



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 02:00 AM UTC

PDB ID : 7PIW / pdb_00007piw
EMDB ID : EMD-13455
Title : Stacked stretched Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-08-23
Resolution : 4.00 Å (reported)
Based on initial model : 6KAC

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:

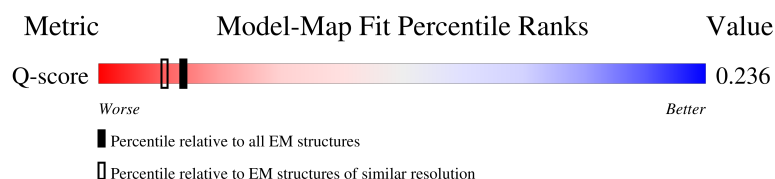
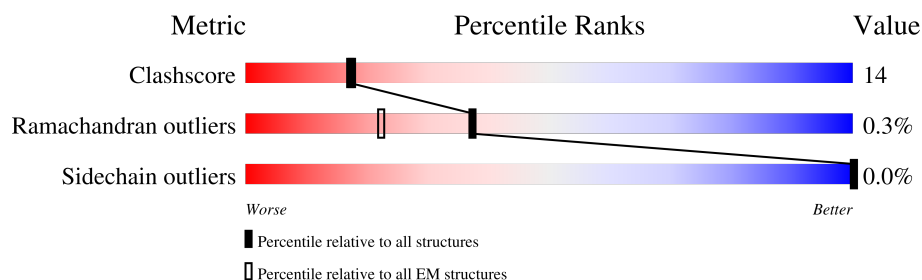
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.00 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	7587 (3.50 - 4.50)

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	336	31% 74% 26%
1	A1	336	16% 61% 39%
1	a	336	37% 68% 32%
1	a1	336	42% 63% 37%

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Mol	Chain	Length	Quality of chain
2	B	484	
2	B1	484	
2	b	484	
2	b1	484	
3	V	32	
3	V1	32	
3	v	32	
3	v1	32	
4	C	449	
4	C1	449	
4	c	449	
4	c1	449	
5	D	348	
5	D1	348	
5	d	348	
5	d1	348	
6	E	76	
6	E1	76	
6	e	76	
6	e1	76	
7	F	31	
7	F1	31	
7	f	31	
7	f1	31	
8	H	67	

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Mol	Chain	Length	Quality of chain
8	H1	67	
8	h	67	
8	h1	67	
9	I	35	
9	I1	35	
9	i	35	
9	i1	35	
10	J	36	
10	J1	36	
10	j	36	
10	j1	36	
11	K	37	
11	K1	37	
11	k	37	
11	k1	37	
12	L	38	
12	L1	38	
12	l	38	
13	M	32	
13	m	32	
14	O	238	
14	O1	238	
14	o	238	
14	o1	238	
15	P	187	

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Mol	Chain	Length	Quality of chain
15	P1	187	94% 77% 23%
15	p	187	100% 87% 13%
15	p1	187	93% 82% 18%
16	T	30	53% 87% 13%
16	T1	30	40% 77% 23%
16	t	30	53% 70% 30%
16	t1	30	63% 70% 30%
17	W	44	68% 84% 16%
17	W1	44	14% 68% 32%
17	w	44	59% 91% 9%
17	w1	44	41% 84% 16%
18	X	30	73% 83% 17%
18	X1	30	20% 83% 17%
18	x	30	73% 83% 17%
18	x1	30	60% 97% .
19	Z	61	75% 82% 18%
19	Z1	61	15% 97% .
19	z	61	92% 79% 21%
19	z1	61	46% 97% .
20	N	222	65% 73% 26%
20	N1	222	9% 78% 22%
20	n	222	88% 73% 26% .
20	n1	222	26% 80% 20%
21	G	221	83% 75% 25%
21	G1	221	10% 78% 22%

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Mol	Chain	Length	Quality of chain
21	g	221	
21	g1	221	
22	R	202	
22	r	202	
23	S	243	
23	S1	243	
23	s	243	
23	s1	243	
24	Y	222	
24	Y1	222	
24	y	222	
24	y1	222	
25	U	27	
25	U1	27	
25	u	27	
25	u1	27	
26	M1	31	
26	m1	31	
27	R1	202	
27	r1	202	

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	A	405	X	-	-	-
31	CLA	A	406	X	-	-	-
31	CLA	A	407	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	A	410	X	-	-	-
31	CLA	A1	405	X	-	-	-
31	CLA	A1	406	X	-	-	-
31	CLA	A1	407	X	-	-	-
31	CLA	A1	410	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	610	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	B	617	X	-	-	-
31	CLA	B1	602	X	-	-	-
31	CLA	B1	603	X	-	-	-
31	CLA	B1	604	X	-	-	-
31	CLA	B1	605	X	-	-	-
31	CLA	B1	606	X	-	-	-
31	CLA	B1	607	X	-	-	-
31	CLA	B1	608	X	-	-	-
31	CLA	B1	609	X	-	-	-
31	CLA	B1	610	X	-	-	-
31	CLA	B1	611	X	-	-	-
31	CLA	B1	612	X	-	-	-
31	CLA	B1	613	X	-	-	-
31	CLA	B1	614	X	-	-	-
31	CLA	B1	615	X	-	-	-
31	CLA	B1	616	X	-	-	-
31	CLA	B1	617	X	-	-	-
31	CLA	C	501	X	-	-	-
31	CLA	C	502	X	-	-	-
31	CLA	C	503	X	-	-	-
31	CLA	C	504	X	-	-	-
31	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	C1	501	X	-	-	-
31	CLA	C1	502	X	-	-	-
31	CLA	C1	503	X	-	-	-
31	CLA	C1	504	X	-	-	-
31	CLA	C1	505	X	-	-	-
31	CLA	C1	506	X	-	-	-
31	CLA	C1	507	X	-	-	-
31	CLA	C1	508	X	-	-	-
31	CLA	C1	509	X	-	-	-
31	CLA	C1	510	X	-	-	-
31	CLA	C1	511	X	-	-	-
31	CLA	C1	512	X	-	-	-
31	CLA	C1	513	X	-	-	-
31	CLA	D	402	X	-	-	-
31	CLA	D	403	X	-	-	-
31	CLA	D1	402	X	-	-	-
31	CLA	D1	403	X	-	-	-
31	CLA	G	602	X	-	-	-
31	CLA	G	603	X	-	-	-
31	CLA	G	604	X	-	-	-
31	CLA	G	610	X	-	-	-
31	CLA	G	611	X	-	-	-
31	CLA	G	612	X	-	-	-
31	CLA	G	613	X	-	-	-
31	CLA	G	614	X	-	-	-
31	CLA	G1	602	X	-	-	-
31	CLA	G1	603	X	-	-	-
31	CLA	G1	604	X	-	-	-
31	CLA	G1	610	X	-	-	-
31	CLA	G1	611	X	-	-	-
31	CLA	G1	612	X	-	-	-
31	CLA	G1	613	X	-	-	-
31	CLA	G1	614	X	-	-	-
31	CLA	N	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	N	603	X	-	-	-
31	CLA	N	604	X	-	-	-
31	CLA	N	610	X	-	-	-
31	CLA	N	611	X	-	-	-
31	CLA	N	612	X	-	-	-
31	CLA	N	613	X	-	-	-
31	CLA	N	614	X	-	-	-
31	CLA	N1	602	X	-	-	-
31	CLA	N1	603	X	-	-	-
31	CLA	N1	604	X	-	-	-
31	CLA	N1	610	X	-	-	-
31	CLA	N1	611	X	-	-	-
31	CLA	N1	612	X	-	-	-
31	CLA	N1	613	X	-	-	-
31	CLA	N1	614	X	-	-	-
31	CLA	R	602	X	-	-	-
31	CLA	R	603	X	-	-	-
31	CLA	R	604	X	-	-	-
31	CLA	R	608	X	-	-	-
31	CLA	R	609	X	-	-	-
31	CLA	R	610	X	-	-	-
31	CLA	R	611	X	-	-	-
31	CLA	R	612	X	-	-	-
31	CLA	R	613	X	-	-	-
31	CLA	R1	602	X	-	-	-
31	CLA	R1	603	X	-	-	-
31	CLA	R1	604	X	-	-	-
31	CLA	R1	608	X	-	-	-
31	CLA	R1	609	X	-	-	-
31	CLA	R1	610	X	-	-	-
31	CLA	R1	612	X	-	-	-
31	CLA	S	602	X	-	-	-
31	CLA	S	603	X	-	-	-
31	CLA	S	604	X	-	-	-
31	CLA	S	605	X	-	-	-
31	CLA	S	609	X	-	-	-
31	CLA	S	610	X	-	-	-
31	CLA	S	611	X	-	-	-
31	CLA	S	612	X	-	-	-
31	CLA	S	613	X	-	-	-
31	CLA	S	614	X	-	-	-
31	CLA	S	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	S1	602	X	-	-	-
31	CLA	S1	603	X	-	-	-
31	CLA	S1	604	X	-	-	-
31	CLA	S1	605	X	-	-	-
31	CLA	S1	609	X	-	-	-
31	CLA	S1	610	X	-	-	-
31	CLA	S1	611	X	-	-	-
31	CLA	S1	612	X	-	-	-
31	CLA	S1	613	X	-	-	-
31	CLA	S1	614	X	-	-	-
31	CLA	S1	617	X	-	-	-
31	CLA	Y	602	X	-	-	-
31	CLA	Y	603	X	-	-	-
31	CLA	Y	604	X	-	-	-
31	CLA	Y	608	X	-	-	-
31	CLA	Y	610	X	-	-	-
31	CLA	Y	611	X	-	-	-
31	CLA	Y	612	X	-	-	-
31	CLA	Y	613	X	-	-	-
31	CLA	Y	614	X	-	-	-
31	CLA	Y1	602	X	-	-	-
31	CLA	Y1	603	X	-	-	-
31	CLA	Y1	604	X	-	-	-
31	CLA	Y1	608	X	-	-	-
31	CLA	Y1	610	X	-	-	-
31	CLA	Y1	611	X	-	-	-
31	CLA	Y1	612	X	-	-	-
31	CLA	Y1	613	X	-	-	-
31	CLA	Y1	614	X	-	-	-
31	CLA	a	405	X	-	-	-
31	CLA	a	406	X	-	-	-
31	CLA	a	407	X	-	-	-
31	CLA	a	410	X	-	-	-
31	CLA	a1	405	X	-	-	-
31	CLA	a1	406	X	-	-	-
31	CLA	a1	407	X	-	-	-
31	CLA	a1	410	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	b	607	X	-	-	-
31	CLA	b	608	X	-	-	-
31	CLA	b	609	X	-	-	-
31	CLA	b	610	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	b	617	X	-	-	-
31	CLA	b1	602	X	-	-	-
31	CLA	b1	603	X	-	-	-
31	CLA	b1	604	X	-	-	-
31	CLA	b1	605	X	-	-	-
31	CLA	b1	606	X	-	-	-
31	CLA	b1	607	X	-	-	-
31	CLA	b1	608	X	-	-	-
31	CLA	b1	609	X	-	-	-
31	CLA	b1	610	X	-	-	-
31	CLA	b1	611	X	-	-	-
31	CLA	b1	612	X	-	-	-
31	CLA	b1	613	X	-	-	-
31	CLA	b1	614	X	-	-	-
31	CLA	b1	615	X	-	-	-
31	CLA	b1	616	X	-	-	-
31	CLA	b1	617	X	-	-	-
31	CLA	c	501	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	-	-	-
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	c1	501	X	-	-	-
31	CLA	c1	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	c1	503	X	-	-	-
31	CLA	c1	504	X	-	-	-
31	CLA	c1	505	X	-	-	-
31	CLA	c1	506	X	-	-	-
31	CLA	c1	507	X	-	-	-
31	CLA	c1	508	X	-	-	-
31	CLA	c1	509	X	-	-	-
31	CLA	c1	510	X	-	-	-
31	CLA	c1	511	X	-	-	-
31	CLA	c1	512	X	-	-	-
31	CLA	c1	513	X	-	-	-
31	CLA	d	402	X	-	-	-
31	CLA	d	403	X	-	-	-
31	CLA	d1	402	X	-	-	-
31	CLA	d1	403	X	-	-	-
31	CLA	g	602	X	-	-	-
31	CLA	g	603	X	-	-	-
31	CLA	g	604	X	-	-	-
31	CLA	g	610	X	-	-	-
31	CLA	g	611	X	-	-	-
31	CLA	g	612	X	-	-	-
31	CLA	g	613	X	-	-	-
31	CLA	g	614	X	-	-	-
31	CLA	g1	602	X	-	-	-
31	CLA	g1	603	X	-	-	-
31	CLA	g1	604	X	-	-	-
31	CLA	g1	610	X	-	-	-
31	CLA	g1	611	X	-	-	-
31	CLA	g1	612	X	-	-	-
31	CLA	g1	613	X	-	-	-
31	CLA	g1	614	X	-	-	-
31	CLA	n	602	X	-	-	-
31	CLA	n	603	X	-	-	-
31	CLA	n	604	X	-	-	-
31	CLA	n	610	X	-	-	-
31	CLA	n	611	X	-	-	-
31	CLA	n	612	X	-	-	-
31	CLA	n	613	X	-	-	-
31	CLA	n	614	X	-	-	-
31	CLA	n1	602	X	-	-	-
31	CLA	n1	603	X	-	-	-
31	CLA	n1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	n1	610	X	-	-	-
31	CLA	n1	611	X	-	-	-
31	CLA	n1	612	X	-	-	-
31	CLA	n1	613	X	-	-	-
31	CLA	n1	614	X	-	-	-
31	CLA	r	602	X	-	-	-
31	CLA	r	603	X	-	-	-
31	CLA	r	604	X	-	-	-
31	CLA	r	608	X	-	-	-
31	CLA	r	609	X	-	-	-
31	CLA	r	610	X	-	-	-
31	CLA	r	611	X	-	-	-
31	CLA	r	612	X	-	-	-
31	CLA	r	613	X	-	-	-
31	CLA	r1	602	X	-	-	-
31	CLA	r1	603	X	-	-	-
31	CLA	r1	604	X	-	-	-
31	CLA	r1	608	X	-	-	-
31	CLA	r1	609	X	-	-	-
31	CLA	r1	610	X	-	-	-
31	CLA	r1	612	X	-	-	-
31	CLA	s	602	X	-	-	-
31	CLA	s	603	X	-	-	-
31	CLA	s	604	X	-	-	-
31	CLA	s	605	X	-	-	-
31	CLA	s	609	X	-	-	-
31	CLA	s	610	X	-	-	-
31	CLA	s	611	X	-	-	-
31	CLA	s	612	X	-	-	-
31	CLA	s	613	X	-	-	-
31	CLA	s	614	X	-	-	-
31	CLA	s	617	X	-	-	-
31	CLA	s1	602	X	-	-	-
31	CLA	s1	603	X	-	-	-
31	CLA	s1	604	X	-	-	-
31	CLA	s1	605	X	-	-	-
31	CLA	s1	609	X	-	-	-
31	CLA	s1	610	X	-	-	-
31	CLA	s1	611	X	-	-	-
31	CLA	s1	612	X	-	-	-
31	CLA	s1	613	X	-	-	-
31	CLA	s1	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	s1	617	X	-	-	-
31	CLA	y	602	X	-	-	-
31	CLA	y	603	X	-	-	-
31	CLA	y	604	X	-	-	-
31	CLA	y	608	X	-	-	-
31	CLA	y	610	X	-	-	-
31	CLA	y	611	X	-	-	-
31	CLA	y	612	X	-	-	-
31	CLA	y	613	X	-	-	-
31	CLA	y	614	X	-	-	-
31	CLA	y1	602	X	-	-	-
31	CLA	y1	603	X	-	-	-
31	CLA	y1	604	X	-	-	-
31	CLA	y1	608	X	-	-	-
31	CLA	y1	610	X	-	-	-
31	CLA	y1	611	X	-	-	-
31	CLA	y1	612	X	-	-	-
31	CLA	y1	613	X	-	-	-
31	CLA	y1	614	X	-	-	-
37	C7Z	B	620	X	-	-	-
37	C7Z	B1	620	X	-	-	-
37	C7Z	b	620	X	-	-	-
37	C7Z	b1	620	X	-	-	-
42	LMK	C	527	X	-	-	-
42	LMK	C1	527	X	-	-	-
42	LMK	c	627	X	-	-	-
42	LMK	c1	527	X	-	-	-
46	RRX	H	101	X	-	X	-
46	RRX	H1	101	X	-	-	-
46	RRX	h	101	X	-	-	-
46	RRX	h1	101	X	-	-	-
47	CHL	G	601	X	-	-	-
47	CHL	G	605	X	-	-	-
47	CHL	G	606	X	-	-	-
47	CHL	G	607	X	-	-	-
47	CHL	G	608	X	-	-	-
47	CHL	G	609	X	-	-	-
47	CHL	G1	601	X	-	-	-
47	CHL	G1	605	X	-	-	-
47	CHL	G1	606	X	-	-	-
47	CHL	G1	607	X	-	-	-
47	CHL	G1	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	CHL	G1	609	X	-	-	-
47	CHL	N	601	X	-	-	-
47	CHL	N	605	X	-	-	-
47	CHL	N	606	X	-	-	-
47	CHL	N	607	X	-	-	-
47	CHL	N	608	X	-	-	-
47	CHL	N	609	X	-	-	-
47	CHL	N1	601	X	-	-	-
47	CHL	N1	605	X	-	-	-
47	CHL	N1	606	X	-	-	-
47	CHL	N1	607	X	-	-	-
47	CHL	N1	608	X	-	-	-
47	CHL	N1	609	X	-	-	-
47	CHL	R	606	X	-	-	-
47	CHL	R	607	X	-	-	-
47	CHL	R1	606	X	-	-	-
47	CHL	R1	607	X	-	-	-
47	CHL	S	601	X	-	-	-
47	CHL	S	606	X	-	-	-
47	CHL	S	607	X	-	-	-
47	CHL	S	608	X	-	-	-
47	CHL	S1	601	X	-	-	-
47	CHL	S1	606	X	-	-	-
47	CHL	S1	607	X	-	-	-
47	CHL	S1	608	X	-	-	-
47	CHL	Y	601	X	-	-	-
47	CHL	Y	605	X	-	-	-
47	CHL	Y	606	X	-	-	-
47	CHL	Y	607	X	-	-	-
47	CHL	Y	609	X	-	-	-
47	CHL	Y1	601	X	-	-	-
47	CHL	Y1	605	X	-	-	-
47	CHL	Y1	606	X	-	-	-
47	CHL	Y1	607	X	-	-	-
47	CHL	Y1	609	X	-	-	-
47	CHL	g	601	X	-	-	-
47	CHL	g	605	X	-	-	-
47	CHL	g	606	X	-	-	-
47	CHL	g	607	X	-	-	-
47	CHL	g	608	X	-	-	-
47	CHL	g	609	X	-	-	-
47	CHL	g1	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	CHL	g1	605	X	-	-	-
47	CHL	g1	606	X	-	-	-
47	CHL	g1	607	X	-	-	-
47	CHL	g1	608	X	-	-	-
47	CHL	g1	609	X	-	-	-
47	CHL	n	601	X	-	-	-
47	CHL	n	605	X	-	-	-
47	CHL	n	606	X	-	-	-
47	CHL	n	607	X	-	-	-
47	CHL	n	608	X	-	-	-
47	CHL	n	609	X	-	-	-
47	CHL	n1	601	X	-	-	-
47	CHL	n1	605	X	-	-	-
47	CHL	n1	606	X	-	-	-
47	CHL	n1	607	X	-	-	-
47	CHL	n1	608	X	-	-	-
47	CHL	n1	609	X	-	-	-
47	CHL	r	606	X	-	-	-
47	CHL	r	607	X	-	-	-
47	CHL	r1	606	X	-	-	-
47	CHL	r1	607	X	-	-	-
47	CHL	s	601	X	-	-	-
47	CHL	s	606	X	-	-	-
47	CHL	s	607	X	-	-	-
47	CHL	s	608	X	-	-	-
47	CHL	s1	601	X	-	-	-
47	CHL	s1	606	X	-	-	-
47	CHL	s1	607	X	-	-	-
47	CHL	s1	608	X	-	-	-
47	CHL	y	601	X	-	-	-
47	CHL	y	605	X	-	-	-
47	CHL	y	606	X	-	-	-
47	CHL	y	607	X	-	-	-
47	CHL	y	609	X	-	-	-
47	CHL	y1	601	X	-	-	-
47	CHL	y1	605	X	-	-	-
47	CHL	y1	606	X	-	-	-
47	CHL	y1	607	X	-	-	-
47	CHL	y1	609	X	-	-	-
48	LUT	G	621	X	-	-	-
48	LUT	R1	620	X	-	-	-
48	LUT	S	620	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	LUT	Y	621	X	-	-	-
48	LUT	g1	621	X	-	-	-
48	LUT	n	621	X	-	-	-
48	LUT	s	620	X	-	-	-
49	XAT	G	622	X	-	-	-
49	XAT	G1	622	X	-	-	-
49	XAT	N	622	X	-	-	-
49	XAT	N1	622	X	-	-	-
49	XAT	R	621	X	-	-	-
49	XAT	Y	622	X	-	-	-
49	XAT	Y1	622	X	-	-	-
49	XAT	g	622	X	-	-	-
49	XAT	g1	622	X	-	-	-
49	XAT	n1	622	X	-	-	-
49	XAT	r	622	X	-	-	-
49	XAT	r1	621	X	-	-	-
56	ERG	R1	626	X	-	-	-
56	ERG	r1	626	X	-	-	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 151508 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	A1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	B1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	298	VAL	LEU	variant	UNP D0FY05
B	415	SER	LEU	variant	UNP D0FY05
b	298	VAL	LEU	variant	UNP D0FY05
b	415	SER	LEU	variant	UNP D0FY05
B1	298	VAL	LEU	variant	UNP D0FY05
B1	415	SER	LEU	variant	UNP D0FY05
b1	298	VAL	LEU	variant	UNP D0FY05
b1	415	SER	LEU	variant	UNP D0FY05

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		
3	V1	32	Total	C	N	O	0	0
			227	152	37	38		
3	v1	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	C1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	D1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	319	ILE	LEU	variant	UNP D0FXW8
d	319	ILE	LEU	variant	UNP D0FXW8
D1	319	ILE	LEU	variant	UNP D0FXW8
d1	319	ILE	LEU	variant	UNP D0FXW8

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		
6	e	76	Total	C	N	O	0	0
			621	404	102	115		
6	E1	76	Total	C	N	O	0	0
			621	404	102	115		
6	e1	76	Total	C	N	O	0	0
			621	404	102	115		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	F1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	H1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	85	ALA	SER	variant	UNP D0FY02
h	85	ALA	SER	variant	UNP D0FY02
H1	85	ALA	SER	variant	UNP D0FY02
h1	85	ALA	SER	variant	UNP D0FY02

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	I1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	36	Total	C	N	O		0	0
			266	183	40	43			
10	j	36	Total	C	N	O		0	0
			266	183	40	43			
10	J1	36	Total	C	N	O		0	0
			266	183	40	43			
10	j1	36	Total	C	N	O		0	0
			266	183	40	43			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	7	ILE	THR	variant	UNP D0FXW2
J	28	ALA	GLY	variant	UNP D0FXW2
J	42	LEU	GLN	variant	UNP D0FXW2
j	7	ILE	THR	variant	UNP D0FXW2
j	28	ALA	GLY	variant	UNP D0FXW2
j	42	LEU	GLN	variant	UNP D0FXW2
J1	7	ILE	THR	variant	UNP D0FXW2
J1	28	ALA	GLY	variant	UNP D0FXW2
J1	42	LEU	GLN	variant	UNP D0FXW2
j1	7	ILE	THR	variant	UNP D0FXW2
j1	28	ALA	GLY	variant	UNP D0FXW2
j1	42	LEU	GLN	variant	UNP D0FXW2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O		0	0
			297	207	43	47			

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Mol	Chain	Residues	Atoms				AltConf	Trace
11	k	37	Total	C	N	O	0	0
			297	207	43	47		
11	K1	37	Total	C	N	O	0	0
			297	207	43	47		
11	k1	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	L1	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	32	Total	C	N	O	0	0
			243	164	34	45		
13	m	32	Total	C	N	O	0	0
			243	164	34	45		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	9	THR	ILE	variant	UNP D0FXZ3
m	9	THR	ILE	variant	UNP D0FXZ3

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	O1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	P1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	T1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	W1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	30	Total	C	N	O	0	0
			201	132	32	37		
18	x	30	Total	C	N	O	0	0
			201	132	32	37		
18	X1	30	Total	C	N	O	0	0
			201	132	32	37		

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Mol	Chain	Residues	Atoms				AltConf	Trace
18	x1	30	Total	C	N	O	0	0
			201	132	32	37		

- Molecule 19 is a protein called PsbZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	Z1	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z1	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	n	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	N1	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	n1	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		

- Molecule 21 is a protein called LHCII M2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	G1	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g1	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		
22	r	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	242	Total	C	N	O	S	0	0
			1849	1195	297	354	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	S1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	Y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	U1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 26 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	M1	31	Total	C	N	O	0	0
			234	159	33	42		
26	m1	31	Total	C	N	O	0	0
			234	159	33	42		

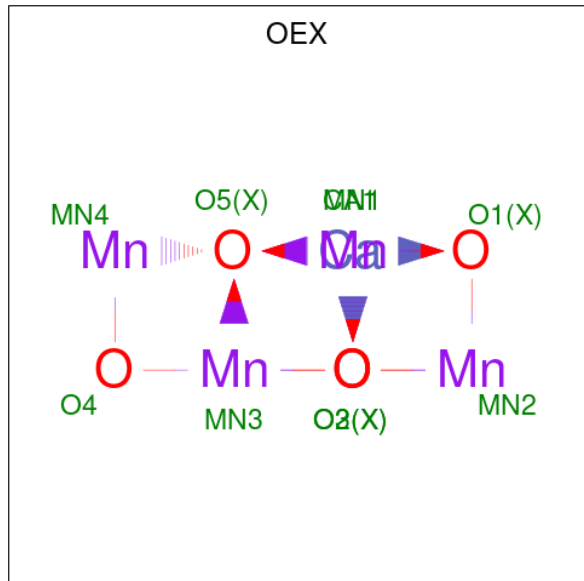
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M1	9	THR	ILE	variant	UNP D0FXZ3
m1	9	THR	ILE	variant	UNP D0FXZ3

- Molecule 27 is a protein called CP29.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	R1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
27	r1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

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Mol	Chain	Residues	Atoms				AltConf
28	A1	1	Total	Ca	Mn	O	0
			10	1	4	5	
28	a1	1	Total	Ca	Mn	O	0
			10	1	4	5	

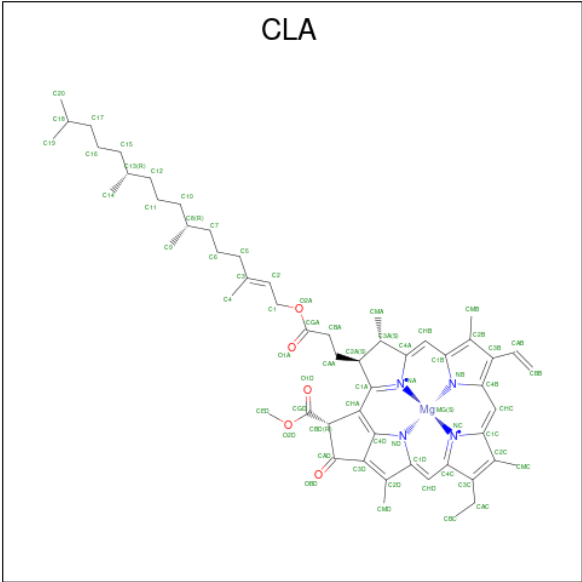
- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	Fe	0
			1	1	
29	a	1	Total	Fe	0
			1	1	
29	A1	1	Total	Fe	0
			1	1	
29	a1	1	Total	Fe	0
			1	1	

- Molecule 30 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
30	A	2	Total	Cl	0
			2	2	
30	a	2	Total	Cl	0
			2	2	
30	A1	2	Total	Cl	0
			2	2	
30	a1	2	Total	Cl	0
			2	2	

- 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
			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	

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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	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 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	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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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	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 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	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	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	A1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	D1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	D1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	N1	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G1	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	S1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	S1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	S1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	S1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	S1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S1	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	S1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	a1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	n1	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g1	1	Total 43	C 35	Mg 1	N 4	O 3	0

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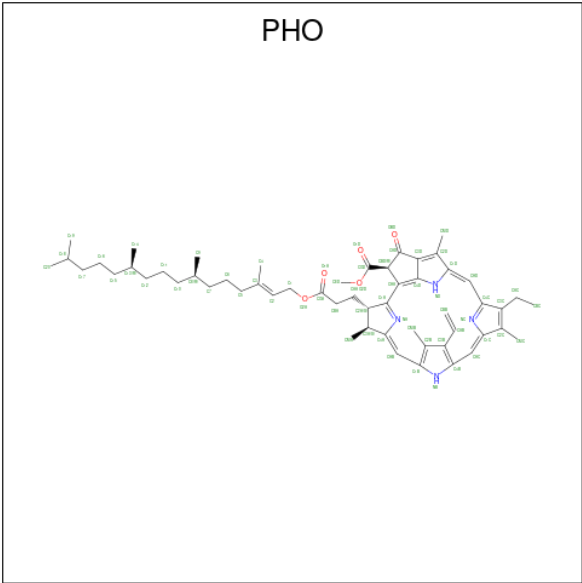
Mol	Chain	Residues	Atoms					AltConf
31	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	s1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	s1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	s1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	s1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s1	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	s1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	y1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



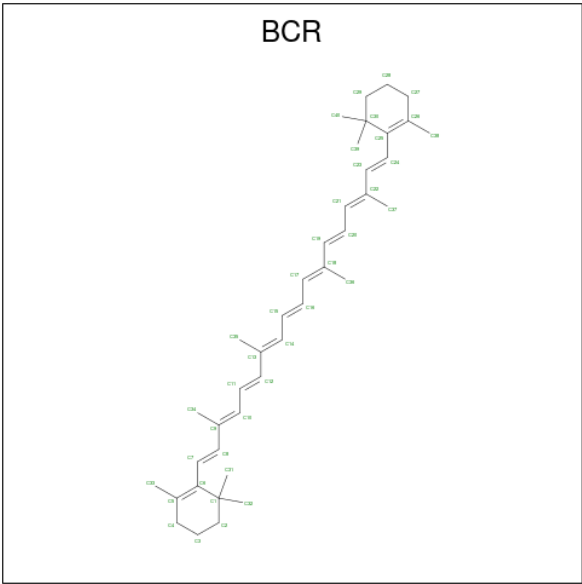
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	N	O	0
			64	55	4	5	
32	A	1	Total	C	N	O	0
			64	55	4	5	
32	a	1	Total	C	N	O	0
			64	55	4	5	

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Mol	Chain	Residues	Atoms				AltConf
32	a	1	Total	C	N	O	0
			64	55	4	5	
32	A1	1	Total	C	N	O	0
			64	55	4	5	
32	A1	1	Total	C	N	O	0
			64	55	4	5	
32	a1	1	Total	C	N	O	0
			64	55	4	5	
32	a1	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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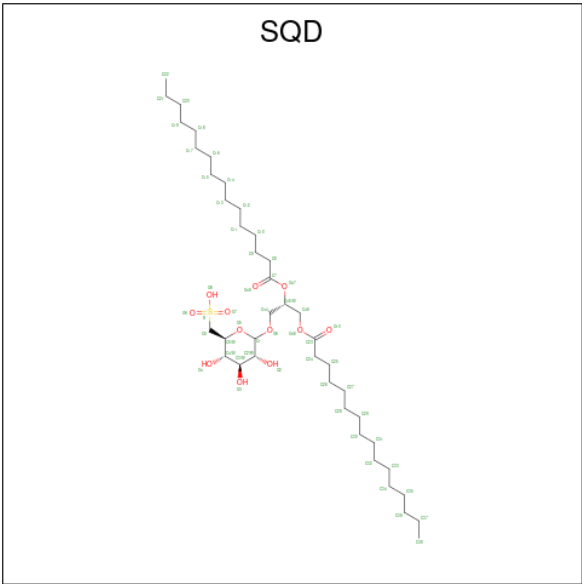
Mol	Chain	Residues	Atoms	AltConf
33	C	1	Total C 40 40	0
33	D	1	Total C 40 40	0
33	a	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	d	1	Total C 40 40	0
33	A1	1	Total C 40 40	0
33	B1	1	Total C 40 40	0
33	B1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	D1	1	Total C 40 40	0
33	a1	1	Total C 40 40	0
33	b1	1	Total C 40 40	0
33	b1	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
33	c1	1	Total	C	0
			40	40	
33	c1	1	Total	C	0
			40	40	
33	c1	1	Total	C	0
			40	40	
33	c1	1	Total	C	0
			40	40	
33	d1	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).



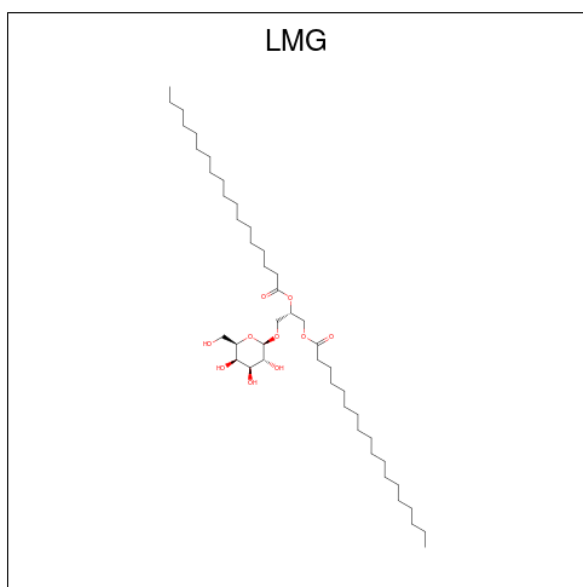
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	S	0
			51	38	12	1	
34	B	1	Total	C	O	S	0
			54	41	12	1	
34	C	1	Total	C	O	S	0
			54	41	12	1	
34	a	1	Total	C	O	S	0
			51	38	12	1	
34	b	1	Total	C	O	S	0
			54	41	12	1	
34	c	1	Total	C	O	S	0
			54	41	12	1	

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Mol	Chain	Residues	Atoms				AltConf
34	A1	1	Total	C	O	S	0
			51	38	12	1	
34	B1	1	Total	C	O	S	0
			42	29	12	1	
34	B1	1	Total	C	O	S	0
			54	41	12	1	
34	C1	1	Total	C	O	S	0
			54	41	12	1	
34	M1	1	Total	C	O	S	0
			42	29	12	1	
34	a1	1	Total	C	O	S	0
			51	38	12	1	
34	b1	1	Total	C	O	S	0
			42	29	12	1	
34	b1	1	Total	C	O	S	0
			54	41	12	1	
34	c1	1	Total	C	O	S	0
			54	41	12	1	
34	m1	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			48	38	10	

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Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total 44	C 34	O 10	0
35	C	1	Total 51	C 41	O 10	0
35	D	1	Total 46	C 36	O 10	0
35	H	1	Total 48	C 38	O 10	0
35	J	1	Total 45	C 35	O 10	0
35	a	1	Total 48	C 38	O 10	0
35	b	1	Total 44	C 34	O 10	0
35	c	1	Total 51	C 41	O 10	0
35	d	1	Total 46	C 36	O 10	0
35	h	1	Total 48	C 38	O 10	0
35	j	1	Total 45	C 35	O 10	0
35	A1	1	Total 48	C 38	O 10	0
35	B1	1	Total 44	C 34	O 10	0
35	C1	1	Total 51	C 41	O 10	0
35	C1	1	Total 55	C 45	O 10	0
35	D1	1	Total 46	C 36	O 10	0
35	H1	1	Total 48	C 38	O 10	0
35	W1	1	Total 39	C 29	O 10	0
35	a1	1	Total 48	C 38	O 10	0
35	b1	1	Total 44	C 34	O 10	0
35	c1	1	Total 51	C 41	O 10	0

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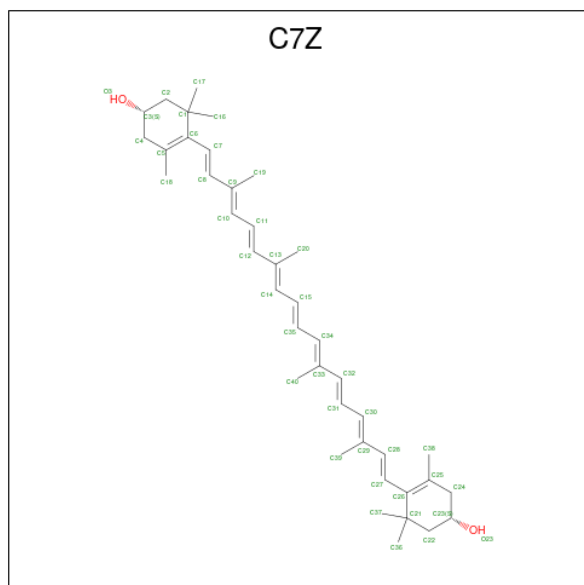
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Mol	Chain	Residues	Atoms			AltConf
35	c1	1	Total	C	O	0
			55	45	10	
35	d1	1	Total	C	O	0
			46	36	10	
35	h1	1	Total	C	O	0
			48	38	10	
35	w1	1	Total	C	O	0
			39	29	10	

- Molecule 36 is SODIUM ION (CCD ID: NA) (formula: Na).

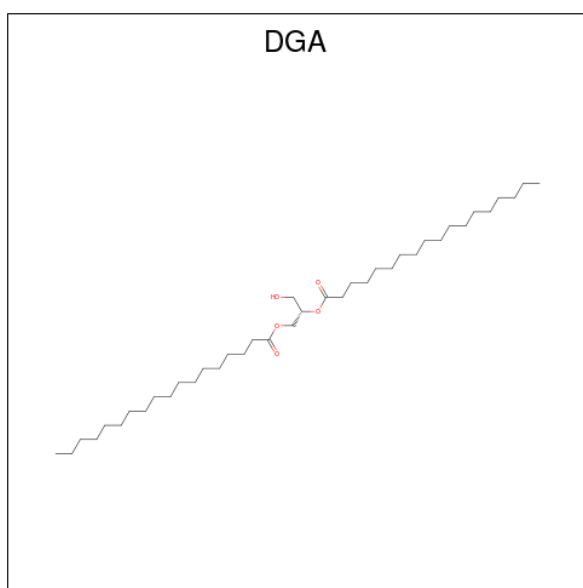
Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Na	0
			1	1	
36	a	1	Total	Na	0
			1	1	
36	A1	1	Total	Na	0
			1	1	
36	a1	1	Total	Na	0
			1	1	

- Molecule 37 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			42	40	2	
37	b	1	Total	C	O	0
			42	40	2	
37	B1	1	Total	C	O	0
			42	40	2	
37	b1	1	Total	C	O	0
			42	40	2	

- Molecule 38 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



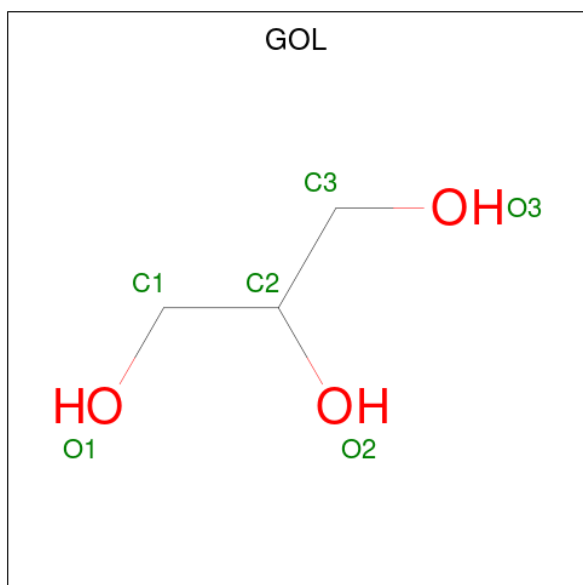
Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			44	39	5	
38	C	1	Total	C	O	0
			44	39	5	
38	b	1	Total	C	O	0
			44	39	5	
38	c	1	Total	C	O	0
			44	39	5	
38	B1	1	Total	C	O	0
			44	39	5	
38	C1	1	Total	C	O	0
			44	39	5	
38	J1	1	Total	C	O	0
			29	24	5	
38	b1	1	Total	C	O	0
			44	39	5	

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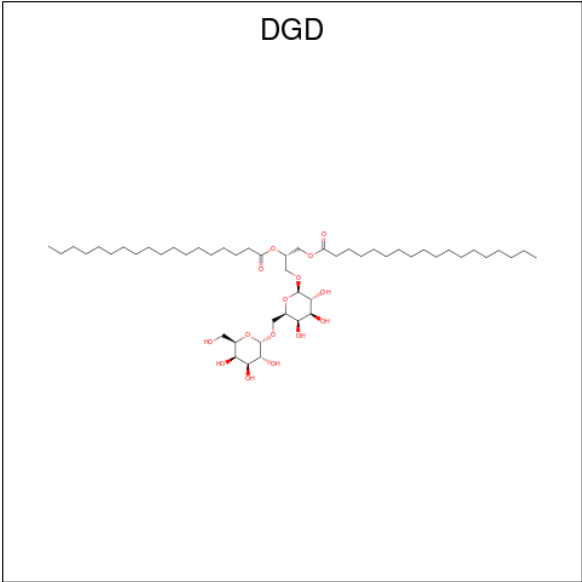
Mol	Chain	Residues	Atoms			AltConf
38	c1	1	Total	C	O	0
			44	39	5	
38	j1	1	Total	C	O	0
			29	24	5	

- Molecule 39 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			6	3	3	
39	b	1	Total	C	O	0
			6	3	3	
39	b	1	Total	C	O	0
			6	3	3	
39	y	1	Total	C	O	0
			6	3	3	
39	I1	1	Total	C	O	0
			6	3	3	

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



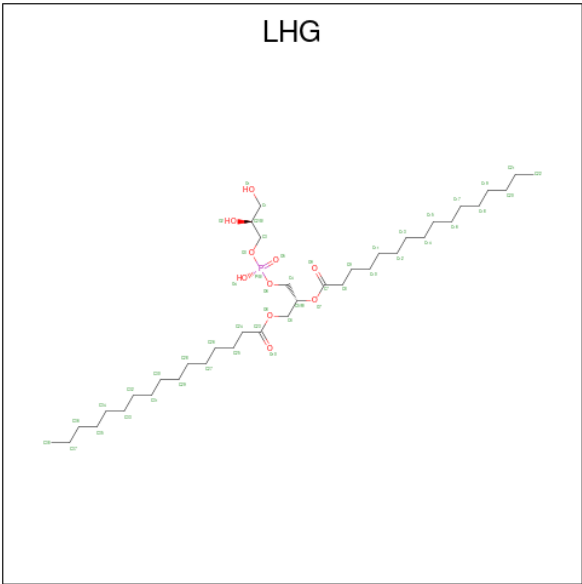
Mol	Chain	Residues	Atoms			AltConf
40	C	1	Total	C	O	0
			55	40	15	
40	C	1	Total	C	O	0
			62	47	15	
40	C	1	Total	C	O	0
			59	44	15	
40	C	1	Total	C	O	0
			66	51	15	
40	c	1	Total	C	O	0
			55	40	15	
40	c	1	Total	C	O	0
			62	47	15	
40	c	1	Total	C	O	0
			59	44	15	
40	c	1	Total	C	O	0
			66	51	15	
40	B1	1	Total	C	O	0
			43	28	15	
40	C1	1	Total	C	O	0
			55	40	15	
40	C1	1	Total	C	O	0
			62	47	15	
40	C1	1	Total	C	O	0
			59	44	15	
40	b1	1	Total	C	O	0
			43	28	15	
40	c1	1	Total	C	O	0
			55	40	15	

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Mol	Chain	Residues	Atoms			AltConf
40	c1	1	Total	C	O	0
			62	47	15	
40	c1	1	Total	C	O	0
			59	44	15	

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
41	C	1	Total	C	O	P	0
			47	36	10	1	
41	D	1	Total	C	O	P	0
			44	33	10	1	
41	D	1	Total	C	O	P	0
			49	38	10	1	
41	D	1	Total	C	O	P	0
			39	28	10	1	
41	L	1	Total	C	O	P	0
			49	38	10	1	
41	N	1	Total	C	O	P	0
			49	38	10	1	
41	G	1	Total	C	O	P	0
			49	38	10	1	
41	S	1	Total	C	O	P	0
			45	34	10	1	
41	Y	1	Total	C	O	P	0
			49	38	10	1	

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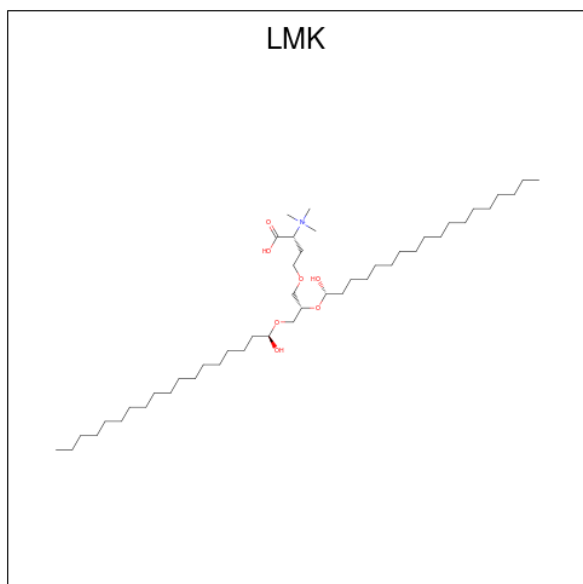
Mol	Chain	Residues	Atoms				AltConf
41	c	1	Total 47	C 36	O 10	P 1	0
41	d	1	Total 44	C 33	O 10	P 1	0
41	d	1	Total 49	C 38	O 10	P 1	0
41	d	1	Total 39	C 28	O 10	P 1	0
41	l	1	Total 49	C 38	O 10	P 1	0
41	n	1	Total 49	C 38	O 10	P 1	0
41	g	1	Total 49	C 38	O 10	P 1	0
41	s	1	Total 45	C 34	O 10	P 1	0
41	y	1	Total 49	C 38	O 10	P 1	0
41	C1	1	Total 47	C 36	O 10	P 1	0
41	D1	1	Total 44	C 33	O 10	P 1	0
41	D1	1	Total 49	C 38	O 10	P 1	0
41	D1	1	Total 39	C 28	O 10	P 1	0
41	L1	1	Total 49	C 38	O 10	P 1	0
41	N1	1	Total 49	C 38	O 10	P 1	0
41	G1	1	Total 49	C 38	O 10	P 1	0
41	S1	1	Total 45	C 34	O 10	P 1	0
41	Y1	1	Total 49	C 38	O 10	P 1	0
41	c1	1	Total 47	C 36	O 10	P 1	0
41	d1	1	Total 44	C 33	O 10	P 1	0
41	d1	1	Total 49	C 38	O 10	P 1	0

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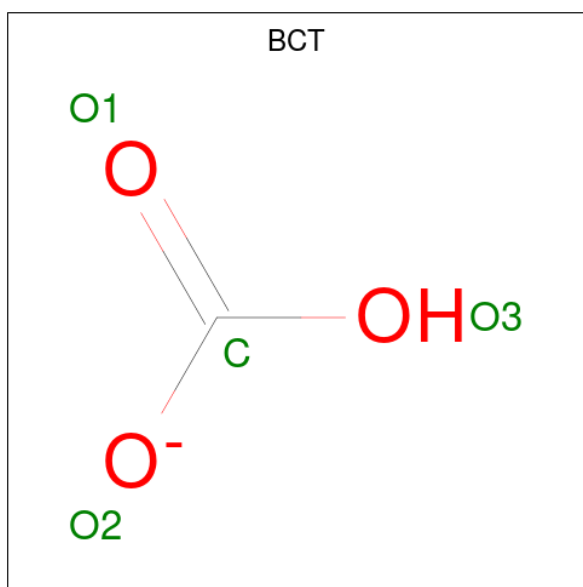
Mol	Chain	Residues	Atoms				AltConf
41	d1	1	Total	C	O	P	0
			39	28	10	1	
41	n1	1	Total	C	O	P	0
			49	38	10	1	
41	g1	1	Total	C	O	P	0
			49	38	10	1	
41	s1	1	Total	C	O	P	0
			45	34	10	1	
41	y1	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 42 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$).



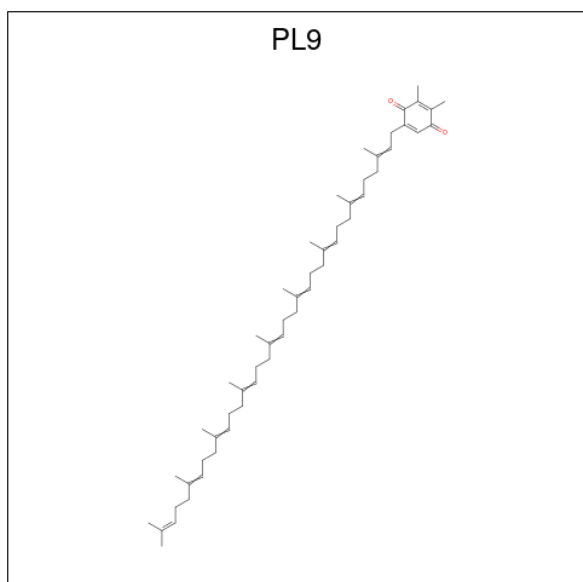
Mol	Chain	Residues	Atoms				AltConf
42	C	1	Total	C	N	O	0
			40	32	1	7	
42	c	1	Total	C	N	O	0
			40	32	1	7	
42	C1	1	Total	C	N	O	0
			40	32	1	7	
42	c1	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 43 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



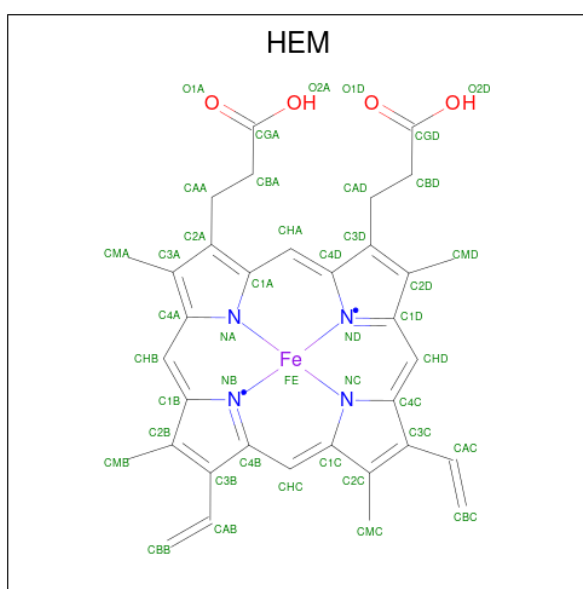
Mol	Chain	Residues	Atoms			AltConf
43	D	1	Total	C	O	0
			4	1	3	
43	d	1	Total	C	O	0
			4	1	3	
43	D1	1	Total	C	O	0
			4	1	3	
43	d1	1	Total	C	O	0
			4	1	3	

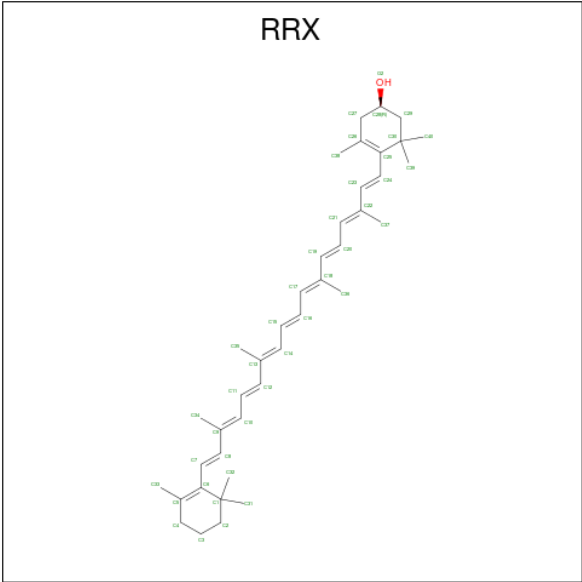
- Molecule 44 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
44	D	1	Total	C	O	0
			55	53	2	
44	d	1	Total	C	O	0
			55	53	2	
44	D1	1	Total	C	O	0
			55	53	2	
44	d1	1	Total	C	O	0
			55	53	2	

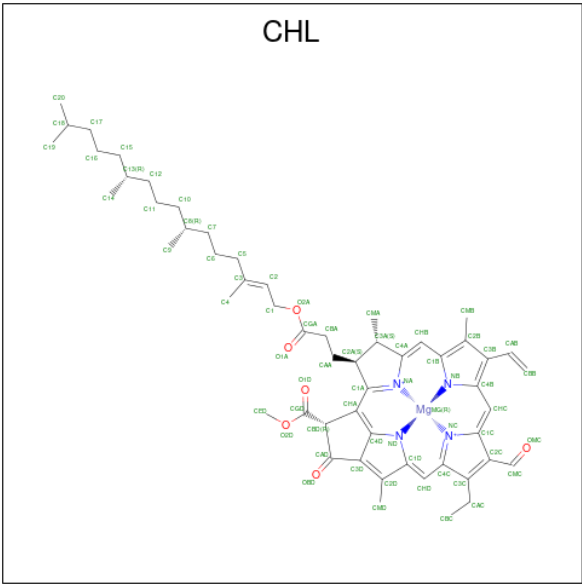
- Molecule 45 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms			AltConf
46	H	1	Total	C	O	0
			41	40	1	
46	h	1	Total	C	O	0
			41	40	1	
46	H1	1	Total	C	O	0
			41	40	1	
46	h1	1	Total	C	O	0
			41	40	1	

- Molecule 47 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
47	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	G	1	Total 48	C 37	Mg 1	N 4	O 6	0
47	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	G	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	R	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
47	S	1	Total 61	C 50	Mg 1	N 4	O 6	0
47	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
47	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
47	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	g	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	r	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	s	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	s	1	Total 43	C 34	Mg 1	N 4	O 4	0
47	s	1	Total 61	C 50	Mg 1	N 4	O 6	0
47	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	y	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
47	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N1	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	G1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	G1	1	Total 48	C 37	Mg 1	N 4	O 6	0
47	G1	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	G1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	G1	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	G1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	R1	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	R1	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	S1	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	S1	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	S1	1	Total 43	C 34	Mg 1	N 4	O 4	0
47	S1	1	Total 61	C 50	Mg 1	N 4	O 6	0

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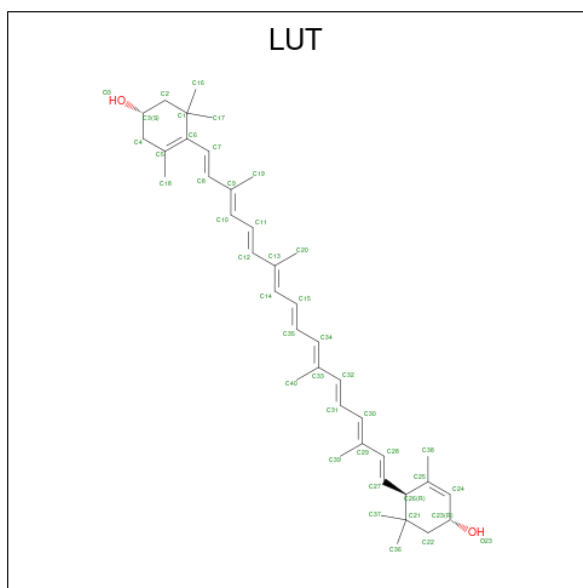
Mol	Chain	Residues	Atoms					AltConf
47	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y1	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n1	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	g1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	g1	1	Total 48	C 37	Mg 1	N 4	O 6	0
47	g1	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	g1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	g1	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	g1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	r1	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	r1	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	s1	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	s1	1	Total 44	C 35	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
47	s1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
47	s1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 48 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			42	40	2	
48	N	1	Total	C	O	0
			42	40	2	
48	G	1	Total	C	O	0
			42	40	2	
48	G	1	Total	C	O	0
			42	40	2	

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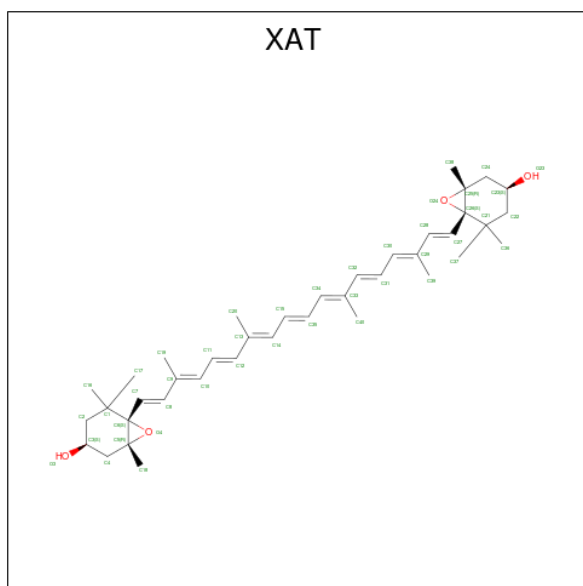
Mol	Chain	Residues	Atoms			AltConf
48	R	1	Total	C	O	0
			42	40	2	
48	S	1	Total	C	O	0
			42	40	2	
48	S	1	Total	C	O	0
			42	40	2	
48	Y	1	Total	C	O	0
			42	40	2	
48	Y	1	Total	C	O	0
			42	40	2	
48	n	1	Total	C	O	0
			42	40	2	
48	n	1	Total	C	O	0
			42	40	2	
48	g	1	Total	C	O	0
			42	40	2	
48	g	1	Total	C	O	0
			42	40	2	
48	r	1	Total	C	O	0
			42	40	2	
48	s	1	Total	C	O	0
			42	40	2	
48	s	1	Total	C	O	0
			42	40	2	
48	y	1	Total	C	O	0
			42	40	2	
48	y	1	Total	C	O	0
			42	40	2	
48	N1	1	Total	C	O	0
			42	40	2	
48	N1	1	Total	C	O	0
			42	40	2	
48	G1	1	Total	C	O	0
			42	40	2	
48	G1	1	Total	C	O	0
			42	40	2	
48	R1	1	Total	C	O	0
			42	40	2	
48	S1	1	Total	C	O	0
			42	40	2	
48	S1	1	Total	C	O	0
			42	40	2	

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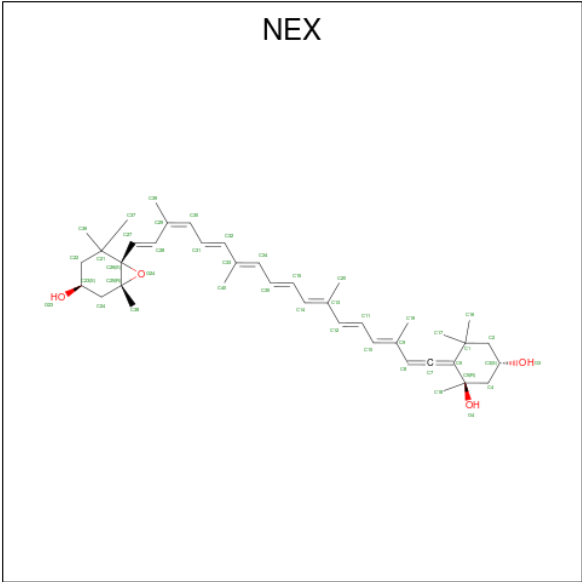
Mol	Chain	Residues	Atoms			AltConf
48	Y1	1	Total	C	O	0
			42	40	2	
48	Y1	1	Total	C	O	0
			42	40	2	
48	n1	1	Total	C	O	0
			42	40	2	
48	n1	1	Total	C	O	0
			42	40	2	
48	g1	1	Total	C	O	0
			42	40	2	
48	g1	1	Total	C	O	0
			42	40	2	
48	r1	1	Total	C	O	0
			42	40	2	
48	s1	1	Total	C	O	0
			42	40	2	
48	s1	1	Total	C	O	0
			42	40	2	
48	y1	1	Total	C	O	0
			42	40	2	
48	y1	1	Total	C	O	0
			42	40	2	

- Molecule 49 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	R	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	
49	n	1	Total	C	O	0
			44	40	4	
49	g	1	Total	C	O	0
			44	40	4	
49	r	1	Total	C	O	0
			44	40	4	
49	y	1	Total	C	O	0
			44	40	4	
49	N1	1	Total	C	O	0
			44	40	4	
49	G1	1	Total	C	O	0
			44	40	4	
49	R1	1	Total	C	O	0
			44	40	4	
49	Y1	1	Total	C	O	0
			44	40	4	
49	n1	1	Total	C	O	0
			44	40	4	
49	g1	1	Total	C	O	0
			44	40	4	
49	r1	1	Total	C	O	0
			44	40	4	
49	y1	1	Total	C	O	0
			44	40	4	

- Molecule 50 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



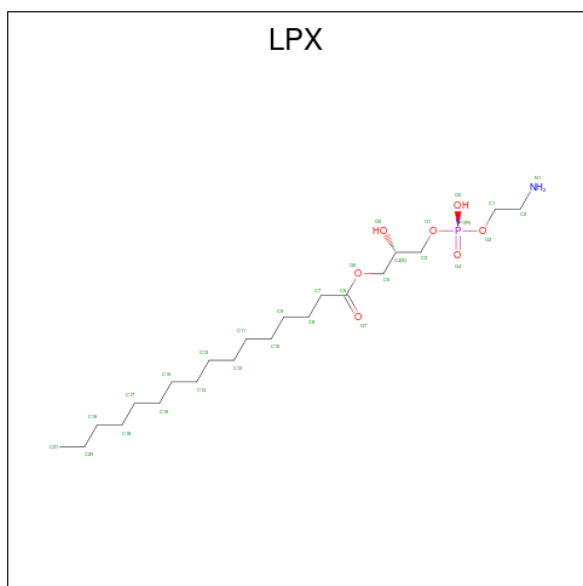
Mol	Chain	Residues	Atoms			AltConf
50	N	1	Total	C	O	0
			44	40	4	
50	G	1	Total	C	O	0
			44	40	4	
50	R	1	Total	C	O	0
			44	40	4	
50	S	1	Total	C	O	0
			44	40	4	
50	Y	1	Total	C	O	0
			44	40	4	
50	n	1	Total	C	O	0
			44	40	4	
50	g	1	Total	C	O	0
			44	40	4	
50	r	1	Total	C	O	0
			44	40	4	
50	s	1	Total	C	O	0
			44	40	4	
50	y	1	Total	C	O	0
			44	40	4	
50	N1	1	Total	C	O	0
			44	40	4	
50	G1	1	Total	C	O	0
			44	40	4	
50	R1	1	Total	C	O	0
			44	40	4	
50	S1	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
50	Y1	1	Total	C	O	0
			44	40	4	
50	n1	1	Total	C	O	0
			44	40	4	
50	g1	1	Total	C	O	0
			44	40	4	
50	r1	1	Total	C	O	0
			44	40	4	
50	s1	1	Total	C	O	0
			44	40	4	
50	y1	1	Total	C	O	0
			44	40	4	

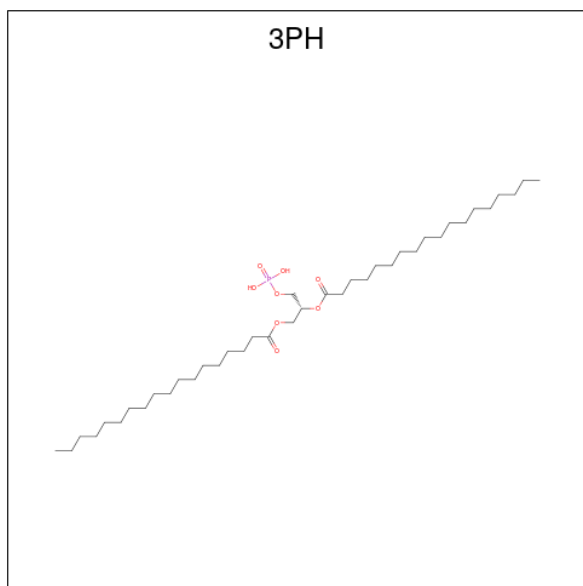
- Molecule 51 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					AltConf
51	S	1	Total	C	N	O	P	0
			30	21	1	7	1	
51	s	1	Total	C	N	O	P	0
			30	21	1	7	1	
51	S1	1	Total	C	N	O	P	0
			30	21	1	7	1	
51	s1	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 52 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula:

$C_{39}H_{77}O_8P$).

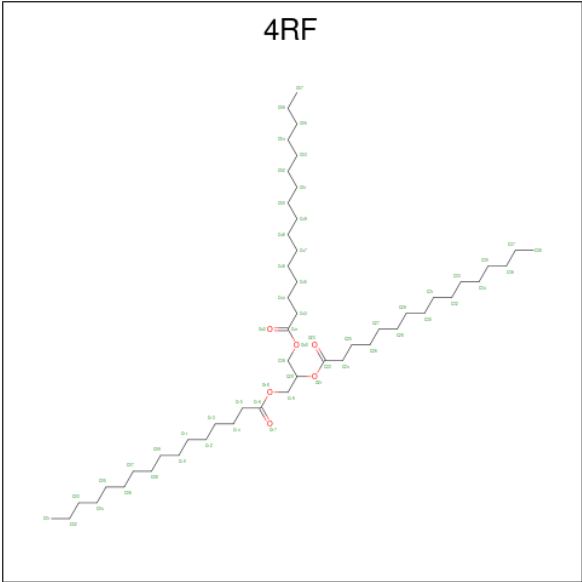


Mol	Chain	Residues	Atoms				AltConf
52	S	1	Total	C	O	P	0
			48	39	8	1	
52	i	1	Total	C	O	P	0
			48	39	8	1	
52	s	1	Total	C	O	P	0
			48	39	8	1	
52	B1	1	Total	C	O	P	0
			48	39	8	1	
52	T1	1	Total	C	O	P	0
			48	39	8	1	
52	S1	1	Total	C	O	P	0
			48	39	8	1	
52	b1	1	Total	C	O	P	0
			48	39	8	1	
52	t1	1	Total	C	O	P	0
			48	39	8	1	
52	s1	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 53 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).

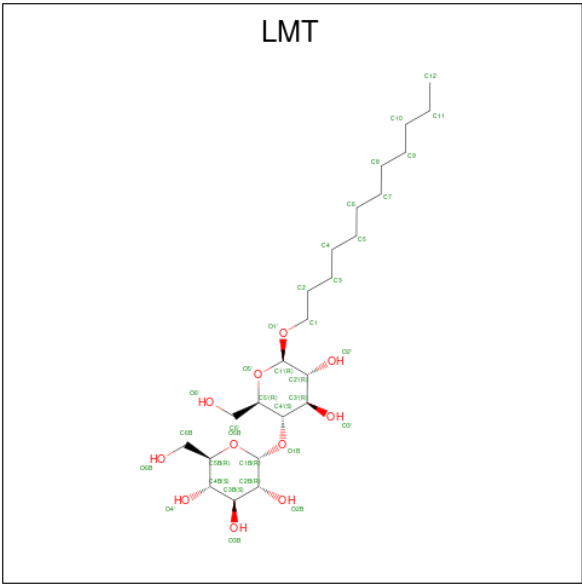


- Molecule 54 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$).



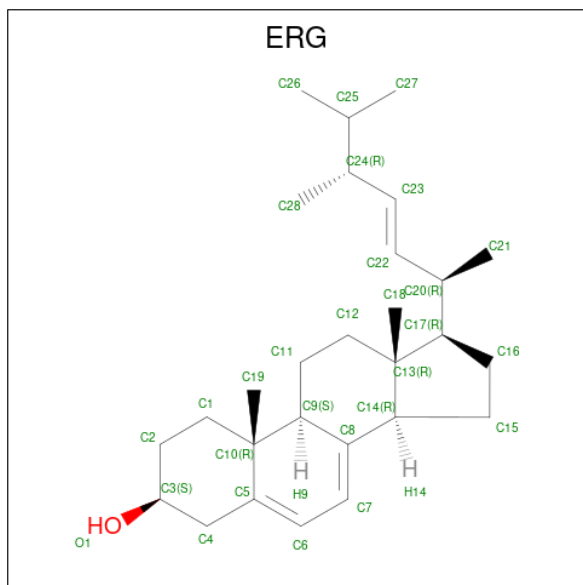
Mol	Chain	Residues	Atoms			AltConf
54	I1	1	Total	C	O	0
			57	51	6	
54	K1	1	Total	C	O	0
			57	51	6	
54	i1	1	Total	C	O	0
			57	51	6	
54	k1	1	Total	C	O	0
			57	51	6	

- Molecule 55 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



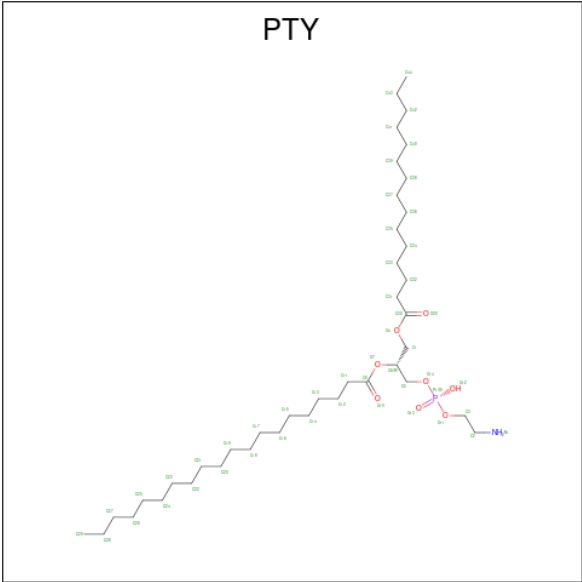
Mol	Chain	Residues	Atoms			AltConf
55	R1	1	Total	C	O	0
			35	24	11	
55	r1	1	Total	C	O	0
			35	24	11	

- Molecule 56 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$).



Mol	Chain	Residues	Atoms			AltConf
56	R1	1	Total	C	O	0
			29	28	1	
56	r1	1	Total	C	O	0
			29	28	1	

- Molecule 57 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
57	Y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
57	Y1	1	Total	C	N	O	P	0
			19	9	1	8	1	
57	y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
57	y1	1	Total	C	N	O	P	0
			19	9	1	8	1	

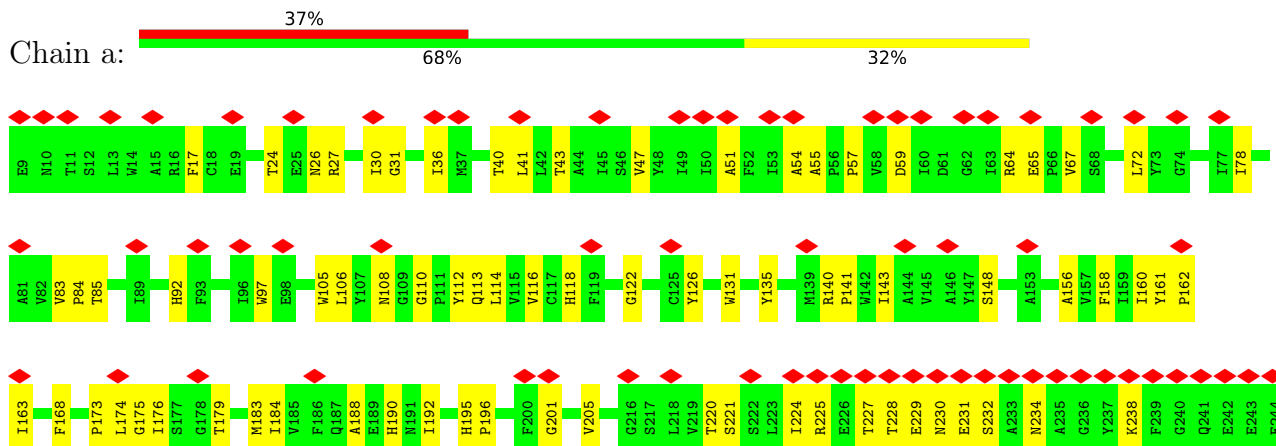
3 Residue-property plots

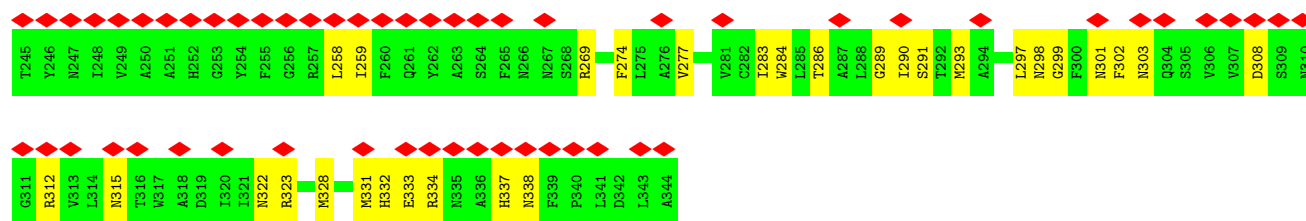
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Photosystem II protein D1

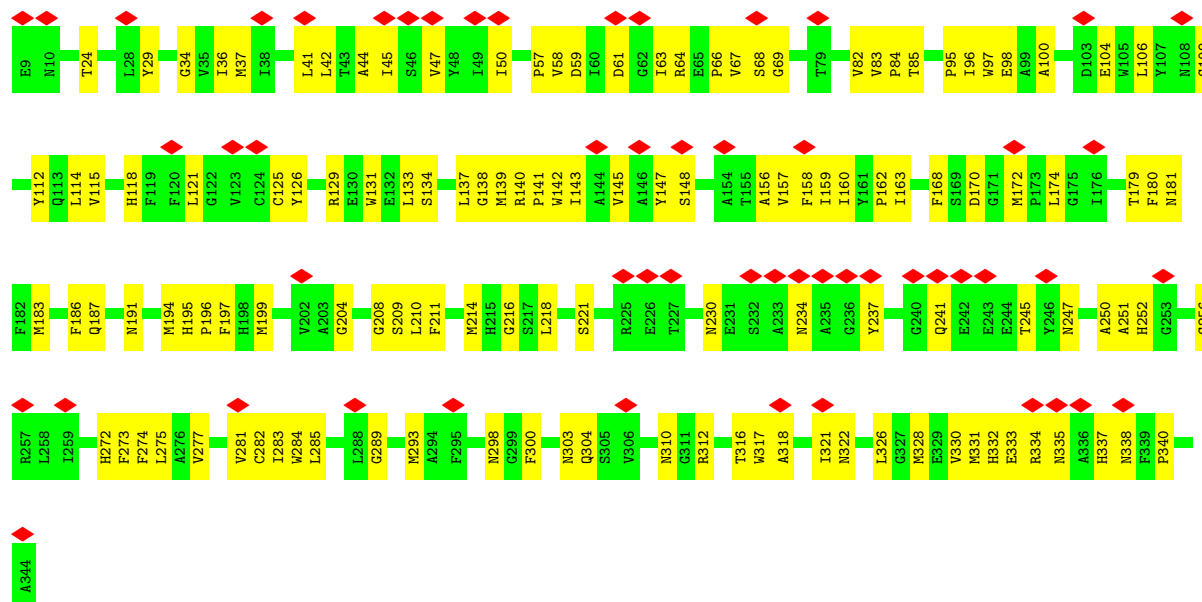


• Molecule 1: Photosystem II protein D1

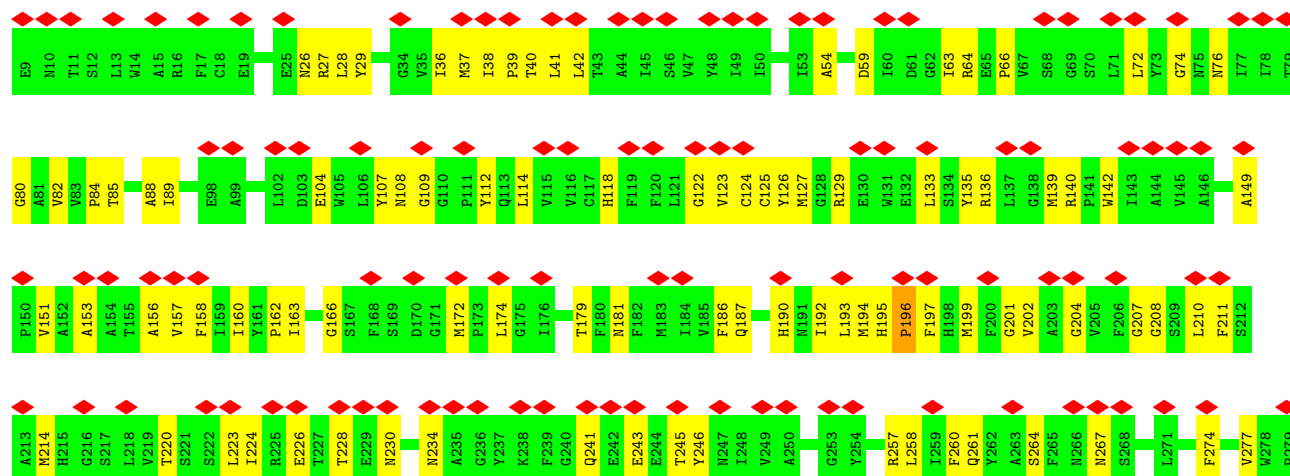
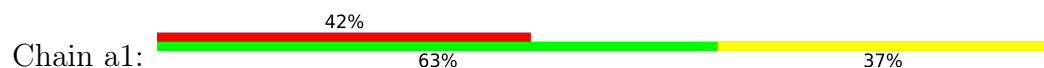


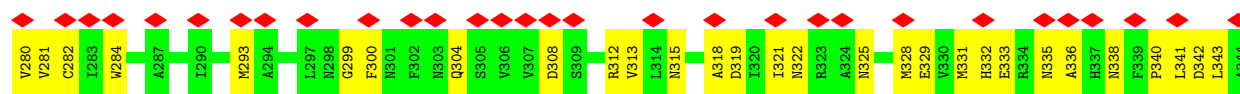


• Molecule 1: Photosystem II protein D1

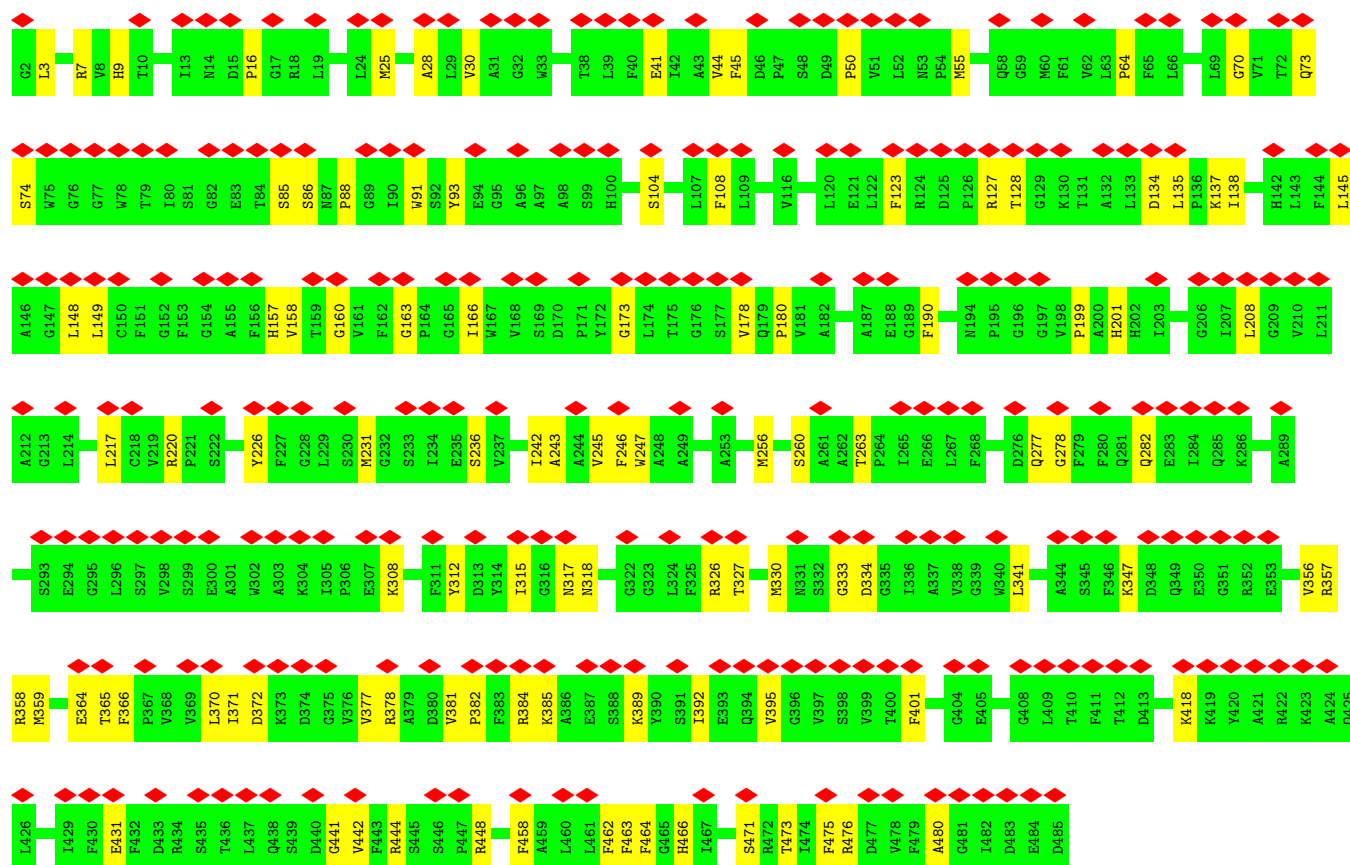
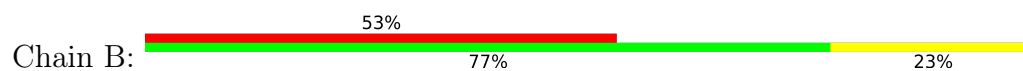


• Molecule 1: Photosystem II protein D1

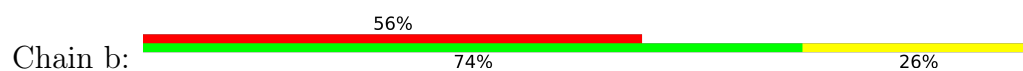


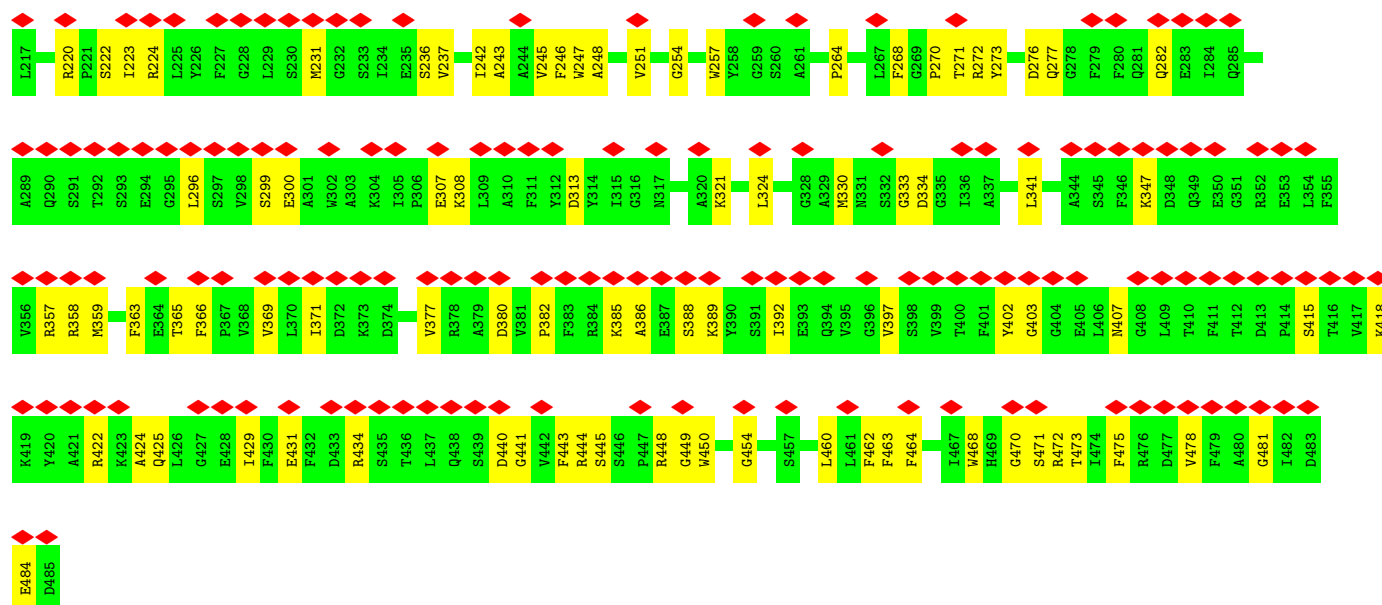


• Molecule 2: Photosystem II CP47 reaction center protein

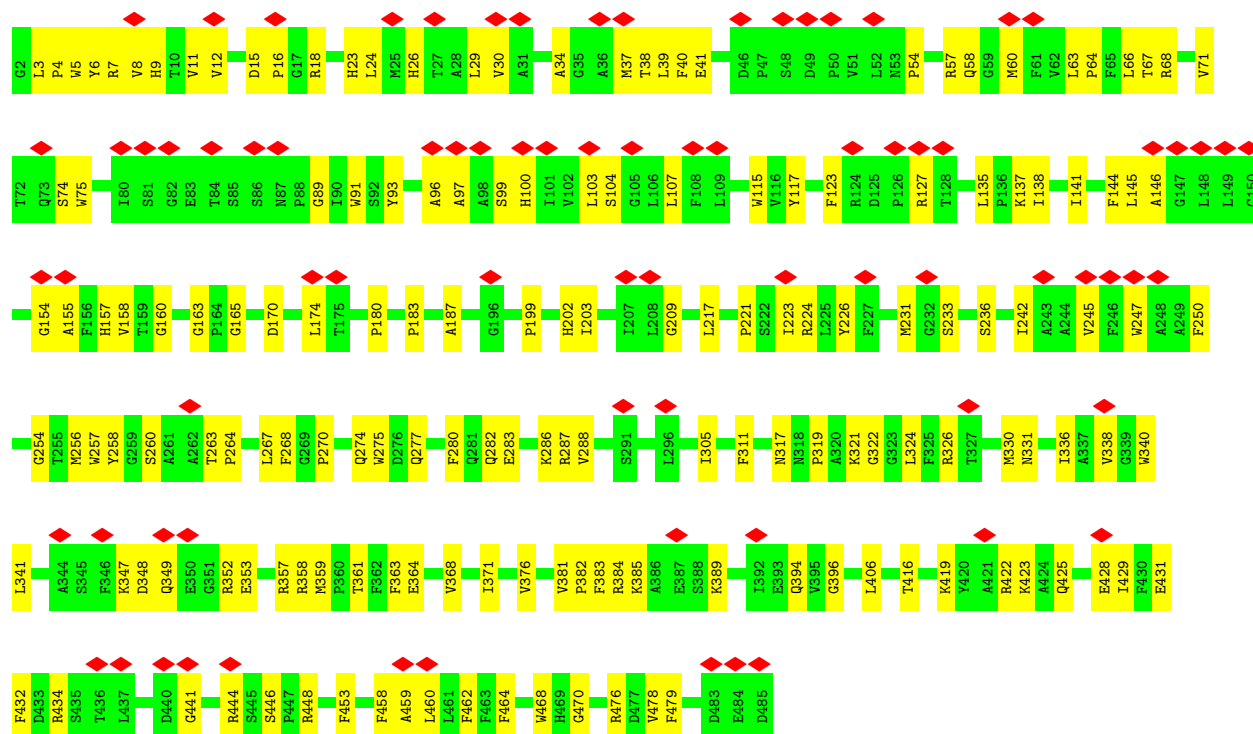


• Molecule 2: Photosystem II CP47 reaction center protein



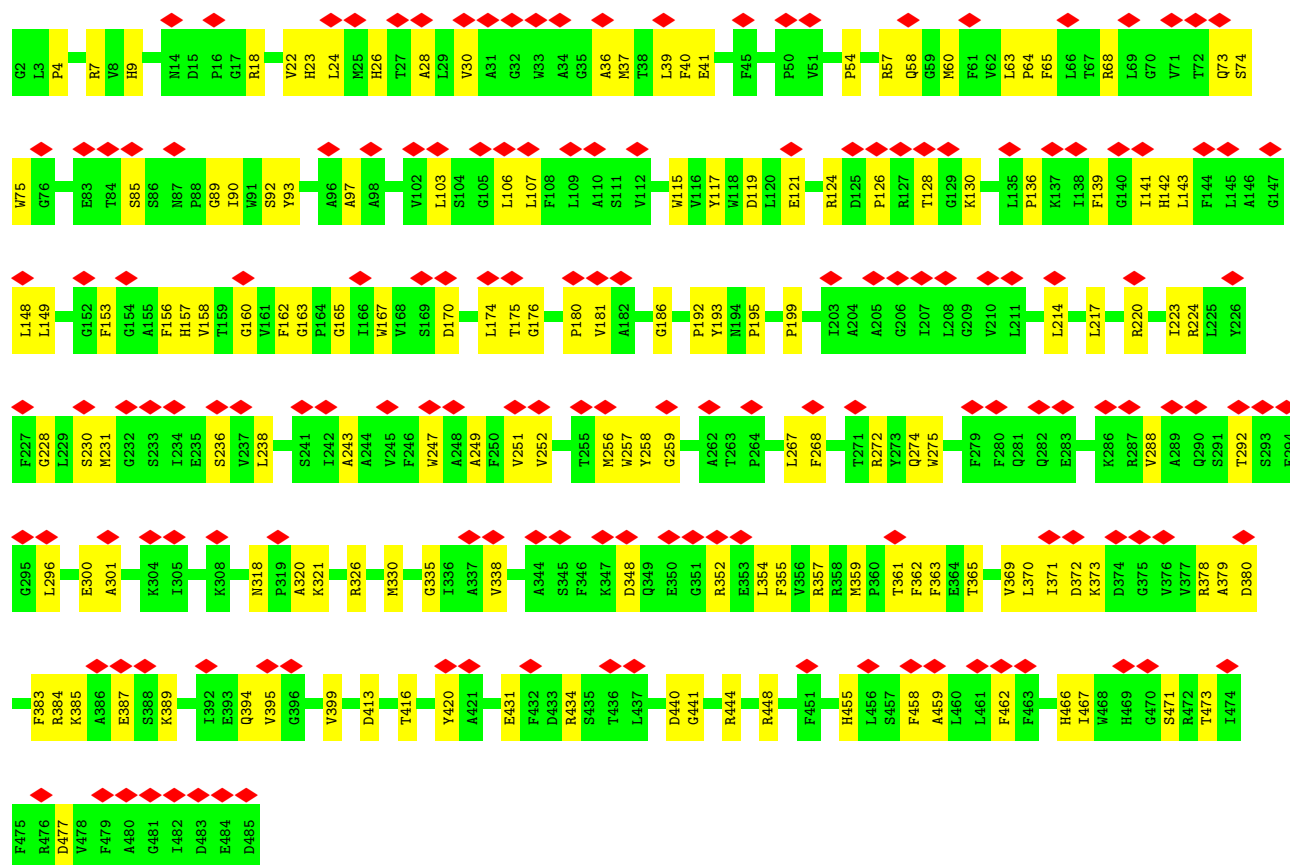


• Molecule 2: Photosystem II CP47 reaction center protein

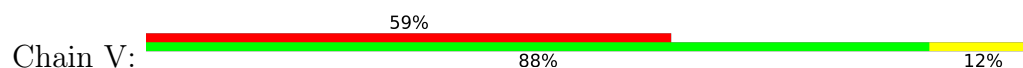


• Molecule 2: Photosystem II CP47 reaction center protein

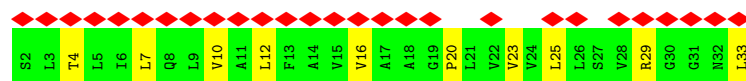
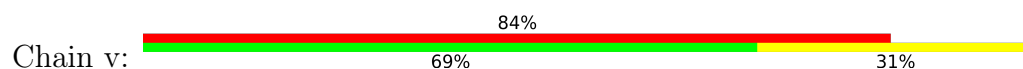




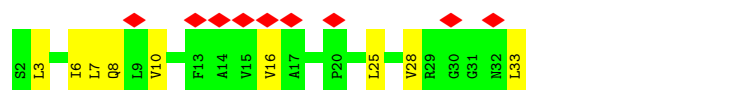
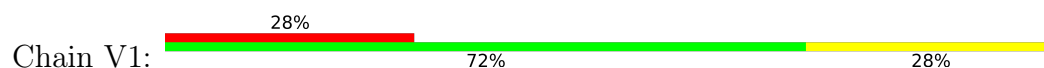
• Molecule 3: Photosystem II reaction center protein Ycf12



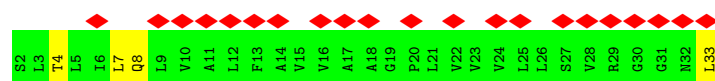
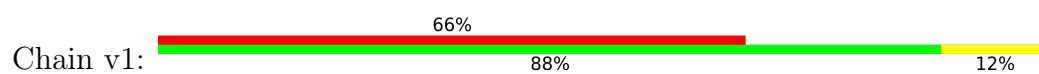
• Molecule 3: Photosystem II reaction center protein Ycf12



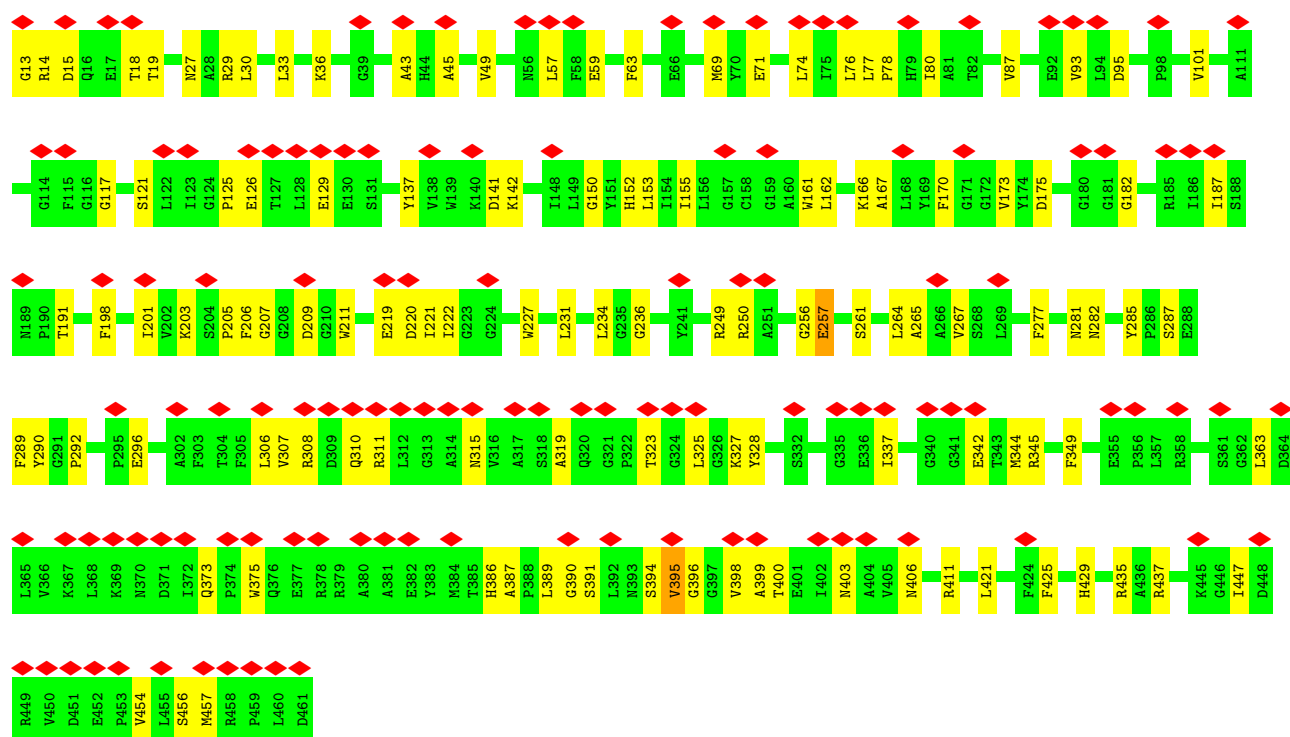
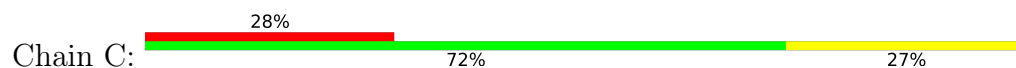
• Molecule 3: Photosystem II reaction center protein Ycf12



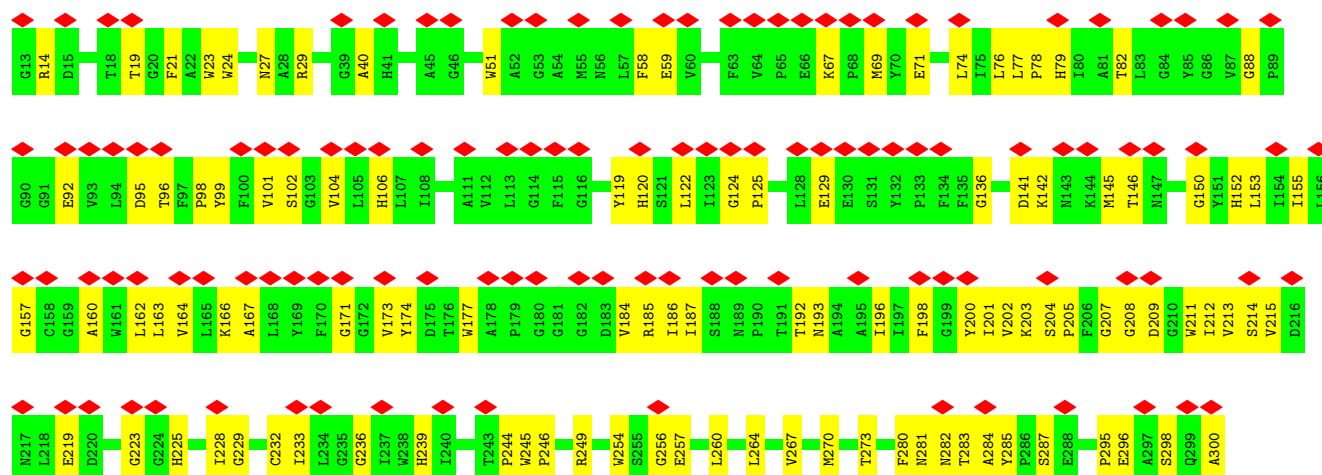
• Molecule 3: Photosystem II reaction center protein Ycf12

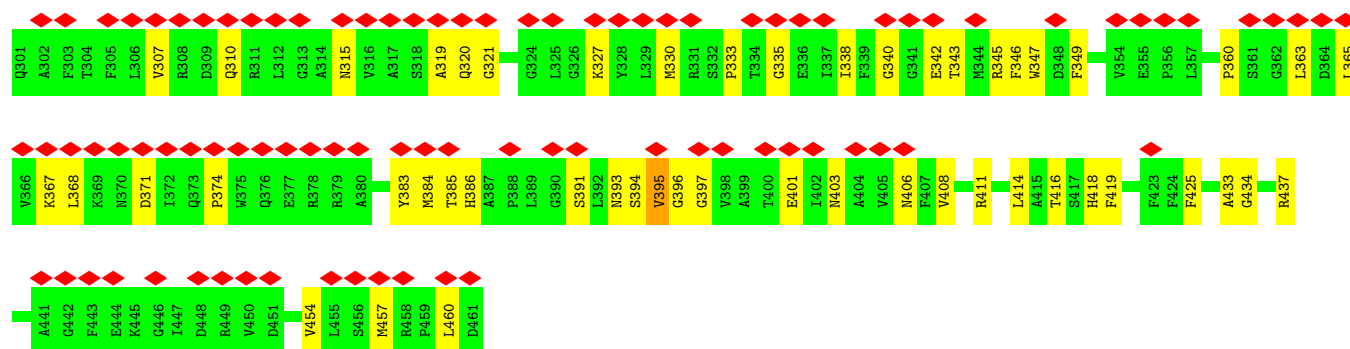


• Molecule 4: Photosystem II CP43 reaction center protein

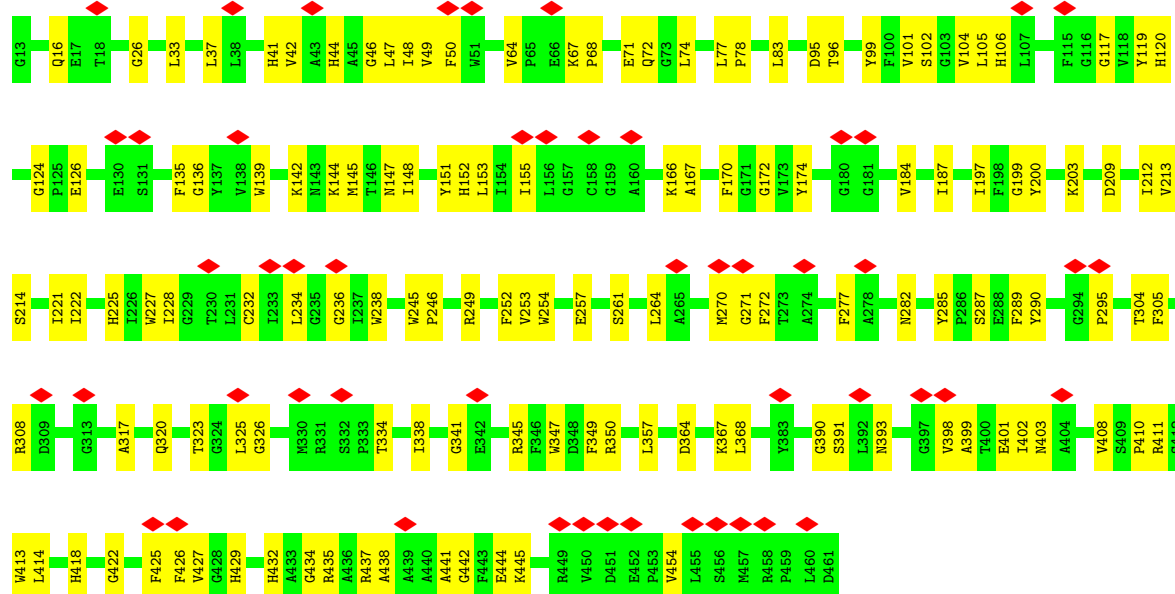


• Molecule 4: Photosystem II CP43 reaction center protein

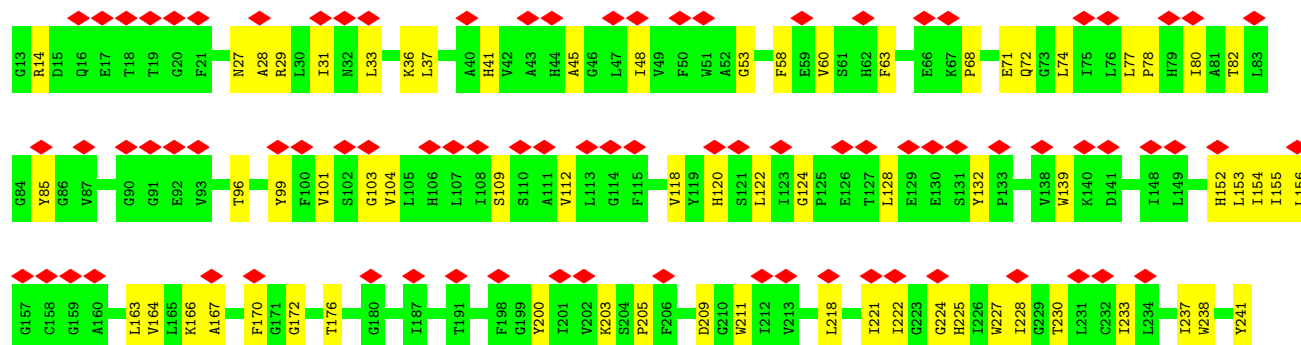


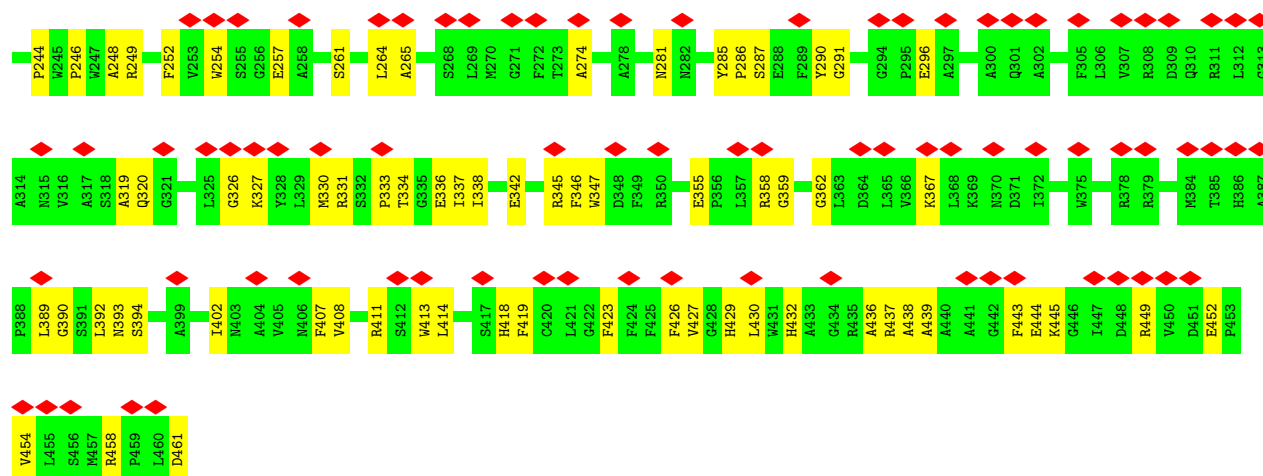


• Molecule 4: Photosystem II CP43 reaction center protein

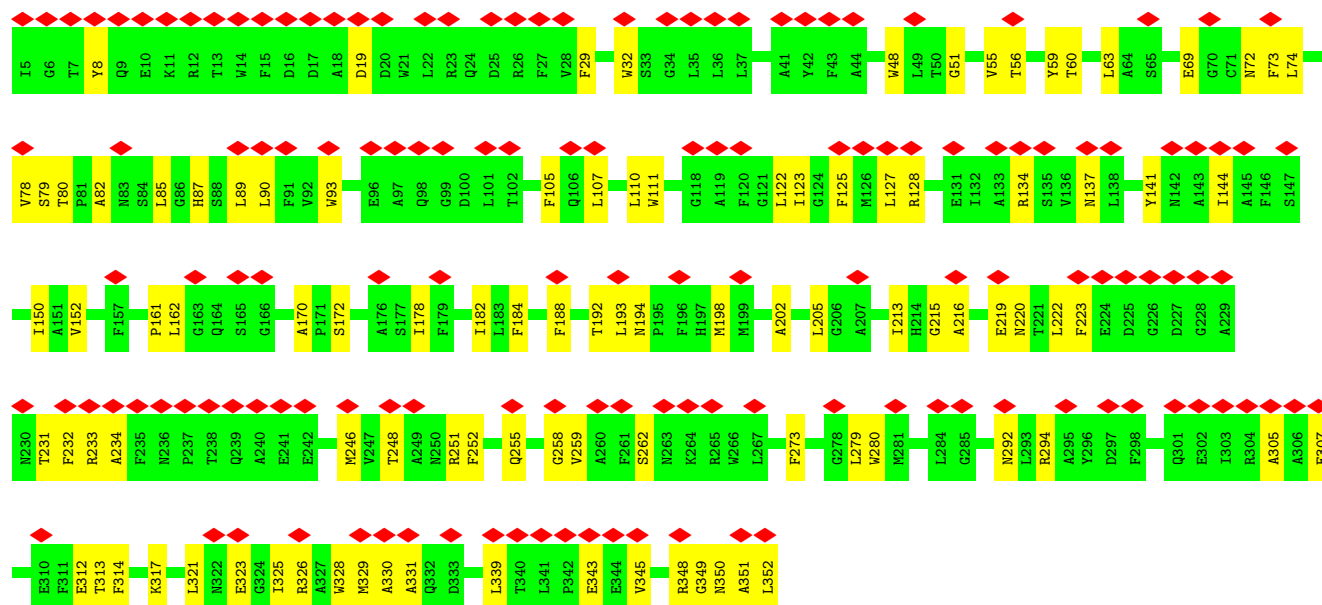
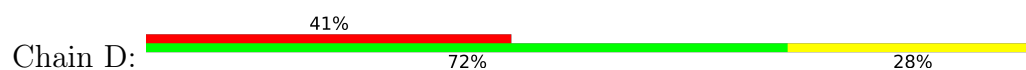


• Molecule 4: Photosystem II CP43 reaction center protein

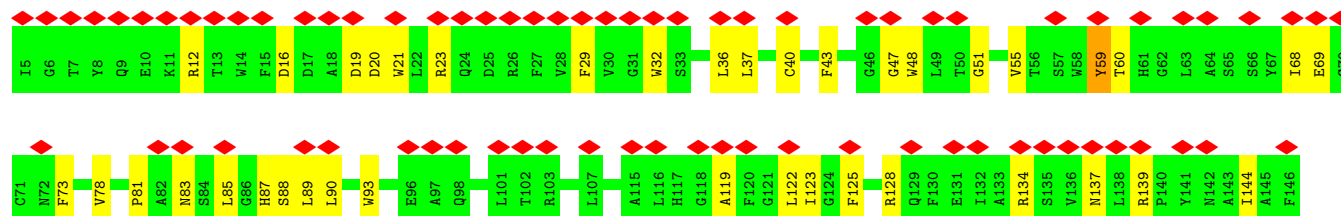


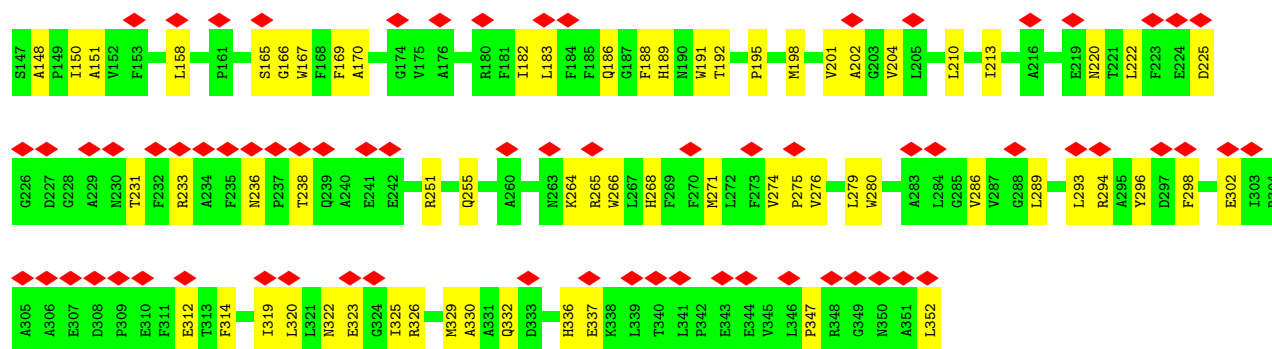


• Molecule 5: Photosystem II D2 protein

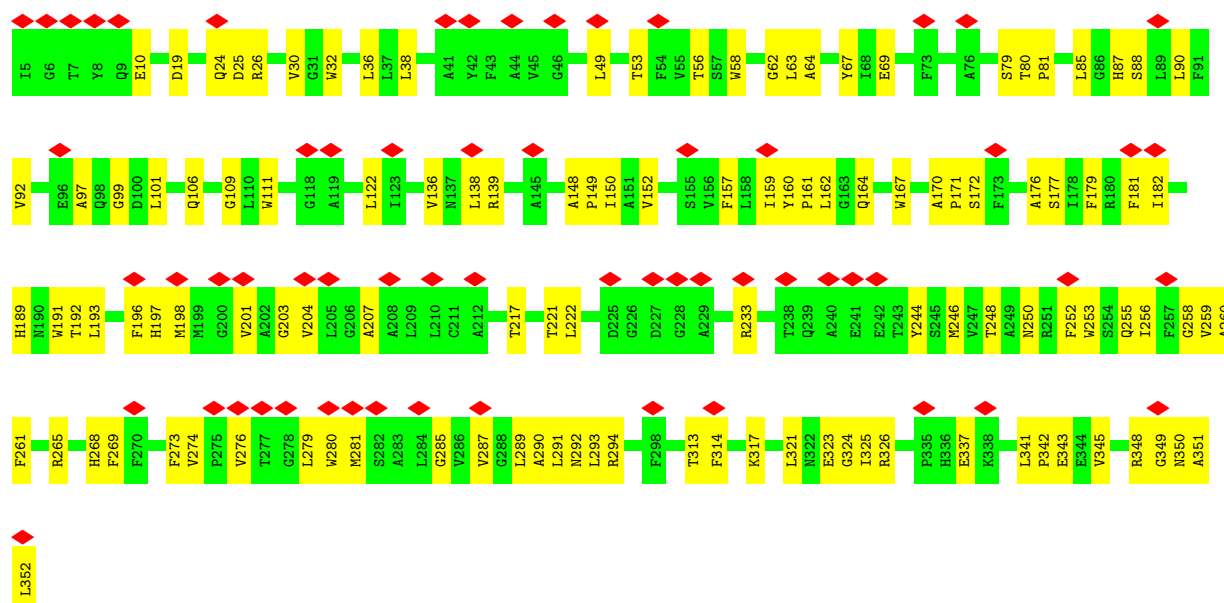


• Molecule 5: Photosystem II D2 protein

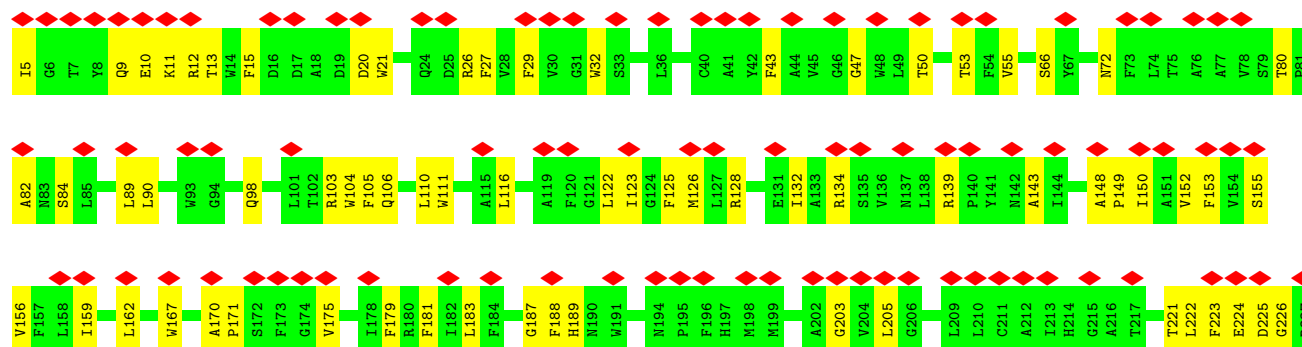
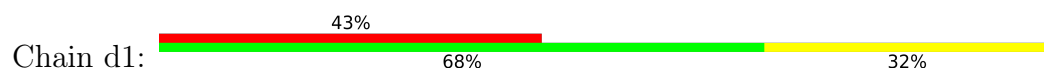


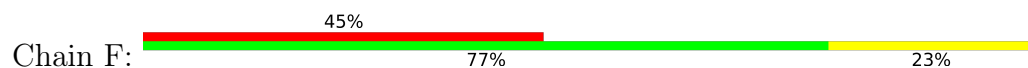


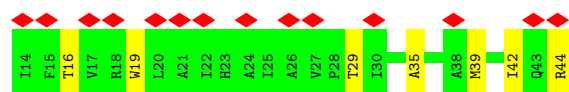
• Molecule 5: Photosystem II D2 protein



• Molecule 5: Photosystem II D2 protein



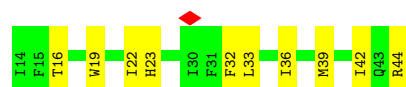




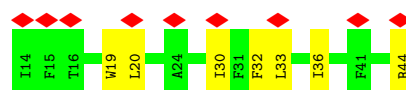
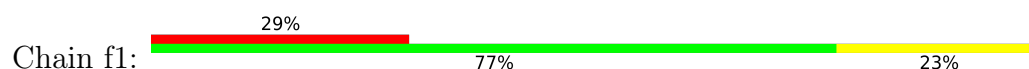
- Molecule 7: Cytochrome b559 subunit beta



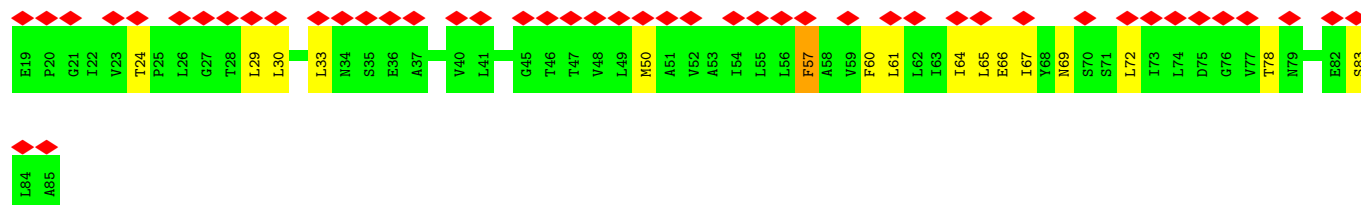
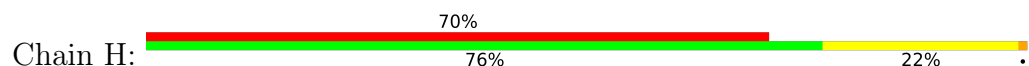
- Molecule 7: Cytochrome b559 subunit beta



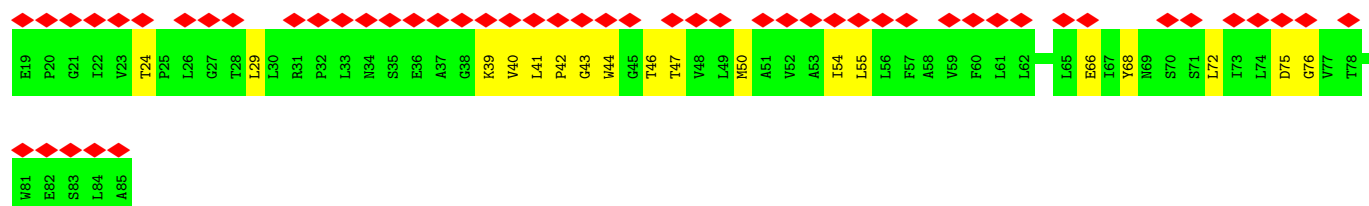
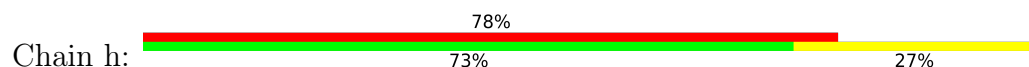
- Molecule 7: Cytochrome b559 subunit beta



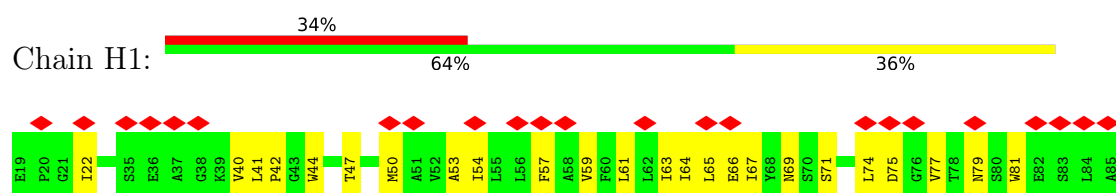
- Molecule 8: Photosystem II reaction center protein H



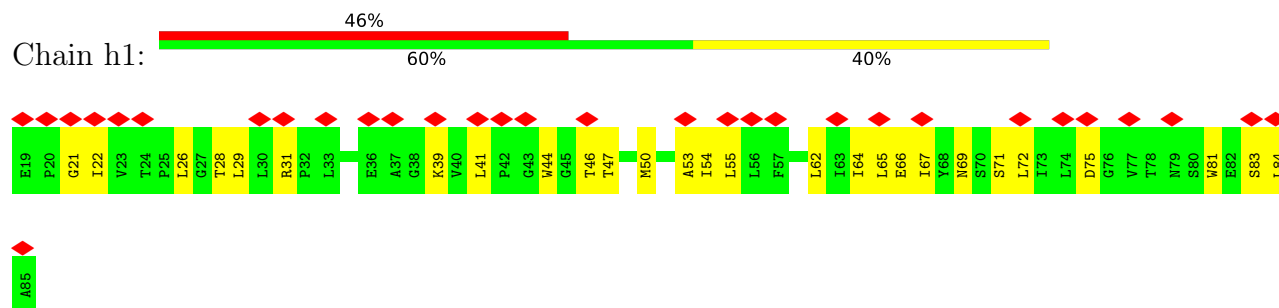
- Molecule 8: Photosystem II reaction center protein H



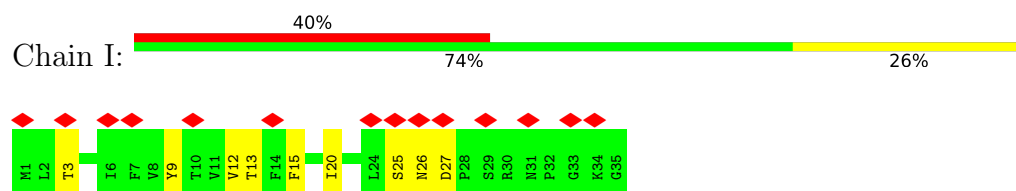
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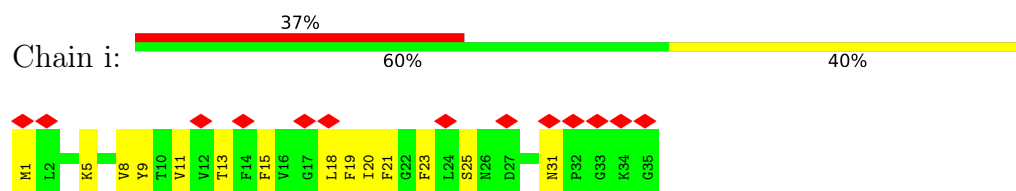
- Molecule 8: Photosystem II reaction center protein H



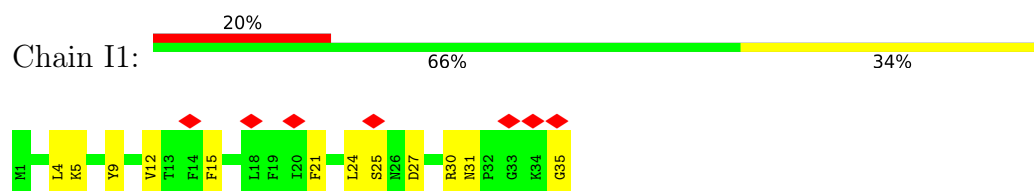
- Molecule 9: Photosystem II reaction center protein I



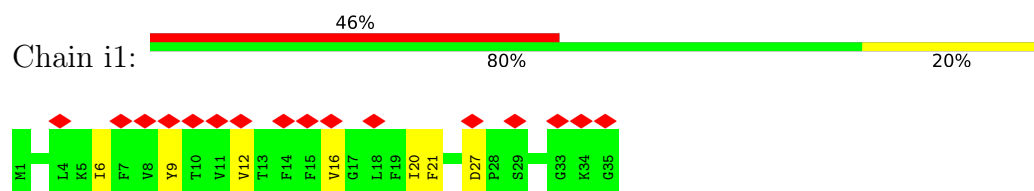
- Molecule 9: Photosystem II reaction center protein I



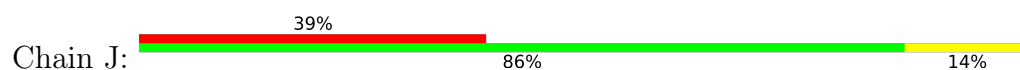
- Molecule 9: Photosystem II reaction center protein I

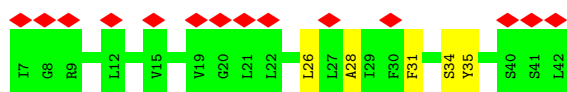


- Molecule 9: Photosystem II reaction center protein I

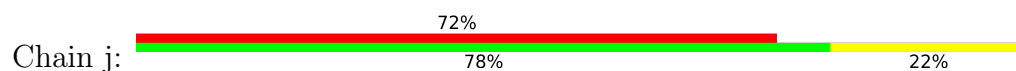


- Molecule 10: Photosystem II reaction center protein J

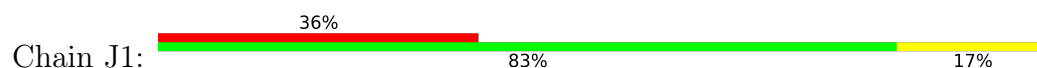




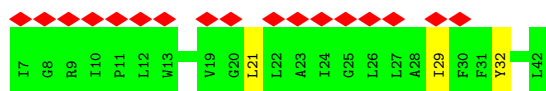
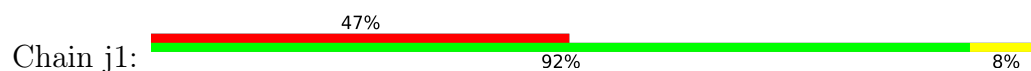
- Molecule 10: Photosystem II reaction center protein J



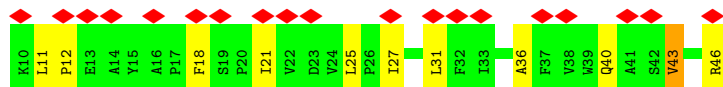
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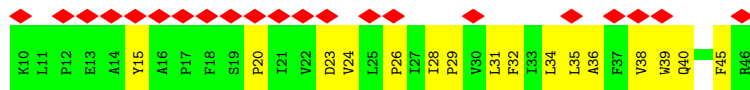
- Molecule 10: Photosystem II reaction center protein J



- Molecule 11: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein K



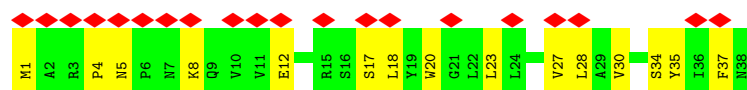
- Molecule 11: Photosystem II reaction center protein K



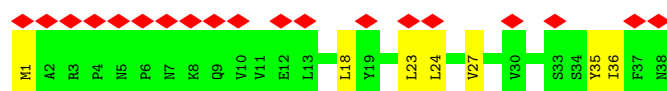
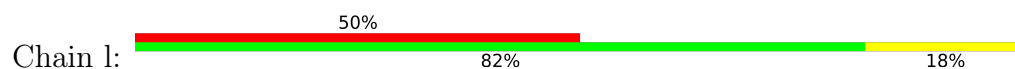
- Molecule 11: Photosystem II reaction center protein K



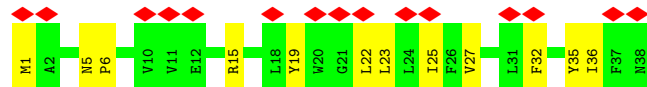
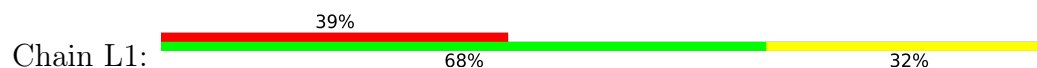
• Molecule 12: Photosystem II reaction center protein L



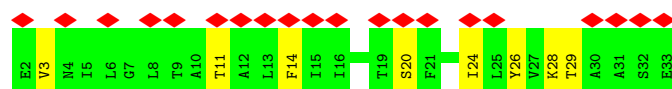
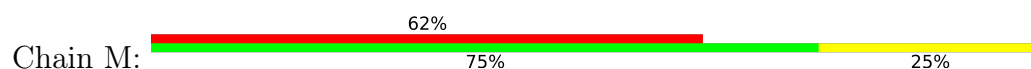
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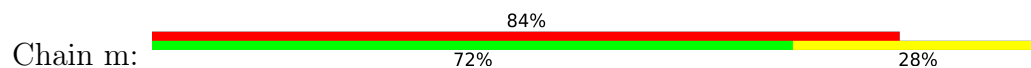
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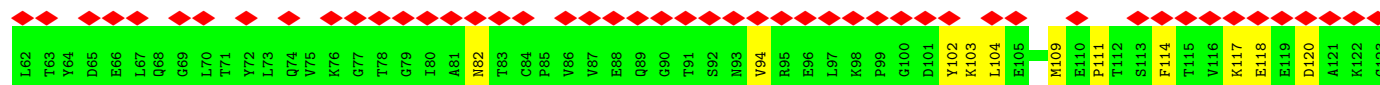
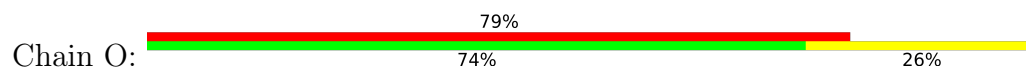
• Molecule 13: Photosystem II reaction center protein M

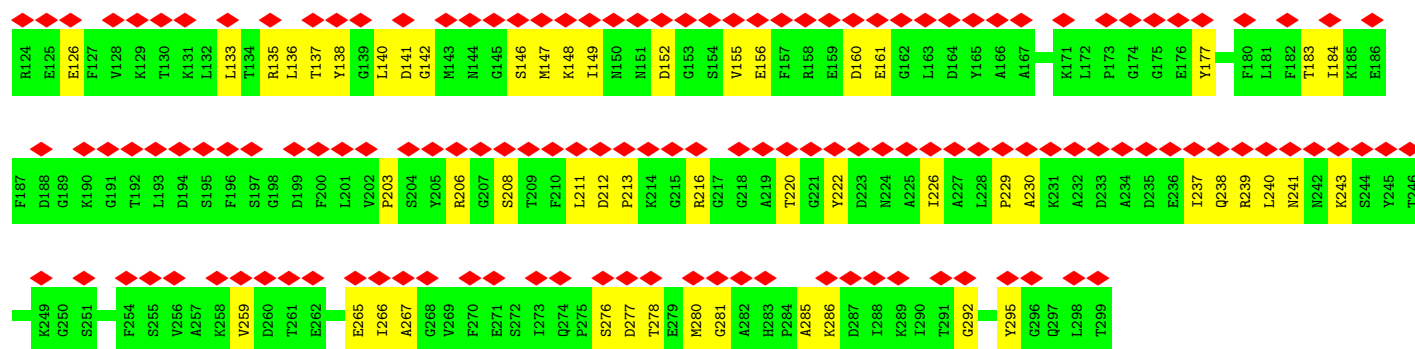


• Molecule 13: Photosystem II reaction center protein M

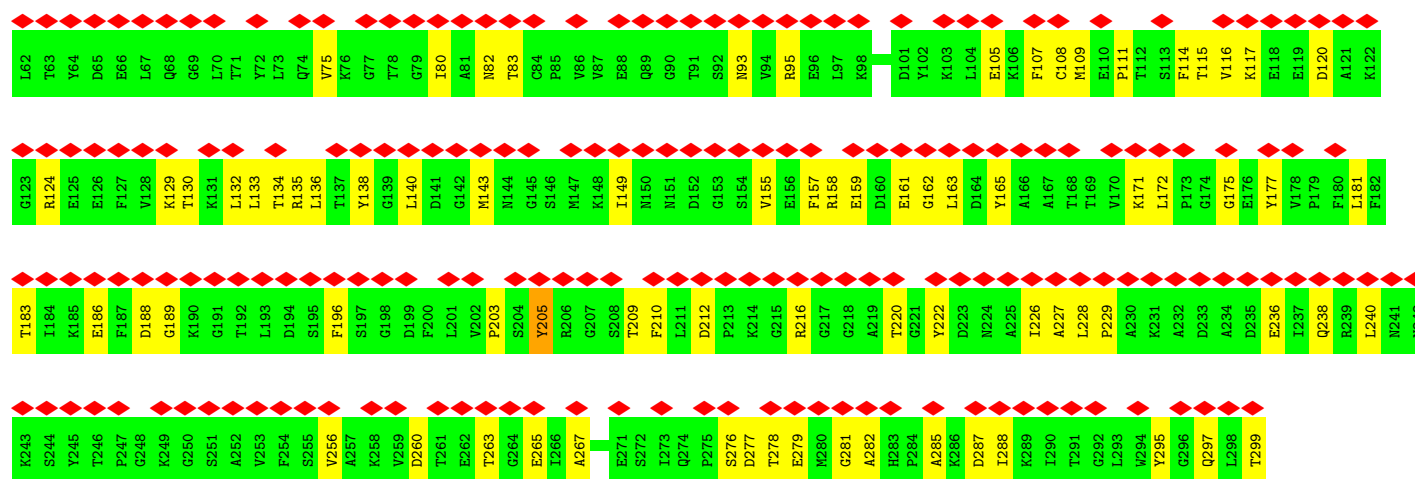
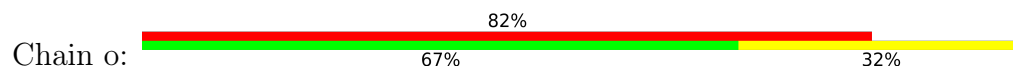


• Molecule 14: PsbO

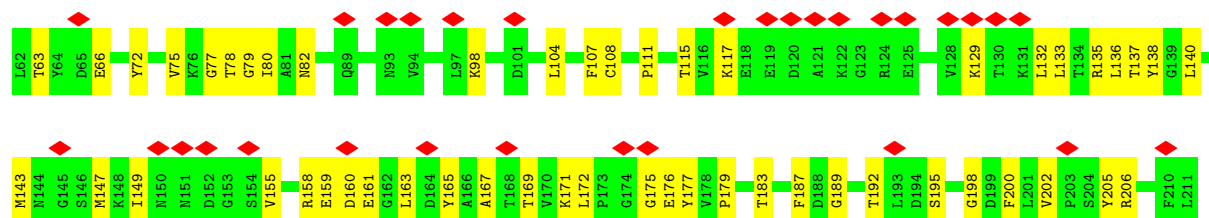
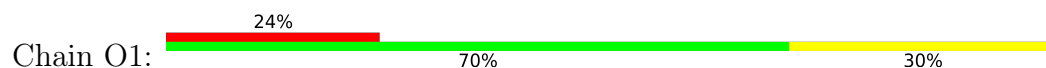




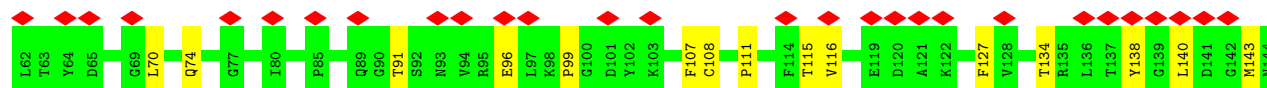
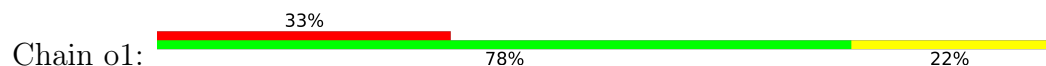
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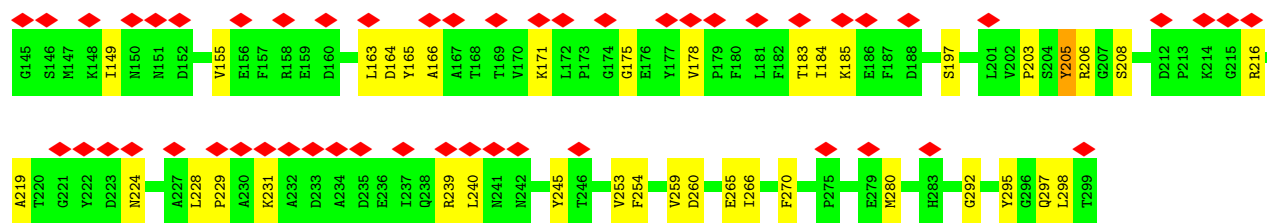


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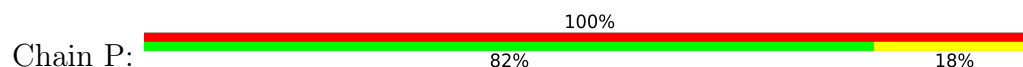


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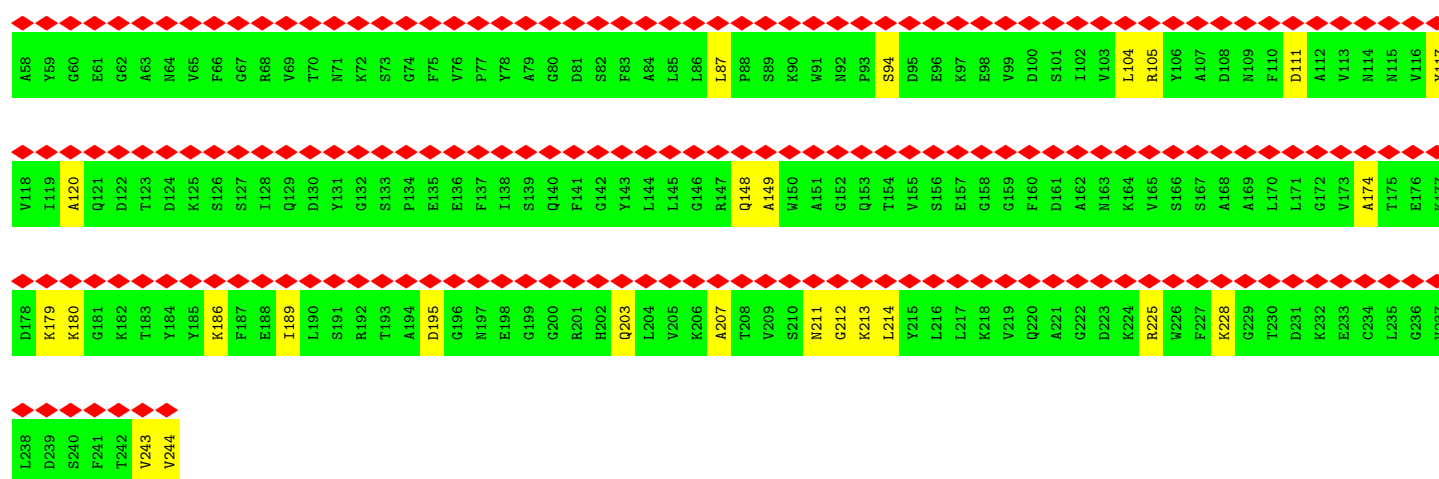
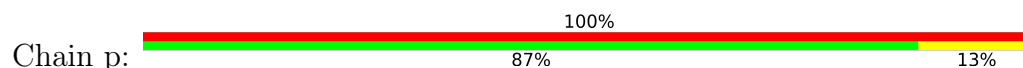




• Molecule 15: PsbP

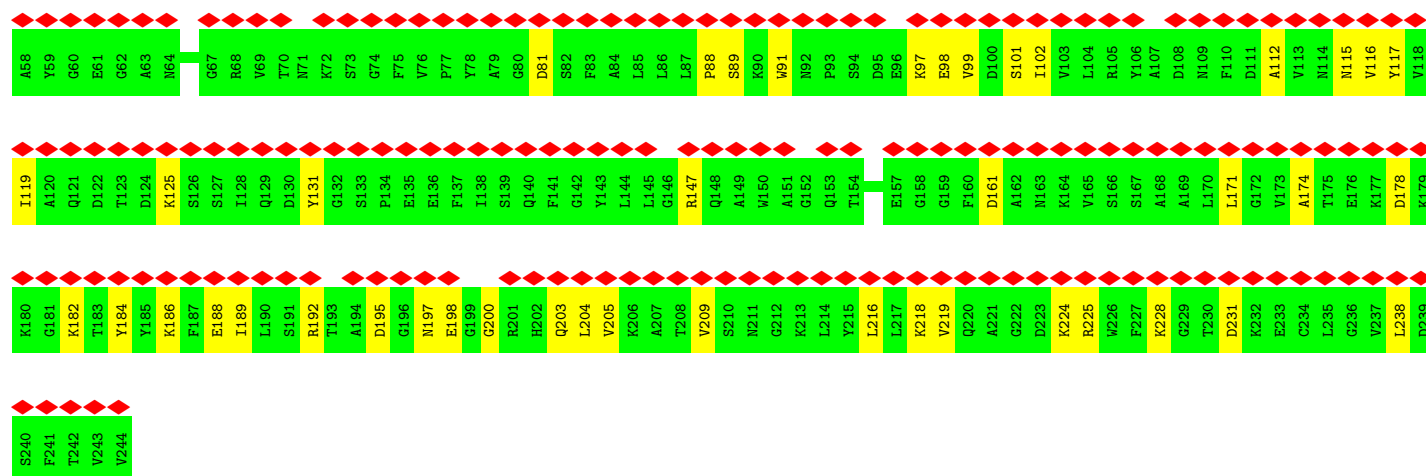


• Molecule 15: PsbP



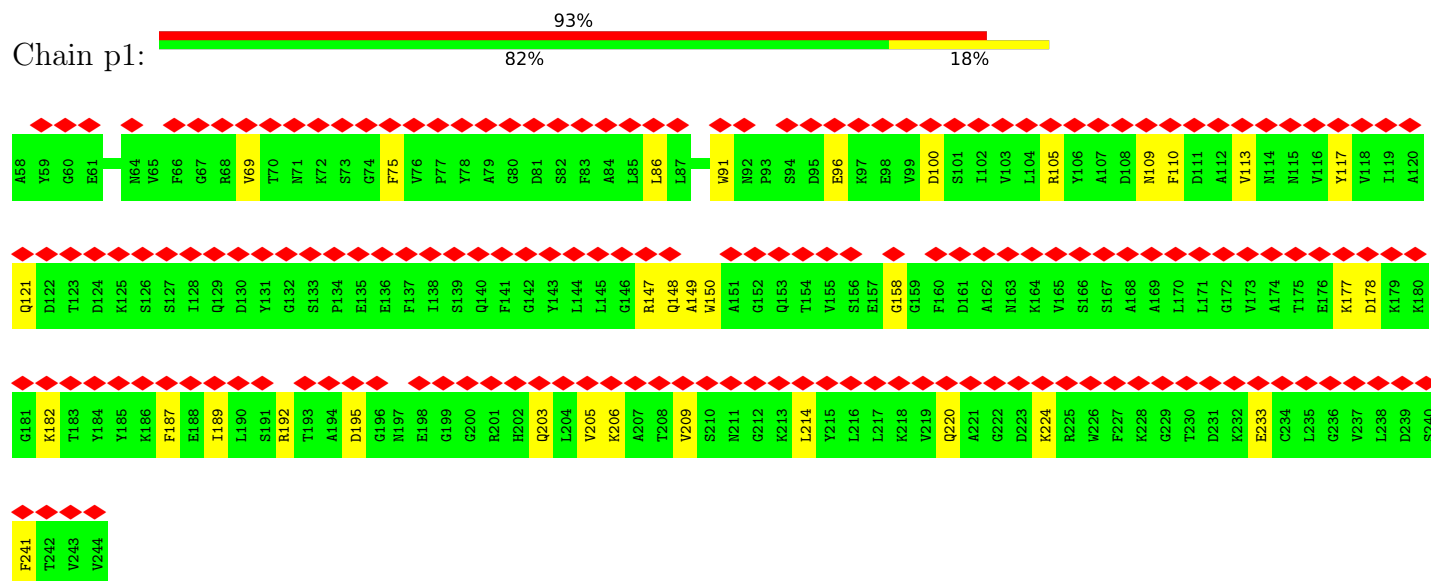
• Molecule 15: PsbP





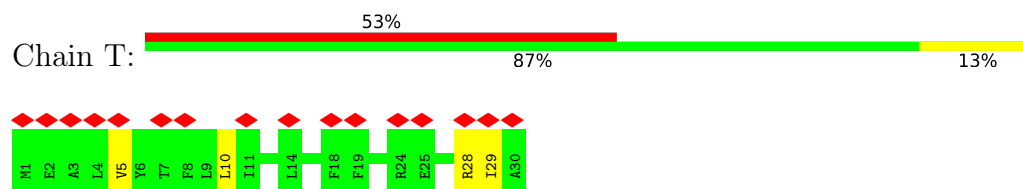
- Molecule 15: PsbP

Chain p1:



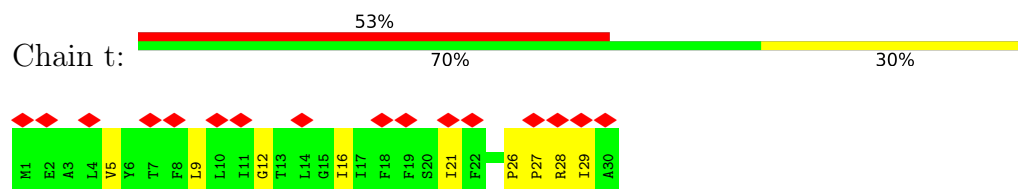
- Molecule 16: Photosystem II reaction center protein T

Chain T:

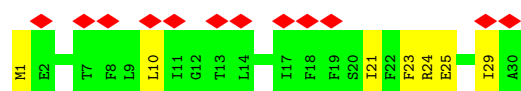
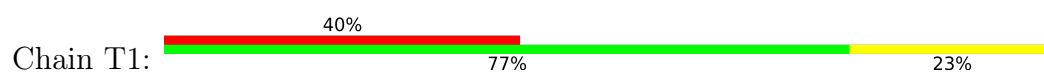


- Molecule 16: Photosystem II reaction center protein T

Chain t:



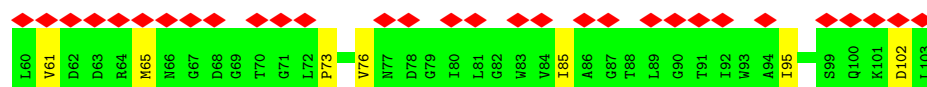
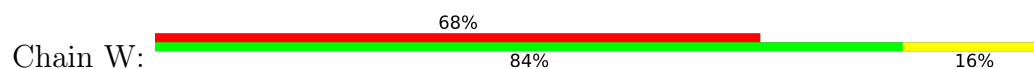
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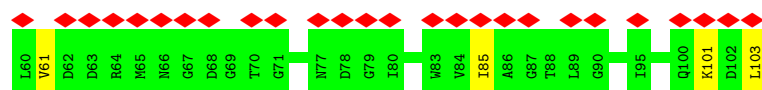
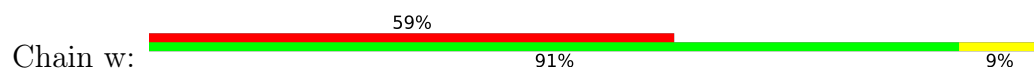
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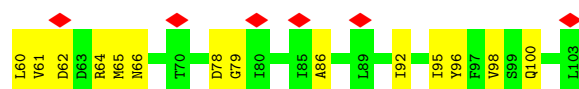
• Molecule 17: PsbW



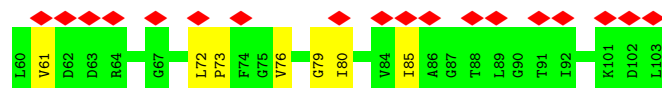
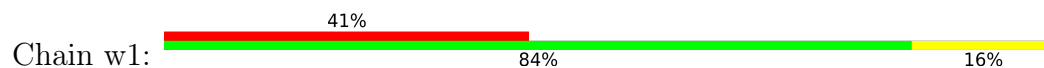
• Molecule 17: PsbW



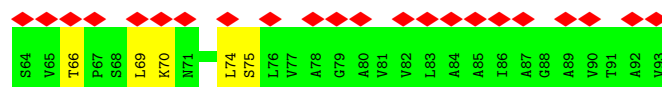
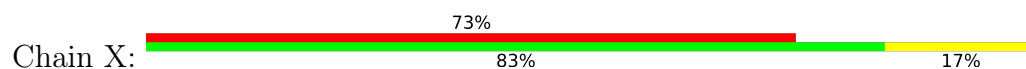
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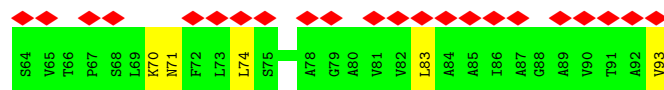
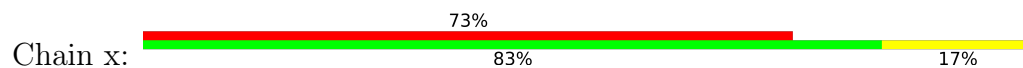
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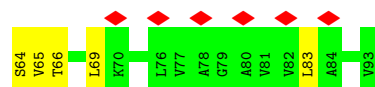
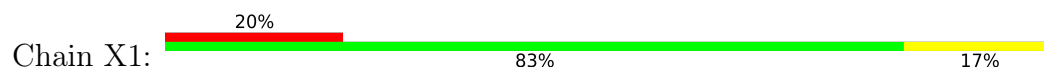
• Molecule 18: PsbX



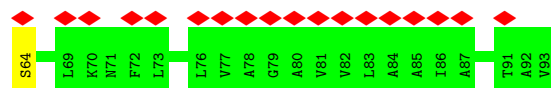
- Molecule 18: PsbX



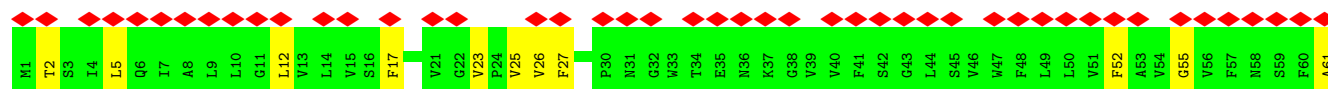
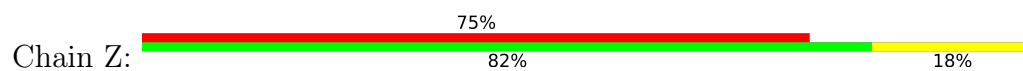
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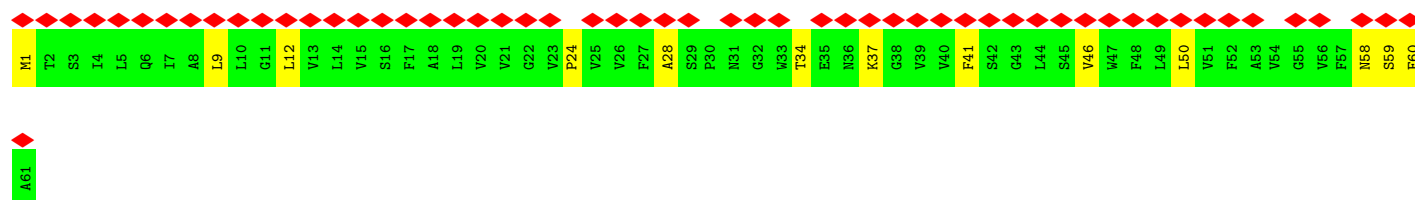
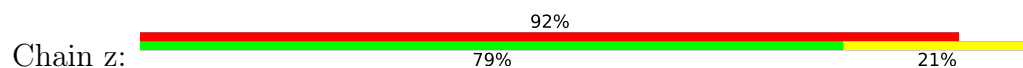
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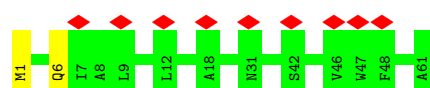
- Molecule 19: PsbZ



- Molecule 19: PsbZ

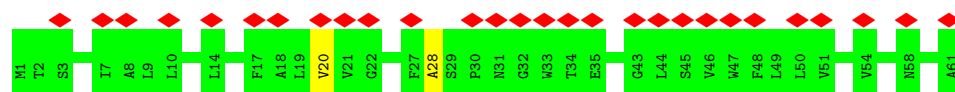


- Molecule 19: PsbZ

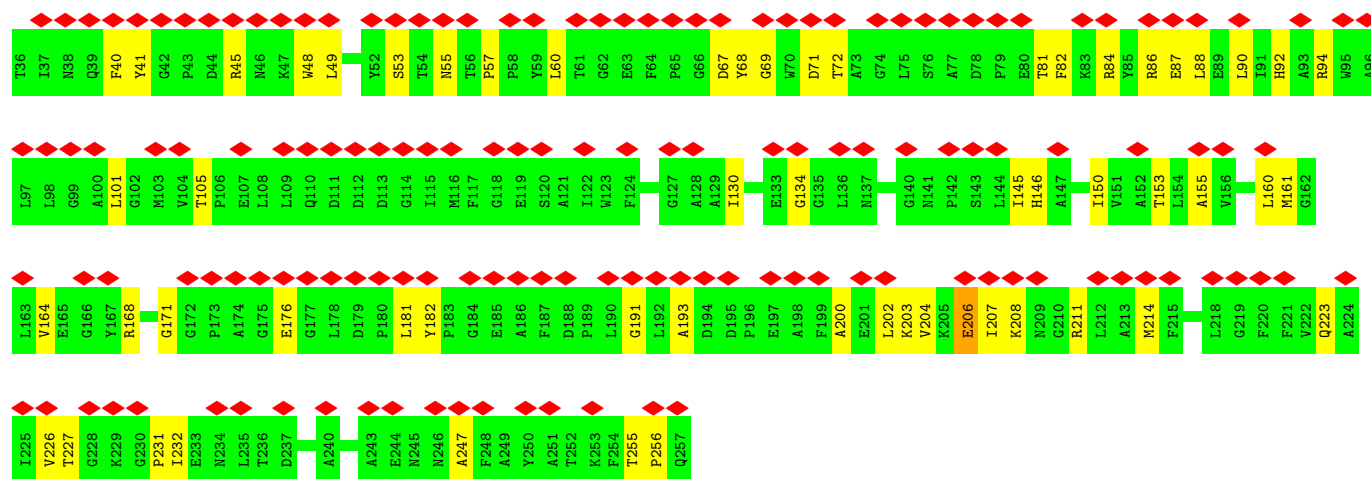
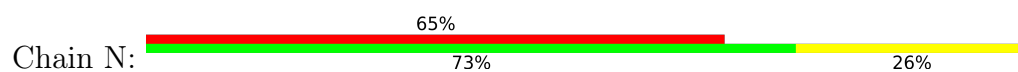


- Molecule 19: PsbZ

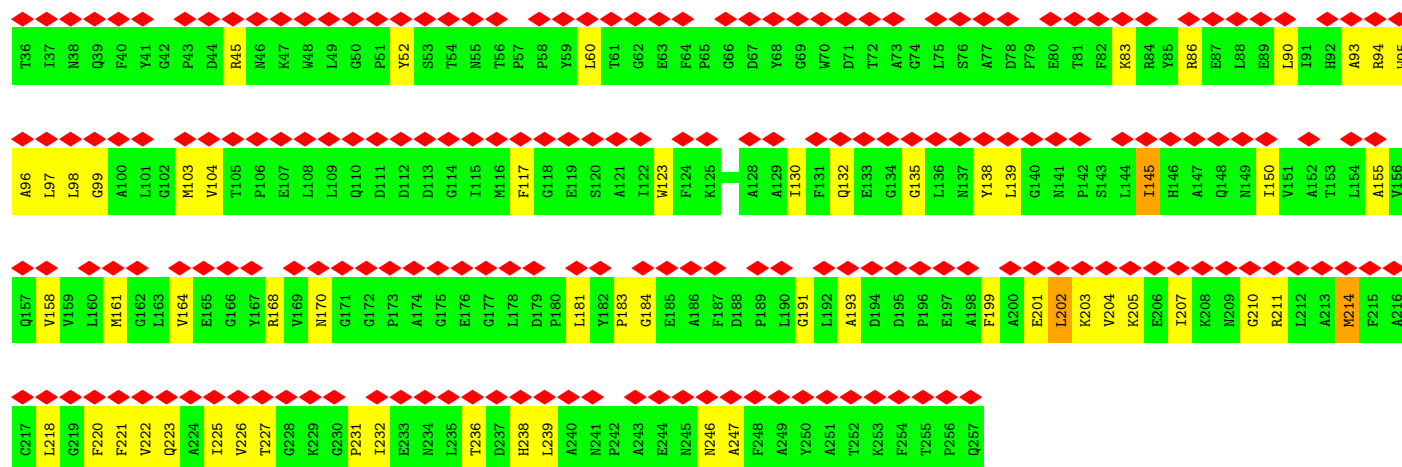
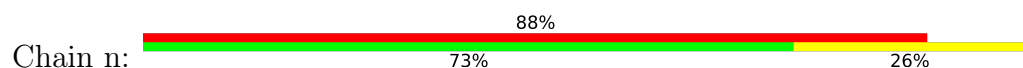




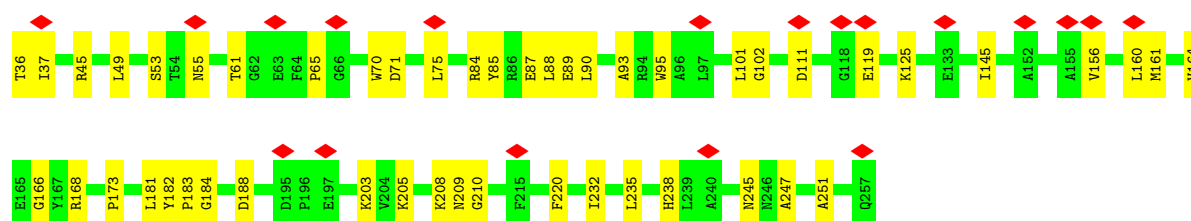
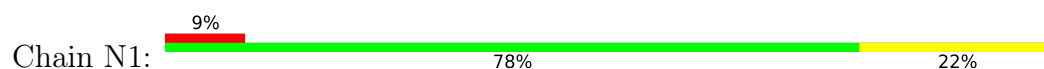
• Molecule 20: LHCII M3



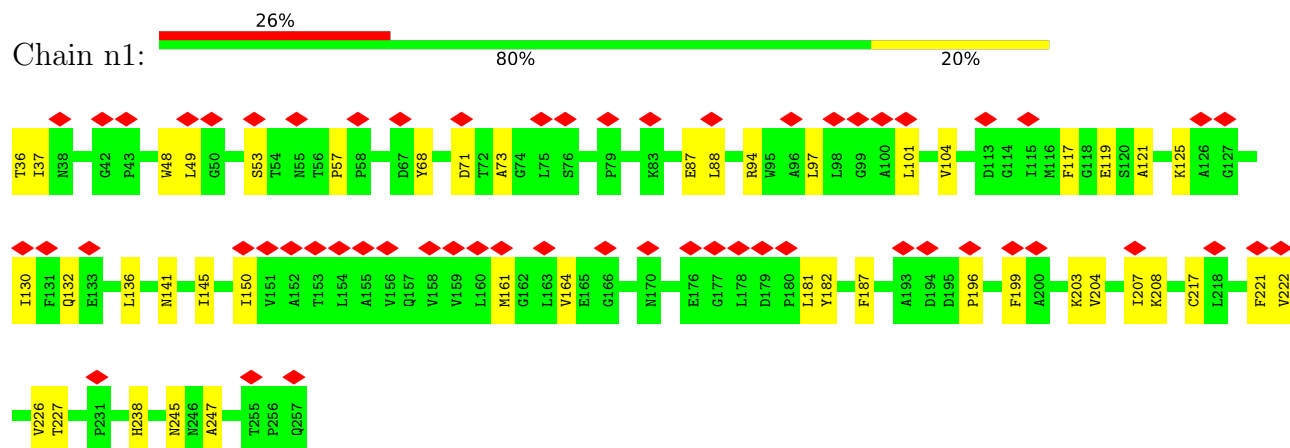
• Molecule 20: LHCII M3



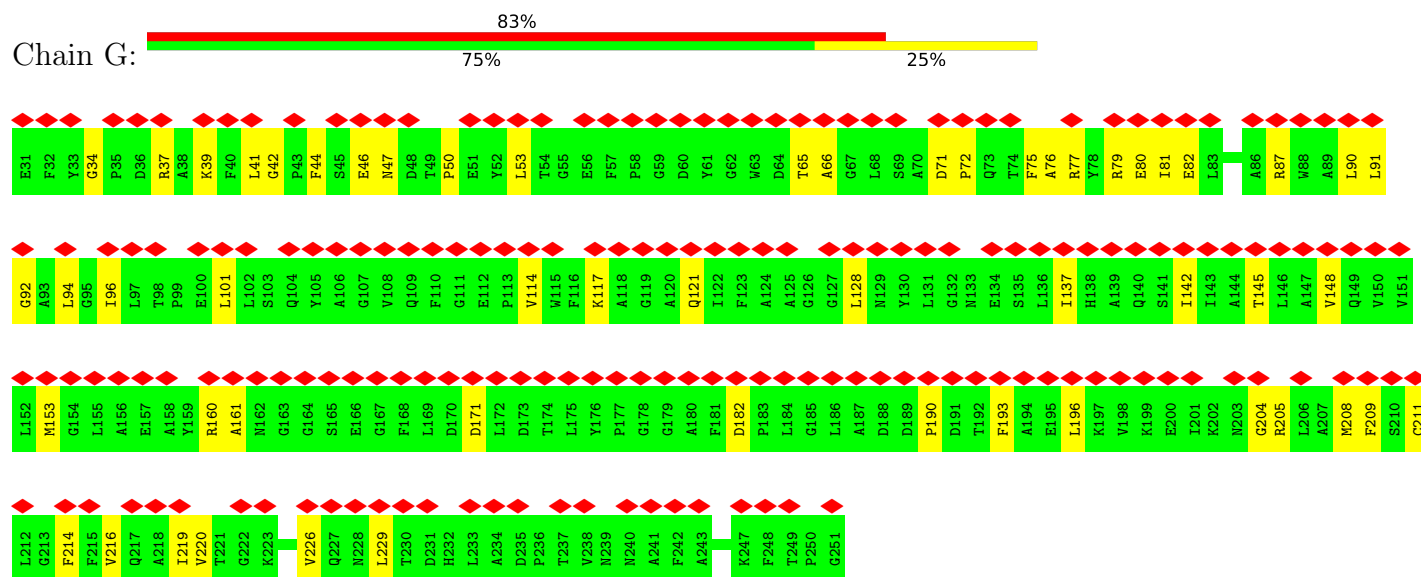
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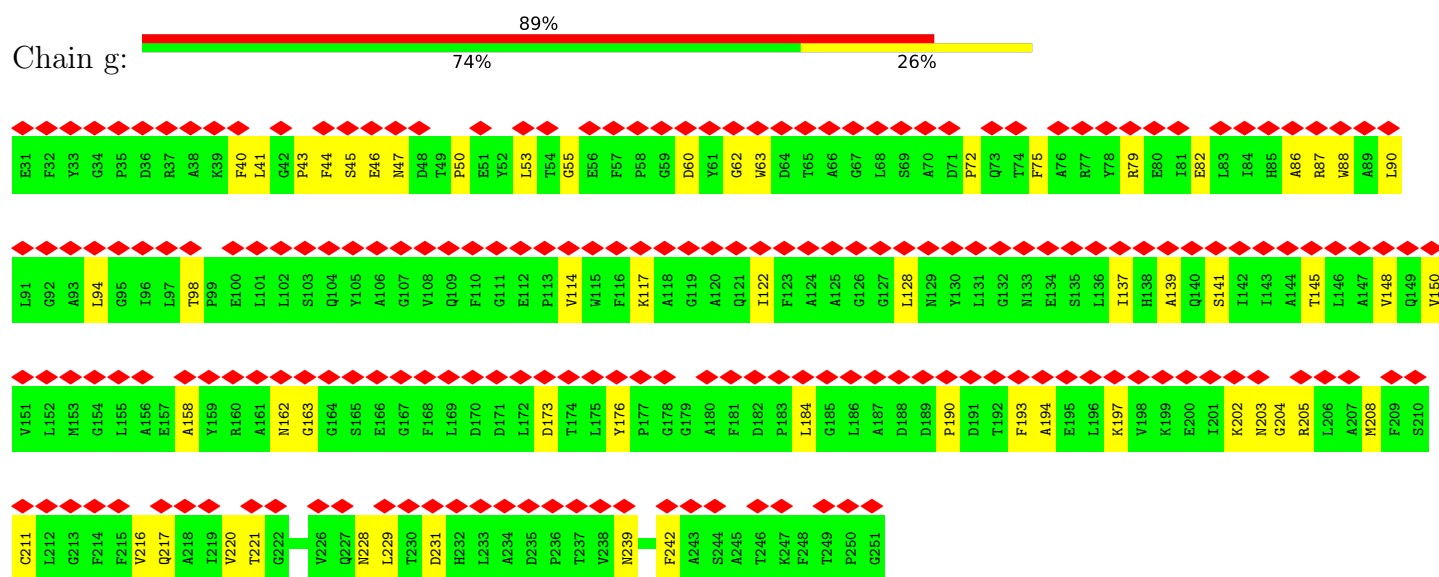
- Molecule 20: LHCII M3



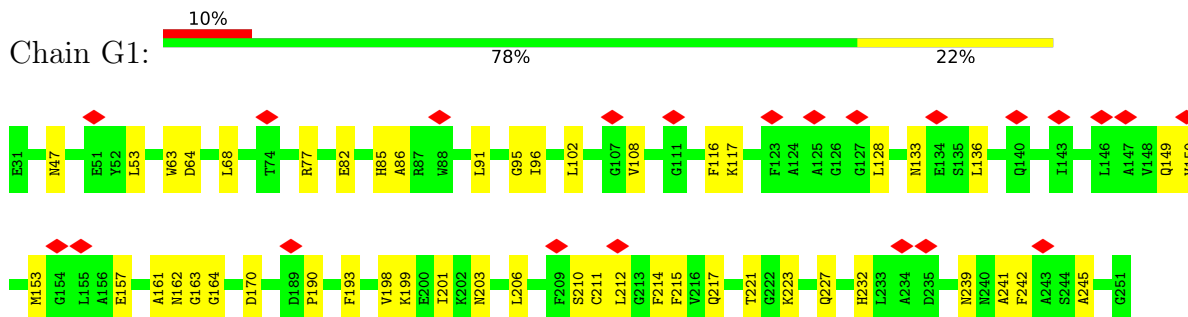
- Molecule 21: LHCII M2



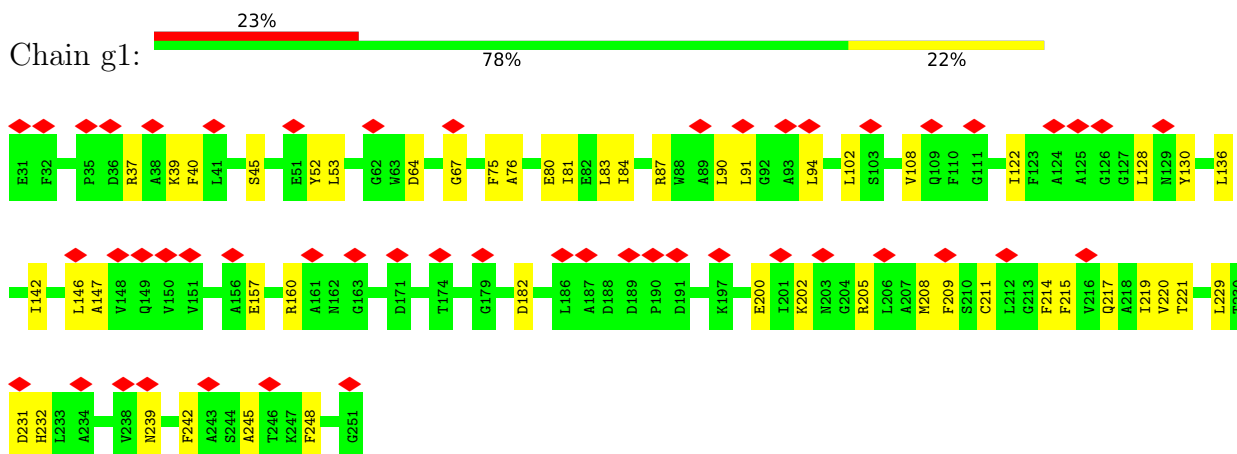
- Molecule 21: LHCII M2



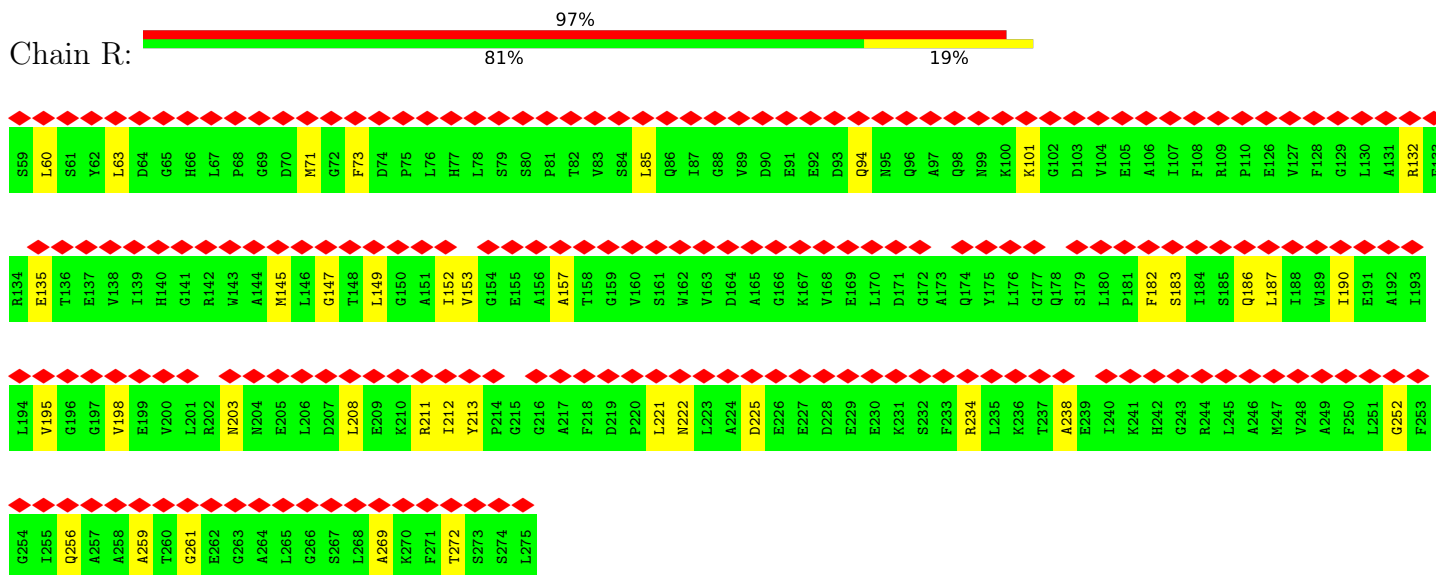
- Molecule 21: LHCII M2



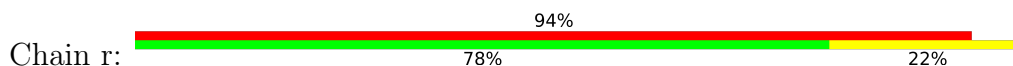
- Molecule 21: LHCII M2

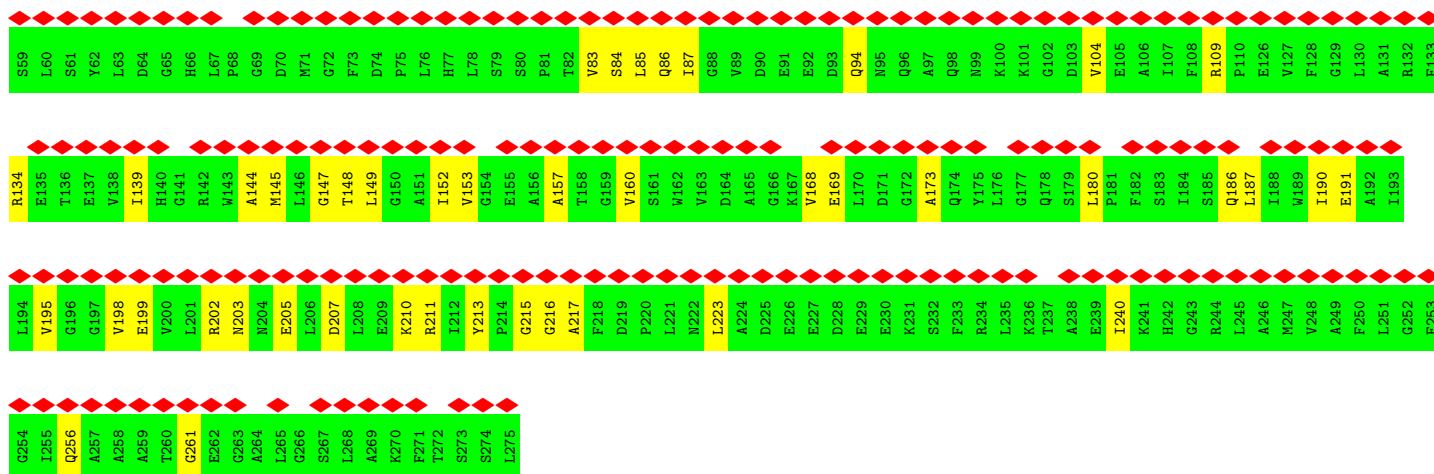


- Molecule 22: CP29

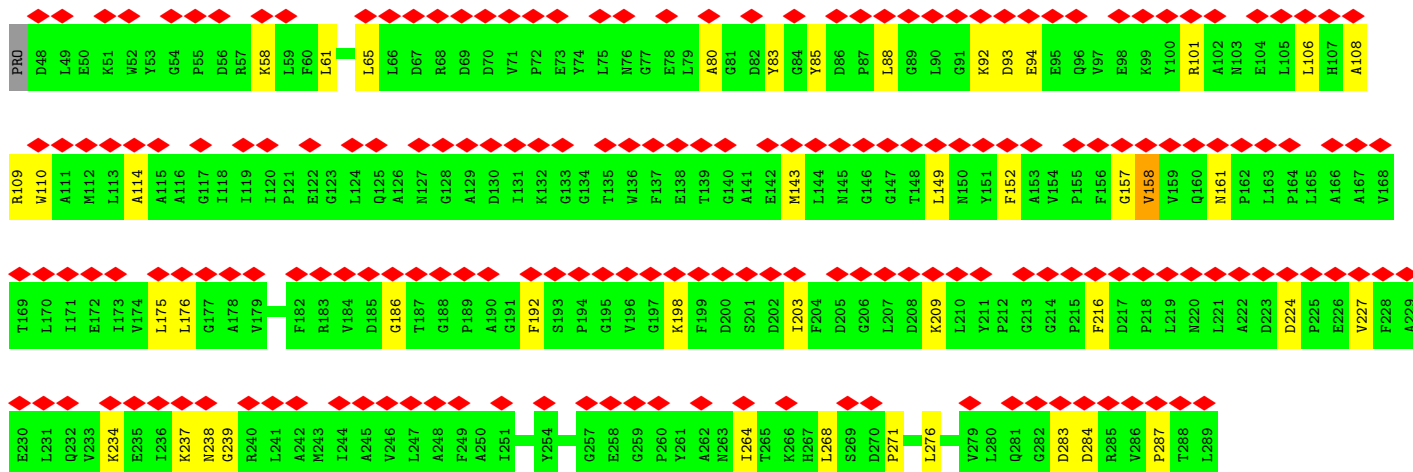
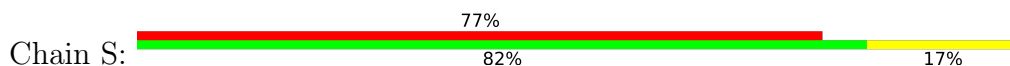


- Molecule 22: CP29

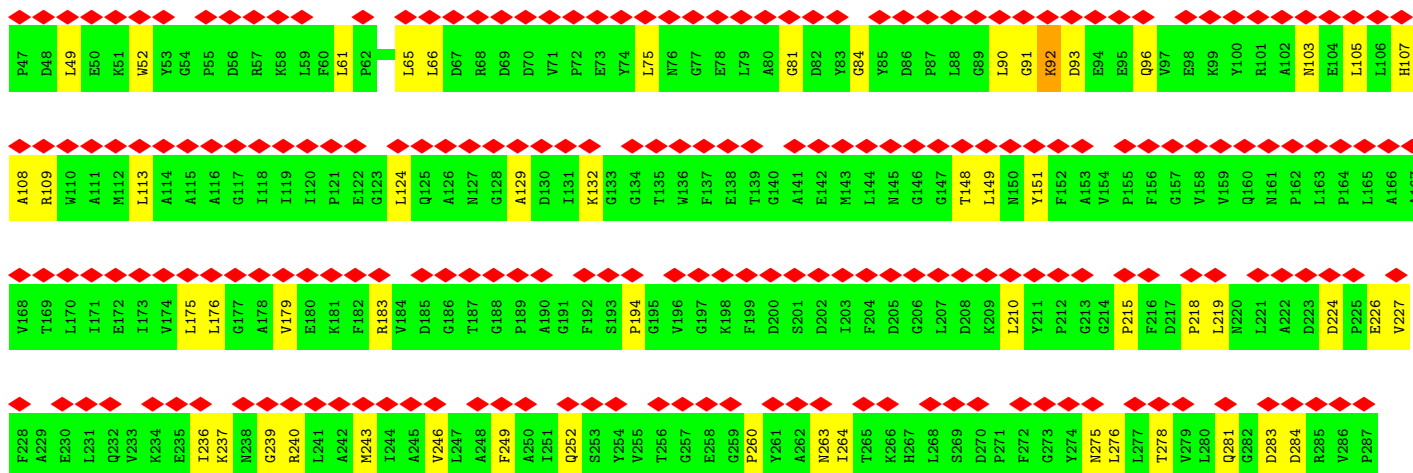
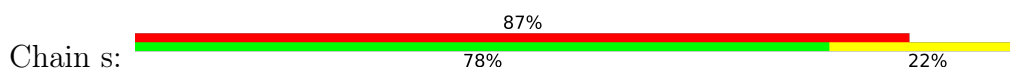




• Molecule 23: CP26

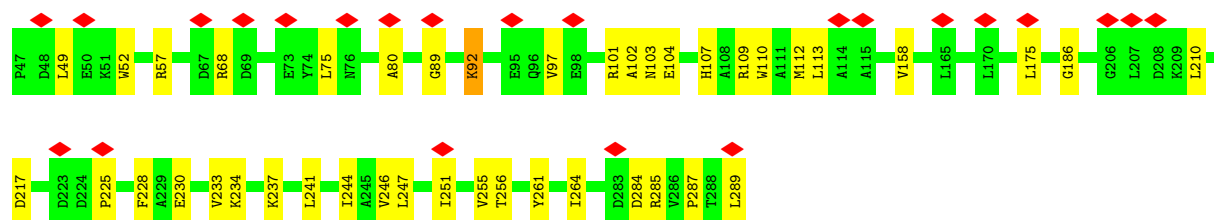
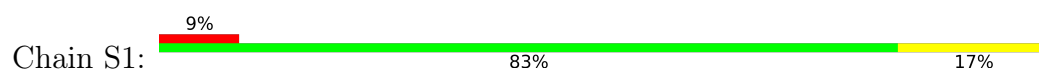


• Molecule 23: CP26

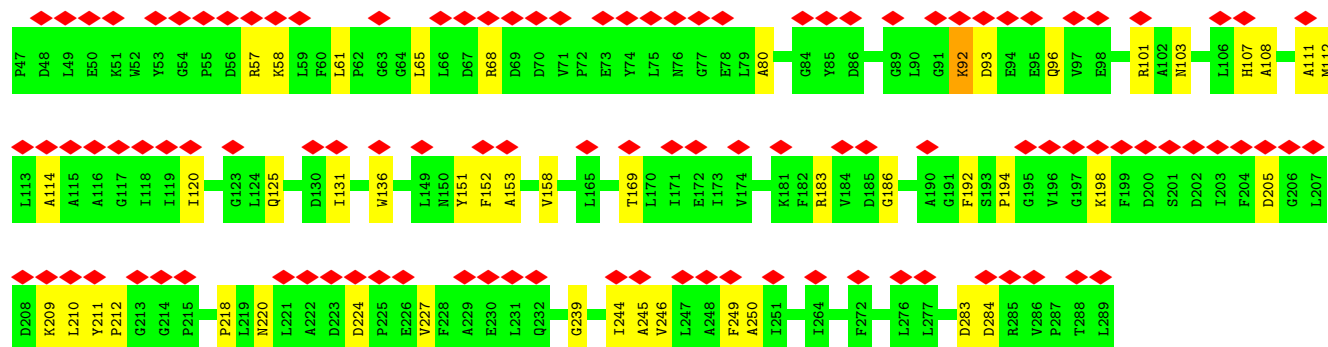
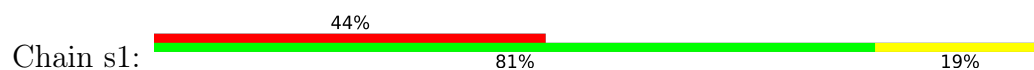




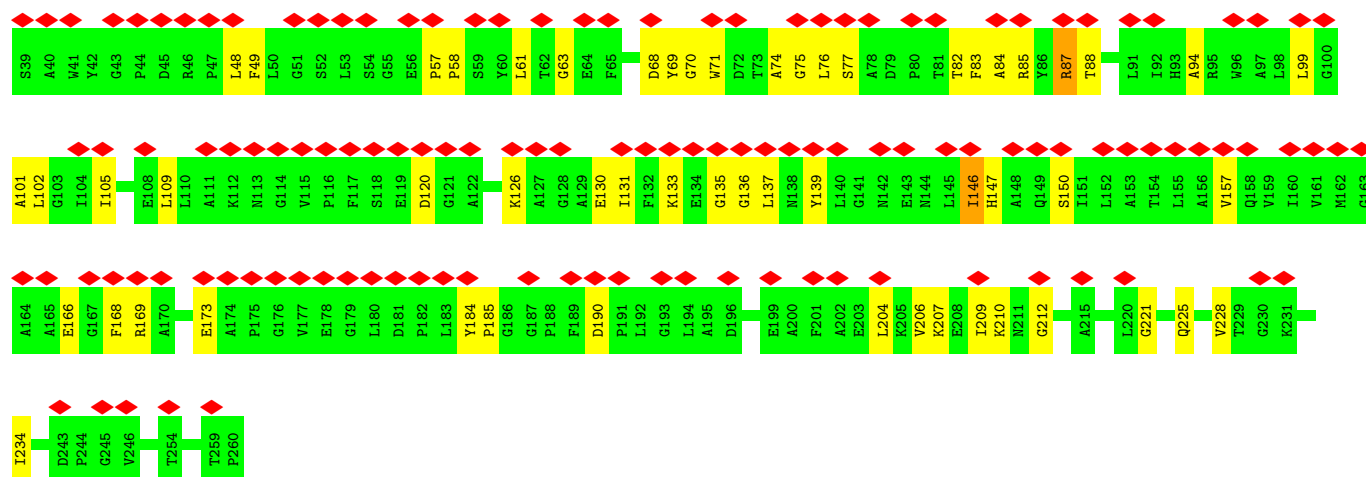
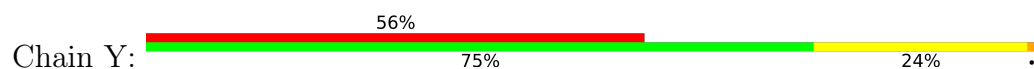
• Molecule 23: CP26



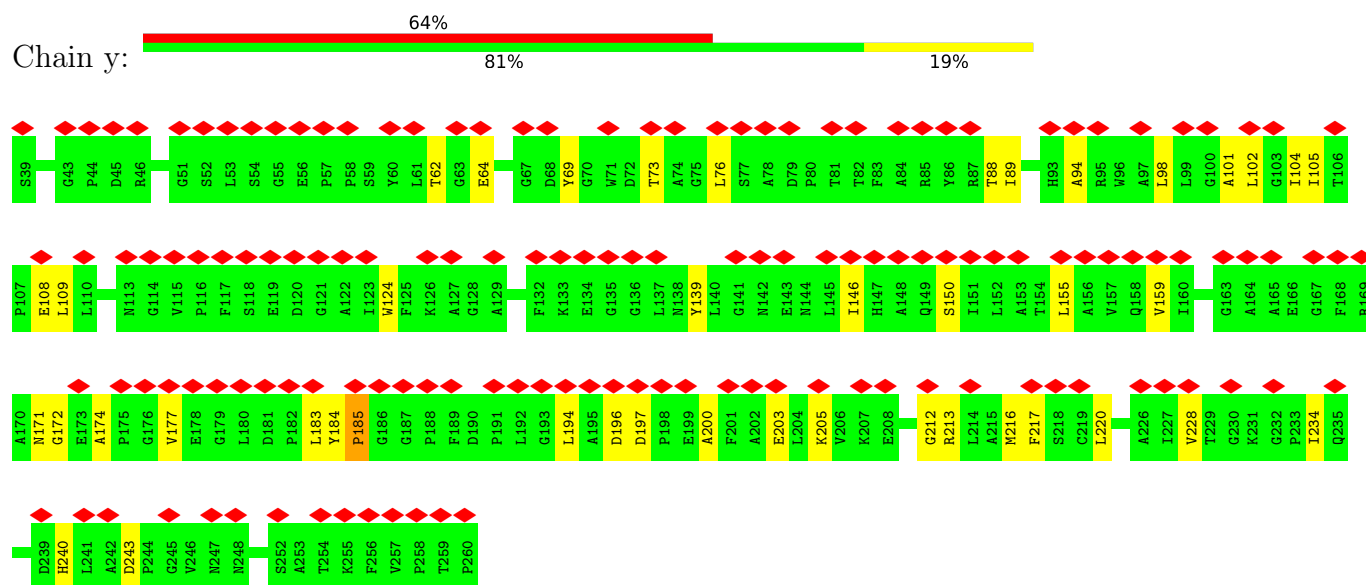
• Molecule 23: CP26



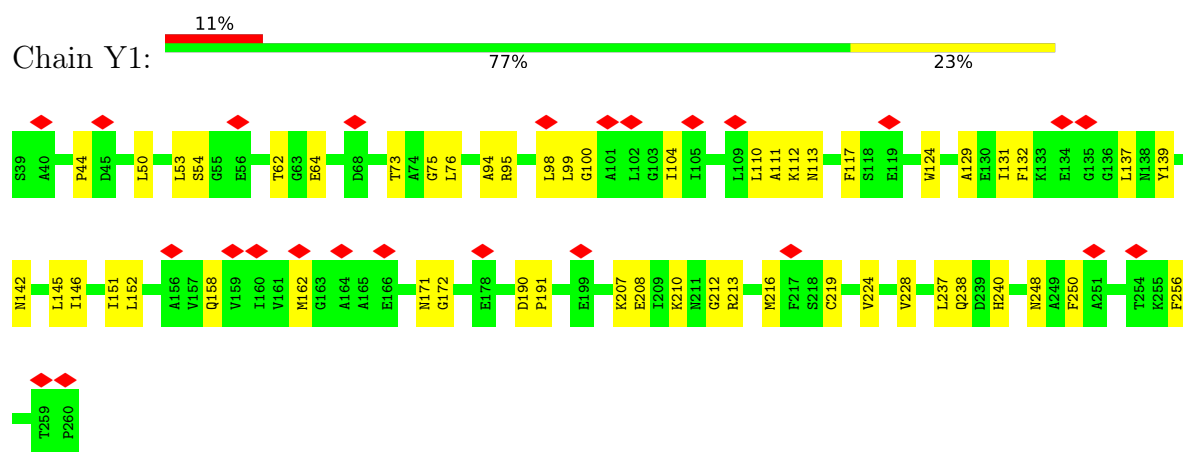
• Molecule 24: LHCII M1



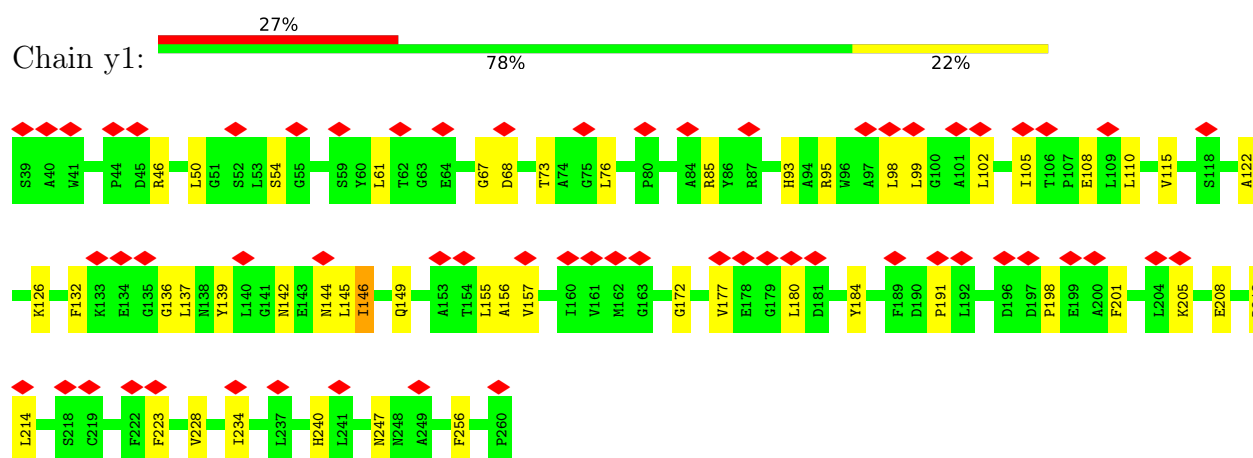
• Molecule 24: LHCII M1



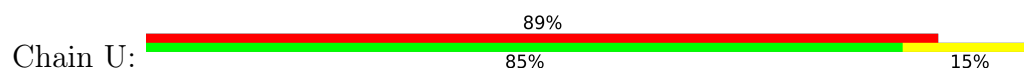
• Molecule 24: LHCII M1

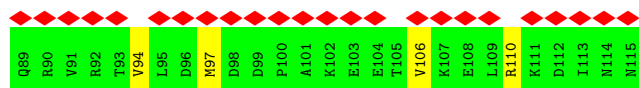


• Molecule 24: LHCII M1

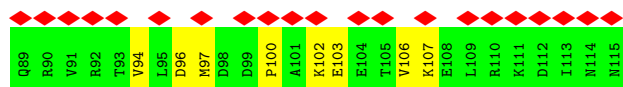
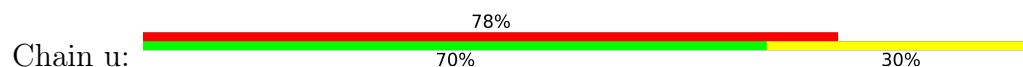


• Molecule 25: PsbU

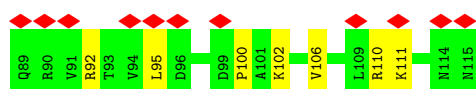
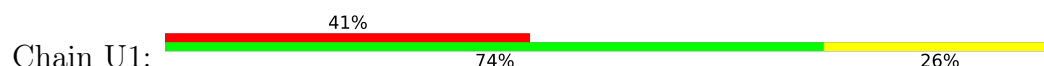




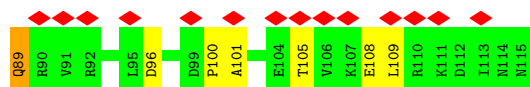
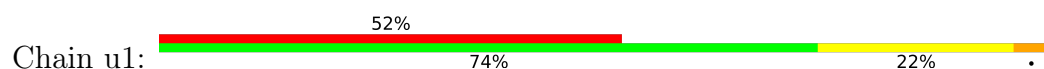
- Molecule 25: PsbU



- Molecule 25: PsbU



- Molecule 25: PsbU



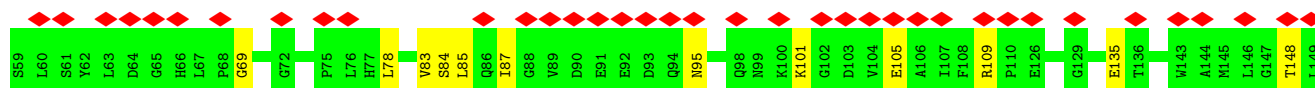
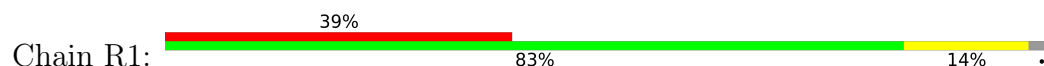
- Molecule 26: Photosystem II reaction center protein M

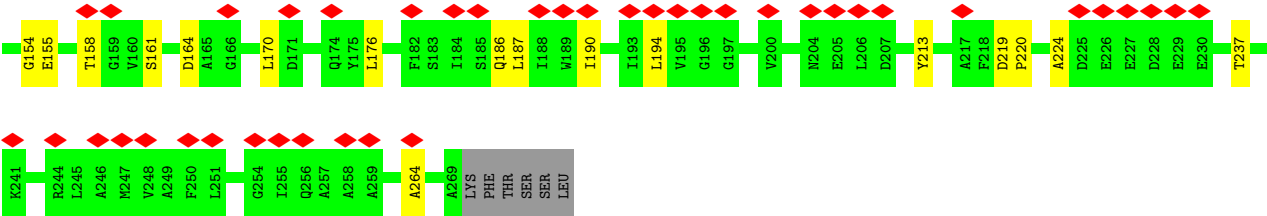


- Molecule 26: Photosystem II reaction center protein M

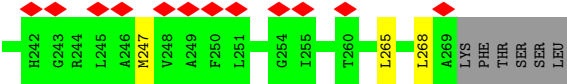
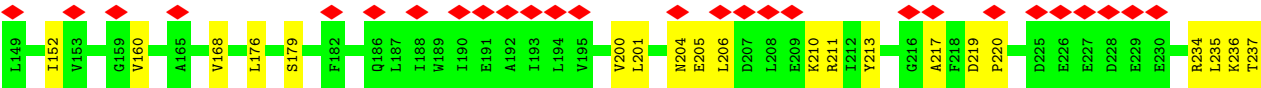
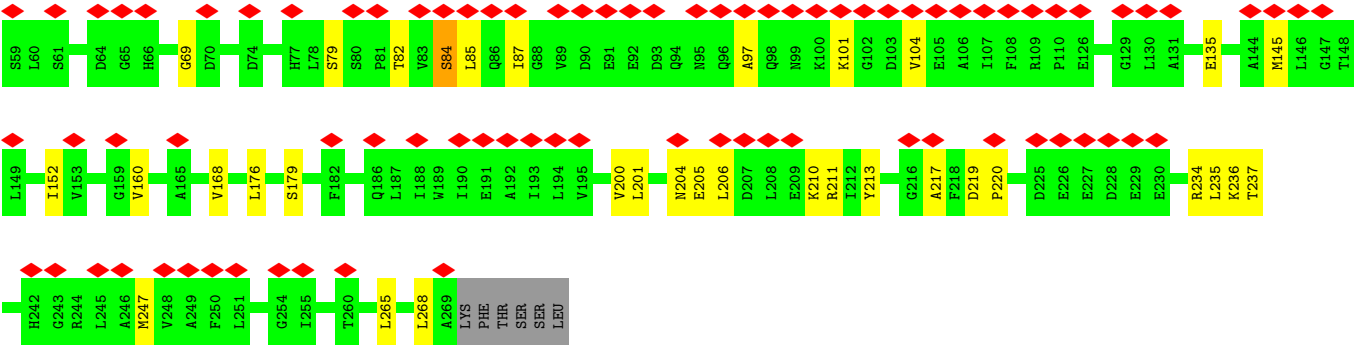
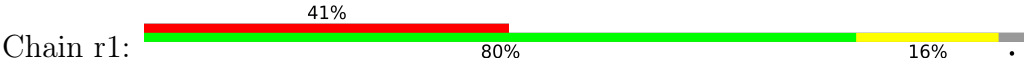


- Molecule 27: CP29





• Molecule 27: CP29



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14307	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 ($e^-/\text{\AA}^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0175	Depositor
Map size ($\text{\AA}$)	460.8, 460.8, 460.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.96, 0.96, 0.96	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SQD, 4RF, LHG, BCR, PHO, DGA, PL9, FE2, LMG, PTY, CHL, CLA, LUT, 3PH, C7Z, CL, LPX, SEP, NA, NEX, SPH, XAT, ERG, BCT, DGD, LMT, OEX, HEM, LMK, RRX

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	0.26	0/2723	0.59	0/3715
1	A1	0.24	0/2723	0.57	0/3715
1	a	0.28	0/2723	0.63	0/3715
1	a1	0.23	0/2723	0.58	3/3715 (0.1%)
2	B	0.33	2/3912 (0.1%)	0.61	6/5327 (0.1%)
2	B1	0.18	0/3912	0.46	0/5327
2	b	0.22	0/3912	0.52	0/5327
2	b1	0.20	0/3912	0.48	0/5327
3	V	0.17	0/228	0.45	0/311
3	V1	0.21	0/228	0.50	0/311
3	v	0.20	0/228	0.52	0/311
3	v1	0.22	0/228	0.49	0/311
4	C	0.23	0/3602	0.54	2/4913 (0.0%)
4	C1	0.19	0/3602	0.48	0/4913
4	c	0.38	1/3602 (0.0%)	0.73	5/4913 (0.1%)
4	c1	0.21	0/3602	0.50	0/4913
5	D	0.24	0/2860	0.58	2/3899 (0.1%)
5	D1	0.21	0/2860	0.54	0/3899
5	d	0.25	0/2860	0.56	2/3899 (0.1%)
5	d1	0.20	0/2860	0.53	0/3899
6	E	0.20	0/639	0.52	0/870
6	E1	0.16	0/639	0.50	0/870
6	e	0.22	0/639	0.59	0/870
6	e1	0.17	0/639	0.44	0/870
7	F	0.23	0/259	0.53	0/351
7	F1	0.20	0/259	0.48	0/351
7	f	0.21	0/259	0.49	0/351
7	f1	0.16	0/259	0.42	0/351
8	H	3.98	6/513 (1.2%)	0.73	1/703 (0.1%)
8	H1	0.17	0/513	0.48	0/703
8	h	0.26	0/513	0.70	2/703 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	h1	0.20	0/513	0.49	0/703
9	I	0.22	0/287	0.52	0/386
9	I1	0.25	0/287	0.57	0/386
9	i	0.24	0/287	0.57	0/386
9	i1	0.17	0/287	0.45	0/386
10	J	0.15	0/272	0.38	0/369
10	J1	0.14	0/272	0.39	0/369
10	j	0.18	0/272	0.39	0/369
10	j1	0.18	0/272	0.43	0/369
11	K	0.27	0/308	0.74	1/423 (0.2%)
11	K1	0.27	0/308	0.69	0/423
11	k	0.29	0/308	0.65	0/423
11	k1	0.29	0/308	0.62	1/423 (0.2%)
12	L	0.36	0/321	0.66	1/435 (0.2%)
12	L1	0.19	0/321	0.53	0/435
12	l	0.18	0/321	0.42	0/435
13	M	0.22	0/246	0.55	0/335
13	m	0.25	0/246	0.62	0/335
14	O	0.22	0/1855	0.55	0/2505
14	O1	0.20	0/1855	0.52	0/2505
14	o	0.21	0/1855	0.55	0/2505
14	o1	0.20	0/1855	0.54	0/2505
15	P	0.18	0/1473	0.50	0/1988
15	P1	0.19	0/1473	0.50	1/1988 (0.1%)
15	p	0.15	0/1473	0.41	0/1988
15	p1	0.16	0/1473	0.50	2/1988 (0.1%)
16	T	0.23	0/254	0.58	0/342
16	T1	0.22	0/254	0.51	0/342
16	t	0.22	0/254	0.61	0/342
16	t1	0.20	0/254	0.49	0/342
17	W	0.20	0/339	0.51	0/460
17	W1	0.19	0/339	0.52	0/460
17	w	0.19	0/339	0.44	0/460
17	w1	0.19	0/339	0.44	0/460
18	X	0.18	0/202	0.44	0/276
18	X1	0.19	0/202	0.49	0/276
18	x	0.20	0/202	0.49	0/276
18	x1	0.19	0/202	0.43	0/276
19	Z	0.21	0/469	0.53	0/641
19	Z1	0.13	0/469	0.39	0/641
19	z	0.18	0/469	0.40	0/641
19	z1	0.16	0/469	0.44	0/641
20	N	0.23	0/1751	0.56	1/2386 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	N1	0.20	0/1751	0.51	0/2386
20	n	0.26	0/1751	0.69	4/2386 (0.2%)
20	n1	0.17	0/1750	0.46	0/2382
21	G	0.22	0/1725	0.61	0/2348
21	G1	0.18	0/1725	0.48	0/2348
21	g	0.22	0/1725	0.53	0/2348
21	g1	0.18	0/1725	0.49	0/2348
22	R	0.18	0/1561	0.46	0/2110
22	r	0.19	0/1561	0.49	0/2110
23	S	0.21	0/1895	0.53	1/2579 (0.0%)
23	S1	0.17	0/1903	0.49	0/2590
23	s	0.20	0/1902	0.53	0/2587
23	s1	0.18	0/1903	0.52	1/2590 (0.0%)
24	Y	0.31	0/1715	0.68	2/2338 (0.1%)
24	Y1	0.22	0/1715	0.49	1/2338 (0.0%)
24	y	0.39	2/1715 (0.1%)	0.73	4/2338 (0.2%)
24	y1	0.18	0/1715	0.47	0/2338
25	U	0.21	0/224	0.56	0/298
25	U1	0.22	0/224	0.54	0/298
25	u	0.23	0/224	0.70	0/298
25	u1	0.27	0/224	0.57	0/298
26	M1	0.23	0/237	0.58	0/323
26	m1	0.23	0/237	0.60	0/323
27	R1	0.16	0/1506	0.39	0/2035
27	r1	0.18	0/1506	0.52	0/2035
All	All	0.35	11/118105 (0.0%)	0.54	43/160649 (0.0%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	57	PHE	CD2-CE2	42.12	2.65	1.38
8	H	57	PHE	CD1-CE1	40.91	2.61	1.38
8	H	57	PHE	CE2-CZ	39.71	2.57	1.38
8	H	57	PHE	CE1-CZ	39.38	2.56	1.38
8	H	57	PHE	CG-CD2	27.71	1.97	1.38

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	185	PRO	N-CD-CG	-17.70	76.65	103.20
4	c	374	PRO	N-CD-CG	-16.63	78.26	103.20
2	B	88	PRO	N-CD-CG	-13.67	82.69	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	185	PRO	CB-CG-CD	12.76	146.92	106.10
24	y	185	PRO	CA-CB-CG	-11.76	82.17	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2638	0	2541	81	0
1	A1	2638	0	2541	119	0
1	a	2638	0	2541	103	0
1	a1	2638	0	2541	108	0
2	B	3783	0	3663	90	0
2	B1	3783	0	3663	138	0
2	b	3783	0	3663	104	0
2	b1	3783	0	3663	126	0
3	V	227	0	261	3	0
3	V1	227	0	261	6	0
3	v	227	0	261	7	0
3	v1	227	0	261	5	0
4	C	3483	0	3376	102	0
4	C1	3483	0	3376	118	0
4	c	3483	0	3376	126	0
4	c1	3483	0	3376	124	0
5	D	2766	0	2654	87	0
5	D1	2766	0	2654	115	0
5	d	2766	0	2655	95	0
5	d1	2766	0	2655	108	0
6	E	621	0	605	8	0
6	E1	621	0	605	13	0
6	e	621	0	605	16	0
6	e1	621	0	605	11	0
7	F	252	0	265	5	0
7	F1	252	0	265	8	0
7	f	252	0	265	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	f1	252	0	265	7	0
8	H	503	0	532	38	0
8	H1	503	0	532	20	0
8	h	503	0	532	15	0
8	h1	503	0	532	29	0
9	I	279	0	288	9	0
9	I1	279	0	288	14	0
9	i	279	0	288	15	0
9	i1	279	0	288	9	0
10	J	266	0	286	4	0
10	J1	266	0	286	6	0
10	j	266	0	286	10	0
10	j1	266	0	286	3	0
11	K	297	0	312	9	0
11	K1	297	0	312	17	0
11	k	297	0	312	14	0
11	k1	297	0	312	15	0
12	L	313	0	325	13	0
12	L1	313	0	325	11	0
12	l	313	0	325	10	0
13	M	243	0	264	6	0
13	m	243	0	264	7	0
14	O	1820	0	1776	52	0
14	O1	1820	0	1776	57	0
14	o	1820	0	1776	56	0
14	o1	1820	0	1776	46	0
15	P	1444	0	1403	23	0
15	P1	1444	0	1403	32	0
15	p	1444	0	1403	16	0
15	p1	1444	0	1403	26	0
16	T	247	0	260	3	0
16	T1	247	0	260	7	0
16	t	247	0	260	6	0
16	t1	247	0	260	8	0
17	W	332	0	323	7	0
17	W1	332	0	323	14	0
17	w	332	0	323	4	0
17	w1	332	0	323	10	0
18	X	201	0	224	3	0
18	X1	201	0	224	5	0
18	x	201	0	224	4	0
18	x1	201	0	224	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Z	457	0	478	10	0
19	Z1	457	0	478	2	0
19	z	457	0	478	11	0
19	z1	457	0	478	2	0
20	N	1703	0	1641	44	0
20	N1	1703	0	1641	40	0
20	n	1703	0	1641	44	0
20	n1	1703	0	1641	30	0
21	G	1680	0	1614	51	0
21	G1	1680	0	1614	37	0
21	g	1680	0	1614	45	0
21	g1	1680	0	1614	42	0
22	R	1533	0	1506	29	0
22	r	1533	0	1506	33	0
23	S	1849	0	1808	41	0
23	S1	1856	0	1816	32	0
23	s	1856	0	1815	41	0
23	s1	1856	0	1816	32	0
24	Y	1667	0	1624	43	0
24	Y1	1667	0	1624	51	0
24	y	1667	0	1624	45	0
24	y1	1667	0	1624	52	0
25	U	224	0	226	5	0
25	U1	224	0	226	5	0
25	u	224	0	226	7	0
25	u1	224	0	226	8	0
26	M1	234	0	258	11	0
26	m1	234	0	258	9	0
27	R1	1490	0	1454	25	0
27	r1	1490	0	1454	27	0
28	A	10	0	0	0	0
28	A1	10	0	0	1	0
28	a	10	0	0	1	0
28	a1	10	0	0	0	0
29	A	1	0	0	0	0
29	A1	1	0	0	0	0
29	a	1	0	0	0	0
29	a1	1	0	0	0	0
30	A	2	0	0	1	0
30	A1	2	0	0	0	0
30	a	2	0	0	1	0
30	a1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	A	239	0	240	23	0
31	A1	240	0	239	16	0
31	B	1040	0	1143	69	0
31	B1	1040	0	1148	77	0
31	C	845	0	934	57	0
31	C1	845	0	929	66	0
31	D	130	0	144	7	0
31	D1	130	0	144	11	0
31	G	446	0	426	22	0
31	G1	466	0	467	24	0
31	N	468	0	467	22	0
31	N1	468	0	468	24	0
31	R	501	0	455	19	0
31	R1	409	0	391	17	0
31	S	625	0	587	24	0
31	S1	625	0	585	27	0
31	Y	570	0	611	33	0
31	Y1	570	0	611	37	0
31	a	239	0	239	14	0
31	a1	239	0	240	18	0
31	b	1040	0	1144	67	0
31	b1	1040	0	1146	88	0
31	c	845	0	930	57	0
31	c1	845	0	930	75	0
31	d	130	0	143	8	0
31	d1	130	0	143	8	0
31	g	446	0	427	22	0
31	g1	466	0	466	24	0
31	n	468	0	467	27	0
31	n1	468	0	468	21	0
31	r	501	0	453	15	0
31	r1	409	0	392	29	0
31	s	625	0	585	25	0
31	s1	625	0	585	28	0
31	y	570	0	612	50	0
31	y1	570	0	613	52	0
32	A	128	0	148	8	0
32	A1	128	0	148	9	0
32	a	128	0	148	9	0
32	a1	128	0	148	10	0
33	A	40	0	53	2	0
33	A1	40	0	53	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	B	80	0	106	6	0
33	B1	80	0	106	9	0
33	C	160	0	211	20	0
33	C1	160	0	211	25	0
33	D	40	0	54	1	0
33	D1	40	0	53	1	0
33	a	40	0	53	4	0
33	a1	40	0	53	4	0
33	b	80	0	106	5	0
33	b1	80	0	106	5	0
33	c	160	0	211	20	0
33	c1	160	0	212	31	0
33	d	40	0	53	5	0
33	d1	40	0	53	5	0
34	A	51	0	68	4	0
34	A1	51	0	68	2	0
34	B	54	0	77	3	0
34	B1	96	0	124	6	0
34	C	54	0	77	2	0
34	C1	54	0	77	2	0
34	M1	42	0	47	6	0
34	a	51	0	68	4	0
34	a1	51	0	68	7	0
34	b	54	0	77	2	0
34	b1	96	0	124	14	0
34	c	54	0	77	2	0
34	c1	54	0	77	5	0
34	m1	42	0	47	3	0
35	A	48	0	66	12	0
35	A1	48	0	66	7	0
35	B	44	0	58	3	0
35	B1	44	0	58	9	0
35	C	51	0	72	7	0
35	C1	106	0	158	14	0
35	D	46	0	62	3	0
35	D1	46	0	62	3	0
35	H	48	0	66	4	0
35	H1	48	0	66	5	0
35	J	45	0	60	2	0
35	W1	39	0	48	4	0
35	a	48	0	66	6	0
35	a1	48	0	66	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	b	44	0	58	5	0
35	b1	44	0	58	6	0
35	c	51	0	72	3	0
35	c1	106	0	158	17	0
35	d	46	0	62	4	0
35	d1	46	0	62	2	0
35	h	48	0	66	6	0
35	h1	48	0	66	3	0
35	j	45	0	60	5	0
35	w1	39	0	48	3	0
36	A	1	0	0	0	0
36	A1	1	0	0	0	0
36	a	1	0	0	0	0
36	a1	1	0	0	0	0
37	B	42	0	0	0	0
37	B1	42	0	0	0	0
37	b	42	0	0	0	0
37	b1	42	0	0	0	0
38	B	44	0	76	4	0
38	B1	44	0	76	5	0
38	C	44	0	76	2	0
38	C1	44	0	76	4	0
38	J1	29	0	40	2	0
38	b	44	0	76	3	0
38	b1	44	0	76	5	0
38	c	44	0	76	0	0
38	c1	44	0	76	3	0
38	j1	29	0	40	3	0
39	B	6	0	8	0	0
39	I1	6	0	8	0	0
39	b	12	0	16	2	0
39	y	6	0	8	0	0
40	B1	43	0	44	5	0
40	C	242	0	322	24	0
40	C1	176	0	226	24	0
40	b1	43	0	44	1	0
40	c	242	0	322	25	0
40	c1	176	0	226	24	0
41	C	47	0	67	1	0
41	C1	47	0	67	9	0
41	D	132	0	183	10	0
41	D1	132	0	183	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	G	49	0	74	6	0
41	G1	49	0	74	3	0
41	L	49	0	74	3	0
41	L1	49	0	74	9	0
41	N	49	0	74	0	0
41	N1	49	0	74	4	0
41	S	45	0	63	8	0
41	S1	45	0	63	6	0
41	Y	49	0	74	4	0
41	Y1	49	0	74	7	0
41	c	47	0	67	4	0
41	c1	47	0	67	9	0
41	d	132	0	183	10	0
41	d1	132	0	183	11	0
41	g	49	0	74	7	0
41	g1	49	0	74	5	0
41	l	49	0	74	9	0
41	n	49	0	74	7	0
41	n1	49	0	74	4	0
41	s	45	0	63	7	0
41	s1	45	0	63	3	0
41	y	49	0	74	7	0
41	y1	49	0	74	7	0
42	C	40	0	0	0	0
42	C1	40	0	0	1	0
42	c	40	0	0	0	0
42	c1	40	0	0	0	0
43	D	4	0	1	0	0
43	D1	4	0	1	0	0
43	d	4	0	1	0	0
43	d1	4	0	1	0	0
44	D	55	0	80	6	0
44	D1	55	0	80	8	0
44	d	55	0	80	4	0
44	d1	55	0	80	6	0
45	F	43	0	30	2	0
45	F1	43	0	30	1	0
45	f	43	0	30	5	0
45	f1	43	0	30	0	0
46	H	41	0	56	26	0
46	H1	41	0	56	5	0
46	h	41	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	h1	41	0	56	9	0
47	G	324	0	274	16	0
47	G1	340	0	305	16	0
47	N	380	0	383	21	0
47	N1	380	0	383	17	0
47	R	94	0	66	4	0
47	R1	94	0	67	4	0
47	S	194	0	144	14	0
47	S1	194	0	145	10	0
47	Y	310	0	307	17	0
47	Y1	310	0	307	14	0
47	g	324	0	274	16	0
47	g1	340	0	305	20	0
47	n	380	0	382	28	0
47	n1	380	0	381	19	0
47	r	94	0	66	3	0
47	r1	94	0	66	3	0
47	s	194	0	144	10	0
47	s1	194	0	144	10	0
47	y	310	0	306	14	0
47	y1	310	0	307	18	0
48	G	84	0	110	16	0
48	G1	84	0	110	7	0
48	N	84	0	110	6	0
48	N1	84	0	110	11	0
48	R	42	0	55	5	0
48	R1	42	0	55	6	0
48	S	84	0	110	9	0
48	S1	84	0	110	11	0
48	Y	84	0	110	10	0
48	Y1	84	0	110	15	0
48	g	84	0	110	14	0
48	g1	84	0	110	10	0
48	n	84	0	110	11	0
48	n1	84	0	110	12	0
48	r	42	0	55	3	0
48	r1	42	0	55	6	0
48	s	84	0	110	14	0
48	s1	84	0	110	9	0
48	y	84	0	110	11	0
48	y1	84	0	110	11	0
49	G	44	0	56	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	G1	44	0	56	8	0
49	N	44	0	56	5	0
49	N1	44	0	56	8	0
49	R	44	0	56	3	0
49	R1	44	0	56	3	0
49	Y	44	0	56	3	0
49	Y1	44	0	56	9	0
49	g	44	0	56	6	0
49	g1	44	0	56	8	0
49	n	44	0	56	5	0
49	n1	44	0	56	8	0
49	r	44	0	56	6	0
49	r1	44	0	56	4	0
49	y	44	0	56	5	0
49	y1	44	0	56	9	0
50	G	44	0	54	3	0
50	G1	44	0	54	0	0
50	N	44	0	54	2	0
50	N1	44	0	54	4	0
50	R	44	0	54	3	0
50	R1	44	0	54	4	0
50	S	44	0	54	2	0
50	S1	44	0	54	4	0
50	Y	44	0	54	0	0
50	Y1	44	0	54	2	0
50	g	44	0	54	0	0
50	g1	44	0	54	1	0
50	n	44	0	54	3	0
50	n1	44	0	54	0	0
50	r	44	0	54	0	0
50	r1	44	0	54	1	0
50	s	44	0	54	2	0
50	s1	44	0	54	1	0
50	y	44	0	54	0	0
50	y1	44	0	54	1	0
51	S	30	0	43	2	0
51	S1	30	0	43	0	0
51	s	30	0	43	1	0
51	s1	30	0	43	2	0
52	B1	48	0	75	10	0
52	S	48	0	75	3	0
52	S1	48	0	75	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	T1	48	0	75	1	0
52	b1	48	0	75	6	0
52	i	48	0	75	1	0
52	s	48	0	75	1	0
52	s1	48	0	75	3	0
52	t1	48	0	75	4	0
53	A1	21	0	37	5	0
53	Y	21	0	37	3	0
53	Y1	21	0	37	3	0
53	a1	21	0	37	5	0
53	y	21	0	37	4	0
53	y1	21	0	37	7	0
54	I1	57	0	98	3	0
54	K1	57	0	98	6	0
54	i1	57	0	98	5	0
54	k1	57	0	98	3	0
55	R1	35	0	45	0	0
55	r1	35	0	46	3	0
56	R1	29	0	38	8	0
56	r1	29	0	38	5	0
57	Y1	69	0	90	7	0
57	y1	69	0	90	5	0
All	All	151508	0	153084	4168	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 14.

The worst 5 of 4168 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)
8:H:57:PHE:CD2	8:H:57:PHE:CG	1.97	1.52
8:H:57:PHE:CG	8:H:57:PHE:CD1	1.96	1.49
56:r1:626:ERG:O1	56:r1:626:ERG:C3	1.70	1.37
56:R1:626:ERG:O1	56:R1:626:ERG:C3	1.70	1.36
24:y:76:LEU:CD1	31:y:602:CLA:H42	1.68	1.22

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	335/336 (100%)	304 (91%)	30 (9%)	1 (0%)	36	70
1	A1	335/336 (100%)	313 (93%)	22 (7%)	0	100	100
1	a	335/336 (100%)	313 (93%)	22 (7%)	0	100	100
1	a1	335/336 (100%)	316 (94%)	19 (6%)	0	100	100
2	B	482/484 (100%)	460 (95%)	21 (4%)	1 (0%)	43	75
2	B1	482/484 (100%)	459 (95%)	23 (5%)	0	100	100
2	b	482/484 (100%)	454 (94%)	28 (6%)	0	100	100
2	b1	482/484 (100%)	462 (96%)	20 (4%)	0	100	100
3	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	V1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	v	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	410 (92%)	34 (8%)	3 (1%)	18	54
4	C1	447/449 (100%)	427 (96%)	20 (4%)	0	100	100
4	c	447/449 (100%)	413 (92%)	31 (7%)	3 (1%)	18	54
4	c1	447/449 (100%)	425 (95%)	22 (5%)	0	100	100
5	D	346/348 (99%)	330 (95%)	15 (4%)	1 (0%)	36	70
5	D1	346/348 (99%)	332 (96%)	14 (4%)	0	100	100
5	d	346/348 (99%)	332 (96%)	13 (4%)	1 (0%)	36	70
5	d1	346/348 (99%)	331 (96%)	15 (4%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	E1	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
6	e	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
6	e1	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	F1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
7	f1	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	H1	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	h	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
8	h1	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	I1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
9	i1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
10	J	34/36 (94%)	34 (100%)	0	0	100	100
10	J1	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
10	j1	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
11	K1	35/37 (95%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	k1	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	L1	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	30/32 (94%)	29 (97%)	0	1 (3%)	3	24
13	m	30/32 (94%)	28 (93%)	1 (3%)	1 (3%)	3	24
14	O	236/238 (99%)	210 (89%)	25 (11%)	1 (0%)	30	65
14	O1	236/238 (99%)	214 (91%)	21 (9%)	1 (0%)	30	65
14	o	236/238 (99%)	215 (91%)	20 (8%)	1 (0%)	30	65
14	o1	236/238 (99%)	217 (92%)	18 (8%)	1 (0%)	30	65
15	P	185/187 (99%)	167 (90%)	17 (9%)	1 (0%)	24	60
15	P1	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	173 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	p1	185/187 (99%)	171 (92%)	14 (8%)	0	100	100
16	T	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	2	23
16	T1	28/30 (93%)	27 (96%)	0	1 (4%)	2	23
16	t	28/30 (93%)	27 (96%)	0	1 (4%)	2	23
16	t1	28/30 (93%)	28 (100%)	0	0	100	100
17	W	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
17	W1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	X1	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
18	x1	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	Z1	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
19	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
19	z1	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24	60
20	N1	220/222 (99%)	201 (91%)	18 (8%)	1 (0%)	24	60
20	n	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	14	48
20	n1	218/222 (98%)	198 (91%)	19 (9%)	1 (0%)	24	60
21	G	219/221 (99%)	203 (93%)	15 (7%)	1 (0%)	24	60
21	G1	219/221 (99%)	201 (92%)	18 (8%)	0	100	100
21	g	219/221 (99%)	209 (95%)	9 (4%)	1 (0%)	24	60
21	g1	219/221 (99%)	202 (92%)	17 (8%)	0	100	100
22	R	198/202 (98%)	188 (95%)	10 (5%)	0	100	100
22	r	198/202 (98%)	181 (91%)	17 (9%)	0	100	100
23	S	240/243 (99%)	218 (91%)	20 (8%)	2 (1%)	16	52
23	S1	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	10	42
23	s	239/243 (98%)	219 (92%)	18 (8%)	2 (1%)	16	52
23	s1	241/243 (99%)	219 (91%)	20 (8%)	2 (1%)	16	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	Y	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	24	60
24	Y1	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	24	60
24	y	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	24	60
24	y1	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	24	60
25	U	25/27 (93%)	25 (100%)	0	0	100	100
25	U1	25/27 (93%)	25 (100%)	0	0	100	100
25	u	25/27 (93%)	25 (100%)	0	0	100	100
25	u1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
26	M1	29/31 (94%)	29 (100%)	0	0	100	100
26	m1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
27	R1	191/202 (95%)	183 (96%)	8 (4%)	0	100	100
27	r1	191/202 (95%)	181 (95%)	10 (5%)	0	100	100
All	All	14651/14872 (98%)	13772 (94%)	839 (6%)	40 (0%)	37	70

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	257	GLU
4	C	395	VAL
14	O	94	VAL
4	c	257	GLU
4	c	395	VAL

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	276/275 (100%)	276 (100%)	0	100	100
1	A1	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	276 (100%)	0	100	100
1	a1	276/275 (100%)	276 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	388/388 (100%)	388 (100%)	0	100	100
2	B1	388/388 (100%)	388 (100%)	0	100	100
2	b	388/388 (100%)	388 (100%)	0	100	100
2	b1	388/388 (100%)	388 (100%)	0	100	100
3	V	25/25 (100%)	25 (100%)	0	100	100
3	V1	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
3	v1	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	C1	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
4	c1	350/350 (100%)	350 (100%)	0	100	100
5	D	279/279 (100%)	279 (100%)	0	100	100
5	D1	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	279 (100%)	0	100	100
5	d1	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	E1	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
6	e1	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	F1	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
7	f1	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	H1	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
8	h1	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	I1	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	i1	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	J1	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
10	j1	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	K1	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
11	k1	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	L1	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	27/27 (100%)	27 (100%)	0	100	100
13	m	27/27 (100%)	27 (100%)	0	100	100
14	O	195/195 (100%)	195 (100%)	0	100	100
14	O1	195/195 (100%)	195 (100%)	0	100	100
14	o	195/195 (100%)	195 (100%)	0	100	100
14	o1	195/195 (100%)	195 (100%)	0	100	100
15	P	151/151 (100%)	151 (100%)	0	100	100
15	P1	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	151 (100%)	0	100	100
15	p1	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	T1	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
16	t1	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	W1	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
17	w1	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X1	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
18	x1	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	Z1	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
19	z1	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
20	N1	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	171 (100%)	0	100	100
20	n1	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	G1	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
21	g1	168/168 (100%)	168 (100%)	0	100	100
22	R	158/158 (100%)	158 (100%)	0	100	100
22	r	158/158 (100%)	158 (100%)	0	100	100
23	S	189/190 (100%)	189 (100%)	0	100	100
23	S1	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
23	s1	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	Y1	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
24	y1	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	U1	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
25	u1	26/26 (100%)	25 (96%)	1 (4%)	29	51
26	M1	26/26 (100%)	26 (100%)	0	100	100
26	m1	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	R1	151/157 (96%)	151 (100%)	0	100	100
27	r1	151/157 (96%)	151 (100%)	0	100	100
All	All	11856/11865 (100%)	11855 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	u1	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
5	d1	239	GLN
14	o1	150	ASN
23	s1	161	ASN
5	d	220	ASN
5	d	189	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
27	SEP	R1	84	27	8,9,10	1.62	1 (12%)	7,12,14	1.53	1 (14%)
27	SEP	r1	84	27	8,9,10	1.62	1 (12%)	7,12,14	1.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SEP	R1	84	27	-	3/6/8/10	-
27	SEP	r1	84	27	-	3/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	r1	84	SEP	P-O1P	3.55	1.61	1.50
27	R1	84	SEP	P-O1P	3.52	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R1	84	SEP	OG-CB-CA	3.54	111.59	108.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	R1	84	SEP	CB-OG-P-O1P
27	R1	84	SEP	CB-OG-P-O2P
27	R1	84	SEP	CB-OG-P-O3P
27	r1	84	SEP	CB-OG-P-O2P
27	r1	84	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	r1	84	SEP	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 703 ligands modelled in this entry, 16 are monoatomic - leaving 687 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
48	LUT	s	620	-	42,43,43	2.49	1 (2%)	51,60,60	2.27	19 (37%)
31	CLA	c	508	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	15 (18%)
31	CLA	g	613	-	69,73,73	1.37	8 (11%)	82,113,113	1.91	19 (23%)
47	CHL	g1	607	-	60,74,74	1.21	8 (13%)	58,114,114	1.77	12 (20%)
33	BCR	C1	514	-	41,41,41	1.62	4 (9%)	56,56,56	4.61	16 (28%)
47	CHL	s1	601	23	40,54,74	1.62	7 (17%)	34,90,114	2.28	10 (29%)
31	CLA	c	507	-	69,73,73	1.37	7 (10%)	82,113,113	1.93	19 (23%)
47	CHL	n1	609	-	60,74,74	1.25	8 (13%)	58,114,114	1.64	10 (17%)
31	CLA	D1	403	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	18 (21%)
52	3PH	t1	101	-	47,47,47	0.88	4 (8%)	50,52,52	1.14	2 (4%)
31	CLA	A	406	-	69,73,73	1.35	6 (8%)	82,113,113	1.94	14 (17%)
33	BCR	D1	404	-	41,41,41	1.59	4 (9%)	56,56,56	4.34	13 (23%)
35	LMG	A	413	-	48,48,55	1.12	5 (10%)	56,56,63	1.15	3 (5%)
31	CLA	Y	612	-	69,73,73	1.37	8 (11%)	82,113,113	1.90	19 (23%)
47	CHL	G	605	21	42,56,74	1.48	7 (16%)	36,92,114	2.10	11 (30%)
48	LUT	s	621	-	42,43,43	2.43	1 (2%)	51,60,60	1.82	14 (27%)
31	CLA	y1	612	-	69,73,73	1.36	8 (11%)	82,113,113	1.88	17 (20%)
48	LUT	N	621	-	42,43,43	2.46	1 (2%)	51,60,60	1.95	12 (23%)
48	LUT	r1	620	-	42,43,43	2.47	1 (2%)	51,60,60	2.12	15 (29%)
31	CLA	R	613	-	50,54,73	1.58	7 (14%)	59,90,113	2.12	17 (28%)
35	LMG	h	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.11	3 (5%)
35	LMG	C1	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.12	4 (6%)
32	PHO	A	408	-	58,69,69	2.13	10 (17%)	55,99,99	1.50	7 (12%)
33	BCR	c	517	-	41,41,41	1.64	4 (9%)	56,56,56	4.50	14 (25%)
31	CLA	R1	610	-	64,68,73	1.39	7 (10%)	76,107,113	1.91	19 (25%)
31	CLA	c1	511	-	69,73,73	1.36	7 (10%)	82,113,113	2.03	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	a1	405	-	69,73,73	1.35	6 (8%)	82,113,113	1.97	22 (26%)
31	CLA	C	509	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	16 (19%)
31	CLA	Y1	610	-	69,73,73	1.33	6 (8%)	82,113,113	1.96	18 (21%)
45	HEM	F1	101	6	50,50,50	1.42	7 (14%)	67,82,82	1.04	1 (1%)
41	LHG	D	408	-	43,43,48	0.42	0	46,49,54	1.08	3 (6%)
47	CHL	y	601	24	60,74,74	1.30	9 (15%)	58,114,114	1.66	13 (22%)
47	CHL	y1	606	-	60,74,74	1.38	8 (13%)	58,114,114	1.63	12 (20%)
31	CLA	r	608	-	64,68,73	1.41	7 (10%)	76,107,113	1.95	16 (21%)
50	NEX	y	623	-	40,46,46	2.62	10 (25%)	50,70,70	1.89	14 (28%)
35	LMG	b	622	-	44,44,55	0.98	3 (6%)	52,52,63	1.12	3 (5%)
31	CLA	b	605	-	69,73,73	1.36	6 (8%)	82,113,113	2.01	17 (20%)
31	CLA	c	510	-	69,73,73	1.36	8 (11%)	82,113,113	1.93	18 (21%)
47	CHL	R1	607	-	44,58,74	1.54	8 (18%)	37,94,114	2.10	12 (32%)
31	CLA	y1	613	-	69,73,73	1.33	6 (8%)	82,113,113	1.89	18 (21%)
31	CLA	b1	616	-	69,73,73	1.37	7 (10%)	82,113,113	1.83	16 (19%)
31	CLA	G1	602	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	18 (21%)
38	DGA	B	625	-	43,43,43	1.16	2 (4%)	45,45,45	1.50	3 (6%)
31	CLA	b1	606	-	69,73,73	1.37	7 (10%)	82,113,113	1.86	17 (20%)
44	PL9	D1	405	-	55,55,55	1.01	5 (9%)	68,69,69	1.59	11 (16%)
31	CLA	r	604	-	53,57,73	1.53	8 (15%)	61,93,113	2.15	17 (27%)
46	RRX	H1	101	-	42,42,42	4.97	24 (57%)	56,58,58	2.72	19 (33%)
31	CLA	b	608	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	17 (20%)
55	LMT	R1	625	-	36,36,36	1.14	5 (13%)	47,47,47	1.01	2 (4%)
39	GOL	b	625	-	5,5,5	0.59	0	5,5,5	0.34	0
31	CLA	g1	603	-	69,73,73	1.35	8 (11%)	82,113,113	1.92	21 (25%)
31	CLA	s	604	-	59,63,73	1.45	6 (10%)	70,101,113	2.04	19 (27%)
34	SQD	A1	412	-	49,51,54	0.81	1 (2%)	59,62,65	0.86	2 (3%)
31	CLA	y	611	-	69,73,73	1.35	7 (10%)	82,113,113	1.87	18 (21%)
31	CLA	b1	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	14 (17%)
31	CLA	B1	605	-	69,73,73	1.33	6 (8%)	82,113,113	1.99	21 (25%)
31	CLA	n1	613	-	69,73,73	1.36	7 (10%)	82,113,113	2.00	21 (25%)
31	CLA	b1	602	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	17 (20%)
31	CLA	S	614	-	59,63,73	1.47	6 (10%)	70,101,113	1.96	16 (22%)
40	DGD	C	518	-	56,56,67	1.07	4 (7%)	70,70,81	1.02	3 (4%)
31	CLA	S1	605	-	54,58,73	1.55	7 (12%)	64,95,113	2.16	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	CHL	Y1	606	-	60,74,74	1.50	7 (11%)	58,114,114	1.75	12 (20%)
31	CLA	g1	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	18 (21%)
50	NEX	g1	623	-	40,46,46	2.71	11 (27%)	50,70,70	2.30	13 (26%)
31	CLA	B	617	-	69,73,73	1.37	6 (8%)	82,113,113	4.00	18 (21%)
31	CLA	R1	608	-	64,68,73	1.42	8 (12%)	76,107,113	1.92	19 (25%)
31	CLA	B1	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	21 (25%)
31	CLA	Y1	608	-	54,58,73	1.55	8 (14%)	64,95,113	2.11	17 (26%)
34	SQD	A	412	-	49,51,54	0.80	0	59,62,65	0.86	2 (3%)
31	CLA	S1	603	-	69,73,73	1.36	6 (8%)	82,113,113	2.00	21 (25%)
56	ERG	r1	626	-	32,32,32	7.98	20 (62%)	45,50,50	3.30	16 (35%)
48	LUT	n1	620	-	42,43,43	2.53	1 (2%)	51,60,60	1.70	12 (23%)
31	CLA	R1	604	-	53,57,73	1.53	7 (13%)	61,93,113	2.23	15 (24%)
33	BCR	a	411	-	41,41,41	1.63	5 (12%)	56,56,56	4.50	14 (25%)
35	LMG	B	622	-	44,44,55	0.96	3 (6%)	52,52,63	1.03	2 (3%)
31	CLA	A	407	-	53,57,73	1.55	7 (13%)	61,93,113	2.13	16 (26%)
31	CLA	b1	615	-	69,73,73	1.37	6 (8%)	82,113,113	1.86	18 (21%)
47	CHL	Y1	601	24	60,74,74	1.37	9 (15%)	58,114,114	1.90	12 (20%)
40	DGD	C	520	-	60,60,67	1.17	6 (10%)	74,74,81	1.00	2 (2%)
31	CLA	B1	614	-	69,73,73	1.35	6 (8%)	82,113,113	1.82	18 (21%)
41	LHG	G	630	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
31	CLA	b	602	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	19 (23%)
31	CLA	b	615	-	69,73,73	1.37	8 (11%)	82,113,113	2.06	19 (23%)
31	CLA	Y	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	18 (21%)
31	CLA	b1	612	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	16 (19%)
48	LUT	n1	621	-	42,43,43	2.50	1 (2%)	51,60,60	2.05	14 (27%)
47	CHL	n1	606	-	60,74,74	1.15	7 (11%)	58,114,114	1.77	11 (18%)
38	DGA	b1	625	-	43,43,43	1.16	3 (6%)	45,45,45	1.47	3 (6%)
31	CLA	s1	603	-	69,73,73	1.36	8 (11%)	82,113,113	2.00	18 (21%)
31	CLA	b	613	-	69,73,73	1.38	6 (8%)	82,113,113	1.80	13 (15%)
33	BCR	d1	404	-	41,41,41	1.62	5 (12%)	56,56,56	4.37	16 (28%)
31	CLA	g	603	-	69,73,73	1.36	7 (10%)	82,113,113	1.96	18 (21%)
41	LHG	n1	624	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
31	CLA	A1	406	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	18 (21%)
33	BCR	b1	619	-	41,41,41	1.61	4 (9%)	56,56,56	4.54	13 (23%)
44	PL9	d1	405	-	55,55,55	1.01	2 (3%)	68,69,69	1.54	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	G1	614	-	53,57,73	1.55	7 (13%)	61,93,113	2.17	16 (26%)
55	LMT	r1	625	-	36,36,36	1.15	6 (16%)	47,47,47	1.00	2 (4%)
47	CHL	y1	601	24	60,74,74	1.43	9 (15%)	58,114,114	1.90	11 (18%)
31	CLA	b	606	-	69,73,73	1.34	7 (10%)	82,113,113	1.96	13 (15%)
35	LMG	c1	523	-	55,55,55	1.28	6 (10%)	63,63,63	1.03	2 (3%)
31	CLA	C1	504	-	69,73,73	1.34	6 (8%)	82,113,113	1.95	16 (19%)
31	CLA	r1	612	-	64,68,73	1.43	8 (12%)	76,107,113	1.92	20 (26%)
49	XAT	G	622	-	41,47,47	0.71	1 (2%)	54,74,74	1.91	14 (25%)
42	LMK	C	527	-	39,39,53	1.55	3 (7%)	39,46,60	1.30	2 (5%)
41	LHG	d	410	-	38,38,48	0.43	0	41,44,54	1.19	3 (7%)
31	CLA	B	609	-	69,73,73	1.39	7 (10%)	82,113,113	1.97	20 (24%)
31	CLA	C	506	-	69,73,73	1.37	7 (10%)	82,113,113	1.91	19 (23%)
31	CLA	b	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.84	15 (18%)
31	CLA	g	604	-	53,57,73	1.57	8 (15%)	61,93,113	2.17	18 (29%)
47	CHL	y1	607	-	60,74,74	1.07	7 (11%)	58,114,114	1.90	12 (20%)
54	4RF	i1	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.93	3 (5%)
31	CLA	b	612	-	69,73,73	1.37	7 (10%)	82,113,113	1.86	18 (21%)
31	CLA	B1	606	-	69,73,73	1.36	7 (10%)	82,113,113	1.98	17 (20%)
31	CLA	B1	608	-	69,73,73	1.37	6 (8%)	82,113,113	1.92	17 (20%)
31	CLA	C	510	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	19 (23%)
47	CHL	r1	606	-	38,52,74	1.82	8 (21%)	31,87,114	2.26	10 (32%)
48	LUT	g1	621	-	42,43,43	2.49	1 (2%)	51,60,60	1.77	11 (21%)
31	CLA	Y1	613	-	69,73,73	1.35	7 (10%)	82,113,113	1.97	17 (20%)
31	CLA	r1	609	-	64,68,73	1.41	6 (9%)	76,107,113	1.96	16 (21%)
31	CLA	B	607	-	69,73,73	1.37	8 (11%)	82,113,113	1.86	18 (21%)
40	DGD	C	519	-	63,63,67	1.23	7 (11%)	77,77,81	1.10	5 (6%)
31	CLA	n	602	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	21 (25%)
41	LHG	D1	409	-	48,48,48	0.39	0	51,54,54	1.11	5 (9%)
47	CHL	N1	605	20	60,74,74	1.44	8 (13%)	58,114,114	1.64	12 (20%)
31	CLA	b	614	-	69,73,73	1.34	6 (8%)	82,113,113	1.83	18 (21%)
52	3PH	S1	626	-	47,47,47	0.87	4 (8%)	50,52,52	4.53	4 (8%)
31	CLA	c	504	-	69,73,73	1.34	6 (8%)	82,113,113	2.02	20 (24%)
31	CLA	S1	610	-	69,73,73	1.38	7 (10%)	82,113,113	1.90	21 (25%)
41	LHG	d1	409	-	48,48,48	0.41	0	51,54,54	1.00	2 (3%)
45	HEM	f	101	6,7	50,50,50	1.44	6 (12%)	67,82,82	1.33	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	CHL	g1	608	-	38,52,74	1.68	8 (21%)	31,87,114	2.24	11 (35%)
31	CLA	s	603	-	69,73,73	1.37	8 (11%)	82,113,113	1.82	17 (20%)
31	CLA	Y1	602	-	69,73,73	1.37	7 (10%)	82,113,113	1.85	19 (23%)
45	HEM	F	101	6,7	50,50,50	1.40	6 (12%)	67,82,82	1.30	8 (11%)
47	CHL	s	608	-	55,69,74	1.33	8 (14%)	52,108,114	1.74	13 (25%)
49	XAT	r	622	-	41,47,47	0.70	1 (2%)	54,74,74	2.12	18 (33%)
31	CLA	G	612	-	47,51,73	1.65	7 (14%)	55,86,113	2.13	14 (25%)
50	NEX	R1	622	-	40,46,46	2.67	11 (27%)	50,70,70	1.83	11 (22%)
47	CHL	g1	609	-	60,74,74	1.42	10 (16%)	58,114,114	1.56	12 (20%)
49	XAT	G1	622	-	41,47,47	0.73	1 (2%)	54,74,74	1.88	14 (25%)
31	CLA	s1	611	-	69,73,73	1.38	7 (10%)	82,113,113	1.90	20 (24%)
31	CLA	c1	507	-	69,73,73	1.38	8 (11%)	82,113,113	1.83	18 (21%)
47	CHL	G1	601	21	60,74,74	1.25	8 (13%)	58,114,114	1.70	12 (20%)
54	4RF	I1	102	-	56,56,56	1.08	3 (5%)	59,59,59	0.97	3 (5%)
31	CLA	C1	506	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	19 (23%)
31	CLA	G	602	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	21 (25%)
31	CLA	a1	407	-	53,57,73	1.53	6 (11%)	61,93,113	2.22	20 (32%)
41	LHG	n	624	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
32	PHO	a1	408	-	58,69,69	2.21	10 (17%)	55,99,99	1.50	8 (14%)
49	XAT	g1	622	-	41,47,47	0.74	1 (2%)	54,74,74	1.85	13 (24%)
31	CLA	y	612	-	69,73,73	1.37	6 (8%)	82,113,113	1.89	14 (17%)
31	CLA	B1	616	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	17 (20%)
41	LHG	D1	408	-	43,43,48	0.41	0	46,49,54	1.09	4 (8%)
31	CLA	n	612	-	49,53,73	1.61	6 (12%)	58,89,113	1.98	18 (31%)
50	NEX	Y	623	-	40,46,46	2.63	11 (27%)	50,70,70	2.03	14 (28%)
50	NEX	G1	623	-	40,46,46	2.69	11 (27%)	50,70,70	1.84	12 (24%)
35	LMG	W1	201	-	39,39,55	0.95	2 (5%)	47,47,63	1.22	2 (4%)
48	LUT	S1	621	-	42,43,43	2.46	1 (2%)	51,60,60	1.93	13 (25%)
31	CLA	N1	611	-	53,57,73	1.55	6 (11%)	61,93,113	2.11	16 (26%)
39	GOL	I1	101	-	5,5,5	0.57	0	5,5,5	0.28	0
50	NEX	s1	623	-	40,46,46	2.78	14 (35%)	50,70,70	1.86	10 (20%)
31	CLA	D1	402	-	69,73,73	1.38	6 (8%)	82,113,113	1.83	17 (20%)
47	CHL	Y1	609	-	60,74,74	1.34	8 (13%)	58,114,114	1.62	12 (20%)
34	SQD	b1	626	-	52,54,54	0.79	0	62,65,65	0.84	2 (3%)
31	CLA	c1	512	-	69,73,73	1.38	6 (8%)	82,113,113	1.88	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	C1	509	-	69,73,73	1.33	6 (8%)	82,113,113	1.89	16 (19%)
47	CHL	S	607	-	37,51,74	1.57	8 (21%)	30,86,114	2.34	11 (36%)
33	BCR	B1	619	-	41,41,41	1.63	4 (9%)	56,56,56	4.58	14 (25%)
31	CLA	c	512	-	69,73,73	1.37	7 (10%)	82,113,113	1.82	19 (23%)
31	CLA	y	602	-	69,73,73	1.33	7 (10%)	82,113,113	2.02	20 (24%)
51	LPX	s	625	-	29,29,29	1.04	2 (6%)	31,33,33	0.97	1 (3%)
47	CHL	R	606	-	38,52,74	1.76	9 (23%)	31,87,114	2.22	9 (29%)
31	CLA	r	612	-	64,68,73	1.42	8 (12%)	76,107,113	1.89	18 (23%)
47	CHL	G1	606	-	44,58,74	1.51	8 (18%)	37,94,114	2.19	11 (29%)
41	LHG	G1	624	-	48,48,48	0.40	0	51,54,54	0.99	3 (5%)
31	CLA	b	607	-	69,73,73	1.37	7 (10%)	82,113,113	2.02	20 (24%)
31	CLA	Y	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.95	22 (26%)
31	CLA	y	613	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	17 (20%)
31	CLA	n	604	-	69,73,73	1.34	6 (8%)	82,113,113	2.00	19 (23%)
31	CLA	y1	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.95	21 (25%)
57	PTY	Y1	627	-	18,18,49	1.32	3 (16%)	21,23,54	1.43	2 (9%)
37	C7Z	b	620	-	43,43,43	5.52	26 (60%)	56,60,60	2.19	15 (26%)
31	CLA	g	612	-	47,51,73	1.64	7 (14%)	55,86,113	2.16	17 (30%)
31	CLA	C1	501	-	69,73,73	1.36	8 (11%)	82,113,113	1.91	19 (23%)
47	CHL	S1	607	-	37,51,74	1.67	8 (21%)	30,86,114	2.20	10 (33%)
31	CLA	G1	604	-	53,57,73	1.56	8 (15%)	61,93,113	2.10	20 (32%)
47	CHL	g	609	-	60,74,74	1.48	10 (16%)	58,114,114	1.61	10 (17%)
47	CHL	s	601	23	40,54,74	1.69	8 (20%)	34,90,114	2.17	10 (29%)
31	CLA	S1	617	23	54,58,73	1.53	7 (12%)	64,95,113	2.13	19 (29%)
43	BCT	d	401	29	3,3,3	1.12	0	2,3,3	4.18	2 (100%)
31	CLA	r	613	-	50,54,73	1.59	6 (12%)	59,90,113	2.12	15 (25%)
47	CHL	s	606	-	38,52,74	1.66	8 (21%)	31,87,114	2.16	10 (32%)
31	CLA	c	502	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	18 (21%)
31	CLA	Y	610	-	69,73,73	1.35	7 (10%)	82,113,113	1.94	20 (24%)
33	BCR	c1	517	-	41,41,41	1.64	4 (9%)	56,56,56	4.64	21 (37%)
31	CLA	c	505	-	69,73,73	1.37	7 (10%)	82,113,113	1.90	15 (18%)
31	CLA	B1	612	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	17 (20%)
31	CLA	s1	610	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	17 (20%)
31	CLA	N1	614	-	53,57,73	1.54	7 (13%)	61,93,113	2.23	20 (32%)
31	CLA	n1	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.95	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	g1	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	20 (24%)
35	LMG	H	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.09	2 (3%)
49	XAT	g	622	-	41,47,47	0.70	1 (2%)	54,74,74	1.96	13 (24%)
31	CLA	b	609	-	69,73,73	1.42	7 (10%)	82,113,113	1.98	19 (23%)
31	CLA	Y1	612	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	21 (25%)
40	DGD	c	523	-	67,67,67	1.29	7 (10%)	81,81,81	0.96	2 (2%)
48	LUT	r	620	-	42,43,43	2.46	1 (2%)	51,60,60	2.08	10 (19%)
31	CLA	y	608	-	54,58,73	1.54	7 (12%)	64,95,113	2.11	18 (28%)
40	DGD	c	519	-	63,63,67	1.21	7 (11%)	77,77,81	1.05	3 (3%)
40	DGD	b1	623	-	44,44,67	0.88	2 (4%)	58,58,81	1.17	4 (6%)
47	CHL	G	607	-	44,58,74	1.38	7 (15%)	37,94,114	2.15	10 (27%)
35	LMG	D	411	-	46,46,55	1.02	4 (8%)	54,54,63	1.18	4 (7%)
48	LUT	S	620	-	42,43,43	2.48	1 (2%)	51,60,60	1.91	13 (25%)
31	CLA	b	604	-	69,73,73	1.37	7 (10%)	82,113,113	1.84	17 (20%)
31	CLA	c1	505	-	69,73,73	1.38	8 (11%)	82,113,113	1.86	16 (19%)
49	XAT	r1	621	-	41,47,47	0.69	1 (2%)	54,74,74	1.93	15 (27%)
47	CHL	N	608	-	44,58,74	1.49	7 (15%)	37,94,114	2.11	11 (29%)
31	CLA	y	614	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
35	LMG	D1	411	-	46,46,55	1.04	4 (8%)	54,54,63	1.08	2 (3%)
47	CHL	y	606	-	60,74,74	1.43	8 (13%)	58,114,114	1.73	12 (20%)
31	CLA	b1	607	-	69,73,73	1.34	6 (8%)	82,113,113	1.88	19 (23%)
50	NEX	N	623	-	40,46,46	2.73	11 (27%)	50,70,70	2.07	13 (26%)
31	CLA	d1	402	-	69,73,73	1.38	8 (11%)	82,113,113	1.79	19 (23%)
34	SQD	a	412	-	49,51,54	0.80	0	59,62,65	0.85	2 (3%)
31	CLA	C	505	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	18 (21%)
31	CLA	R	611	-	50,54,73	1.60	8 (16%)	59,90,113	2.10	16 (27%)
31	CLA	S	617	-	54,58,73	1.54	8 (14%)	64,95,113	2.10	18 (28%)
48	LUT	S1	620	-	42,43,43	2.43	1 (2%)	51,60,60	2.01	10 (19%)
57	PTY	y1	626	-	49,49,49	0.90	4 (8%)	52,54,54	1.07	2 (3%)
31	CLA	c	509	-	69,73,73	1.39	6 (8%)	82,113,113	1.88	14 (17%)
31	CLA	y1	614	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
31	CLA	c	503	-	69,73,73	1.37	7 (10%)	82,113,113	1.97	21 (25%)
42	LMK	C1	527	-	39,39,53	1.53	2 (5%)	39,46,60	1.46	2 (5%)
47	CHL	N	606	-	60,74,74	1.36	8 (13%)	58,114,114	1.74	13 (22%)
35	LMG	w1	201	-	39,39,55	0.95	2 (5%)	47,47,63	1.21	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	HEM	f1	101	-	50,50,50	1.45	9 (18%)	67,82,82	1.10	2 (2%)
31	CLA	G	614	-	53,57,73	1.53	7 (13%)	61,93,113	2.17	18 (29%)
31	CLA	N1	602	-	69,73,73	1.32	7 (10%)	82,113,113	1.90	19 (23%)
31	CLA	N1	613	-	69,73,73	1.37	8 (11%)	82,113,113	1.87	17 (20%)
49	XAT	y1	622	-	41,47,47	0.71	1 (2%)	54,74,74	3.69	14 (25%)
54	4RF	K1	101	-	56,56,56	1.06	4 (7%)	59,59,59	0.86	3 (5%)
31	CLA	S	613	-	59,63,73	1.48	6 (10%)	70,101,113	2.23	19 (27%)
47	CHL	n1	608	-	44,58,74	1.38	7 (15%)	37,94,114	2.17	11 (29%)
50	NEX	S1	623	-	40,46,46	2.69	12 (30%)	50,70,70	1.83	12 (24%)
54	4RF	k1	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.91	3 (5%)
57	PTY	Y1	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)
47	CHL	S	601	-	40,54,74	1.74	9 (22%)	34,90,114	2.18	11 (32%)
31	CLA	s	617	-	54,58,73	1.52	8 (14%)	64,95,113	2.12	20 (31%)
34	SQD	c	626	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
31	CLA	s	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	19 (23%)
31	CLA	N1	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	15 (18%)
47	CHL	r	607	-	44,58,74	1.58	8 (18%)	37,94,114	2.18	12 (32%)
31	CLA	B1	615	-	69,73,73	1.38	8 (11%)	82,113,113	1.88	16 (19%)
49	XAT	N1	622	-	41,47,47	0.67	1 (2%)	54,74,74	2.03	12 (22%)
41	LHG	C	525	-	46,46,48	0.39	0	49,52,54	1.08	3 (6%)
46	RRX	h1	101	-	42,42,42	5.04	24 (57%)	56,58,58	2.60	20 (35%)
48	LUT	R1	620	-	42,43,43	2.44	1 (2%)	51,60,60	2.22	14 (27%)
39	GOL	B	627	-	5,5,5	0.57	0	5,5,5	0.29	0
33	BCR	C	515	-	41,41,41	1.62	4 (9%)	56,56,56	4.45	14 (25%)
40	DGD	c1	518	-	56,56,67	1.08	4 (7%)	70,70,81	0.97	3 (4%)
31	CLA	B1	613	-	69,73,73	1.35	6 (8%)	82,113,113	1.86	16 (19%)
47	CHL	s1	607	-	37,51,74	1.67	7 (18%)	30,86,114	2.37	11 (36%)
31	CLA	B	605	-	69,73,73	1.35	7 (10%)	82,113,113	2.04	20 (24%)
31	CLA	y1	602	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	18 (21%)
31	CLA	B	616	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	22 (26%)
31	CLA	g1	612	-	47,51,73	1.63	6 (12%)	55,86,113	2.12	15 (27%)
33	BCR	A	411	-	41,41,41	1.61	4 (9%)	56,56,56	4.42	11 (19%)
48	LUT	S	621	-	42,43,43	2.44	1 (2%)	51,60,60	1.97	16 (31%)
31	CLA	r	609	-	64,68,73	1.40	6 (9%)	76,107,113	1.93	18 (23%)
35	LMG	H1	102	-	48,48,55	1.13	6 (12%)	56,56,63	1.10	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	s1	614	-	59,63,73	1.47	6 (10%)	70,101,113	1.92	14 (20%)
41	LHG	Y	624	-	48,48,48	0.38	0	51,54,54	1.06	3 (5%)
41	LHG	S	624	-	44,44,48	0.42	0	47,50,54	1.15	3 (6%)
31	CLA	G1	613	-	69,73,73	1.35	6 (8%)	82,113,113	1.93	18 (21%)
31	CLA	s1	609	-	64,68,73	1.41	8 (12%)	76,107,113	1.97	19 (25%)
47	CHL	N	609	-	60,74,74	1.27	8 (13%)	58,114,114	1.69	11 (18%)
48	LUT	R	620	-	42,43,43	2.43	1 (2%)	51,60,60	2.15	12 (23%)
31	CLA	g	614	-	53,57,73	1.55	7 (13%)	61,93,113	2.17	17 (27%)
31	CLA	Y	602	24	69,73,73	1.37	7 (10%)	82,113,113	1.80	15 (18%)
31	CLA	B	608	-	69,73,73	1.36	7 (10%)	82,113,113	1.84	17 (20%)
31	CLA	s1	602	-	64,68,73	1.40	7 (10%)	76,107,113	1.91	21 (27%)
31	CLA	y1	610	-	69,73,73	1.35	6 (8%)	82,113,113	1.86	16 (19%)
49	XAT	n1	622	-	41,47,47	0.71	1 (2%)	54,74,74	1.89	13 (24%)
31	CLA	C	511	-	69,73,73	1.37	8 (11%)	82,113,113	1.95	18 (21%)
40	DGD	C1	518	-	56,56,67	1.06	4 (7%)	70,70,81	0.94	2 (2%)
31	CLA	s	614	-	59,63,73	1.45	6 (10%)	70,101,113	2.10	17 (24%)
31	CLA	a	410	-	64,68,73	1.41	7 (10%)	76,107,113	2.03	19 (25%)
31	CLA	Y	604	-	69,73,73	1.35	8 (11%)	82,113,113	1.95	19 (23%)
31	CLA	s1	604	-	59,63,73	1.47	8 (13%)	70,101,113	2.06	19 (27%)
47	CHL	n	605	-	60,74,74	1.46	9 (15%)	58,114,114	1.61	10 (17%)
41	LHG	d1	410	-	38,38,48	0.42	0	41,44,54	1.18	3 (7%)
47	CHL	N1	609	-	60,74,74	1.21	8 (13%)	58,114,114	1.80	11 (18%)
52	3PH	B1	624	-	47,47,47	0.87	4 (8%)	50,52,52	1.13	2 (4%)
33	BCR	B1	618	-	41,41,41	1.62	4 (9%)	56,56,56	4.67	17 (30%)
47	CHL	s	607	-	37,51,74	1.55	7 (18%)	30,86,114	2.27	10 (33%)
48	LUT	G1	620	-	42,43,43	2.44	1 (2%)	51,60,60	1.94	12 (23%)
31	CLA	a	406	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	14 (17%)
51	LPX	S1	625	-	29,29,29	1.06	2 (6%)	31,33,33	0.97	1 (3%)
47	CHL	N	607	-	60,74,74	1.16	7 (11%)	58,114,114	1.84	13 (22%)
31	CLA	C	507	-	69,73,73	1.38	7 (10%)	82,113,113	1.84	18 (21%)
47	CHL	g	601	21	60,74,74	1.37	8 (13%)	58,114,114	1.67	12 (20%)
31	CLA	A1	410	-	64,68,73	1.40	7 (10%)	76,107,113	2.03	21 (27%)
31	CLA	R1	602	-	64,68,73	1.40	6 (9%)	76,107,113	2.04	21 (27%)
38	DGA	J1	101	-	28,28,43	1.32	3 (10%)	30,30,45	1.28	2 (6%)
31	CLA	r1	610	-	64,68,73	1.42	8 (12%)	76,107,113	1.89	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMG	C	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.09	4 (6%)
48	LUT	G1	621	-	42,43,43	2.46	1 (2%)	51,60,60	2.02	13 (25%)
31	CLA	S	605	-	54,58,73	1.53	6 (11%)	64,95,113	2.24	20 (31%)
47	CHL	g	607	-	44,58,74	1.34	7 (15%)	37,94,114	2.06	12 (32%)
31	CLA	s	605	-	54,58,73	1.56	8 (14%)	64,95,113	2.19	21 (32%)
34	SQD	B1	626	-	52,54,54	0.79	0	62,65,65	0.84	2 (3%)
47	CHL	r1	607	-	44,58,74	1.53	8 (18%)	37,94,114	2.15	12 (32%)
47	CHL	s1	608	-	55,69,74	1.45	8 (14%)	52,108,114	1.69	12 (23%)
31	CLA	n1	612	-	49,53,73	1.61	7 (14%)	58,89,113	2.02	16 (27%)
49	XAT	N	622	-	41,47,47	0.70	1 (2%)	54,74,74	1.90	12 (22%)
31	CLA	c	513	-	69,73,73	1.38	7 (10%)	82,113,113	1.87	17 (20%)
31	CLA	Y	614	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	17 (20%)
35	LMG	d1	411	-	46,46,55	1.03	4 (8%)	54,54,63	1.18	2 (3%)
47	CHL	g	608	-	38,52,74	1.64	8 (21%)	31,87,114	2.27	11 (35%)
31	CLA	r	603	-	64,68,73	1.41	7 (10%)	76,107,113	1.92	16 (21%)
31	CLA	S	603	-	69,73,73	1.37	8 (11%)	82,113,113	1.83	16 (19%)
35	LMG	A1	413	-	48,48,55	1.13	5 (10%)	56,56,63	1.18	4 (7%)
31	CLA	B1	617	-	69,73,73	1.37	7 (10%)	82,113,113	1.84	20 (24%)
31	CLA	n1	614	-	53,57,73	1.55	7 (13%)	61,93,113	2.18	19 (31%)
47	CHL	g1	606	-	44,58,74	1.71	9 (20%)	37,94,114	2.14	12 (32%)
31	CLA	B1	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	20 (24%)
31	CLA	C1	502	-	69,73,73	1.37	7 (10%)	82,113,113	1.90	18 (21%)
31	CLA	b1	604	-	69,73,73	1.33	6 (8%)	82,113,113	1.92	20 (24%)
47	CHL	R	607	-	44,58,74	1.52	8 (18%)	37,94,114	2.17	12 (32%)
31	CLA	c1	513	-	69,73,73	1.36	7 (10%)	82,113,113	1.97	22 (26%)
31	CLA	A	405	-	69,73,73	1.37	6 (8%)	82,113,113	1.86	16 (19%)
28	OEX	A	401	4,1	0,15,15	-	-	-	-	-
31	CLA	R	612	-	64,68,73	1.41	7 (10%)	76,107,113	1.94	21 (27%)
31	CLA	b1	609	-	69,73,73	1.39	7 (10%)	82,113,113	1.94	20 (24%)
31	CLA	r1	608	-	64,68,73	1.43	7 (10%)	76,107,113	1.93	16 (21%)
41	LHG	C1	525	-	46,46,48	0.40	0	49,52,54	1.12	2 (4%)
31	CLA	C1	505	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	16 (19%)
37	C7Z	b1	620	-	43,43,43	5.43	26 (60%)	56,60,60	2.28	21 (37%)
48	LUT	G	620	-	42,43,43	2.45	1 (2%)	51,60,60	1.93	10 (19%)
31	CLA	B1	609	-	69,73,73	1.38	6 (8%)	82,113,113	1.92	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PHO	a	408	-	58,69,69	2.16	10 (17%)	55,99,99	1.55	7 (12%)
37	C7Z	B	620	-	43,43,43	5.50	26 (60%)	56,60,60	2.19	14 (25%)
47	CHL	n	606	-	60,74,74	1.42	8 (13%)	58,114,114	1.75	12 (20%)
31	CLA	c	501	-	69,73,73	1.35	8 (11%)	82,113,113	1.92	19 (23%)
31	CLA	R1	603	-	64,68,73	1.42	8 (12%)	76,107,113	1.87	16 (21%)
43	BCT	D1	401	-	3,3,3	1.11	0	2,3,3	4.27	2 (100%)
31	CLA	Y1	603	-	69,73,73	1.37	7 (10%)	82,113,113	1.98	20 (24%)
47	CHL	G	606	-	44,58,74	1.58	9 (20%)	37,94,114	2.09	12 (32%)
35	LMG	a1	413	-	48,48,55	1.13	5 (10%)	56,56,63	1.06	2 (3%)
35	LMG	b1	622	-	44,44,55	0.97	3 (6%)	52,52,63	1.17	3 (5%)
31	CLA	N	614	-	53,57,73	1.54	7 (13%)	61,93,113	2.16	19 (31%)
47	CHL	n1	607	-	60,74,74	1.14	7 (11%)	58,114,114	1.82	12 (20%)
31	CLA	Y	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.82	15 (18%)
31	CLA	D	403	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	21 (25%)
31	CLA	s	609	-	64,68,73	1.42	8 (12%)	76,107,113	1.92	17 (22%)
44	PL9	D	405	-	55,55,55	1.25	4 (7%)	68,69,69	1.52	12 (17%)
50	NEX	N1	623	-	40,46,46	2.69	11 (27%)	50,70,70	1.69	11 (22%)
38	DGA	j1	101	-	28,28,43	1.32	3 (10%)	30,30,45	1.31	2 (6%)
31	CLA	B	615	-	69,73,73	1.35	6 (8%)	82,113,113	2.03	17 (20%)
47	CHL	S	608	-	55,69,74	1.32	8 (14%)	52,108,114	1.78	12 (23%)
41	LHG	L	101	-	48,48,48	0.41	0	51,54,54	0.97	2 (3%)
47	CHL	y1	609	-	60,74,74	1.30	8 (13%)	58,114,114	1.71	12 (20%)
48	LUT	n	620	-	42,43,43	2.45	1 (2%)	51,60,60	2.07	13 (25%)
33	BCR	c	514	-	41,41,41	1.65	4 (9%)	56,56,56	4.67	19 (33%)
48	LUT	n	621	-	42,43,43	2.49	1 (2%)	51,60,60	1.90	12 (23%)
31	CLA	g1	602	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	21 (25%)
31	CLA	r	611	-	50,54,73	1.59	8 (16%)	59,90,113	2.07	15 (25%)
31	CLA	G	613	-	69,73,73	1.37	8 (11%)	82,113,113	2.01	24 (29%)
35	LMG	J	101	-	45,45,55	1.00	3 (6%)	53,53,63	1.09	3 (5%)
31	CLA	S	610	-	69,73,73	1.39	8 (11%)	82,113,113	1.88	17 (20%)
31	CLA	y1	604	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	19 (23%)
33	BCR	b	618	-	41,41,41	1.61	4 (9%)	56,56,56	4.50	14 (25%)
34	SQD	c1	526	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
33	BCR	C1	515	-	41,41,41	1.60	4 (9%)	56,56,56	4.52	14 (25%)
31	CLA	y1	611	-	69,73,73	1.38	7 (10%)	82,113,113	1.87	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	CHL	S1	608	-	55,69,74	1.34	8 (14%)	52,108,114	1.83	13 (25%)
48	LUT	y1	620	-	42,43,43	2.49	1 (2%)	51,60,60	1.83	10 (19%)
47	CHL	y1	605	-	40,54,74	1.49	8 (20%)	34,90,114	2.24	11 (32%)
50	NEX	r	623	-	40,46,46	2.66	11 (27%)	50,70,70	1.65	7 (14%)
38	DGA	c	524	-	43,43,43	1.16	3 (6%)	45,45,45	1.51	3 (6%)
41	LHG	L1	101	-	48,48,48	0.38	0	51,54,54	4.52	5 (9%)
48	LUT	N1	620	-	42,43,43	2.50	1 (2%)	51,60,60	1.73	13 (25%)
34	SQD	C	526	-	52,54,54	0.78	1 (1%)	62,65,65	0.83	2 (3%)
47	CHL	n1	601	20	60,74,74	1.25	8 (13%)	58,114,114	1.80	12 (20%)
31	CLA	C1	507	-	69,73,73	1.35	7 (10%)	82,113,113	1.93	18 (21%)
47	CHL	g1	605	-	42,56,74	1.58	7 (16%)	36,92,114	2.10	11 (30%)
32	PHO	a1	409	-	58,69,69	2.14	9 (15%)	55,99,99	1.79	11 (20%)
31	CLA	S1	602	-	64,68,73	1.40	7 (10%)	76,107,113	1.99	21 (27%)
50	NEX	y1	623	-	40,46,46	2.71	11 (27%)	50,70,70	1.98	12 (24%)
41	LHG	d	408	-	43,43,48	0.41	0	46,49,54	1.14	3 (6%)
31	CLA	b	617	-	69,73,73	1.36	6 (8%)	82,113,113	3.98	18 (21%)
47	CHL	G1	605	-	42,56,74	1.49	8 (19%)	36,92,114	2.13	11 (30%)
34	SQD	B	621	-	52,54,54	0.78	0	62,65,65	0.84	2 (3%)
31	CLA	R	604	-	53,57,73	1.55	6 (11%)	61,93,113	2.14	16 (26%)
31	CLA	y	610	-	69,73,73	1.38	7 (10%)	82,113,113	1.93	18 (21%)
41	LHG	c	625	-	46,46,48	0.41	0	49,52,54	1.05	4 (8%)
48	LUT	y	620	-	42,43,43	2.43	1 (2%)	51,60,60	2.03	14 (27%)
48	LUT	N1	621	-	42,43,43	2.44	1 (2%)	51,60,60	1.91	11 (21%)
49	XAT	y	622	-	41,47,47	0.69	1 (2%)	54,74,74	3.73	18 (33%)
31	CLA	d	402	-	69,73,73	1.37	7 (10%)	82,113,113	1.79	18 (21%)
35	LMG	c1	521	-	51,51,55	1.21	6 (11%)	59,59,63	1.14	3 (5%)
31	CLA	C	508	-	69,73,73	1.37	6 (8%)	82,113,113	1.84	17 (20%)
50	NEX	r1	622	-	40,46,46	2.75	12 (30%)	50,70,70	2.34	11 (22%)
31	CLA	S1	609	-	64,68,73	1.40	7 (10%)	76,107,113	1.99	20 (26%)
31	CLA	B	612	-	69,73,73	1.38	7 (10%)	82,113,113	1.81	15 (18%)
41	LHG	s1	624	-	44,44,48	0.41	0	47,50,54	1.03	3 (6%)
31	CLA	a1	406	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	17 (20%)
31	CLA	c	506	-	69,73,73	1.38	7 (10%)	82,113,113	1.92	20 (24%)
31	CLA	G1	603	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	17 (20%)
41	LHG	g	624	-	48,48,48	0.39	0	51,54,54	1.10	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	NEX	Y1	623	-	40,46,46	2.76	11 (27%)	50,70,70	1.98	12 (24%)
33	BCR	c	515	-	41,41,41	1.64	5 (12%)	56,56,56	4.43	18 (32%)
47	CHL	n1	605	-	60,74,74	1.23	8 (13%)	58,114,114	1.67	12 (20%)
47	CHL	G1	608	-	38,52,74	1.65	8 (21%)	31,87,114	2.20	11 (35%)
35	LMG	a	413	-	48,48,55	1.13	5 (10%)	56,56,63	1.22	4 (7%)
38	DGA	b	623	-	43,43,43	1.15	2 (4%)	45,45,45	1.53	3 (6%)
52	3PH	T1	101	-	47,47,47	0.86	4 (8%)	50,52,52	1.12	2 (4%)
57	PTY	y1	627	-	18,18,49	1.33	3 (16%)	21,23,54	1.46	2 (9%)
31	CLA	B	613	-	69,73,73	1.37	7 (10%)	82,113,113	1.89	15 (18%)
48	LUT	s1	621	-	42,43,43	2.43	1 (2%)	51,60,60	2.12	13 (25%)
32	PHO	A1	408	-	58,69,69	2.17	10 (17%)	55,99,99	1.53	7 (12%)
31	CLA	c1	502	-	69,73,73	1.34	6 (8%)	82,113,113	1.95	21 (25%)
31	CLA	B	602	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	18 (21%)
31	CLA	S	602	23	64,68,73	1.40	6 (9%)	76,107,113	1.91	17 (22%)
47	CHL	G	601	-	60,74,74	1.77	9 (15%)	58,114,114	1.63	11 (18%)
31	CLA	G1	610	-	69,73,73	1.34	6 (8%)	82,113,113	1.91	19 (23%)
47	CHL	G	609	-	60,74,74	1.62	9 (15%)	58,114,114	1.56	12 (20%)
52	3PH	s1	626	-	47,47,47	0.89	4 (8%)	50,52,52	4.52	4 (8%)
33	BCR	c1	515	-	41,41,41	1.63	5 (12%)	56,56,56	4.46	16 (28%)
33	BCR	b	619	-	41,41,41	1.64	4 (9%)	56,56,56	4.59	19 (33%)
31	CLA	g	611	-	49,53,73	1.61	7 (14%)	58,89,113	2.16	16 (27%)
31	CLA	C	502	-	69,73,73	1.35	7 (10%)	82,113,113	1.94	19 (23%)
31	CLA	N	612	-	49,53,73	1.62	7 (14%)	58,89,113	2.05	12 (20%)
31	CLA	c1	508	-	69,73,73	1.35	7 (10%)	82,113,113	1.83	15 (18%)
31	CLA	b	603	-	69,73,73	1.36	8 (11%)	82,113,113	1.92	21 (25%)
34	SQD	m1	101	-	40,42,54	0.89	0	50,53,65	0.90	2 (4%)
33	BCR	C	517	-	41,41,41	1.62	4 (9%)	56,56,56	4.40	11 (19%)
31	CLA	S1	612	-	49,53,73	1.60	6 (12%)	58,89,113	2.09	15 (25%)
47	CHL	n	601	-	60,74,74	1.34	9 (15%)	58,114,114	1.75	12 (20%)
32	PHO	A1	409	-	58,69,69	2.13	9 (15%)	55,99,99	1.63	8 (14%)
49	XAT	Y1	622	-	41,47,47	0.69	1 (2%)	54,74,74	3.78	19 (35%)
31	CLA	G	611	-	49,53,73	1.61	6 (12%)	58,89,113	2.13	18 (31%)
31	CLA	s1	605	23	54,58,73	1.56	7 (12%)	64,95,113	2.15	18 (28%)
31	CLA	B	611	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	18 (21%)
31	CLA	S	611	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	B1	610	-	69,73,73	1.37	7 (10%)	82,113,113	1.85	18 (21%)
31	CLA	C1	512	-	69,73,73	1.37	7 (10%)	82,113,113	1.95	21 (25%)
40	DGD	C	523	-	67,67,67	1.29	7 (10%)	81,81,81	1.07	3 (3%)
47	CHL	Y	605	24	40,54,74	1.74	7 (17%)	34,90,114	2.09	10 (29%)
50	NEX	g	623	-	40,46,46	2.68	11 (27%)	50,70,70	2.27	14 (28%)
31	CLA	b	611	-	69,73,73	1.37	8 (11%)	82,113,113	1.92	21 (25%)
34	SQD	B1	621	-	40,42,54	0.86	0	50,53,65	0.88	2 (4%)
31	CLA	A	410	-	64,68,73	1.42	7 (10%)	76,107,113	2.02	19 (25%)
31	CLA	C	512	-	69,73,73	1.36	7 (10%)	82,113,113	1.79	17 (20%)
31	CLA	n	603	-	69,73,73	1.35	6 (8%)	82,113,113	2.00	19 (23%)
52	3PH	i	101	-	47,47,47	0.87	4 (8%)	50,52,52	1.20	2 (4%)
42	LMK	c	627	-	39,39,53	1.53	3 (7%)	39,46,60	1.39	2 (5%)
49	XAT	n	622	-	41,47,47	0.70	1 (2%)	54,74,74	1.93	10 (18%)
31	CLA	c1	510	-	69,73,73	1.37	6 (8%)	82,113,113	1.85	16 (19%)
31	CLA	g1	614	-	53,57,73	1.55	8 (15%)	61,93,113	2.18	17 (27%)
31	CLA	N	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.96	20 (24%)
31	CLA	r	610	-	64,68,73	1.42	7 (10%)	76,107,113	1.95	22 (28%)
31	CLA	G	603	-	69,73,73	1.33	6 (8%)	82,113,113	2.00	21 (25%)
33	BCR	B	618	-	41,41,41	1.60	4 (9%)	56,56,56	4.57	14 (25%)
31	CLA	N	604	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	20 (24%)
43	BCT	d1	401	-	3,3,3	1.15	0	2,3,3	4.40	2 (100%)
31	CLA	a	405	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	19 (23%)
41	LHG	N1	624	-	48,48,48	0.39	0	51,54,54	1.10	4 (7%)
47	CHL	Y	601	-	60,74,74	1.37	9 (15%)	58,114,114	1.70	11 (18%)
46	RRX	h	101	-	42,42,42	5.03	24 (57%)	56,58,58	1.97	18 (32%)
35	LMG	h1	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.11	2 (3%)
31	CLA	N1	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.95	19 (23%)
31	CLA	b1	613	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	15 (18%)
34	SQD	M1	101	-	40,42,54	0.87	0	50,53,65	0.89	2 (4%)
47	CHL	G1	607	-	60,74,74	1.25	8 (13%)	58,114,114	1.79	13 (22%)
50	NEX	S	622	-	40,46,46	2.68	11 (27%)	50,70,70	1.91	12 (24%)
41	LHG	S1	624	-	44,44,48	0.41	0	47,50,54	1.12	4 (8%)
31	CLA	B	610	-	69,73,73	1.37	7 (10%)	82,113,113	1.88	16 (19%)
31	CLA	s1	617	-	54,58,73	1.52	7 (12%)	64,95,113	2.12	20 (31%)
47	CHL	r	606	-	38,52,74	1.73	9 (23%)	31,87,114	2.27	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	n1	611	-	53,57,73	1.53	7 (13%)	61,93,113	2.18	17 (27%)
40	DGD	C1	519	-	63,63,67	1.24	7 (11%)	77,77,81	1.00	3 (3%)
31	CLA	y	603	-	69,73,73	1.34	6 (8%)	82,113,113	1.97	20 (24%)
31	CLA	g	610	-	69,73,73	1.34	6 (8%)	82,113,113	1.91	19 (23%)
31	CLA	G	604	-	53,57,73	1.56	8 (15%)	61,93,113	2.19	17 (27%)
31	CLA	S1	604	-	59,63,73	1.48	6 (10%)	70,101,113	2.11	19 (27%)
33	BCR	c1	516	-	41,41,41	1.59	4 (9%)	56,56,56	4.60	16 (28%)
31	CLA	d1	403	-	69,73,73	1.37	8 (11%)	82,113,113	1.93	19 (23%)
31	CLA	R	603	-	64,68,73	1.42	8 (12%)	76,107,113	2.01	18 (23%)
47	CHL	y	609	-	60,74,74	1.31	9 (15%)	58,114,114	1.70	12 (20%)
50	NEX	s	623	-	40,46,46	2.75	14 (35%)	50,70,70	1.80	12 (24%)
34	SQD	b	621	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
56	ERG	R1	626	-	32,32,32	7.93	20 (62%)	45,50,50	2.88	20 (44%)
40	DGD	C1	520	-	60,60,67	1.17	6 (10%)	74,74,81	1.00	4 (5%)
50	NEX	G	623	-	40,46,46	2.74	11 (27%)	50,70,70	1.82	11 (22%)
49	XAT	R1	621	-	41,47,47	0.65	1 (2%)	54,74,74	1.88	13 (24%)
31	CLA	a1	410	-	64,68,73	1.41	6 (9%)	76,107,113	1.92	18 (23%)
31	CLA	S1	614	-	59,63,73	1.46	6 (10%)	70,101,113	1.99	17 (24%)
33	BCR	C	516	-	41,41,41	1.62	4 (9%)	56,56,56	4.52	15 (26%)
32	PHO	A	409	-	58,69,69	2.15	9 (15%)	55,99,99	1.63	8 (14%)
41	LHG	y1	624	-	48,48,48	0.40	0	51,54,54	0.99	2 (3%)
47	CHL	G1	609	-	60,74,74	1.43	8 (13%)	58,114,114	1.62	12 (20%)
31	CLA	b1	614	-	69,73,73	1.37	8 (11%)	82,113,113	1.81	18 (21%)
51	LPX	S	625	-	29,29,29	1.03	2 (6%)	31,33,33	0.97	1 (3%)
31	CLA	n	611	-	53,57,73	1.56	7 (13%)	61,93,113	2.22	18 (29%)
33	BCR	a1	411	-	41,41,41	1.60	4 (9%)	56,56,56	4.60	14 (25%)
31	CLA	n	610	-	69,73,73	1.36	6 (8%)	82,113,113	1.96	19 (23%)
47	CHL	G	608	-	38,52,74	1.76	9 (23%)	31,87,114	2.25	10 (32%)
31	CLA	B	614	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	17 (20%)
31	CLA	D	402	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
33	BCR	b1	618	-	41,41,41	1.61	4 (9%)	56,56,56	4.65	18 (32%)
33	BCR	d	404	-	41,41,41	1.59	4 (9%)	56,56,56	4.28	17 (30%)
35	LMG	j	101	-	45,45,55	1.00	4 (8%)	53,53,63	1.06	2 (3%)
41	LHG	D	409	-	48,48,48	0.40	0	51,54,54	1.08	3 (5%)
47	CHL	Y	606	-	60,74,74	1.31	8 (13%)	58,114,114	1.76	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	c1	504	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	20 (24%)
39	GOL	b	624	-	5,5,5	0.59	0	5,5,5	0.26	0
31	CLA	g1	604	-	53,57,73	1.55	7 (13%)	61,93,113	2.13	20 (32%)
31	CLA	r	602	-	64,68,73	1.43	8 (12%)	76,107,113	1.94	19 (25%)
47	CHL	n	607	-	60,74,74	1.17	7 (11%)	58,114,114	1.85	13 (22%)
31	CLA	C	503	-	69,73,73	1.37	8 (11%)	82,113,113	1.91	19 (23%)
47	CHL	N1	608	-	44,58,74	1.74	7 (15%)	37,94,114	2.01	12 (32%)
31	CLA	G1	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	18 (21%)
34	SQD	C1	526	-	52,54,54	0.77	0	62,65,65	0.85	2 (3%)
48	LUT	Y	620	-	42,43,43	2.48	1 (2%)	51,60,60	1.90	13 (25%)
46	RRX	H	101	-	42,42,42	7.86	26 (61%)	56,58,58	6.26	22 (39%)
50	NEX	n	623	-	40,46,46	2.69	11 (27%)	50,70,70	1.80	13 (26%)
47	CHL	y	605	24	40,54,74	1.59	7 (17%)	34,90,114	2.06	10 (29%)
48	LUT	y	621	-	42,43,43	2.40	1 (2%)	51,60,60	1.87	13 (25%)
38	DGA	c1	524	-	43,43,43	1.16	3 (6%)	45,45,45	1.53	4 (8%)
33	BCR	A1	411	-	41,41,41	1.61	4 (9%)	56,56,56	4.57	13 (23%)
41	LHG	Y1	624	-	48,48,48	0.39	0	51,54,54	1.01	3 (5%)
31	CLA	S	604	-	59,63,73	1.45	6 (10%)	70,101,113	2.05	19 (27%)
31	CLA	R1	612	-	64,68,73	1.42	8 (12%)	76,107,113	1.97	20 (26%)
31	CLA	g	602	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	21 (25%)
38	DGA	C	524	-	43,43,43	1.15	3 (6%)	45,45,45	1.52	3 (6%)
47	CHL	N1	601	20	60,74,74	1.38	8 (13%)	58,114,114	1.63	13 (22%)
31	CLA	s	610	-	69,73,73	1.37	6 (8%)	82,113,113	1.90	18 (21%)
38	DGA	B1	625	-	43,43,43	1.16	2 (4%)	45,45,45	1.45	3 (6%)
31	CLA	C1	508	-	69,73,73	1.34	6 (8%)	82,113,113	1.85	17 (20%)
41	LHG	N	624	-	48,48,48	0.37	0	51,54,54	1.17	3 (5%)
47	CHL	R1	606	-	38,52,74	1.91	9 (23%)	31,87,114	2.31	11 (35%)
50	NEX	n1	623	-	40,46,46	2.64	11 (27%)	50,70,70	1.72	10 (20%)
31	CLA	n	613	-	69,73,73	1.36	8 (11%)	82,113,113	1.98	21 (25%)
31	CLA	Y1	614	-	69,73,73	1.38	8 (11%)	82,113,113	1.83	18 (21%)
40	DGD	c1	519	-	63,63,67	1.23	7 (11%)	77,77,81	0.99	5 (6%)
31	CLA	B1	602	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	17 (20%)
31	CLA	R1	609	-	64,68,73	1.40	7 (10%)	76,107,113	4.17	22 (28%)
47	CHL	N	605	-	60,74,74	1.38	9 (15%)	58,114,114	1.63	10 (17%)
31	CLA	N	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	b1	617	-	69,73,73	1.39	7 (10%)	82,113,113	1.91	16 (19%)
47	CHL	n	609	-	60,74,74	1.45	9 (15%)	58,114,114	1.70	14 (24%)
35	LMG	c	521	-	51,51,55	1.21	6 (11%)	59,59,63	1.20	4 (6%)
52	3PH	b1	624	-	47,47,47	0.87	4 (8%)	50,52,52	1.18	2 (4%)
48	LUT	G	621	-	42,43,43	2.46	1 (2%)	51,60,60	2.05	16 (31%)
31	CLA	s	613	-	59,63,73	1.47	6 (10%)	70,101,113	2.18	14 (20%)
31	CLA	R	610	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	20 (26%)
37	C7Z	B1	620	-	43,43,43	5.46	26 (60%)	56,60,60	2.36	19 (33%)
31	CLA	b1	608	-	69,73,73	1.36	6 (8%)	82,113,113	1.86	18 (21%)
40	DGD	c1	520	-	60,60,67	1.17	6 (10%)	74,74,81	1.01	3 (4%)
47	CHL	y	607	-	60,74,74	1.12	7 (11%)	58,114,114	1.79	13 (22%)
35	LMG	d	411	-	46,46,55	1.02	4 (8%)	54,54,63	1.21	3 (5%)
31	CLA	y	604	-	69,73,73	1.36	6 (8%)	82,113,113	1.86	16 (19%)
31	CLA	d	403	-	69,73,73	1.37	6 (8%)	82,113,113	1.91	17 (20%)
31	CLA	Y1	604	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	22 (26%)
39	GOL	y	626	-	5,5,5	0.54	0	5,5,5	0.37	0
33	BCR	C1	517	-	41,41,41	1.66	4 (9%)	56,56,56	4.76	16 (28%)
31	CLA	B	604	-	69,73,73	1.41	9 (13%)	82,113,113	1.83	18 (21%)
48	LUT	N	620	-	42,43,43	2.46	1 (2%)	51,60,60	2.00	16 (31%)
41	LHG	l	101	-	48,48,48	0.40	0	51,54,54	0.97	2 (3%)
31	CLA	c1	501	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	20 (24%)
33	BCR	B	619	-	41,41,41	1.62	4 (9%)	56,56,56	4.51	19 (33%)
41	LHG	d	409	-	48,48,48	0.40	0	51,54,54	0.99	2 (3%)
31	CLA	S	609	-	64,68,73	1.42	8 (12%)	76,107,113	1.91	20 (26%)
31	CLA	c1	506	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	16 (19%)
31	CLA	C	513	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	19 (23%)
31	CLA	B	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.96	20 (24%)
41	LHG	c1	525	-	46,46,48	0.40	0	49,52,54	1.03	3 (6%)
31	CLA	C	501	-	69,73,73	1.36	7 (10%)	82,113,113	1.99	19 (23%)
38	DGA	C1	524	-	43,43,43	1.16	3 (6%)	45,45,45	1.52	3 (6%)
40	DGD	c	520	-	60,60,67	1.16	6 (10%)	74,74,81	1.03	2 (2%)
31	CLA	n1	610	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	18 (21%)
31	CLA	r1	603	-	64,68,73	1.43	7 (10%)	76,107,113	1.89	15 (19%)
53	SPH	y	625	-	19,20,20	0.66	0	18,21,21	1.15	2 (11%)
31	CLA	R	608	-	64,68,73	1.41	7 (10%)	76,107,113	1.92	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	a	407	-	53,57,73	1.56	7 (13%)	61,93,113	2.14	18 (29%)
31	CLA	r1	602	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	22 (28%)
31	CLA	Y	608	-	54,58,73	1.54	9 (16%)	64,95,113	2.07	17 (26%)
31	CLA	r1	604	-	53,57,73	1.53	6 (11%)	61,93,113	2.20	18 (29%)
31	CLA	A1	405	-	69,73,73	1.41	7 (10%)	82,113,113	2.03	20 (24%)
47	CHL	g	605	-	42,56,74	1.58	8 (19%)	36,92,114	2.11	11 (30%)
28	OEX	A1	401	4,1	0,15,15	-	-	-	-	-
31	CLA	C1	511	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	17 (20%)
31	CLA	c1	503	-	69,73,73	1.36	6 (8%)	82,113,113	1.97	23 (28%)
31	CLA	y1	608	-	54,58,73	1.53	8 (14%)	64,95,113	2.11	19 (29%)
31	CLA	B1	604	-	69,73,73	1.38	8 (11%)	82,113,113	1.82	19 (23%)
31	CLA	C1	510	-	69,73,73	1.37	6 (8%)	82,113,113	1.85	16 (19%)
31	CLA	G1	612	-	47,51,73	1.65	8 (17%)	55,86,113	2.10	14 (25%)
31	CLA	b1	605	-	69,73,73	1.34	6 (8%)	82,113,113	2.16	21 (25%)
47	CHL	N	601	20	60,74,74	1.46	8 (13%)	58,114,114	1.73	11 (18%)
49	XAT	Y	622	-	41,47,47	0.70	1 (2%)	54,74,74	3.76	16 (29%)
41	LHG	s	624	-	44,44,48	0.41	0	47,50,54	1.13	3 (6%)
31	CLA	A1	407	-	54,58,73	1.53	7 (12%)	64,95,113	2.10	22 (34%)
35	LMG	B1	622	-	44,44,55	0.97	3 (6%)	52,52,63	1.14	3 (5%)
31	CLA	G	610	-	69,73,73	1.34	6 (8%)	82,113,113	1.98	20 (24%)
31	CLA	S1	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	18 (21%)
31	CLA	s	612	-	49,53,73	1.61	7 (14%)	58,89,113	2.10	16 (27%)
31	CLA	N	610	-	69,73,73	1.38	7 (10%)	82,113,113	1.95	20 (24%)
33	BCR	c1	514	-	41,41,41	1.60	4 (9%)	56,56,56	4.60	16 (28%)
47	CHL	Y	609	-	60,74,74	1.29	9 (15%)	58,114,114	1.72	12 (20%)
31	CLA	B	606	-	69,73,73	1.36	8 (11%)	82,113,113	1.88	19 (23%)
31	CLA	b	616	-	69,73,73	1.37	6 (8%)	82,113,113	1.85	17 (20%)
33	BCR	C1	516	-	41,41,41	1.53	5 (12%)	56,56,56	4.46	18 (32%)
33	BCR	C	514	-	41,41,41	1.62	4 (9%)	56,56,56	4.55	13 (23%)
52	3PH	S	626	-	47,47,47	0.88	4 (8%)	50,52,52	1.12	2 (4%)
31	CLA	N1	604	-	69,73,73	1.37	7 (10%)	82,113,113	1.95	20 (24%)
53	SPH	A1	414	-	19,20,20	0.68	1 (5%)	18,21,21	0.92	0
48	LUT	y1	621	-	42,43,43	2.48	1 (2%)	51,60,60	1.90	13 (25%)
52	3PH	s	626	-	47,47,47	0.87	4 (8%)	50,52,52	1.14	2 (4%)
31	CLA	s	602	-	64,68,73	1.39	6 (9%)	76,107,113	1.94	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	PL9	d	405	-	55,55,55	1.26	6 (10%)	68,69,69	1.47	13 (19%)
31	CLA	c1	509	-	69,73,73	1.36	6 (8%)	82,113,113	1.84	16 (19%)
41	LHG	y	624	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
43	BCT	D	401	29	3,3,3	1.16	0	2,3,3	4.58	2 (100%)
41	LHG	D	410	-	38,38,48	0.44	0	41,44,54	1.04	2 (4%)
47	CHL	n	608	-	44,58,74	1.31	8 (18%)	37,94,114	2.16	11 (29%)
31	CLA	s1	612	-	49,53,73	1.59	6 (12%)	58,89,113	2.14	16 (27%)
48	LUT	Y	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.88	14 (27%)
41	LHG	g1	624	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
31	CLA	R	602	-	64,68,73	1.42	7 (10%)	76,107,113	1.92	20 (26%)
31	CLA	n	614	-	53,57,73	1.54	7 (13%)	61,93,113	2.16	19 (31%)
31	CLA	g1	613	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	21 (25%)
47	CHL	N1	607	-	60,74,74	1.08	7 (11%)	58,114,114	1.77	14 (24%)
49	XAT	R	621	-	41,47,47	0.71	1 (2%)	54,74,74	2.02	13 (24%)
31	CLA	C1	503	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	18 (21%)
32	PHO	a	409	-	58,69,69	2.14	9 (15%)	55,99,99	1.71	8 (14%)
47	CHL	s1	606	-	38,52,74	1.61	7 (18%)	31,87,114	2.22	9 (29%)
50	NEX	R	622	-	40,46,46	2.82	13 (32%)	50,70,70	1.93	10 (20%)
40	DGD	B1	623	-	44,44,67	0.84	1 (2%)	58,58,81	1.25	4 (6%)
47	CHL	g	606	-	44,58,74	1.44	8 (18%)	37,94,114	2.19	11 (29%)
31	CLA	s1	613	-	59,63,73	1.49	7 (11%)	70,101,113	2.02	16 (22%)
28	OEX	a	401	4,1	0,15,15	-	-	-	-	-
48	LUT	g1	620	-	42,43,43	2.46	1 (2%)	51,60,60	1.84	11 (21%)
42	LMK	c1	527	-	39,39,53	1.55	3 (7%)	39,46,60	1.35	2 (5%)
47	CHL	S	606	-	38,52,74	1.63	8 (21%)	31,87,114	2.21	11 (35%)
48	LUT	g	620	-	42,43,43	2.47	1 (2%)	51,60,60	1.98	12 (23%)
31	CLA	N	611	-	53,57,73	1.56	8 (15%)	61,93,113	2.22	18 (29%)
31	CLA	b1	611	-	69,73,73	1.35	7 (10%)	82,113,113	1.84	18 (21%)
34	SQD	a1	412	-	49,51,54	0.80	0	59,62,65	0.84	2 (3%)
31	CLA	n1	602	-	69,73,73	1.35	6 (8%)	82,113,113	1.92	19 (23%)
53	SPH	Y1	625	-	19,20,20	0.66	0	18,21,21	1.07	1 (5%)
48	LUT	s1	620	-	42,43,43	2.48	1 (2%)	51,60,60	1.94	13 (25%)
31	CLA	c	511	-	69,73,73	1.38	8 (11%)	82,113,113	1.93	21 (25%)
34	SQD	b1	621	-	40,42,54	0.87	0	50,53,65	0.88	2 (4%)
31	CLA	C	504	-	69,73,73	1.33	7 (10%)	82,113,113	1.96	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	n1	604	-	69,73,73	1.35	6 (8%)	82,113,113	1.87	21 (25%)
33	BCR	D	404	-	41,41,41	1.60	4 (9%)	56,56,56	4.34	19 (33%)
48	LUT	g	621	-	42,43,43	2.45	1 (2%)	51,60,60	1.98	9 (17%)
53	SPH	a1	414	-	19,20,20	0.68	0	18,21,21	1.04	1 (5%)
47	CHL	S1	606	-	38,52,74	1.87	9 (23%)	31,87,114	2.19	9 (29%)
53	SPH	y1	625	-	19,20,20	0.66	0	18,21,21	1.06	1 (5%)
41	LHG	D1	410	-	38,38,48	0.43	0	41,44,54	1.10	3 (7%)
31	CLA	S1	613	-	59,63,73	1.47	6 (10%)	70,101,113	2.02	16 (22%)
41	LHG	d1	408	-	43,43,48	0.42	0	46,49,54	1.07	3 (6%)
31	CLA	R	609	-	64,68,73	1.41	7 (10%)	76,107,113	1.93	18 (23%)
48	LUT	Y1	620	-	42,43,43	2.46	1 (2%)	51,60,60	1.88	14 (27%)
31	CLA	Y1	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	15 (18%)
47	CHL	S1	601	23	40,54,74	1.66	8 (20%)	34,90,114	2.19	11 (32%)
33	BCR	c	516	-	41,41,41	1.58	4 (9%)	56,56,56	4.43	19 (33%)
51	LPX	s1	625	-	29,29,29	1.06	2 (6%)	31,33,33	0.97	1 (3%)
53	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.14	1 (5%)
31	CLA	C1	513	-	69,73,73	1.36	8 (11%)	82,113,113	1.92	21 (25%)
31	CLA	N1	612	-	49,53,73	1.60	7 (14%)	58,89,113	2.07	15 (25%)
31	CLA	B1	607	-	69,73,73	1.37	7 (10%)	82,113,113	1.81	17 (20%)
31	CLA	S	612	-	49,53,73	1.63	6 (12%)	58,89,113	2.05	15 (25%)
47	CHL	Y1	607	-	60,74,74	1.11	7 (11%)	58,114,114	1.77	11 (18%)
47	CHL	g1	601	-	60,74,74	1.29	8 (13%)	58,114,114	1.71	12 (20%)
28	OEX	a1	401	4,1	0,15,15	-	-	-	-	-
31	CLA	N	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.87	20 (24%)
31	CLA	b1	603	-	69,73,73	1.37	7 (10%)	82,113,113	2.05	18 (21%)
47	CHL	Y1	605	24	40,54,74	1.53	8 (20%)	34,90,114	2.19	10 (29%)
40	DGD	c	518	-	56,56,67	1.06	4 (7%)	70,70,81	0.98	2 (2%)
47	CHL	Y	607	-	60,74,74	1.12	7 (11%)	58,114,114	1.73	11 (18%)
48	LUT	Y1	621	-	42,43,43	2.47	1 (2%)	51,60,60	1.80	11 (21%)
35	LMG	C1	523	-	55,55,55	1.27	6 (10%)	63,63,63	1.11	3 (4%)
47	CHL	N1	606	-	60,74,74	1.34	8 (13%)	58,114,114	1.66	12 (20%)

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
48	LUT	s	620	-	1/1/12/27	2/29/67/67	0/2/2/2
31	CLA	c	508	-	1/1/15/20	11/39/115/115	-
31	CLA	g	613	-	1/1/15/20	19/39/115/115	-
47	CHL	g1	607	-	4/4/20/26	8/39/137/137	-
33	BCR	C1	514	-	-	15/29/63/63	0/2/2/2
47	CHL	s1	601	23	3/3/16/26	5/15/113/137	-
31	CLA	c	507	-	1/1/15/20	21/39/115/115	-
47	CHL	n1	609	-	4/4/20/26	3/39/137/137	-
31	CLA	D1	403	-	1/1/15/20	19/39/115/115	-
52	3PH	t1	101	-	-	27/49/49/49	-
31	CLA	A	406	-	1/1/15/20	14/39/115/115	-
33	BCR	D1	404	-	-	11/29/63/63	0/2/2/2
35	LMG	A	413	-	-	12/43/63/70	0/1/1/1
31	CLA	Y	612	-	1/1/15/20	11/39/115/115	-
47	CHL	G	605	21	3/3/16/26	1/18/116/137	-
48	LUT	s	621	-	-	1/29/67/67	0/2/2/2
31	CLA	y1	612	-	1/1/15/20	15/39/115/115	-
48	LUT	N	621	-	-	3/29/67/67	0/2/2/2
48	LUT	r1	620	-	-	6/29/67/67	0/2/2/2
31	CLA	R	613	-	1/1/11/20	10/17/93/115	-
35	LMG	h	102	-	-	13/43/63/70	0/1/1/1
35	LMG	C1	521	-	-	12/46/66/70	0/1/1/1
32	PHO	A	408	-	-	5/37/103/103	0/5/6/6
33	BCR	c	517	-	-	9/29/63/63	0/2/2/2
31	CLA	R1	610	-	1/1/14/20	11/33/109/115	-
31	CLA	c1	511	-	1/1/15/20	14/39/115/115	-
31	CLA	a1	405	-	1/1/15/20	13/39/115/115	-
31	CLA	C	509	-	1/1/15/20	11/39/115/115	-
31	CLA	Y1	610	-	1/1/15/20	15/39/115/115	-
47	CHL	y	601	24	4/4/20/26	6/39/137/137	-
41	LHG	D	408	-	-	29/48/48/53	-
47	CHL	y1	606	-	4/4/20/26	7/39/137/137	-
45	HEM	F1	101	6	-	1/14/54/54	-
31	CLA	r	608	-	1/1/14/20	16/33/109/115	-
50	NEX	y	623	-	-	5/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	b	622	-	-	12/39/59/70	0/1/1/1
31	CLA	b	605	-	1/1/15/20	17/39/115/115	-
31	CLA	c	510	-	1/1/15/20	13/39/115/115	-
47	CHL	R1	607	-	3/3/16/26	4/20/118/137	-
31	CLA	y1	613	-	1/1/15/20	23/39/115/115	-
31	CLA	b1	616	-	1/1/15/20	9/39/115/115	-
31	CLA	G1	602	-	1/1/15/20	18/39/115/115	-
46	RRX	H1	101	-	1/1/11/25	4/29/65/65	0/2/2/2
31	CLA	b1	606	-	1/1/15/20	9/39/115/115	-
38	DGA	B	625	-	-	25/45/45/45	-
31	CLA	r	604	-	1/1/11/20	10/20/96/115	-
44	PL9	D1	405	-	-	17/53/73/73	0/1/1/1
31	CLA	b	608	-	1/1/15/20	25/39/115/115	-
55	LMT	R1	625	-	-	9/21/61/61	0/2/2/2
39	GOL	b	625	-	-	2/4/4/4	-
31	CLA	g1	603	-	1/1/15/20	23/39/115/115	-
31	CLA	s	604	-	1/1/13/20	11/27/103/115	-
34	SQD	A1	412	-	-	15/46/66/69	0/1/1/1
31	CLA	y	611	-	1/1/15/20	18/39/115/115	-
31	CLA	b1	610	-	1/1/15/20	15/39/115/115	-
31	CLA	B1	605	-	1/1/15/20	14/39/115/115	-
31	CLA	n1	613	-	1/1/15/20	21/39/115/115	-
31	CLA	b1	602	-	1/1/15/20	17/39/115/115	-
31	CLA	S	614	-	1/1/13/20	10/27/103/115	-
40	DGD	C	518	-	-	12/44/84/95	0/2/2/2
31	CLA	S1	605	-	1/1/12/20	8/21/97/115	-
47	CHL	Y1	606	-	4/4/20/26	6/39/137/137	-
31	CLA	g1	611	-	1/1/15/20	16/39/115/115	-
50	NEX	g1	623	-	-	3/27/83/83	0/3/3/3
31	CLA	B	617	-	1/1/15/20	15/39/115/115	-
31	CLA	R1	608	-	1/1/14/20	13/33/109/115	-
31	CLA	B1	603	-	1/1/15/20	15/39/115/115	-
31	CLA	Y1	608	-	1/1/12/20	9/21/97/115	-
34	SQD	A	412	-	-	17/46/66/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	S1	603	-	1/1/15/20	17/39/115/115	-
56	ERG	r1	626	-	5/5/11/15	8/13/71/71	0/4/4/4
48	LUT	n1	620	-	-	4/29/67/67	0/2/2/2
31	CLA	R1	604	-	1/1/11/20	10/20/96/115	-
33	BCR	a	411	-	-	10/29/63/63	0/2/2/2
35	LMG	B	622	-	-	11/39/59/70	0/1/1/1
31	CLA	A	407	-	1/1/11/20	4/20/96/115	-
31	CLA	b1	615	-	1/1/15/20	18/39/115/115	-
47	CHL	Y1	601	24	4/4/20/26	0/39/137/137	-
40	DGD	C	520	-	-	13/48/88/95	0/2/2/2
31	CLA	B1	614	-	1/1/15/20	11/39/115/115	-
41	LHG	G	630	-	-	29/53/53/53	-
31	CLA	b	602	-	1/1/15/20	22/39/115/115	-
31	CLA	b	615	-	1/1/15/20	11/39/115/115	-
31	CLA	Y	613	-	1/1/15/20	16/39/115/115	-
31	CLA	b1	612	-	1/1/15/20	10/39/115/115	-
48	LUT	n1	621	-	-	3/29/67/67	0/2/2/2
47	CHL	n1	606	-	4/4/20/26	5/39/137/137	-
38	DGA	b1	625	-	-	23/45/45/45	-
31	CLA	s1	603	-	1/1/15/20	19/39/115/115	-
31	CLA	b	613	-	1/1/15/20	17/39/115/115	-
33	BCR	d1	404	-	-	12/29/63/63	0/2/2/2
31	CLA	g	603	-	1/1/15/20	17/39/115/115	-
41	LHG	n1	624	-	-	34/53/53/53	-
31	CLA	A1	406	-	1/1/15/20	12/39/115/115	-
33	BCR	b1	619	-	-	5/29/63/63	0/2/2/2
44	PL9	d1	405	-	-	22/53/73/73	0/1/1/1
31	CLA	G1	614	-	1/1/11/20	11/20/96/115	-
55	LMT	r1	625	-	-	9/21/61/61	0/2/2/2
47	CHL	y1	601	24	4/4/20/26	0/39/137/137	-
31	CLA	b	606	-	1/1/15/20	14/39/115/115	-
35	LMG	c1	523	-	-	14/50/70/70	0/1/1/1
31	CLA	C1	504	-	1/1/15/20	15/39/115/115	-
31	CLA	r1	612	-	1/1/14/20	17/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	XAT	G	622	-	2/2/12/26	0/31/93/93	0/4/4/4
42	LMK	C	527	-	1/1/6/6	12/46/46/60	-
41	LHG	d	410	-	-	32/43/43/53	-
31	CLA	B	609	-	1/1/15/20	19/39/115/115	-
31	CLA	C	506	-	1/1/15/20	21/39/115/115	-
31	CLA	b	610	-	1/1/15/20	16/39/115/115	-
31	CLA	g	604	-	1/1/11/20	8/20/96/115	-
47	CHL	y1	607	-	4/4/20/26	6/39/137/137	-
54	4RF	i1	101	-	-	28/59/59/59	-
31	CLA	b	612	-	1/1/15/20	18/39/115/115	-
31	CLA	B1	606	-	1/1/15/20	8/39/115/115	-
31	CLA	B1	608	-	1/1/15/20	25/39/115/115	-
31	CLA	C	510	-	1/1/15/20	18/39/115/115	-
47	CHL	r1	606	-	3/3/15/26	2/13/111/137	-
48	LUT	g1	621	-	1/1/12/27	3/29/67/67	0/2/2/2
31	CLA	Y1	613	-	1/1/15/20	19/39/115/115	-
31	CLA	r1	609	-	1/1/14/20	13/33/109/115	-
31	CLA	B	607	-	1/1/15/20	20/39/115/115	-
40	DGD	C	519	-	-	18/51/91/95	0/2/2/2
31	CLA	n	602	-	1/1/15/20	18/39/115/115	-
47	CHL	N1	605	20	4/4/20/26	5/39/137/137	-
41	LHG	D1	409	-	-	29/53/53/53	-
31	CLA	b	614	-	1/1/15/20	14/39/115/115	-
52	3PH	S1	626	-	-	22/49/49/49	-
31	CLA	c	504	-	1/1/15/20	13/39/115/115	-
31	CLA	S1	610	-	1/1/15/20	20/39/115/115	-
47	CHL	g1	608	-	3/3/15/26	1/13/111/137	-
41	LHG	d1	409	-	-	31/53/53/53	-
45	HEM	f	101	6,7	-	2/14/54/54	-
31	CLA	s	603	-	1/1/15/20	16/39/115/115	-
31	CLA	Y1	602	-	1/1/15/20	22/39/115/115	-
45	HEM	F	101	6,7	-	3/14/54/54	-
47	CHL	s	608	-	4/4/19/26	2/33/131/137	-
49	XAT	r	622	-	1/1/12/26	12/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	G	612	-	1/1/10/20	6/13/89/115	-
50	NEX	R1	622	-	-	6/27/83/83	0/3/3/3
47	CHL	g1	609	-	4/4/20/26	7/39/137/137	-
49	XAT	G1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
31	CLA	s1	611	-	1/1/15/20	16/39/115/115	-
31	CLA	c1	507	-	1/1/15/20	20/39/115/115	-
47	CHL	G1	601	21	4/4/20/26	10/39/137/137	-
54	4RF	I1	102	-	-	35/59/59/59	-
31	CLA	C1	506	-	1/1/15/20	18/39/115/115	-
31	CLA	G	602	-	1/1/15/20	21/39/115/115	-
31	CLA	a1	407	-	1/1/11/20	8/20/96/115	-
49	XAT	g1	622	-	2/2/12/26	0/31/93/93	0/4/4/4
32	PHO	a1	408	-	-	4/37/103/103	0/5/6/6
41	LHG	n	624	-	-	30/53/53/53	-
31	CLA	y	612	-	1/1/15/20	14/39/115/115	-
31	CLA	B1	616	-	1/1/15/20	10/39/115/115	-
41	LHG	D1	408	-	-	30/48/48/53	-
31	CLA	n	612	-	1/1/11/20	4/15/91/115	-
50	NEX	Y	623	-	-	2/27/83/83	0/3/3/3
50	NEX	G1	623	-	-	2/27/83/83	0/3/3/3
35	LMG	W1	201	-	-	16/34/54/70	0/1/1/1
48	LUT	S1	621	-	-	2/29/67/67	0/2/2/2
31	CLA	N1	611	-	1/1/11/20	9/20/96/115	-
39	GOL	I1	101	-	-	0/4/4/4	-
50	NEX	s1	623	-	-	3/27/83/83	0/3/3/3
31	CLA	D1	402	-	1/1/15/20	22/39/115/115	-
47	CHL	Y1	609	-	4/4/20/26	6/39/137/137	-
34	SQD	b1	626	-	-	23/49/69/69	0/1/1/1
31	CLA	c1	512	-	1/1/15/20	18/39/115/115	-
31	CLA	C1	509	-	1/1/15/20	14/39/115/115	-
47	CHL	S	607	-	4/4/15/26	1/12/110/137	-
33	BCR	B1	619	-	-	8/29/63/63	0/2/2/2
31	CLA	c	512	-	1/1/15/20	20/39/115/115	-
31	CLA	y	602	-	1/1/15/20	24/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	LPX	s	625	-	-	13/31/31/31	-
47	CHL	R	606	-	3/3/15/26	3/13/111/137	-
31	CLA	r	612	-	1/1/14/20	14/33/109/115	-
47	CHL	G1	606	-	3/3/16/26	2/20/118/137	-
41	LHG	G1	624	-	-	29/53/53/53	-
31	CLA	b	607	-	1/1/15/20	18/39/115/115	-
31	CLA	Y	603	-	1/1/15/20	18/39/115/115	-
31	CLA	y	613	-	1/1/15/20	18/39/115/115	-
31	CLA	n	604	-	1/1/15/20	14/39/115/115	-
31	CLA	y1	603	-	1/1/15/20	17/39/115/115	-
57	PTY	Y1	627	-	-	10/20/20/53	-
37	C7Z	b	620	-	1/1/12/26	8/29/67/67	0/2/2/2
31	CLA	g	612	-	1/1/10/20	8/13/89/115	-
31	CLA	C1	501	-	1/1/15/20	12/39/115/115	-
47	CHL	S1	607	-	3/3/15/26	0/12/110/137	-
31	CLA	G1	604	-	1/1/11/20	7/20/96/115	-
47	CHL	g	609	-	4/4/20/26	5/39/137/137	-
47	CHL	s	601	23	3/3/16/26	4/15/113/137	-
31	CLA	S1	617	23	1/1/12/20	8/21/97/115	-
47	CHL	s	606	-	3/3/15/26	0/13/111/137	-
31	CLA	r	613	-	1/1/11/20	10/17/93/115	-
31	CLA	c	502	-	1/1/15/20	11/39/115/115	-
31	CLA	Y	610	-	1/1/15/20	18/39/115/115	-
33	BCR	c1	517	-	-	8/29/63/63	0/2/2/2
31	CLA	c	505	-	1/1/15/20	18/39/115/115	-
31	CLA	B1	612	-	1/1/15/20	9/39/115/115	-
31	CLA	s1	610	-	1/1/15/20	18/39/115/115	-
31	CLA	N1	614	-	1/1/11/20	7/20/96/115	-
31	CLA	n1	603	-	1/1/15/20	18/39/115/115	-
31	CLA	g1	610	-	1/1/15/20	16/39/115/115	-
35	LMG	H	102	-	-	10/43/63/70	0/1/1/1
49	XAT	g	622	-	2/2/12/26	1/31/93/93	0/4/4/4
31	CLA	b	609	-	1/1/15/20	11/39/115/115	-
31	CLA	Y1	612	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	DGD	c	523	-	-	17/55/95/95	0/2/2/2
48	LUT	r	620	-	-	8/29/67/67	0/2/2/2
31	CLA	y	608	-	1/1/12/20	6/21/97/115	-
47	CHL	G	607	-	3/3/16/26	3/20/118/137	-
48	LUT	S	620	-	1/1/12/27	3/29/67/67	0/2/2/2
40	DGD	c	519	-	-	22/51/91/95	0/2/2/2
35	LMG	D	411	-	-	9/41/61/70	0/1/1/1
40	DGD	b1	623	-	-	11/32/72/95	0/2/2/2
31	CLA	b	604	-	1/1/15/20	19/39/115/115	-
31	CLA	c1	505	-	1/1/15/20	17/39/115/115	-
49	XAT	r1	621	-	1/1/12/26	2/31/93/93	0/4/4/4
47	CHL	N	608	-	3/3/16/26	4/20/118/137	-
31	CLA	y	614	-	1/1/15/20	15/39/115/115	-
47	CHL	y	606	-	4/4/20/26	8/39/137/137	-
35	LMG	D1	411	-	-	11/41/61/70	0/1/1/1
31	CLA	b1	607	-	1/1/15/20	15/39/115/115	-
50	NEX	N	623	-	-	7/27/83/83	0/3/3/3
31	CLA	d1	402	-	1/1/15/20	14/39/115/115	-
34	SQD	a	412	-	-	12/46/66/69	0/1/1/1
31	CLA	C	505	-	1/1/15/20	15/39/115/115	-
31	CLA	R	611	-	1/1/11/20	6/17/93/115	-
31	CLA	S	617	-	1/1/12/20	7/21/97/115	-
48	LUT	S1	620	-	-	2/29/67/67	0/2/2/2
57	PTY	y1	626	-	-	22/53/53/53	-
31	CLA	c	509	-	1/1/15/20	15/39/115/115	-
31	CLA	y1	614	-	1/1/15/20	14/39/115/115	-
31	CLA	c	503	-	1/1/15/20	20/39/115/115	-
42	LMK	C1	527	-	2/2/6/6	16/46/46/60	-
47	CHL	N	606	-	4/4/20/26	6/39/137/137	-
35	LMG	w1	201	-	-	16/34/54/70	0/1/1/1
45	HEM	f1	101	-	-	0/14/54/54	-
31	CLA	G	614	-	1/1/11/20	9/20/96/115	-
31	CLA	N1	602	-	1/1/15/20	11/39/115/115	-
31	CLA	N1	613	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	XAT	y1	622	-	-	4/31/93/93	0/4/4/4
54	4RF	K1	101	-	-	29/59/59/59	-
31	CLA	S	613	-	1/1/13/20	13/27/103/115	-
47	CHL	n1	608	-	3/3/16/26	3/20/118/137	-
50	NEX	S1	623	-	-	3/27/83/83	0/3/3/3
54	4RF	k1	101	-	-	35/59/59/59	-
57	PTY	Y1	626	-	-	18/53/53/53	-
47	CHL	S	601	-	3/3/16/26	4/15/113/137	-
31	CLA	s	617	-	1/1/12/20	9/21/97/115	-
34	SQD	c	626	-	-	19/49/69/69	0/1/1/1
31	CLA	s	611	-	1/1/15/20	16/39/115/115	-
31	CLA	N1	610	-	1/1/15/20	18/39/115/115	-
47	CHL	r	607	-	3/3/16/26	4/20/118/137	-
31	CLA	B1	615	-	1/1/15/20	18/39/115/115	-
49	XAT	N1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
41	LHG	C	525	-	-	28/51/51/53	-
46	RRX	h1	101	-	1/1/11/25	9/29/65/65	0/2/2/2
48	LUT	R1	620	-	1/1/12/27	5/29/67/67	0/2/2/2
39	GOL	B	627	-	-	0/4/4/4	-
33	BCR	C	515	-	-	11/29/63/63	0/2/2/2
40	DGD	c1	518	-	-	16/44/84/95	0/2/2/2
31	CLA	B1	613	-	1/1/15/20	17/39/115/115	-
47	CHL	s1	607	-	3/3/15/26	2/12/110/137	-
31	CLA	B	605	-	1/1/15/20	17/39/115/115	-
31	CLA	y1	602	-	1/1/15/20	17/39/115/115	-
31	CLA	B	616	-	1/1/15/20	15/39/115/115	-
31	CLA	g1	612	-	1/1/10/20	6/13/89/115	-
33	BCR	A	411	-	-	11/29/63/63	0/2/2/2
48	LUT	S	621	-	-	1/29/67/67	0/2/2/2
31	CLA	r	609	-	1/1/14/20	17/33/109/115	-
35	LMG	H1	102	-	-	13/43/63/70	0/1/1/1
31	CLA	s1	614	-	1/1/13/20	11/27/103/115	-
41	LHG	Y	624	-	-	31/53/53/53	-
41	LHG	S	624	-	-	27/49/49/53	-
31	CLA	G1	613	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	s1	609	-	1/1/14/20	16/33/109/115	-
47	CHL	N	609	-	4/4/20/26	10/39/137/137	-
48	LUT	R	620	-	-	9/29/67/67	0/2/2/2
31	CLA	g	614	-	1/1/11/20	10/20/96/115	-
31	CLA	Y	602	24	1/1/15/20	18/39/115/115	-
31	CLA	B	608	-	1/1/15/20	19/39/115/115	-
31	CLA	s1	602	-	1/1/14/20	12/33/109/115	-
31	CLA	y1	610	-	1/1/15/20	11/39/115/115	-
49	XAT	n1	622	-	1/1/12/26	5/31/93/93	0/4/4/4
31	CLA	C	511	-	1/1/15/20	9/39/115/115	-
40	DGD	C1	518	-	-	14/44/84/95	0/2/2/2
31	CLA	s	614	-	1/1/13/20	11/27/103/115	-
31	CLA	a	410	-	1/1/14/20	7/33/109/115	-
31	CLA	Y	604	-	1/1/15/20	17/39/115/115	-
31	CLA	s1	604	-	1/1/13/20	14/27/103/115	-
47	CHL	n	605	-	4/4/20/26	5/39/137/137	-
47	CHL	N1	609	-	4/4/20/26	6/39/137/137	-
41	LHG	d1	410	-	-	25/43/43/53	-
52	3PH	B1	624	-	-	23/49/49/49	-
33	BCR	B1	618	-	-	11/29/63/63	0/2/2/2
47	CHL	s	607	-	4/4/15/26	3/12/110/137	-
48	LUT	G1	620	-	-	4/29/67/67	0/2/2/2
31	CLA	a	406	-	1/1/15/20	9/39/115/115	-
51	LPX	S1	625	-	-	9/31/31/31	-
47	CHL	N	607	-	4/4/20/26	6/39/137/137	-
31	CLA	C	507	-	1/1/15/20	18/39/115/115	-
47	CHL	g	601	21	4/4/20/26	5/39/137/137	-
31	CLA	A1	410	-	1/1/14/20	8/33/109/115	-
31	CLA	R1	602	-	1/1/14/20	15/33/109/115	-
38	DGA	J1	101	-	-	10/30/30/45	-
31	CLA	r1	610	-	1/1/14/20	16/33/109/115	-
35	LMG	C	521	-	-	20/46/66/70	0/1/1/1
48	LUT	G1	621	-	-	4/29/67/67	0/2/2/2
31	CLA	S	605	-	1/1/12/20	12/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	CHL	g	607	-	3/3/16/26	3/20/118/137	-
31	CLA	s	605	-	1/1/12/20	10/21/97/115	-
34	SQD	B1	626	-	-	25/49/69/69	0/1/1/1
47	CHL	r1	607	-	3/3/16/26	4/20/118/137	-
47	CHL	s1	608	-	4/4/19/26	4/33/131/137	-
31	CLA	n1	612	-	1/1/11/20	8/15/91/115	-
49	XAT	N	622	-	1/1/12/26	3/31/93/93	0/4/4/4
31	CLA	c	513	-	1/1/15/20	21/39/115/115	-
31	CLA	Y	614	-	1/1/15/20	13/39/115/115	-
47	CHL	g	608	-	3/3/15/26	1/13/111/137	-
35	LMG	d1	411	-	-	11/41/61/70	0/1/1/1
31	CLA	r	603	-	1/1/14/20	16/33/109/115	-
31	CLA	S	603	-	1/1/15/20	12/39/115/115	-
35	LMG	A1	413	-	-	15/43/63/70	0/1/1/1
31	CLA	B1	617	-	1/1/15/20	17/39/115/115	-
31	CLA	n1	614	-	1/1/11/20	7/20/96/115	-
47	CHL	g1	606	-	3/3/16/26	4/20/118/137	-
31	CLA	B1	611	-	1/1/15/20	15/39/115/115	-
31	CLA	C1	502	-	1/1/15/20	13/39/115/115	-
31	CLA	b1	604	-	1/1/15/20	17/39/115/115	-
47	CHL	R	607	-	3/3/16/26	2/20/118/137	-
31	CLA	c1	513	-	1/1/15/20	21/39/115/115	-
31	CLA	A	405	-	1/1/15/20	11/39/115/115	-
31	CLA	R	612	-	1/1/14/20	13/33/109/115	-
31	CLA	b1	609	-	1/1/15/20	11/39/115/115	-
31	CLA	r1	608	-	1/1/14/20	22/33/109/115	-
41	LHG	C1	525	-	-	32/51/51/53	-
31	CLA	C1	505	-	1/1/15/20	21/39/115/115	-
37	C7Z	b1	620	-	1/1/12/26	15/29/67/67	0/2/2/2
48	LUT	G	620	-	-	3/29/67/67	0/2/2/2
31	CLA	B1	609	-	1/1/15/20	17/39/115/115	-
32	PHO	a	408	-	-	12/37/103/103	0/5/6/6
37	C7Z	B	620	-	1/1/12/26	11/29/67/67	0/2/2/2
47	CHL	n	606	-	4/4/20/26	6/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	501	-	1/1/15/20	17/39/115/115	-
31	CLA	R1	603	-	1/1/14/20	11/33/109/115	-
31	CLA	Y1	603	-	1/1/15/20	21/39/115/115	-
47	CHL	G	606	-	4/4/16/26	5/20/118/137	-
35	LMG	a1	413	-	-	15/43/63/70	0/1/1/1
35	LMG	b1	622	-	-	15/39/59/70	0/1/1/1
31	CLA	N	614	-	1/1/11/20	8/20/96/115	-
47	CHL	n1	607	-	4/4/20/26	7/39/137/137	-
31	CLA	Y	611	-	1/1/15/20	15/39/115/115	-
31	CLA	D	403	-	1/1/15/20	17/39/115/115	-
31	CLA	s	609	-	1/1/14/20	14/33/109/115	-
44	PL9	D	405	-	-	22/53/73/73	0/1/1/1
50	NEX	N1	623	-	-	5/27/83/83	0/3/3/3
38	DGA	j1	101	-	-	15/30/30/45	-
31	CLA	B	615	-	1/1/15/20	8/39/115/115	-
47	CHL	S	608	-	4/4/19/26	4/33/131/137	-
41	LHG	L	101	-	-	32/53/53/53	-
47	CHL	y1	609	-	4/4/20/26	7/39/137/137	-
48	LUT	n	620	-	-	6/29/67/67	0/2/2/2
48	LUT	n	621	-	1/1/12/27	4/29/67/67	0/2/2/2
33	BCR	c	514	-	-	12/29/63/63	0/2/2/2
31	CLA	g1	602	-	1/1/15/20	23/39/115/115	-
31	CLA	r	611	-	1/1/11/20	7/17/93/115	-
31	CLA	G	613	-	1/1/15/20	17/39/115/115	-
35	LMG	J	101	-	-	14/40/60/70	0/1/1/1
31	CLA	S	610	-	1/1/15/20	14/39/115/115	-
31	CLA	y1	604	-	1/1/15/20	17/39/115/115	-
33	BCR	b	618	-	-	10/29/63/63	0/2/2/2
34	SQD	c1	526	-	-	17/49/69/69	0/1/1/1
33	BCR	C1	515	-	-	10/29/63/63	0/2/2/2
31	CLA	y1	611	-	1/1/15/20	14/39/115/115	-
47	CHL	S1	608	-	4/4/19/26	8/33/131/137	-
48	LUT	y1	620	-	-	3/29/67/67	0/2/2/2
47	CHL	y1	605	-	3/3/16/26	1/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	NEX	r	623	-	-	8/27/83/83	0/3/3/3
38	DGA	c	524	-	-	22/45/45/45	-
41	LHG	L1	101	-	-	34/53/53/53	-
48	LUT	N1	620	-	-	5/29/67/67	0/2/2/2
47	CHL	n1	601	20	4/4/20/26	8/39/137/137	-
34	SQD	C	526	-	-	17/49/69/69	0/1/1/1
31	CLA	C1	507	-	1/1/15/20	18/39/115/115	-
47	CHL	g1	605	-	4/4/16/26	4/18/116/137	-
32	PHO	a1	409	-	-	11/37/103/103	0/5/6/6
31	CLA	S1	602	-	1/1/14/20	19/33/109/115	-
50	NEX	y1	623	-	-	7/27/83/83	0/3/3/3
41	LHG	d	408	-	-	28/48/48/53	-
31	CLA	b	617	-	1/1/15/20	14/39/115/115	-
47	CHL	G1	605	-	4/4/16/26	3/18/116/137	-
34	SQD	B	621	-	-	18/49/69/69	0/1/1/1
31	CLA	R	604	-	1/1/11/20	10/20/96/115	-
31	CLA	y	610	-	1/1/15/20	15/39/115/115	-
41	LHG	c	625	-	-	33/51/51/53	-
48	LUT	y	620	-	-	0/29/67/67	0/2/2/2
48	LUT	N1	621	-	-	5/29/67/67	0/2/2/2
49	XAT	y	622	-	-	3/31/93/93	0/4/4/4
31	CLA	d	402	-	1/1/15/20	18/39/115/115	-
35	LMG	c1	521	-	-	12/46/66/70	0/1/1/1
31	CLA	C	508	-	1/1/15/20	11/39/115/115	-
50	NEX	r1	622	-	-	9/27/83/83	0/3/3/3
31	CLA	S1	609	-	1/1/14/20	14/33/109/115	-
31	CLA	B	612	-	1/1/15/20	21/39/115/115	-
41	LHG	s1	624	-	-	22/49/49/53	-
31	CLA	a1	406	-	1/1/15/20	13/39/115/115	-
31	CLA	c	506	-	1/1/15/20	22/39/115/115	-
31	CLA	G1	603	-	1/1/15/20	18/39/115/115	-
41	LHG	g	624	-	-	27/53/53/53	-
50	NEX	Y1	623	-	-	8/27/83/83	0/3/3/3
47	CHL	n1	605	-	4/4/20/26	9/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	BCR	c	515	-	-	10/29/63/63	0/2/2/2
47	CHL	G1	608	-	3/3/15/26	3/13/111/137	-
35	LMG	a	413	-	-	18/43/63/70	0/1/1/1
38	DGA	b	623	-	-	27/45/45/45	-
52	3PH	T1	101	-	-	28/49/49/49	-
57	PTY	y1	627	-	-	14/20/20/53	-
31	CLA	B	613	-	1/1/15/20	14/39/115/115	-
48	LUT	s1	621	-	-	2/29/67/67	0/2/2/2
32	PHO	A1	408	-	-	6/37/103/103	0/5/6/6
31	CLA	c1	502	-	1/1/15/20	13/39/115/115	-
31	CLA	B	602	-	1/1/15/20	21/39/115/115	-
31	CLA	S	602	23	1/1/14/20	13/33/109/115	-
47	CHL	G	601	-	4/4/20/26	3/39/137/137	-
31	CLA	G1	610	-	1/1/15/20	14/39/115/115	-
47	CHL	G	609	-	4/4/20/26	10/39/137/137	-
52	3PH	s1	626	-	-	24/49/49/49	-
33	BCR	c1	515	-	-	13/29/63/63	0/2/2/2
33	BCR	b	619	-	-	9/29/63/63	0/2/2/2
31	CLA	g	611	-	1/1/11/20	7/15/91/115	-
31	CLA	C	502	-	1/1/15/20	18/39/115/115	-
31	CLA	N	612	-	1/1/11/20	7/15/91/115	-
31	CLA	c1	508	-	1/1/15/20	12/39/115/115	-
31	CLA	b	603	-	1/1/15/20	19/39/115/115	-
34	SQD	m1	101	-	-	21/37/57/69	0/1/1/1
33	BCR	C	517	-	-	8/29/63/63	0/2/2/2
31	CLA	S1	612	-	1/1/11/20	6/15/91/115	-
47	CHL	n	601	-	4/4/20/26	5/39/137/137	-
32	PHO	A1	409	-	-	13/37/103/103	0/5/6/6
49	XAT	Y1	622	-	2/2/12/26	2/31/93/93	0/4/4/4
31	CLA	G	611	-	1/1/11/20	6/15/91/115	-
31	CLA	s1	605	23	1/1/12/20	9/21/97/115	-
31	CLA	B	611	-	1/1/15/20	10/39/115/115	-
31	CLA	S	611	-	1/1/15/20	15/39/115/115	-
31	CLA	B1	610	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	C1	512	-	1/1/15/20	18/39/115/115	-
40	DGD	C	523	-	-	16/55/95/95	0/2/2/2
47	CHL	Y	605	24	3/3/16/26	0/15/113/137	-
50	NEX	g	623	-	-	4/27/83/83	0/3/3/3
31	CLA	b	611	-	1/1/15/20	10/39/115/115	-
34	SQD	B1	621	-	-	13/37/57/69	0/1/1/1
31	CLA	A	410	-	1/1/14/20	12/33/109/115	-
31	CLA	C	512	-	1/1/15/20	16/39/115/115	-
31	CLA	n	603	-	1/1/15/20	24/39/115/115	-
52	3PH	i	101	-	-	21/49/49/49	-
42	LMK	c	627	-	1/1/6/6	11/46/46/60	-
49	XAT	n	622	-	-	1/31/93/93	0/4/4/4
31	CLA	c1	510	-	1/1/15/20	17/39/115/115	-
31	CLA	g1	614	-	1/1/11/20	11/20/96/115	-
31	CLA	N	603	-	1/1/15/20	16/39/115/115	-
31	CLA	r	610	-	1/1/14/20	15/33/109/115	-
31	CLA	G	603	-	1/1/15/20	21/39/115/115	-
33	BCR	B	618	-	-	11/29/63/63	0/2/2/2
31	CLA	N	604	-	1/1/15/20	17/39/115/115	-
31	CLA	a	405	-	1/1/15/20	15/39/115/115	-
41	LHG	N1	624	-	-	39/53/53/53	-
47	CHL	Y	601	-	4/4/20/26	5/39/137/137	-
46	RRX	h	101	-	1/1/11/25	7/29/65/65	0/2/2/2
35	LMG	h1	102	-	-	14/43/63/70	0/1/1/1
31	CLA	N1	603	-	1/1/15/20	17/39/115/115	-
31	CLA	b1	613	-	1/1/15/20	20/39/115/115	-
34	SQD	M1	101	-	-	17/37/57/69	0/1/1/1
47	CHL	G1	607	-	4/4/20/26	12/39/137/137	-
50	NEX	S	622	-	-	12/27/83/83	0/3/3/3
41	LHG	S1	624	-	-	25/49/49/53	-
31	CLA	B	610	-	1/1/15/20	20/39/115/115	-
31	CLA	s1	617	-	1/1/12/20	10/21/97/115	-
47	CHL	r	606	-	3/3/15/26	1/13/111/137	-
31	CLA	n1	611	-	1/1/11/20	10/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	DGD	C1	519	-	-	21/51/91/95	0/2/2/2
31	CLA	y	603	-	1/1/15/20	10/39/115/115	-
31	CLA	g	610	-	1/1/15/20	12/39/115/115	-
31	CLA	G	604	-	1/1/11/20	9/20/96/115	-
31	CLA	S1	604	-	1/1/13/20	9/27/103/115	-
33	BCR	c1	516	-	-	12/29/63/63	0/2/2/2
31	CLA	d1	403	-	1/1/15/20	11/39/115/115	-
31	CLA	R	603	-	1/1/14/20	16/33/109/115	-
47	CHL	y	609	-	4/4/20/26	4/39/137/137	-
50	NEX	s	623	-	-	7/27/83/83	0/3/3/3
56	ERG	R1	626	-	5/5/11/15	7/13/71/71	0/4/4/4
34	SQD	b	621	-	-	18/49/69/69	0/1/1/1
40	DGD	C1	520	-	-	14/48/88/95	0/2/2/2
50	NEX	G	623	-	-	4/27/83/83	0/3/3/3
49	XAT	R1	621	-	-	2/31/93/93	0/4/4/4
31	CLA	a1	410	-	1/1/14/20	9/33/109/115	-
31	CLA	S1	614	-	1/1/13/20	11/27/103/115	-
33	BCR	C	516	-	-	15/29/63/63	0/2/2/2
32	PHO	A	409	-	-	8/37/103/103	0/5/6/6
41	LHG	y1	624	-	-	26/53/53/53	-
47	CHL	G1	609	-	4/4/20/26	7/39/137/137	-
31	CLA	b1	614	-	1/1/15/20	11/39/115/115	-
51	LPX	S	625	-	-	12/31/31/31	-
31	CLA	n	611	-	1/1/11/20	15/20/96/115	-
47	CHL	G	608	-	3/3/15/26	0/13/111/137	-
31	CLA	n	610	-	1/1/15/20	13/39/115/115	-
33	BCR	a1	411	-	-	13/29/63/63	0/2/2/2
31	CLA	B	614	-	1/1/15/20	13/39/115/115	-
31	CLA	D	402	-	1/1/15/20	17/39/115/115	-
47	CHL	Y	606	-	4/4/20/26	6/39/137/137	-
33	BCR	d	404	-	-	11/29/63/63	0/2/2/2
33	BCR	b1	618	-	-	8/29/63/63	0/2/2/2
35	LMG	j	101	-	-	14/40/60/70	0/1/1/1
41	LHG	D	409	-	-	31/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c1	504	-	1/1/15/20	16/39/115/115	-
39	GOL	b	624	-	-	1/4/4/4	-
31	CLA	g1	604	-	1/1/11/20	10/20/96/115	-
31	CLA	r	602	-	1/1/14/20	7/33/109/115	-
47	CHL	n	607	-	4/4/20/26	9/39/137/137	-
31	CLA	C	503	-	1/1/15/20	20/39/115/115	-
47	CHL	N1	608	-	3/3/16/26	3/20/118/137	-
31	CLA	G1	611	-	1/1/15/20	16/39/115/115	-
34	SQD	C1	526	-	-	24/49/69/69	0/1/1/1
48	LUT	Y	620	-	-	6/29/67/67	0/2/2/2
46	RRX	H	101	-	1/1/11/25	10/29/65/65	0/2/2/2
50	NEX	n	623	-	-	5/27/83/83	0/3/3/3
47	CHL	y	605	24	3/3/16/26	5/15/113/137	-
48	LUT	y	621	-	-	3/29/67/67	0/2/2/2
38	DGA	c1	524	-	-	22/45/45/45	-
33	BCR	A1	411	-	-	11/29/63/63	0/2/2/2
41	LHG	Y1	624	-	-	25/53/53/53	-
31	CLA	S	604	-	1/1/13/20	11/27/103/115	-
31	CLA	R1	612	-	1/1/14/20	15/33/109/115	-
31	CLA	g	602	-	1/1/15/20	21/39/115/115	-
47	CHL	N1	601	20	4/4/20/26	2/39/137/137	-
38	DGA	C	524	-	-	26/45/45/45	-
31	CLA	s	610	-	1/1/15/20	21/39/115/115	-
38	DGA	B1	625	-	-	23/45/45/45	-
31	CLA	C1	508	-	1/1/15/20	11/39/115/115	-
47	CHL	R1	606	-	3/3/15/26	1/13/111/137	-
41	LHG	N	624	-	-	24/53/53/53	-
50	NEX	n1	623	-	-	5/27/83/83	1/3/3/3
31	CLA	n	613	-	1/1/15/20	17/39/115/115	-
31	CLA	Y1	614	-	1/1/15/20	16/39/115/115	-
40	DGD	c1	519	-	-	18/51/91/95	0/2/2/2
31	CLA	B1	602	-	1/1/15/20	22/39/115/115	-
31	CLA	R1	609	-	1/1/14/20	10/33/109/115	-
47	CHL	N	605	-	4/4/20/26	8/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	N	613	-	1/1/15/20	18/39/115/115	-
31	CLA	b1	617	-	1/1/15/20	18/39/115/115	-
47	CHL	n	609	-	4/4/20/26	12/39/137/137	-
35	LMG	c	521	-	-	20/46/66/70	0/1/1/1
52	3PH	b1	624	-	-	19/49/49/49	-
48	LUT	G	621	-	1/1/12/27	6/29/67/67	0/2/2/2
31	CLA	s	613	-	1/1/13/20	12/27/103/115	-
31	CLA	R	610	-	1/1/14/20	13/33/109/115	-
37	C7Z	B1	620	-	1/1/12/26	11/29/67/67	0/2/2/2
31	CLA	b1	608	-	1/1/15/20	21/39/115/115	-
40	DGD	c1	520	-	-	12/48/88/95	0/2/2/2
47	CHL	y	607	-	4/4/20/26	9/39/137/137	-
35	LMG	d	411	-	-	10/41/61/70	0/1/1/1
31	CLA	y	604	-	1/1/15/20	19/39/115/115	-
31	CLA	d	403	-	1/1/15/20	13/39/115/115	-
31	CLA	Y1	604	-	1/1/15/20	17/39/115/115	-
39	GOL	y	626	-	-	0/4/4/4	-
33	BCR	C1	517	-	-	12/29/63/63	0/2/2/2
31	CLA	B	604	-	1/1/15/20	17/39/115/115	-
48	LUT	N	620	-	-	4/29/67/67	0/2/2/2
41	LHG	l	101	-	-	28/53/53/53	-
31	CLA	c1	501	-	1/1/15/20	15/39/115/115	-
33	BCR	B	619	-	-	3/29/63/63	0/2/2/2
41	LHG	d	409	-	-	27/53/53/53	-
31	CLA	S	609	-	1/1/14/20	12/33/109/115	-
31	CLA	c1	506	-	1/1/15/20	17/39/115/115	-
31	CLA	C	513	-	1/1/15/20	20/39/115/115	-
31	CLA	B	603	-	1/1/15/20	18/39/115/115	-
41	LHG	c1	525	-	-	33/51/51/53	-
31	CLA	C	501	-	1/1/15/20	17/39/115/115	-
38	DGA	C1	524	-	-	35/45/45/45	-
40	DGD	c	520	-	-	15/48/88/95	0/2/2/2
31	CLA	n1	610	-	1/1/15/20	16/39/115/115	-
31	CLA	r1	603	-	1/1/14/20	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	SPH	y	625	-	-	13/21/21/21	-
31	CLA	R	608	-	1/1/14/20	18/33/109/115	-
31	CLA	a	407	-	1/1/11/20	5/20/96/115	-
31	CLA	r1	602	-	1/1/14/20	15/33/109/115	-
31	CLA	Y	608	-	1/1/12/20	8/21/97/115	-
31	CLA	r1	604	-	1/1/11/20	8/20/96/115	-
31	CLA	A1	405	-	1/1/15/20	12/39/115/115	-
47	CHL	g	605	-	3/3/16/26	1/18/116/137	-
31	CLA	C1	511	-	1/1/15/20	10/39/115/115	-
31	CLA	c1	503	-	1/1/15/20	18/39/115/115	-
31	CLA	y1	608	-	1/1/12/20	9/21/97/115	-
31	CLA	B1	604	-	1/1/15/20	21/39/115/115	-
31	CLA	C1	510	-	1/1/15/20	18/39/115/115	-
31	CLA	G1	612	-	1/1/10/20	7/13/89/115	-
31	CLA	b1	605	-	1/1/15/20	20/39/115/115	-
47	CHL	N	601	20	4/4/20/26	3/39/137/137	-
49	XAT	Y	622	-	1/1/12/26	3/31/93/93	0/4/4/4
41	LHG	s	624	-	-	26/49/49/53	-
31	CLA	A1	407	-	1/1/12/20	6/21/97/115	-
35	LMG	B1	622	-	-	17/39/59/70	0/1/1/1
31	CLA	G	610	-	1/1/15/20	13/39/115/115	-
31	CLA	S1	611	-	1/1/15/20	17/39/115/115	-
31	CLA	s	612	-	1/1/11/20	10/15/91/115	-
31	CLA	N	610	-	1/1/15/20	9/39/115/115	-
33	BCR	c1	514	-	-	13/29/63/63	0/2/2/2
47	CHL	Y	609	-	4/4/20/26	9/39/137/137	-
31	CLA	B	606	-	1/1/15/20	15/39/115/115	-
31	CLA	b	616	-	1/1/15/20	11/39/115/115	-
33	BCR	C1	516	-	-	15/29/63/63	0/2/2/2
33	BCR	C	514	-	-	9/29/63/63	0/2/2/2
52	3PH	S	626	-	-	19/49/49/49	-
31	CLA	N1	604	-	1/1/15/20	14/39/115/115	-
53	SPH	A1	414	-	-	13/21/21/21	-
48	LUT	y1	621	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3PH	s	626	-	-	30/49/49/49	-
31	CLA	s	602	-	1/1/14/20	12/33/109/115	-
44	PL9	d	405	-	-	10/53/73/73	0/1/1/1
31	CLA	c1	509	-	1/1/15/20	15/39/115/115	-
41	LHG	y	624	-	-	28/53/53/53	-
41	LHG	D	410	-	-	27/43/43/53	-
47	CHL	n	608	-	3/3/16/26	4/20/118/137	-
31	CLA	s1	612	-	1/1/11/20	6/15/91/115	-
48	LUT	Y	621	-	1/1/12/27	2/29/67/67	0/2/2/2
41	LHG	g1	624	-	-	29/53/53/53	-
31	CLA	R	602	-	1/1/14/20	12/33/109/115	-
31	CLA	n	614	-	1/1/11/20	7/20/96/115	-
31	CLA	g1	613	-	1/1/15/20	15/39/115/115	-
47	CHL	N1	607	-	4/4/20/26	6/39/137/137	-
49	XAT	R	621	-	1/1/12/26	14/31/93/93	0/4/4/4
31	CLA	C1	503	-	1/1/15/20	14/39/115/115	-
32	PHO	a	409	-	-	9/37/103/103	0/5/6/6
47	CHL	s1	606	-	3/3/15/26	1/13/111/137	-
50	NEX	R	622	-	-	11/27/83/83	0/3/3/3
40	DGD	B1	623	-	-	16/32/72/95	0/2/2/2
47	CHL	g	606	-	3/3/16/26	4/20/118/137	-
31	CLA	s1	613	-	1/1/13/20	9/27/103/115	-
48	LUT	g1	620	-	-	3/29/67/67	0/2/2/2
42	LMK	c1	527	-	2/2/6/6	13/46/46/60	-
47	CHL	S	606	-	3/3/15/26	1/13/111/137	-
48	LUT	g	620	-	-	6/29/67/67	0/2/2/2
31	CLA	N	611	-	1/1/11/20	12/20/96/115	-
31	CLA	b1	611	-	1/1/15/20	11/39/115/115	-
34	SQD	a1	412	-	-	18/46/66/69	0/1/1/1
31	CLA	n1	602	-	1/1/15/20	21/39/115/115	-
53	SPH	Y1	625	-	-	11/21/21/21	-
48	LUT	s1	620	-	-	4/29/67/67	0/2/2/2
31	CLA	c	511	-	1/1/15/20	15/39/115/115	-
34	SQD	b1	621	-	-	18/37/57/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	C	504	-	1/1/15/20	15/39/115/115	-
31	CLA	n1	604	-	1/1/15/20	15/39/115/115	-
33	BCR	D	404	-	-	12/29/63/63	0/2/2/2
48	LUT	g	621	-	-	3/29/67/67	0/2/2/2
53	SPH	a1	414	-	-	12/21/21/21	-
47	CHL	S1	606	-	3/3/15/26	2/13/111/137	-
53	SPH	y1	625	-	-	11/21/21/21	-
41	LHG	D1	410	-	-	23/43/43/53	-
31	CLA	S1	613	-	1/1/13/20	8/27/103/115	-
41	LHG	d1	408	-	-	28/48/48/53	-
31	CLA	R	609	-	1/1/14/20	17/33/109/115	-
48	LUT	Y1	620	-	-	3/29/67/67	0/2/2/2
31	CLA	Y1	611	-	1/1/15/20	14/39/115/115	-
47	CHL	S1	601	23	3/3/16/26	0/15/113/137	-
33	BCR	c	516	-	-	11/29/63/63	0/2/2/2
51	LPX	s1	625	-	-	14/31/31/31	-
53	SPH	Y	625	-	-	12/21/21/21	-
31	CLA	C1	513	-	1/1/15/20	18/39/115/115	-
31	CLA	N1	612	-	1/1/11/20	9/15/91/115	-
31	CLA	B1	607	-	1/1/15/20	15/39/115/115	-
31	CLA	S	612	-	1/1/11/20	6/15/91/115	-
47	CHL	Y1	607	-	4/4/20/26	10/39/137/137	-
47	CHL	g1	601	-	4/4/20/26	14/39/137/137	-
31	CLA	N	602	-	1/1/15/20	14/39/115/115	-
31	CLA	b1	603	-	1/1/15/20	15/39/115/115	-
47	CHL	Y1	605	24	3/3/16/26	1/15/113/137	-
40	DGD	c	518	-	-	9/44/84/95	0/2/2/2
47	CHL	Y	607	-	4/4/20/26	7/39/137/137	-
48	LUT	Y1	621	-	-	2/29/67/67	0/2/2/2
35	LMG	C1	523	-	-	16/50/70/70	0/1/1/1
47	CHL	N1	606	-	4/4/20/26	13/39/137/137	-

The worst 5 of 4002 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H	101	RRX	C21-C22	38.28	2.24	1.35
56	R1	626	ERG	C1-C10	-24.08	1.10	1.54
56	r1	626	ERG	C1-C10	-23.87	1.10	1.54
56	r1	626	ERG	C10-C9	-21.39	1.28	1.55
56	R1	626	ERG	C10-C9	-20.86	1.29	1.55

The worst 5 of 8887 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	H	101	RRX	C37-C22-C23	-31.76	69.57	118.09
41	L1	101	LHG	O7-C7-C8	23.31	161.90	111.48
52	S1	626	3PH	O21-C21-C22	22.43	160.00	111.48
52	s1	626	3PH	O21-C21-C22	22.34	159.81	111.48
31	R1	609	CLA	C4-C3-C5	-22.08	76.90	115.23

5 of 694 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	A	405	CLA	ND
31	A	406	CLA	ND
31	A	407	CLA	ND
31	A	410	CLA	ND
31	B	602	CLA	ND

5 of 8548 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	A	405	CLA	CBD-CGD-O2D-CED
31	A	406	CLA	C1A-C2A-CAA-CBA
31	A	406	CLA	C3A-C2A-CAA-CBA
31	A	407	CLA	C2B-C3B-CAB-CBB
31	A	407	CLA	C4B-C3B-CAB-CBB

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	n1	623	NEX	C1-C2-C3-C4-C5-C6

637 monomers are involved in 2147 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	s	620	LUT	8	0
31	c	508	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	g	613	CLA	5	0
47	g1	607	CHL	3	0
33	C1	514	BCR	9	0
47	s1	601	CHL	1	0
31	c	507	CLA	4	0
47	n1	609	CHL	3	0
31	D1	403	CLA	1	0
52	t1	101	3PH	4	0
31	A	406	CLA	6	0
33	D1	404	BCR	1	0
35	A	413	LMG	12	0
31	Y	612	CLA	4	0
47	G	605	CHL	2	0
48	s	621	LUT	6	0
31	y1	612	CLA	6	0
48	N	621	LUT	3	0
48	r1	620	LUT	6	0
35	h	102	LMG	6	0
35	C1	521	LMG	9	0
32	A	408	PHO	6	0
33	c	517	BCR	6	0
31	R1	610	CLA	3	0
31	c1	511	CLA	9	0
31	a1	405	CLA	7	0
31	C	509	CLA	4	0
31	Y1	610	CLA	2	0
45	F1	101	HEM	1	0
41	D	408	LHG	3	0
47	y	601	CHL	5	0
47	y1	606	CHL	1	0
31	r	608	CLA	3	0
35	b	622	LMG	5	0
31	b	605	CLA	6	0
31	c	510	CLA	3	0
47	R1	607	CHL	1	0
31	y1	613	CLA	5	0
31	b1	616	CLA	8	0
31	G1	602	CLA	6	0
38	B	625	DGA	4	0
31	b1	606	CLA	4	0
44	D1	405	PL9	8	0
31	r	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	H1	101	RRX	5	0
31	b	608	CLA	6	0
39	b	625	GOL	1	0
31	g1	603	CLA	2	0
31	s	604	CLA	2	0
34	A1	412	SQD	2	0
31	y	611	CLA	1	0
31	b1	610	CLA	10	0
31	B1	605	CLA	8	0
31	n1	613	CLA	5	0
31	b1	602	CLA	7	0
31	S	614	CLA	2	0
40	C	518	DGD	6	0
31	S1	605	CLA	2	0
47	Y1	606	CHL	4	0
31	g1	611	CLA	3	0
50	g1	623	NEX	1	0
31	B	617	CLA	4	0
31	R1	608	CLA	3	0
31	B1	603	CLA	7	0
31	Y1	608	CLA	1	0
34	A	412	SQD	4	0
31	S1	603	CLA	3	0
56	r1	626	ERG	5	0
48	n1	620	LUT	4	0
31	R1	604	CLA	2	0
33	a	411	BCR	4	0
35	B	622	LMG	3	0
31	A	407	CLA	2	0
31	b1	615	CLA	8	0
47	Y1	601	CHL	3	0
40	C	520	DGD	5	0
31	B1	614	CLA	3	0
41	G	630	LHG	6	0
31	b	602	CLA	2	0
31	b	615	CLA	2	0
31	Y	613	CLA	3	0
31	b1	612	CLA	4	0
48	n1	621	LUT	8	0
47	n1	606	CHL	1	0
38	b1	625	DGA	5	0
31	s1	603	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b	613	CLA	2	0
33	d1	404	BCR	5	0
31	g	603	CLA	4	0
41	n1	624	LHG	4	0
31	A1	406	CLA	7	0
33	b1	619	BCR	2	0
44	d1	405	PL9	6	0
31	G1	614	CLA	1	0
55	r1	625	LMT	3	0
47	y1	601	CHL	4	0
31	b	606	CLA	5	0
35	c1	523	LMG	10	0
31	C1	504	CLA	8	0
31	r1	612	CLA	3	0
49	G	622	XAT	7	0
41	d	410	LHG	5	0
31	B	609	CLA	4	0
31	C	506	CLA	4	0
31	b	610	CLA	9	0
31	g	604	CLA	1	0
47	y1	607	CHL	6	0
54	i1	101	4RF	5	0
31	b	612	CLA	8	0
31	B1	606	CLA	4	0
31	B1	608	CLA	5	0
31	C	510	CLA	4	0
47	r1	606	CHL	2	0
48	g1	621	LUT	5	0
31	Y1	613	CLA	8	0
31	r1	609	CLA	7	0
31	B	607	CLA	5	0
40	C	519	DGD	8	0
31	n	602	CLA	4	0
41	D1	409	LHG	6	0
47	N1	605	CHL	2	0
31	b	614	CLA	3	0
52	S1	626	3PH	2	0
31	c	504	CLA	3	0
31	S1	610	CLA	4	0
41	d1	409	LHG	3	0
45	f	101	HEM	5	0
47	g1	608	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	s	603	CLA	1	0
31	Y1	602	CLA	13	0
45	F	101	HEM	2	0
47	s	608	CHL	5	0
49	r	622	XAT	6	0
50	R1	622	NEX	4	0
47	g1	609	CHL	3	0
49	G1	622	XAT	8	0
31	s1	611	CLA	5	0
31	c1	507	CLA	4	0
47	G1	601	CHL	3	0
54	I1	102	4RF	3	0
31	C1	506	CLA	7	0
31	G	602	CLA	9	0
31	a1	407	CLA	4	0
41	n	624	LHG	7	0
32	a1	408	PHO	7	0
49	g1	622	XAT	8	0
31	y	612	CLA	4	0
31	B1	616	CLA	5	0
41	D1	408	LHG	2	0
35	W1	201	LMG	4	0
48	S1	621	LUT	6	0
31	N1	611	CLA	1	0
50	s1	623	NEX	1	0
31	D1	402	CLA	10	0
47	Y1	609	CHL	2	0
34	b1	626	SQD	9	0
31	c1	512	CLA	5	0
31	C1	509	CLA	3	0
47	S	607	CHL	2	0
33	B1	619	BCR	3	0
31	c	512	CLA	1	0
31	y	602	CLA	20	0
51	s	625	LPX	1	0
47	R	606	CHL	2	0
31	r	612	CLA	1	0
47	G1	606	CHL	2	0
41	G1	624	LHG	3	0
31	b	607	CLA	2	0
31	Y	603	CLA	7	0
31	y	613	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	n	604	CLA	4	0
31	y1	603	CLA	4	0
57	Y1	627	PTY	1	0
31	C1	501	CLA	7	0
47	S1	607	CHL	2	0
31	G1	604	CLA	2	0
47	g	609	CHL	4	0
47	s	601	CHL	2	0
47	s	606	CHL	2	0
31	c	502	CLA	3	0
31	Y	610	CLA	4	0
33	c1	517	BCR	5	0
31	c	505	CLA	5	0
31	B1	612	CLA	4	0
31	s1	610	CLA	6	0
31	N1	614	CLA	1	0
31	n1	603	CLA	5	0
31	g1	610	CLA	2	0
35	H	102	LMG	4	0
49	g	622	XAT	6	0
31	b	609	CLA	9	0
31	Y1	612	CLA	3	0
40	c	523	DGD	6	0
48	r	620	LUT	3	0
31	y	608	CLA	2	0
40	c	519	DGD	8	0
40	b1	623	DGD	1	0
35	D	411	LMG	3	0
48	S	620	LUT	3	0
31	b	604	CLA	3	0
31	c1	505	CLA	9	0
49	r1	621	XAT	4	0
47	N	608	CHL	3	0
31	y	614	CLA	2	0
35	D1	411	LMG	3	0
47	y	606	CHL	2	0
31	b1	607	CLA	5	0
50	N	623	NEX	2	0
31	d1	402	CLA	6	0
34	a	412	SQD	4	0
31	C	505	CLA	7	0
31	R	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	S	617	CLA	1	0
48	S1	620	LUT	5	0
57	y1	626	PTY	5	0
31	c	509	CLA	6	0
31	y1	614	CLA	7	0
31	c	503	CLA	1	0
42	C1	527	LMK	1	0
47	N	606	CHL	3	0
35	w1	201	LMG	3	0
31	G	614	CLA	1	0
31	N1	602	CLA	5	0
31	N1	613	CLA	2	0
49	y1	622	XAT	9	0
54	K1	101	4RF	6	0
31	S	613	CLA	4	0
47	n1	608	CHL	1	0
50	S1	623	NEX	4	0
54	k1	101	4RF	3	0
57	Y1	626	PTY	6	0
47	S	601	CHL	3	0
31	s	617	CLA	2	0
34	c	626	SQD	2	0
31	s	611	CLA	4	0
31	N1	610	CLA	8	0
47	r	607	CHL	2	0
31	B1	615	CLA	7	0
49	N1	622	XAT	8	0
41	C	525	LHG	1	0
46	h1	101	RRX	9	0
48	R1	620	LUT	6	0
33	C	515	BCR	3	0
40	c1	518	DGD	7	0
31	B1	613	CLA	10	0
47	s1	607	CHL	3	0
31	B	605	CLA	8	0
31	y1	602	CLA	13	0
31	B	616	CLA	2	0
31	g1	612	CLA	1	0
33	A	411	BCR	2	0
48	S	621	LUT	6	0
31	r	609	CLA	3	0
35	H1	102	LMG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	Y	624	LHG	4	0
41	S	624	LHG	8	0
31	G1	613	CLA	5	0
31	s1	609	CLA	3	0
47	N	609	CHL	2	0
48	R	620	LUT	5	0
31	Y	602	CLA	8	0
31	B	608	CLA	6	0
31	s1	602	CLA	4	0
31	y1	610	CLA	9	0
49	n1	622	XAT	8	0
31	C	511	CLA	6	0
40	C1	518	DGD	10	0
31	s	614	CLA	2	0
31	a	410	CLA	5	0
31	Y	604	CLA	4	0
31	s1	604	CLA	4	0
47	n	605	CHL	4	0
41	d1	410	LHG	6	0
47	N1	609	CHL	3	0
52	B1	624	3PH	10	0
33	B1	618	BCR	6	0
47	s	607	CHL	1	0
48	G1	620	LUT	2	0
31	a	406	CLA	5	0
47	N	607	CHL	5	0
31	C	507	CLA	6	0
47	g	601	CHL	4	0
31	A1	410	CLA	5	0
38	J1	101	DGA	2	0
31	r1	610	CLA	6	0
35	C	521	LMG	7	0
48	G1	621	LUT	5	0
31	S	605	CLA	2	0
31	s	605	CLA	1	0
34	B1	626	SQD	2	0
47	r1	607	CHL	2	0
47	s1	608	CHL	5	0
49	N	622	XAT	5	0
31	c	513	CLA	7	0
31	Y	614	CLA	2	0
35	d1	411	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	g	608	CHL	5	0
31	r	603	CLA	1	0
31	S	603	CLA	1	0
35	A1	413	LMG	7	0
31	B1	617	CLA	2	0
31	n1	614	CLA	1	0
47	g1	606	CHL	2	0
31	B1	611	CLA	6	0
31	C1	502	CLA	1	0
31	b1	604	CLA	5	0
47	R	607	CHL	2	0
31	c1	513	CLA	10	0
31	A	405	CLA	11	0
31	R	612	CLA	5	0
31	b1	609	CLA	9	0
31	r1	608	CLA	5	0
41	C1	525	LHG	9	0
31	C1	505	CLA	9	0
48	G	620	LUT	6	0
31	B1	609	CLA	7	0
32	a	408	PHO	4	0
47	n	606	CHL	3	0
31	c	501	CLA	5	0
31	R1	603	CLA	4	0
31	Y1	603	CLA	2	0
47	G	606	CHL	1	0
35	a1	413	LMG	7	0
35	b1	622	LMG	6	0
47	n1	607	CHL	4	0
31	Y	611	CLA	1	0
31	D	403	CLA	1	0
31	s	609	CLA	4	0
44	D	405	PL9	6	0
50	N1	623	NEX	4	0
38	j1	101	DGA	3	0
31	B	615	CLA	3	0
47	S	608	CHL	7	0
41	L	101	LHG	3	0
47	y1	609	CHL	3	0
48	n	620	LUT	5	0
33	c	514	BCR	4	0
48	n	621	LUT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	g1	602	CLA	6	0
31	G	613	CLA	2	0
35	J	101	LMG	2	0
31	S	610	CLA	2	0
31	y1	604	CLA	3	0
33	b	618	BCR	4	0
34	c1	526	SQD	5	0
33	C1	515	BCR	6	0
31	y1	611	CLA	7	0
47	S1	608	CHL	5	0
48	y1	620	LUT	5	0
47	y1	605	CHL	4	0
41	L1	101	LHG	9	0
48	N1	620	LUT	4	0
34	C	526	SQD	2	0
47	n1	601	CHL	5	0
31	C1	507	CLA	10	0
47	g1	605	CHL	2	0
32	a1	409	PHO	3	0
31	S1	602	CLA	4	0
50	y1	623	NEX	1	0
41	d	408	LHG	2	0
31	b	617	CLA	4	0
47	G1	605	CHL	2	0
34	B	621	SQD	3	0
31	R	604	CLA	1	0
31	y	610	CLA	6	0
41	c	625	LHG	4	0
48	y	620	LUT	5	0
48	N1	621	LUT	7	0
49	y	622	XAT	5	0
31	d	402	CLA	5	0
35	c1	521	LMG	7	0
31	C	508	CLA	3	0
50	r1	622	NEX	1	0
31	S1	609	CLA	2	0
31	B	612	CLA	9	0
41	s1	624	LHG	3	0
31	a1	406	CLA	4	0
31	c	506	CLA	7	0
31	G1	603	CLA	7	0
41	g	624	LHG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	Y1	623	NEX	2	0
33	c	515	BCR	5	0
47	n1	605	CHL	5	0
47	G1	608	CHL	2	0
35	a	413	LMG	6	0
38	b	623	DGA	3	0
52	T1	101	3PH	1	0
31	B	613	CLA	6	0
48	s1	621	LUT	7	0
32	A1	408	PHO	5	0
31	c1	502	CLA	4	0
31	B	602	CLA	2	0
31	S	602	CLA	2	0
47	G	601	CHL	6	0
31	G1	610	CLA	1	0
47	G	609	CHL	3	0
52	s1	626	3PH	3	0
33	c1	515	BCR	7	0
33	b	619	BCR	1	0
31	g	611	CLA	2	0
31	C	502	CLA	5	0
31	c1	508	CLA	9	0
31	b	603	CLA	3	0
34	m1	101	SQD	3	0
33	C	517	BCR	7	0
31	S1	612	CLA	1	0
47	n	601	CHL	7	0
32	A1	409	PHO	4	0
49	Y1	622	XAT	9	0
31	s1	605	CLA	2	0
31	B	611	CLA	3	0
31	S	611	CLA	3	0
31	B1	610	CLA	4	0
31	C1	512	CLA	7	0
40	C	523	DGD	5	0
47	Y	605	CHL	3	0
31	b	611	CLA	7	0
34	B1	621	SQD	4	0
31	A	410	CLA	8	0
31	C	512	CLA	5	0
31	n	603	CLA	9	0
52	i	101	3PH	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	n	622	XAT	5	0
31	c1	510	CLA	5	0
31	g1	614	CLA	1	0
31	N	603	CLA	4	0
31	r	610	CLA	3	0
31	G	603	CLA	4	0
33	B	618	BCR	4	0
31	N	604	CLA	3	0
31	a	405	CLA	4	0
41	N1	624	LHG	4	0
47	Y	601	CHL	2	0
46	h	101	RRX	3	0
35	h1	102	LMG	3	0
31	N1	603	CLA	2	0
31	b1	613	CLA	7	0
34	M1	101	SQD	6	0
47	G1	607	CHL	4	0
50	S	622	NEX	2	0
41	S1	624	LHG	6	0
31	B	610	CLA	5	0
47	r	606	CHL	1	0
31	n1	611	CLA	1	0
40	C1	519	DGD	8	0
31	y	603	CLA	10	0
31	g	610	CLA	1	0
31	G	604	CLA	6	0
31	S1	604	CLA	4	0
33	c1	516	BCR	7	0
31	d1	403	CLA	2	0
31	R	603	CLA	1	0
47	y	609	CHL	3	0
50	s	623	NEX	2	0
34	b	621	SQD	2	0
56	R1	626	ERG	8	0
40	C1	520	DGD	6	0
50	G	623	NEX	3	0
49	R1	621	XAT	3	0
31	a1	410	CLA	5	0
31	S1	614	CLA	1	0
33	C	516	BCR	4	0
32	A	409	PHO	2	0
41	y1	624	LHG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	G1	609	CHL	3	0
31	b1	614	CLA	3	0
51	S	625	LPX	2	0
33	a1	411	BCR	4	0
31	n	610	CLA	3	0
47	G	608	CHL	4	0
31	B	614	CLA	1	0
31	D	402	CLA	6	0
33	b1	618	BCR	3	0
33	d	404	BCR	5	0
35	j	101	LMG	5	0
41	D	409	LHG	6	0
47	Y	606	CHL	2	0
31	c1	504	CLA	7	0
39	b	624	GOL	1	0
31	g1	604	CLA	4	0
31	r	602	CLA	3	0
47	n	607	CHL	6	0
31	C	503	CLA	4	0
47	N1	608	CHL	4	0
31	G1	611	CLA	3	0
34	C1	526	SQD	2	0
48	Y	620	LUT	4	0
46	H	101	RRX	26	0
50	n	623	NEX	3	0
47	y	605	CHL	2	0
48	y	621	LUT	6	0
38	c1	524	DGA	3	0
33	A1	411	BCR	4	0
41	Y1	624	LHG	7	0
31	S	604	CLA	3	0
31	R1	612	CLA	2	0
31	g	602	CLA	9	0
38	C	524	DGA	2	0
47	N1	601	CHL	4	0
31	s	610	CLA	3	0
38	B1	625	DGA	5	0
31	C1	508	CLA	8	0
47	R1	606	CHL	3	0
31	n	613	CLA	7	0
31	Y1	614	CLA	7	0
40	c1	519	DGD	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B1	602	CLA	4	0
31	R1	609	CLA	3	0
47	N	605	CHL	7	0
31	N	613	CLA	5	0
31	b1	617	CLA	2	0
47	n	609	CHL	8	0
35	c	521	LMG	3	0
52	b1	624	3PH	6	0
48	G	621	LUT	10	0
31	s	613	CLA	3	0
31	R	610	CLA	3	0
31	b1	608	CLA	11	0
40	c1	520	DGD	8	0
47	y	607	CHL	2	0
35	d	411	LMG	4	0
31	y	604	CLA	2	0
31	d	403	CLA	3	0
31	Y1	604	CLA	3	0
33	C1	517	BCR	5	0
31	B	604	CLA	4	0
48	N	620	LUT	3	0
41	l	101	LHG	9	0
31	c1	501	CLA	4	0
33	B	619	BCR	2	0
41	d	409	LHG	3	0
31	S	609	CLA	4	0
31	c1	506	CLA	7	0
31	C	513	CLA	6	0
31	B	603	CLA	9	0
41	c1	525	LHG	9	0
31	C	501	CLA	6	0
38	C1	524	DGA	4	0
40	c	520	DGD	5	0
31	n1	610	CLA	5	0
31	r1	603	CLA	7	0
53	y	625	SPH	4	0
31	R	608	CLA	2	0
31	r1	602	CLA	2	0
31	Y	608	CLA	2	0
31	A1	405	CLA	3	0
47	g	605	CHL	2	0
28	A1	401	OEX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	C1	511	CLA	3	0
31	c1	503	CLA	5	0
31	y1	608	CLA	2	0
31	B1	604	CLA	8	0
31	C1	510	CLA	5	0
31	b1	605	CLA	4	0
47	N	601	CHL	3	0
49	Y	622	XAT	3	0
41	s	624	LHG	7	0
31	A1	407	CLA	2	0
35	B1	622	LMG	9	0
31	G	610	CLA	1	0
31	S1	611	CLA	6	0
31	s	612	CLA	2	0
31	N	610	CLA	5	0
33	c1	514	BCR	12	0
47	Y	609	CHL	6	0
31	B	606	CLA	7	0
31	b	616	CLA	6	0
33	C1	516	BCR	6	0
33	C	514	BCR	6	0
52	S	626	3PH	3	0
31	N1	604	CLA	5	0
53	A1	414	SPH	5	0
48	y1	621	LUT	6	0
52	s	626	3PH	1	0
31	s	602	CLA	3	0
44	d	405	PL9	4	0
31	c1	509	CLA	5	0
41	y	624	LHG	7	0
41	D	410	LHG	1	0
47	n	608	CHL	2	0
31	s1	612	CLA	1	0
48	Y	621	LUT	6	0
41	g1	624	LHG	5	0
31	R	602	CLA	3	0
31	g1	613	CLA	7	0
47	N1	607	CHL	1	0
49	R	621	XAT	3	0
31	C1	503	CLA	3	0
32	a	409	PHO	5	0
47	s1	606	CHL	2	0

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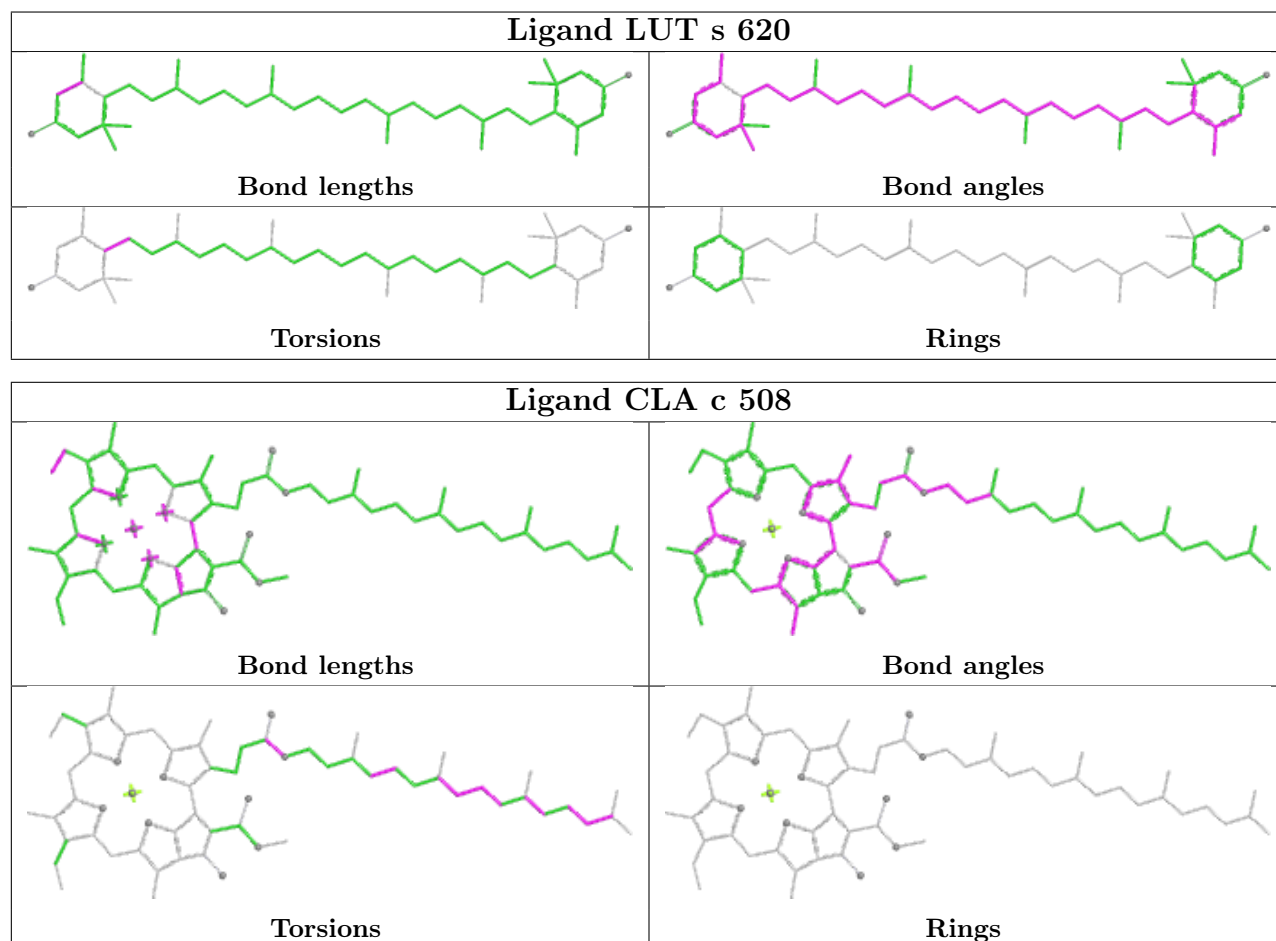
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50	R	622	NEX	3	0
40	B1	623	DGD	5	0
47	g	606	CHL	1	0
31	s1	613	CLA	1	0
28	a	401	OEX	1	0
48	g1	620	LUT	5	0
47	S	606	CHL	3	0
48	g	620	LUT	4	0
31	N	611	CLA	2	0
31	b1	611	CLA	6	0
34	a1	412	SQD	7	0
31	n1	602	CLA	4	0
53	Y1	625	SPH	3	0
48	s1	620	LUT	2	0
31	c	511	CLA	6	0
34	b1	621	SQD	5	0
31	C	504	CLA	5	0
31	n1	604	CLA	1	0
33	D	404	BCR	1	0
48	g	621	LUT	10	0
53	a1	414	SPH	5	0
47	S1	606	CHL	3	0
53	y1	625	SPH	7	0
41	D1	410	LHG	3	0
31	S1	613	CLA	3	0
41	d1	408	LHG	2	0
31	R	609	CLA	3	0
48	Y1	620	LUT	7	0
31	Y1	611	CLA	1	0
47	S1	601	CHL	1	0
33	c	516	BCR	5	0
51	s1	625	LPX	2	0
53	Y	625	SPH	3	0
31	C1	513	CLA	7	0
31	N1	612	CLA	1	0
31	B1	607	CLA	4	0
31	S	612	CLA	2	0
47	Y1	607	CHL	5	0
47	g1	601	CHL	7	0
31	N	602	CLA	4	0
31	b1	603	CLA	6	0
47	Y1	605	CHL	1	0

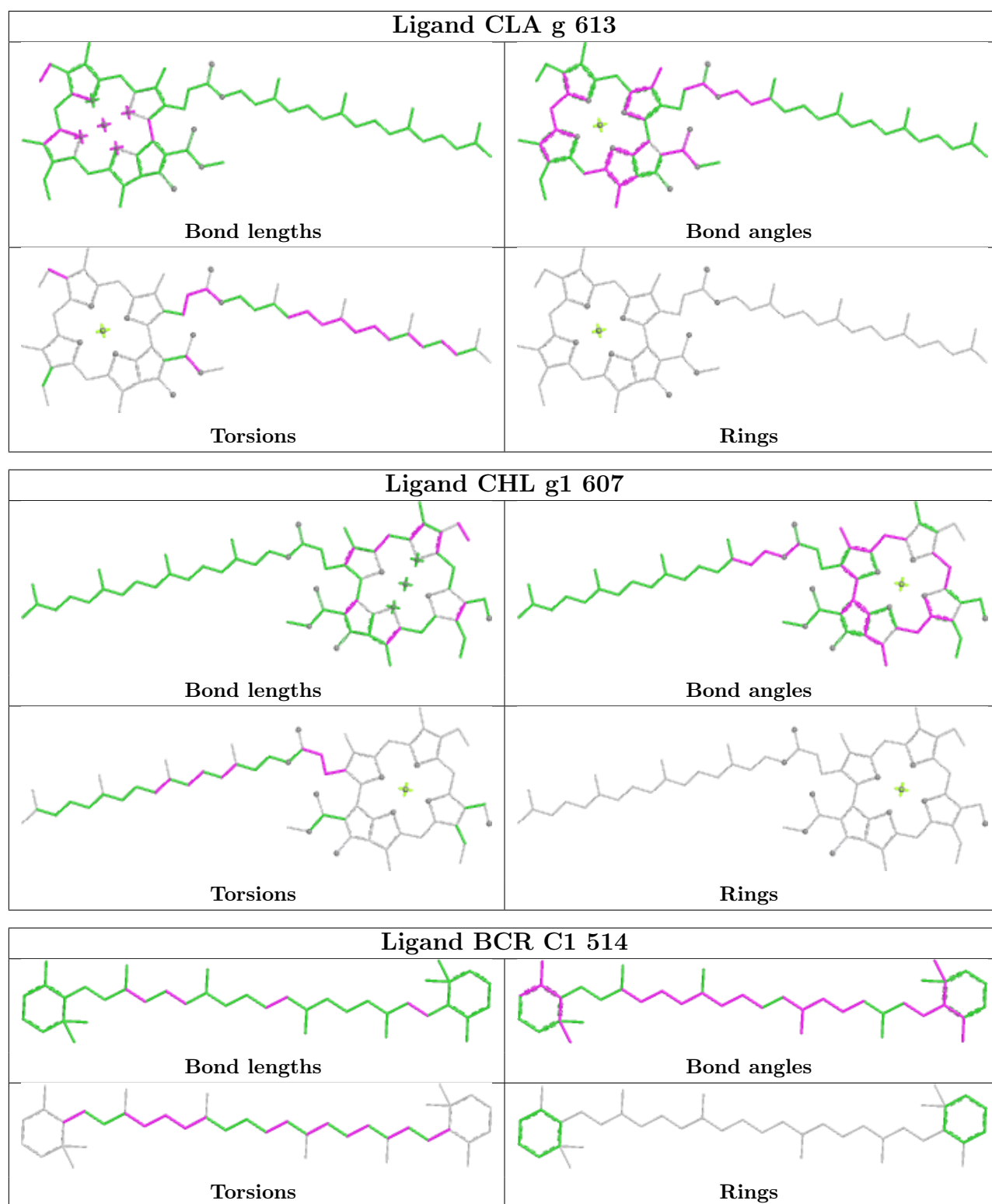
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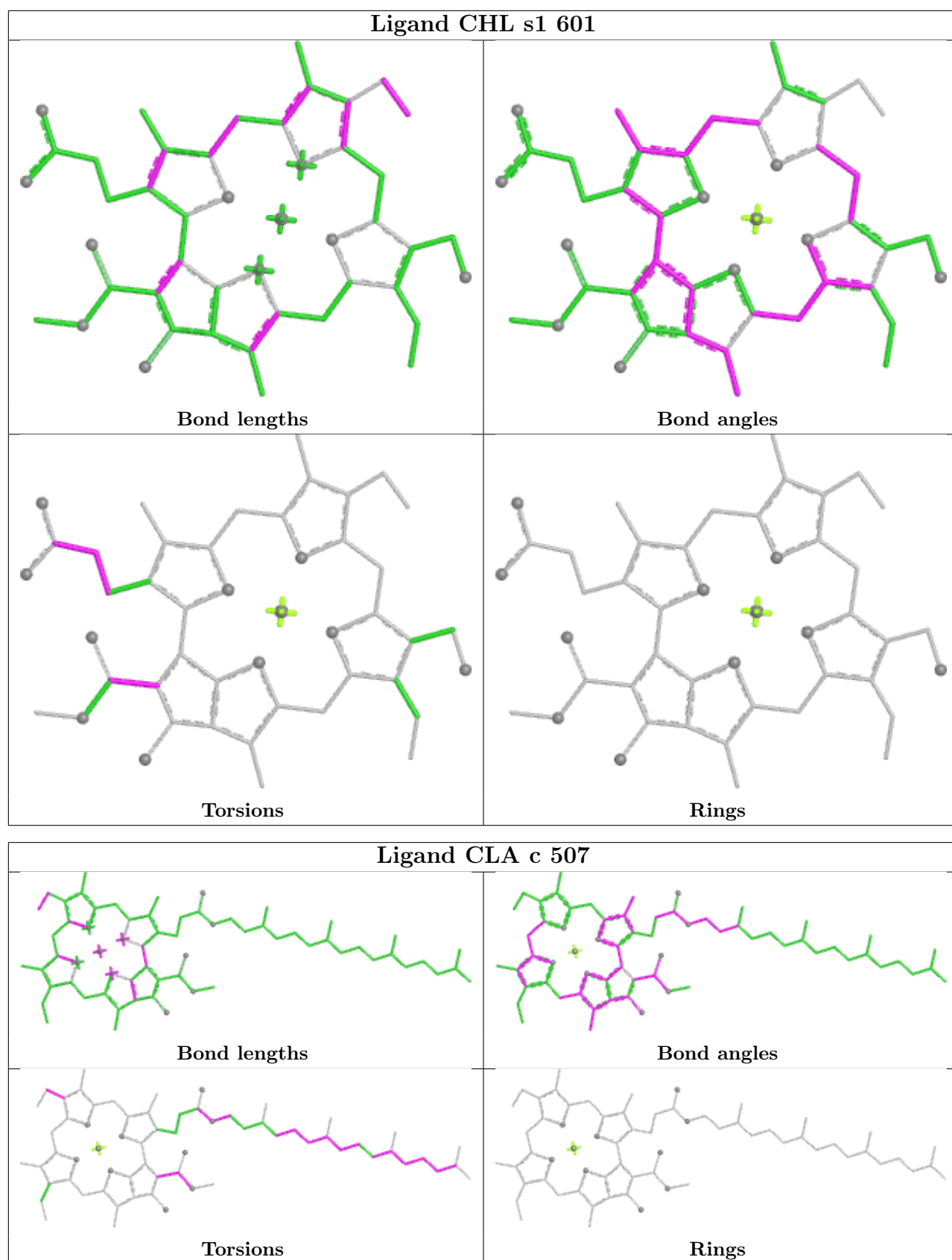
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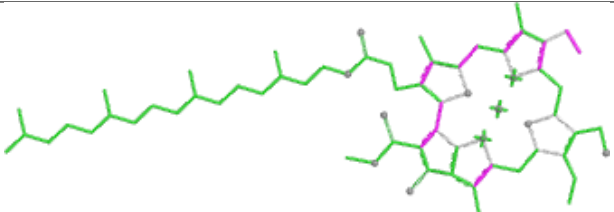
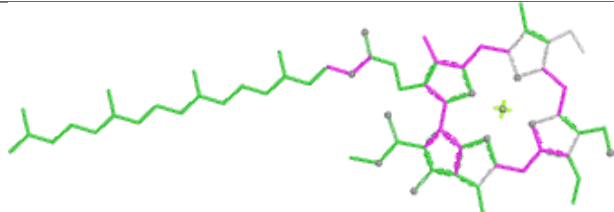
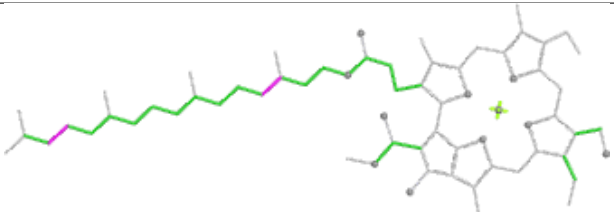
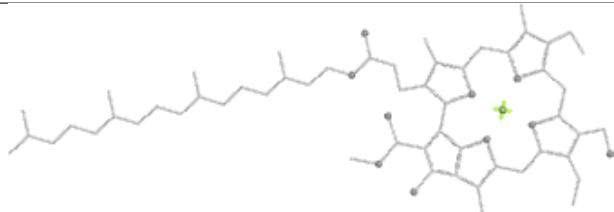
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	c	518	DGD	6	0
47	Y	607	CHL	5	0
48	Y1	621	LUT	8	0
35	C1	523	LMG	5	0
47	N1	606	CHL	4	0

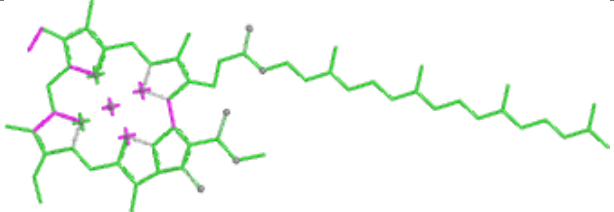
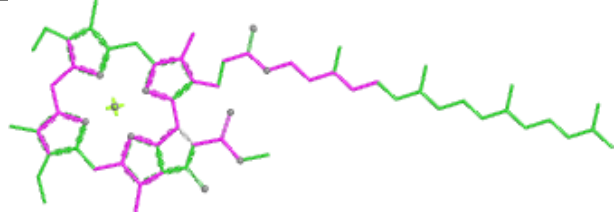
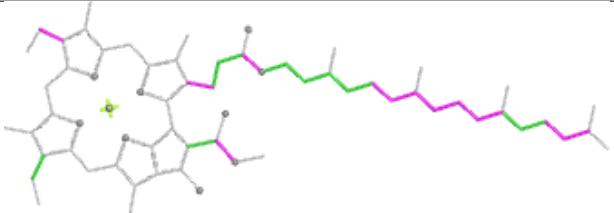
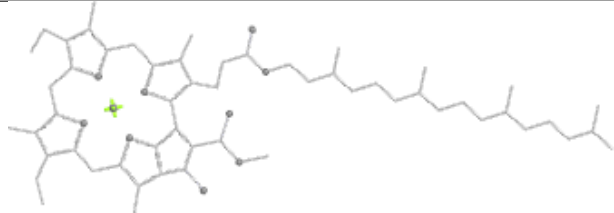
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

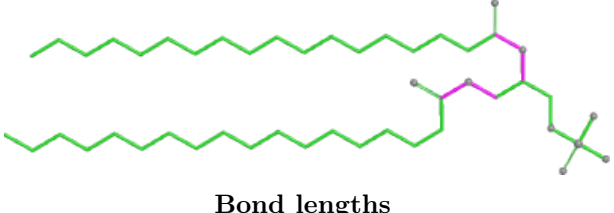
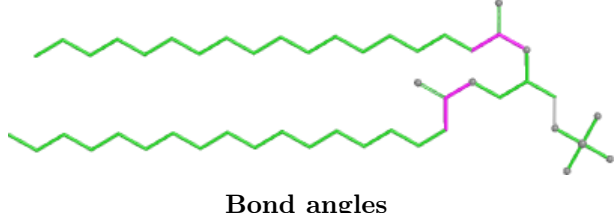
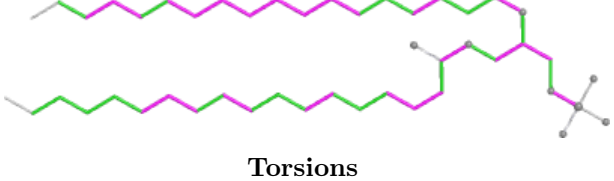


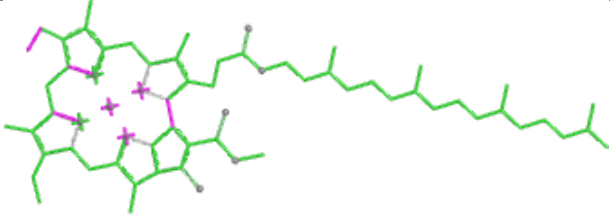
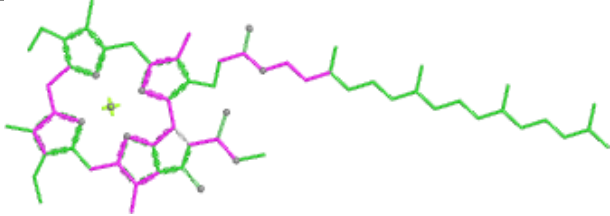
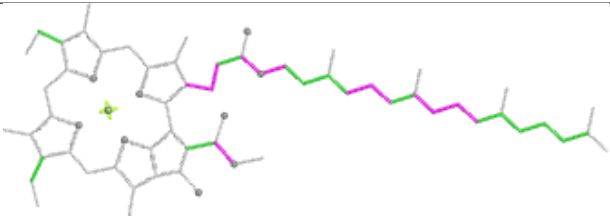
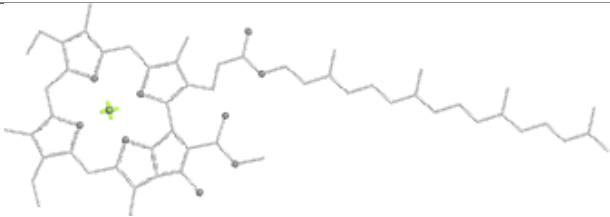
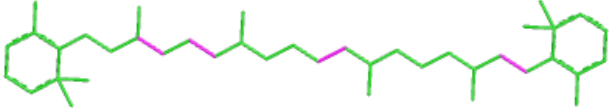
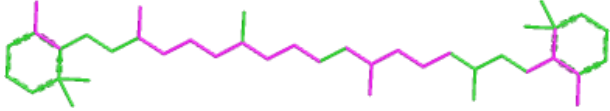
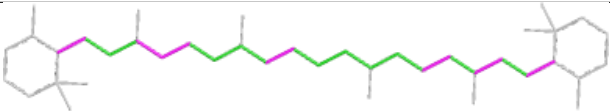
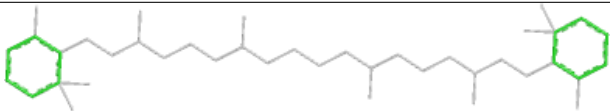
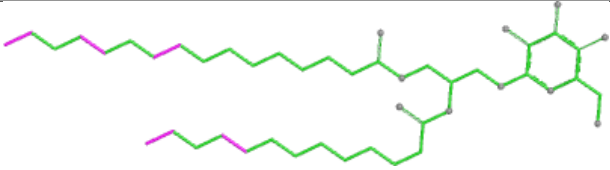
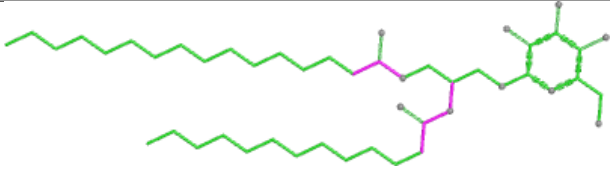
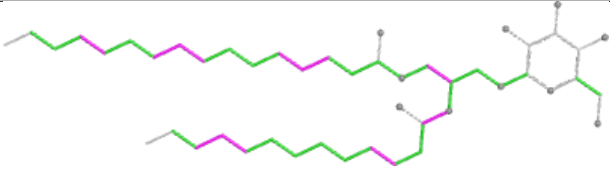
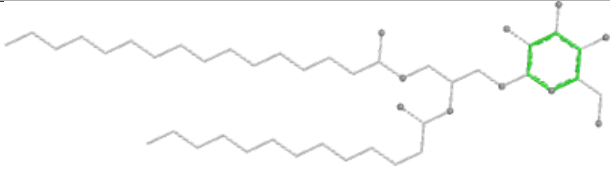


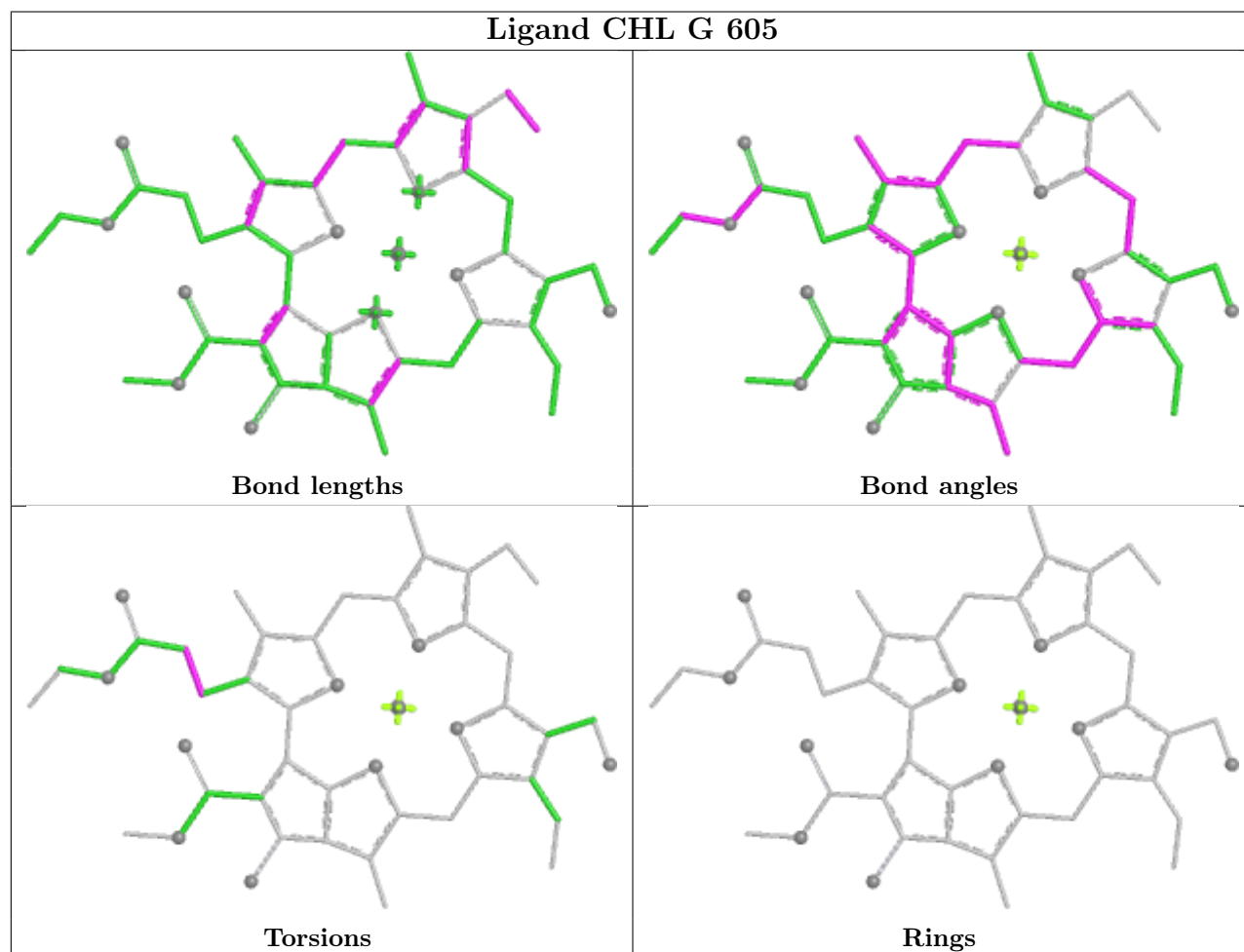
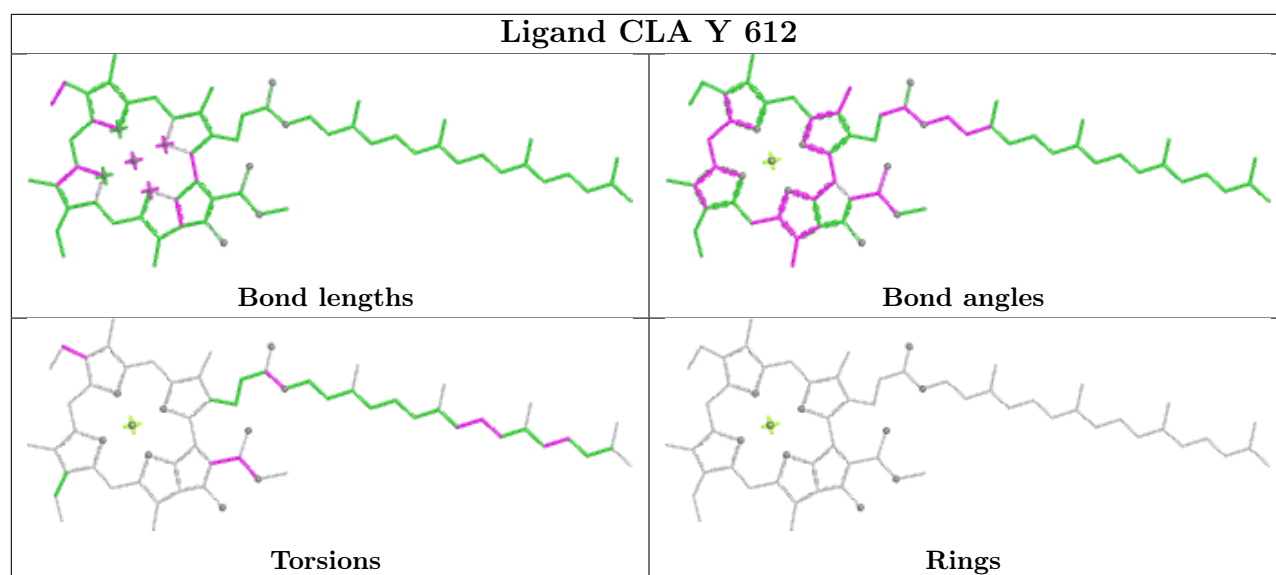


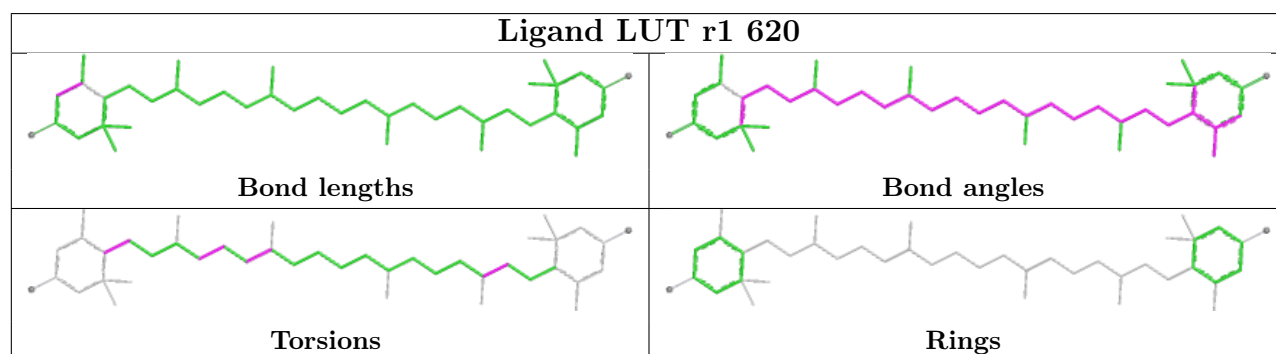
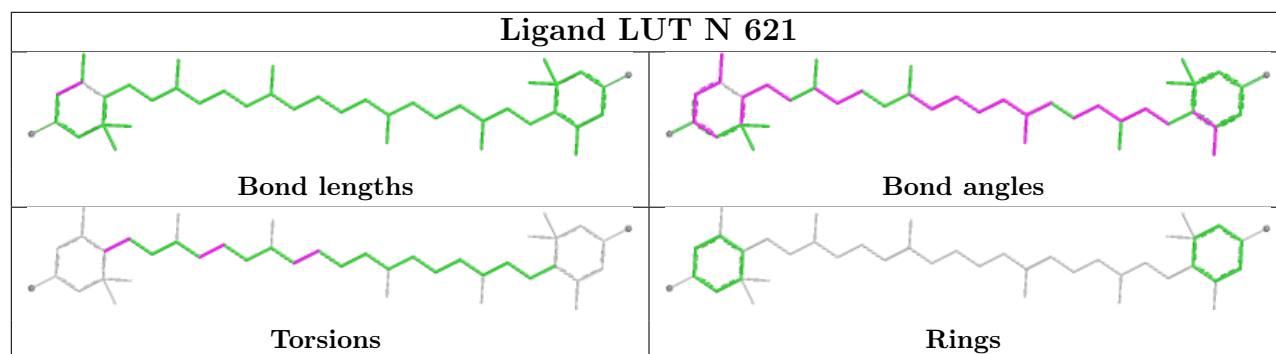
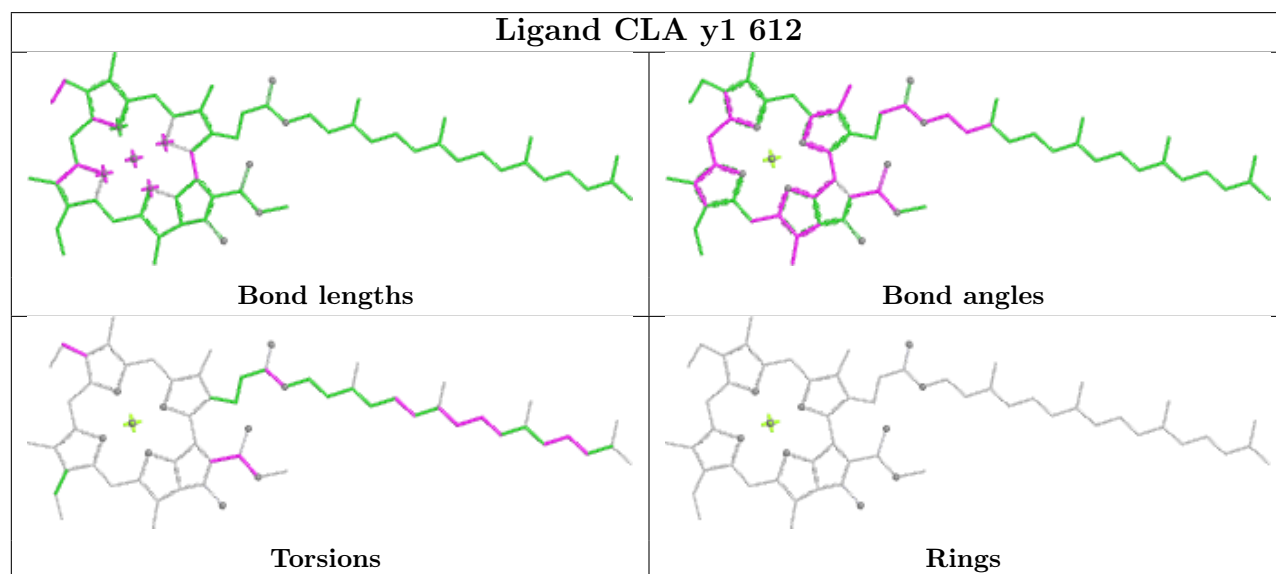
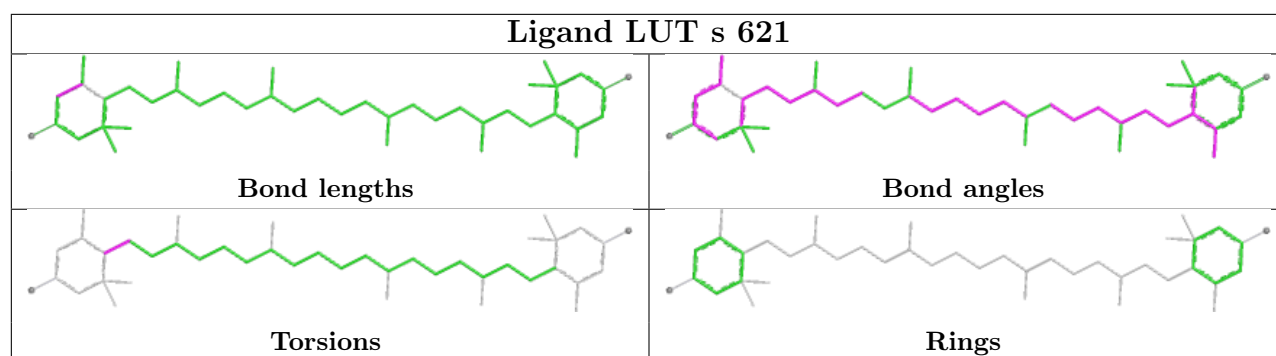
Ligand CHL n1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

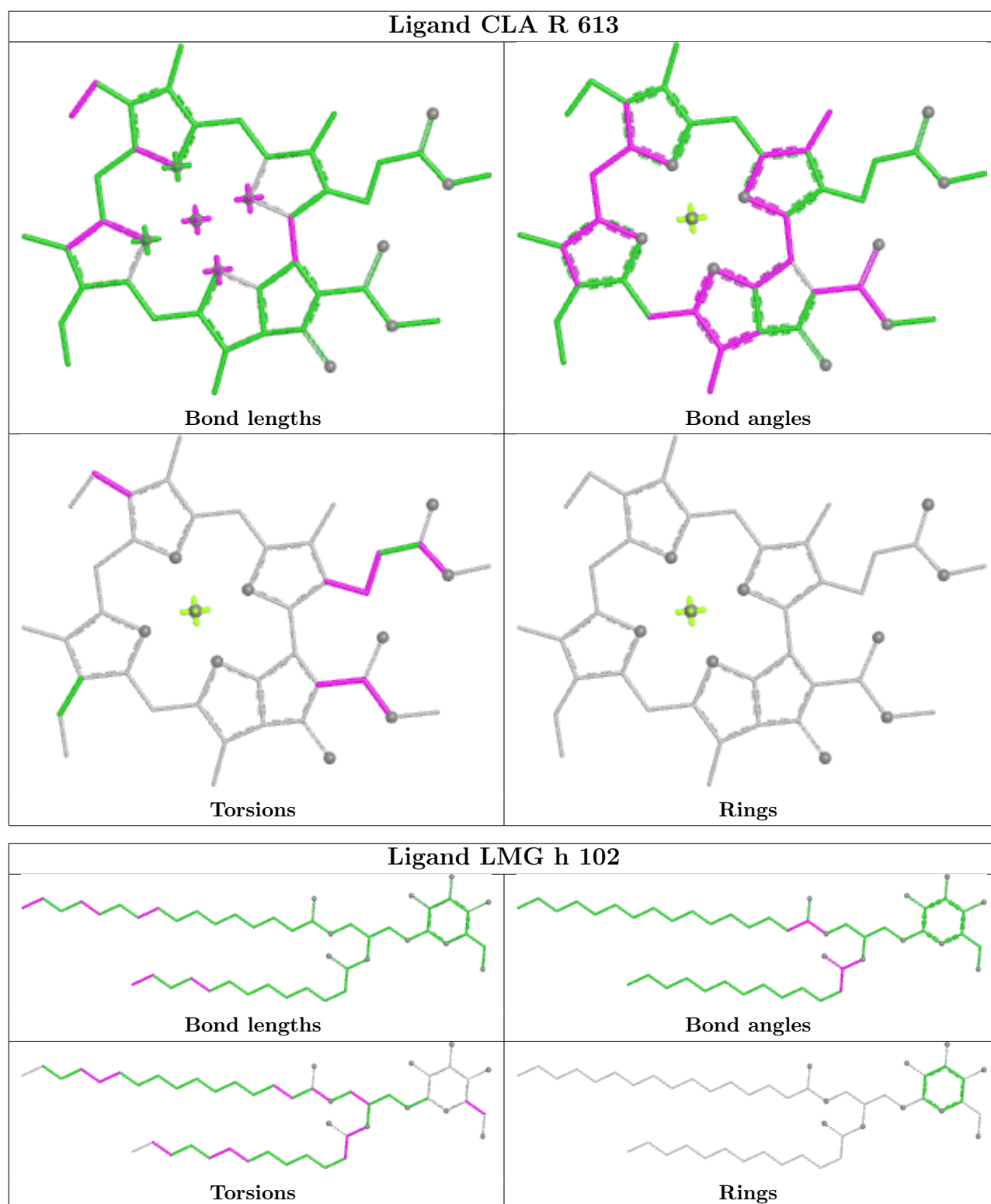
Ligand CLA D1 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

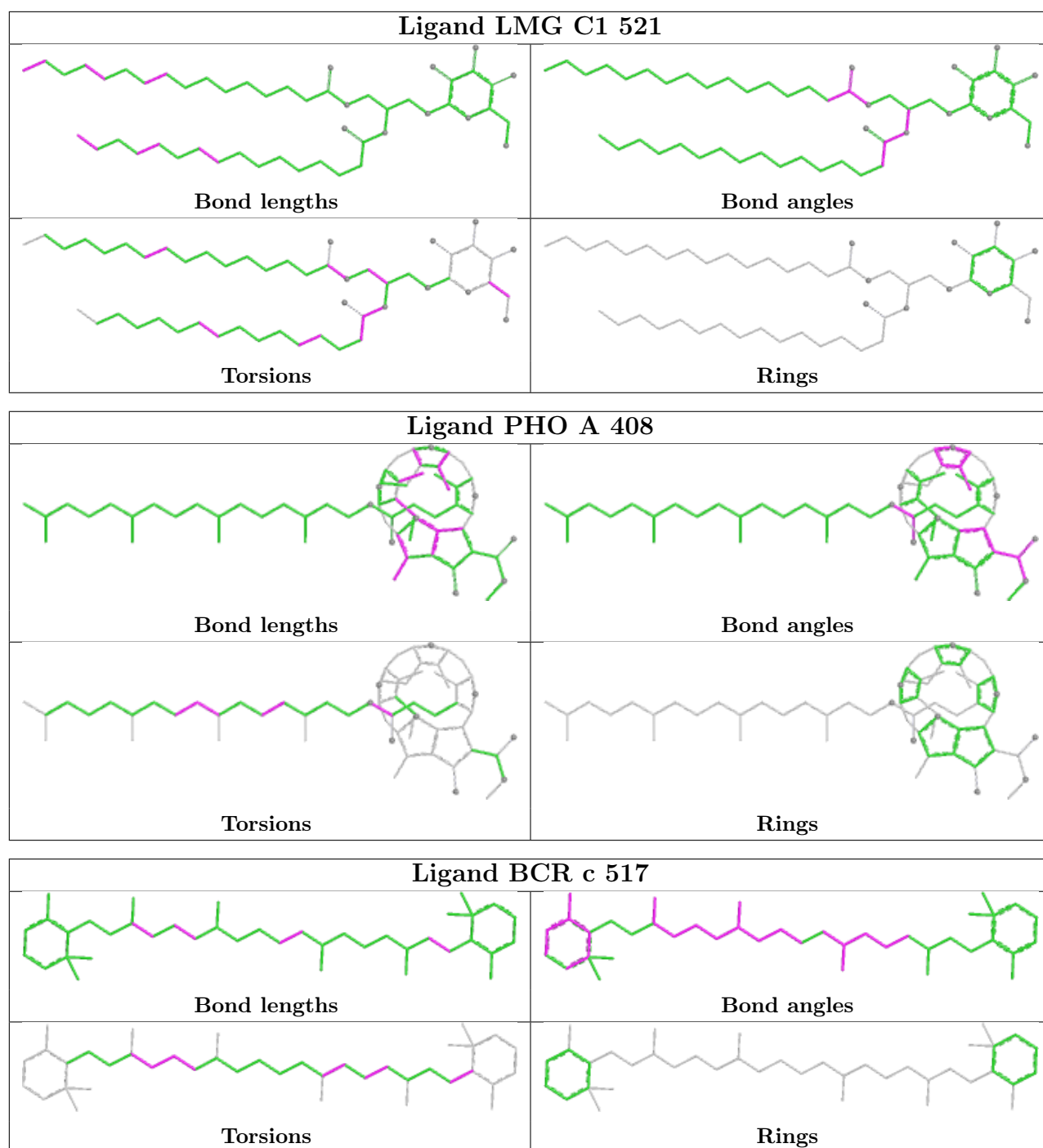
Ligand 3PH t1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

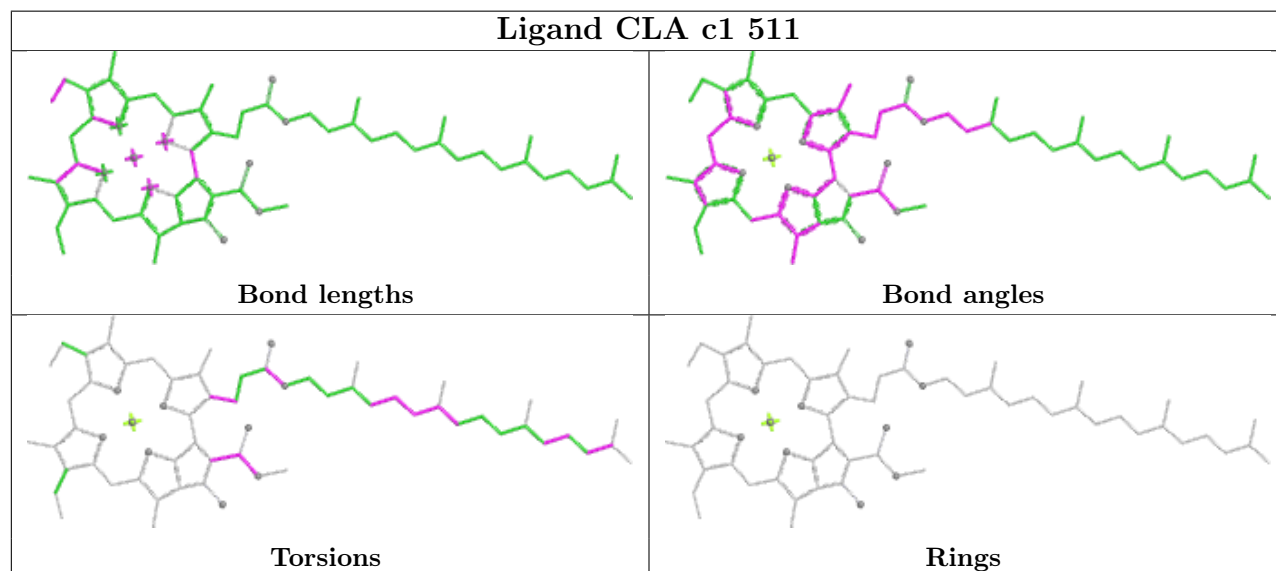
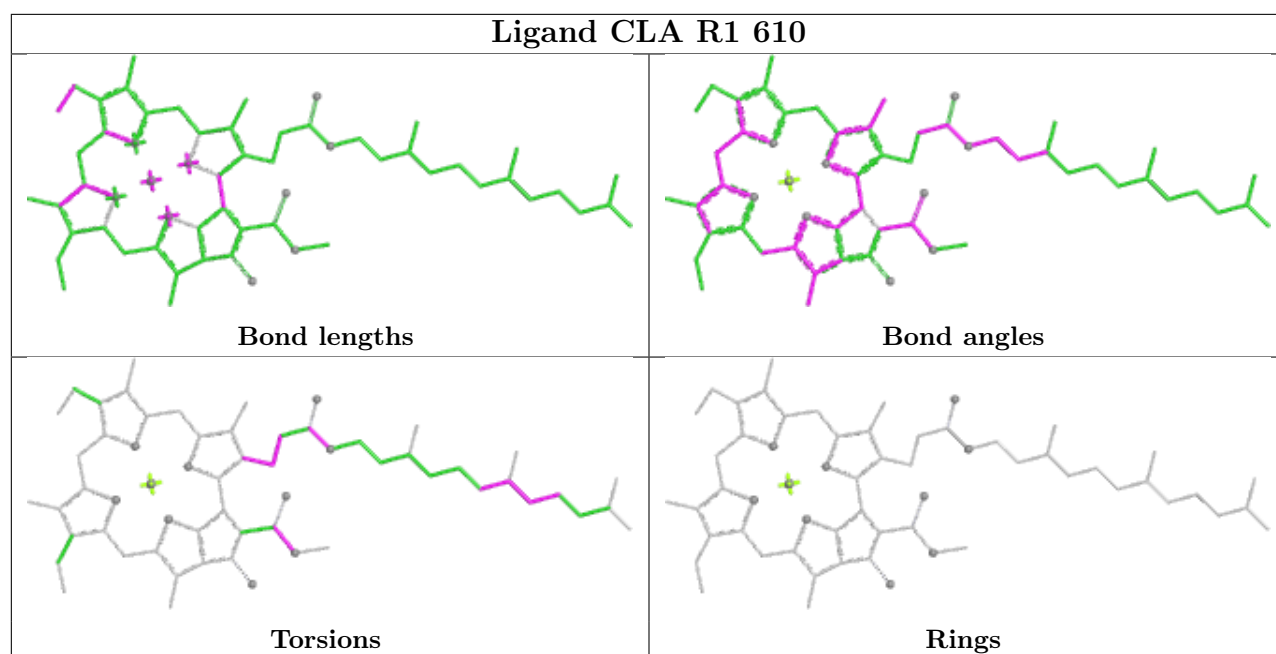
Ligand CLA A 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D1 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG A 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

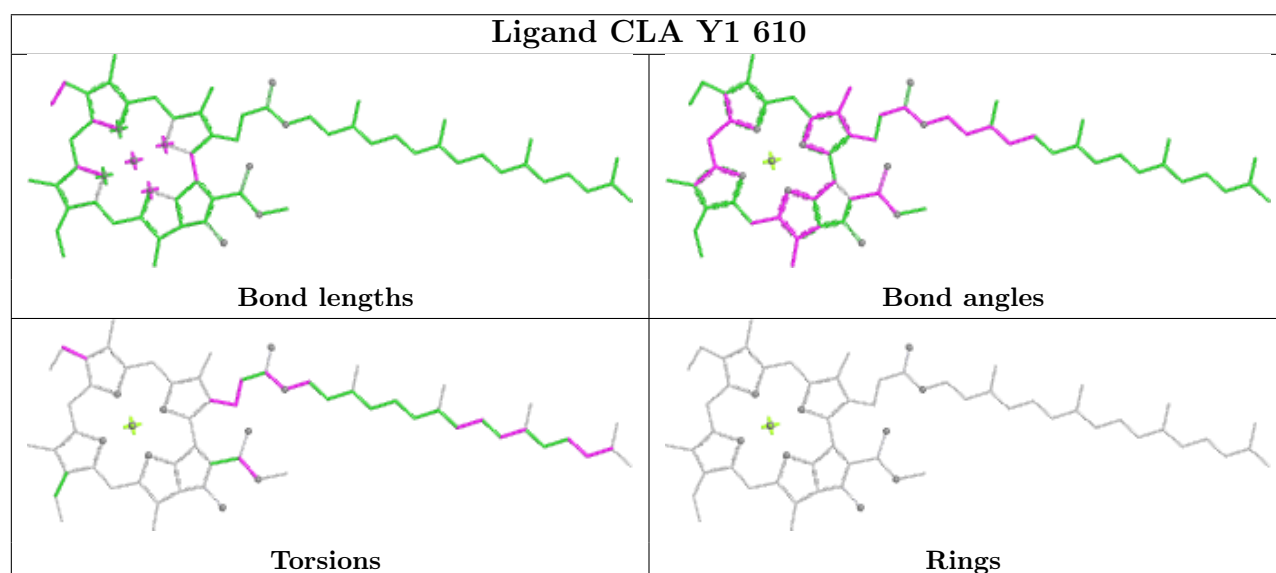
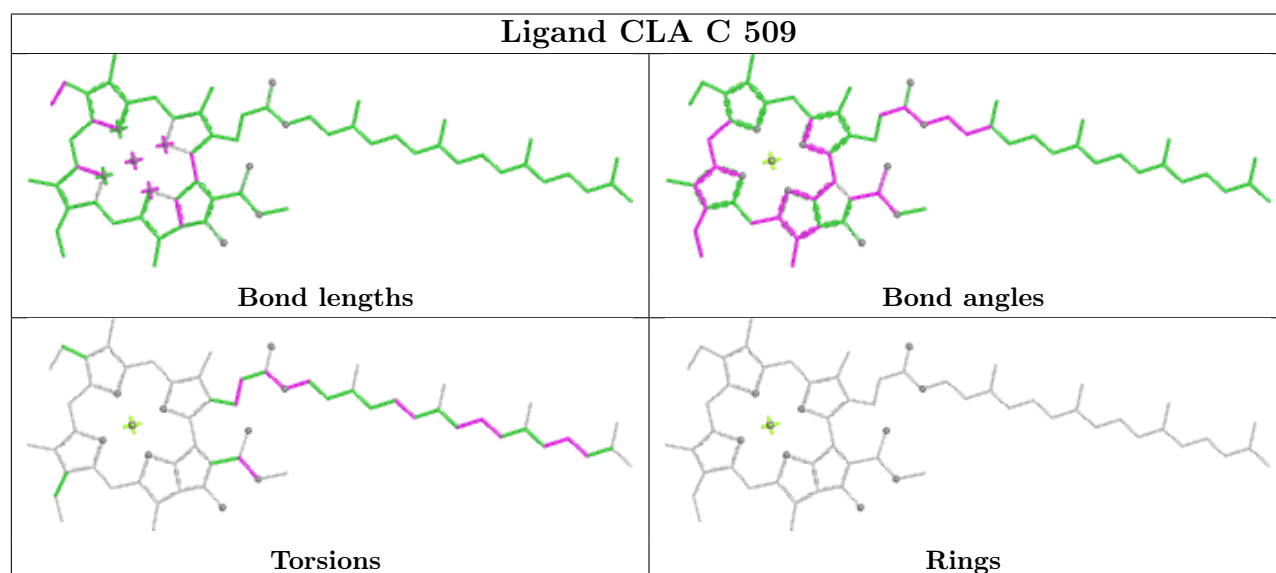
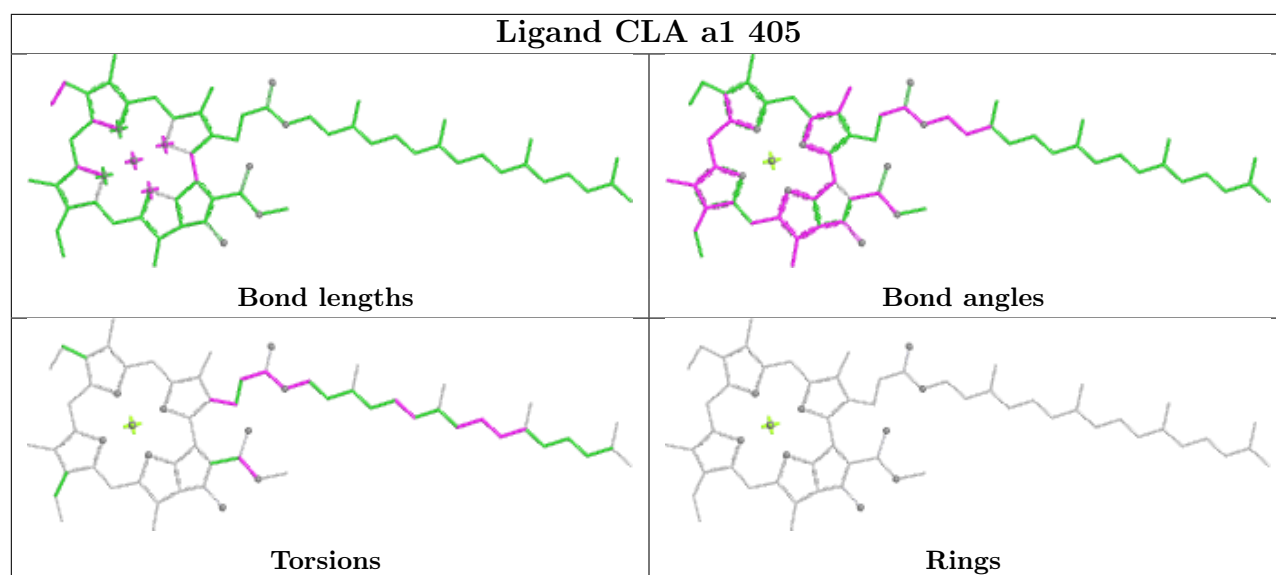




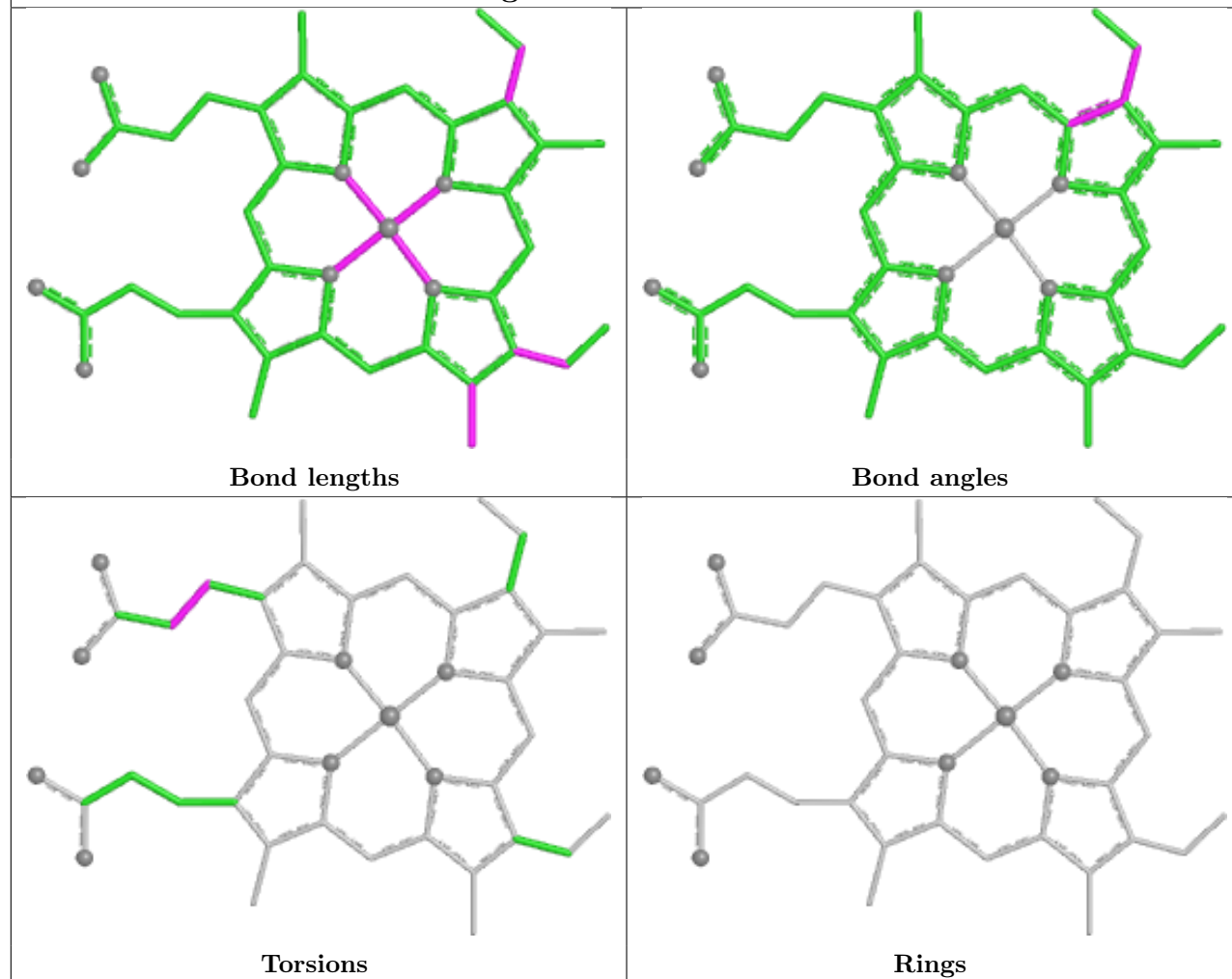


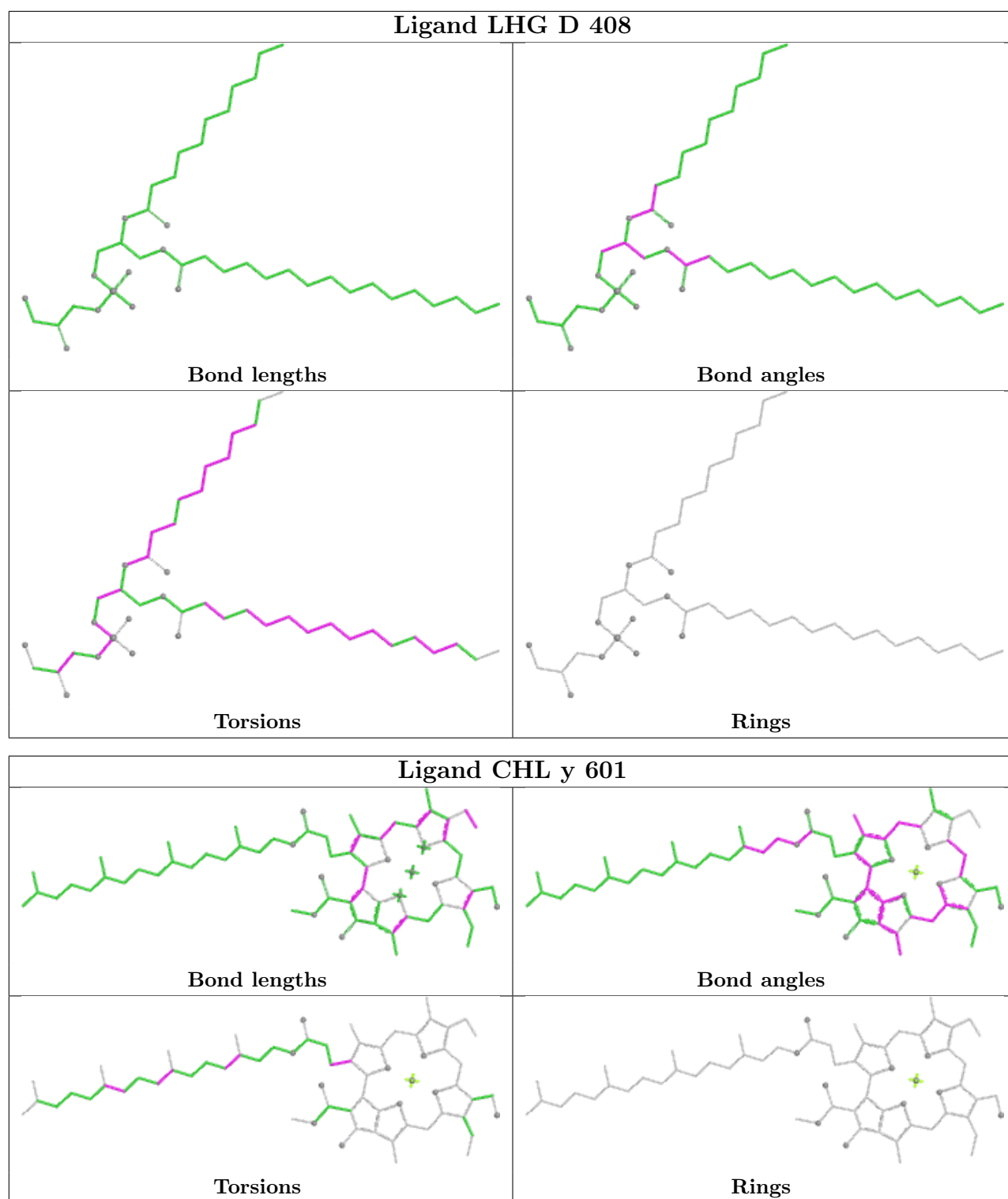


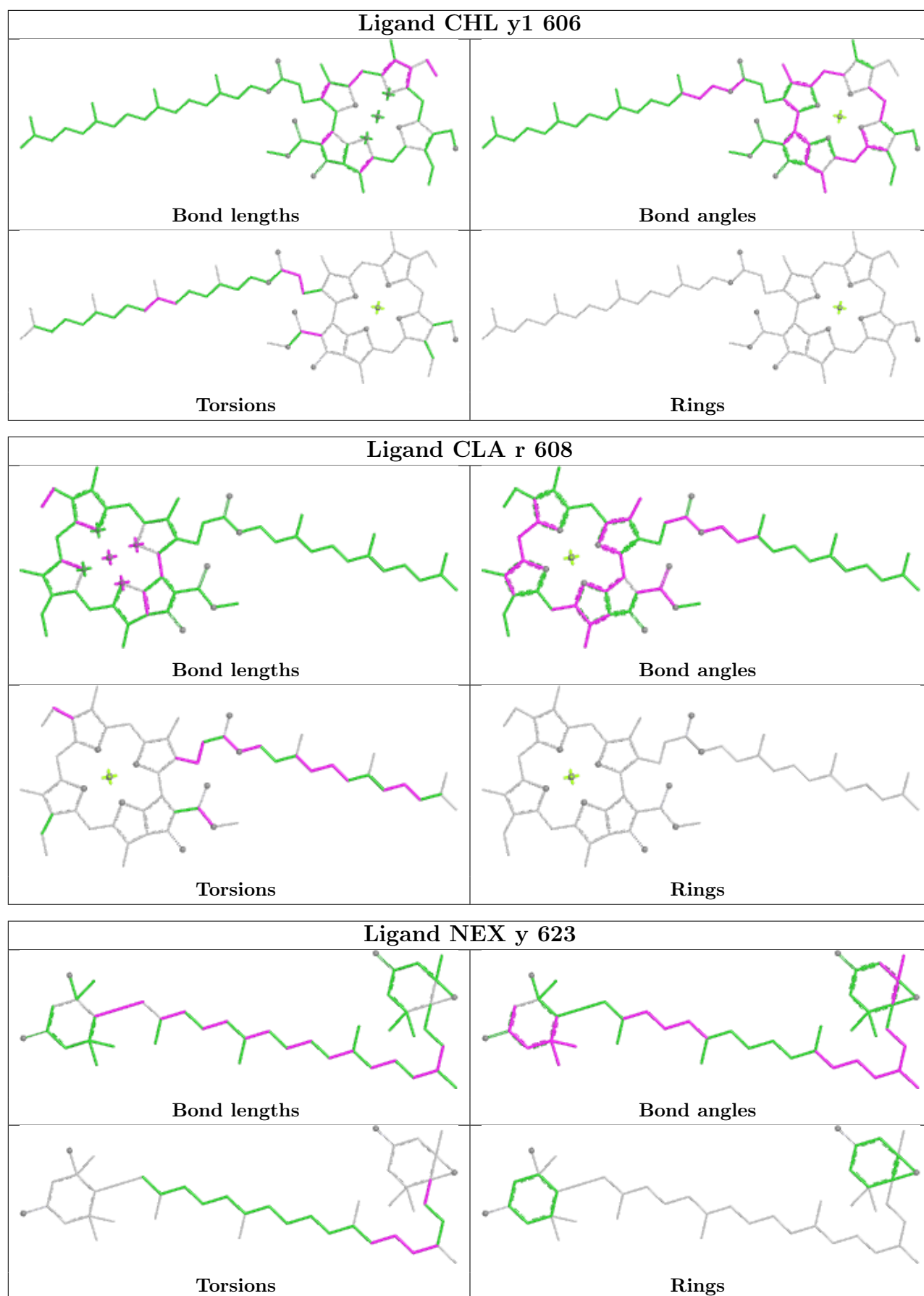


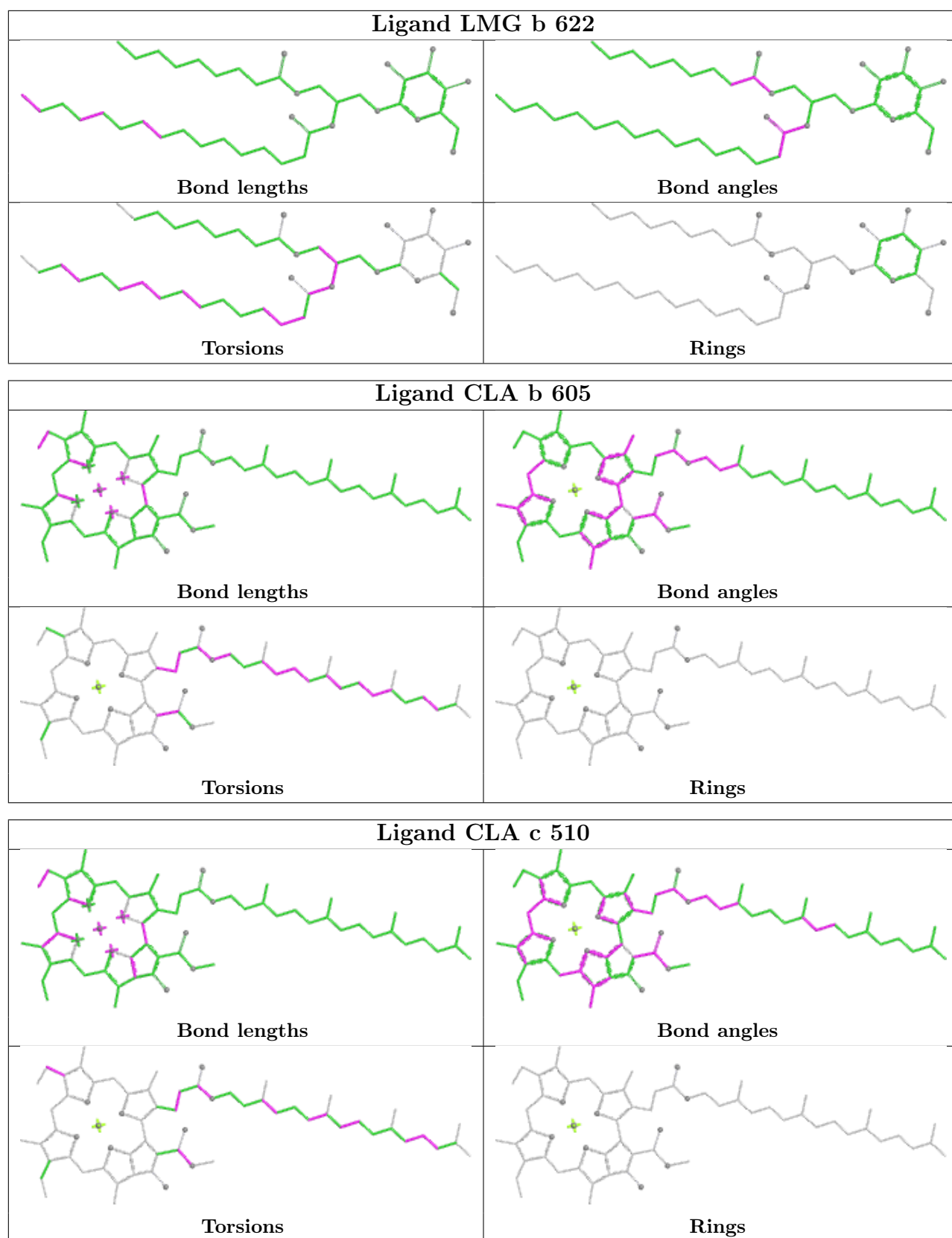


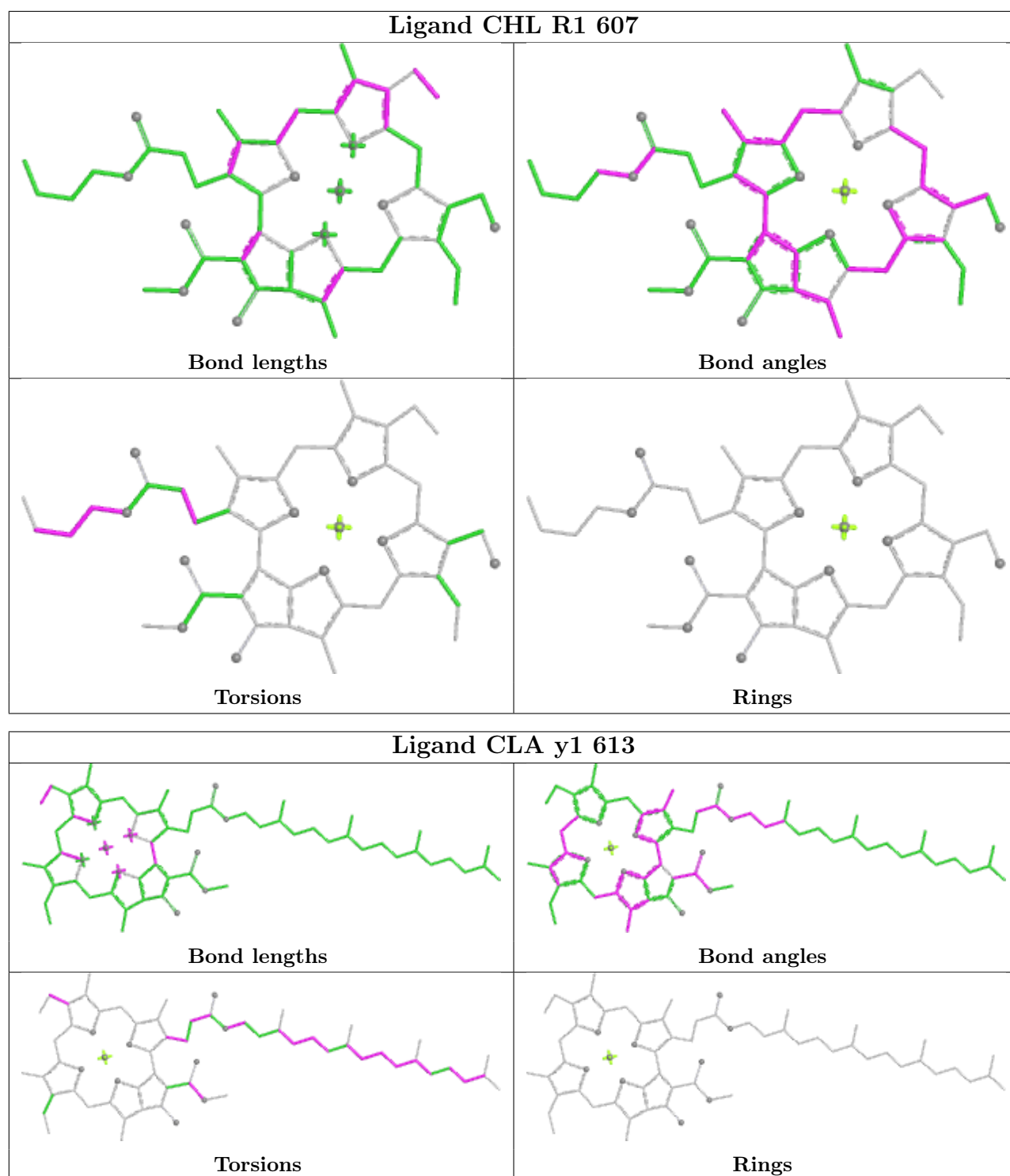
Ligand HEM F1 101

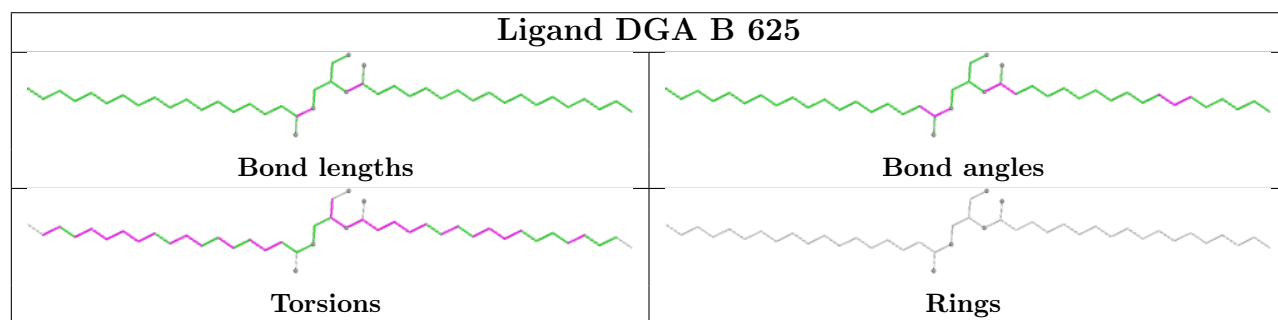
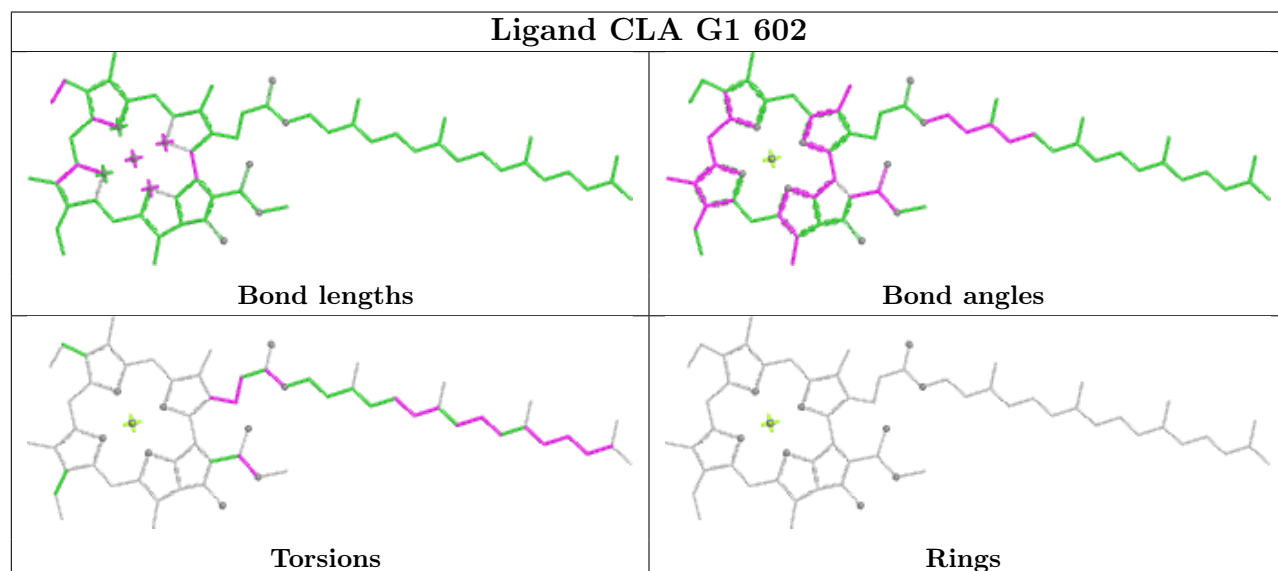
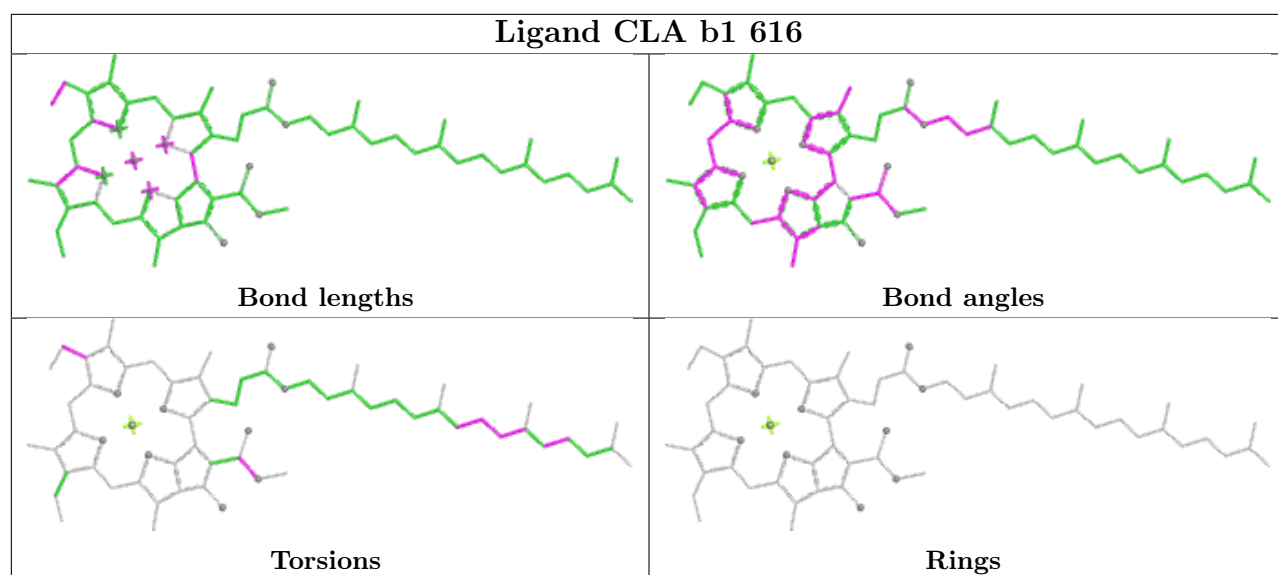


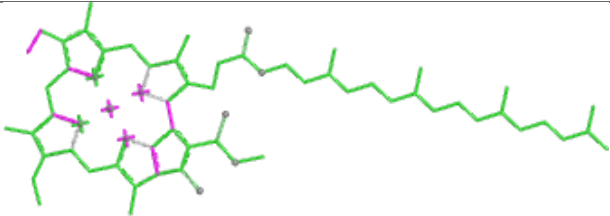
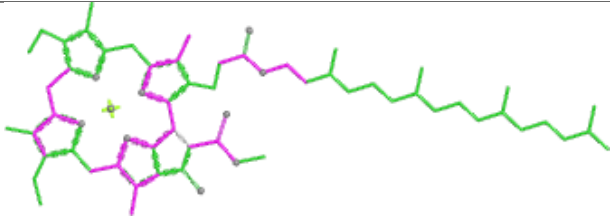
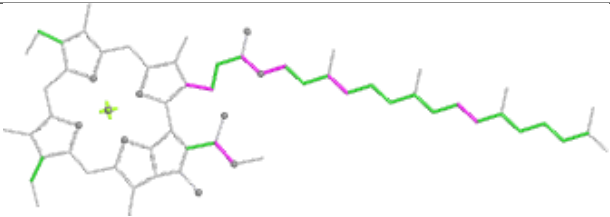
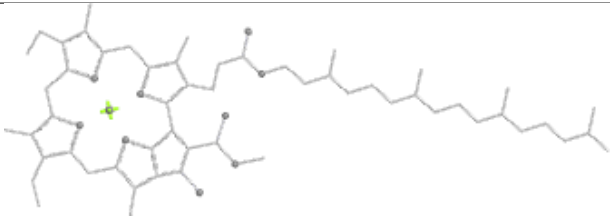
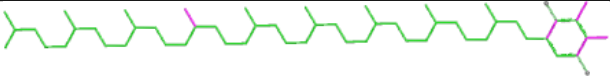
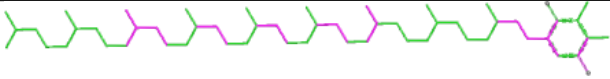
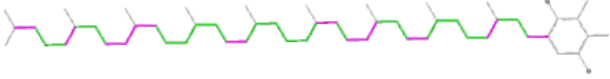
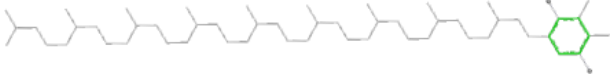


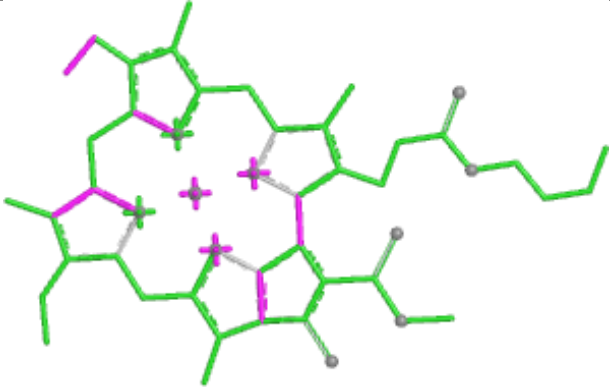
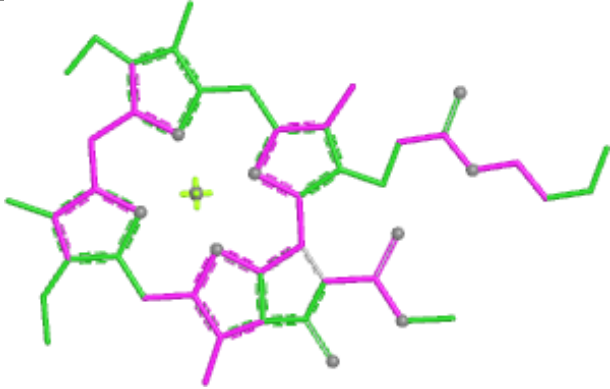
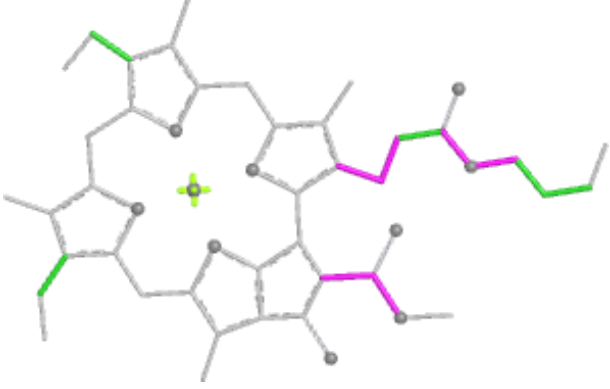
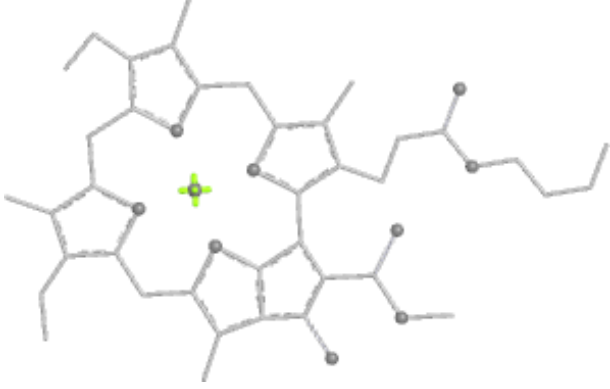
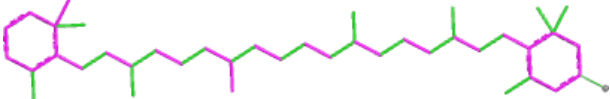
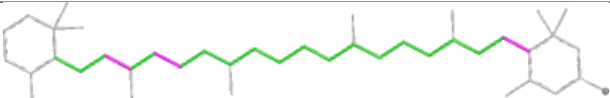
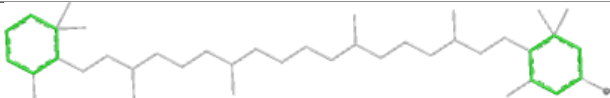


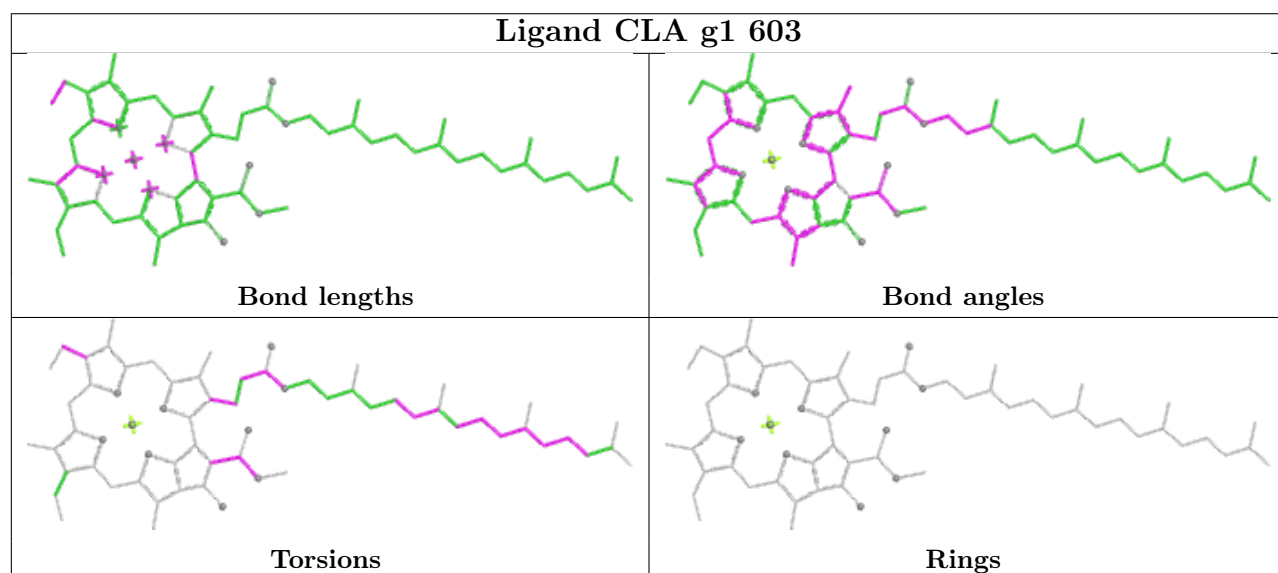
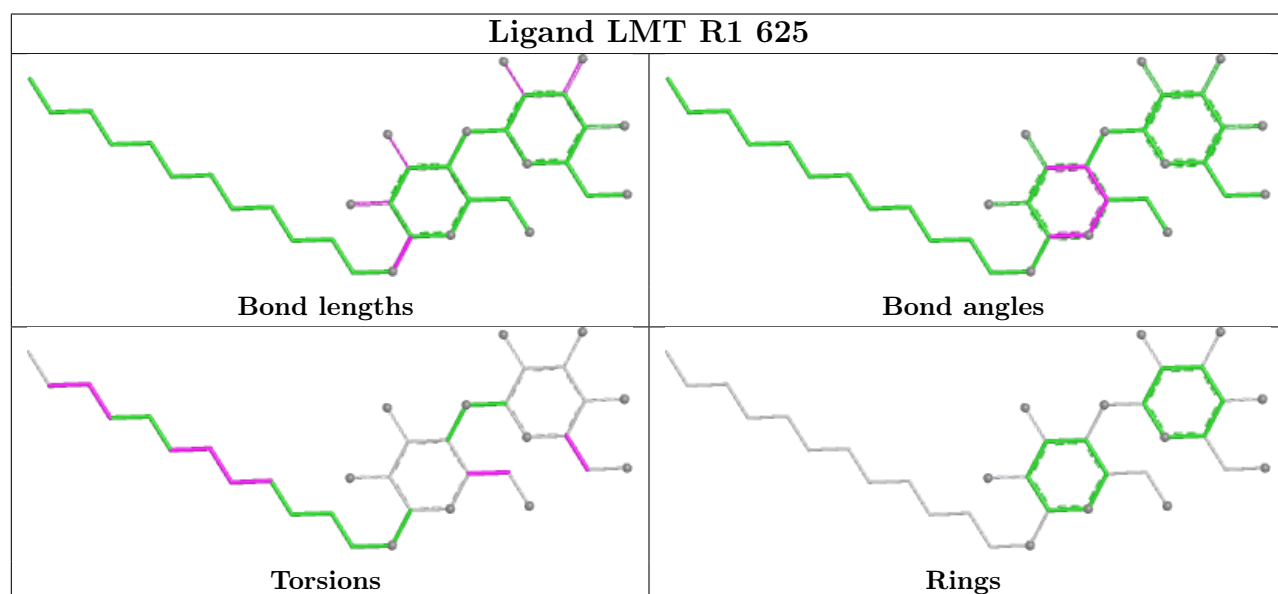
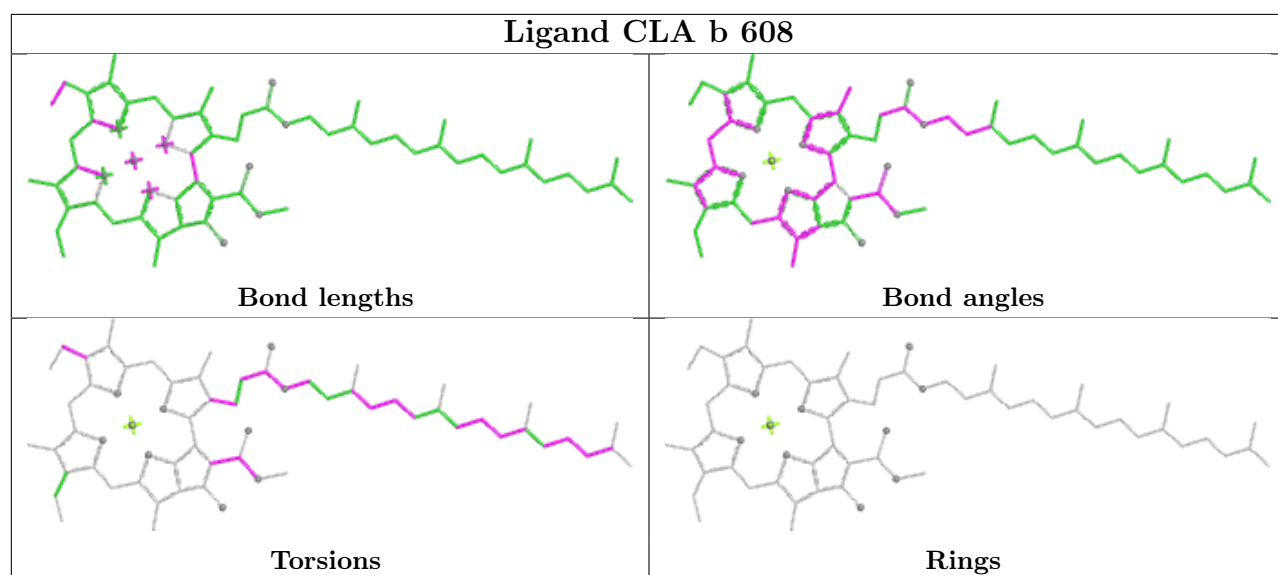


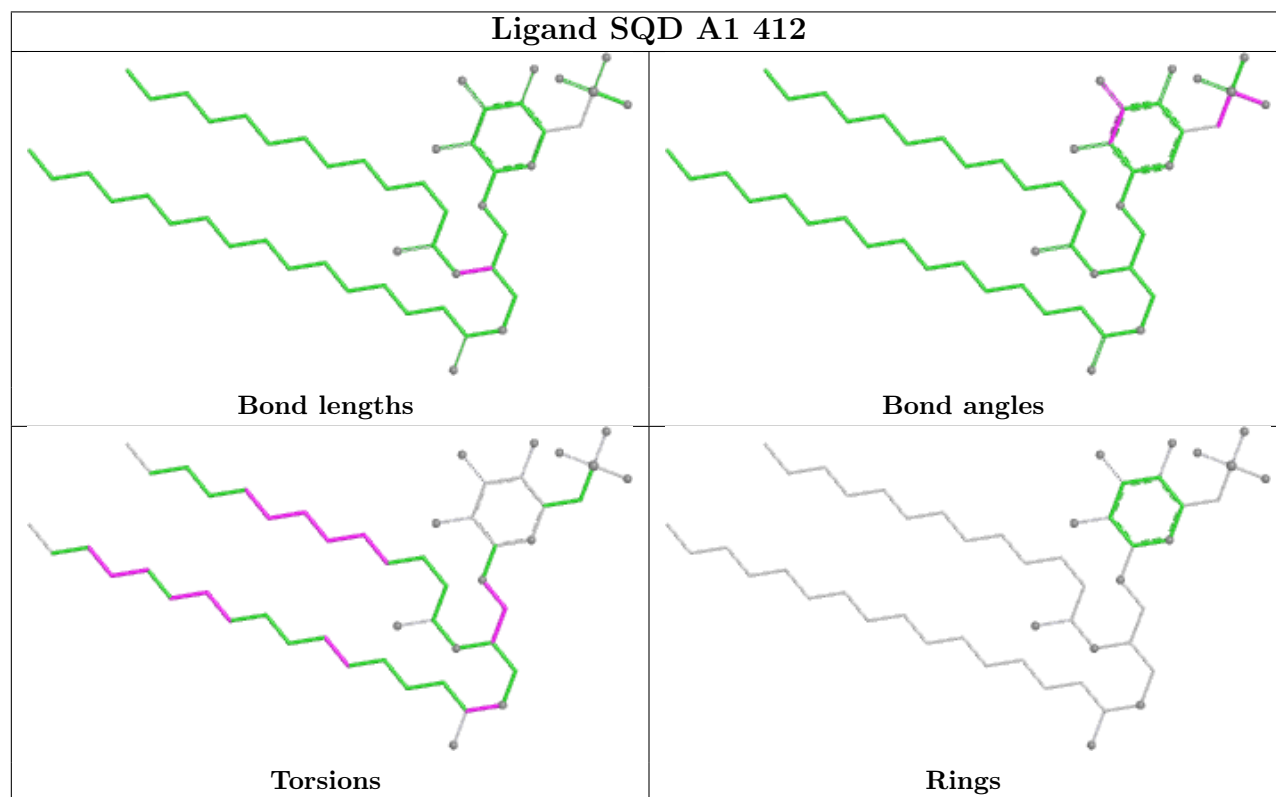
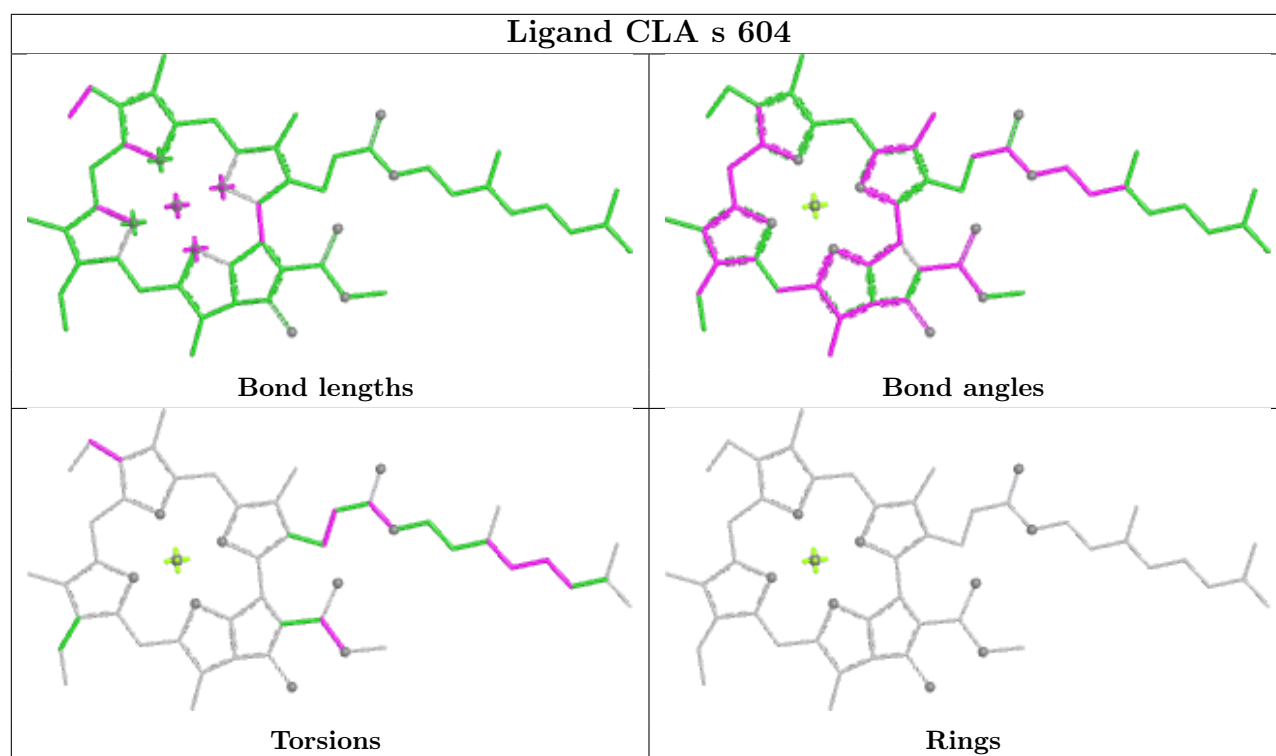


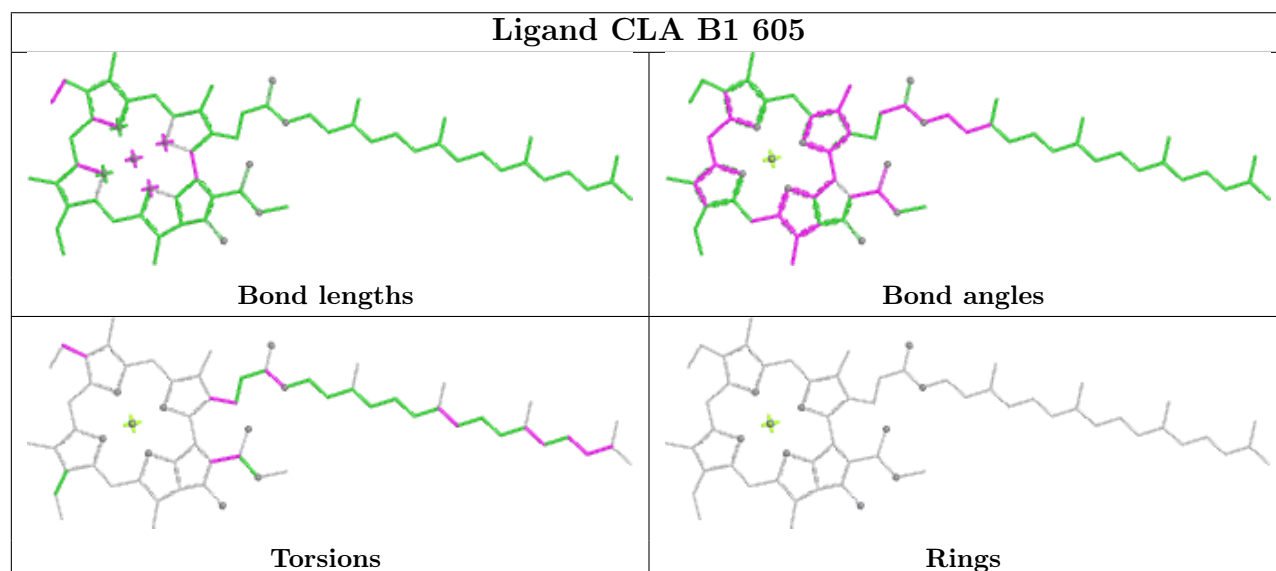
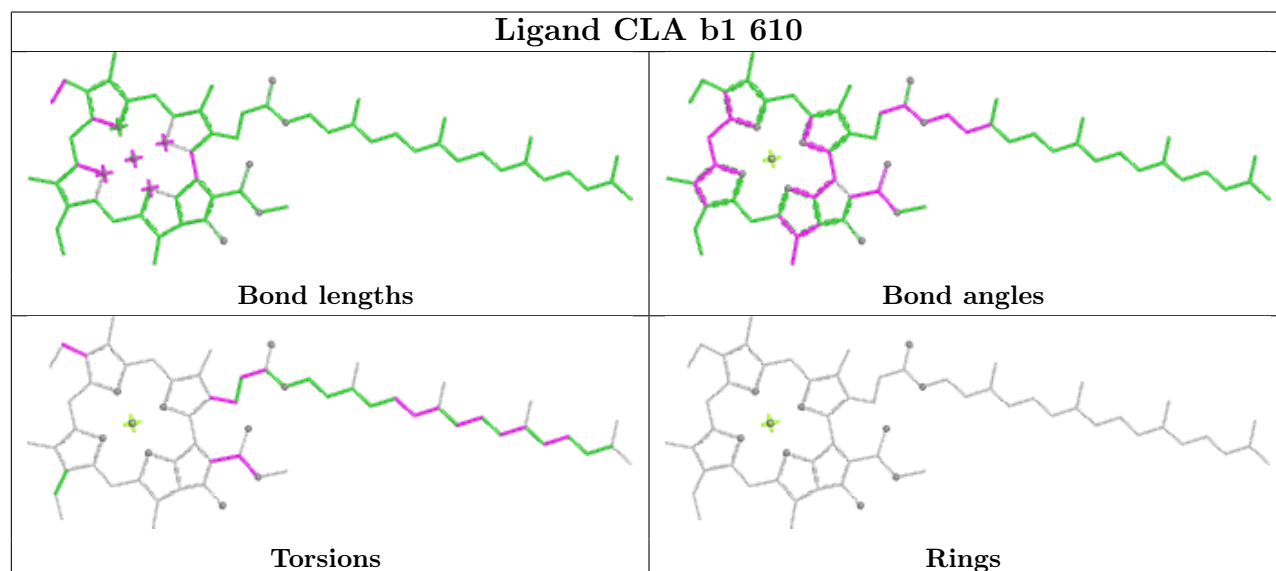
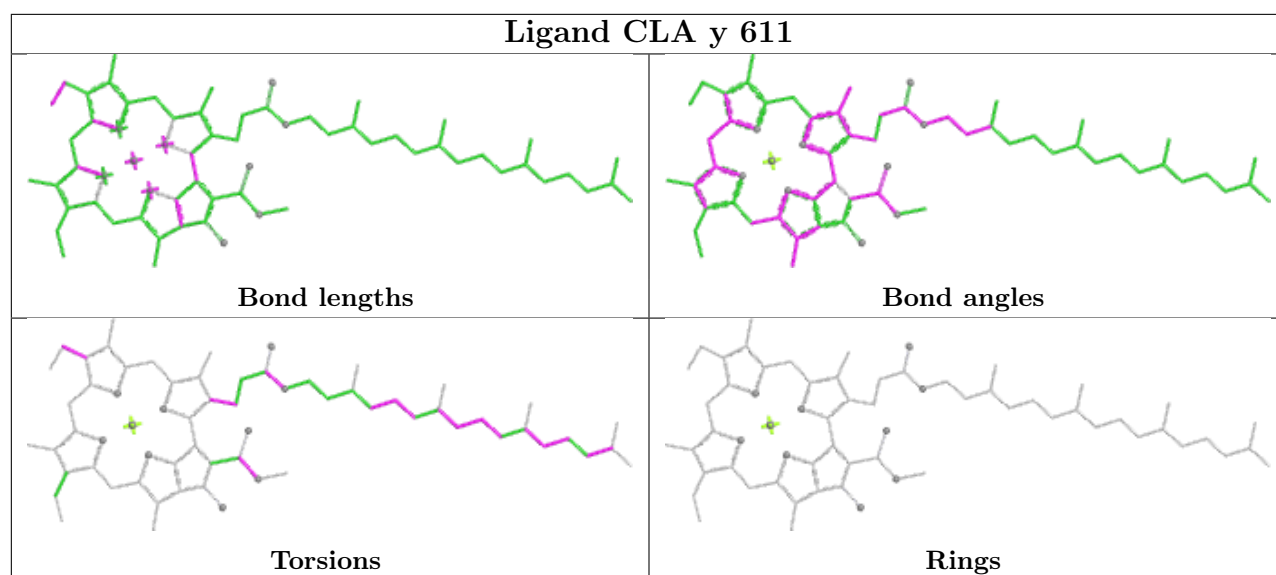


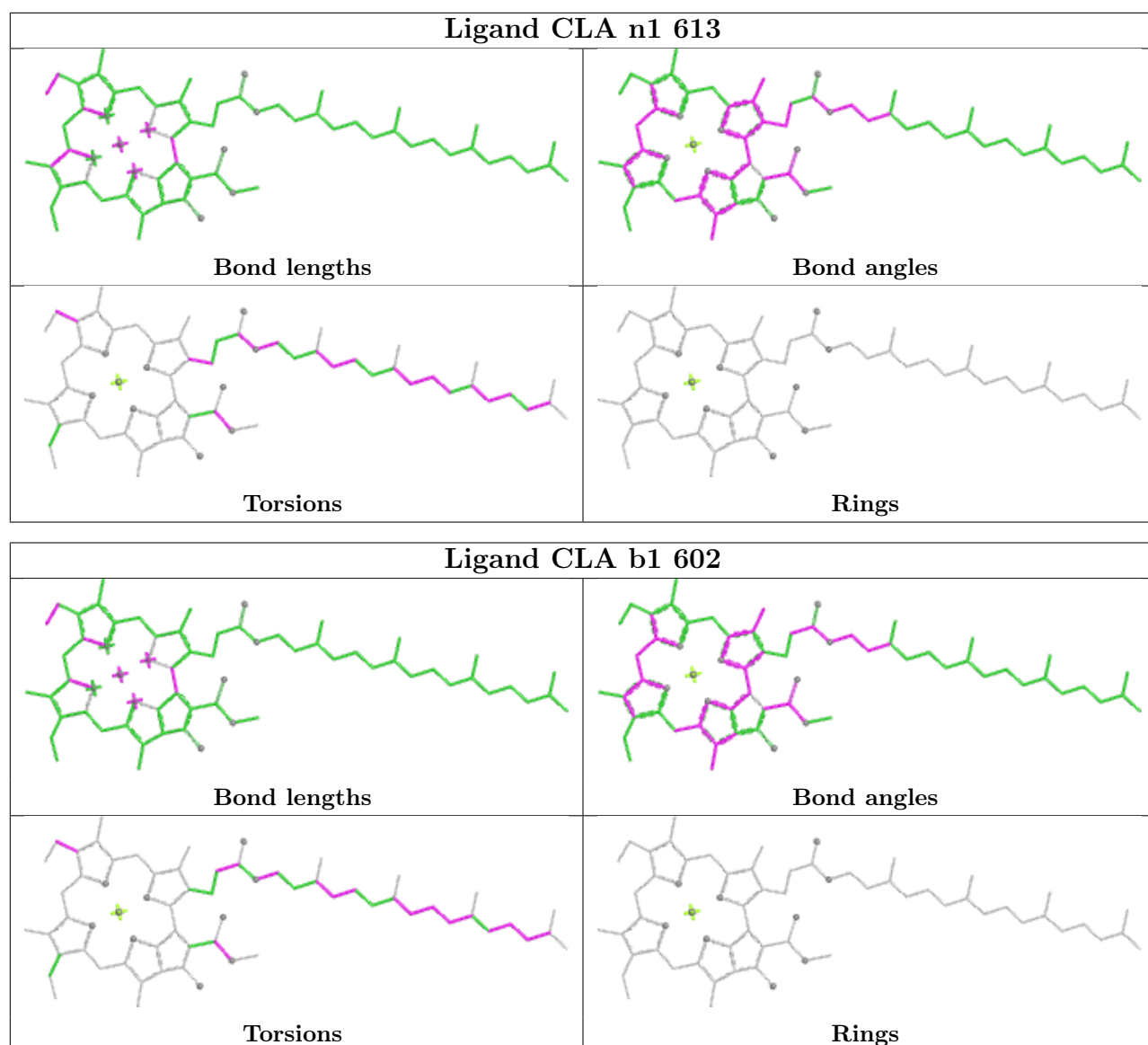
Ligand CLA b1 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D1 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 604	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand RRX H1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

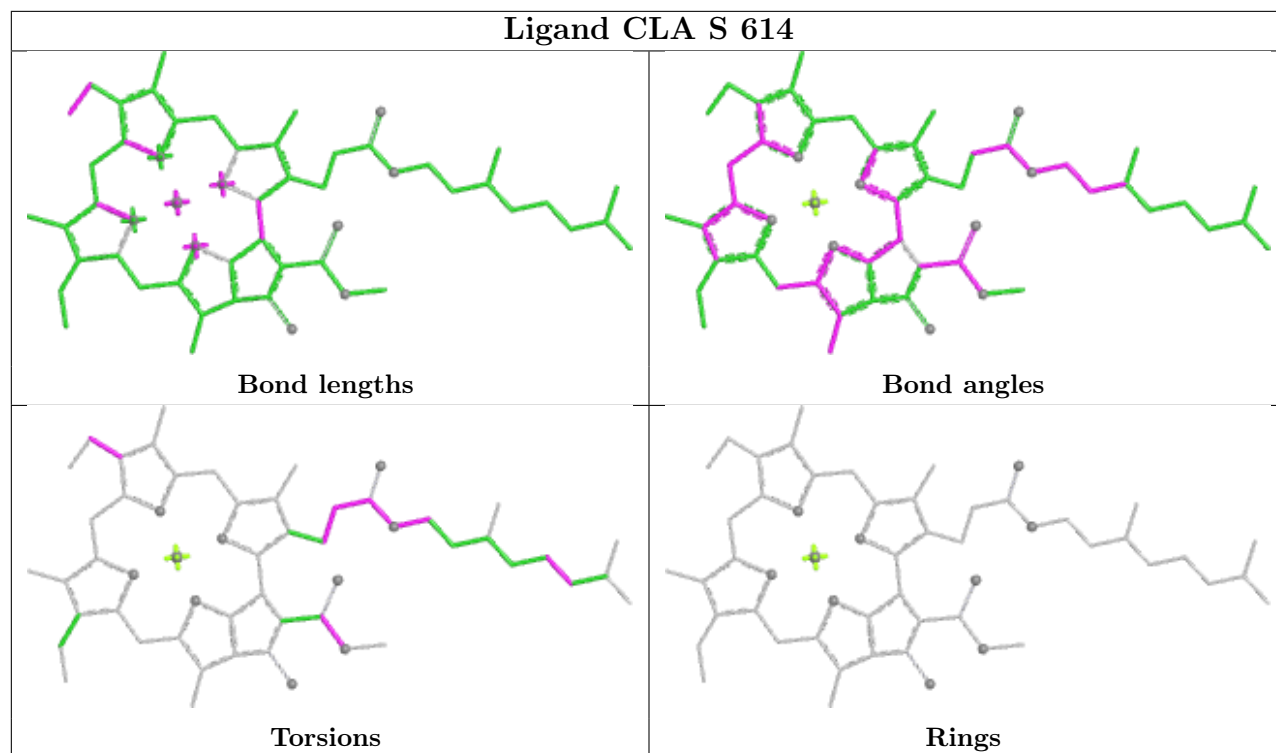




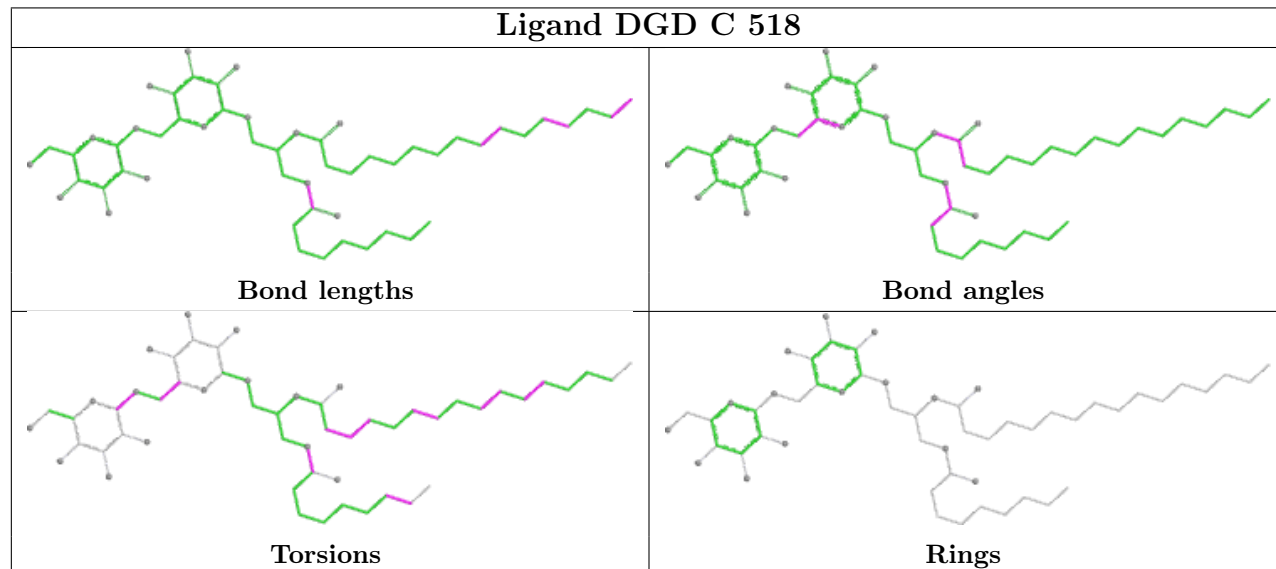


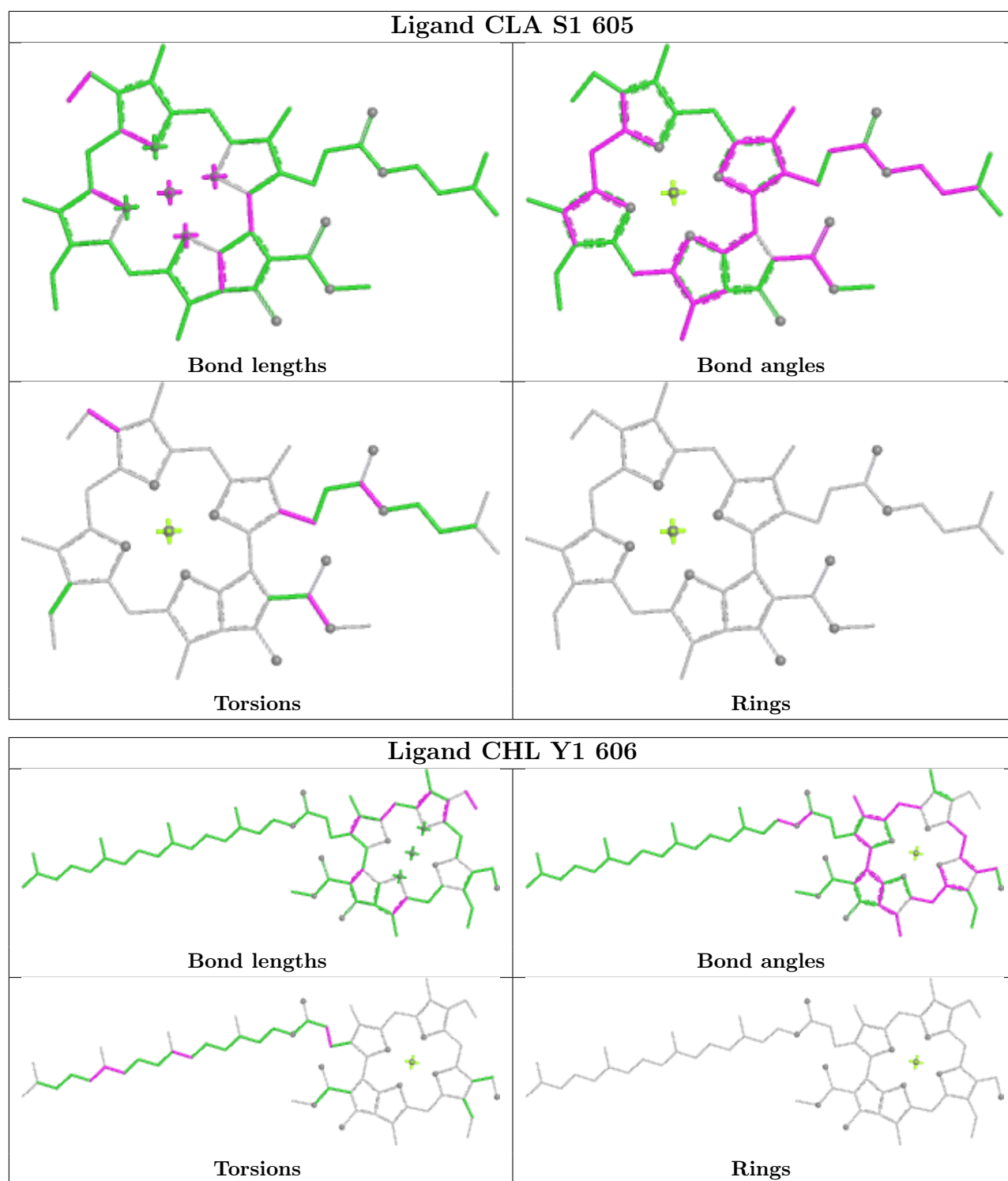


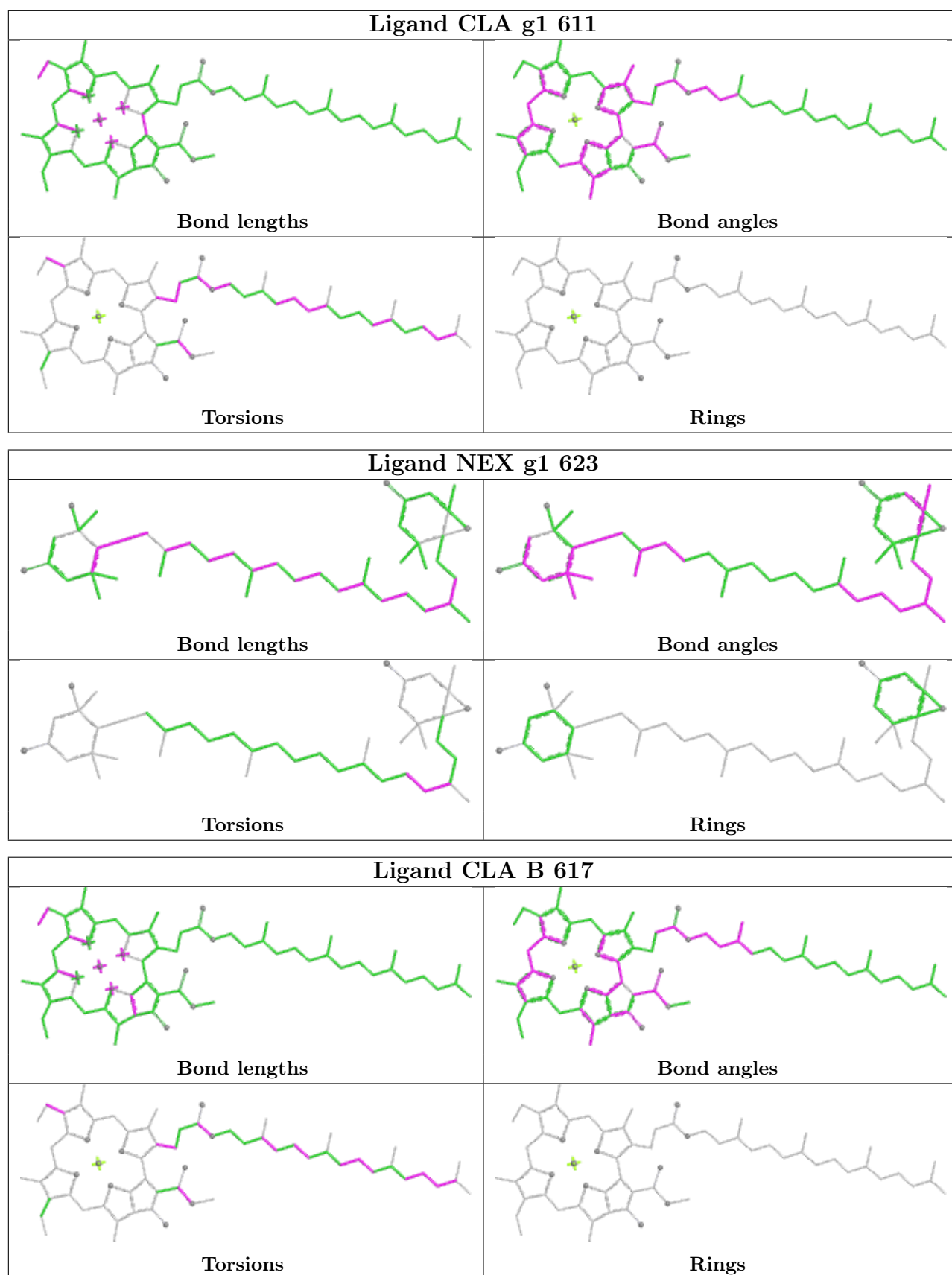
Ligand CLA S 614

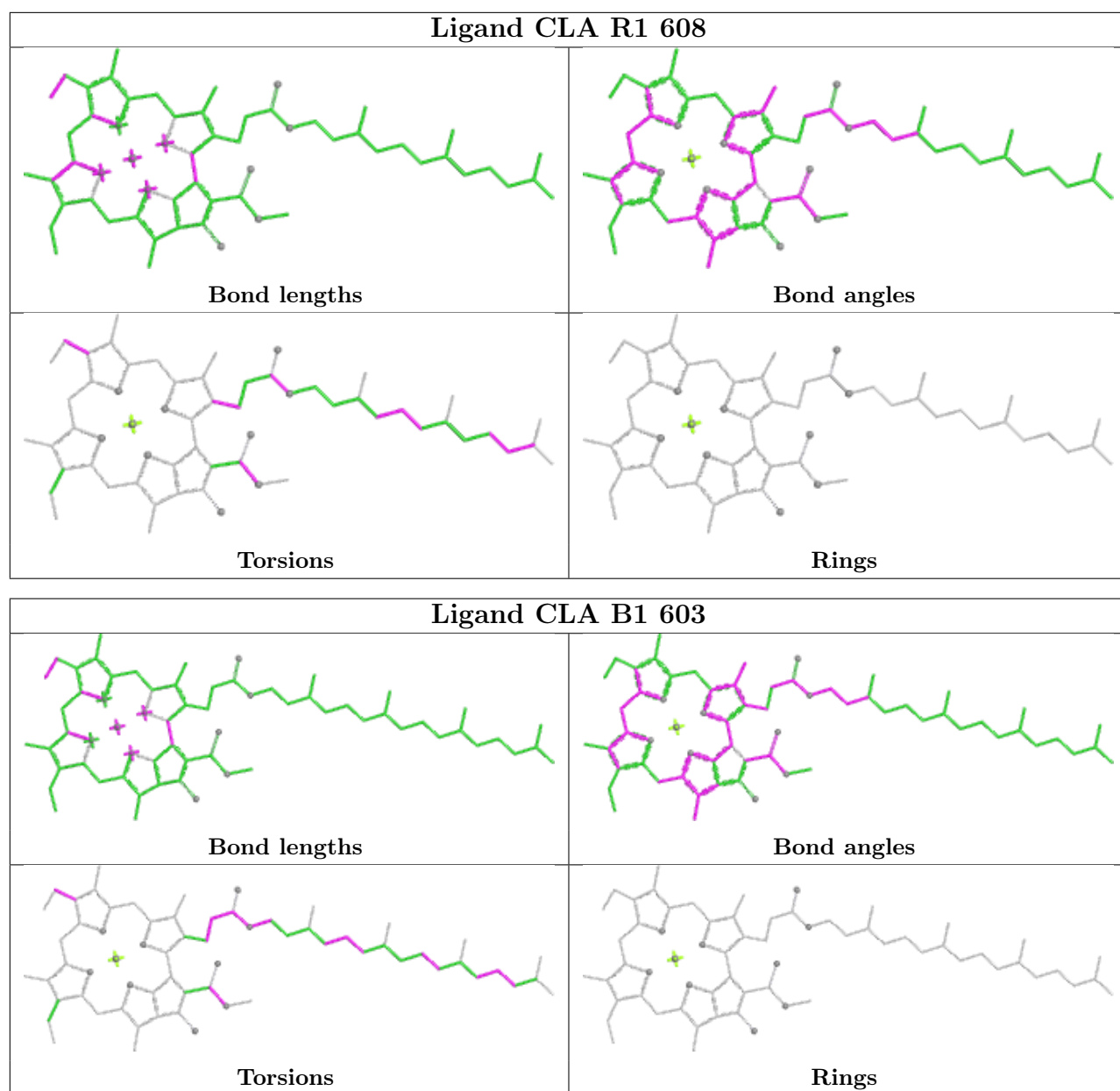


Ligand DGD C 518

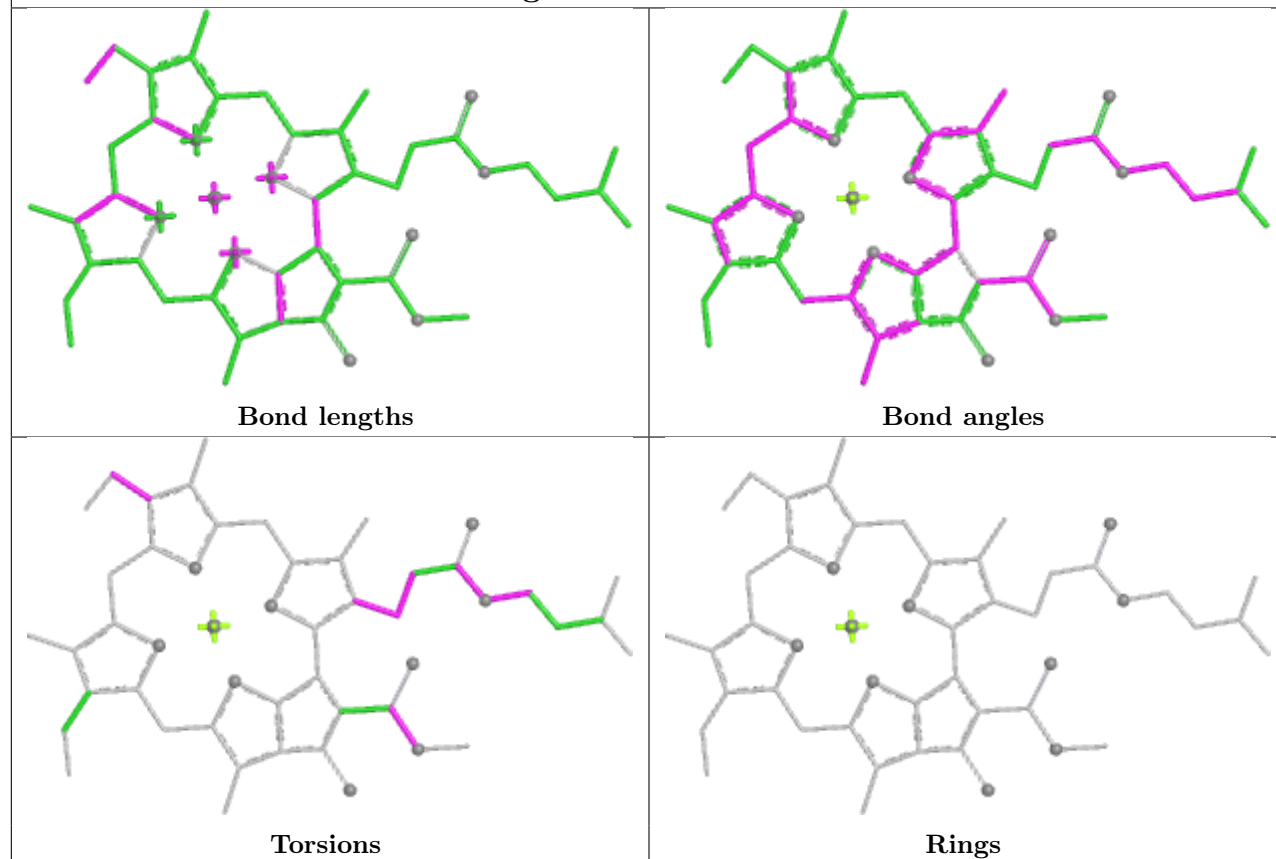




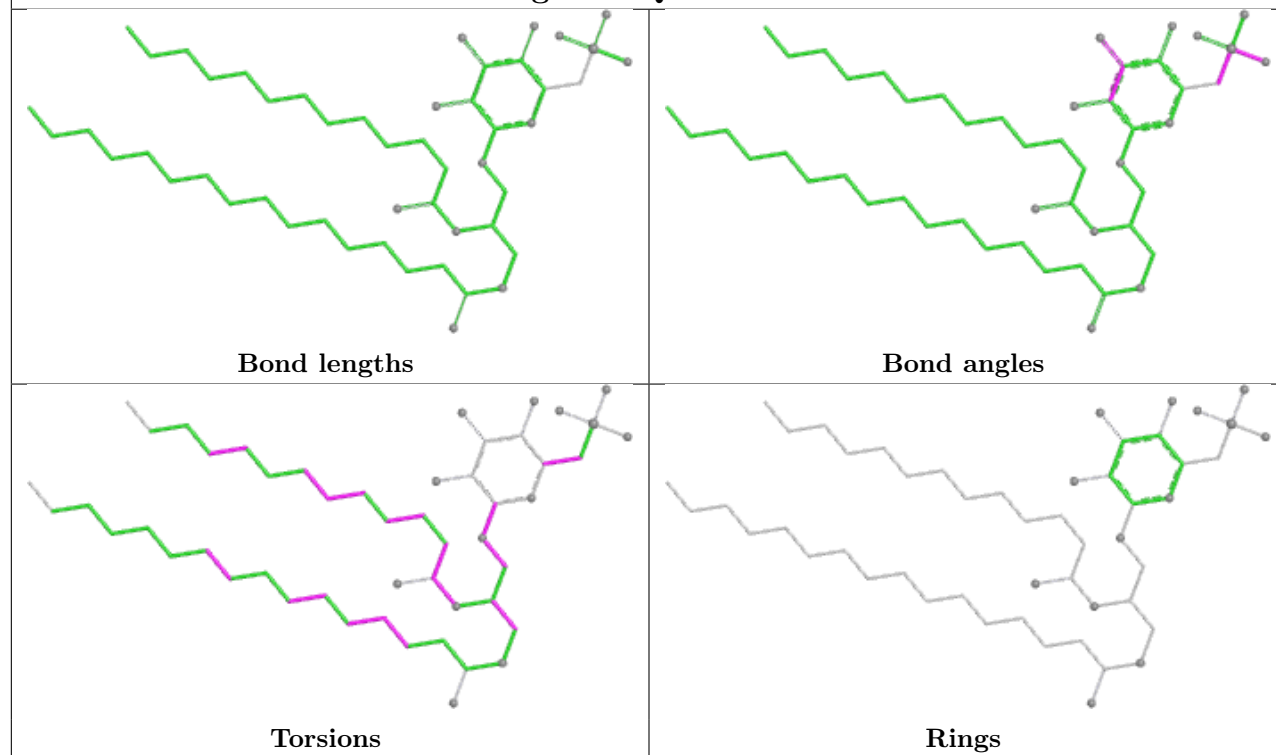


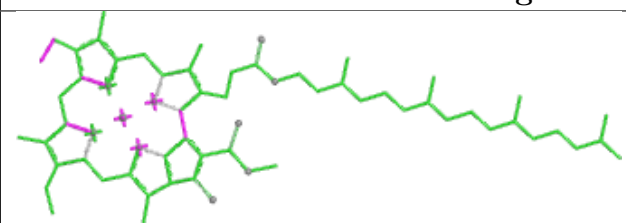
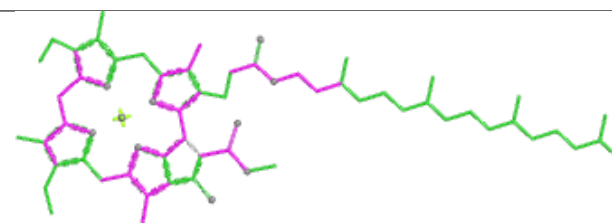
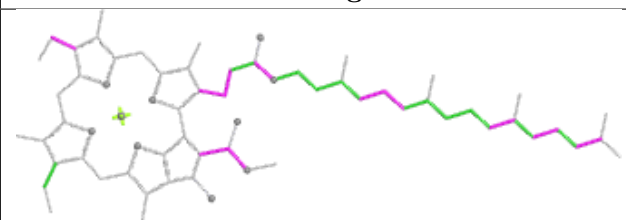
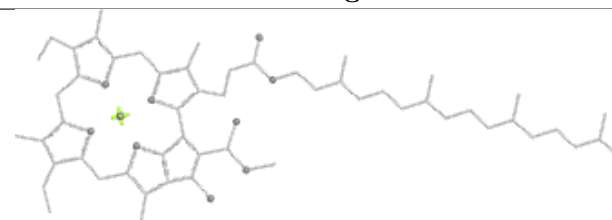


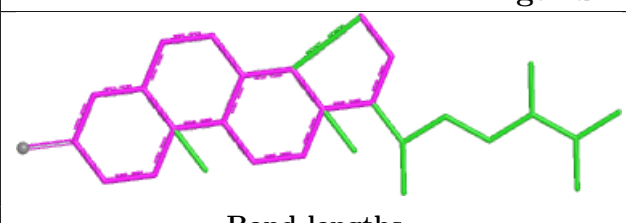
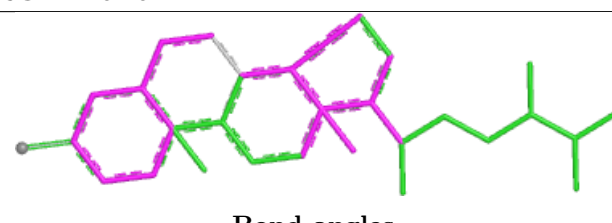
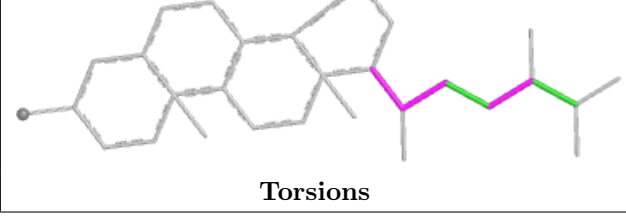
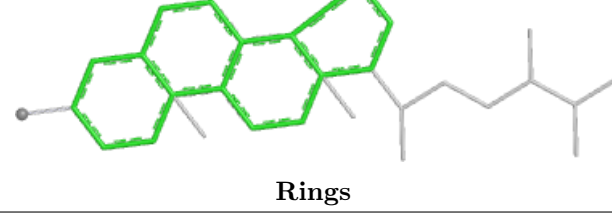
Ligand CLA Y1 608

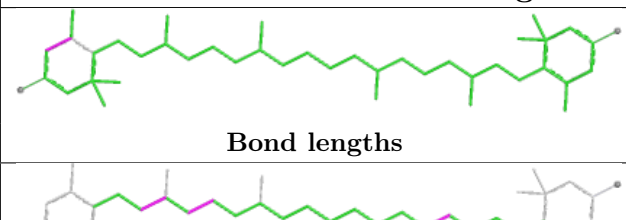
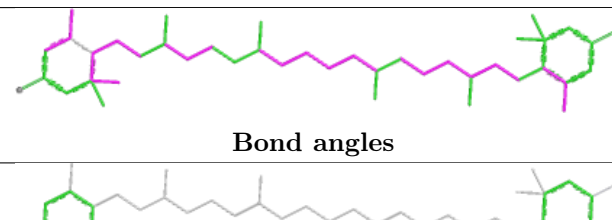
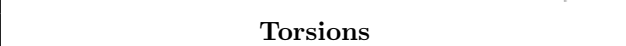


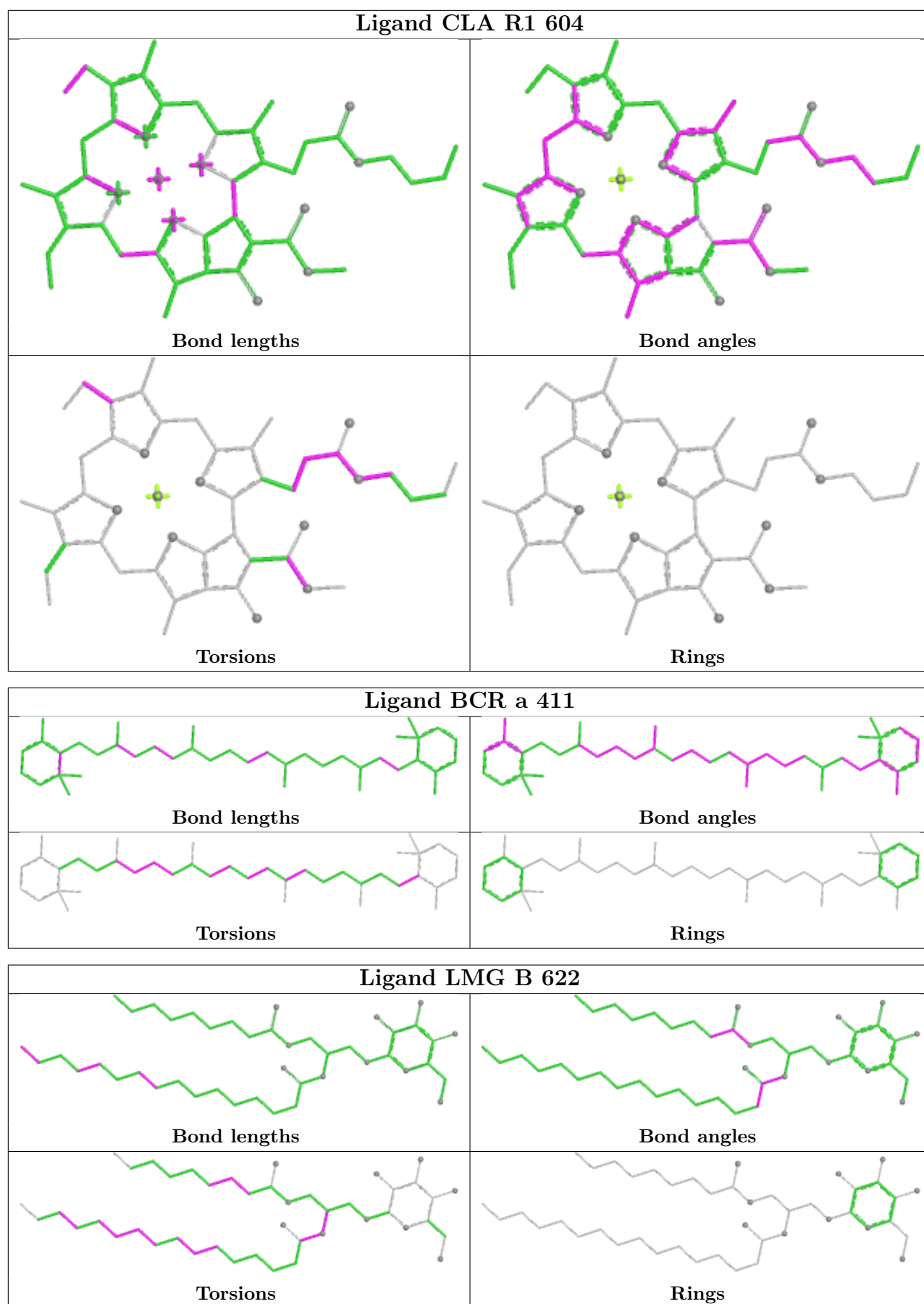
Ligand SQD A 412



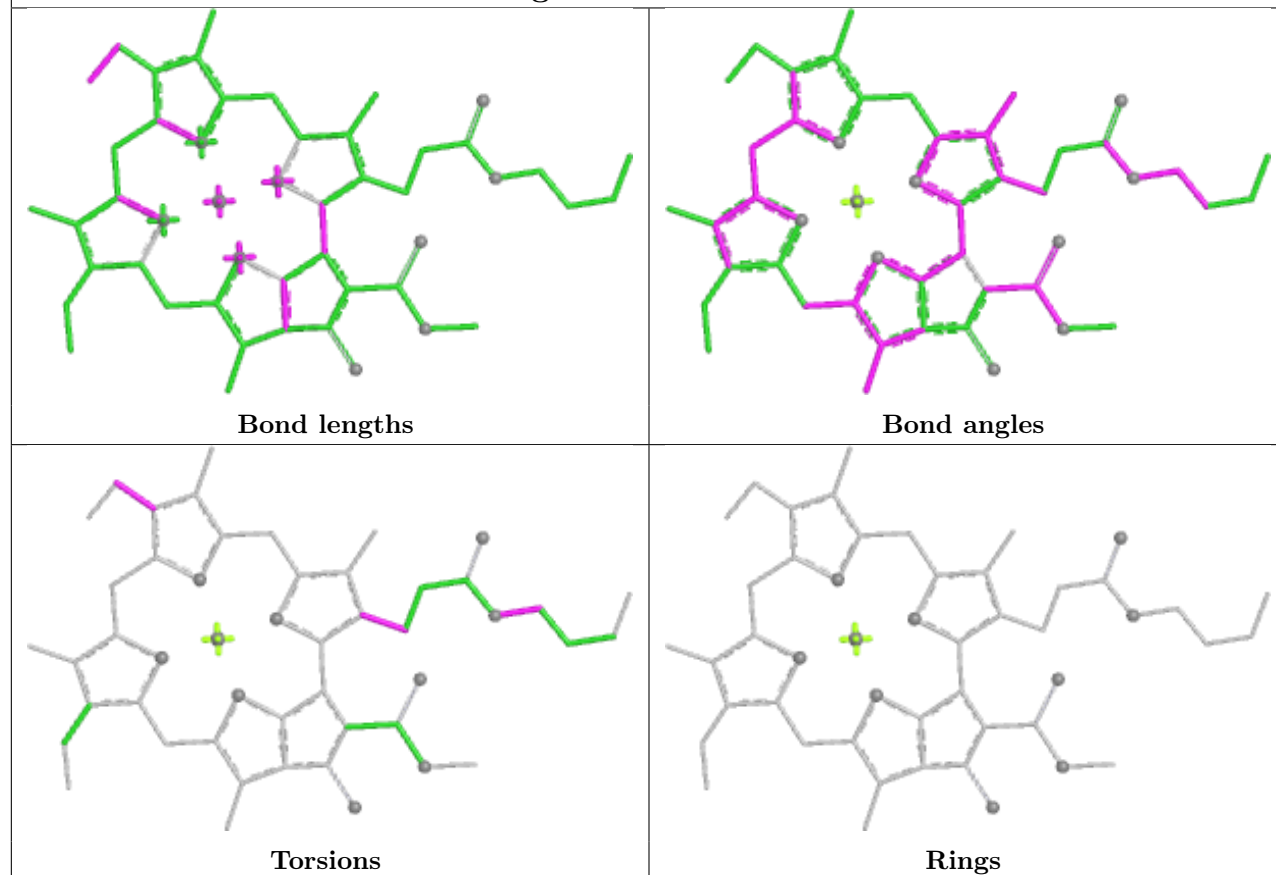
Ligand CLA S1 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ERG r1 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

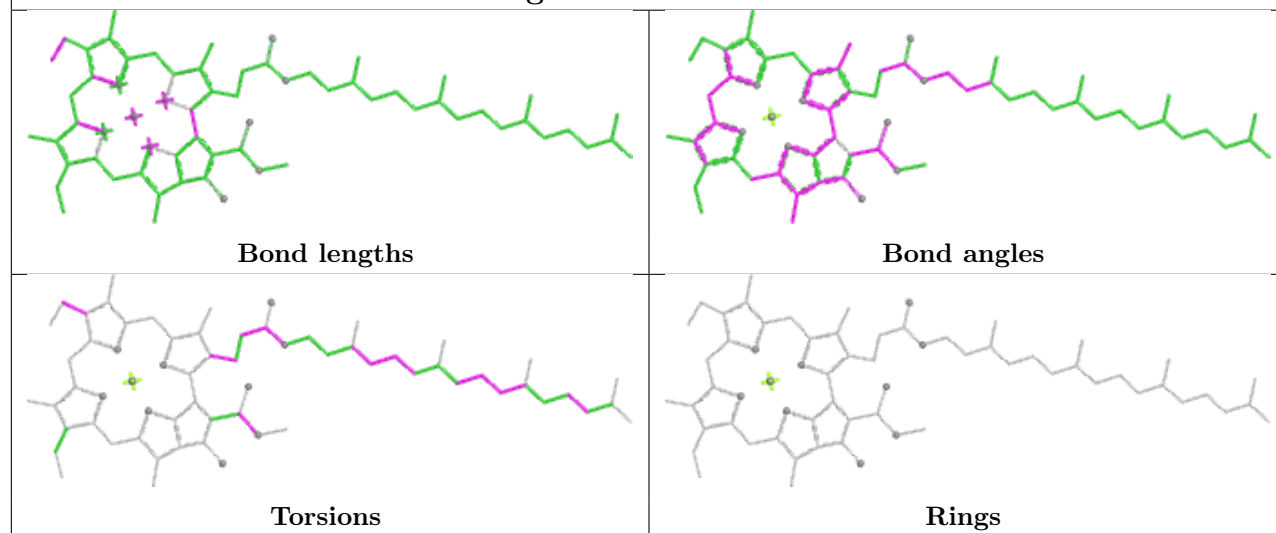
Ligand LUT n1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

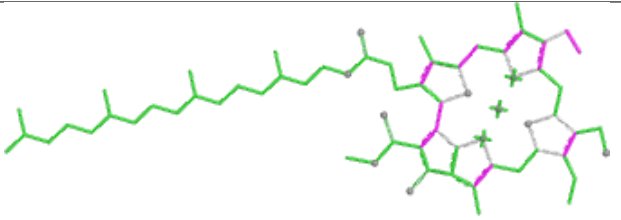
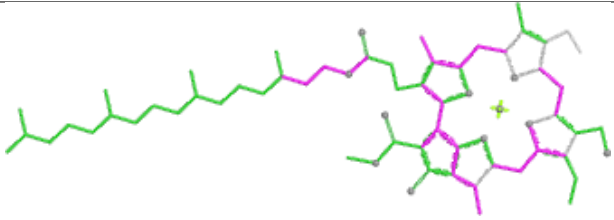
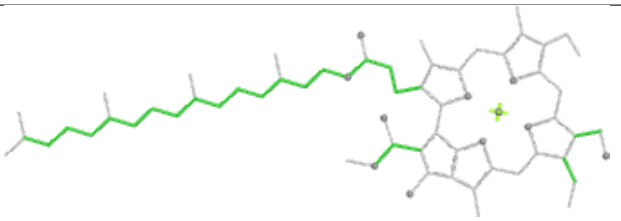
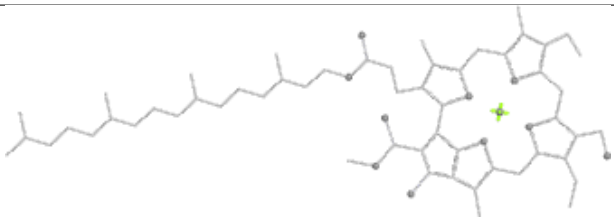


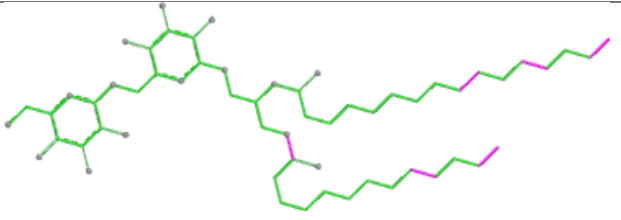
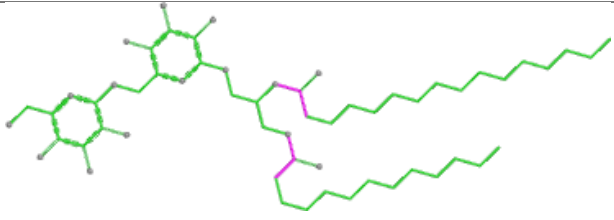
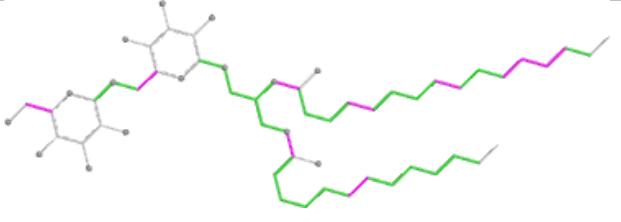
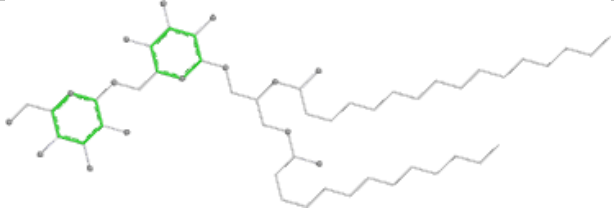
Ligand CLA A 407

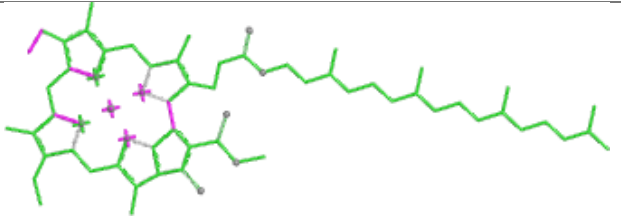
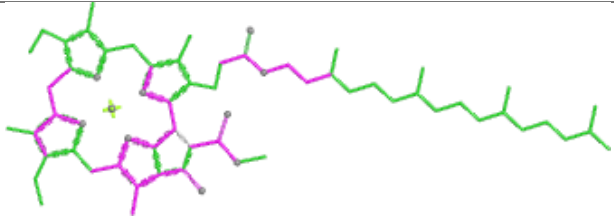
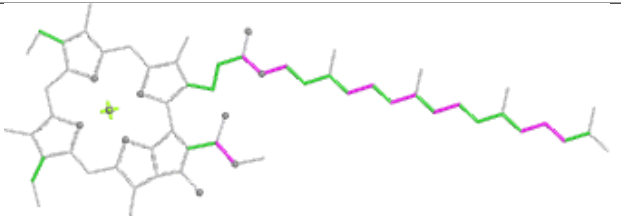
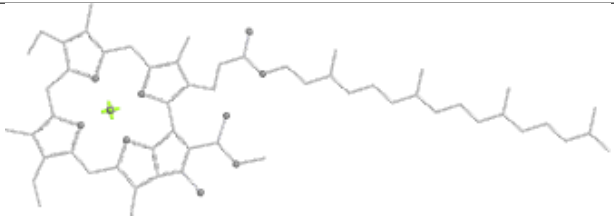


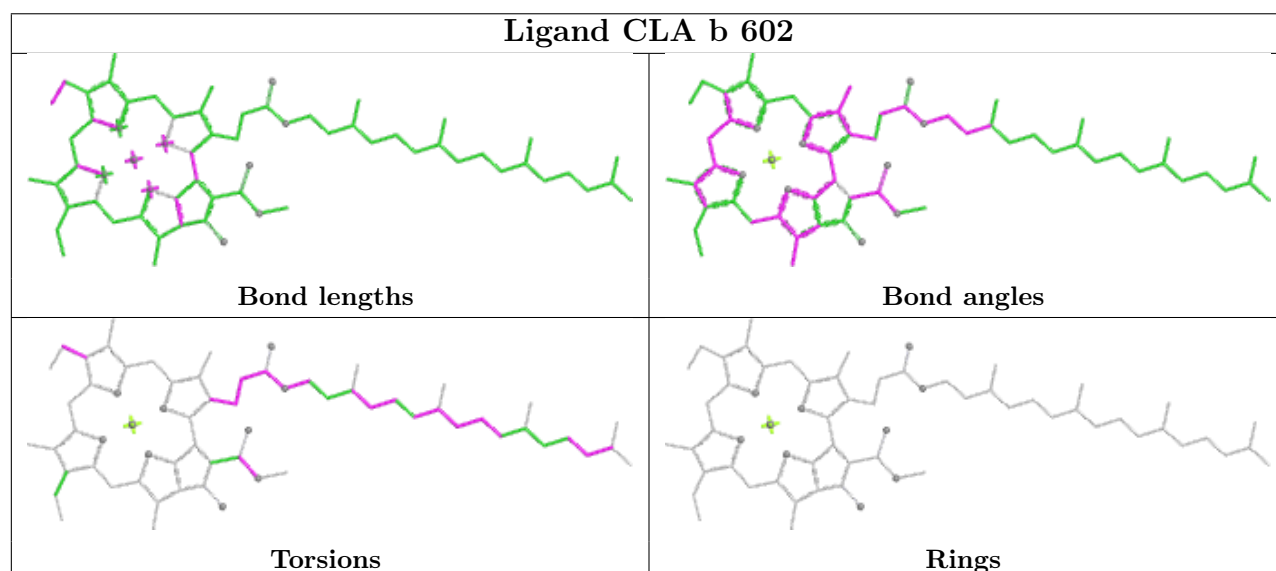
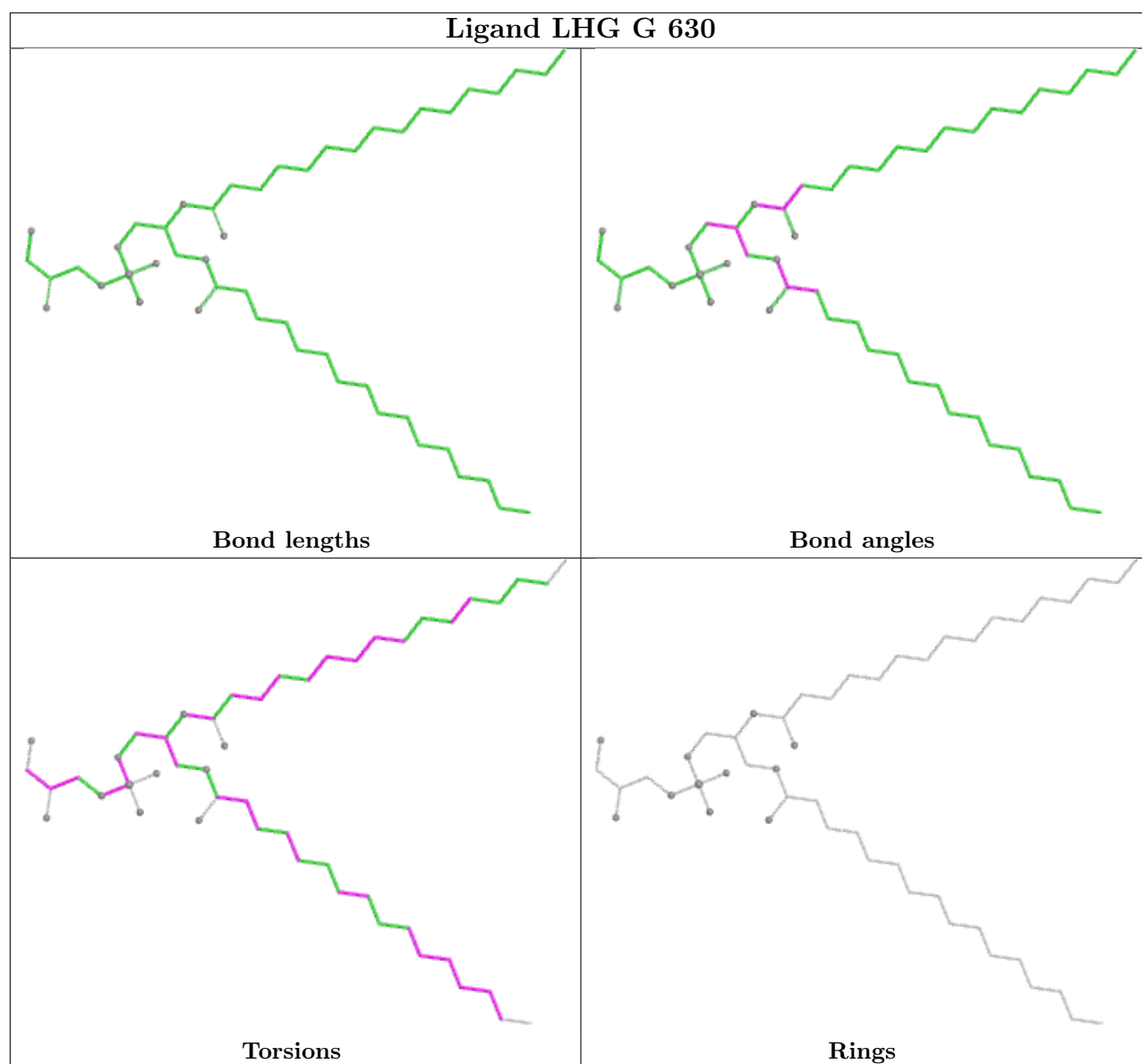
Ligand CLA b1 615

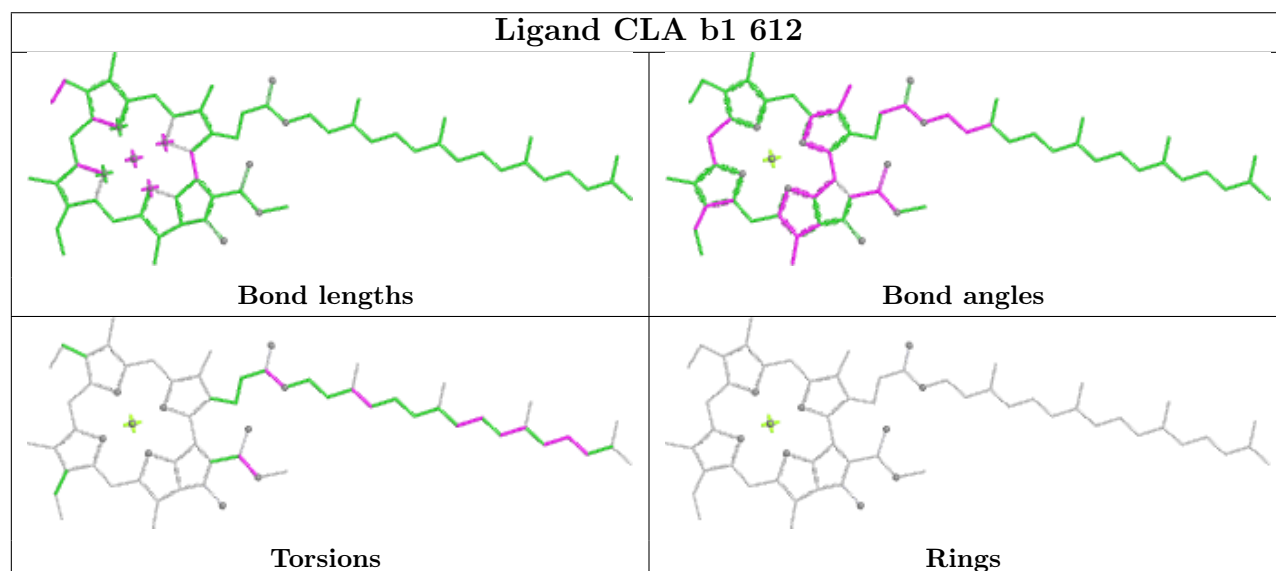
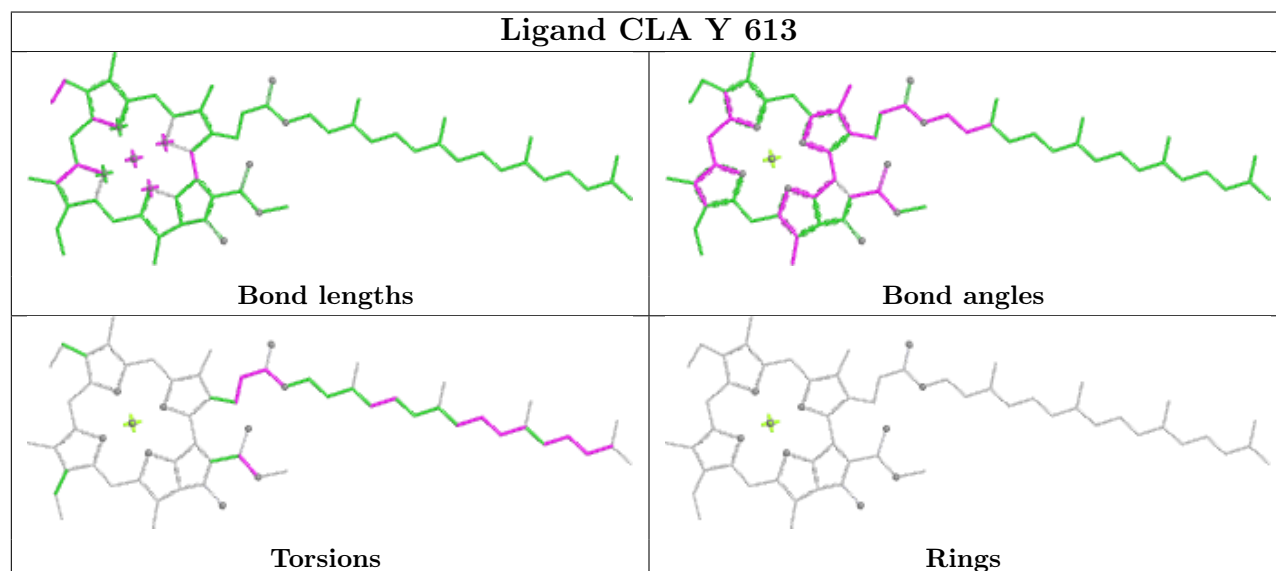
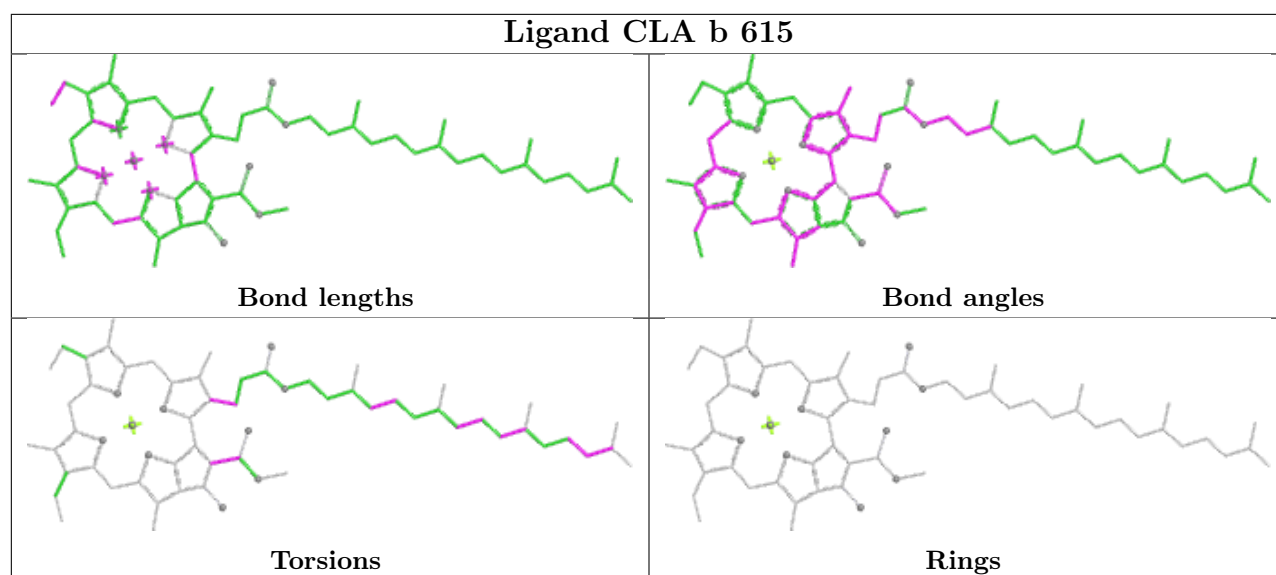


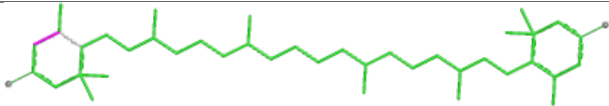
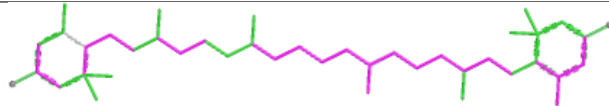
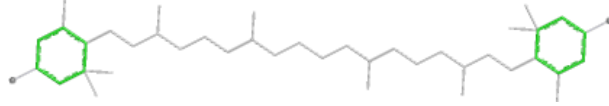
Ligand CHL Y1 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

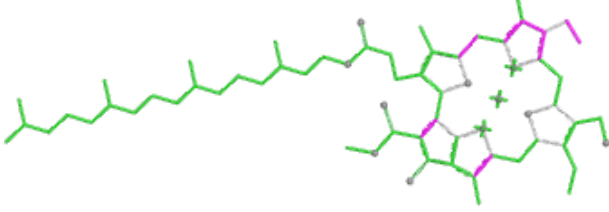
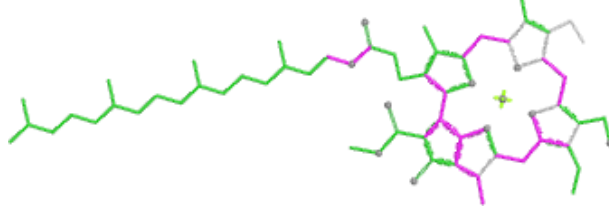
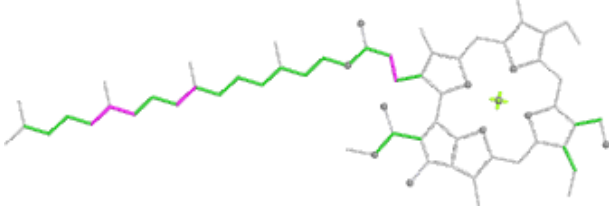
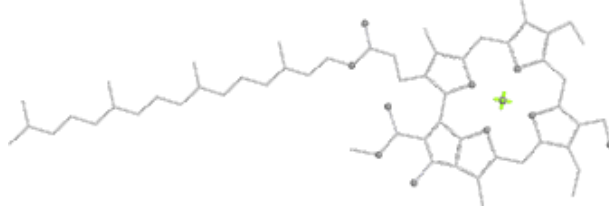
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Bond lengths	Bond angles
	
Torsions	Rings

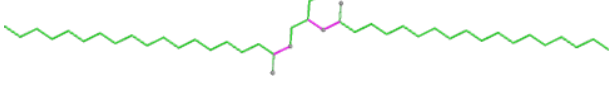
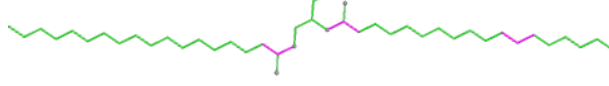
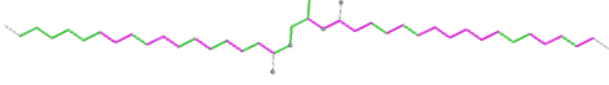
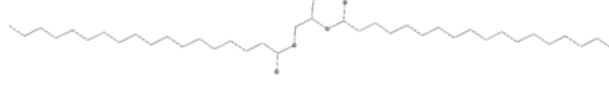
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Bond lengths	Bond angles
	
Torsions	Rings

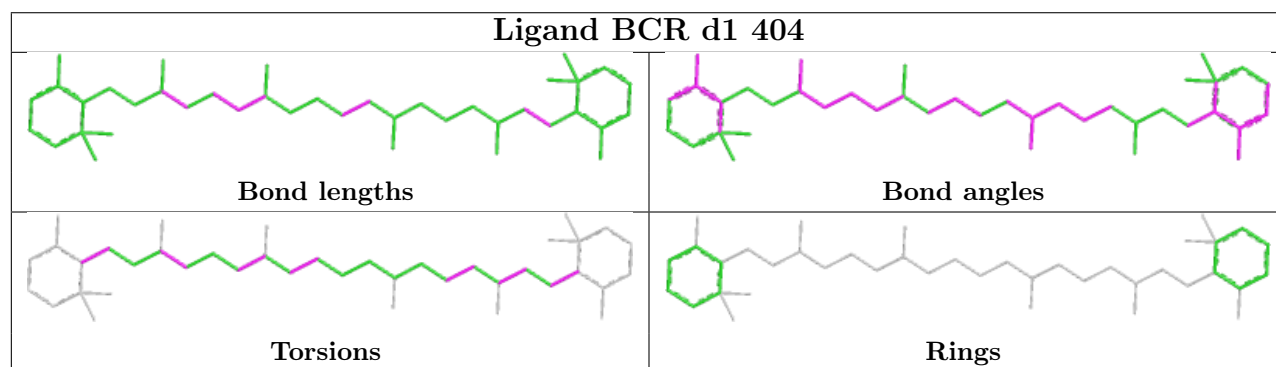
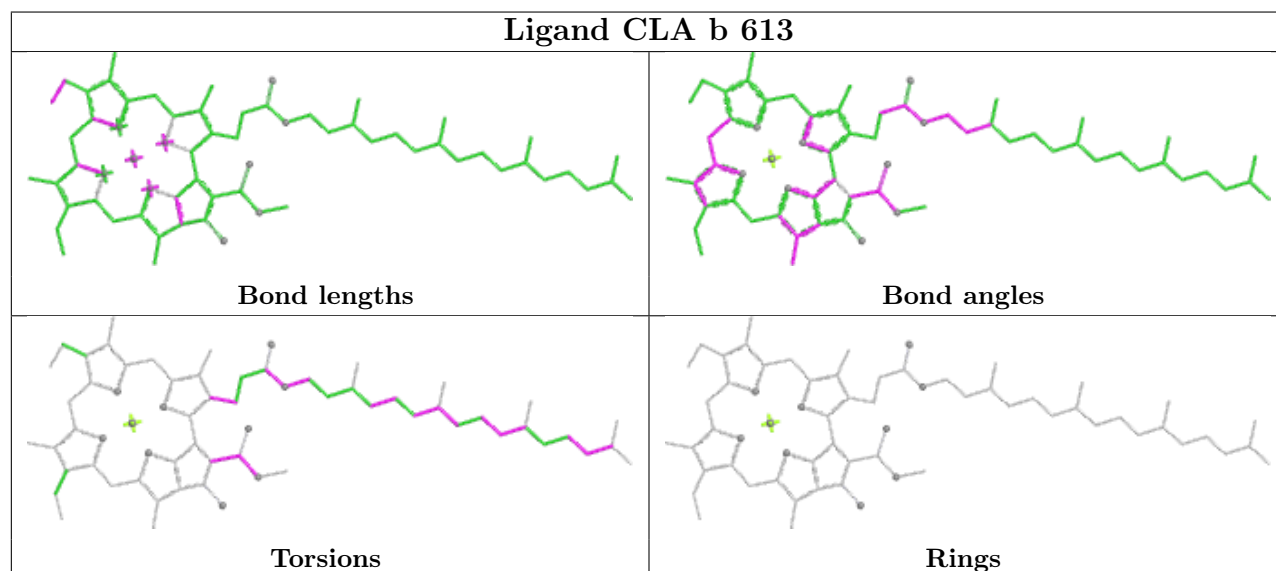
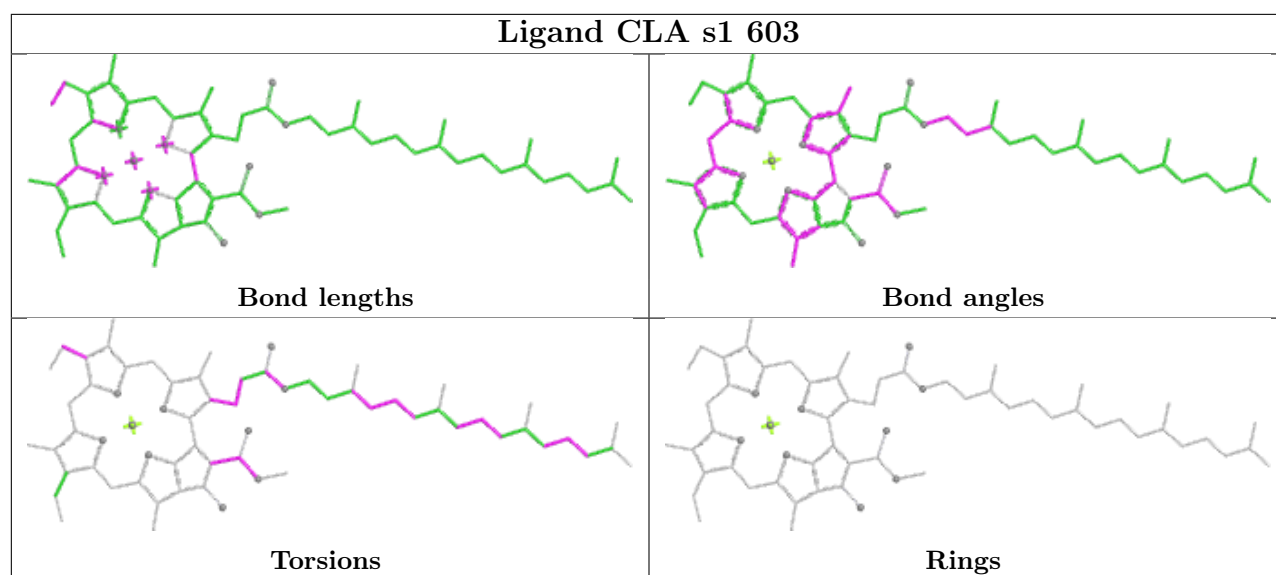


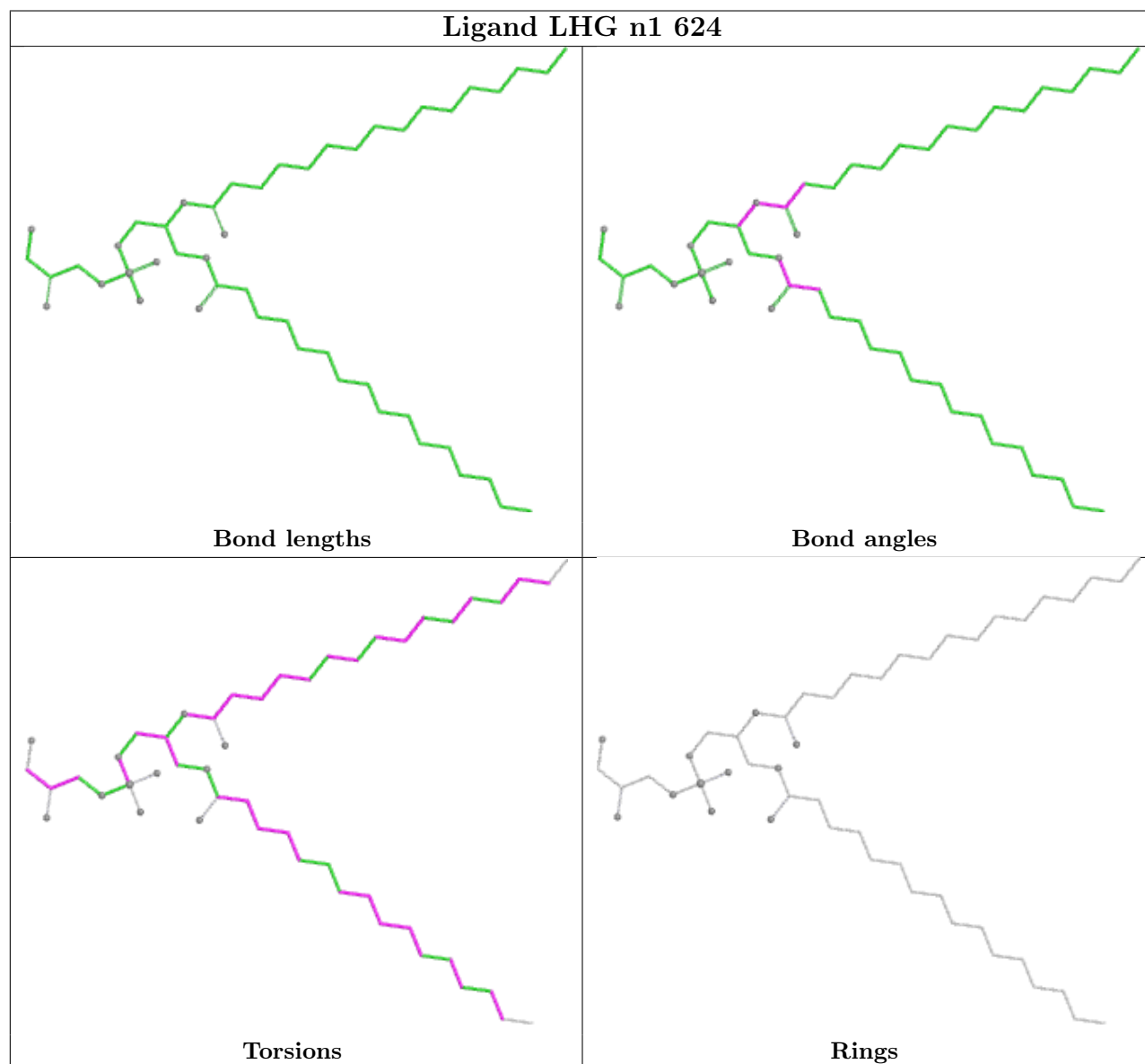
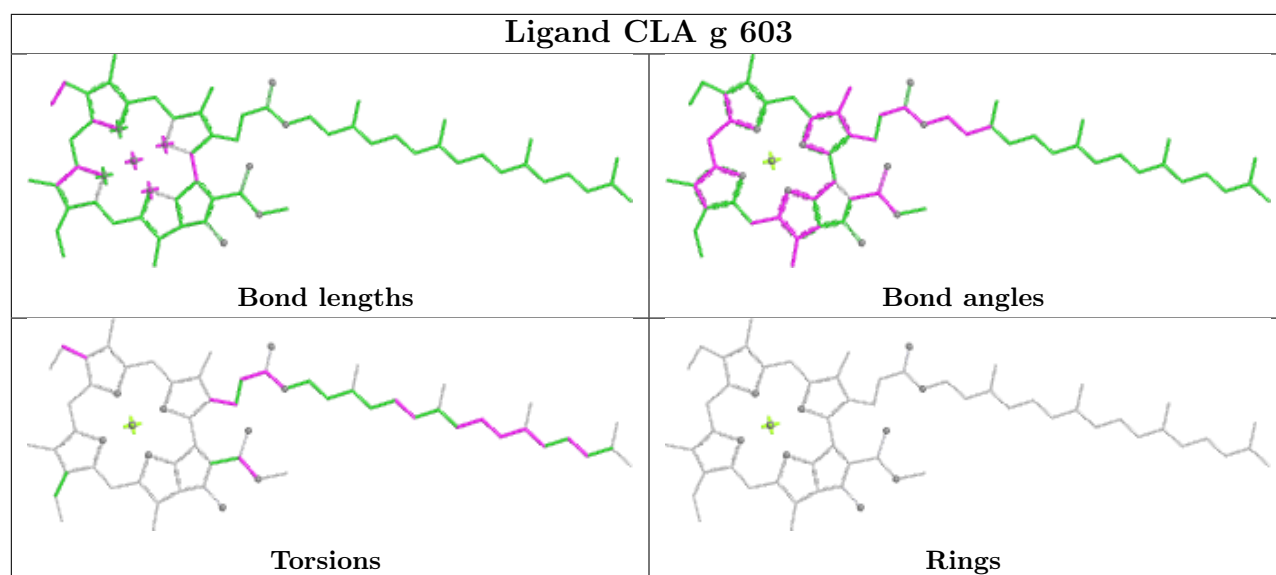


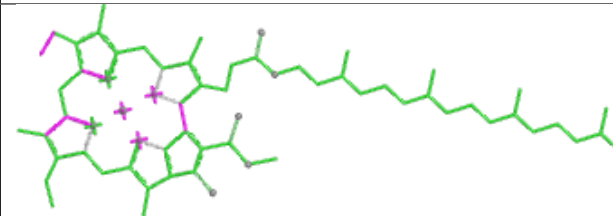
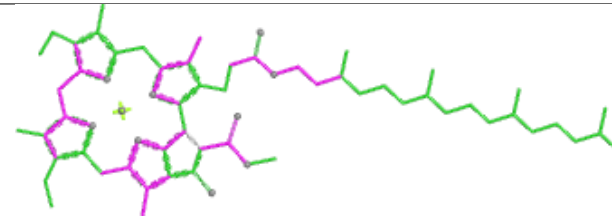
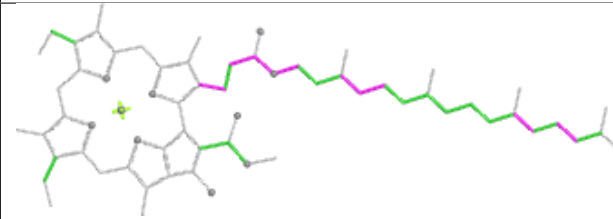
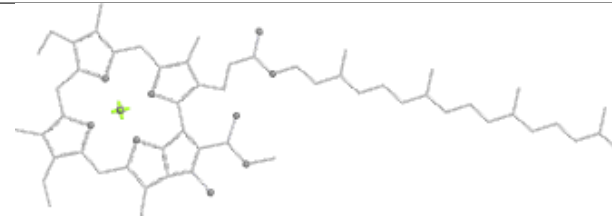
Ligand LUT n1 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

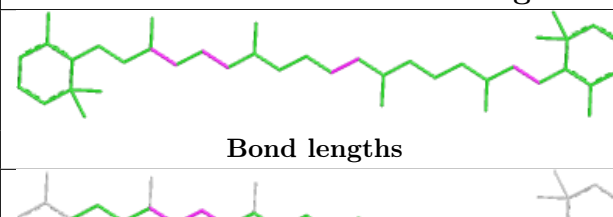
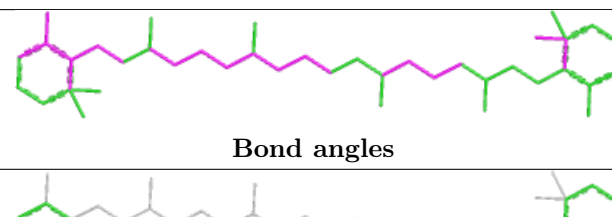
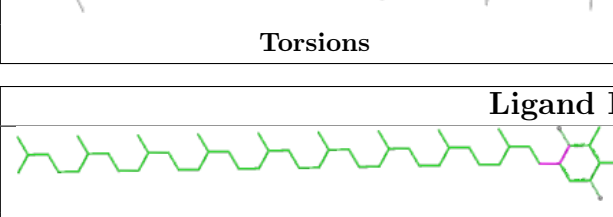
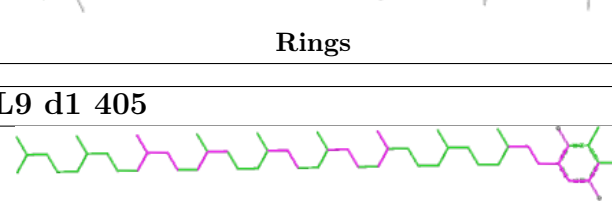
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Bond lengths	Bond angles
	
Torsions	Rings

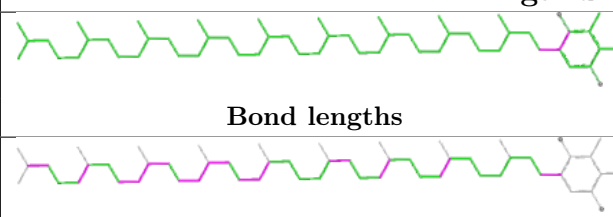
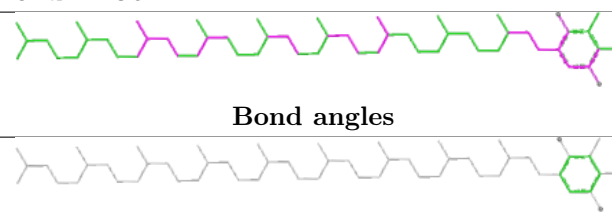
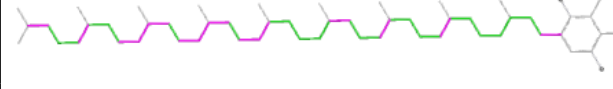
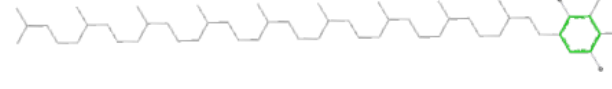
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Bond lengths	Bond angles
	
Torsions	Rings

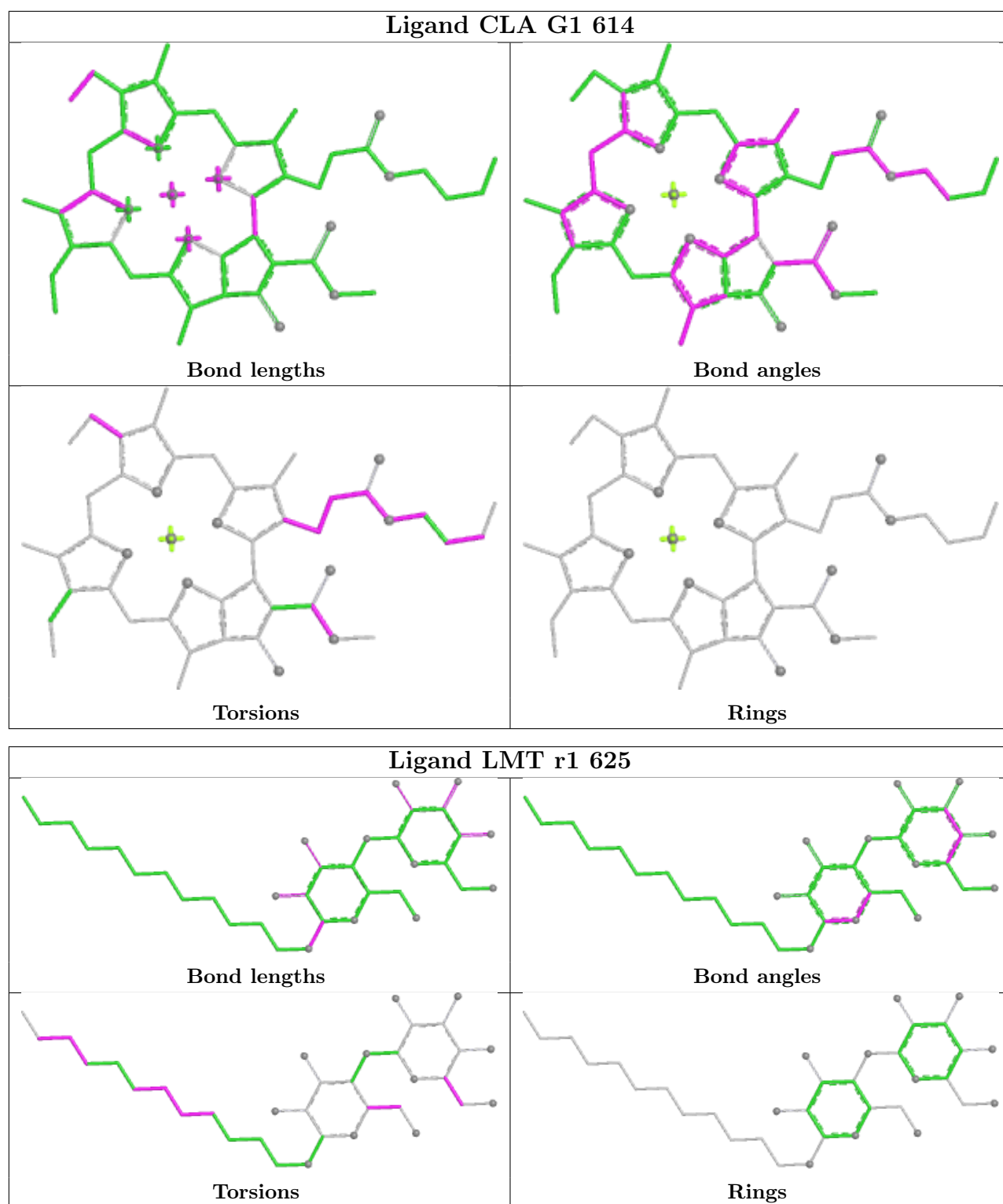


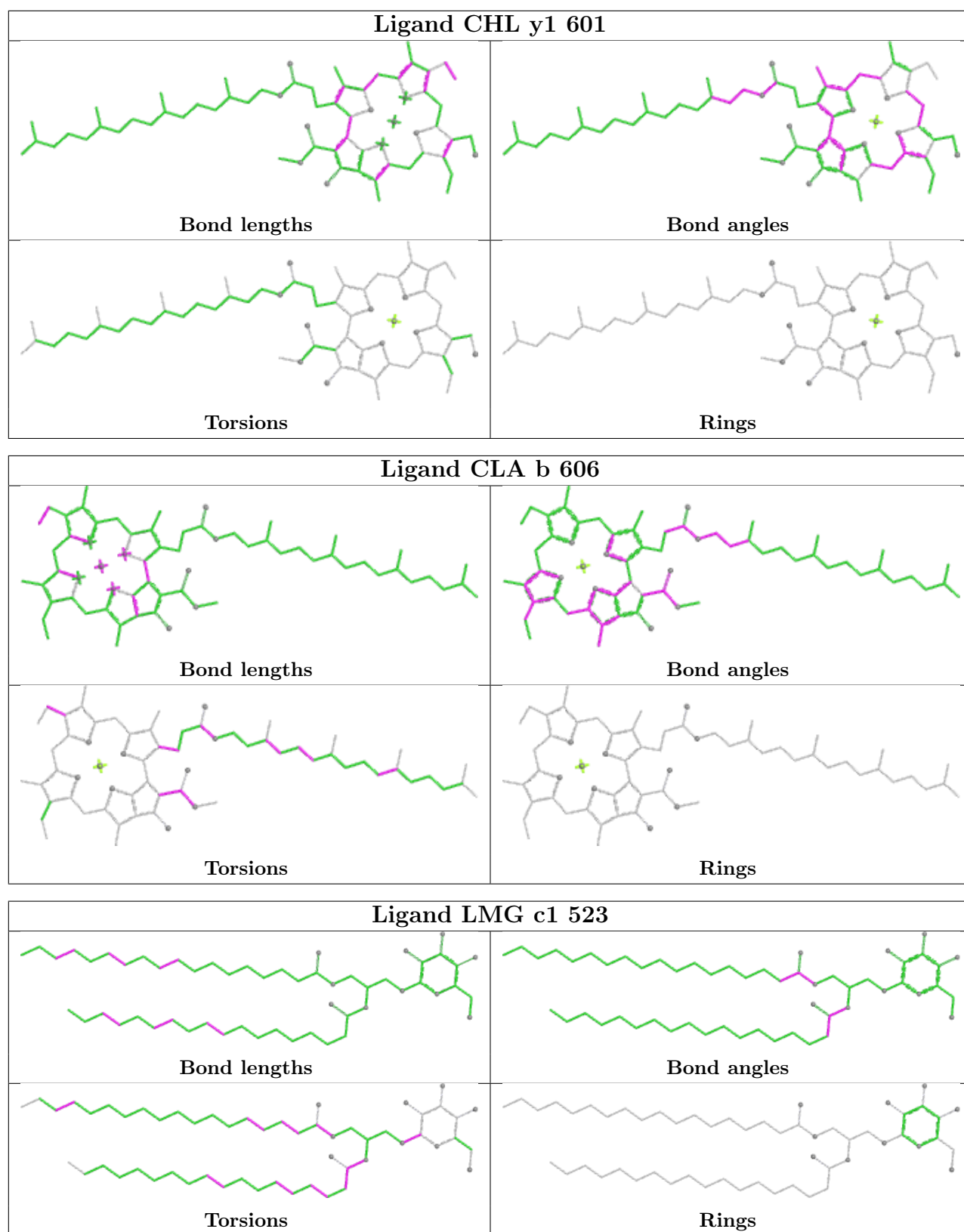


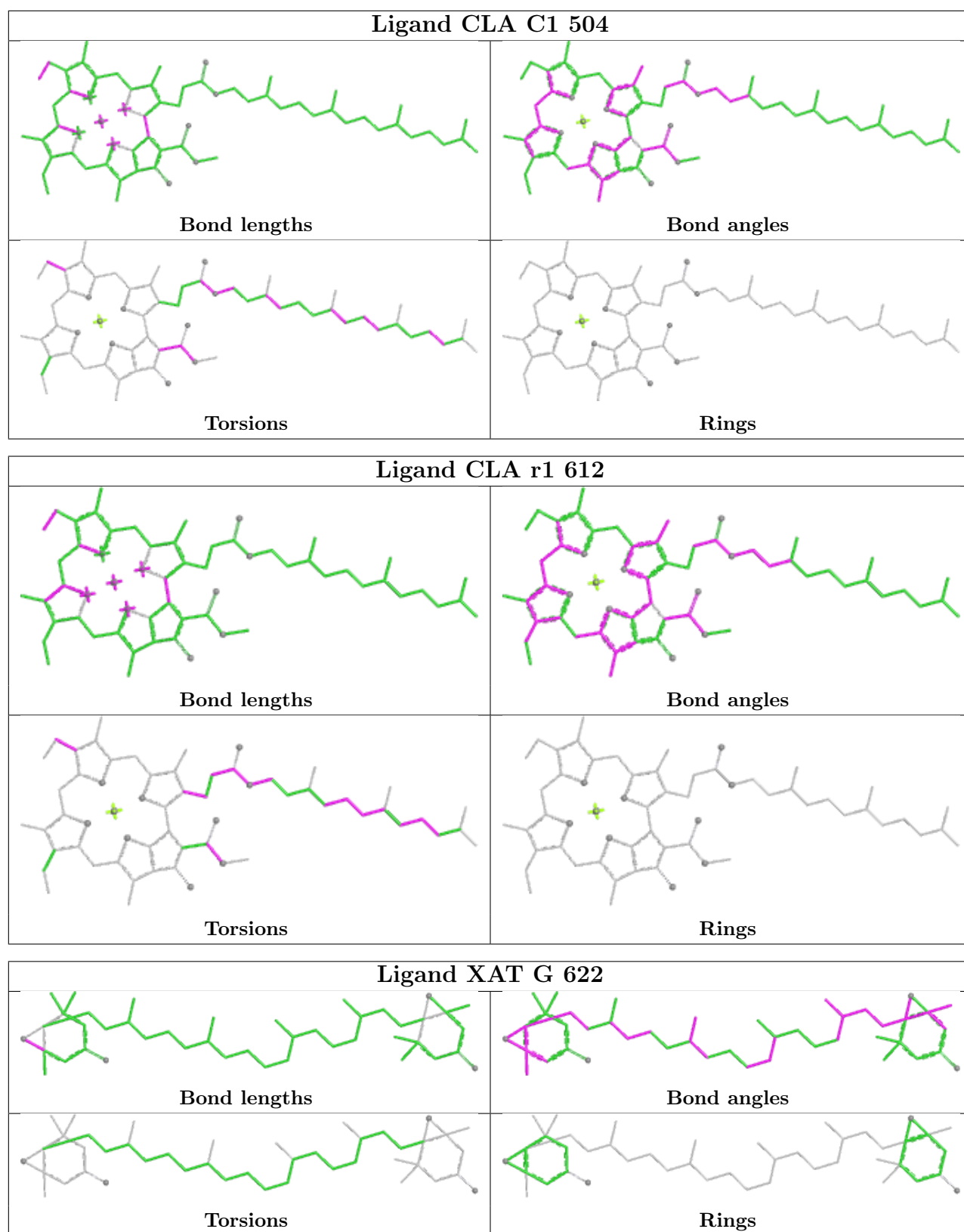
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Bond lengths	Bond angles
	
Torsions	Rings

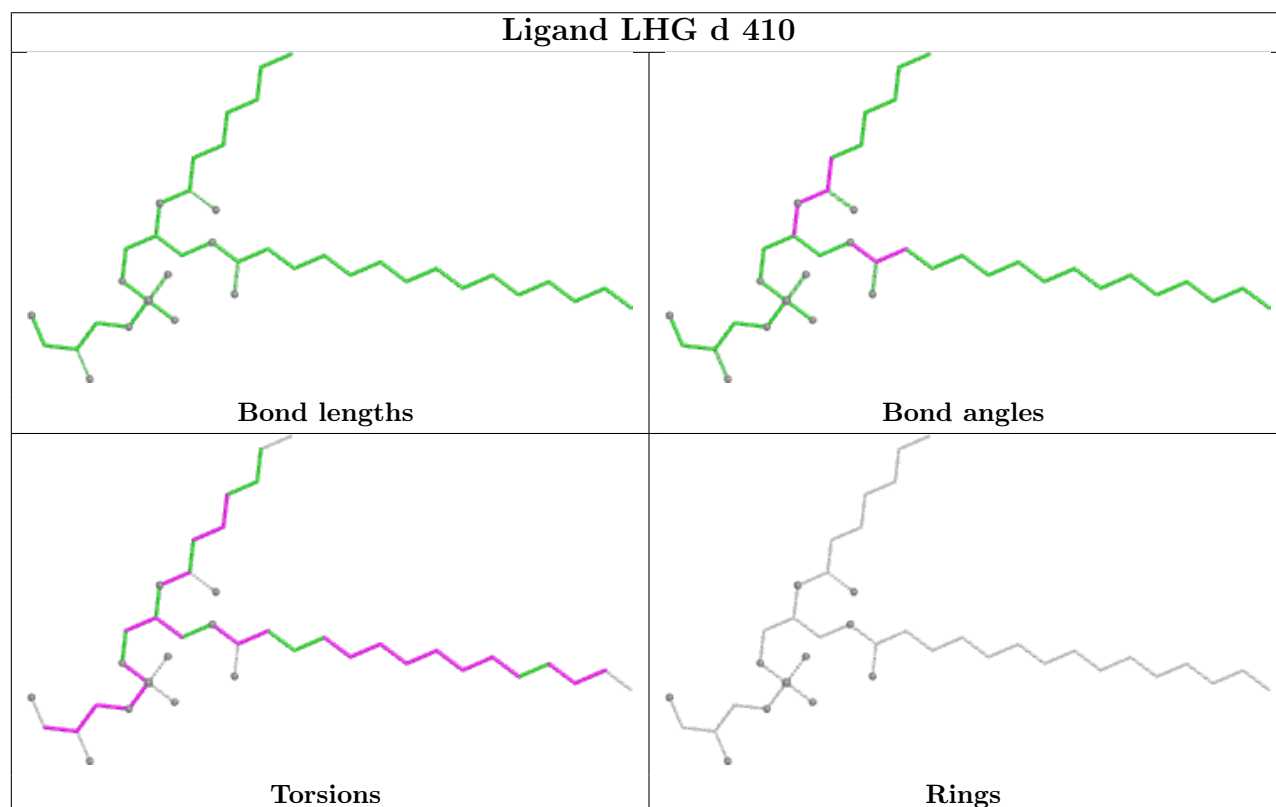
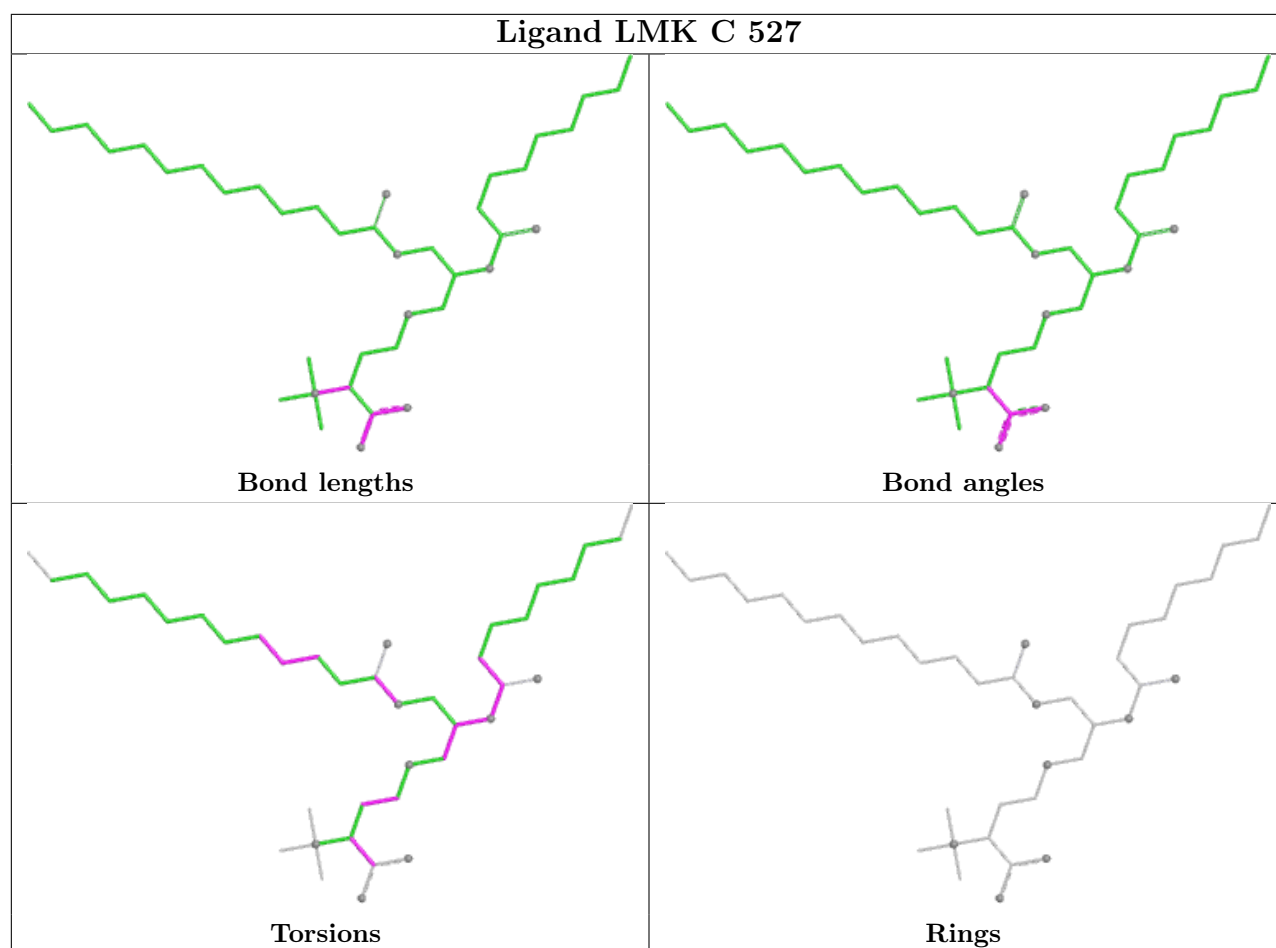
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Bond lengths	Bond angles
	
Torsions	Rings

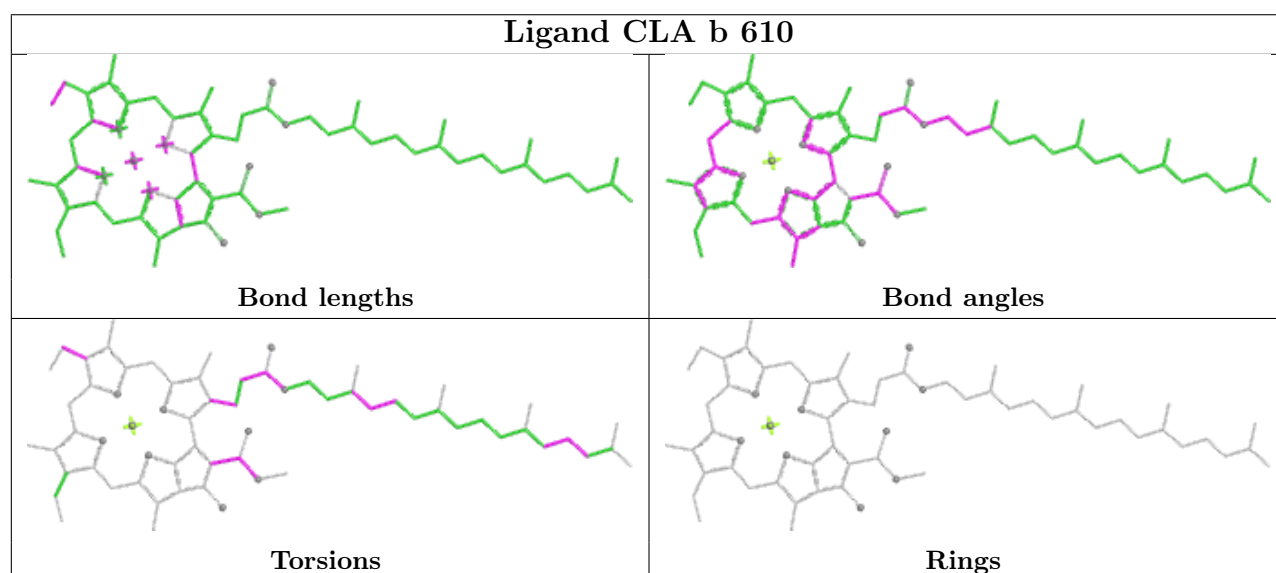
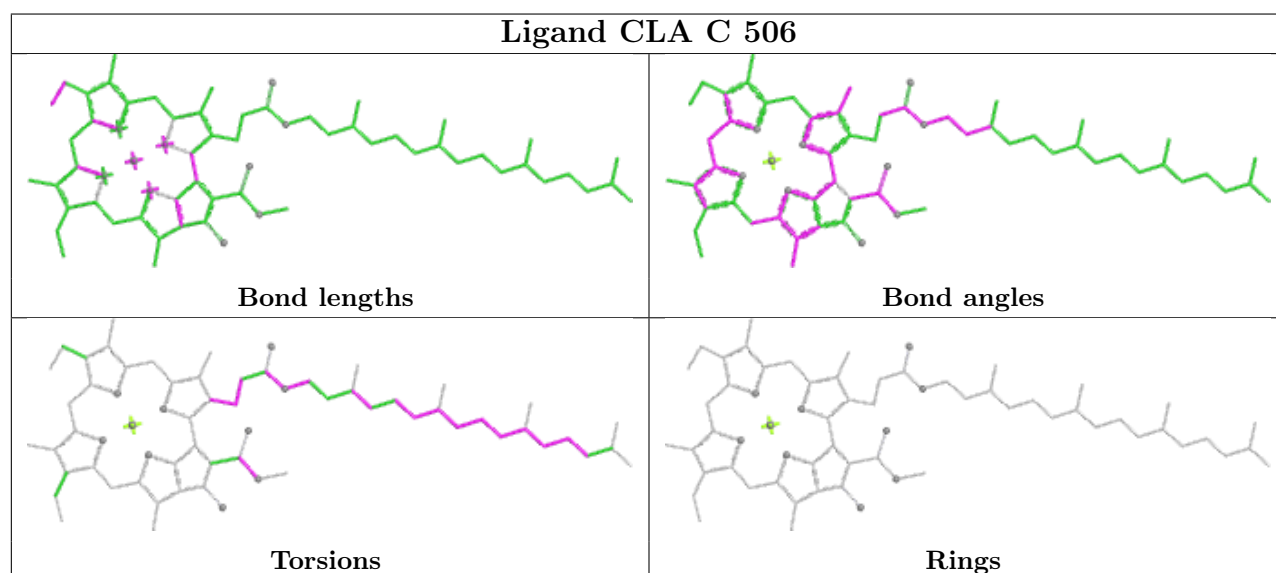
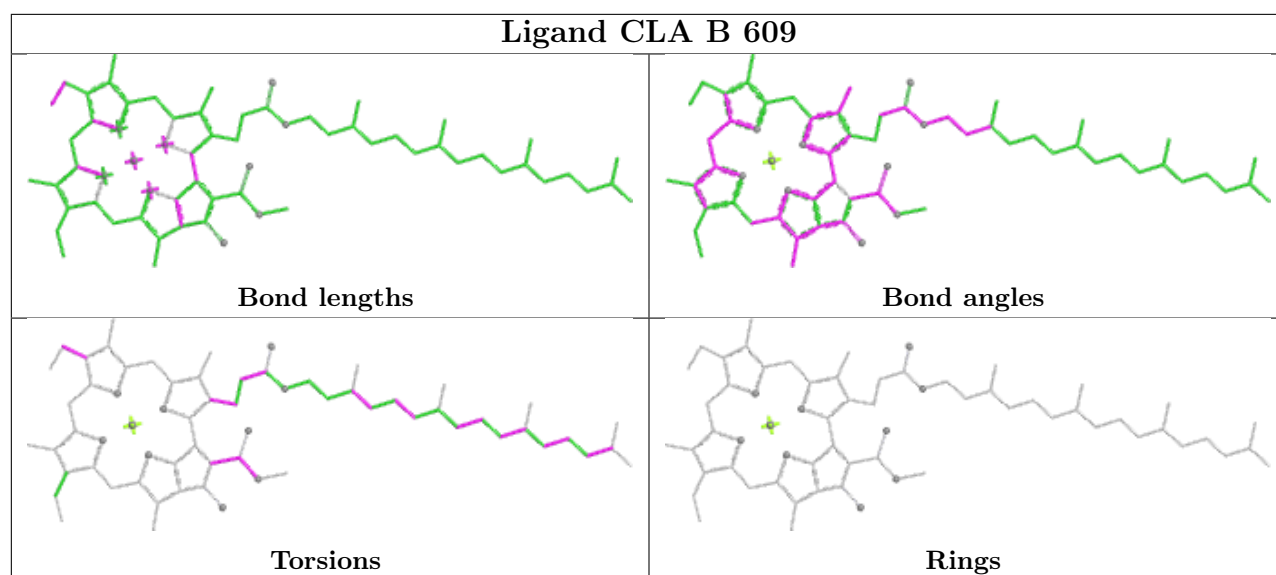
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Bond lengths	Bond angles
	
Torsions	Rings

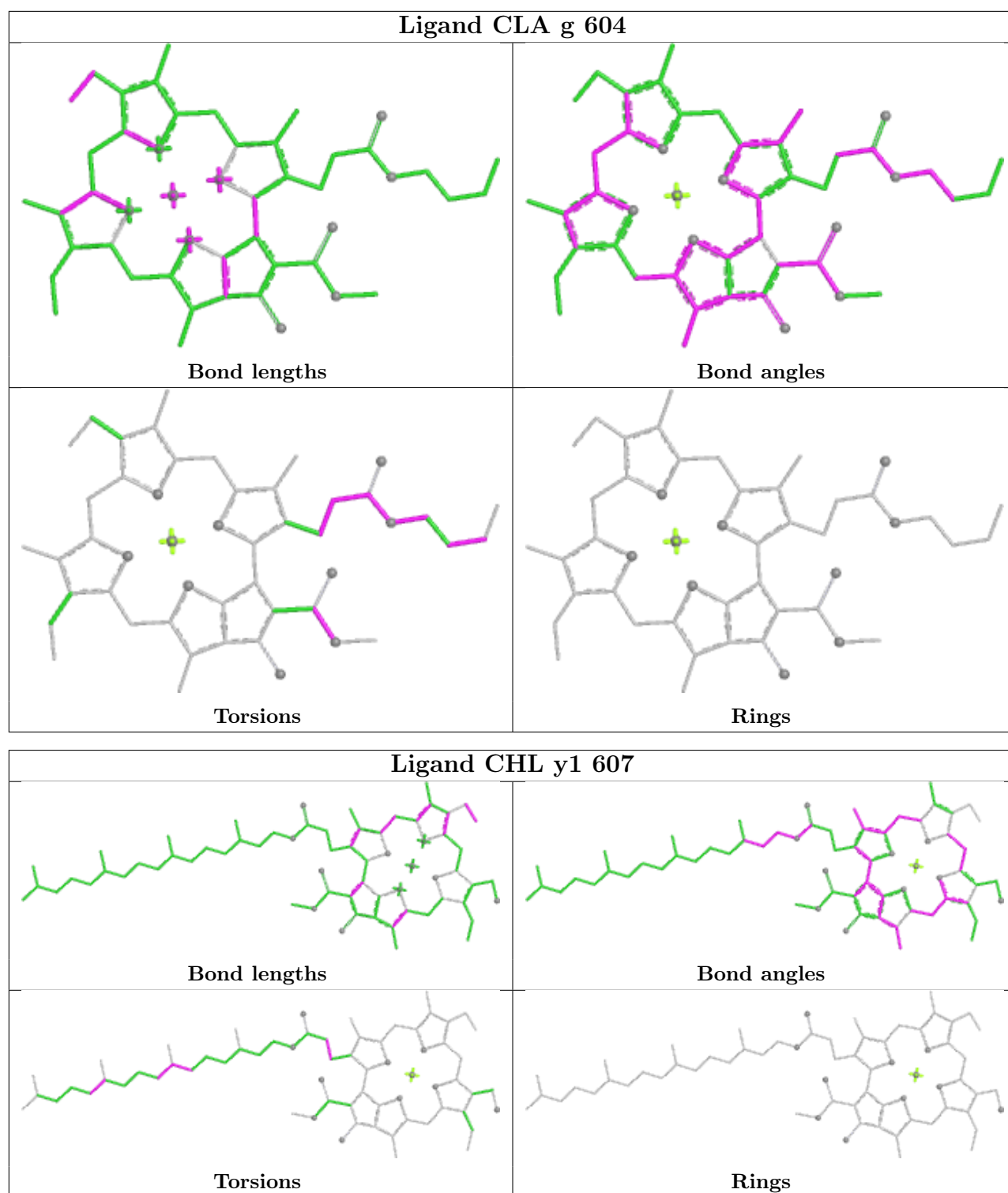


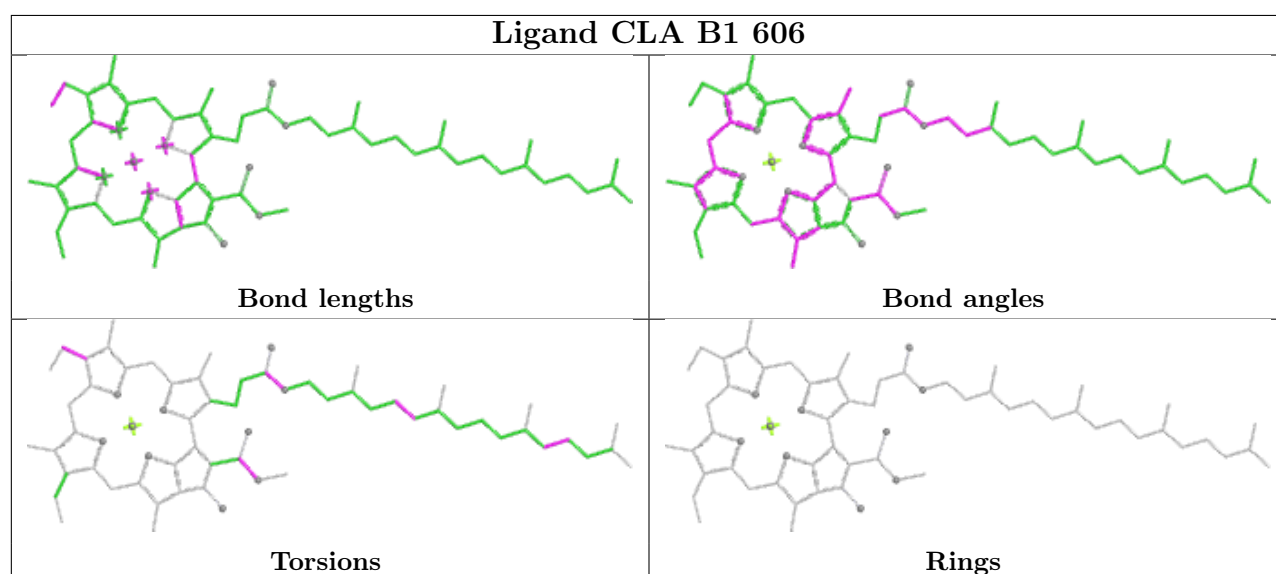
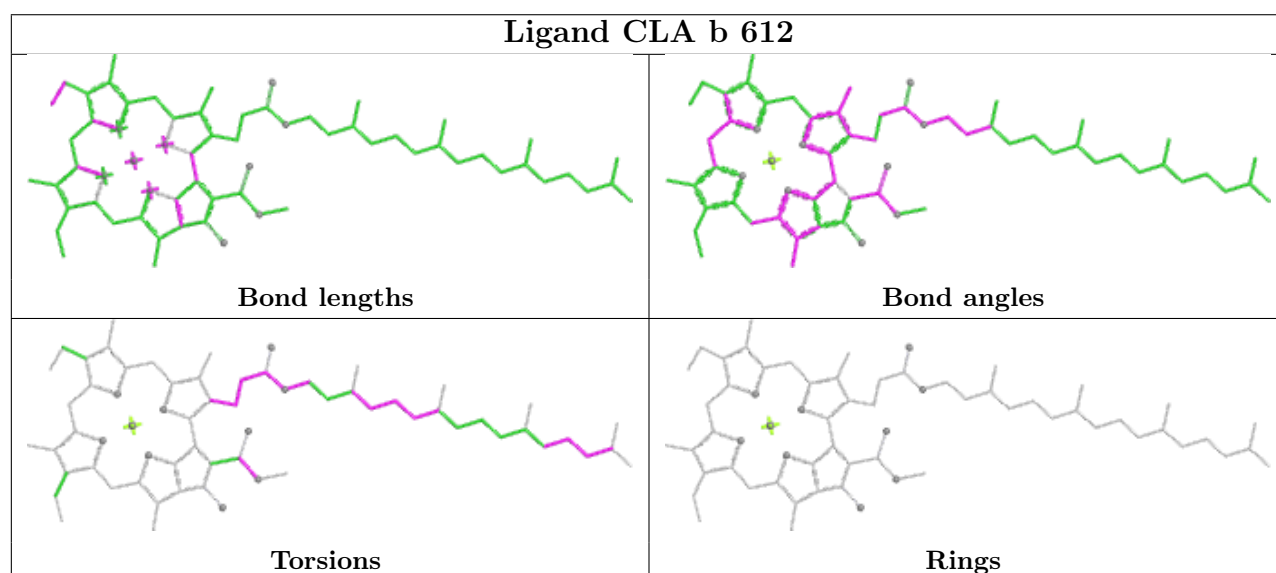
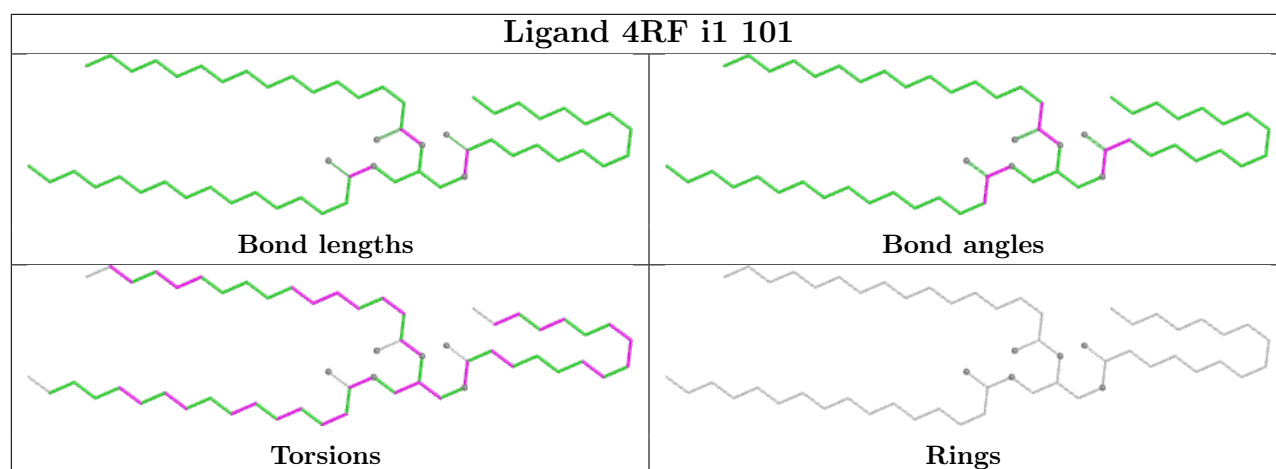


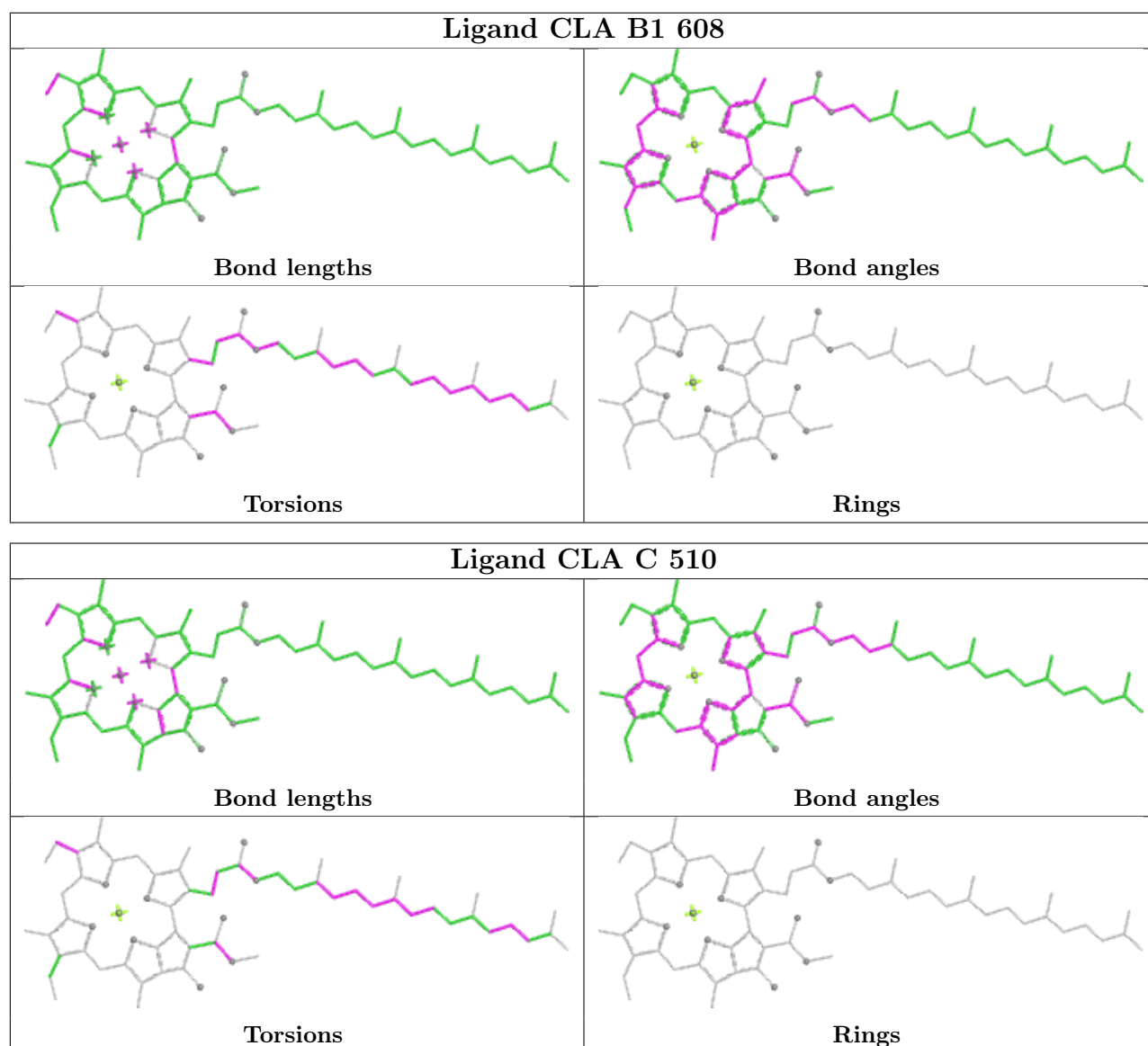


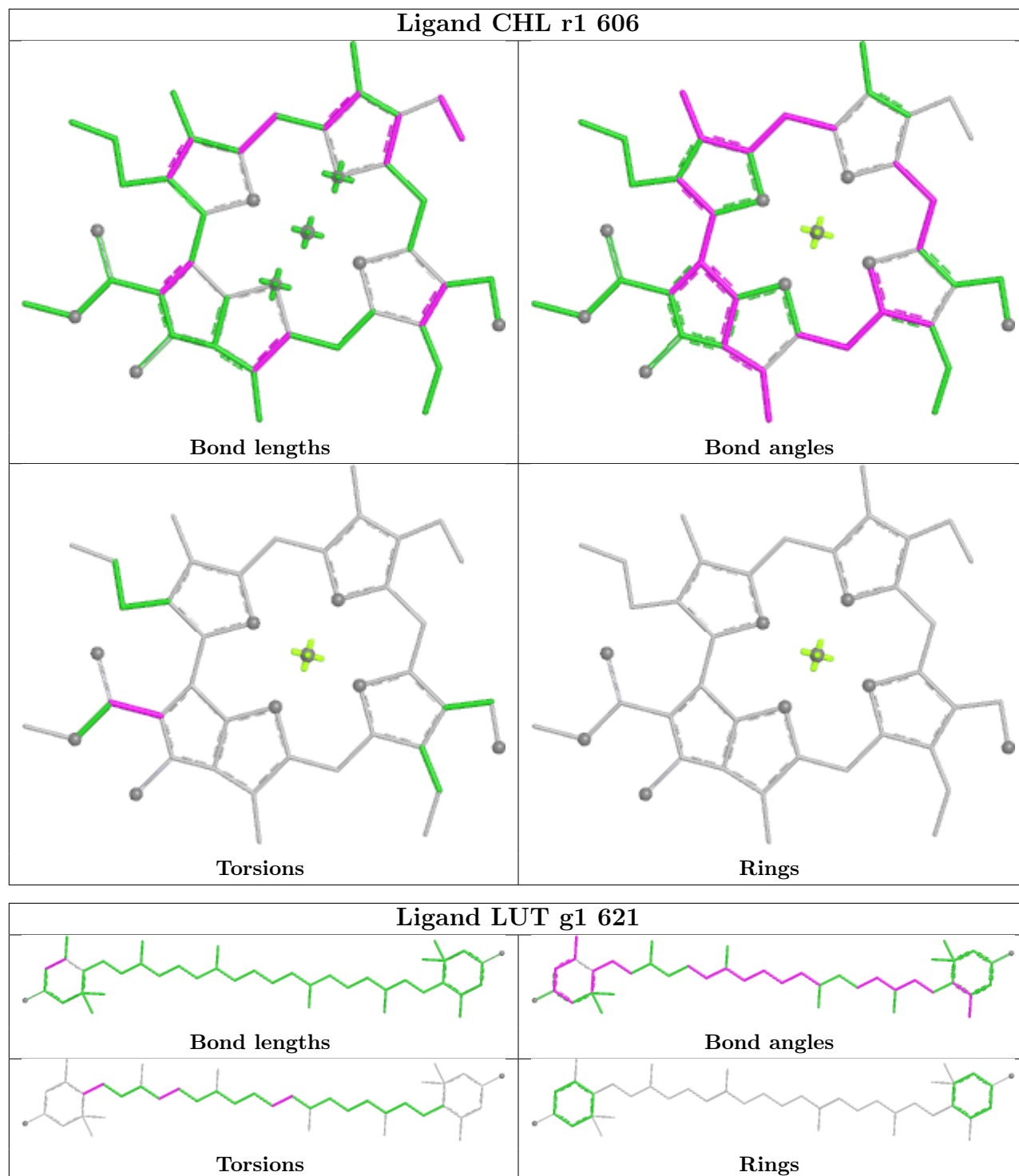


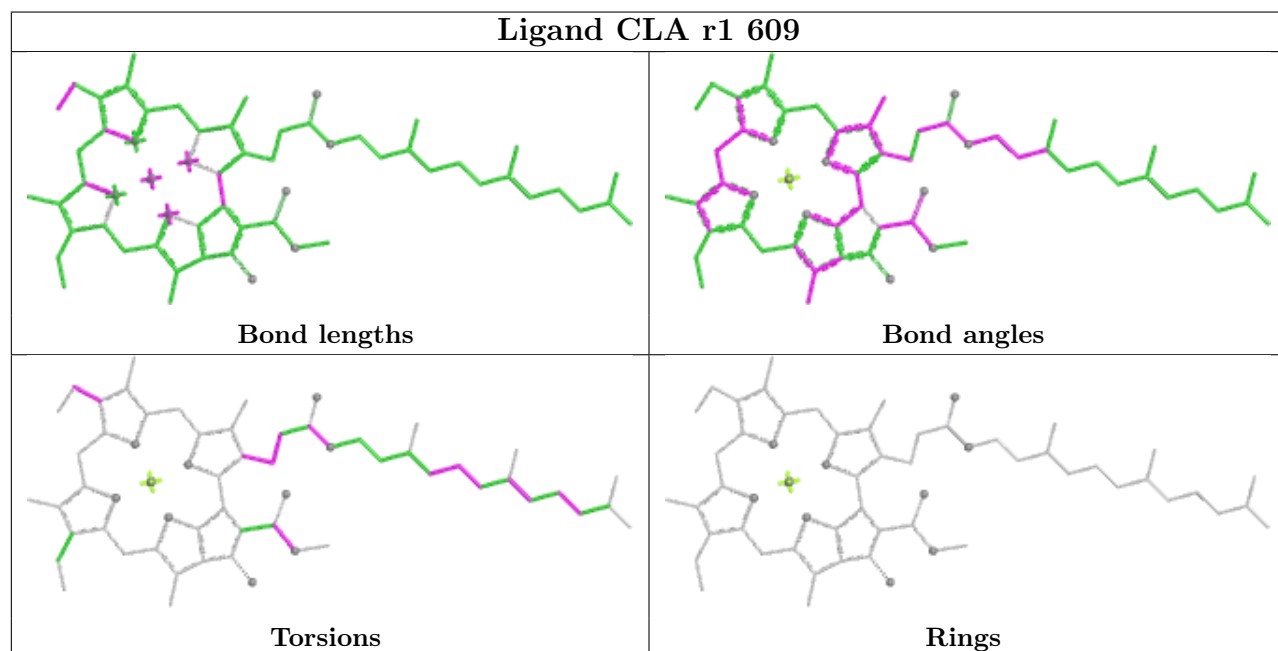
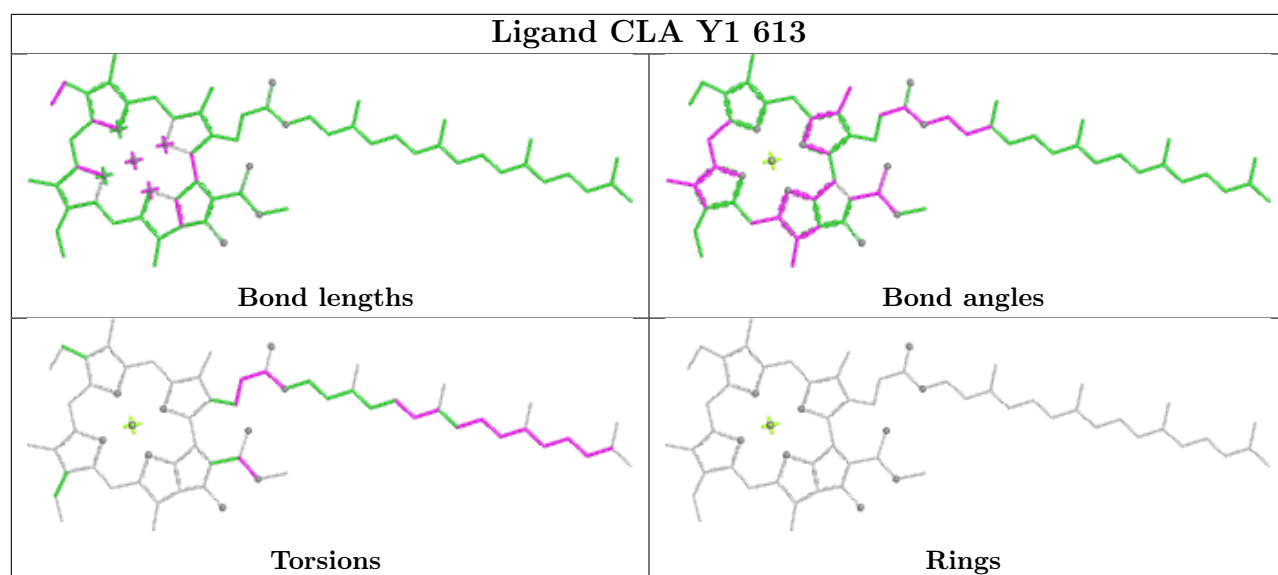


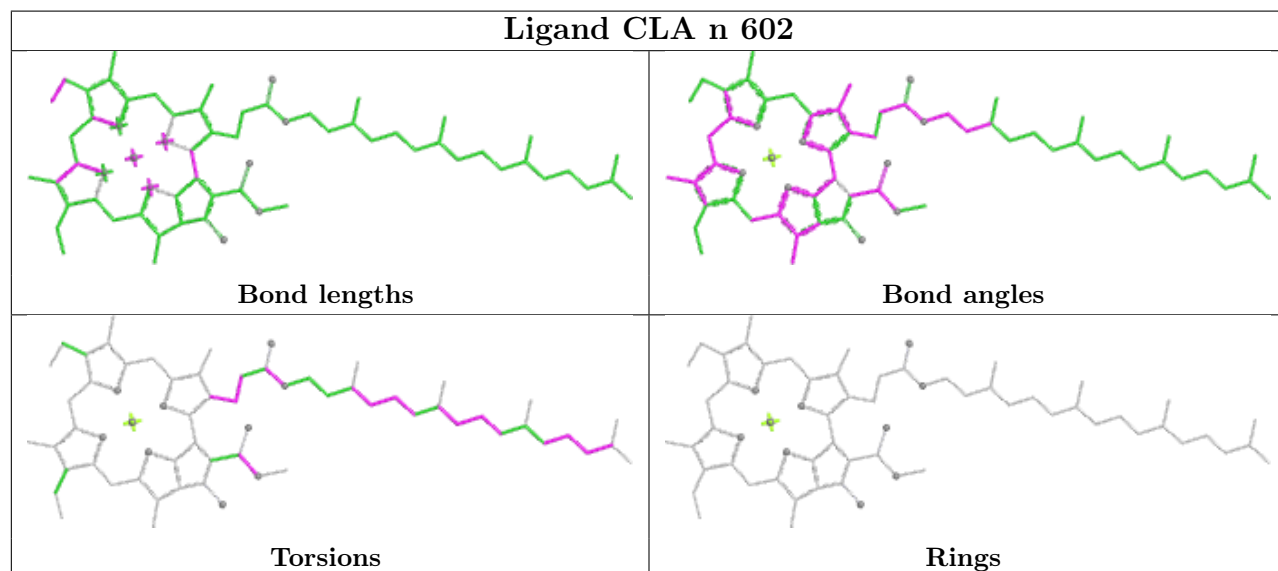
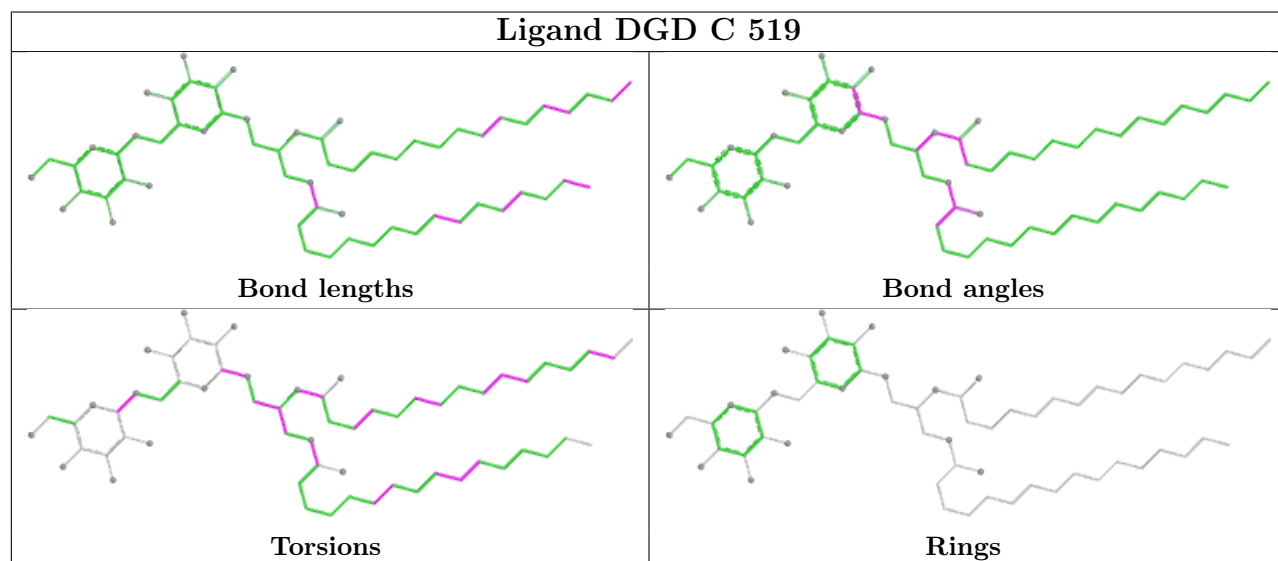
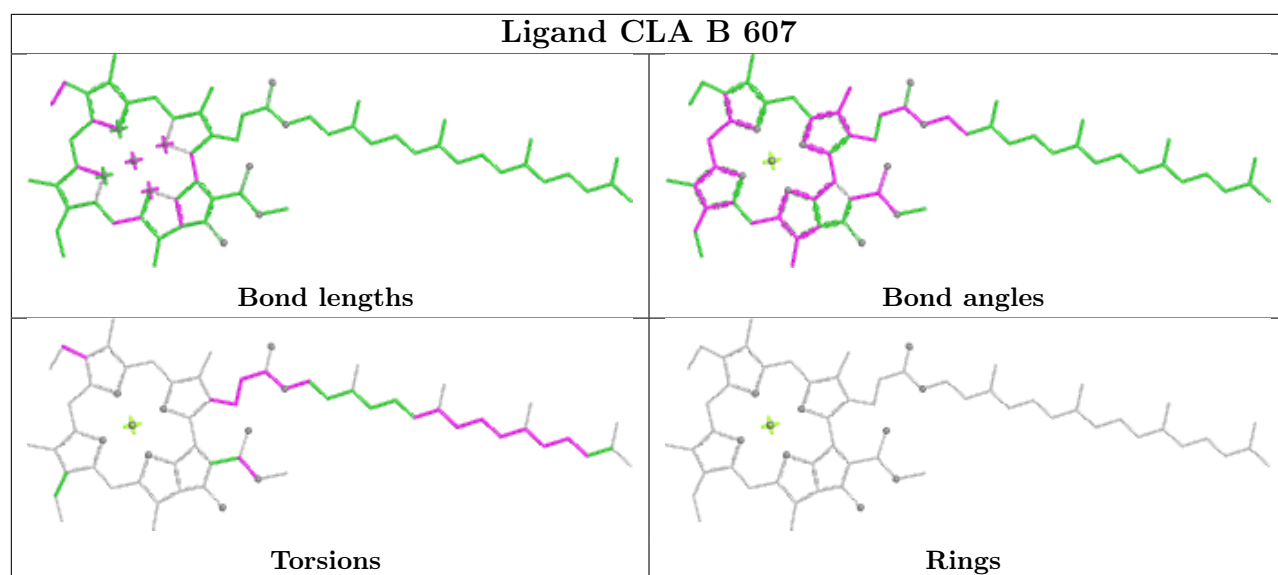


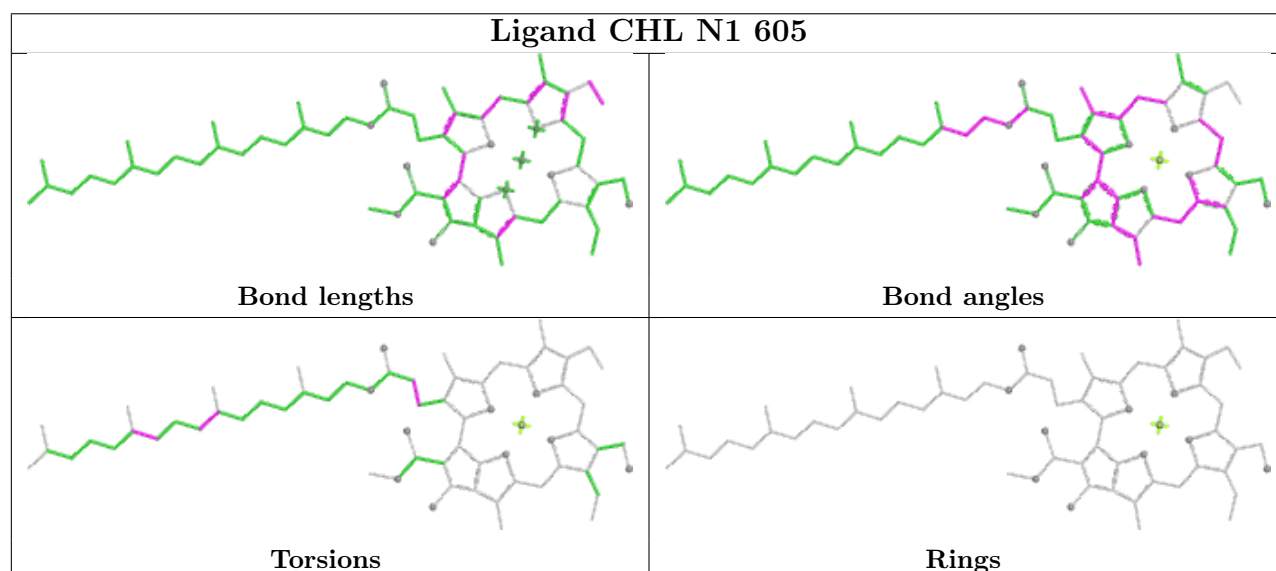
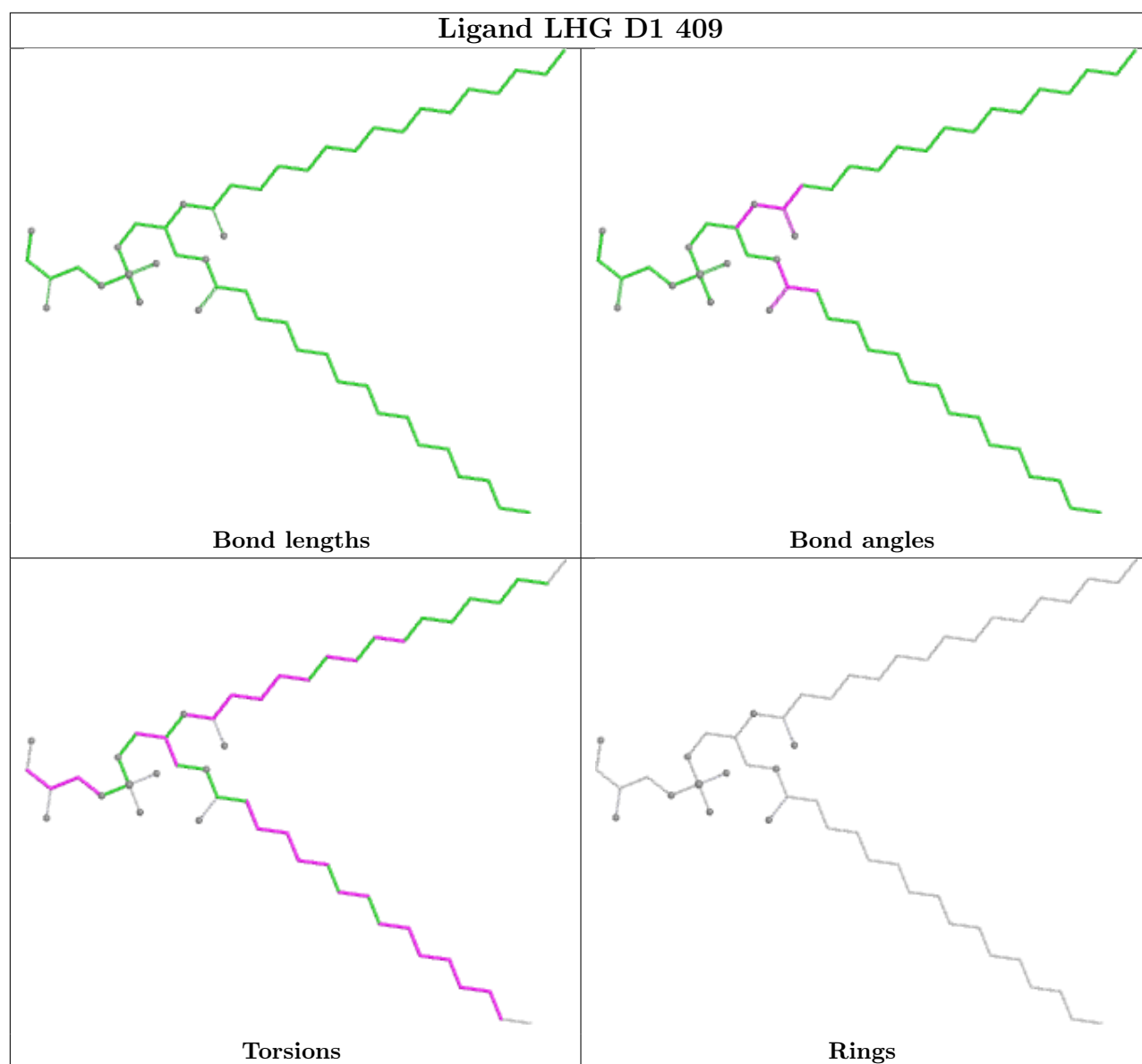


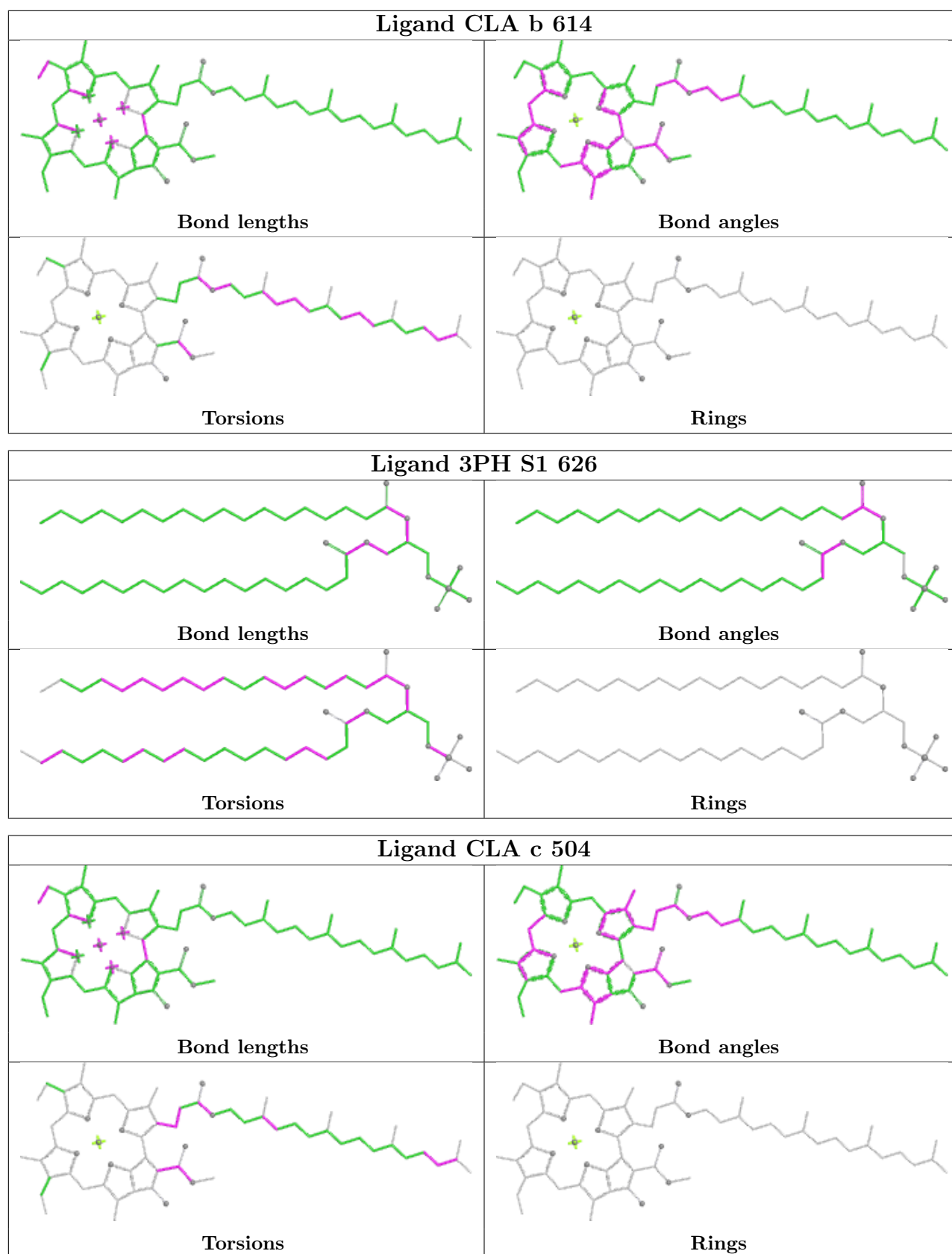


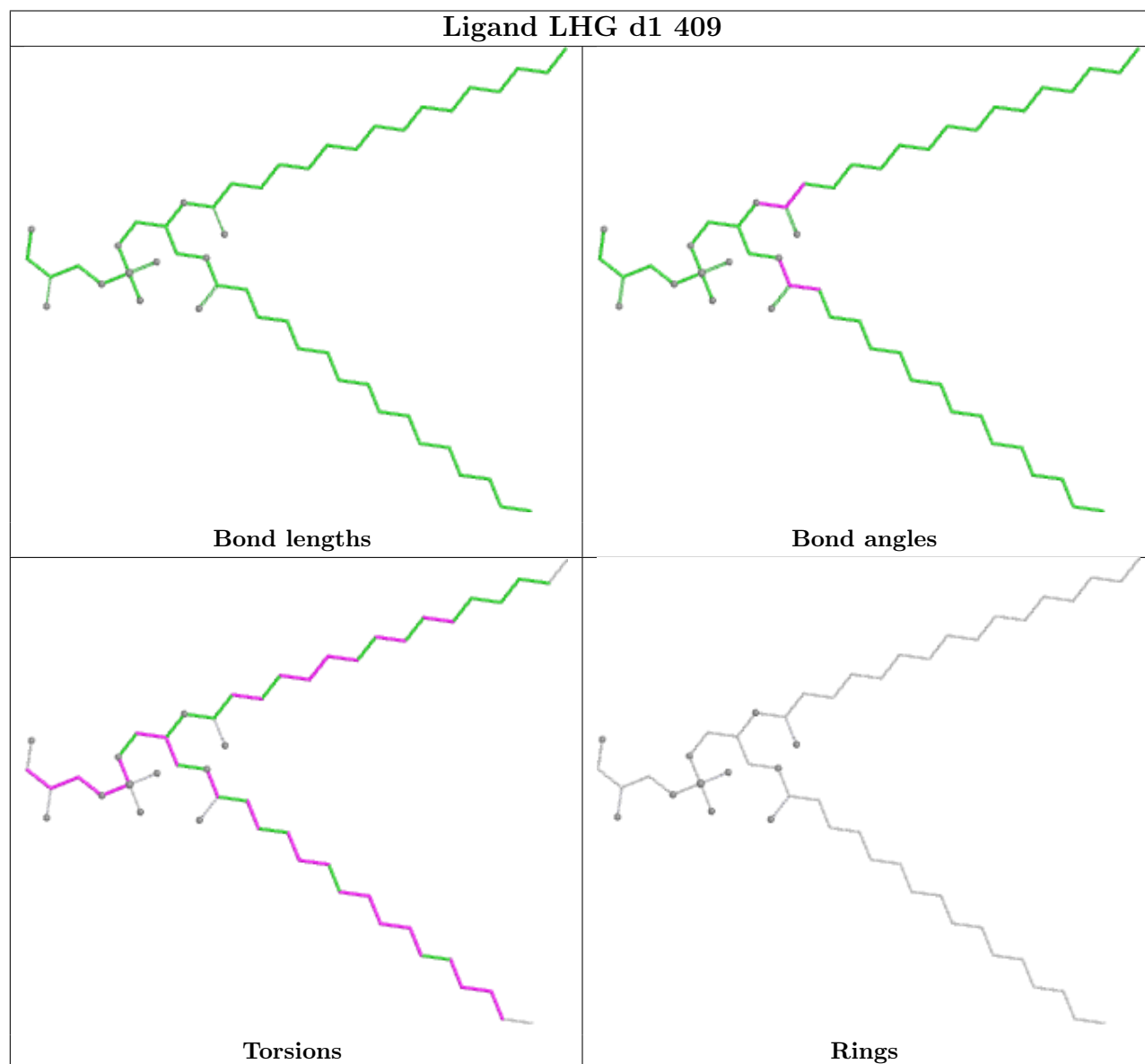
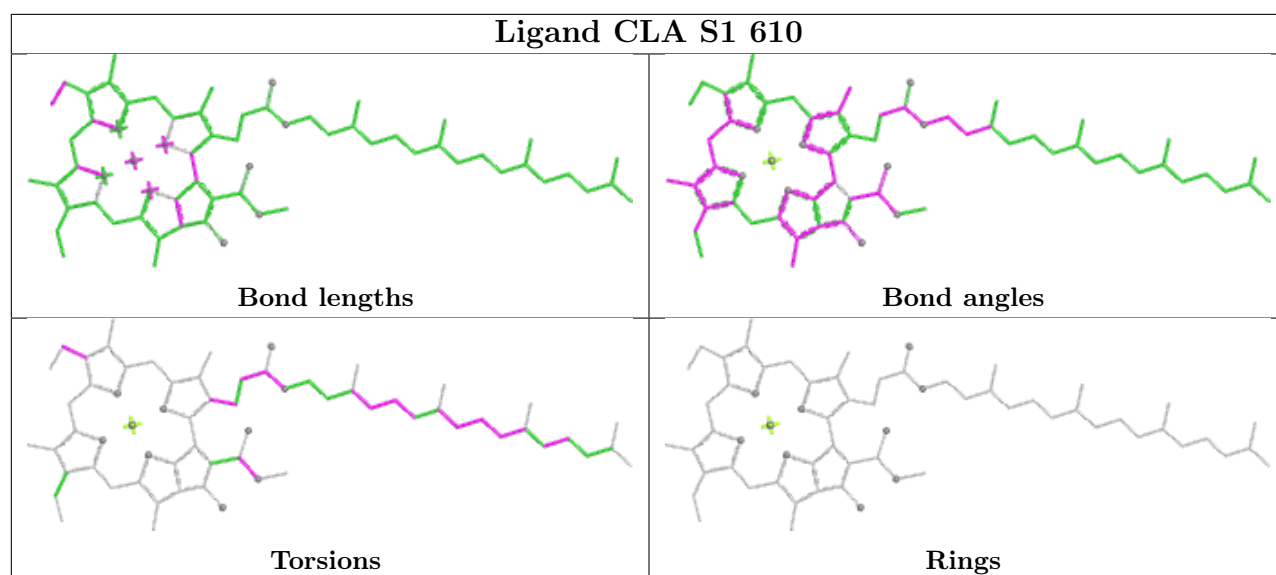


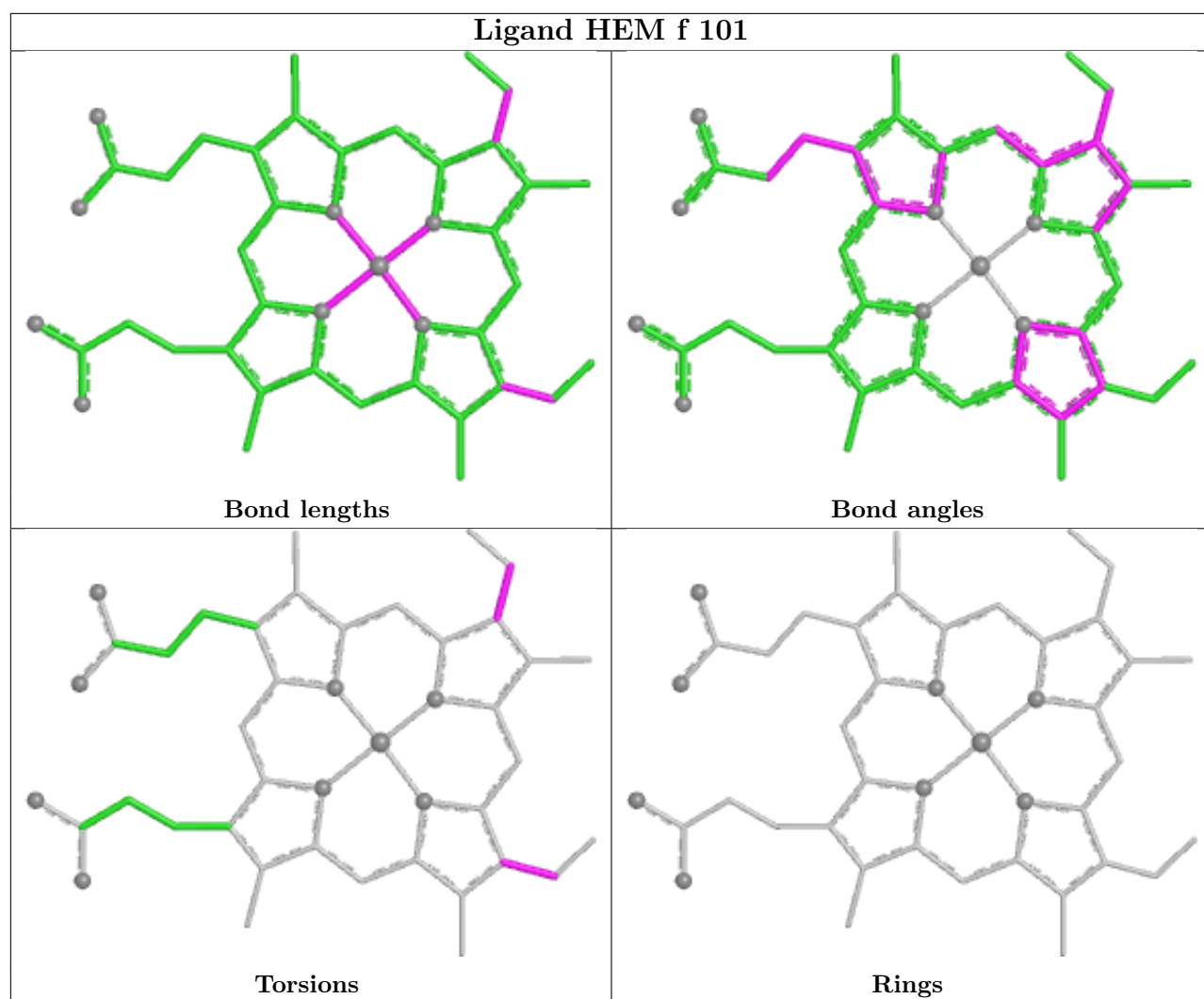


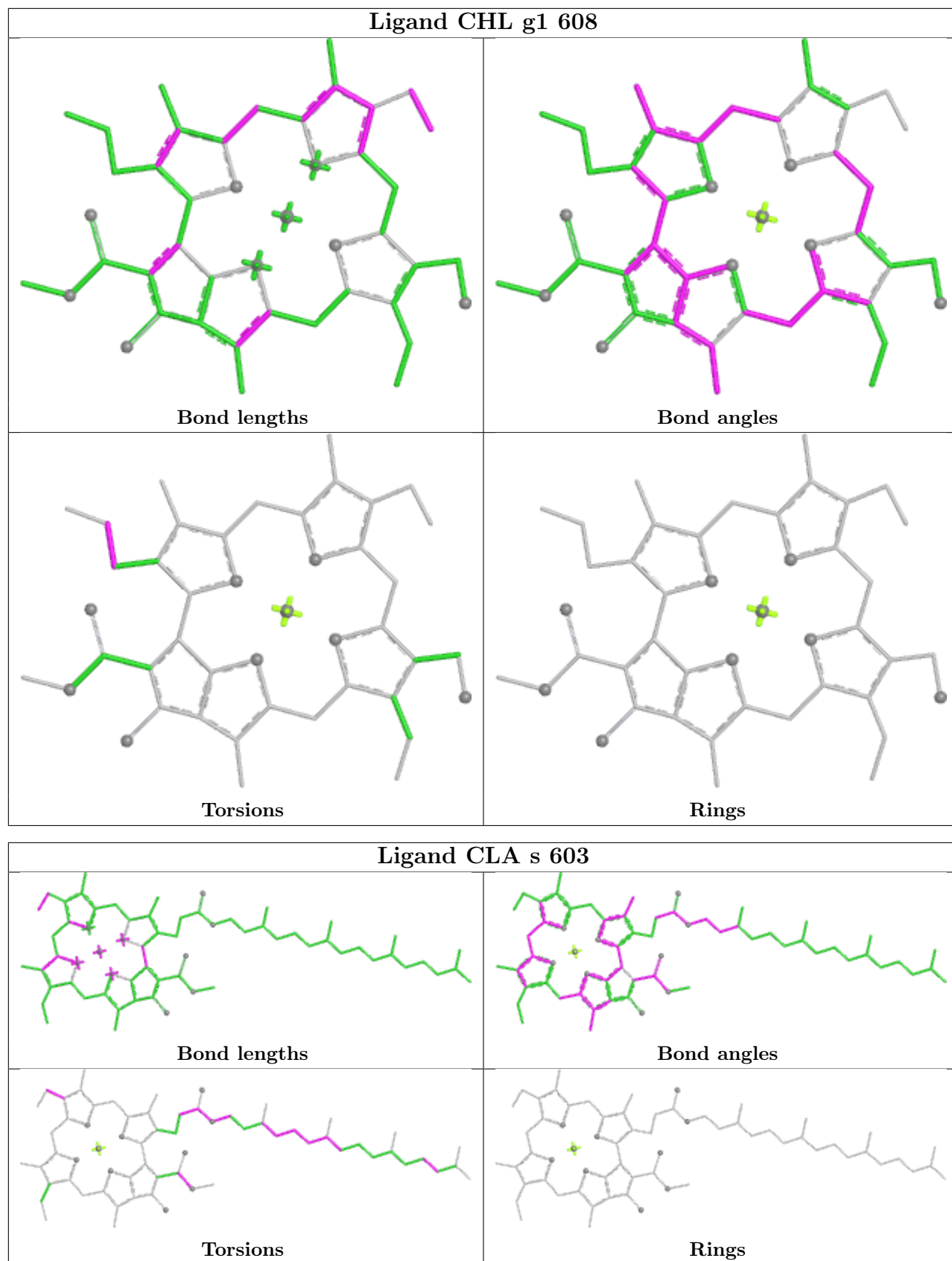


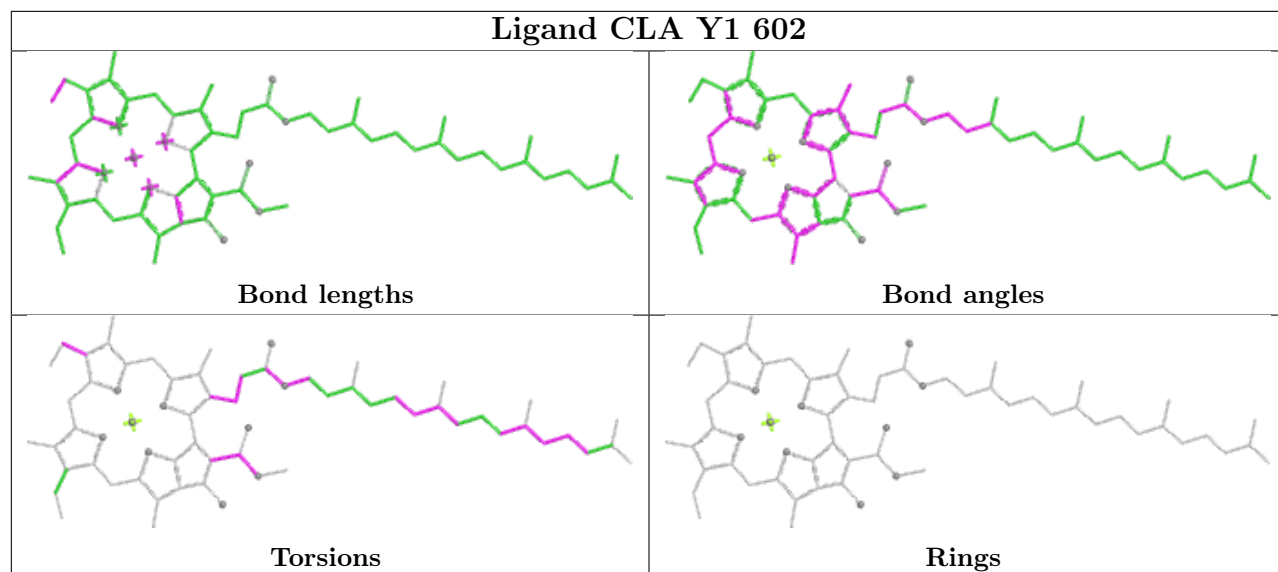
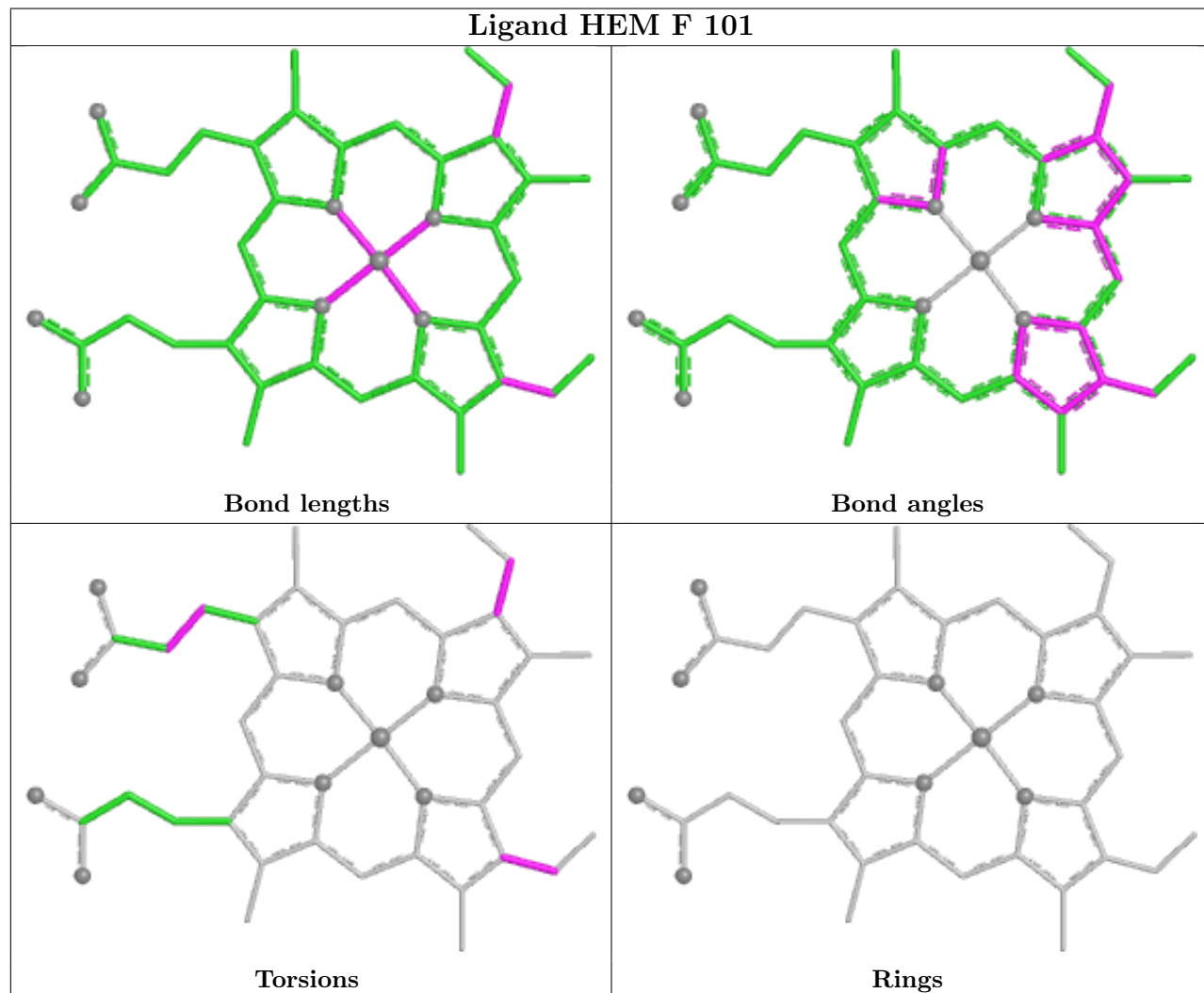


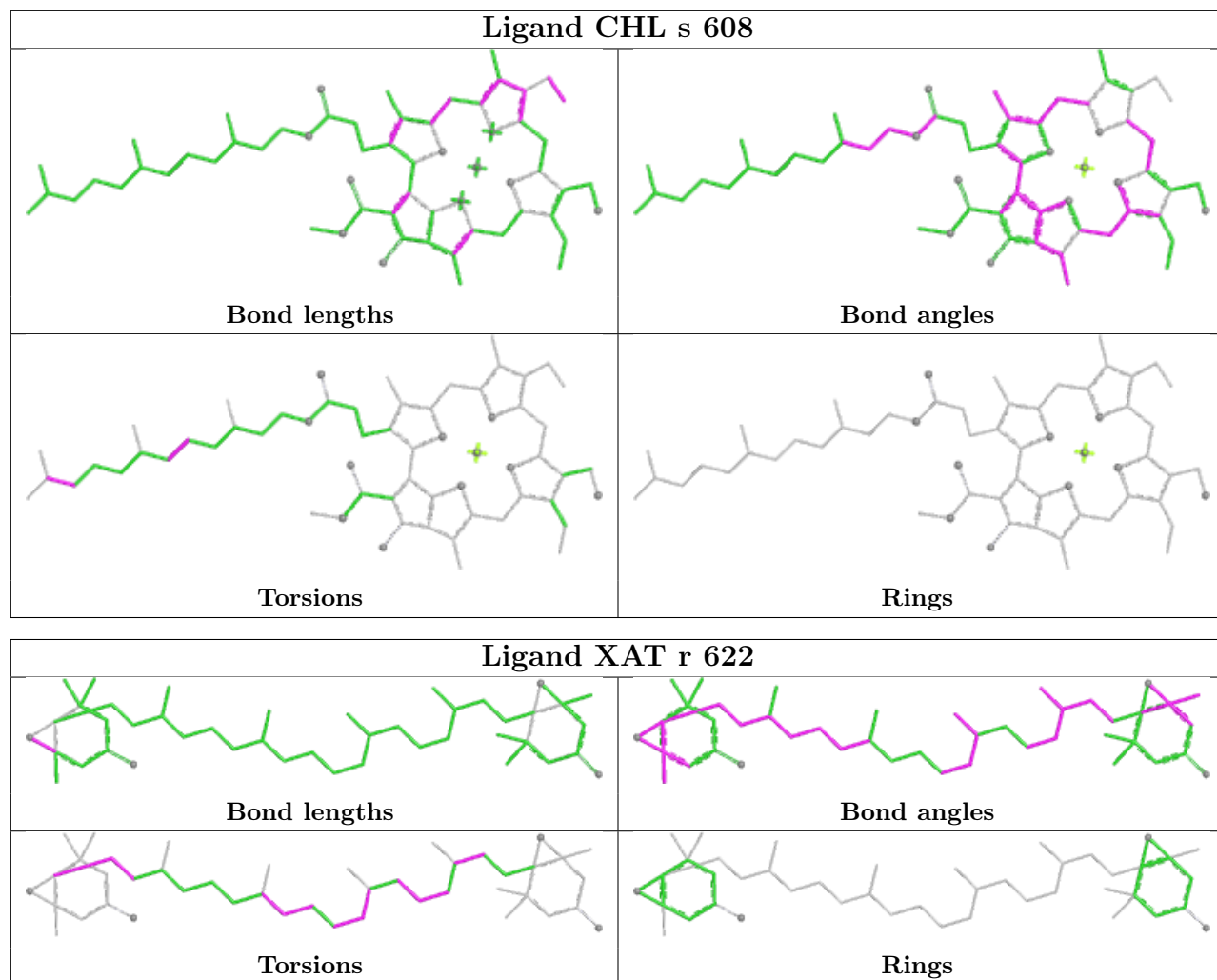


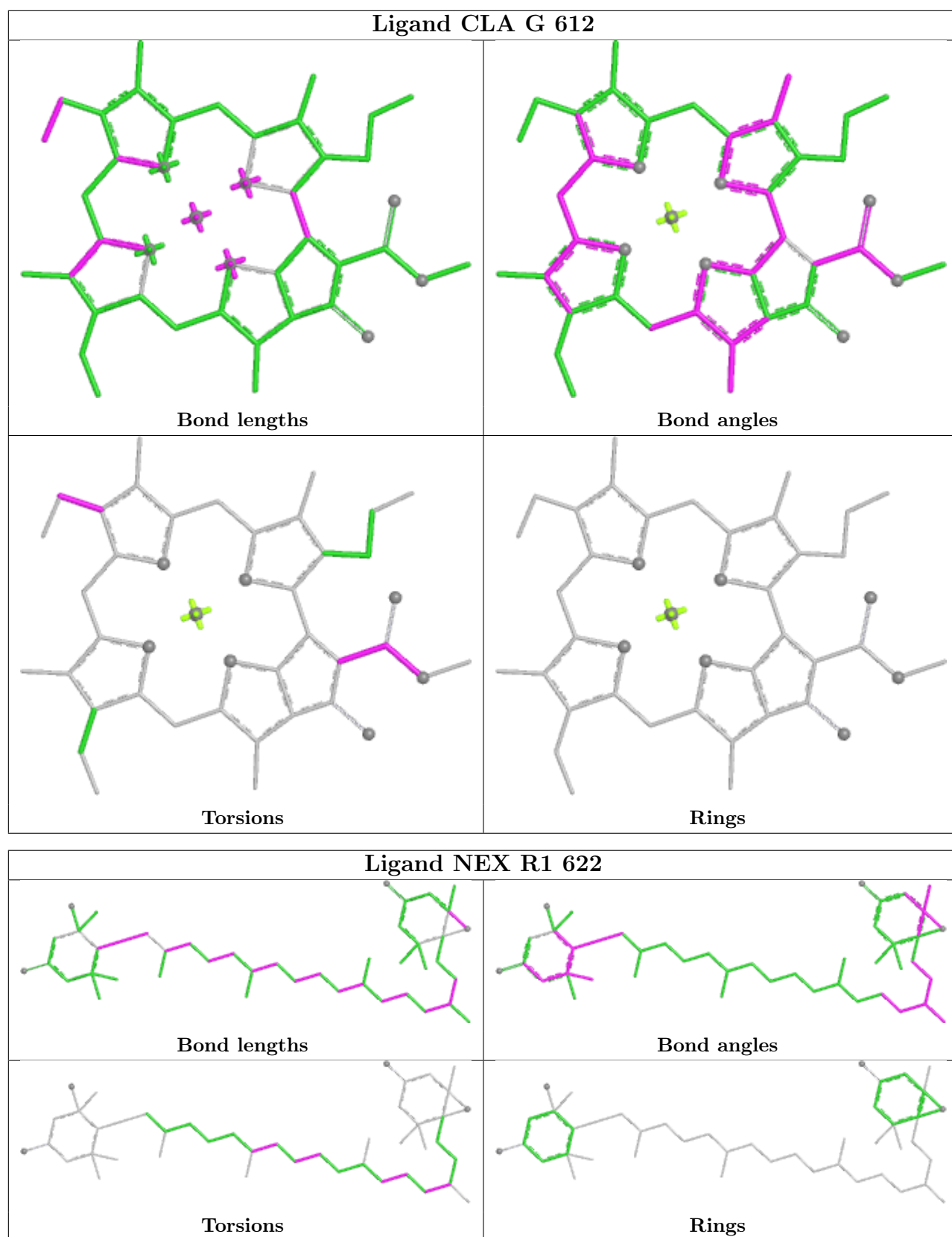


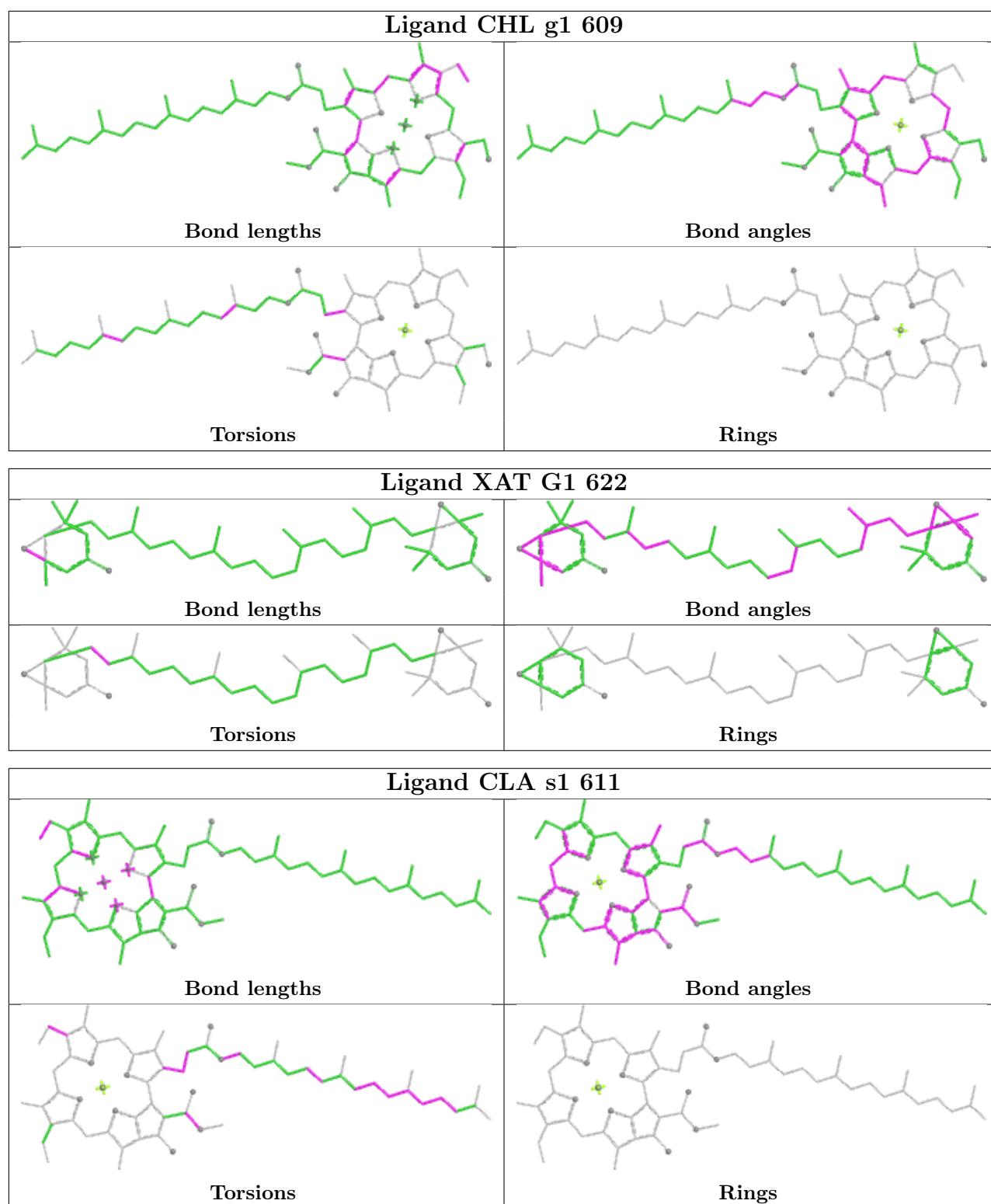


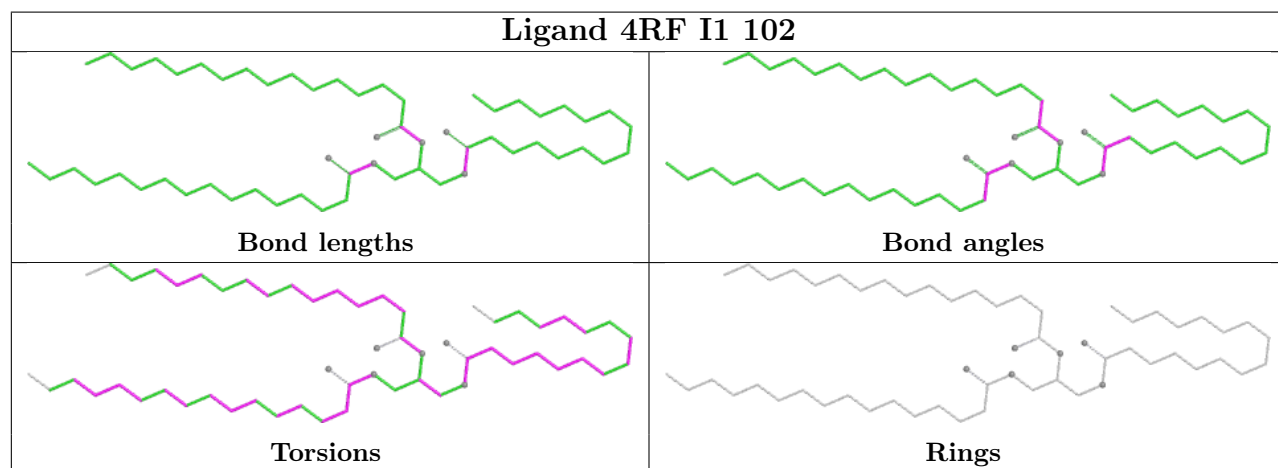
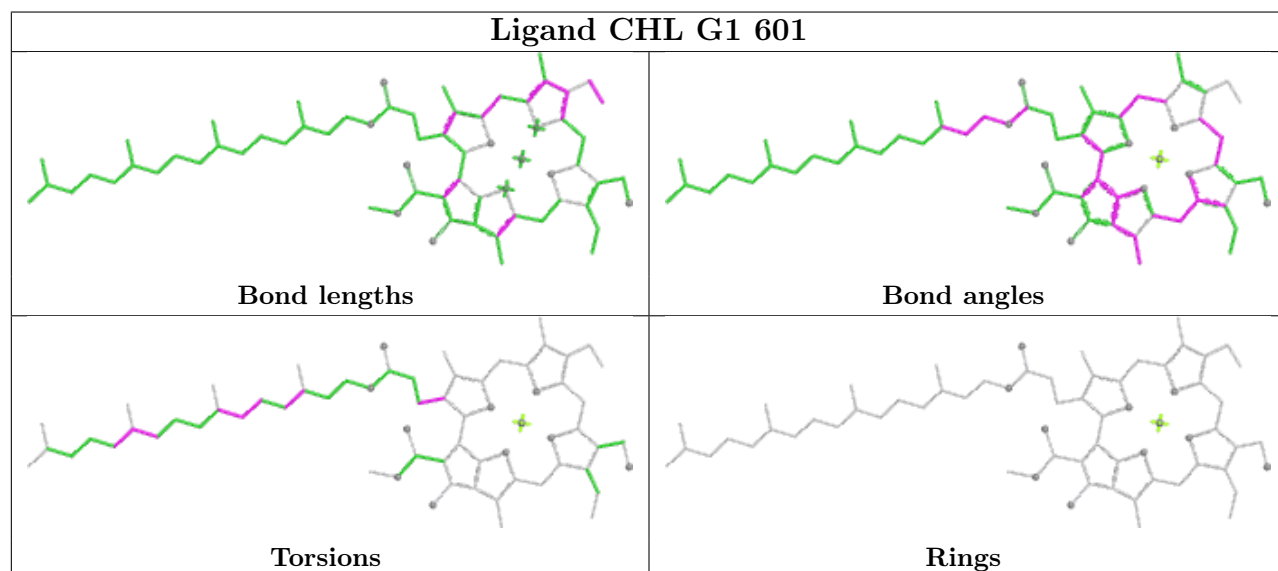
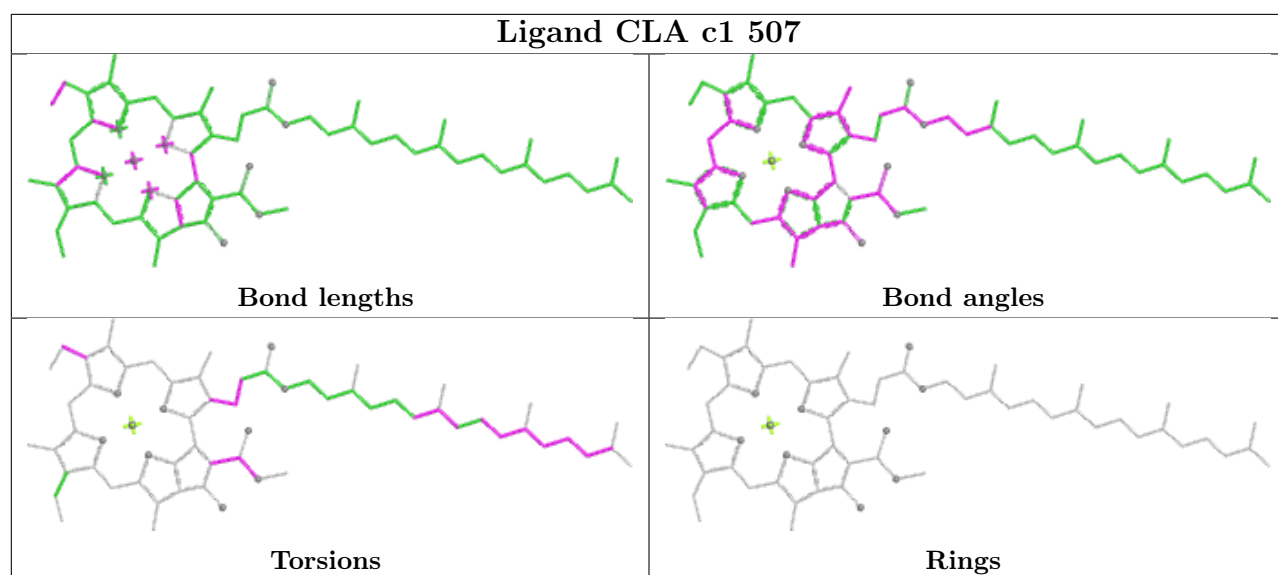


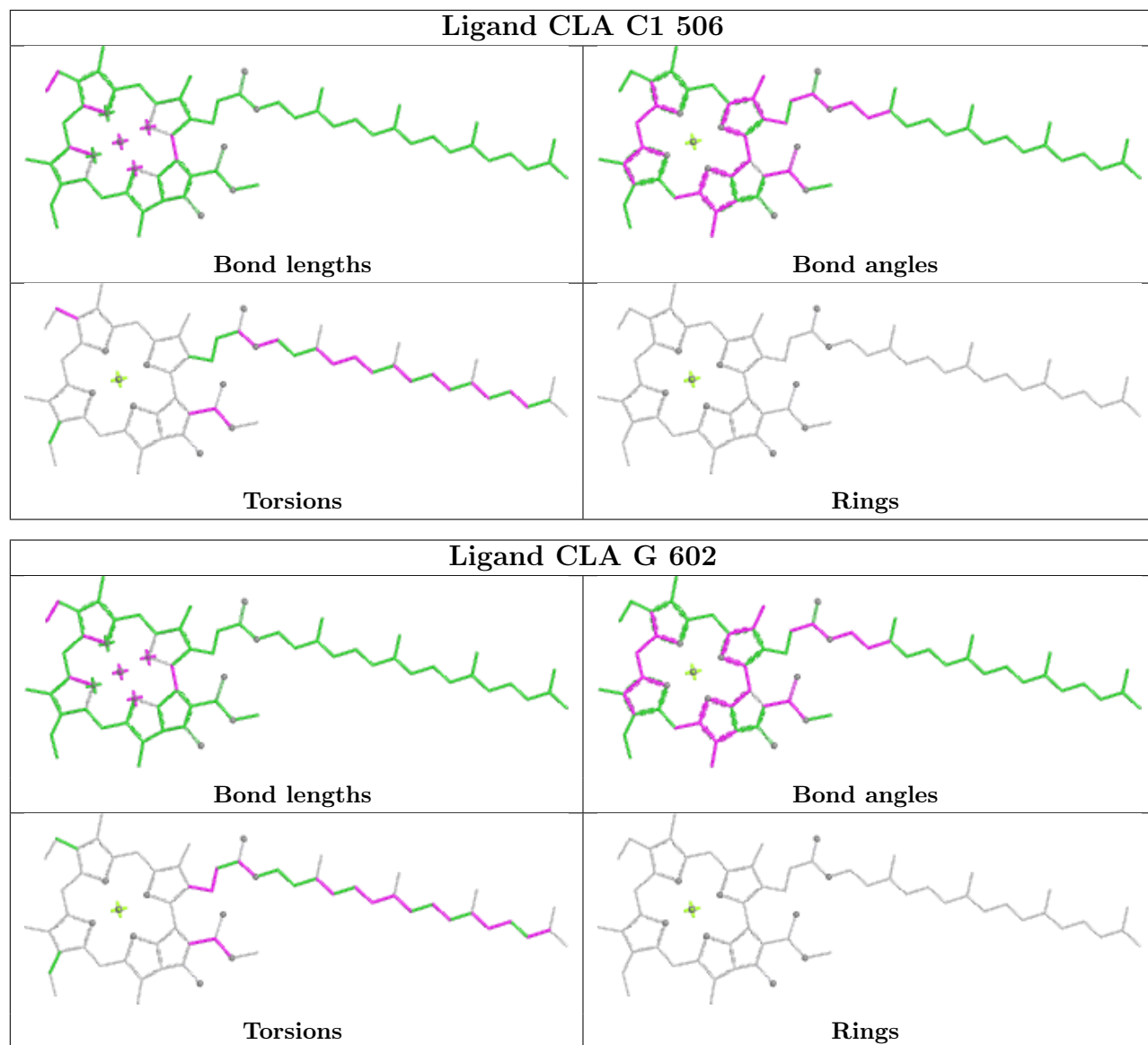
Ligand CLA Y1 602**Ligand HEM F 101**

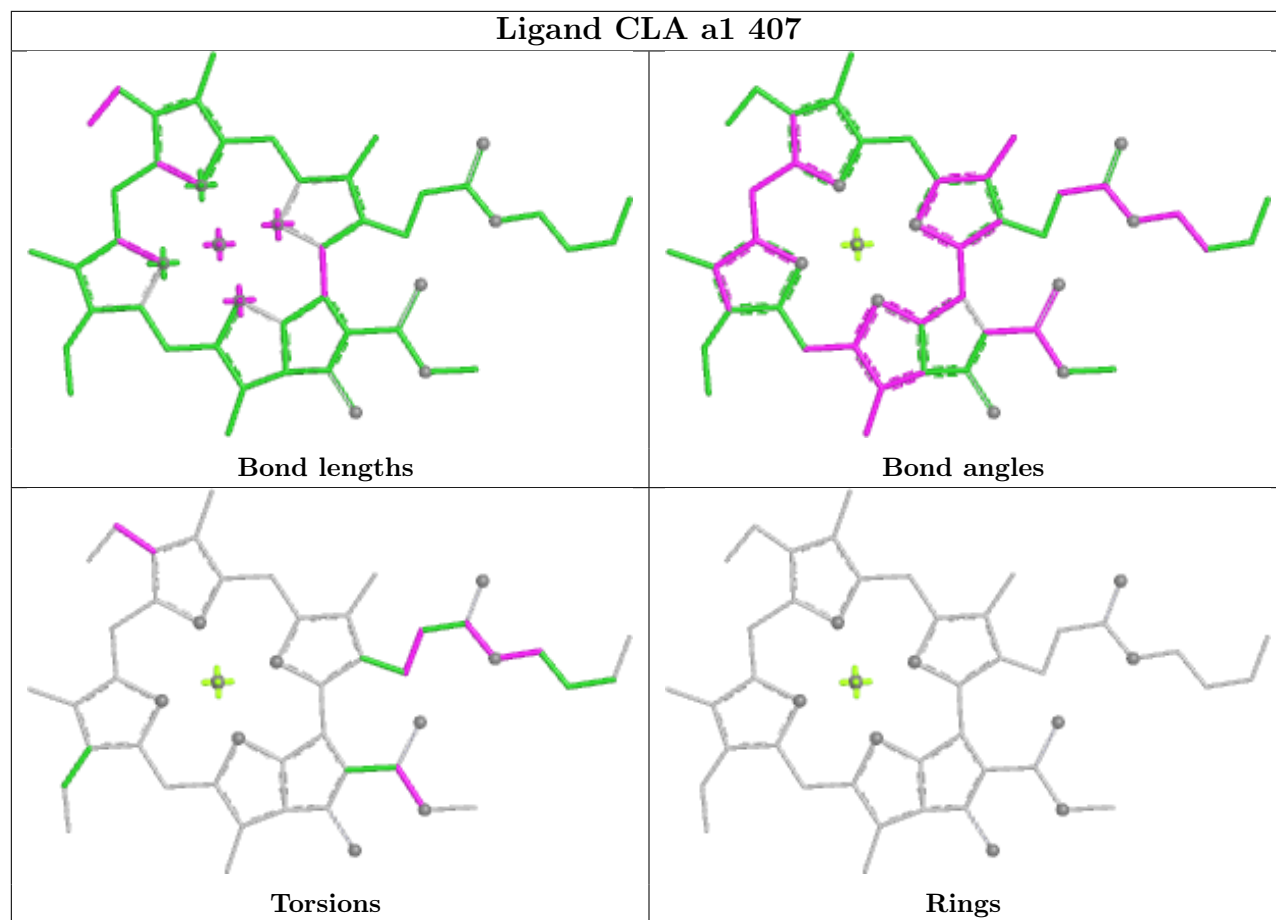


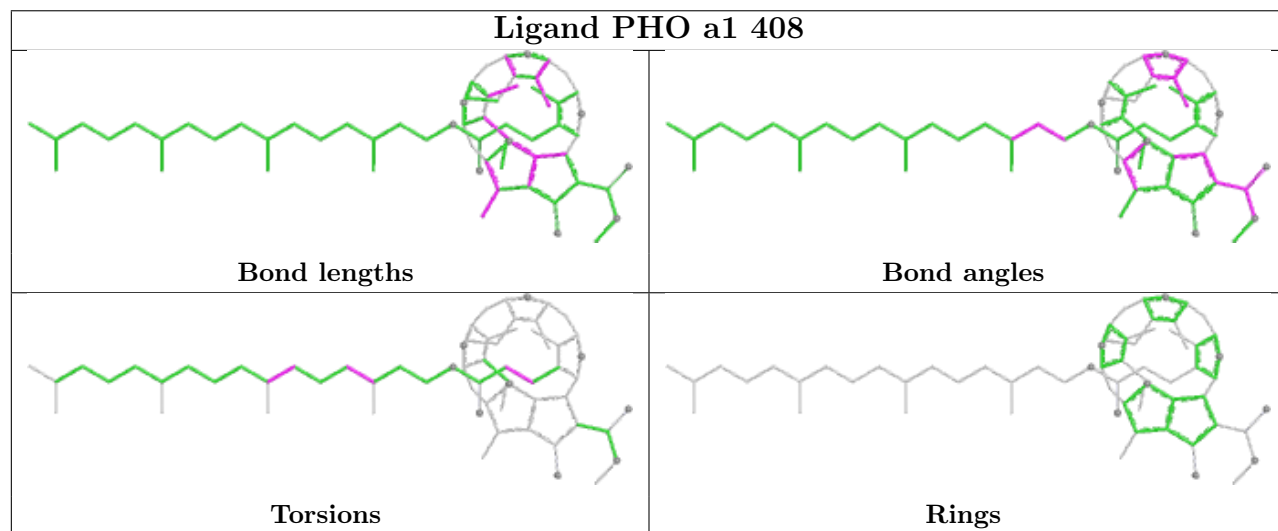
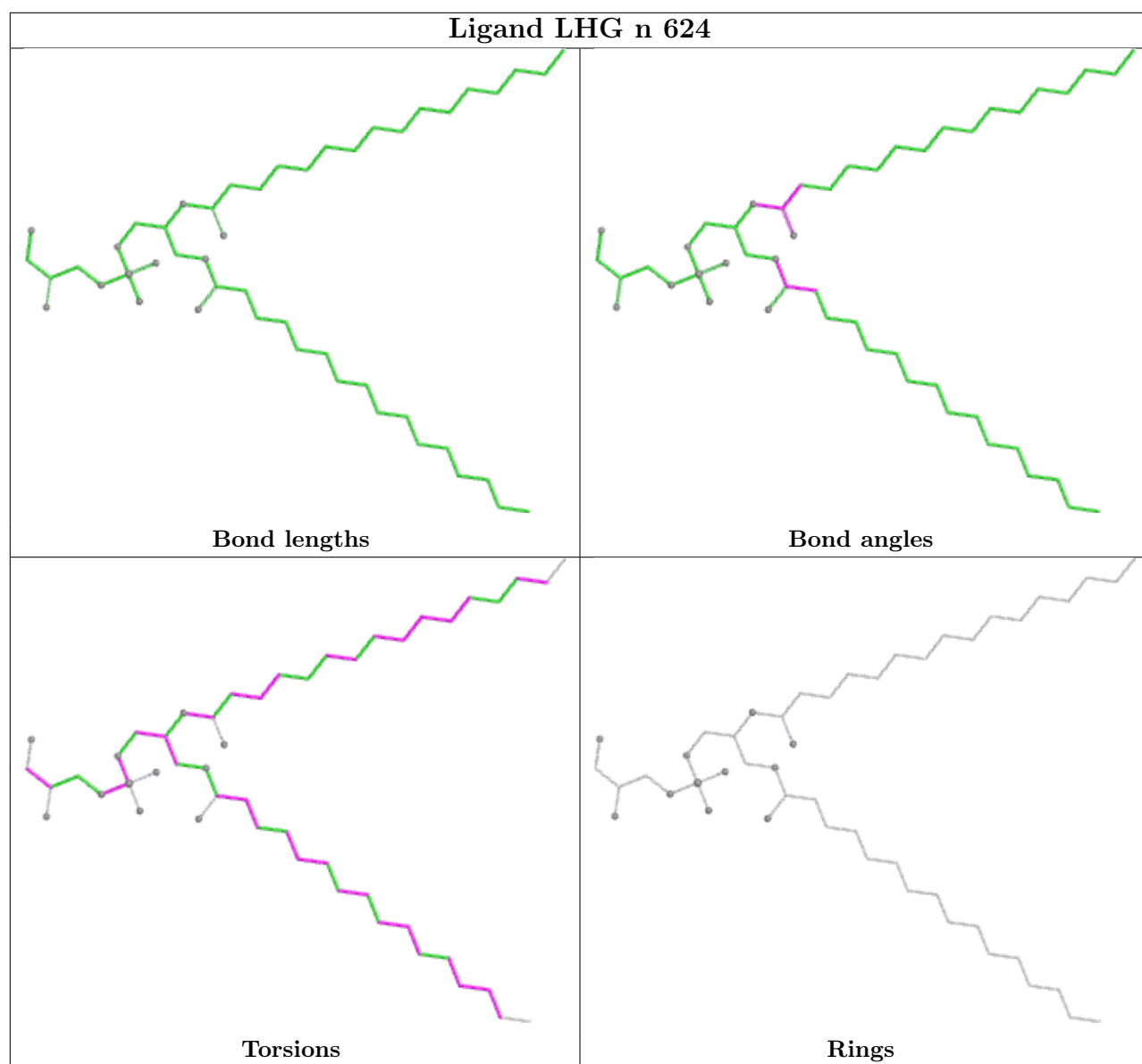


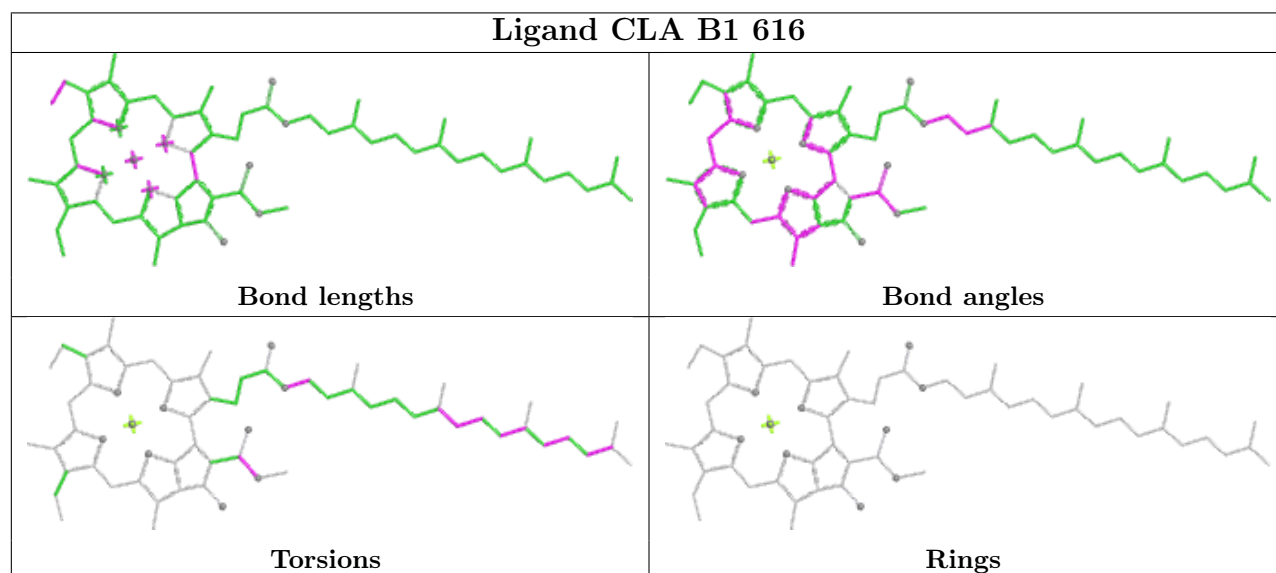
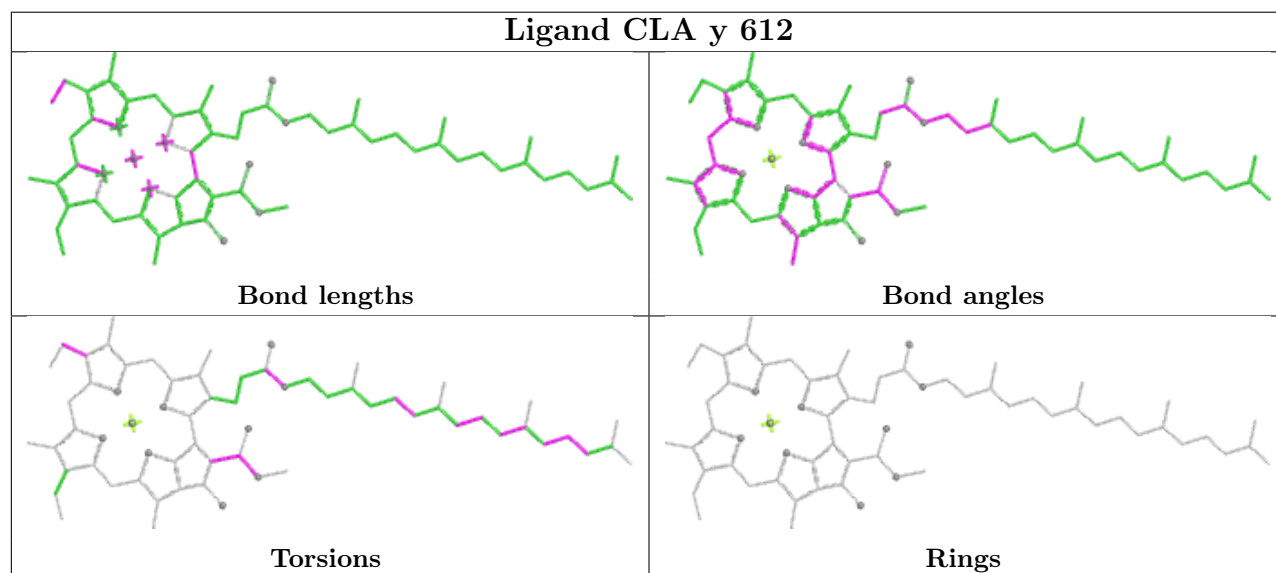
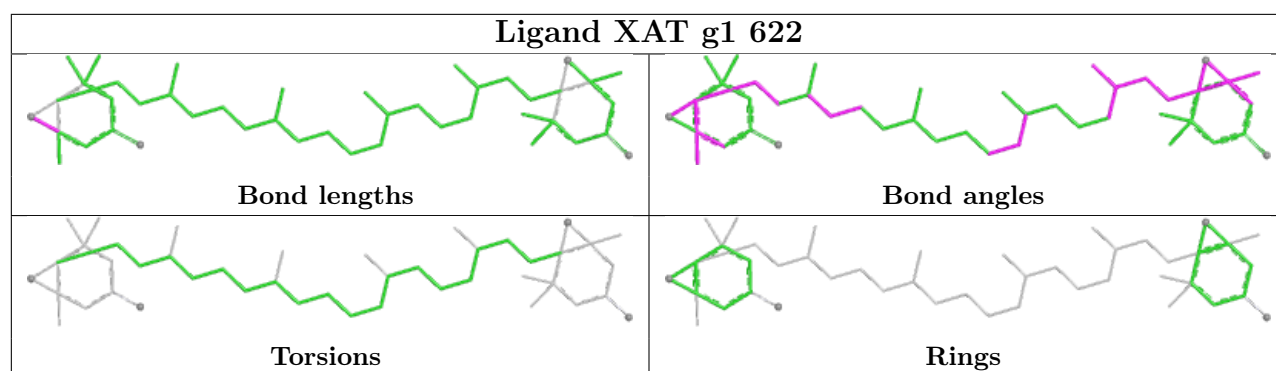


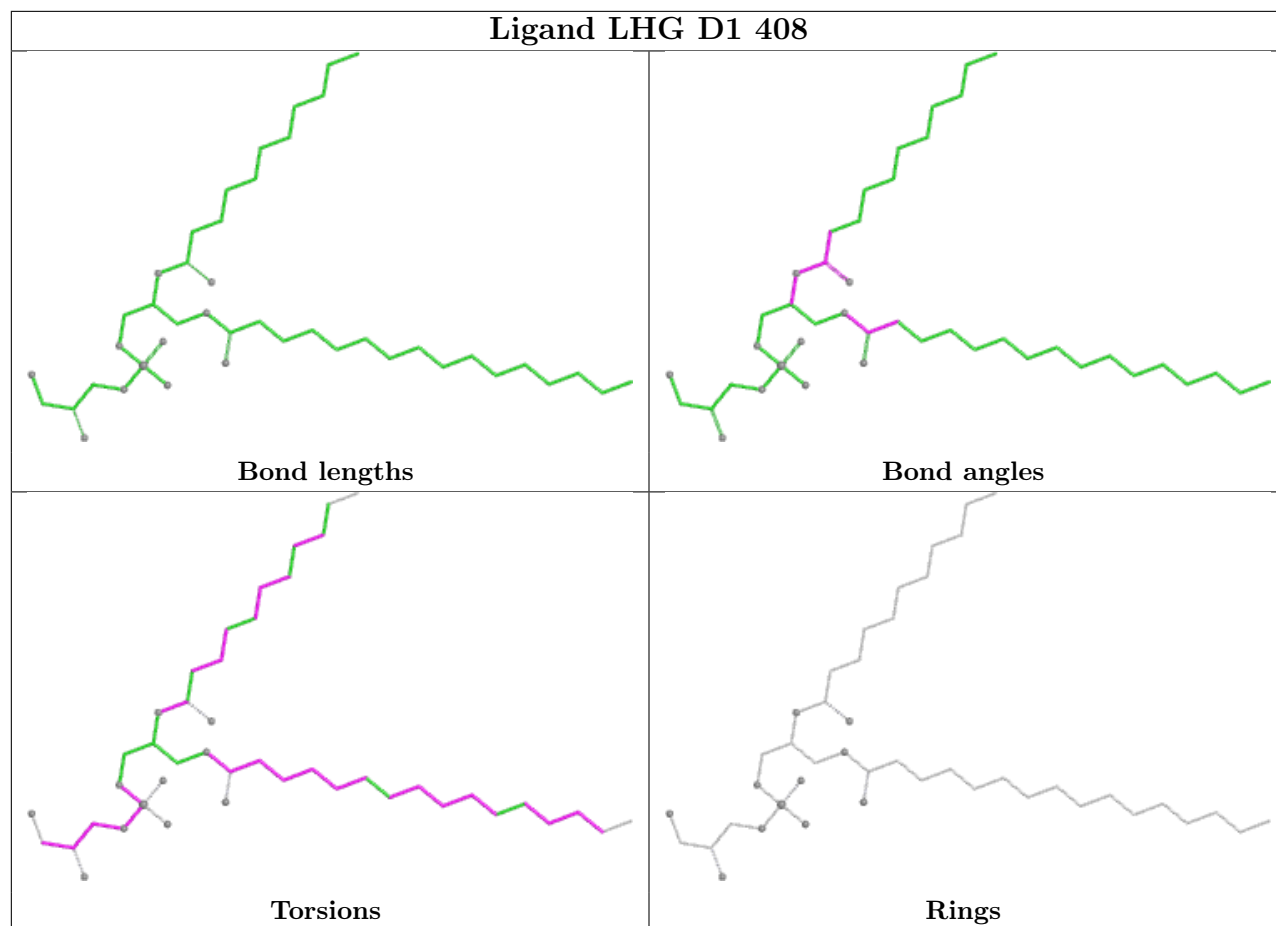




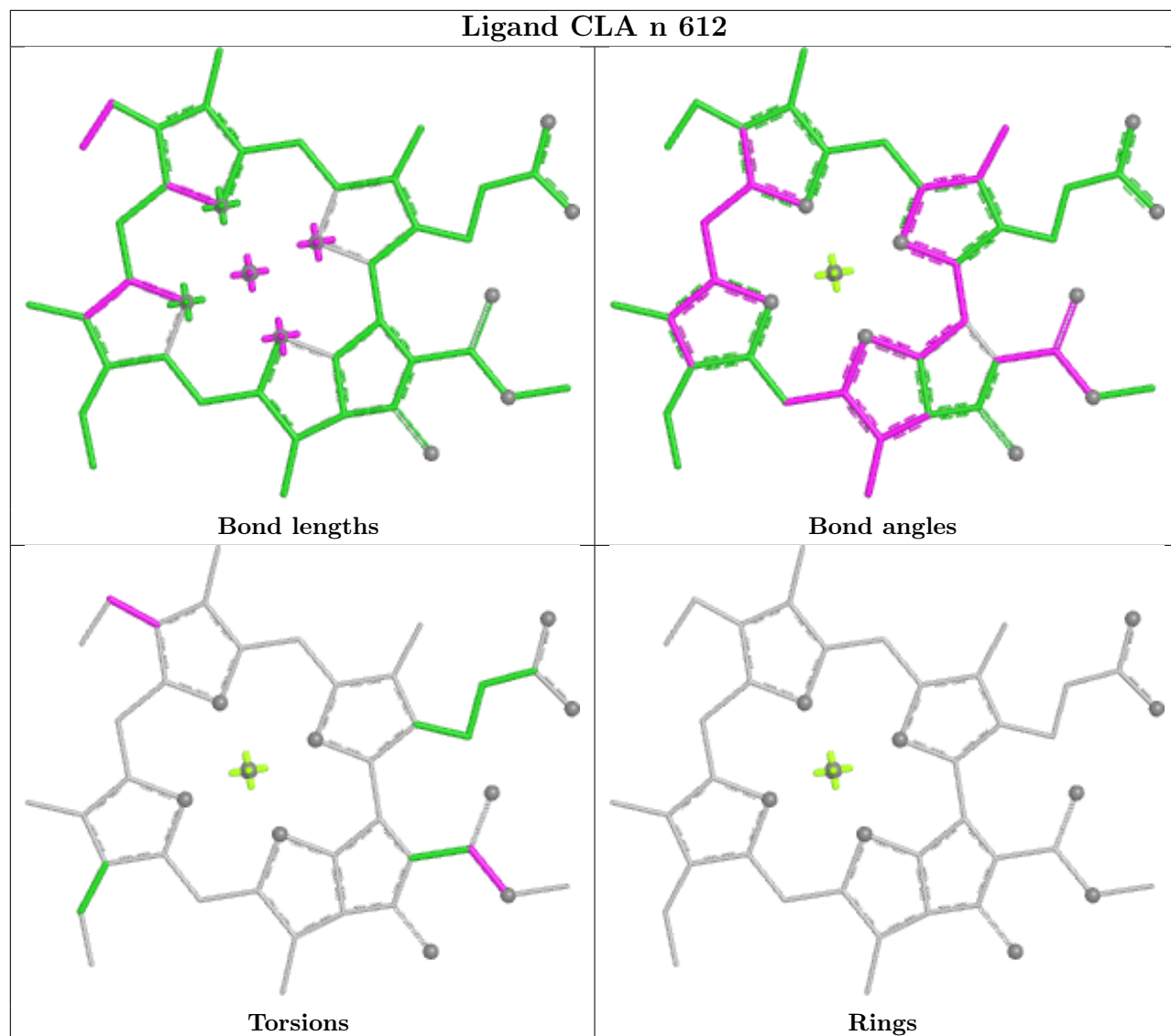




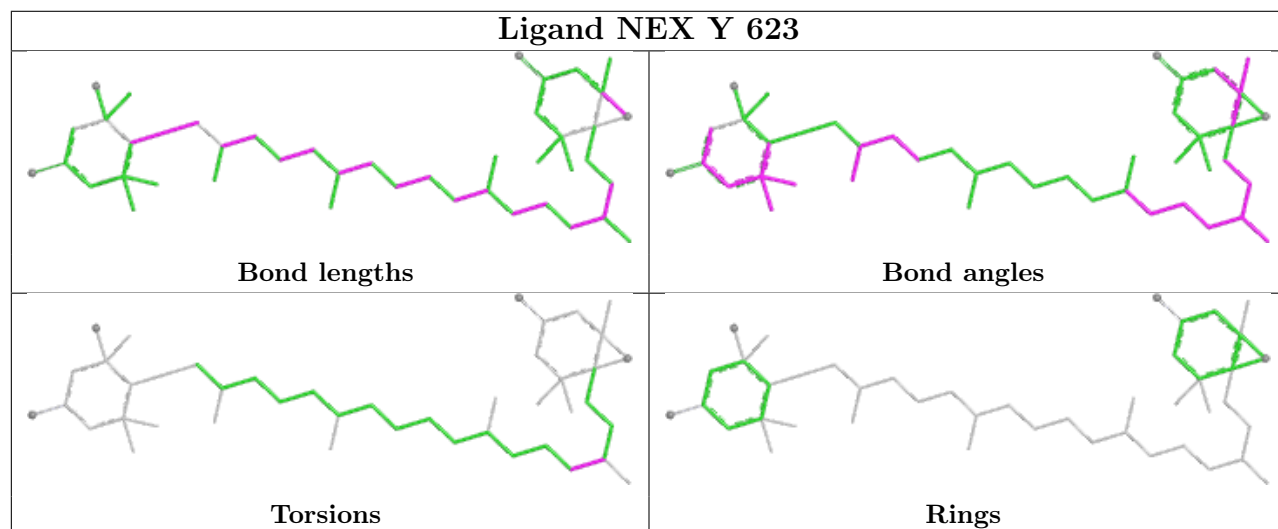


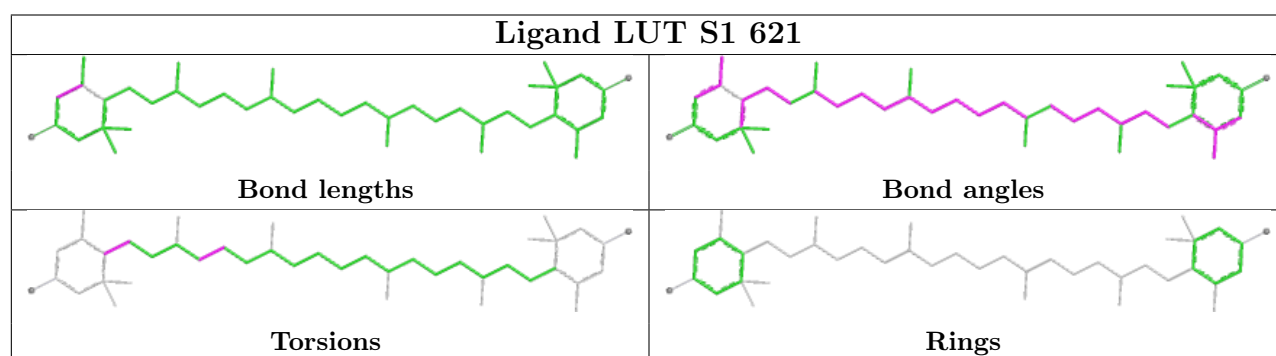
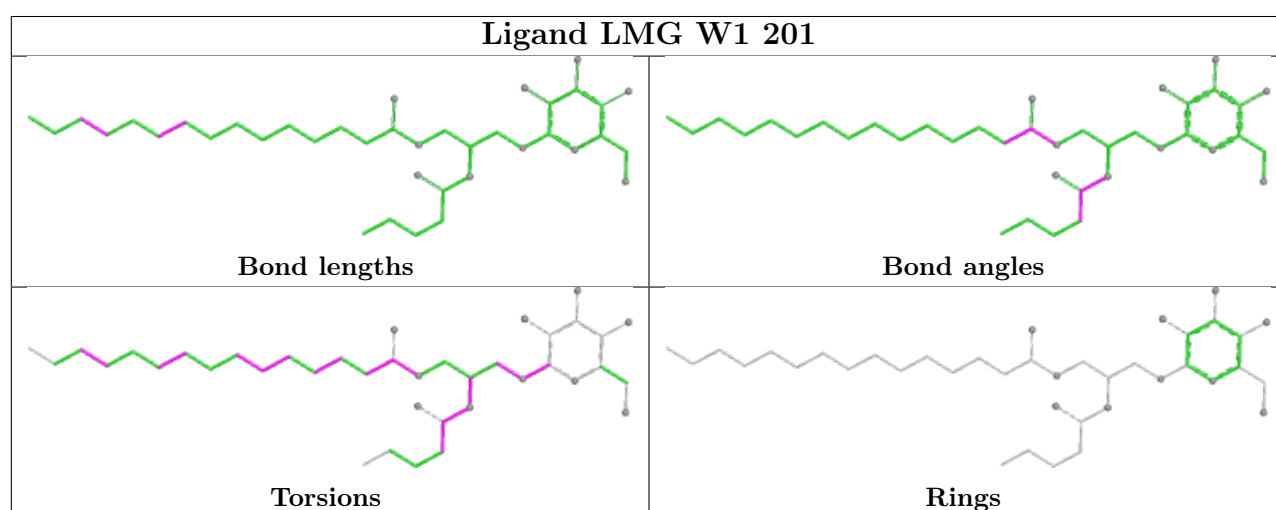
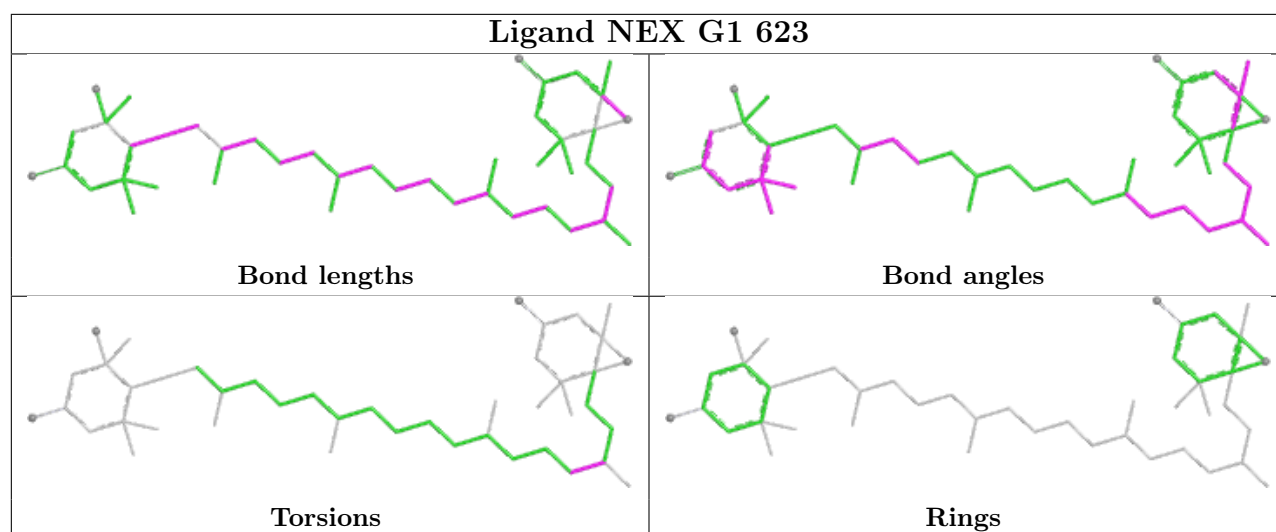


Ligand CLA n 612

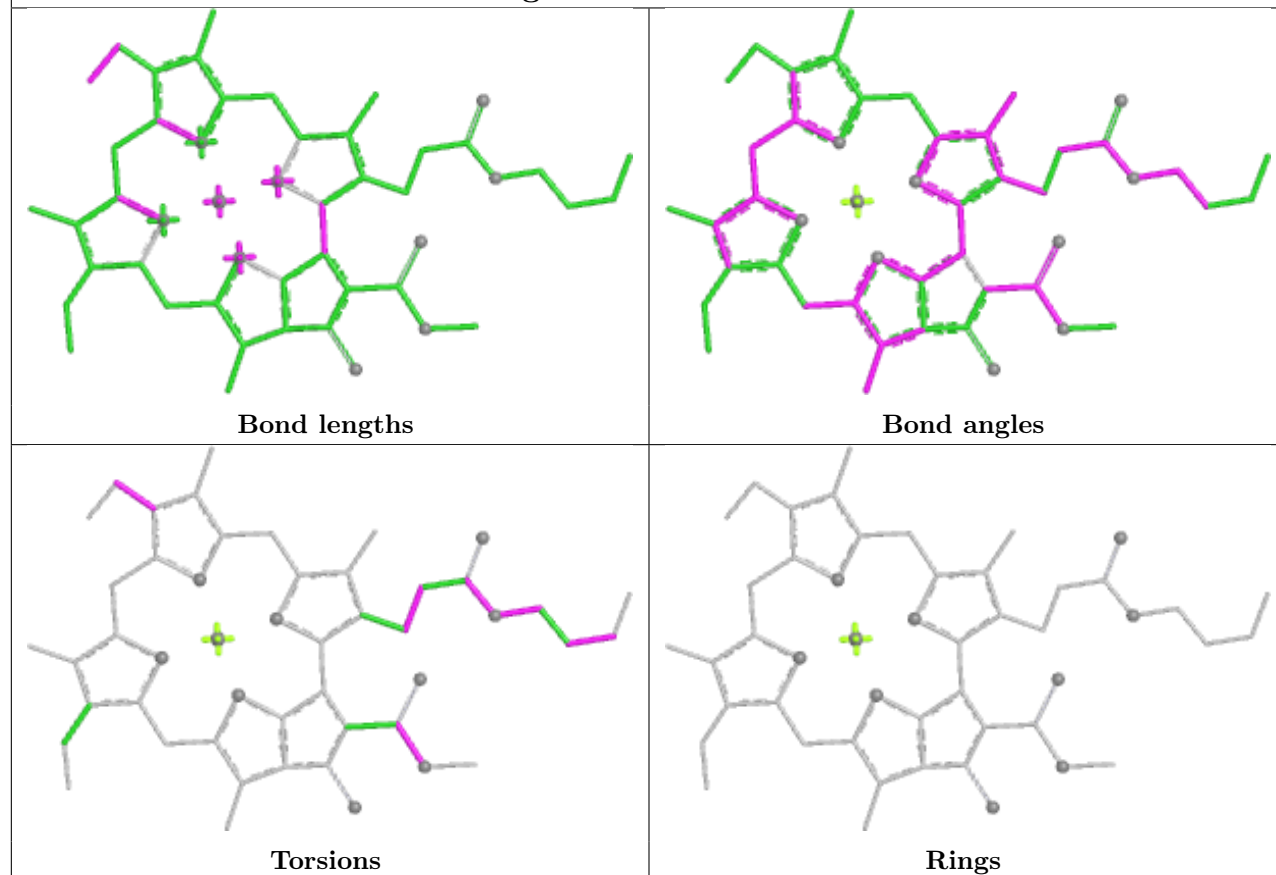


Ligand NEX Y 623

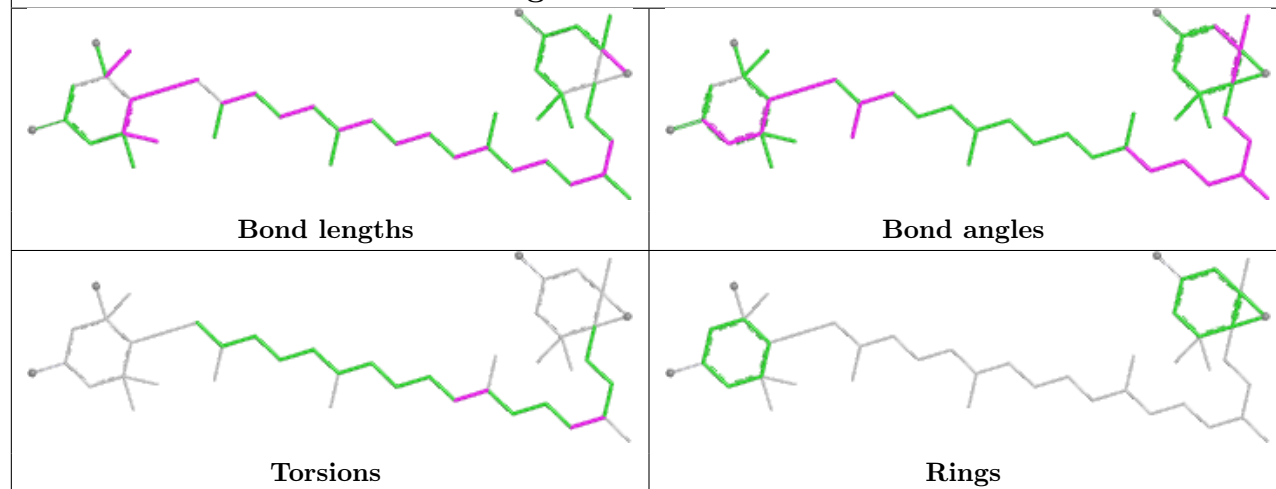


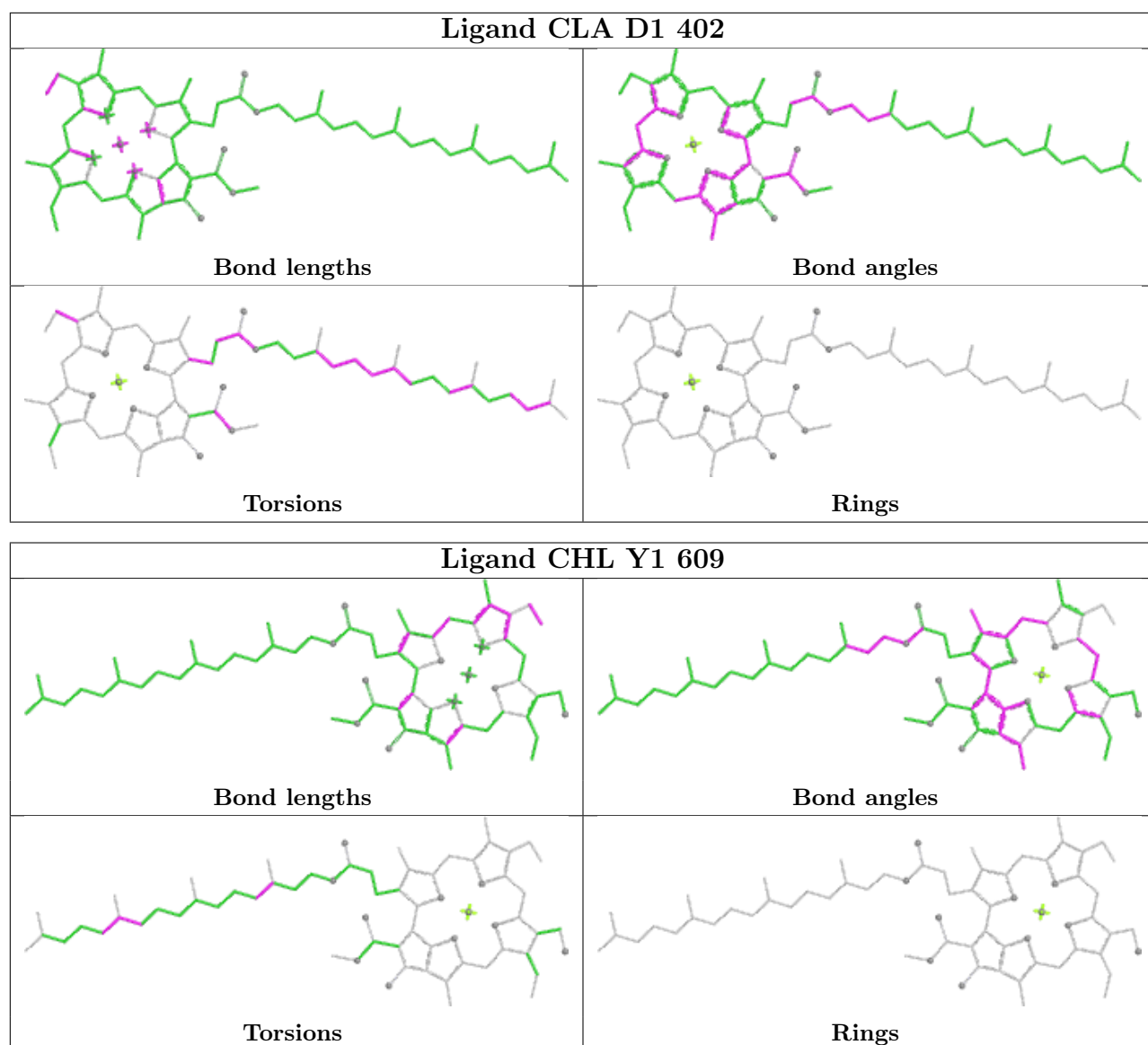


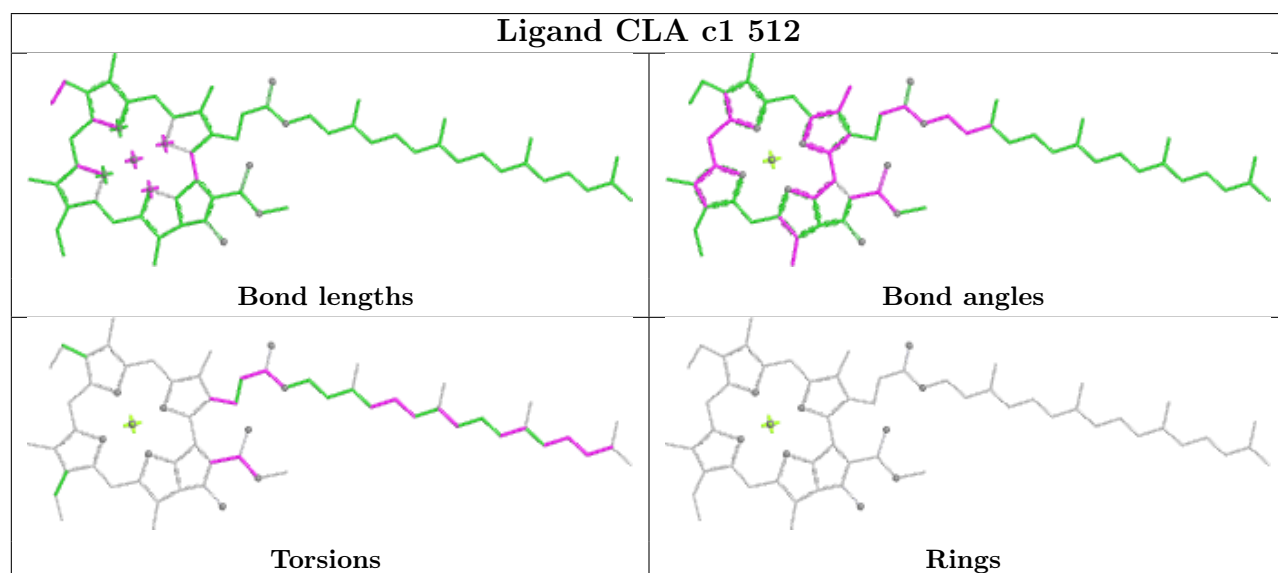
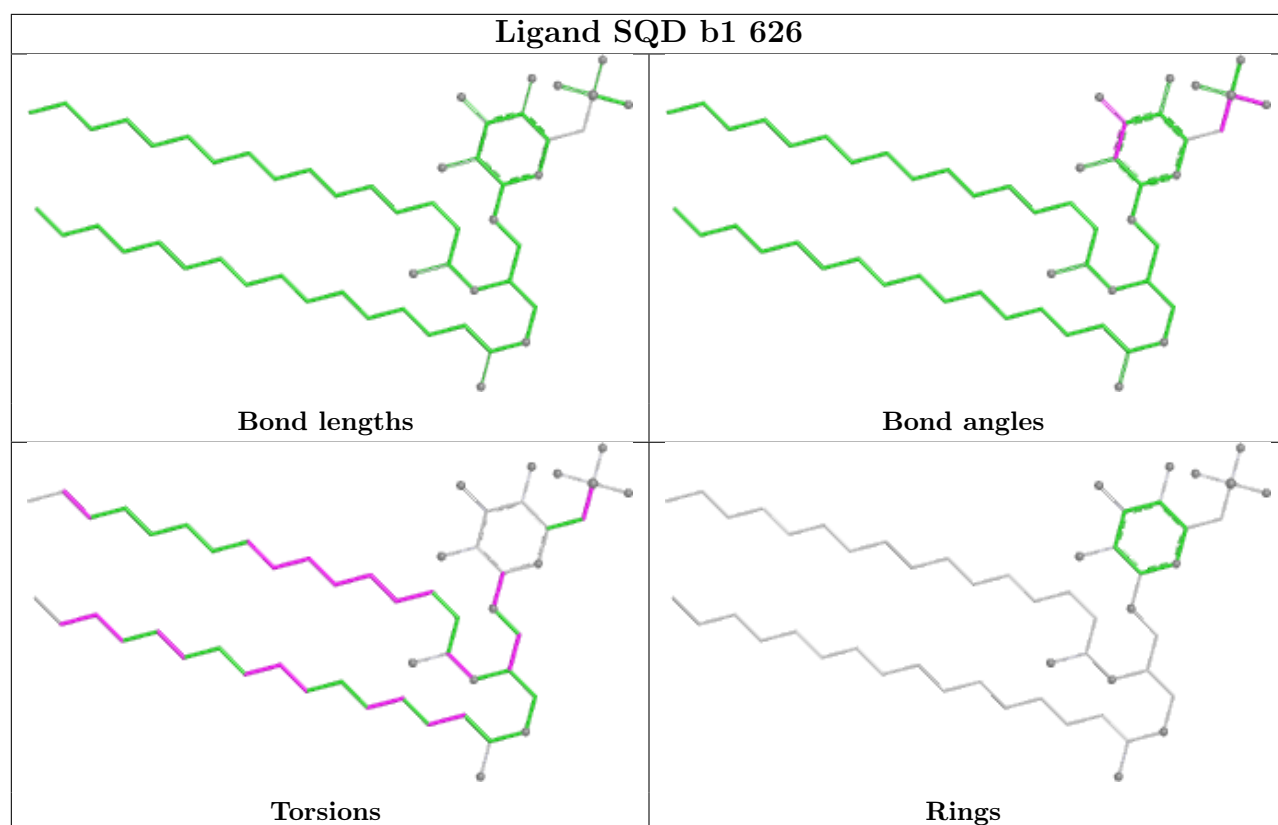
Ligand CLA N1 611

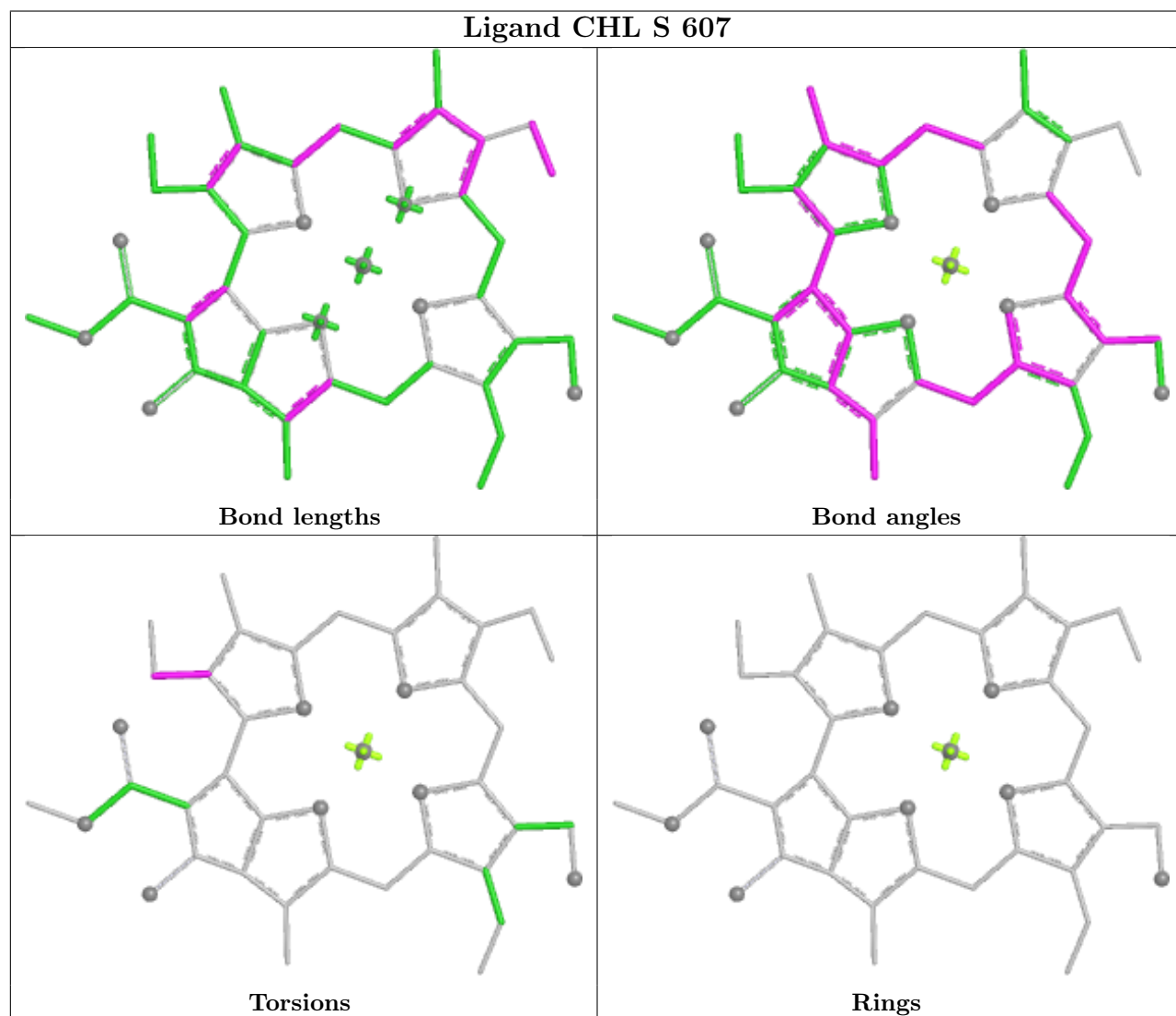
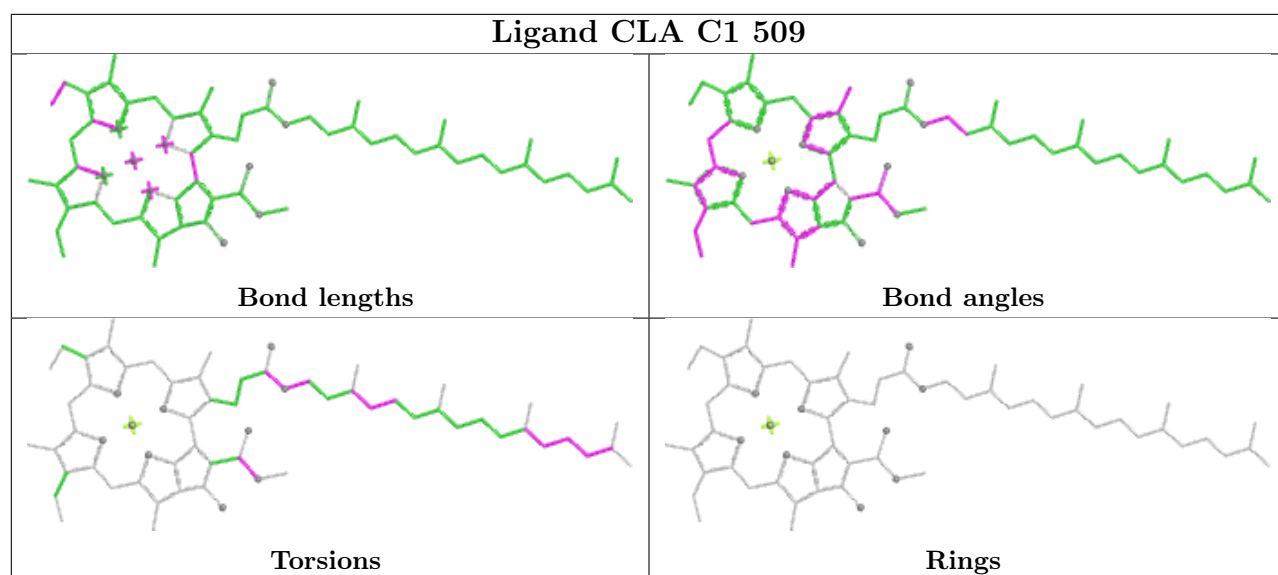


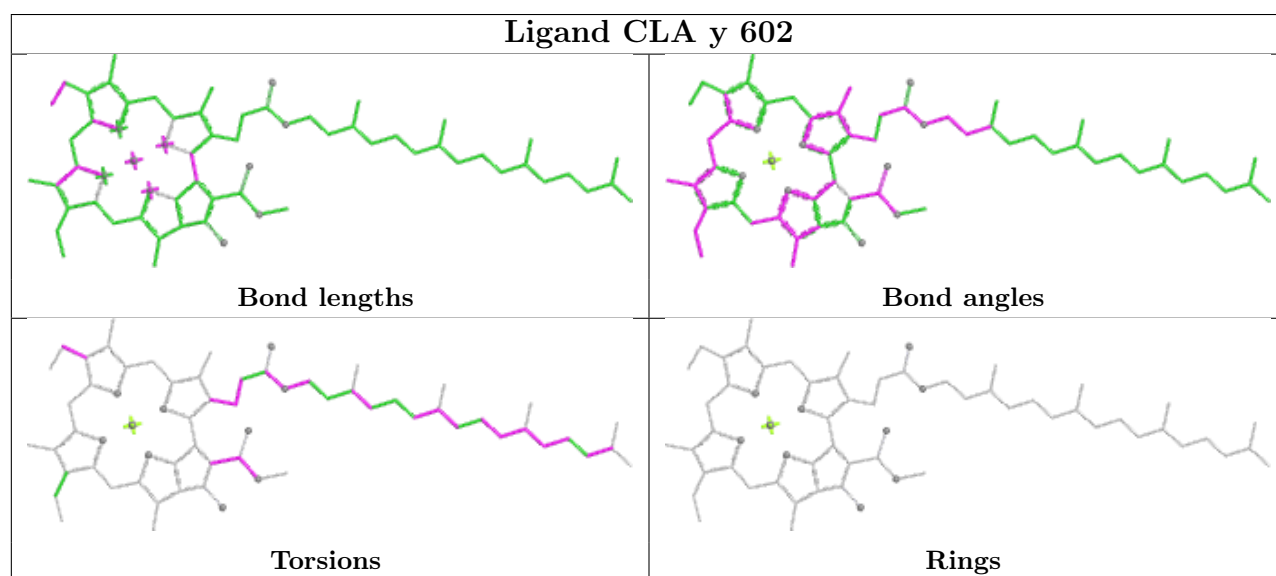
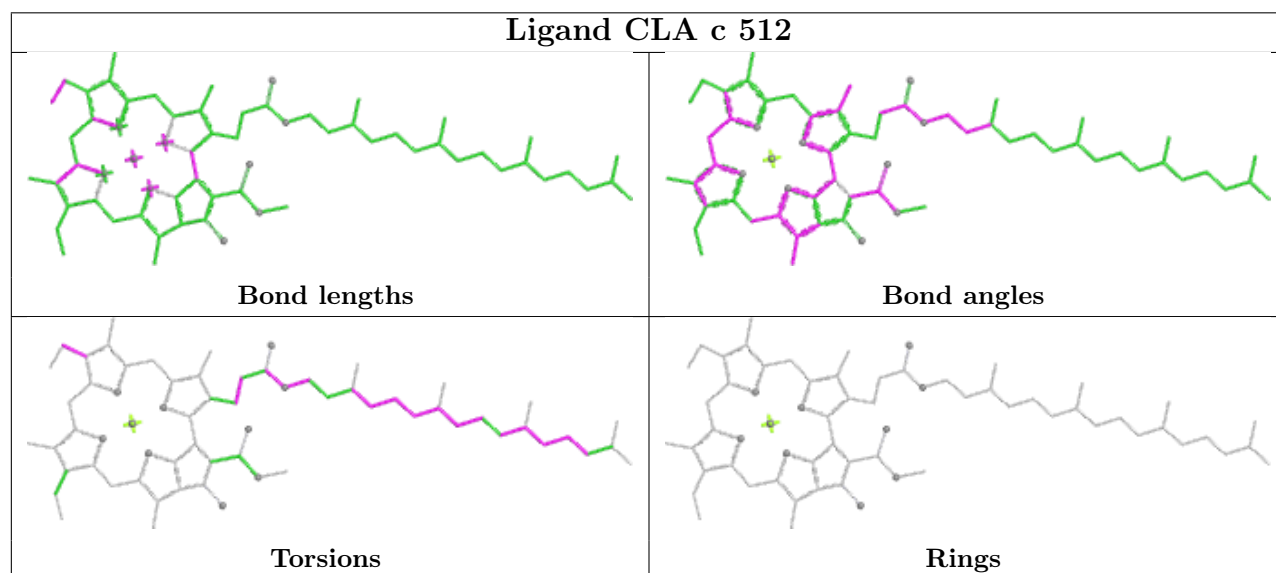
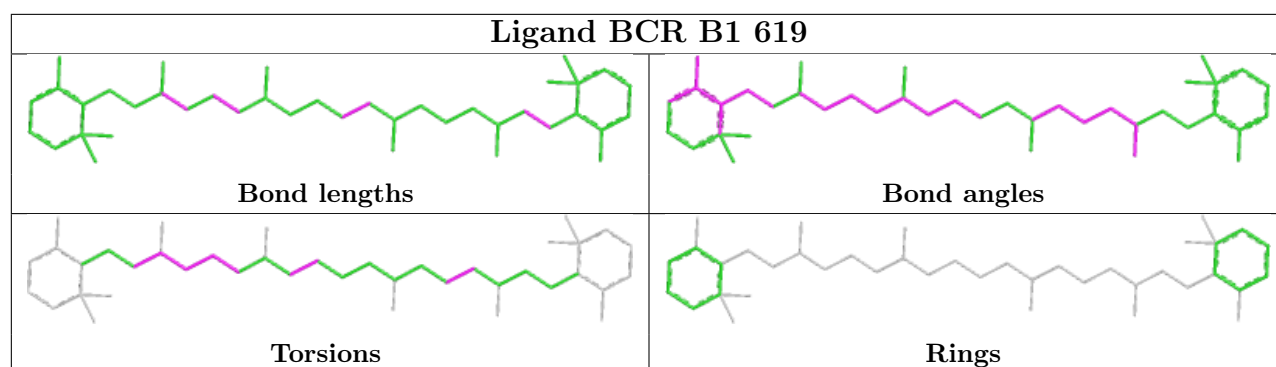
Ligand NEX s1 623



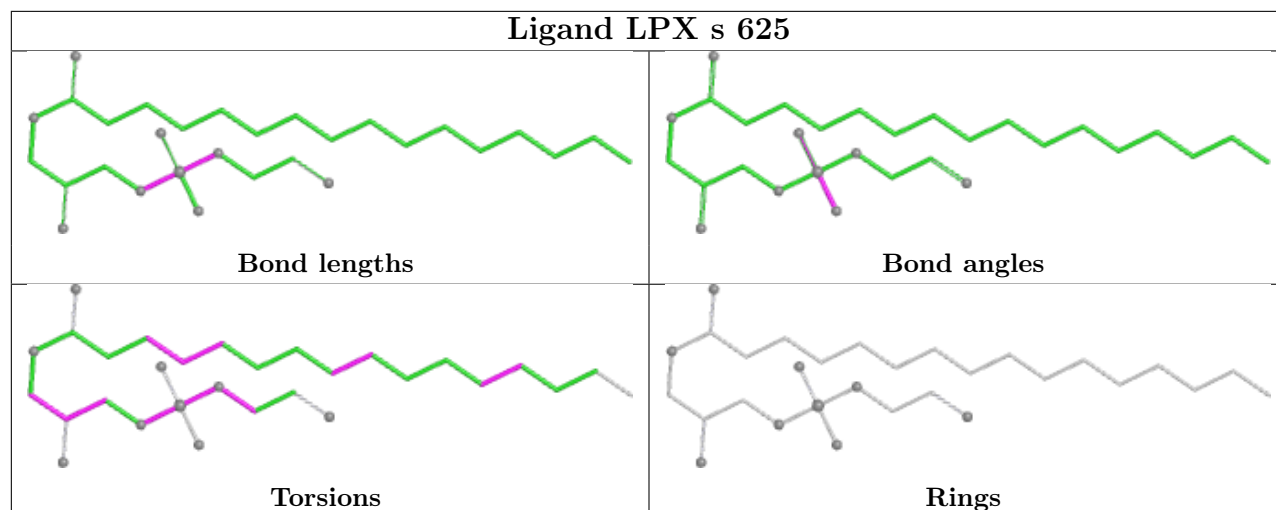




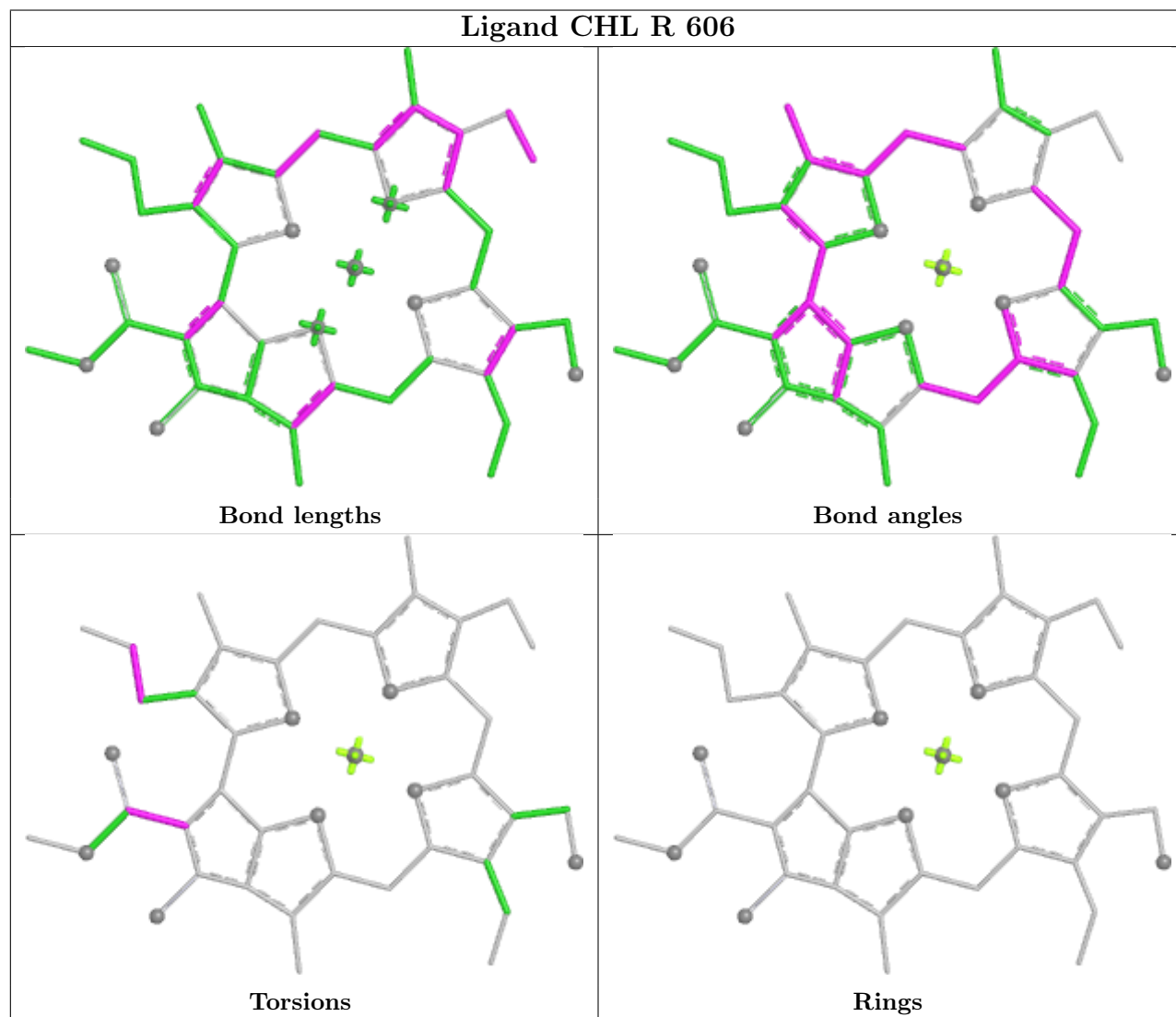


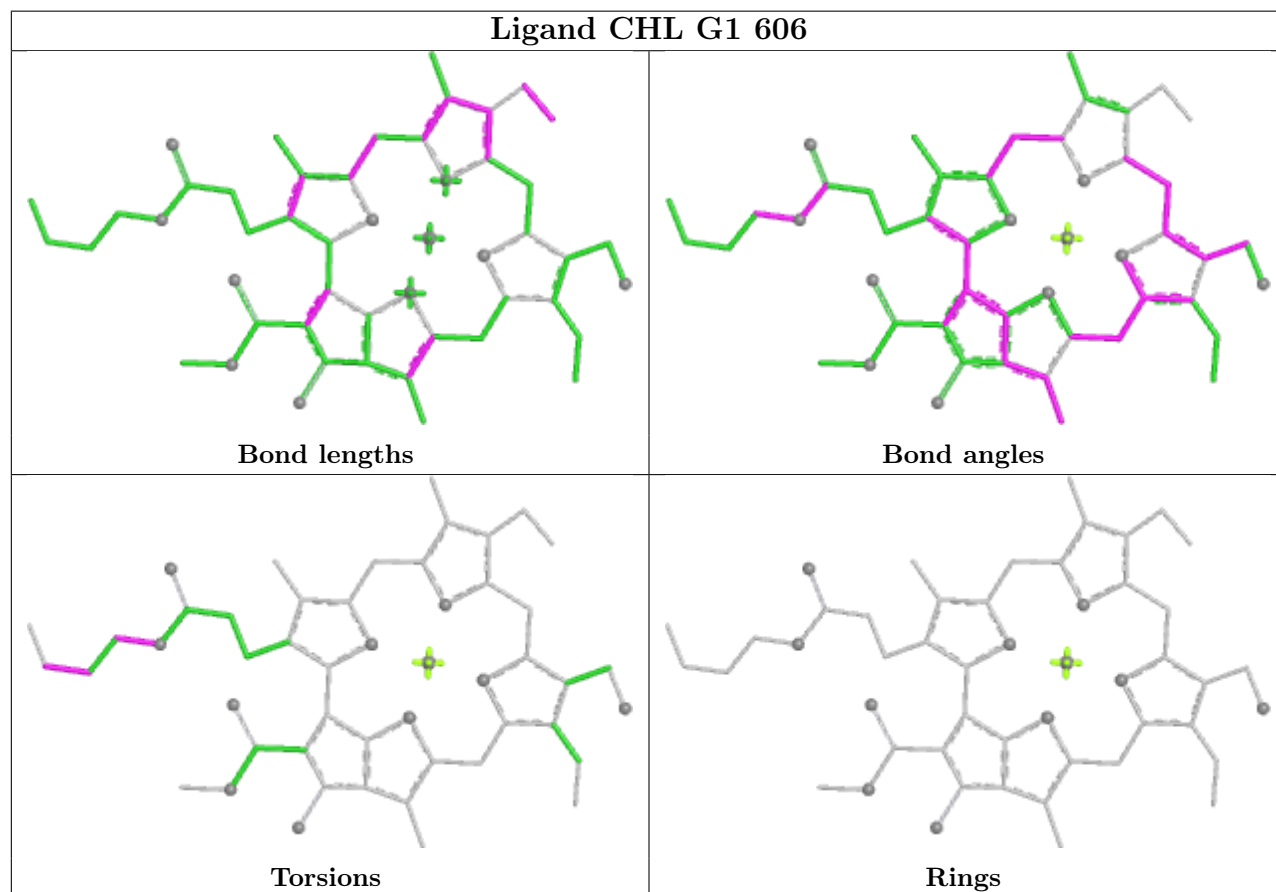
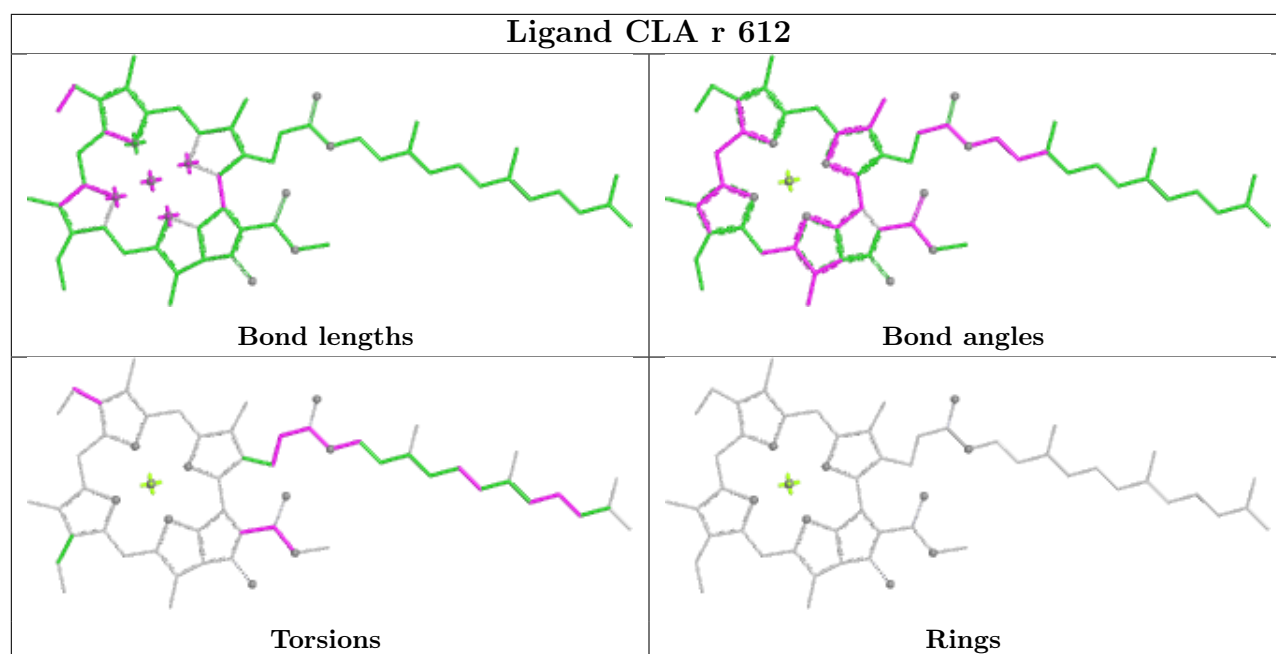


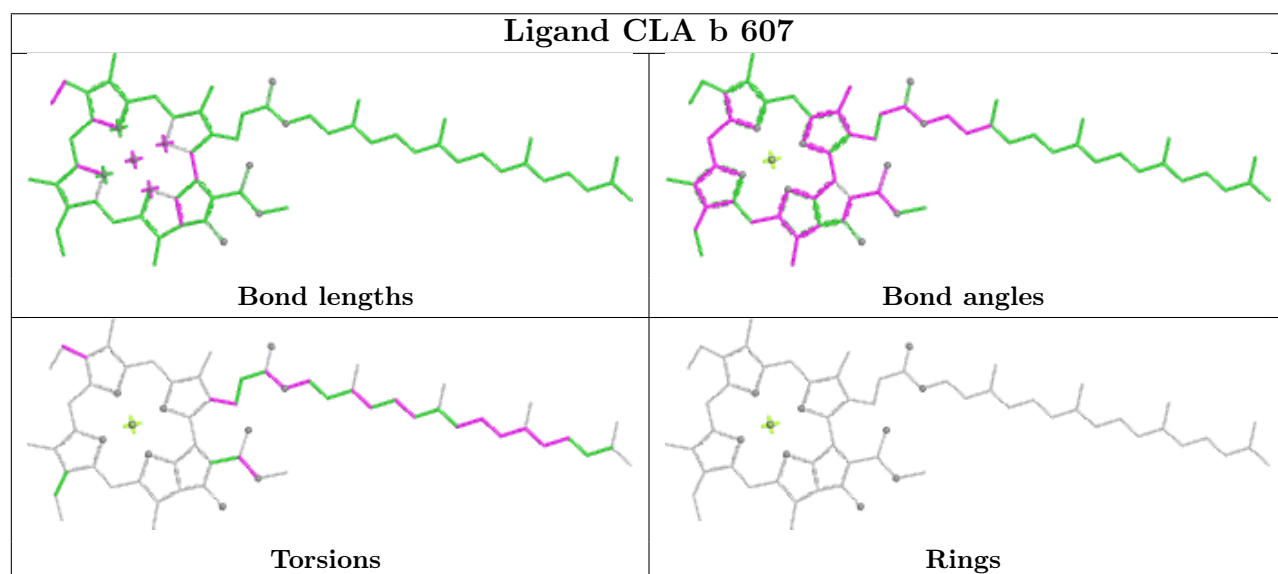
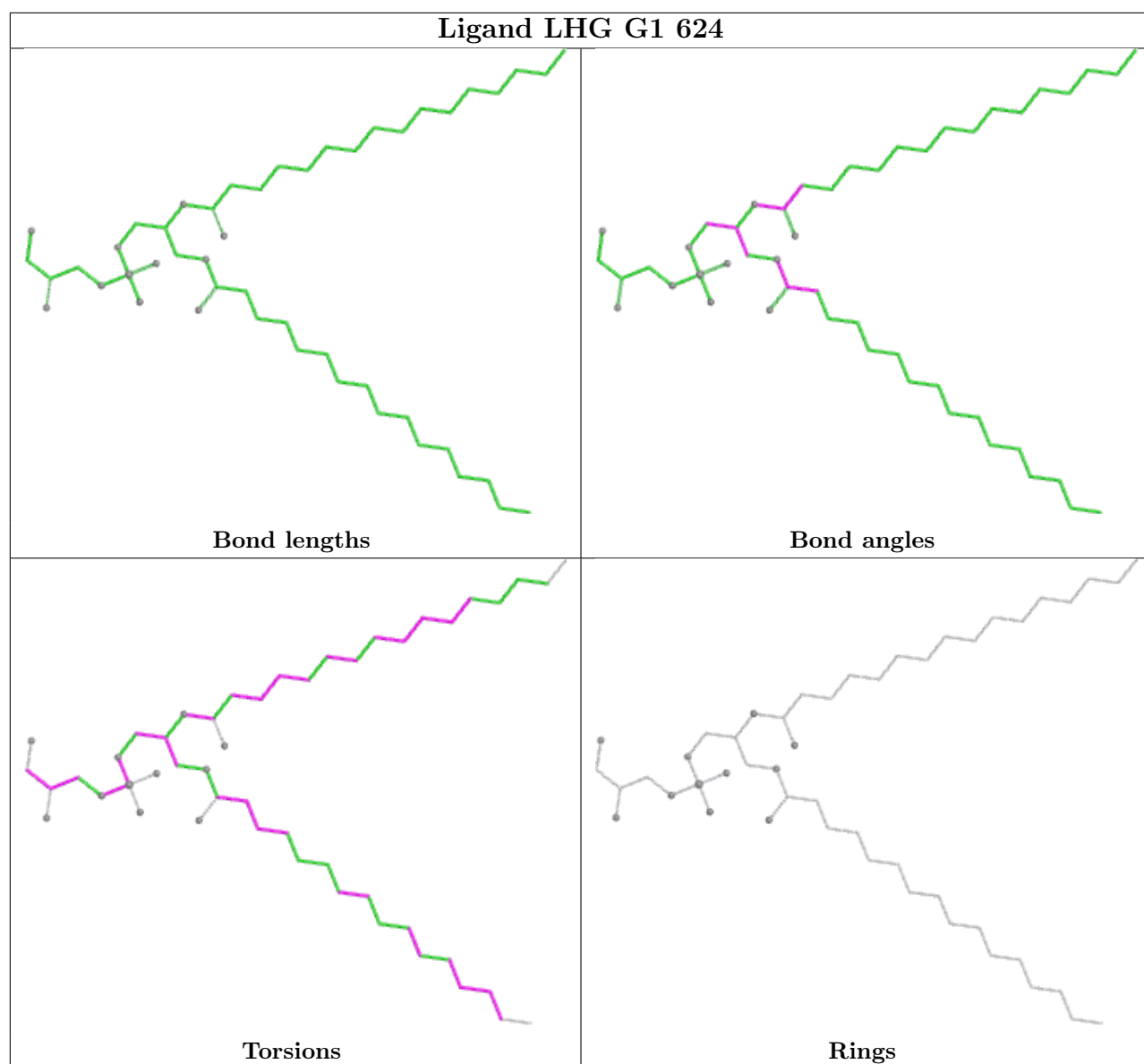
Ligand LPX s 625

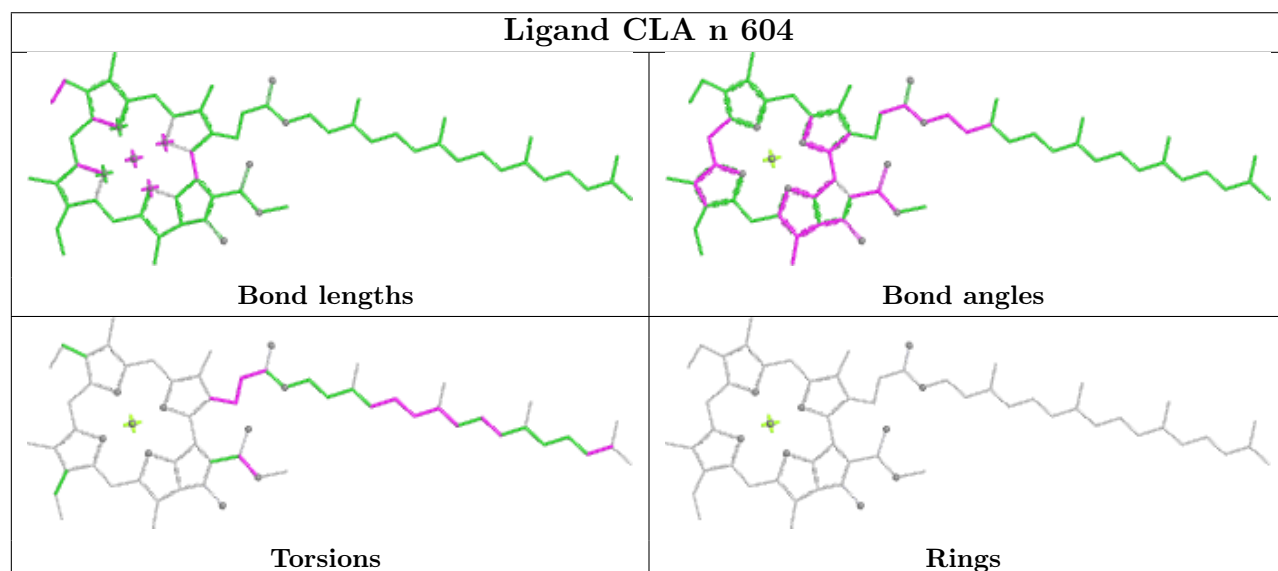
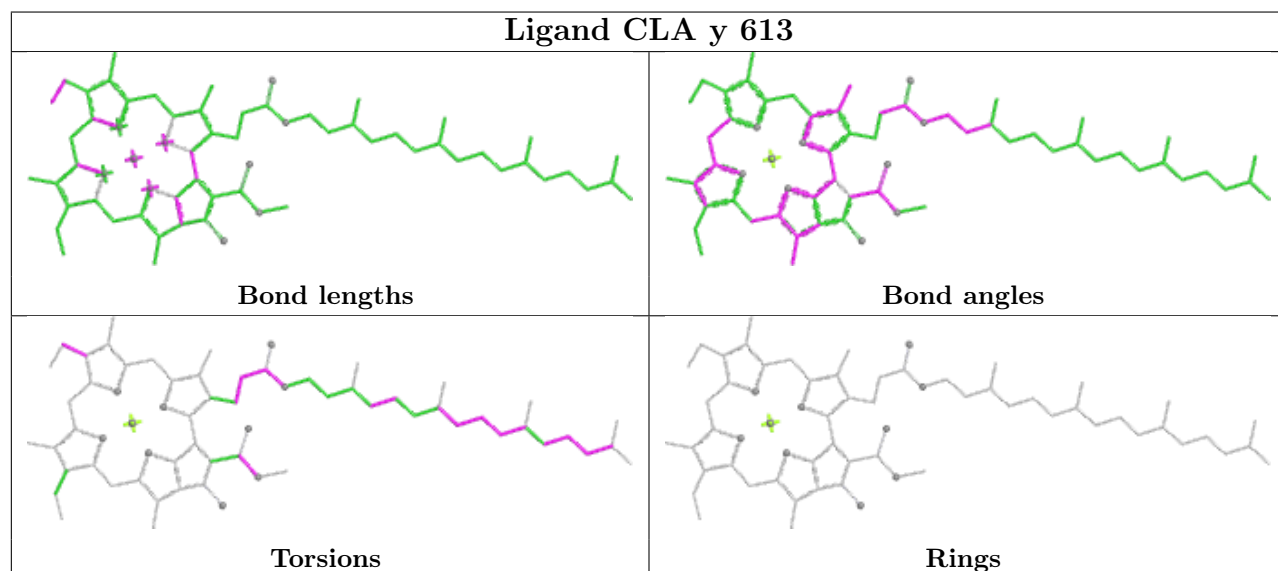
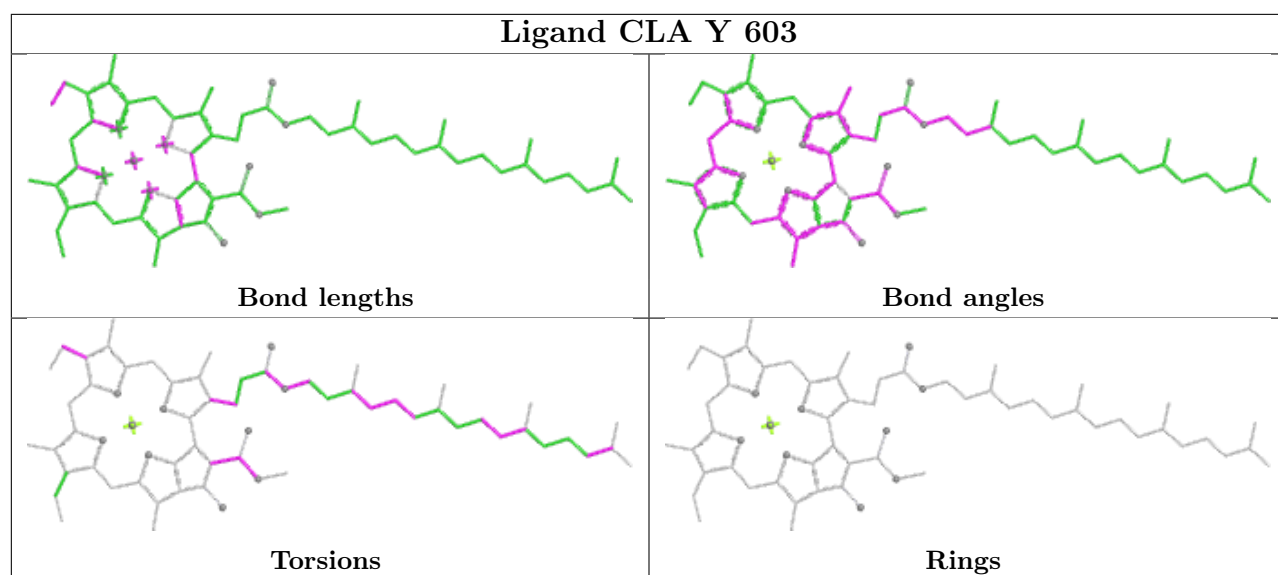


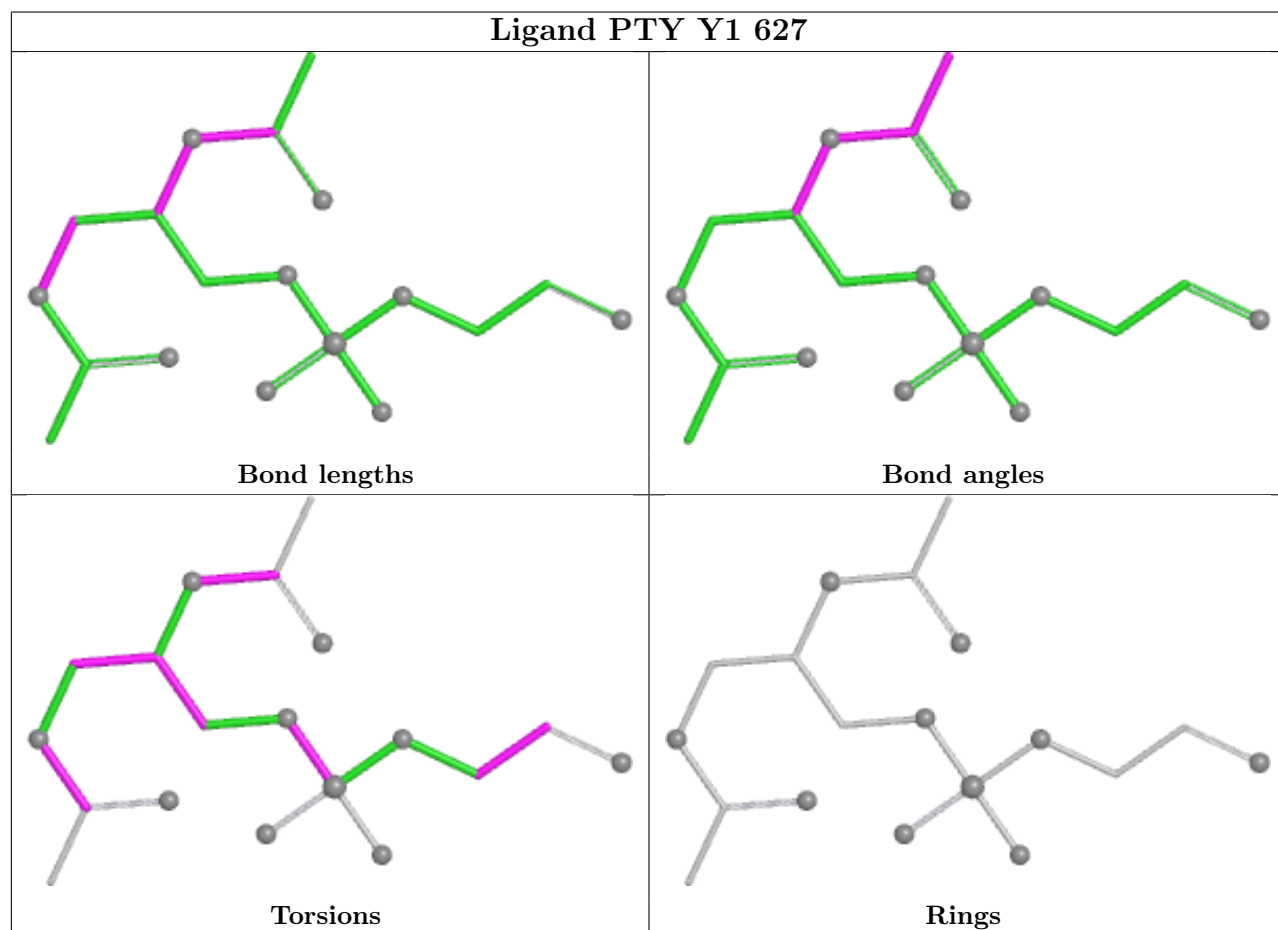
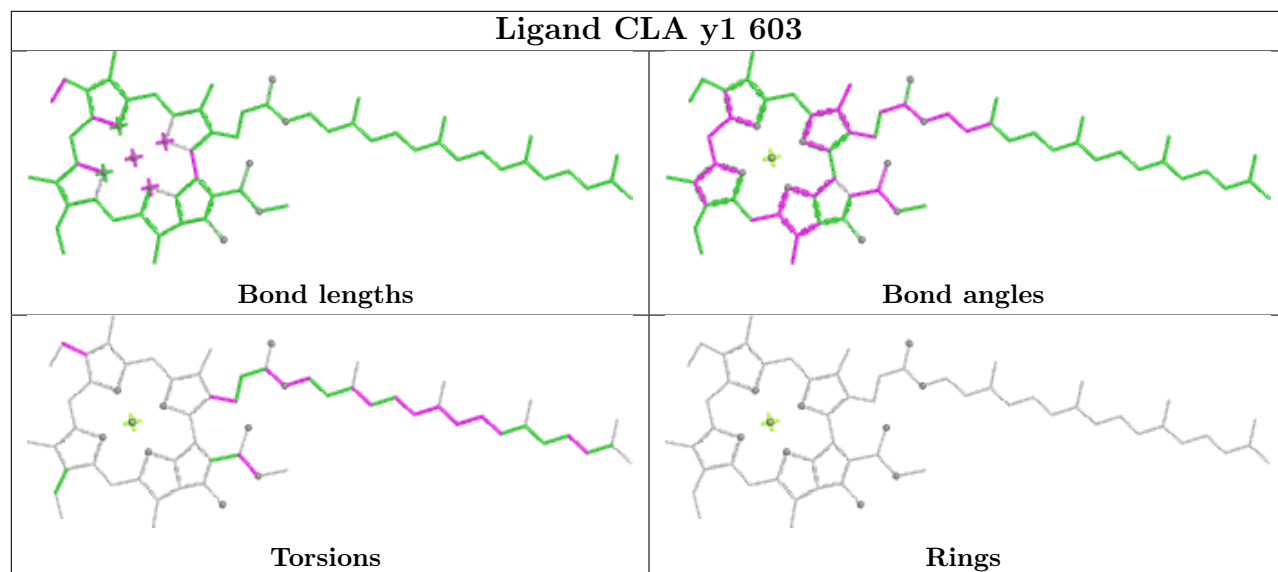
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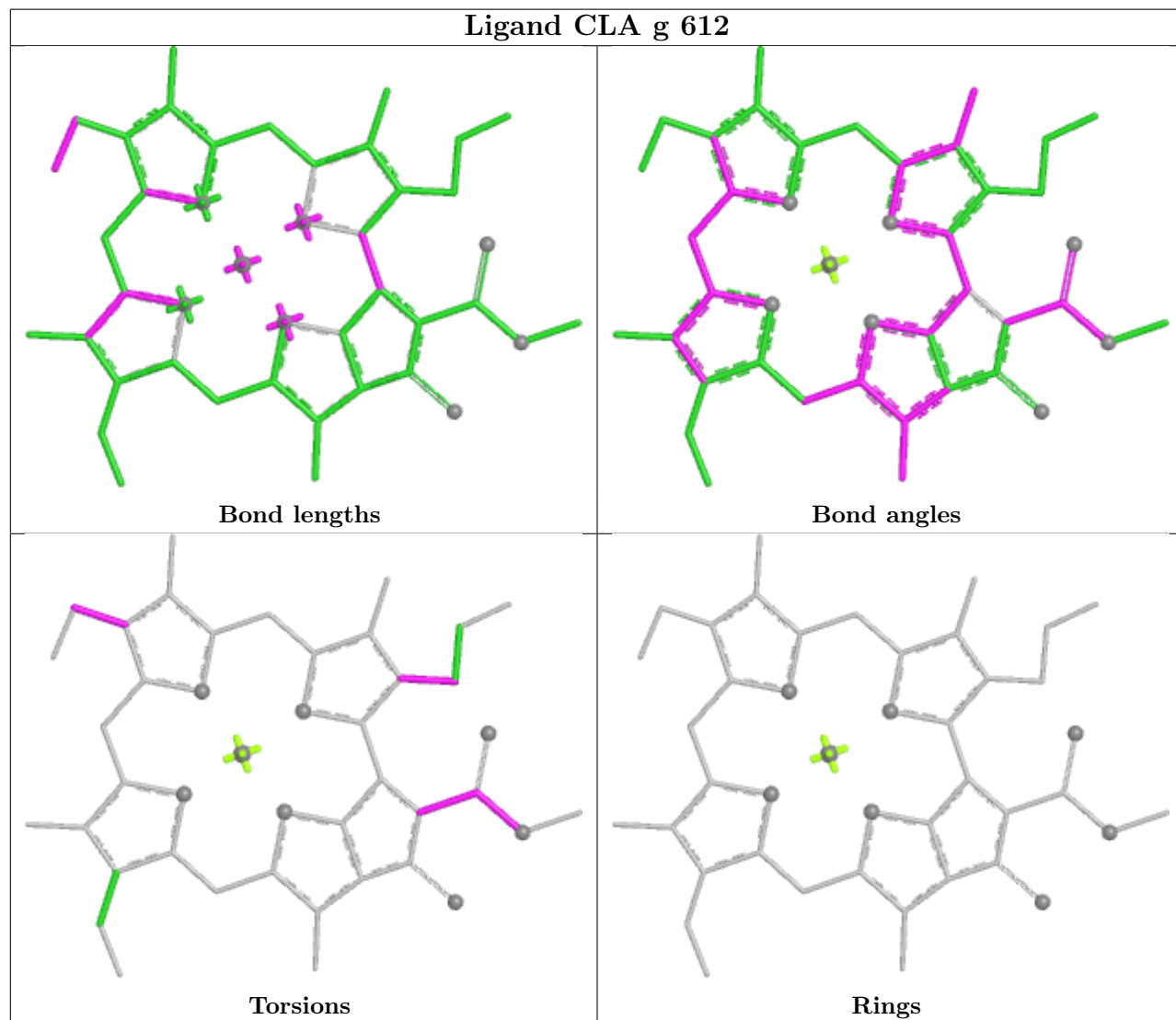
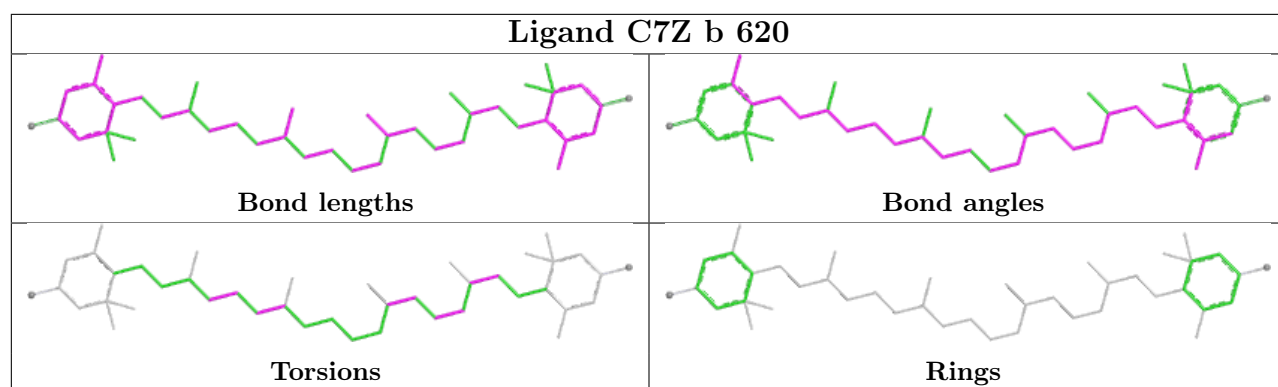




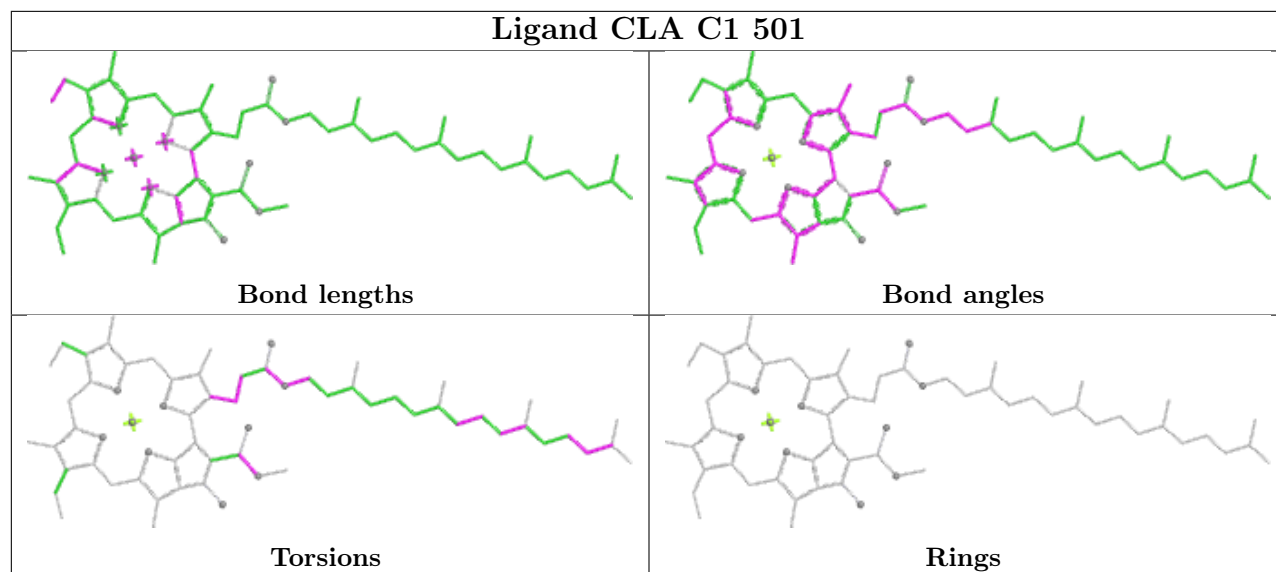




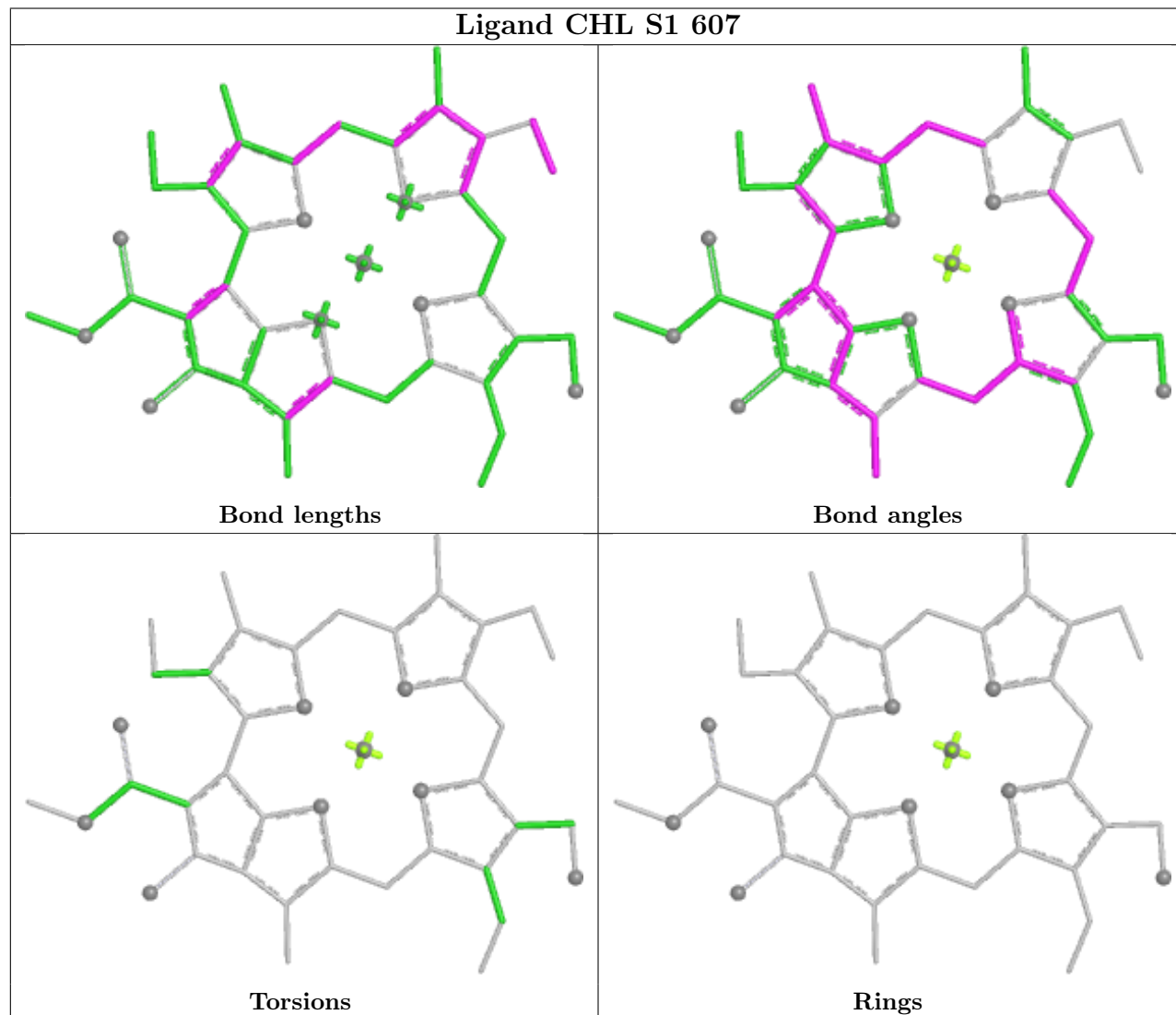




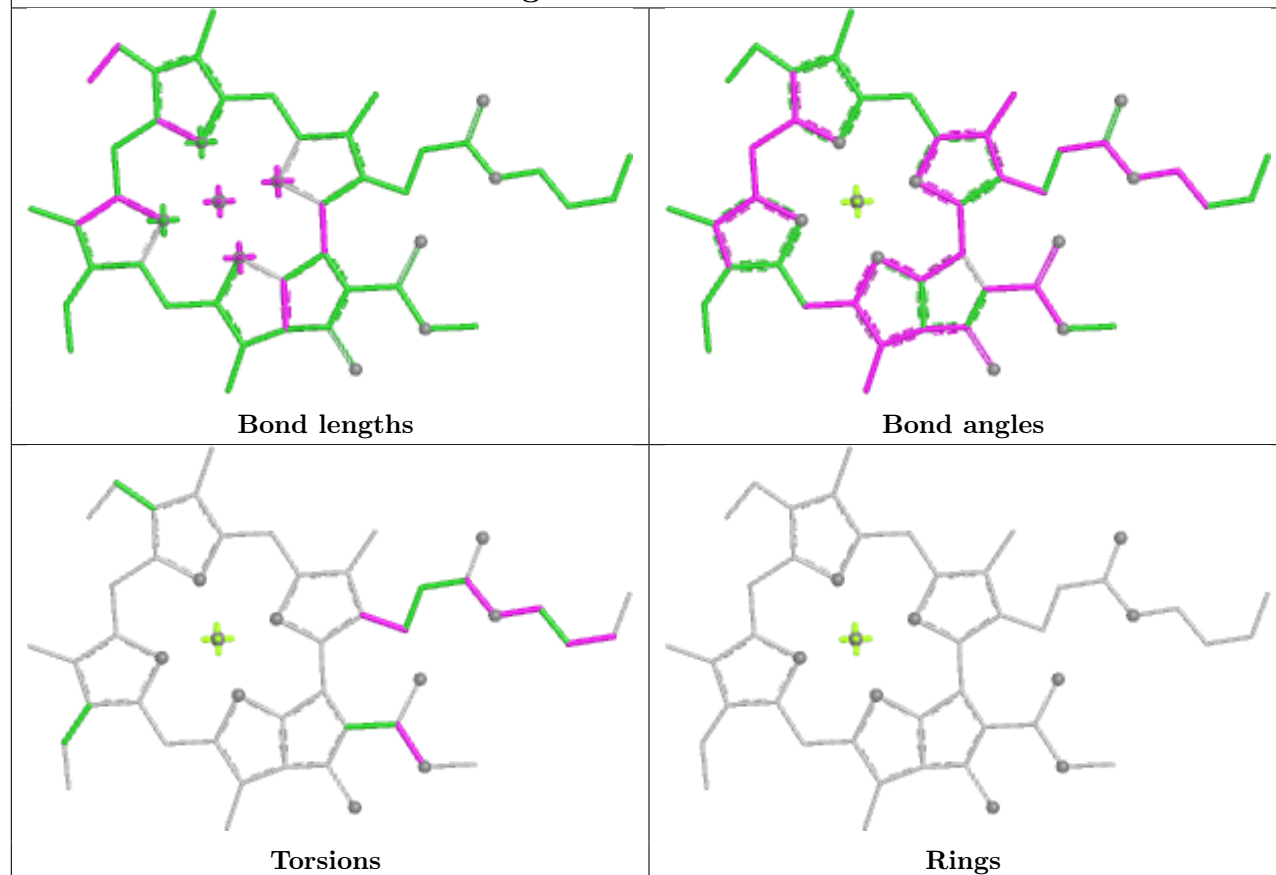
Ligand CLA C1 501



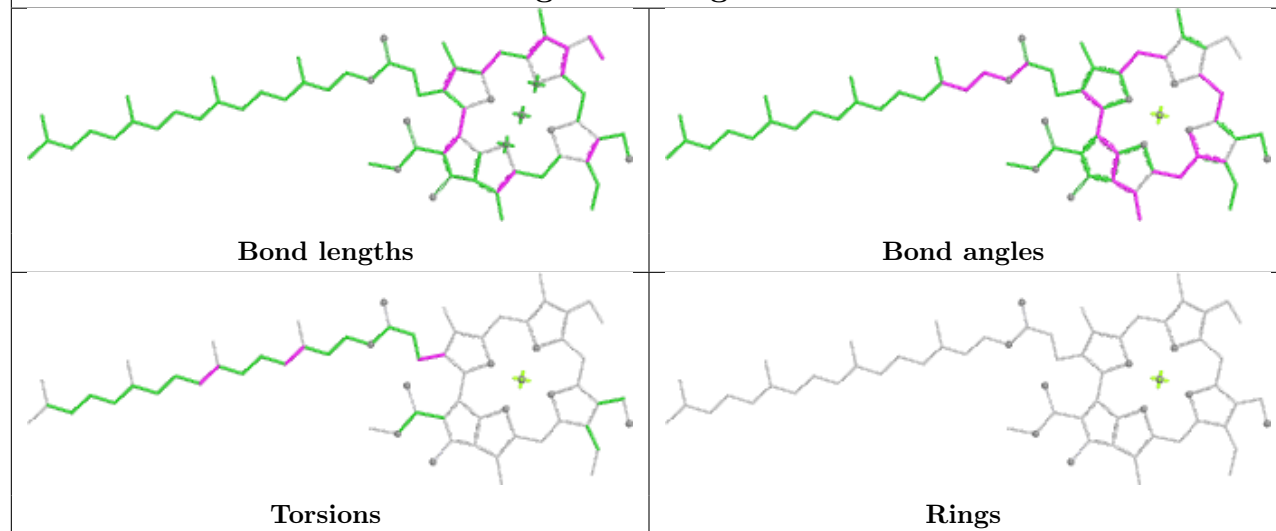
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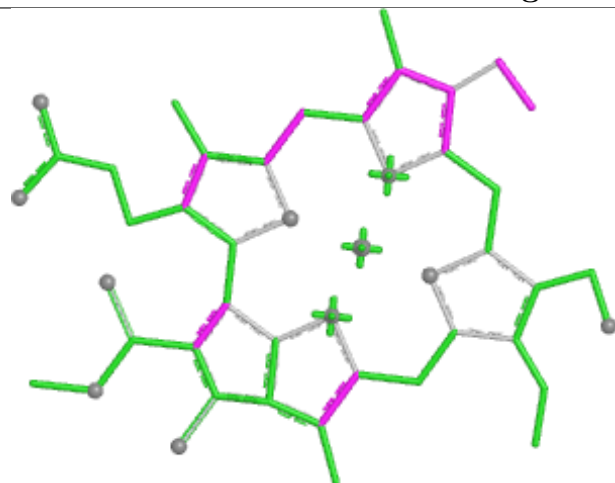
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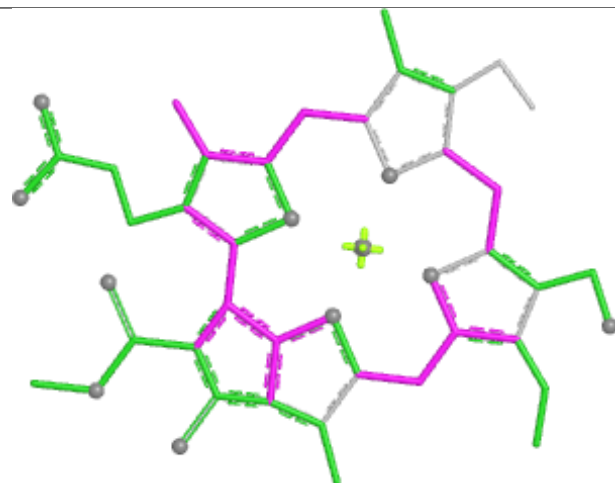
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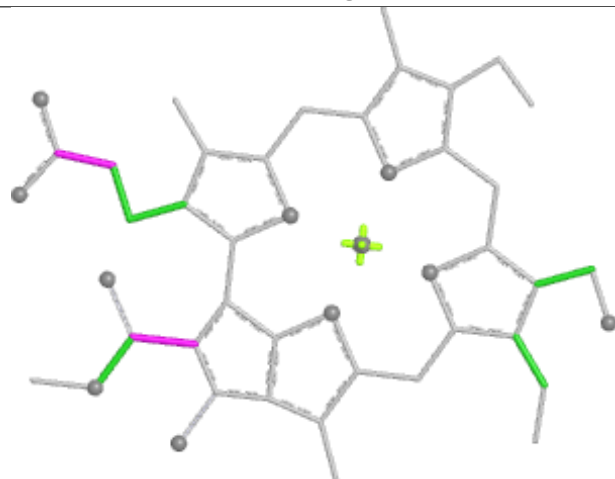
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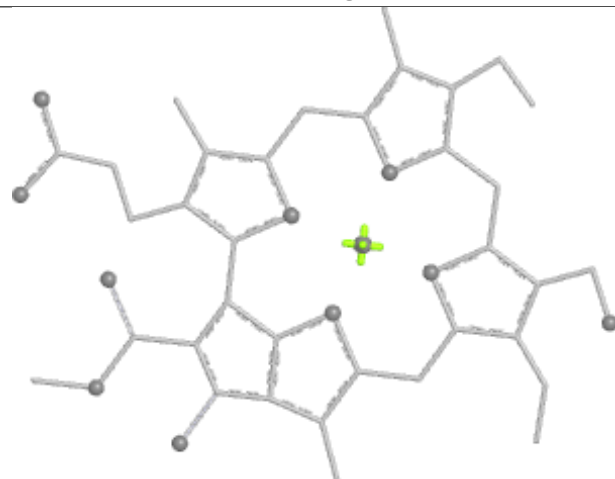
Bond lengths



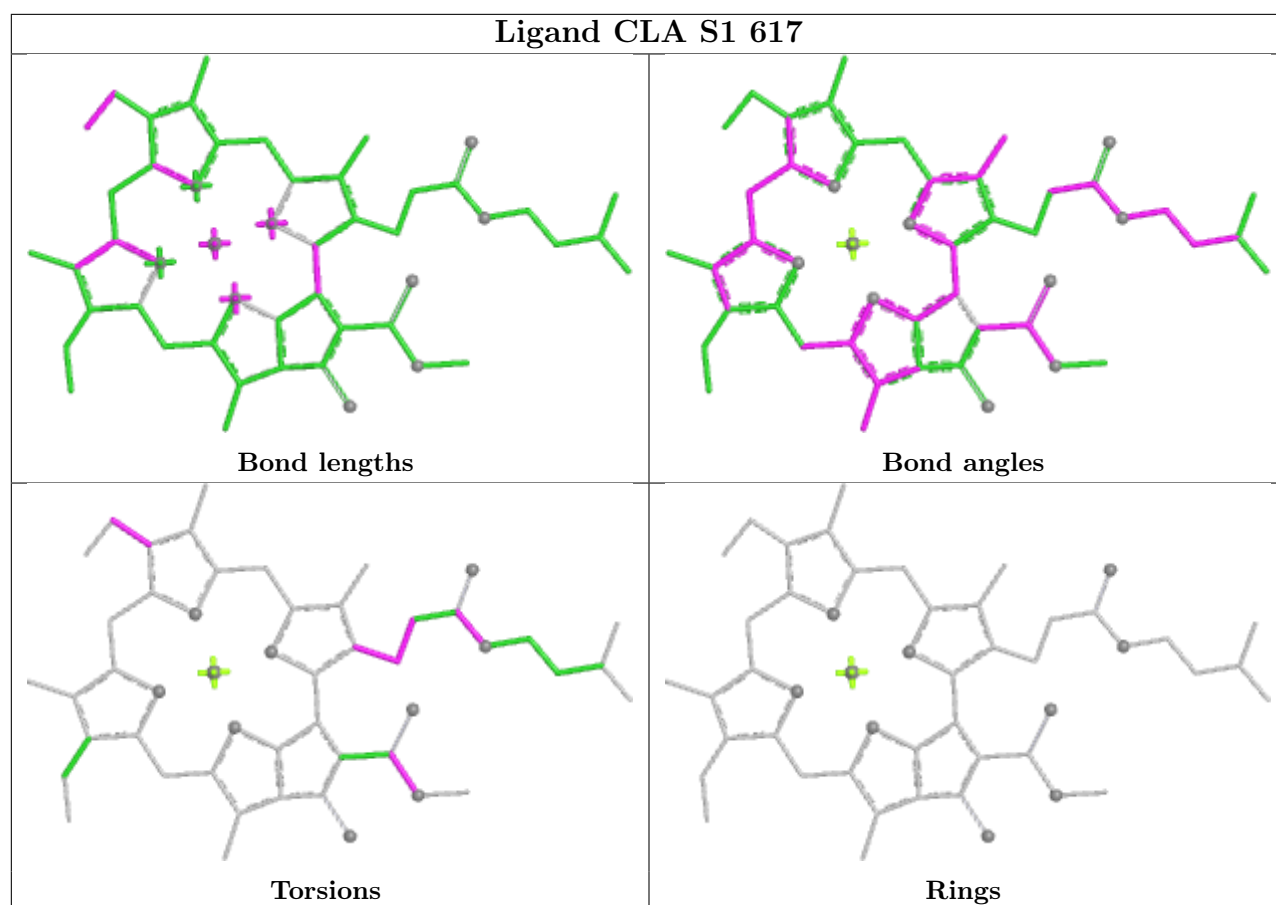
Bond angles



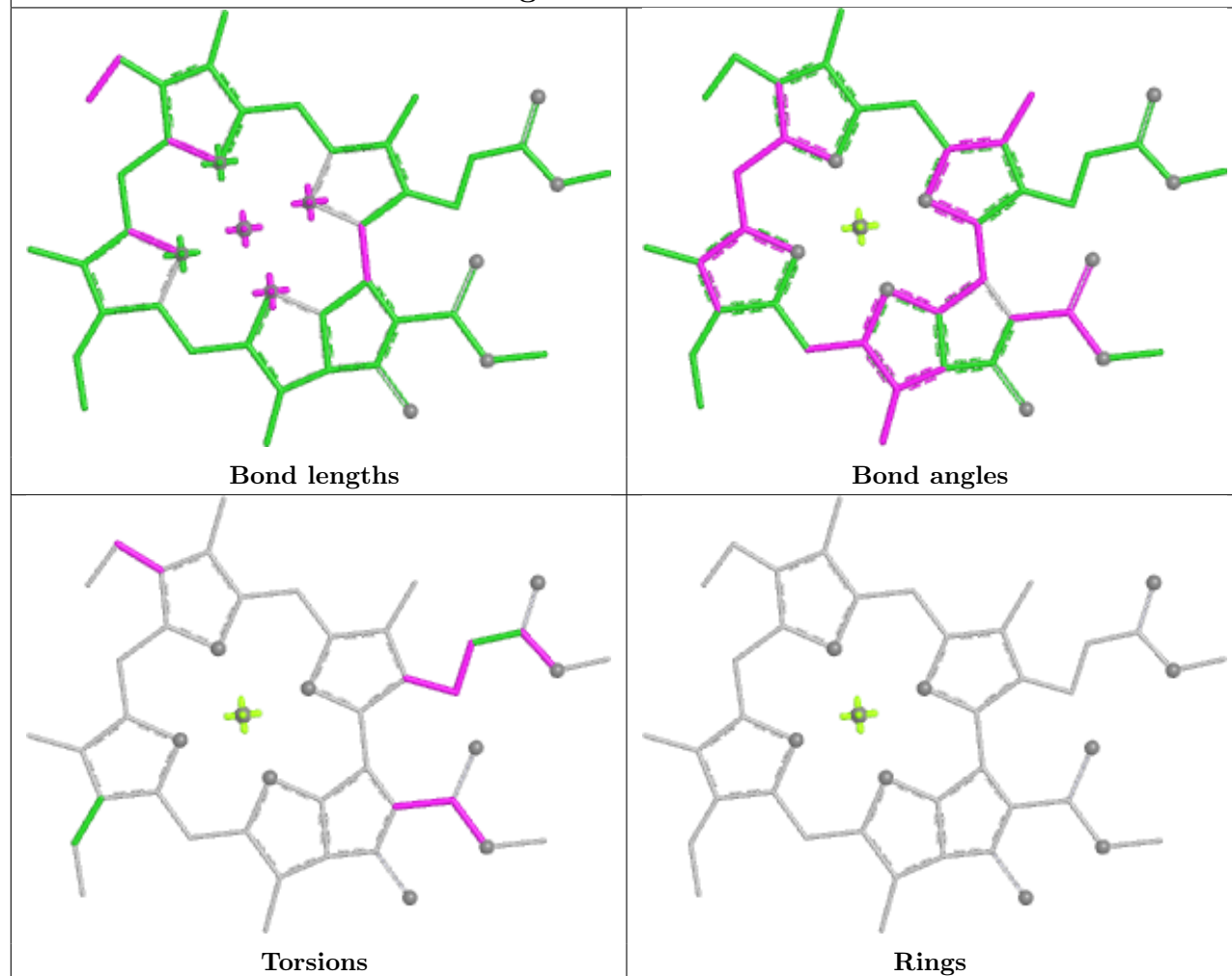
Torsions



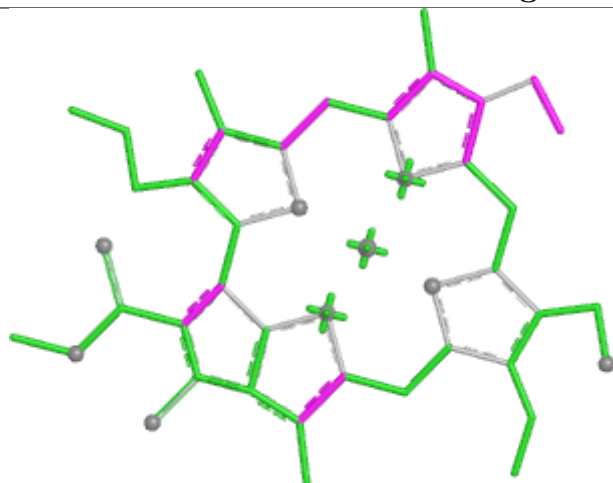
Rings



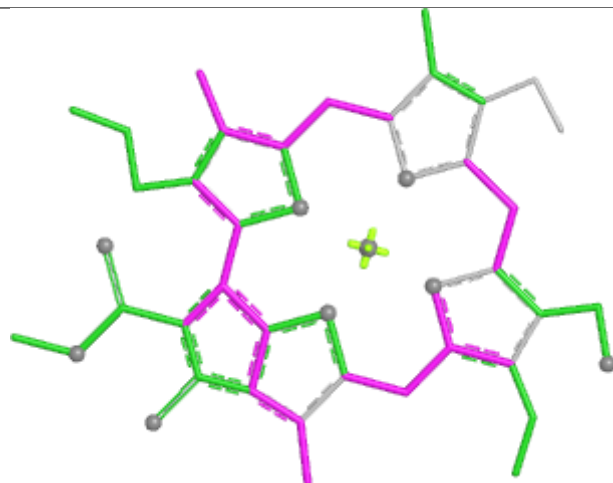
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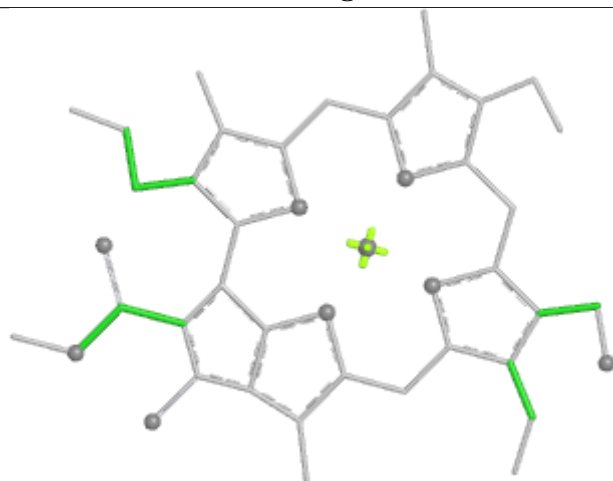
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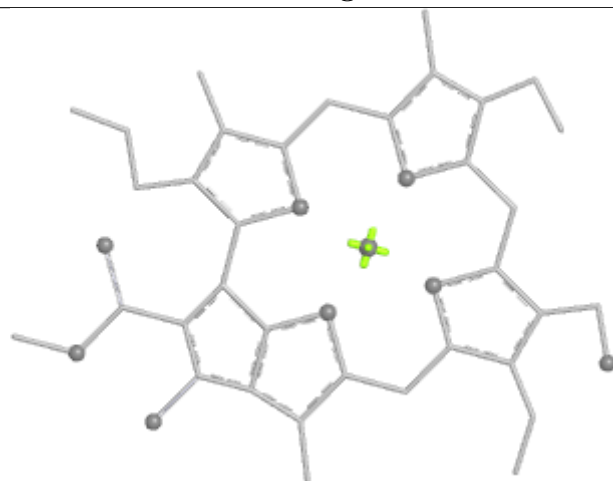
Bond lengths



Bond angles

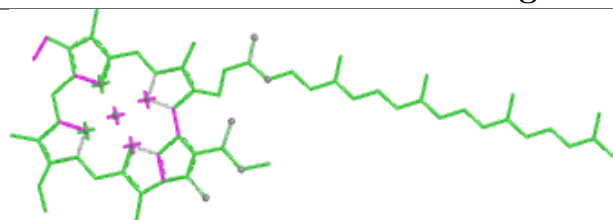


Torsions

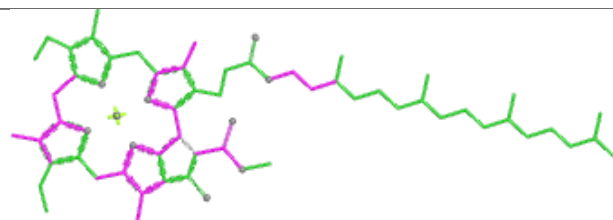


Rings

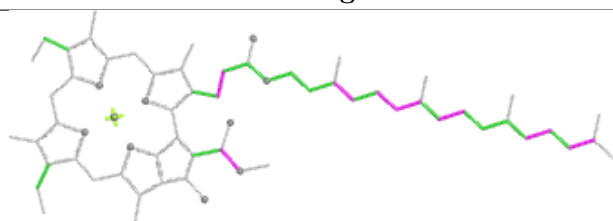
Ligand CLA c 502



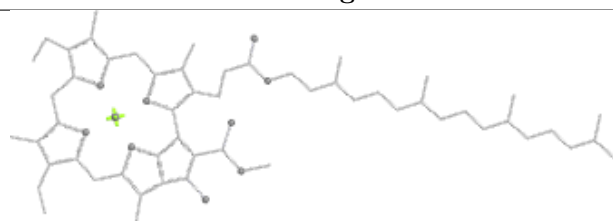
Bond lengths



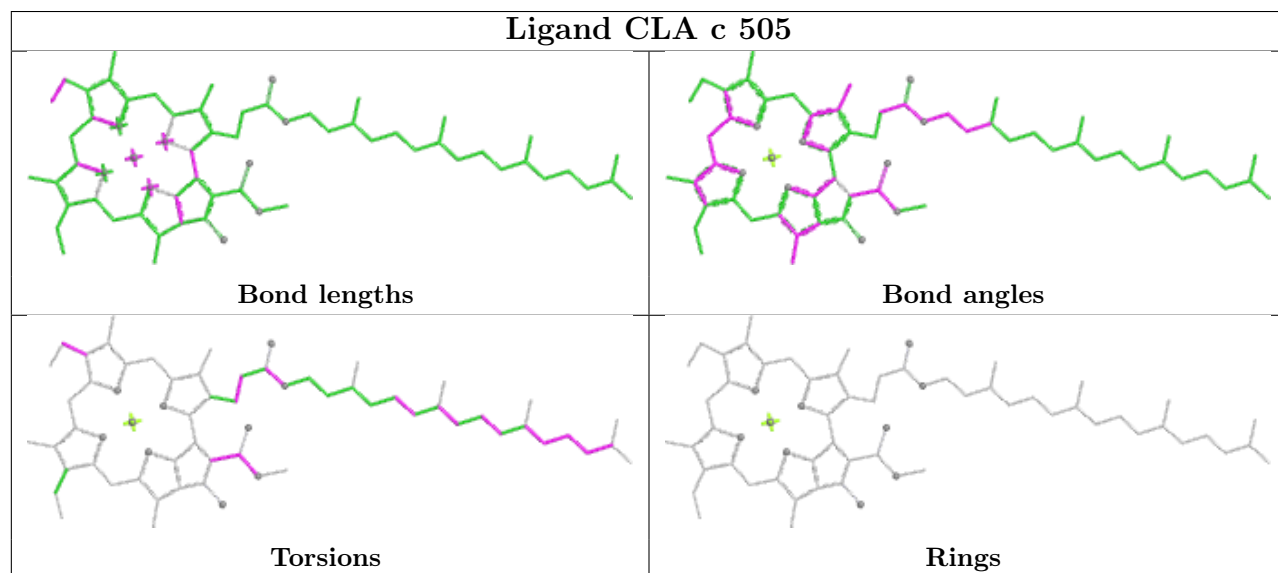
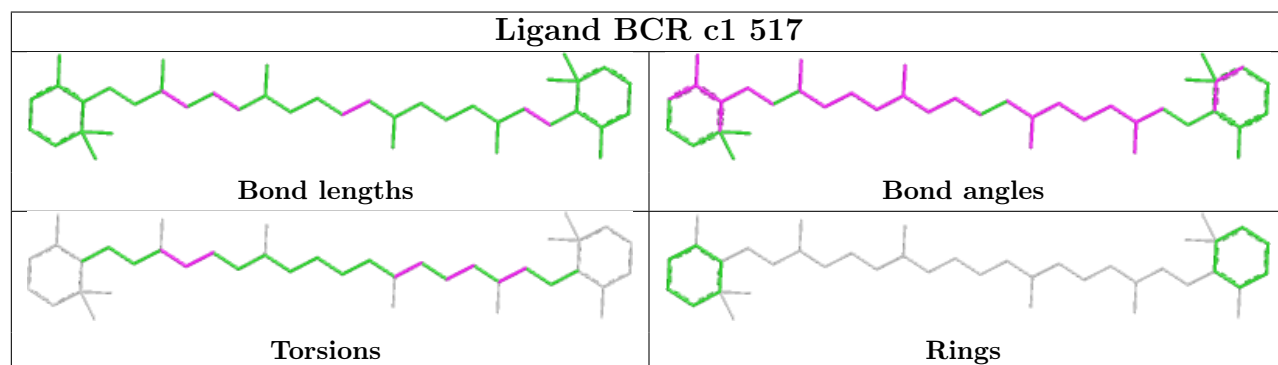
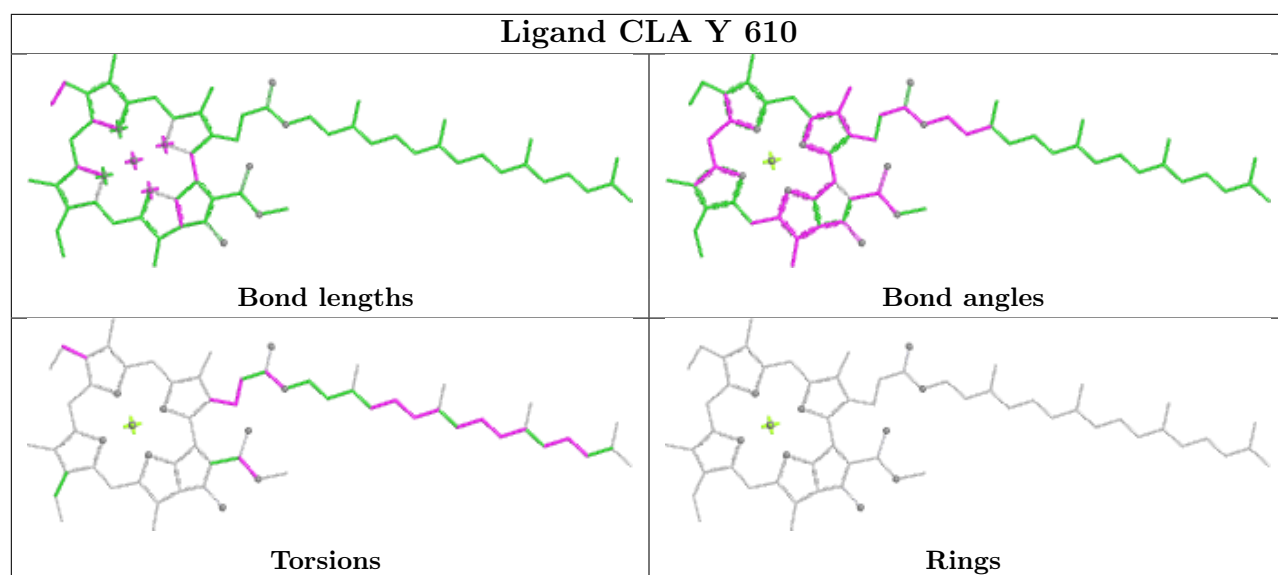
Bond angles

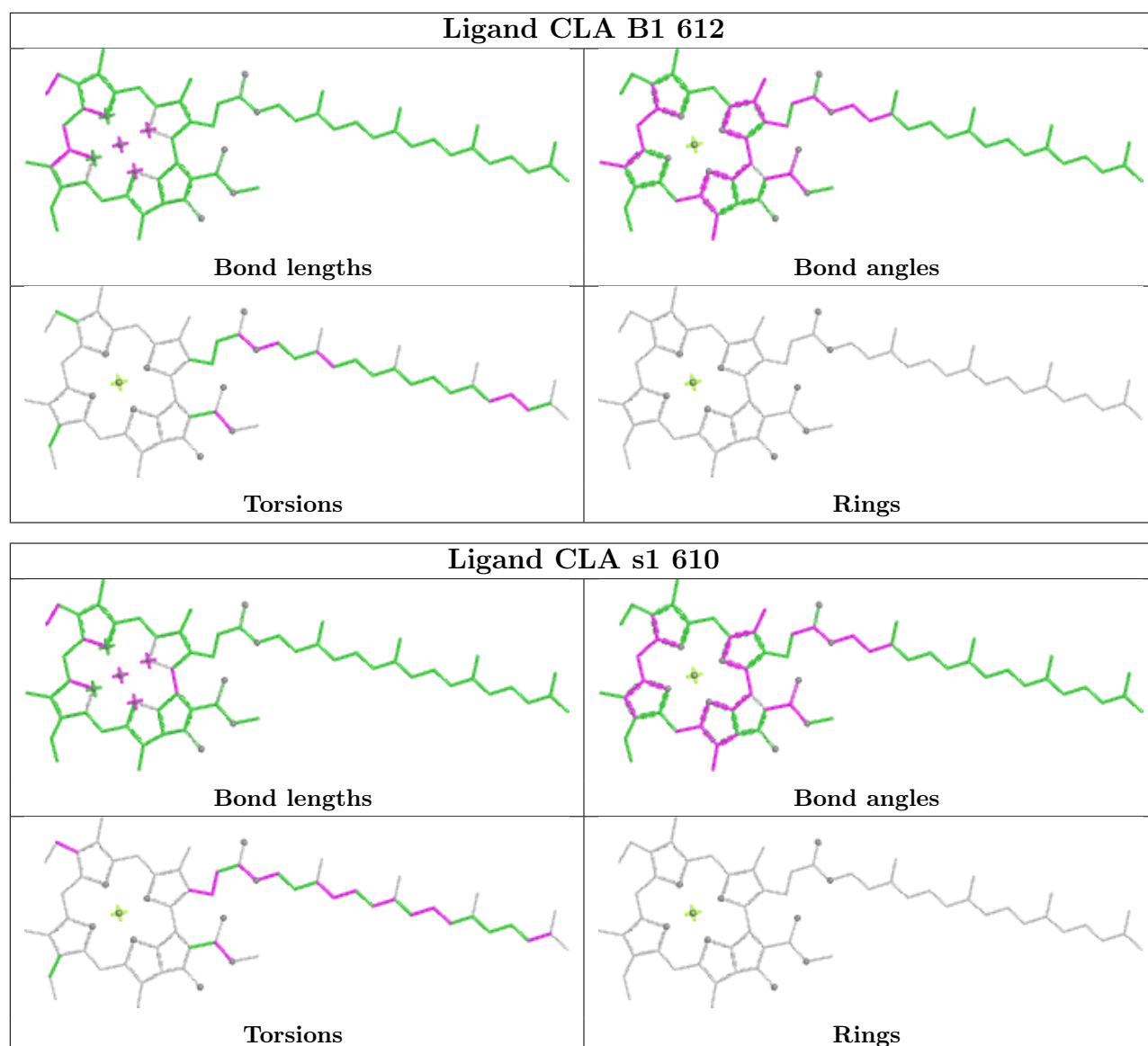


Torsions

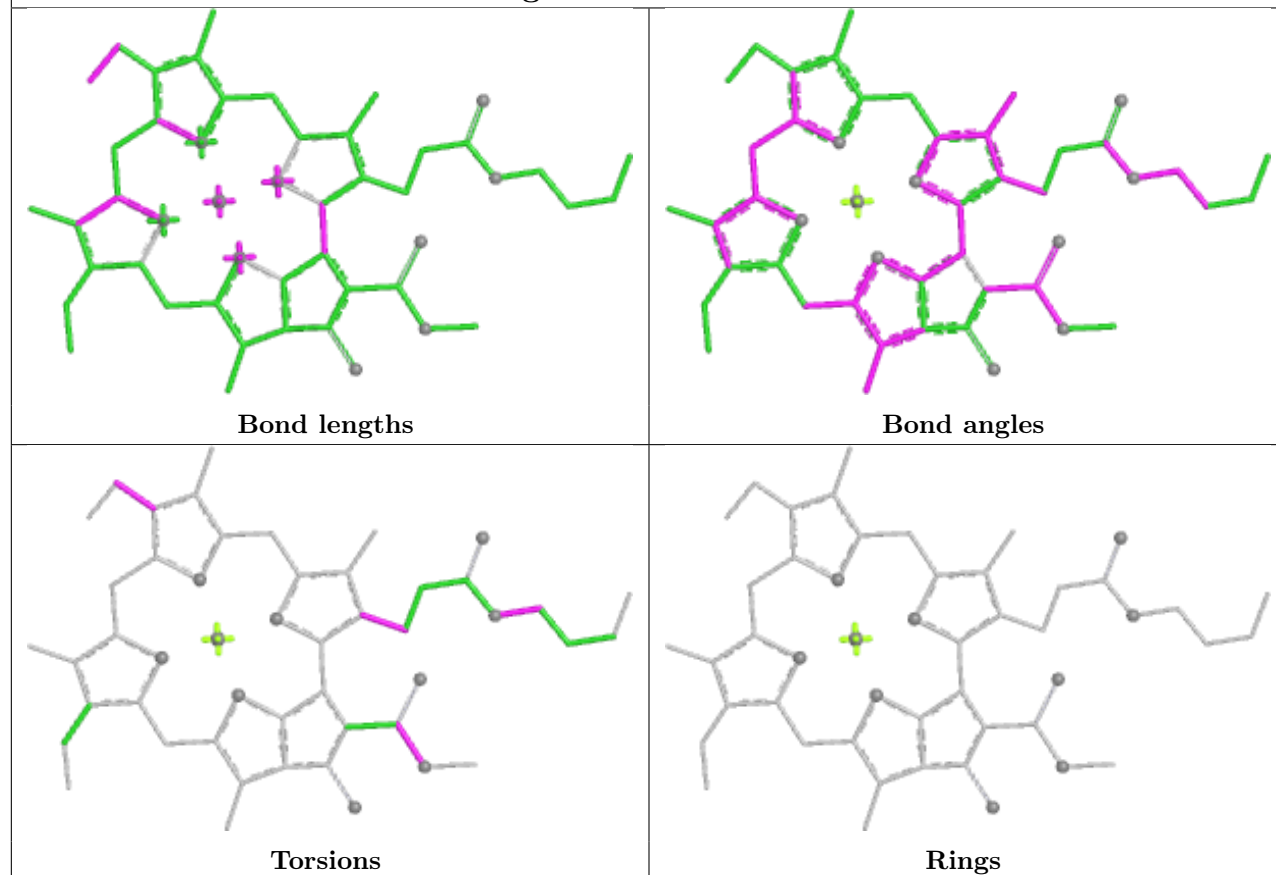


Rings

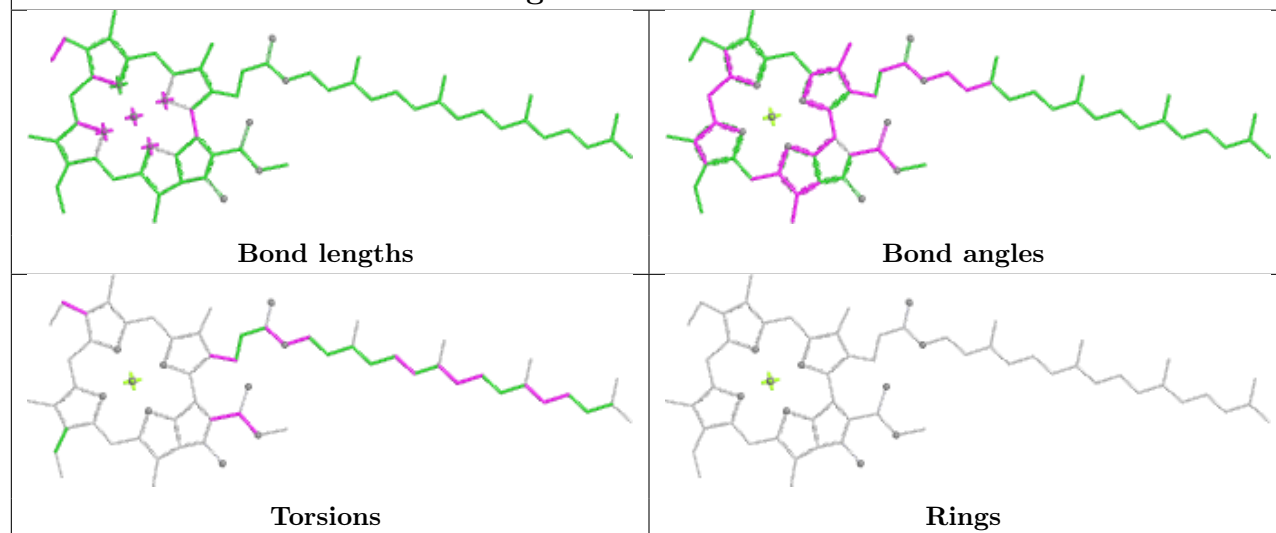


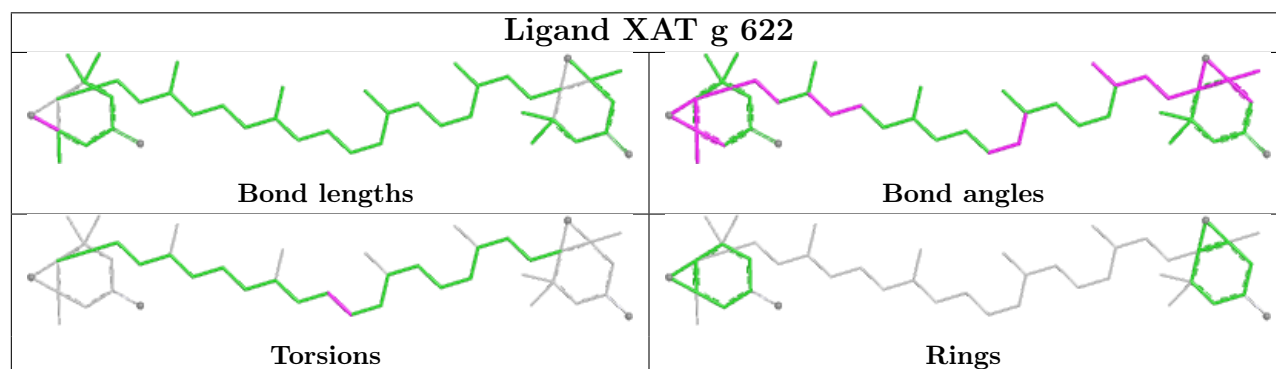
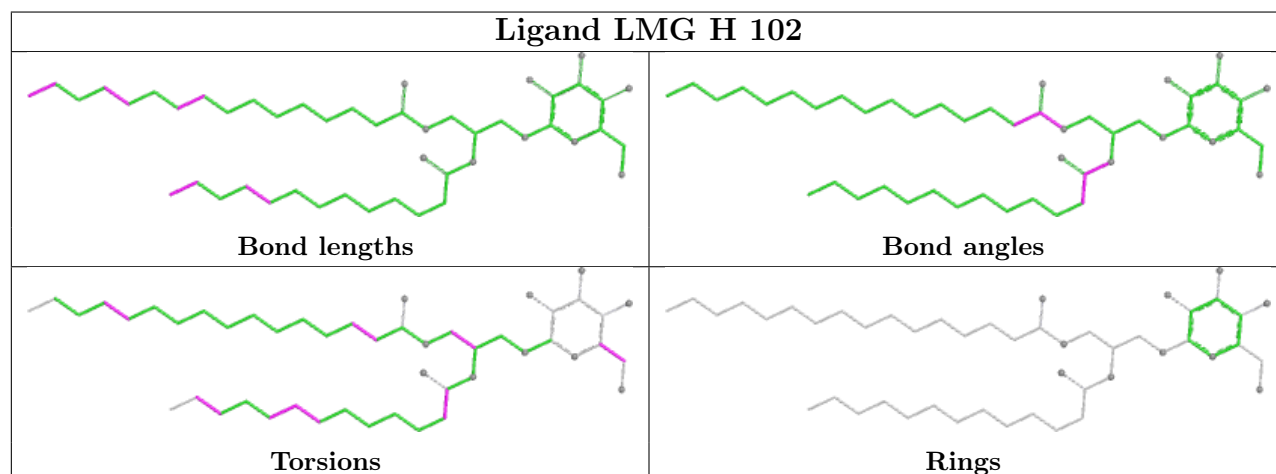
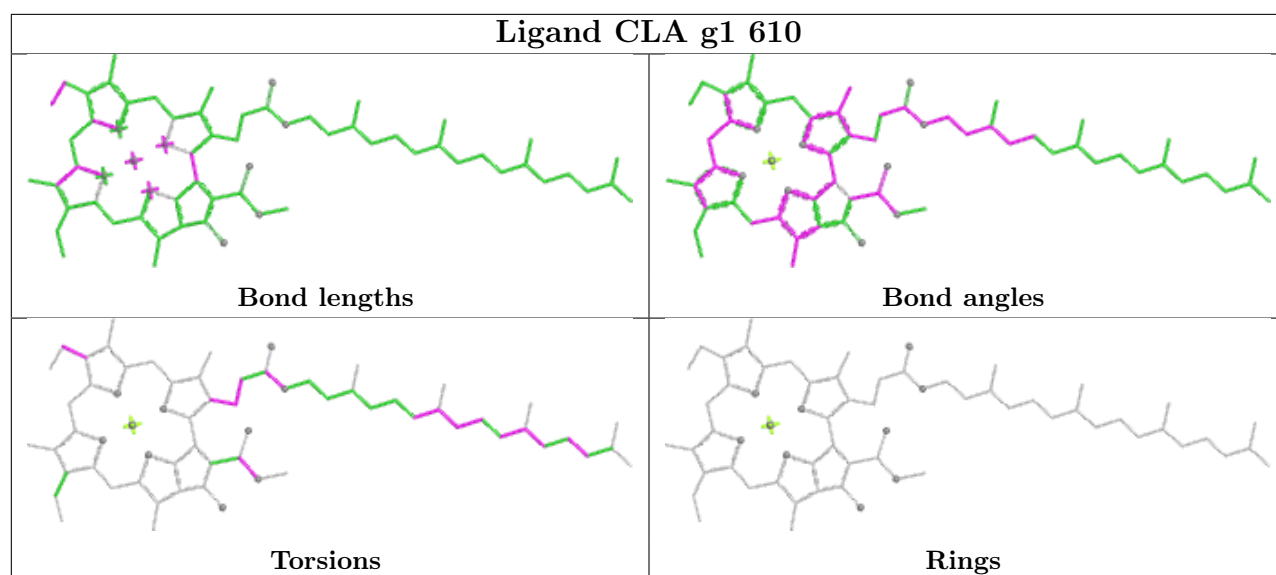


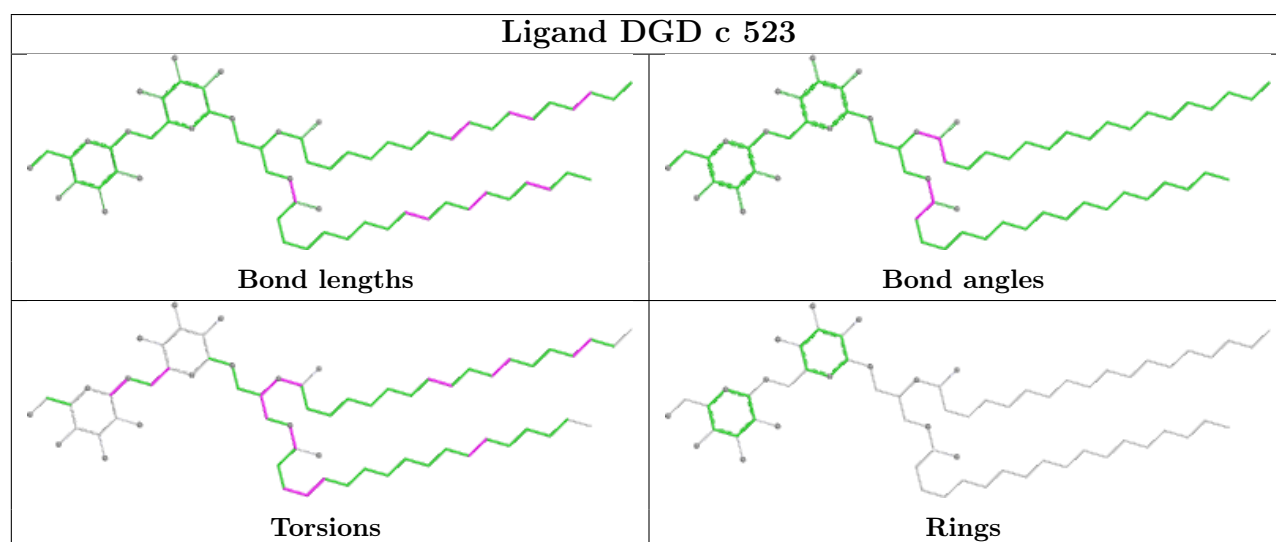
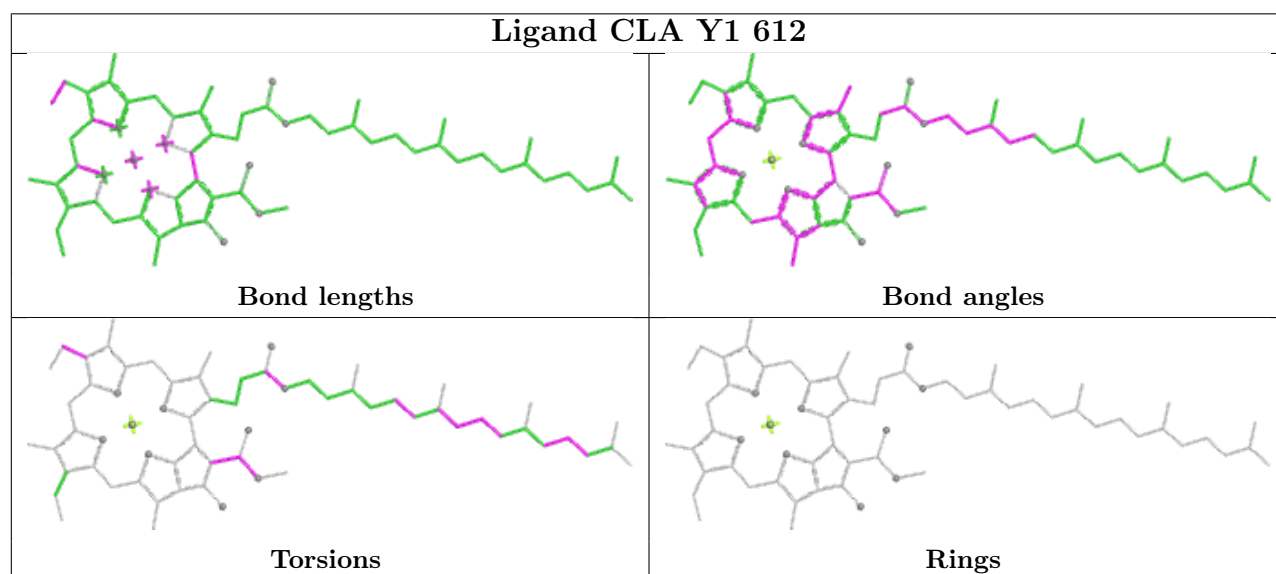
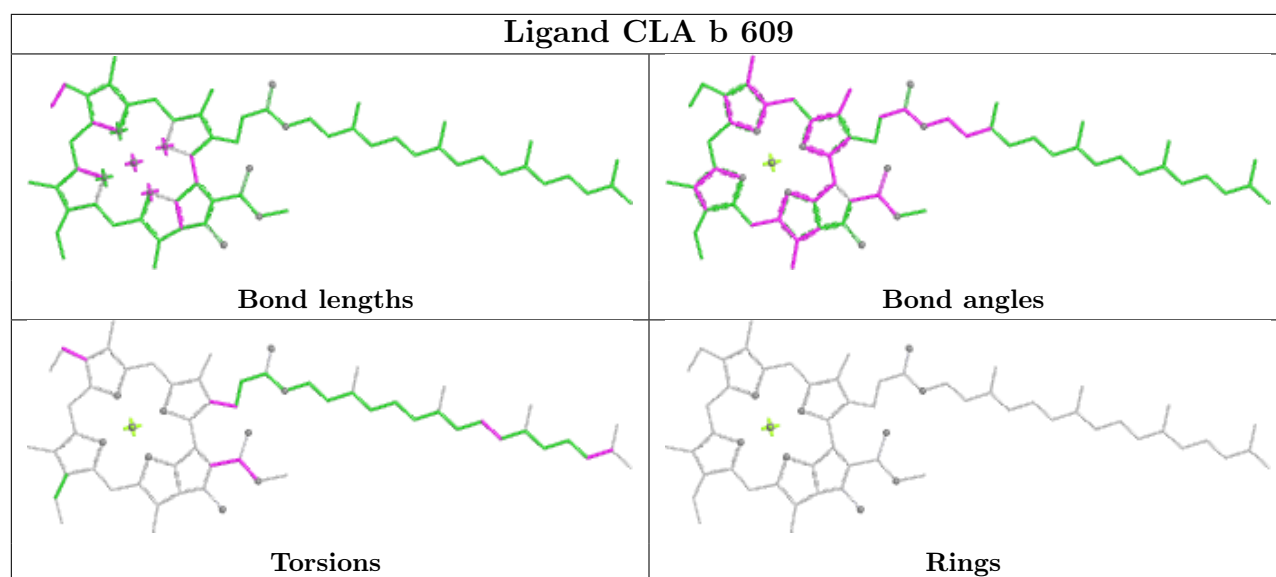
Ligand CLA N1 614

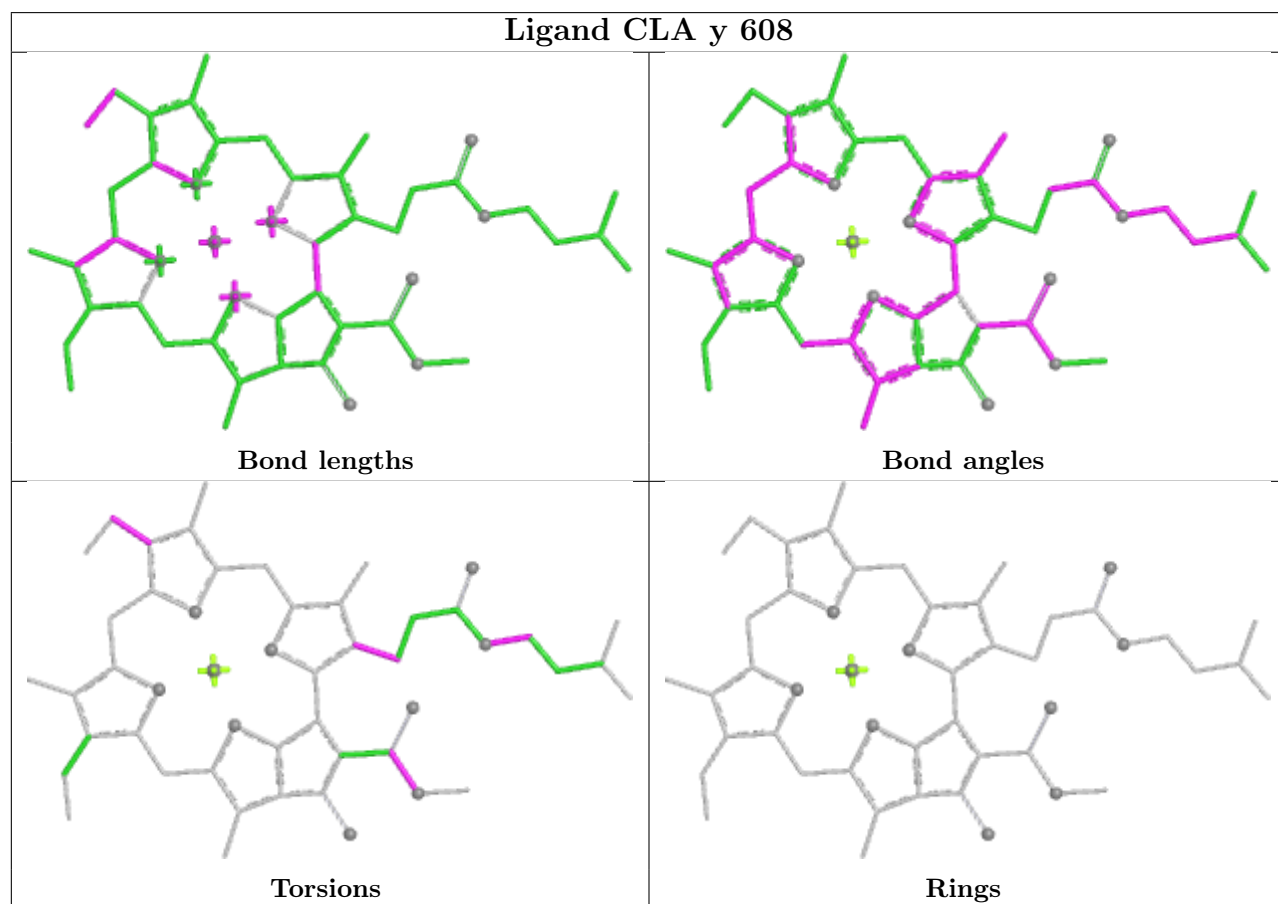
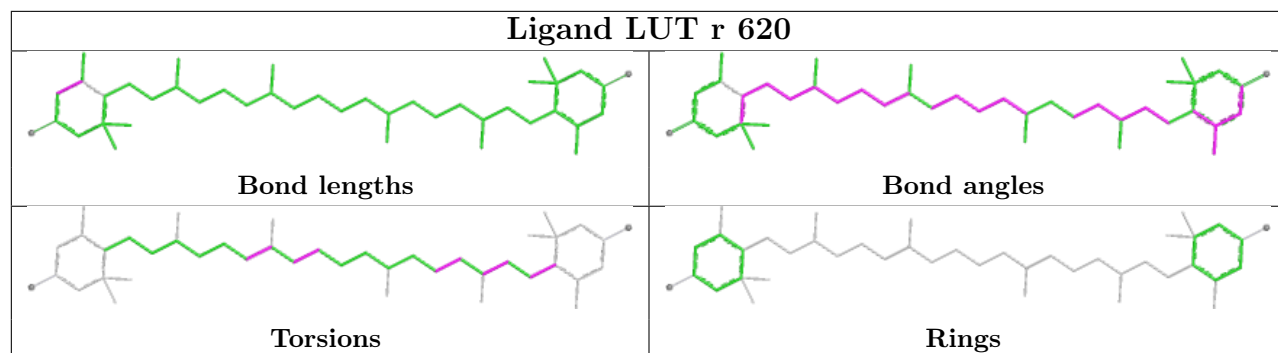


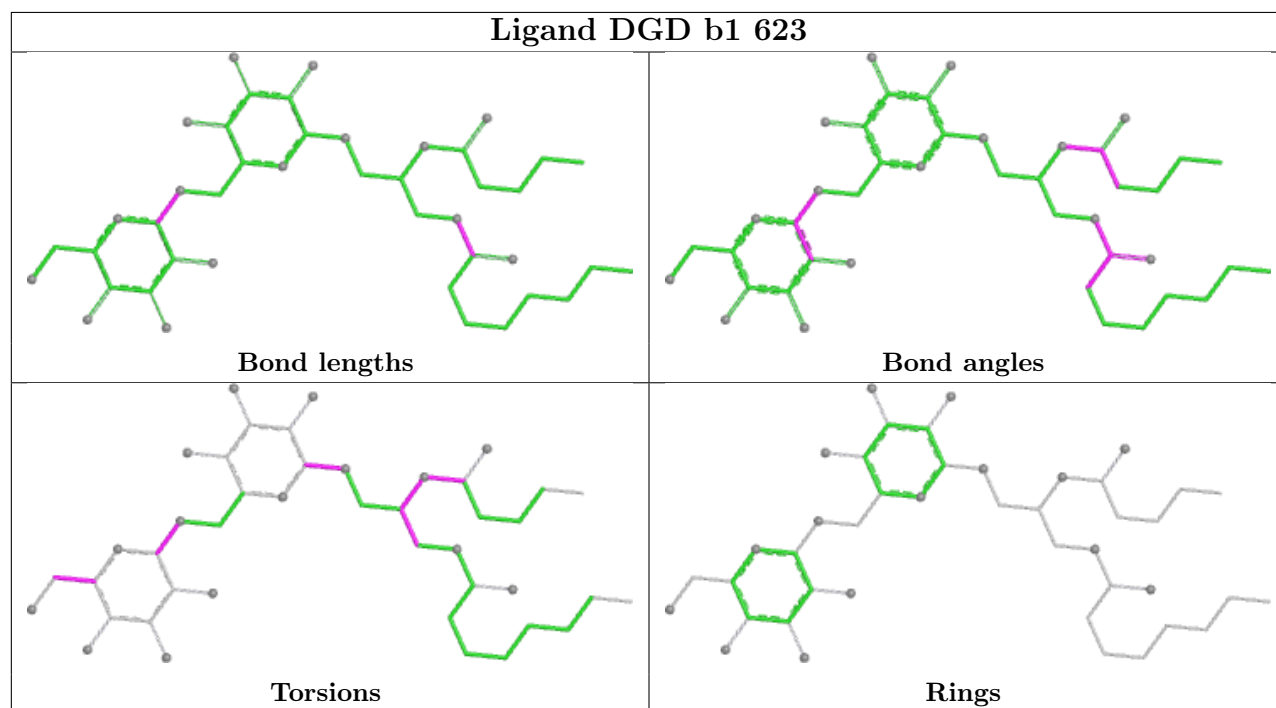
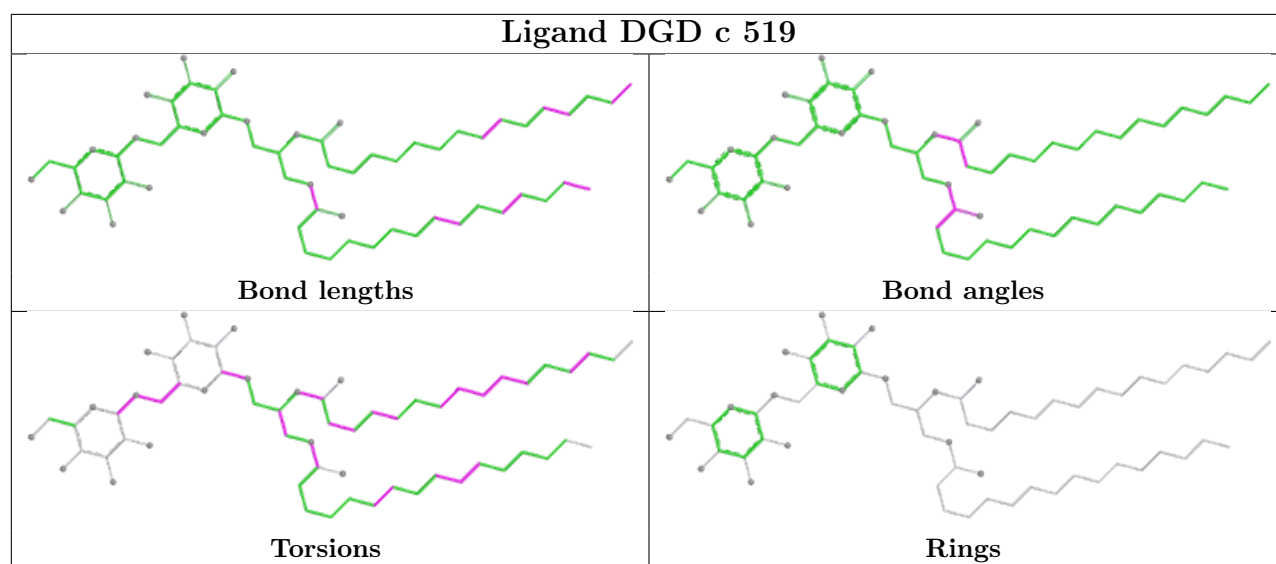
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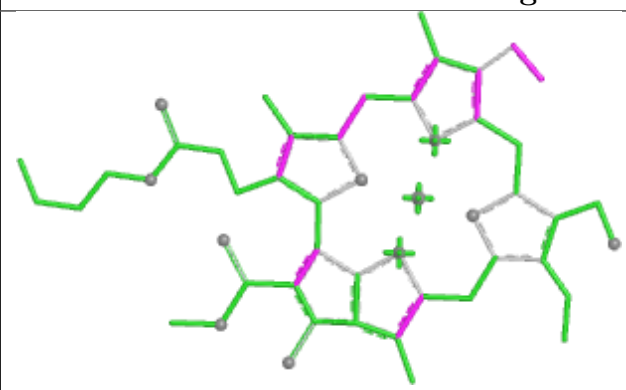
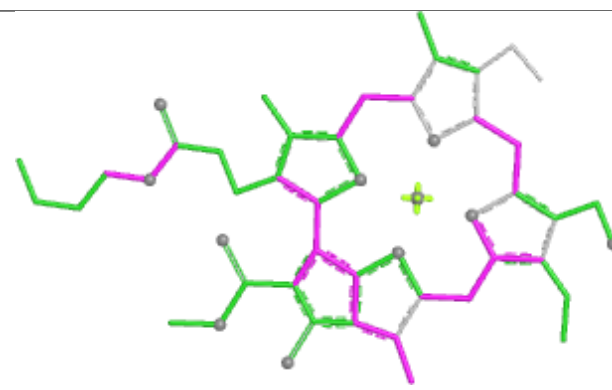
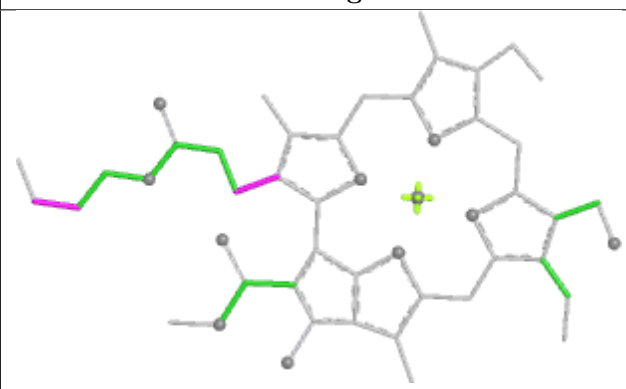
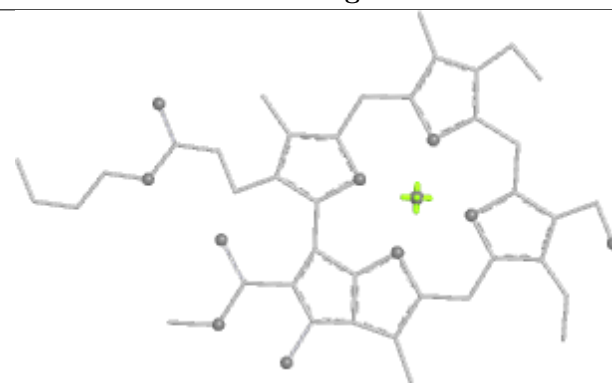


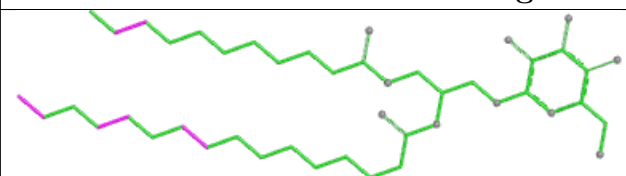
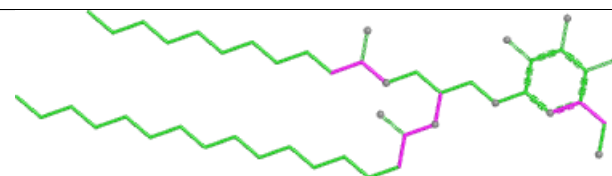
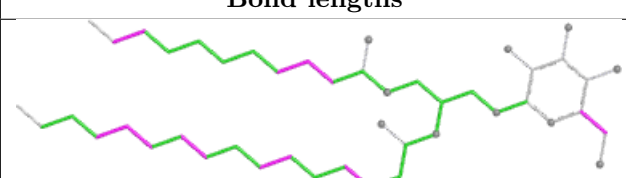
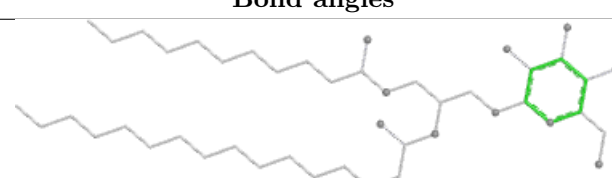


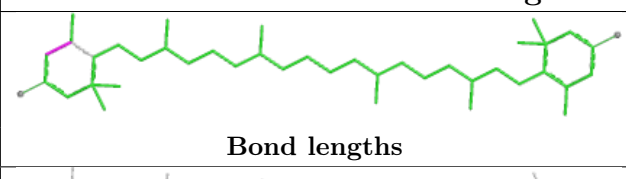
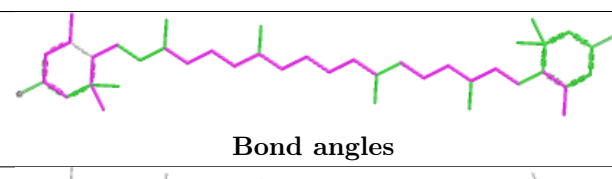
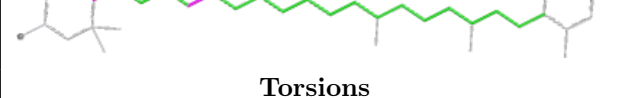


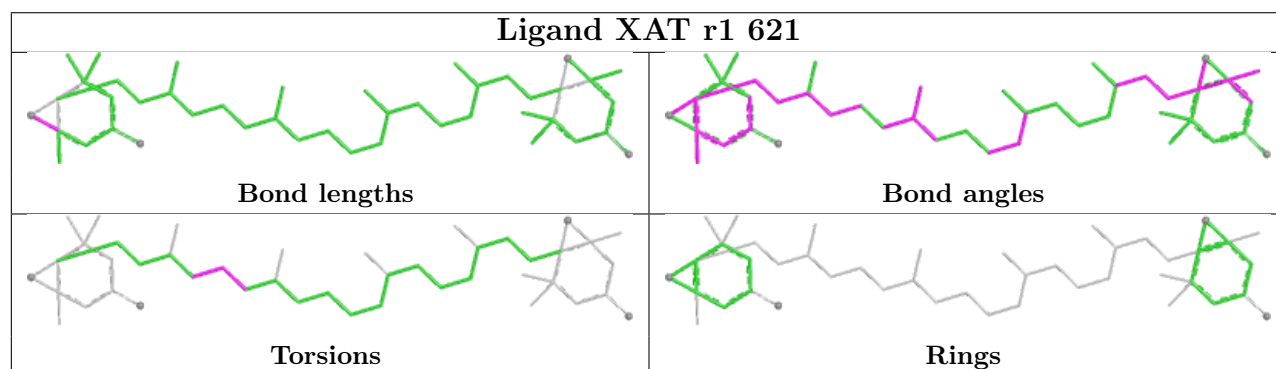
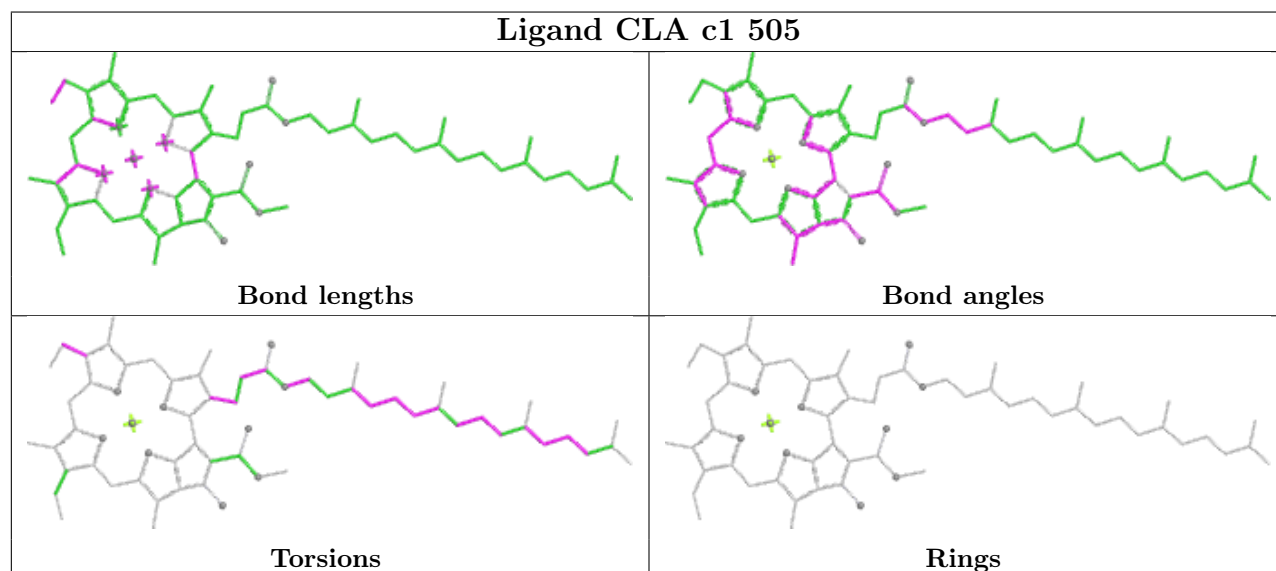
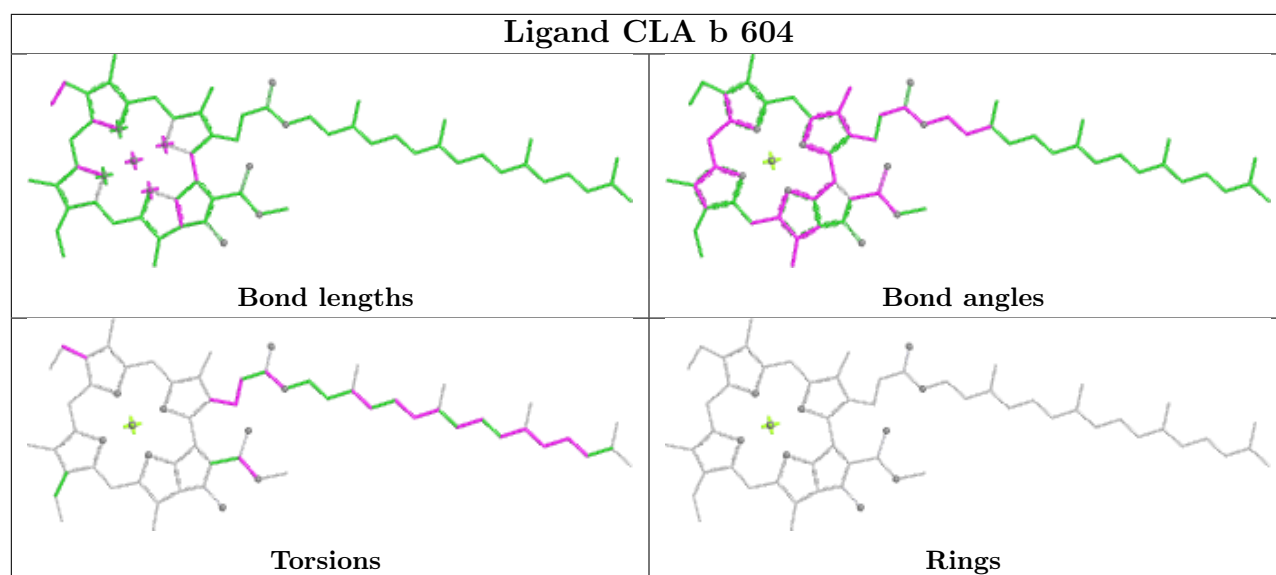


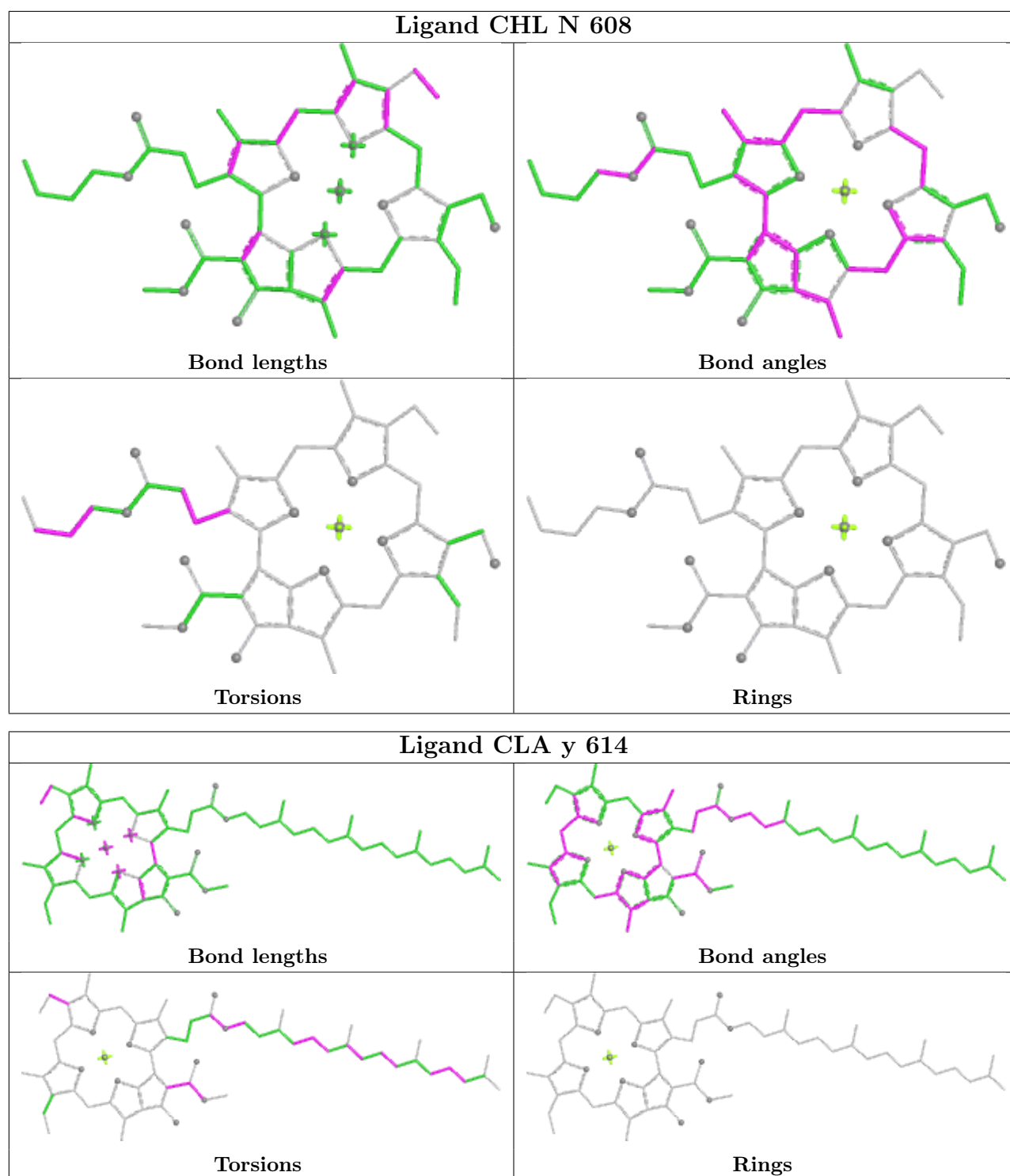


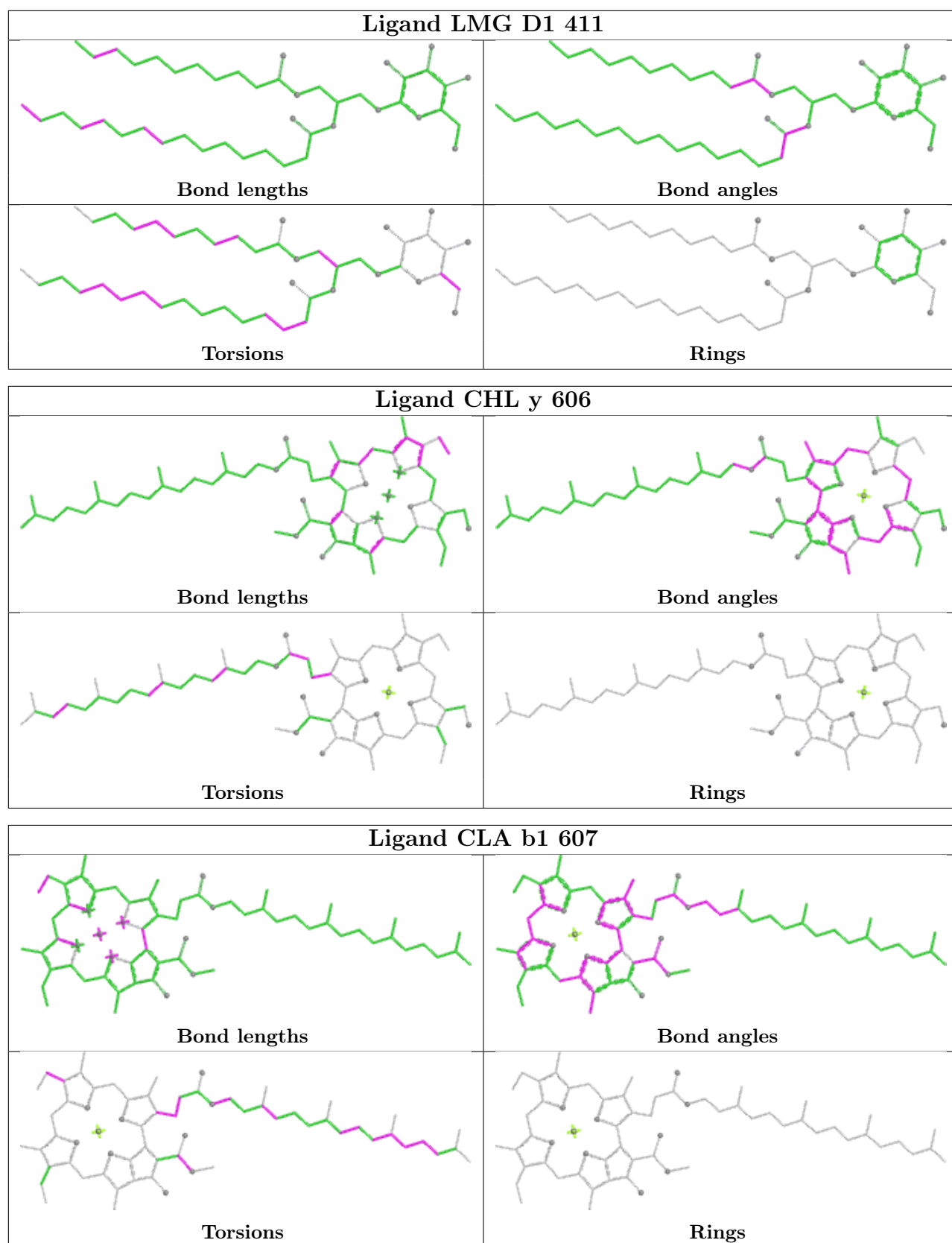
Ligand CHL G 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

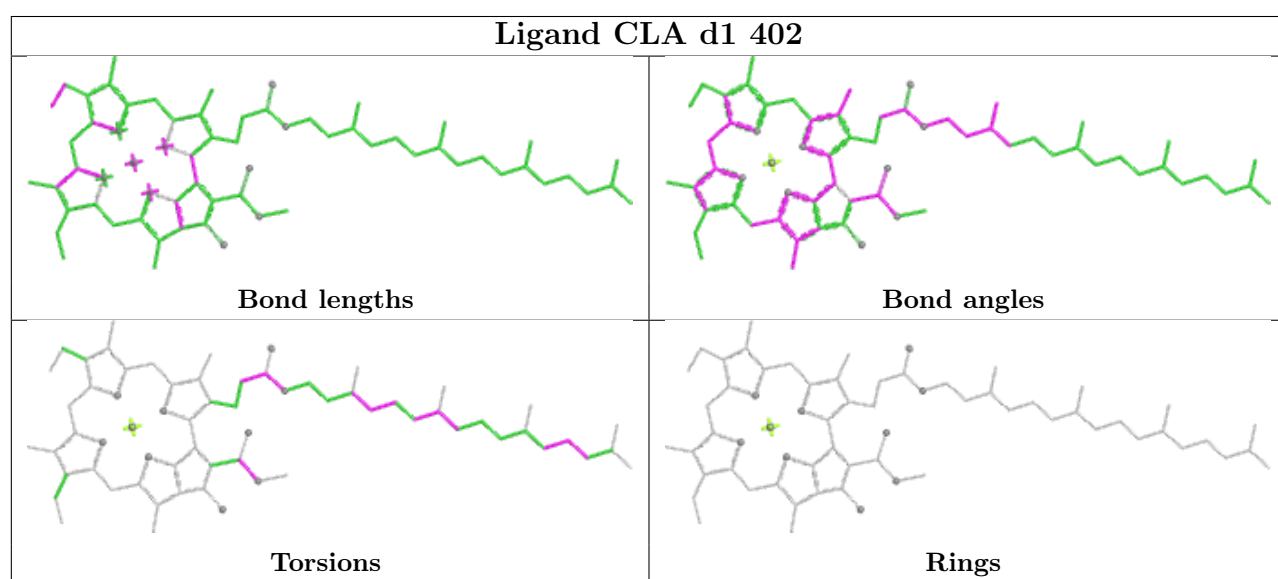
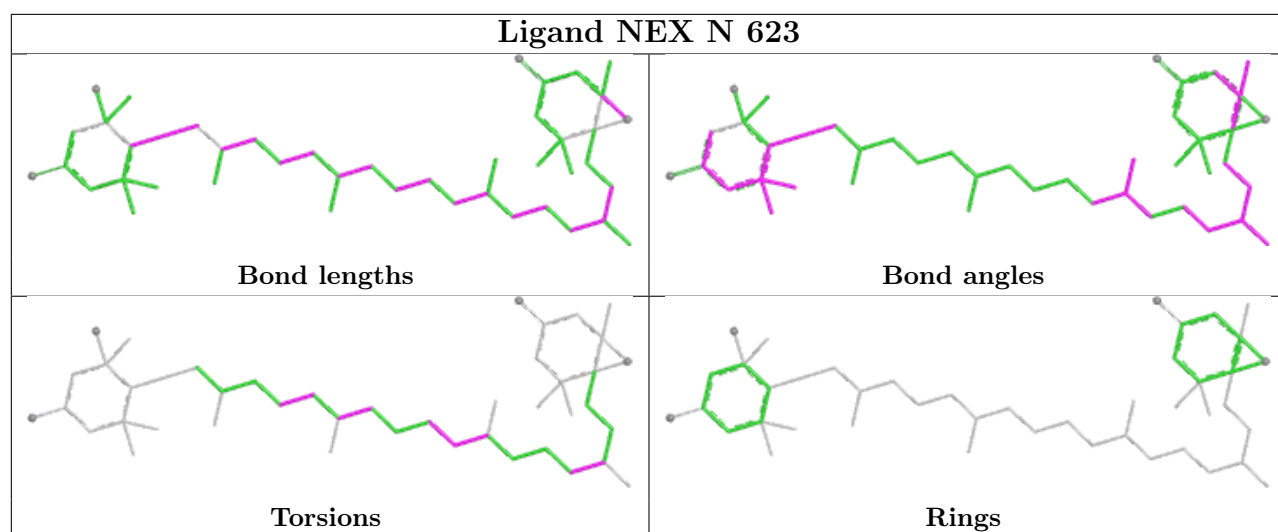
Ligand LMG D 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

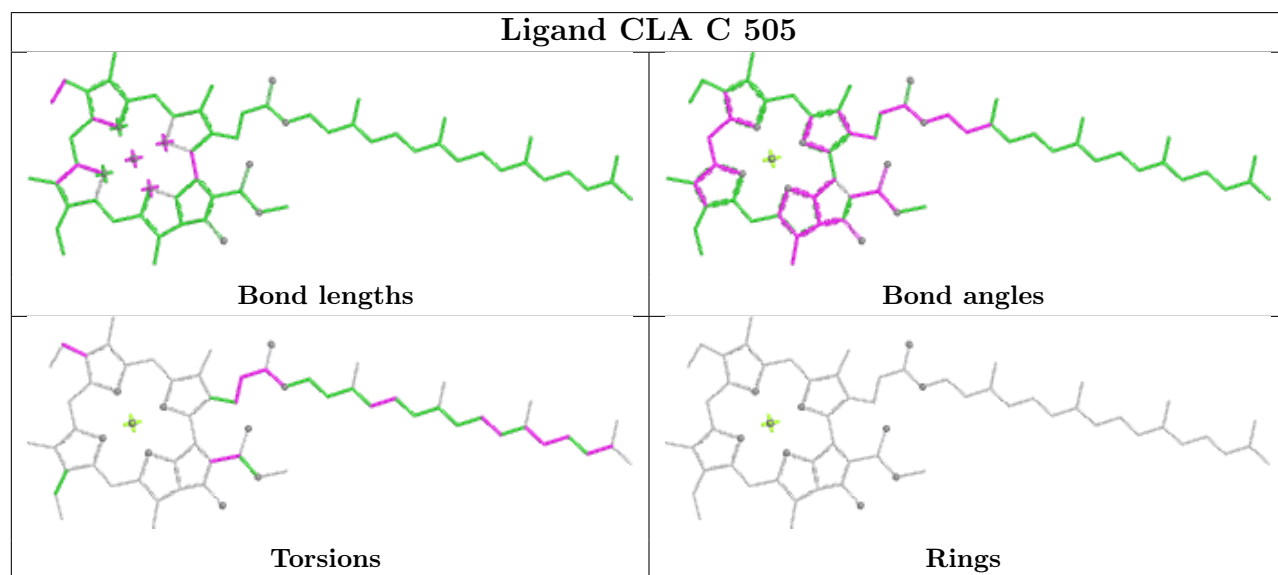
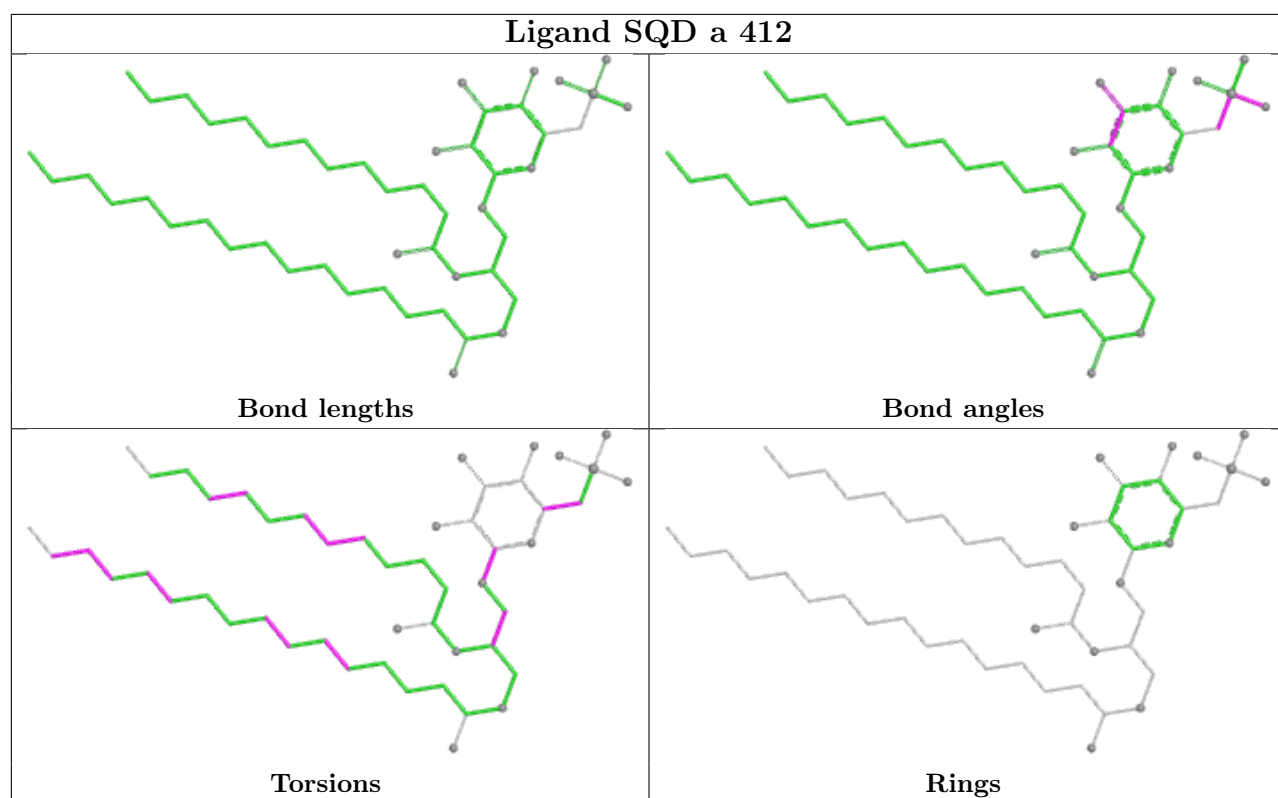
Ligand LUT S 620	
	
Bond lengths	Bond angles
	
Torsions	Rings



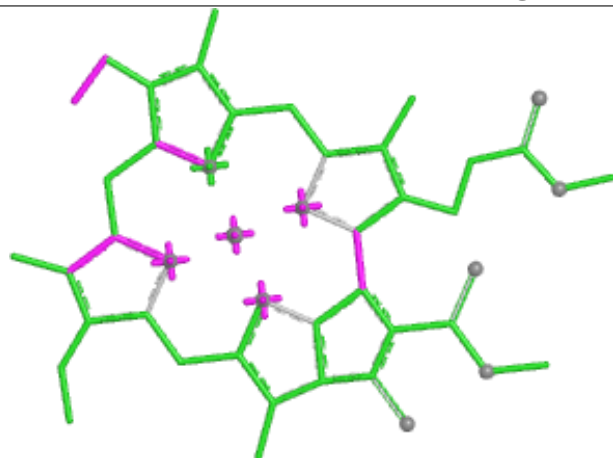




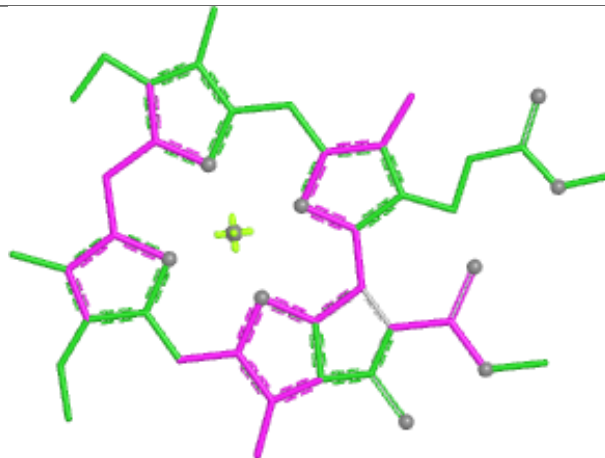




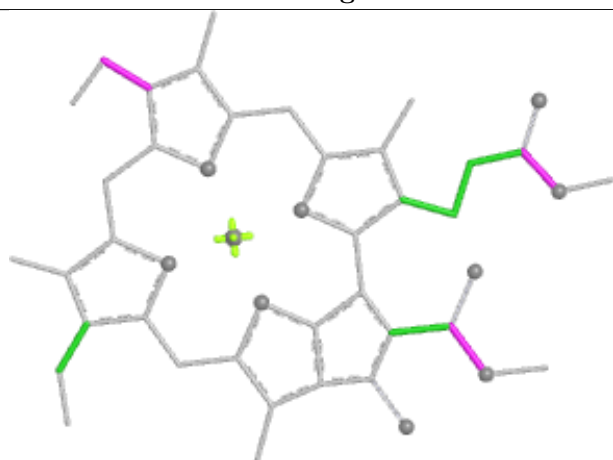
Ligand CLA R 611



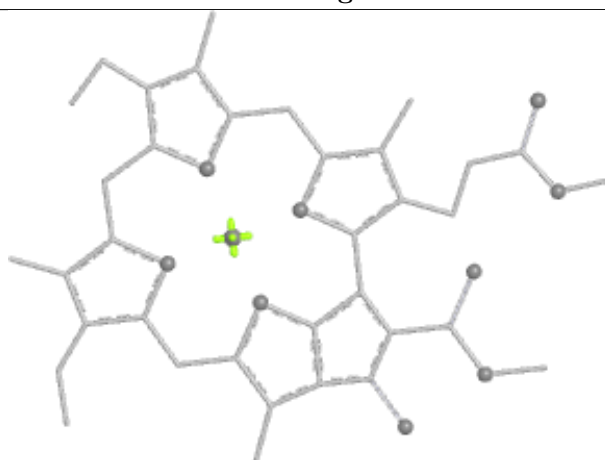
Bond lengths



Bond angles

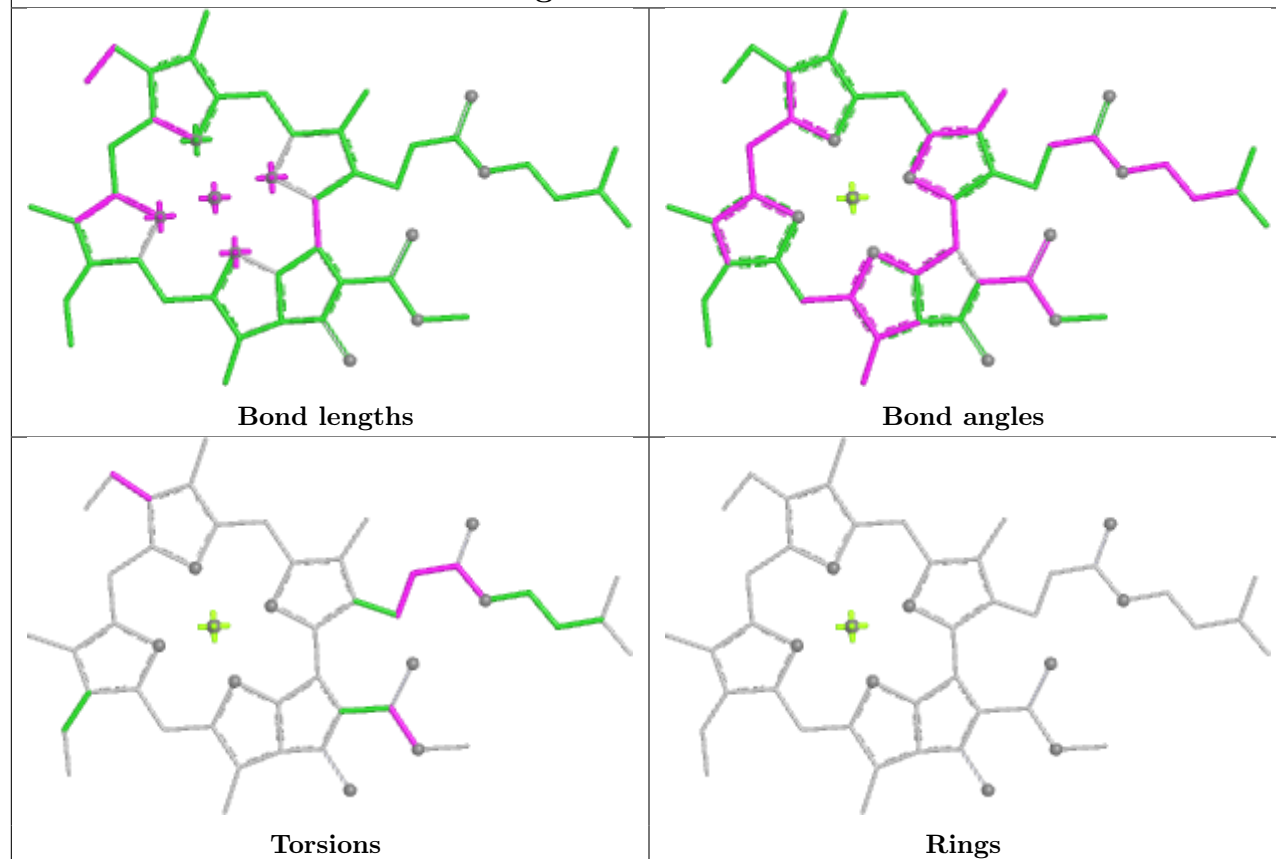


Torsions

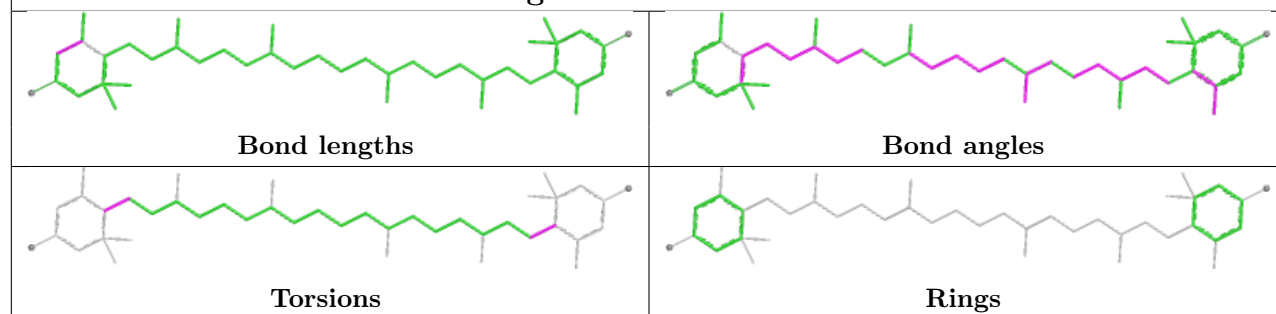


Rings

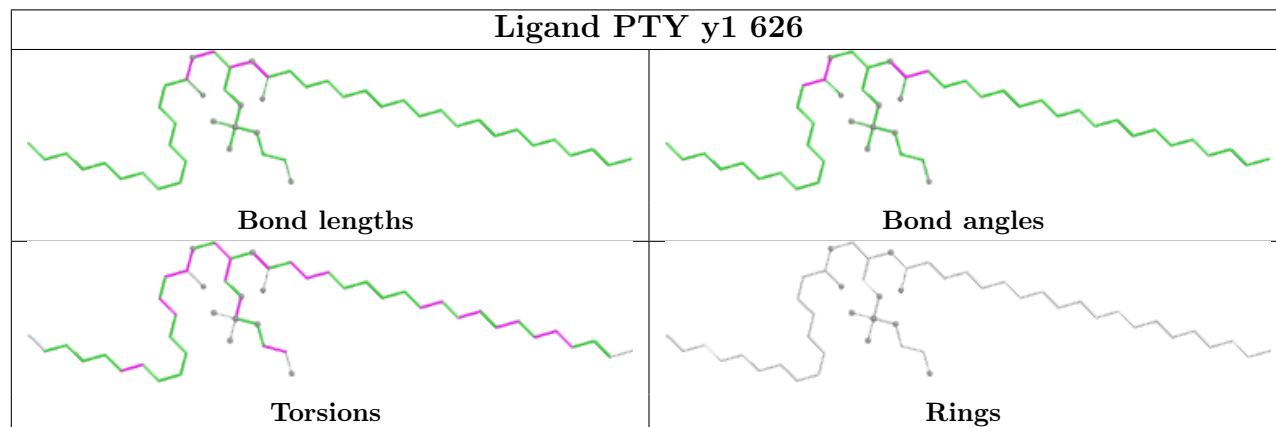
Ligand CLA S 617

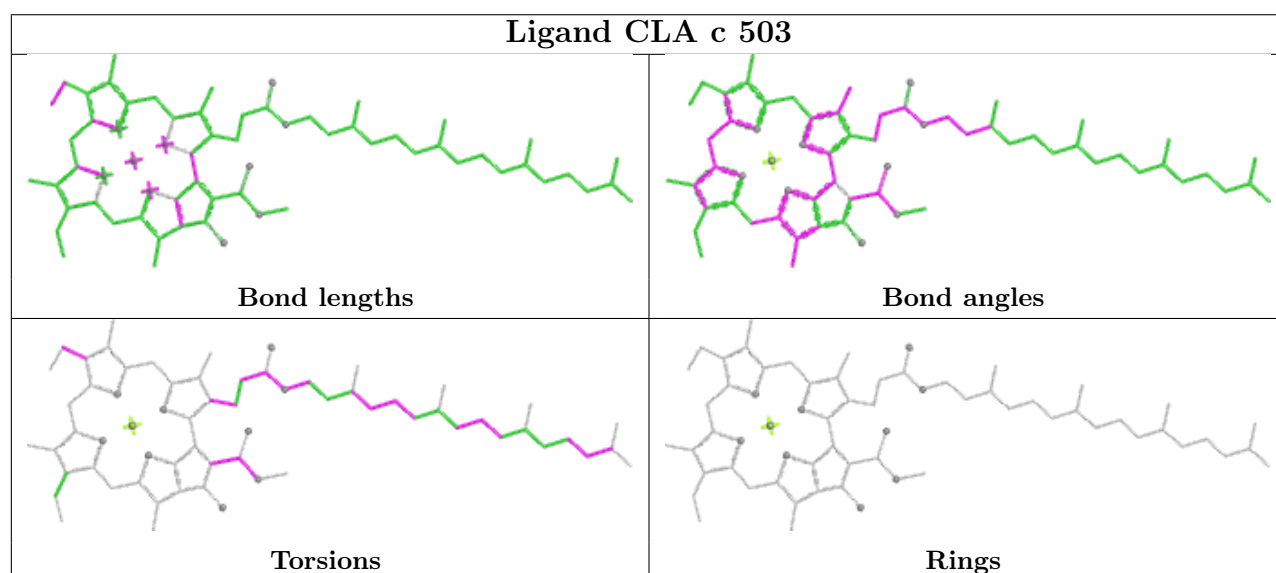
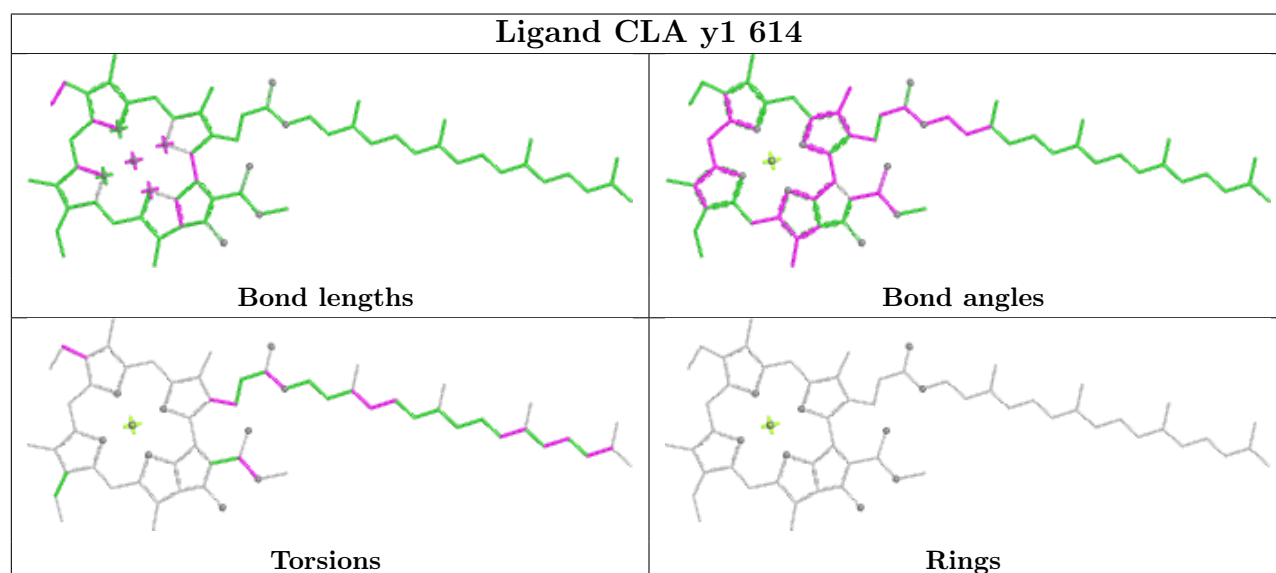
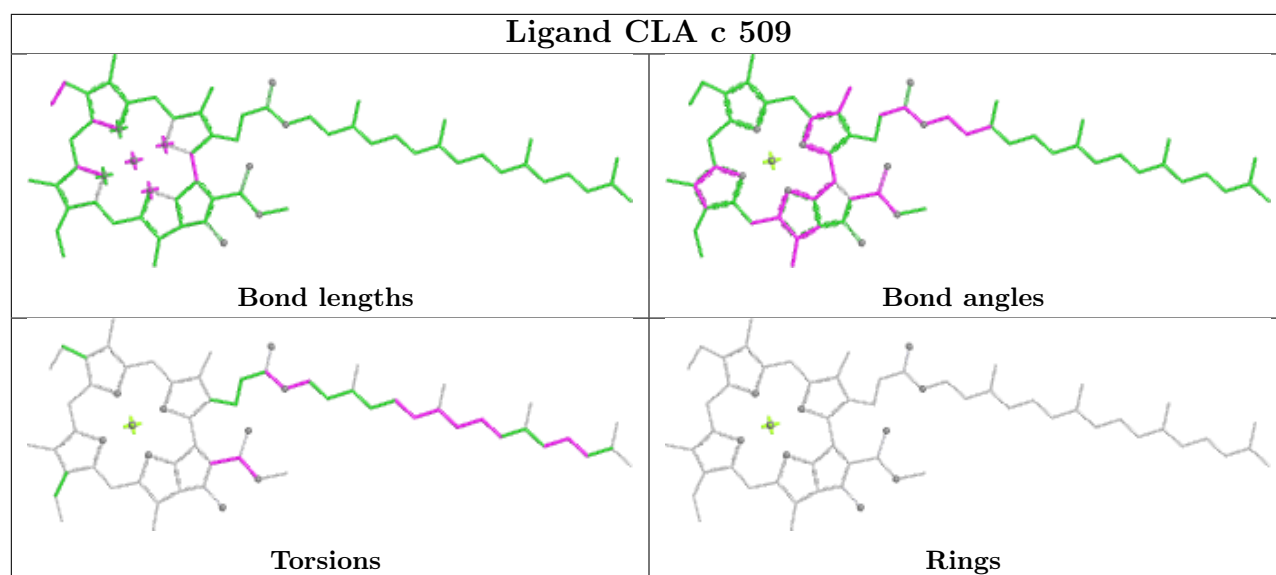


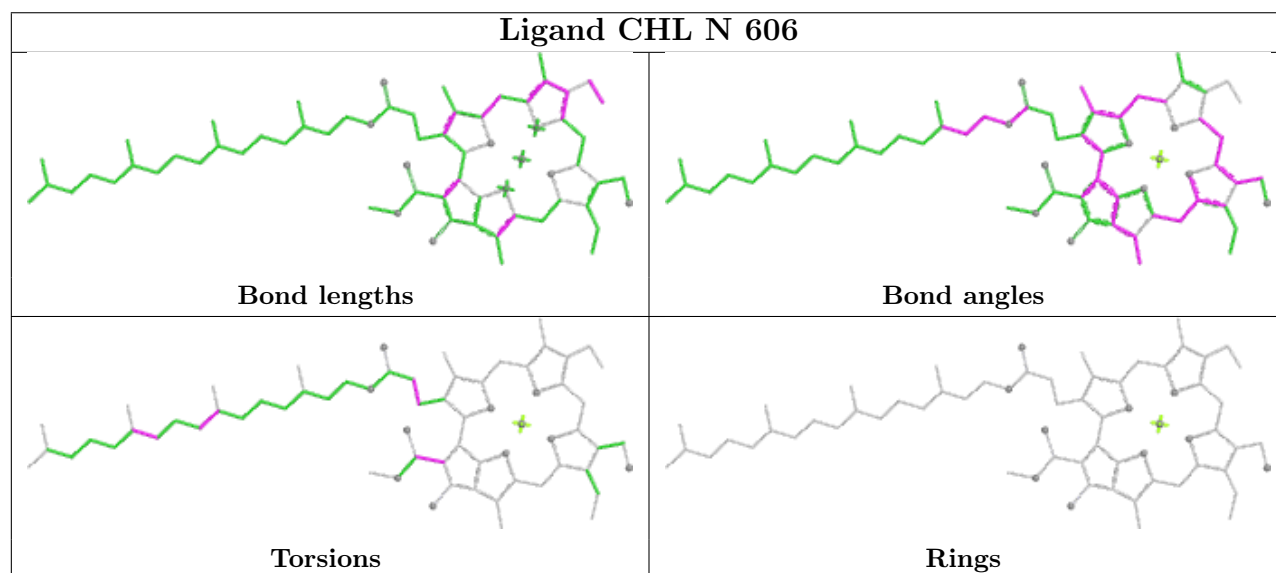
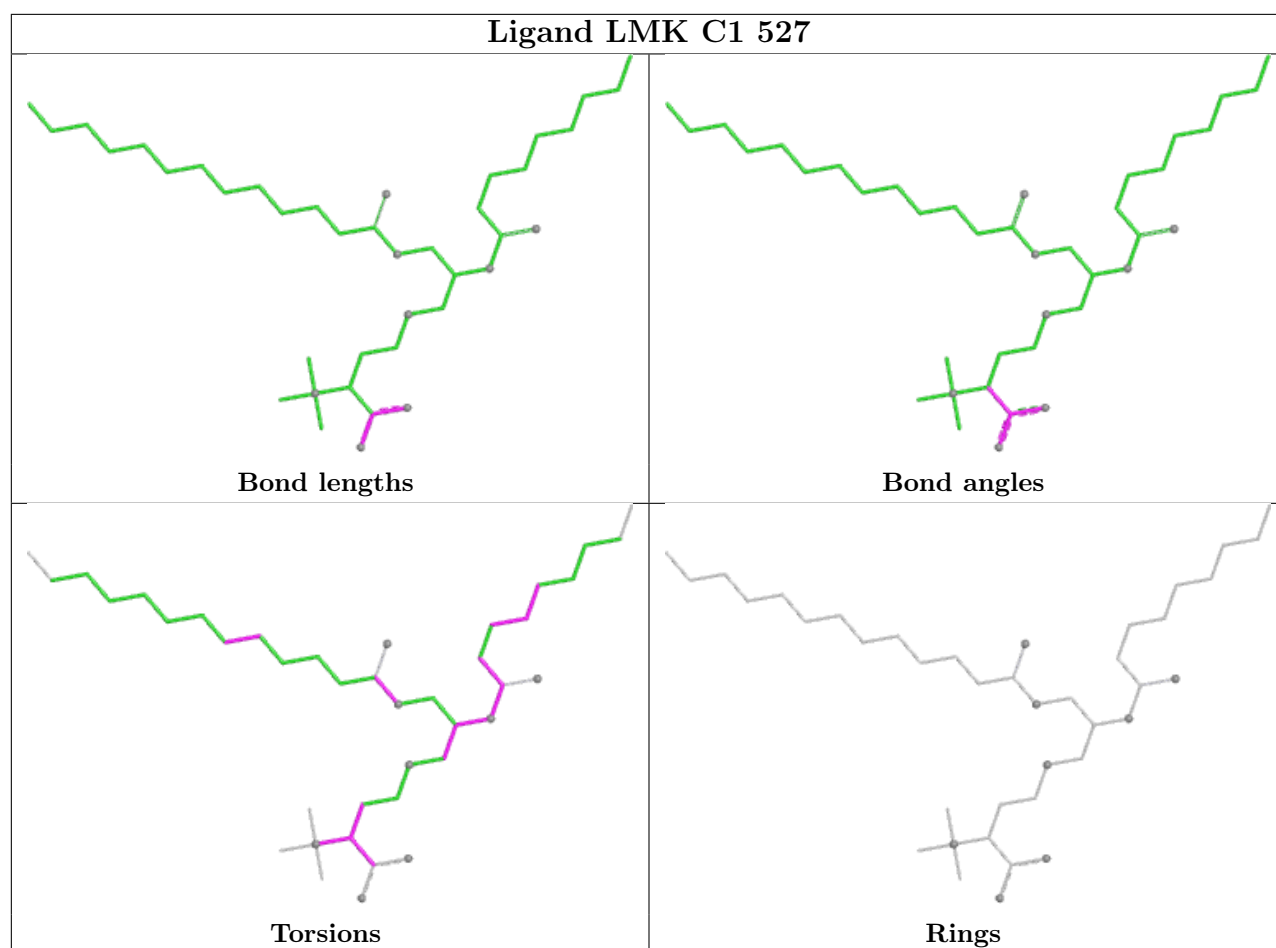
Ligand LUT S1 620

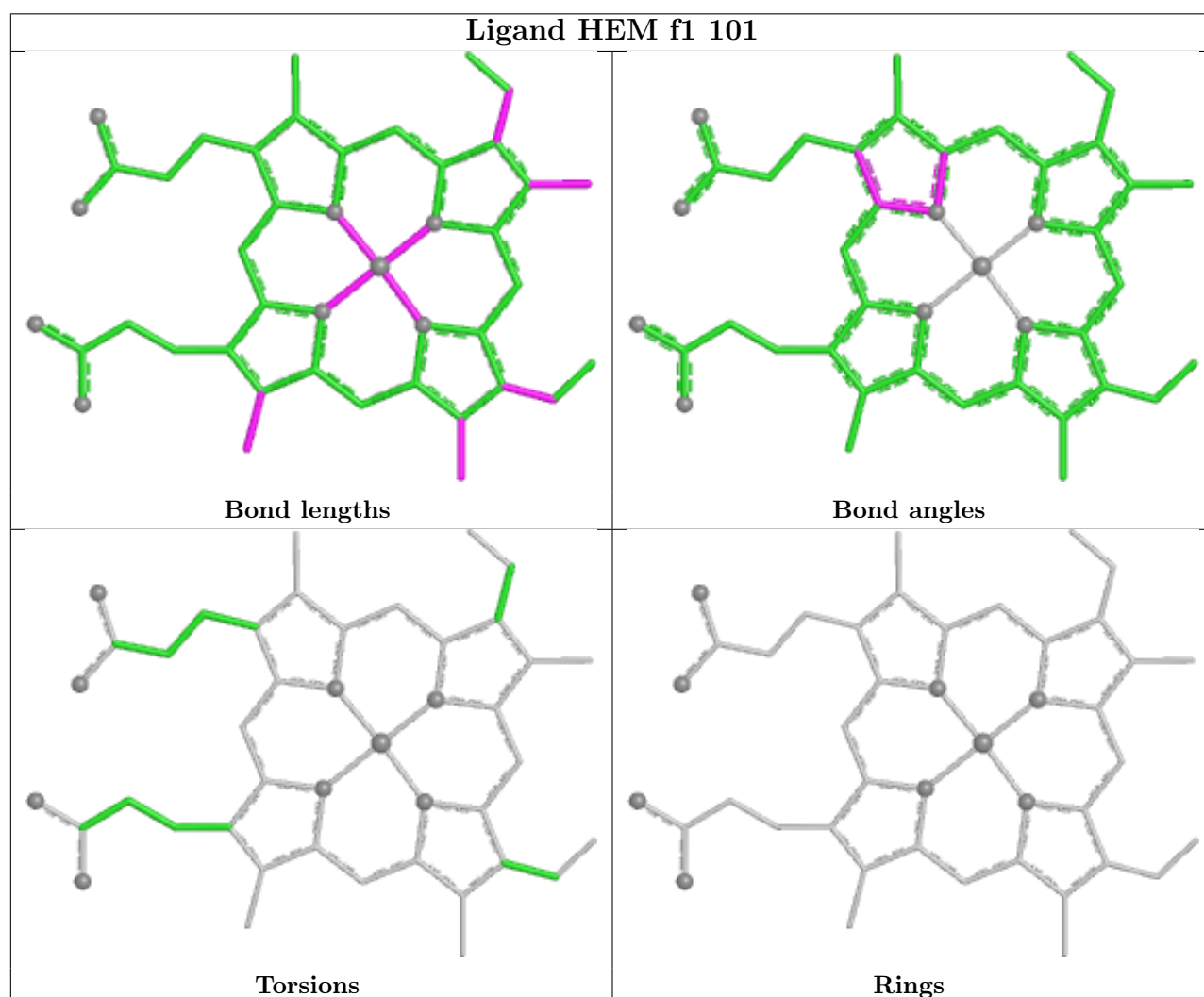
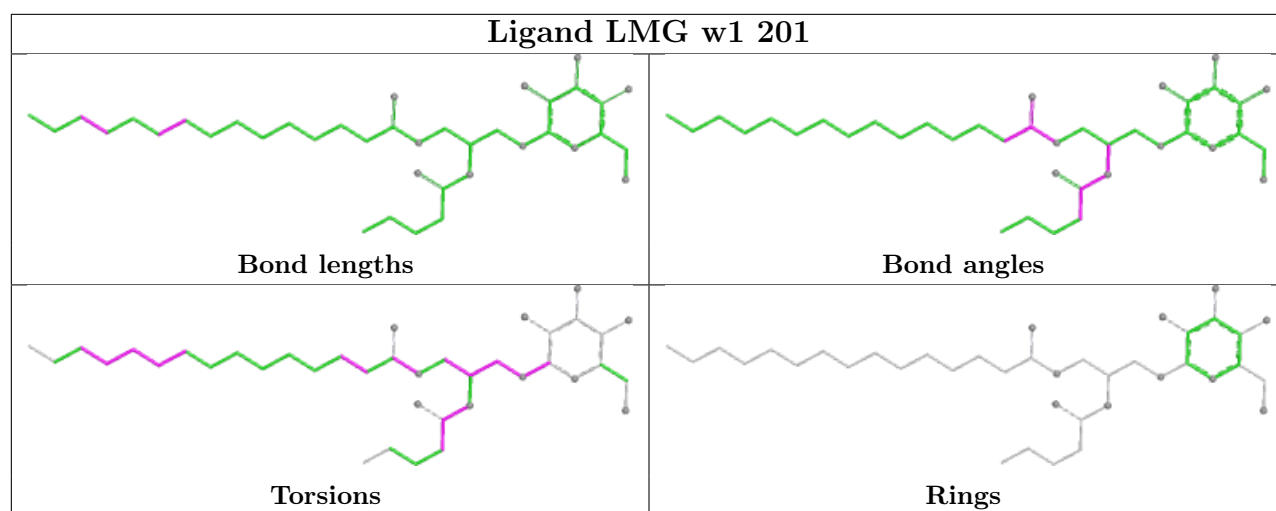


Ligand PTY y1 626

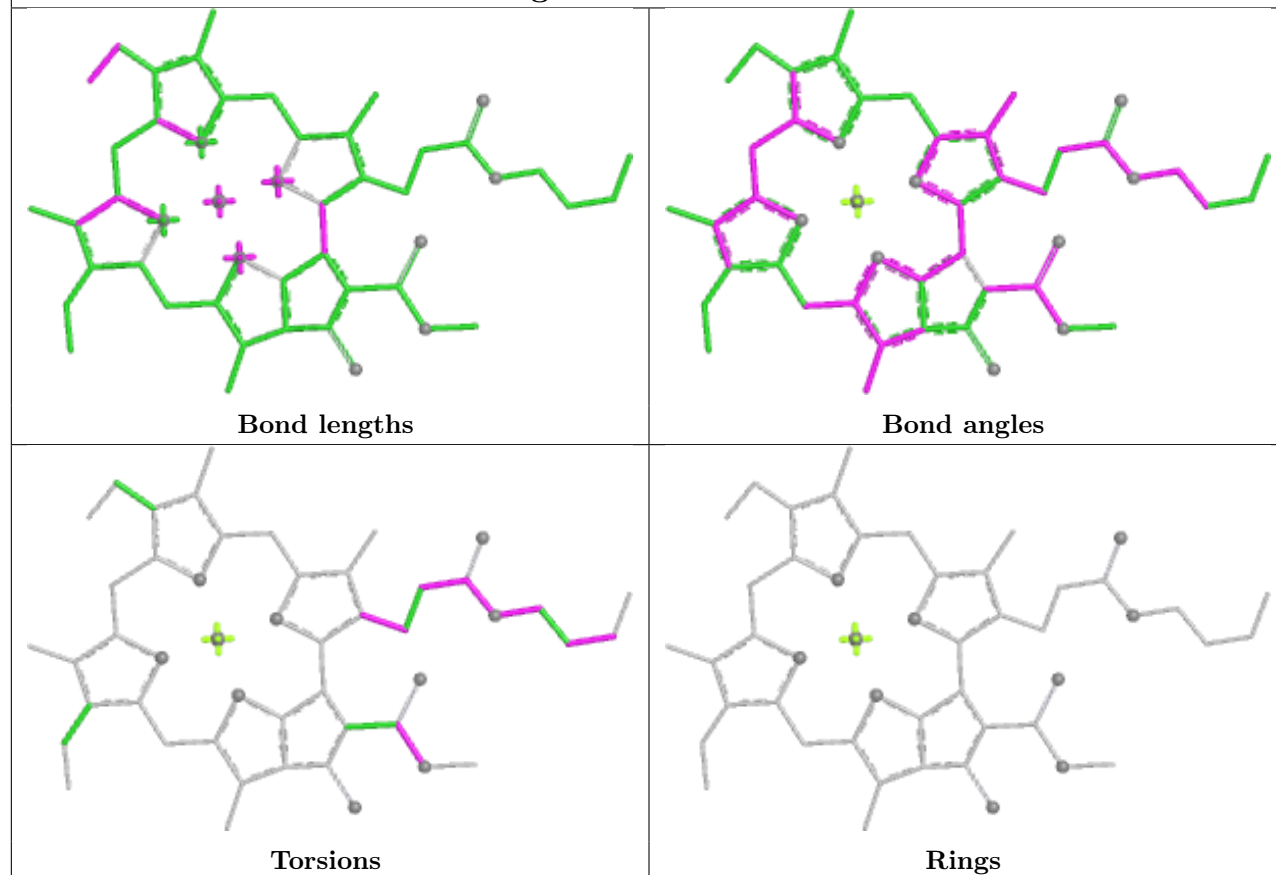




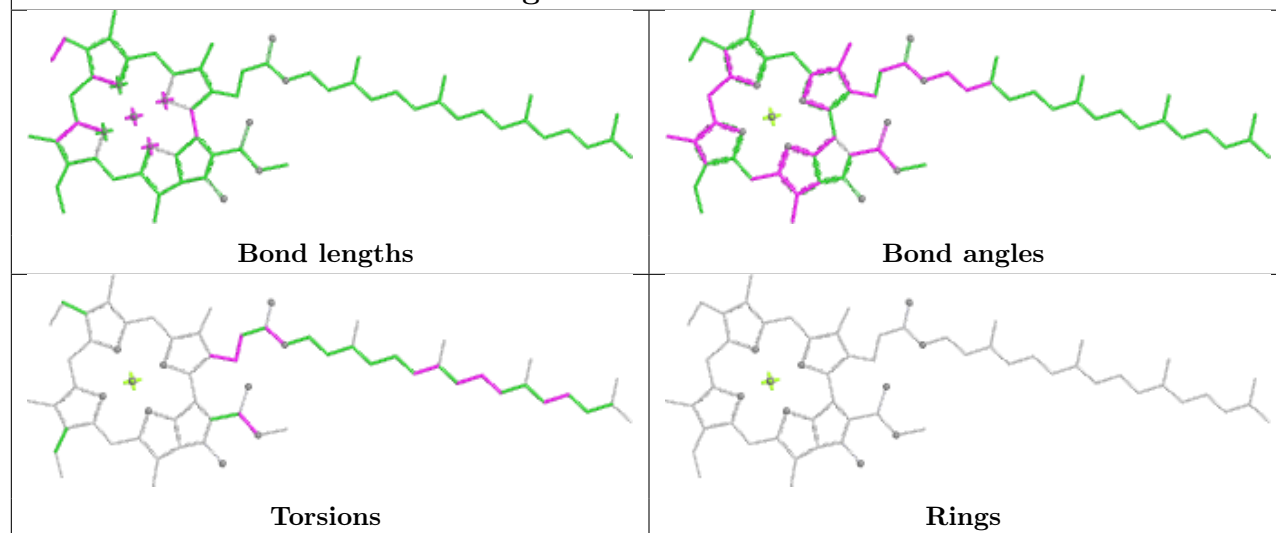


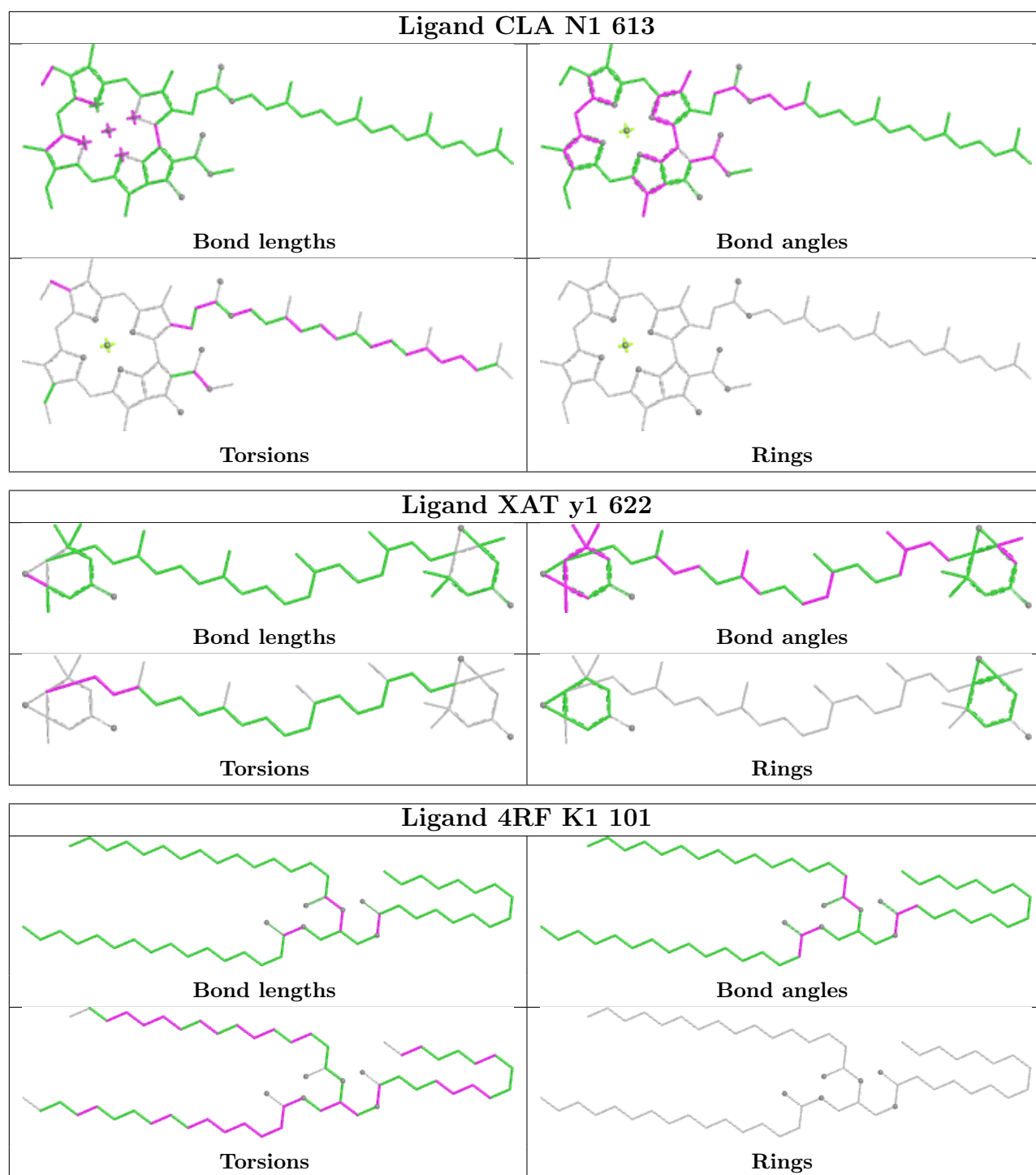


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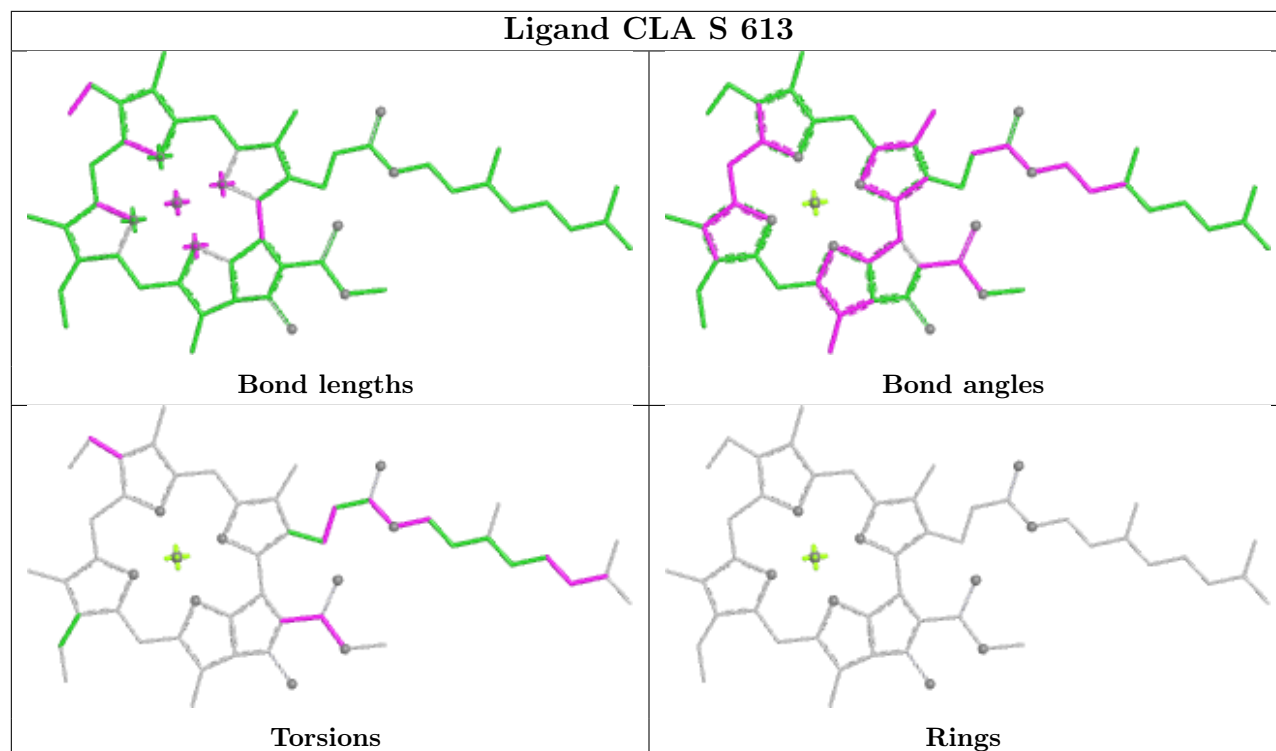


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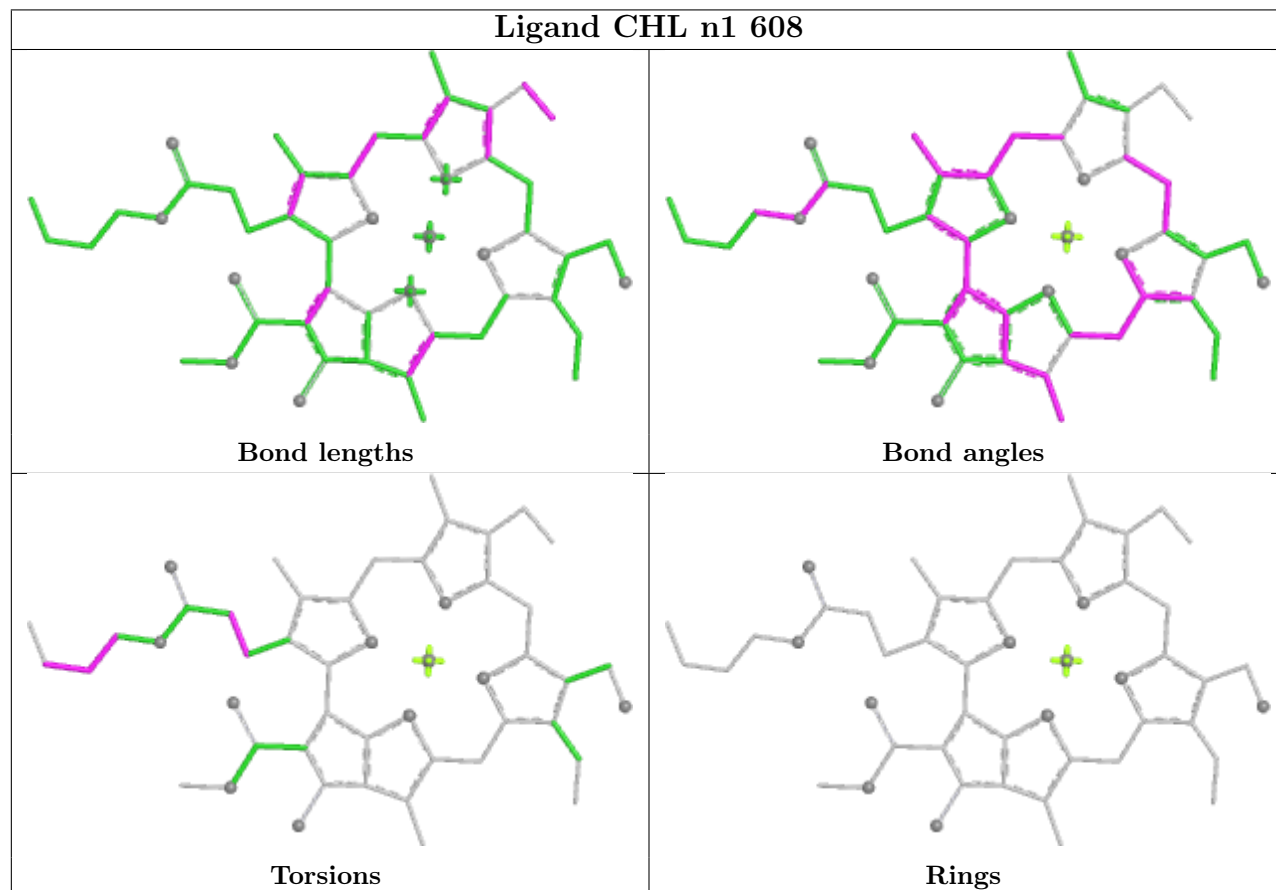


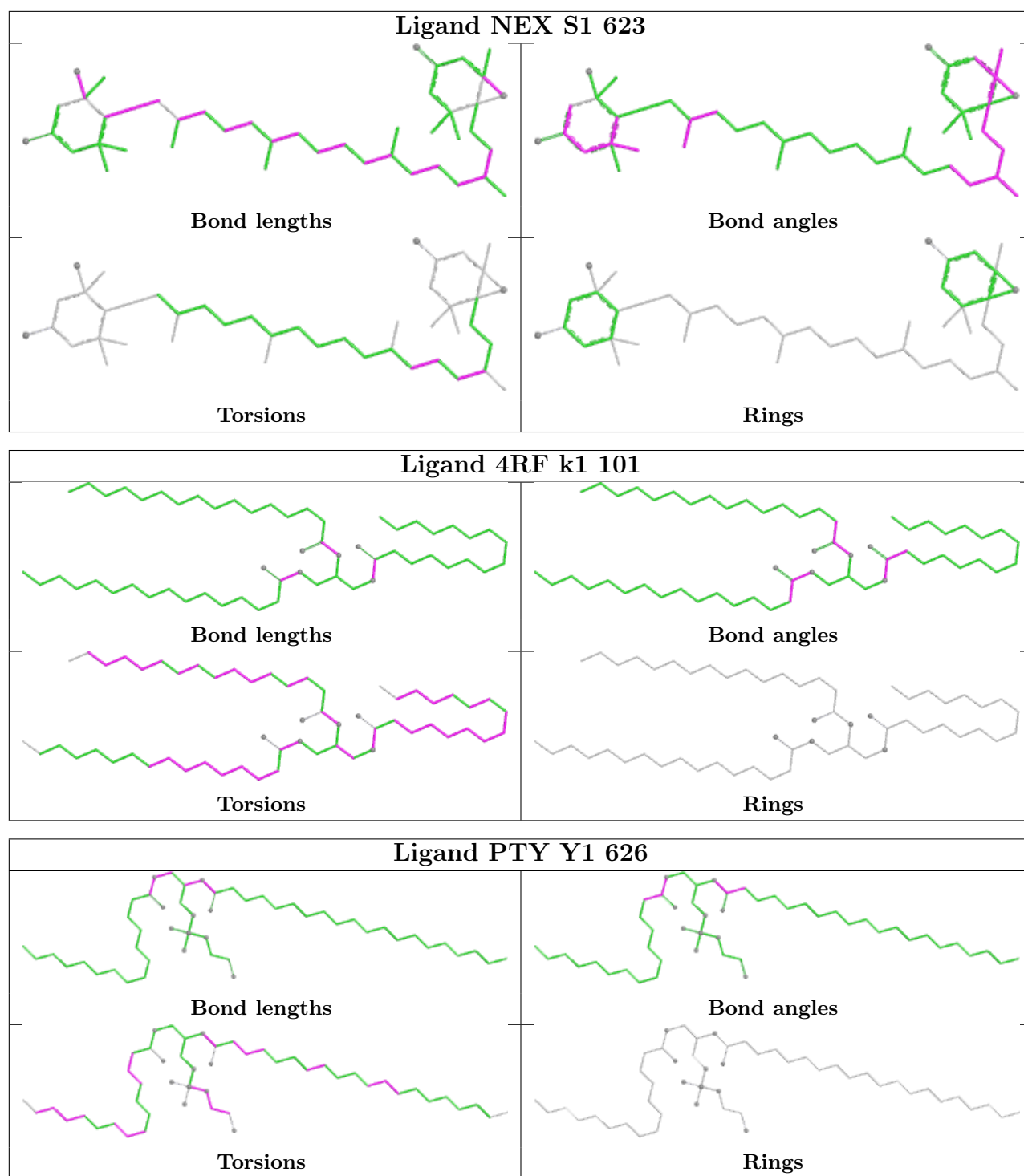


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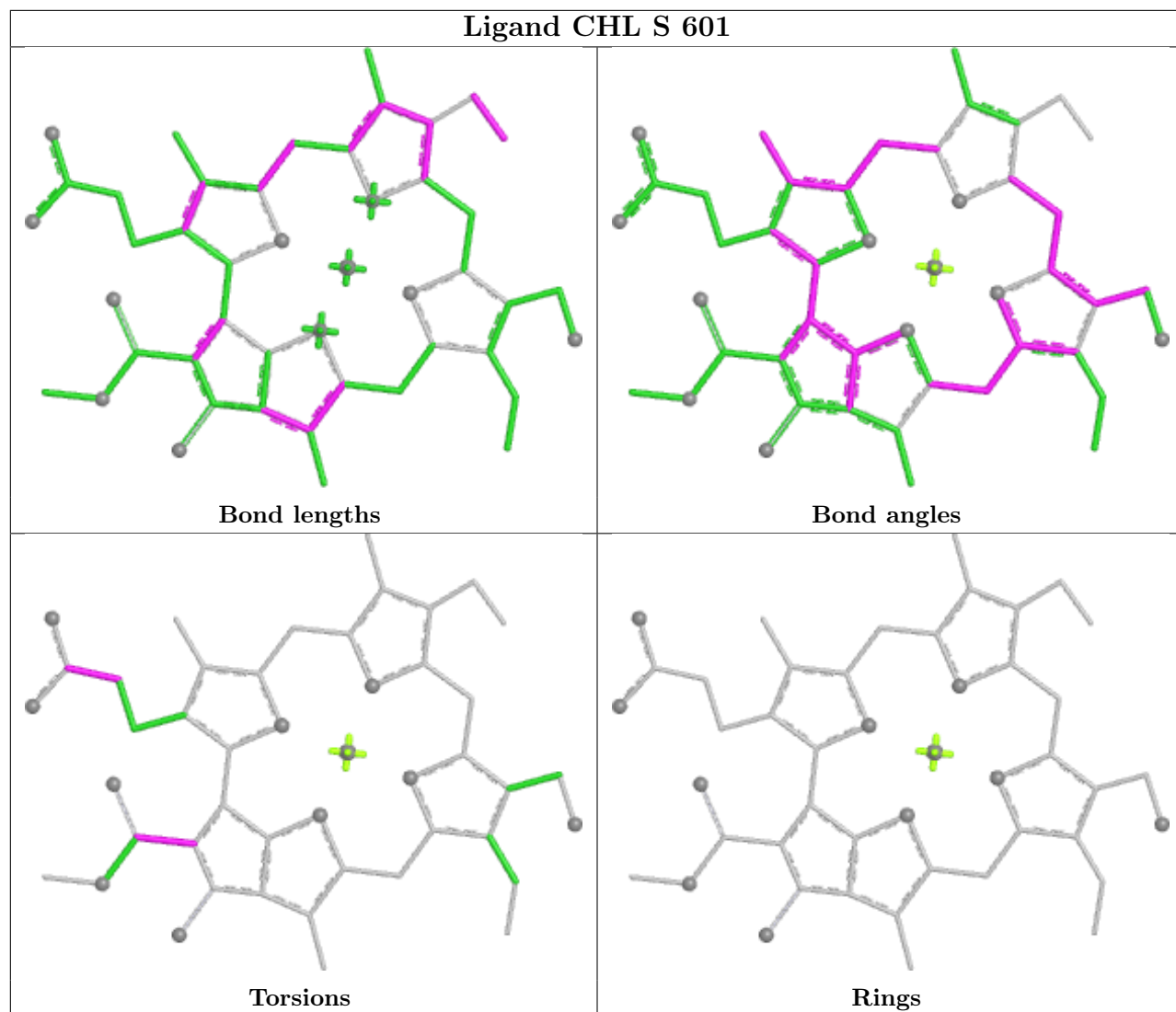


Ligand CHL n1 608

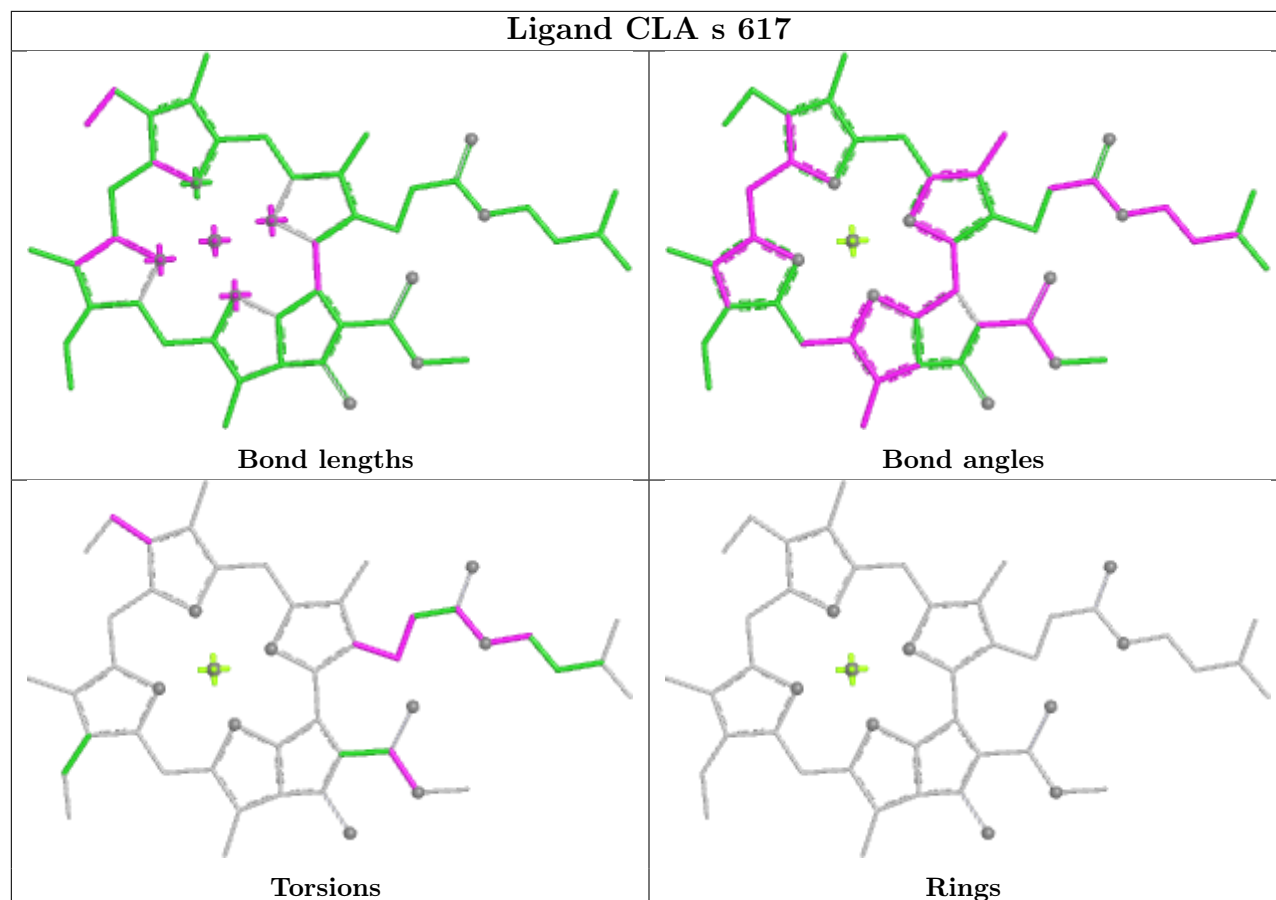




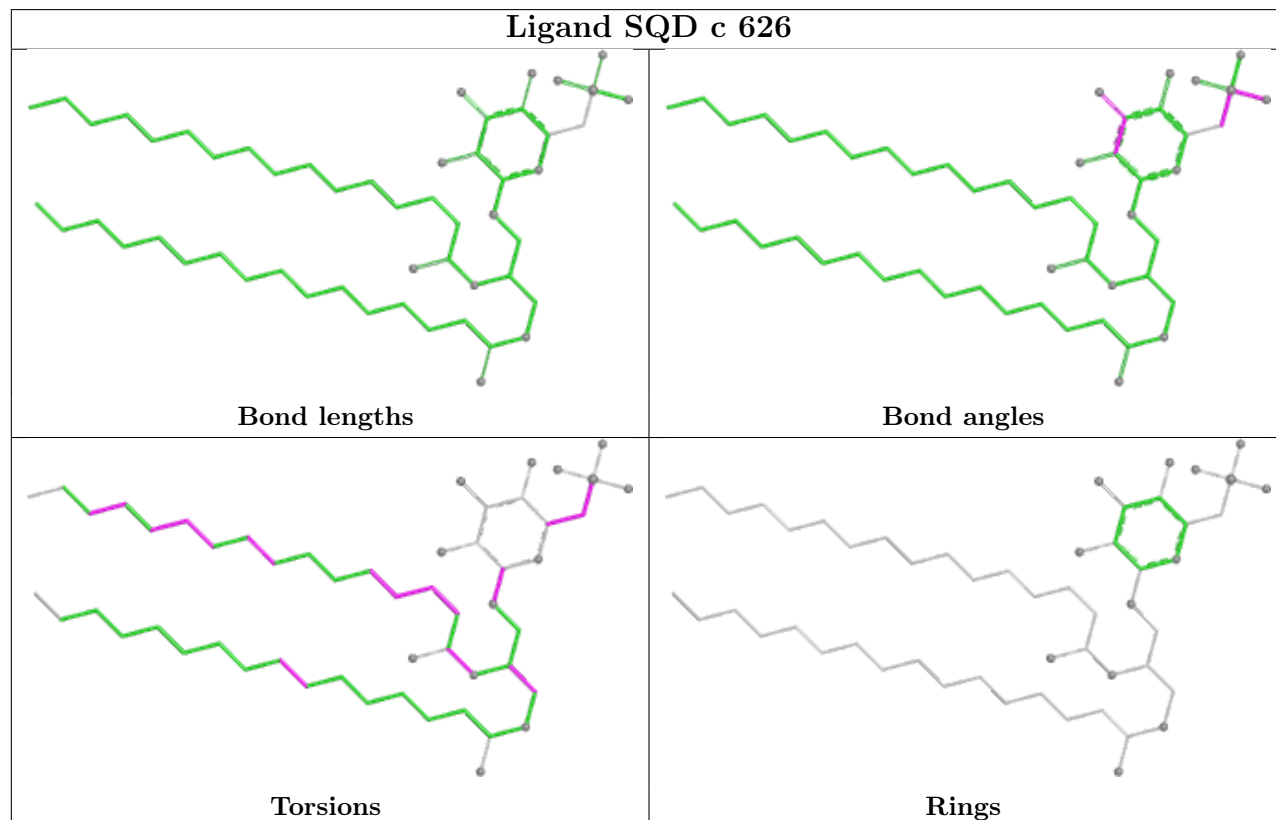
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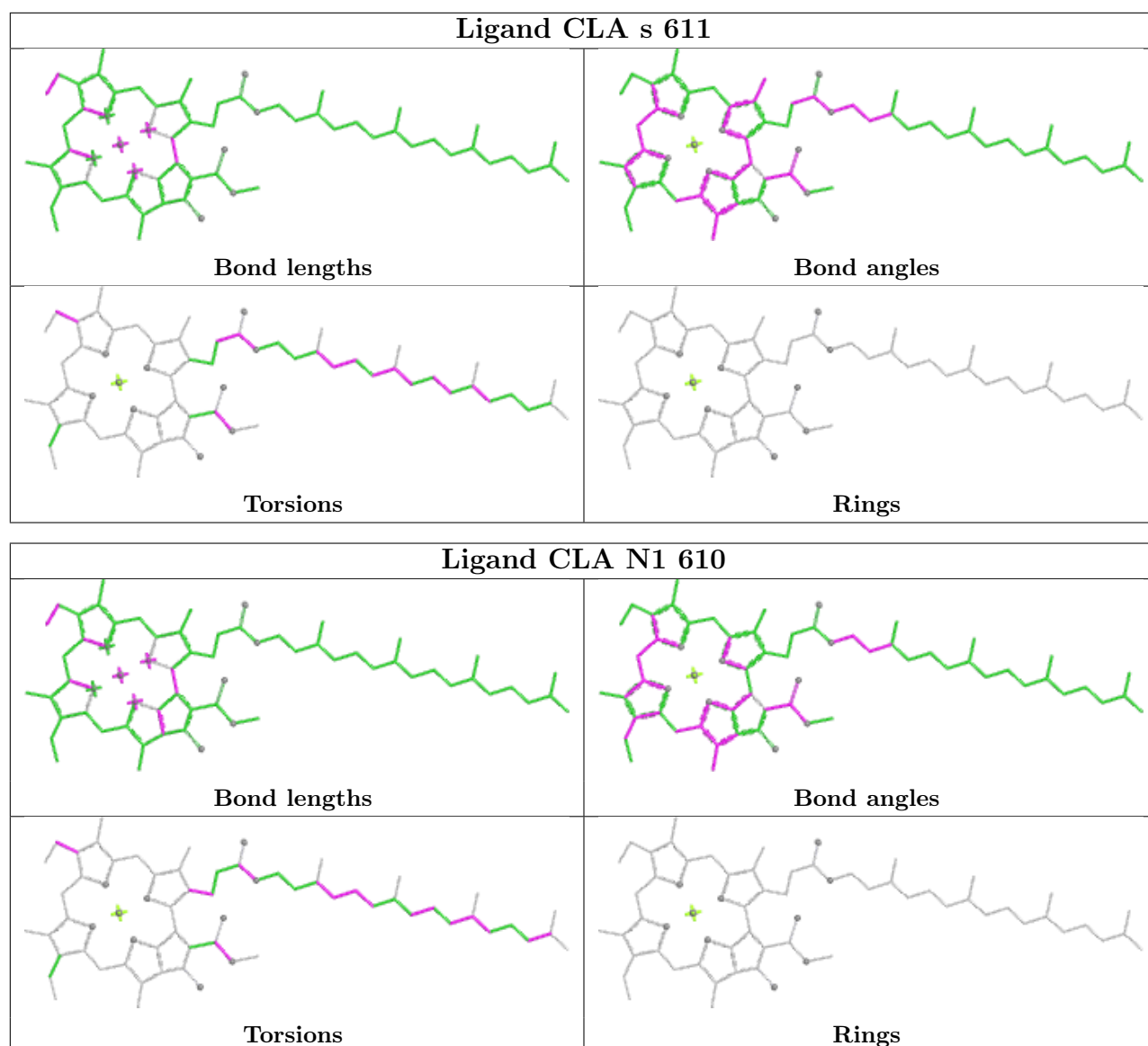


Ligand CLA s 617

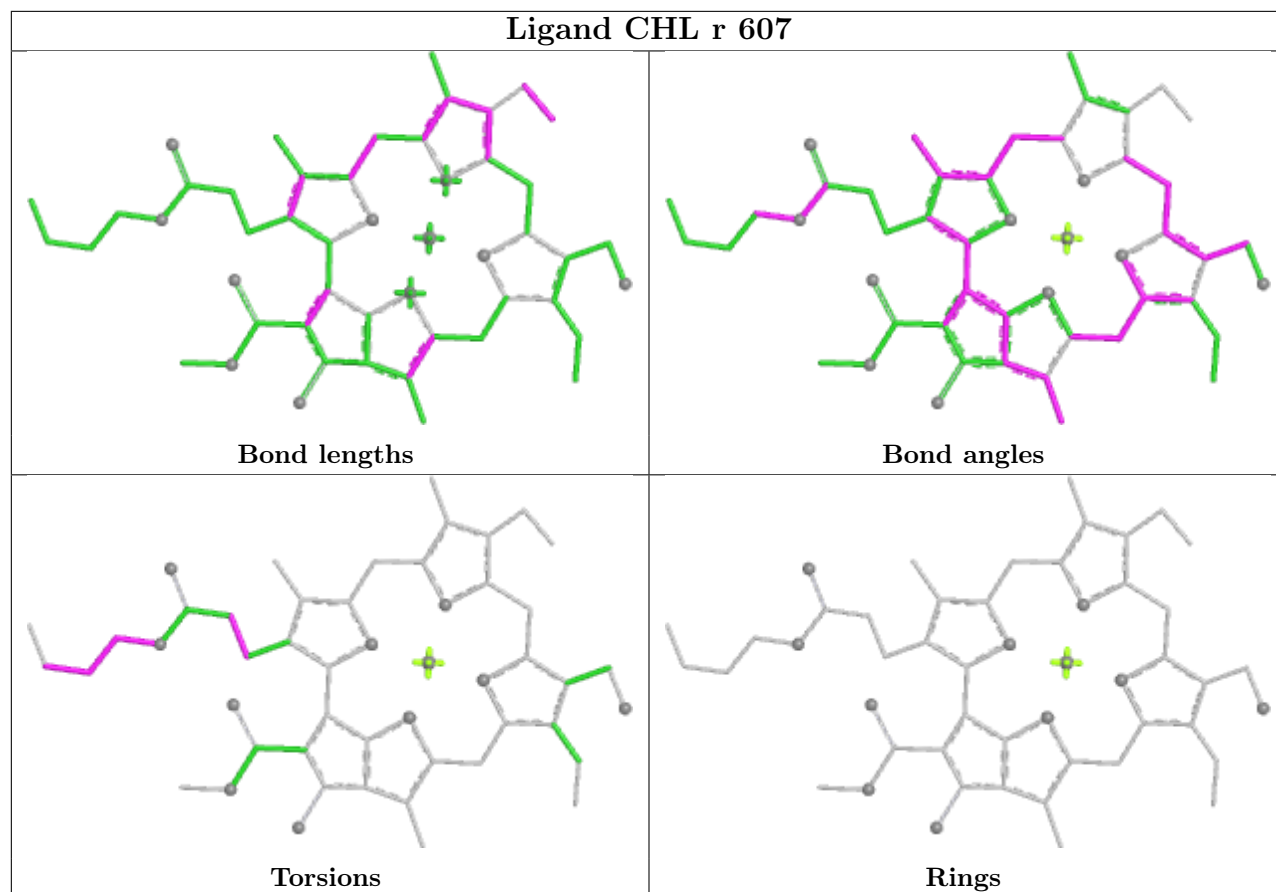


Ligand SQD c 626

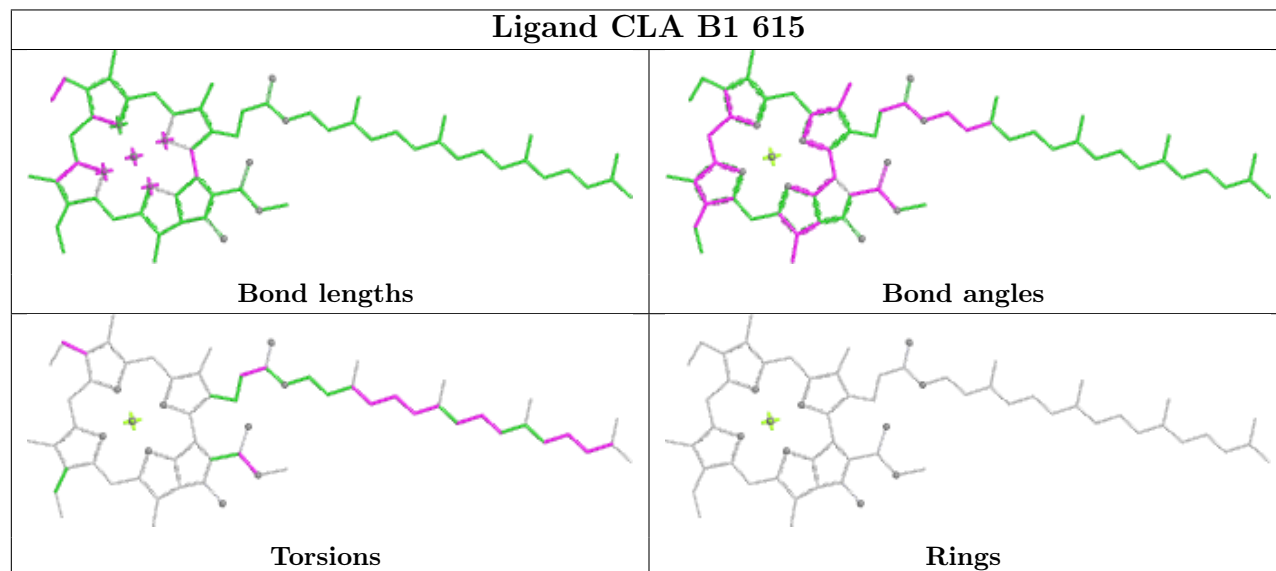


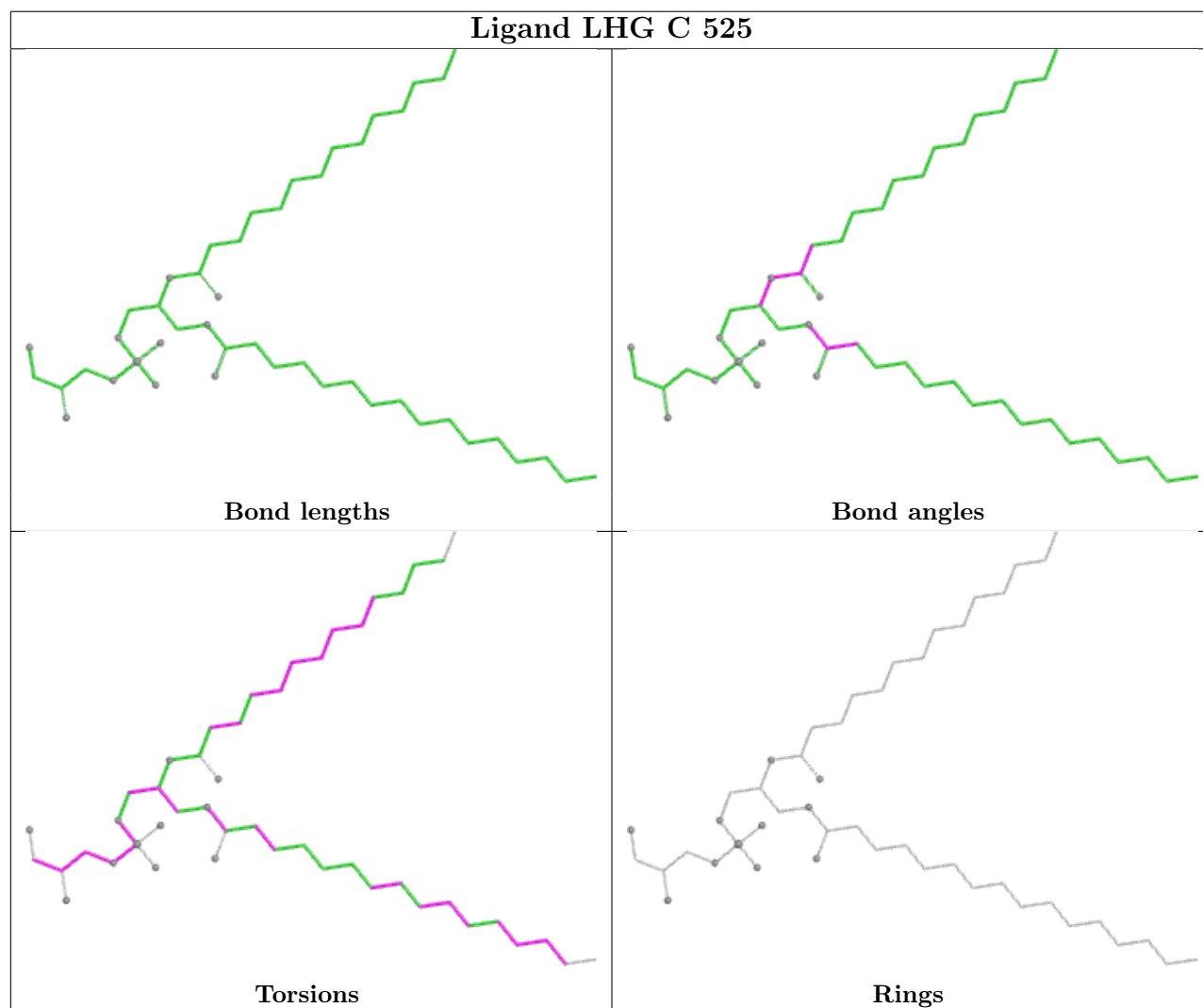
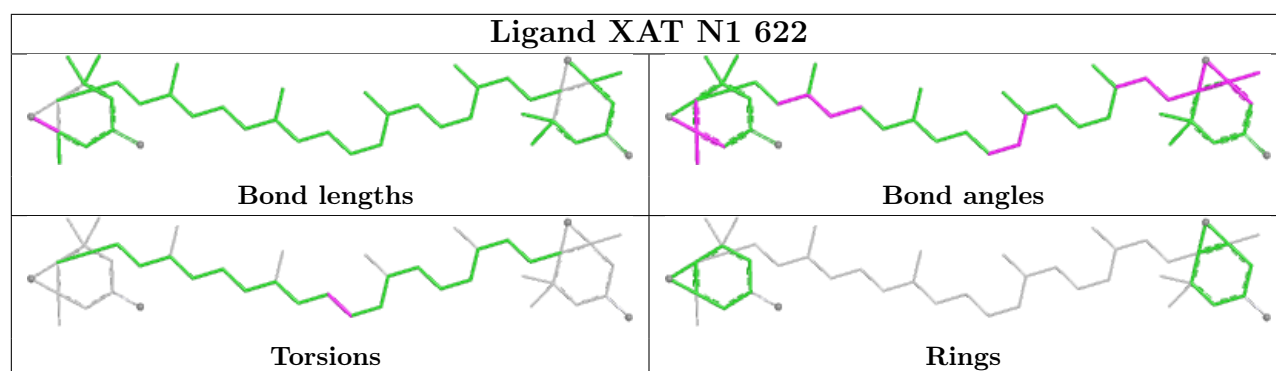


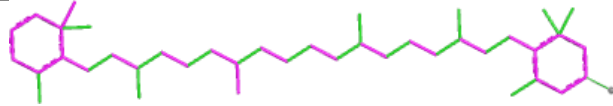
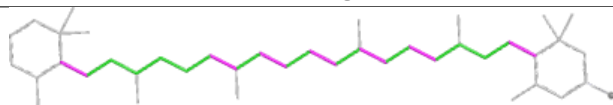
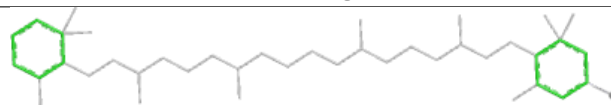
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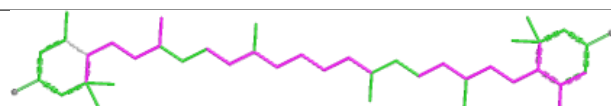
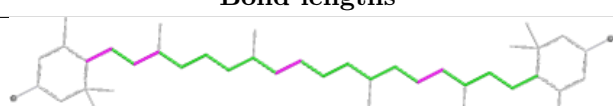
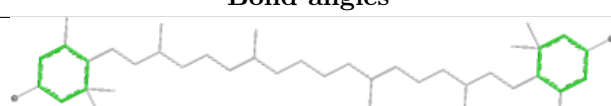


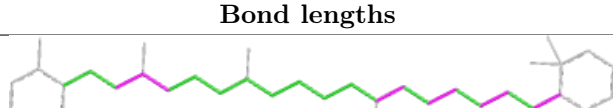
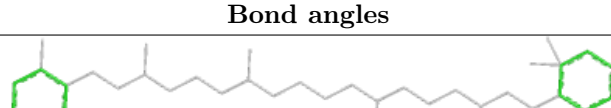
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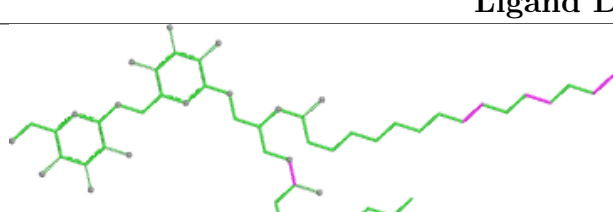
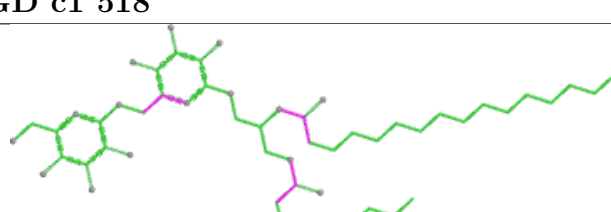
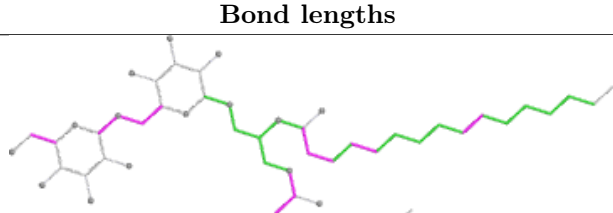
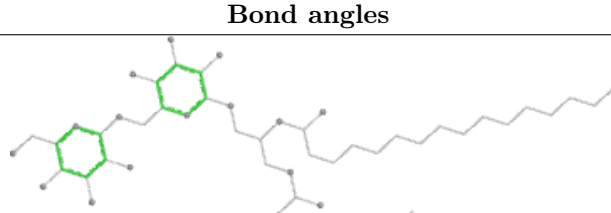


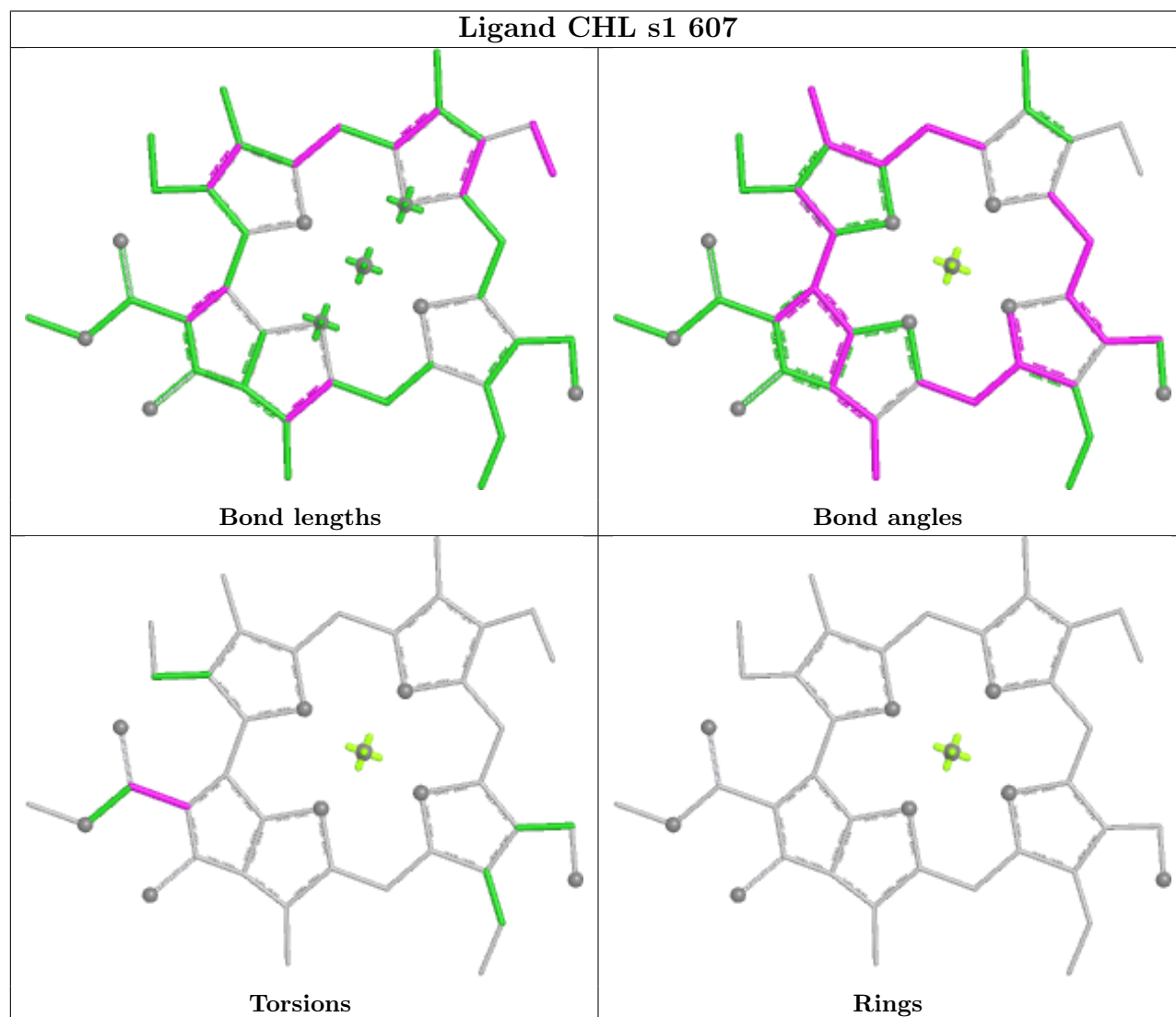
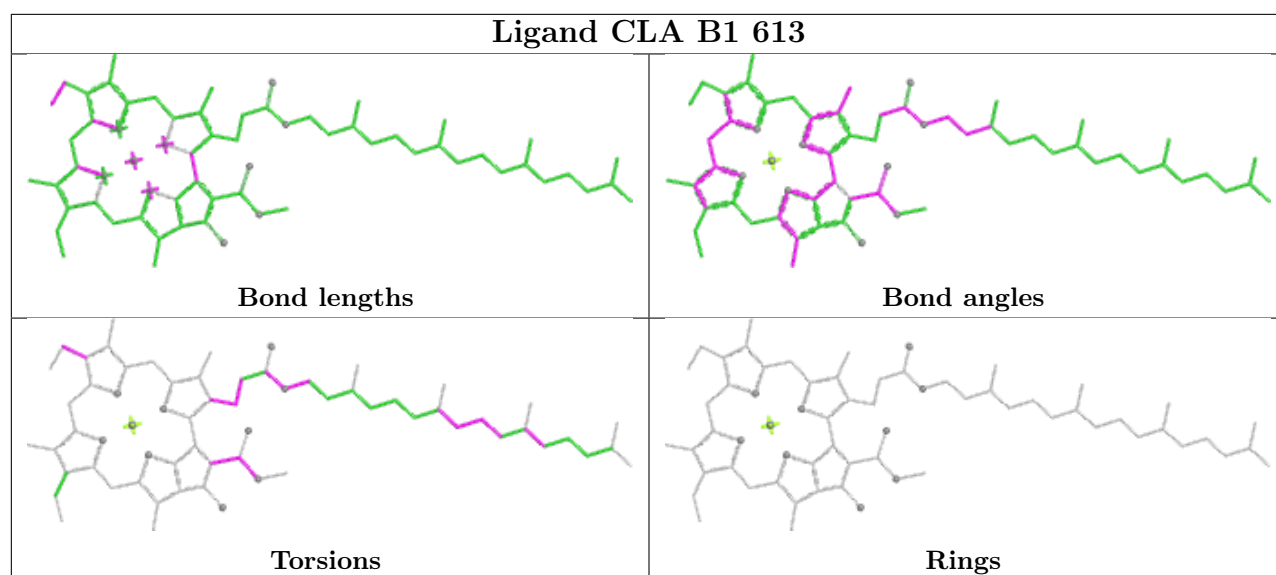


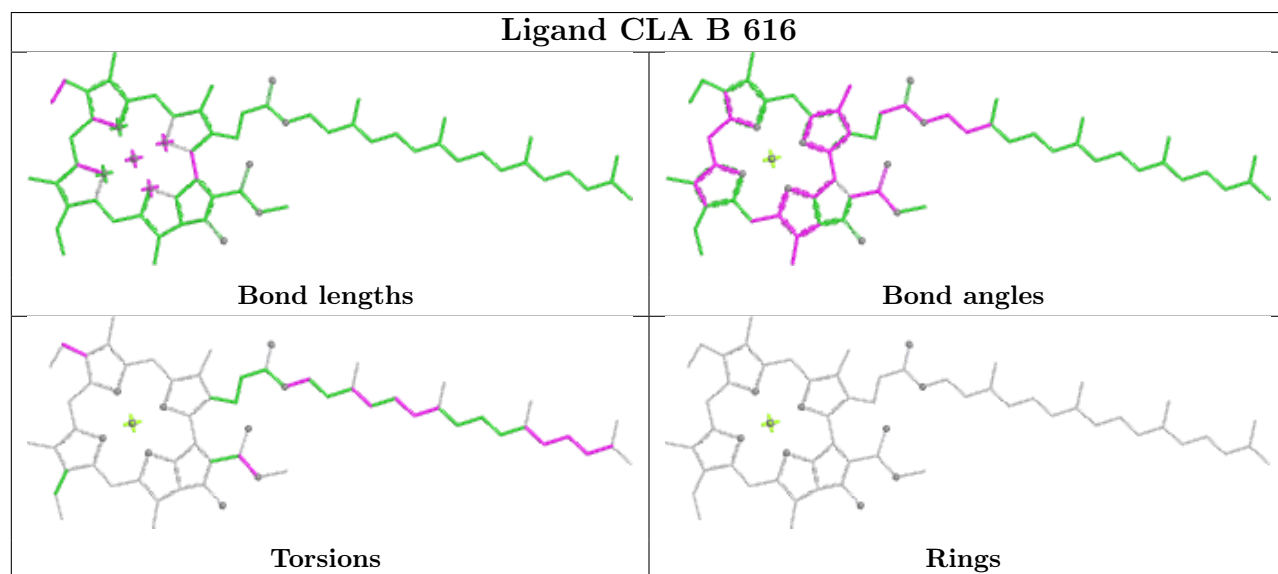
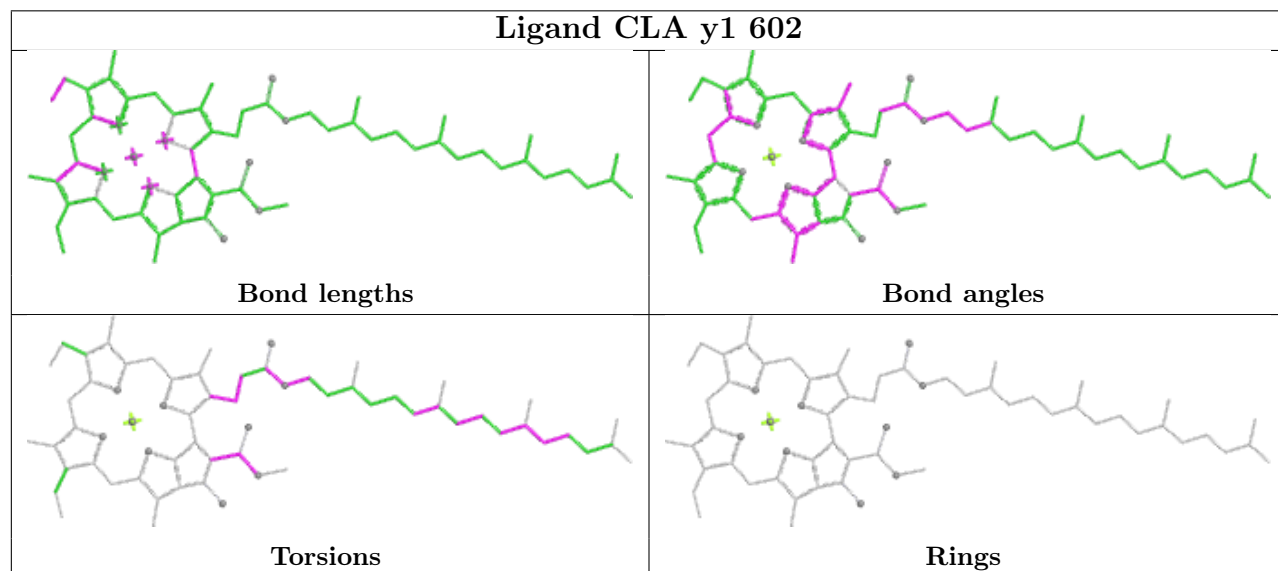
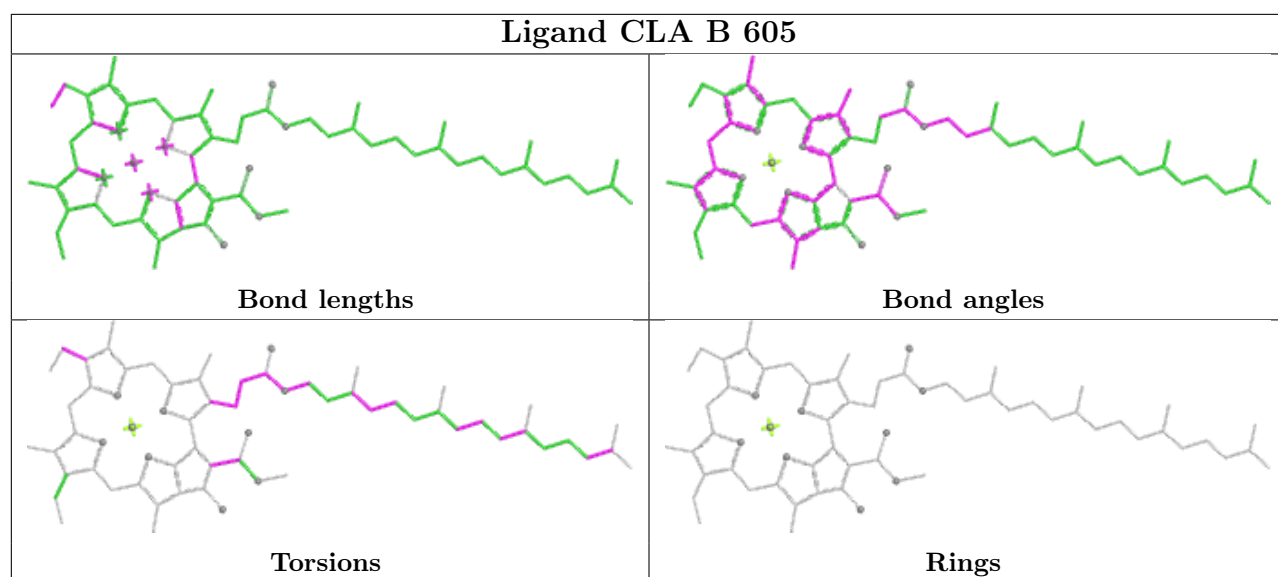
Ligand RRX h1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

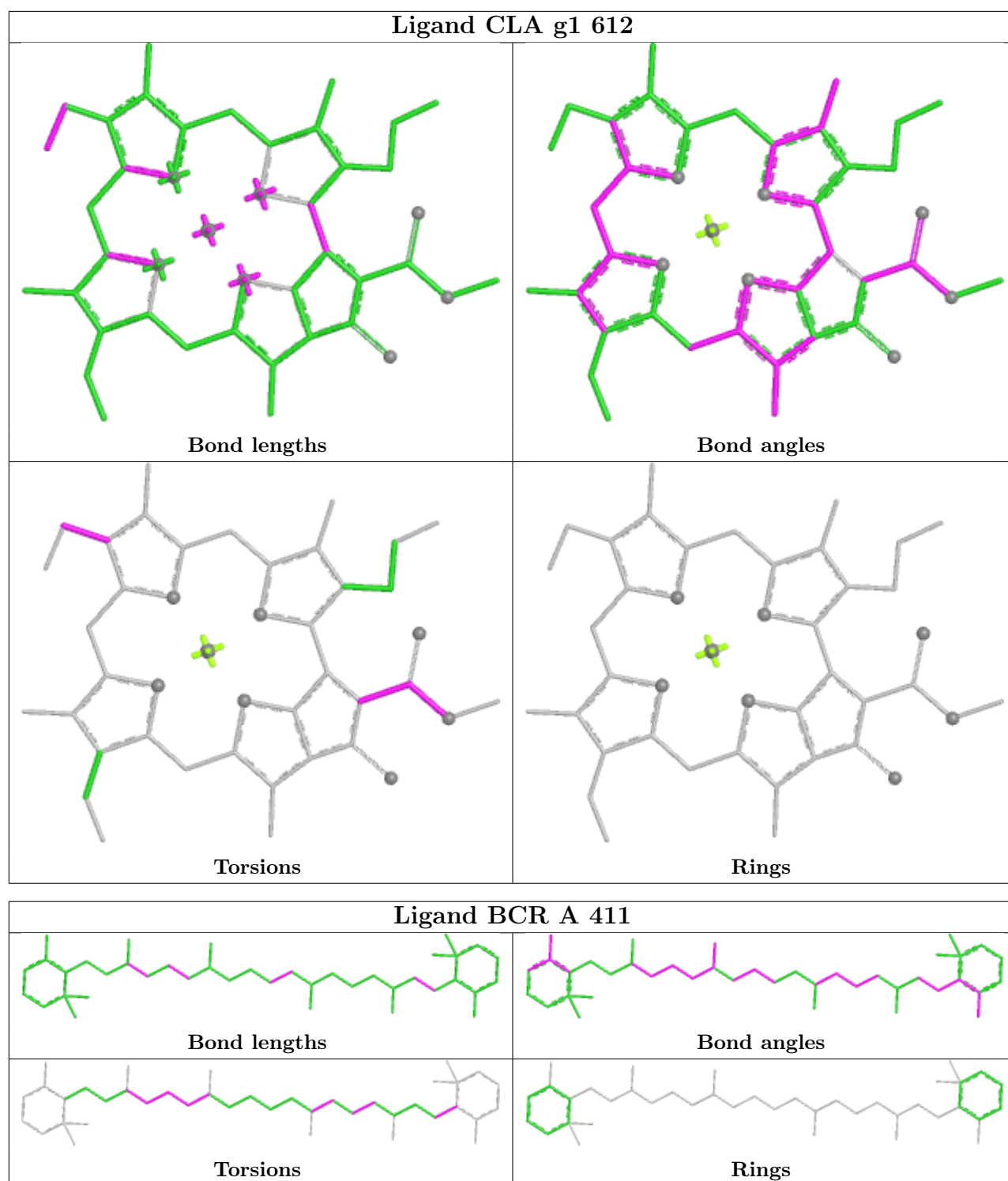
Ligand LUT R1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

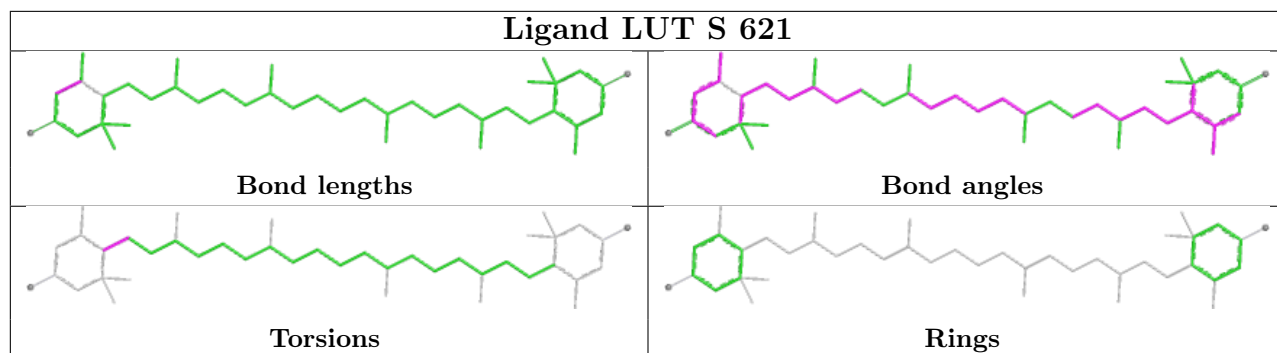
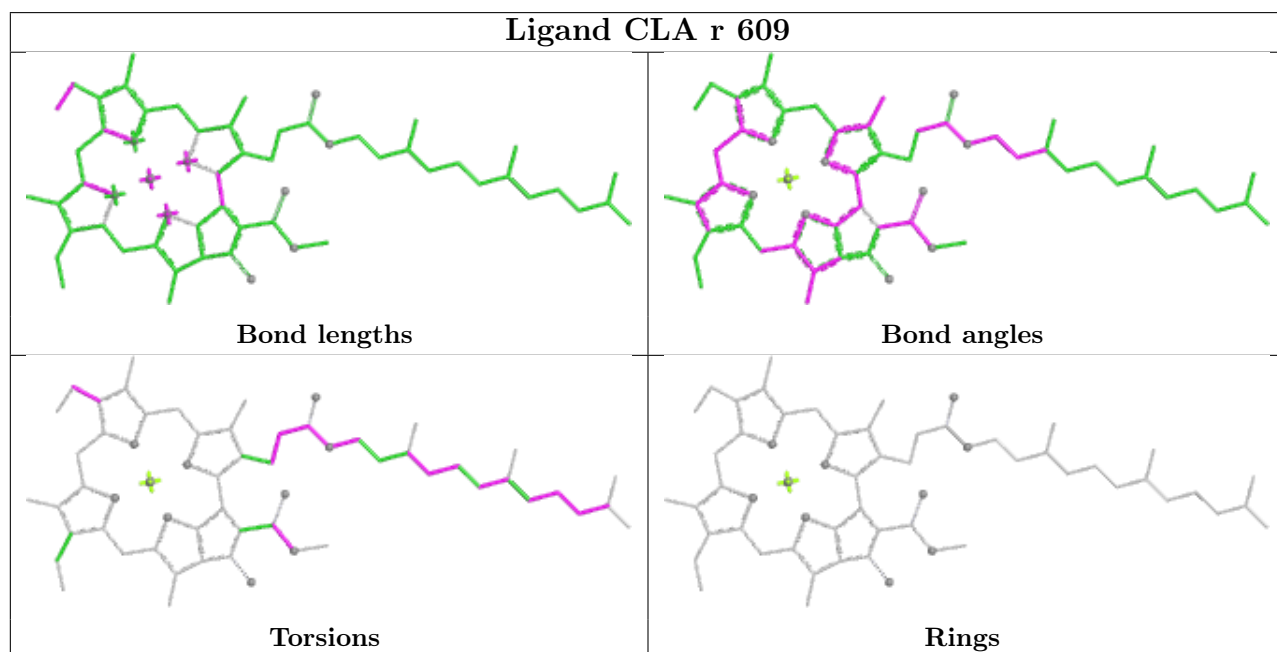
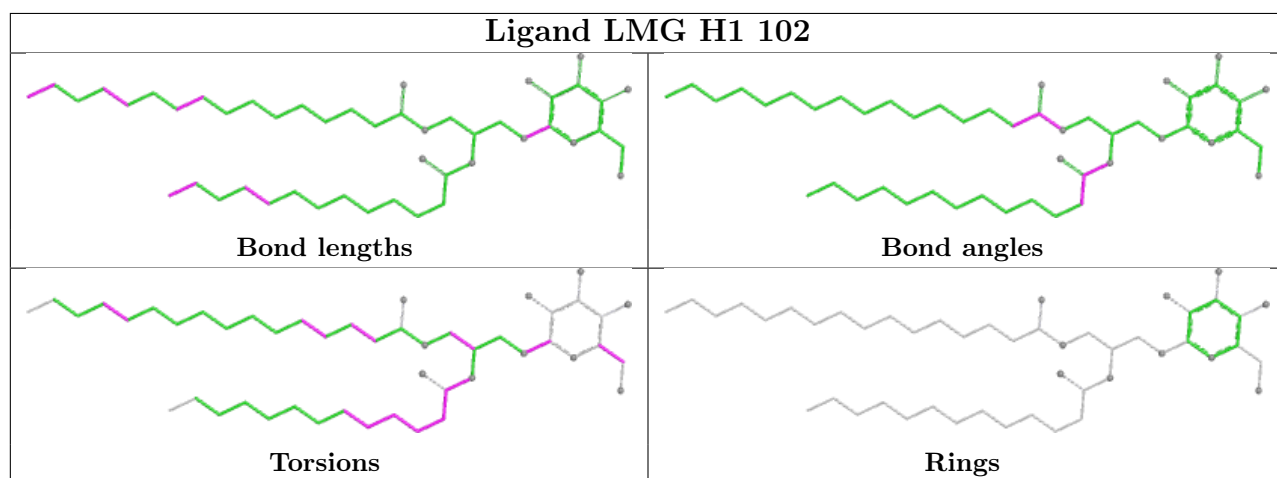
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

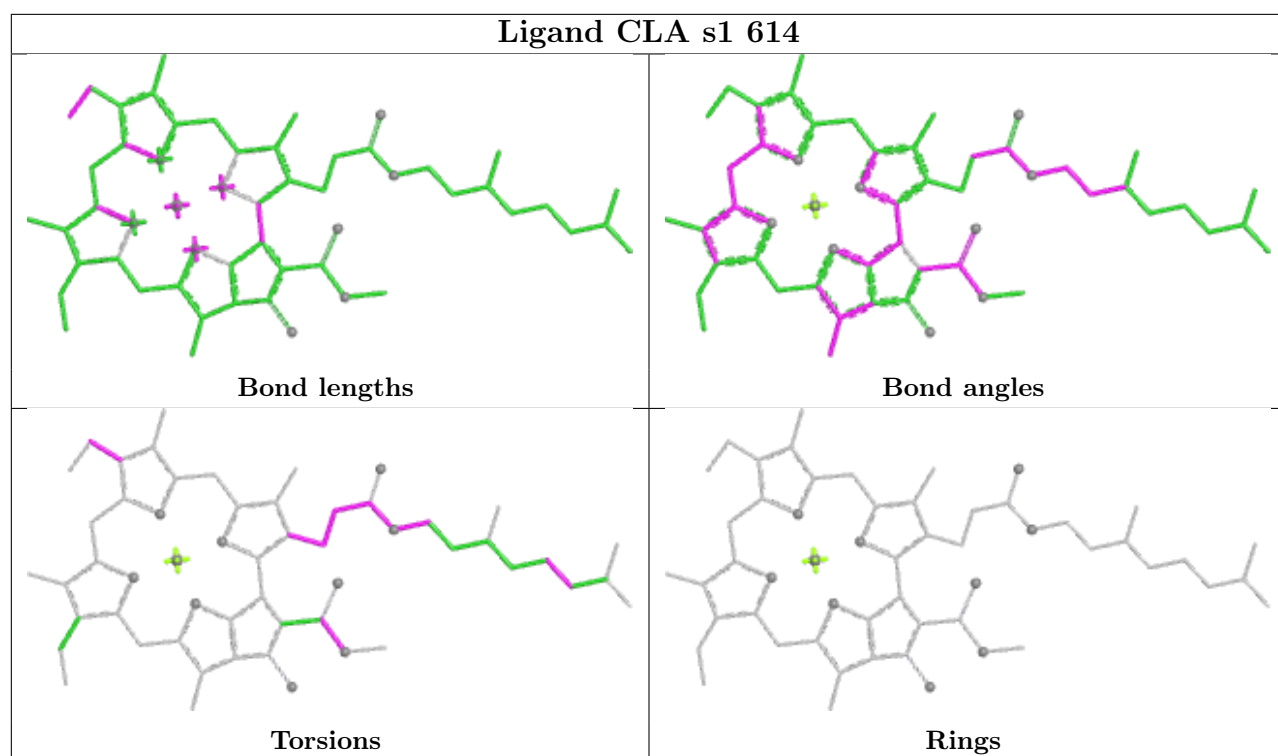
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Bond lengths	Bond angles
	
Torsions	Rings

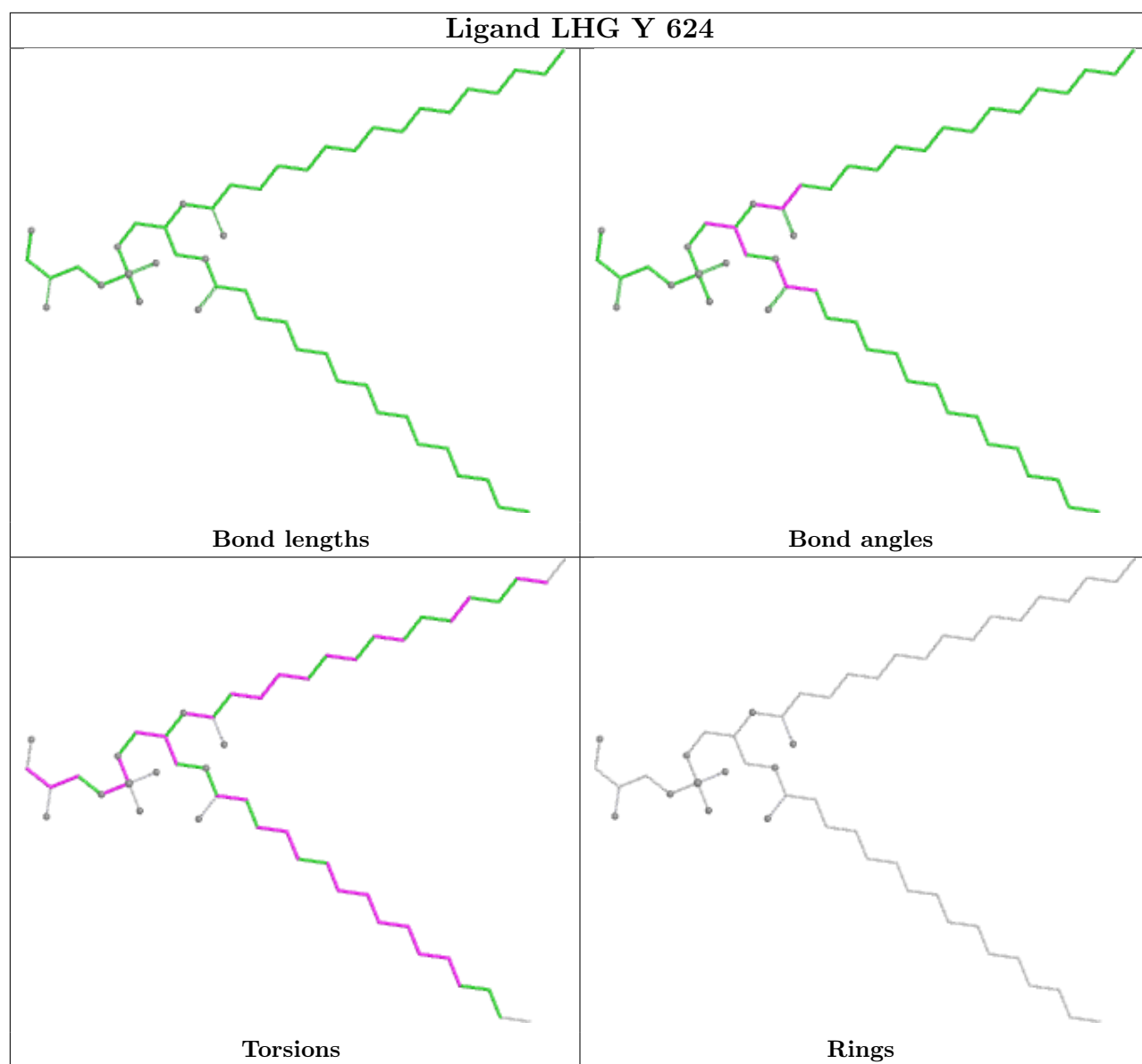


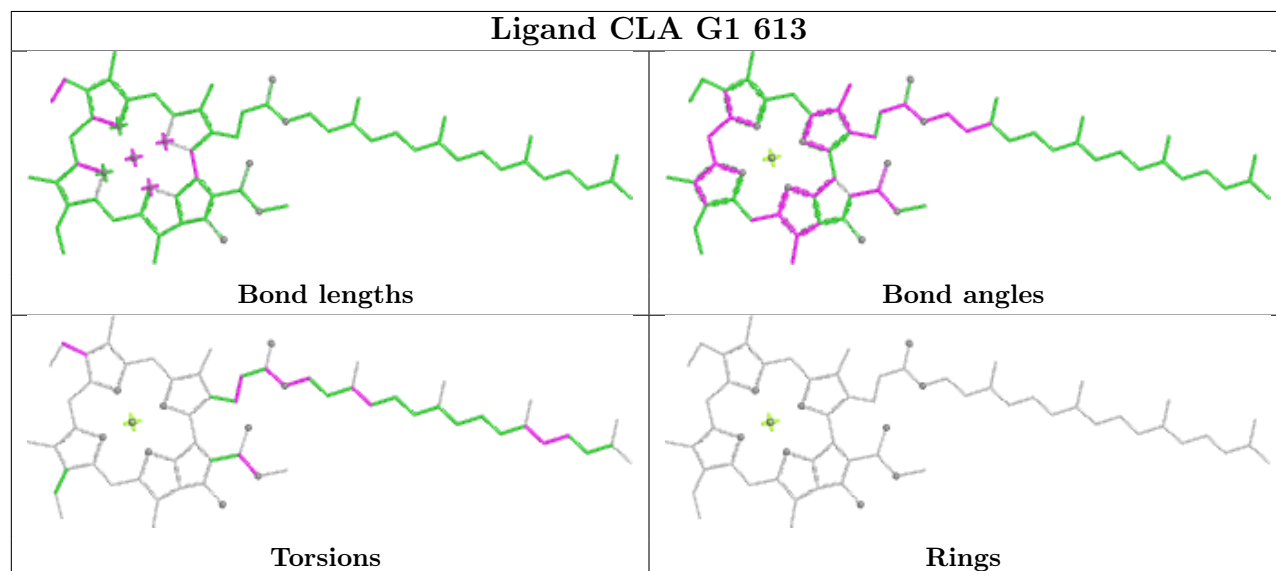
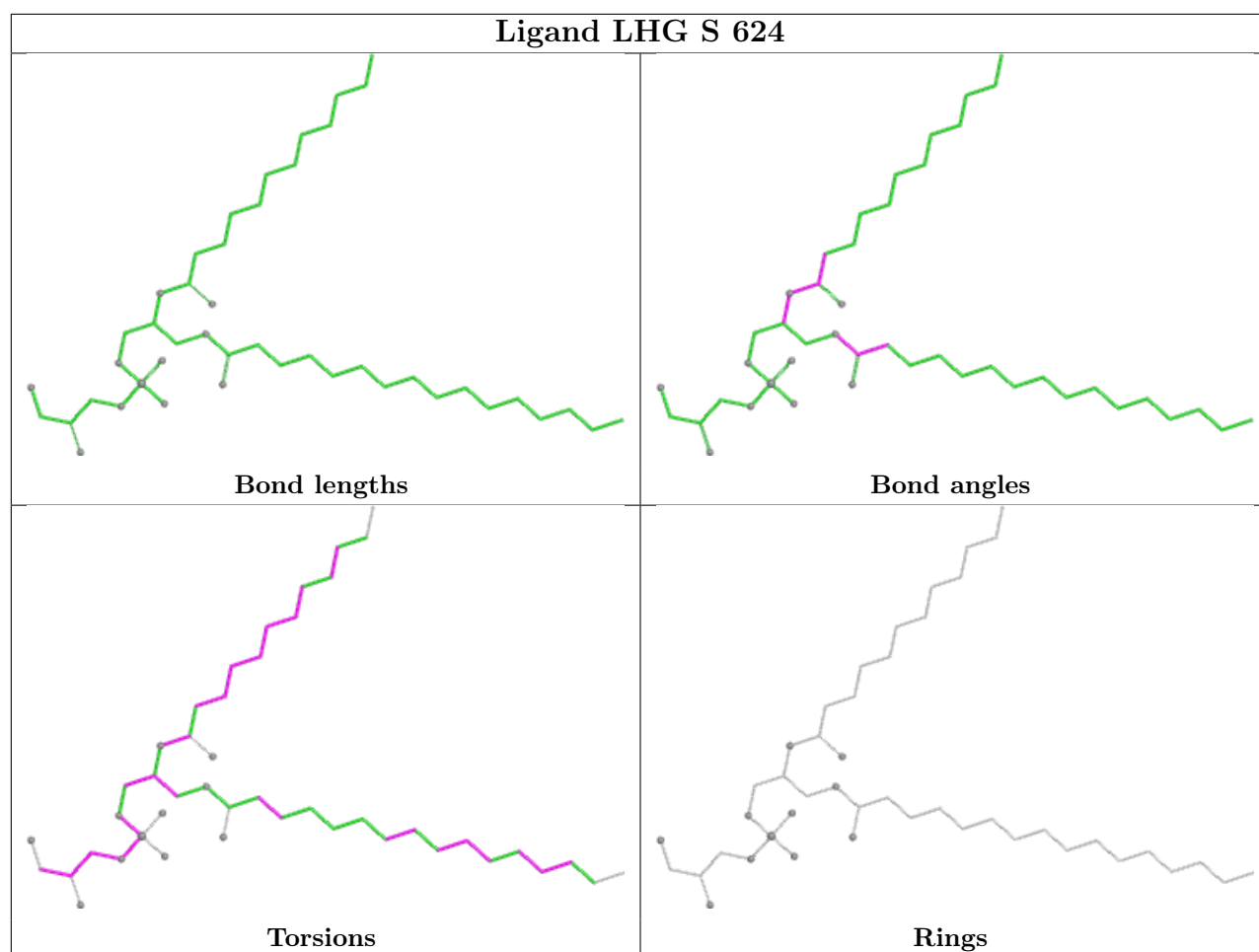


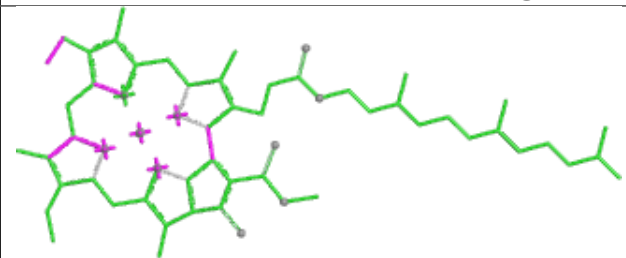
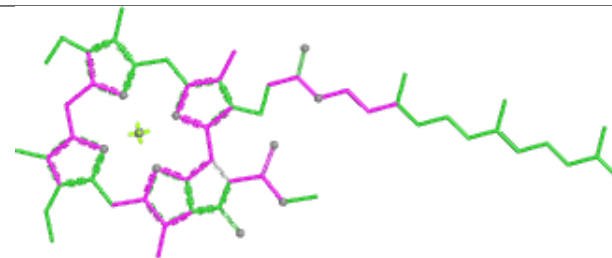
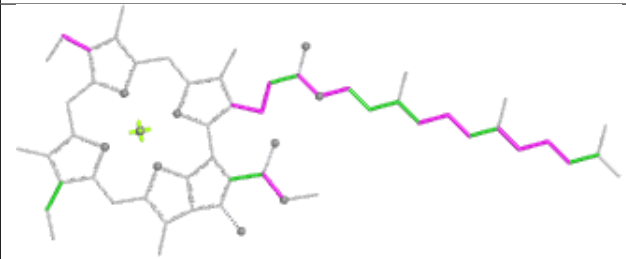
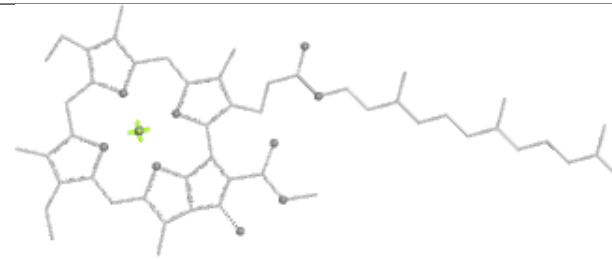
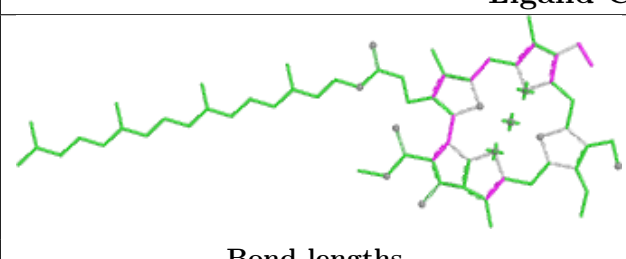
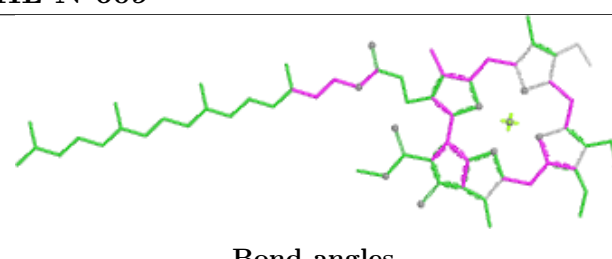
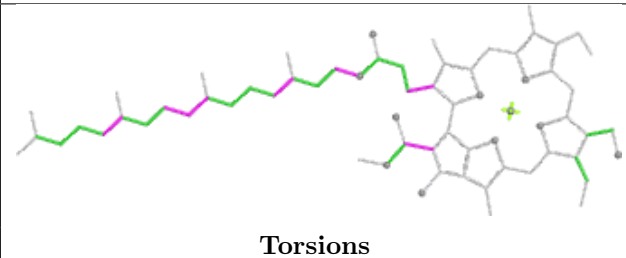
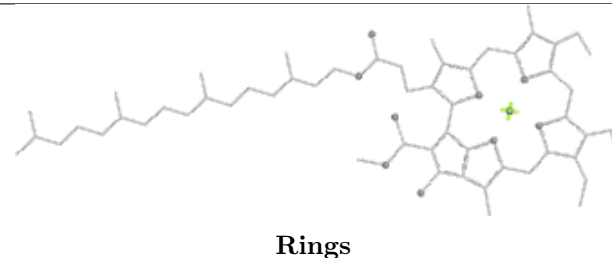
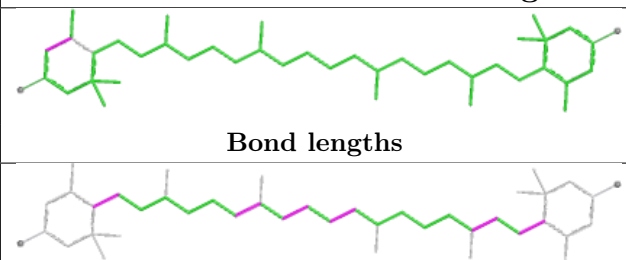
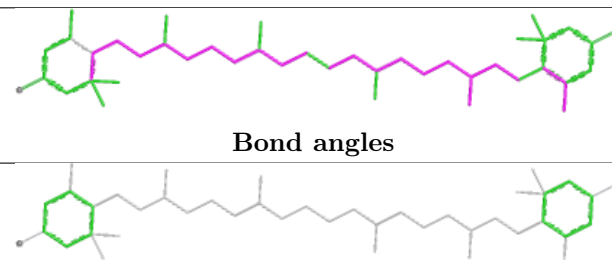


Ligand LUT S 621**Ligand CLA r 609****Ligand LMG H1 102**

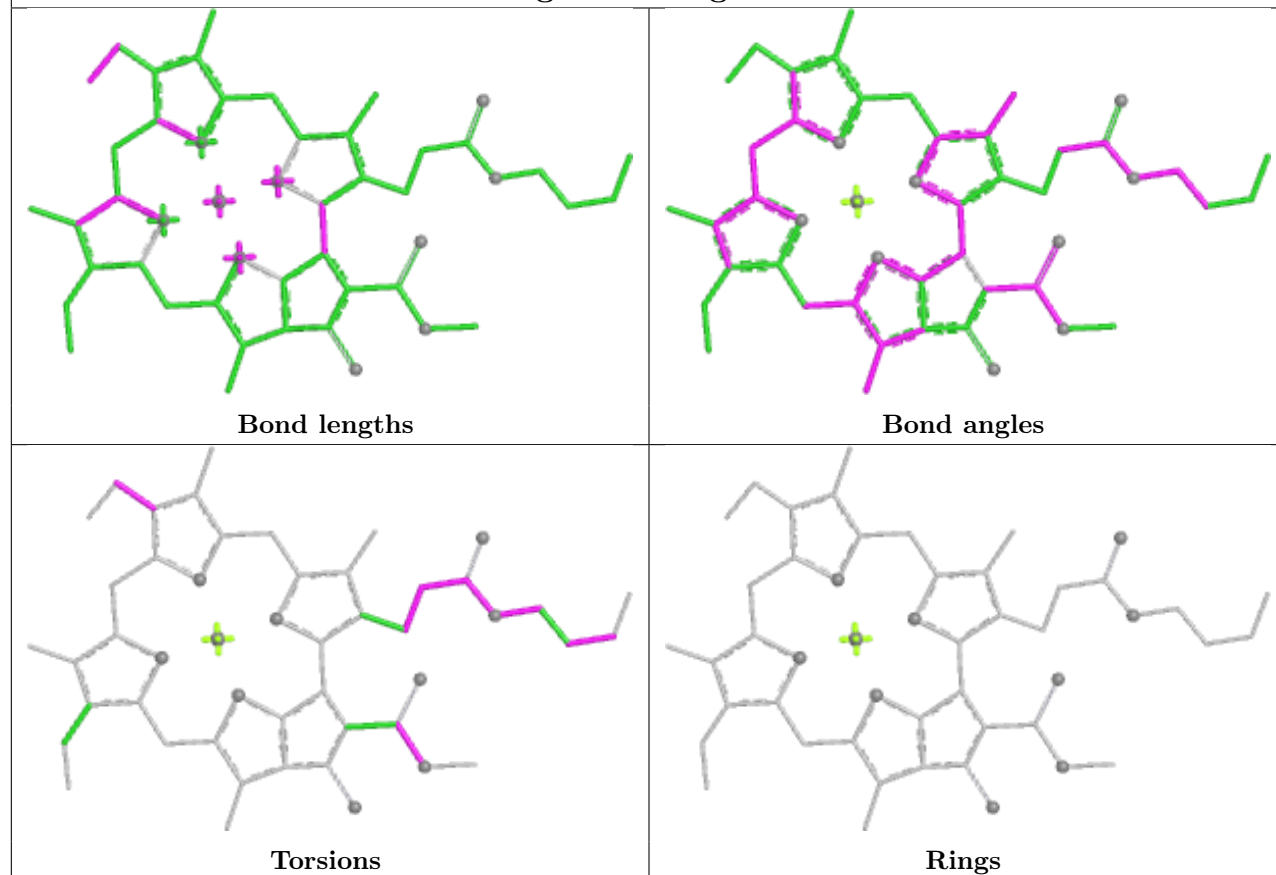




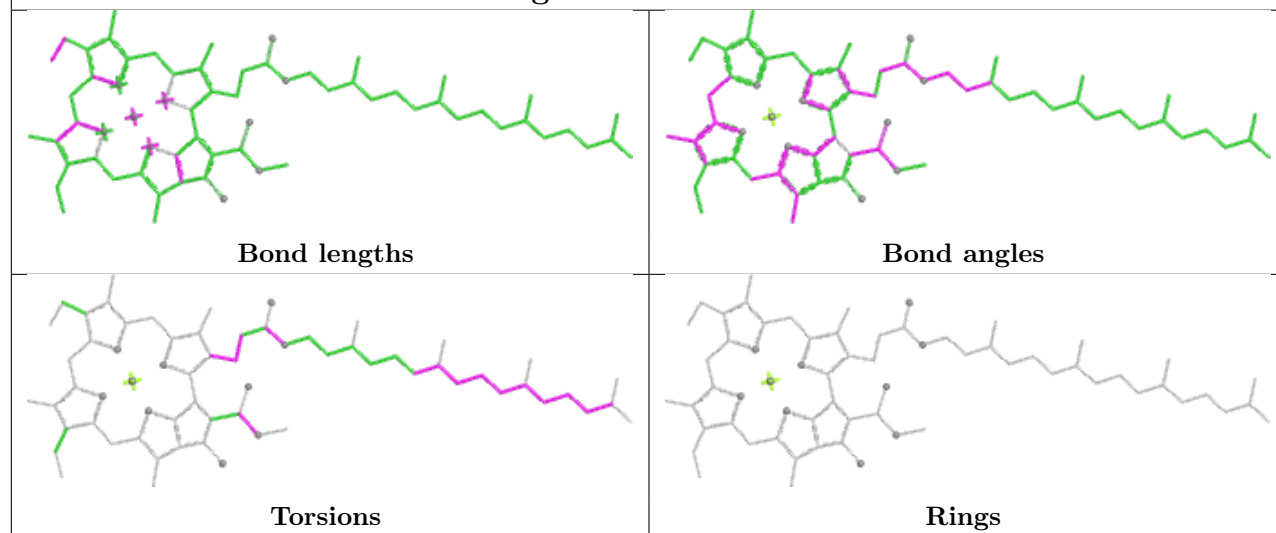


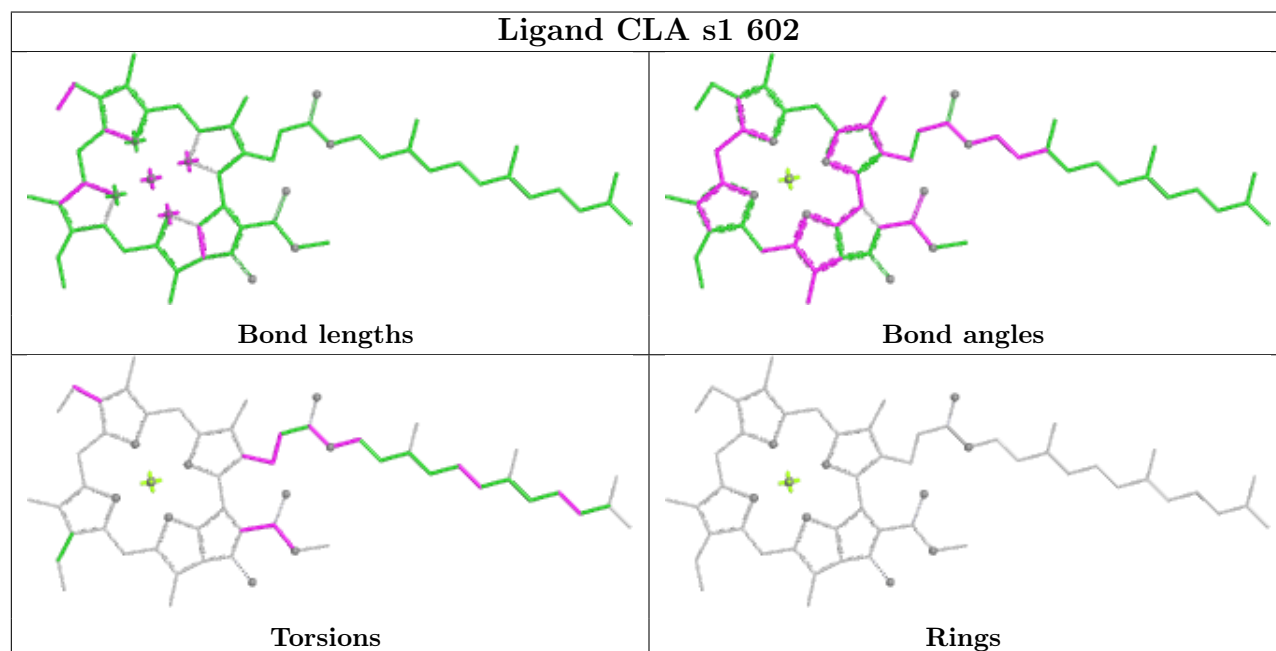
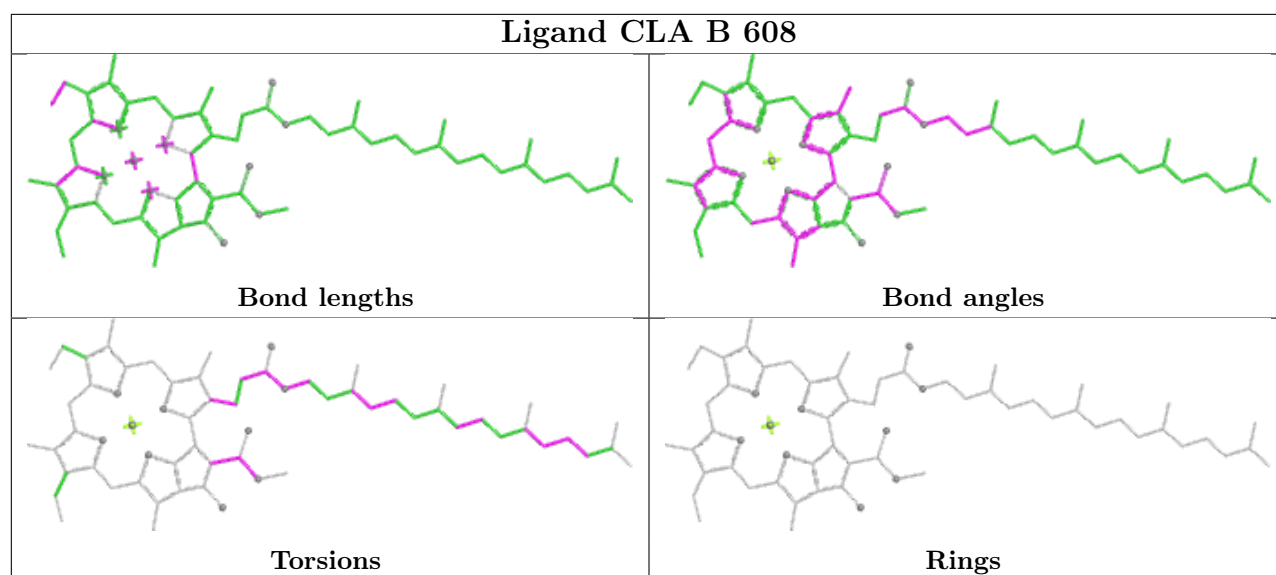
Ligand CLA s1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CHL N 609	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand LUT R 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

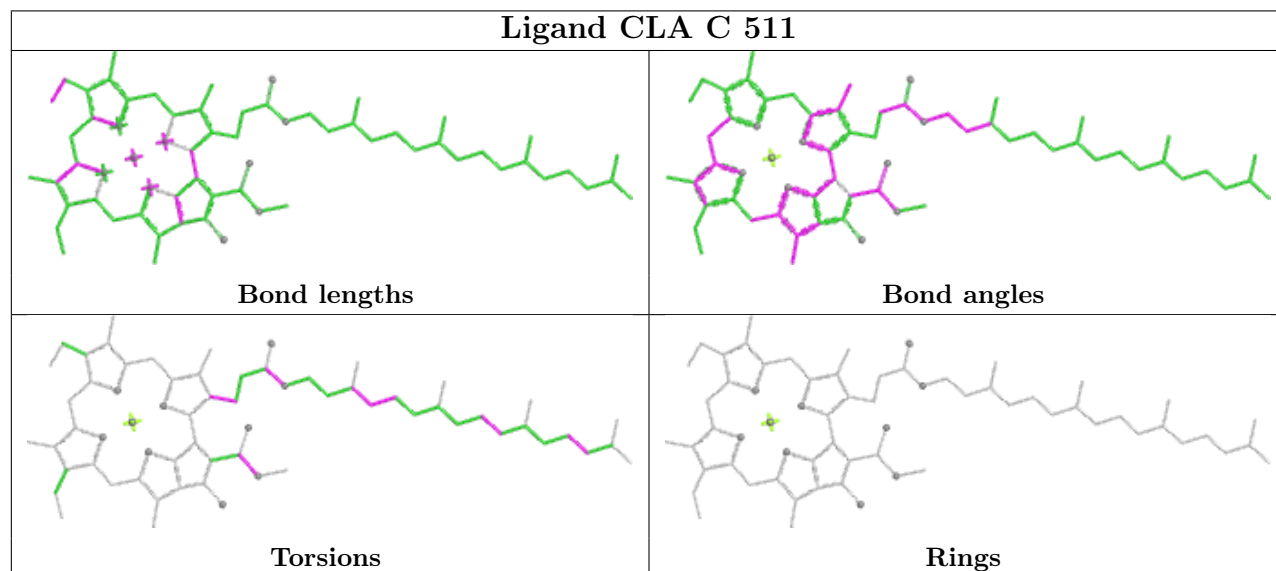
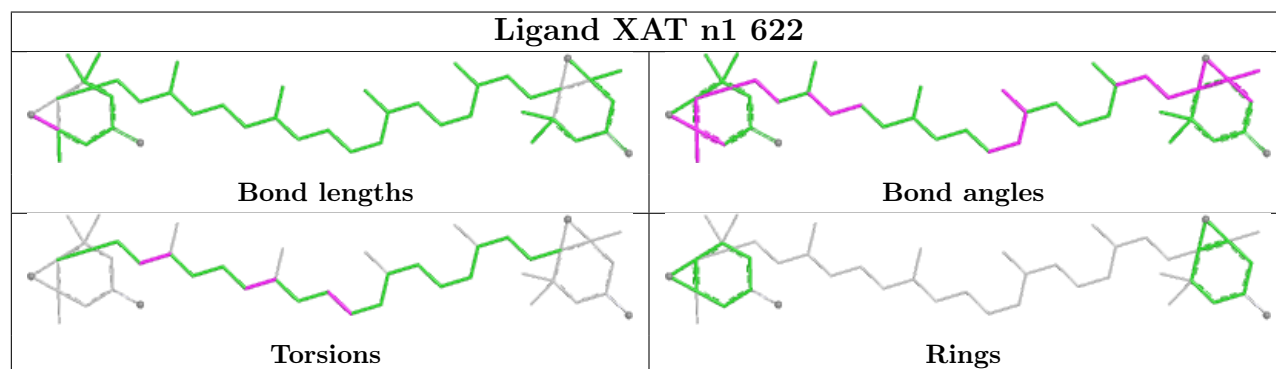
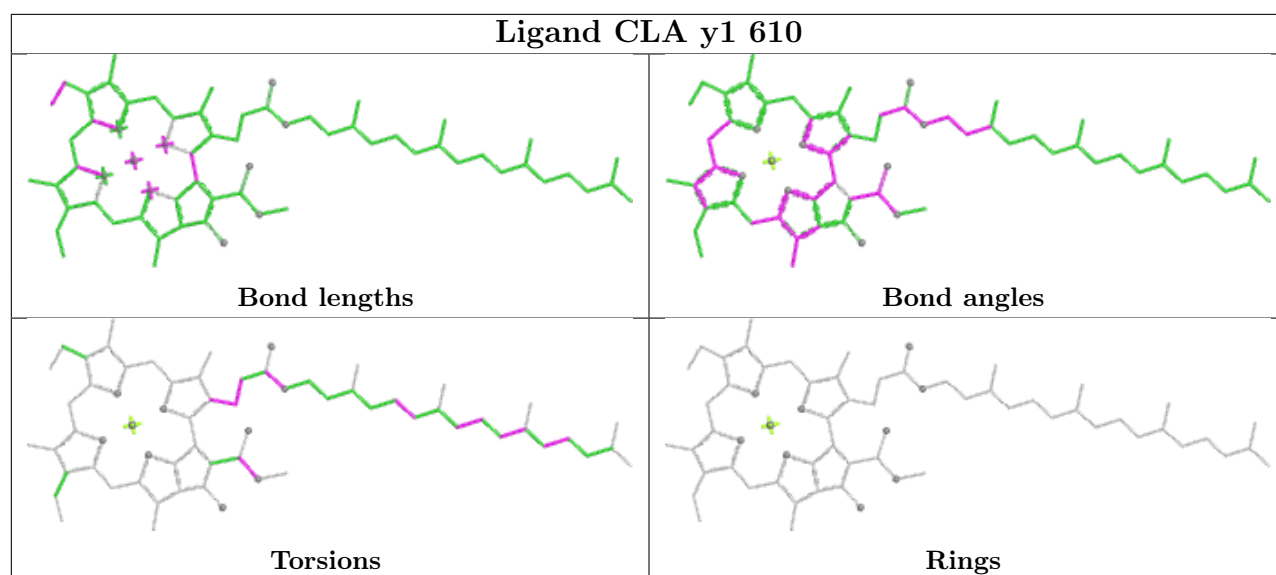
Ligand CLA g 614

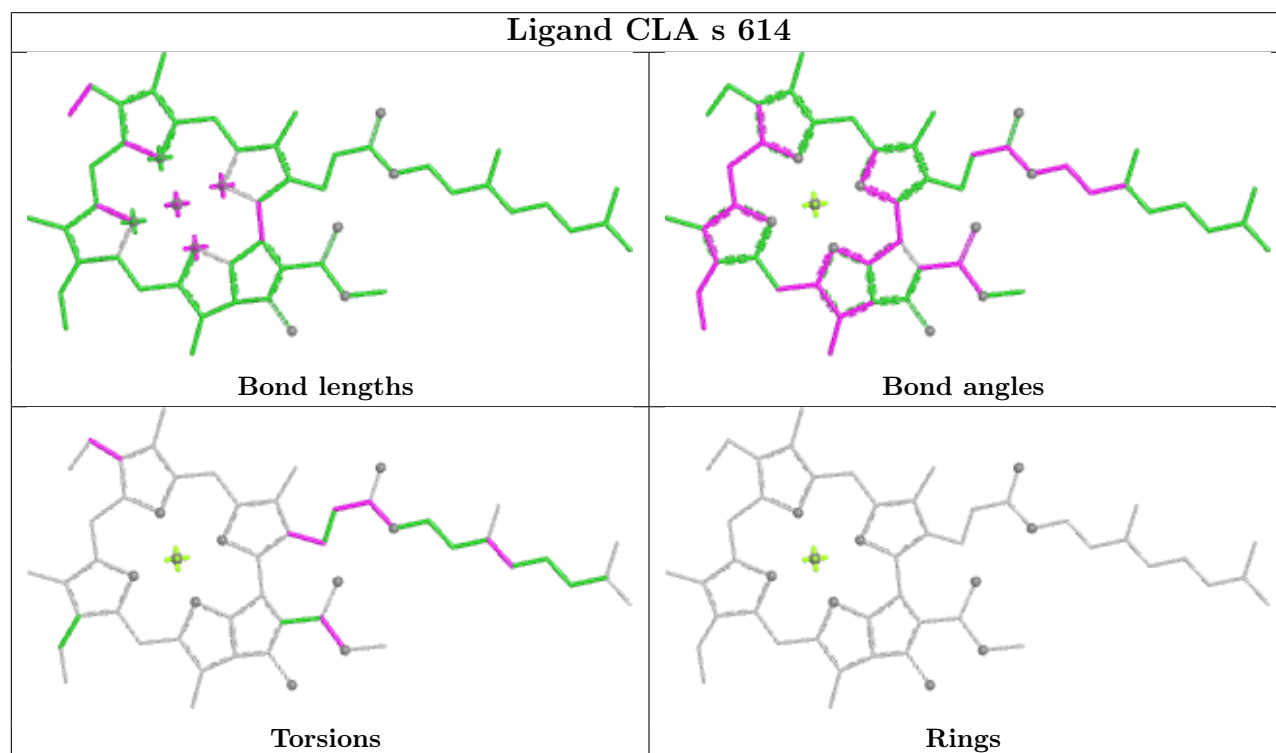
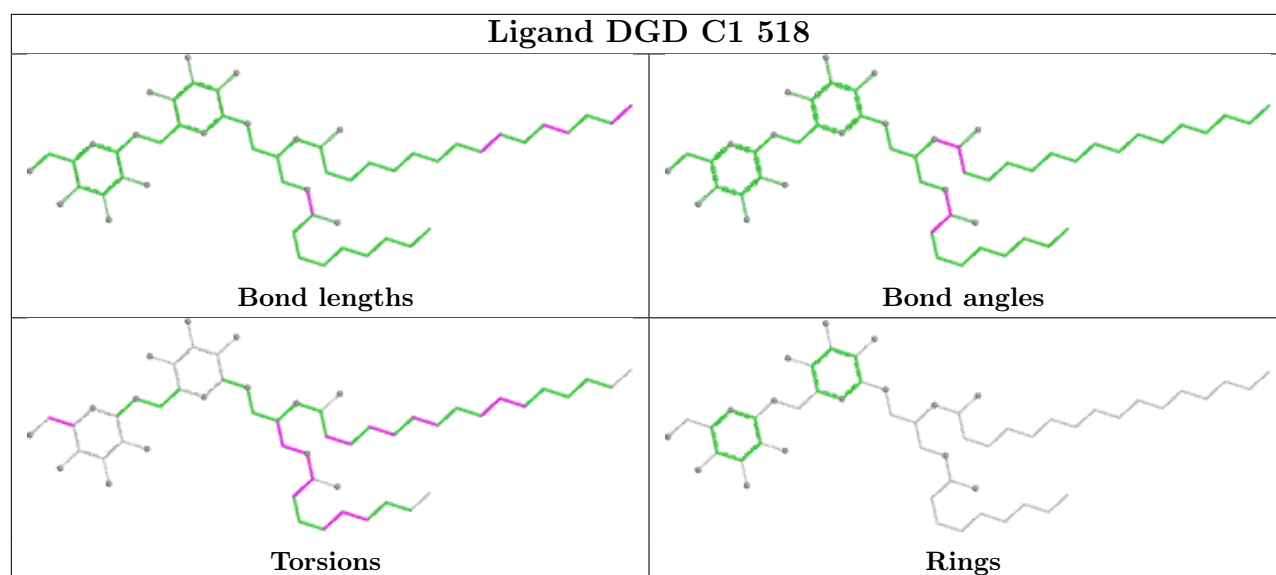


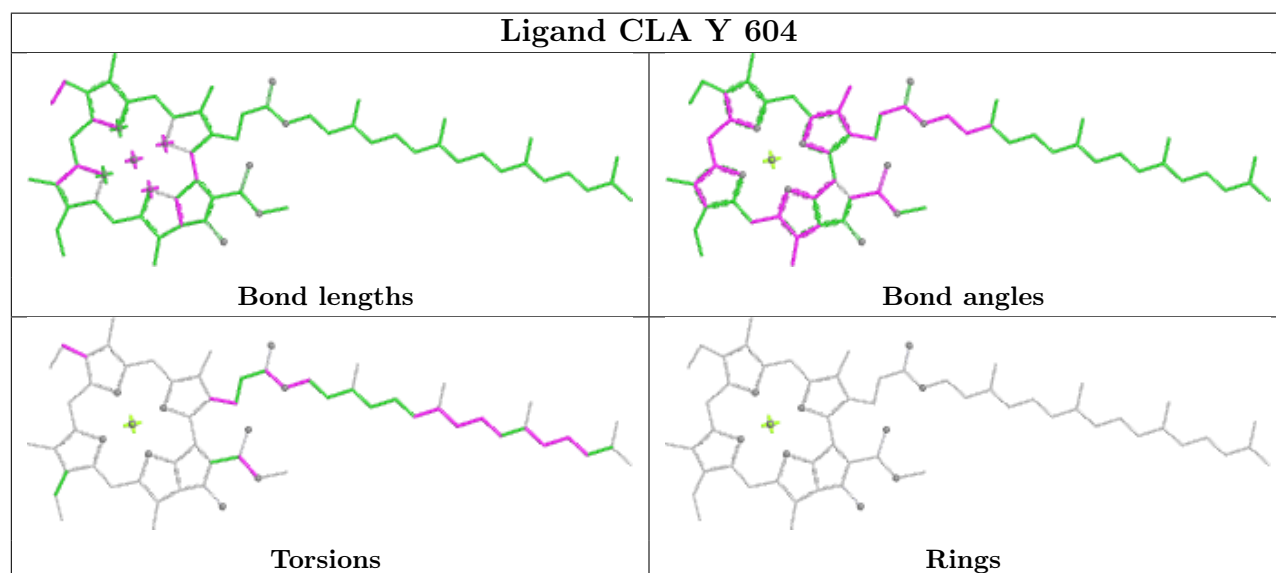
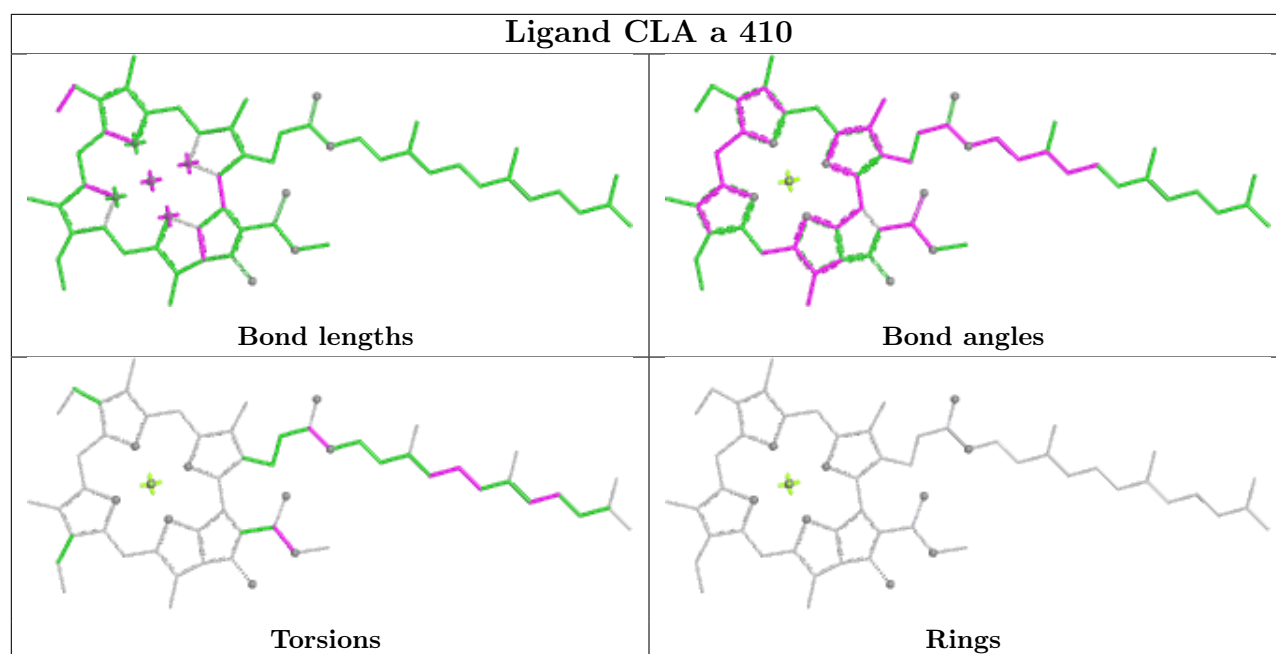
Ligand CLA Y 602

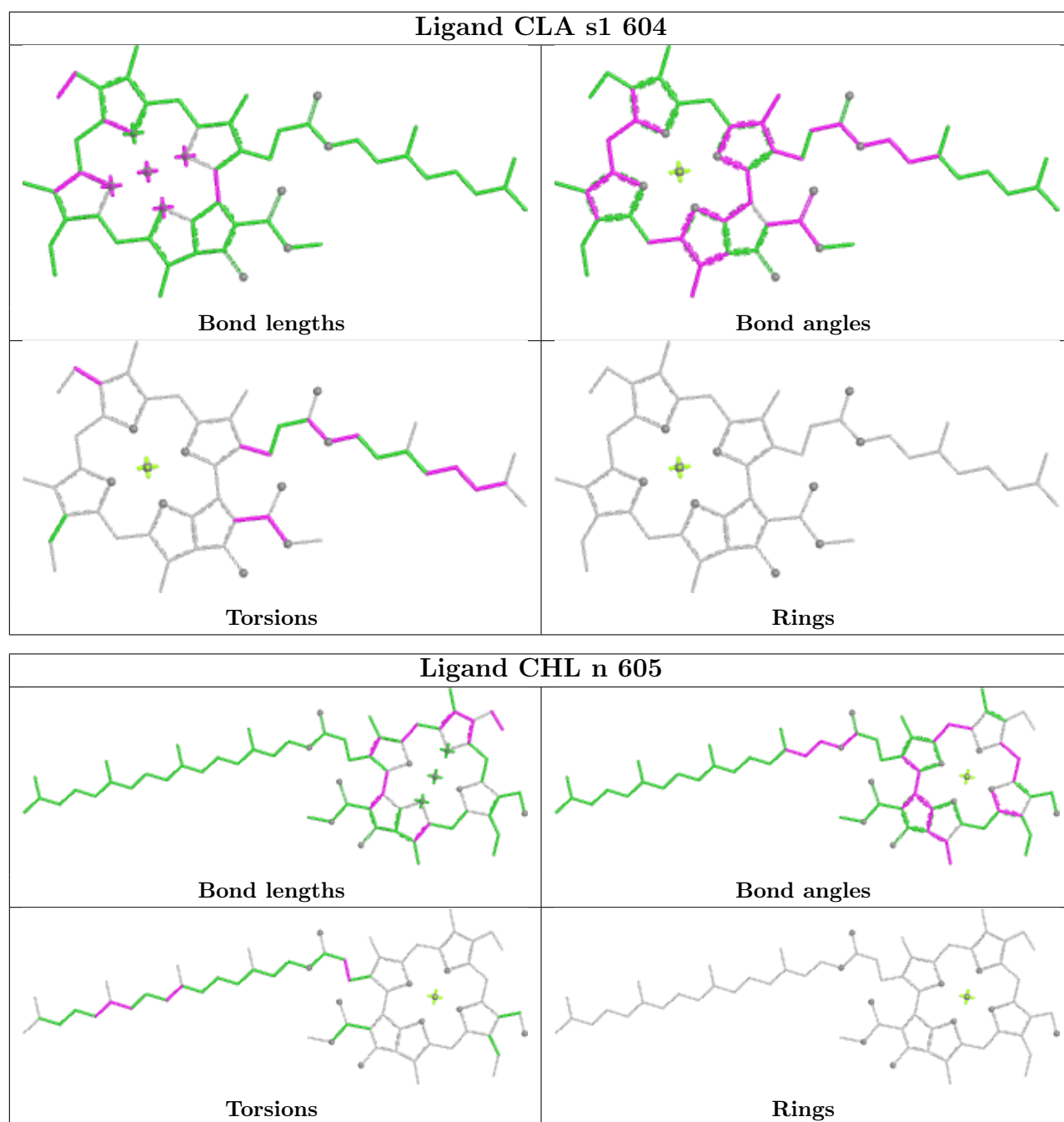


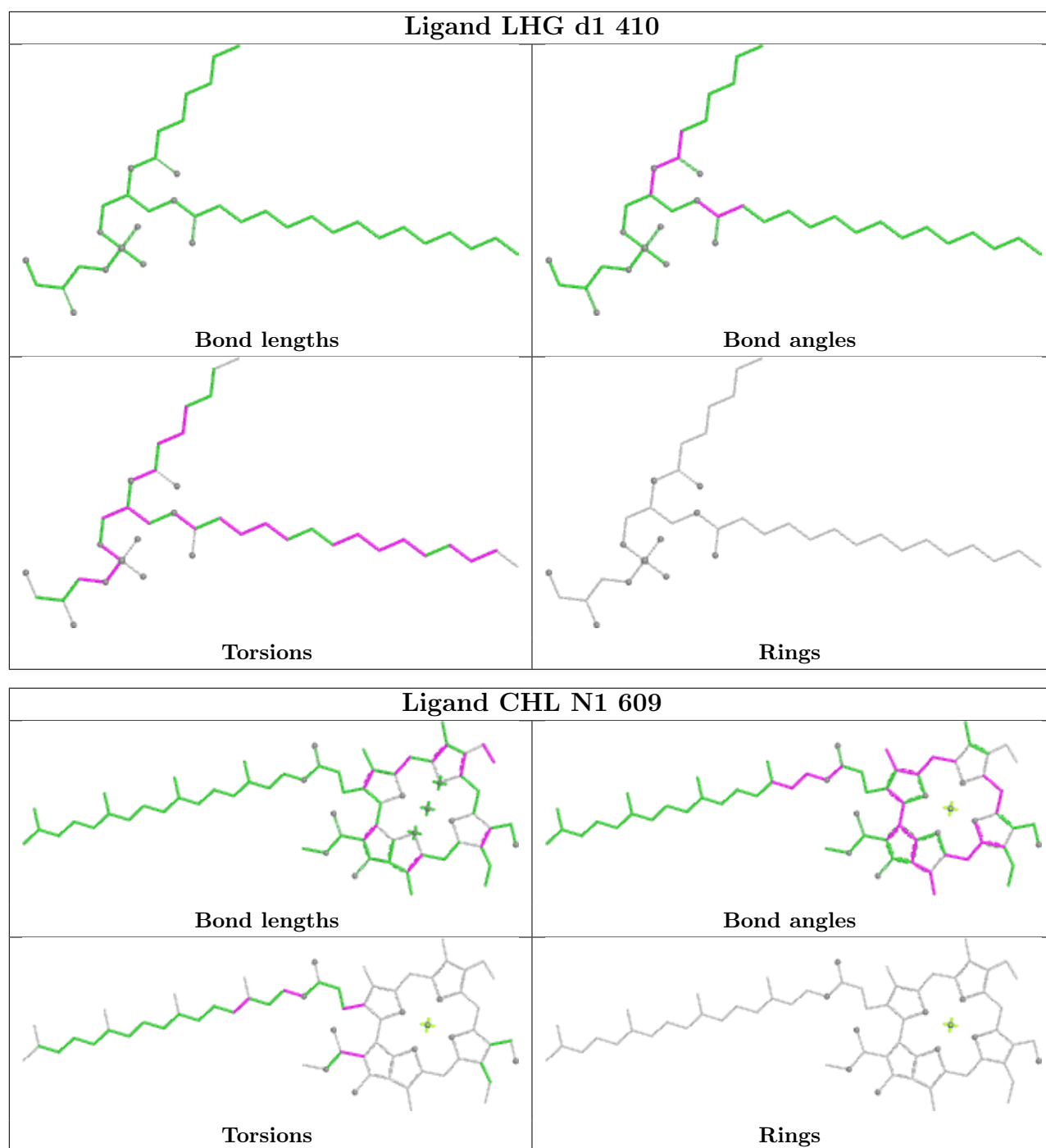


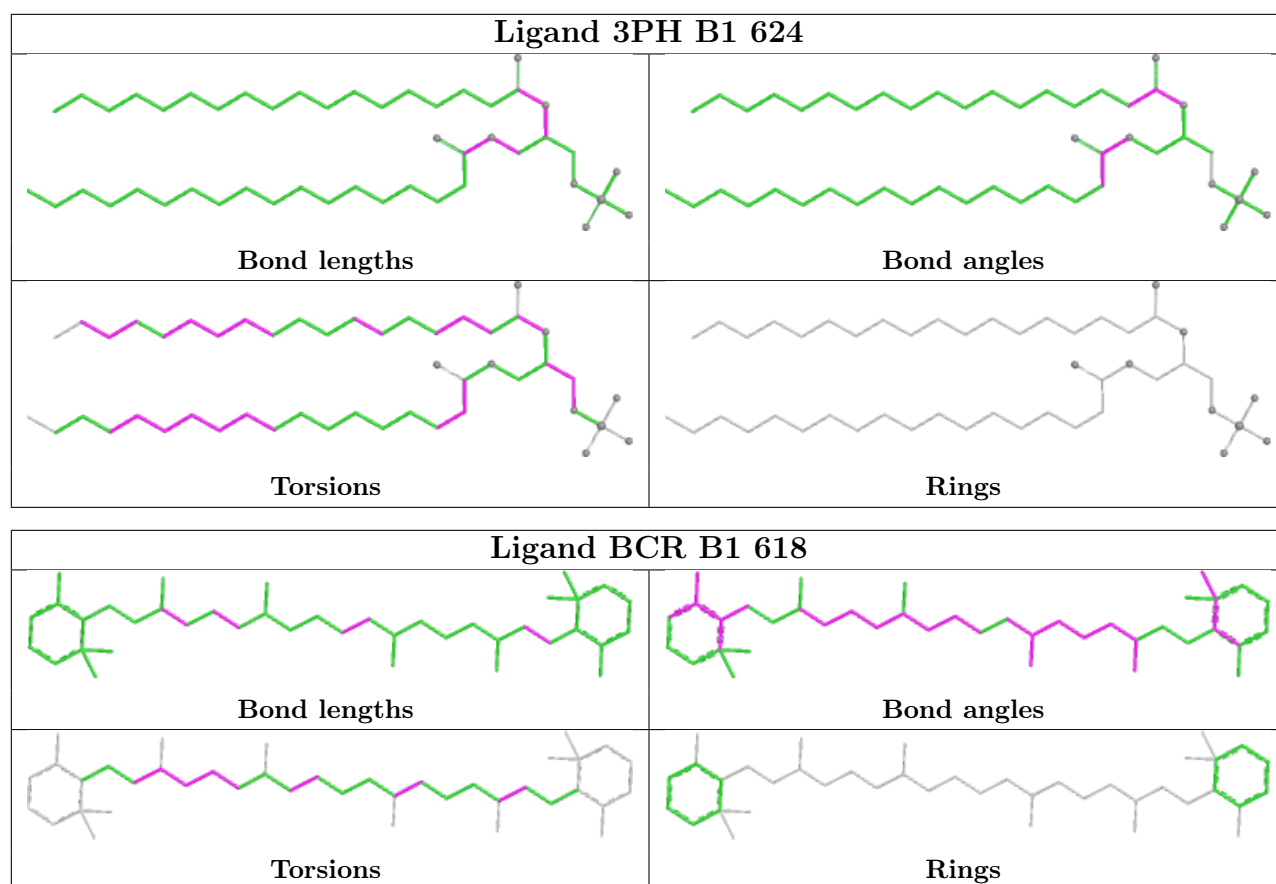




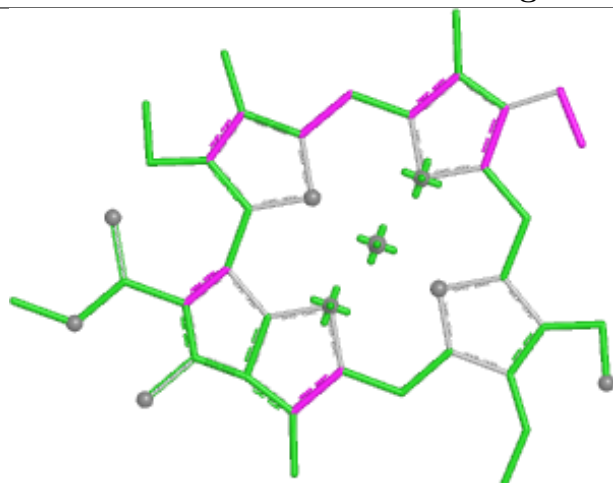




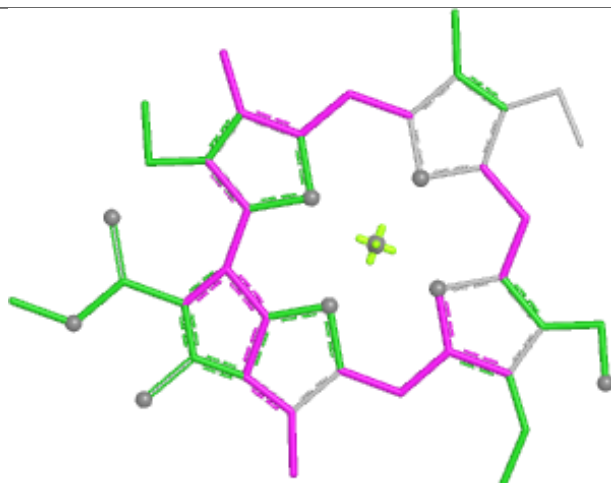




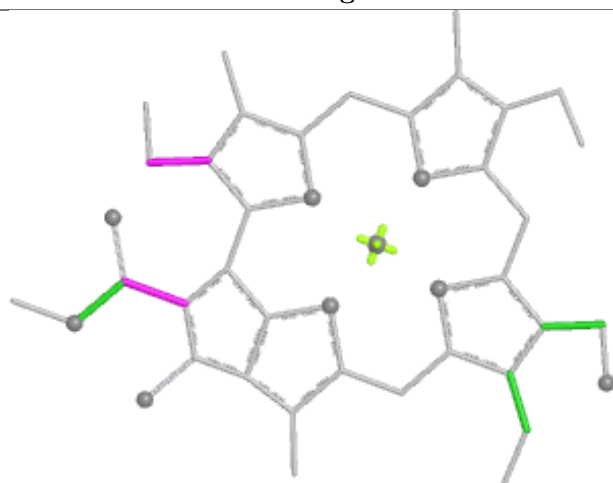
Ligand CHL s 607



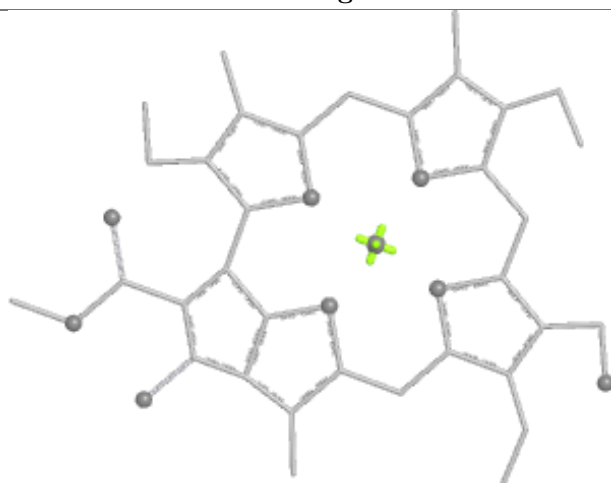
Bond lengths



Bond angles

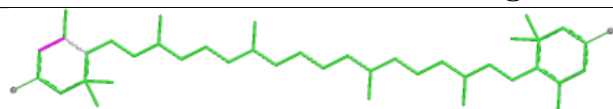


Torsions

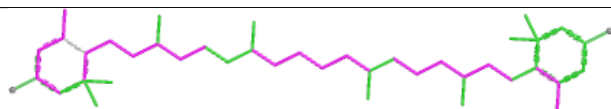


Rings

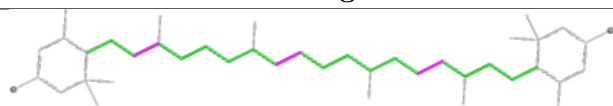
Ligand LUT G1 620



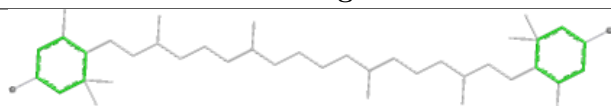
Bond lengths



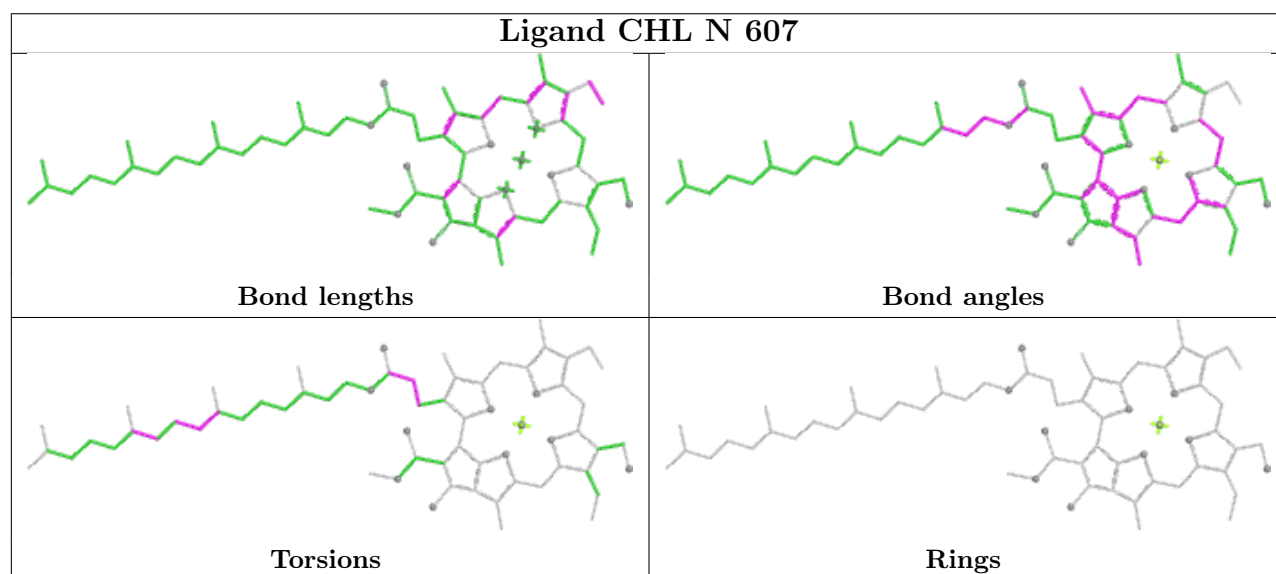
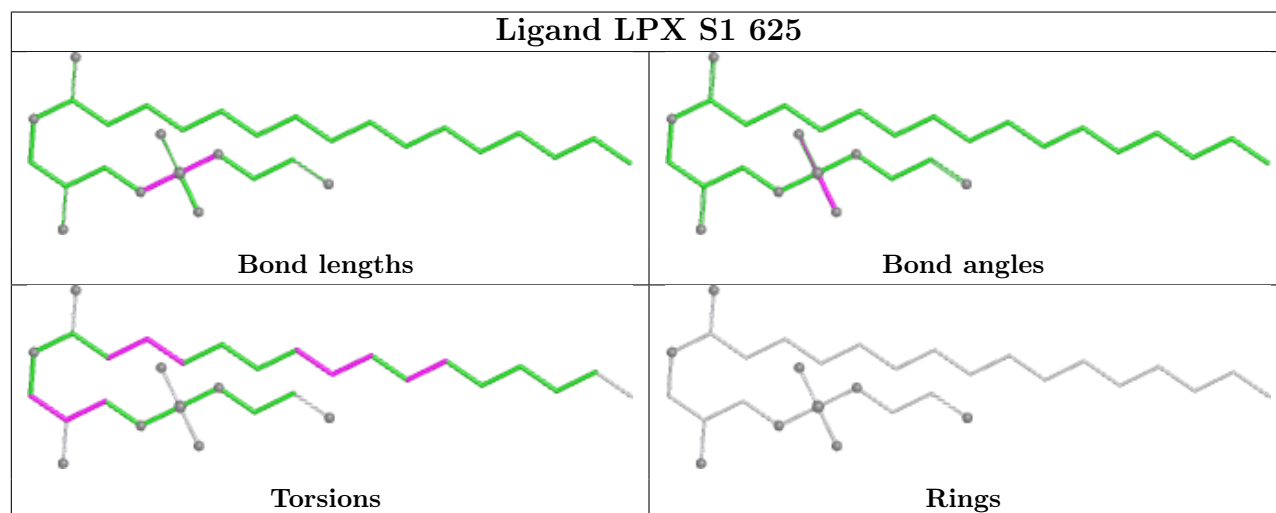
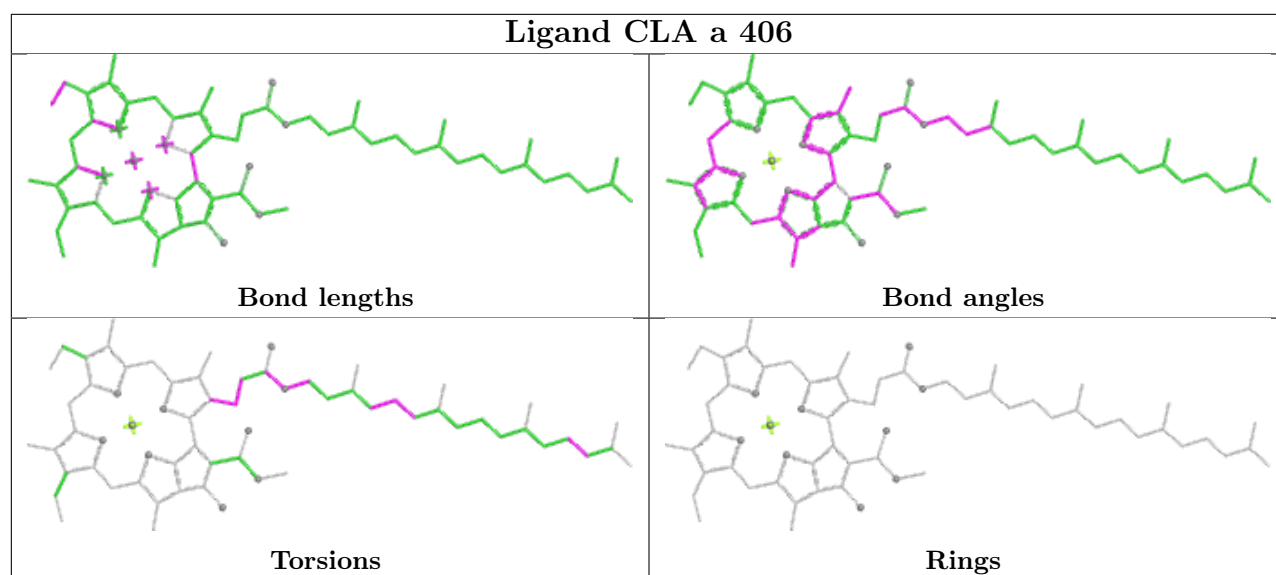
Bond angles

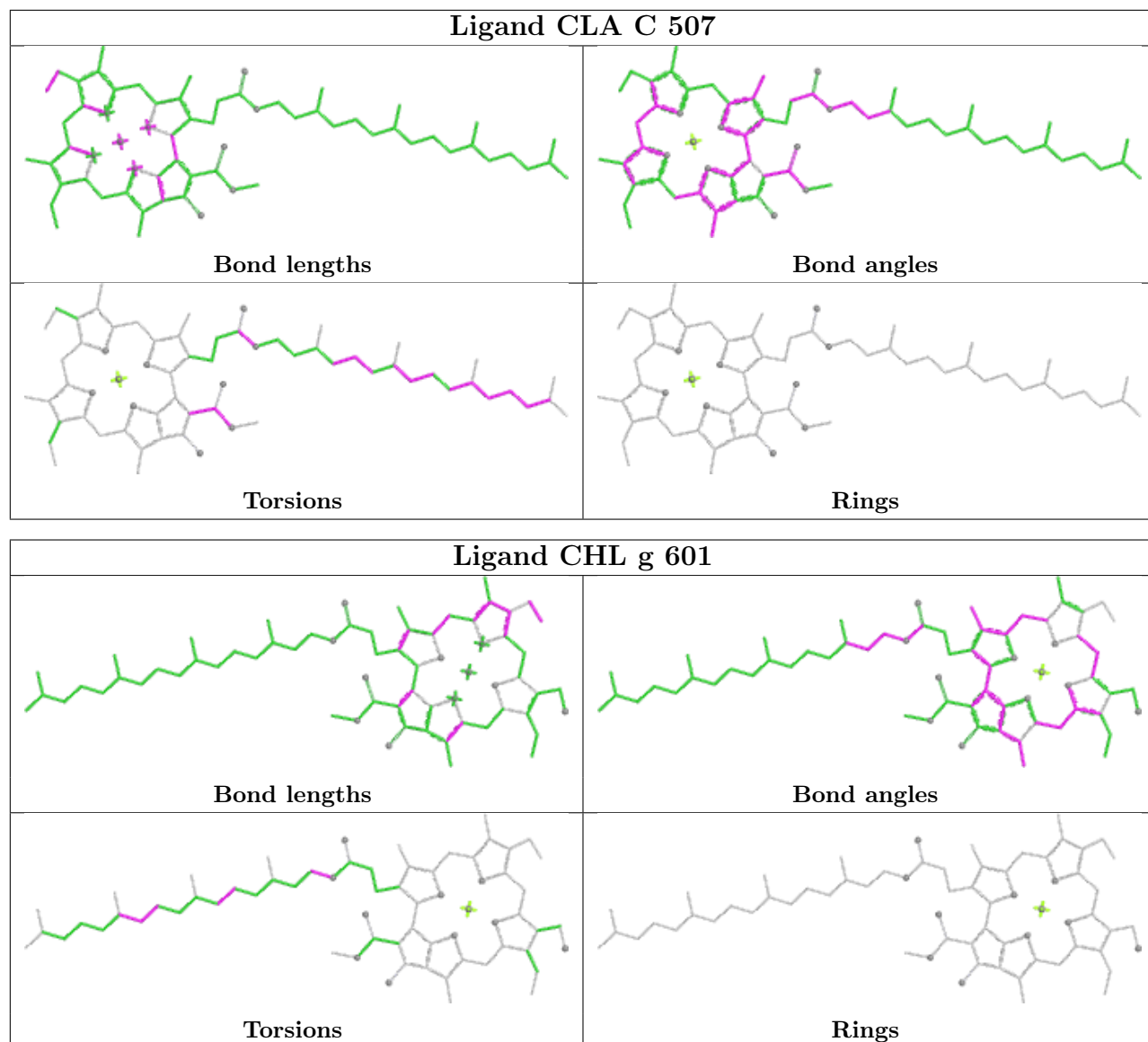


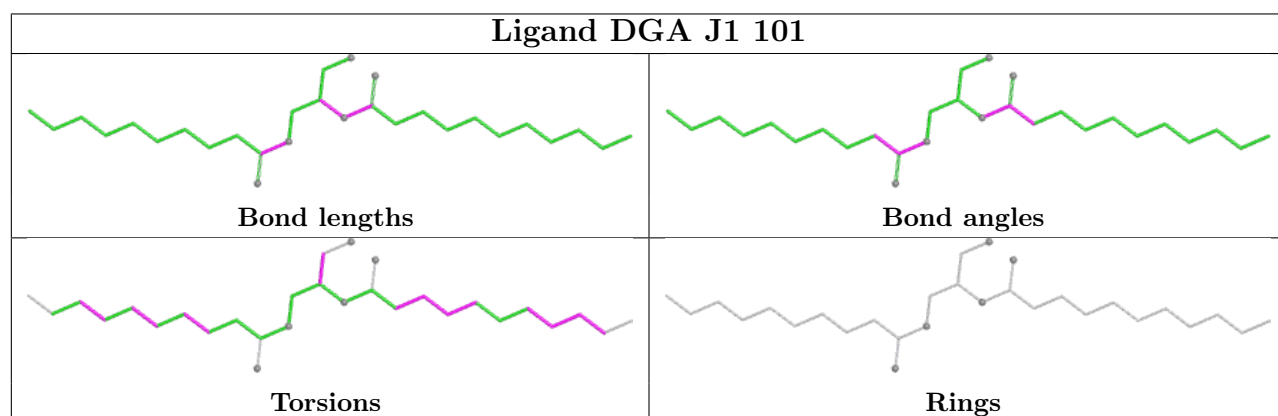
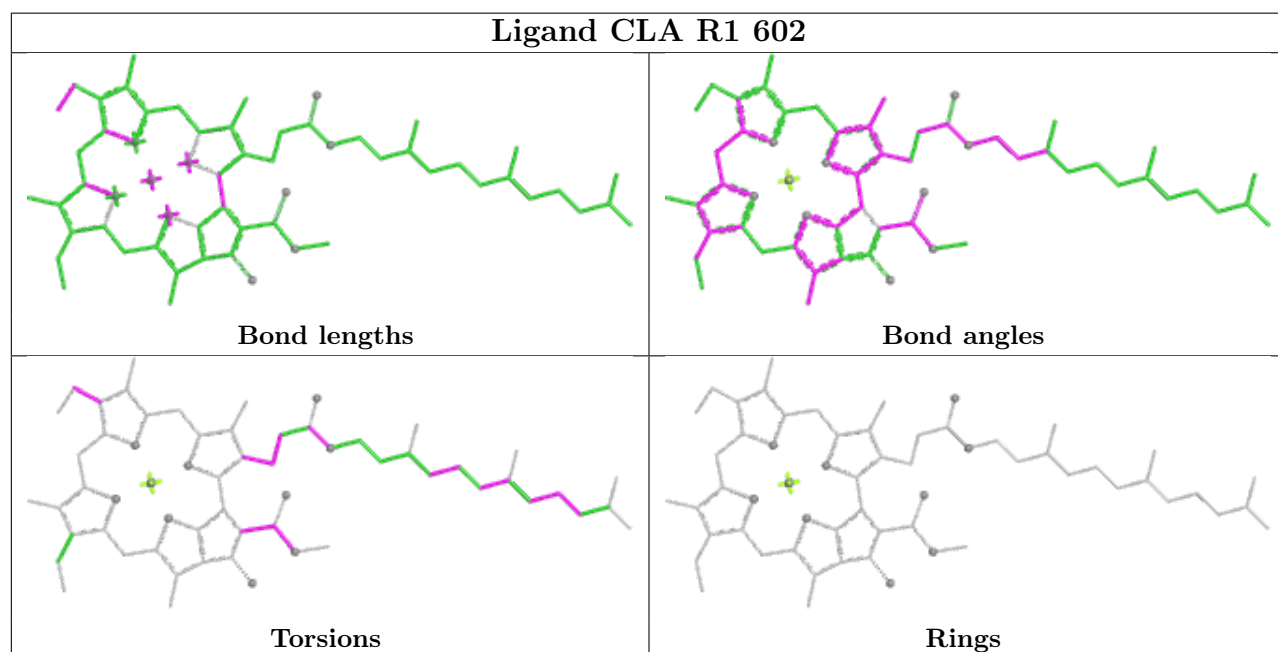
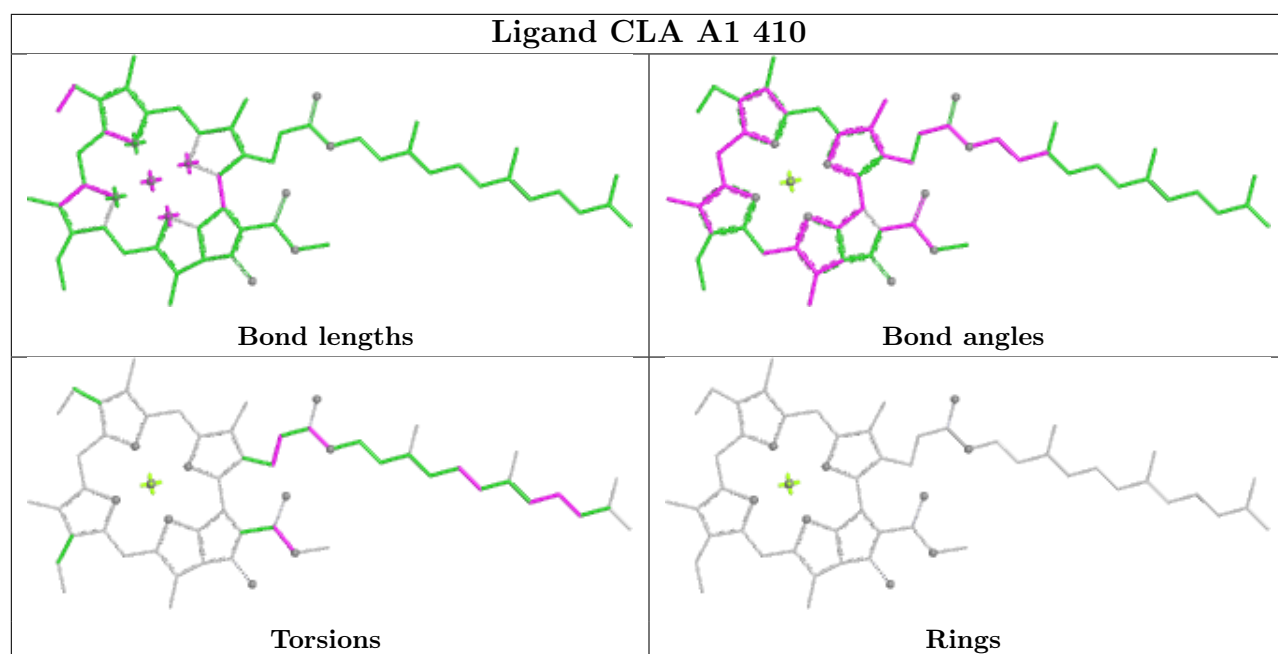
Torsions

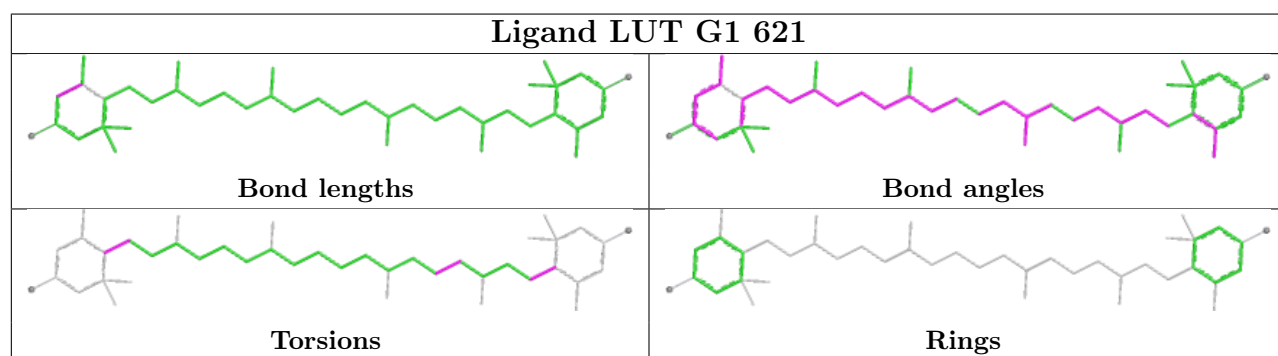
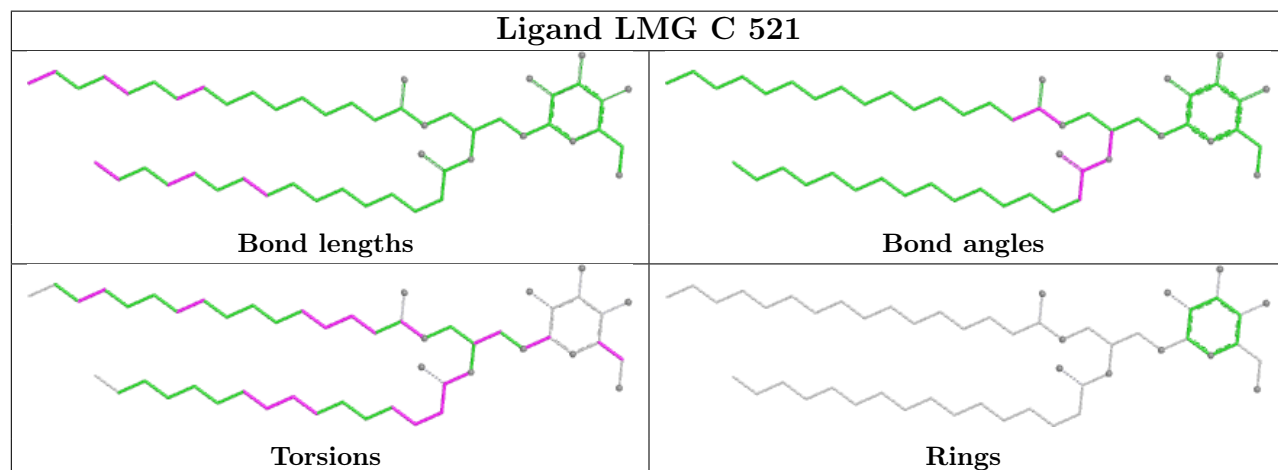
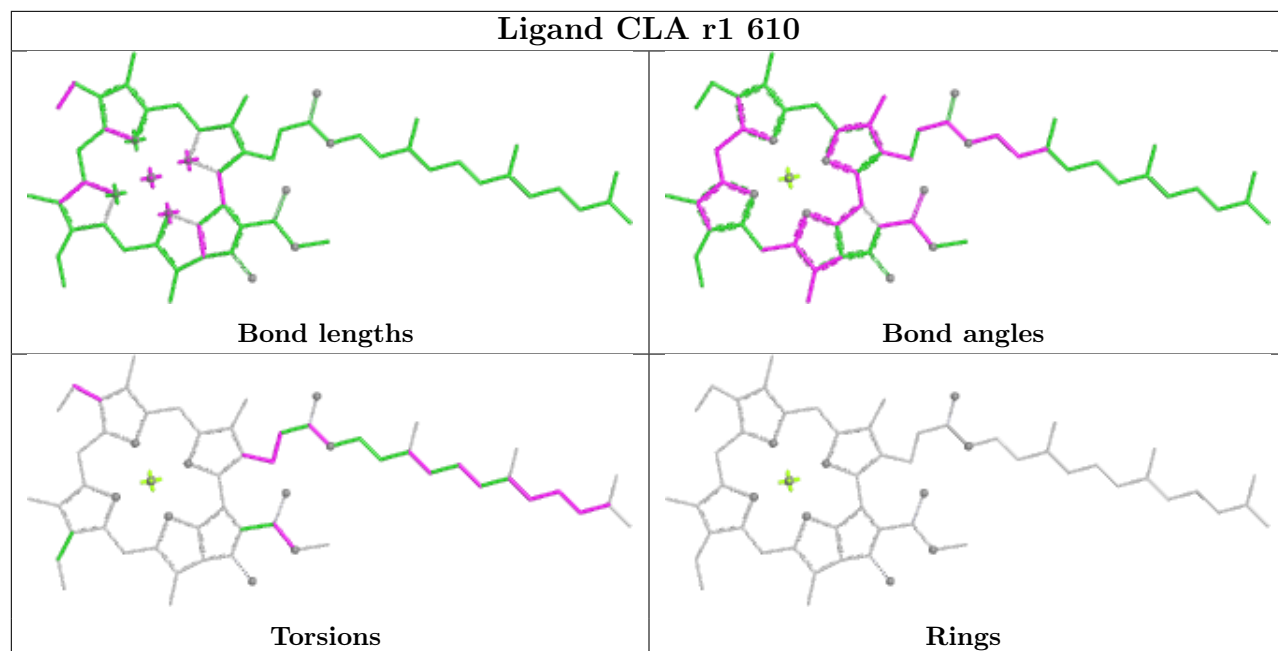


Rings

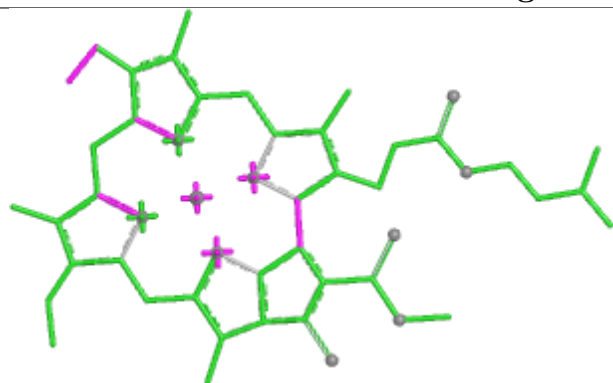




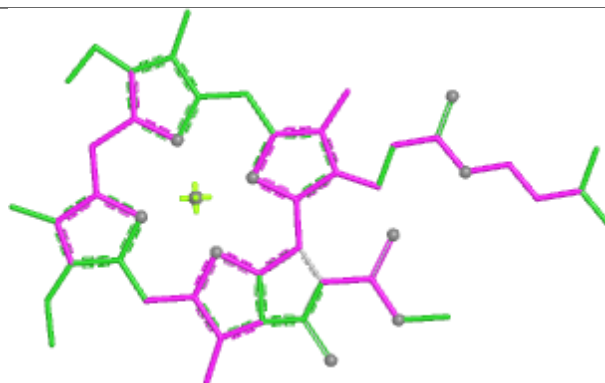




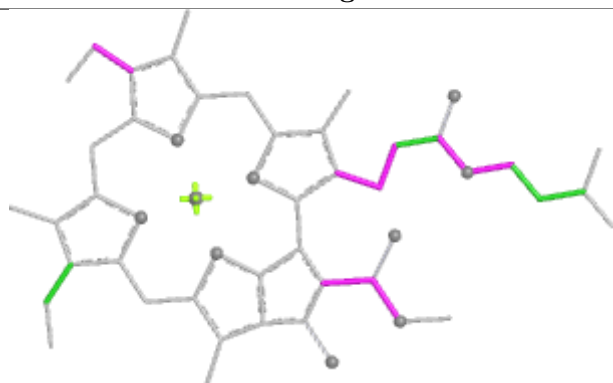
Ligand CLA S 605



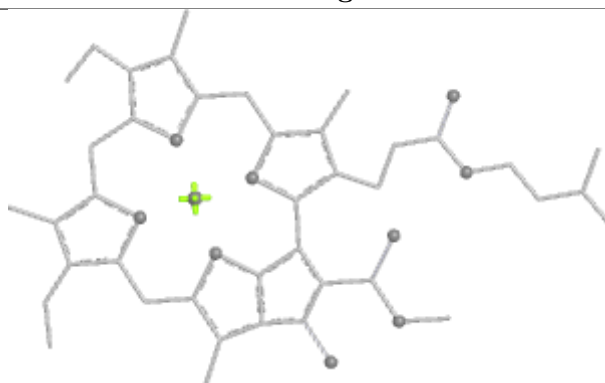
Bond lengths



Bond angles

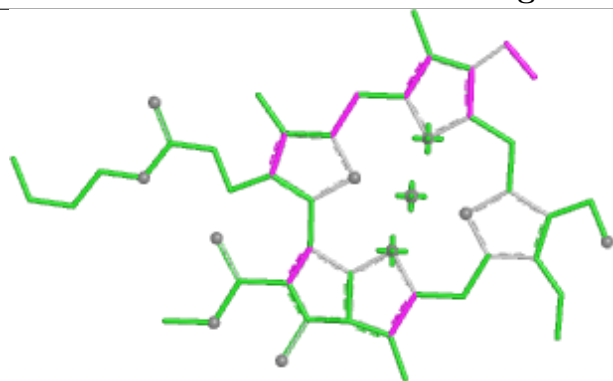


Torsions

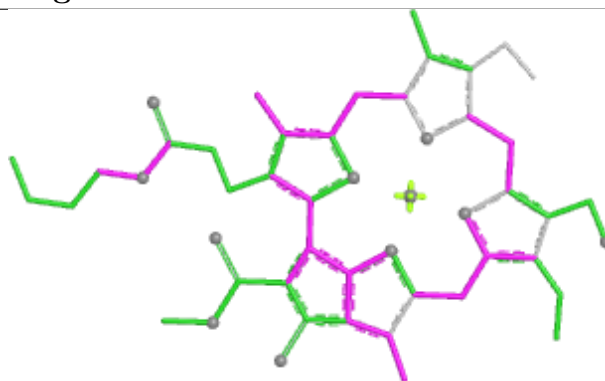


Rings

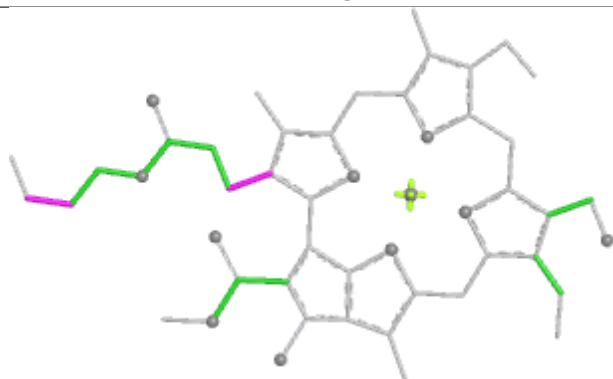
Ligand CHL g 607



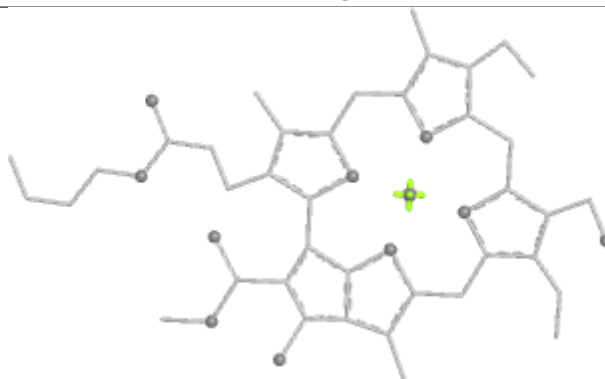
Bond lengths



Bond angles

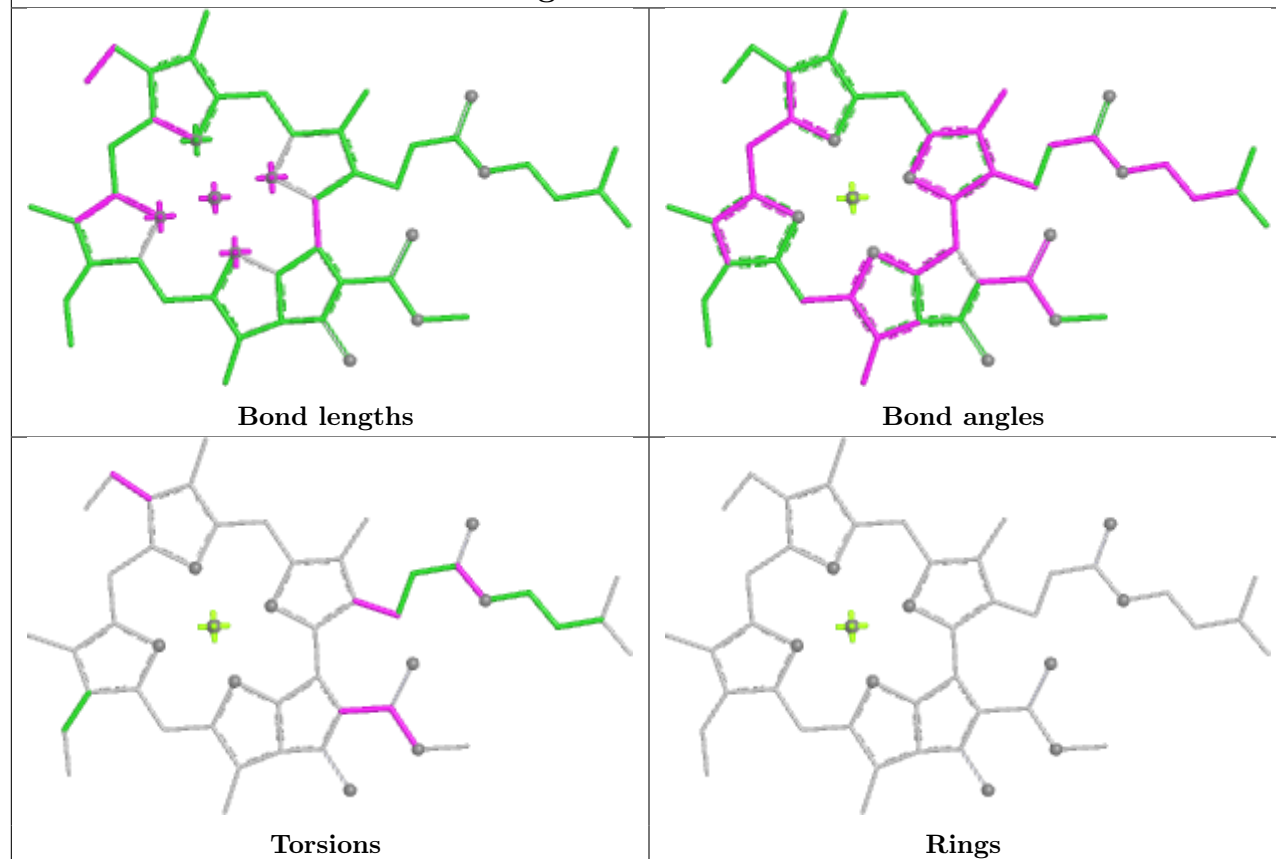


Torsions

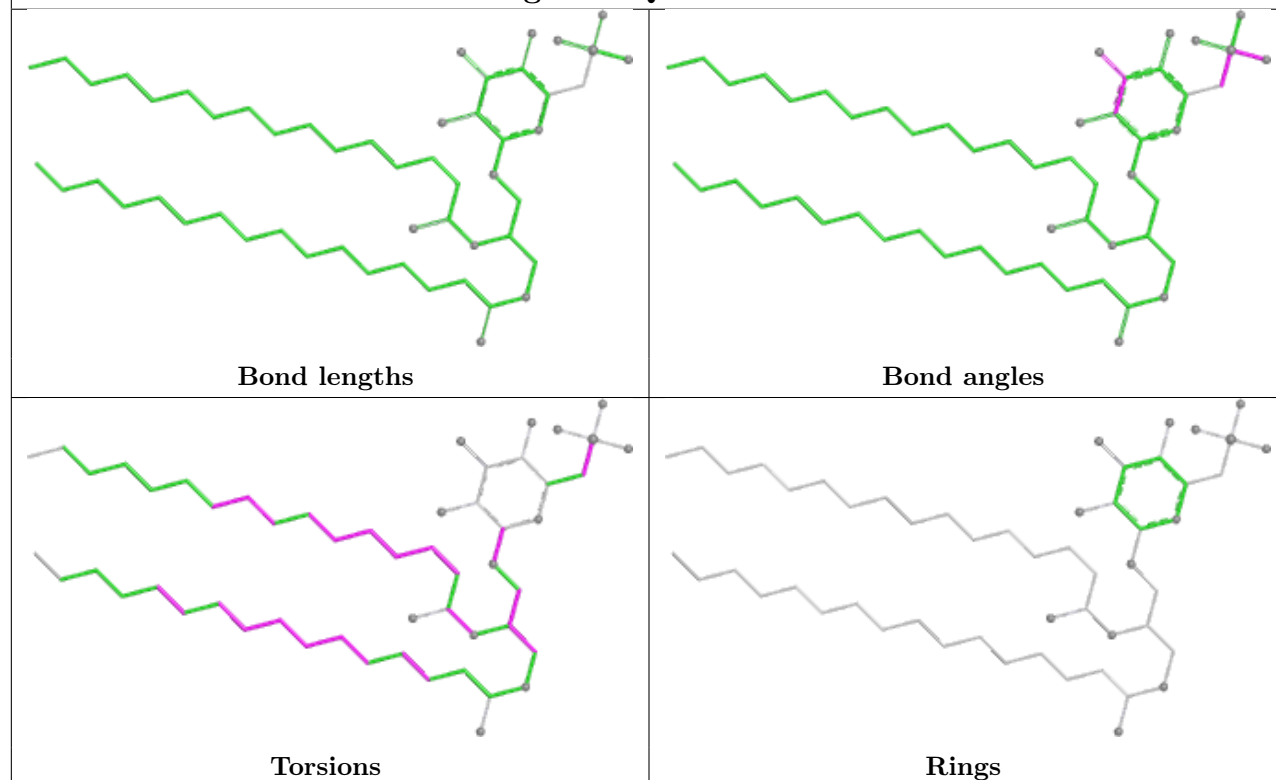


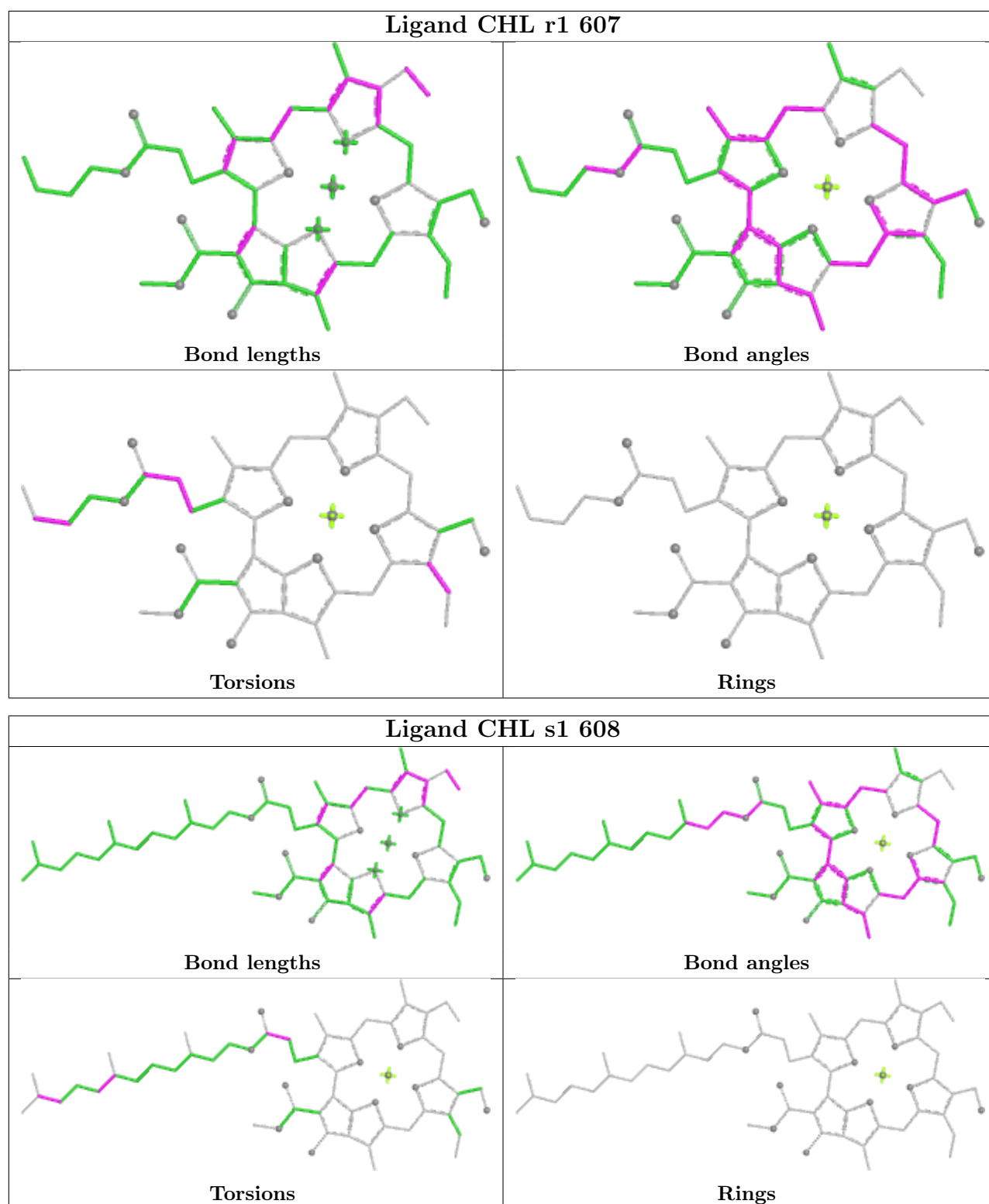
Rings

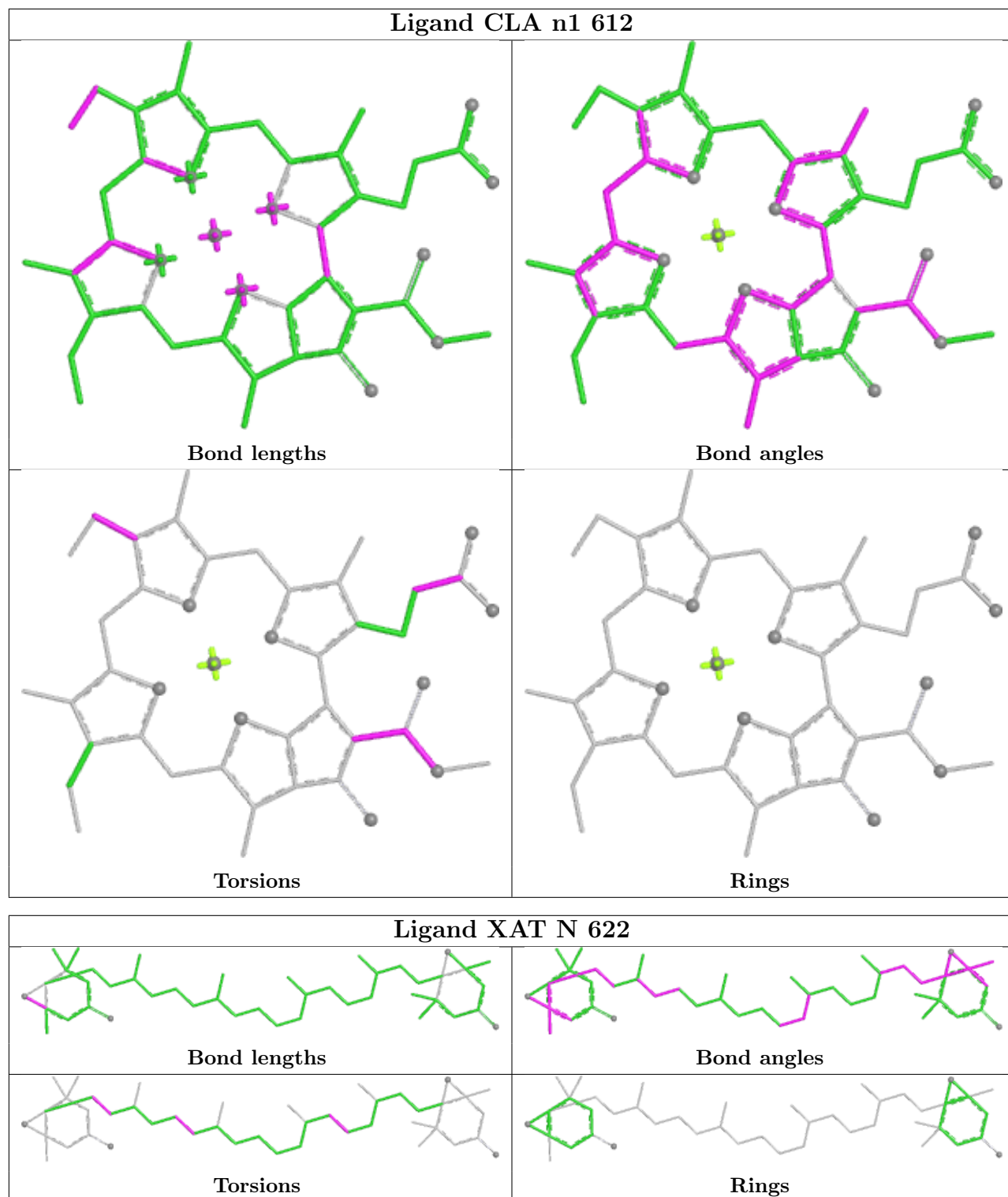
Ligand CLA s 605

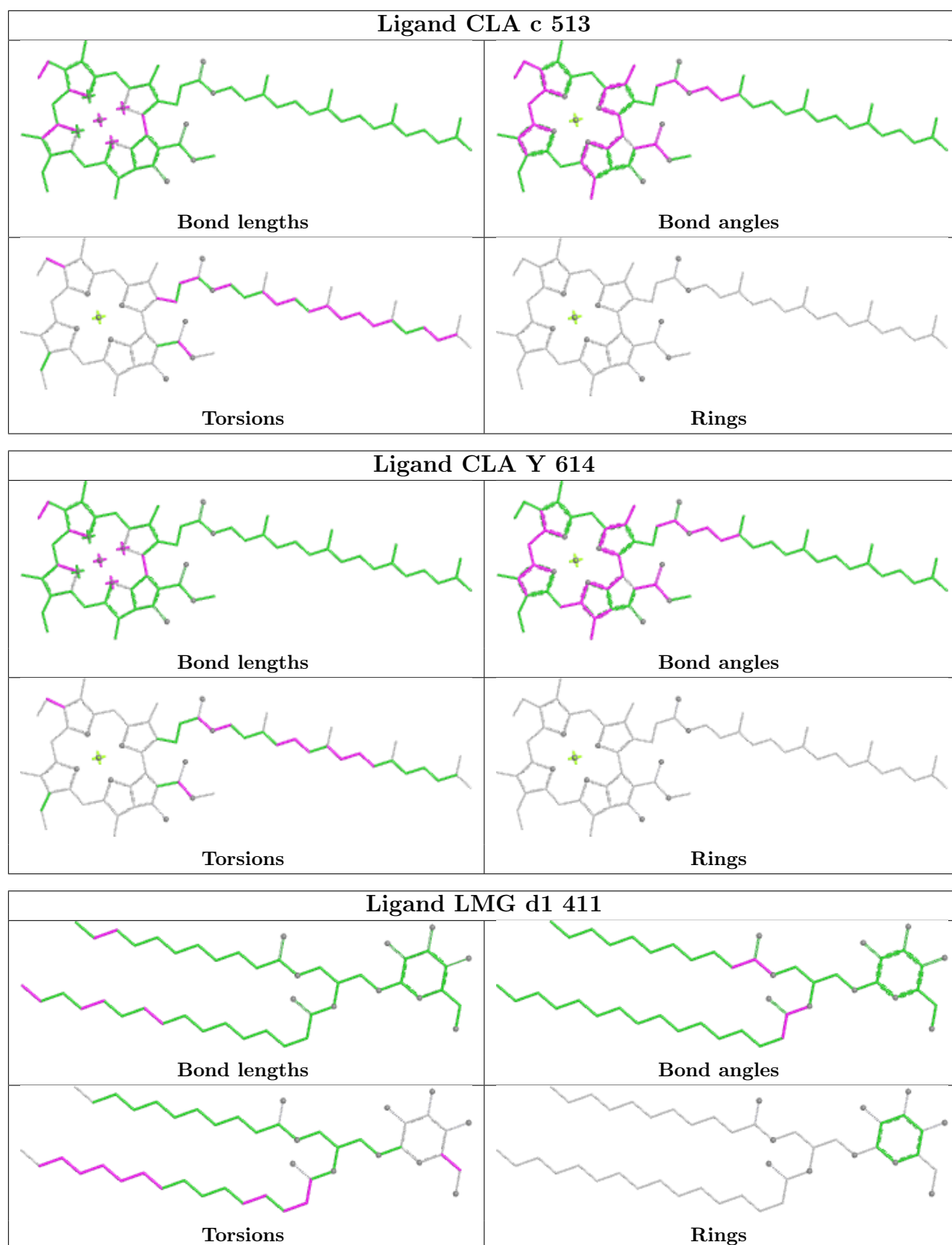


Ligand SQD B1 626

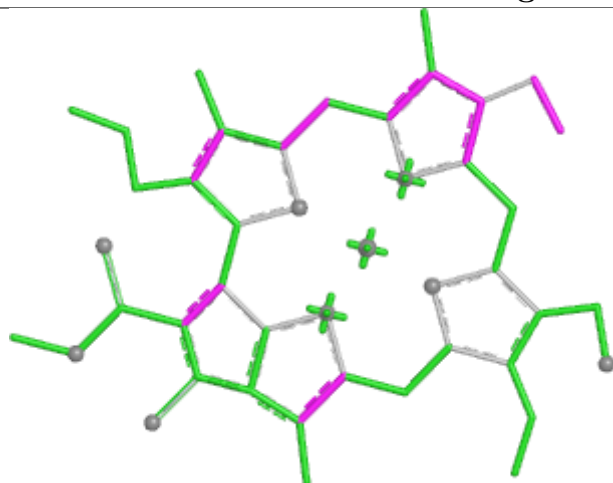




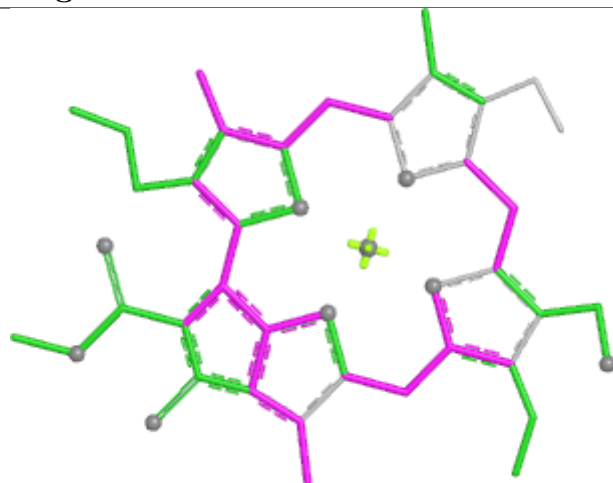




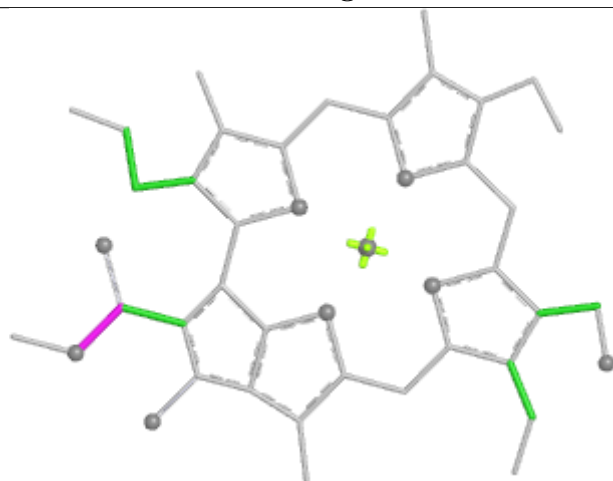
Ligand CHL g 608



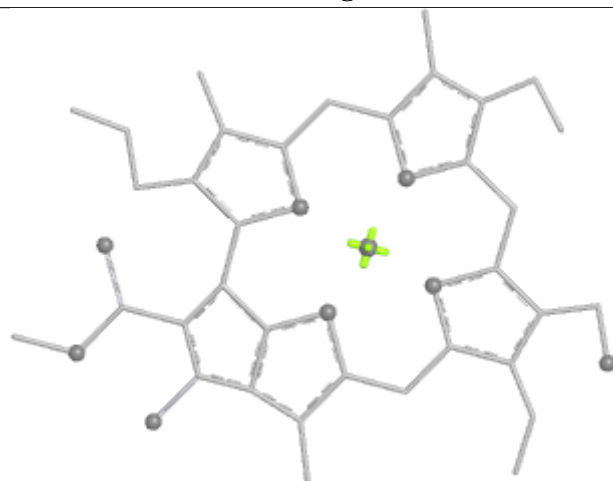
Bond lengths



Bond angles

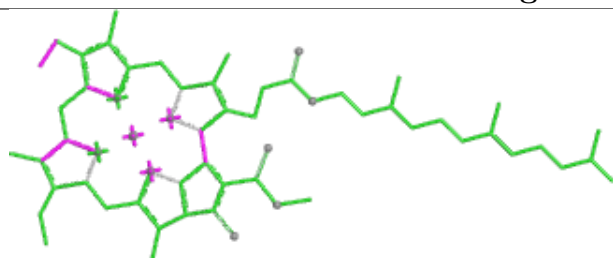


Torsions

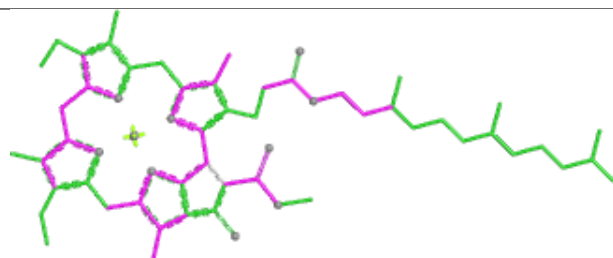


Rings

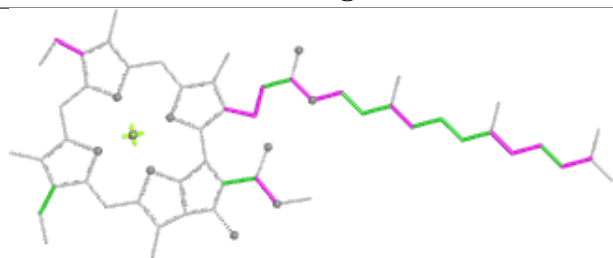
Ligand CLA r 603



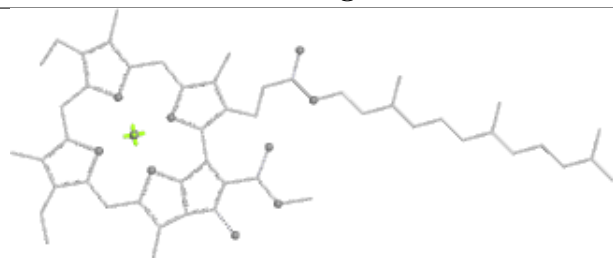
Bond lengths



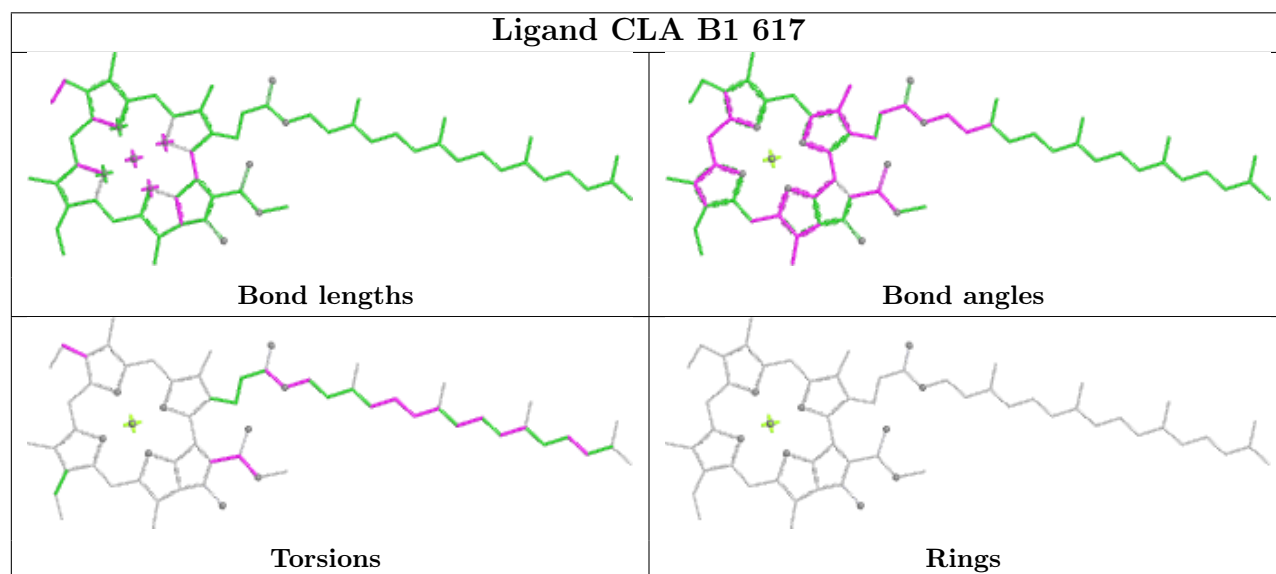
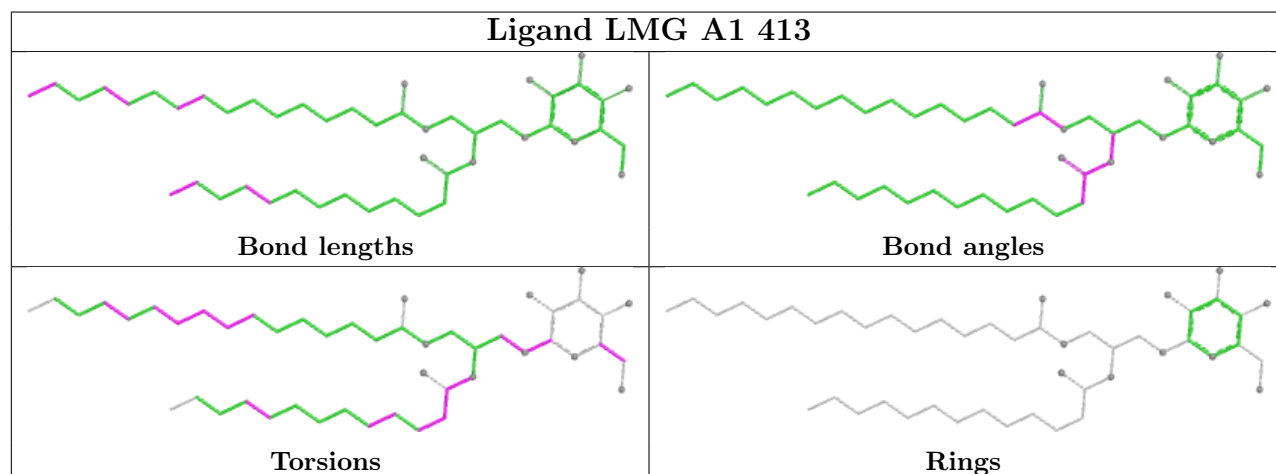
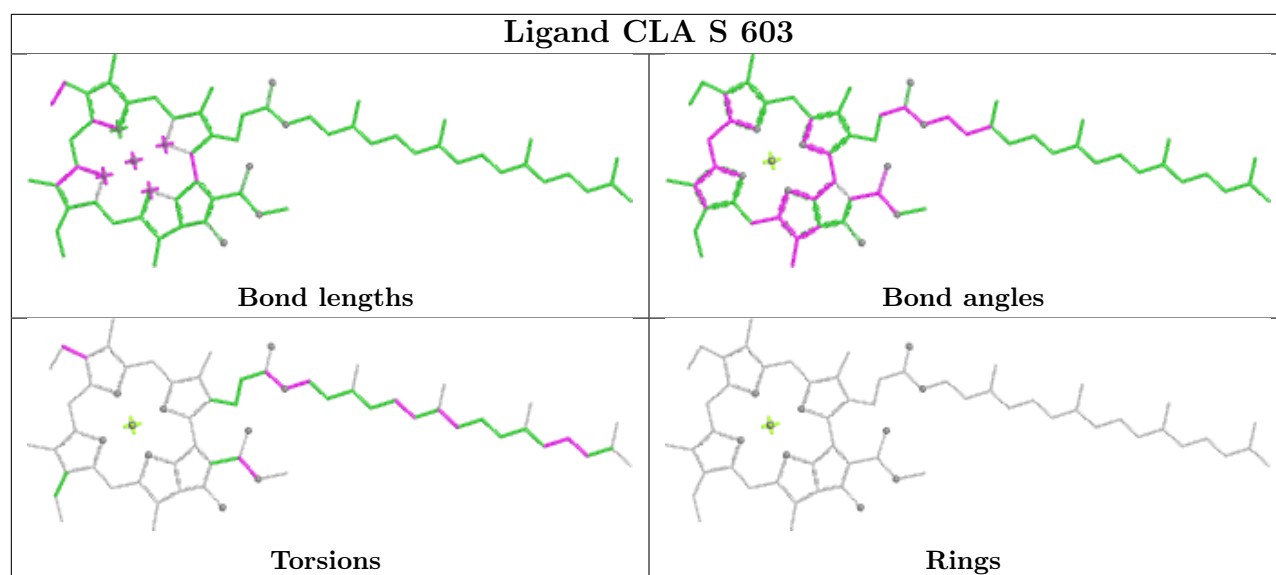
Bond angles

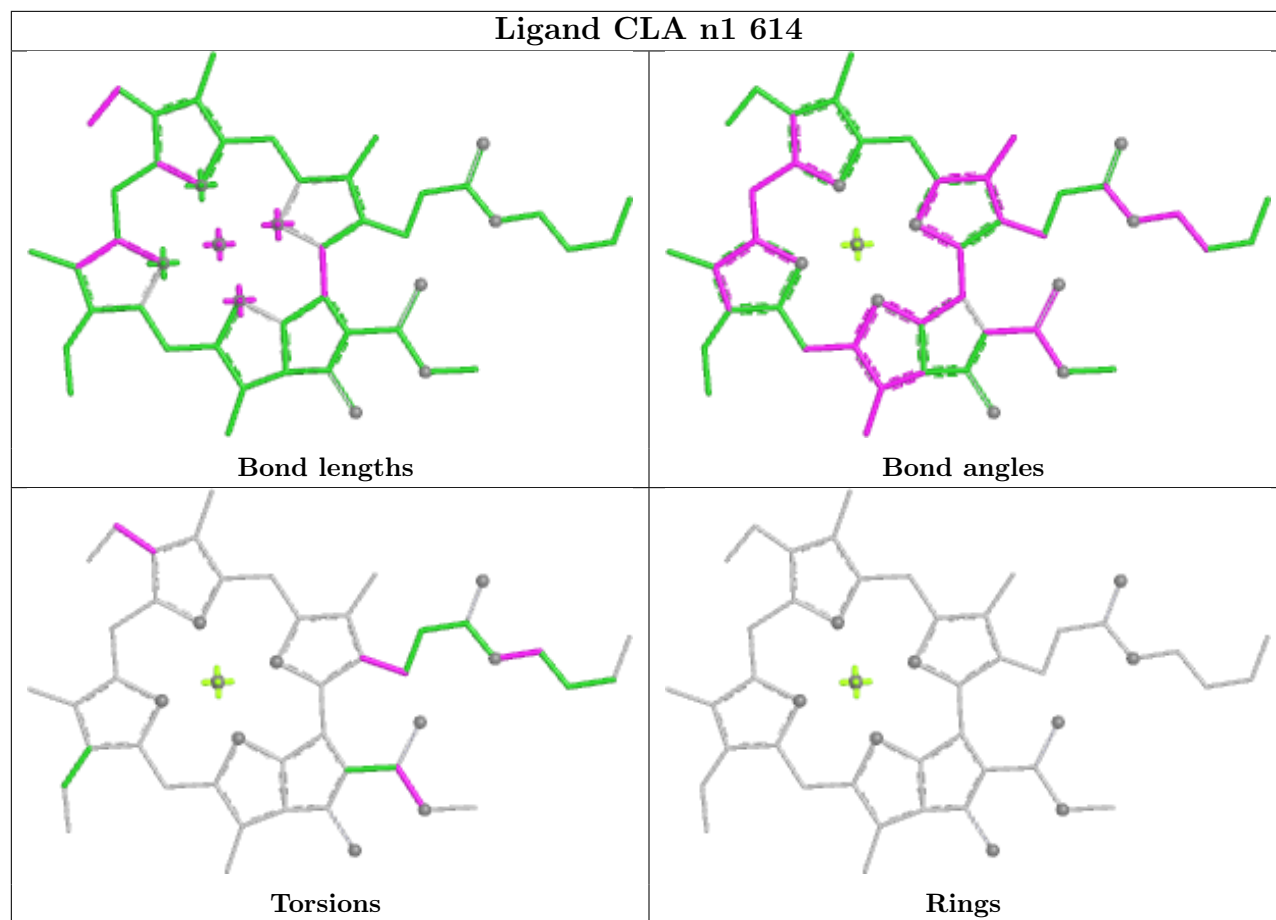


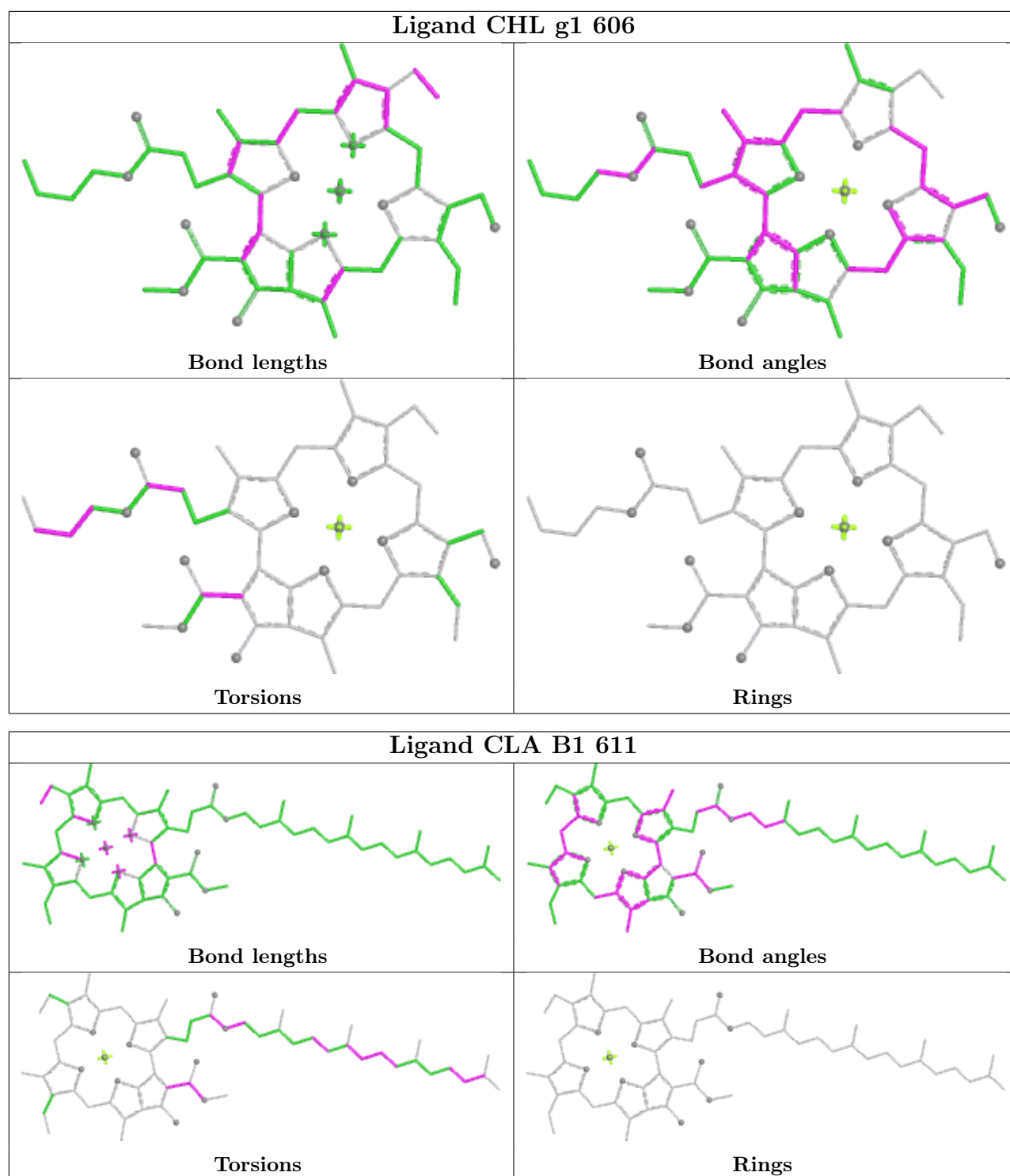
Torsions

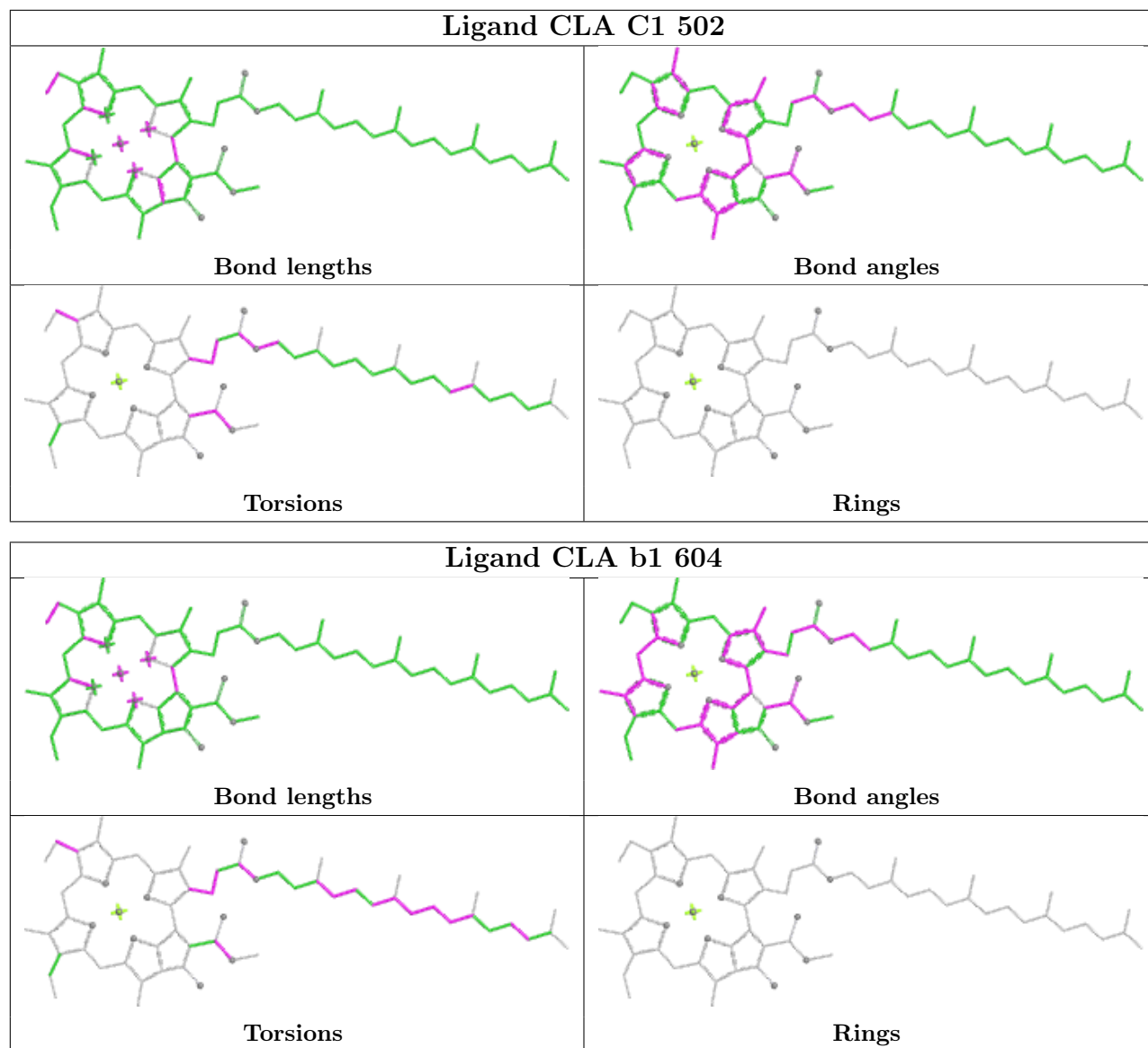


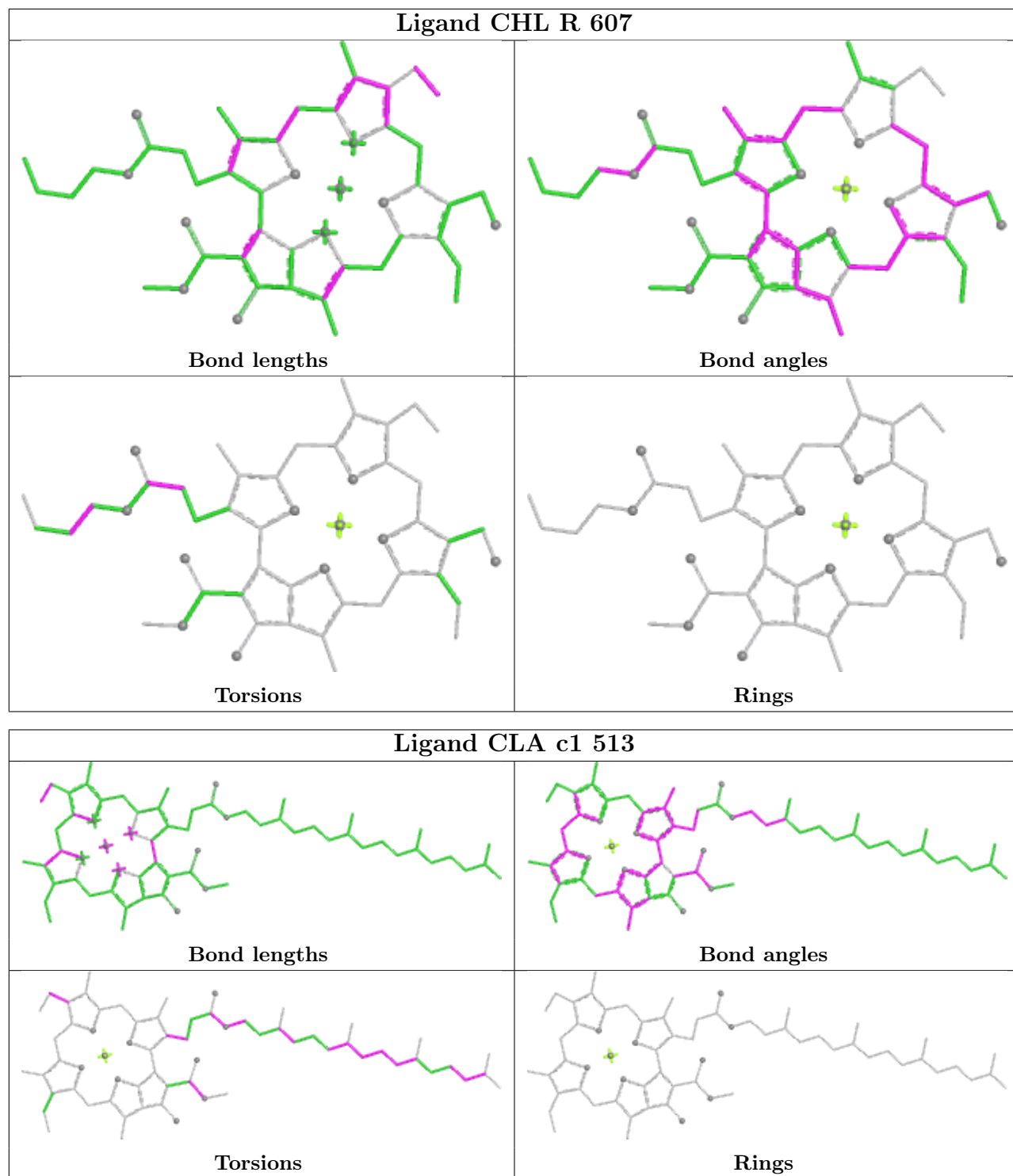
Rings

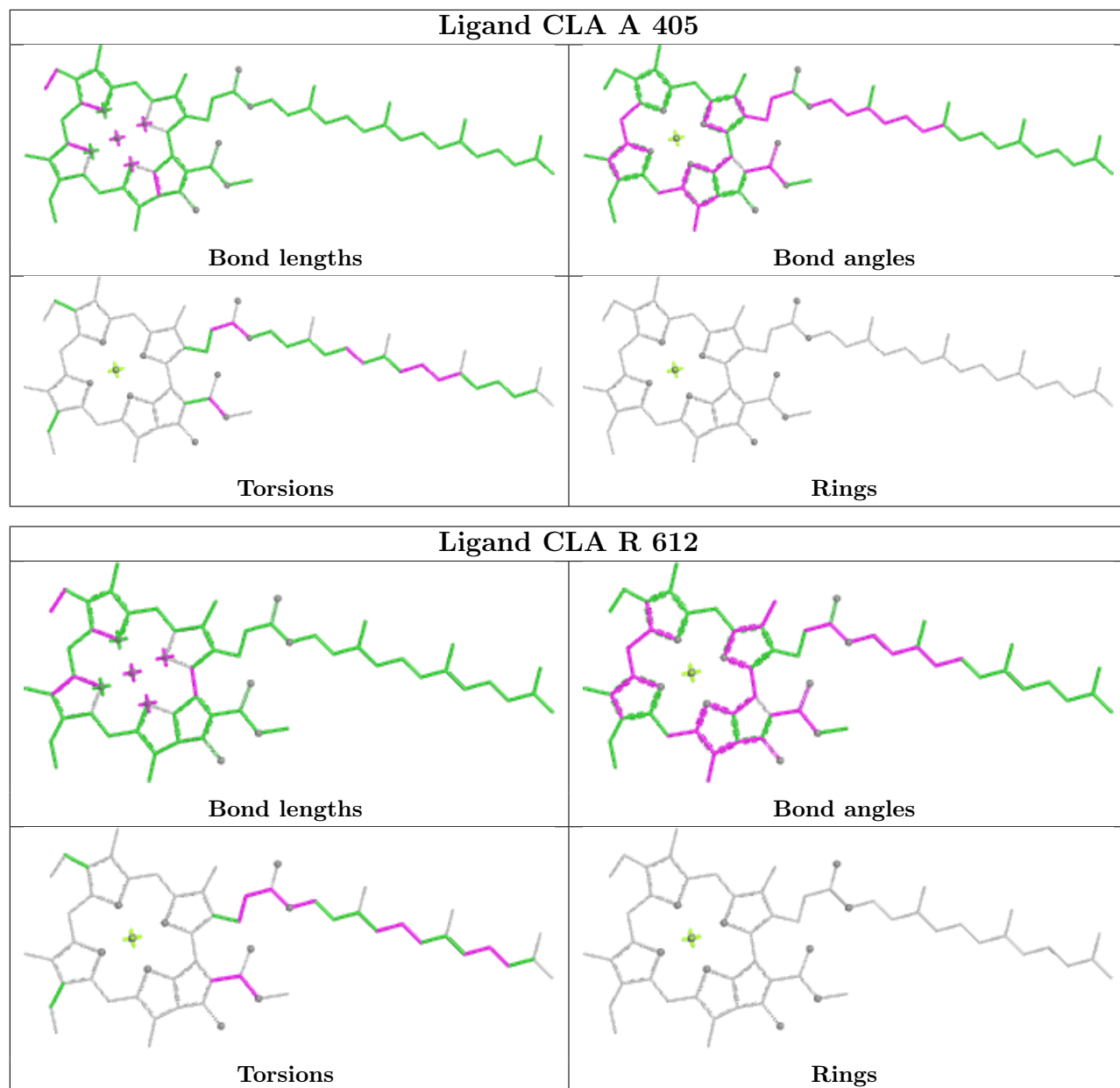


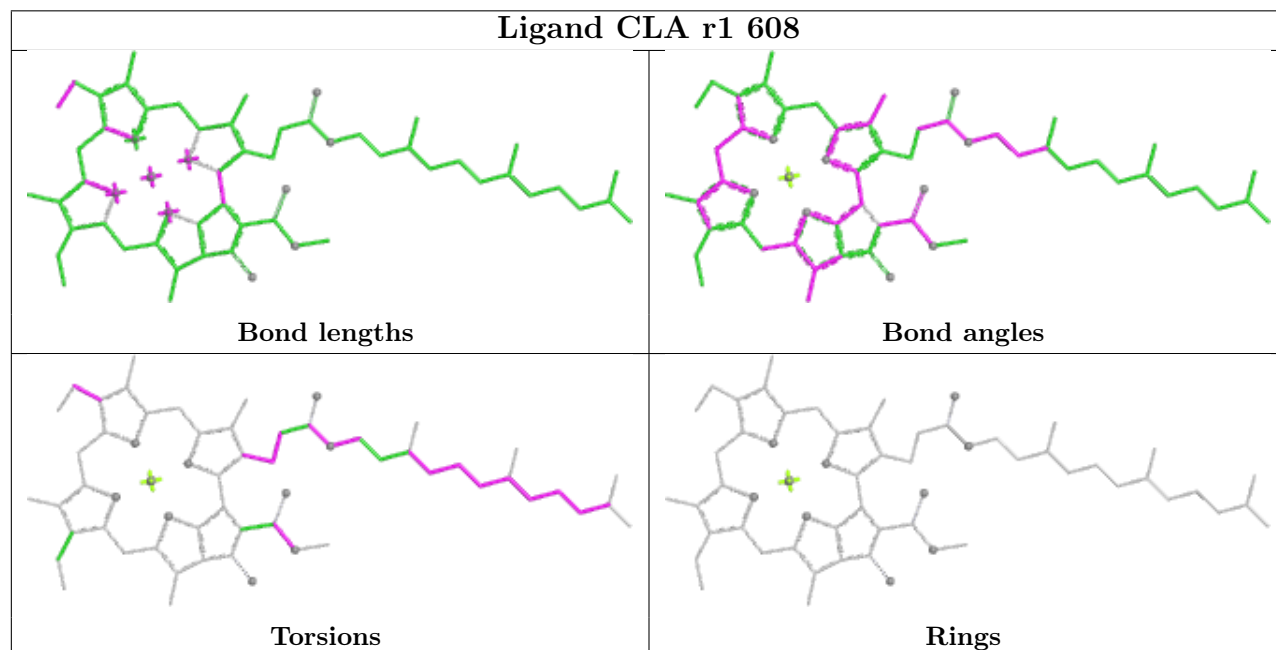
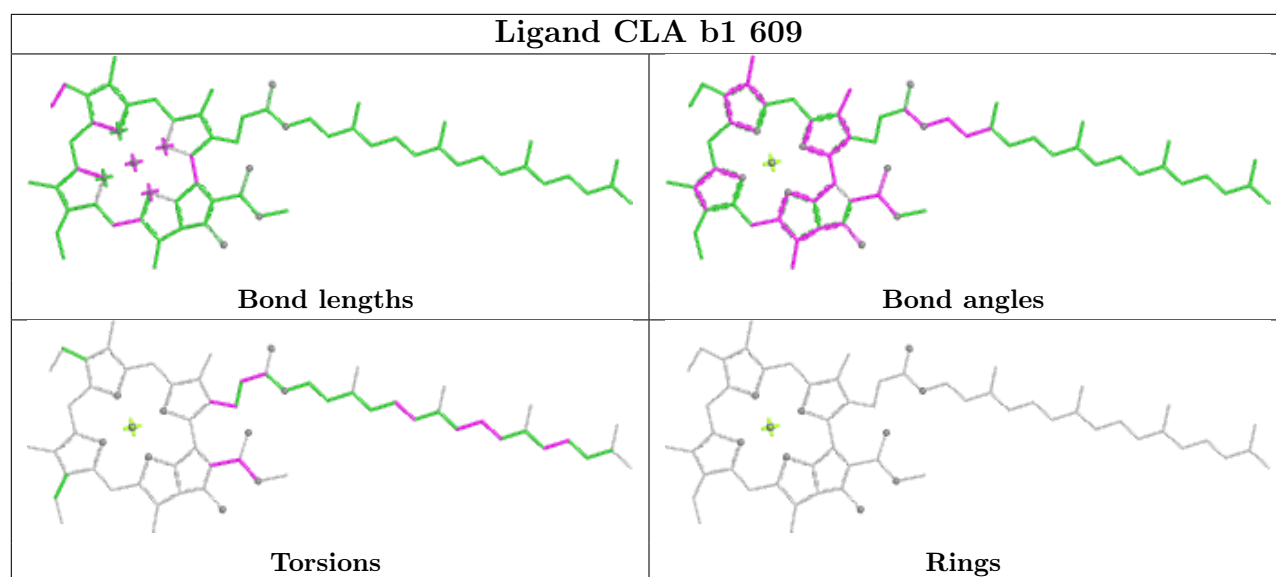


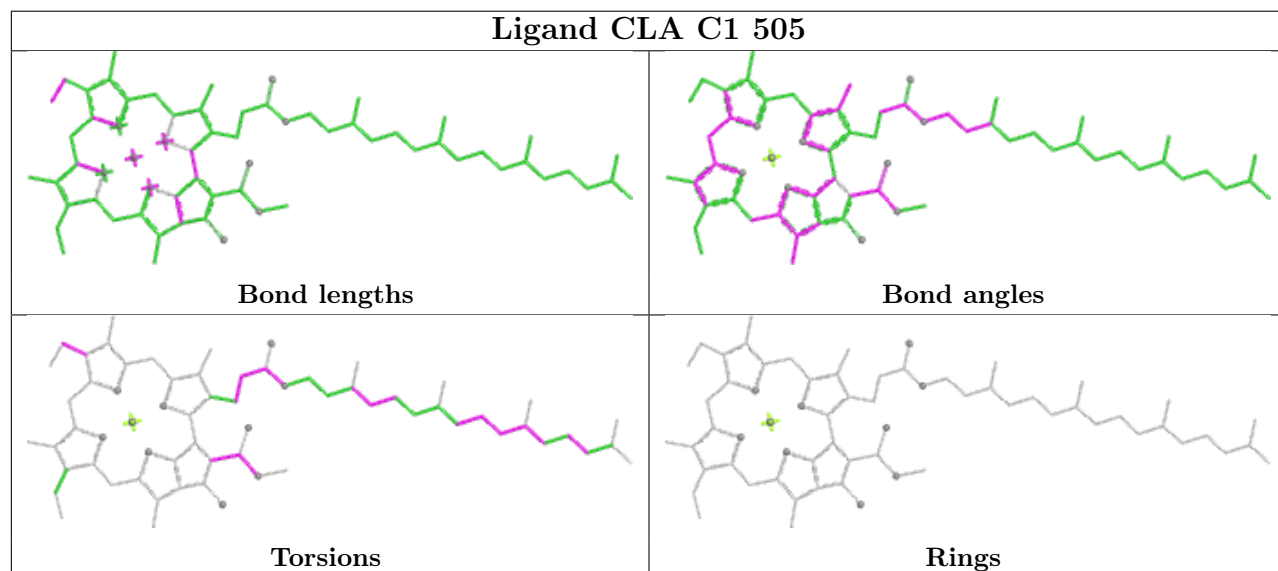
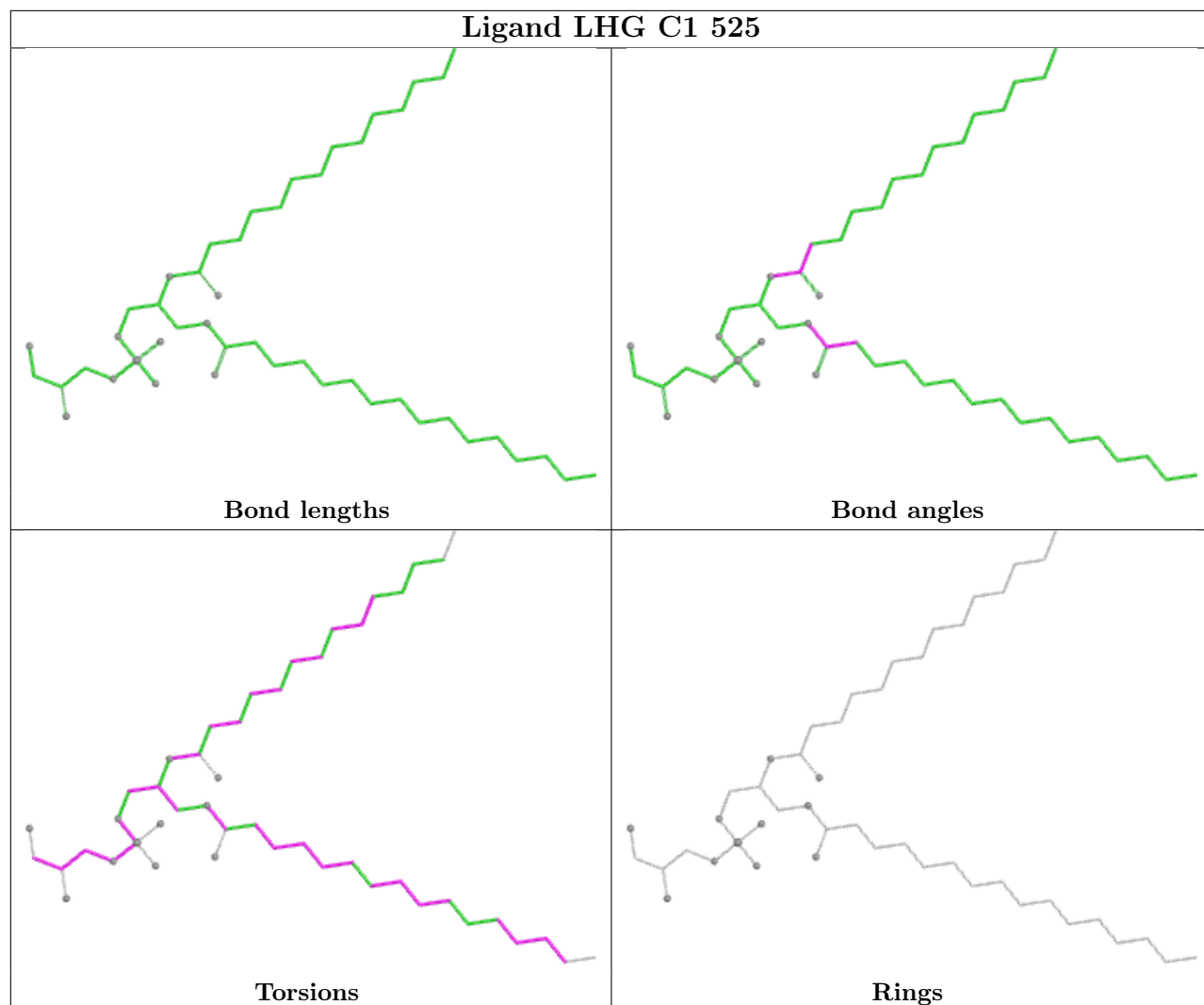


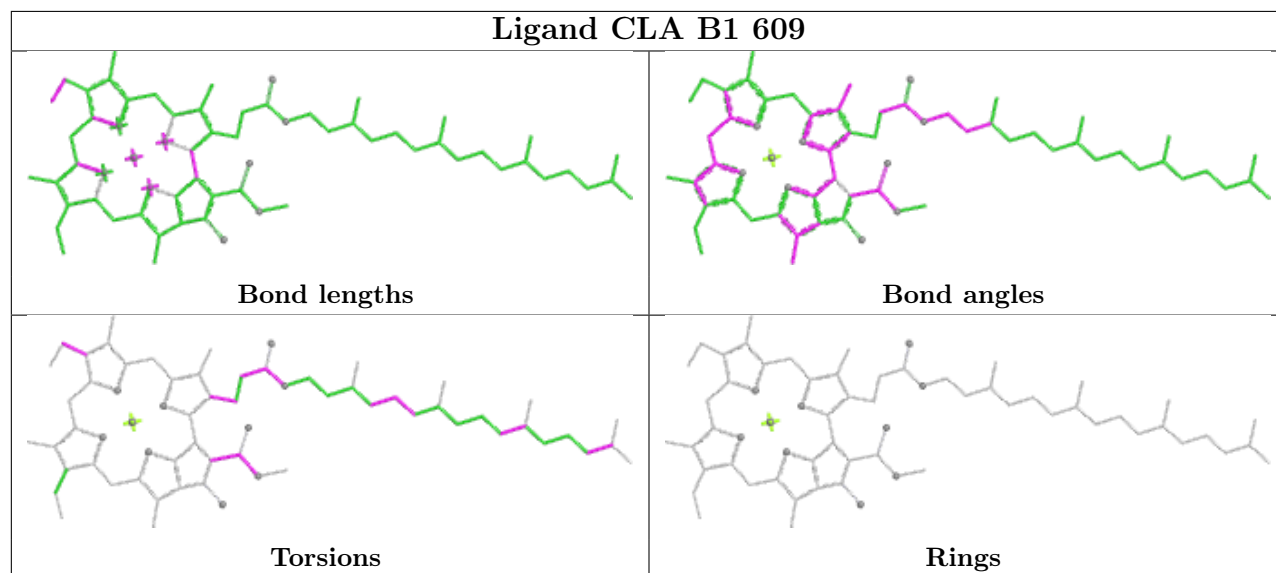
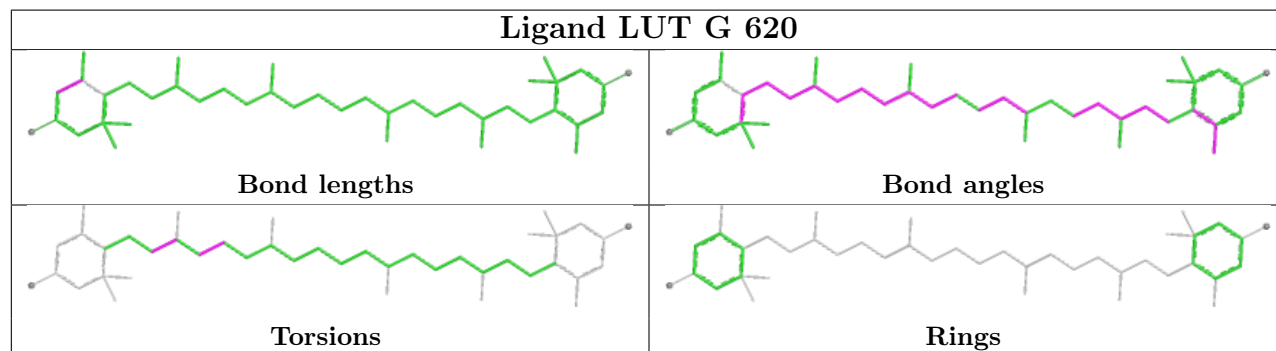
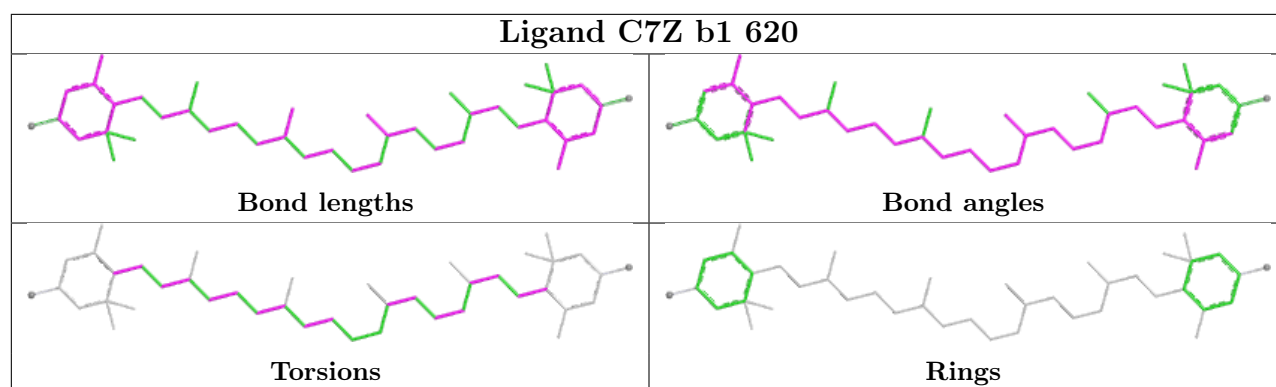


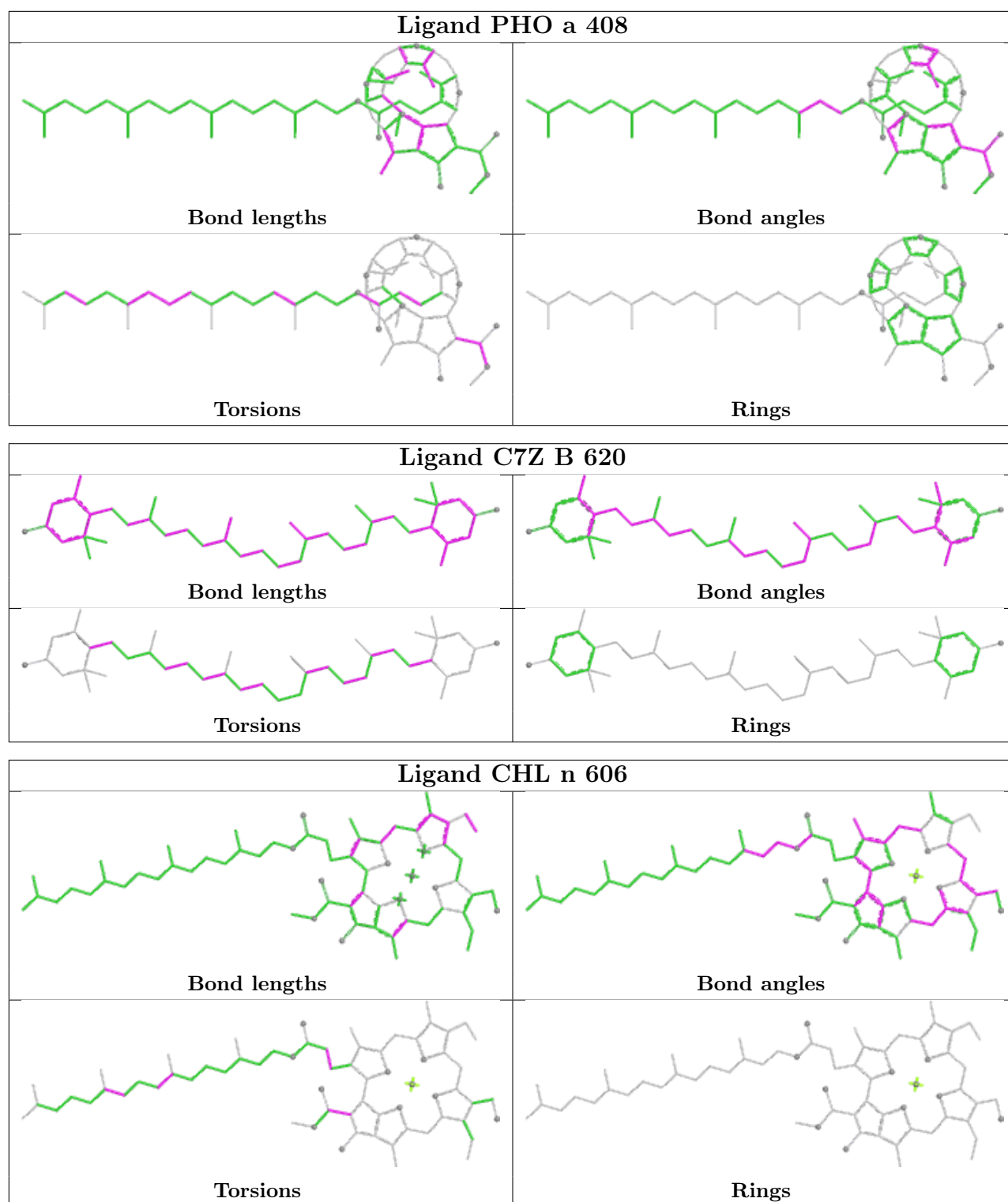


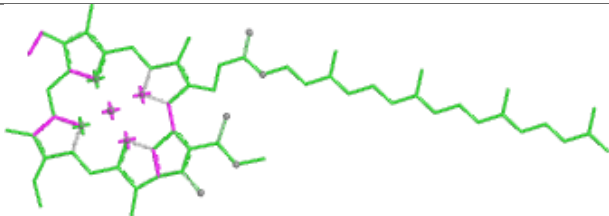
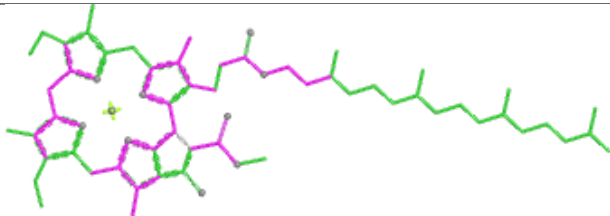
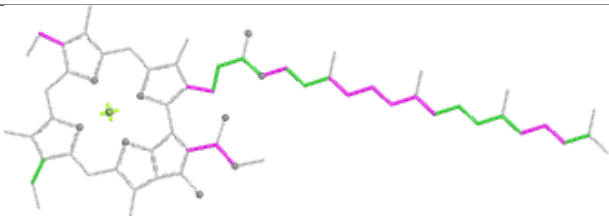
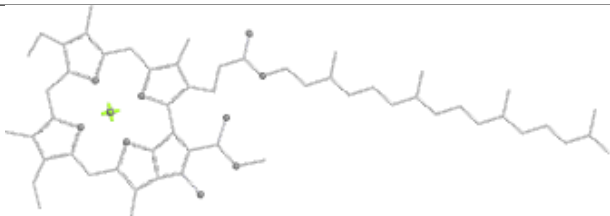


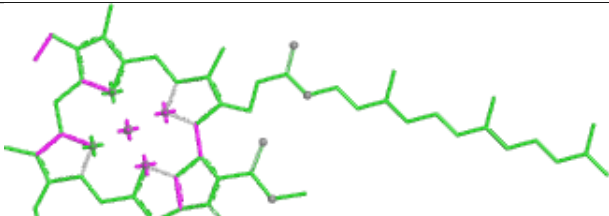
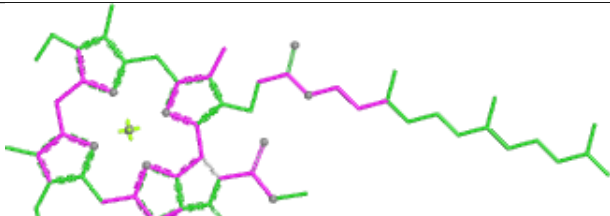
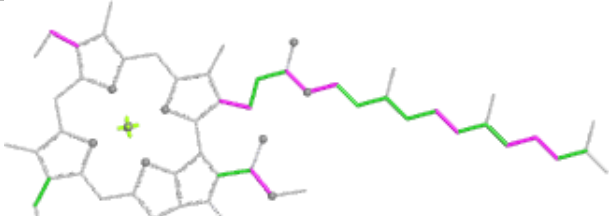
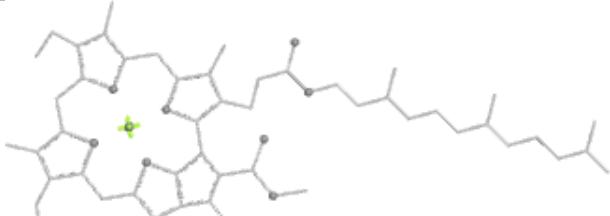


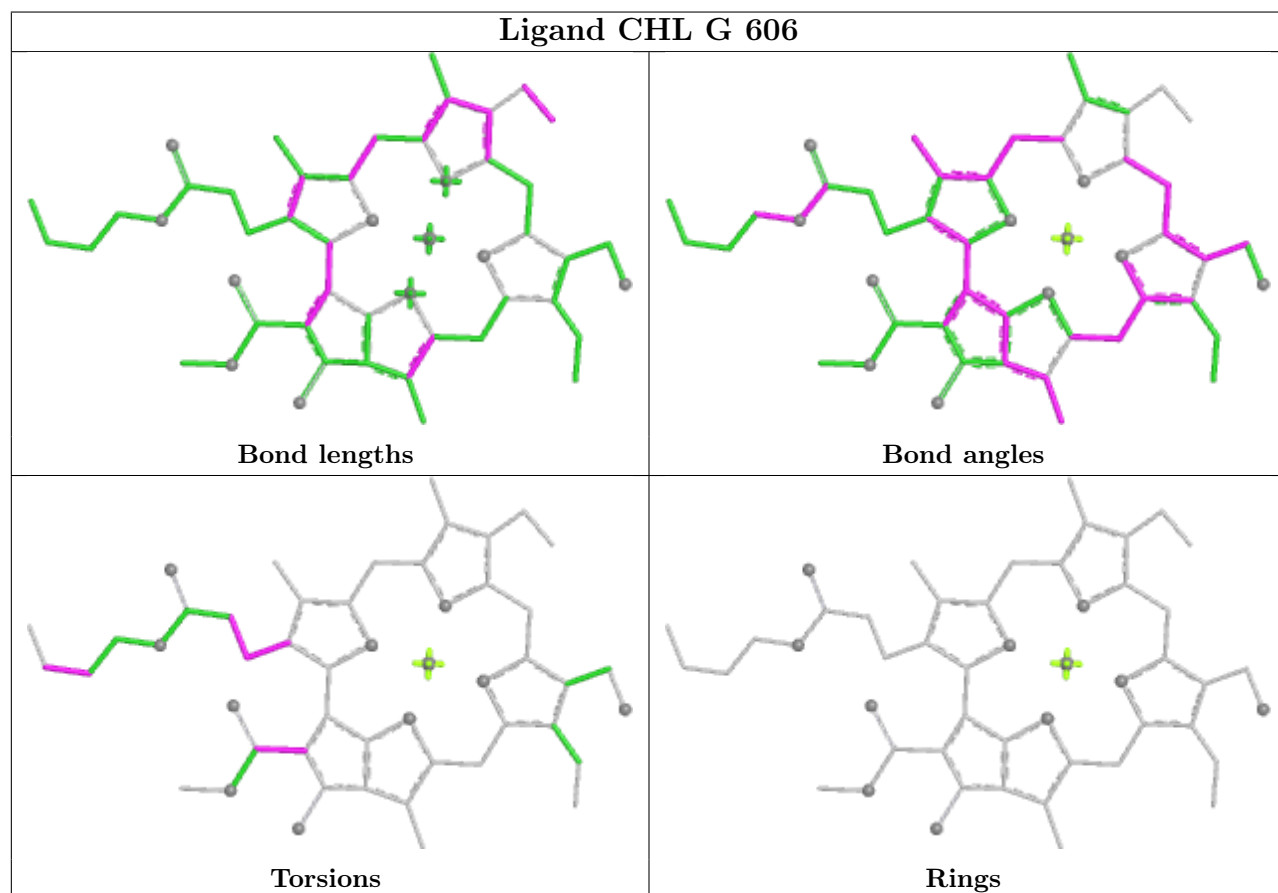
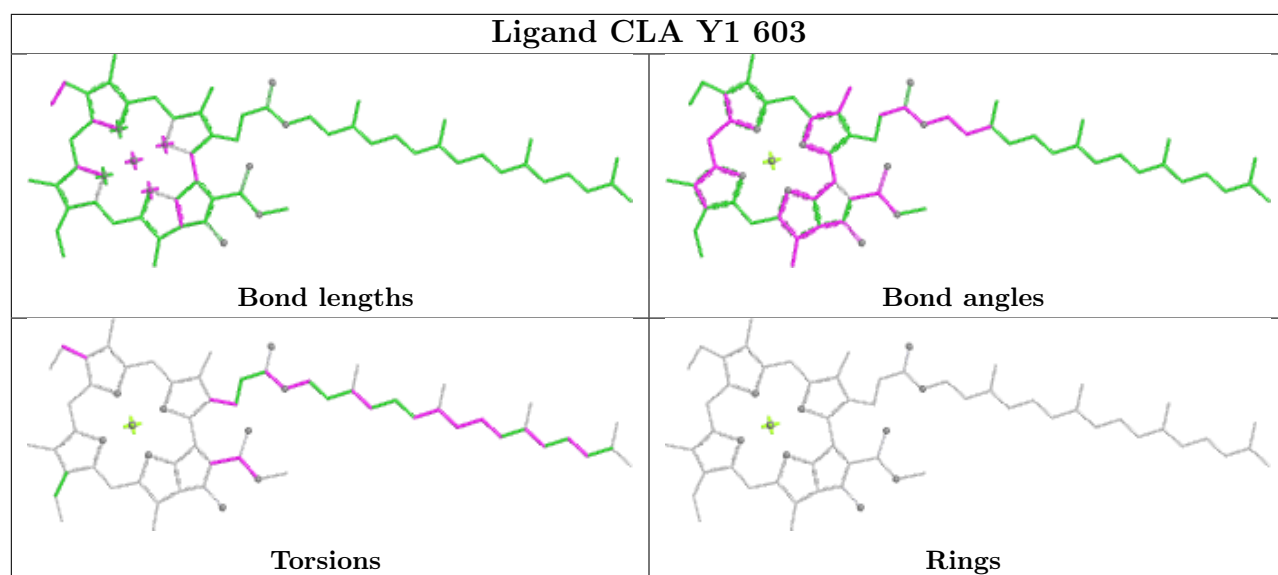


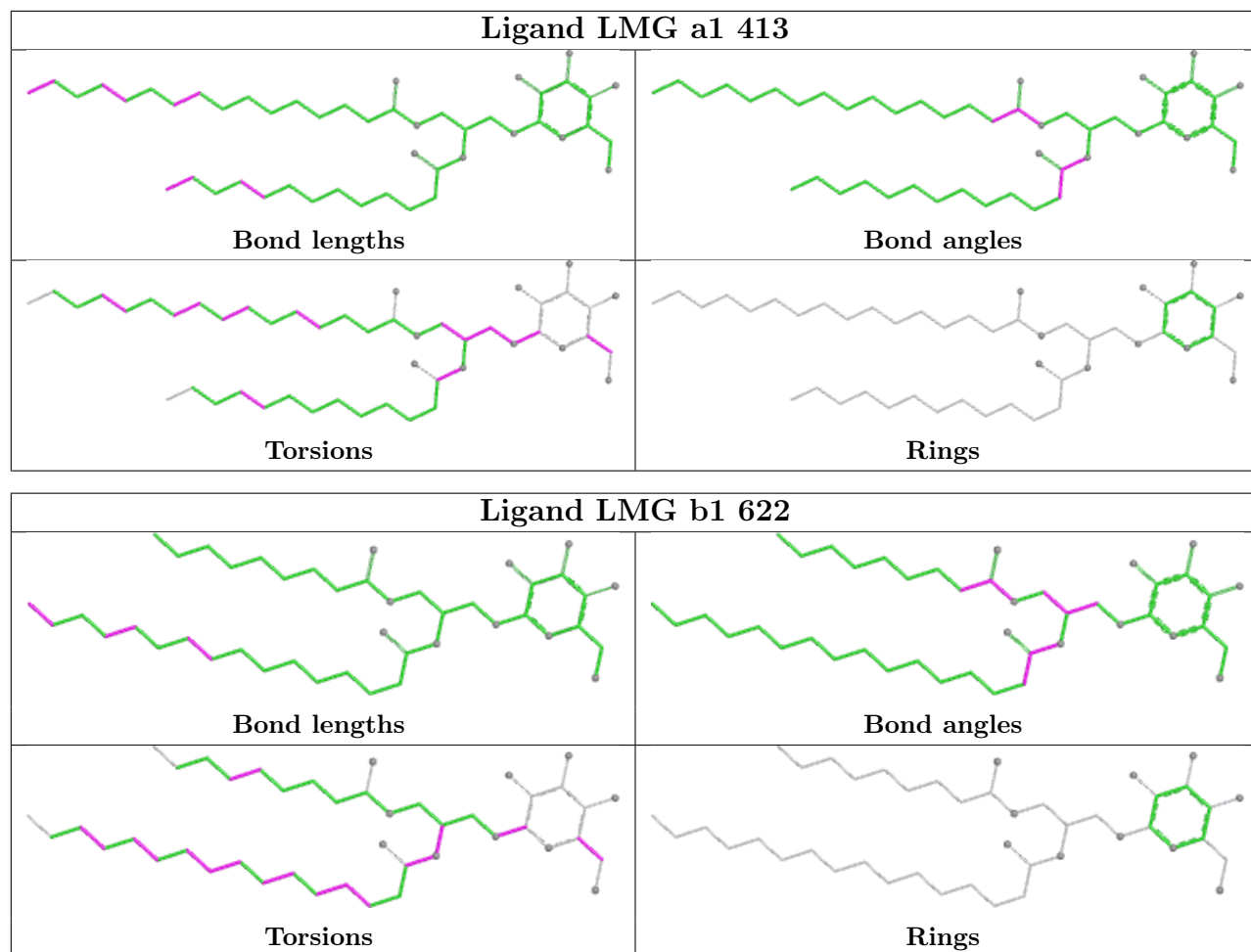




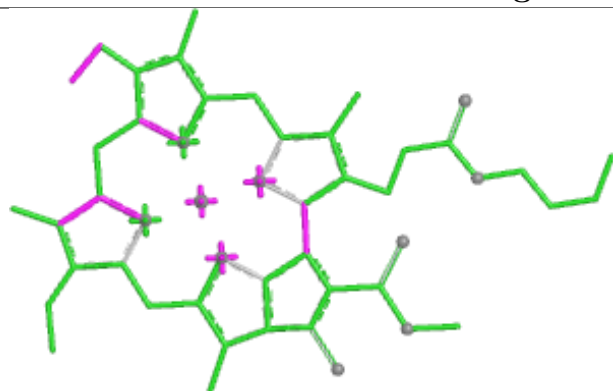
Ligand CLA c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R1 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

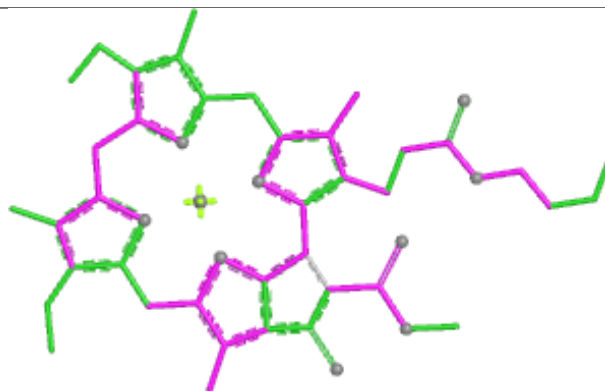




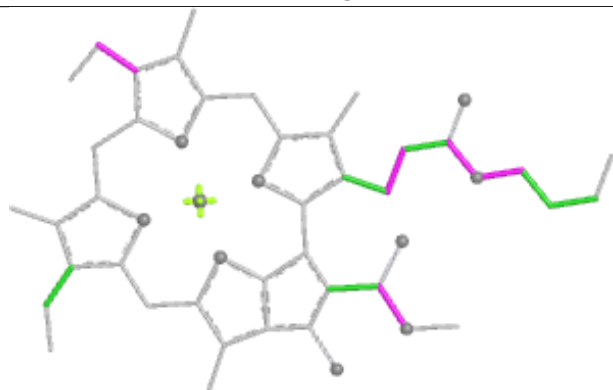
Ligand CLA N 614



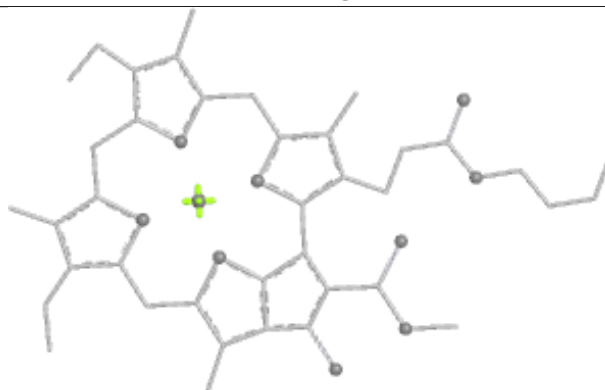
Bond lengths



Bond angles

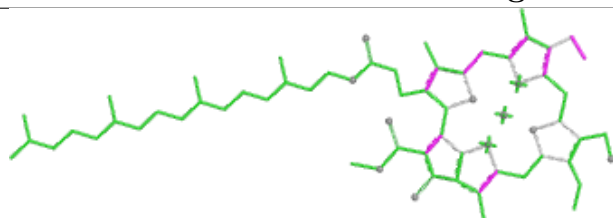


Torsions

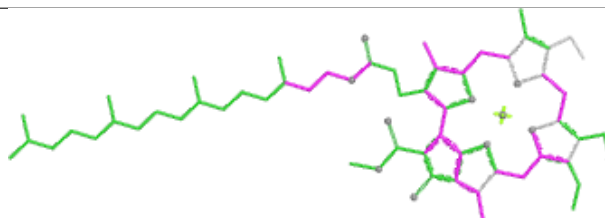


Rings

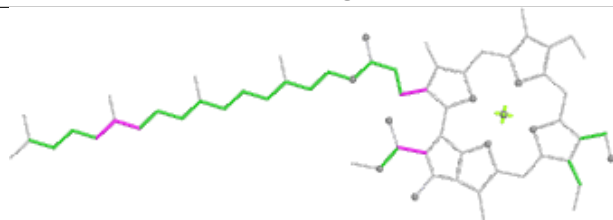
Ligand CHL n1 607



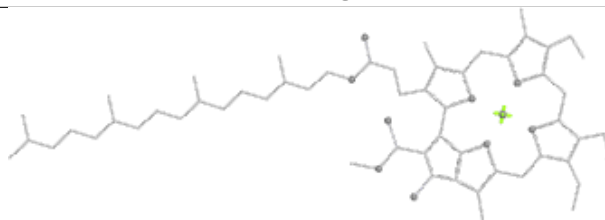
Bond lengths



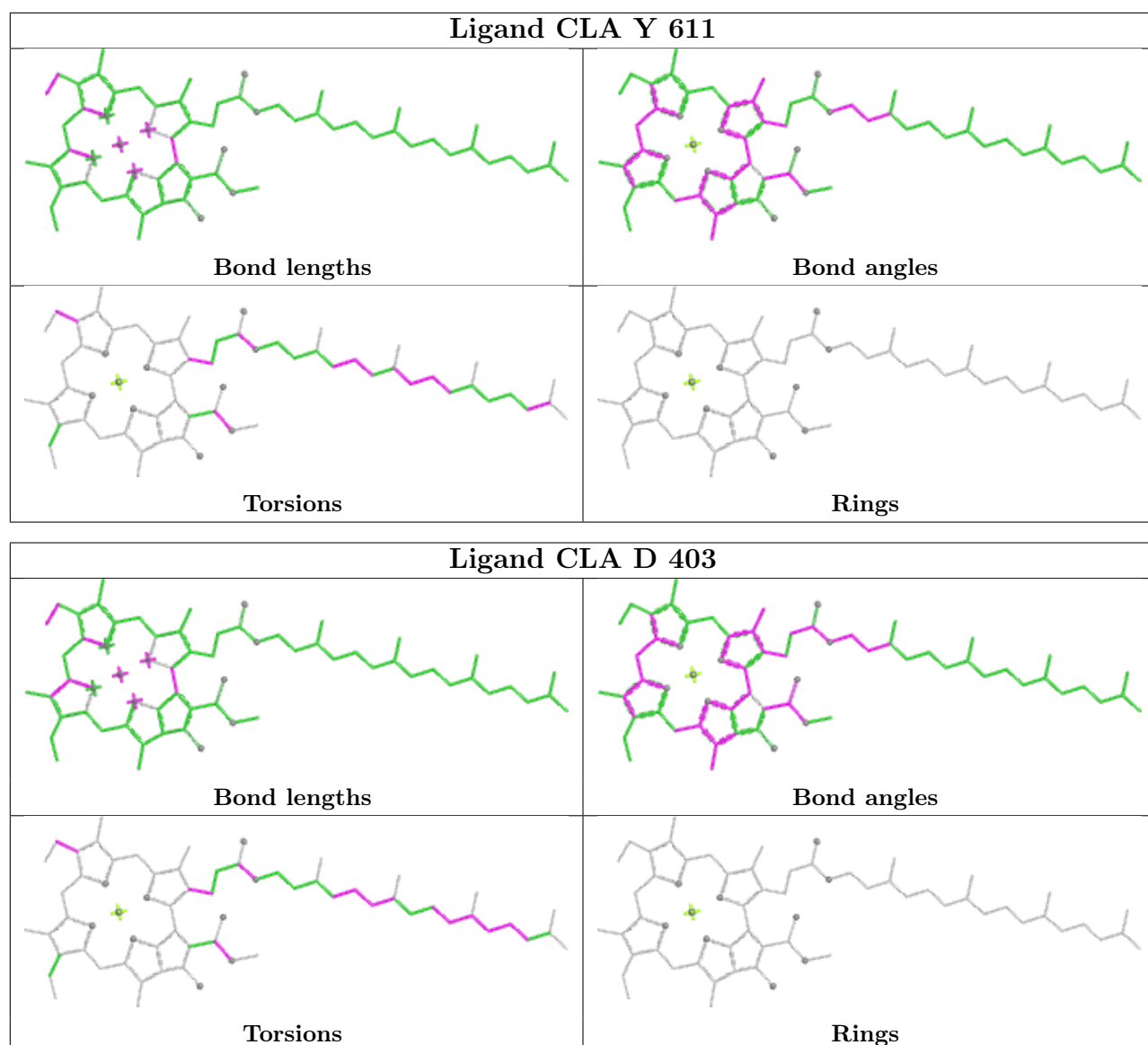
Bond angles

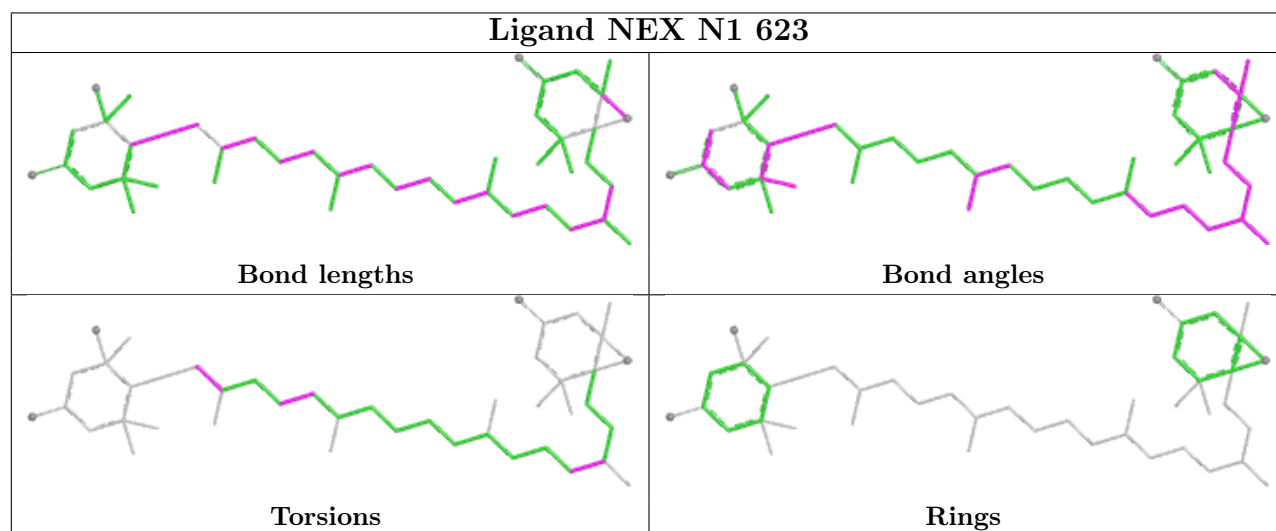
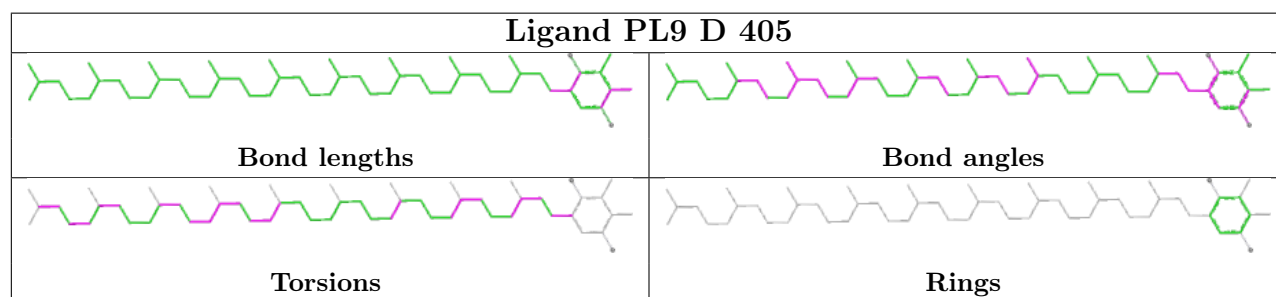
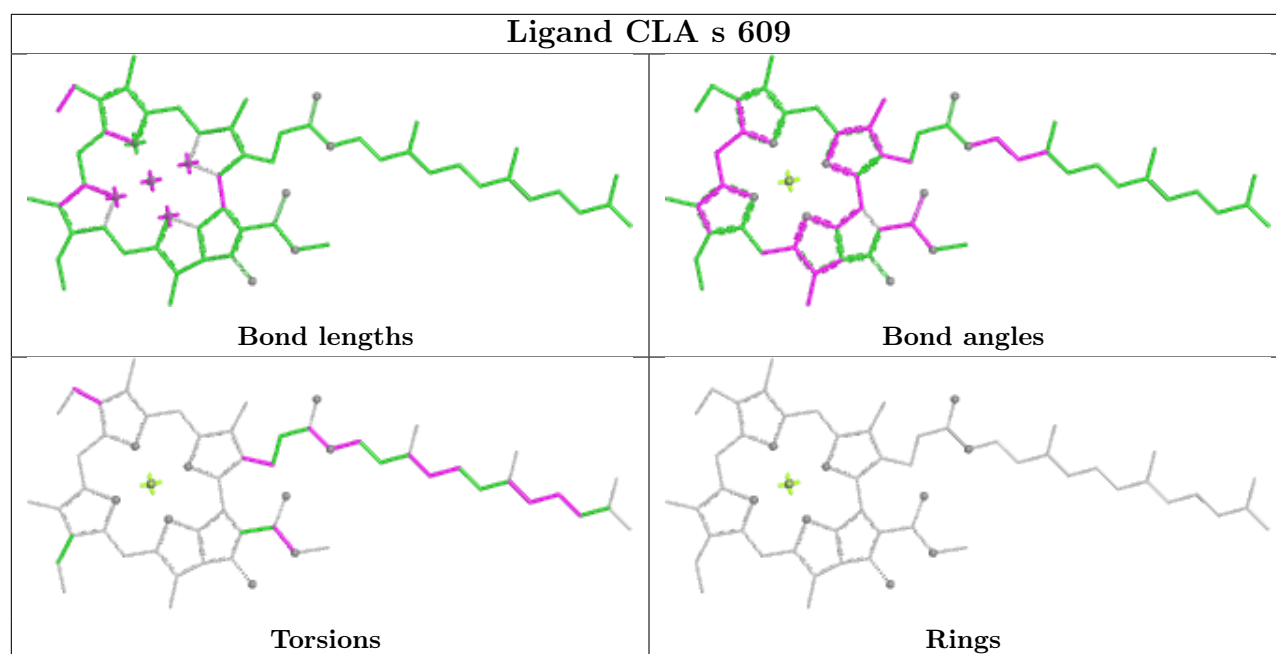


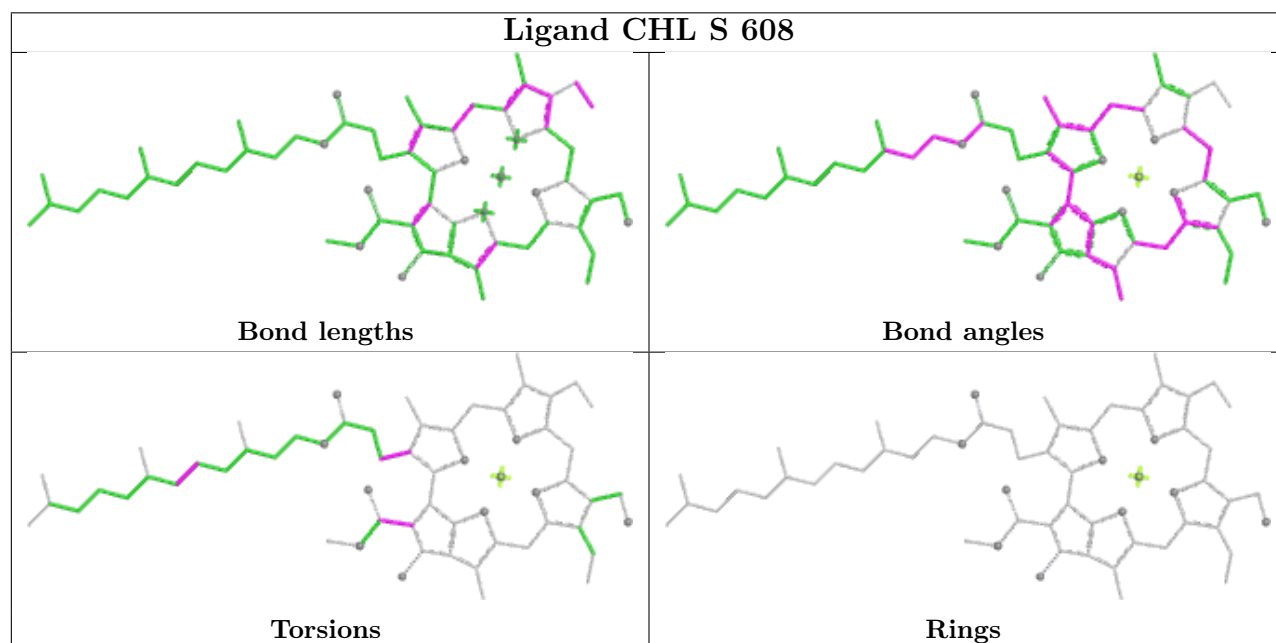
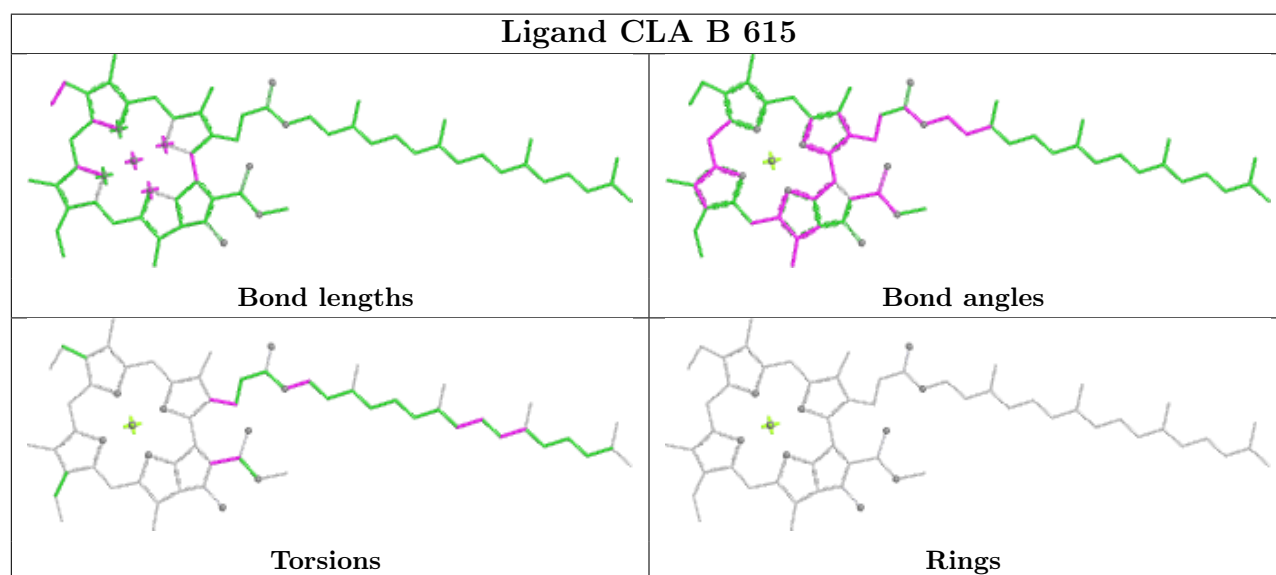
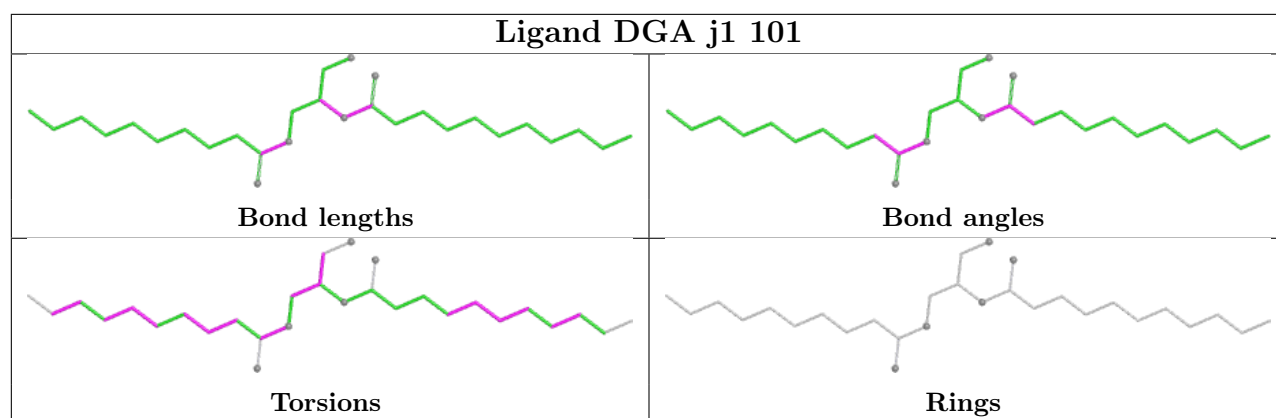
Torsions

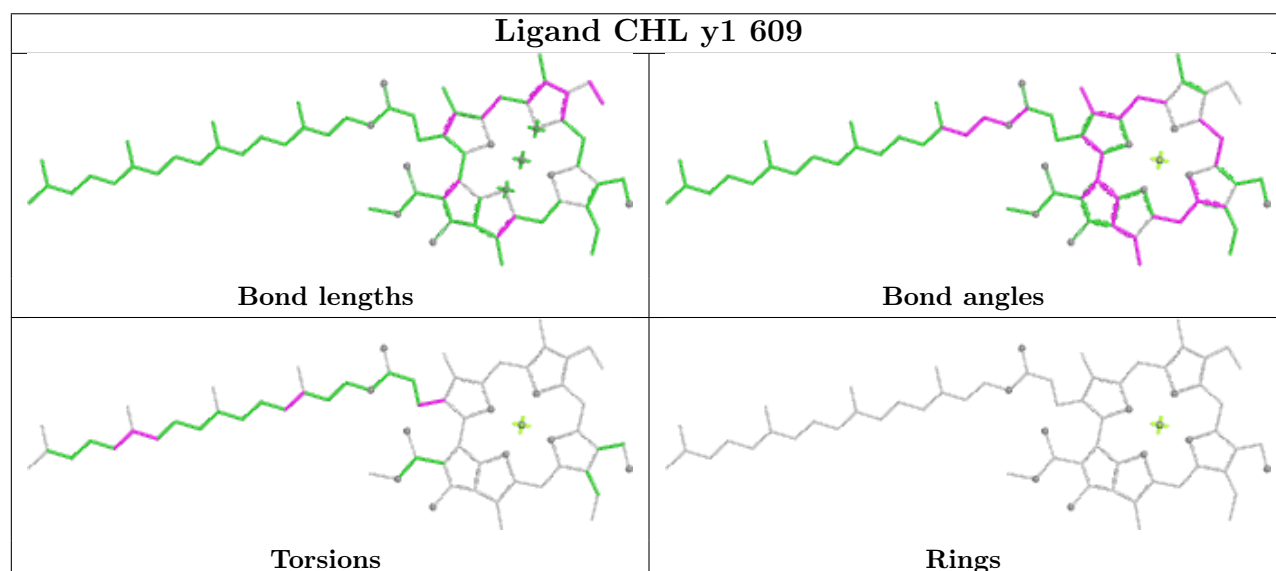
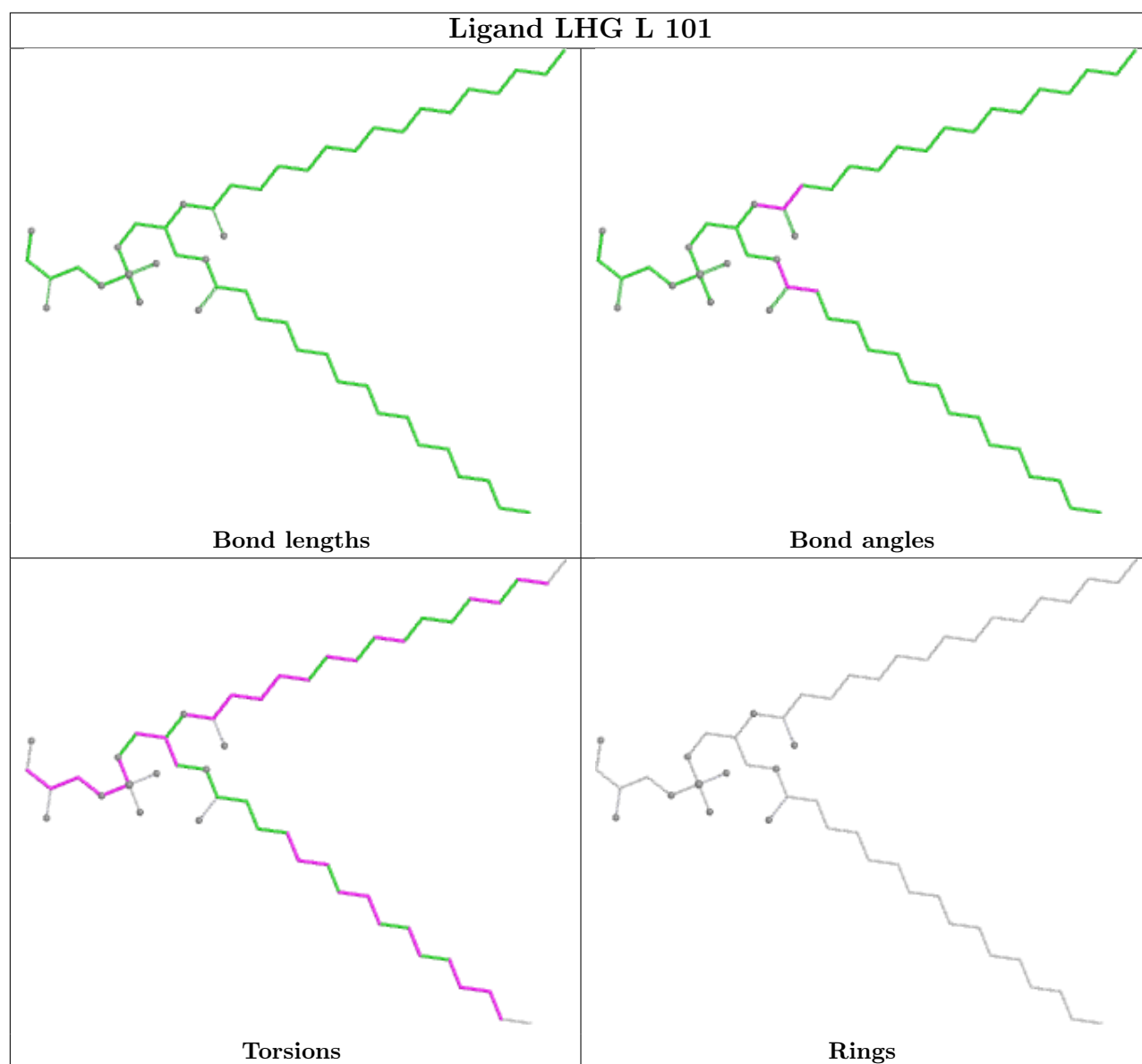


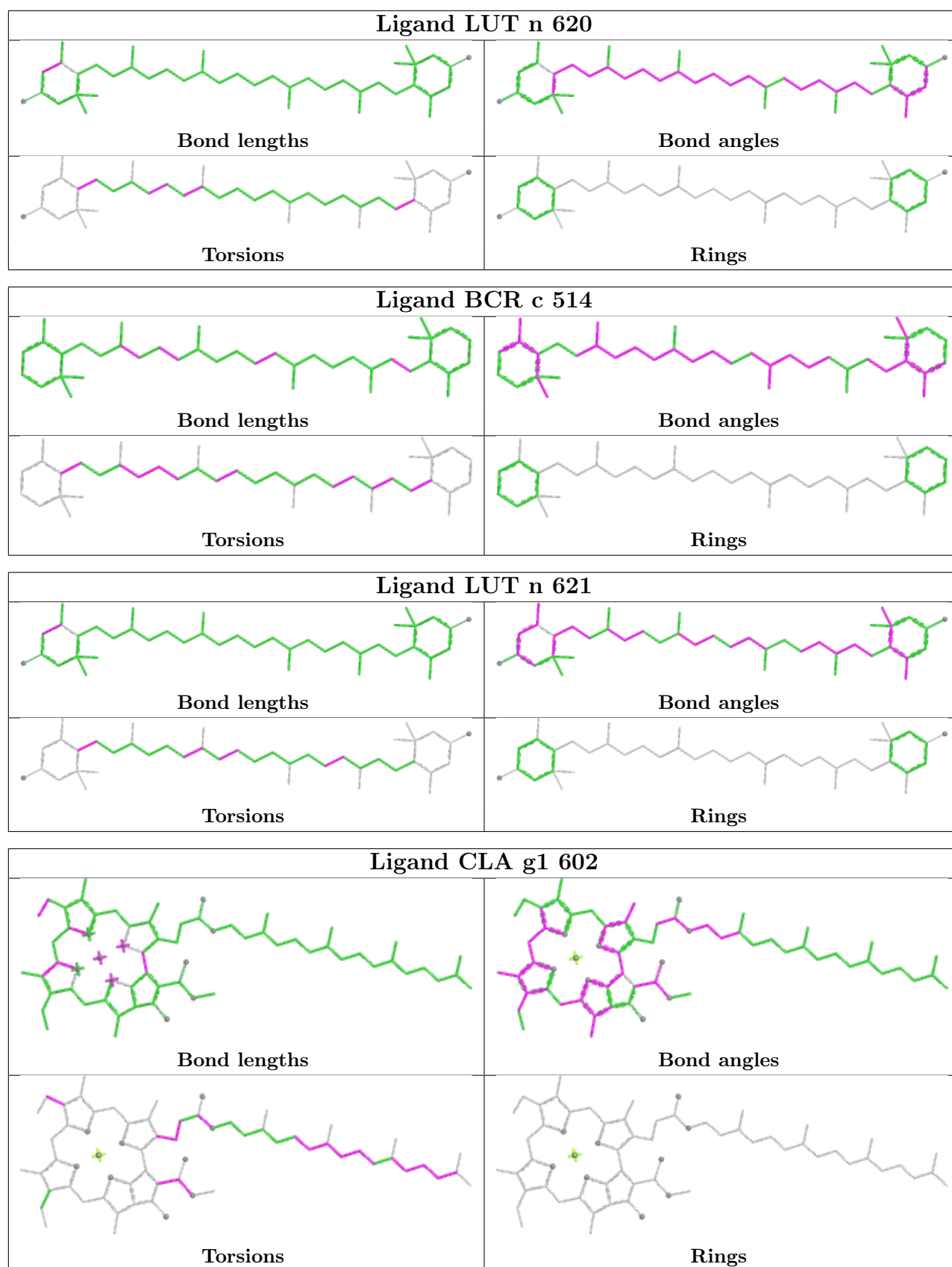
Rings



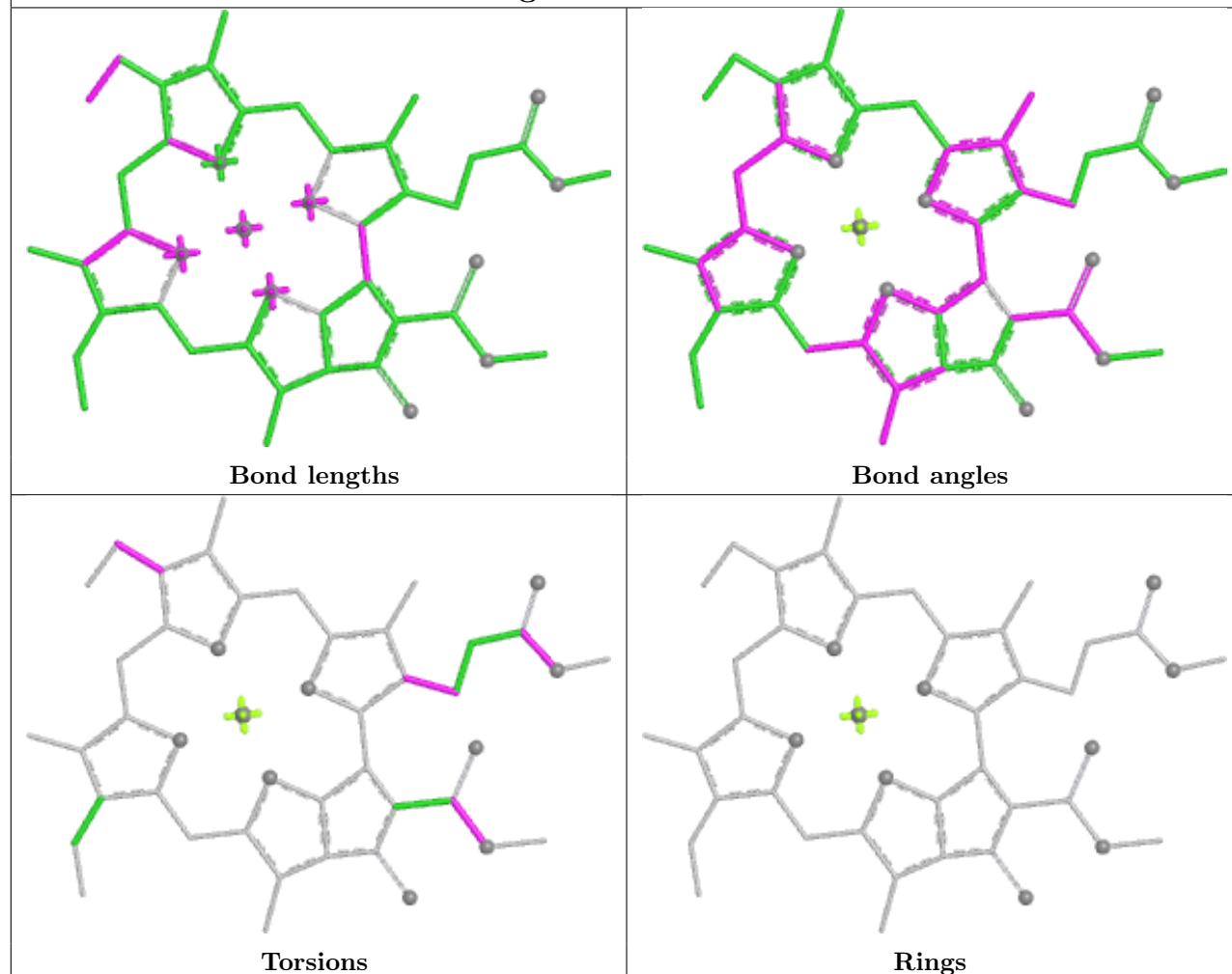




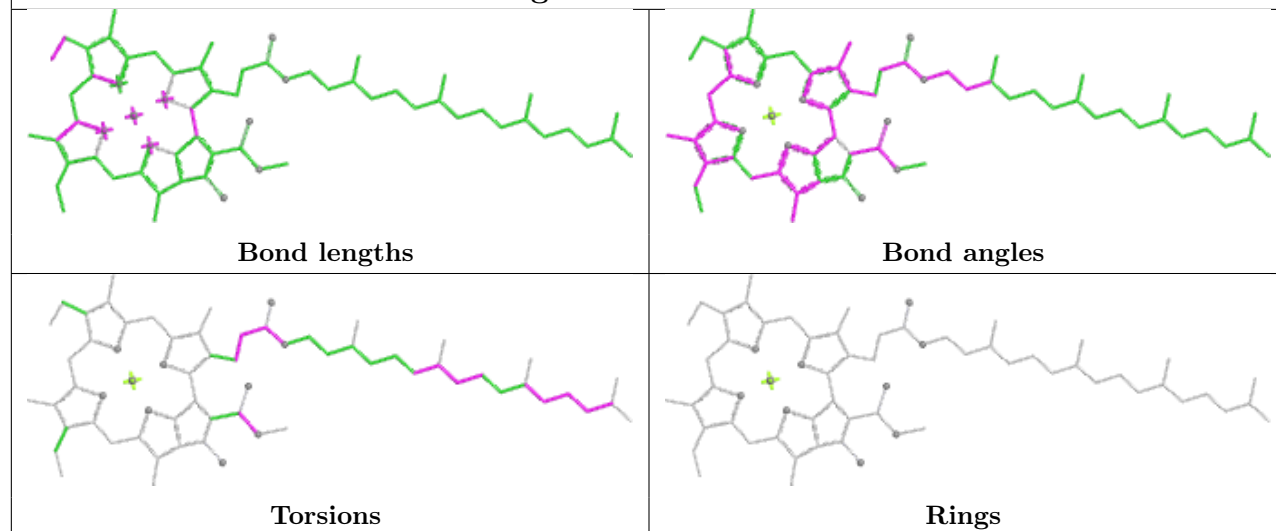


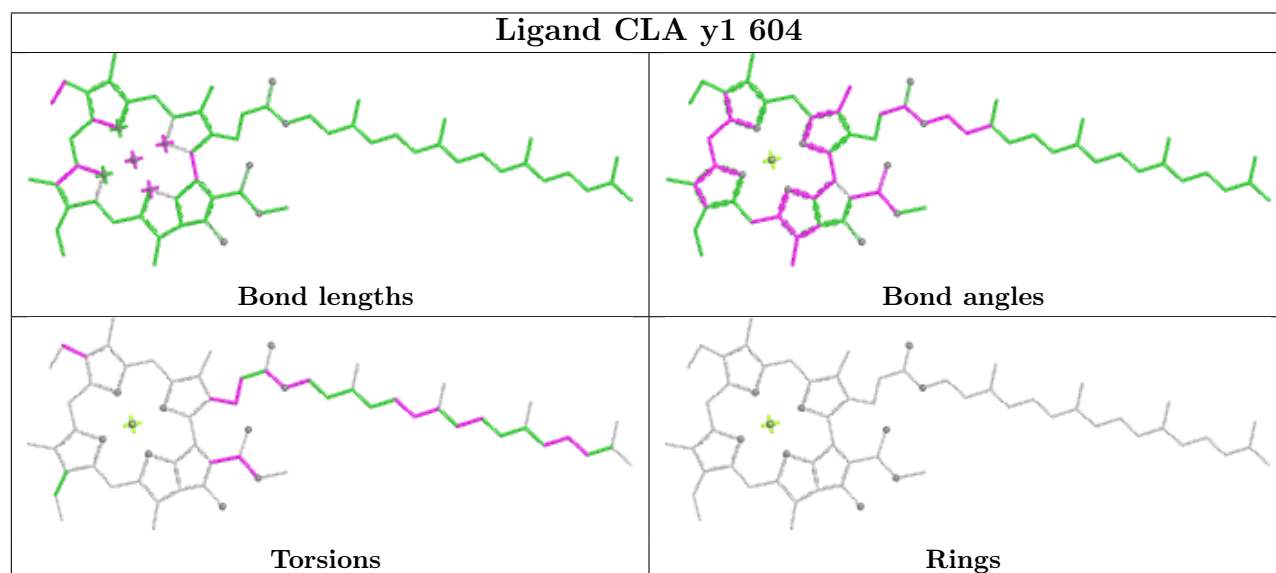
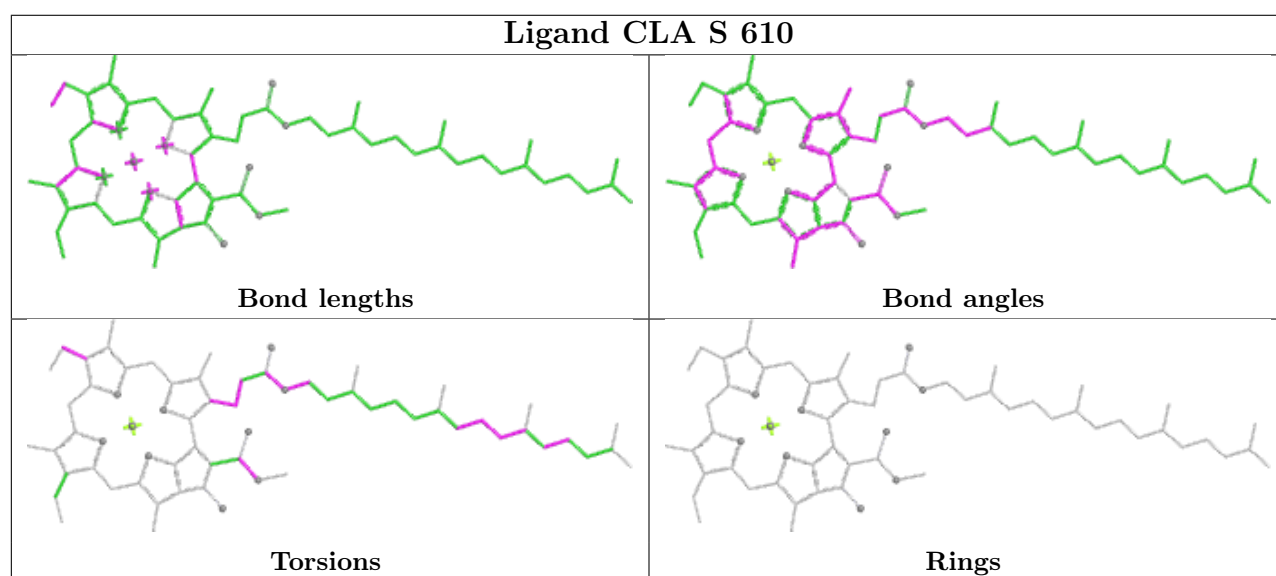
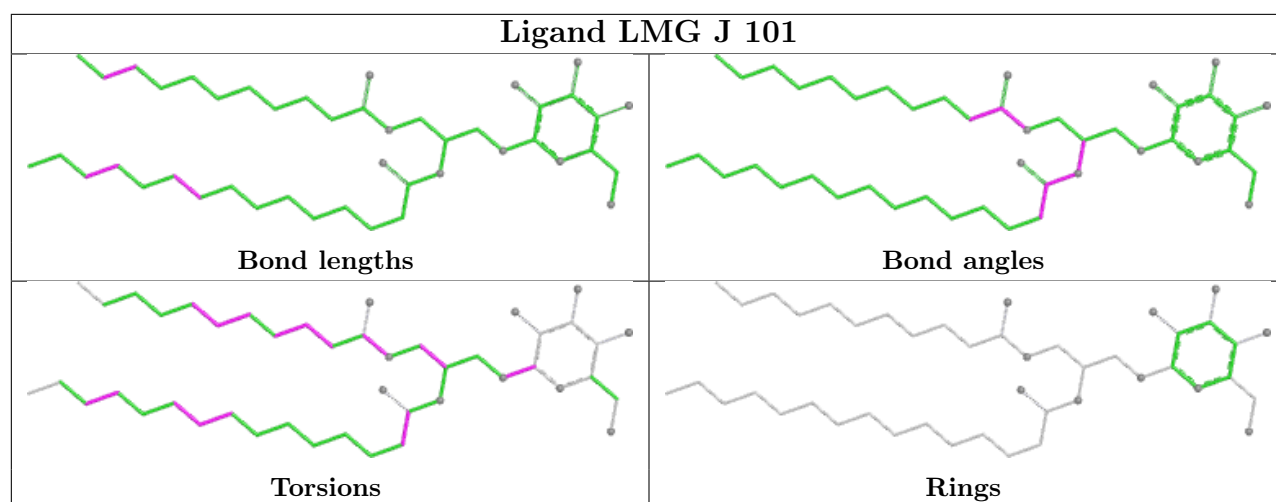


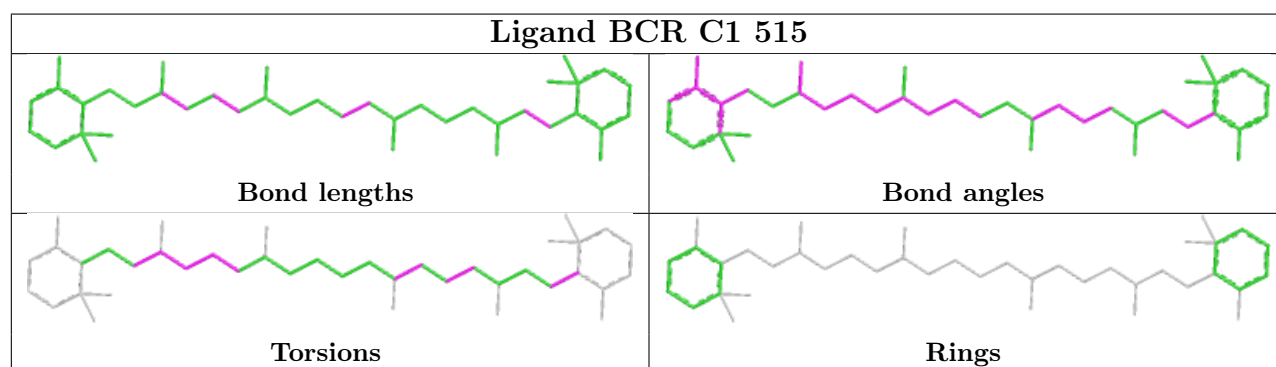
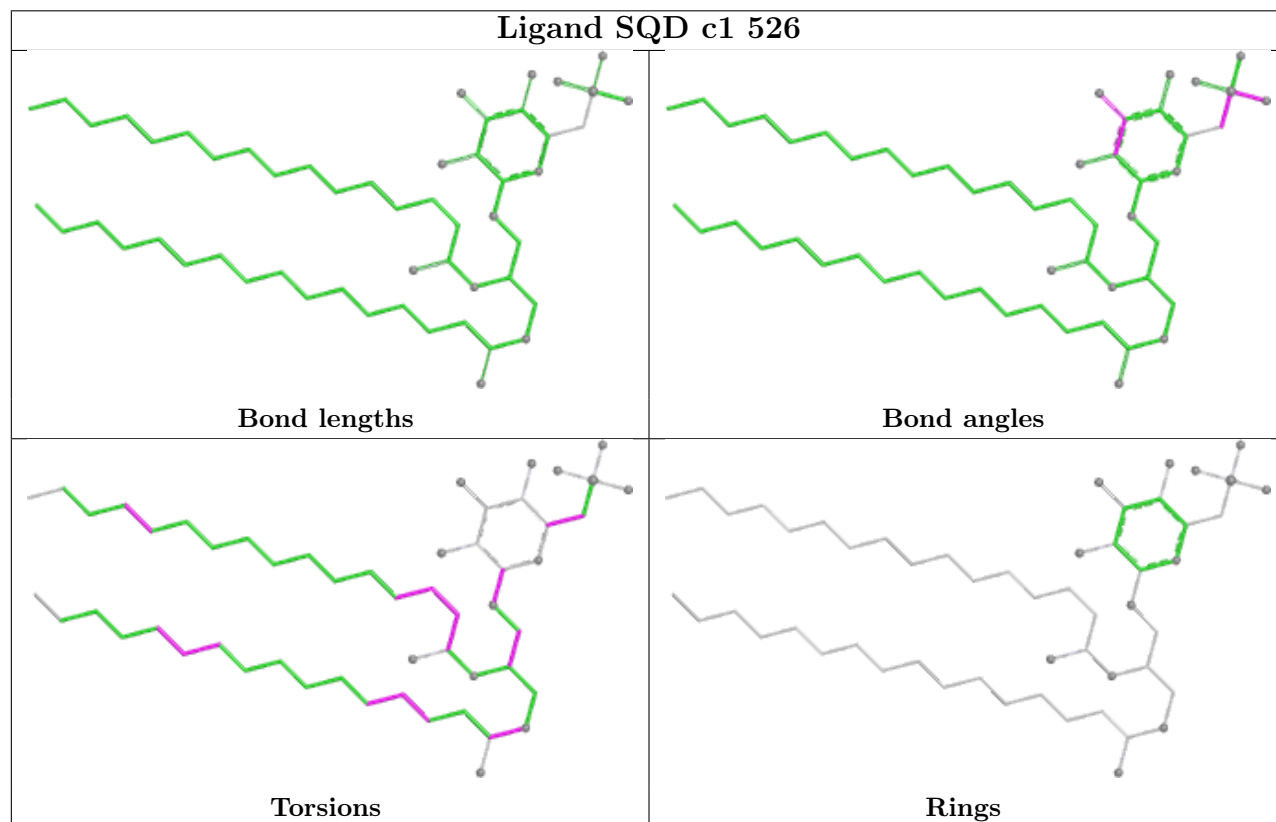
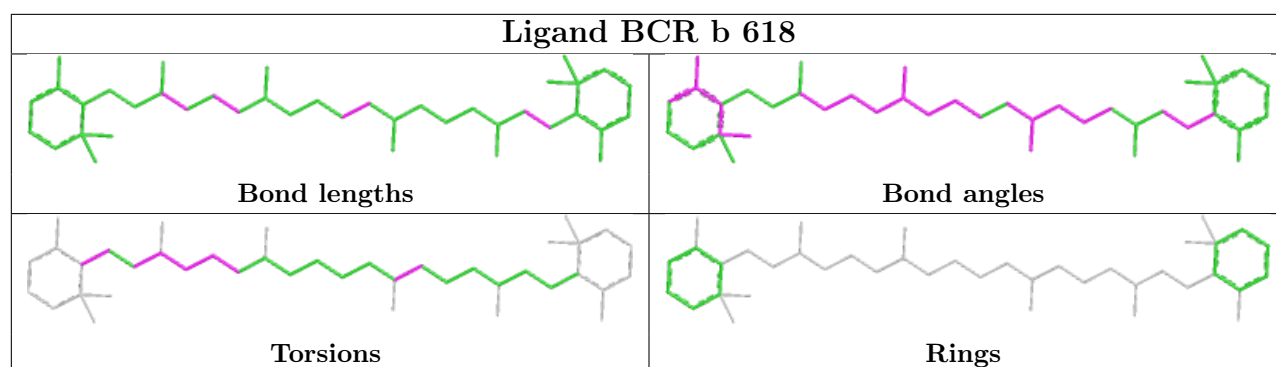
Ligand CLA r 611

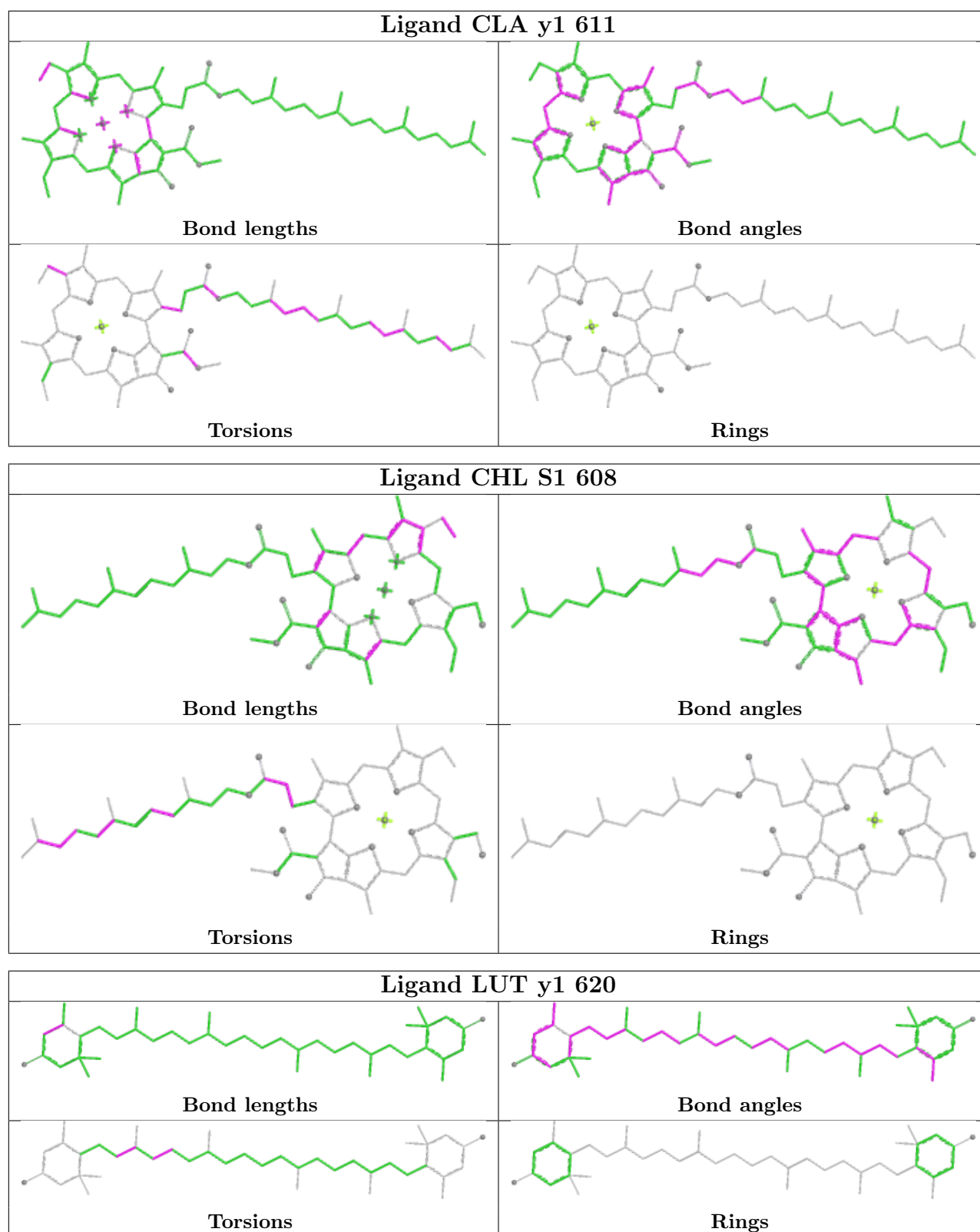


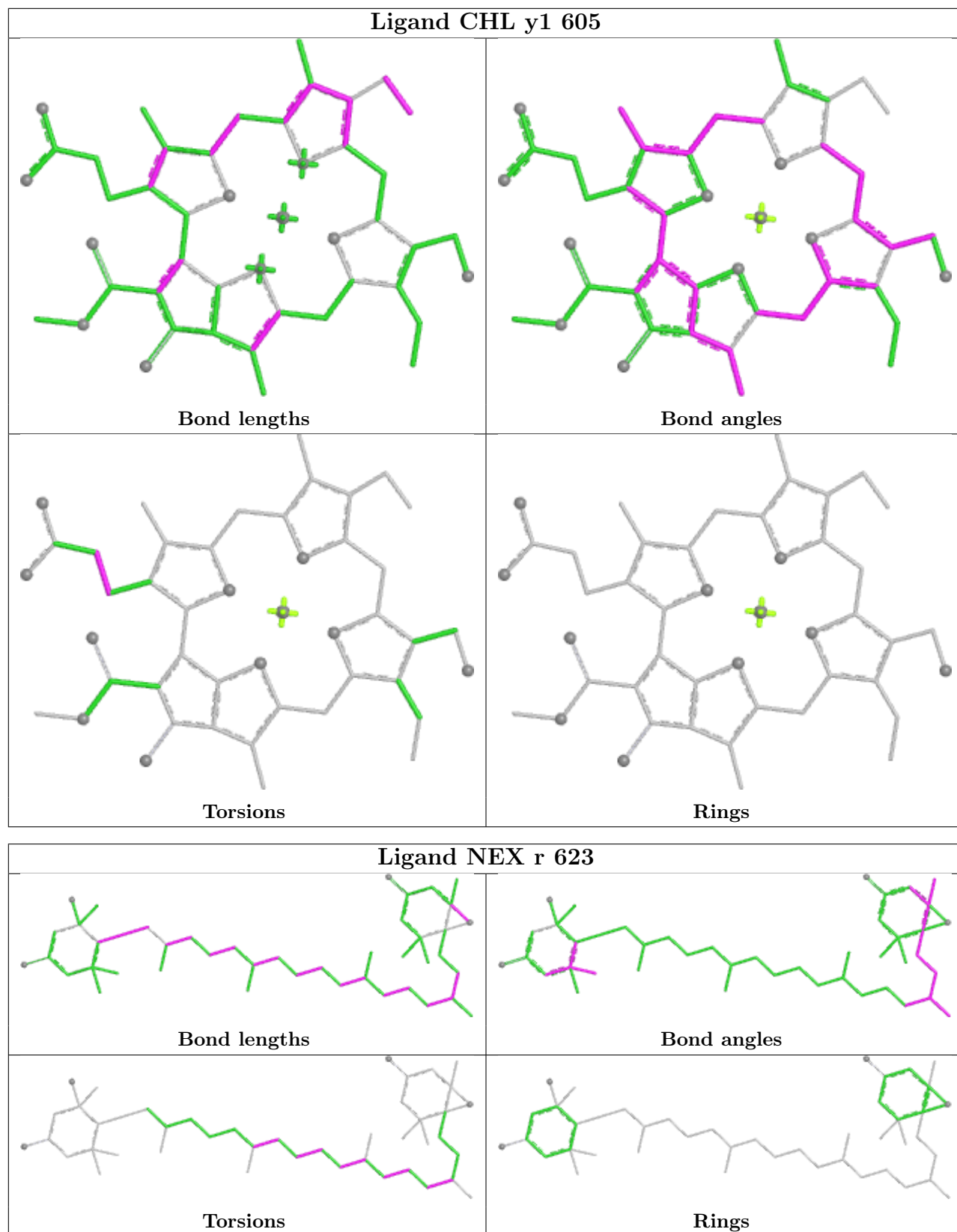
Ligand CLA G 613

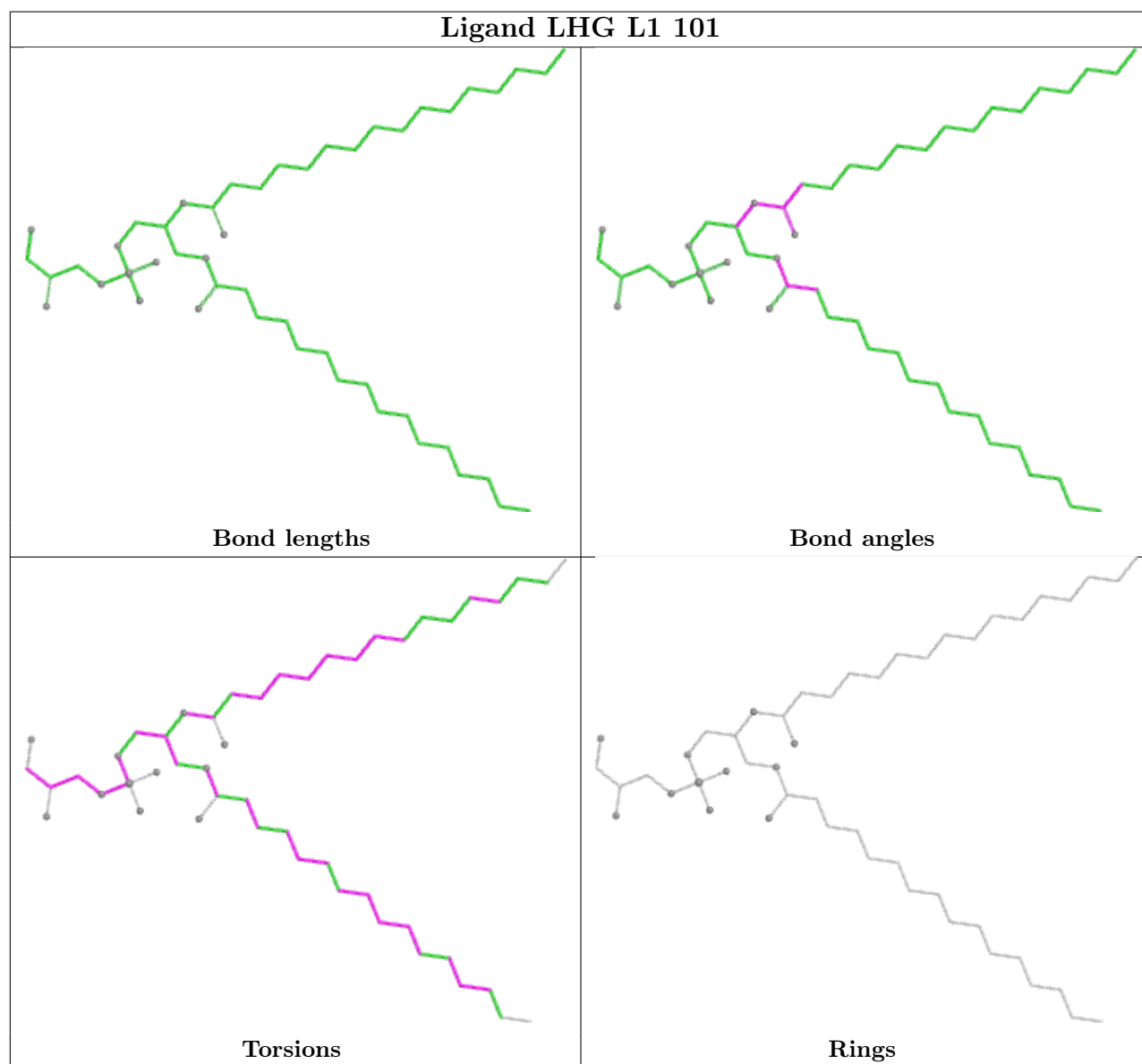
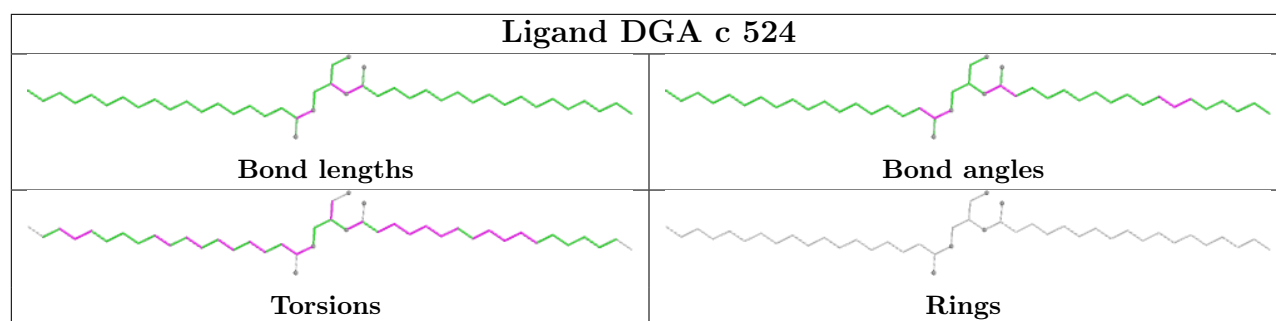


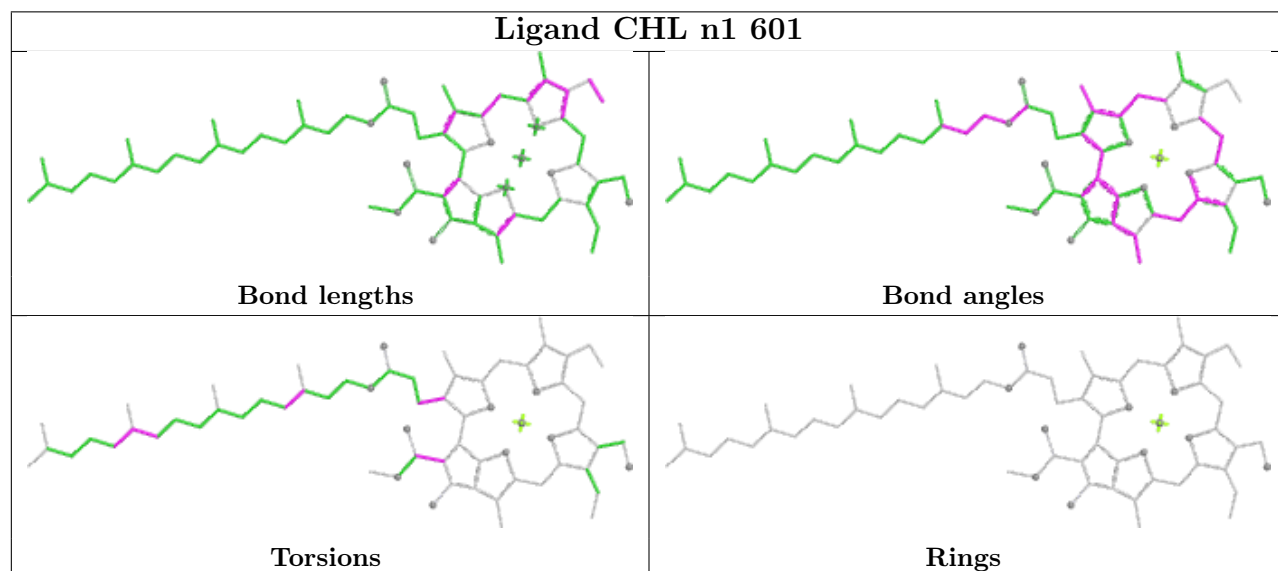
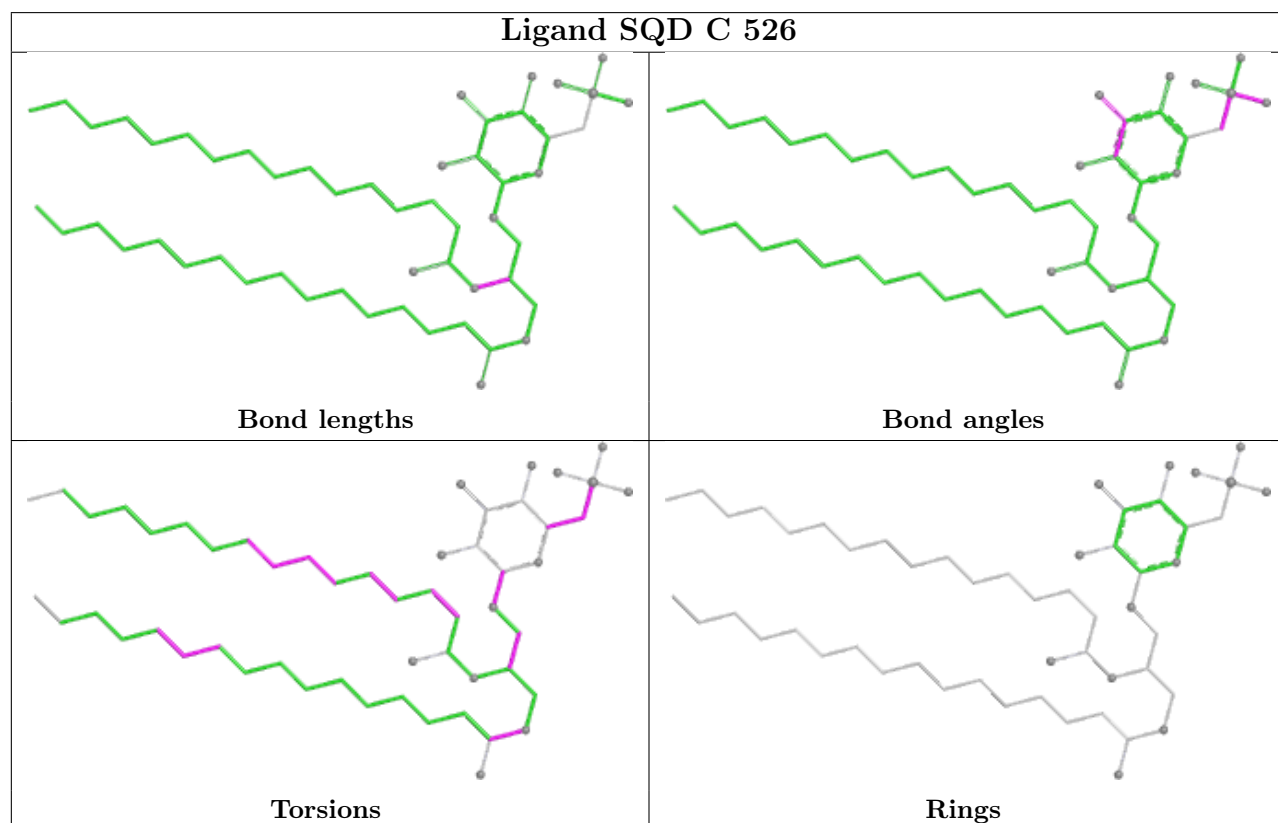
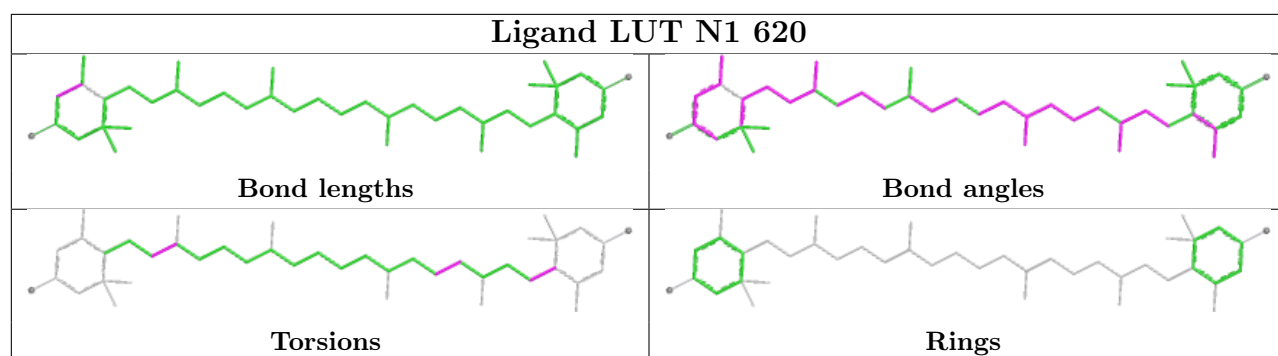


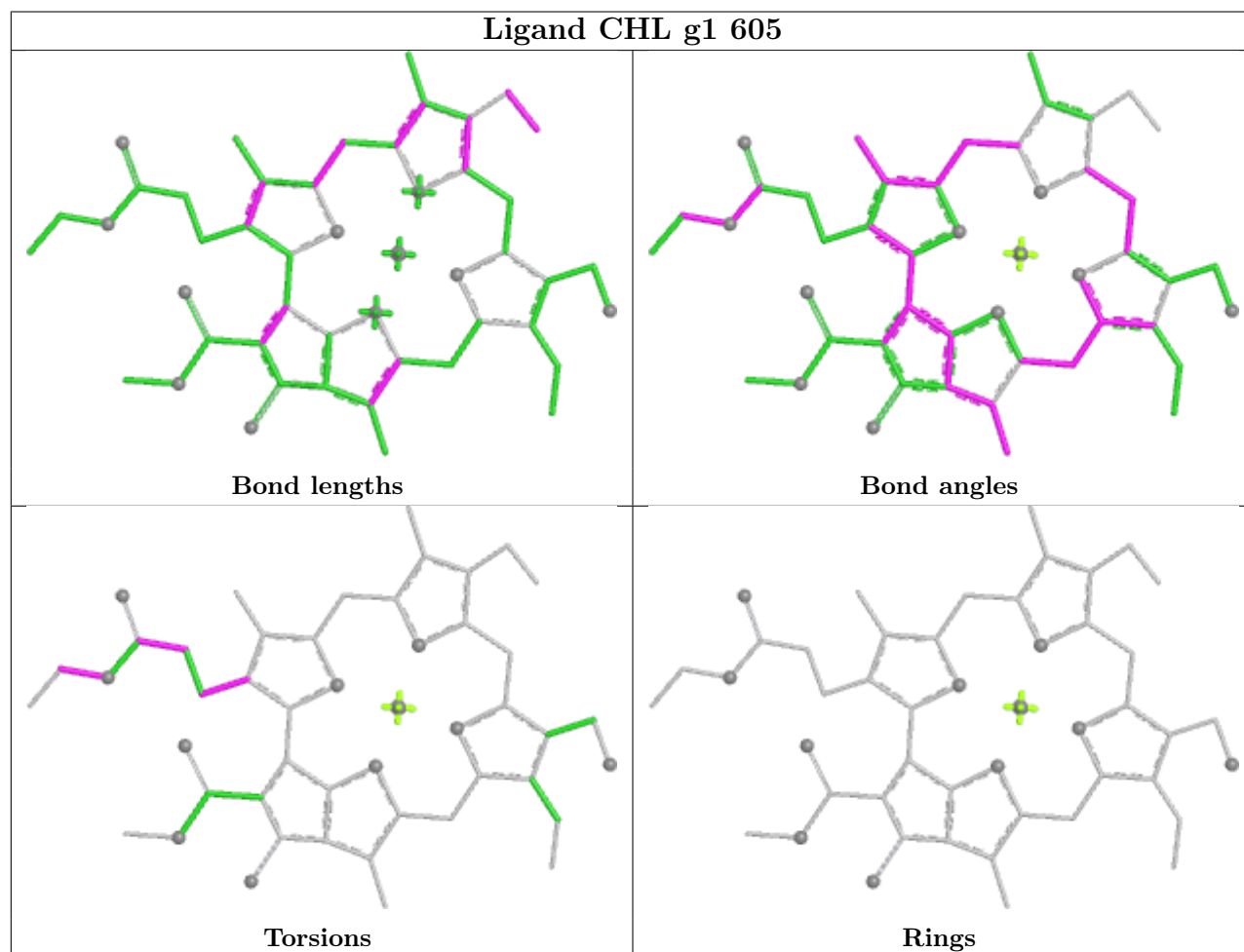
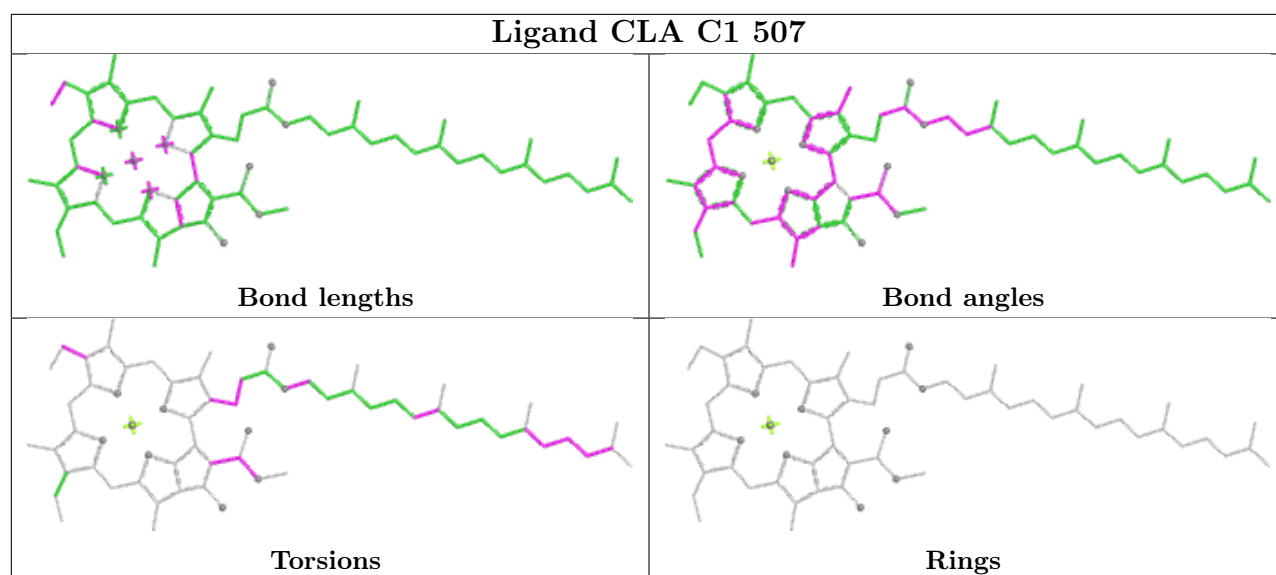


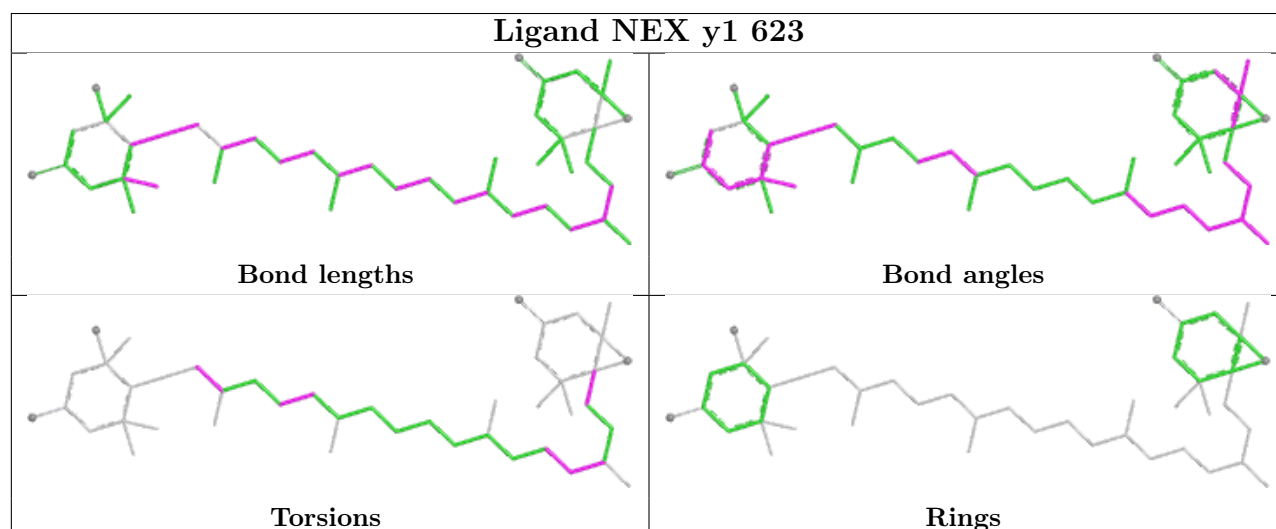
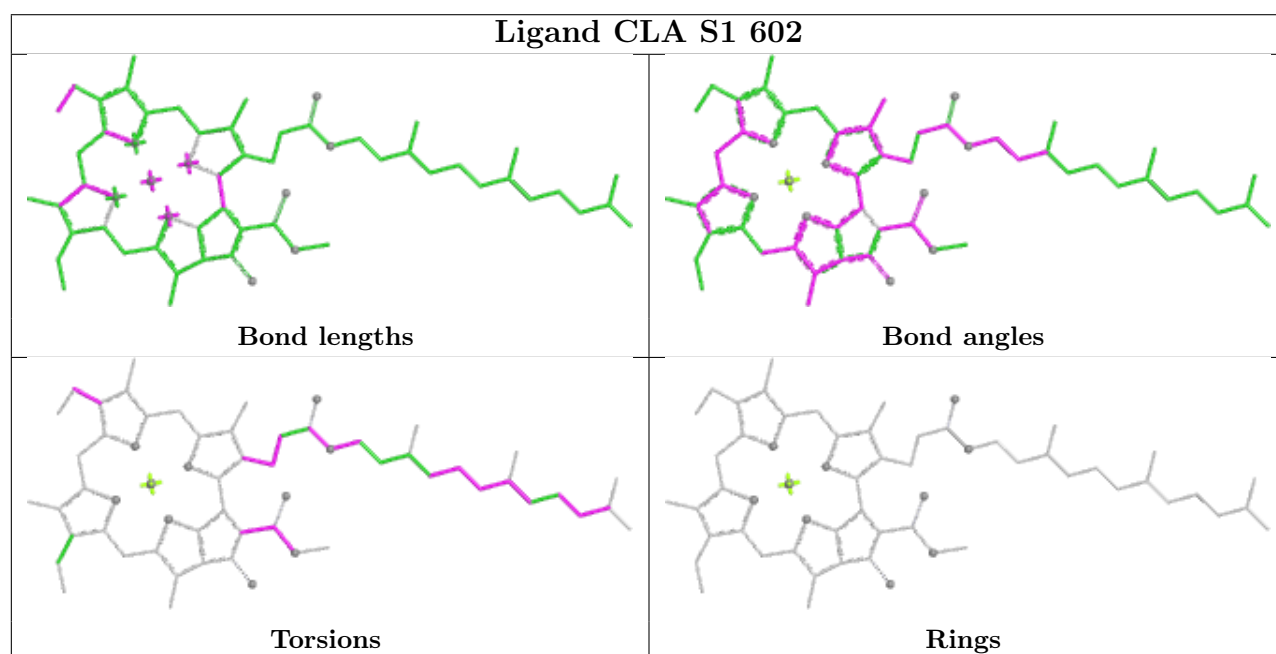
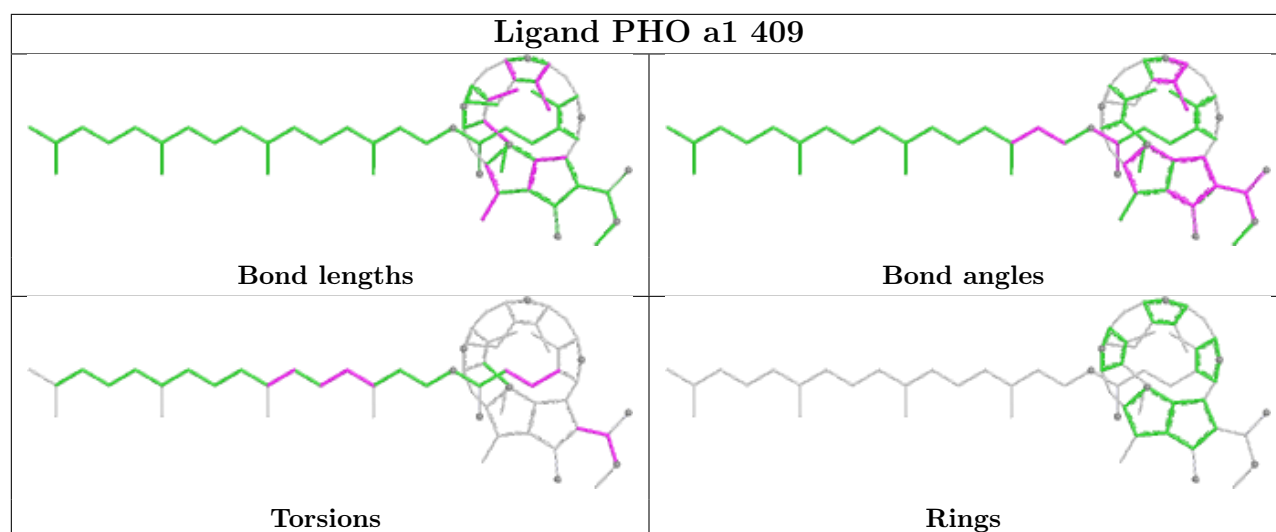


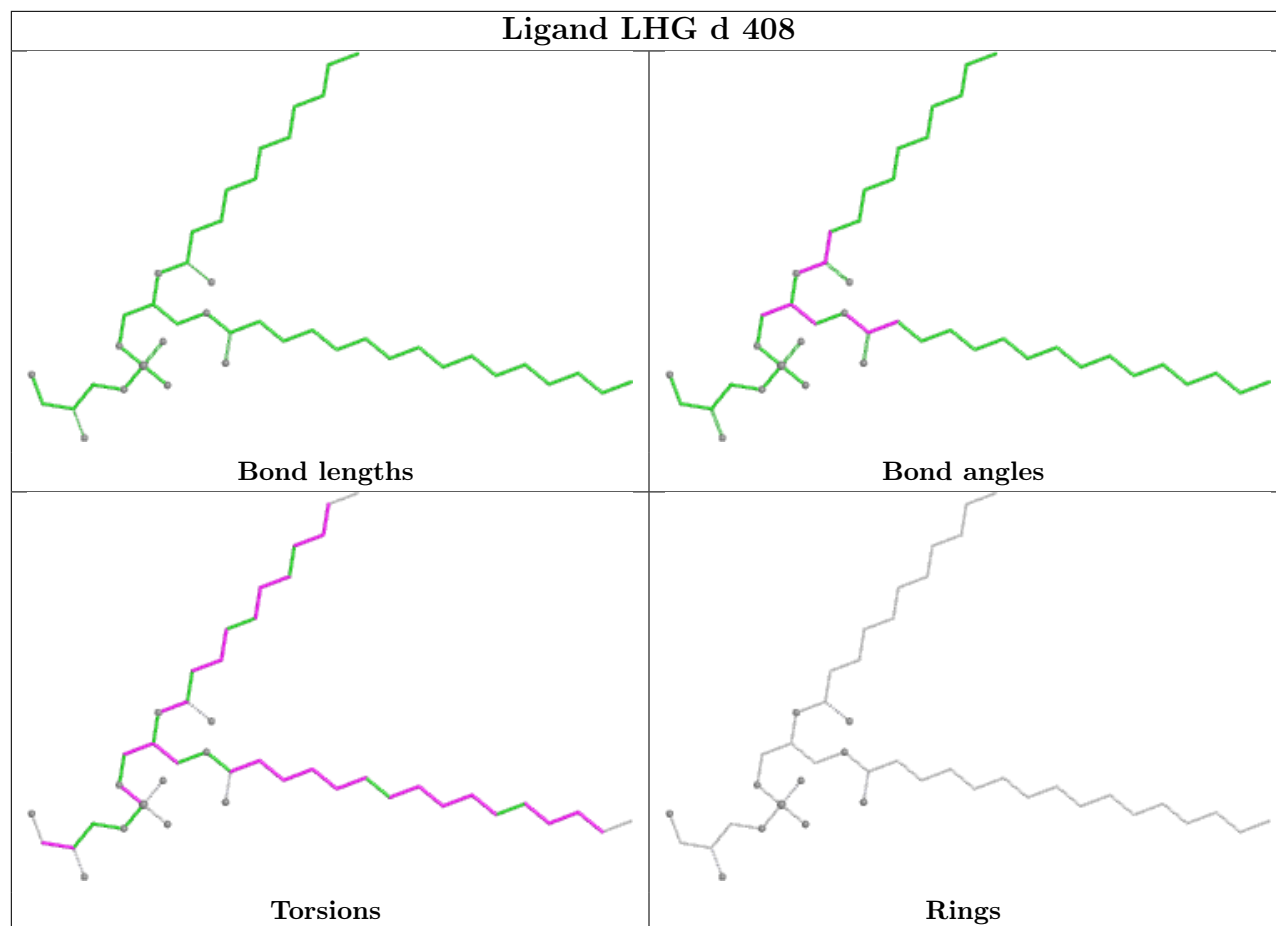
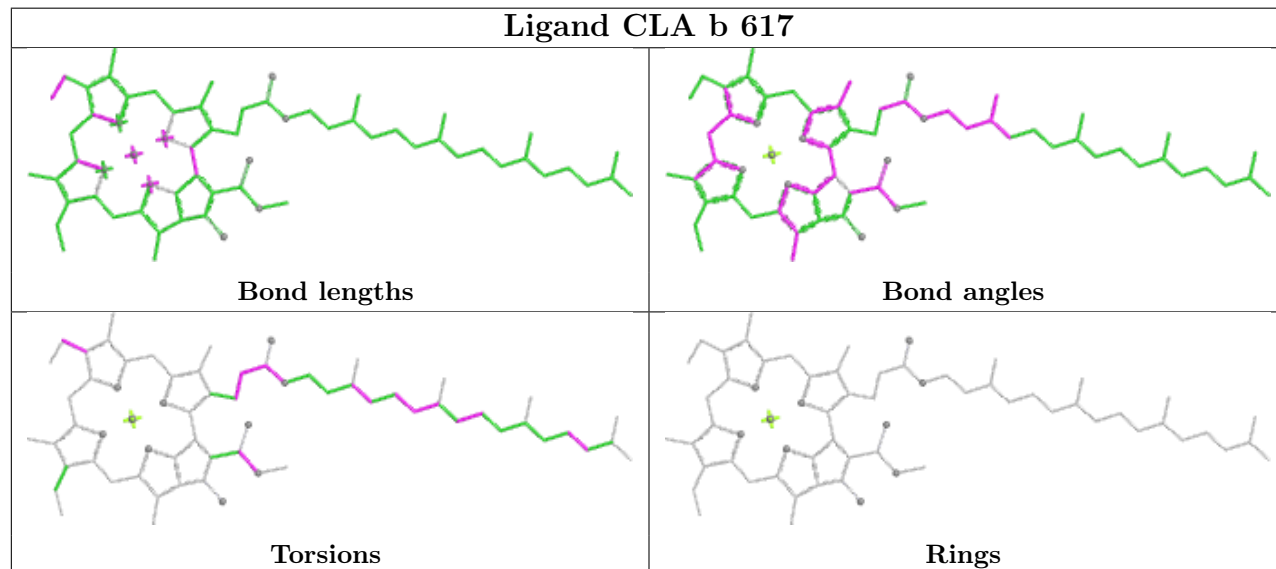


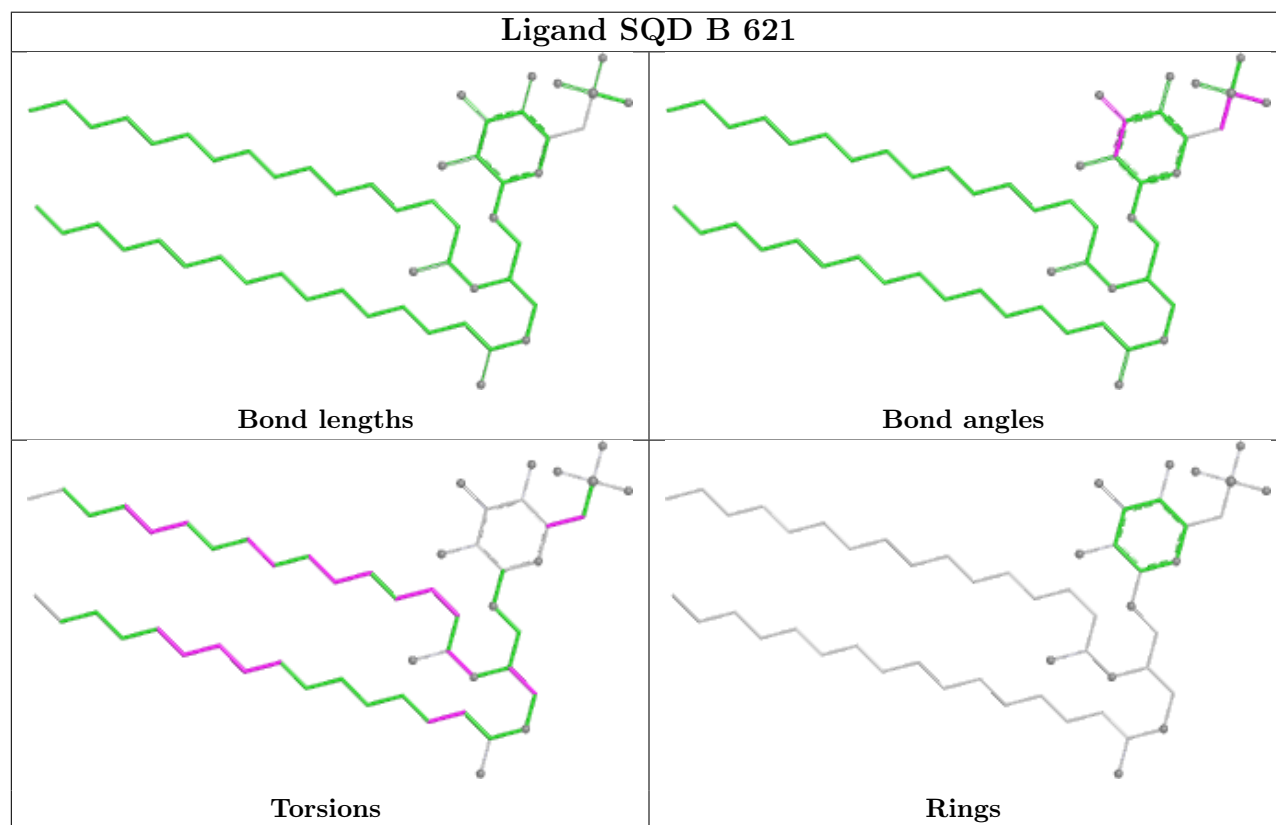
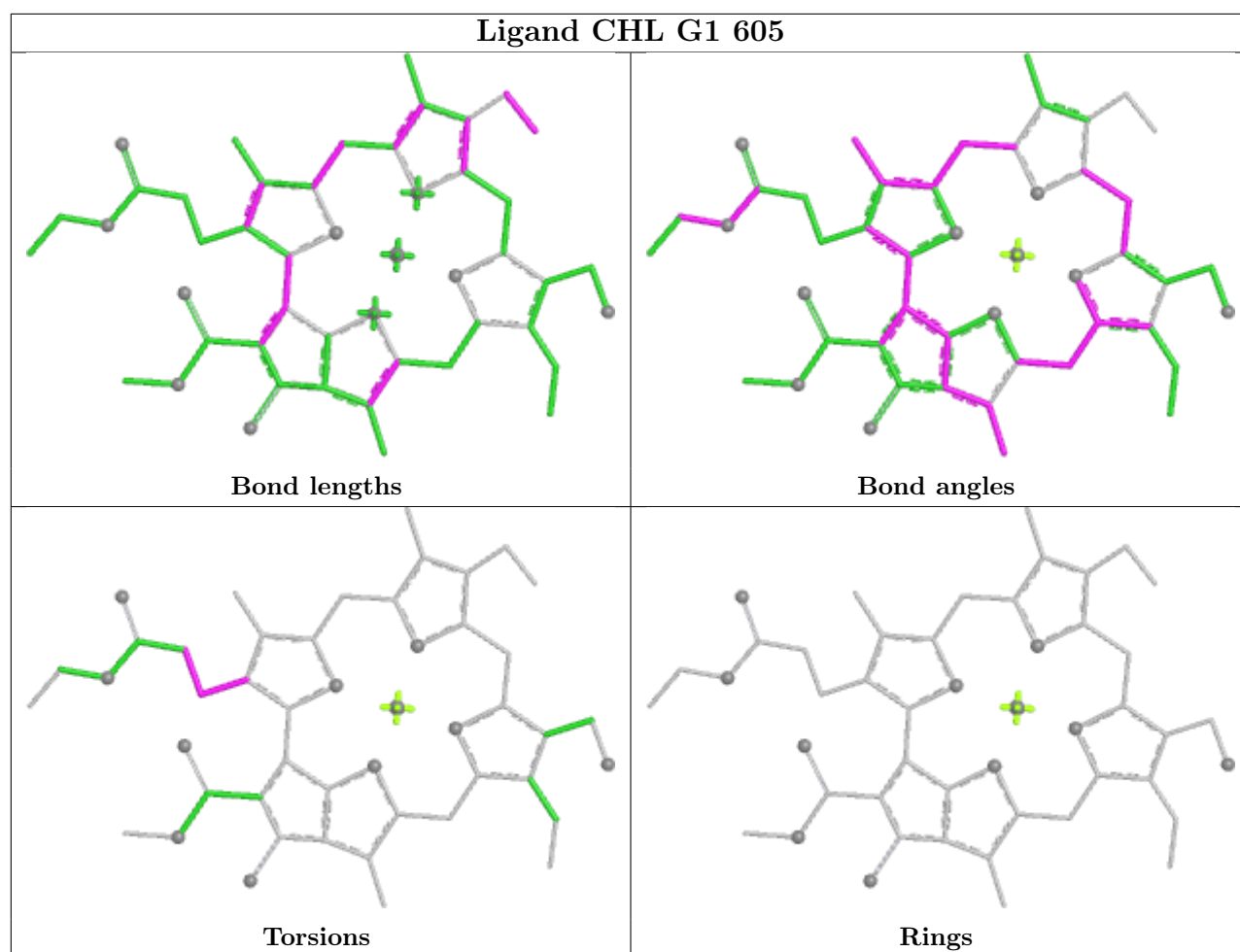




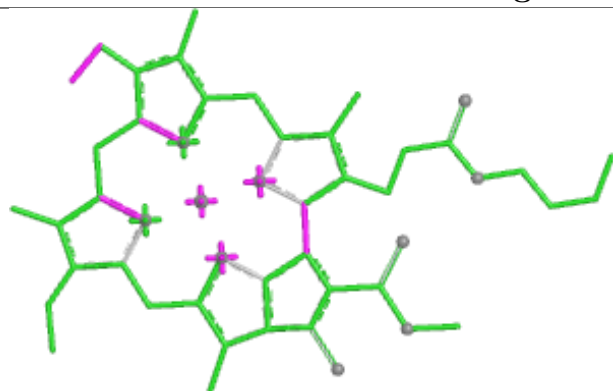




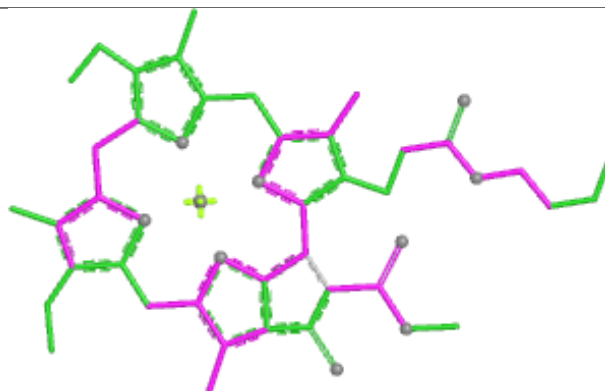
Ligand LHG d 408**Ligand CLA b 617**



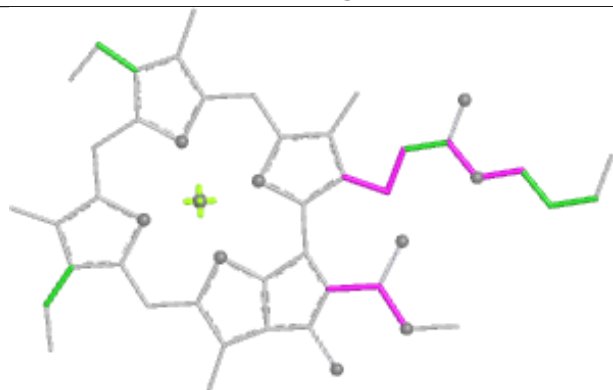
Ligand CLA R 604



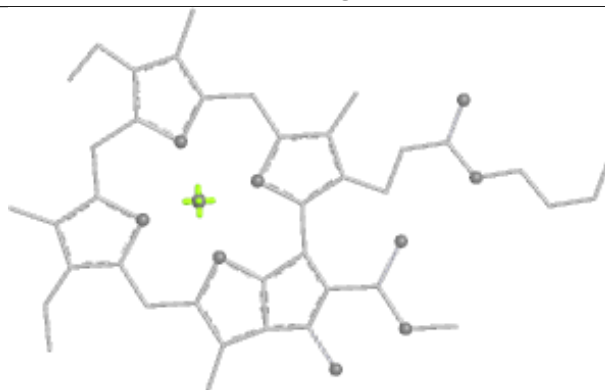
Bond lengths



Bond angles

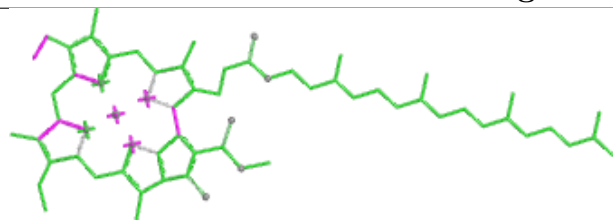


Torsions

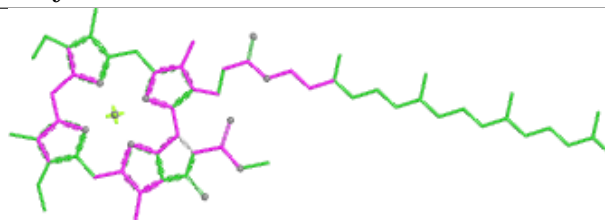


Rings

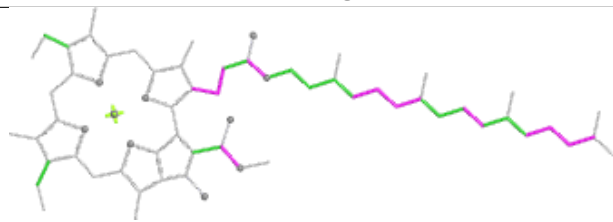
Ligand CLA y 610



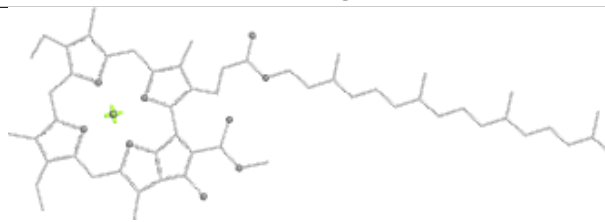
Bond lengths



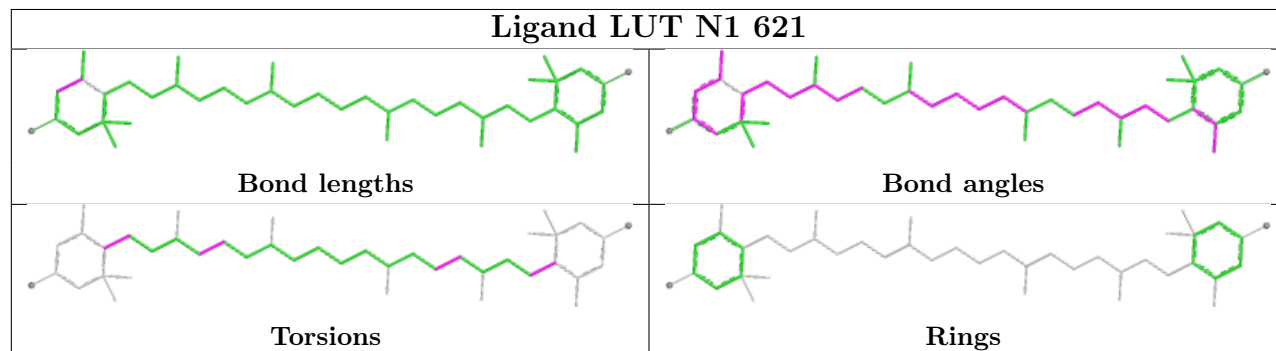
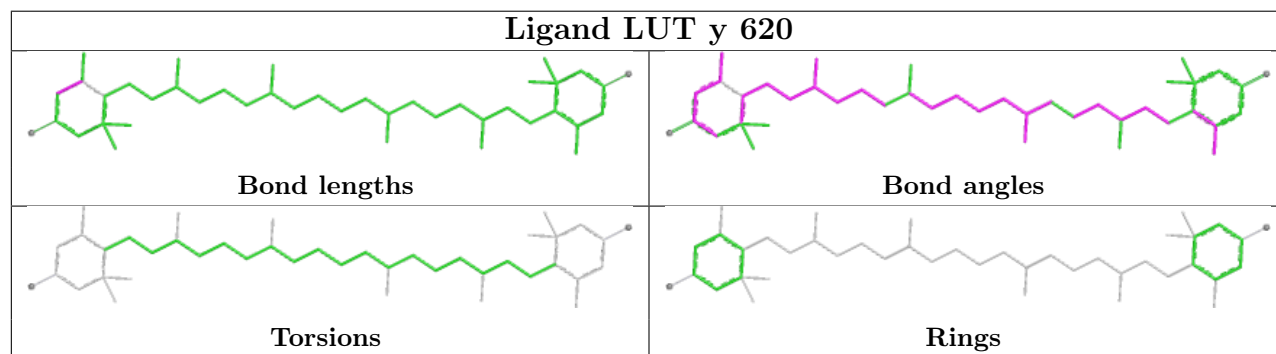
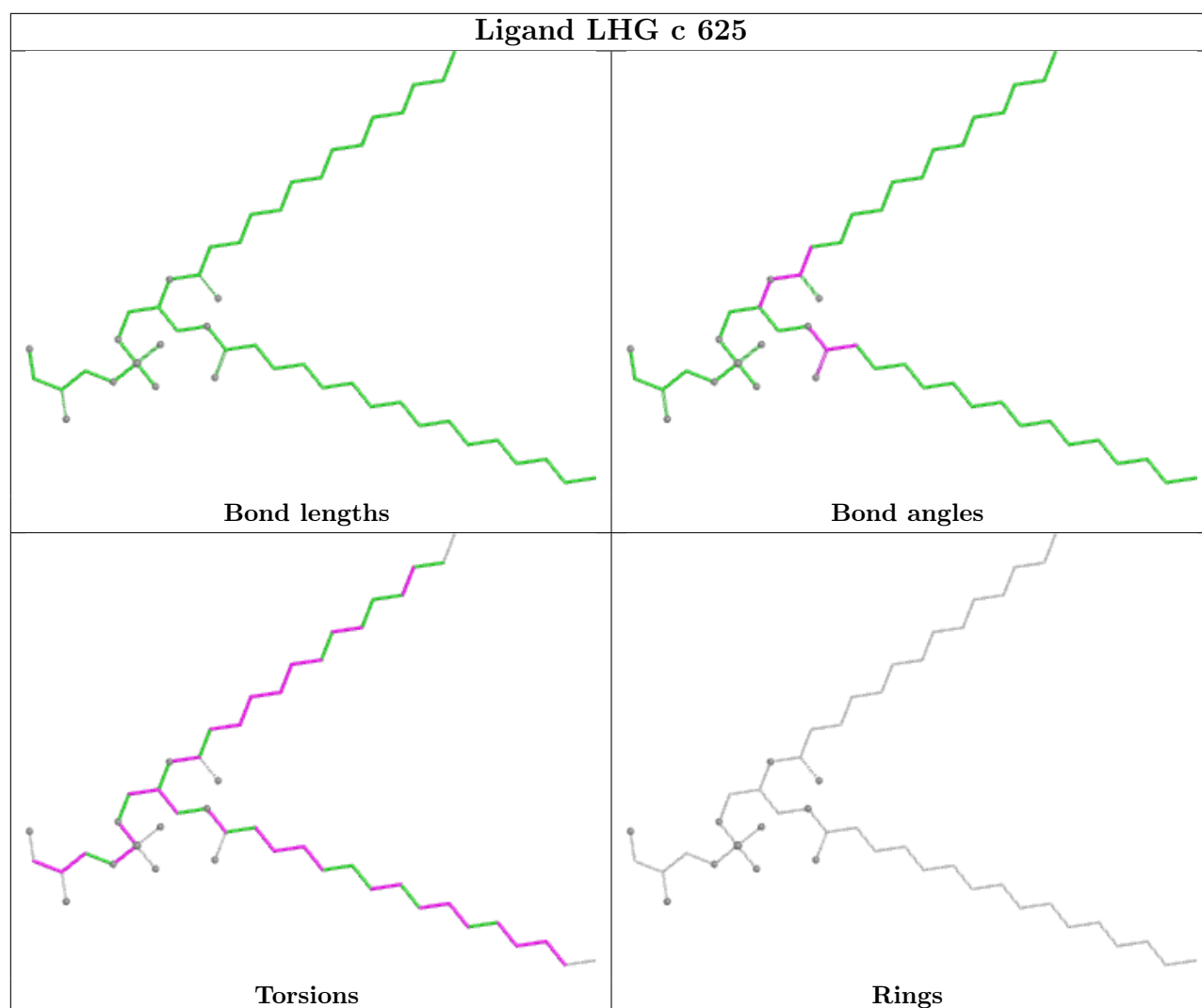
Bond angles

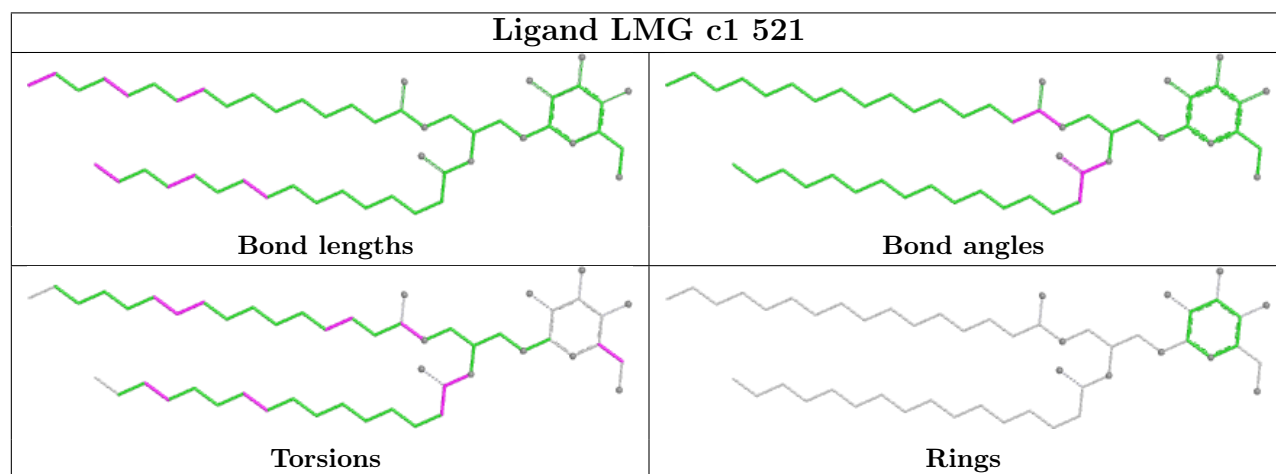
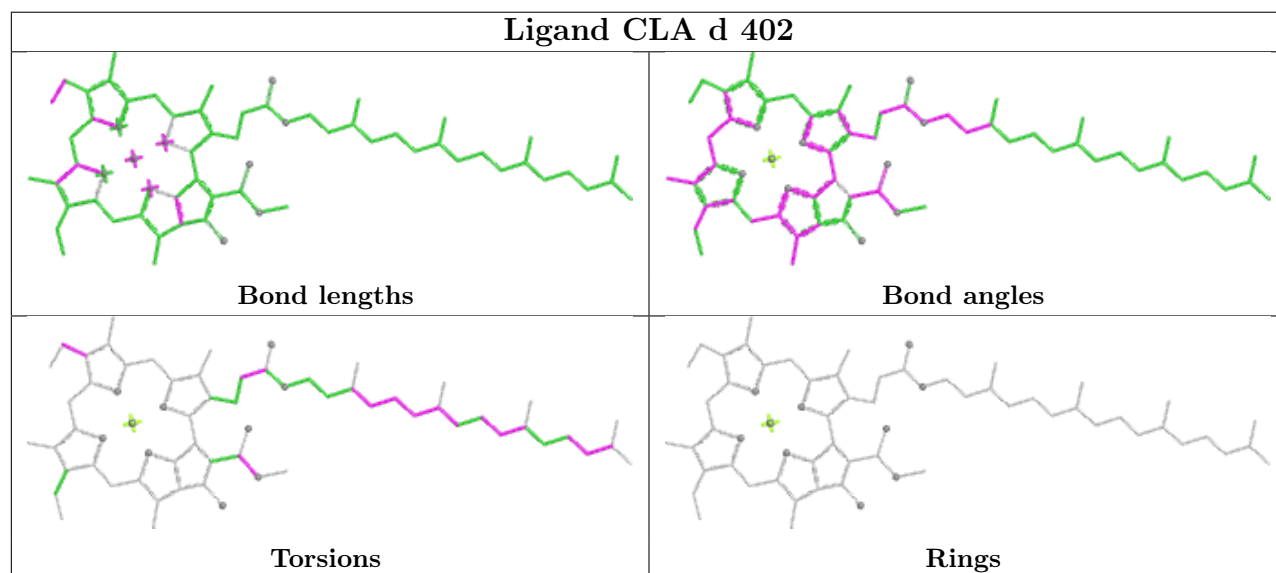
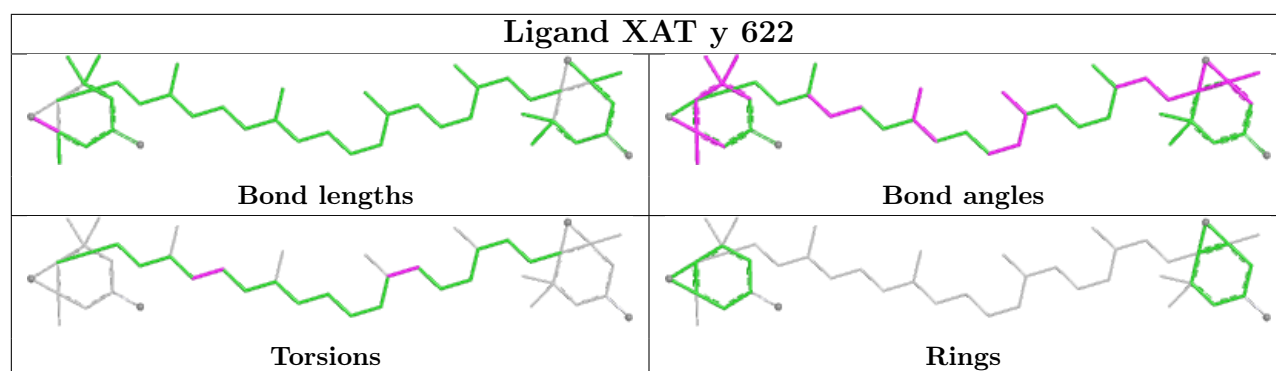


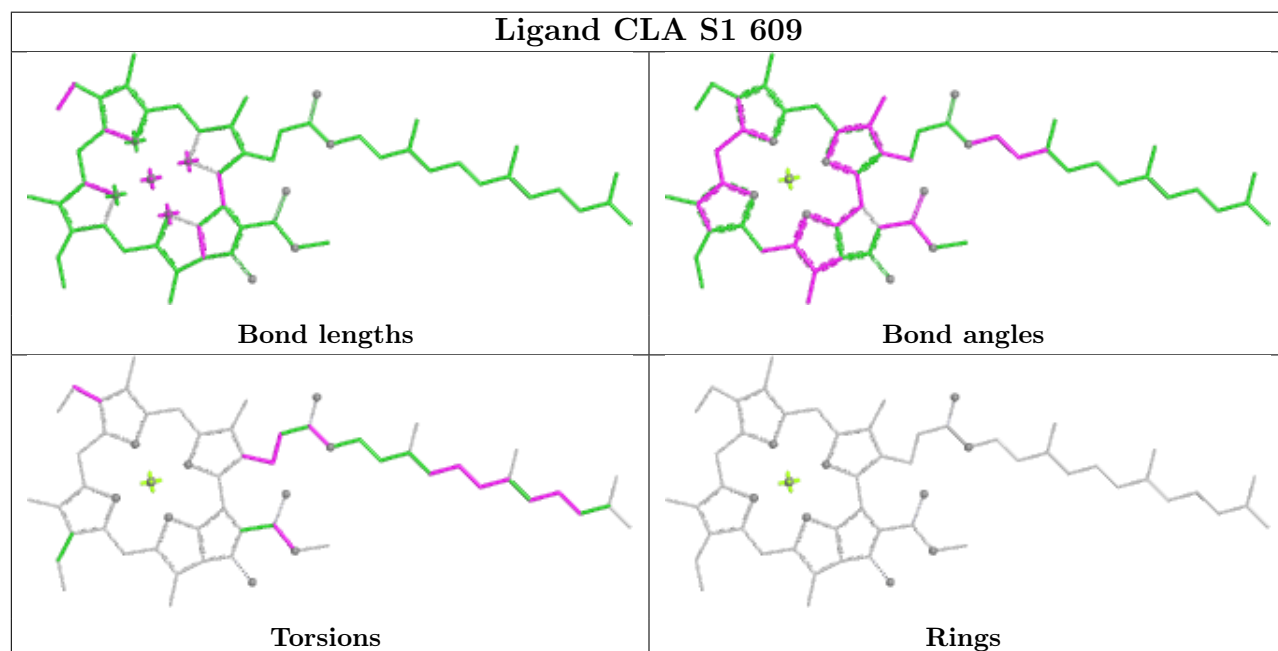
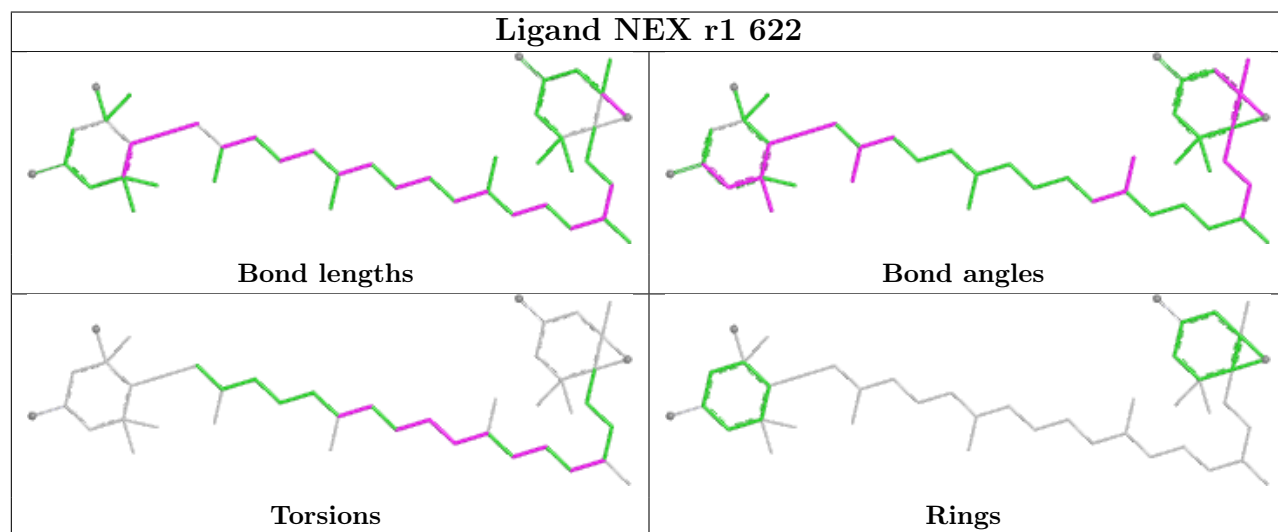
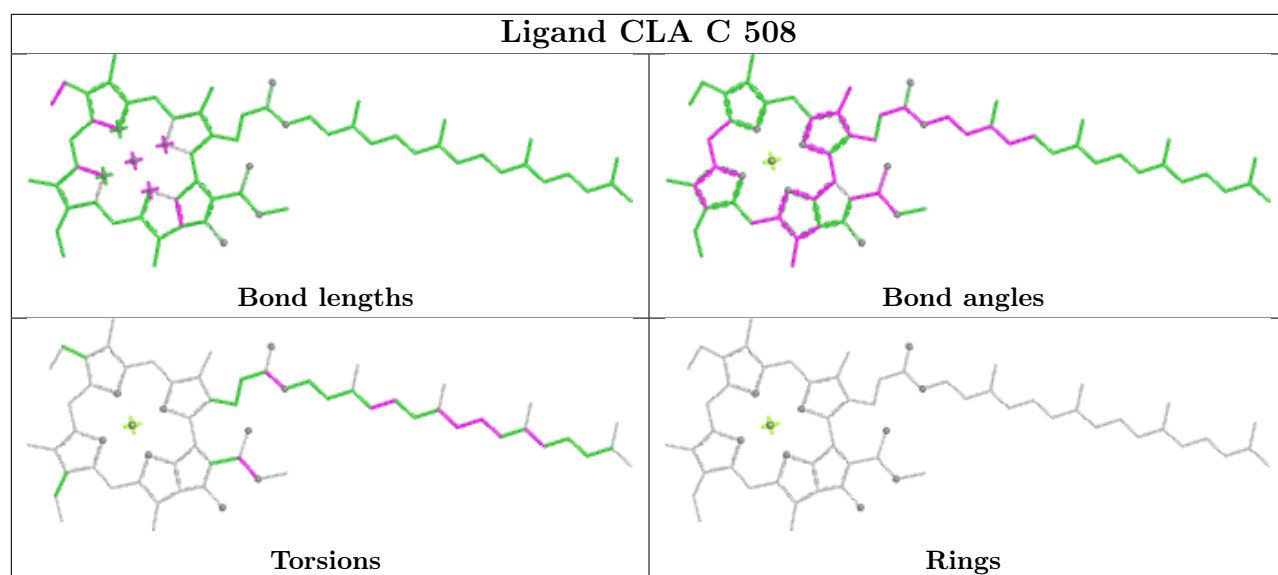
Torsions

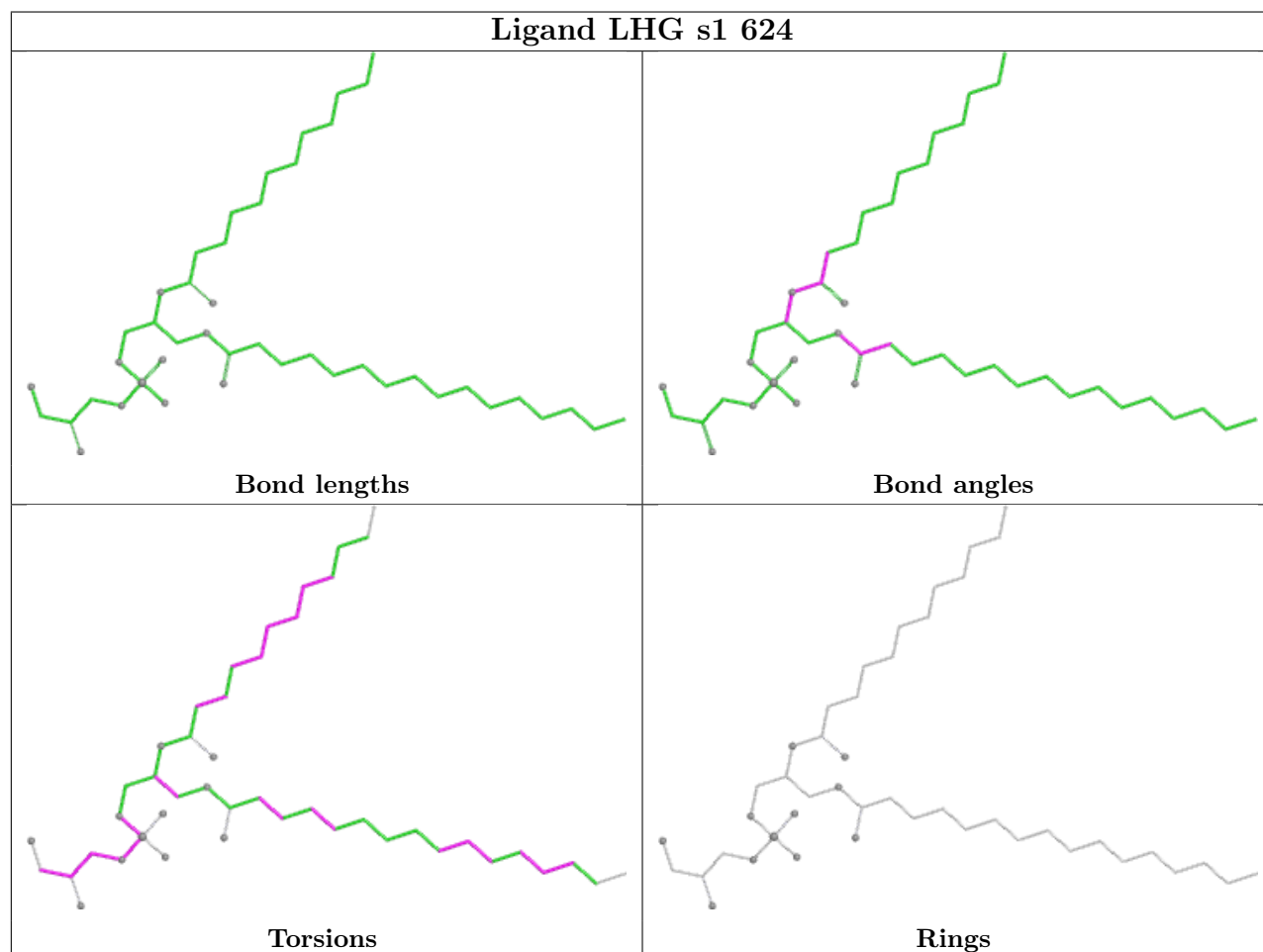
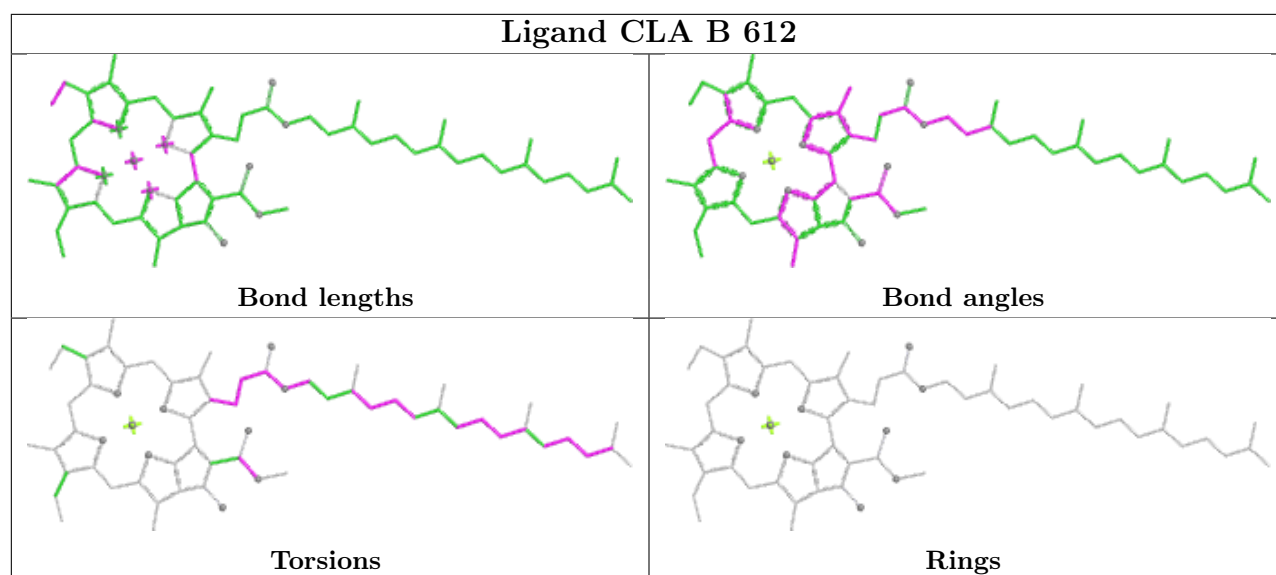


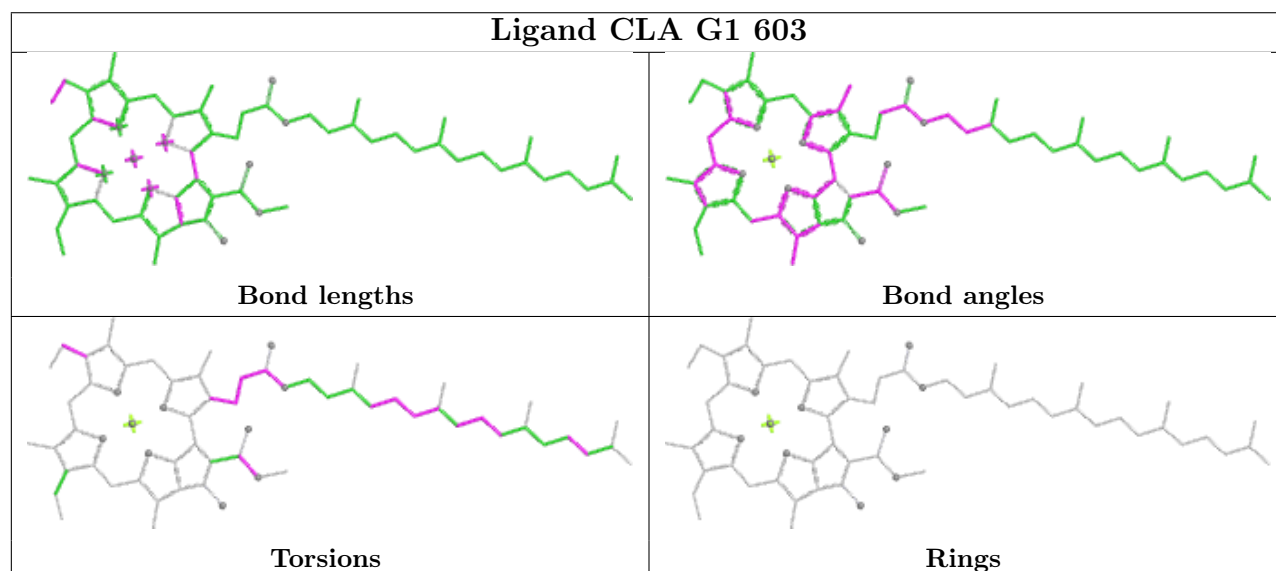
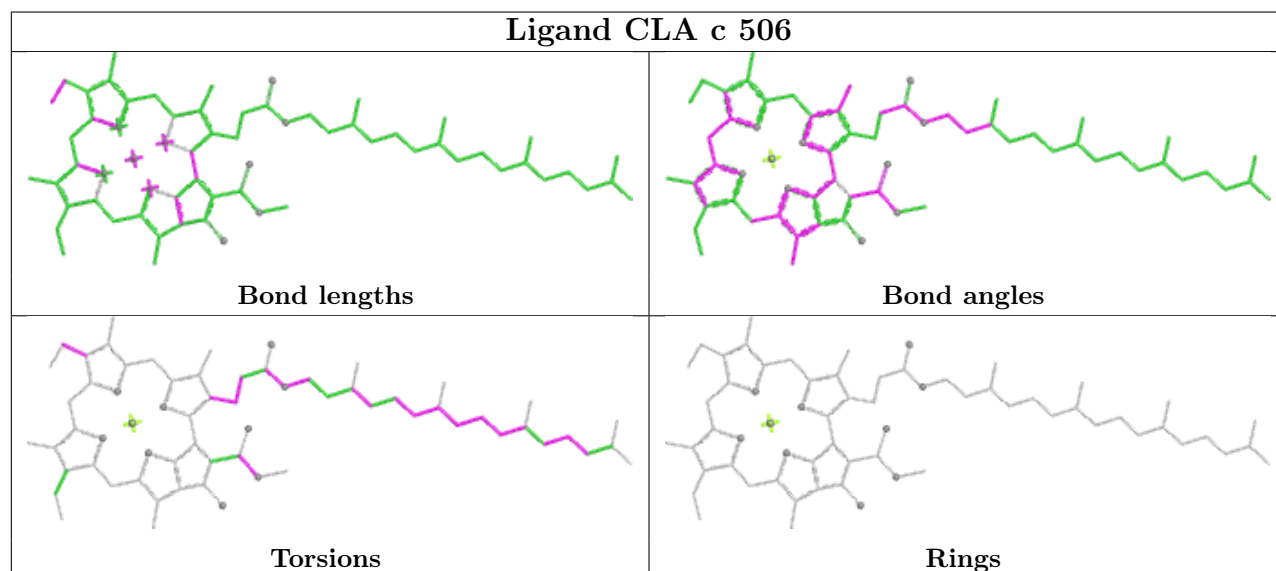
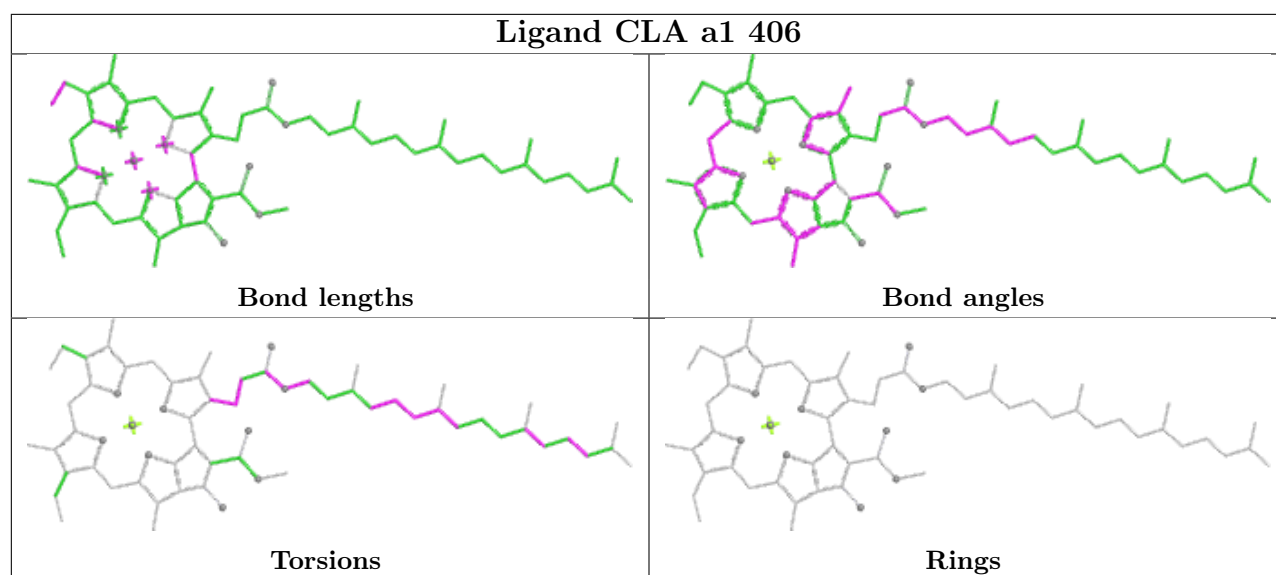
Rings

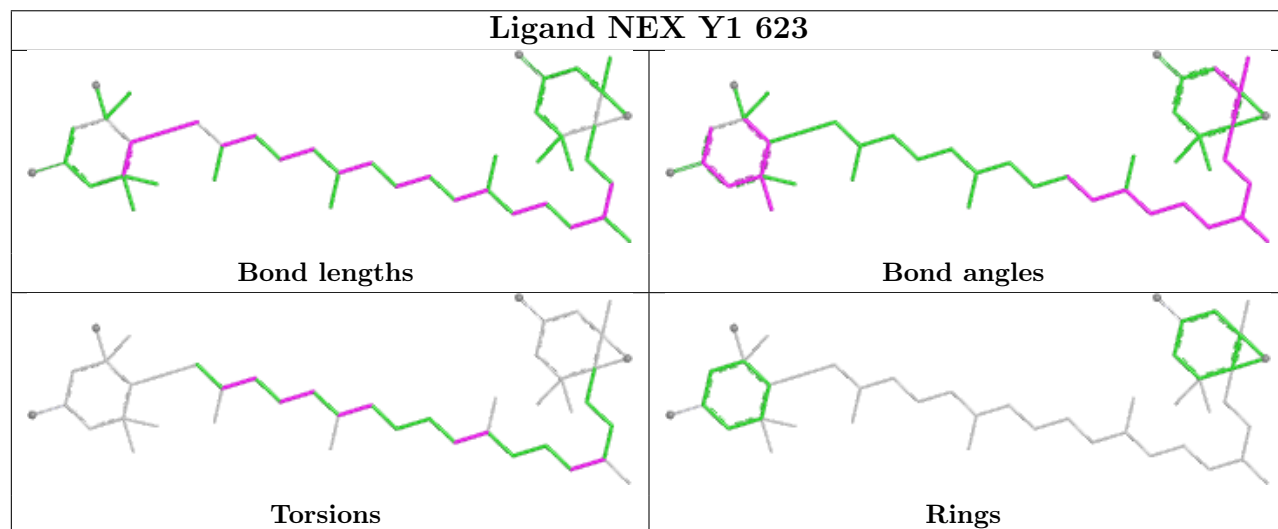
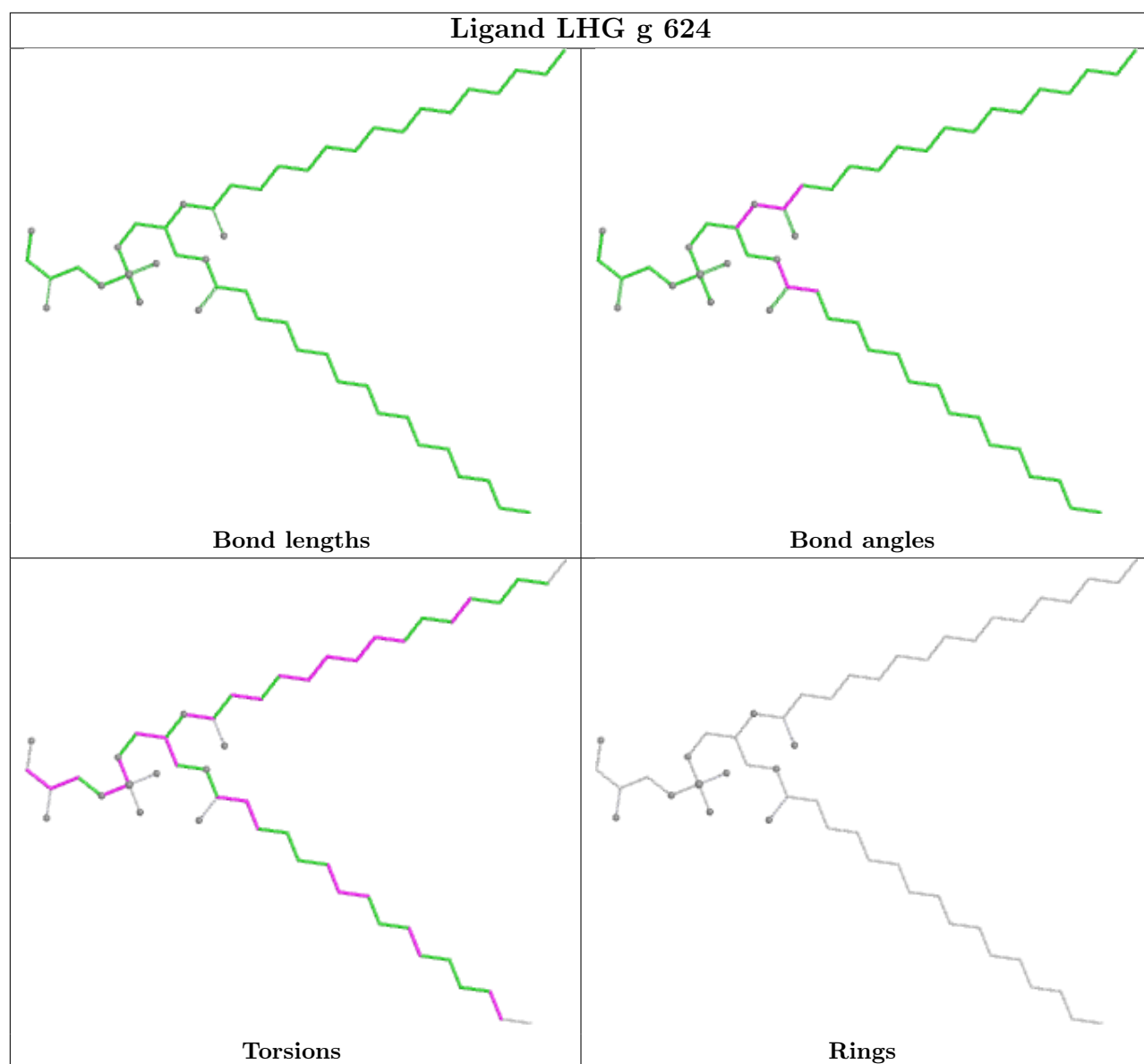


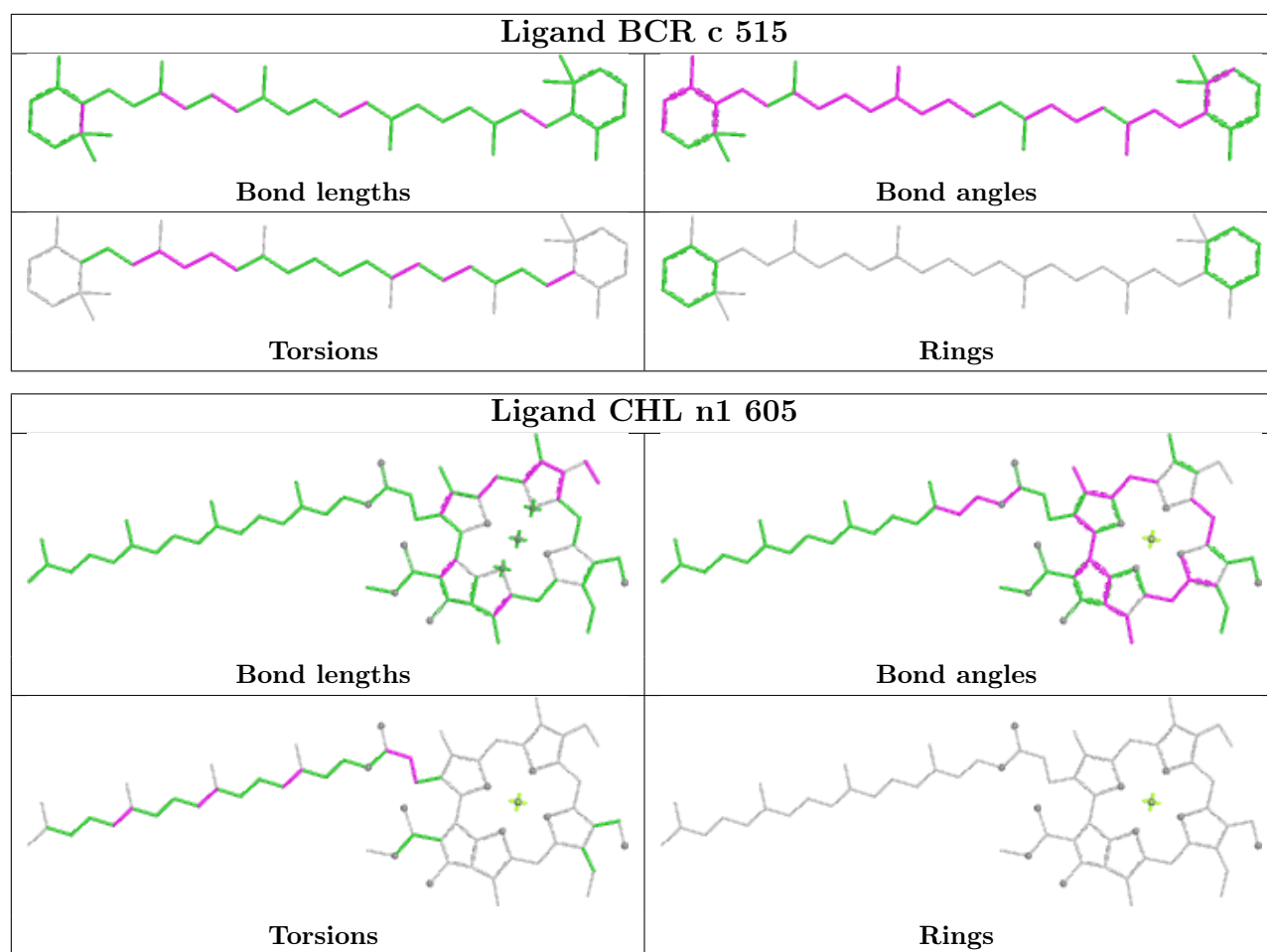




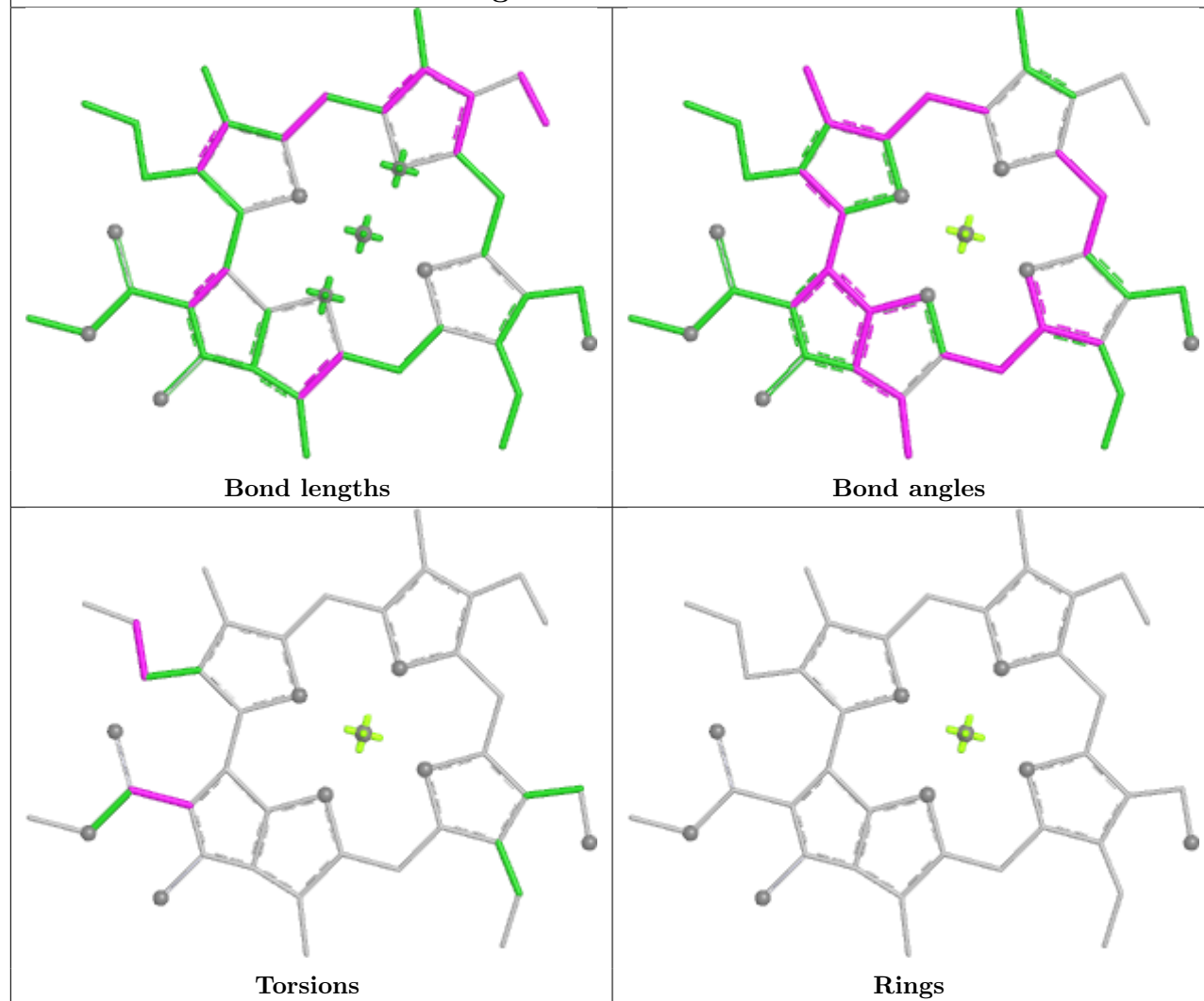




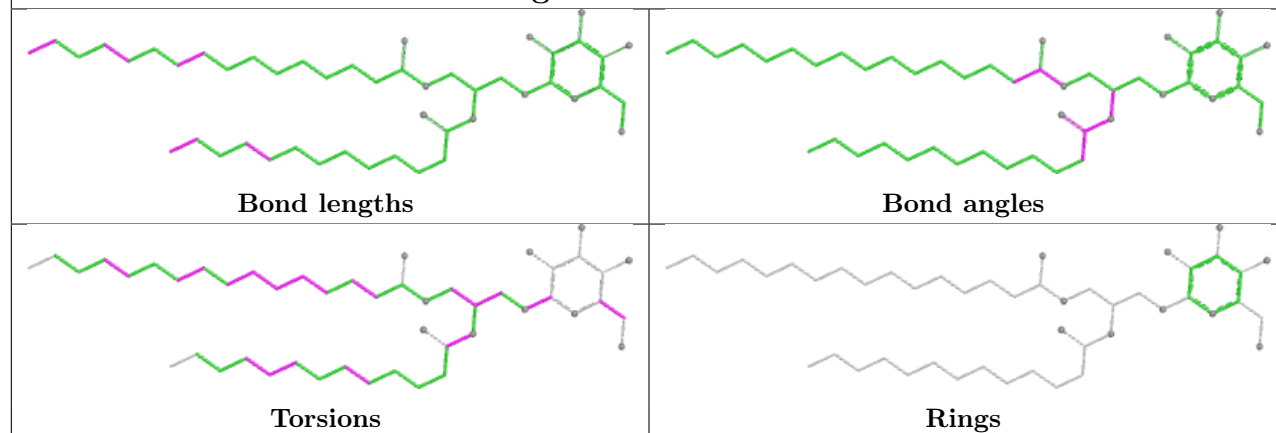


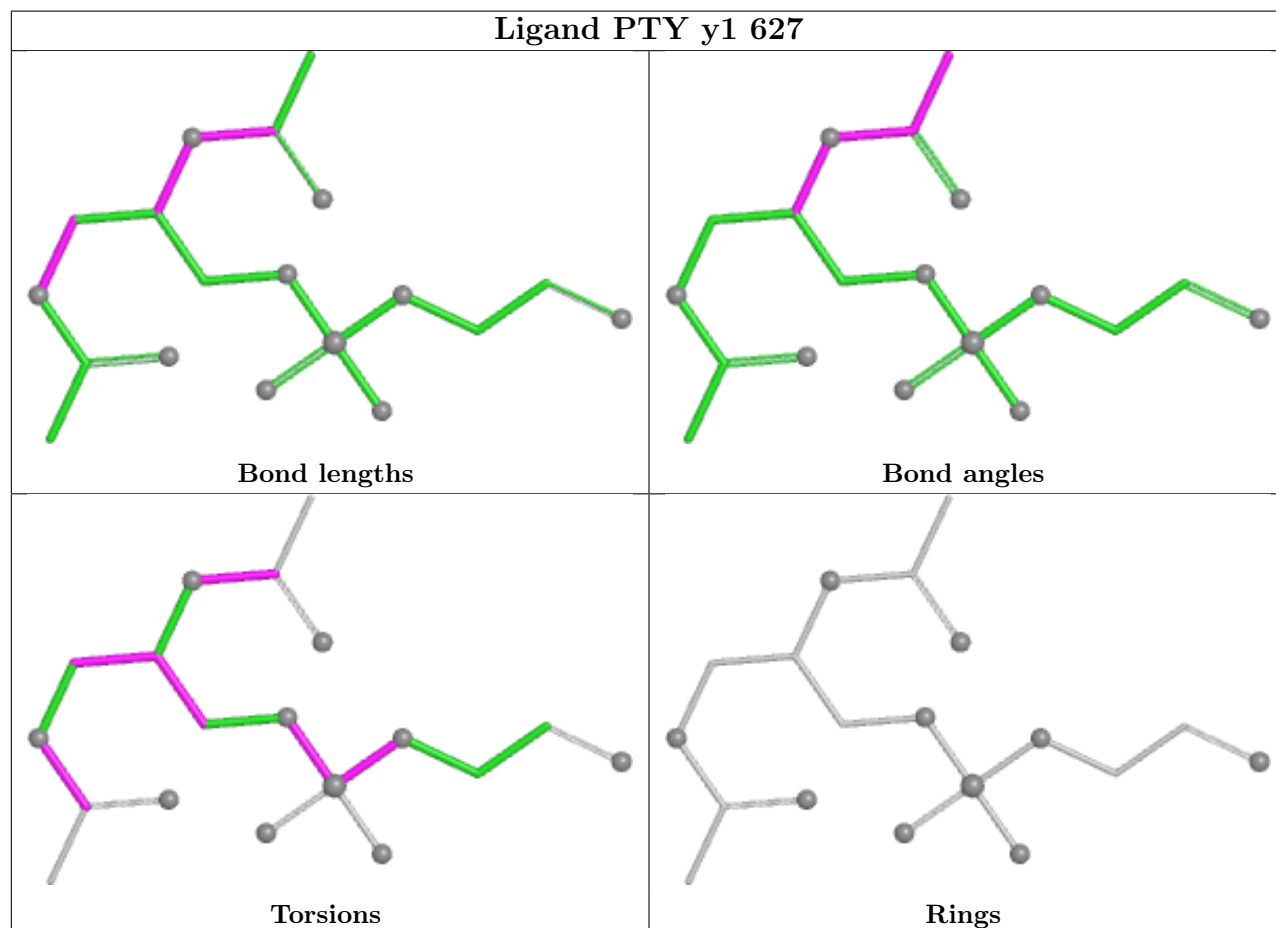
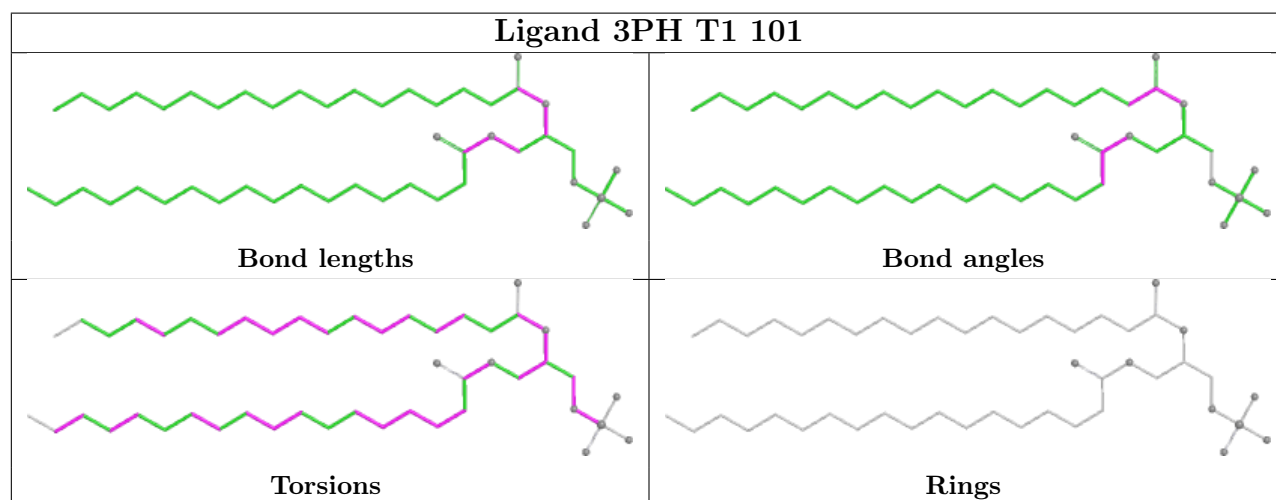
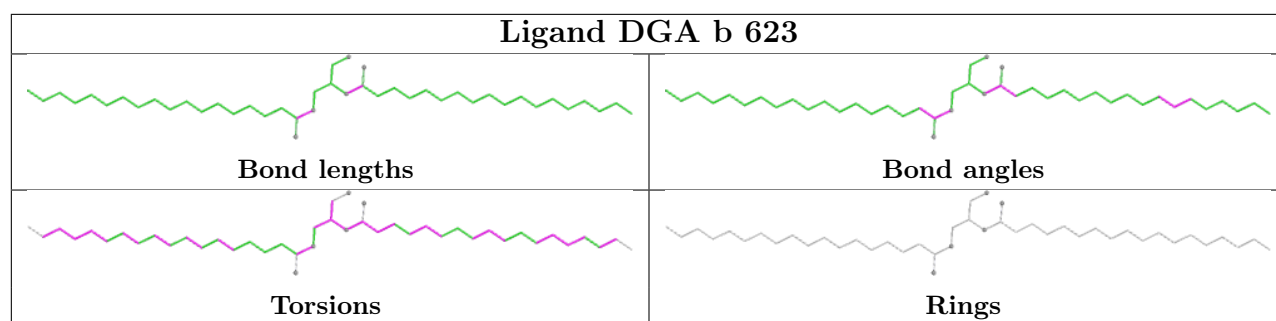


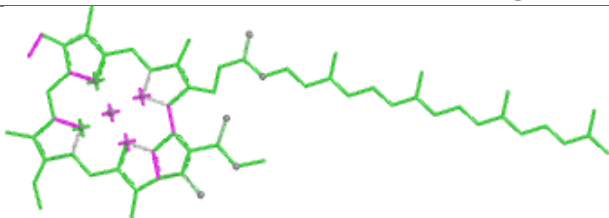
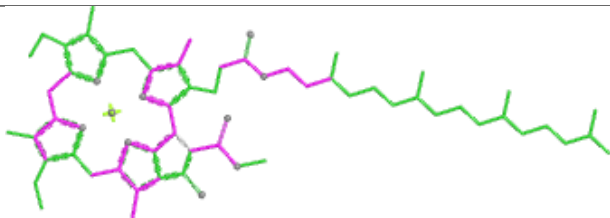
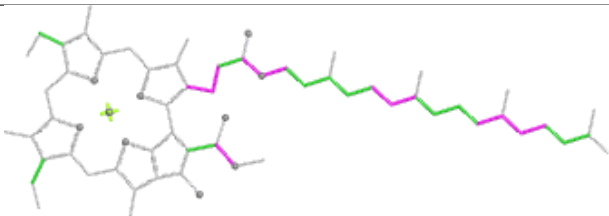
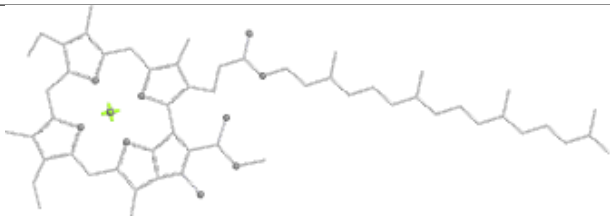
Ligand CHL G1 608

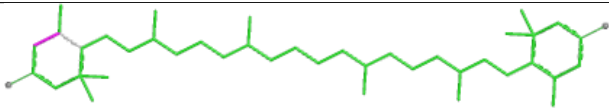
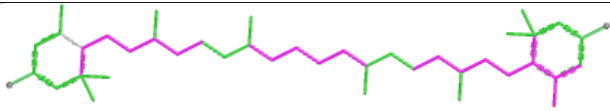
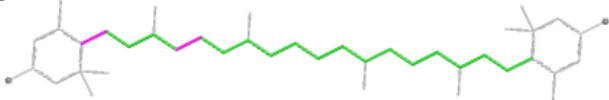
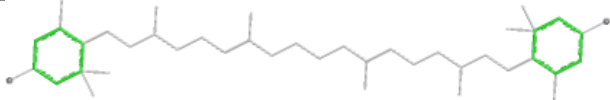


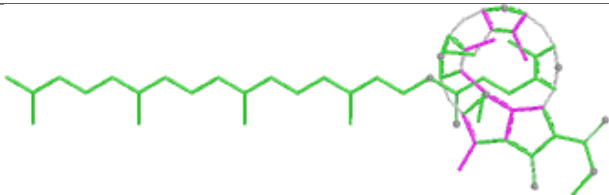
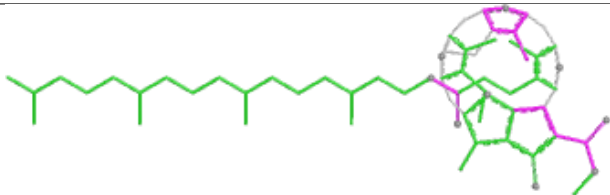
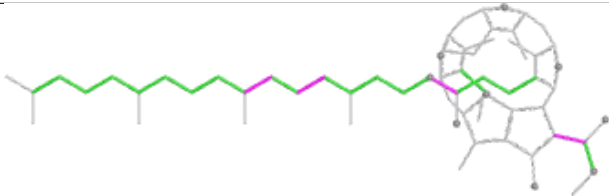
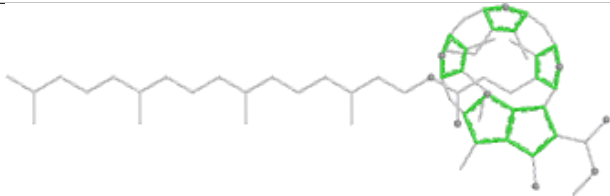
Ligand LMG a 413

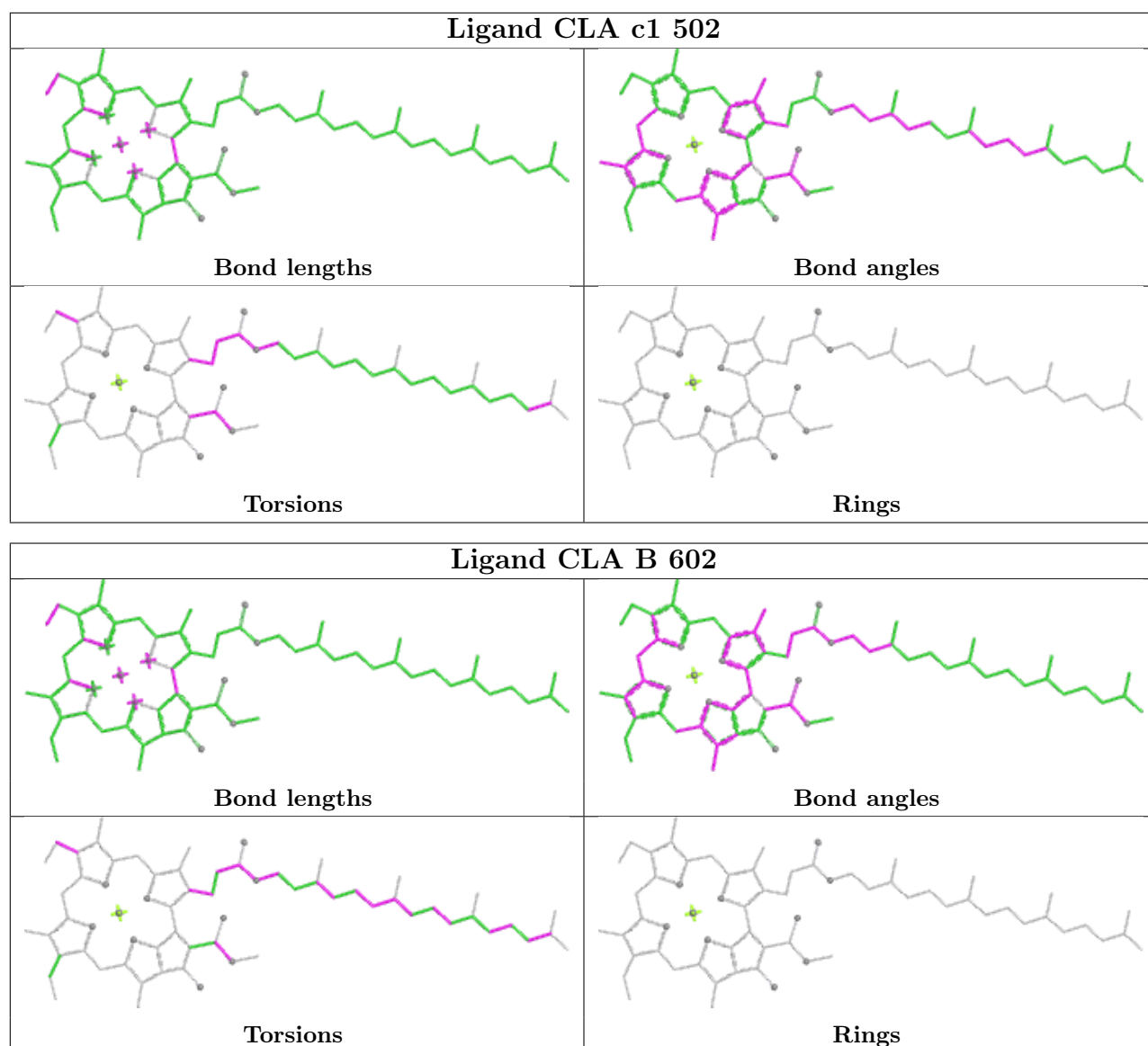


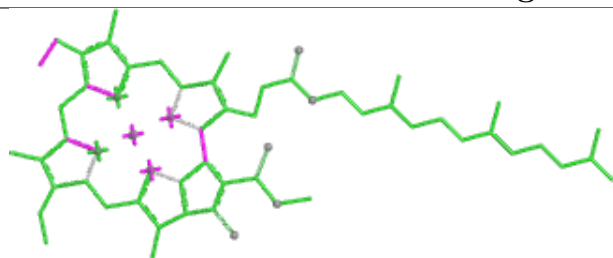
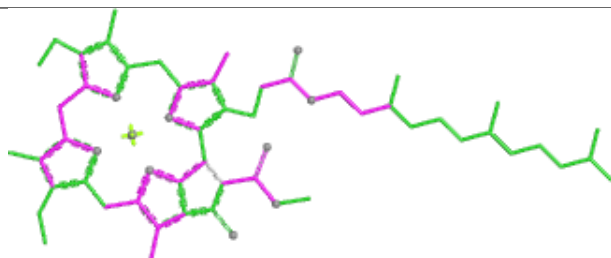
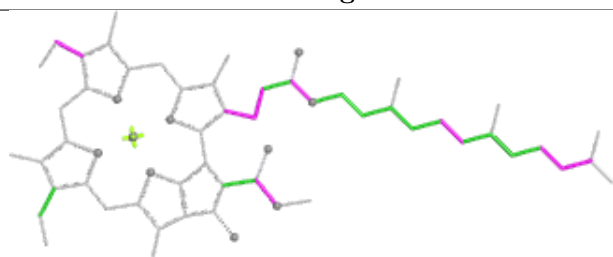
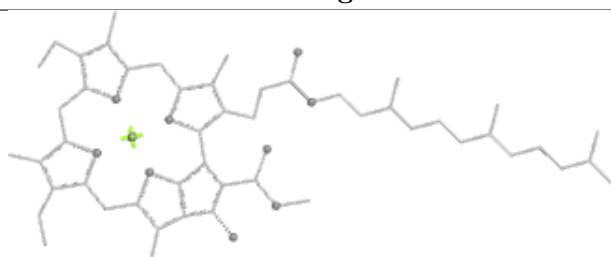
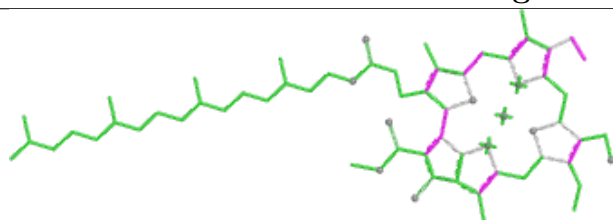
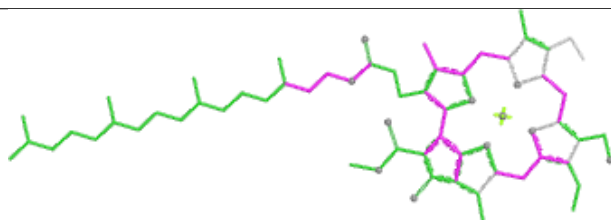
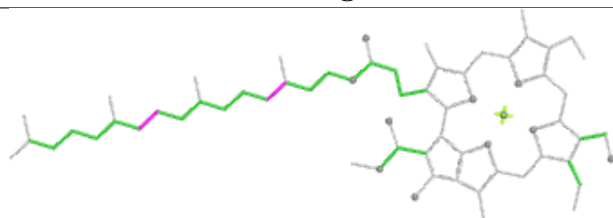
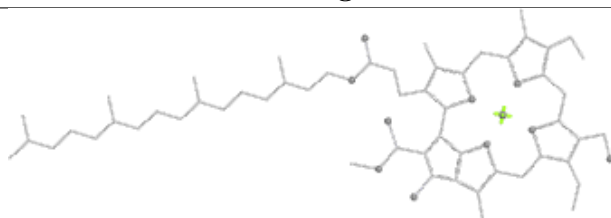


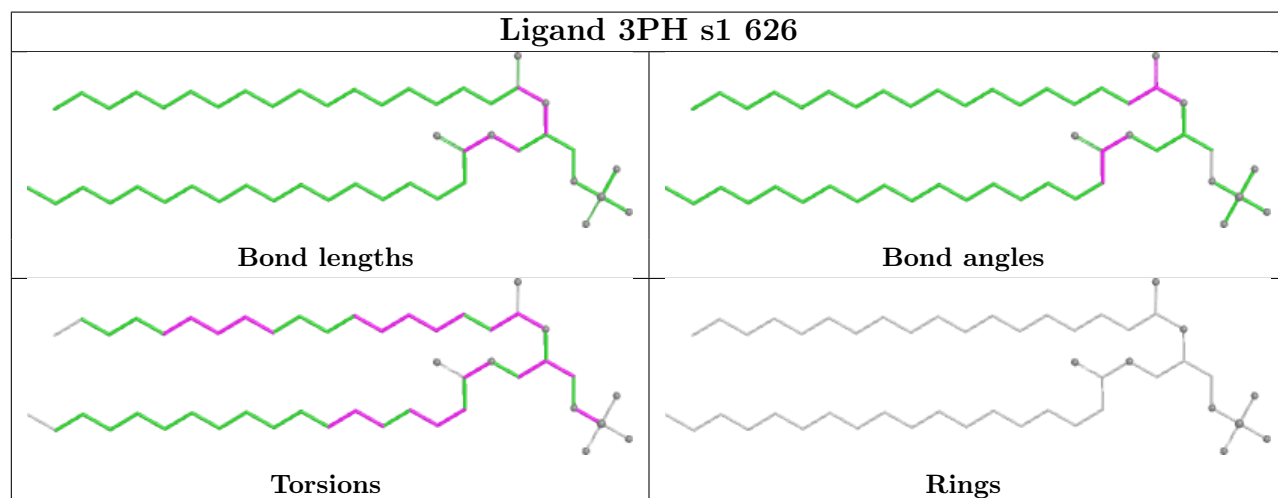
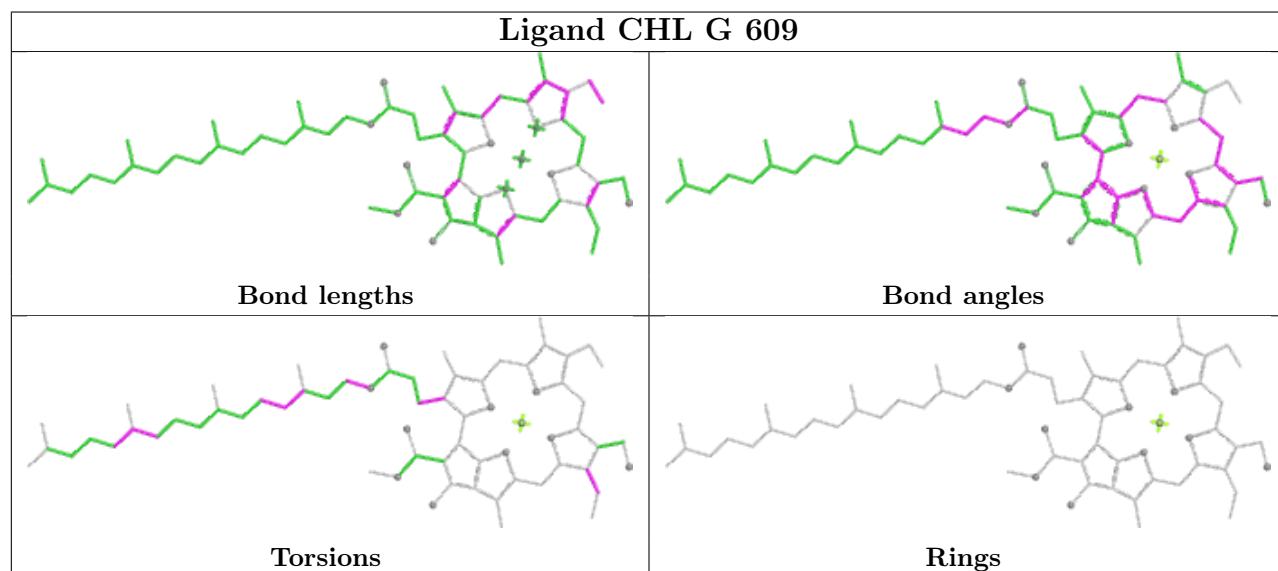
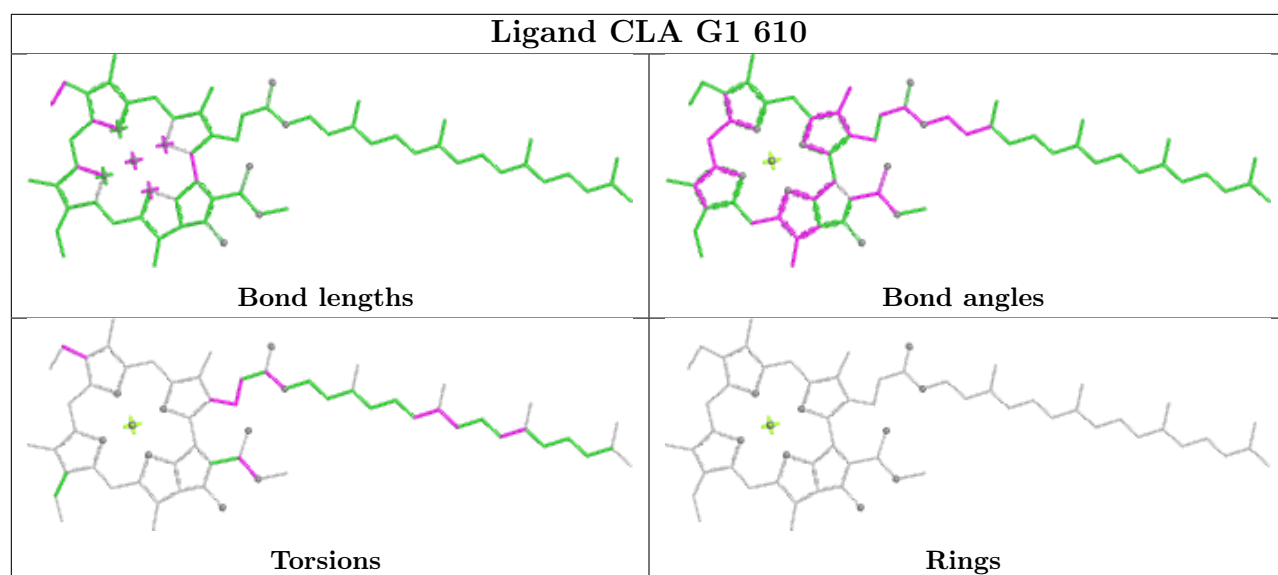
Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

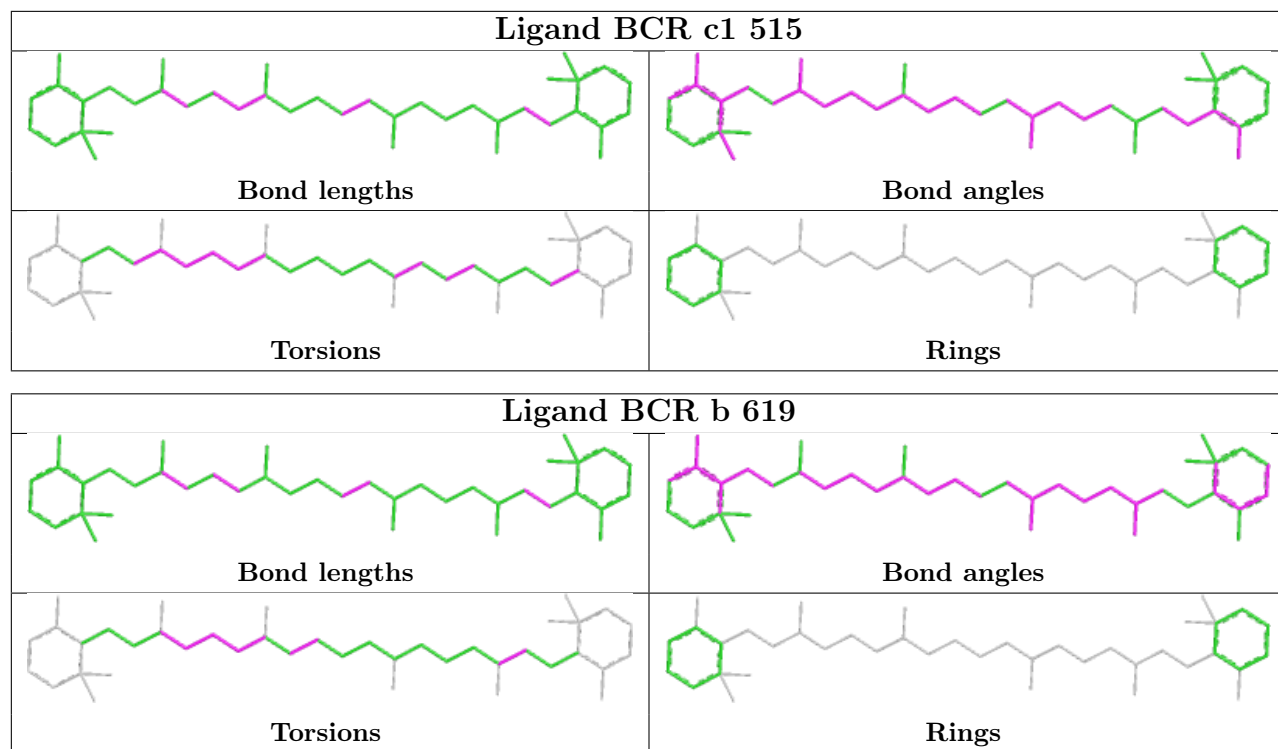
Ligand LUT s1 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO A1 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

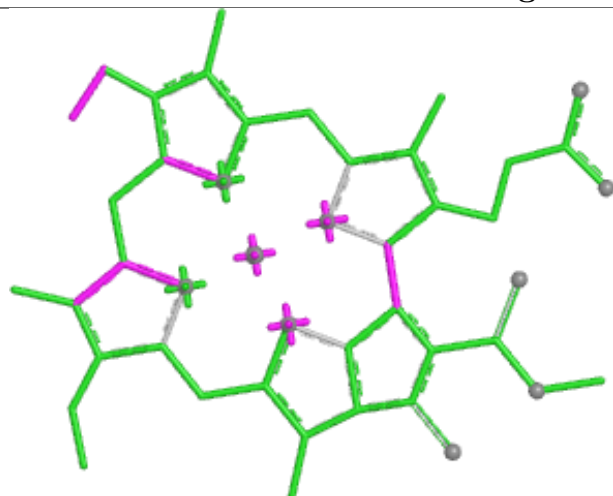


Ligand CLA S 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CHL G 601****Bond lengths****Bond angles****Torsions****Rings**

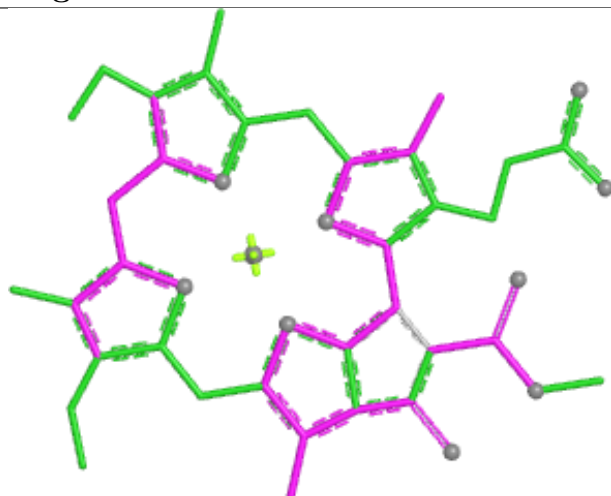




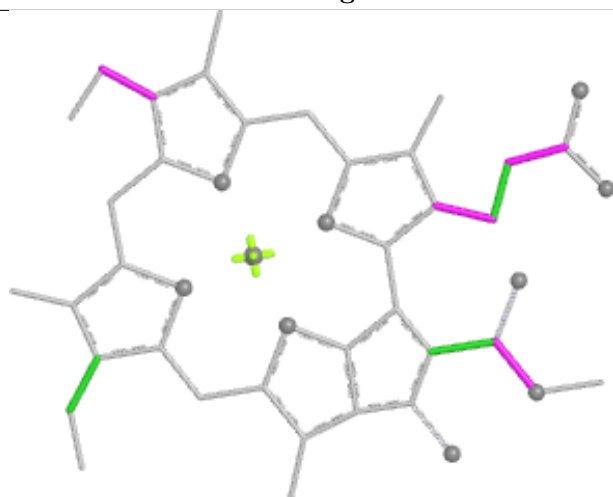
Ligand CLA g 611



Bond lengths



Bond angles

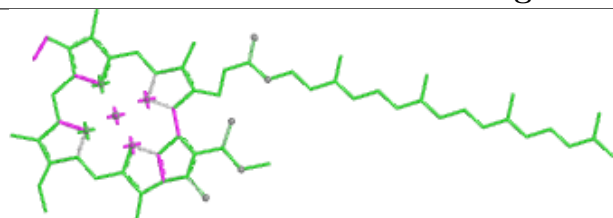


Torsions

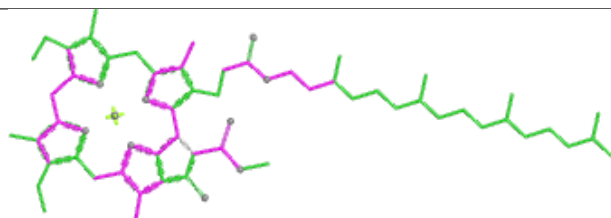


Rings

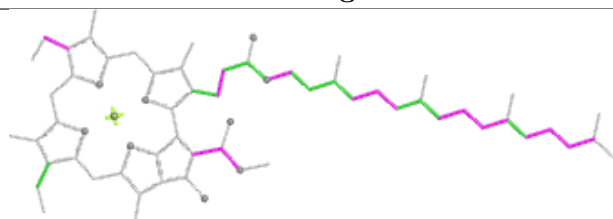
Ligand CLA C 502



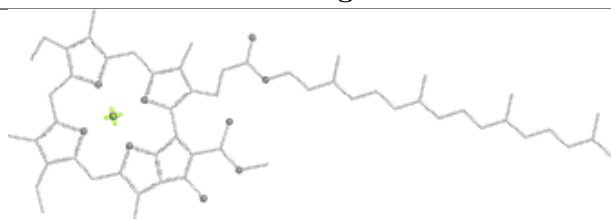
Bond lengths



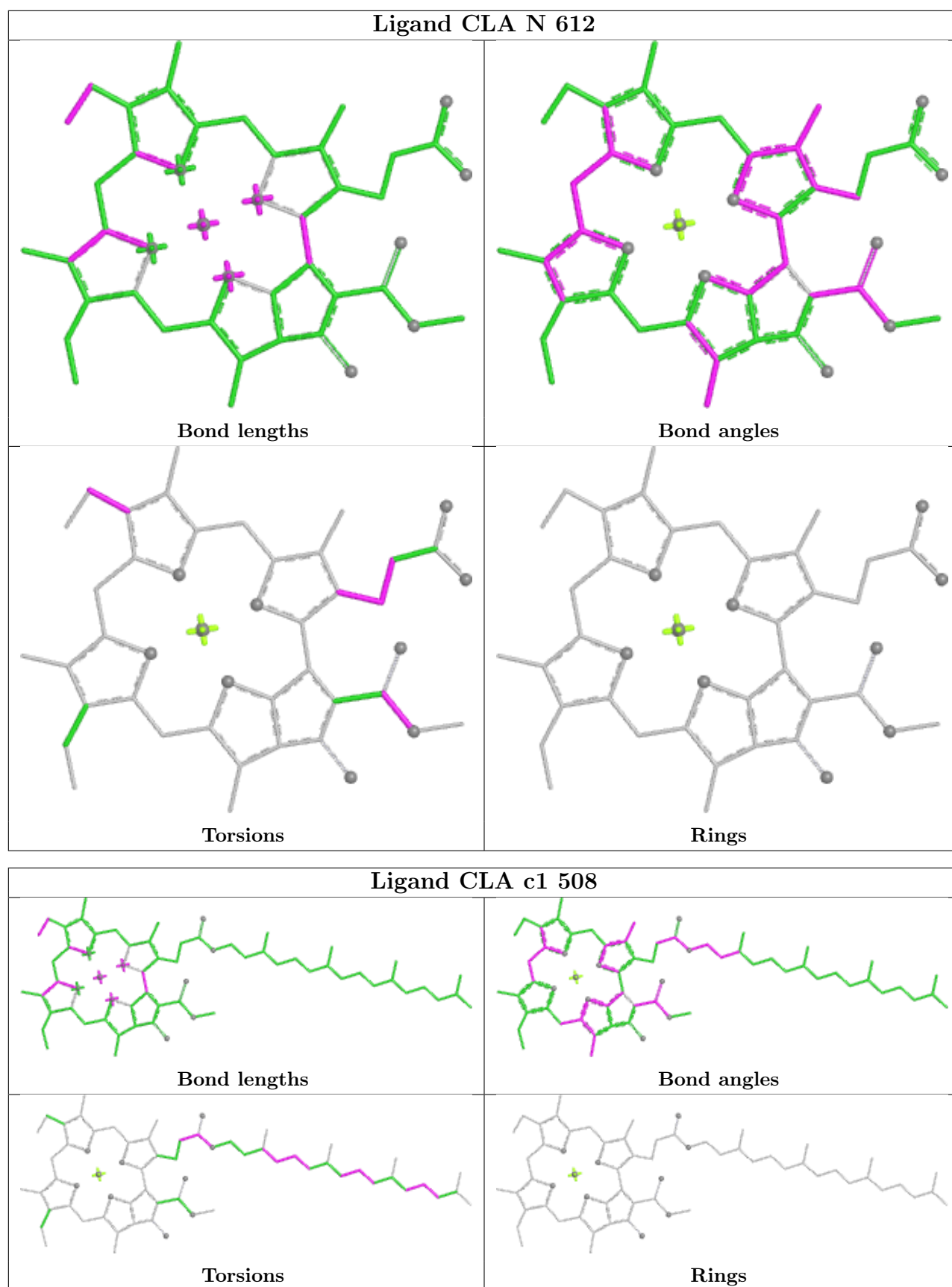
Bond angles

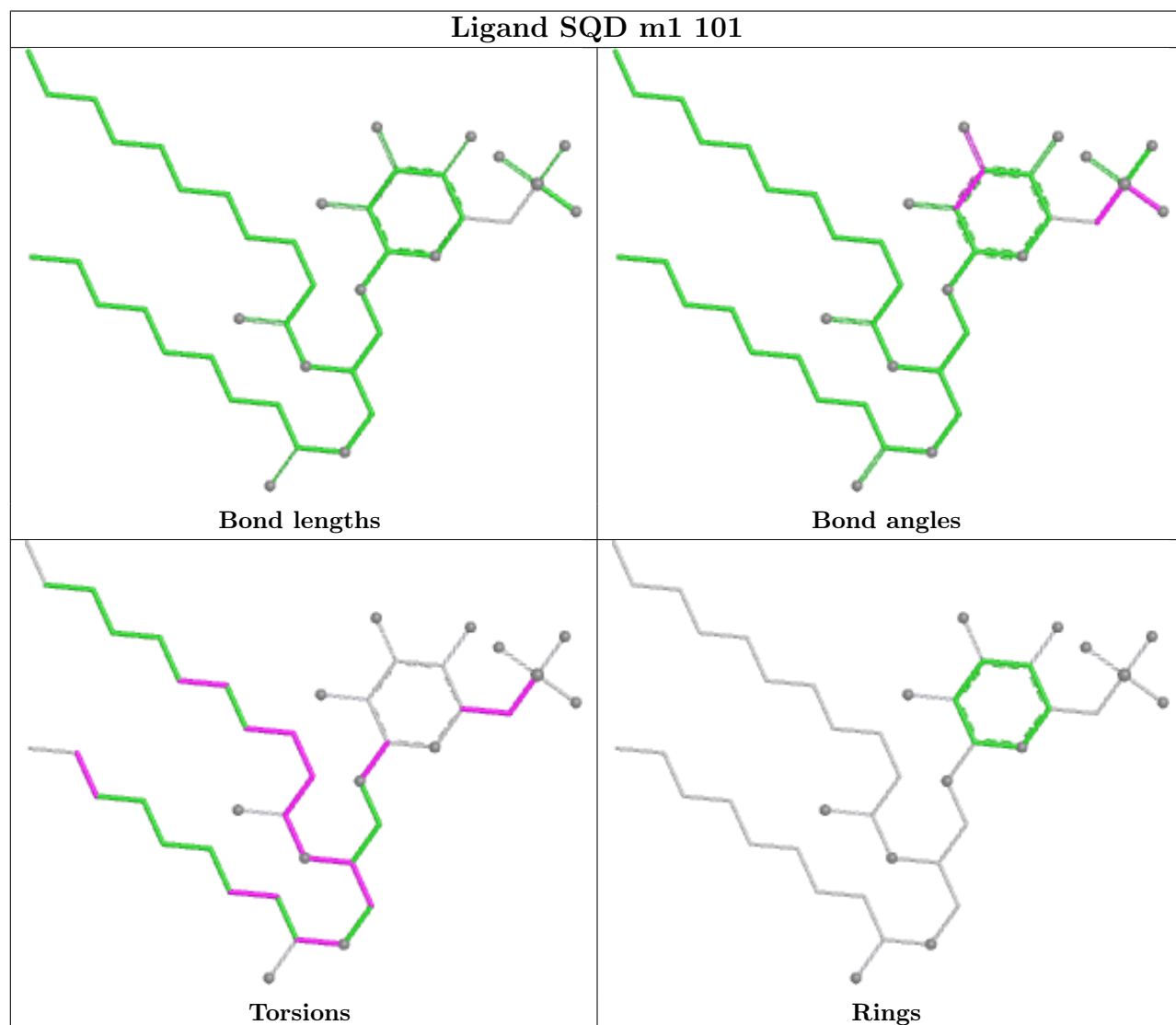
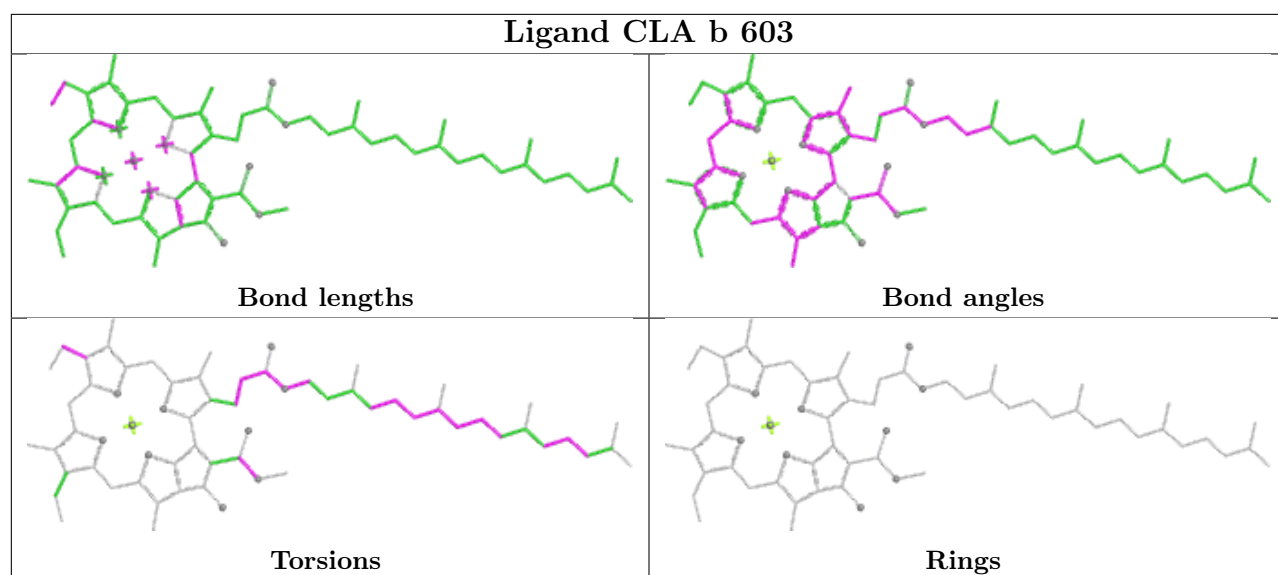


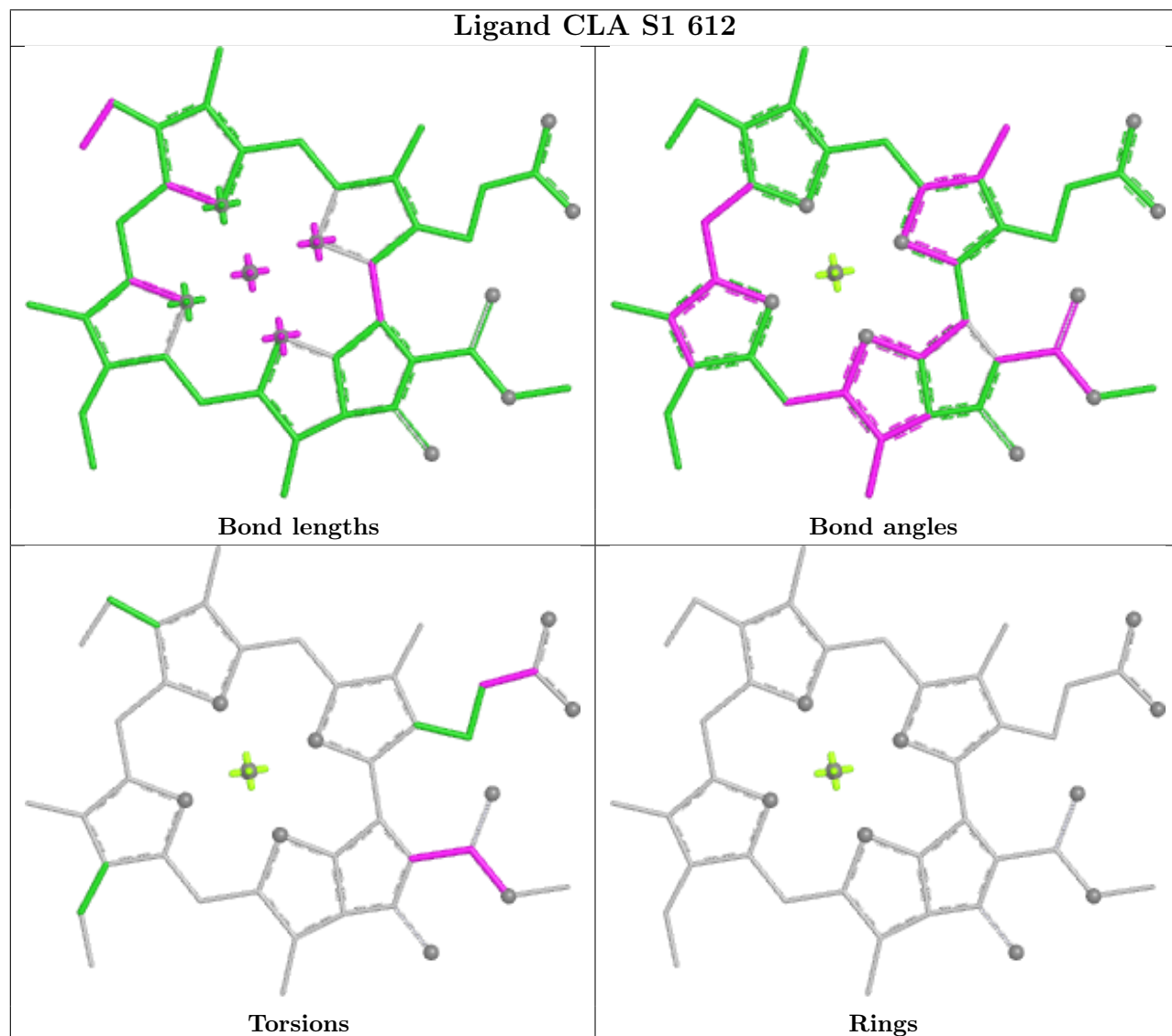
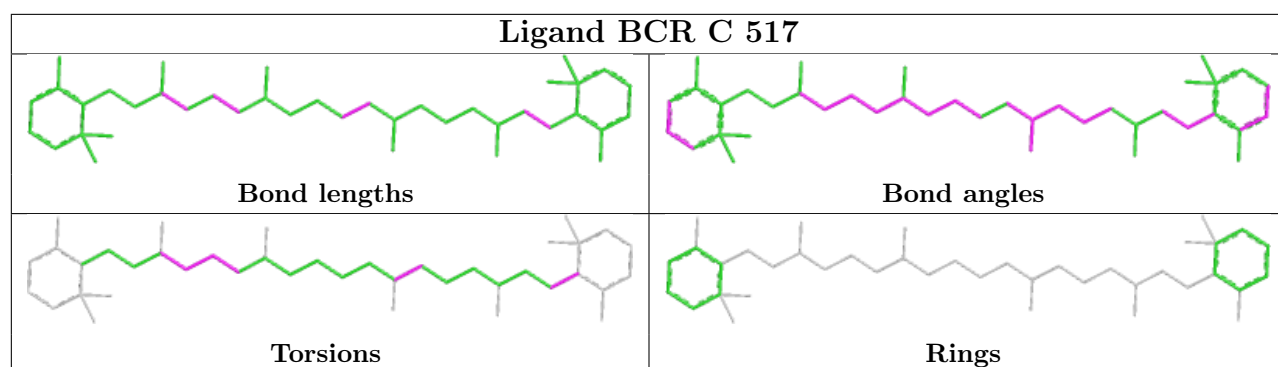
Torsions

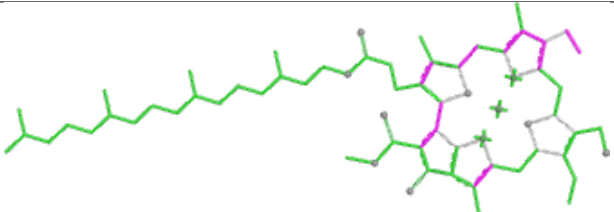
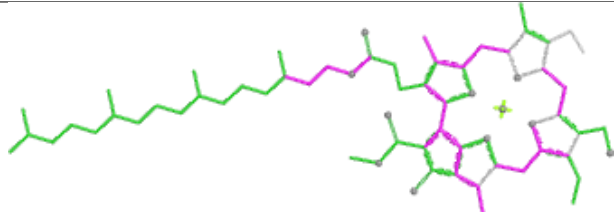
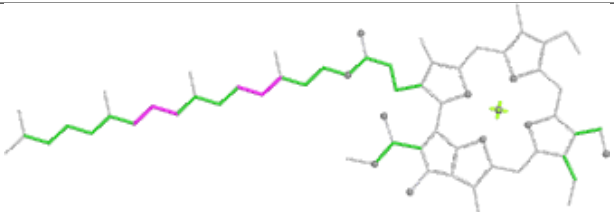
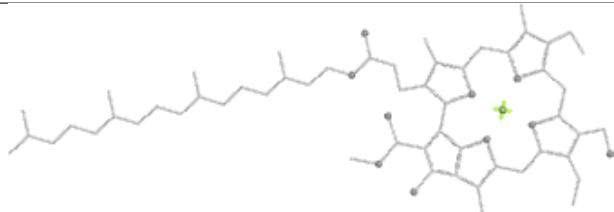


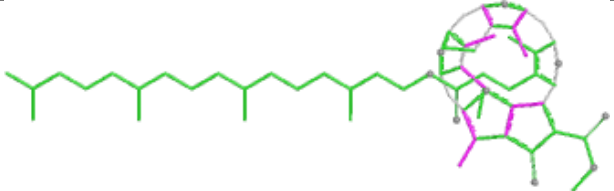
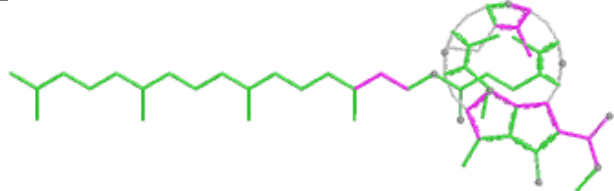
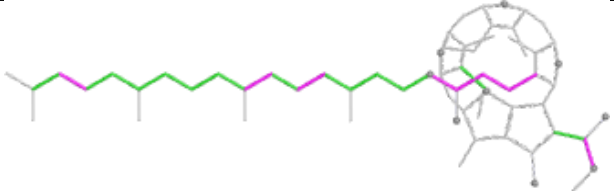
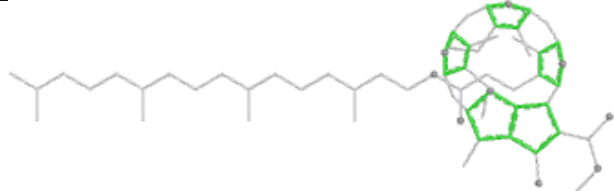
Rings

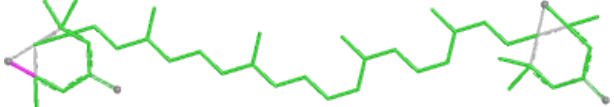
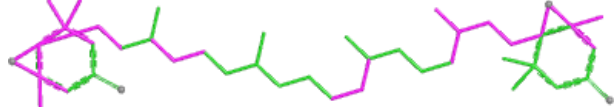
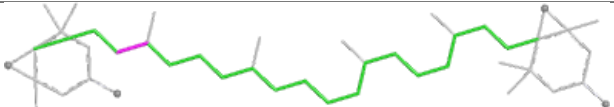
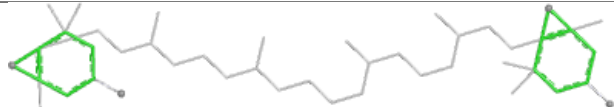


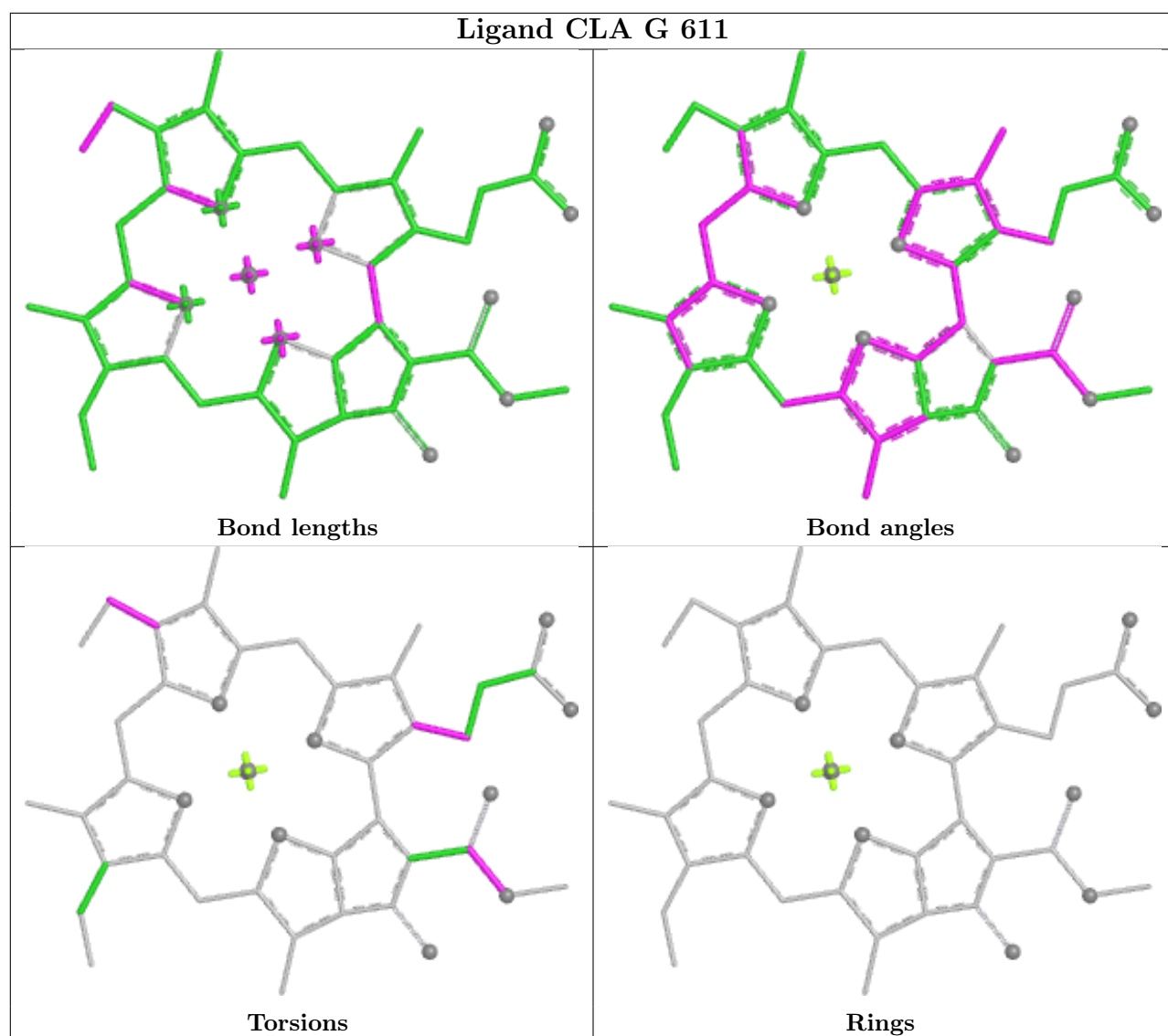


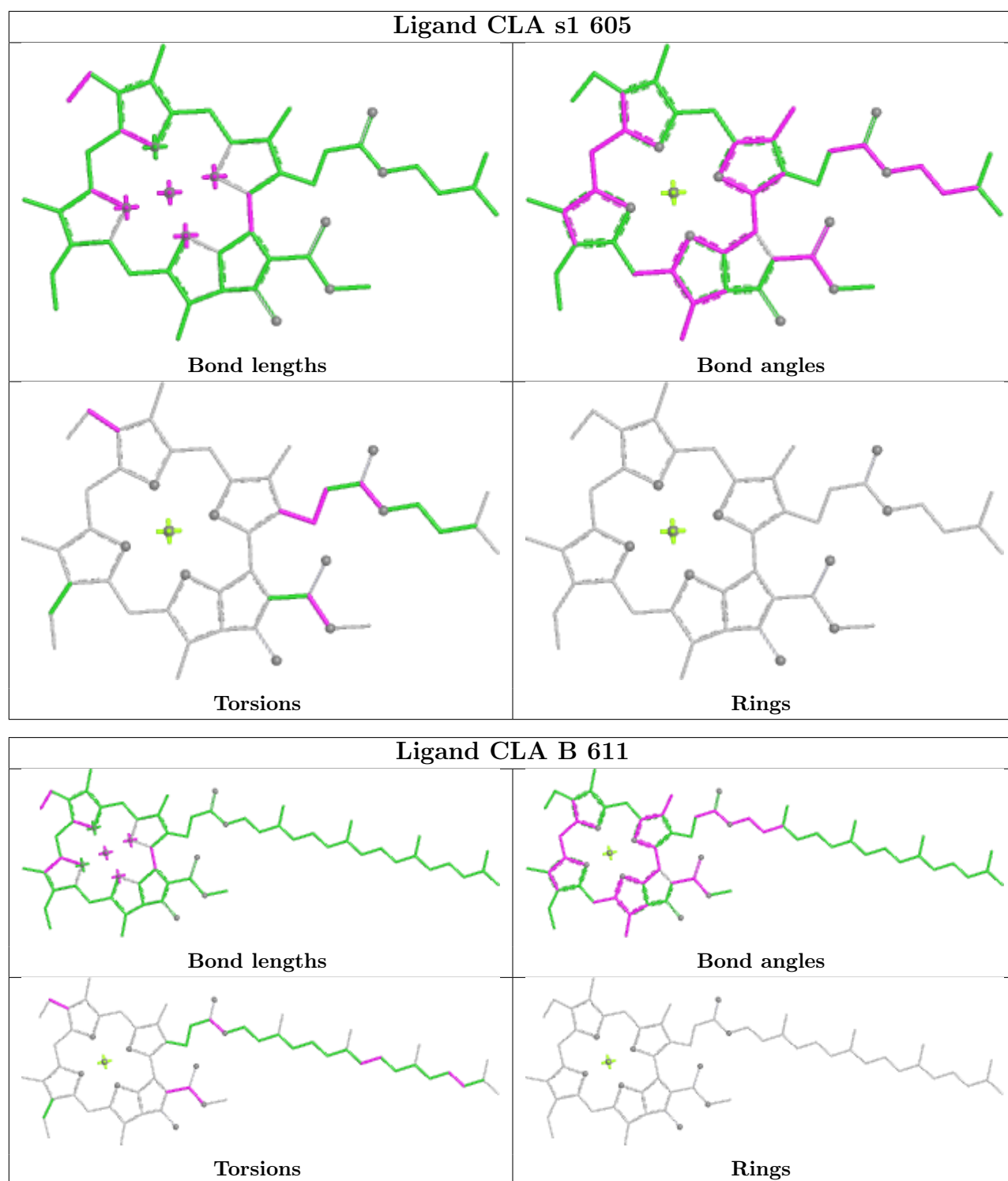


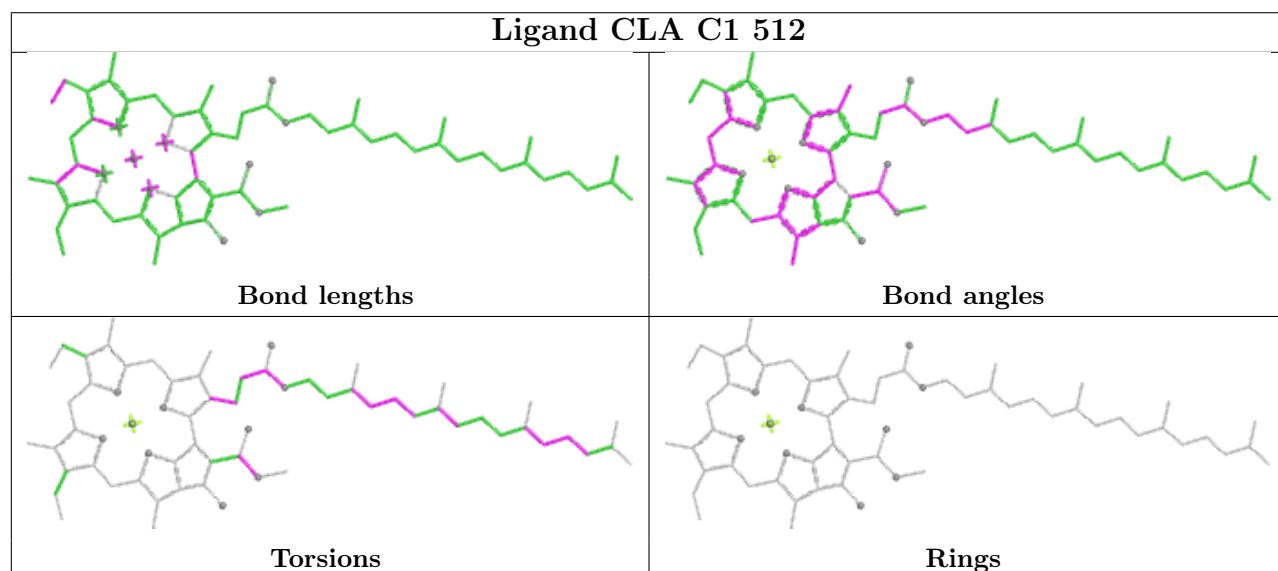
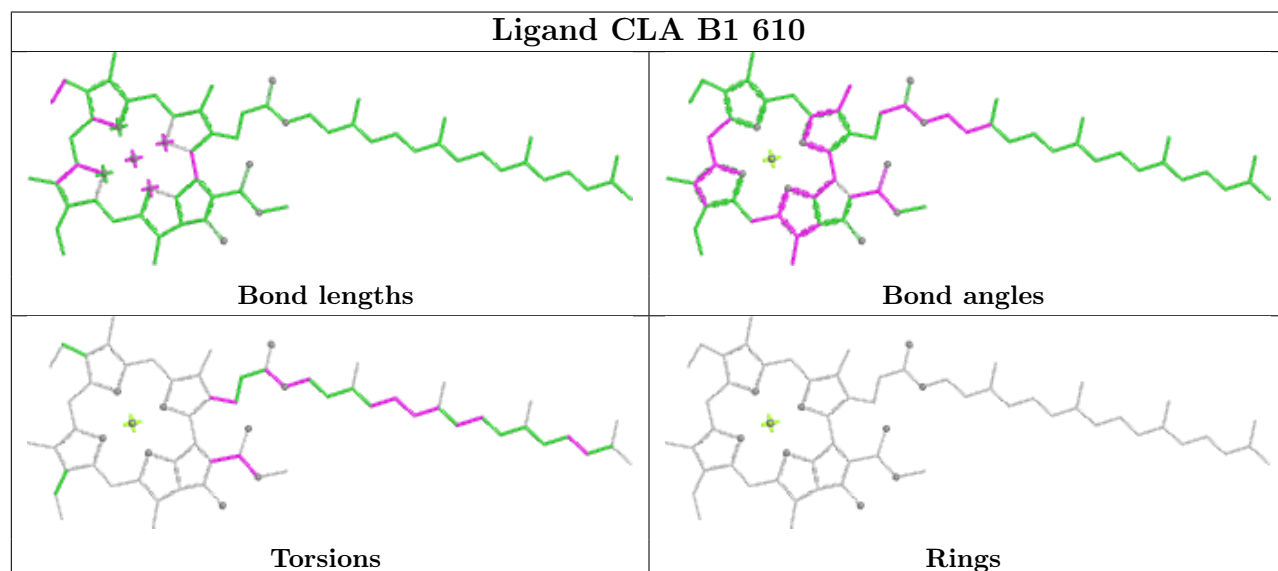
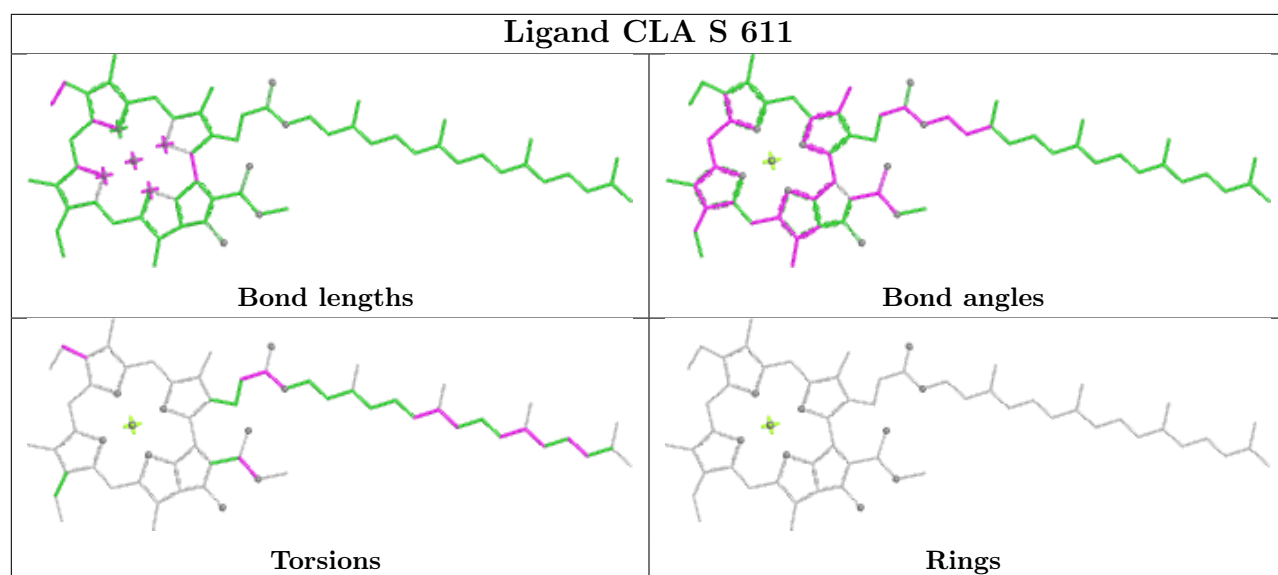
Ligand CHL n 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

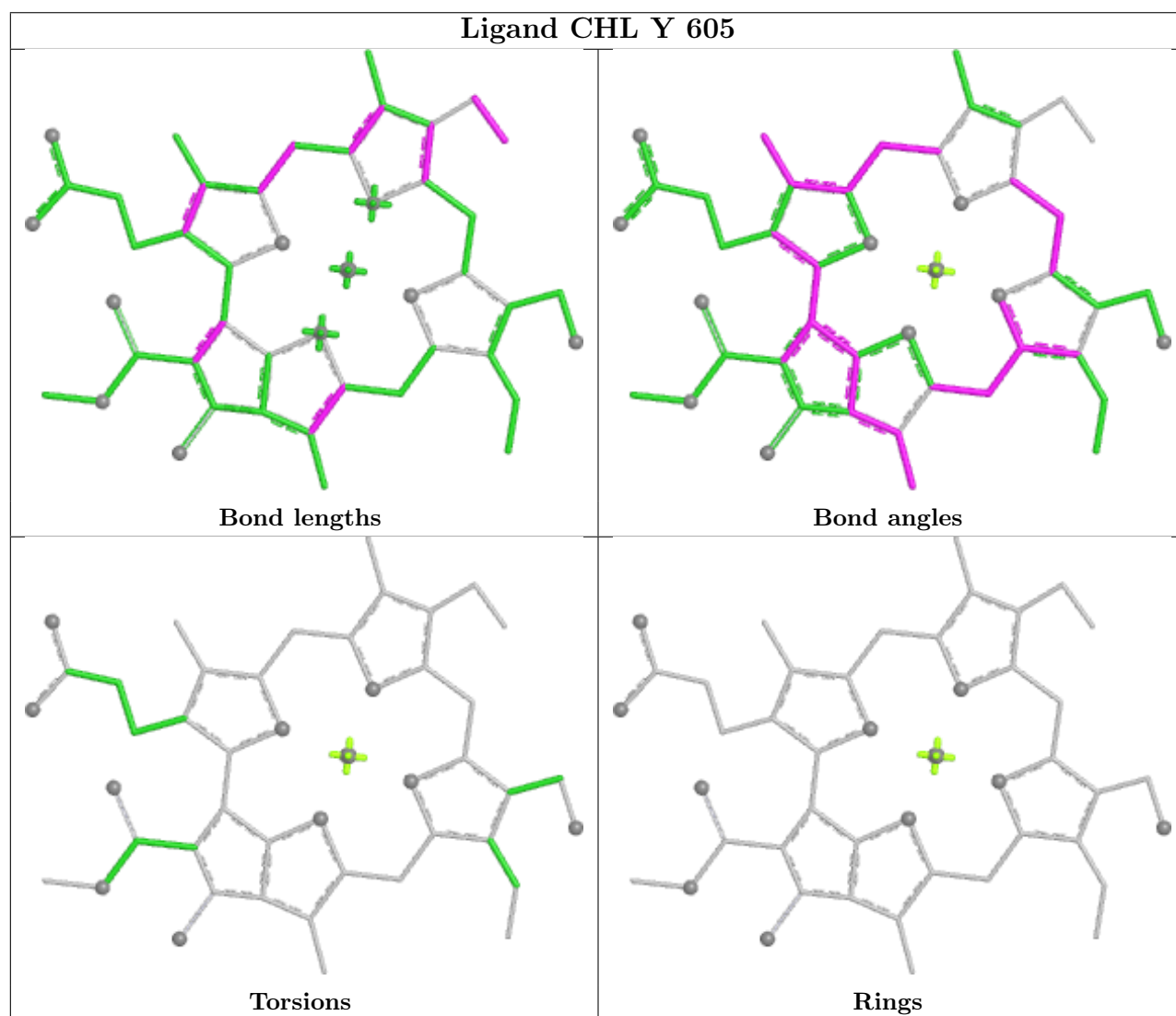
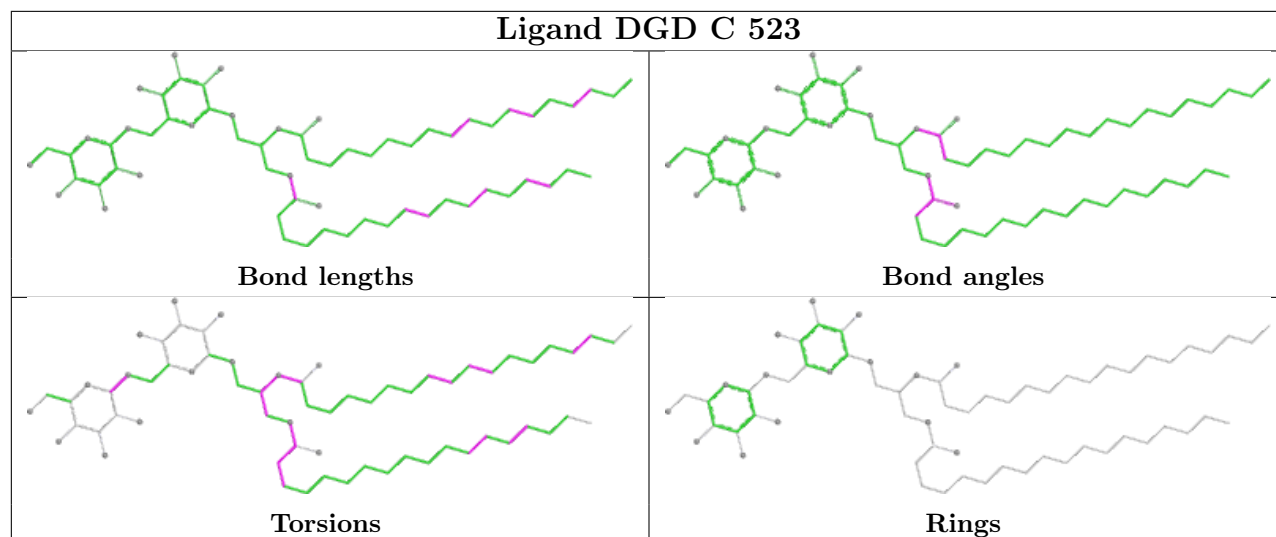
Ligand PHO A1 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

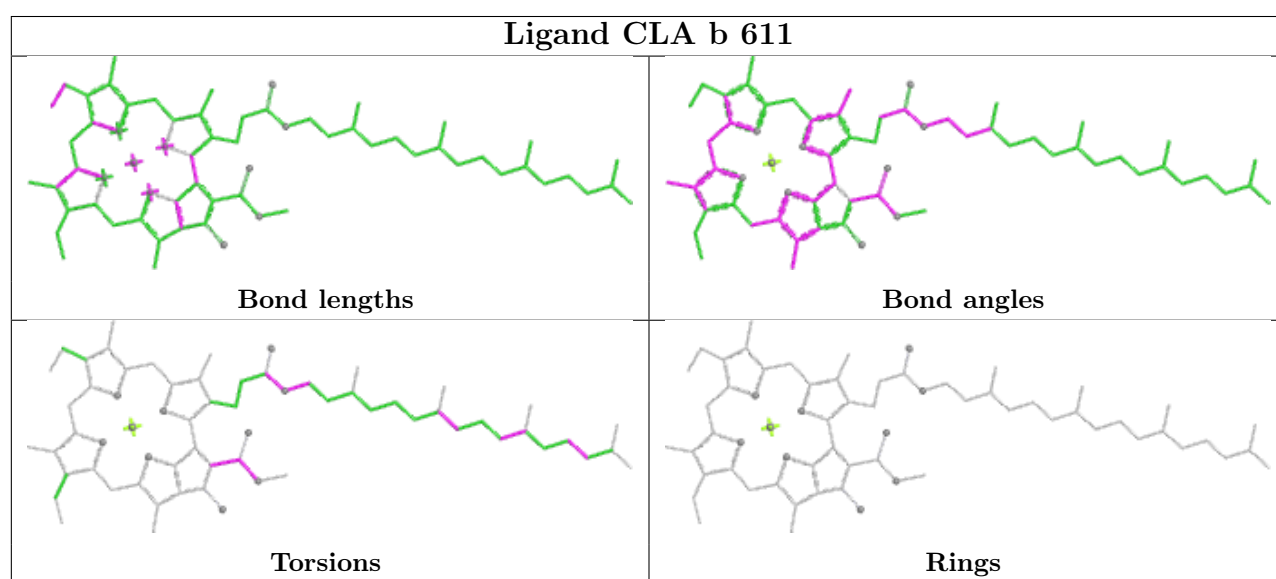
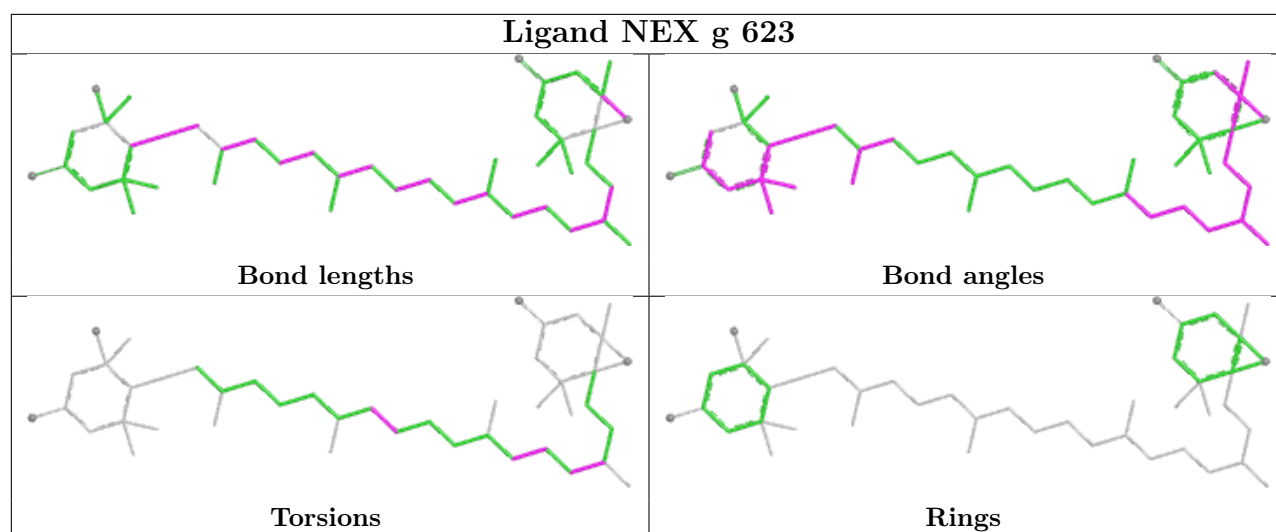
Ligand XAT Y1 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

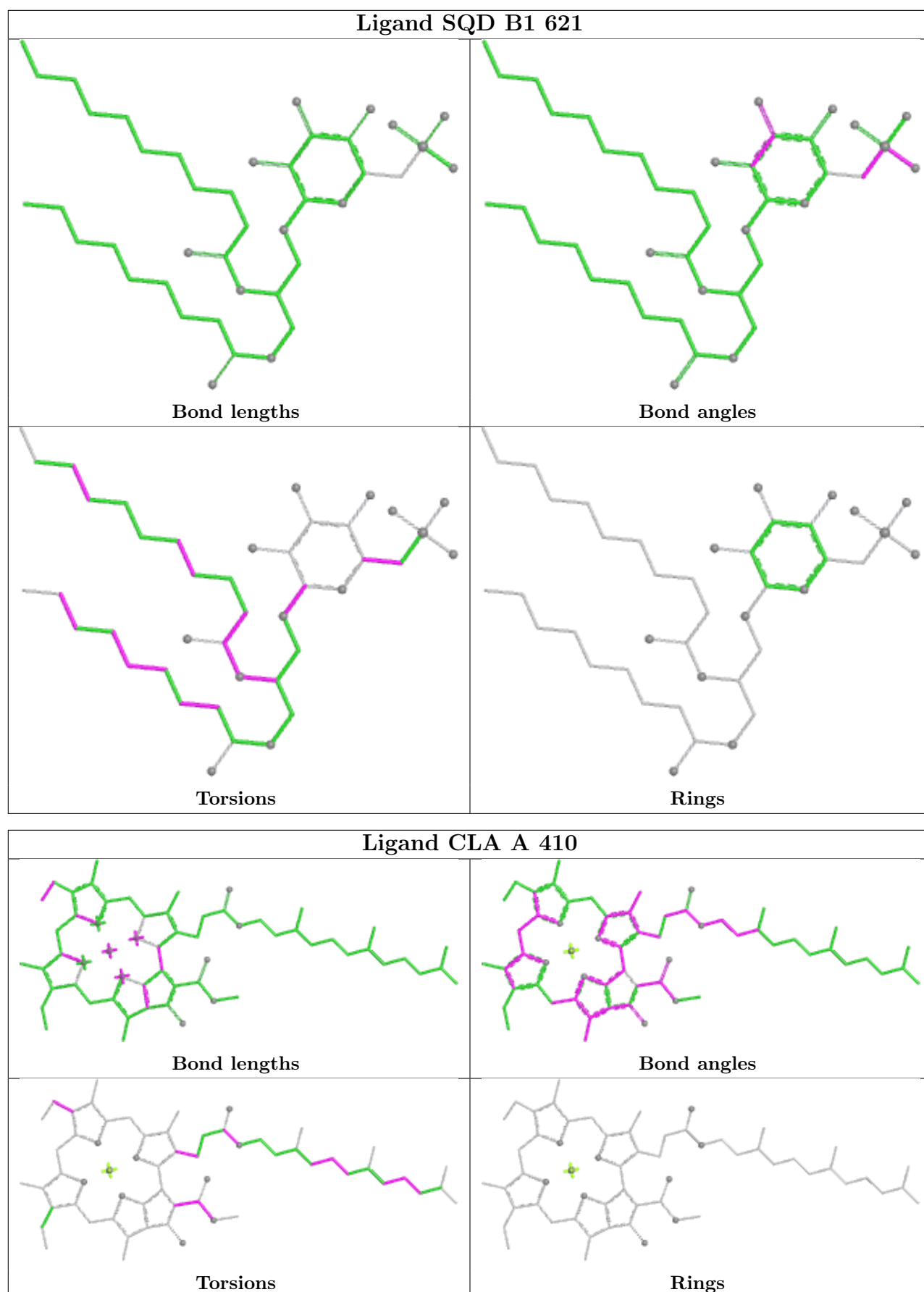


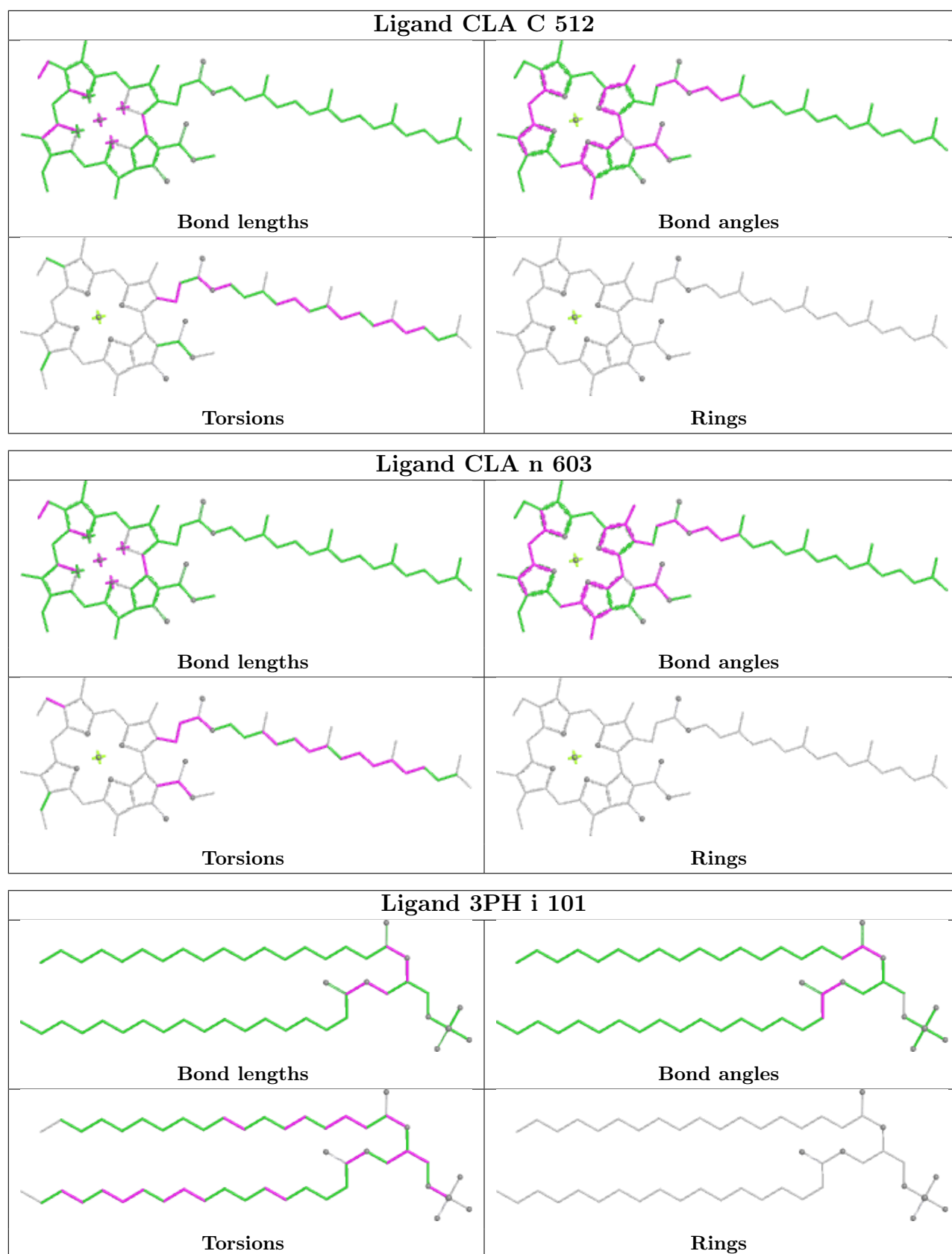


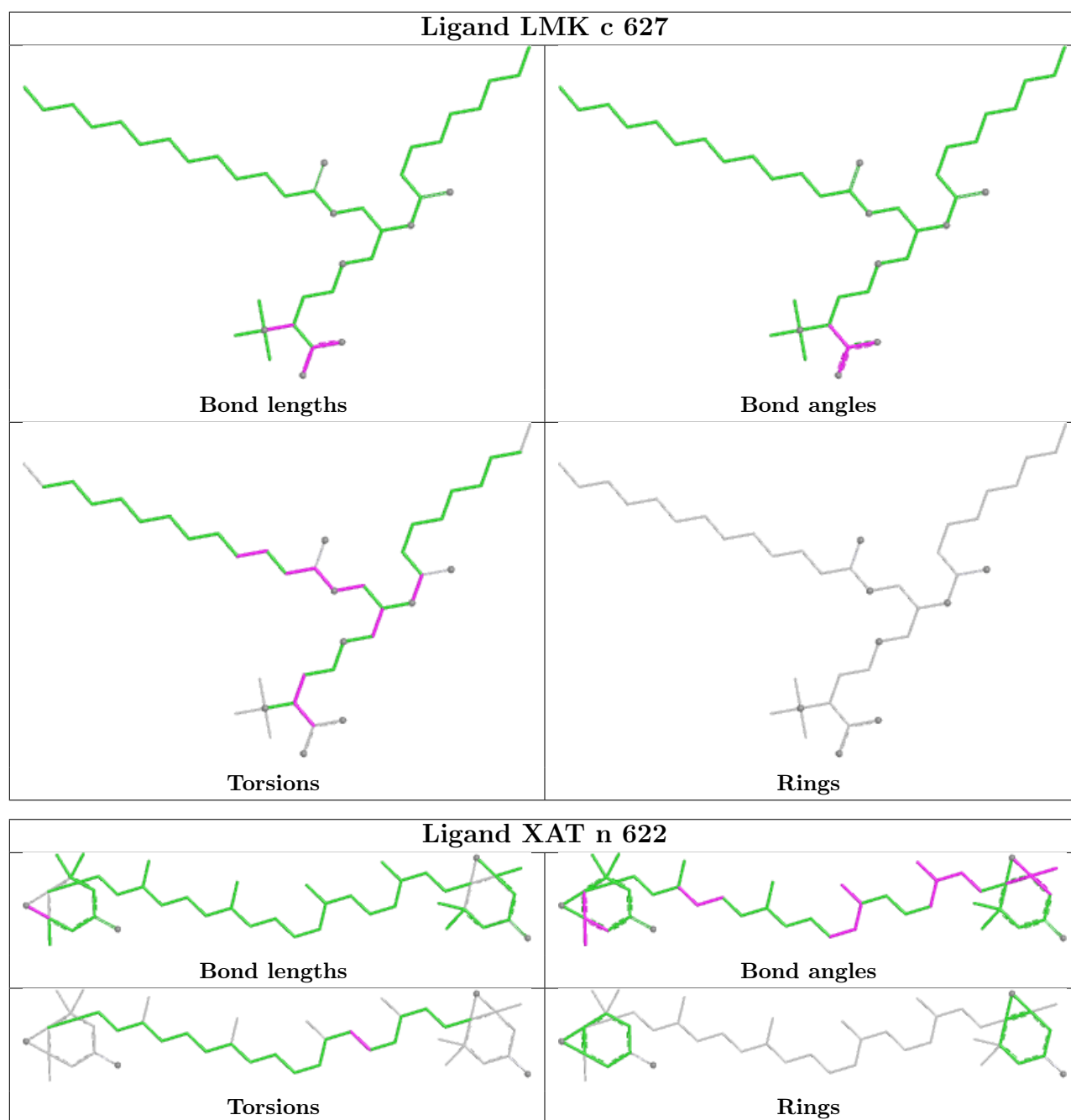


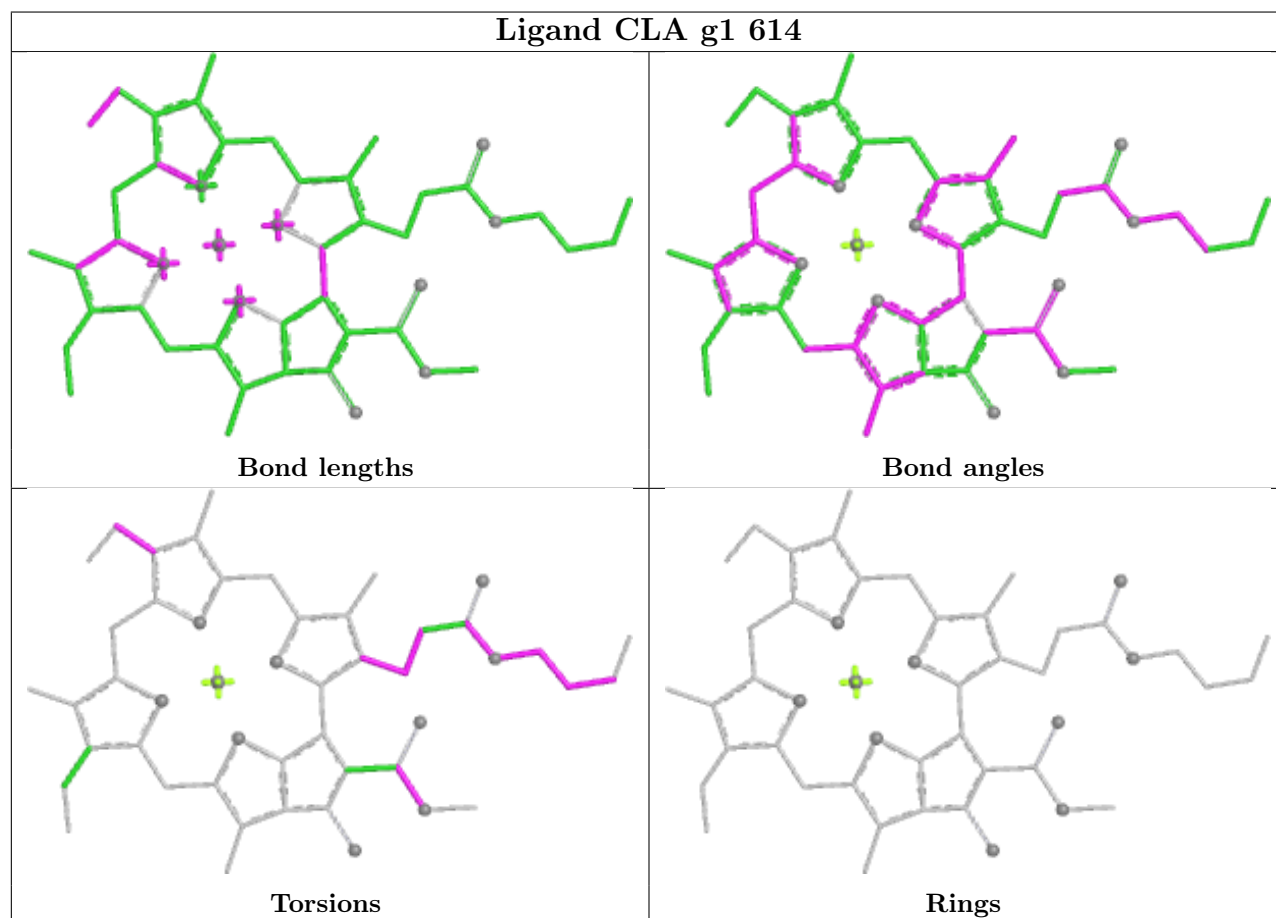
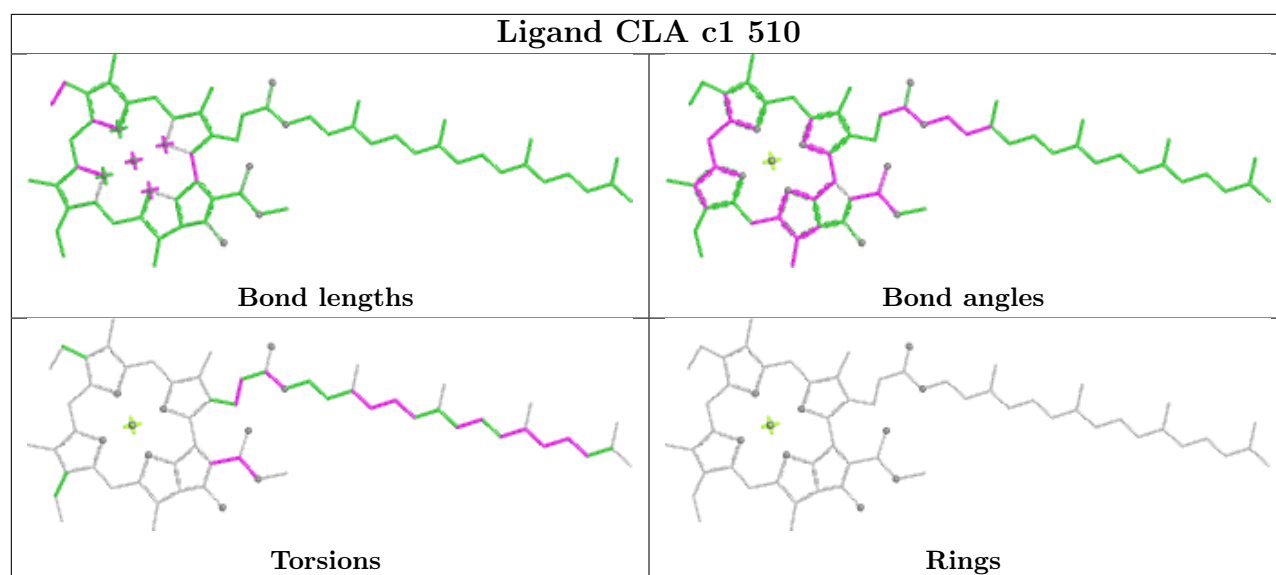


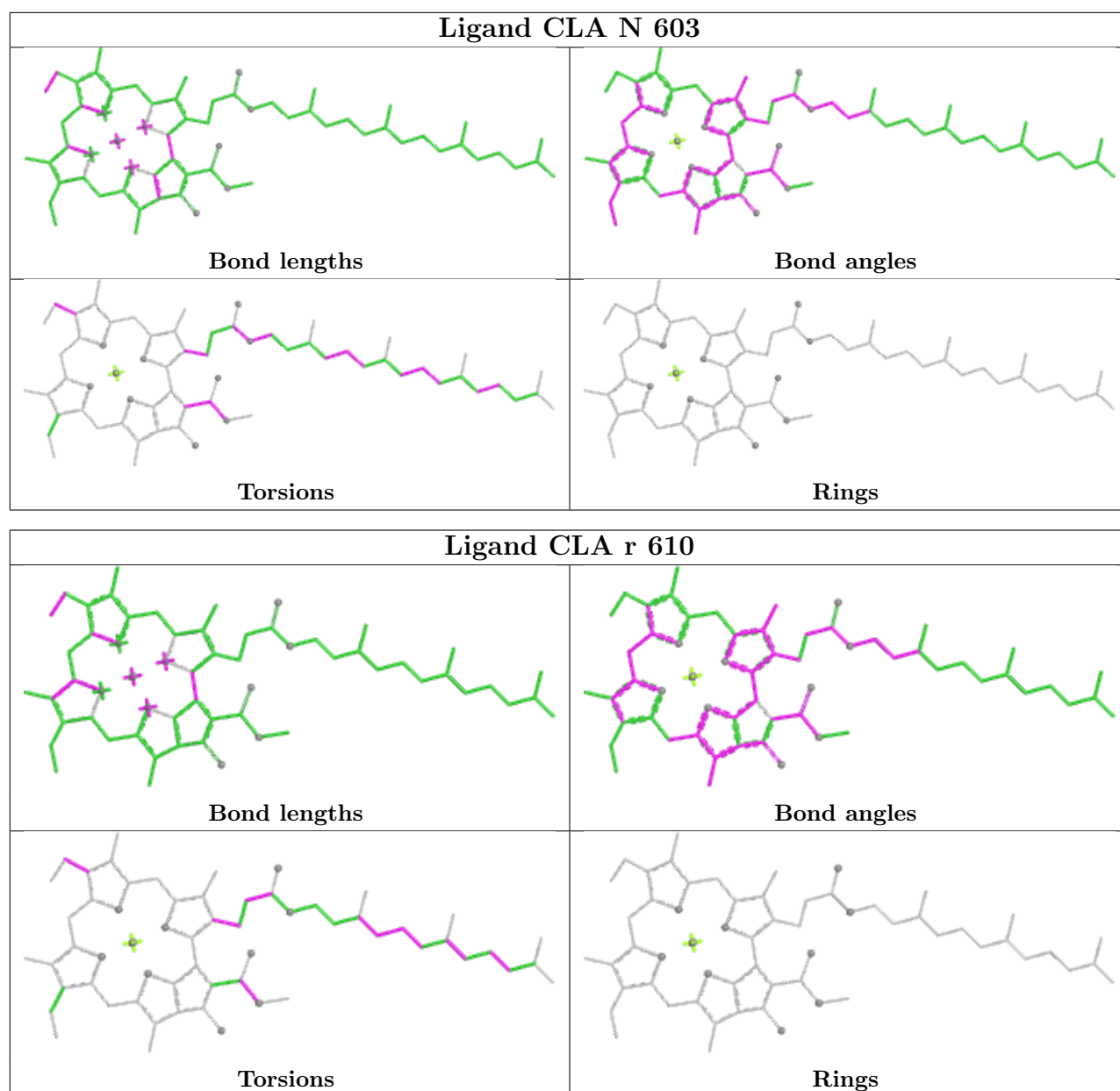


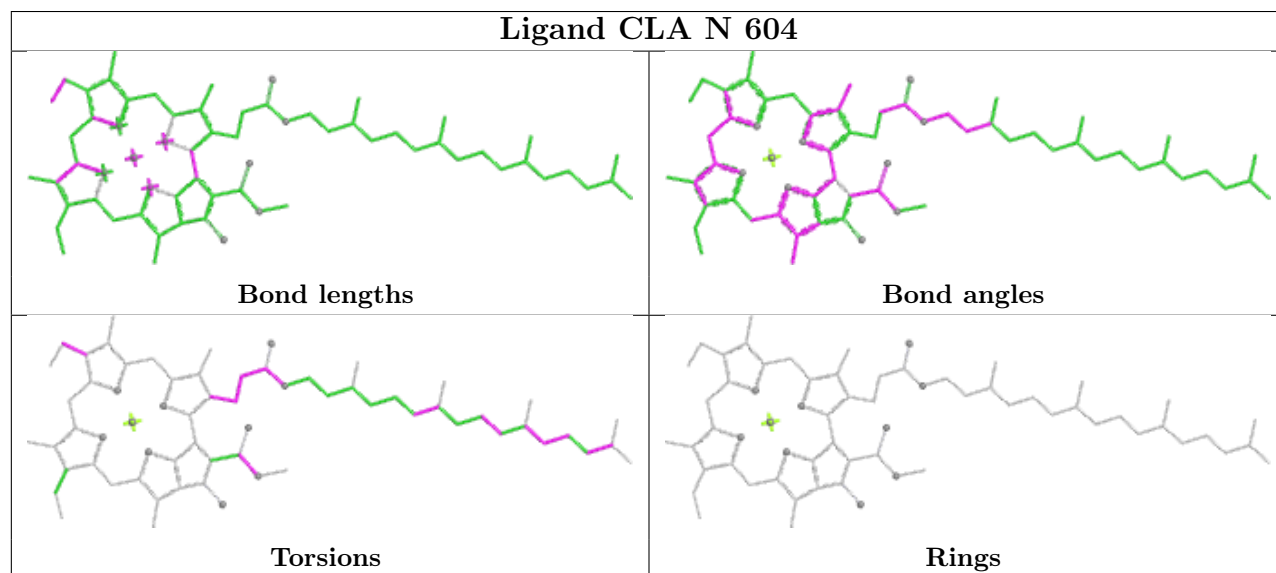
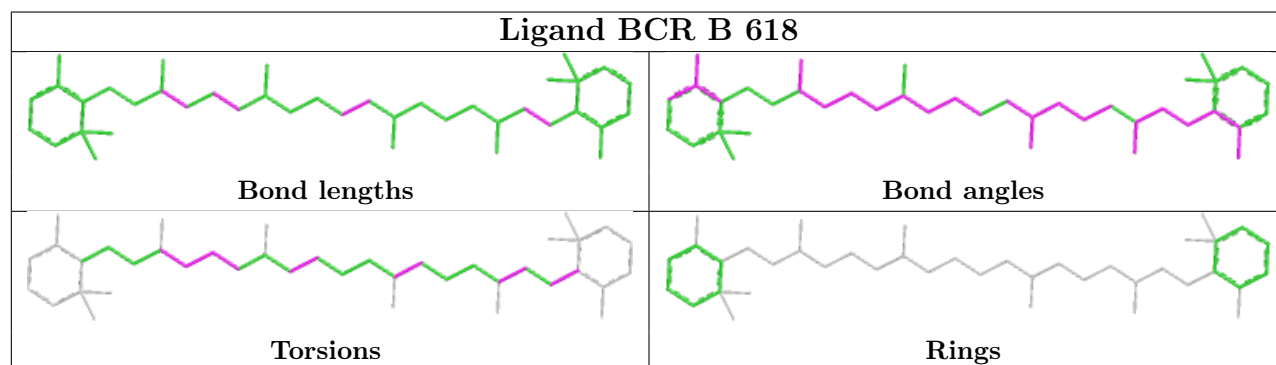
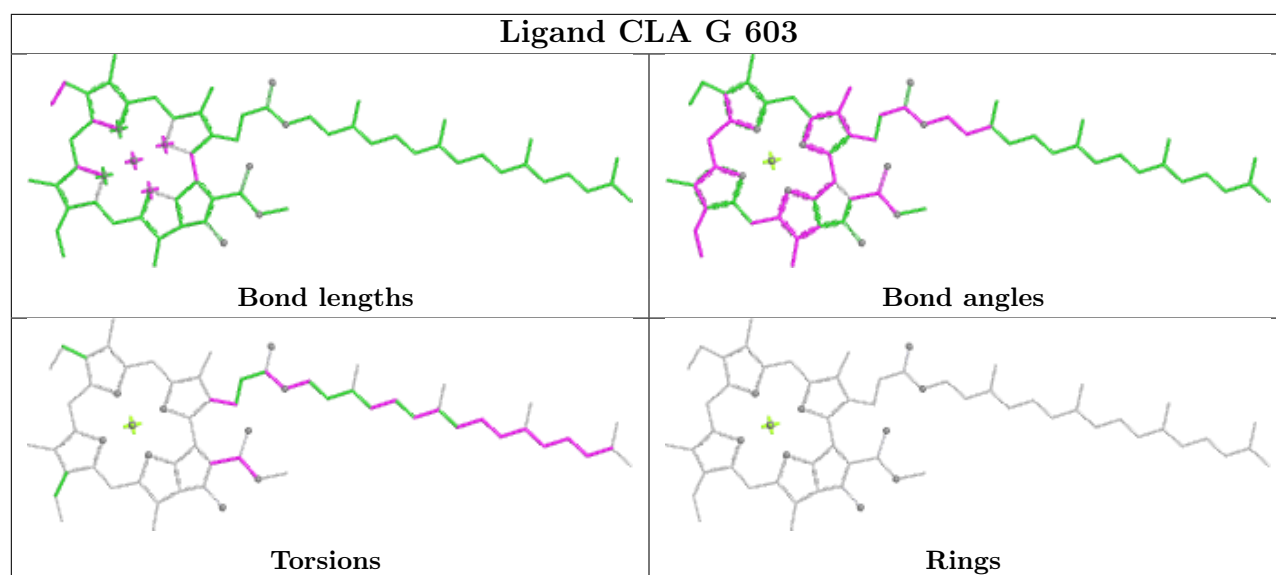


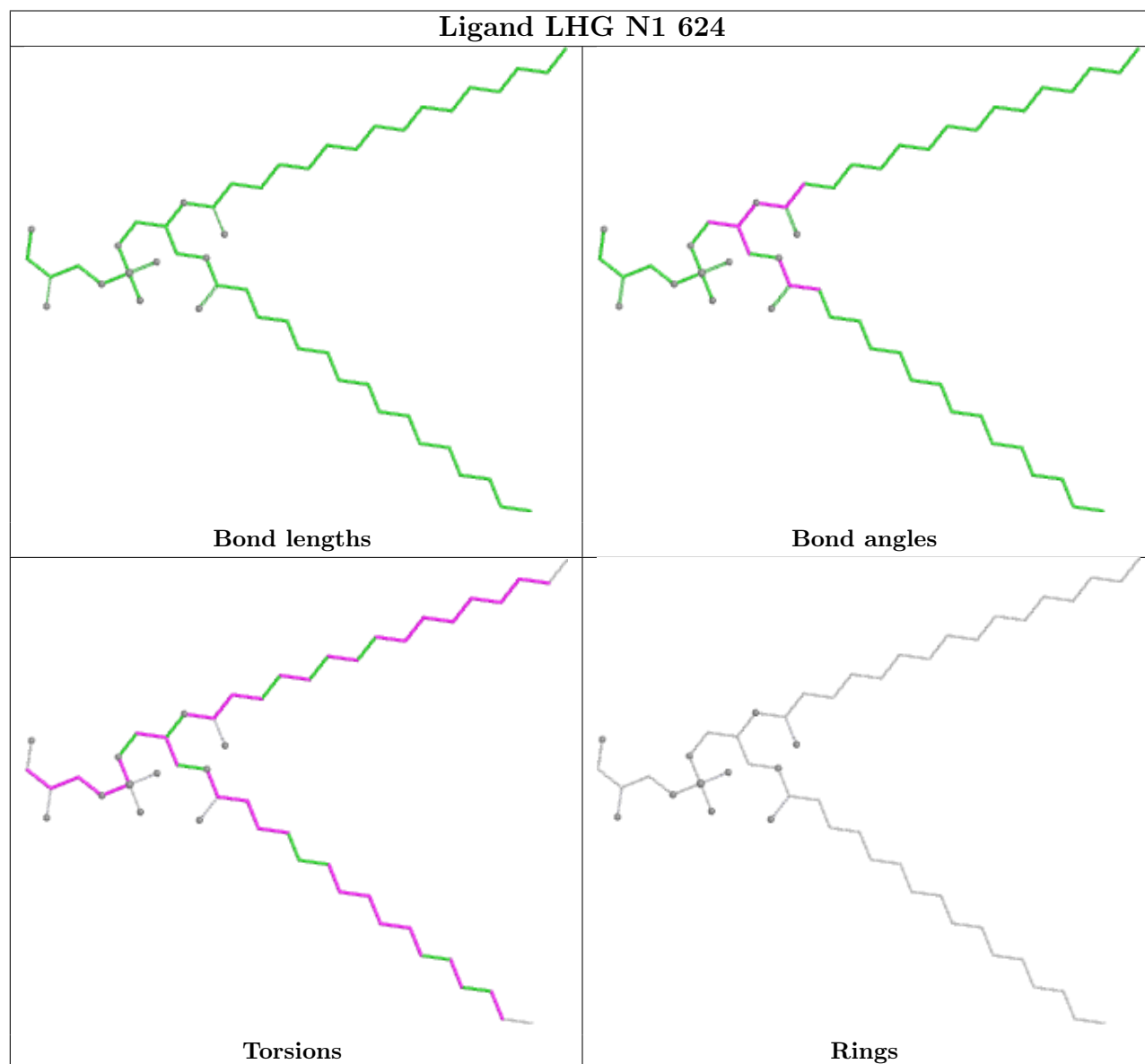
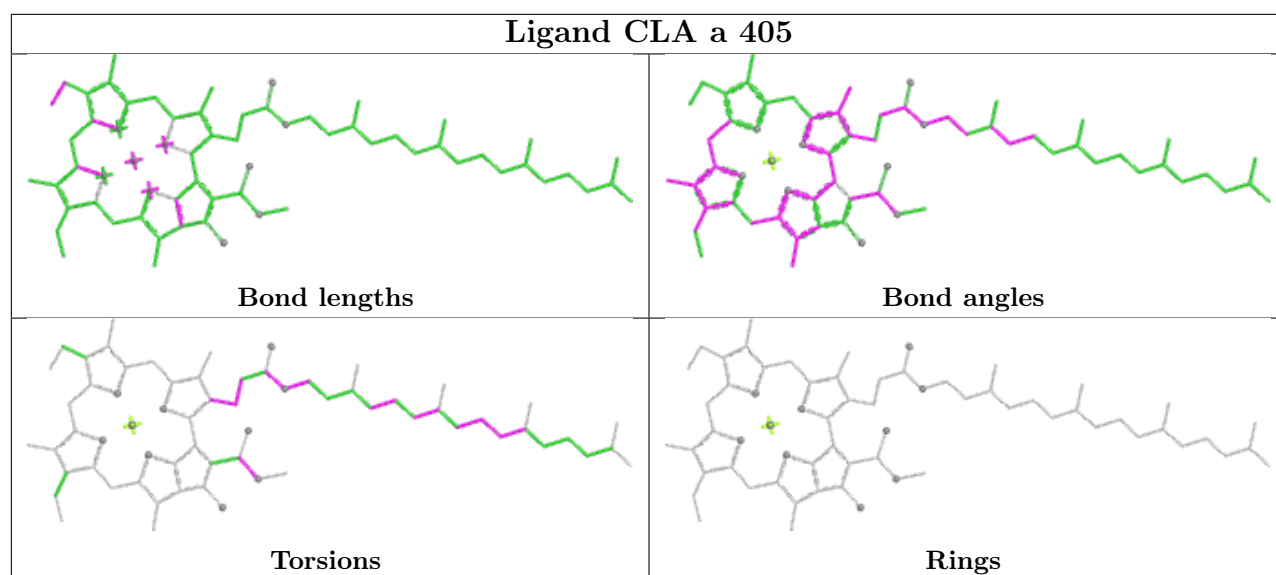


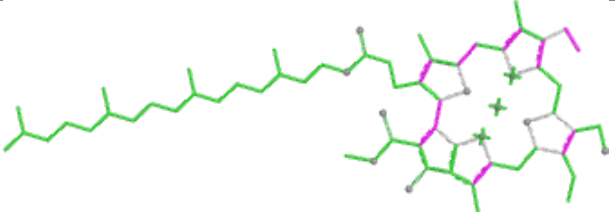
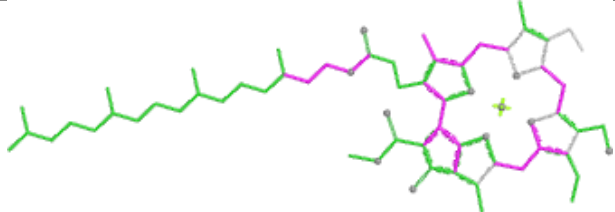
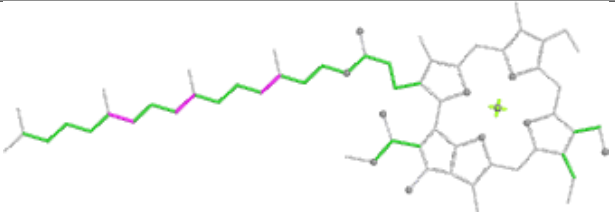
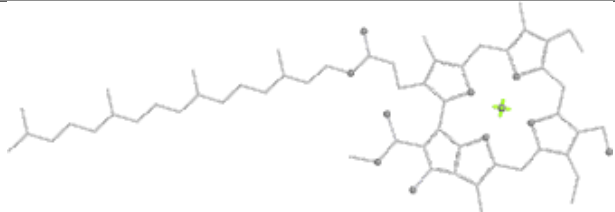
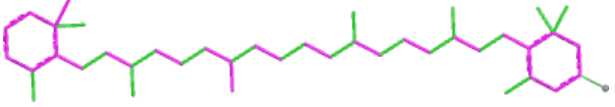
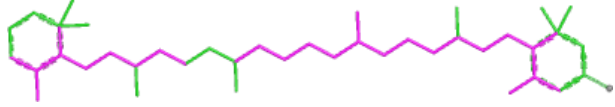
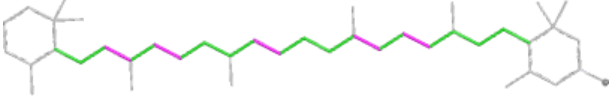
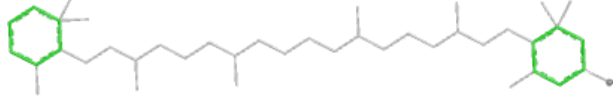
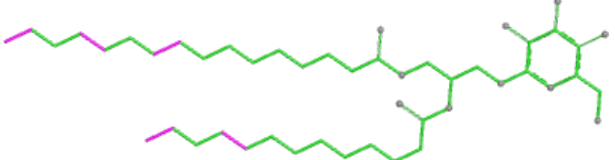
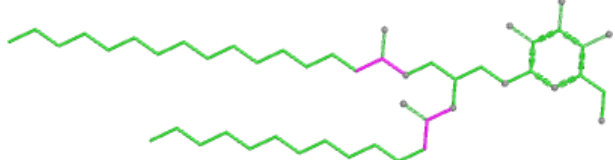
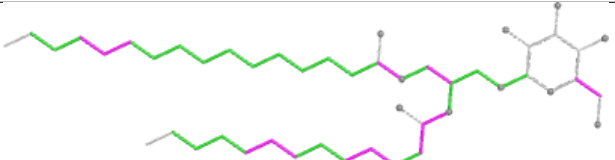
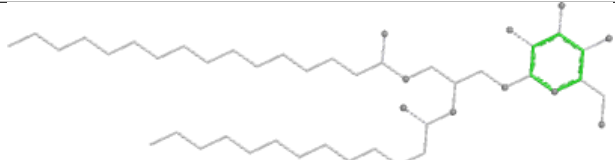


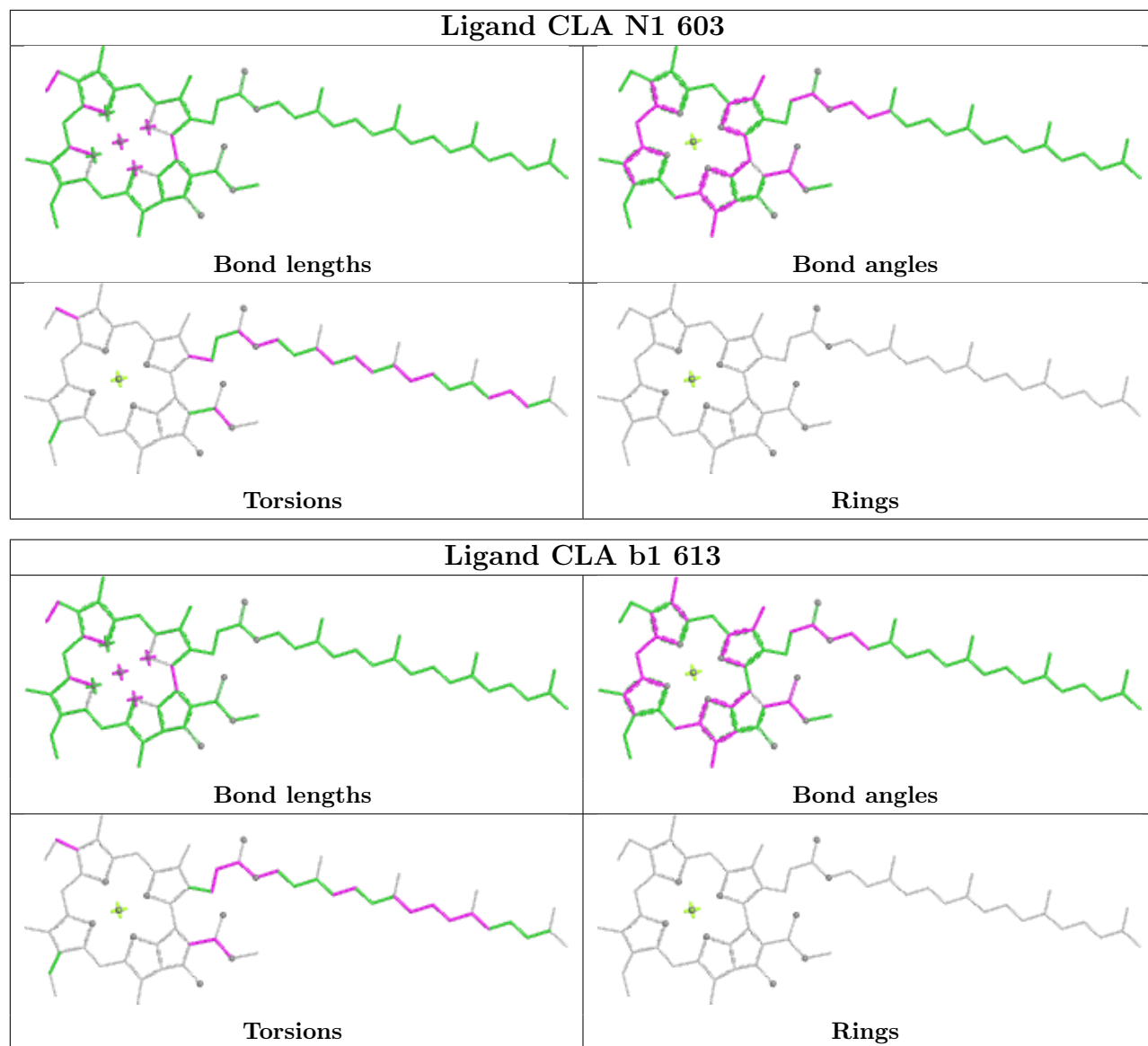


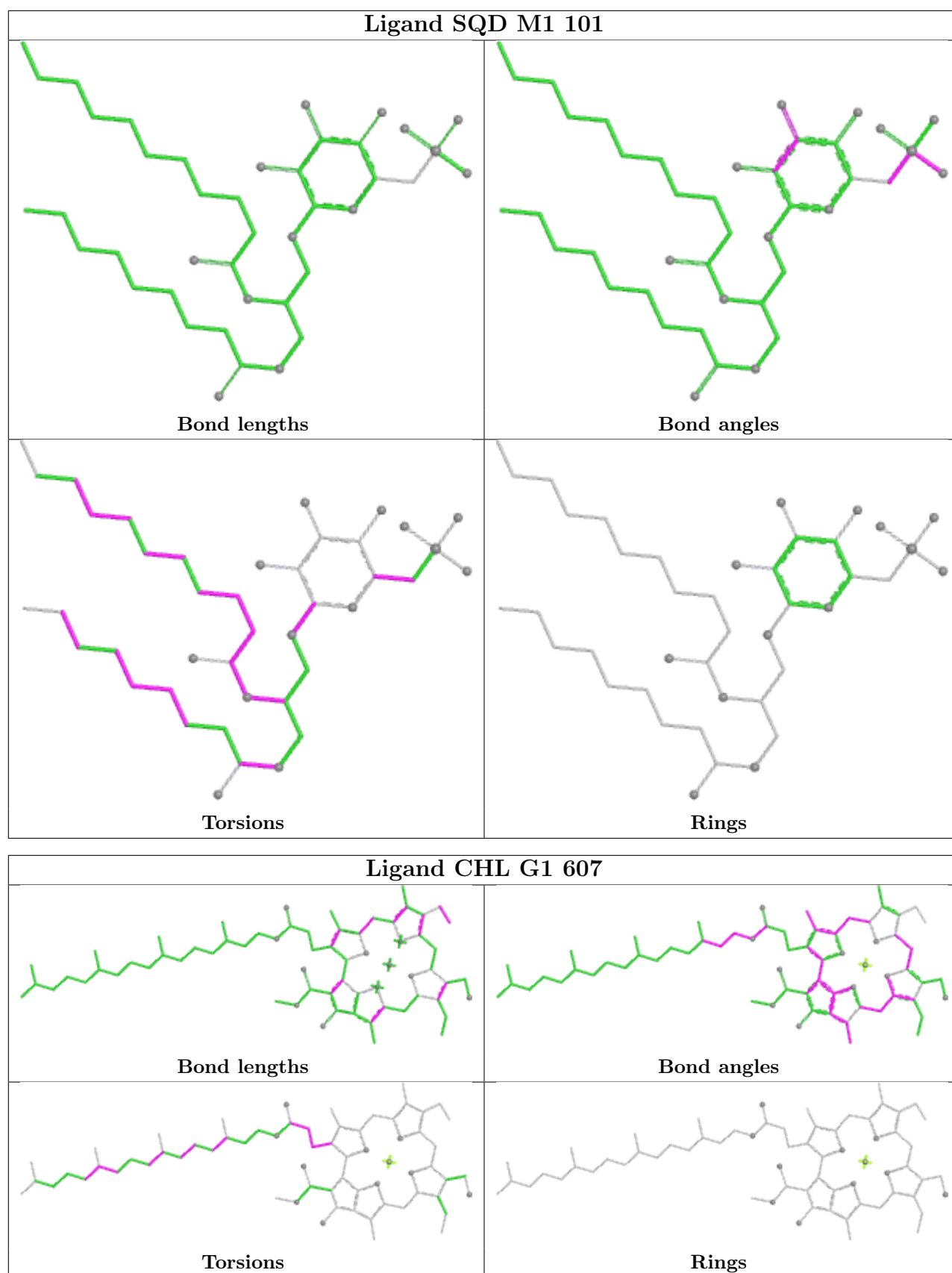


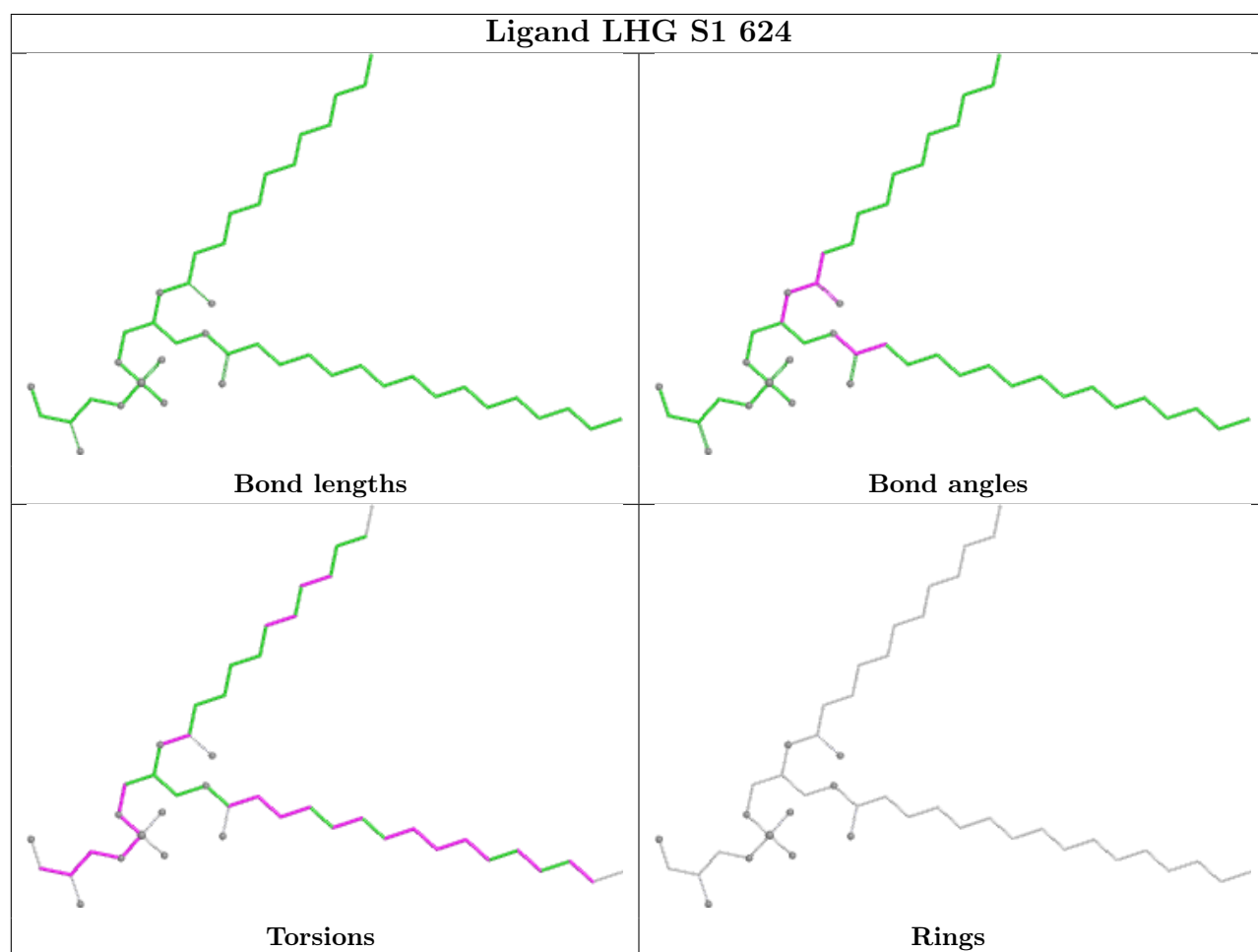
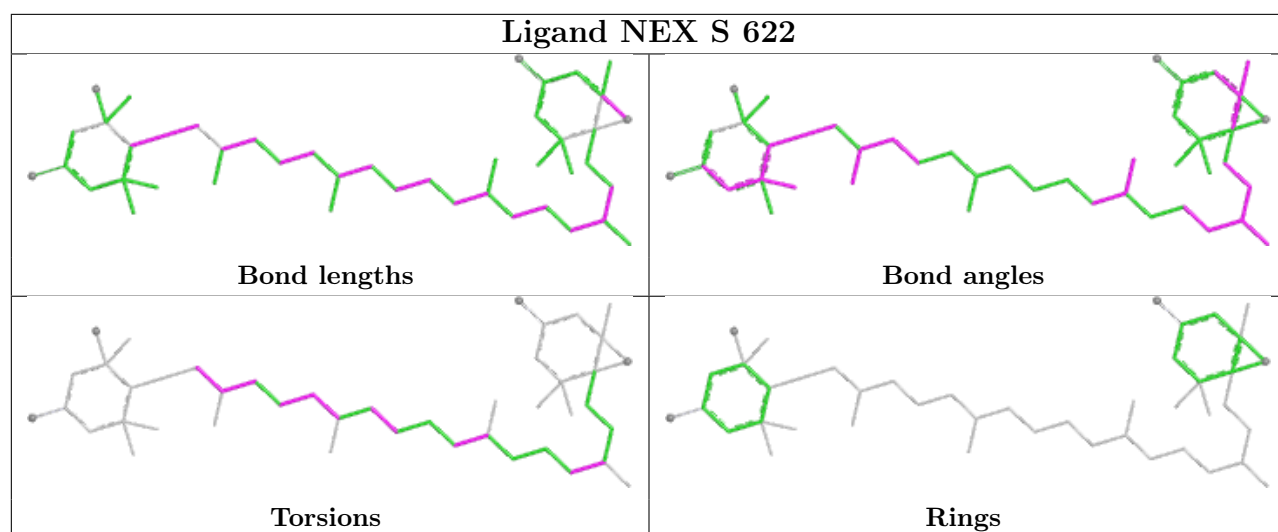




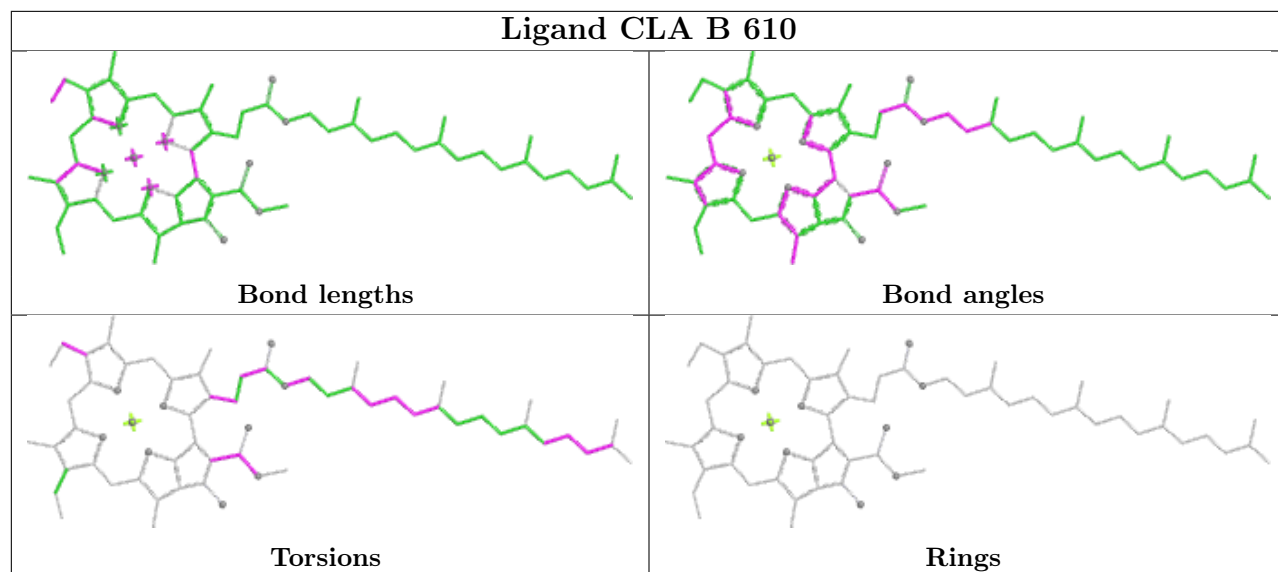
Ligand CHL Y 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand RRX h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG h1 102	
 Bond lengths	 Bond angles
 Torsions	 Rings



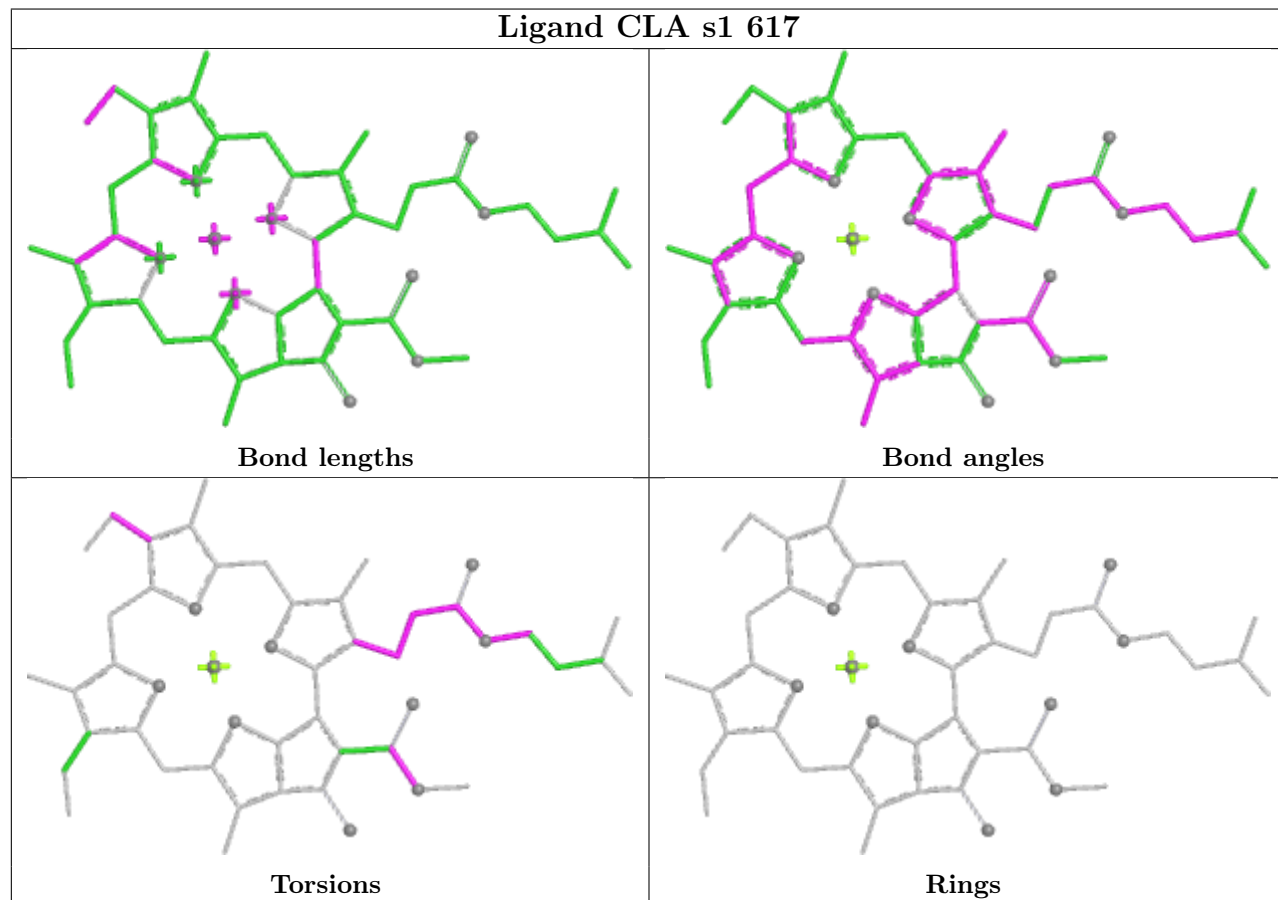




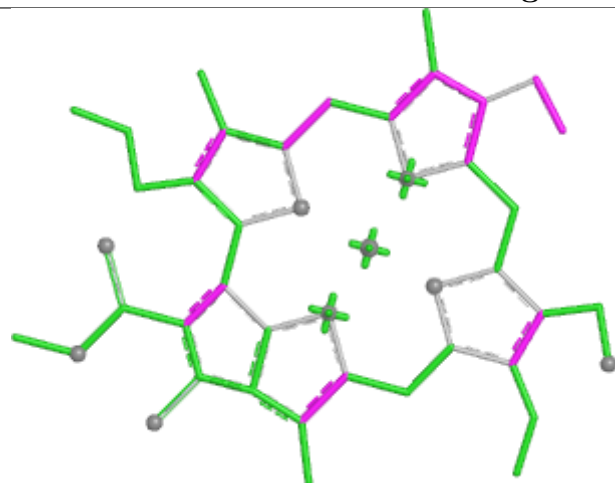
Ligand CLA B 610



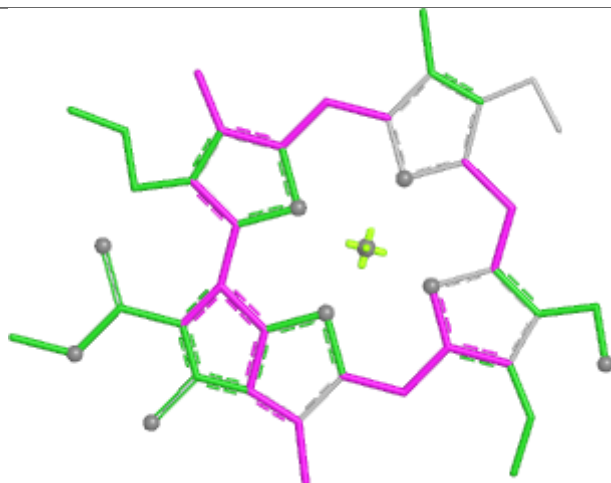
Ligand CLA s1 617



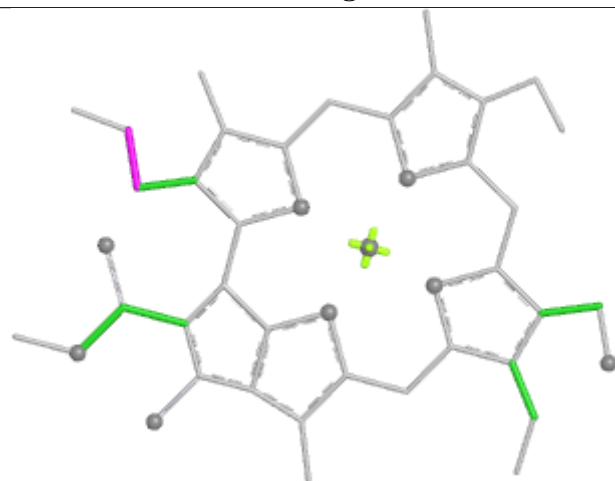
Ligand CHL r 606



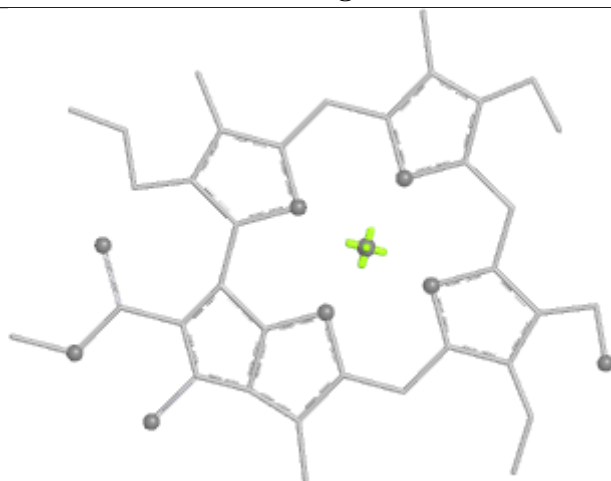
Bond lengths



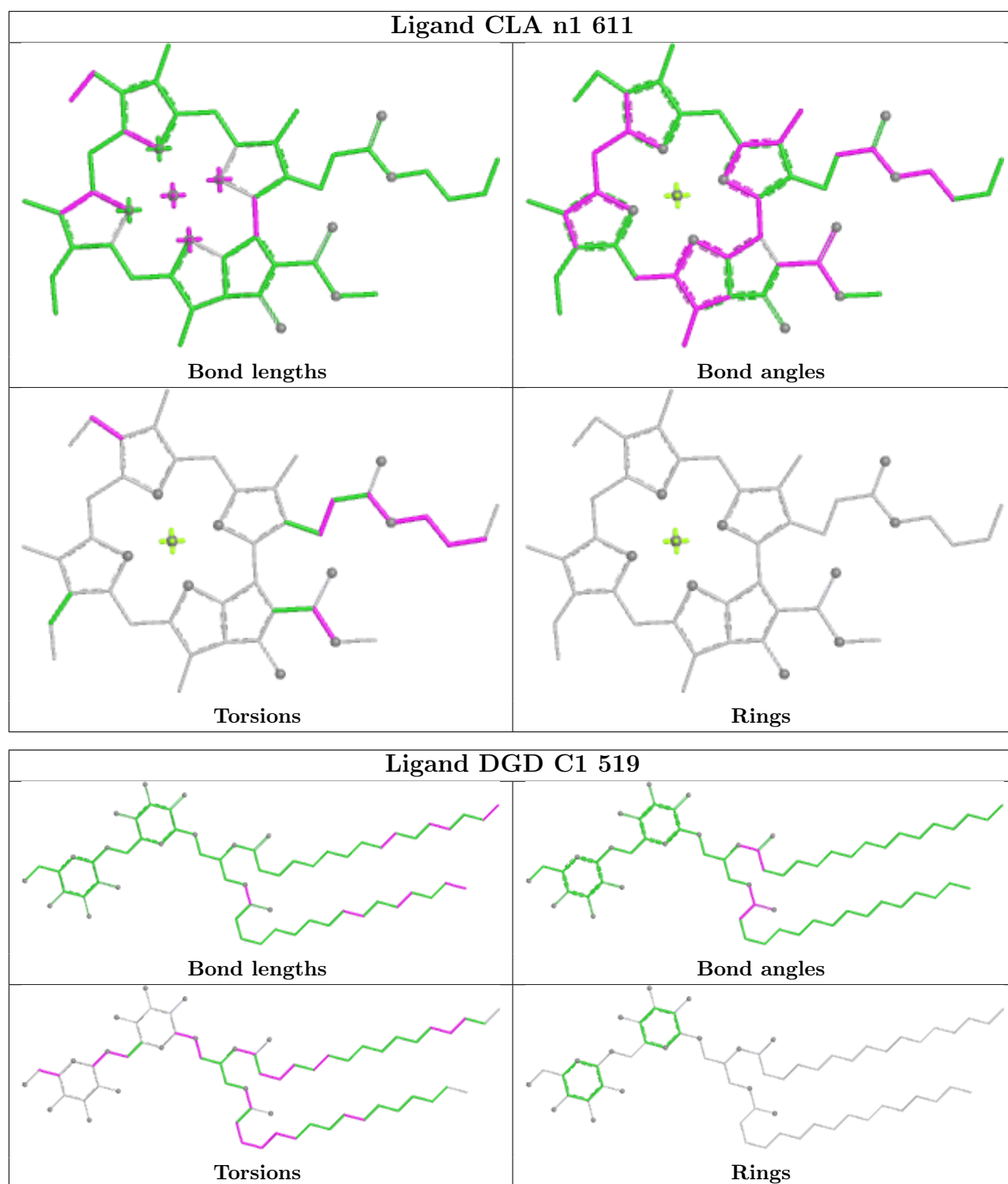
Bond angles

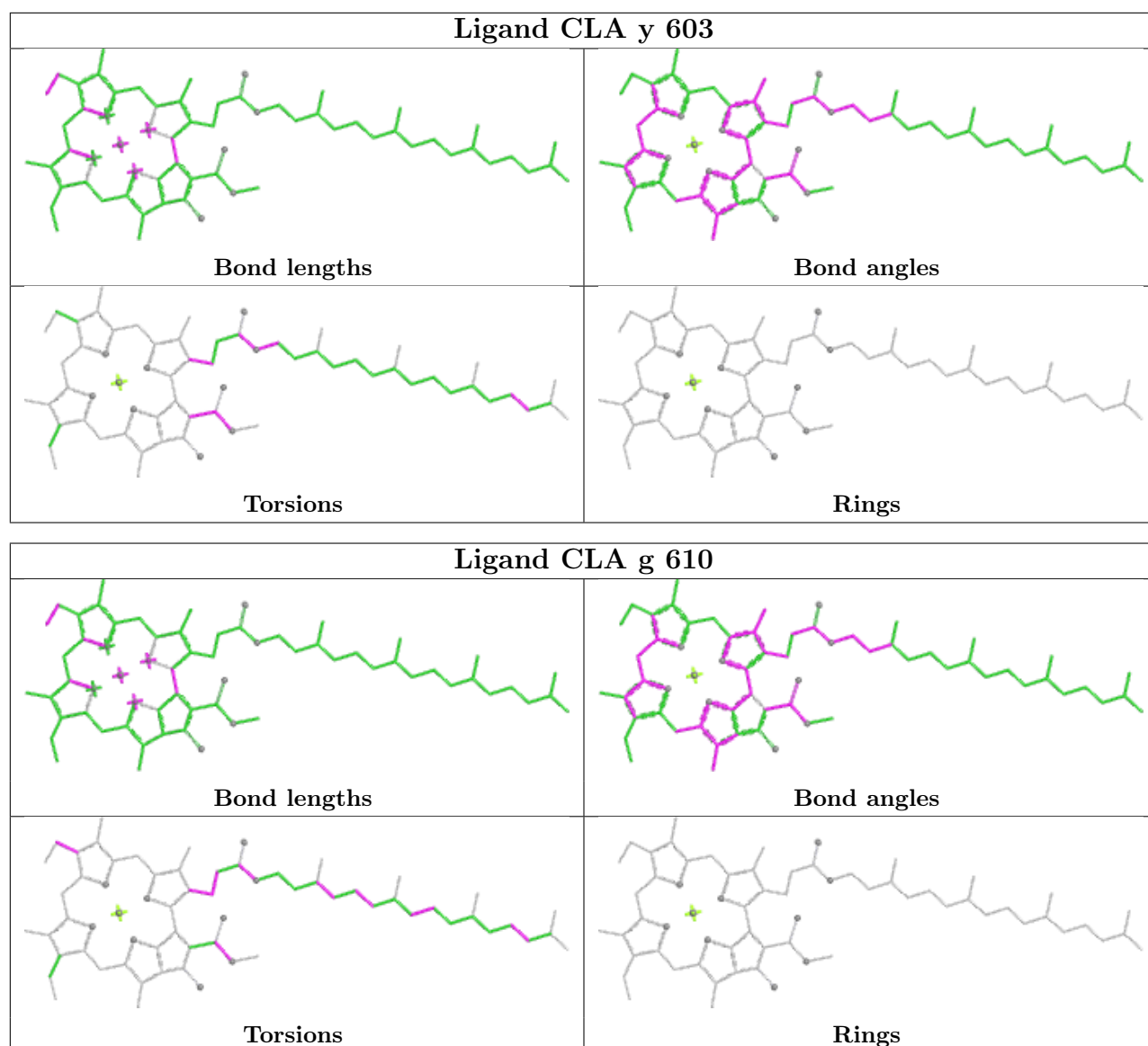


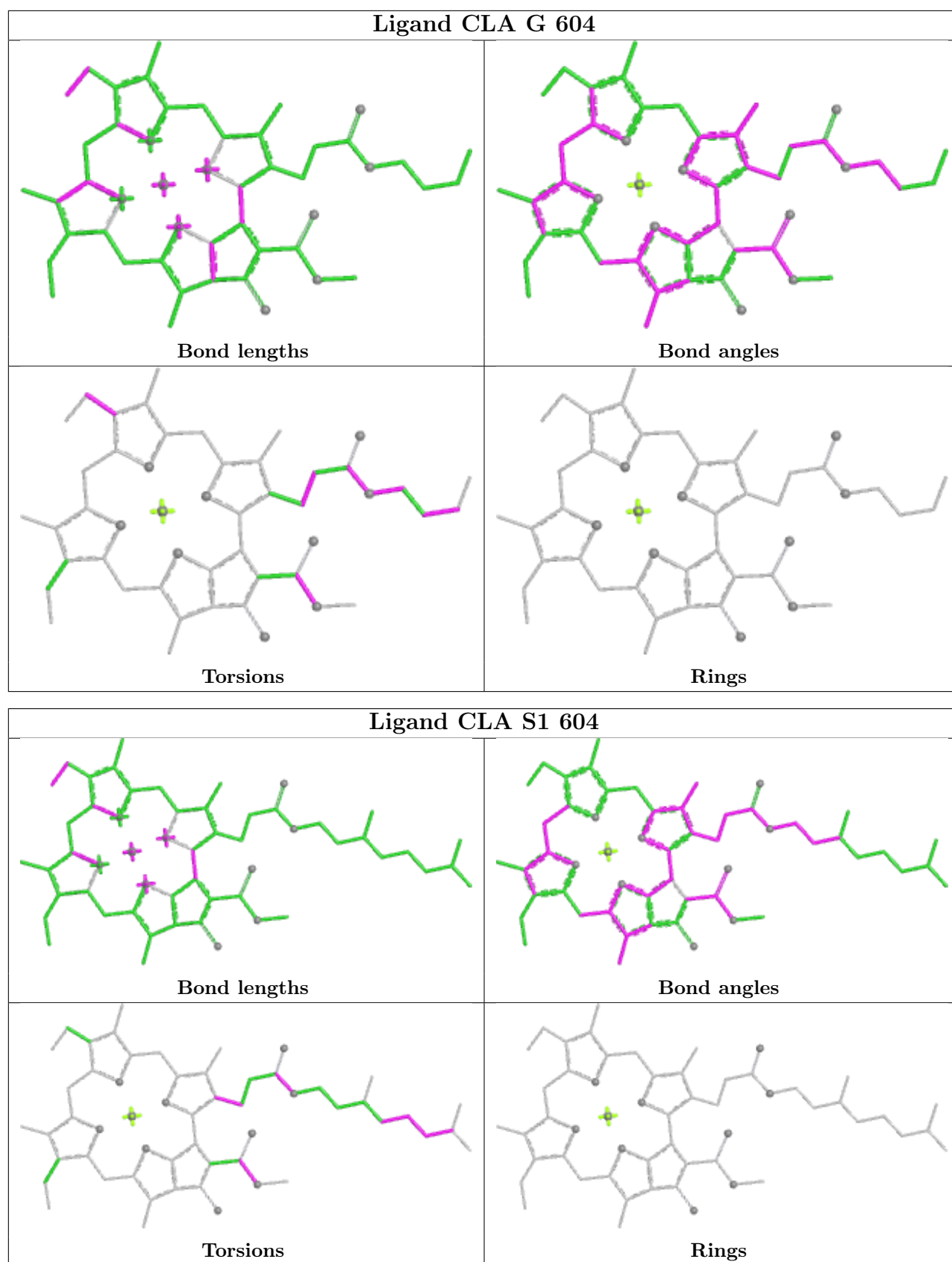
Torsions

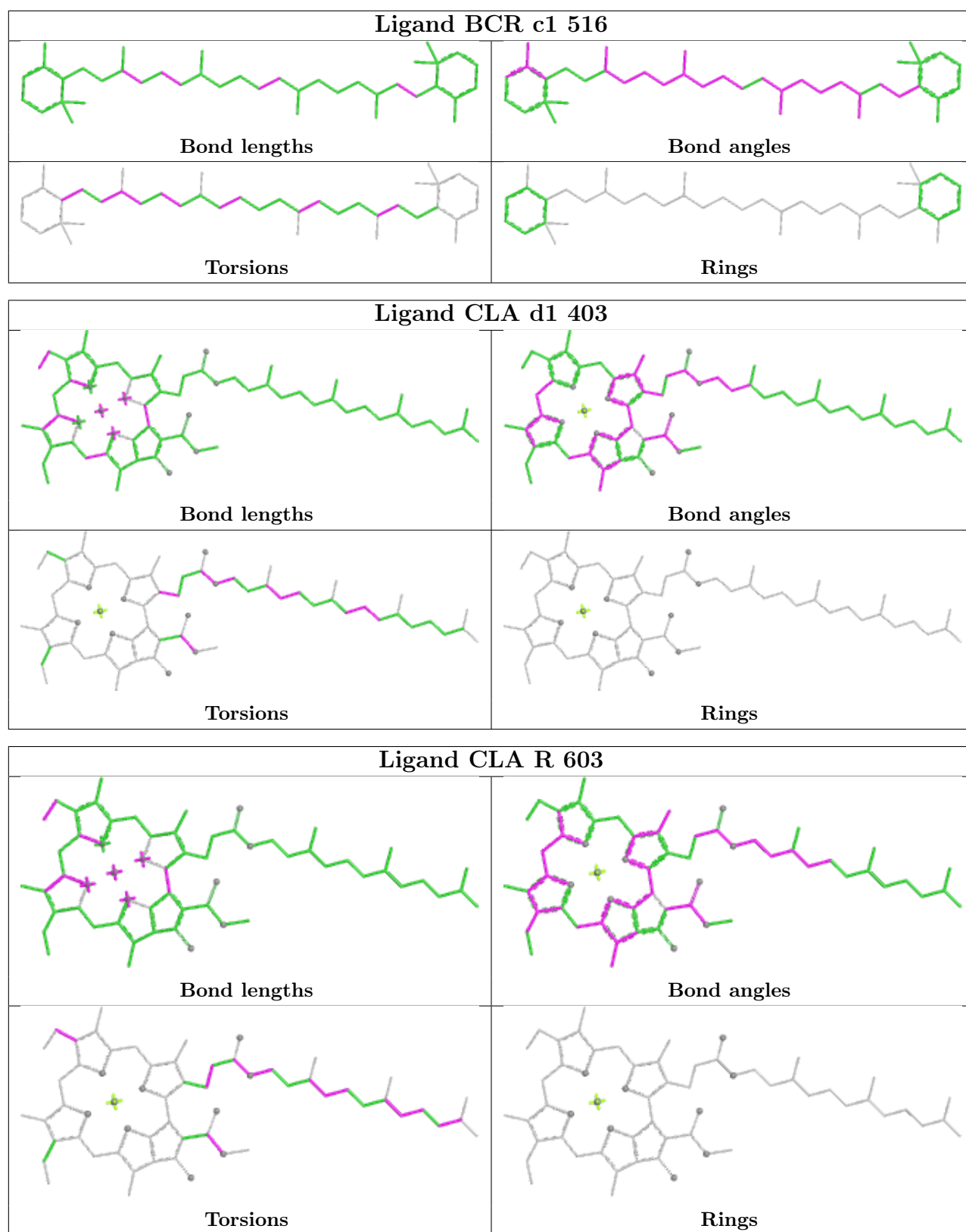


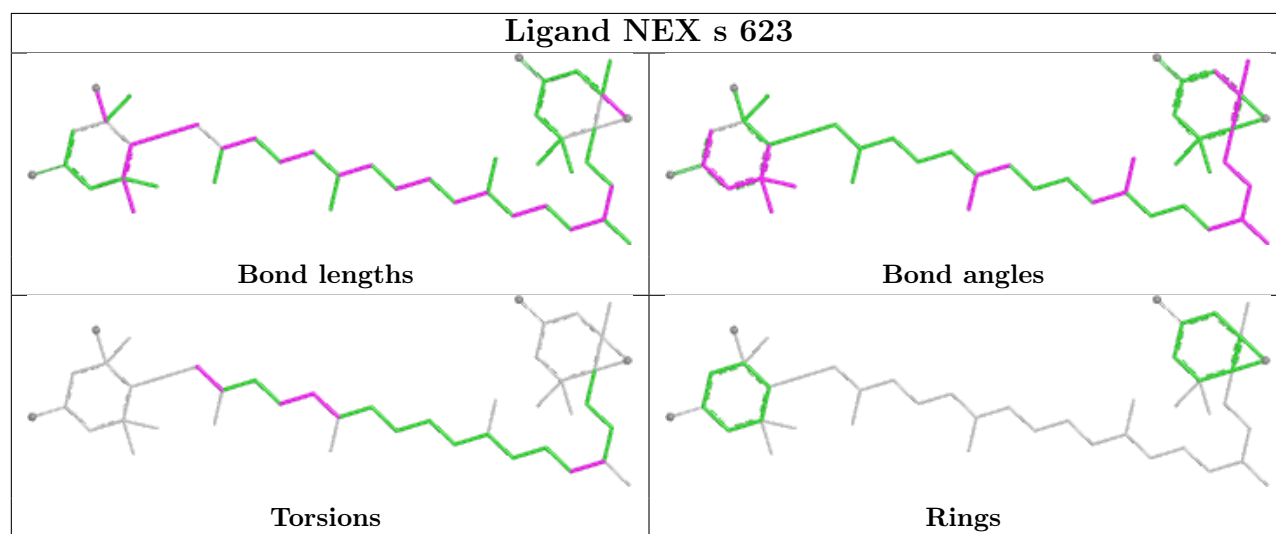
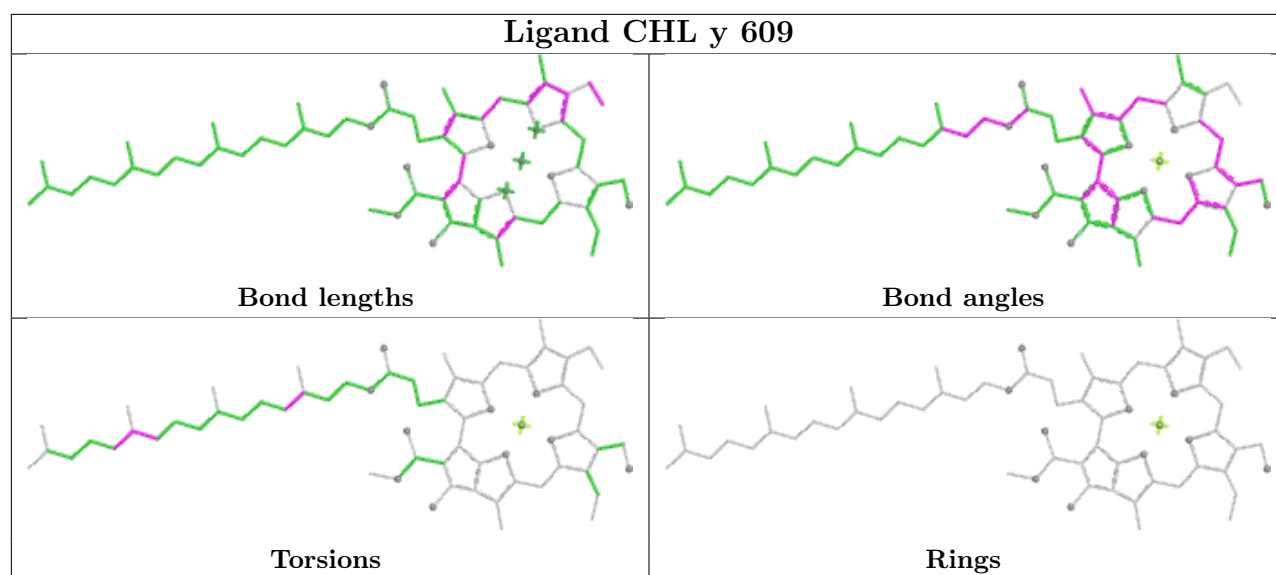
Rings

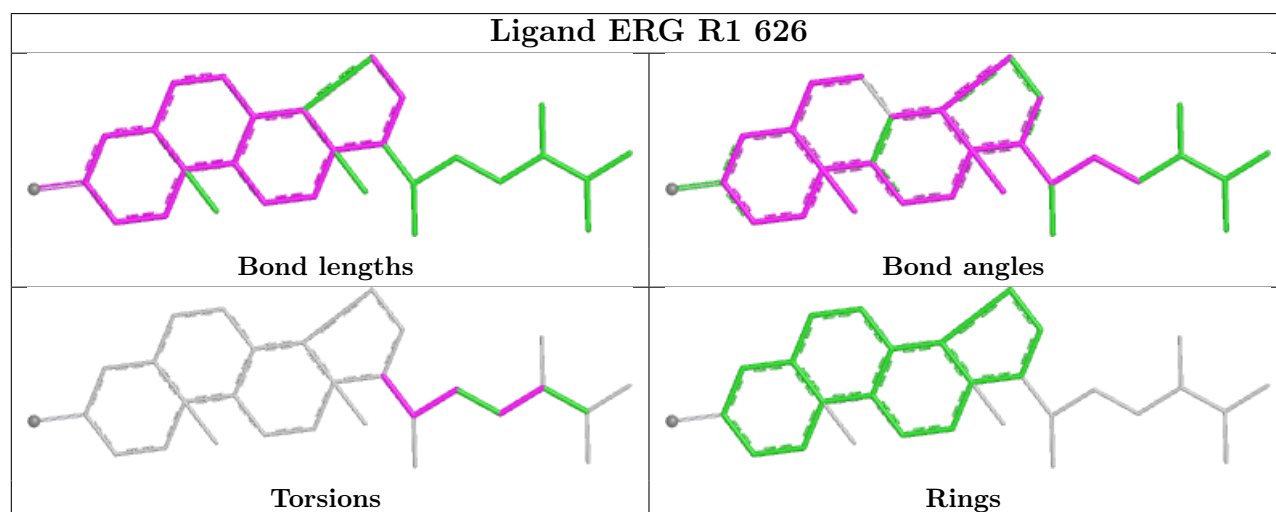
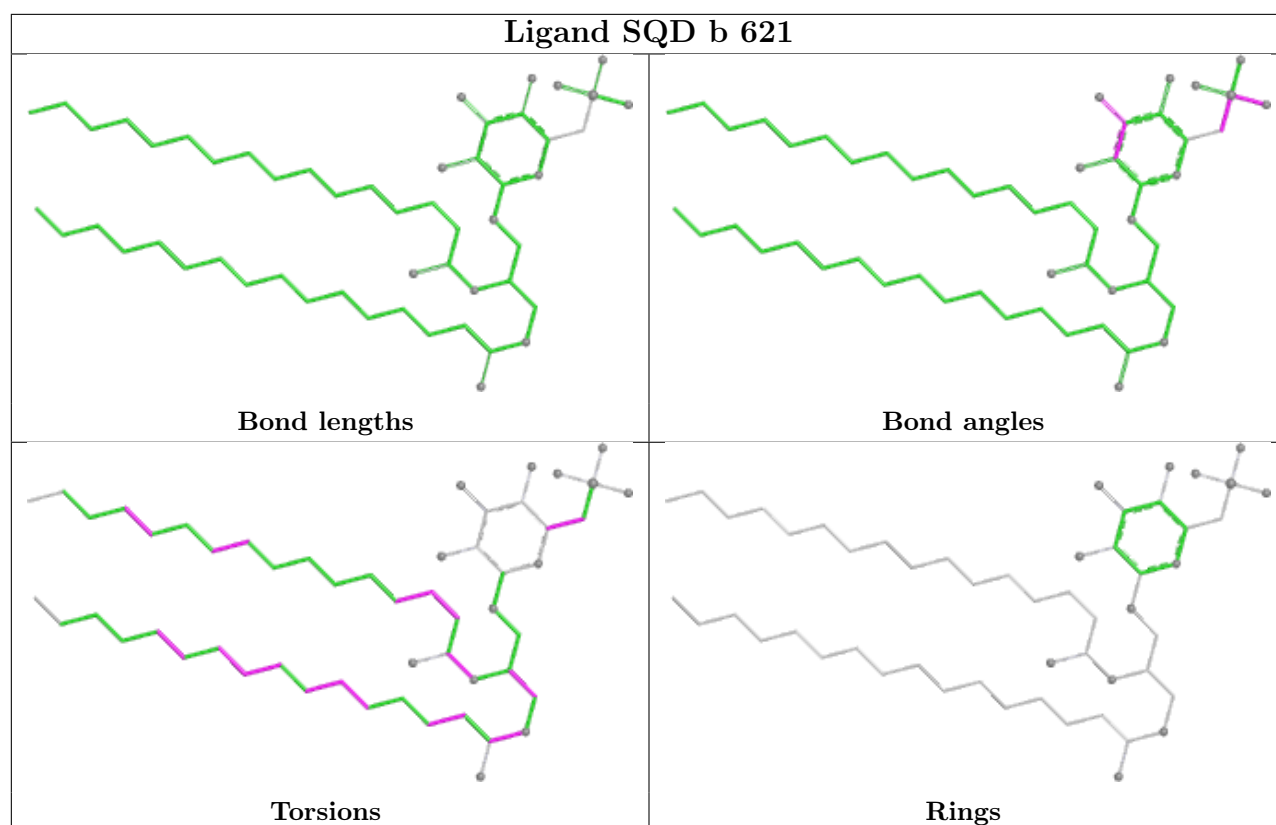


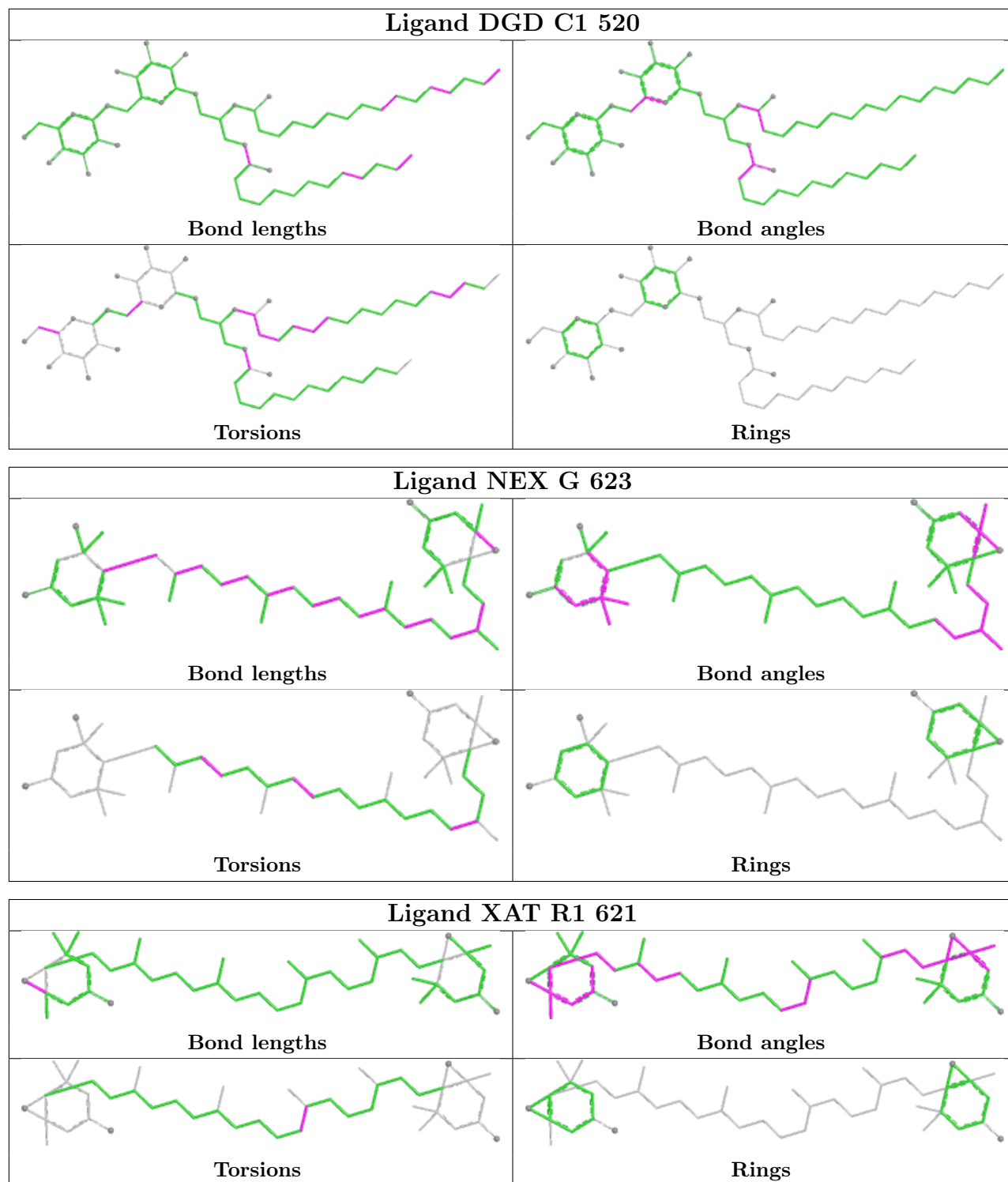


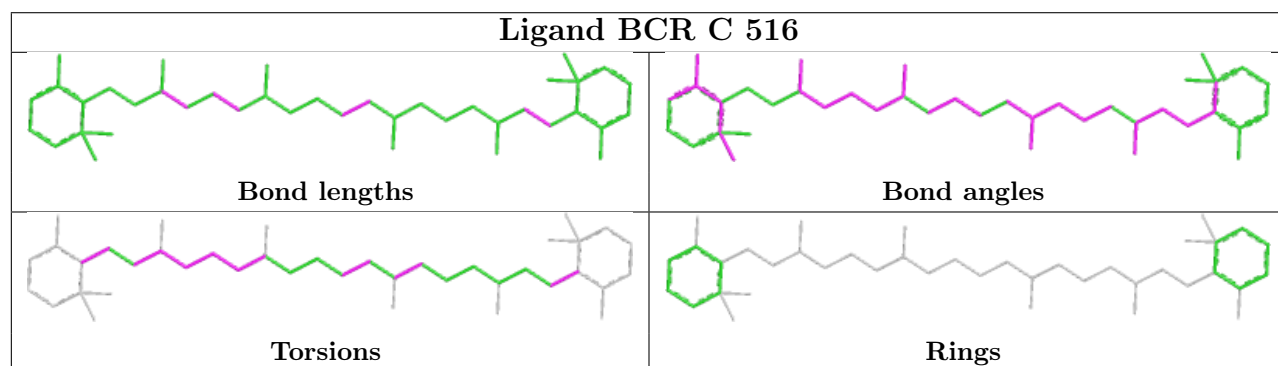
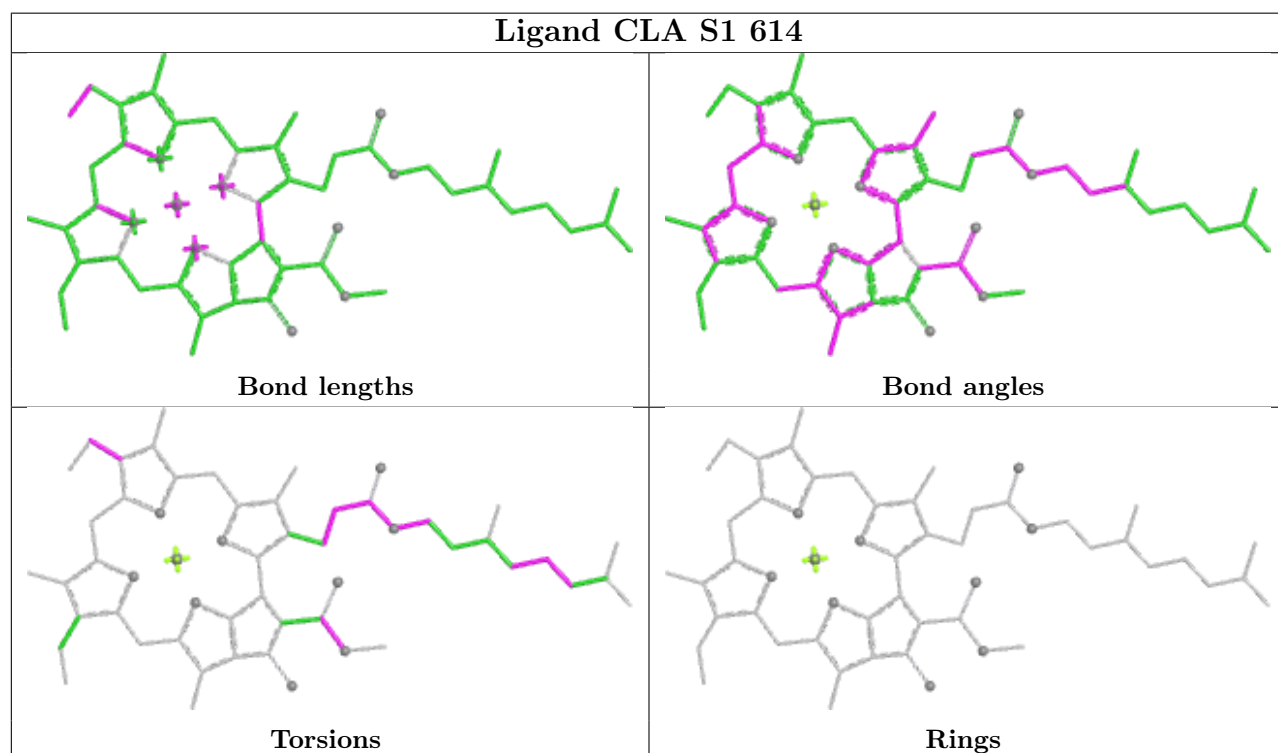
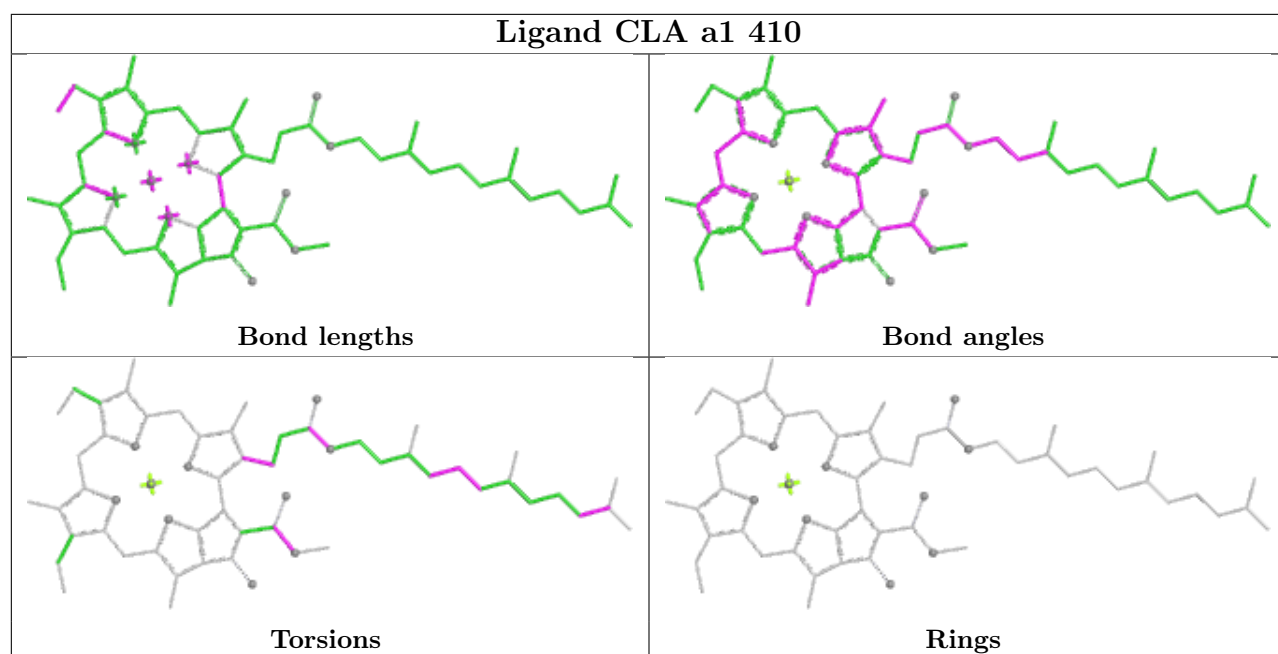


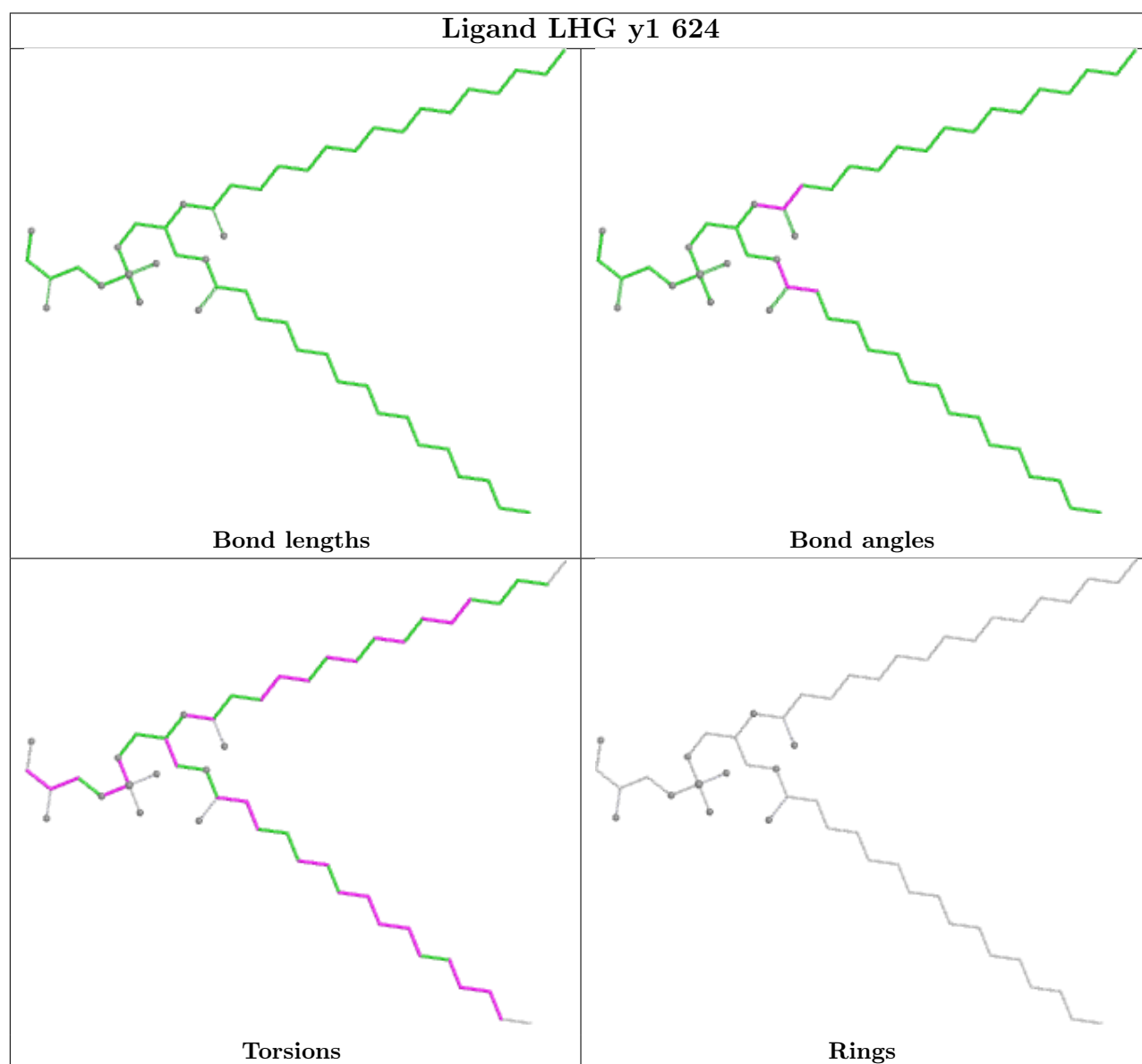
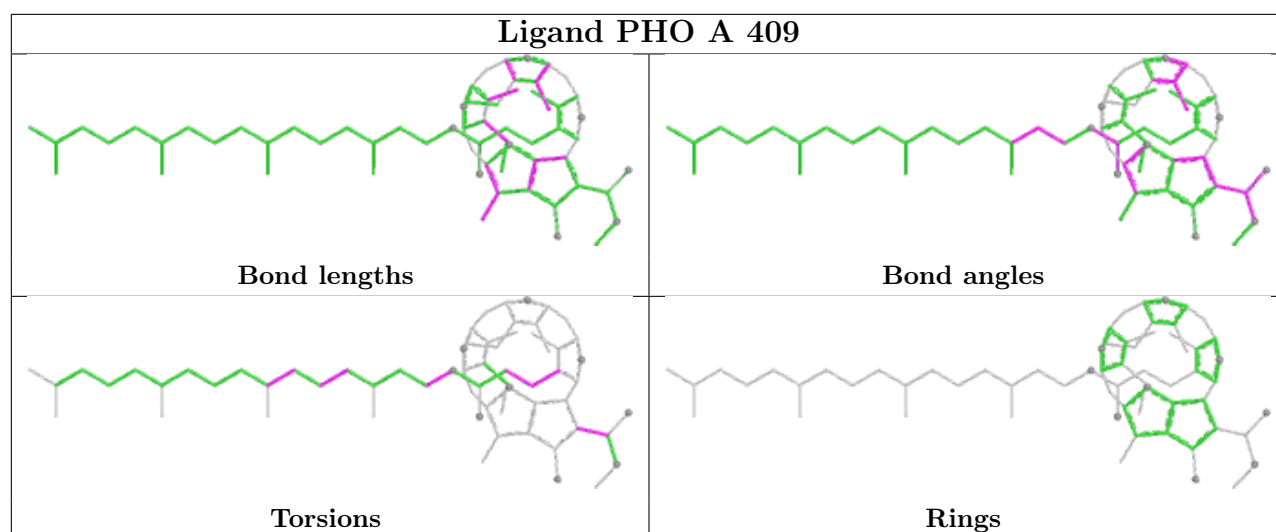


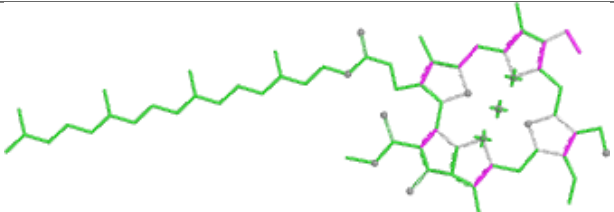
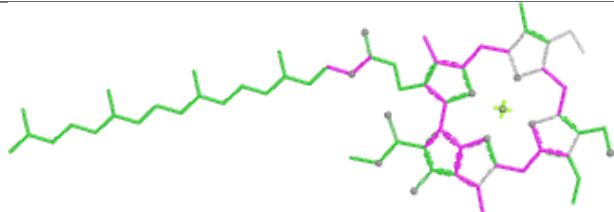
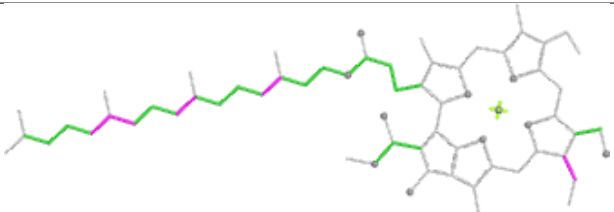
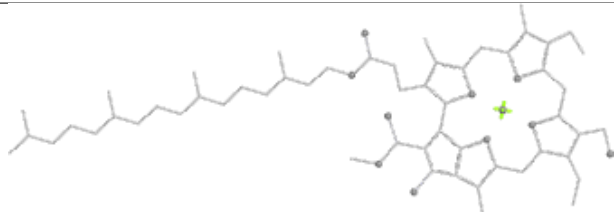


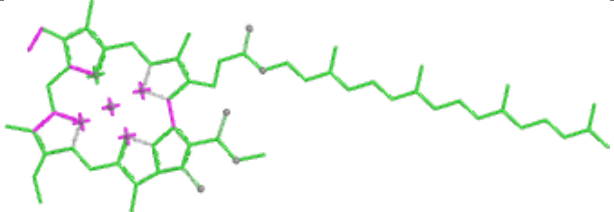
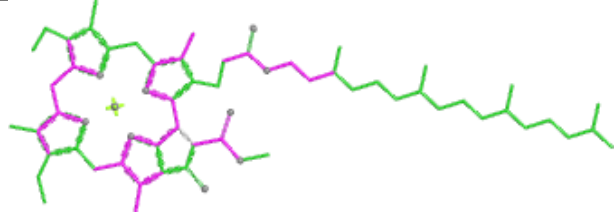
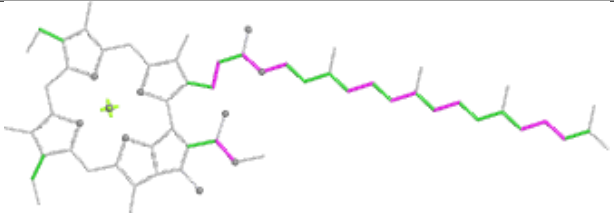
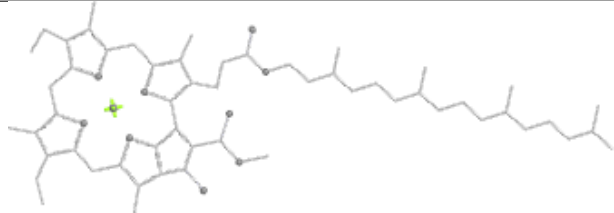


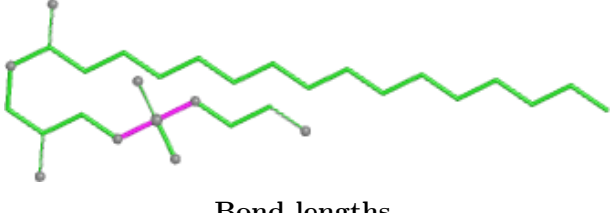
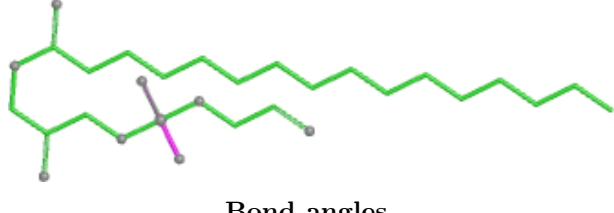
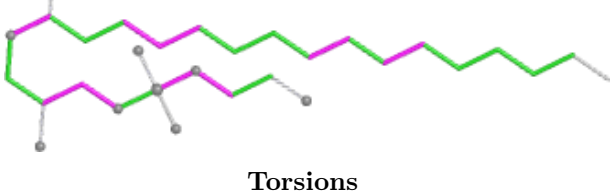
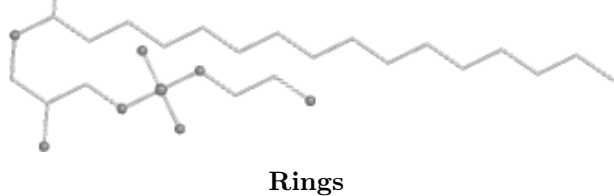


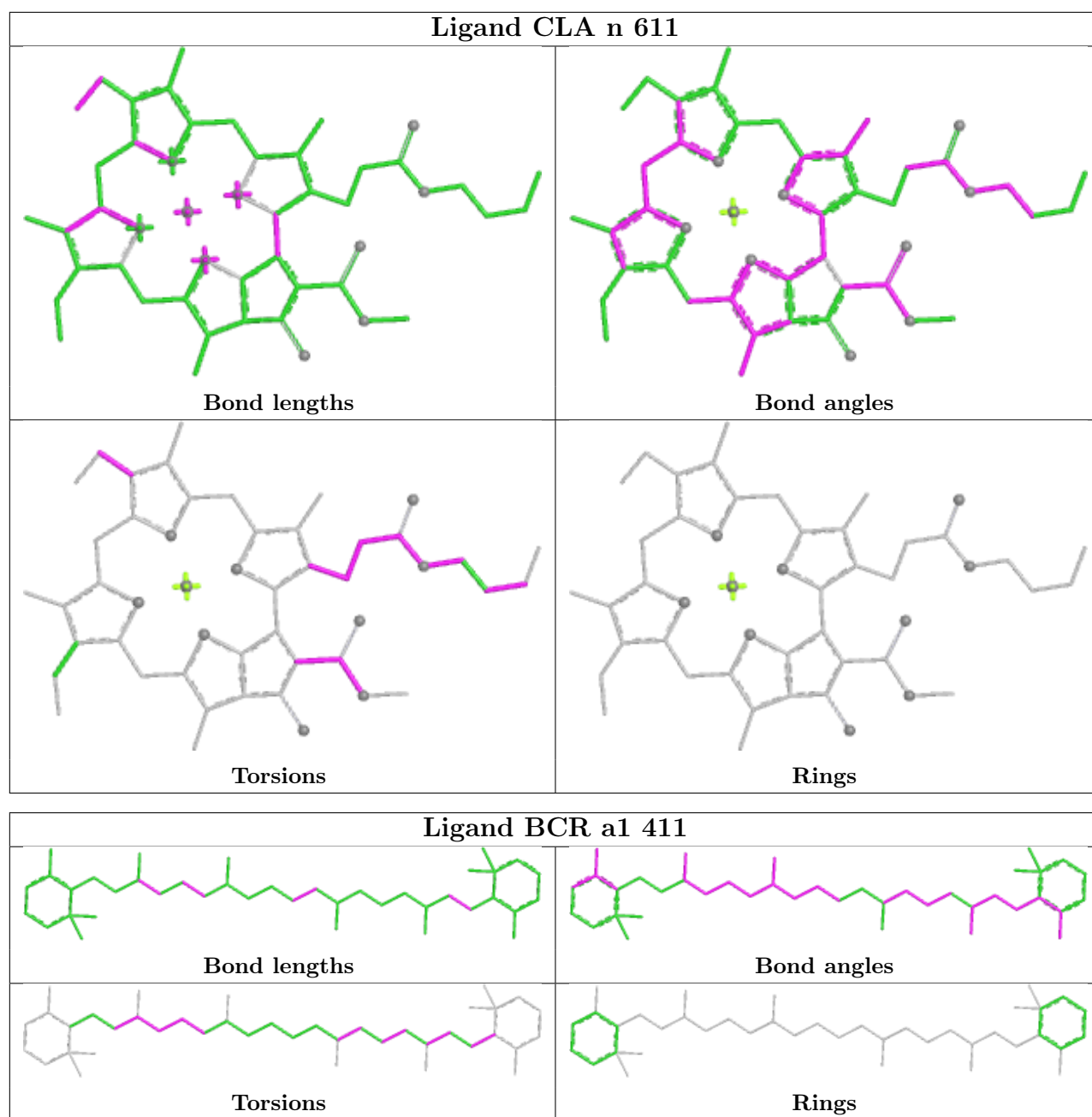




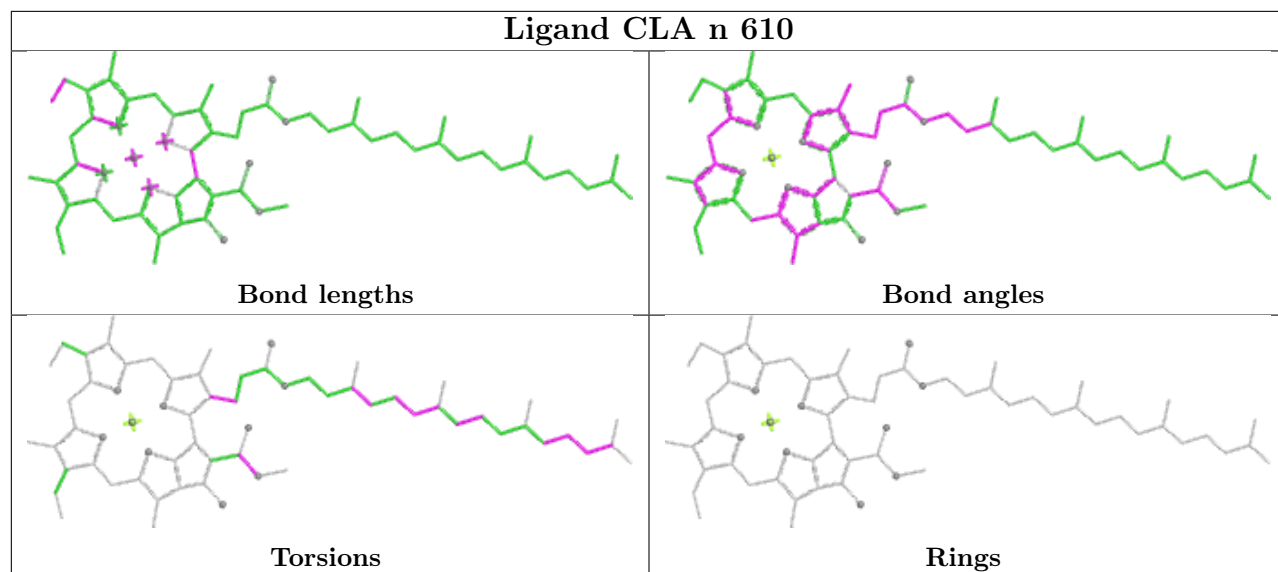
Ligand CHL G1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b1 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

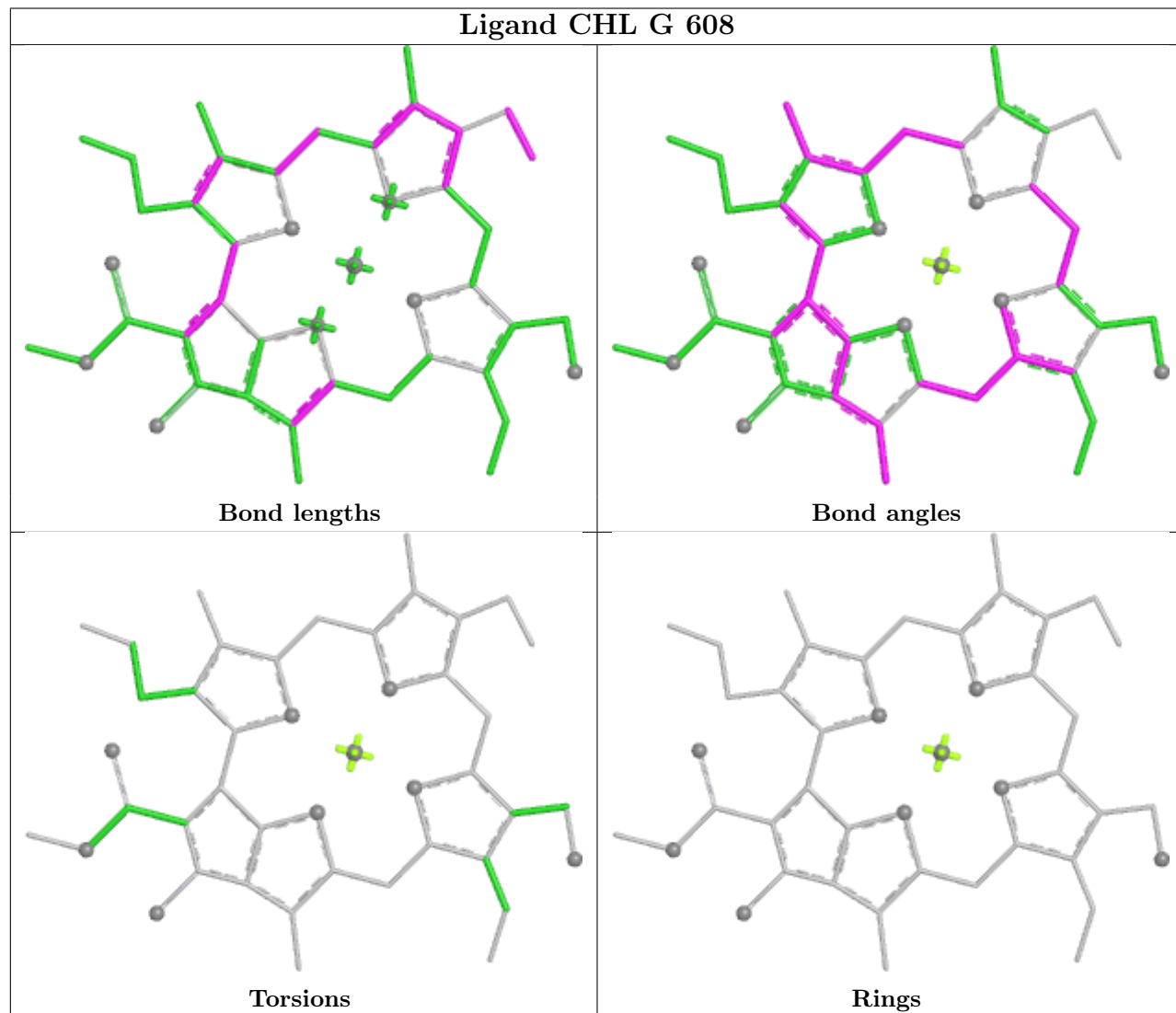
Ligand LPX S 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

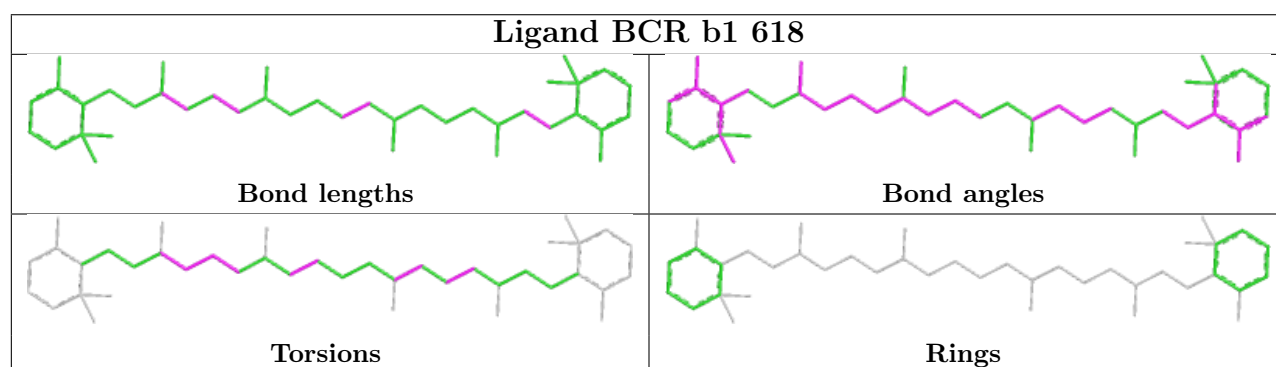
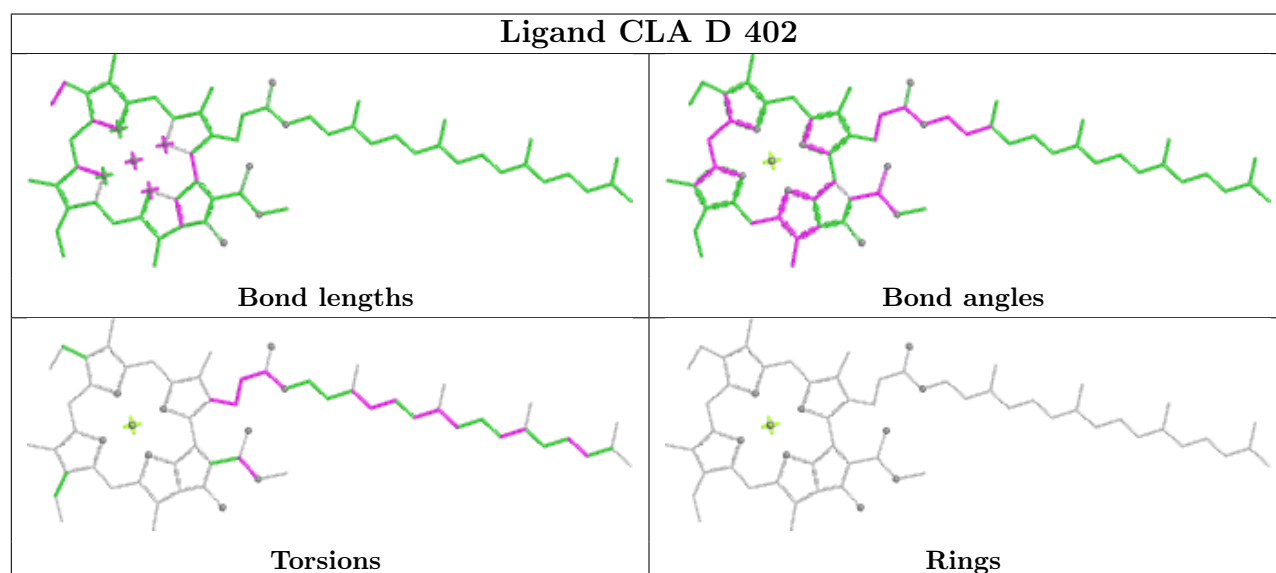
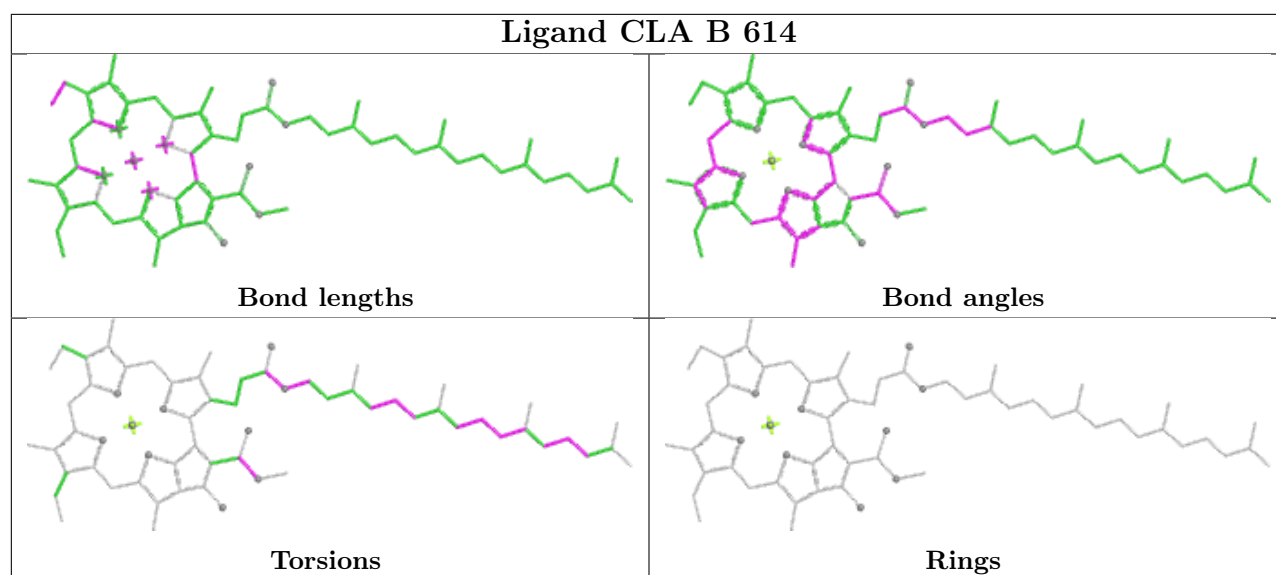


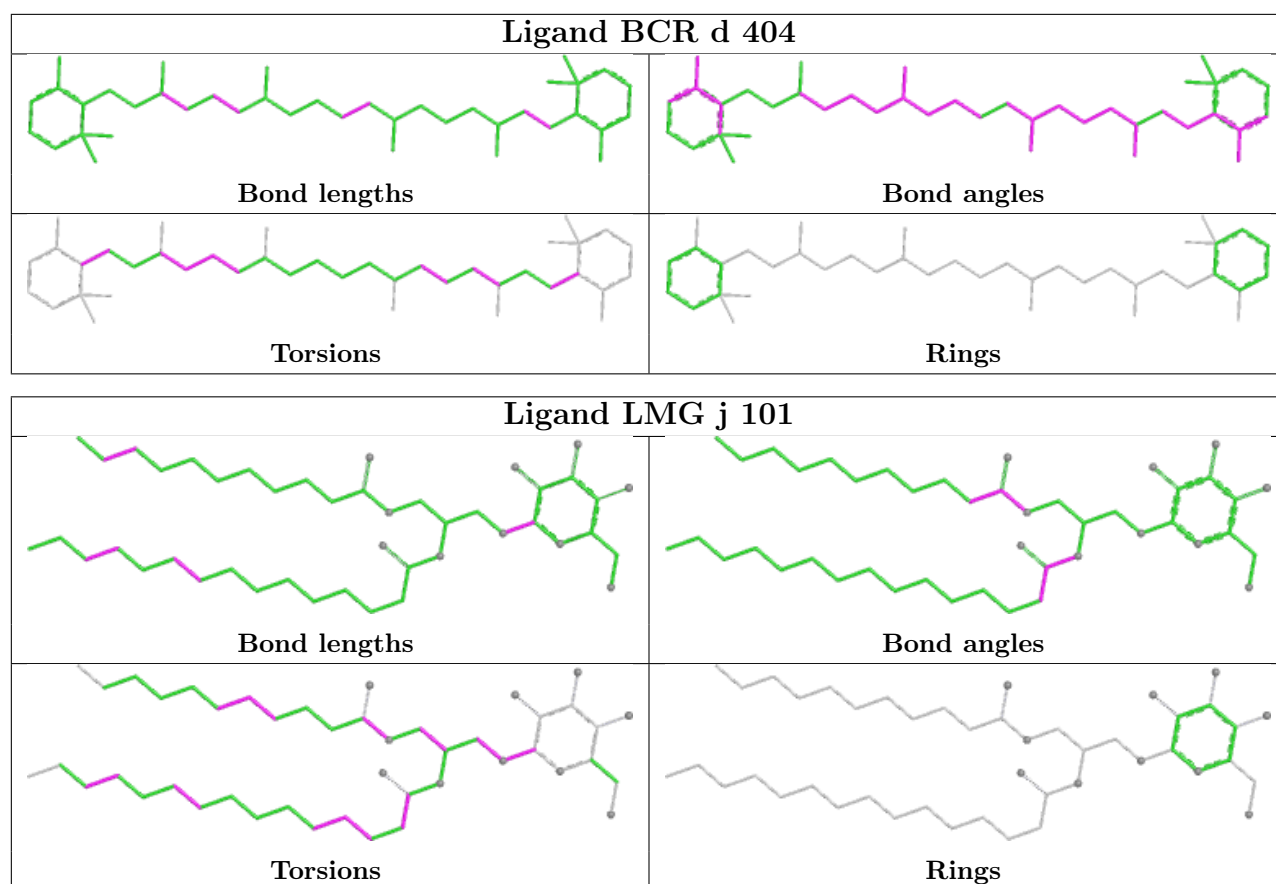
Ligand CLA n 610

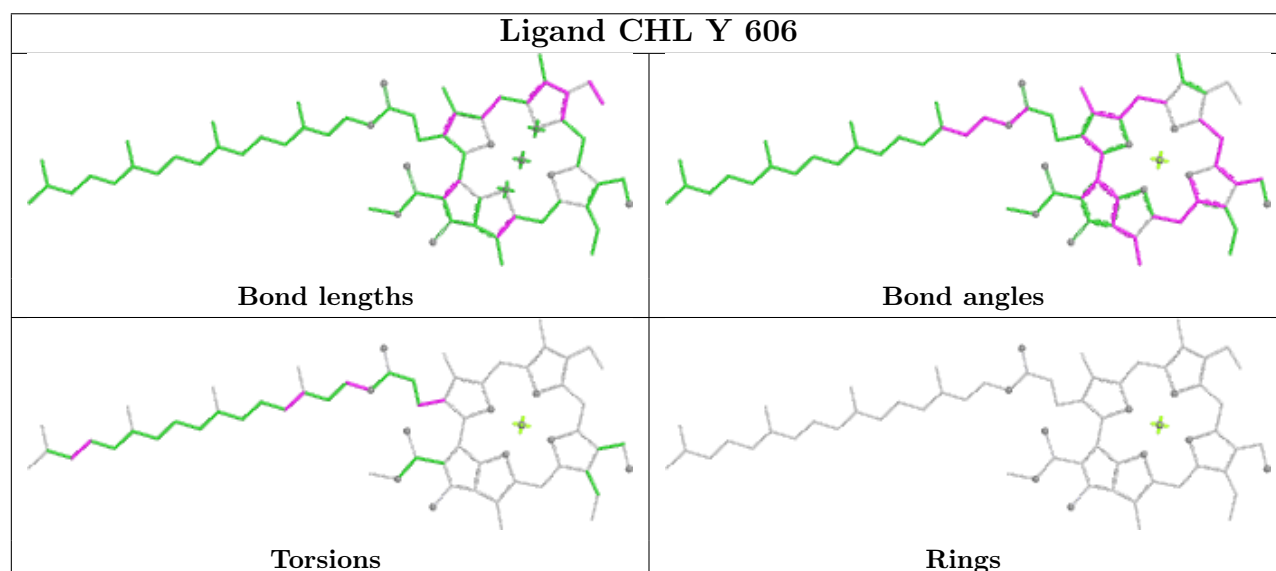
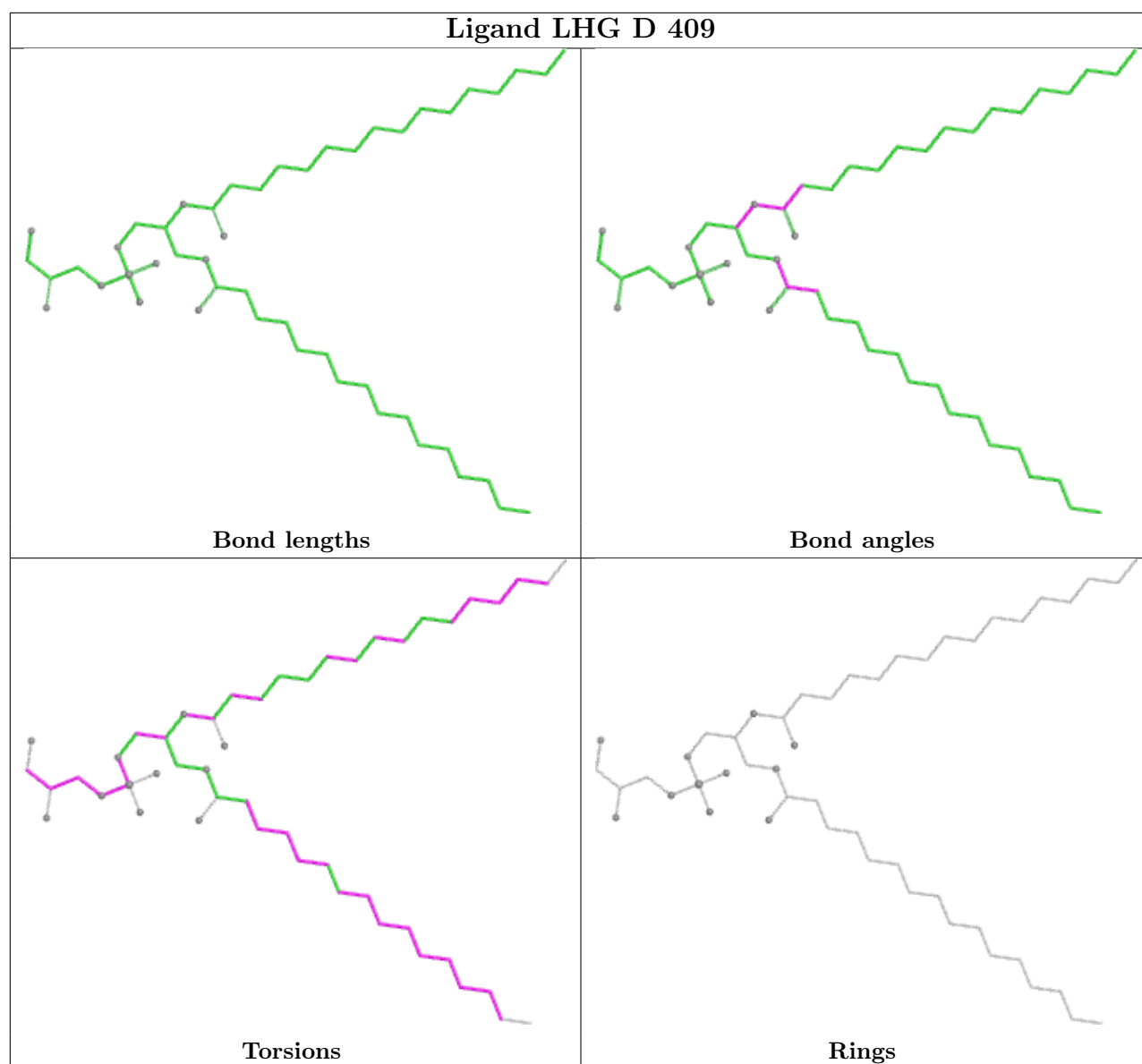


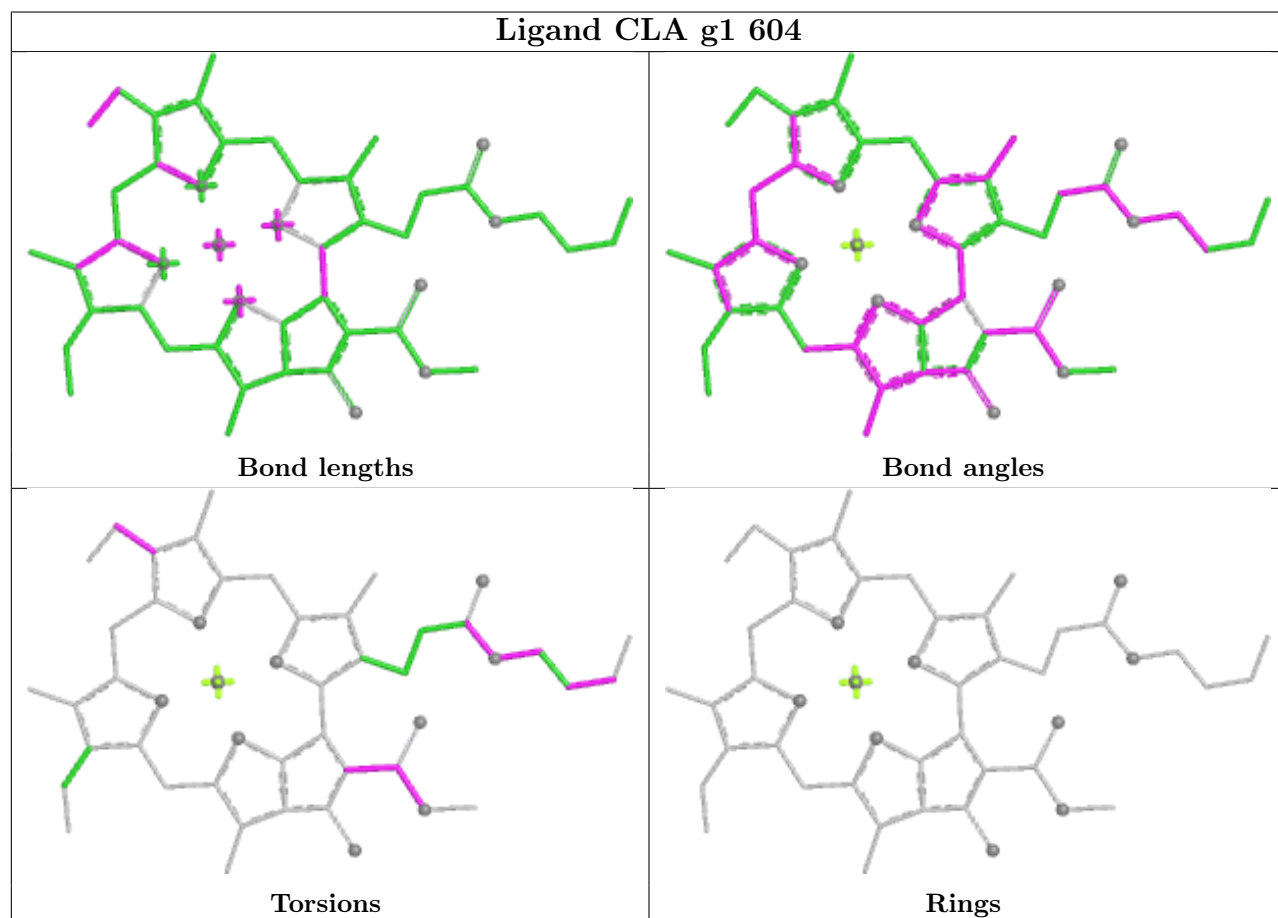
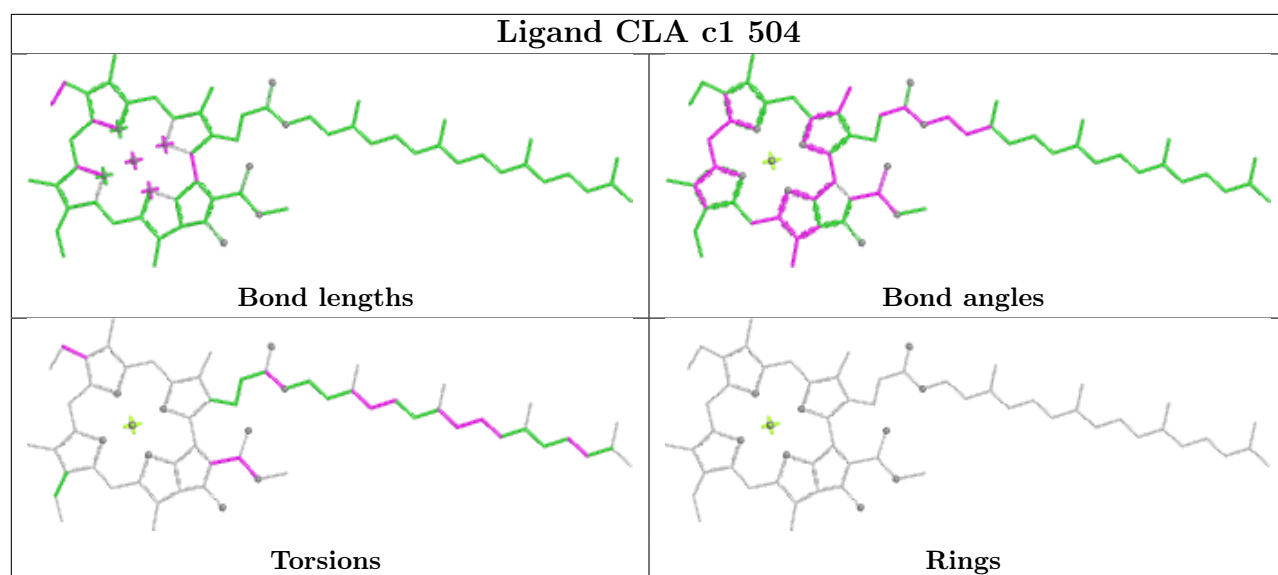
Ligand CHL G 608

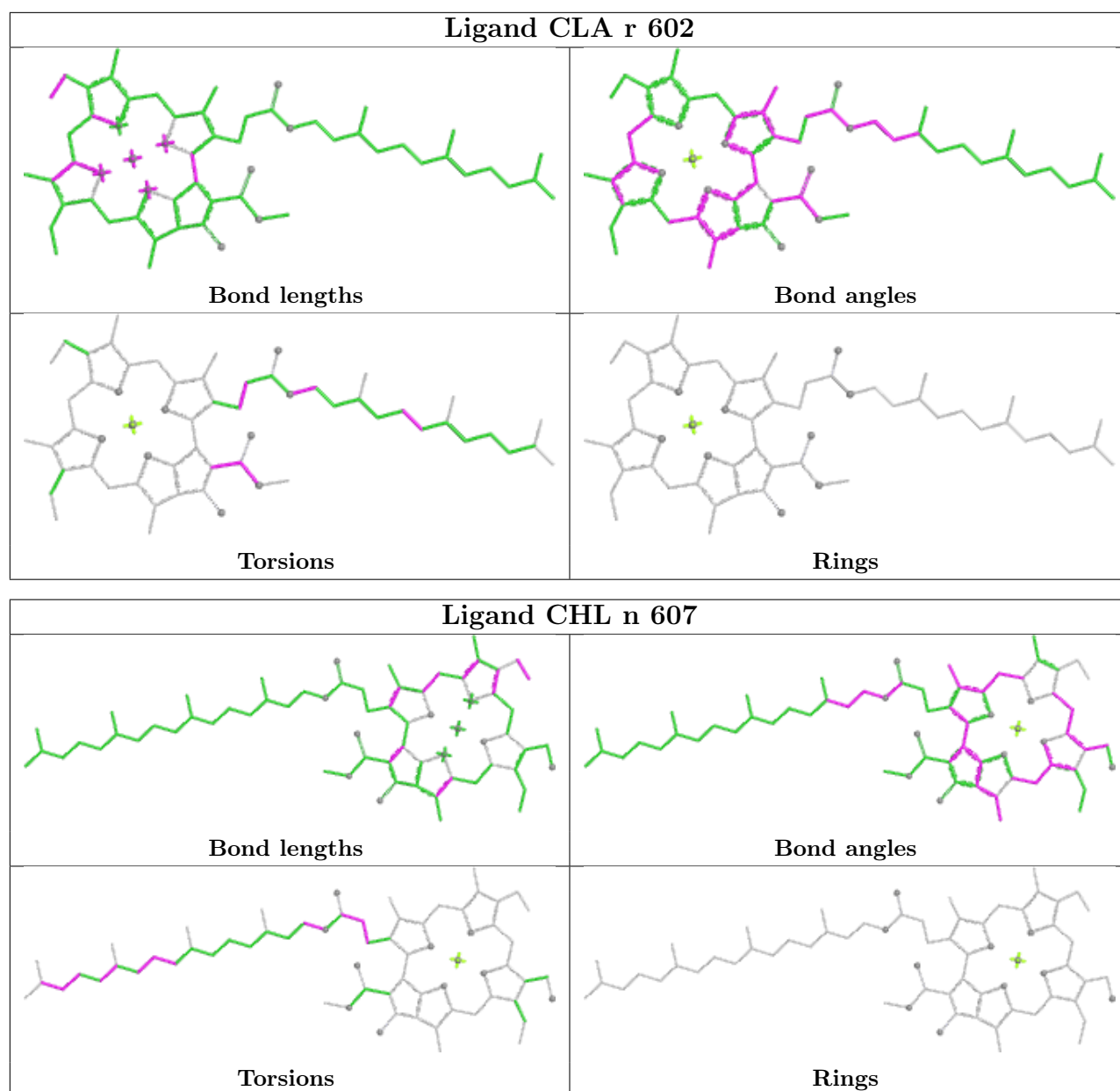


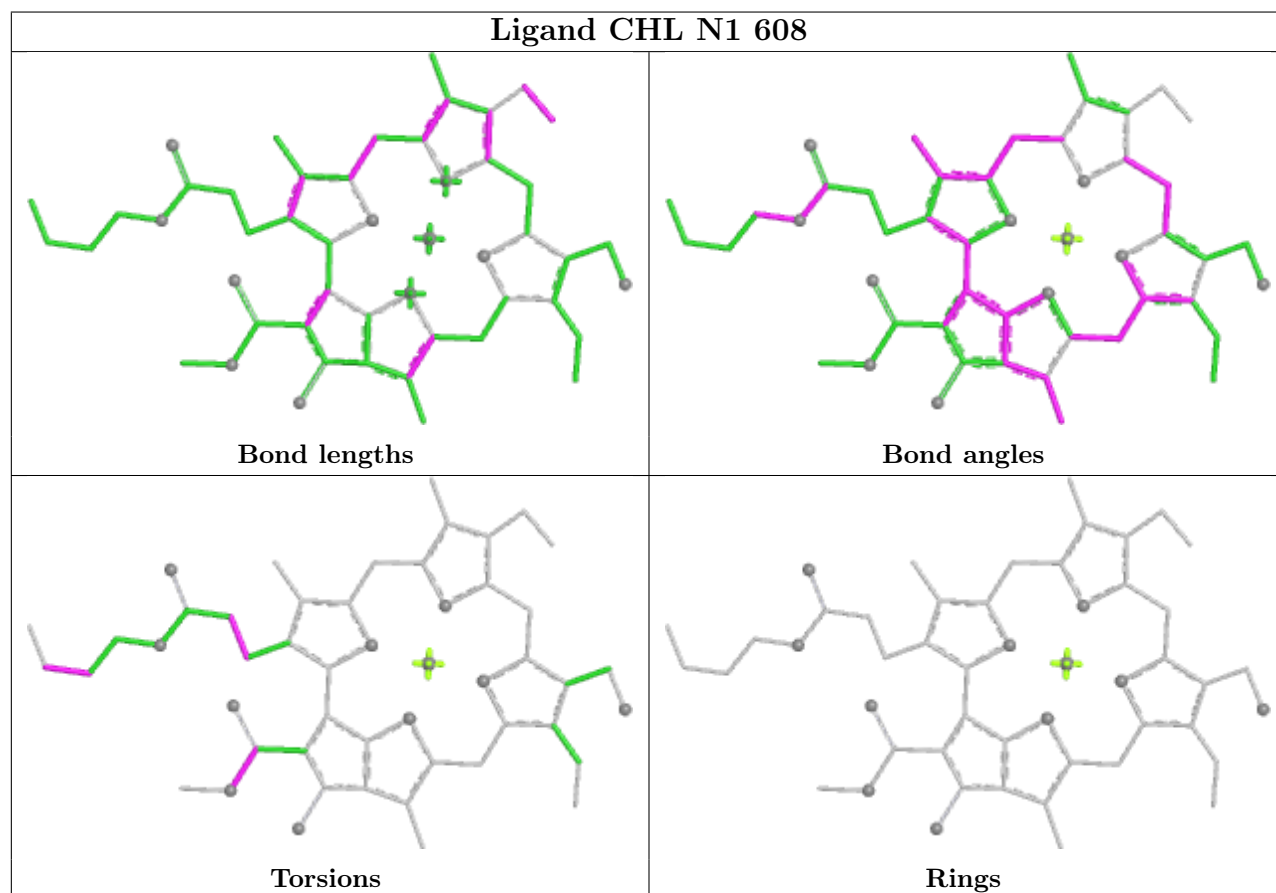
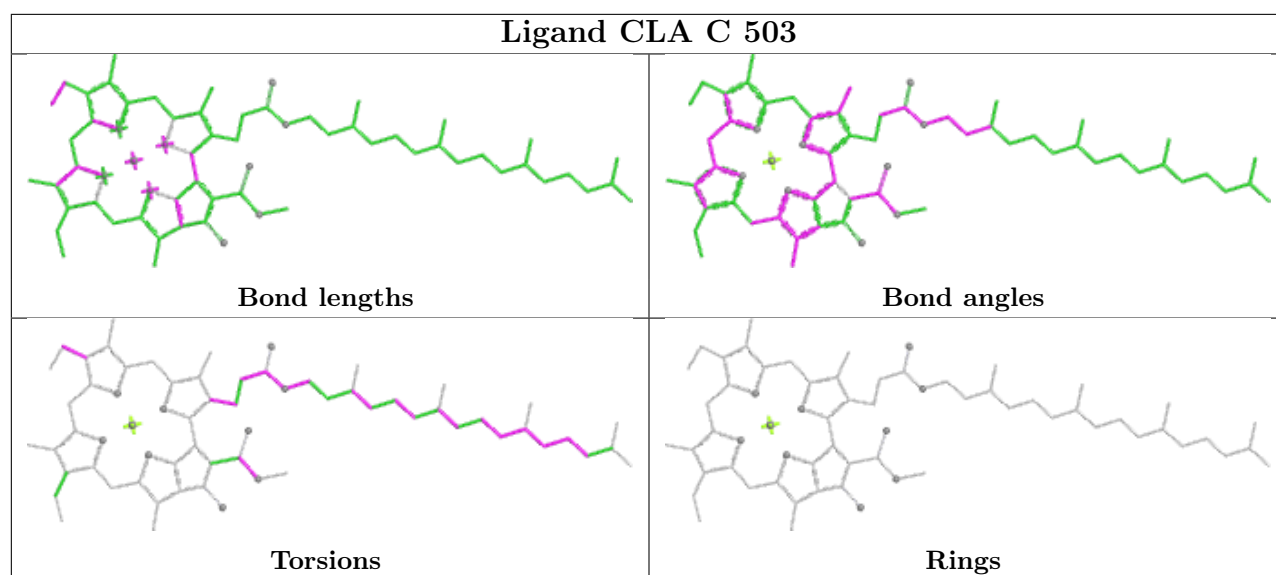


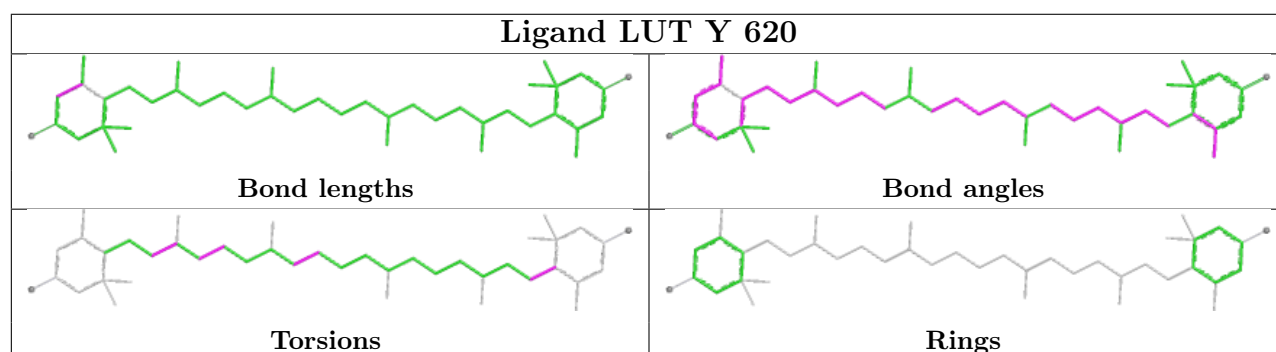
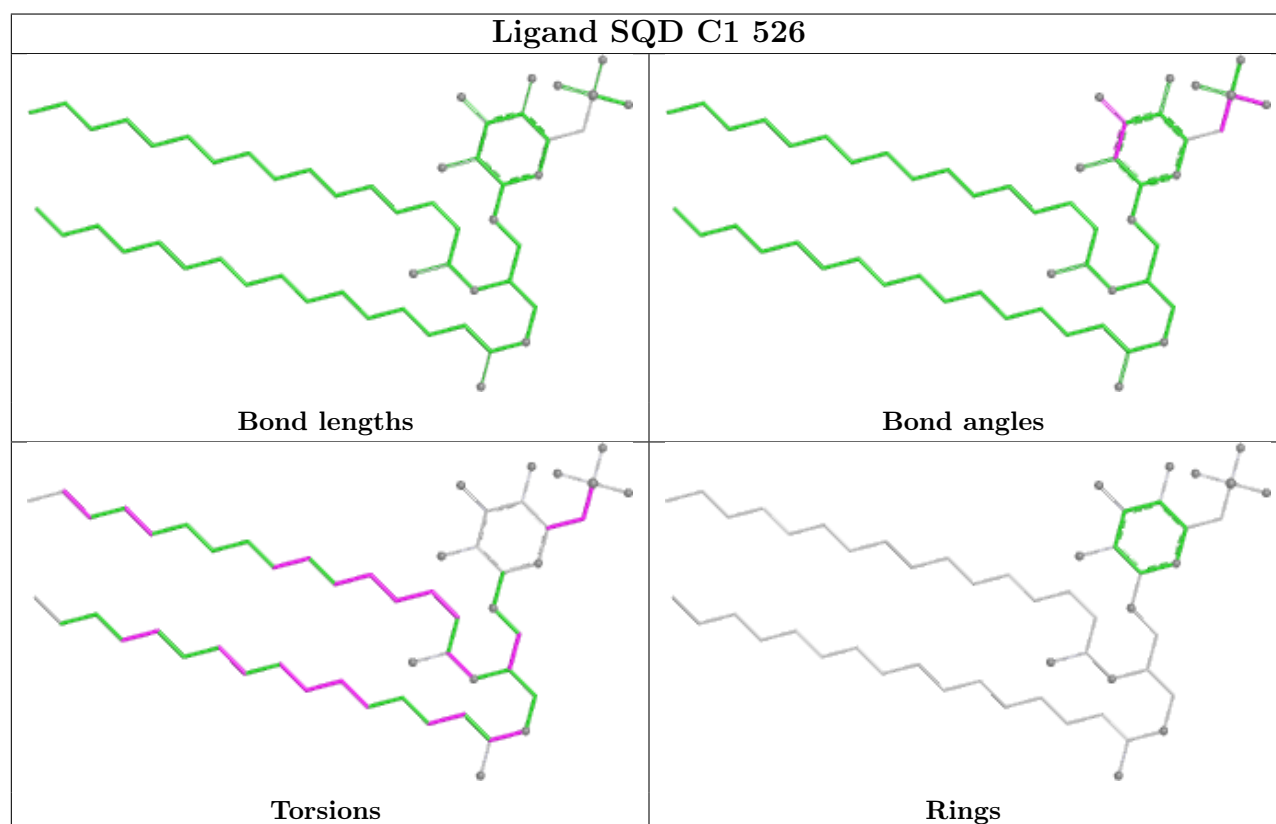
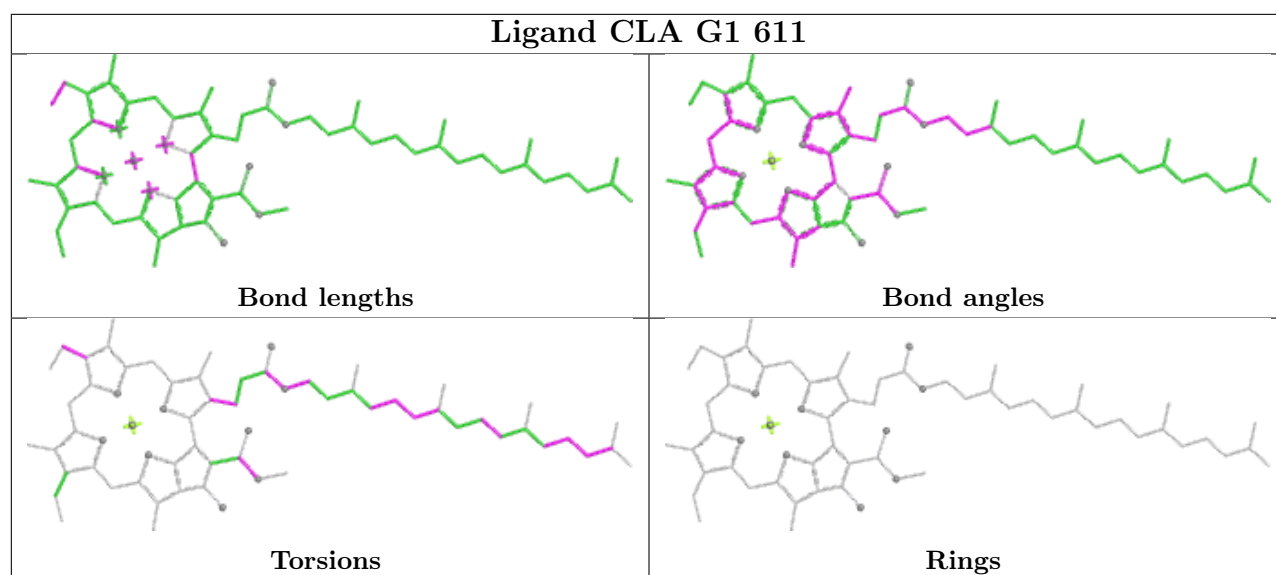


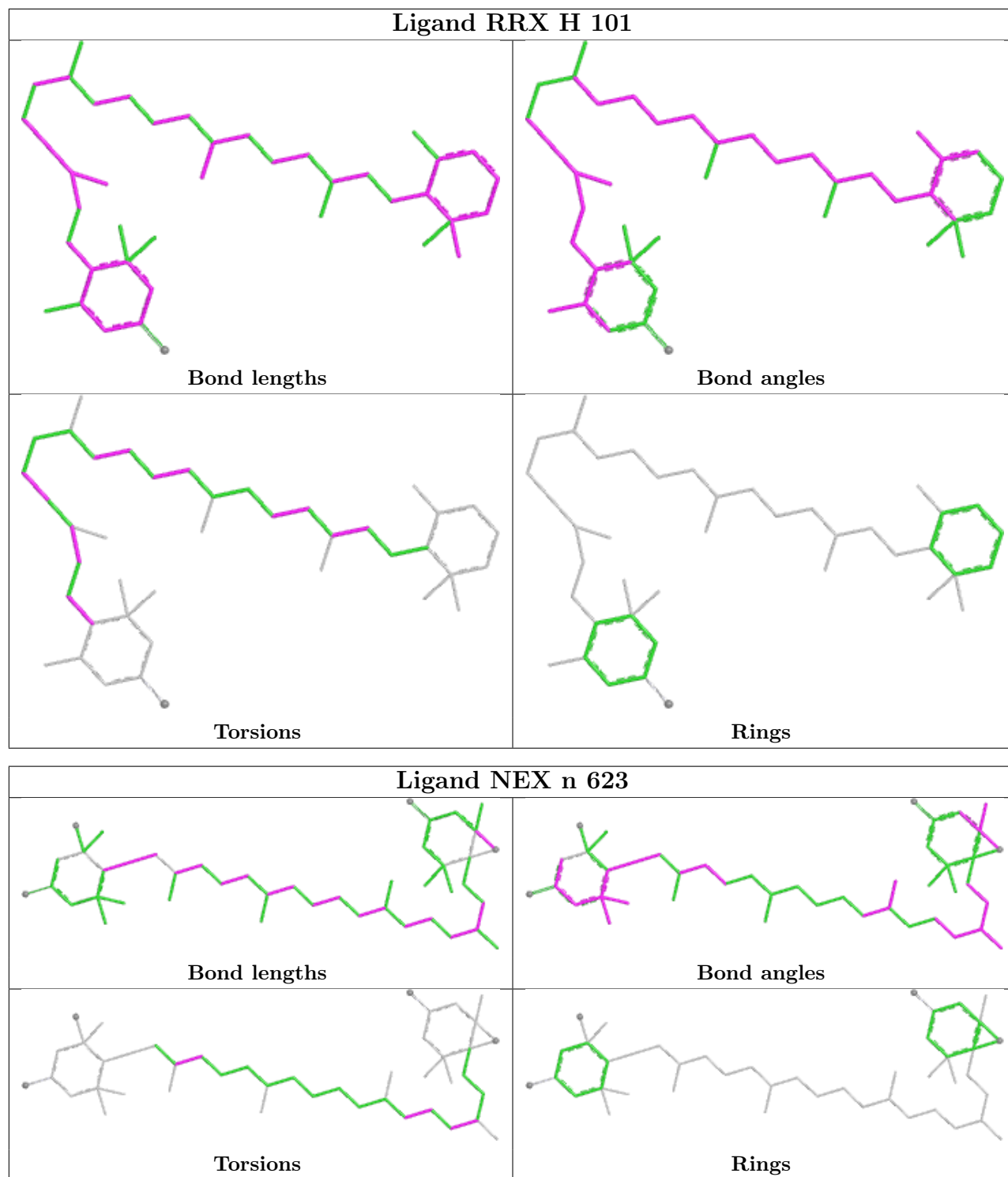


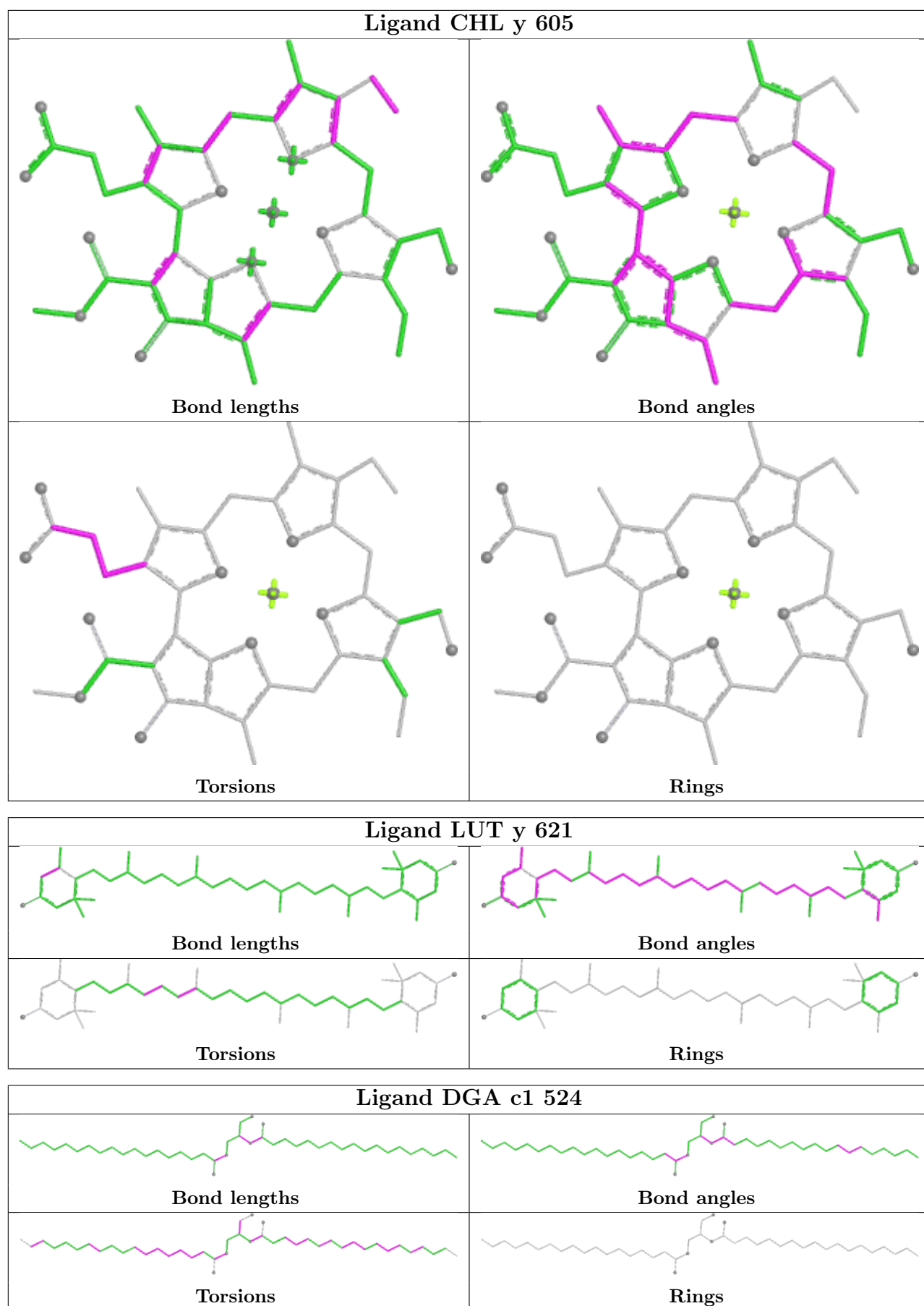


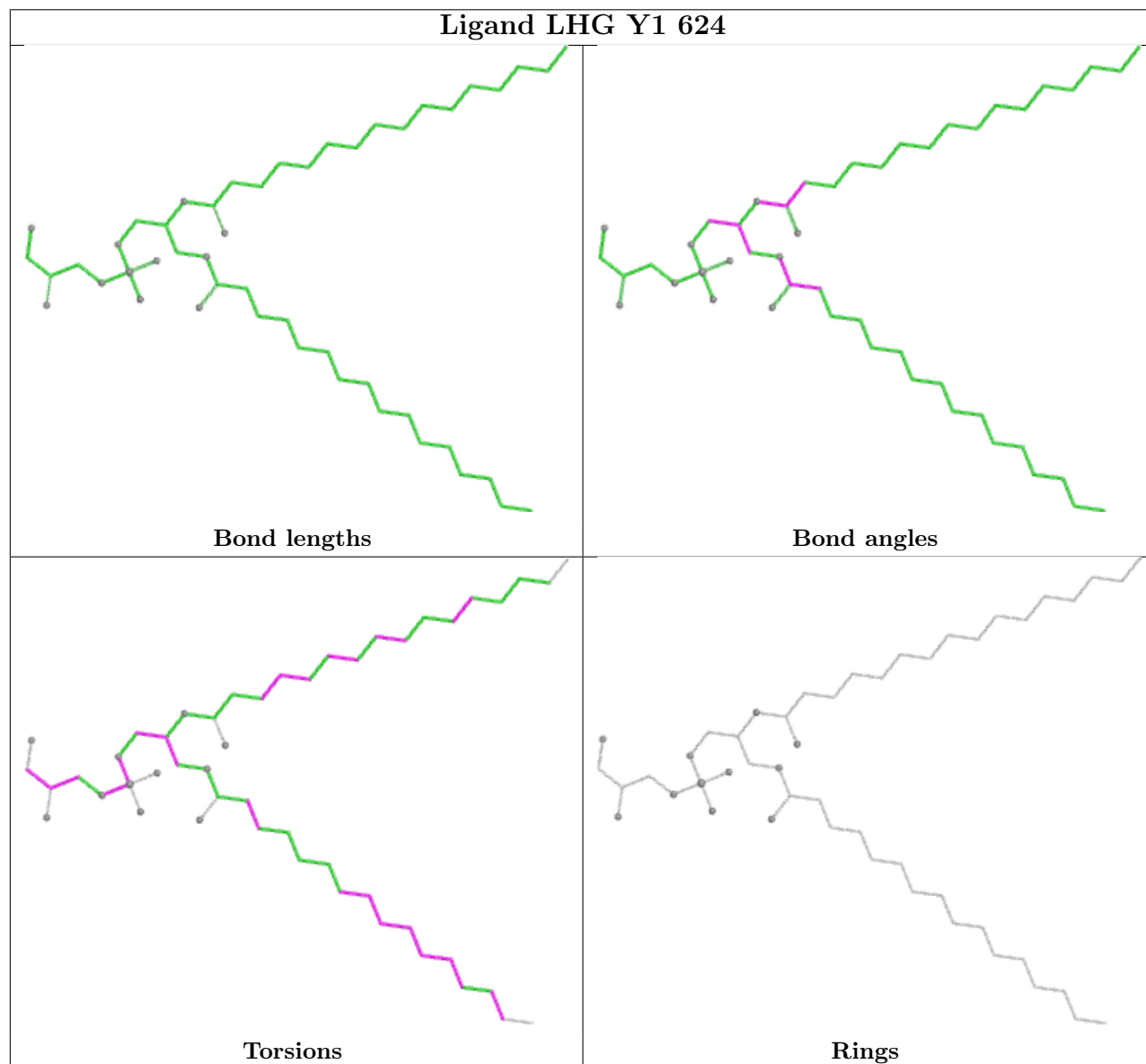
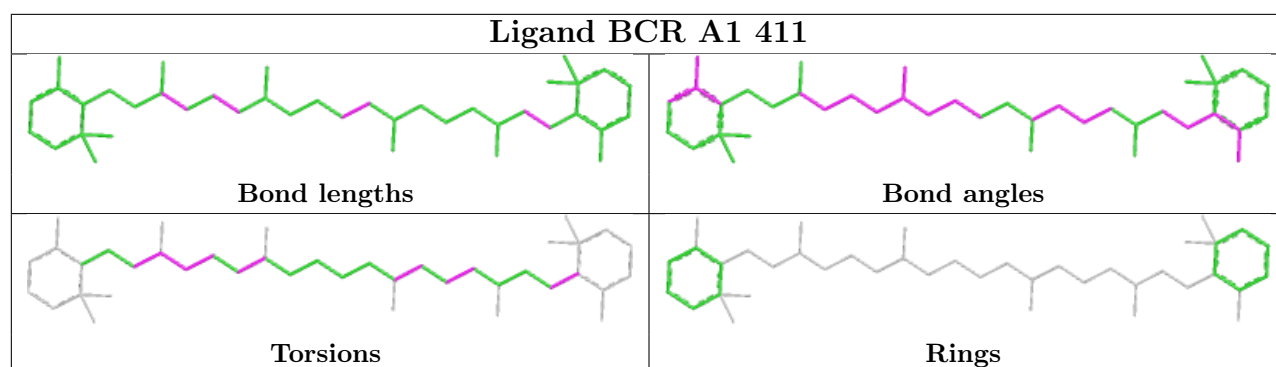




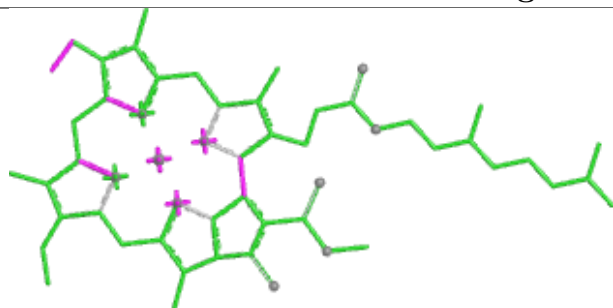




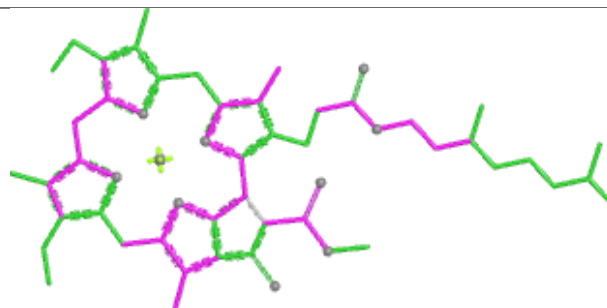




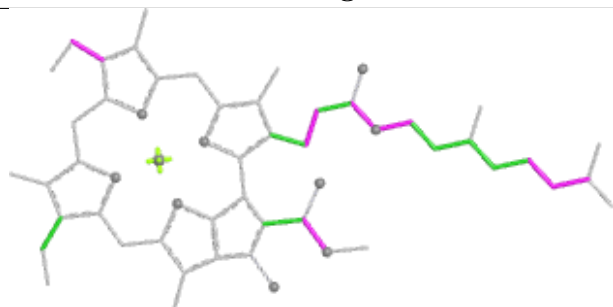
Ligand CLA S 604



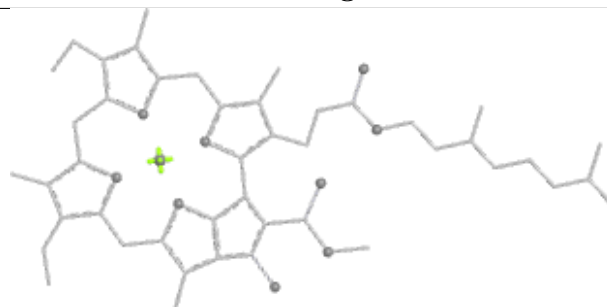
Bond lengths



Bond angles

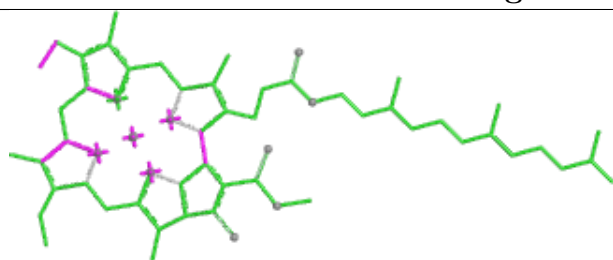


Torsions

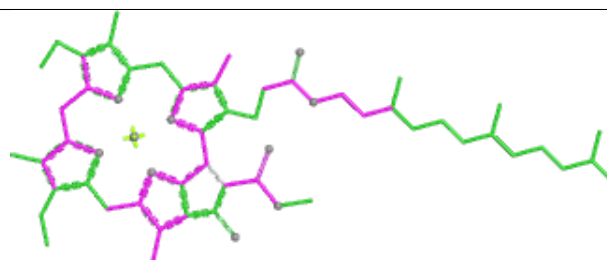


Rings

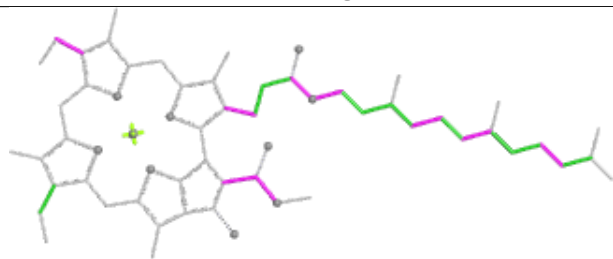
Ligand CLA R1 612



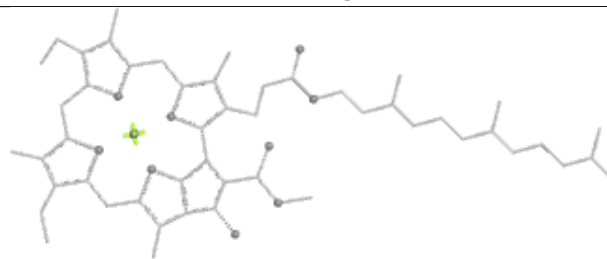
Bond lengths



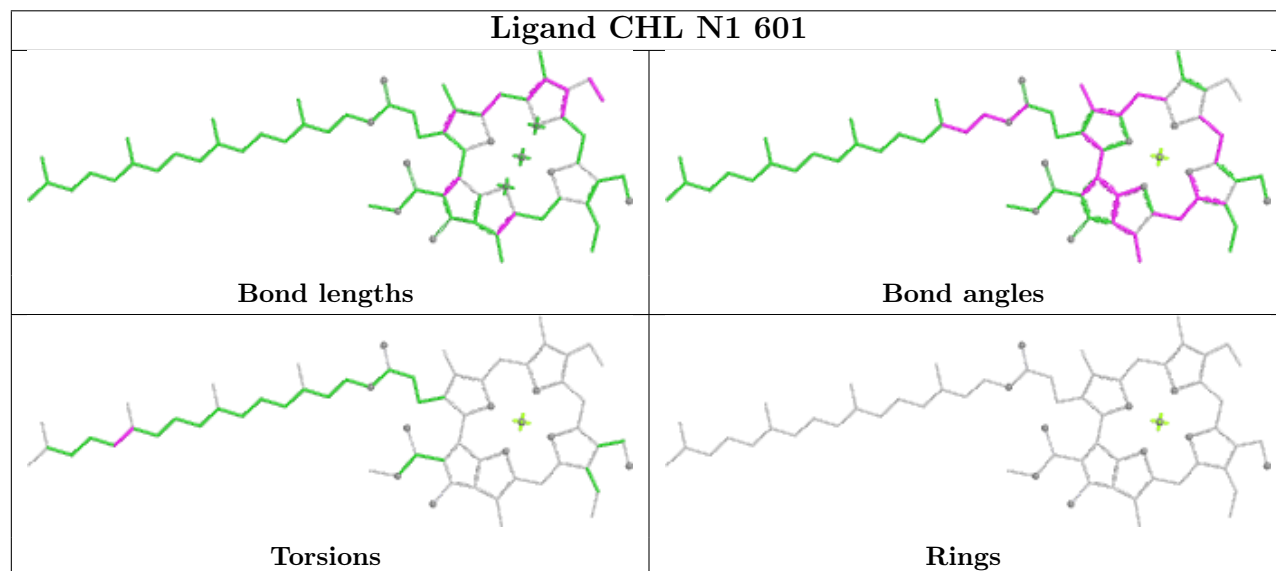
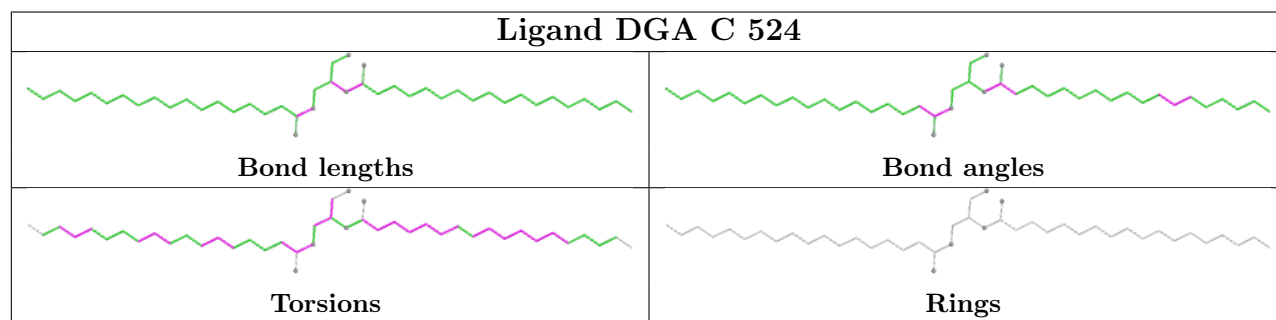
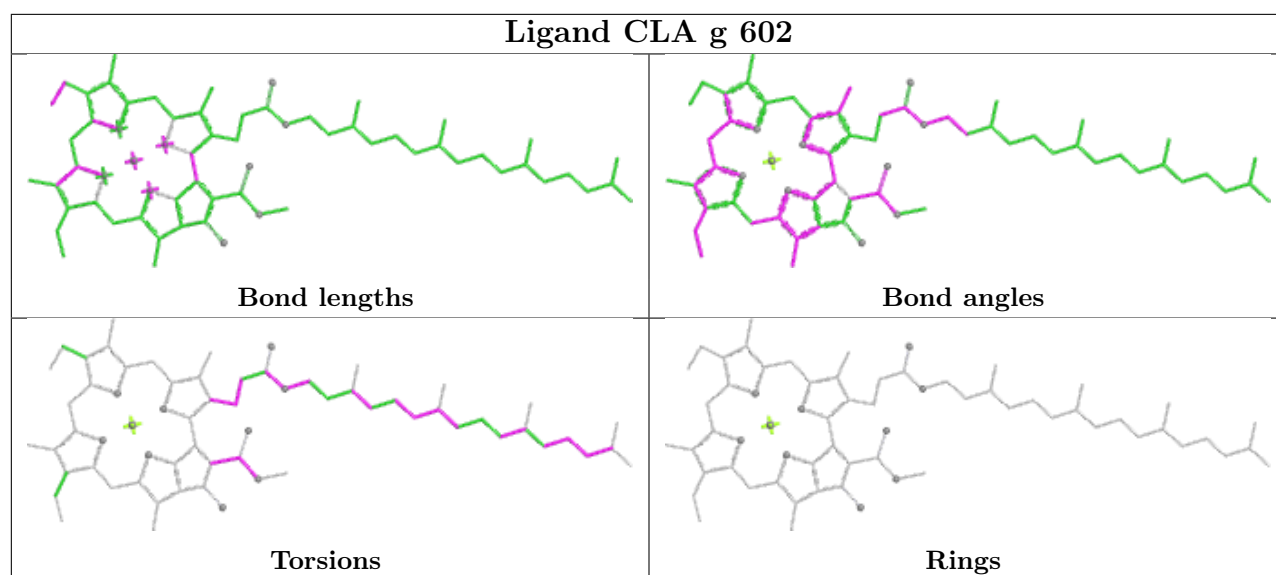
Bond angles

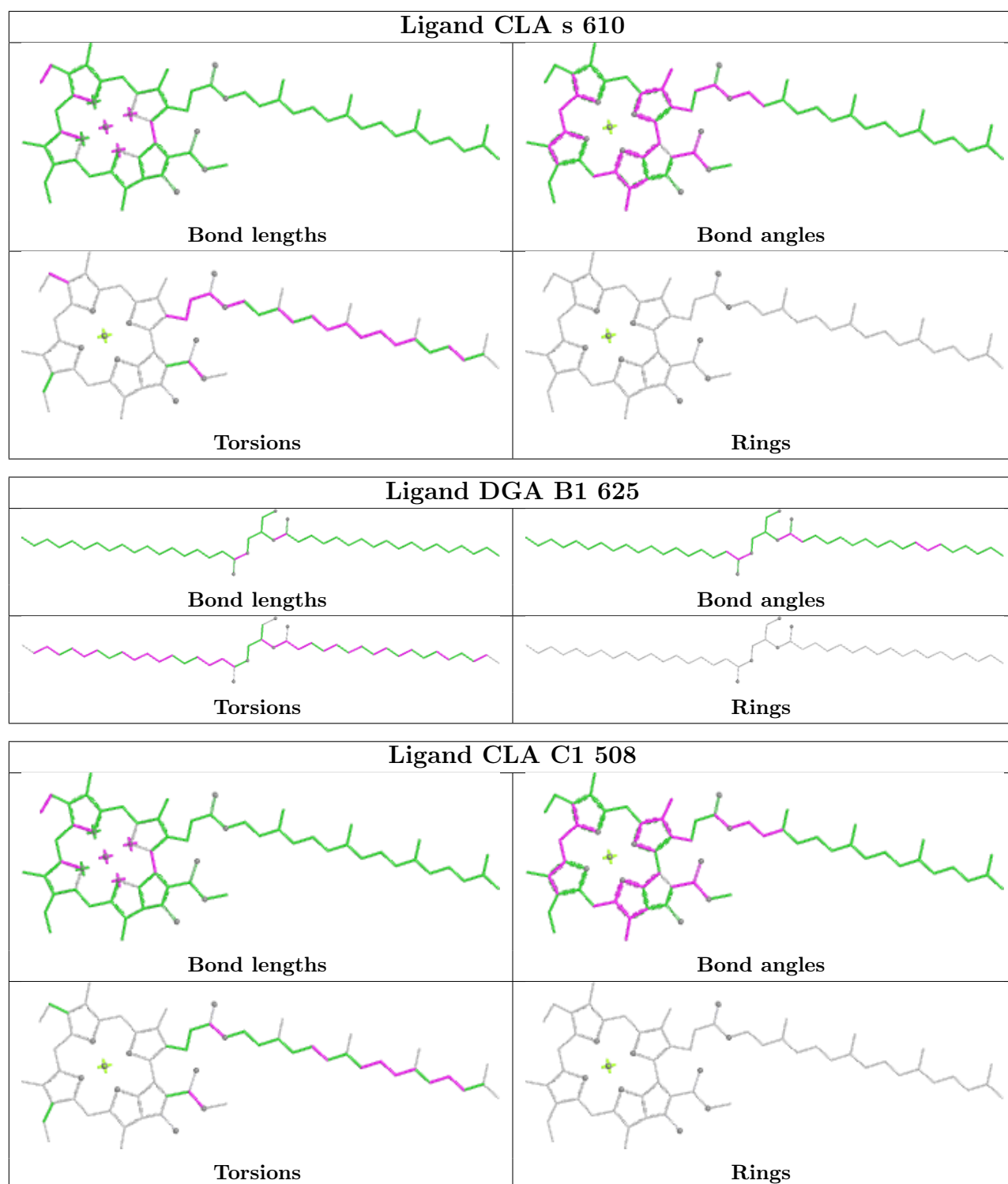


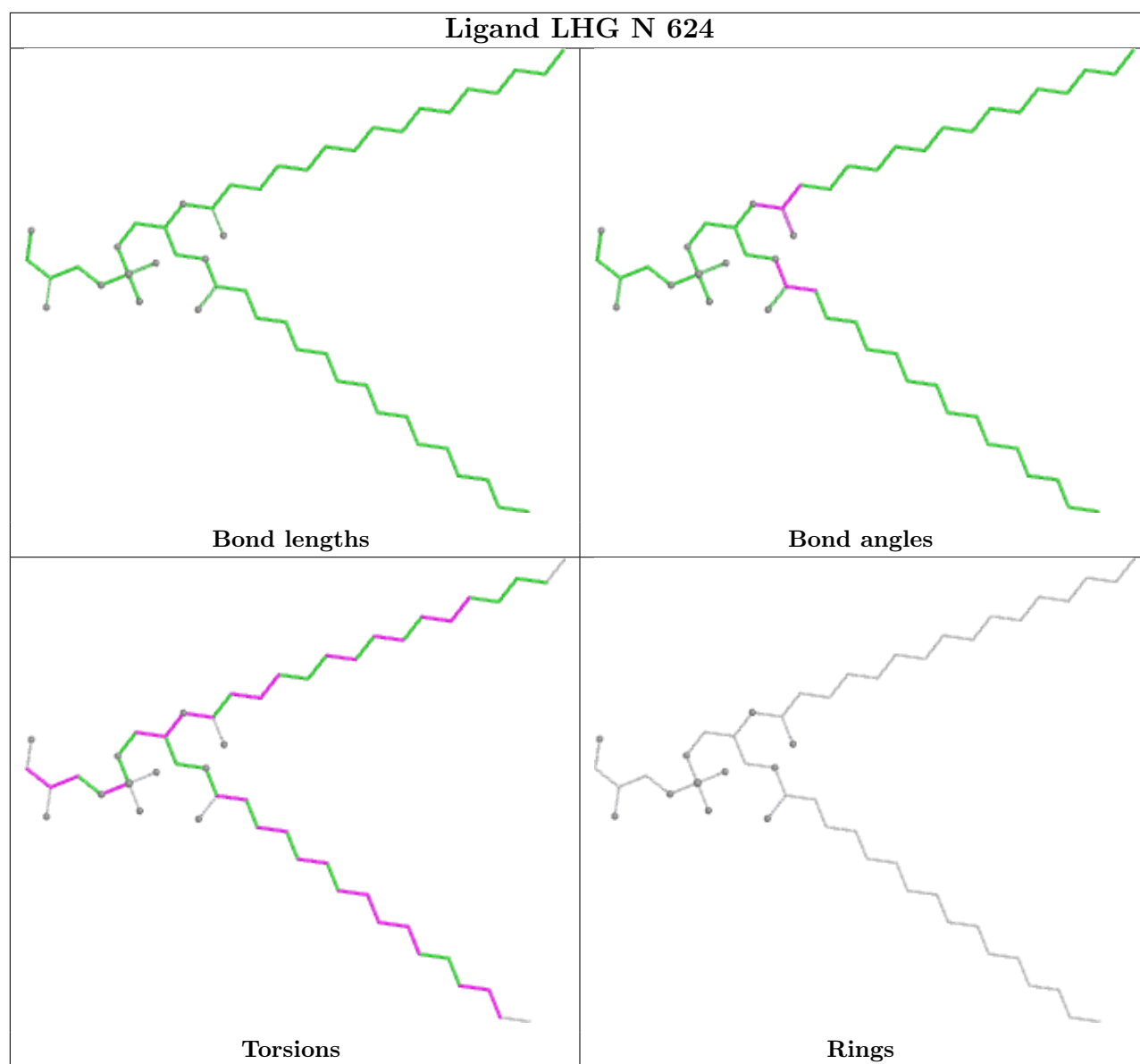
Torsions



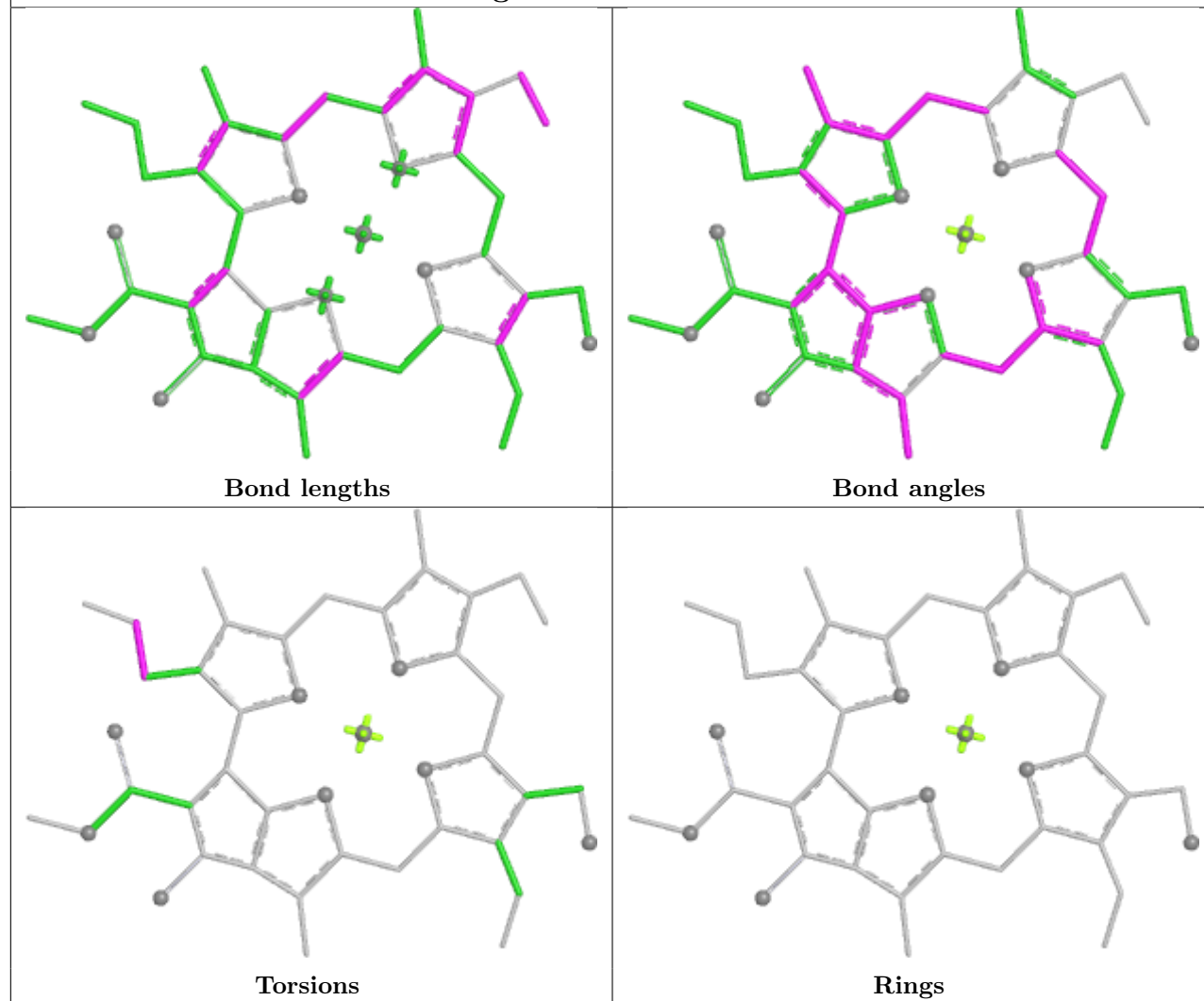
Rings



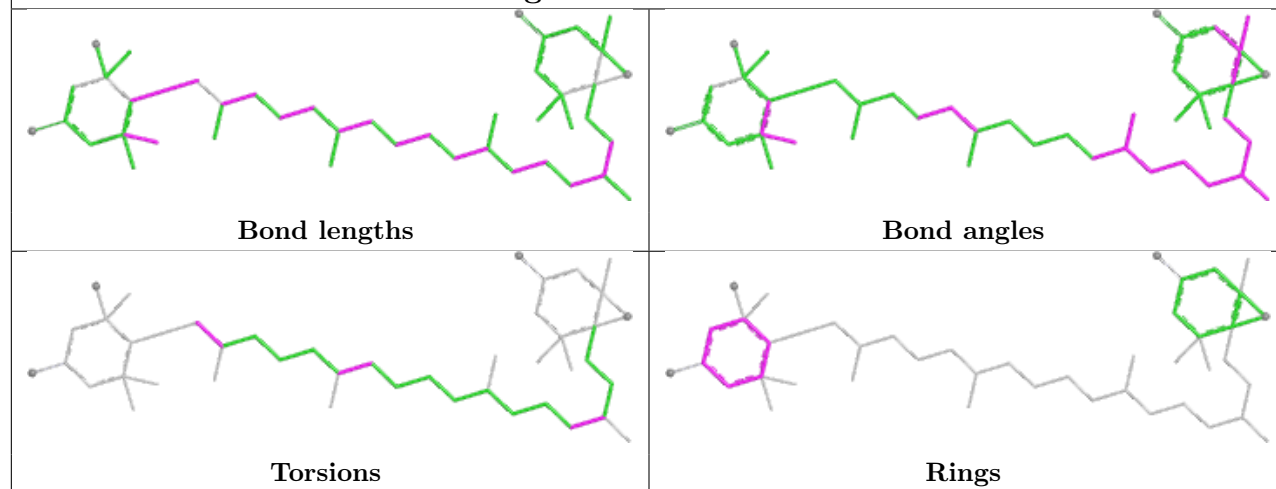


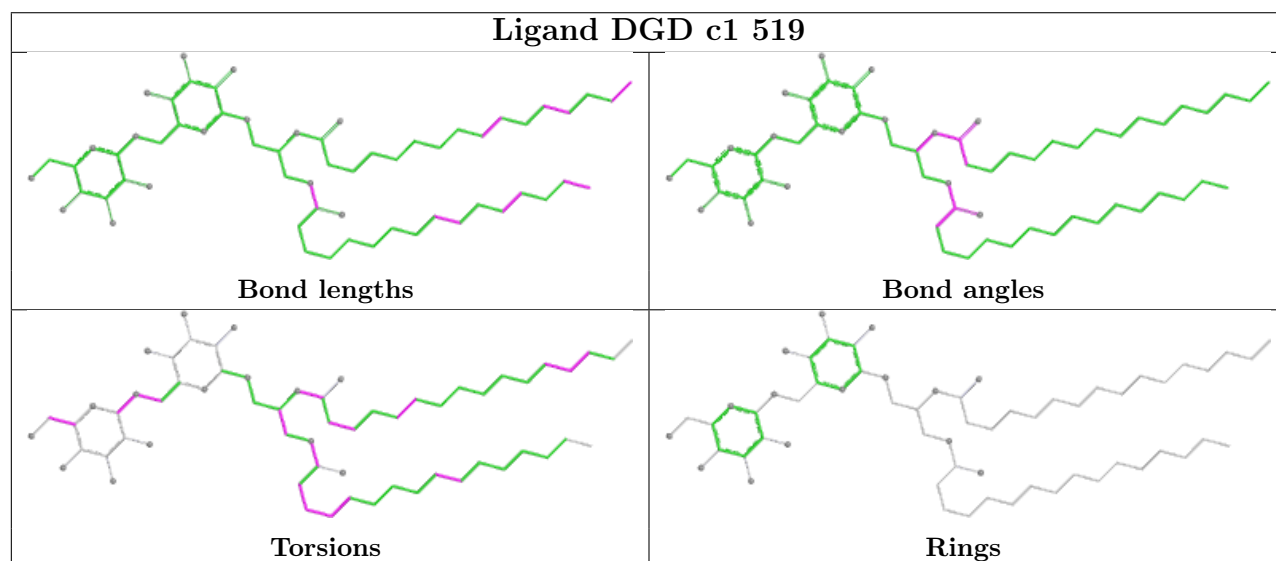
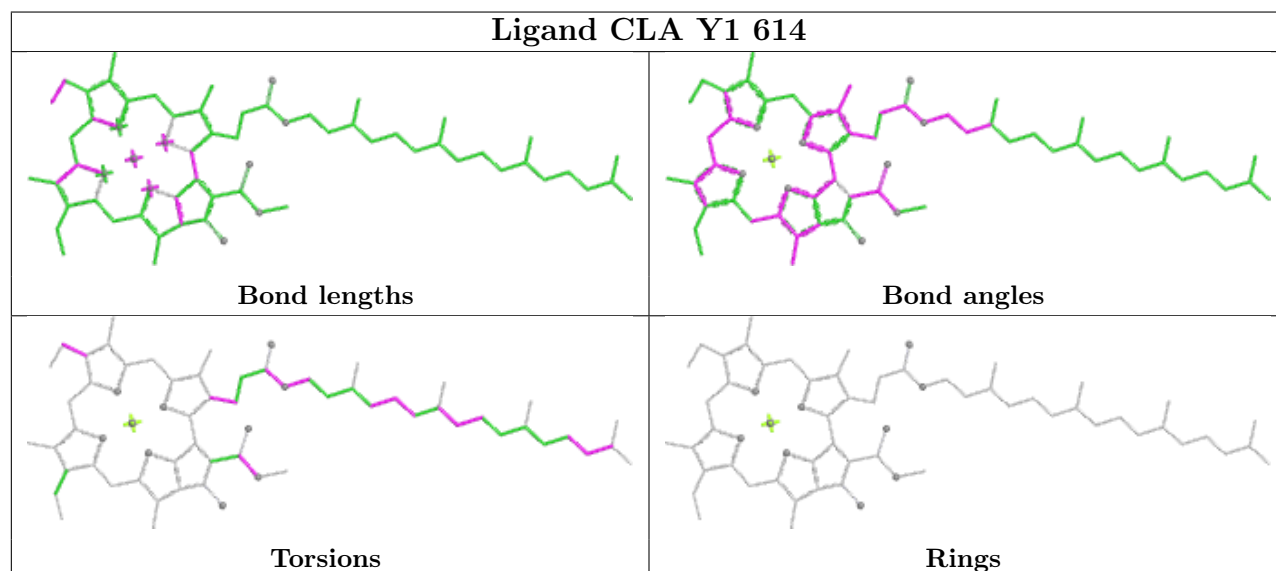
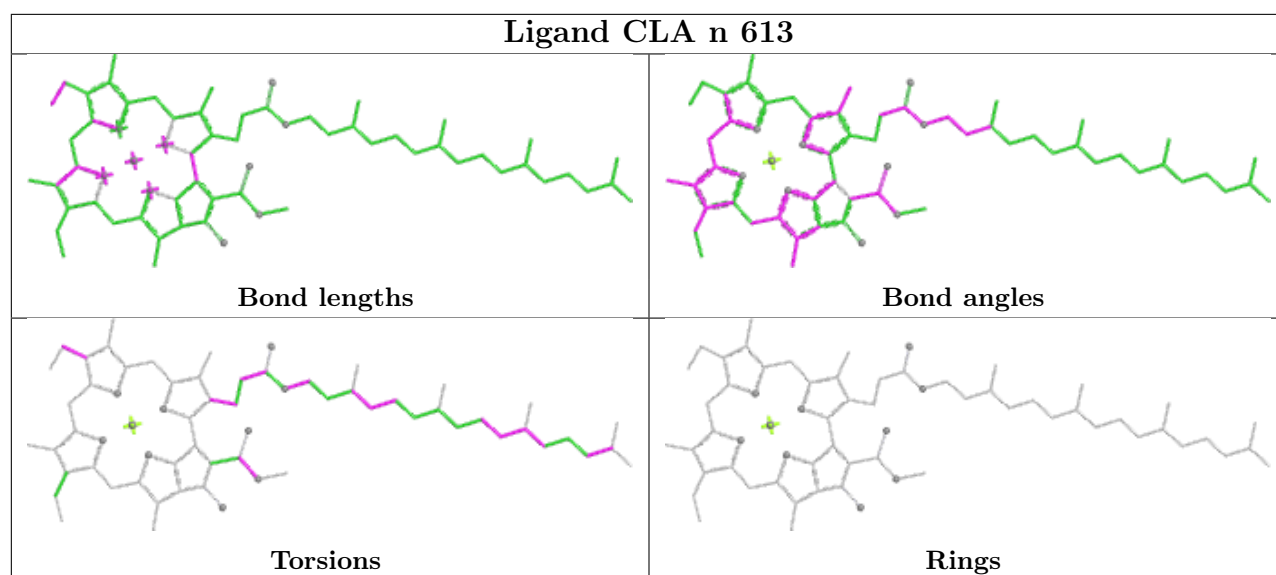


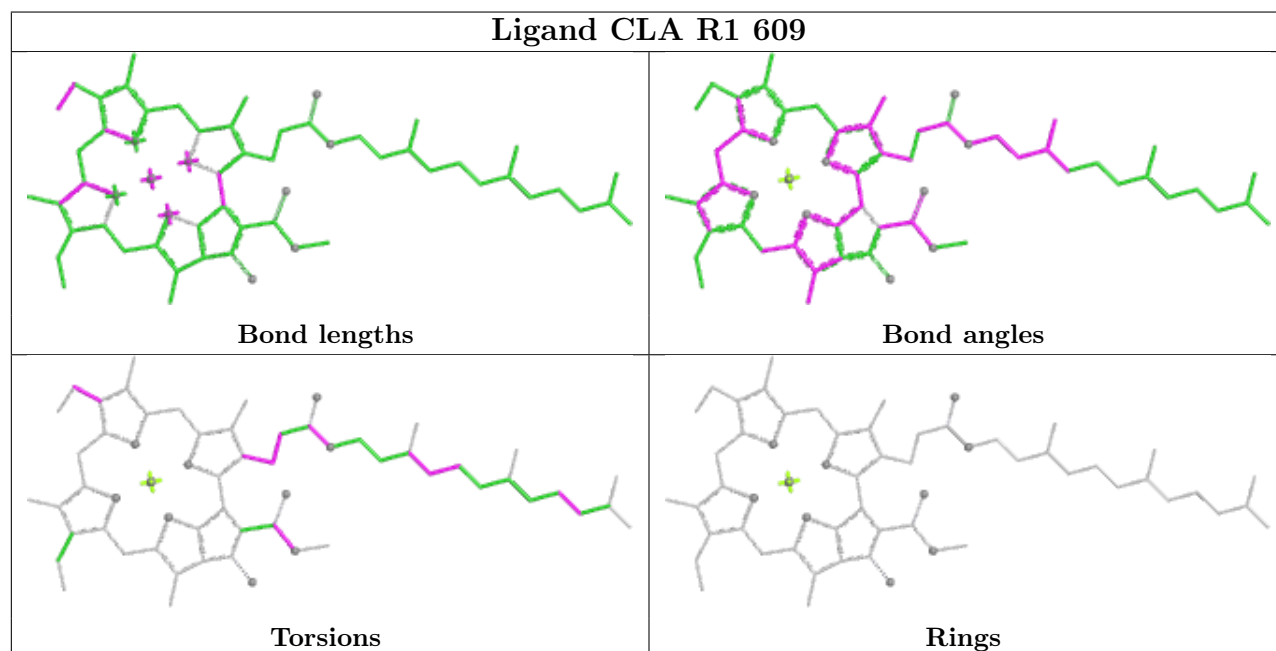
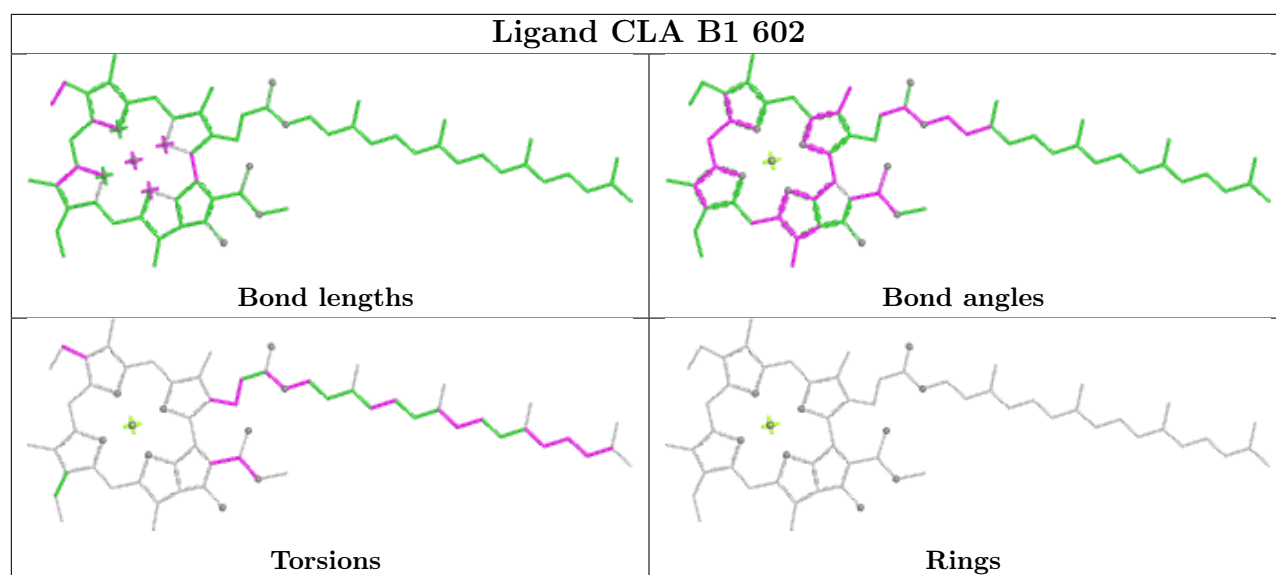
Ligand CHL R1 606

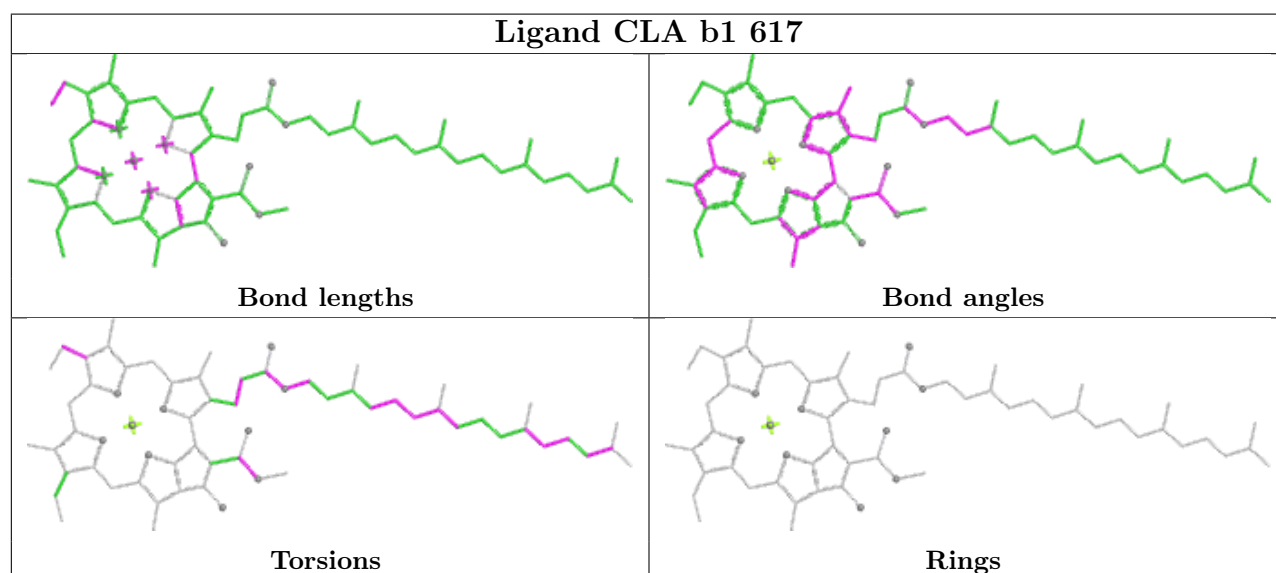
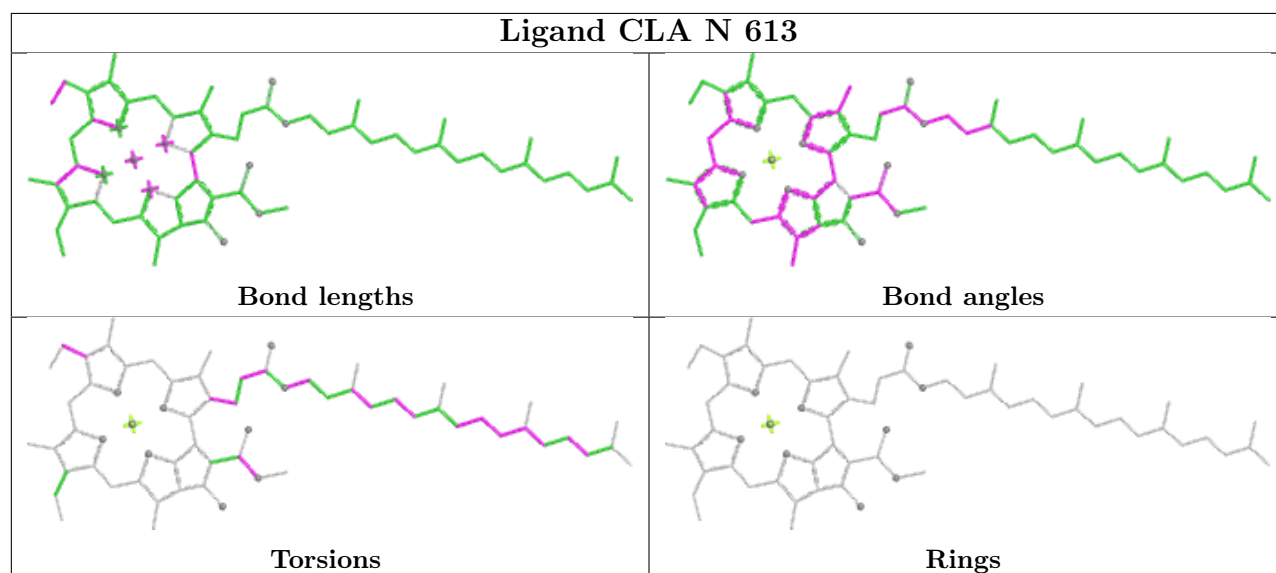
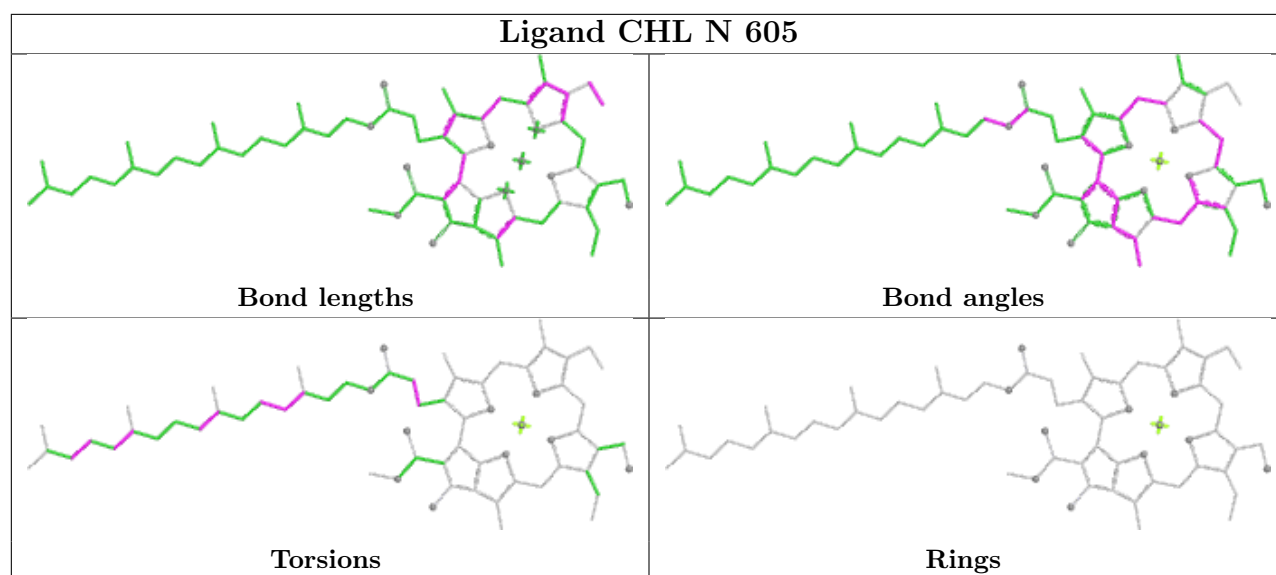


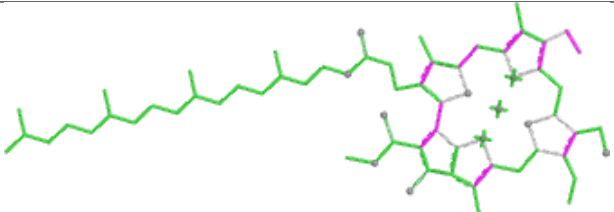
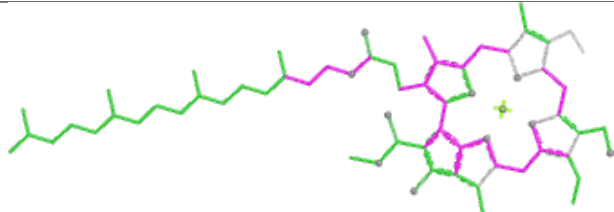
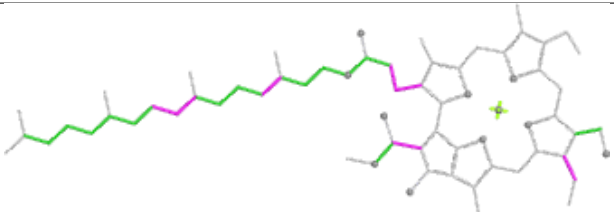
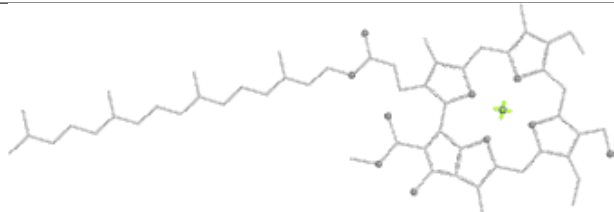
Ligand NEX n1 623

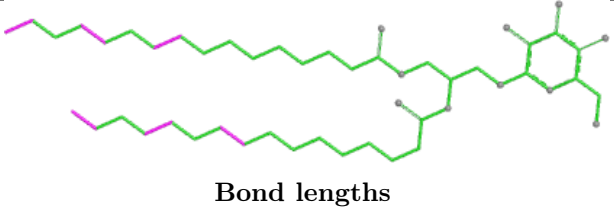
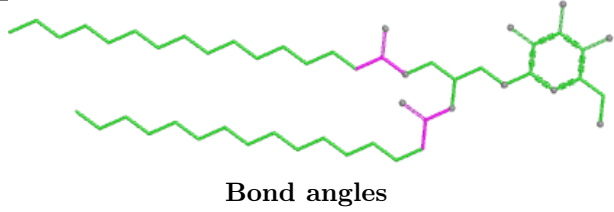
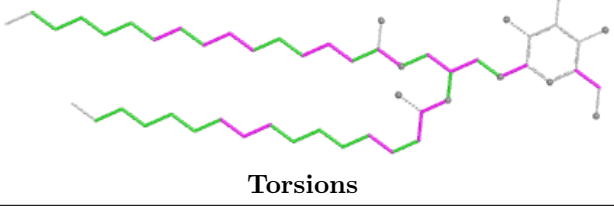
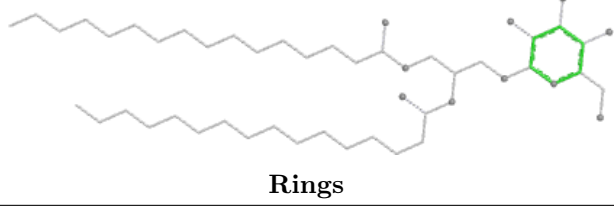


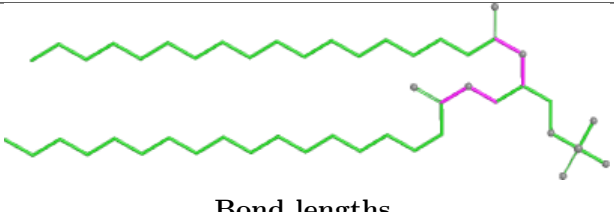
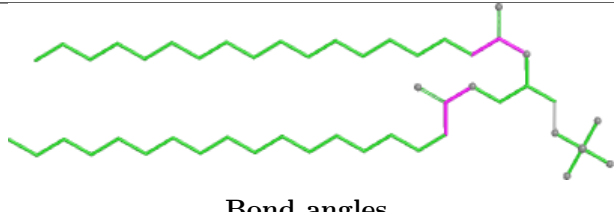
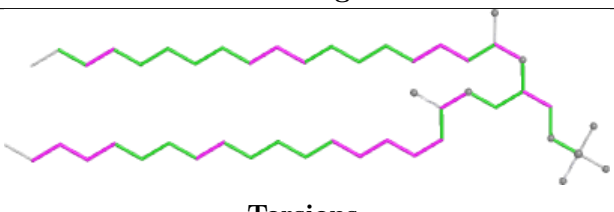
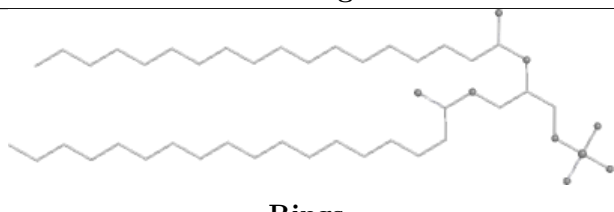


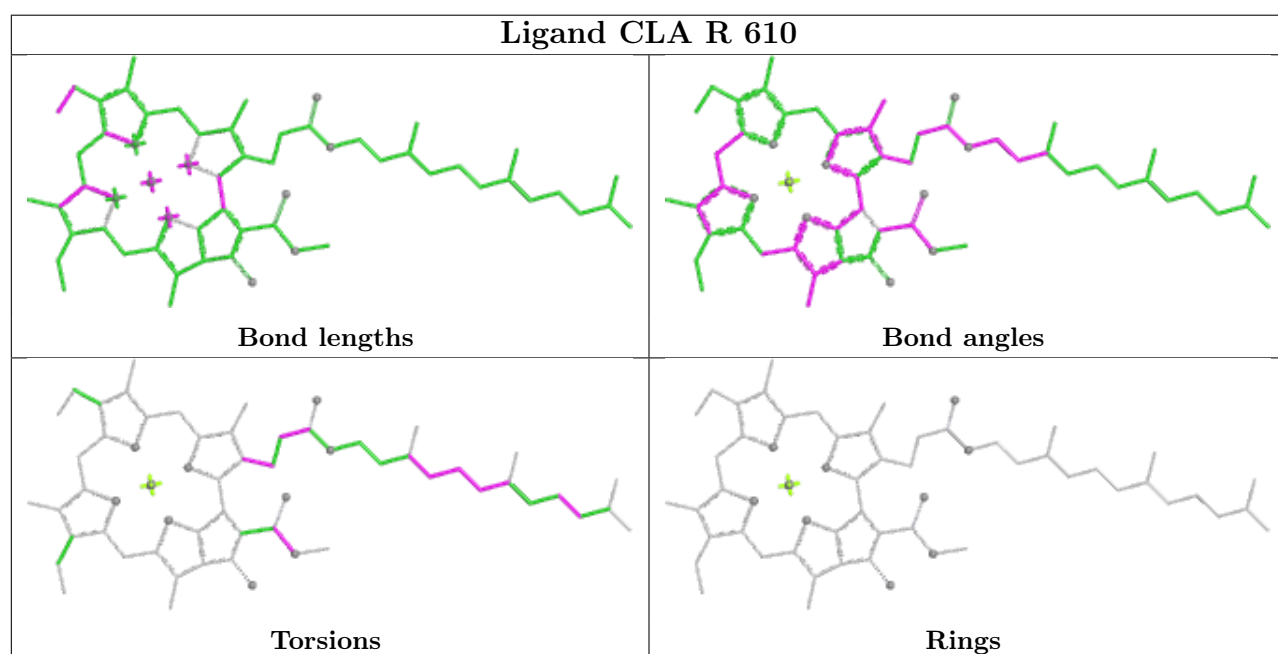
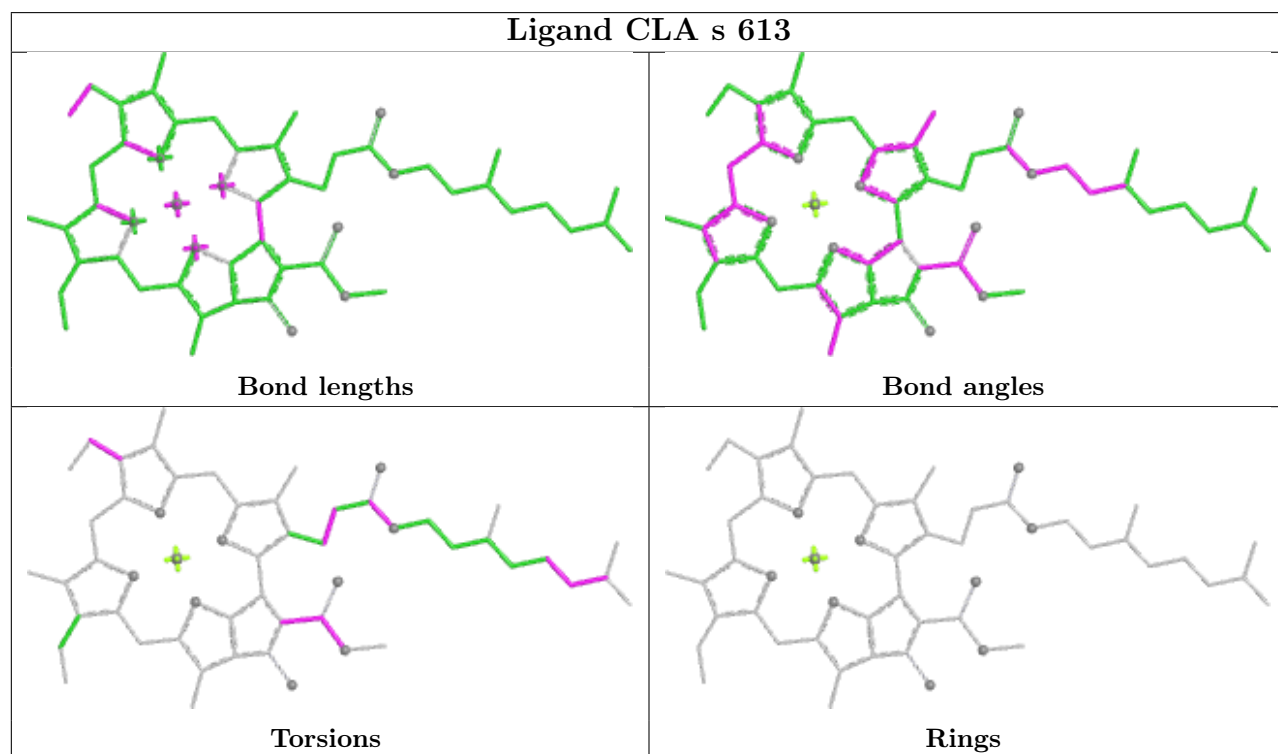
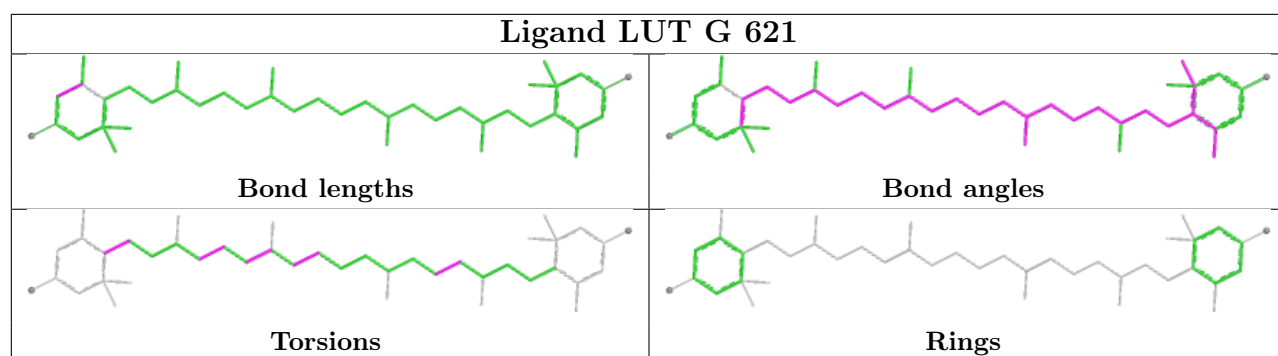


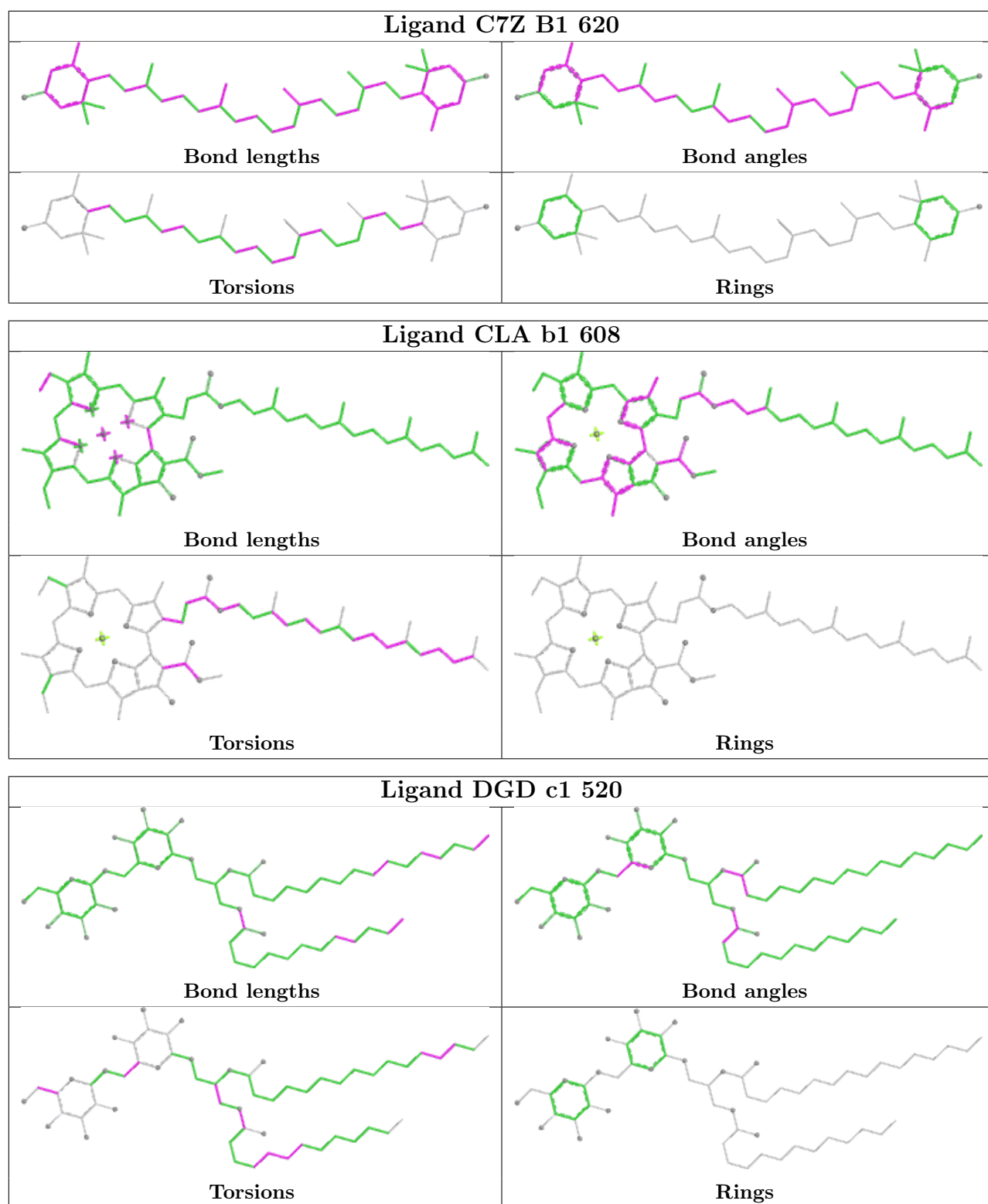


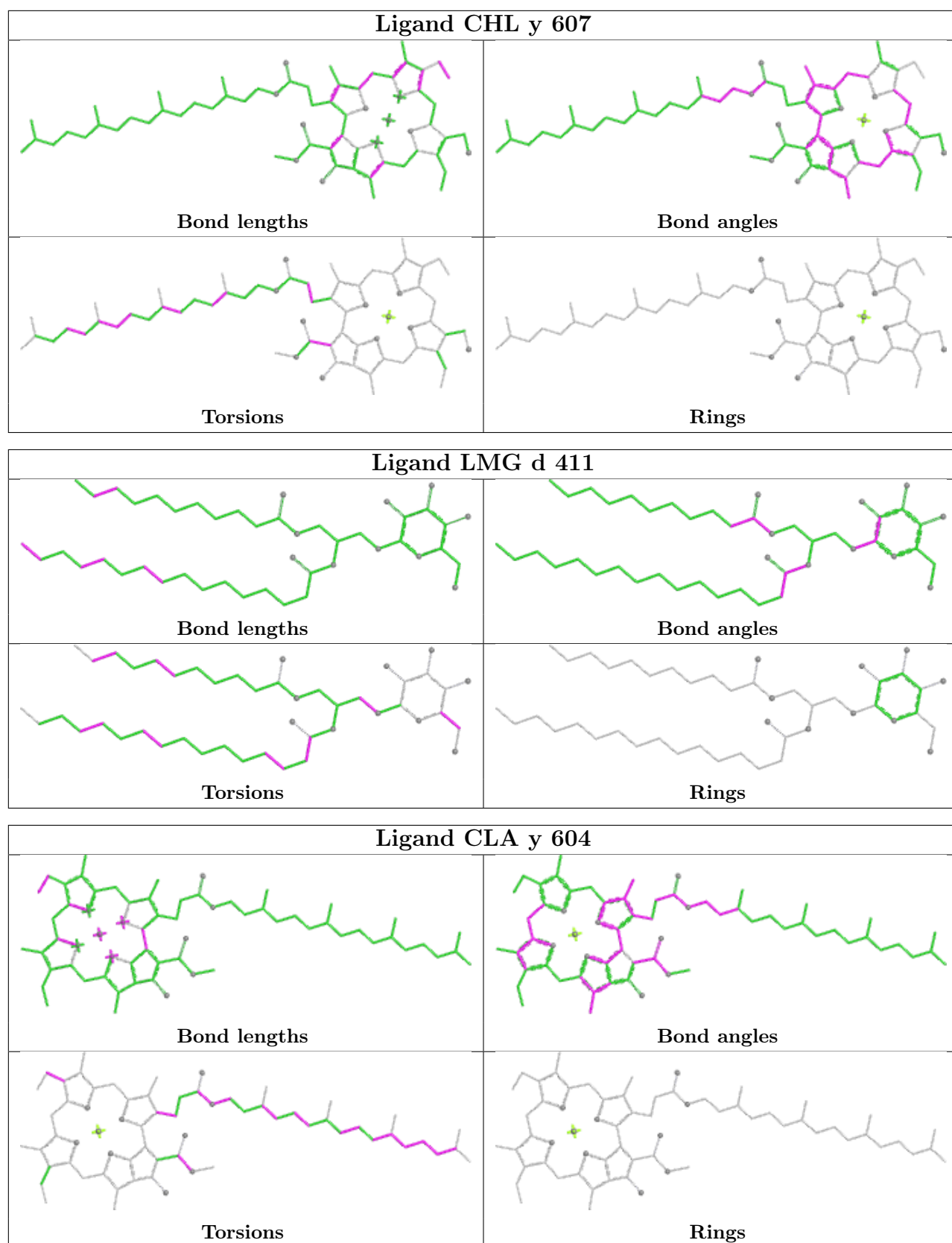
Ligand CHL n 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

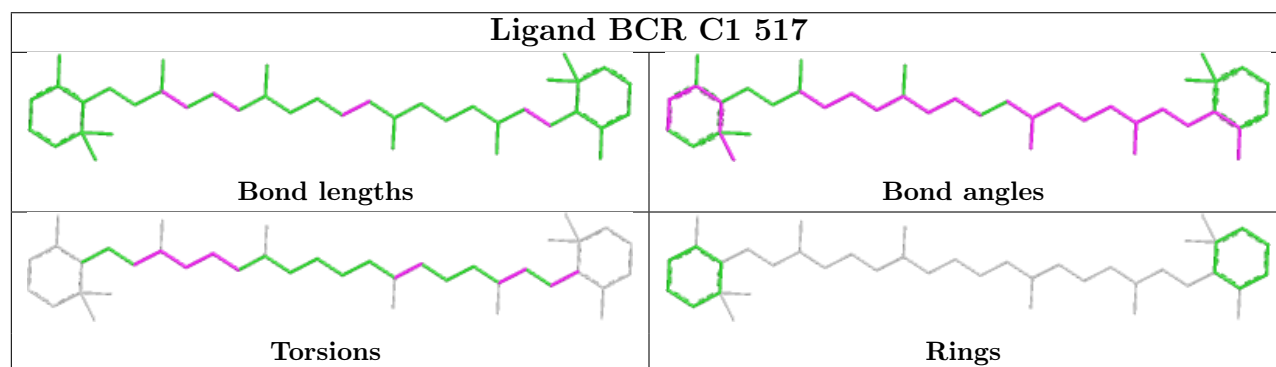
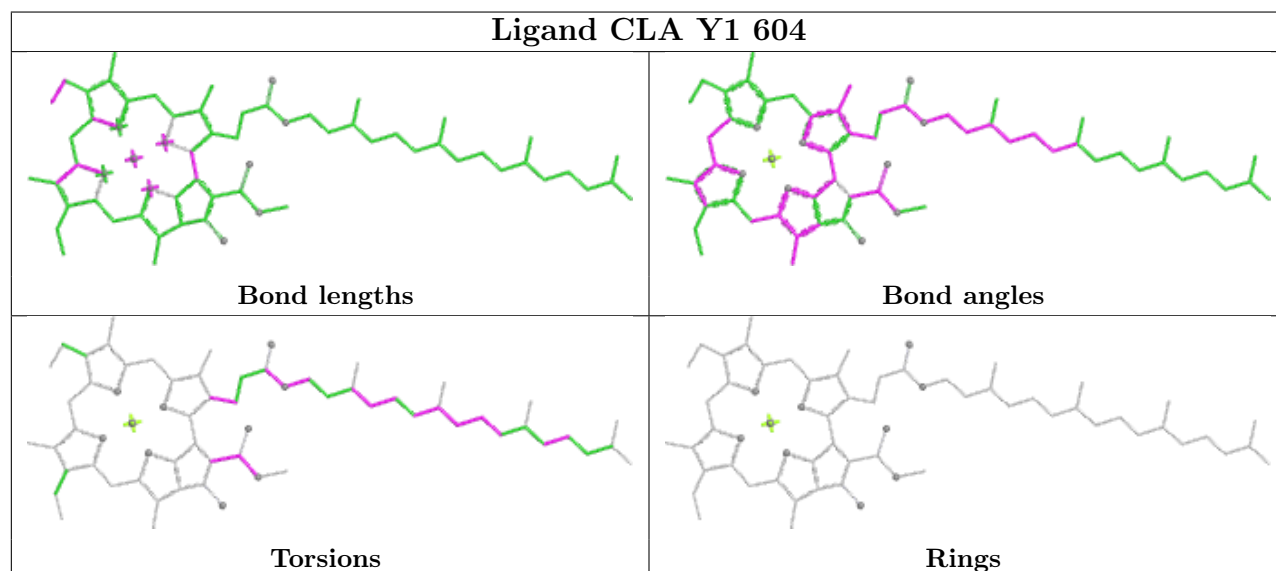
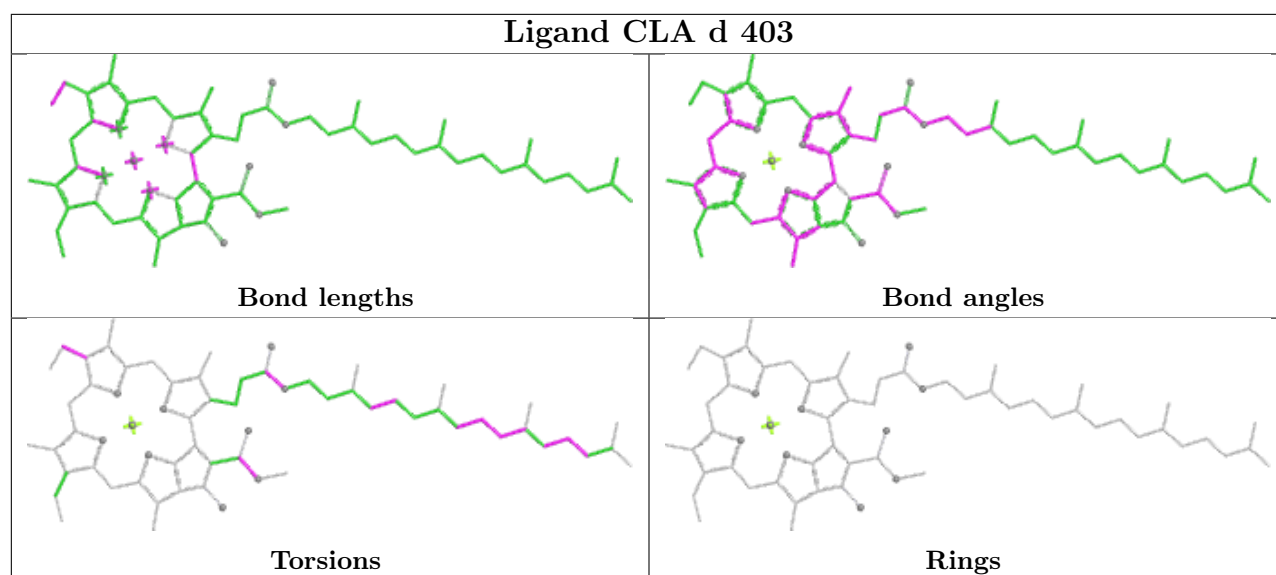
Ligand LMG c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

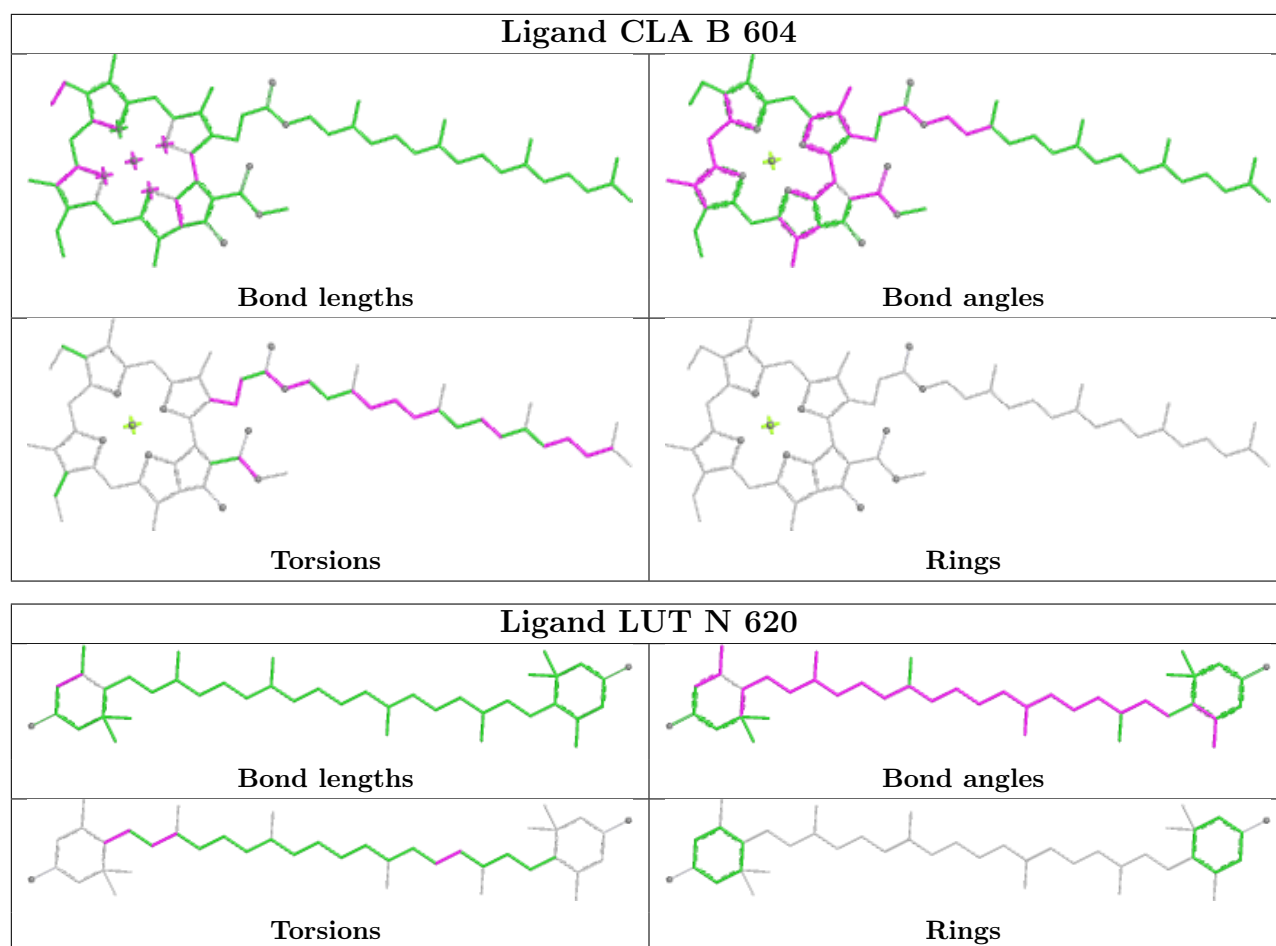
Ligand 3PH b1 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

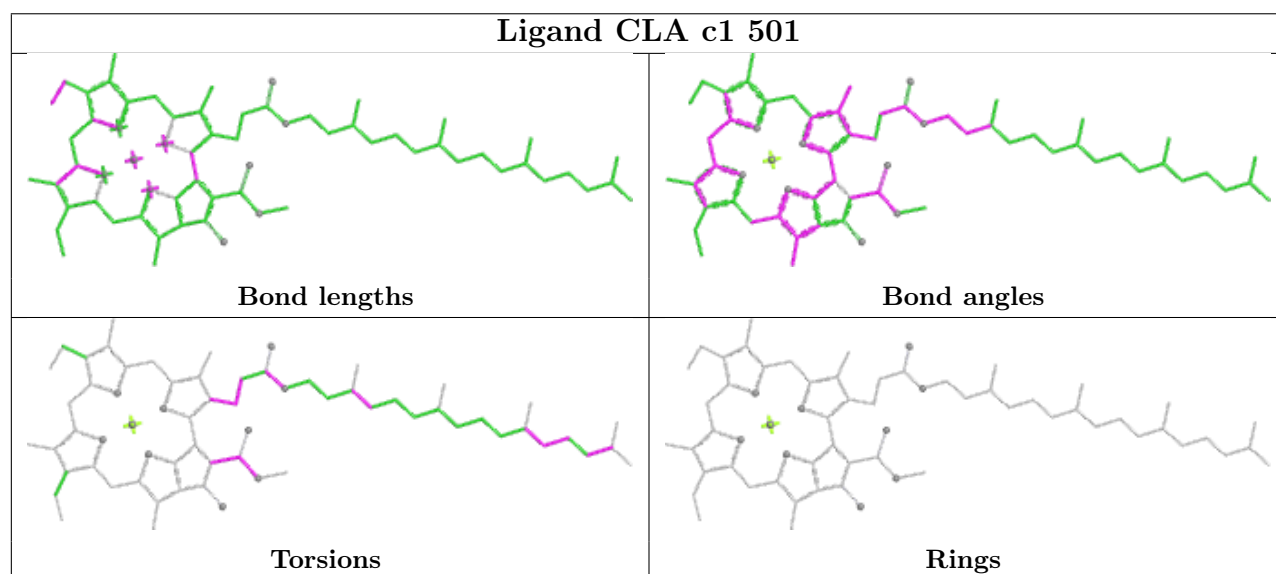
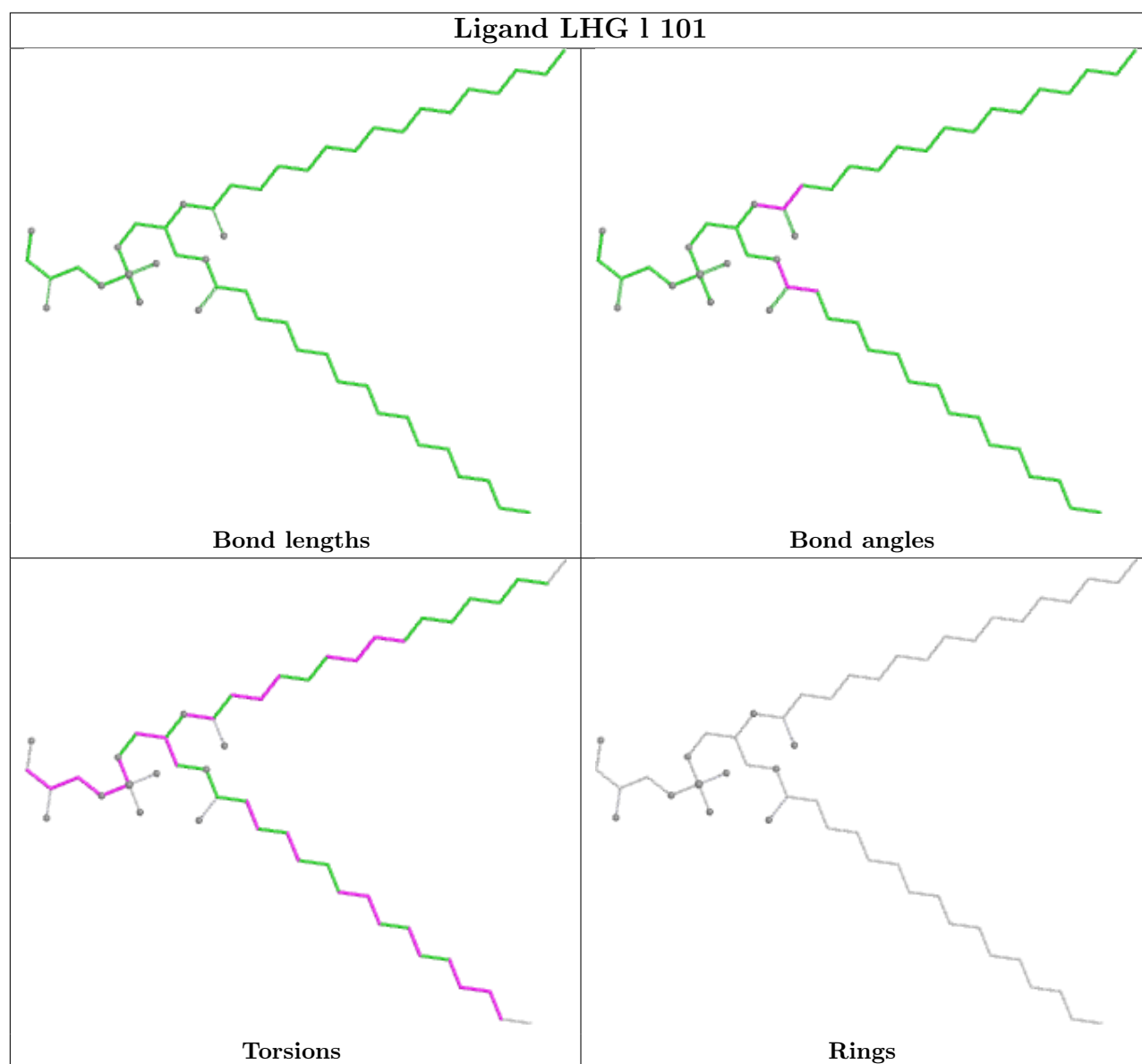


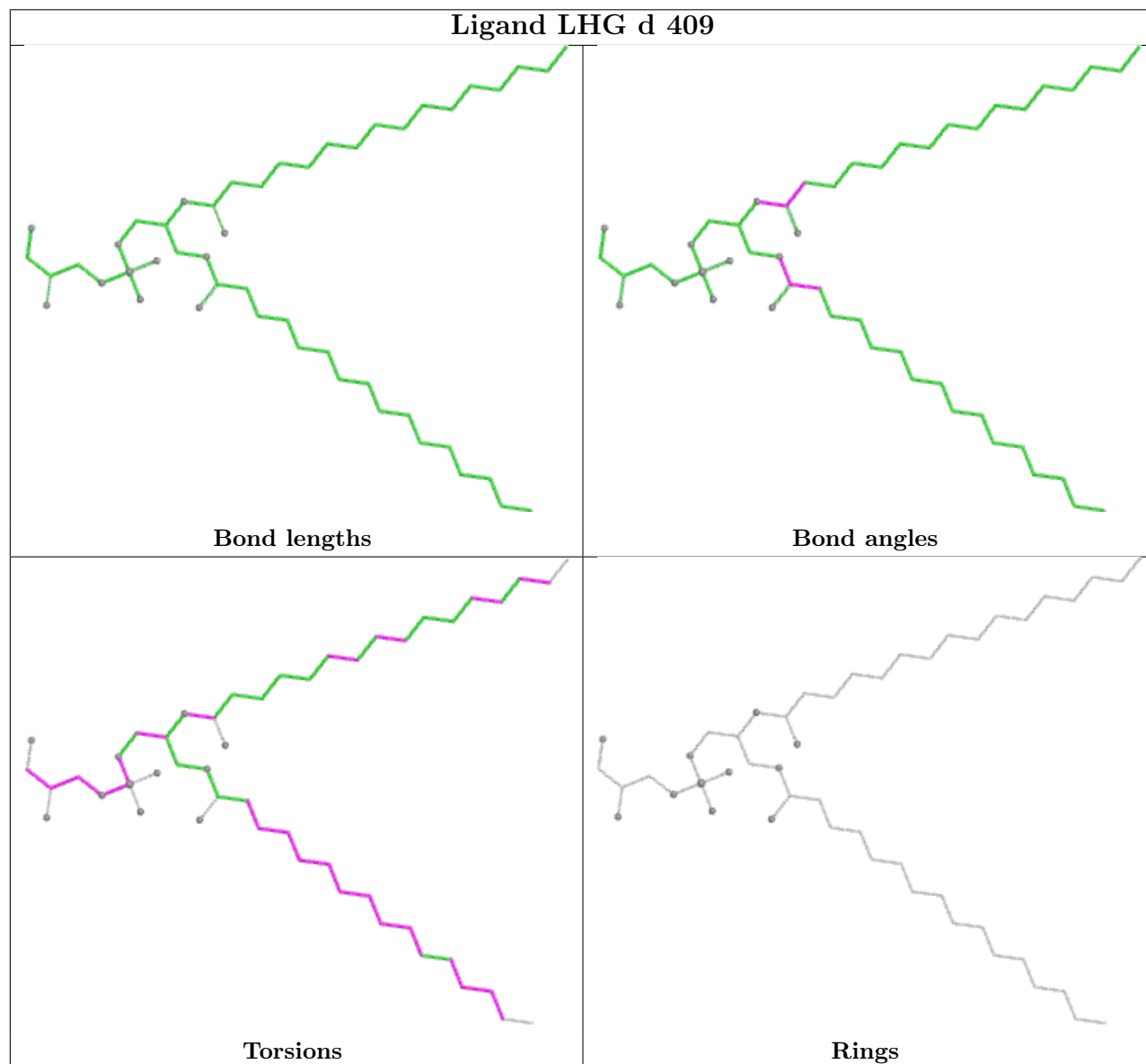
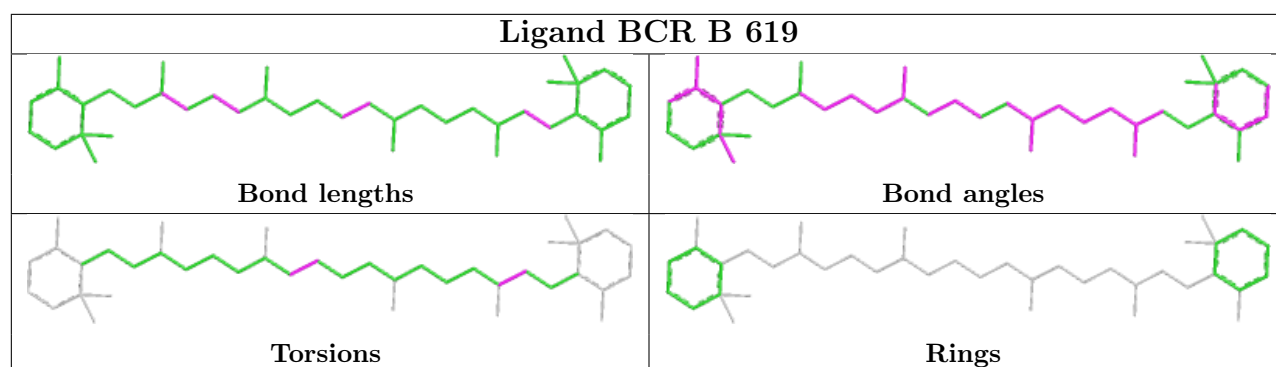




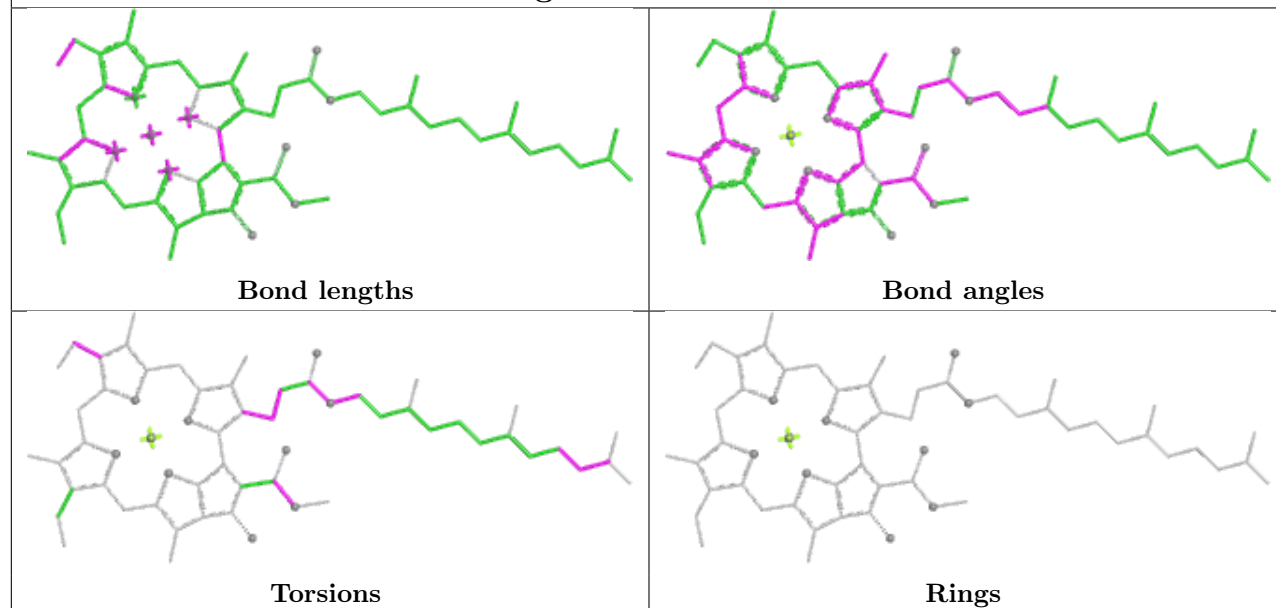




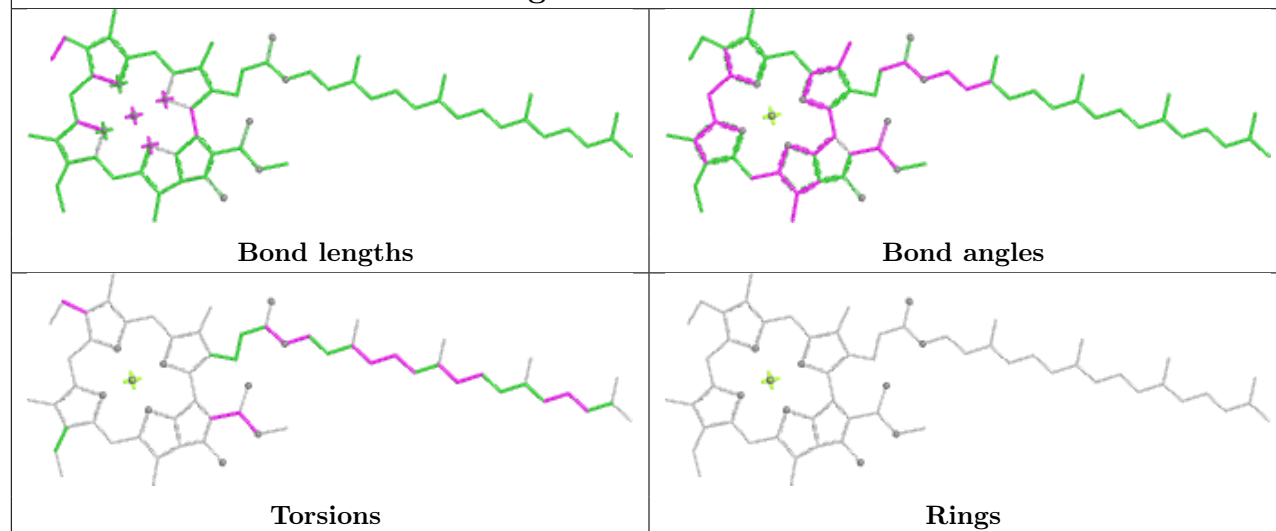


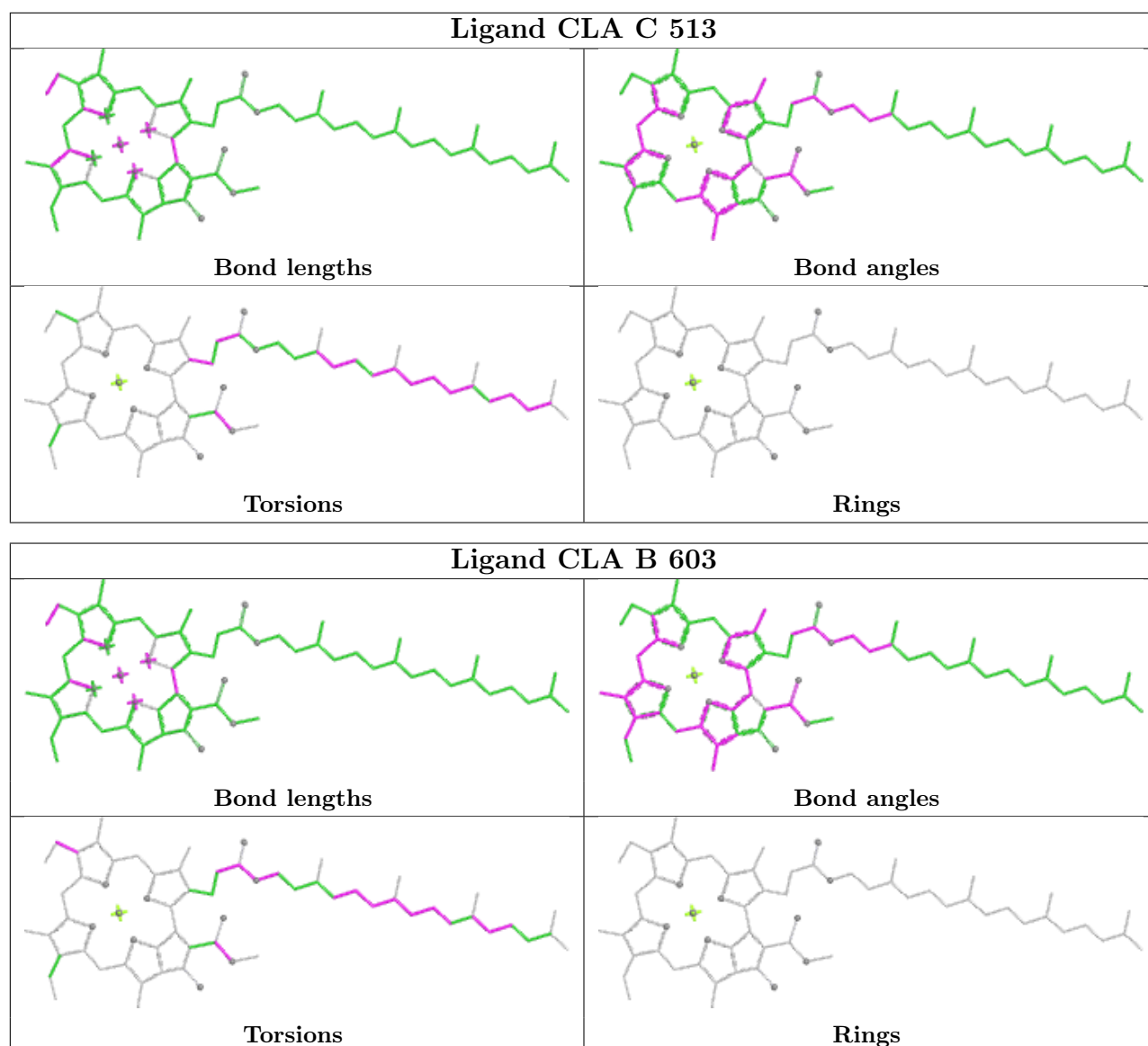


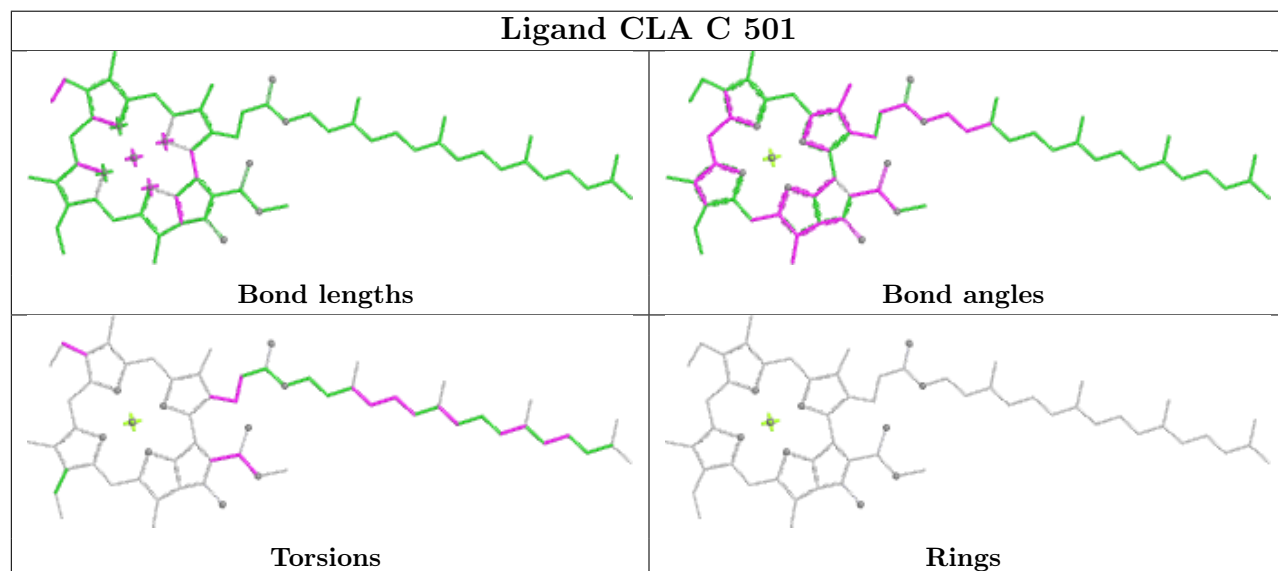
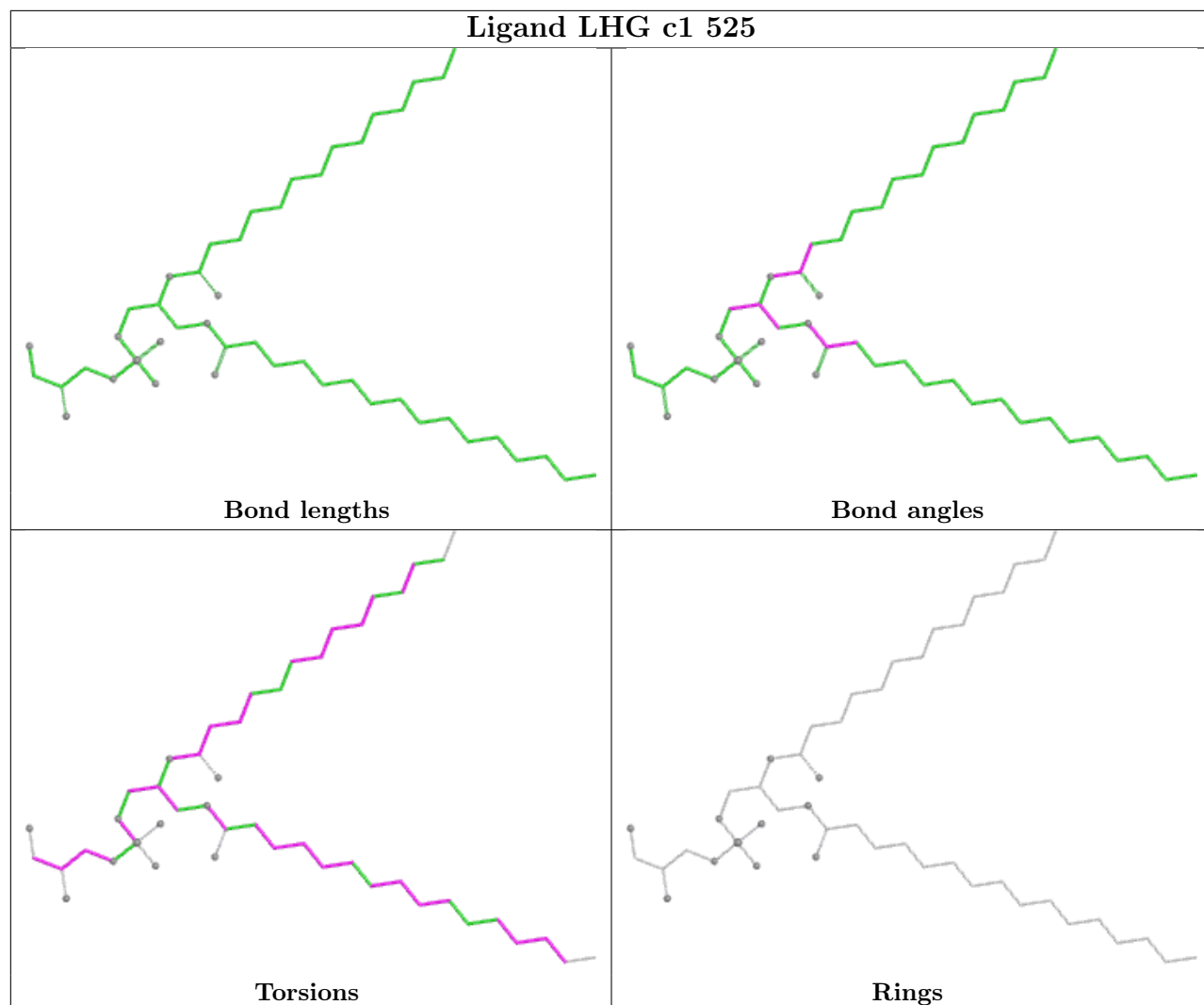
Ligand CLA S 609

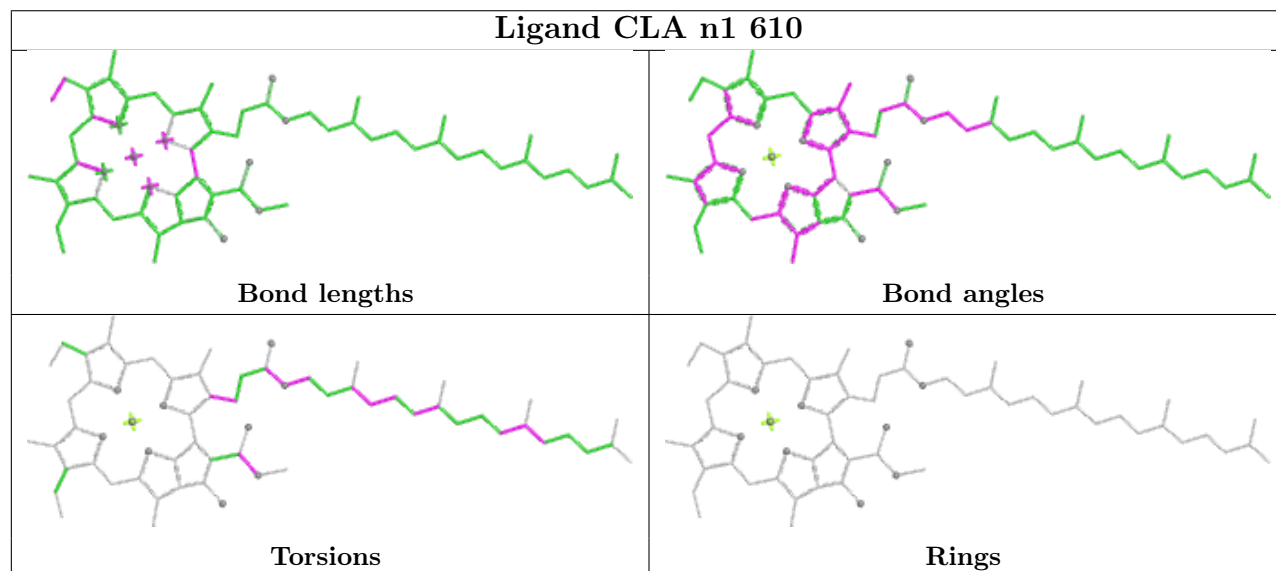
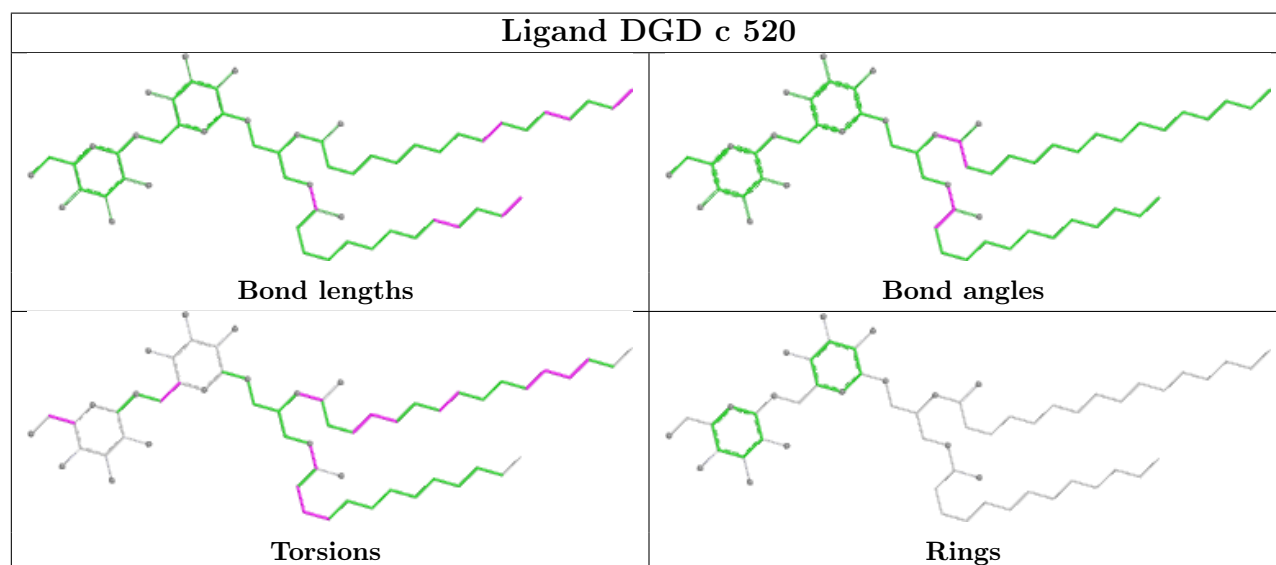
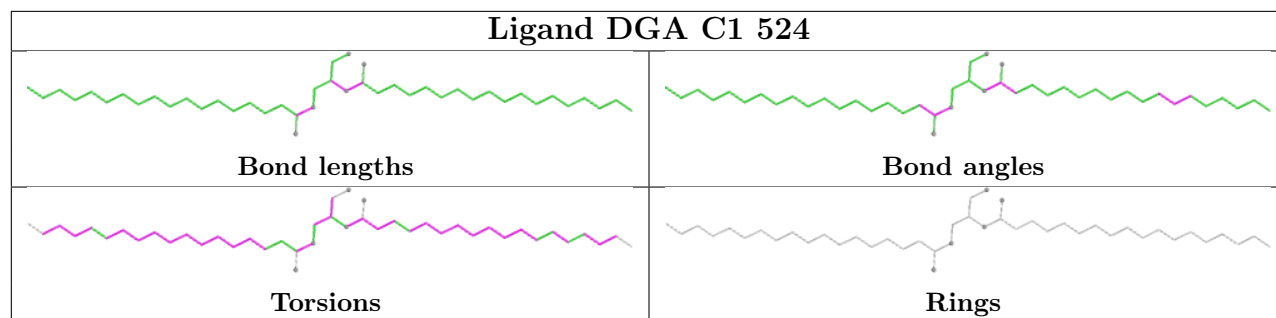


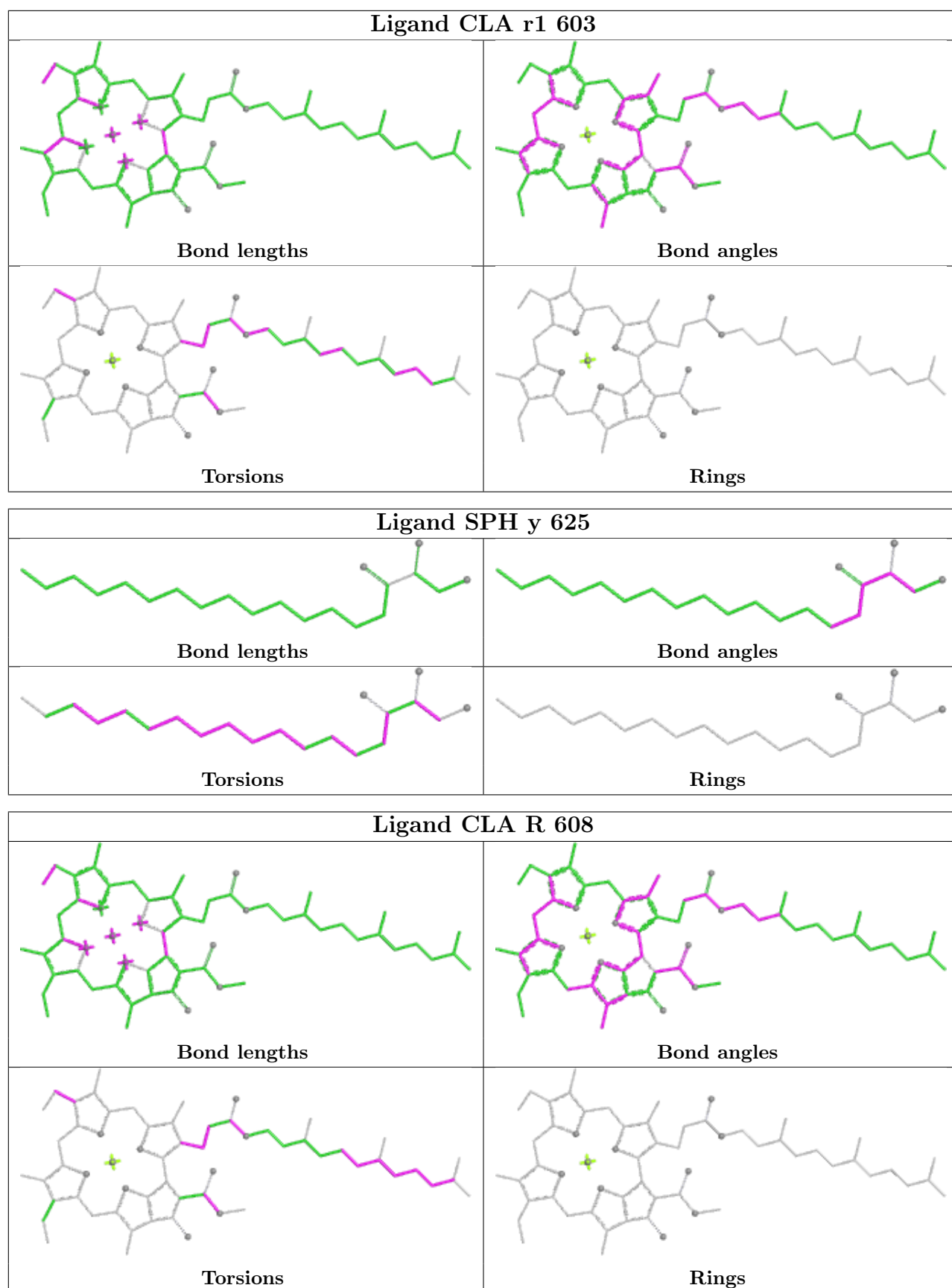
Ligand CLA c1 506



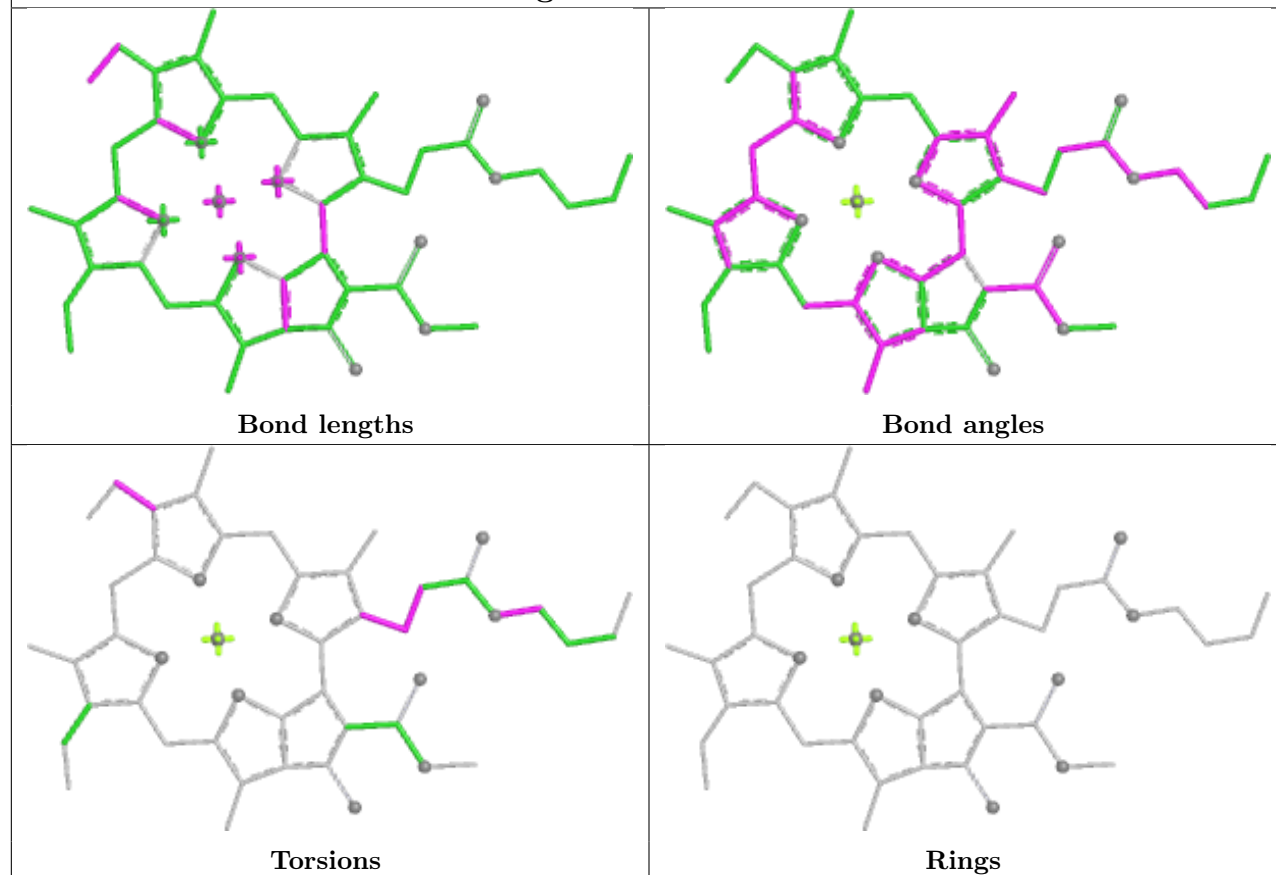




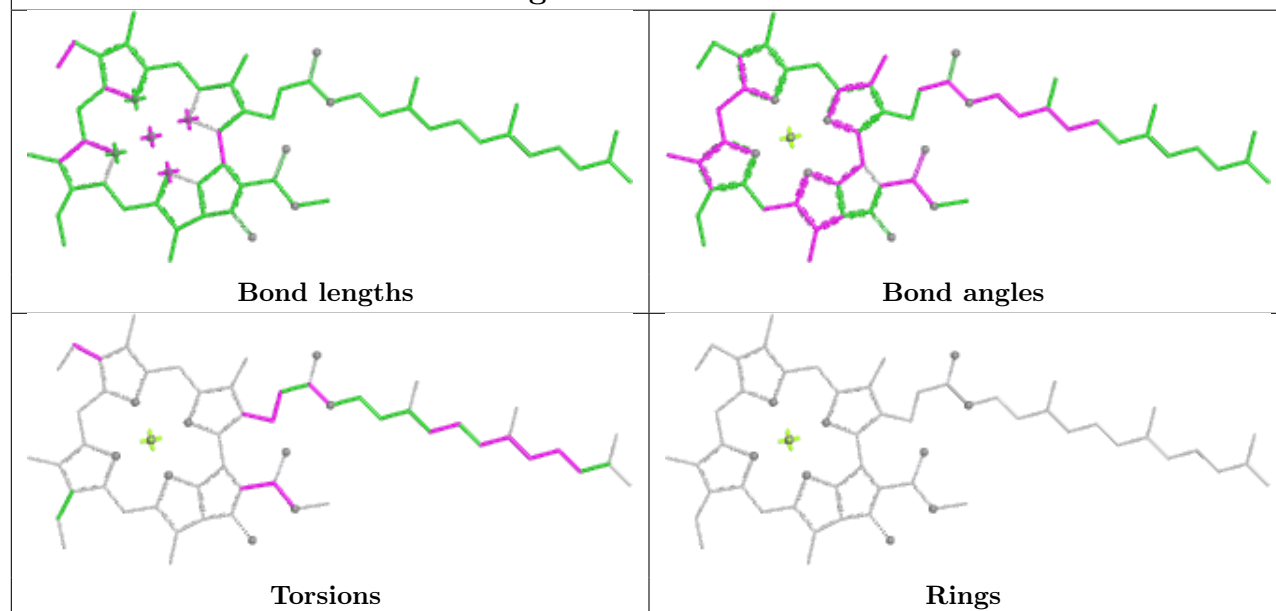


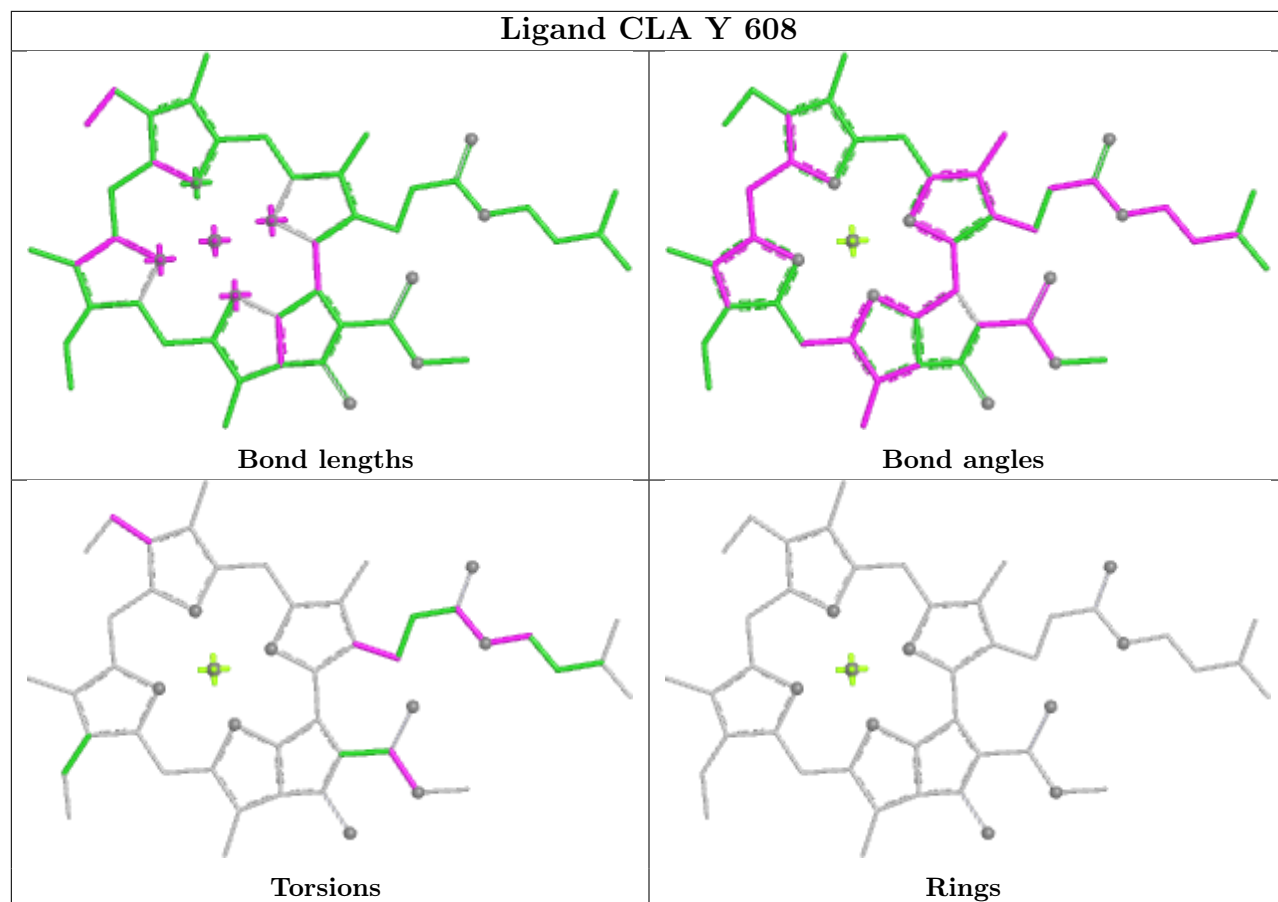


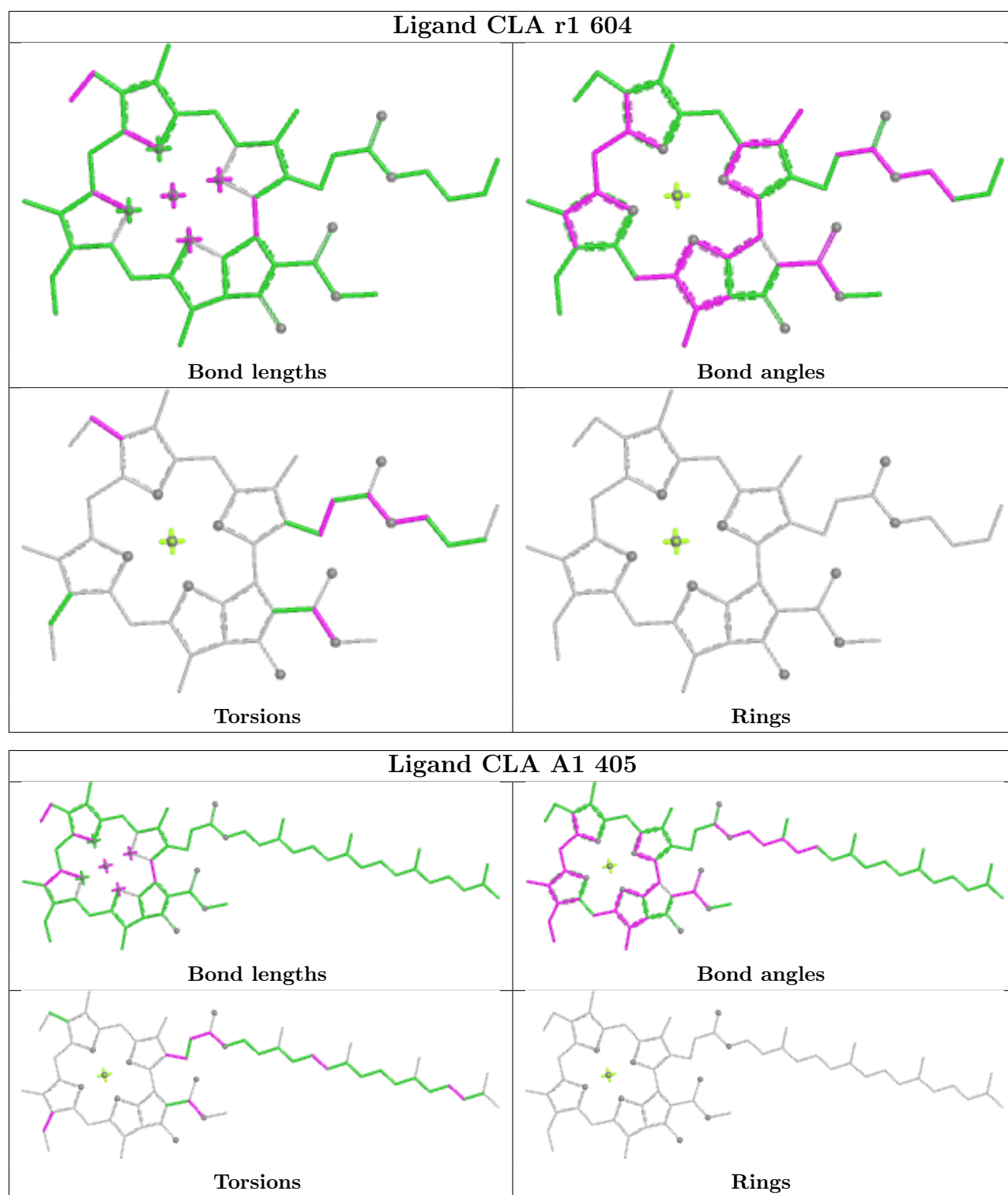
Ligand CLA a 407



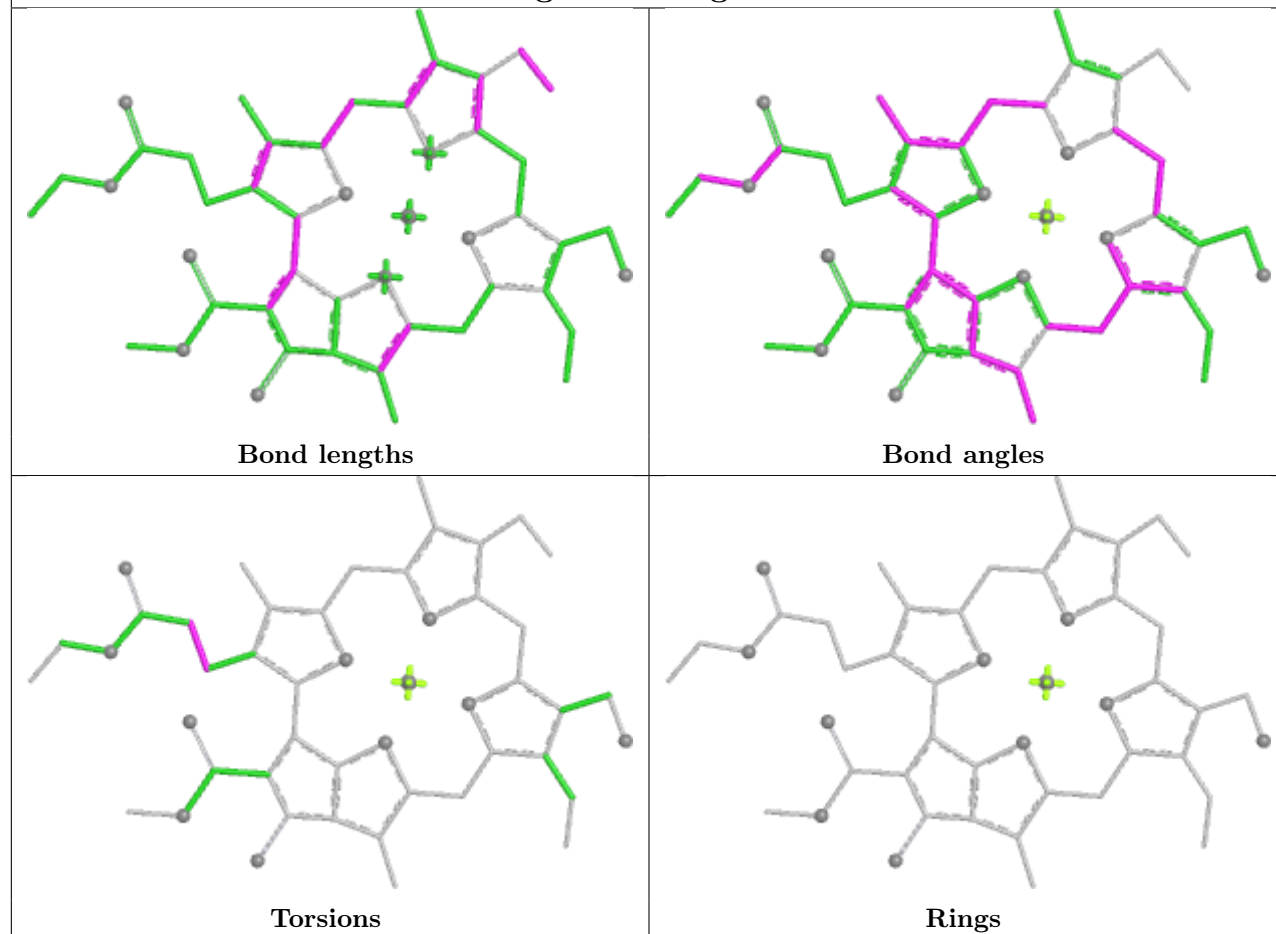
Ligand CLA r1 602



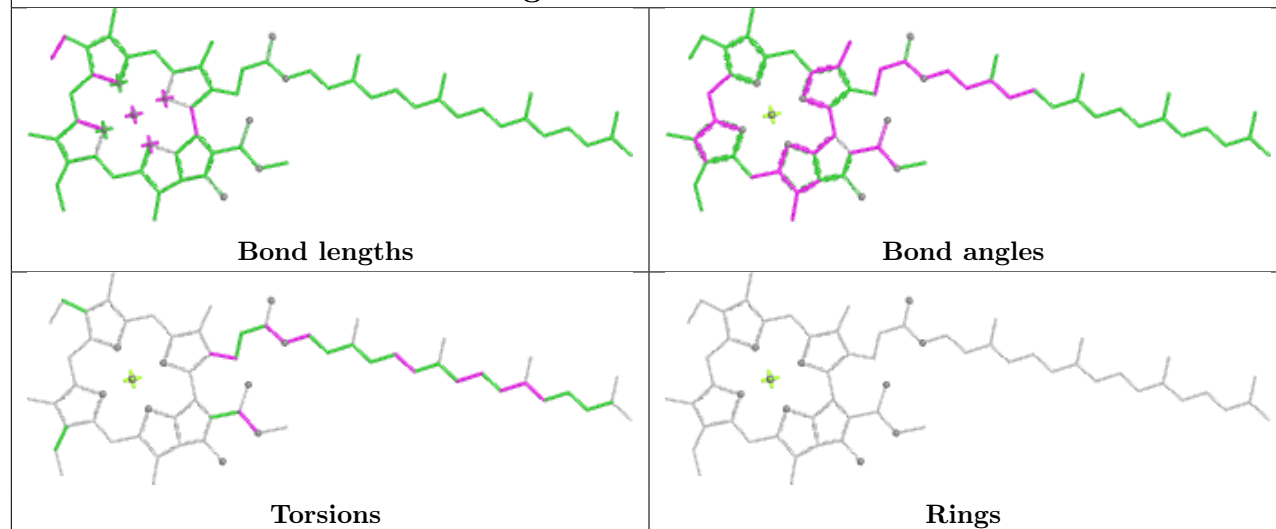


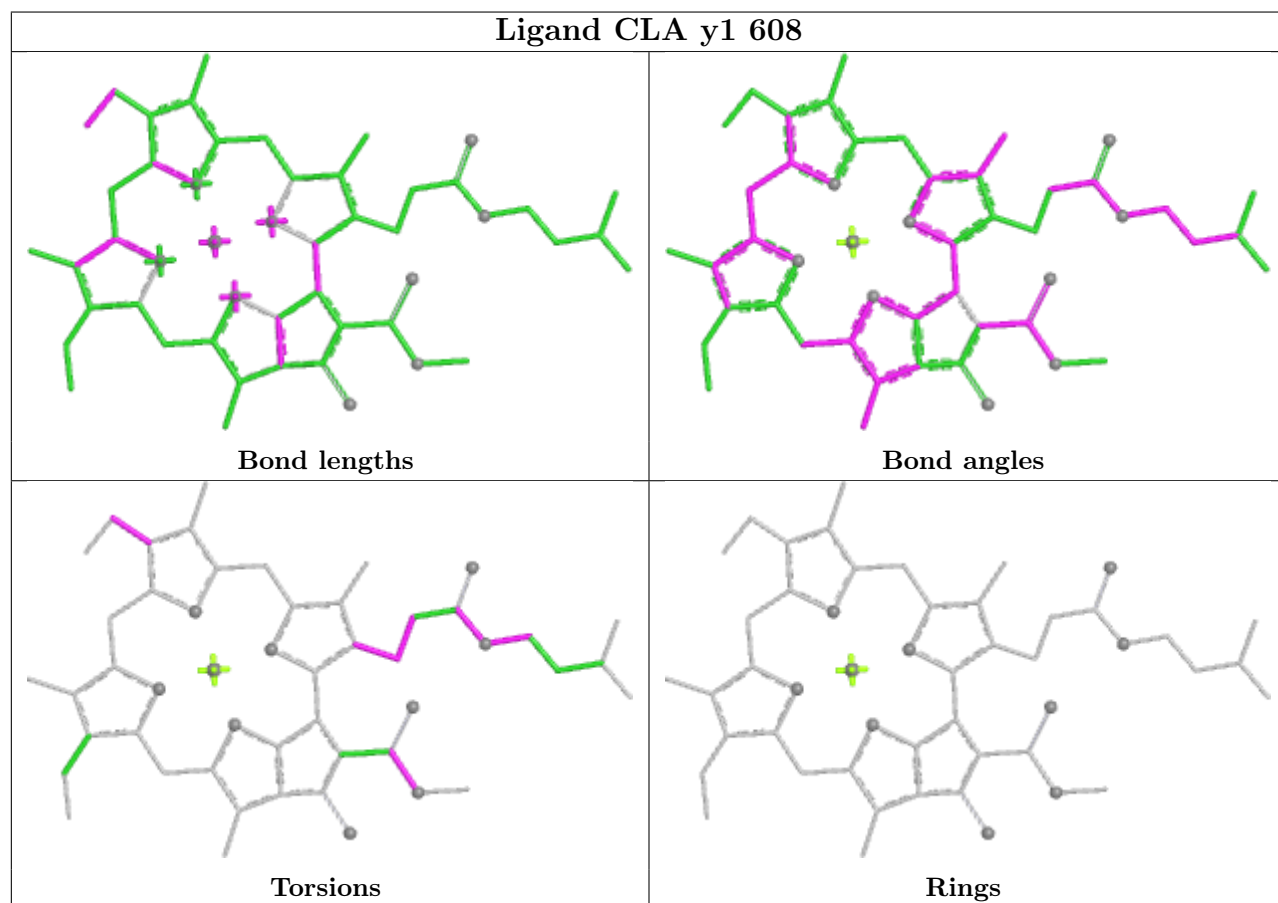
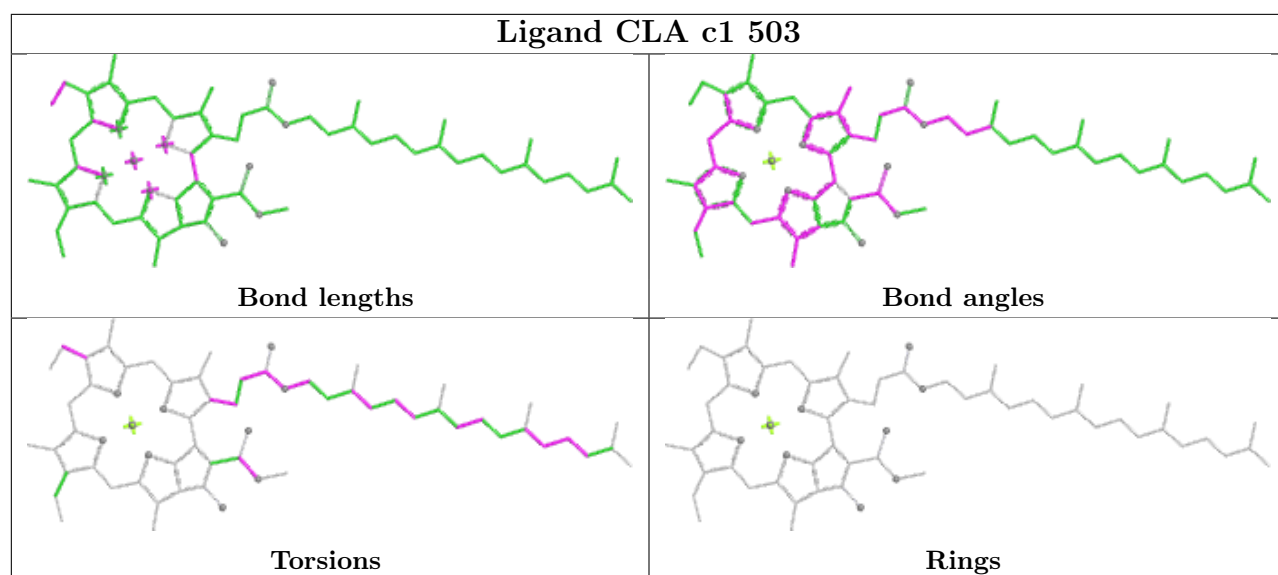


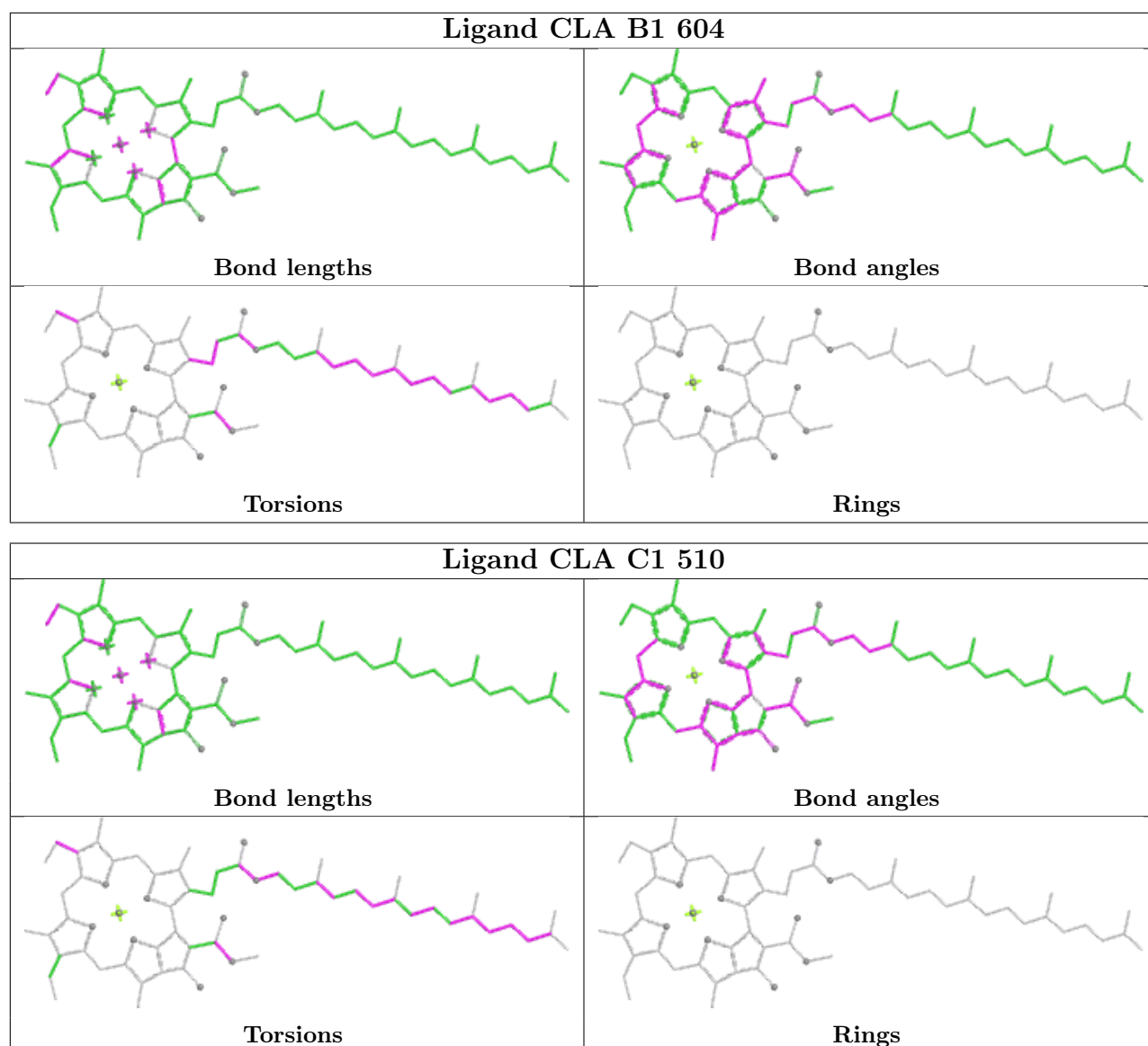
Ligand CHL g 605



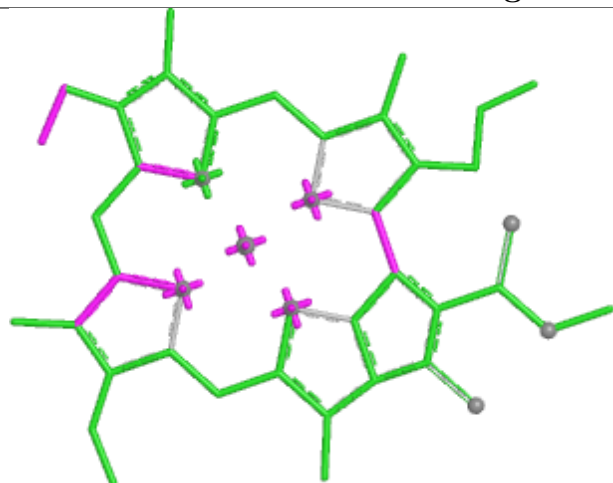
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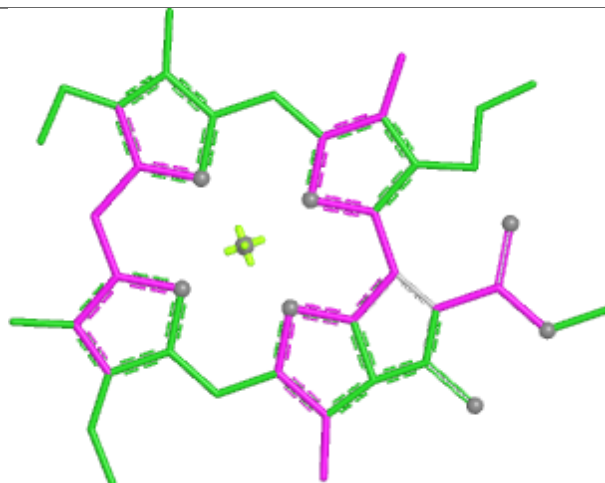




Ligand CLA G1 612



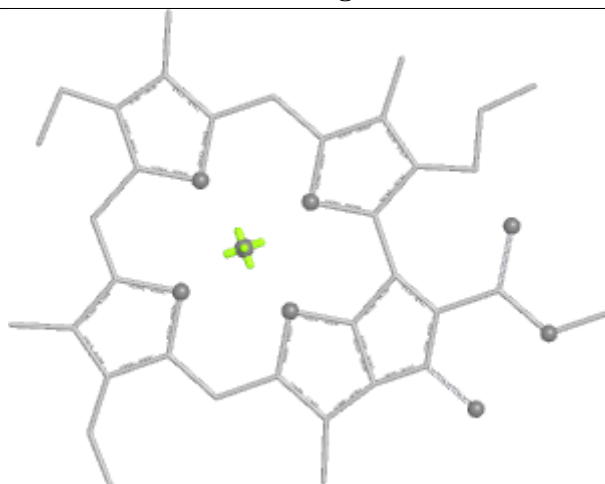
Bond lengths



Bond angles

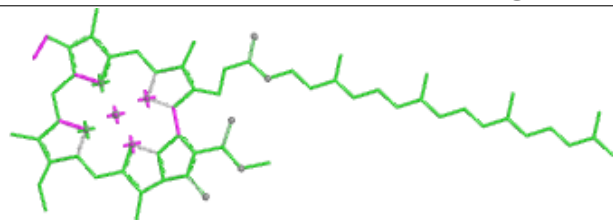


Torsions

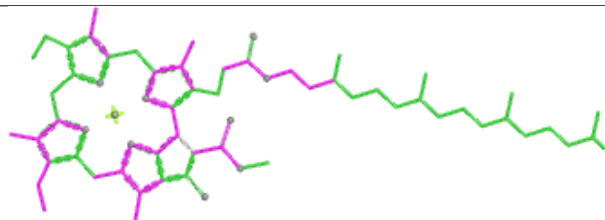


Rings

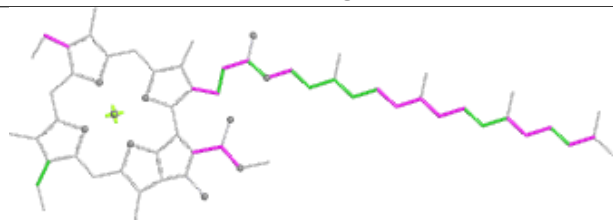
Ligand CLA b1 605



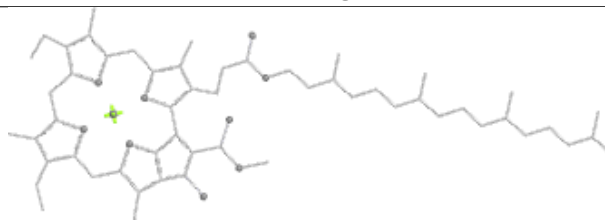
Bond lengths



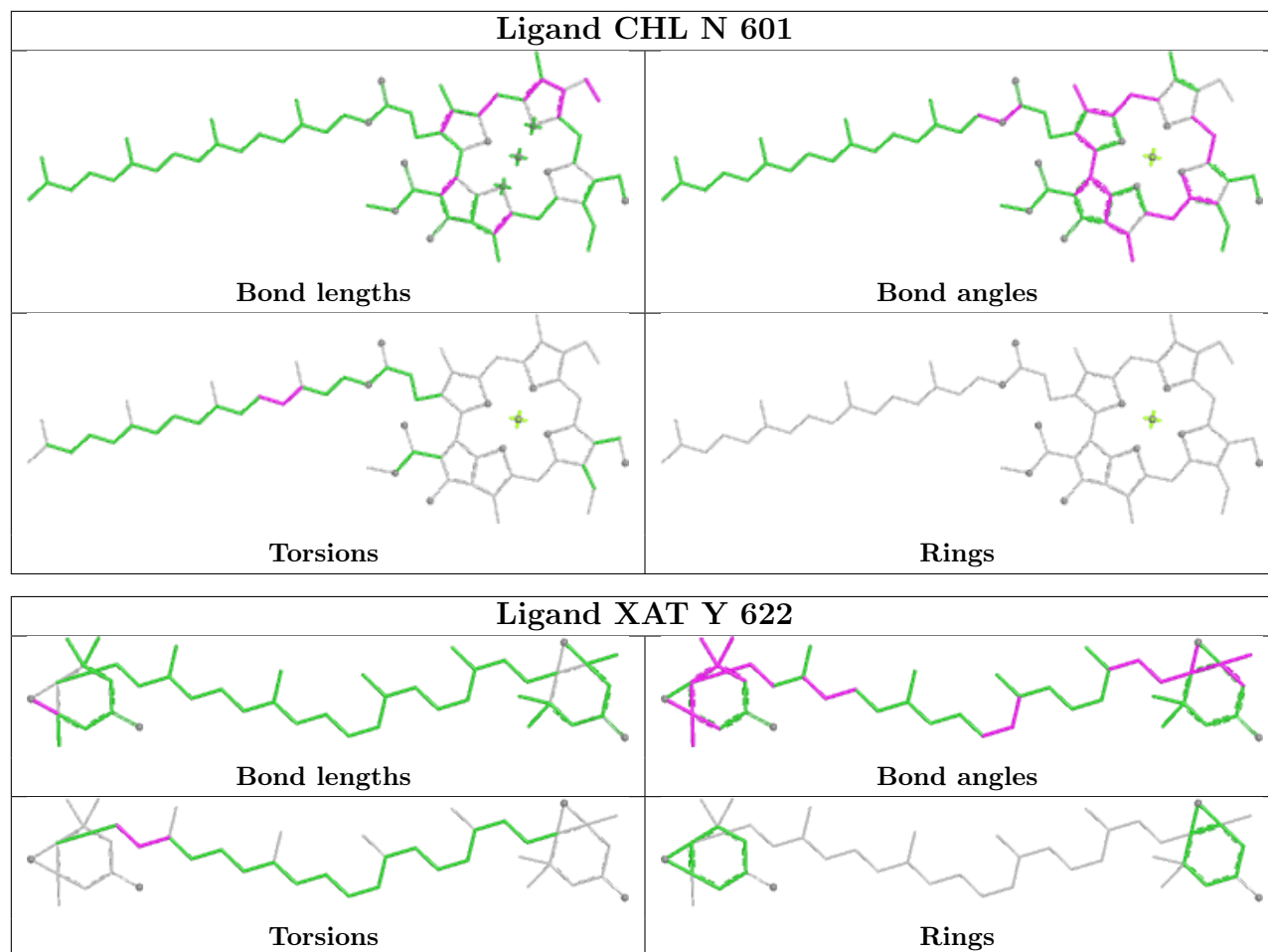
Bond angles

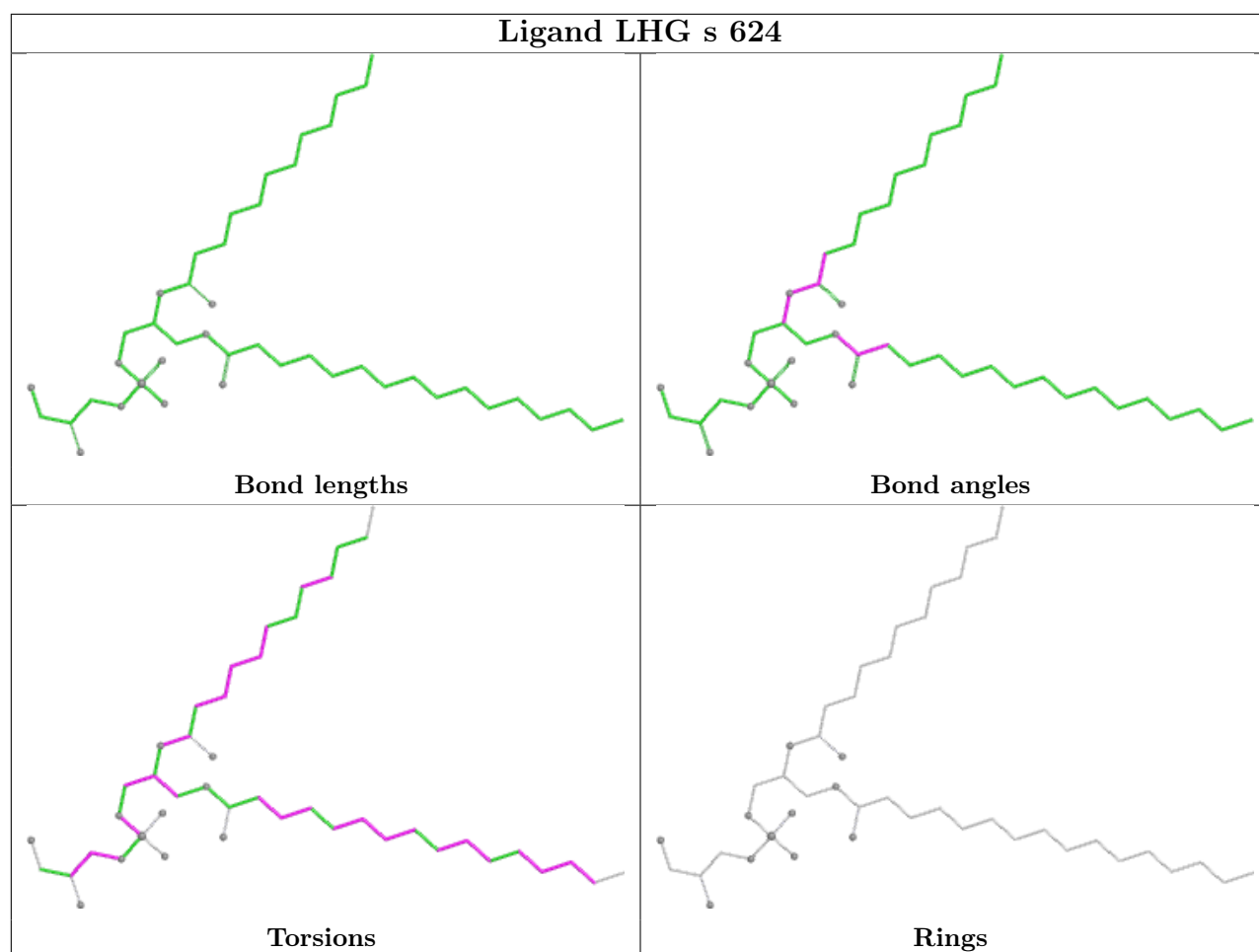


Torsions

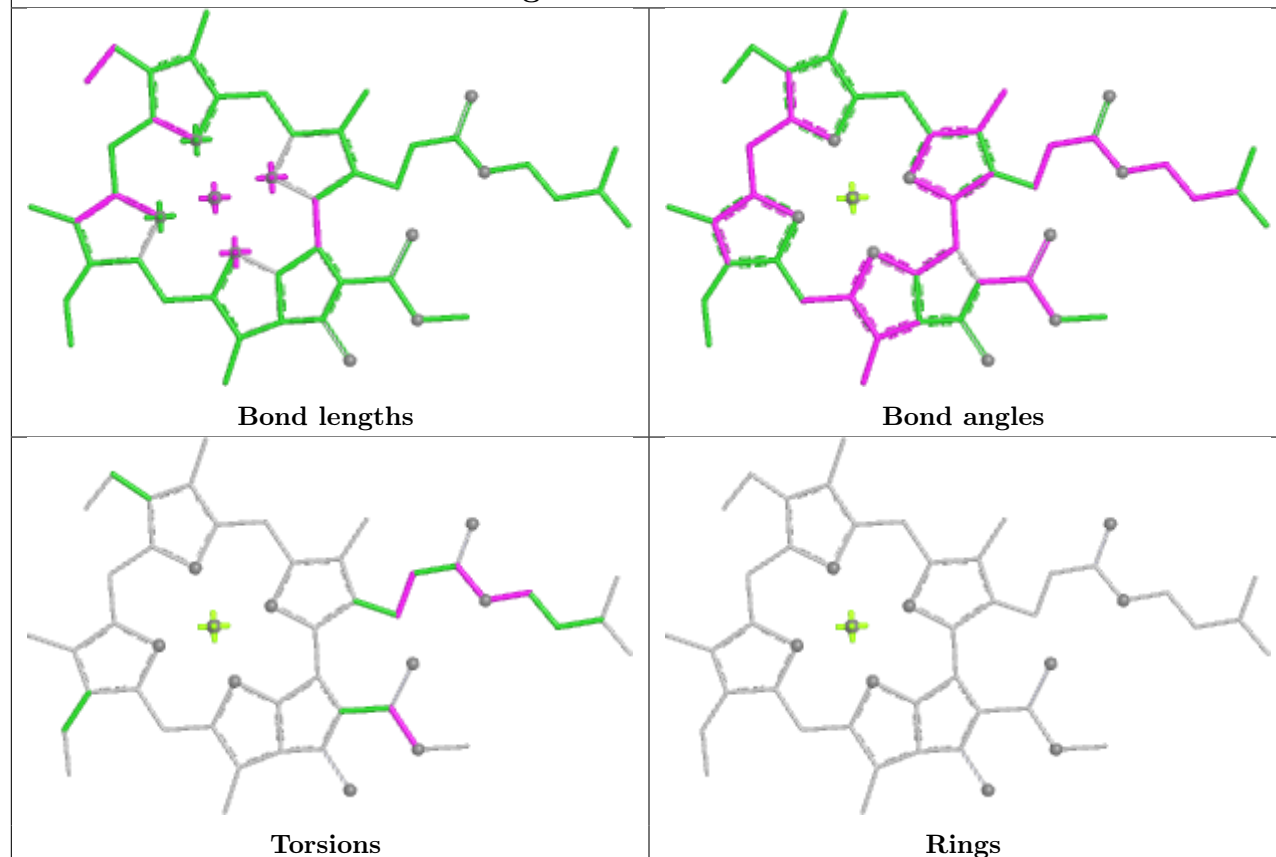


Rings

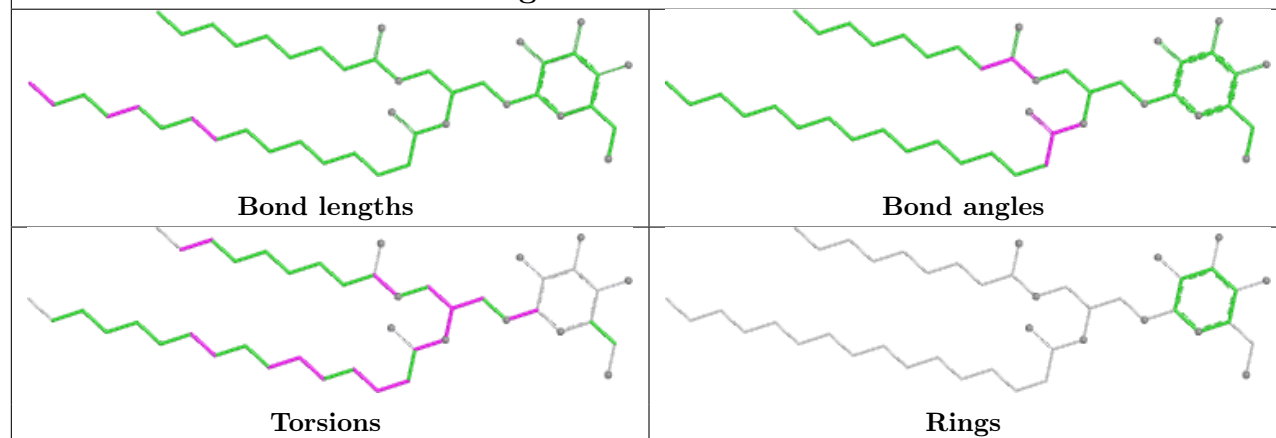


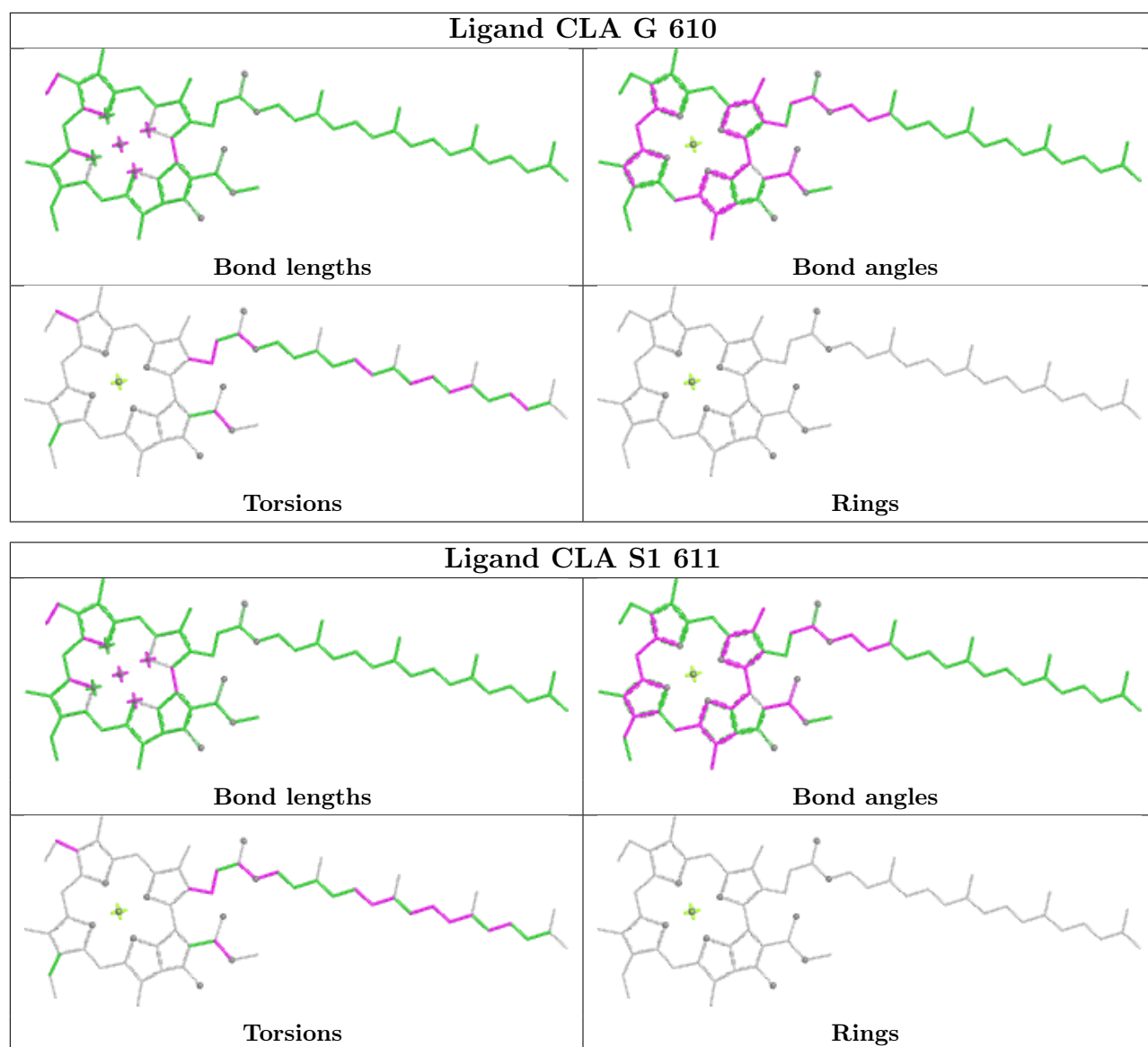


Ligand CLA A1 407

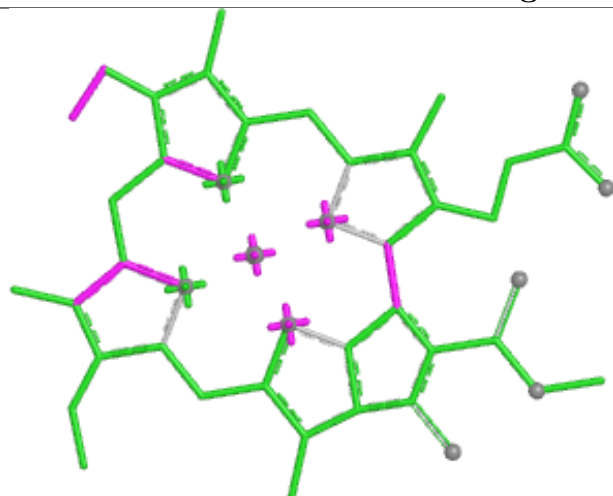


Ligand LMG B1 622

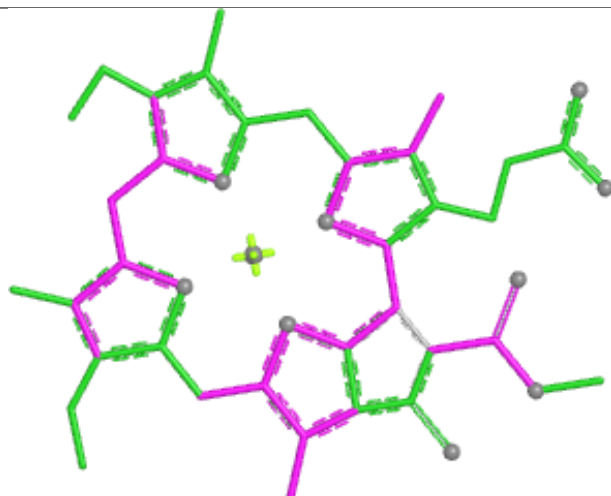




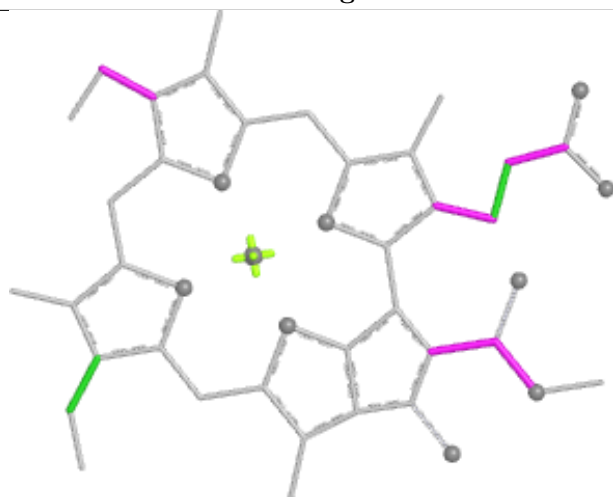
Ligand CLA s 612



Bond lengths



Bond angles

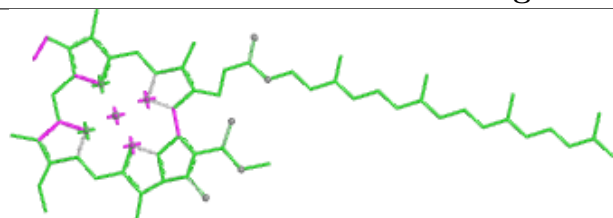


Torsions

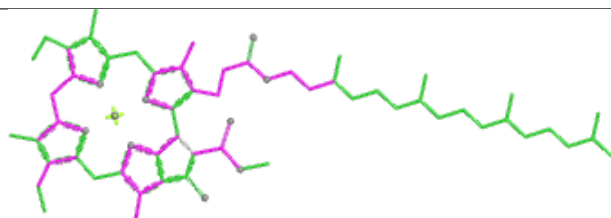


Rings

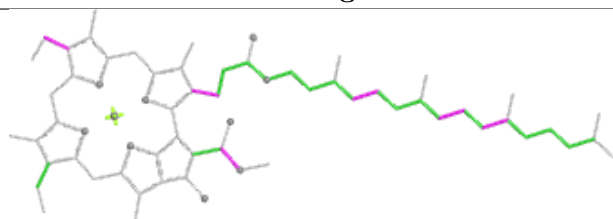
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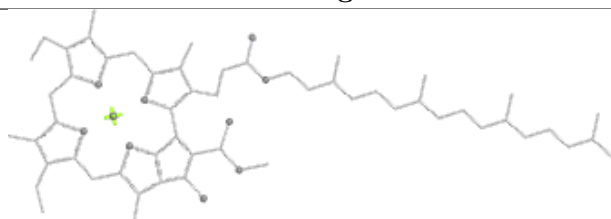
Bond lengths



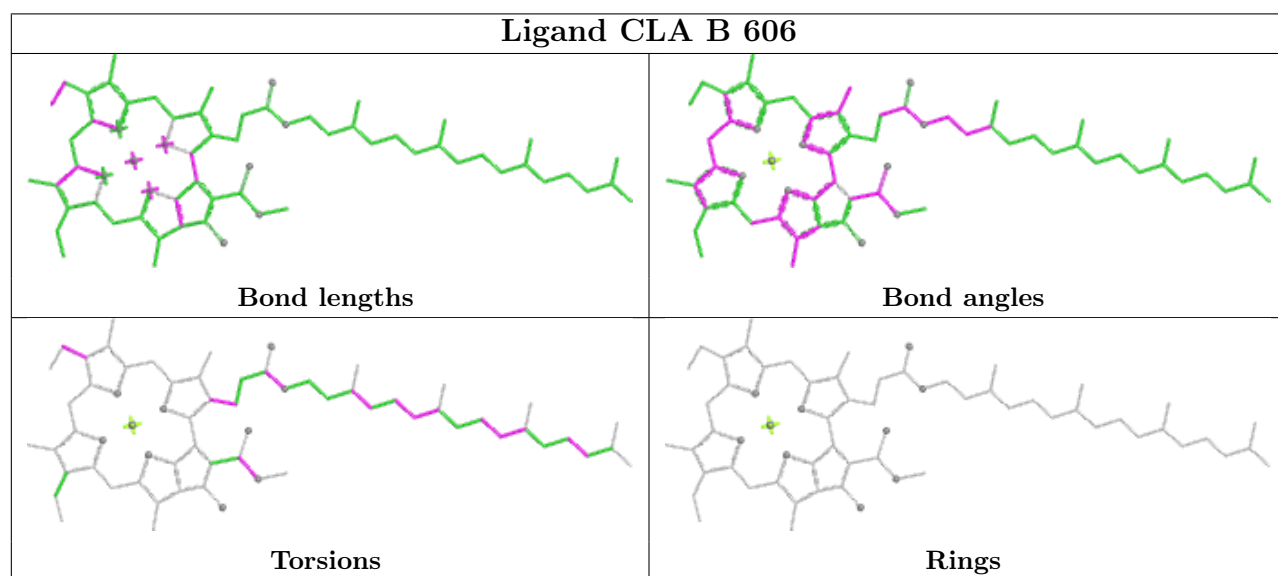
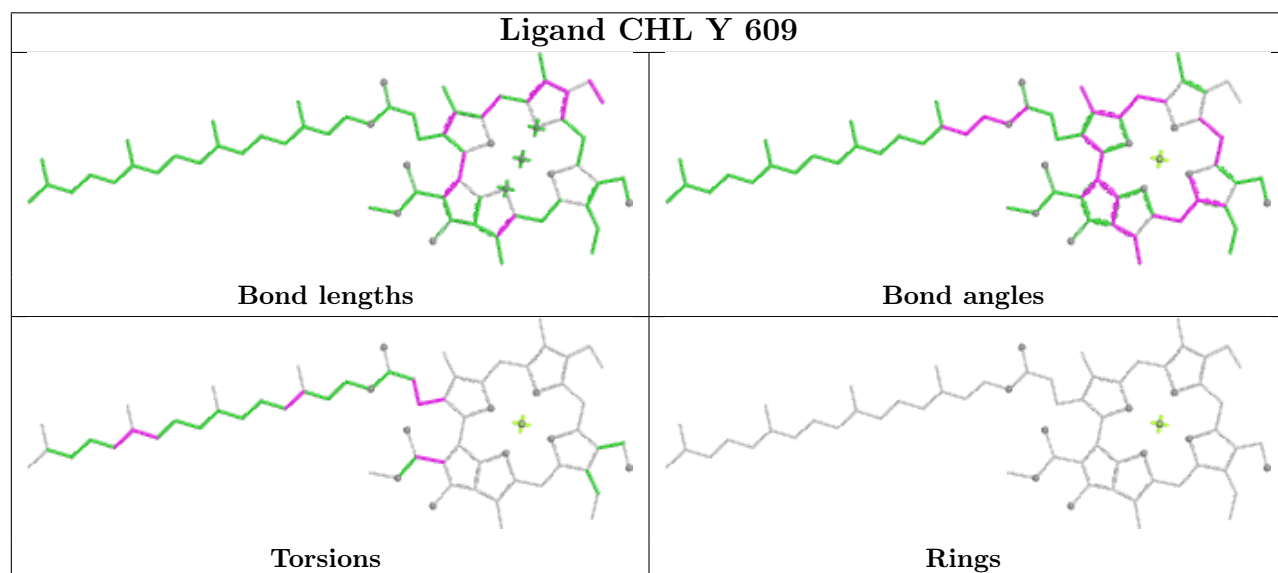
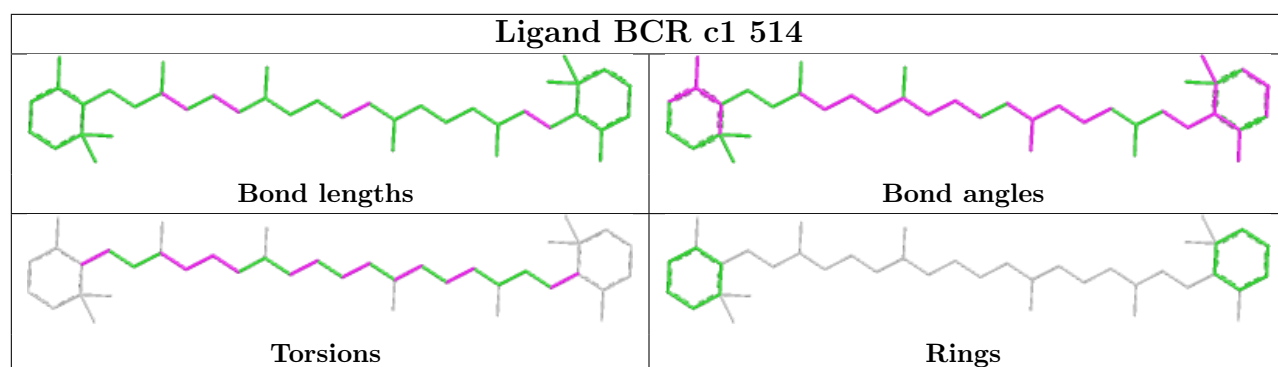
Bond angles

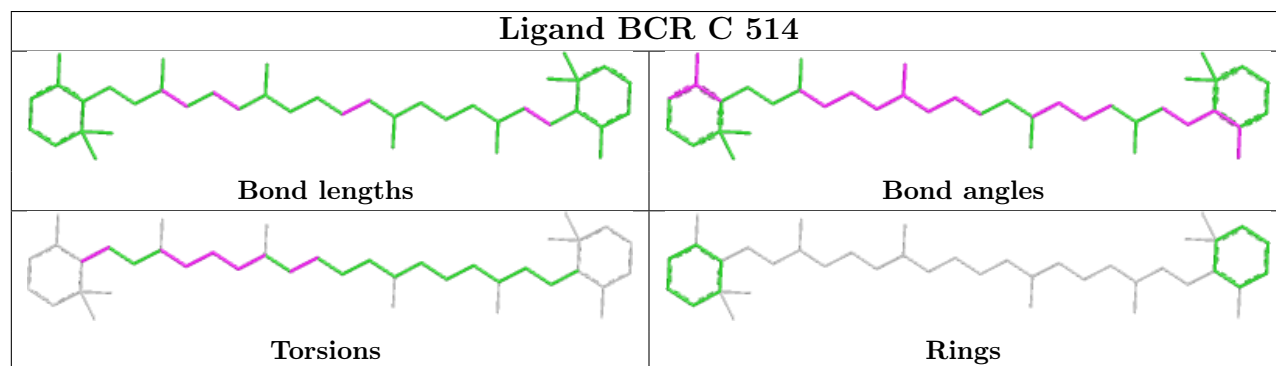
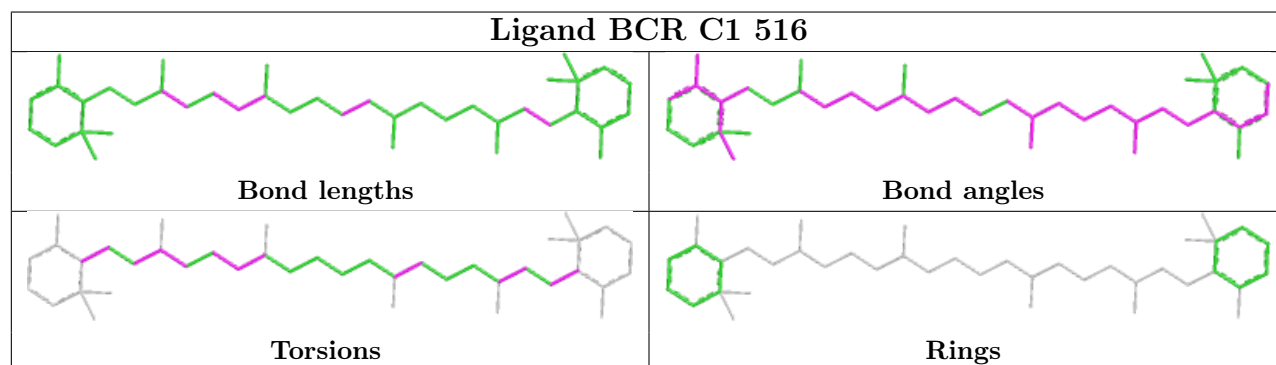
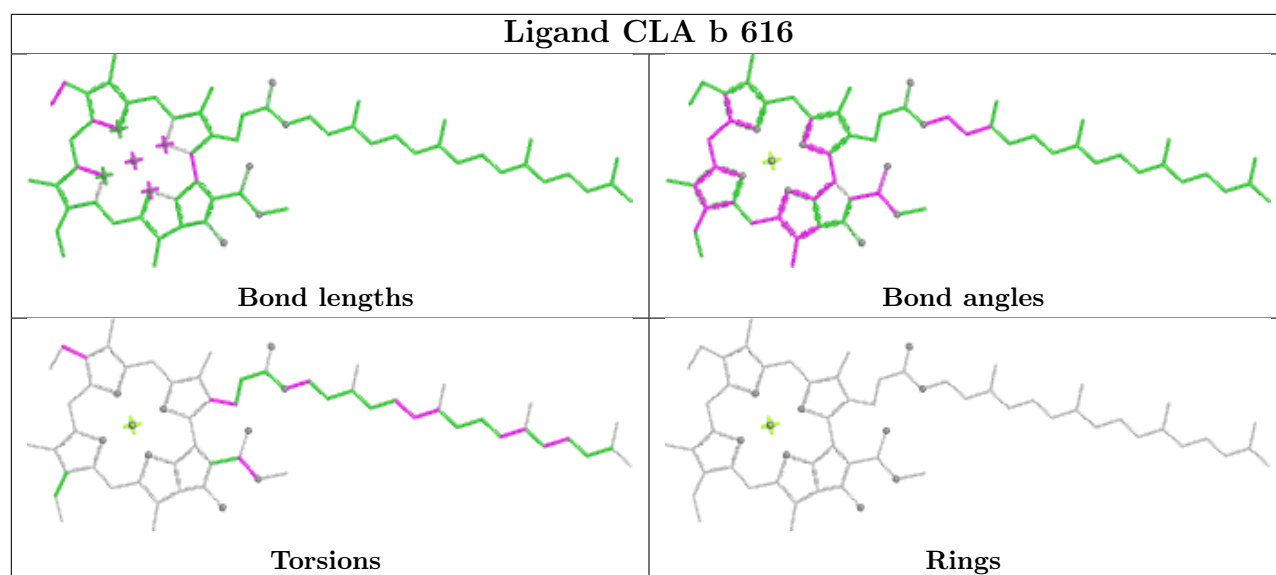


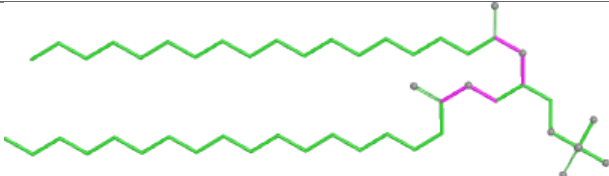
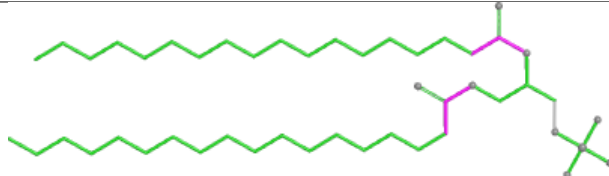
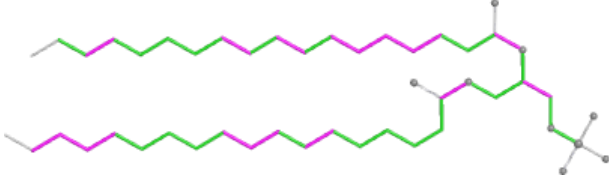
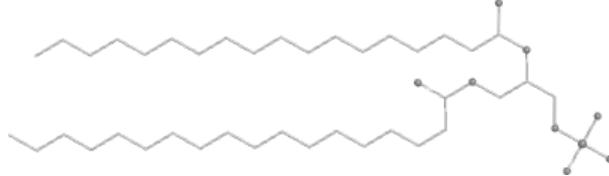
Torsions

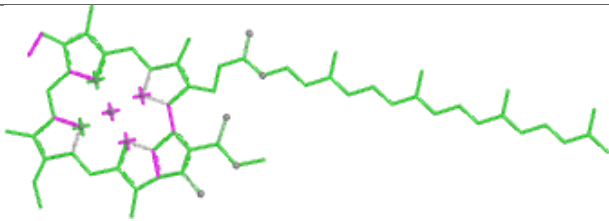
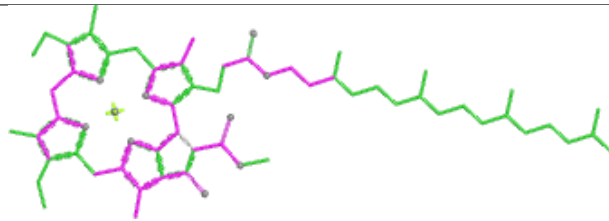
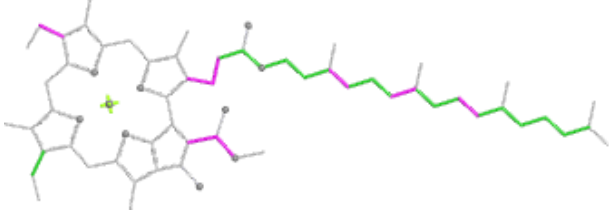
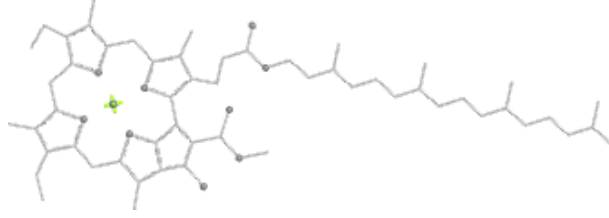


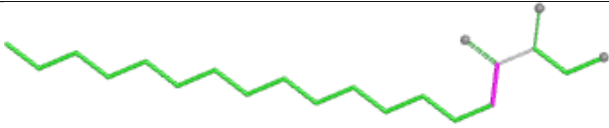
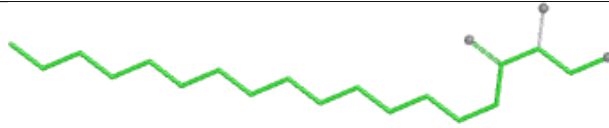
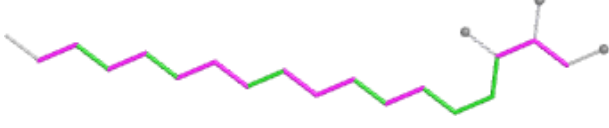
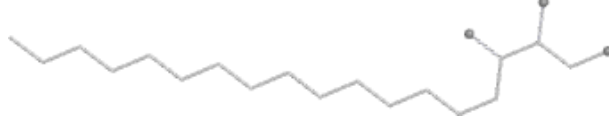
Rings

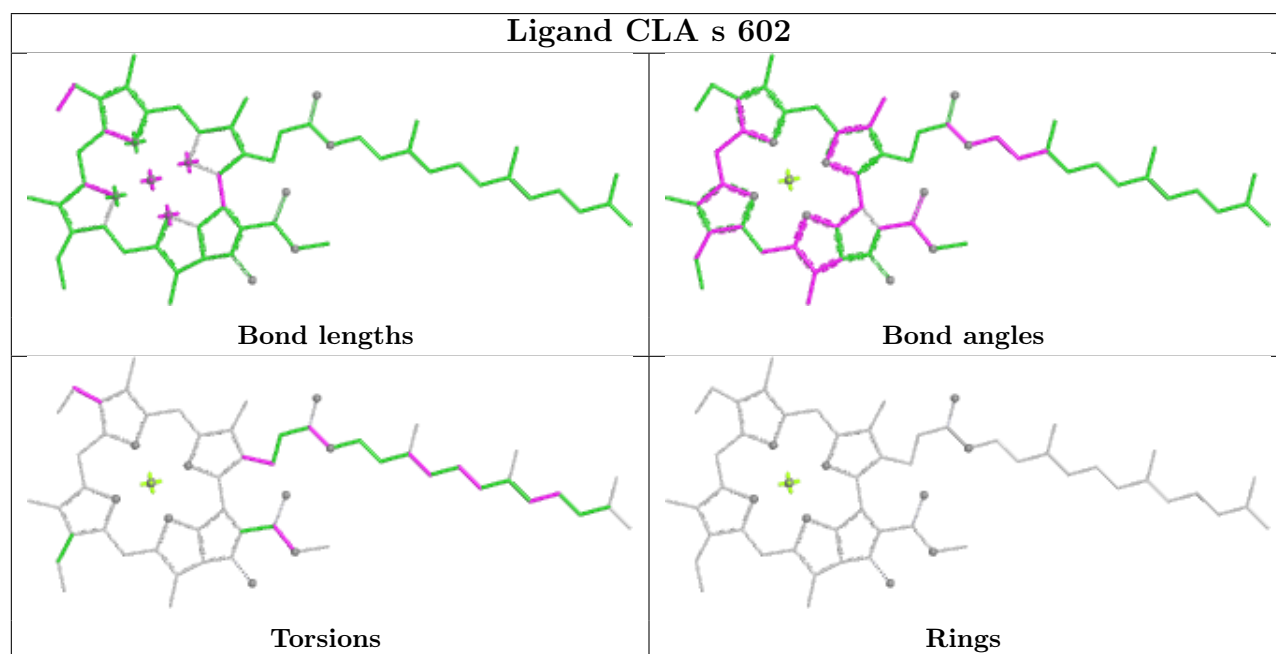
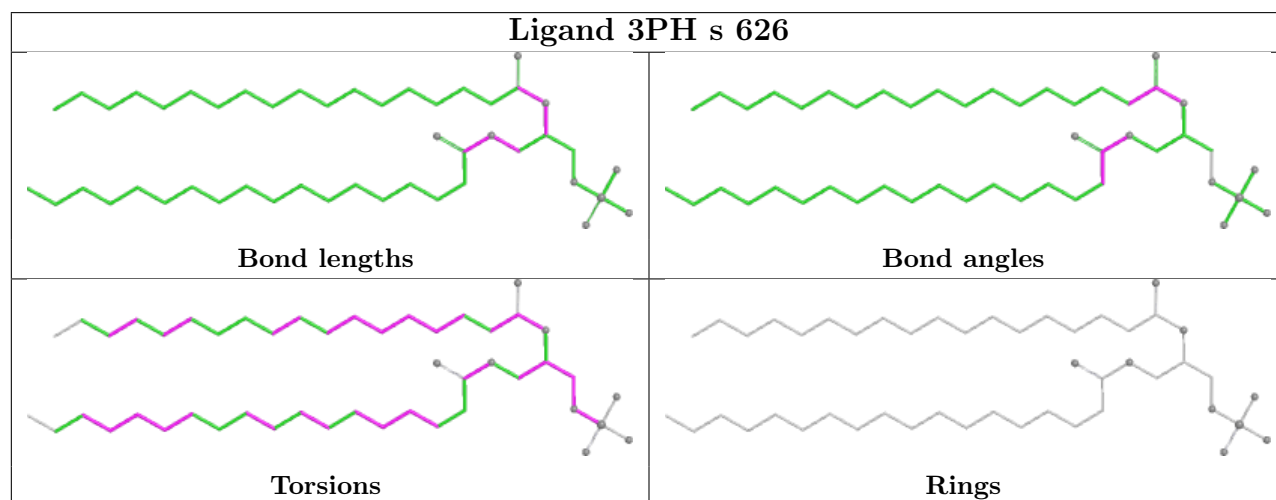
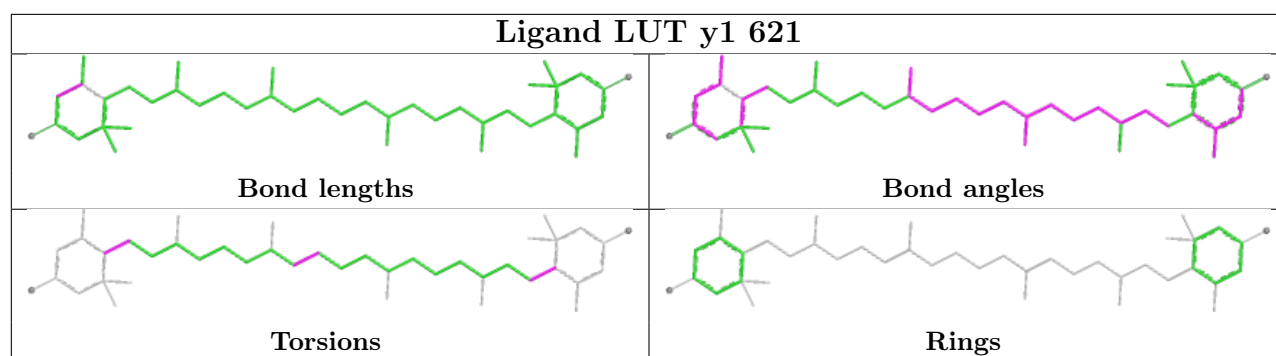


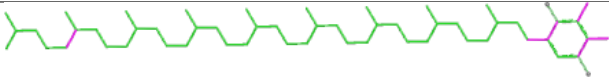
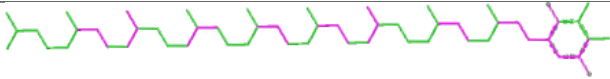
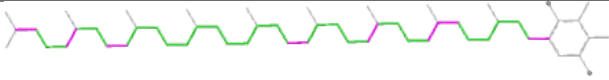
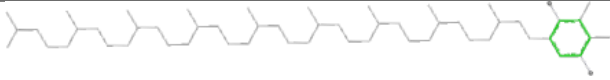


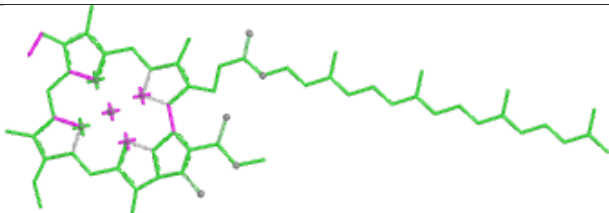
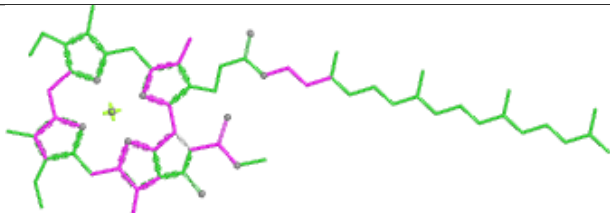
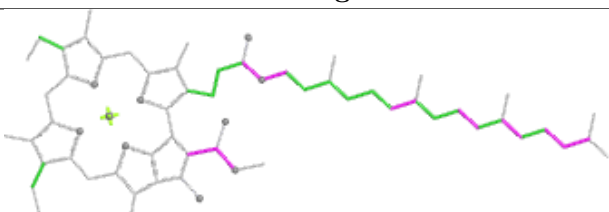
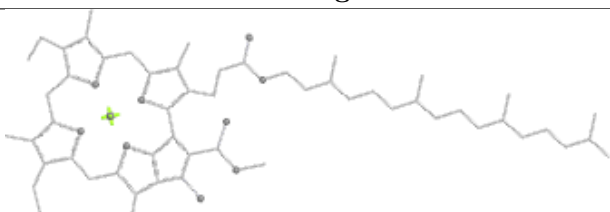
Ligand 3PH S 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

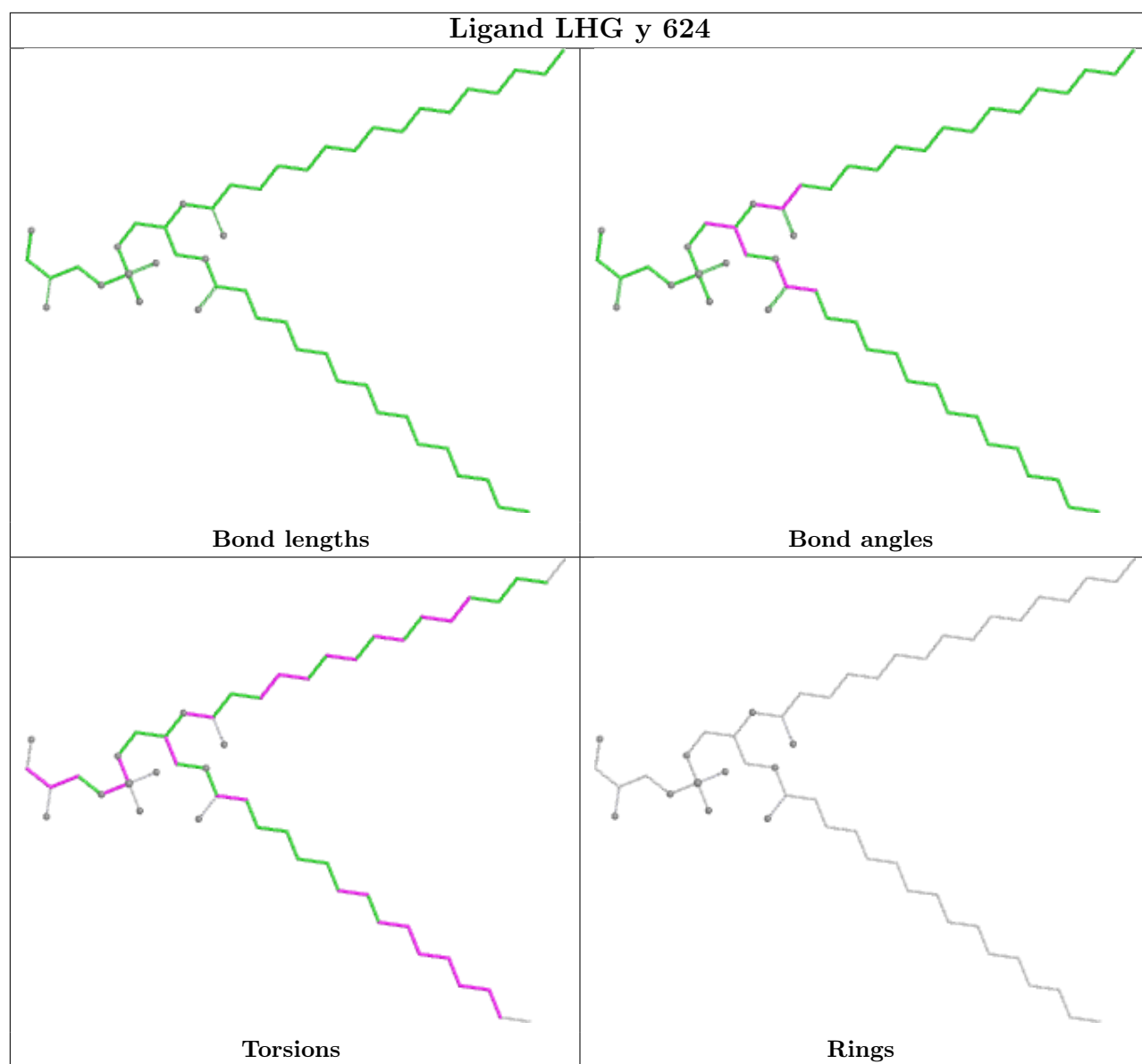
Ligand CLA N1 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

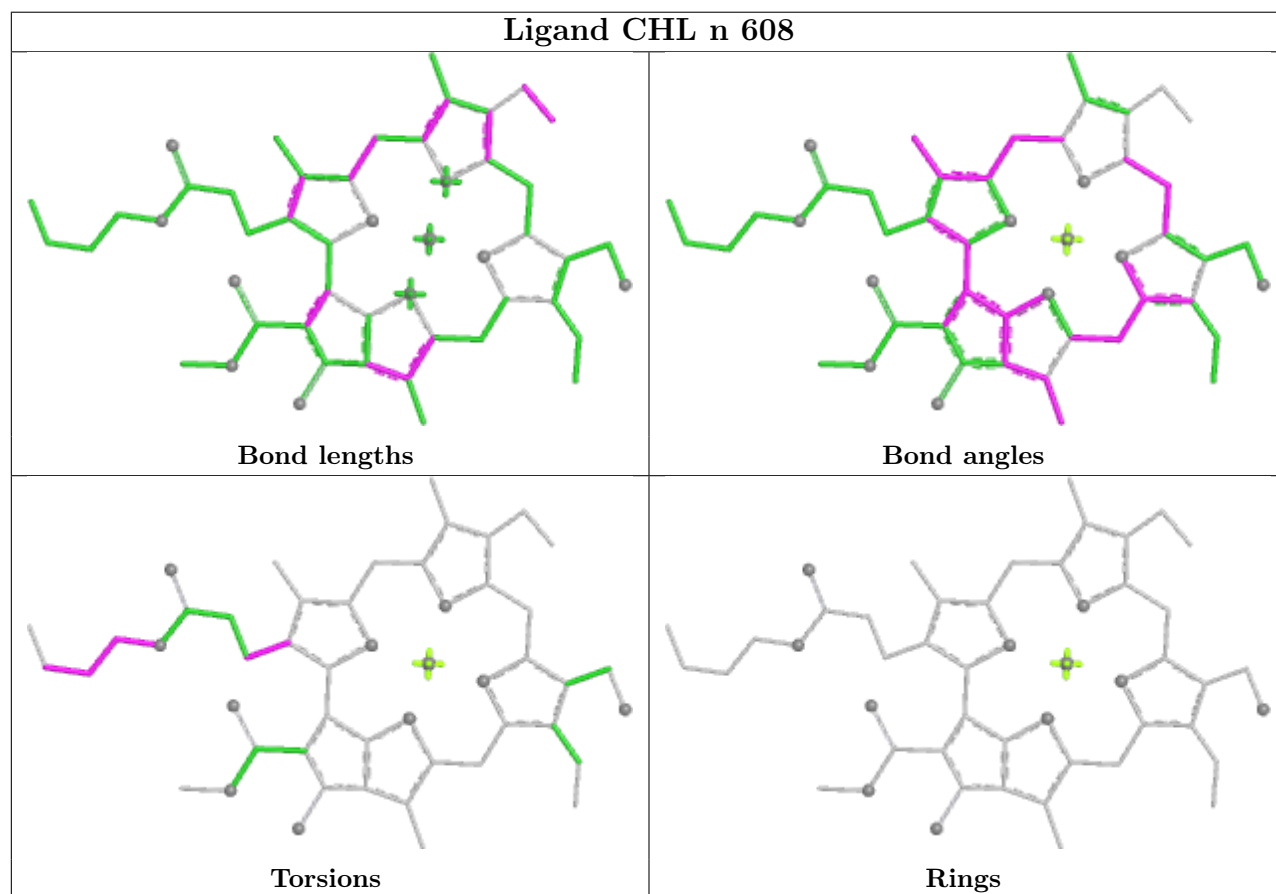
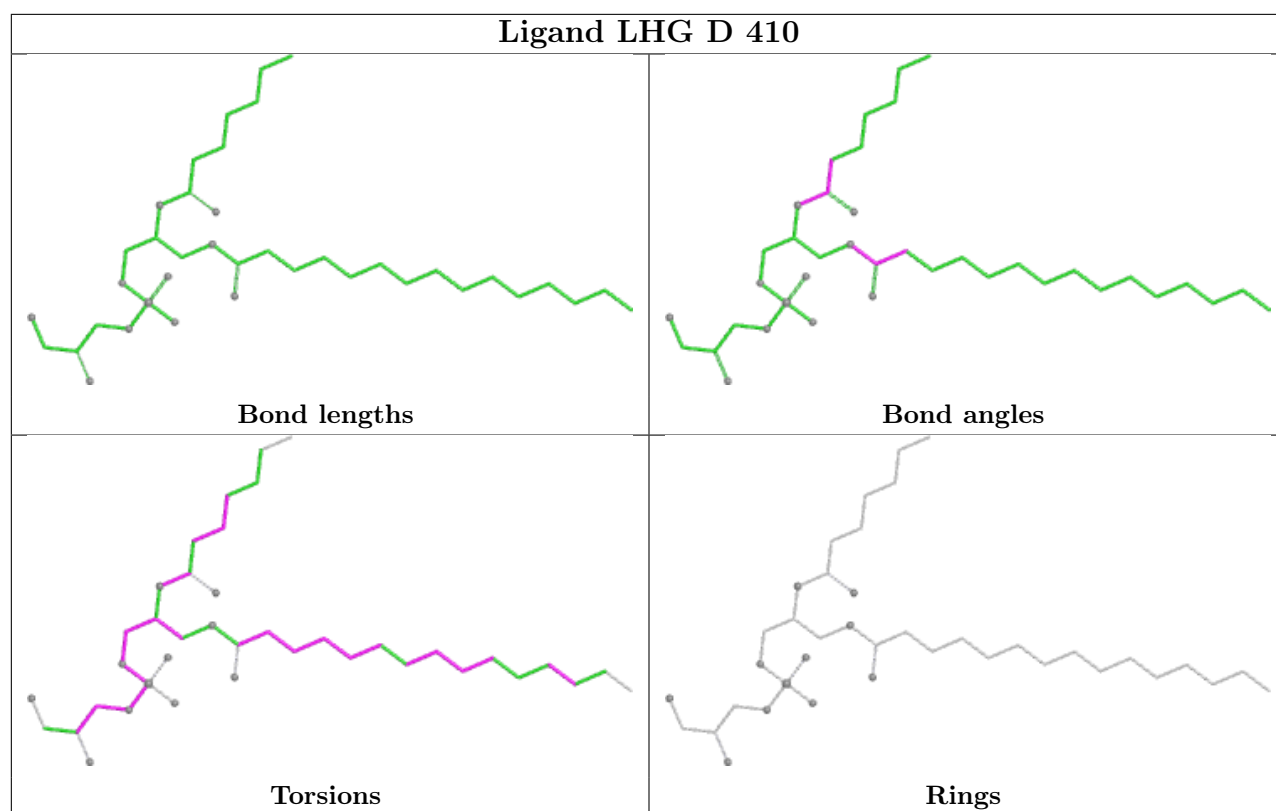
Ligand SPH A1 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

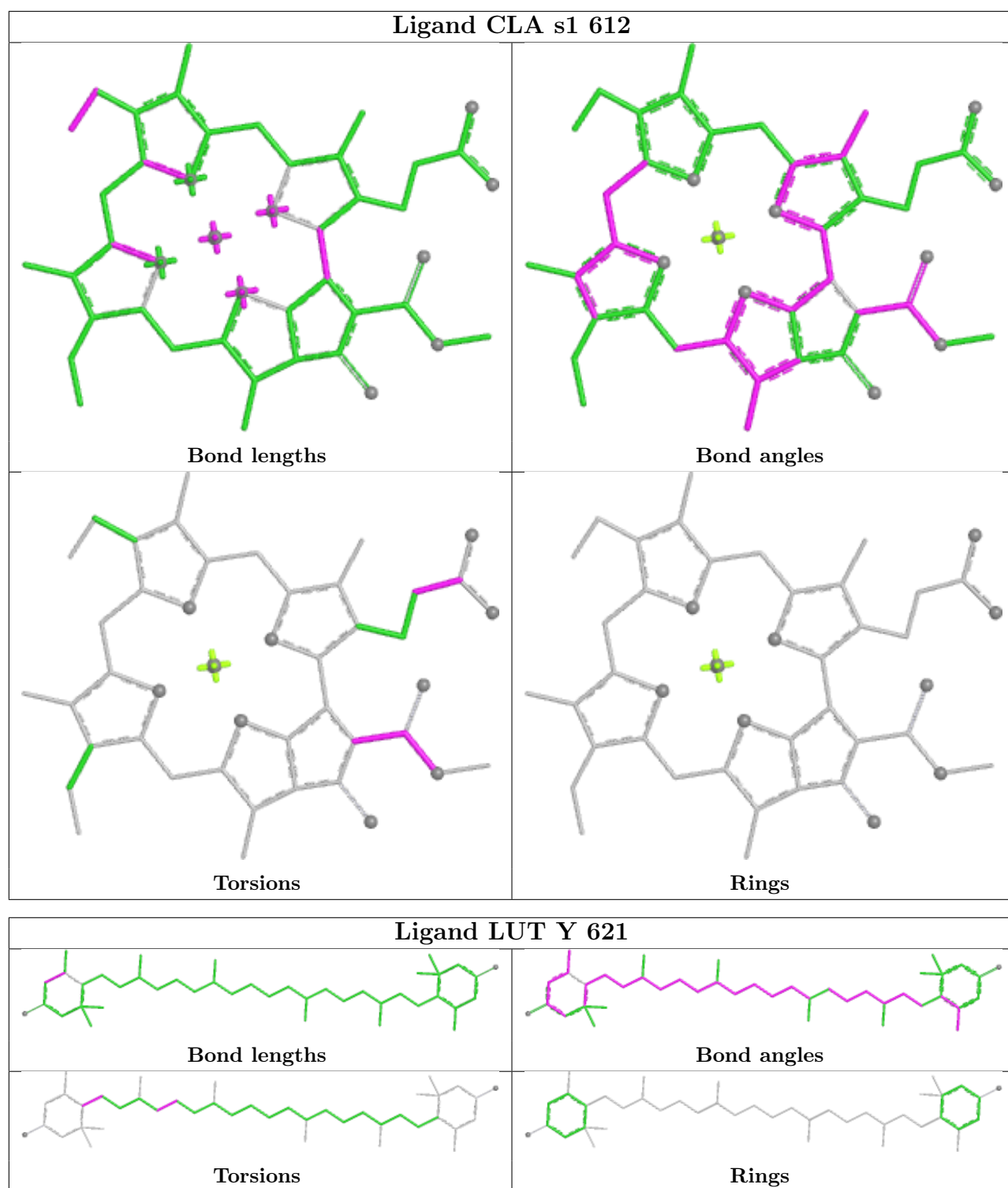


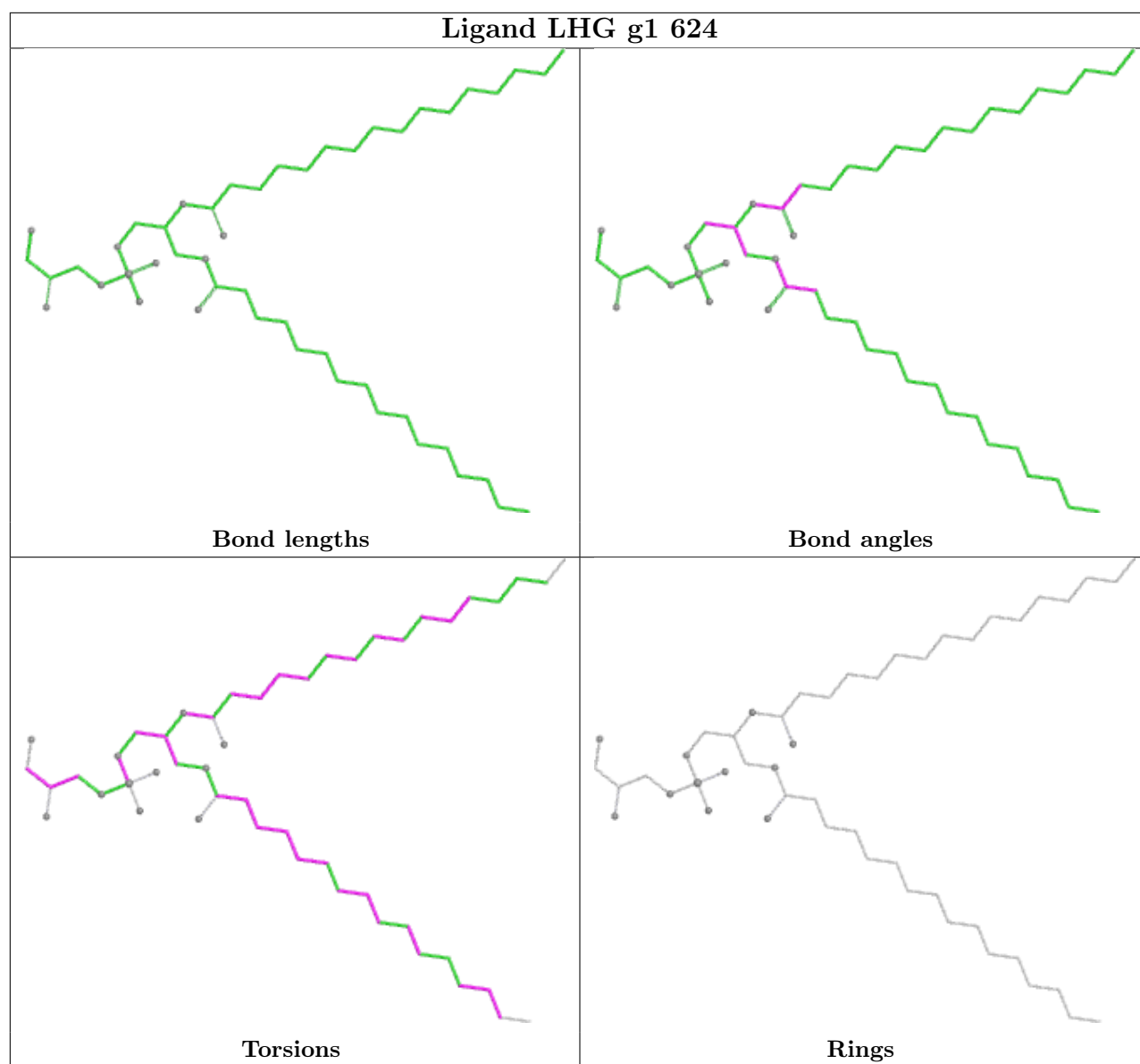
Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c1 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

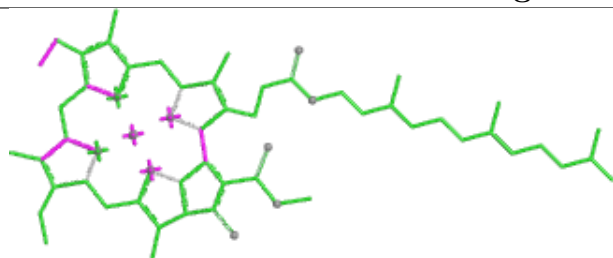




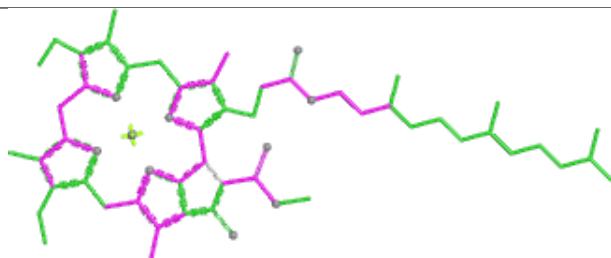




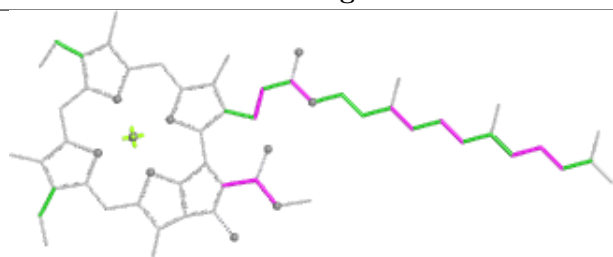
Ligand CLA R 602



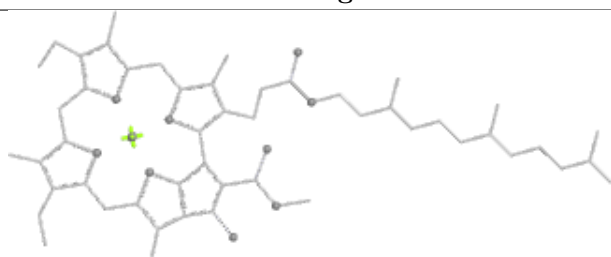
Bond lengths



Bond angles

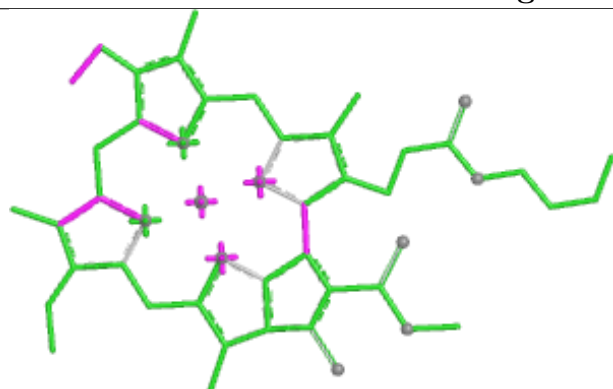


Torsions

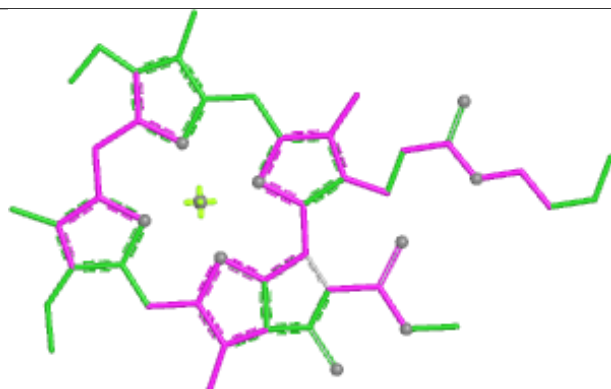


Rings

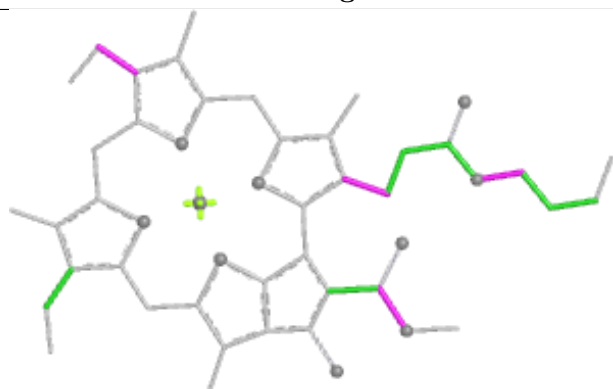
Ligand CLA n 614



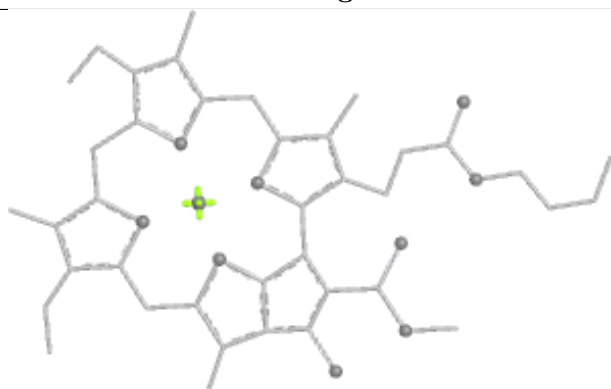
Bond lengths



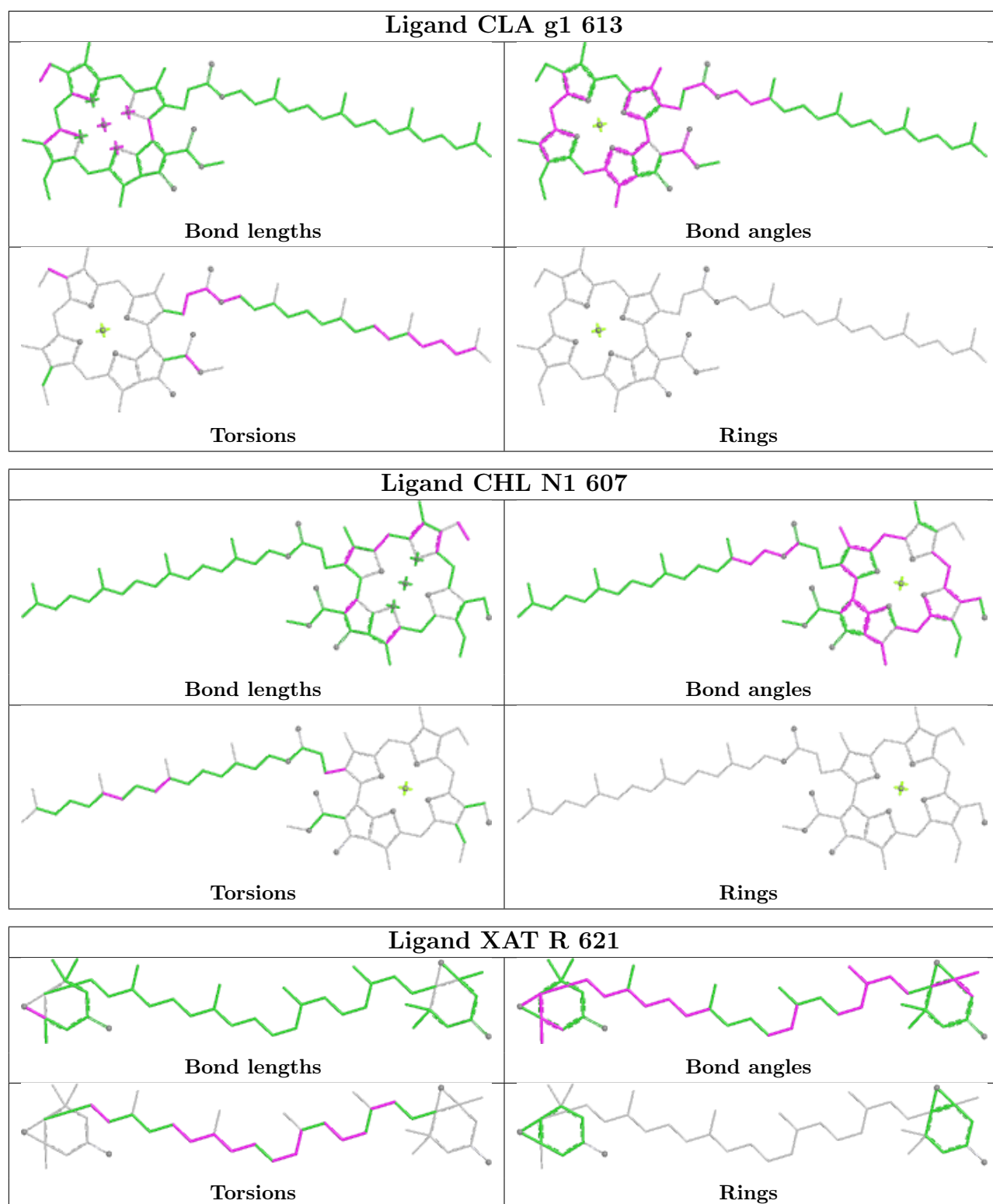
Bond angles

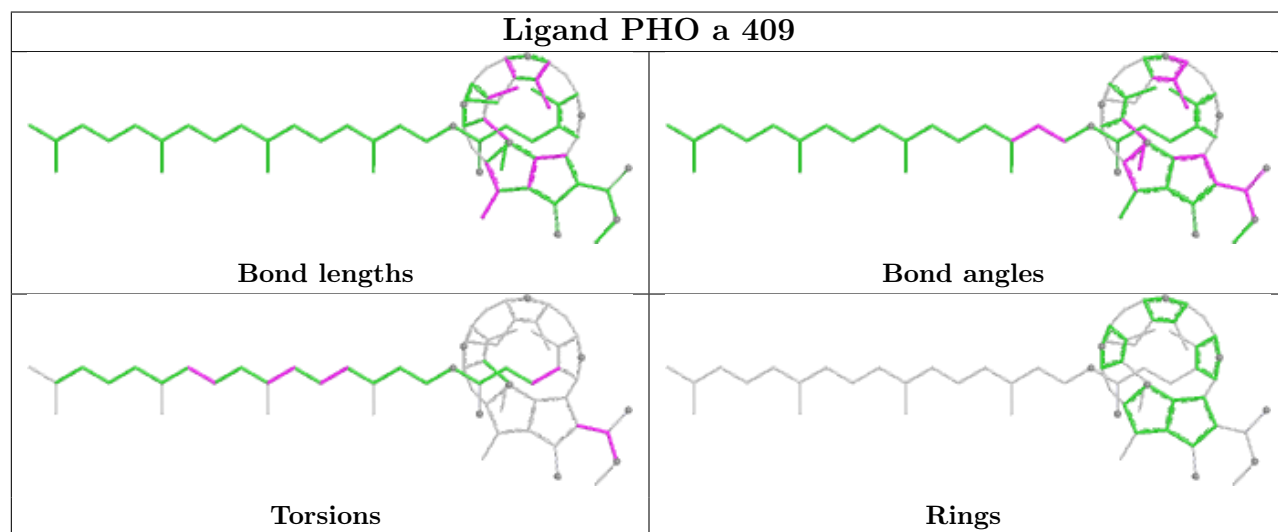
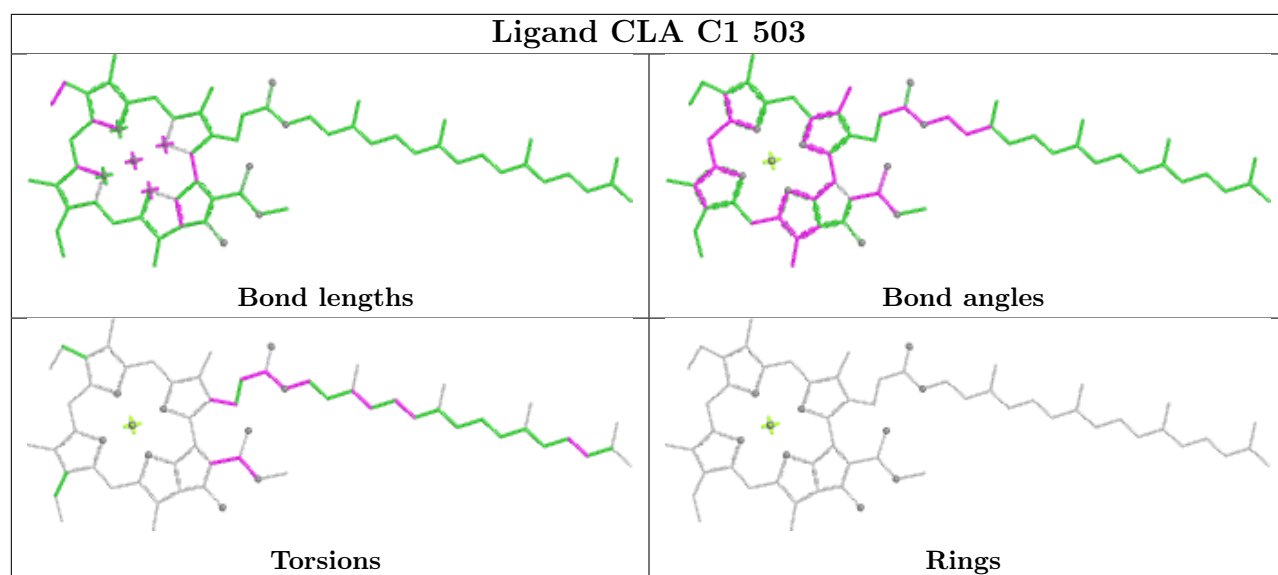


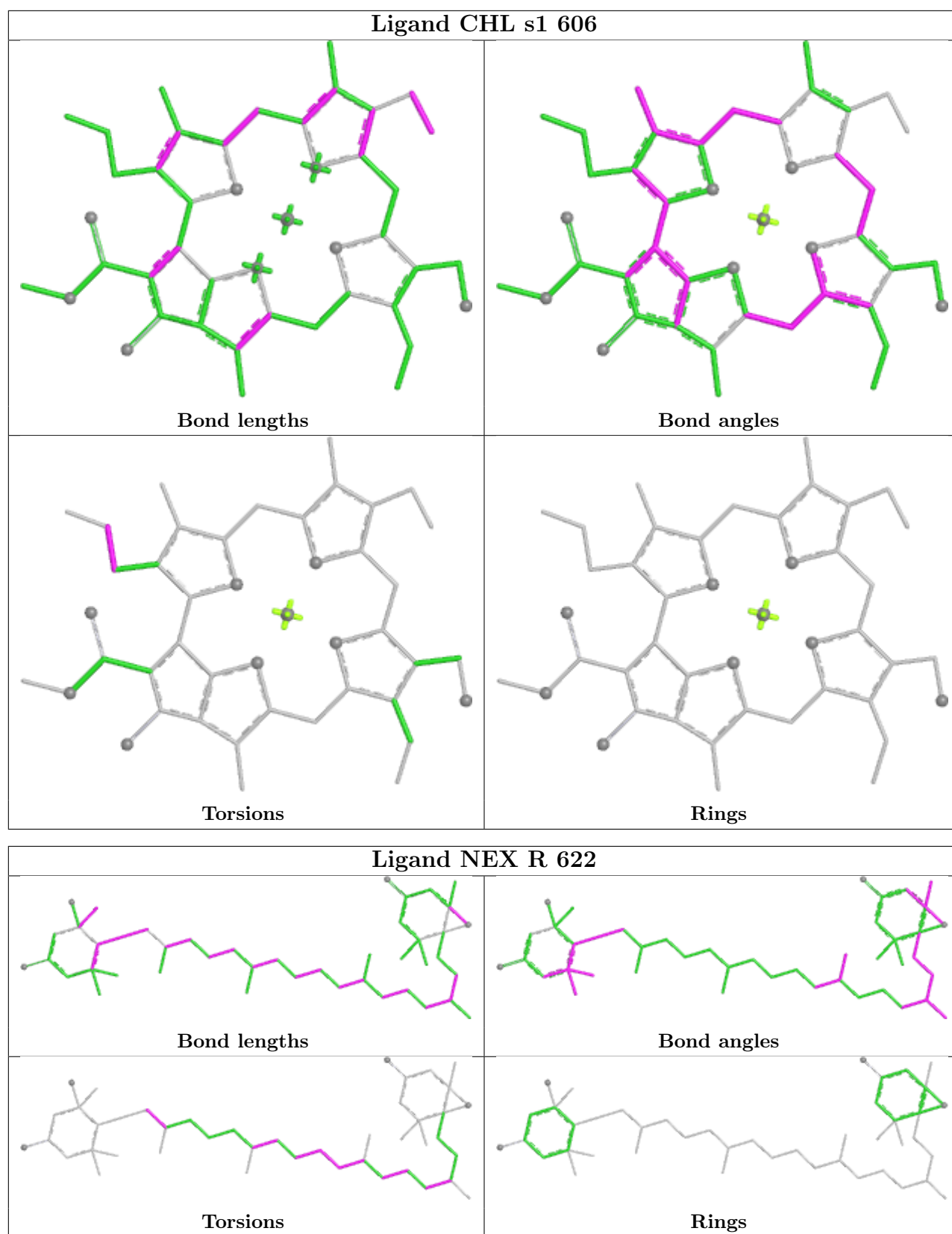
Torsions

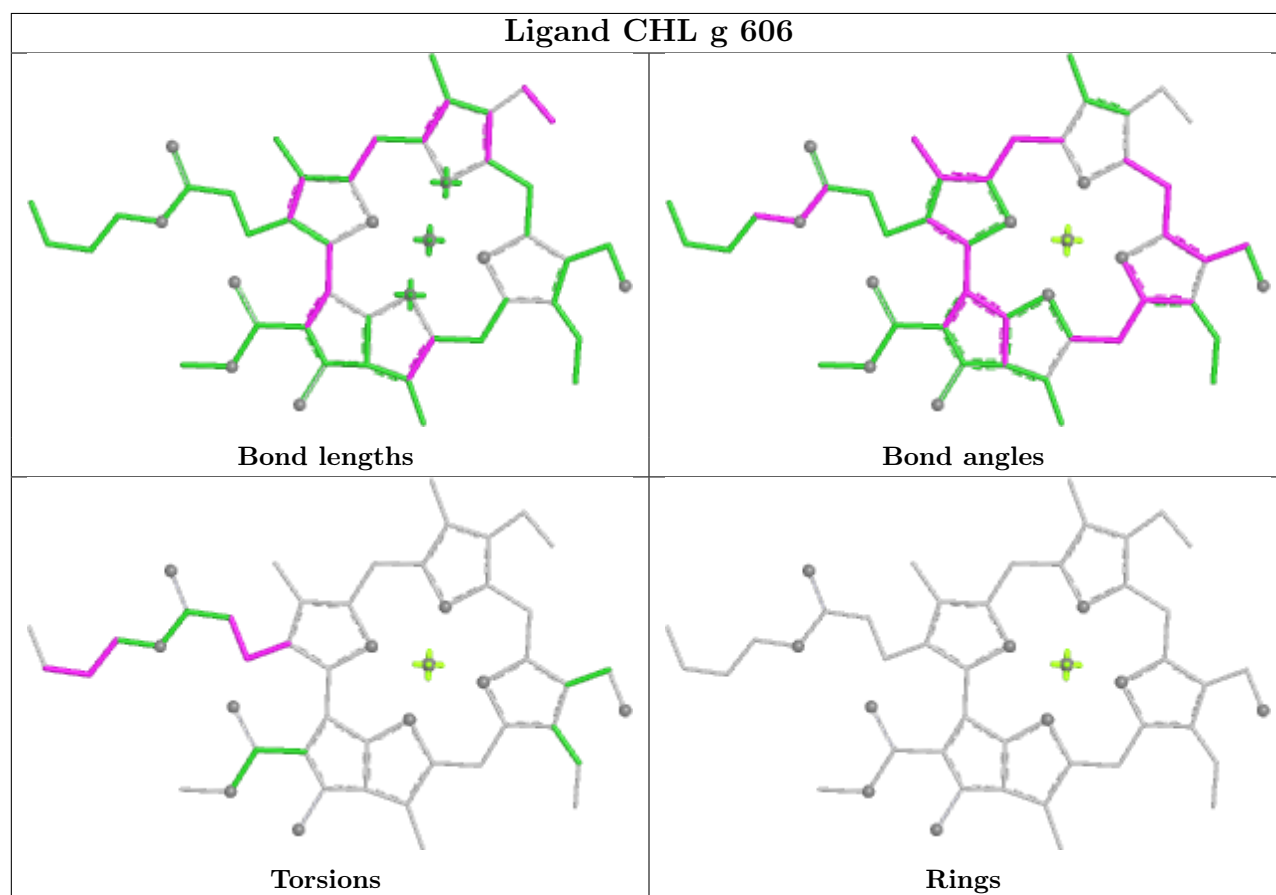
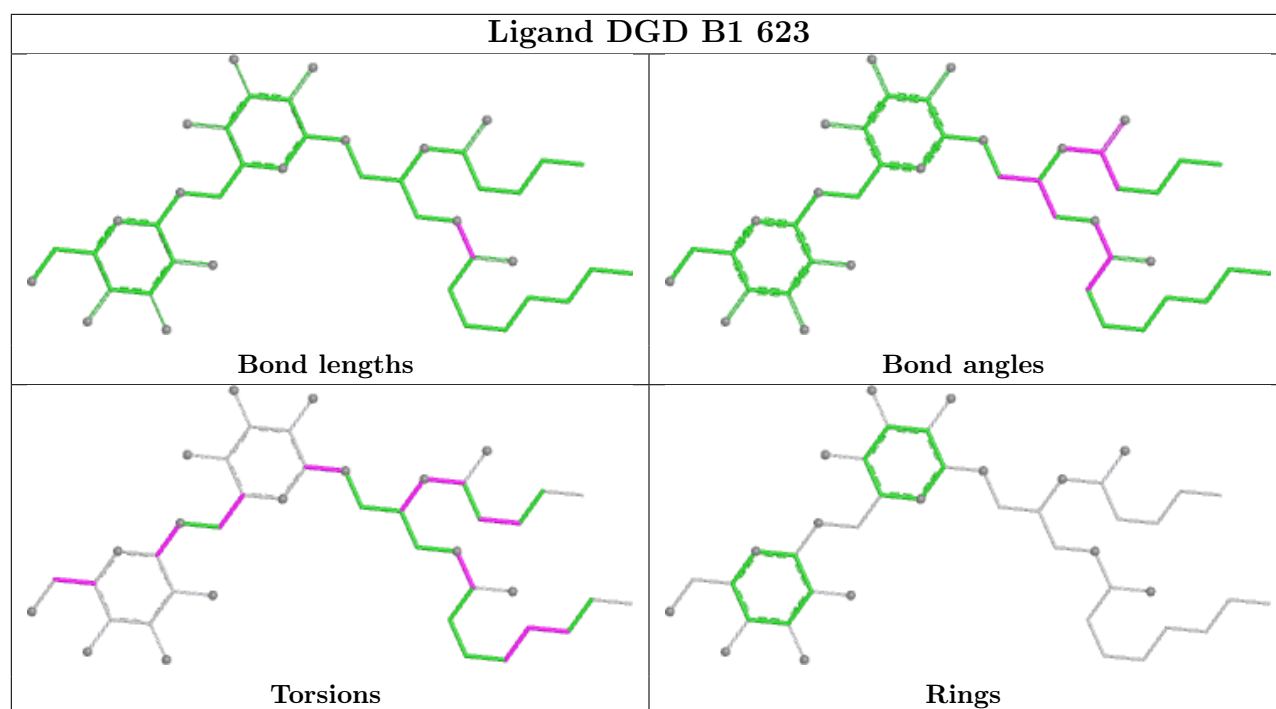


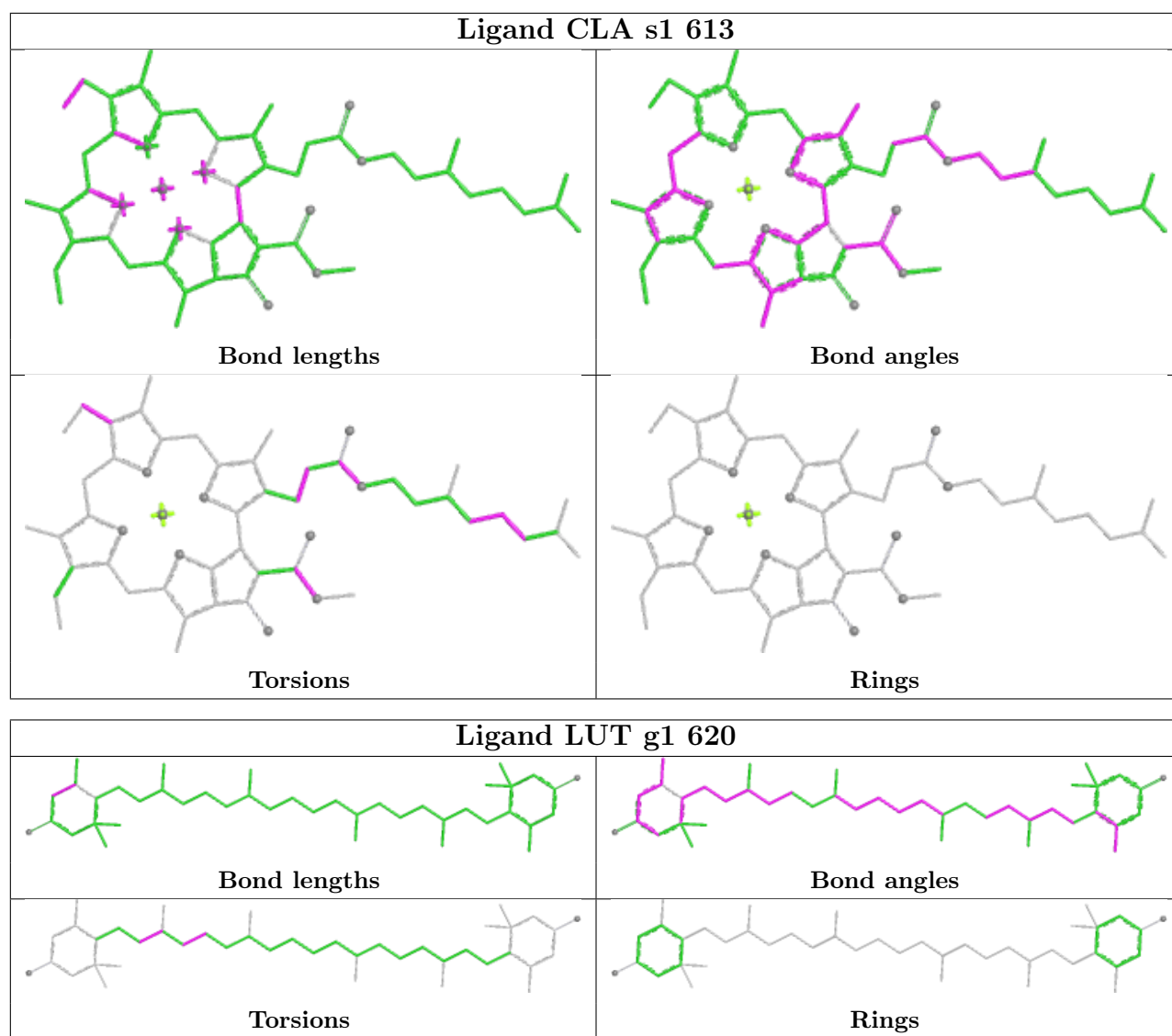
Rings

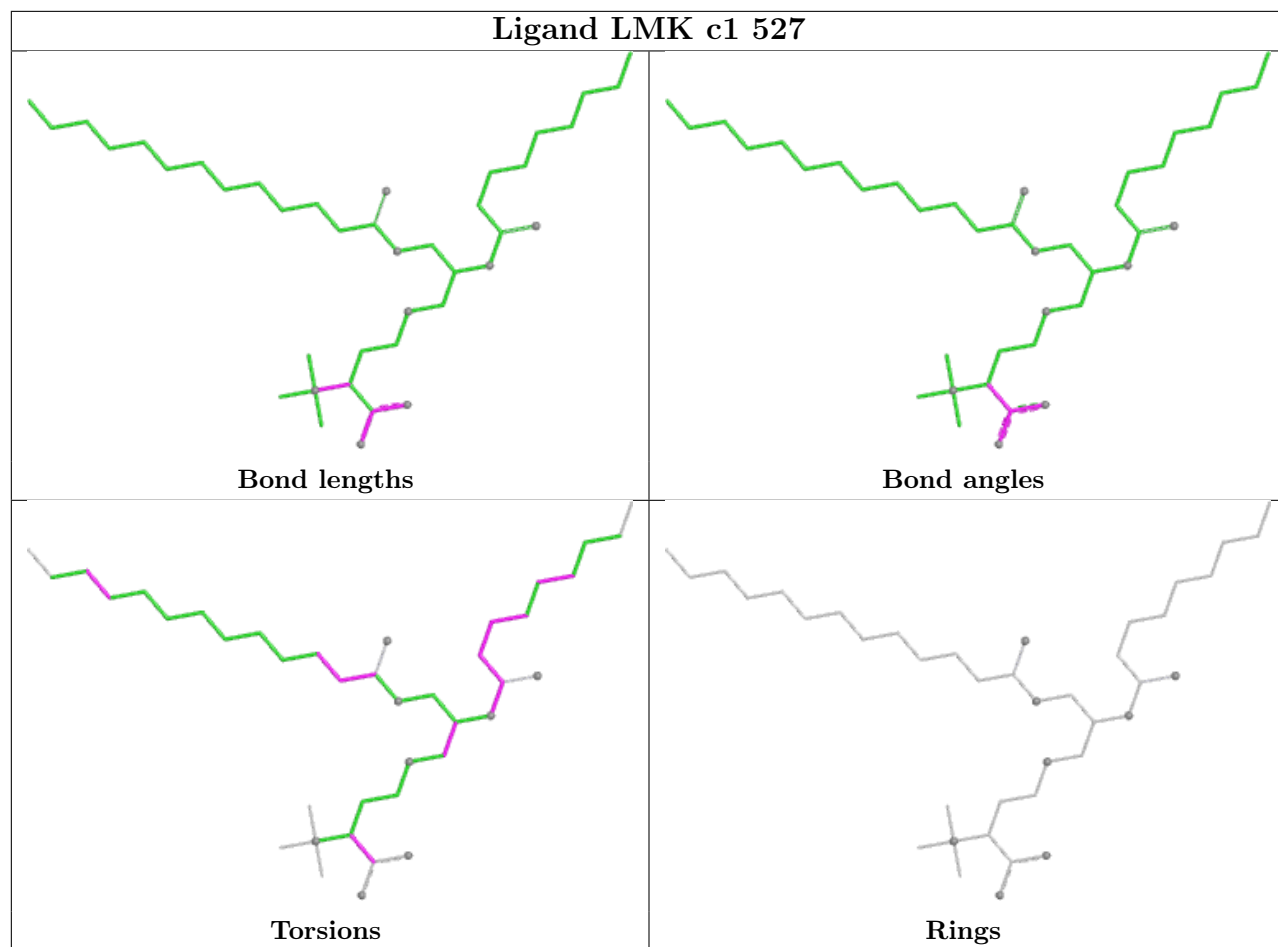




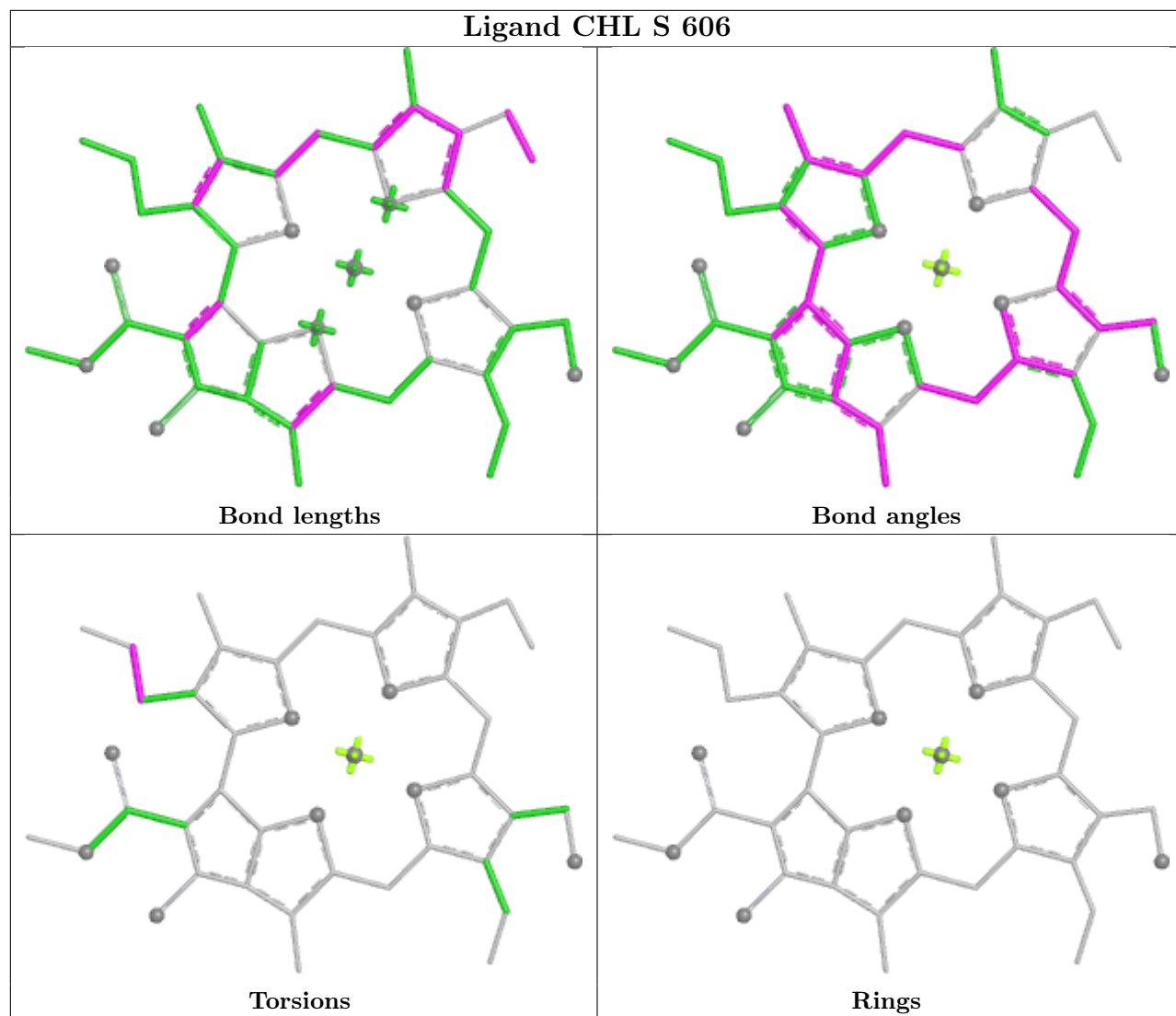




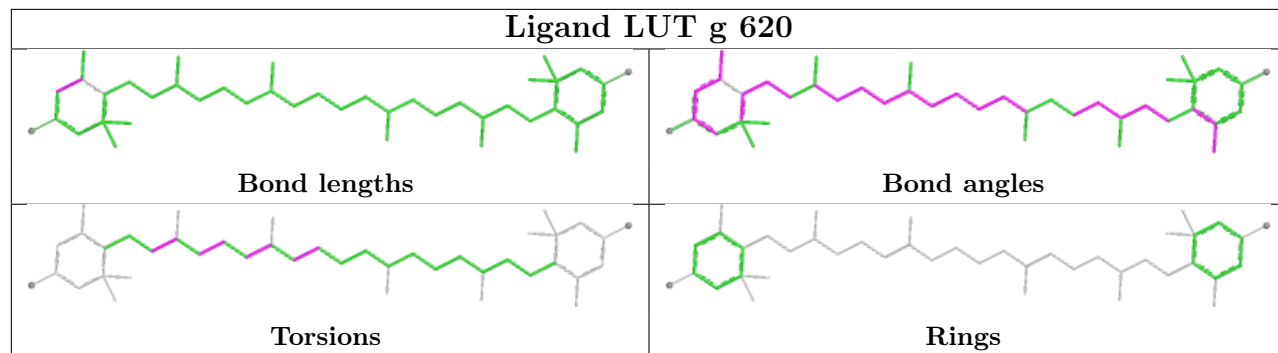




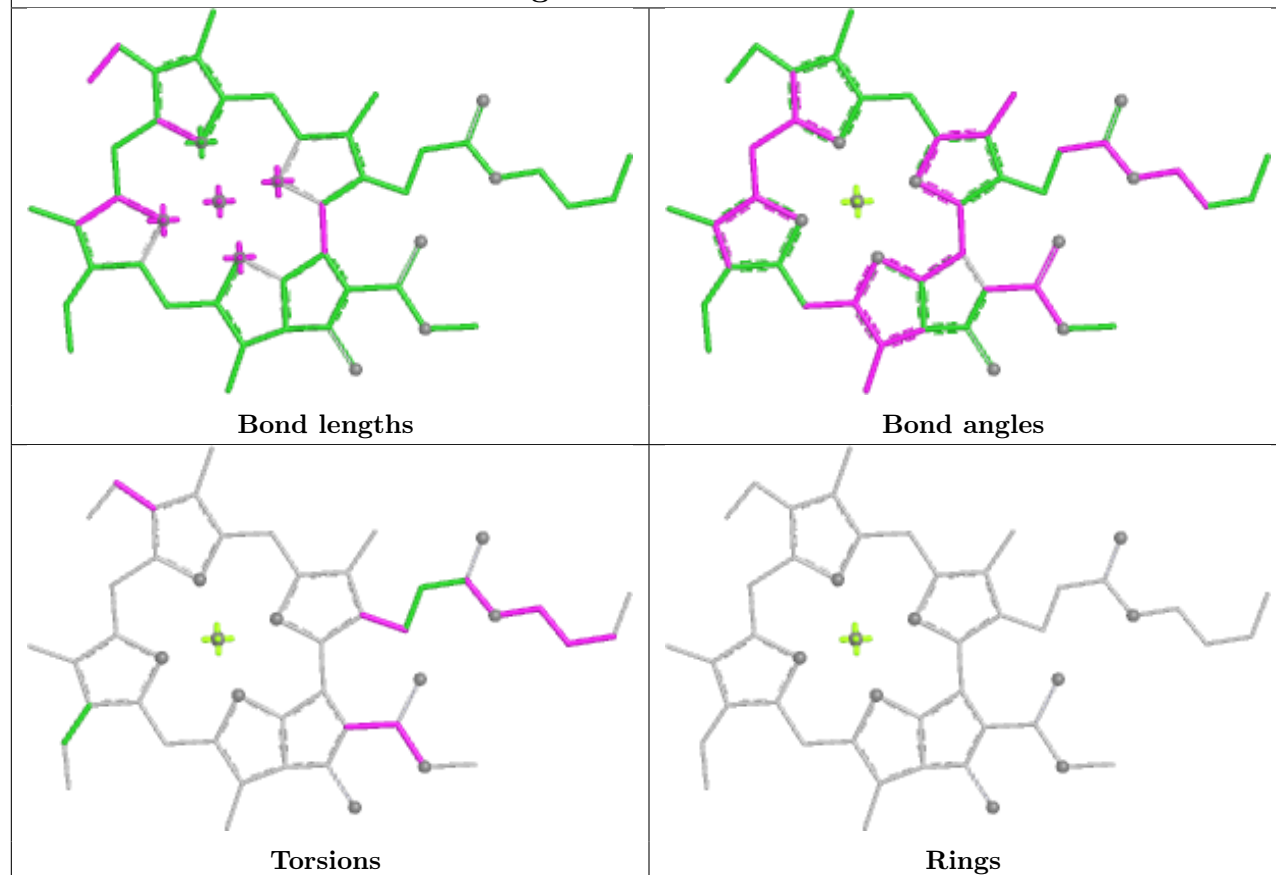
Ligand CHL S 606



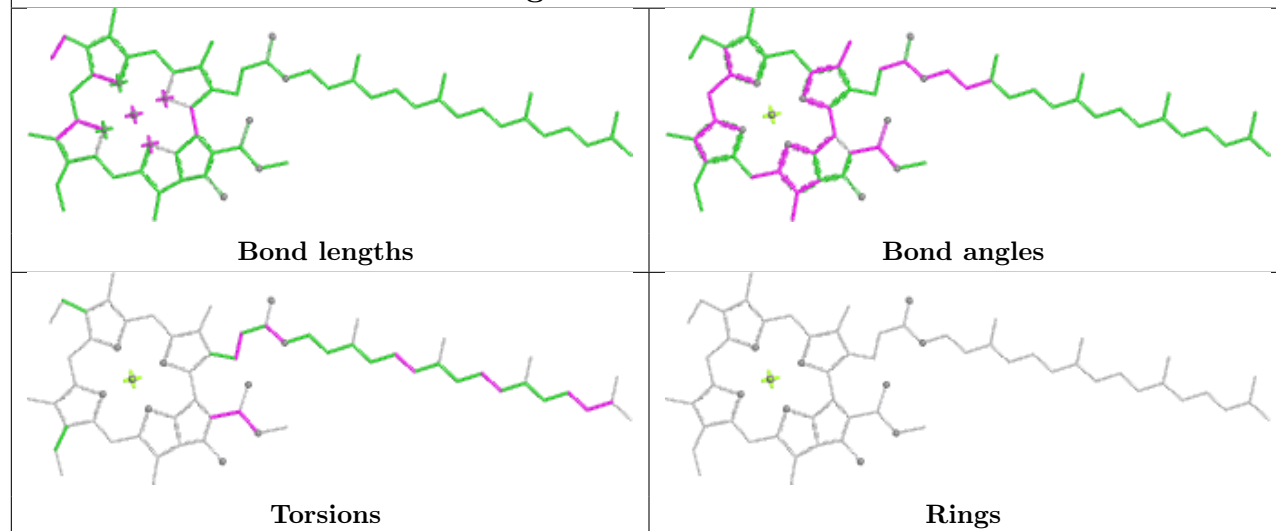
Ligand LUT g 620

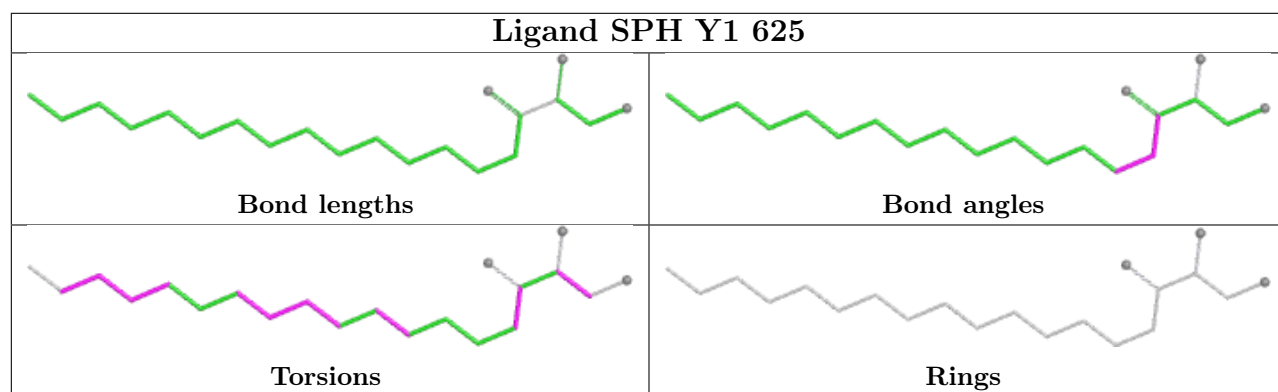
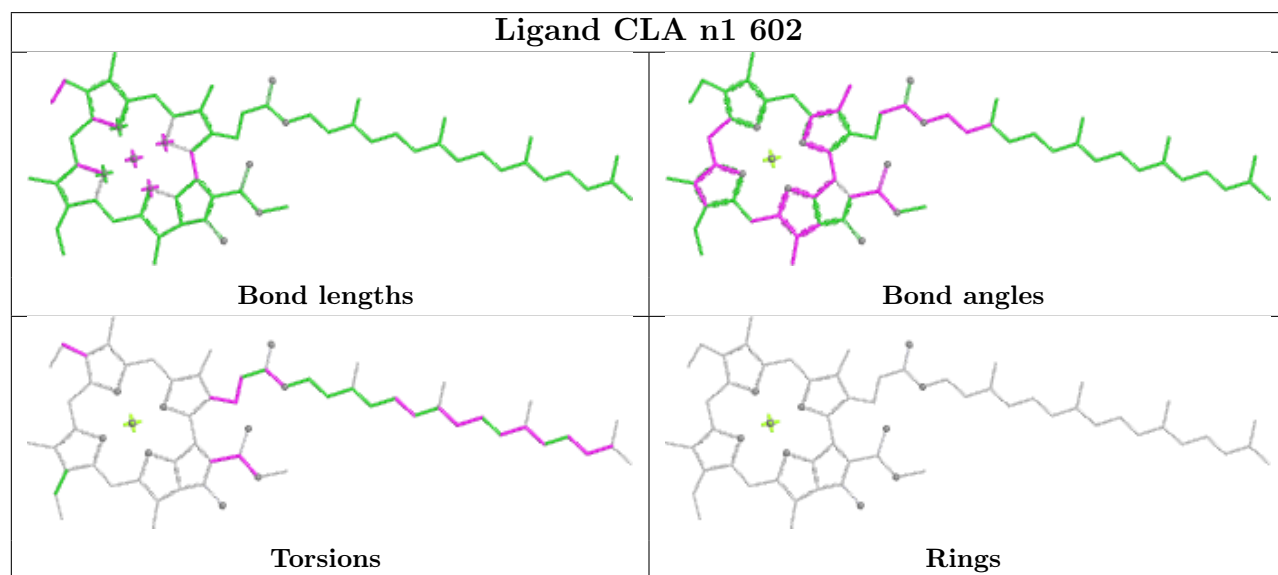
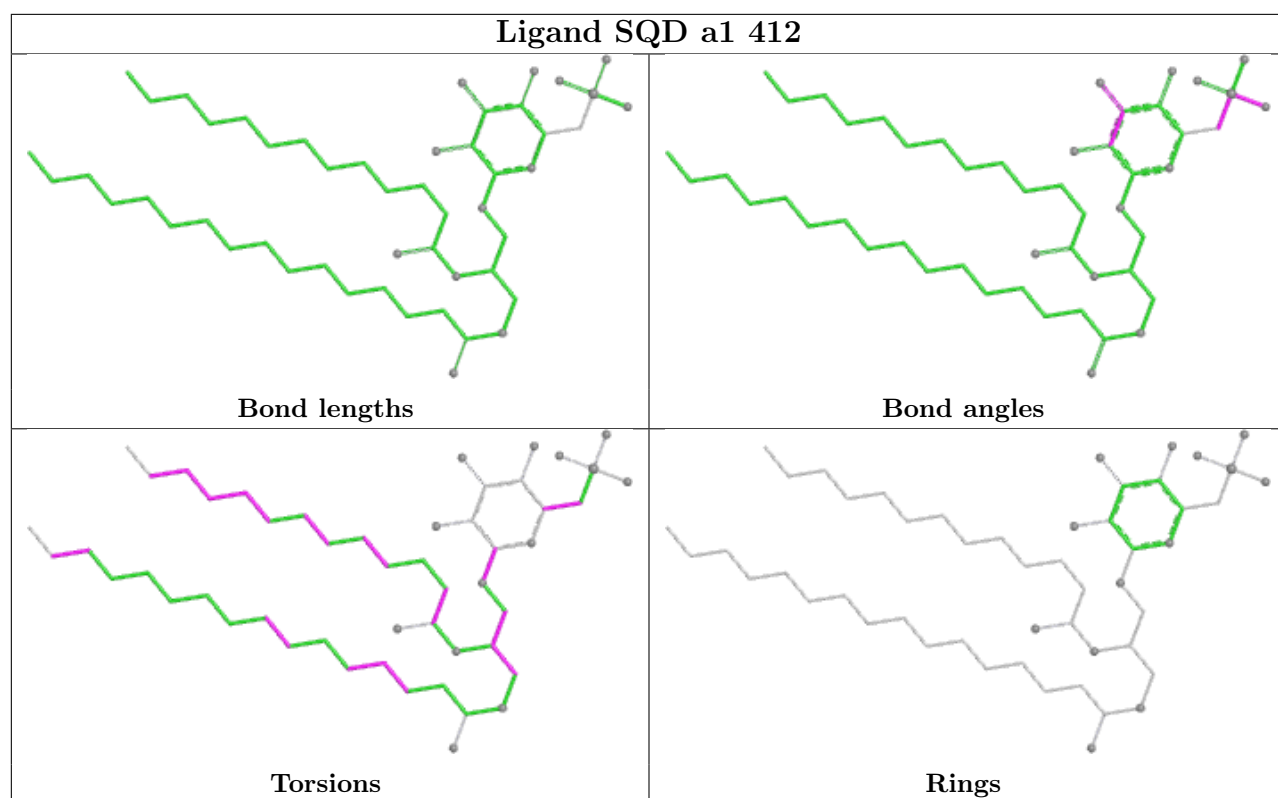


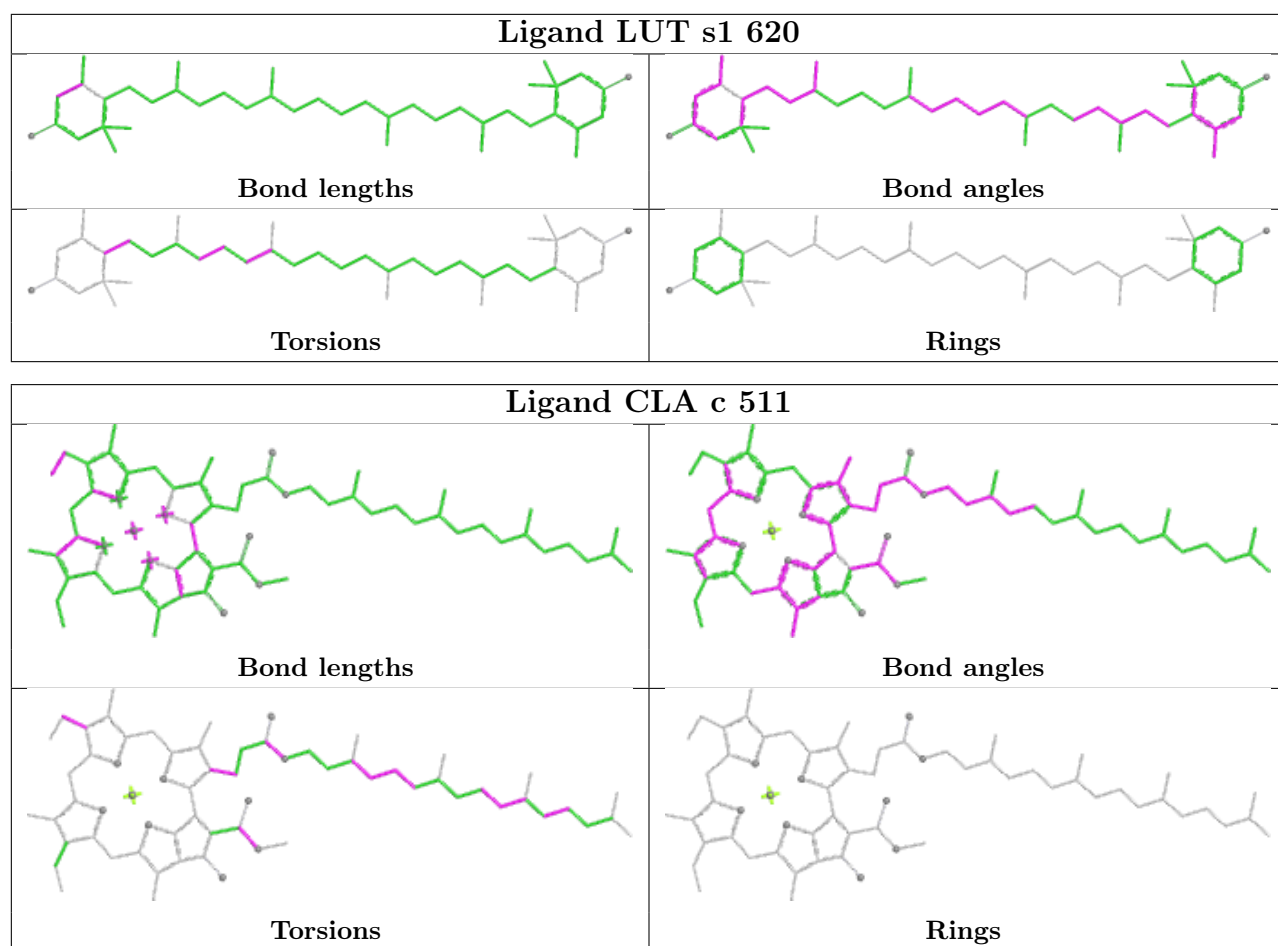
Ligand CLA N 611

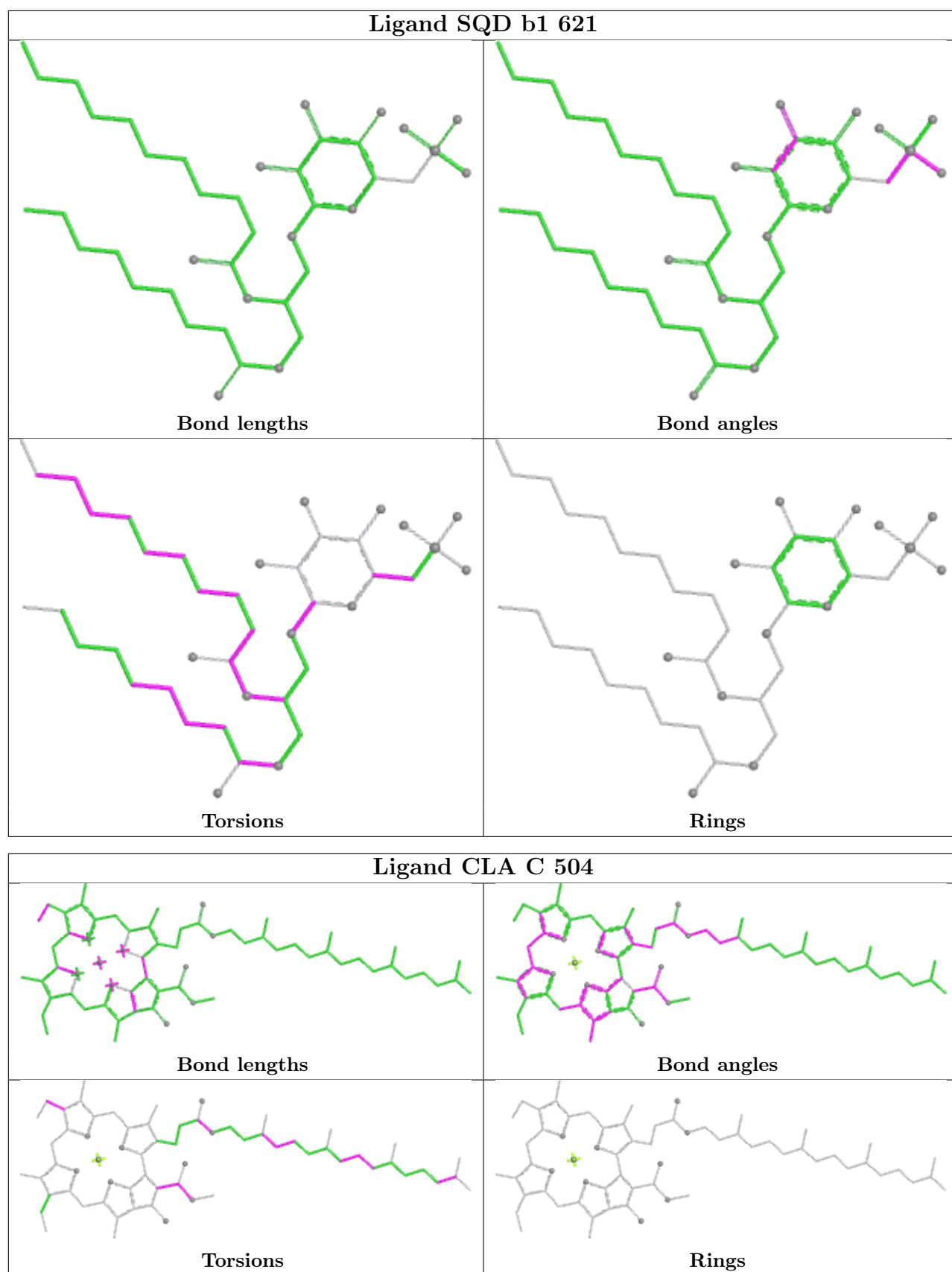


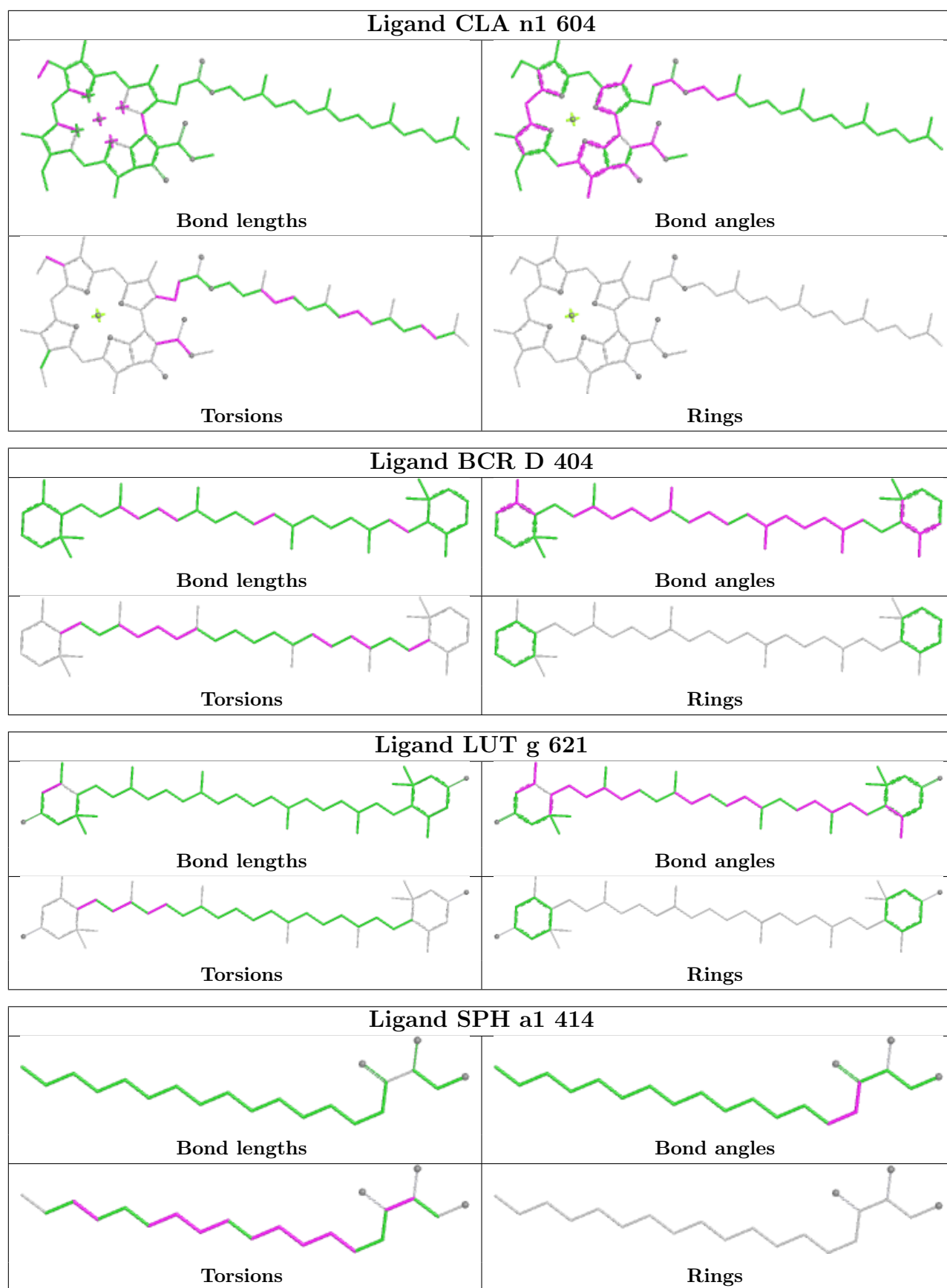
Ligand CLA b1 611

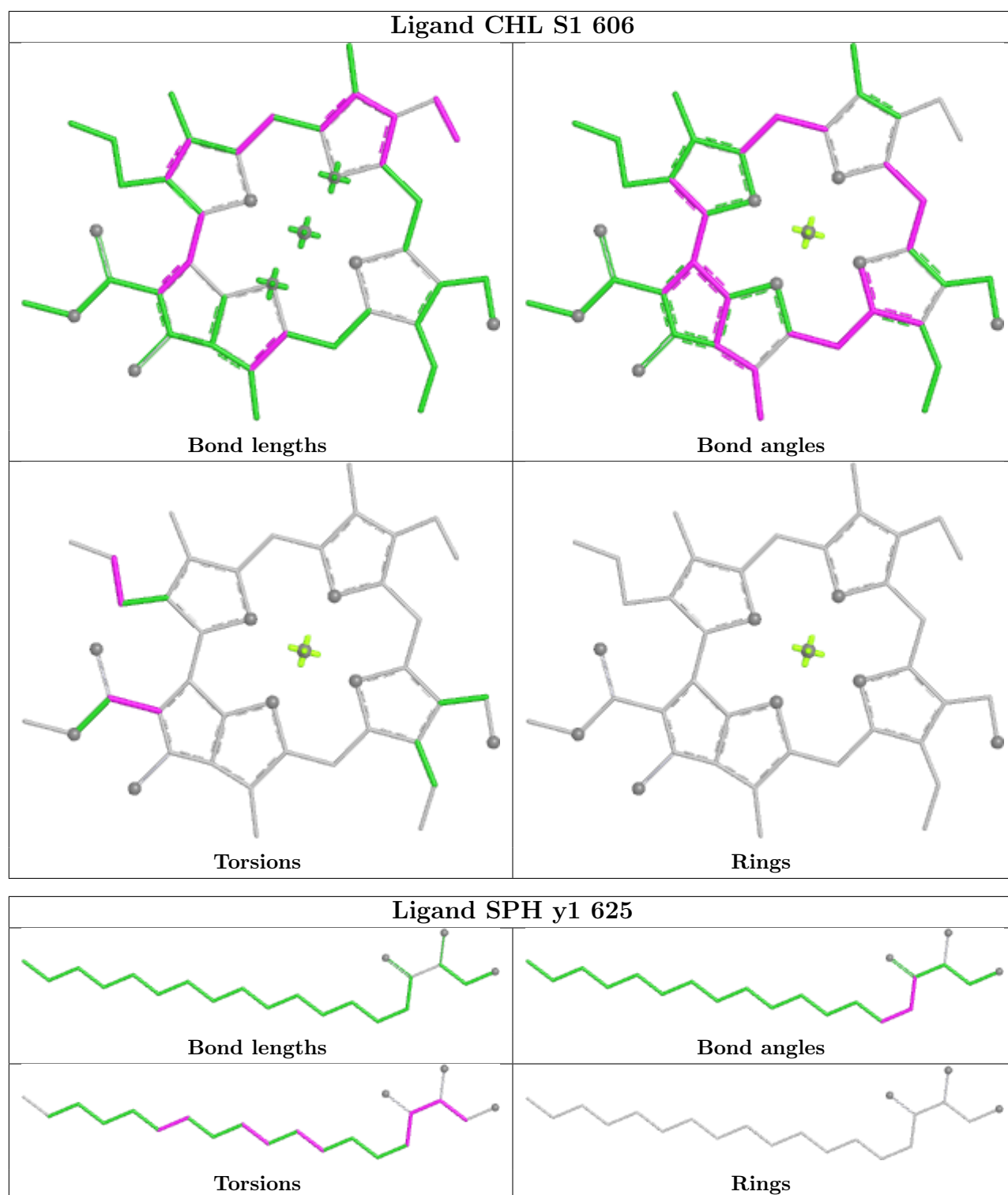


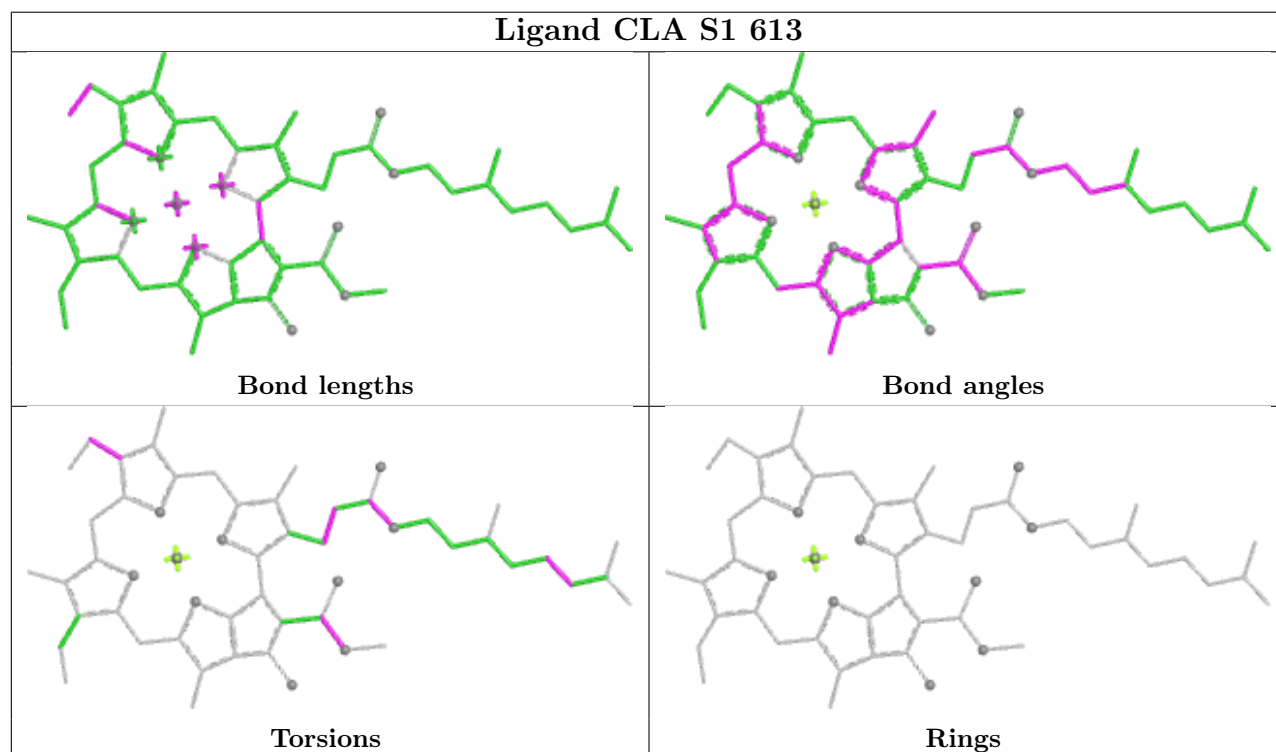
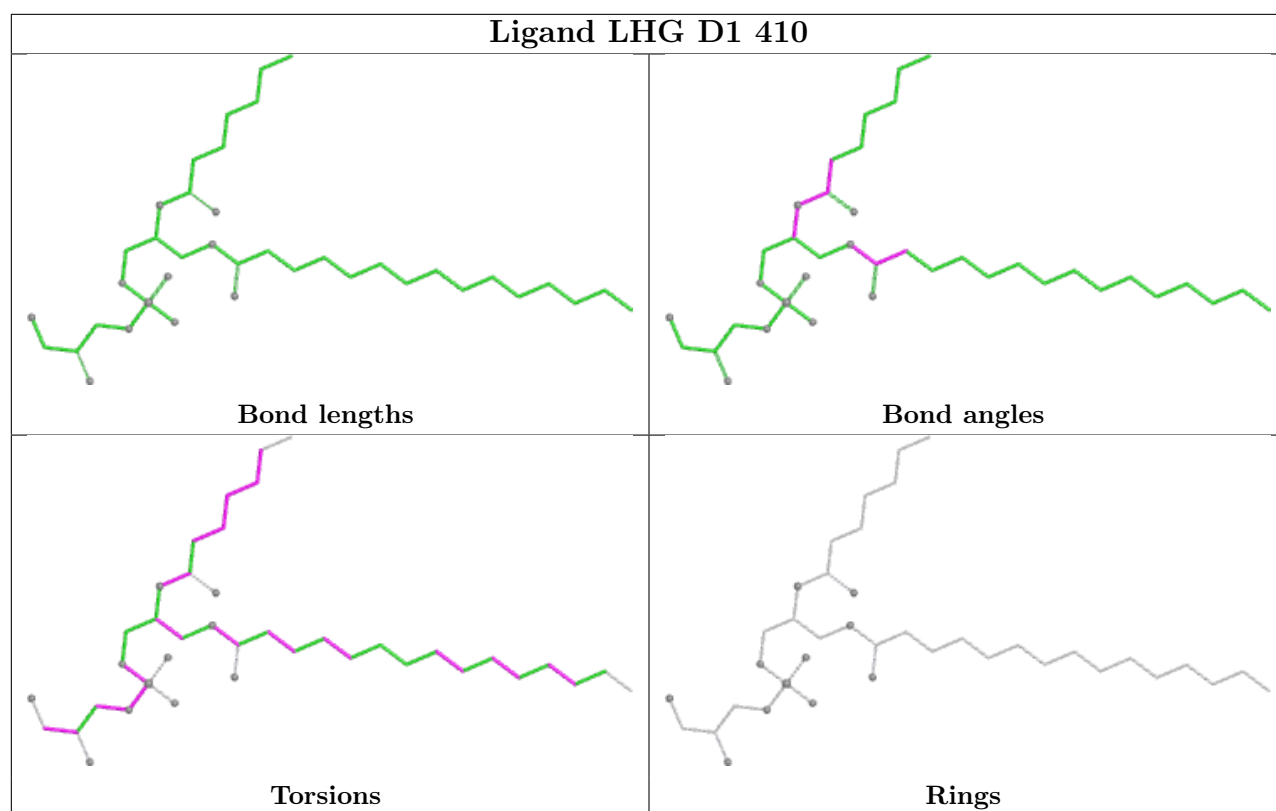


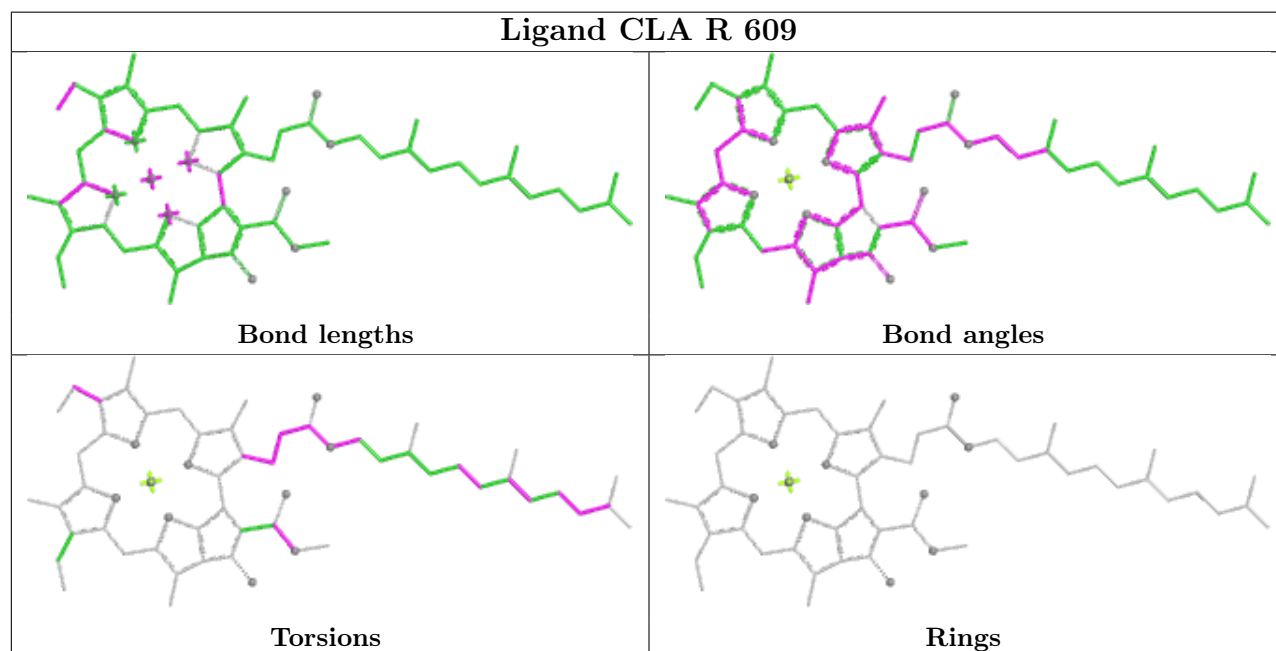
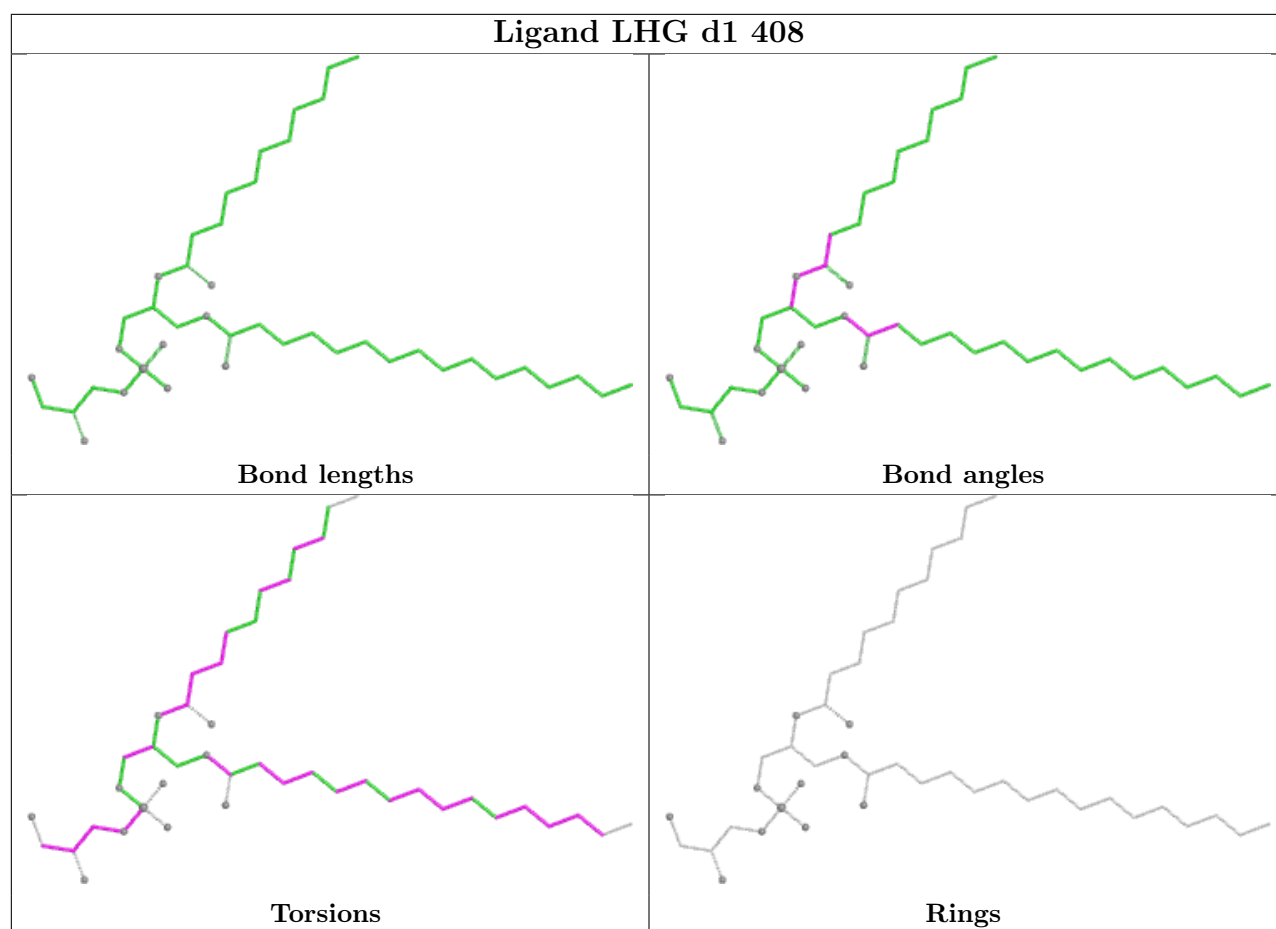


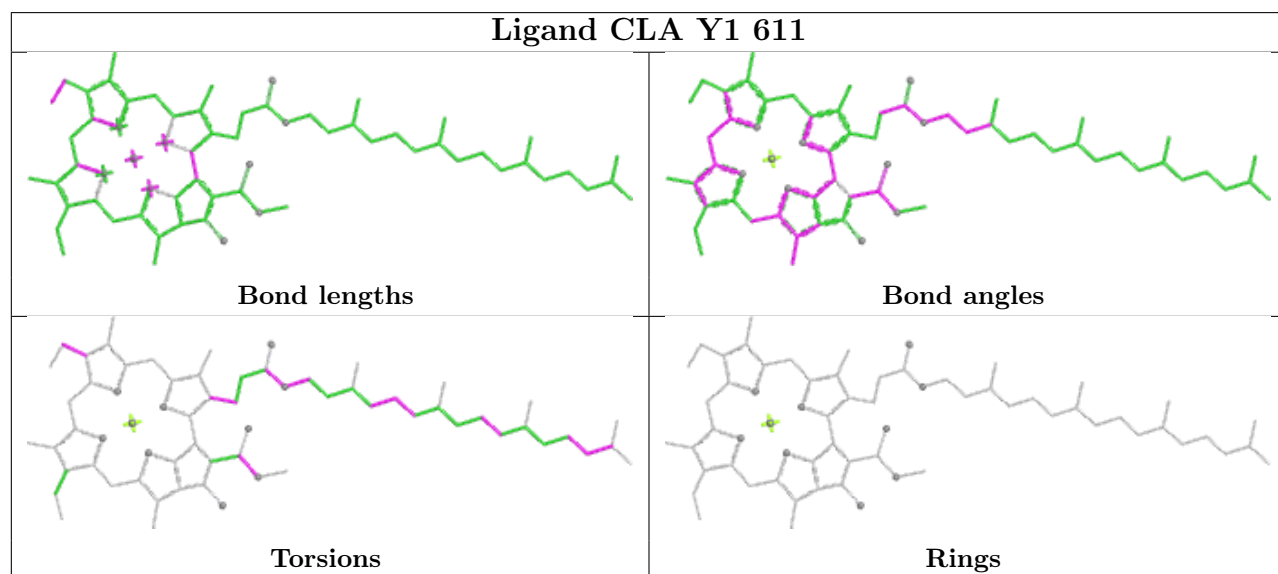
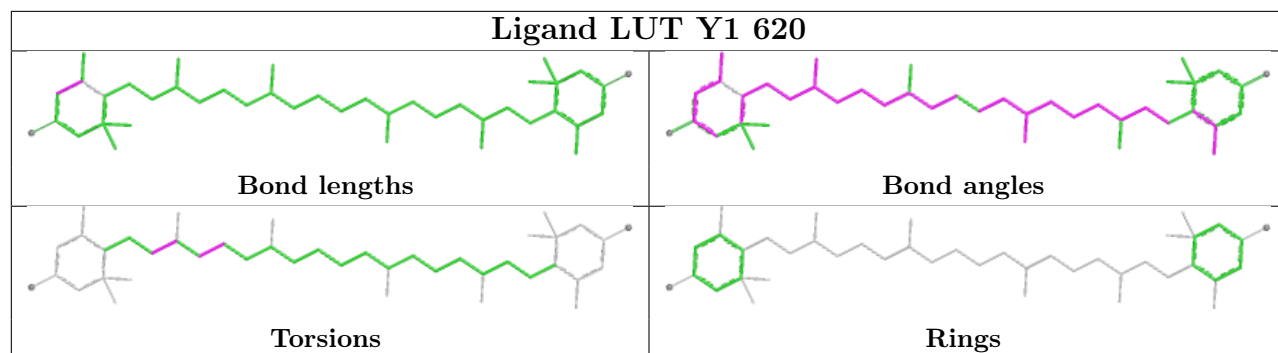


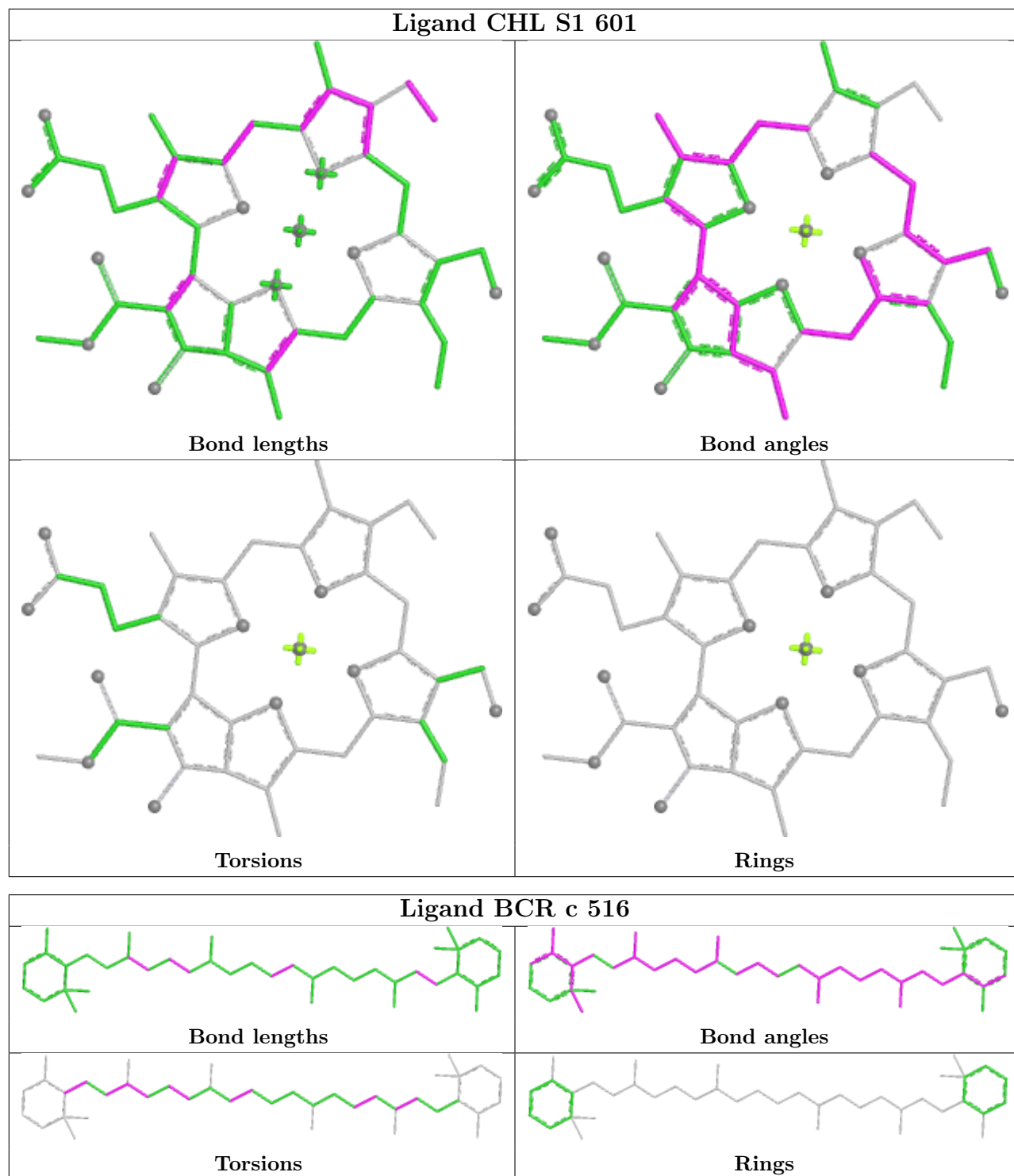


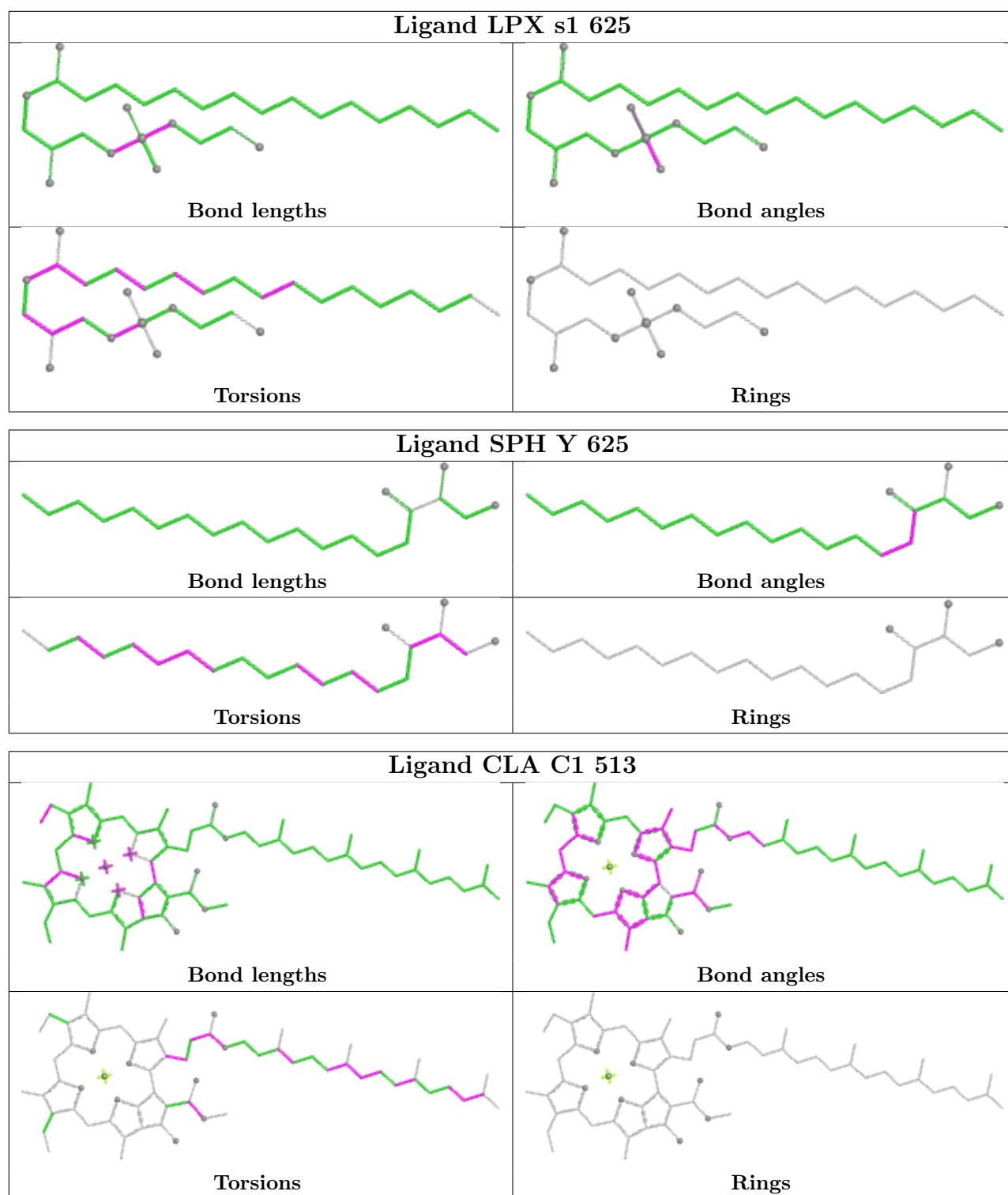




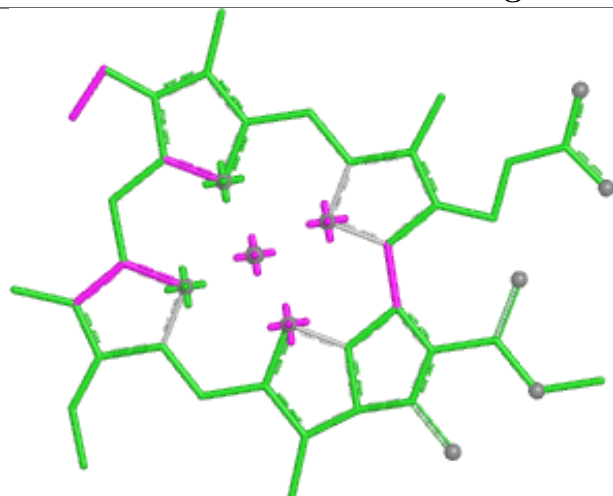




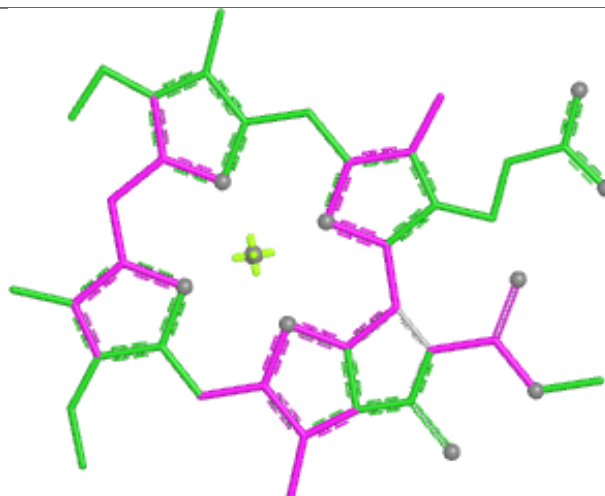




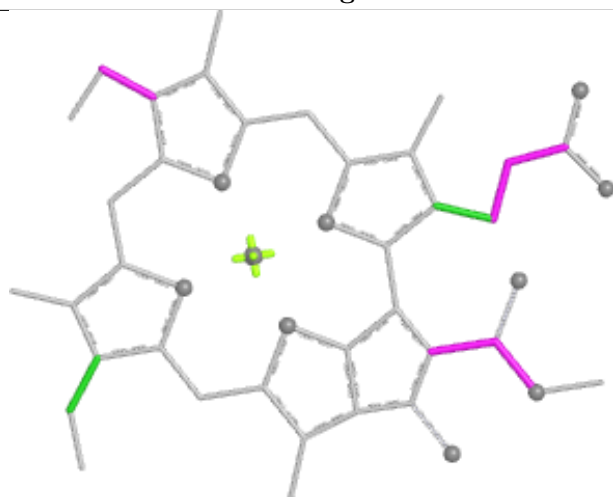
Ligand CLA N1 612



Bond lengths



Bond angles

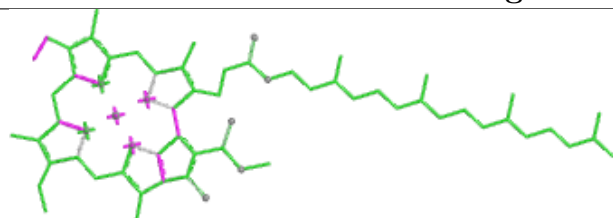


Torsions

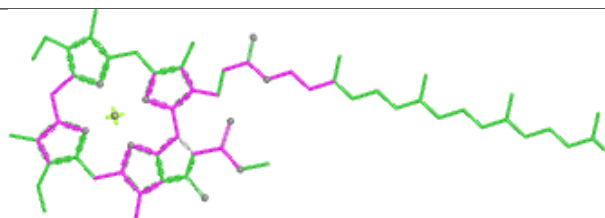


Rings

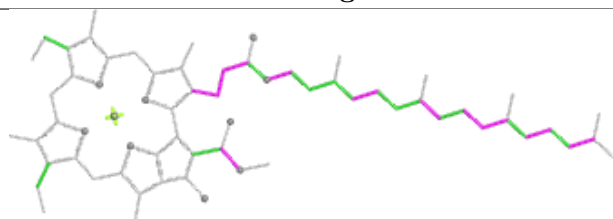
Ligand CLA B1 607



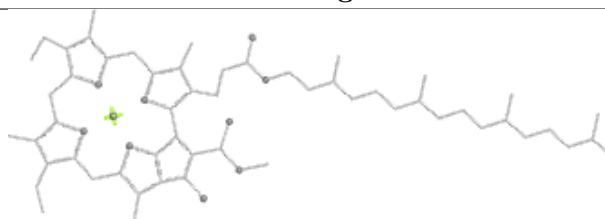
Bond lengths



Bond angles

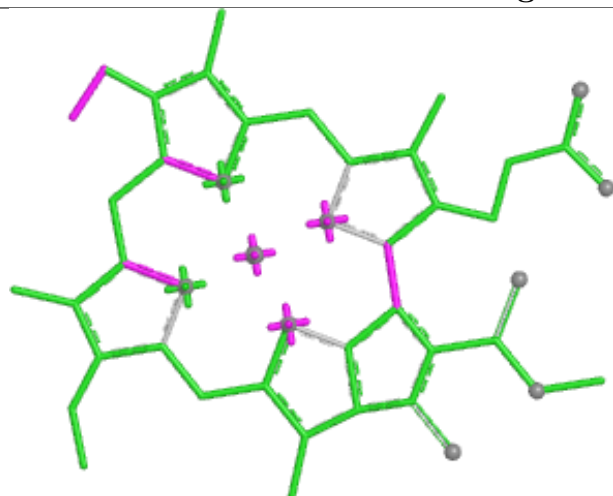


Torsions

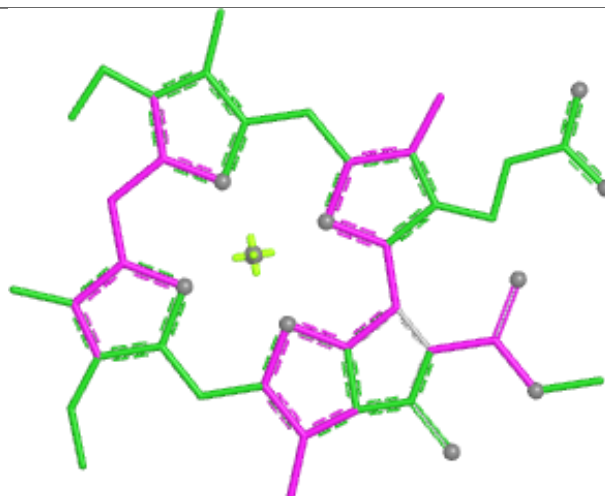


Rings

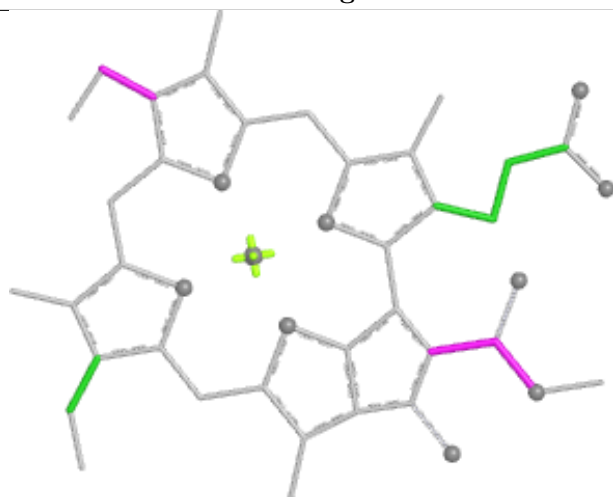
Ligand CLA S 612



Bond lengths



Bond angles

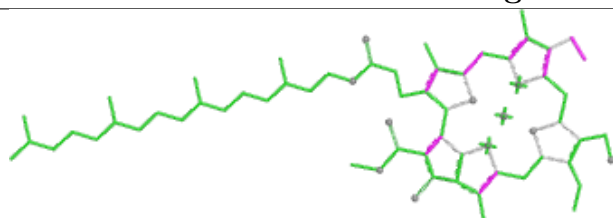


Torsions

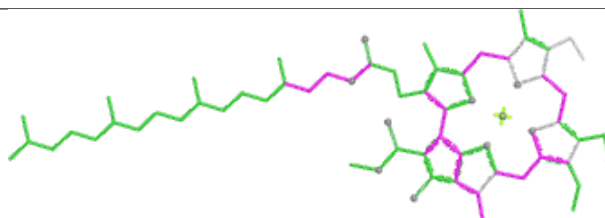


Rings

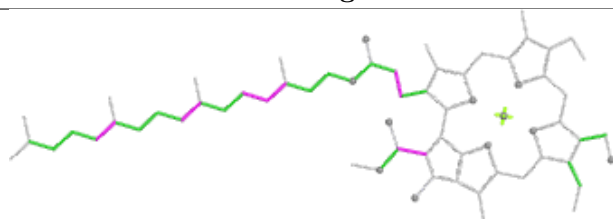
Ligand CHL Y1 607



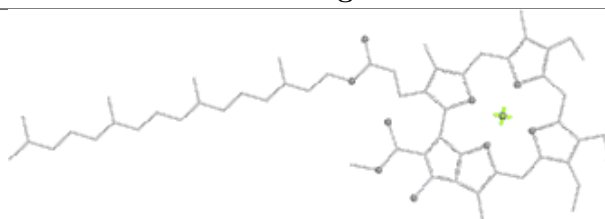
Bond lengths



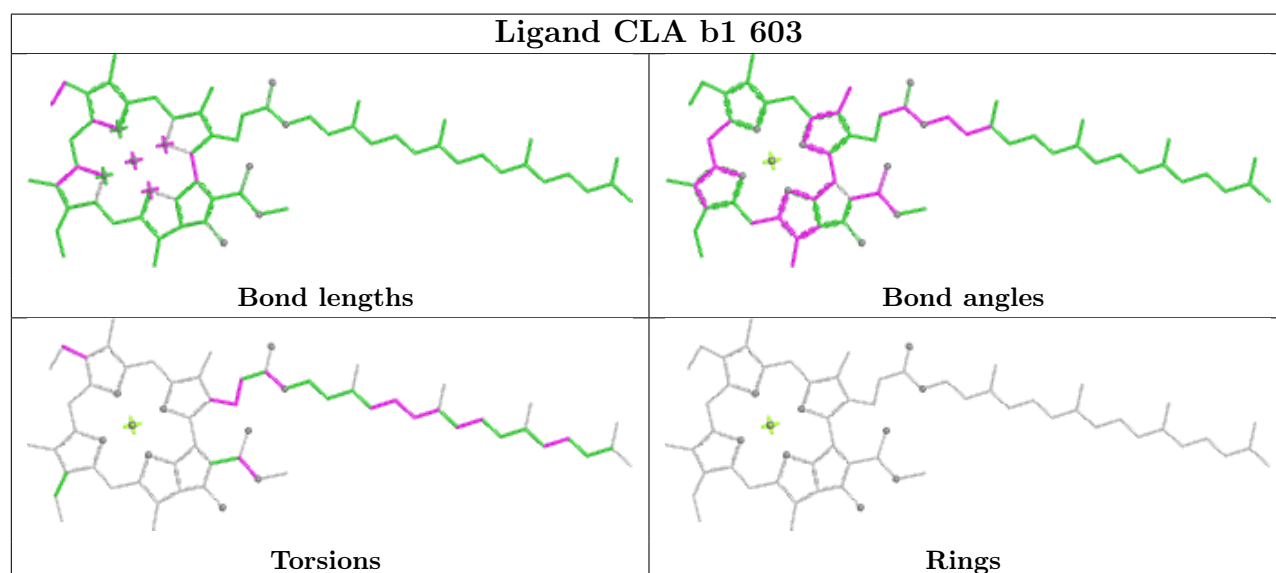
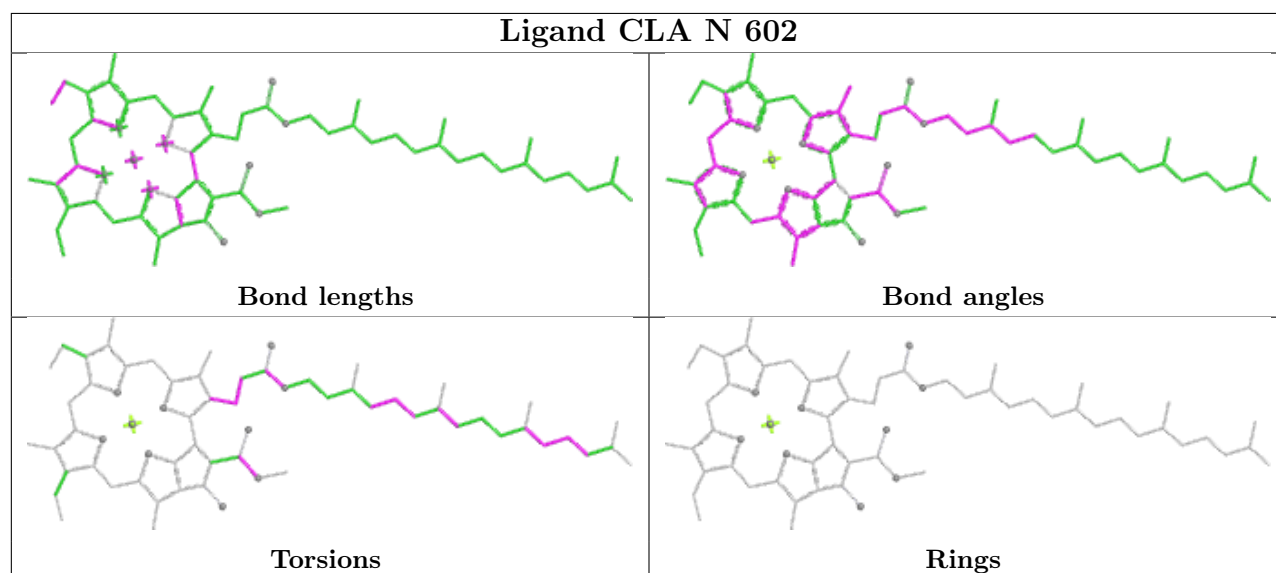
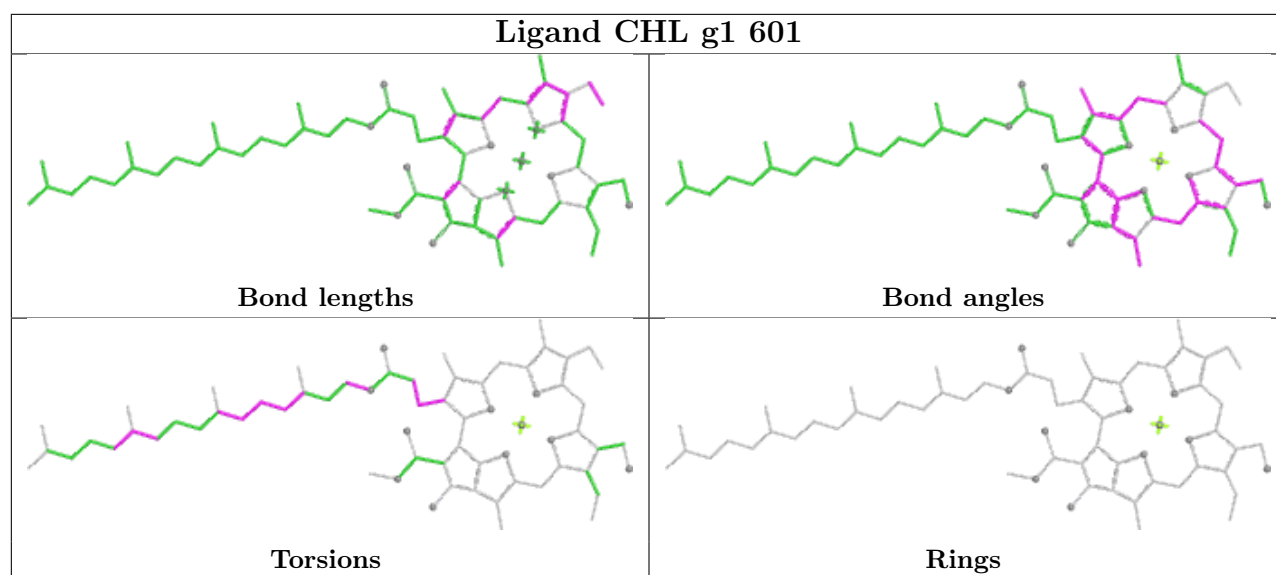
Bond angles



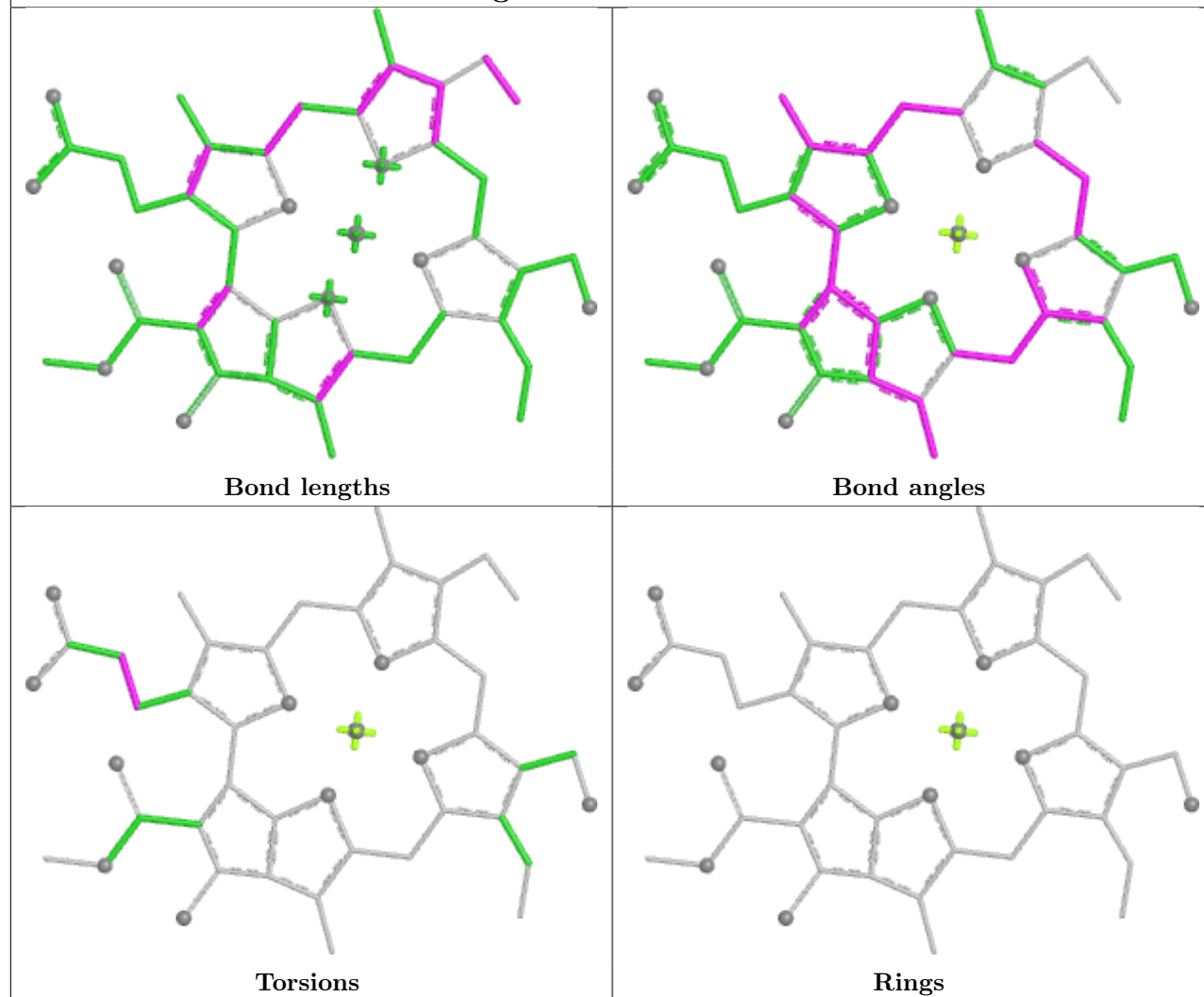
Torsions



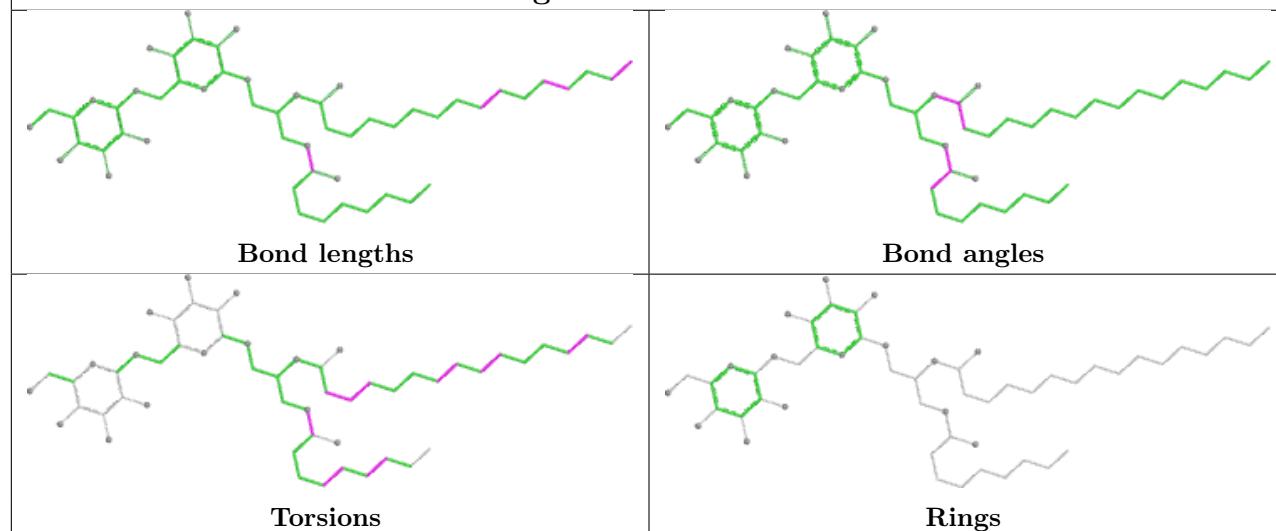
Rings

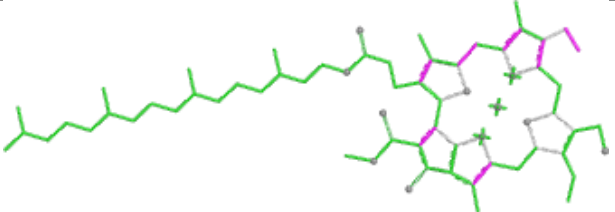
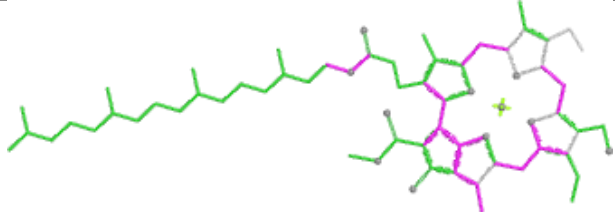
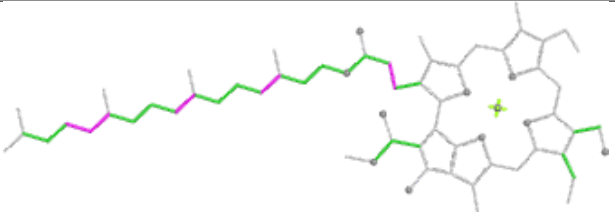
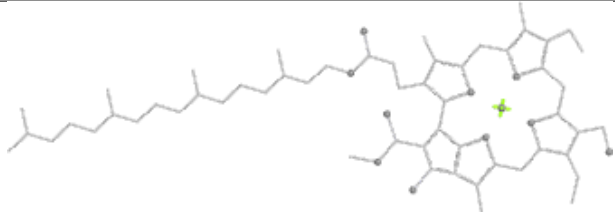
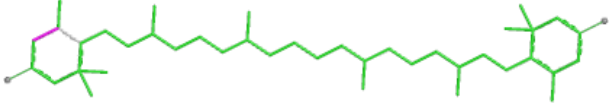
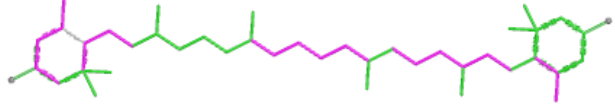
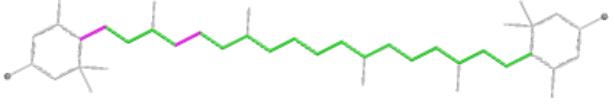
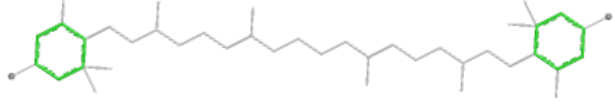
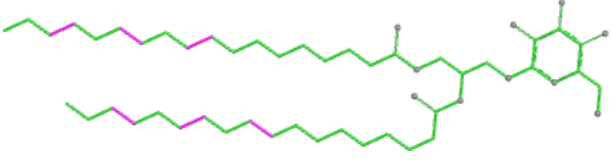
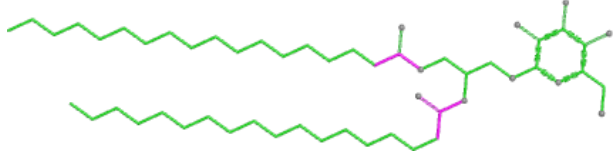
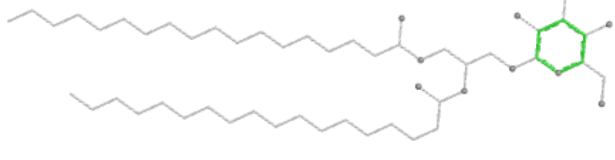


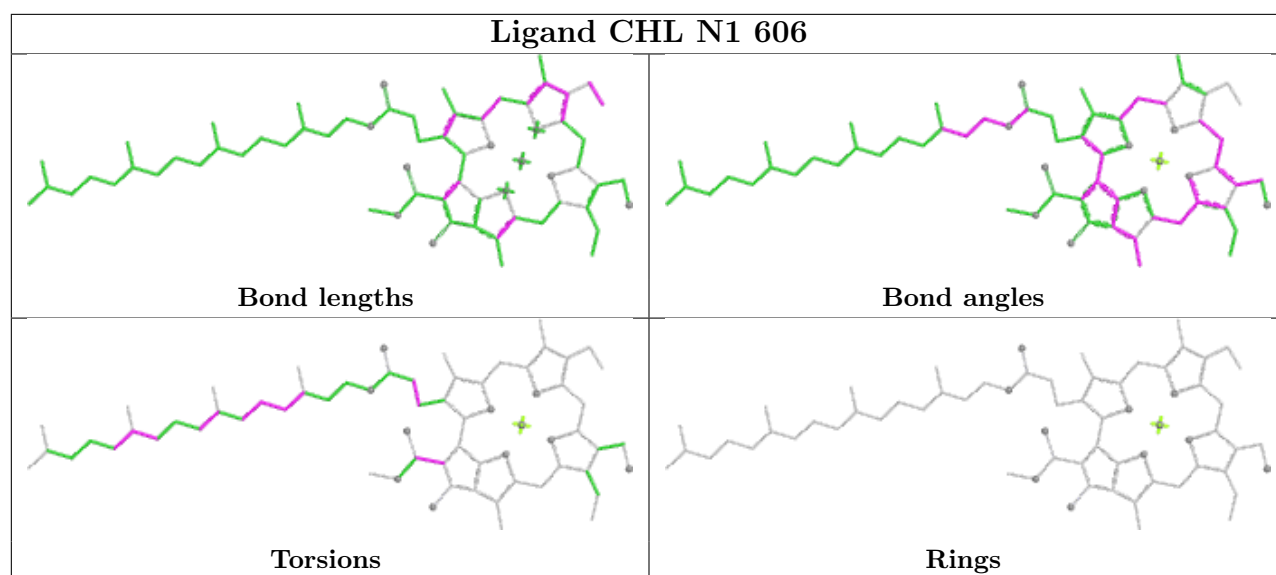
Ligand CHL Y1 605



Ligand DGD c 518



Ligand CHL Y 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT Y1 621	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C1 523	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	R	1
27	r1	1
27	R1	1
23	s	1
20	n1	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	18.97
1	R	110:PRO	C	126:GLU	N	18.01
1	r1	110:PRO	C	126:GLU	N	12.33
1	R1	110:PRO	C	126:GLU	N	11.82
1	s	285:ARG	C	286:VAL	N	3.41

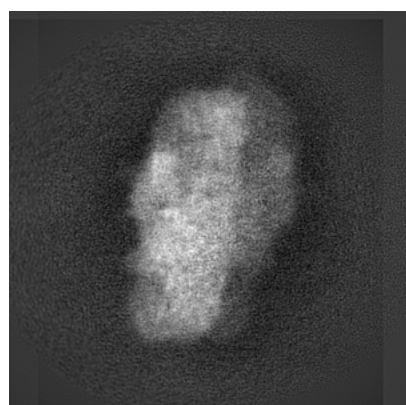
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13455. These allow visual inspection of the internal detail of the map and identification of artifacts.

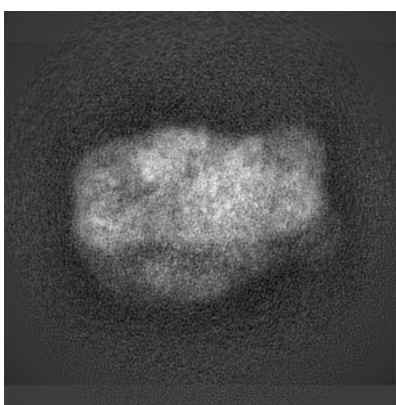
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

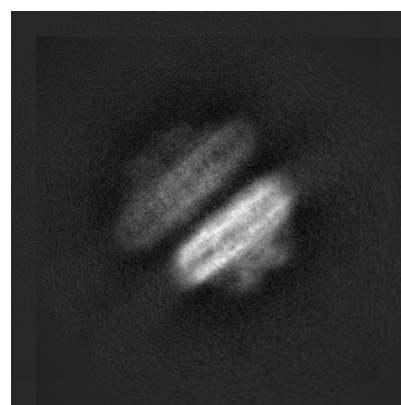
6.1.1 Primary map



X



Y

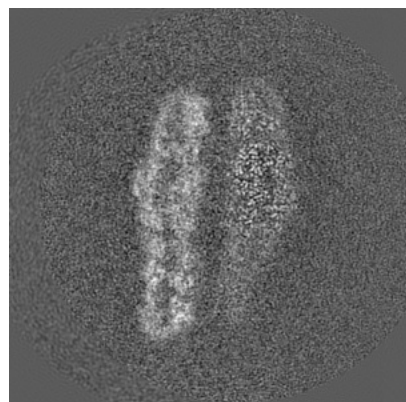


Z

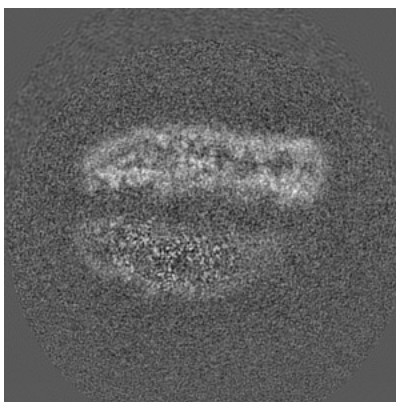
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

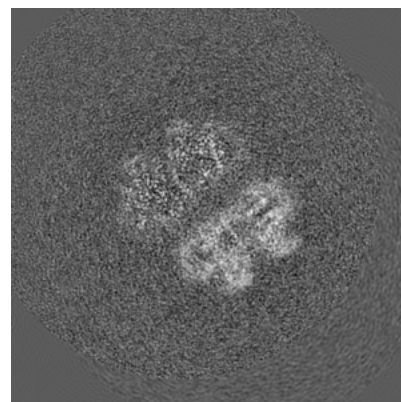
6.2.1 Primary map



X Index: 240



Y Index: 240

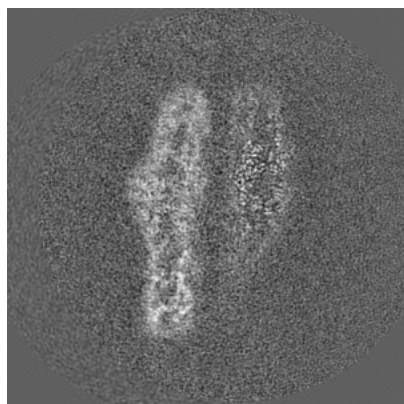


Z Index: 240

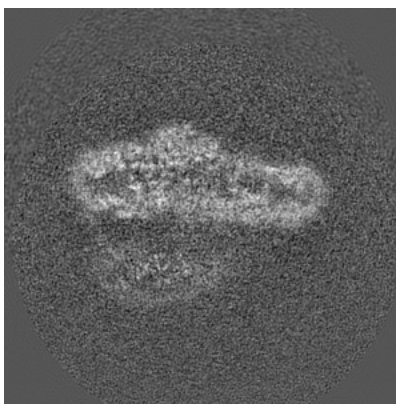
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

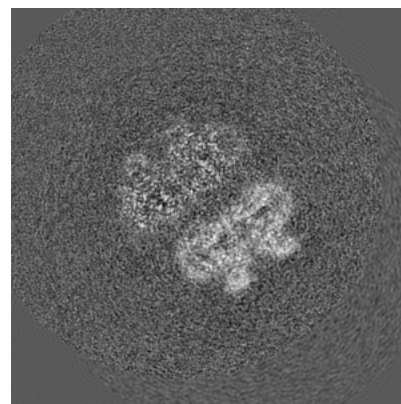
6.3.1 Primary map



X Index: 246



Y Index: 215

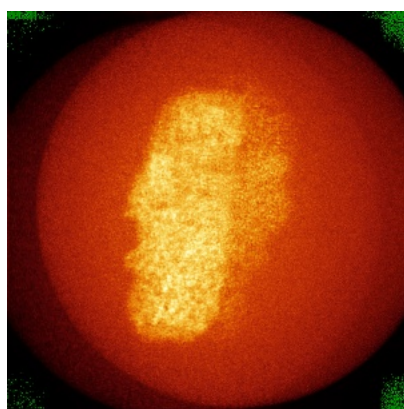


Z Index: 238

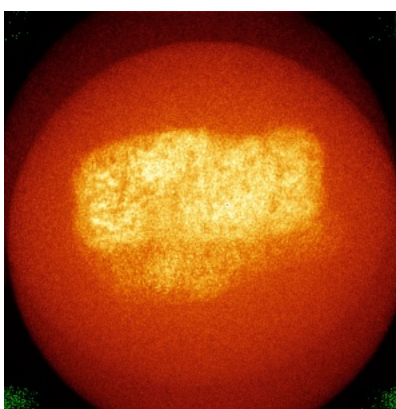
The images above show the largest variance slices of the map in three orthogonal directions.

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

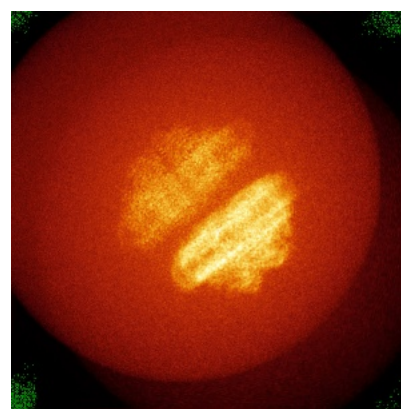
6.4.1 Primary map



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

This section was not generated.

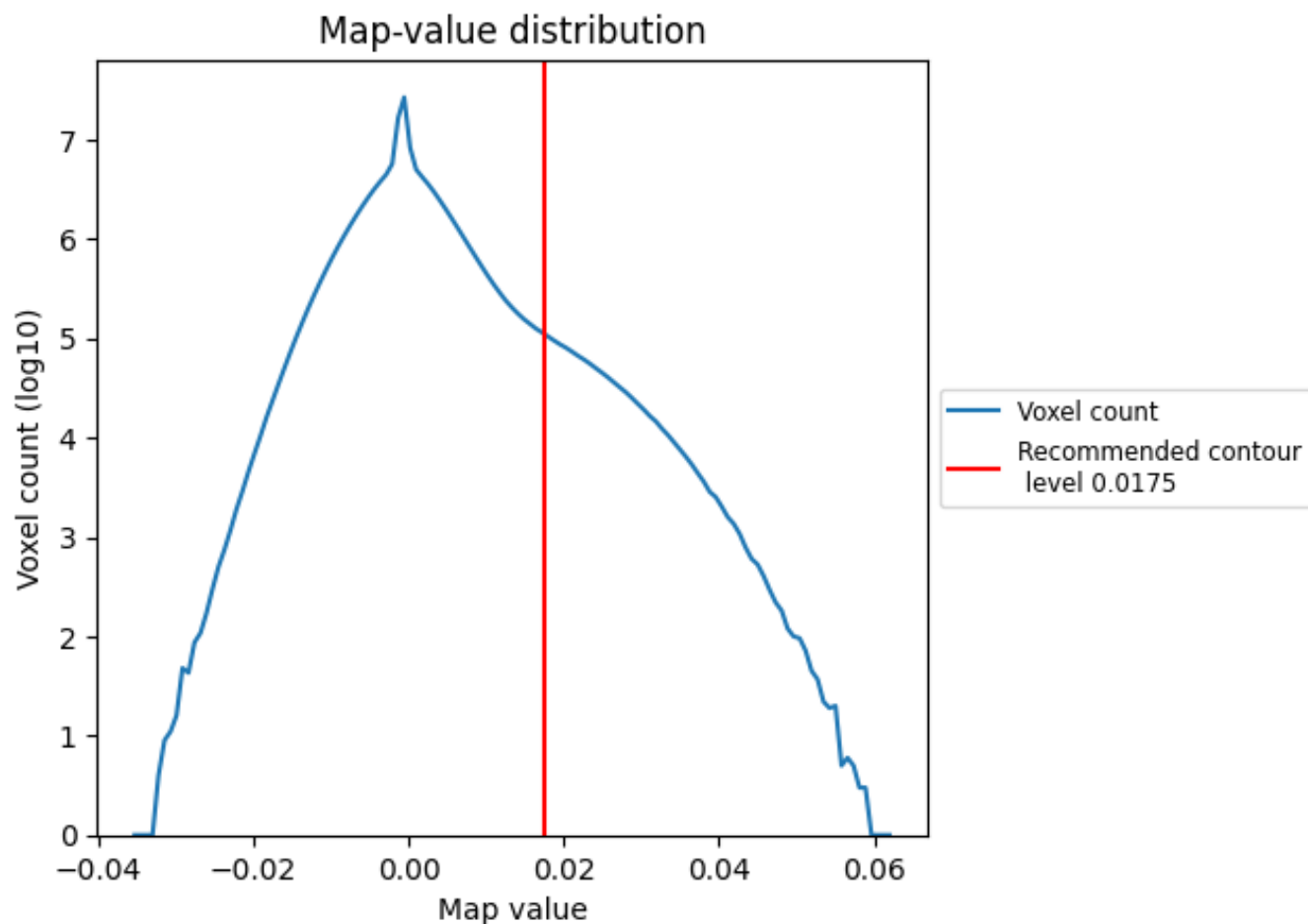
6.6 Mask visualisation

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

7 Map analysis [i](#)

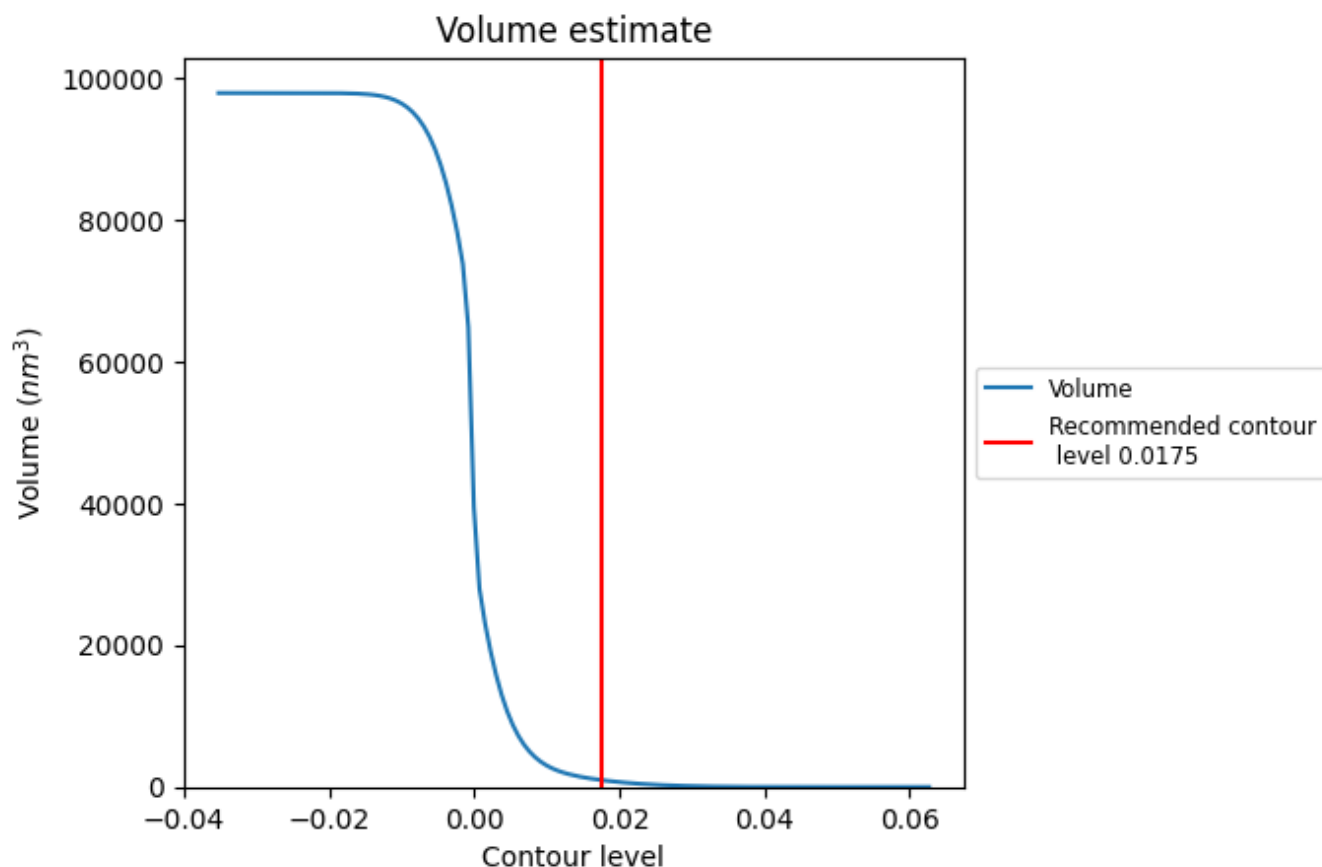
This section contains the results of statistical analysis of the map.

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.

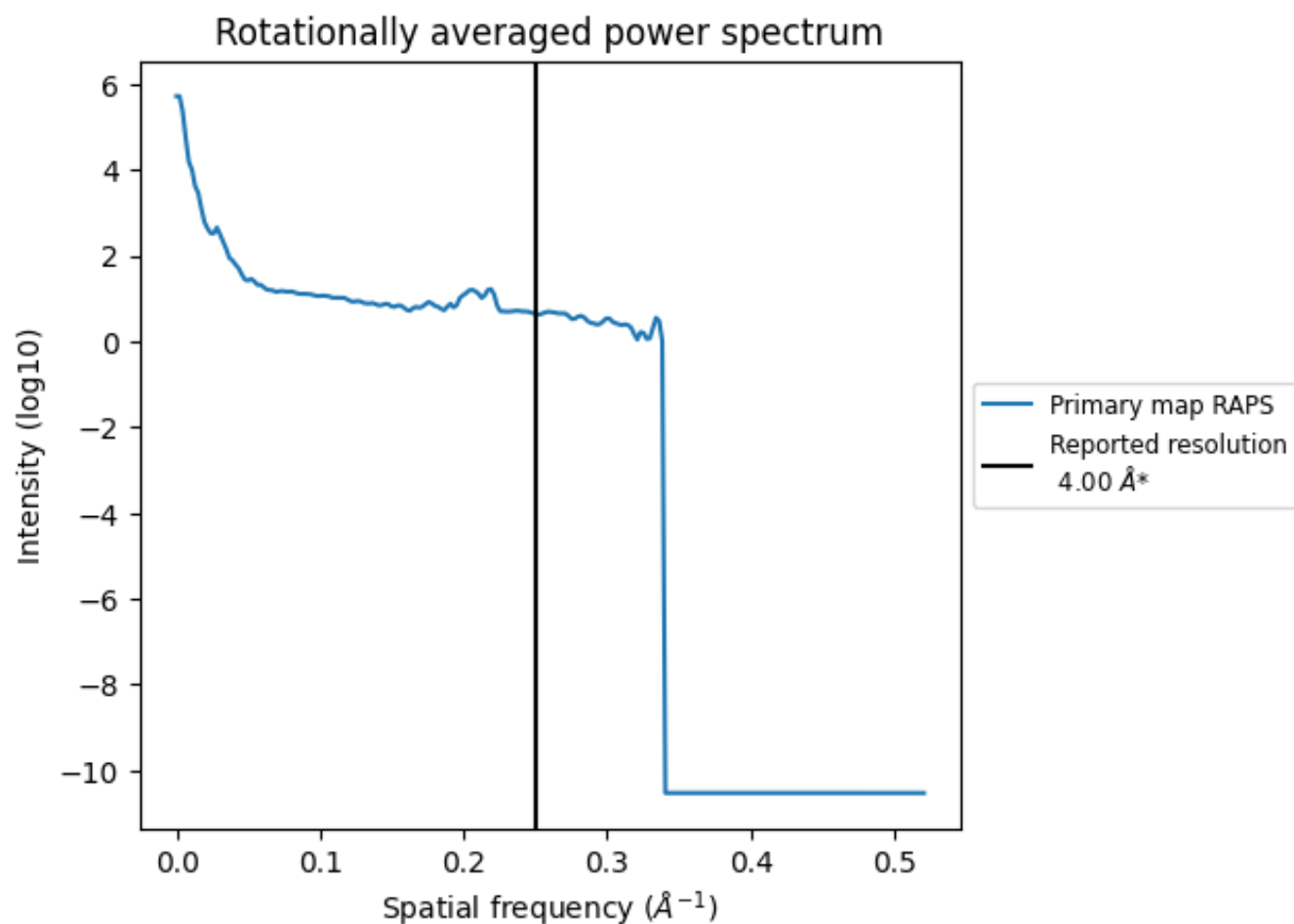
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 976 nm^3 ; this corresponds to an approximate mass of 881 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 ⓘ

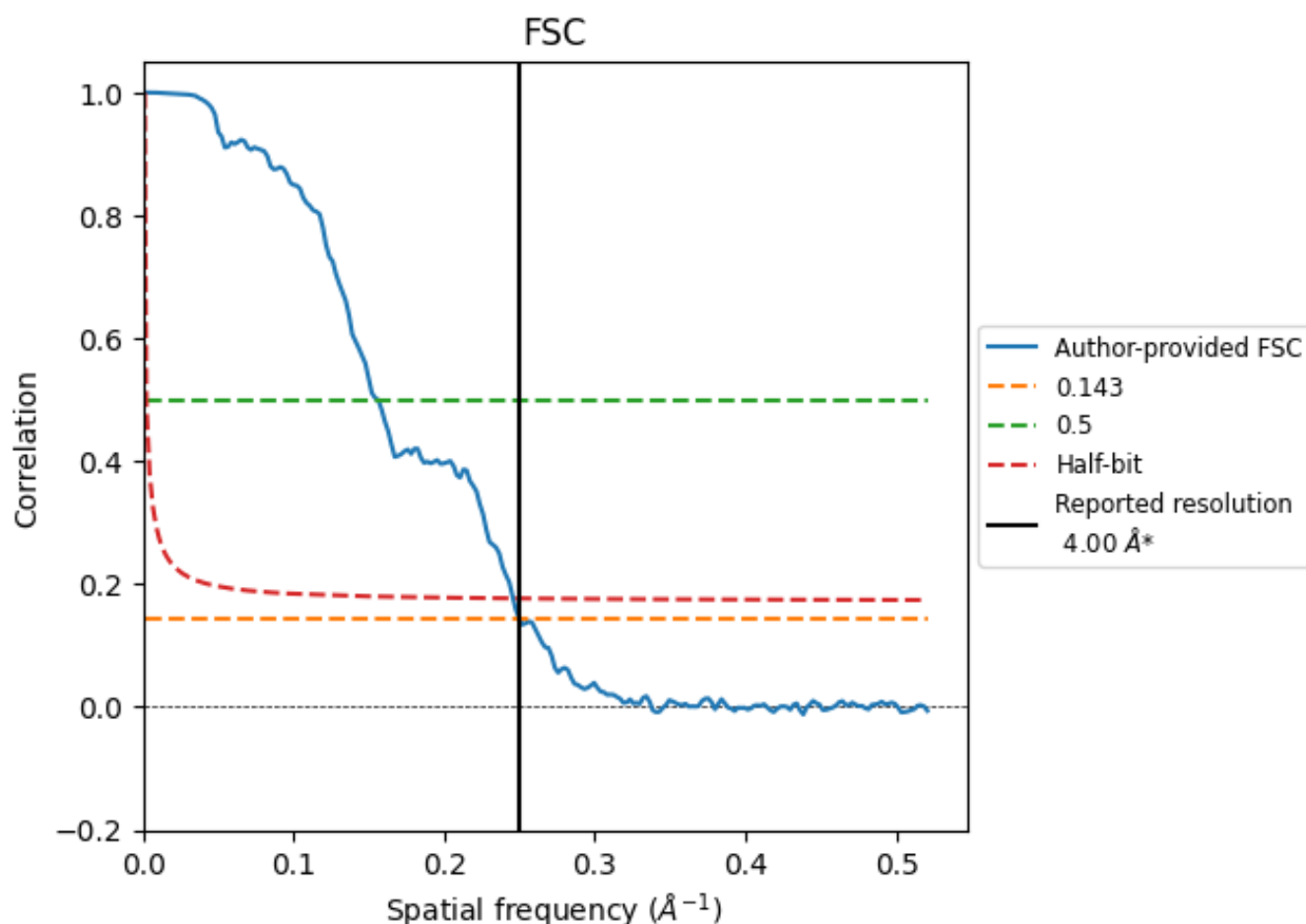


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

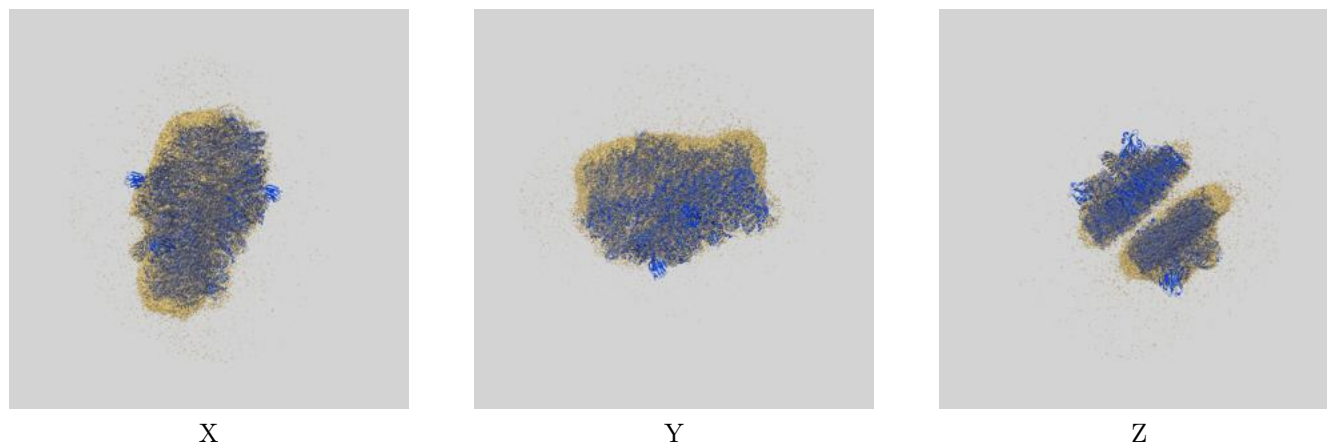
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	6.41	4.07
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

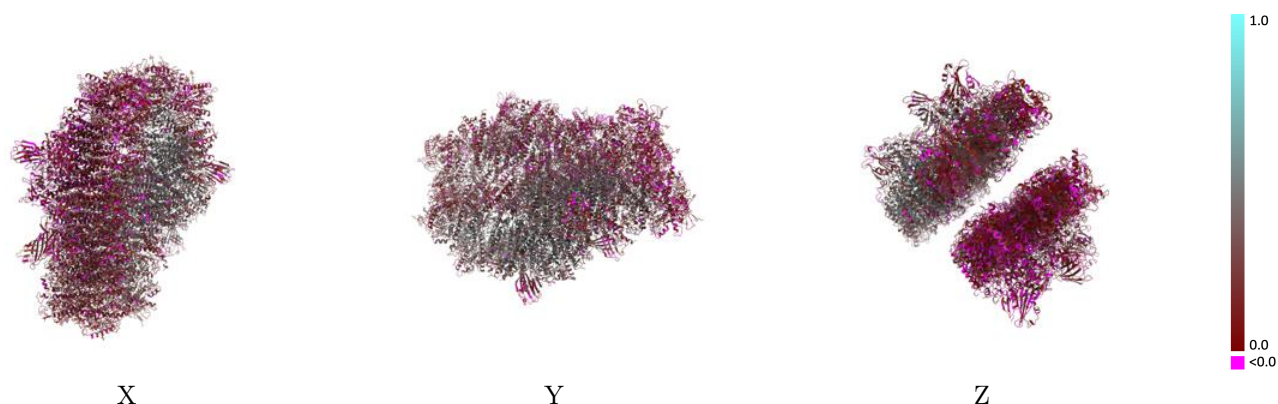
This section contains information regarding the fit between EMDB map EMD-13455 and PDB model 7PIW. Per-residue inclusion information can be found in section [3](#) on page [74](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0175 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](#)

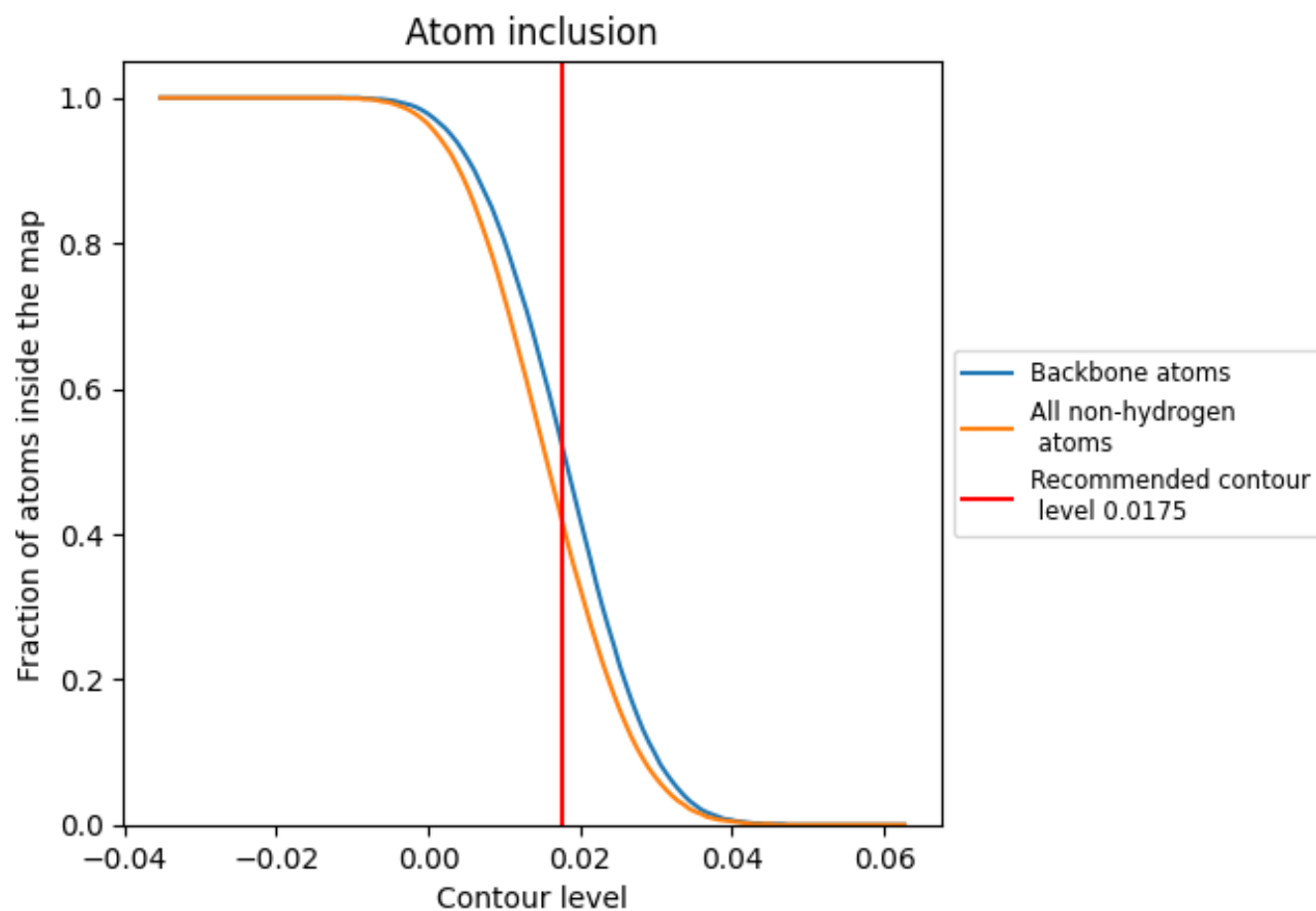


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 42% 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 (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4230	 0.2360
A	 0.4920	 0.4320
A1	 0.6120	 0.1910
B	 0.3740	 0.4030
B1	 0.5830	 0.1700
C	 0.4930	 0.4560
C1	 0.6260	 0.2020
D	 0.4420	 0.4380
D1	 0.5980	 0.1890
E	 0.3810	 0.3710
E1	 0.7460	 0.2080
F	 0.4090	 0.3800
F1	 0.7590	 0.2050
G	 0.1980	 0.2600
G1	 0.6690	 0.1600
H	 0.2980	 0.3500
H1	 0.5310	 0.1360
I	 0.4670	 0.4330
I1	 0.5400	 0.1970
J	 0.3820	 0.4050
J1	 0.5240	 0.1330
K	 0.4160	 0.4140
K1	 0.6510	 0.1960
L	 0.3520	 0.4110
L1	 0.4340	 0.1560
M	 0.3310	 0.3640
M1	 0.3820	 0.1470
N	 0.2960	 0.3340
N1	 0.6720	 0.1820
O	 0.2270	 0.3310
O1	 0.6070	 0.1800
P	 0.0180	 0.2020
P1	 0.0950	 0.1420
R	 0.1040	 0.1750
R1	 0.4660	 0.1110



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Chain	Atom inclusion	Q-score
S	 0.2680	 0.3030
S1	 0.6810	 0.1710
T	 0.3590	 0.4290
T1	 0.3960	 0.2160
U	 0.2200	 0.3330
U1	 0.5410	 0.2320
V	 0.3600	 0.3860
V1	 0.6090	 0.1950
W	 0.3150	 0.3650
W1	 0.6040	 0.2360
X	 0.2690	 0.2770
X1	 0.6270	 0.1450
Y	 0.3620	 0.3620
Y1	 0.6270	 0.1880
Z	 0.2730	 0.3710
Z1	 0.6530	 0.1750
a	 0.4670	 0.4160
a1	 0.4720	 0.1010
b	 0.3610	 0.3830
b1	 0.4930	 0.1120
c	 0.4000	 0.3630
c1	 0.4770	 0.0910
d	 0.4390	 0.4230
d1	 0.4440	 0.1090
e	 0.2430	 0.2560
e1	 0.4650	 0.1240
f	 0.3670	 0.3420
f1	 0.5450	 0.1770
g	 0.1420	 0.1520
g1	 0.5720	 0.0970
h	 0.2440	 0.3270
h1	 0.4570	 0.1090
i	 0.4500	 0.4350
i1	 0.4140	 0.1420
j	 0.2450	 0.3000
j1	 0.4380	 0.1210
k	 0.3480	 0.3170
k1	 0.4060	 0.0940
l	 0.3920	 0.4300
m	 0.2480	 0.3610
m1	 0.3740	 0.1220
n	 0.1660	 0.1610

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Chain	Atom inclusion	Q-score
n1	 0.5480	 0.1050
o	 0.2180	 0.2800
o1	 0.5320	 0.1330
p	 0.0080	 0.1570
p1	 0.0860	 0.0850
r	 0.1200	 0.1900
r1	 0.4780	 0.1150
s	 0.1610	 0.1410
s1	 0.4600	 0.0870
t	 0.3590	 0.3890
t1	 0.3090	 0.1070
u	 0.2060	 0.3570
u1	 0.4130	 0.1420
v	 0.2090	 0.2760
v1	 0.3330	 0.1020
w	 0.3360	 0.3470
w1	 0.4700	 0.1230
x	 0.2590	 0.2950
x1	 0.3830	 0.0660
y	 0.3310	 0.3270
y1	 0.5280	 0.1190
z	 0.1600	 0.1980
z1	 0.4240	 0.1280