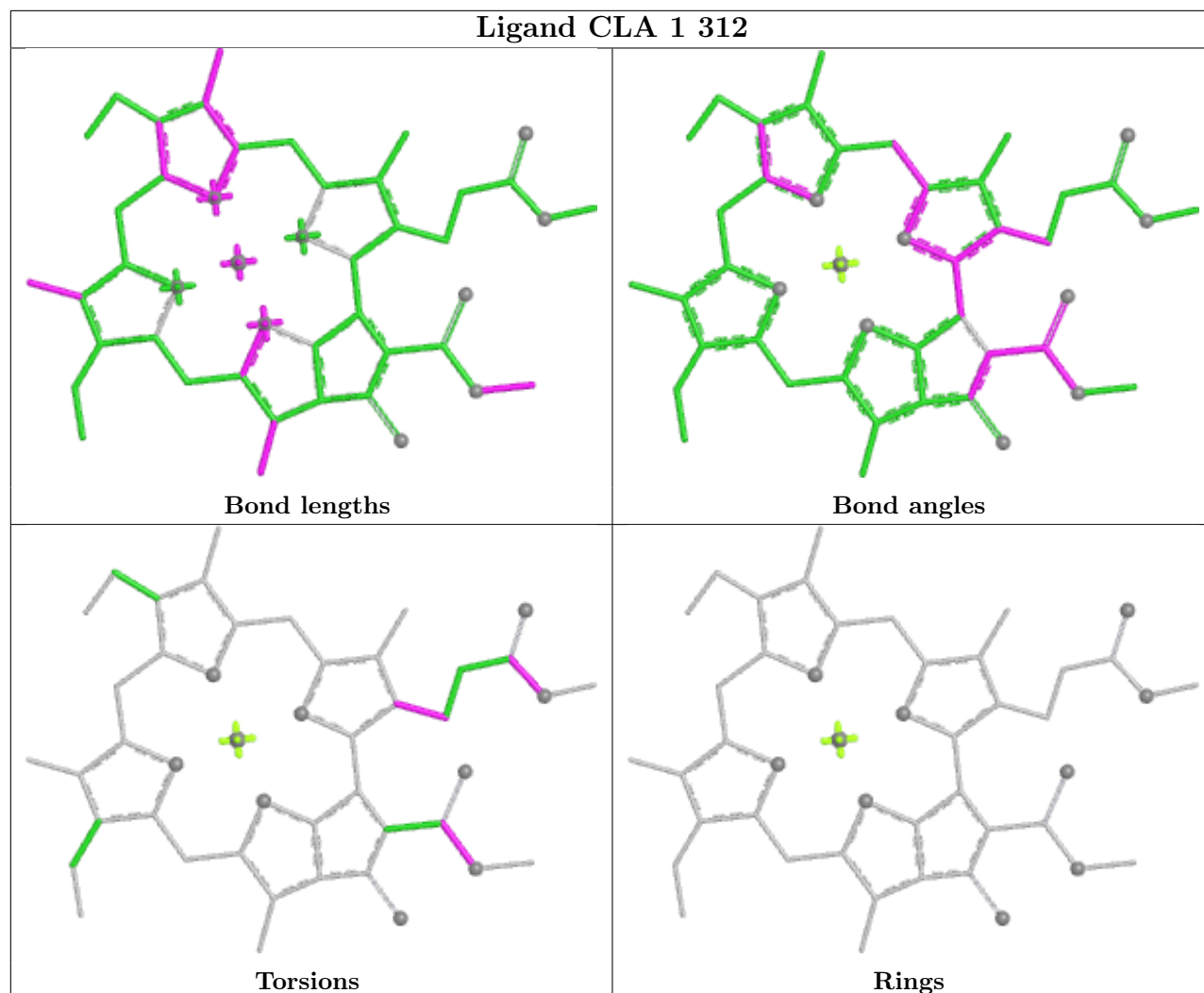
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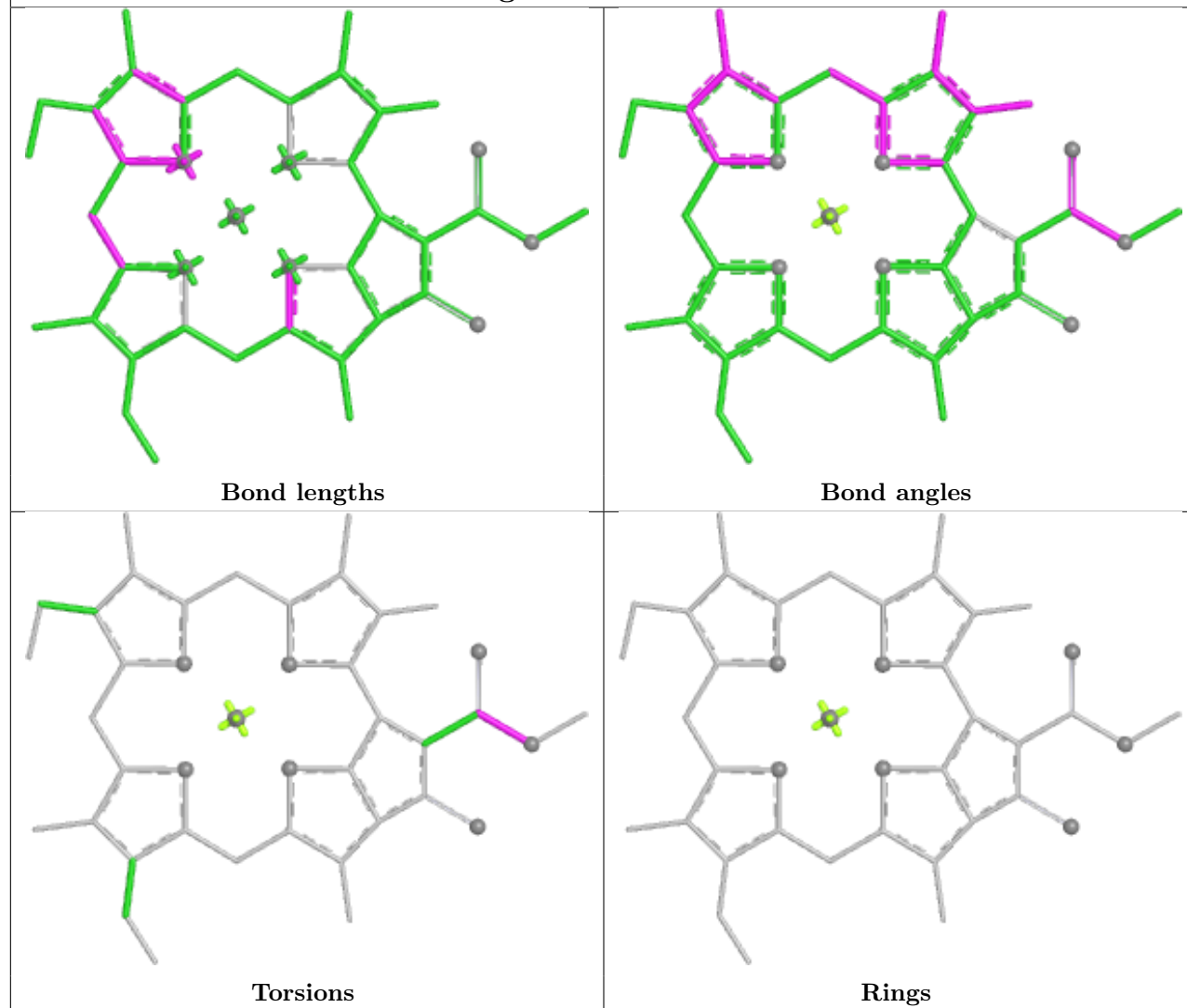
Ligand A86 0 303



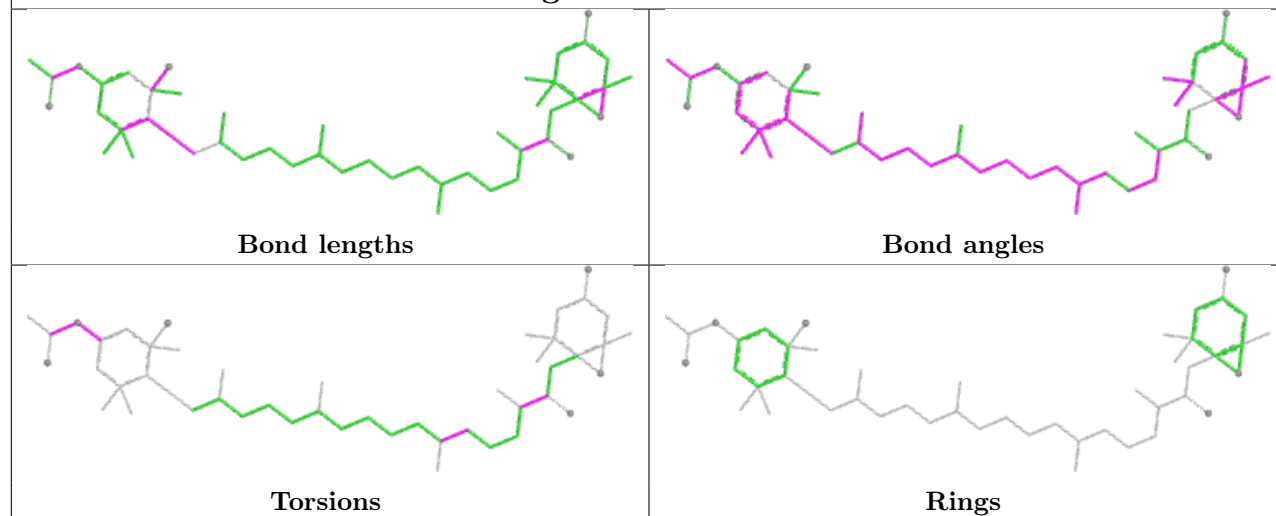
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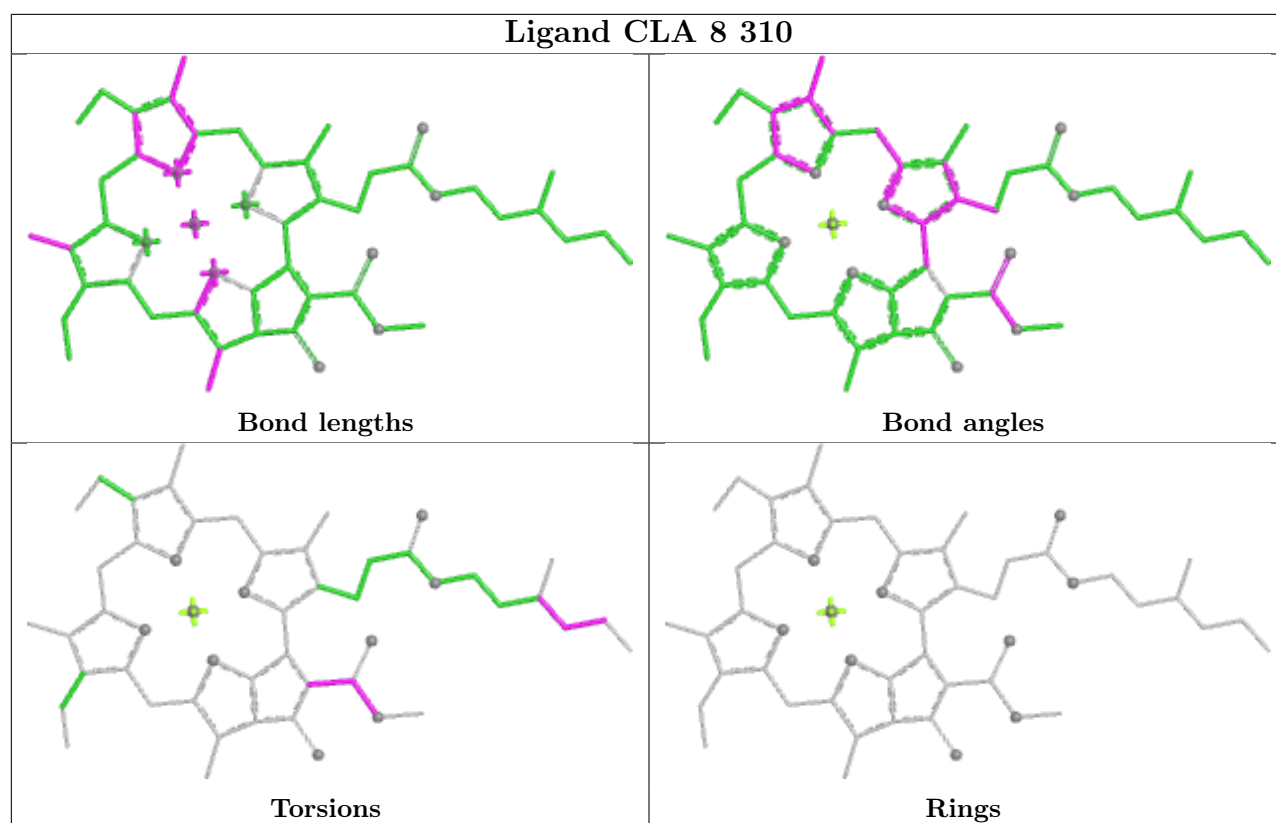


Ligand CLA 3 310

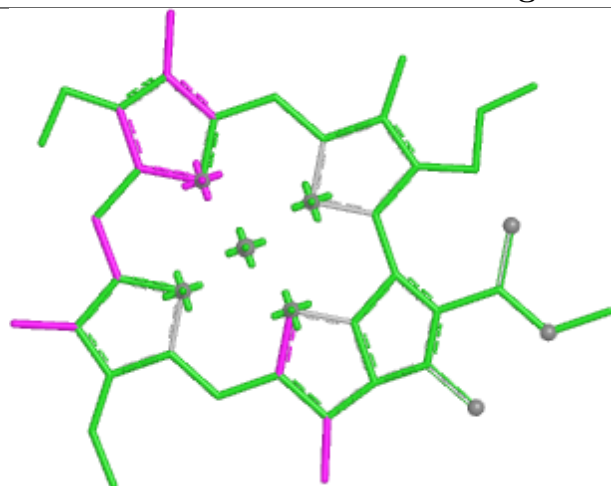


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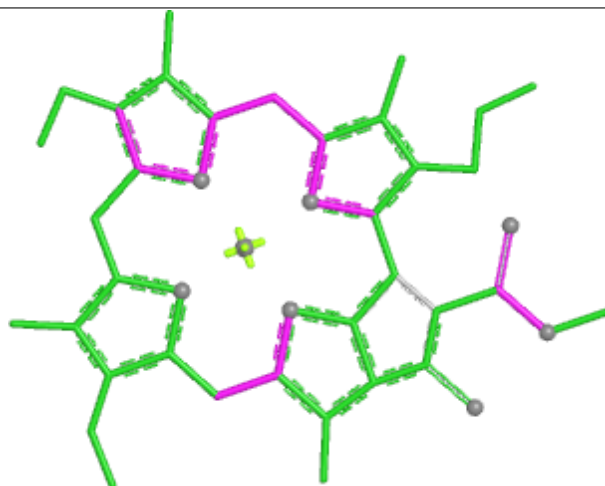




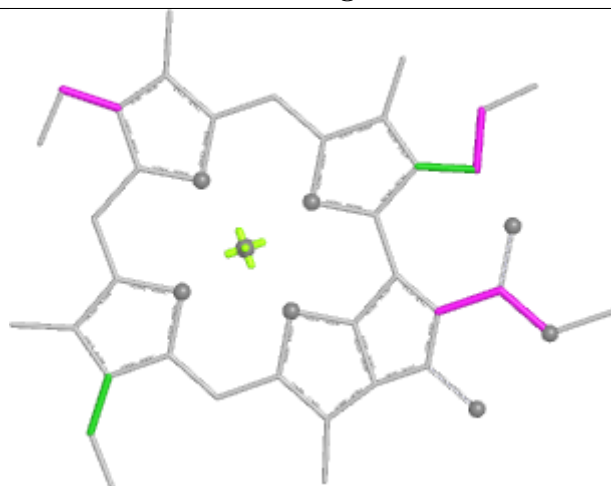
Ligand CLA 4 314



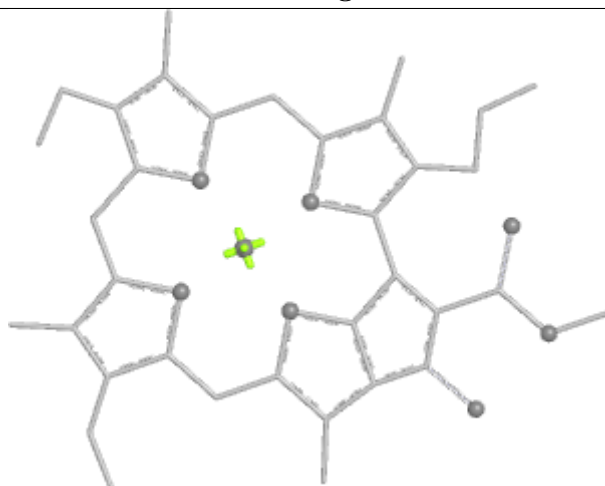
Bond lengths



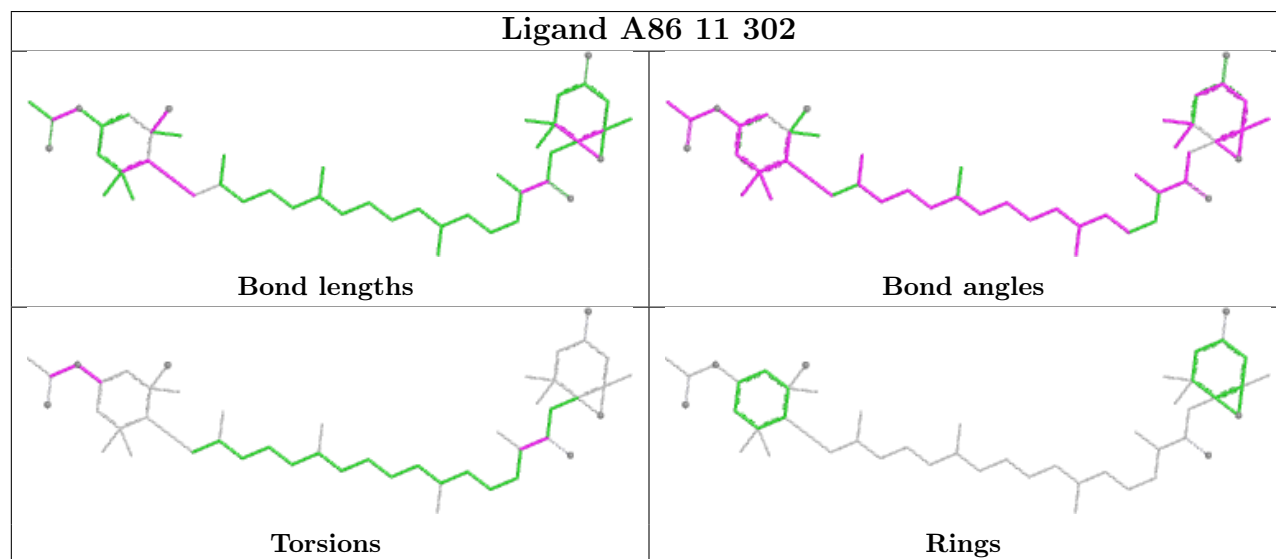
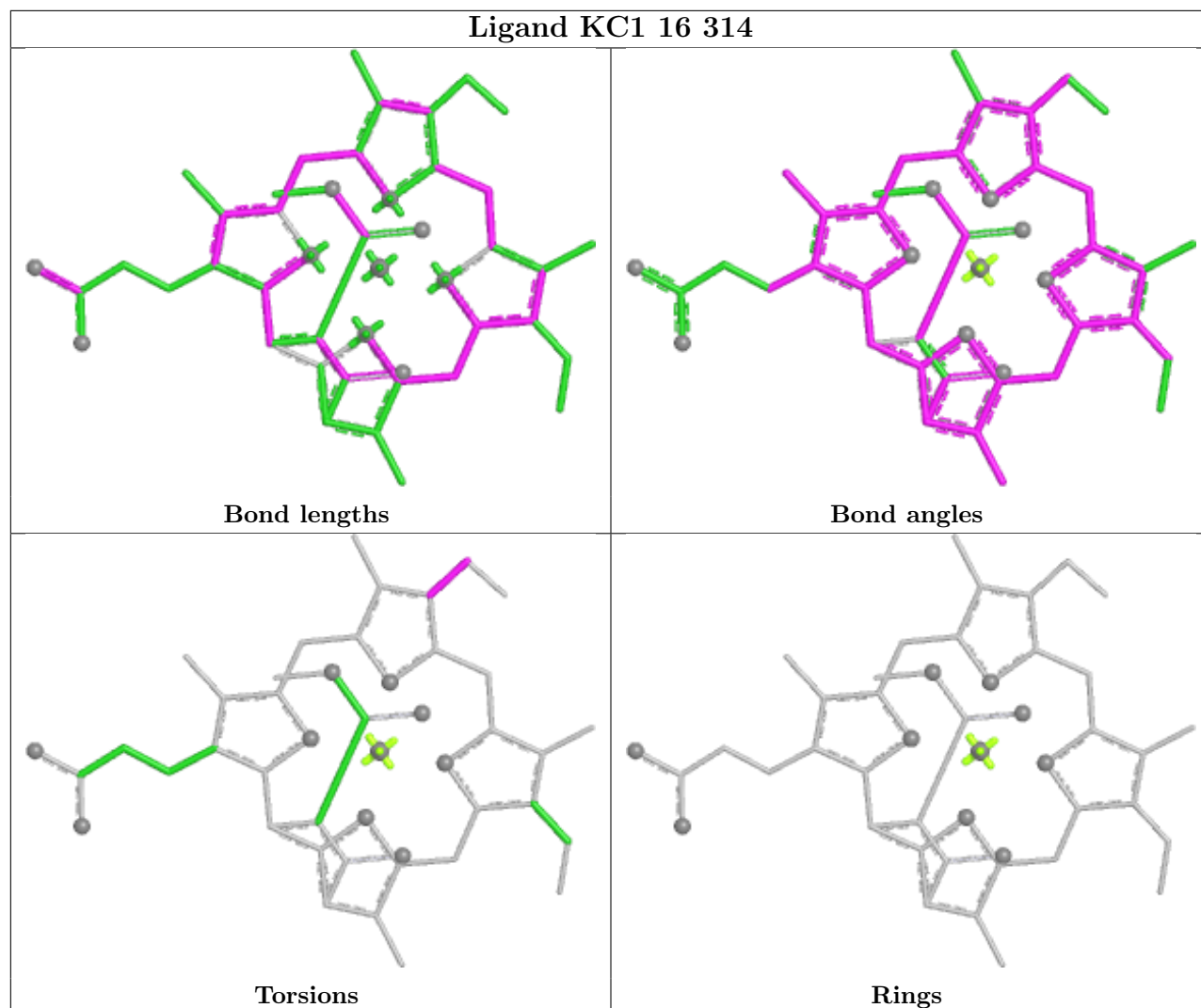
Bond angles

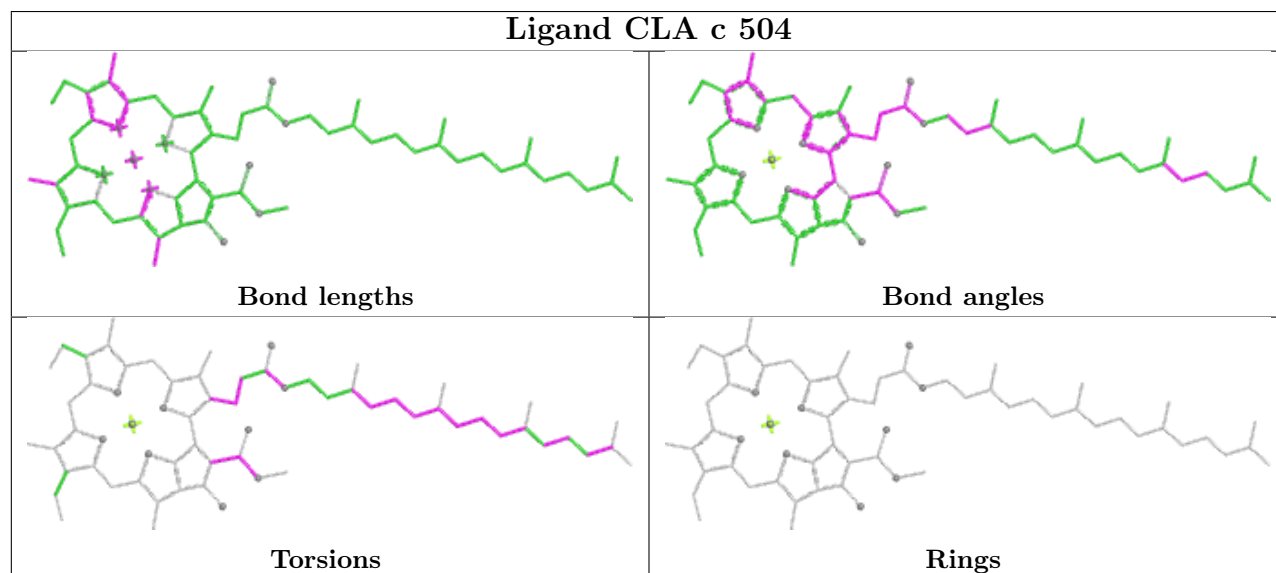
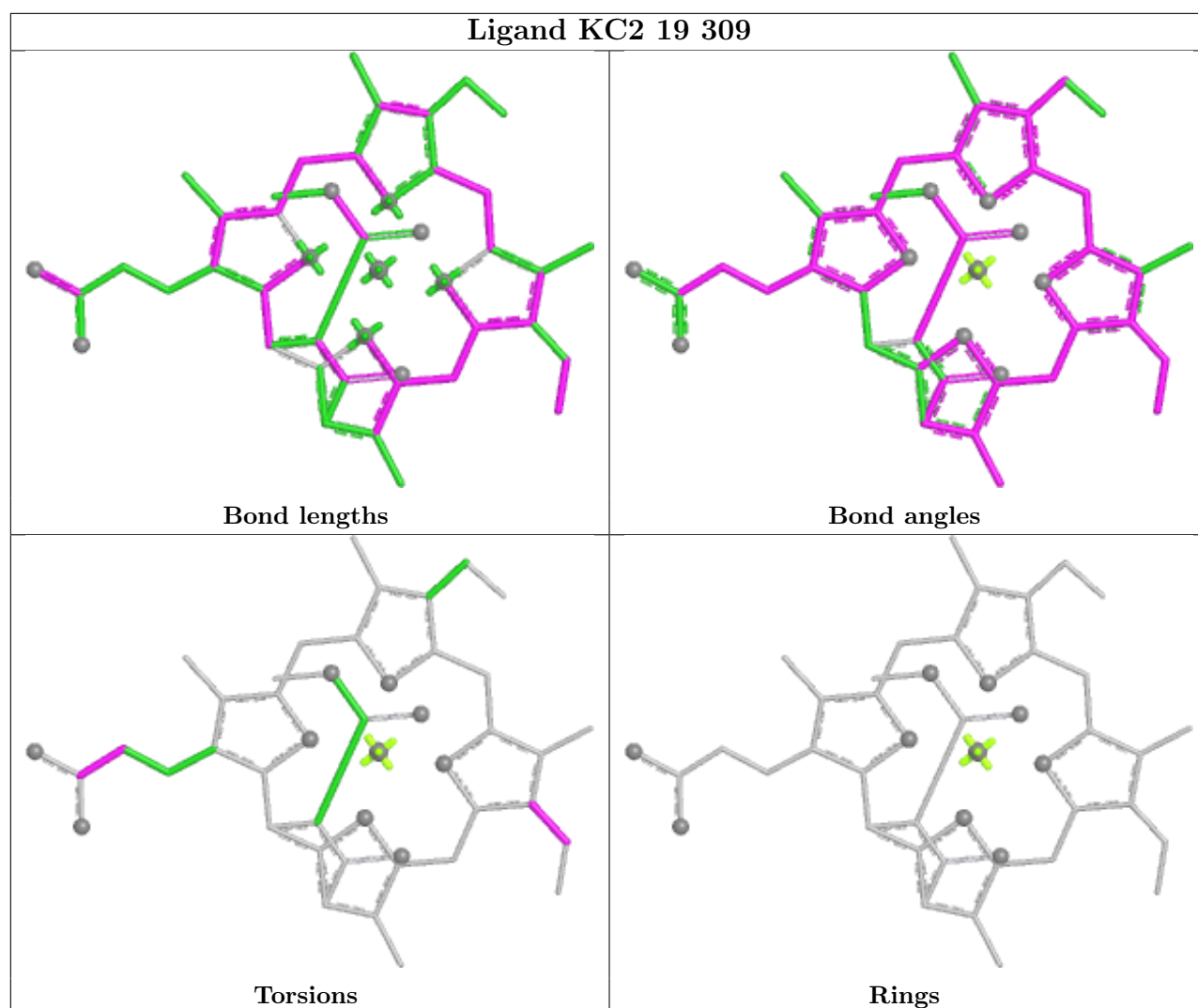


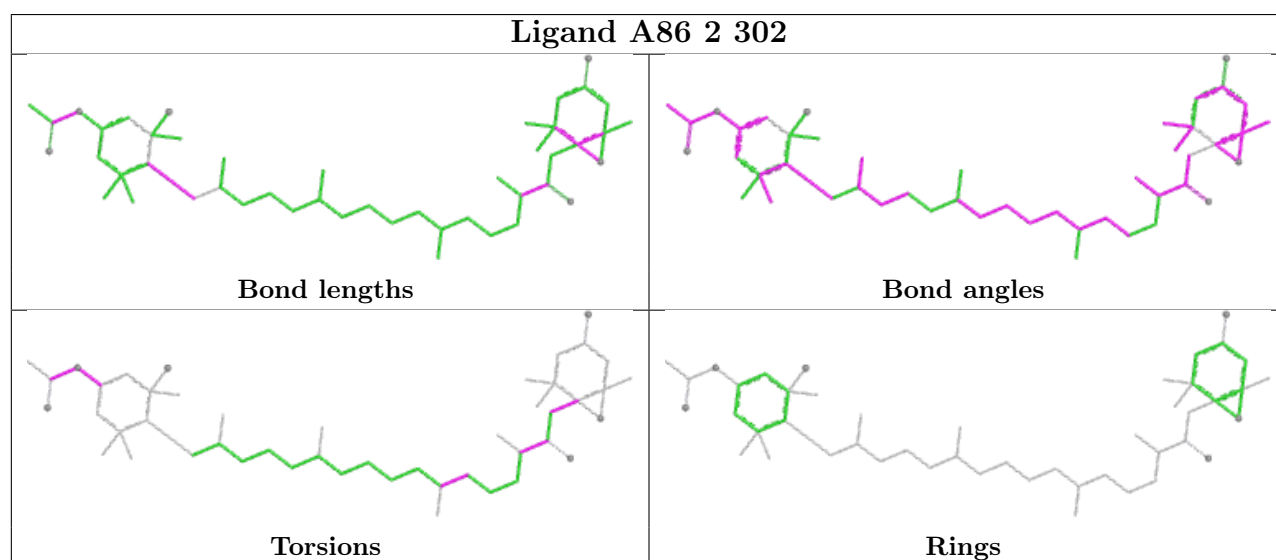
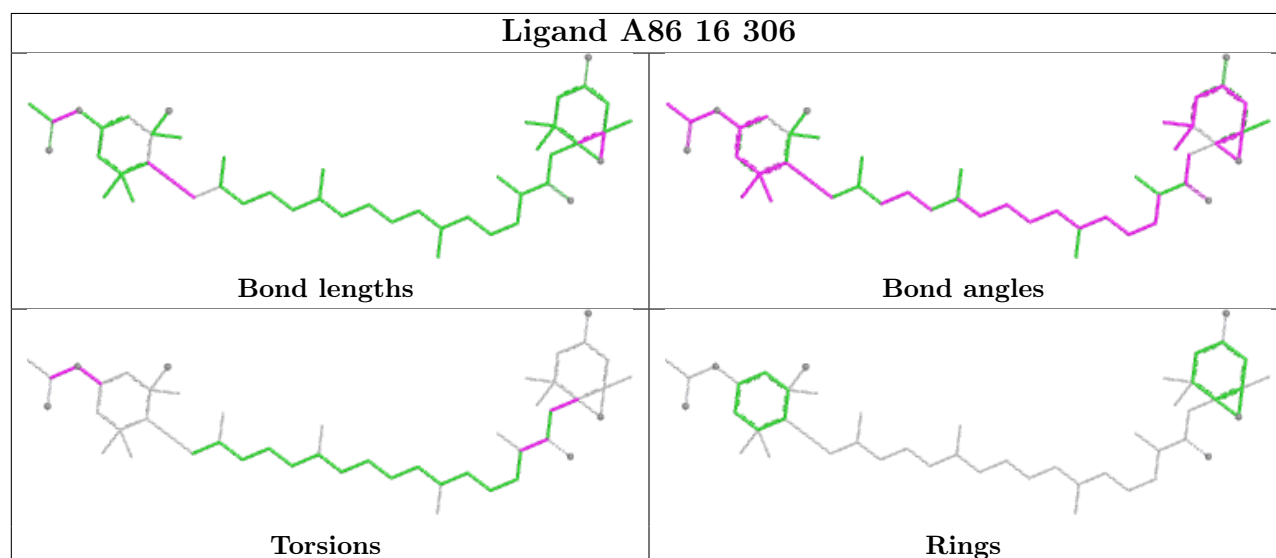
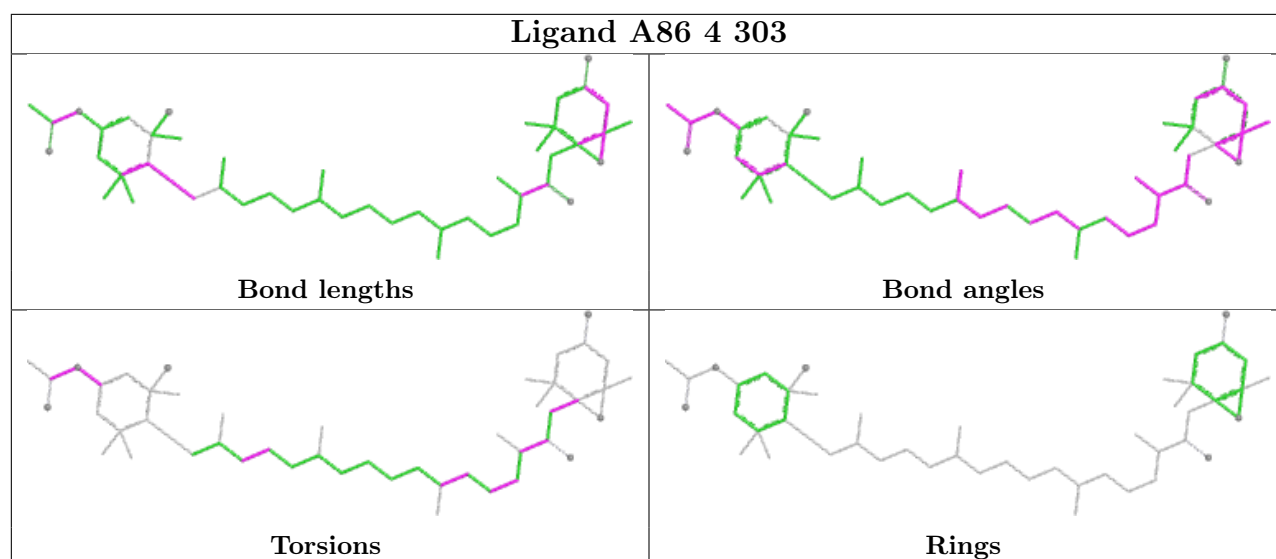
Torsions



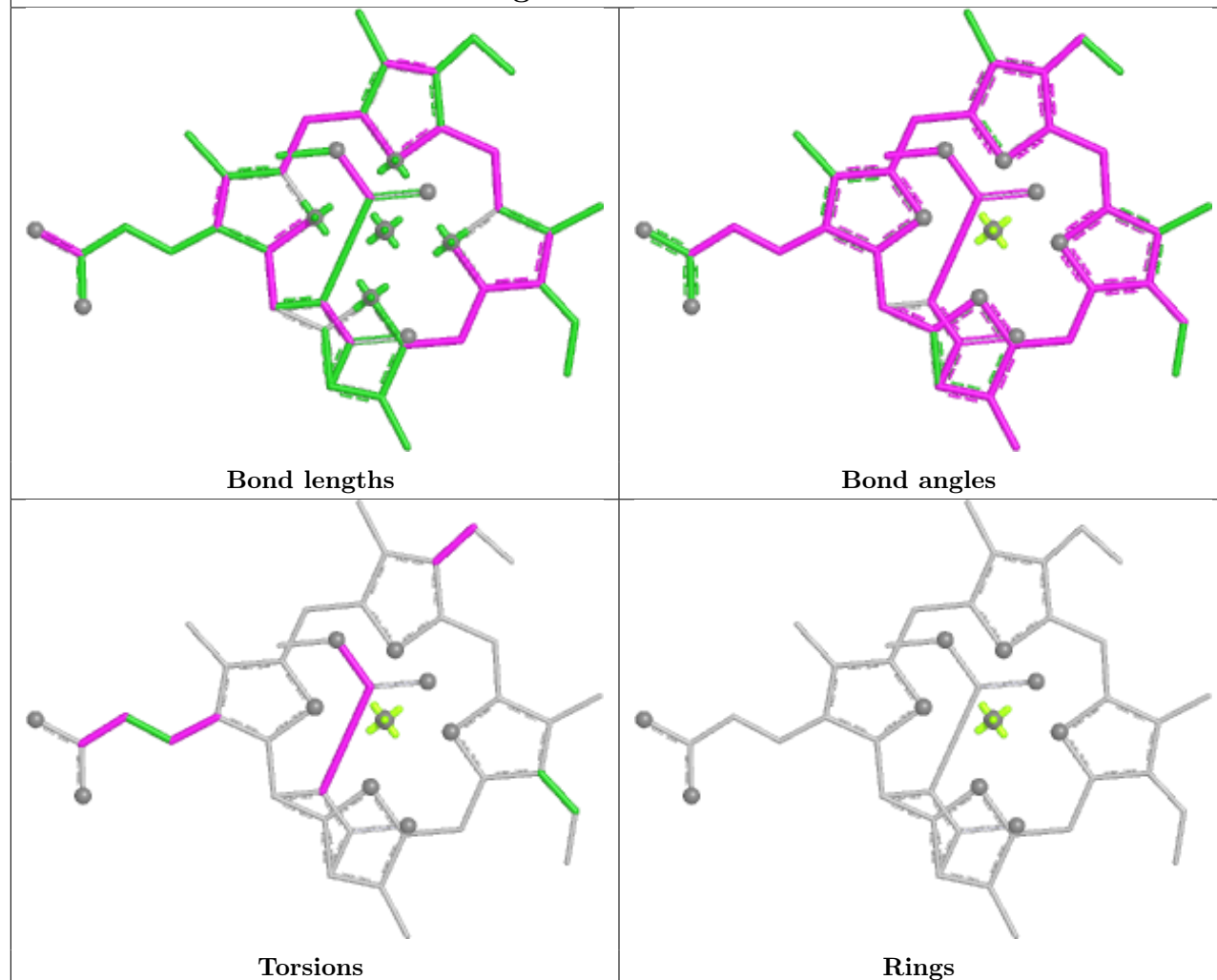
Rings



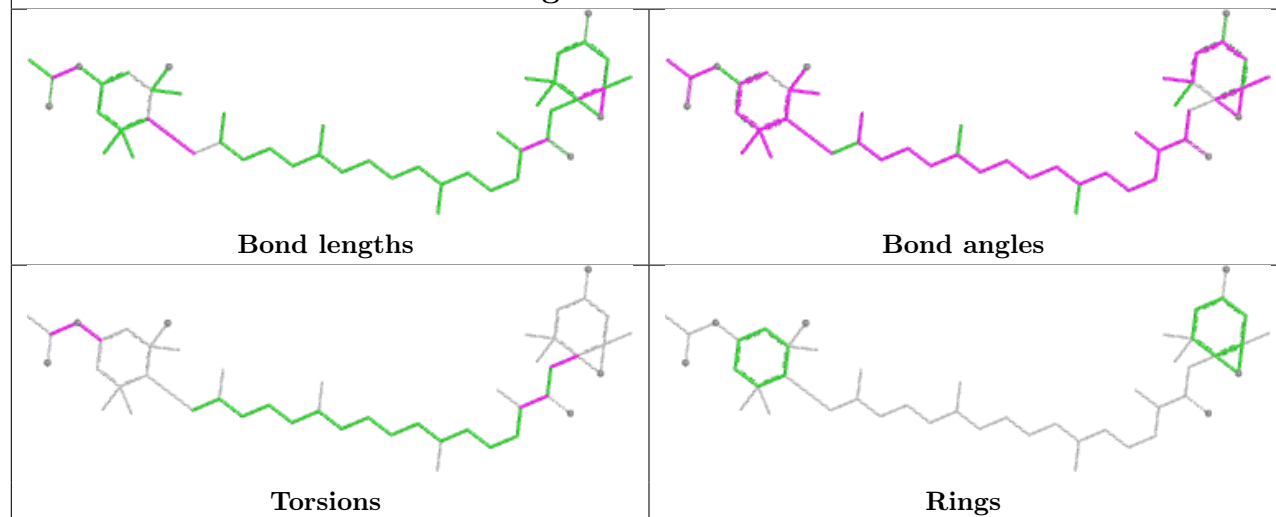


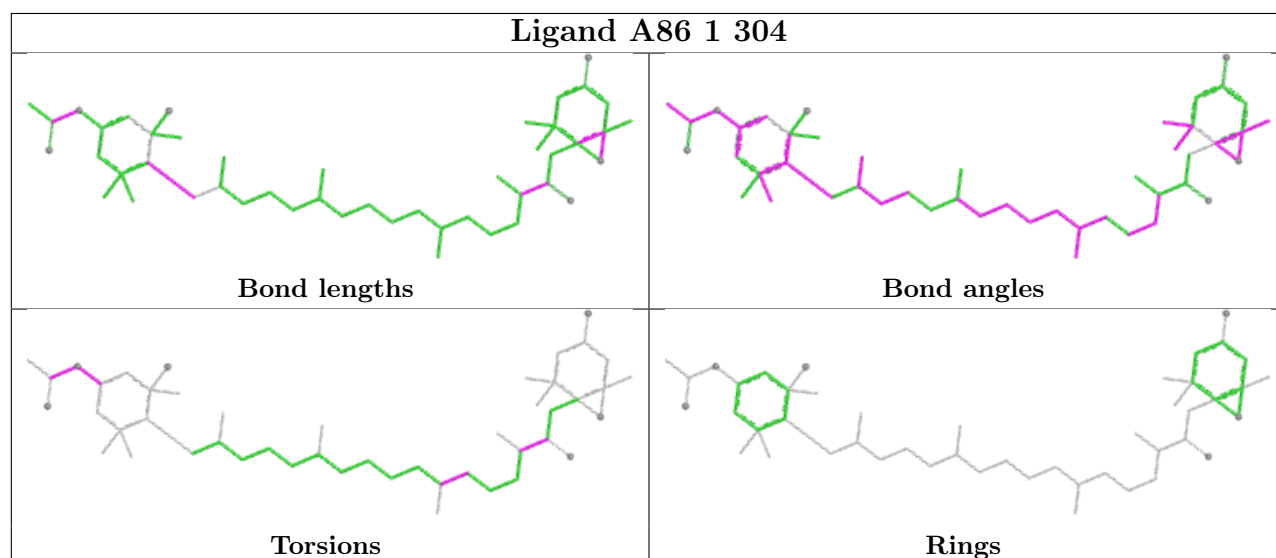
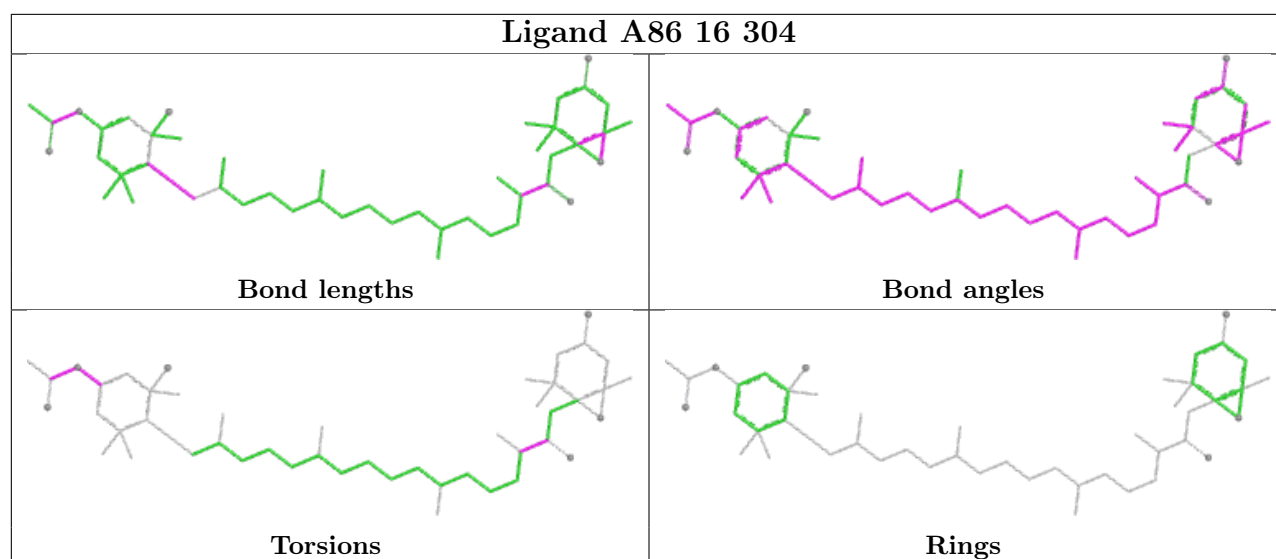


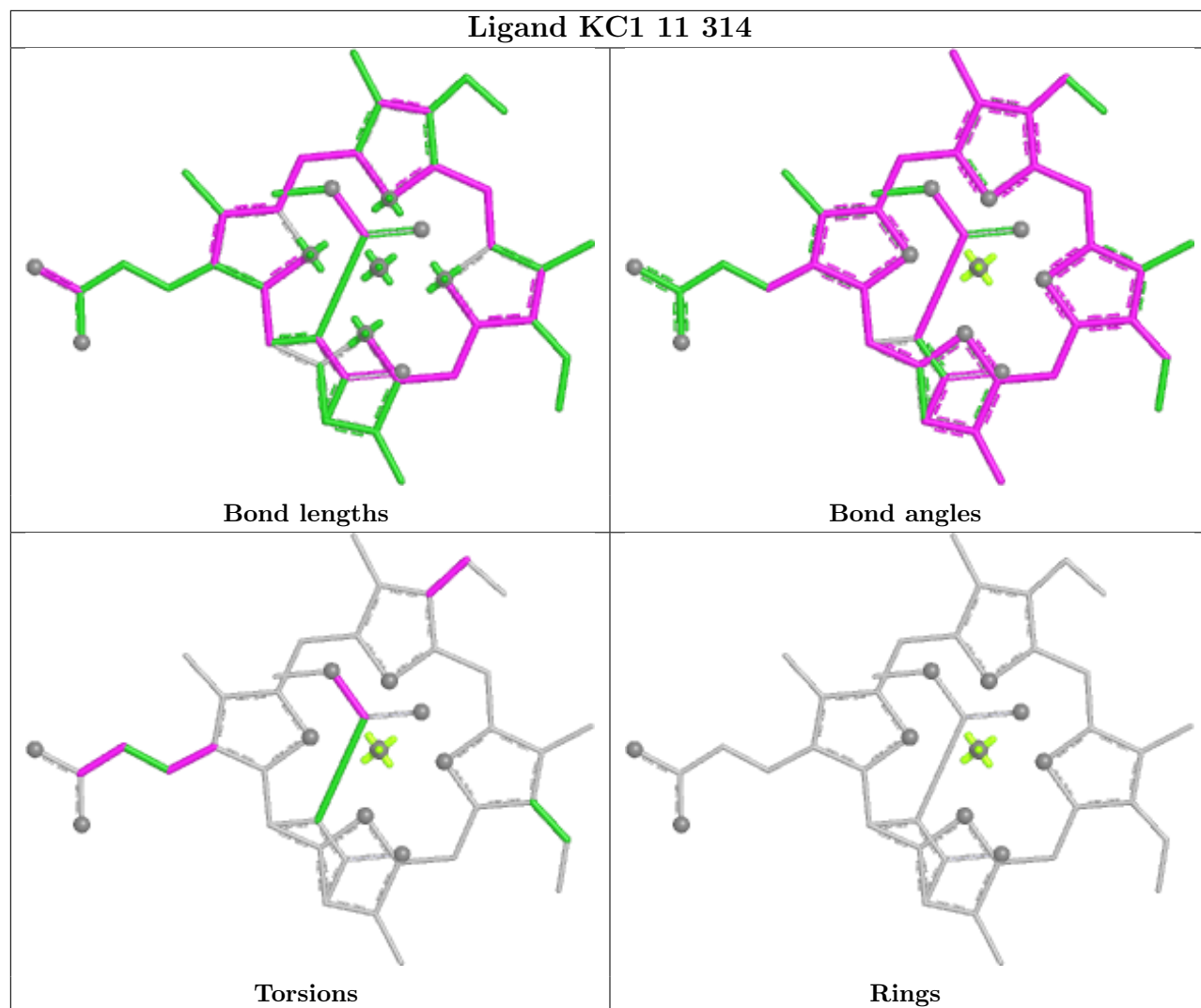
Ligand KC1 4 313



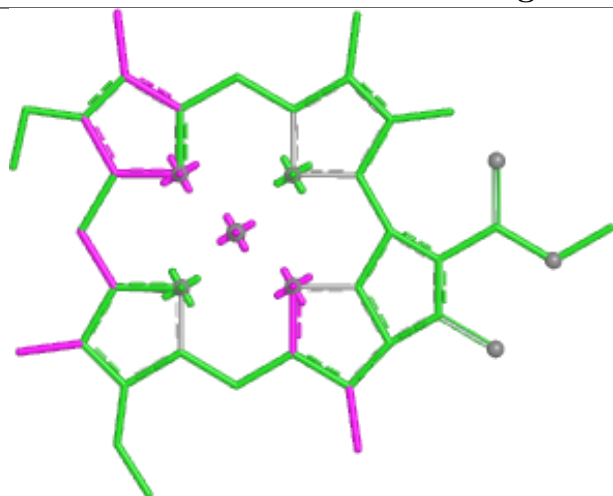
Ligand A86 0 305



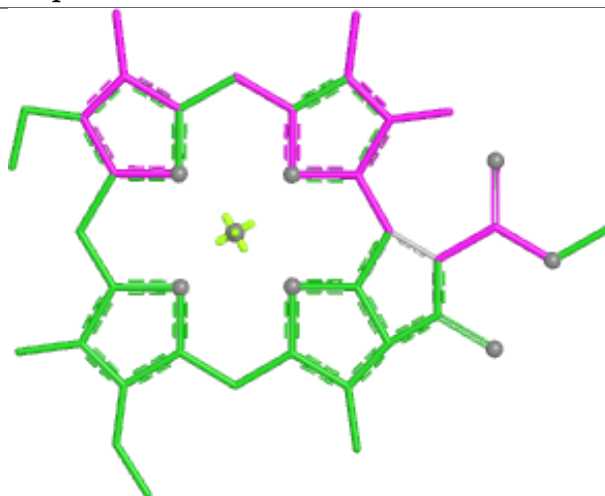




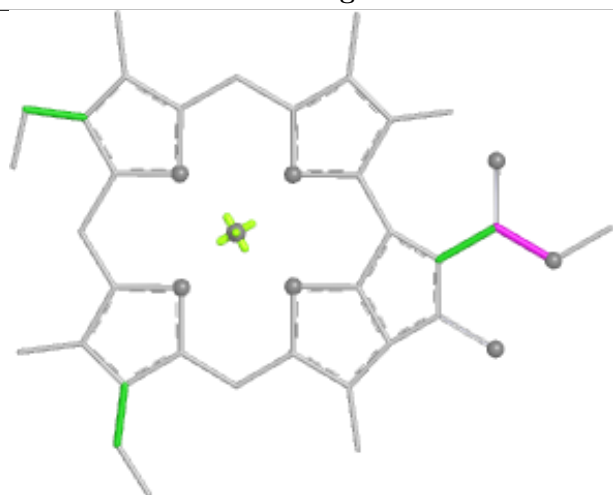
Ligand CLA p 610



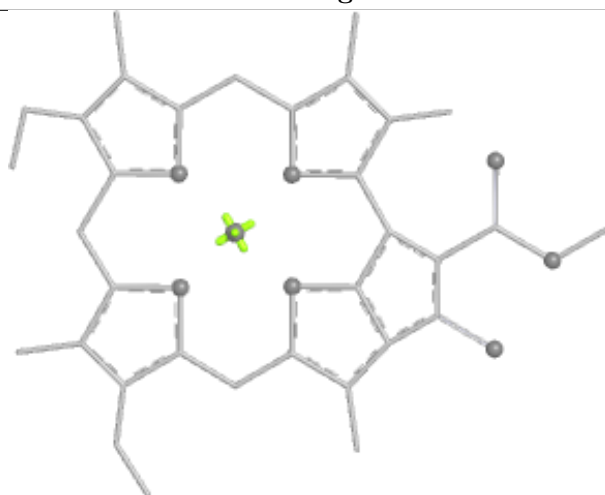
Bond lengths



Bond angles

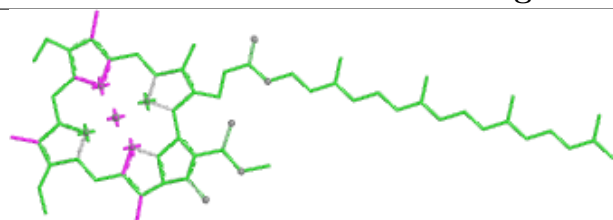


Torsions

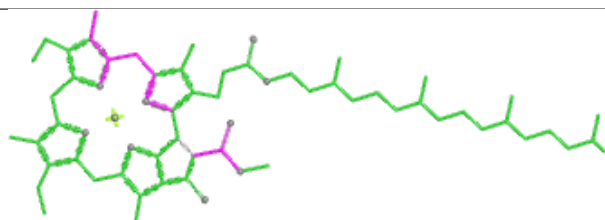


Rings

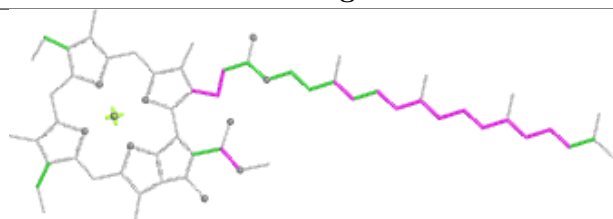
Ligand CLA B 607



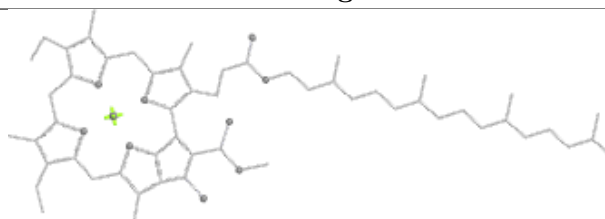
Bond lengths



Bond angles

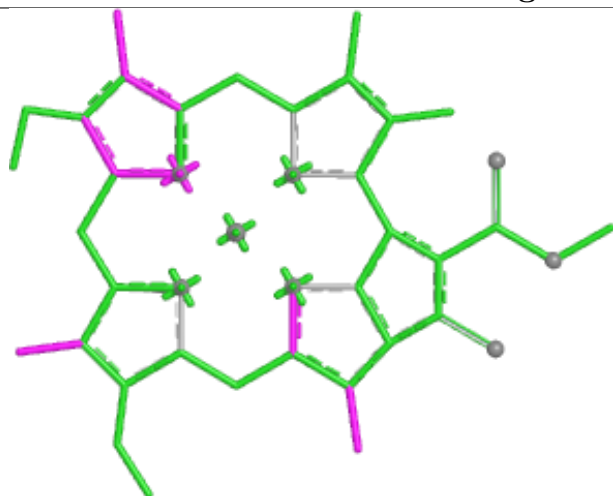


Torsions

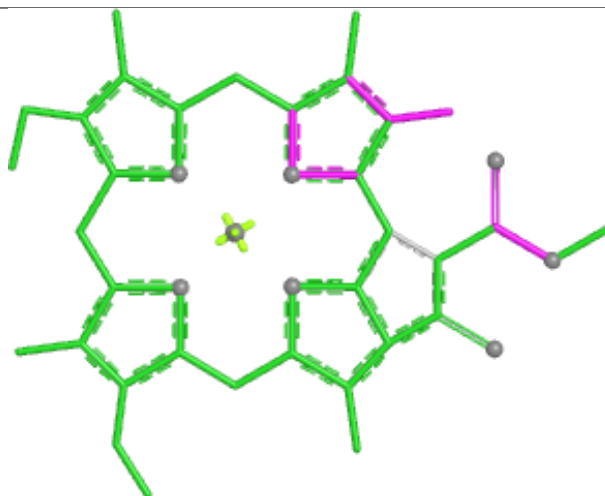


Rings

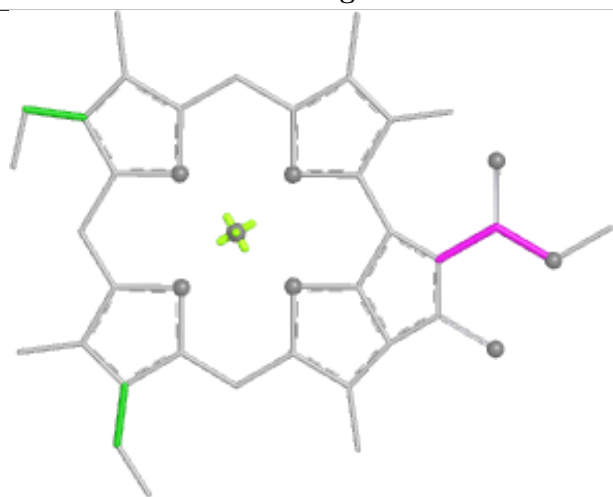
Ligand CLA 1 315



Bond lengths



Bond angles

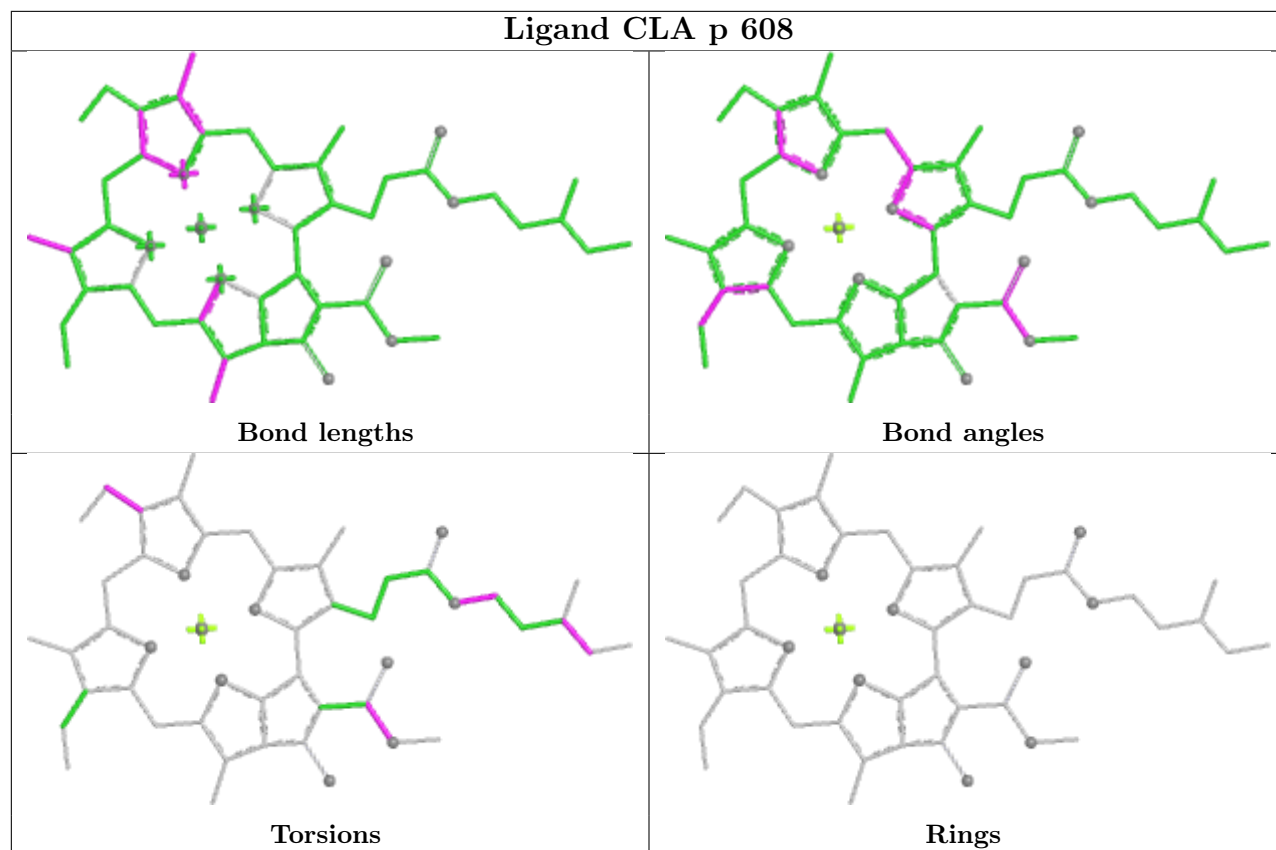


Torsions

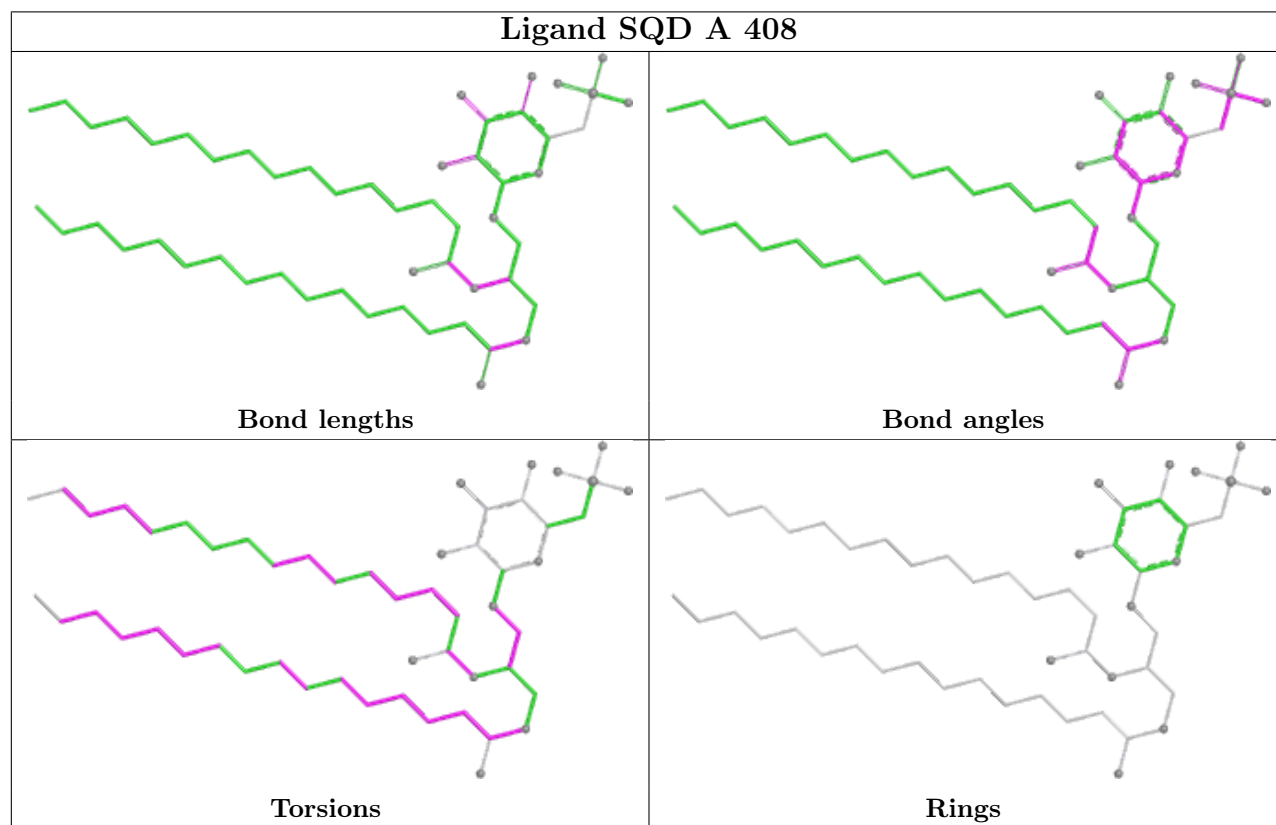


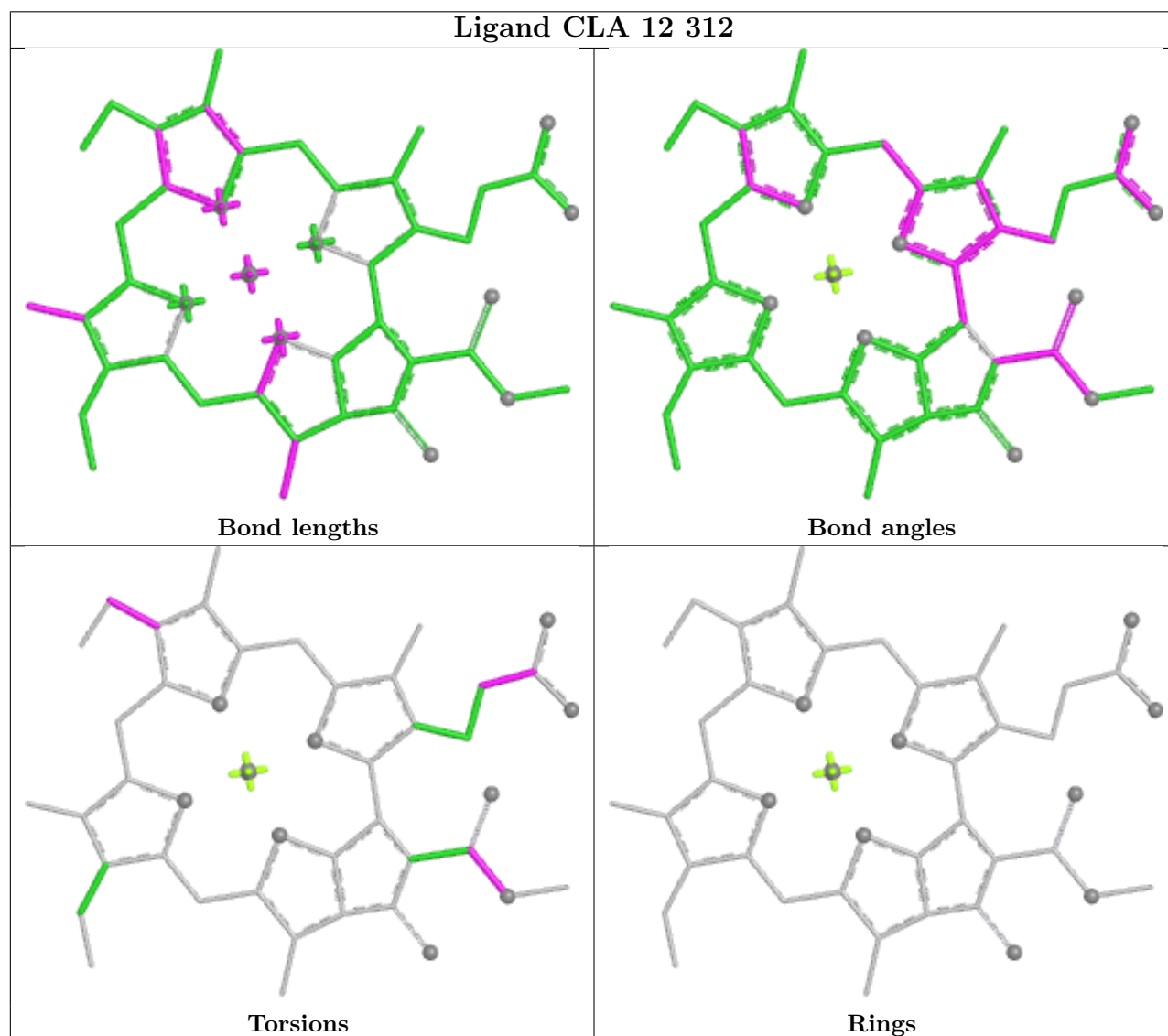
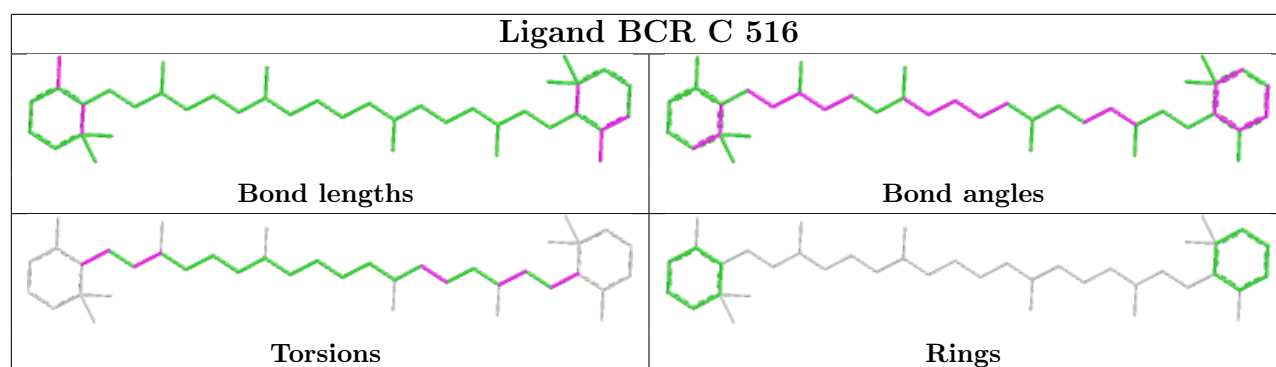
Rings

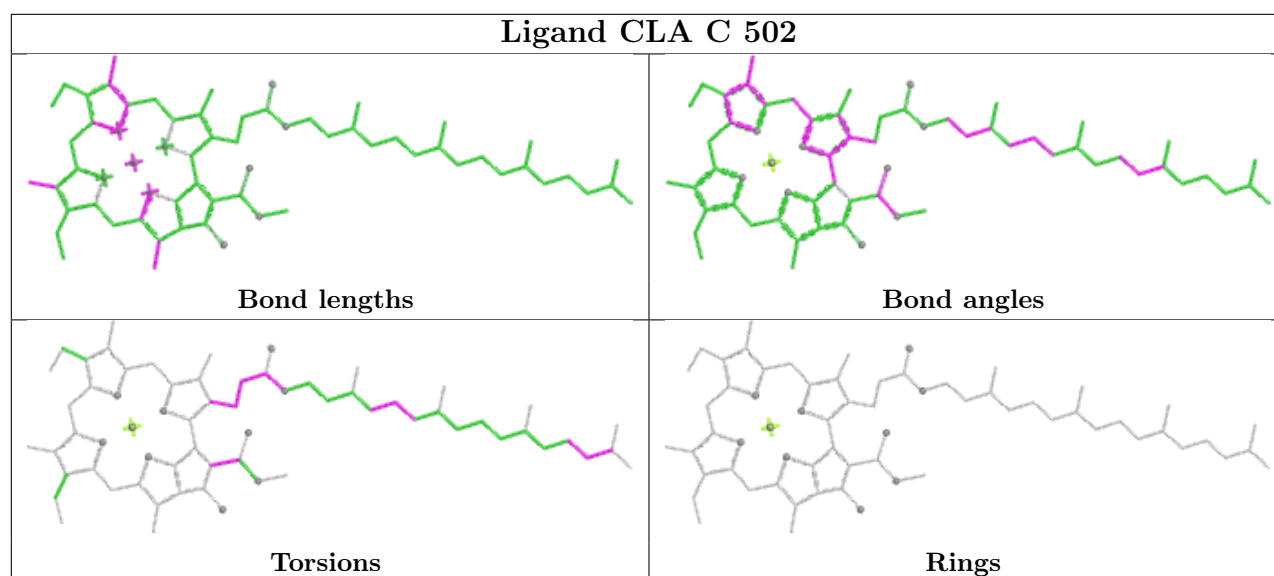
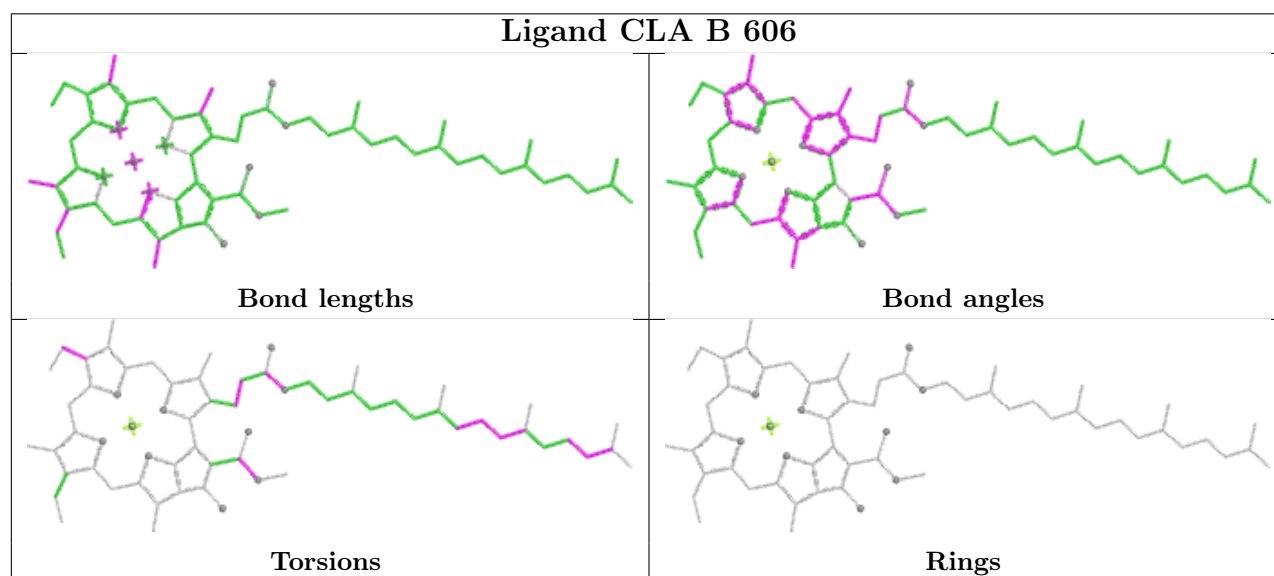
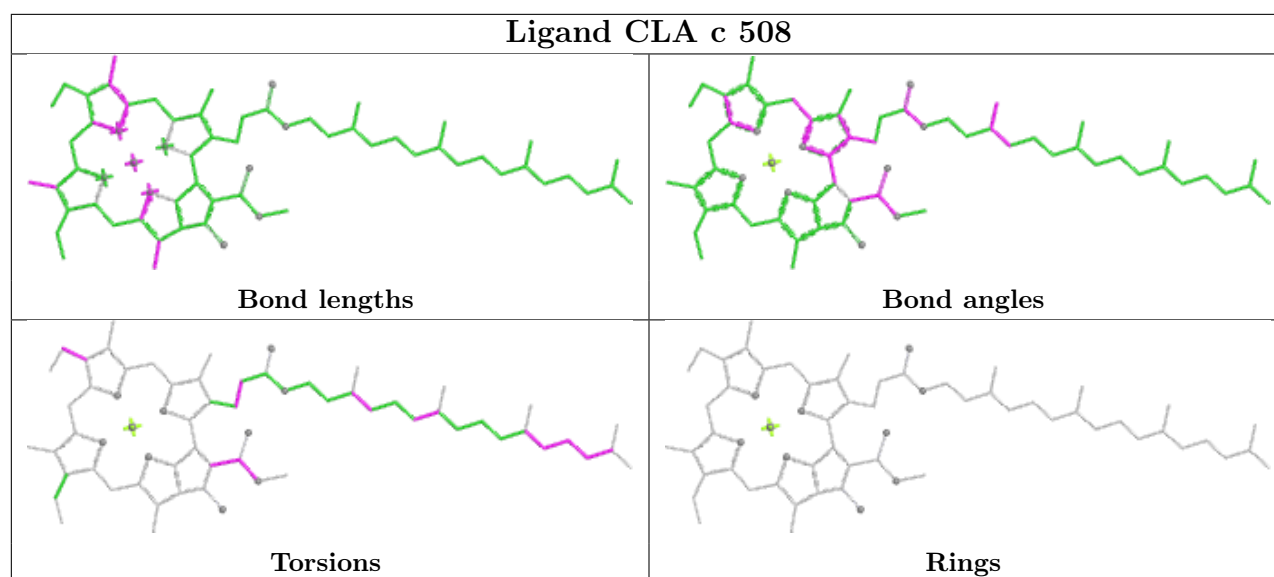
Ligand CLA p 608

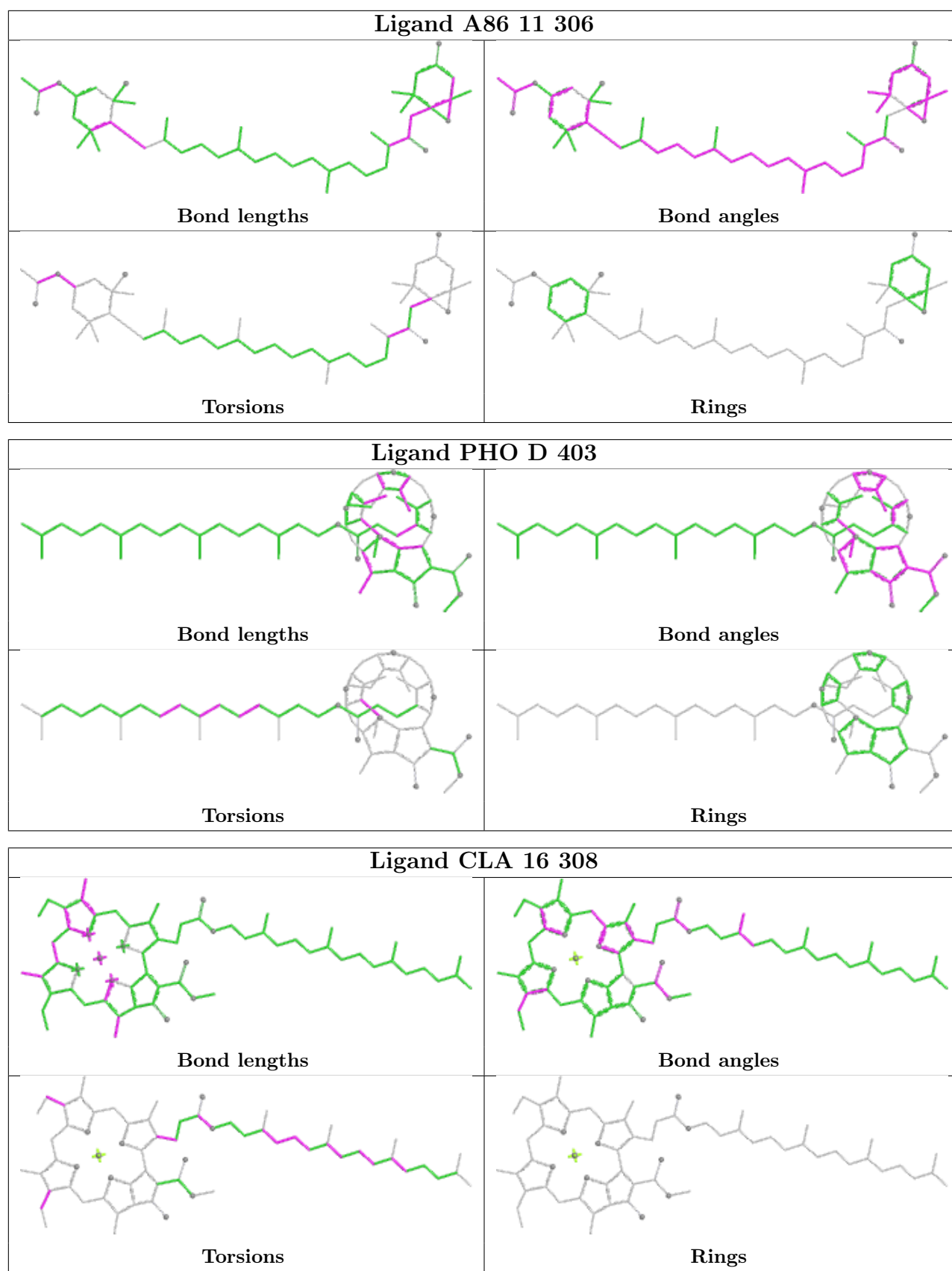


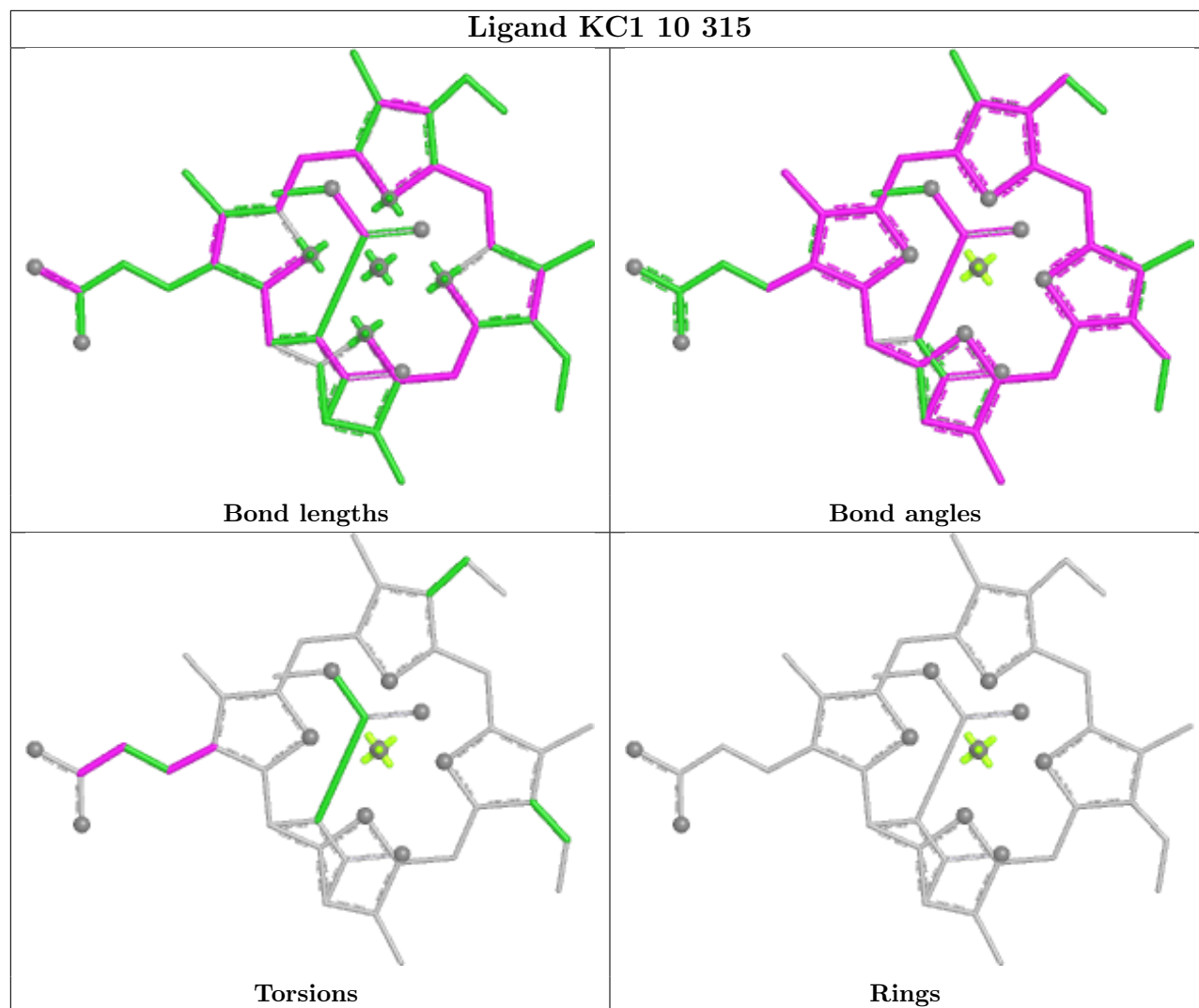
Ligand SQD A 408

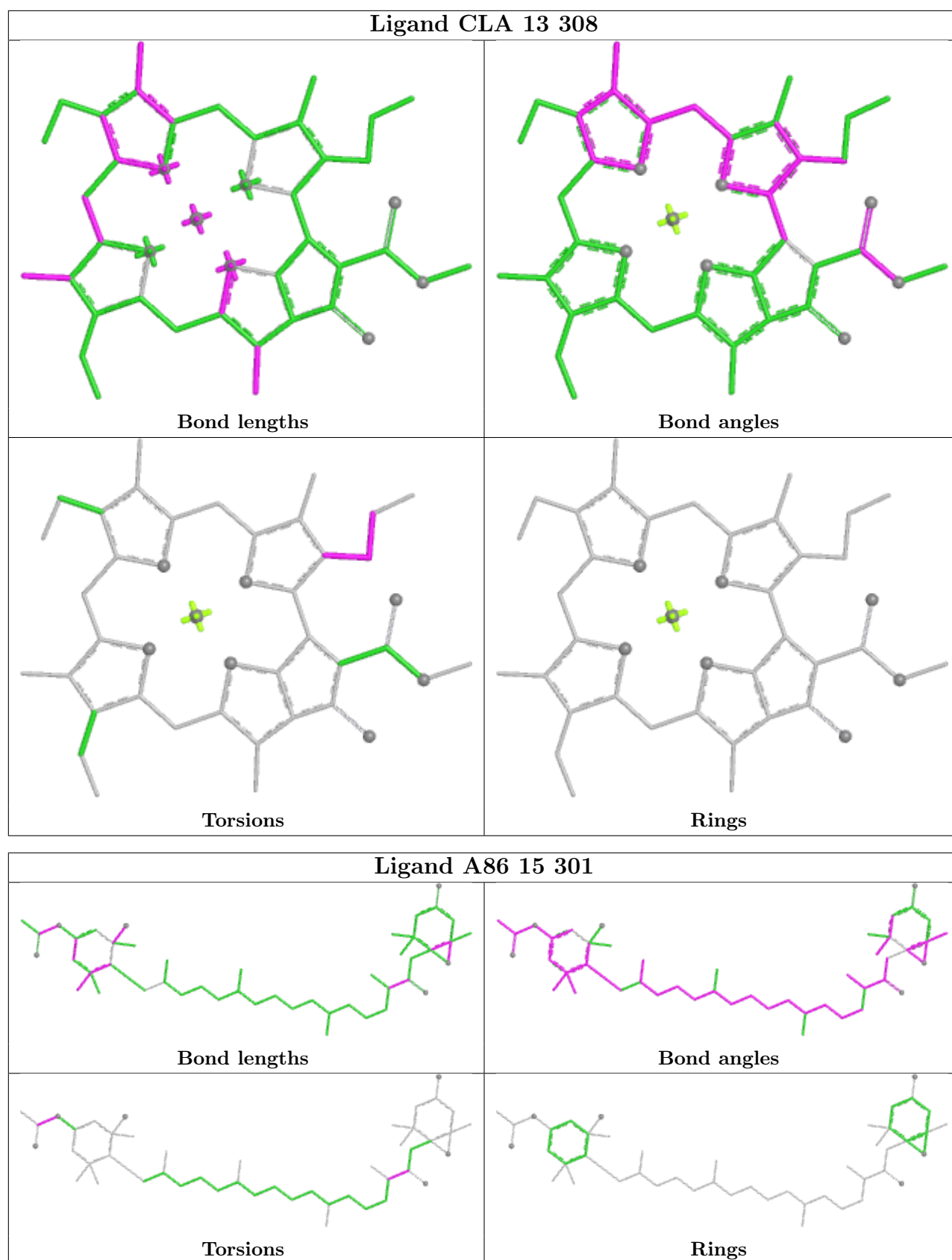


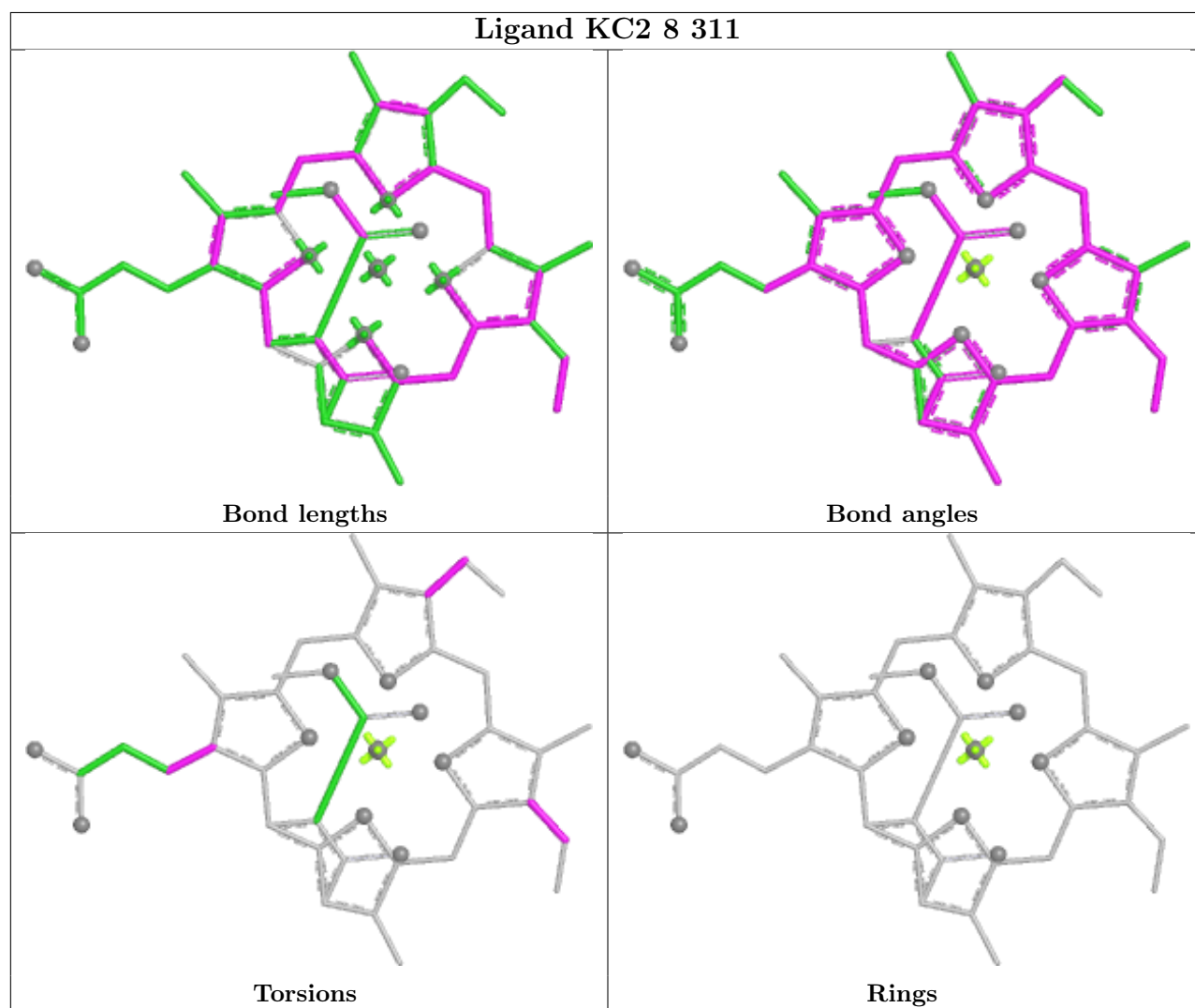
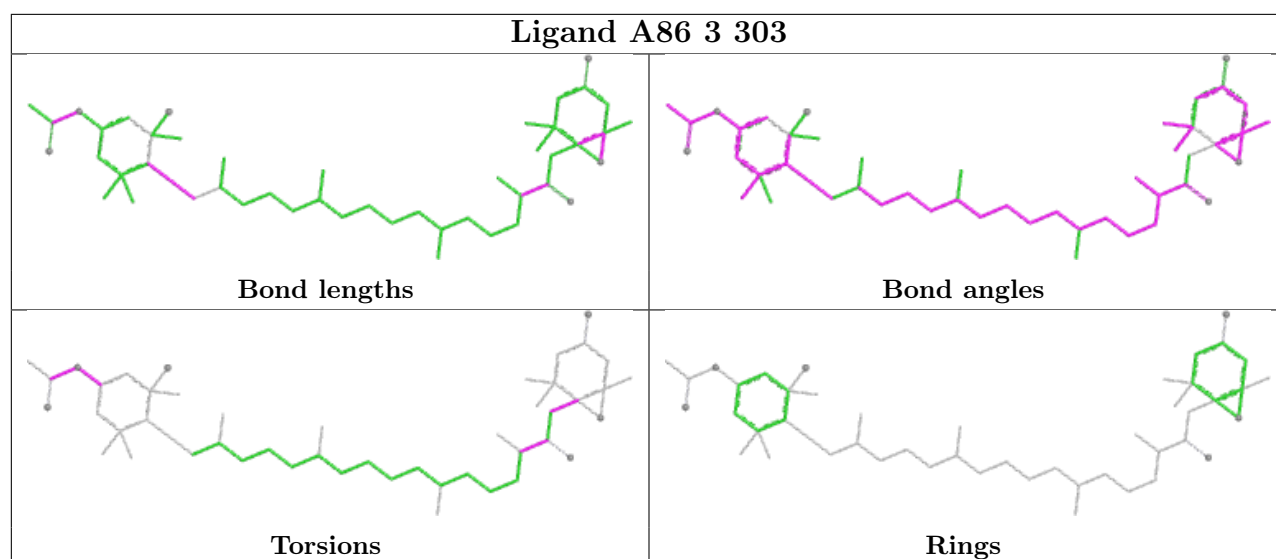


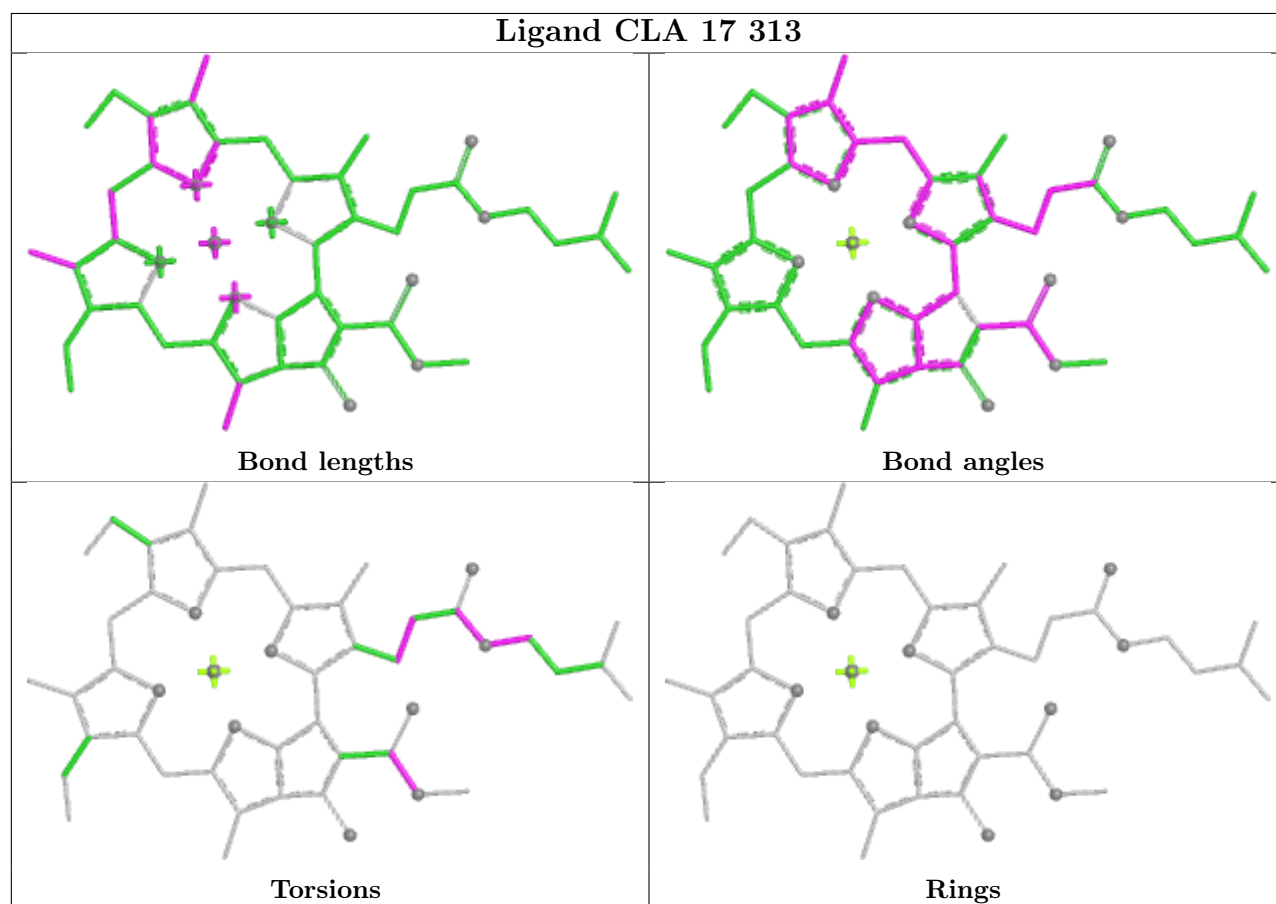
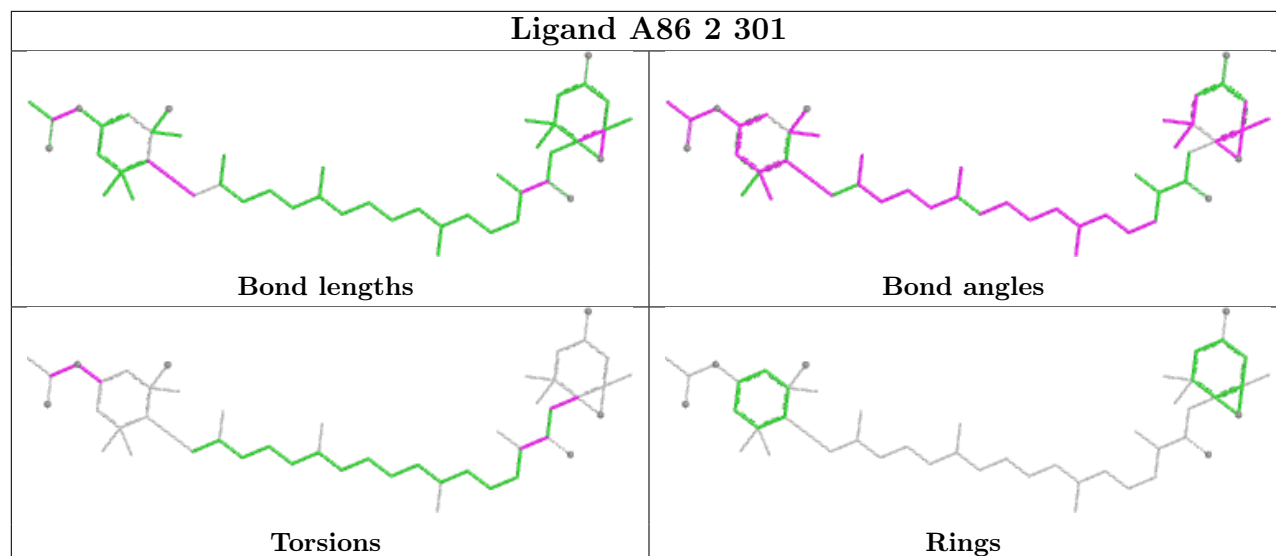


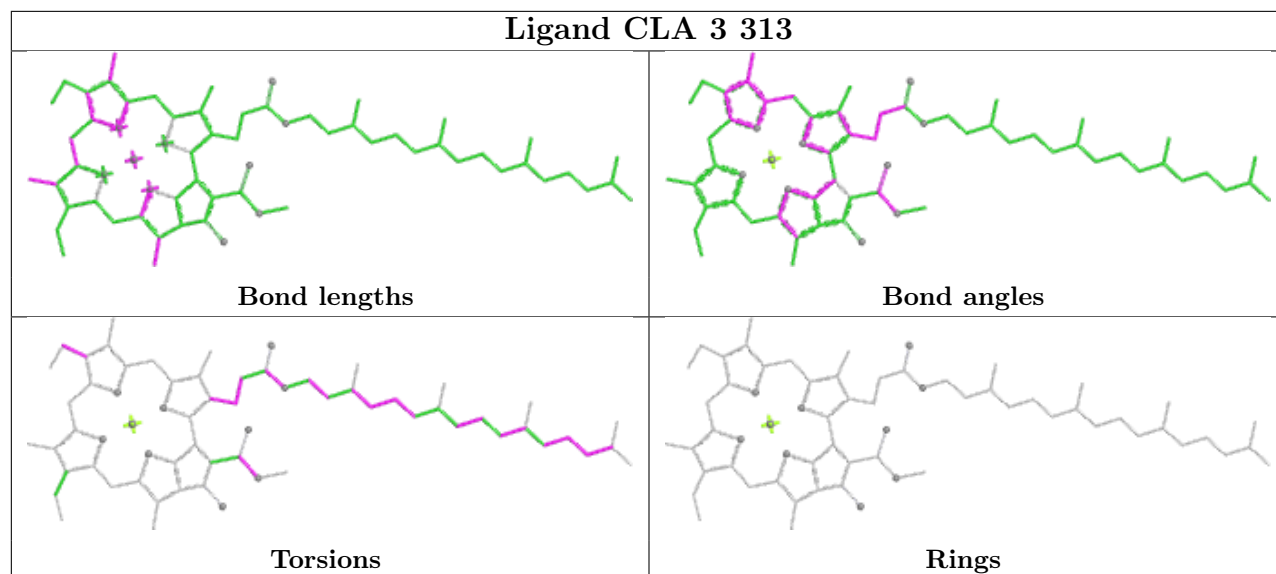
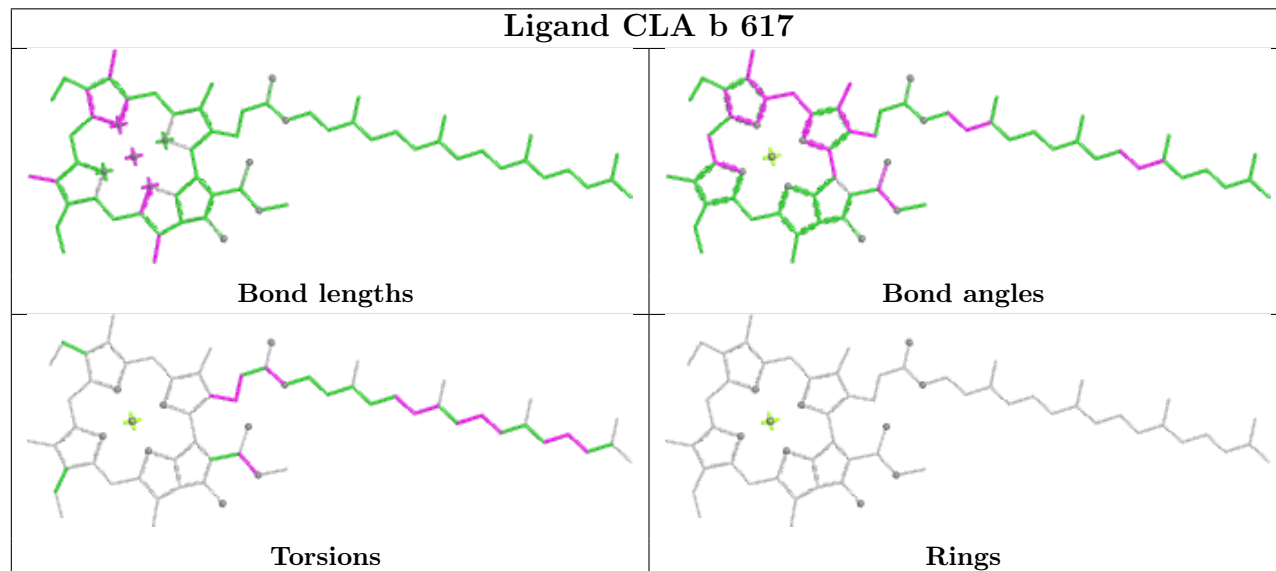




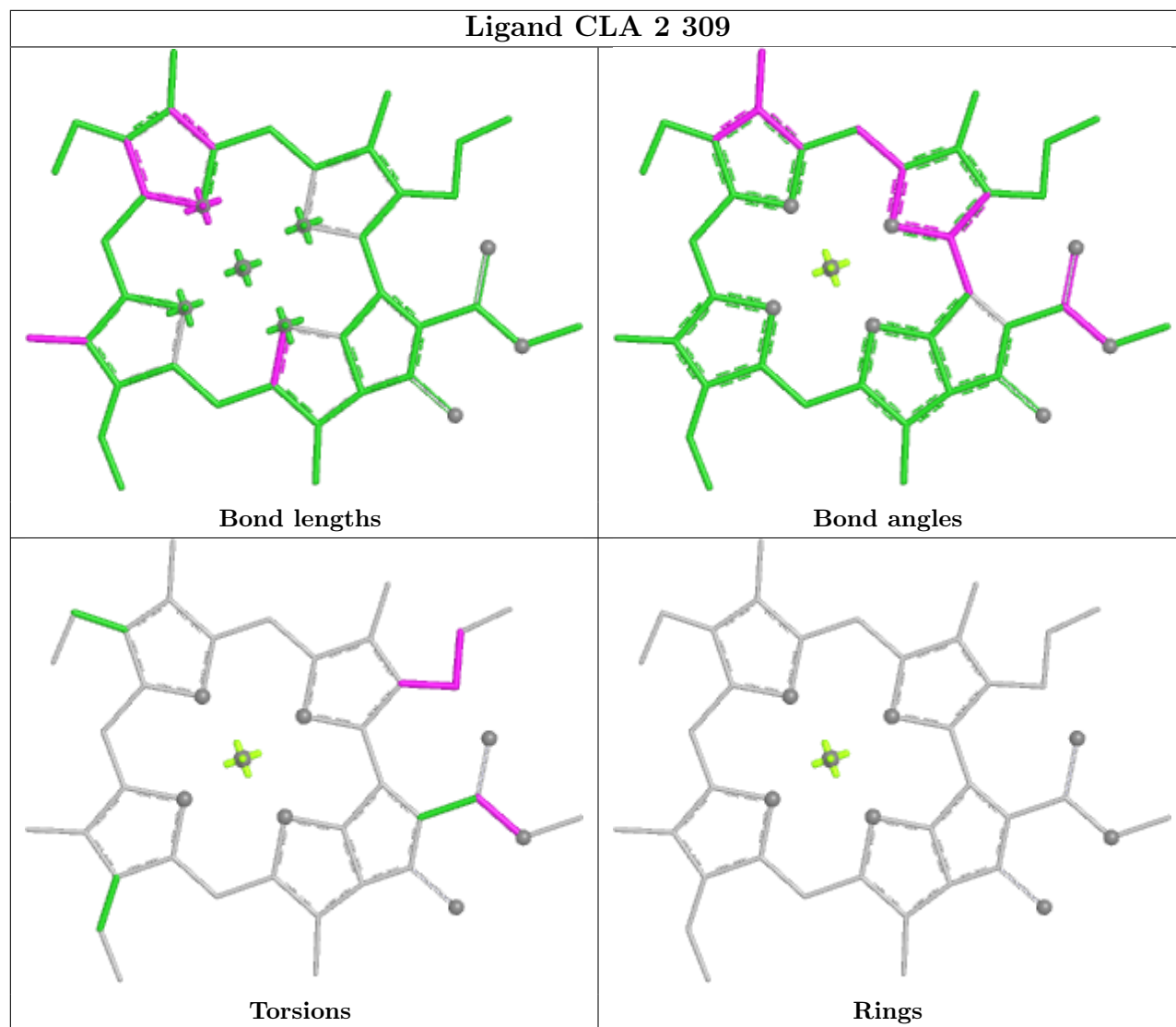


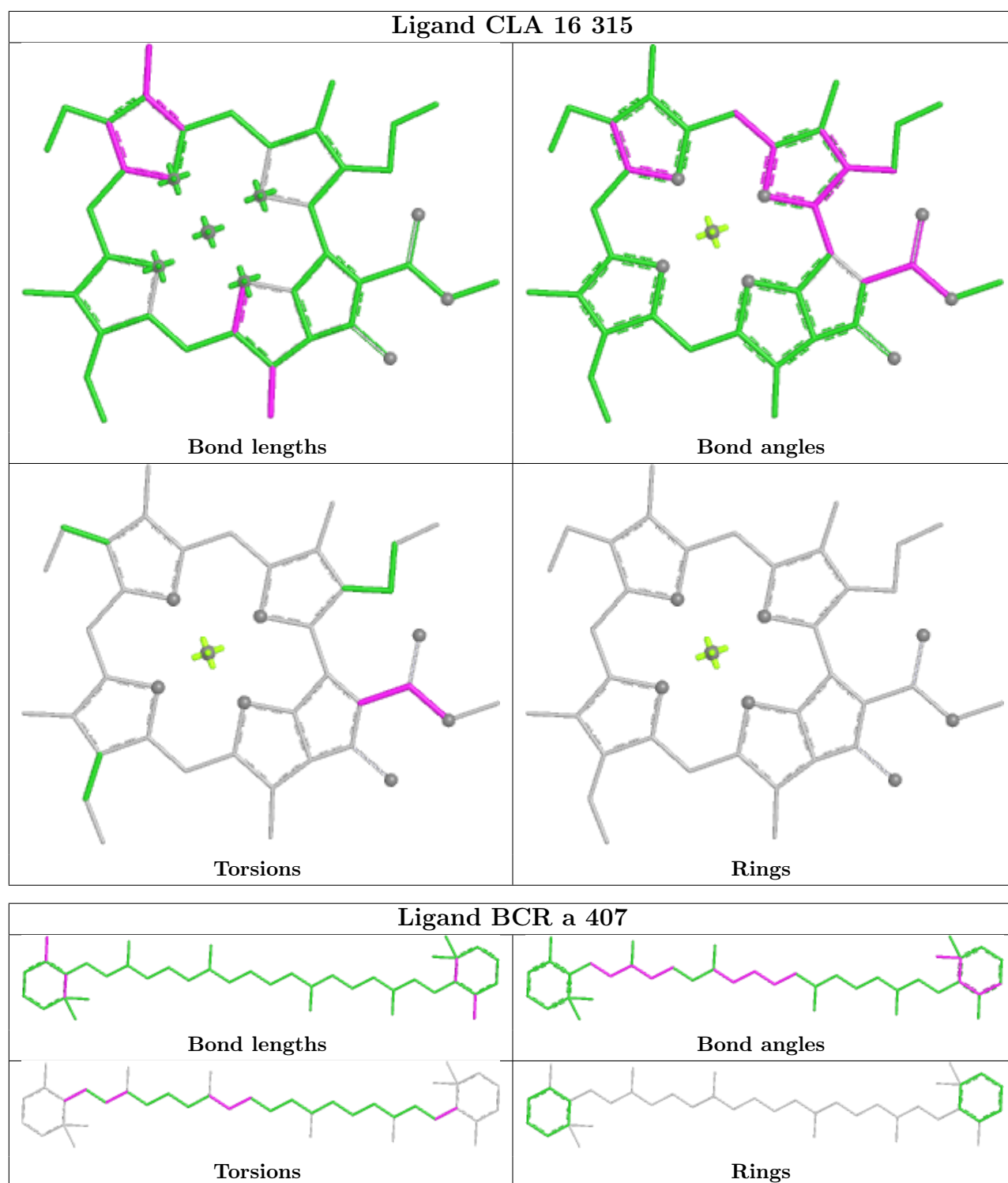


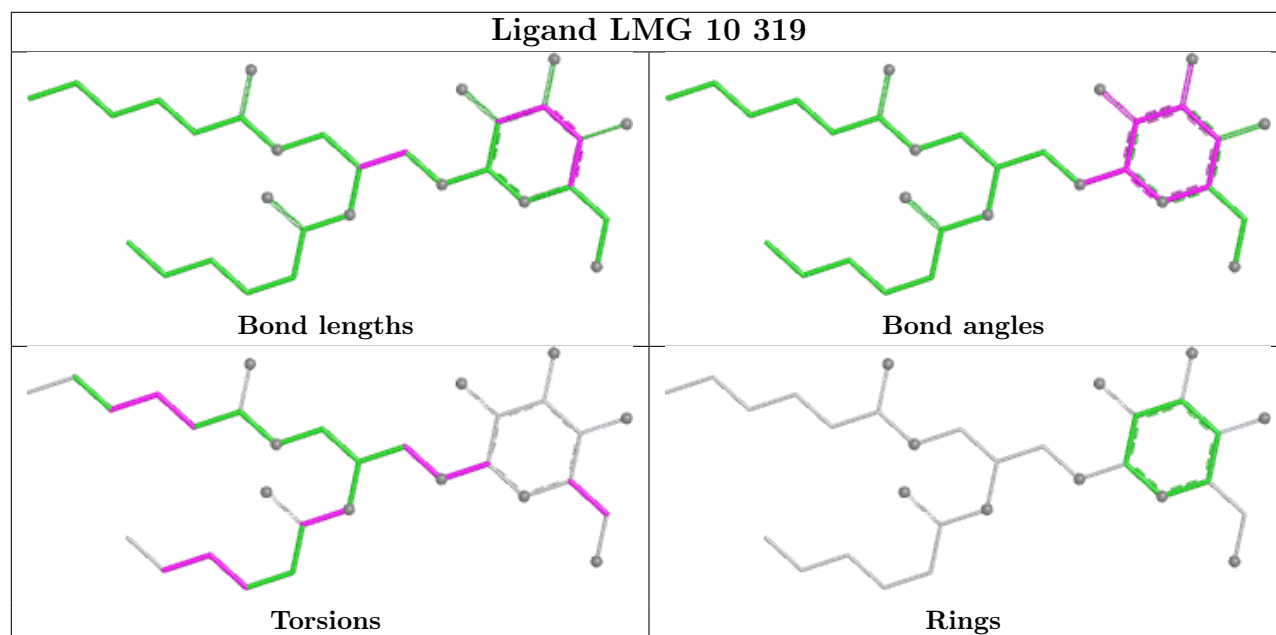
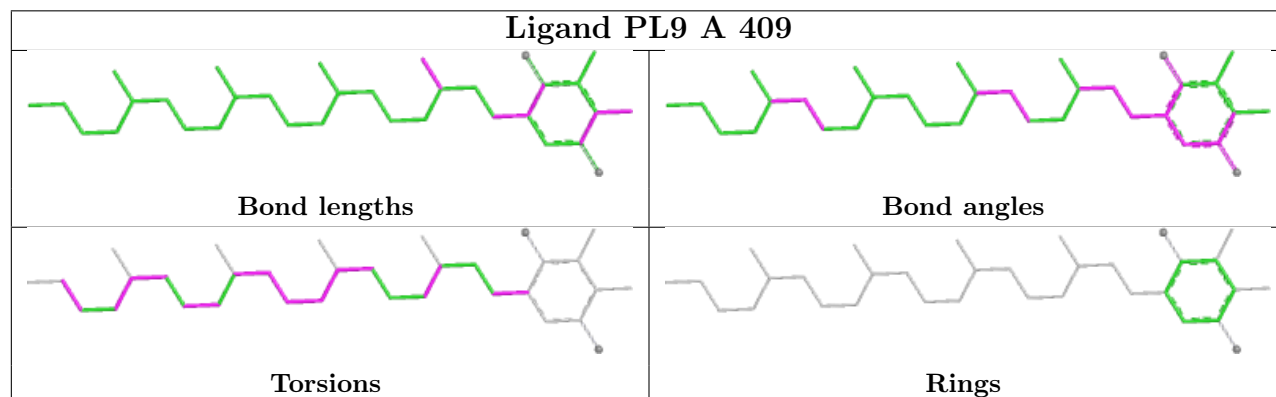
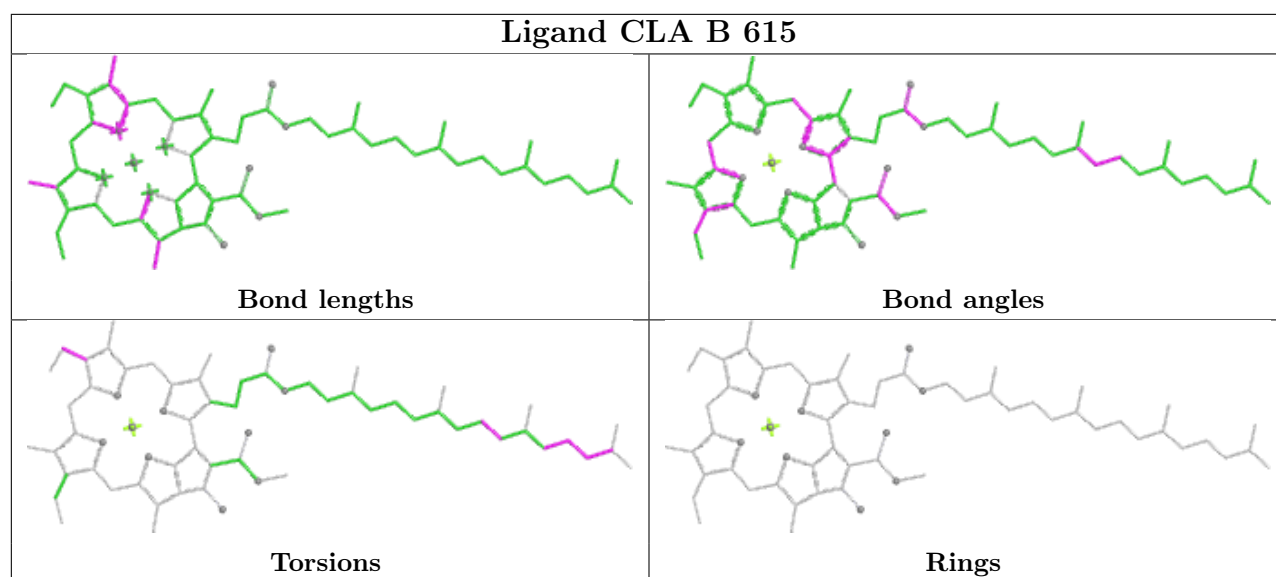


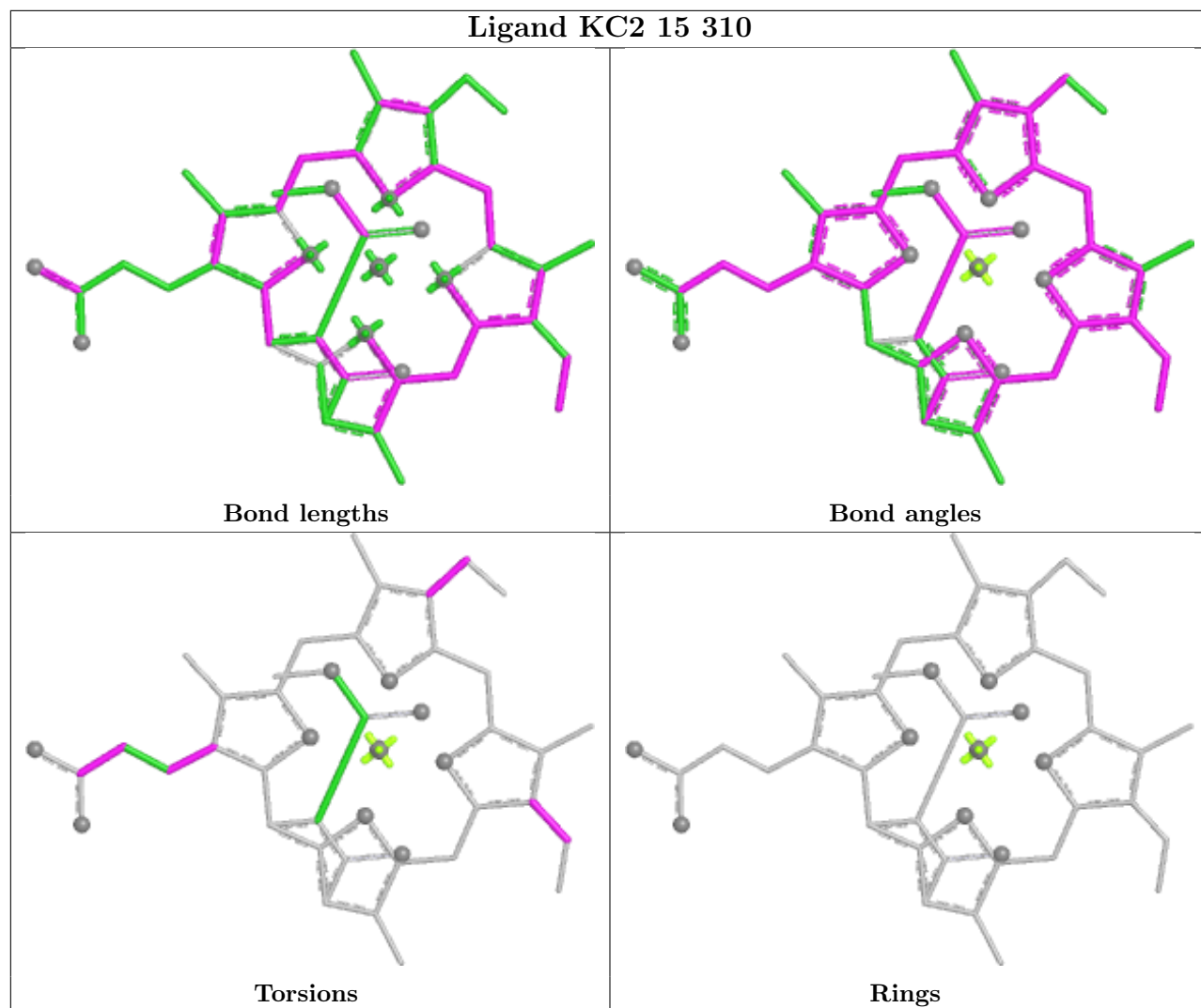
Ligand CLA 3 313**Ligand CLA b 617**

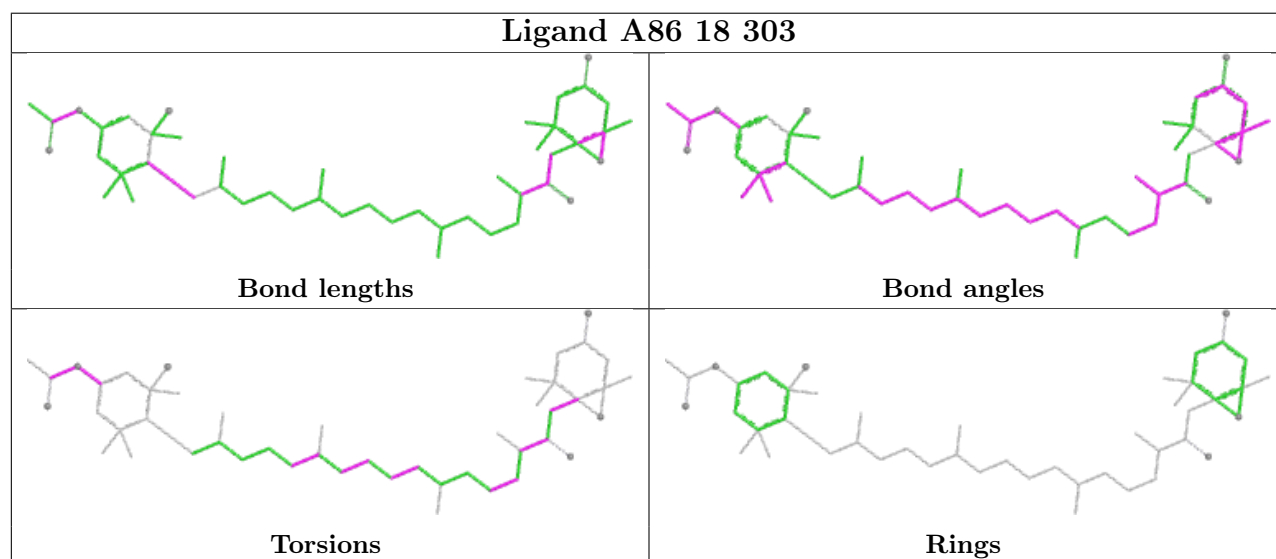
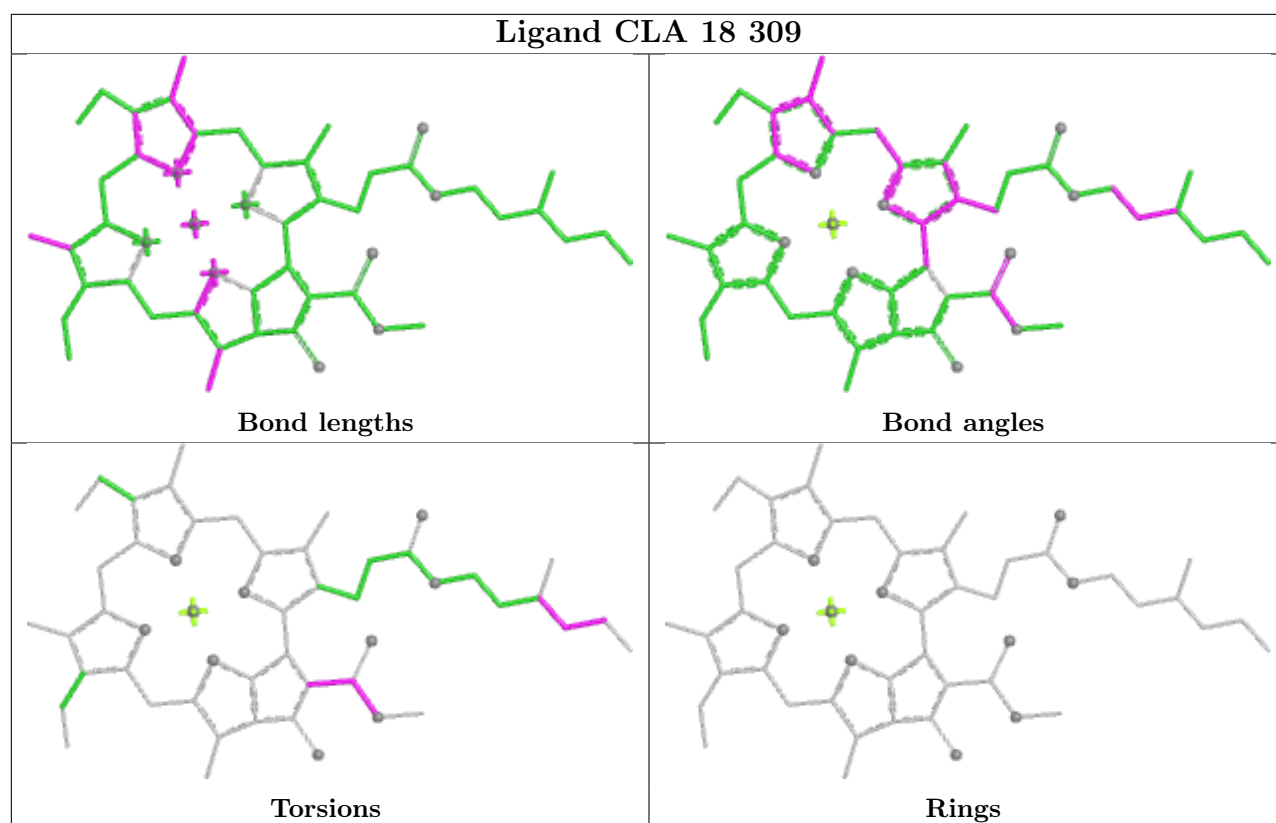
Ligand CLA 2 309

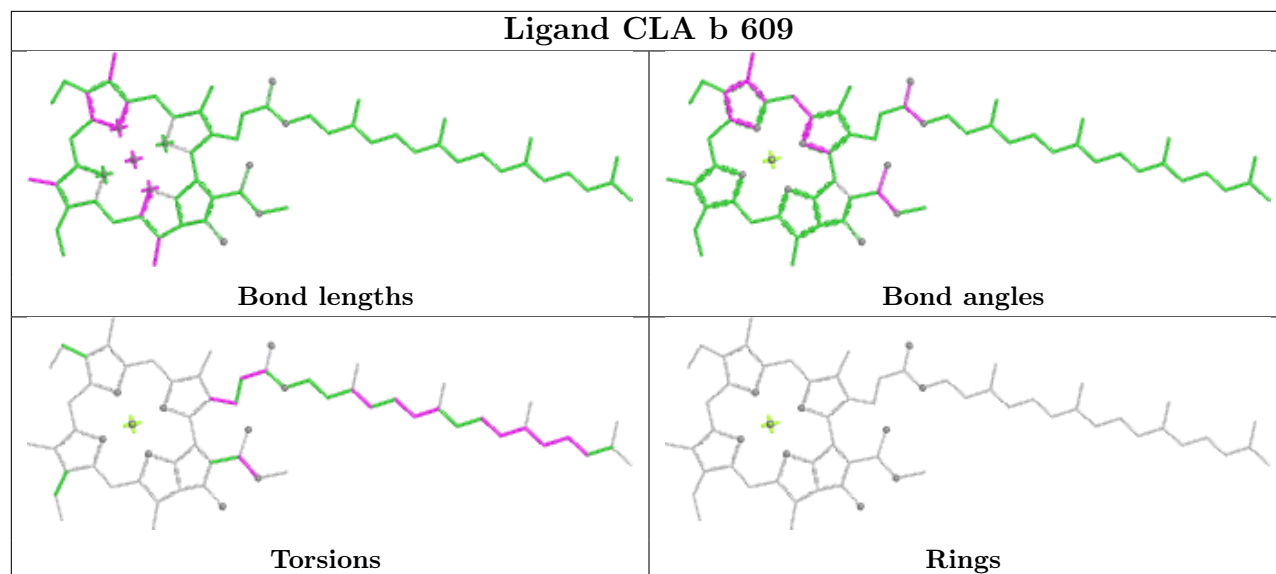
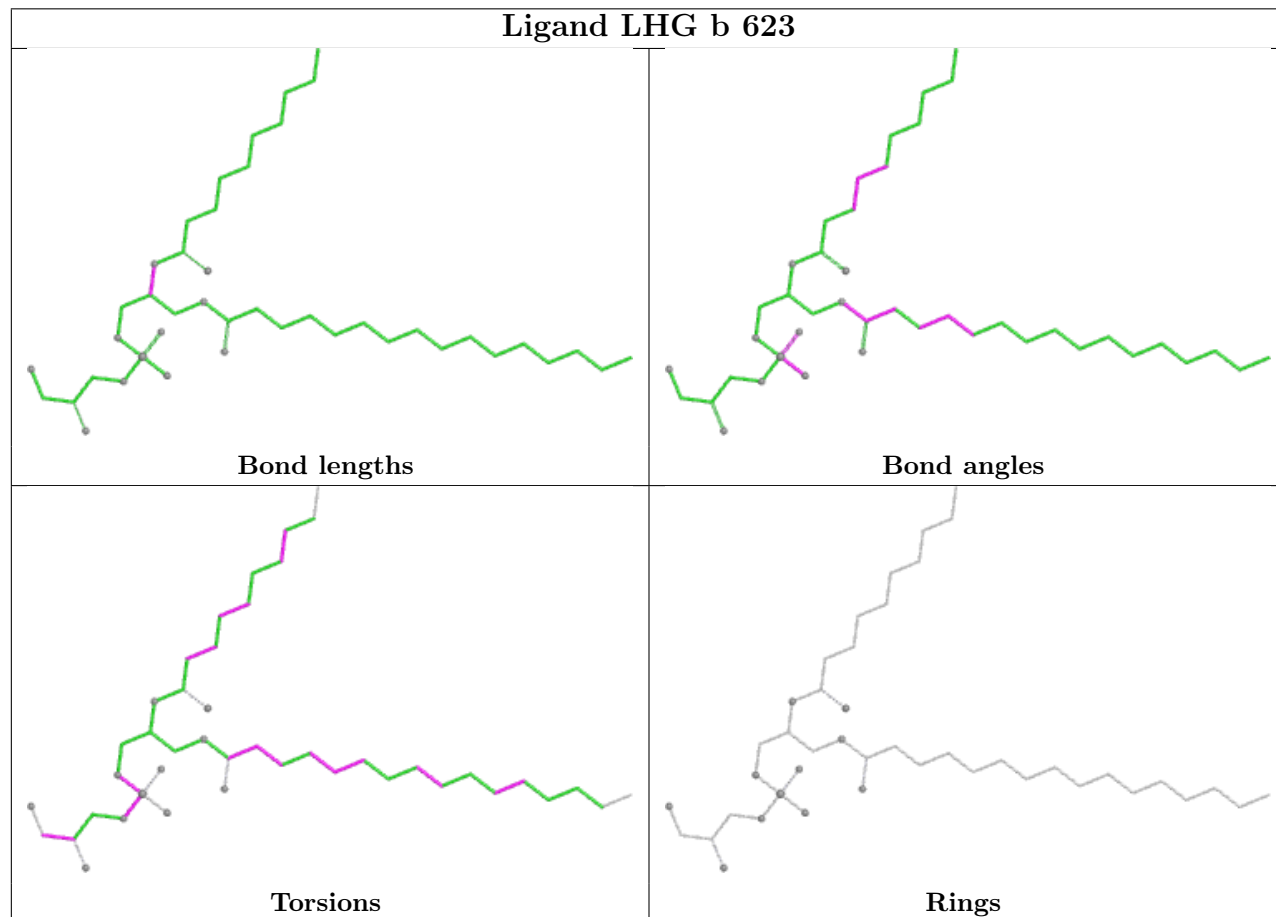


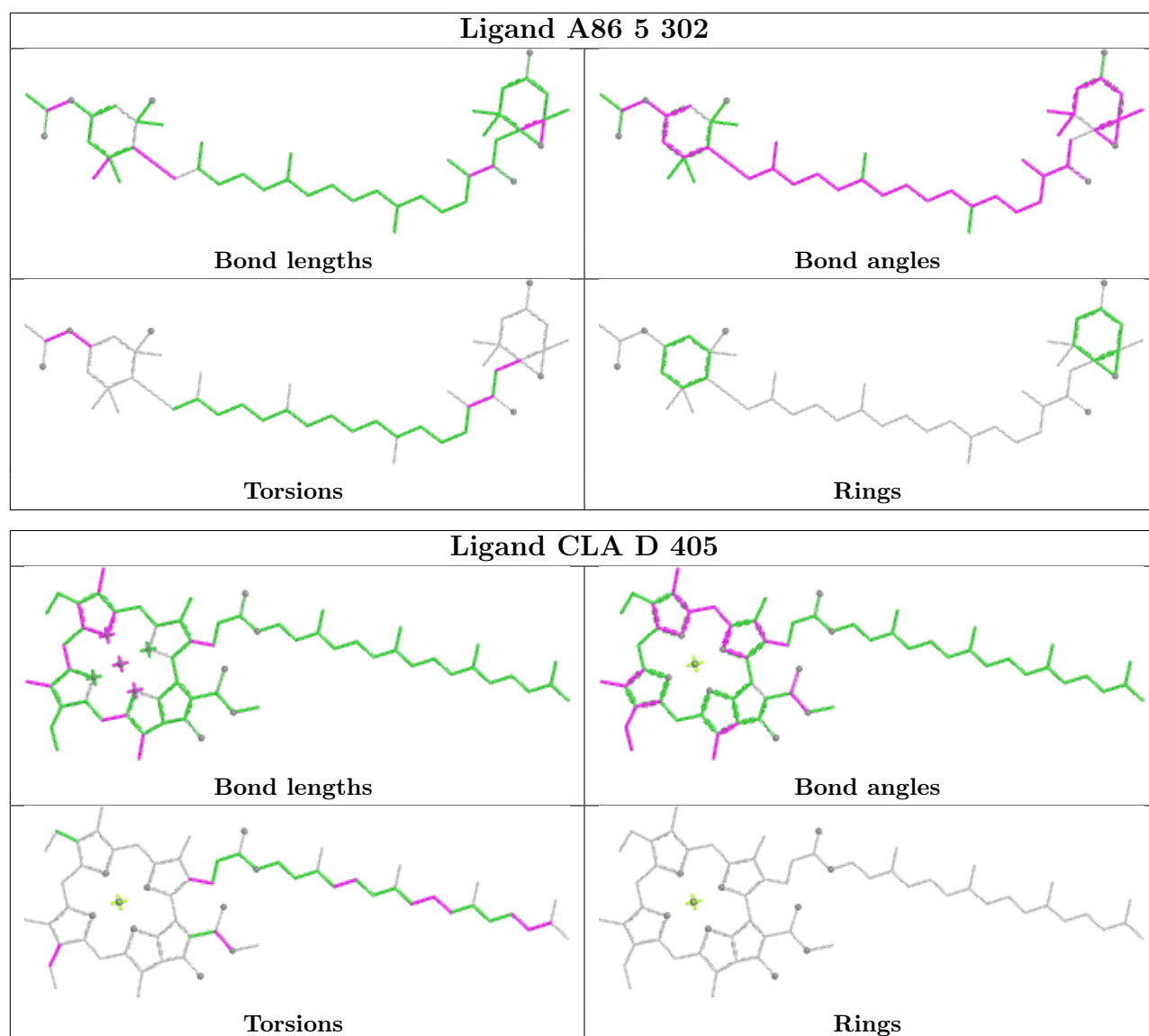




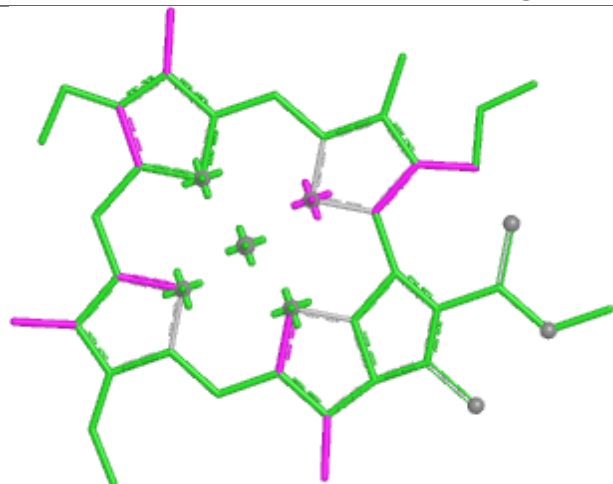




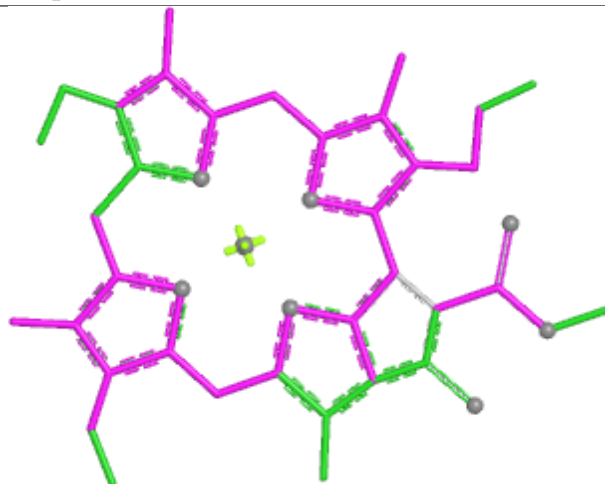
Ligand CLA b 609**Ligand LHG b 623**



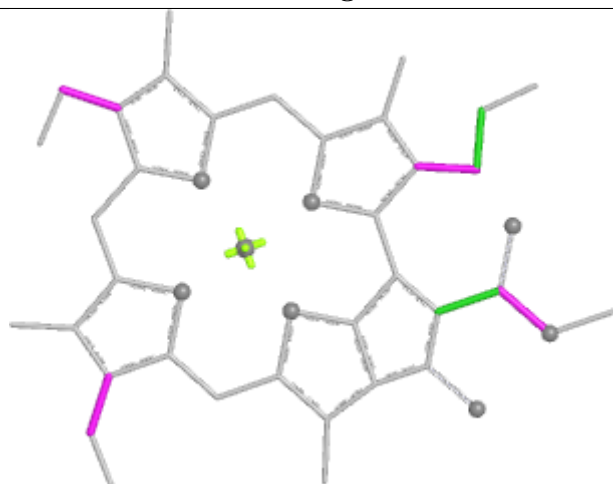
Ligand CLA p 606



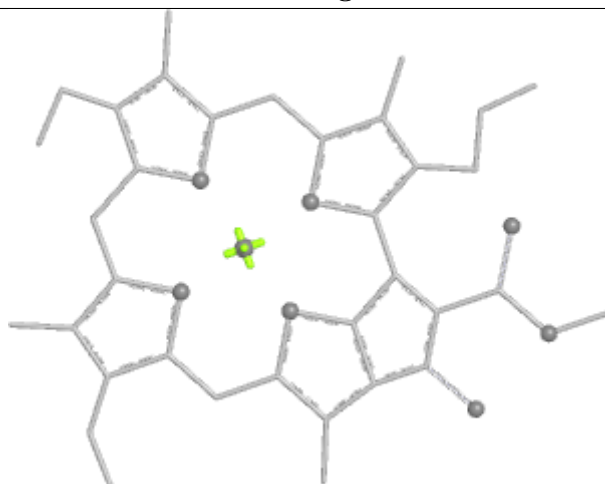
Bond lengths



Bond angles

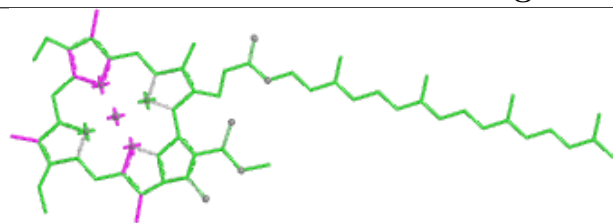


Torsions

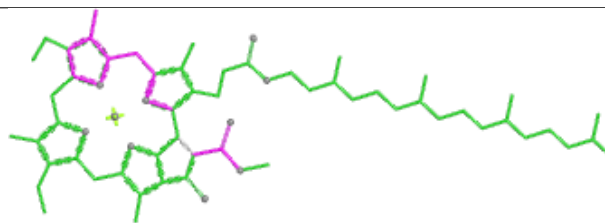


Rings

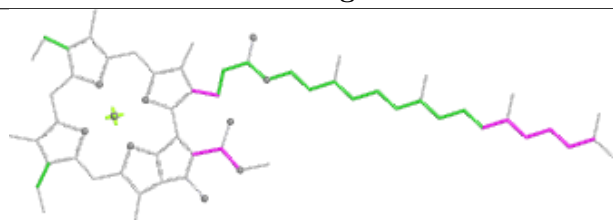
Ligand CLA C 507



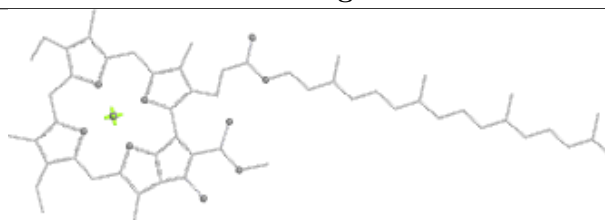
Bond lengths



Bond angles

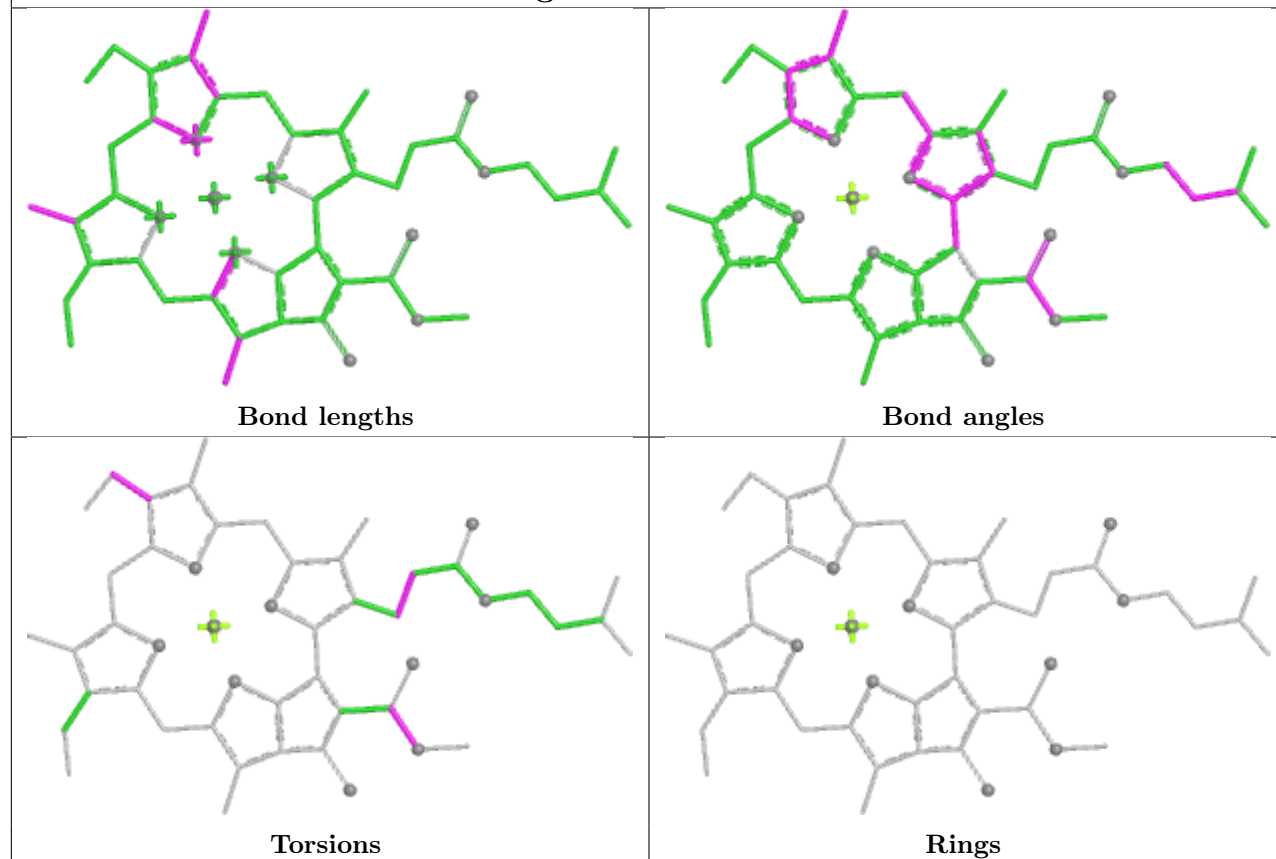


Torsions

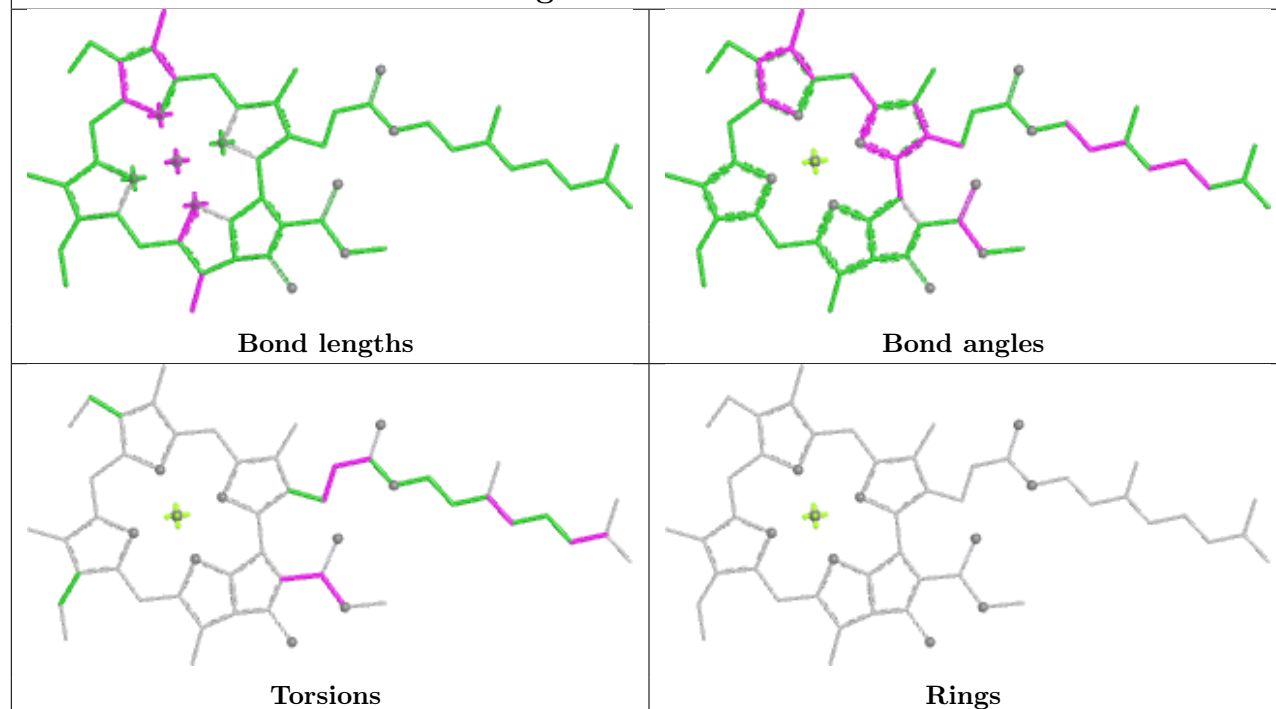


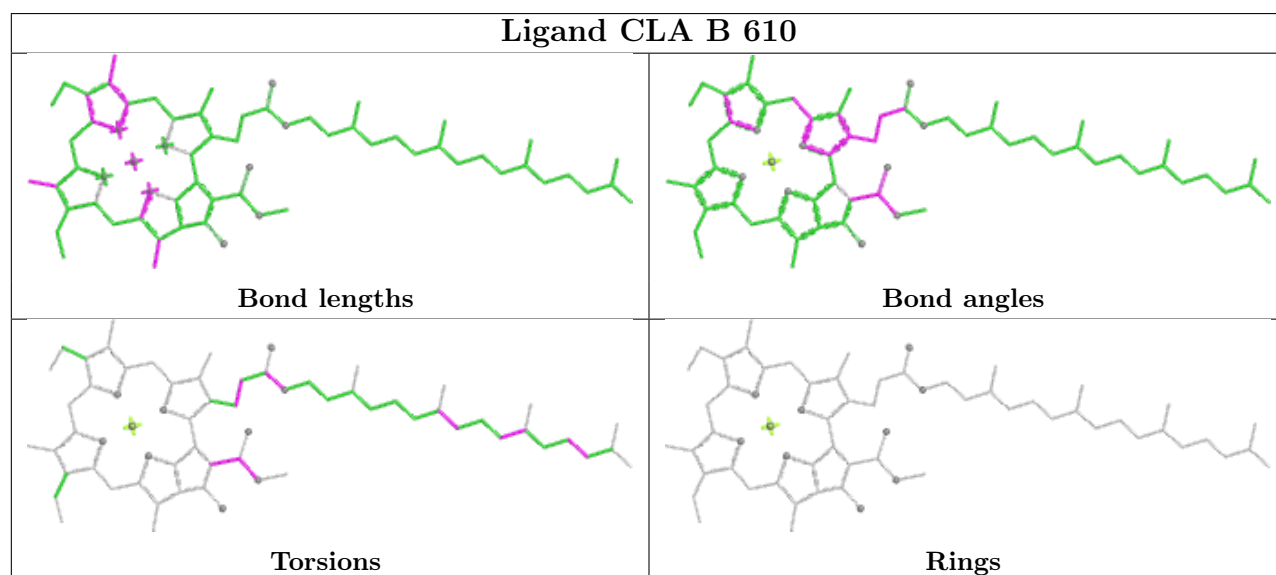
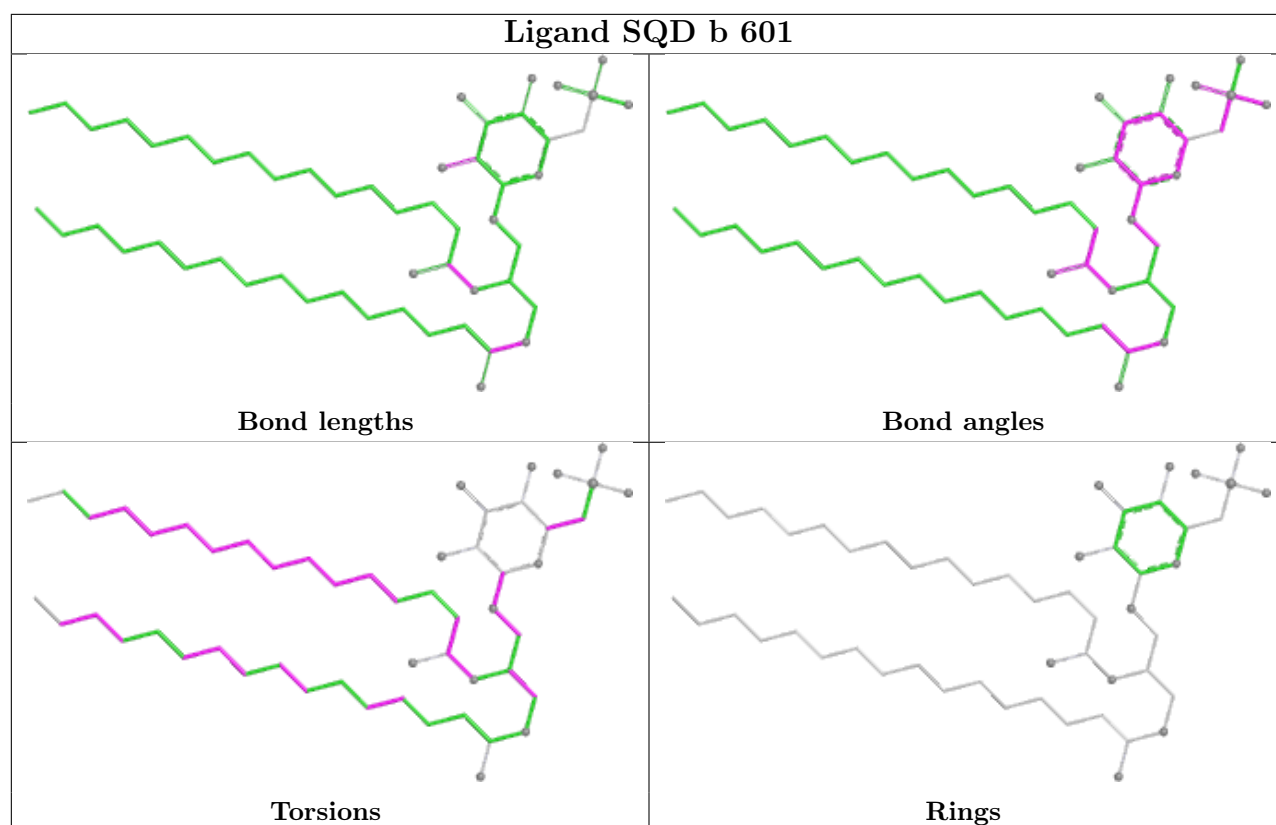
Rings

Ligand CLA 1 310

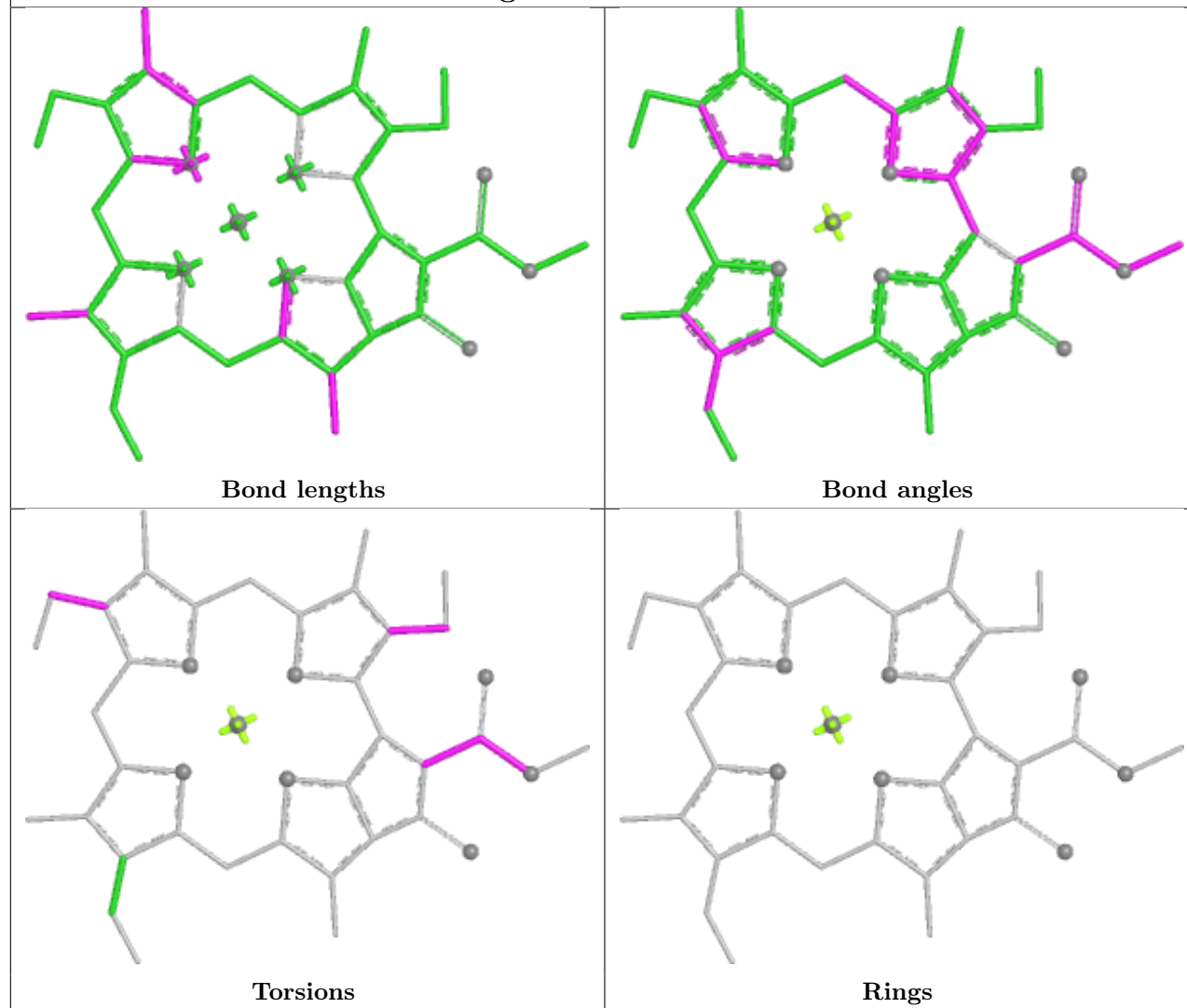


Ligand CLA 5 309

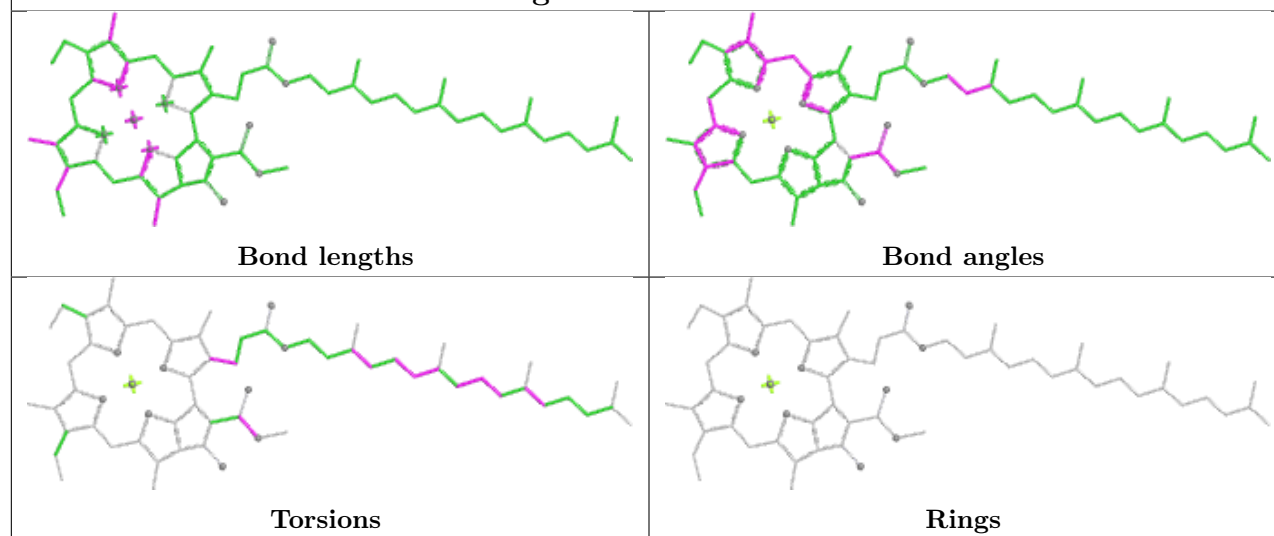


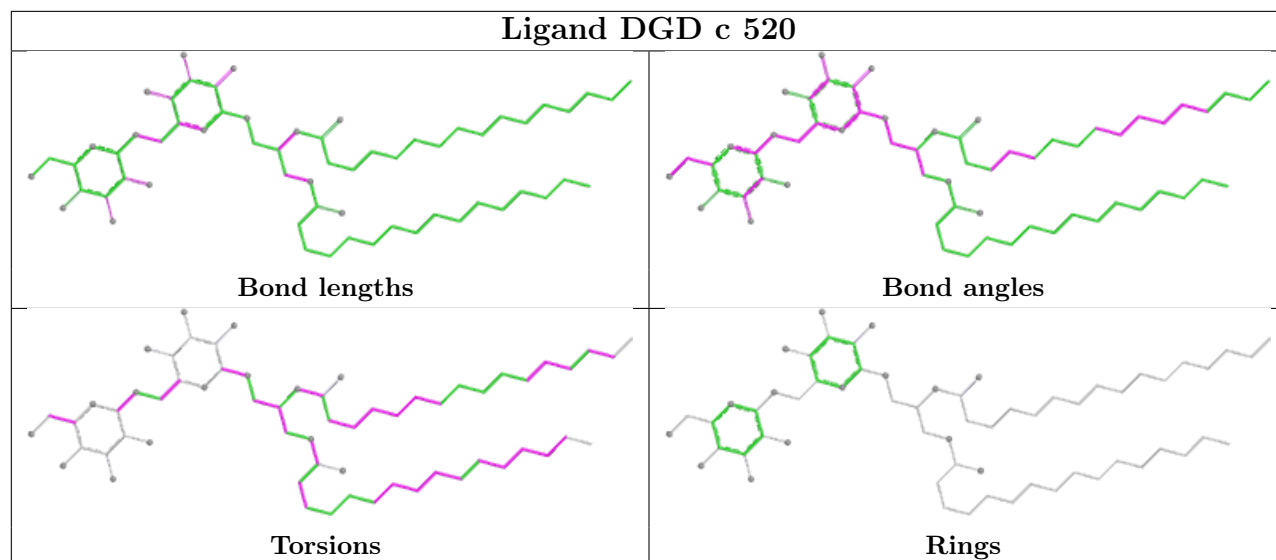
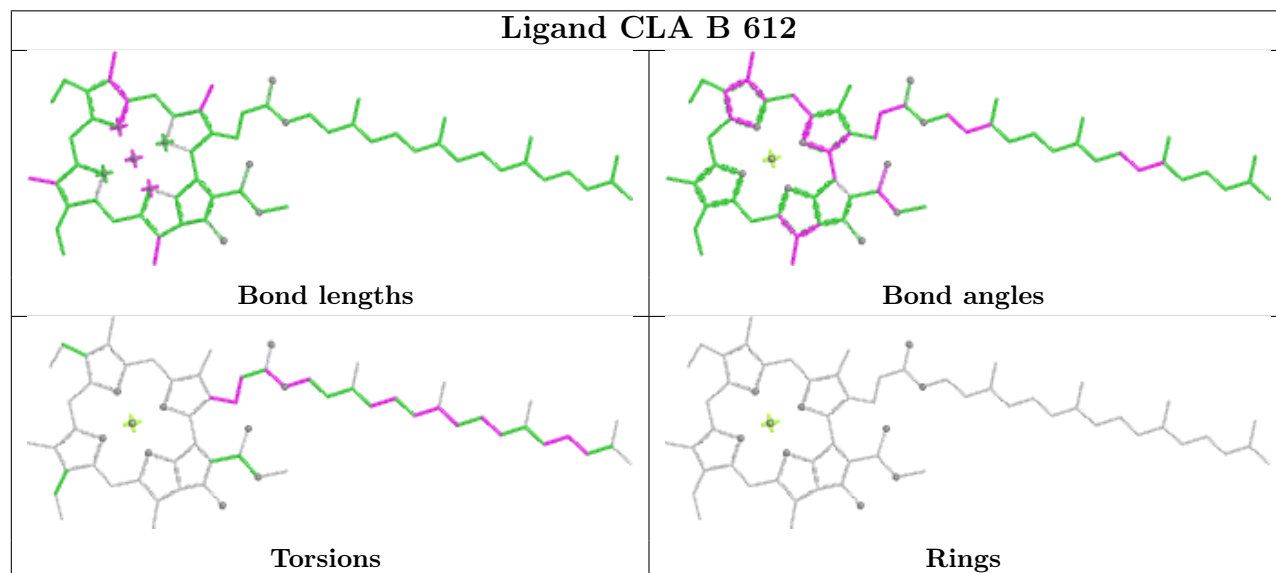
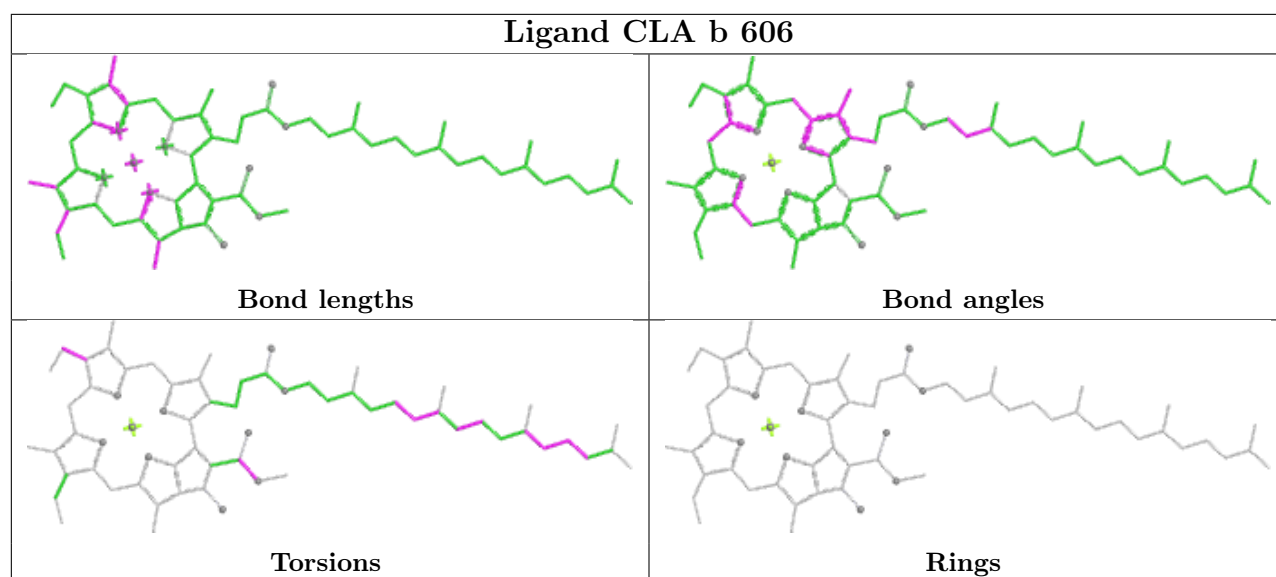


Ligand CLA 6 308

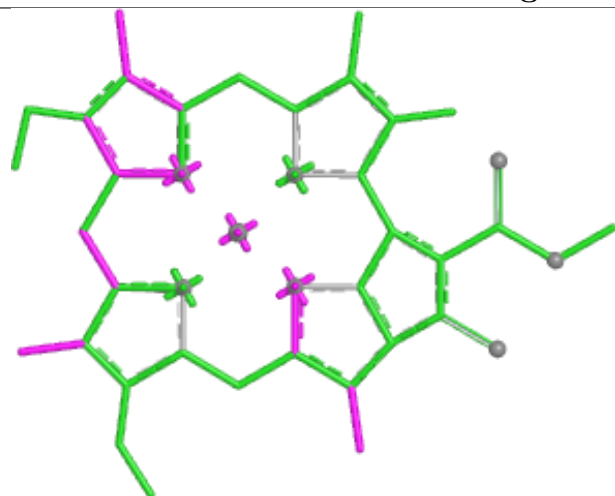


Ligand CLA B 611

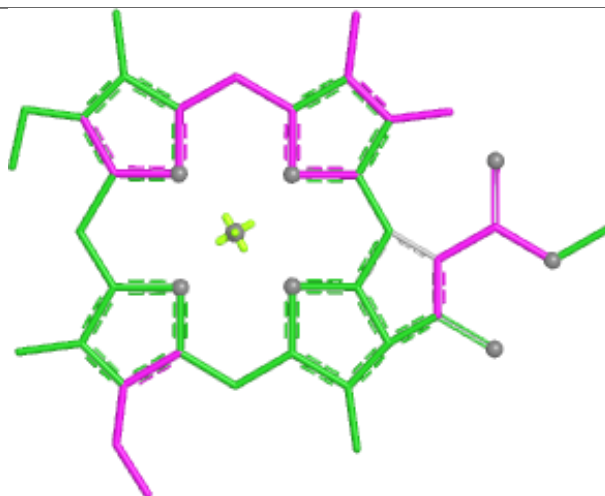




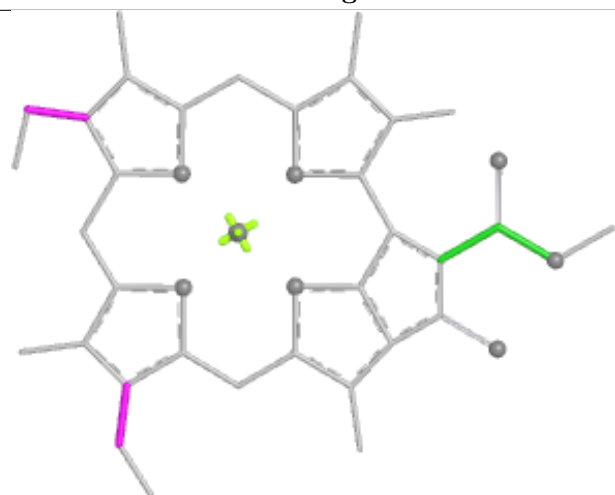
Ligand CLA 7 308



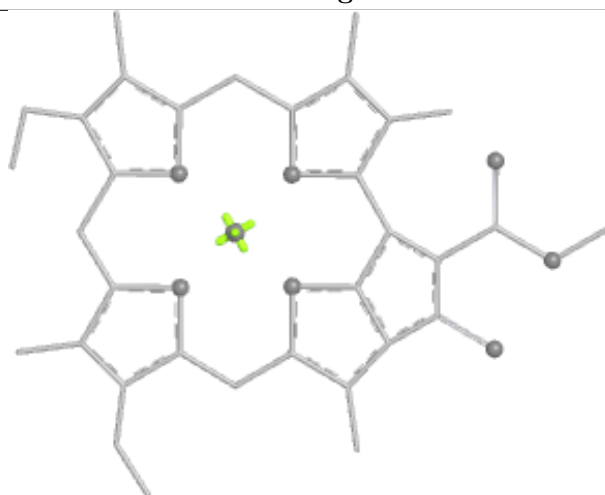
Bond lengths



Bond angles

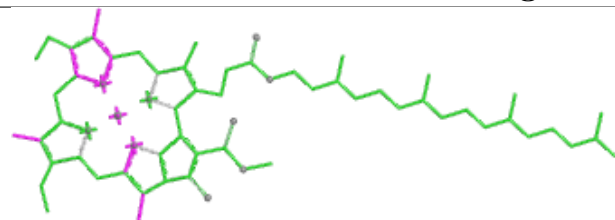


Torsions

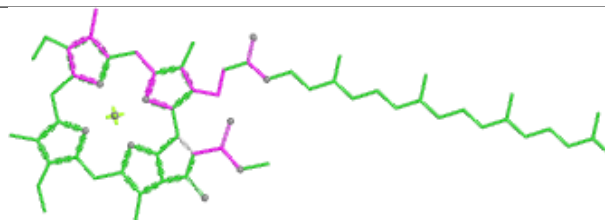


Rings

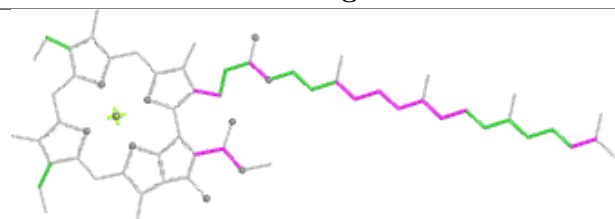
Ligand CLA b 615



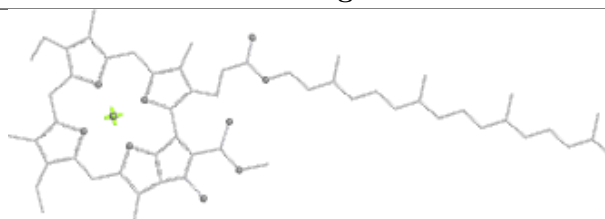
Bond lengths



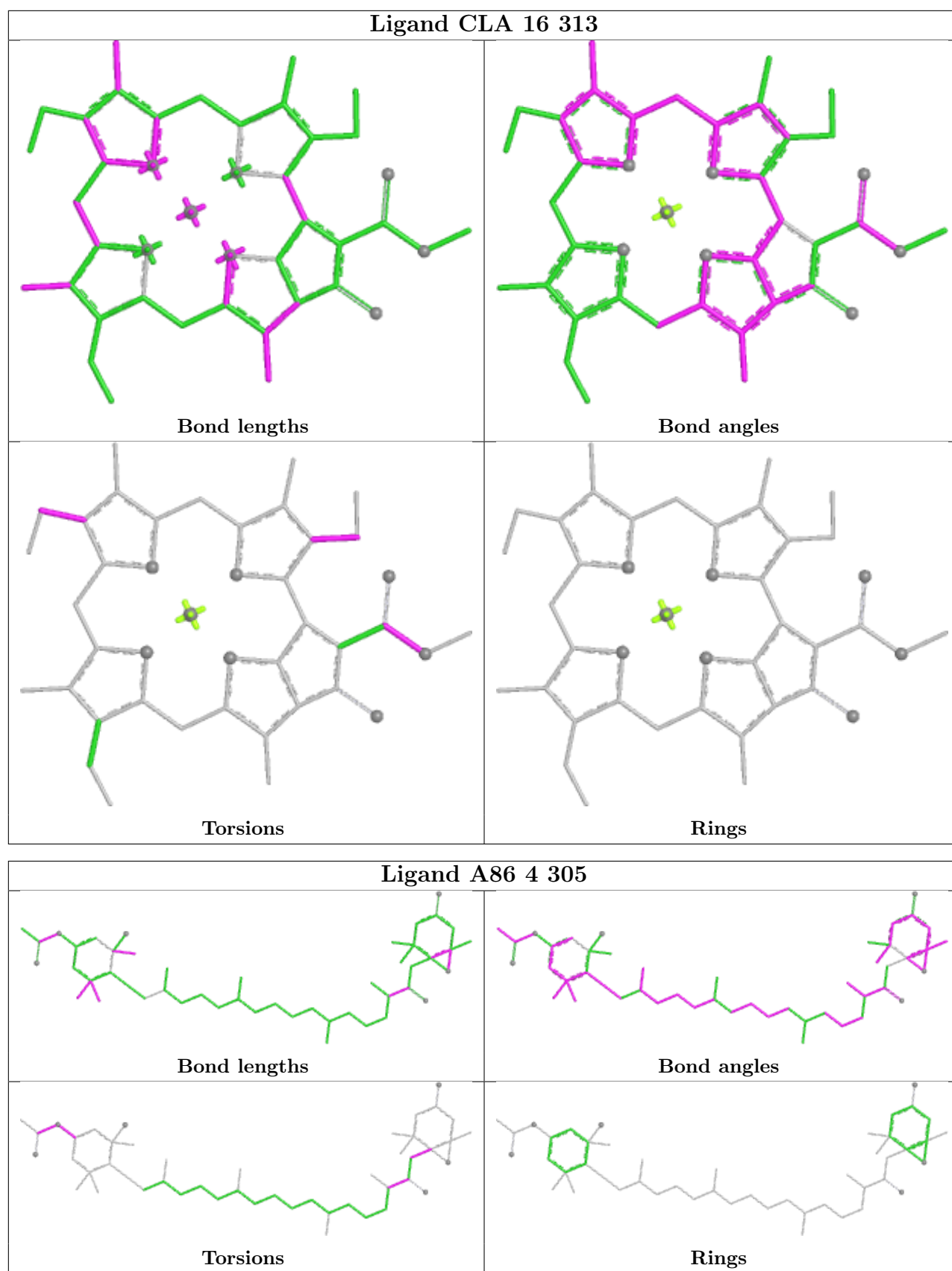
Bond angles

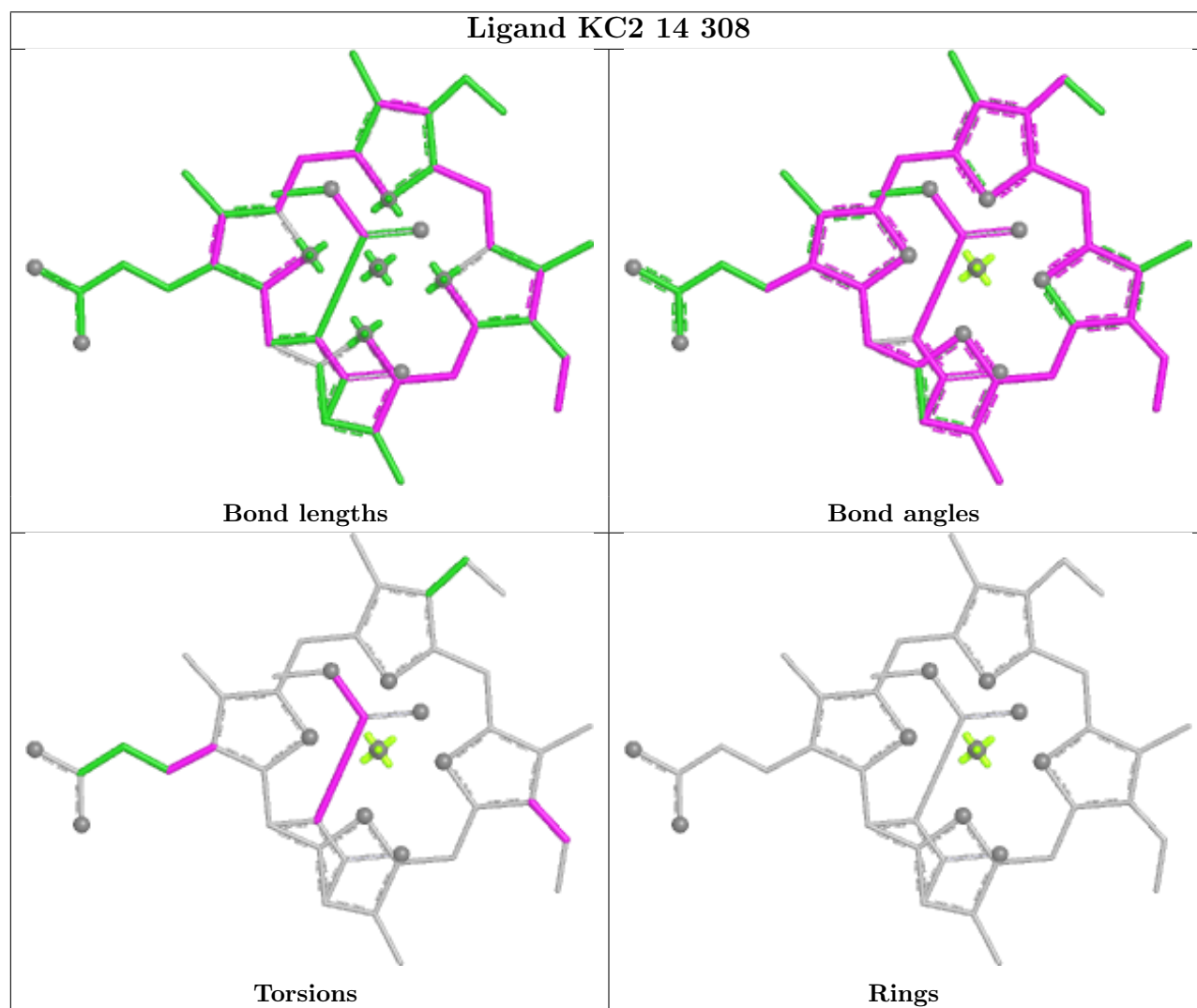
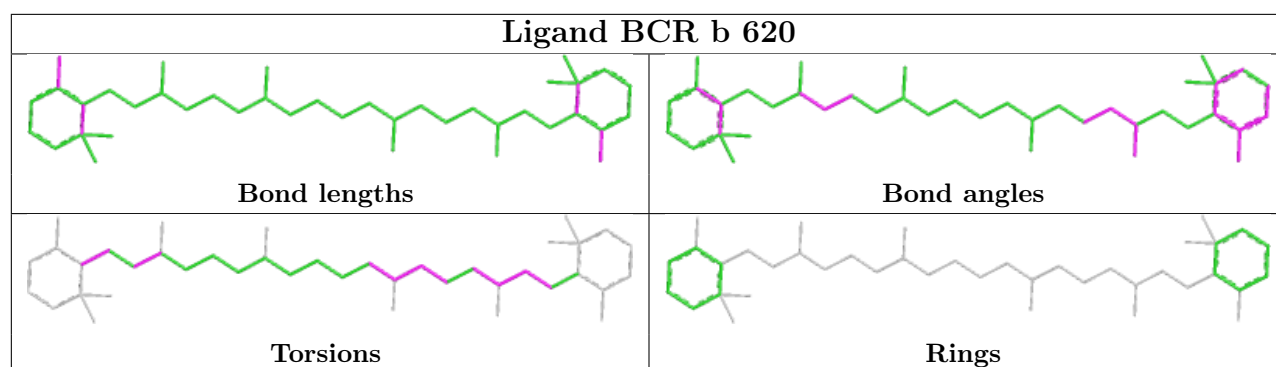


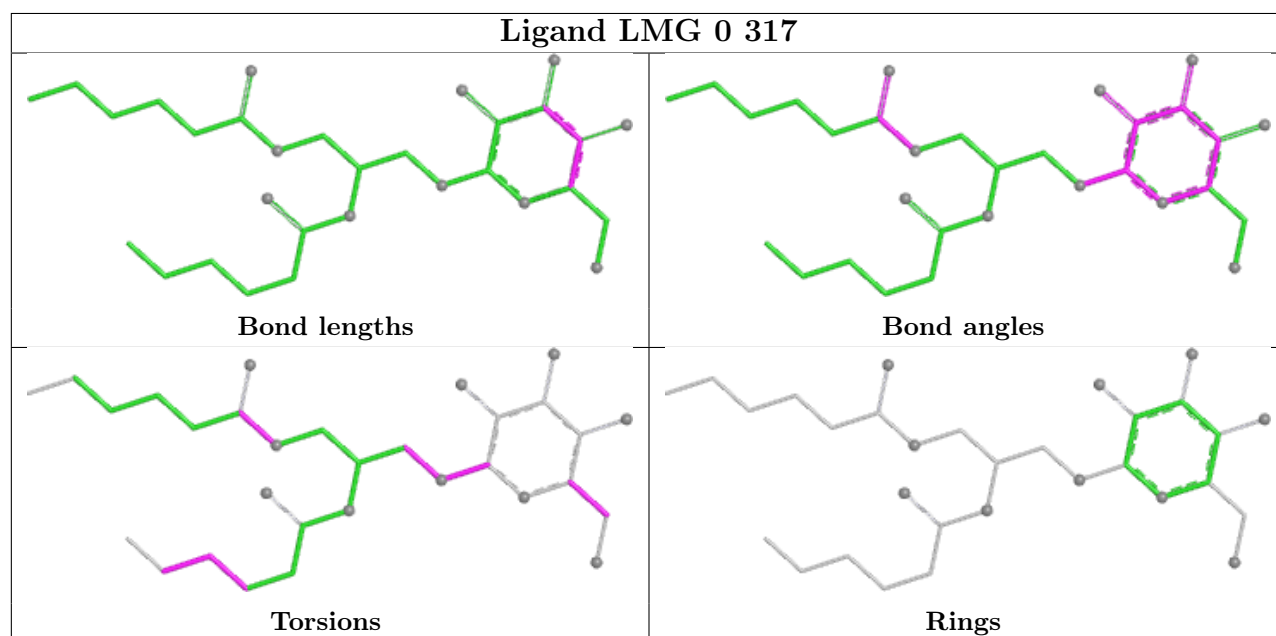
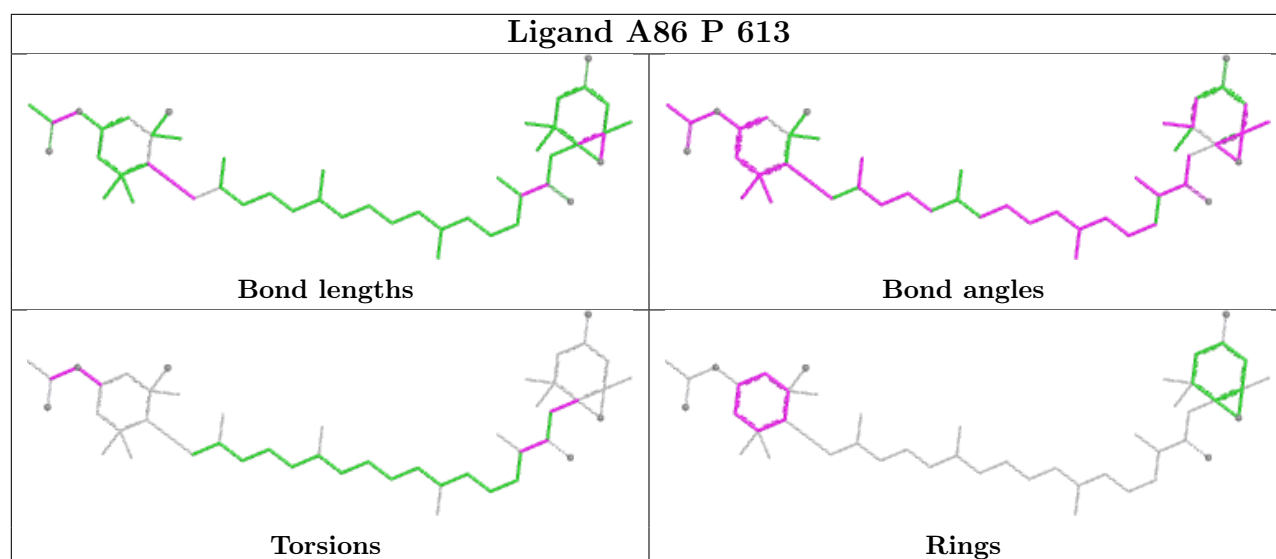
Torsions

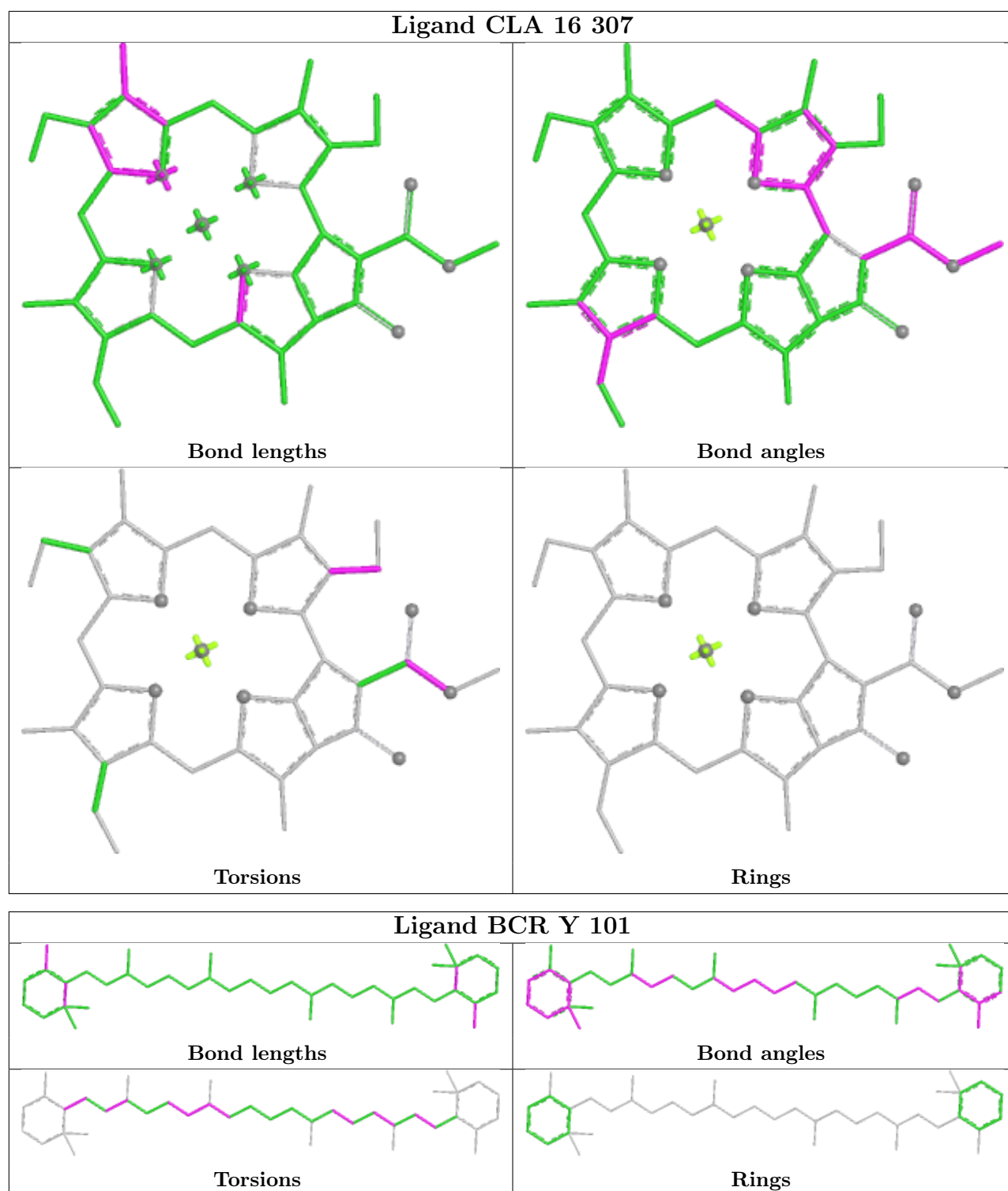


Rings

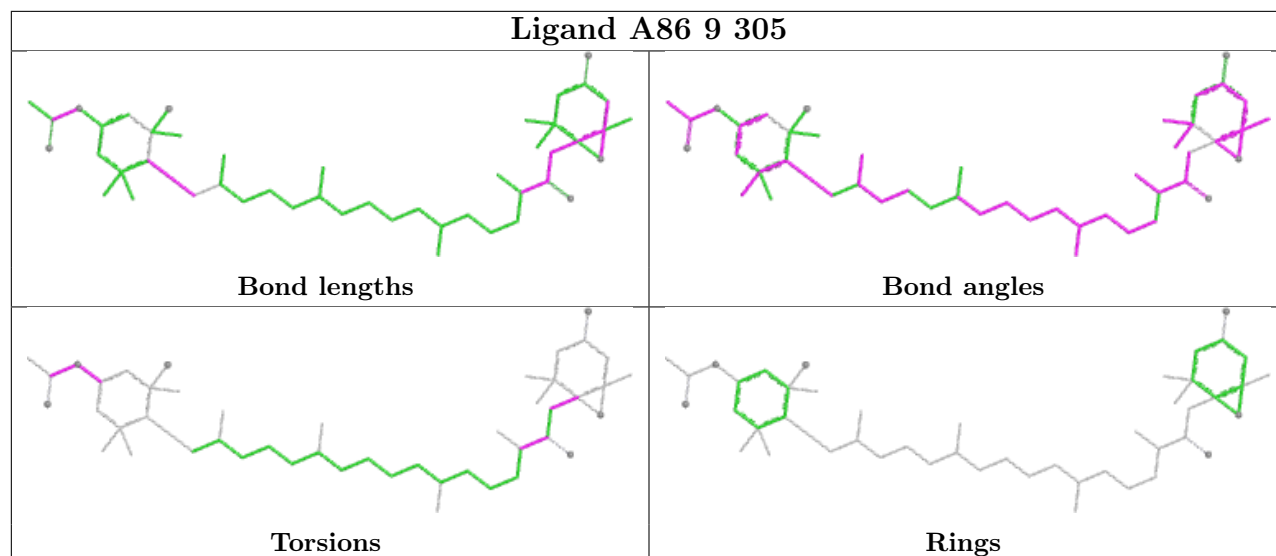




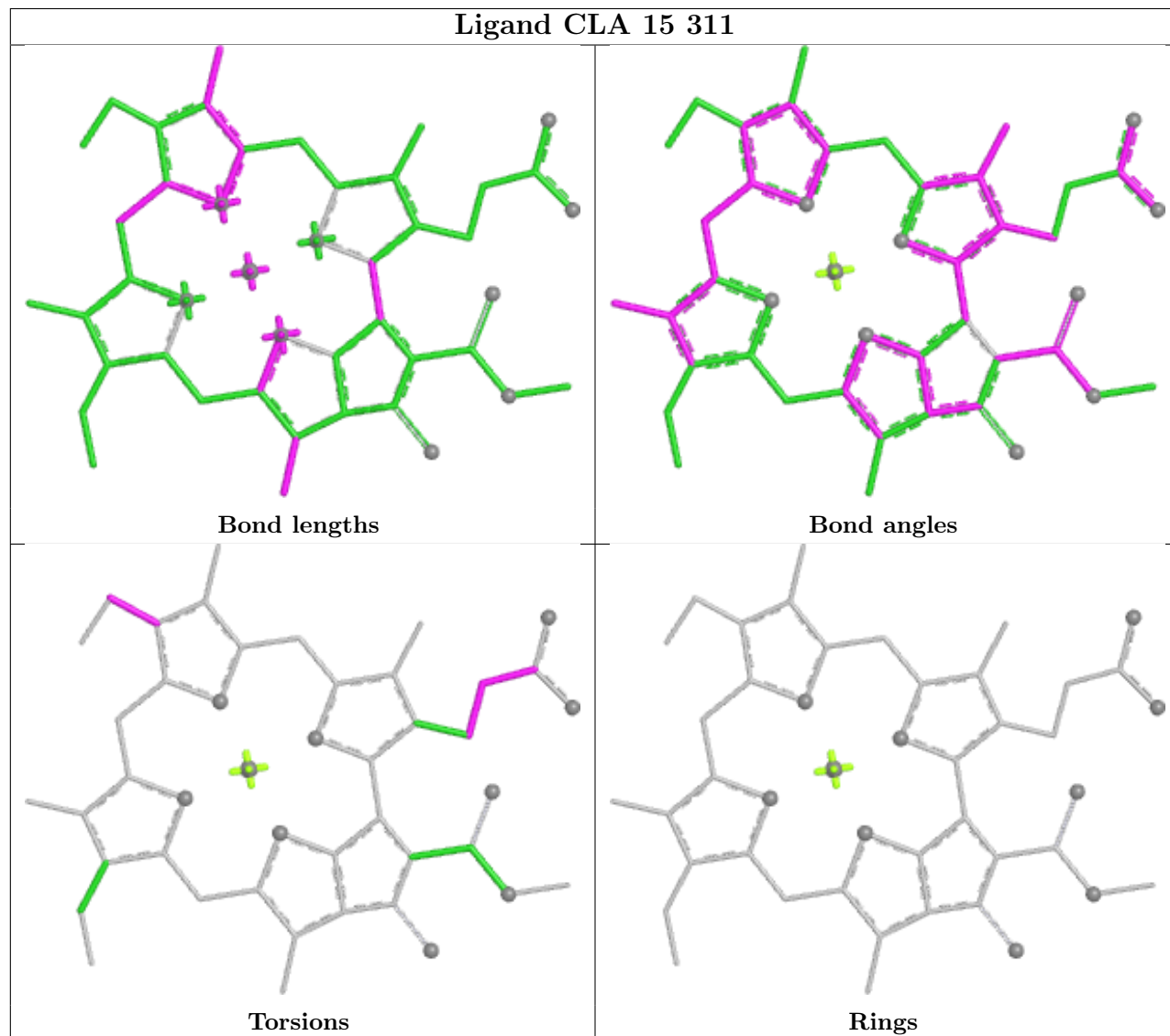


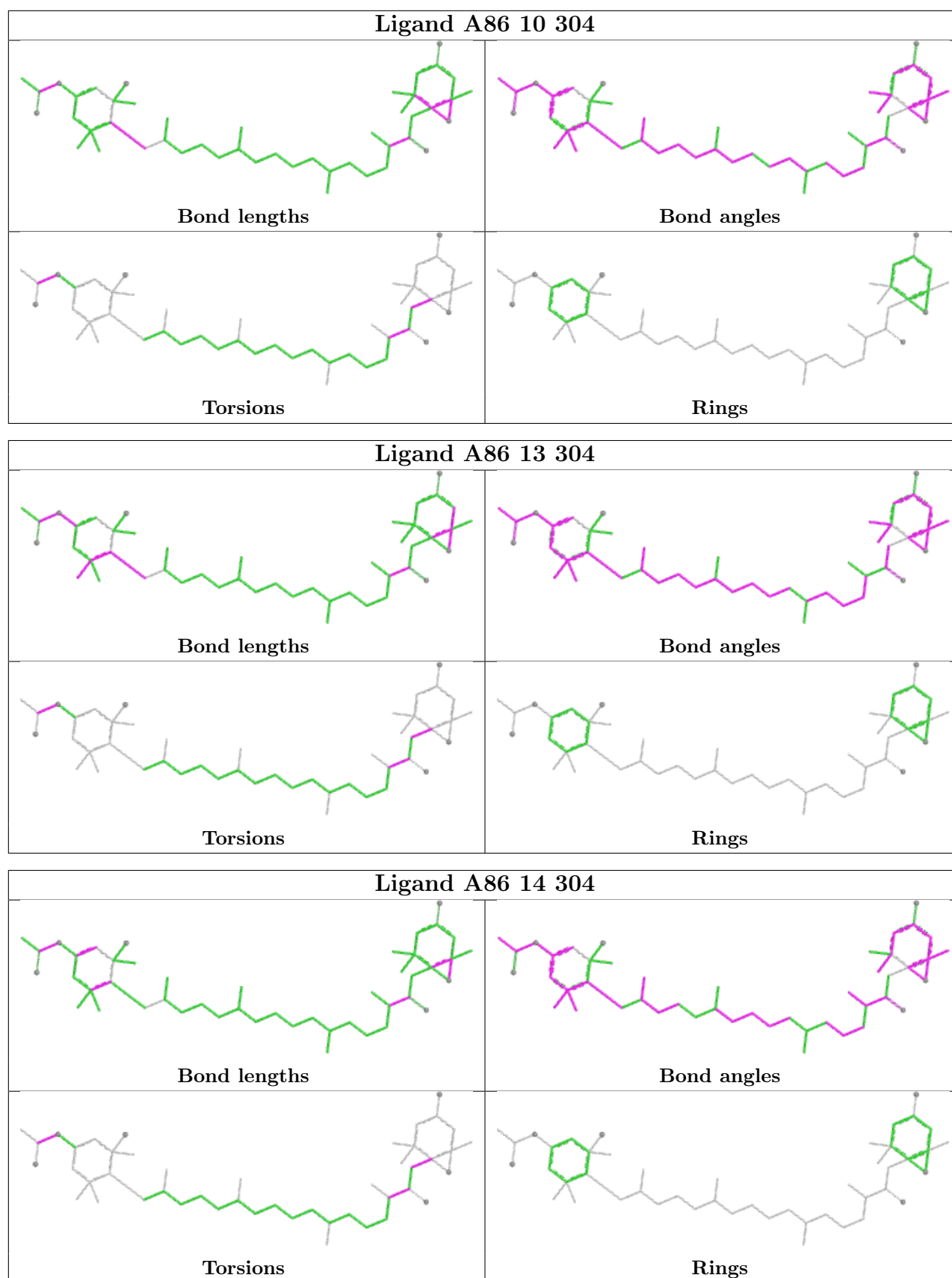


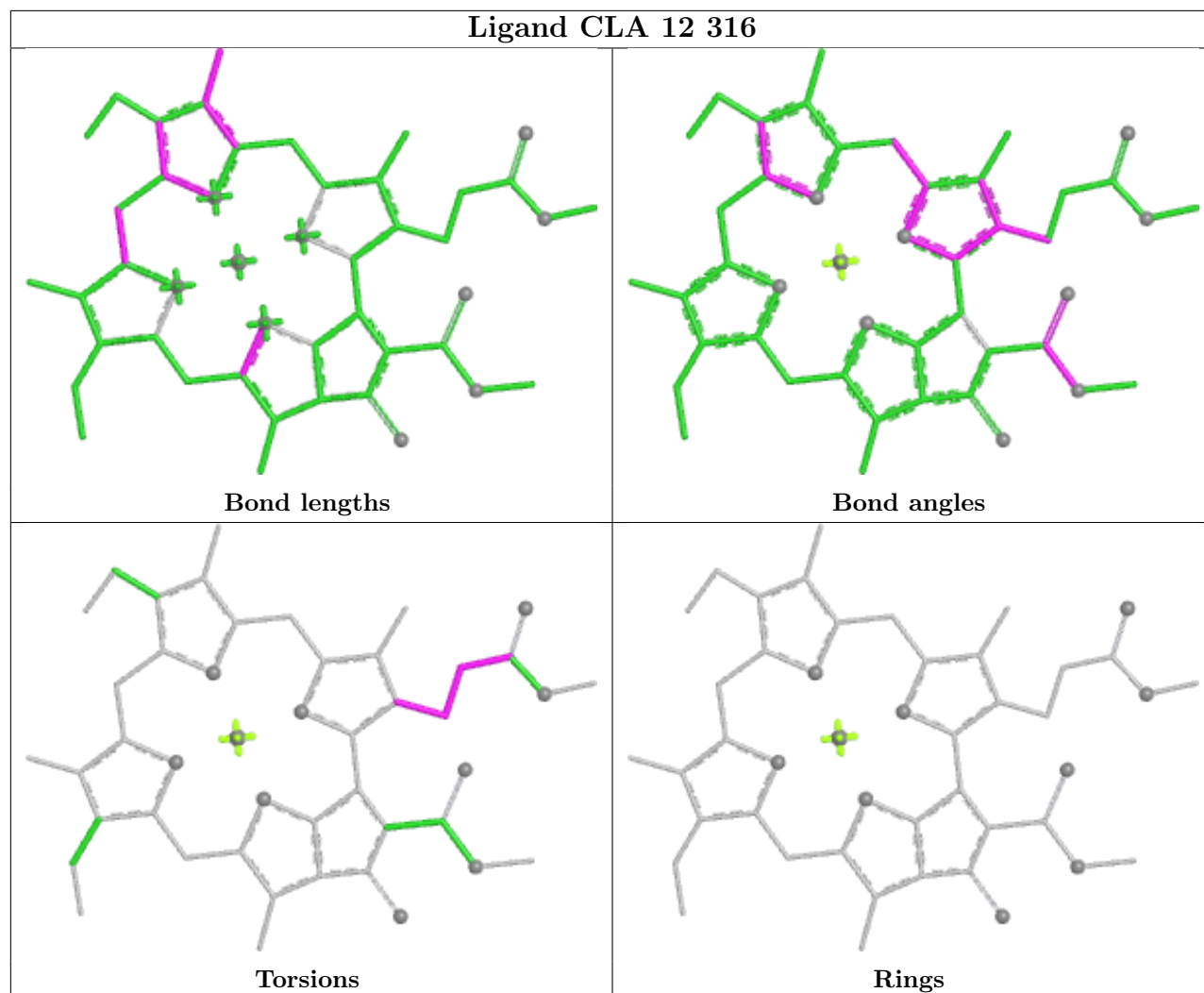
Ligand A86 9 305

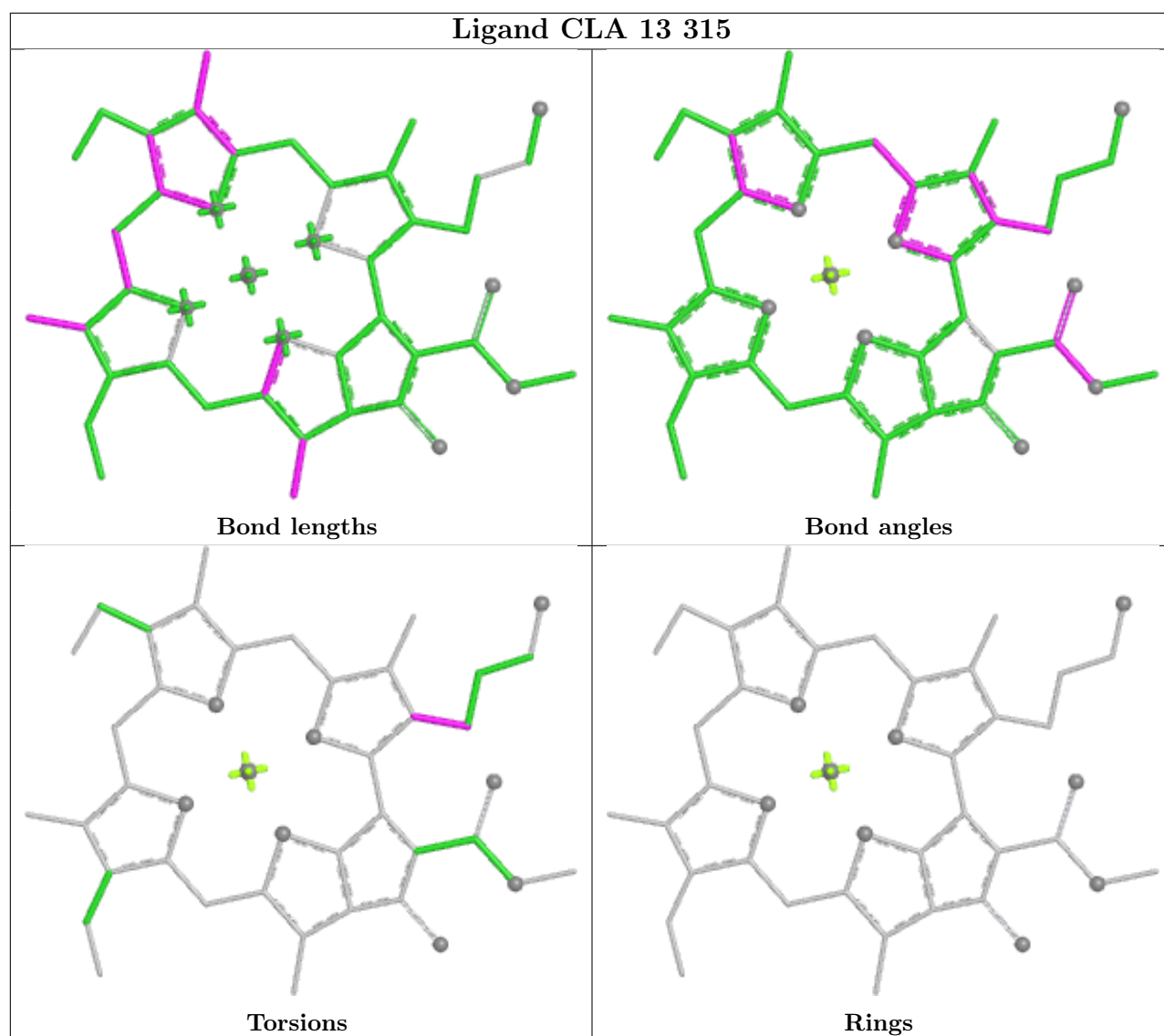


Ligand CLA 15 311

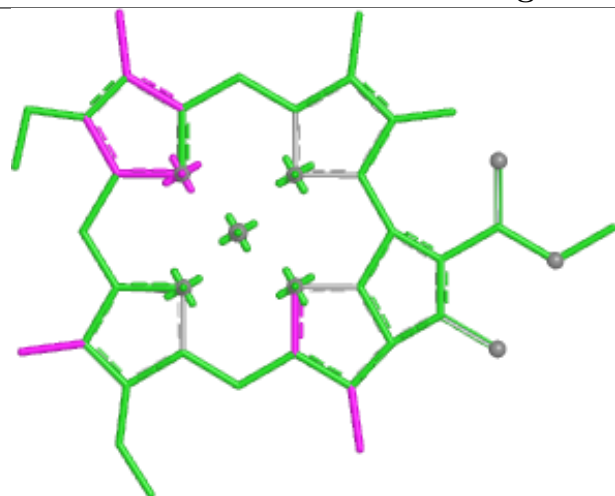




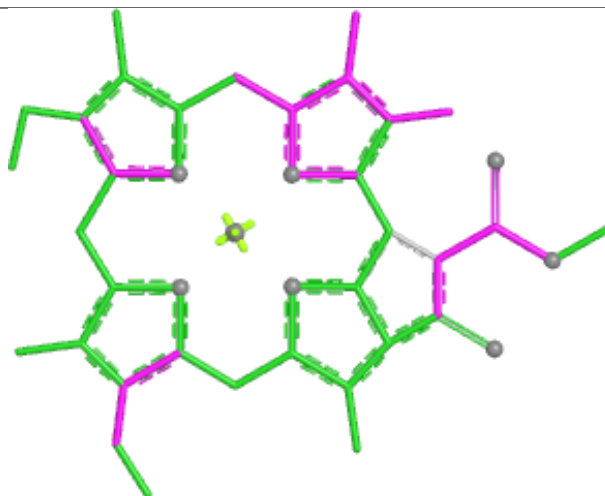




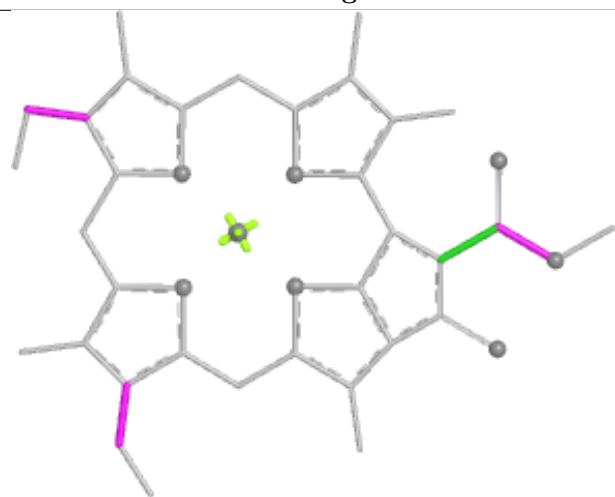
Ligand CLA P 605



Bond lengths



Bond angles

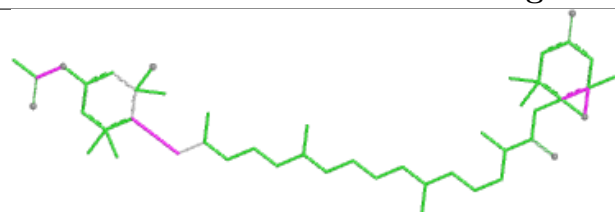


Torsions

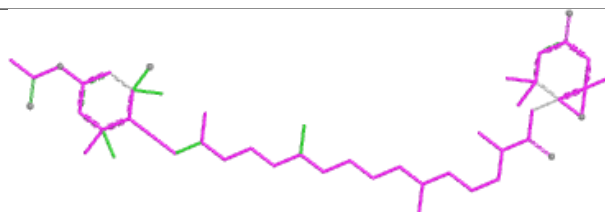


Rings

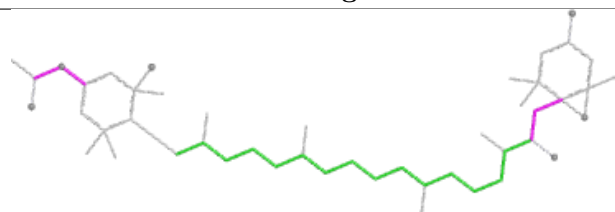
Ligand A86 1 302



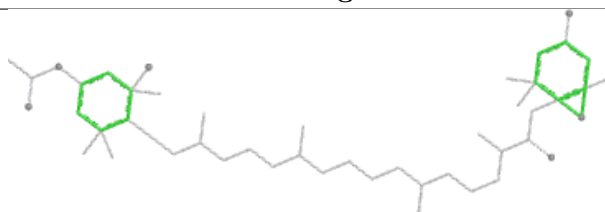
Bond lengths



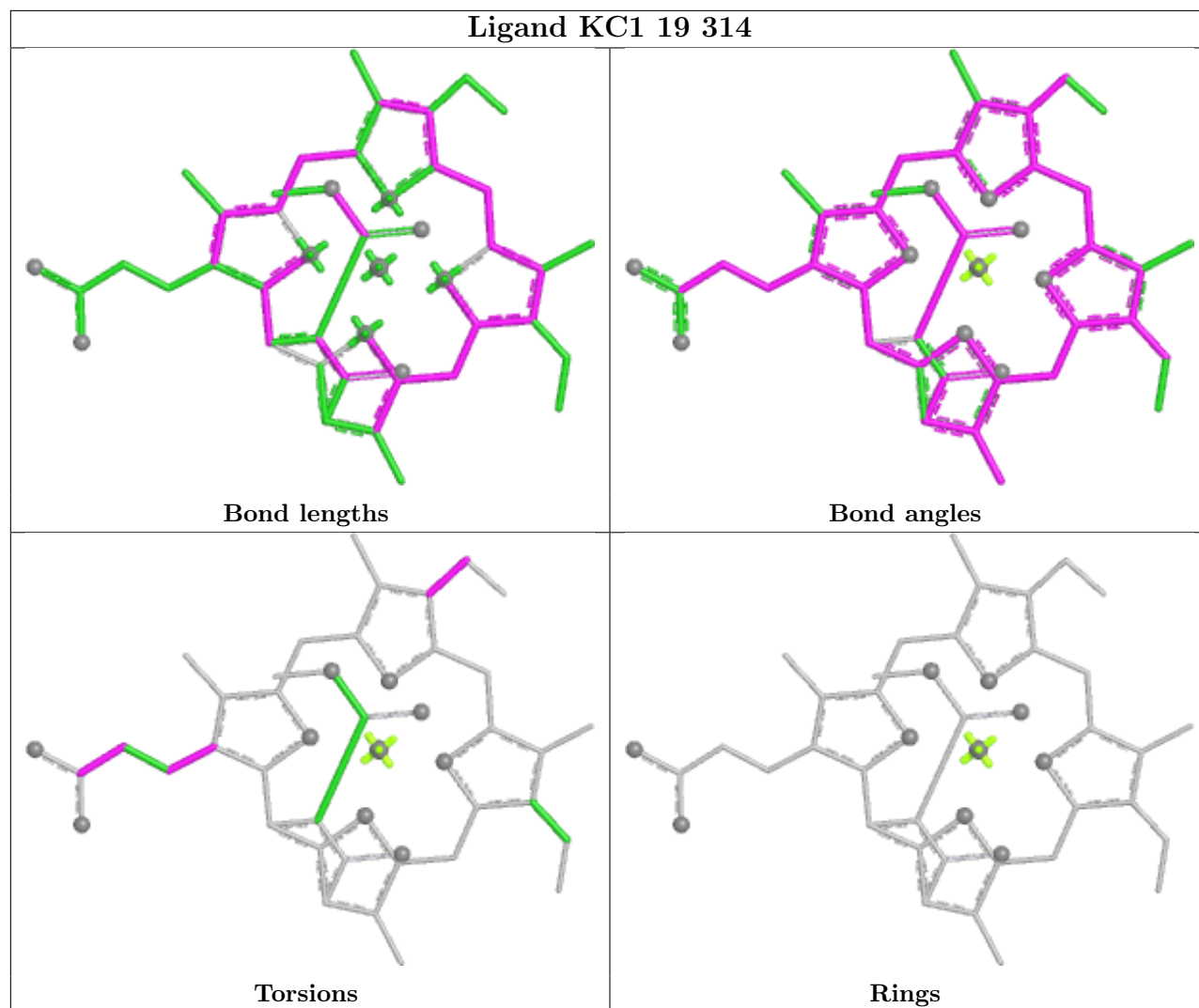
Bond angles



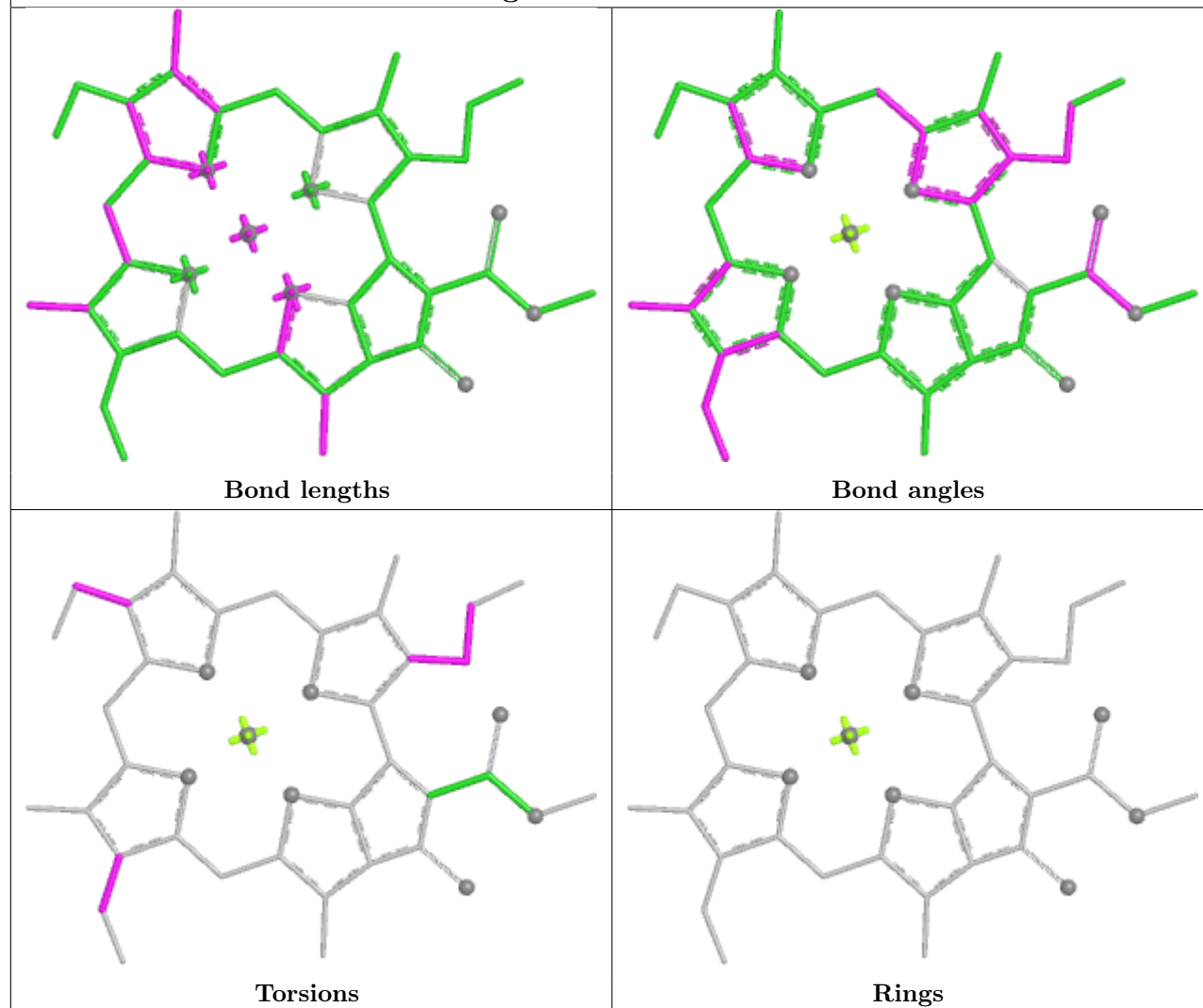
Torsions



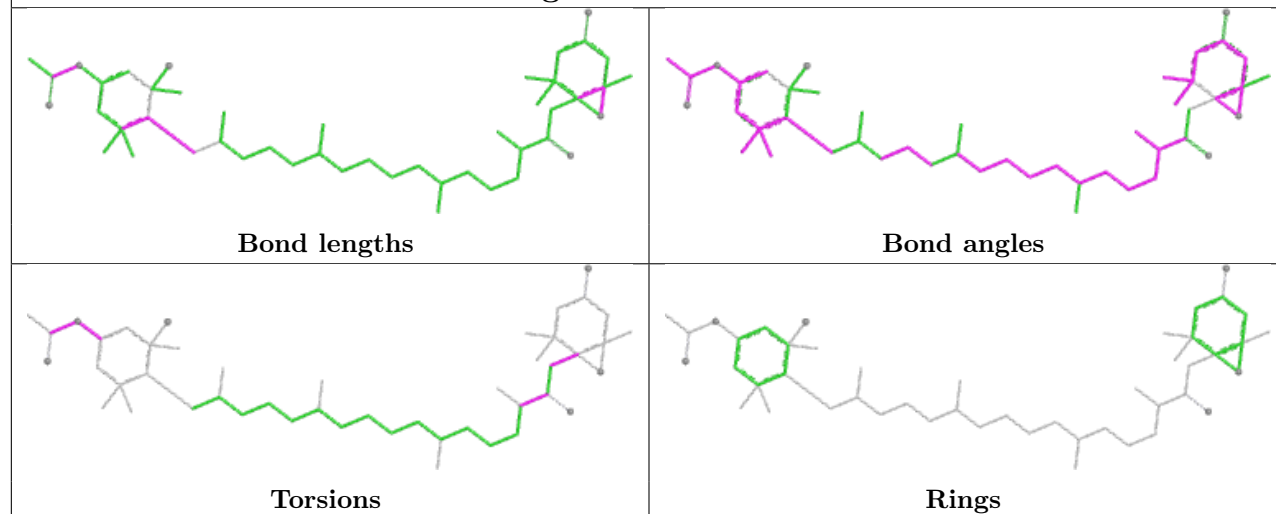
Rings

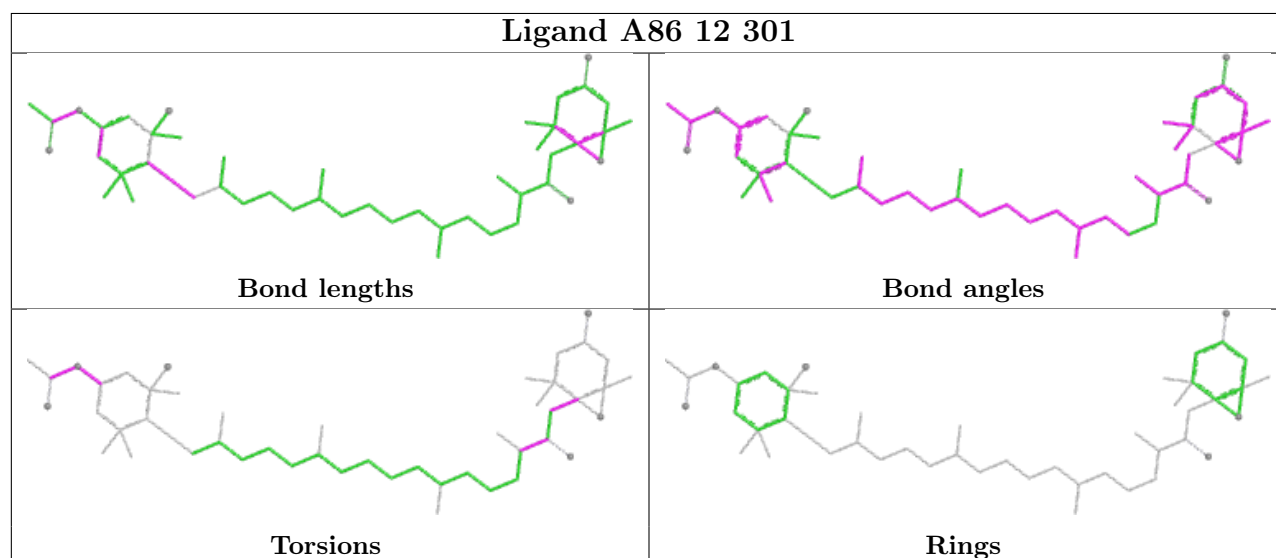
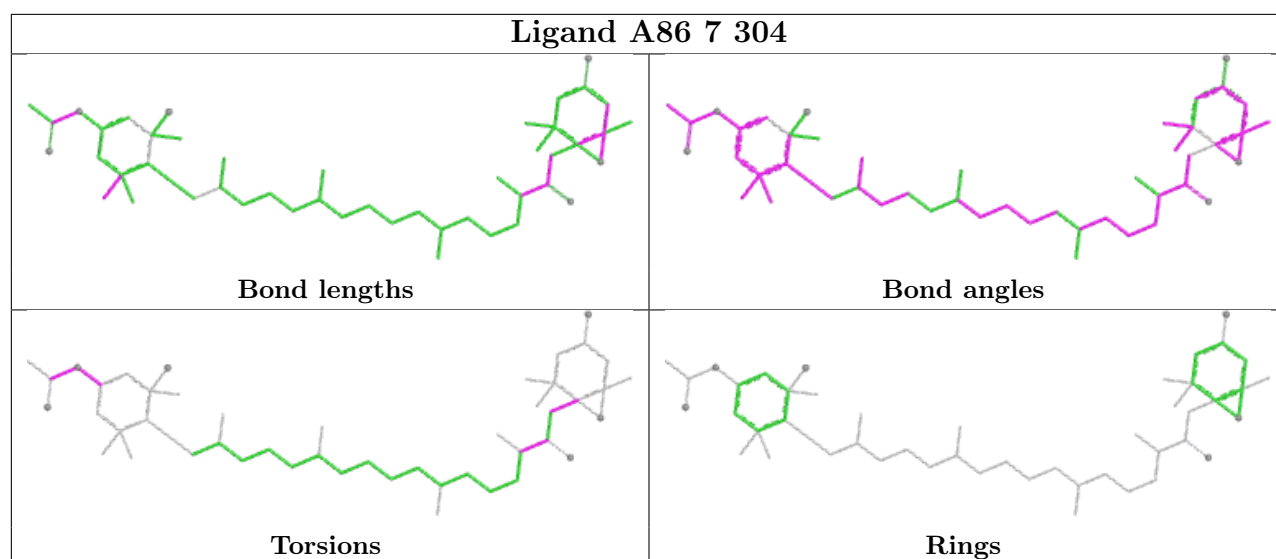


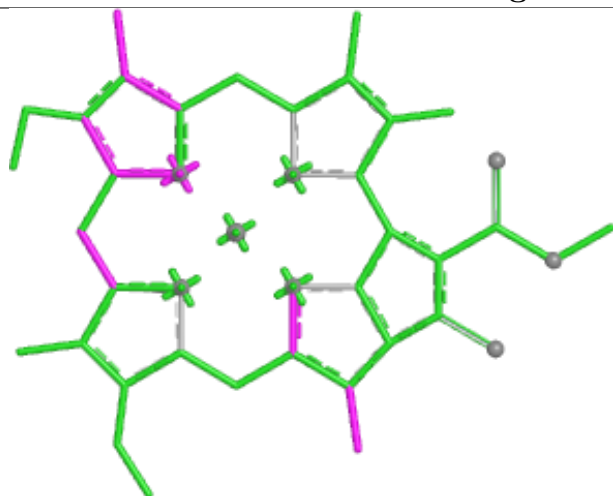
Ligand CLA P 607



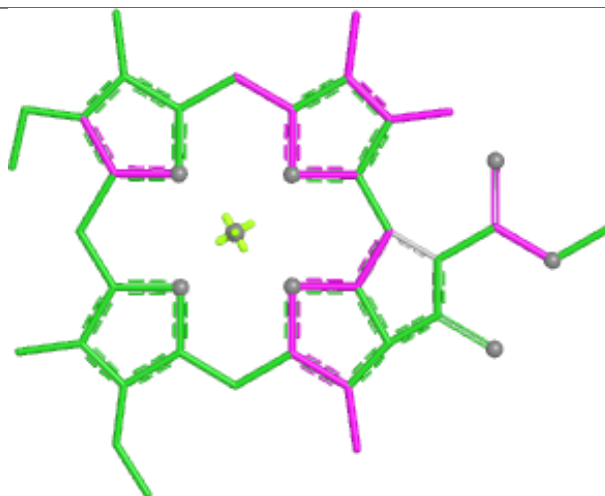
Ligand A86 7 305



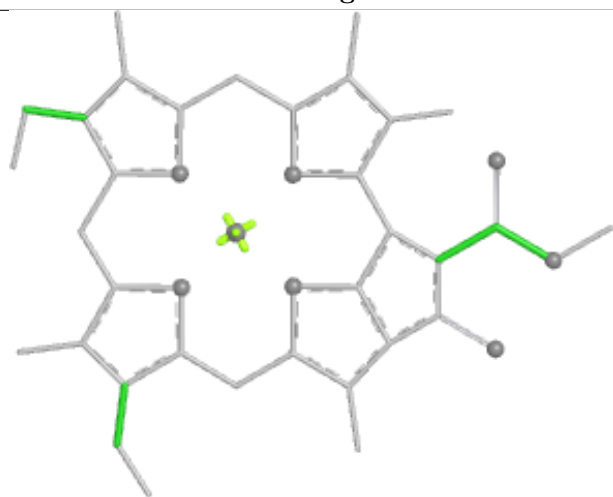


Ligand CLA 15 313

Bond lengths



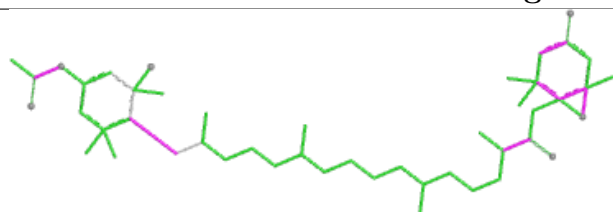
Bond angles



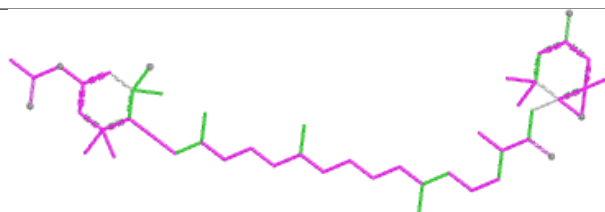
Torsions



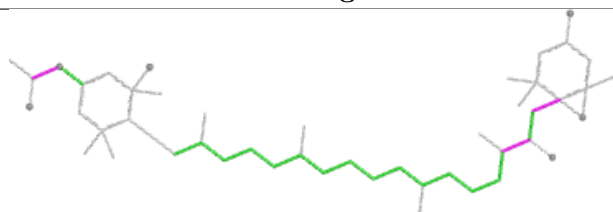
Rings

Ligand A86 8 303

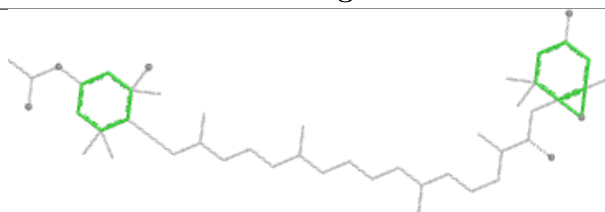
Bond lengths



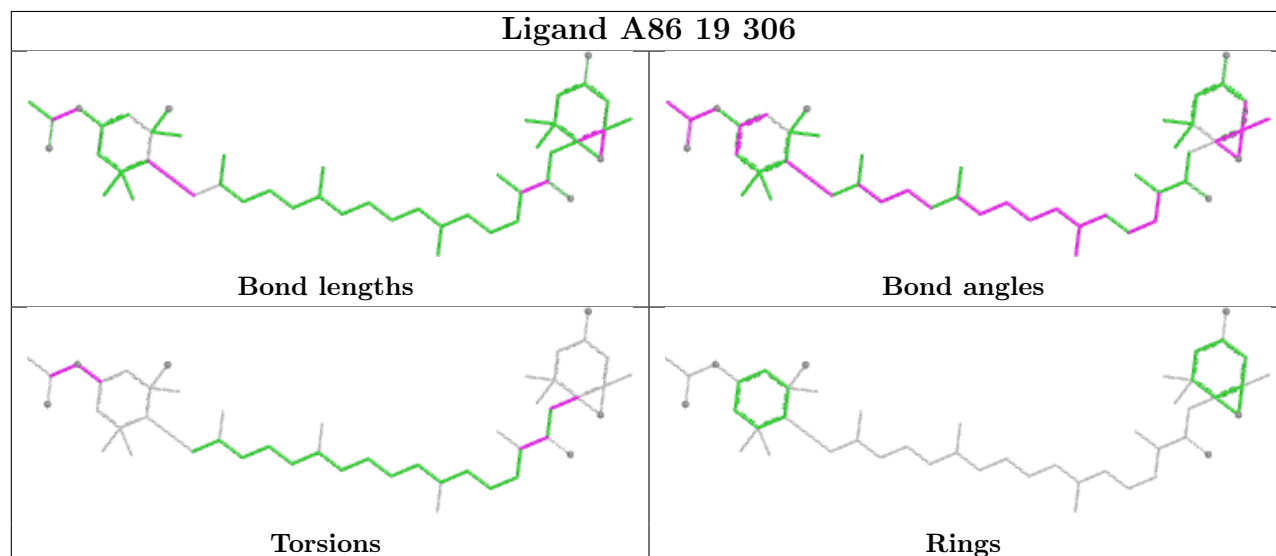
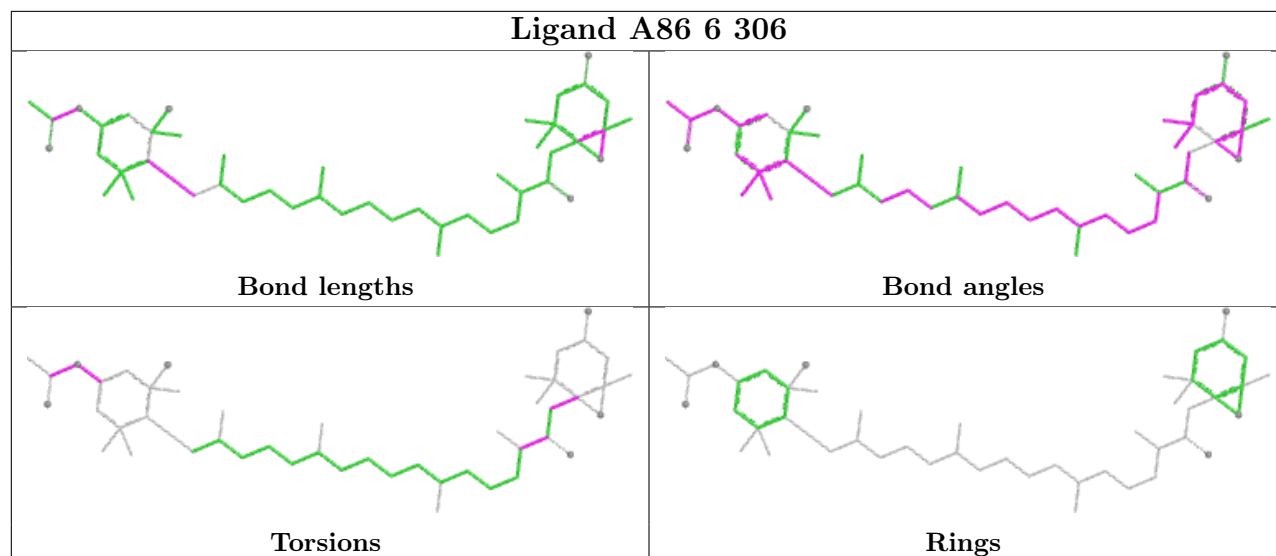
Bond angles



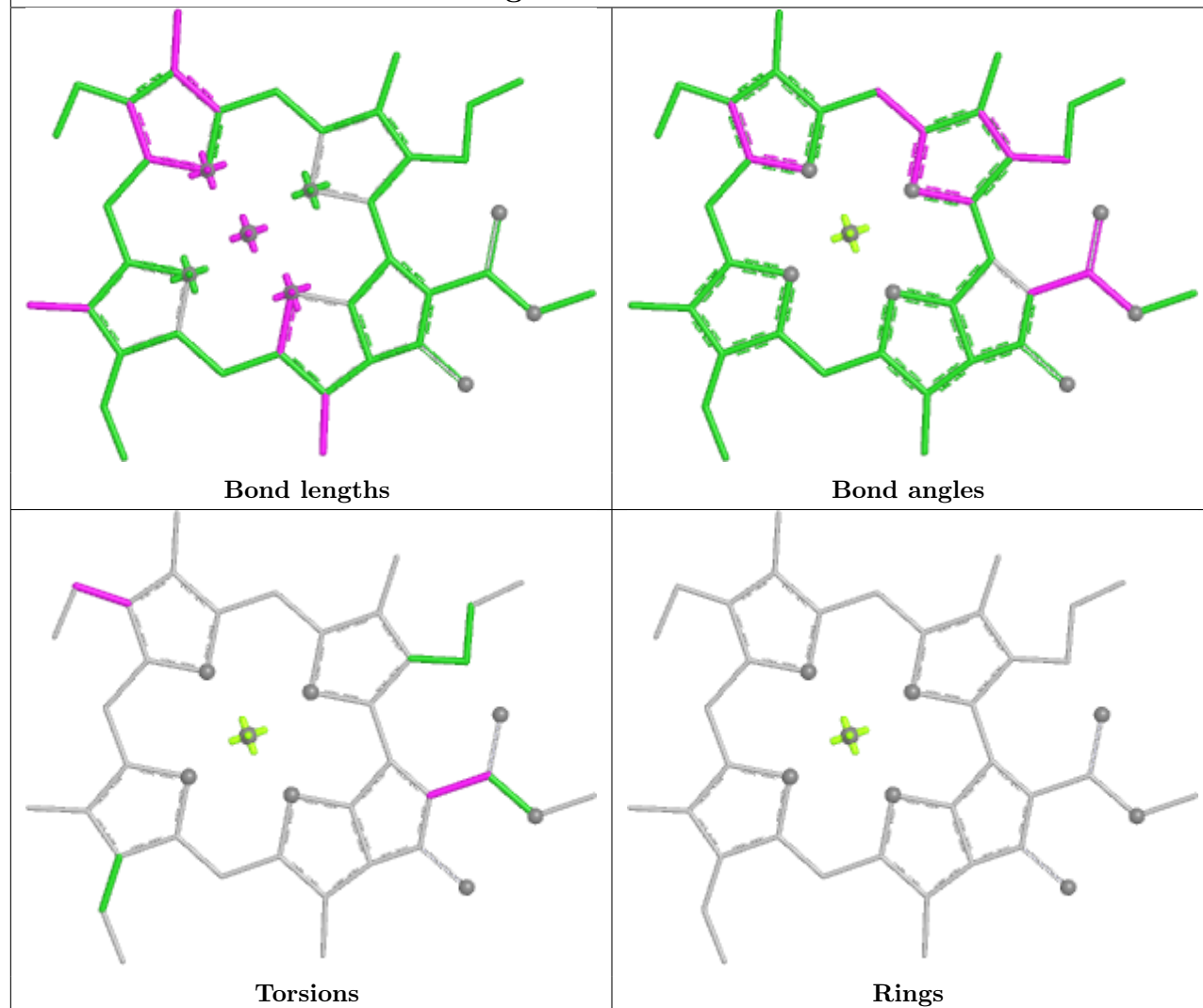
Torsions



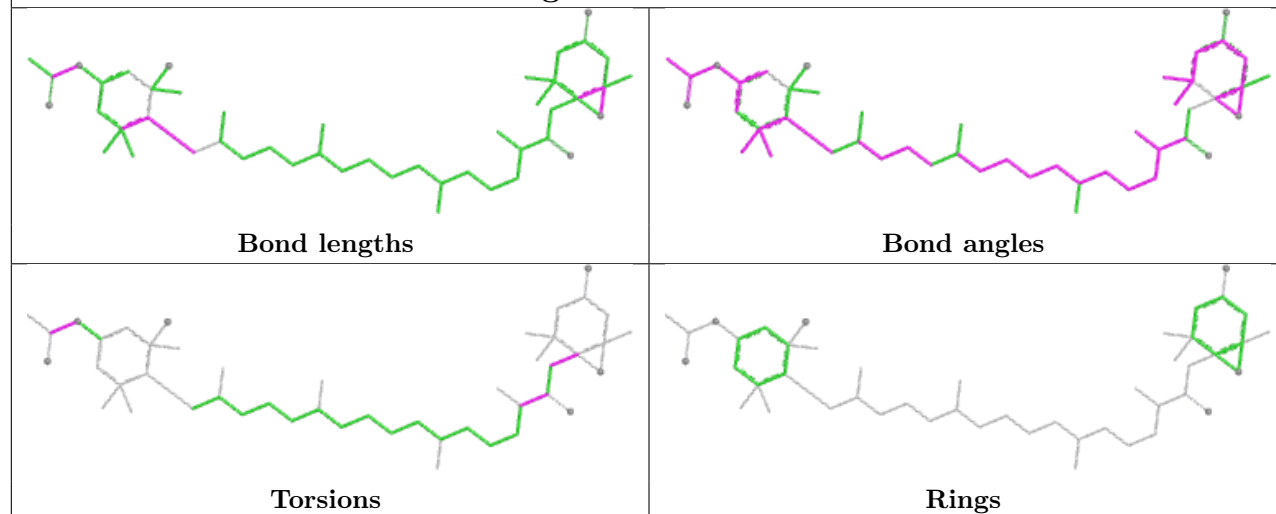
Rings



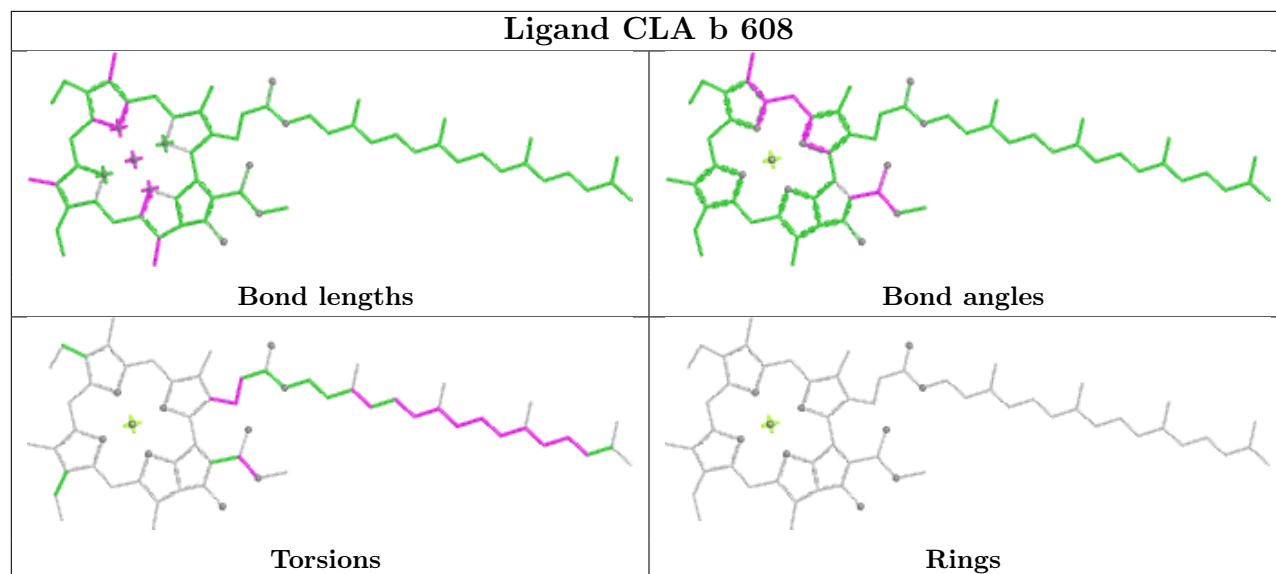
Ligand CLA 8 315



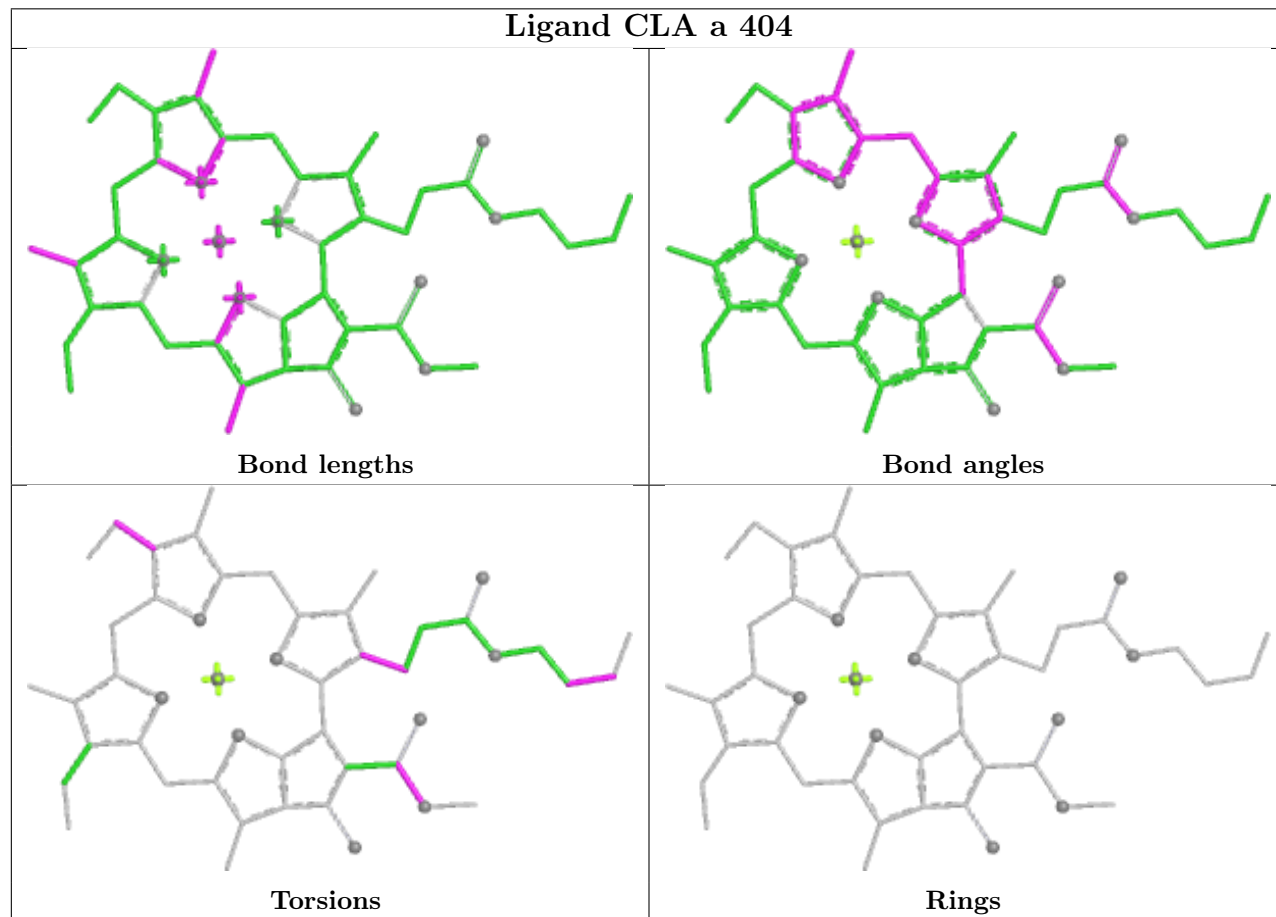
Ligand A86 2 305



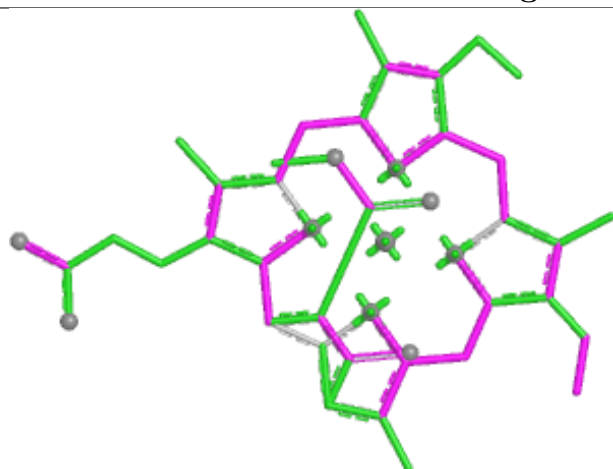
Ligand CLA b 608



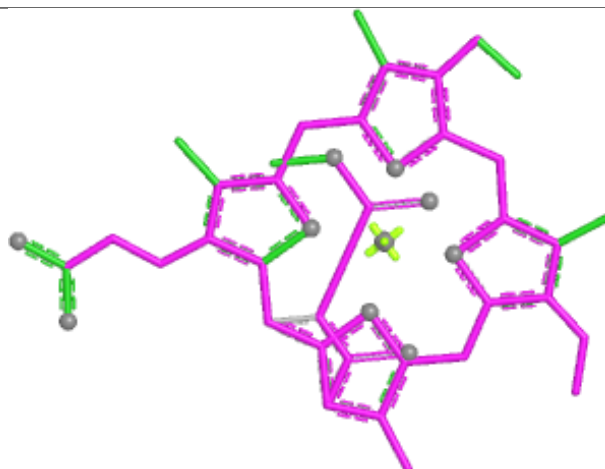
Ligand CLA a 404



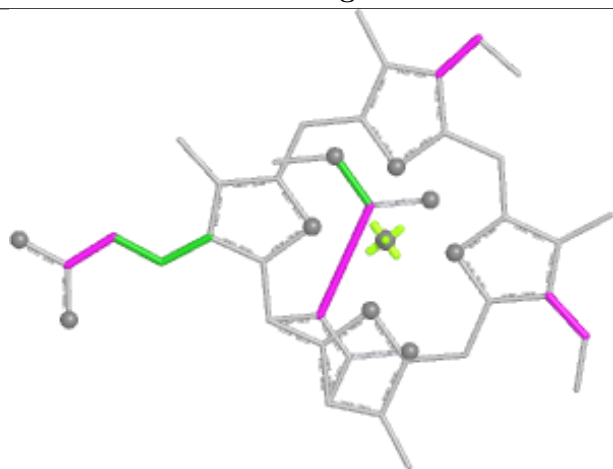
Ligand KC2 4 310



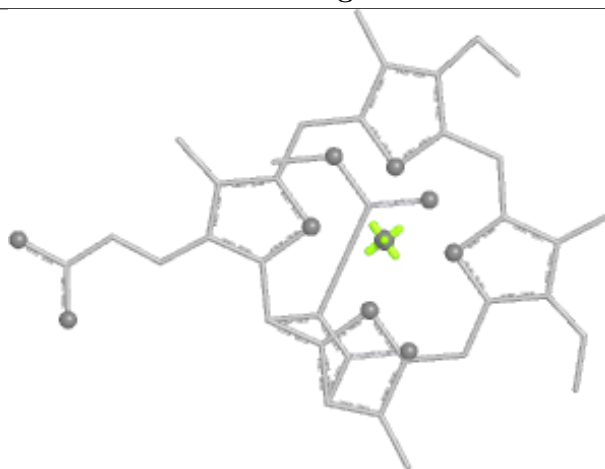
Bond lengths



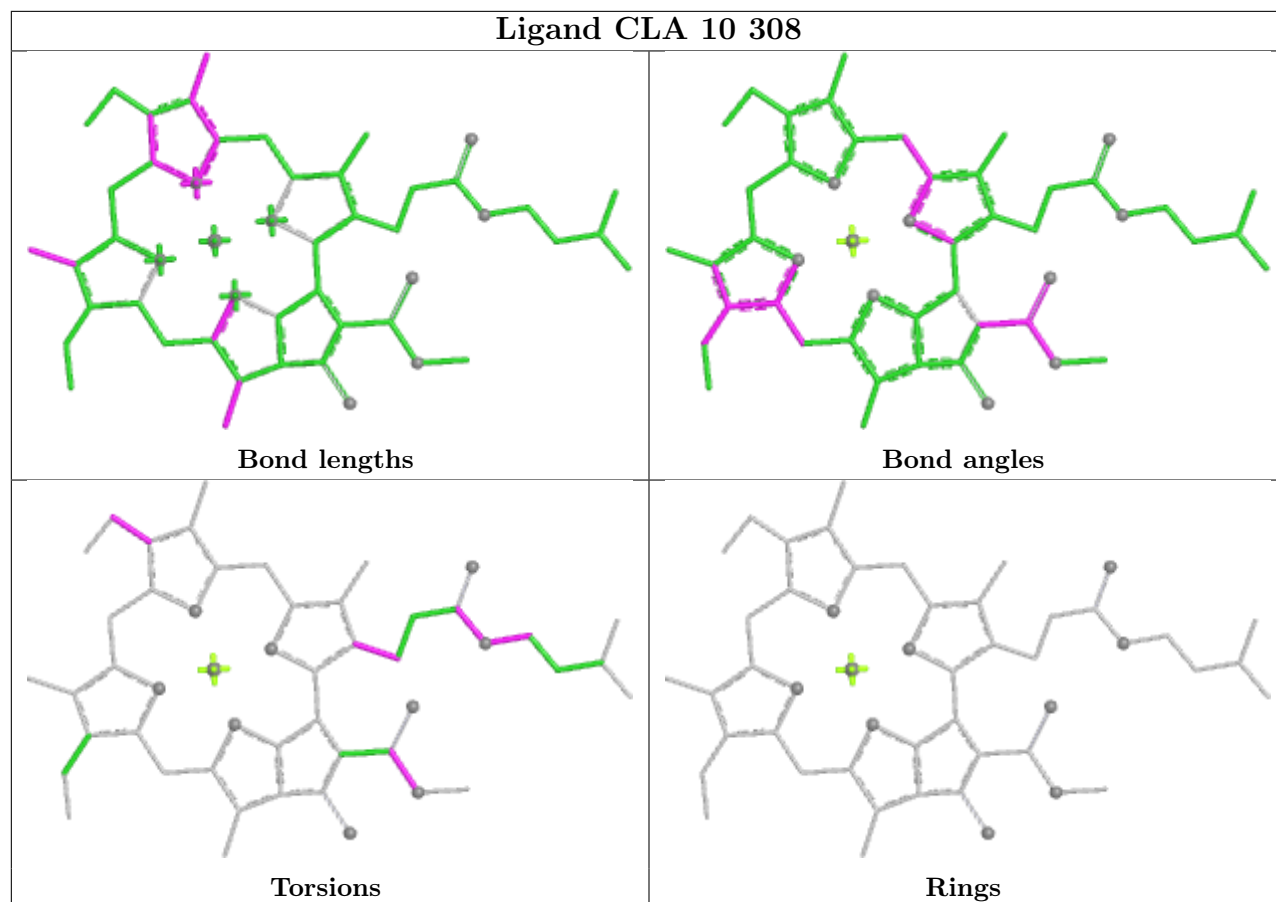
Bond angles



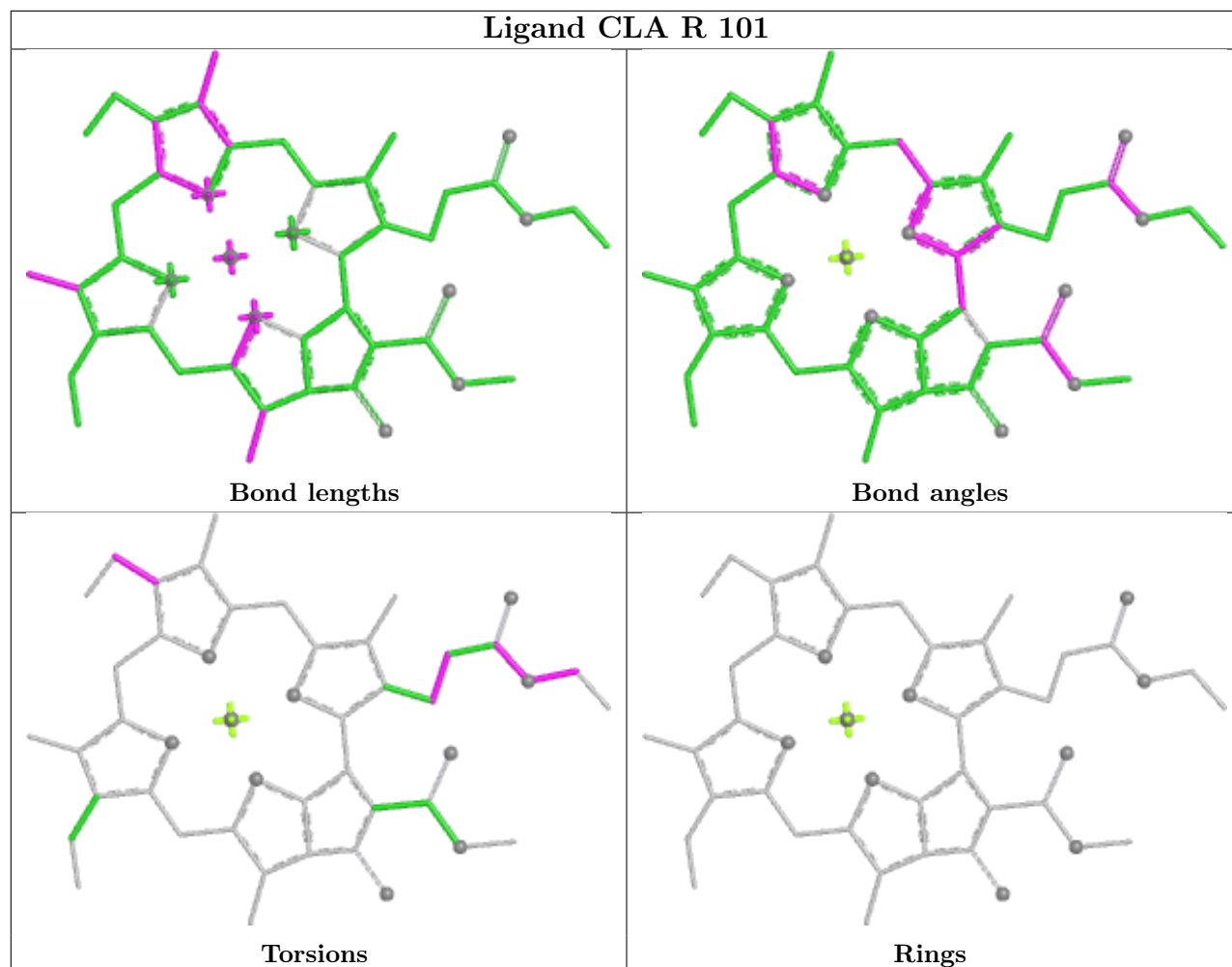
Torsions



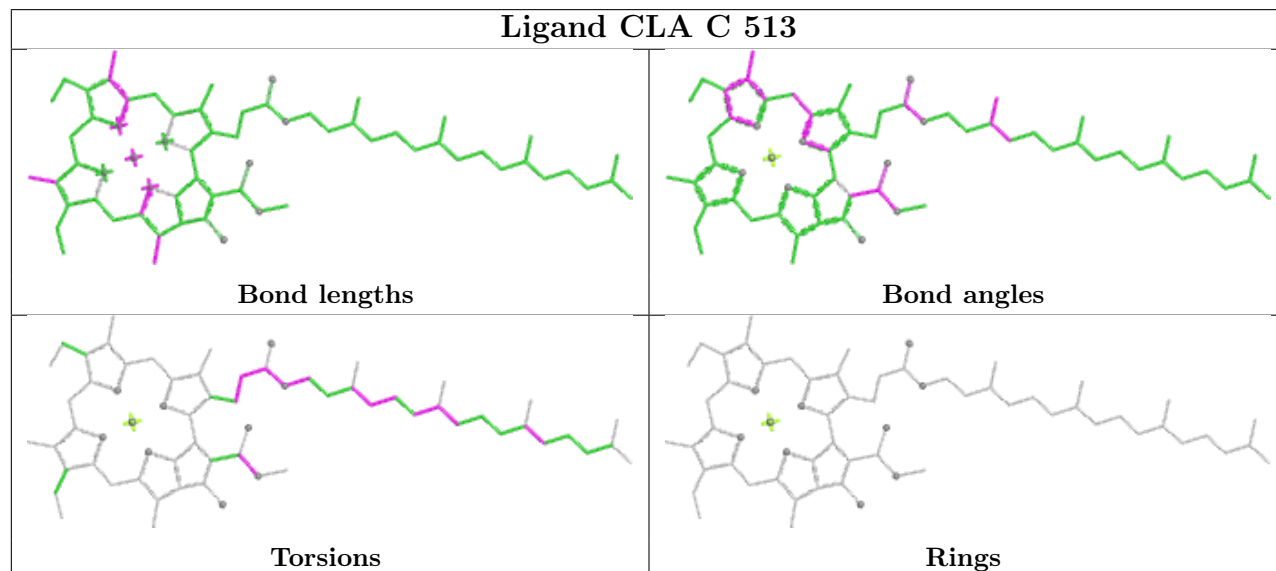
Rings

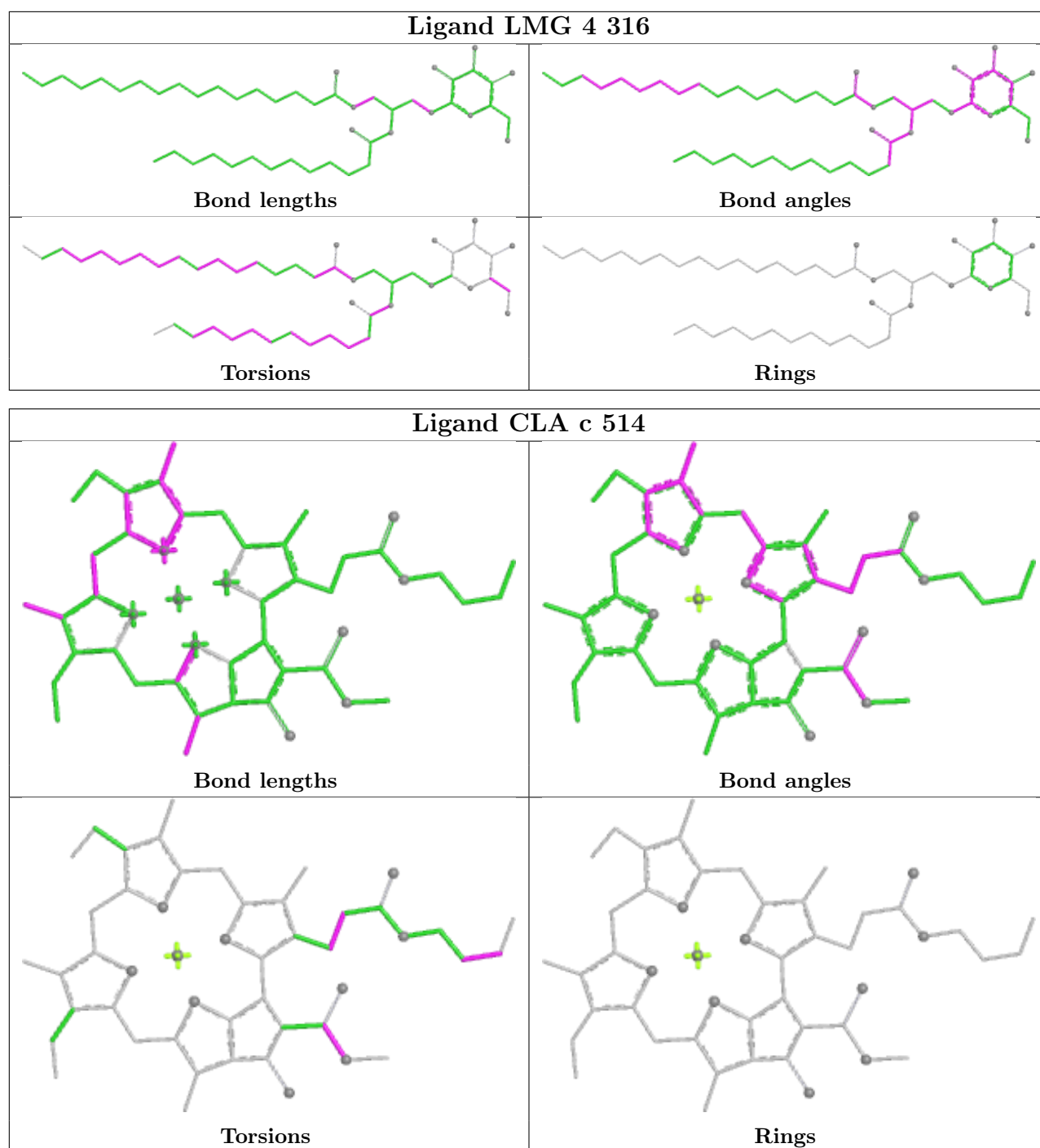


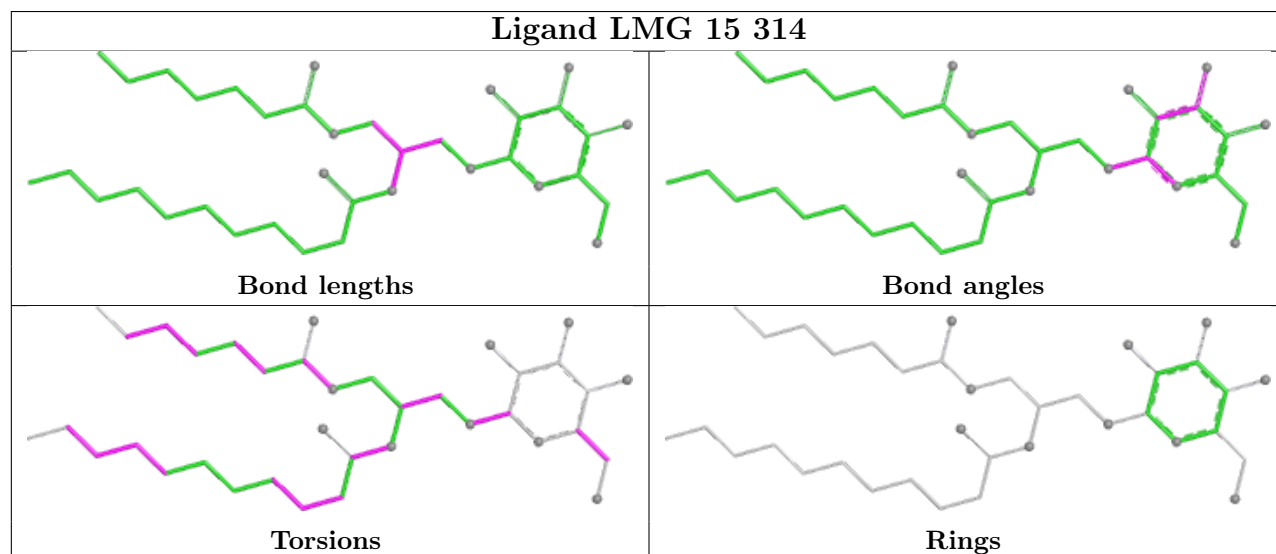
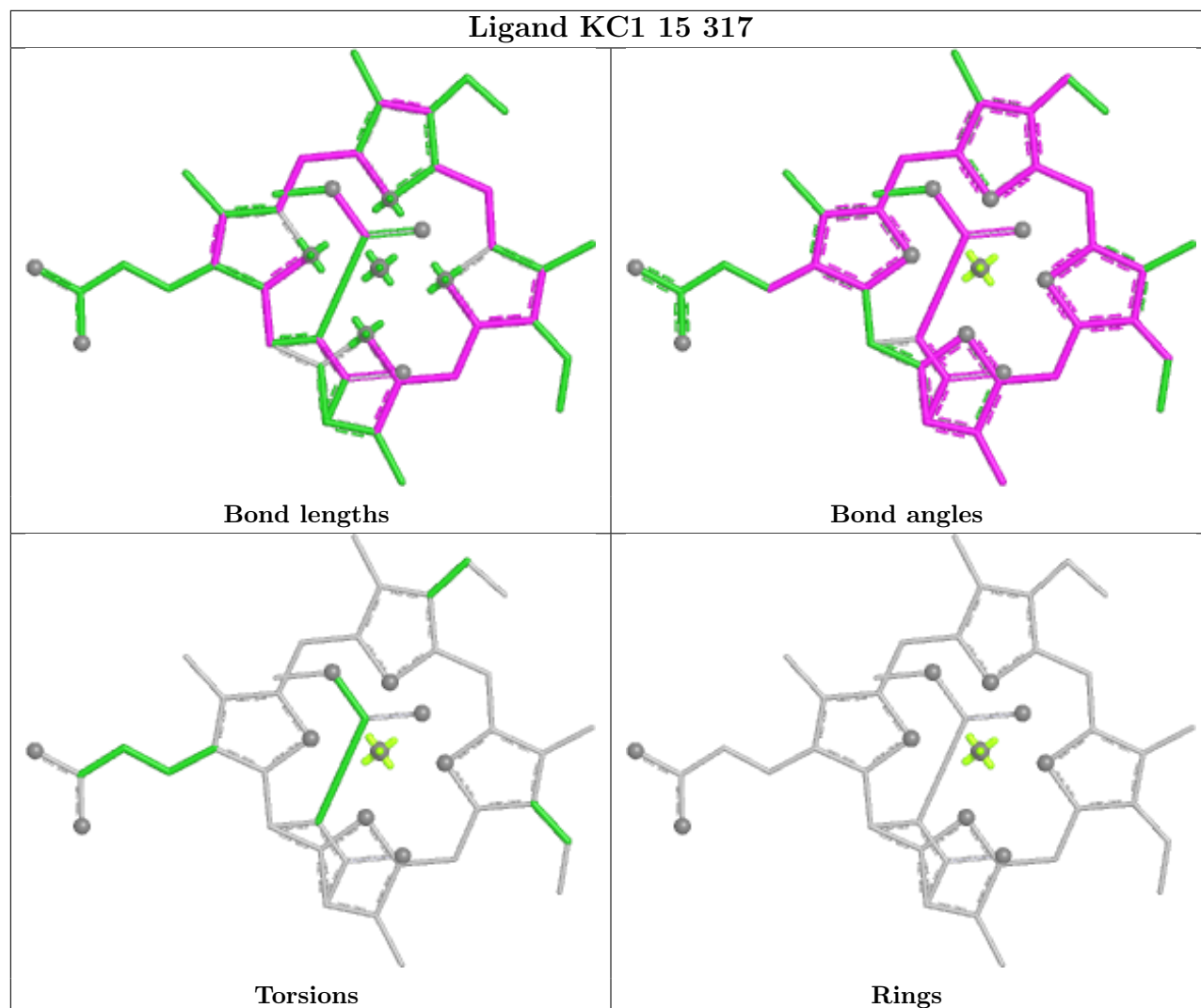
Ligand CLA R 101

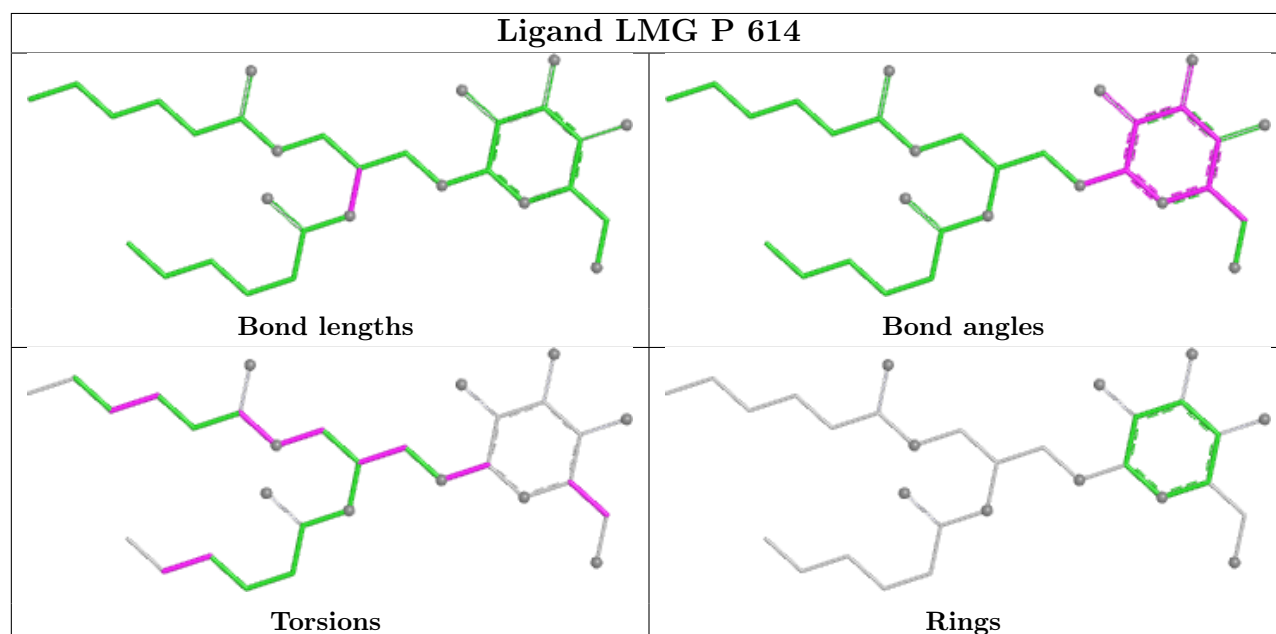
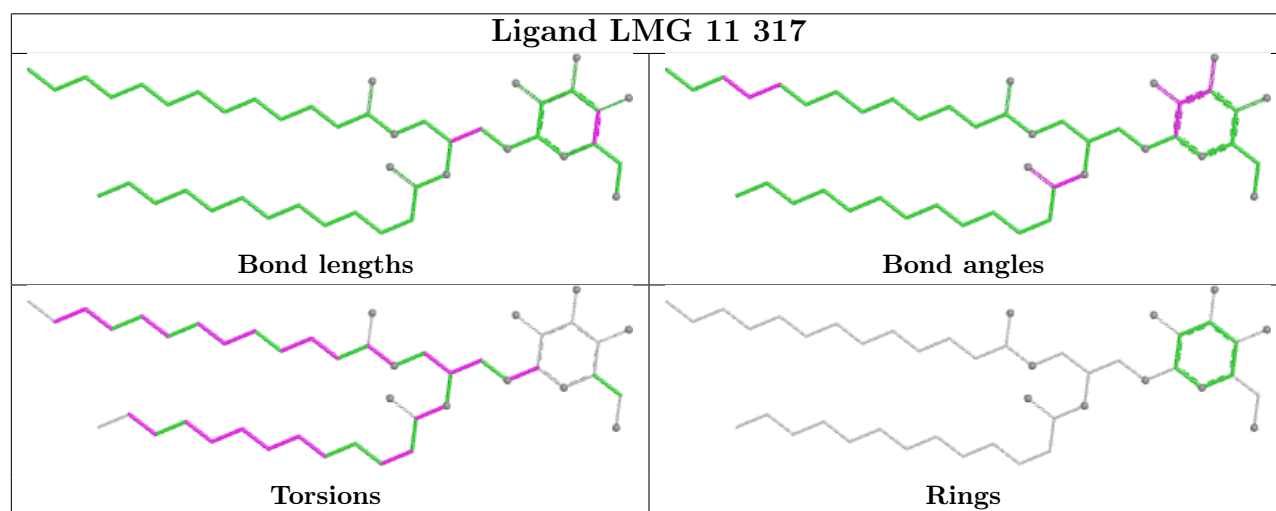
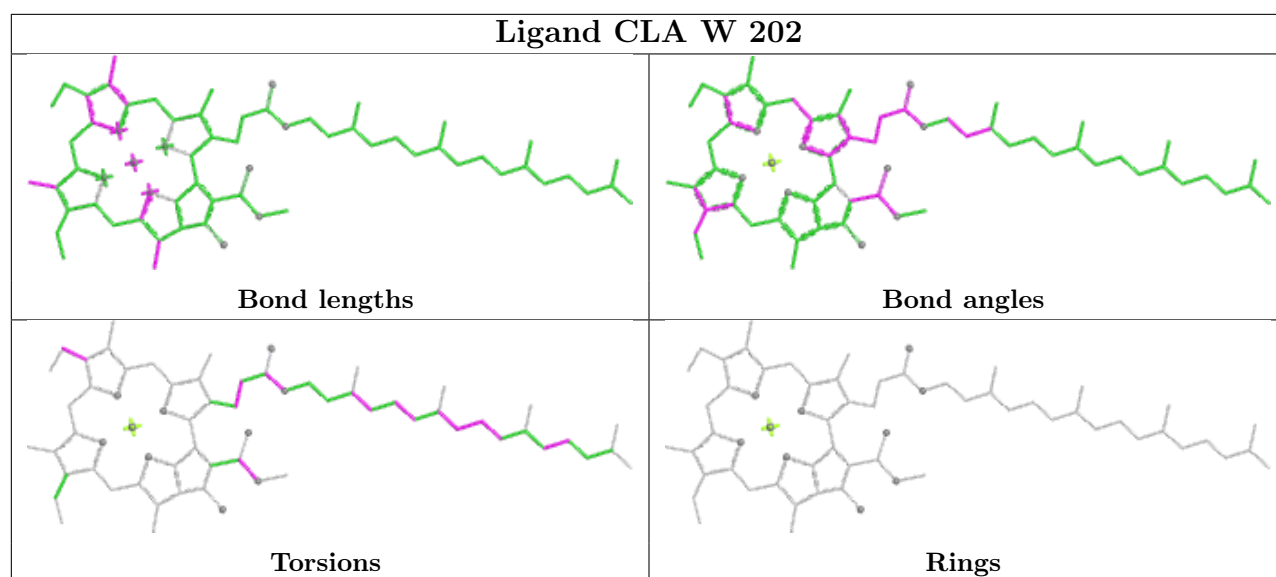


Ligand CLA C 513

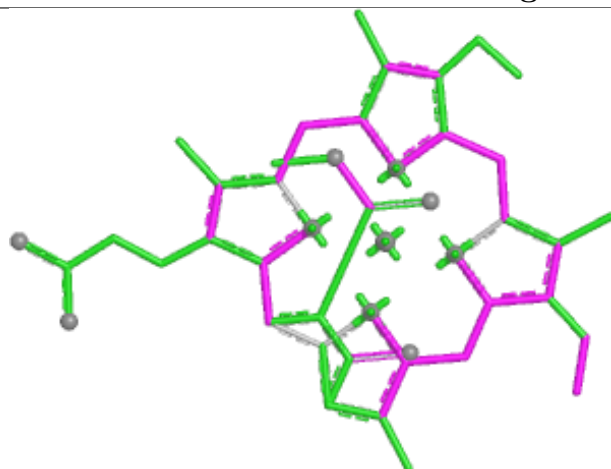




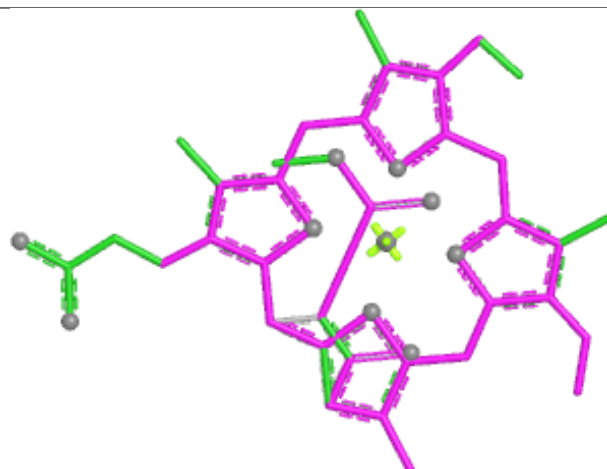




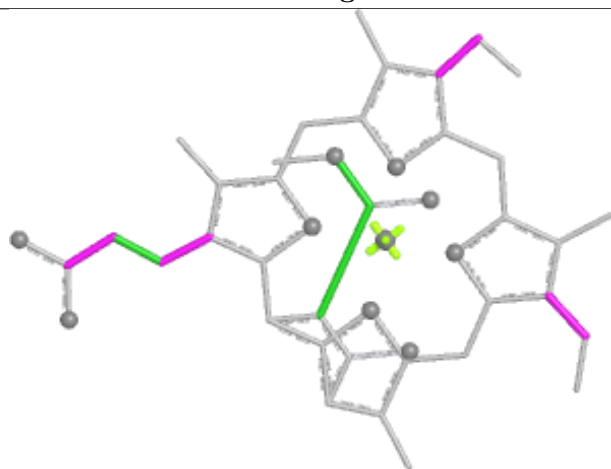
Ligand KC2 2 310



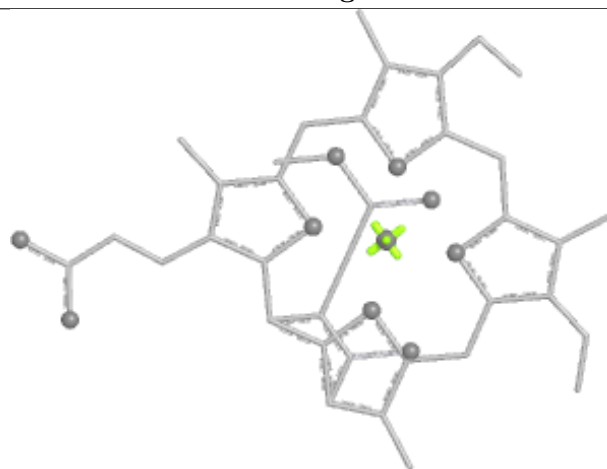
Bond lengths



Bond angles

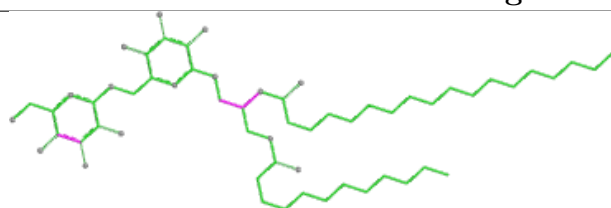


Torsions

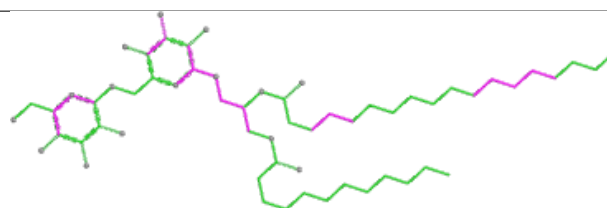


Rings

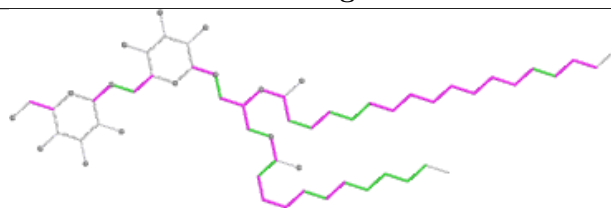
Ligand DGD 11 318



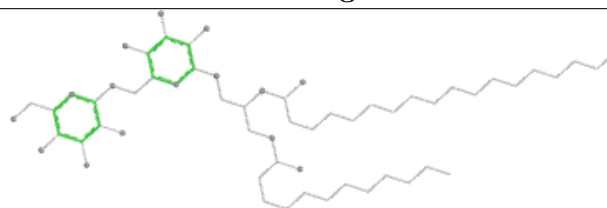
Bond lengths



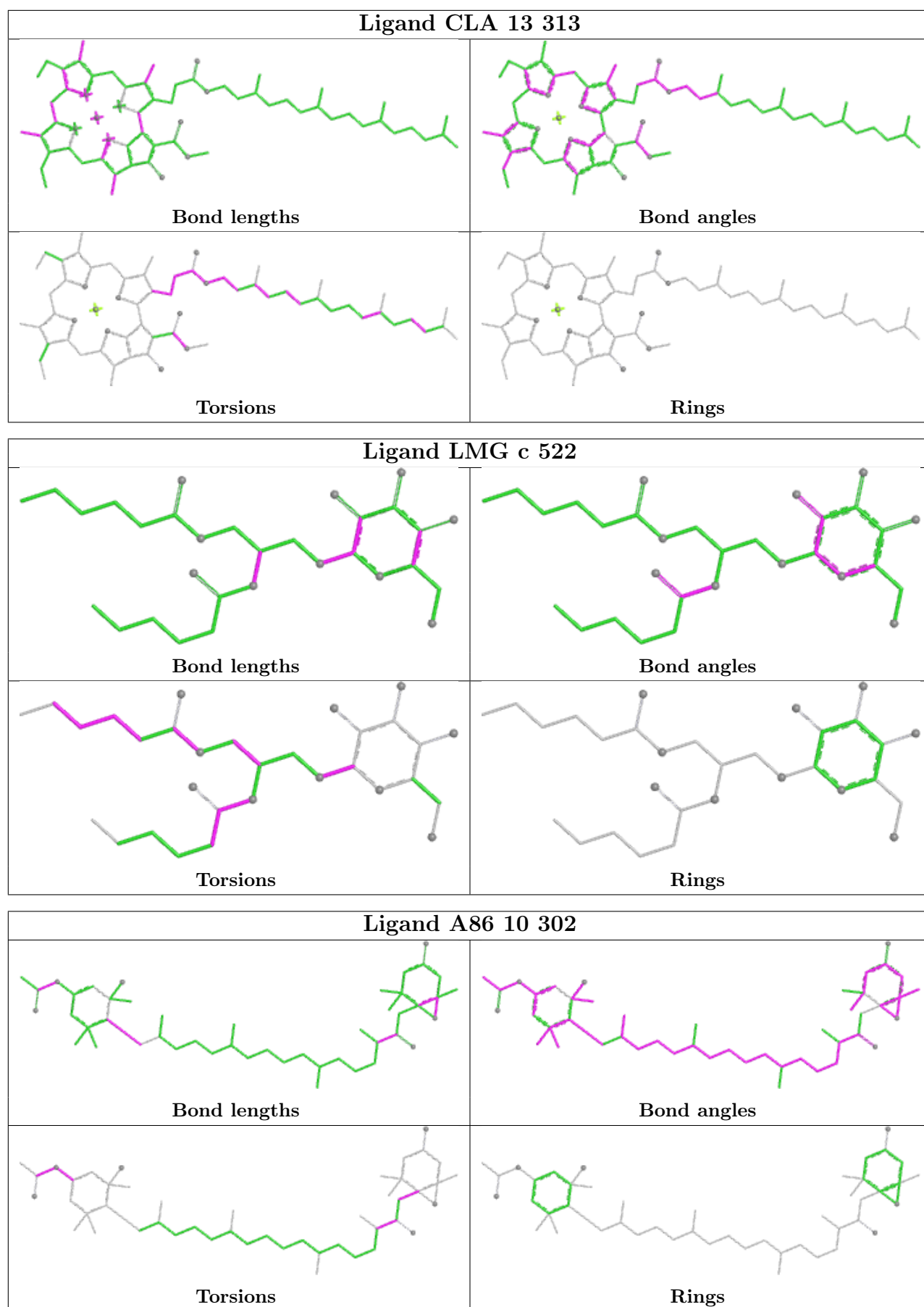
Bond angles

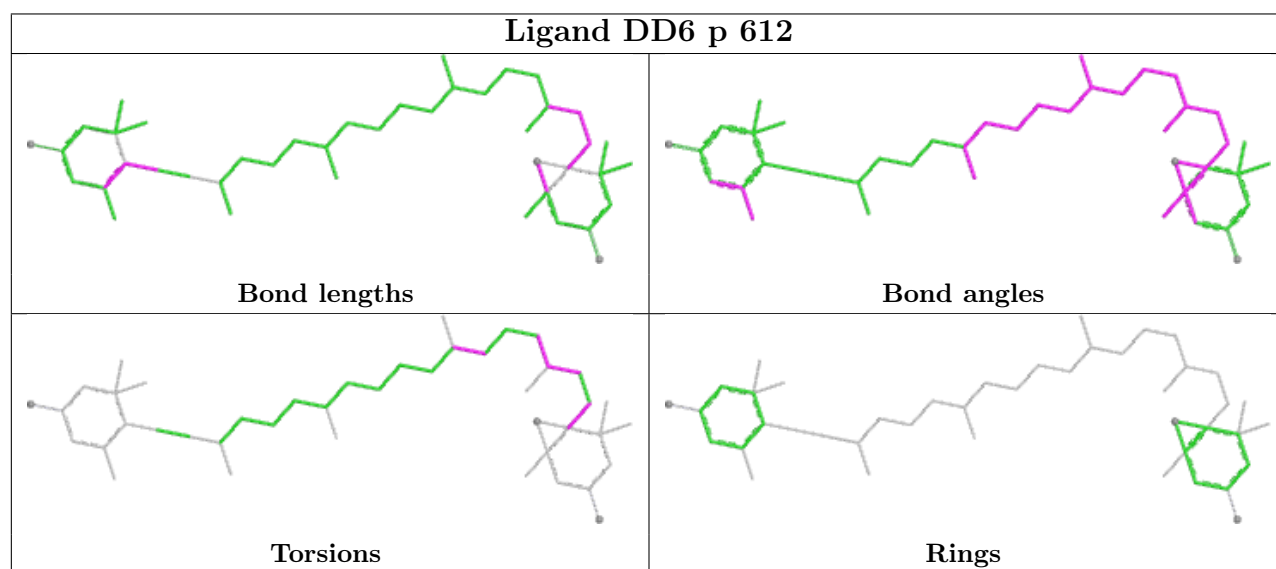
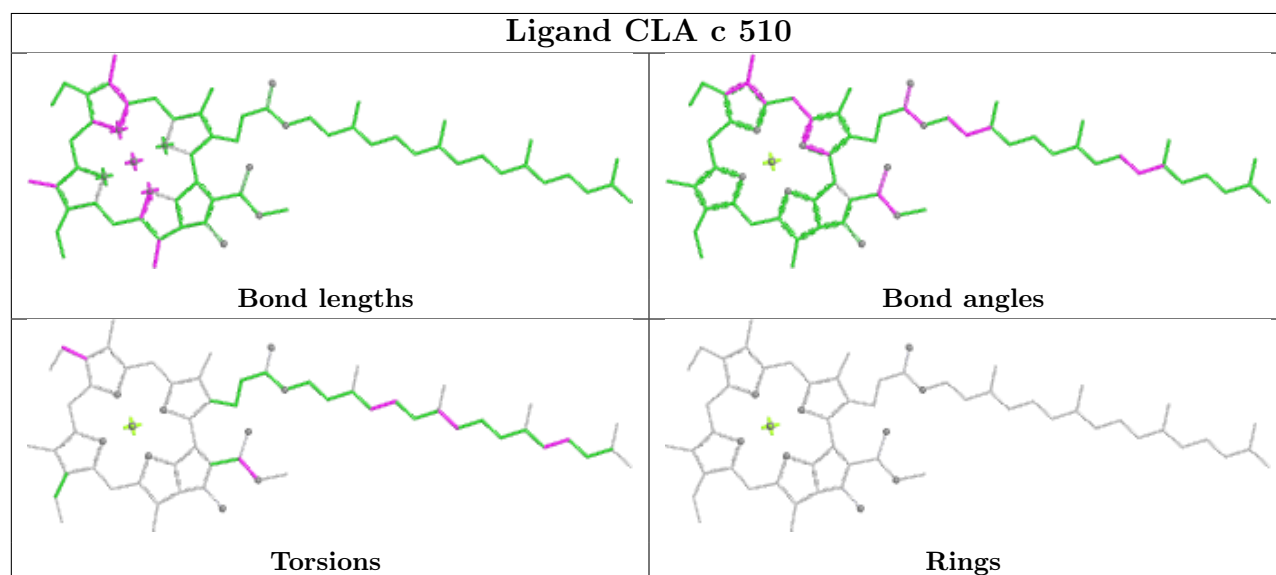
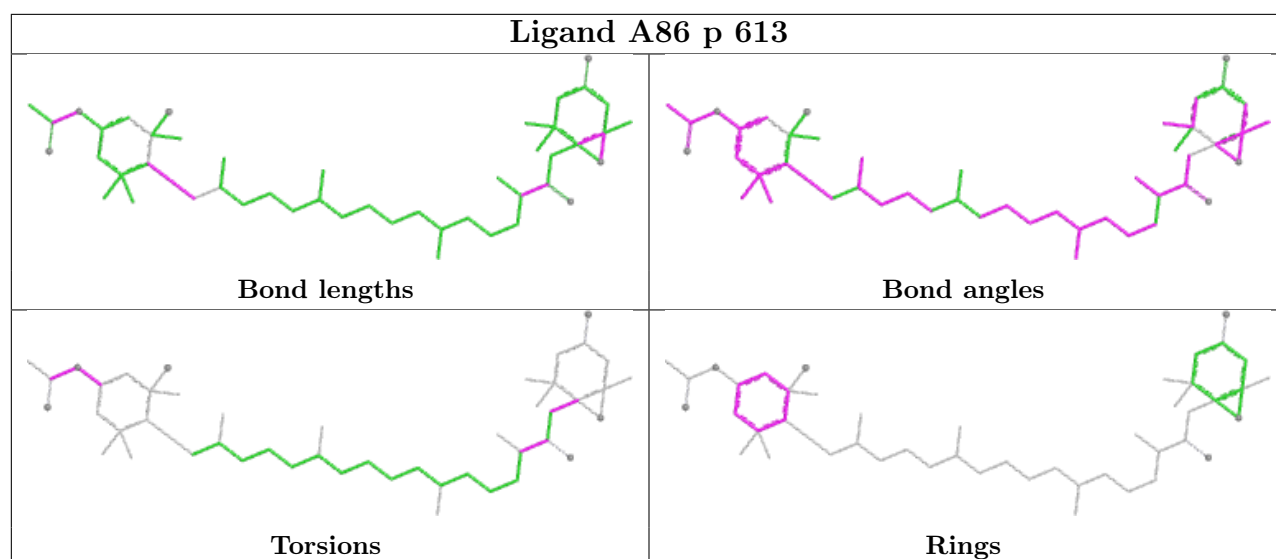


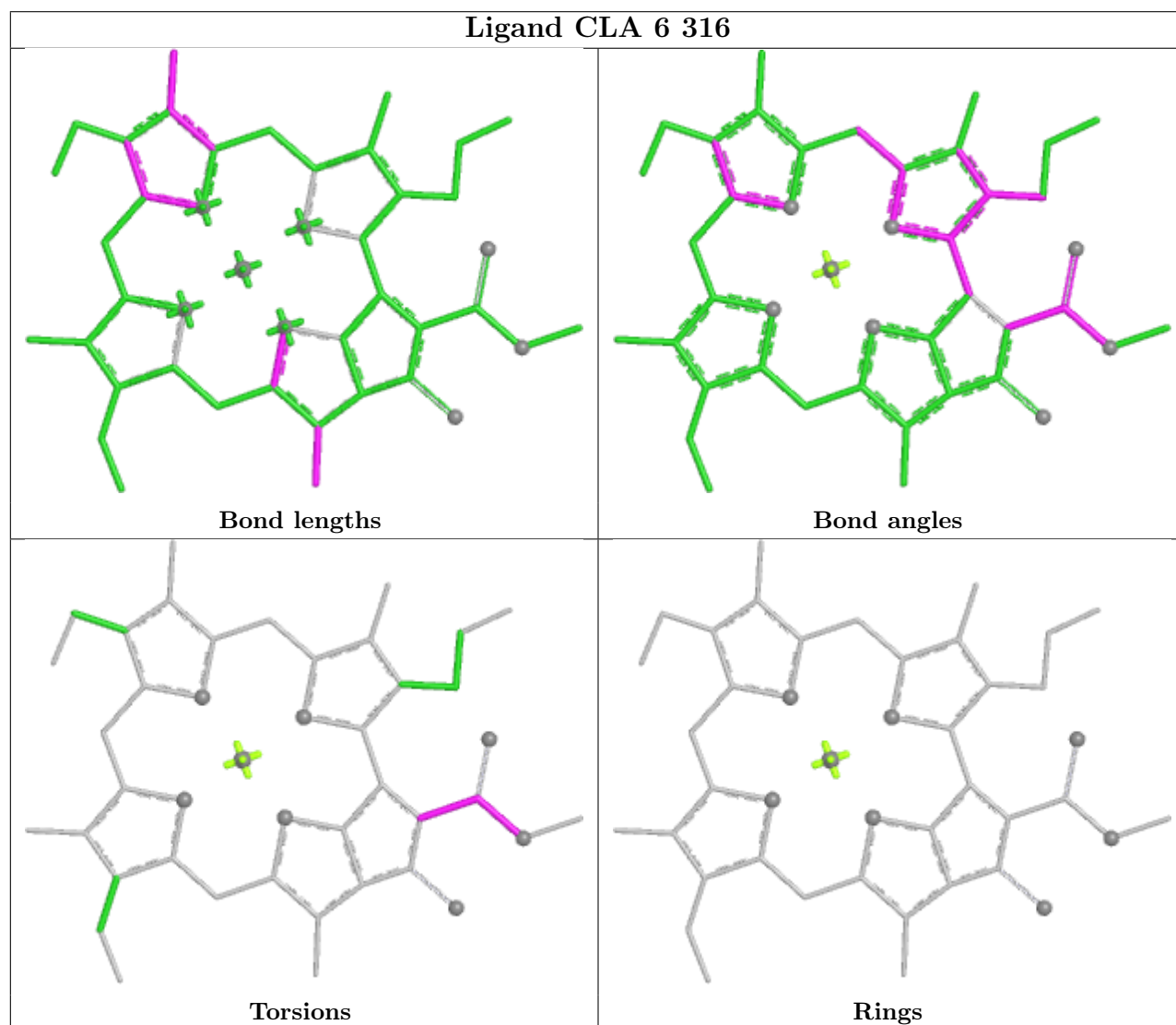
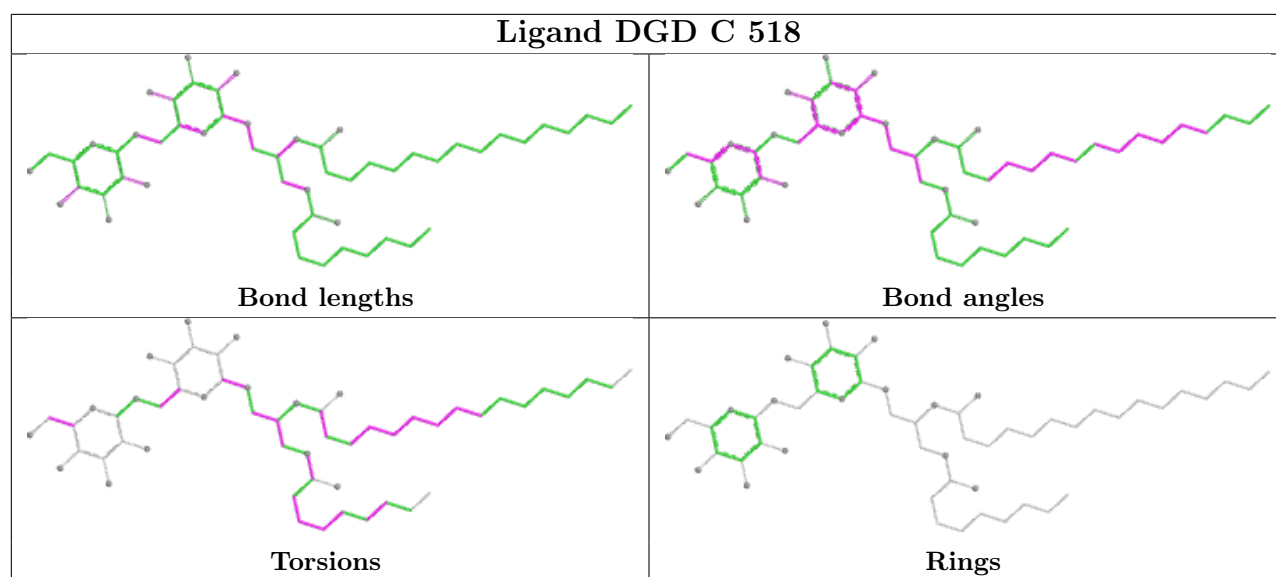
Torsions

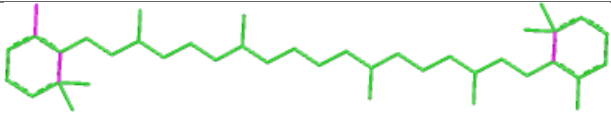
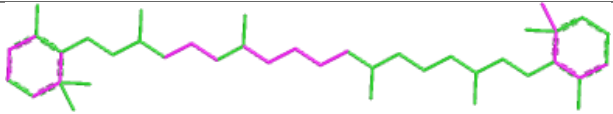
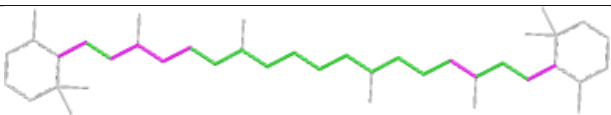
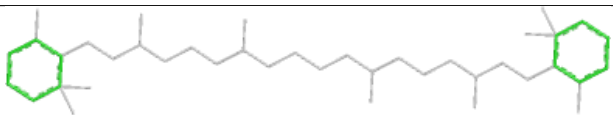


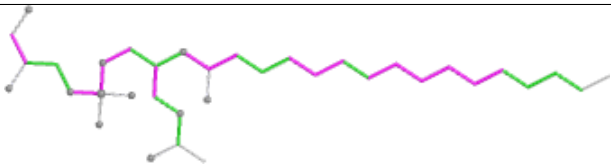
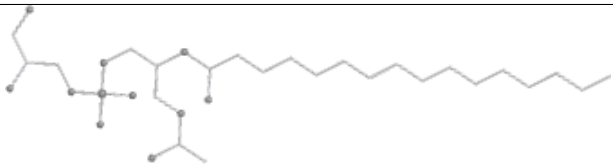
Rings

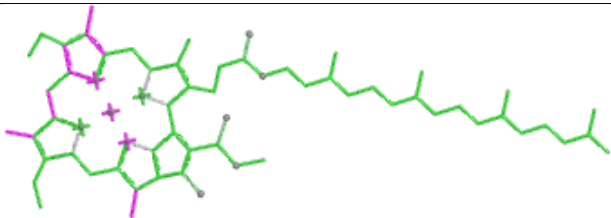
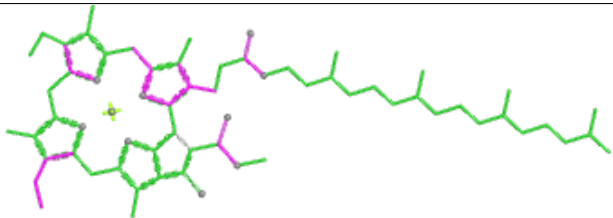
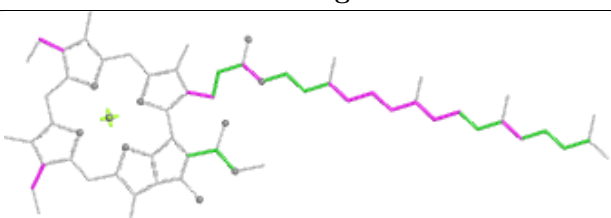
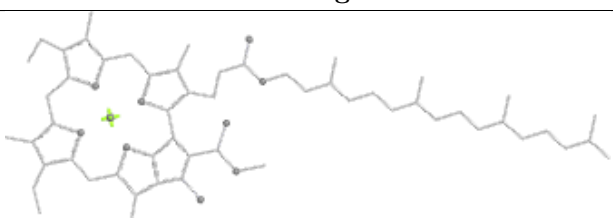


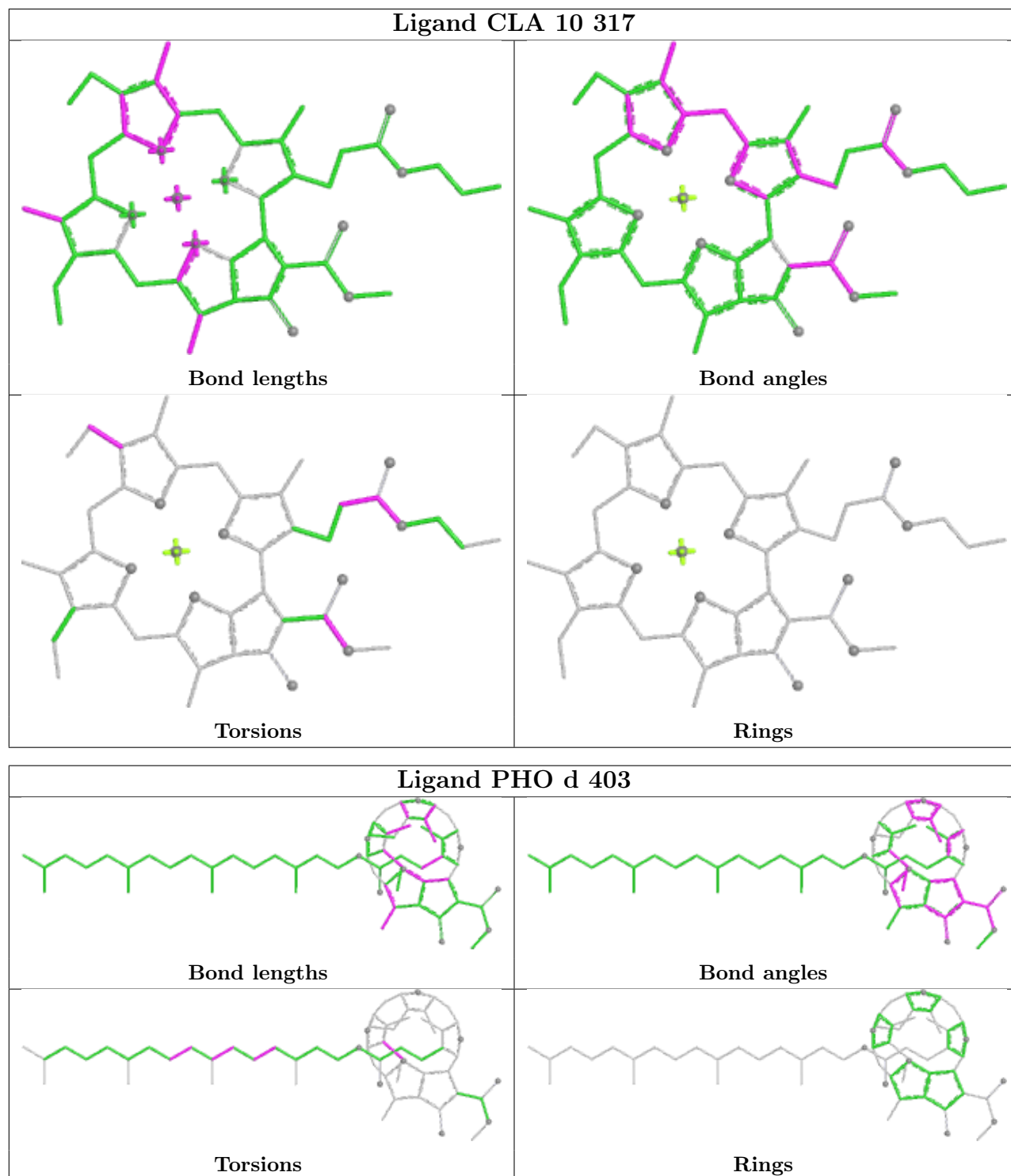


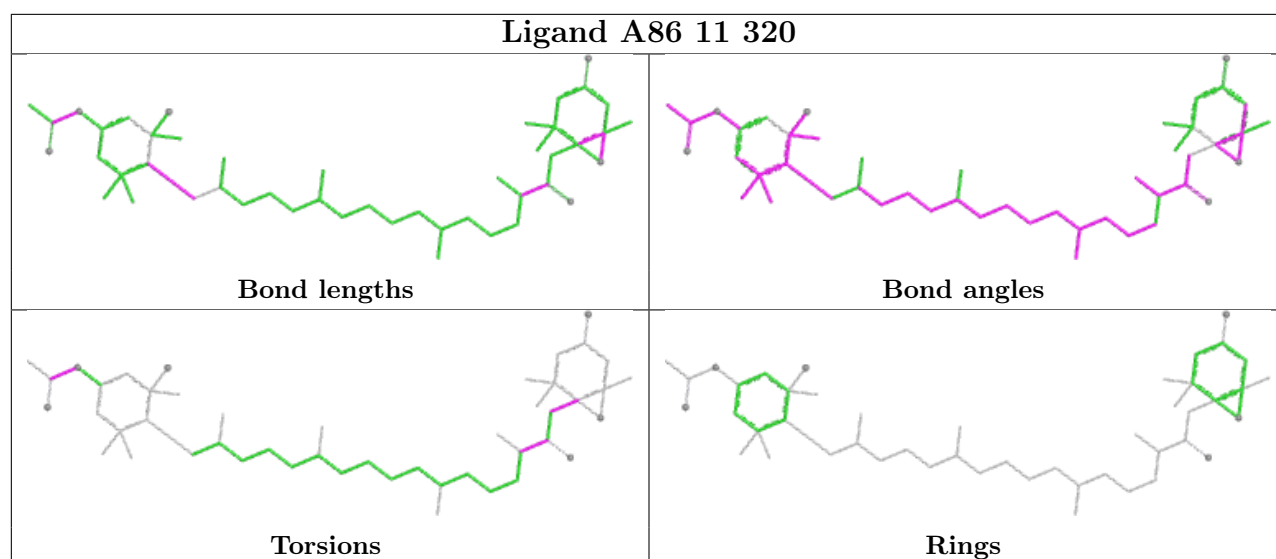
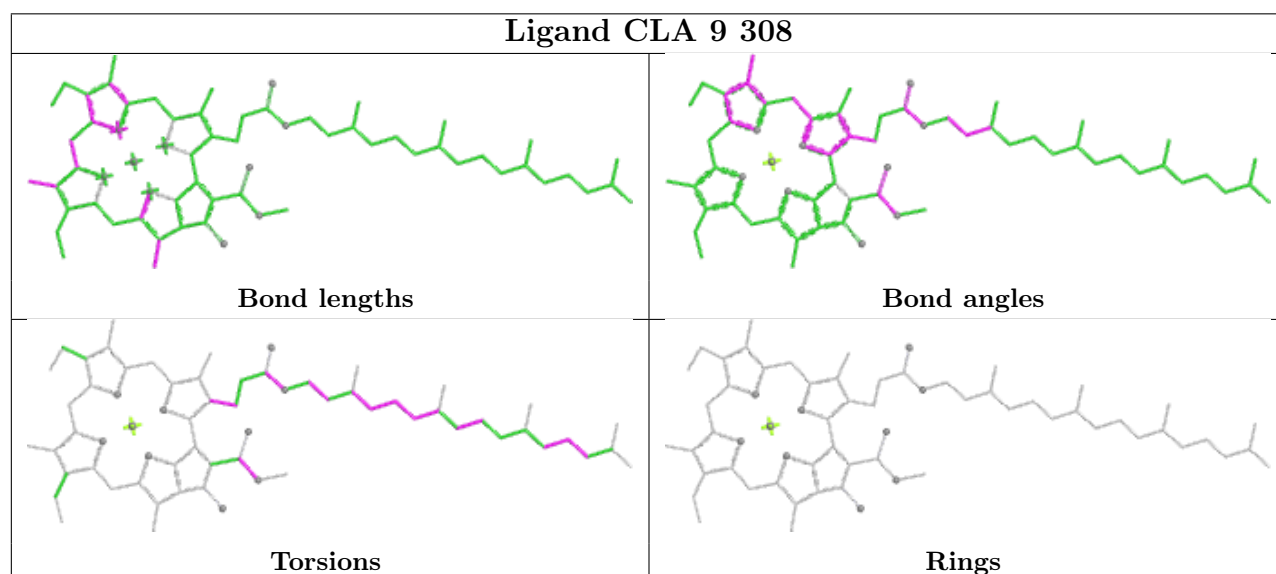
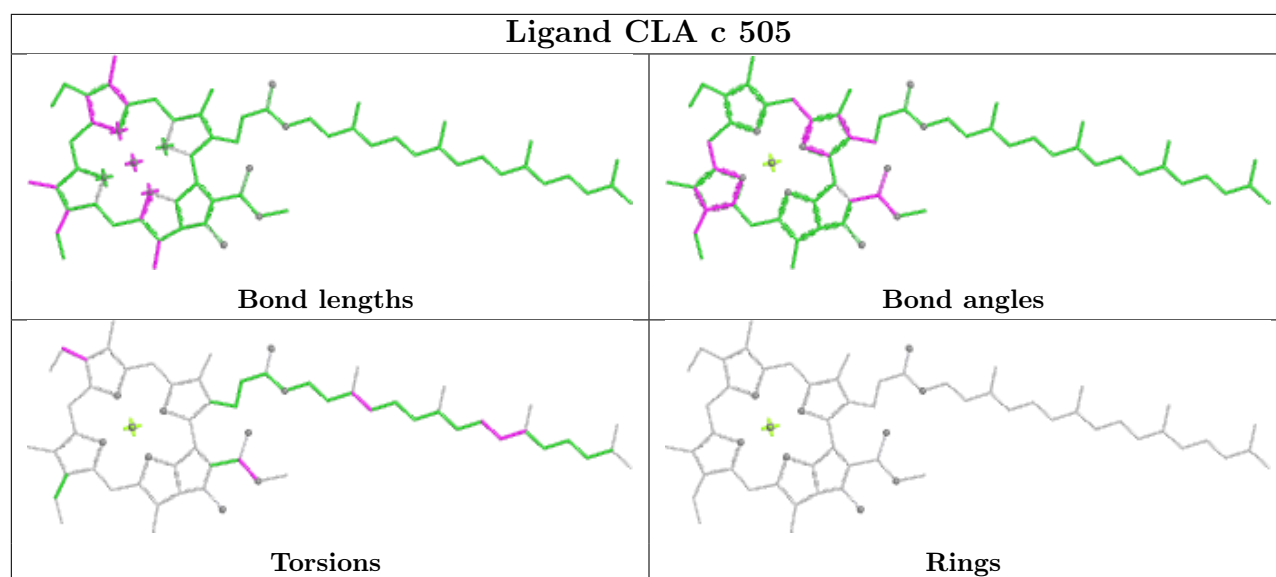


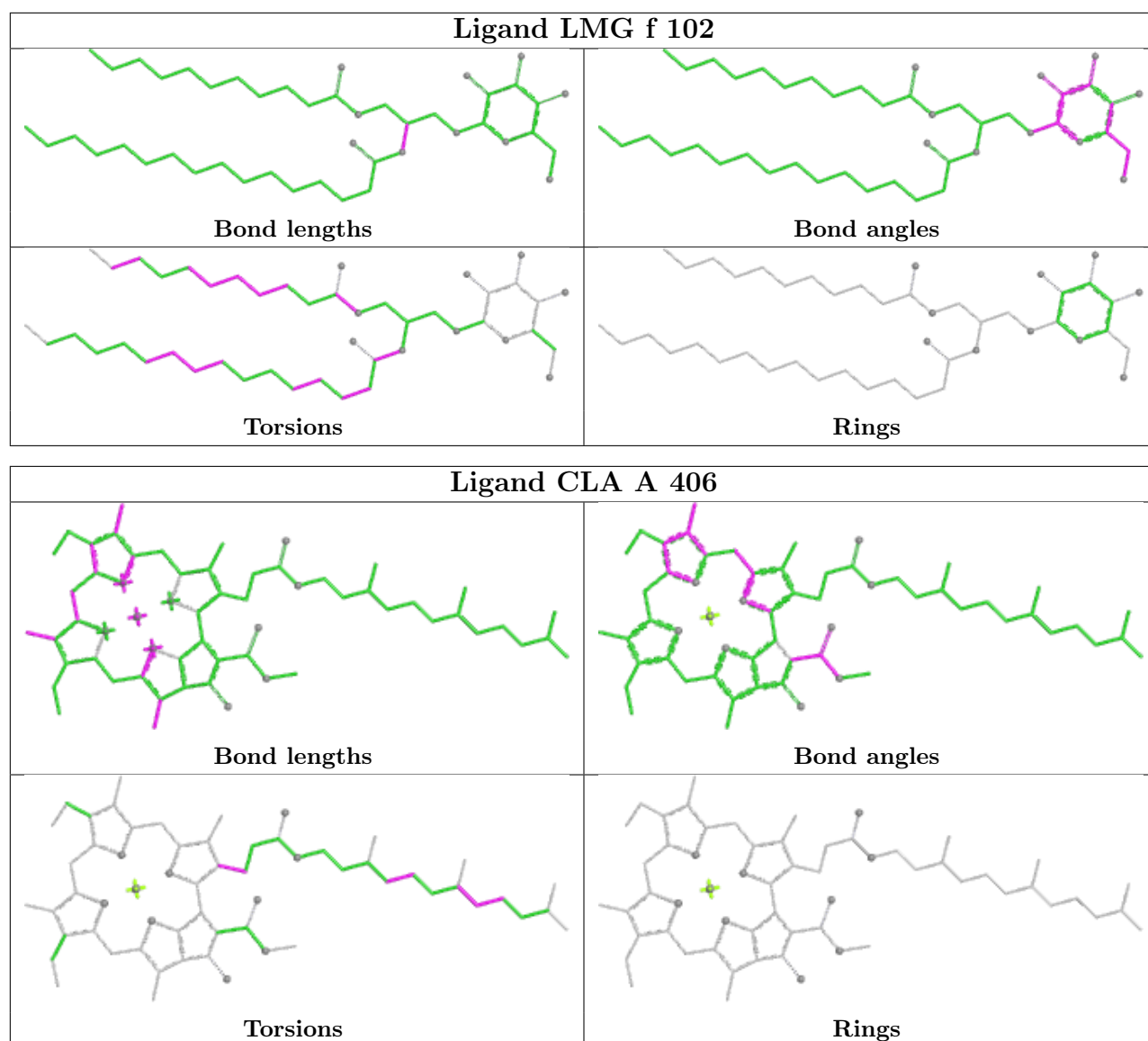
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

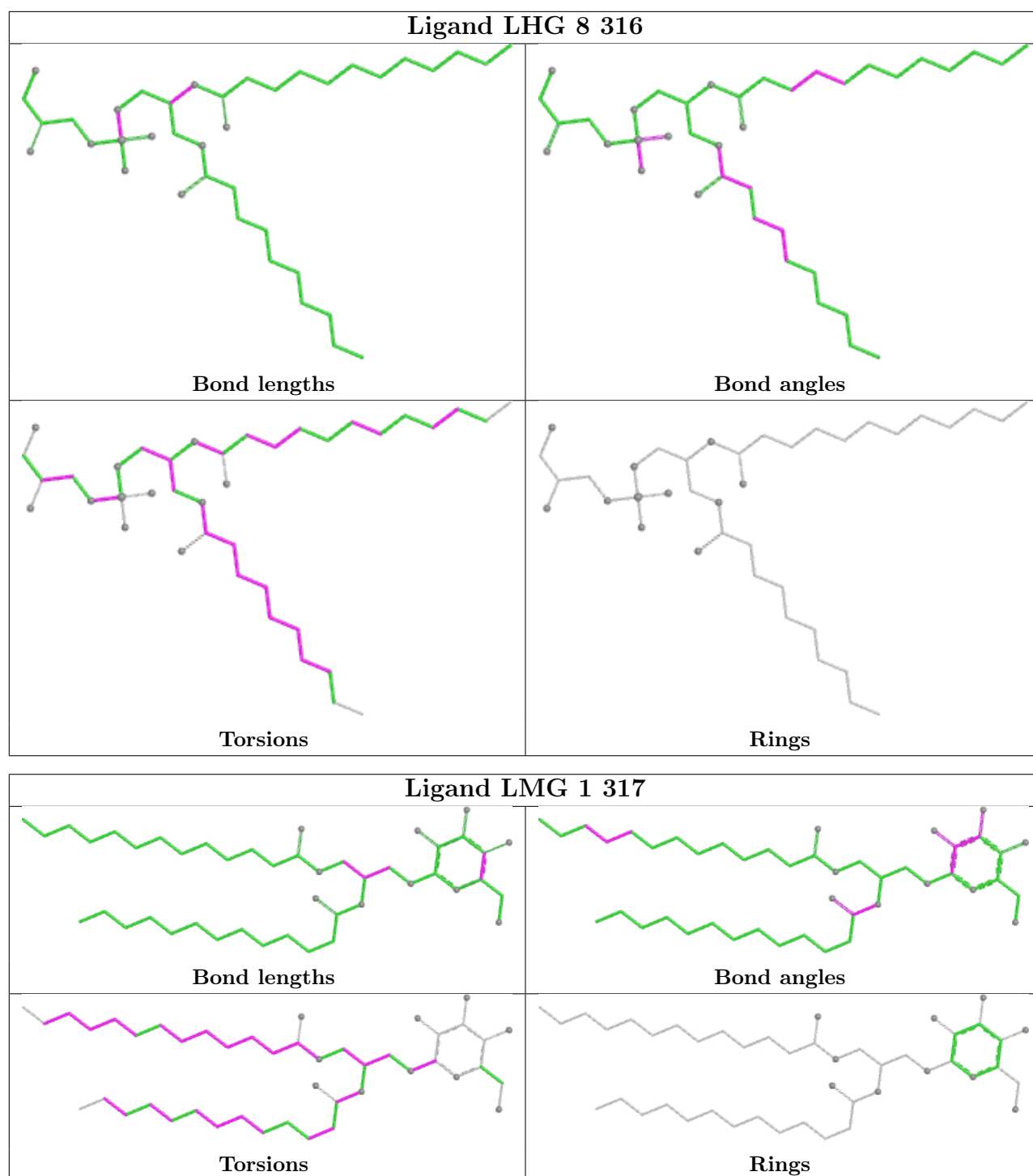
Ligand LHG 4 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

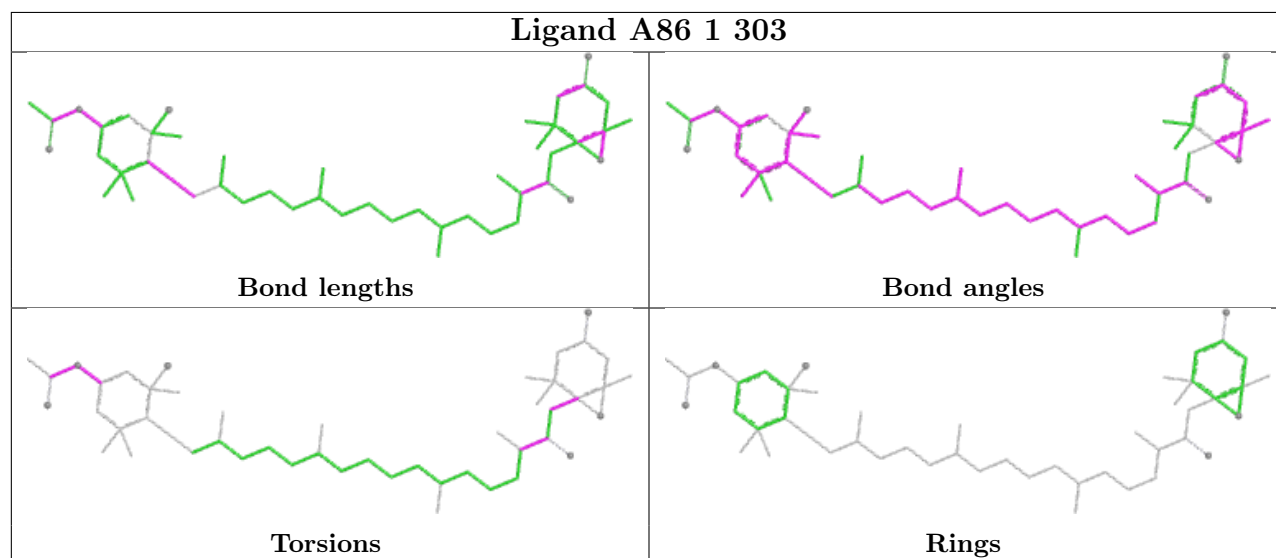
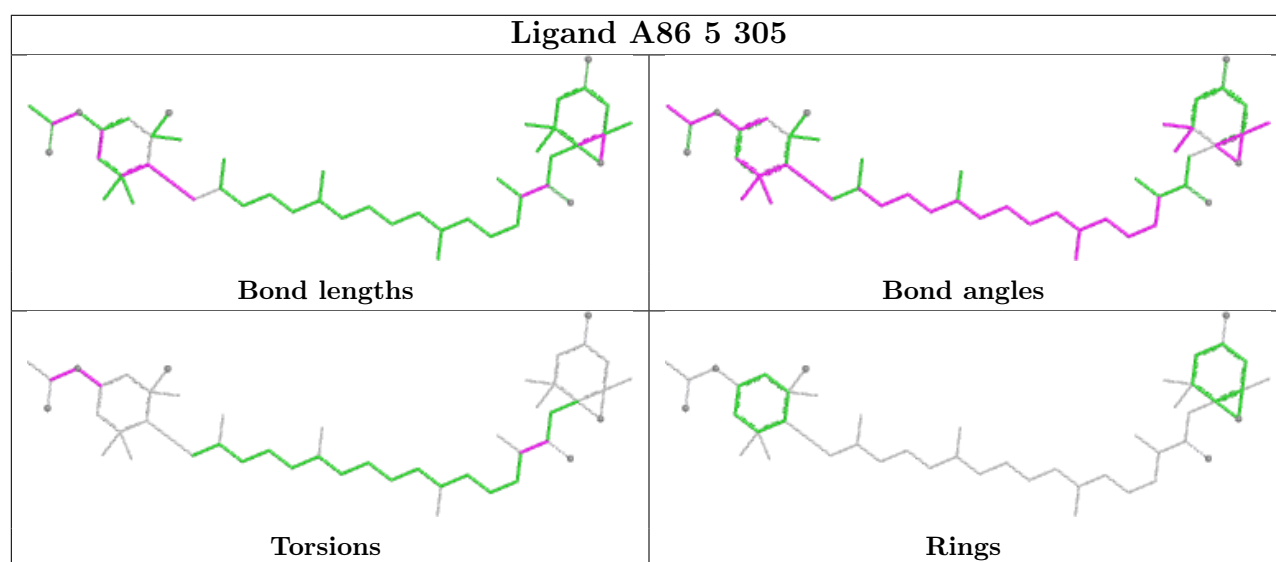
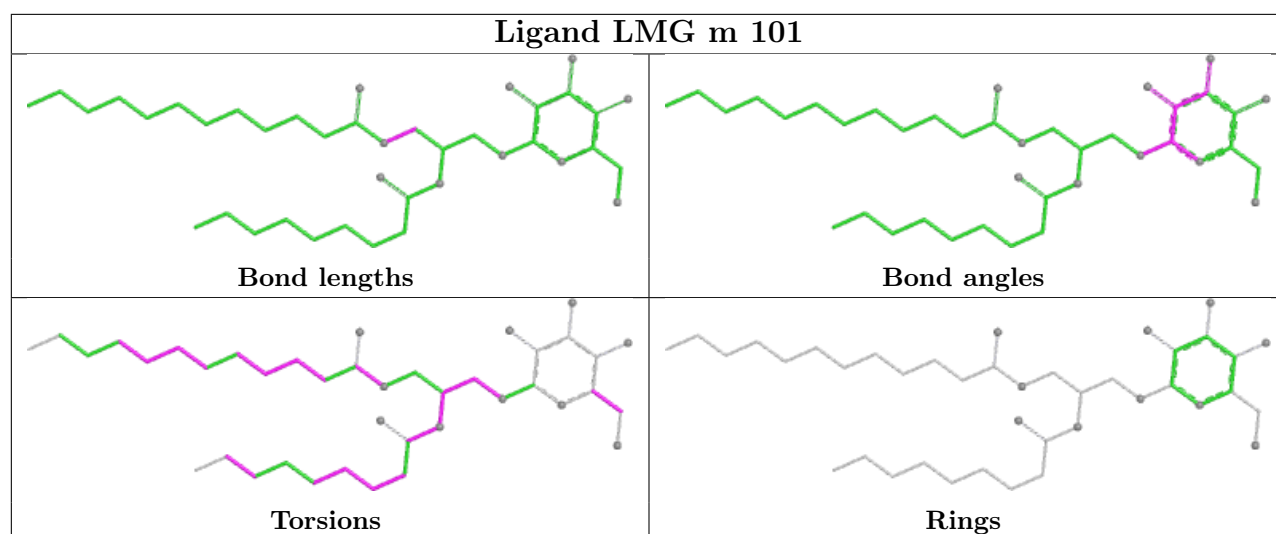
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Bond lengths	Bond angles
	
Torsions	Rings



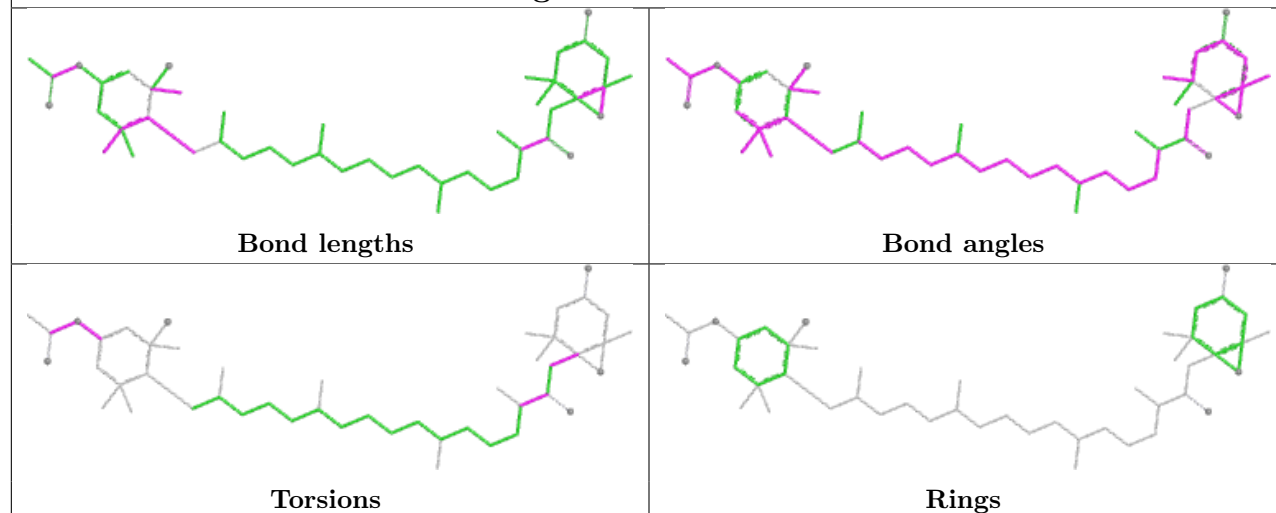




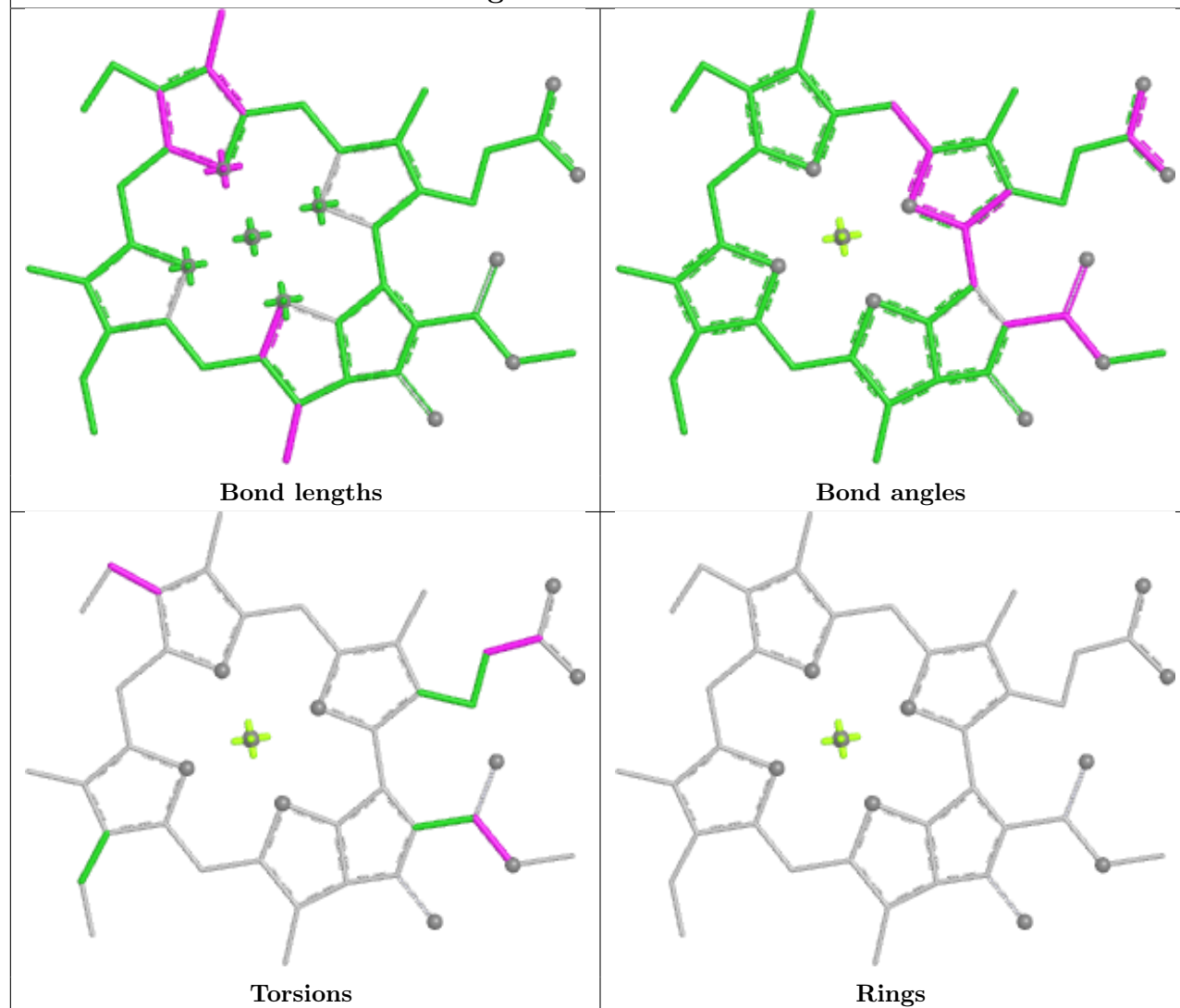




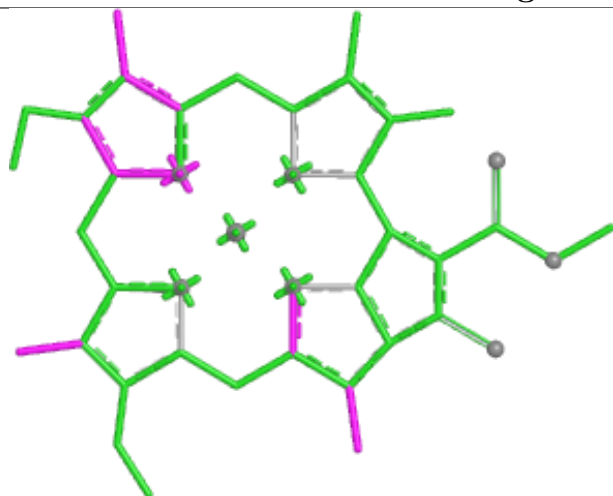
Ligand A86 17 301



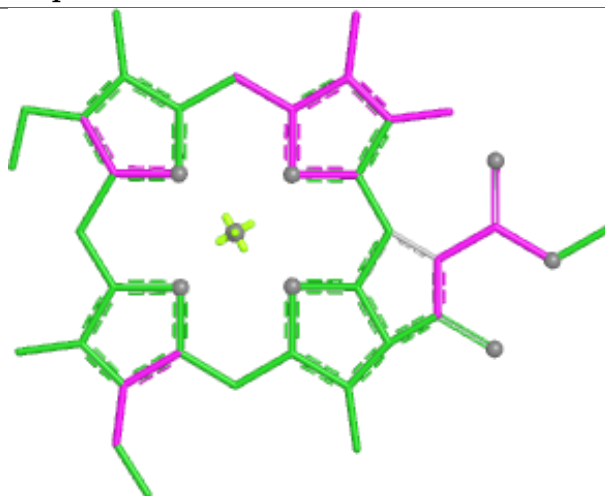
Ligand CLA 13 312



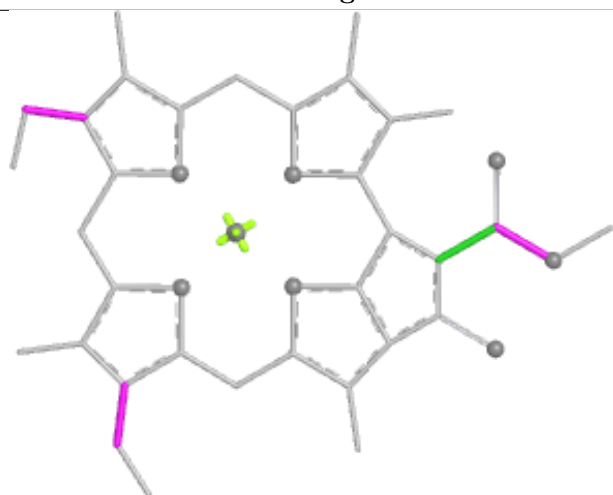
Ligand CLA p 605



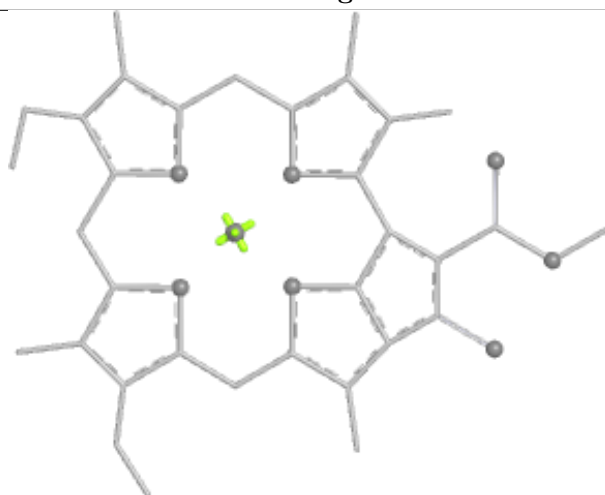
Bond lengths



Bond angles

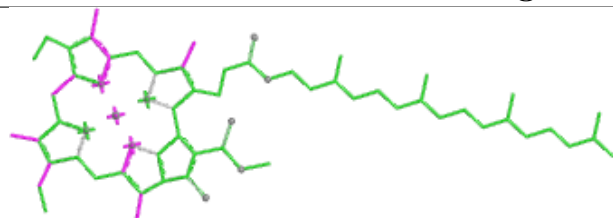


Torsions

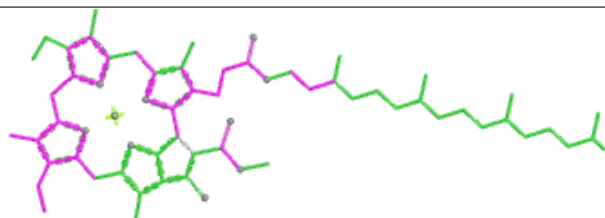


Rings

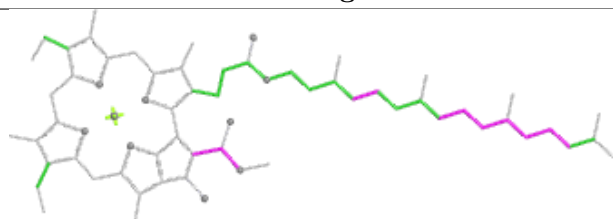
Ligand CLA b 605



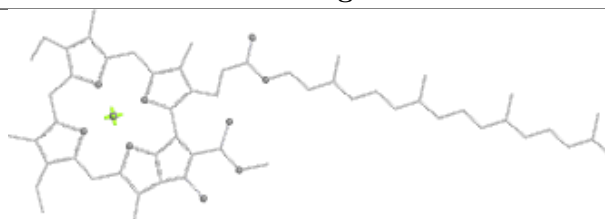
Bond lengths



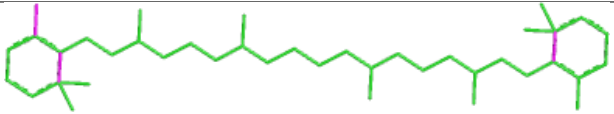
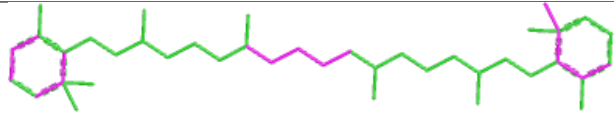
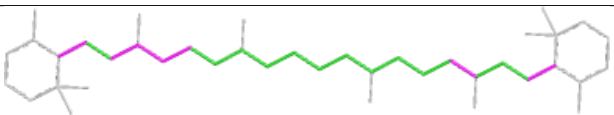
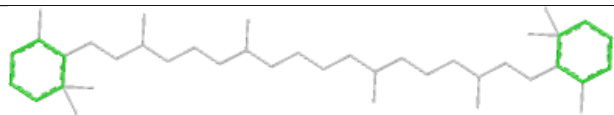
Bond angles

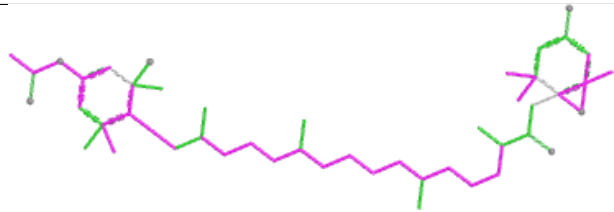
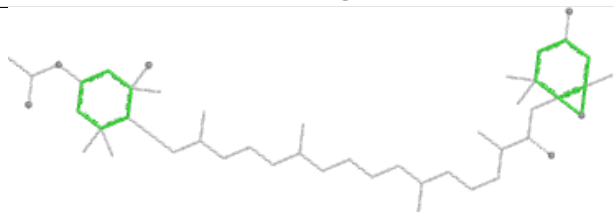


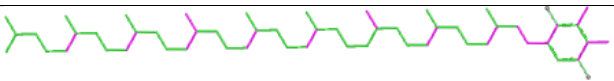
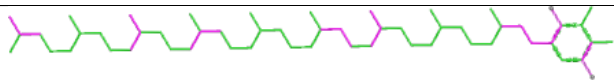
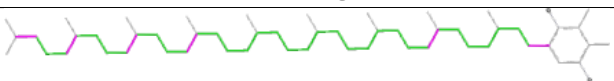
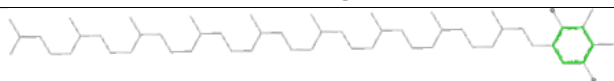
Torsions

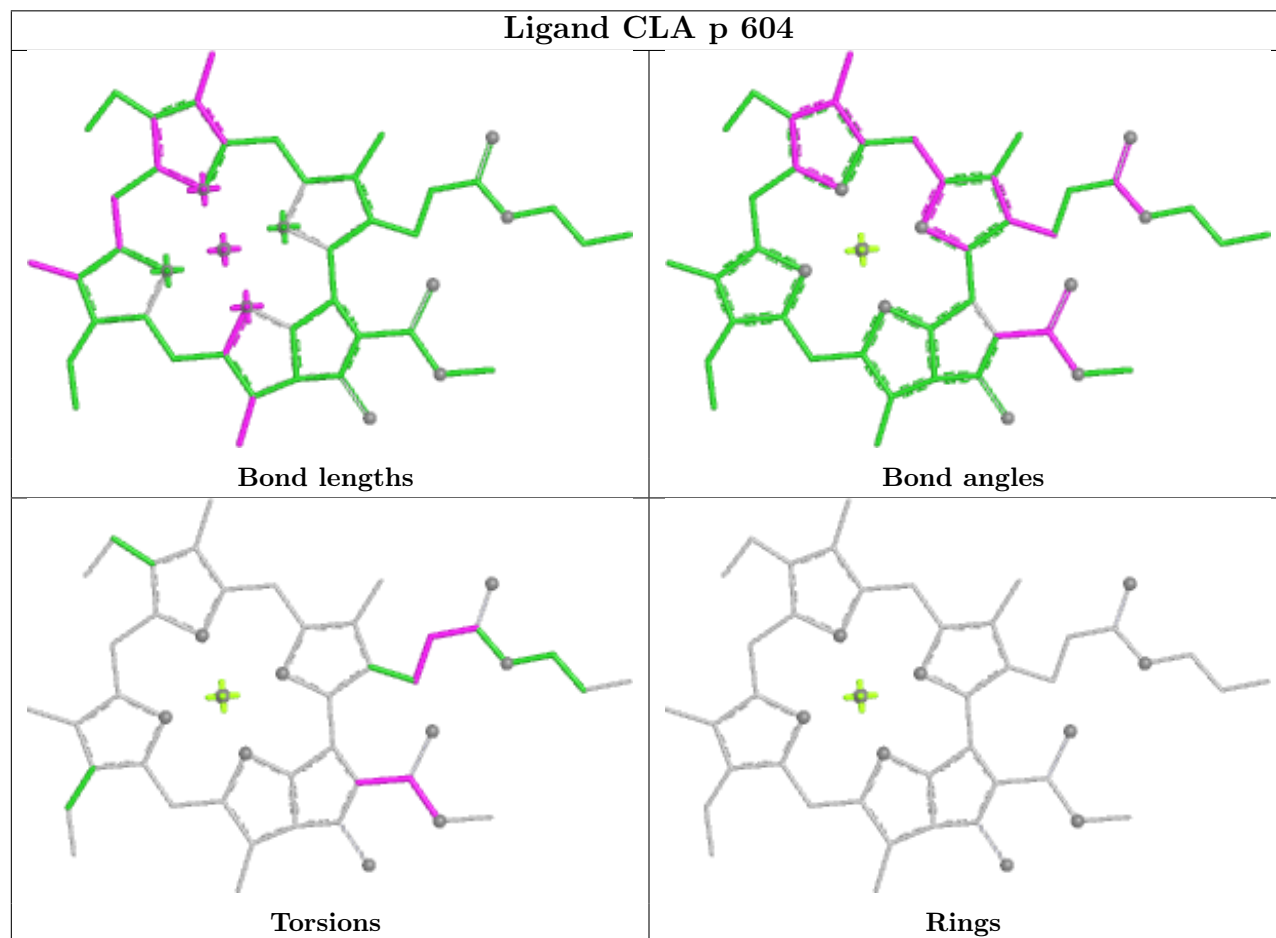
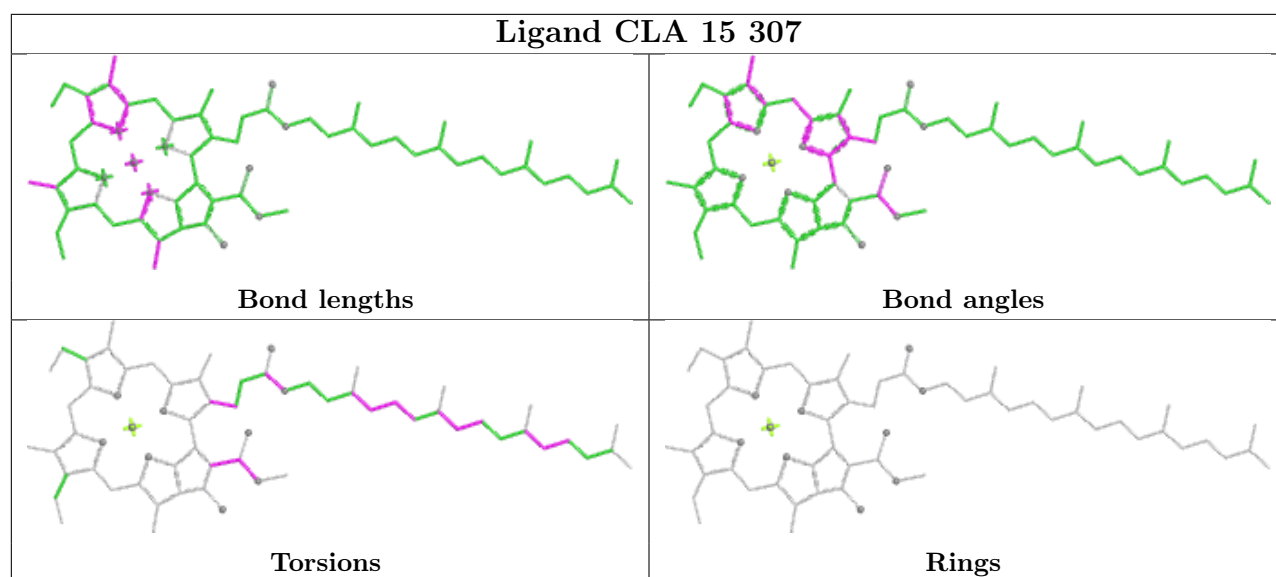


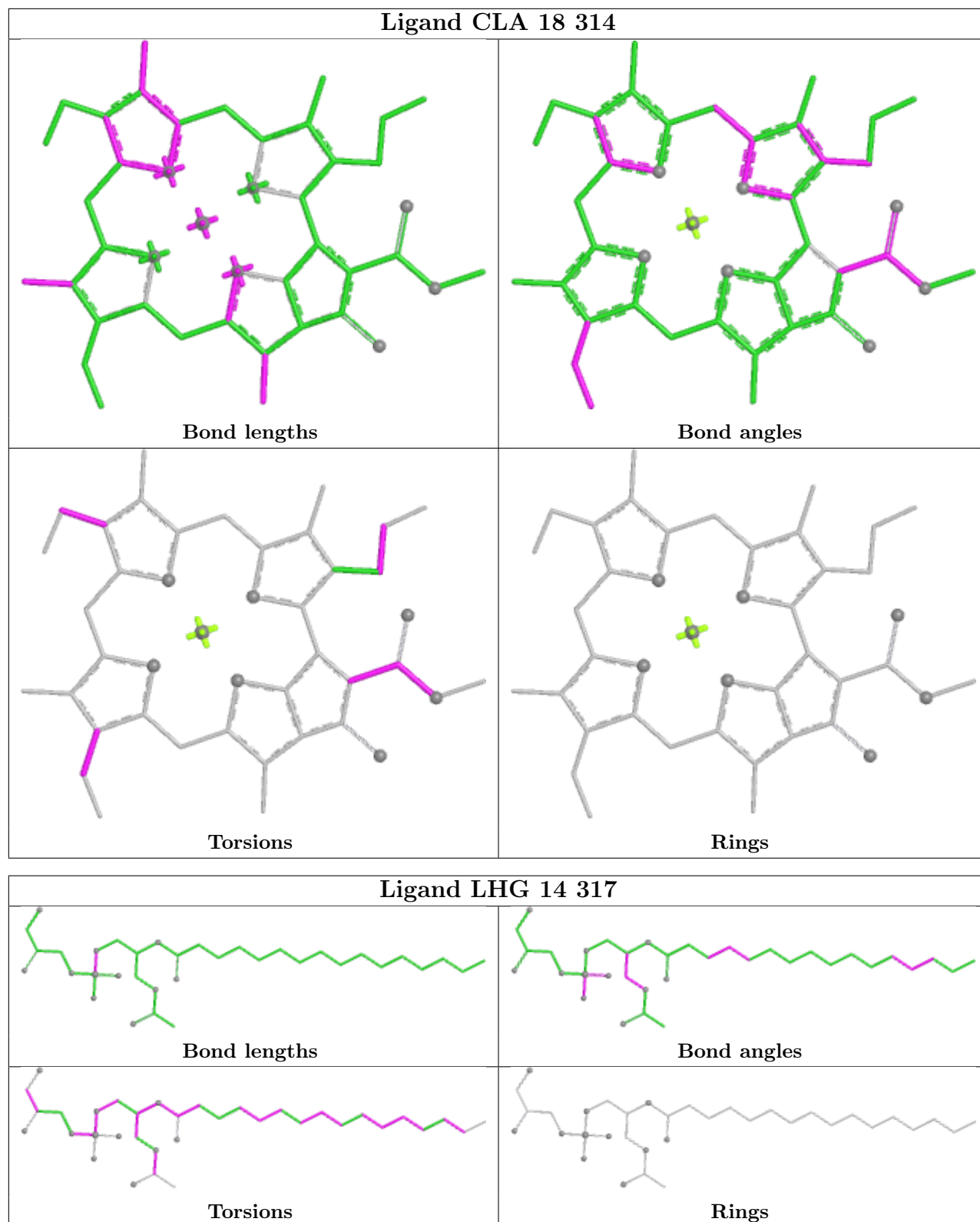
Rings

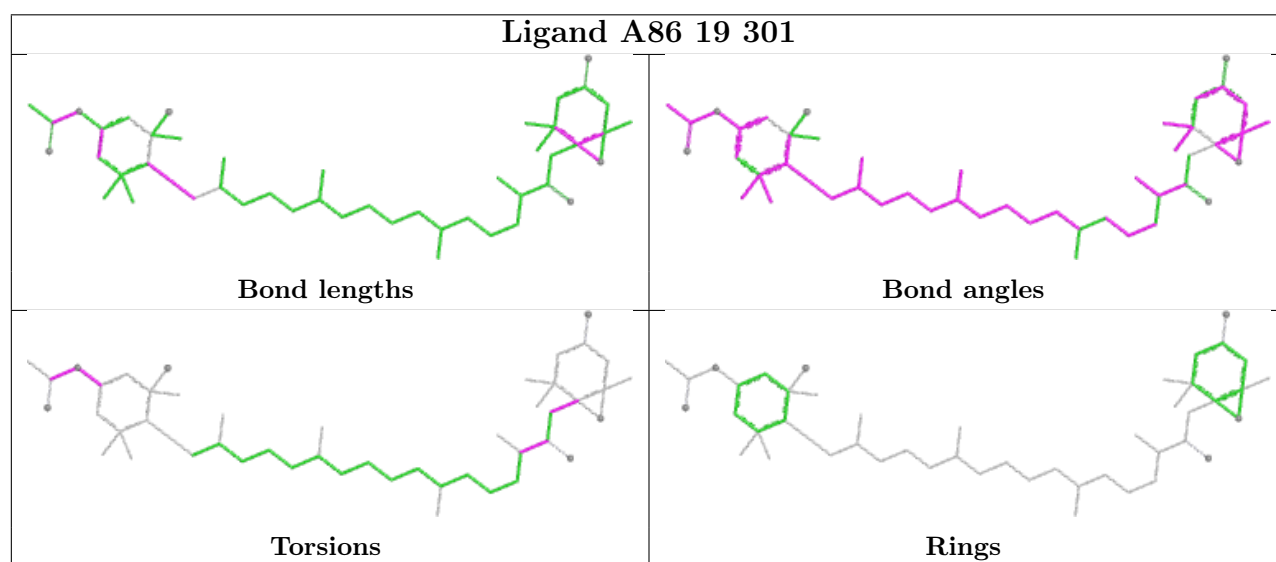
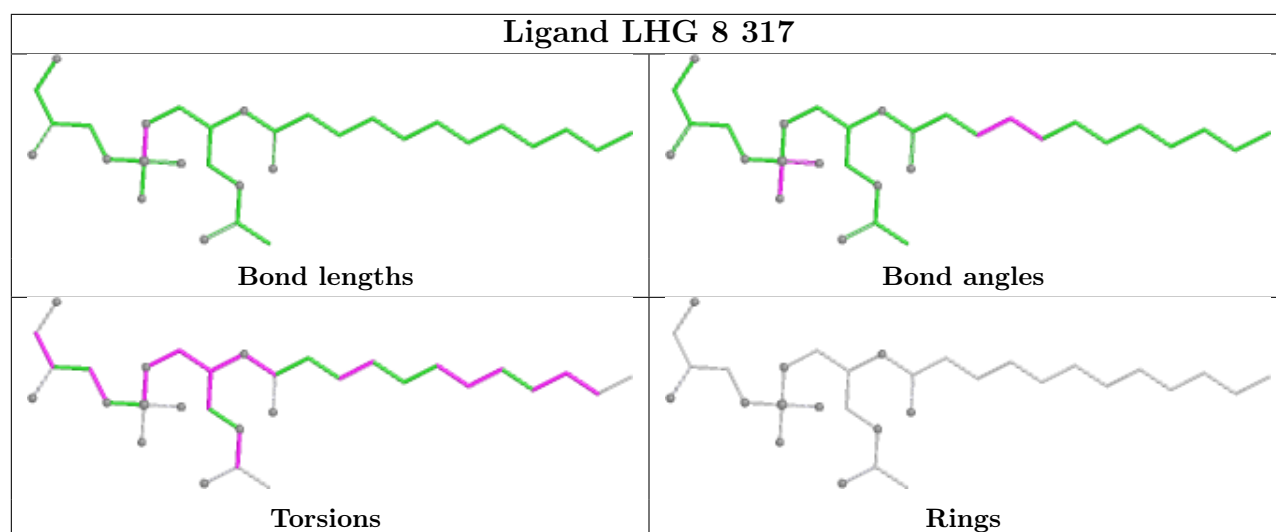
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

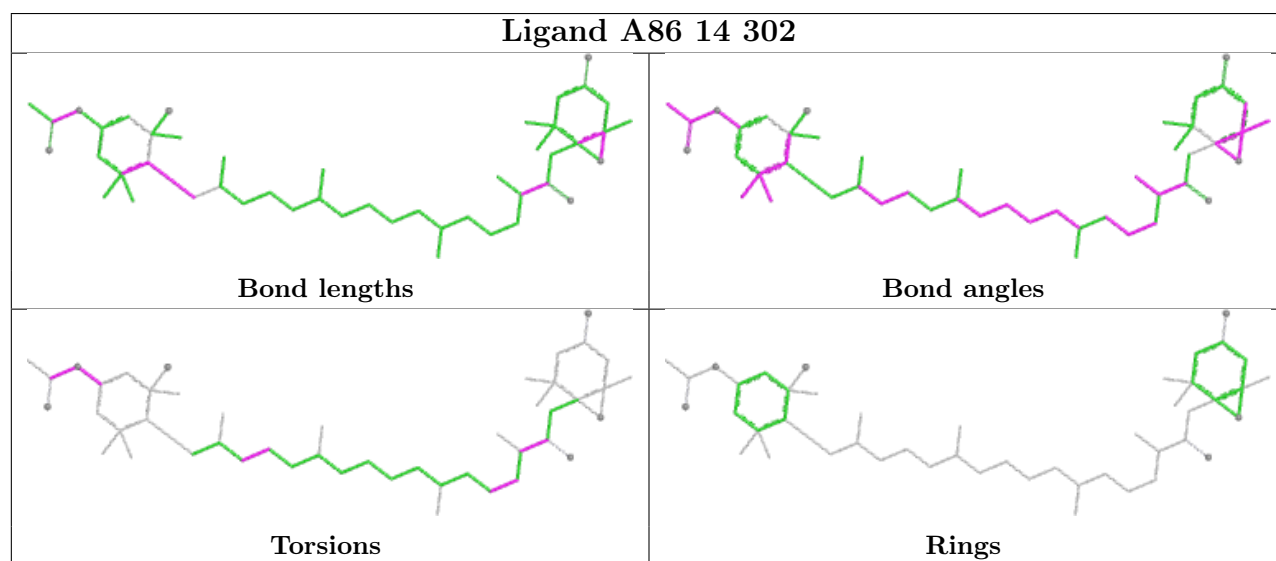
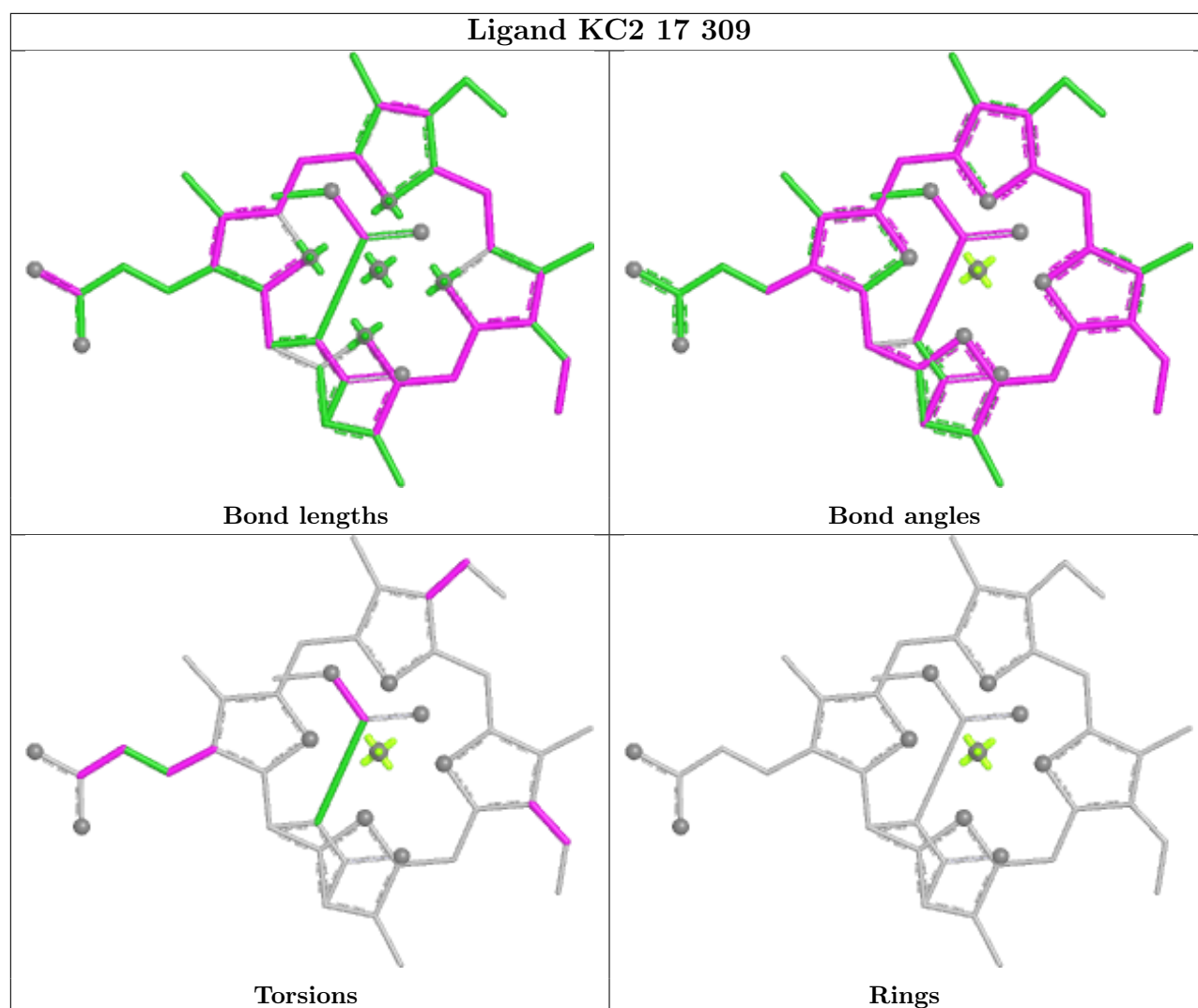
Ligand A86 0 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

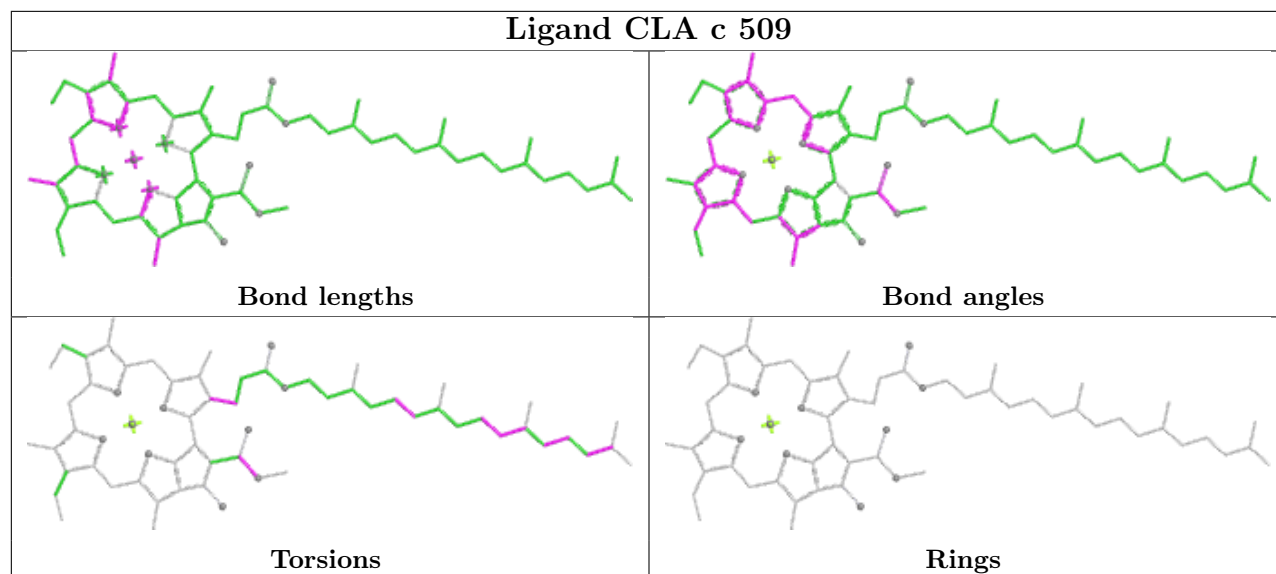
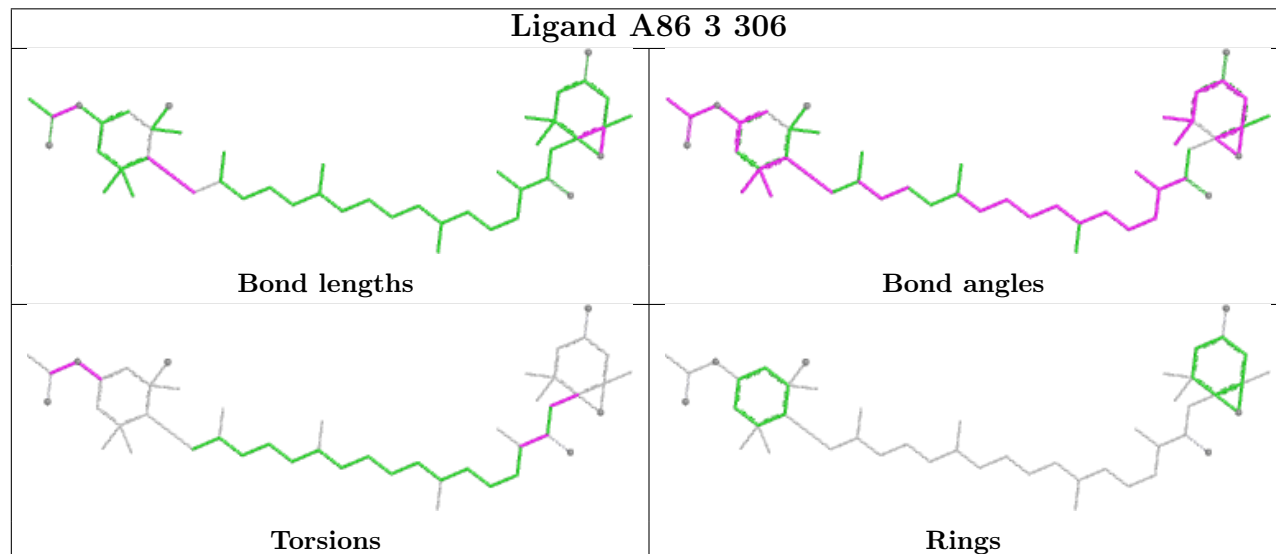
Ligand PL9 d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings



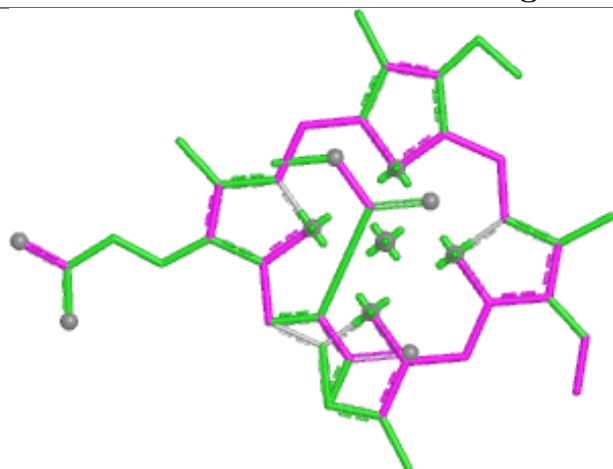




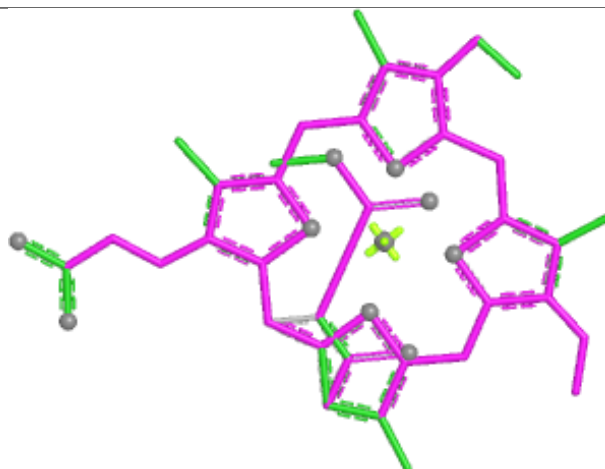


Ligand CLA c 509**Ligand A86 3 306**

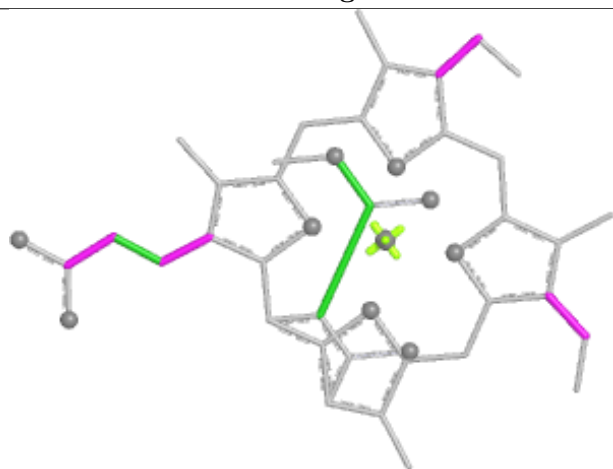
Ligand KC2 5 310



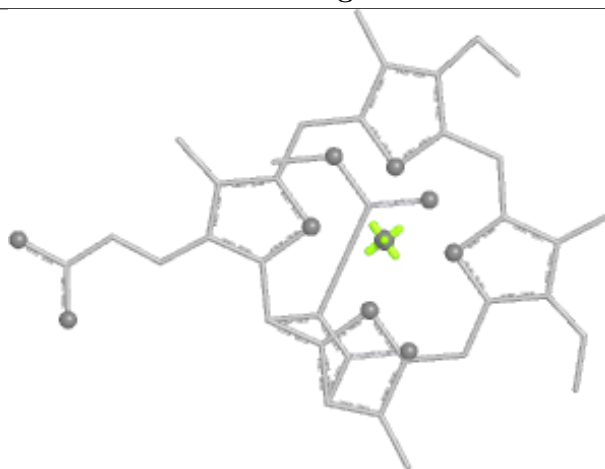
Bond lengths



Bond angles

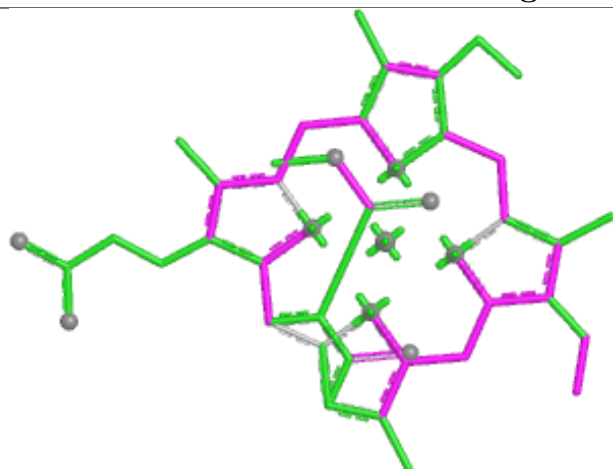


Torsions

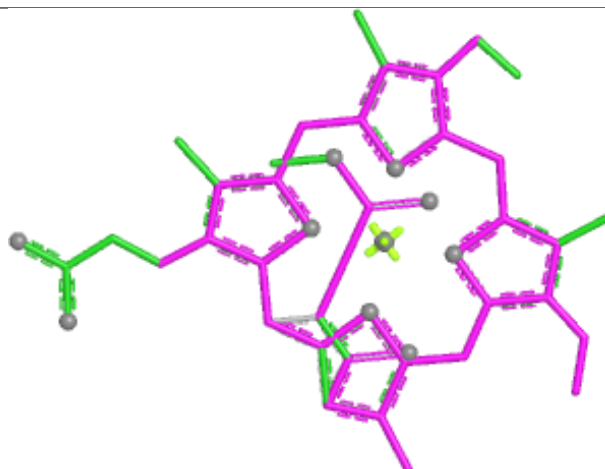


Rings

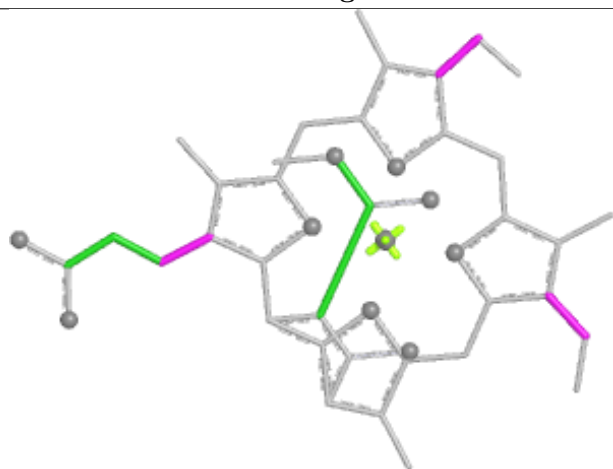
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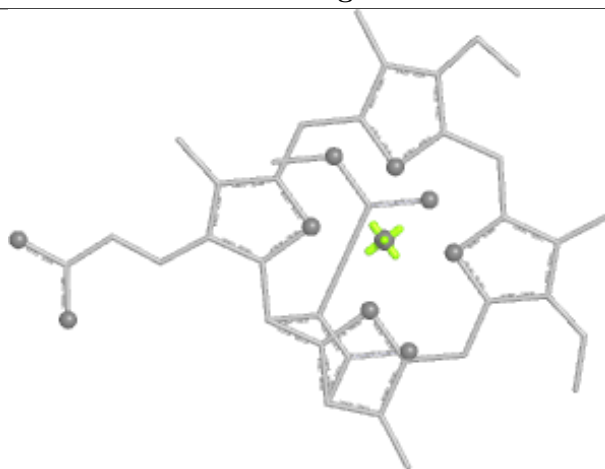
Bond lengths



Bond angles

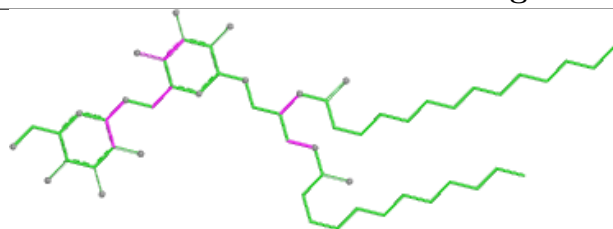


Torsions

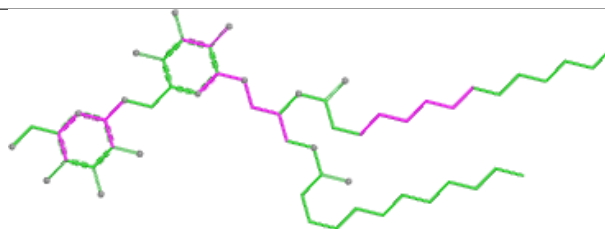


Rings

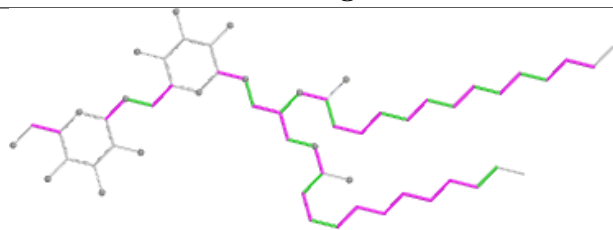
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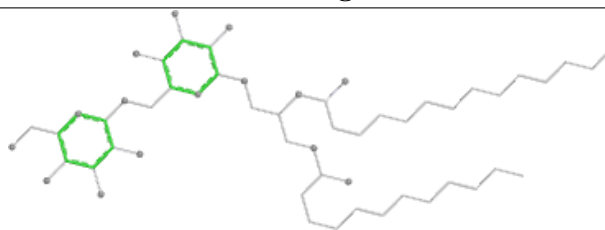
Bond lengths



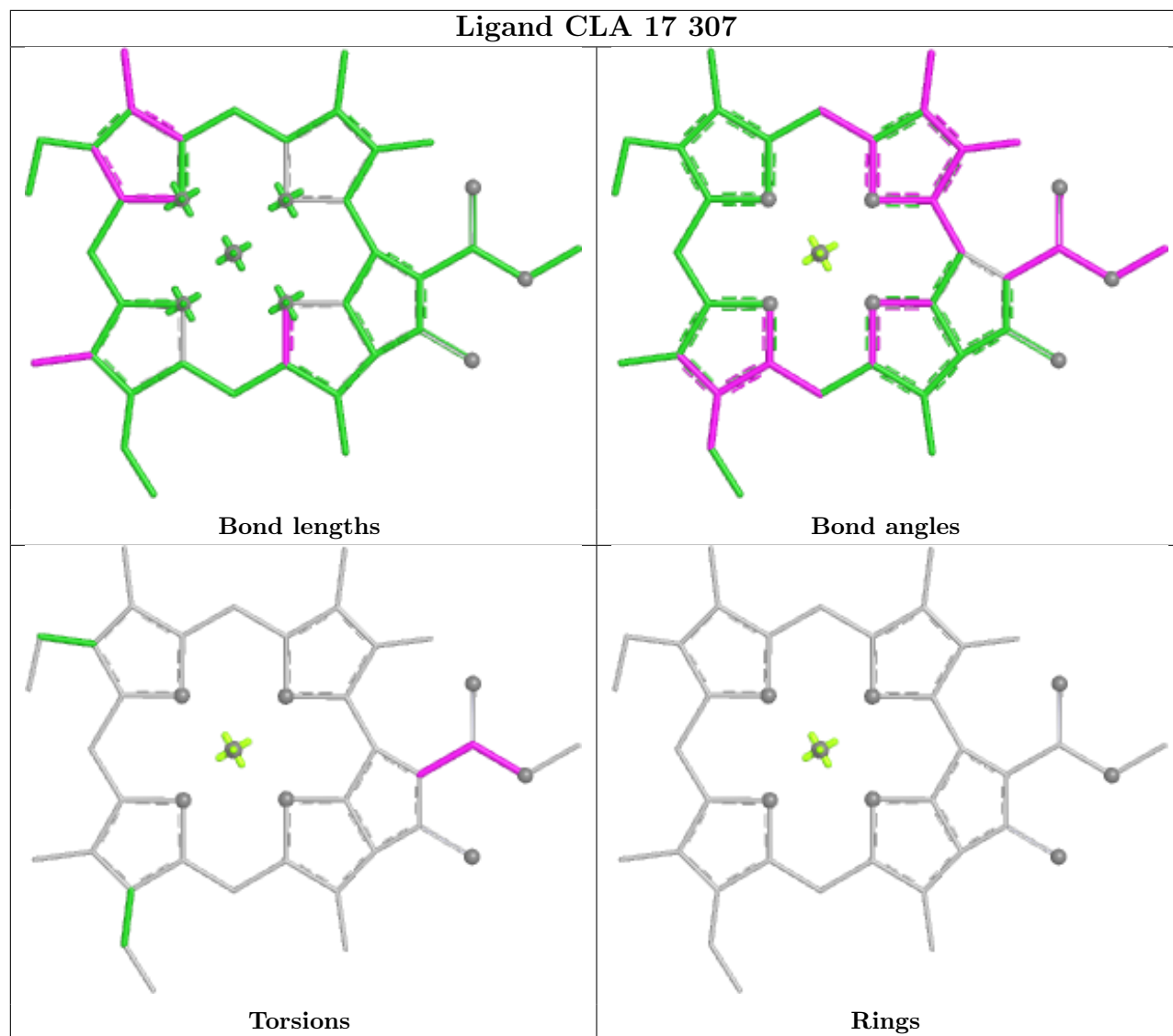
Bond angles



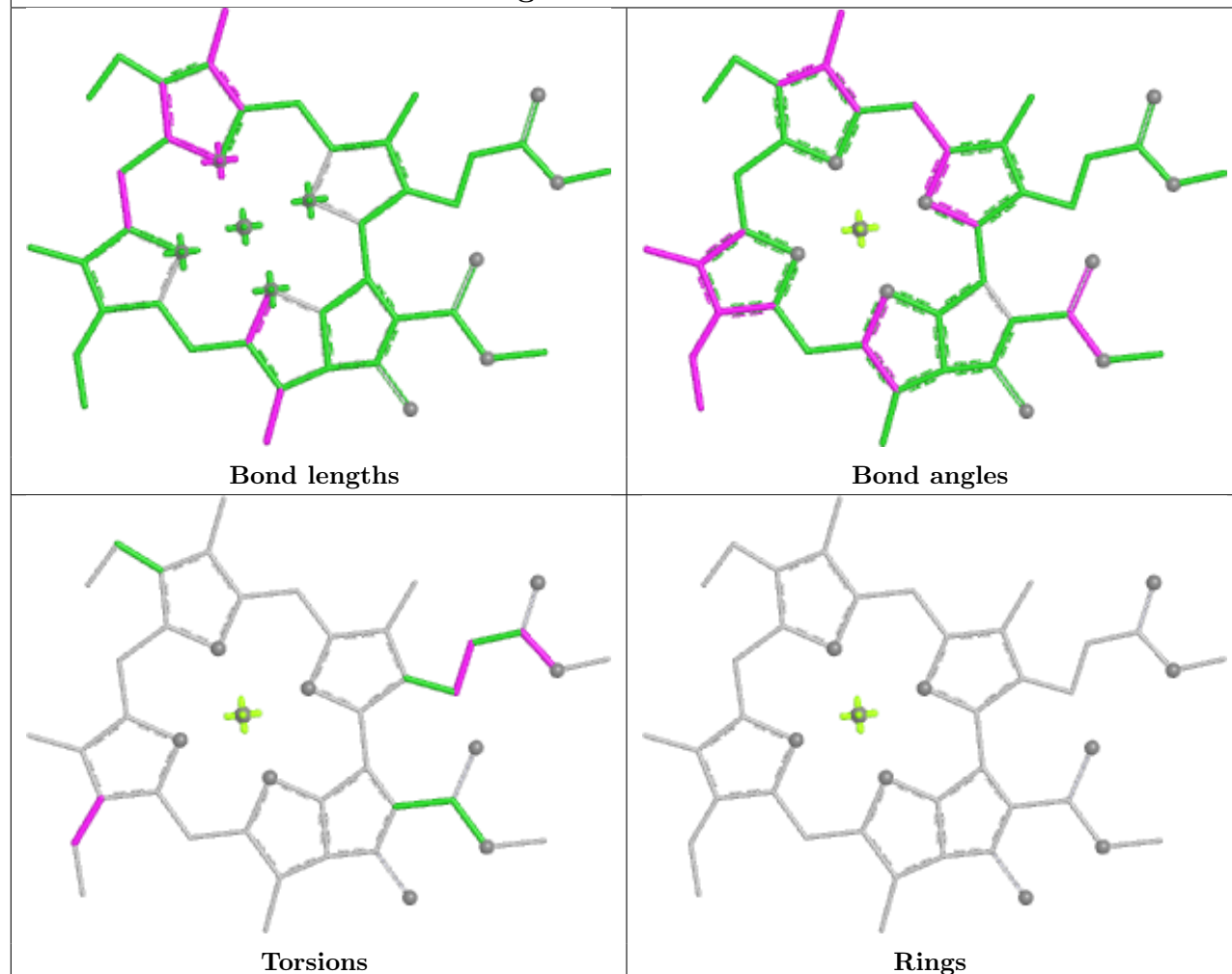
Torsions



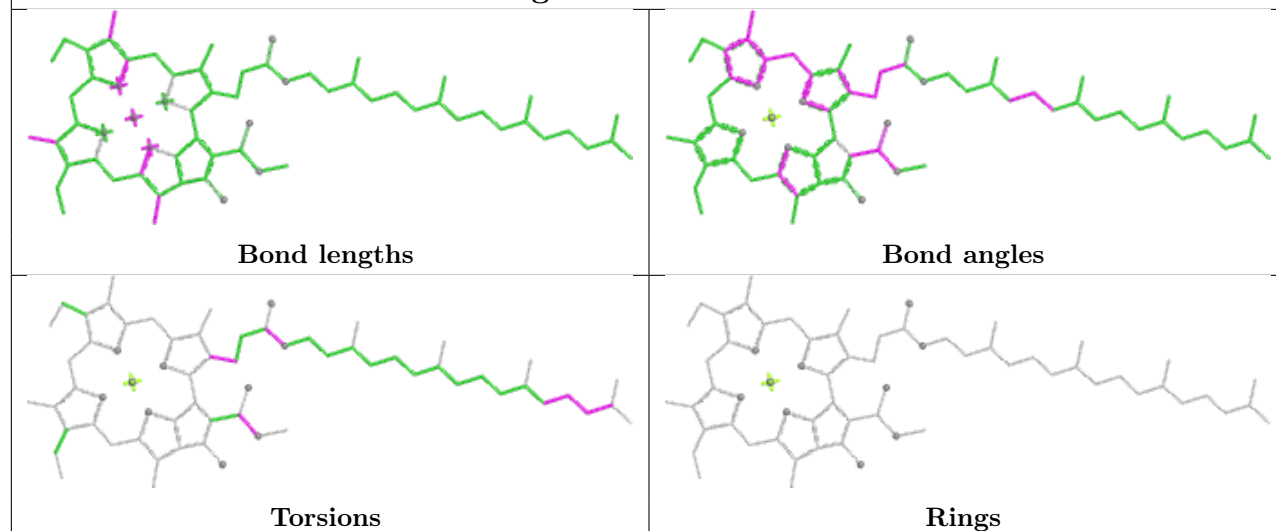
Rings

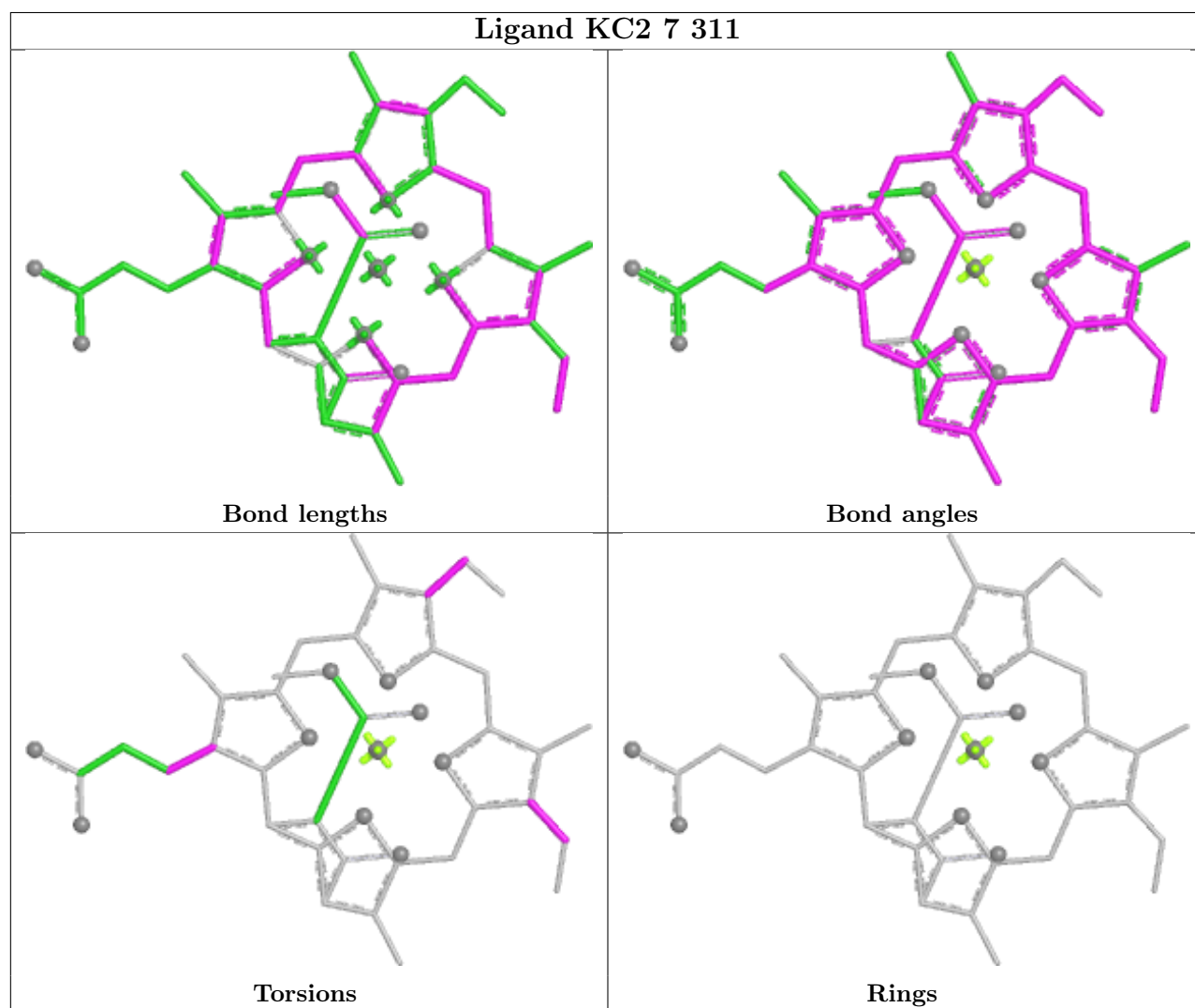
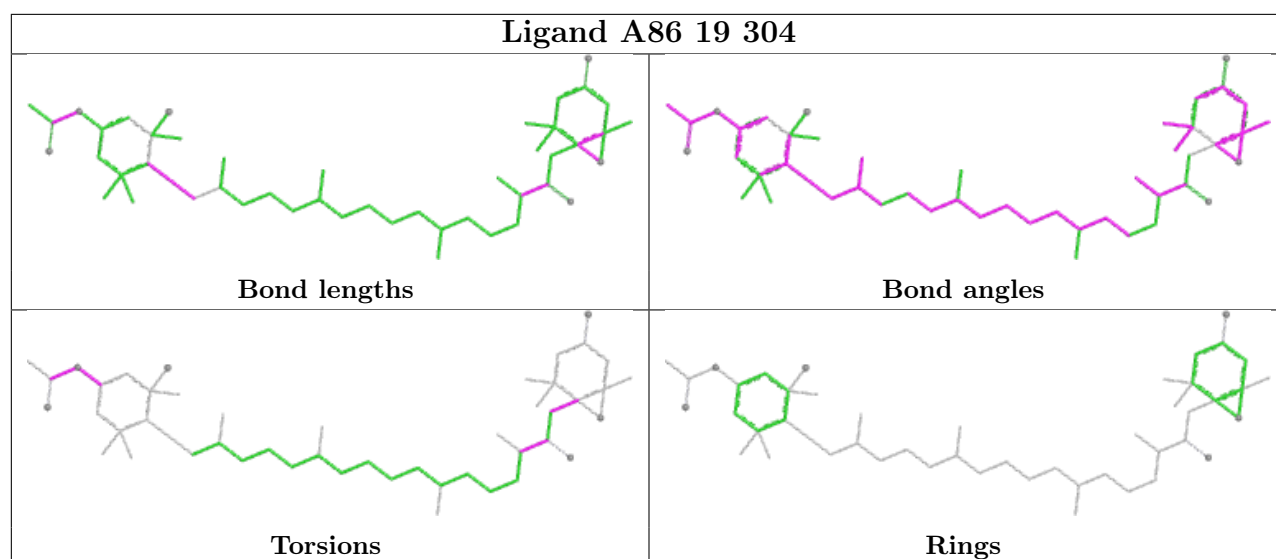


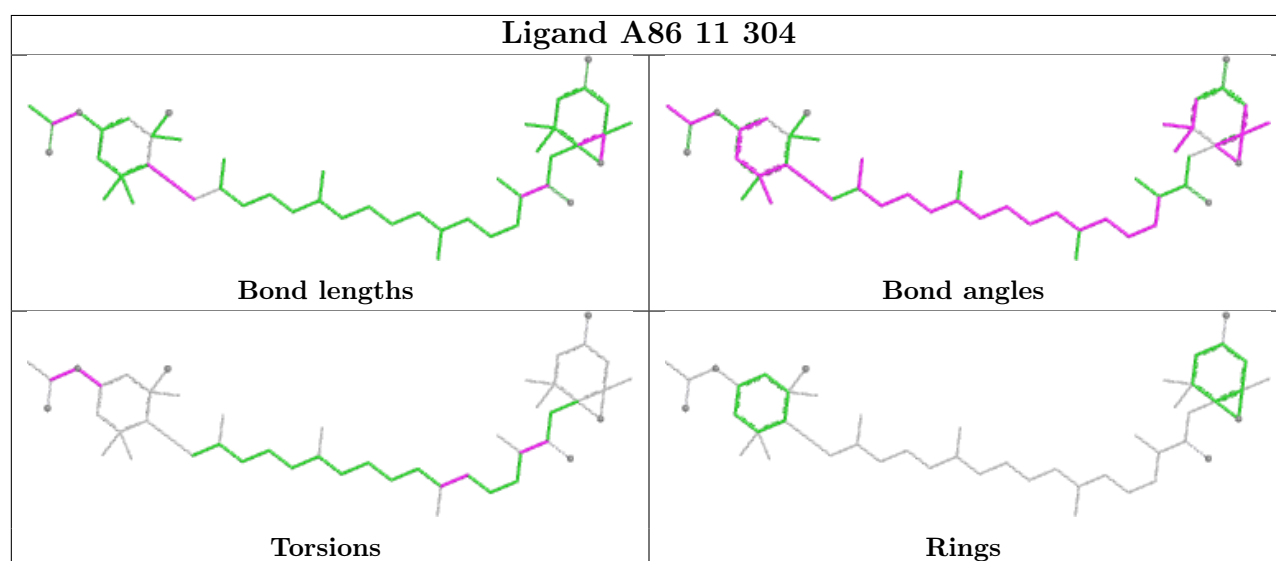
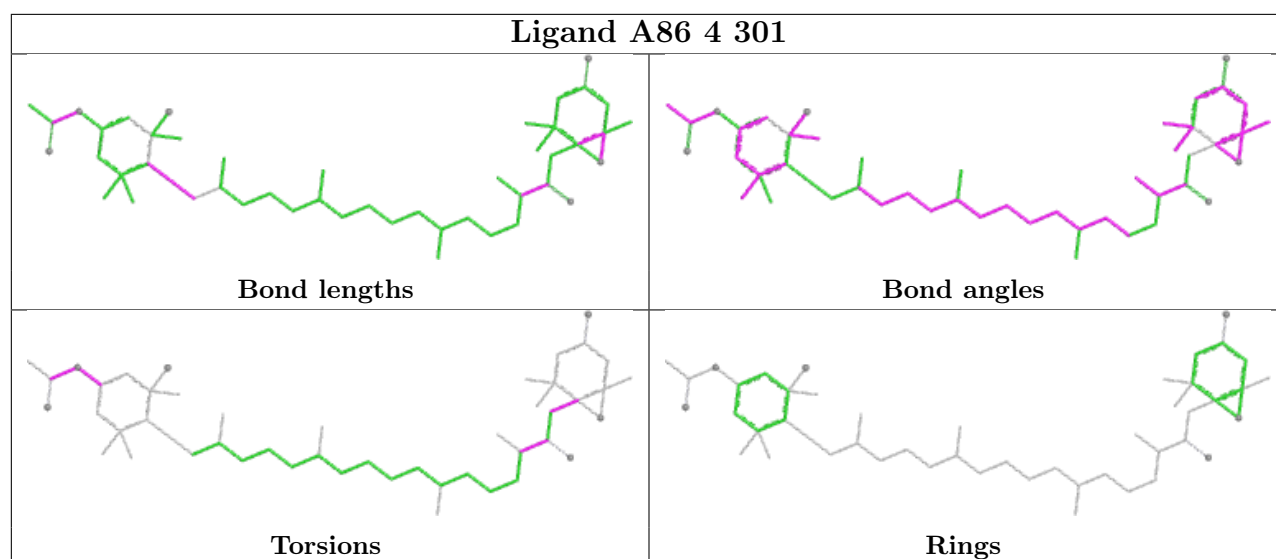
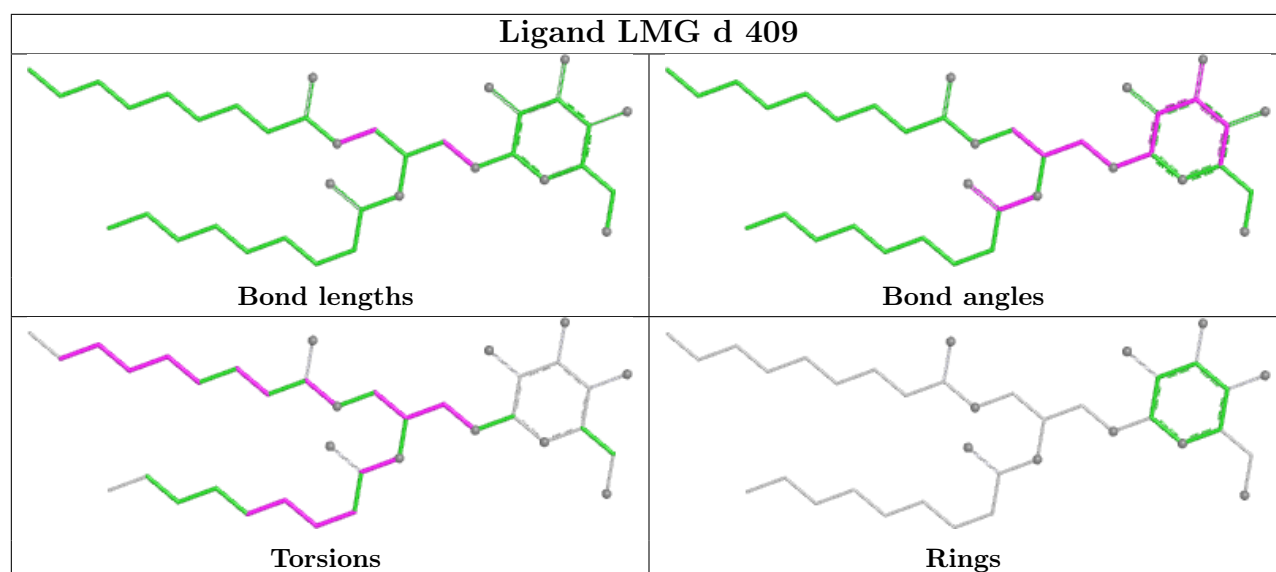
Ligand CLA 0 312

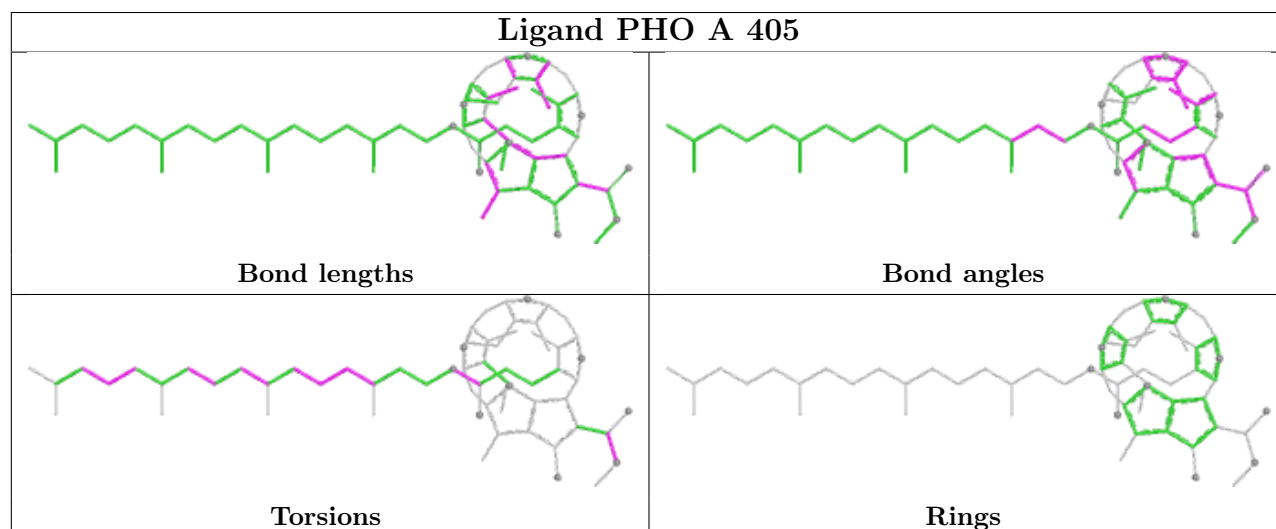
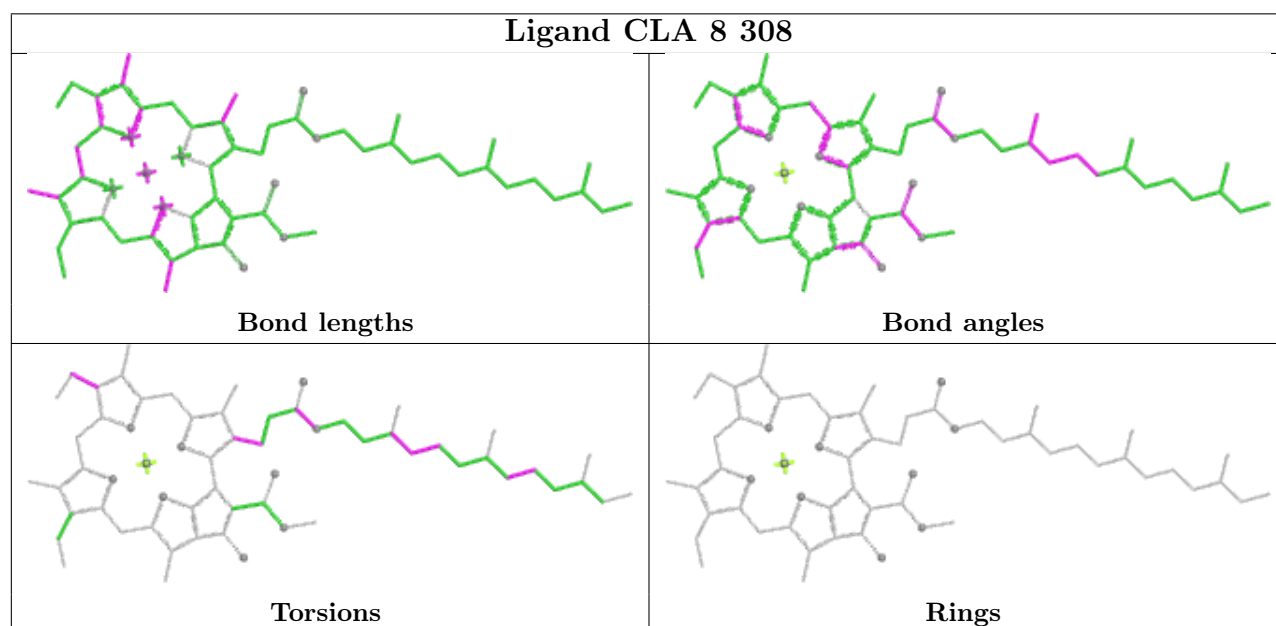
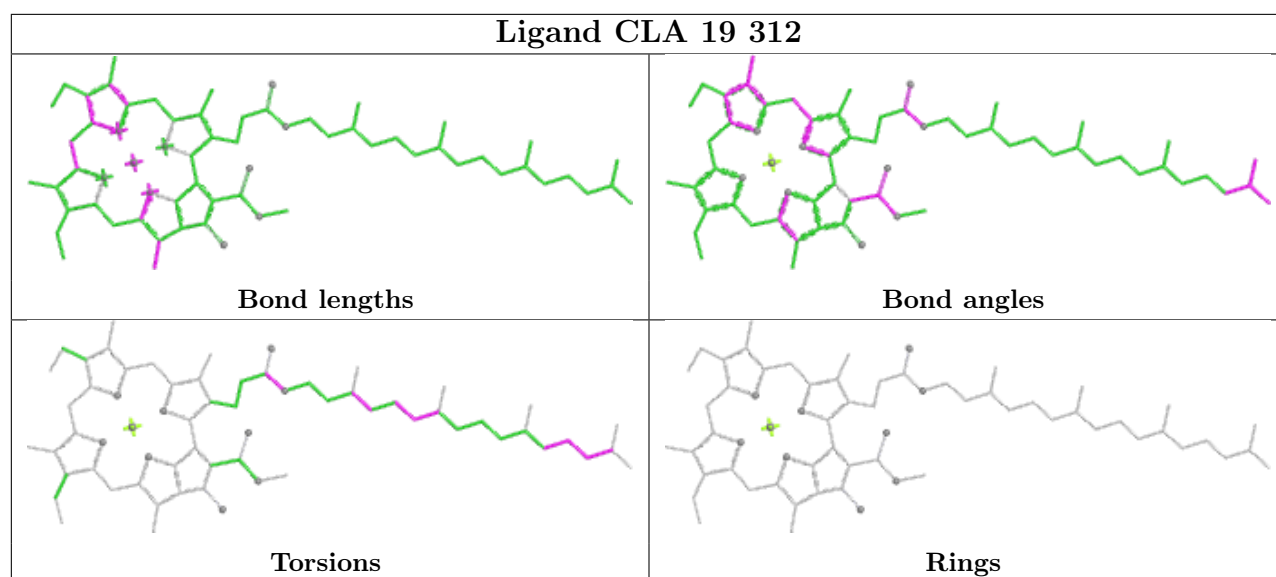


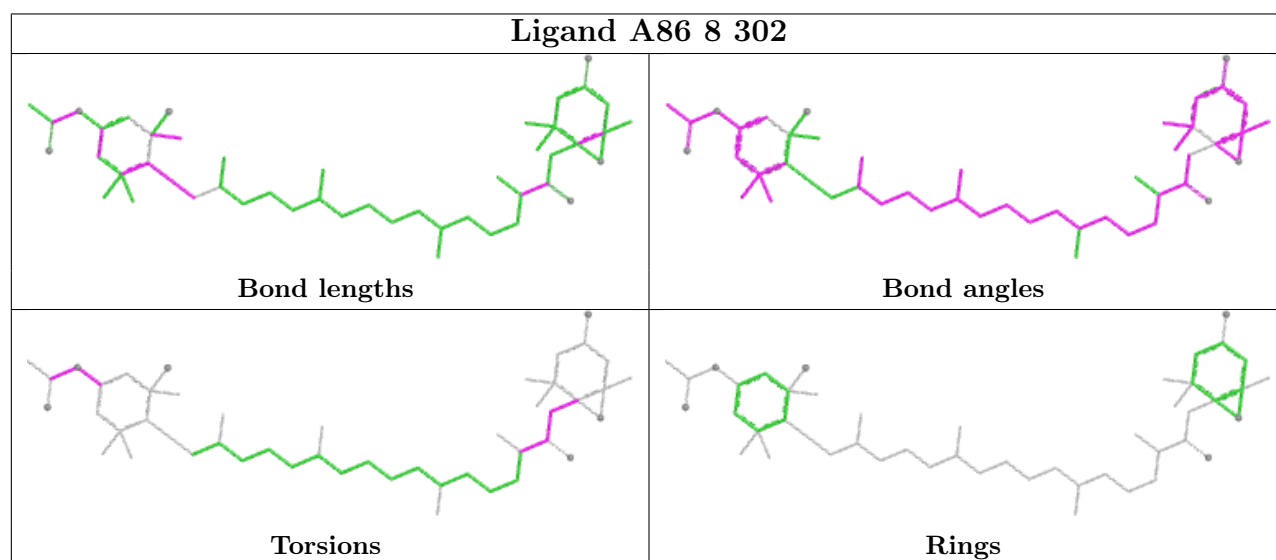
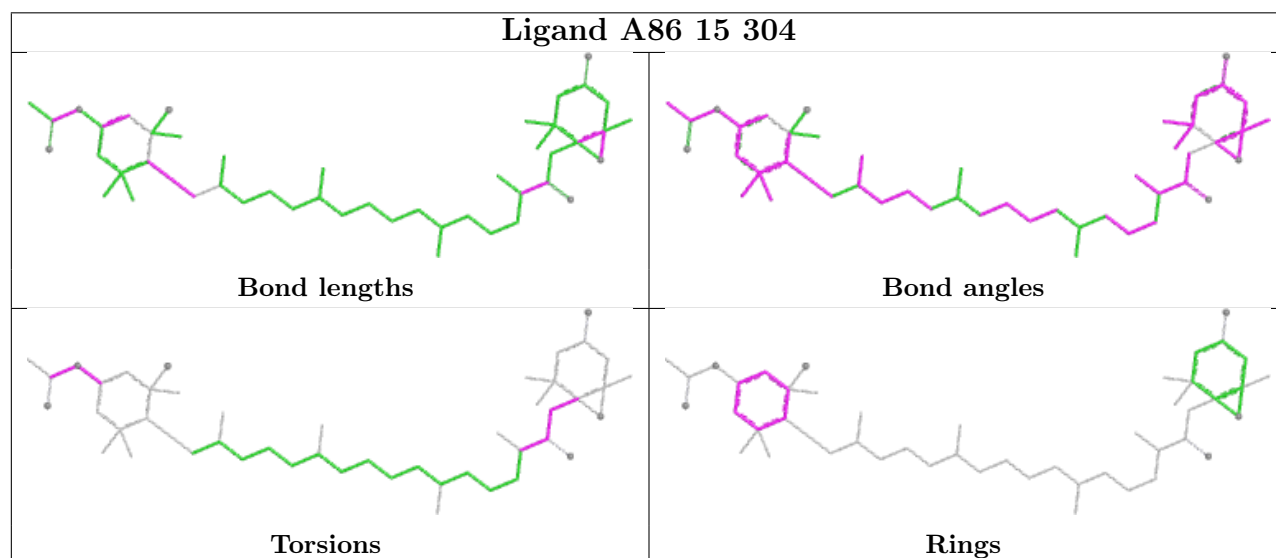
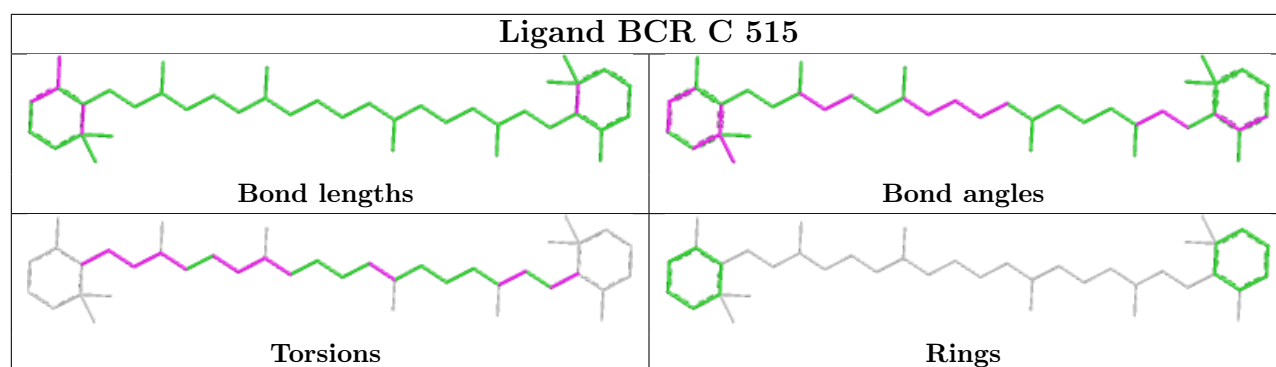
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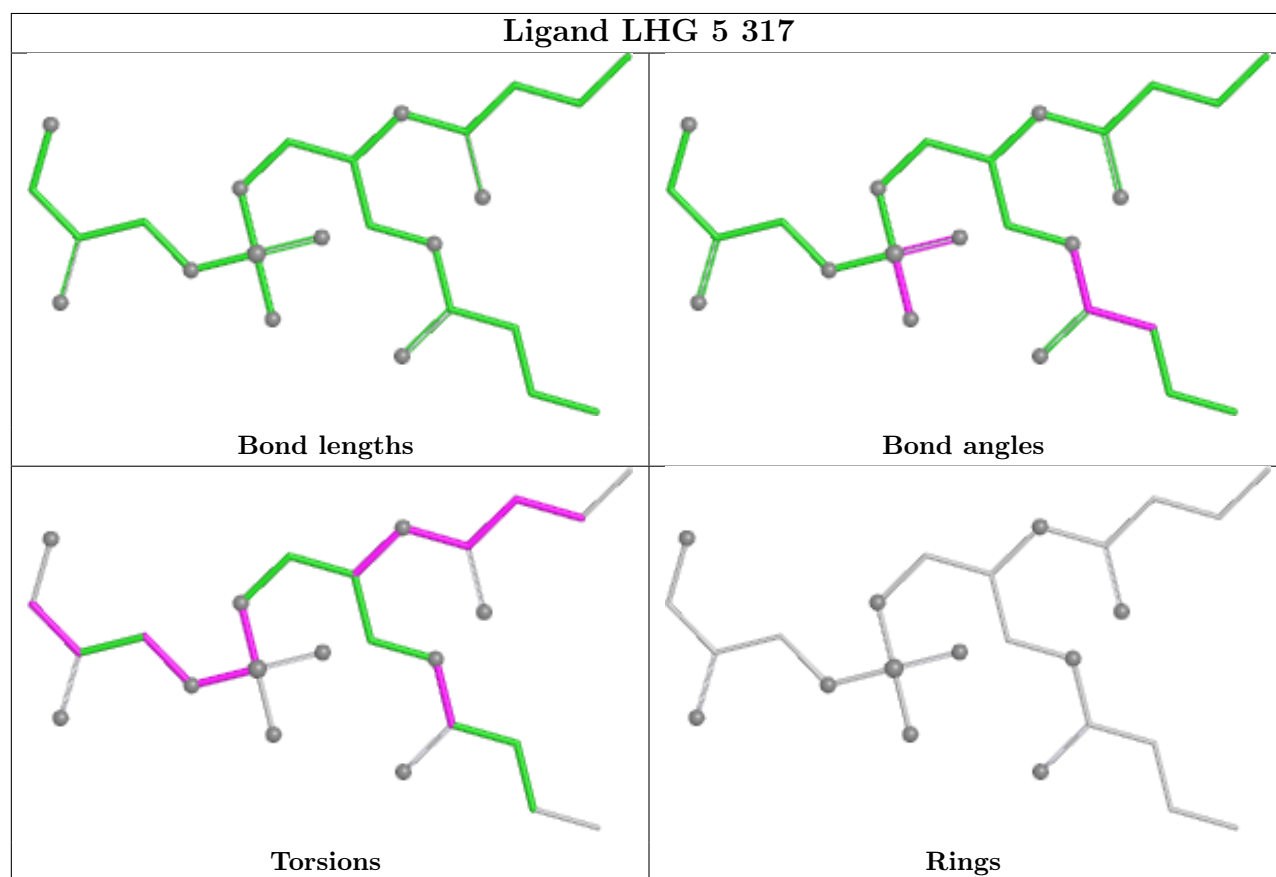
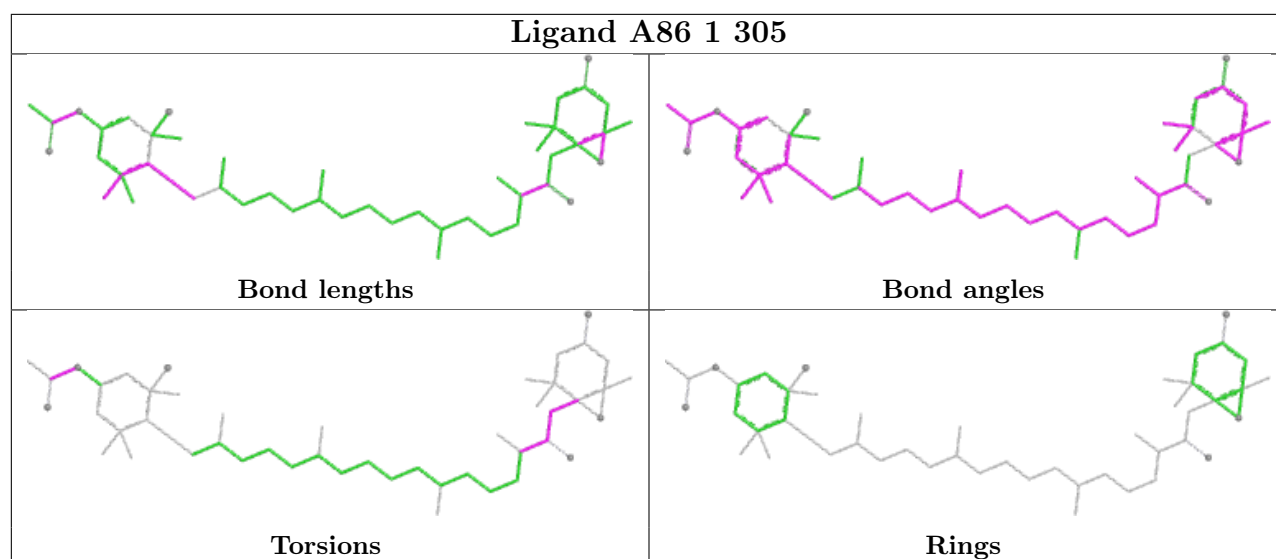


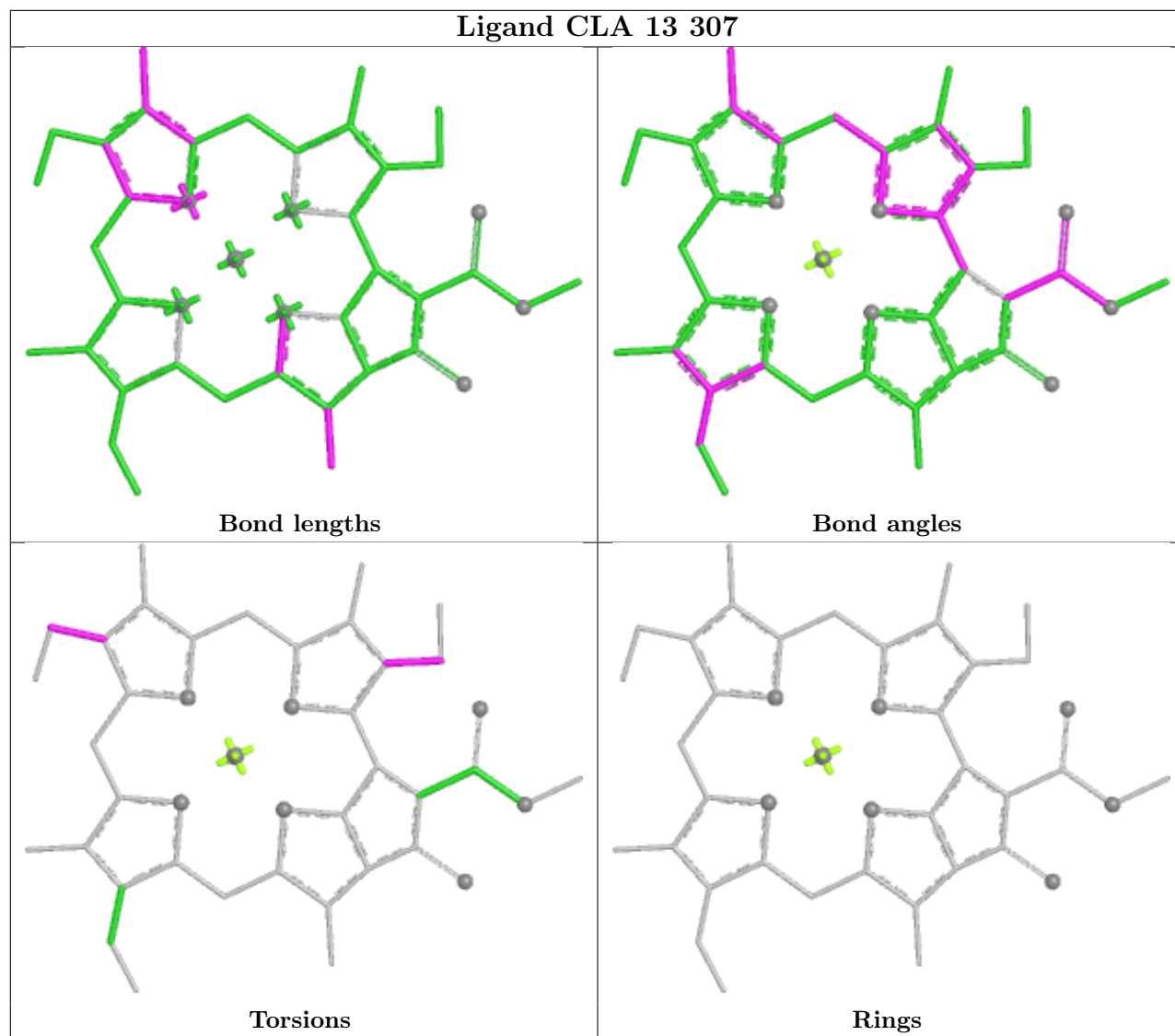


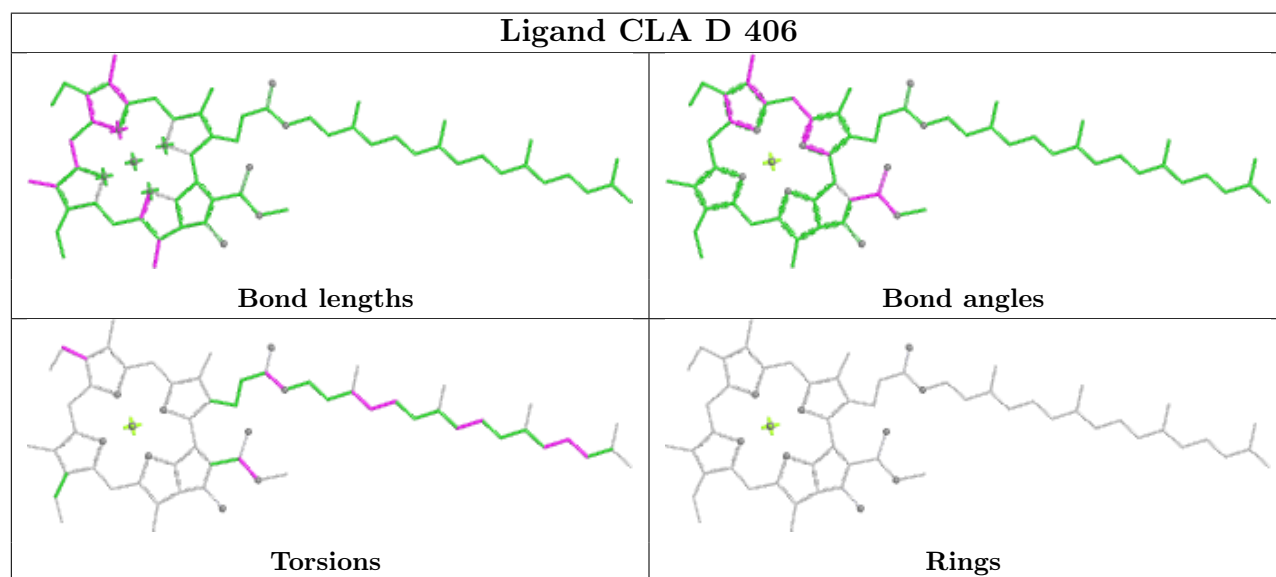
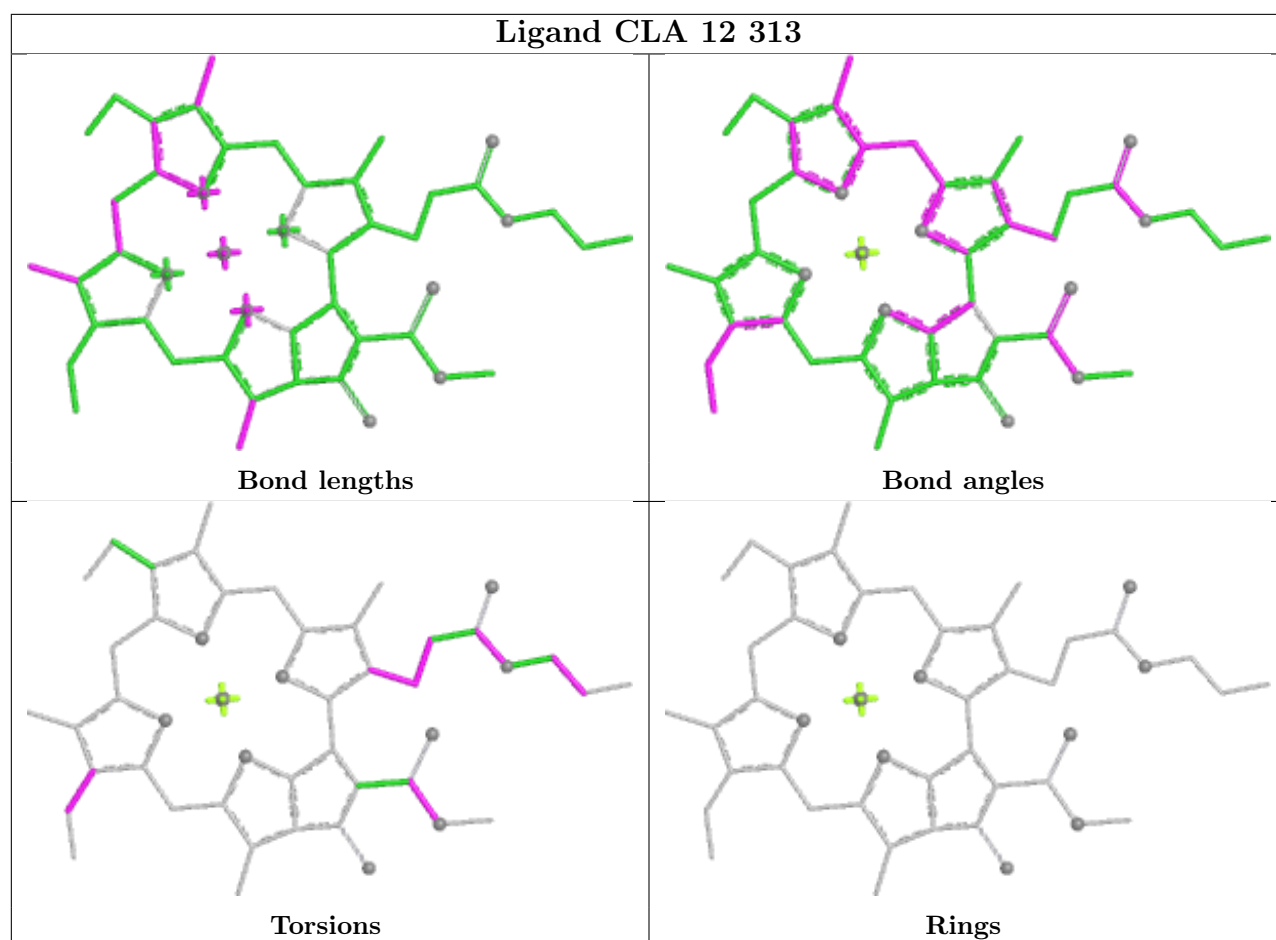




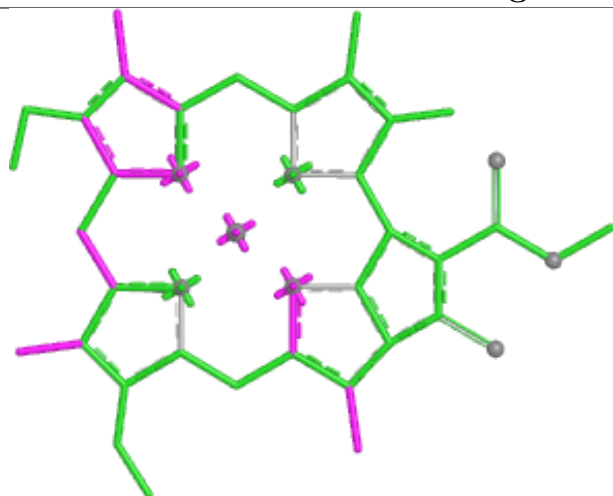




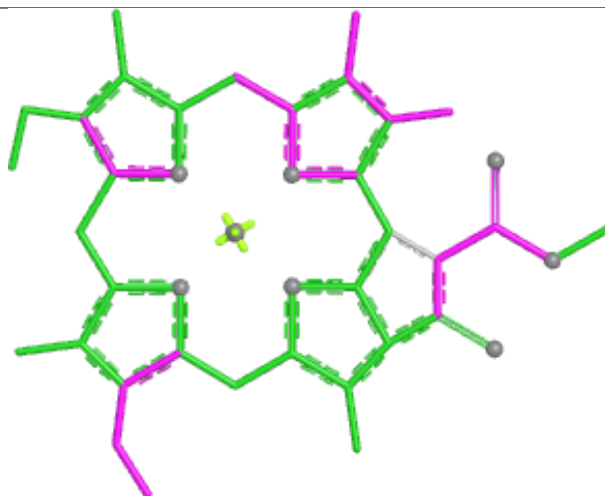




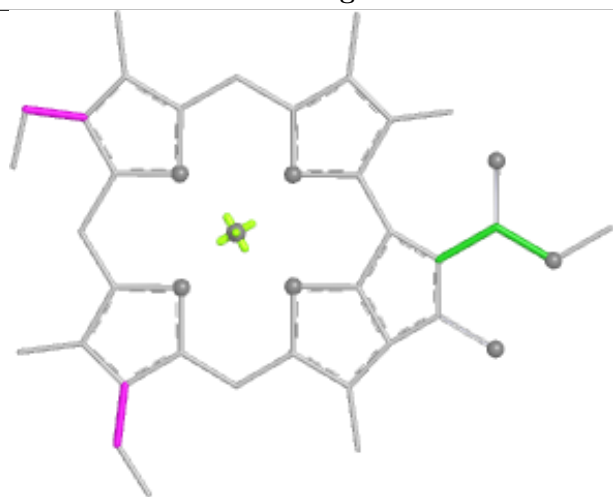
Ligand CLA 17 308



Bond lengths



Bond angles

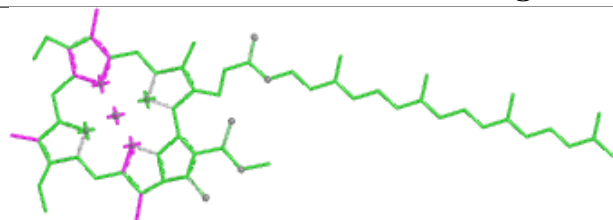


Torsions

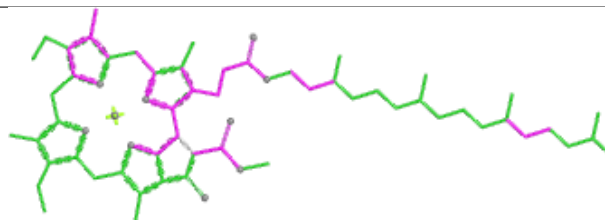


Rings

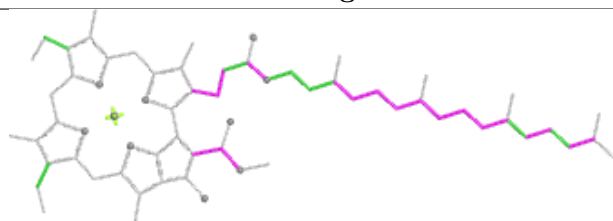
Ligand CLA C 504



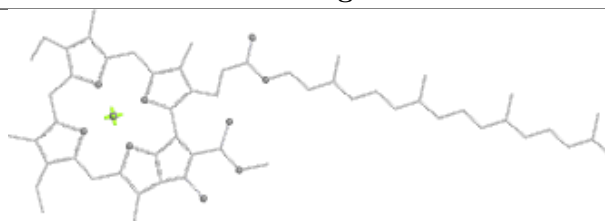
Bond lengths



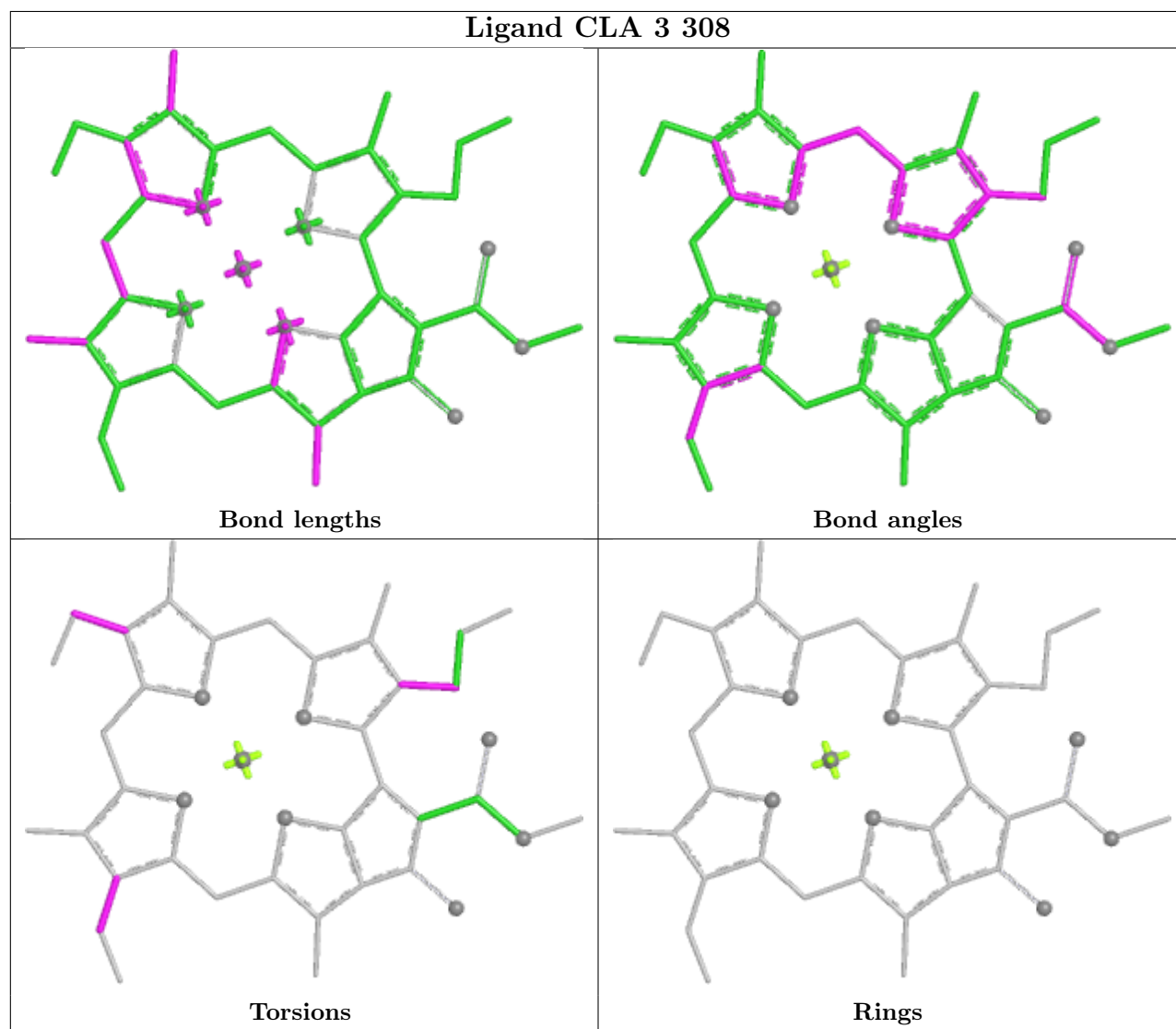
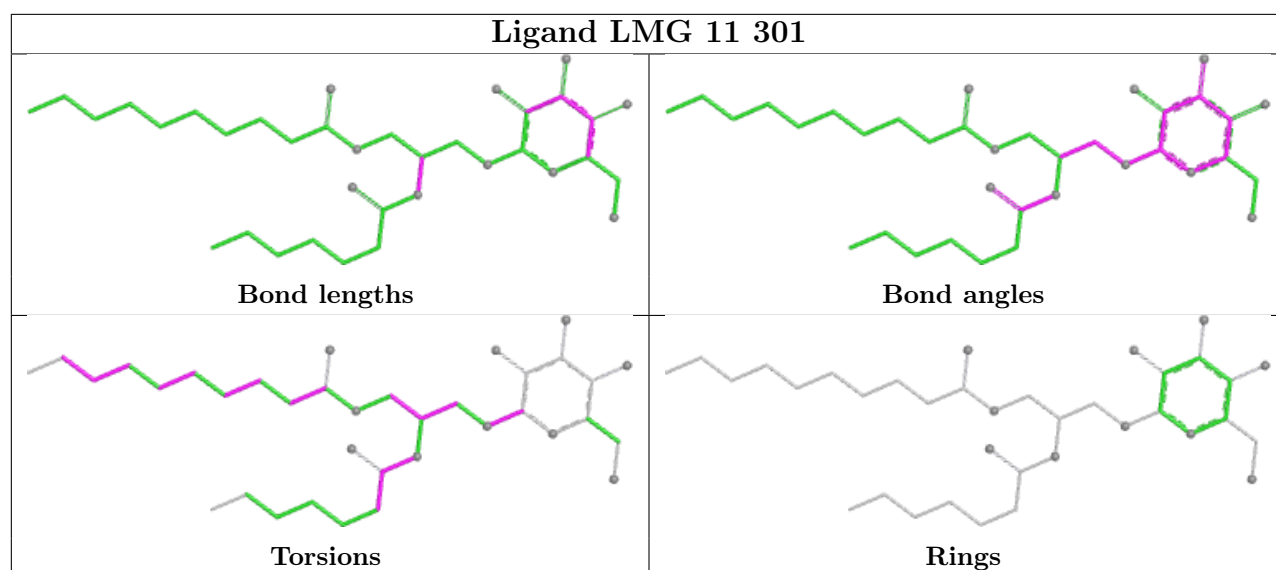
Bond angles

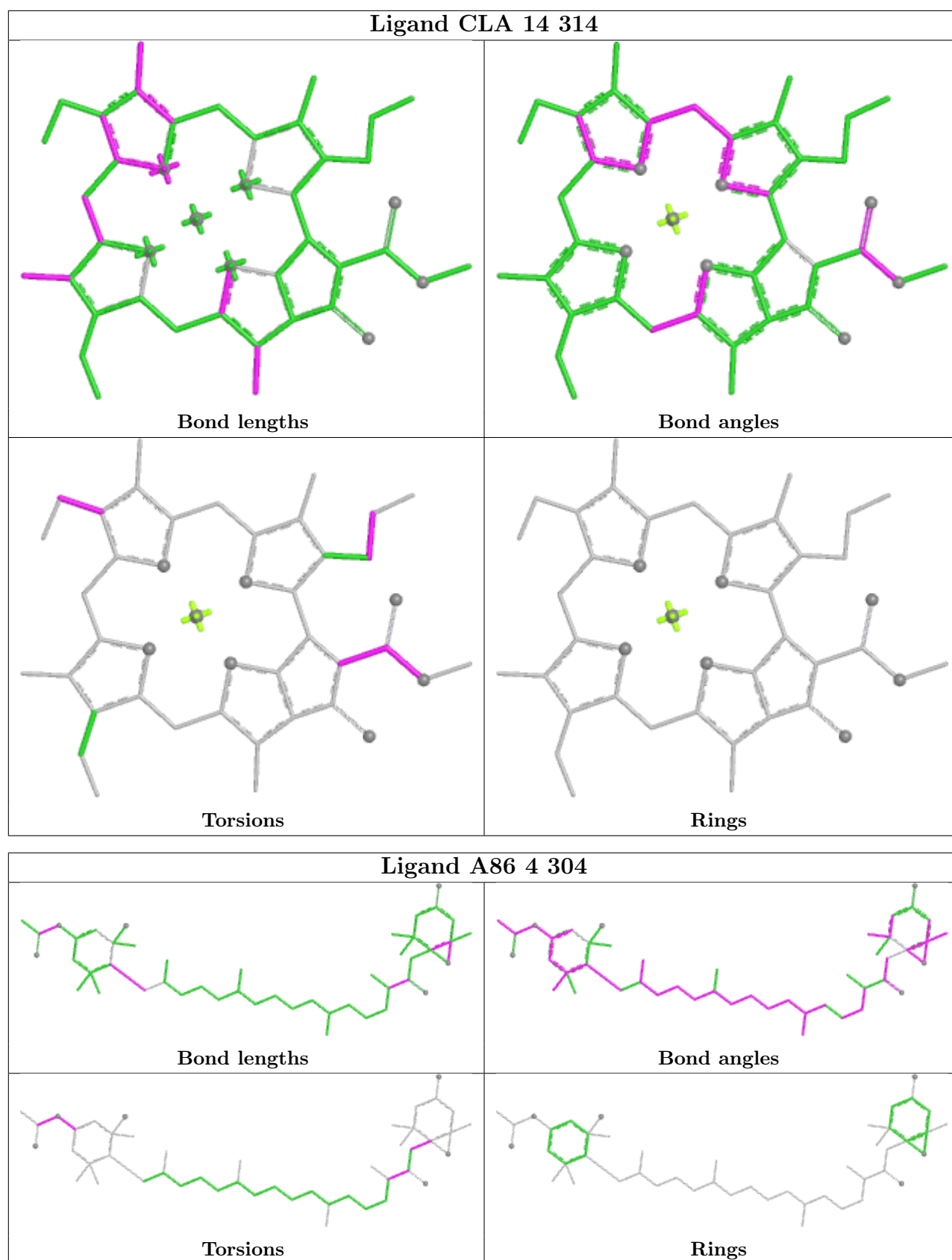


Torsions

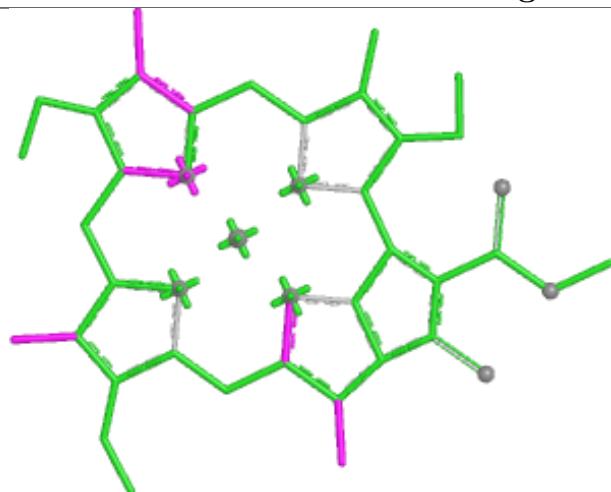


Rings

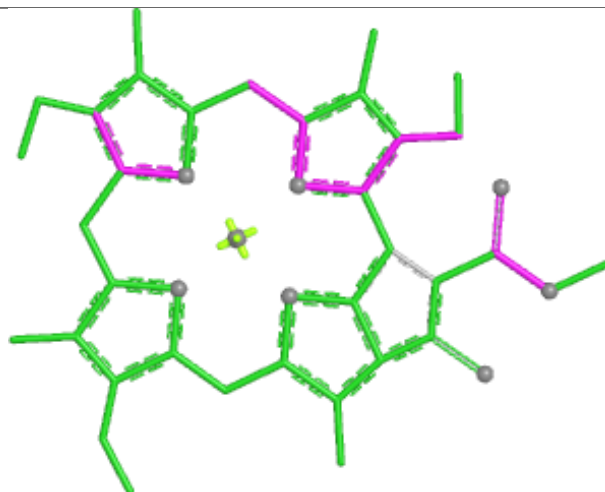




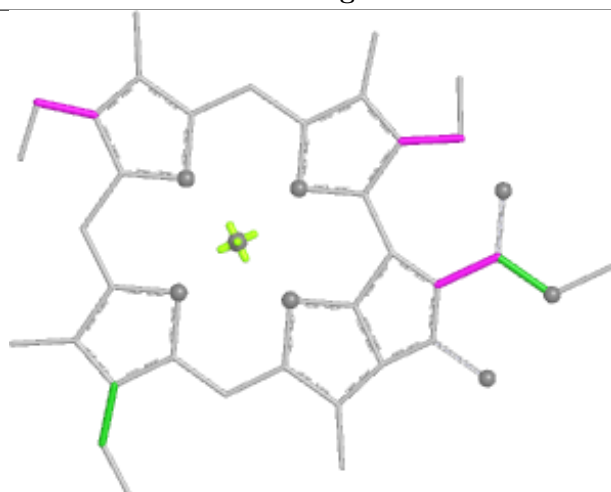
Ligand CLA 1 316



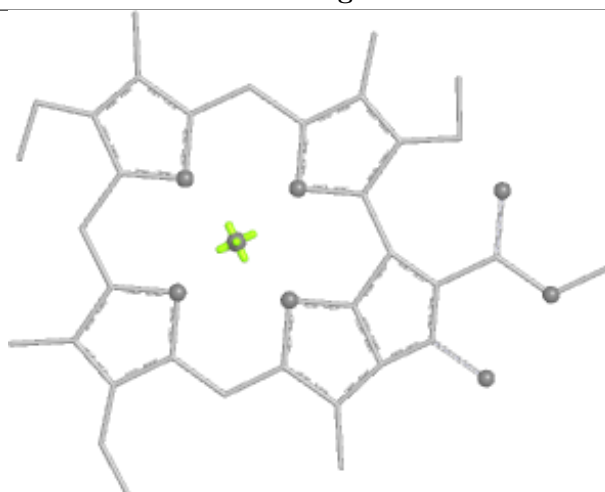
Bond lengths



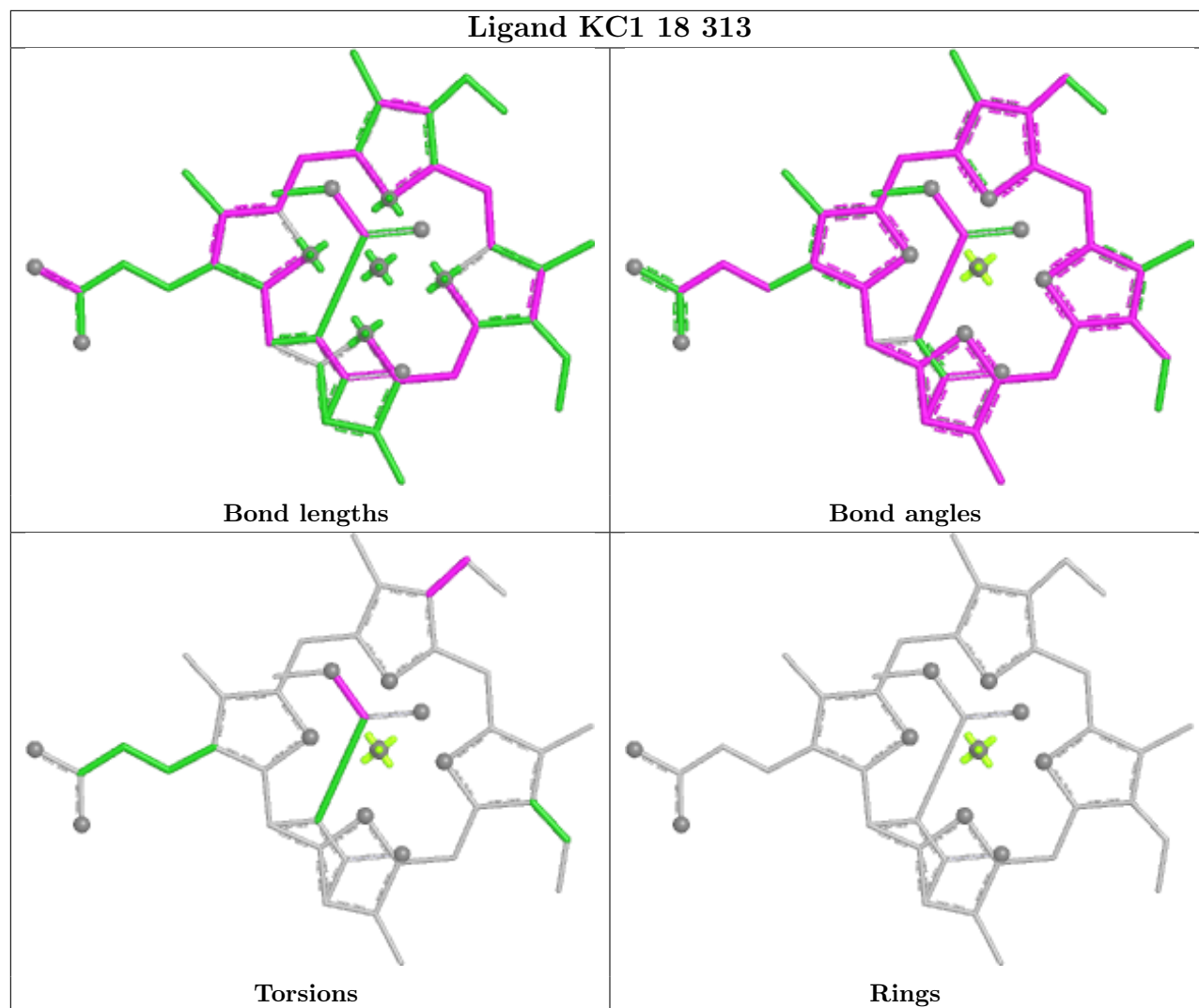
Bond angles



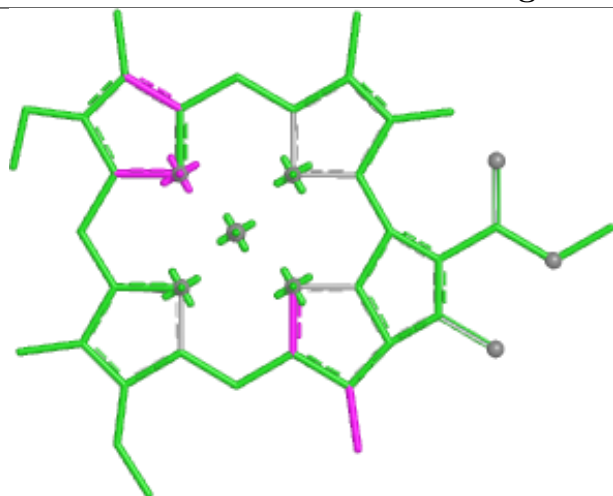
Torsions



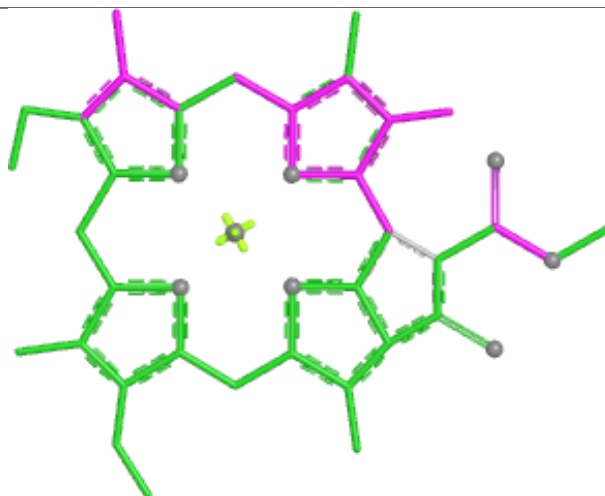
Rings



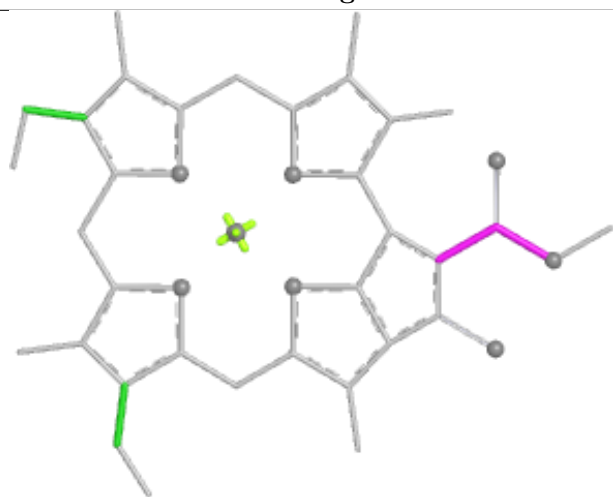
Ligand CLA 6 311



Bond lengths



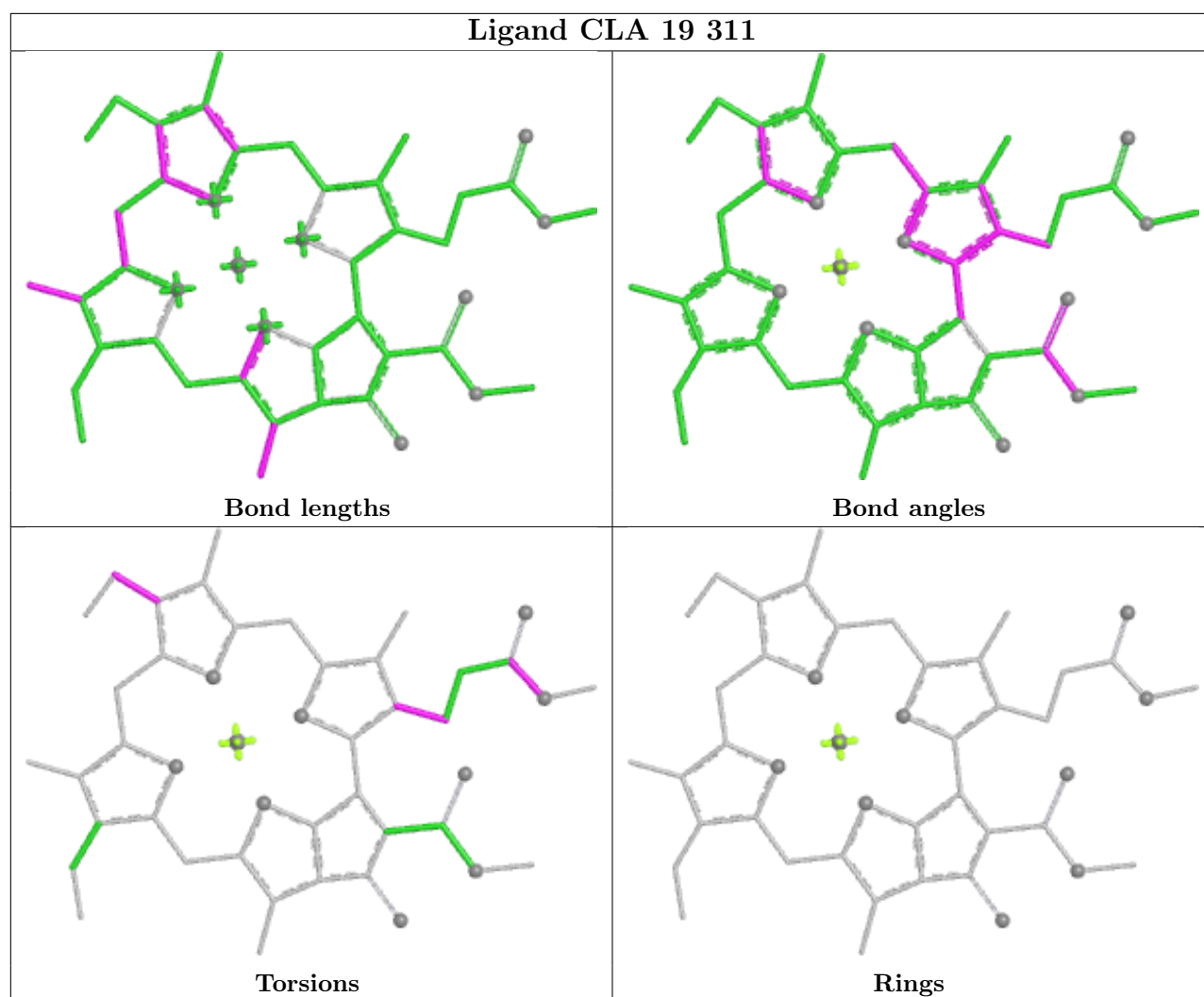
Bond angles



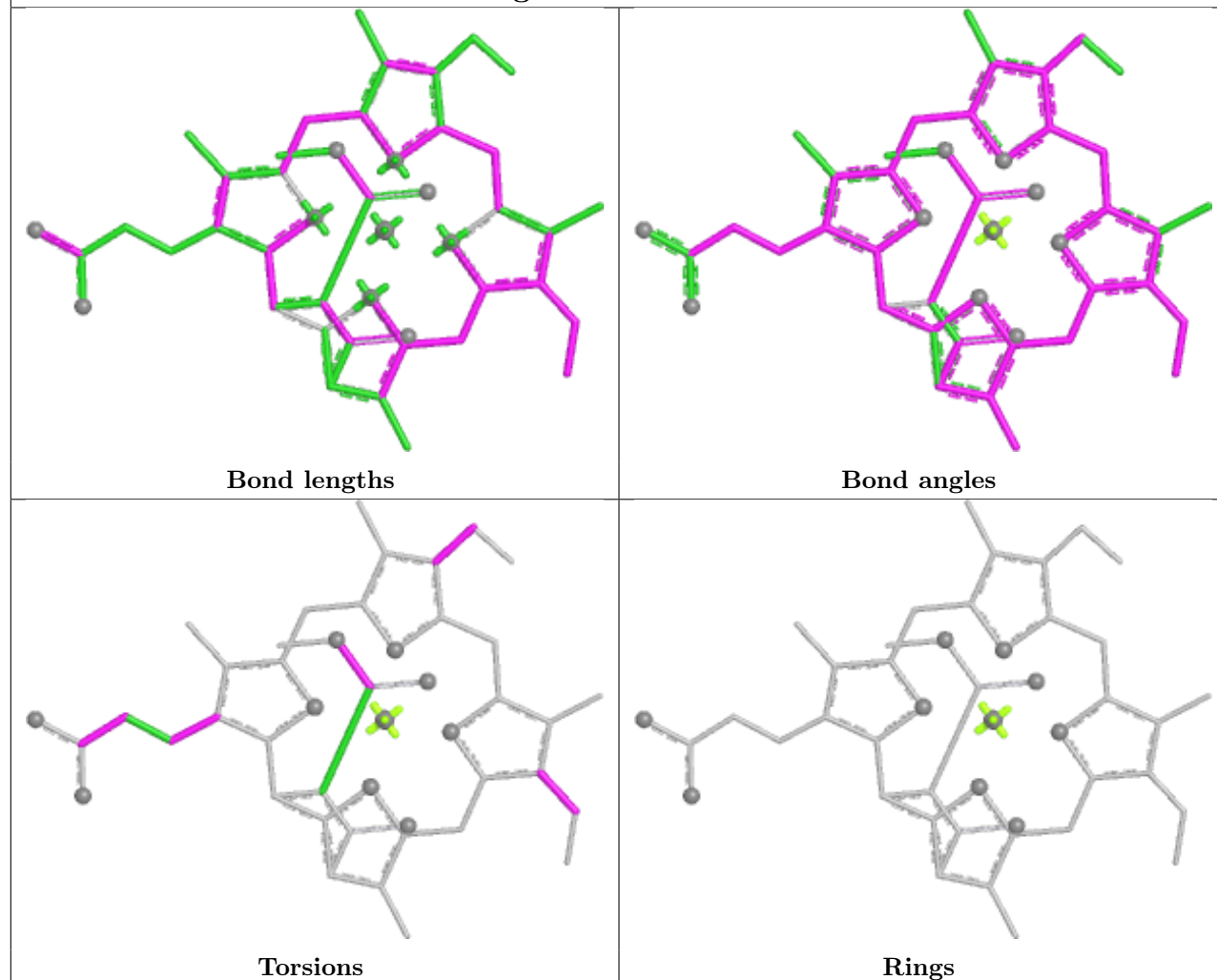
Torsions



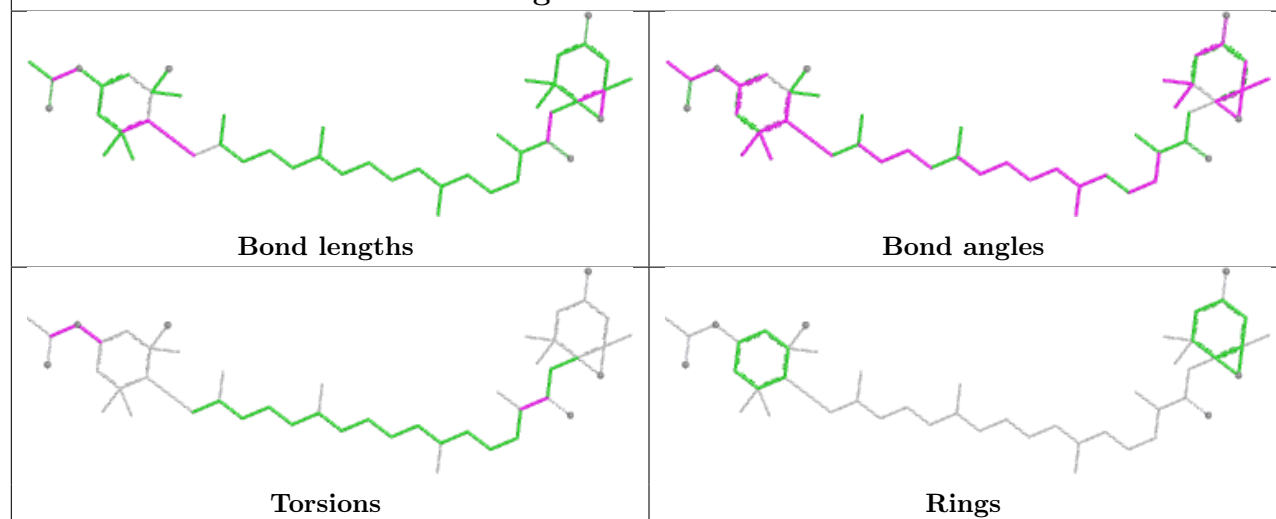
Rings

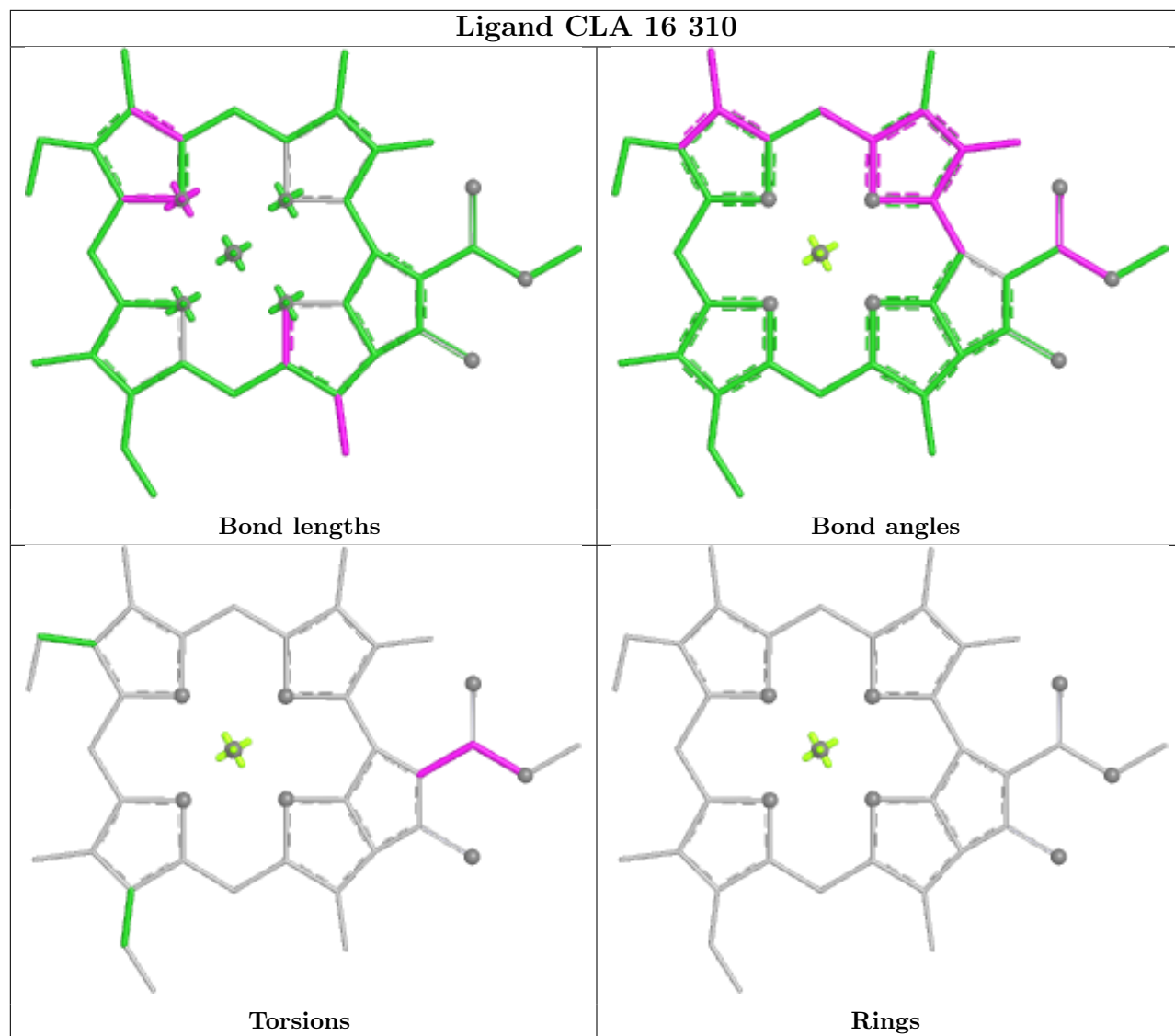


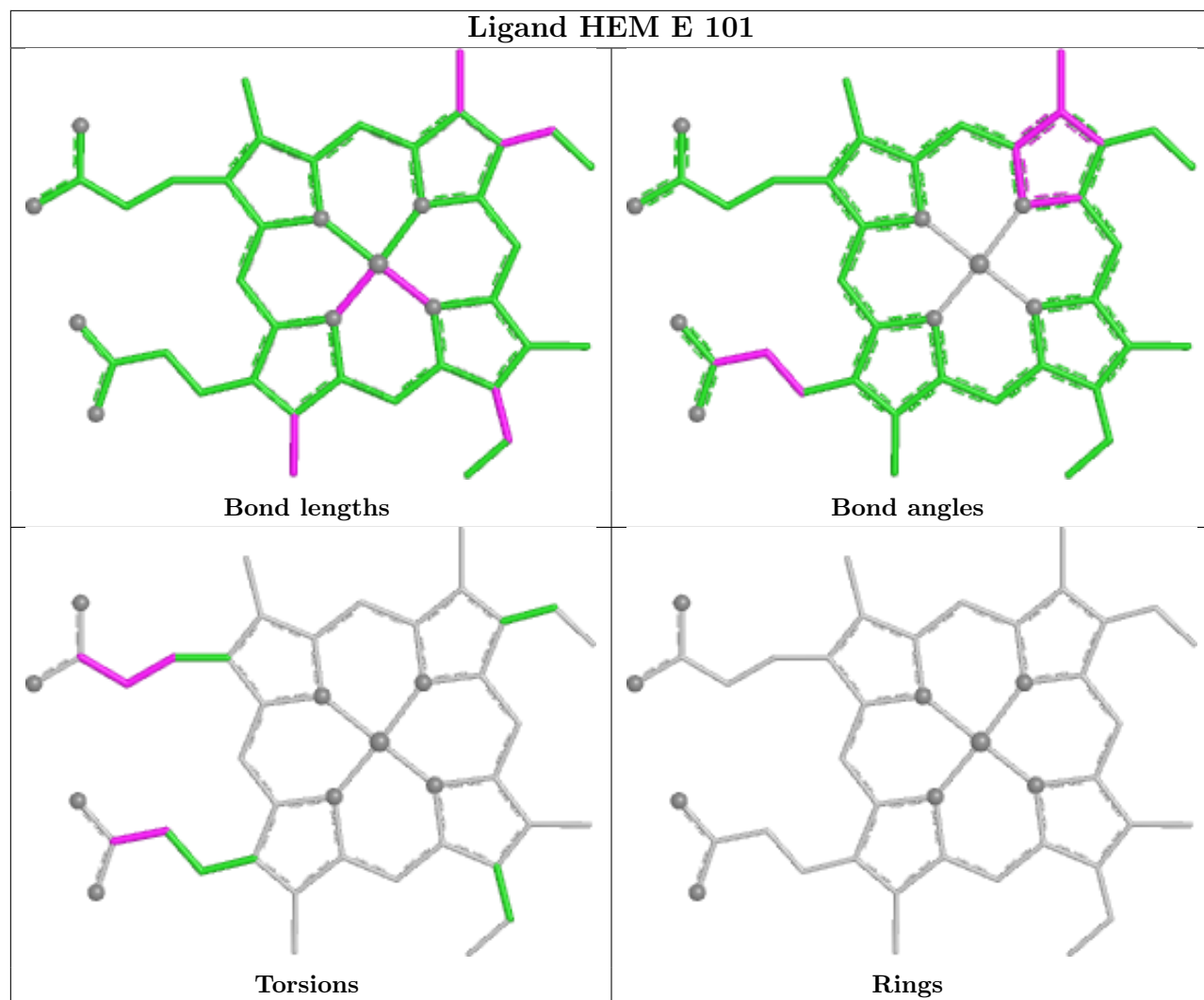
Ligand KC2 3 309

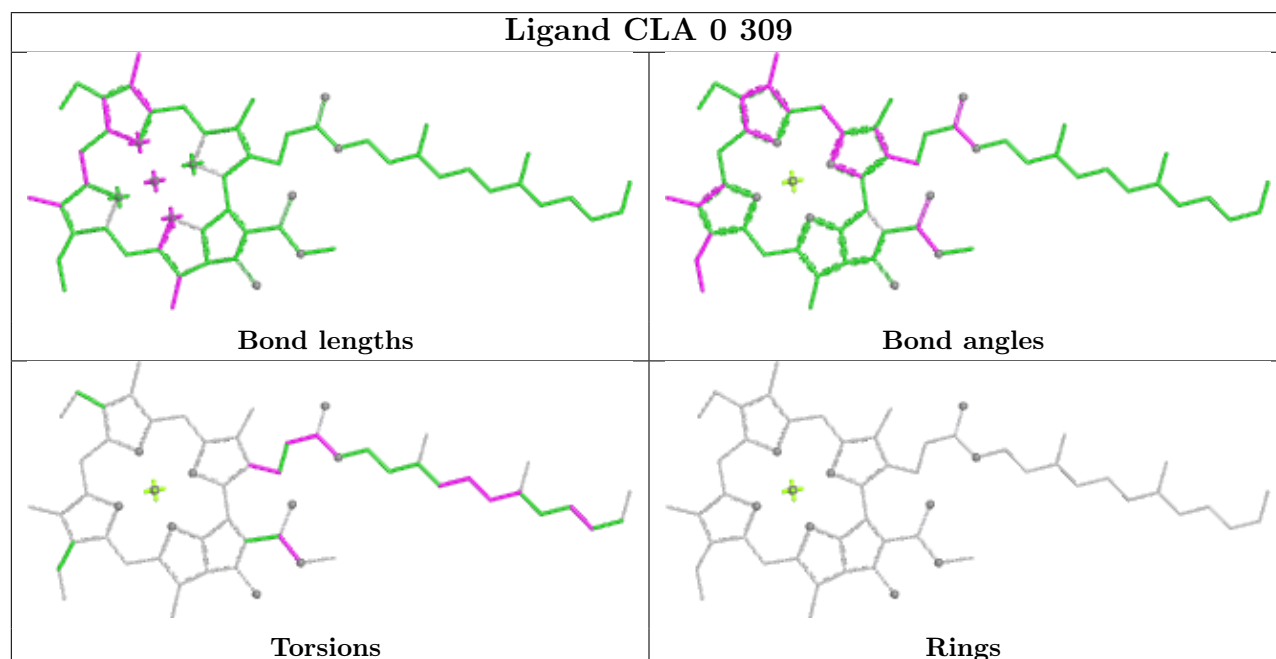
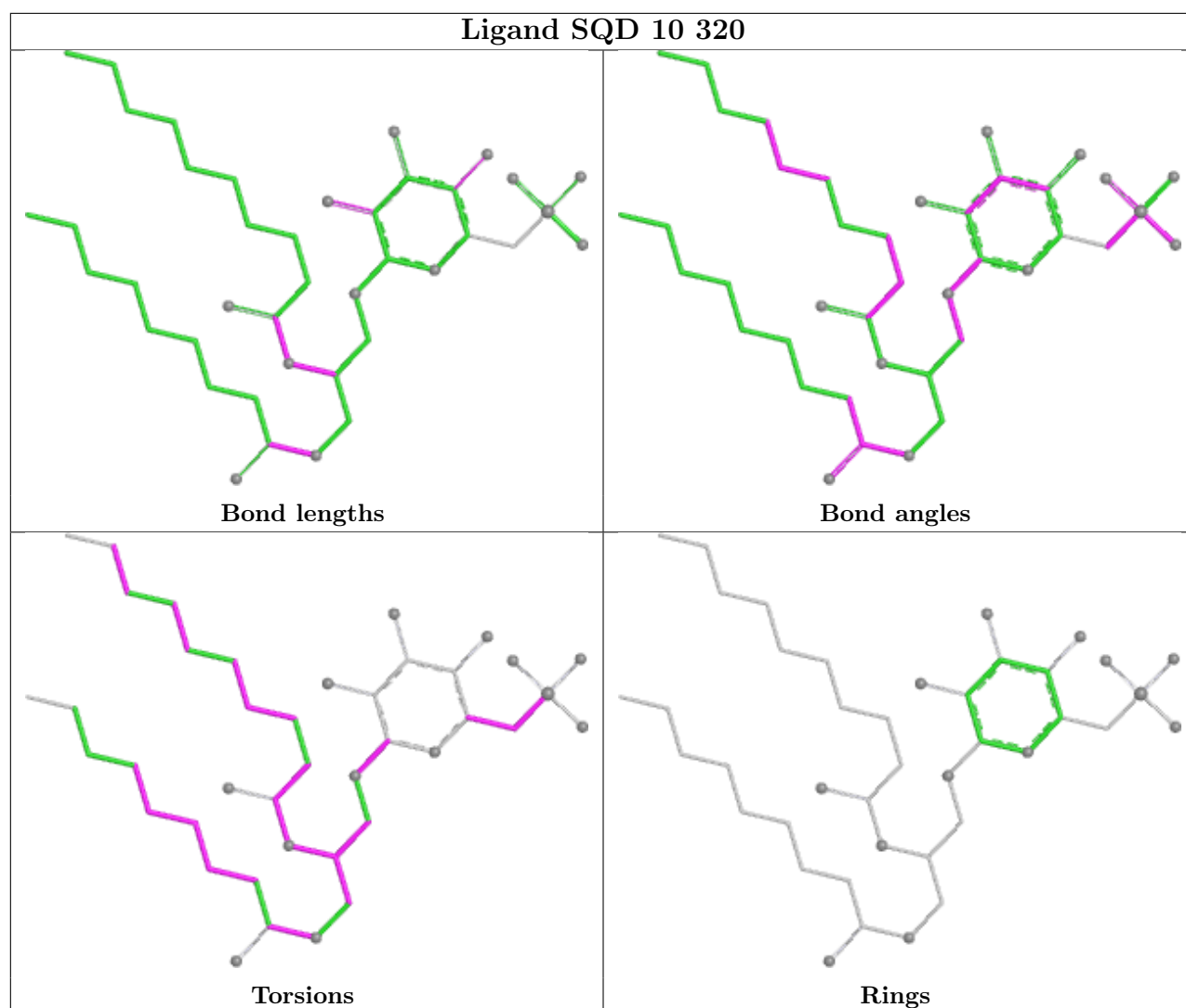


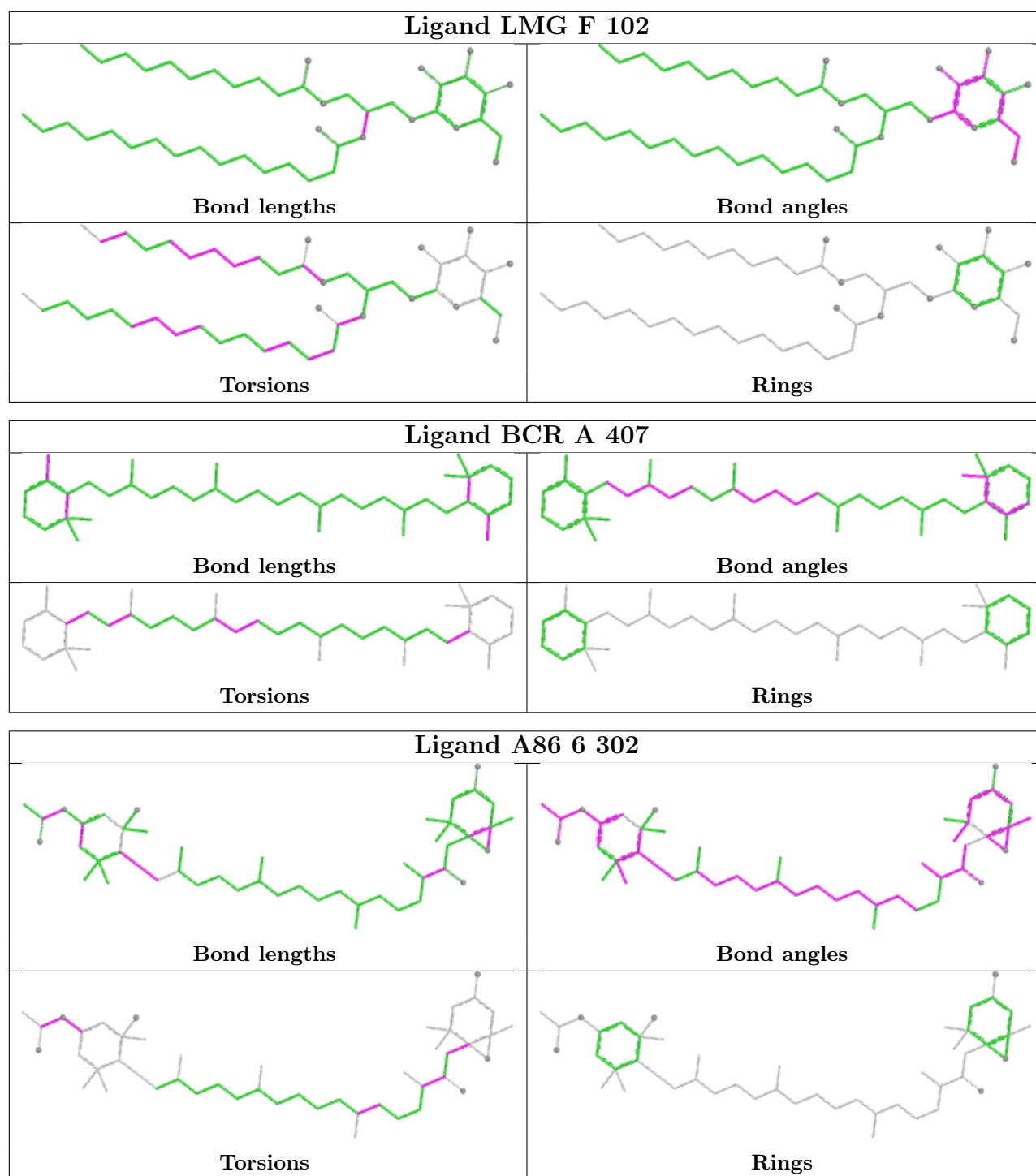
Ligand A86 15 305

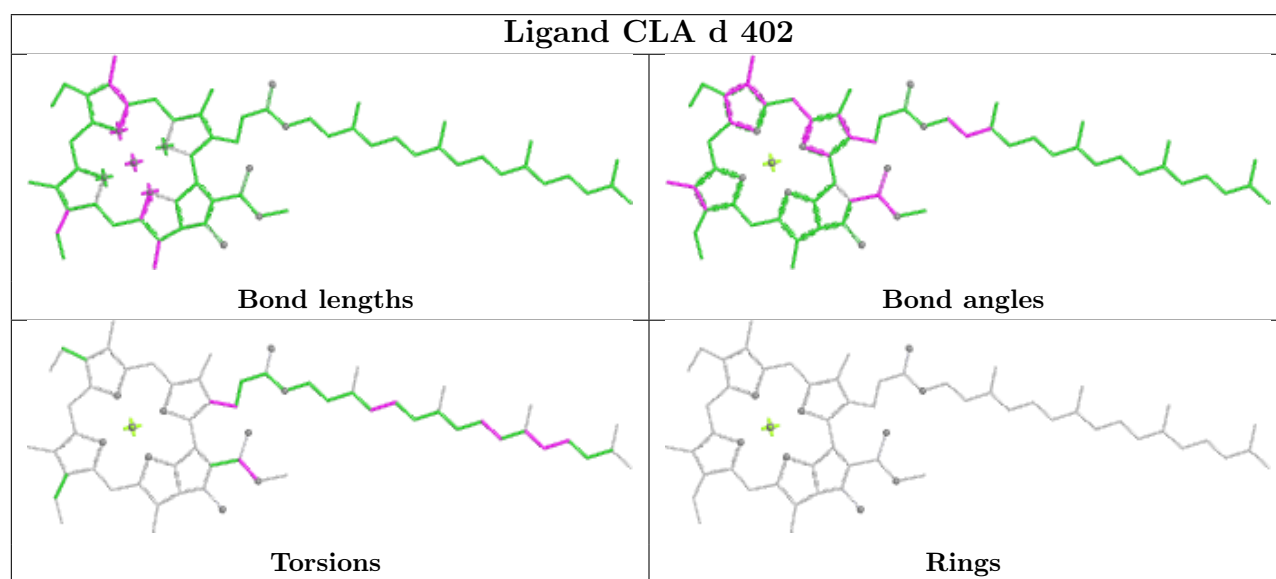
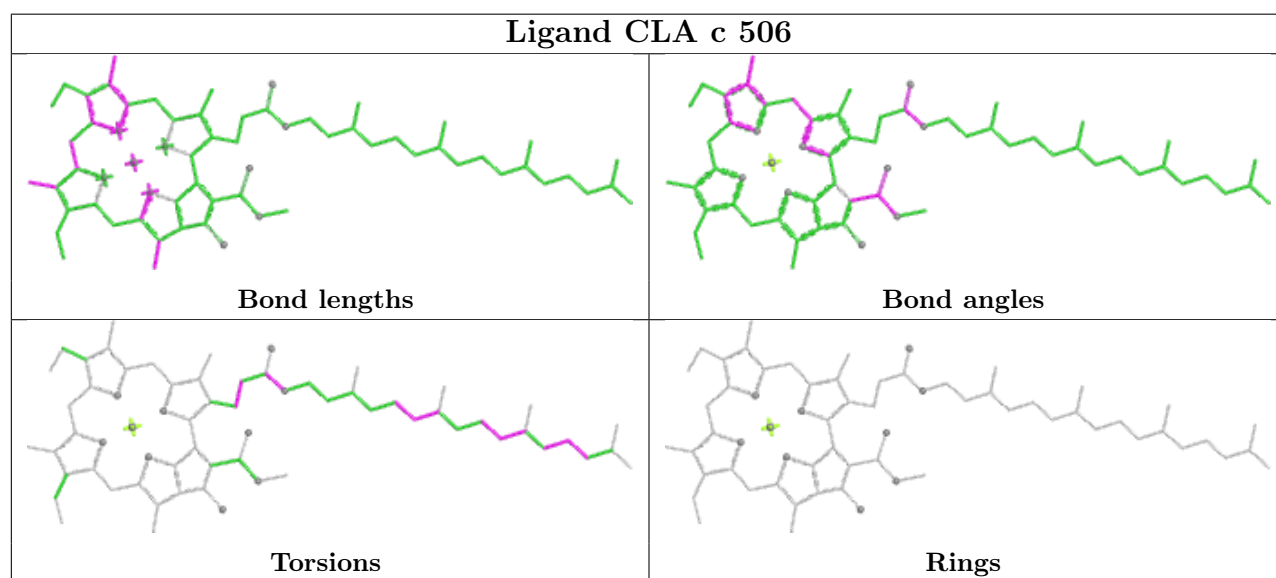
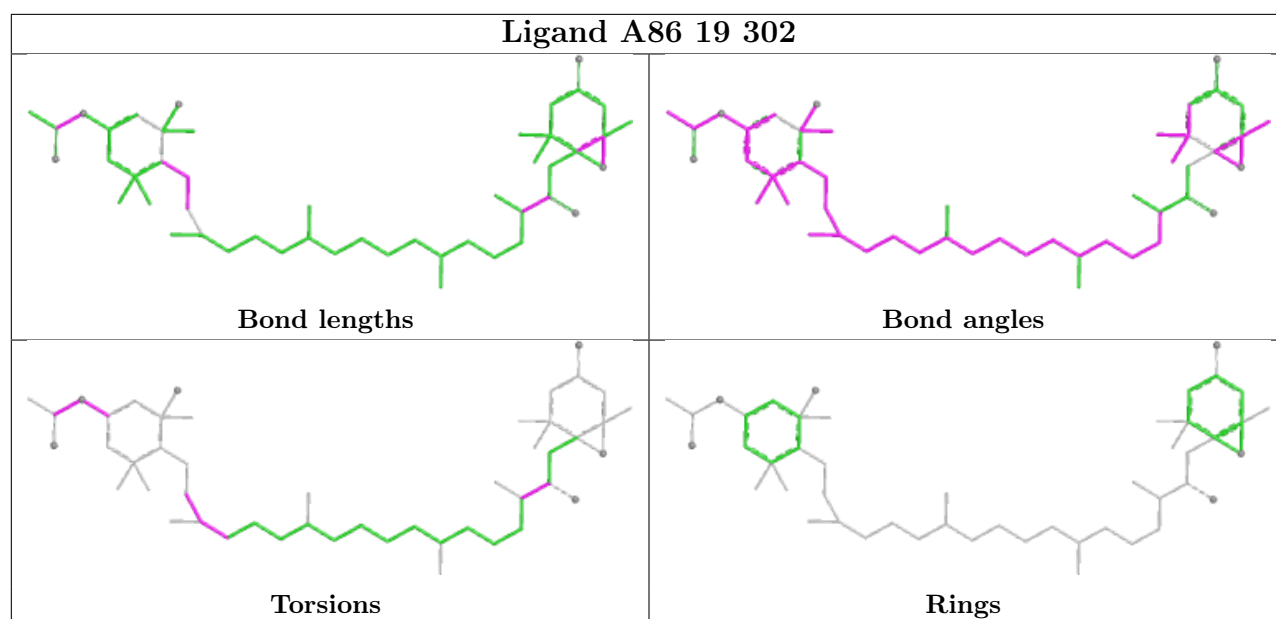


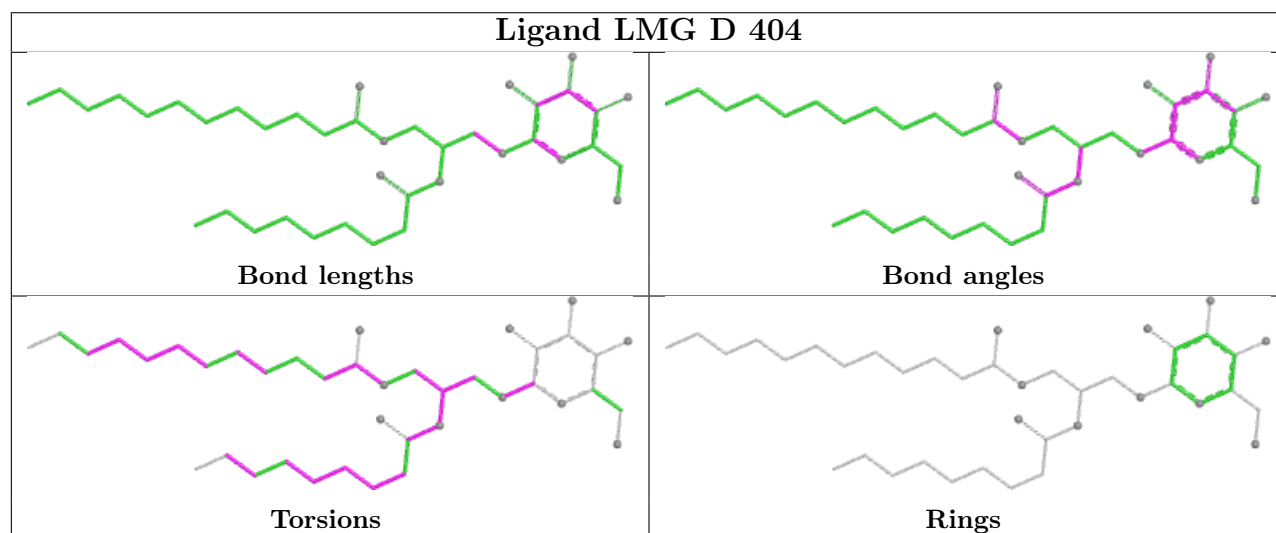
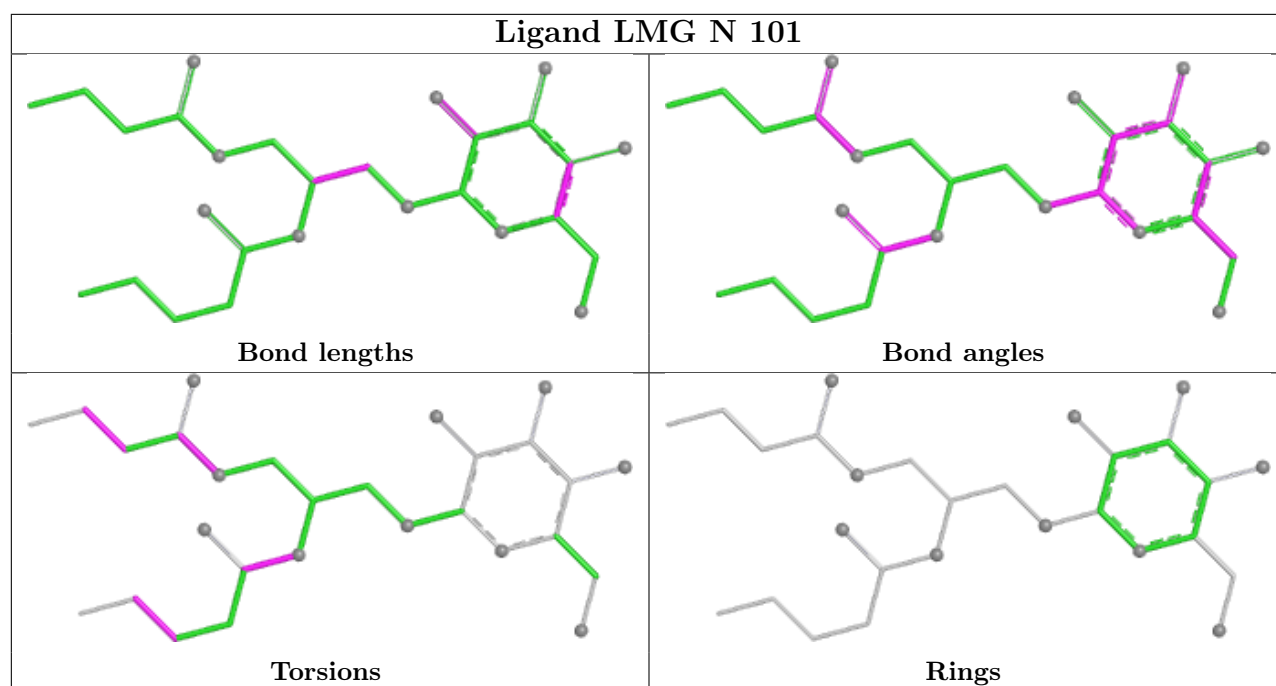


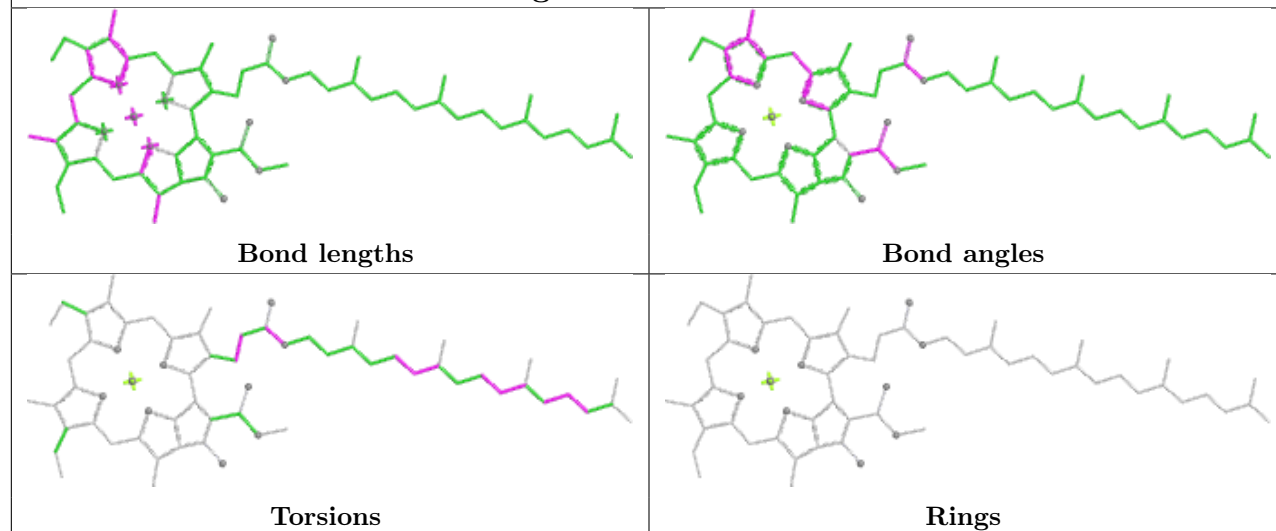
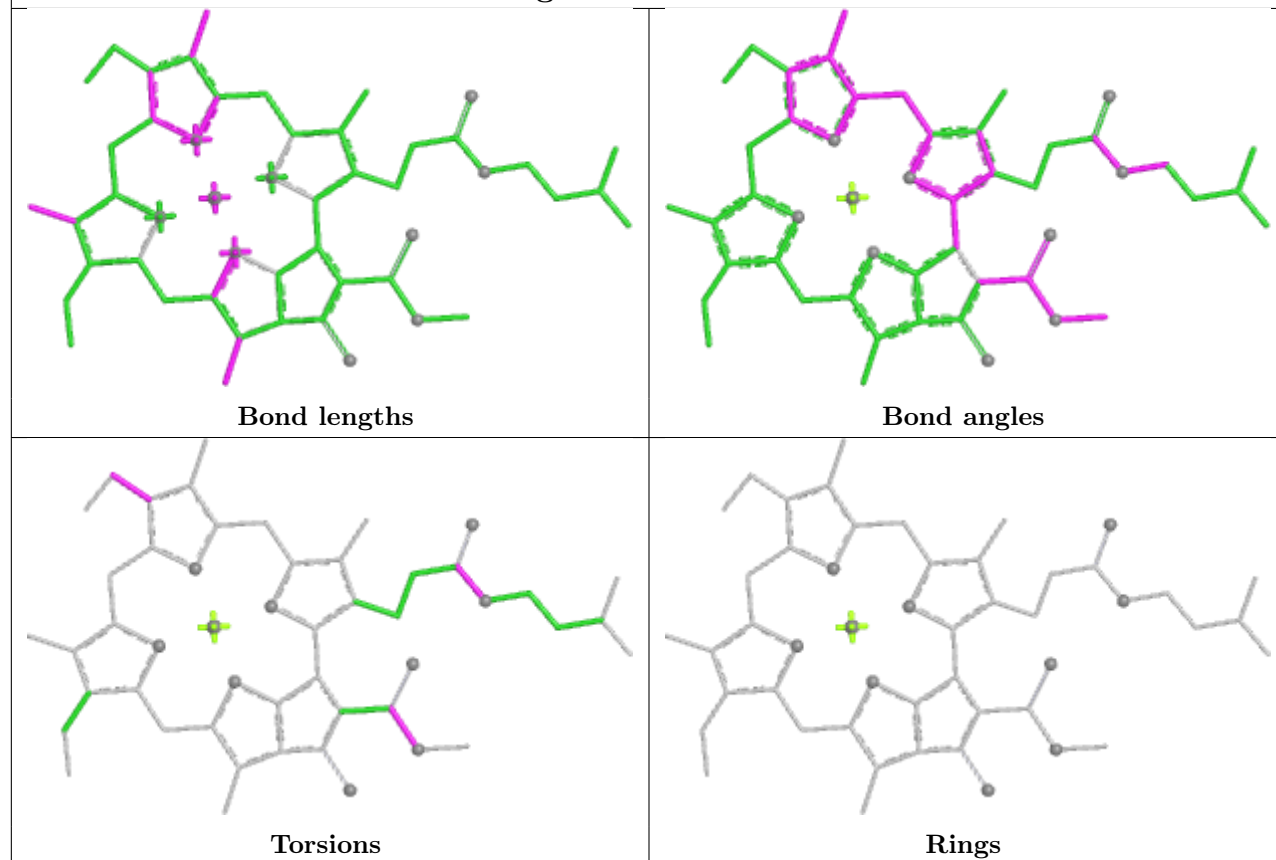


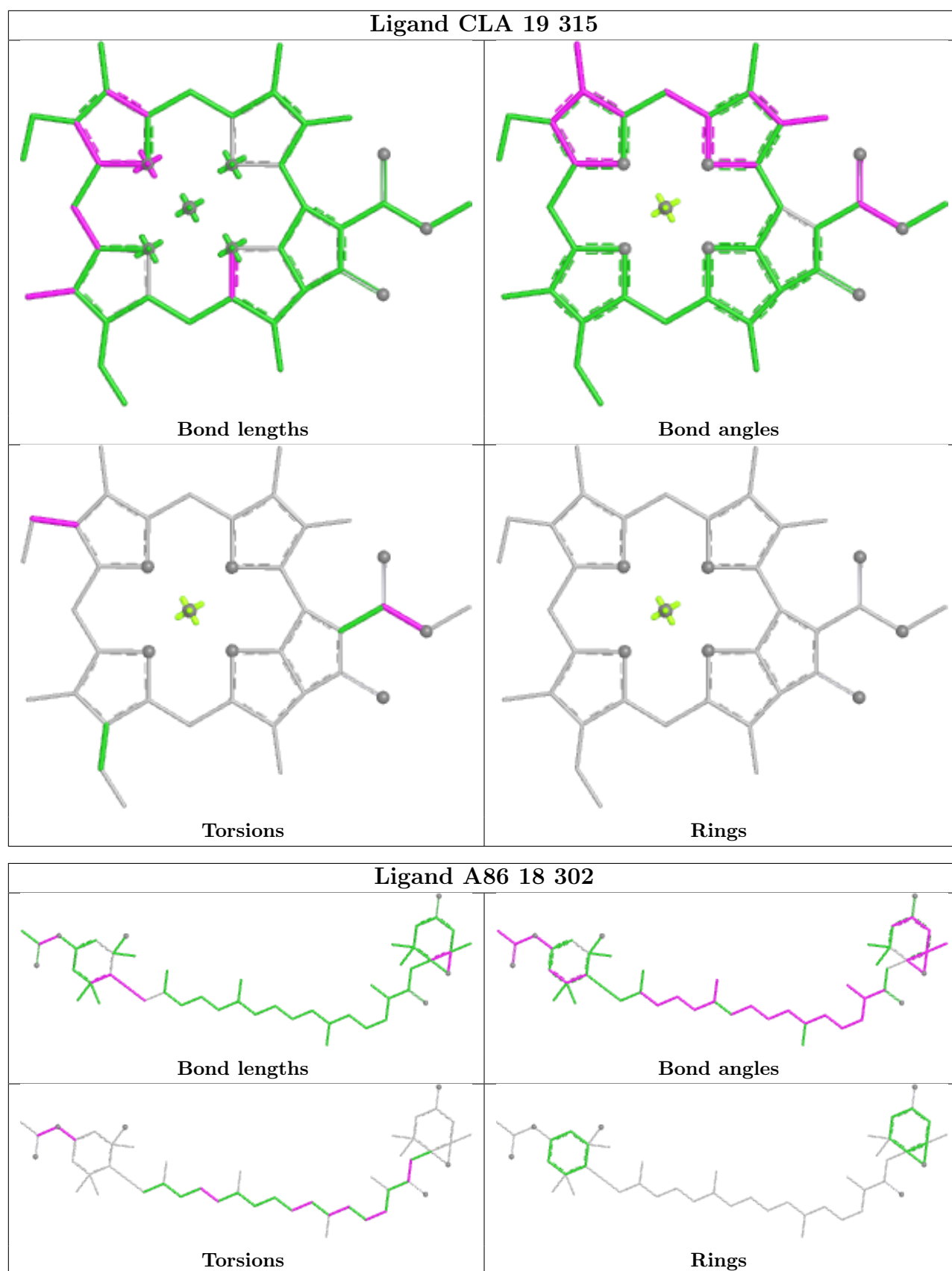


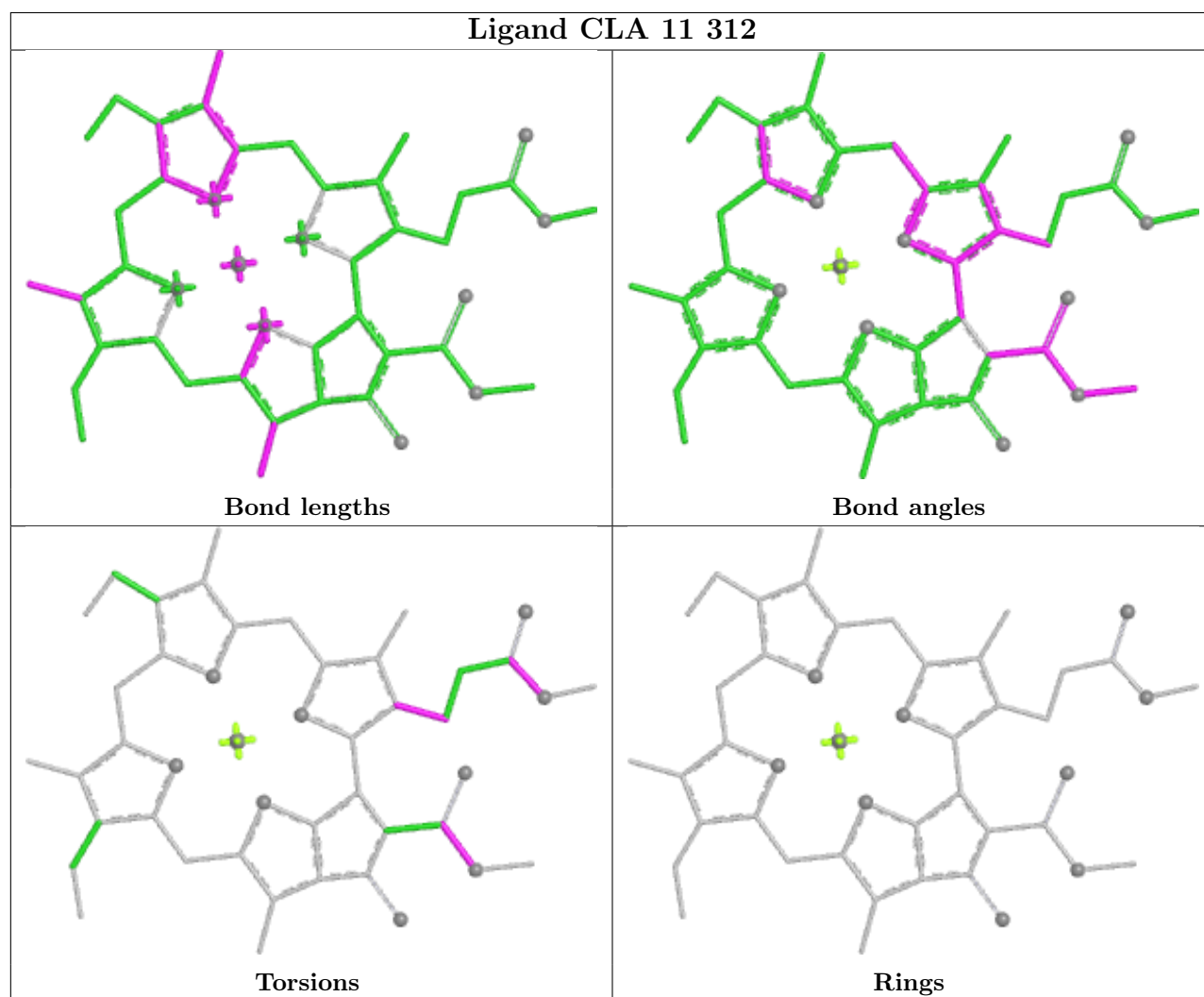
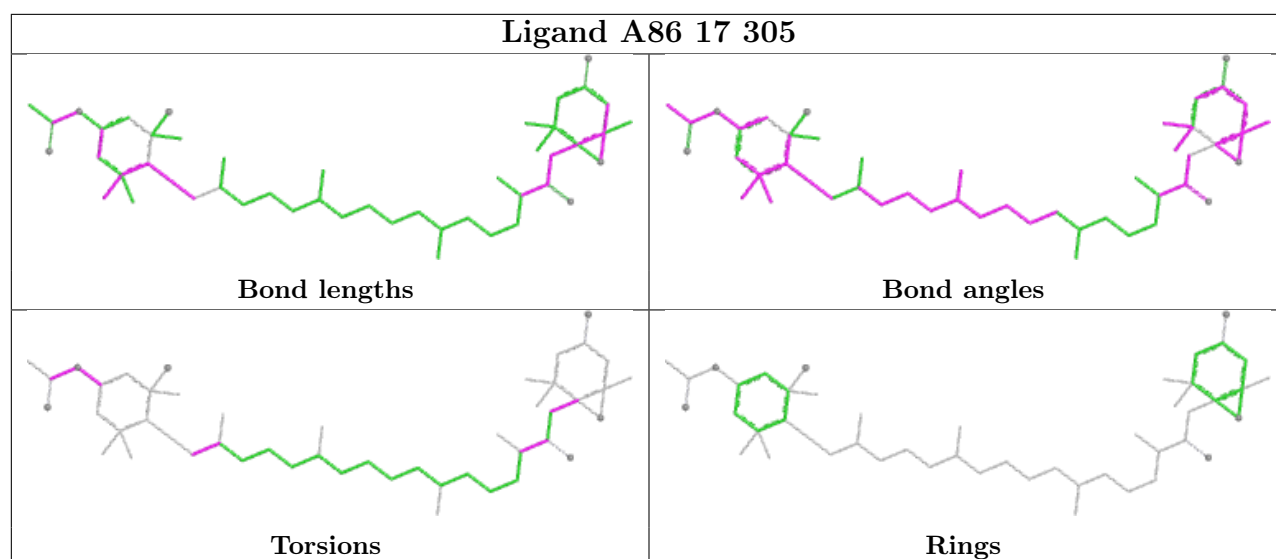




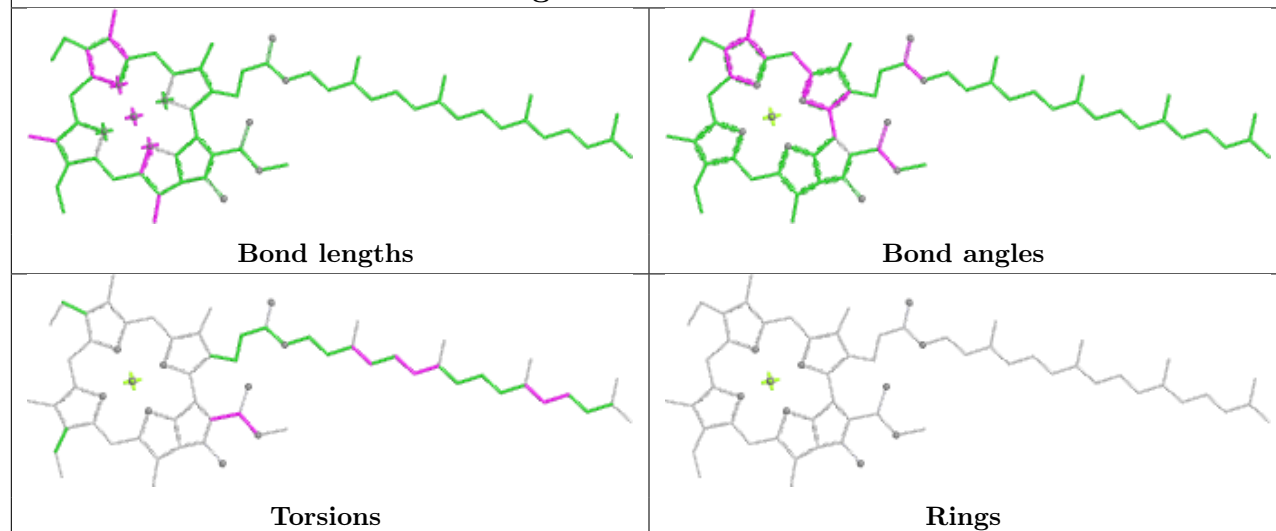


Ligand CLA C 506**Ligand CLA 8 307**

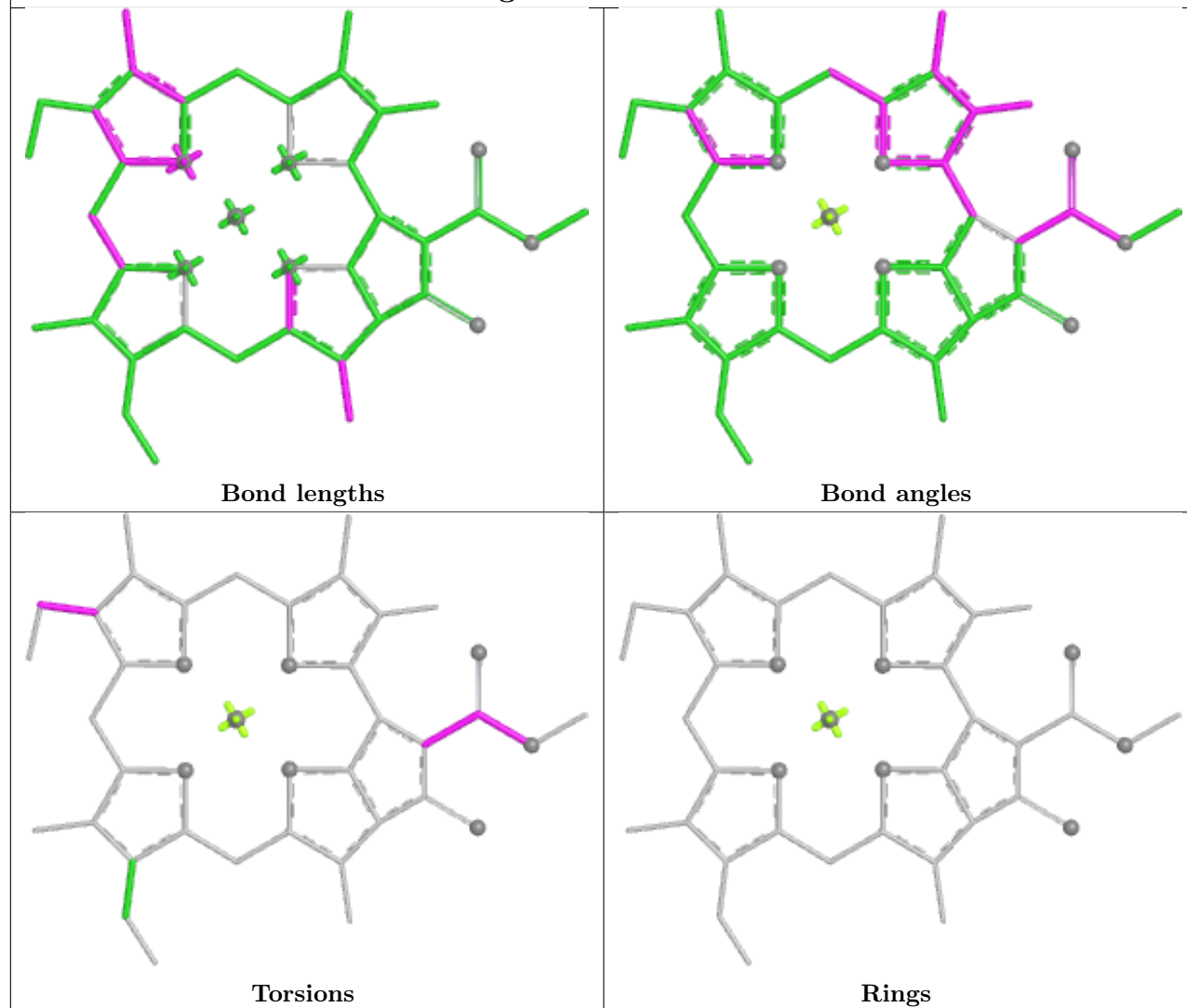


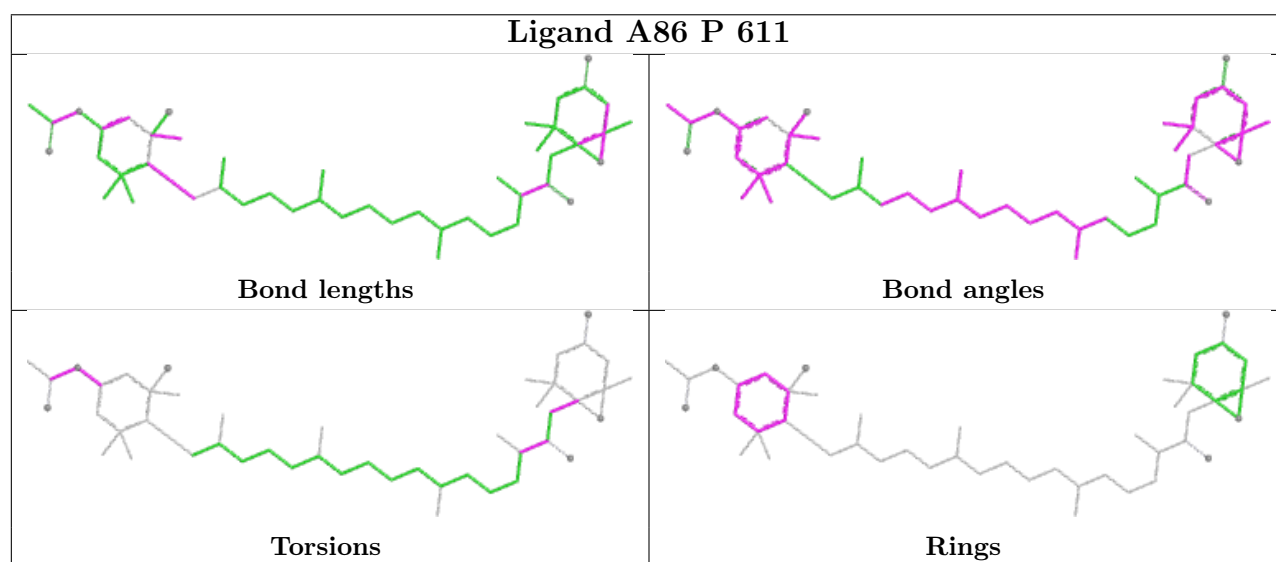
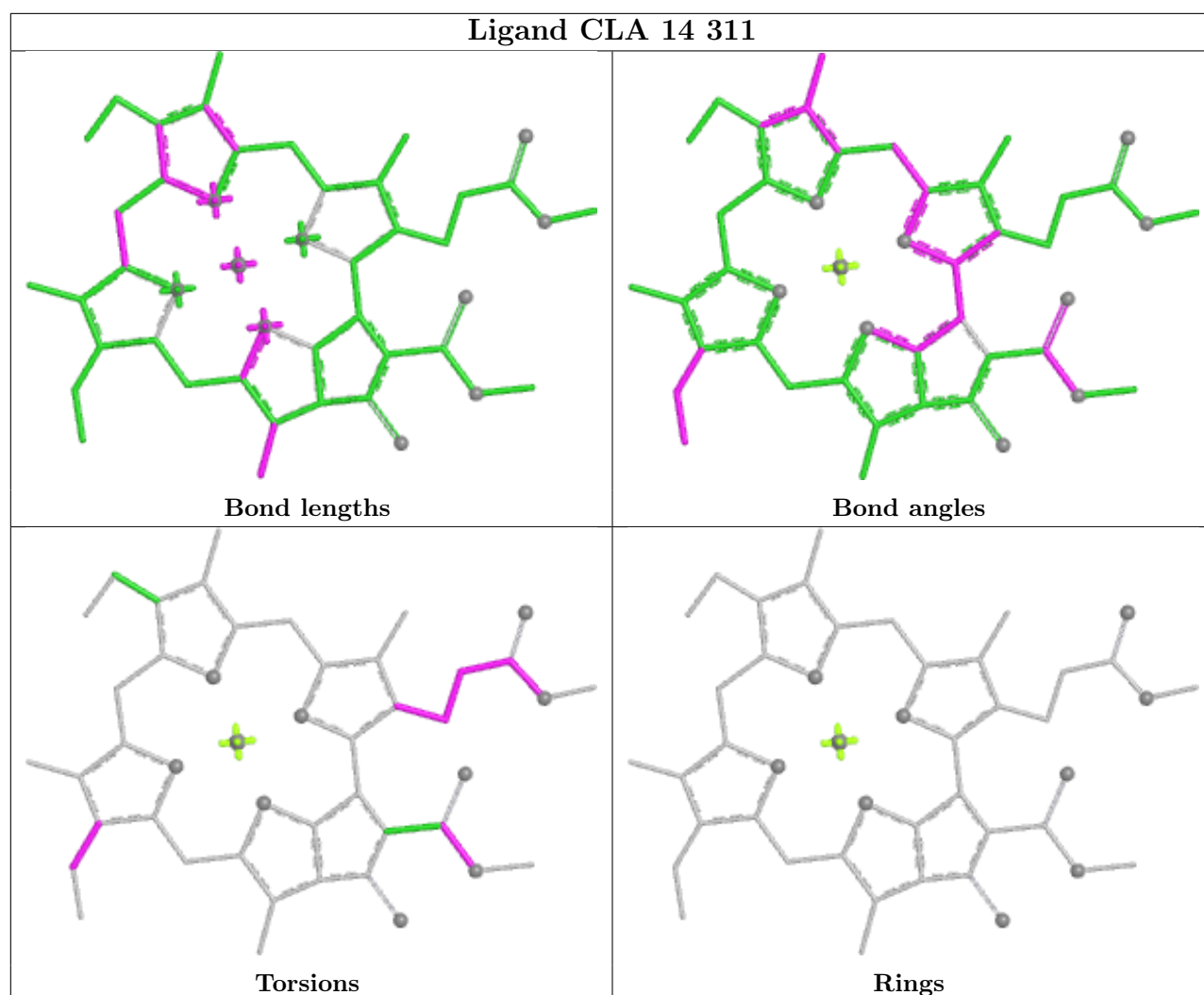


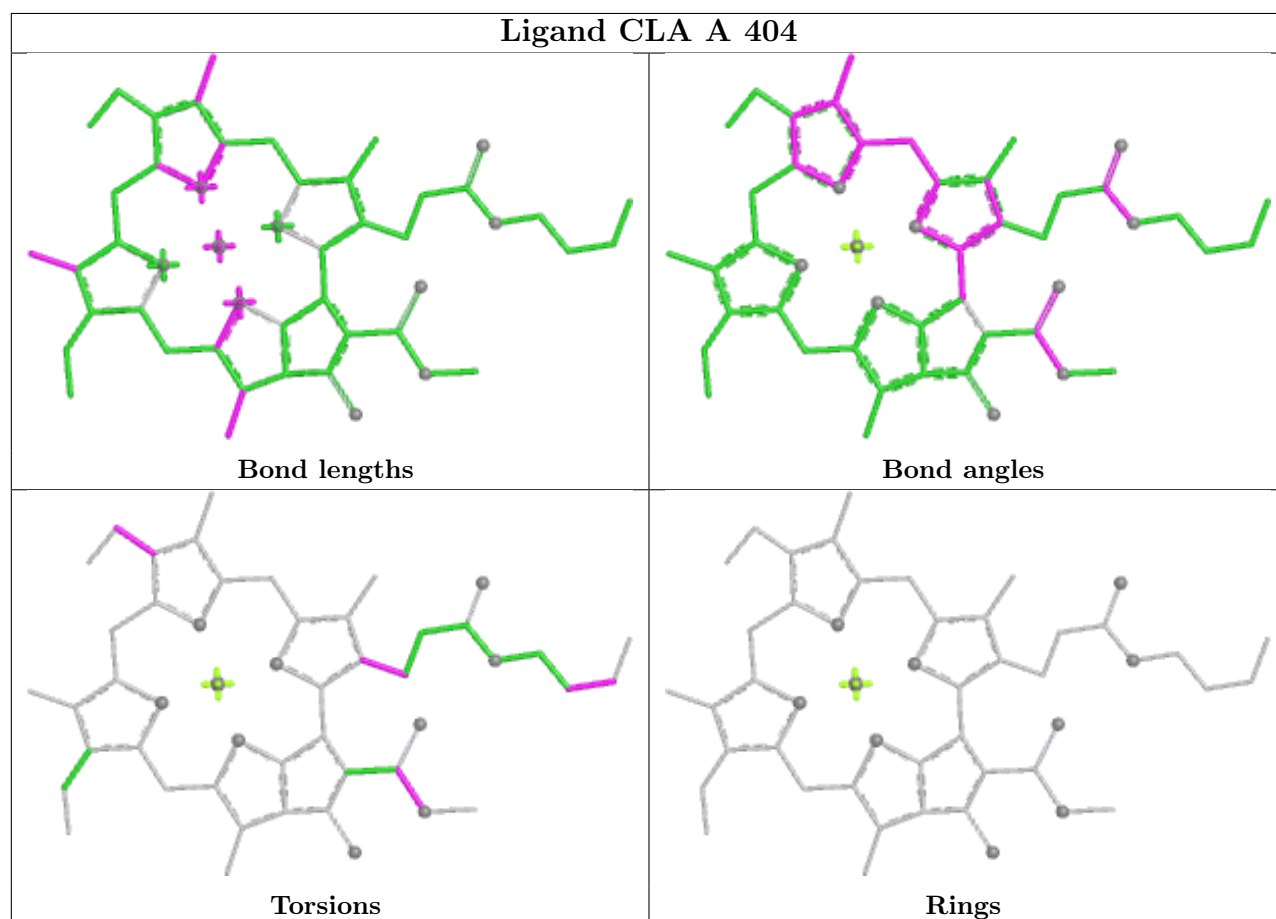
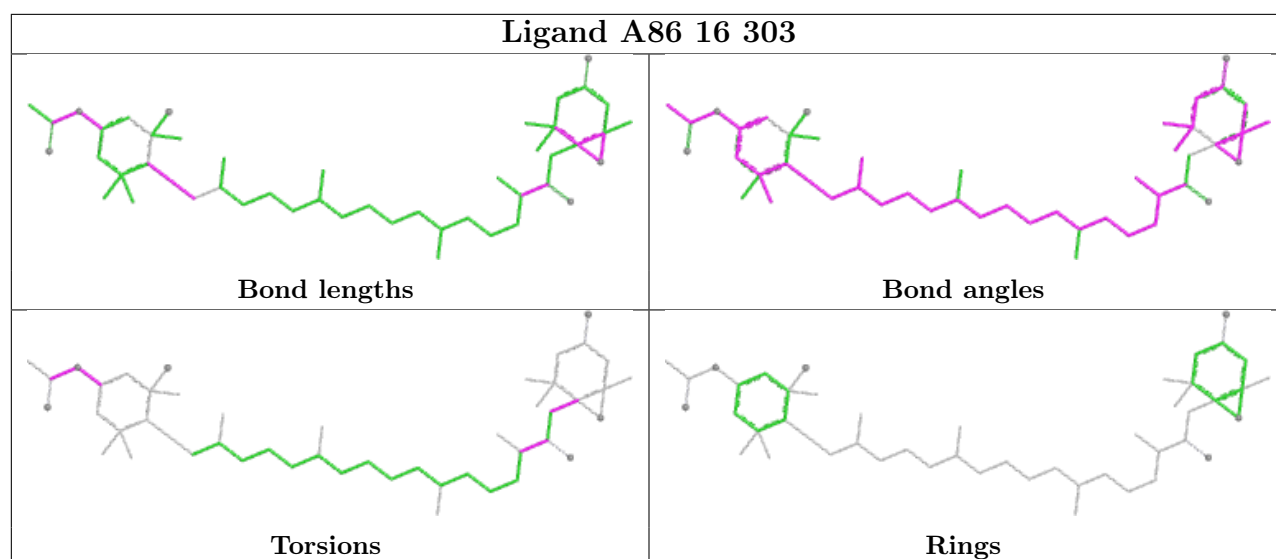
Ligand CLA B 609

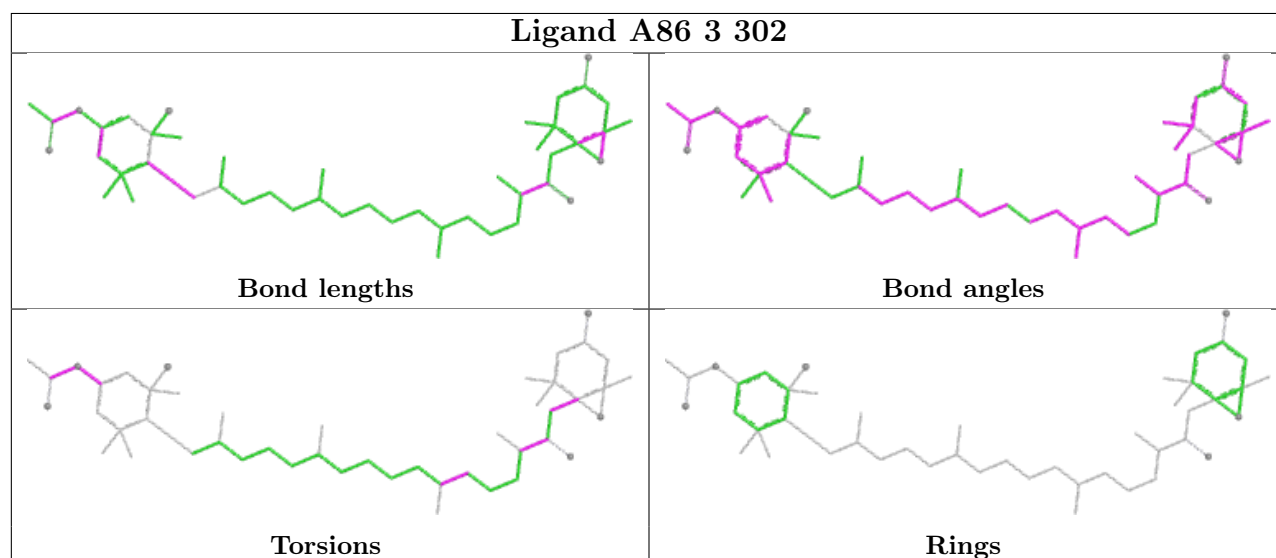
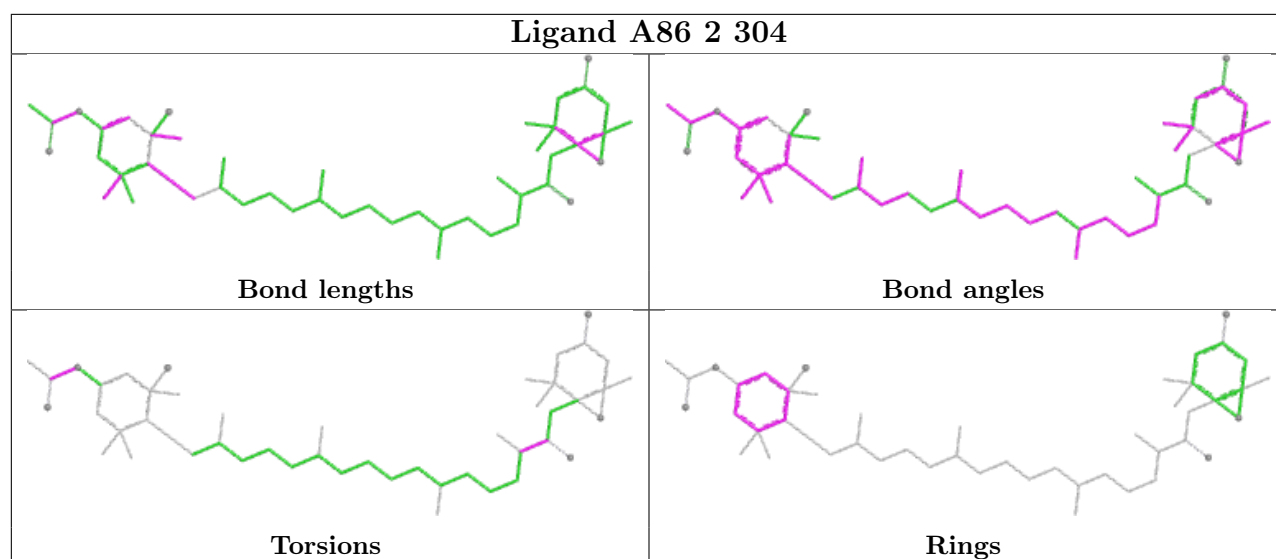


Ligand CLA 2 314

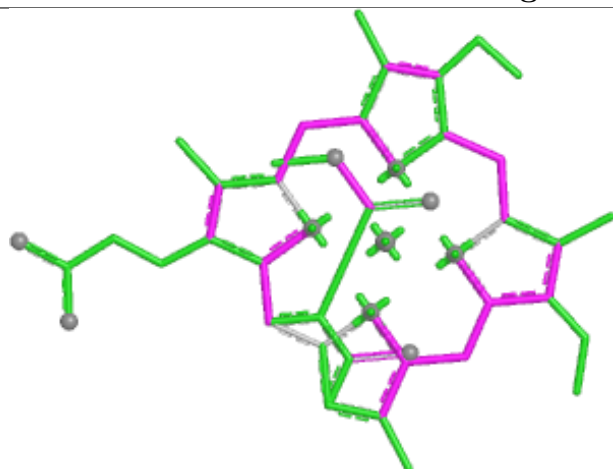




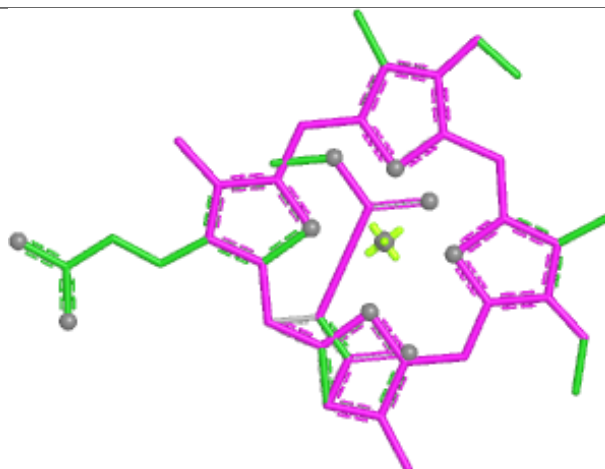




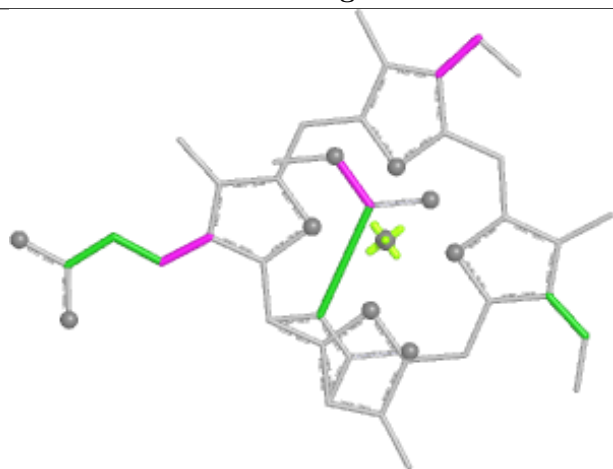
Ligand KC1 2 313



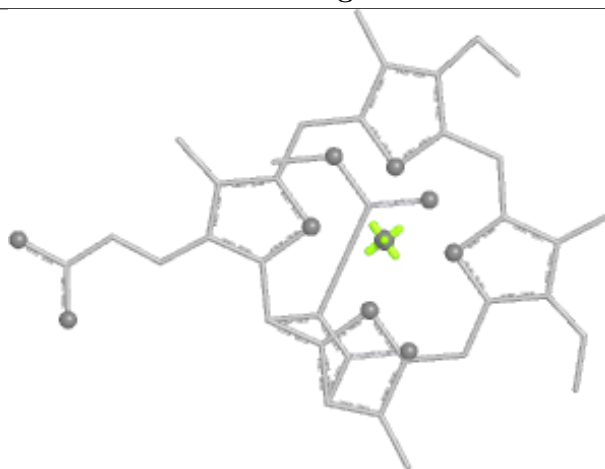
Bond lengths



Bond angles

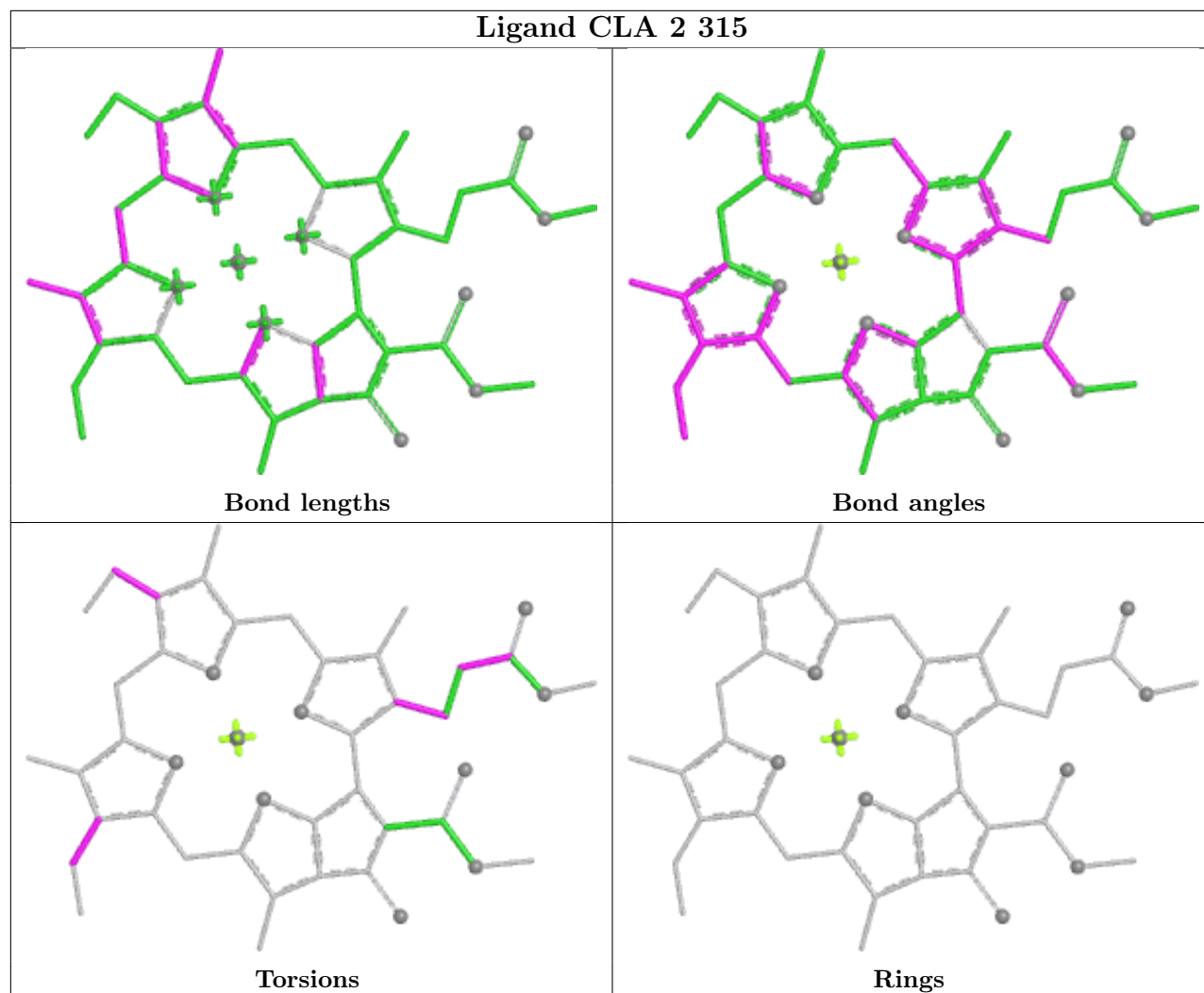


Torsions

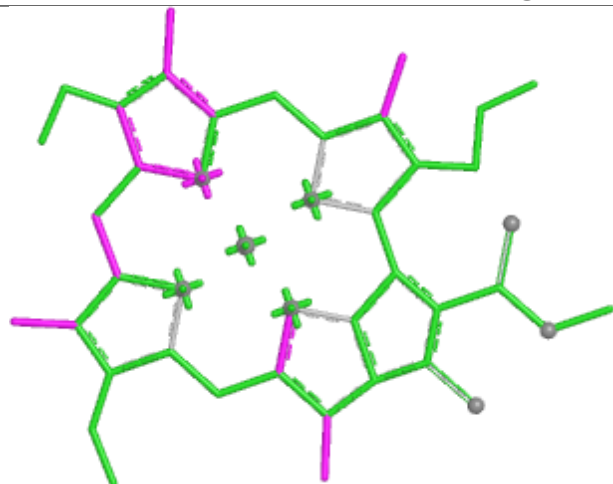


Rings

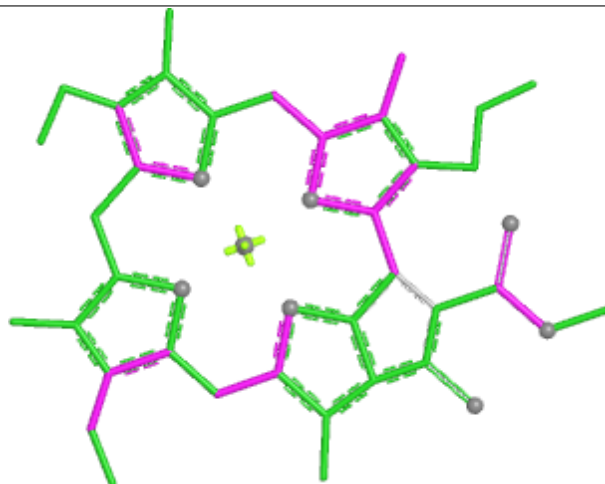
Ligand CLA 2 315



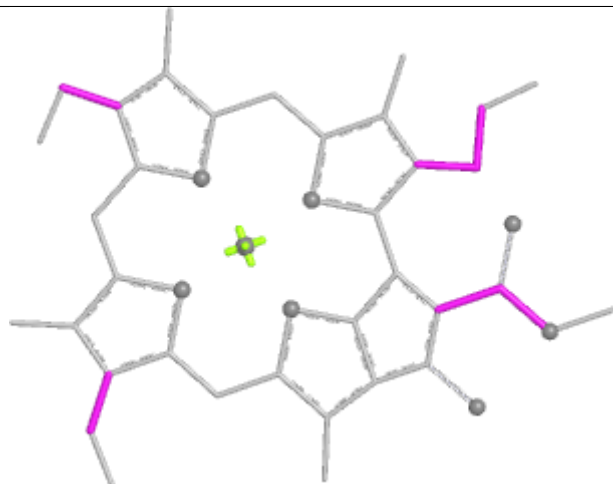
Ligand CLA 4 315



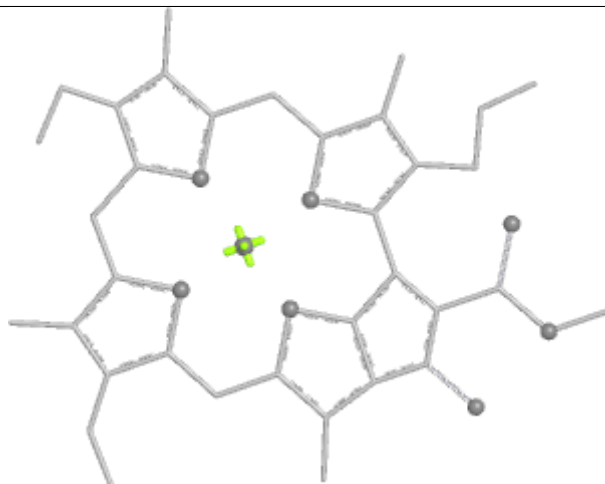
Bond lengths



Bond angles

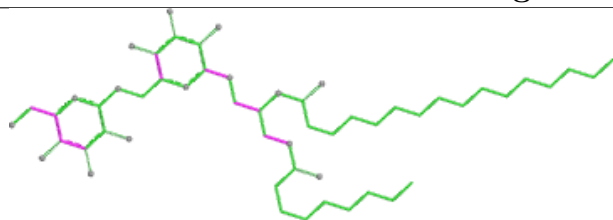


Torsions

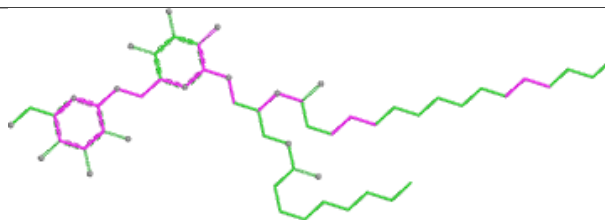


Rings

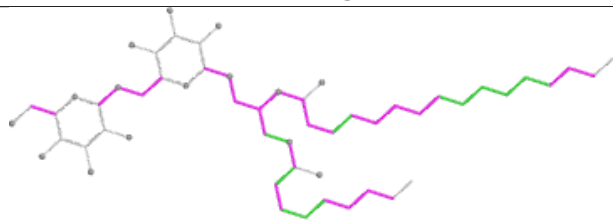
Ligand DGD b 622



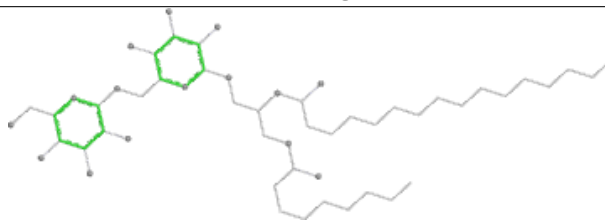
Bond lengths



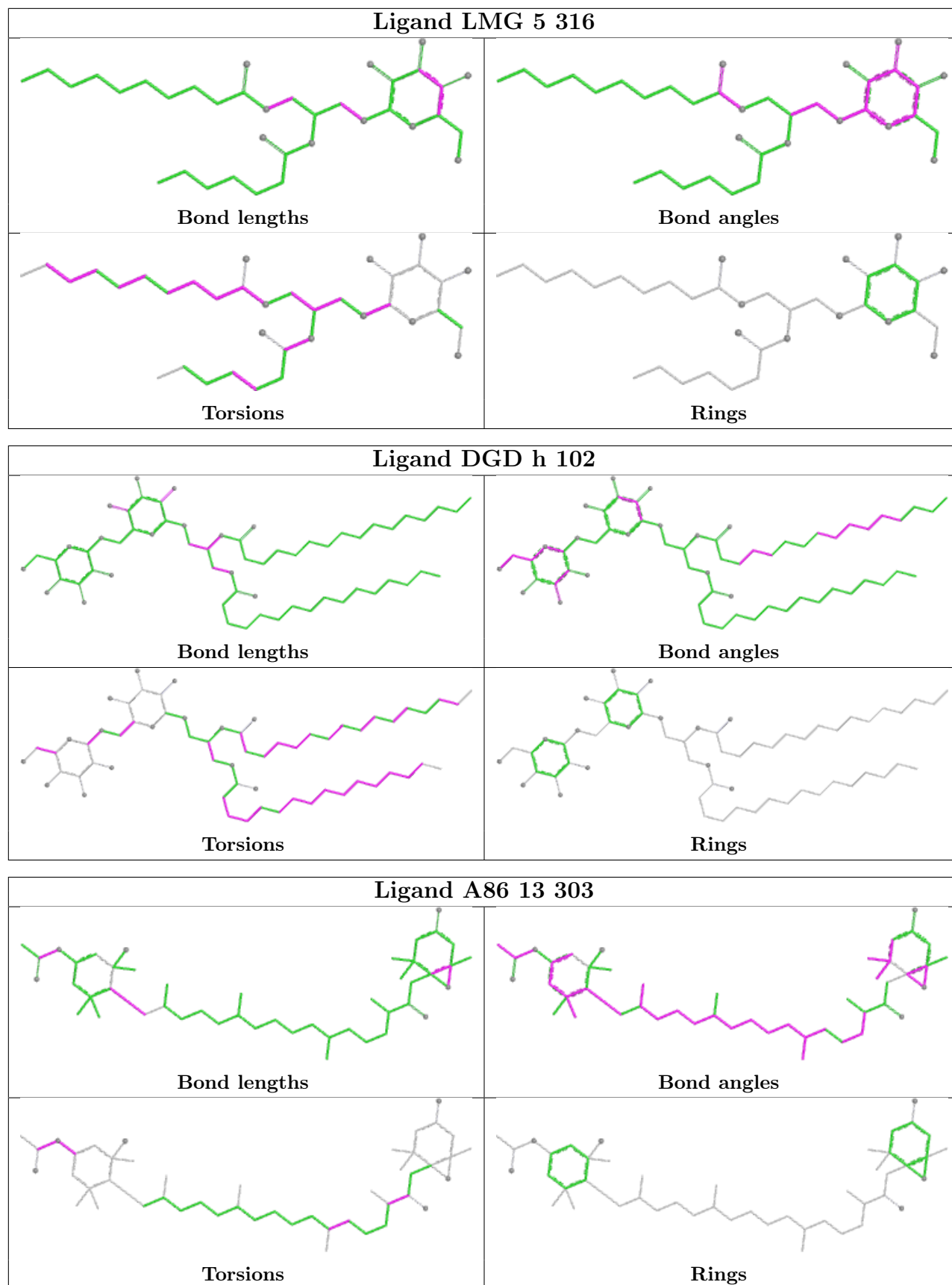
Bond angles

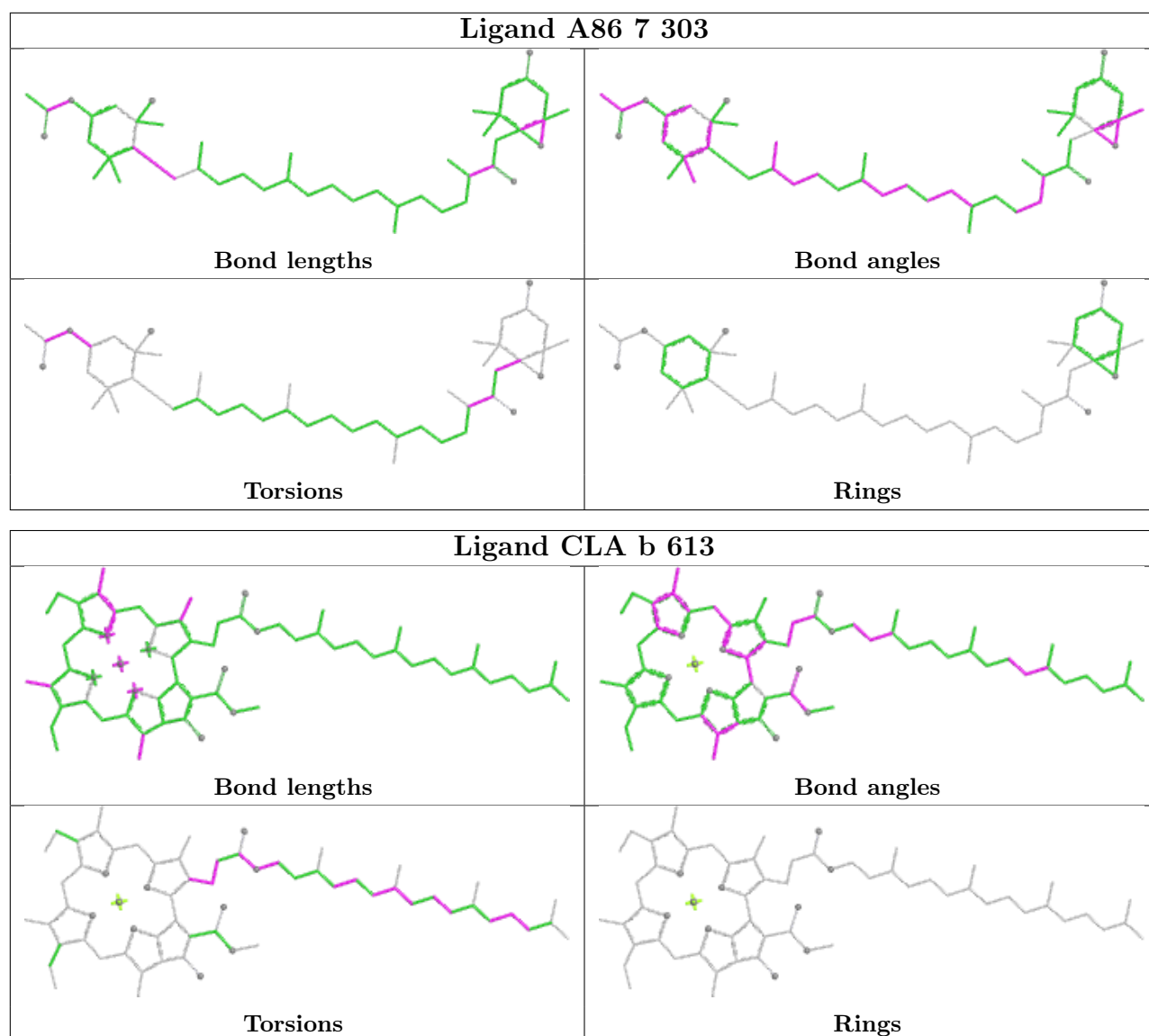


Torsions

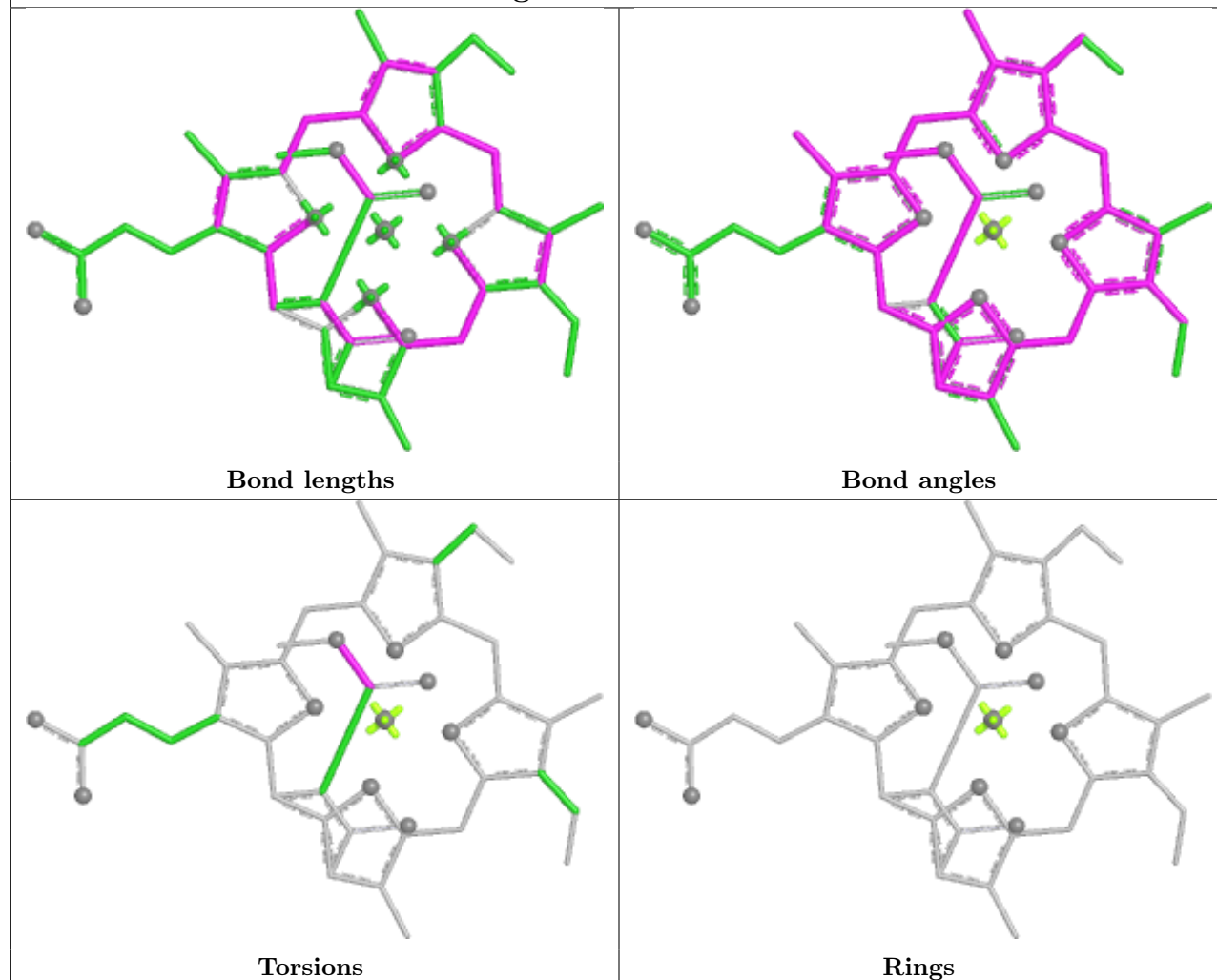


Rings

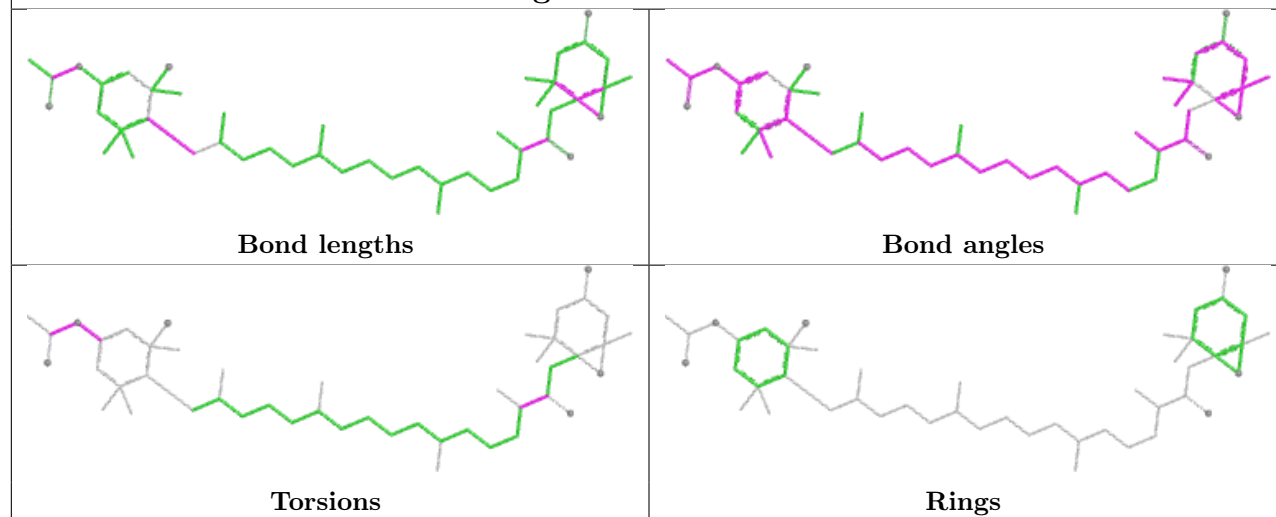


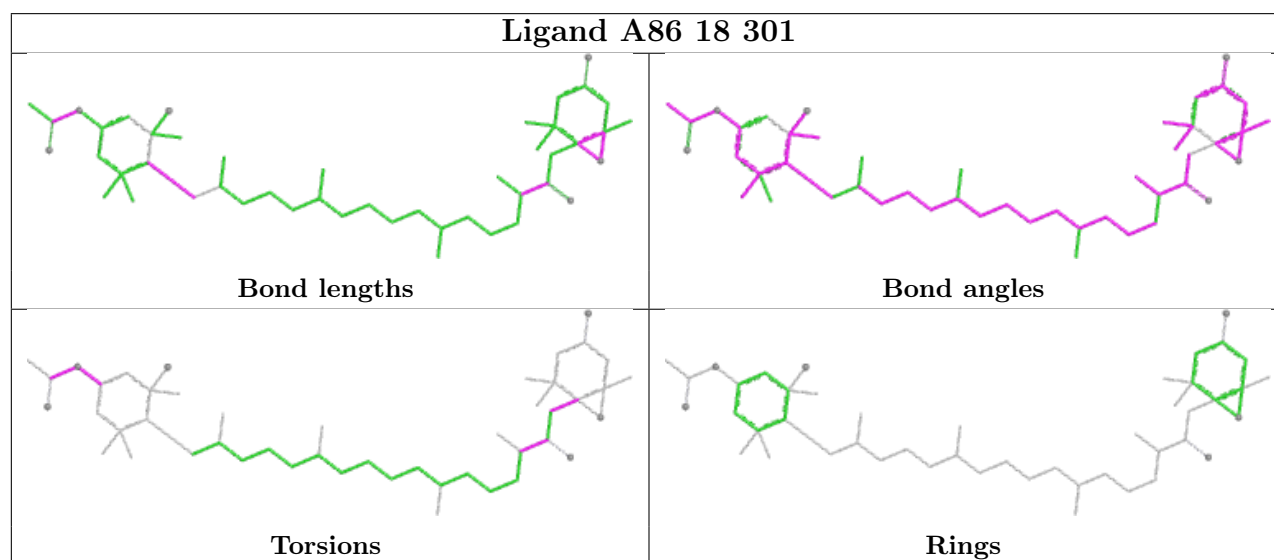
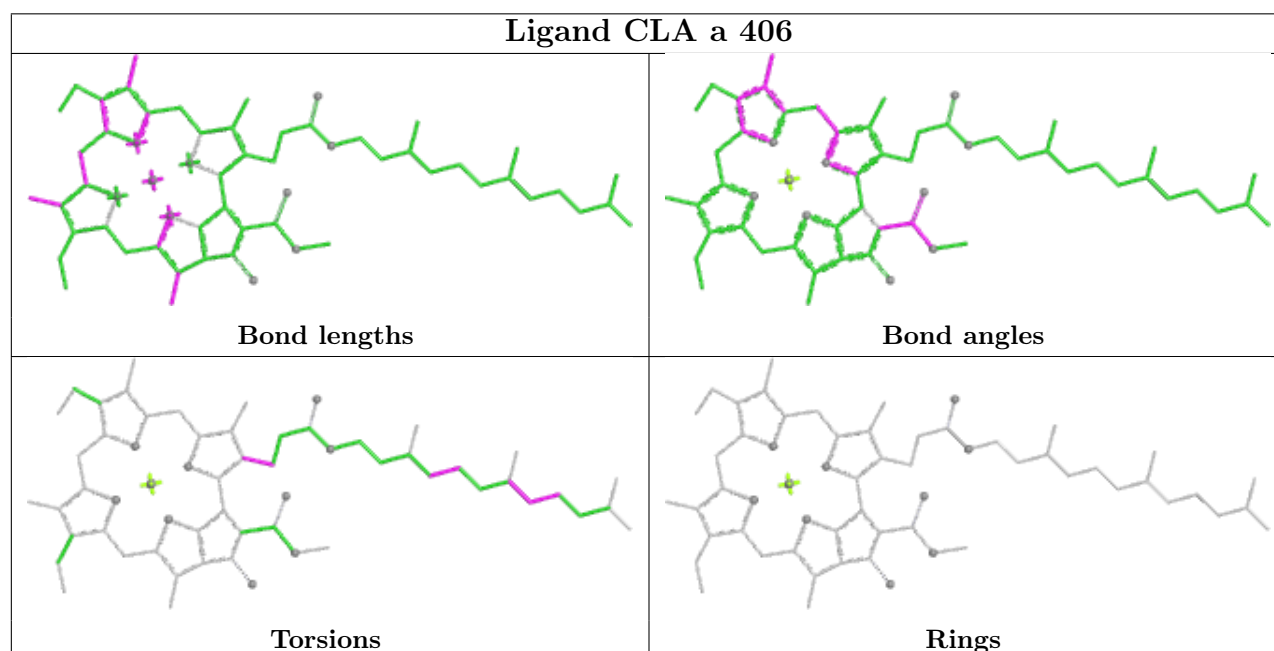
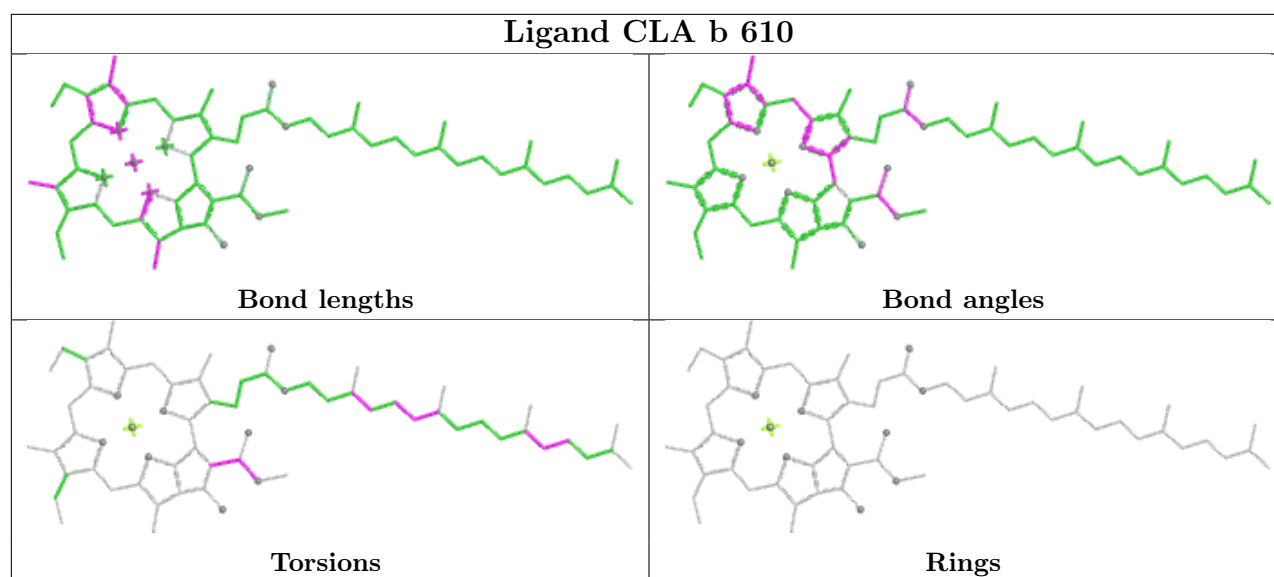


Ligand KC1 7 314

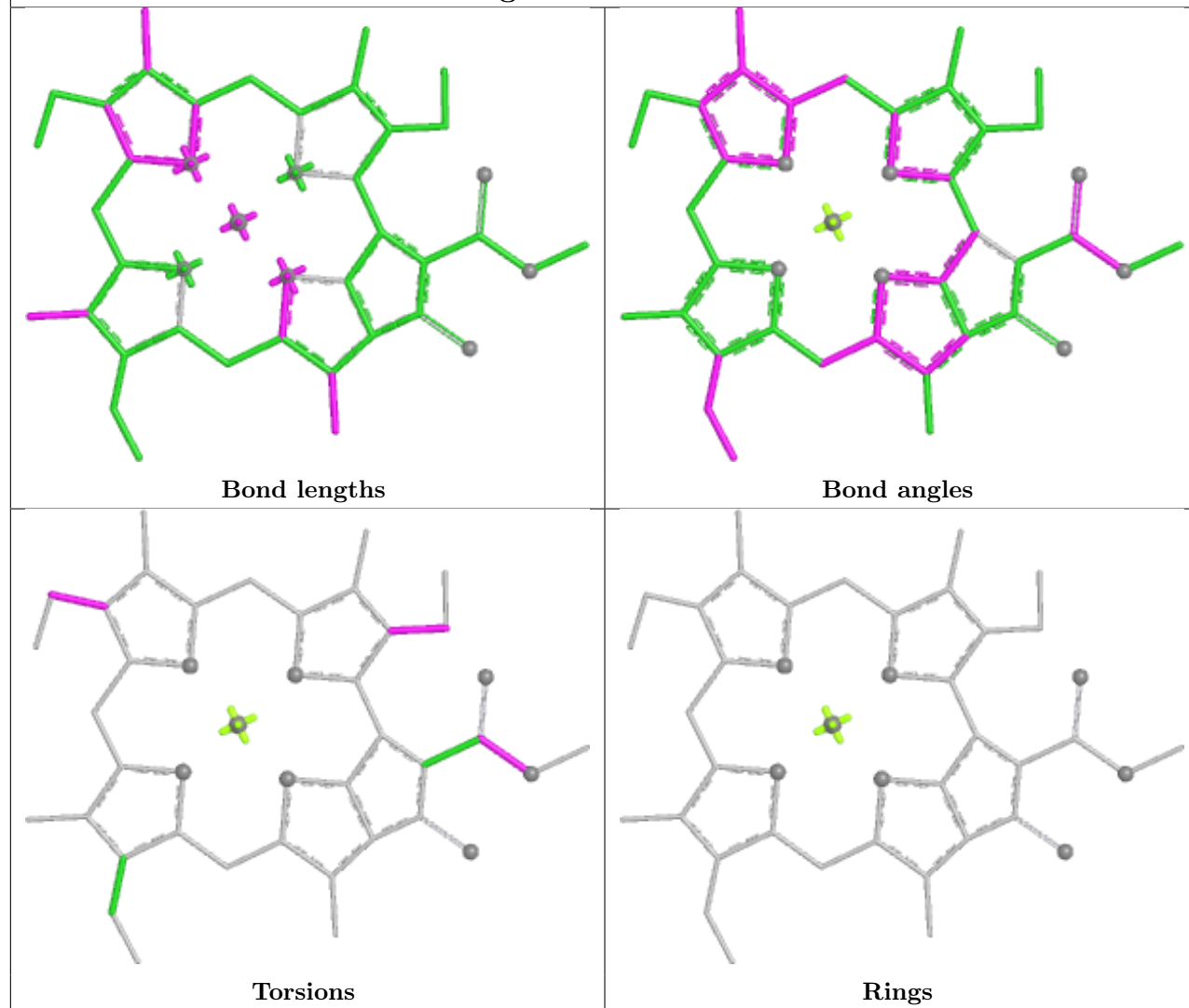


Ligand A86 10 301

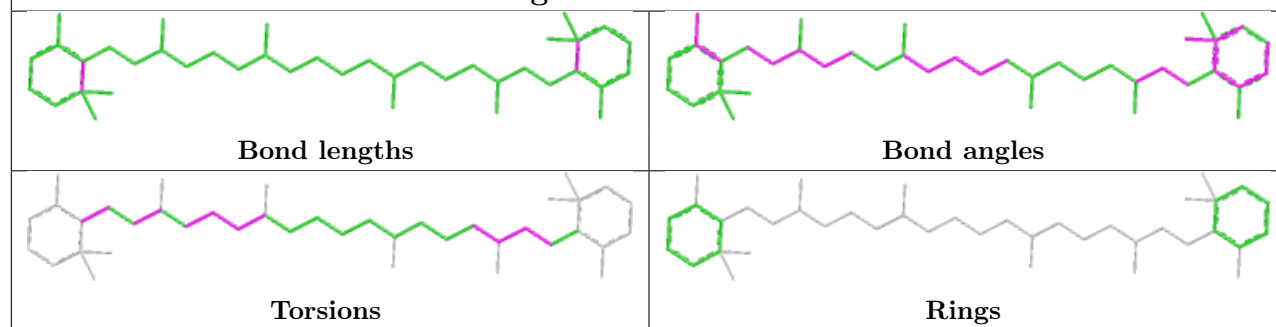




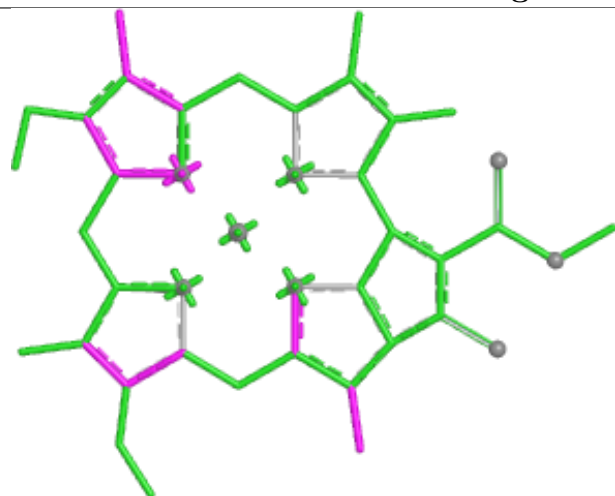
Ligand CLA 6 314



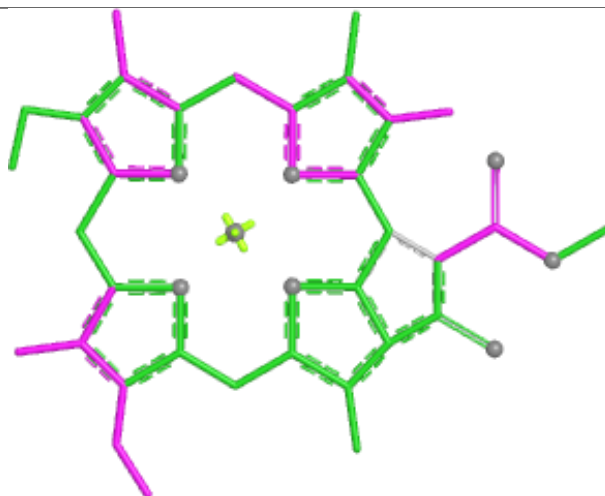
Ligand BCR B 617



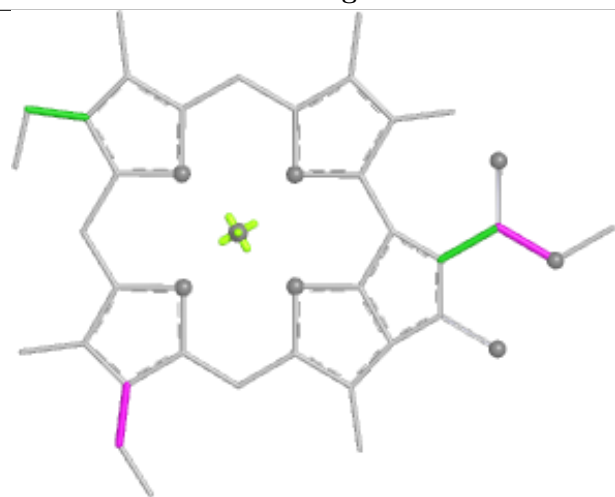
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Bond lengths



Bond angles

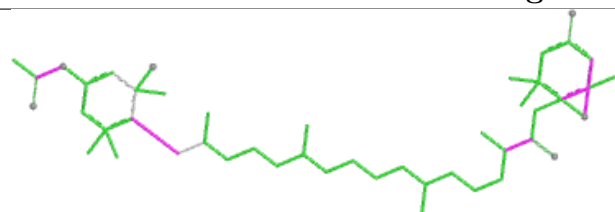


Torsions

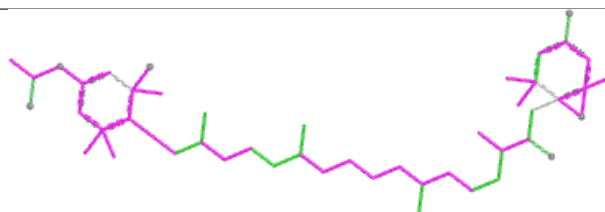


Rings

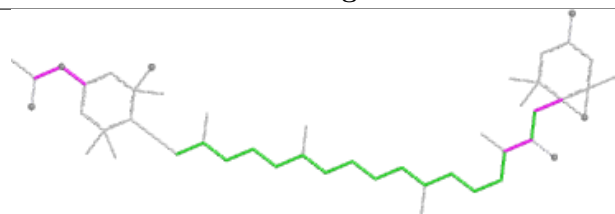
Ligand A86 7 306



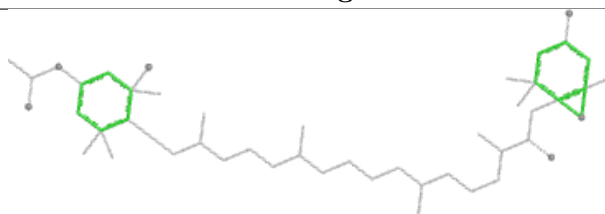
Bond lengths



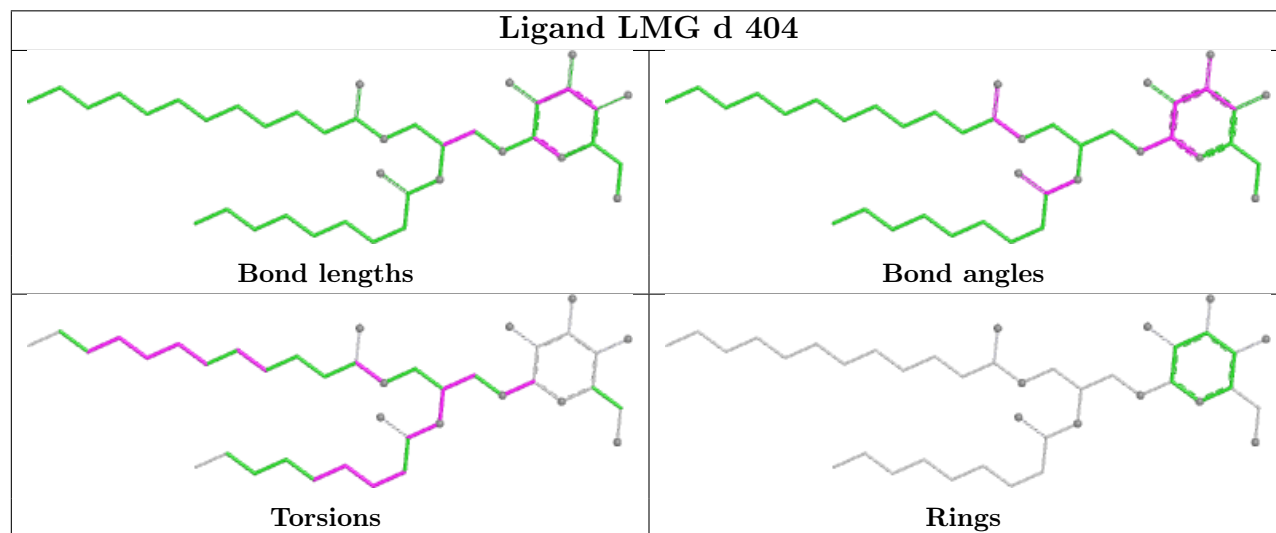
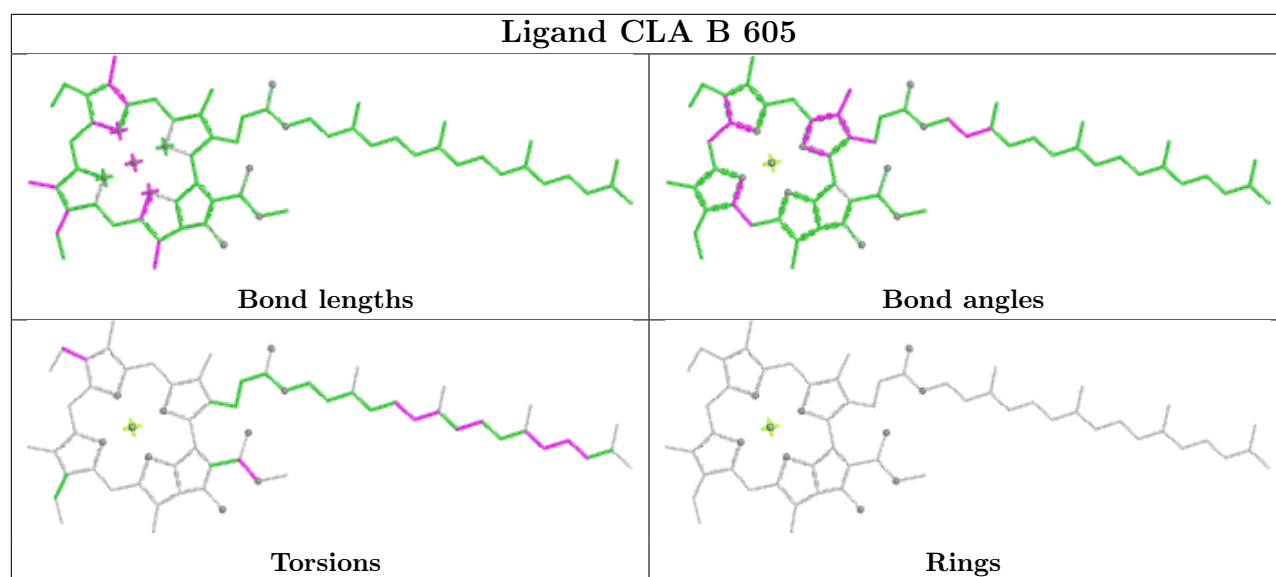
Bond angles

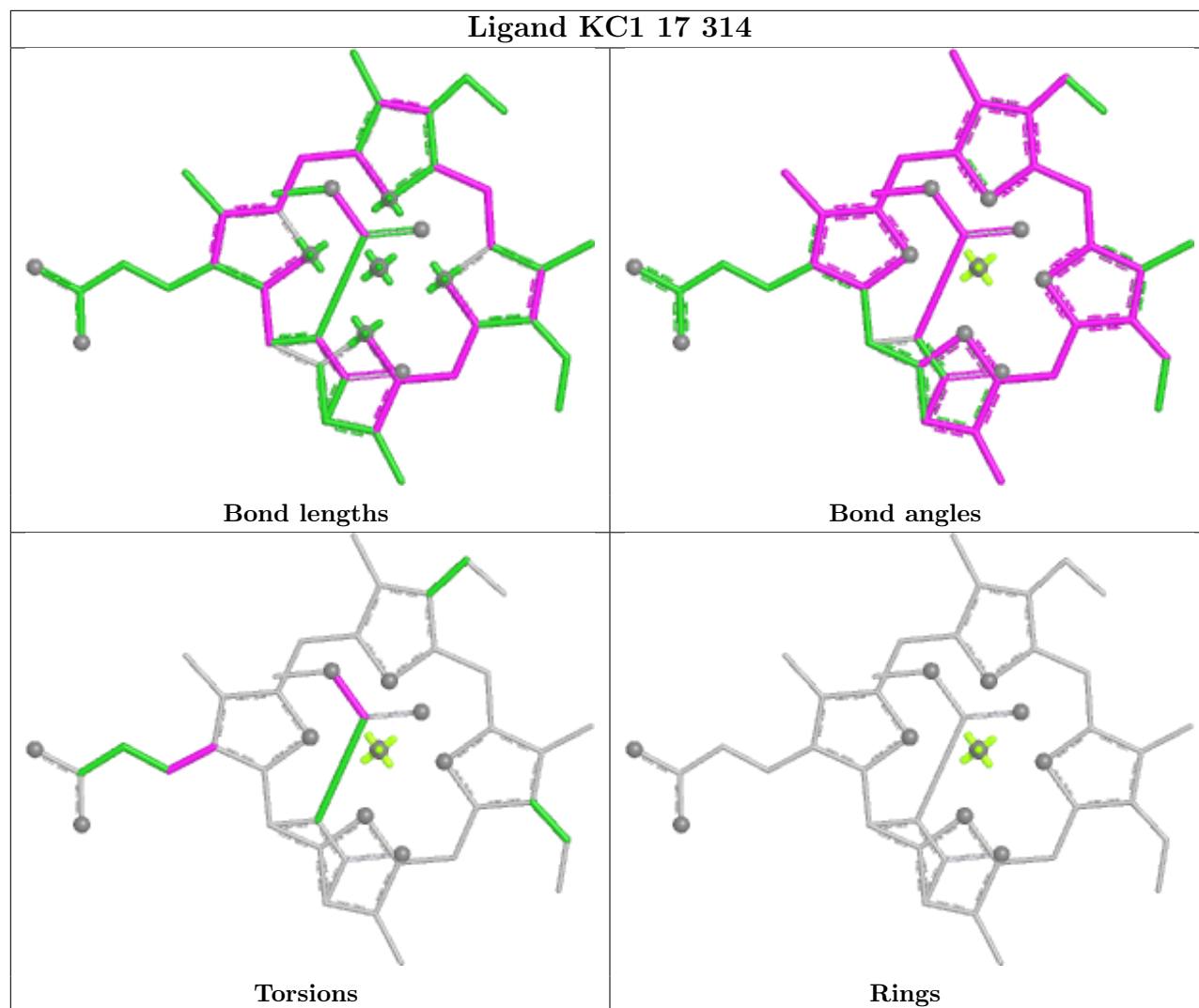


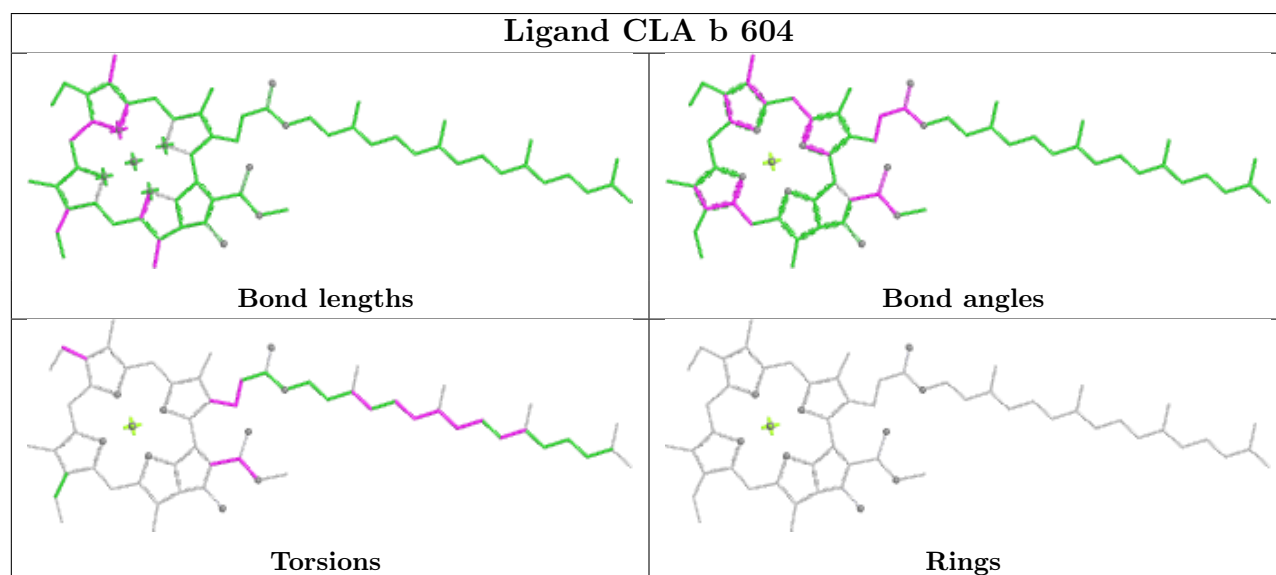
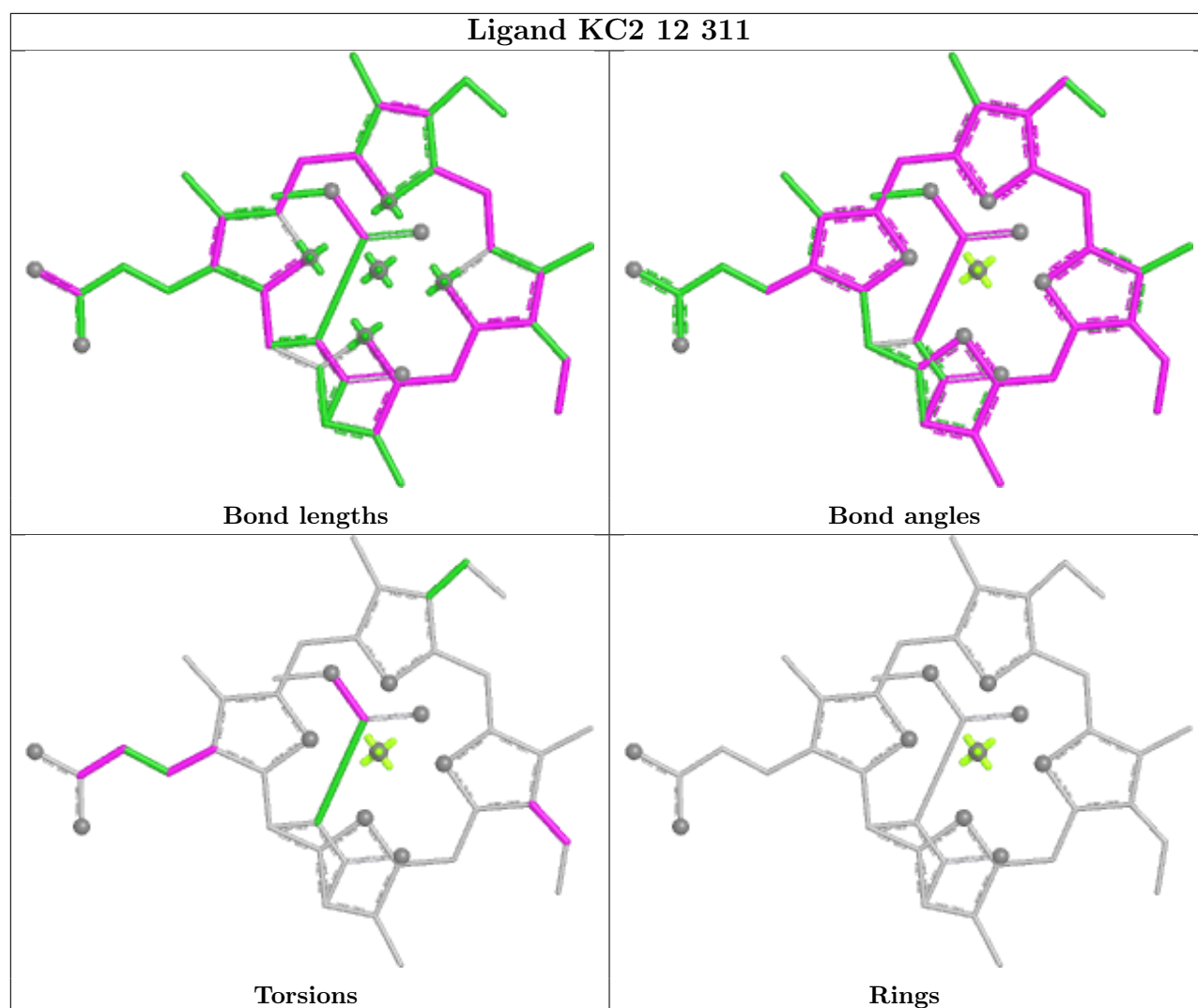
Torsions



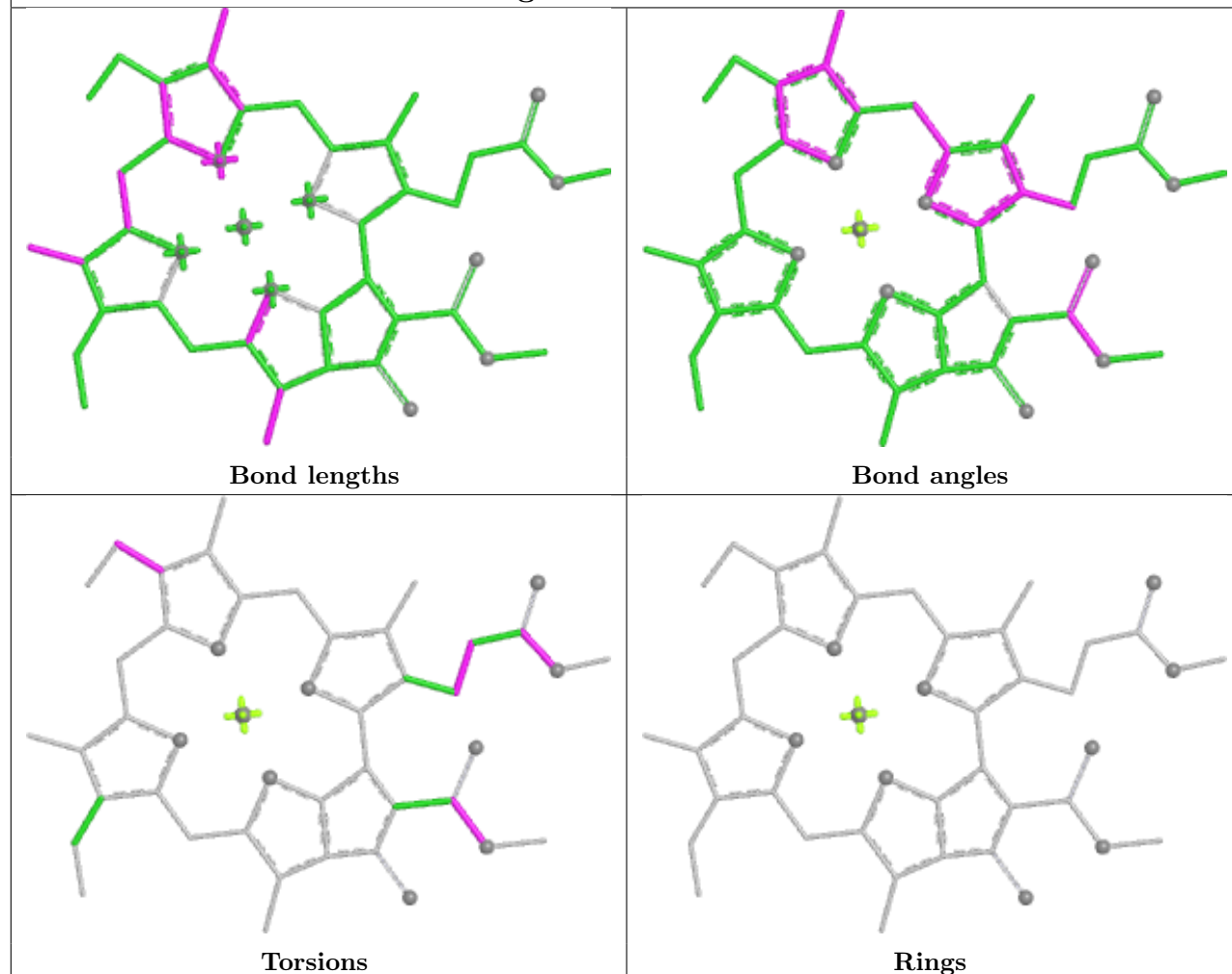
Rings



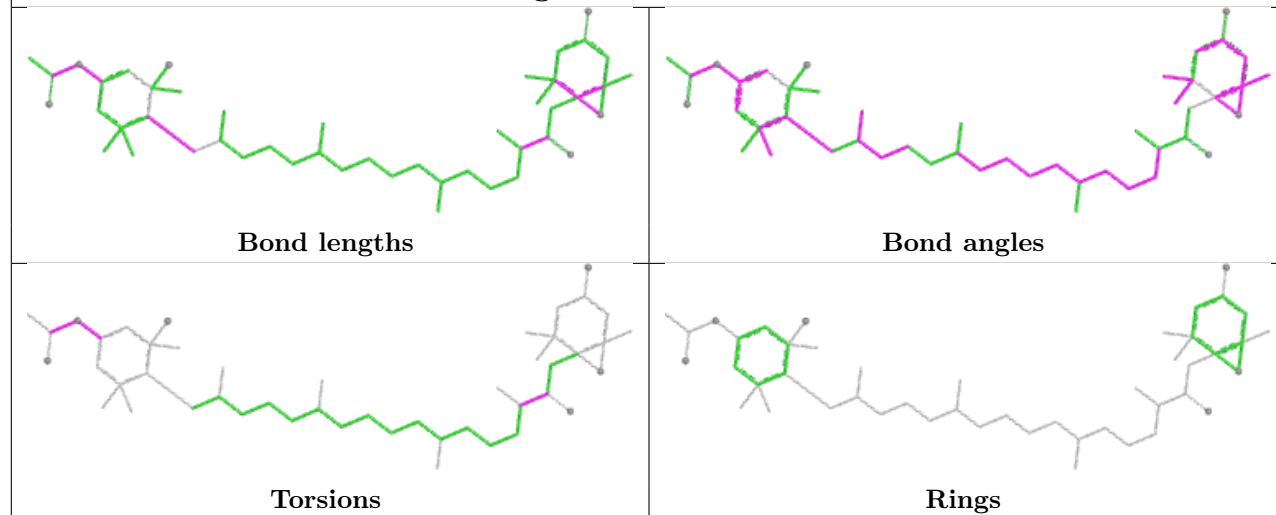


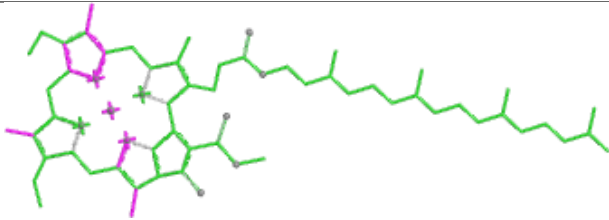
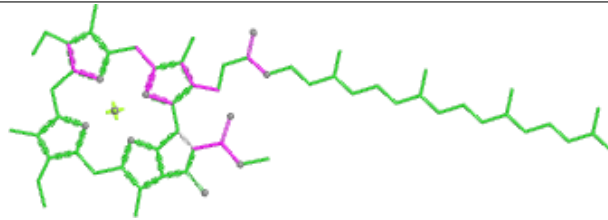
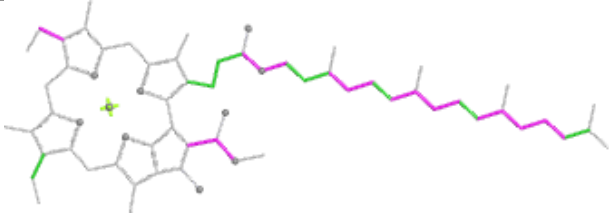
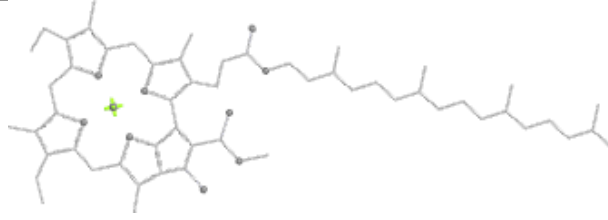


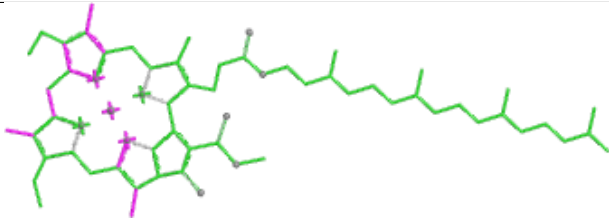
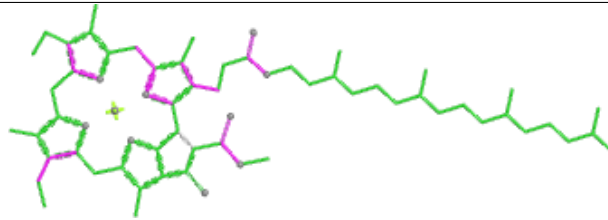
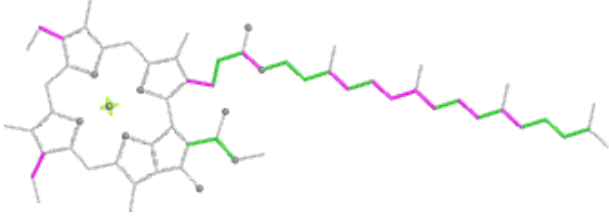
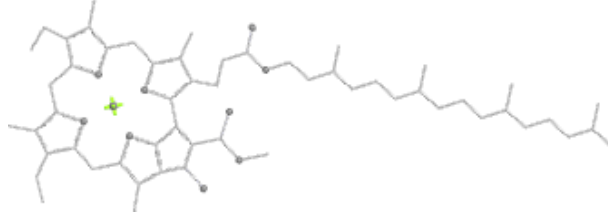
Ligand CLA 0 316

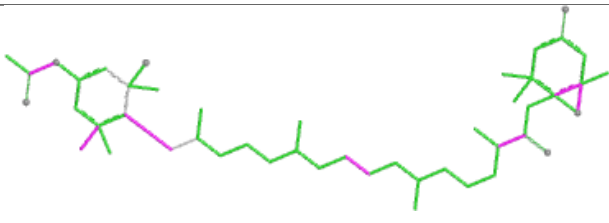
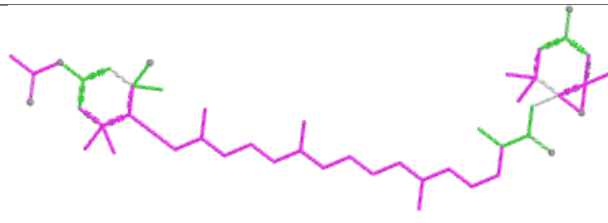
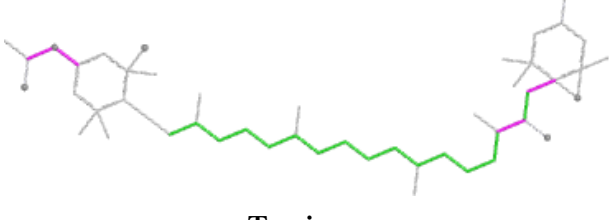
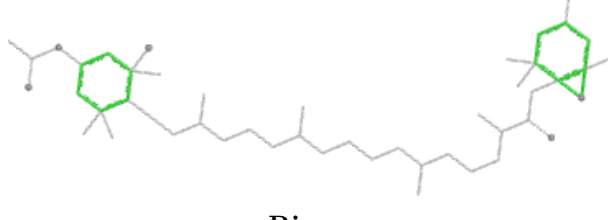


Ligand A86 12 304

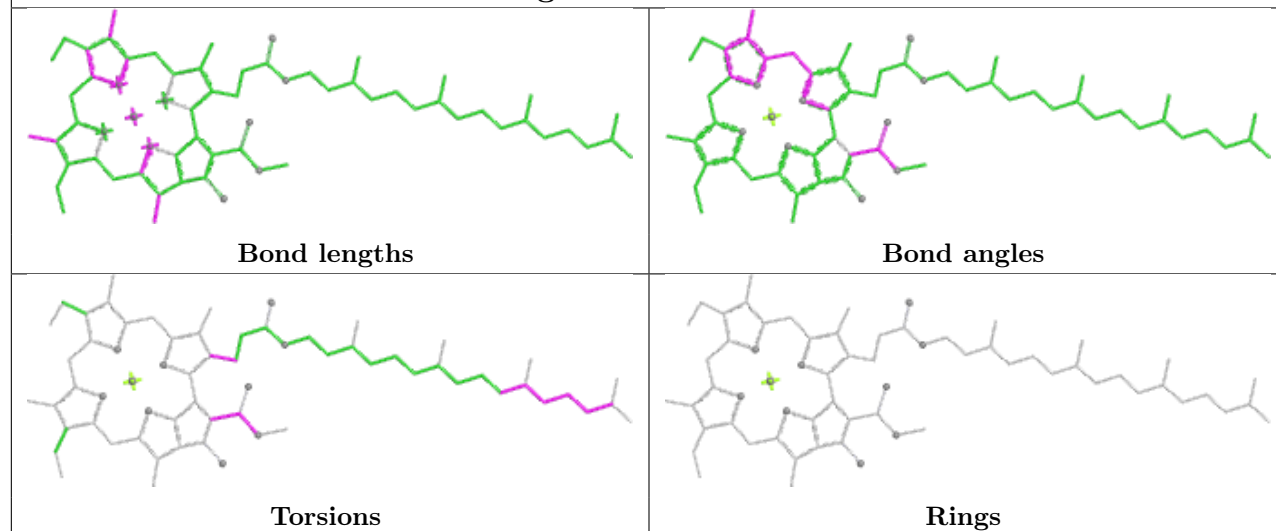


Ligand CLA P 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

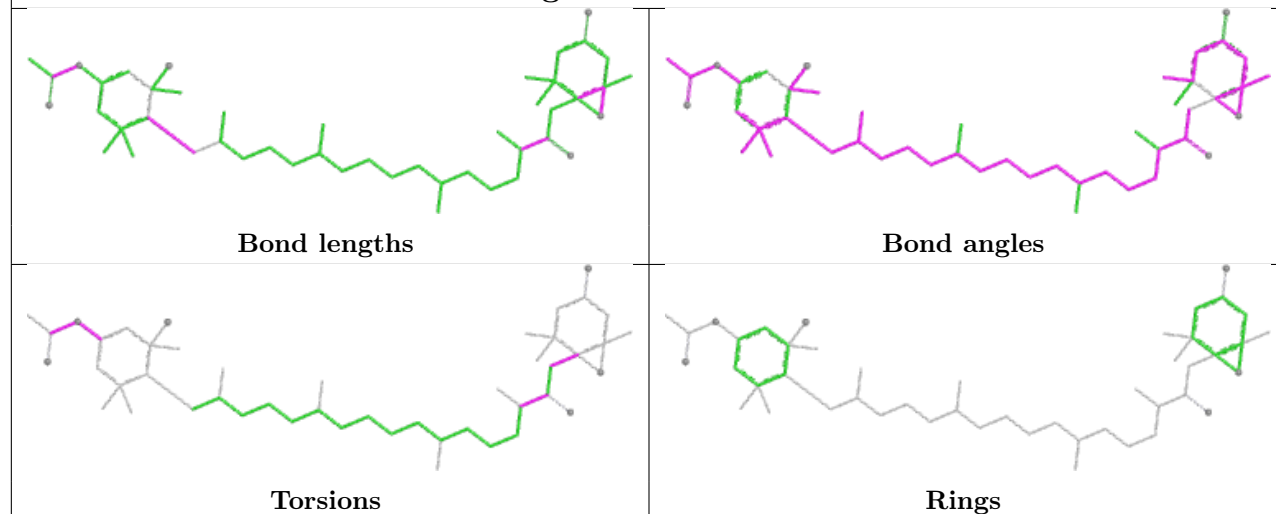
Ligand CLA 6 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A86 3 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

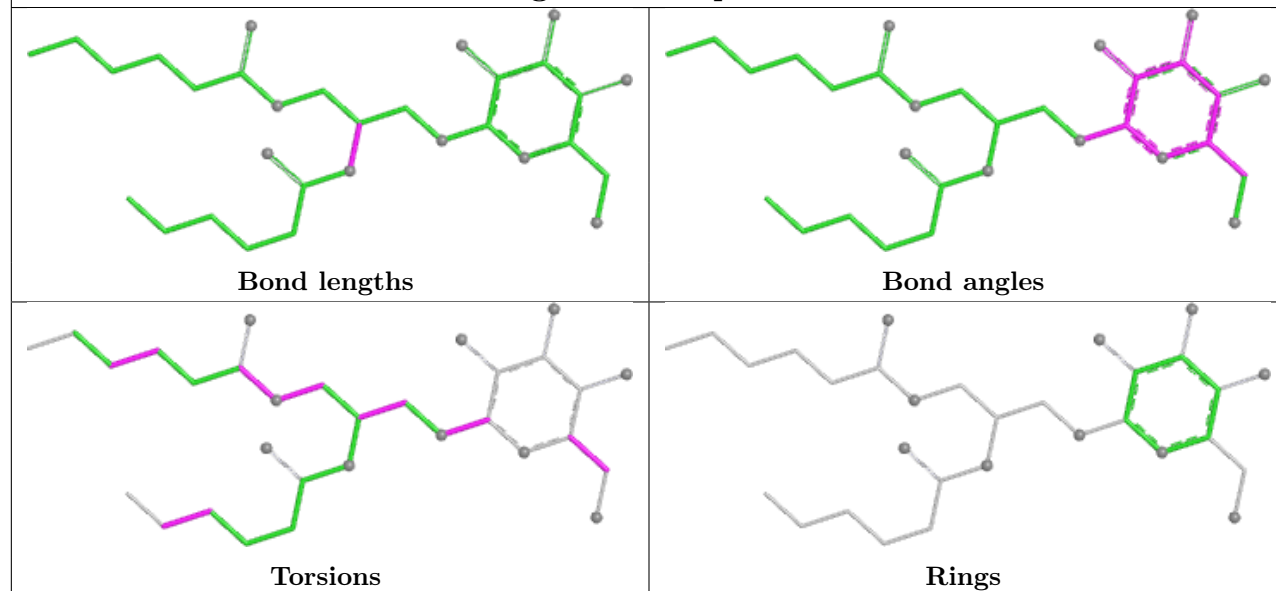
Ligand CLA c 507



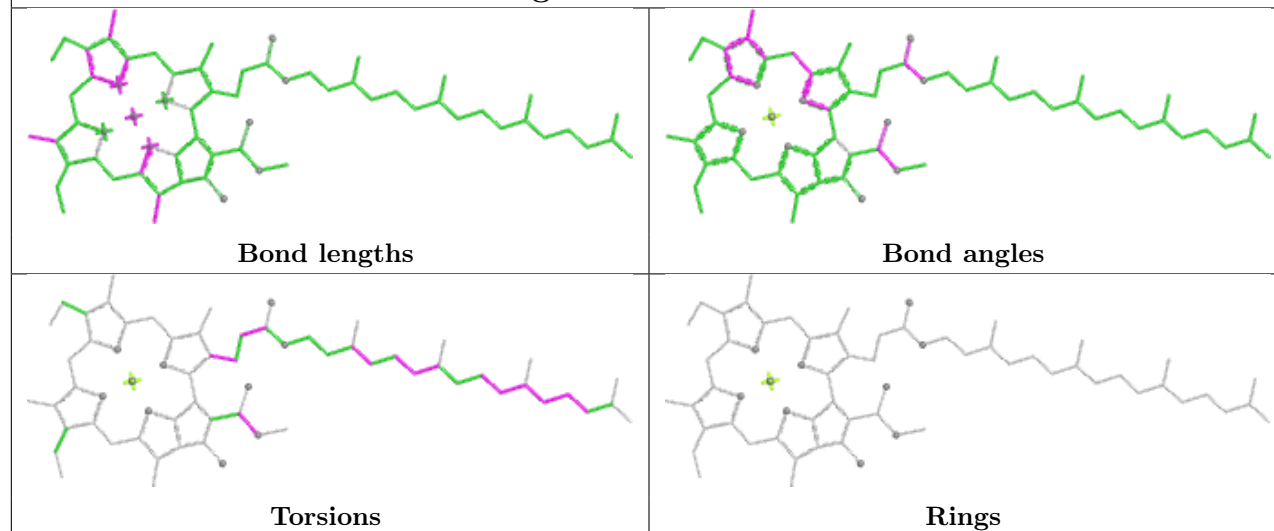
Ligand A86 6 301



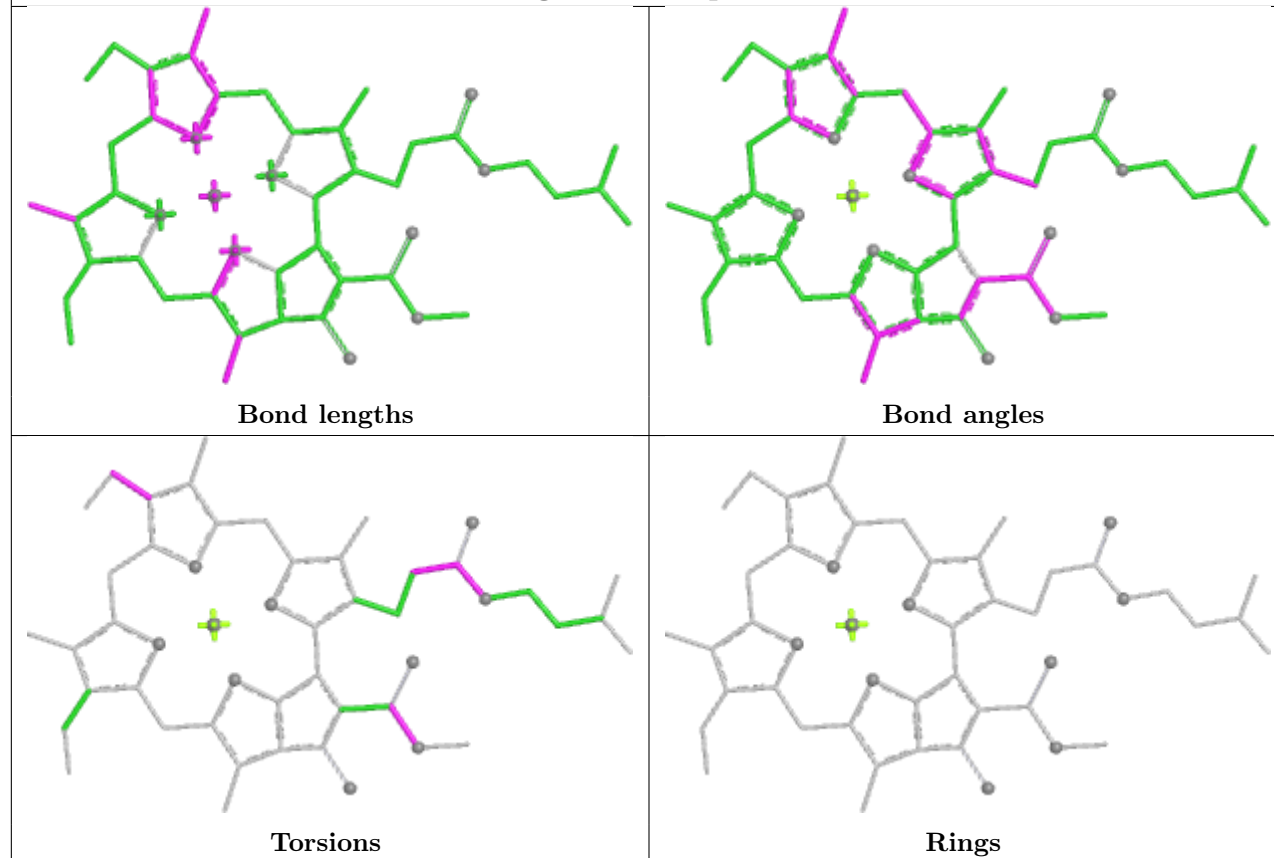
Ligand LMG p 614

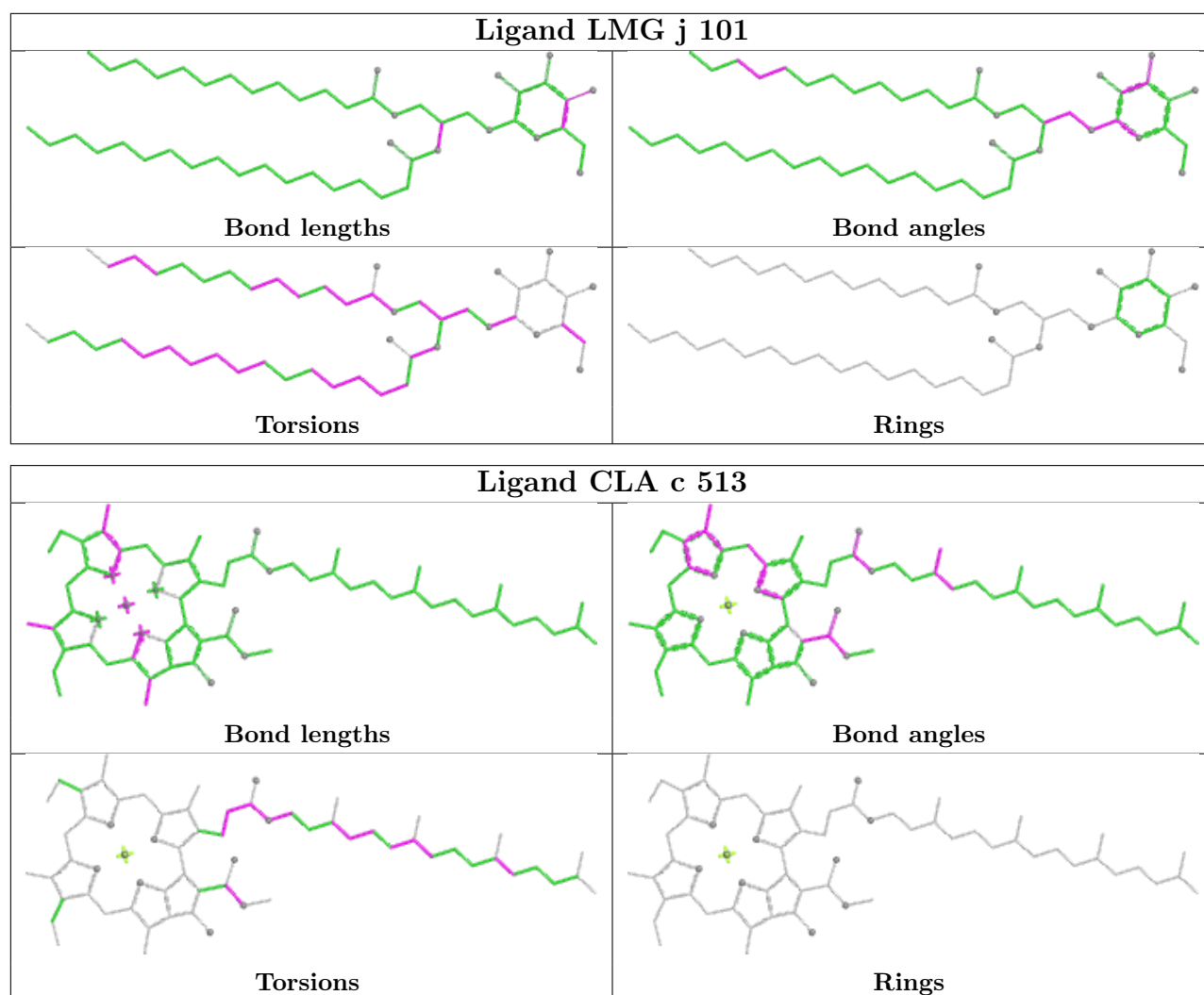


Ligand CLA B 608

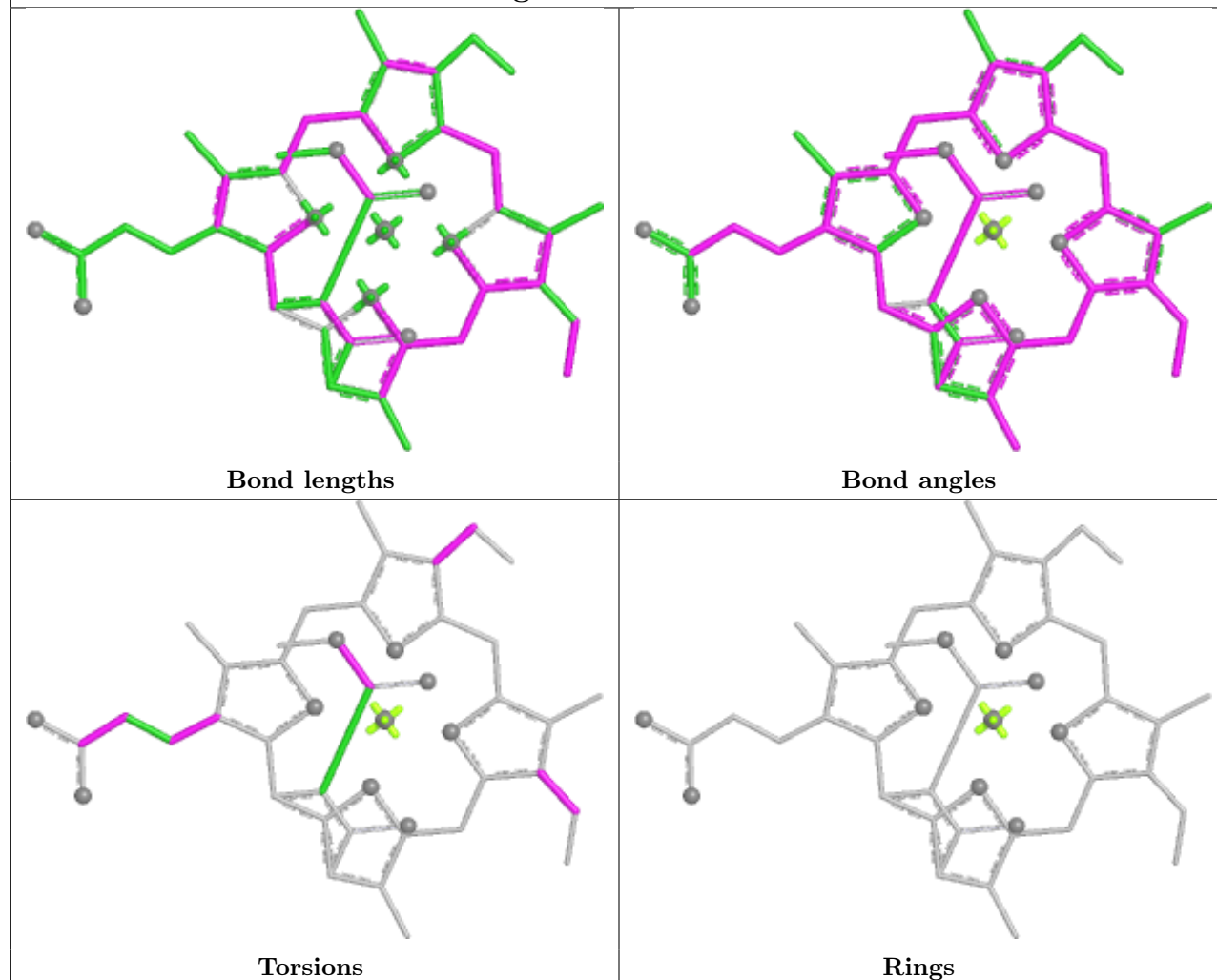


Ligand CLA p 603

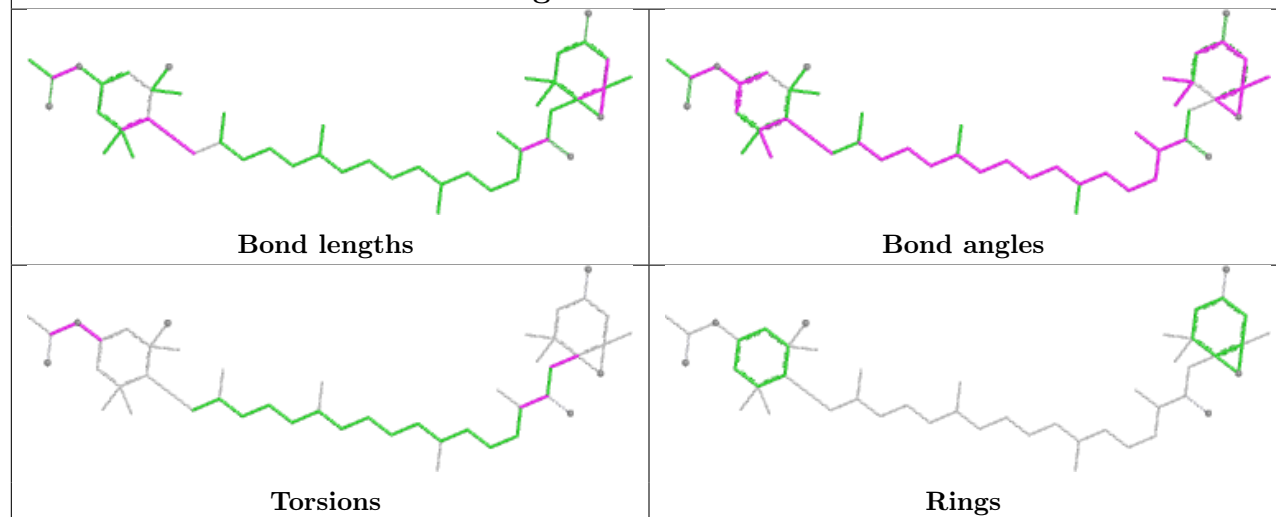


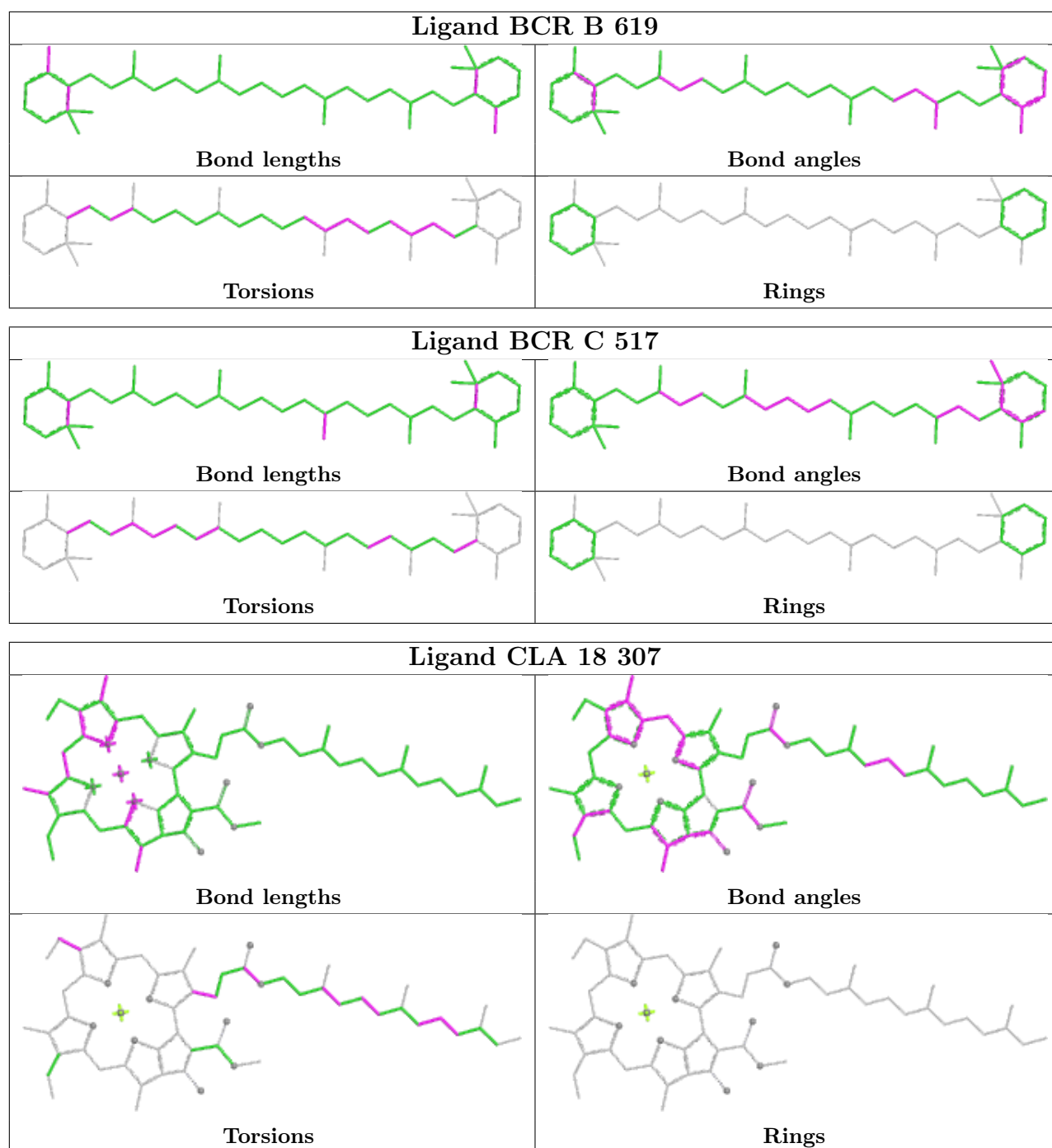


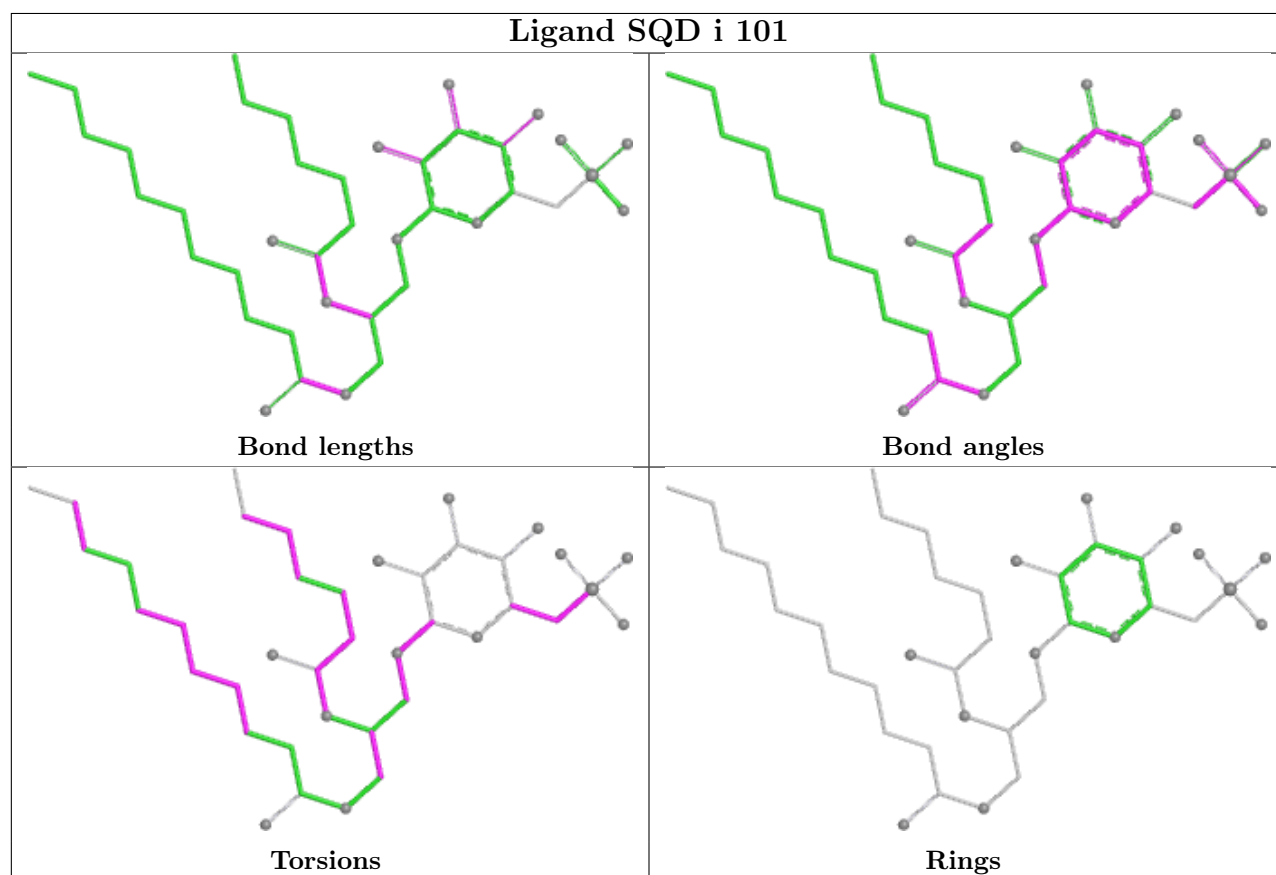
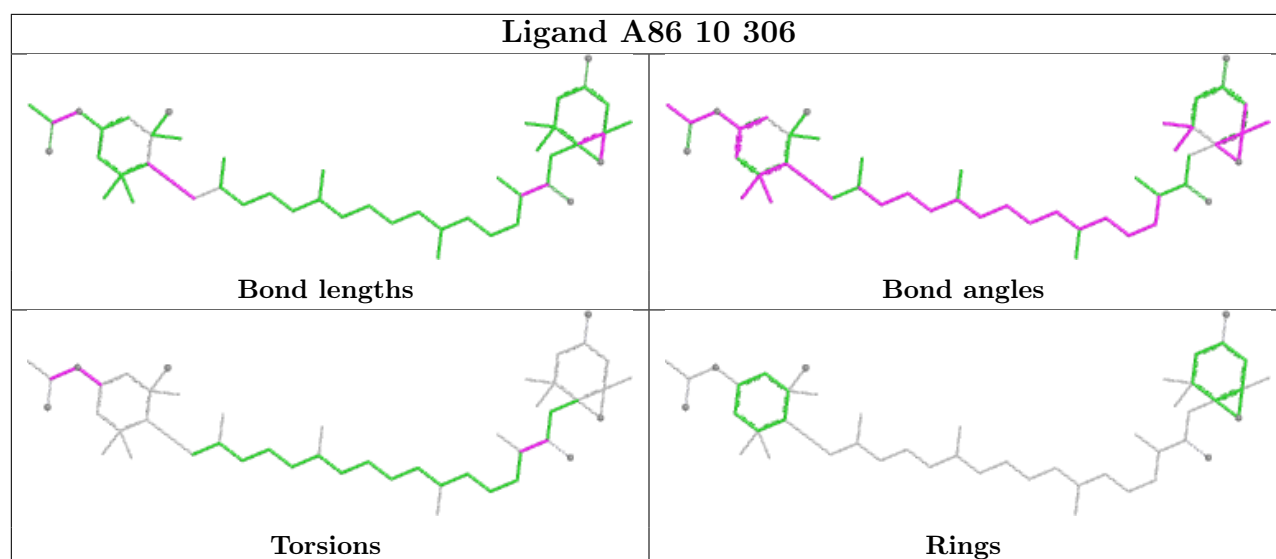
Ligand KC2 6 310



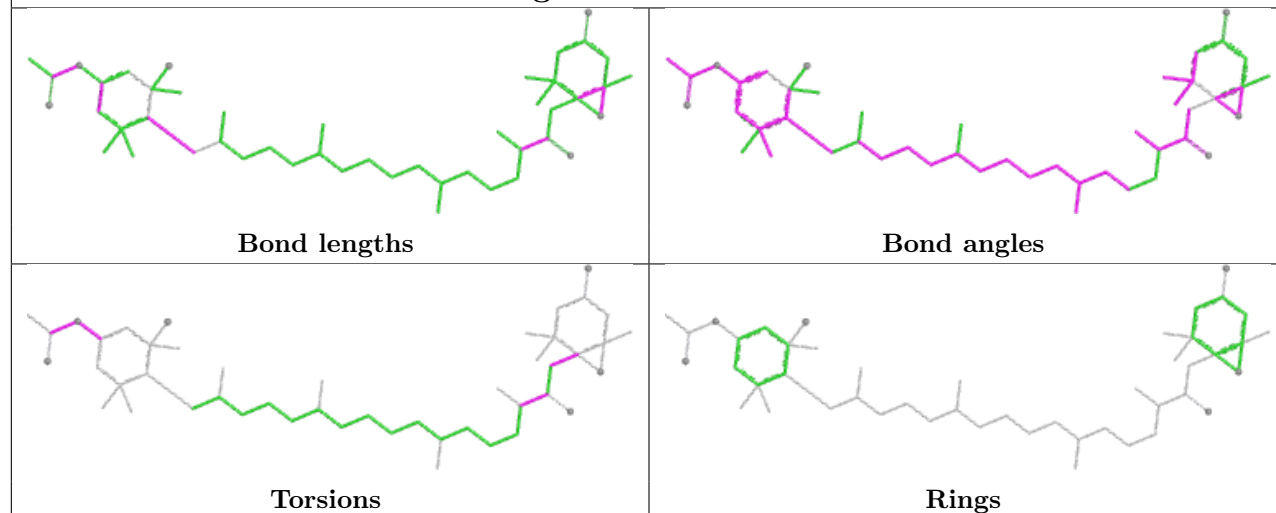
Ligand A86 17 303



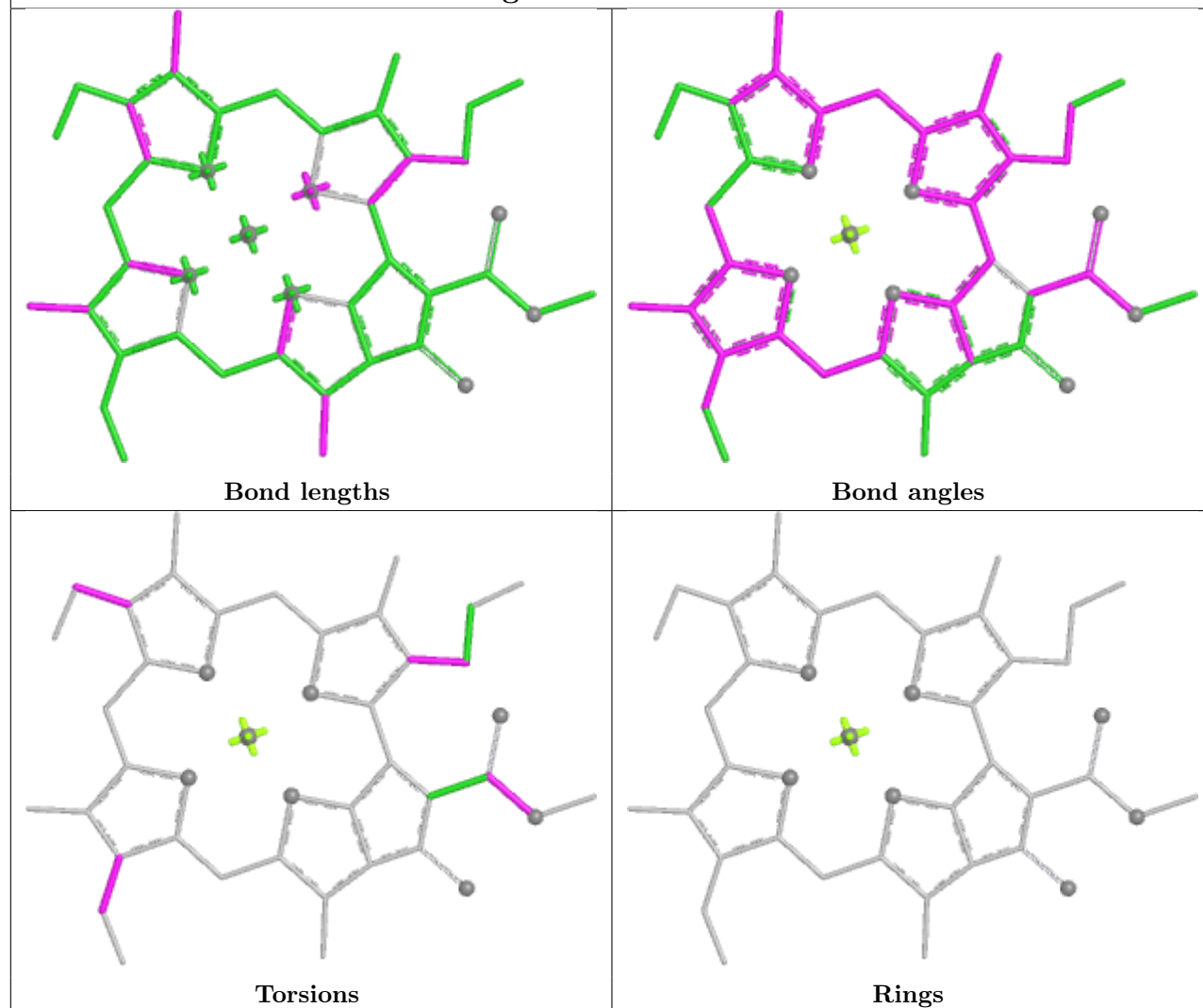


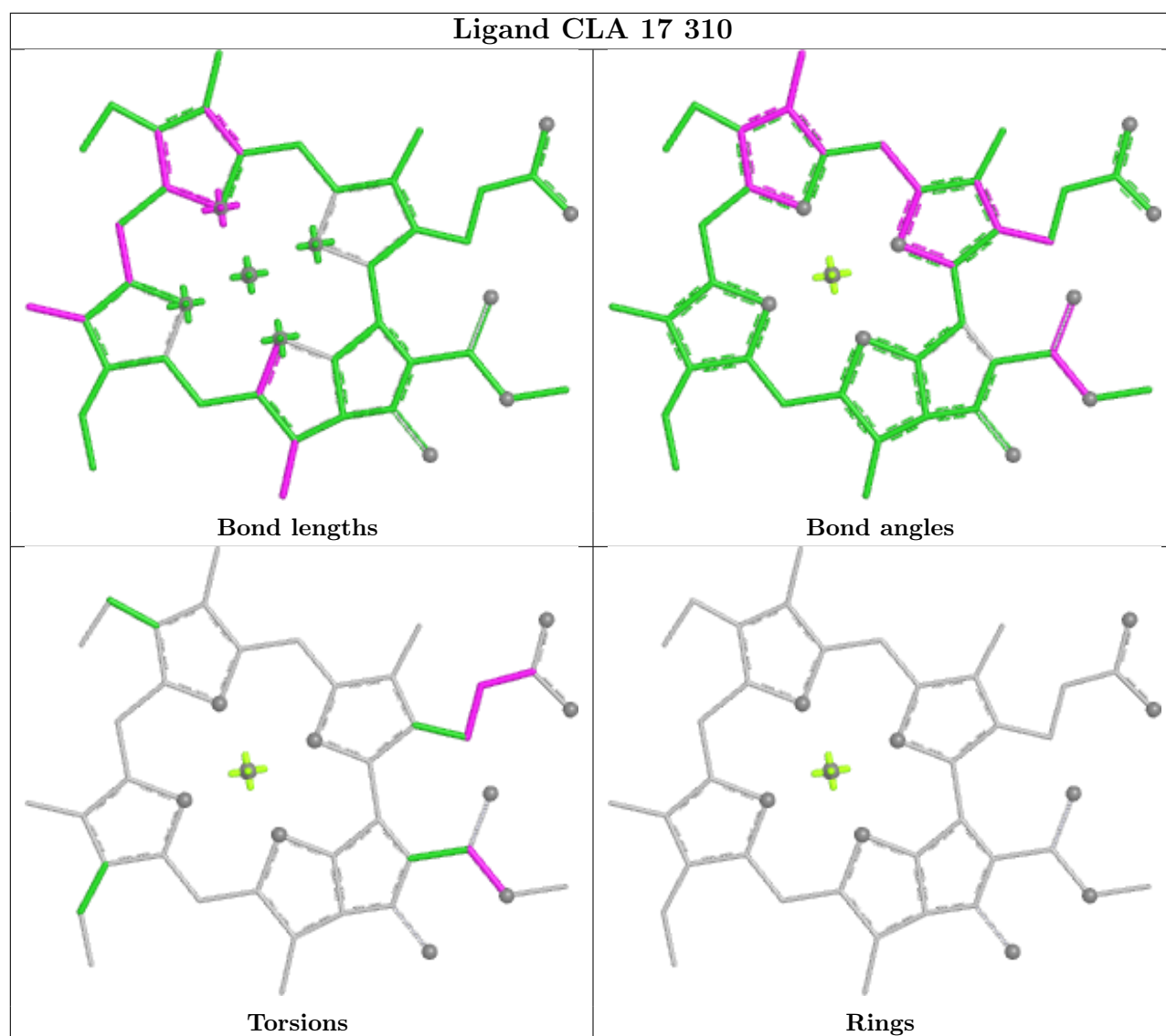


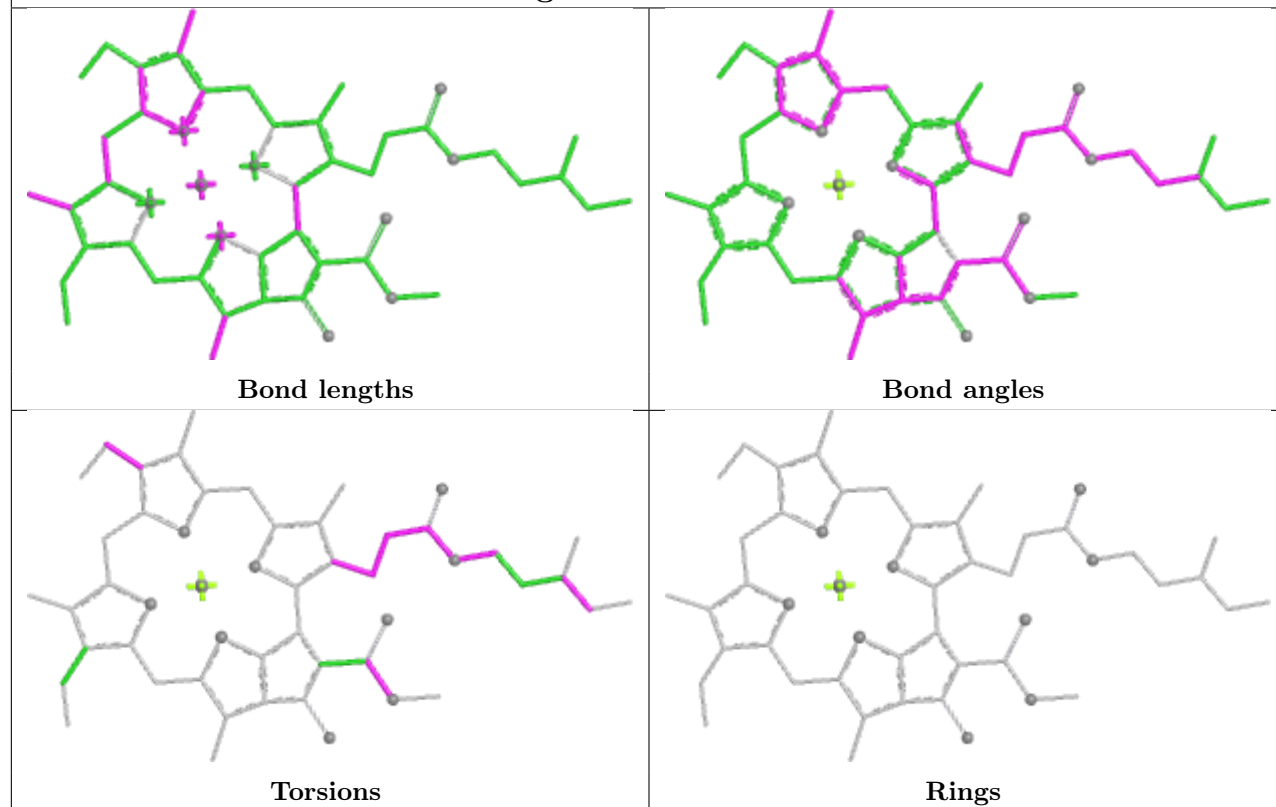
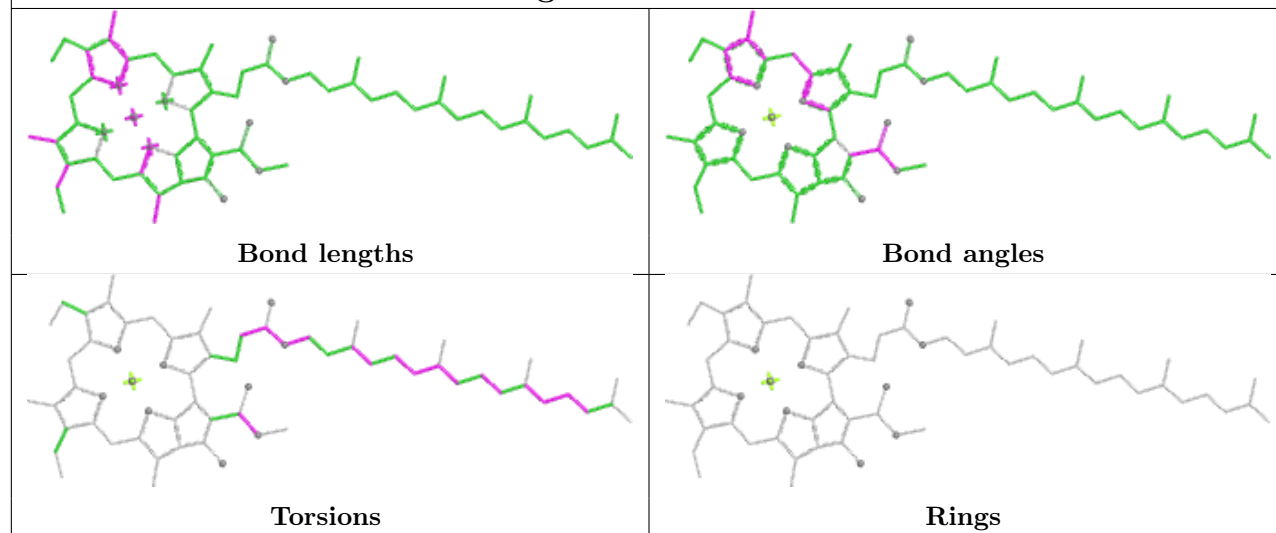
Ligand A86 13 301

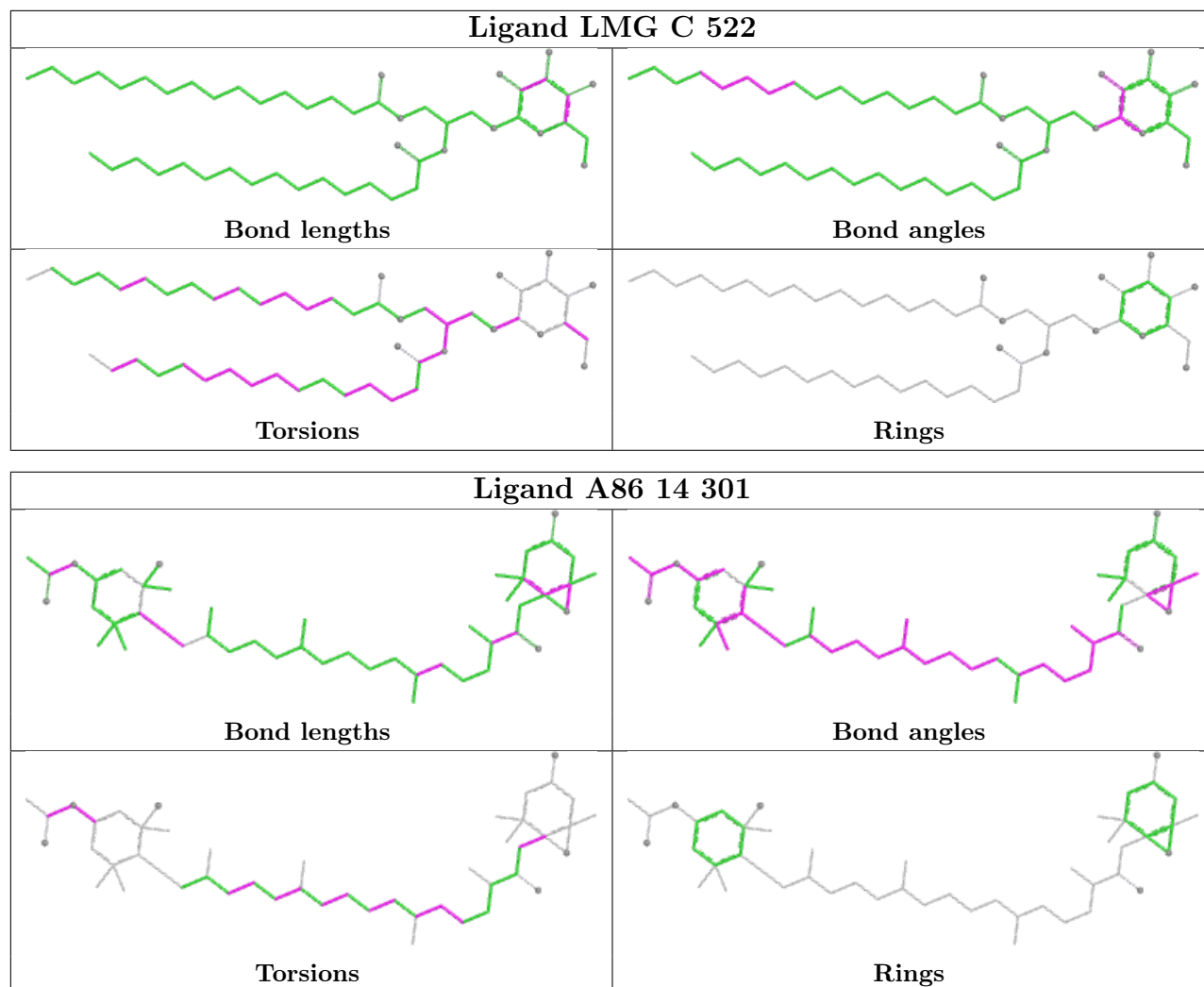


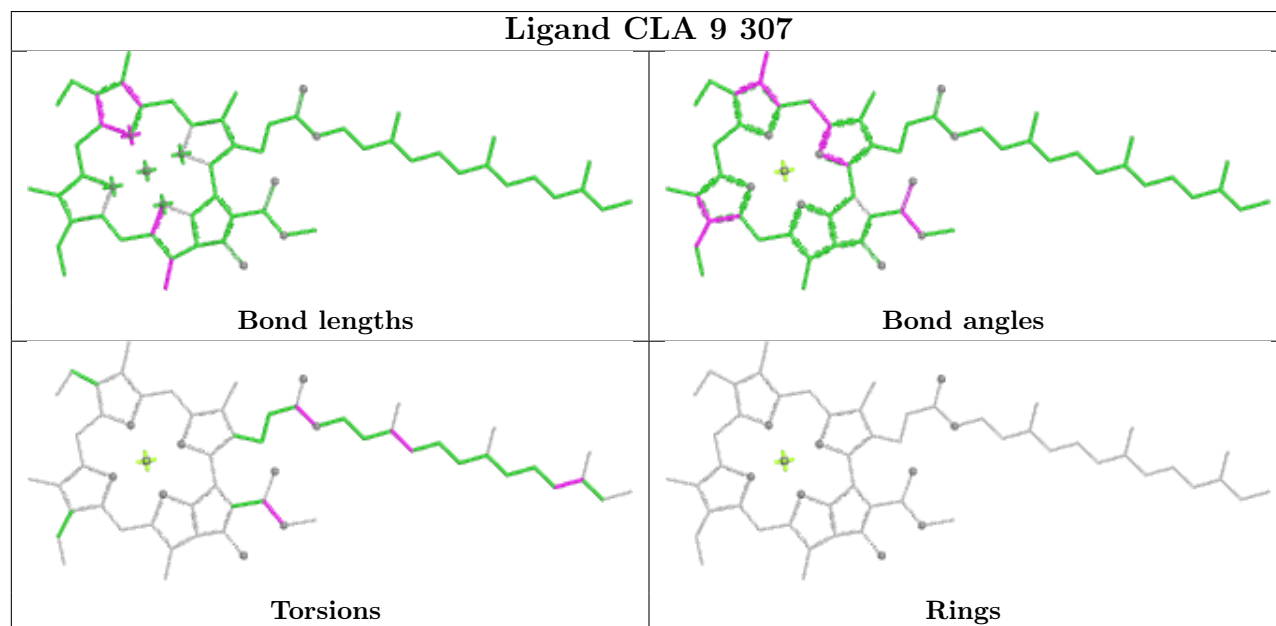
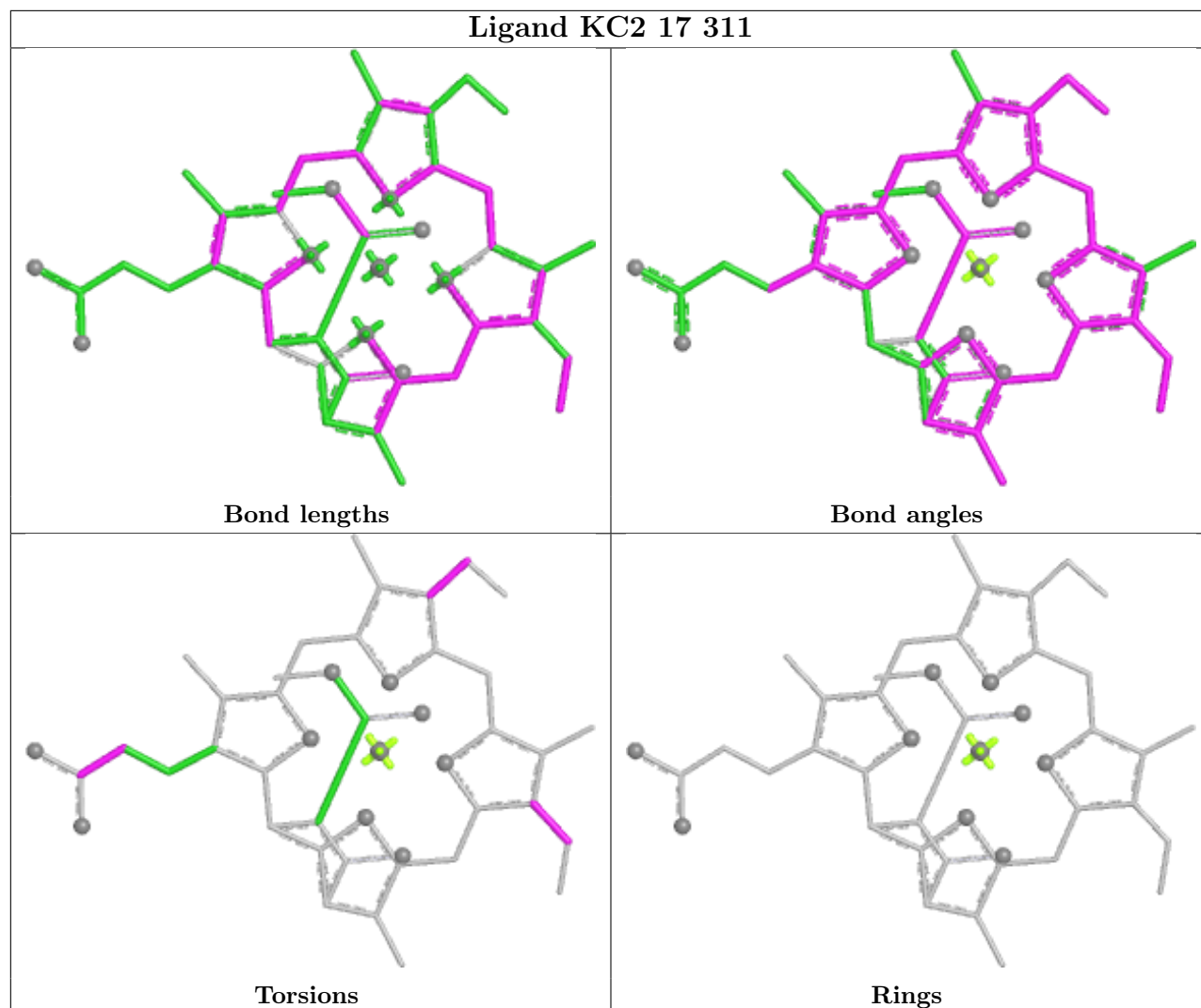
Ligand CLA P 606



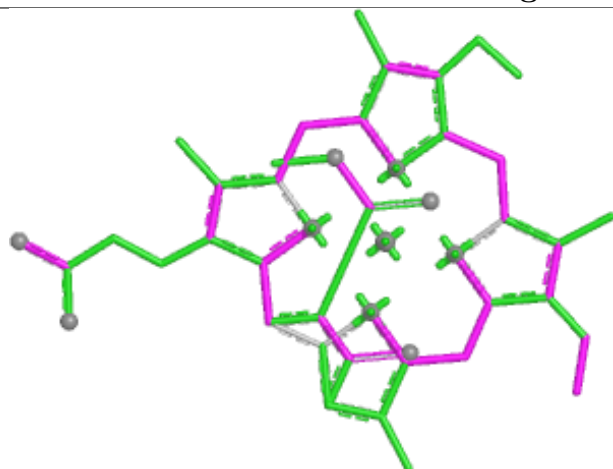


Ligand CLA 4 312**Ligand CLA c 511**

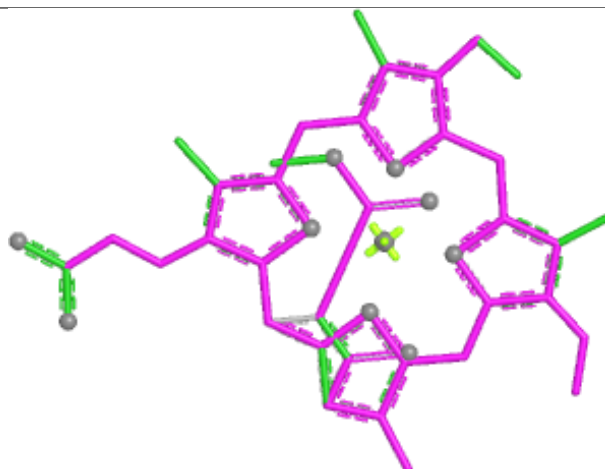




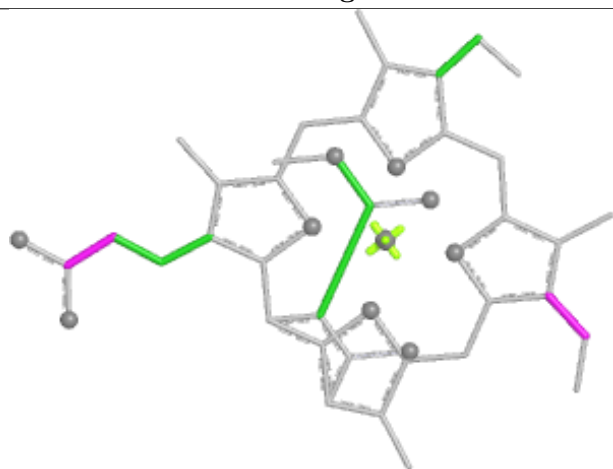
Ligand KC2 1 311



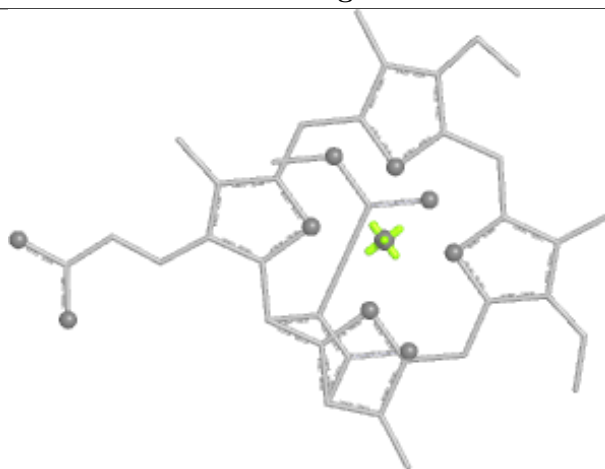
Bond lengths



Bond angles

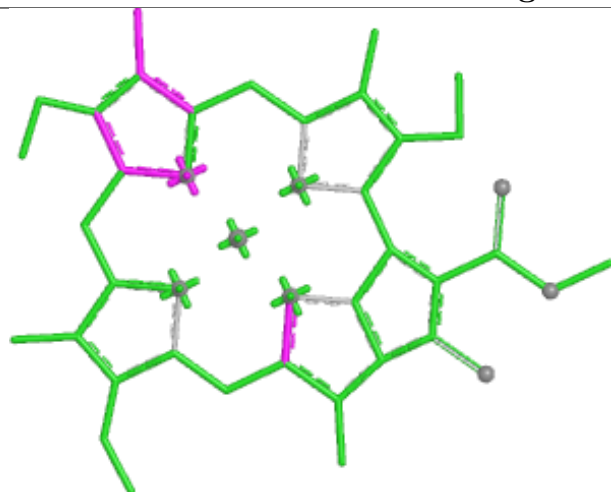


Torsions

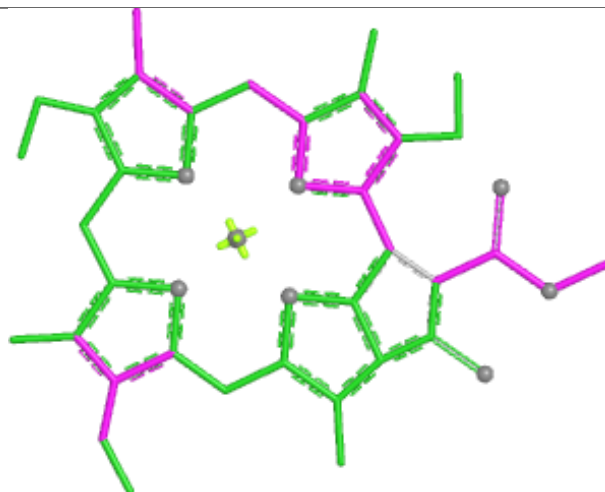


Rings

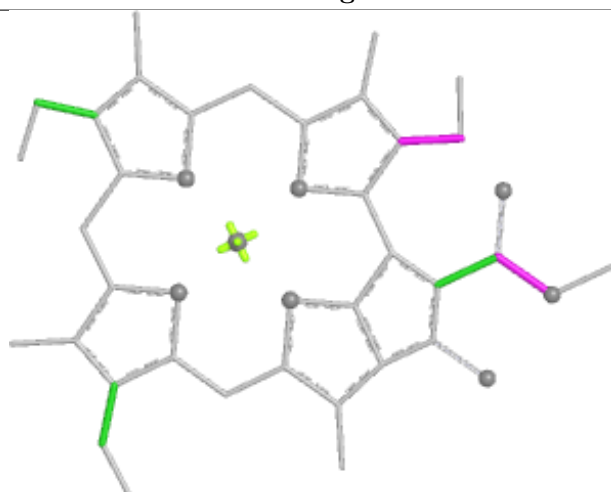
Ligand CLA 3 307



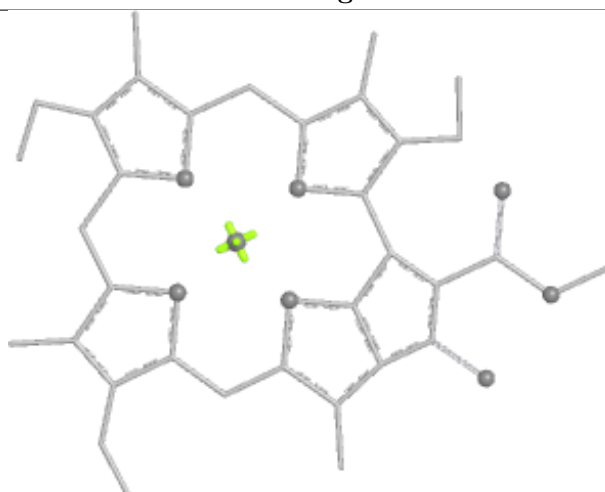
Bond lengths



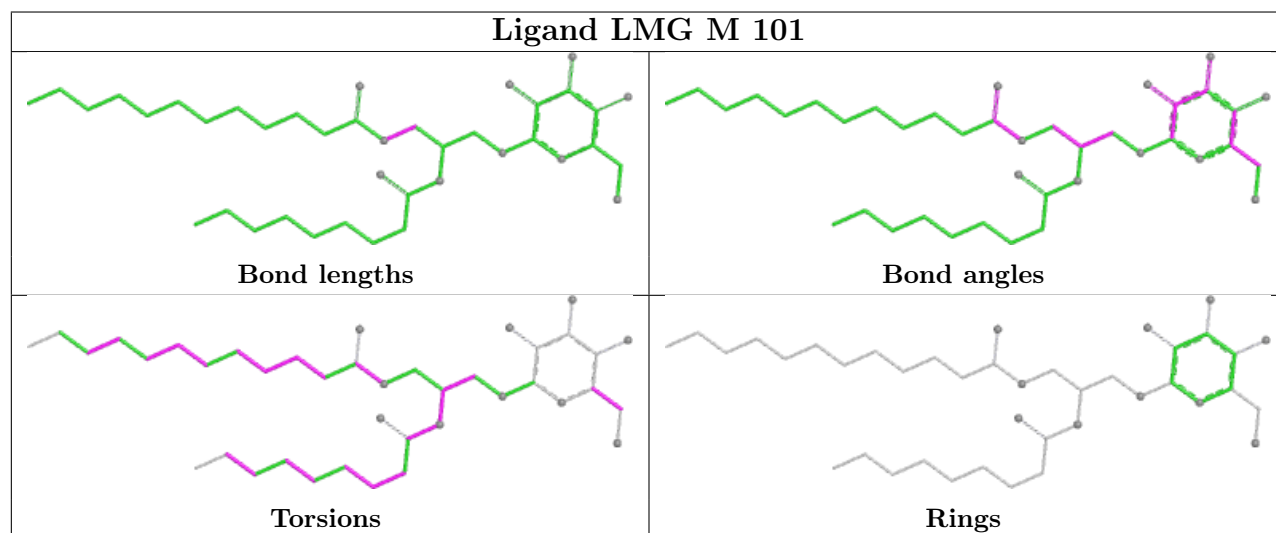
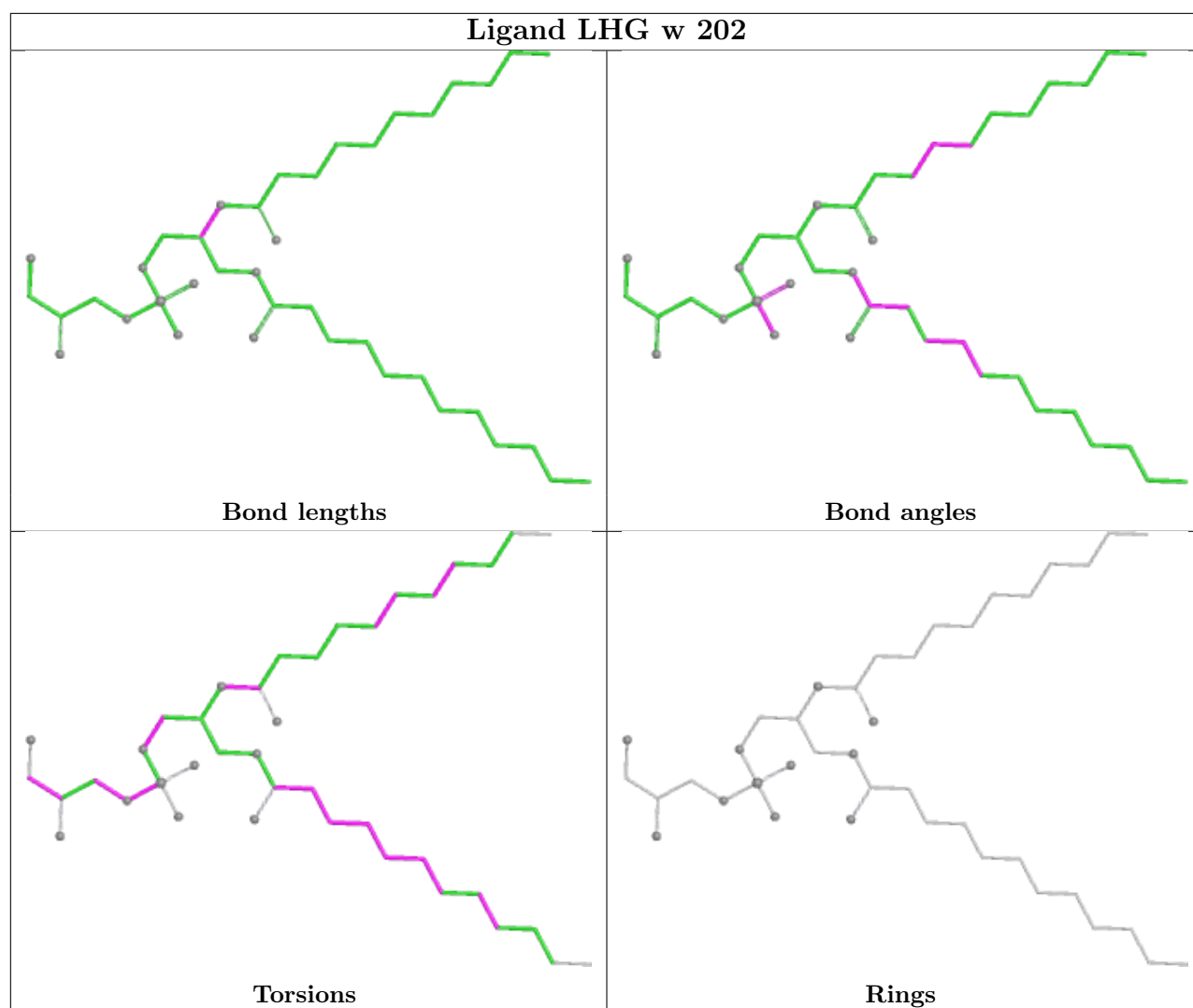
Bond angles



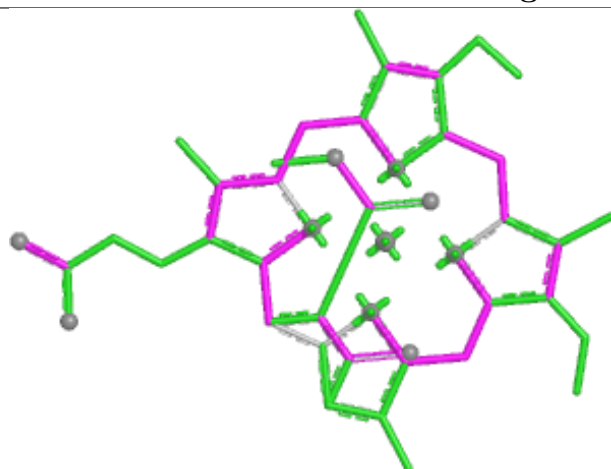
Torsions



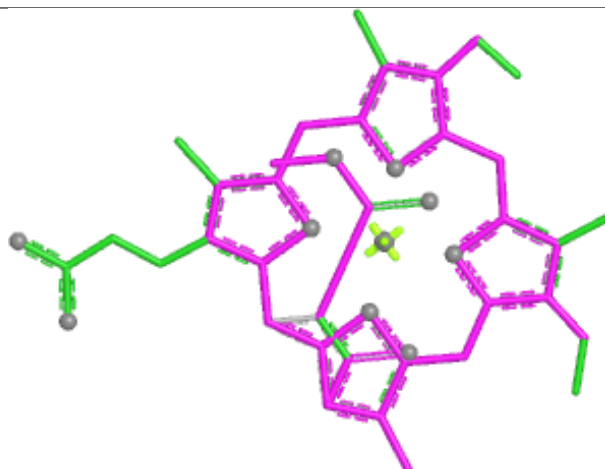
Rings



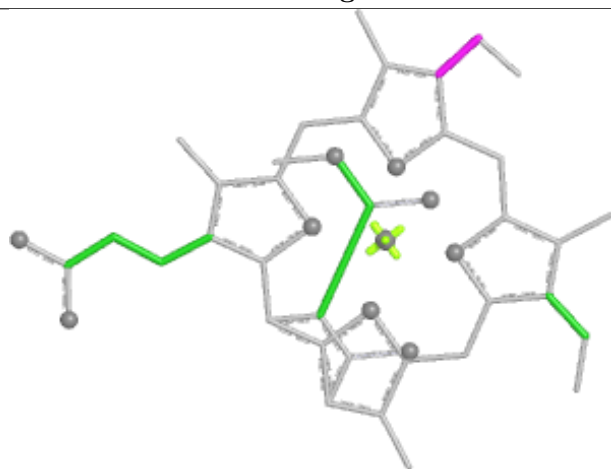
Ligand KC1 3 314



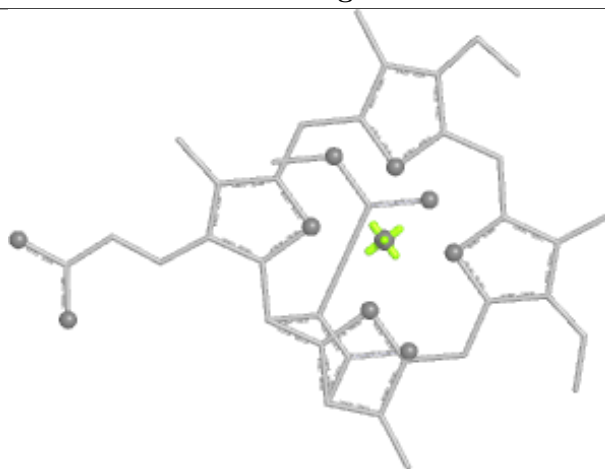
Bond lengths



Bond angles

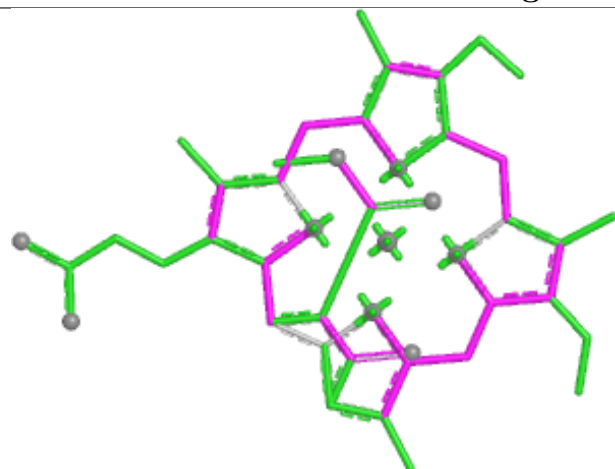


Torsions

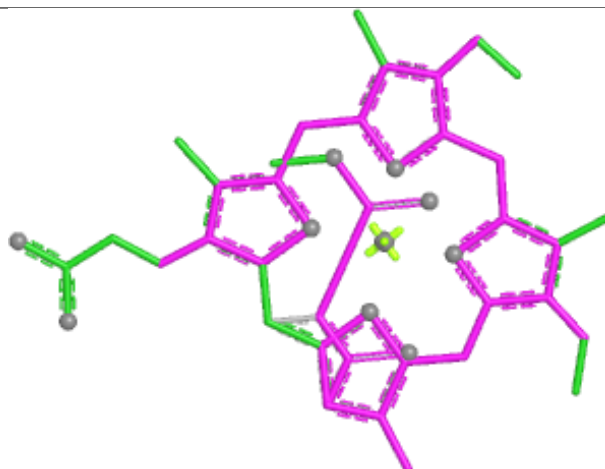


Rings

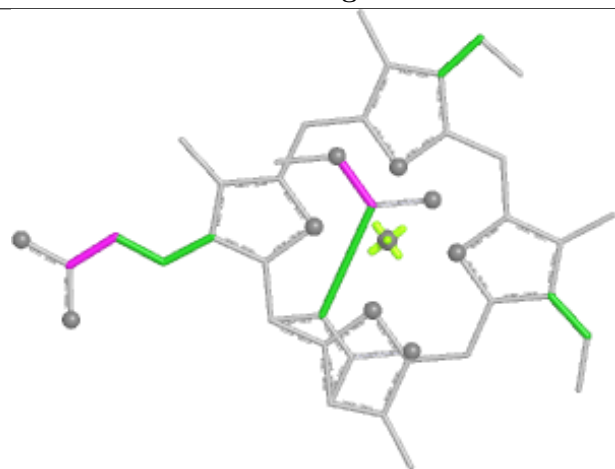
Ligand KC1 5 313



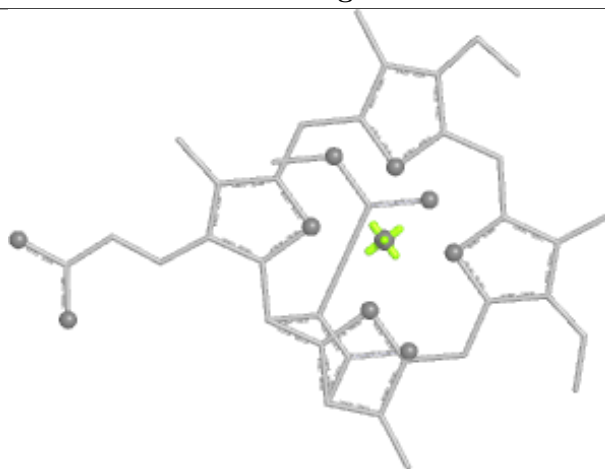
Bond lengths



Bond angles

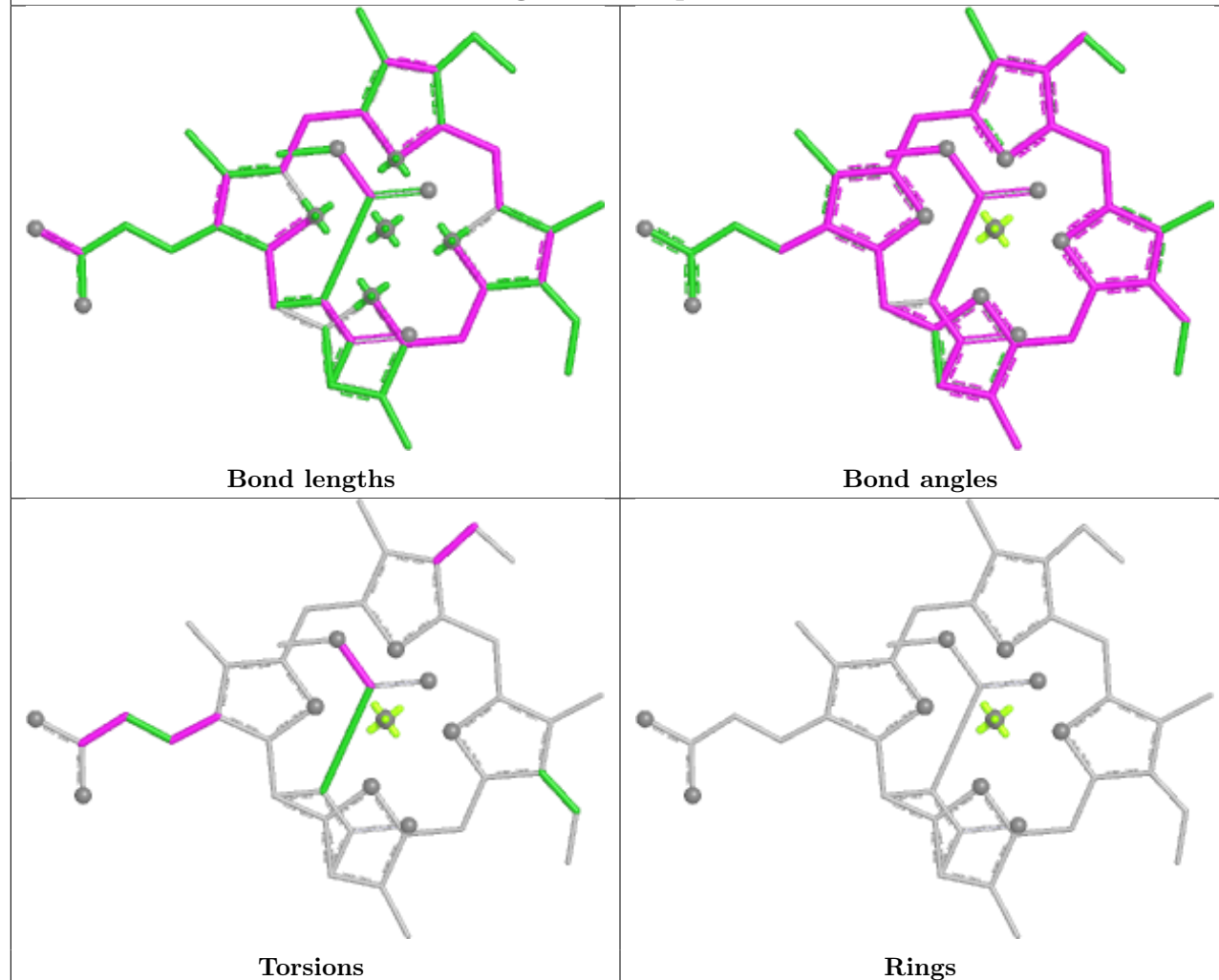


Torsions

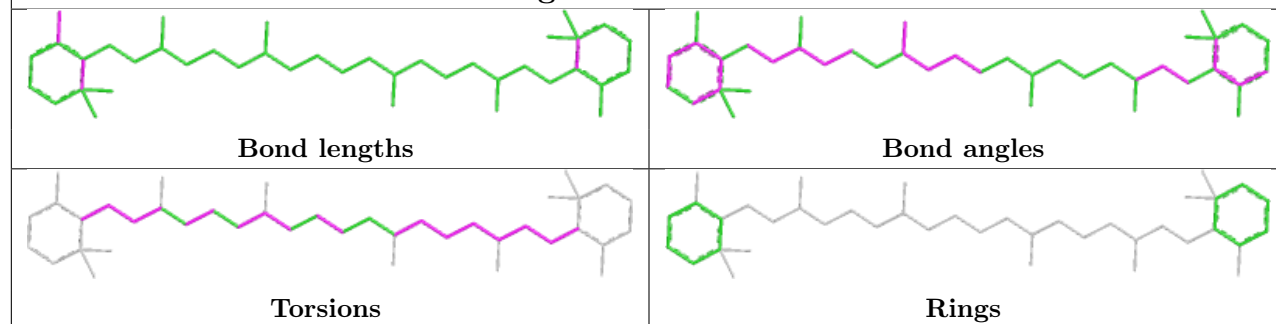


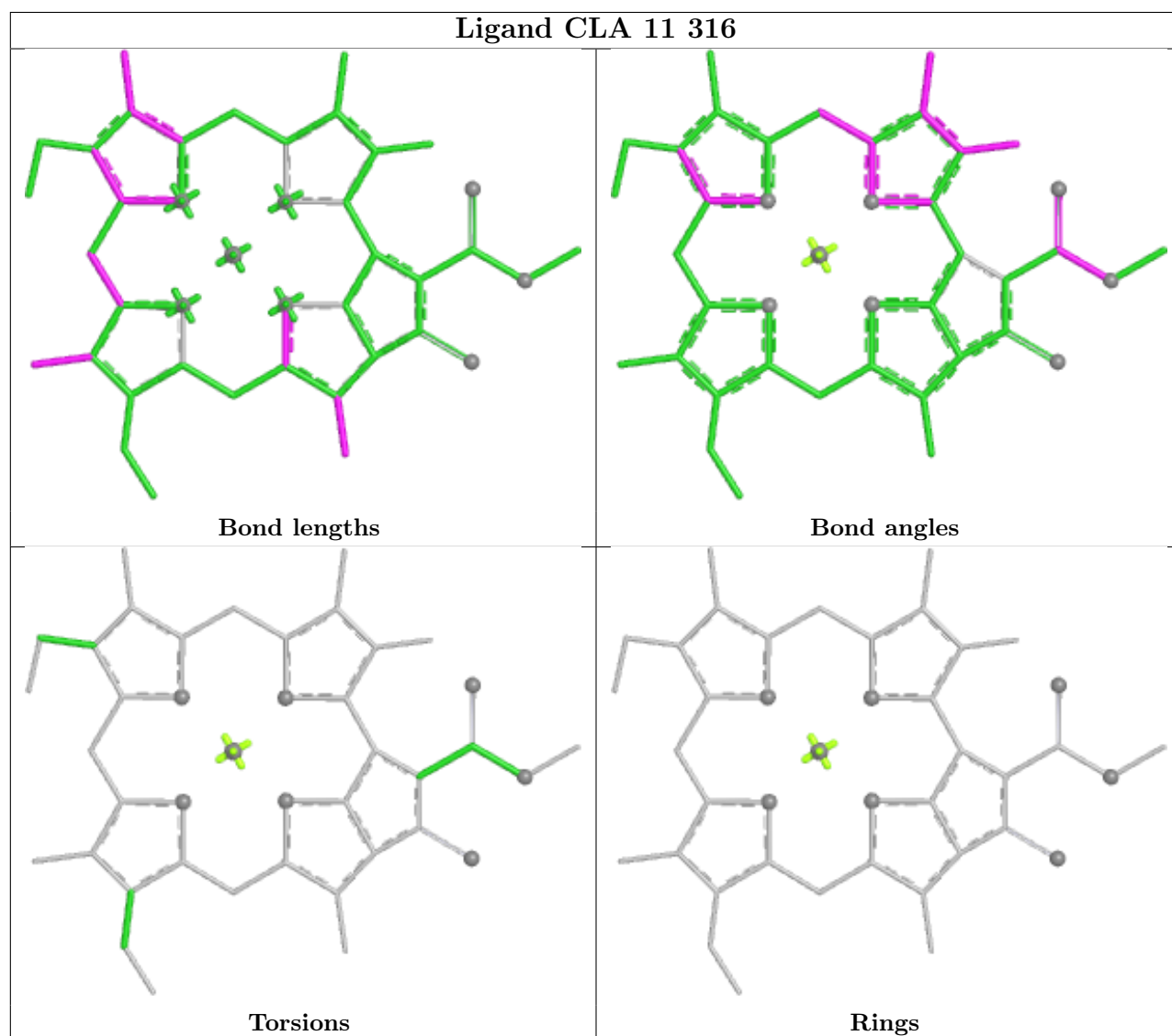
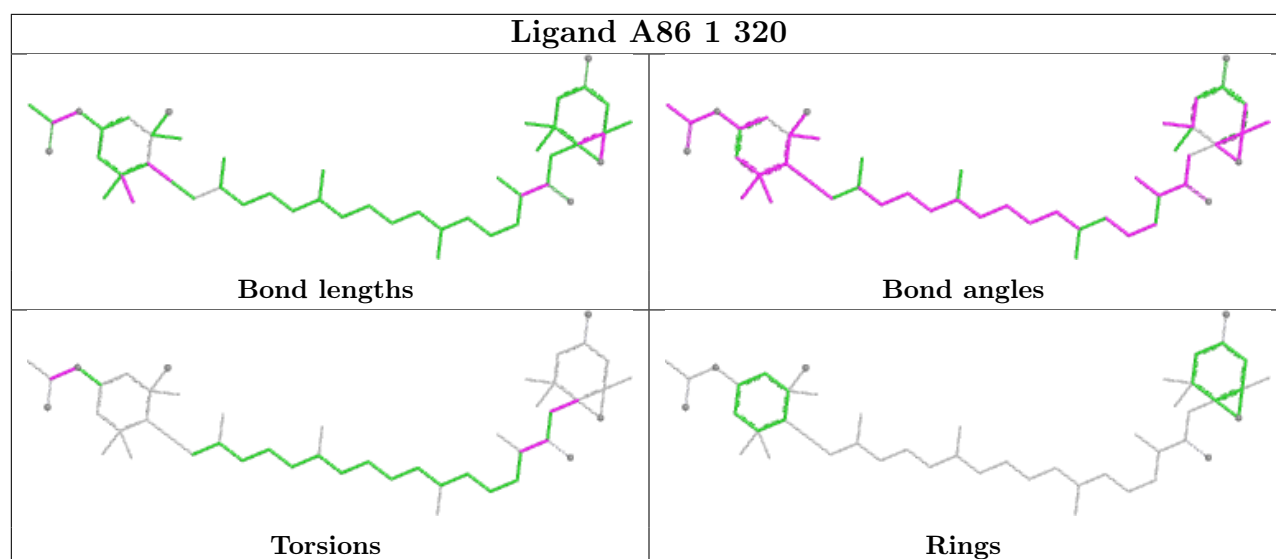
Rings

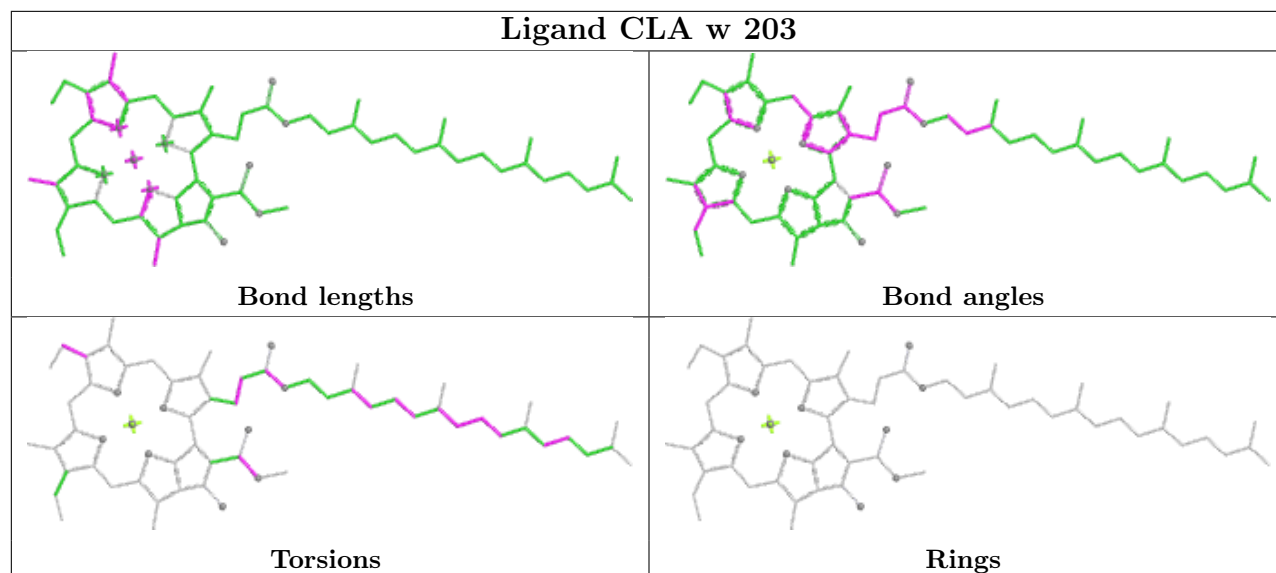
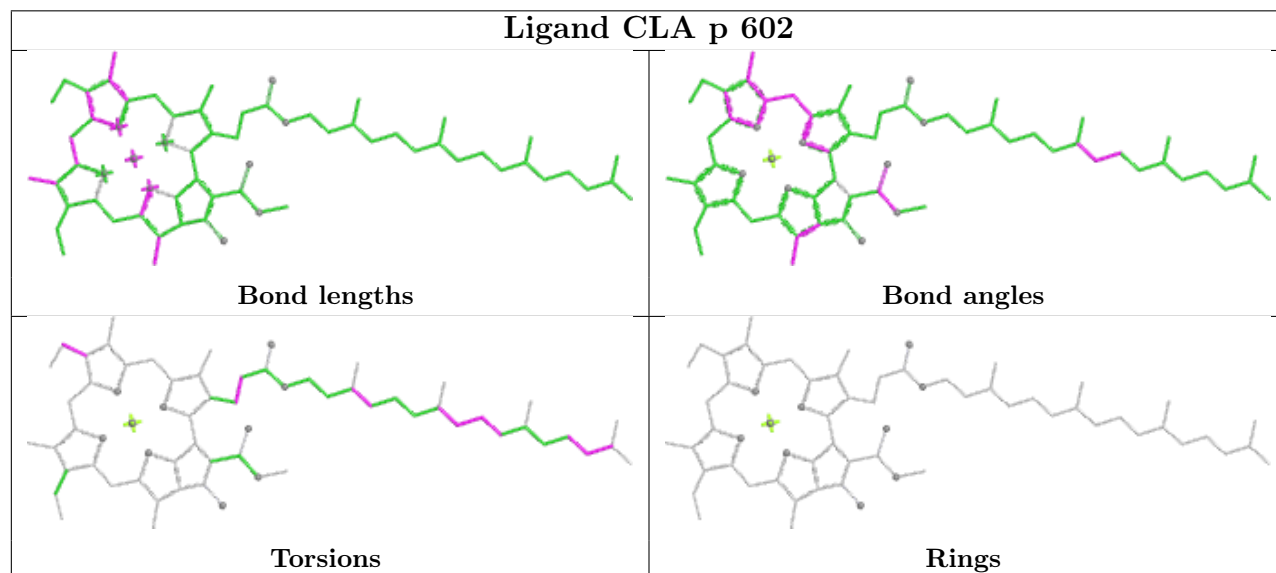
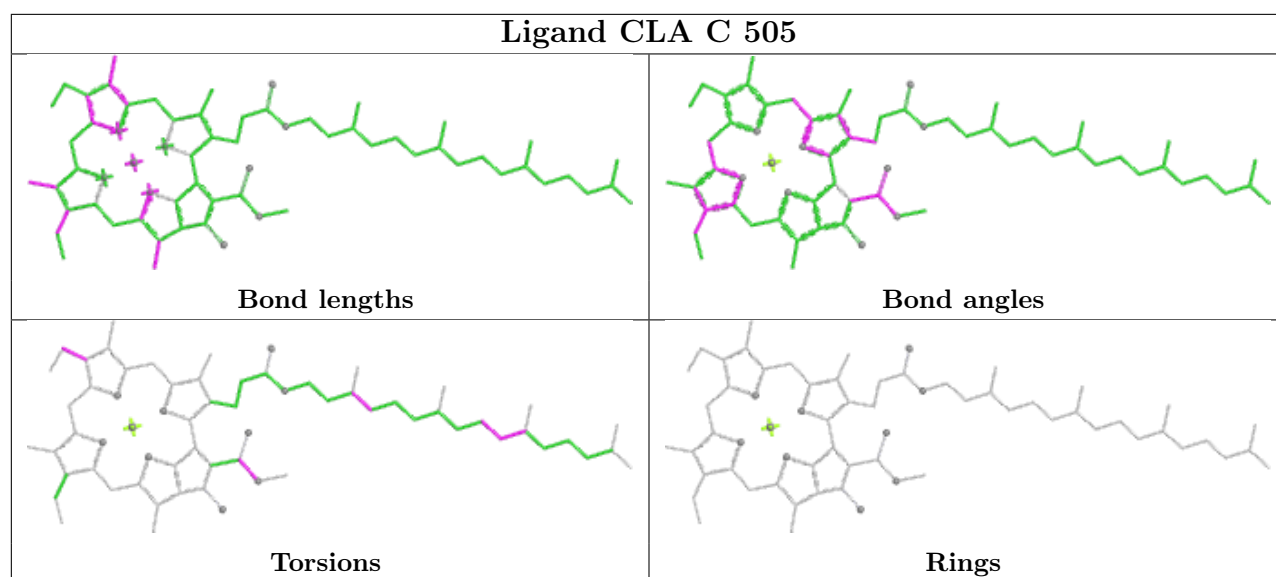
Ligand KC1 p 609



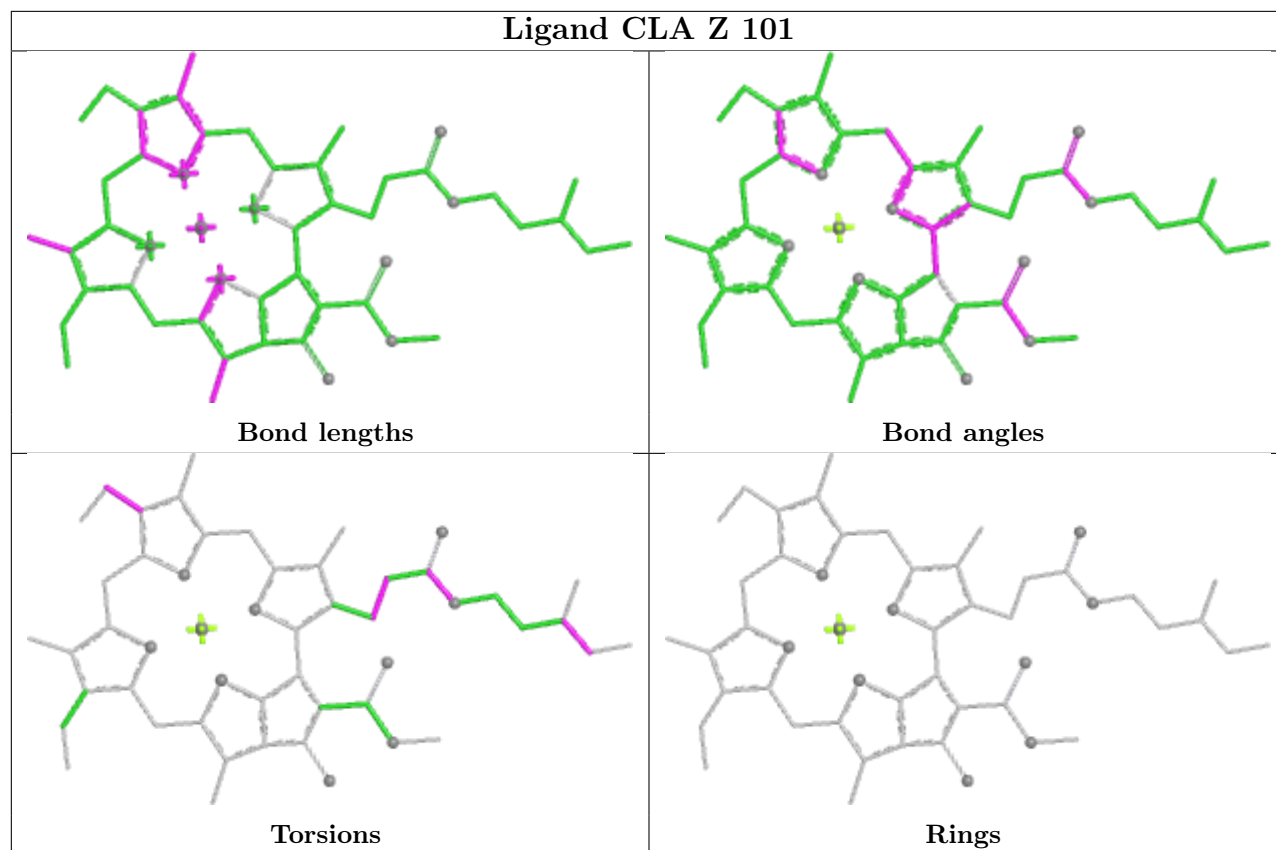
Ligand BCR f 101



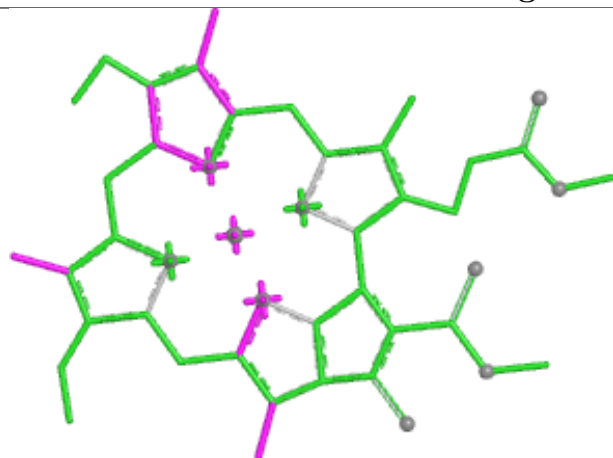




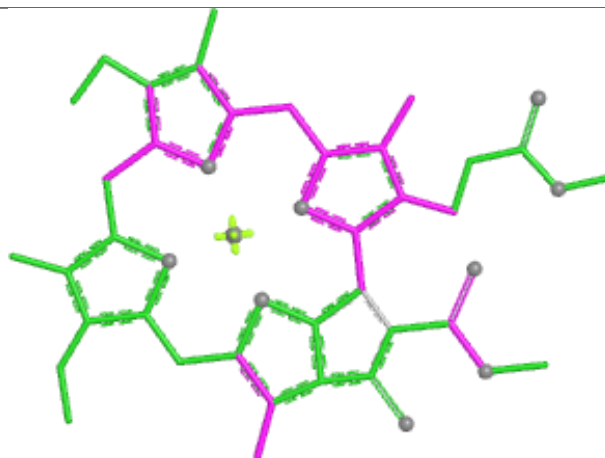
Ligand CLA Z 101



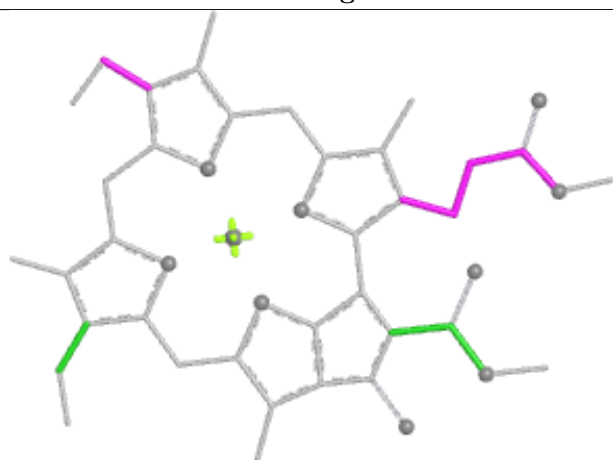
Ligand CLA 8 312



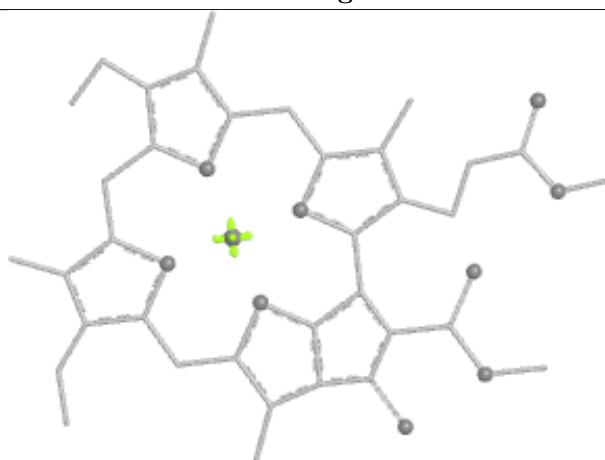
Bond lengths



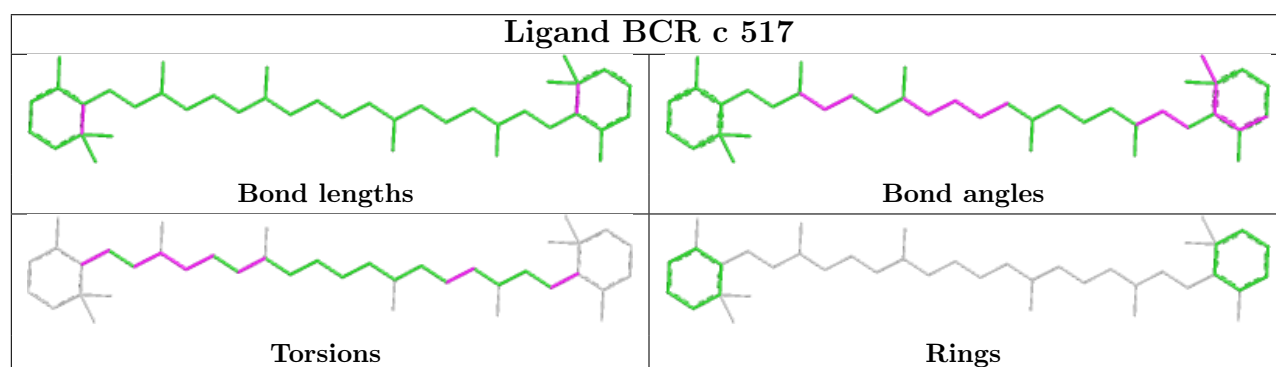
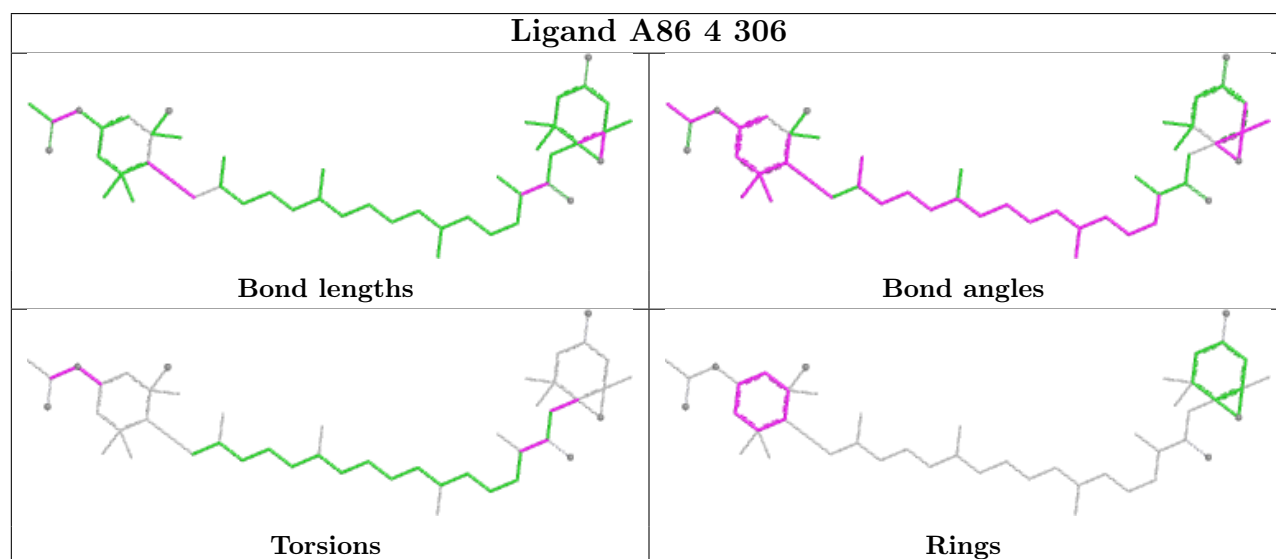
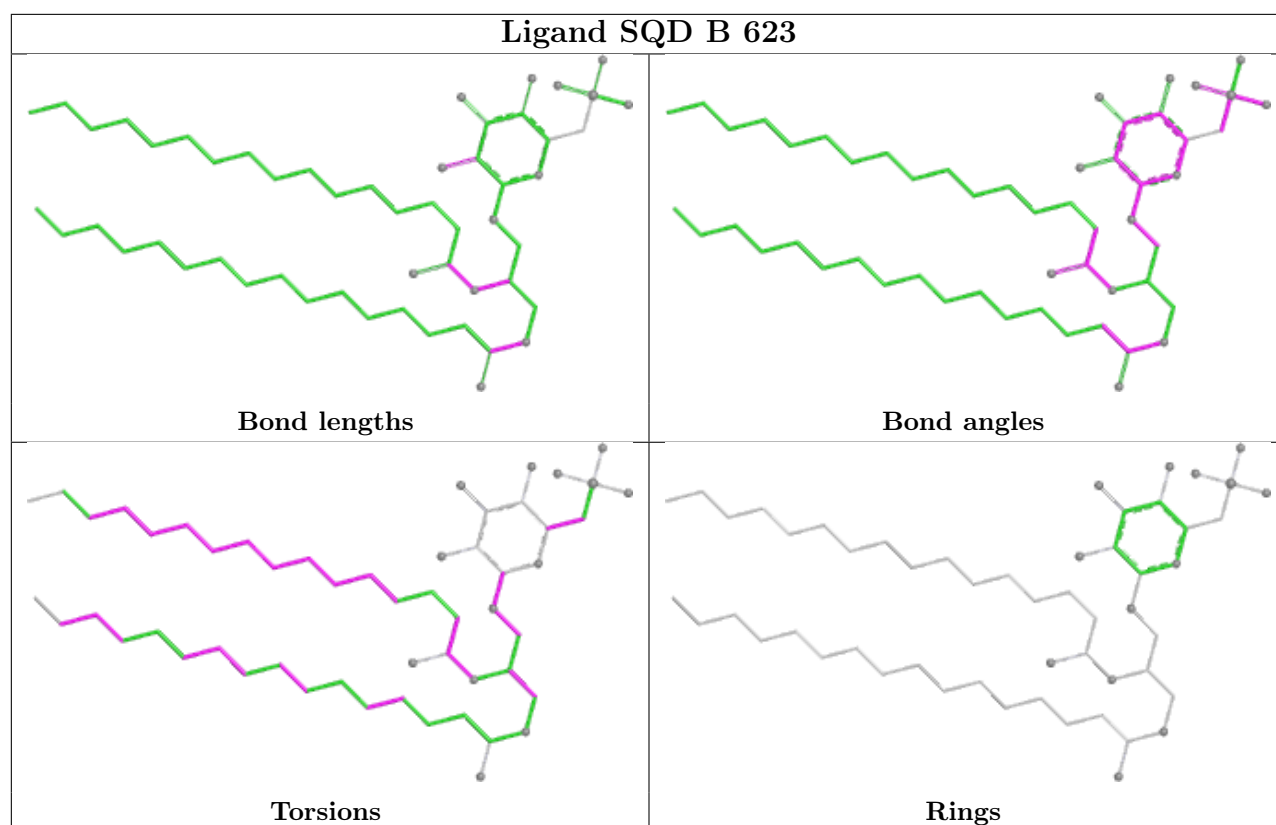
Bond angles



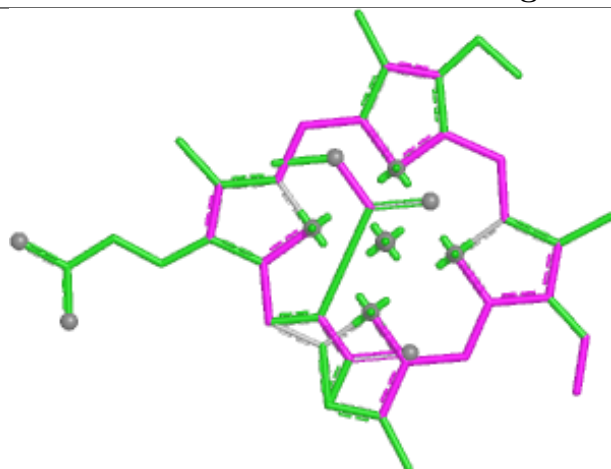
Torsions



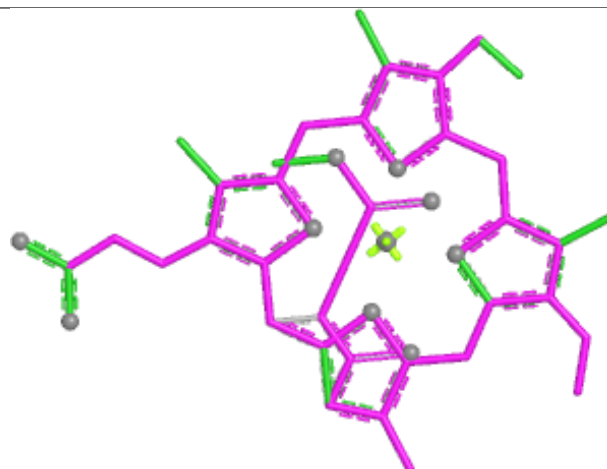
Rings



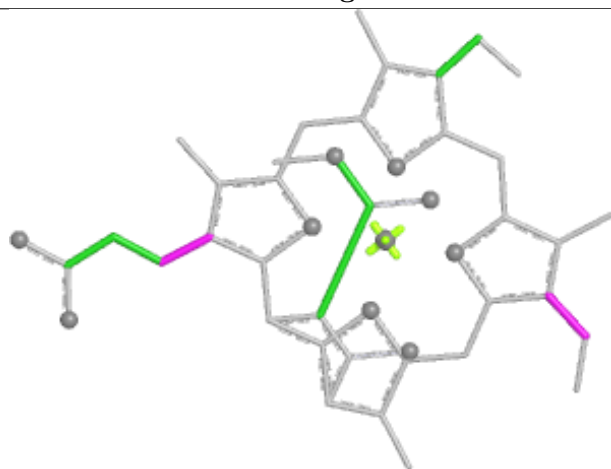
Ligand KC2 4 308



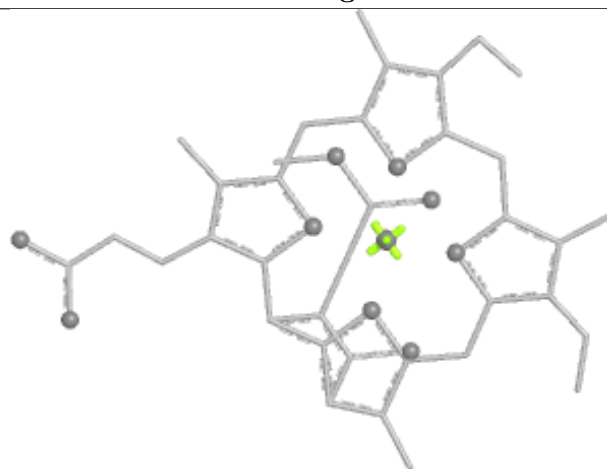
Bond lengths



Bond angles

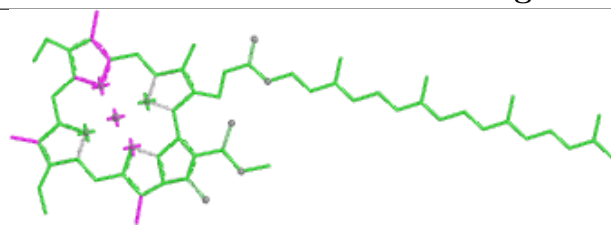


Torsions

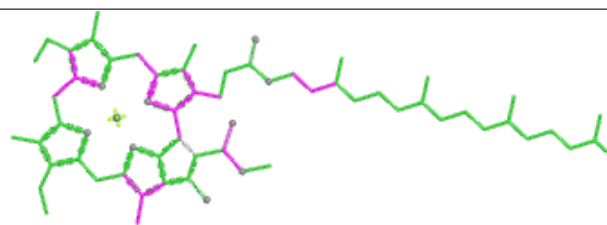


Rings

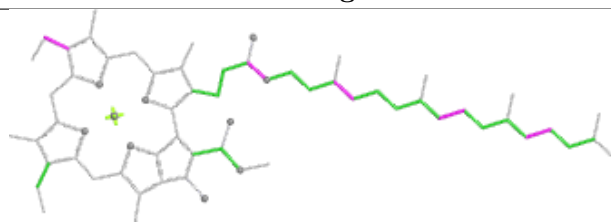
Ligand CLA C 512



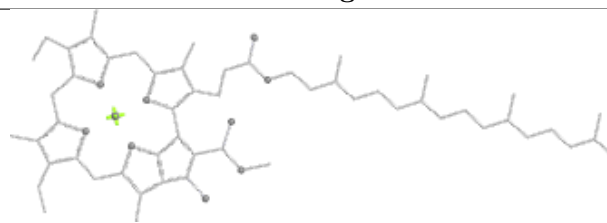
Bond lengths



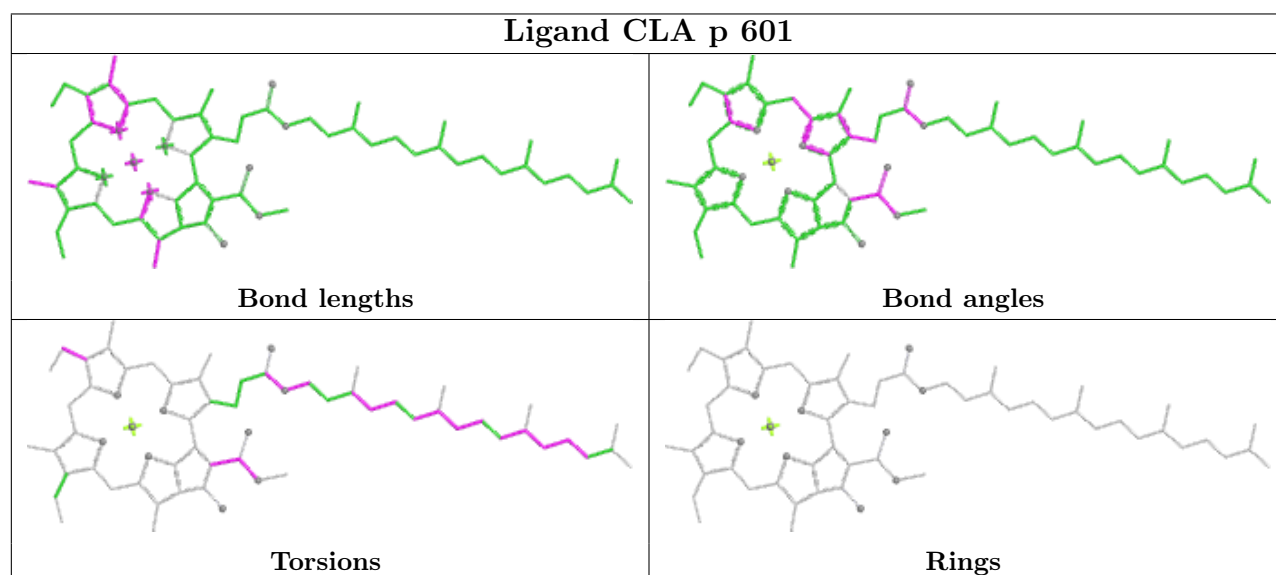
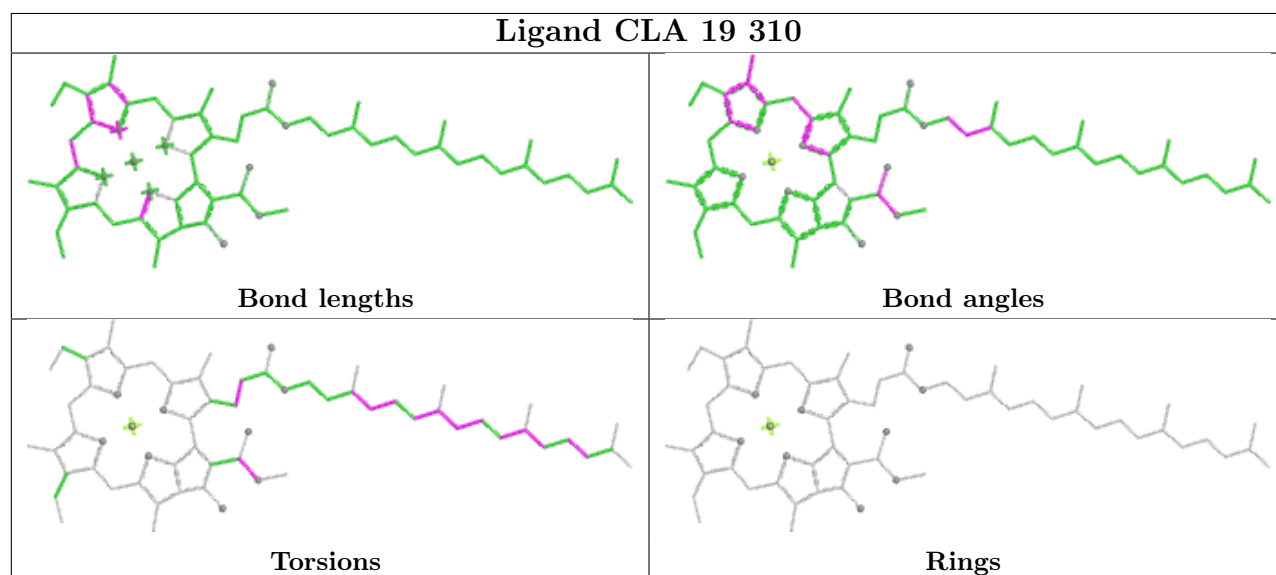
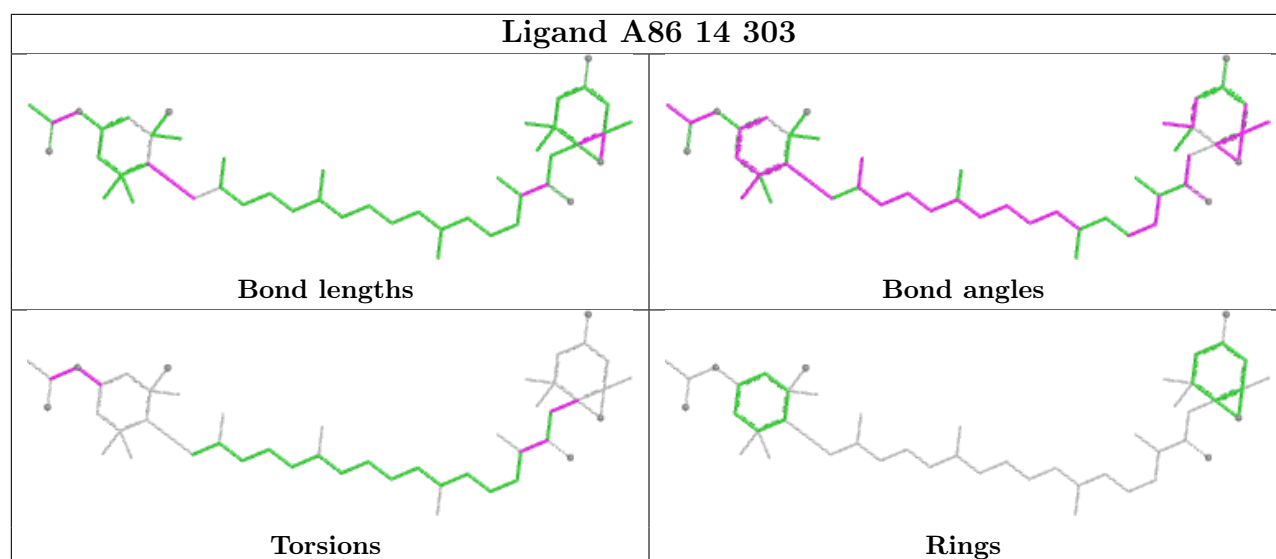
Bond angles



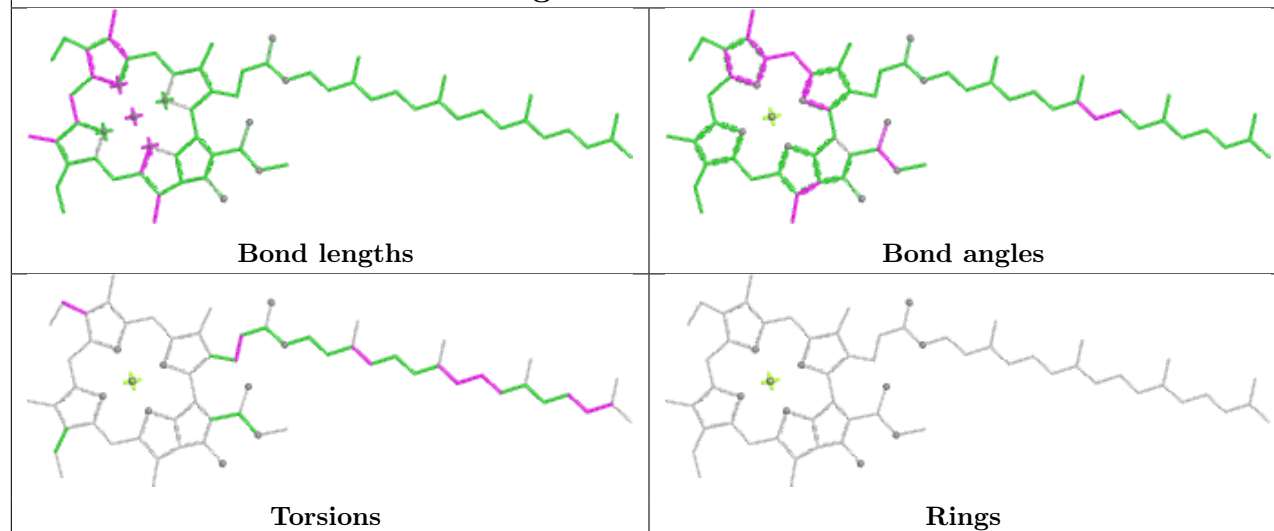
Torsions



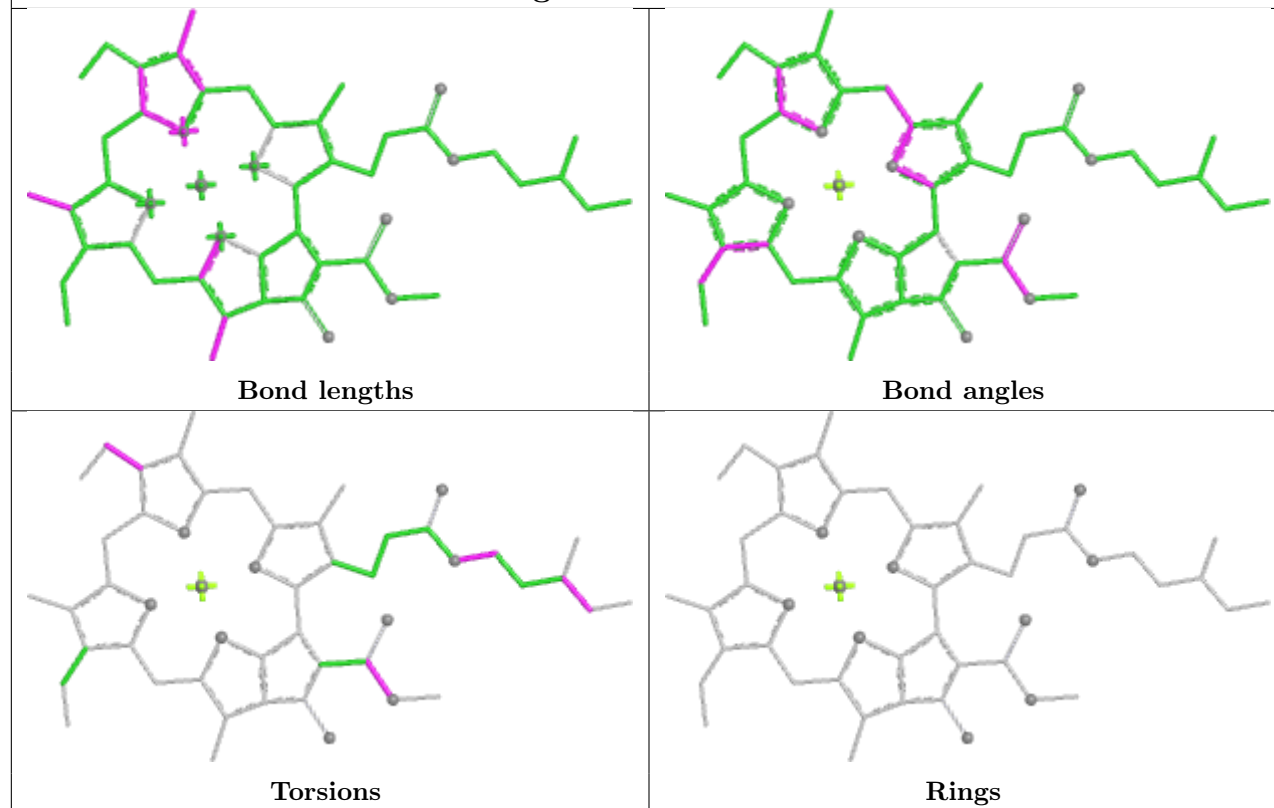
Rings

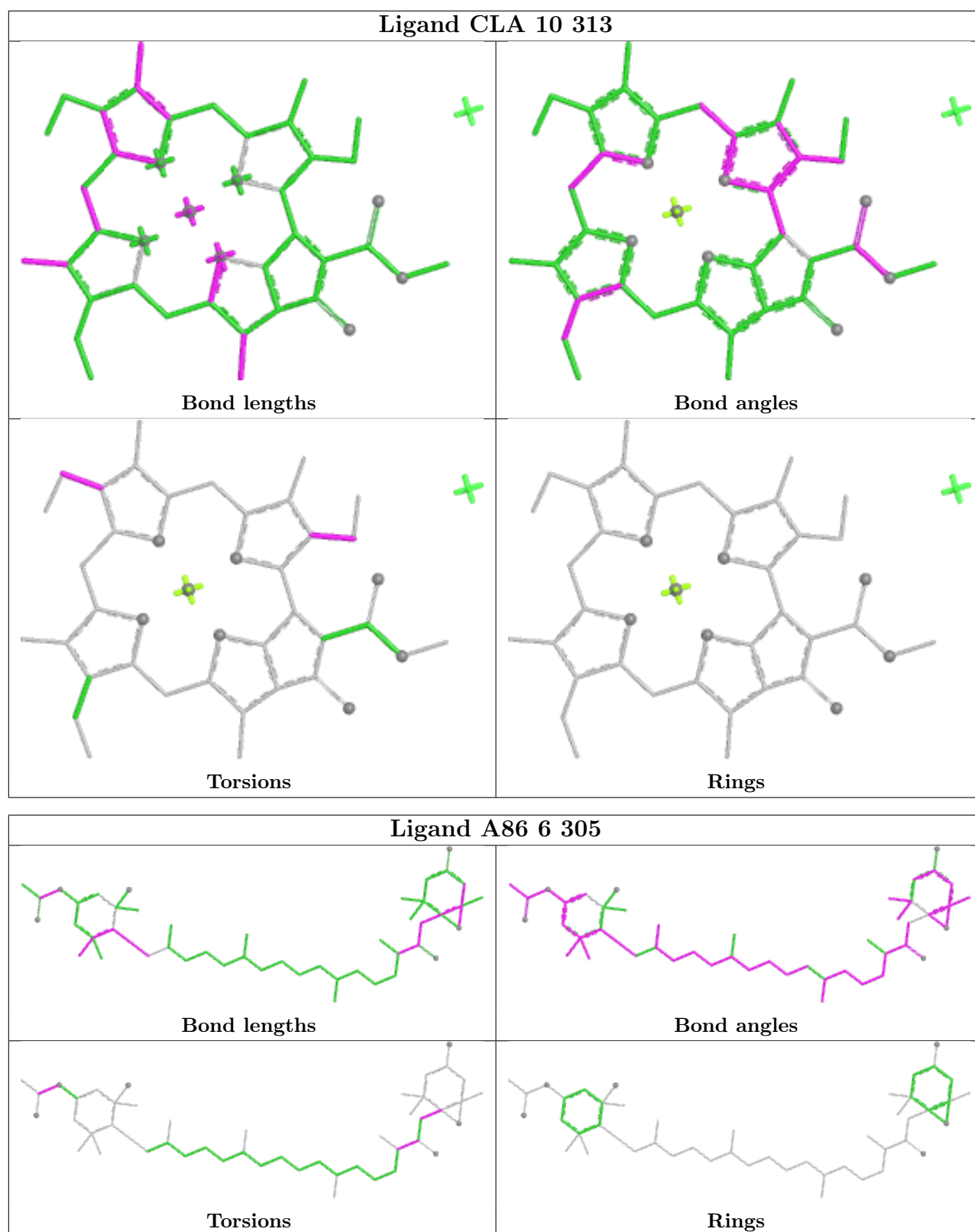


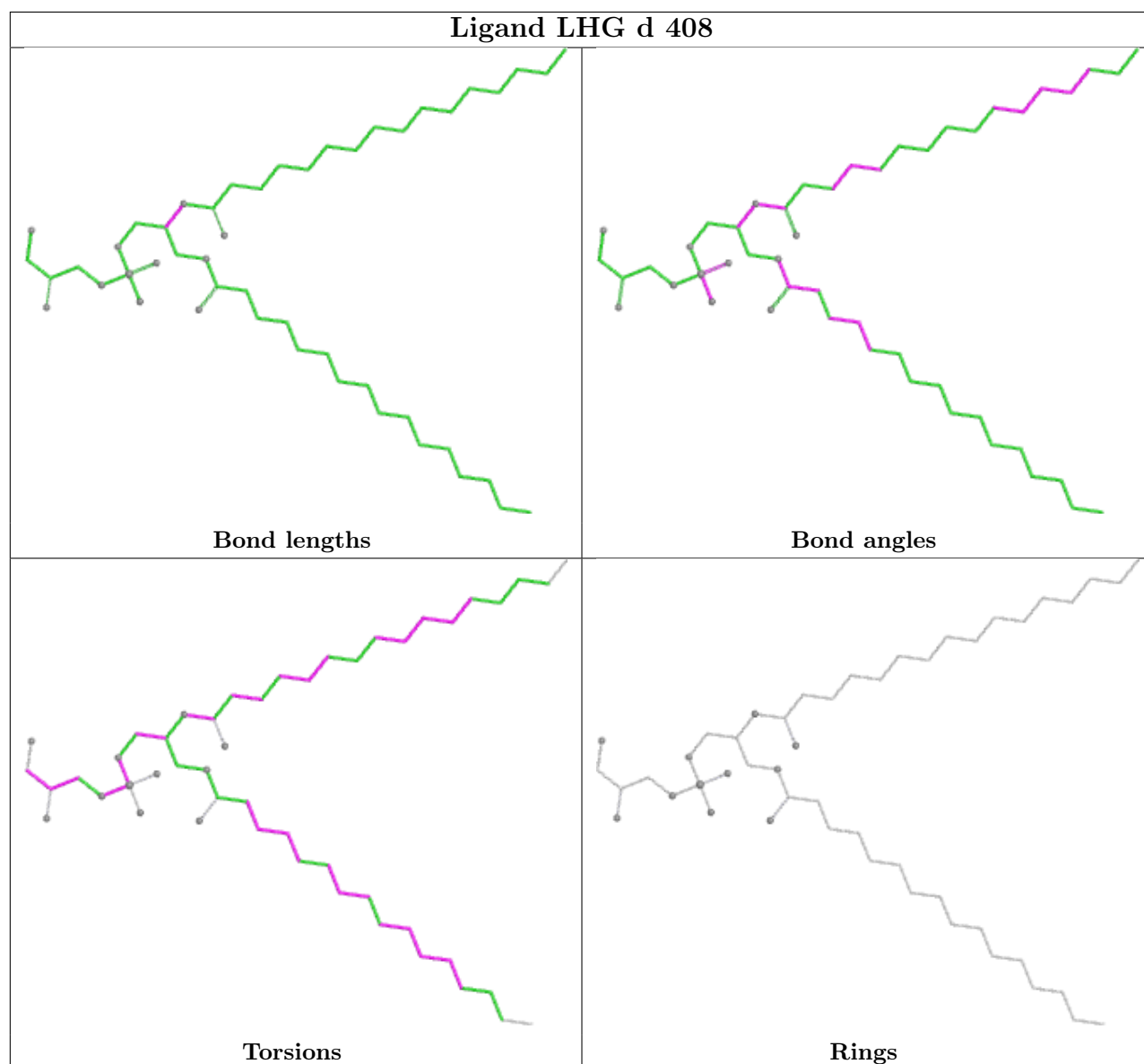
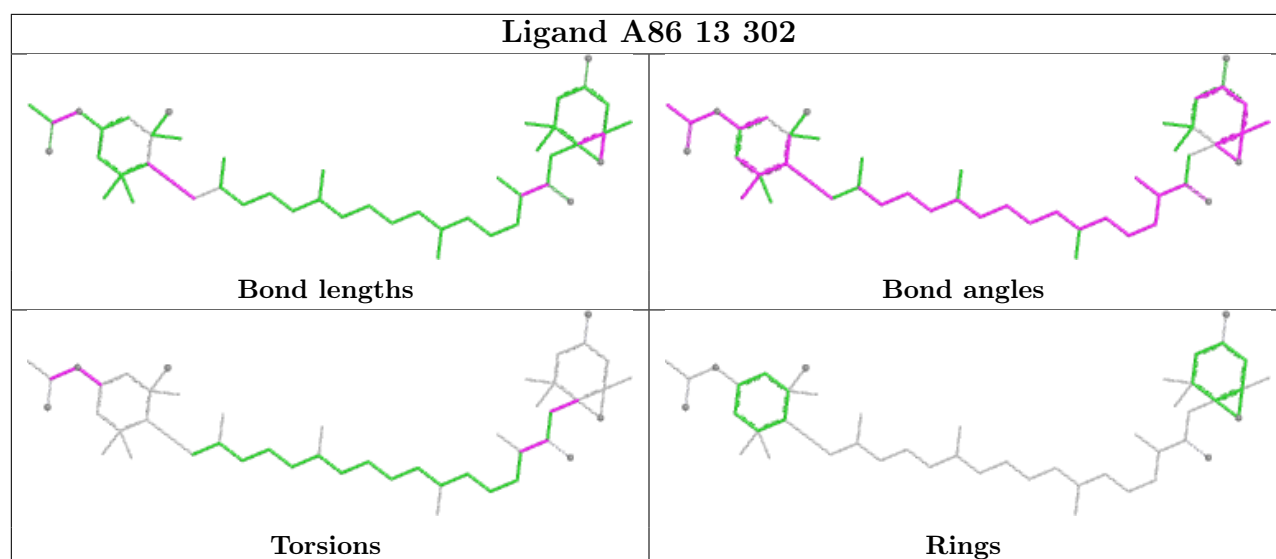
Ligand CLA P 602



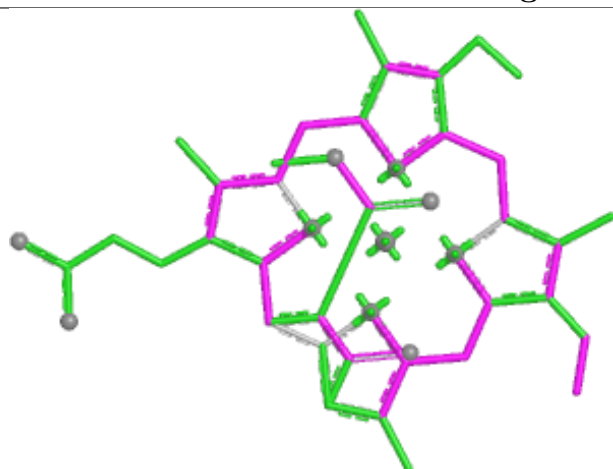
Ligand CLA P 608



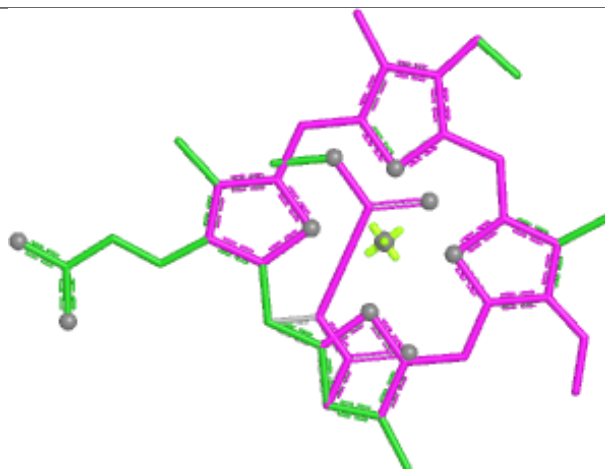




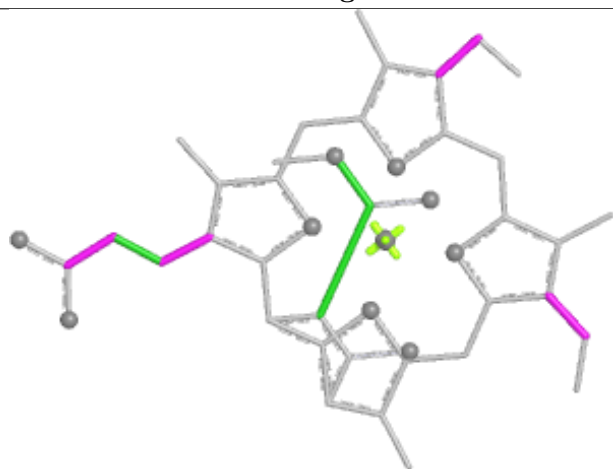
Ligand KC2 0 310



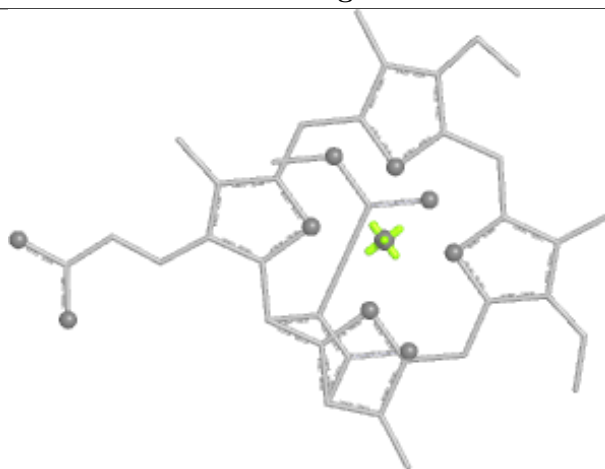
Bond lengths



Bond angles

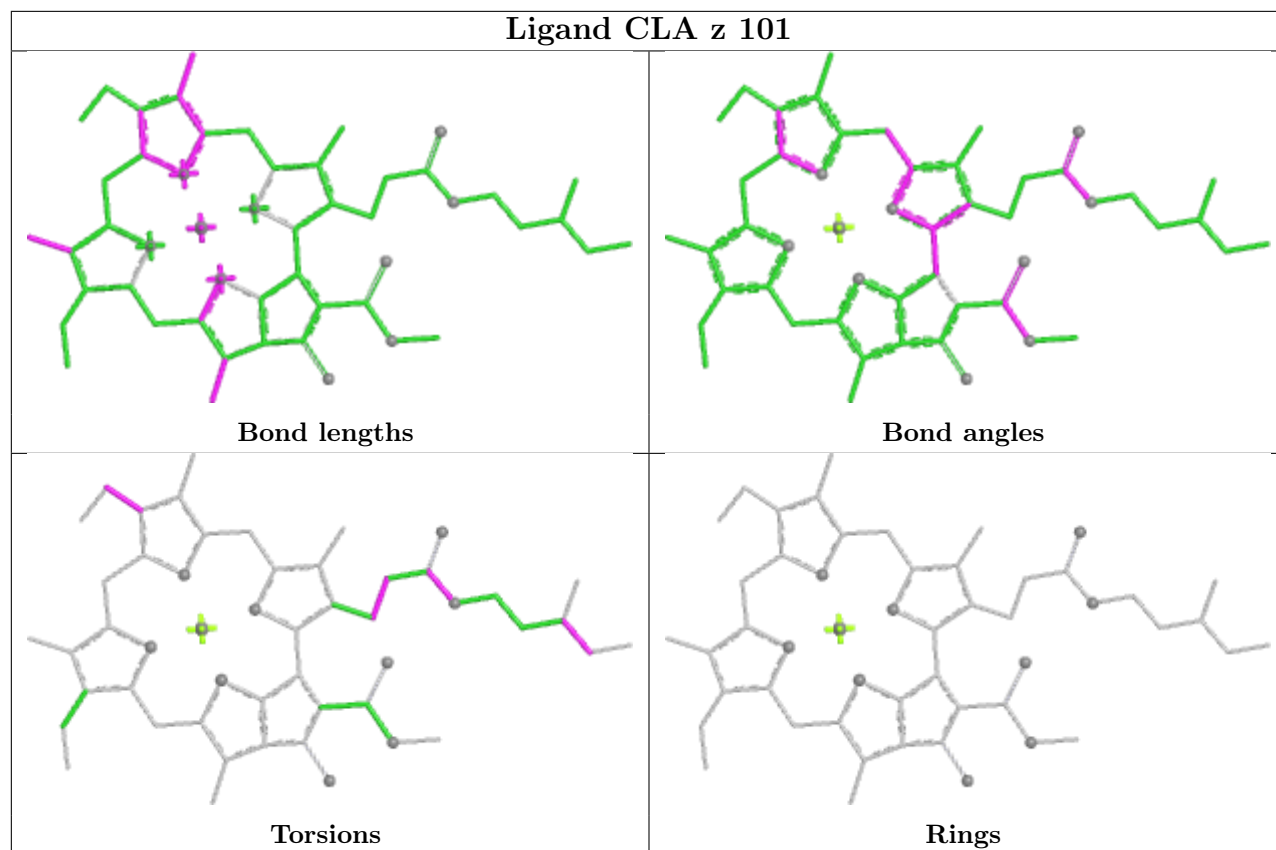


Torsions

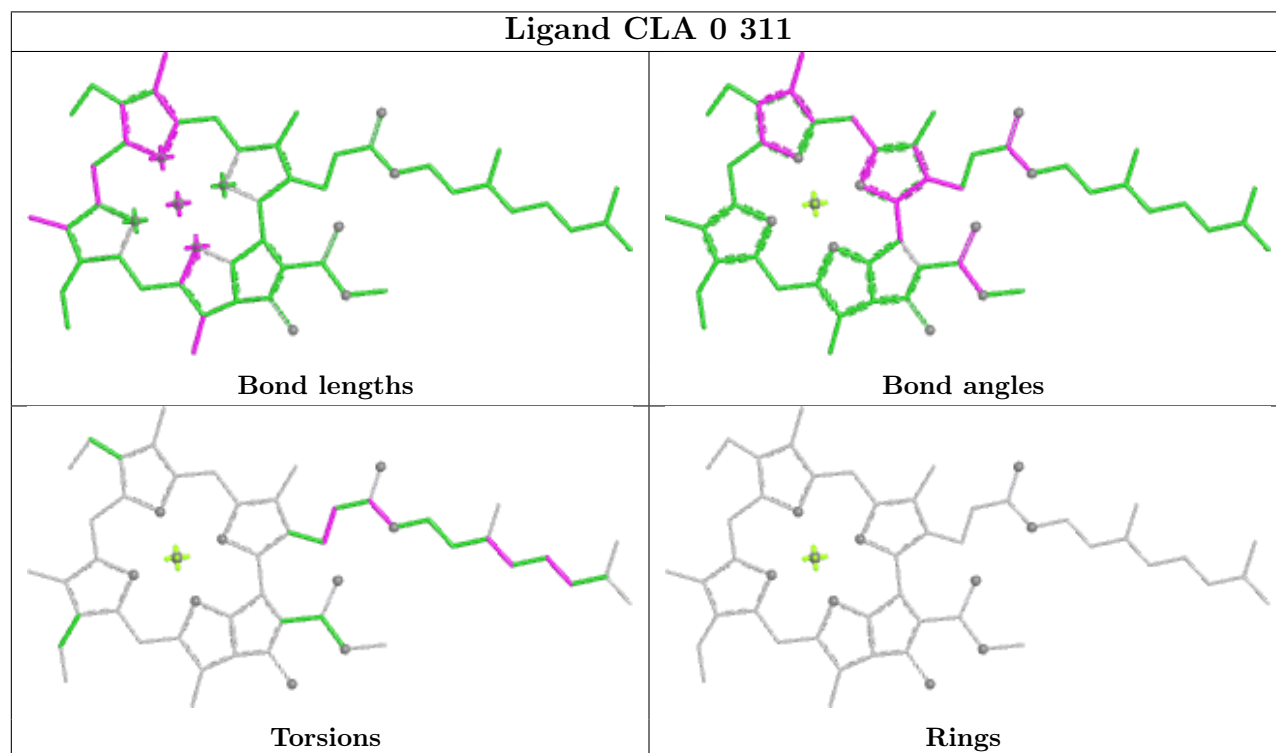


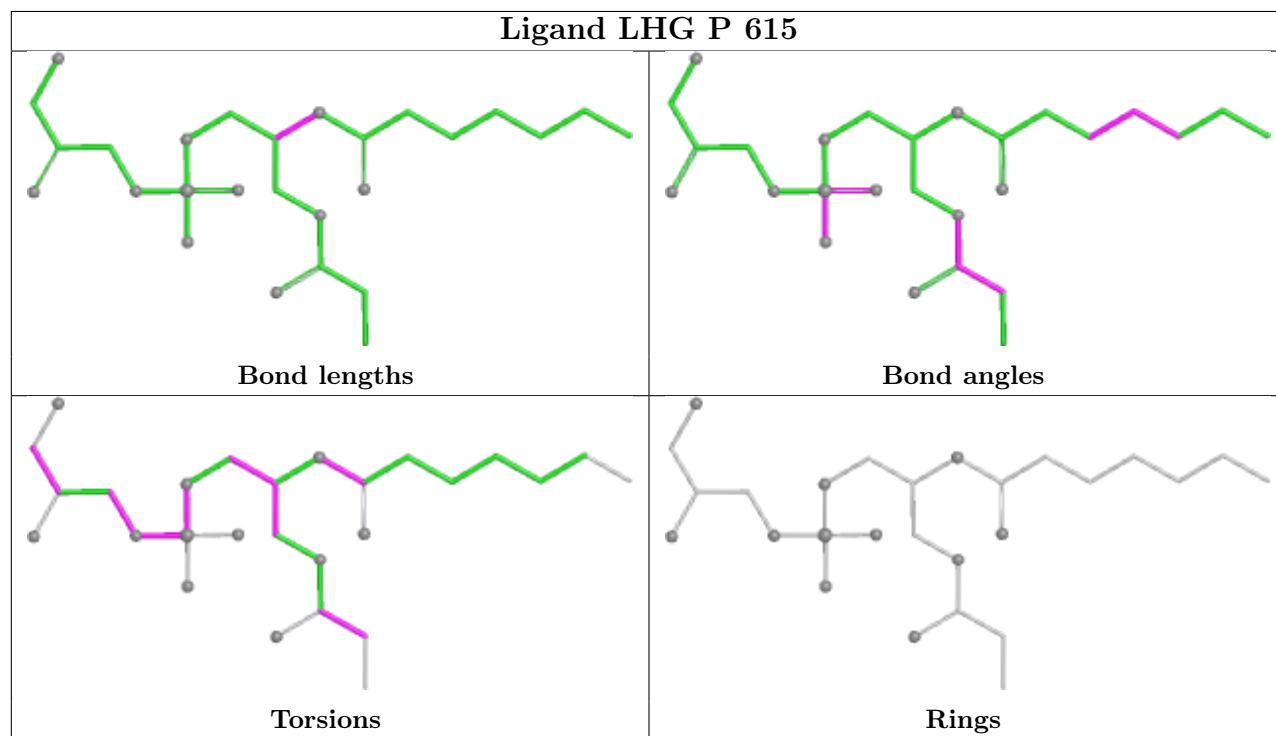
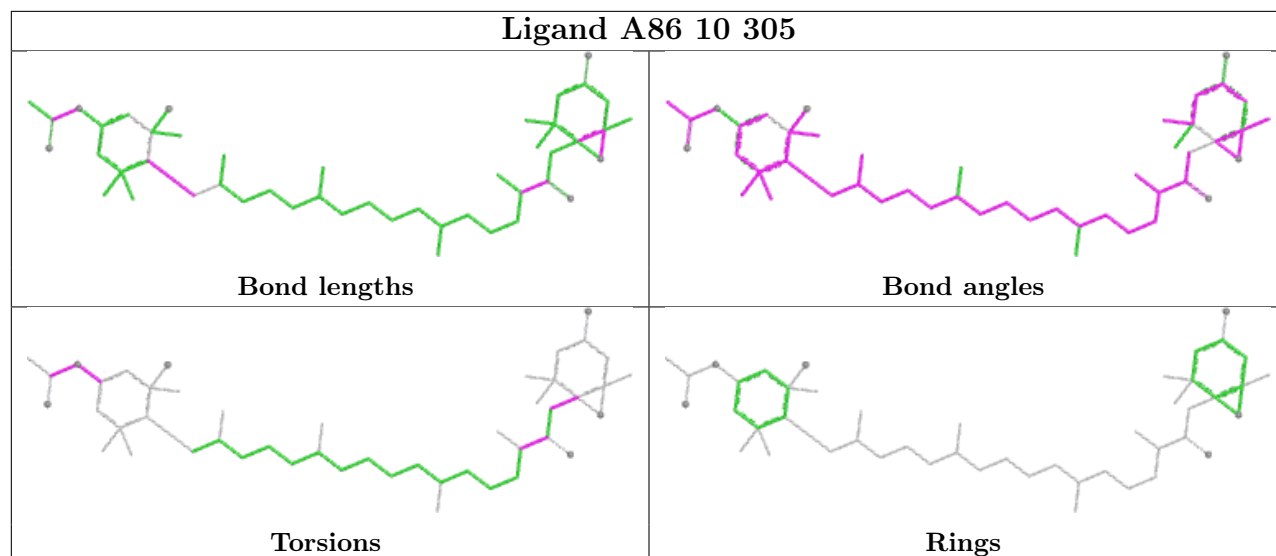
Rings

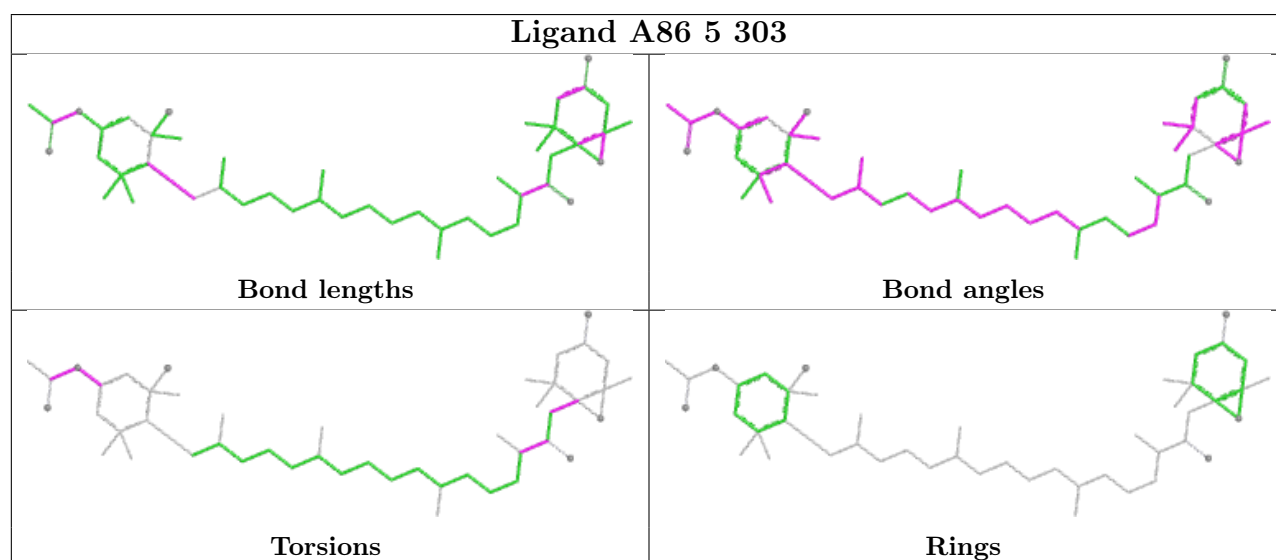
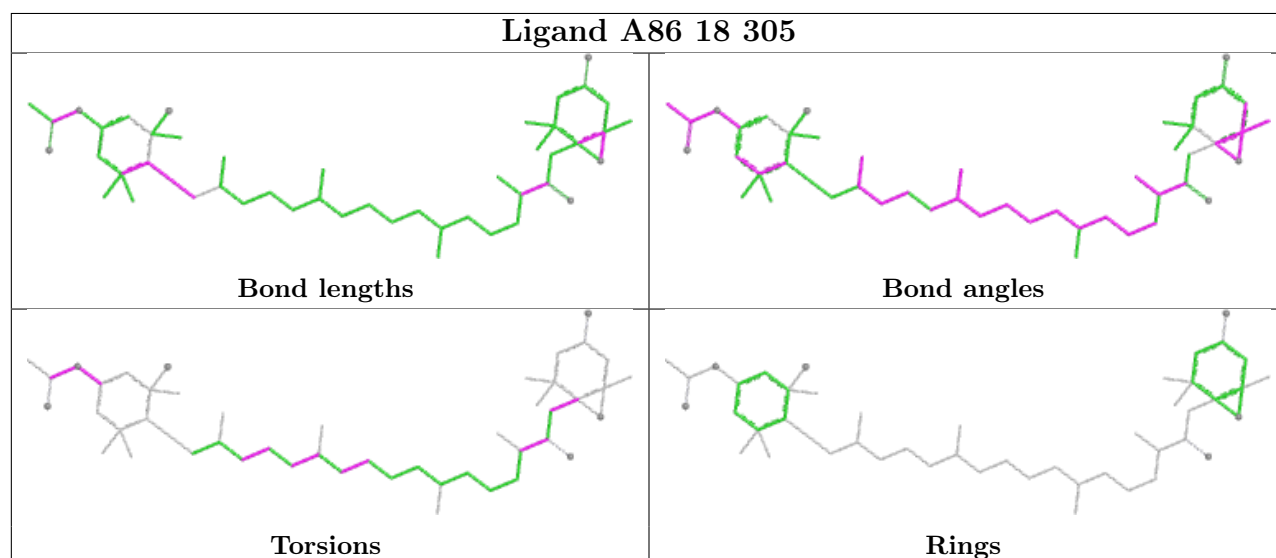
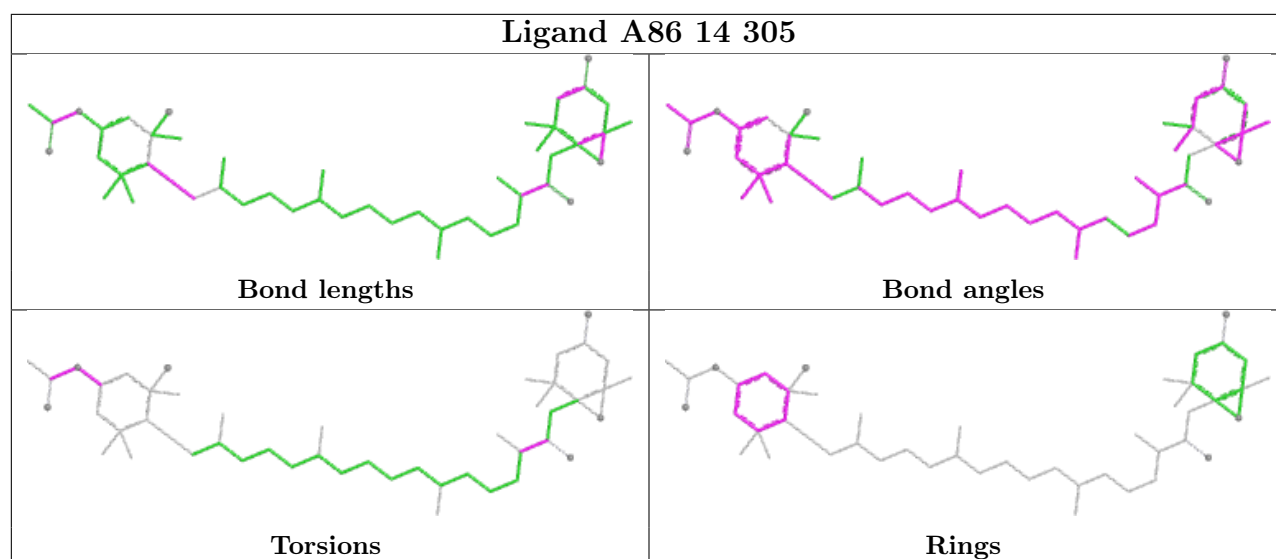
Ligand CLA z 101

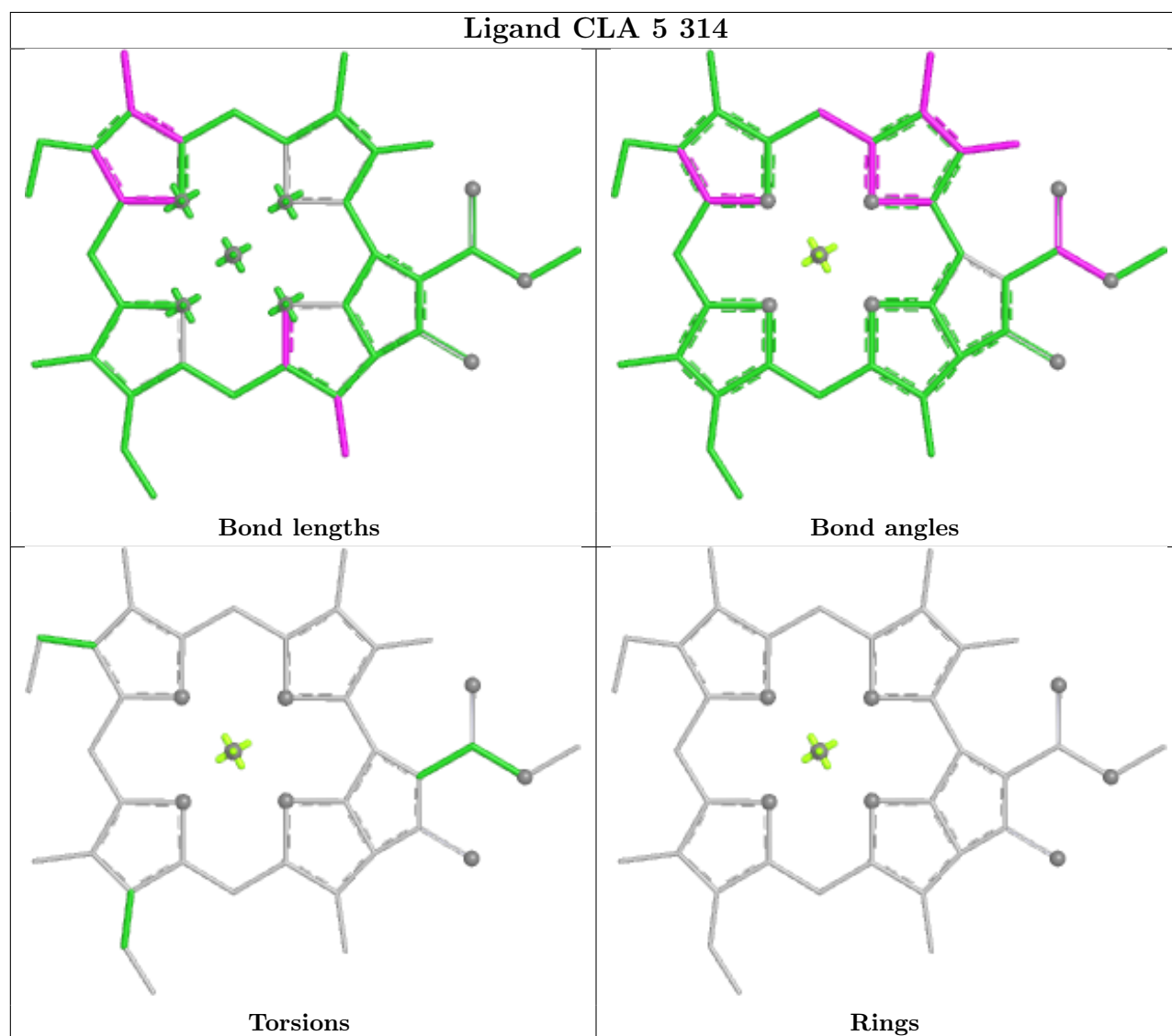
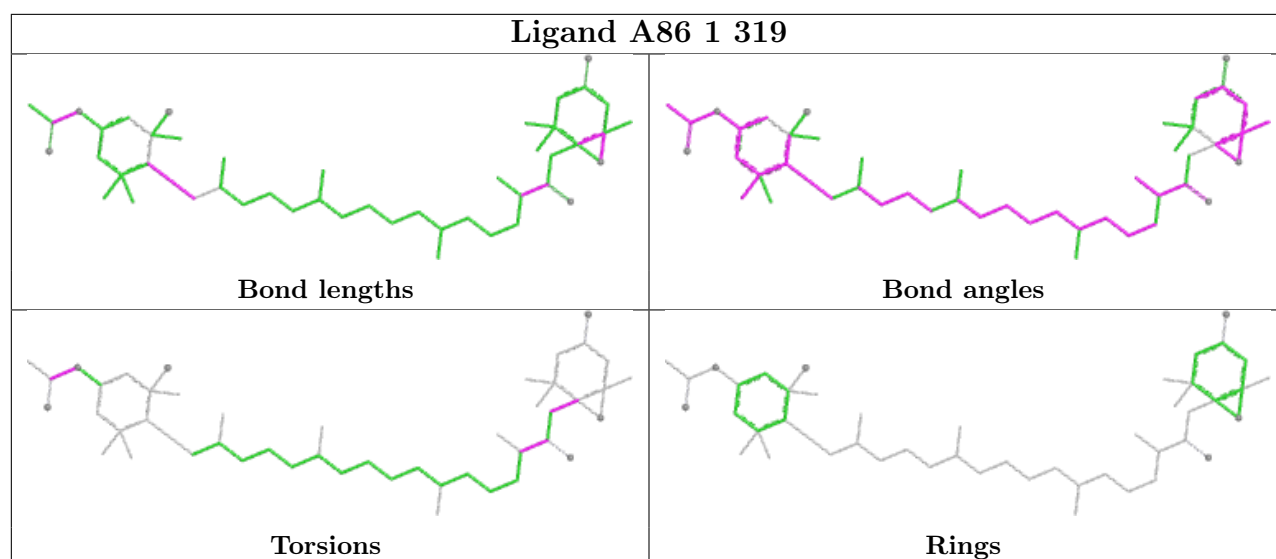


Ligand CLA 0 311

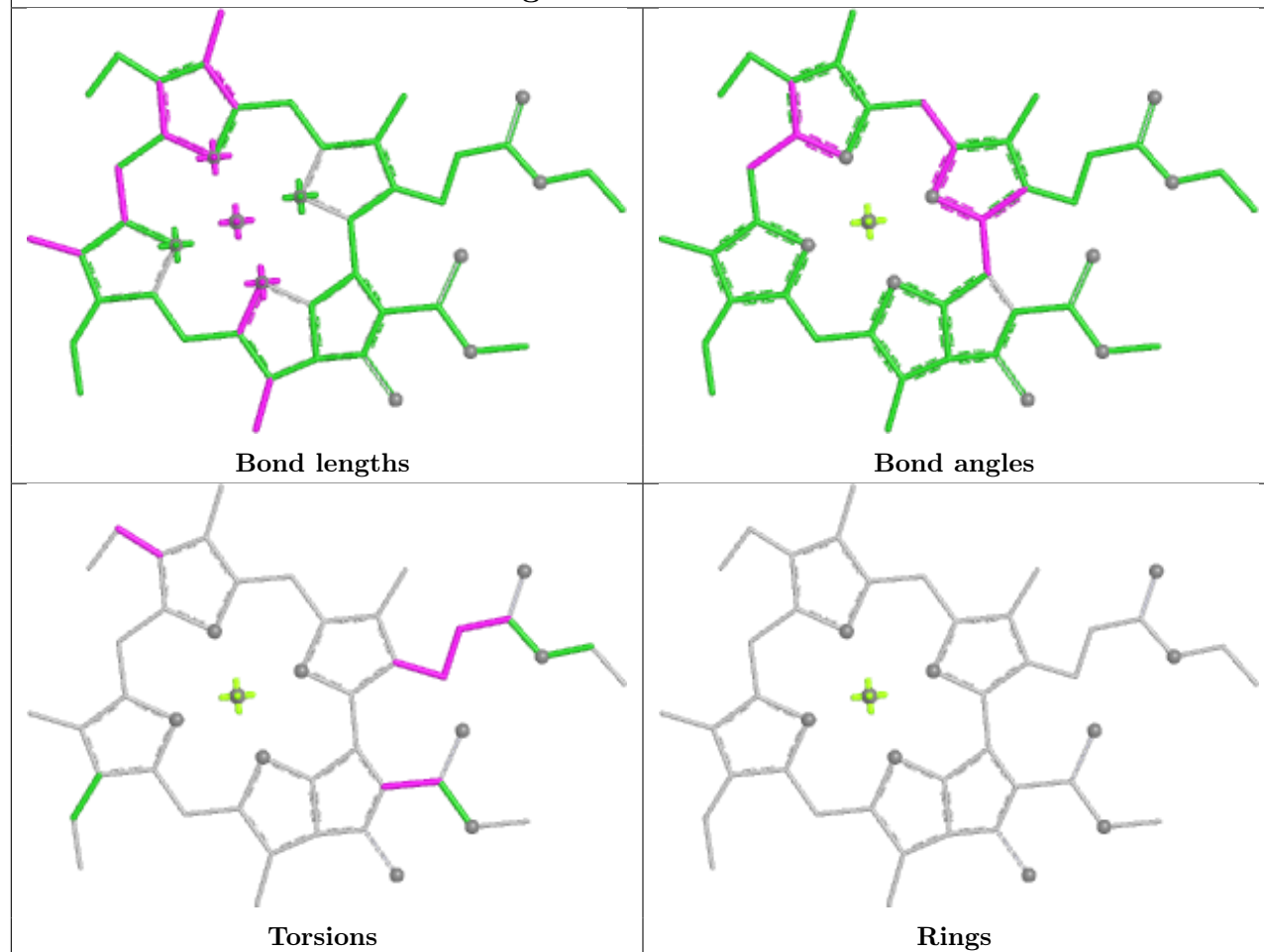




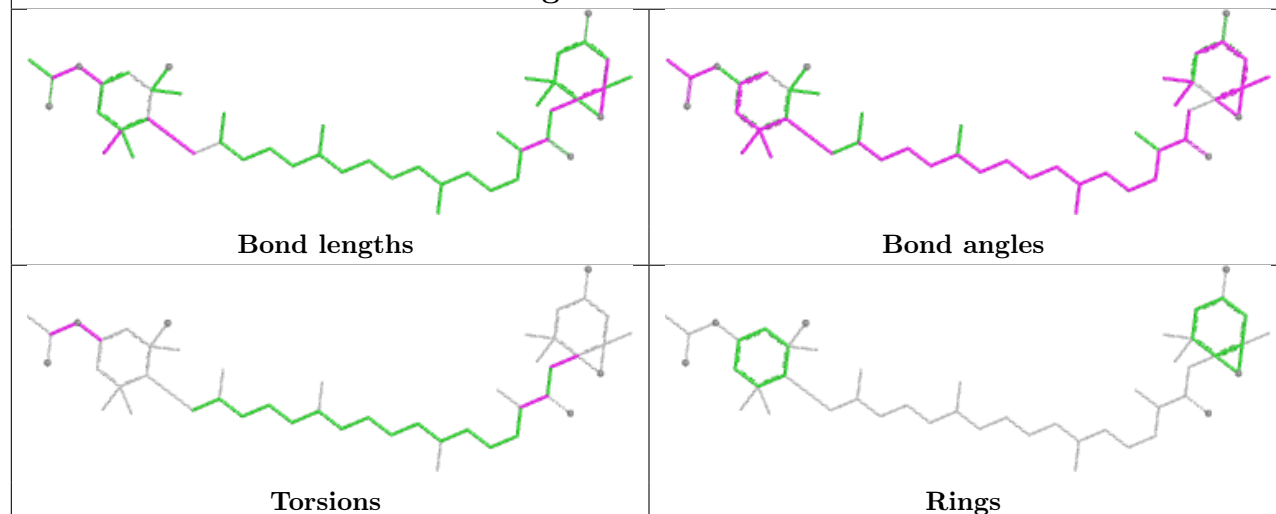




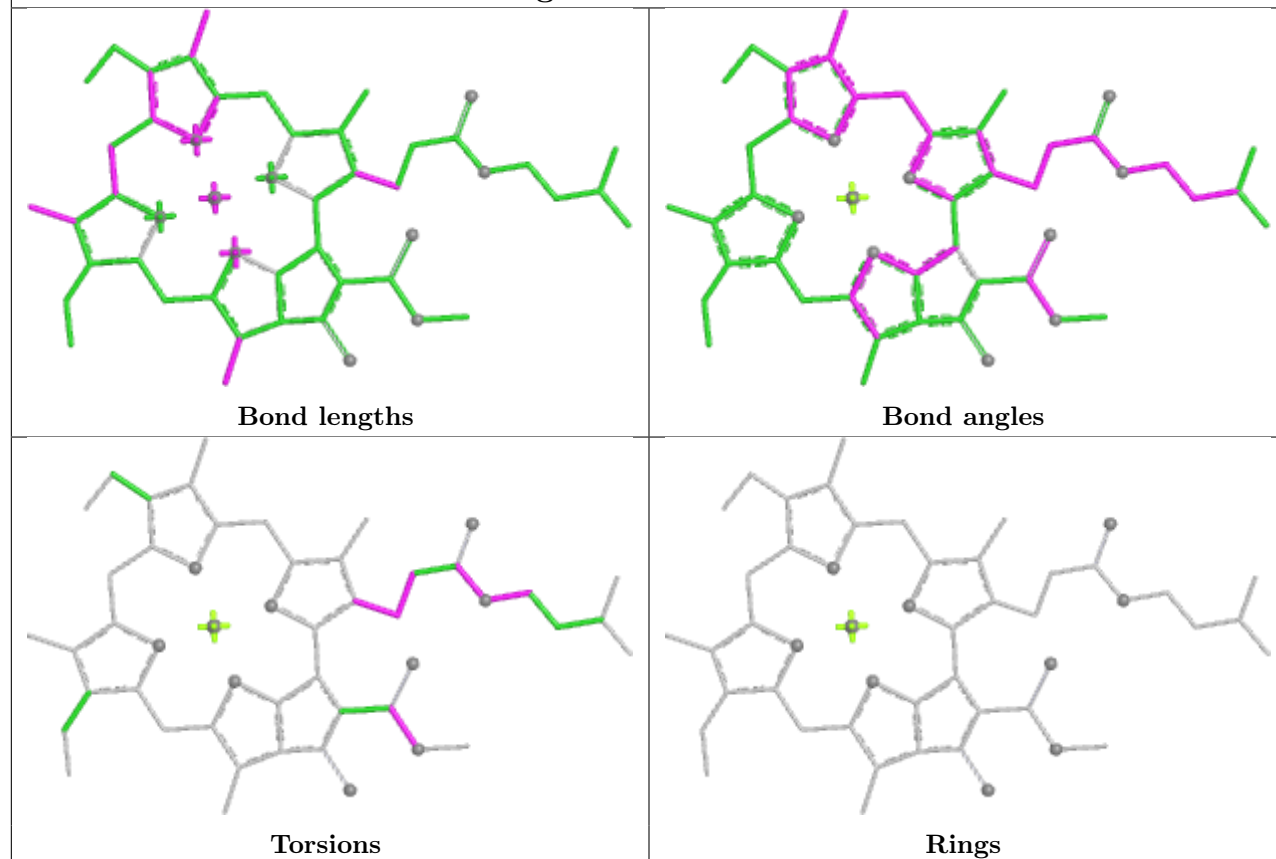
Ligand CLA 16 312



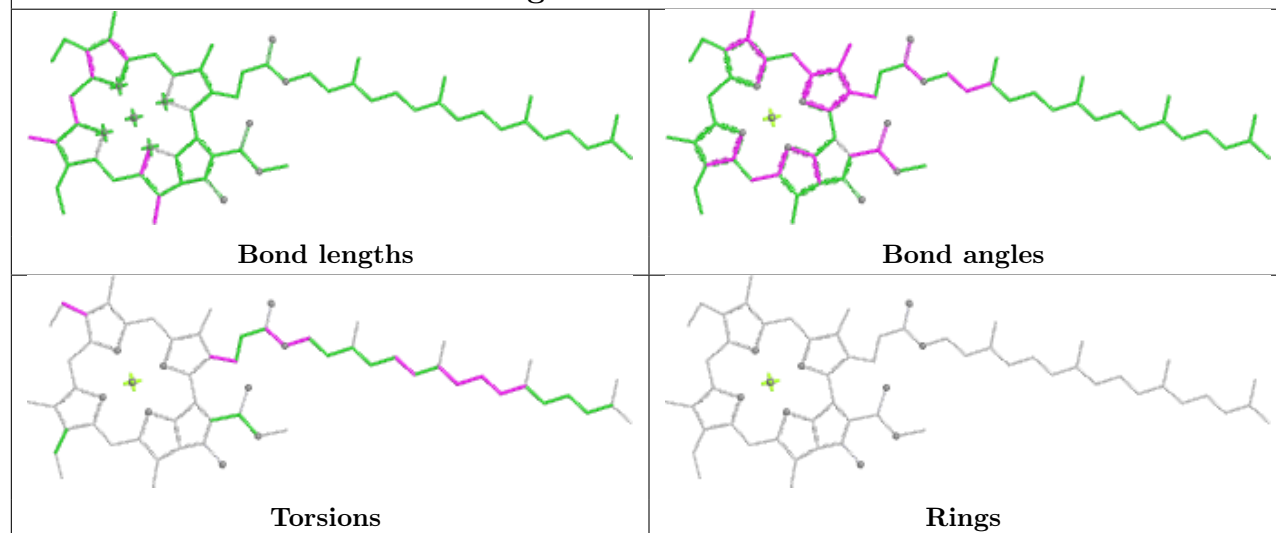
Ligand A86 3 305



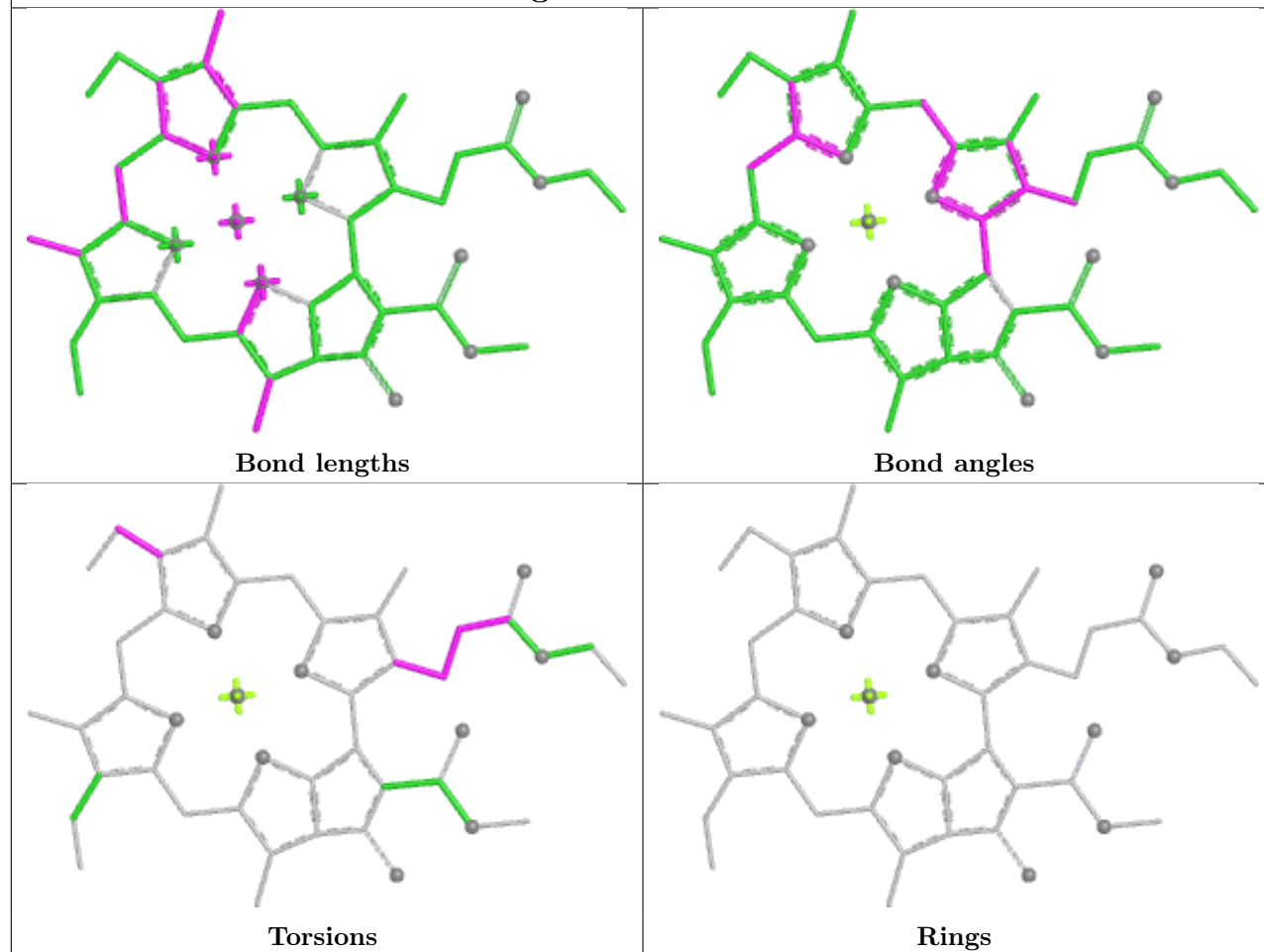
Ligand CLA 7 313



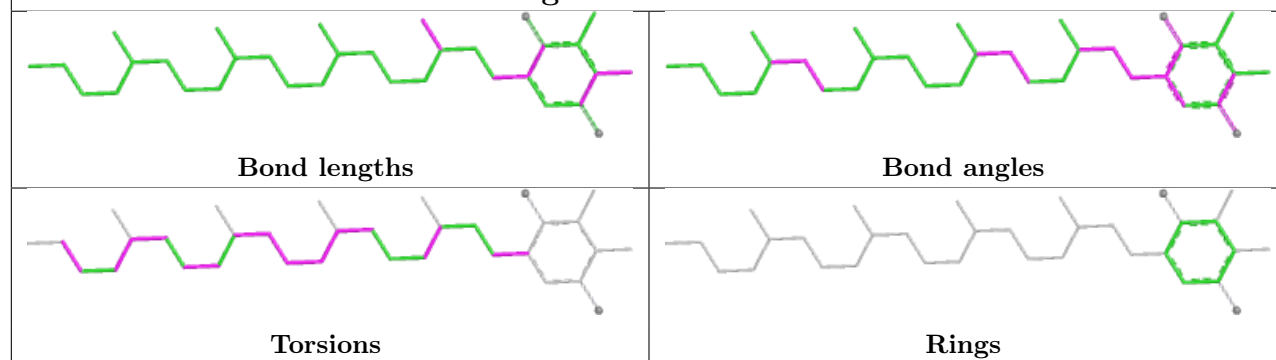
Ligand CLA 19 313

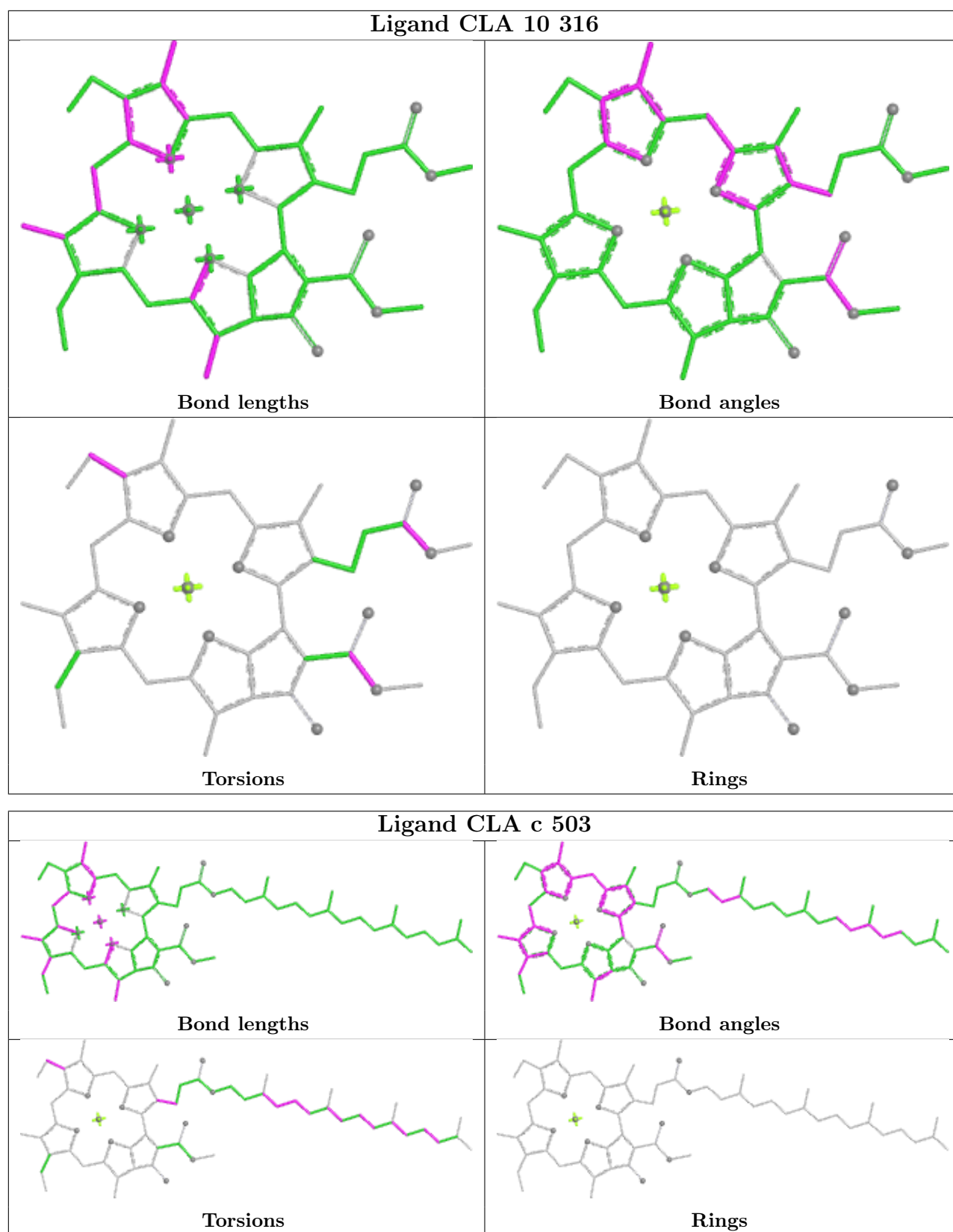


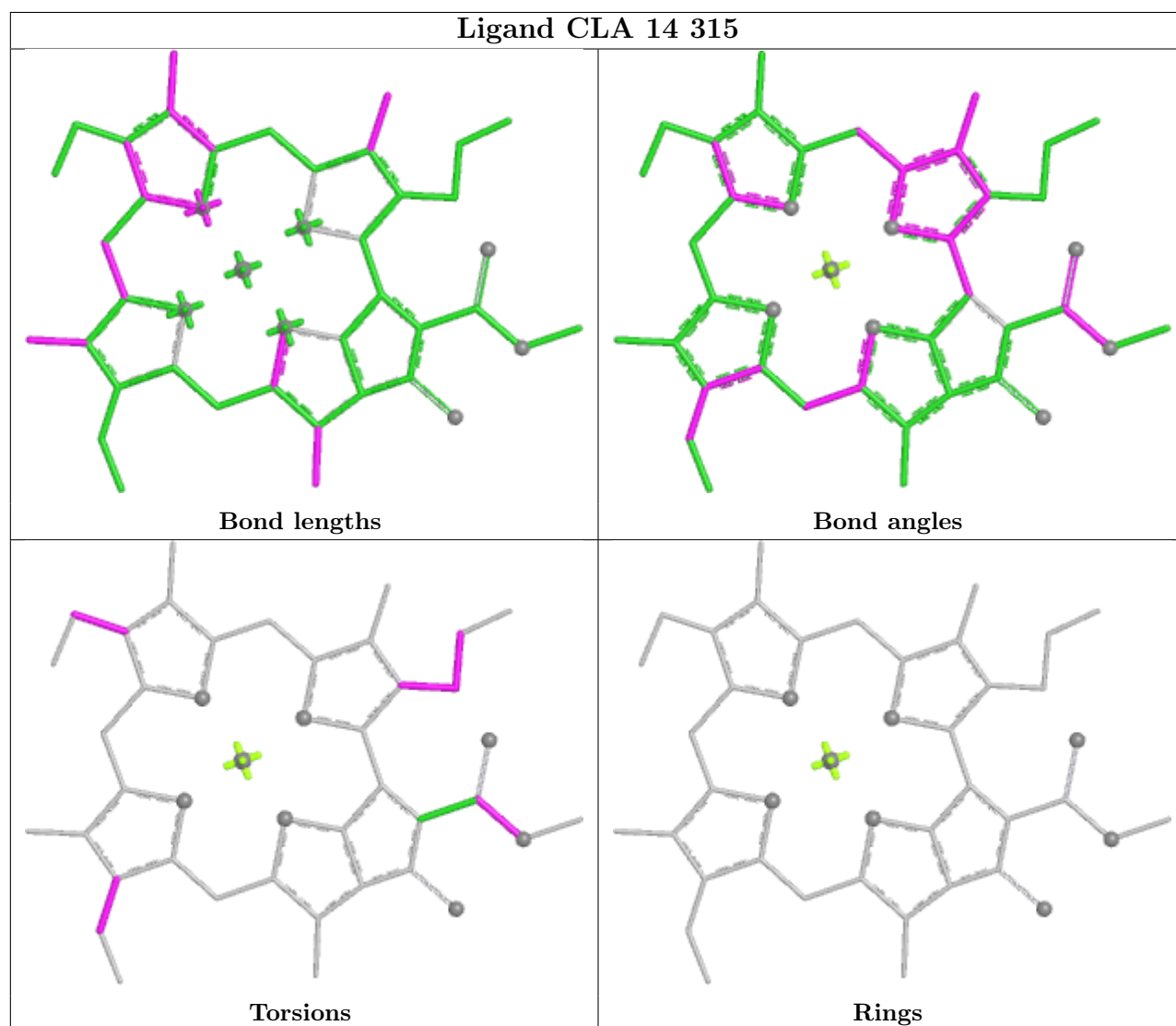
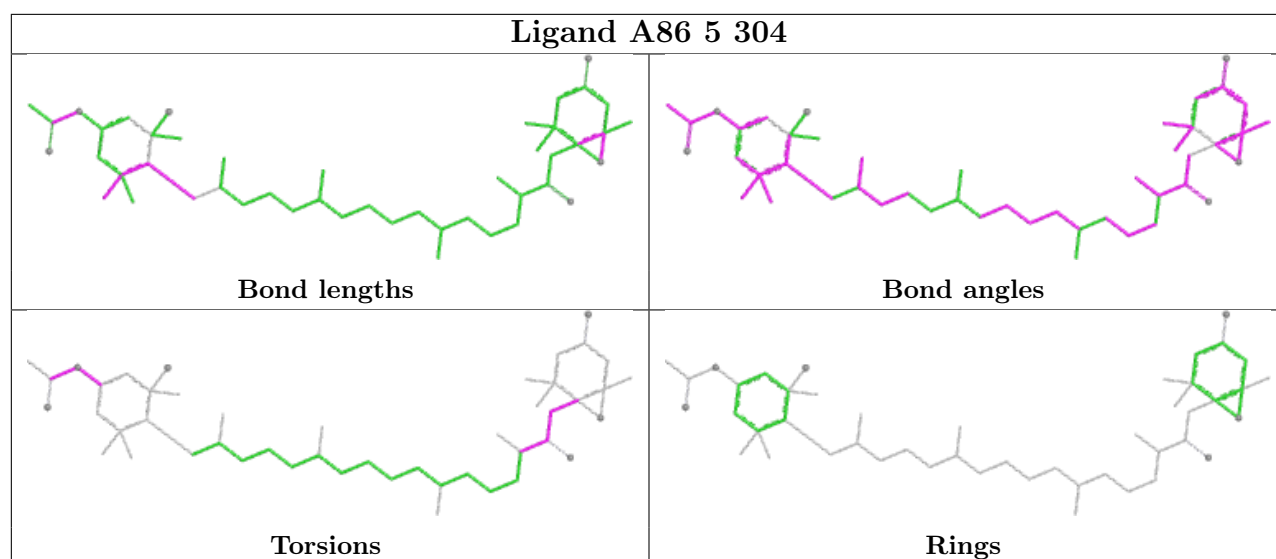
Ligand CLA 6 313

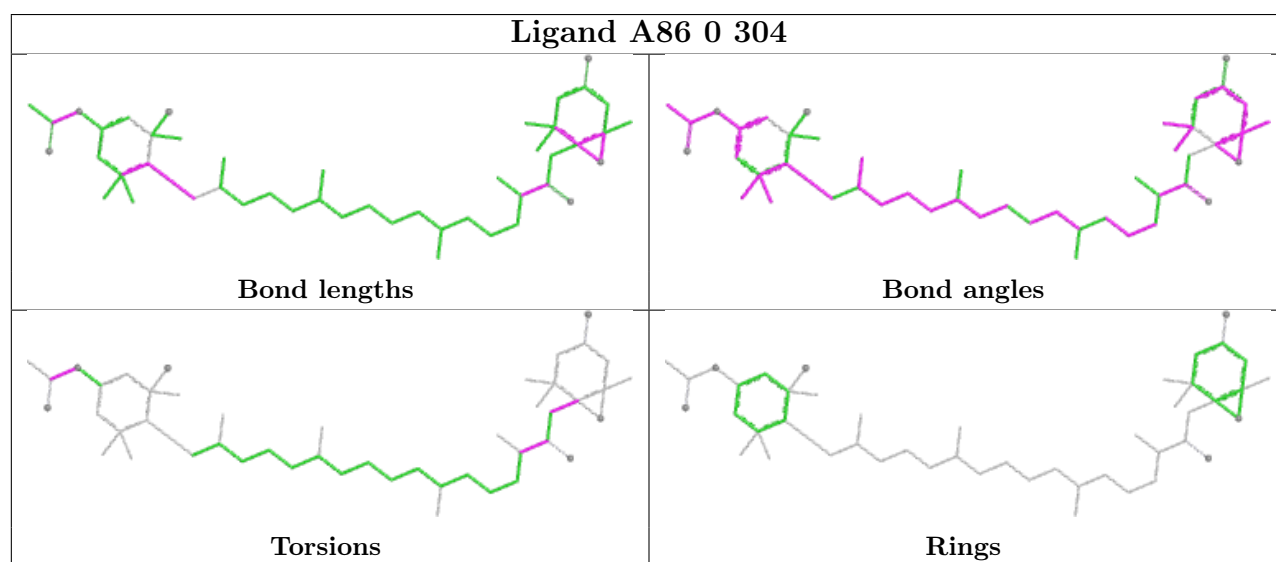
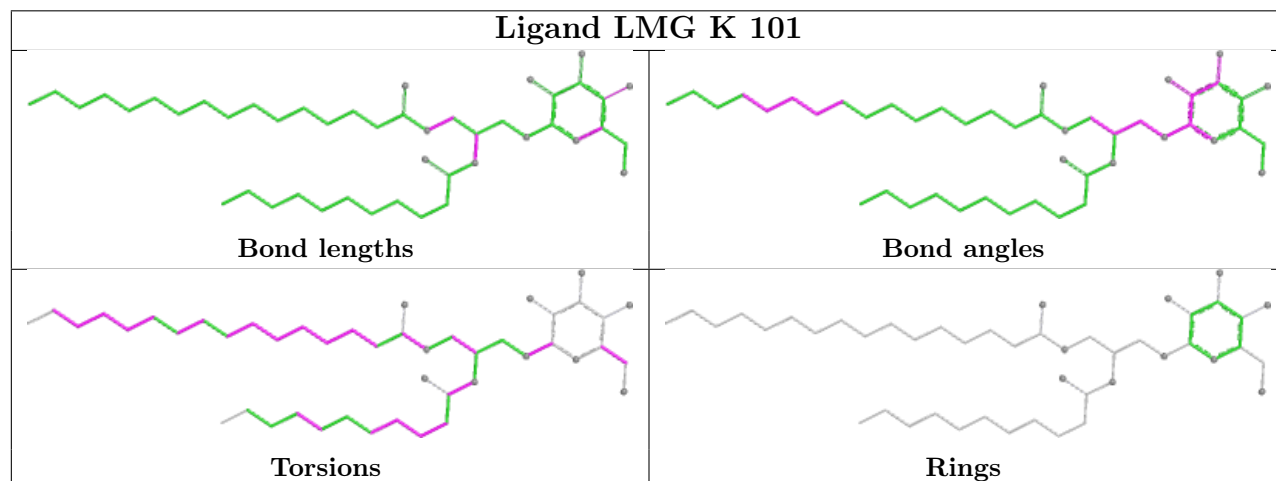
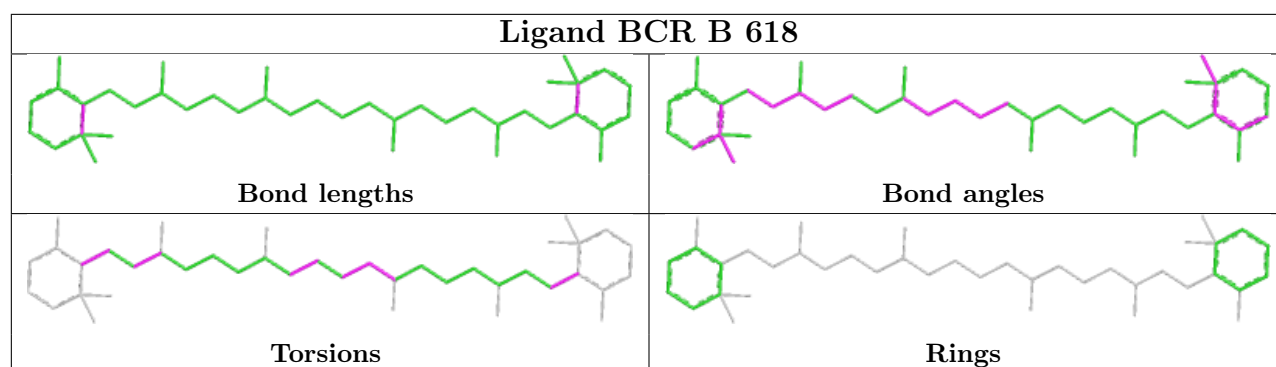


Ligand PL9 a 409

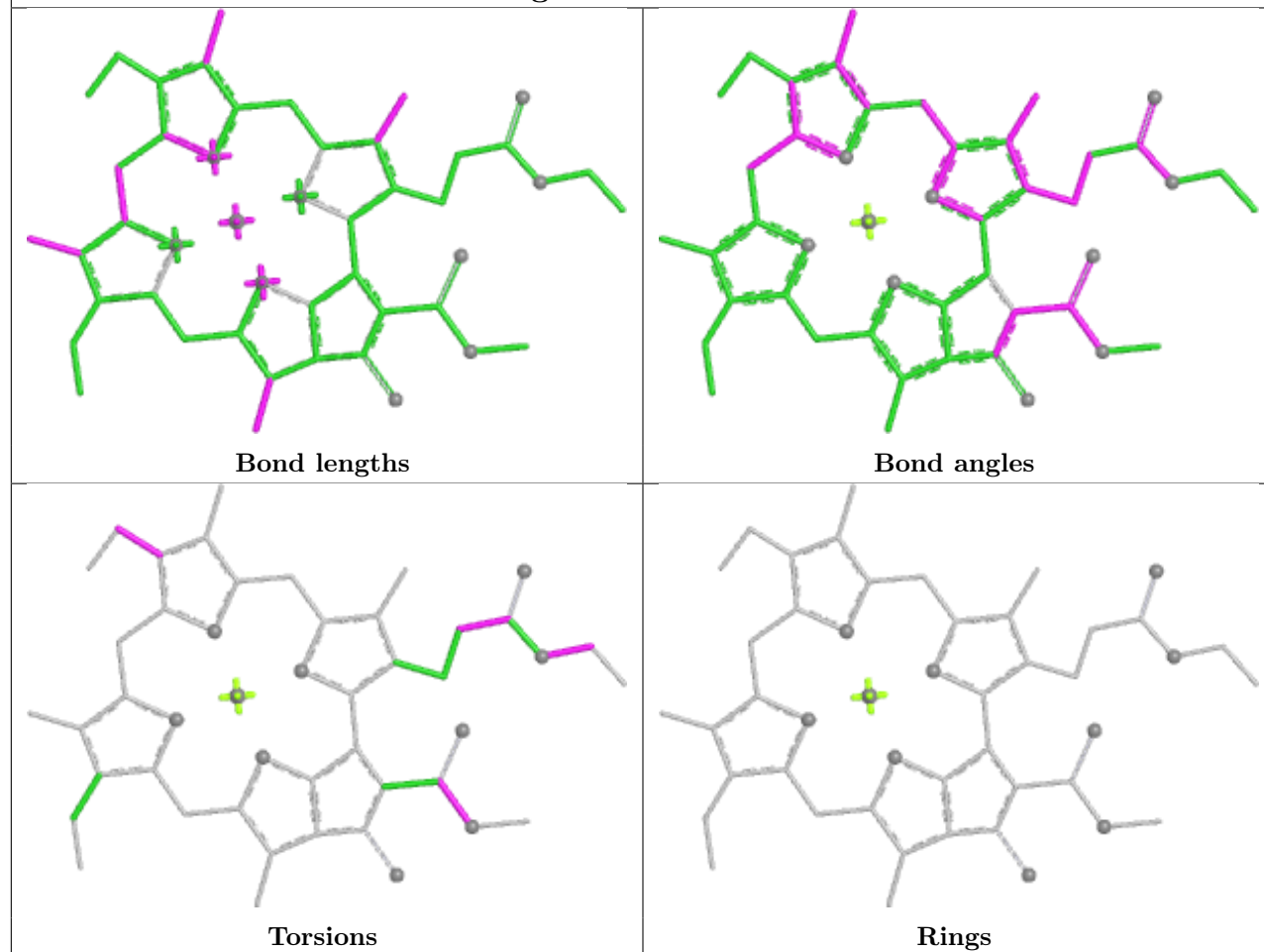




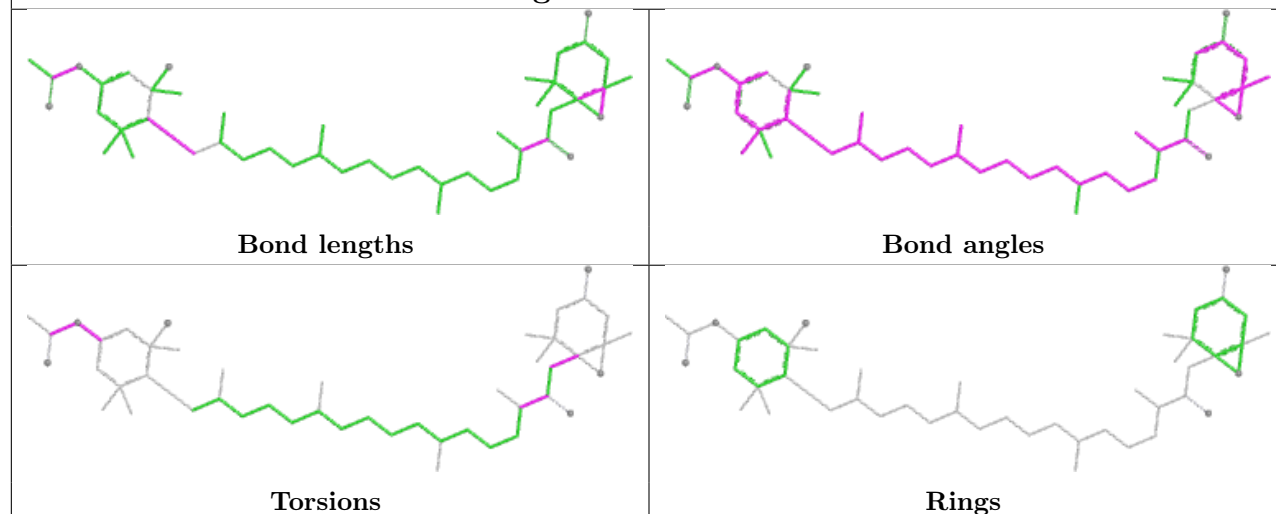


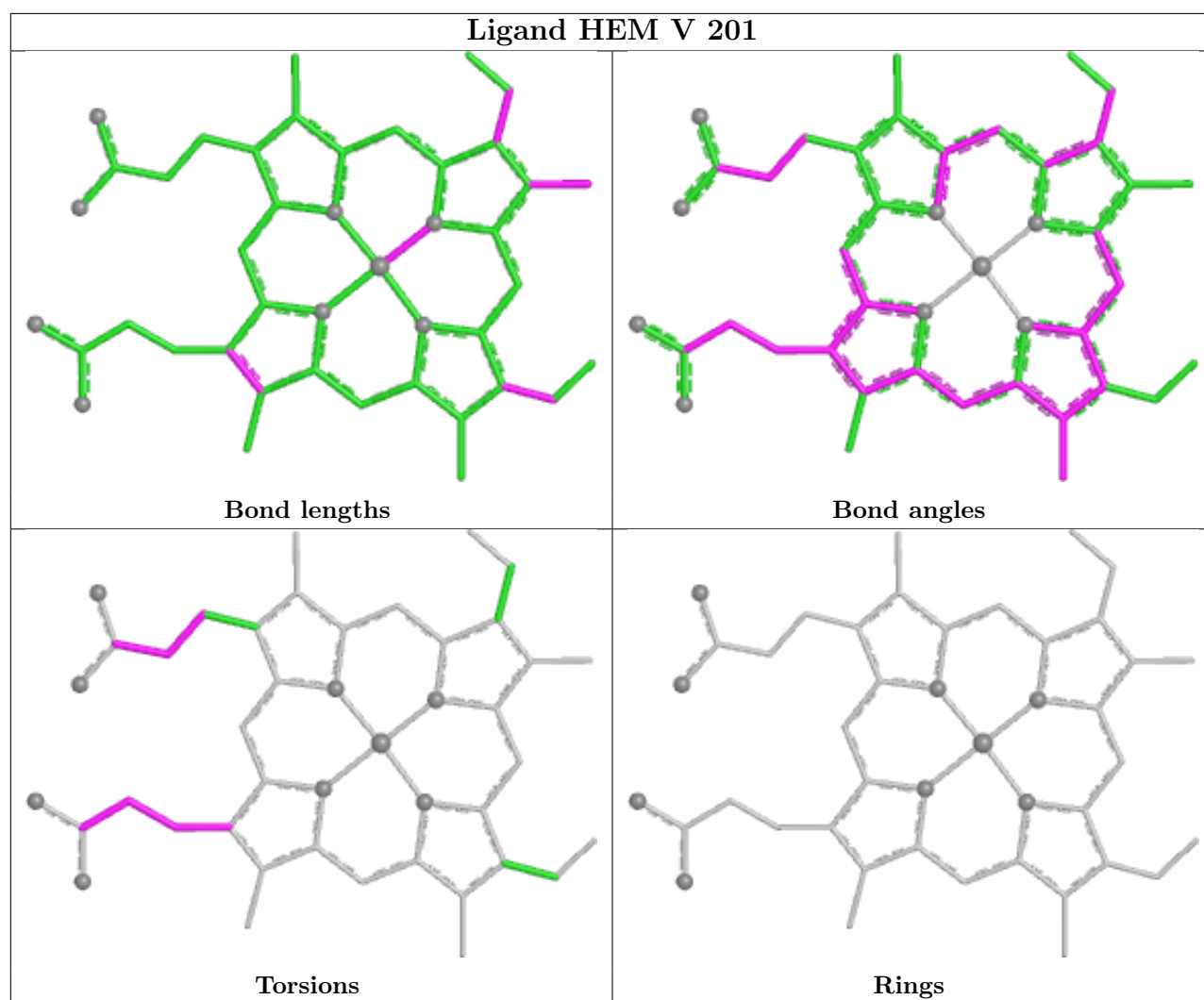


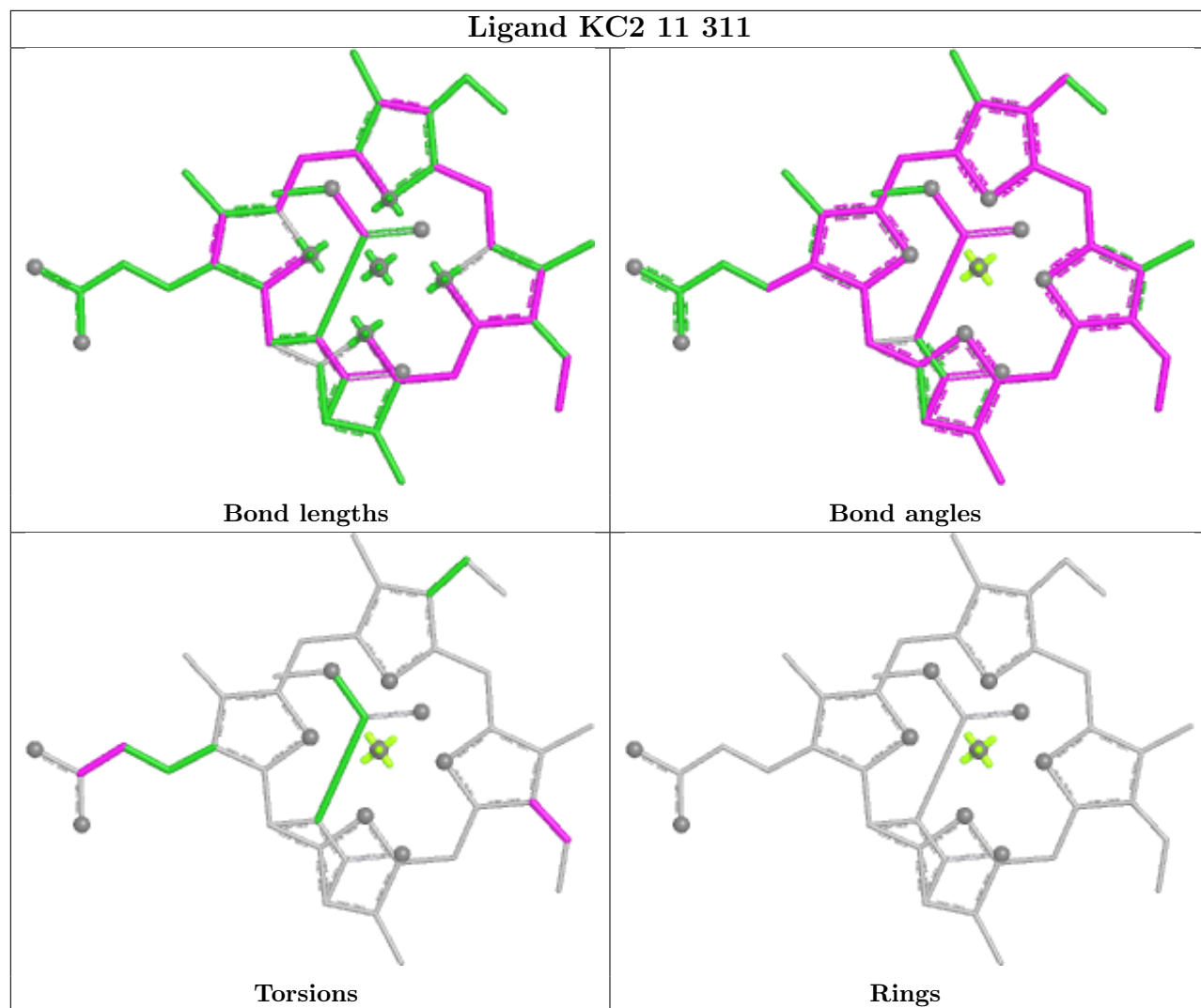
Ligand CLA 5 312



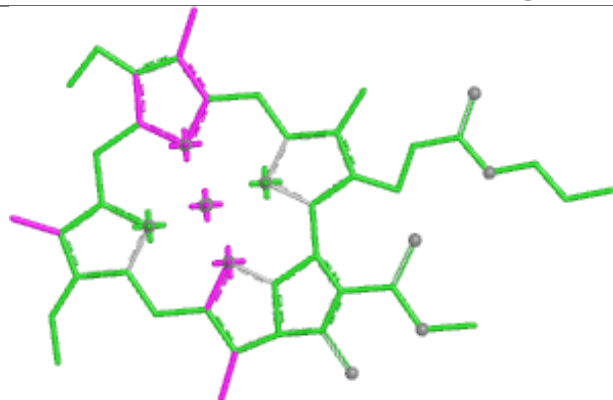
Ligand A86 11 303



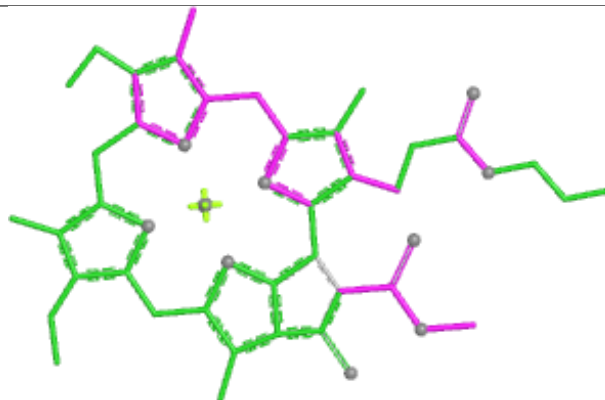




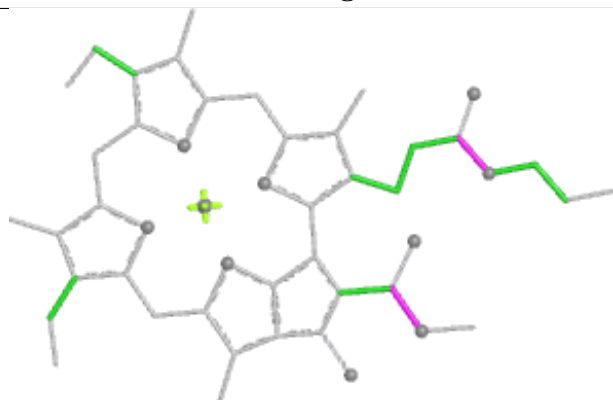
Ligand CLA z 103



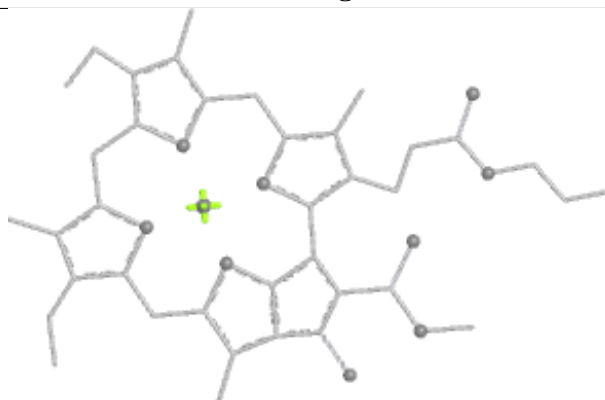
Bond lengths



Bond angles

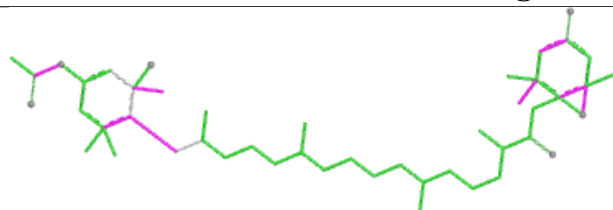


Torsions

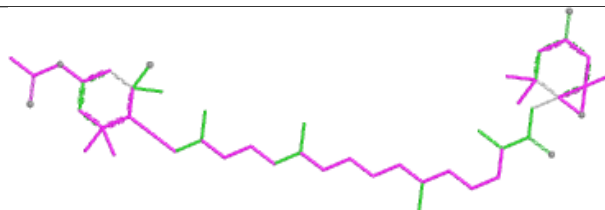


Rings

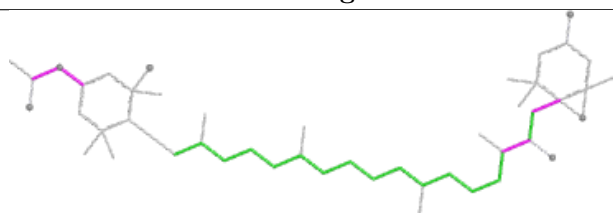
Ligand A86 10 318



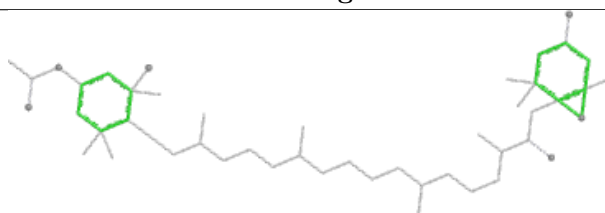
Bond lengths



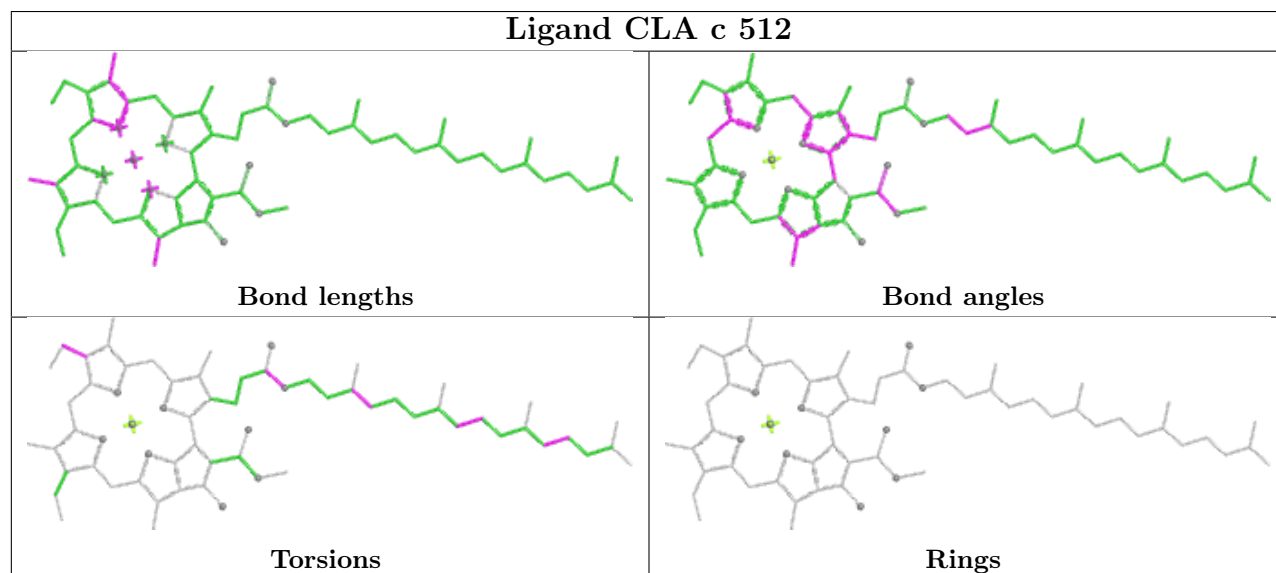
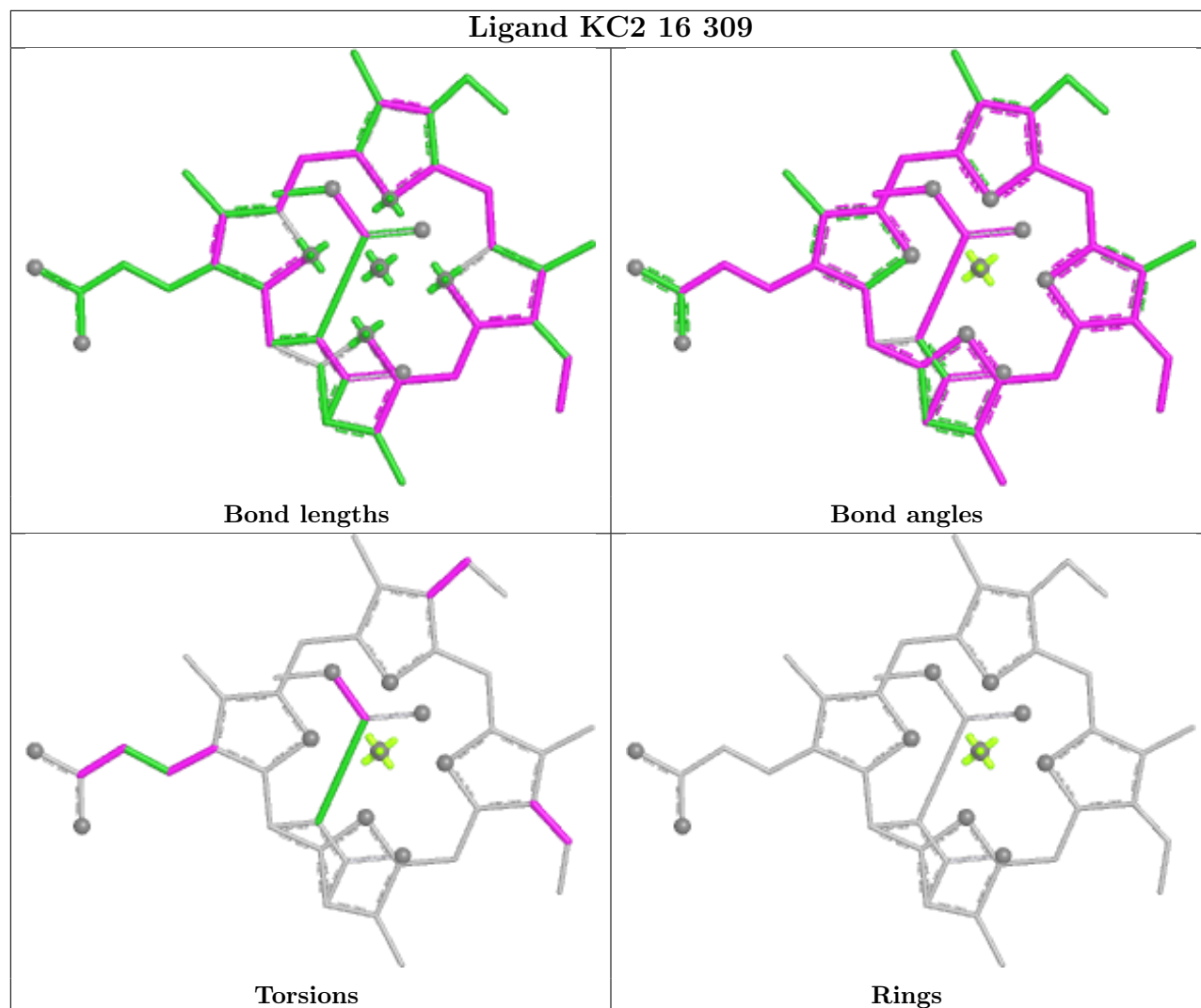
Bond angles

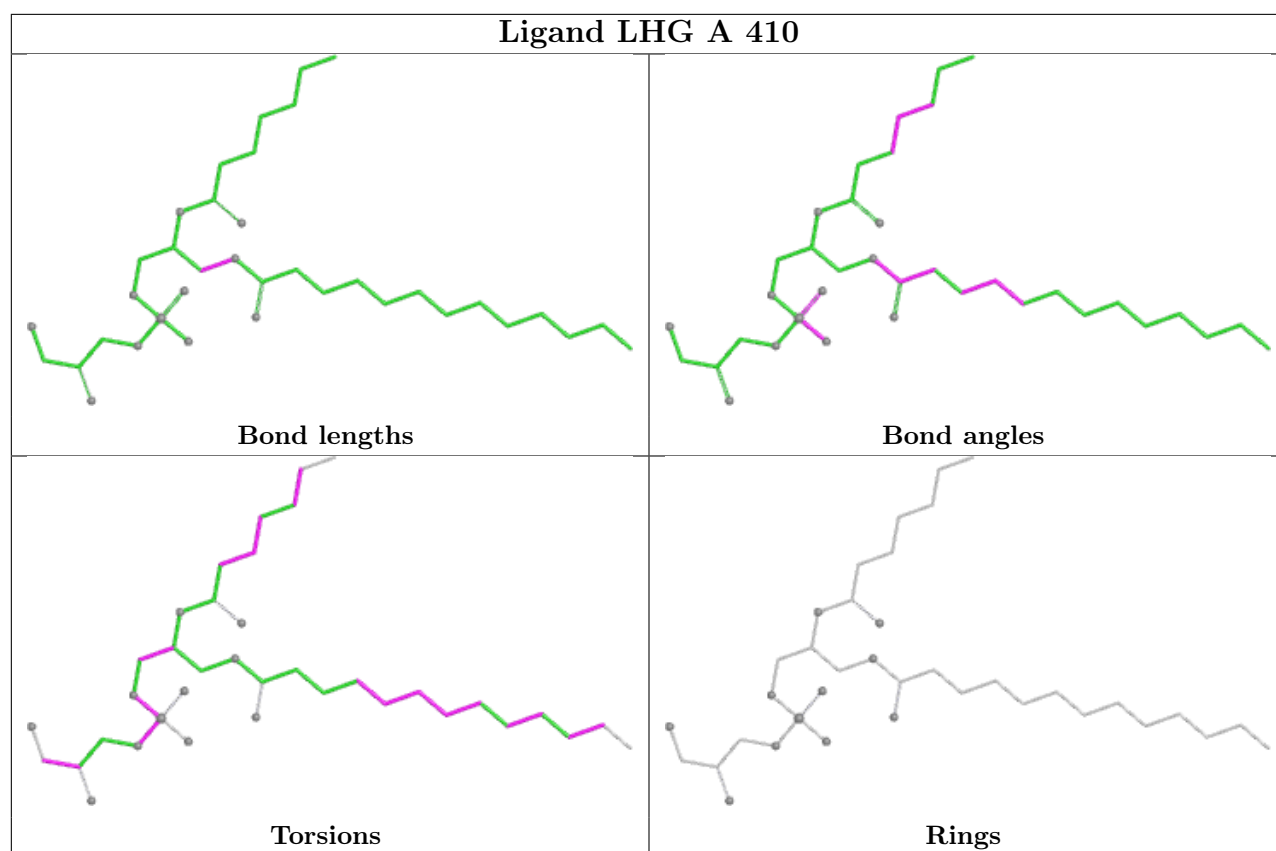


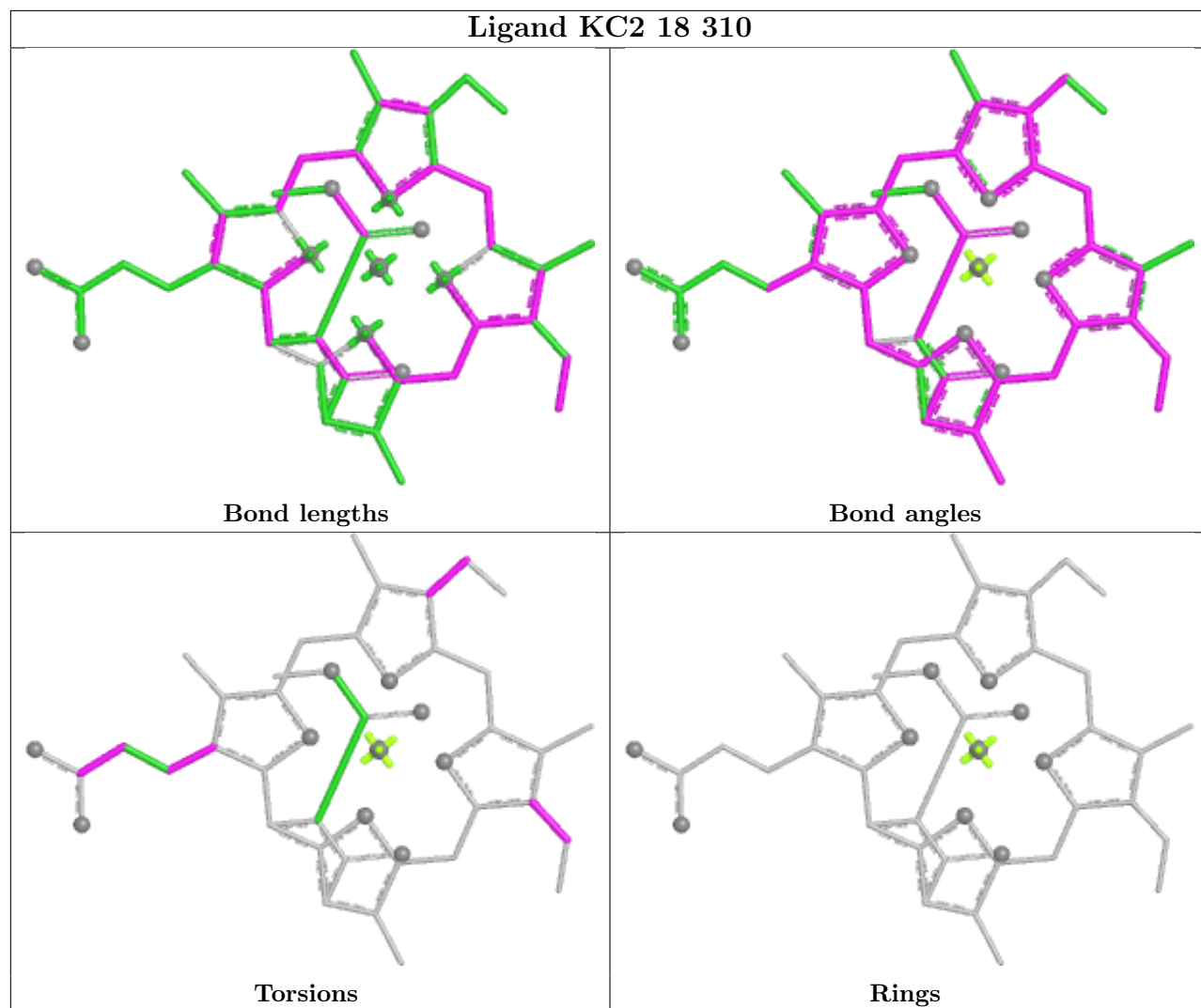
Torsions



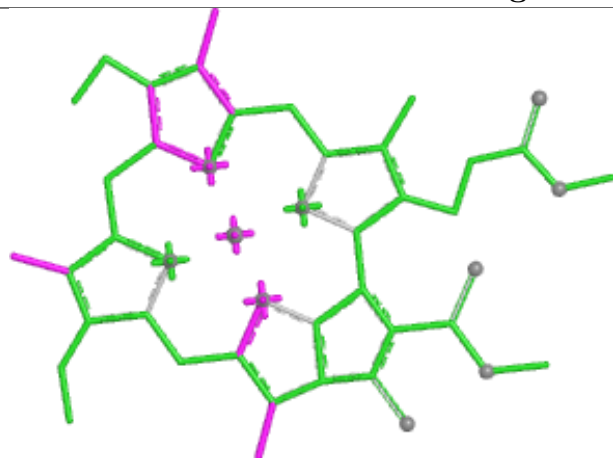
Rings



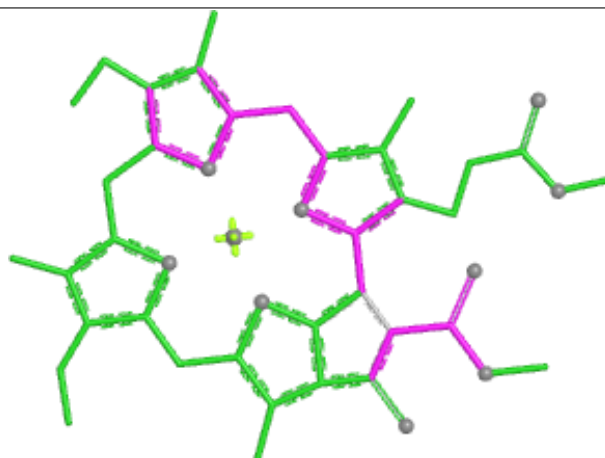




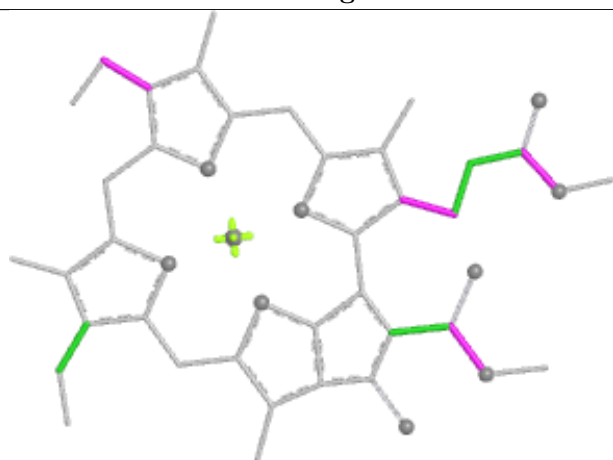
Ligand CLA 18 311



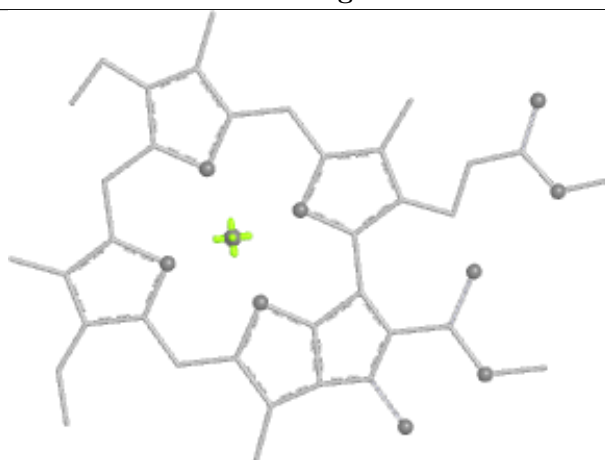
Bond lengths



Bond angles

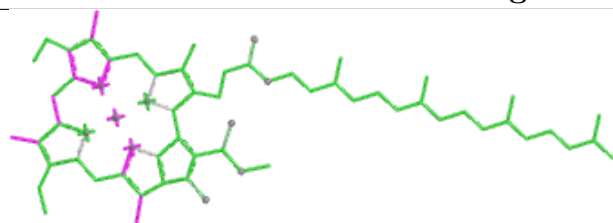


Torsions

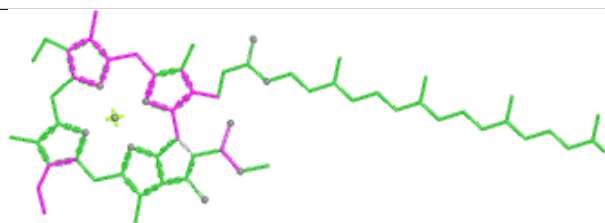


Rings

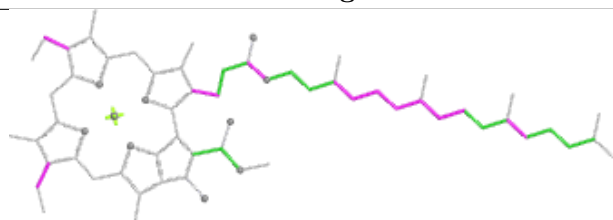
Ligand CLA 12 308



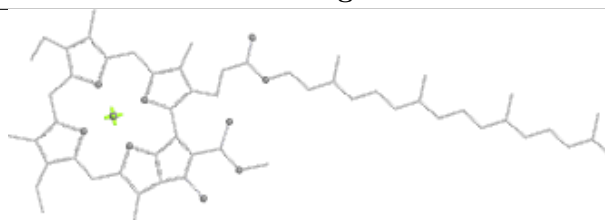
Bond lengths



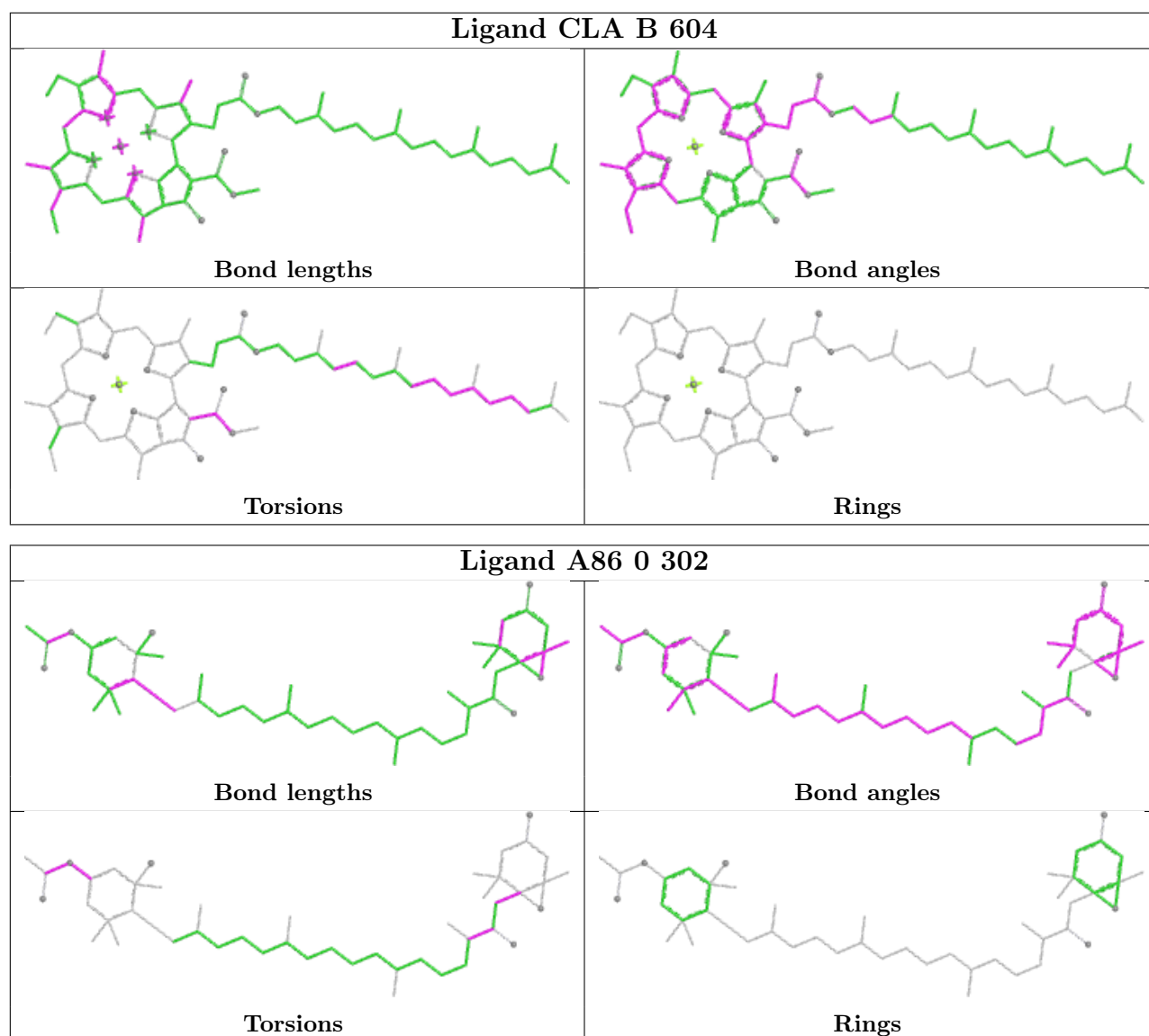
Bond angles



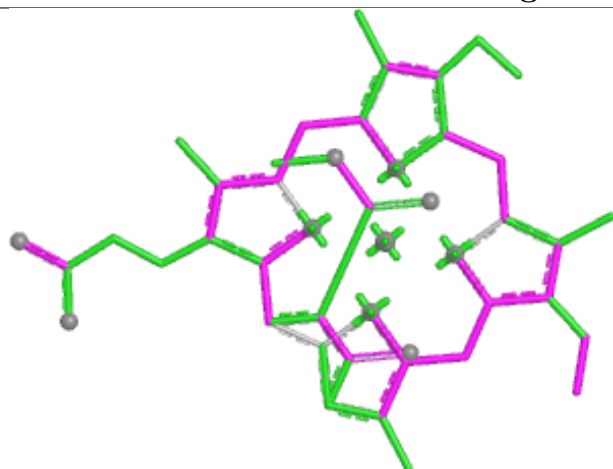
Torsions



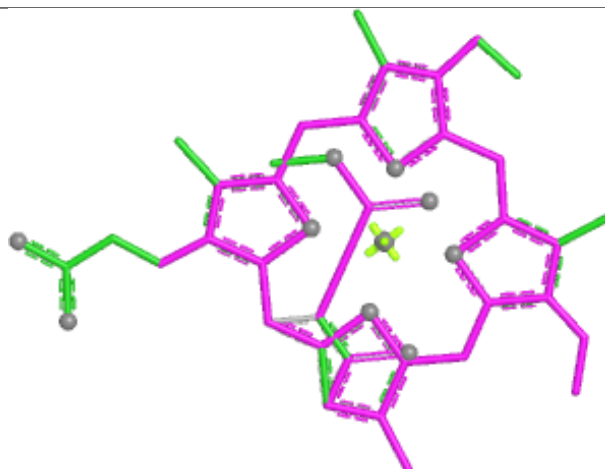
Rings



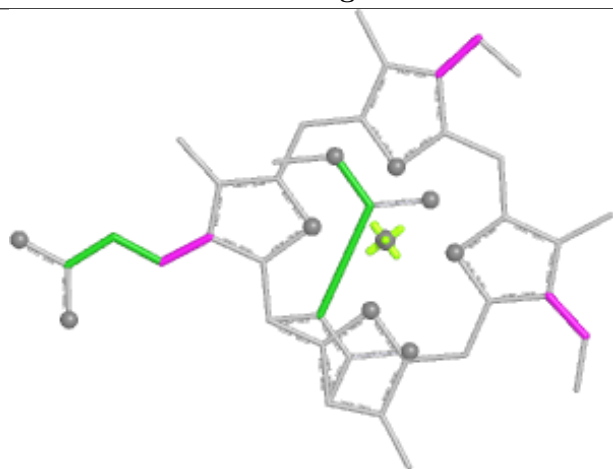
Ligand KC2 6 312



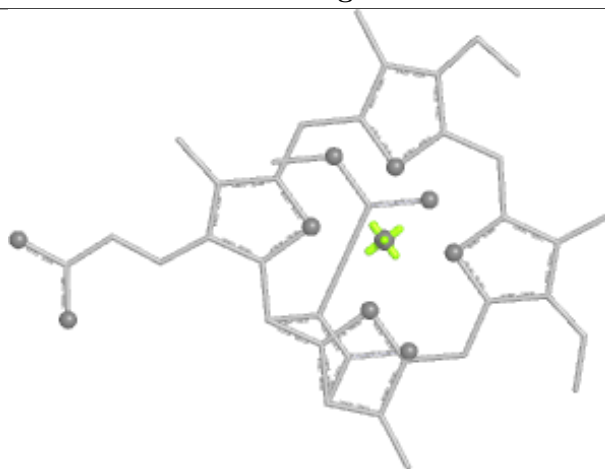
Bond lengths



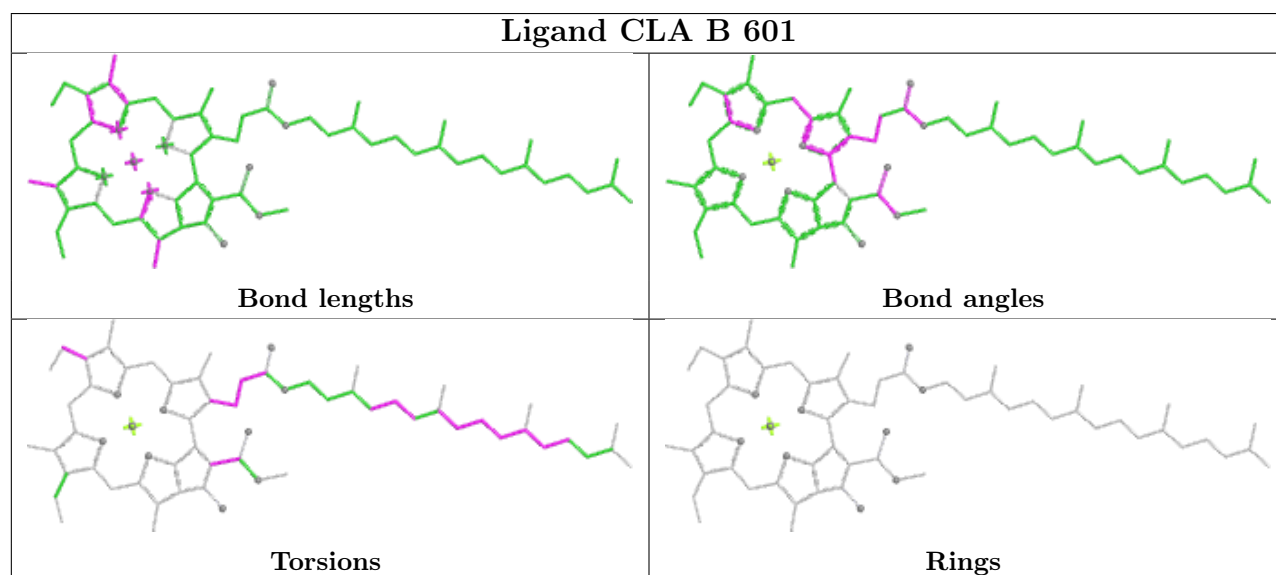
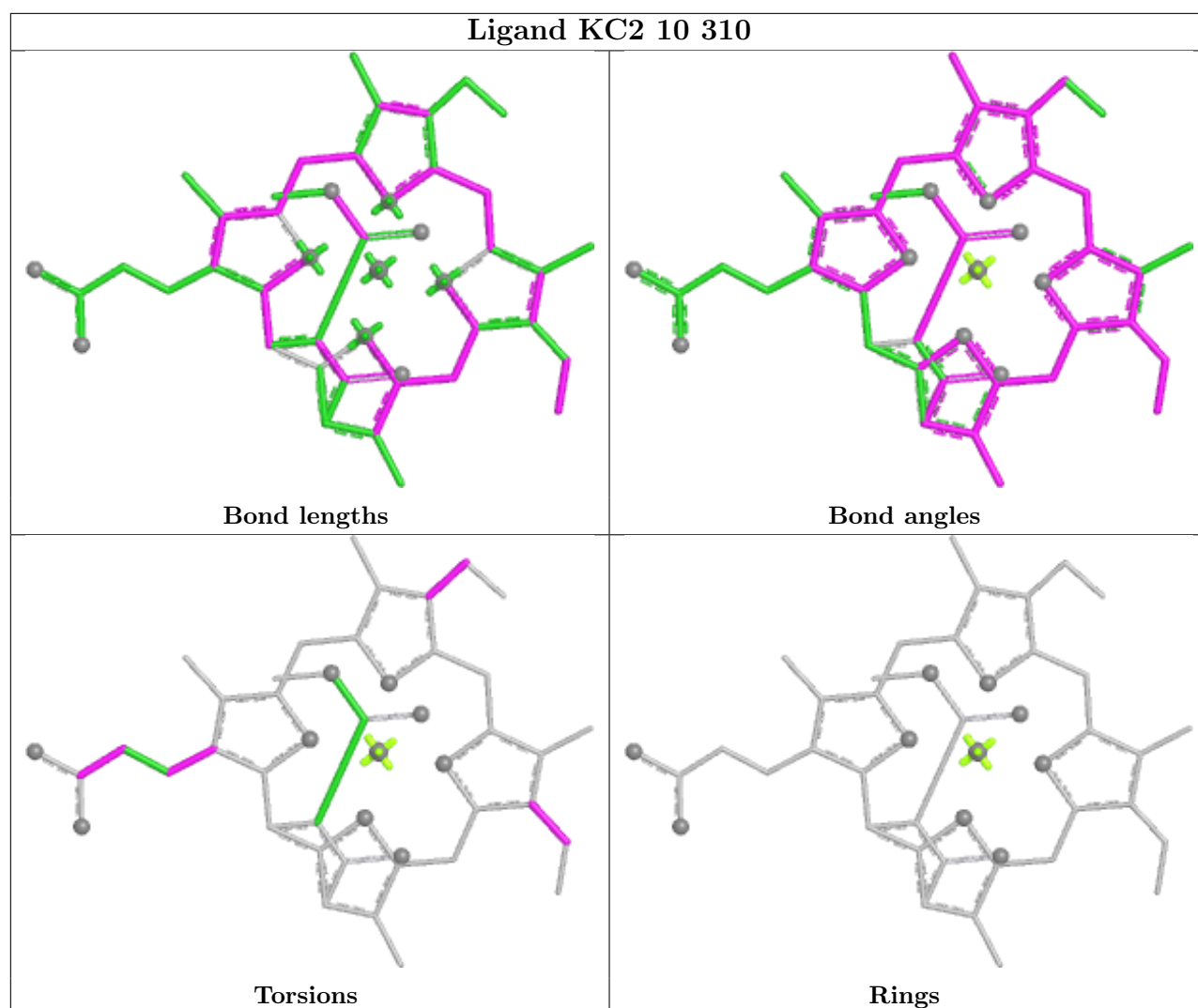
Bond angles

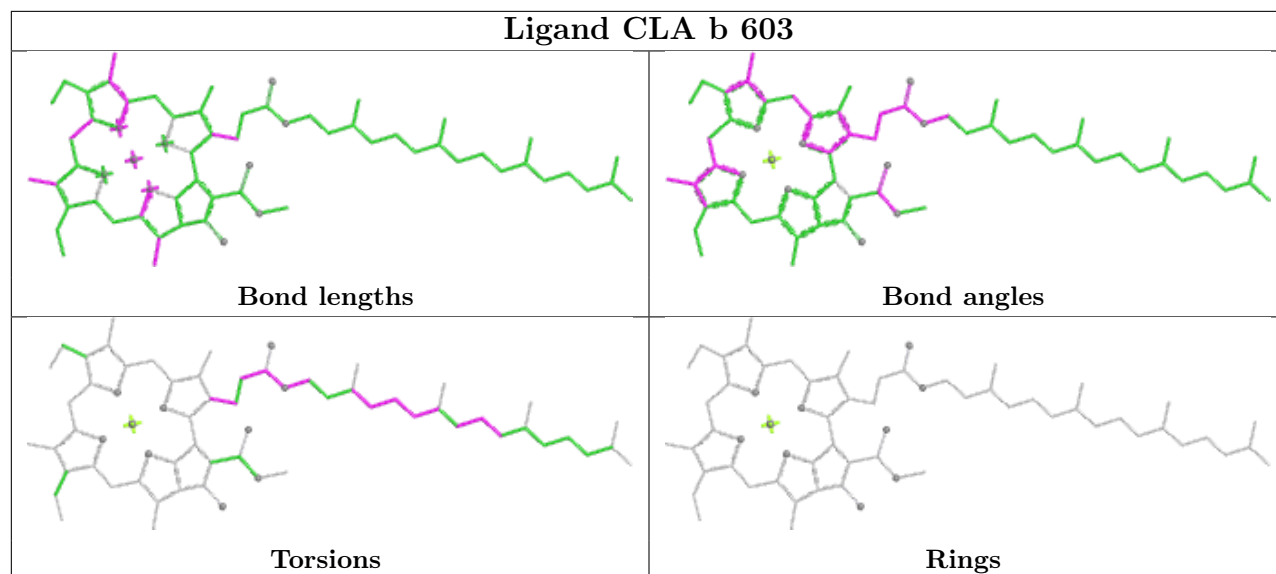
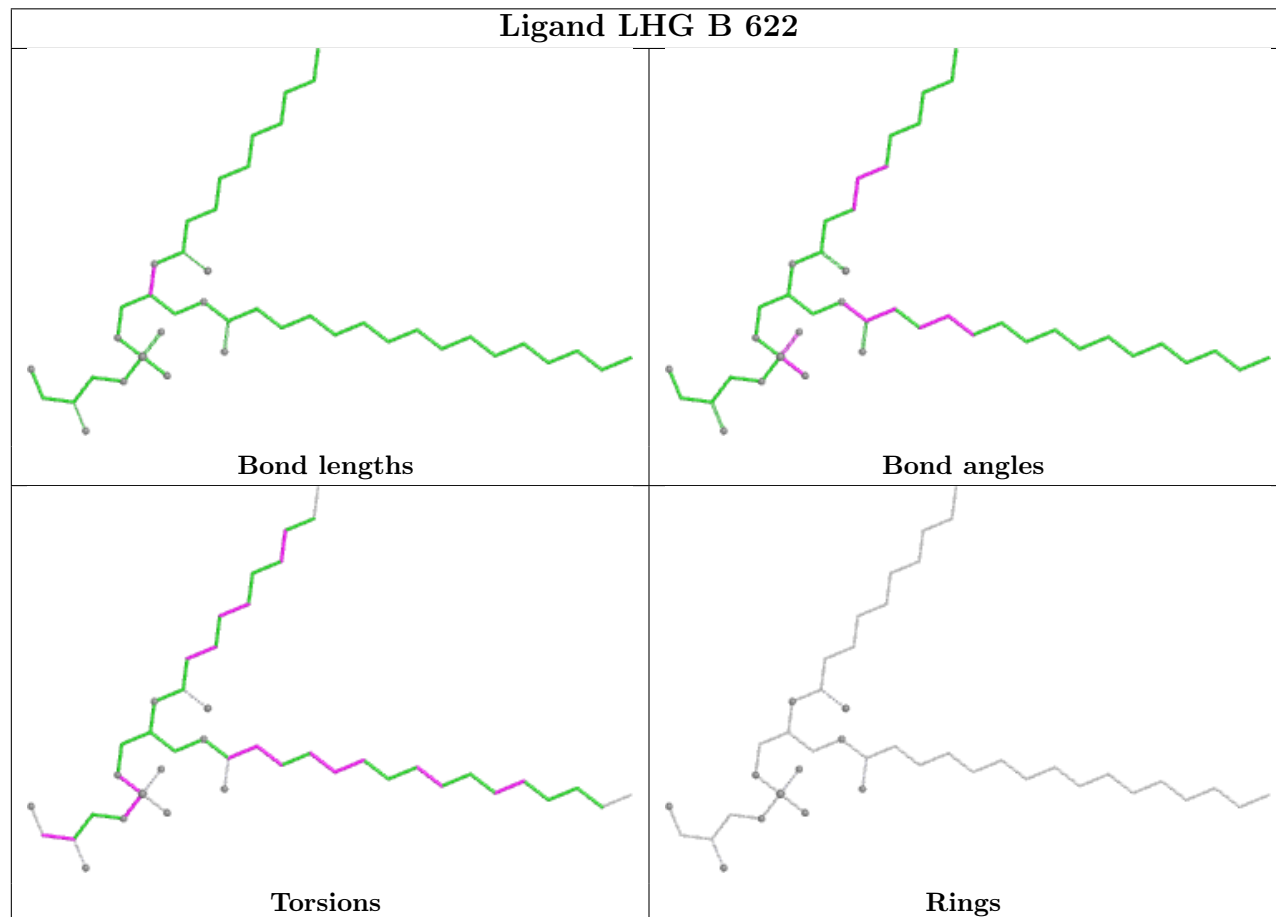


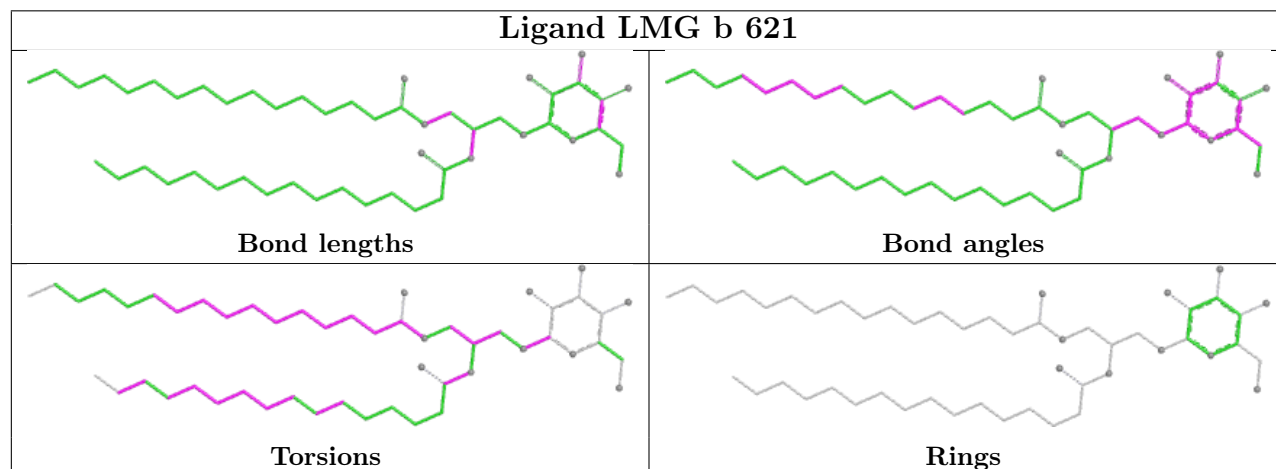
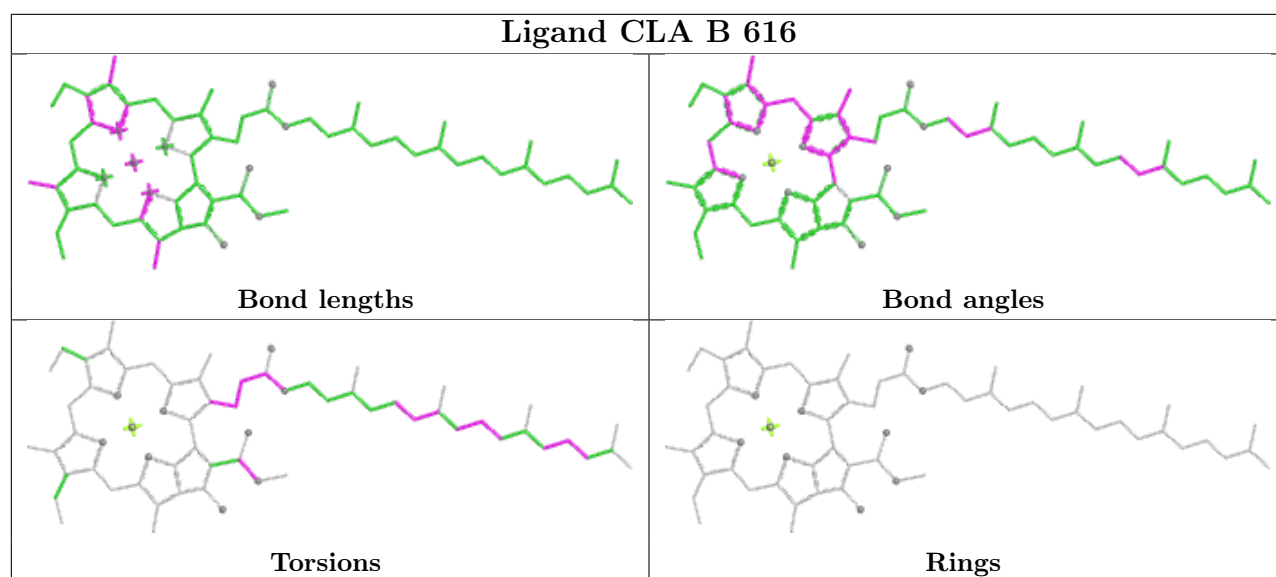
Torsions



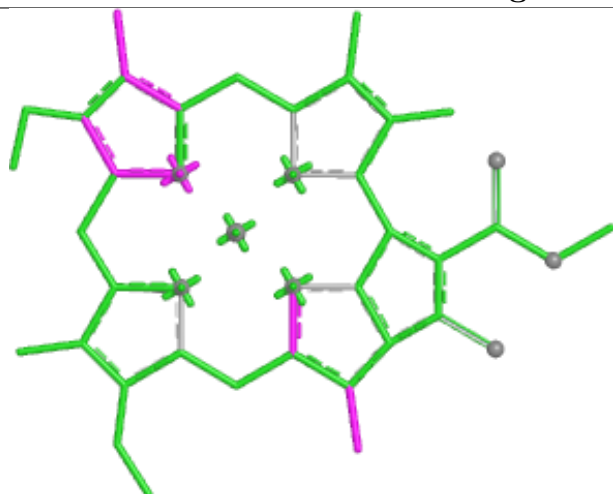
Rings



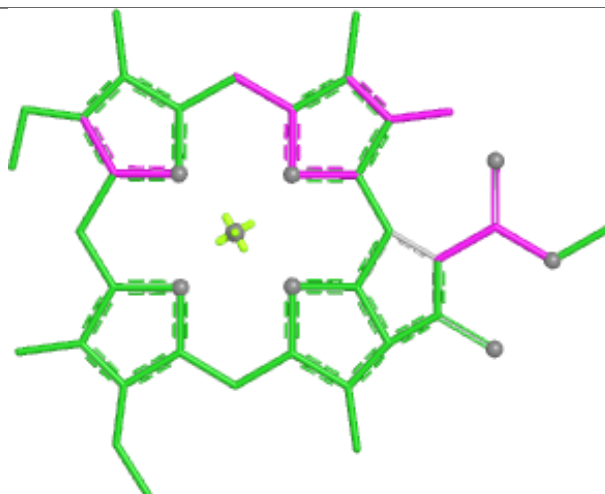
Ligand CLA b 603**Ligand LHG B 622**



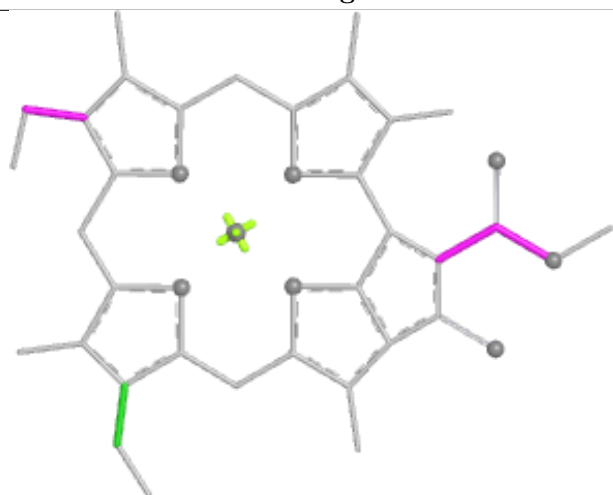
Ligand CLA 17 315



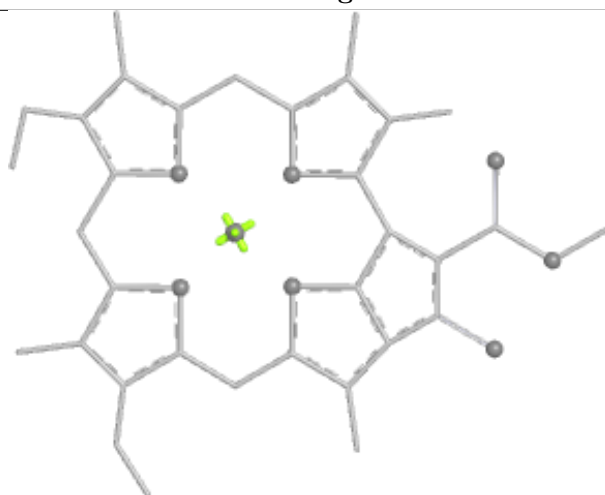
Bond lengths



Bond angles

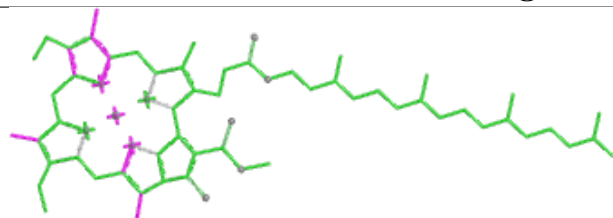


Torsions

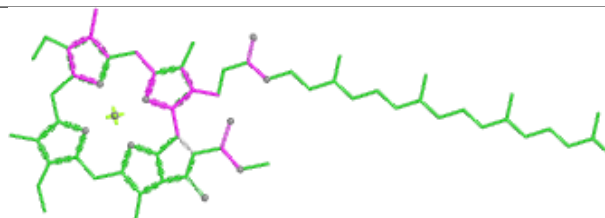


Rings

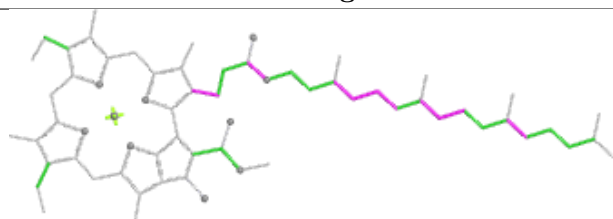
Ligand CLA 5 307



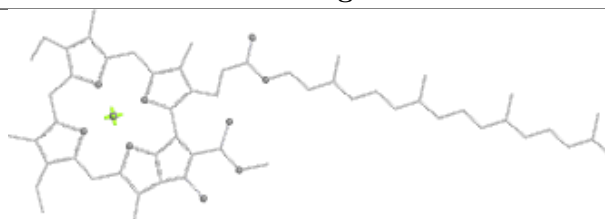
Bond lengths



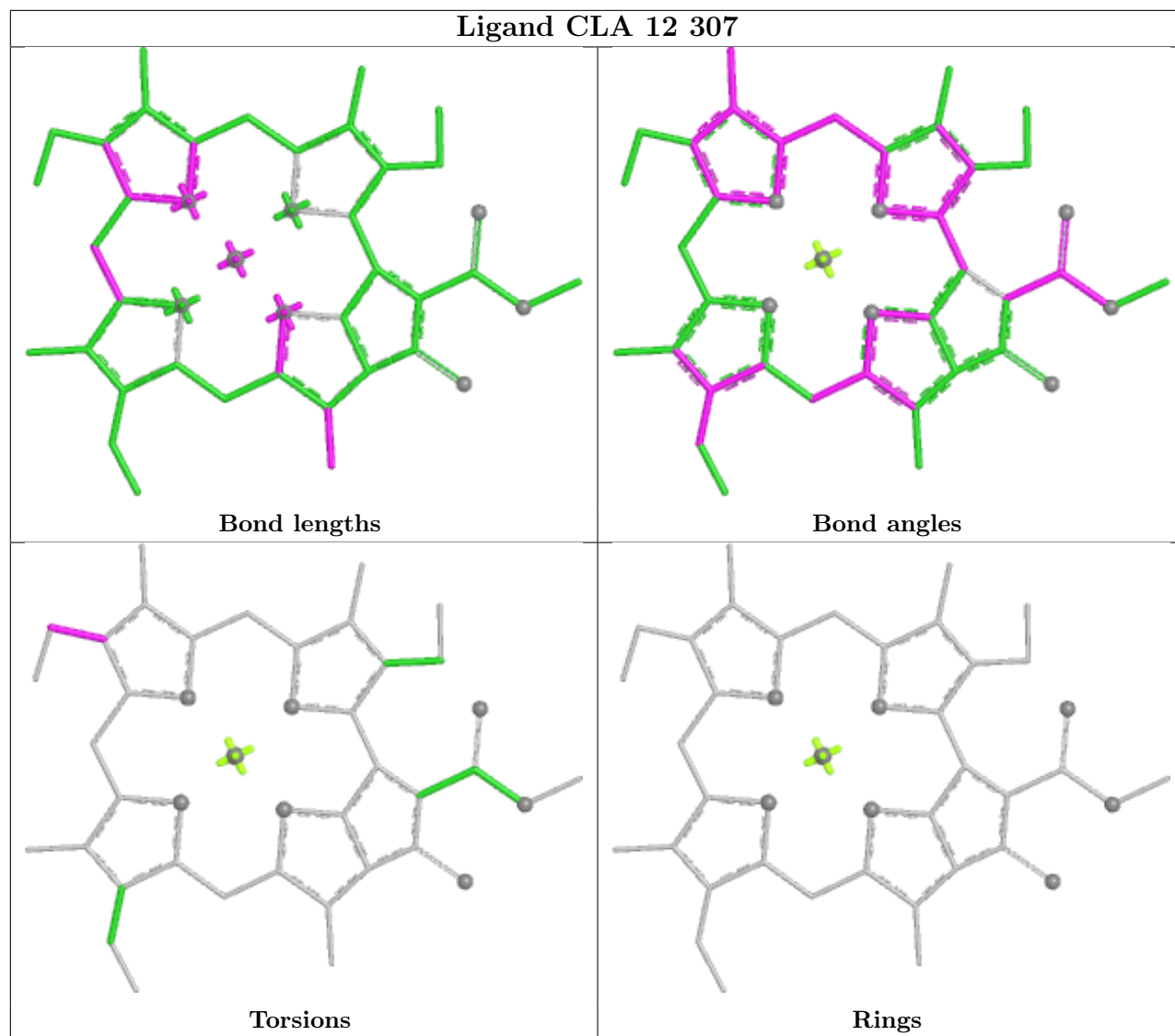
Bond angles

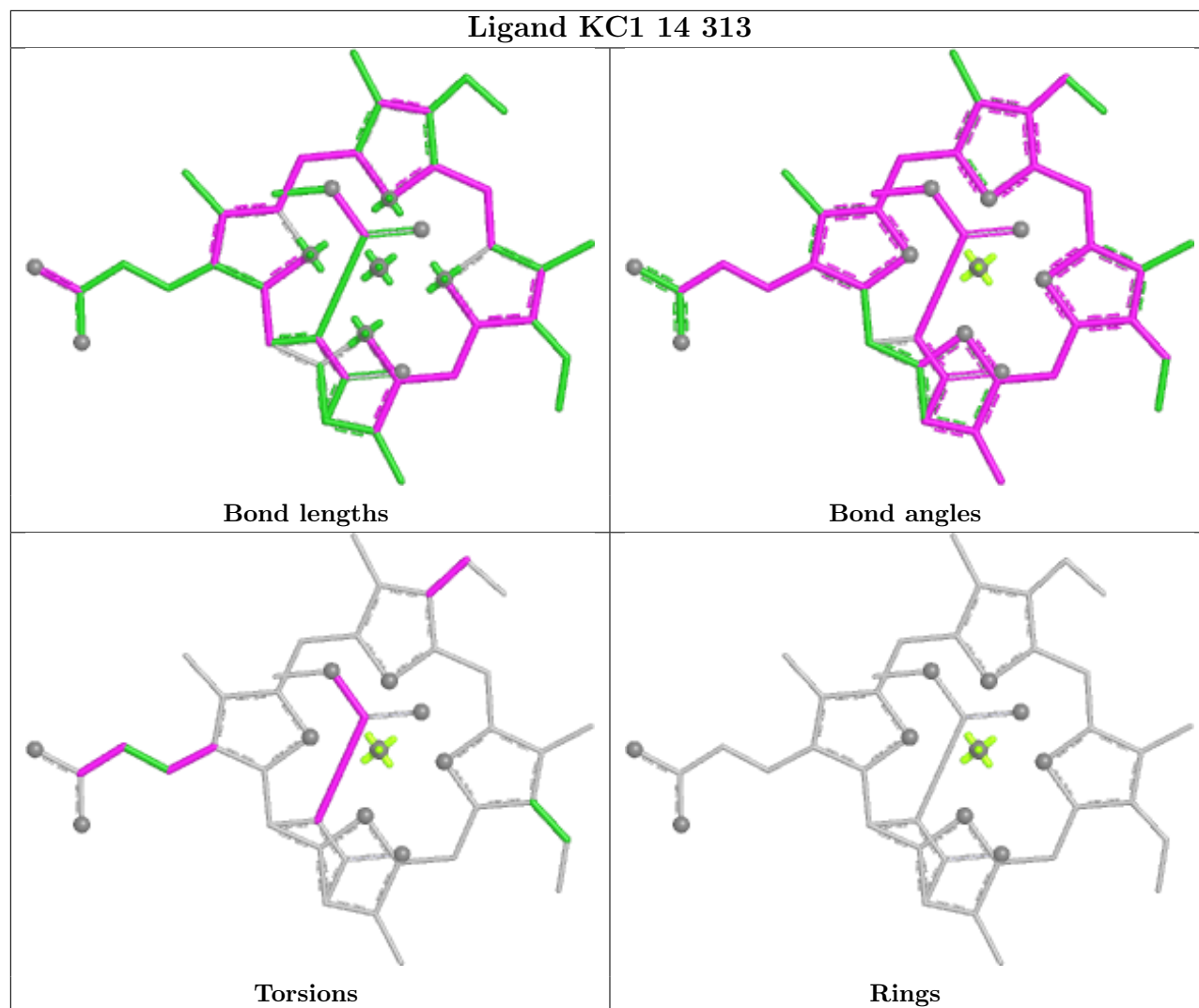


Torsions

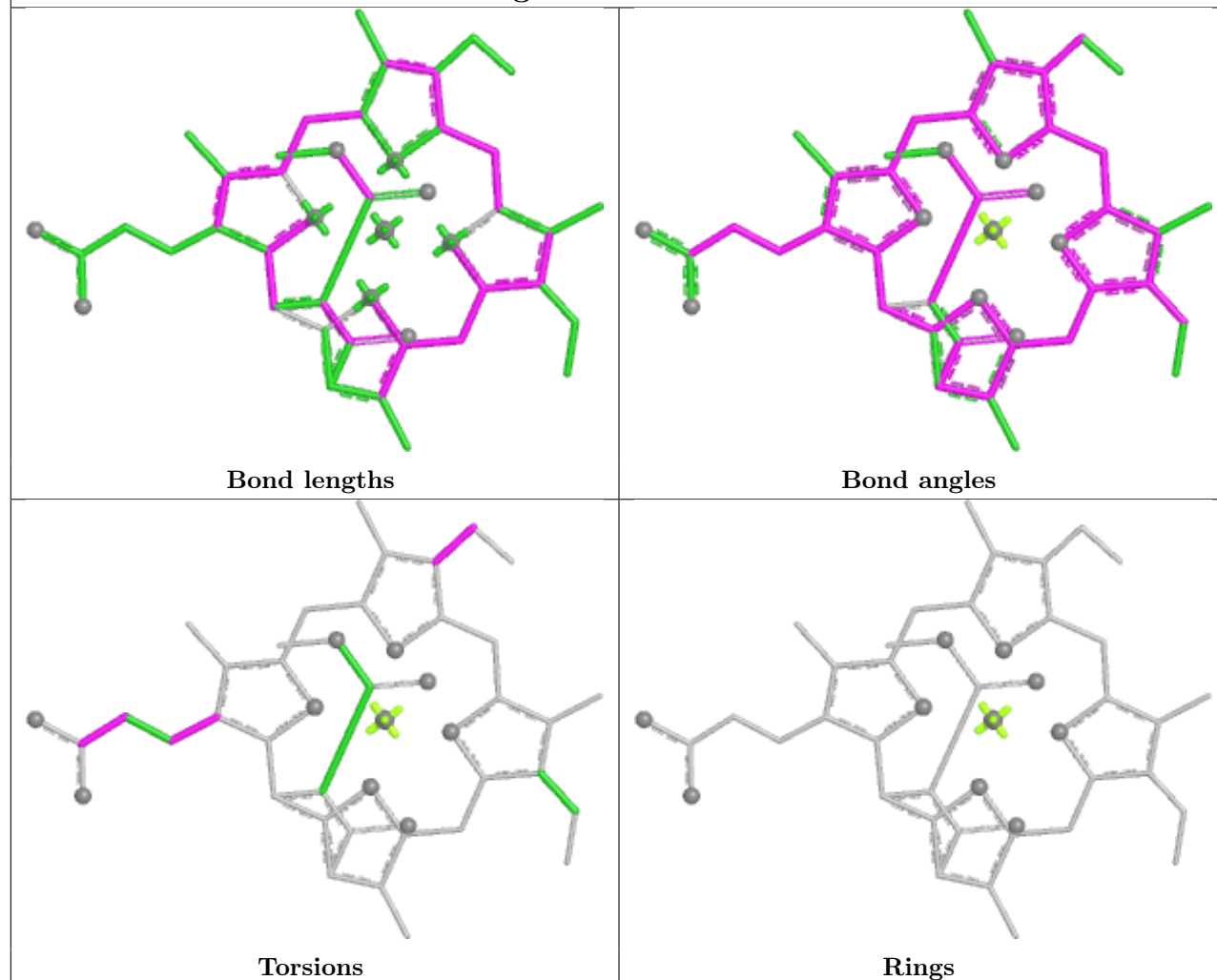


Rings

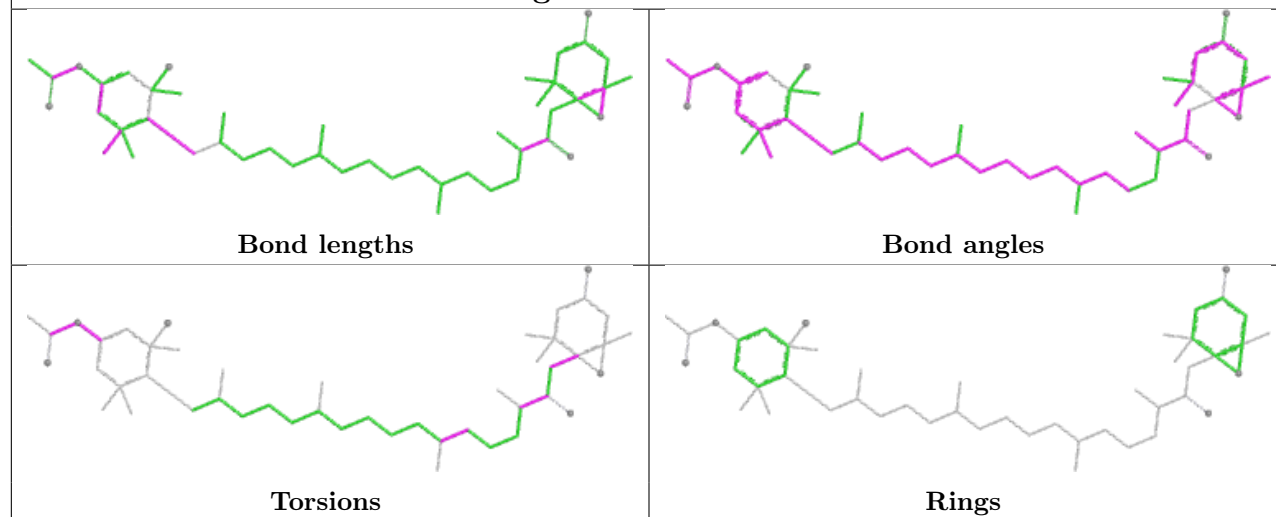


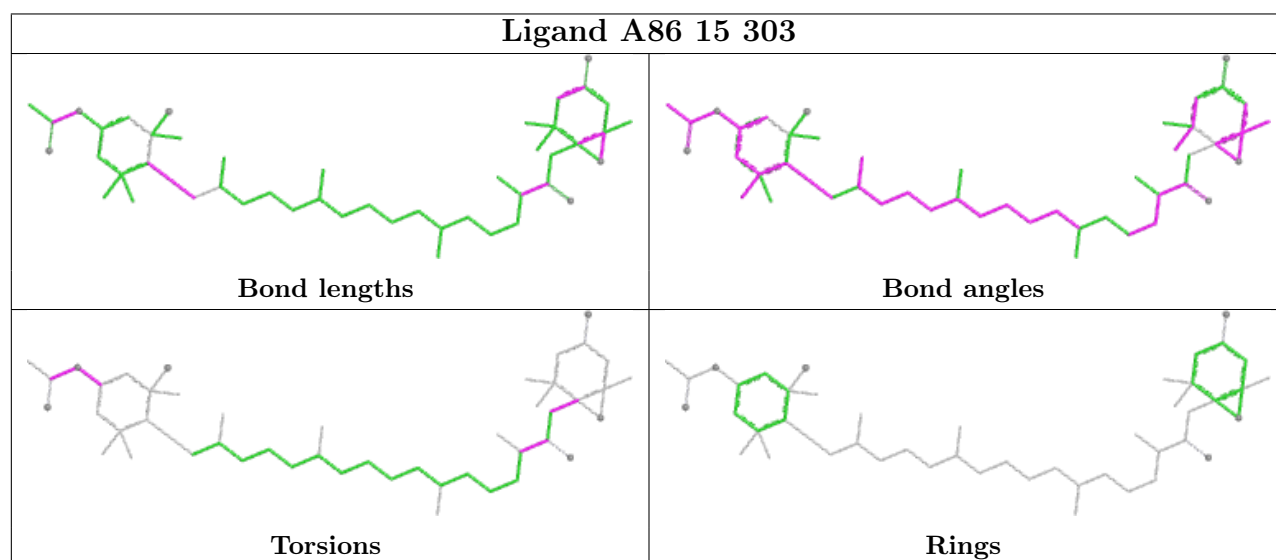
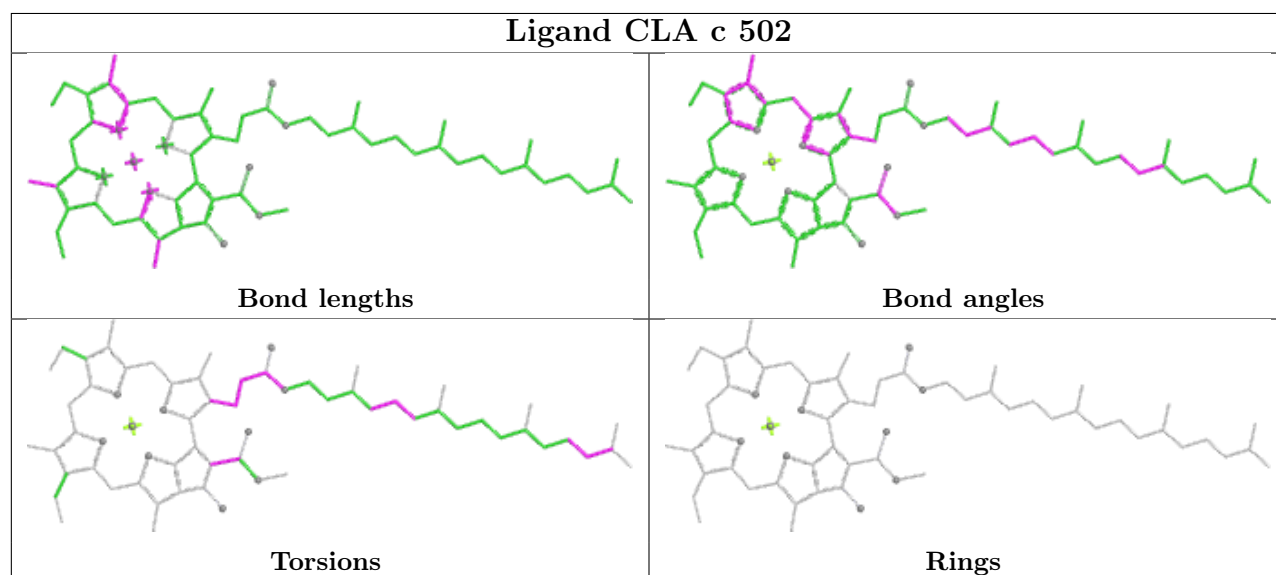
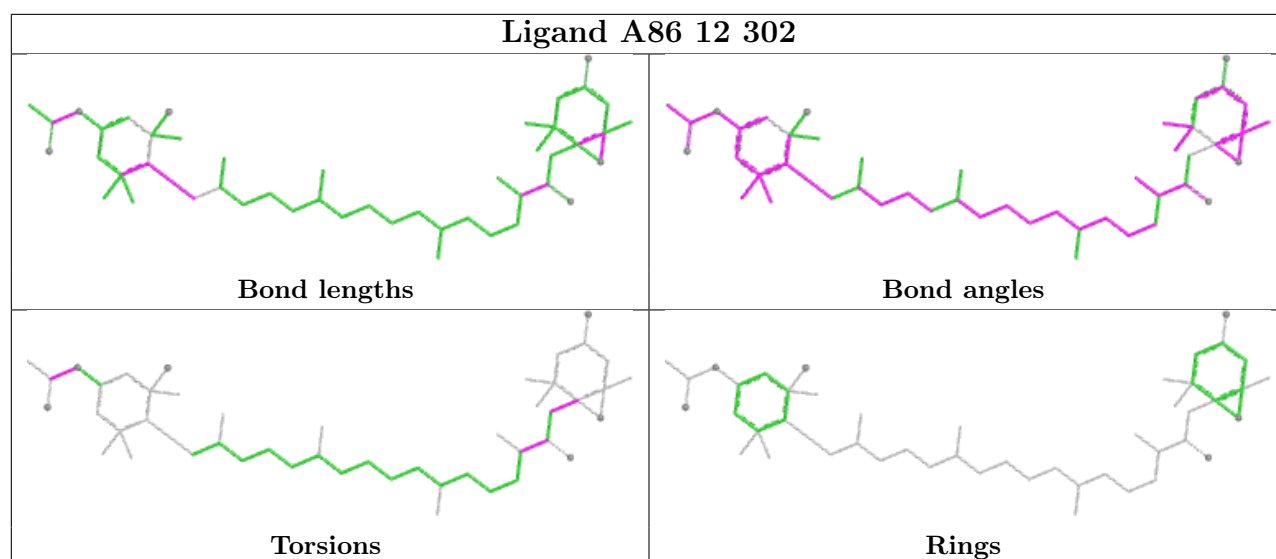


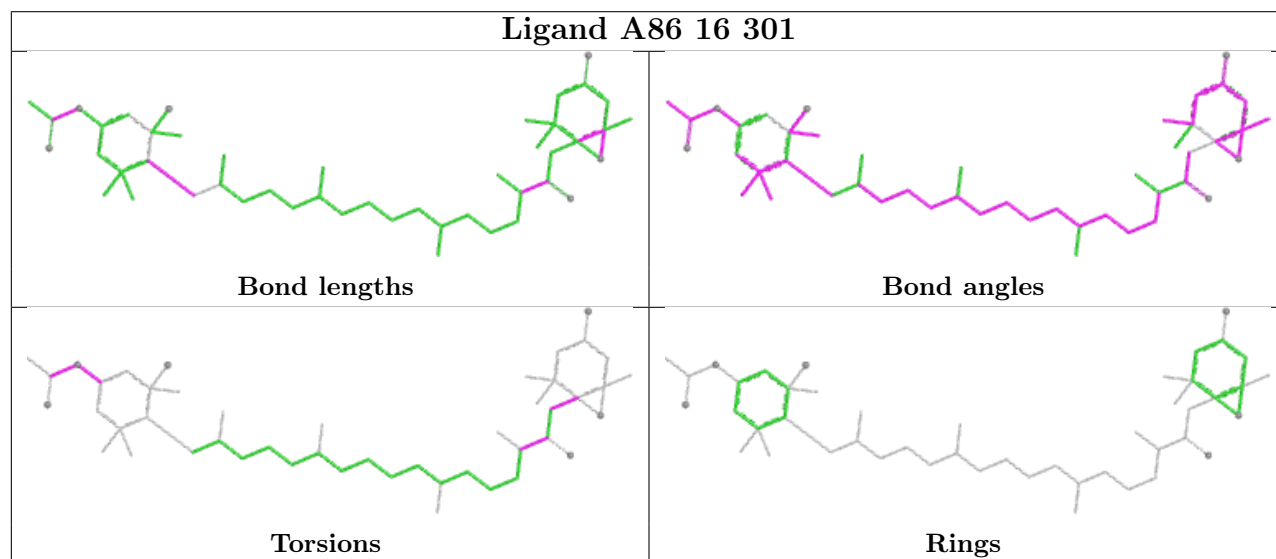
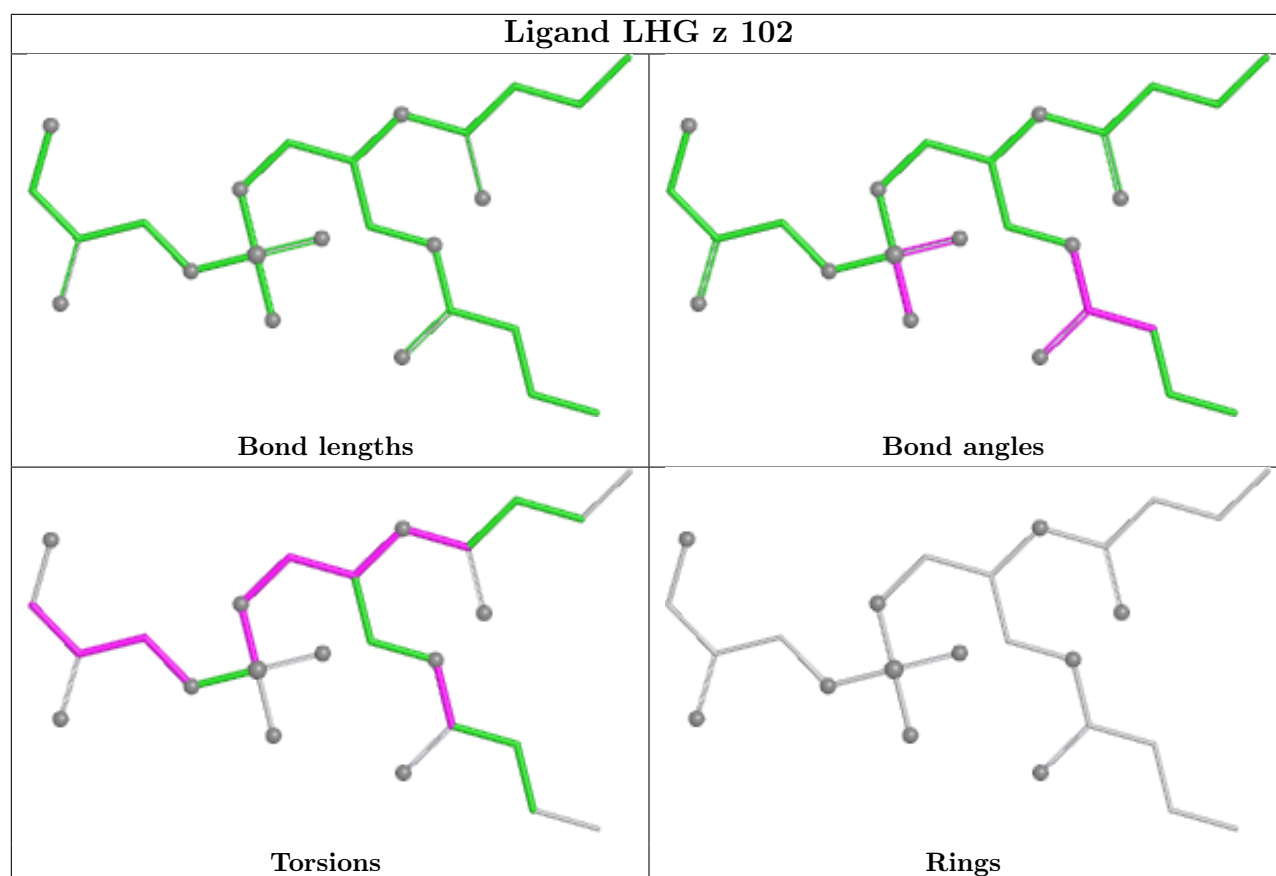
Ligand KC1 9 314

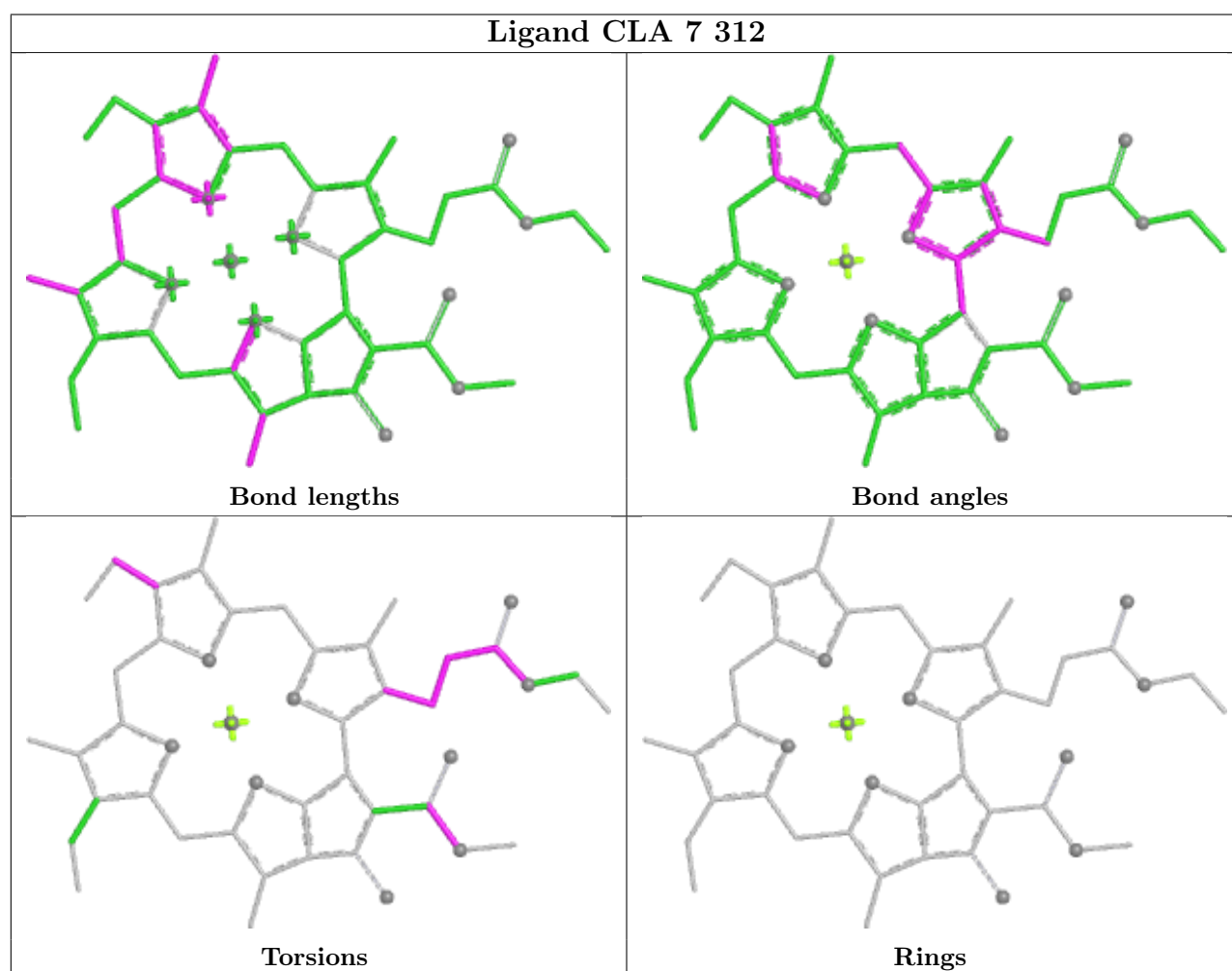
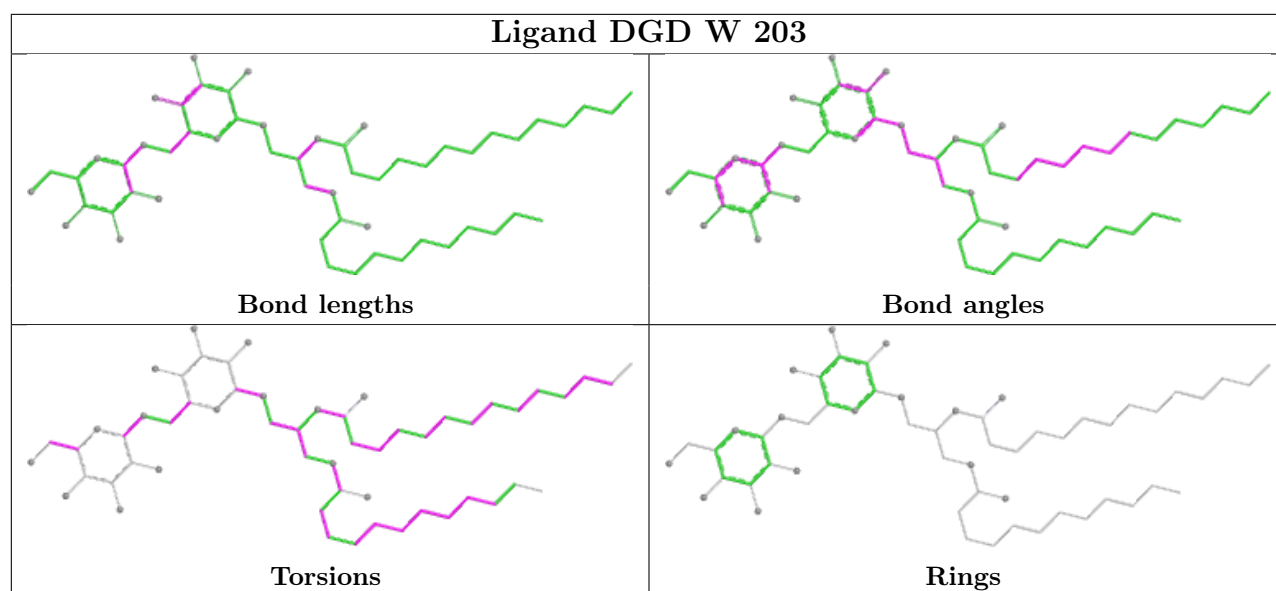


Ligand A86 16 302

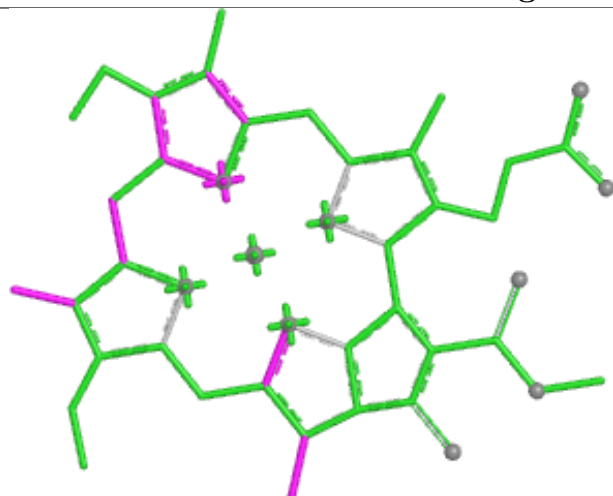




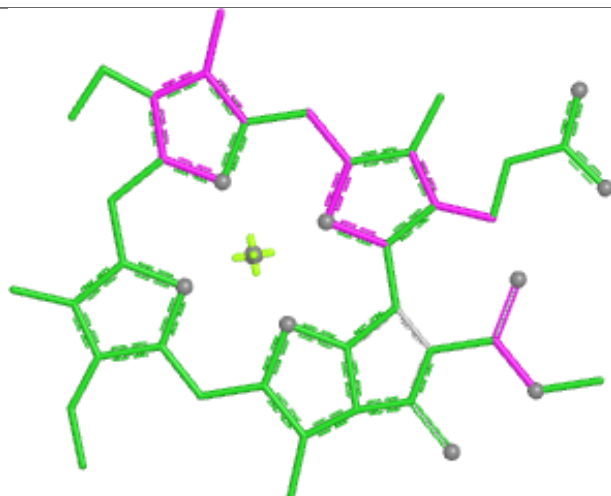




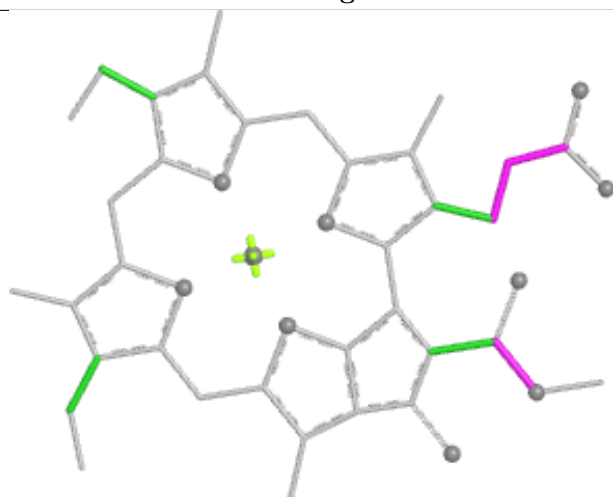
Ligand CLA 7 310



Bond lengths



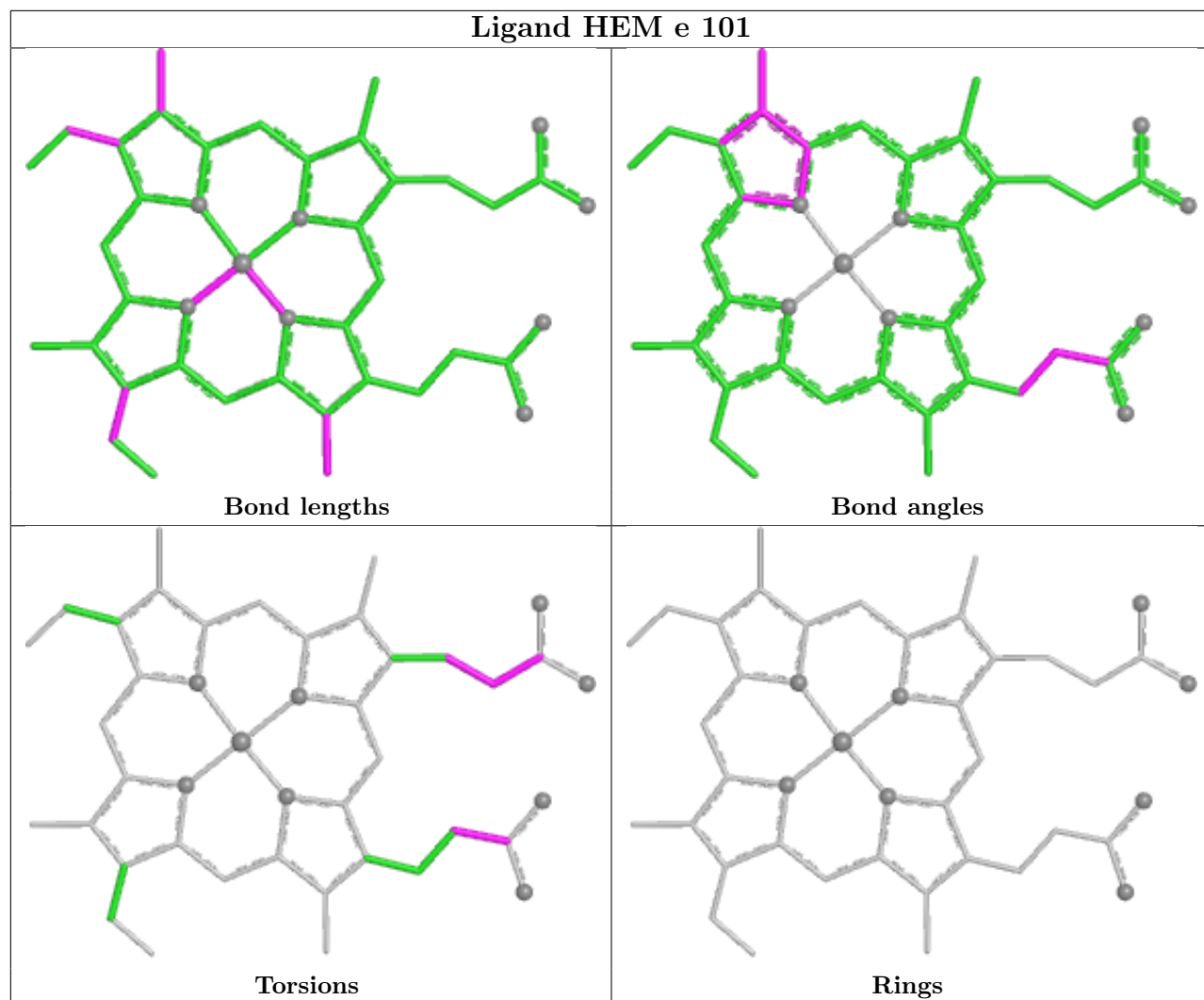
Bond angles

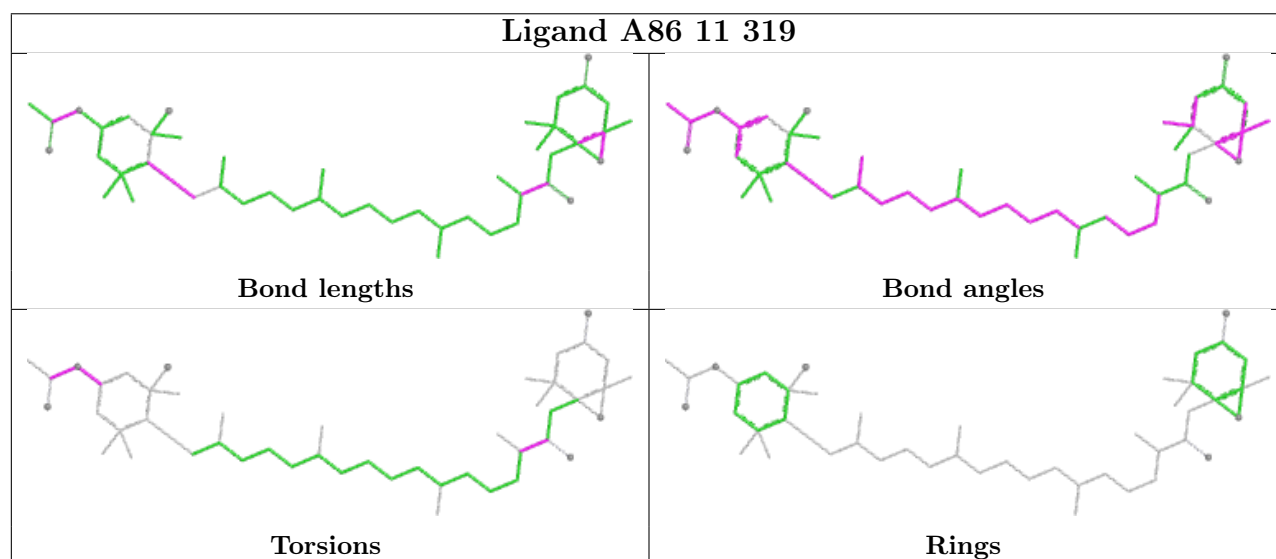
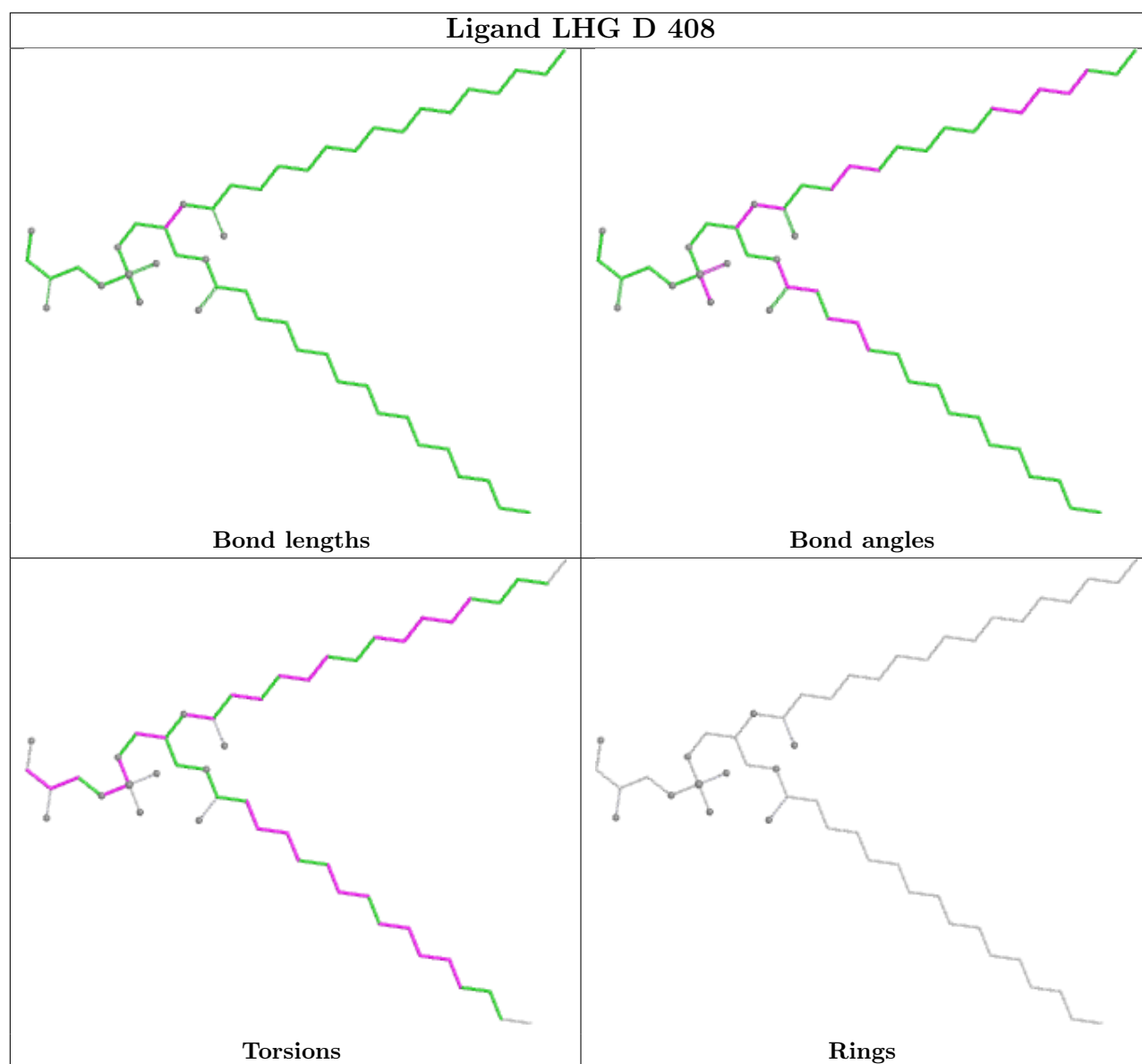


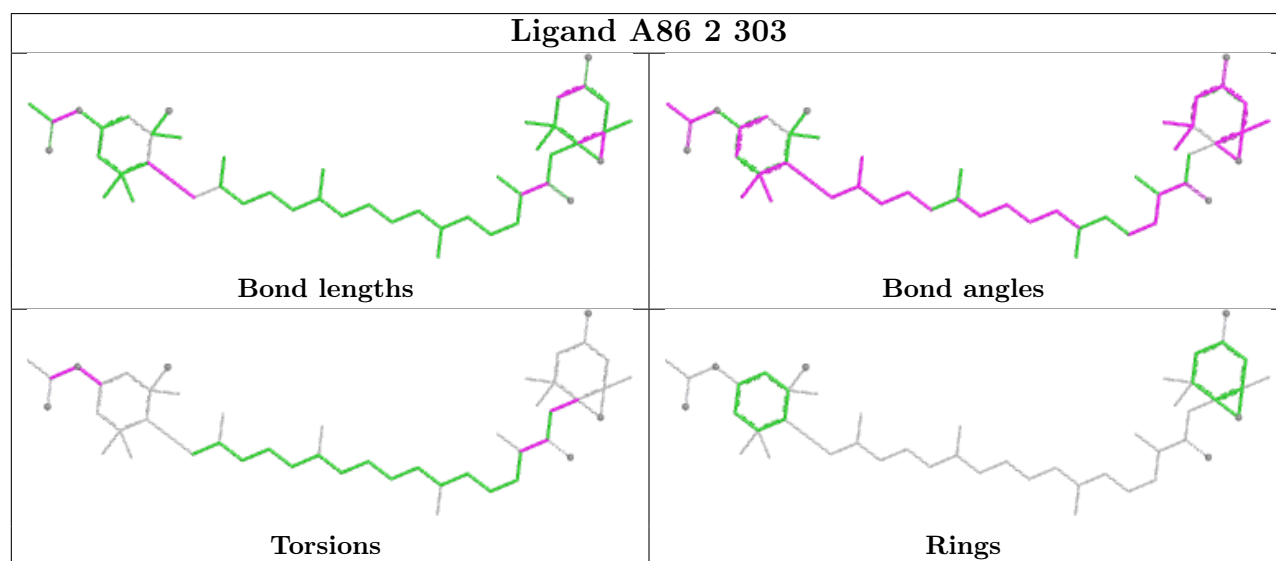
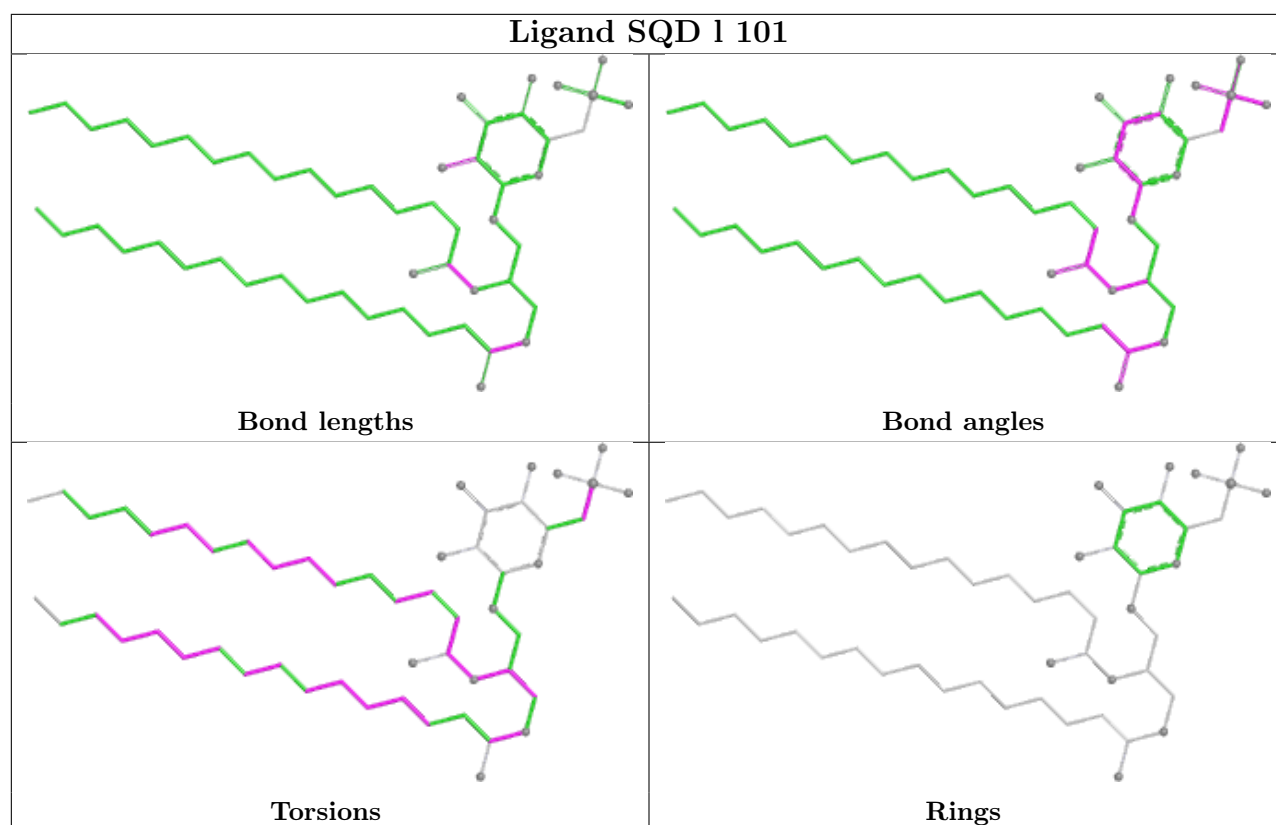
Torsions



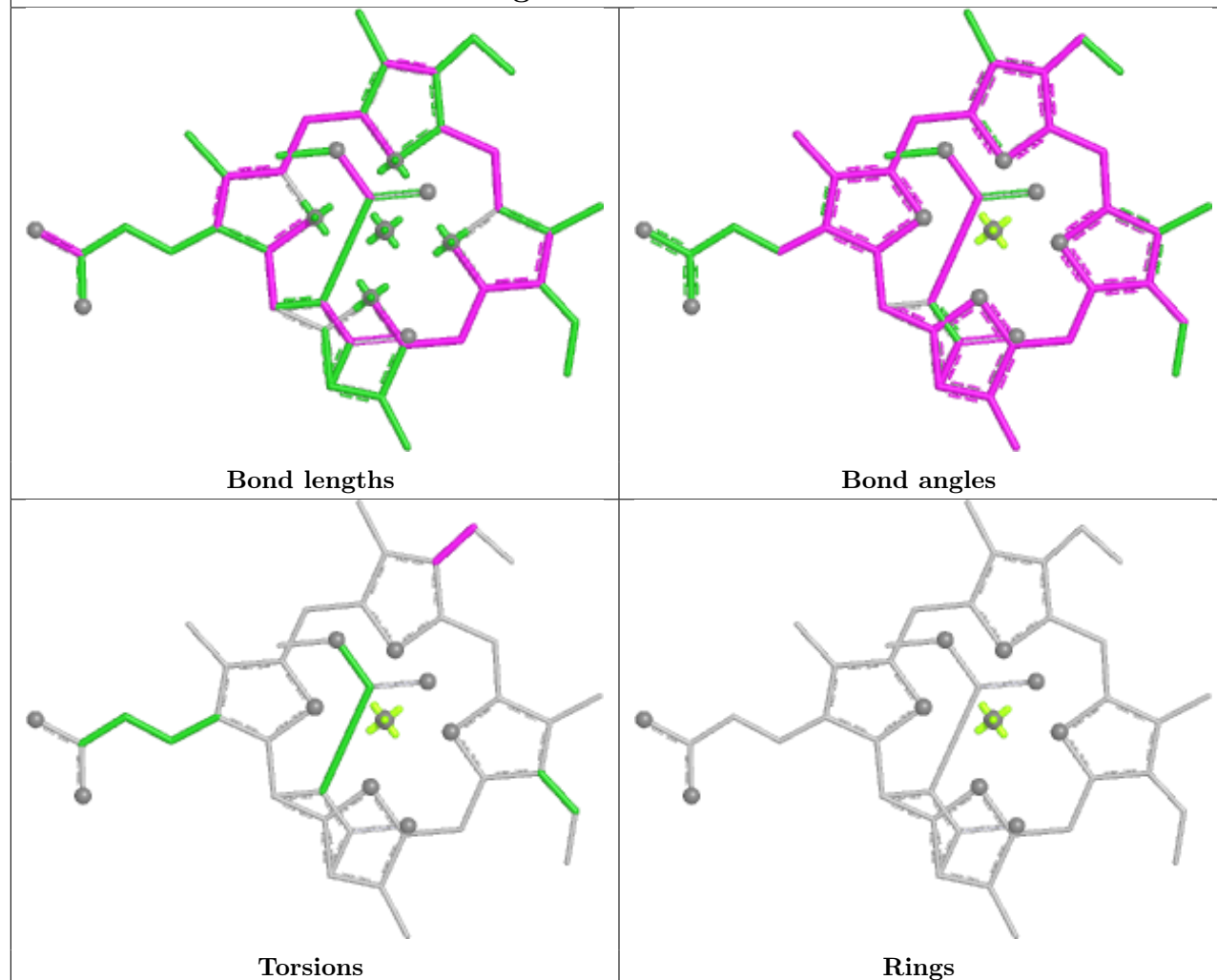
Rings



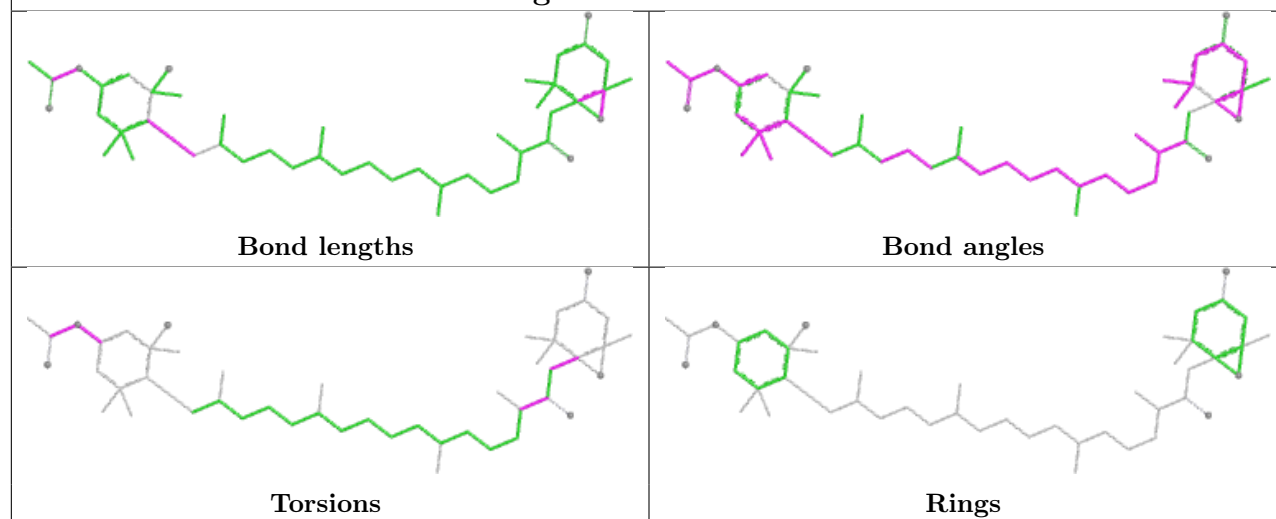


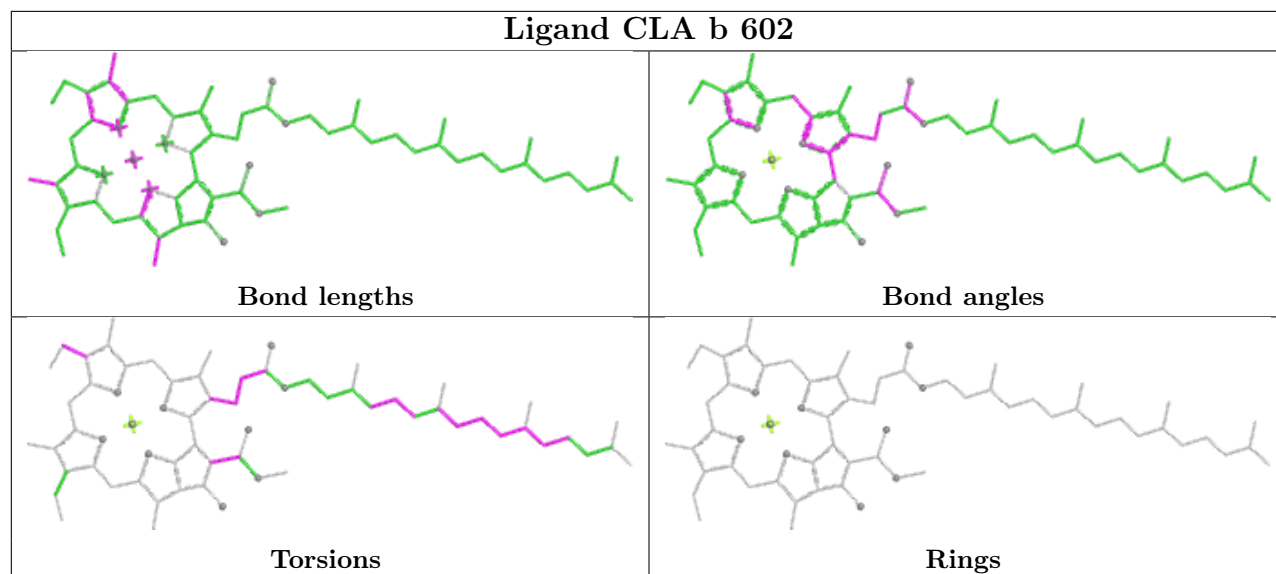
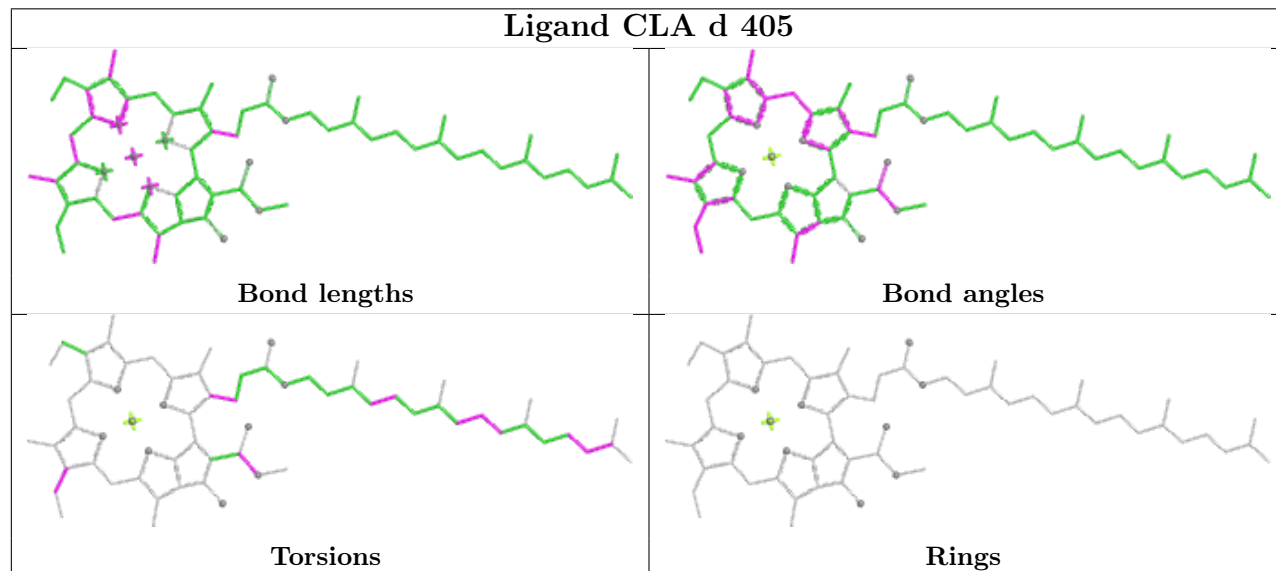


Ligand KC1 6 315

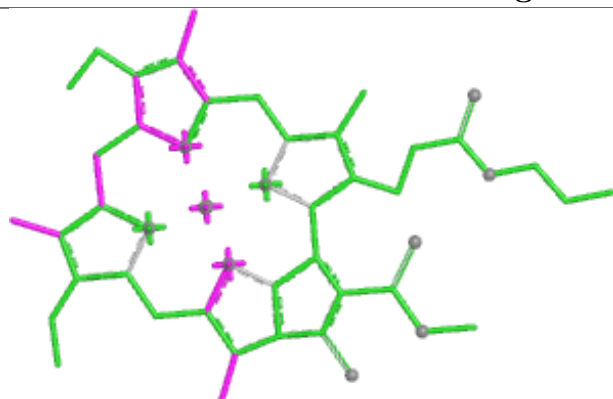


Ligand A86 17 306

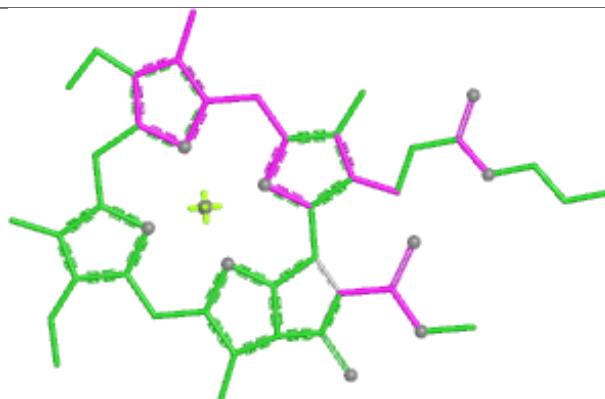


Ligand CLA b 602**Ligand CLA d 405**

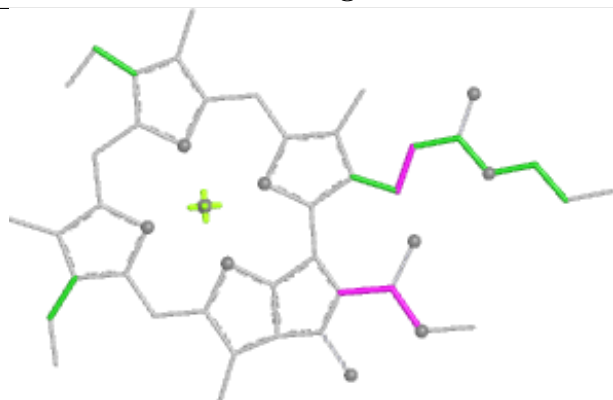
Ligand CLA P 604



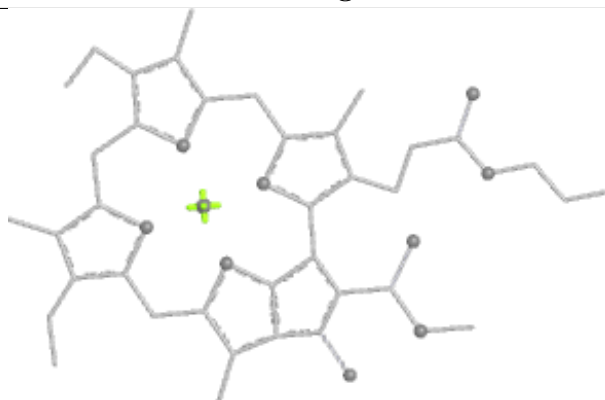
Bond lengths



Bond angles

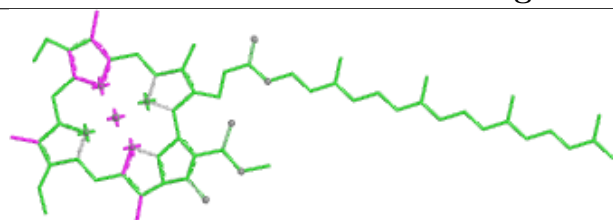


Torsions



Rings

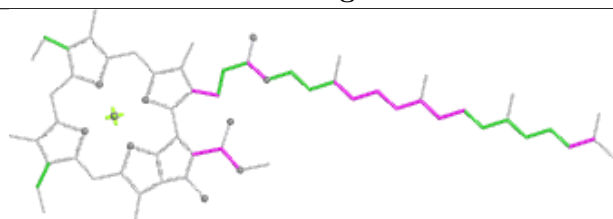
Ligand CLA B 614



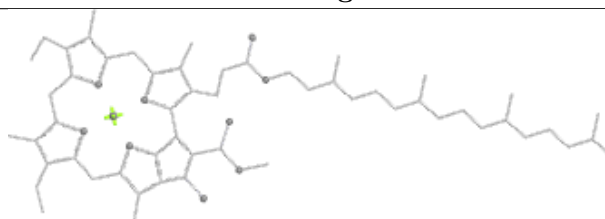
Bond lengths



Bond angles

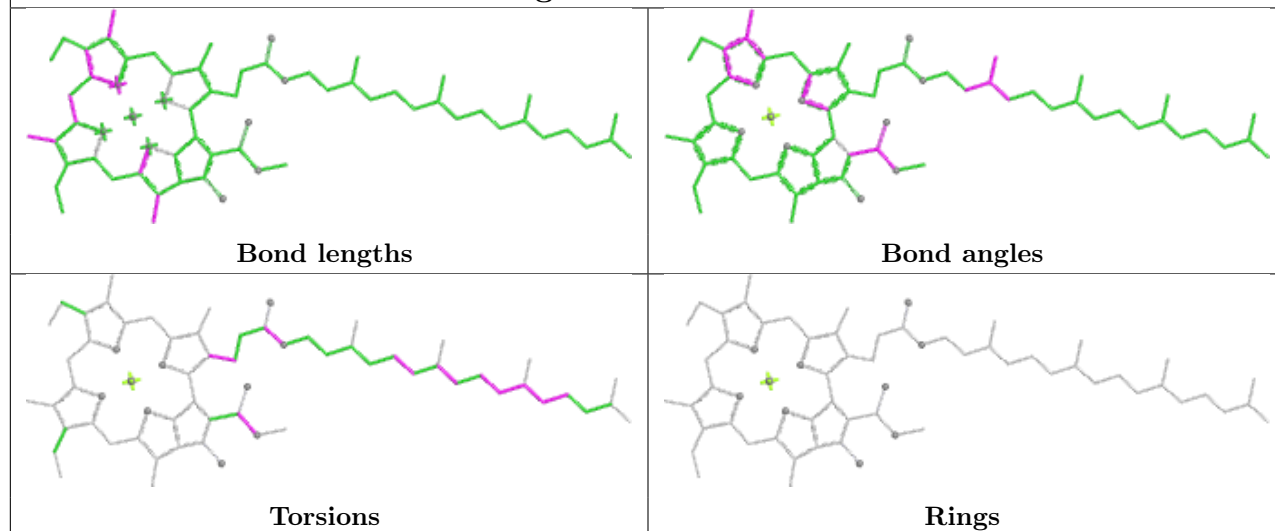


Torsions

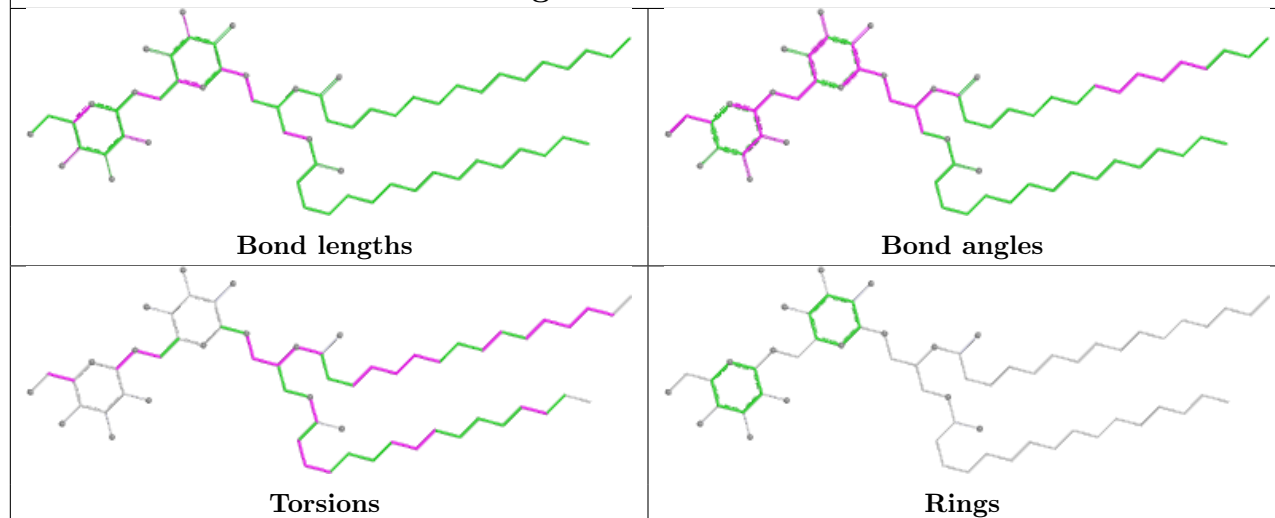


Rings

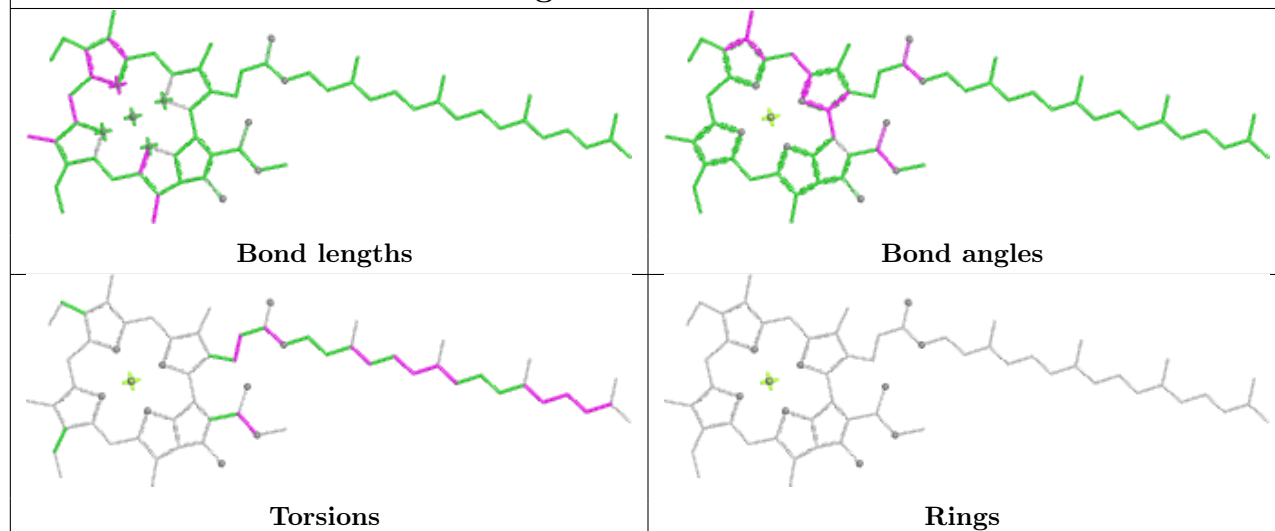
Ligand CLA 1 308

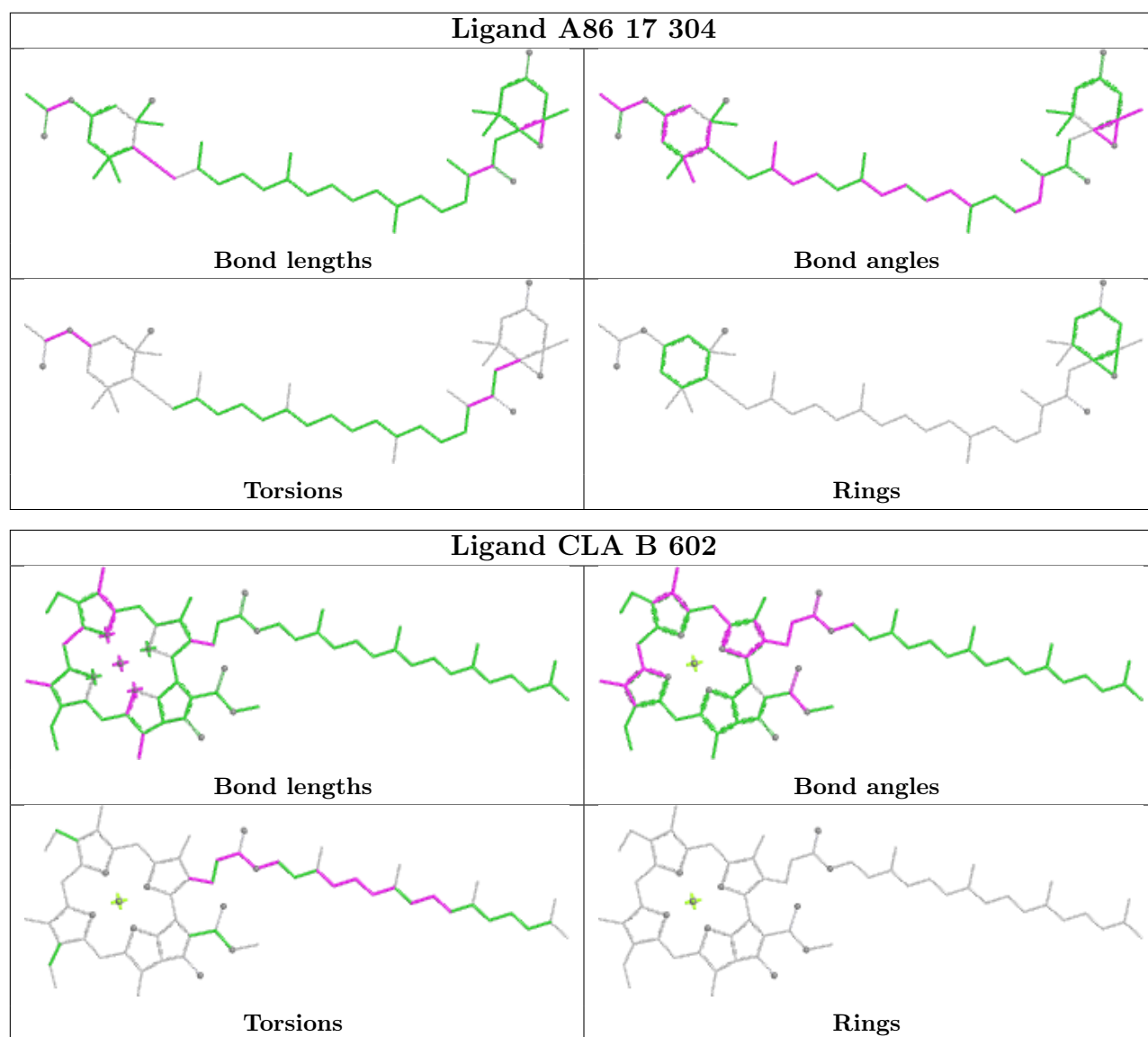


Ligand DGD c 519

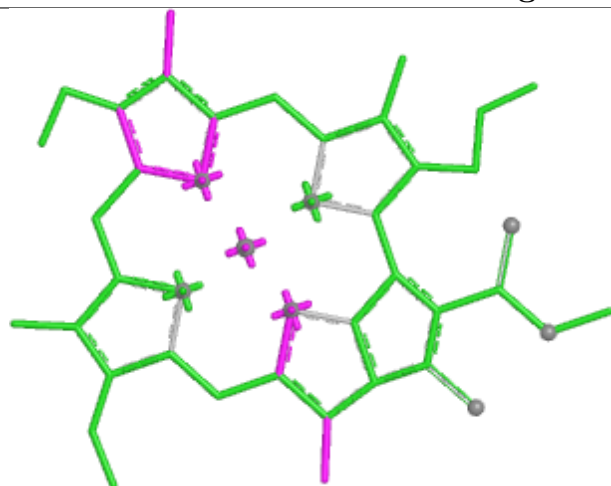


Ligand CLA 4 309

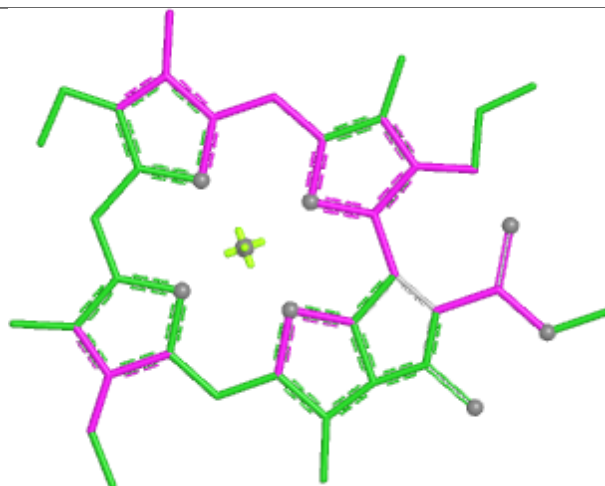




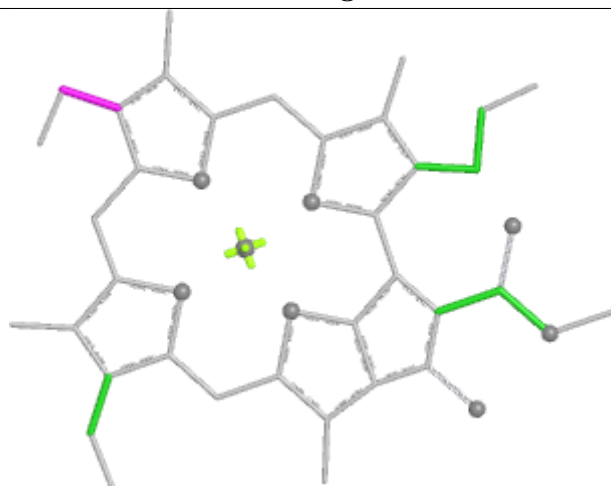
Ligand CLA 1 307



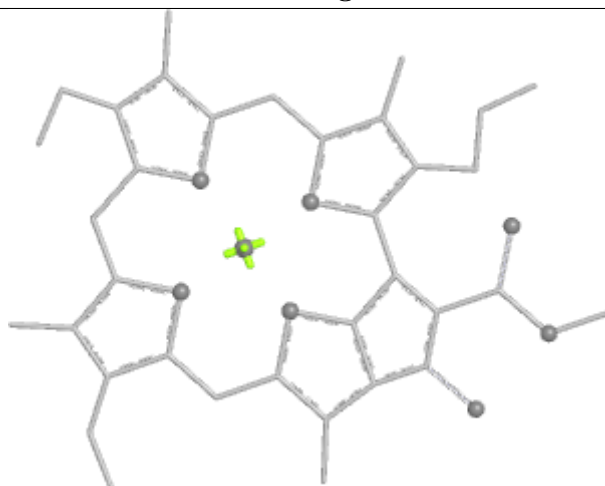
Bond lengths



Bond angles

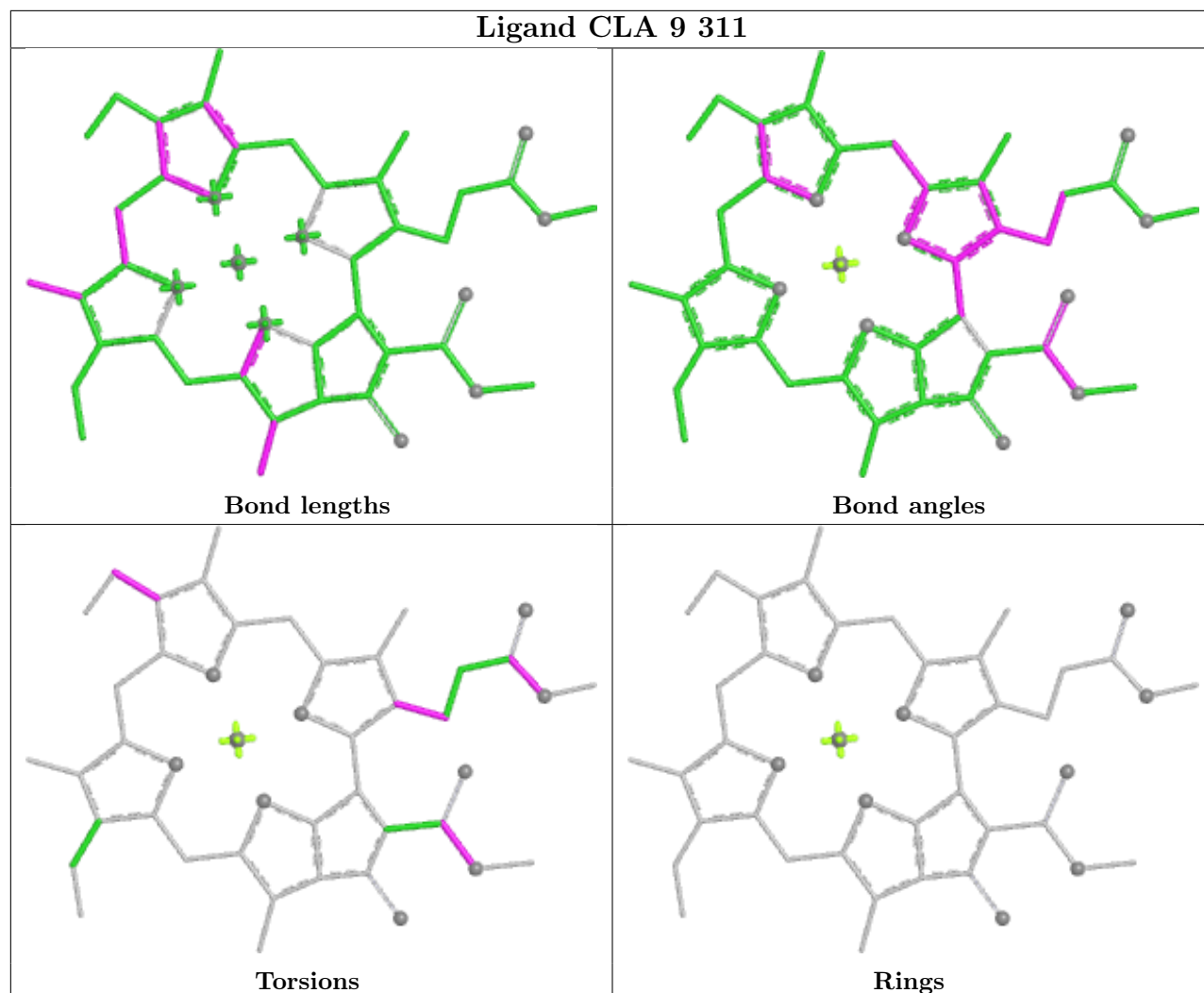


Torsions

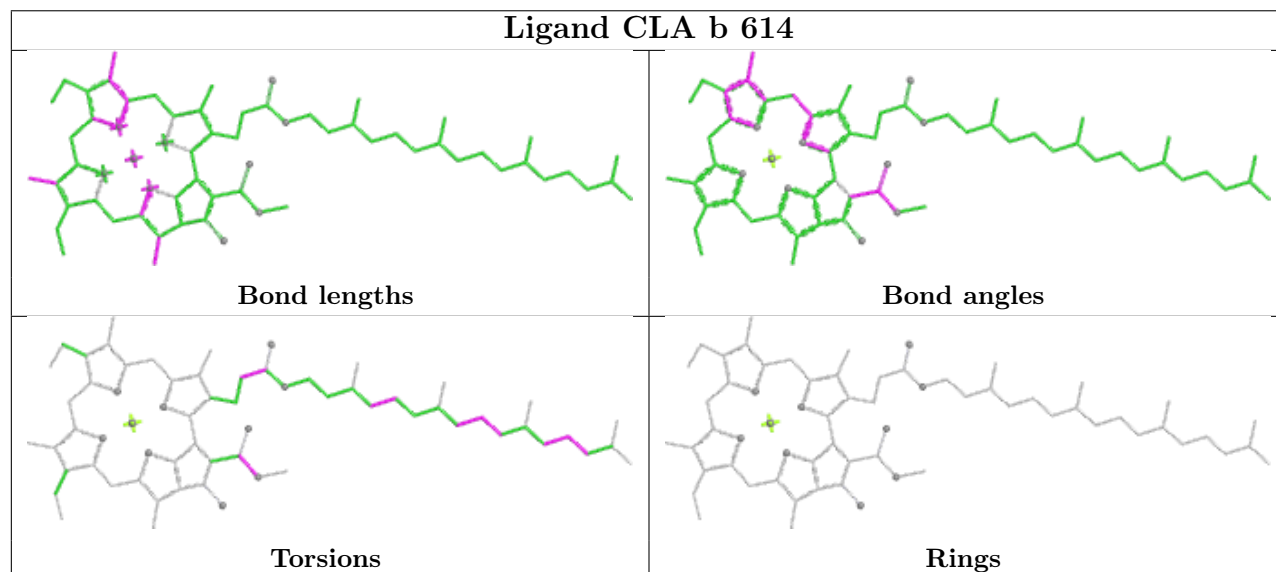


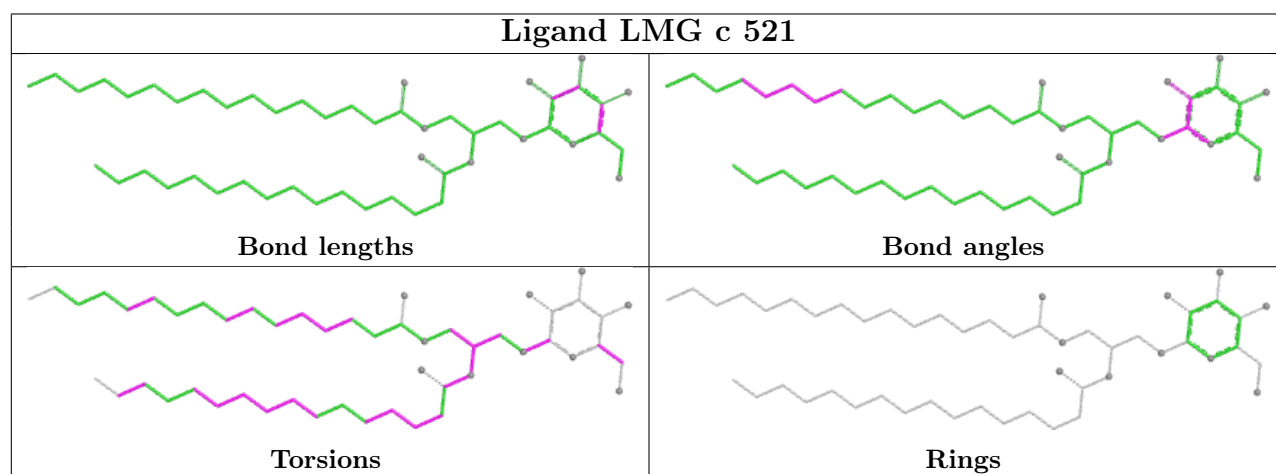
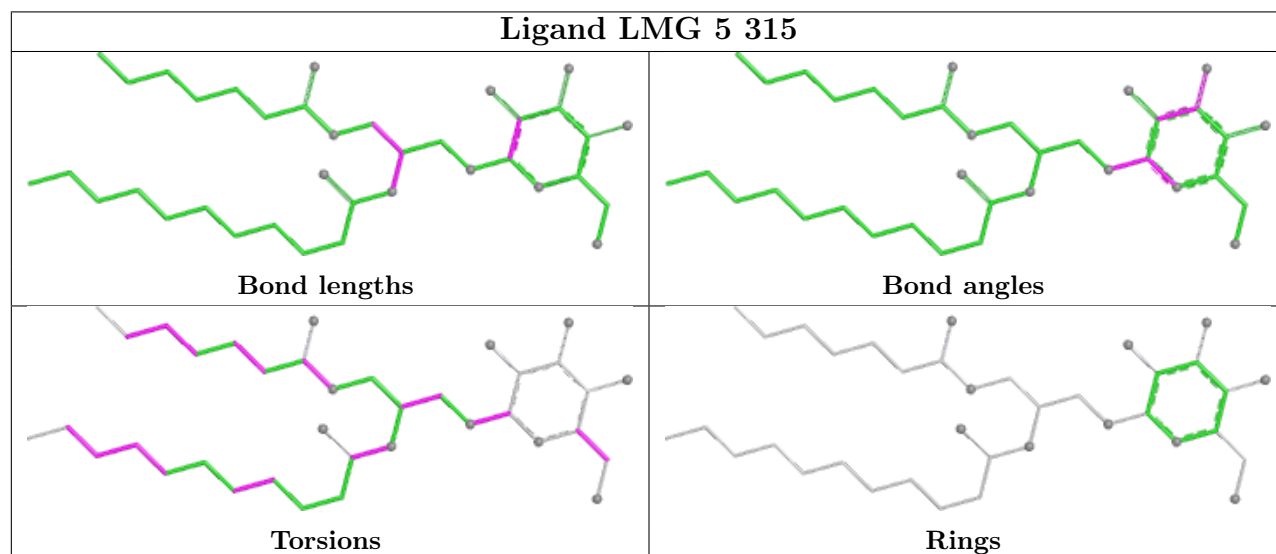
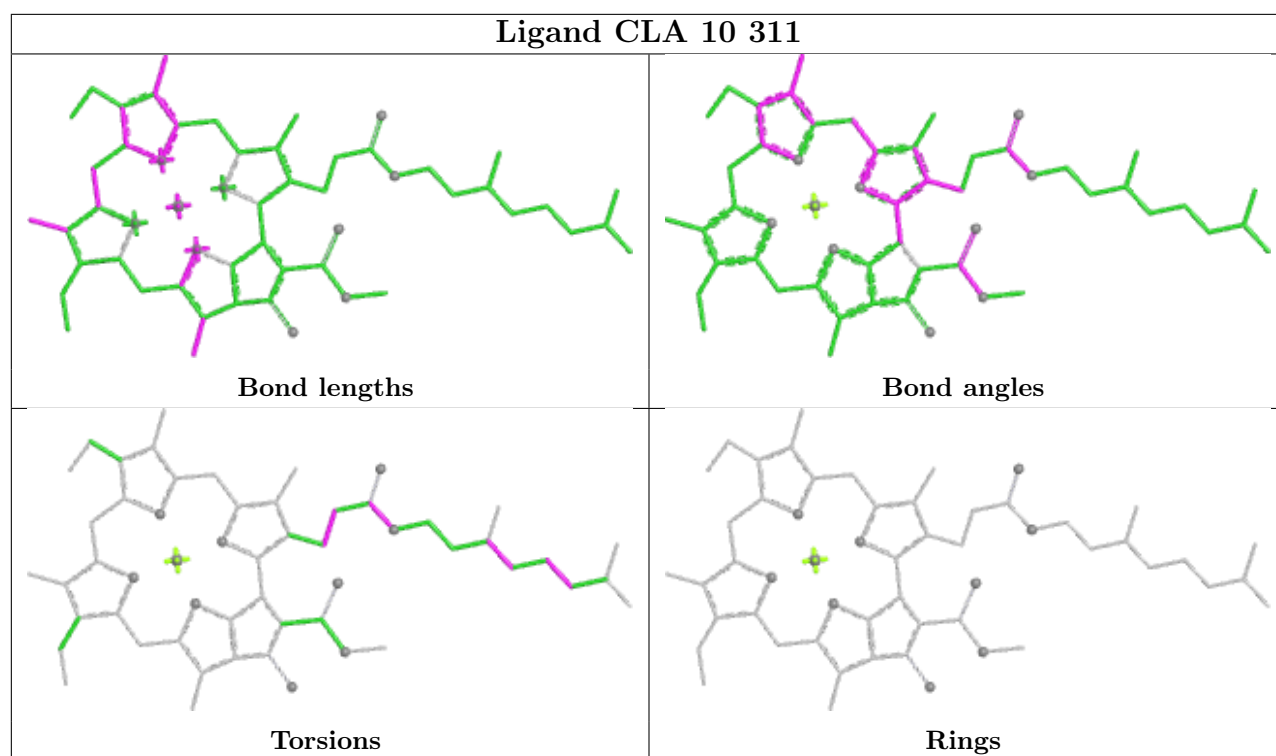
Rings

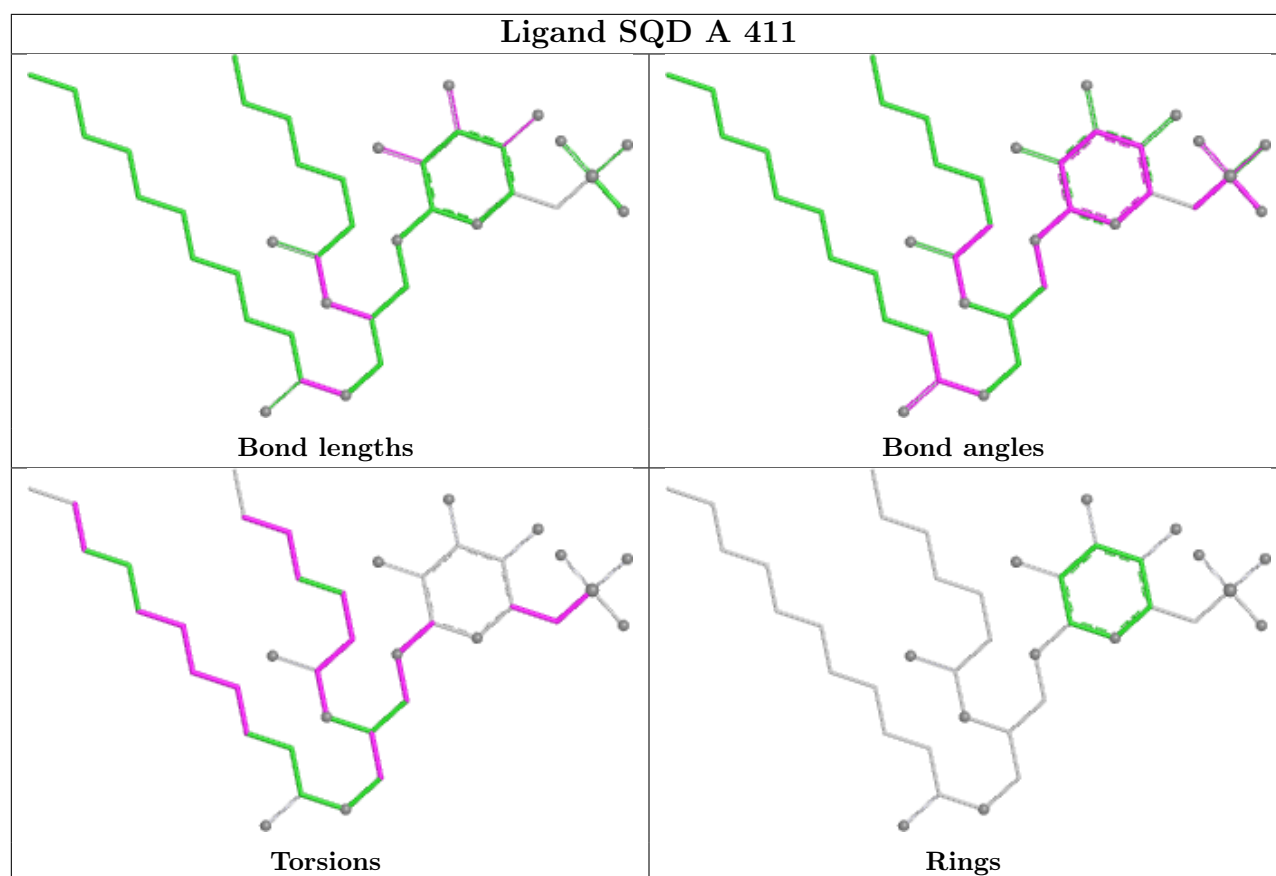
Ligand CLA 9 311

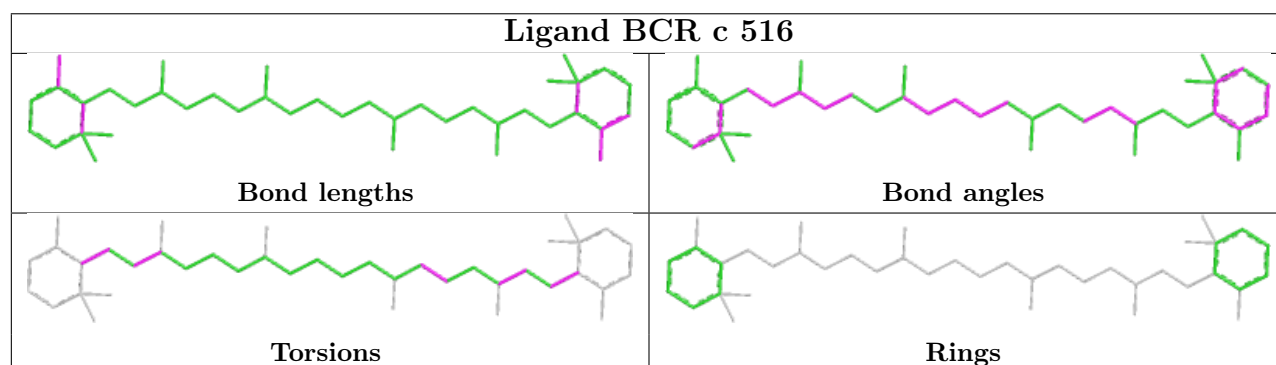
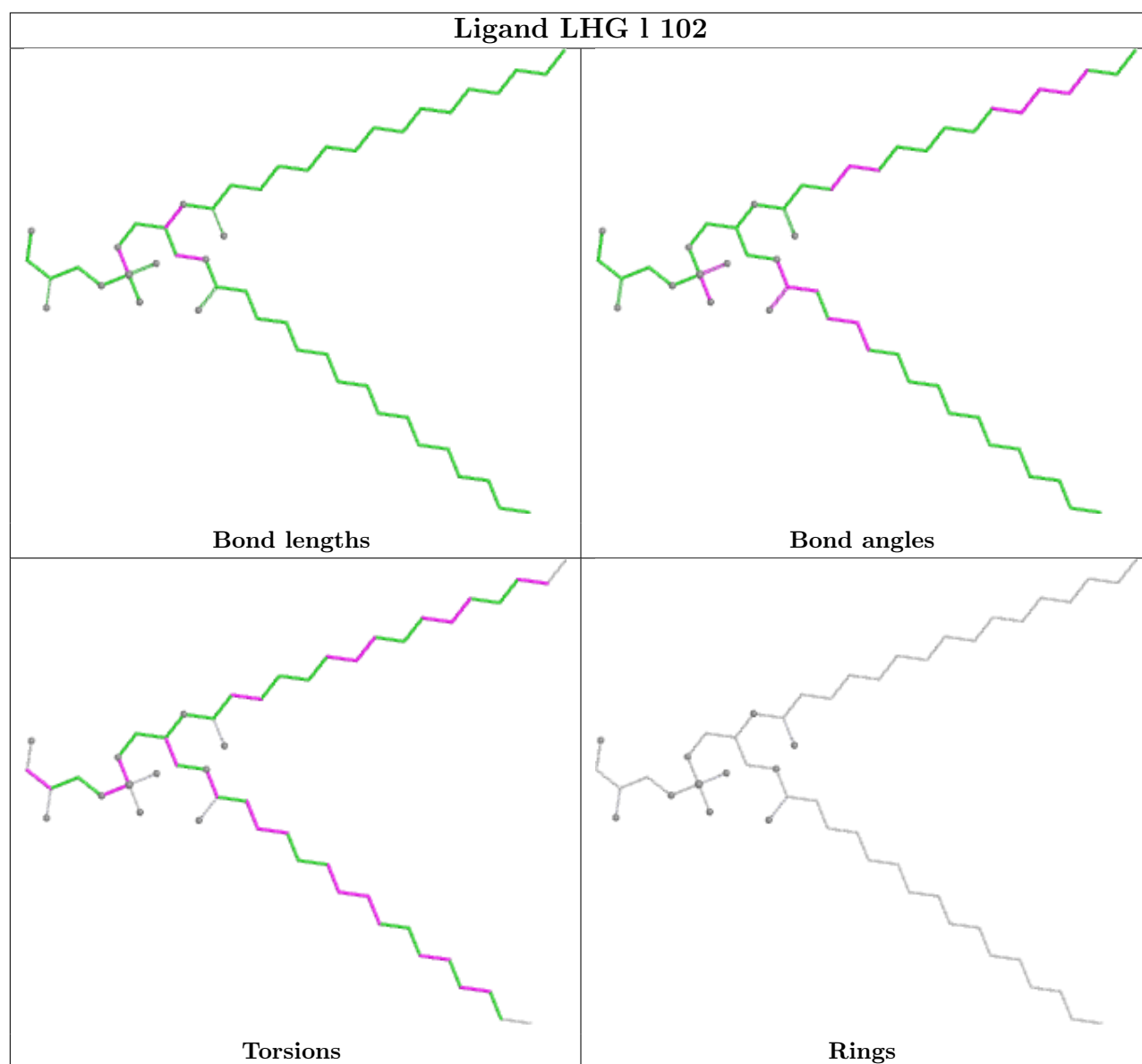


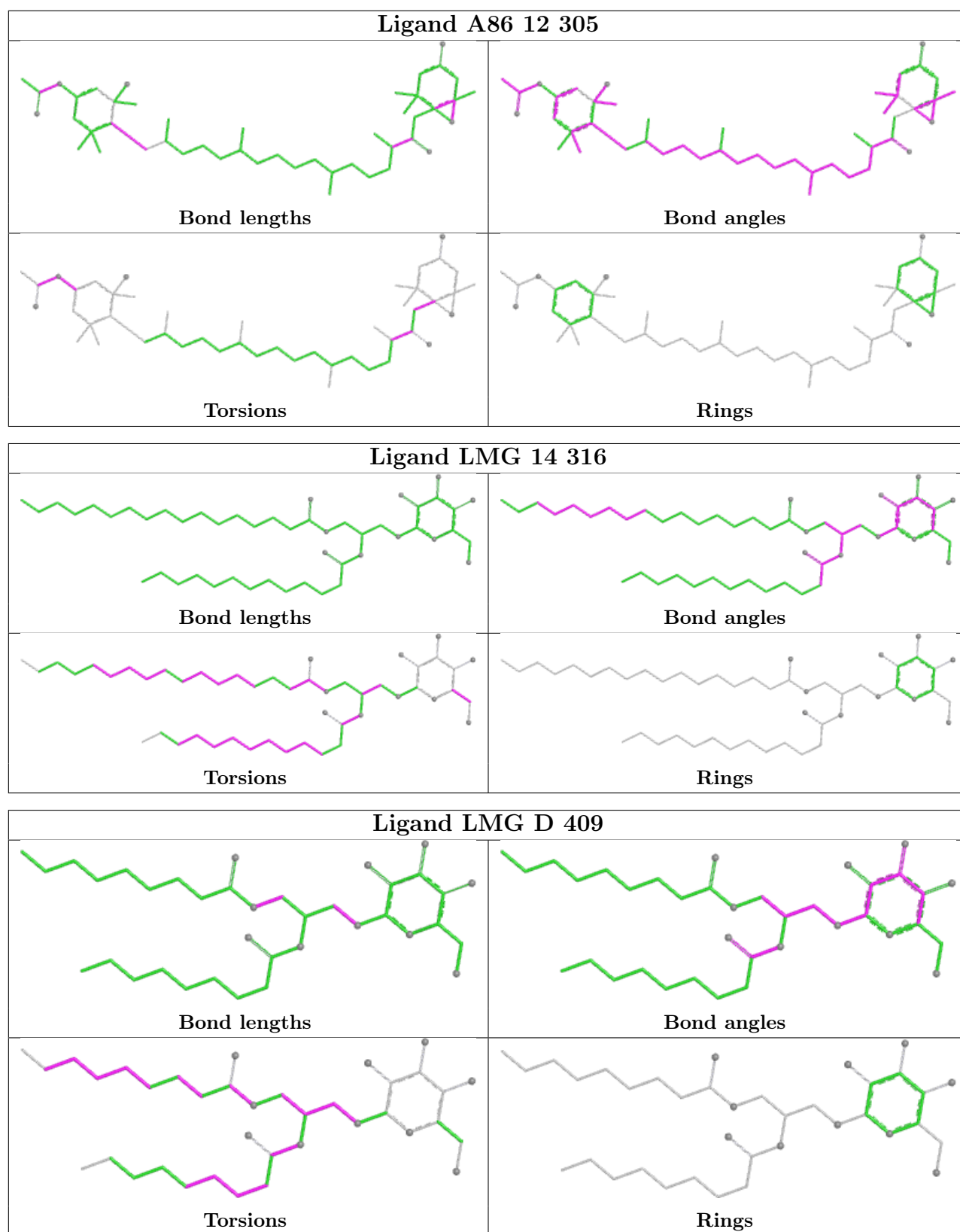
Ligand CLA b 614

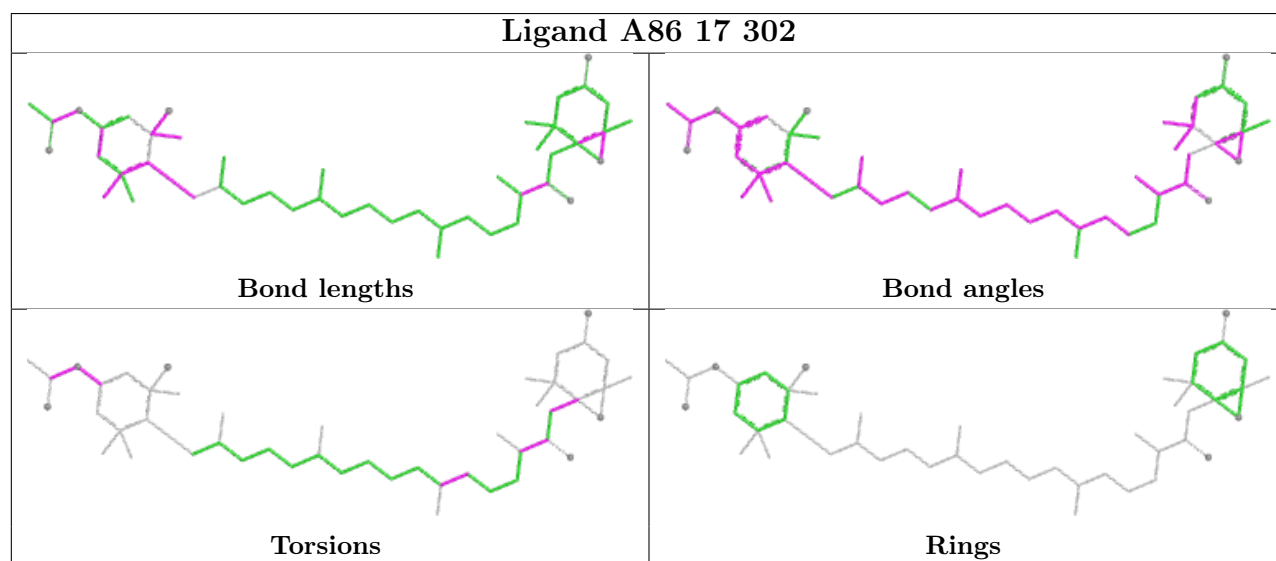
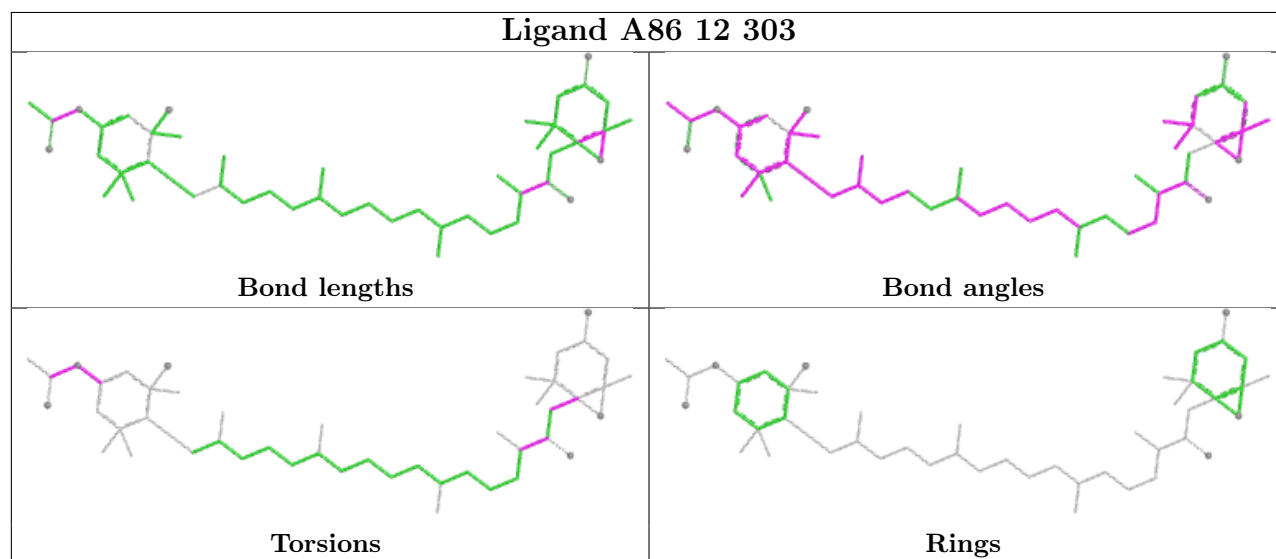
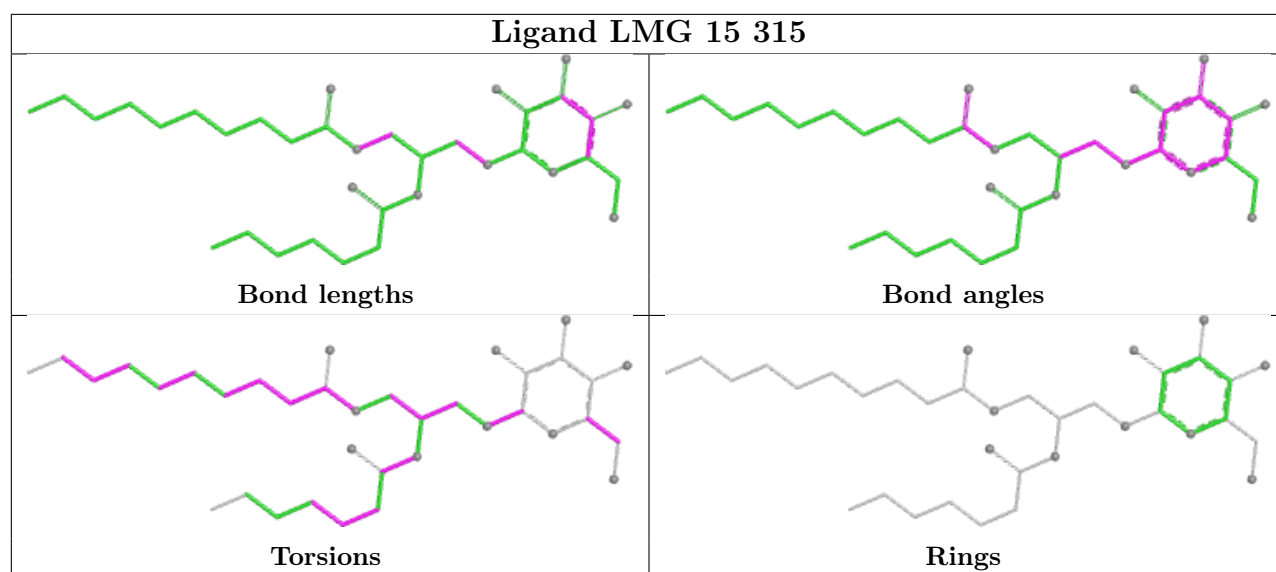


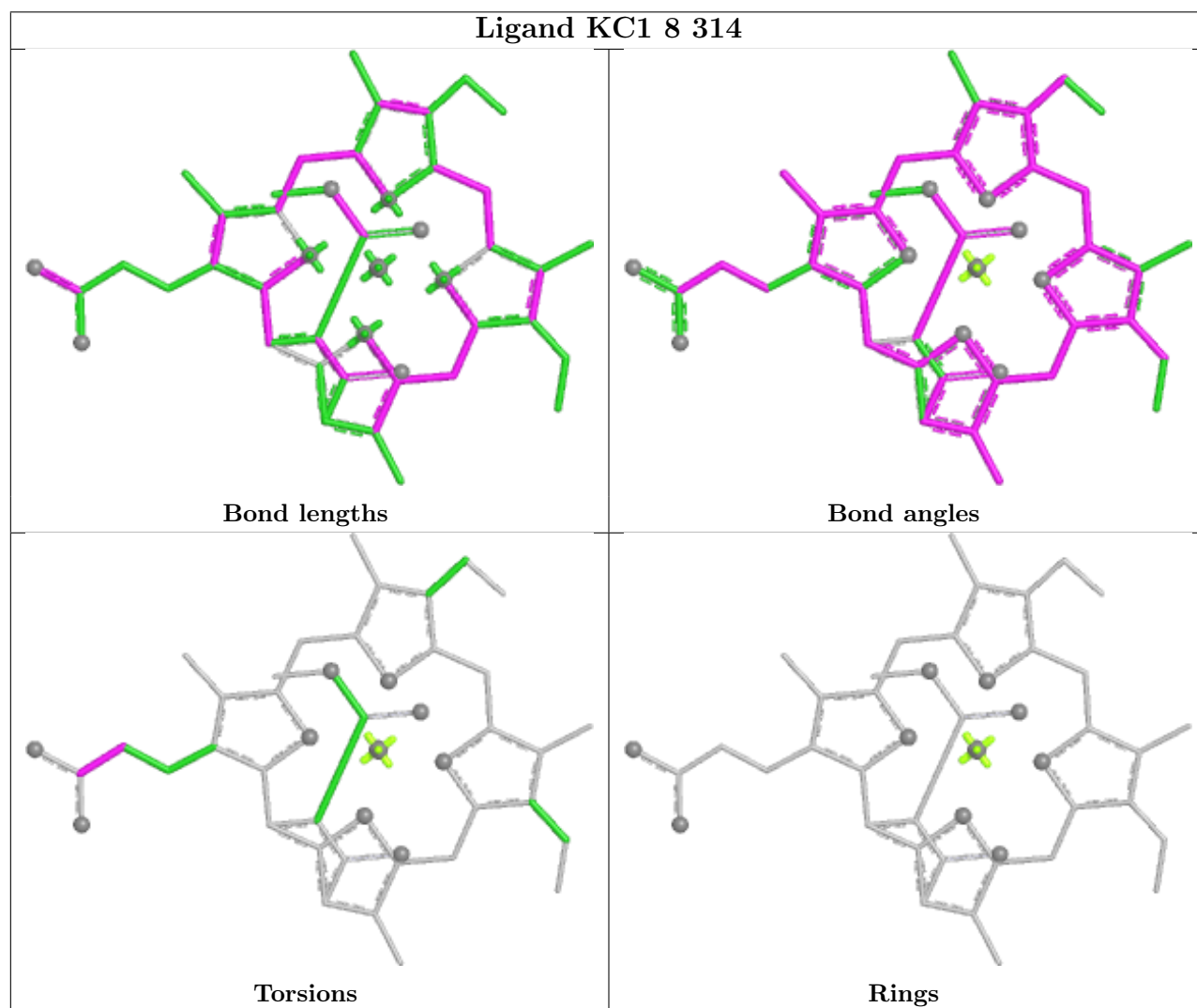
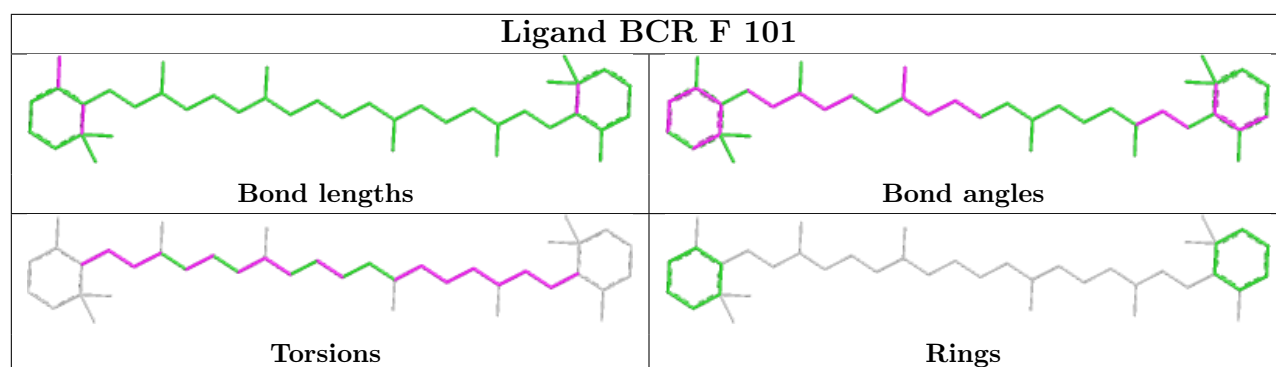


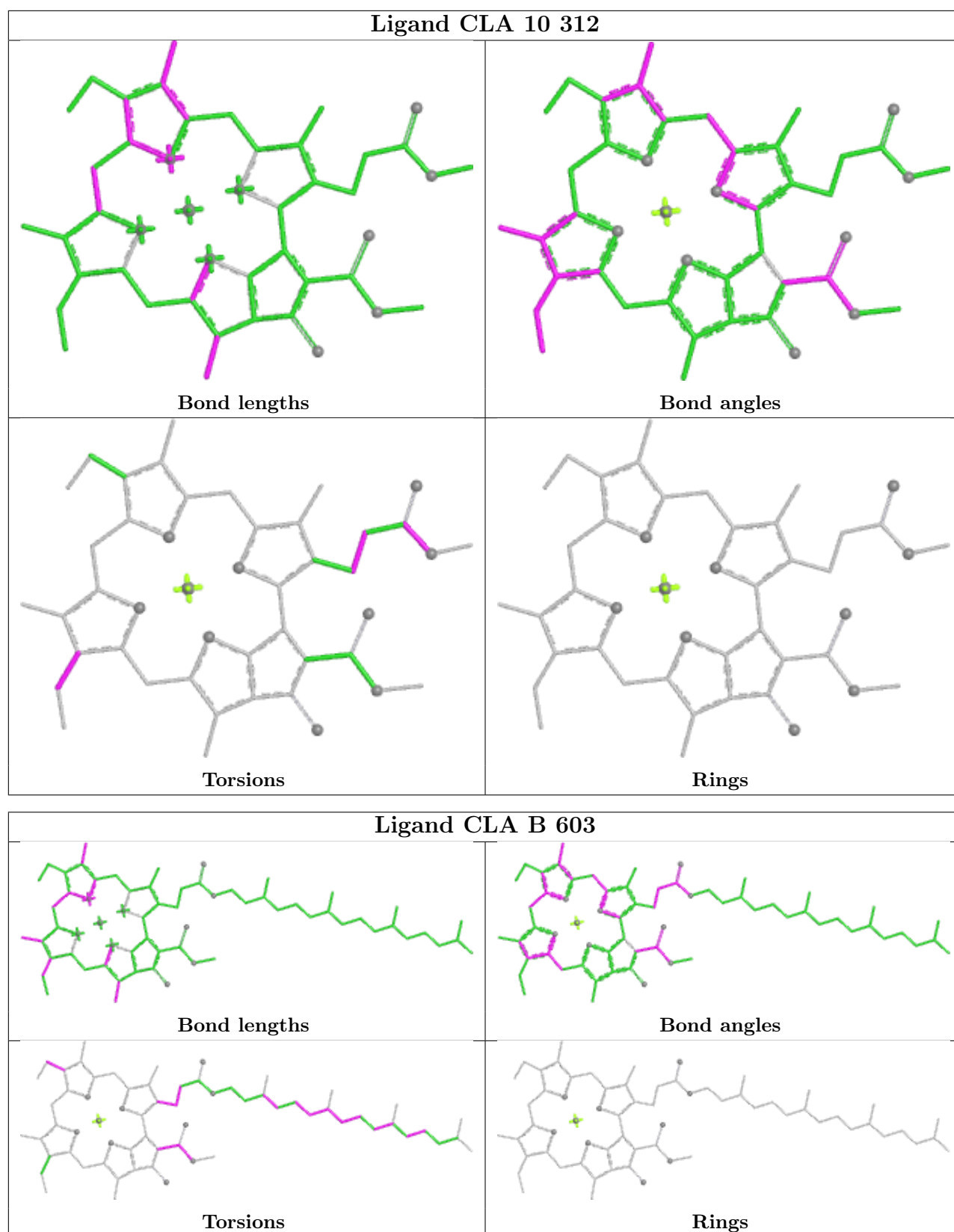


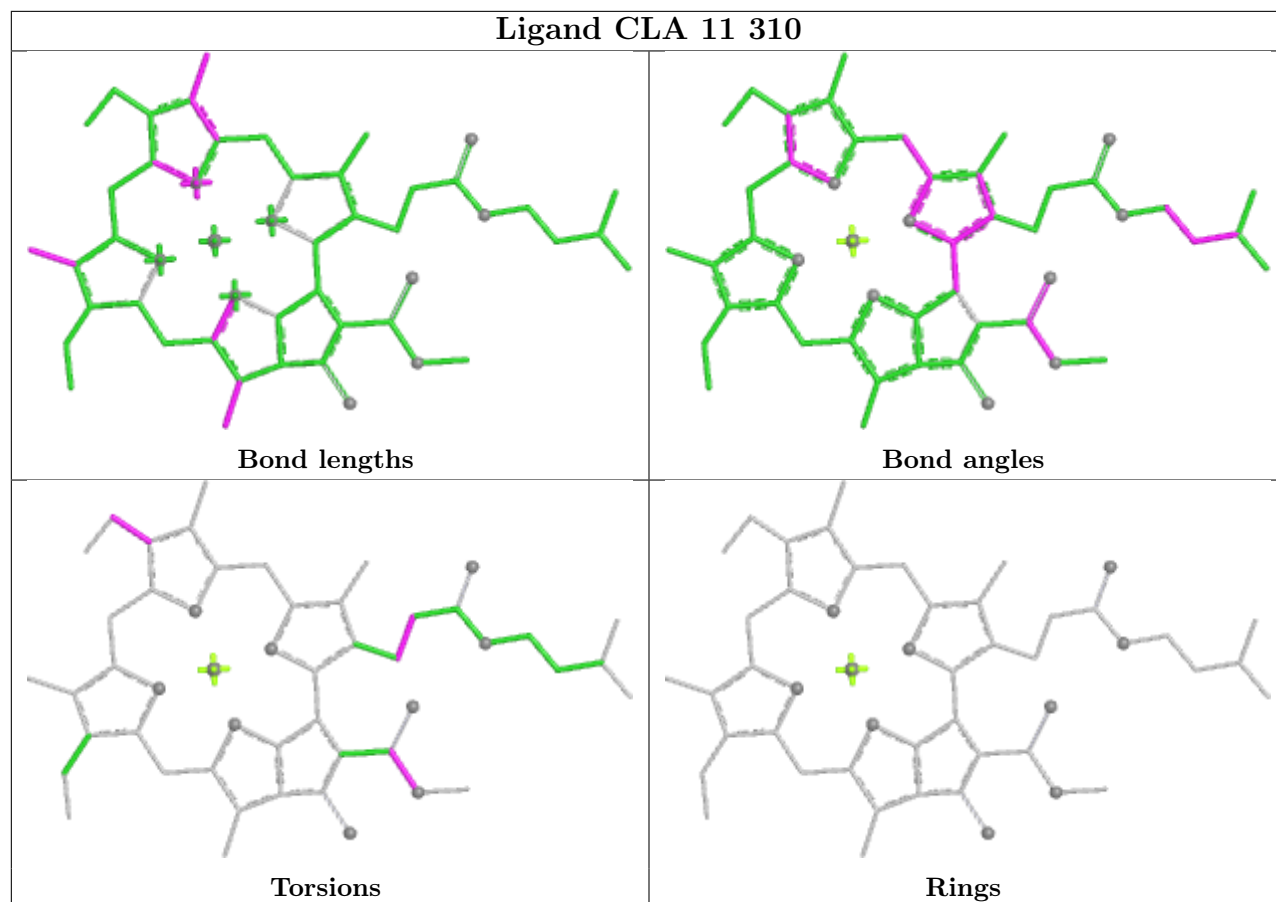




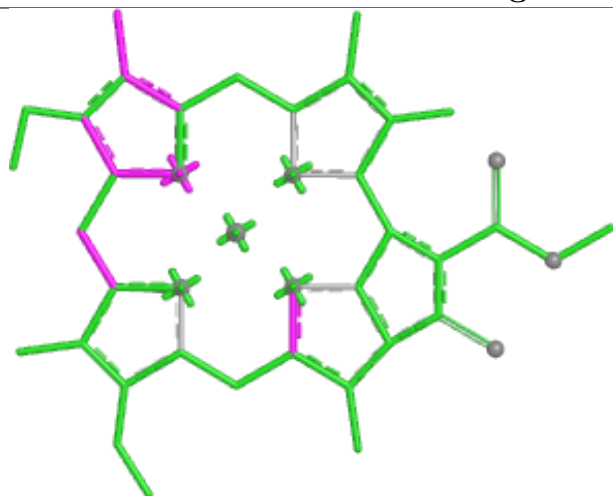




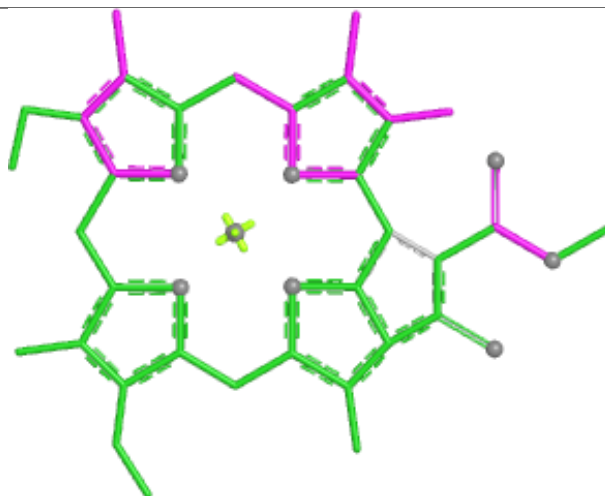




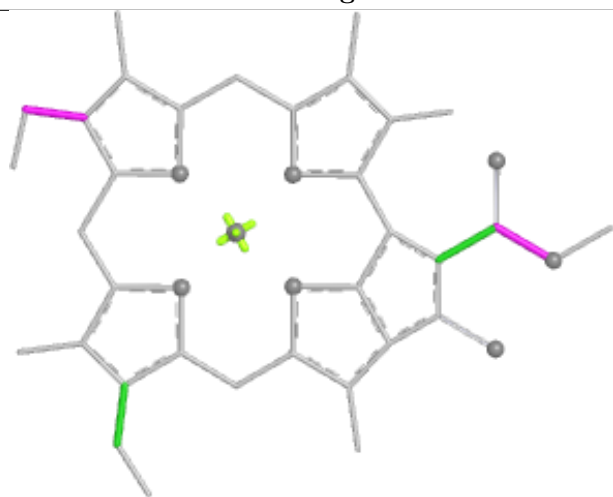
Ligand CLA 13 310



Bond lengths



Bond angles

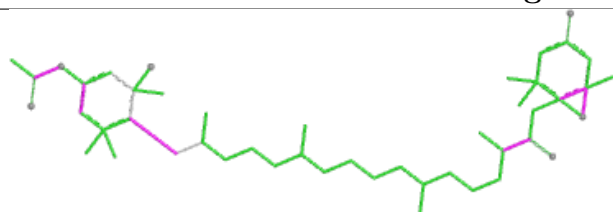


Torsions

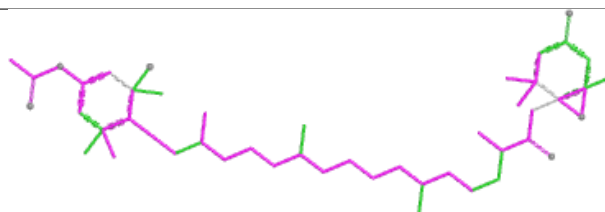


Rings

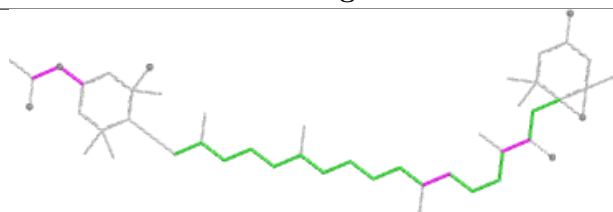
Ligand A86 7 301



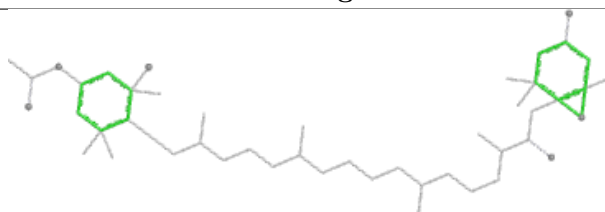
Bond lengths



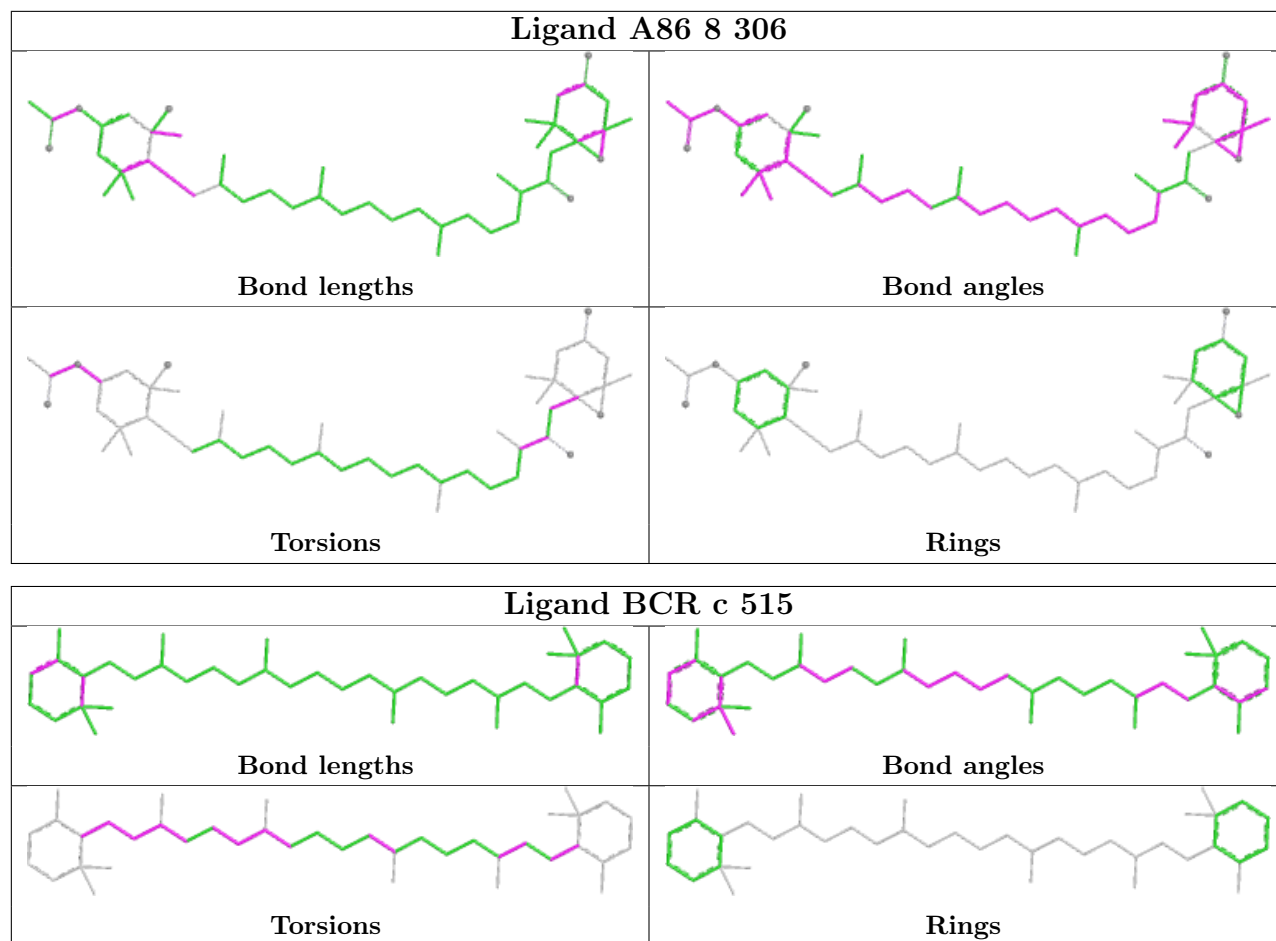
Bond angles

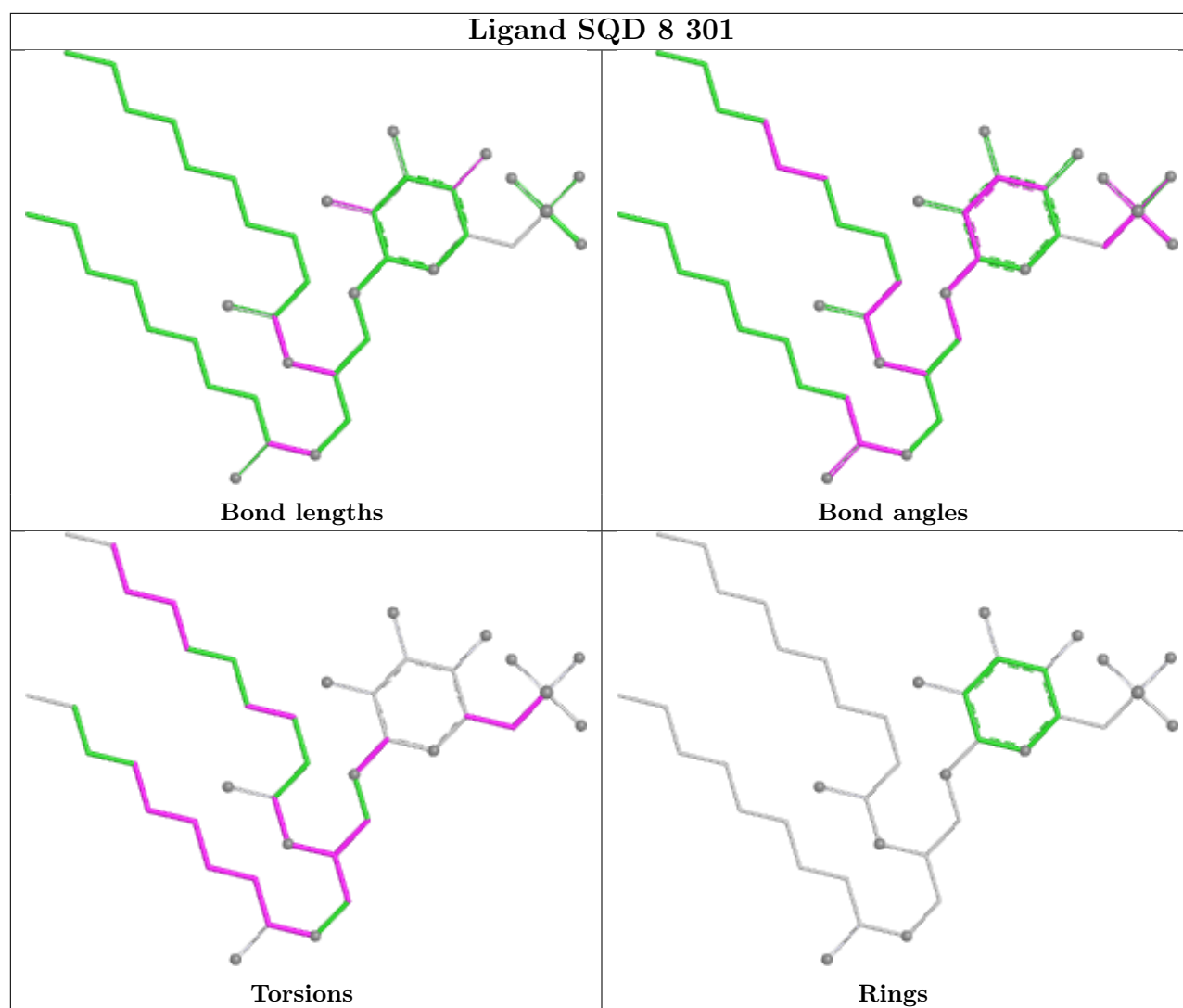


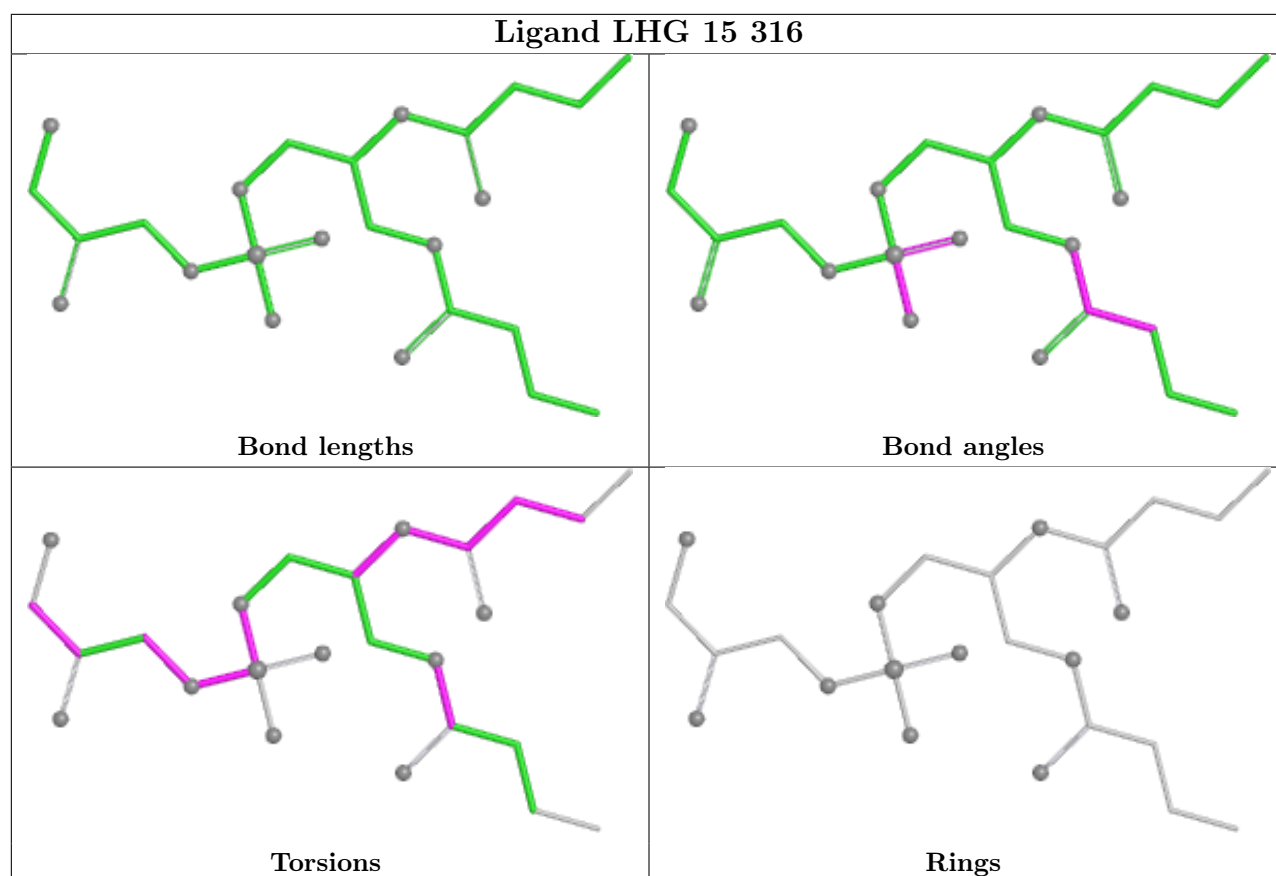
Torsions



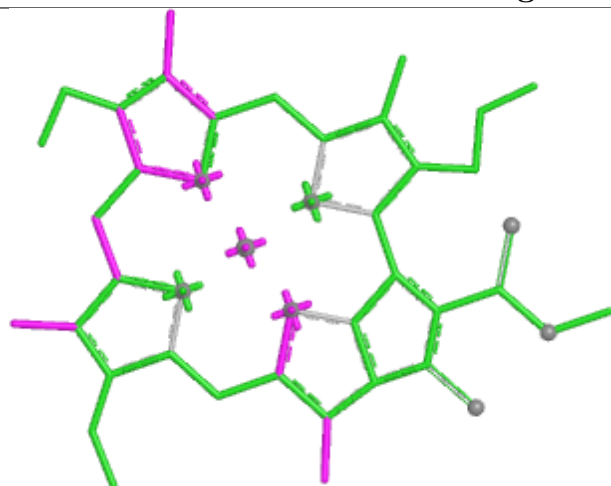
Rings



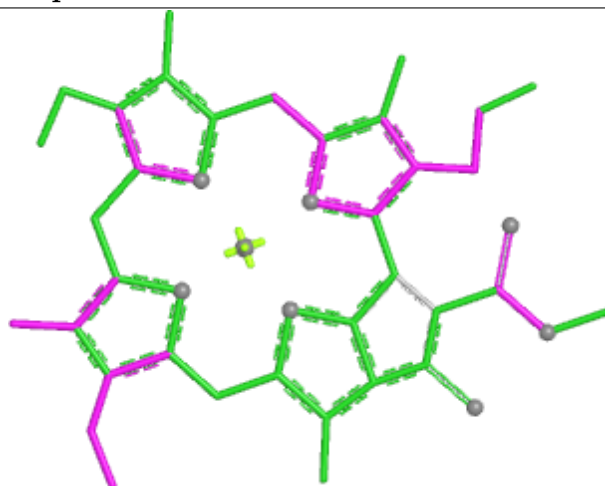




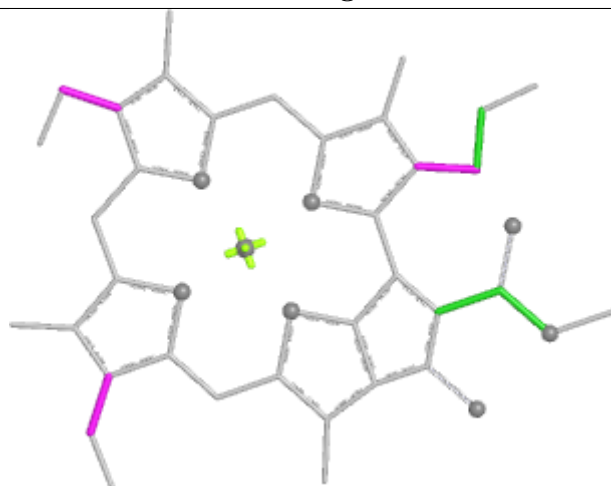
Ligand CLA p 607



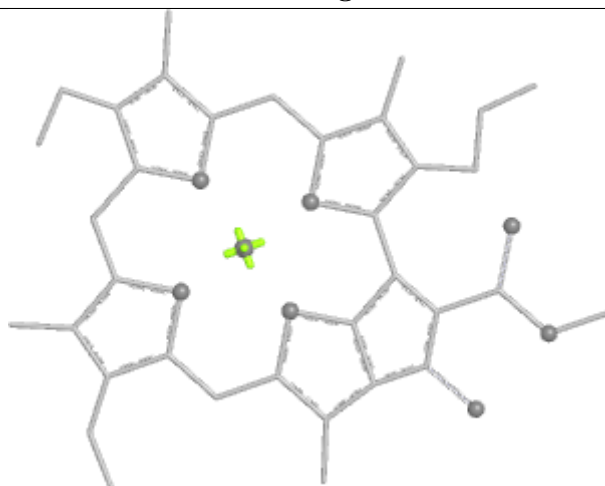
Bond lengths



Bond angles

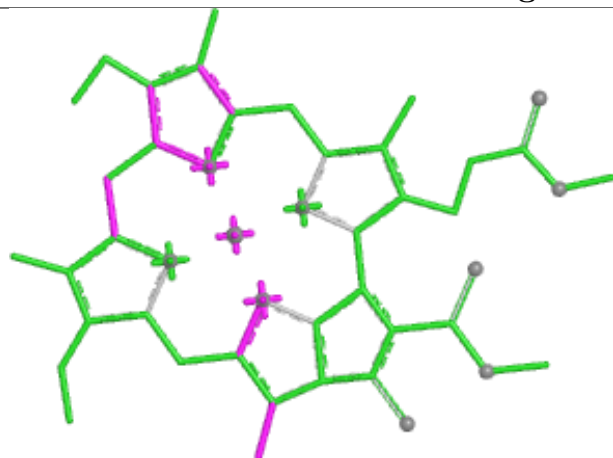


Torsions

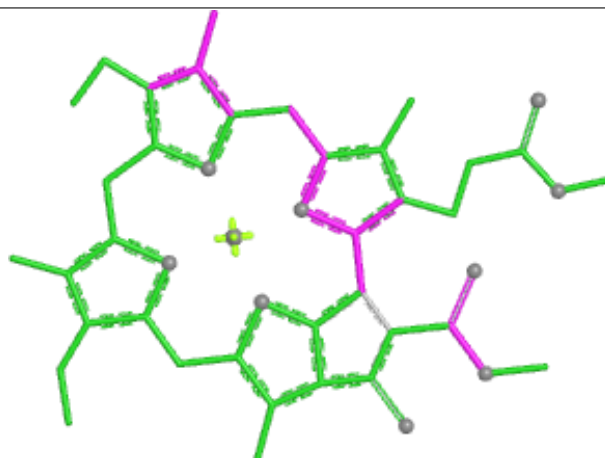


Rings

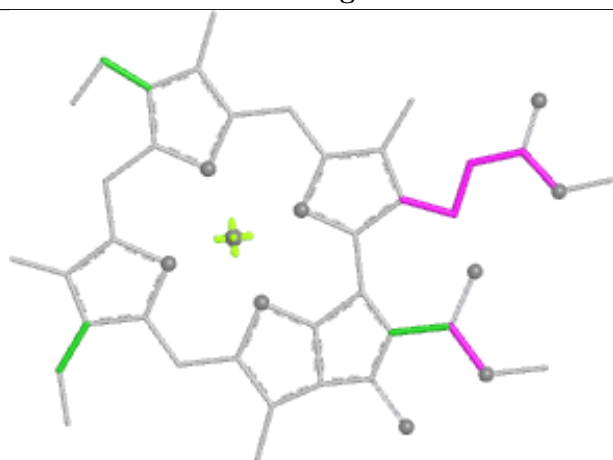
Ligand CLA 4 311



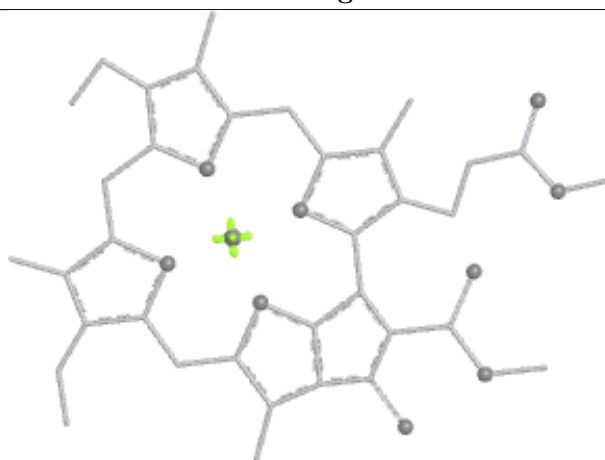
Bond lengths



Bond angles

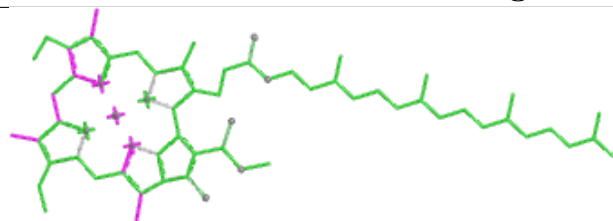


Torsions

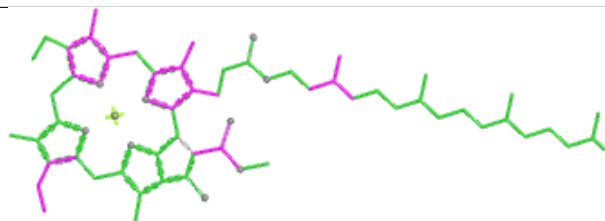


Rings

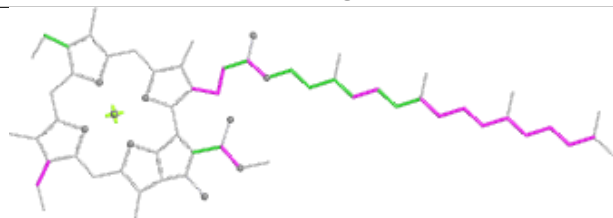
Ligand CLA 11 308



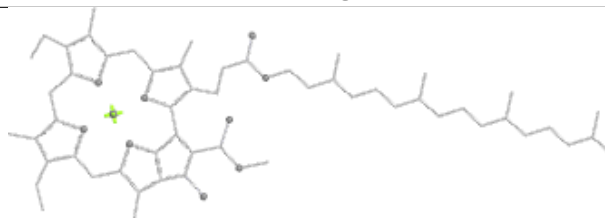
Bond lengths



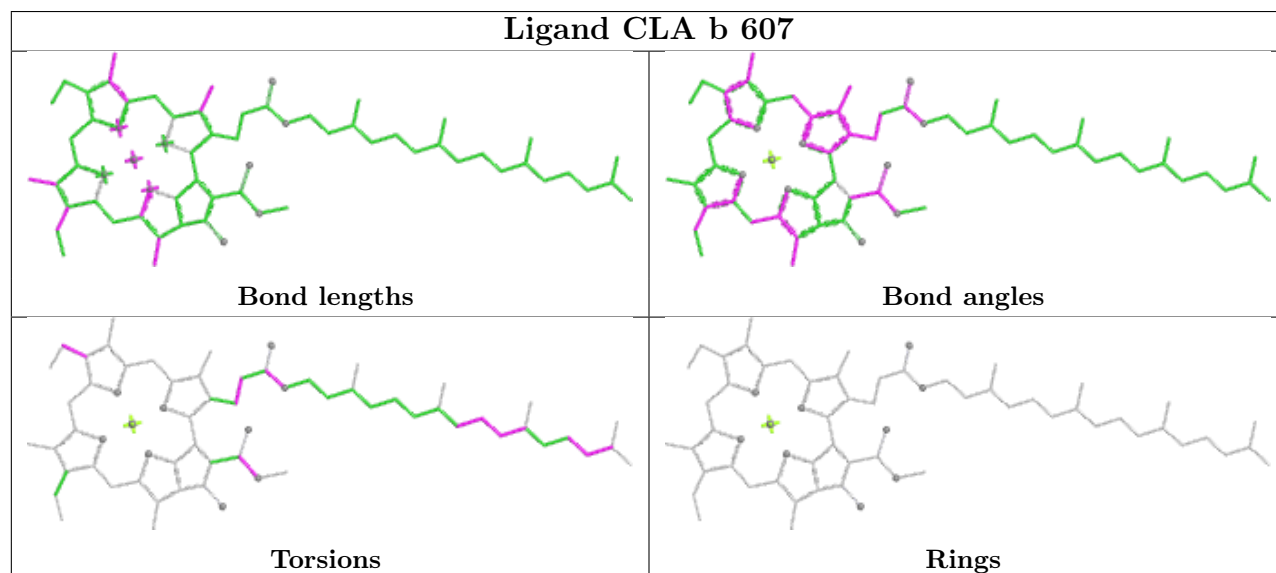
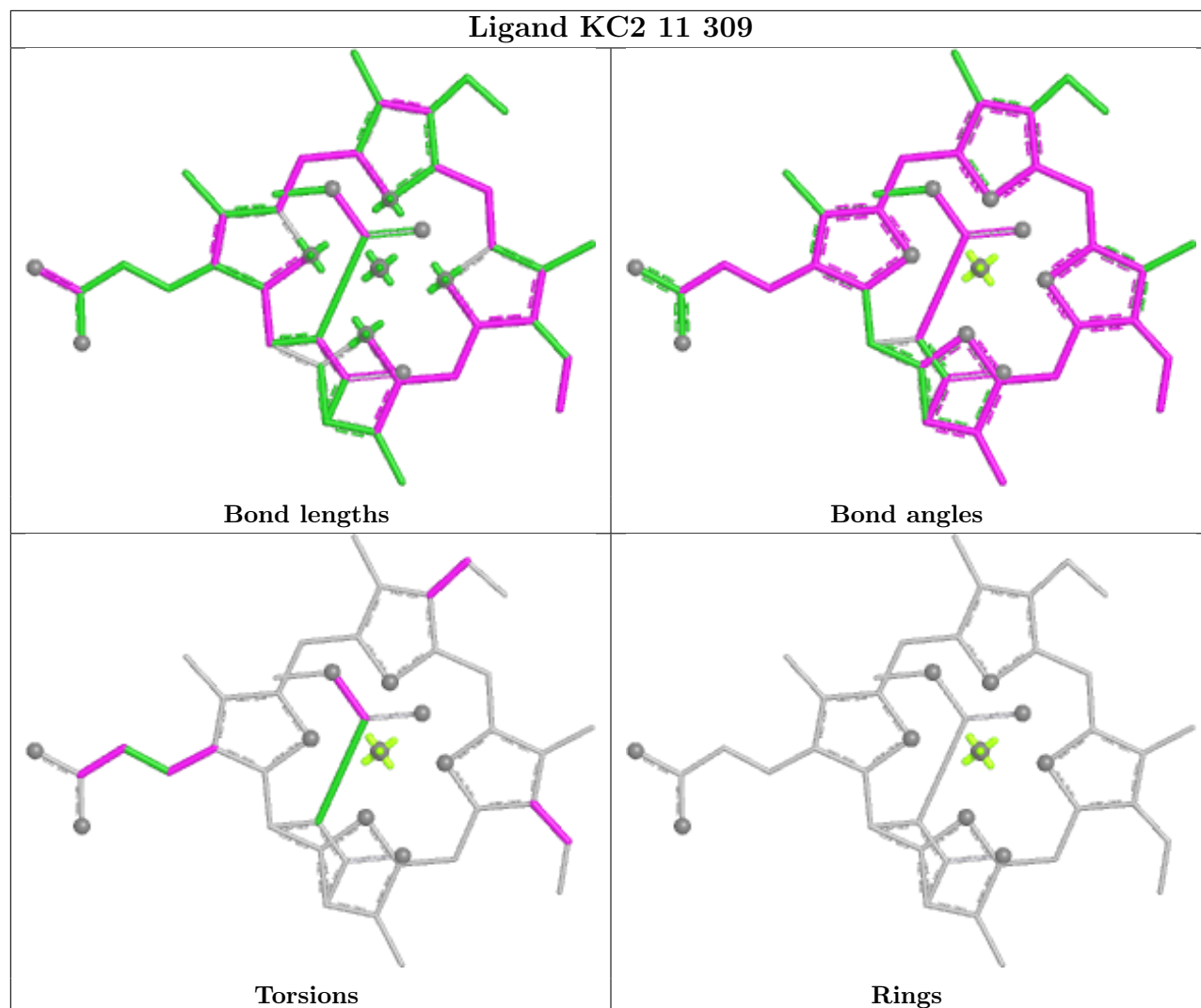
Bond angles



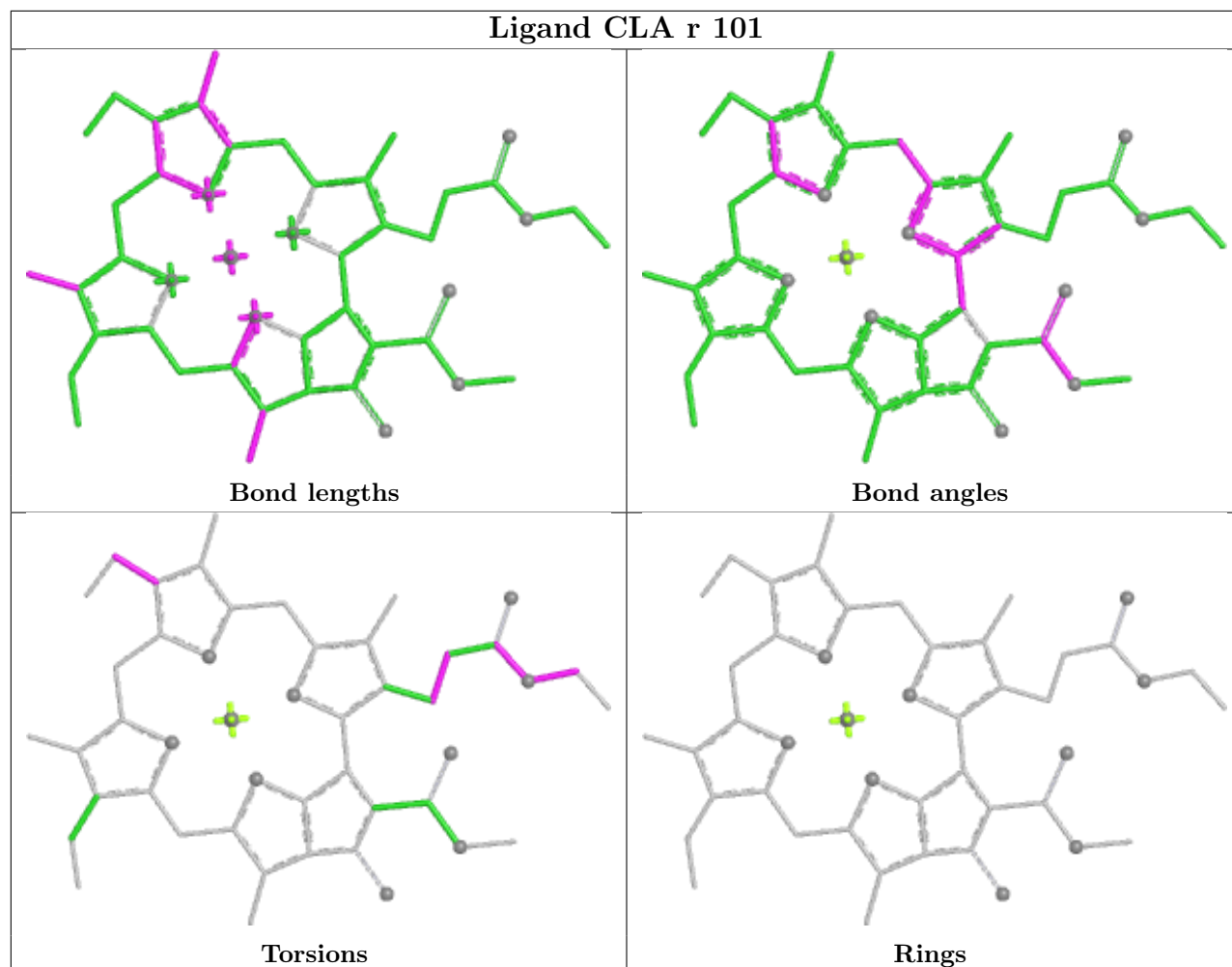
Torsions

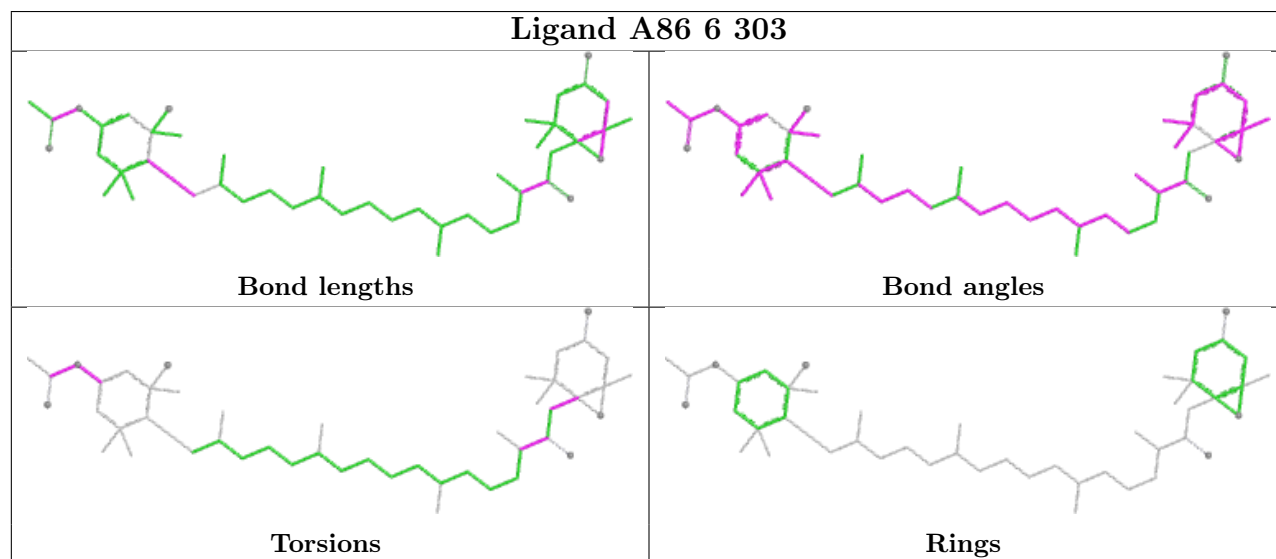
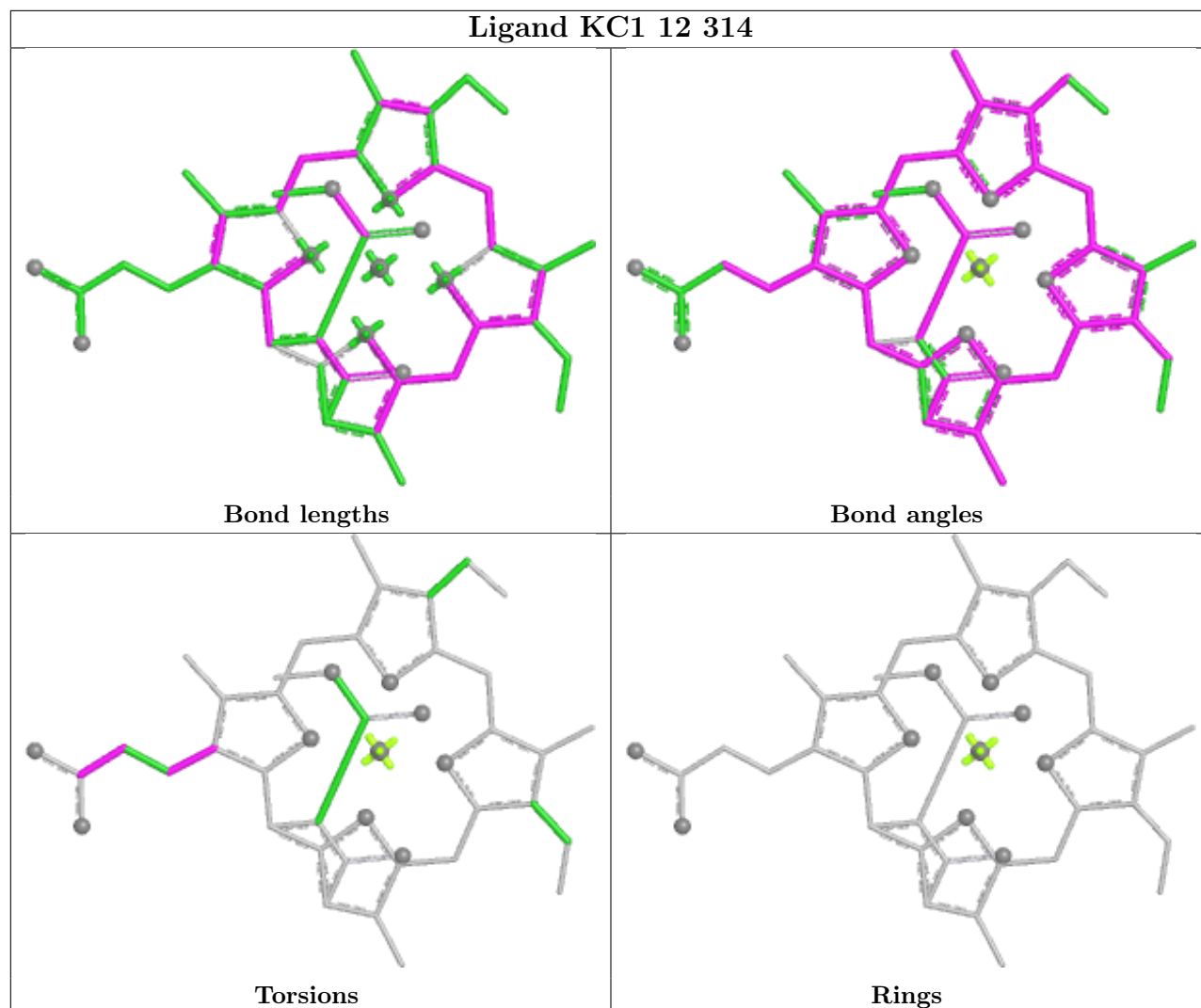


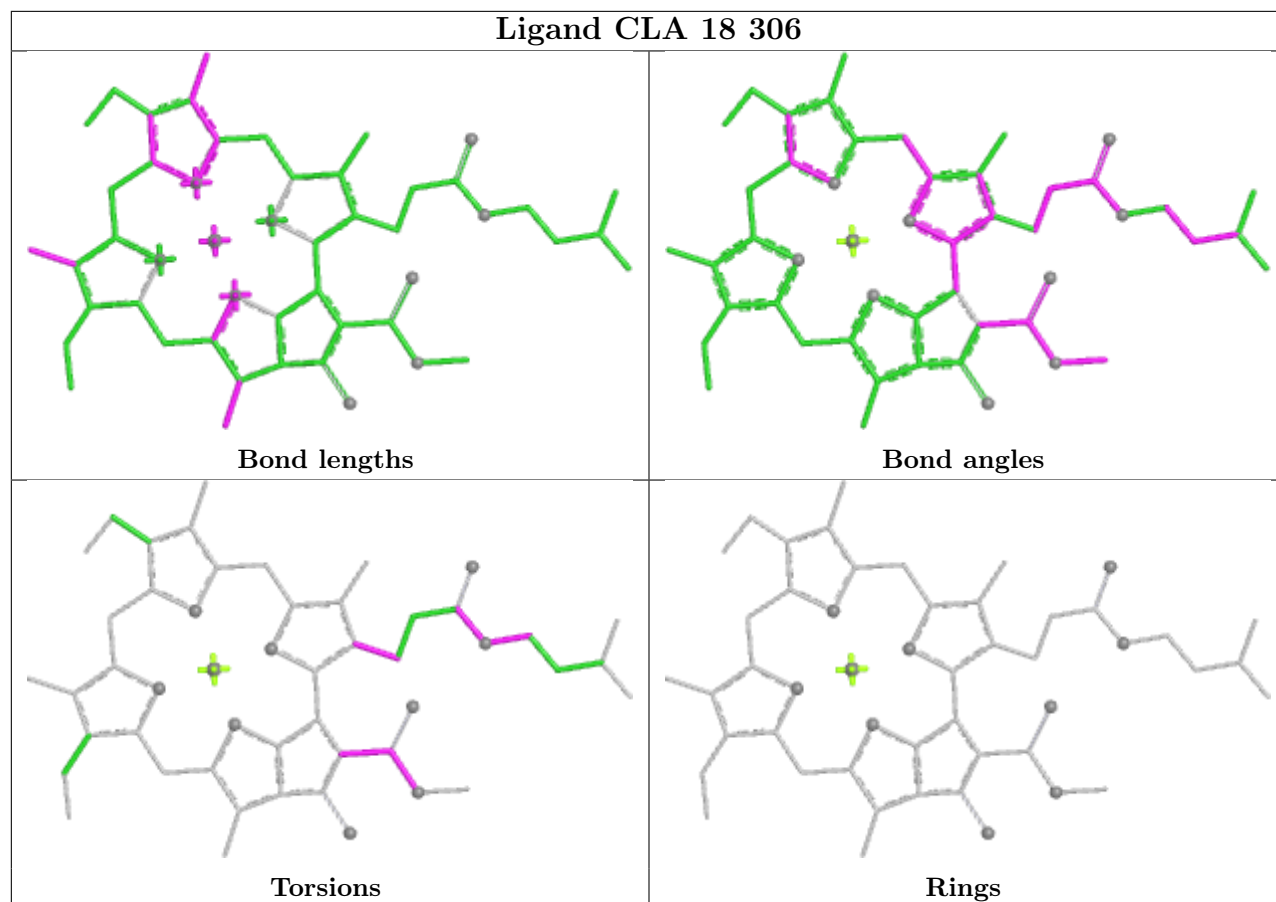
Rings



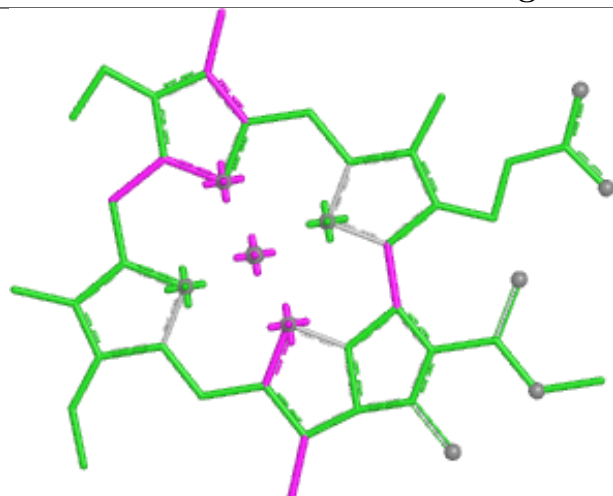
Ligand CLA r 101



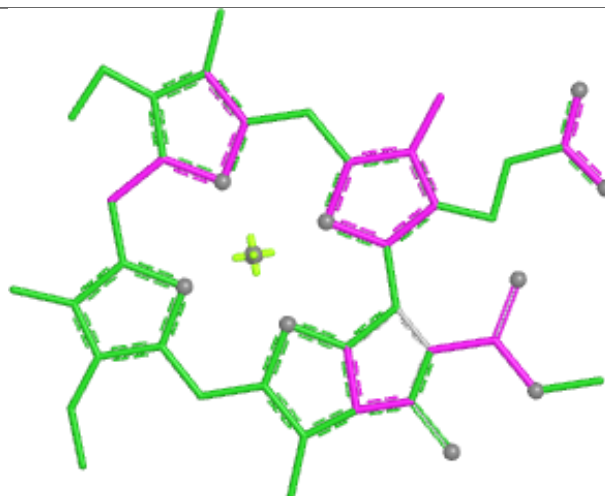




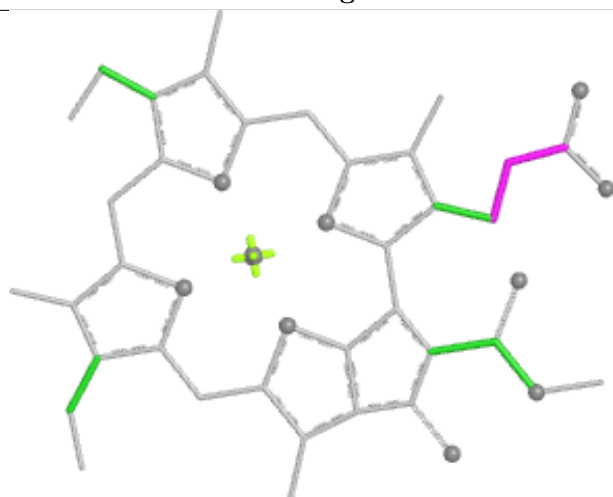
Ligand CLA 5 311



Bond lengths



Bond angles

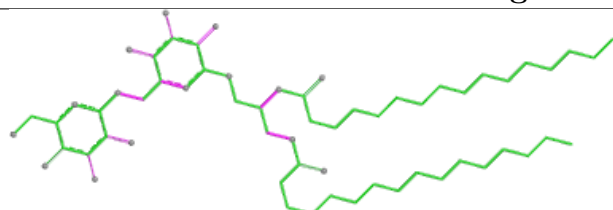


Torsions

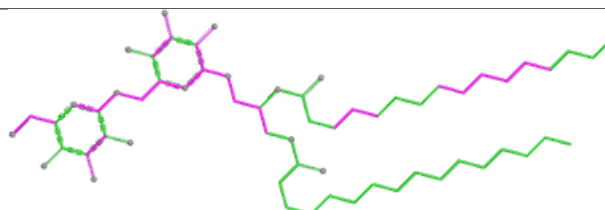


Rings

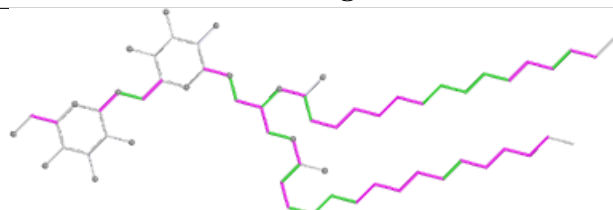
Ligand DGD C 520



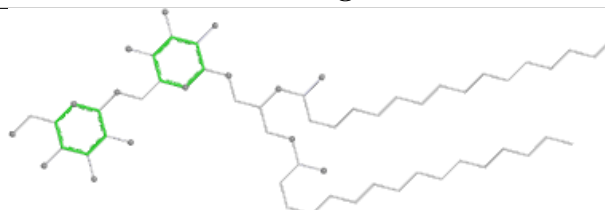
Bond lengths



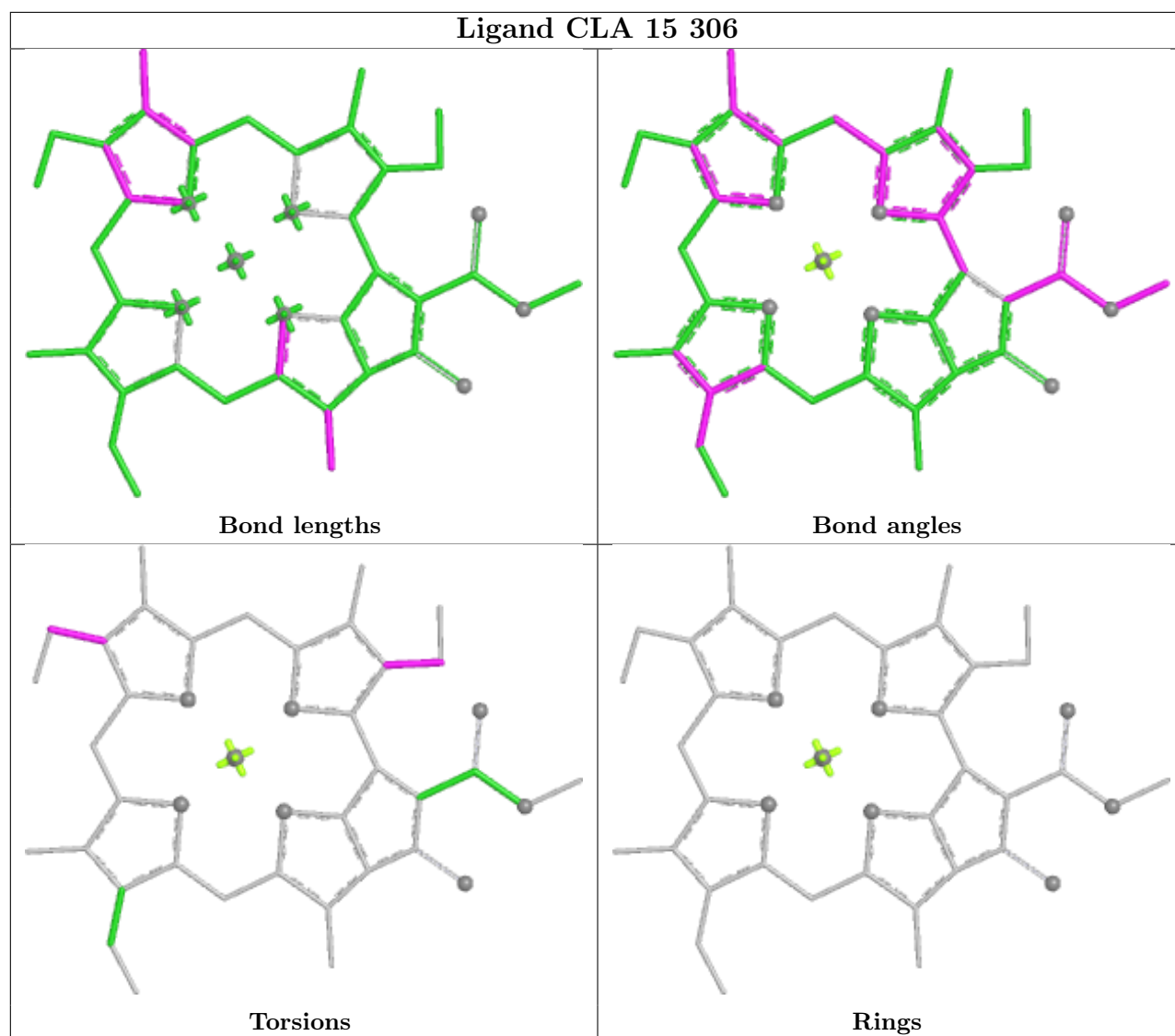
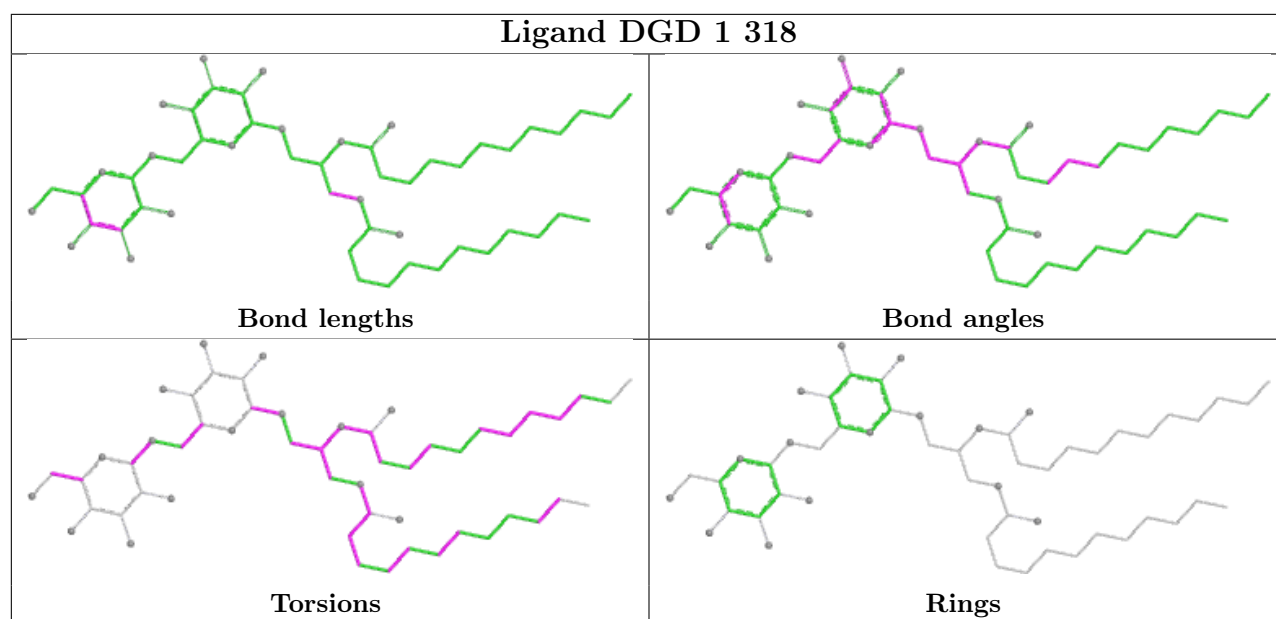
Bond angles

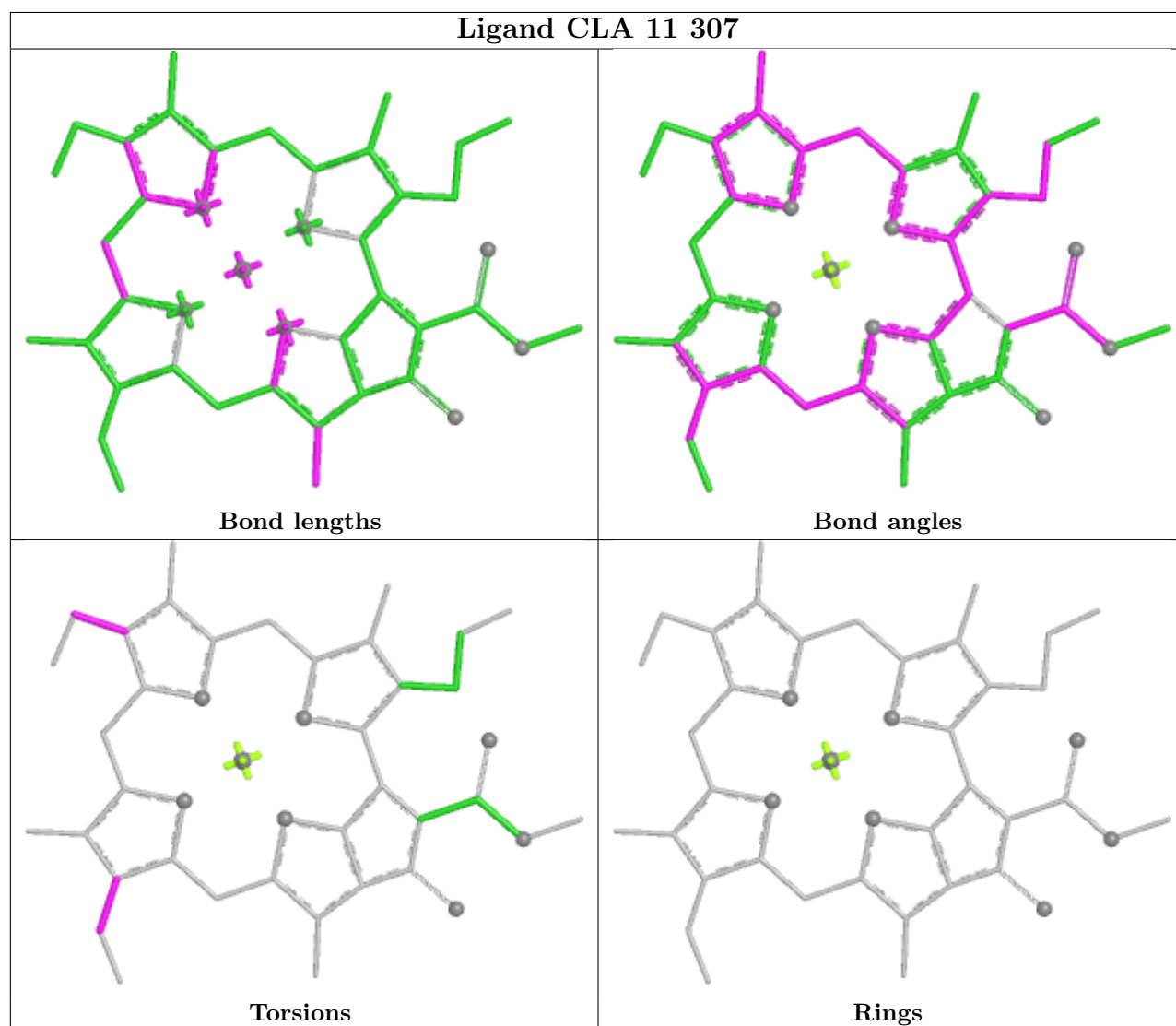
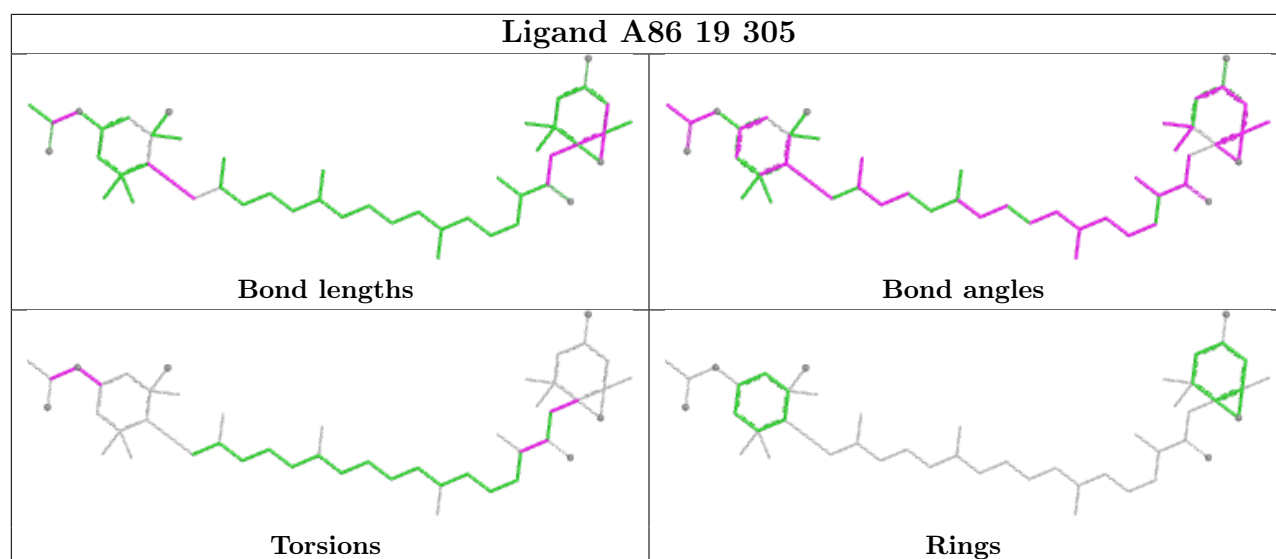


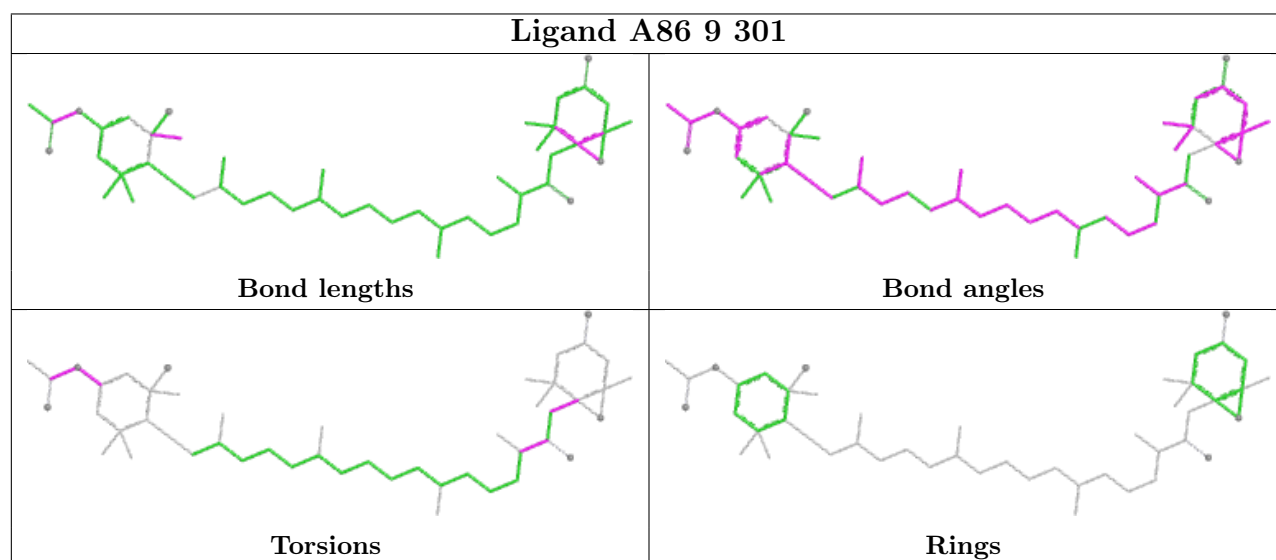
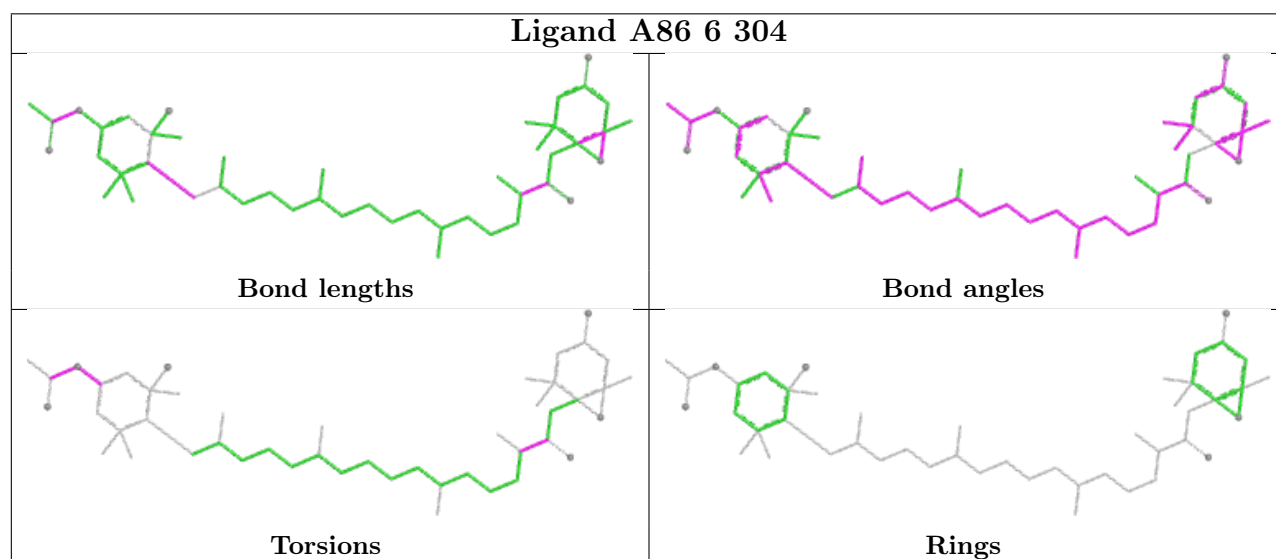
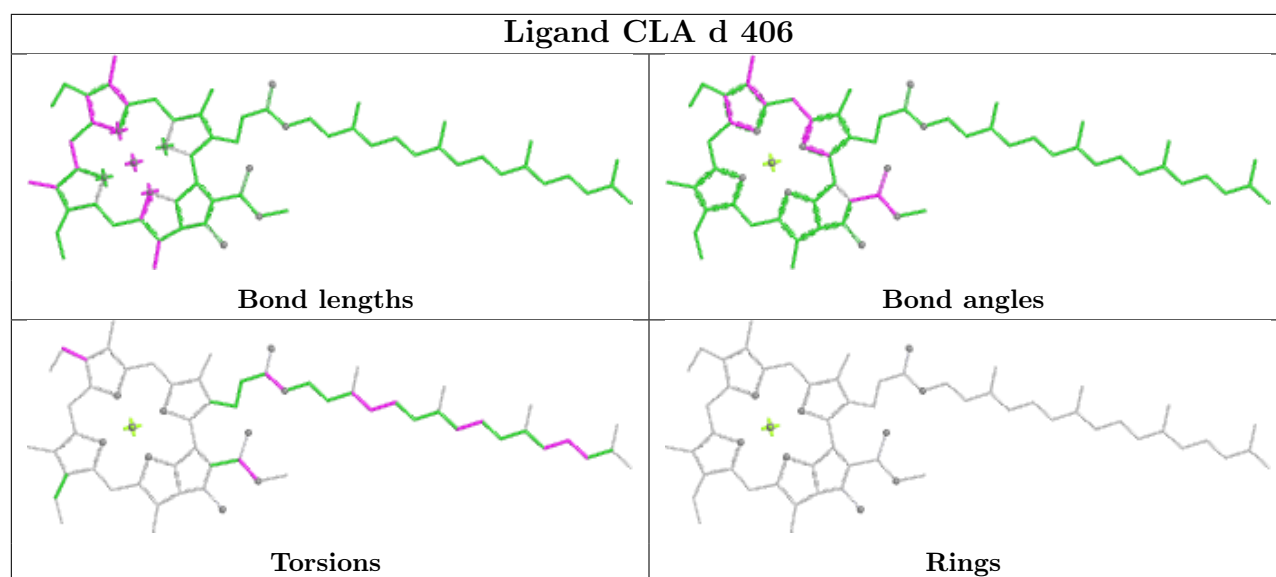
Torsions

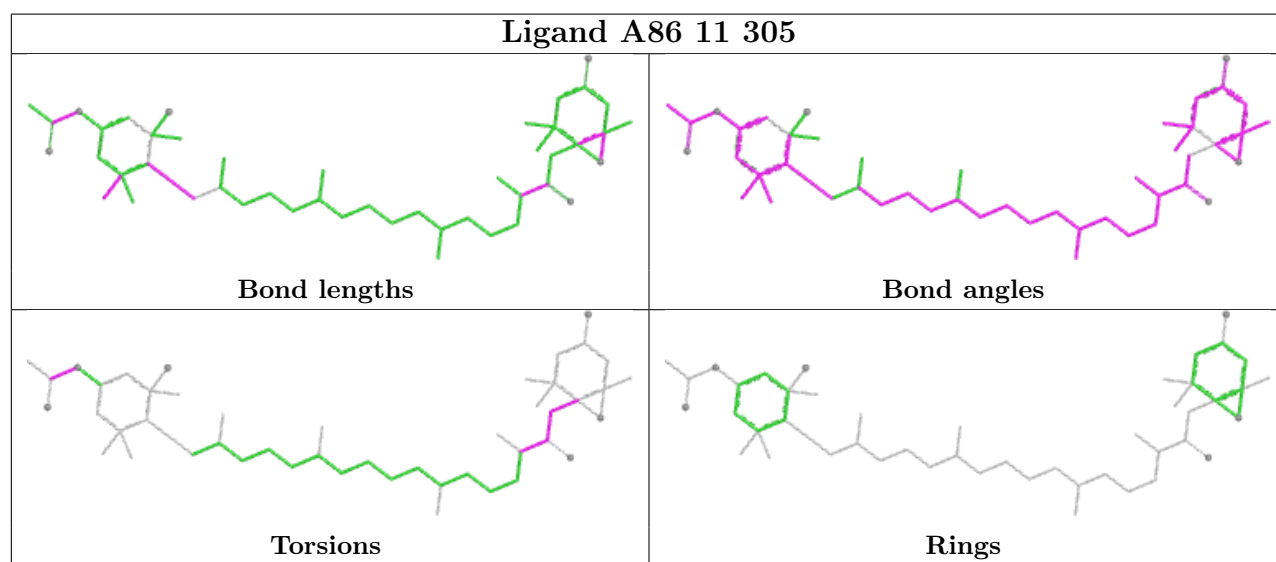
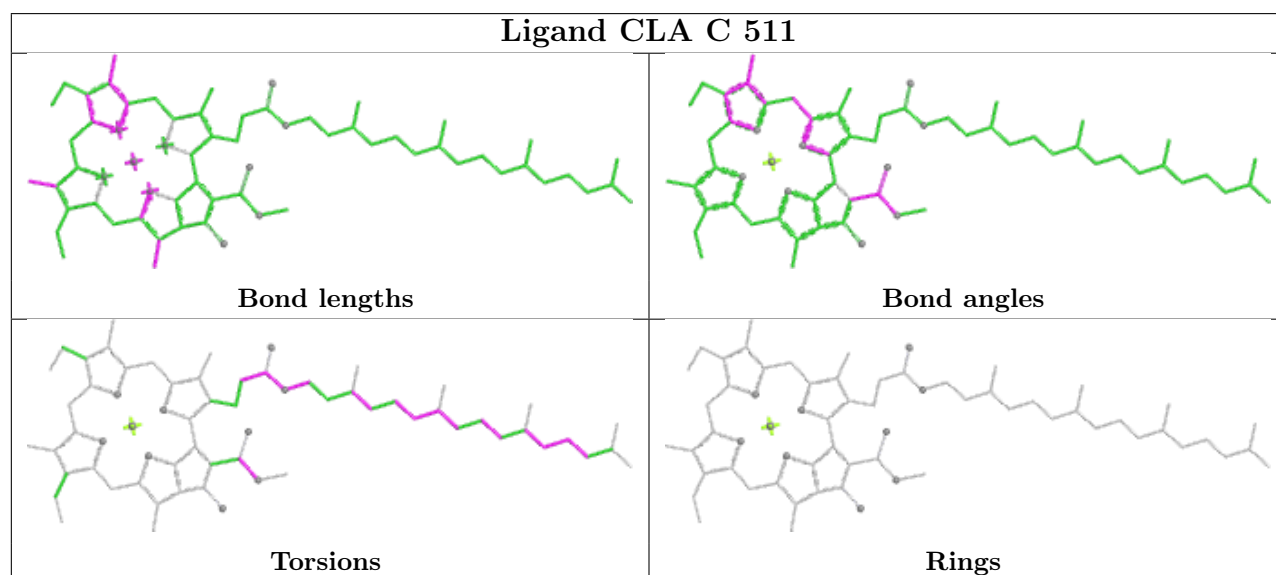
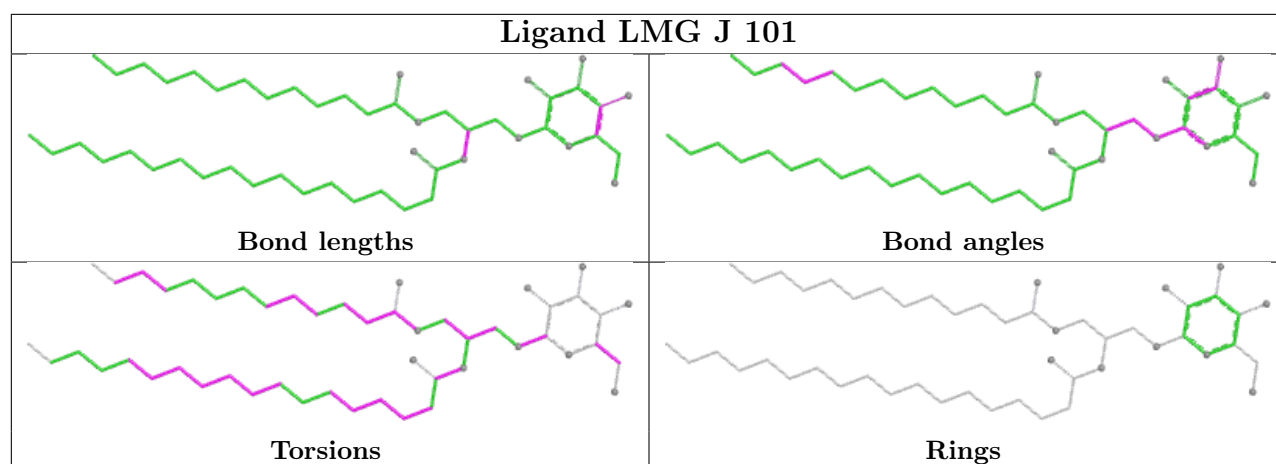


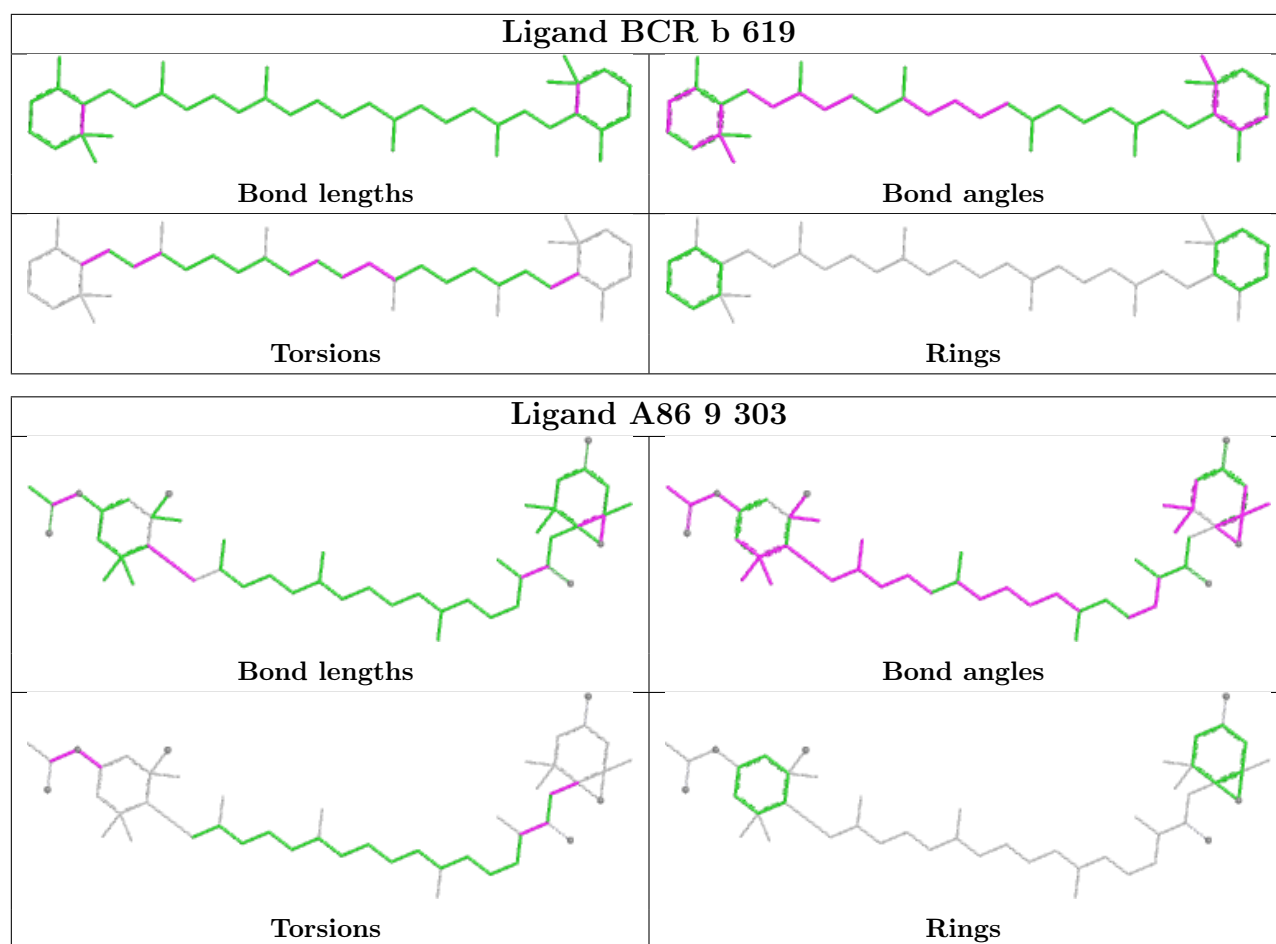
Rings

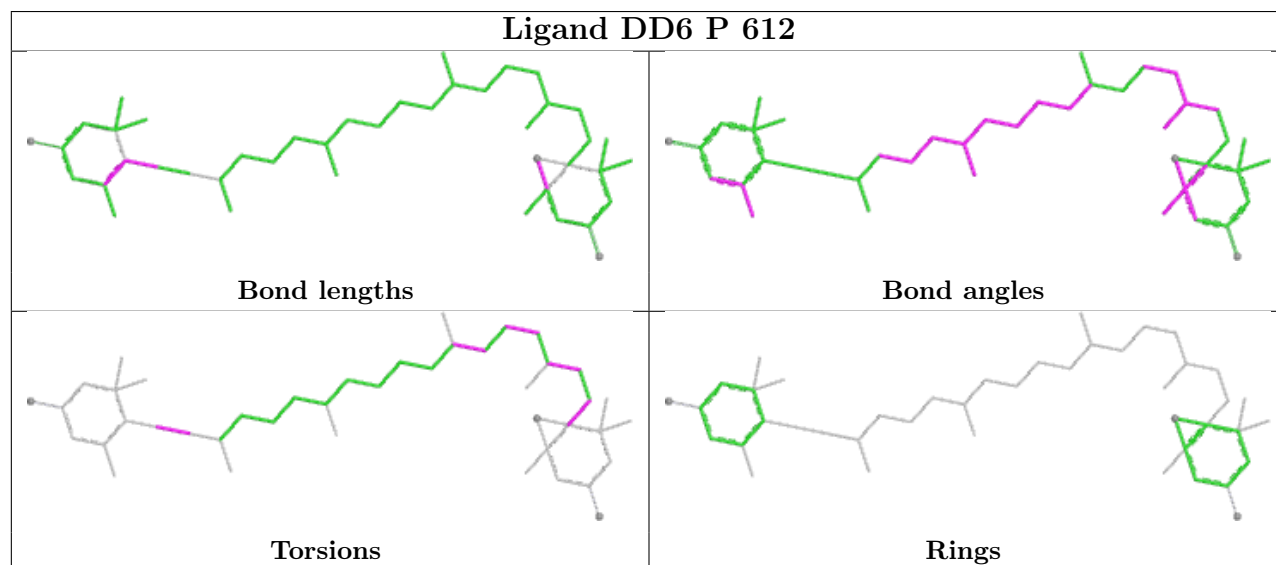
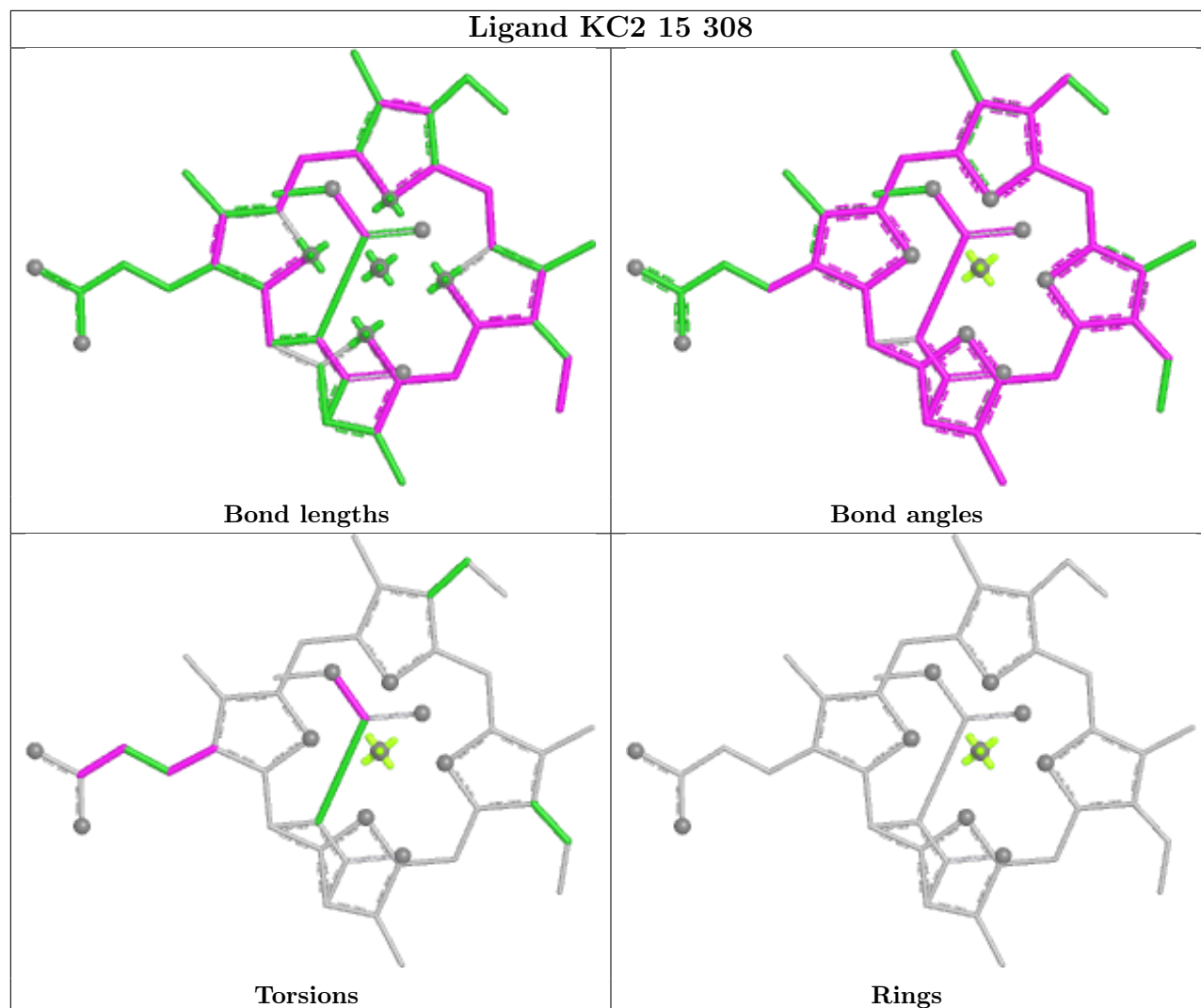




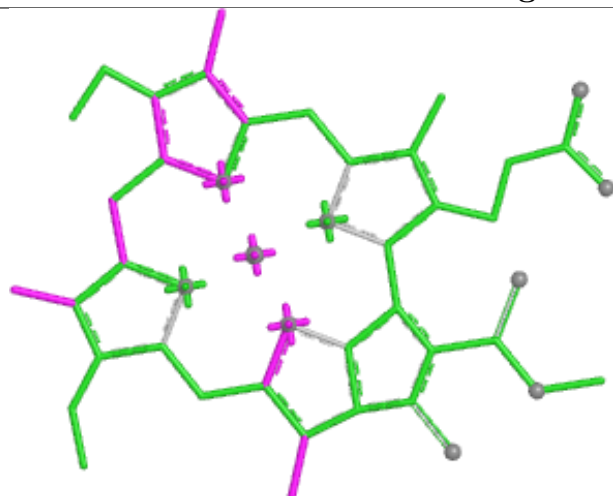




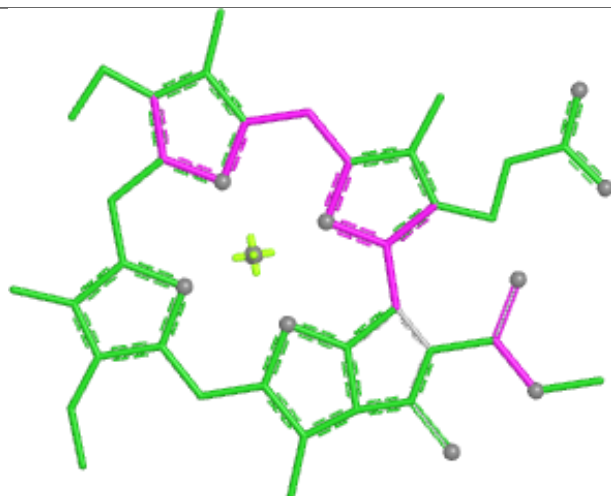




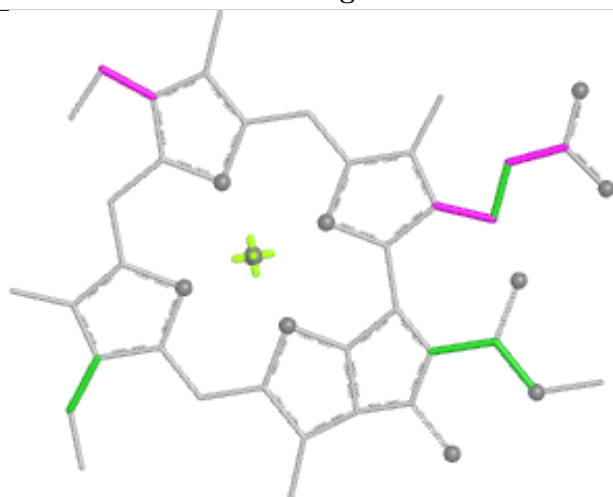
Ligand CLA 2 311



Bond lengths



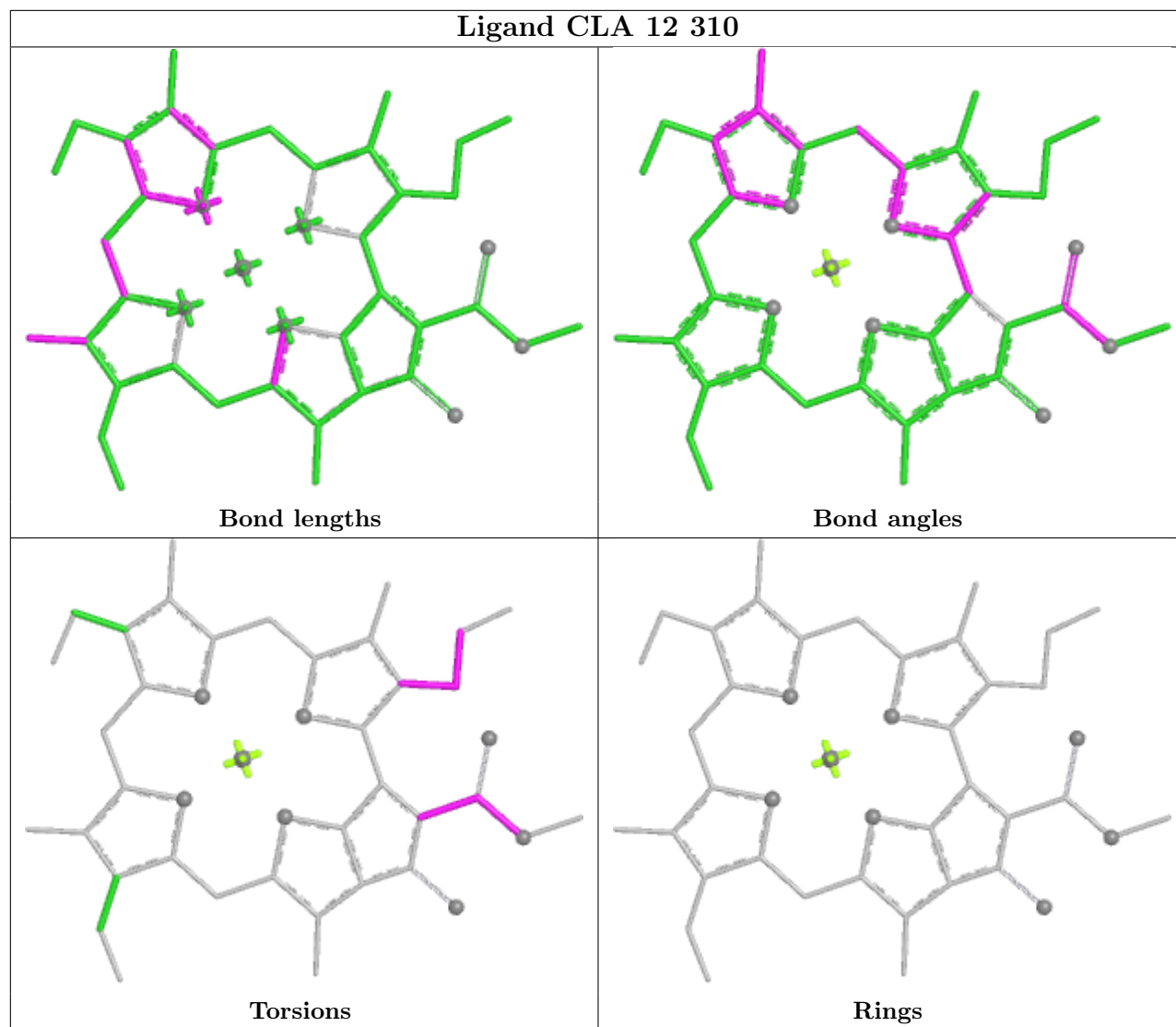
Bond angles



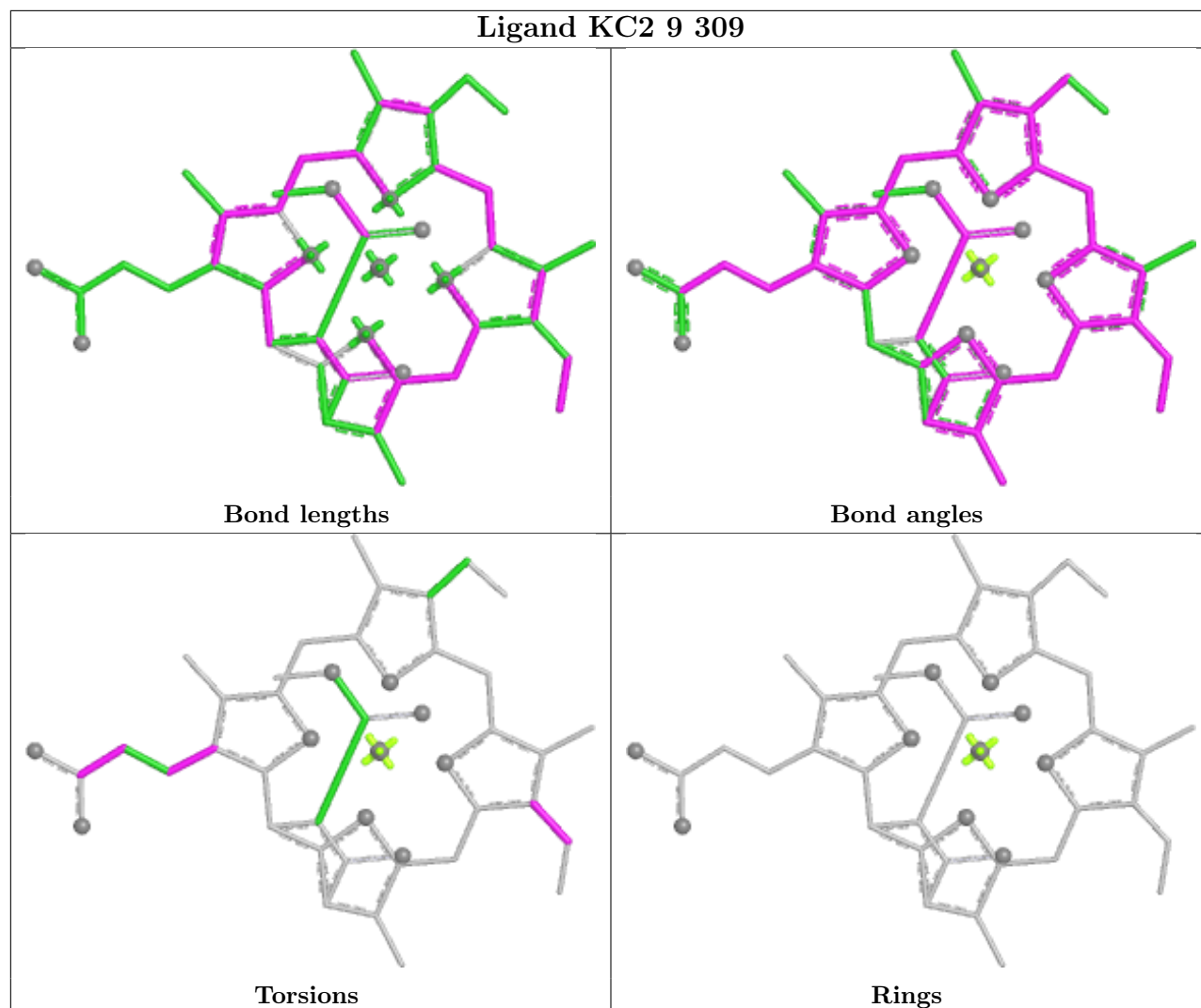
Torsions



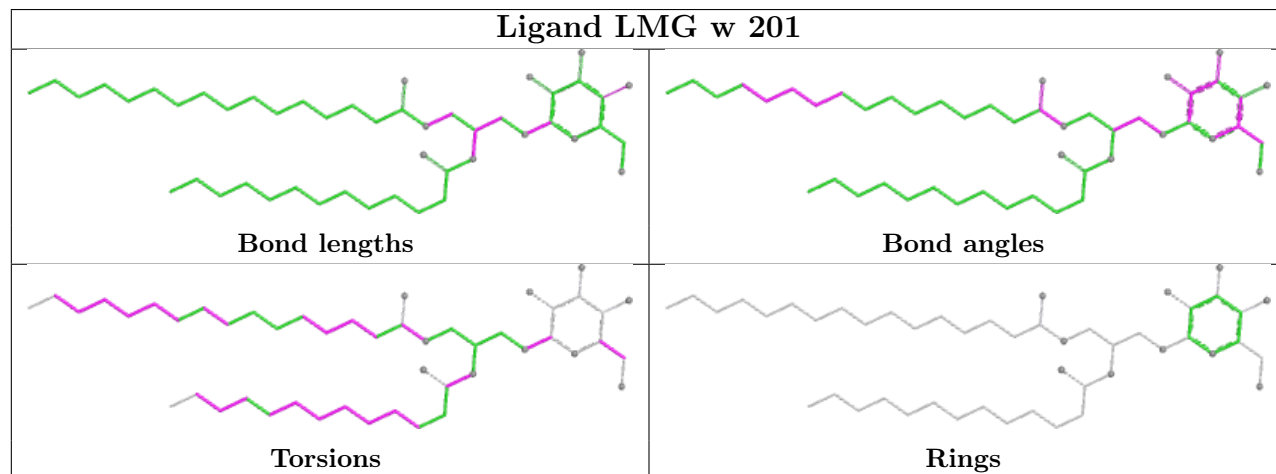
Rings

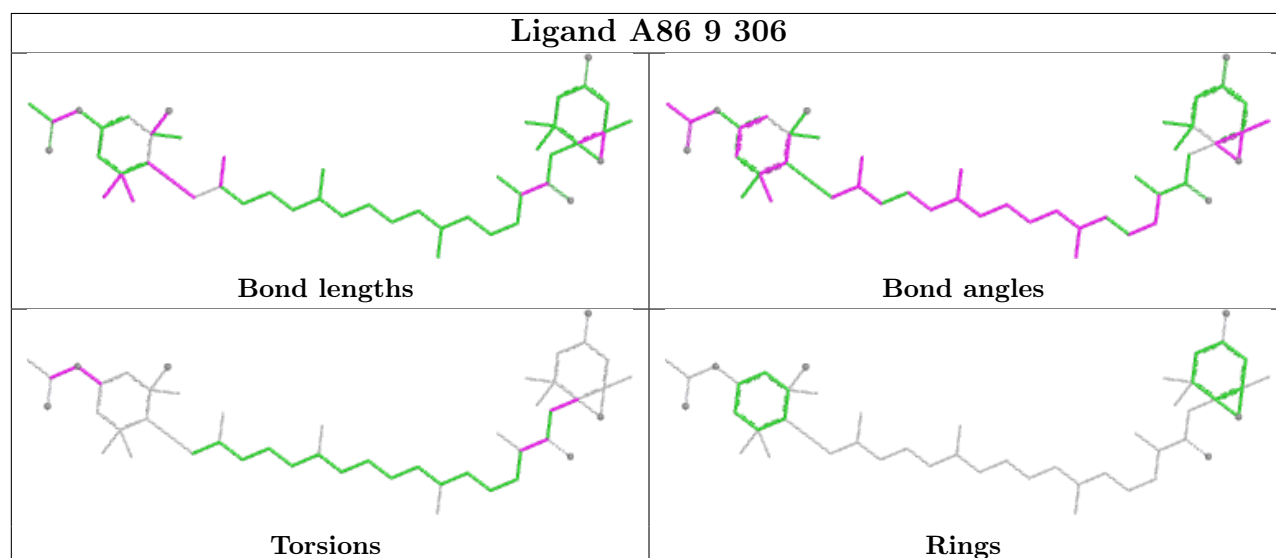
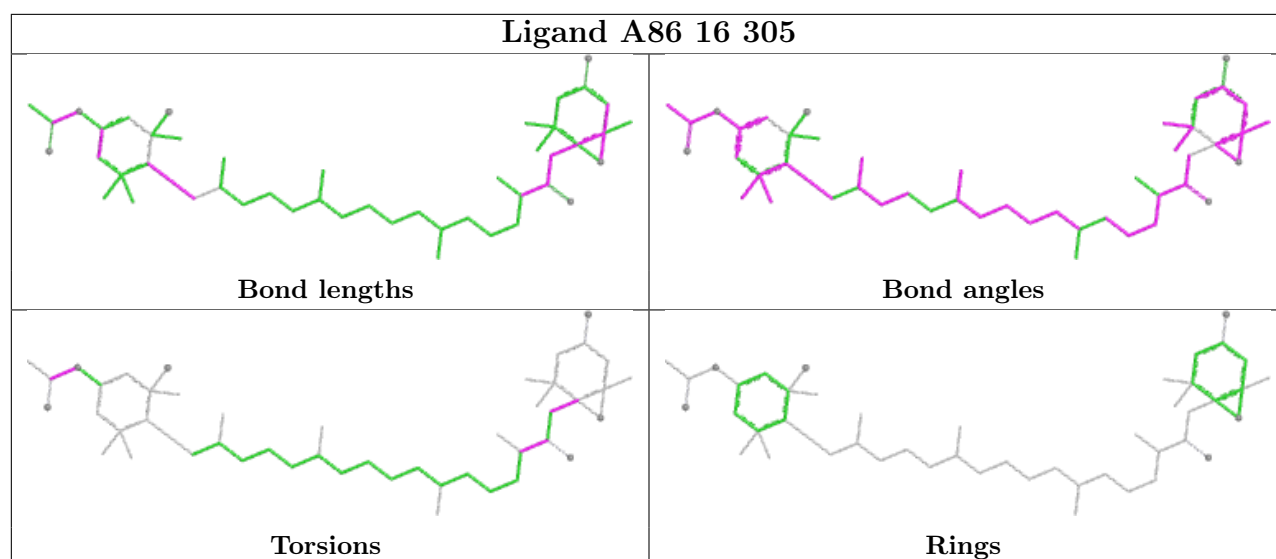


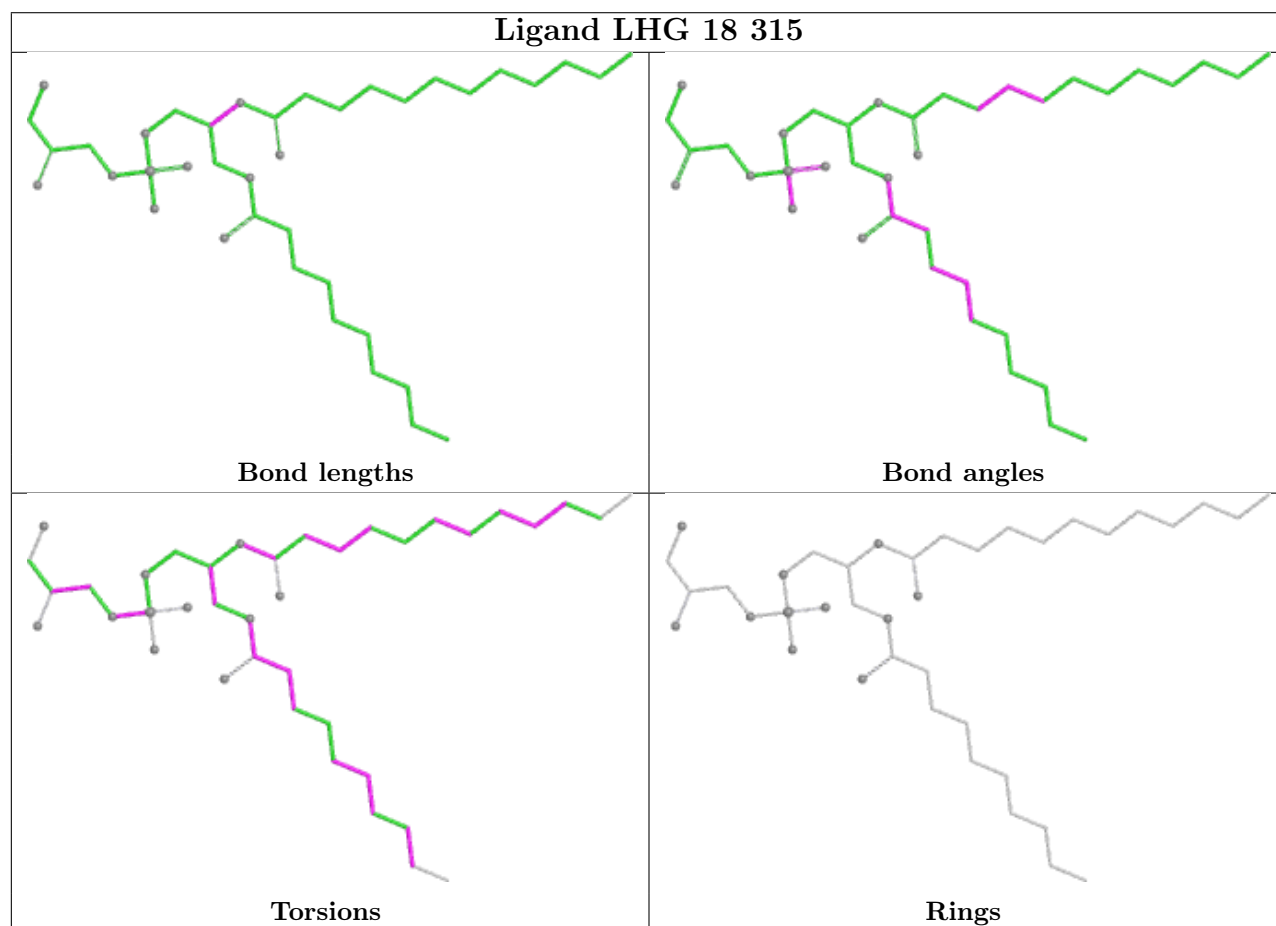
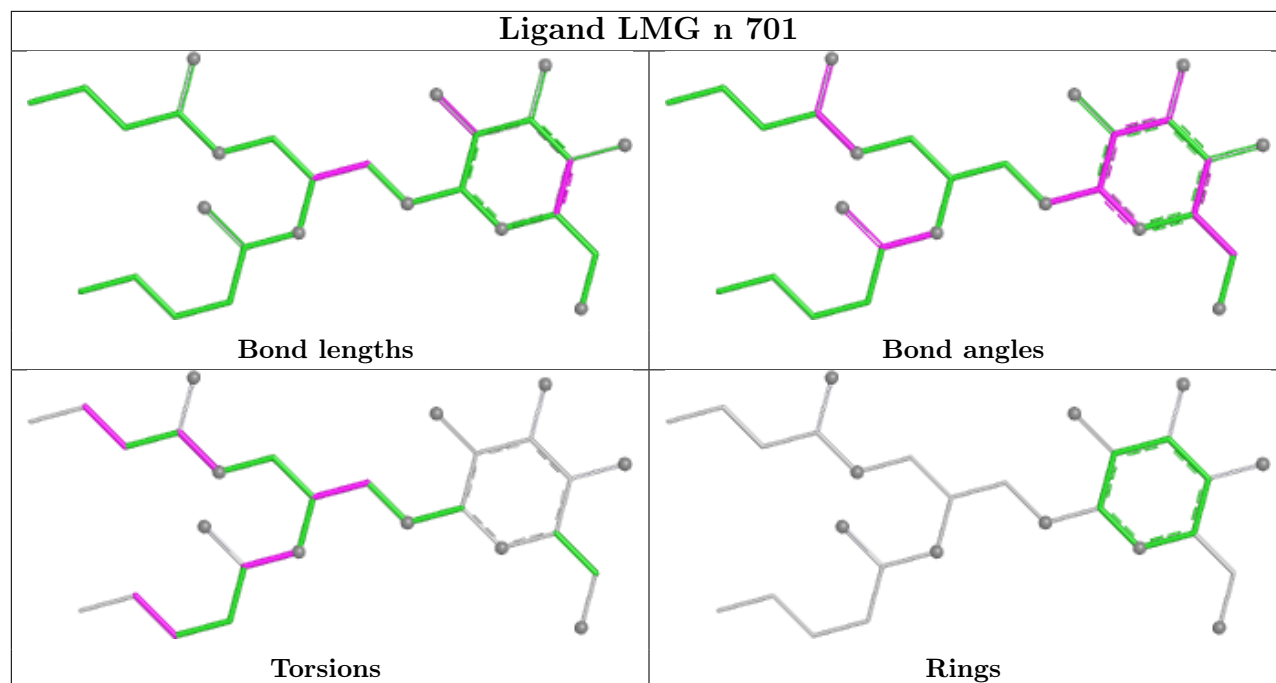
Ligand KC2 9 309



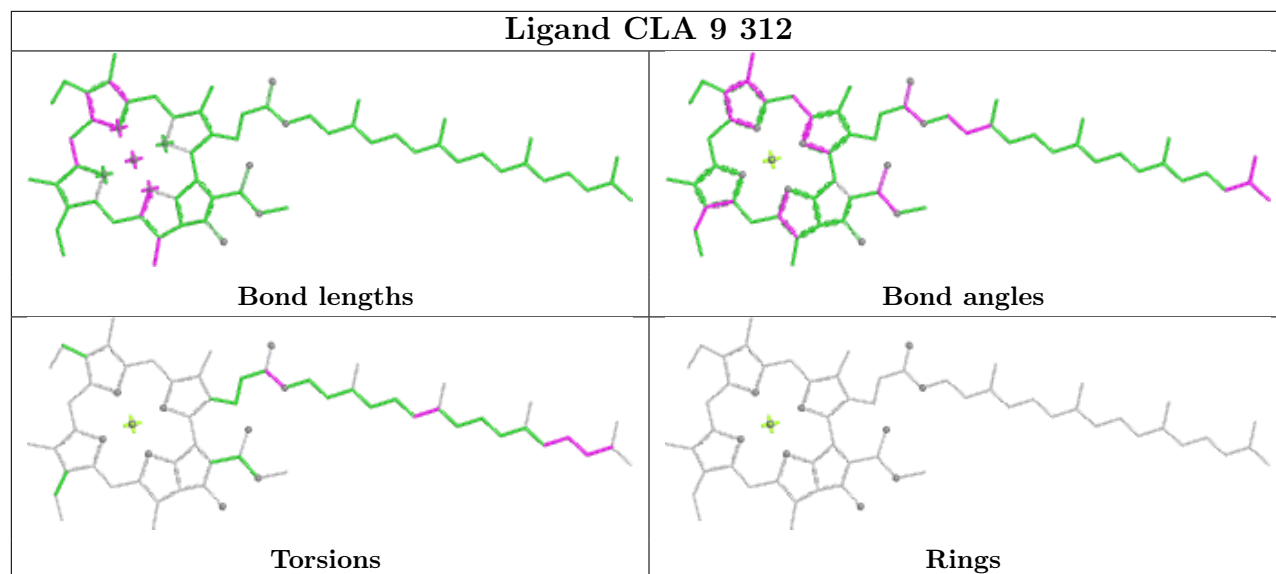
Ligand LMG w 201



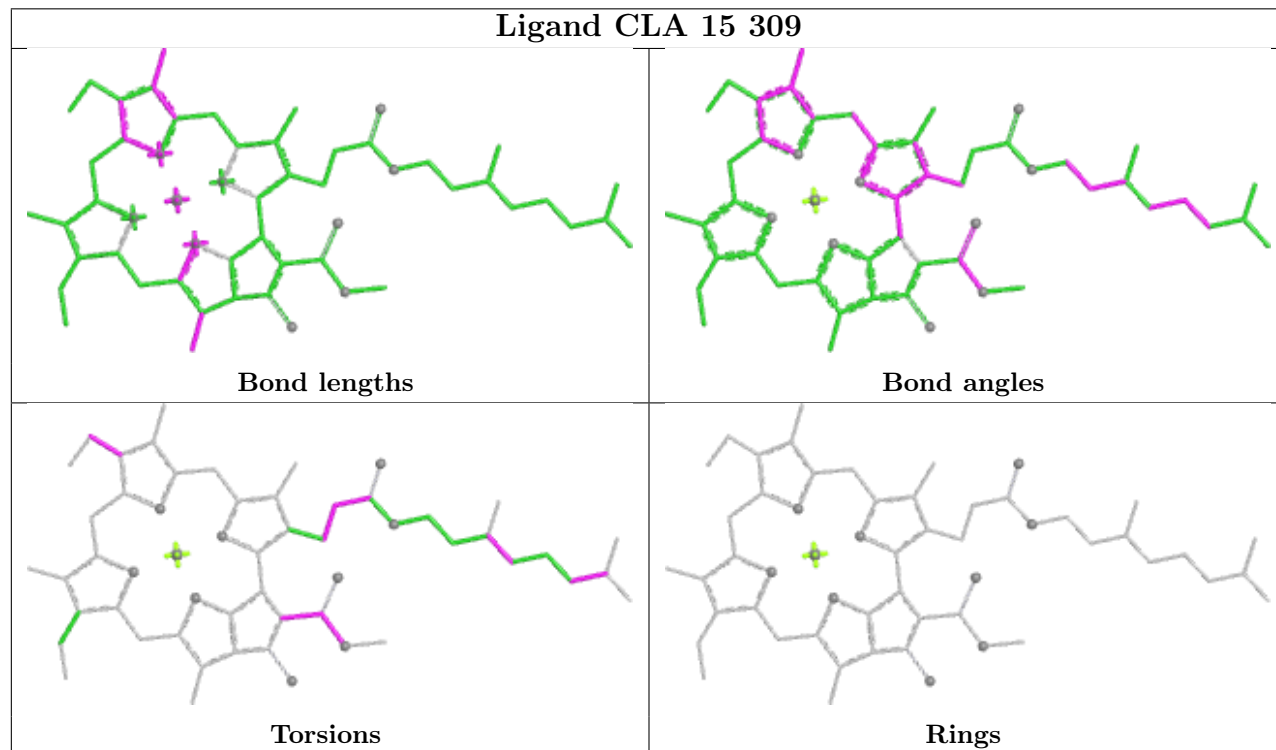




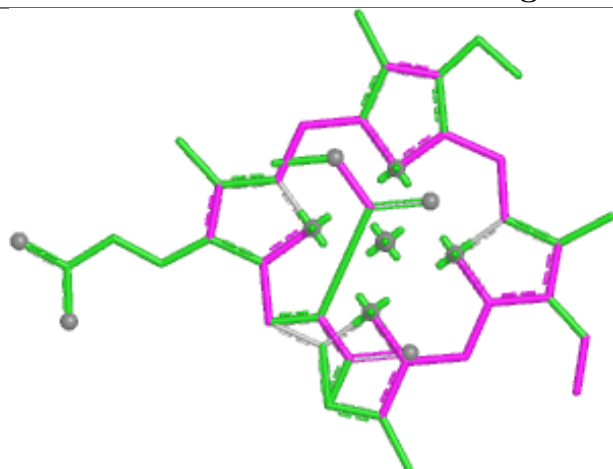
Ligand CLA 9 312



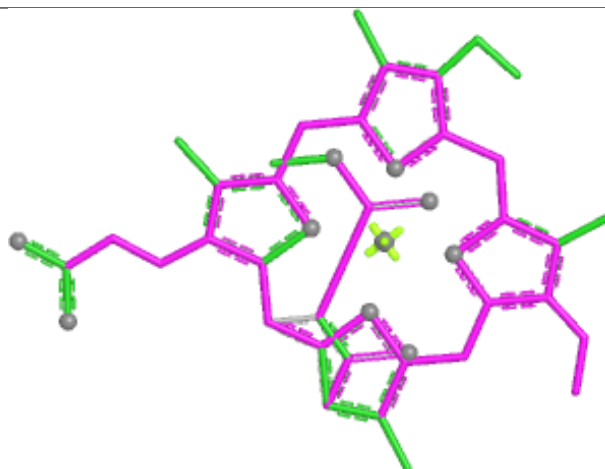
Ligand CLA 15 309



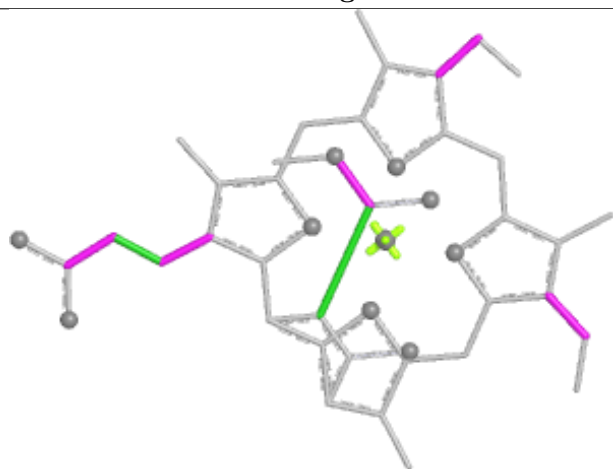
Ligand KC2 1 309



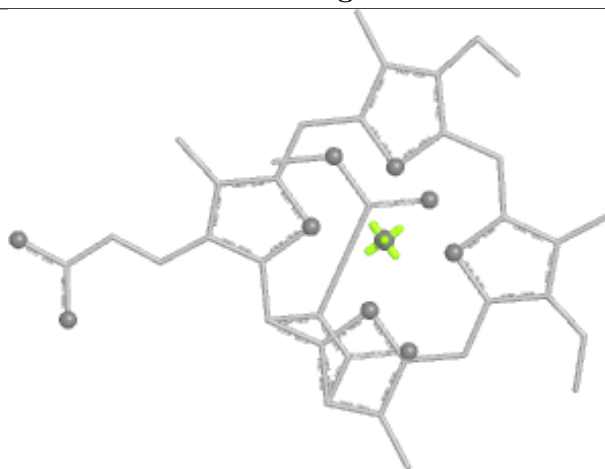
Bond lengths



Bond angles

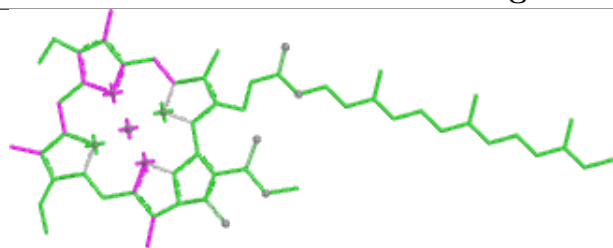


Torsions

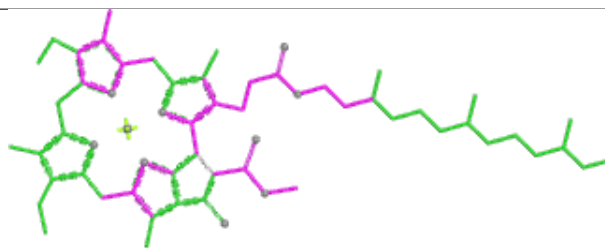


Rings

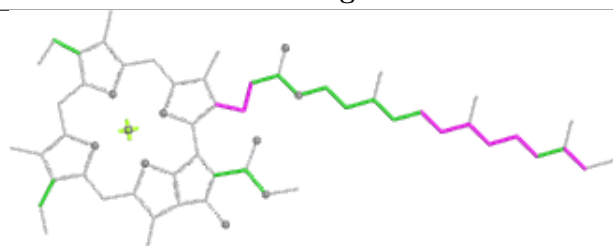
Ligand CLA 14 306



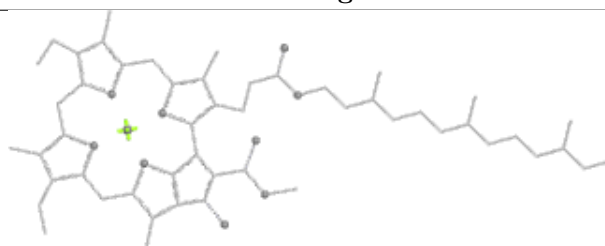
Bond lengths



Bond angles

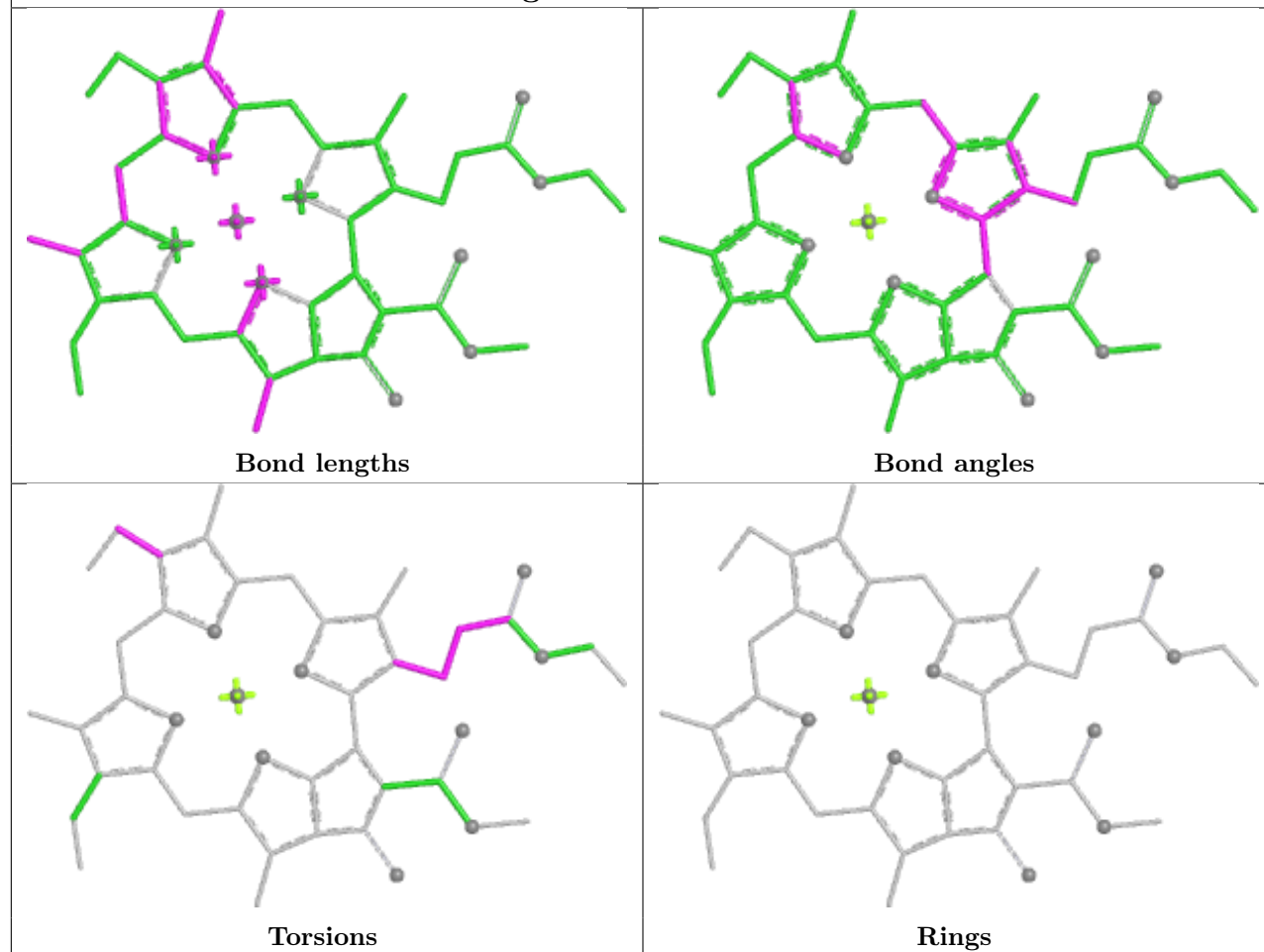


Torsions

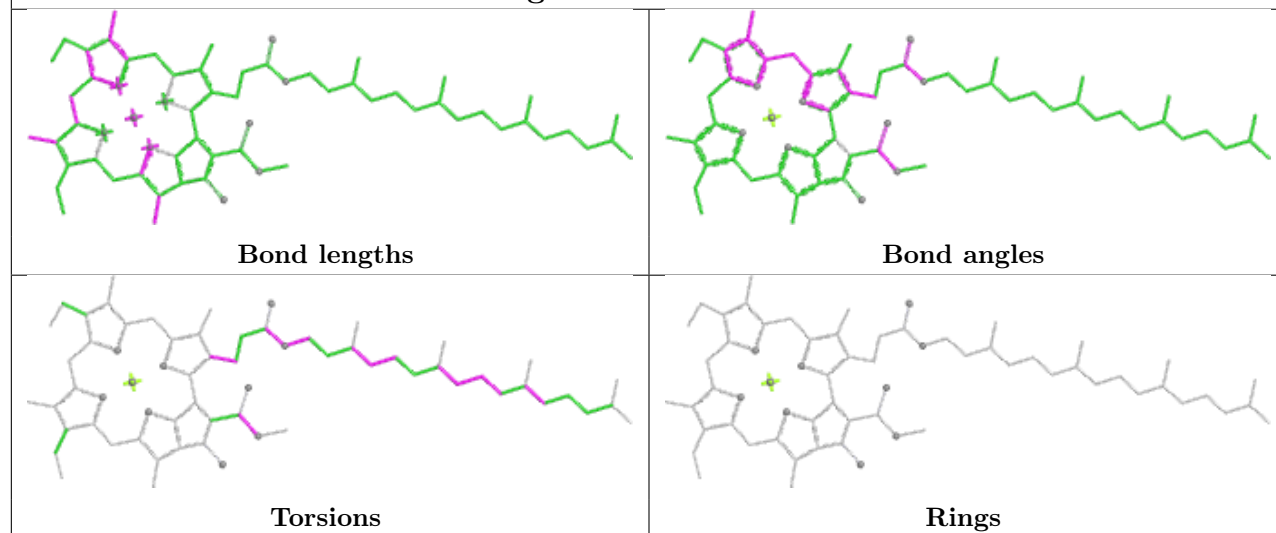


Rings

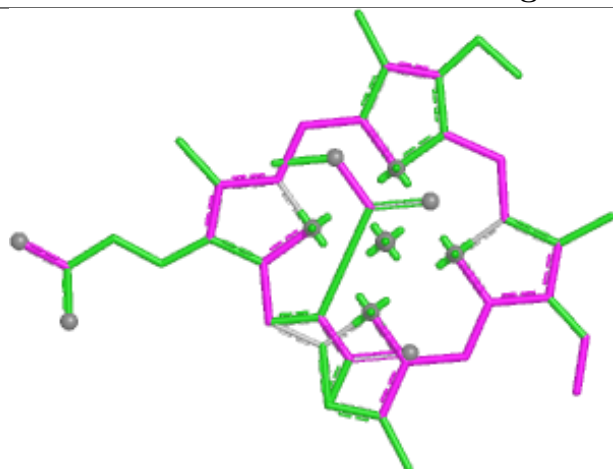
Ligand CLA 17 312



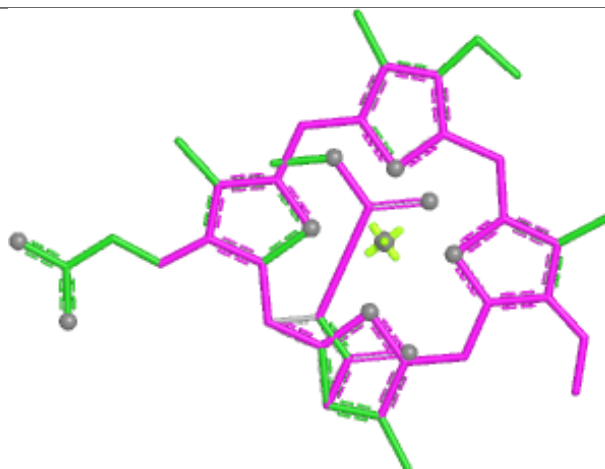
Ligand CLA 14 307



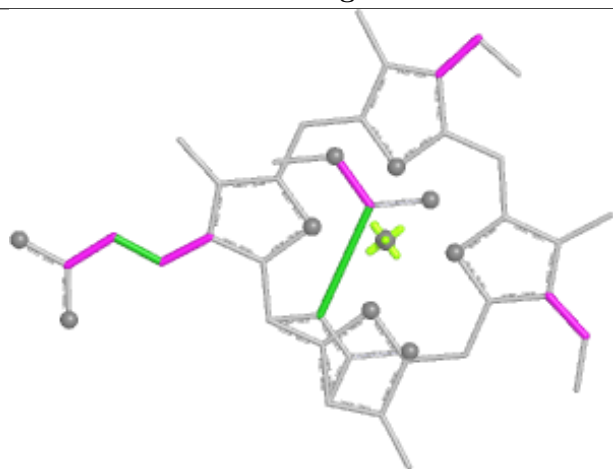
Ligand KC2 7 309



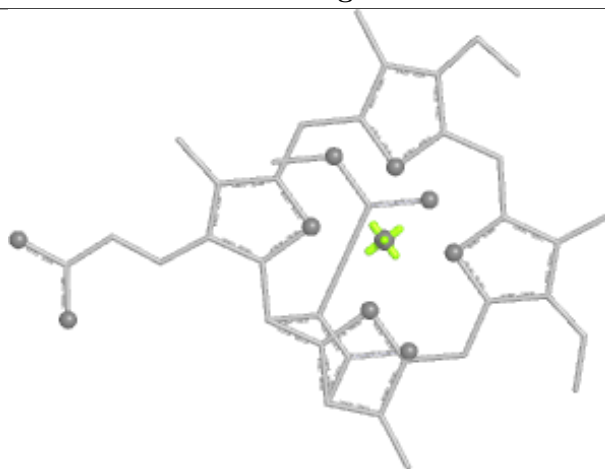
Bond lengths



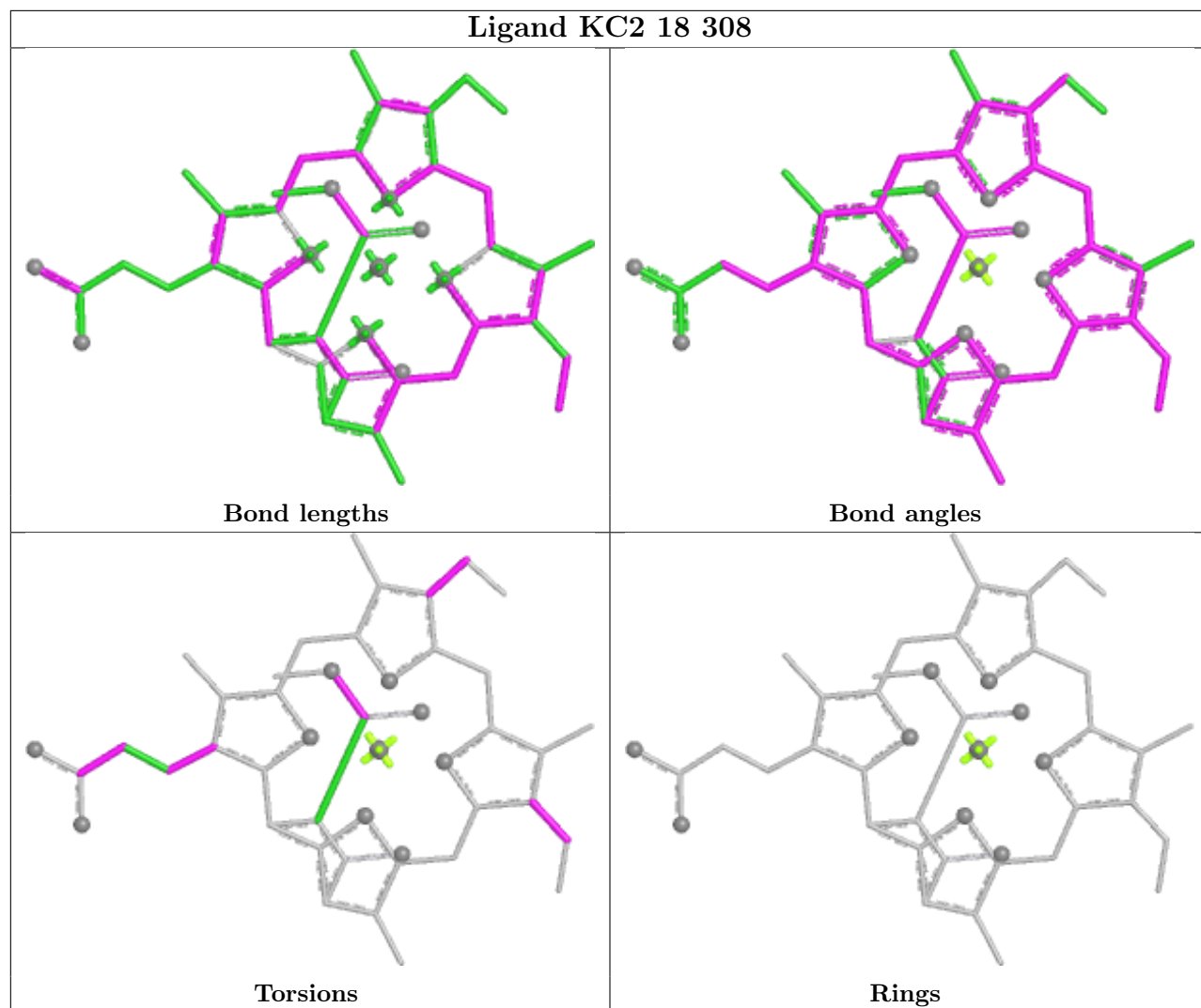
Bond angles



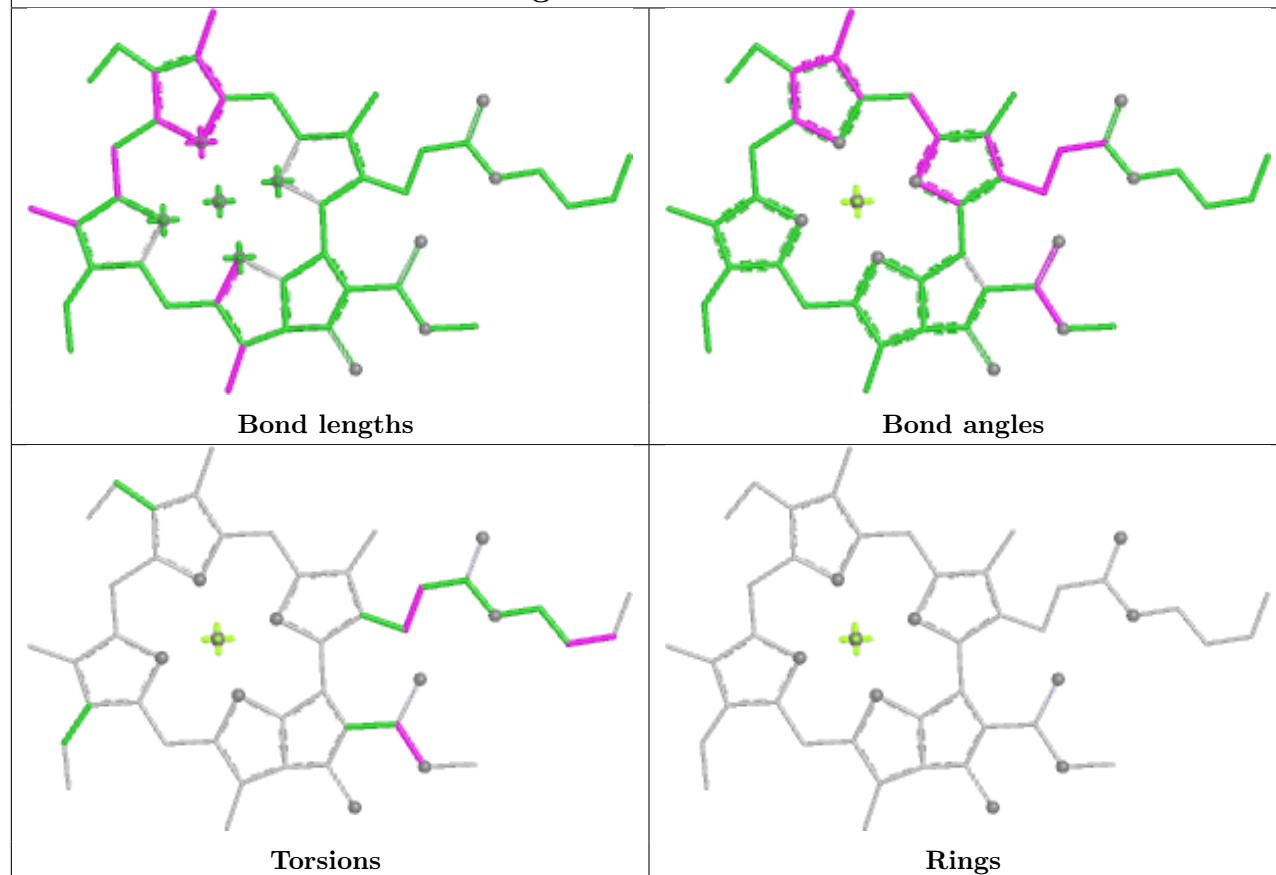
Torsions



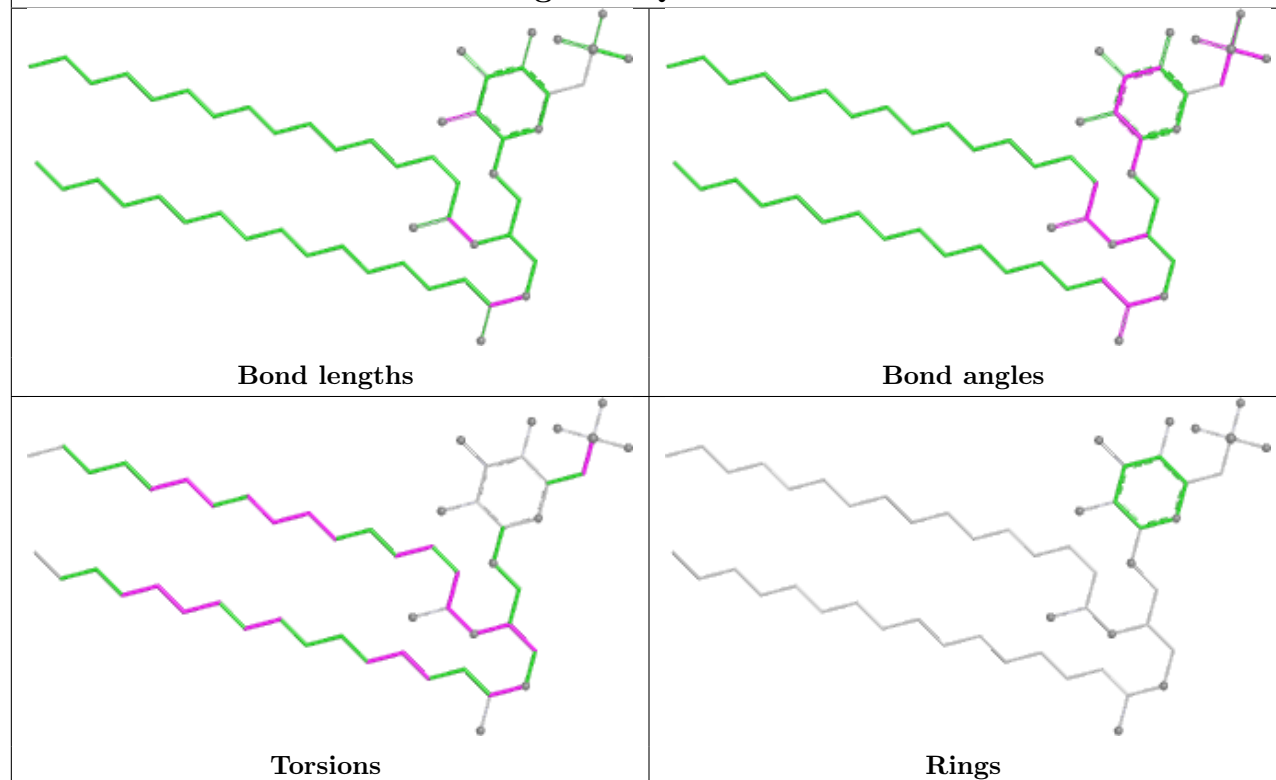
Rings

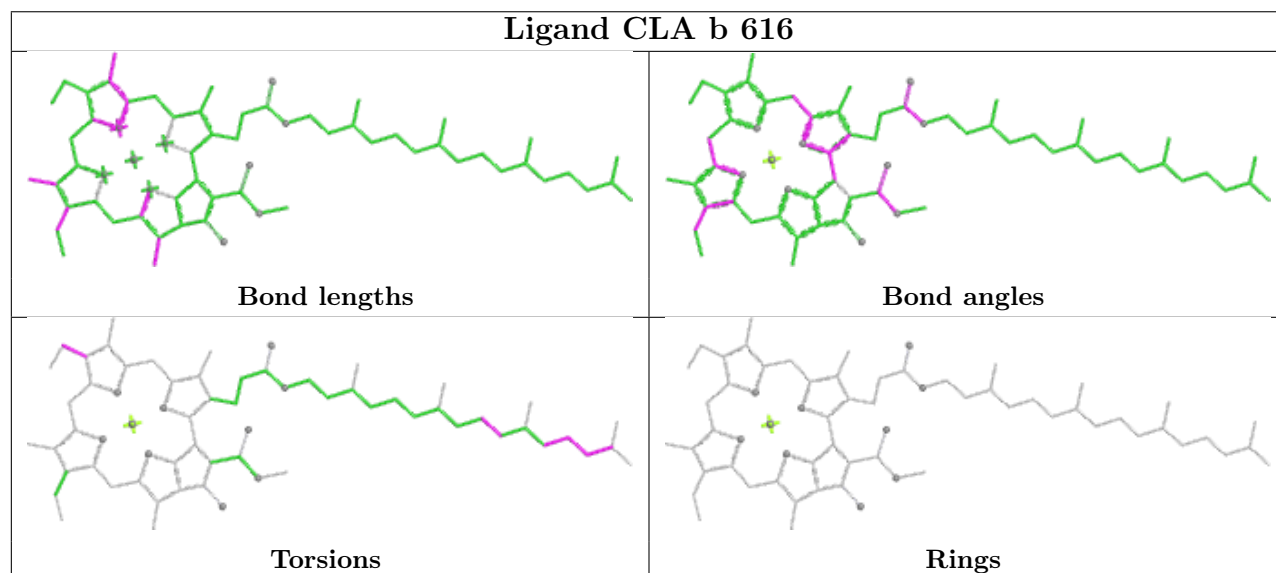
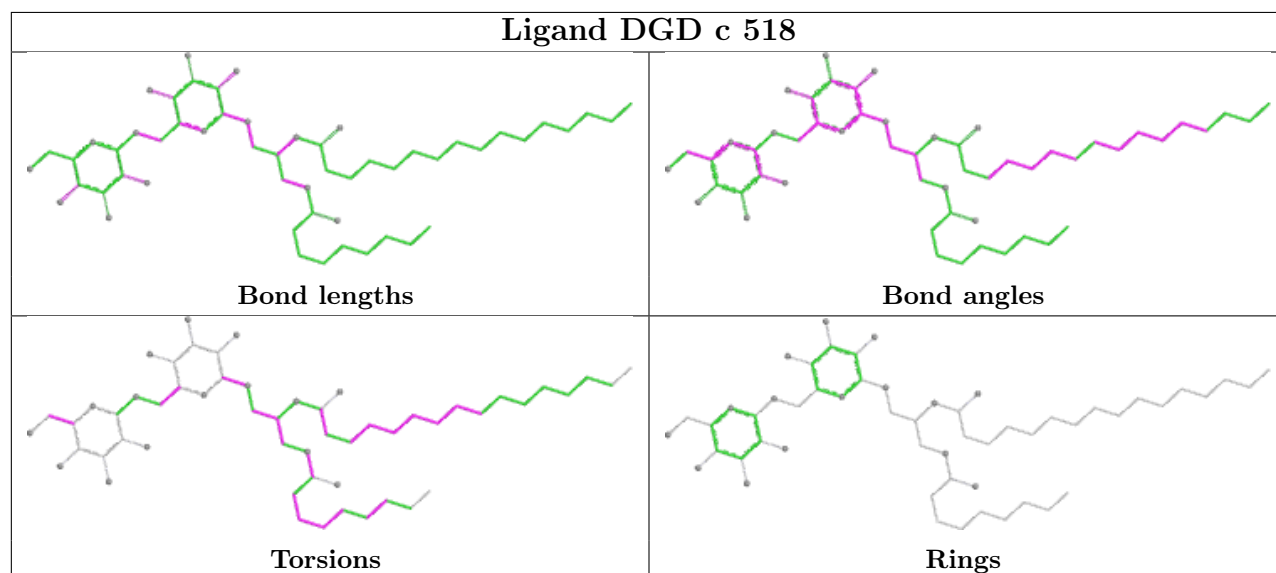
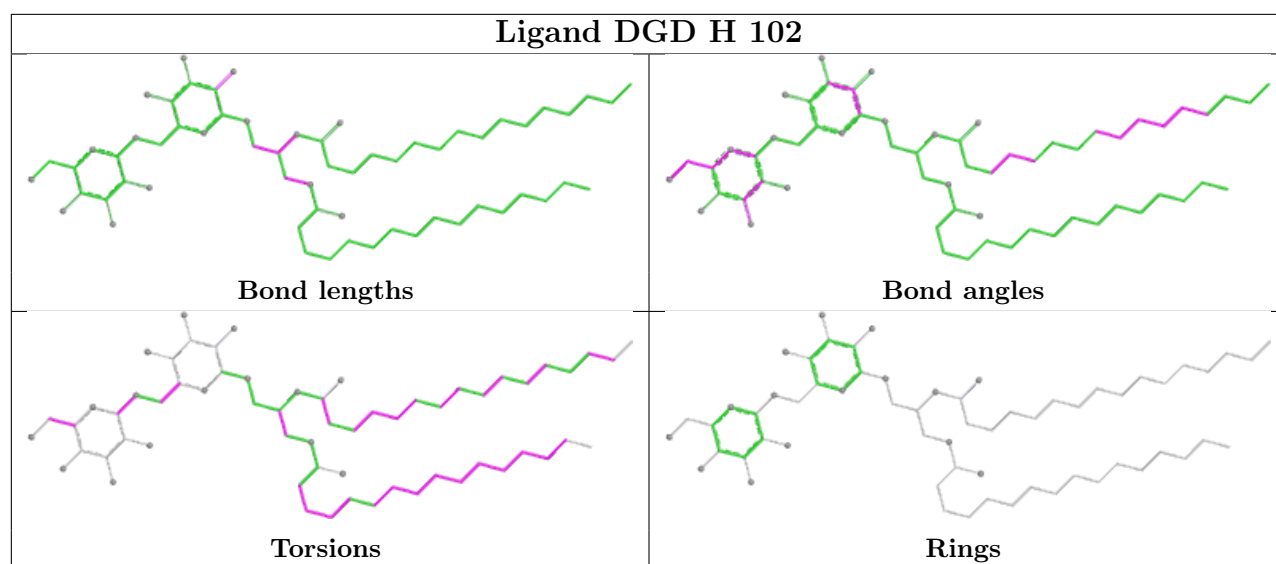


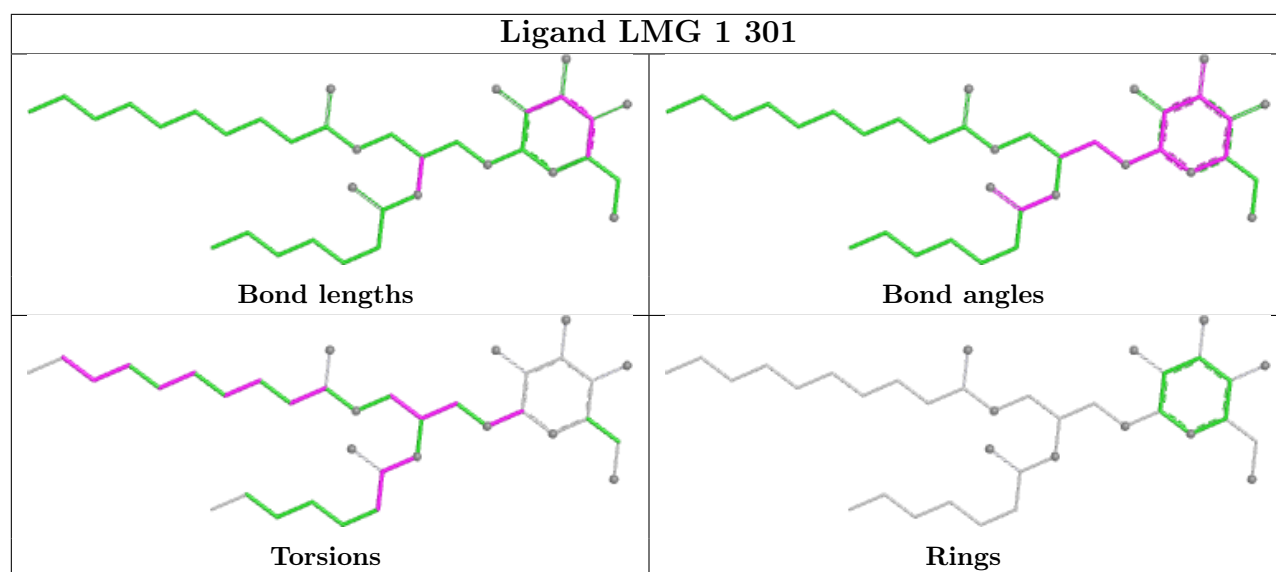
Ligand CLA C 514



Ligand SQD L 102







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.

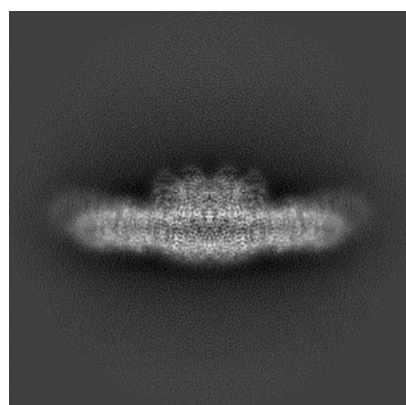
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9839. These allow visual inspection of the internal detail of the map and identification of artifacts.

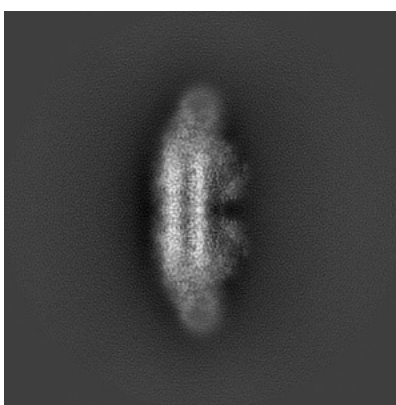
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

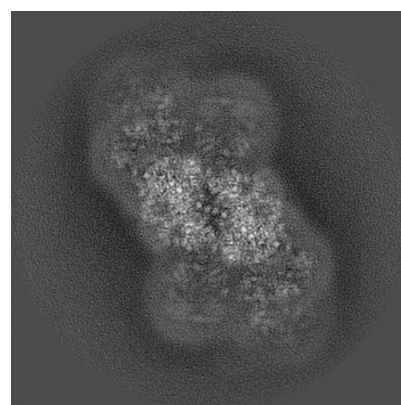
6.1.1 Primary map



X



Y

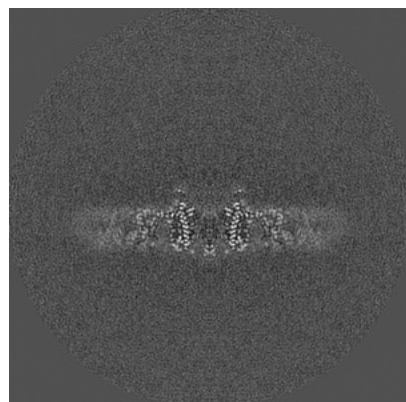


Z

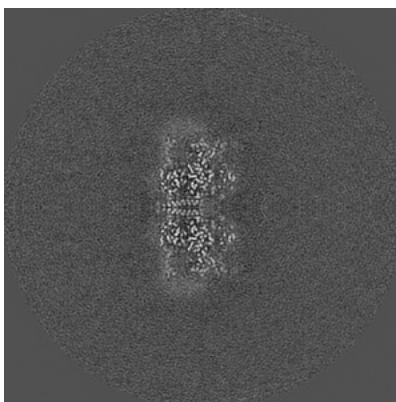
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

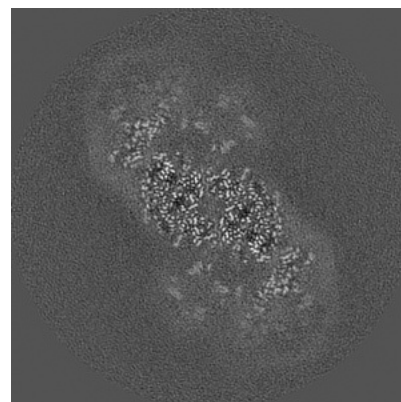
6.2.1 Primary map



X Index: 170



Y Index: 170

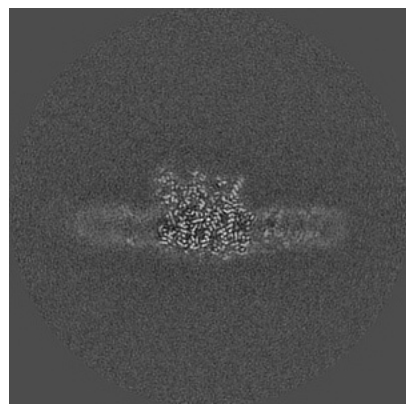


Z Index: 170

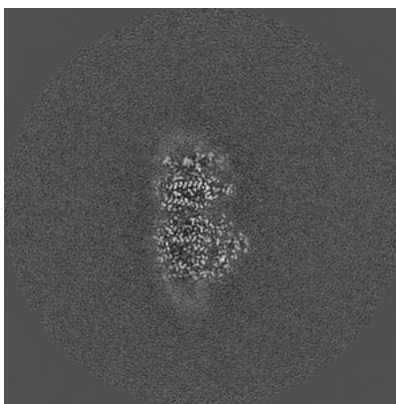
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

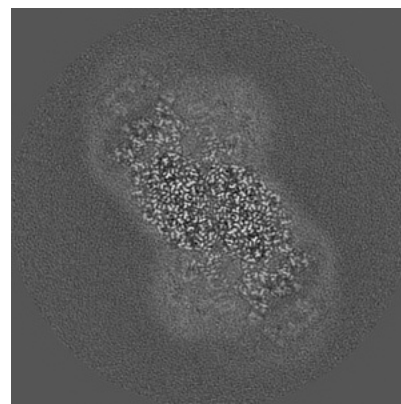
6.3.1 Primary map



X Index: 191



Y Index: 187

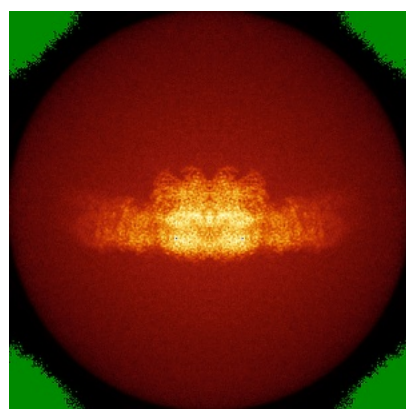


Z Index: 165

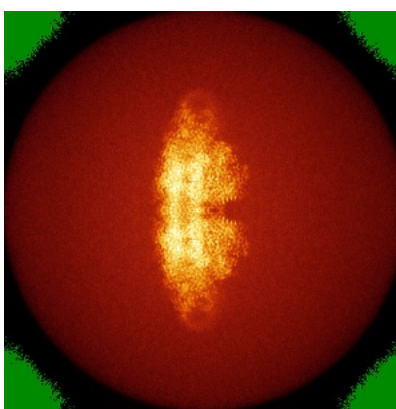
The images above show the largest variance slices of the map in three orthogonal directions.

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

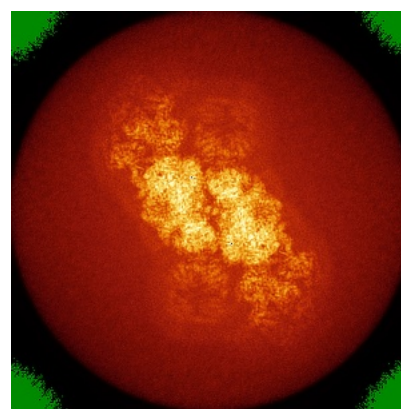
6.4.1 Primary map



X



Y

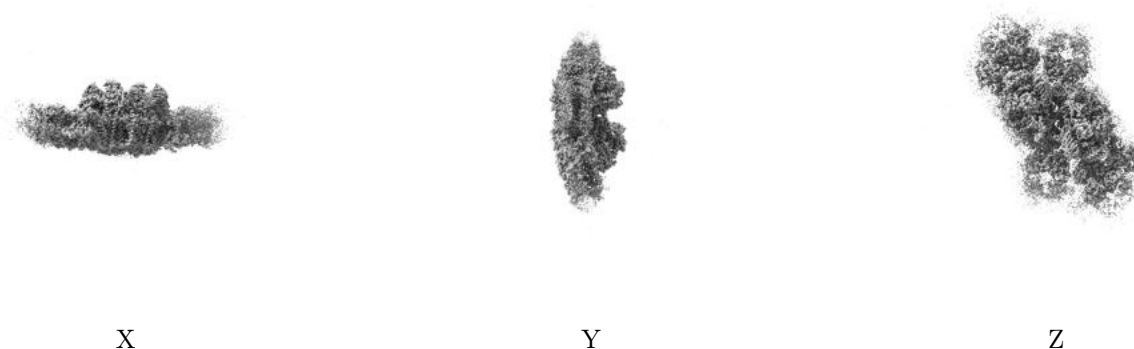


Z

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

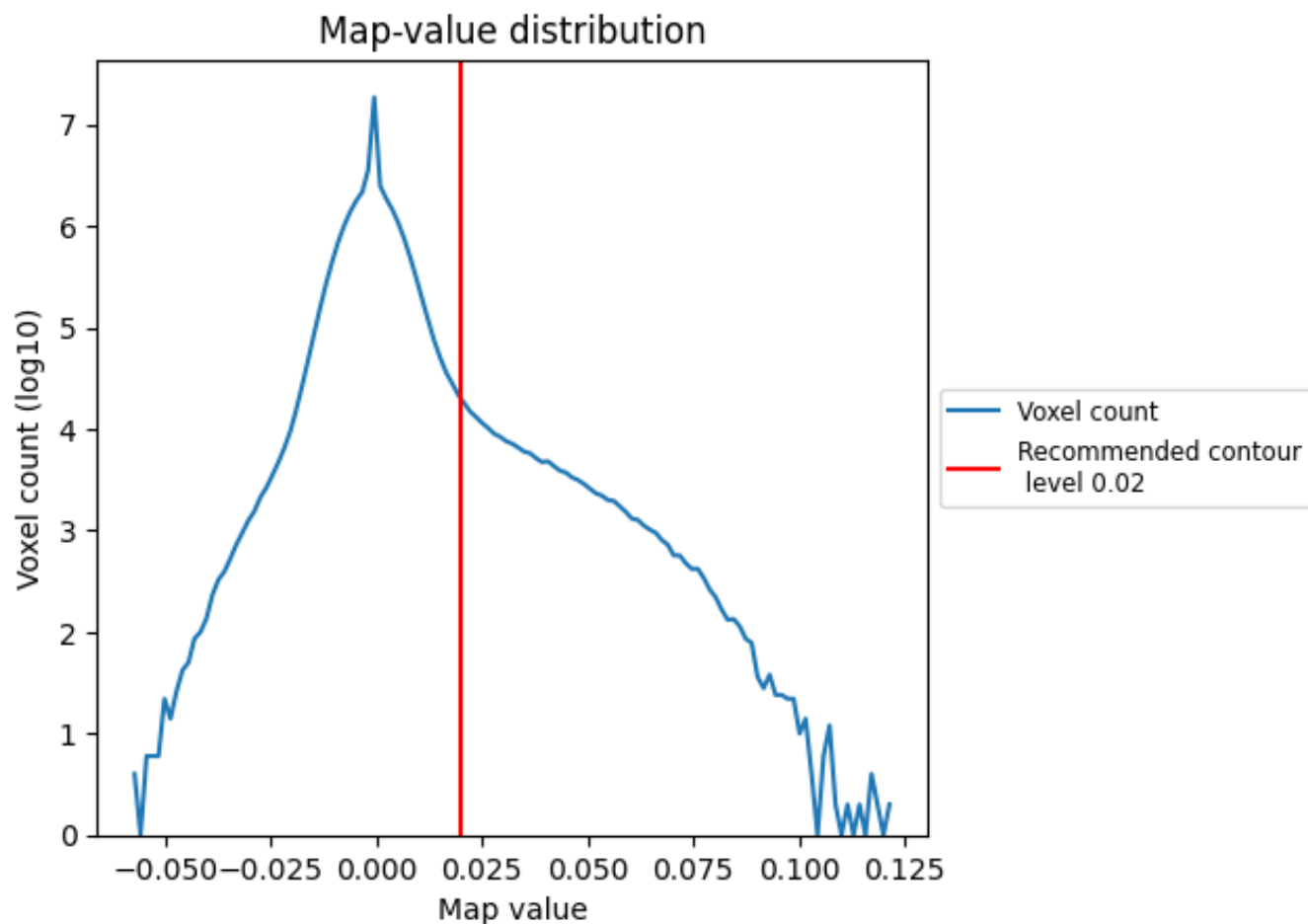
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

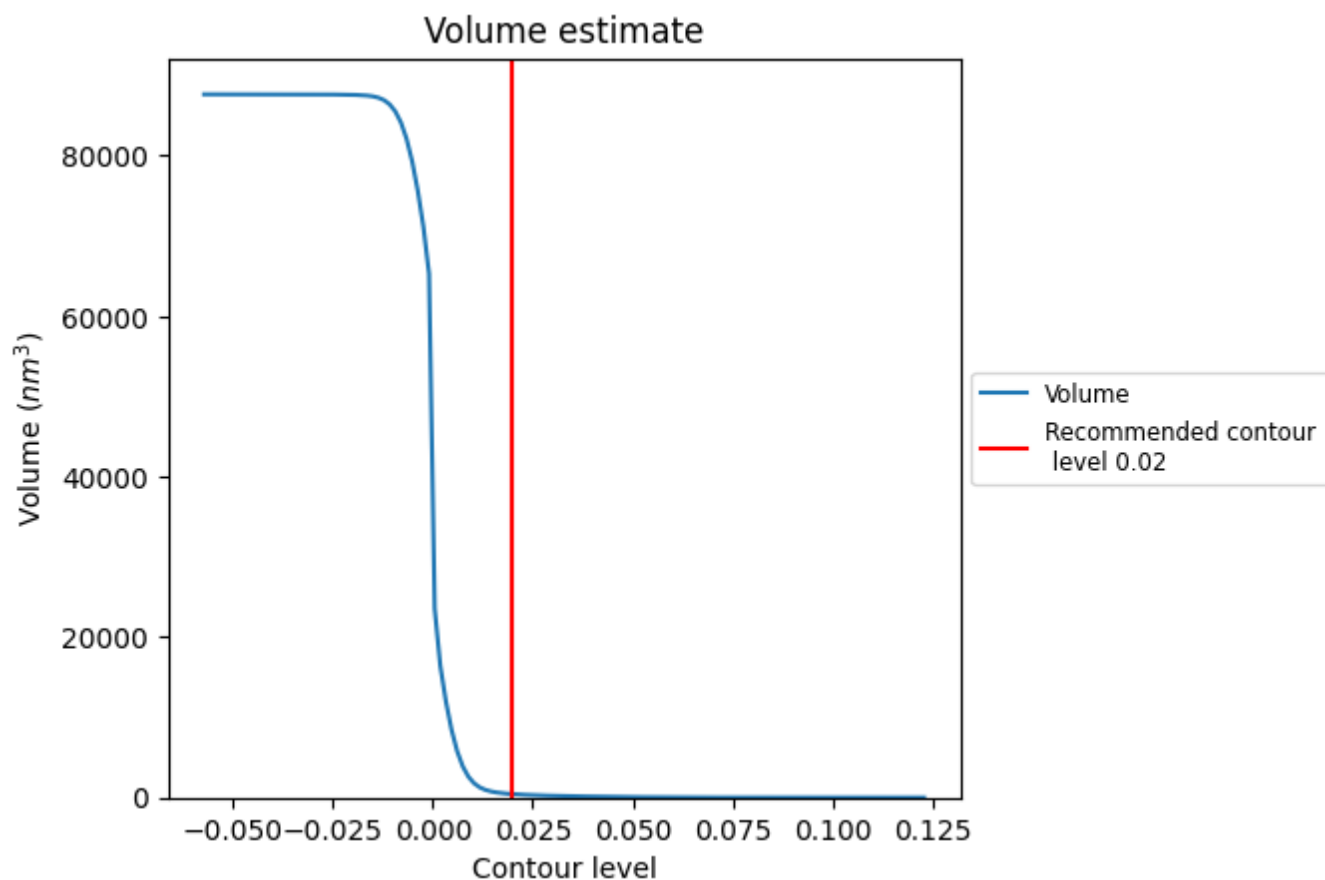
This section contains the results of statistical analysis of the map.

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.

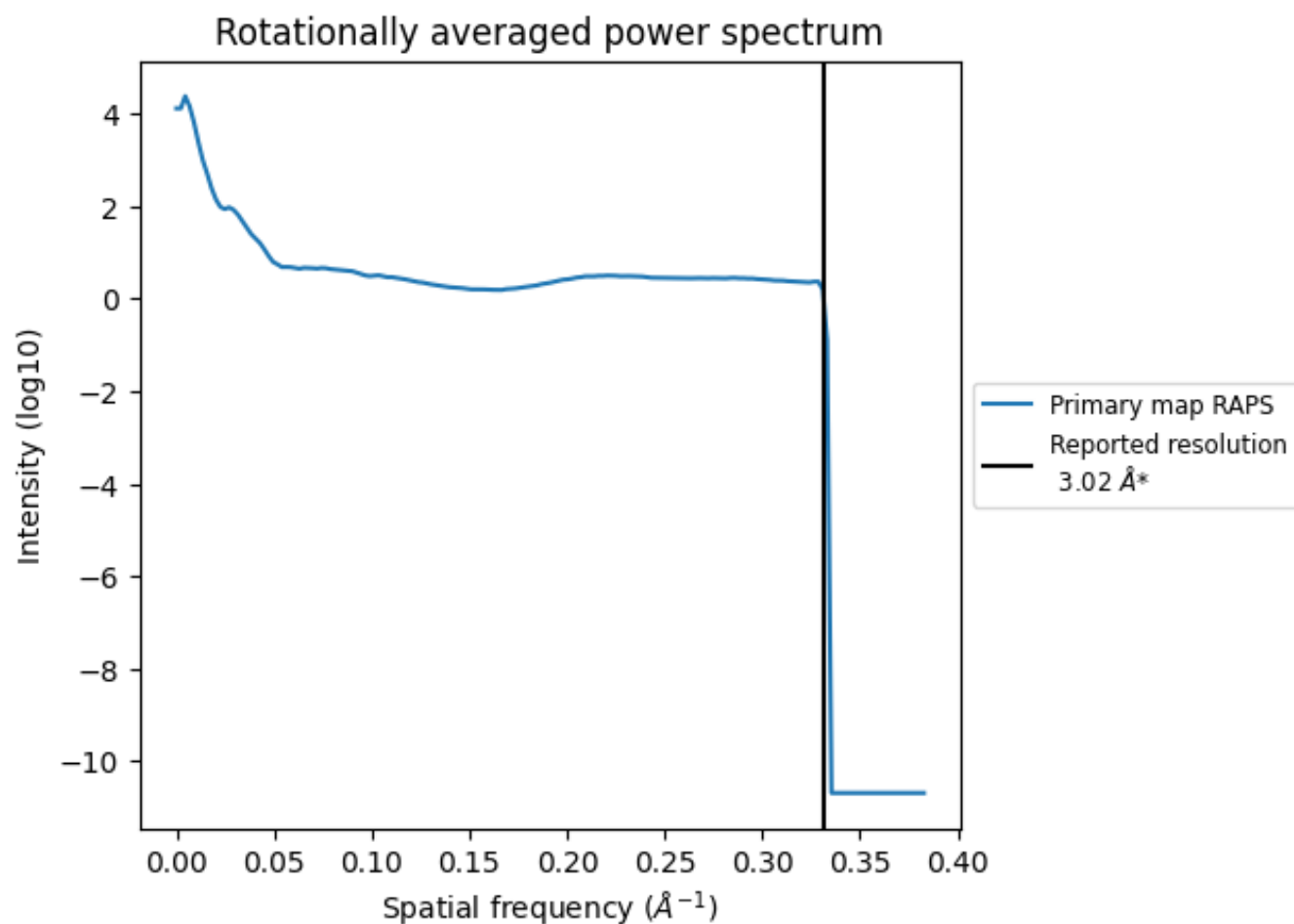
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 428 nm³; this corresponds to an approximate mass of 387 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 0.331 Å⁻¹

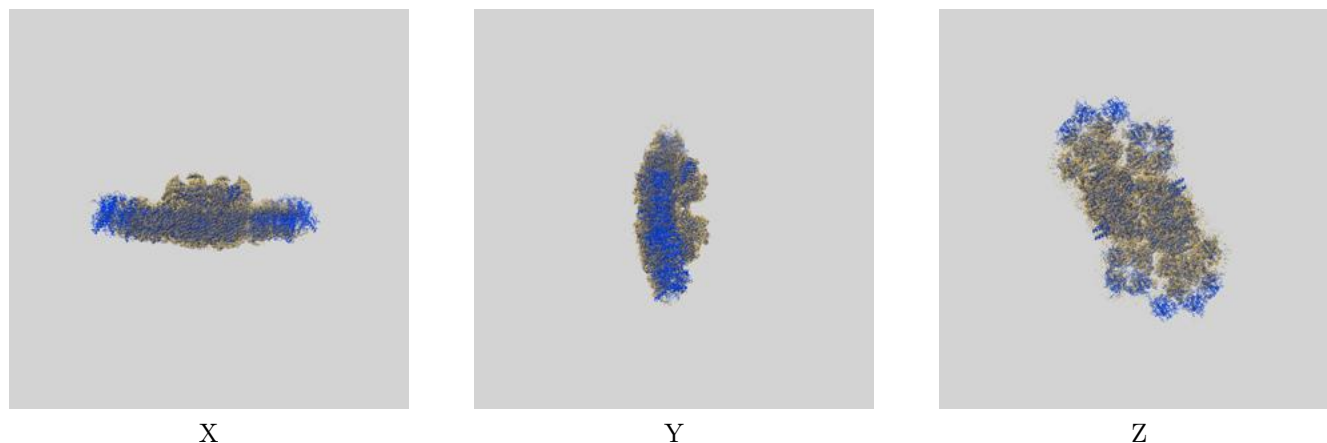
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

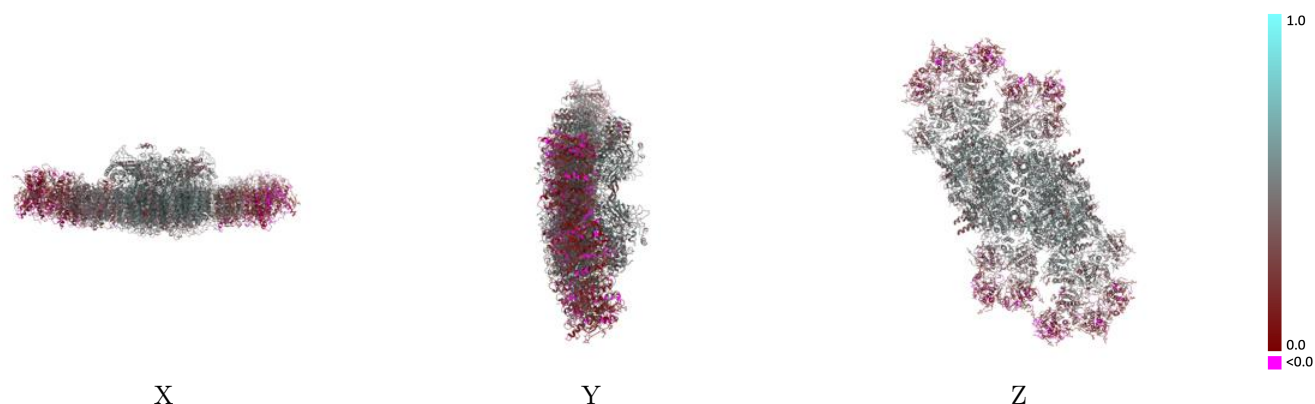
This section contains information regarding the fit between EMDB map EMD-9839 and PDB model 6JLU. Per-residue inclusion information can be found in section [3](#) on page [52](#).

9.1 Map-model overlay [i](#)



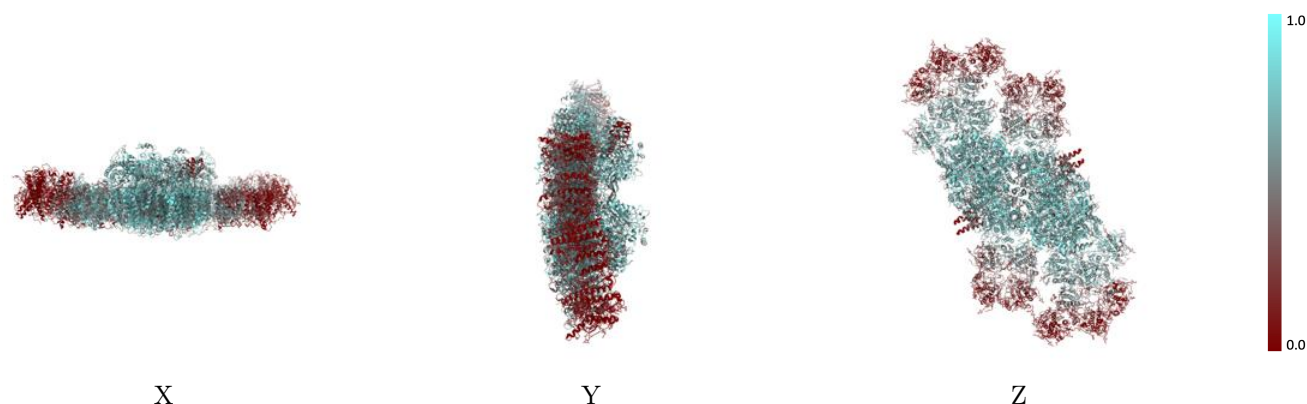
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



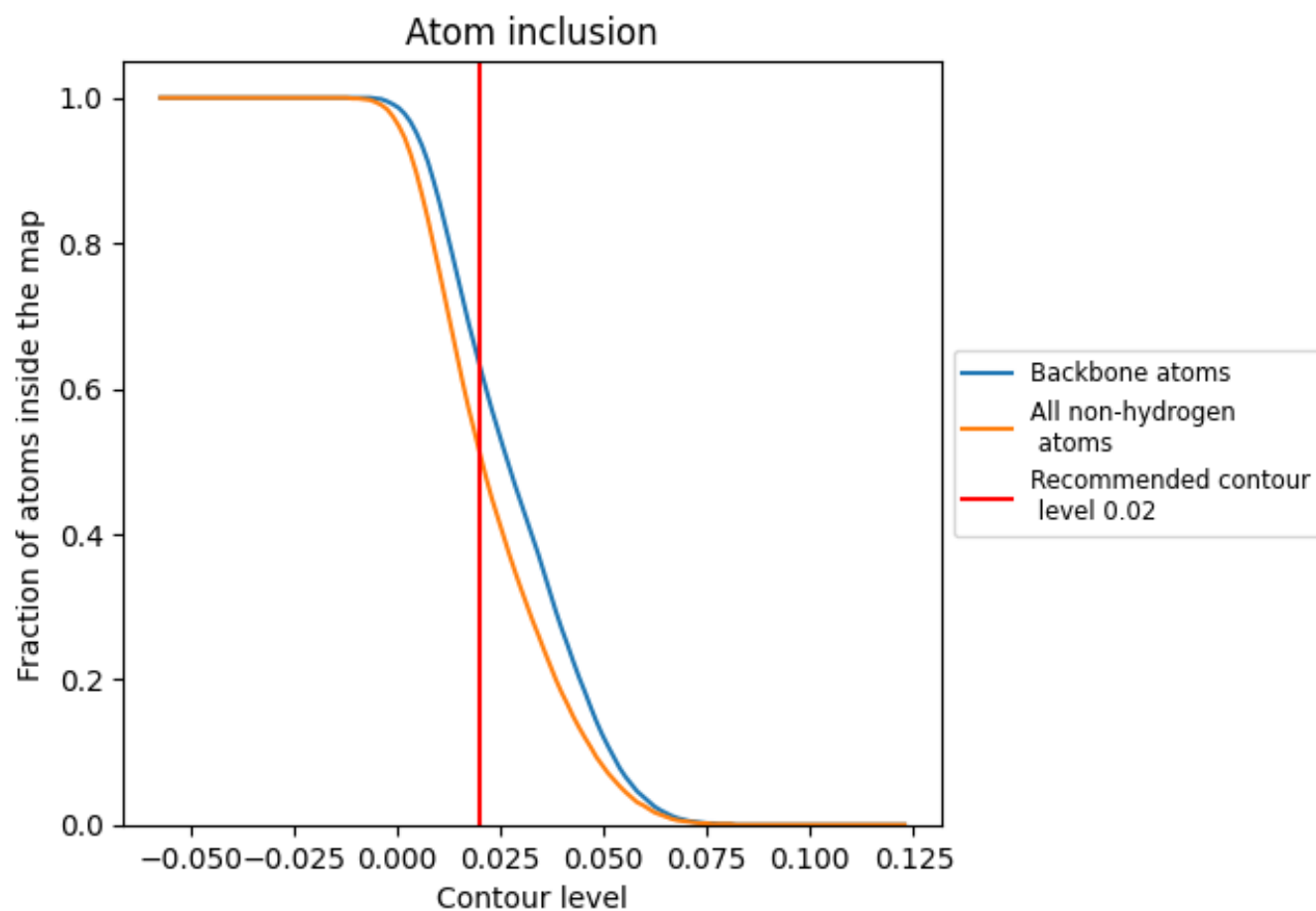
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5130	 0.3850
0	 0.5870	 0.3810
1	 0.3470	 0.2950
10	 0.5900	 0.3960
11	 0.3310	 0.2880
12	 0.0900	 0.1210
13	 0.0840	 0.1180
14	 0.4270	 0.3380
15	 0.4080	 0.2930
16	 0.0380	 0.1490
17	 0.0840	 0.1710
18	 0.5780	 0.3840
19	 0.0060	 0.0800
2	 0.0910	 0.1220
3	 0.0880	 0.1170
4	 0.4240	 0.3460
5	 0.4000	 0.2960
6	 0.0350	 0.1540
7	 0.0820	 0.1720
8	 0.5890	 0.3800
9	 0.0050	 0.0870
A	 0.7640	 0.5220
B	 0.7290	 0.5140
C	 0.7560	 0.5300
D	 0.7530	 0.5220
E	 0.6500	 0.4390
F	 0.5790	 0.4350
G	 0.2400	 0.3790
H	 0.7270	 0.4870
I	 0.7470	 0.5030
J	 0.5510	 0.4140
K	 0.6550	 0.4860
L	 0.6270	 0.5090
M	 0.5940	 0.4760
N	 0.7580	 0.4700



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Chain	Atom inclusion	Q-score
O	 0.6790	 0.4660
P	 0.6380	 0.4460
Q	 0.6190	 0.4260
R	 0.6270	 0.4430
T	 0.6530	 0.4970
U	 0.6900	 0.4650
V	 0.7300	 0.4920
W	 0.5480	 0.4210
X	 0.4670	 0.4270
Y	 0.5190	 0.3660
Z	 0.6110	 0.4460
a	 0.7710	 0.5220
b	 0.7290	 0.5140
c	 0.7560	 0.5280
d	 0.7550	 0.5240
e	 0.6530	 0.4420
f	 0.5790	 0.4530
g	 0.2390	 0.3770
h	 0.7290	 0.4920
i	 0.6740	 0.5100
j	 0.5820	 0.4360
k	 0.6550	 0.4750
l	 0.6370	 0.5090
m	 0.5940	 0.4720
n	 0.7810	 0.4780
o	 0.6820	 0.4700
p	 0.6380	 0.4490
q	 0.6230	 0.4290
r	 0.6300	 0.4490
t	 0.6610	 0.4960
u	 0.6950	 0.4680
v	 0.7350	 0.4920
w	 0.5290	 0.4240
x	 0.4830	 0.4400
y	 0.5220	 0.3540
z	 0.6340	 0.4460