



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 04:25 AM JST

PDB ID : 6JEO / pdb_00006jeo
EMDB ID : EMD-9807
Title : Structure of PSI tetramer from Anabaena
Authors : Kato, K.; Nagao, R.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on : 2019-02-06
Resolution : 3.30 Å(reported)
Based on initial model : 1JB0

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

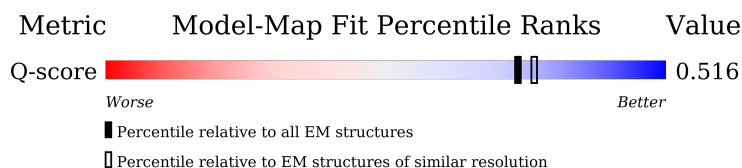
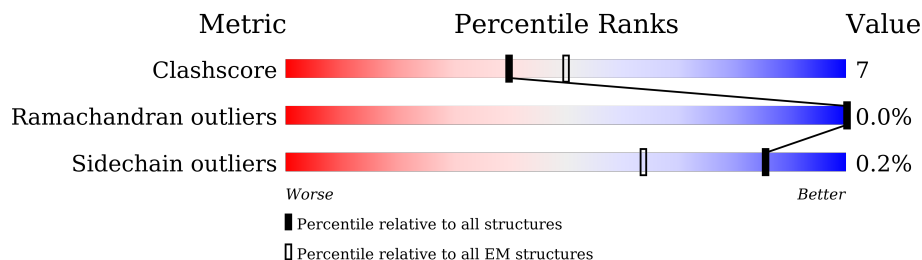
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	aA	752	26% 86% 12% .
1	bA	752	19% 86% 12% .
1	cA	752	26% 85% 13% .
1	dA	752	20% 86% 13% .

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Mol	Chain	Length	Quality of chain
2	aB	741	
2	bB	741	
2	cB	741	
2	dB	741	
3	aC	81	
3	bC	81	
3	cC	81	
3	dC	81	
4	aD	139	
4	bD	139	
4	cD	139	
4	dD	139	
5	aE	70	
5	bE	70	
5	cE	70	
5	dE	70	
6	aF	164	
6	bF	164	
6	cF	164	
6	dF	164	
7	aI	46	
7	bI	46	
7	cI	46	
7	dI	46	
8	aJ	49	

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Mol	Chain	Length	Quality of chain
8	bJ	49	
8	cJ	49	
8	dJ	49	
9	aK	86	
9	bK	86	
9	cK	86	
9	dK	86	
10	aL	172	
10	bL	172	
10	cL	172	
10	dL	172	
11	aM	40	
11	bM	40	
11	cM	40	
11	dM	40	
12	aX	44	
12	bX	44	
12	cX	44	
12	dX	44	

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
13	CL0	aA	801	-	-	X	-
13	CL0	bA	801	-	-	X	-
13	CL0	cA	801	-	-	X	-
15	PQN	bA	843	-	-	X	-
15	PQN	dA	843	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	SF4	aC	102	-	-	X	-
16	SF4	bC	102	-	-	X	-
16	SF4	cC	102	-	-	X	-
16	SF4	dC	102	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 94576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		
1	bA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		
1	cA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		
1	dA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		
2	bB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		
2	cB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		
2	dB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	bC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	cC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	dC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	73	Total	C	N	O	S	0	0
			581	378	97	105	1		
4	bD	96	Total	C	N	O	S	0	0
			740	479	122	138	1		
4	cD	73	Total	C	N	O	S	0	0
			581	378	97	105	1		
4	dD	96	Total	C	N	O	S	0	0
			740	479	122	138	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	aE	61	Total	C	N	O	0	0
			490	313	84	93		
5	bE	61	Total	C	N	O	0	0
			490	313	84	93		
5	cE	61	Total	C	N	O	0	0
			490	313	84	93		
5	dE	61	Total	C	N	O	0	0
			490	313	84	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	140	Total	C	N	O	S	0	0
			1072	684	183	203	2		
6	bF	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		
6	cF	140	Total	C	N	O	S	0	0
			1072	684	183	203	2		
6	dF	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	aI	31	Total	C	N	O	0	0
			253	177	35	41		
7	bI	31	Total	C	N	O	0	0
			253	177	35	41		
7	cI	31	Total	C	N	O	0	0
			253	177	35	41		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	dI	31	Total	C	N	O	0	0
			253	177	35	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	aJ	43	Total	C	N	O	0	0
			347	236	52	59		
8	bJ	43	Total	C	N	O	0	0
			347	236	52	59		
8	cJ	43	Total	C	N	O	0	0
			347	236	52	59		
8	dJ	43	Total	C	N	O	0	0
			347	236	52	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aK	66	Total	C	N	O	S	0	0
			480	322	78	79	1		
9	bK	66	Total	C	N	O	S	0	0
			480	322	78	79	1		
9	cK	66	Total	C	N	O	S	0	0
			480	322	78	79	1		
9	dK	66	Total	C	N	O	S	0	0
			480	322	78	79	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	140	Total	C	N	O	S	0	0
			1037	684	172	180	1		
10	bL	161	Total	C	N	O	S	0	0
			1210	792	206	211	1		
10	cL	140	Total	C	N	O	S	0	0
			1037	684	172	180	1		
10	dL	161	Total	C	N	O	S	0	0
			1210	792	206	211	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	aM	30	Total 235	C 157	N 36	O 42	0	0
11	bM	30	Total 235	C 157	N 36	O 42	0	0
11	cM	30	Total 235	C 157	N 36	O 42	0	0
11	dM	30	Total 235	C 157	N 36	O 42	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
aM	1	MET	-	see sequence details	UNP Q8YNB0
aM	2	PRO	-	see sequence details	UNP Q8YNB0
aM	3	THR	-	see sequence details	UNP Q8YNB0
aM	4	LEU	-	see sequence details	UNP Q8YNB0
aM	5	TYR	-	see sequence details	UNP Q8YNB0
aM	6	LEU	-	see sequence details	UNP Q8YNB0
aM	7	ALA	-	see sequence details	UNP Q8YNB0
aM	8	GLN	-	see sequence details	UNP Q8YNB0
aM	9	VAL	-	see sequence details	UNP Q8YNB0
bM	1	MET	-	see sequence details	UNP Q8YNB0
bM	2	PRO	-	see sequence details	UNP Q8YNB0
bM	3	THR	-	see sequence details	UNP Q8YNB0
bM	4	LEU	-	see sequence details	UNP Q8YNB0
bM	5	TYR	-	see sequence details	UNP Q8YNB0
bM	6	LEU	-	see sequence details	UNP Q8YNB0
bM	7	ALA	-	see sequence details	UNP Q8YNB0
bM	8	GLN	-	see sequence details	UNP Q8YNB0
bM	9	VAL	-	see sequence details	UNP Q8YNB0
cM	1	MET	-	see sequence details	UNP Q8YNB0
cM	2	PRO	-	see sequence details	UNP Q8YNB0
cM	3	THR	-	see sequence details	UNP Q8YNB0
cM	4	LEU	-	see sequence details	UNP Q8YNB0
cM	5	TYR	-	see sequence details	UNP Q8YNB0
cM	6	LEU	-	see sequence details	UNP Q8YNB0
cM	7	ALA	-	see sequence details	UNP Q8YNB0
cM	8	GLN	-	see sequence details	UNP Q8YNB0
cM	9	VAL	-	see sequence details	UNP Q8YNB0
dM	1	MET	-	see sequence details	UNP Q8YNB0
dM	2	PRO	-	see sequence details	UNP Q8YNB0
dM	3	THR	-	see sequence details	UNP Q8YNB0
dM	4	LEU	-	see sequence details	UNP Q8YNB0

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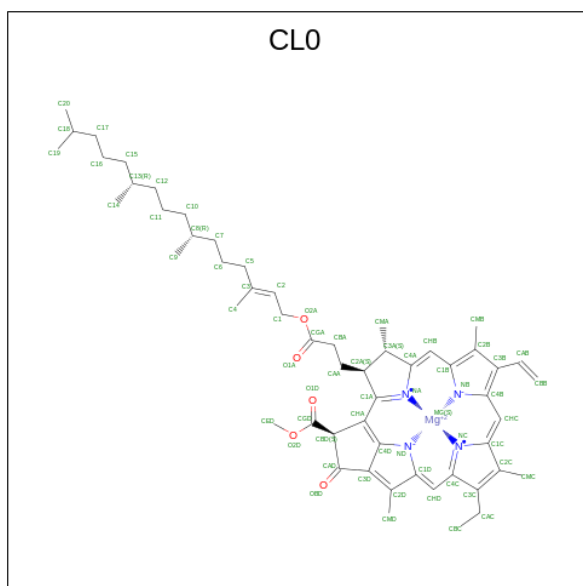
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Chain	Residue	Modelled	Actual	Comment	Reference
dM	5	TYR	-	see sequence details	UNP Q8YNB0
dM	6	LEU	-	see sequence details	UNP Q8YNB0
dM	7	ALA	-	see sequence details	UNP Q8YNB0
dM	8	GLN	-	see sequence details	UNP Q8YNB0
dM	9	VAL	-	see sequence details	UNP Q8YNB0

- Molecule 12 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	aX	29	Total	C	N	O	0	0
			243	170	37	36		
12	bX	29	Total	C	N	O	0	0
			243	170	37	36		
12	cX	29	Total	C	N	O	0	0
			243	170	37	36		
12	dX	29	Total	C	N	O	0	0
			243	170	37	36		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



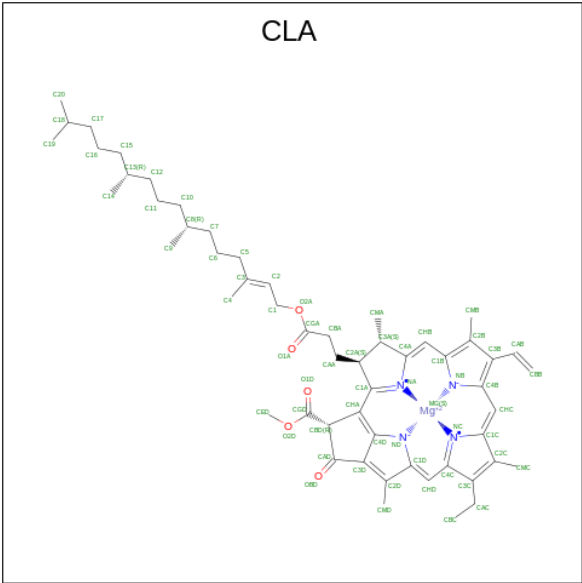
Mol	Chain	Residues	Atoms				AltConf
13	aA	1	Total	C	Mg	N	O
			65	55	1	4	5
13	bA	1	Total	C	Mg	N	O
			65	55	1	4	5
13	cA	1	Total	C	Mg	N	O
			65	55	1	4	5

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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	aA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aF	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	aF	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aJ	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	aK	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	aK	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aL	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	aX	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bB	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	bB	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bF	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	bF	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bJ	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	bK	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	bK	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bL	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	bL	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bX	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cA	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cB	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cB	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	cF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	cK	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
14	cK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	cX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	dA	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	dA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	dA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	dA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	dA	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	dA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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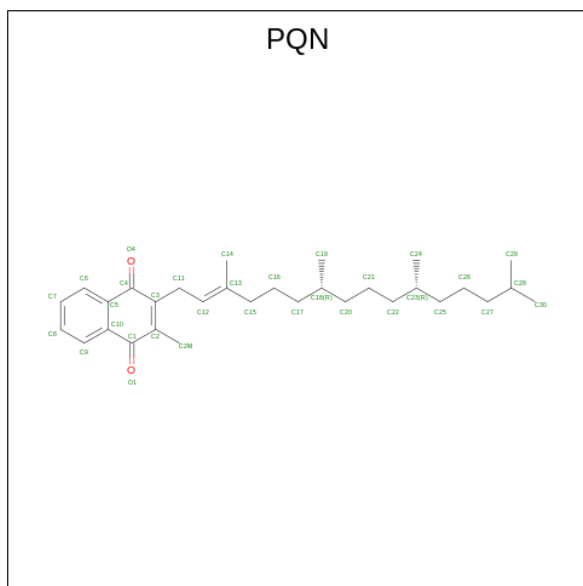
Mol	Chain	Residues	Atoms					AltConf
14	dB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	dF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	dJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	dK	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
14	dK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dL	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	dL	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



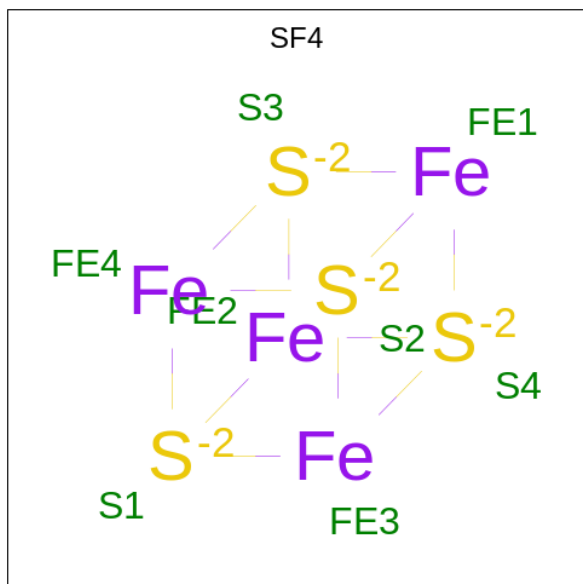
Mol	Chain	Residues	Atoms			AltConf
15	aA	1	Total	C	O	0
			33	31	2	
15	aB	1	Total	C	O	0
			33	31	2	

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Mol	Chain	Residues	Atoms			AltConf
15	bA	1	Total	C	O	0
			33	31	2	
15	bB	1	Total	C	O	0
			33	31	2	
15	cA	1	Total	C	O	0
			33	31	2	
15	cB	1	Total	C	O	0
			33	31	2	
15	dA	1	Total	C	O	0
			33	31	2	
15	dB	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



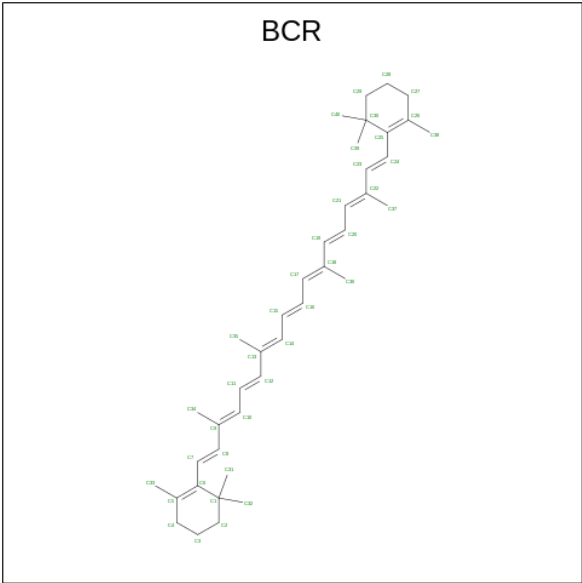
Mol	Chain	Residues	Atoms			AltConf
16	aA	1	Total	Fe	S	0
			8	4	4	
16	aC	1	Total	Fe	S	0
			8	4	4	
16	aC	1	Total	Fe	S	0
			8	4	4	
16	bA	1	Total	Fe	S	0
			8	4	4	
16	bC	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
16	bC	1	Total	Fe	S	0
			8	4	4	
16	cA	1	Total	Fe	S	0
			8	4	4	
16	cC	1	Total	Fe	S	0
			8	4	4	
16	cC	1	Total	Fe	S	0
			8	4	4	
16	dA	1	Total	Fe	S	0
			8	4	4	
16	dC	1	Total	Fe	S	0
			8	4	4	
16	dC	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
17	aA	1	Total C 40 40	0
17	aA	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aF	1	Total C 40 40	0
17	aF	1	Total C 40 40	0
17	aI	1	Total C 40 40	0
17	aJ	1	Total C 40 40	0
17	aJ	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	aM	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bI	1	Total C 40 40	0
17	bJ	1	Total C 40 40	0
17	bJ	1	Total C 40 40	0
17	bK	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bM	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0

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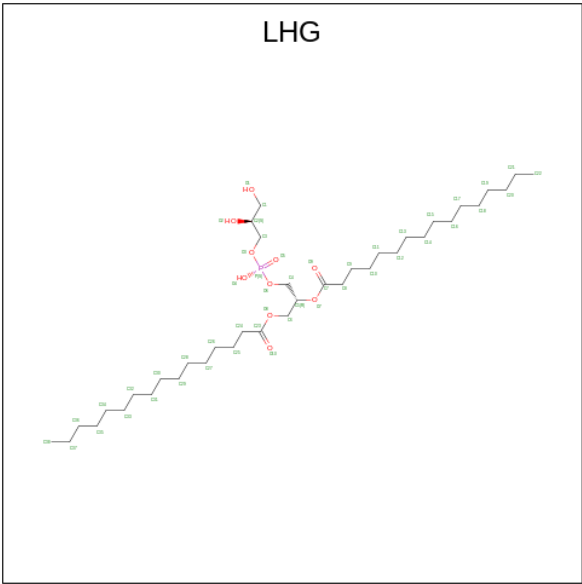
Mol	Chain	Residues	Atoms	AltConf
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cJ	1	Total C 40 40	0
17	cJ	1	Total C 40 40	0
17	cL	1	Total C 40 40	0
17	cL	1	Total C 40 40	0
17	cL	1	Total C 40 40	0
17	cM	1	Total C 40 40	0
17	dA	1	Total C 40 40	0

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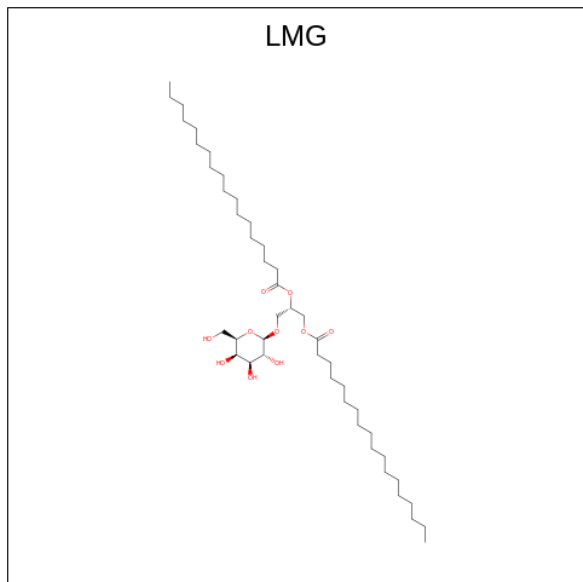
Mol	Chain	Residues	Atoms	AltConf
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17	dA	1	Total C 40 40	0
17	dA	1	Total C 40 40	0
17	dA	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dF	1	Total C 40 40	0
17	dF	1	Total C 40 40	0
17	dI	1	Total C 40 40	0
17	dJ	1	Total C 40 40	0
17	dJ	1	Total C 40 40	0
17	dK	1	Total C 40 40	0
17	dL	1	Total C 40 40	0
17	dL	1	Total C 40 40	0
17	dL	1	Total C 40 40	0
17	dM	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
18	aA	1	Total	C	O	P	0
			49	38	10	1	
18	aA	1	Total	C	O	P	0
			27	16	10	1	
18	aB	1	Total	C	O	P	0
			23	12	10	1	
18	bA	1	Total	C	O	P	0
			49	38	10	1	
18	bA	1	Total	C	O	P	0
			27	16	10	1	
18	bB	1	Total	C	O	P	0
			23	12	10	1	
18	cA	1	Total	C	O	P	0
			49	38	10	1	
18	cA	1	Total	C	O	P	0
			27	16	10	1	
18	cB	1	Total	C	O	P	0
			23	12	10	1	
18	dA	1	Total	C	O	P	0
			49	38	10	1	
18	dA	1	Total	C	O	P	0
			27	16	10	1	
18	dB	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

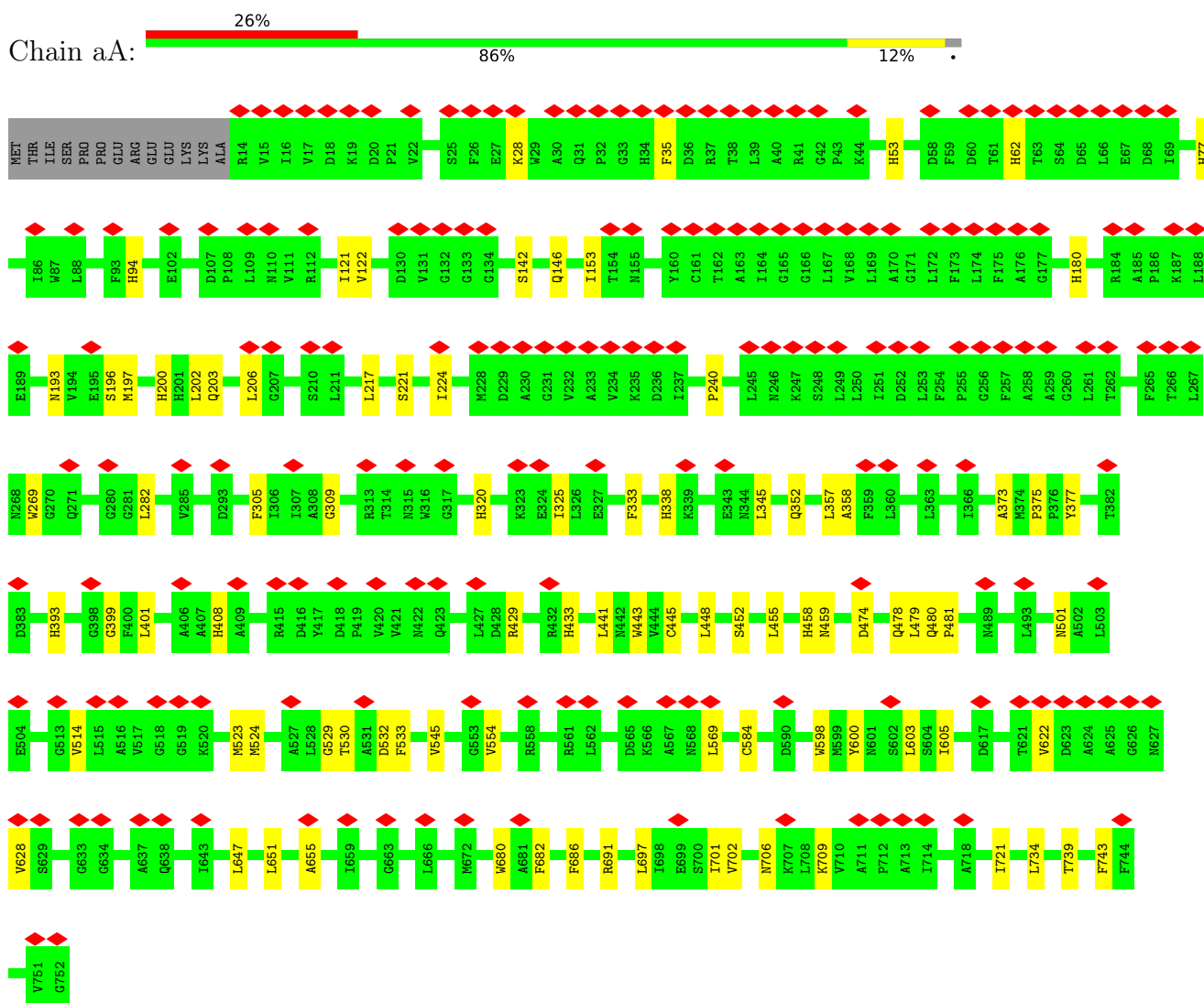


Mol	Chain	Residues	Atoms			AltConf
19	aB	1	Total	C	O	0
			55	45	10	
19	bB	1	Total	C	O	0
			55	45	10	
19	cB	1	Total	C	O	0
			55	45	10	
19	dB	1	Total	C	O	0
			55	45	10	

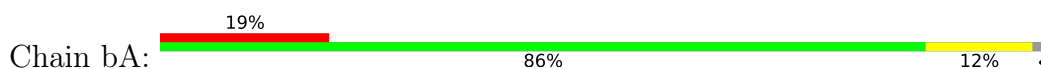
3 Residue-property plots

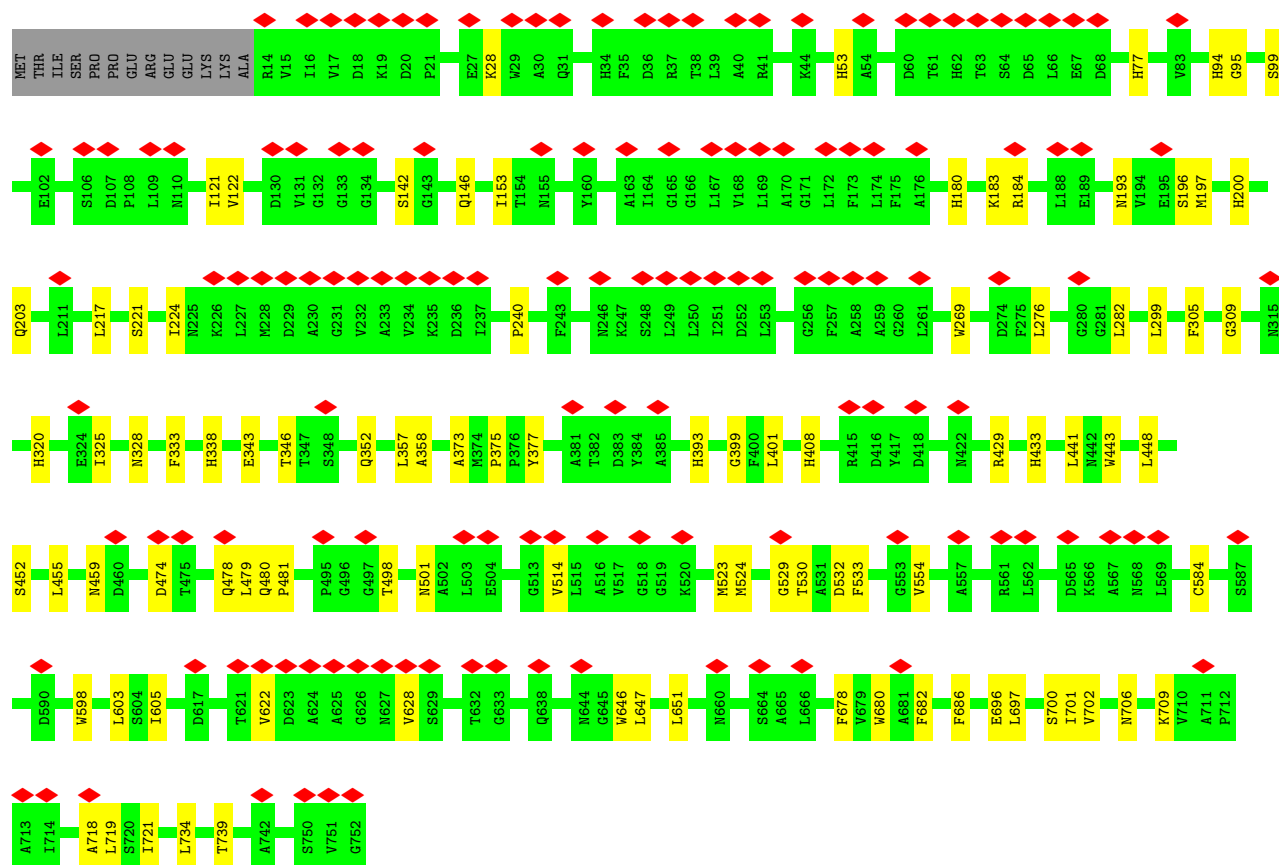
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

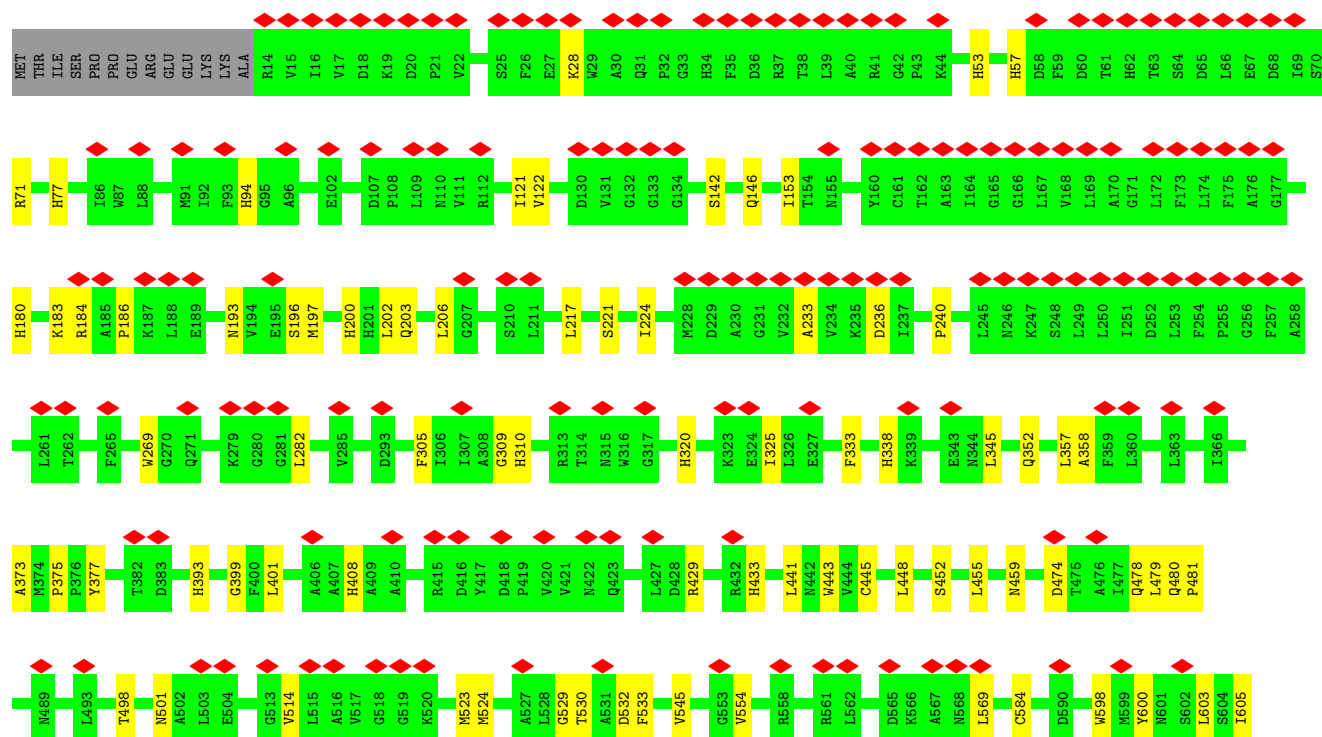
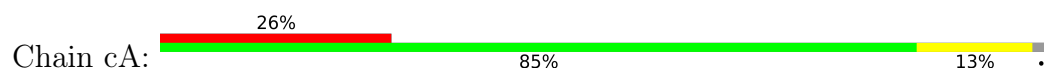


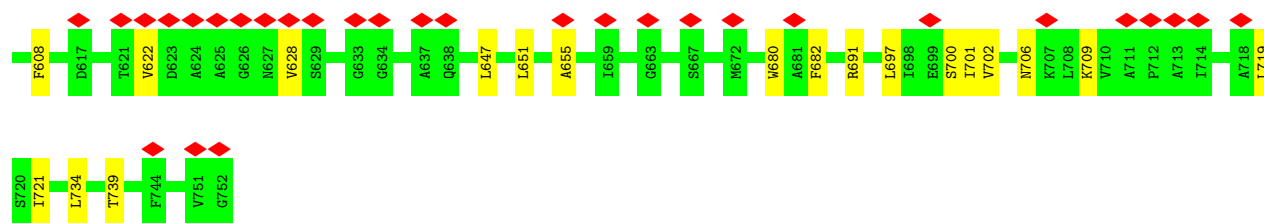
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



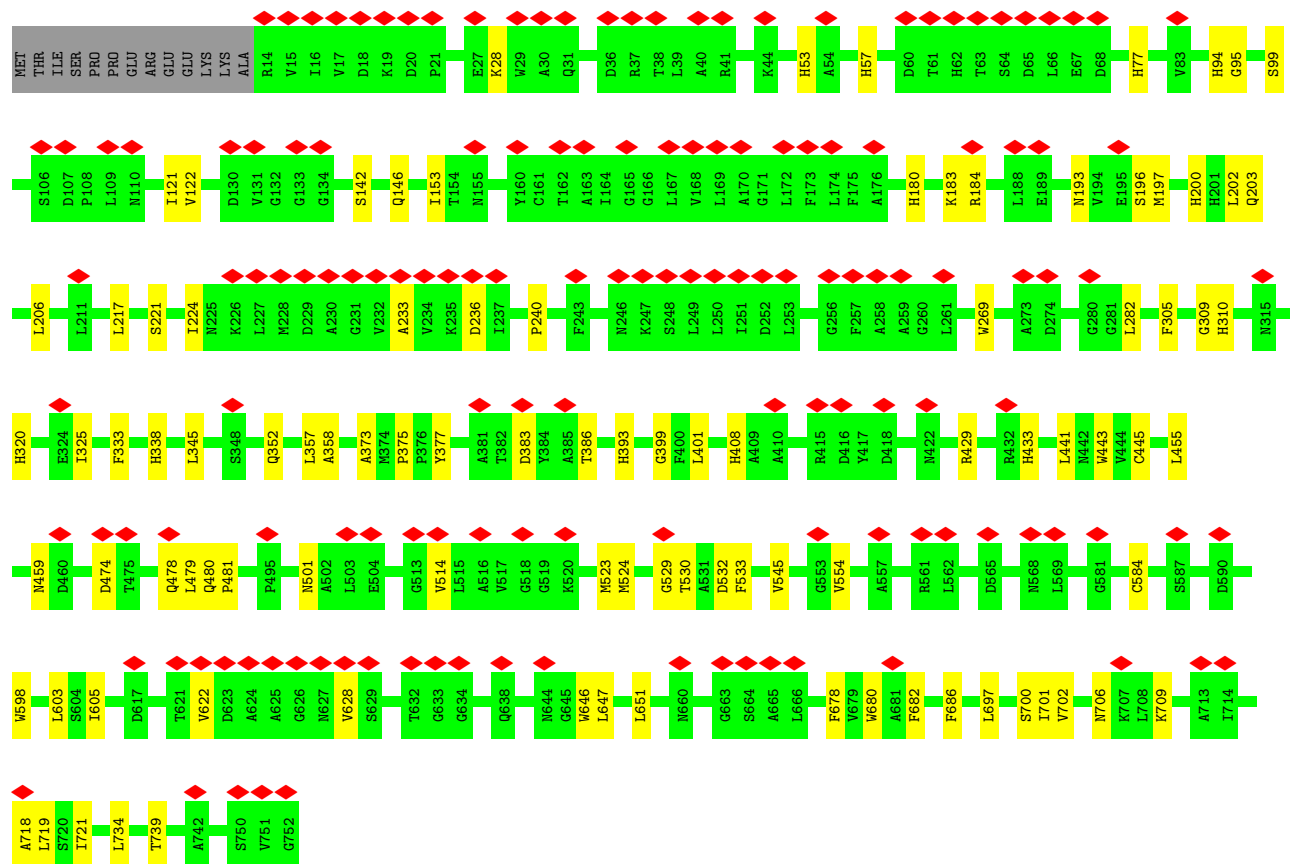
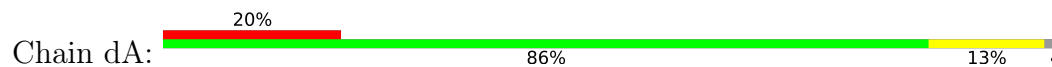


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

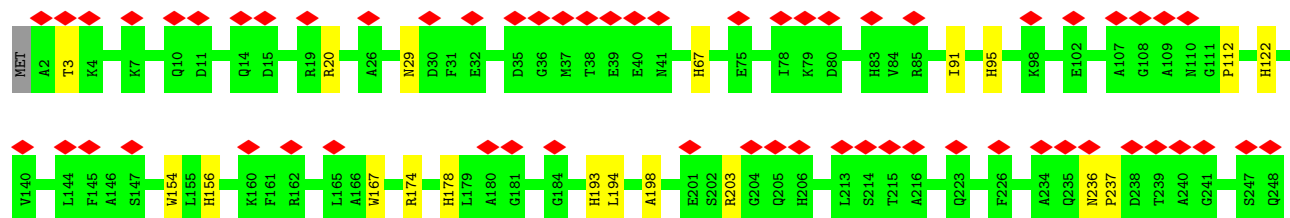


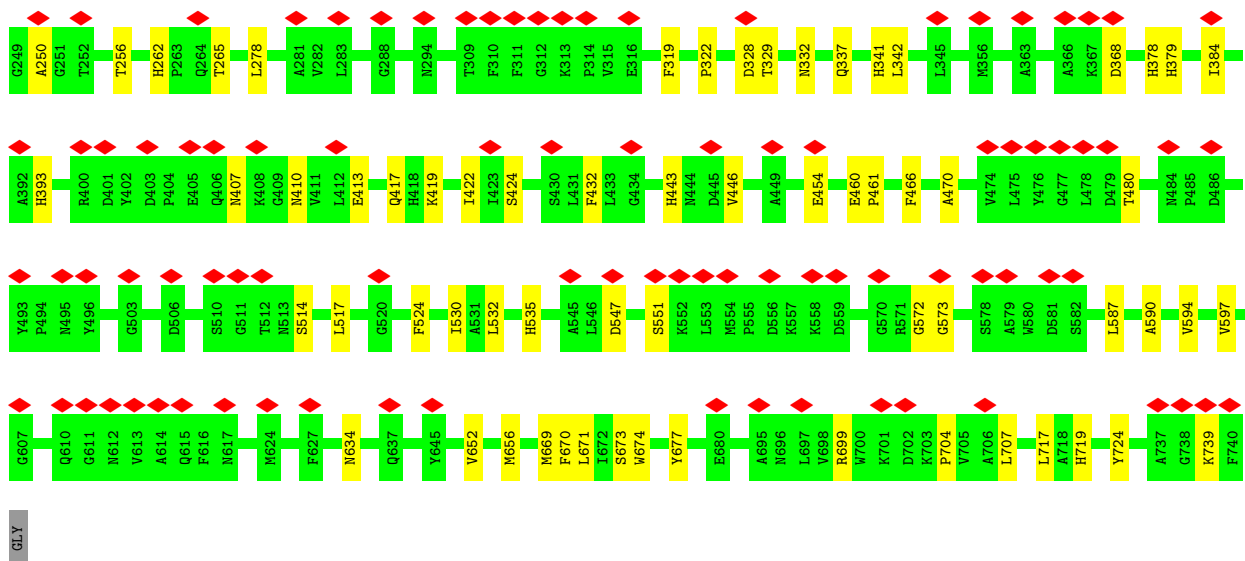


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

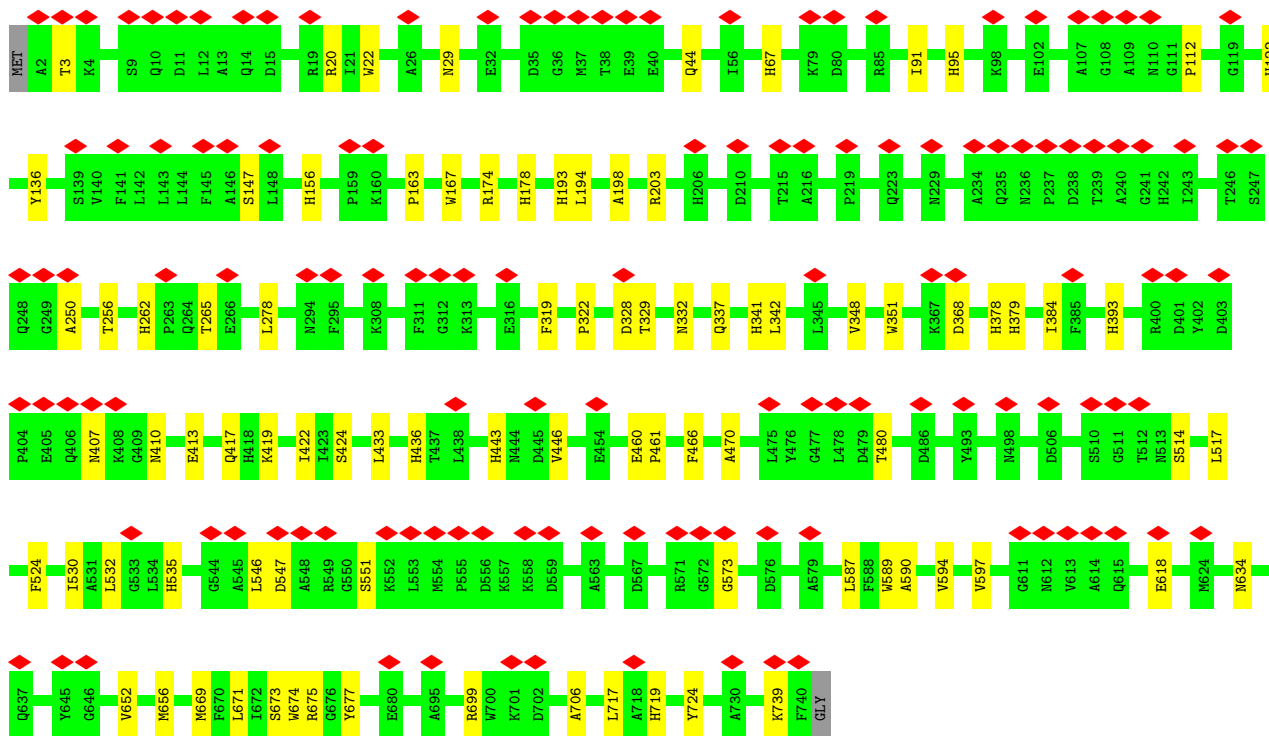
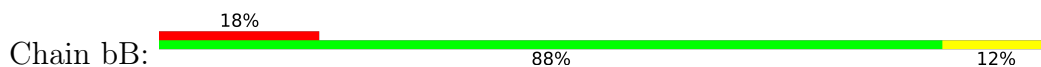


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

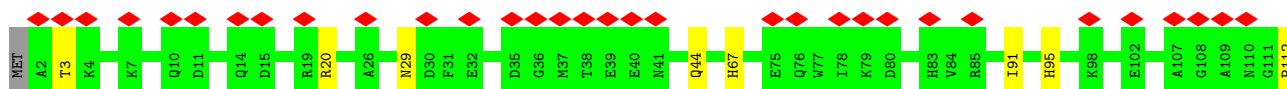
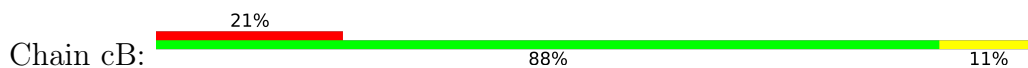


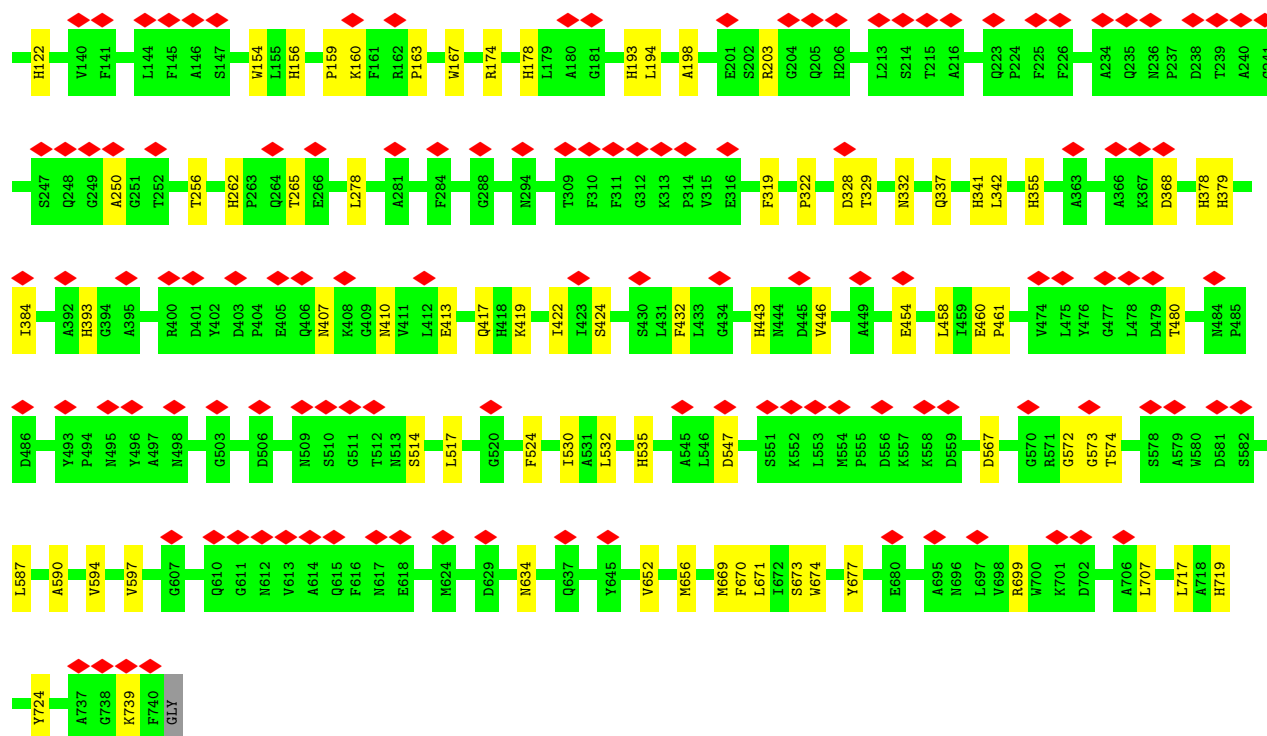


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

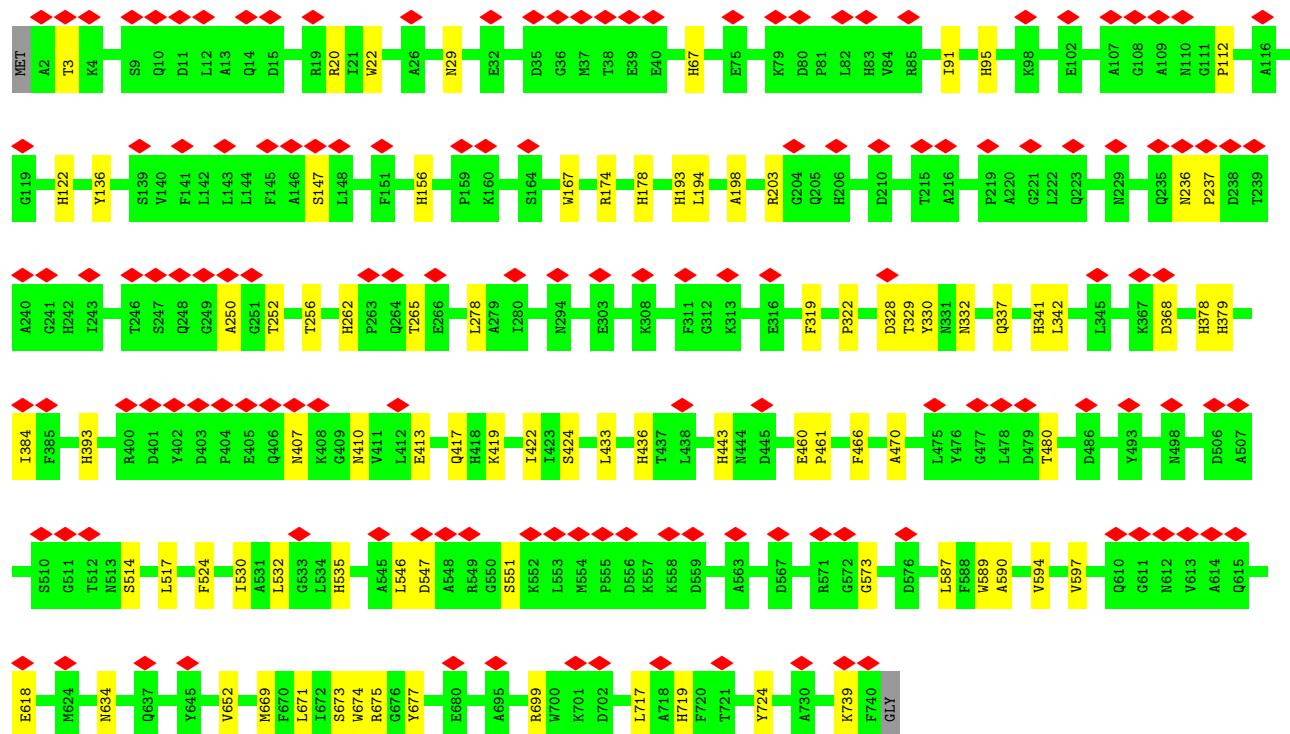
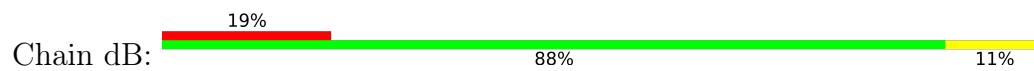


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

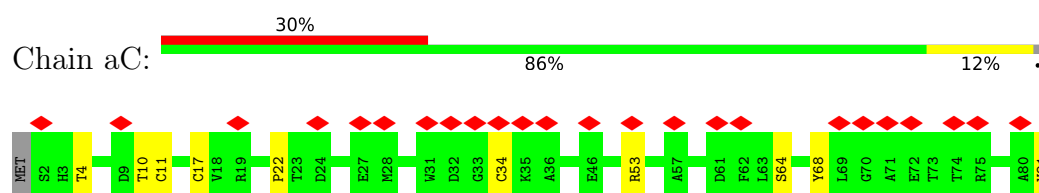




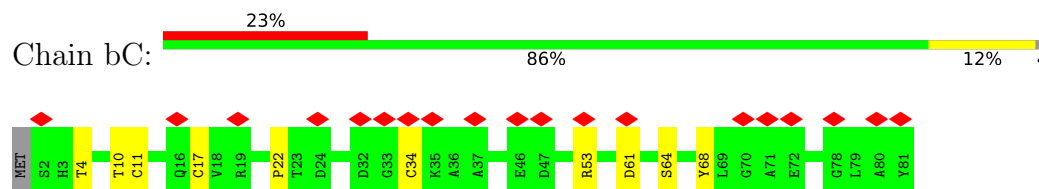
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1



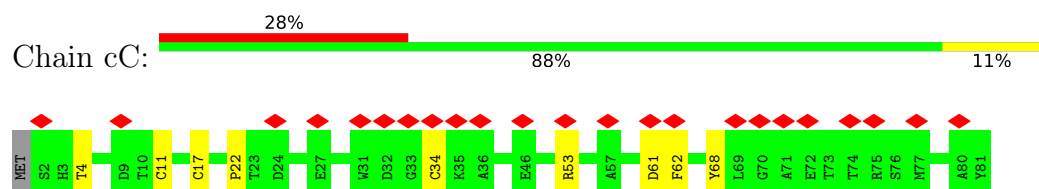
• Molecule 3: Photosystem I iron-sulfur center



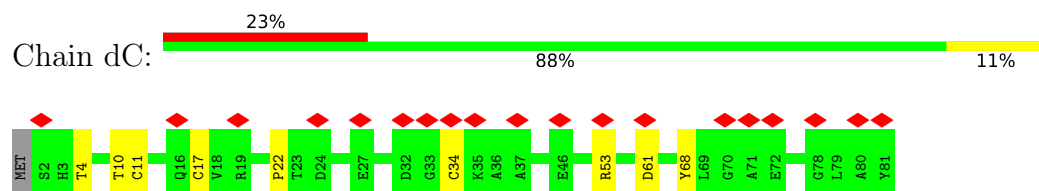
- Molecule 3: Photosystem I iron-sulfur center



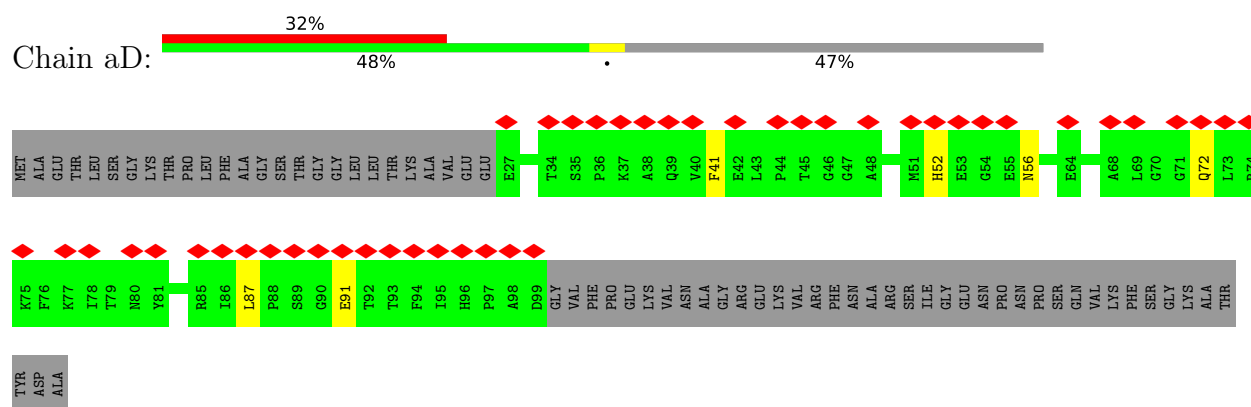
- Molecule 3: Photosystem I iron-sulfur center



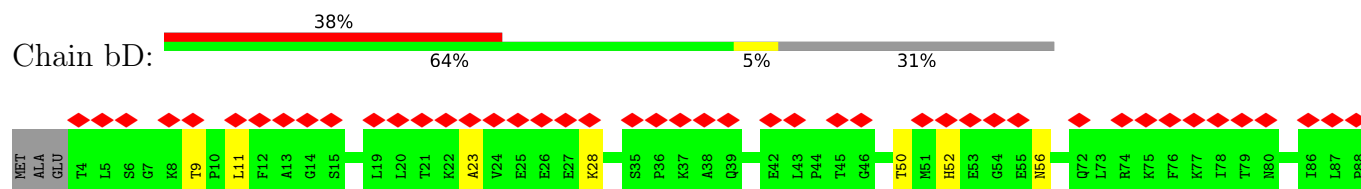
- Molecule 3: Photosystem I iron-sulfur center

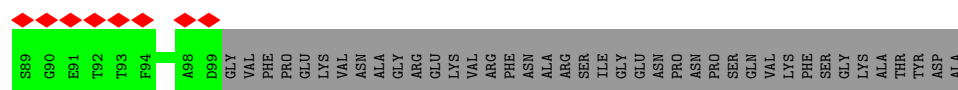


- Molecule 4: Photosystem I reaction center subunit II

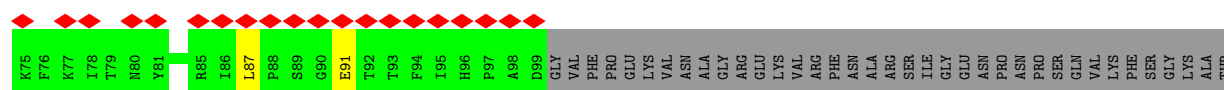
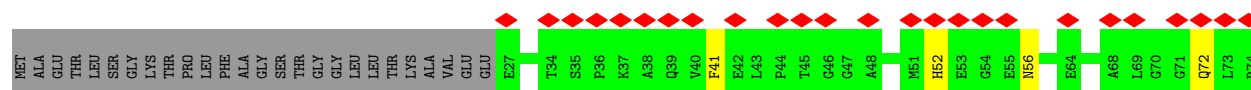


- Molecule 4: Photosystem I reaction center subunit II

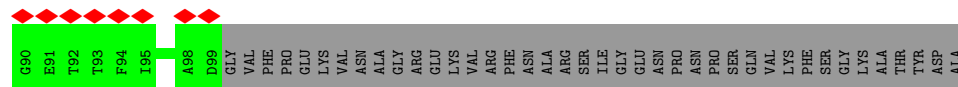
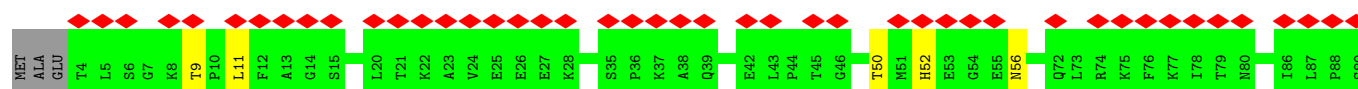
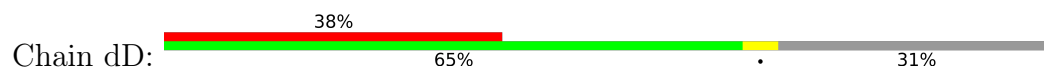




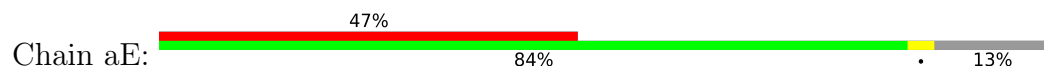
- Molecule 4: Photosystem I reaction center subunit II



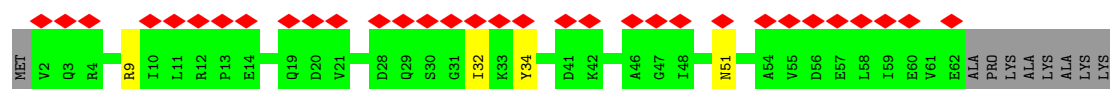
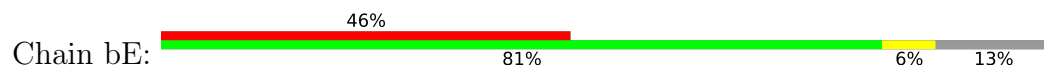
- Molecule 4: Photosystem I reaction center subunit II



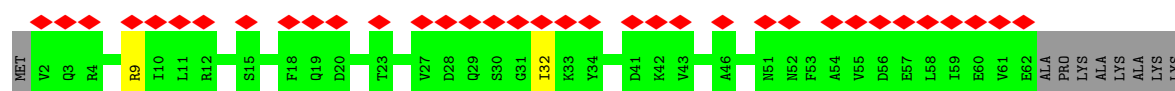
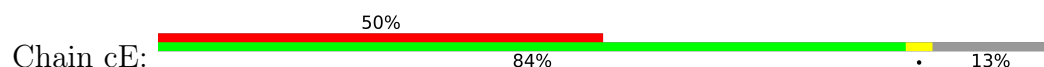
- Molecule 5: Photosystem I reaction center subunit IV



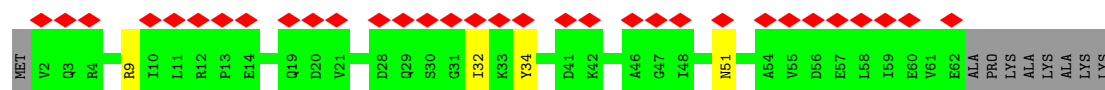
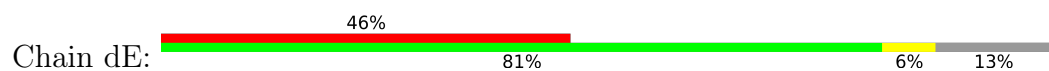
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 5: Photosystem I reaction center subunit IV



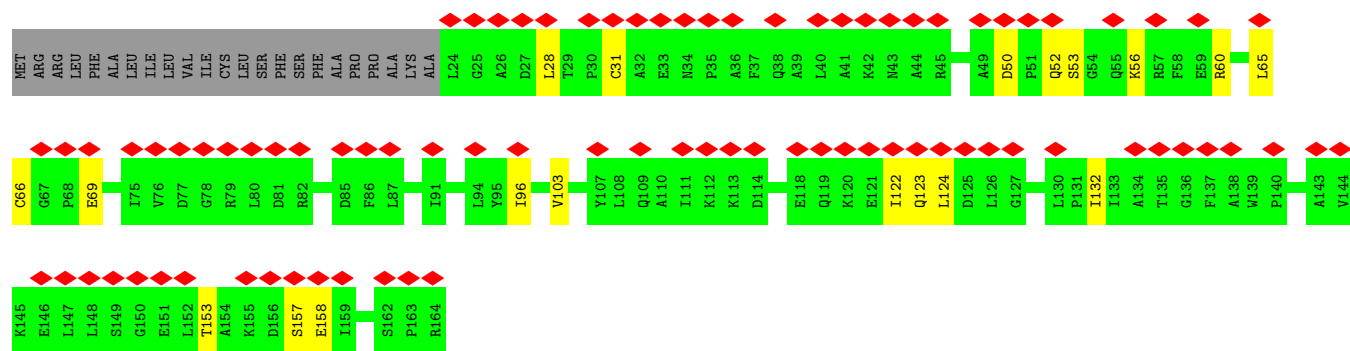
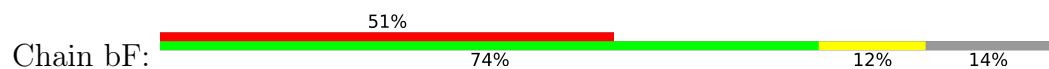
- Molecule 5: Photosystem I reaction center subunit IV



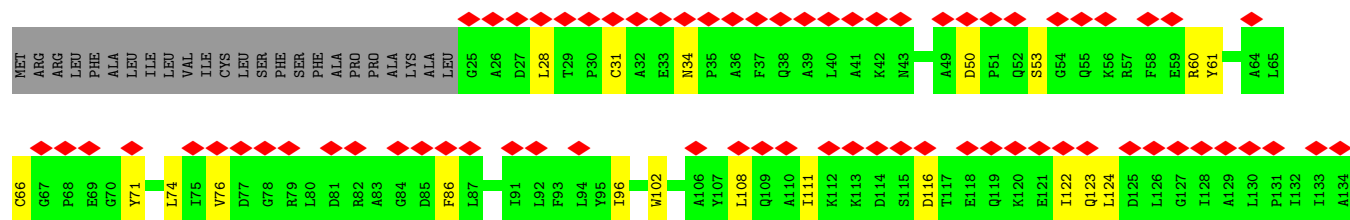
- Molecule 6: Photosystem I reaction center subunit III

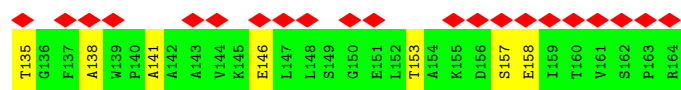


- Molecule 6: Photosystem I reaction center subunit III

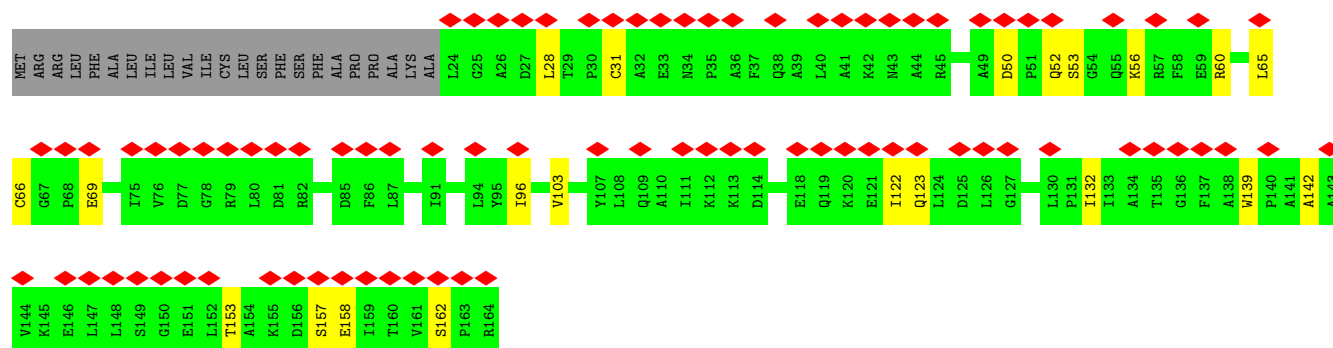
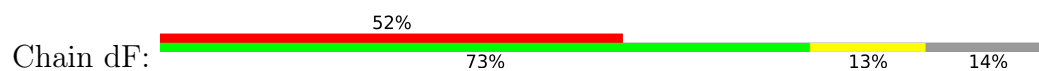


- Molecule 6: Photosystem I reaction center subunit III





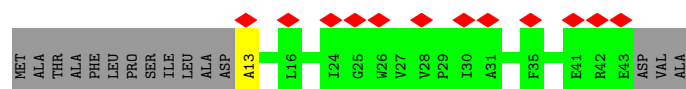
• Molecule 6: Photosystem I reaction center subunit III



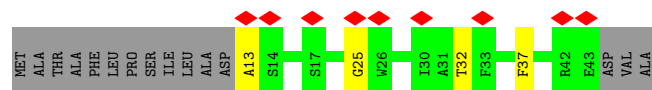
• Molecule 7: Photosystem I reaction center subunit VIII



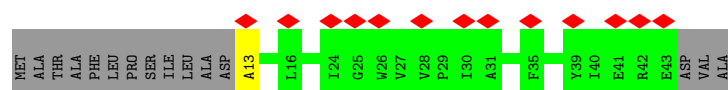
• Molecule 7: Photosystem I reaction center subunit VIII



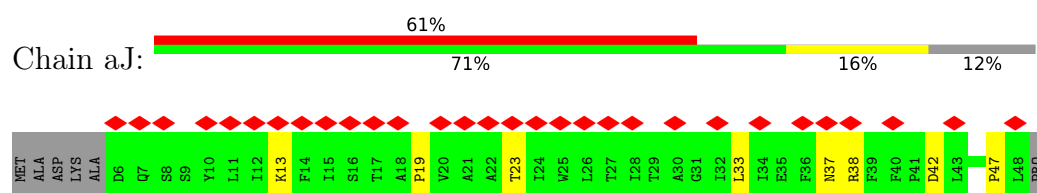
• Molecule 7: Photosystem I reaction center subunit VIII



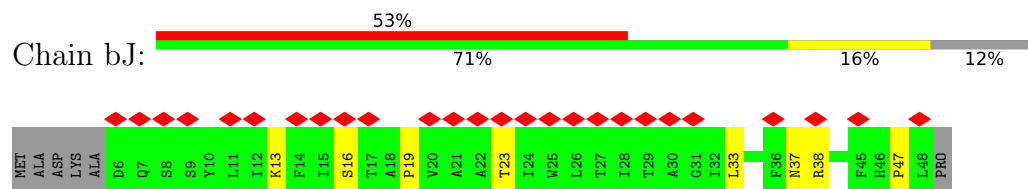
• Molecule 7: Photosystem I reaction center subunit VIII



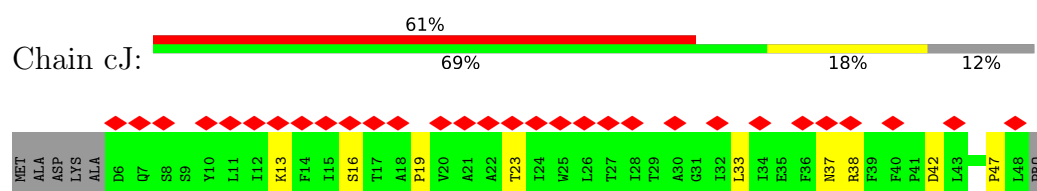
• Molecule 8: Photosystem I reaction center subunit IX



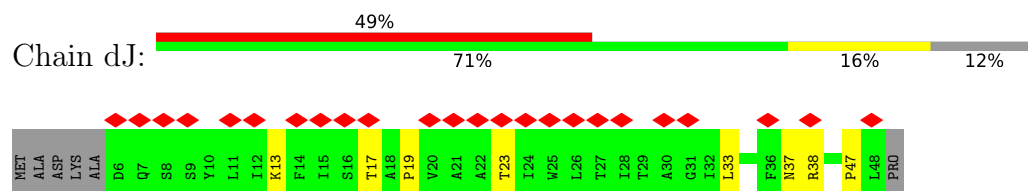
- Molecule 8: Photosystem I reaction center subunit IX



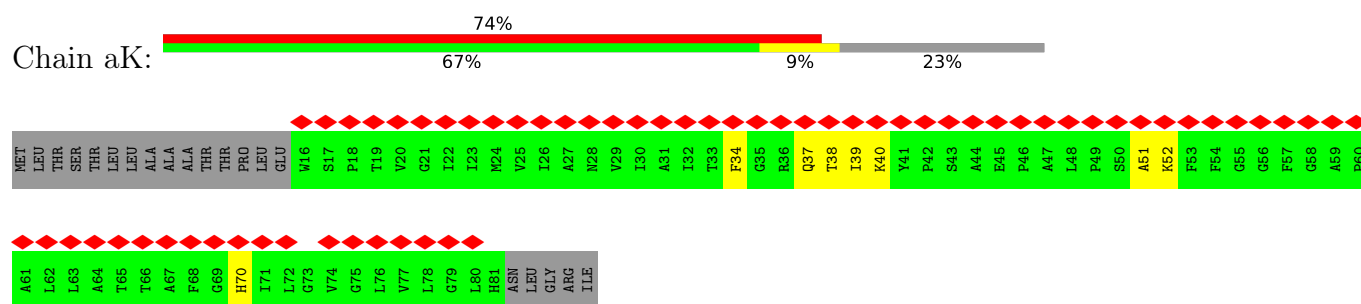
- Molecule 8: Photosystem I reaction center subunit IX



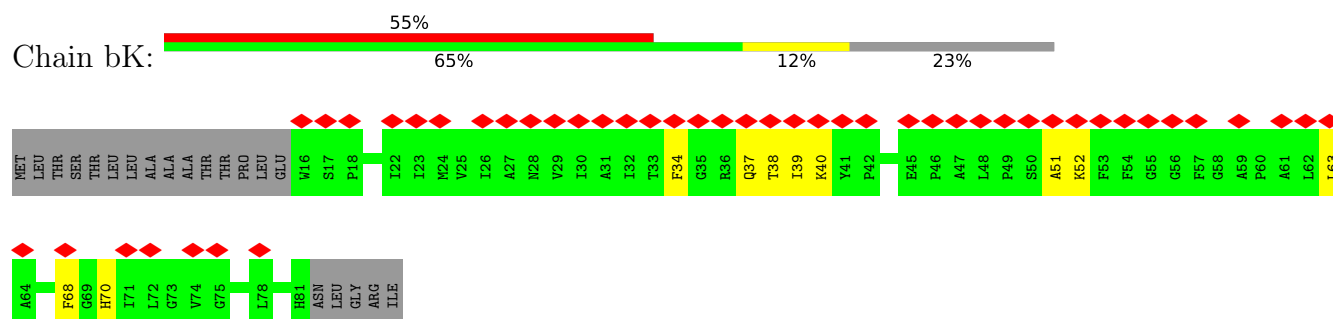
- Molecule 8: Photosystem I reaction center subunit IX



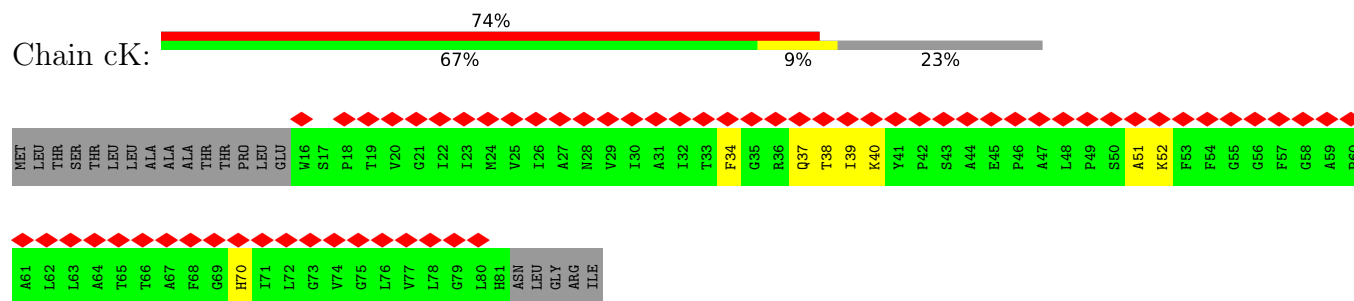
- Molecule 9: Photosystem I reaction center subunit PsaK 1



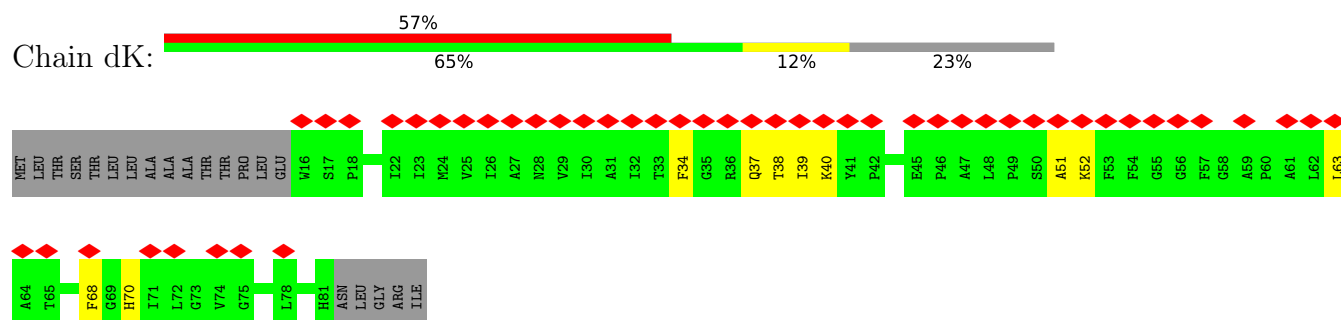
- Molecule 9: Photosystem I reaction center subunit PsaK 1



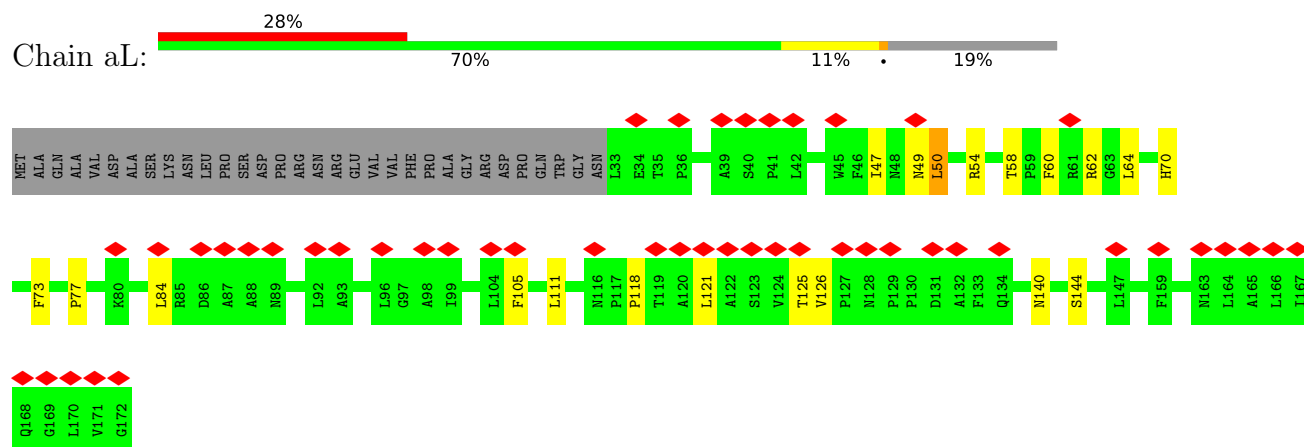
- Molecule 9: Photosystem I reaction center subunit PsaK 1



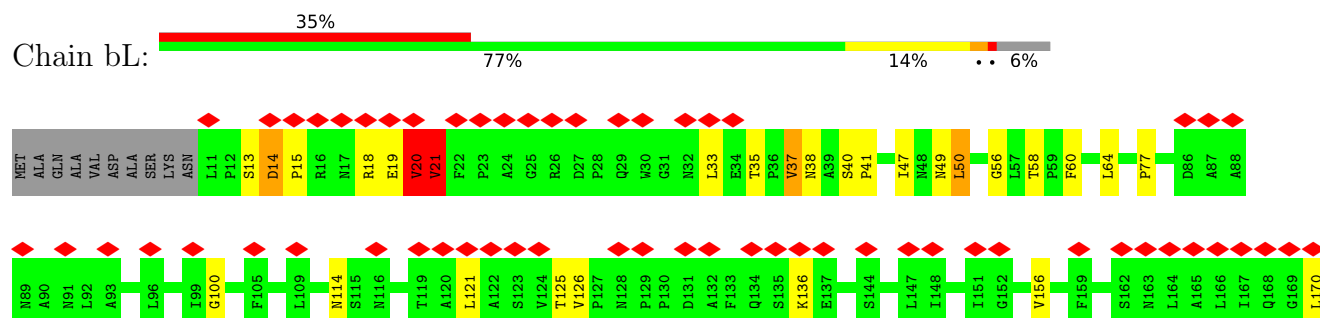
- Molecule 9: Photosystem I reaction center subunit PsaK 1



- Molecule 10: Photosystem I reaction center subunit XI

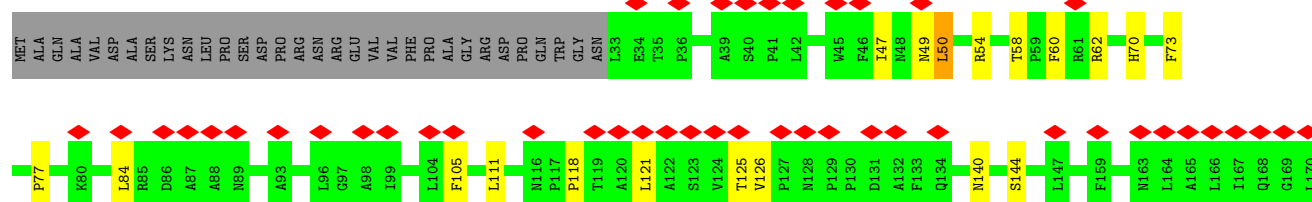


- Molecule 10: Photosystem I reaction center subunit XI

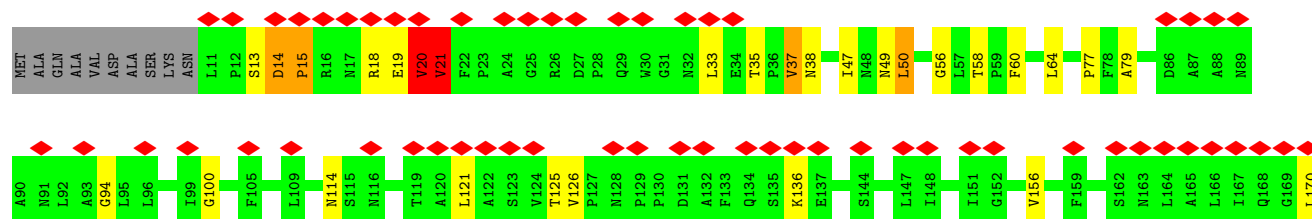
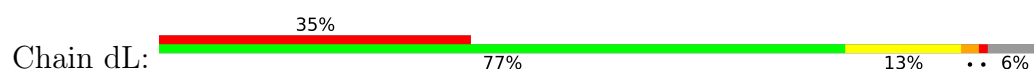




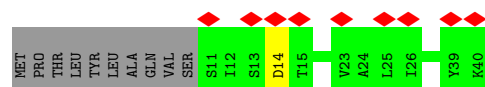
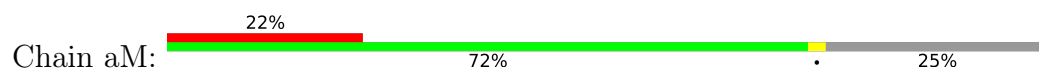
- Molecule 10: Photosystem I reaction center subunit XI



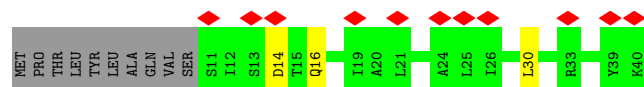
- Molecule 10: Photosystem I reaction center subunit XI



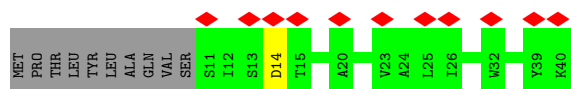
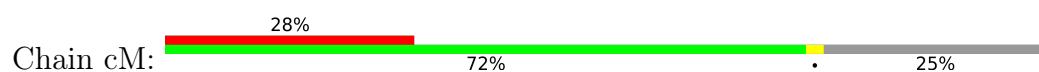
- Molecule 11: Photosystem I reaction center subunit XII



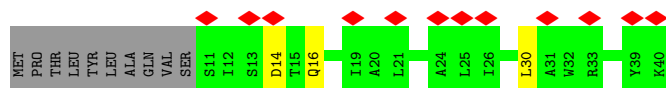
- Molecule 11: Photosystem I reaction center subunit XII



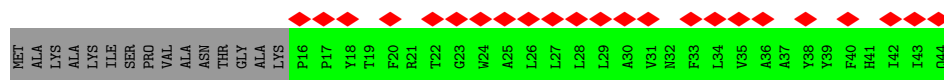
- Molecule 11: Photosystem I reaction center subunit XII



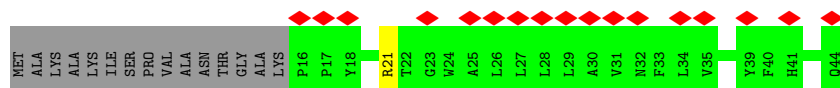
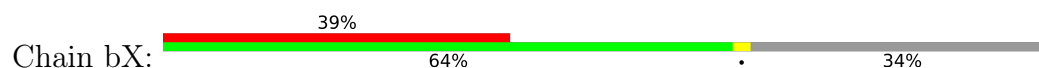
- Molecule 11: Photosystem I reaction center subunit XII



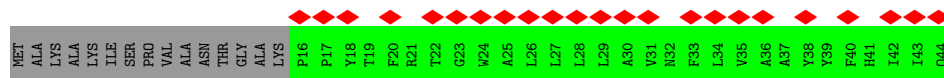
- Molecule 12: Photosystem I 4.8 kDa protein



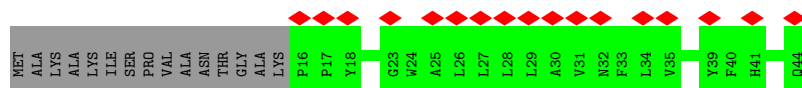
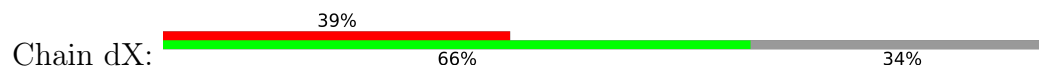
- Molecule 12: Photosystem I 4.8 kDa protein



- Molecule 12: Photosystem I 4.8 kDa protein



- Molecule 12: Photosystem I 4.8 kDa protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	111400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.260	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	492.8, 492.8, 492.8	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	aA	0.35	0/6000	0.50	1/8187 (0.0%)
1	bA	0.35	0/6000	0.50	1/8187 (0.0%)
1	cA	0.35	0/6000	0.50	1/8187 (0.0%)
1	dA	0.35	0/6000	0.50	1/8187 (0.0%)
2	aB	0.37	0/6143	0.53	0/8398
2	bB	0.37	0/6143	0.53	0/8398
2	cB	0.37	0/6143	0.53	0/8398
2	dB	0.37	0/6143	0.53	0/8398
3	aC	0.30	0/609	0.54	0/826
3	bC	0.30	0/609	0.53	0/826
3	cC	0.30	0/609	0.53	0/826
3	dC	0.30	0/609	0.54	0/826
4	aD	0.24	0/596	0.48	0/806
4	bD	0.29	0/757	0.56	0/1024
4	cD	0.24	0/596	0.49	0/806
4	dD	0.29	0/757	0.56	0/1024
5	aE	0.29	0/499	0.49	0/677
5	bE	0.29	0/499	0.49	0/677
5	cE	0.29	0/499	0.49	0/677
5	dE	0.29	0/499	0.49	0/677
6	aF	0.29	0/1096	0.60	2/1489 (0.1%)
6	bF	0.32	0/1104	0.62	0/1500
6	cF	0.28	0/1096	0.60	2/1489 (0.1%)
6	dF	0.32	0/1104	0.62	0/1500
7	aI	0.34	0/262	0.57	0/358
7	bI	0.34	0/262	0.57	0/358
7	cI	0.34	0/262	0.57	0/358
7	dI	0.34	0/262	0.57	0/358
8	aJ	0.26	0/358	0.49	0/490
8	bJ	0.27	0/358	0.50	0/490
8	cJ	0.27	0/358	0.50	0/490
8	dJ	0.27	0/358	0.50	0/490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	aK	0.30	0/494	0.68	0/675
9	bK	0.29	0/494	0.68	0/675
9	cK	0.30	0/494	0.68	0/675
9	dK	0.30	0/494	0.68	0/675
10	aL	0.32	0/1067	0.51	0/1462
10	bL	0.38	0/1247	0.70	2/1710 (0.1%)
10	cL	0.32	0/1067	0.53	0/1462
10	dL	0.38	0/1247	0.71	2/1710 (0.1%)
11	aM	0.28	0/239	0.50	0/326
11	bM	0.28	0/239	0.50	0/326
11	cM	0.28	0/239	0.50	0/326
11	dM	0.28	0/239	0.50	0/326
12	aX	0.23	0/253	0.38	0/347
12	bX	0.23	0/253	0.38	0/347
12	cX	0.23	0/253	0.38	0/347
12	dX	0.23	0/253	0.38	0/347
All	All	0.34	0/71162	0.53	12/97118 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	aB	0	1
2	bB	0	1
2	cB	0	1
2	dB	0	1
6	aF	0	1
6	cF	0	1
10	bL	0	3
10	dL	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	dL	21	VAL	CG1-CB-CG2	-7.18	95.00	110.80
10	bL	21	VAL	CG1-CB-CG2	-7.18	95.01	110.80
10	bL	37	VAL	N-CA-C	-6.03	106.94	112.96
10	dL	37	VAL	N-CA-C	-6.00	106.96	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	cF	116	ASP	CA-C-N	5.97	132.94	121.54

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	aB	480	THR	Peptide
6	aF	135	THR	Peptide
2	bB	480	THR	Peptide
10	bL	14	ASP	Peptide
10	bL	19	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5801	0	5667	78	0
1	bA	5801	0	5667	77	0
1	cA	5801	0	5667	87	0
1	dA	5801	0	5667	77	0
2	aB	5919	0	5675	65	0
2	bB	5919	0	5675	72	0
2	cB	5919	0	5675	68	0
2	dB	5919	0	5675	69	0
3	aC	599	0	577	8	0
3	bC	599	0	577	9	0
3	cC	599	0	577	7	0
3	dC	599	0	577	7	0
4	aD	581	0	584	3	0
4	bD	740	0	751	4	0
4	cD	581	0	584	3	0
4	dD	740	0	751	3	0
5	aE	490	0	484	3	0
5	bE	490	0	484	5	0
5	cE	490	0	484	3	0
5	dE	490	0	484	5	0
6	aF	1072	0	1065	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	bF	1080	0	1076	15	0
6	cF	1072	0	1065	19	0
6	dF	1080	0	1076	17	0
7	aI	253	0	255	4	0
7	bI	253	0	255	1	0
7	cI	253	0	255	4	0
7	dI	253	0	255	1	0
8	aJ	347	0	352	7	0
8	bJ	347	0	352	7	0
8	cJ	347	0	352	8	0
8	dJ	347	0	352	7	0
9	aK	480	0	501	5	0
9	bK	480	0	501	9	0
9	cK	480	0	501	5	0
9	dK	480	0	501	9	0
10	aL	1037	0	1051	16	0
10	bL	1210	0	1213	21	0
10	cL	1037	0	1051	16	0
10	dL	1210	0	1213	22	0
11	aM	235	0	251	1	0
11	bM	235	0	251	3	0
11	cM	235	0	251	1	0
11	dM	235	0	251	3	0
12	aX	243	0	244	0	0
12	bX	243	0	244	1	0
12	cX	243	0	244	0	0
12	dX	243	0	244	0	0
13	aA	65	0	72	29	0
13	bA	65	0	72	21	0
13	cA	65	0	72	32	0
13	dA	65	0	72	19	0
14	aA	2332	0	2197	68	0
14	aB	2340	0	2282	73	0
14	aF	96	0	74	3	0
14	aJ	82	0	58	1	0
14	aK	86	0	62	1	0
14	aL	182	0	187	4	0
14	aX	45	0	33	1	0
14	bA	2280	0	2154	75	0
14	bB	2405	0	2354	83	0
14	bF	96	0	74	10	0
14	bJ	82	0	58	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	bK	86	0	62	1	0
14	bL	299	0	301	9	0
14	bX	45	0	33	0	0
14	cA	2332	0	2197	74	0
14	cB	2340	0	2282	79	0
14	cF	96	0	74	3	0
14	cJ	82	0	58	1	0
14	cK	86	0	62	1	0
14	cL	182	0	187	4	0
14	cX	45	0	33	1	0
14	dA	2280	0	2154	70	0
14	dB	2405	0	2354	82	0
14	dF	96	0	74	10	0
14	dJ	82	0	58	0	0
14	dK	86	0	62	2	0
14	dL	299	0	301	10	0
14	dX	45	0	33	0	0
15	aA	33	0	46	12	0
15	aB	33	0	46	6	0
15	bA	33	0	46	30	0
15	bB	33	0	46	19	0
15	cA	33	0	46	12	0
15	cB	33	0	46	7	0
15	dA	33	0	46	26	0
15	dB	33	0	46	10	0
16	aA	8	0	0	1	0
16	aC	16	0	0	2	0
16	bA	8	0	0	1	0
16	bC	16	0	0	3	0
16	cA	8	0	0	1	0
16	cC	16	0	0	2	0
16	dA	8	0	0	1	0
16	dC	16	0	0	2	0
17	aA	240	0	336	13	0
17	aB	280	0	392	18	0
17	aF	80	0	112	2	0
17	aI	40	0	56	1	0
17	aJ	80	0	112	3	0
17	aL	120	0	168	6	0
17	aM	40	0	56	1	0
17	bA	200	0	280	10	0
17	bB	280	0	392	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	bF	80	0	112	5	0
17	bI	40	0	56	5	0
17	bJ	80	0	112	3	0
17	bK	40	0	56	5	0
17	bL	120	0	168	5	0
17	bM	40	0	56	0	0
17	cA	240	0	336	16	0
17	cB	280	0	392	15	0
17	cF	80	0	112	3	0
17	cI	40	0	56	1	0
17	cJ	80	0	112	5	0
17	cL	120	0	168	3	0
17	cM	40	0	56	1	0
17	dA	200	0	280	11	0
17	dB	280	0	392	13	0
17	dF	80	0	112	3	0
17	dI	40	0	56	5	0
17	dJ	80	0	112	3	0
17	dK	40	0	56	5	0
17	dL	120	0	168	5	0
17	dM	40	0	56	2	0
18	aA	76	0	98	1	0
18	aB	23	0	16	0	0
18	bA	76	0	98	1	0
18	bB	23	0	16	1	0
18	cA	76	0	98	1	0
18	cB	23	0	16	0	0
18	dA	76	0	98	1	0
18	dB	23	0	16	0	0
19	aB	55	0	86	1	0
19	bB	55	0	86	2	0
19	cB	55	0	86	2	0
19	dB	55	0	86	1	0
All	All	94576	0	93746	1339	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 7.

The worst 5 of 1339 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)
14:aA:841:CLA:H92	15:aA:844:PQN:C19	1.48	1.41
14:cA:841:CLA:H92	15:cA:844:PQN:C19	1.61	1.29
14:aA:841:CLA:C9	15:aA:844:PQN:H191	1.63	1.27
14:cA:841:CLA:H92	15:cA:844:PQN:H191	1.19	1.16
1:dA:605:ILE:HD11	13:dA:801:CL0:H69	1.35	1.06

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	aA	737/752 (98%)	704 (96%)	33 (4%)	0	100	100
1	bA	737/752 (98%)	703 (95%)	34 (5%)	0	100	100
1	cA	737/752 (98%)	704 (96%)	33 (4%)	0	100	100
1	dA	737/752 (98%)	703 (95%)	34 (5%)	0	100	100
2	aB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	bB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	cB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	dB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
3	aC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	bC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	cC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	dC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	aD	71/139 (51%)	69 (97%)	2 (3%)	0	100	100
4	bD	94/139 (68%)	89 (95%)	5 (5%)	0	100	100
4	cD	71/139 (51%)	69 (97%)	2 (3%)	0	100	100
4	dD	94/139 (68%)	89 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	aE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
5	bE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
5	cE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
5	dE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
6	aF	138/164 (84%)	129 (94%)	9 (6%)	0	100	100
6	bF	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
6	cF	138/164 (84%)	130 (94%)	8 (6%)	0	100	100
6	dF	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
7	aI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
7	bI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
7	cI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
7	dI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
8	aJ	41/49 (84%)	41 (100%)	0	0	100	100
8	bJ	41/49 (84%)	41 (100%)	0	0	100	100
8	cJ	41/49 (84%)	41 (100%)	0	0	100	100
8	dJ	41/49 (84%)	41 (100%)	0	0	100	100
9	aK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
9	bK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
9	cK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
9	dK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
10	aL	138/172 (80%)	134 (97%)	4 (3%)	0	100	100
10	bL	159/172 (92%)	145 (91%)	12 (8%)	2 (1%)	9	35
10	cL	138/172 (80%)	134 (97%)	4 (3%)	0	100	100
10	dL	159/172 (92%)	144 (91%)	13 (8%)	2 (1%)	9	35
11	aM	28/40 (70%)	28 (100%)	0	0	100	100
11	bM	28/40 (70%)	28 (100%)	0	0	100	100
11	cM	28/40 (70%)	28 (100%)	0	0	100	100
11	dM	28/40 (70%)	28 (100%)	0	0	100	100
12	aX	27/44 (61%)	27 (100%)	0	0	100	100
12	bX	27/44 (61%)	27 (100%)	0	0	100	100
12	cX	27/44 (61%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	dX	27/44 (61%)	27 (100%)	0	0	100	100
All	All	8678/9536 (91%)	8260 (95%)	414 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	bL	15	PRO
10	dL	15	PRO
10	dL	21	VAL
10	bL	21	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	593/605 (98%)	592 (100%)	1 (0%)	87	88
1	bA	593/605 (98%)	592 (100%)	1 (0%)	87	88
1	cA	593/605 (98%)	592 (100%)	1 (0%)	87	88
1	dA	593/605 (98%)	592 (100%)	1 (0%)	87	88
2	aB	601/602 (100%)	600 (100%)	1 (0%)	87	88
2	bB	601/602 (100%)	600 (100%)	1 (0%)	87	88
2	cB	601/602 (100%)	600 (100%)	1 (0%)	87	88
2	dB	601/602 (100%)	600 (100%)	1 (0%)	87	88
3	aC	68/69 (99%)	68 (100%)	0	100	100
3	bC	68/69 (99%)	68 (100%)	0	100	100
3	cC	68/69 (99%)	68 (100%)	0	100	100
3	dC	68/69 (99%)	68 (100%)	0	100	100
4	aD	59/110 (54%)	59 (100%)	0	100	100
4	bD	76/110 (69%)	76 (100%)	0	100	100
4	cD	59/110 (54%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	dD	76/110 (69%)	76 (100%)	0	100	100
5	aE	54/60 (90%)	54 (100%)	0	100	100
5	bE	54/60 (90%)	54 (100%)	0	100	100
5	cE	54/60 (90%)	54 (100%)	0	100	100
5	dE	54/60 (90%)	54 (100%)	0	100	100
6	aF	109/129 (84%)	109 (100%)	0	100	100
6	bF	110/129 (85%)	110 (100%)	0	100	100
6	cF	109/129 (84%)	109 (100%)	0	100	100
6	dF	110/129 (85%)	110 (100%)	0	100	100
7	aI	28/39 (72%)	28 (100%)	0	100	100
7	bI	28/39 (72%)	28 (100%)	0	100	100
7	cI	28/39 (72%)	28 (100%)	0	100	100
7	dI	28/39 (72%)	28 (100%)	0	100	100
8	aJ	38/42 (90%)	38 (100%)	0	100	100
8	bJ	38/42 (90%)	38 (100%)	0	100	100
8	cJ	38/42 (90%)	38 (100%)	0	100	100
8	dJ	38/42 (90%)	38 (100%)	0	100	100
9	aK	48/64 (75%)	48 (100%)	0	100	100
9	bK	48/64 (75%)	48 (100%)	0	100	100
9	cK	48/64 (75%)	48 (100%)	0	100	100
9	dK	48/64 (75%)	48 (100%)	0	100	100
10	aL	105/131 (80%)	103 (98%)	2 (2%)	50	68
10	bL	124/131 (95%)	121 (98%)	3 (2%)	43	65
10	cL	105/131 (80%)	104 (99%)	1 (1%)	68	76
10	dL	124/131 (95%)	121 (98%)	3 (2%)	43	65
11	aM	25/34 (74%)	25 (100%)	0	100	100
11	bM	25/34 (74%)	25 (100%)	0	100	100
11	cM	25/34 (74%)	25 (100%)	0	100	100
11	dM	25/34 (74%)	25 (100%)	0	100	100
12	aX	24/34 (71%)	24 (100%)	0	100	100
12	bX	24/34 (71%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	cX	24/34 (71%)	24 (100%)	0	100	100
12	dX	24/34 (71%)	24 (100%)	0	100	100
All	All	7082/7676 (92%)	7065 (100%)	17 (0%)	85	88

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	dL	20	VAL
10	dL	64	LEU
10	bL	50	LEU
10	bL	64	LEU
1	cA	153	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
2	cB	229	ASN
1	dA	356	ASN
2	cB	262	HIS
4	cD	56	ASN
1	dA	695	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

504 ligands 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	$\# Z > 2$
17	BCR	bA	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.22	3 (5%)
14	CLA	cA	816	-	53,57,73	1.41	8 (15%)	62,93,113	1.48	4 (6%)
17	BCR	dF	202	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
17	BCR	cA	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	8 (14%)
14	CLA	dL	206	-	69,73,73	1.25	10 (14%)	83,113,113	1.27	6 (7%)
14	CLA	bB	808	2	69,73,73	1.24	10 (14%)	83,113,113	1.35	9 (10%)
17	BCR	dM	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	6 (10%)
14	CLA	aB	833	2	62,66,73	1.31	8 (12%)	74,104,113	1.38	8 (10%)
14	CLA	aA	817	1	58,62,73	1.35	9 (15%)	69,99,113	1.43	7 (10%)
15	PQN	aB	842	-	34,34,34	1.52	2 (5%)	42,45,45	1.23	5 (11%)
14	CLA	aK	101	9	46,49,73	1.47	9 (19%)	55,83,113	1.48	6 (10%)
17	BCR	cL	205	-	41,41,41	1.18	2 (4%)	56,56,56	1.37	9 (16%)
14	CLA	dB	801	-	69,73,73	1.28	11 (15%)	83,113,113	1.26	7 (8%)
14	CLA	aA	833	1	69,73,73	1.25	11 (15%)	83,113,113	1.41	8 (9%)
14	CLA	dB	842	2	69,73,73	1.24	9 (13%)	83,113,113	1.43	5 (6%)
17	BCR	dL	203	-	41,41,41	1.24	3 (7%)	56,56,56	1.25	5 (8%)
14	CLA	dB	832	2	53,57,73	1.40	10 (18%)	62,93,113	1.48	8 (12%)
14	CLA	aB	824	2	58,62,73	1.40	11 (18%)	69,99,113	1.37	8 (11%)
14	CLA	dA	809	1	49,53,73	1.48	11 (22%)	59,89,113	1.57	6 (10%)
14	CLA	dB	802	2	69,73,73	1.25	10 (14%)	83,113,113	1.28	5 (6%)
14	CLA	cB	826	2	69,73,73	1.25	11 (15%)	83,113,113	1.33	7 (8%)
17	BCR	dL	208	-	41,41,41	1.12	2 (4%)	56,56,56	1.38	10 (17%)
14	CLA	dX	101	12	49,53,73	1.46	9 (18%)	59,89,113	1.51	4 (6%)
14	CLA	aA	813	1	49,53,73	1.47	9 (18%)	59,89,113	1.57	10 (16%)
14	CLA	bB	811	2	69,73,73	1.25	11 (15%)	83,113,113	1.28	5 (6%)
14	CLA	cA	821	14	69,73,73	1.24	10 (14%)	83,113,113	1.41	7 (8%)
16	SF4	bA	844	1,2	0,12,12	-	-	-	-	-
16	SF4	dC	102	3	0,12,12	-	-	-	-	-
14	CLA	cB	803	-	69,73,73	1.25	12 (17%)	83,113,113	1.25	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dA	840	1	69,73,73	1.22	9 (13%)	83,113,113	1.39	6 (7%)
15	PQN	cB	842	-	34,34,34	1.52	2 (5%)	42,45,45	1.23	5 (11%)
14	CLA	bB	816	2	49,53,73	1.45	10 (20%)	59,89,113	1.56	8 (13%)
14	CLA	dB	819	2	64,68,73	1.29	9 (14%)	77,107,113	1.36	8 (10%)
14	CLA	aA	815	1	49,53,73	1.47	8 (16%)	59,89,113	1.54	5 (8%)
17	BCR	cB	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	6 (10%)
14	CLA	dB	840	2	51,55,73	1.41	9 (17%)	61,91,113	1.54	8 (13%)
17	BCR	dB	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.32	5 (8%)
17	BCR	aL	201	-	41,41,41	1.23	3 (7%)	56,56,56	1.26	5 (8%)
15	PQN	cA	844	-	34,34,34	1.52	2 (5%)	42,45,45	1.27	5 (11%)
17	BCR	cA	851	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	6 (10%)
14	CLA	cB	840	-	69,73,73	1.26	11 (15%)	83,113,113	1.27	6 (7%)
14	CLA	aB	816	2	59,63,73	1.35	9 (15%)	71,101,113	1.37	8 (11%)
14	CLA	cB	837	2	64,68,73	1.29	10 (15%)	77,107,113	1.39	8 (10%)
14	CLA	dB	813	2	49,53,73	1.48	10 (20%)	59,89,113	1.52	5 (8%)
17	BCR	cA	848	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	8 (14%)
14	CLA	dB	810	2	69,73,73	1.28	10 (14%)	83,113,113	1.36	7 (8%)
17	BCR	dK	102	-	41,41,41	1.19	3 (7%)	56,56,56	1.42	10 (17%)
14	CLA	bB	801	-	69,73,73	1.28	11 (15%)	83,113,113	1.26	7 (8%)
14	CLA	aA	806	1	69,73,73	1.28	10 (14%)	83,113,113	1.37	8 (9%)
14	CLA	aB	812	2	49,53,73	1.48	10 (20%)	59,89,113	1.52	5 (8%)
14	CLA	bB	804	-	69,73,73	1.25	11 (15%)	83,113,113	1.64	12 (14%)
17	BCR	cA	846	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	11 (19%)
14	CLA	dB	817	2	59,63,73	1.34	9 (15%)	71,101,113	1.37	8 (11%)
14	CLA	bA	824	1	51,55,73	1.44	8 (15%)	61,91,113	1.51	6 (9%)
14	CLA	dJ	101	-	49,53,73	1.47	9 (18%)	59,89,113	1.51	5 (8%)
17	BCR	dA	848	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	6 (10%)
14	CLA	dB	811	2	69,73,73	1.25	11 (15%)	83,113,113	1.28	6 (7%)
16	SF4	bC	102	3	0,12,12	-	-	-	-	-
17	BCR	cJ	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	6 (10%)
14	CLA	cA	828	1	69,73,73	1.22	11 (15%)	83,113,113	1.44	8 (9%)
17	BCR	cB	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	aJ	101	-	49,53,73	1.46	9 (18%)	59,89,113	1.51	5 (8%)
14	CLA	cA	815	1	49,53,73	1.47	8 (16%)	59,89,113	1.55	5 (8%)
17	BCR	bL	203	-	41,41,41	1.23	3 (7%)	56,56,56	1.25	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	aA	808	1	49,53,73	1.44	10 (20%)	59,89,113	1.52	6 (10%)
14	CLA	aB	832	2	69,73,73	1.27	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	bB	819	2	64,68,73	1.29	9 (14%)	77,107,113	1.37	8 (10%)
17	BCR	bB	849	-	41,41,41	1.21	2 (4%)	56,56,56	1.17	4 (7%)
17	BCR	bL	208	-	41,41,41	1.12	2 (4%)	56,56,56	1.38	10 (17%)
14	CLA	dB	827	2	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
17	BCR	dF	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	8 (14%)
14	CLA	dA	815	1	49,53,73	1.46	8 (16%)	59,89,113	1.55	5 (8%)
14	CLA	dB	841	-	69,73,73	1.26	11 (15%)	83,113,113	1.27	6 (7%)
14	CLA	cL	203	10	69,73,73	1.21	10 (14%)	83,113,113	1.48	9 (10%)
14	CLA	dB	815	2	60,64,73	1.32	9 (15%)	72,102,113	1.41	6 (8%)
17	BCR	aB	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	6 (10%)
17	BCR	cL	206	-	41,41,41	1.07	1 (2%)	56,56,56	1.33	7 (12%)
14	CLA	bB	812	2	49,53,73	1.46	9 (18%)	59,89,113	1.51	4 (6%)
14	CLA	aB	819	-	69,73,73	1.23	10 (14%)	83,113,113	1.39	7 (8%)
14	CLA	dA	817	1	58,62,73	1.34	9 (15%)	69,99,113	1.44	7 (10%)
14	CLA	dA	841	1	69,73,73	1.24	9 (13%)	83,113,113	1.37	5 (6%)
14	CLA	bA	827	14,1	69,73,73	1.26	10 (14%)	83,113,113	1.40	6 (7%)
14	CLA	aA	810	1	49,53,73	1.44	8 (16%)	59,89,113	1.46	5 (8%)
14	CLA	dB	838	2	64,68,73	1.30	10 (15%)	77,107,113	1.40	8 (10%)
14	CLA	aA	819	1	69,73,73	1.24	10 (14%)	83,113,113	1.41	10 (12%)
14	CLA	cA	822	1	53,57,73	1.41	11 (20%)	62,93,113	1.51	6 (9%)
14	CLA	bA	814	1	49,53,73	1.47	9 (18%)	59,89,113	1.51	8 (13%)
14	CLA	bA	820	1	65,69,73	1.29	10 (15%)	78,108,113	1.42	7 (8%)
14	CLA	bB	832	2	53,57,73	1.40	10 (18%)	62,93,113	1.49	8 (12%)
14	CLA	aB	813	2	69,73,73	1.25	10 (14%)	83,113,113	1.41	9 (10%)
14	CLA	bB	814	2	69,73,73	1.26	10 (14%)	83,113,113	1.41	9 (10%)
16	SF4	bC	101	3	0,12,12	-	-	-	-	-
14	CLA	aB	822	-	59,63,73	1.33	10 (16%)	71,101,113	1.47	4 (5%)
14	CLA	cA	817	1	58,62,73	1.35	9 (15%)	69,99,113	1.44	7 (10%)
14	CLA	dA	827	14,1	69,73,73	1.25	10 (14%)	83,113,113	1.41	6 (7%)
18	LHG	bA	851	14	26,26,48	0.87	1 (3%)	29,32,54	1.31	3 (10%)
17	BCR	aB	845	-	41,41,41	1.17	3 (7%)	56,56,56	1.17	3 (5%)
14	CLA	dA	821	14	69,73,73	1.25	10 (14%)	83,113,113	1.41	7 (8%)
14	CLA	bF	203	-	49,53,73	1.46	10 (20%)	59,89,113	1.52	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	bA	808	1	49,53,73	1.44	10 (20%)	59,89,113	1.53	6 (10%)
17	BCR	aA	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	8 (14%)
14	CLA	dB	828	2	69,73,73	1.23	10 (14%)	83,113,113	1.38	8 (9%)
14	CLA	cB	827	2	69,73,73	1.23	10 (14%)	83,113,113	1.39	8 (9%)
14	CLA	bB	806	2	69,73,73	1.22	11 (15%)	83,113,113	1.44	8 (9%)
14	CLA	bA	806	1	69,73,73	1.27	10 (14%)	83,113,113	1.38	8 (9%)
14	CLA	bB	829	2	69,73,73	1.23	10 (14%)	83,113,113	1.34	6 (7%)
14	CLA	cB	832	2	69,73,73	1.27	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	cB	816	2	59,63,73	1.35	10 (16%)	71,101,113	1.38	8 (11%)
15	PQN	dB	843	-	34,34,34	1.52	2 (5%)	42,45,45	1.27	4 (9%)
17	BCR	cB	845	-	41,41,41	1.17	2 (4%)	56,56,56	1.16	3 (5%)
14	CLA	cB	828	2	69,73,73	1.23	10 (14%)	83,113,113	1.34	6 (7%)
18	LHG	dA	850	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
14	CLA	cB	805	2	58,62,73	1.35	11 (18%)	69,99,113	1.45	8 (11%)
17	BCR	bA	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	bA	818	1	58,62,73	1.36	10 (17%)	69,99,113	1.49	9 (13%)
18	LHG	aA	853	14	26,26,48	0.86	1 (3%)	29,32,54	1.31	3 (10%)
16	SF4	aC	102	3	0,12,12	-	-	-	-	-
14	CLA	dA	835	1	58,62,73	1.35	9 (15%)	69,99,113	1.46	8 (11%)
14	CLA	bA	828	1	69,73,73	1.22	11 (15%)	83,113,113	1.44	9 (10%)
14	CLA	dA	810	1	49,53,73	1.45	8 (16%)	59,89,113	1.46	4 (6%)
13	CL0	dA	801	1	69,73,73	2.02	20 (28%)	83,113,113	2.88	30 (36%)
14	CLA	bB	830	2	69,73,73	1.27	10 (14%)	83,113,113	1.53	9 (10%)
14	CLA	bB	817	2	59,63,73	1.34	10 (16%)	71,101,113	1.38	8 (11%)
14	CLA	bA	816	-	53,57,73	1.41	8 (15%)	62,93,113	1.48	4 (6%)
14	CLA	bB	833	2	69,73,73	1.27	11 (15%)	83,113,113	1.33	7 (8%)
17	BCR	cB	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.38	8 (14%)
14	CLA	cA	826	-	59,63,73	1.36	11 (18%)	71,101,113	1.41	9 (12%)
14	CLA	aA	826	-	59,63,73	1.37	12 (20%)	71,101,113	1.41	9 (12%)
14	CLA	dB	839	2	69,73,73	1.25	10 (14%)	83,113,113	1.48	10 (12%)
14	CLA	dA	836	1	49,53,73	1.46	9 (18%)	59,89,113	1.62	7 (11%)
17	BCR	aA	848	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	cB	831	2	53,57,73	1.40	10 (18%)	62,93,113	1.48	8 (12%)
17	BCR	cF	202	-	41,41,41	1.16	2 (4%)	56,56,56	1.30	5 (8%)
14	CLA	cB	824	2	58,62,73	1.40	11 (18%)	69,99,113	1.37	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dB	836	-	49,53,73	1.51	9 (18%)	59,89,113	1.56	9 (15%)
14	CLA	dA	816	-	53,57,73	1.42	8 (15%)	62,93,113	1.48	4 (6%)
17	BCR	cJ	104	-	41,41,41	1.14	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	cA	803	1	49,53,73	1.46	9 (18%)	59,89,113	1.56	8 (13%)
15	PQN	aA	844	-	34,34,34	1.52	2 (5%)	42,45,45	1.26	5 (11%)
17	BCR	bF	202	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
14	CLA	aA	802	-	49,53,73	1.45	11 (22%)	59,89,113	1.58	7 (11%)
16	SF4	aA	845	1,2	0,12,12	-	-	-		
14	CLA	cB	836	-	49,53,73	1.48	10 (20%)	59,89,113	1.42	5 (8%)
14	CLA	cA	813	1	49,53,73	1.48	10 (20%)	59,89,113	1.57	11 (18%)
14	CLA	cB	804	-	69,73,73	1.25	11 (15%)	83,113,113	1.64	12 (14%)
14	CLA	dL	202	18,10	56,60,73	1.40	11 (19%)	67,97,113	1.96	10 (14%)
14	CLA	dL	201	2,10	69,73,73	1.25	11 (15%)	83,113,113	1.28	6 (7%)
14	CLA	aB	818	2	64,68,73	1.29	10 (15%)	77,107,113	1.36	8 (10%)
14	CLA	bB	815	2	60,64,73	1.32	9 (15%)	72,102,113	1.40	6 (8%)
14	CLA	dB	821	2	51,55,73	1.41	10 (19%)	61,91,113	1.46	5 (8%)
14	CLA	cF	203	-	49,53,73	1.48	10 (20%)	59,89,113	1.50	6 (10%)
16	SF4	cC	102	3	0,12,12	-	-	-		
14	CLA	dA	837	1	55,59,73	1.38	11 (20%)	66,96,113	1.52	9 (13%)
17	BCR	aB	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	5 (8%)
14	CLA	bL	202	18,10	56,60,73	1.40	11 (19%)	67,97,113	1.96	11 (16%)
14	CLA	aA	840	1	69,73,73	1.22	9 (13%)	83,113,113	1.39	6 (7%)
14	CLA	dB	837	-	49,53,73	1.48	10 (20%)	59,89,113	1.43	6 (10%)
14	CLA	aB	830	2	49,53,73	1.46	9 (18%)	59,89,113	1.47	5 (8%)
14	CLA	cB	806	2	69,73,73	1.22	11 (15%)	83,113,113	1.44	8 (9%)
14	CLA	bB	810	2	69,73,73	1.28	10 (14%)	83,113,113	1.36	7 (8%)
14	CLA	aJ	102	-	42,45,73	1.53	9 (21%)	50,78,113	1.52	5 (10%)
14	CLA	cF	201	-	55,59,73	1.38	9 (16%)	66,96,113	1.49	6 (9%)
14	CLA	bK	101	9	46,49,73	1.47	9 (19%)	55,83,113	1.47	6 (10%)
14	CLA	bB	842	2	69,73,73	1.24	9 (13%)	83,113,113	1.44	5 (6%)
14	CLA	bF	201	-	55,59,73	1.38	9 (16%)	66,96,113	1.48	6 (9%)
14	CLA	cB	812	2	49,53,73	1.49	10 (20%)	59,89,113	1.53	6 (10%)
14	CLA	bB	834	2	62,66,73	1.31	8 (12%)	74,104,113	1.37	8 (10%)
17	BCR	bB	852	-	41,41,41	1.19	2 (4%)	56,56,56	1.37	8 (14%)
14	CLA	bB	818	2	63,67,73	1.31	11 (17%)	75,105,113	1.45	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	aL	206	-	41,41,41	1.08	1 (2%)	56,56,56	1.32	7 (12%)
14	CLA	bB	831	2	49,53,73	1.46	9 (18%)	59,89,113	1.48	5 (8%)
14	CLA	aB	806	2	69,73,73	1.23	11 (15%)	83,113,113	1.43	8 (9%)
14	CLA	aA	830	1	69,73,73	1.28	10 (14%)	83,113,113	1.43	7 (8%)
14	CLA	cB	802	2	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
14	CLA	bB	838	2	64,68,73	1.30	9 (14%)	77,107,113	1.40	8 (10%)
14	CLA	bA	842	-	69,73,73	1.26	10 (14%)	83,113,113	1.37	7 (8%)
14	CLA	bA	832	1	69,73,73	1.25	11 (15%)	83,113,113	1.36	10 (12%)
14	CLA	dL	204	10	56,60,73	1.39	9 (16%)	67,97,113	1.53	8 (11%)
14	CLA	bB	807	2	69,73,73	1.27	11 (15%)	83,113,113	1.36	6 (7%)
17	BCR	bA	845	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	8 (14%)
14	CLA	dB	830	2	69,73,73	1.27	10 (14%)	83,113,113	1.54	9 (10%)
17	BCR	dB	849	-	41,41,41	1.21	2 (4%)	56,56,56	1.16	4 (7%)
17	BCR	bB	844	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	6 (10%)
14	CLA	dB	803	-	69,73,73	1.25	12 (17%)	83,113,113	1.25	6 (7%)
14	CLA	bB	841	-	69,73,73	1.26	11 (15%)	83,113,113	1.27	6 (7%)
14	CLA	dA	807	1	55,59,73	1.38	9 (16%)	66,96,113	1.47	6 (9%)
14	CLA	dB	835	2	49,53,73	1.44	10 (20%)	59,89,113	1.67	7 (11%)
14	CLA	aB	817	2	63,67,73	1.30	10 (15%)	75,105,113	1.45	9 (12%)
14	CLA	cB	818	2	64,68,73	1.29	10 (15%)	77,107,113	1.36	8 (10%)
14	CLA	dA	832	1	69,73,73	1.26	11 (15%)	83,113,113	1.36	10 (12%)
17	BCR	dA	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	bL	201	2,10	69,73,73	1.25	11 (15%)	83,113,113	1.27	5 (6%)
18	LHG	bB	851	-	22,22,48	0.89	1 (4%)	25,28,54	1.20	1 (4%)
19	LMG	aB	849	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
14	CLA	bA	819	1	69,73,73	1.24	10 (14%)	83,113,113	1.41	10 (12%)
14	CLA	bA	833	1	69,73,73	1.24	11 (15%)	83,113,113	1.41	8 (9%)
14	CLA	cA	842	-	69,73,73	1.26	10 (14%)	83,113,113	1.35	7 (8%)
14	CLA	dB	809	2	69,73,73	1.24	12 (17%)	83,113,113	1.51	7 (8%)
14	CLA	cB	813	2	69,73,73	1.26	11 (15%)	83,113,113	1.41	9 (10%)
17	BCR	dB	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	3 (5%)
14	CLA	cA	806	1	69,73,73	1.28	10 (14%)	83,113,113	1.37	8 (9%)
17	BCR	dA	849	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	6 (10%)
14	CLA	aX	101	12	49,53,73	1.47	9 (18%)	59,89,113	1.52	4 (6%)
14	CLA	cB	829	2	69,73,73	1.27	10 (14%)	83,113,113	1.53	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	LMG	dB	850	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
14	CLA	bA	834	1	69,73,73	1.23	9 (13%)	83,113,113	1.35	7 (8%)
17	BCR	cF	204	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	8 (14%)
14	CLA	aA	809	1	49,53,73	1.48	11 (22%)	59,89,113	1.57	6 (10%)
14	CLA	cA	824	1	51,55,73	1.44	8 (15%)	61,91,113	1.50	6 (9%)
14	CLA	dB	826	-	50,54,73	1.42	11 (22%)	60,90,113	1.54	8 (13%)
14	CLA	bA	813	1	49,53,73	1.48	9 (18%)	59,89,113	1.57	10 (16%)
17	BCR	bF	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
14	CLA	aB	801	-	69,73,73	1.28	11 (15%)	83,113,113	1.27	7 (8%)
14	CLA	bB	825	2	58,62,73	1.40	11 (18%)	69,99,113	1.36	8 (11%)
14	CLA	aB	820	2	51,55,73	1.41	10 (19%)	61,91,113	1.45	5 (8%)
14	CLA	bA	804	14,1	49,53,73	1.48	11 (22%)	59,89,113	1.60	9 (15%)
14	CLA	dA	824	1	51,55,73	1.43	8 (15%)	61,91,113	1.50	6 (9%)
16	SF4	aC	101	3	0,12,12	-	-	-	-	-
14	CLA	dB	822	2	49,53,73	1.45	10 (20%)	59,89,113	1.54	7 (11%)
17	BCR	aF	204	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	9 (16%)
14	CLA	cK	102	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	6 (10%)
14	CLA	dK	101	9	46,49,73	1.47	9 (19%)	55,83,113	1.48	6 (10%)
17	BCR	cA	850	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	5 (8%)
18	LHG	aB	850	-	22,22,48	0.89	1 (4%)	25,28,54	1.20	1 (4%)
14	CLA	bL	204	10	56,60,73	1.39	9 (16%)	67,97,113	1.53	8 (11%)
18	LHG	bA	850	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
14	CLA	bB	803	-	69,73,73	1.24	12 (17%)	83,113,113	1.25	6 (7%)
14	CLA	bA	817	1	58,62,73	1.34	9 (15%)	69,99,113	1.43	7 (10%)
14	CLA	cA	841	1	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
14	CLA	aB	810	2	69,73,73	1.28	10 (14%)	83,113,113	1.36	7 (8%)
14	CLA	aA	805	1	49,53,73	1.52	11 (22%)	59,89,113	1.62	7 (11%)
14	CLA	bK	103	-	49,53,73	1.47	10 (20%)	59,89,113	1.50	6 (10%)
17	BCR	aB	848	-	41,41,41	1.22	2 (4%)	56,56,56	1.16	4 (7%)
17	BCR	bJ	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	7 (12%)
14	CLA	cB	807	2	69,73,73	1.28	11 (15%)	83,113,113	1.37	6 (7%)
17	BCR	dL	207	-	41,41,41	1.17	3 (7%)	56,56,56	1.43	7 (12%)
14	CLA	aB	834	2	49,53,73	1.43	9 (18%)	59,89,113	1.67	7 (11%)
14	CLA	cJ	102	-	42,45,73	1.53	9 (21%)	50,78,113	1.52	5 (10%)
17	BCR	bB	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	cA	804	14,1	49,53,73	1.48	11 (22%)	59,89,113	1.62	8 (13%)
14	CLA	bB	820	-	69,73,73	1.23	10 (14%)	83,113,113	1.38	7 (8%)
17	BCR	cB	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	5 (8%)
14	CLA	bB	826	-	50,54,73	1.41	11 (22%)	60,90,113	1.55	8 (13%)
14	CLA	cX	101	12	49,53,73	1.47	9 (18%)	59,89,113	1.52	4 (6%)
17	BCR	bK	102	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)
14	CLA	dA	806	1	69,73,73	1.27	10 (14%)	83,113,113	1.37	8 (9%)
14	CLA	aA	828	1	69,73,73	1.23	11 (15%)	83,113,113	1.44	8 (9%)
14	CLA	cA	811	14,1	69,73,73	1.23	9 (13%)	83,113,113	1.31	7 (8%)
14	CLA	bL	205	10	69,73,73	1.21	9 (13%)	83,113,113	1.47	9 (10%)
14	CLA	cB	830	2	49,53,73	1.47	10 (20%)	59,89,113	1.47	5 (8%)
14	CLA	dA	828	1	69,73,73	1.23	11 (15%)	83,113,113	1.45	9 (10%)
14	CLA	aA	834	1	69,73,73	1.23	9 (13%)	83,113,113	1.34	7 (8%)
14	CLA	bB	839	2	69,73,73	1.24	10 (14%)	83,113,113	1.47	10 (12%)
14	CLA	aB	826	2	69,73,73	1.24	11 (15%)	83,113,113	1.34	7 (8%)
14	CLA	aA	831	1	54,58,73	1.38	11 (20%)	65,95,113	1.53	8 (12%)
14	CLA	cB	808	2	69,73,73	1.23	10 (14%)	83,113,113	1.35	9 (10%)
14	CLA	aB	811	2	49,53,73	1.45	9 (18%)	59,89,113	1.51	4 (6%)
14	CLA	aB	823	2	49,53,73	1.48	10 (20%)	59,89,113	1.40	6 (10%)
14	CLA	cB	833	2	62,66,73	1.30	8 (12%)	74,104,113	1.37	8 (10%)
14	CLA	aA	822	1	53,57,73	1.41	10 (18%)	62,93,113	1.51	5 (8%)
14	CLA	aA	823	1	55,59,73	1.38	8 (14%)	66,96,113	1.43	7 (10%)
14	CLA	aB	839	2	51,55,73	1.40	9 (17%)	61,91,113	1.53	8 (13%)
14	CLA	aA	825	-	69,73,73	1.25	11 (15%)	83,113,113	1.40	11 (13%)
14	CLA	cB	820	2	51,55,73	1.42	10 (19%)	61,91,113	1.46	5 (8%)
17	BCR	aB	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.31	5 (8%)
17	BCR	dA	845	-	41,41,41	1.14	3 (7%)	56,56,56	1.29	8 (14%)
14	CLA	dA	808	1	49,53,73	1.45	10 (20%)	59,89,113	1.53	6 (10%)
14	CLA	cA	812	1	58,62,73	1.36	10 (17%)	69,99,113	1.44	4 (5%)
14	CLA	dA	814	1	49,53,73	1.46	10 (20%)	59,89,113	1.51	8 (13%)
18	LHG	cA	853	14	26,26,48	0.87	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	aK	102	-	49,53,73	1.47	10 (20%)	59,89,113	1.50	6 (10%)
17	BCR	cM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	6 (10%)
14	CLA	bA	810	1	49,53,73	1.45	8 (16%)	59,89,113	1.47	5 (8%)
14	CLA	bJ	102	-	42,45,73	1.53	9 (21%)	50,78,113	1.53	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	dB	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.15	5 (8%)
14	CLA	aA	841	1	69,73,73	1.24	9 (13%)	83,113,113	1.37	6 (7%)
14	CLA	cA	814	1	49,53,73	1.45	10 (20%)	59,89,113	1.50	9 (15%)
14	CLA	cB	838	2	69,73,73	1.24	10 (14%)	83,113,113	1.47	10 (12%)
14	CLA	dB	805	2	58,62,73	1.34	10 (17%)	69,99,113	1.45	9 (13%)
14	CLA	bB	840	2	51,55,73	1.40	9 (17%)	61,91,113	1.54	8 (13%)
14	CLA	cA	843	18	56,60,73	1.40	11 (19%)	67,97,113	1.96	10 (14%)
14	CLA	cB	839	2	51,55,73	1.41	9 (17%)	61,91,113	1.54	8 (13%)
14	CLA	cJ	101	-	49,53,73	1.46	9 (18%)	59,89,113	1.50	5 (8%)
14	CLA	bA	829	1	69,73,73	1.25	11 (15%)	83,113,113	1.26	5 (6%)
14	CLA	cA	827	14,1	69,73,73	1.25	10 (14%)	83,113,113	1.41	6 (7%)
19	LMG	bB	850	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
16	SF4	dA	844	1,2	0,12,12	-	-	-	-	-
14	CLA	cA	832	1	69,73,73	1.25	11 (15%)	83,113,113	1.36	10 (12%)
14	CLA	aF	203	-	49,53,73	1.47	10 (20%)	59,89,113	1.50	6 (10%)
14	CLA	cA	831	1	54,58,73	1.39	10 (18%)	65,95,113	1.52	8 (12%)
14	CLA	cA	820	1	65,69,73	1.28	9 (13%)	78,108,113	1.41	6 (7%)
14	CLA	bA	812	1	58,62,73	1.36	11 (18%)	69,99,113	1.45	4 (5%)
14	CLA	bX	101	12	49,53,73	1.47	9 (18%)	59,89,113	1.50	4 (6%)
14	CLA	aB	831	2	53,57,73	1.40	9 (16%)	62,93,113	1.48	8 (12%)
14	CLA	aL	202	10	69,73,73	1.26	8 (11%)	83,113,113	1.30	8 (9%)
14	CLA	aB	804	-	69,73,73	1.25	11 (15%)	83,113,113	1.65	12 (14%)
17	BCR	aB	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.38	8 (14%)
14	CLA	aB	802	2	69,73,73	1.25	9 (13%)	83,113,113	1.29	4 (4%)
14	CLA	bA	830	1	69,73,73	1.27	10 (14%)	83,113,113	1.43	7 (8%)
17	BCR	bB	847	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
17	BCR	aJ	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	6 (10%)
16	SF4	dC	101	3	0,12,12	-	-	-	-	-
14	CLA	aB	809	2	69,73,73	1.25	11 (15%)	83,113,113	1.52	7 (8%)
14	CLA	bA	811	14,1	69,73,73	1.23	9 (13%)	83,113,113	1.31	7 (8%)
14	CLA	cK	101	9	46,49,73	1.47	9 (19%)	55,83,113	1.48	6 (10%)
14	CLA	cA	808	1	49,53,73	1.45	10 (20%)	59,89,113	1.54	6 (10%)
14	CLA	dA	822	1	53,57,73	1.41	11 (20%)	62,93,113	1.51	6 (9%)
14	CLA	bA	839	1	69,73,73	1.25	9 (13%)	83,113,113	1.40	8 (9%)
14	CLA	dA	804	14,1	49,53,73	1.48	11 (22%)	59,89,113	1.61	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	cB	811	2	49,53,73	1.45	9 (18%)	59,89,113	1.50	4 (6%)
14	CLA	dB	804	-	69,73,73	1.25	11 (15%)	83,113,113	1.65	12 (14%)
14	CLA	aB	840	-	69,73,73	1.26	11 (15%)	83,113,113	1.27	6 (7%)
19	LMG	cB	849	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
14	CLA	cB	819	-	69,73,73	1.23	10 (14%)	83,113,113	1.38	7 (8%)
17	BCR	aA	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	3 (5%)
14	CLA	bB	805	2	58,62,73	1.35	11 (18%)	69,99,113	1.45	8 (11%)
14	CLA	aA	837	1	55,59,73	1.39	11 (20%)	66,96,113	1.52	9 (13%)
17	BCR	aA	846	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	11 (19%)
14	CLA	aA	818	1	58,62,73	1.35	10 (17%)	69,99,113	1.48	9 (13%)
14	CLA	dB	823	-	59,63,73	1.33	10 (16%)	71,101,113	1.46	4 (5%)
17	BCR	bA	849	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	6 (10%)
17	BCR	aF	202	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	5 (8%)
17	BCR	bJ	104	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	5 (8%)
14	CLA	cB	841	2	69,73,73	1.24	9 (13%)	83,113,113	1.44	5 (6%)
14	CLA	bB	809	2	69,73,73	1.25	12 (17%)	83,113,113	1.51	7 (8%)
14	CLA	aB	805	2	58,62,73	1.35	10 (17%)	69,99,113	1.46	8 (11%)
14	CLA	aA	812	1	58,62,73	1.36	10 (17%)	69,99,113	1.44	4 (5%)
14	CLA	cB	801	-	69,73,73	1.28	11 (15%)	83,113,113	1.26	7 (8%)
14	CLA	dA	812	1	58,62,73	1.37	11 (18%)	69,99,113	1.44	4 (5%)
14	CLA	bA	822	1	53,57,73	1.41	10 (18%)	62,93,113	1.50	6 (9%)
14	CLA	bB	835	2	49,53,73	1.44	10 (20%)	59,89,113	1.67	7 (11%)
14	CLA	bB	824	2	49,53,73	1.48	10 (20%)	59,89,113	1.40	6 (10%)
14	CLA	cA	837	1	55,59,73	1.38	11 (20%)	66,96,113	1.52	9 (13%)
14	CLA	cA	818	1	58,62,73	1.36	10 (17%)	69,99,113	1.50	9 (13%)
14	CLA	bA	826	-	59,63,73	1.37	11 (18%)	71,101,113	1.41	9 (12%)
14	CLA	cB	814	2	60,64,73	1.32	10 (16%)	72,102,113	1.41	6 (8%)
14	CLA	bB	821	2	51,55,73	1.41	10 (19%)	61,91,113	1.46	5 (8%)
17	BCR	dJ	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	7 (12%)
14	CLA	bJ	101	-	49,53,73	1.46	9 (18%)	59,89,113	1.50	5 (8%)
14	CLA	dB	807	2	69,73,73	1.27	11 (15%)	83,113,113	1.35	6 (7%)
14	CLA	cA	805	1	49,53,73	1.52	11 (22%)	59,89,113	1.62	7 (11%)
17	BCR	dI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
14	CLA	aB	829	2	69,73,73	1.27	10 (14%)	83,113,113	1.53	9 (10%)
14	CLA	bB	836	-	49,53,73	1.50	9 (18%)	59,89,113	1.56	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dF	203	-	49,53,73	1.46	10 (20%)	59,89,113	1.52	8 (13%)
17	BCR	bB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	5 (8%)
14	CLA	bA	840	1	69,73,73	1.22	9 (13%)	83,113,113	1.39	6 (7%)
14	CLA	bB	828	2	69,73,73	1.23	10 (14%)	83,113,113	1.38	8 (9%)
14	CLA	dA	842	-	69,73,73	1.26	10 (14%)	83,113,113	1.36	7 (8%)
14	CLA	cA	802	-	49,53,73	1.46	11 (22%)	59,89,113	1.58	7 (11%)
14	CLA	cA	807	1	55,59,73	1.38	8 (14%)	66,96,113	1.48	6 (9%)
13	CL0	aA	801	1	69,73,73	2.03	21 (30%)	83,113,113	2.84	27 (32%)
17	BCR	dB	847	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
14	CLA	aF	201	-	55,59,73	1.38	9 (16%)	66,96,113	1.49	6 (9%)
14	CLA	dA	818	1	58,62,73	1.36	11 (18%)	69,99,113	1.48	9 (13%)
14	CLA	dB	806	2	69,73,73	1.22	11 (15%)	83,113,113	1.44	8 (9%)
14	CLA	cB	835	-	49,53,73	1.50	9 (18%)	59,89,113	1.55	8 (13%)
17	BCR	aA	850	-	41,41,41	1.20	2 (4%)	56,56,56	1.21	5 (8%)
14	CLA	cL	202	10	69,73,73	1.26	8 (11%)	83,113,113	1.31	8 (9%)
14	CLA	aL	204	-	56,60,73	1.37	9 (16%)	67,97,113	1.45	7 (10%)
14	CLA	bB	823	-	59,63,73	1.33	10 (16%)	71,101,113	1.46	4 (5%)
17	BCR	bA	848	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	6 (10%)
14	CLA	dA	831	1	54,58,73	1.37	10 (18%)	65,95,113	1.53	9 (13%)
14	CLA	aB	821	2	49,53,73	1.45	9 (18%)	59,89,113	1.54	7 (11%)
14	CLA	aB	838	2	69,73,73	1.24	10 (14%)	83,113,113	1.48	10 (12%)
14	CLA	cA	835	1	58,62,73	1.36	9 (15%)	69,99,113	1.45	8 (11%)
14	CLA	bA	809	1	49,53,73	1.47	11 (22%)	59,89,113	1.56	6 (10%)
14	CLA	bL	206	-	69,73,73	1.25	10 (14%)	83,113,113	1.27	5 (6%)
14	CLA	cA	809	1	49,53,73	1.47	10 (20%)	59,89,113	1.57	6 (10%)
14	CLA	aB	841	2	69,73,73	1.24	9 (13%)	83,113,113	1.44	5 (6%)
14	CLA	dA	829	1	69,73,73	1.25	11 (15%)	83,113,113	1.26	5 (6%)
17	BCR	bI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
14	CLA	dK	103	-	49,53,73	1.48	10 (20%)	59,89,113	1.50	6 (10%)
14	CLA	cA	810	1	49,53,73	1.45	8 (16%)	59,89,113	1.47	4 (6%)
17	BCR	aJ	104	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	dB	829	2	69,73,73	1.23	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	bA	803	1	49,53,73	1.46	9 (18%)	59,89,113	1.57	7 (11%)
14	CLA	dA	830	1	69,73,73	1.28	10 (14%)	83,113,113	1.43	7 (8%)
17	BCR	aA	851	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dB	824	2	49,53,73	1.48	10 (20%)	59,89,113	1.41	6 (10%)
17	BCR	aI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
14	CLA	bA	831	1	54,58,73	1.38	10 (18%)	65,95,113	1.53	9 (13%)
14	CLA	cB	815	2	49,53,73	1.44	10 (20%)	59,89,113	1.55	8 (13%)
14	CLA	dA	813	1	49,53,73	1.48	8 (16%)	59,89,113	1.56	10 (16%)
13	CL0	cA	801	1	69,73,73	2.02	21 (30%)	83,113,113	2.84	28 (33%)
14	CLA	aA	824	1	51,55,73	1.44	8 (15%)	61,91,113	1.51	6 (9%)
14	CLA	cA	829	1	69,73,73	1.25	11 (15%)	83,113,113	1.27	6 (7%)
14	CLA	aB	827	2	69,73,73	1.22	10 (14%)	83,113,113	1.37	8 (9%)
14	CLA	bB	822	2	49,53,73	1.45	9 (18%)	59,89,113	1.54	7 (11%)
14	CLA	dB	825	2	58,62,73	1.40	11 (18%)	69,99,113	1.36	8 (11%)
14	CLA	bB	802	2	69,73,73	1.25	9 (13%)	83,113,113	1.29	5 (6%)
14	CLA	aA	827	14,1	69,73,73	1.26	10 (14%)	83,113,113	1.42	6 (7%)
14	CLA	dA	833	1	69,73,73	1.24	11 (15%)	83,113,113	1.42	8 (9%)
17	BCR	cB	848	-	41,41,41	1.22	2 (4%)	56,56,56	1.16	4 (7%)
14	CLA	aB	814	2	60,64,73	1.32	9 (15%)	72,102,113	1.40	6 (8%)
14	CLA	dF	201	-	55,59,73	1.38	9 (16%)	66,96,113	1.50	7 (10%)
14	CLA	aA	832	1	69,73,73	1.25	11 (15%)	83,113,113	1.36	10 (12%)
14	CLA	aB	815	2	49,53,73	1.44	10 (20%)	59,89,113	1.57	8 (13%)
14	CLA	aA	820	1	65,69,73	1.29	9 (13%)	78,108,113	1.42	6 (7%)
14	CLA	cA	823	1	55,59,73	1.38	8 (14%)	66,96,113	1.42	7 (10%)
14	CLA	dB	833	2	69,73,73	1.27	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	aB	825	-	50,54,73	1.41	11 (22%)	60,90,113	1.54	8 (13%)
17	BCR	cB	846	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
16	SF4	cC	101	3	0,12,12	-	-	-	-	-
14	CLA	dA	825	-	69,73,73	1.25	11 (15%)	83,113,113	1.41	12 (14%)
14	CLA	aA	821	14	69,73,73	1.25	10 (14%)	83,113,113	1.41	7 (8%)
14	CLA	aA	839	1	69,73,73	1.25	9 (13%)	83,113,113	1.39	8 (9%)
14	CLA	cA	830	1	69,73,73	1.27	10 (14%)	83,113,113	1.43	7 (8%)
14	CLA	aB	835	-	49,53,73	1.50	9 (18%)	59,89,113	1.55	9 (15%)
14	CLA	bA	841	1	69,73,73	1.24	9 (13%)	83,113,113	1.38	6 (7%)
14	CLA	cA	834	1	69,73,73	1.23	9 (13%)	83,113,113	1.35	7 (8%)
15	PQN	bB	843	-	34,34,34	1.53	2 (5%)	42,45,45	1.20	4 (9%)
14	CLA	aB	803	-	69,73,73	1.24	11 (15%)	83,113,113	1.24	6 (7%)
14	CLA	dL	205	10	69,73,73	1.21	9 (13%)	83,113,113	1.48	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	aA	835	1	58,62,73	1.36	9 (15%)	69,99,113	1.45	8 (11%)
14	CLA	bB	813	2	49,53,73	1.48	10 (20%)	59,89,113	1.53	5 (8%)
14	CLA	bA	837	1	55,59,73	1.39	11 (20%)	66,96,113	1.52	9 (13%)
14	CLA	cA	833	1	69,73,73	1.24	11 (15%)	83,113,113	1.41	8 (9%)
14	CLA	dB	814	2	69,73,73	1.26	10 (14%)	83,113,113	1.41	9 (10%)
14	CLA	aL	203	10	69,73,73	1.21	10 (14%)	83,113,113	1.48	9 (10%)
17	BCR	dB	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	6 (10%)
17	BCR	aL	205	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	7 (12%)
14	CLA	cB	817	2	63,67,73	1.31	9 (14%)	75,105,113	1.44	9 (12%)
18	LHG	cA	852	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
14	CLA	cA	825	-	69,73,73	1.24	11 (15%)	83,113,113	1.41	12 (14%)
15	PQN	dA	843	-	34,34,34	1.50	2 (5%)	42,45,45	1.27	6 (14%)
14	CLA	bA	802	-	49,53,73	1.46	11 (22%)	59,89,113	1.58	7 (11%)
14	CLA	aB	828	2	69,73,73	1.23	10 (14%)	83,113,113	1.34	7 (8%)
14	CLA	aB	836	-	49,53,73	1.49	10 (20%)	59,89,113	1.42	6 (10%)
18	LHG	dB	851	-	22,22,48	0.90	1 (4%)	25,28,54	1.20	1 (4%)
18	LHG	aA	852	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
14	CLA	cB	809	2	69,73,73	1.25	12 (17%)	83,113,113	1.51	7 (8%)
14	CLA	aA	836	1	49,53,73	1.46	9 (18%)	59,89,113	1.61	7 (11%)
14	CLA	dB	808	2	69,73,73	1.24	11 (15%)	83,113,113	1.36	9 (10%)
14	CLA	aA	804	14,1	49,53,73	1.48	11 (22%)	59,89,113	1.61	8 (13%)
14	CLA	cA	839	1	69,73,73	1.26	8 (11%)	83,113,113	1.40	8 (9%)
14	CLA	dA	805	1	49,53,73	1.53	11 (22%)	59,89,113	1.62	7 (11%)
14	CLA	dA	820	1	65,69,73	1.28	10 (15%)	78,108,113	1.41	6 (7%)
17	BCR	cL	201	-	41,41,41	1.24	3 (7%)	56,56,56	1.25	5 (8%)
14	CLA	aA	816	-	53,57,73	1.41	8 (15%)	62,93,113	1.48	4 (6%)
14	CLA	dA	826	-	59,63,73	1.36	11 (18%)	71,101,113	1.41	9 (12%)
14	CLA	cL	204	-	56,60,73	1.37	9 (16%)	67,97,113	1.44	6 (8%)
14	CLA	dA	802	-	49,53,73	1.46	11 (22%)	59,89,113	1.58	7 (11%)
17	BCR	dJ	104	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	aA	811	14,1	69,73,73	1.23	9 (13%)	83,113,113	1.31	7 (8%)
14	CLA	dB	820	-	69,73,73	1.23	10 (14%)	83,113,113	1.38	7 (8%)
14	CLA	aA	838	1	69,73,73	1.25	9 (13%)	83,113,113	1.43	8 (9%)
17	BCR	bB	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	5 (8%)
15	PQN	bA	843	-	34,34,34	1.51	2 (5%)	42,45,45	1.27	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dA	838	1	69,73,73	1.26	10 (14%)	83,113,113	1.43	8 (9%)
14	CLA	dB	818	2	63,67,73	1.31	9 (14%)	75,105,113	1.45	9 (12%)
17	BCR	dB	852	-	41,41,41	1.18	2 (4%)	56,56,56	1.38	8 (14%)
14	CLA	dJ	102	-	42,45,73	1.53	9 (21%)	50,78,113	1.52	5 (10%)
14	CLA	dA	839	1	69,73,73	1.25	8 (11%)	83,113,113	1.40	8 (9%)
14	CLA	bA	835	1	58,62,73	1.36	10 (17%)	69,99,113	1.44	8 (11%)
14	CLA	cA	836	1	49,53,73	1.46	9 (18%)	59,89,113	1.62	7 (11%)
14	CLA	aB	837	2	64,68,73	1.30	10 (15%)	77,107,113	1.39	8 (10%)
14	CLA	bA	807	1	55,59,73	1.37	8 (14%)	66,96,113	1.47	6 (9%)
18	LHG	cB	850	-	22,22,48	0.89	1 (4%)	25,28,54	1.20	1 (4%)
14	CLA	dA	803	1	49,53,73	1.46	9 (18%)	59,89,113	1.56	7 (11%)
14	CLA	bA	805	1	49,53,73	1.52	11 (22%)	59,89,113	1.62	7 (11%)
14	CLA	dA	834	1	69,73,73	1.23	9 (13%)	83,113,113	1.35	7 (8%)
14	CLA	cA	838	1	69,73,73	1.25	10 (14%)	83,113,113	1.43	8 (9%)
14	CLA	cB	810	2	69,73,73	1.28	10 (14%)	83,113,113	1.37	7 (8%)
17	BCR	cI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
14	CLA	bA	823	1	55,59,73	1.38	8 (14%)	66,96,113	1.43	7 (10%)
14	CLA	dB	834	2	62,66,73	1.30	8 (12%)	74,104,113	1.37	7 (9%)
14	CLA	bA	836	1	49,53,73	1.46	9 (18%)	59,89,113	1.61	7 (11%)
14	CLA	dA	819	1	69,73,73	1.24	10 (14%)	83,113,113	1.41	10 (12%)
16	SF4	cA	845	1,2	0,12,12	-	-	-	-	-
14	CLA	aA	843	18	56,60,73	1.40	11 (19%)	67,97,113	1.96	10 (14%)
14	CLA	cB	834	2	49,53,73	1.44	10 (20%)	59,89,113	1.66	7 (11%)
14	CLA	cA	819	1	69,73,73	1.24	10 (14%)	83,113,113	1.41	10 (12%)
18	LHG	dA	851	14	26,26,48	0.87	1 (3%)	29,32,54	1.31	3 (10%)
17	BCR	cA	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	3 (5%)
14	CLA	aA	814	1	49,53,73	1.46	9 (18%)	59,89,113	1.51	8 (13%)
14	CLA	dB	831	2	49,53,73	1.46	9 (18%)	59,89,113	1.47	5 (8%)
14	CLA	bB	827	2	69,73,73	1.25	11 (15%)	83,113,113	1.34	7 (8%)
14	CLA	bA	838	1	69,73,73	1.25	9 (13%)	83,113,113	1.43	8 (9%)
14	CLA	dA	811	14,1	69,73,73	1.23	9 (13%)	83,113,113	1.31	7 (8%)
14	CLA	dA	823	1	55,59,73	1.38	9 (16%)	66,96,113	1.43	7 (10%)
14	CLA	bB	837	-	49,53,73	1.48	10 (20%)	59,89,113	1.43	6 (10%)
13	CL0	bA	801	1	69,73,73	2.02	20 (28%)	83,113,113	2.88	30 (36%)
14	CLA	aA	842	-	69,73,73	1.26	10 (14%)	83,113,113	1.37	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dB	812	2	49,53,73	1.45	9 (18%)	59,89,113	1.51	4 (6%)
14	CLA	cB	825	-	50,54,73	1.42	11 (22%)	60,90,113	1.54	8 (13%)
14	CLA	aB	808	2	69,73,73	1.24	10 (14%)	83,113,113	1.35	9 (10%)
14	CLA	cA	840	1	69,73,73	1.22	9 (13%)	83,113,113	1.38	6 (7%)
14	CLA	bA	815	1	49,53,73	1.47	8 (16%)	59,89,113	1.54	5 (8%)
17	BCR	dA	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	3 (5%)
17	BCR	bL	207	-	41,41,41	1.18	3 (7%)	56,56,56	1.42	7 (12%)
14	CLA	cB	821	2	49,53,73	1.45	10 (20%)	59,89,113	1.54	7 (11%)
14	CLA	bA	825	-	69,73,73	1.25	11 (15%)	83,113,113	1.42	12 (14%)
14	CLA	aB	807	2	69,73,73	1.28	11 (15%)	83,113,113	1.36	6 (7%)
17	BCR	aM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	6 (10%)
17	BCR	bM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	6 (10%)
14	CLA	cB	822	-	59,63,73	1.33	10 (16%)	71,101,113	1.46	4 (5%)
14	CLA	cB	823	2	49,53,73	1.47	10 (20%)	59,89,113	1.40	6 (10%)
14	CLA	aA	807	1	55,59,73	1.38	9 (16%)	66,96,113	1.47	6 (9%)
14	CLA	dB	816	2	49,53,73	1.44	10 (20%)	59,89,113	1.57	8 (13%)
14	CLA	bA	821	14	69,73,73	1.25	11 (15%)	83,113,113	1.41	7 (8%)
17	BCR	aB	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	4 (7%)
14	CLA	aA	829	1	69,73,73	1.24	11 (15%)	83,113,113	1.26	5 (6%)
14	CLA	aA	803	1	49,53,73	1.47	9 (18%)	59,89,113	1.56	8 (13%)

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
17	BCR	bA	847	-	-	18/29/63/63	0/2/2/2
14	CLA	cA	816	-	-	10/20/96/115	-
17	BCR	dF	202	-	-	11/29/63/63	0/2/2/2
17	BCR	cA	847	-	-	7/29/63/63	0/2/2/2
14	CLA	dL	206	-	-	22/39/115/115	-
14	CLA	bB	808	2	-	8/39/115/115	-
17	BCR	dM	101	-	-	9/29/63/63	0/2/2/2
14	CLA	aB	833	2	-	13/31/107/115	-
14	CLA	aA	817	1	-	10/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PQN	aB	842	-	-	9/23/43/43	0/2/2/2
14	CLA	aK	101	9	-	3/9/81/115	-
17	BCR	cL	205	-	-	9/29/63/63	0/2/2/2
14	CLA	dB	801	-	-	14/39/115/115	-
14	CLA	aA	833	1	-	11/39/115/115	-
14	CLA	dB	842	2	-	22/39/115/115	-
17	BCR	dL	203	-	-	13/29/63/63	0/2/2/2
14	CLA	dB	832	2	-	11/20/96/115	-
14	CLA	aB	824	2	-	7/26/102/115	-
14	CLA	dA	809	1	-	7/15/91/115	-
14	CLA	dB	802	2	-	14/39/115/115	-
14	CLA	cB	826	2	-	22/39/115/115	-
17	BCR	dL	208	-	-	15/29/63/63	0/2/2/2
14	CLA	dX	101	12	-	9/15/91/115	-
14	CLA	aA	813	1	-	8/15/91/115	-
14	CLA	bB	811	2	-	8/39/115/115	-
14	CLA	cA	821	14	-	16/39/115/115	-
16	SF4	bA	844	1,2	-	-	0/6/5/5
16	SF4	dC	102	3	-	-	0/6/5/5
14	CLA	cB	803	-	-	18/39/115/115	-
14	CLA	dA	840	1	-	14/39/115/115	-
15	PQN	cB	842	-	-	9/23/43/43	0/2/2/2
14	CLA	bB	816	2	-	7/15/91/115	-
14	CLA	dB	819	2	-	10/33/109/115	-
14	CLA	aA	815	1	-	6/15/91/115	-
17	BCR	cB	843	-	-	10/29/63/63	0/2/2/2
14	CLA	dB	840	2	-	1/18/94/115	-
17	BCR	dB	848	-	-	10/29/63/63	0/2/2/2
17	BCR	aL	201	-	-	13/29/63/63	0/2/2/2
15	PQN	cA	844	-	-	8/23/43/43	0/2/2/2
17	BCR	cA	851	-	-	20/29/63/63	0/2/2/2
14	CLA	cB	840	-	-	5/39/115/115	-
14	CLA	aB	816	2	-	10/27/103/115	-
14	CLA	cB	837	2	-	10/33/109/115	-
14	CLA	dB	813	2	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	cA	848	-	-	8/29/63/63	0/2/2/2
14	CLA	dB	810	2	-	10/39/115/115	-
17	BCR	dK	102	-	-	6/29/63/63	0/2/2/2
14	CLA	bB	801	-	-	14/39/115/115	-
14	CLA	aA	806	1	-	12/39/115/115	-
14	CLA	aB	812	2	-	8/15/91/115	-
14	CLA	bB	804	-	-	13/39/115/115	-
17	BCR	cA	846	-	-	6/29/63/63	0/2/2/2
14	CLA	dB	817	2	-	10/27/103/115	-
14	CLA	bA	824	1	-	7/18/94/115	-
14	CLA	dJ	101	-	-	12/15/91/115	-
17	BCR	dA	848	-	-	9/29/63/63	0/2/2/2
14	CLA	dB	811	2	-	8/39/115/115	-
16	SF4	bC	102	3	-	-	0/6/5/5
17	BCR	cJ	103	-	-	15/29/63/63	0/2/2/2
14	CLA	cA	828	1	-	6/39/115/115	-
17	BCR	cB	847	-	-	9/29/63/63	0/2/2/2
14	CLA	aJ	101	-	-	12/15/91/115	-
14	CLA	cA	815	1	-	6/15/91/115	-
17	BCR	bL	203	-	-	13/29/63/63	0/2/2/2
14	CLA	aA	808	1	-	6/15/91/115	-
14	CLA	aB	832	2	-	15/39/115/115	-
14	CLA	bB	819	2	-	10/33/109/115	-
17	BCR	bB	849	-	-	7/29/63/63	0/2/2/2
17	BCR	bL	208	-	-	15/29/63/63	0/2/2/2
14	CLA	dB	827	2	-	22/39/115/115	-
17	BCR	dF	204	-	-	13/29/63/63	0/2/2/2
14	CLA	dA	815	1	-	6/15/91/115	-
14	CLA	dB	841	-	-	4/39/115/115	-
14	CLA	cL	203	10	-	14/39/115/115	-
14	CLA	dB	815	2	-	2/29/105/115	-
17	BCR	aB	843	-	-	10/29/63/63	0/2/2/2
17	BCR	cL	206	-	-	11/29/63/63	0/2/2/2
14	CLA	bB	812	2	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aB	819	-	-	9/39/115/115	-
14	CLA	dA	817	1	-	10/26/102/115	-
14	CLA	dA	841	1	-	14/39/115/115	-
14	CLA	bA	827	14,1	-	14/39/115/115	-
14	CLA	aA	810	1	-	5/15/91/115	-
14	CLA	dB	838	2	-	10/33/109/115	-
14	CLA	aA	819	1	-	19/39/115/115	-
14	CLA	cA	822	1	-	13/20/96/115	-
14	CLA	bA	814	1	-	7/15/91/115	-
14	CLA	bA	820	1	-	13/35/111/115	-
14	CLA	bB	832	2	-	11/20/96/115	-
14	CLA	aB	813	2	-	15/39/115/115	-
14	CLA	bB	814	2	-	15/39/115/115	-
16	SF4	bC	101	3	-	-	0/6/5/5
14	CLA	aB	822	-	-	15/27/103/115	-
14	CLA	cA	817	1	-	9/26/102/115	-
14	CLA	dA	827	14,1	-	14/39/115/115	-
18	LHG	bA	851	14	-	10/31/31/53	-
17	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
14	CLA	dA	821	14	-	16/39/115/115	-
14	CLA	bF	203	-	-	5/15/91/115	-
14	CLA	bA	808	1	-	6/15/91/115	-
17	BCR	aA	847	-	-	7/29/63/63	0/2/2/2
14	CLA	dB	828	2	-	14/39/115/115	-
14	CLA	cB	827	2	-	14/39/115/115	-
14	CLA	bB	806	2	-	15/39/115/115	-
14	CLA	bA	806	1	-	12/39/115/115	-
14	CLA	bB	829	2	-	11/39/115/115	-
14	CLA	cB	832	2	-	15/39/115/115	-
14	CLA	cB	816	2	-	10/27/103/115	-
15	PQN	dB	843	-	-	5/23/43/43	0/2/2/2
17	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
14	CLA	cB	828	2	-	11/39/115/115	-
18	LHG	dA	850	-	-	18/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cB	805	2	-	7/26/102/115	-
17	BCR	bA	846	-	-	8/29/63/63	0/2/2/2
14	CLA	bA	818	1	-	7/26/102/115	-
18	LHG	aA	853	14	-	10/31/31/53	-
16	SF4	aC	102	3	-	-	0/6/5/5
14	CLA	dA	835	1	-	7/26/102/115	-
14	CLA	bA	828	1	-	6/39/115/115	-
14	CLA	dA	810	1	-	5/15/91/115	-
13	CL0	dA	801	1	-	13/39/115/115	-
14	CLA	bB	830	2	-	13/39/115/115	-
14	CLA	bB	817	2	-	10/27/103/115	-
14	CLA	bA	816	-	-	10/20/96/115	-
14	CLA	bB	833	2	-	15/39/115/115	-
17	BCR	cB	851	-	-	8/29/63/63	0/2/2/2
14	CLA	cA	826	-	-	6/27/103/115	-
14	CLA	aA	826	-	-	6/27/103/115	-
14	CLA	dB	839	2	-	8/39/115/115	-
14	CLA	dA	836	1	-	7/15/91/115	-
17	BCR	aA	848	-	-	8/29/63/63	0/2/2/2
14	CLA	cB	831	2	-	11/20/96/115	-
17	BCR	cF	202	-	-	11/29/63/63	0/2/2/2
14	CLA	cB	824	2	-	7/26/102/115	-
14	CLA	dB	836	-	-	4/15/91/115	-
14	CLA	dA	816	-	-	10/20/96/115	-
17	BCR	cJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	cA	803	1	-	8/15/91/115	-
15	PQN	aA	844	-	-	8/23/43/43	0/2/2/2
17	BCR	bF	202	-	-	11/29/63/63	0/2/2/2
14	CLA	aA	802	-	-	3/15/91/115	-
16	SF4	aA	845	1,2	-	-	0/6/5/5
14	CLA	cB	836	-	-	8/15/91/115	-
14	CLA	cA	813	1	-	8/15/91/115	-
14	CLA	cB	804	-	-	13/39/115/115	-
14	CLA	dL	202	18,10	-	13/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	dL	201	2,10	-	8/39/115/115	-
14	CLA	aB	818	2	-	10/33/109/115	-
14	CLA	bB	815	2	-	2/29/105/115	-
14	CLA	dB	821	2	-	10/18/94/115	-
14	CLA	cF	203	-	-	6/15/91/115	-
16	SF4	cC	102	3	-	-	0/6/5/5
14	CLA	dA	837	1	-	7/23/99/115	-
17	BCR	aB	844	-	-	9/29/63/63	0/2/2/2
14	CLA	bL	202	18,10	-	13/24/100/115	-
14	CLA	aA	840	1	-	14/39/115/115	-
14	CLA	dB	837	-	-	8/15/91/115	-
14	CLA	aB	830	2	-	8/15/91/115	-
14	CLA	cB	806	2	-	15/39/115/115	-
14	CLA	bB	810	2	-	10/39/115/115	-
14	CLA	aJ	102	-	-	2/4/76/115	-
14	CLA	cF	201	-	-	7/23/99/115	-
14	CLA	bK	101	9	-	3/9/81/115	-
14	CLA	bB	842	2	-	22/39/115/115	-
14	CLA	bF	201	-	-	7/23/99/115	-
14	CLA	cB	812	2	-	8/15/91/115	-
14	CLA	bB	834	2	-	13/31/107/115	-
17	BCR	bB	852	-	-	8/29/63/63	0/2/2/2
14	CLA	bB	818	2	-	11/32/108/115	-
17	BCR	aL	206	-	-	11/29/63/63	0/2/2/2
14	CLA	bB	831	2	-	8/15/91/115	-
14	CLA	aB	806	2	-	15/39/115/115	-
14	CLA	aA	830	1	-	14/39/115/115	-
14	CLA	cB	802	2	-	15/39/115/115	-
14	CLA	bB	838	2	-	10/33/109/115	-
14	CLA	bA	842	-	-	14/39/115/115	-
14	CLA	bA	832	1	-	13/39/115/115	-
14	CLA	dL	204	10	-	9/24/100/115	-
14	CLA	bB	807	2	-	20/39/115/115	-
17	BCR	bA	845	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	dB	830	2	-	13/39/115/115	-
17	BCR	dB	849	-	-	7/29/63/63	0/2/2/2
17	BCR	bB	844	-	-	10/29/63/63	0/2/2/2
14	CLA	dB	803	-	-	18/39/115/115	-
14	CLA	bB	841	-	-	5/39/115/115	-
14	CLA	dA	807	1	-	4/23/99/115	-
14	CLA	dB	835	2	-	4/15/91/115	-
14	CLA	aB	817	2	-	11/32/108/115	-
14	CLA	cB	818	2	-	10/33/109/115	-
14	CLA	dA	832	1	-	13/39/115/115	-
17	BCR	dA	846	-	-	8/29/63/63	0/2/2/2
14	CLA	bL	201	2,10	-	8/39/115/115	-
18	LHG	bB	851	-	-	11/26/26/53	-
19	LMG	aB	849	-	-	23/50/70/70	0/1/1/1
14	CLA	bA	819	1	-	19/39/115/115	-
14	CLA	bA	833	1	-	11/39/115/115	-
14	CLA	cA	842	-	-	14/39/115/115	-
14	CLA	dB	809	2	-	11/39/115/115	-
14	CLA	cB	813	2	-	15/39/115/115	-
17	BCR	dB	846	-	-	12/29/63/63	0/2/2/2
14	CLA	cA	806	1	-	12/39/115/115	-
17	BCR	dA	849	-	-	20/29/63/63	0/2/2/2
14	CLA	aX	101	12	-	9/15/91/115	-
14	CLA	cB	829	2	-	13/39/115/115	-
19	LMG	dB	850	-	-	23/50/70/70	0/1/1/1
14	CLA	bA	834	1	-	11/39/115/115	-
17	BCR	cF	204	-	-	14/29/63/63	0/2/2/2
14	CLA	aA	809	1	-	7/15/91/115	-
14	CLA	cA	824	1	-	7/18/94/115	-
14	CLA	dB	826	-	-	8/17/93/115	-
14	CLA	bA	813	1	-	8/15/91/115	-
17	BCR	bF	204	-	-	13/29/63/63	0/2/2/2
14	CLA	aB	801	-	-	14/39/115/115	-
14	CLA	bB	825	2	-	7/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aB	820	2	-	10/18/94/115	-
14	CLA	bA	804	14,1	-	6/15/91/115	-
14	CLA	dA	824	1	-	7/18/94/115	-
16	SF4	aC	101	3	-	-	0/6/5/5
14	CLA	dB	822	2	-	7/15/91/115	-
17	BCR	aF	204	-	-	14/29/63/63	0/2/2/2
14	CLA	cK	102	-	-	5/15/91/115	-
14	CLA	dK	101	9	-	3/9/81/115	-
17	BCR	cA	850	-	-	9/29/63/63	0/2/2/2
18	LHG	aB	850	-	-	11/26/26/53	-
14	CLA	bL	204	10	-	9/24/100/115	-
18	LHG	bA	850	-	-	18/53/53/53	-
14	CLA	bB	803	-	-	18/39/115/115	-
14	CLA	bA	817	1	-	10/26/102/115	-
14	CLA	cA	841	1	-	14/39/115/115	-
14	CLA	aB	810	2	-	10/39/115/115	-
14	CLA	aA	805	1	-	7/15/91/115	-
14	CLA	bK	103	-	-	5/15/91/115	-
17	BCR	aB	848	-	-	7/29/63/63	0/2/2/2
17	BCR	bJ	103	-	-	15/29/63/63	0/2/2/2
14	CLA	cB	807	2	-	20/39/115/115	-
17	BCR	dL	207	-	-	9/29/63/63	0/2/2/2
14	CLA	aB	834	2	-	4/15/91/115	-
14	CLA	cJ	102	-	-	2/4/76/115	-
17	BCR	bB	846	-	-	12/29/63/63	0/2/2/2
14	CLA	cA	804	14,1	-	6/15/91/115	-
14	CLA	bB	820	-	-	9/39/115/115	-
17	BCR	cB	844	-	-	9/29/63/63	0/2/2/2
14	CLA	bB	826	-	-	8/17/93/115	-
14	CLA	cX	101	12	-	9/15/91/115	-
17	BCR	bK	102	-	-	6/29/63/63	0/2/2/2
14	CLA	dA	806	1	-	12/39/115/115	-
14	CLA	aA	828	1	-	6/39/115/115	-
14	CLA	cA	811	14,1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bL	205	10	-	12/39/115/115	-
14	CLA	cB	830	2	-	8/15/91/115	-
14	CLA	dA	828	1	-	6/39/115/115	-
14	CLA	aA	834	1	-	11/39/115/115	-
14	CLA	bB	839	2	-	8/39/115/115	-
14	CLA	aB	826	2	-	22/39/115/115	-
14	CLA	aA	831	1	-	4/21/97/115	-
14	CLA	cB	808	2	-	8/39/115/115	-
14	CLA	aB	811	2	-	6/15/91/115	-
14	CLA	aB	823	2	-	8/15/91/115	-
14	CLA	cB	833	2	-	13/31/107/115	-
14	CLA	aA	822	1	-	13/20/96/115	-
14	CLA	aA	823	1	-	14/23/99/115	-
14	CLA	aB	839	2	-	1/18/94/115	-
14	CLA	aA	825	-	-	13/39/115/115	-
14	CLA	cB	820	2	-	10/18/94/115	-
17	BCR	aB	847	-	-	9/29/63/63	0/2/2/2
17	BCR	dA	845	-	-	7/29/63/63	0/2/2/2
14	CLA	dA	808	1	-	6/15/91/115	-
14	CLA	cA	812	1	-	13/26/102/115	-
14	CLA	dA	814	1	-	7/15/91/115	-
18	LHG	cA	853	14	-	10/31/31/53	-
14	CLA	aK	102	-	-	5/15/91/115	-
17	BCR	cM	101	-	-	9/29/63/63	0/2/2/2
14	CLA	bA	810	1	-	5/15/91/115	-
14	CLA	bJ	102	-	-	2/4/76/115	-
17	BCR	dB	845	-	-	9/29/63/63	0/2/2/2
14	CLA	aA	841	1	-	14/39/115/115	-
14	CLA	cA	814	1	-	7/15/91/115	-
14	CLA	cB	838	2	-	8/39/115/115	-
14	CLA	dB	805	2	-	7/26/102/115	-
14	CLA	bB	840	2	-	1/18/94/115	-
14	CLA	cA	843	18	-	13/24/100/115	-
14	CLA	cB	839	2	-	1/18/94/115	-
14	CLA	cJ	101	-	-	12/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bA	829	1	-	16/39/115/115	-
14	CLA	cA	827	14,1	-	14/39/115/115	-
19	LMG	bB	850	-	-	23/50/70/70	0/1/1/1
16	SF4	dA	844	1,2	-	-	0/6/5/5
14	CLA	cA	832	1	-	14/39/115/115	-
14	CLA	aF	203	-	-	6/15/91/115	-
14	CLA	cA	831	1	-	4/21/97/115	-
14	CLA	cA	820	1	-	13/35/111/115	-
14	CLA	bA	812	1	-	13/26/102/115	-
14	CLA	bX	101	12	-	9/15/91/115	-
14	CLA	aB	831	2	-	11/20/96/115	-
14	CLA	aL	202	10	-	12/39/115/115	-
14	CLA	aB	804	-	-	13/39/115/115	-
17	BCR	aB	851	-	-	8/29/63/63	0/2/2/2
14	CLA	aB	802	2	-	14/39/115/115	-
14	CLA	bA	830	1	-	14/39/115/115	-
17	BCR	bB	847	-	-	17/29/63/63	0/2/2/2
17	BCR	aJ	103	-	-	15/29/63/63	0/2/2/2
16	SF4	dC	101	3	-	-	0/6/5/5
14	CLA	aB	809	2	-	11/39/115/115	-
14	CLA	bA	811	14,1	-	13/39/115/115	-
14	CLA	cK	101	9	-	3/9/81/115	-
14	CLA	cA	808	1	-	6/15/91/115	-
14	CLA	dA	822	1	-	13/20/96/115	-
14	CLA	bA	839	1	-	12/39/115/115	-
14	CLA	dA	804	14,1	-	6/15/91/115	-
14	CLA	cB	811	2	-	6/15/91/115	-
14	CLA	dB	804	-	-	13/39/115/115	-
14	CLA	aB	840	-	-	4/39/115/115	-
19	LMG	cB	849	-	-	23/50/70/70	0/1/1/1
14	CLA	cB	819	-	-	9/39/115/115	-
17	BCR	aA	849	-	-	18/29/63/63	0/2/2/2
14	CLA	bB	805	2	-	7/26/102/115	-
14	CLA	aA	837	1	-	7/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	aA	846	-	-	6/29/63/63	0/2/2/2
14	CLA	aA	818	1	-	7/26/102/115	-
14	CLA	dB	823	-	-	13/27/103/115	-
17	BCR	bA	849	-	-	20/29/63/63	0/2/2/2
17	BCR	aF	202	-	-	11/29/63/63	0/2/2/2
17	BCR	bJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	cB	841	2	-	22/39/115/115	-
14	CLA	bB	809	2	-	11/39/115/115	-
14	CLA	aB	805	2	-	7/26/102/115	-
14	CLA	aA	812	1	-	13/26/102/115	-
14	CLA	cB	801	-	-	14/39/115/115	-
14	CLA	dA	812	1	-	13/26/102/115	-
14	CLA	bA	822	1	-	13/20/96/115	-
14	CLA	bB	835	2	-	4/15/91/115	-
14	CLA	bB	824	2	-	8/15/91/115	-
14	CLA	cA	837	1	-	7/23/99/115	-
14	CLA	cA	818	1	-	7/26/102/115	-
14	CLA	bA	826	-	-	6/27/103/115	-
14	CLA	cB	814	2	-	2/29/105/115	-
14	CLA	bB	821	2	-	10/18/94/115	-
17	BCR	dJ	103	-	-	15/29/63/63	0/2/2/2
14	CLA	bJ	101	-	-	12/15/91/115	-
14	CLA	dB	807	2	-	20/39/115/115	-
14	CLA	cA	805	1	-	7/15/91/115	-
17	BCR	dI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	aB	829	2	-	13/39/115/115	-
14	CLA	bB	836	-	-	4/15/91/115	-
14	CLA	dF	203	-	-	5/15/91/115	-
17	BCR	bB	845	-	-	9/29/63/63	0/2/2/2
14	CLA	bA	840	1	-	14/39/115/115	-
14	CLA	bB	828	2	-	14/39/115/115	-
14	CLA	dA	842	-	-	14/39/115/115	-
14	CLA	cA	802	-	-	3/15/91/115	-
14	CLA	cA	807	1	-	4/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL0	aA	801	1	-	17/39/115/115	-
17	BCR	dB	847	-	-	17/29/63/63	0/2/2/2
14	CLA	aF	201	-	-	7/23/99/115	-
14	CLA	dA	818	1	-	7/26/102/115	-
14	CLA	dB	806	2	-	15/39/115/115	-
14	CLA	cB	835	-	-	4/15/91/115	-
17	BCR	aA	850	-	-	9/29/63/63	0/2/2/2
14	CLA	cL	202	10	-	12/39/115/115	-
14	CLA	aL	204	-	-	10/24/100/115	-
14	CLA	bB	823	-	-	15/27/103/115	-
17	BCR	bA	848	-	-	9/29/63/63	0/2/2/2
14	CLA	dA	831	1	-	4/21/97/115	-
14	CLA	aB	821	2	-	7/15/91/115	-
14	CLA	aB	838	2	-	8/39/115/115	-
14	CLA	cA	835	1	-	7/26/102/115	-
14	CLA	bA	809	1	-	7/15/91/115	-
14	CLA	bL	206	-	-	22/39/115/115	-
14	CLA	cA	809	1	-	7/15/91/115	-
14	CLA	aB	841	2	-	22/39/115/115	-
14	CLA	dA	829	1	-	16/39/115/115	-
17	BCR	bI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	dK	103	-	-	5/15/91/115	-
14	CLA	cA	810	1	-	5/15/91/115	-
17	BCR	aJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	dB	829	2	-	11/39/115/115	-
14	CLA	bA	803	1	-	8/15/91/115	-
14	CLA	dA	830	1	-	14/39/115/115	-
17	BCR	aA	851	-	-	20/29/63/63	0/2/2/2
14	CLA	dB	824	2	-	8/15/91/115	-
17	BCR	aI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	bA	831	1	-	4/21/97/115	-
14	CLA	cB	815	2	-	7/15/91/115	-
14	CLA	dA	813	1	-	8/15/91/115	-
13	CL0	cA	801	1	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aA	824	1	-	7/18/94/115	-
14	CLA	cA	829	1	-	16/39/115/115	-
14	CLA	aB	827	2	-	14/39/115/115	-
14	CLA	bB	822	2	-	7/15/91/115	-
14	CLA	dB	825	2	-	7/26/102/115	-
14	CLA	bB	802	2	-	14/39/115/115	-
14	CLA	aA	827	14,1	-	14/39/115/115	-
14	CLA	dA	833	1	-	11/39/115/115	-
17	BCR	cB	848	-	-	7/29/63/63	0/2/2/2
14	CLA	aB	814	2	-	2/29/105/115	-
14	CLA	dF	201	-	-	7/23/99/115	-
14	CLA	aA	832	1	-	13/39/115/115	-
14	CLA	aB	815	2	-	7/15/91/115	-
14	CLA	aA	820	1	-	13/35/111/115	-
14	CLA	cA	823	1	-	14/23/99/115	-
14	CLA	dB	833	2	-	15/39/115/115	-
14	CLA	aB	825	-	-	8/17/93/115	-
17	BCR	cB	846	-	-	17/29/63/63	0/2/2/2
16	SF4	cC	101	3	-	-	0/6/5/5
14	CLA	dA	825	-	-	13/39/115/115	-
14	CLA	aA	821	14	-	16/39/115/115	-
14	CLA	aA	839	1	-	12/39/115/115	-
14	CLA	cA	830	1	-	14/39/115/115	-
14	CLA	aB	835	-	-	4/15/91/115	-
14	CLA	bA	841	1	-	14/39/115/115	-
14	CLA	cA	834	1	-	11/39/115/115	-
15	PQN	bB	843	-	-	7/23/43/43	0/2/2/2
14	CLA	aB	803	-	-	18/39/115/115	-
14	CLA	dL	205	10	-	12/39/115/115	-
14	CLA	aA	835	1	-	7/26/102/115	-
14	CLA	bB	813	2	-	8/15/91/115	-
14	CLA	bA	837	1	-	7/23/99/115	-
14	CLA	cA	833	1	-	11/39/115/115	-
14	CLA	dB	814	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aL	203	10	-	14/39/115/115	-
17	BCR	dB	844	-	-	10/29/63/63	0/2/2/2
17	BCR	aL	205	-	-	9/29/63/63	0/2/2/2
14	CLA	cB	817	2	-	11/32/108/115	-
18	LHG	cA	852	-	-	18/53/53/53	-
14	CLA	cA	825	-	-	13/39/115/115	-
15	PQN	dA	843	-	-	5/23/43/43	0/2/2/2
14	CLA	bA	802	-	-	3/15/91/115	-
14	CLA	aB	828	2	-	11/39/115/115	-
14	CLA	aB	836	-	-	8/15/91/115	-
18	LHG	dB	851	-	-	11/26/26/53	-
18	LHG	aA	852	-	-	18/53/53/53	-
14	CLA	cB	809	2	-	11/39/115/115	-
14	CLA	aA	836	1	-	7/15/91/115	-
14	CLA	dB	808	2	-	8/39/115/115	-
14	CLA	aA	804	14,1	-	6/15/91/115	-
14	CLA	cA	839	1	-	12/39/115/115	-
14	CLA	dA	805	1	-	7/15/91/115	-
14	CLA	dA	820	1	-	13/35/111/115	-
17	BCR	cL	201	-	-	13/29/63/63	0/2/2/2
14	CLA	aA	816	-	-	10/20/96/115	-
14	CLA	dA	826	-	-	6/27/103/115	-
14	CLA	cL	204	-	-	9/24/100/115	-
14	CLA	dA	802	-	-	3/15/91/115	-
17	BCR	dJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	aA	811	14,1	-	13/39/115/115	-
14	CLA	dB	820	-	-	9/39/115/115	-
14	CLA	aA	838	1	-	16/39/115/115	-
17	BCR	bB	848	-	-	10/29/63/63	0/2/2/2
15	PQN	bA	843	-	-	5/23/43/43	0/2/2/2
14	CLA	dA	838	1	-	16/39/115/115	-
14	CLA	dB	818	2	-	11/32/108/115	-
17	BCR	dB	852	-	-	8/29/63/63	0/2/2/2
14	CLA	dJ	102	-	-	2/4/76/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	dA	839	1	-	12/39/115/115	-
14	CLA	bA	835	1	-	7/26/102/115	-
14	CLA	cA	836	1	-	7/15/91/115	-
14	CLA	aB	837	2	-	10/33/109/115	-
14	CLA	bA	807	1	-	4/23/99/115	-
18	LHG	cB	850	-	-	11/26/26/53	-
14	CLA	dA	803	1	-	8/15/91/115	-
14	CLA	bA	805	1	-	7/15/91/115	-
14	CLA	dA	834	1	-	11/39/115/115	-
14	CLA	cA	838	1	-	16/39/115/115	-
14	CLA	cB	810	2	-	10/39/115/115	-
17	BCR	cI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	bA	823	1	-	14/23/99/115	-
14	CLA	dB	834	2	-	13/31/107/115	-
14	CLA	bA	836	1	-	7/15/91/115	-
14	CLA	dA	819	1	-	19/39/115/115	-
16	SF4	cA	845	1,2	-	-	0/6/5/5
14	CLA	aA	843	18	-	13/24/100/115	-
14	CLA	cB	834	2	-	4/15/91/115	-
14	CLA	cA	819	1	-	19/39/115/115	-
18	LHG	dA	851	14	-	10/31/31/53	-
17	BCR	cA	849	-	-	18/29/63/63	0/2/2/2
14	CLA	aA	814	1	-	7/15/91/115	-
14	CLA	dB	831	2	-	8/15/91/115	-
14	CLA	bB	827	2	-	22/39/115/115	-
14	CLA	bA	838	1	-	16/39/115/115	-
14	CLA	dA	811	14,1	-	13/39/115/115	-
14	CLA	dA	823	1	-	14/23/99/115	-
14	CLA	bB	837	-	-	8/15/91/115	-
13	CL0	bA	801	1	-	14/39/115/115	-
14	CLA	aA	842	-	-	14/39/115/115	-
14	CLA	dB	812	2	-	6/15/91/115	-
14	CLA	cB	825	-	-	8/17/93/115	-
14	CLA	aB	808	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cA	840	1	-	14/39/115/115	-
14	CLA	bA	815	1	-	6/15/91/115	-
17	BCR	dA	847	-	-	18/29/63/63	0/2/2/2
17	BCR	bL	207	-	-	9/29/63/63	0/2/2/2
14	CLA	cB	821	2	-	7/15/91/115	-
14	CLA	bA	825	-	-	13/39/115/115	-
14	CLA	aB	807	2	-	20/39/115/115	-
17	BCR	aM	101	-	-	9/29/63/63	0/2/2/2
17	BCR	bM	101	-	-	9/29/63/63	0/2/2/2
14	CLA	cB	822	-	-	13/27/103/115	-
14	CLA	cB	823	2	-	8/15/91/115	-
14	CLA	aA	807	1	-	4/23/99/115	-
14	CLA	dB	816	2	-	7/15/91/115	-
14	CLA	bA	821	14	-	16/39/115/115	-
17	BCR	aB	846	-	-	17/29/63/63	0/2/2/2
14	CLA	aA	829	1	-	16/39/115/115	-
14	CLA	aA	803	1	-	8/15/91/115	-

The worst 5 of 4017 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	843	PQN	C3-C2	7.39	1.48	1.35
15	dB	843	PQN	C3-C2	7.35	1.48	1.35
15	cA	844	PQN	C3-C2	7.31	1.48	1.35
15	aA	844	PQN	C3-C2	7.29	1.48	1.35
15	aB	842	PQN	C3-C2	7.26	1.48	1.35

The worst 5 of 3437 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	aB	804	CLA	C4A-NA-C1A	9.40	110.93	106.71
14	dB	804	CLA	C4A-NA-C1A	9.36	110.91	106.71
14	bB	804	CLA	C4A-NA-C1A	9.30	110.89	106.71
14	cB	804	CLA	C4A-NA-C1A	9.28	110.88	106.71
13	aA	801	CL0	C1D-ND-C4D	-8.96	99.97	106.33

There are no chirality outliers.

5 of 5146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	dA	801	CL0	C4B-C3B-CAB-CBB
14	aA	803	CLA	CHA-CBD-CGD-O1D
14	aA	803	CLA	CHA-CBD-CGD-O2D
14	aA	805	CLA	C1A-C2A-CAA-CBA
14	aA	805	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

398 monomers are involved in 936 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	bA	847	BCR	3	0
17	dF	202	BCR	1	0
17	cA	847	BCR	2	0
14	dL	206	CLA	2	0
14	bB	808	CLA	2	0
17	dM	101	BCR	2	0
14	aB	833	CLA	2	0
14	aA	817	CLA	1	0
15	aB	842	PQN	6	0
14	aK	101	CLA	1	0
17	cL	205	BCR	1	0
14	dB	801	CLA	1	0
14	aA	833	CLA	2	0
14	dB	842	CLA	9	0
17	dL	203	BCR	1	0
14	dB	802	CLA	6	0
14	cB	826	CLA	1	0
17	dL	208	BCR	2	0
14	bB	811	CLA	3	0
14	cA	821	CLA	4	0
16	bA	844	SF4	1	0
16	dC	102	SF4	2	0
14	cB	803	CLA	5	0
14	dA	840	CLA	2	0
15	cB	842	PQN	7	0
14	dB	819	CLA	3	0
17	cB	843	BCR	1	0
14	dB	840	CLA	1	0
17	dB	848	BCR	1	0
17	aL	201	BCR	3	0
15	cA	844	PQN	12	0
17	cA	851	BCR	3	0
14	cB	840	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aB	816	CLA	1	0
17	cA	848	BCR	2	0
14	dB	810	CLA	3	0
17	dK	102	BCR	5	0
14	bB	801	CLA	1	0
14	aA	806	CLA	2	0
14	bB	804	CLA	4	0
17	cA	846	BCR	3	0
14	dB	817	CLA	1	0
14	bA	824	CLA	1	0
17	dA	848	BCR	4	0
14	dB	811	CLA	3	0
16	bC	102	SF4	3	0
17	cJ	103	BCR	1	0
14	cA	828	CLA	5	0
17	cB	847	BCR	1	0
14	aJ	101	CLA	1	0
17	bL	203	BCR	1	0
14	aA	808	CLA	1	0
14	aB	832	CLA	2	0
14	bB	819	CLA	3	0
17	bB	849	BCR	4	0
17	bL	208	BCR	2	0
14	dB	827	CLA	1	0
17	dF	204	BCR	2	0
14	dB	841	CLA	1	0
14	dB	815	CLA	1	0
17	aB	843	BCR	1	0
14	bB	812	CLA	3	0
14	dA	817	CLA	1	0
14	dA	841	CLA	11	0
14	bA	827	CLA	3	0
14	aA	810	CLA	1	0
14	dB	838	CLA	1	0
14	aA	819	CLA	2	0
14	cA	822	CLA	1	0
14	bA	820	CLA	3	0
14	aB	813	CLA	2	0
14	bB	814	CLA	3	0
14	aB	822	CLA	2	0
14	cA	817	CLA	1	0
14	dA	827	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	bA	851	LHG	1	0
17	aB	845	BCR	1	0
14	dA	821	CLA	4	0
14	bF	203	CLA	3	0
14	bA	808	CLA	1	0
17	aA	847	BCR	1	0
14	dB	828	CLA	4	0
14	cB	827	CLA	5	0
14	bB	806	CLA	2	0
14	bA	806	CLA	2	0
14	bB	829	CLA	3	0
14	cB	832	CLA	2	0
14	cB	816	CLA	1	0
15	dB	843	PQN	10	0
17	cB	845	BCR	2	0
14	cB	828	CLA	3	0
14	cB	805	CLA	1	0
17	bA	846	BCR	1	0
14	bA	818	CLA	1	0
18	aA	853	LHG	1	0
16	aC	102	SF4	2	0
14	dA	835	CLA	2	0
14	bA	828	CLA	4	0
14	dA	810	CLA	1	0
13	dA	801	CL0	19	0
14	bB	830	CLA	4	0
14	bB	817	CLA	1	0
14	bB	833	CLA	3	0
17	cB	851	BCR	3	0
14	dB	839	CLA	2	0
14	dA	836	CLA	3	0
17	cF	202	BCR	2	0
14	cB	824	CLA	1	0
14	dB	836	CLA	1	0
17	cJ	104	BCR	4	0
14	cA	803	CLA	3	0
15	aA	844	PQN	12	0
17	bF	202	BCR	2	0
14	aA	802	CLA	1	0
16	aA	845	SF4	1	0
14	cB	836	CLA	1	0
14	cB	804	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	dL	201	CLA	3	0
14	aB	818	CLA	3	0
14	bB	815	CLA	1	0
14	dB	821	CLA	1	0
14	cF	203	CLA	2	0
16	cC	102	SF4	2	0
17	aB	844	BCR	2	0
14	aA	840	CLA	3	0
14	dB	837	CLA	1	0
14	aB	830	CLA	3	0
14	cB	806	CLA	2	0
14	bB	810	CLA	3	0
14	cF	201	CLA	1	0
14	bK	101	CLA	1	0
14	bB	842	CLA	8	0
14	bF	201	CLA	7	0
14	bB	834	CLA	2	0
17	bB	852	BCR	4	0
14	bB	818	CLA	1	0
14	bB	831	CLA	3	0
14	aB	806	CLA	2	0
14	aA	830	CLA	4	0
14	cB	802	CLA	4	0
14	bA	842	CLA	2	0
14	bA	832	CLA	2	0
14	dL	204	CLA	4	0
14	bB	807	CLA	4	0
17	bA	845	BCR	1	0
14	dB	830	CLA	3	0
17	dB	849	BCR	3	0
14	dB	803	CLA	5	0
14	bB	841	CLA	3	0
14	dA	807	CLA	1	0
14	aB	817	CLA	1	0
14	cB	818	CLA	3	0
14	dA	832	CLA	2	0
14	bL	201	CLA	3	0
18	bB	851	LHG	1	0
19	aB	849	LMG	1	0
14	bA	819	CLA	2	0
14	bA	833	CLA	2	0
14	cA	842	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	dB	809	CLA	2	0
14	cB	813	CLA	3	0
17	dB	846	BCR	2	0
14	cA	806	CLA	2	0
17	dA	849	BCR	2	0
14	aX	101	CLA	1	0
14	cB	829	CLA	4	0
19	dB	850	LMG	1	0
14	bA	834	CLA	1	0
17	cF	204	BCR	1	0
14	cA	824	CLA	2	0
17	bF	204	BCR	3	0
14	aB	801	CLA	2	0
14	bA	804	CLA	2	0
14	dA	824	CLA	2	0
17	aF	204	BCR	1	0
14	dK	101	CLA	2	0
17	cA	850	BCR	3	0
14	bL	204	CLA	3	0
14	bB	803	CLA	5	0
14	bA	817	CLA	1	0
14	cA	841	CLA	11	0
14	aB	810	CLA	3	0
14	aA	805	CLA	1	0
17	aB	848	BCR	6	0
14	cB	807	CLA	4	0
17	dL	207	BCR	2	0
14	cA	804	CLA	2	0
14	bB	820	CLA	1	0
17	cB	844	BCR	1	0
14	cX	101	CLA	1	0
17	bK	102	BCR	5	0
14	dA	806	CLA	2	0
14	aA	828	CLA	3	0
14	cA	811	CLA	3	0
14	cB	830	CLA	3	0
14	dA	828	CLA	4	0
14	aA	834	CLA	3	0
14	aA	831	CLA	1	0
14	cB	808	CLA	3	0
14	aB	811	CLA	3	0
14	aB	823	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	cB	833	CLA	2	0
14	aA	822	CLA	1	0
14	aA	823	CLA	1	0
14	aB	839	CLA	2	0
14	aA	825	CLA	4	0
14	cB	820	CLA	1	0
17	aB	847	BCR	2	0
17	dA	845	BCR	2	0
14	dA	808	CLA	1	0
14	cA	812	CLA	2	0
18	cA	853	LHG	1	0
17	cM	101	BCR	1	0
14	bA	810	CLA	2	0
17	dB	845	BCR	1	0
14	aA	841	CLA	14	0
14	cB	838	CLA	2	0
14	dB	805	CLA	1	0
14	bB	840	CLA	1	0
14	cB	839	CLA	2	0
14	cJ	101	CLA	1	0
14	cA	827	CLA	2	0
19	bB	850	LMG	2	0
16	dA	844	SF4	1	0
14	cA	832	CLA	3	0
14	aF	203	CLA	2	0
14	cA	831	CLA	1	0
14	cA	820	CLA	2	0
14	bA	812	CLA	1	0
14	aL	202	CLA	3	0
14	aB	804	CLA	3	0
17	aB	851	BCR	4	0
14	aB	802	CLA	3	0
14	bA	830	CLA	3	0
17	bB	847	BCR	2	0
14	aB	809	CLA	2	0
14	bA	811	CLA	4	0
14	cK	101	CLA	1	0
14	cA	808	CLA	1	0
14	bA	839	CLA	4	0
14	dA	804	CLA	3	0
14	cB	811	CLA	3	0
14	dB	804	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aB	840	CLA	1	0
19	cB	849	LMG	2	0
17	aA	849	BCR	3	0
14	bB	805	CLA	1	0
17	aA	846	BCR	2	0
14	dB	823	CLA	2	0
17	bA	849	BCR	2	0
17	aF	202	BCR	1	0
17	bJ	104	BCR	3	0
14	cB	841	CLA	5	0
14	bB	809	CLA	2	0
14	aB	805	CLA	1	0
14	aA	812	CLA	2	0
14	cB	801	CLA	2	0
14	dA	812	CLA	1	0
14	bA	822	CLA	1	0
14	bB	824	CLA	3	0
14	cA	818	CLA	1	0
14	cB	814	CLA	1	0
14	bB	821	CLA	1	0
17	dJ	103	BCR	1	0
14	bJ	101	CLA	1	0
14	dB	807	CLA	4	0
14	cA	805	CLA	1	0
17	dI	101	BCR	5	0
14	aB	829	CLA	4	0
14	bB	836	CLA	1	0
14	dF	203	CLA	3	0
17	bB	845	BCR	2	0
14	bA	840	CLA	2	0
14	bB	828	CLA	5	0
14	dA	842	CLA	1	0
14	cA	802	CLA	1	0
14	cA	807	CLA	1	0
13	aA	801	CL0	29	0
17	dB	847	BCR	3	0
14	aF	201	CLA	1	0
14	dA	818	CLA	1	0
14	dB	806	CLA	2	0
14	cB	835	CLA	1	0
17	aA	850	BCR	4	0
14	cL	202	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	aL	204	CLA	1	0
14	bB	823	CLA	2	0
17	bA	848	BCR	3	0
14	dA	831	CLA	1	0
14	aB	838	CLA	3	0
14	cA	835	CLA	2	0
14	bL	206	CLA	3	0
14	aB	841	CLA	6	0
17	bI	101	BCR	5	0
14	cA	810	CLA	1	0
17	aJ	104	BCR	3	0
14	dB	829	CLA	3	0
14	bA	803	CLA	3	0
14	dA	830	CLA	3	0
17	aA	851	BCR	3	0
14	dB	824	CLA	3	0
17	aI	101	BCR	1	0
14	bA	831	CLA	1	0
14	cB	815	CLA	1	0
13	cA	801	CL0	32	0
14	aA	824	CLA	2	0
14	aB	827	CLA	5	0
14	bB	802	CLA	6	0
14	aA	827	CLA	2	0
14	dA	833	CLA	2	0
17	cB	848	BCR	5	0
14	aB	814	CLA	1	0
14	dF	201	CLA	7	0
14	aA	832	CLA	1	0
14	aA	820	CLA	2	0
14	cA	823	CLA	1	0
14	dB	833	CLA	2	0
17	cB	846	BCR	2	0
14	dA	825	CLA	4	0
14	aA	821	CLA	3	0
14	aA	839	CLA	4	0
14	cA	830	CLA	4	0
14	aB	835	CLA	1	0
14	bA	841	CLA	14	0
14	cA	834	CLA	2	0
15	bB	843	PQN	19	0
14	aB	803	CLA	5	0

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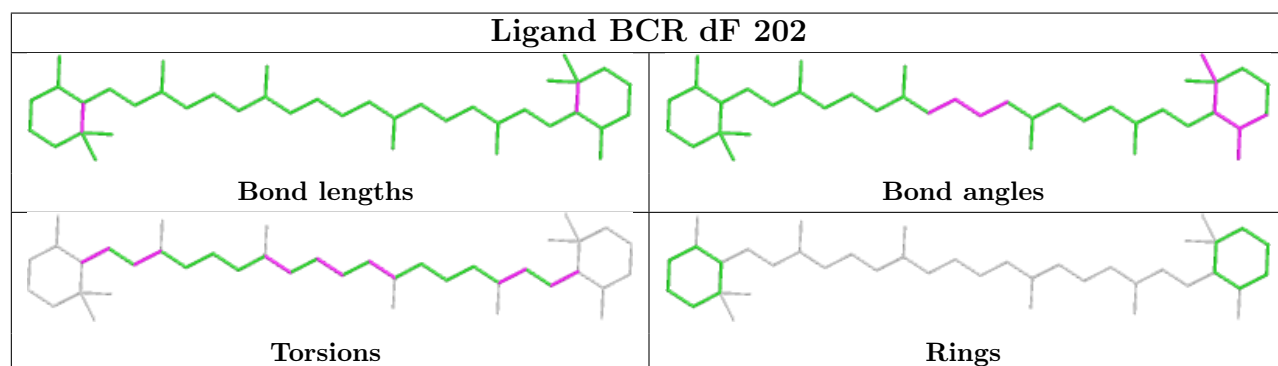
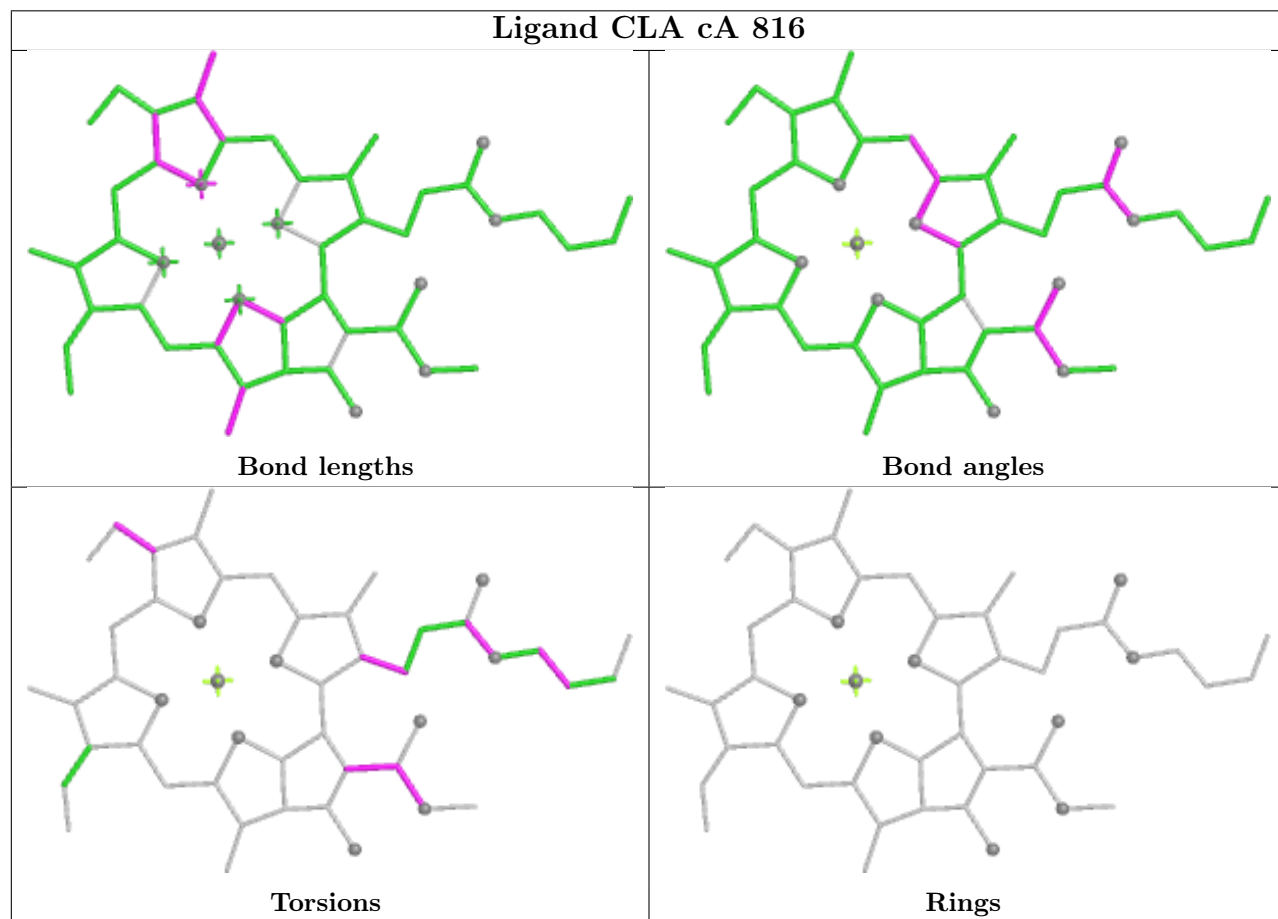
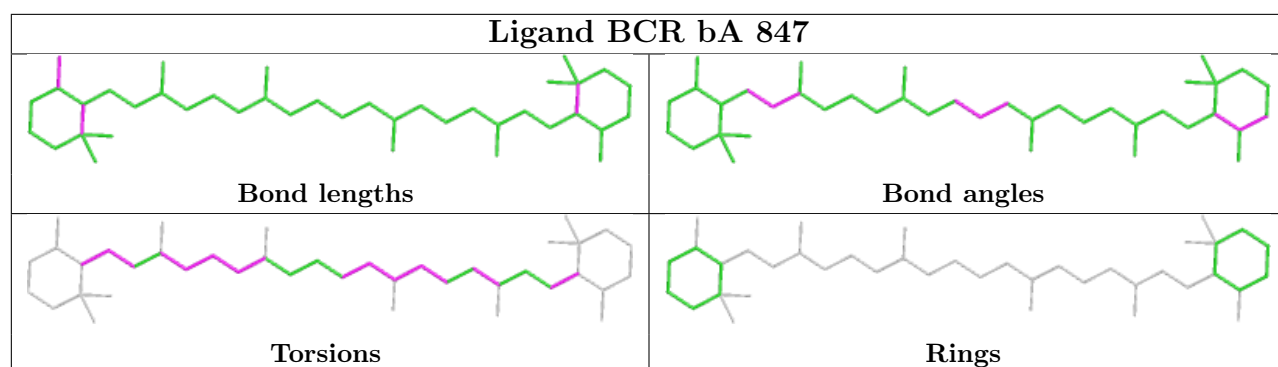
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	dL	205	CLA	1	0
14	aA	835	CLA	1	0
14	cA	833	CLA	2	0
14	dB	814	CLA	3	0
17	dB	844	BCR	1	0
17	aL	205	BCR	3	0
14	cB	817	CLA	1	0
14	cA	825	CLA	4	0
15	dA	843	PQN	26	0
14	bA	802	CLA	2	0
14	aB	828	CLA	3	0
14	aB	836	CLA	1	0
14	cB	809	CLA	2	0
14	aA	836	CLA	3	0
14	dB	808	CLA	3	0
14	aA	804	CLA	1	0
14	cA	839	CLA	4	0
14	dA	805	CLA	1	0
14	dA	820	CLA	4	0
17	cL	201	BCR	2	0
14	cL	204	CLA	1	0
14	dA	802	CLA	2	0
17	dJ	104	BCR	2	0
14	aA	811	CLA	3	0
14	aA	838	CLA	3	0
17	bB	848	BCR	1	0
15	bA	843	PQN	30	0
14	dA	838	CLA	3	0
14	dB	818	CLA	1	0
17	dB	852	BCR	2	0
14	dA	839	CLA	4	0
14	bA	835	CLA	3	0
14	cA	836	CLA	3	0
14	bA	807	CLA	1	0
14	dA	803	CLA	3	0
14	bA	805	CLA	1	0
14	dA	834	CLA	1	0
14	cA	838	CLA	3	0
14	cB	810	CLA	4	0
17	cI	101	BCR	1	0
14	bA	823	CLA	2	0
14	dB	834	CLA	1	0

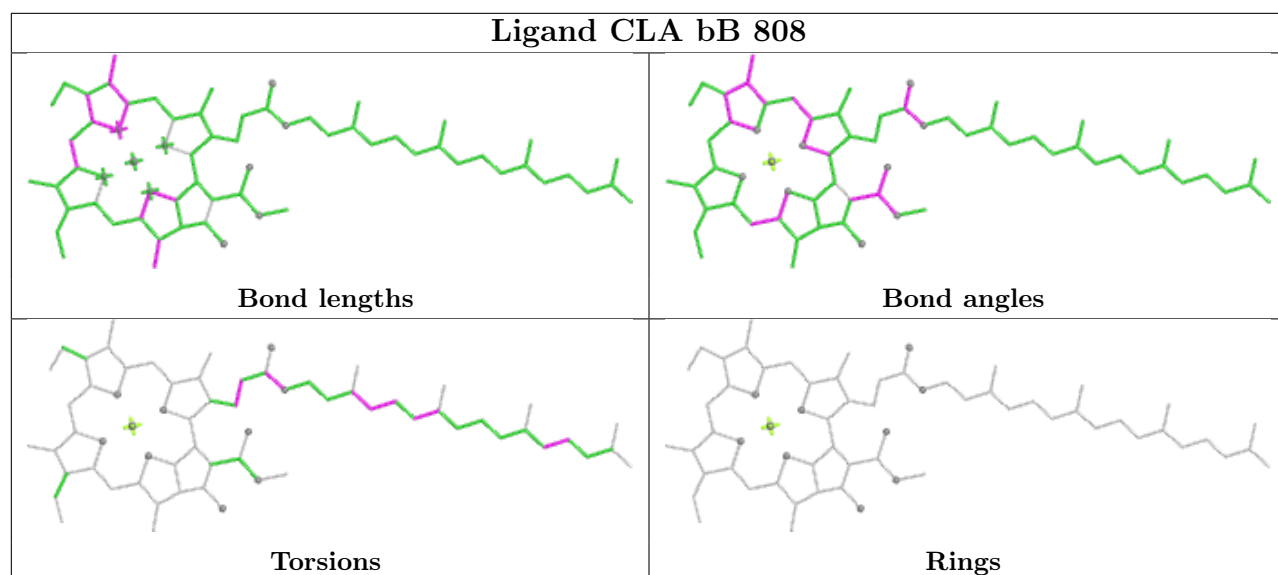
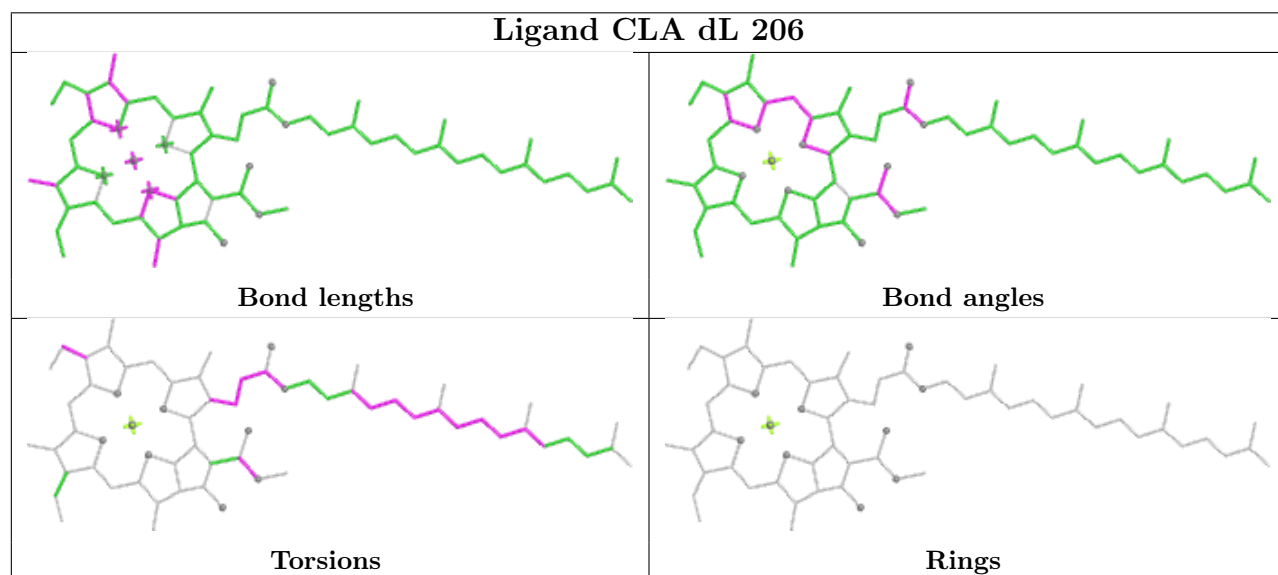
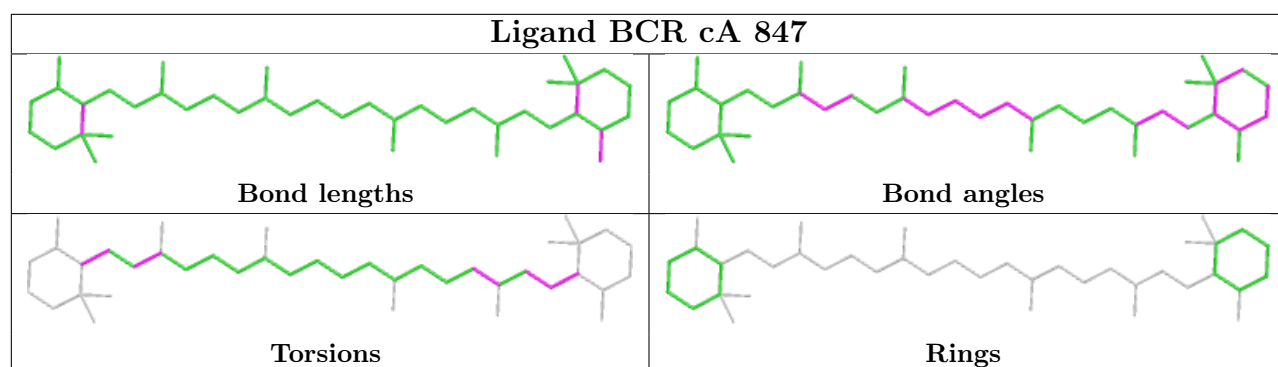
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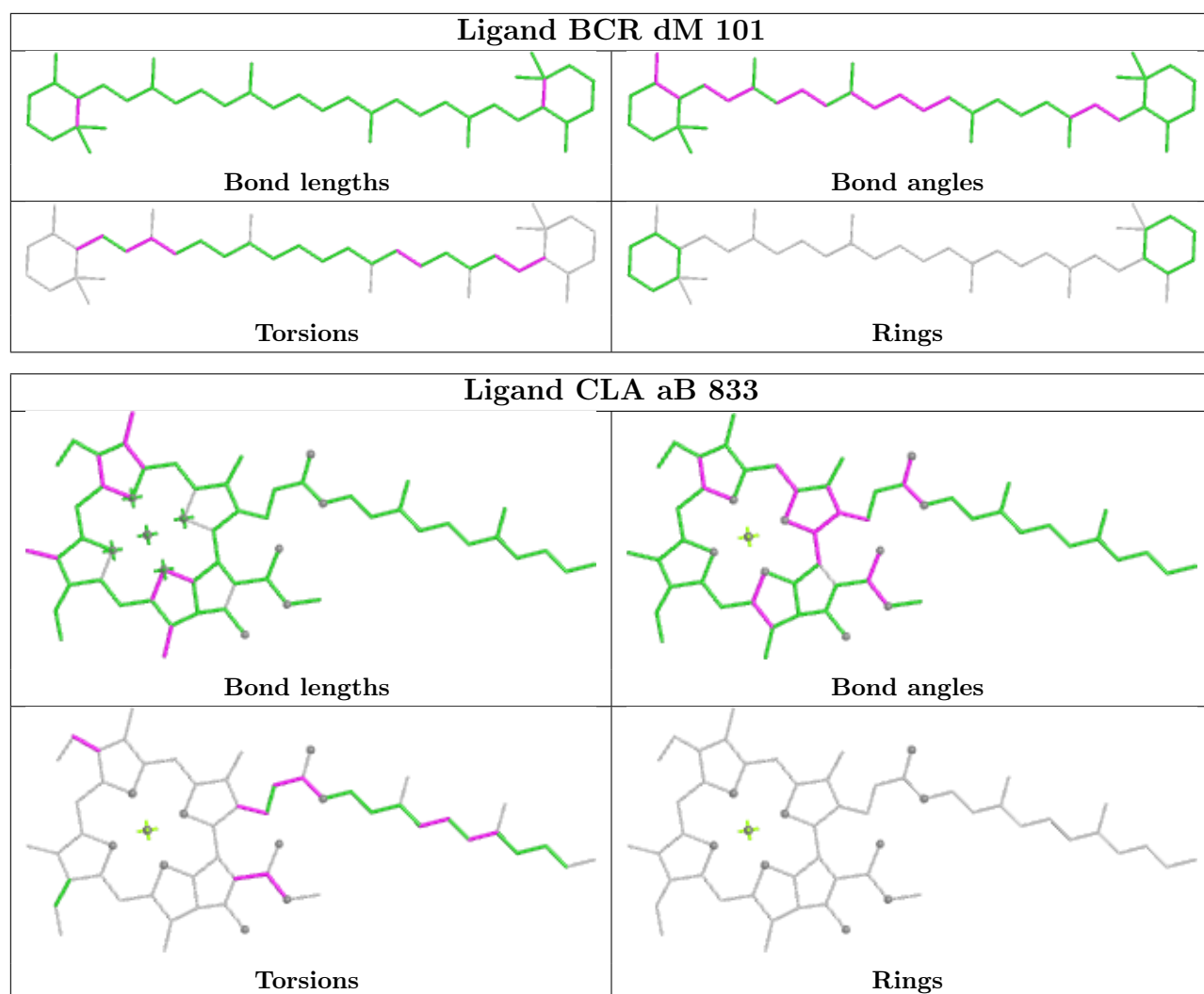
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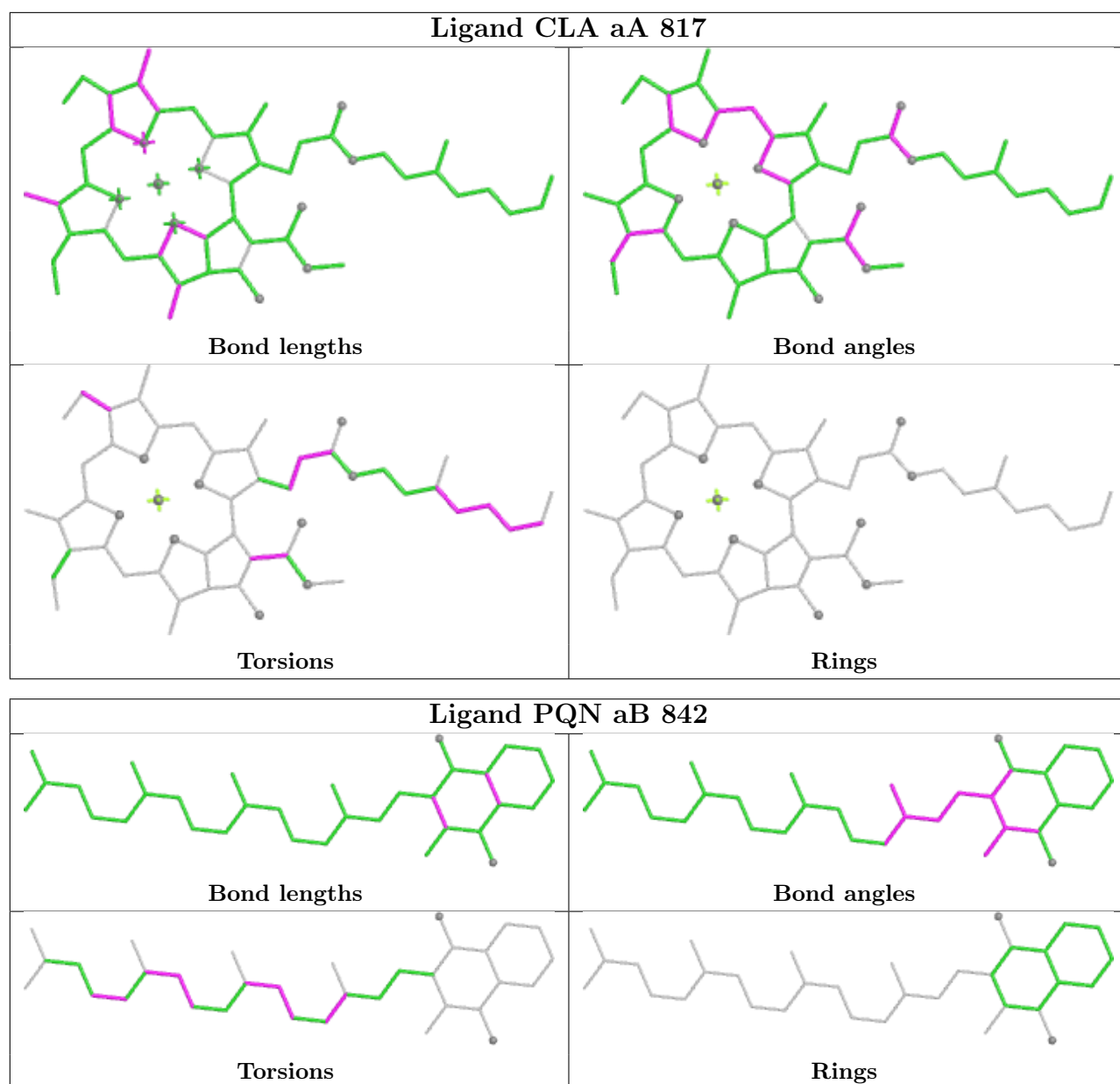
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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14	dA	819	CLA	2	0
16	cA	845	SF4	1	0
14	cA	819	CLA	1	0
18	dA	851	LHG	1	0
17	cA	849	BCR	3	0
14	dB	831	CLA	3	0
14	bB	827	CLA	1	0
14	bA	838	CLA	2	0
14	dA	811	CLA	4	0
14	dA	823	CLA	1	0
14	bB	837	CLA	1	0
13	bA	801	CL0	21	0
14	aA	842	CLA	1	0
14	dB	812	CLA	3	0
14	aB	808	CLA	3	0
14	cA	840	CLA	5	0
17	dA	847	BCR	3	0
17	bL	207	BCR	2	0
14	bA	825	CLA	6	0
14	aB	807	CLA	4	0
17	aM	101	BCR	1	0
14	cB	822	CLA	2	0
14	cB	823	CLA	3	0
14	aA	807	CLA	1	0
14	dB	816	CLA	1	0
14	bA	821	CLA	3	0
17	aB	846	BCR	2	0
14	aA	803	CLA	3	0

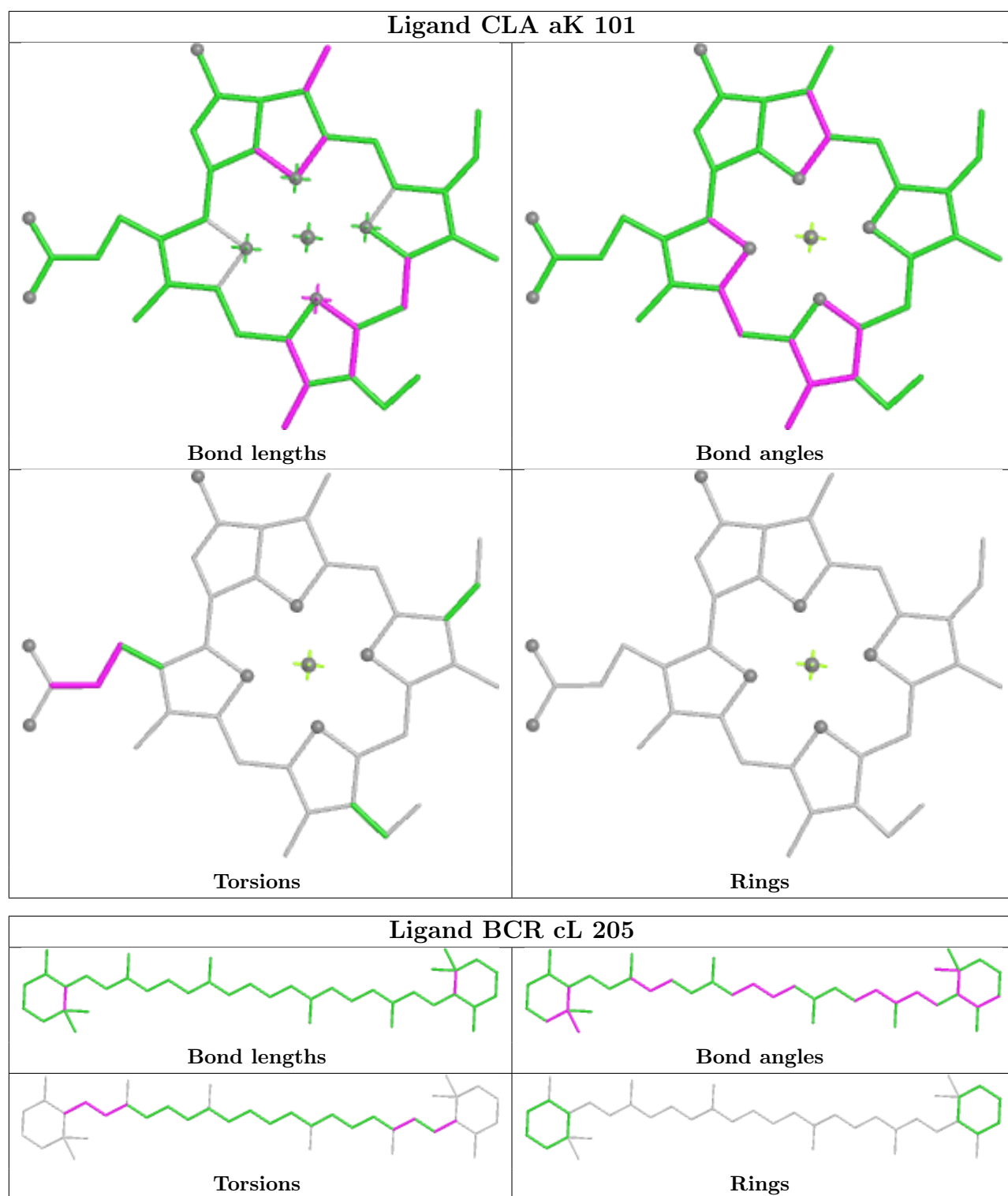
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

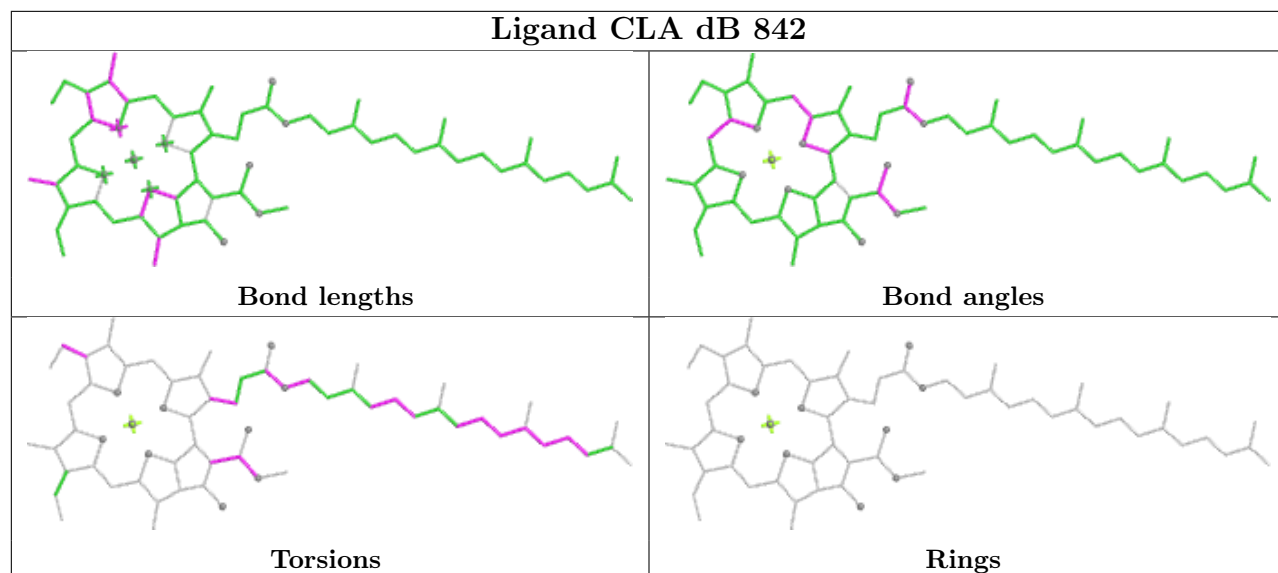
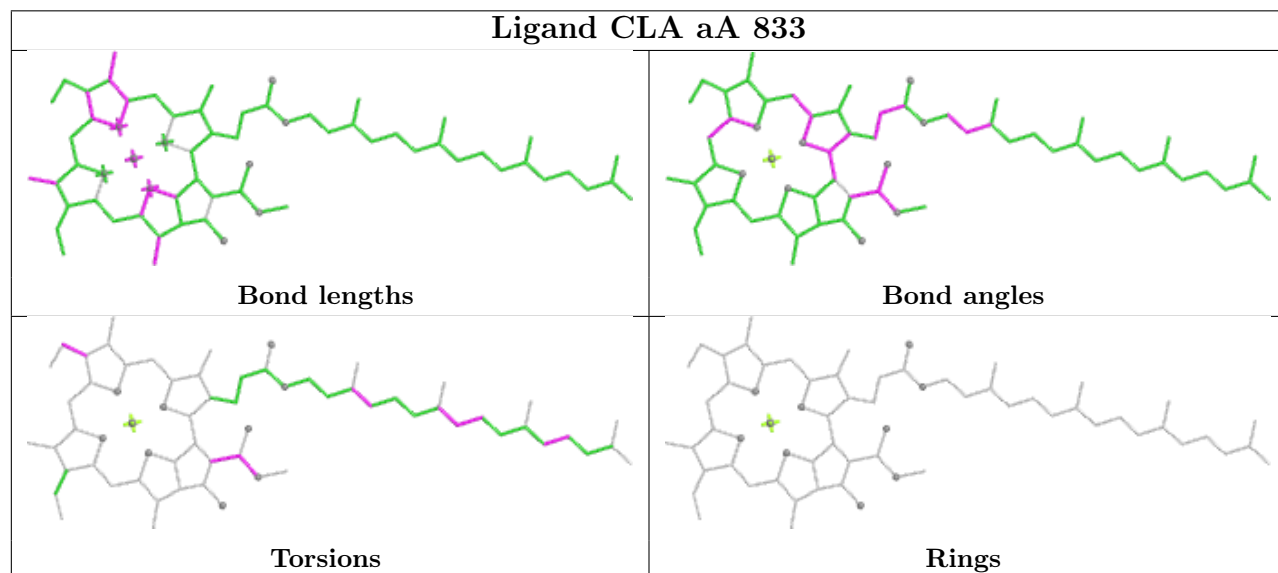
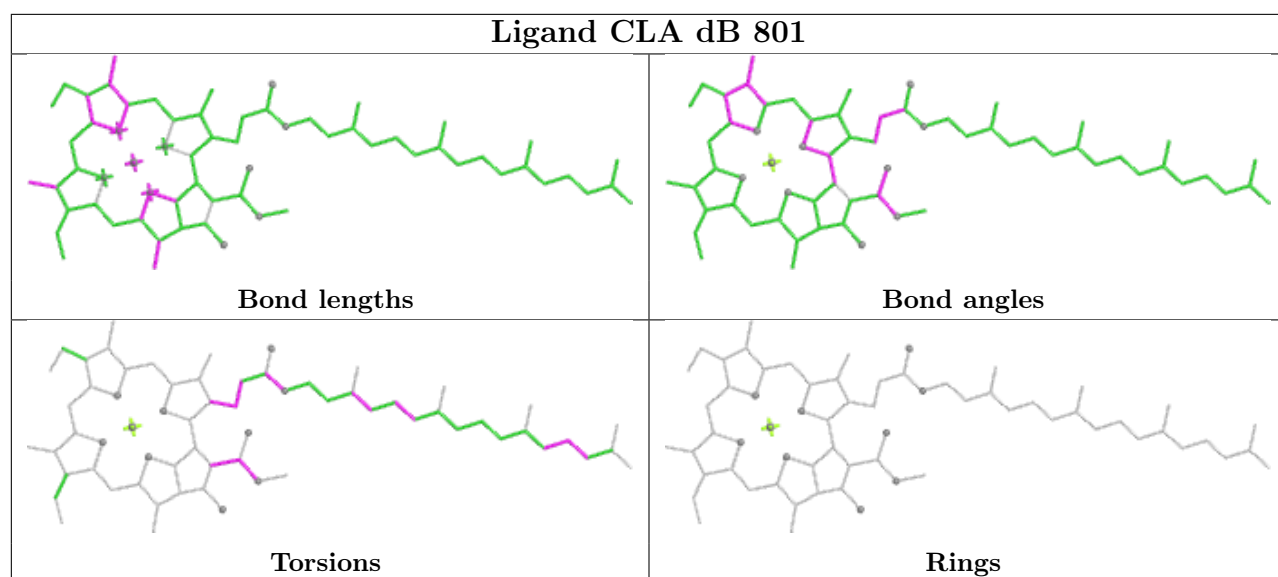


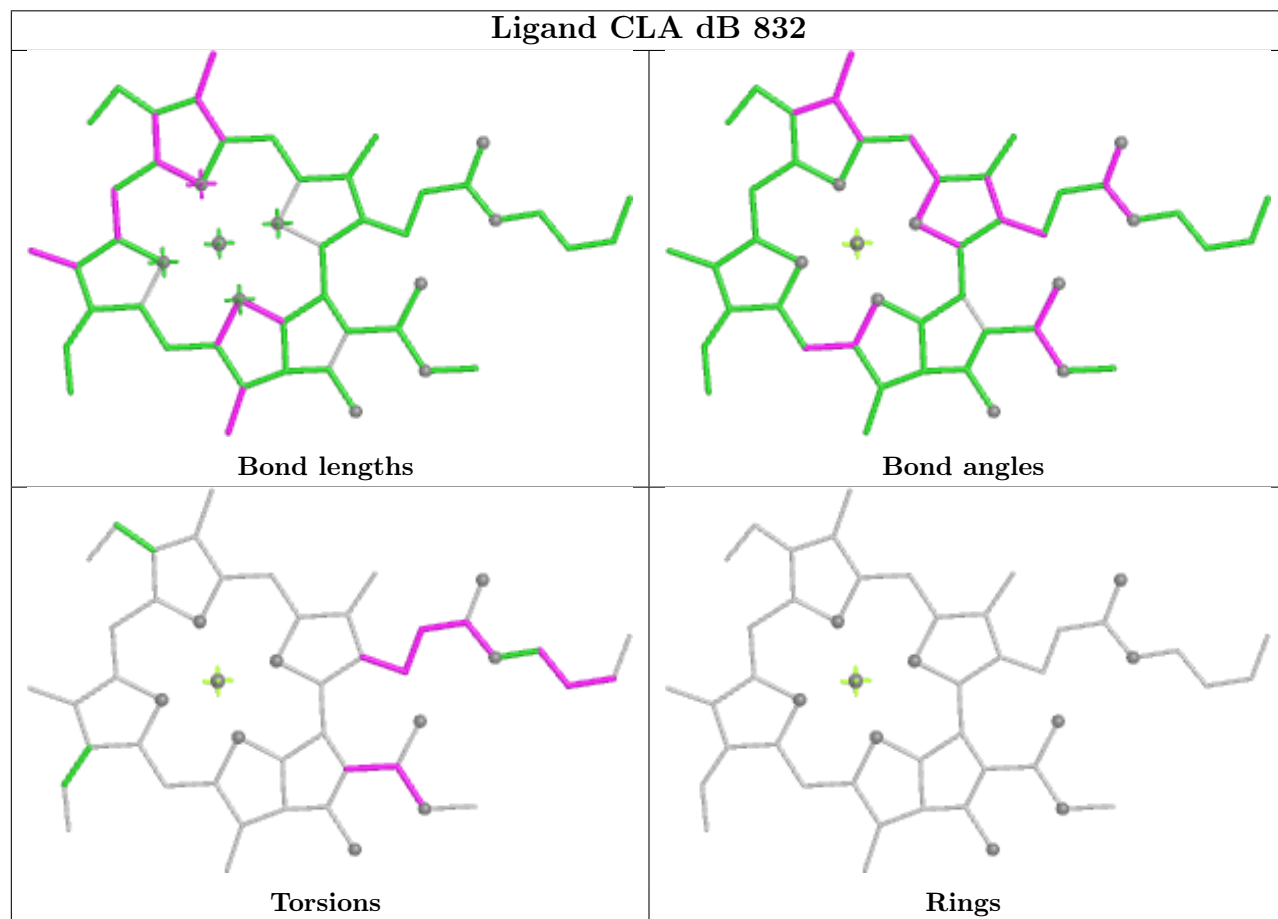
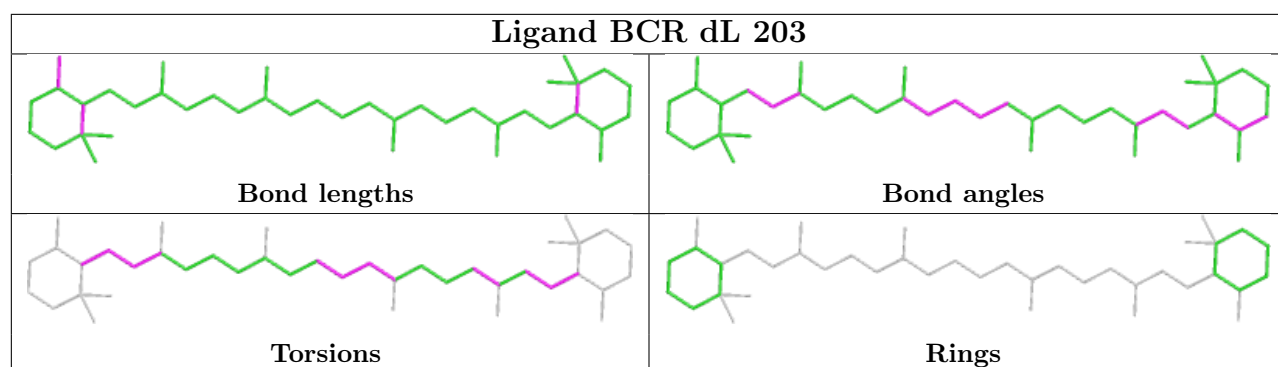


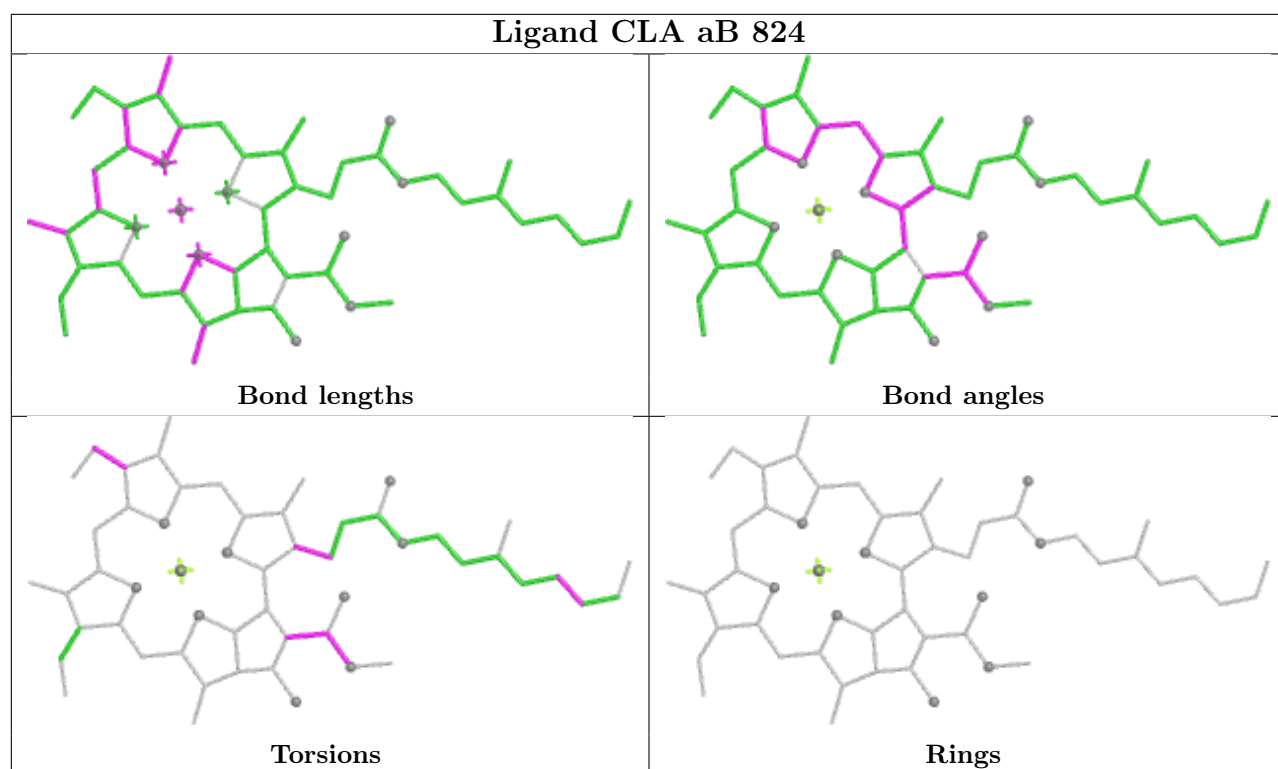




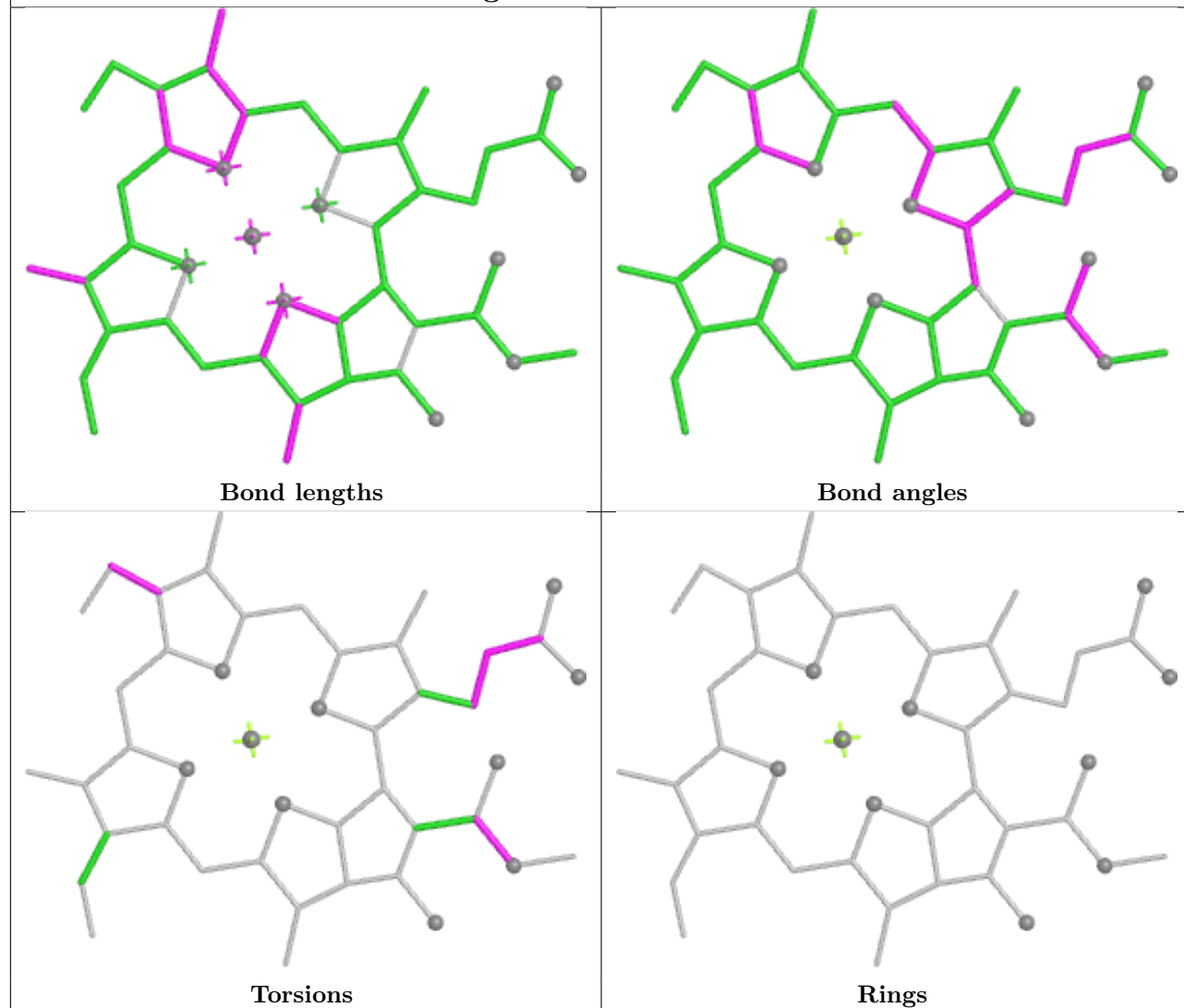




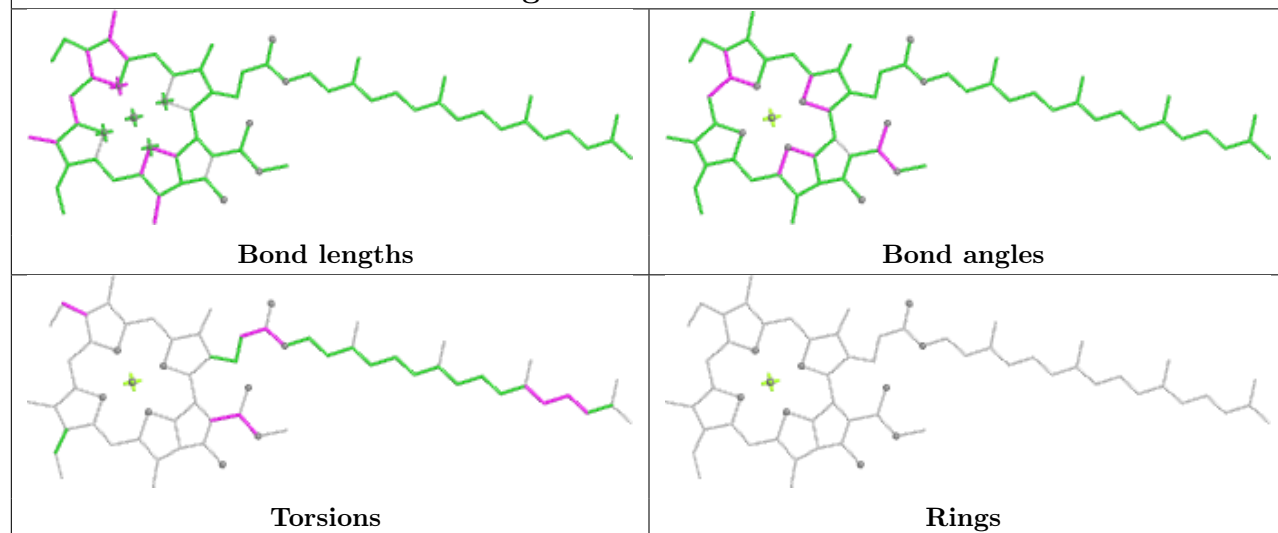


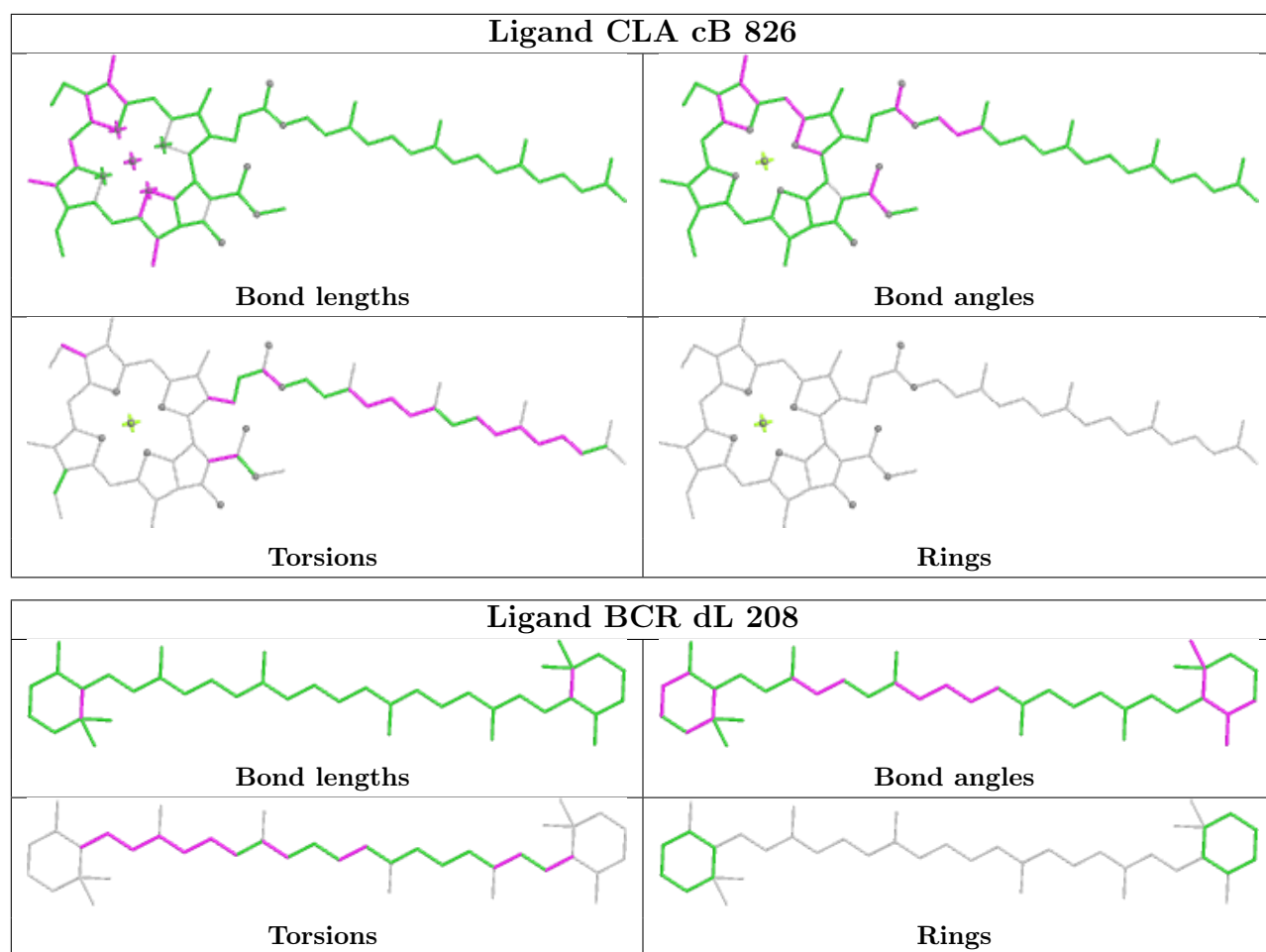


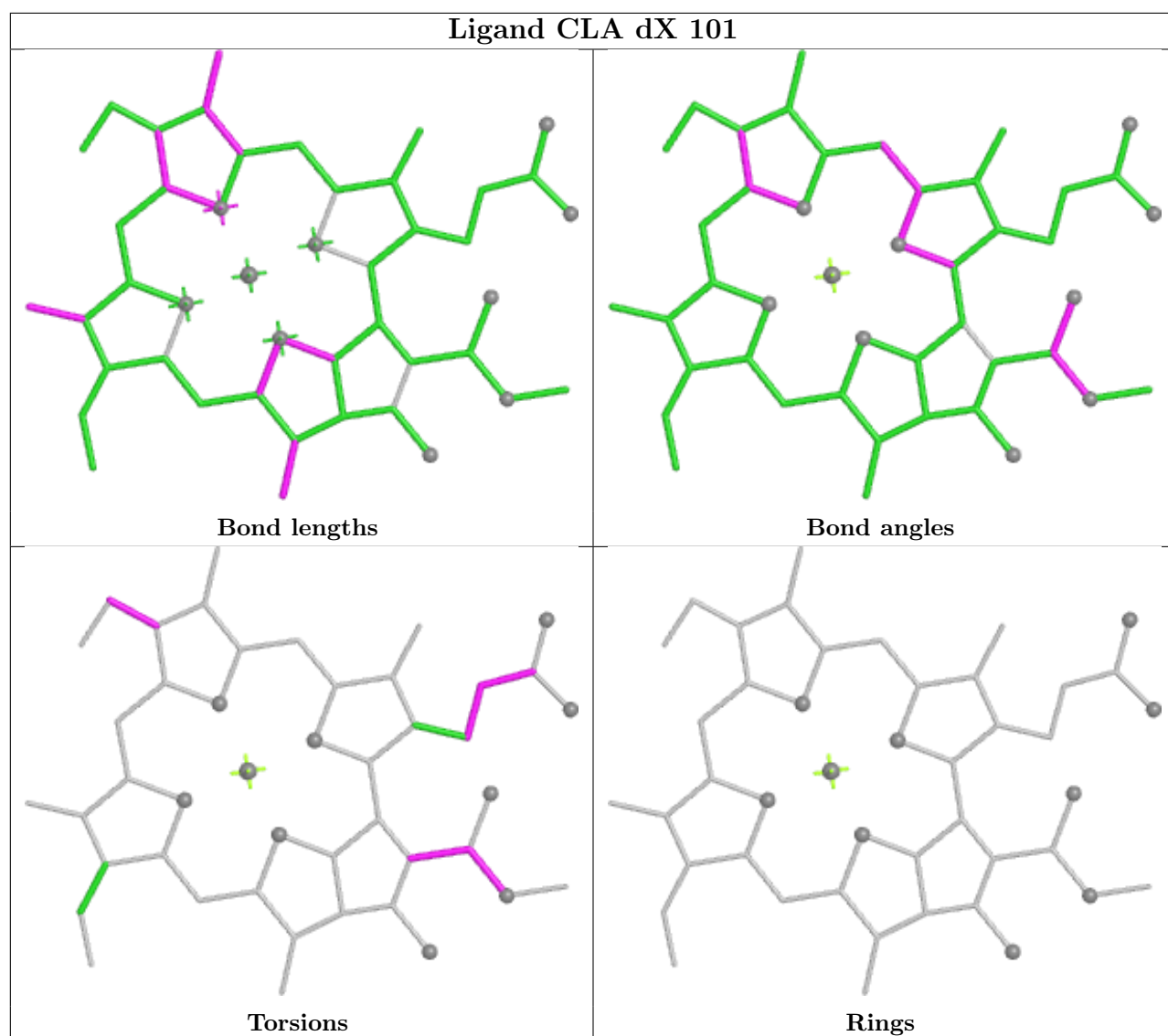
Ligand CLA dA 809



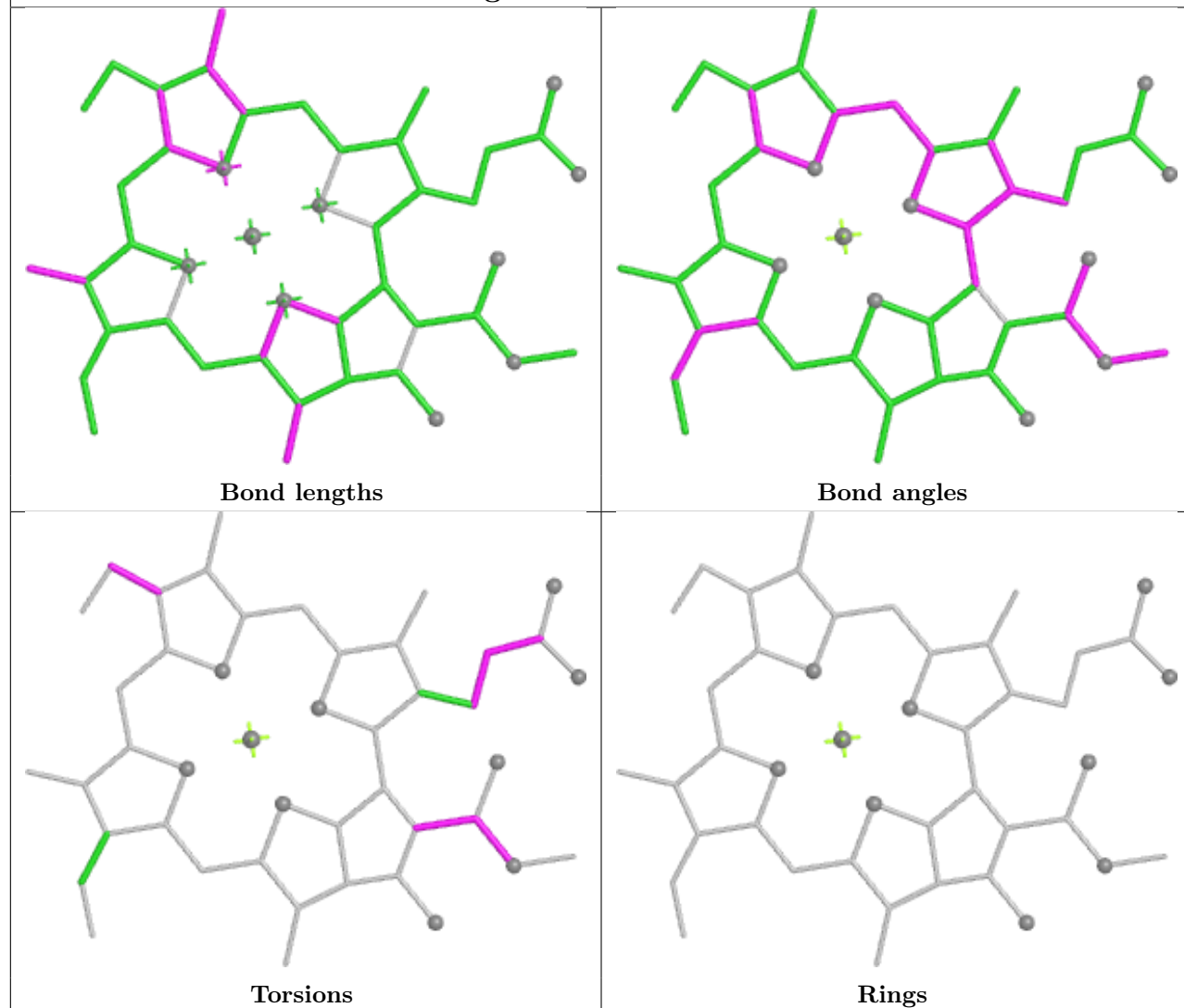
Ligand CLA dB 802



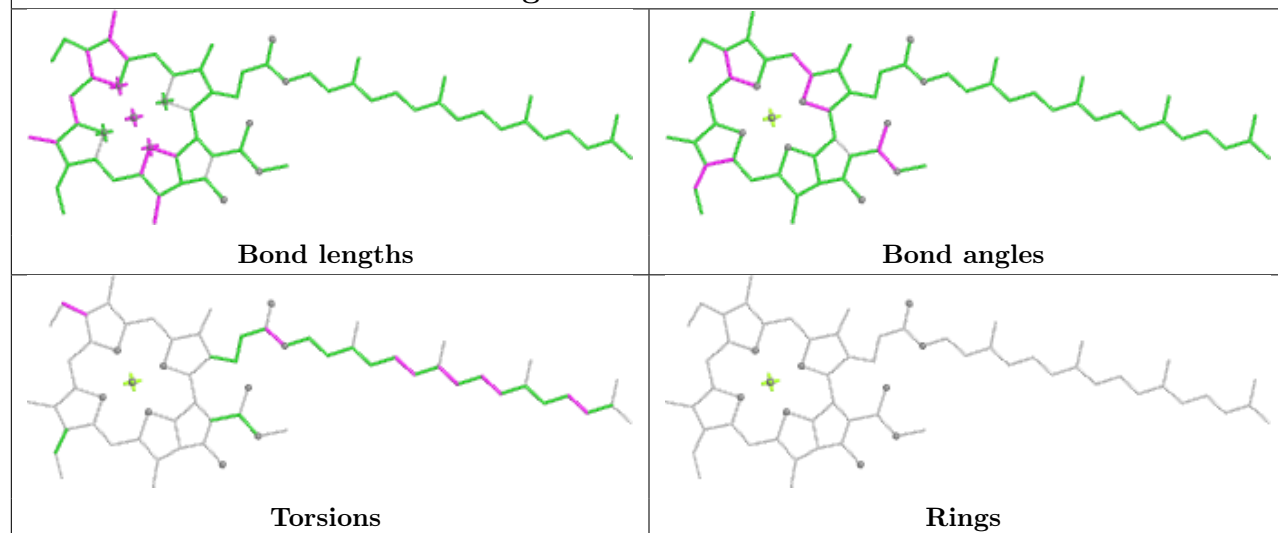


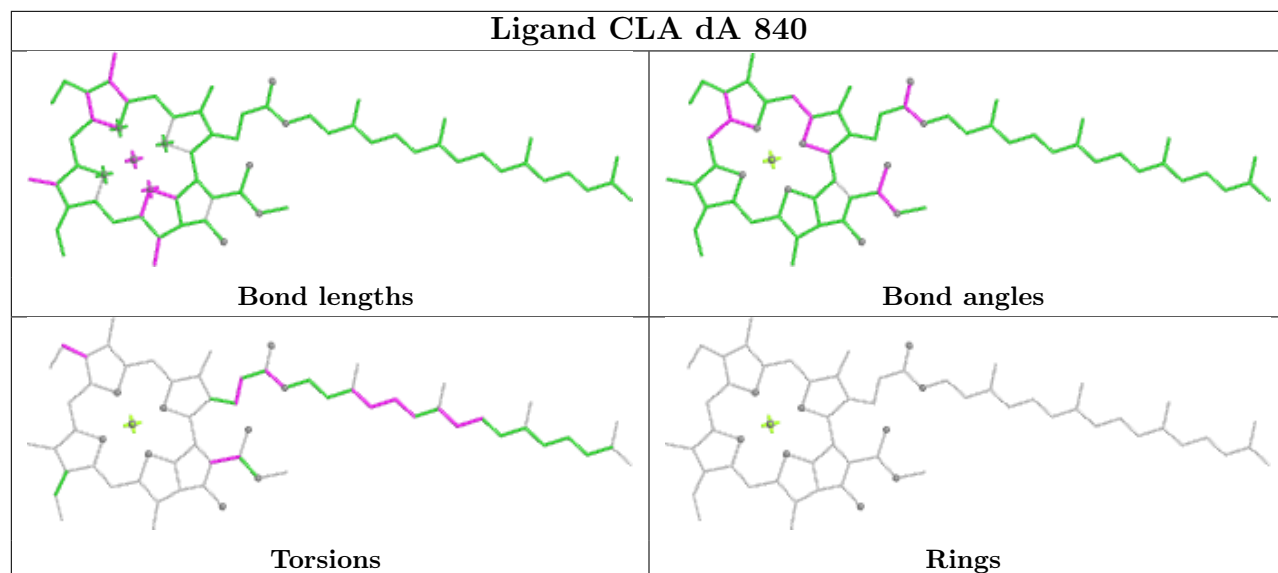
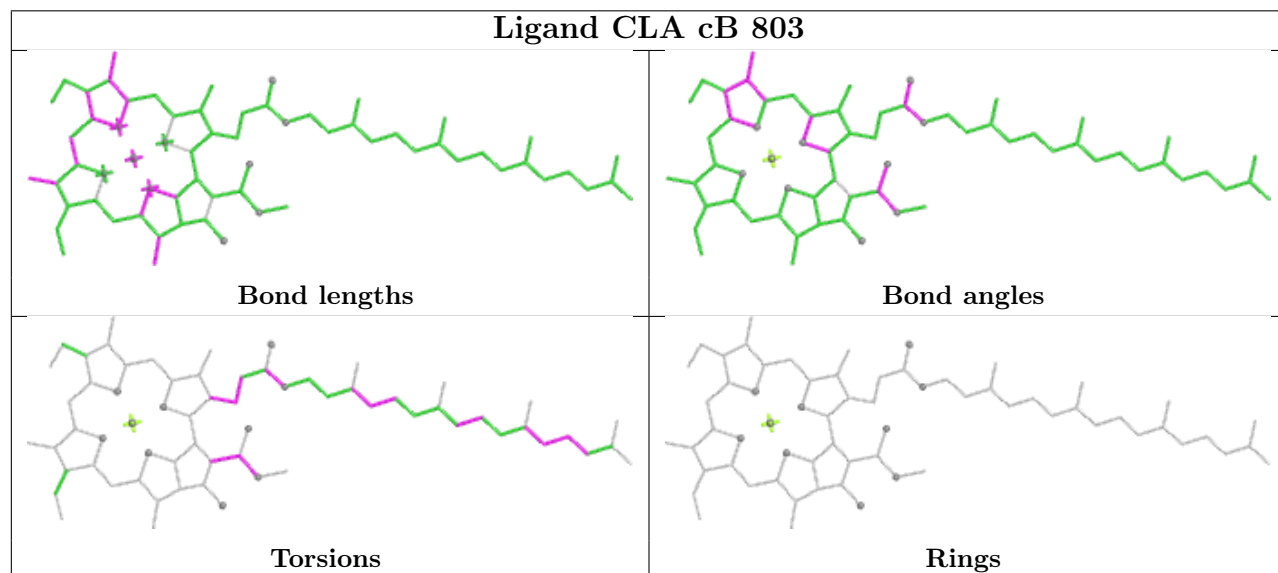
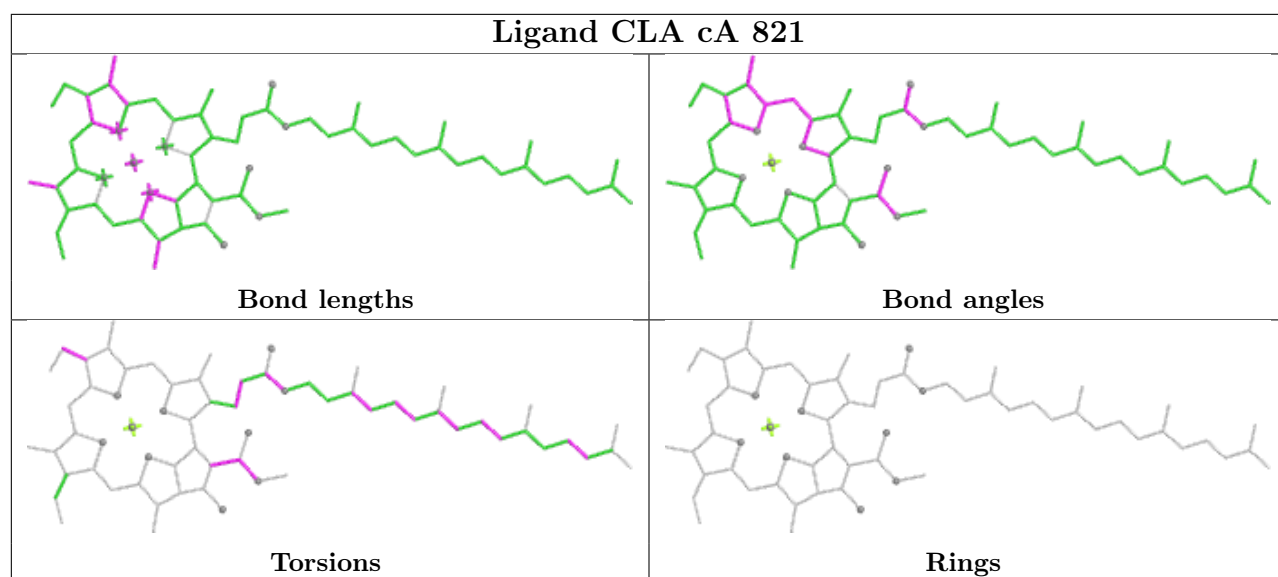


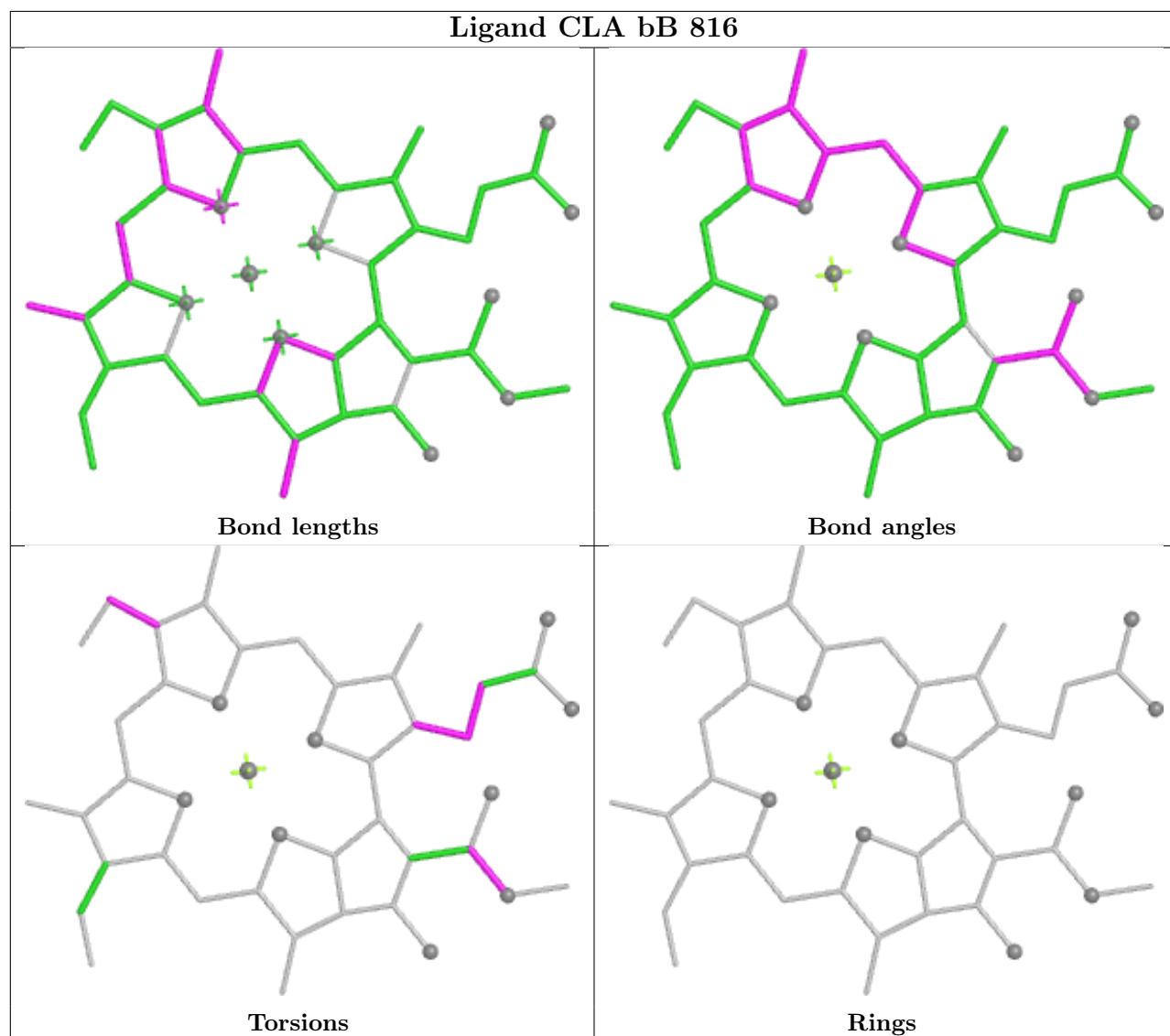
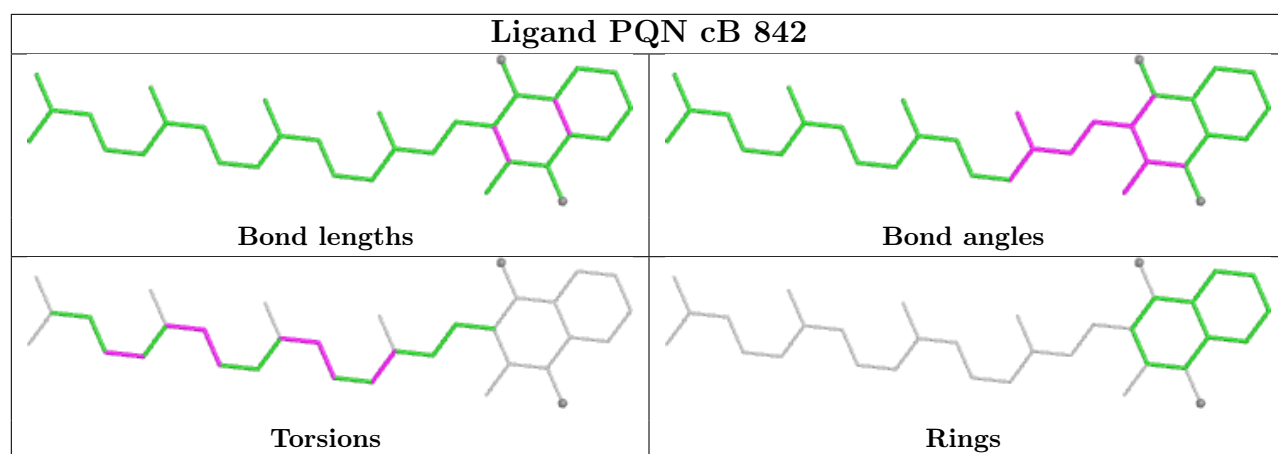
Ligand CLA aA 813



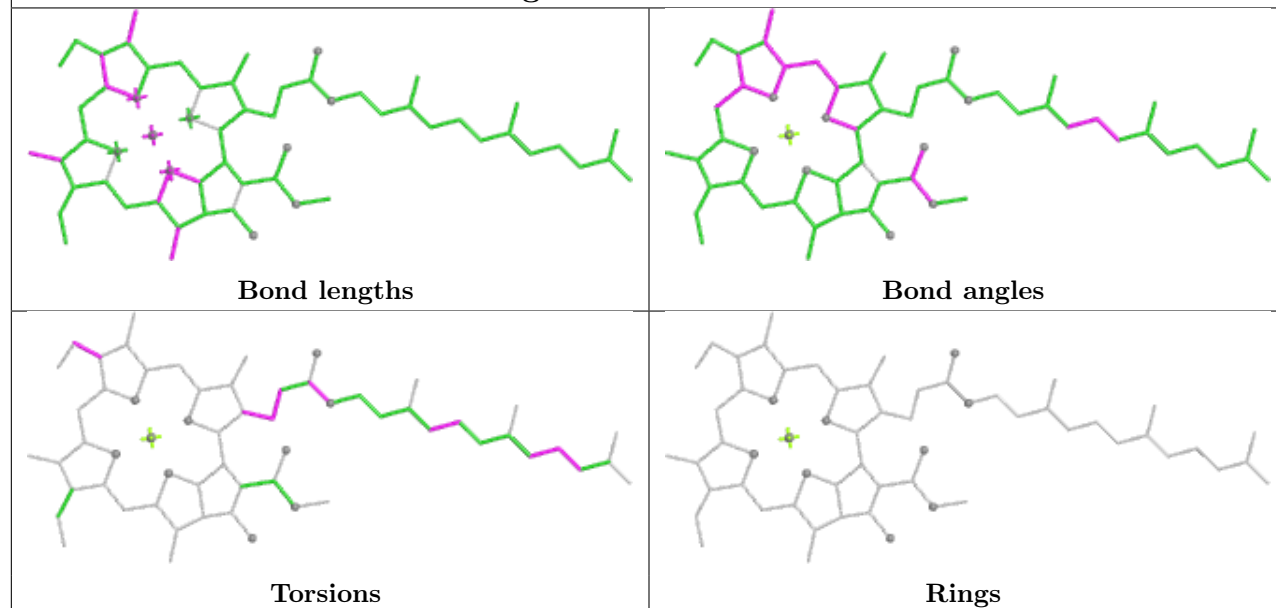
Ligand CLA bB 811



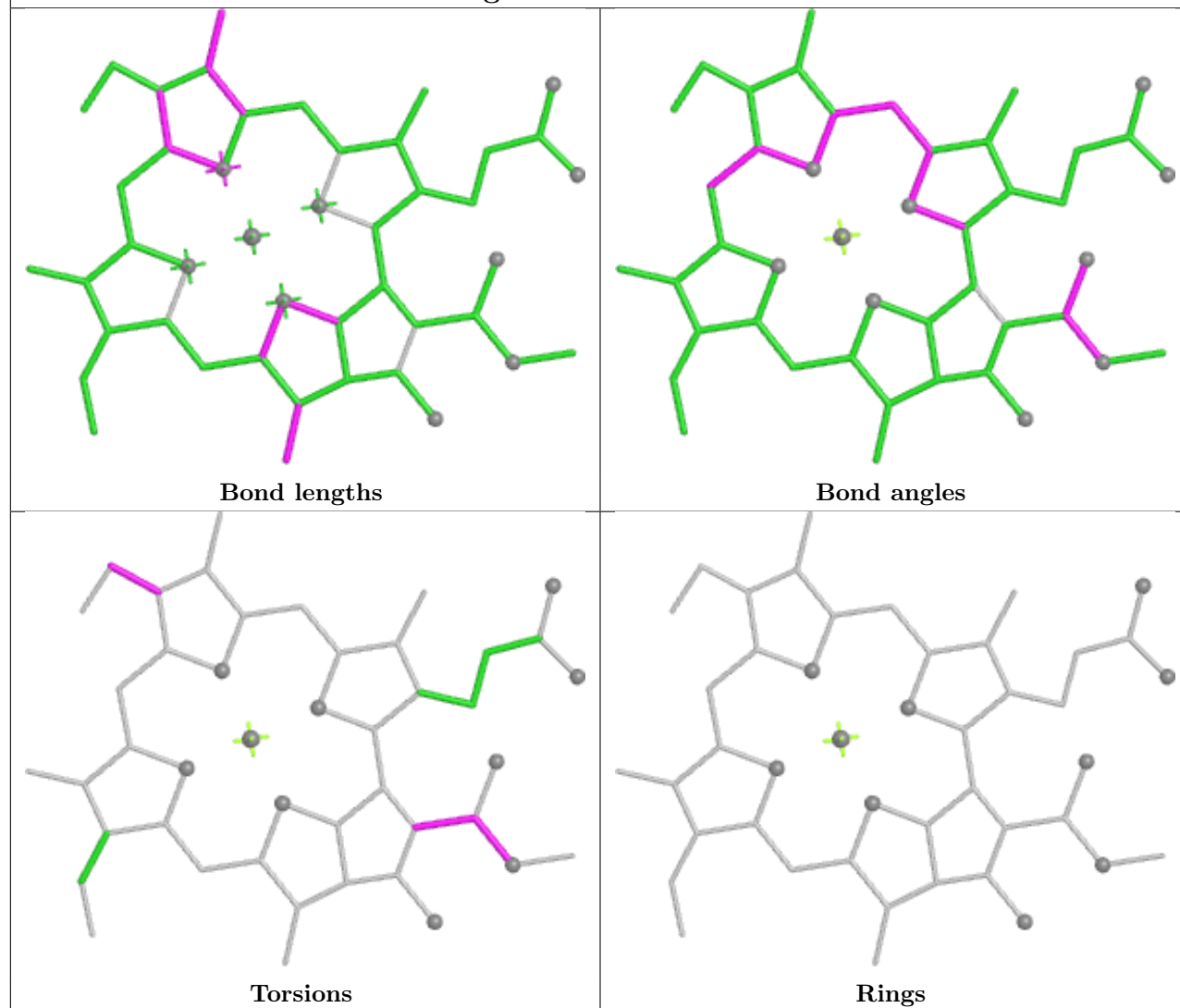


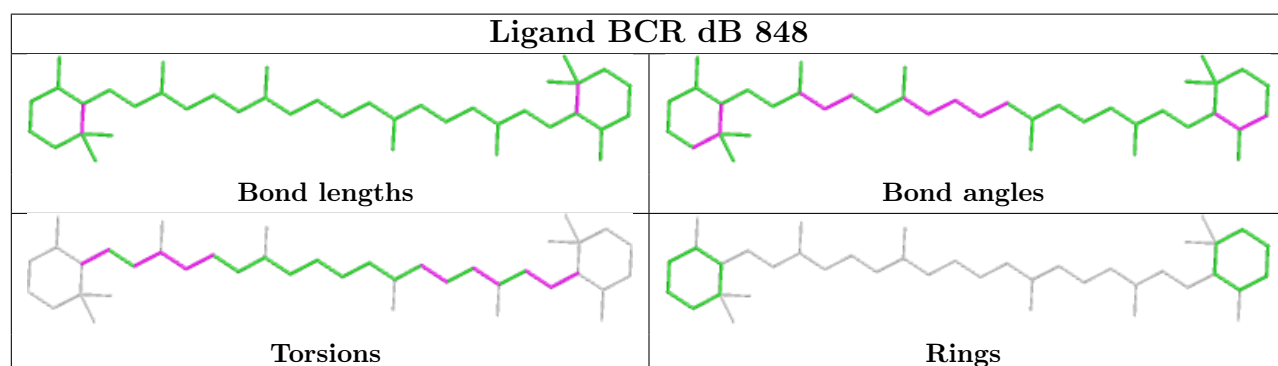
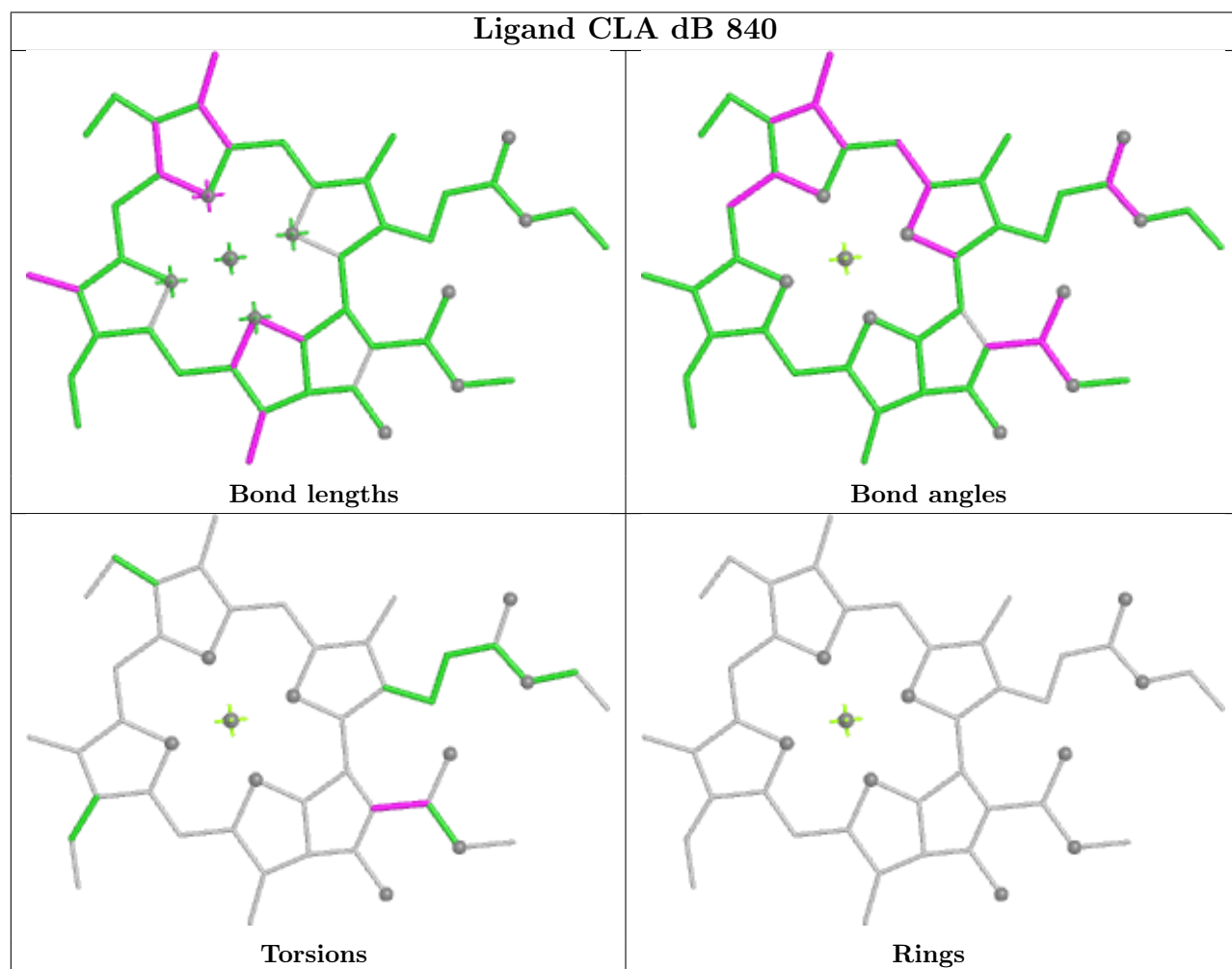
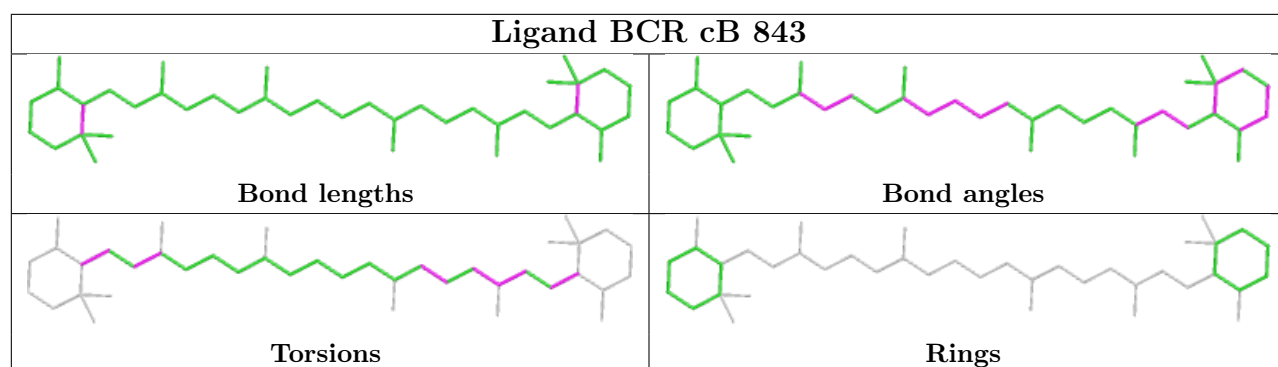


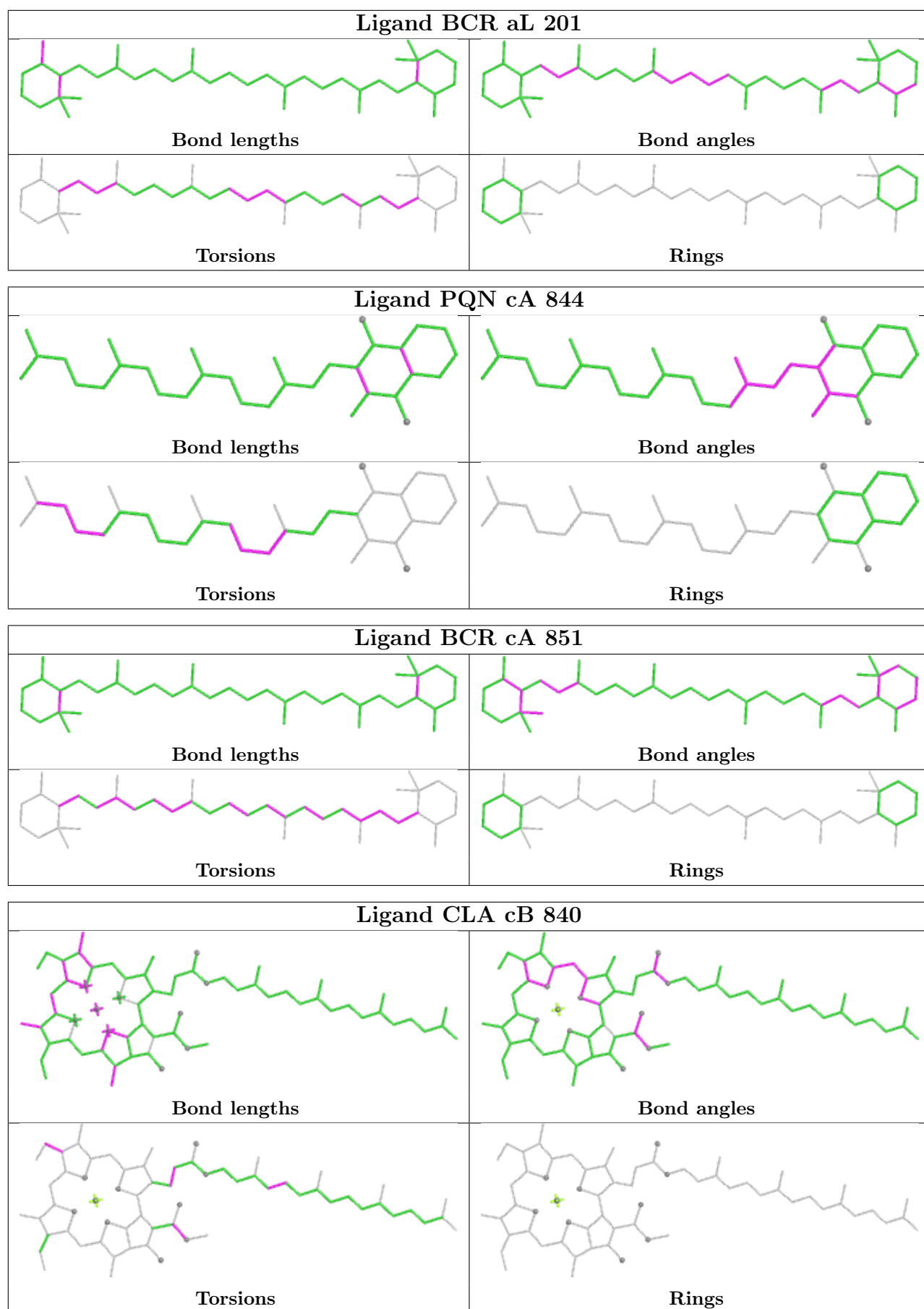
Ligand CLA dB 819

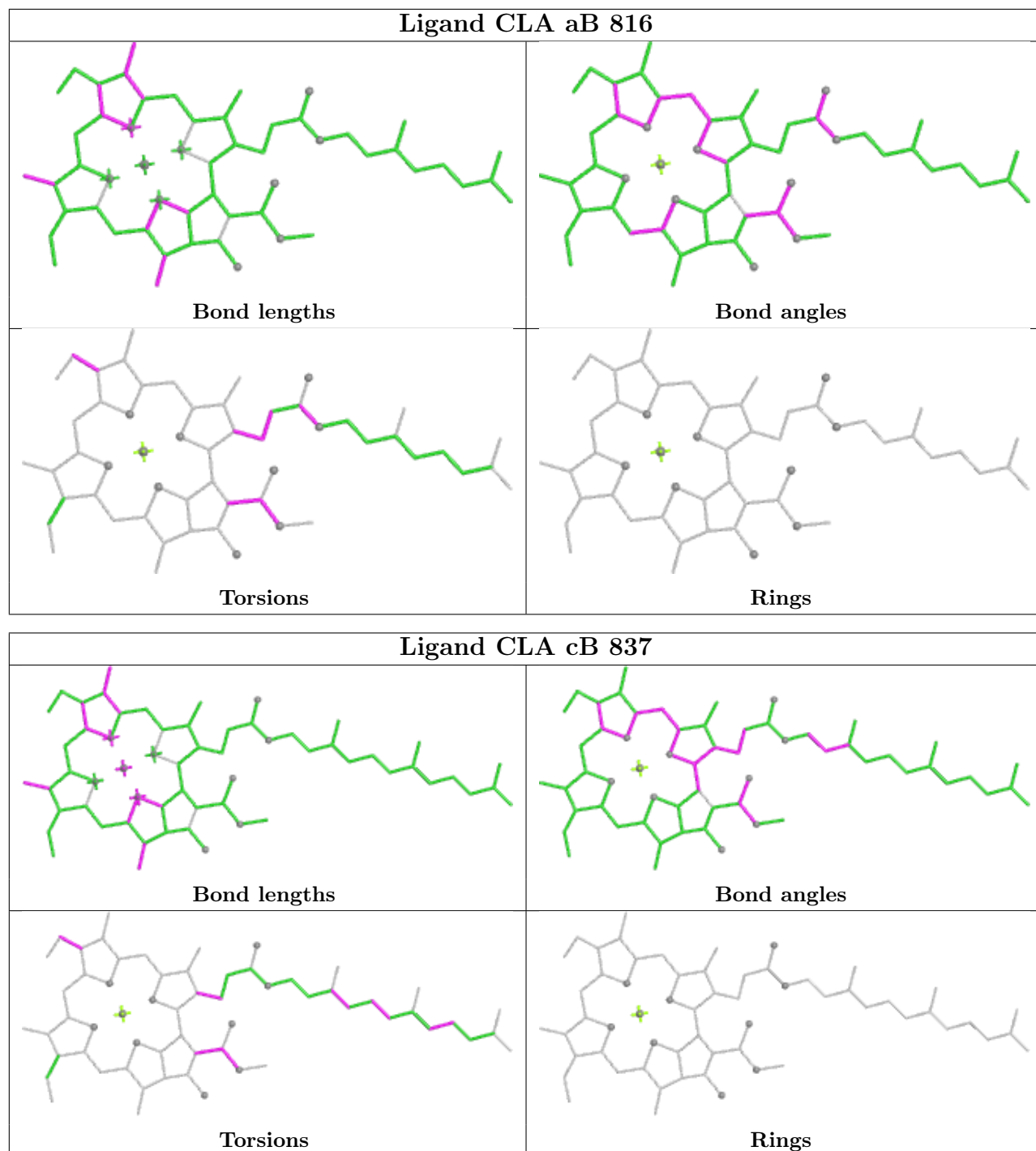


Ligand CLA aA 815

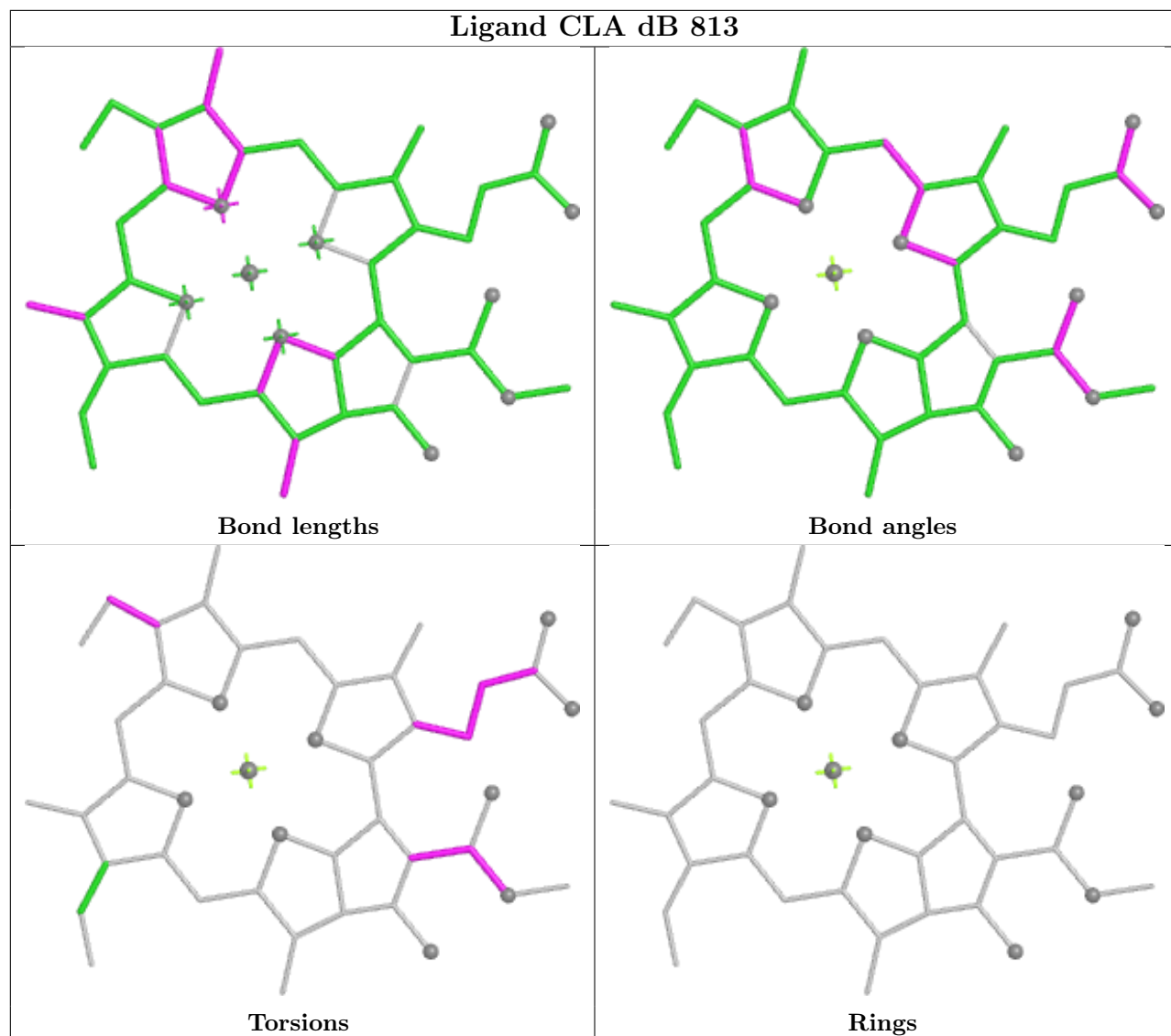




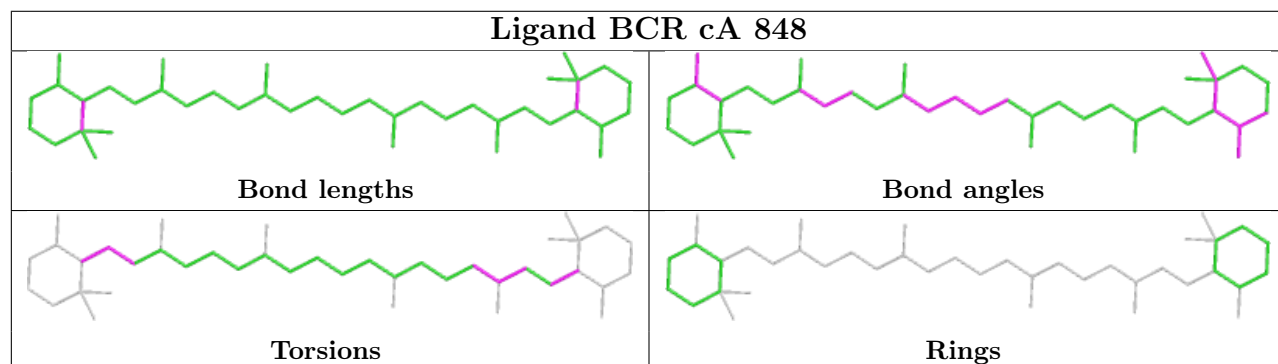


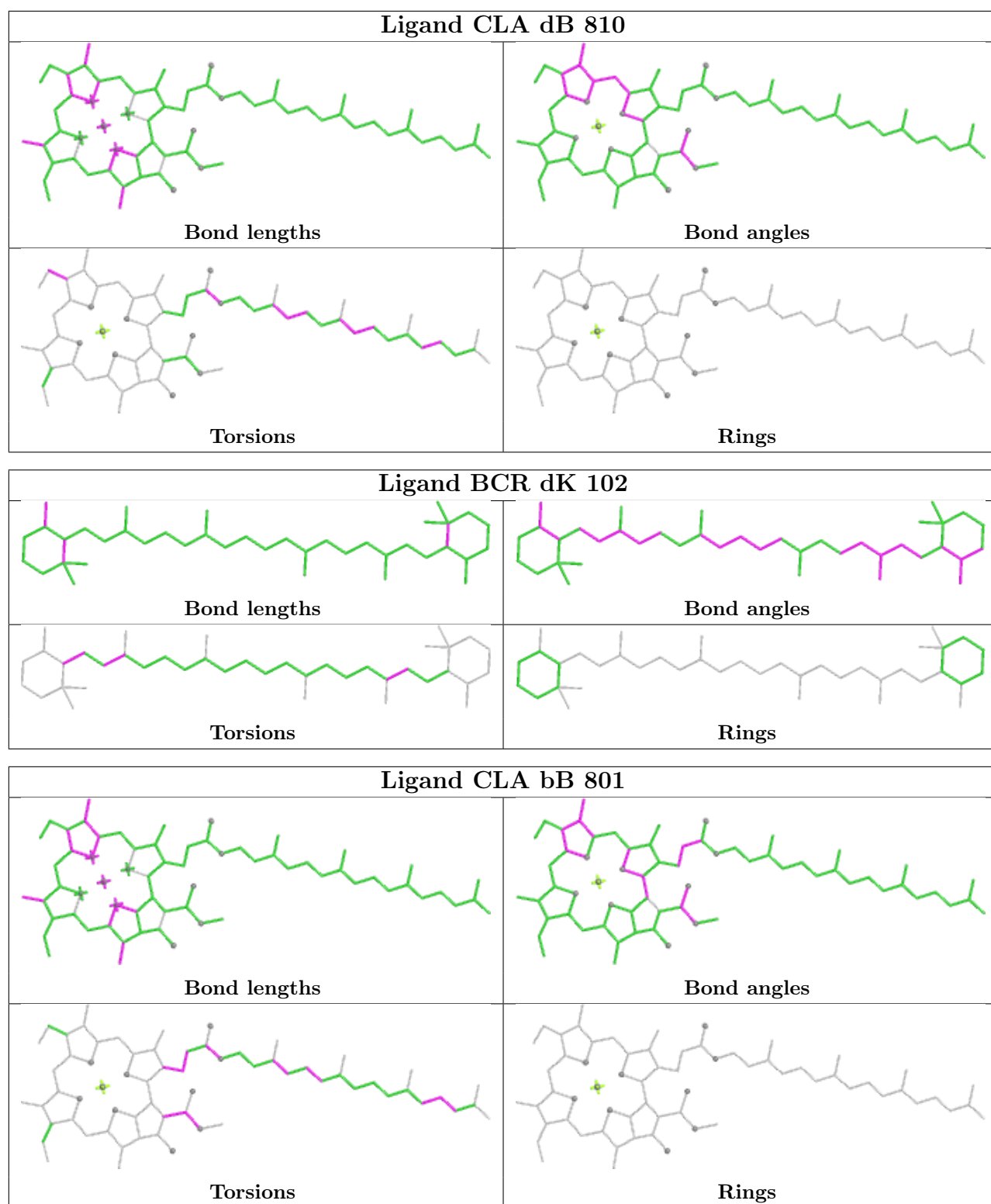


Ligand CLA dB 813

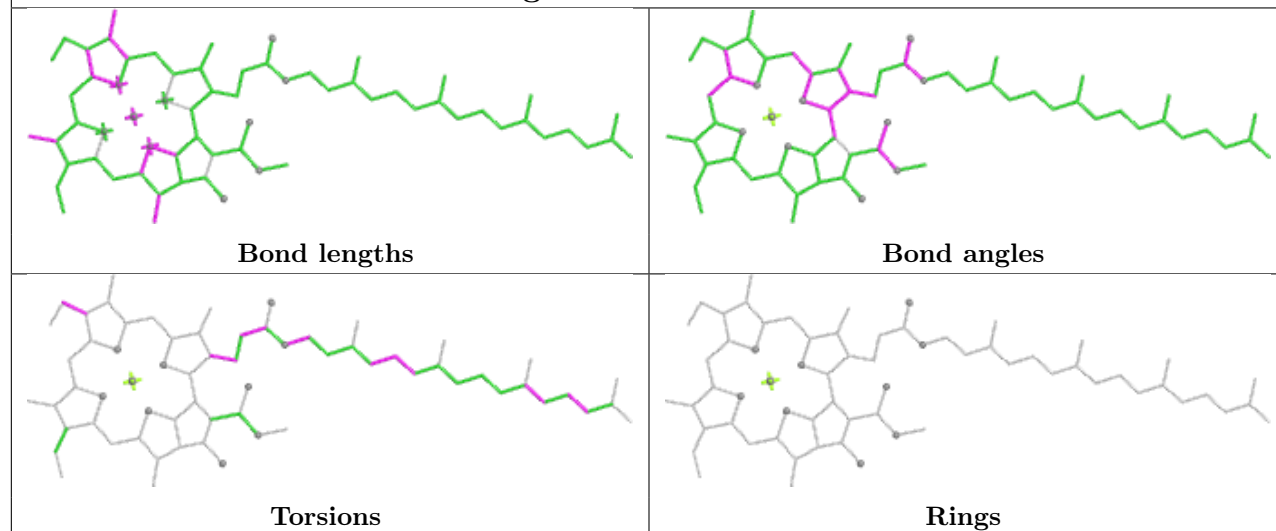


Ligand BCR cA 848

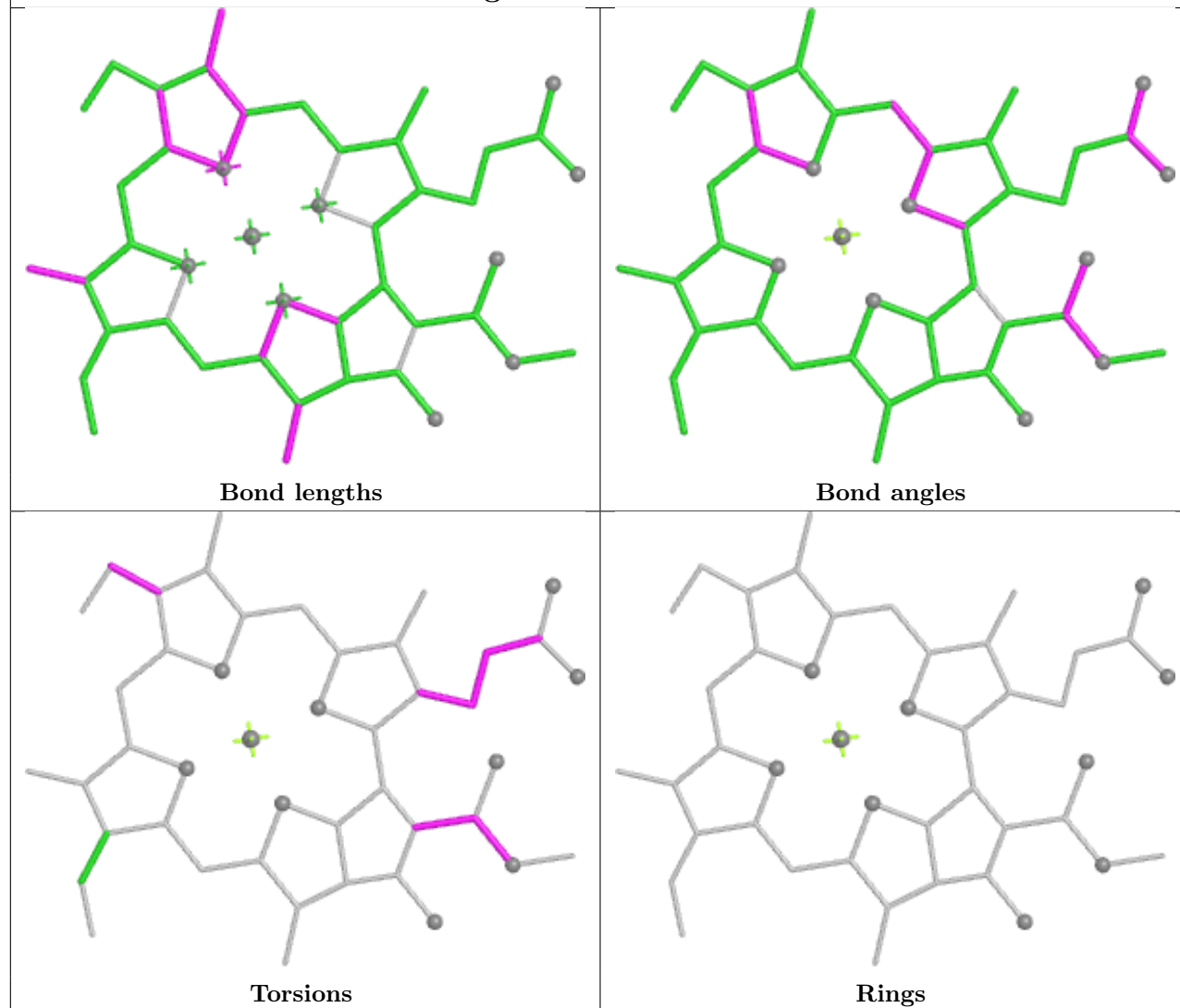


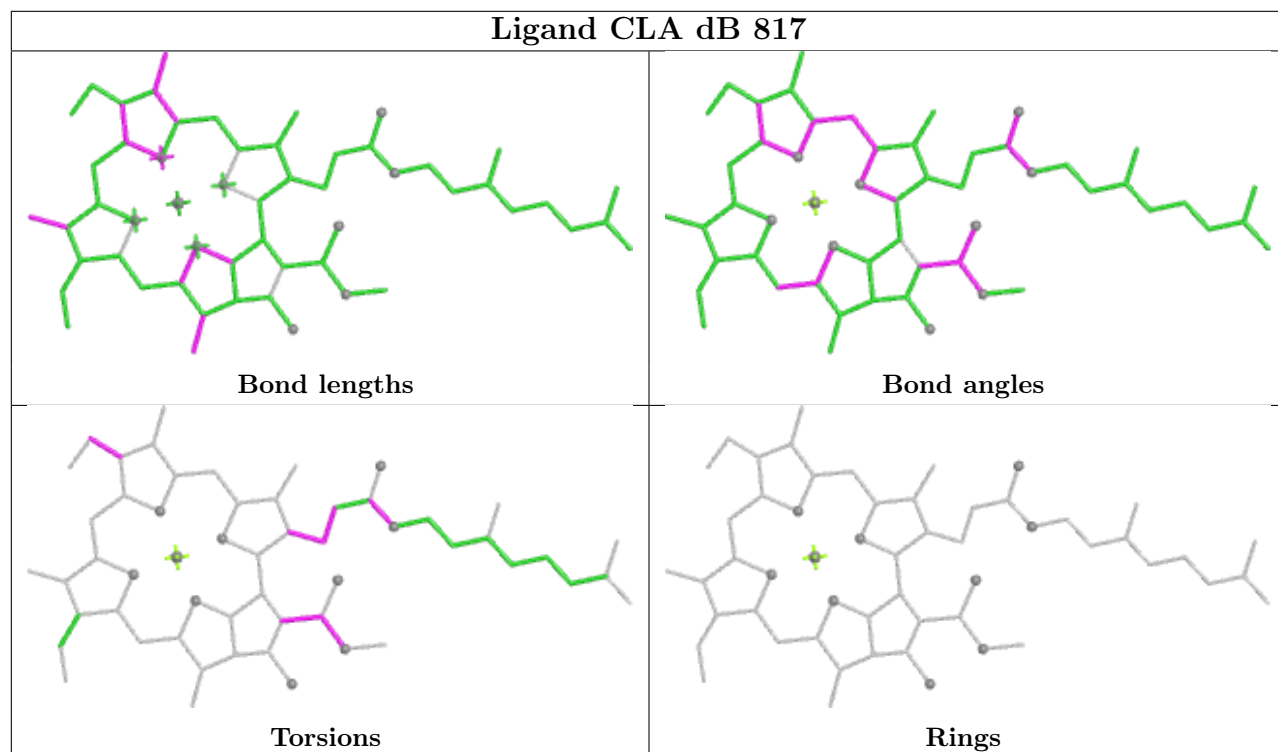
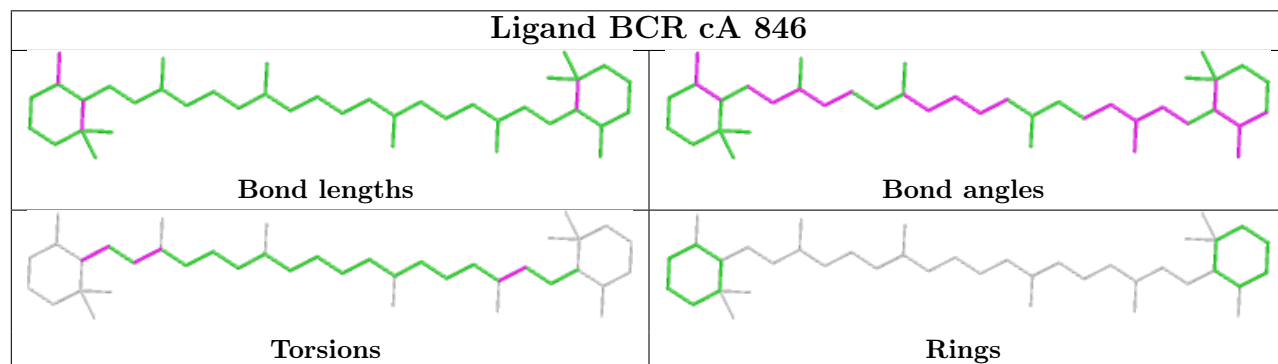
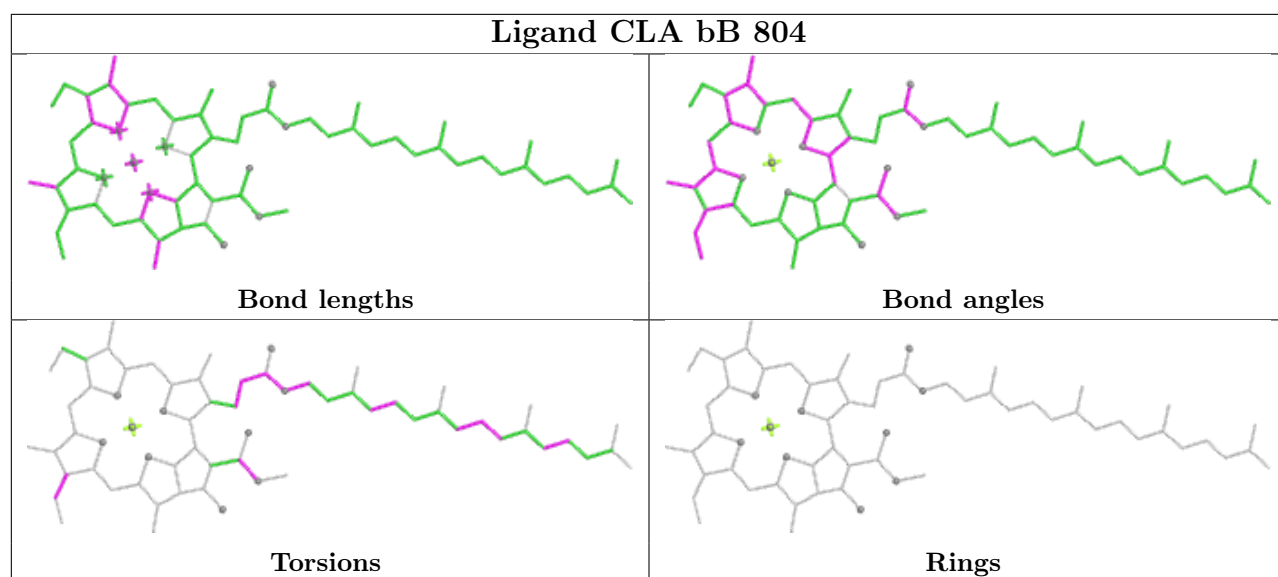


Ligand CLA aA 806

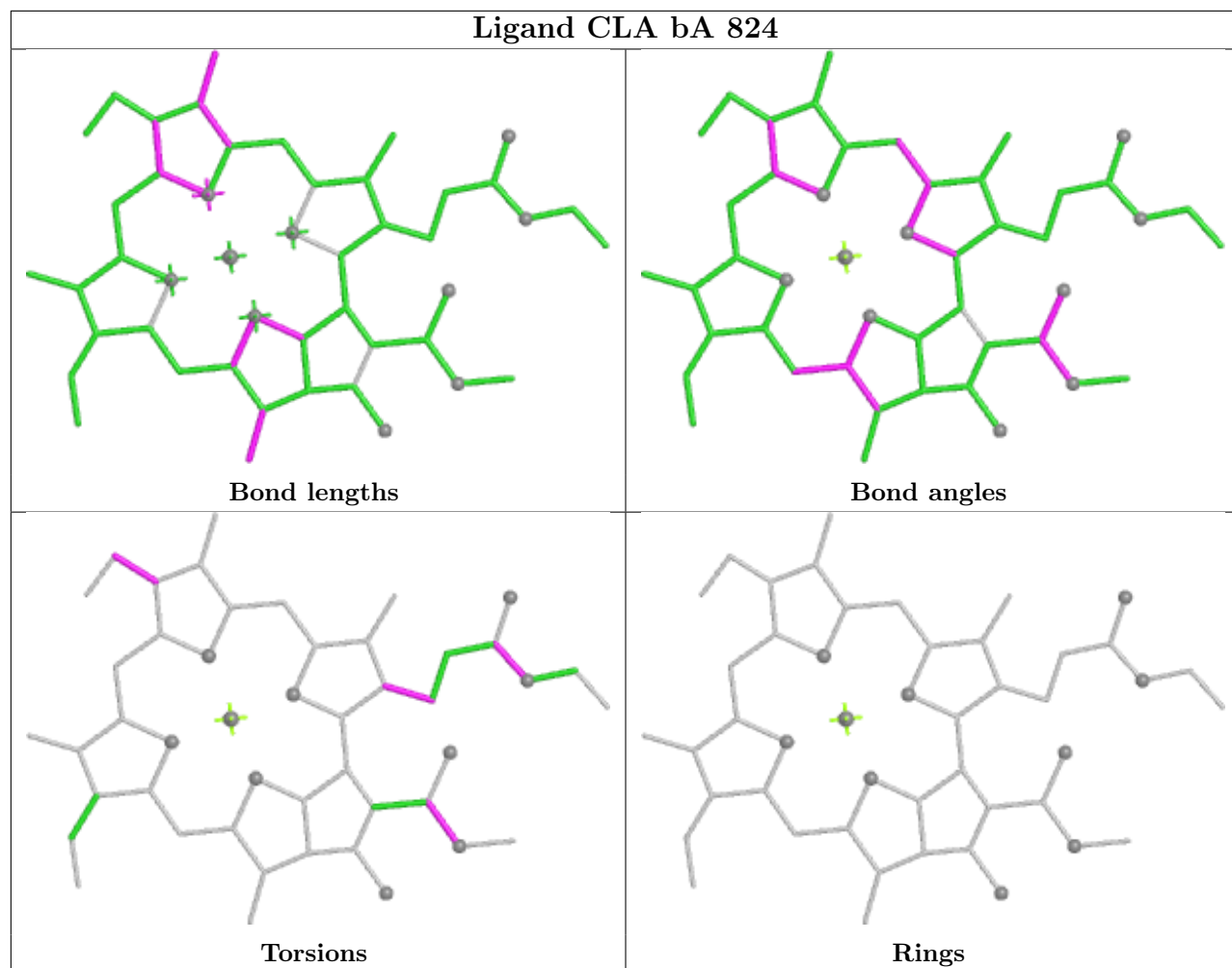


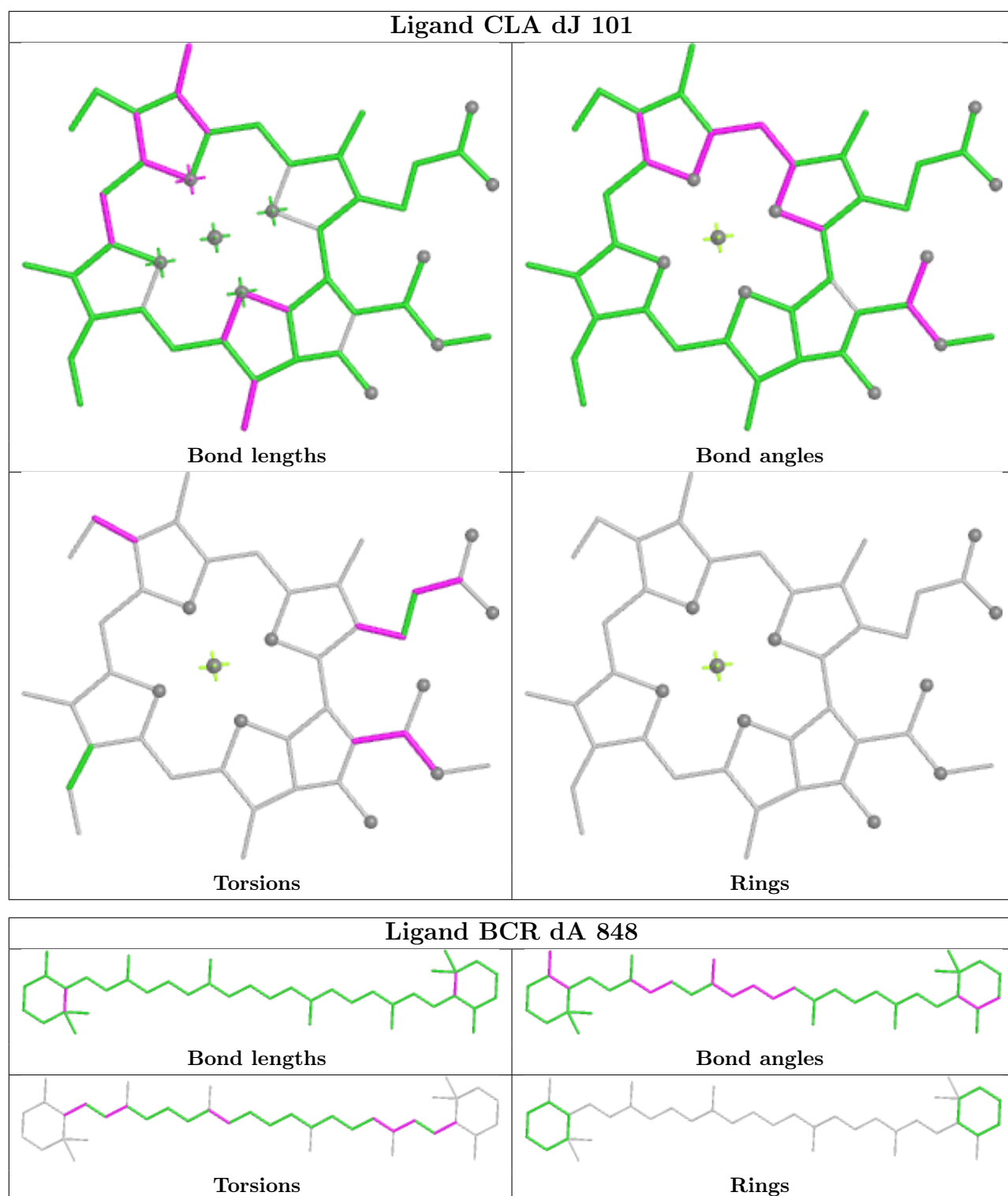
Ligand CLA aB 812

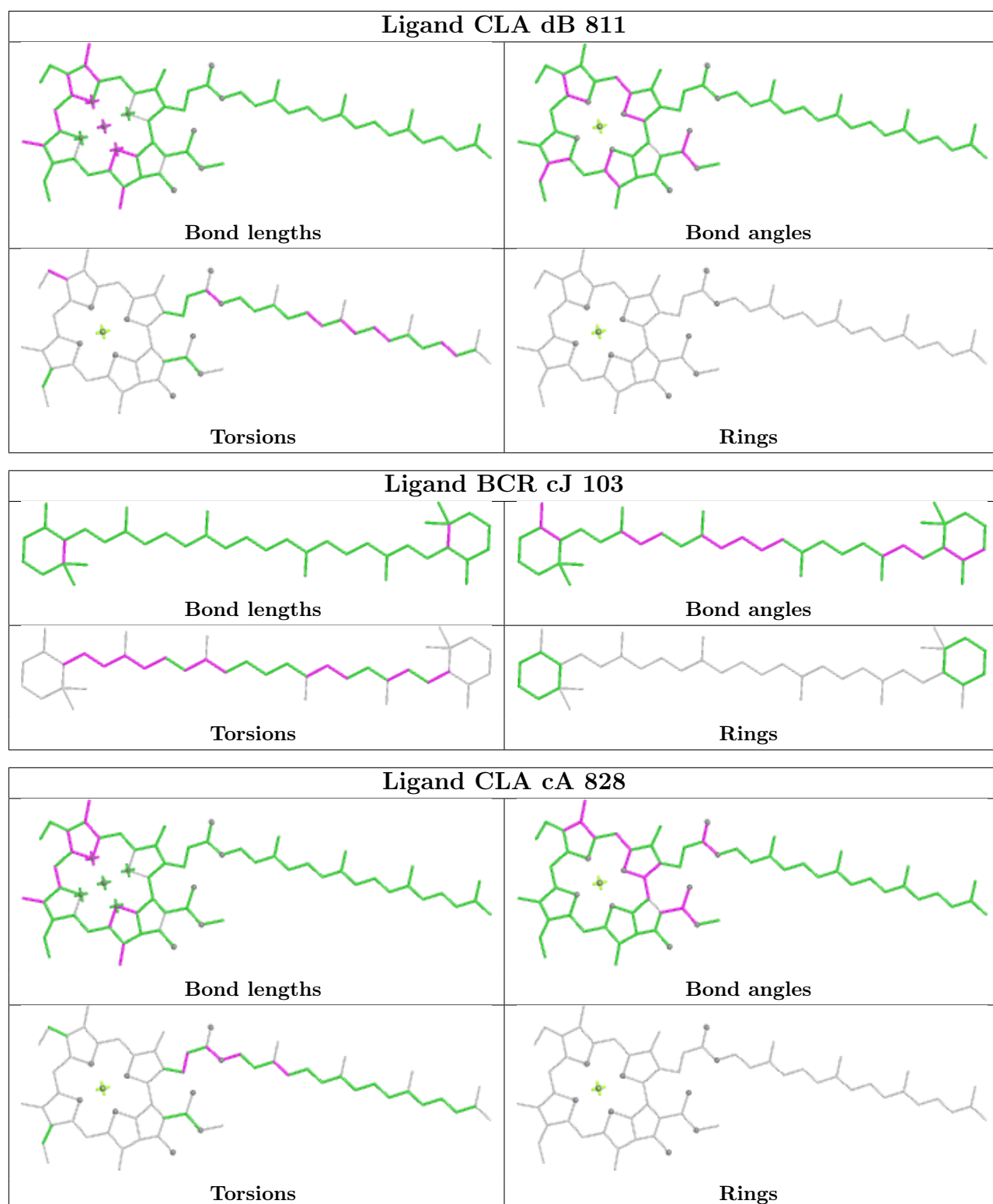


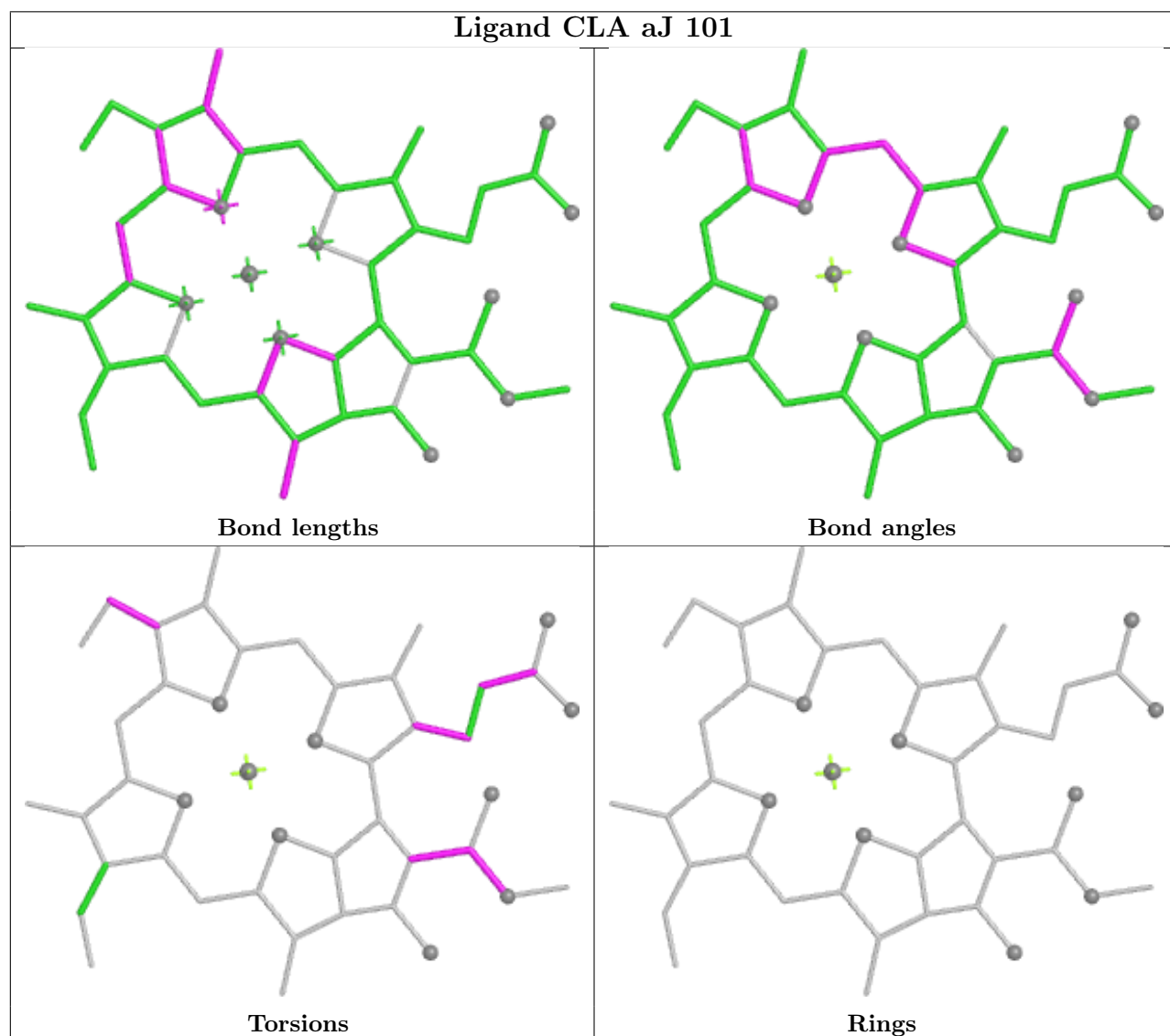
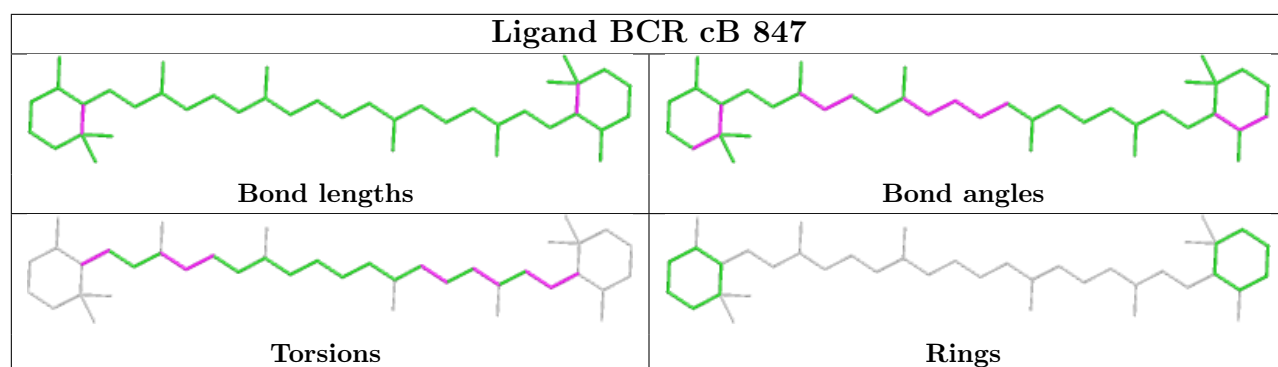


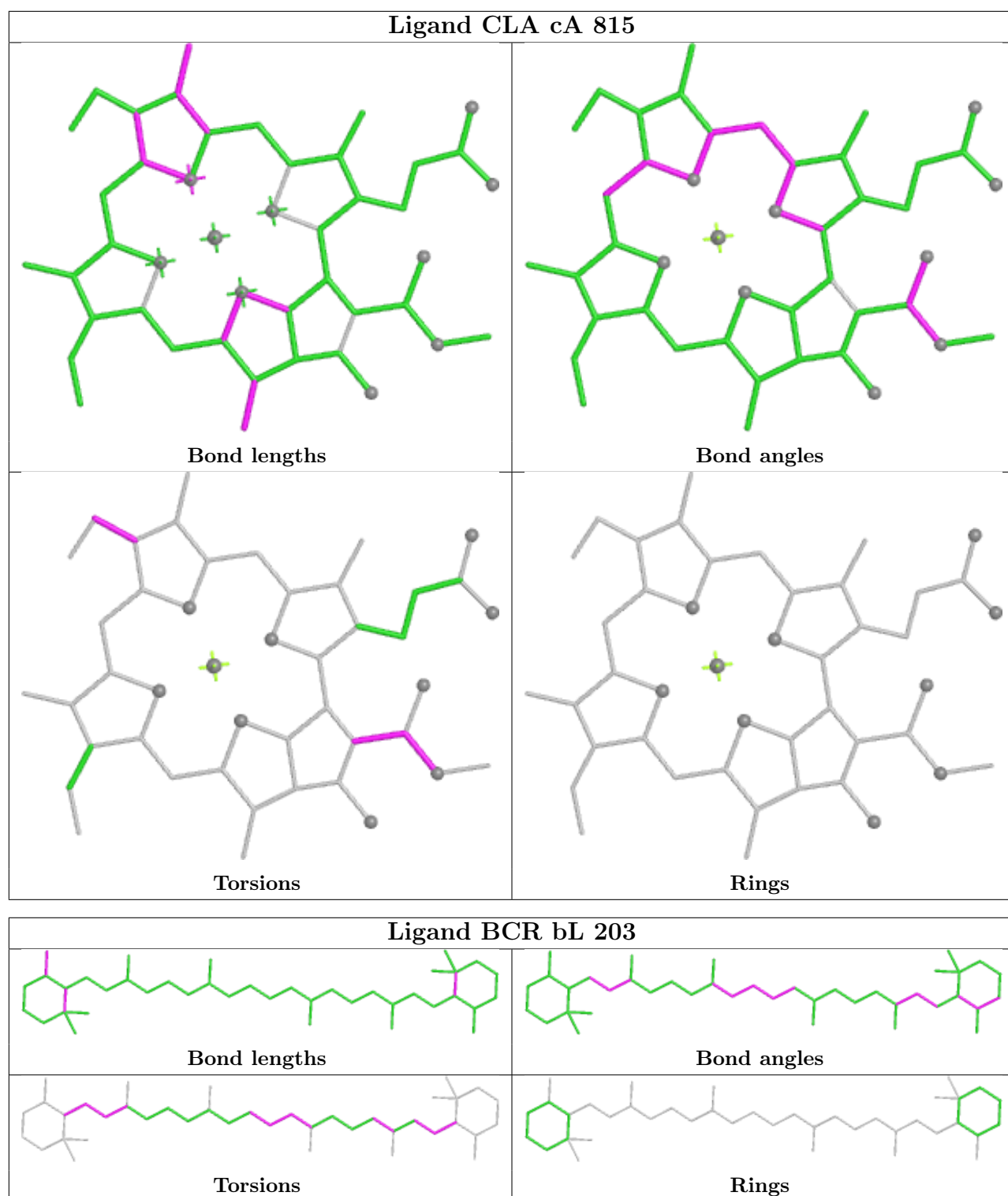
Ligand CLA bA 824

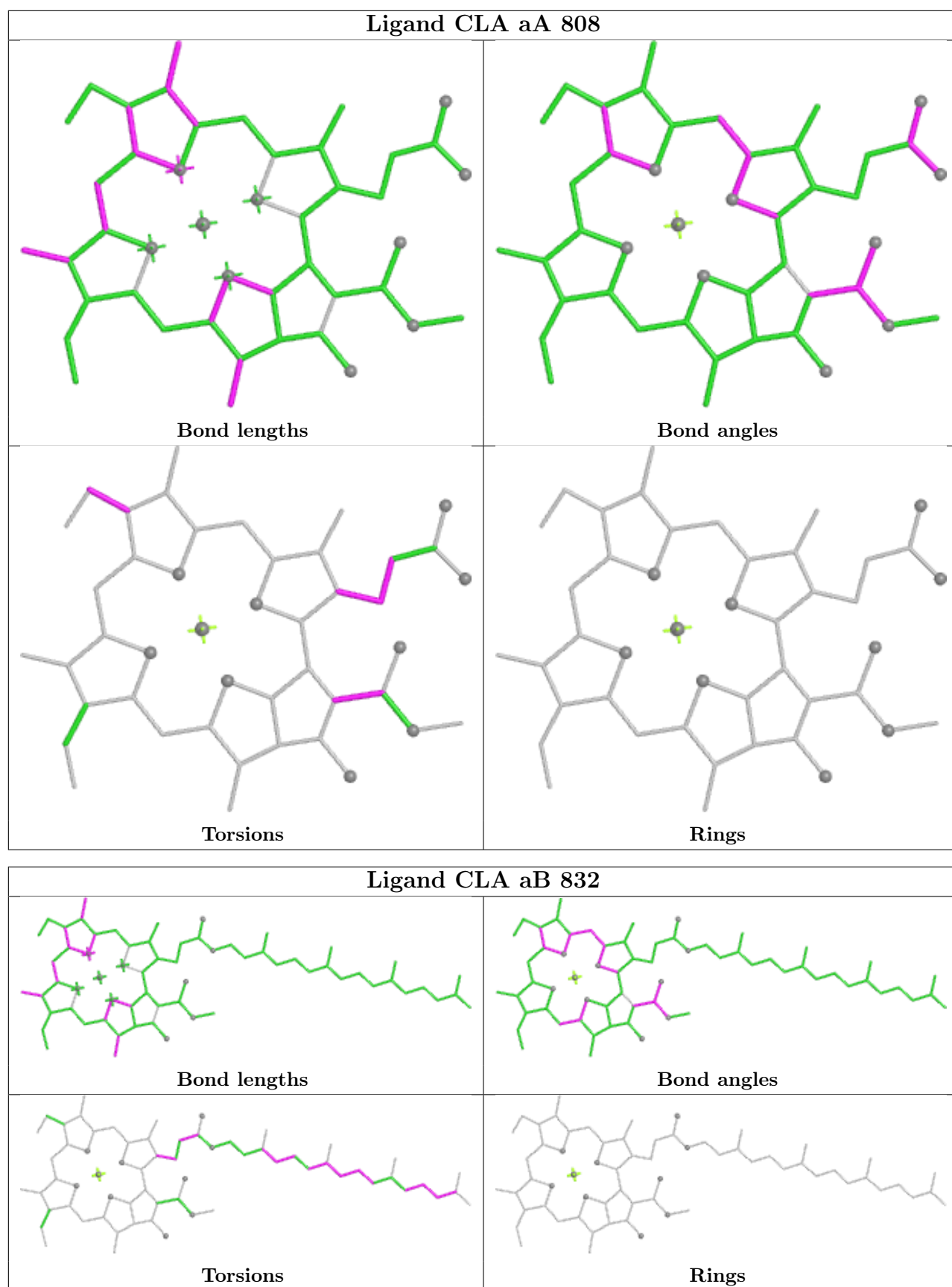


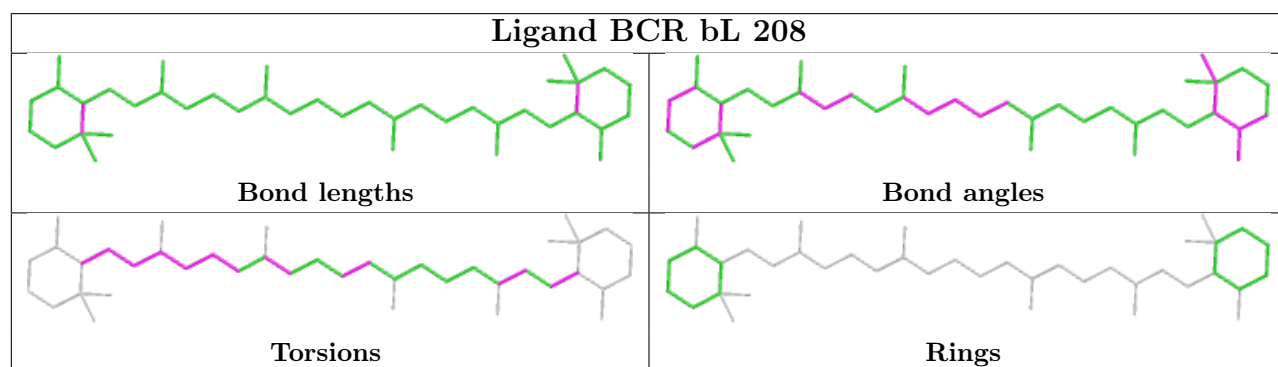
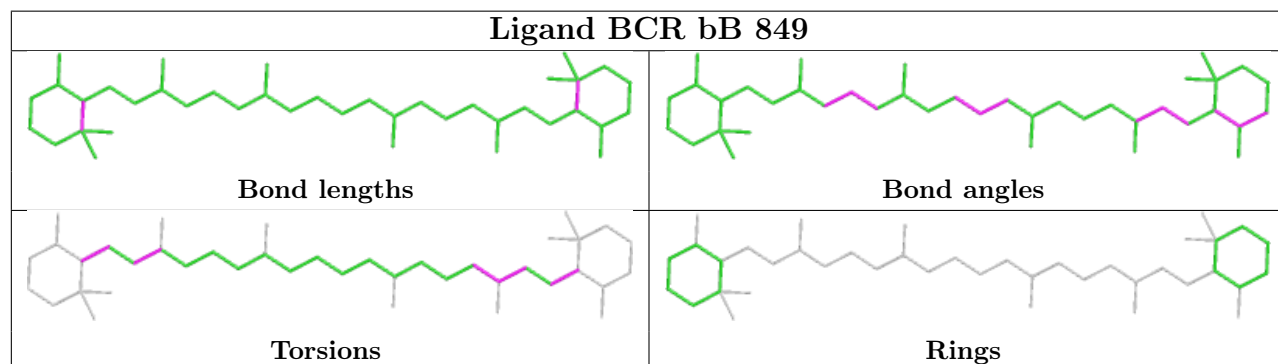
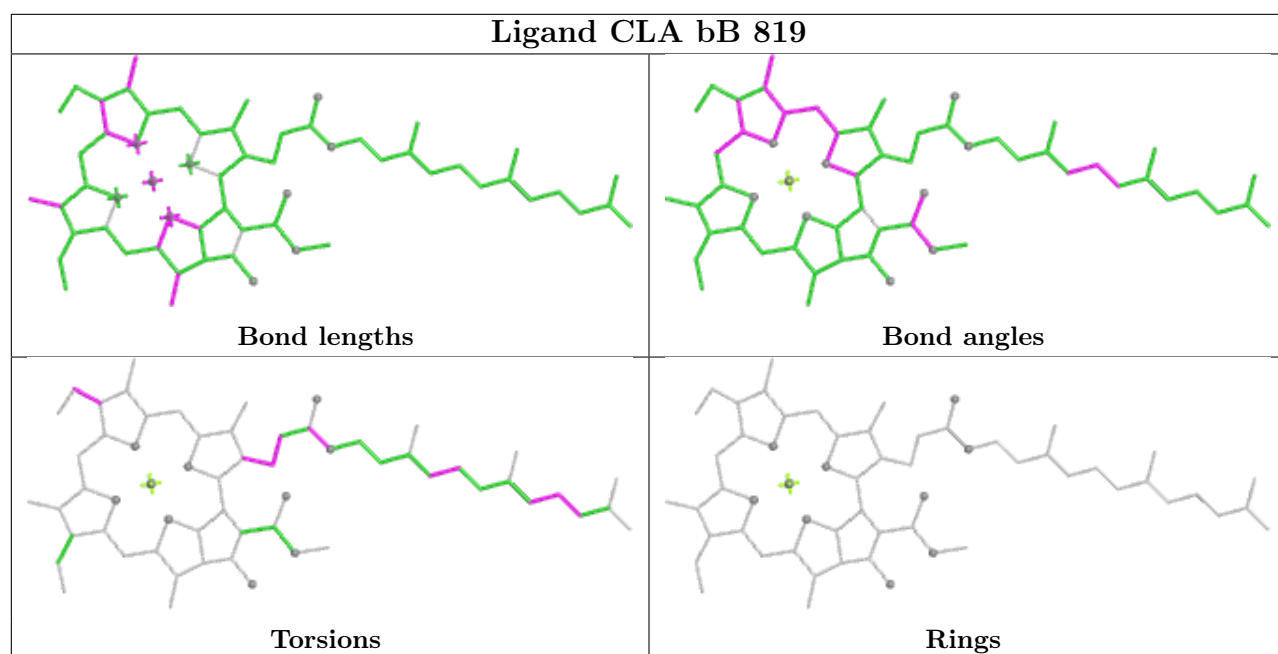


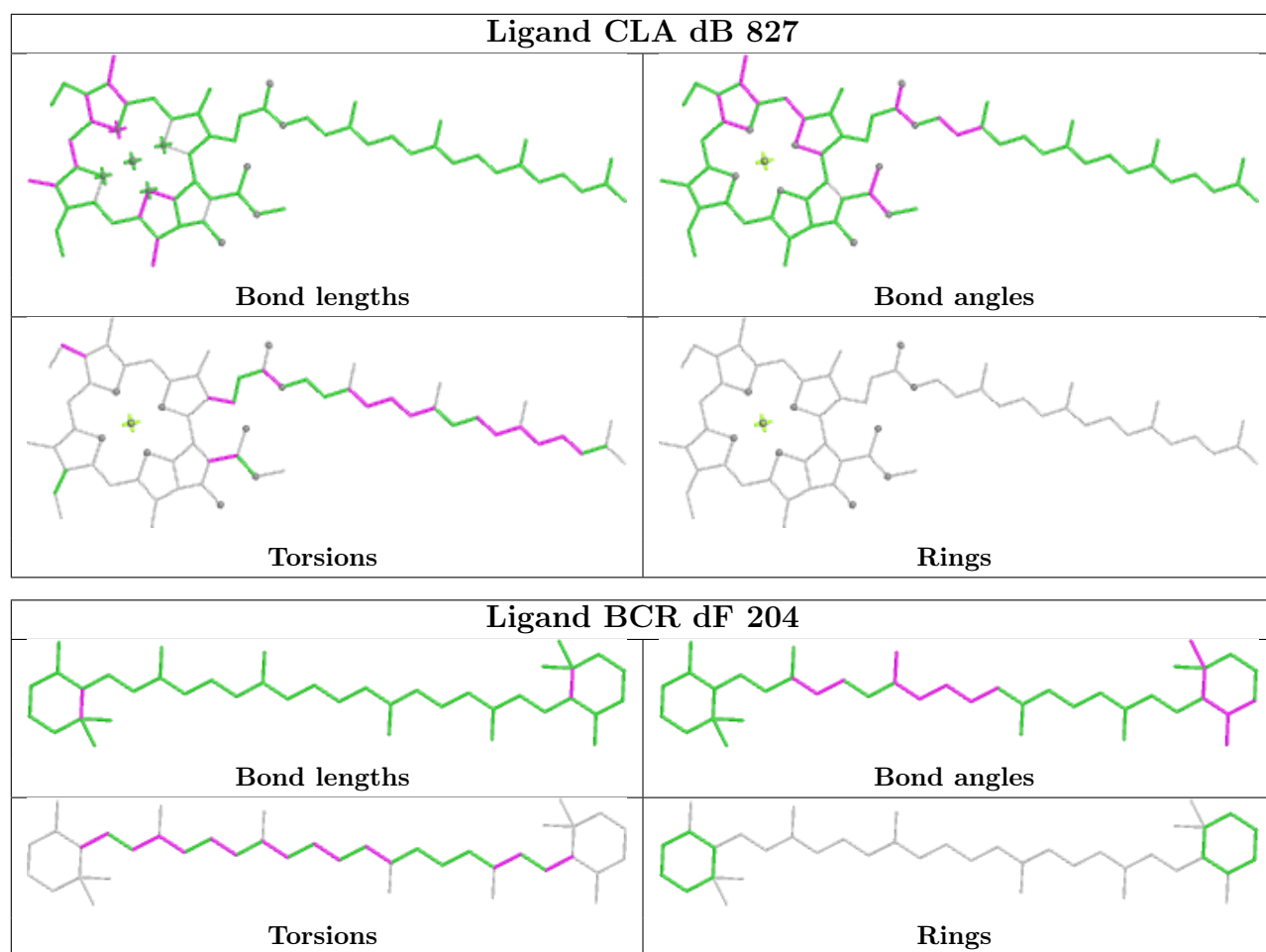




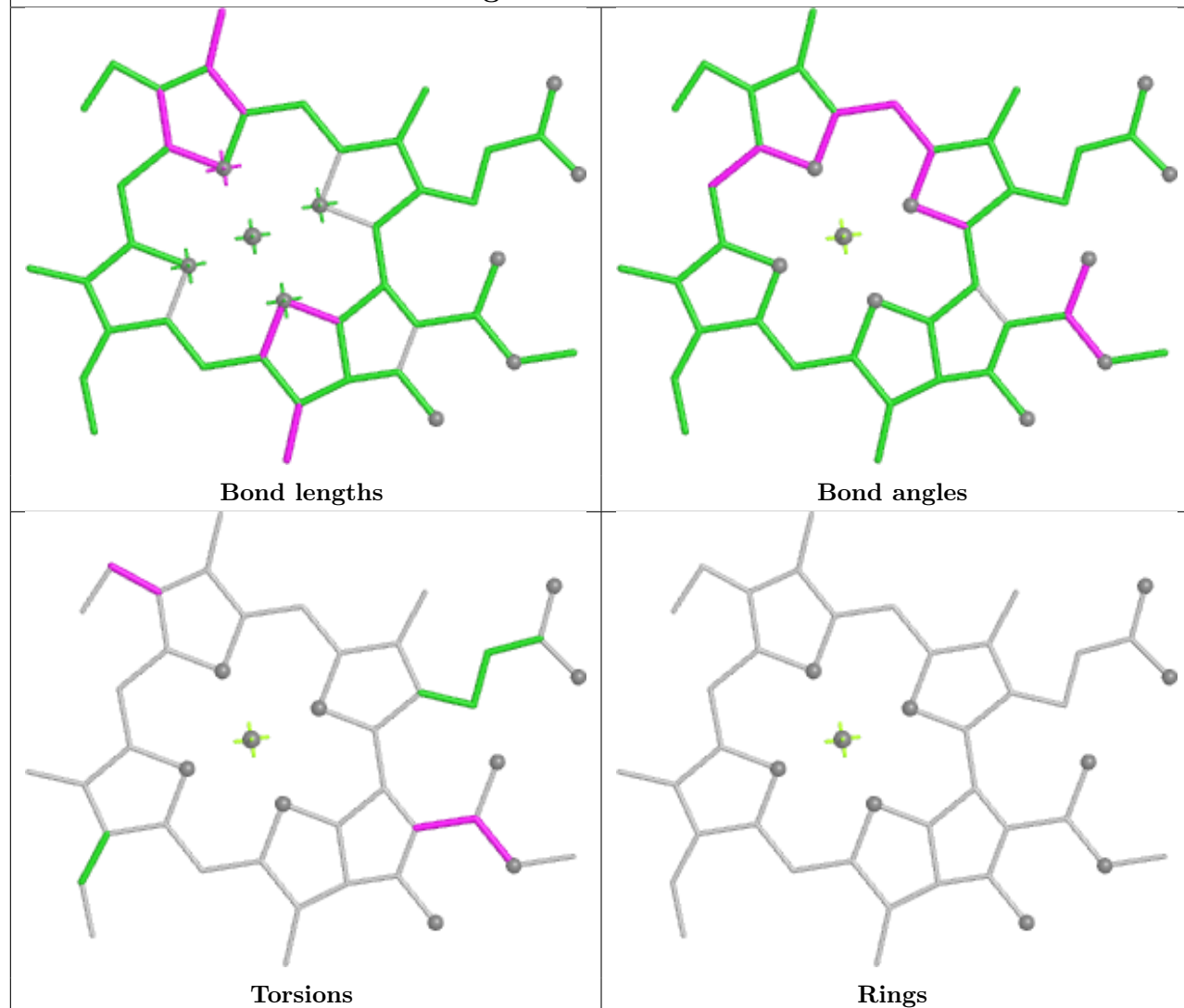




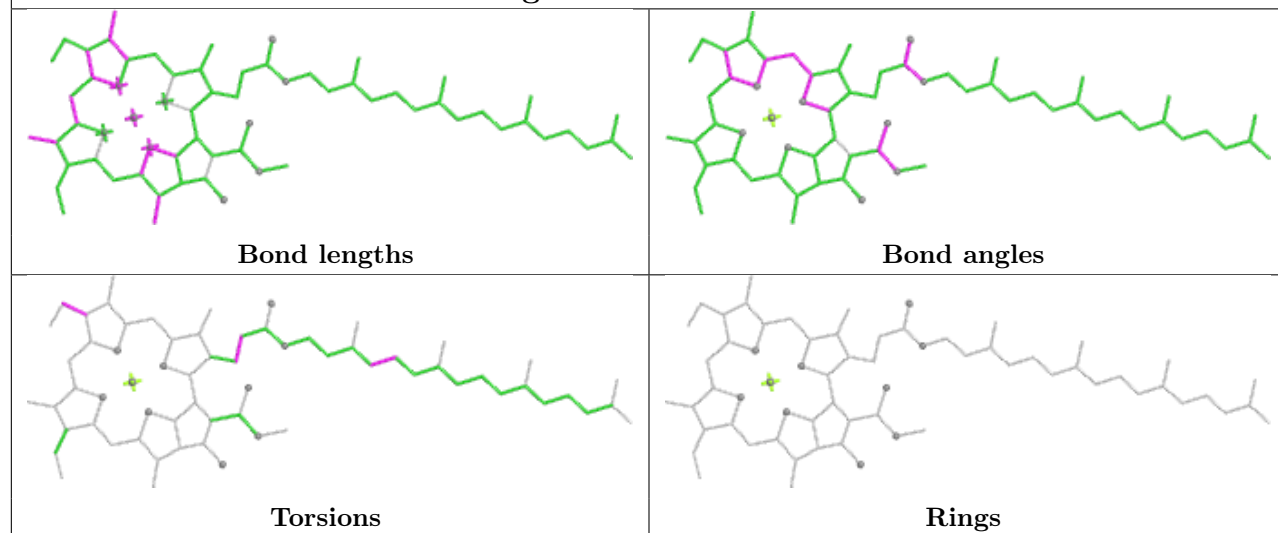


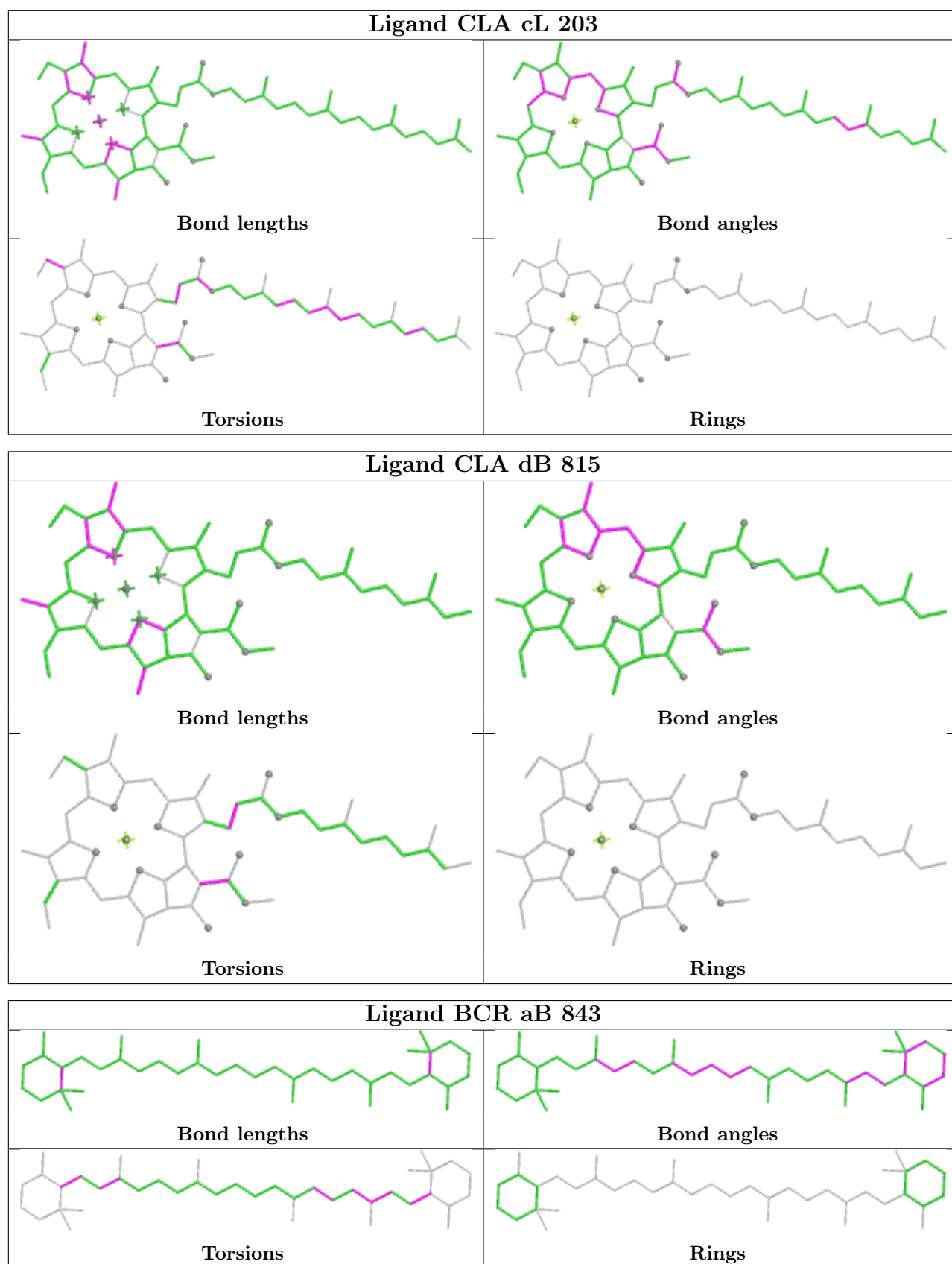


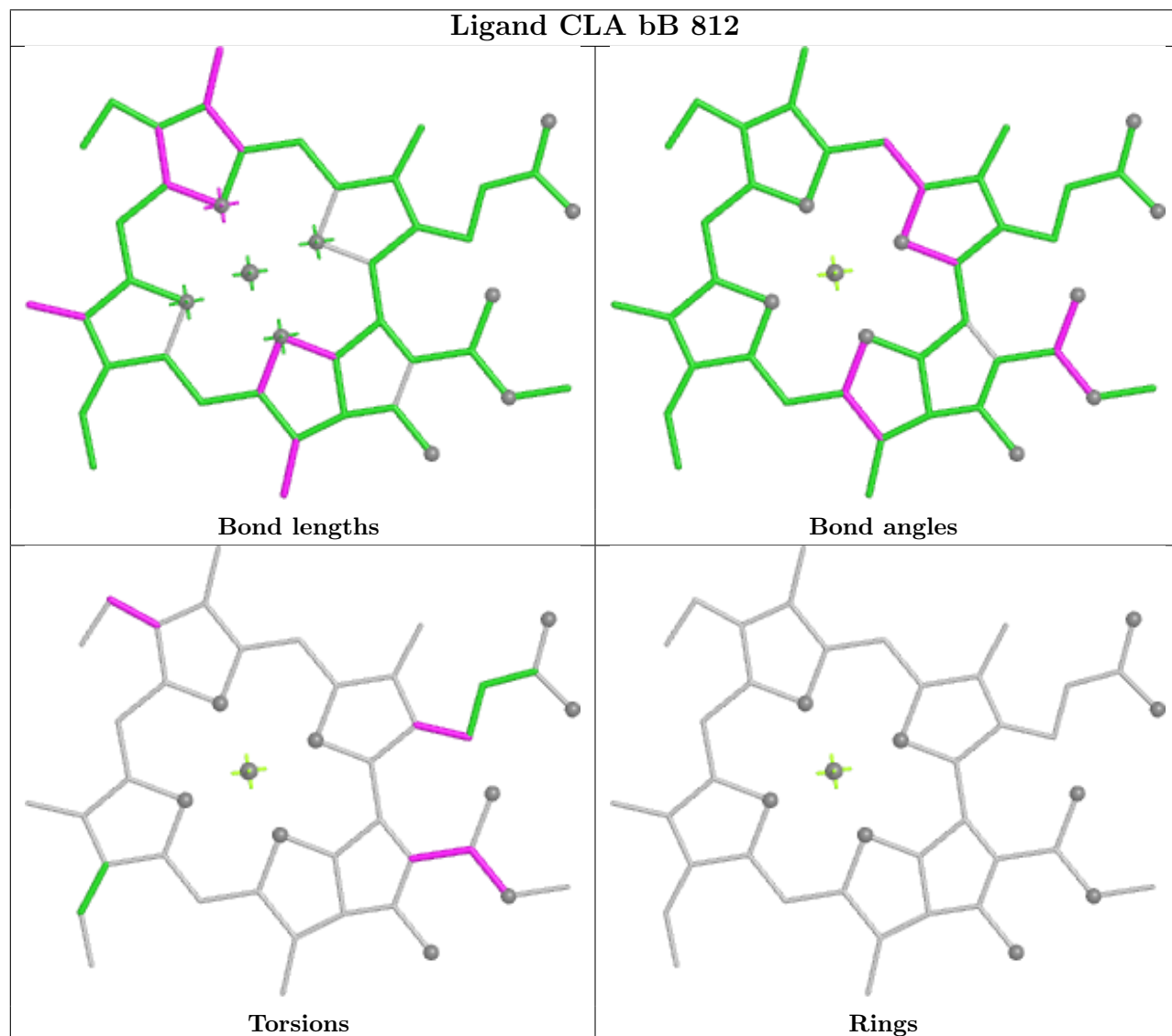
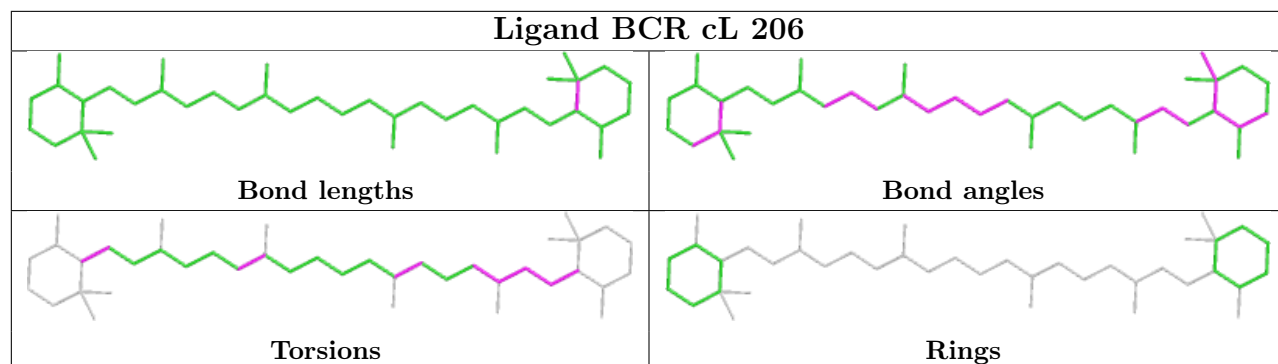
Ligand CLA dA 815

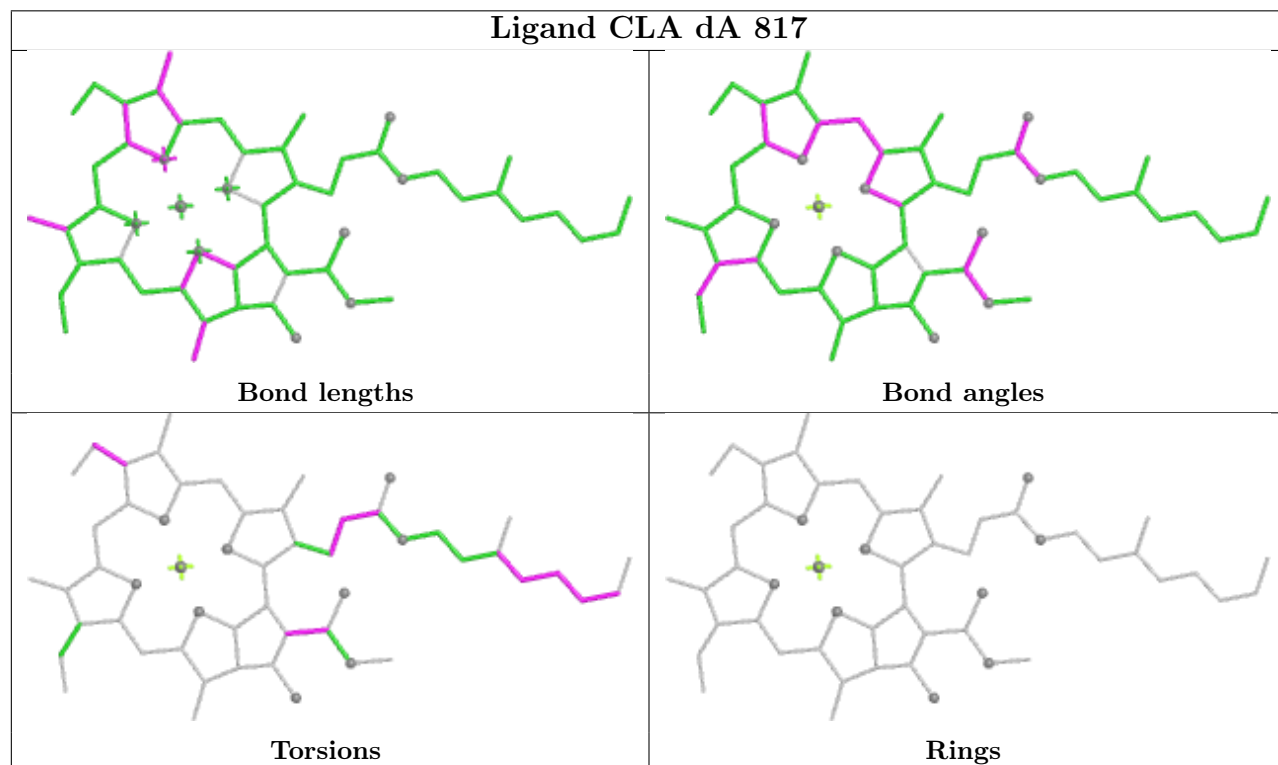
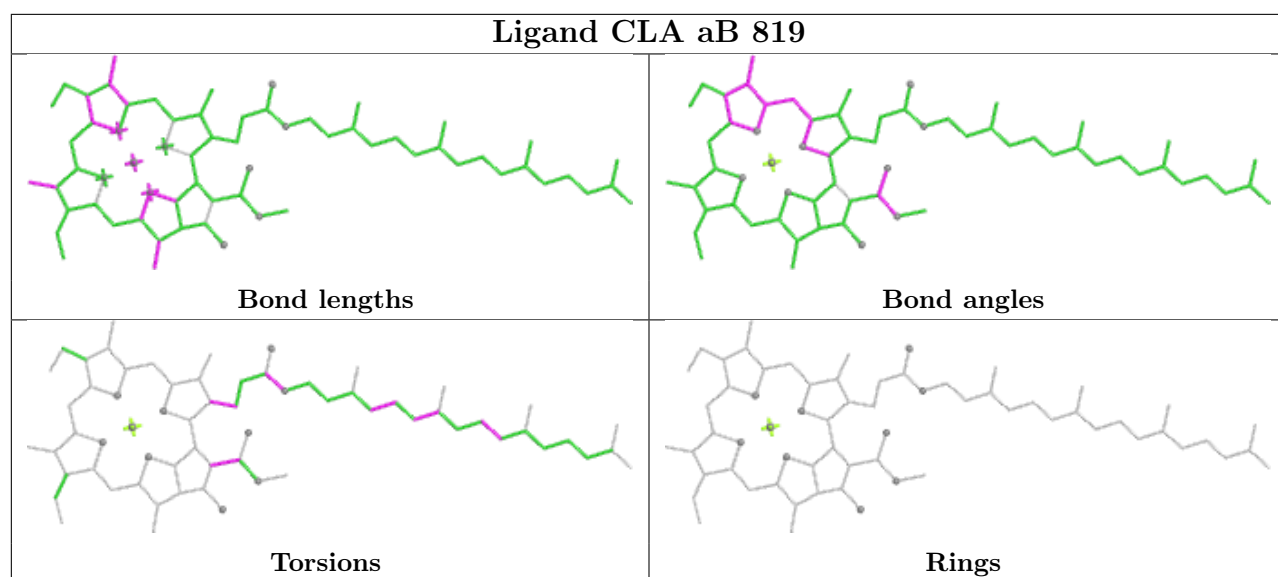


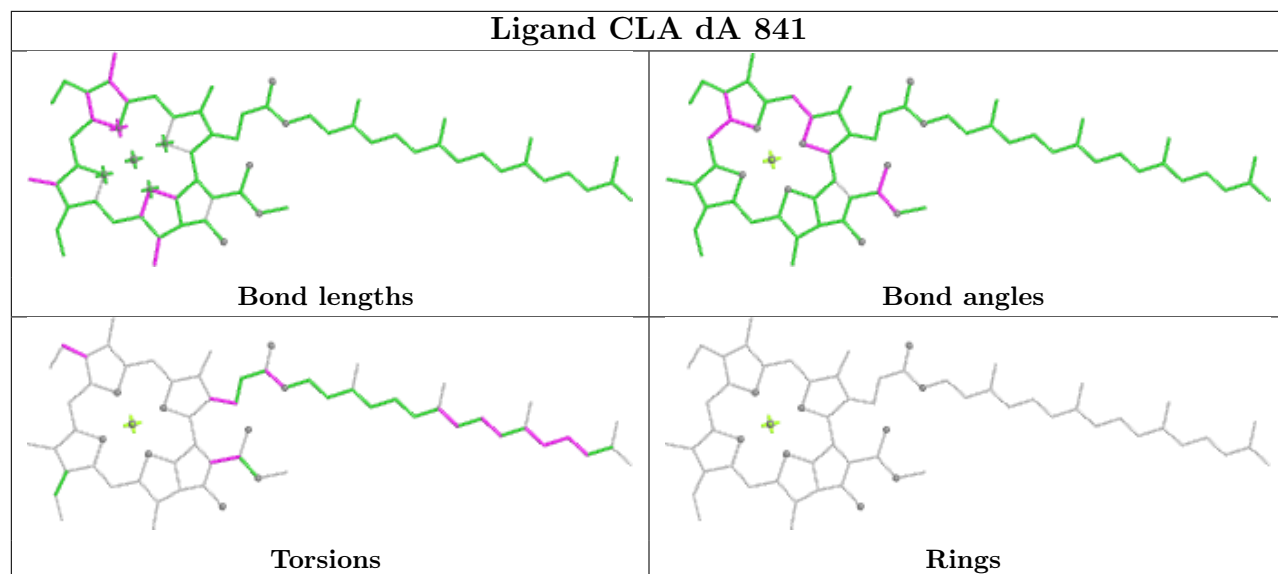
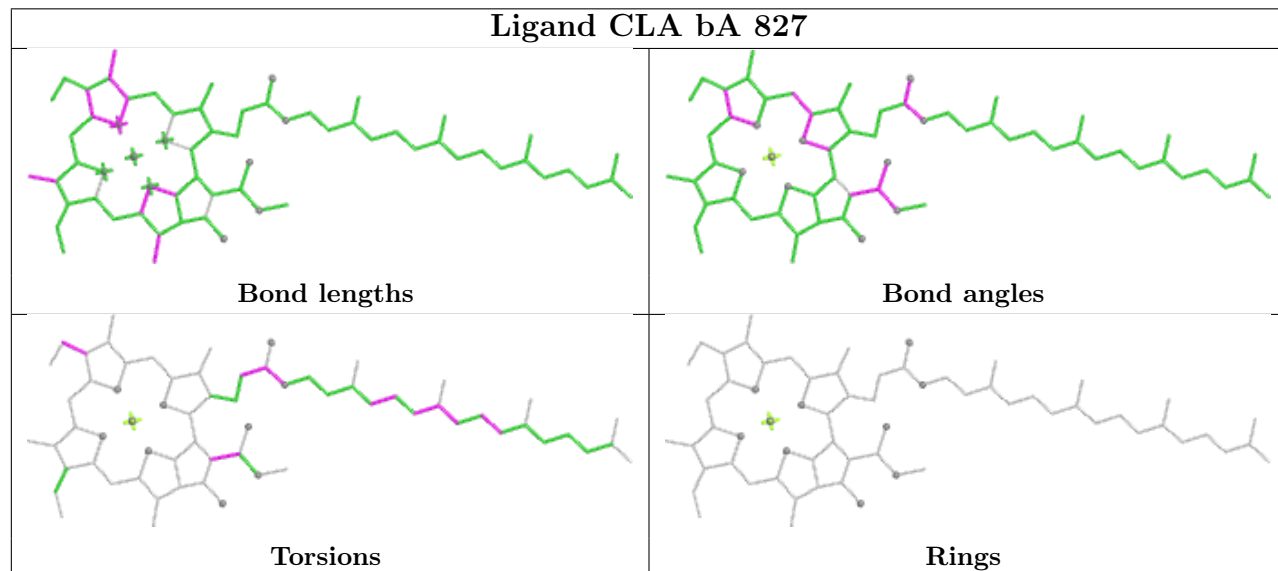
Ligand CLA dB 841



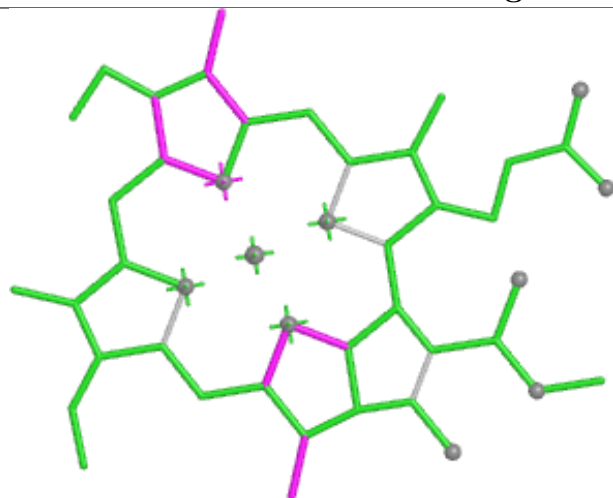




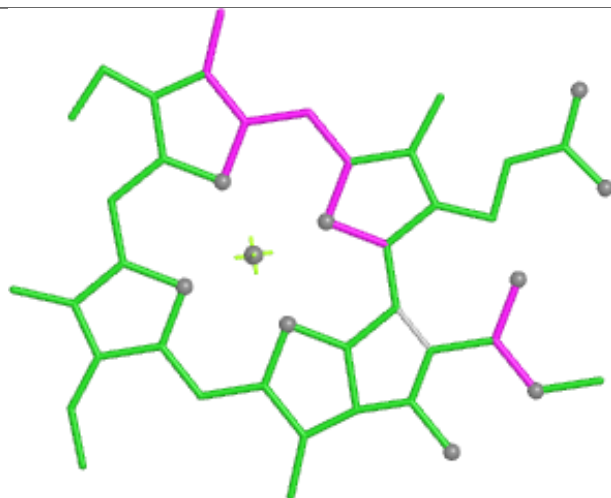


Ligand CLA dA 841**Ligand CLA bA 827**

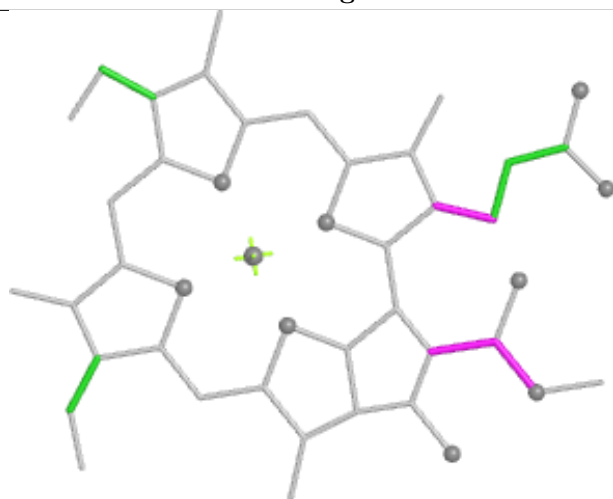
Ligand CLA aA 810



Bond lengths



Bond angles

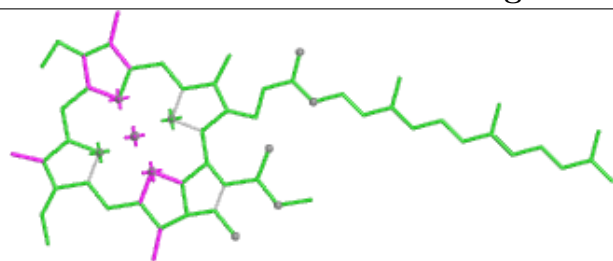


Torsions

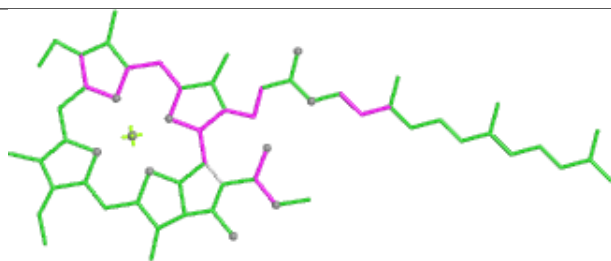


Rings

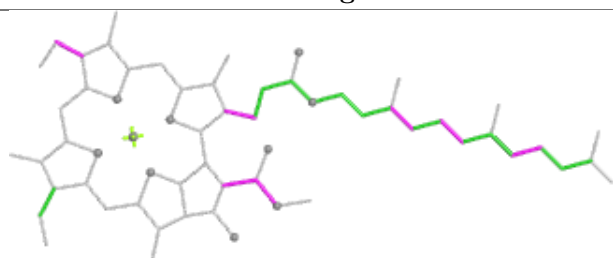
Ligand CLA dB 838



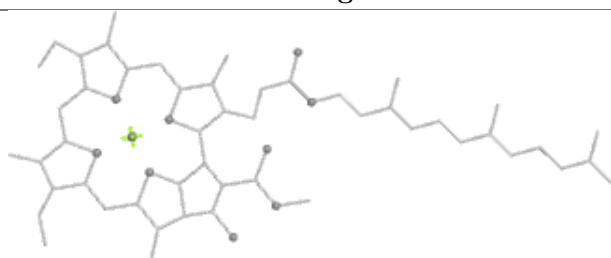
Bond lengths



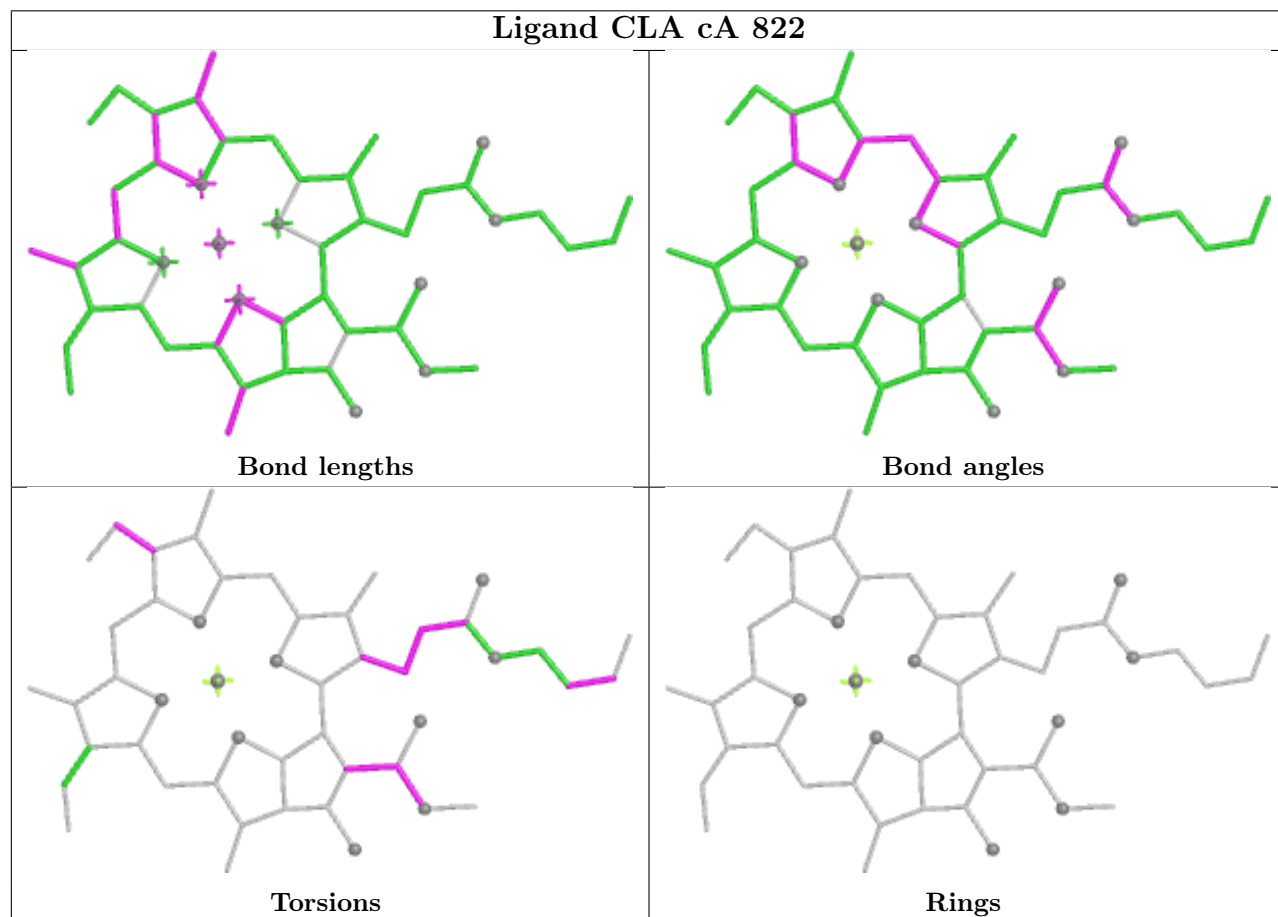
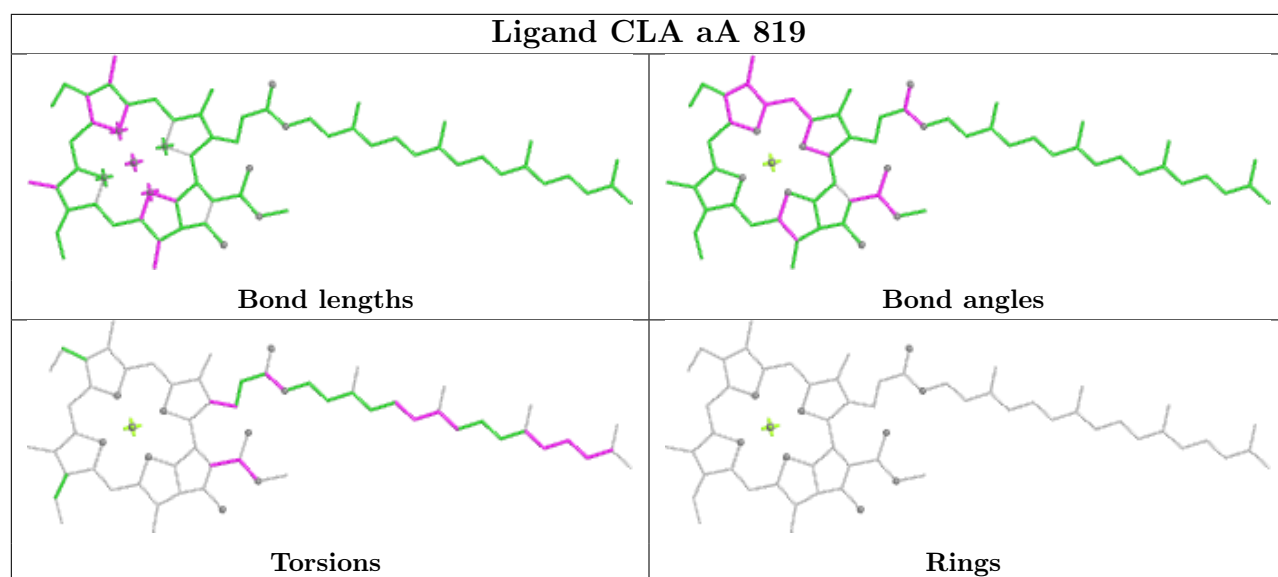
Bond angles



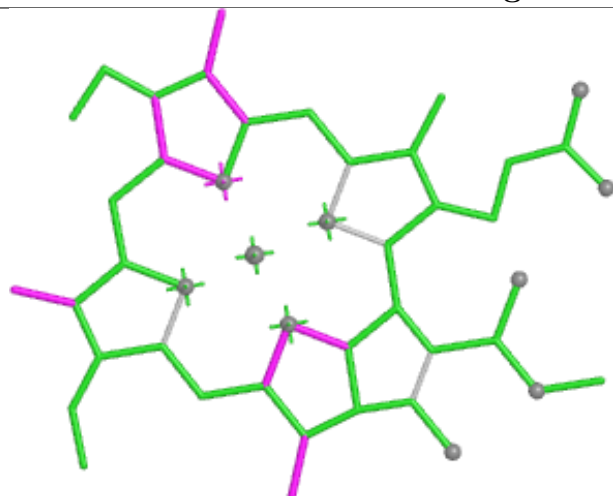
Torsions



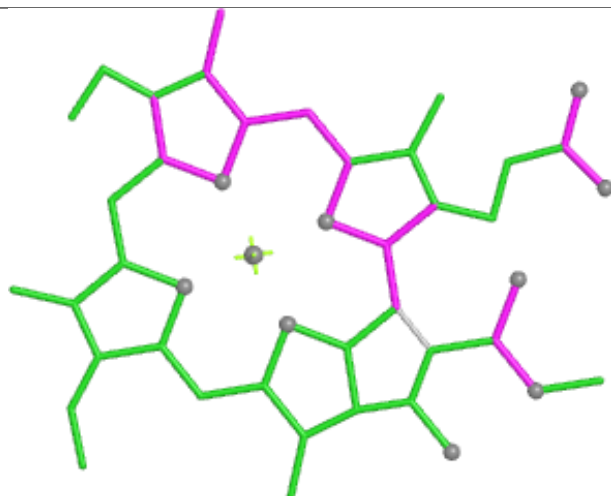
Rings



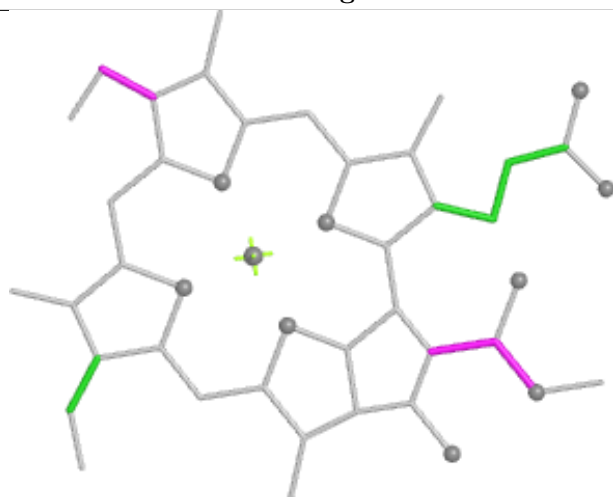
Ligand CLA bA 814



Bond lengths



Bond angles

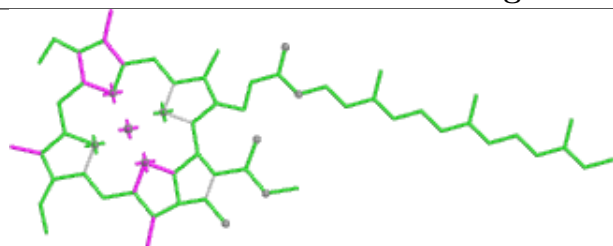


Torsions

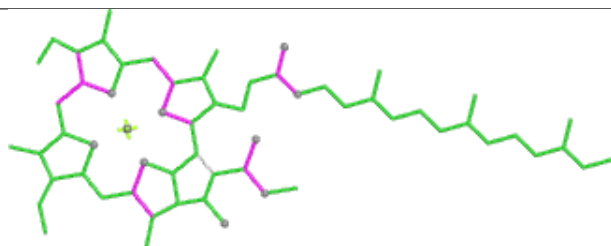


Rings

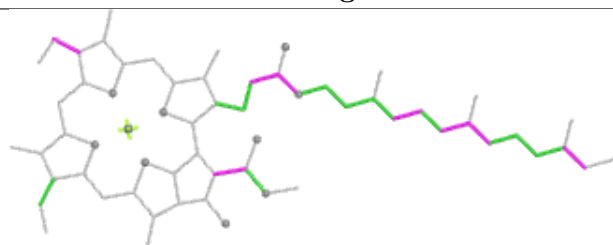
Ligand CLA bA 820



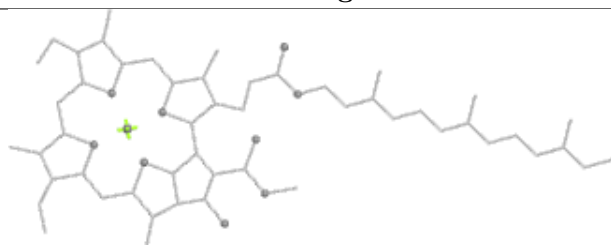
Bond lengths



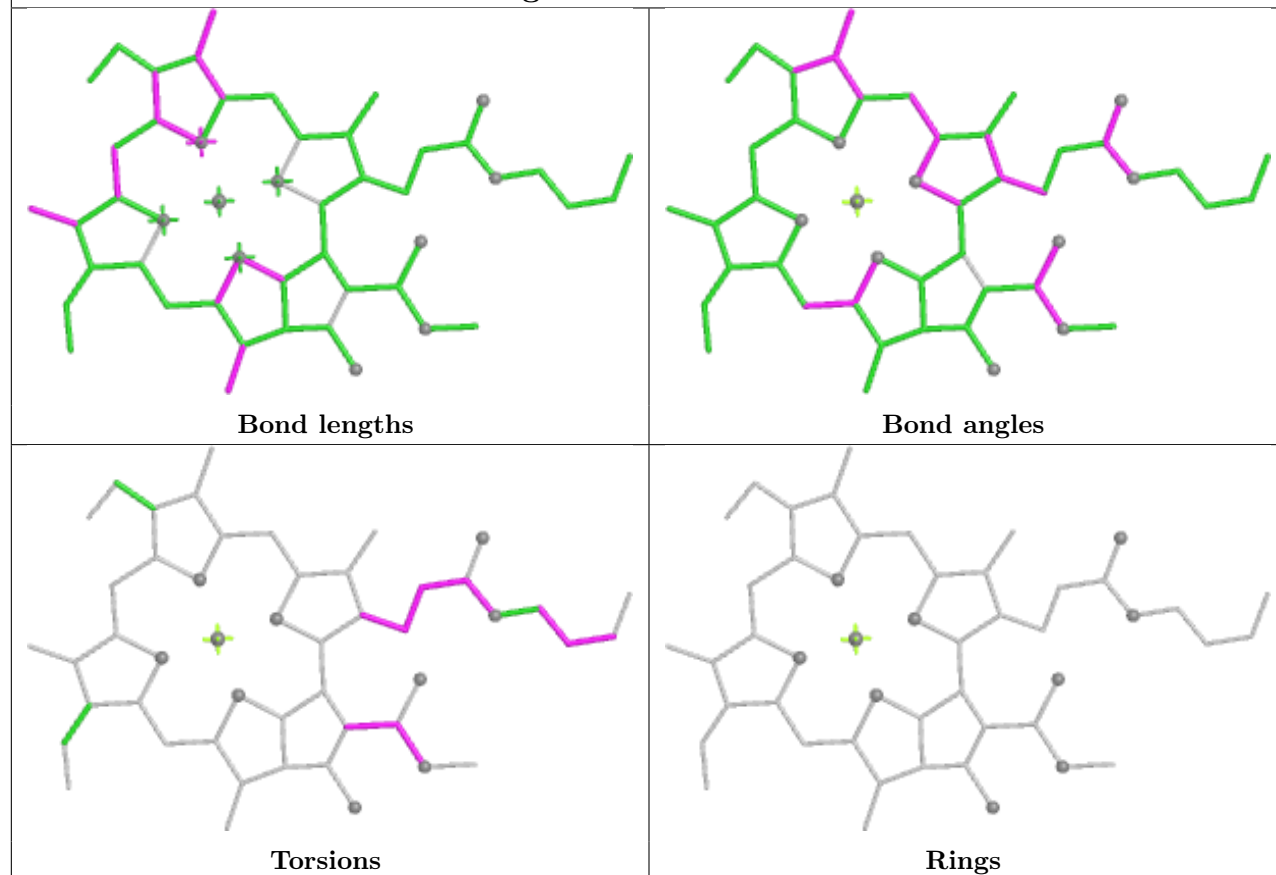
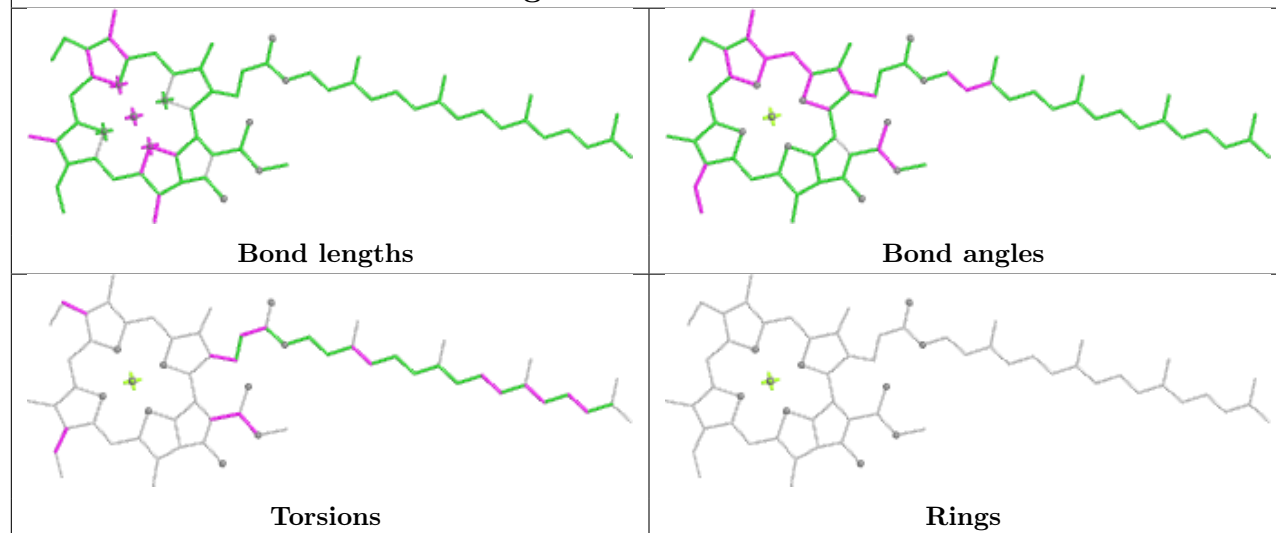
Bond angles

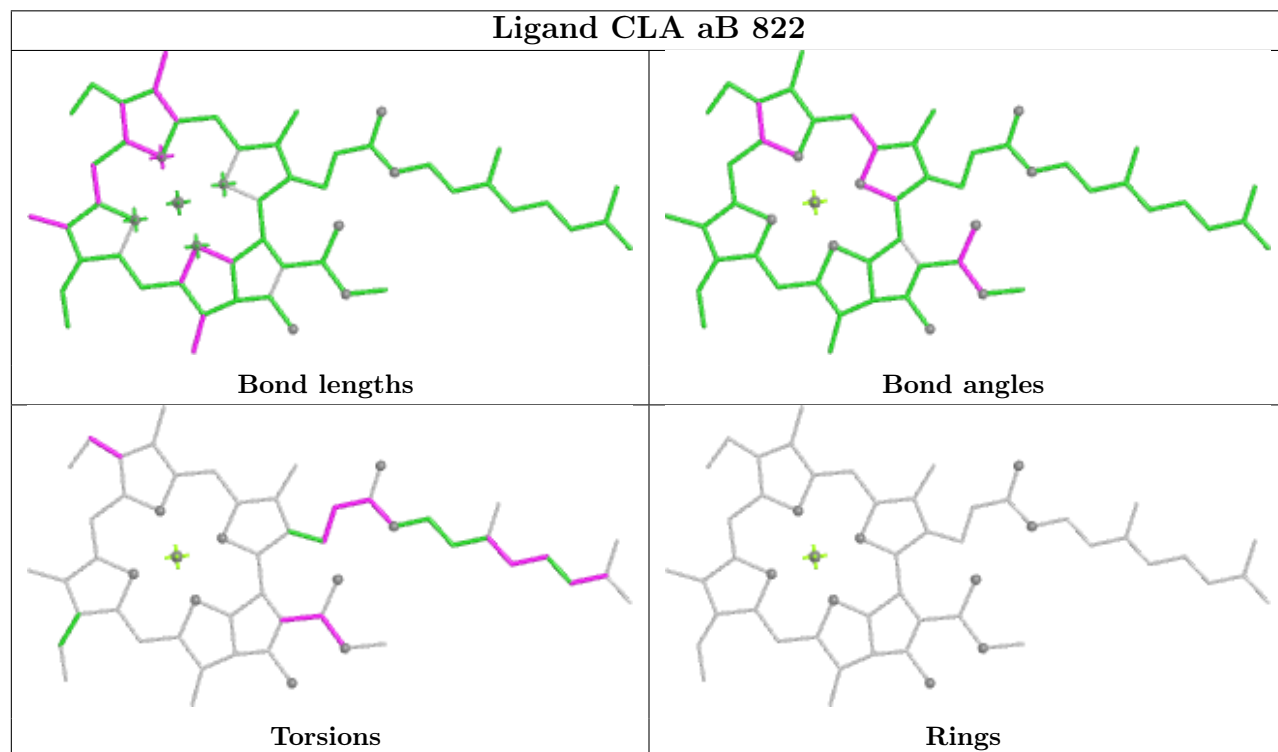
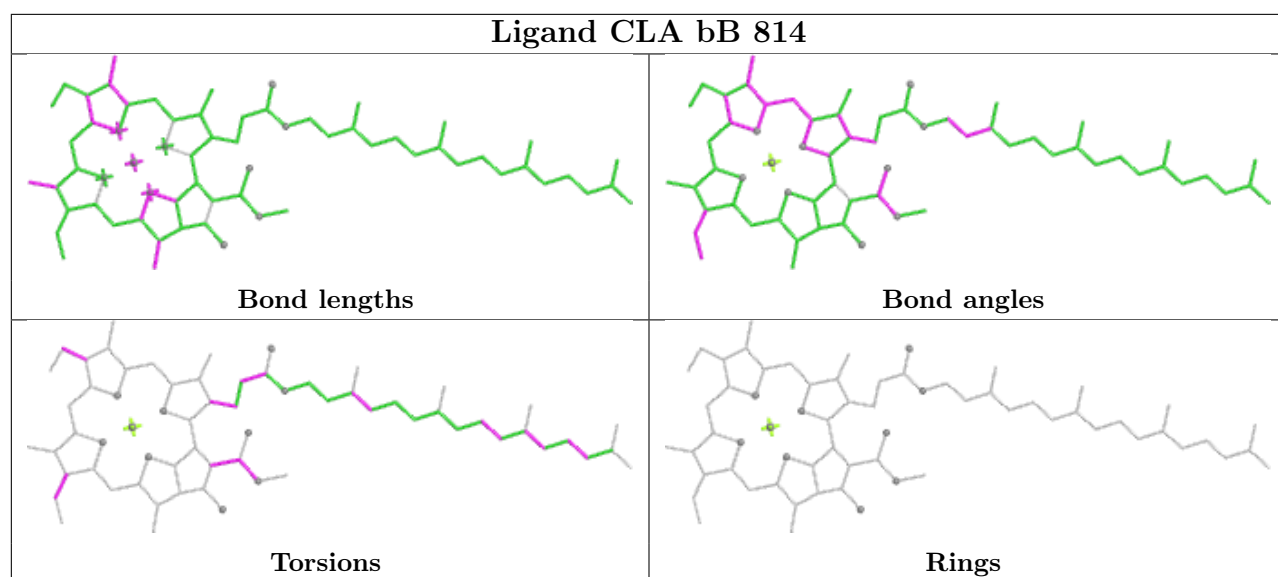


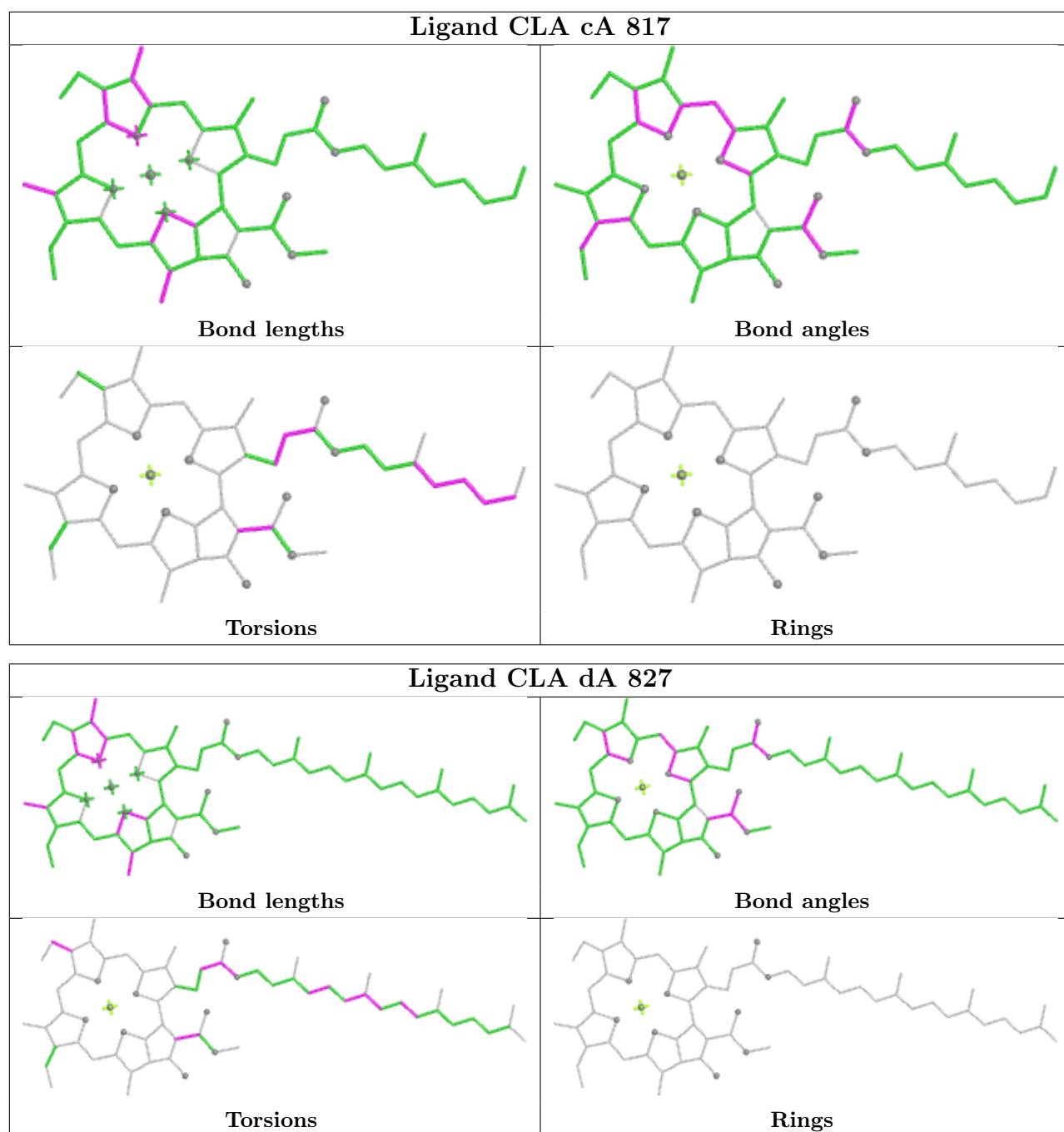
Torsions

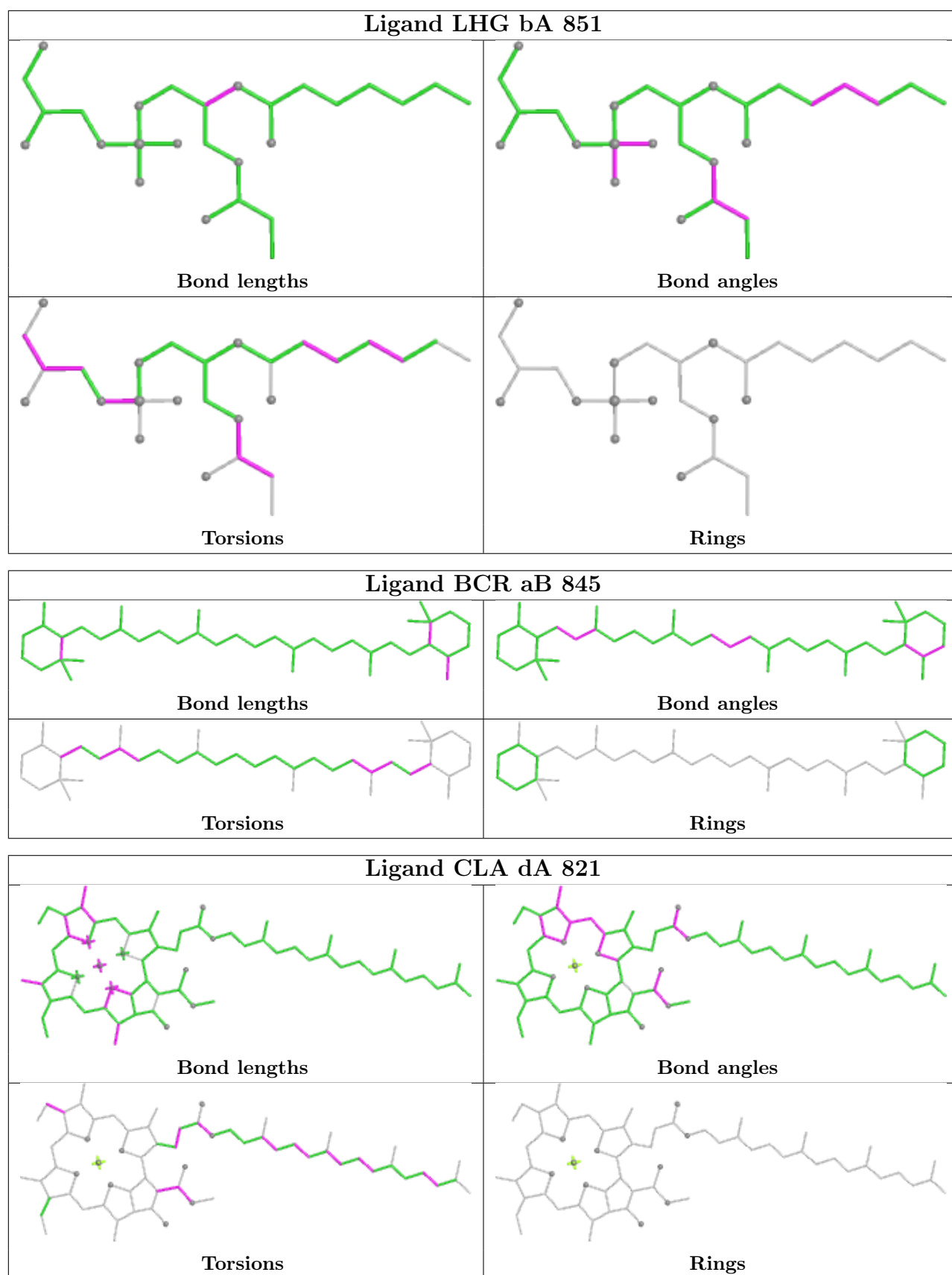


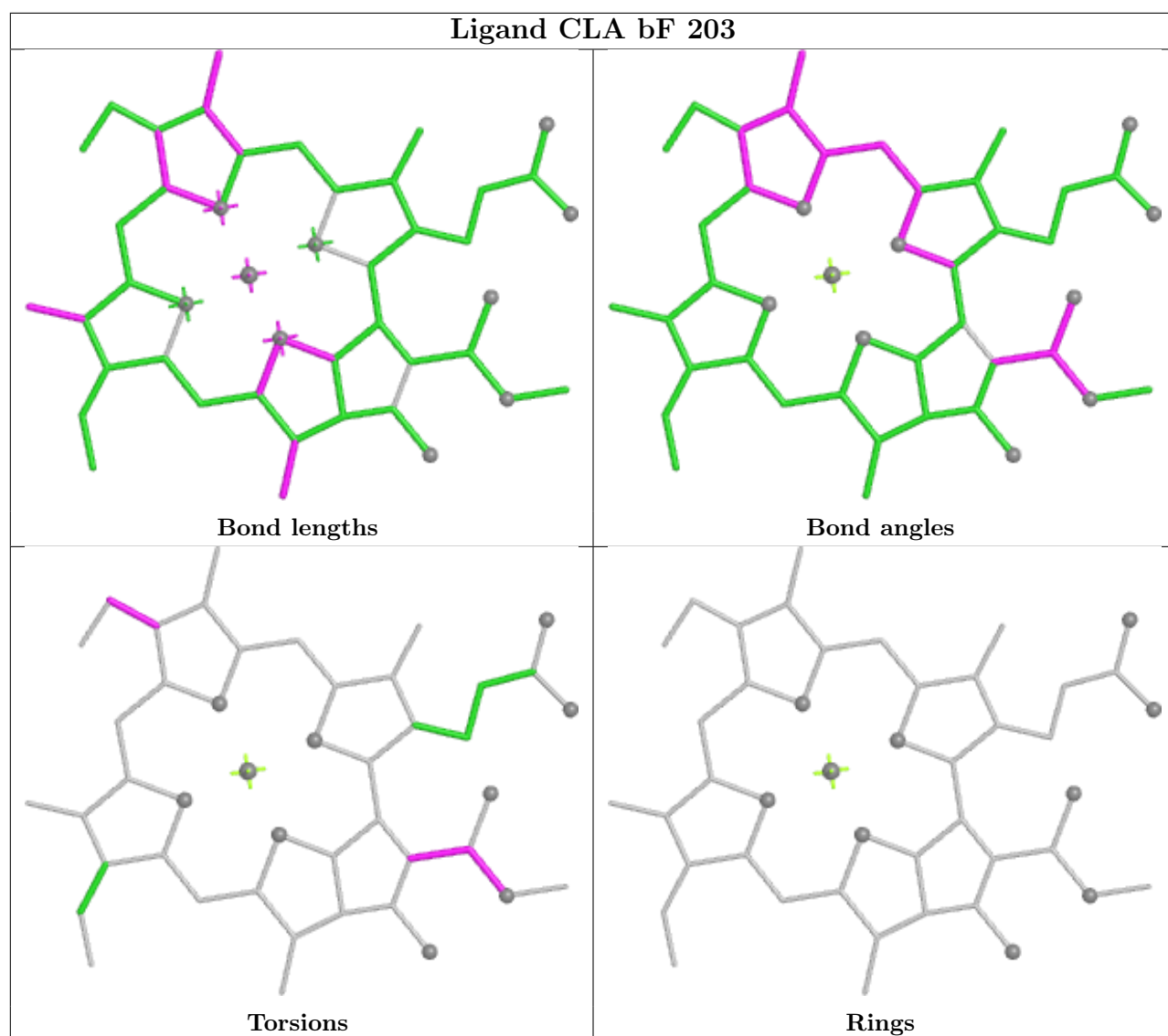
Rings

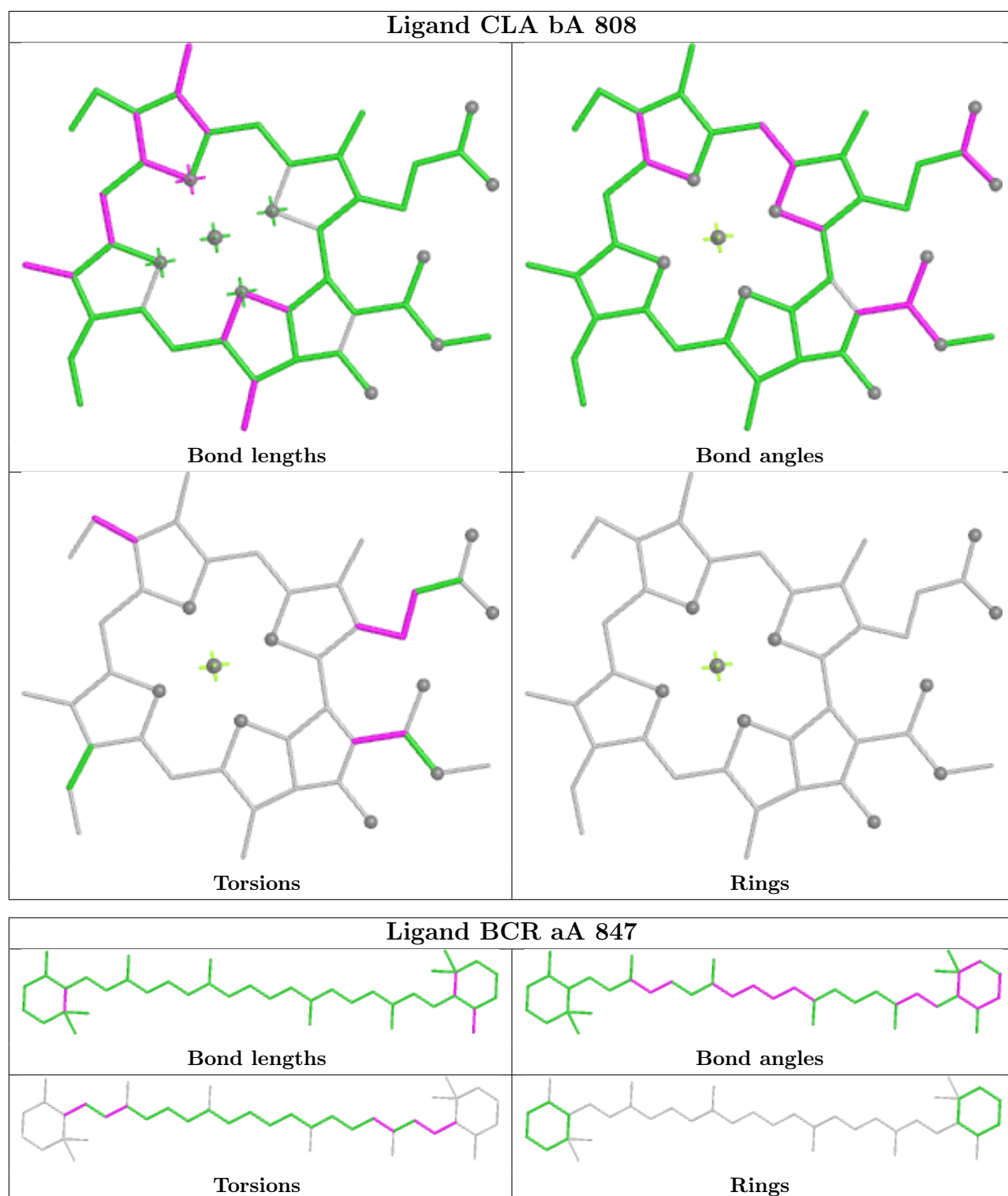
Ligand CLA bB 832**Ligand CLA aB 813**

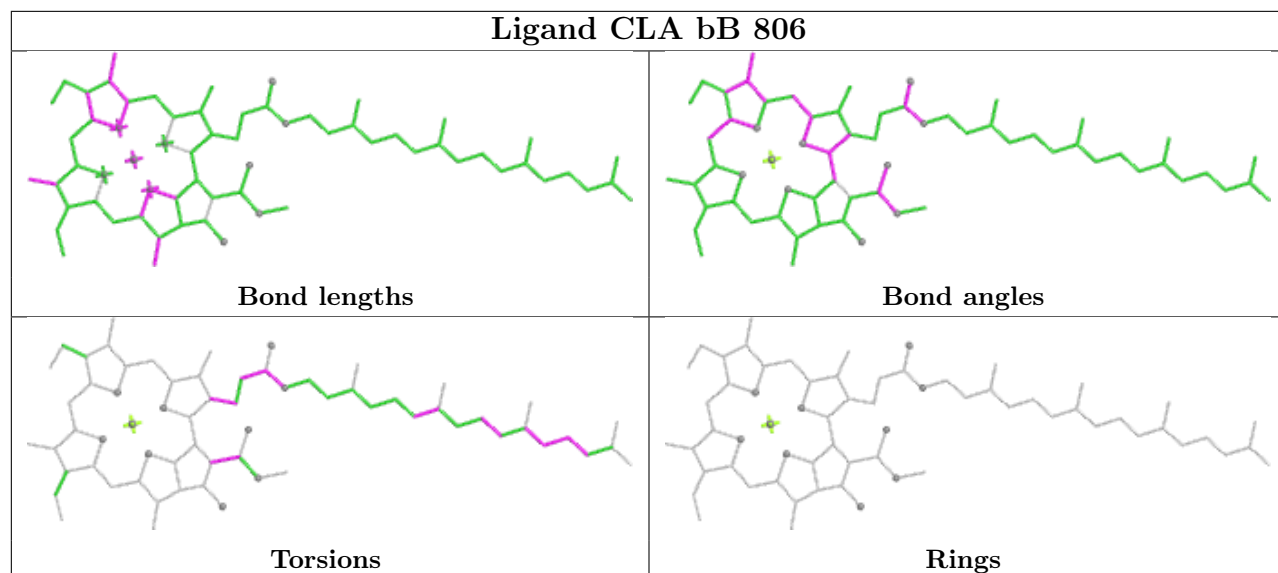
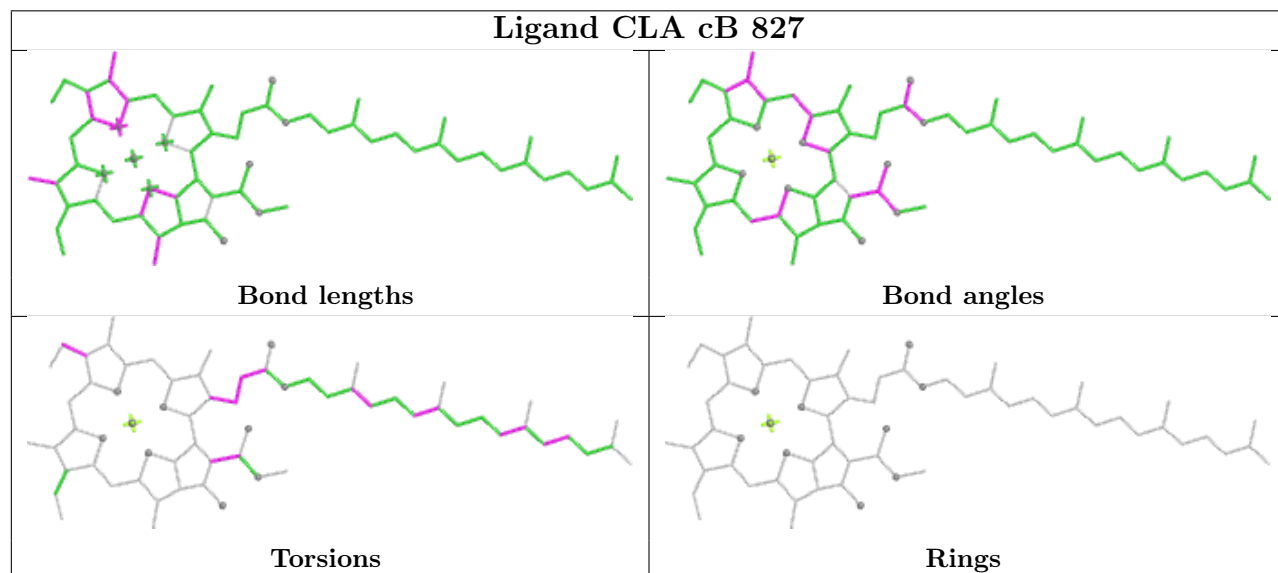
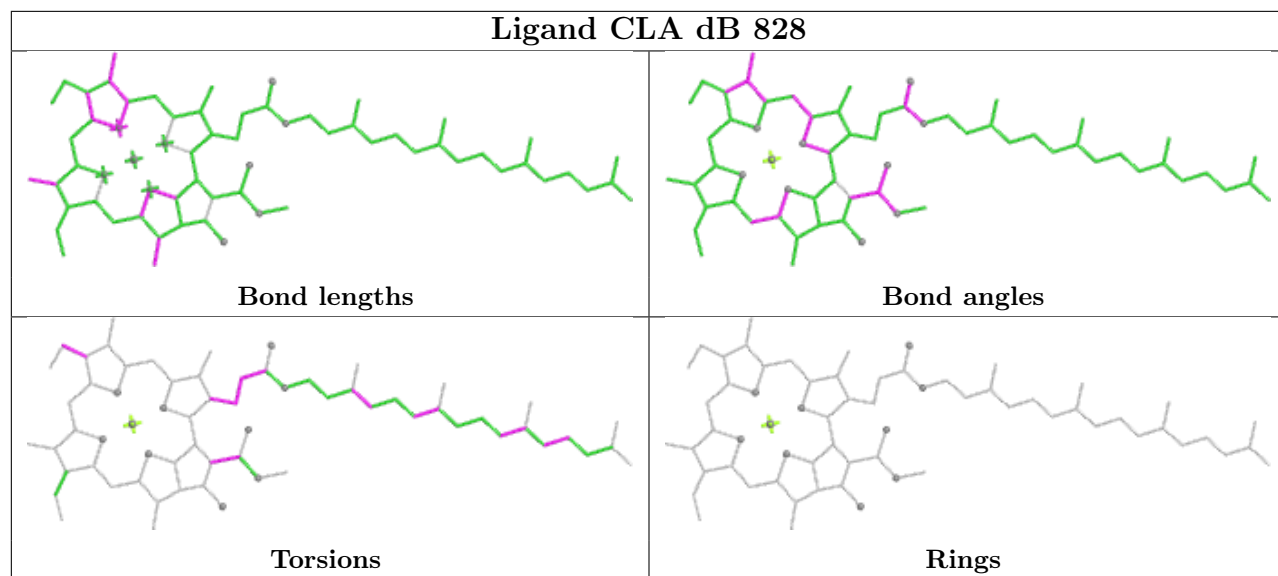


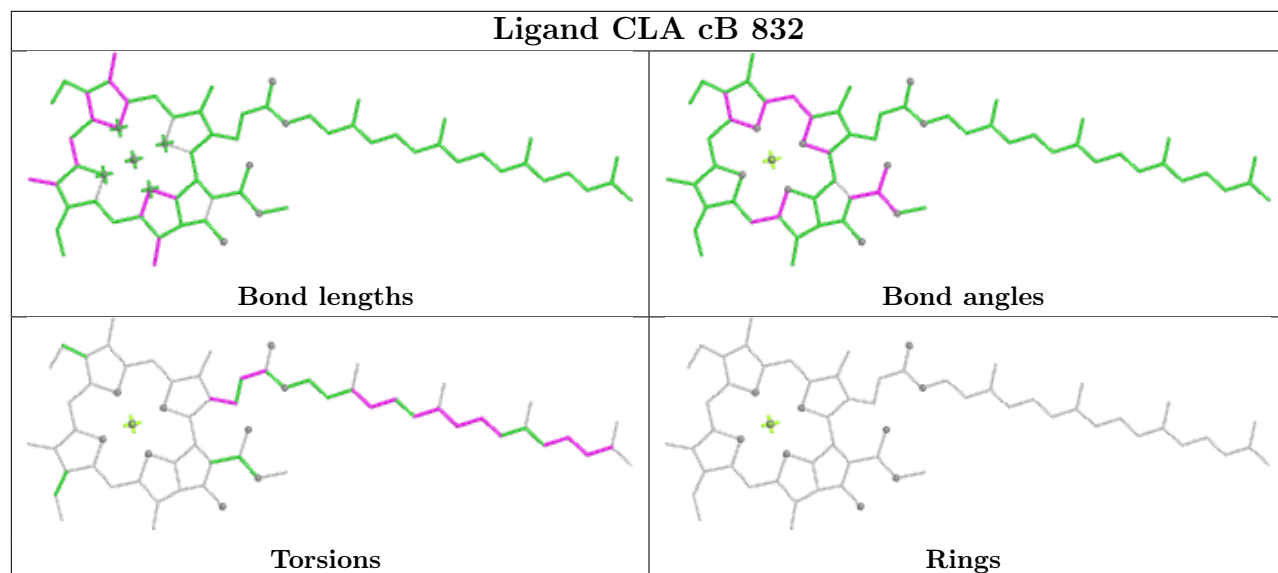
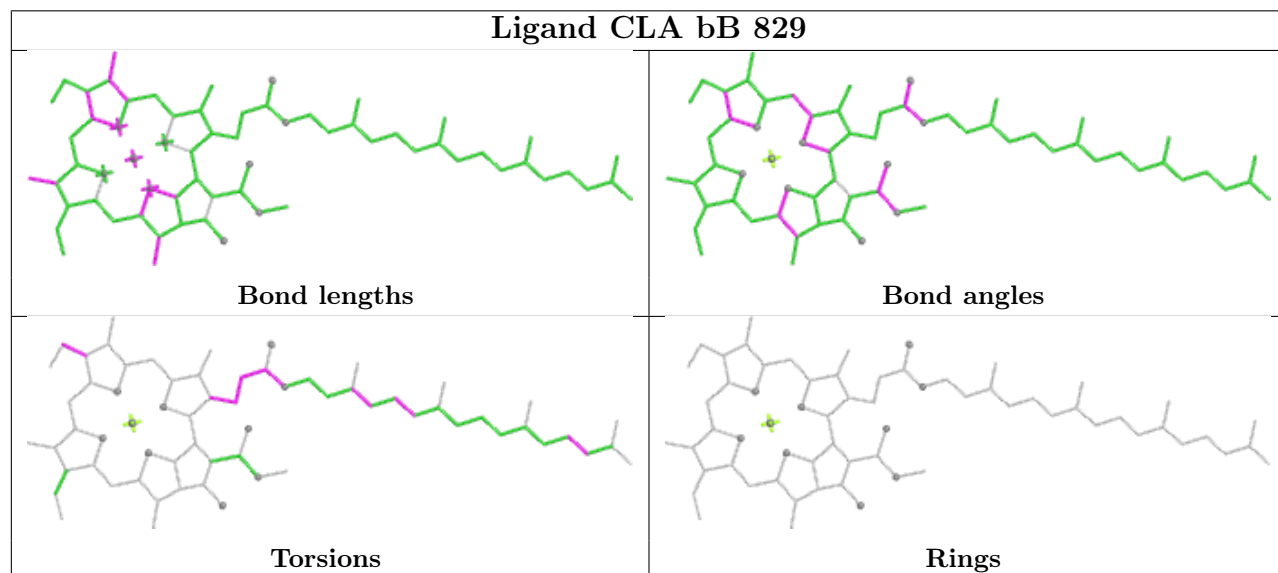
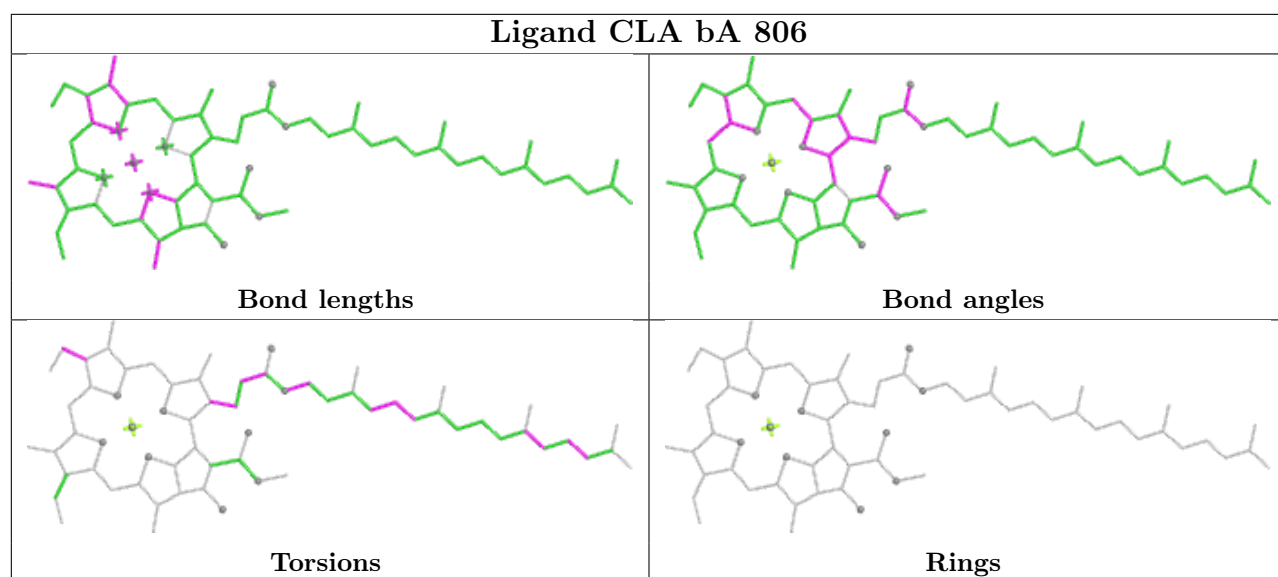


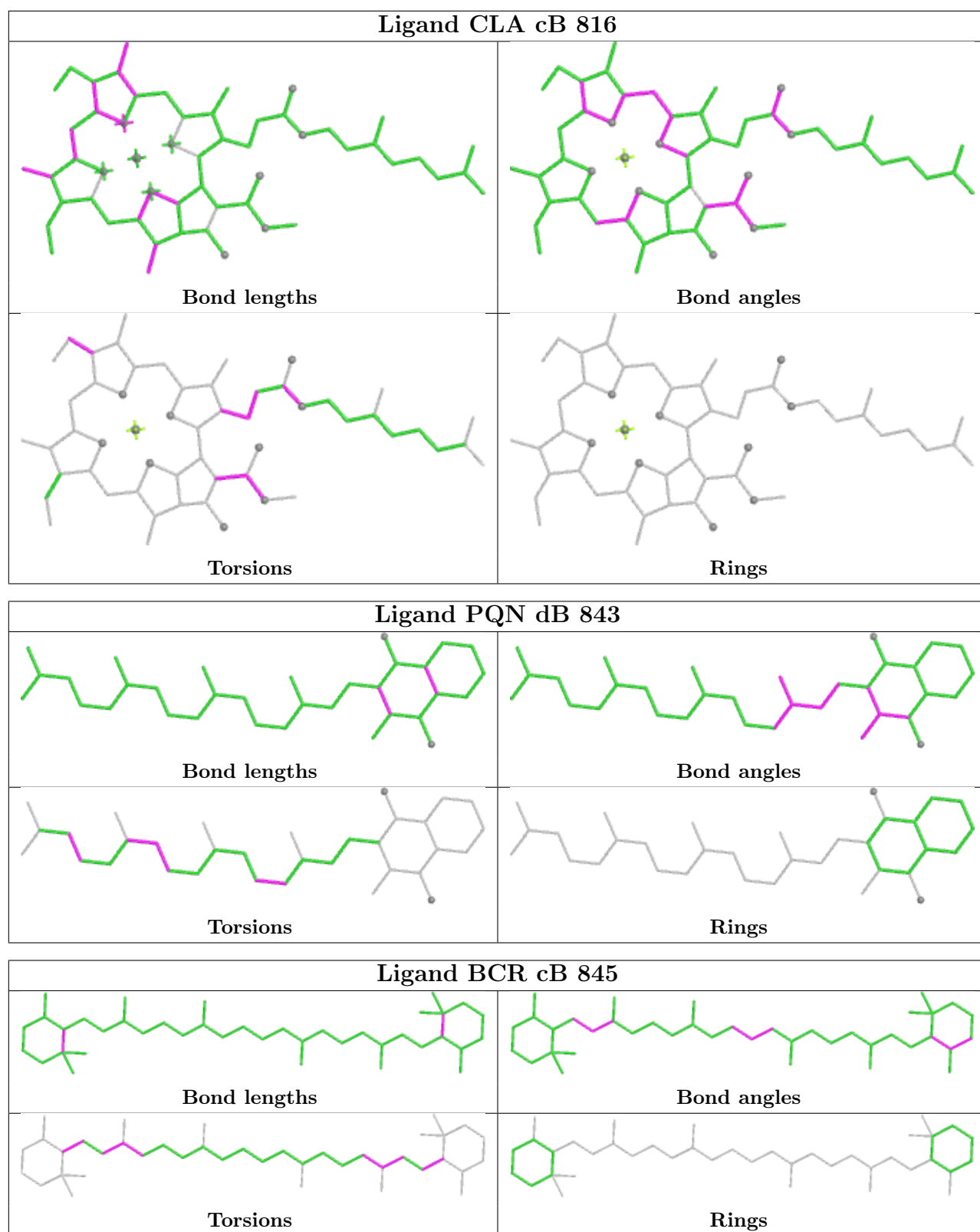


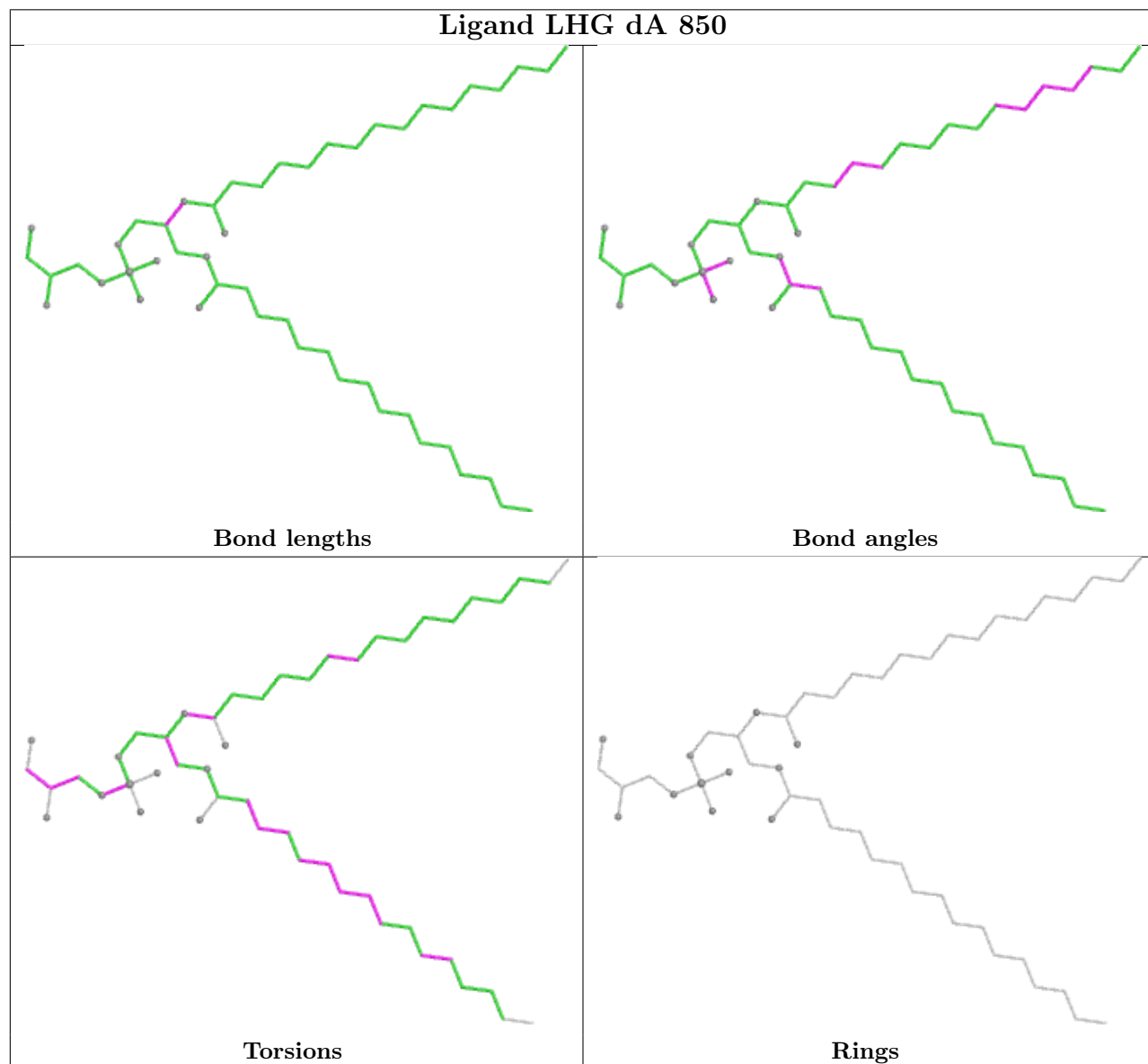
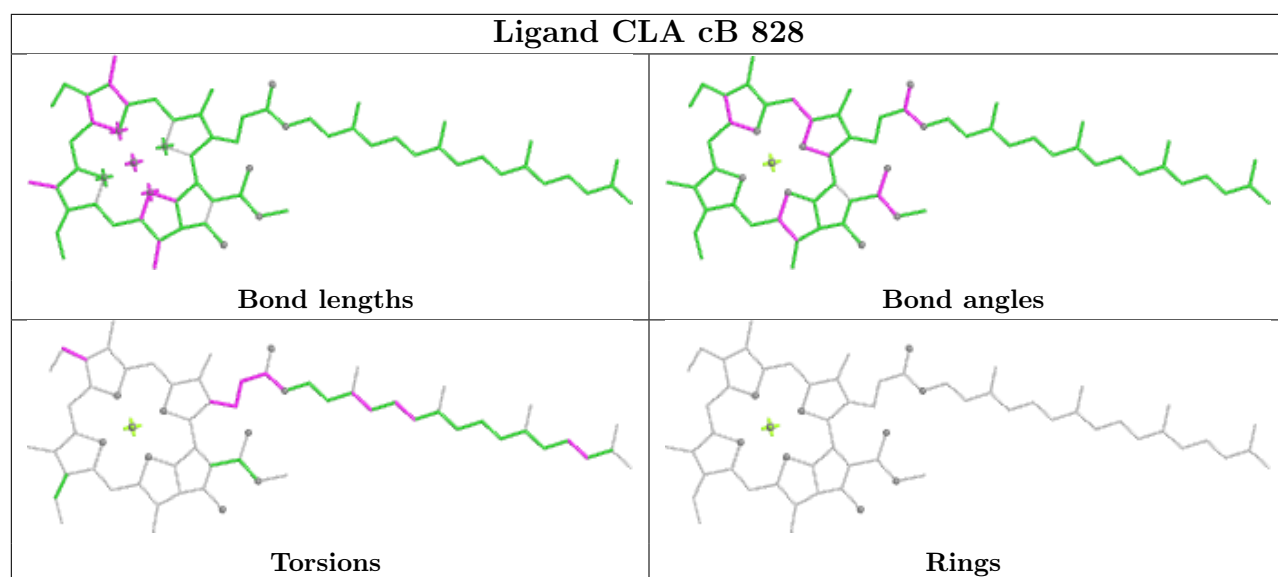


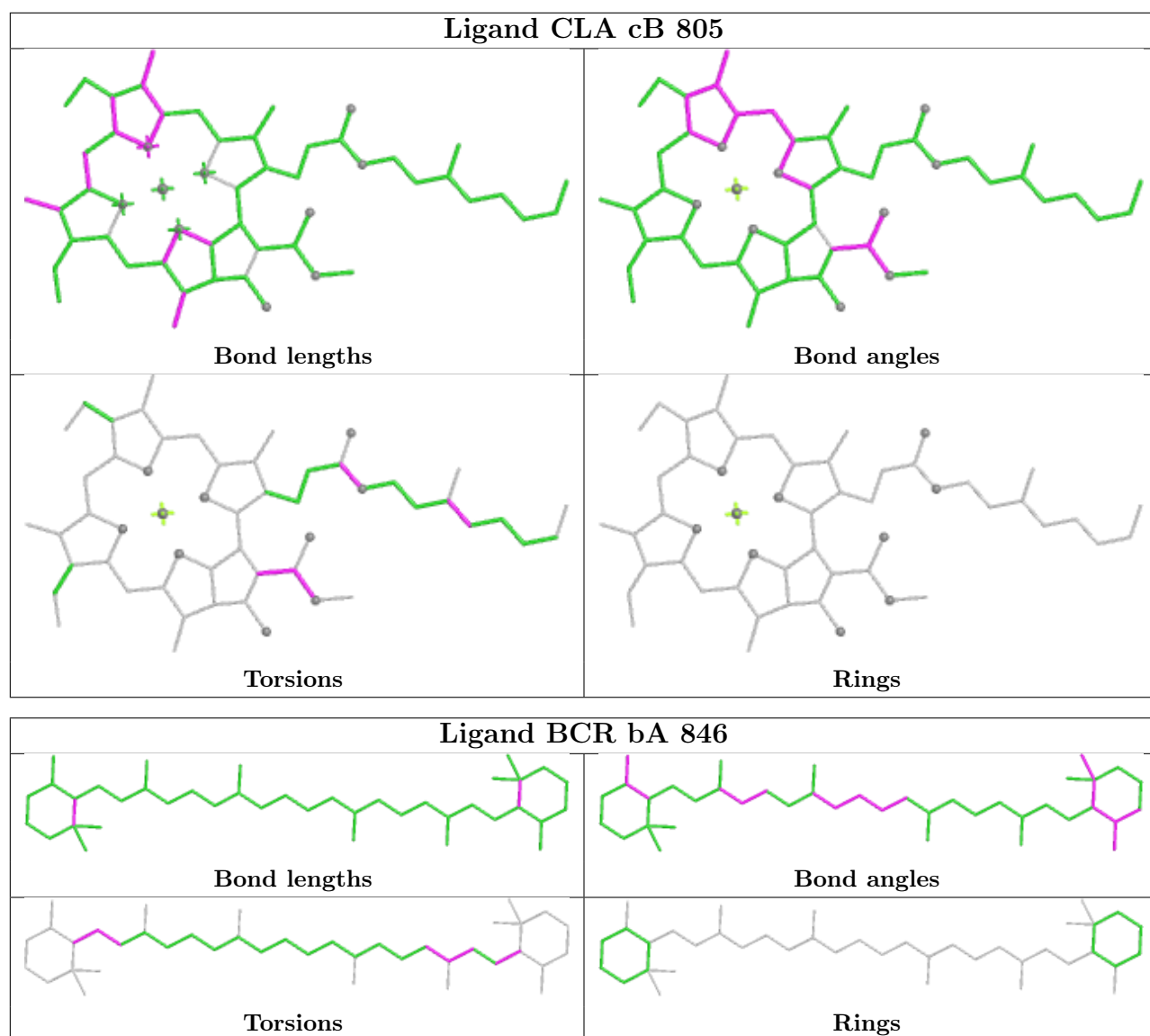


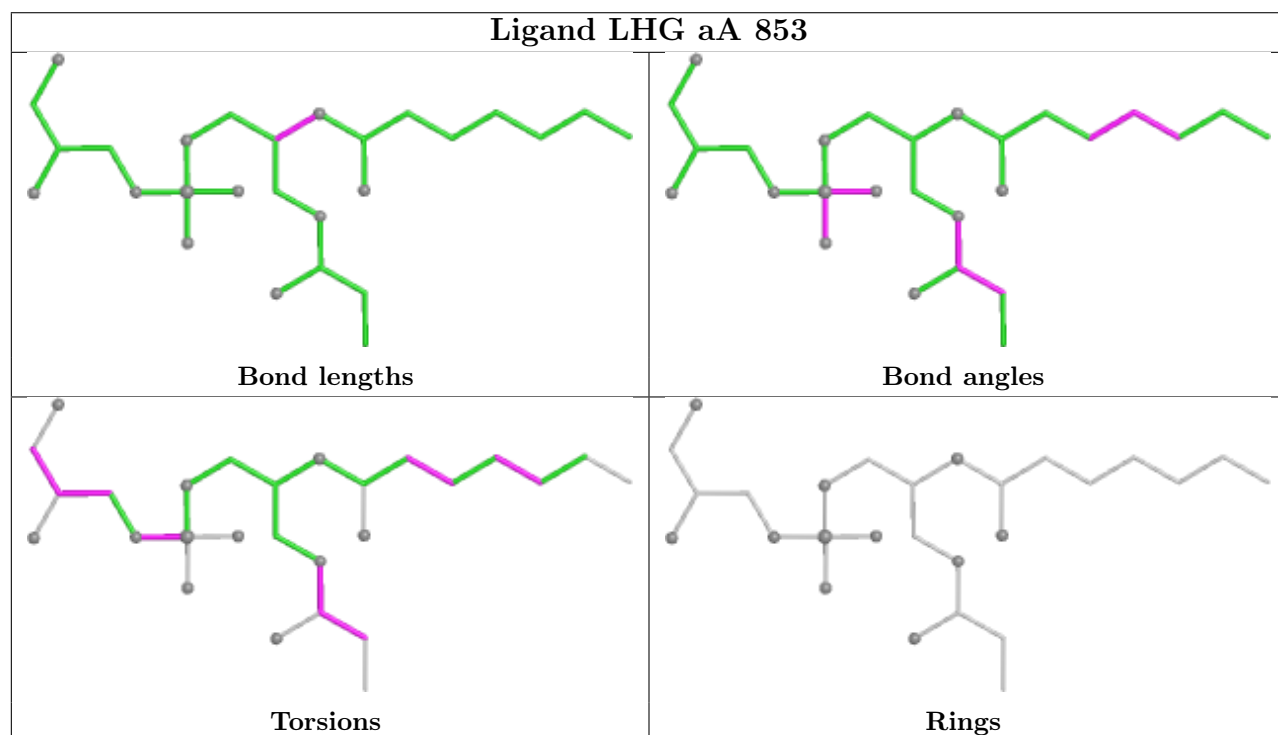
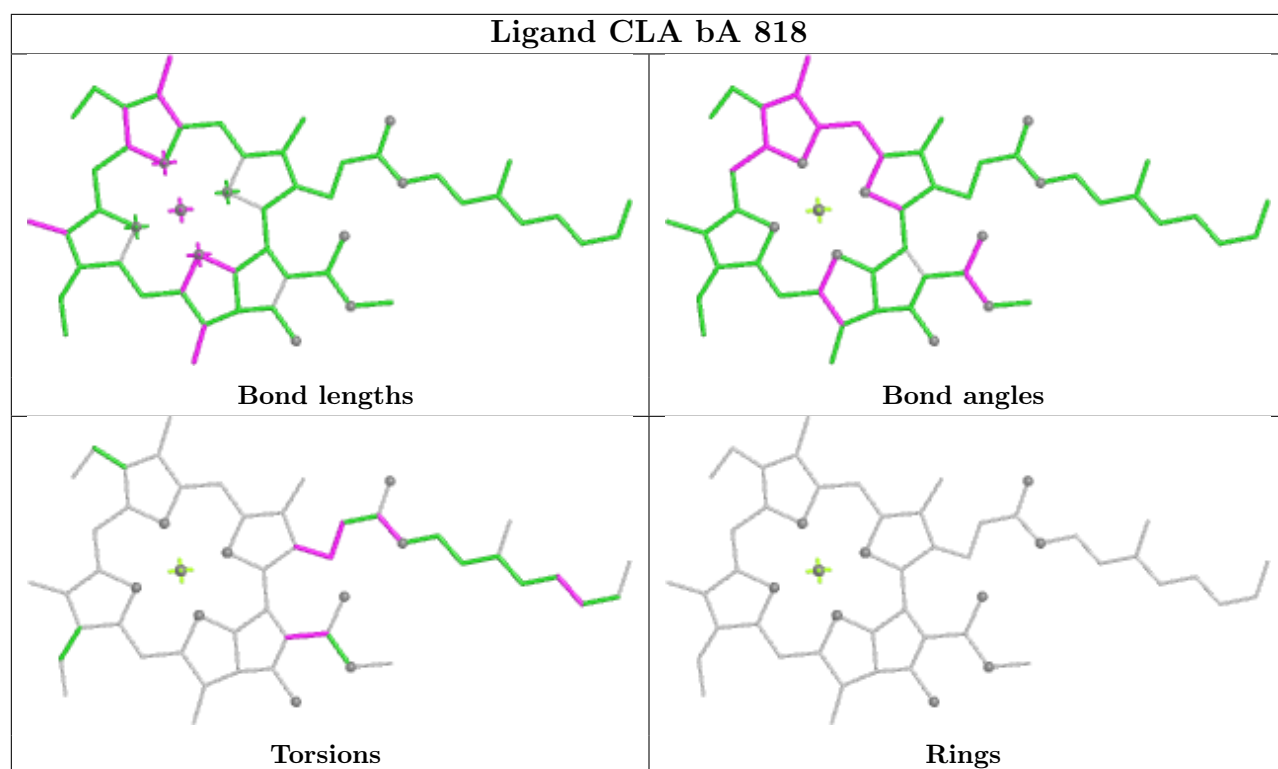


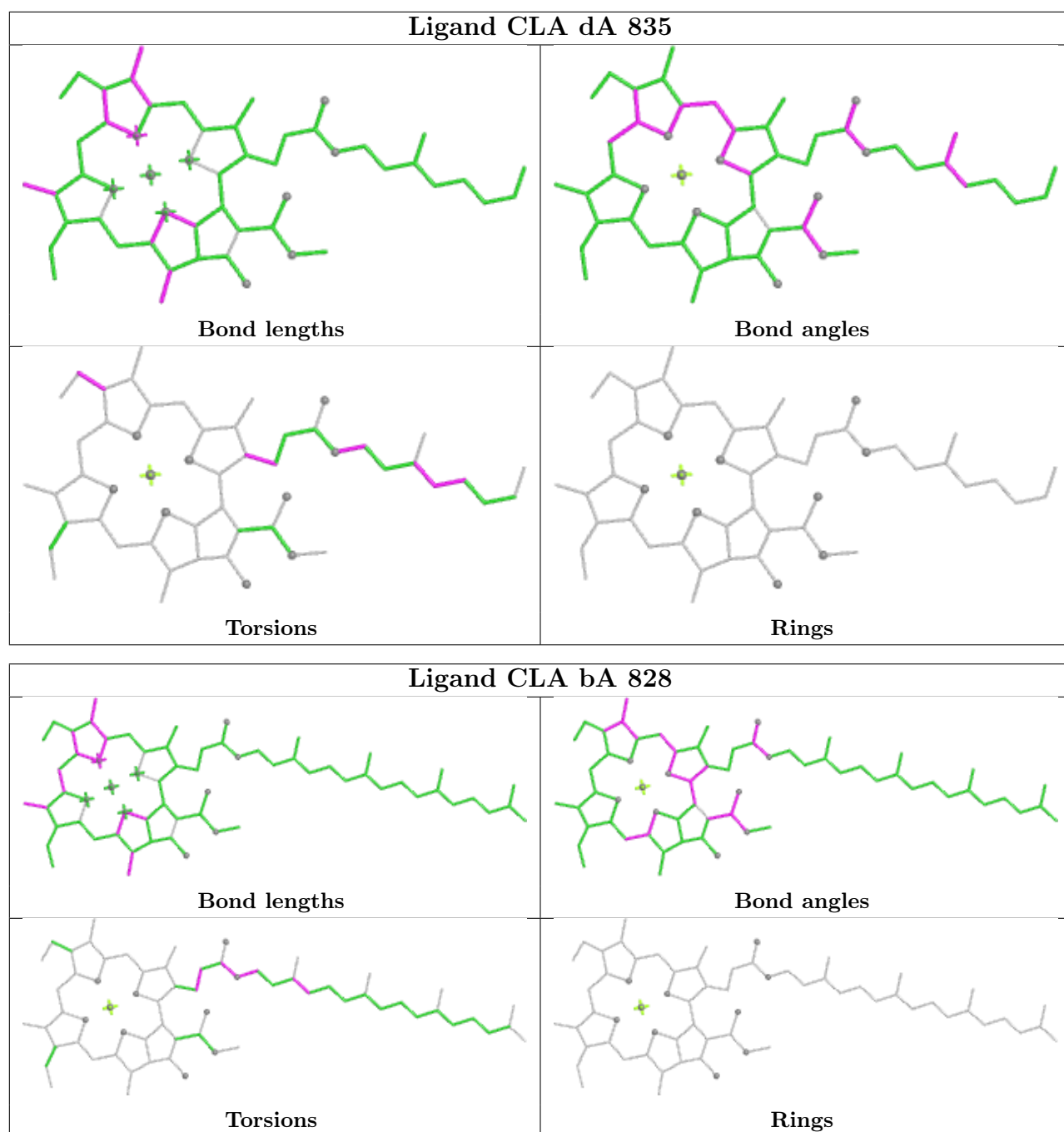


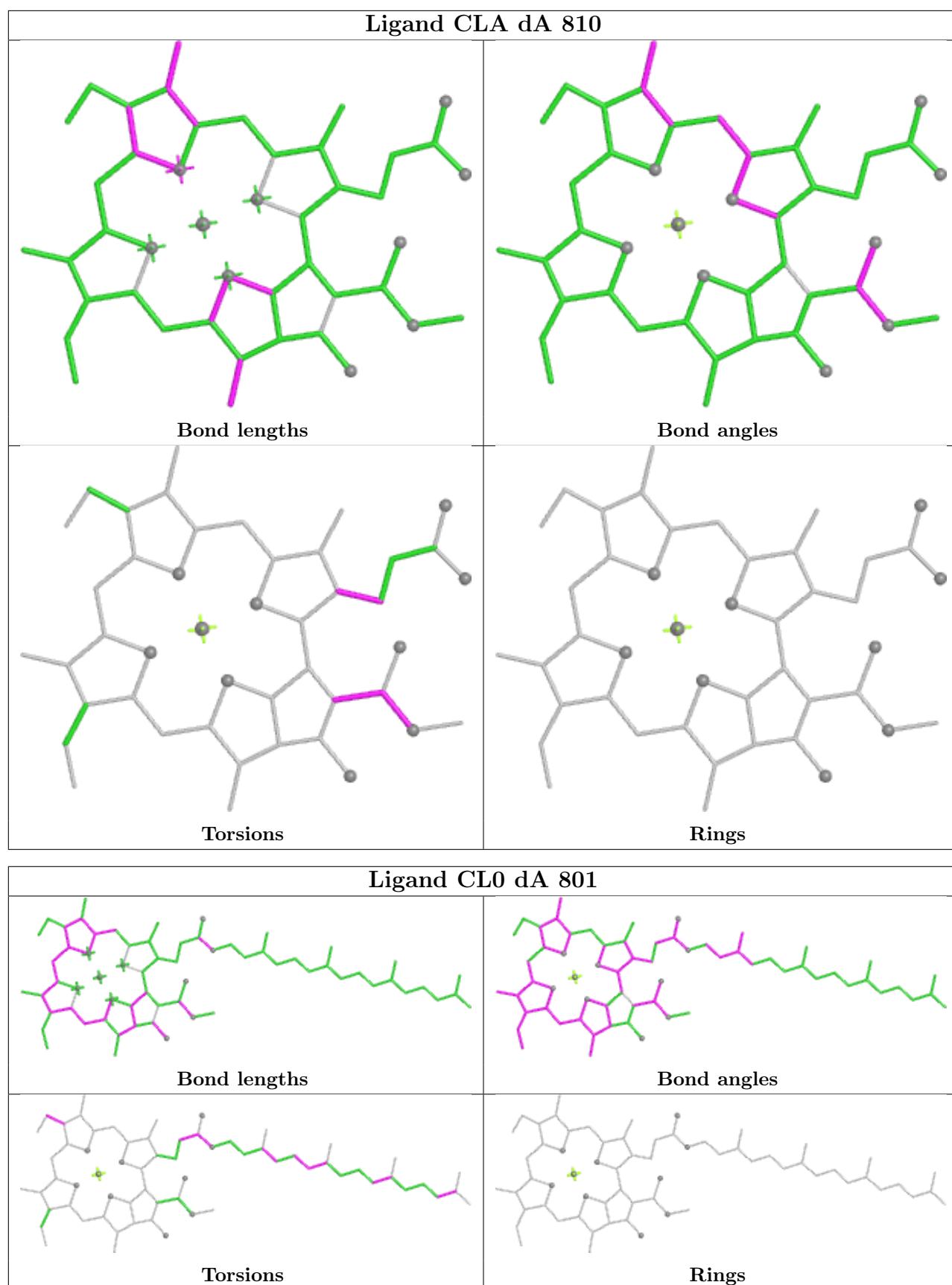


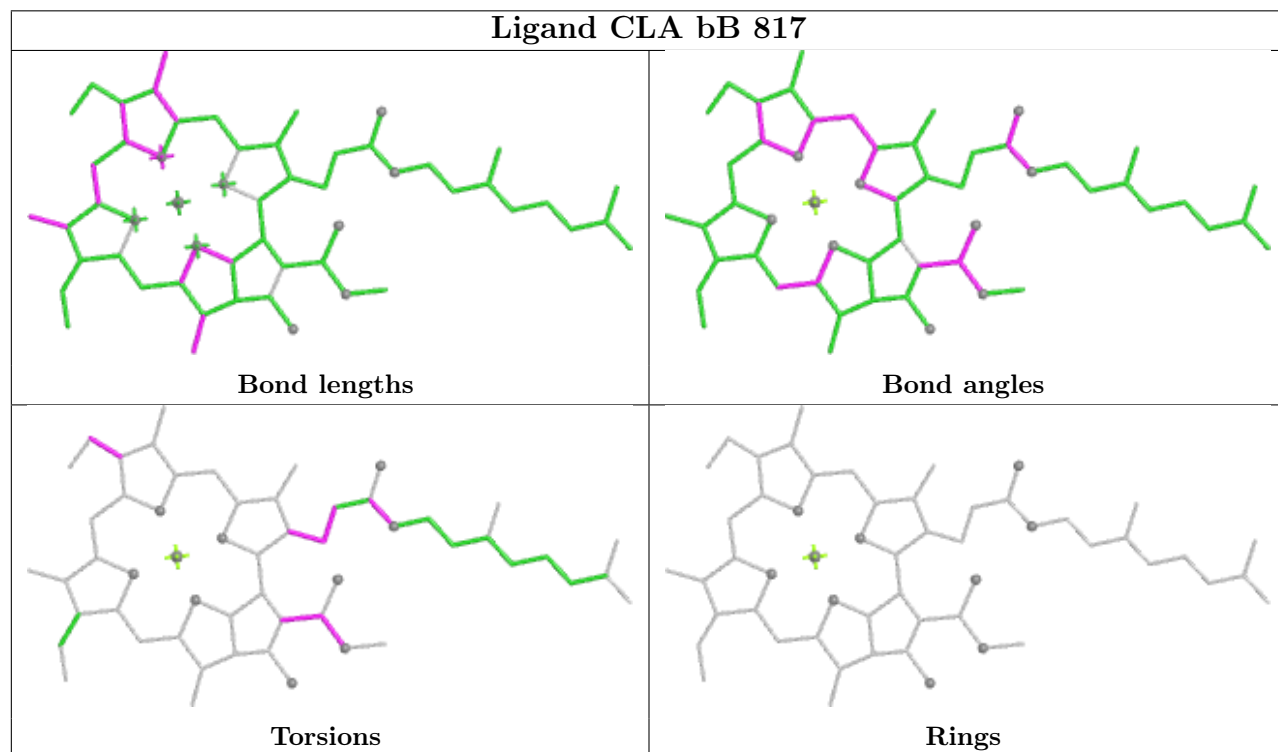
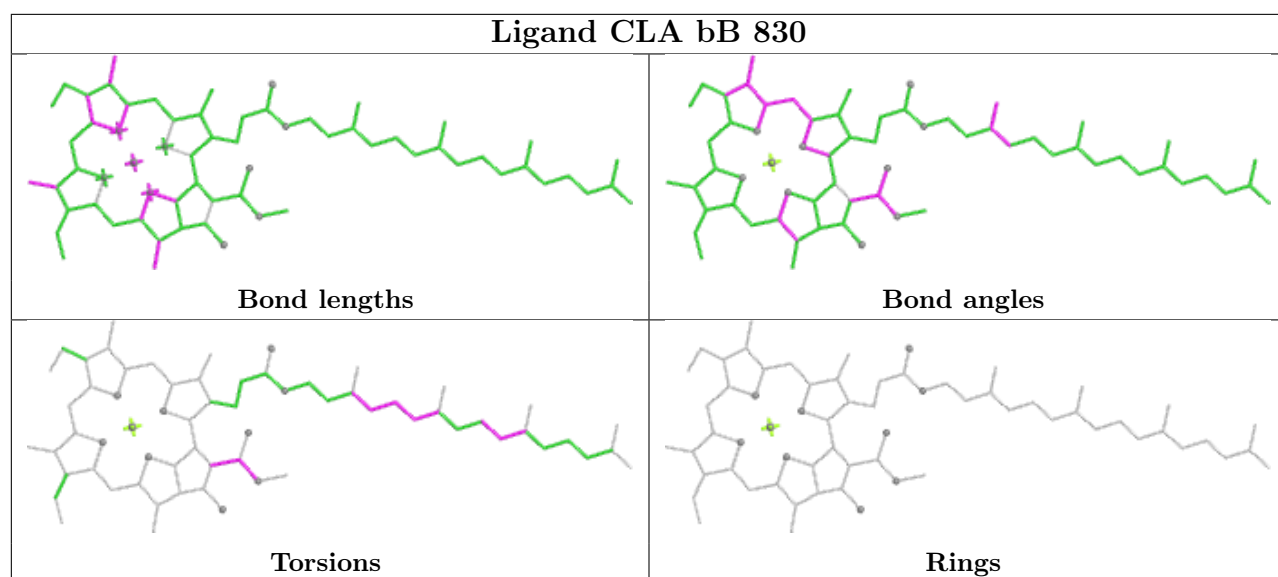




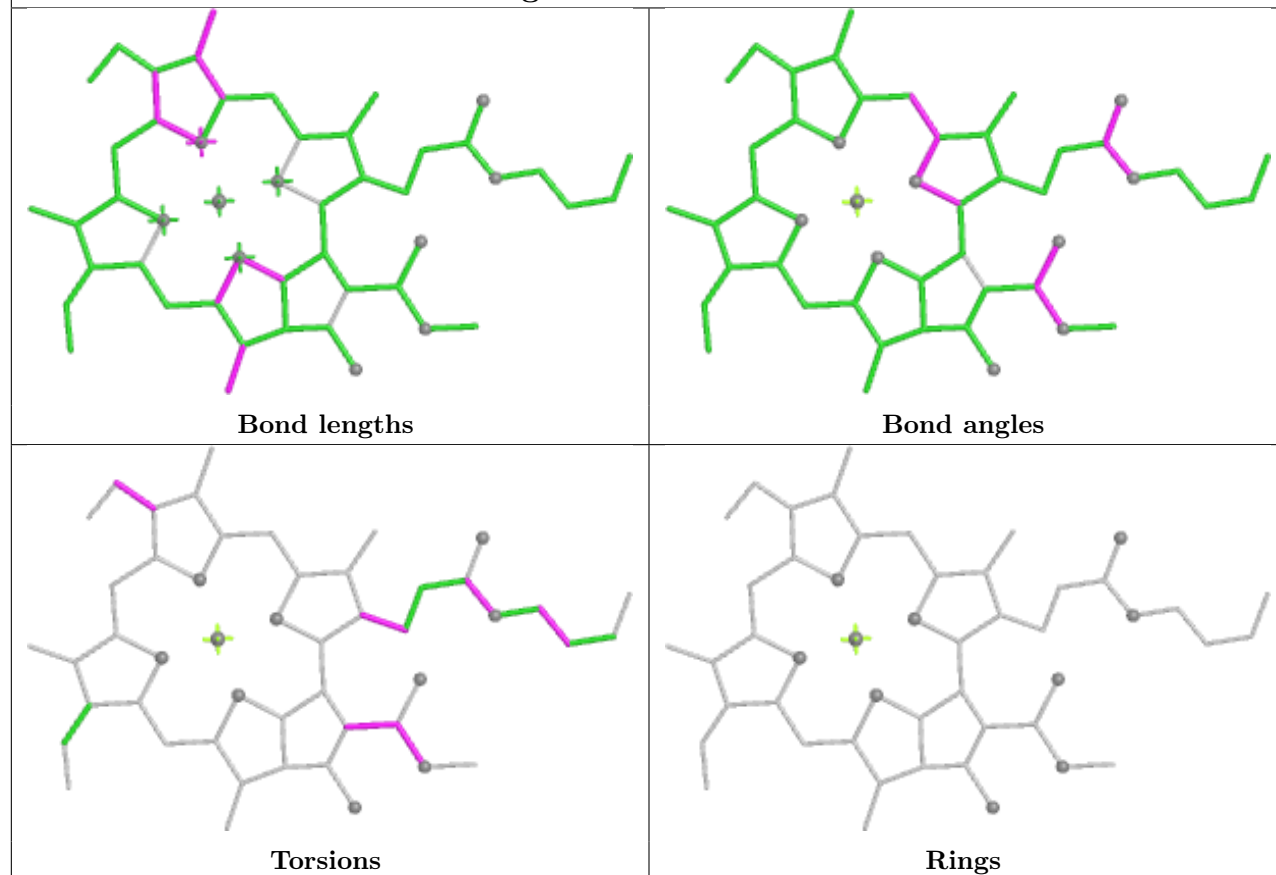




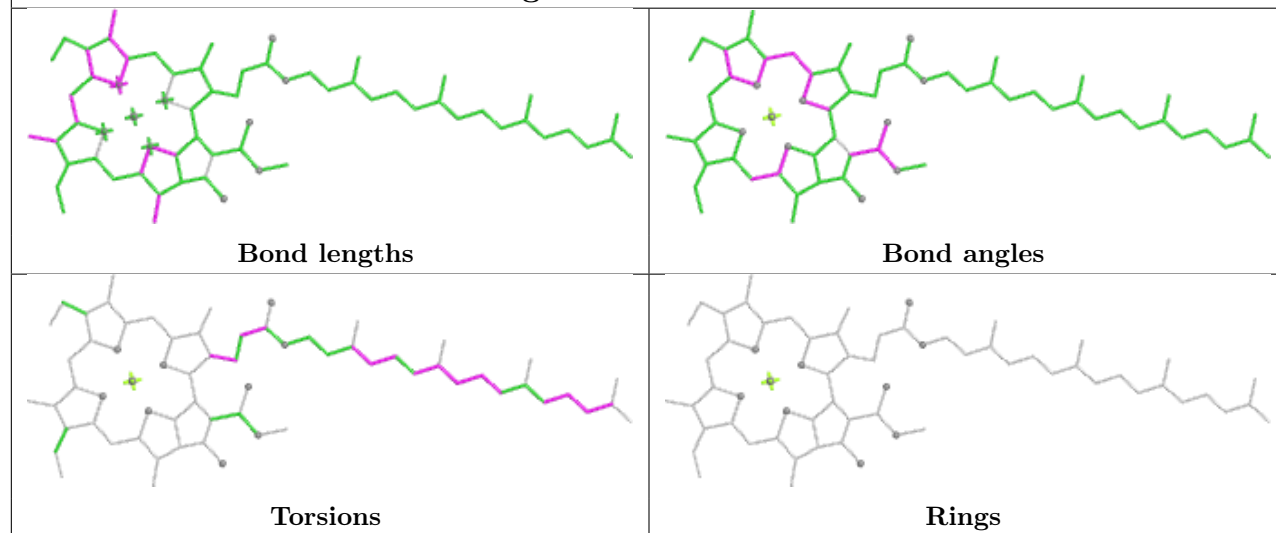


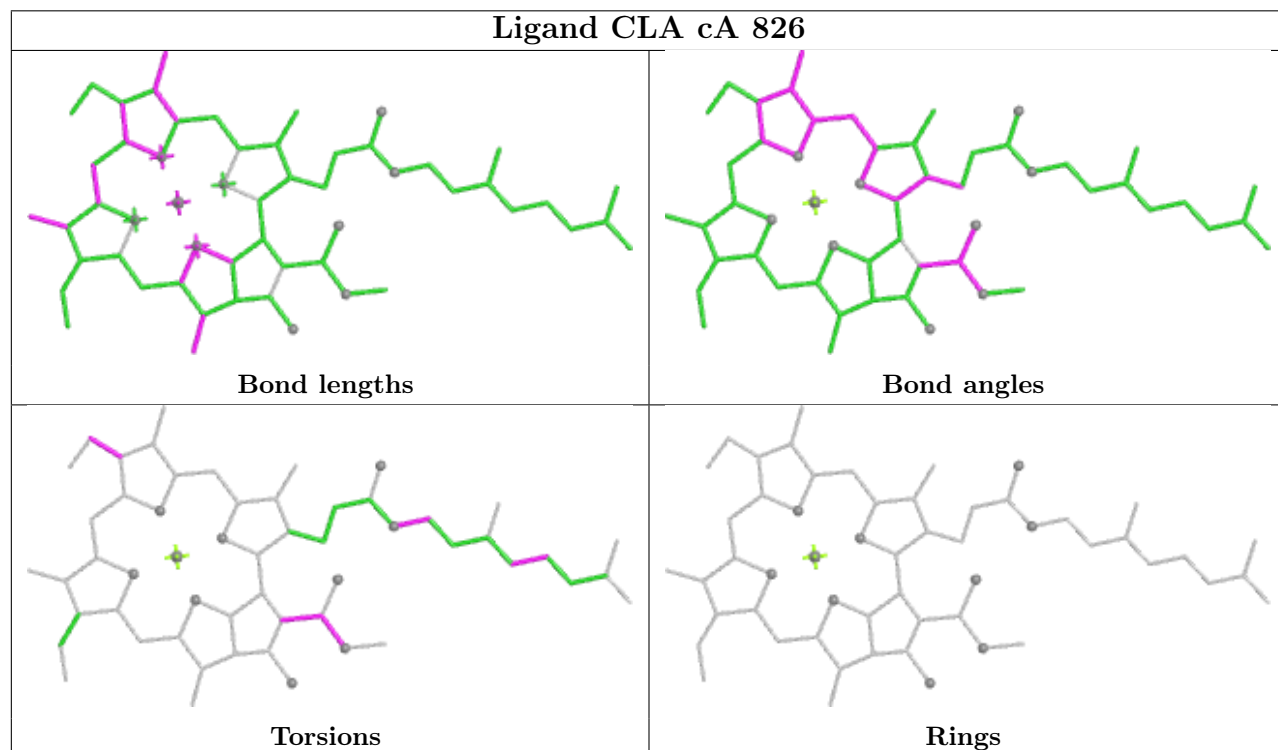
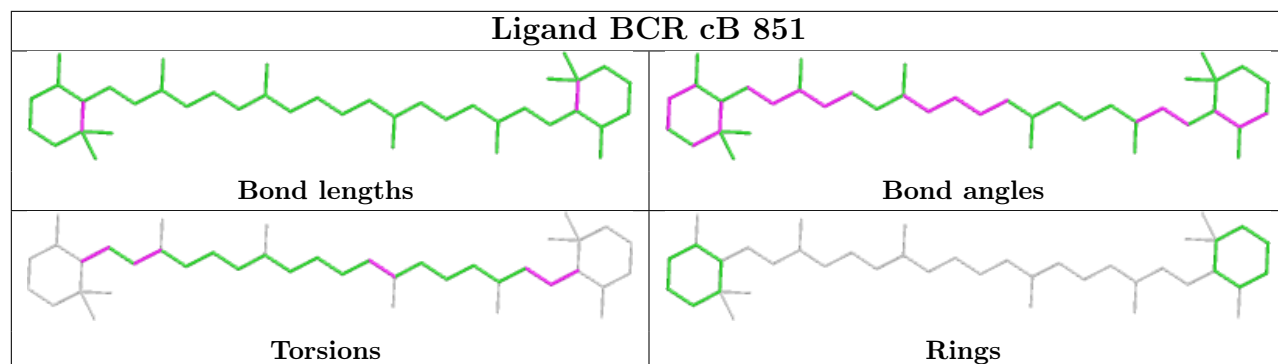


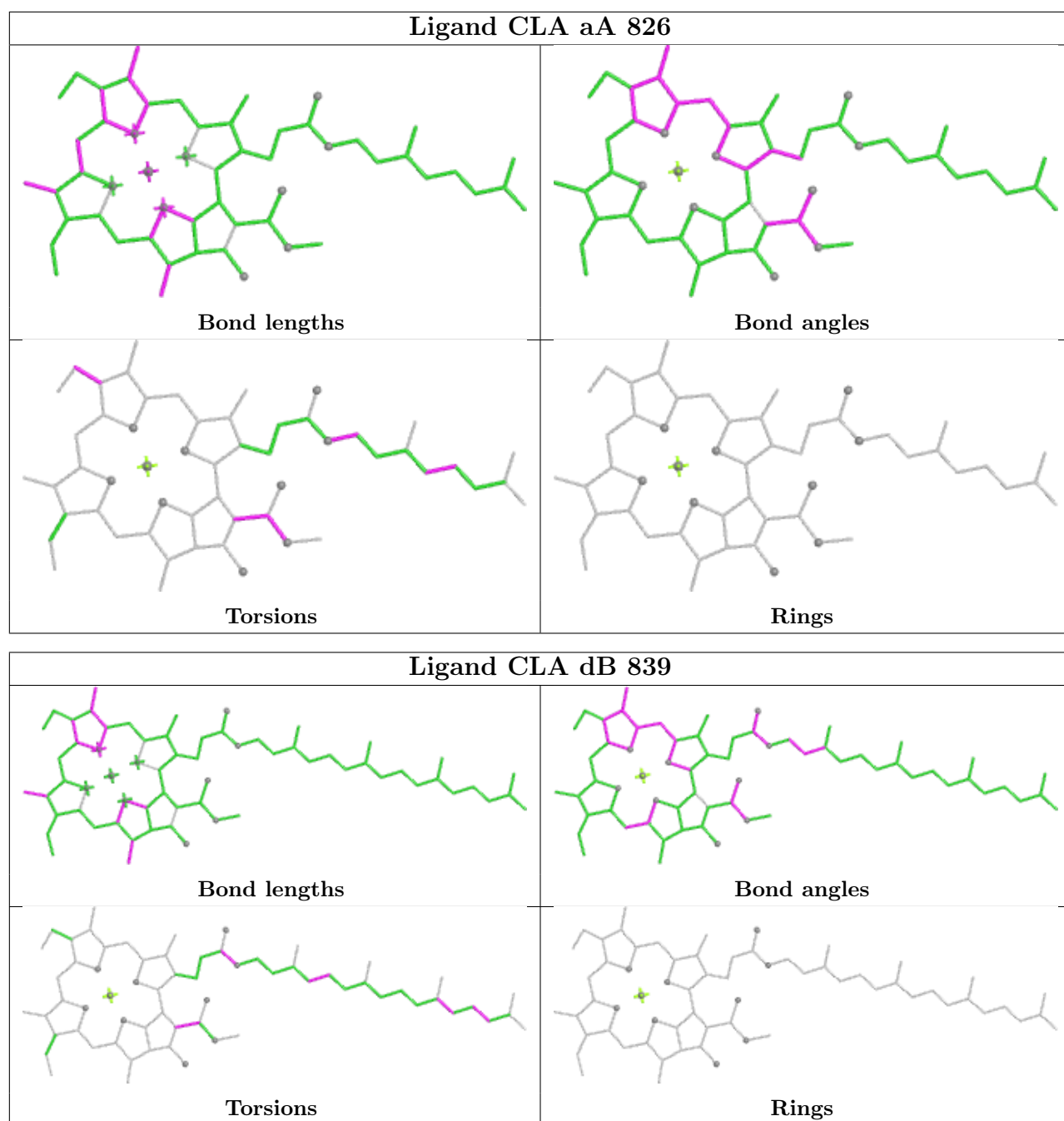
Ligand CLA bA 816



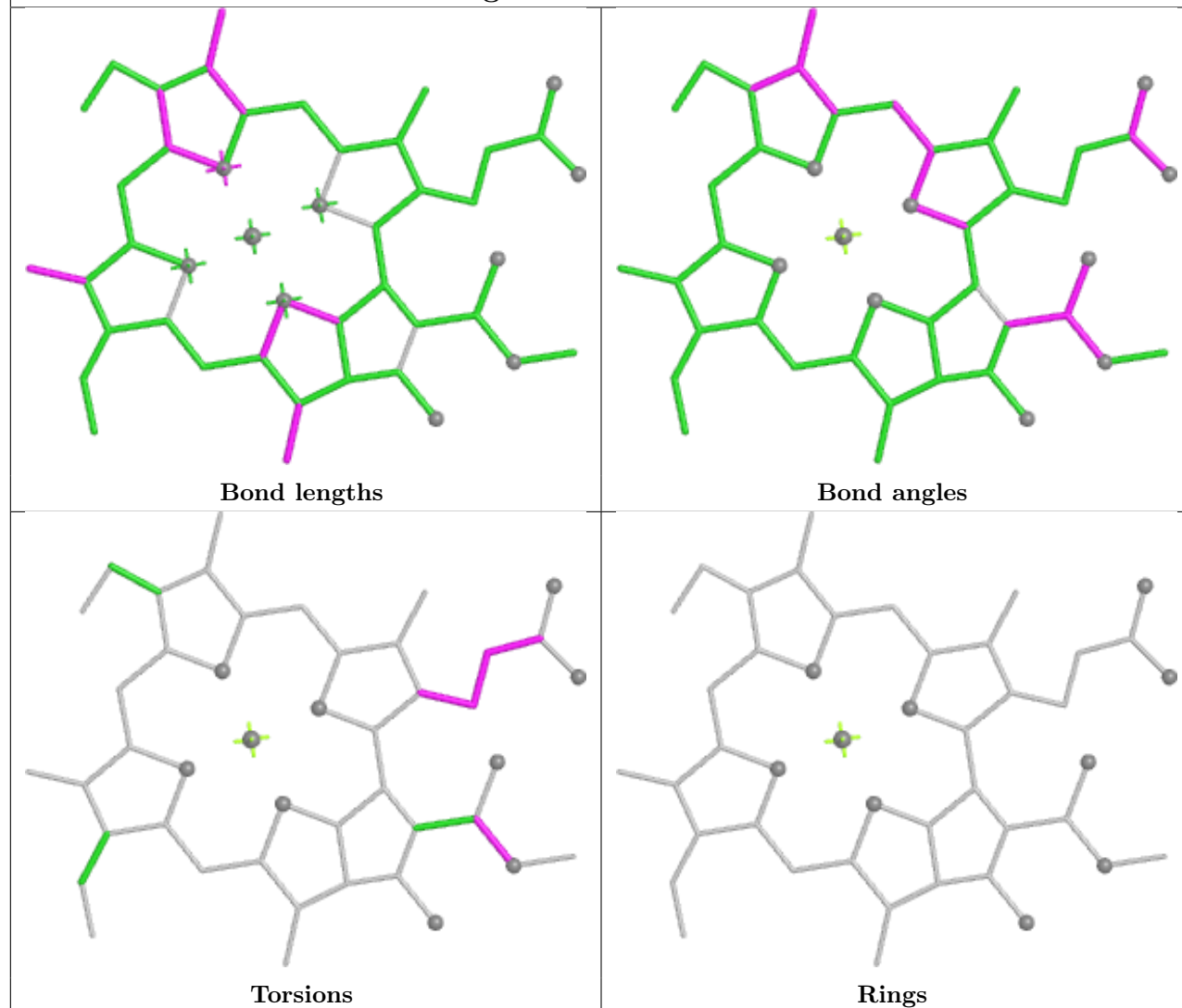
Ligand CLA bB 833



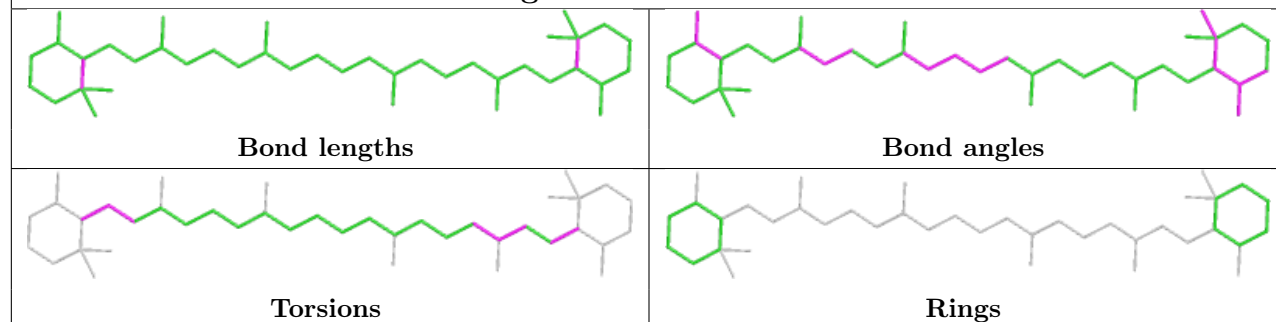


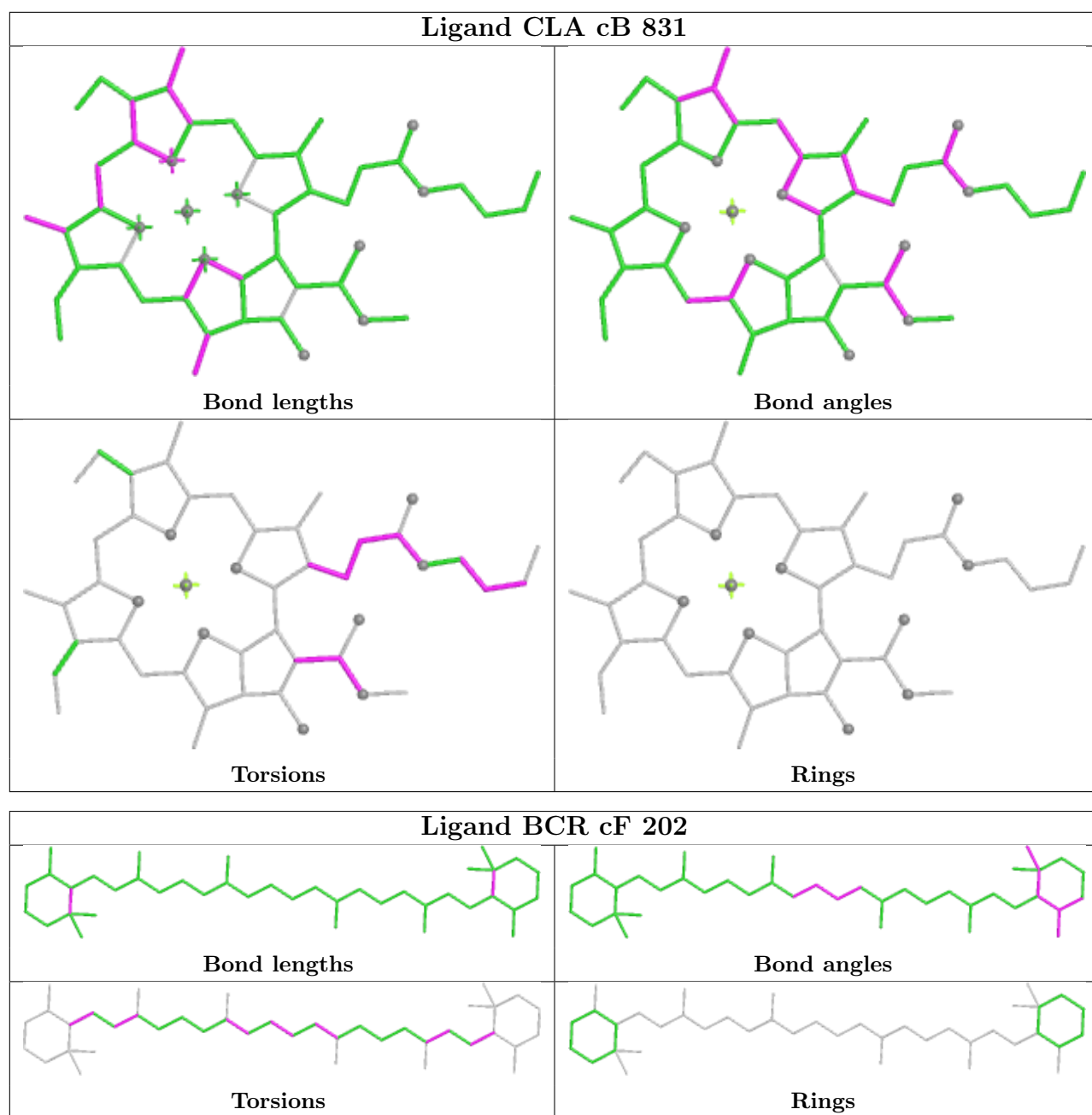


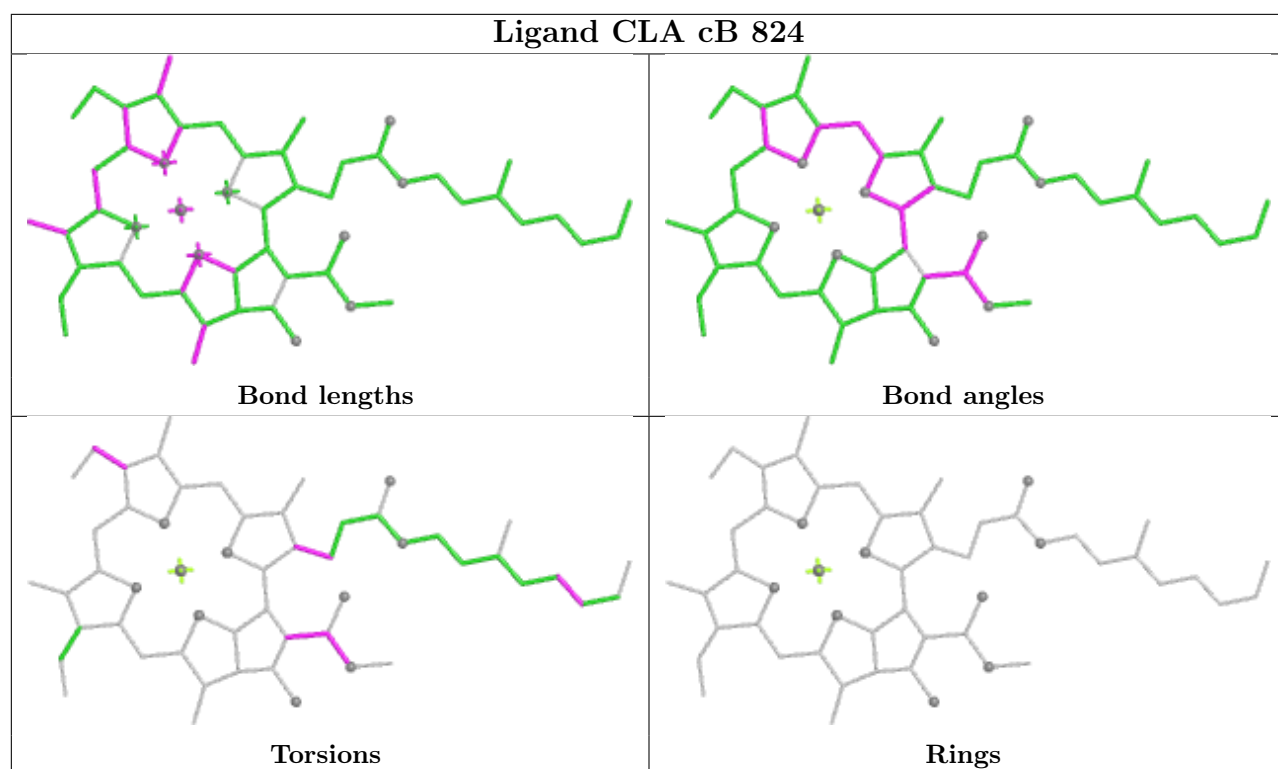
Ligand CLA dA 836



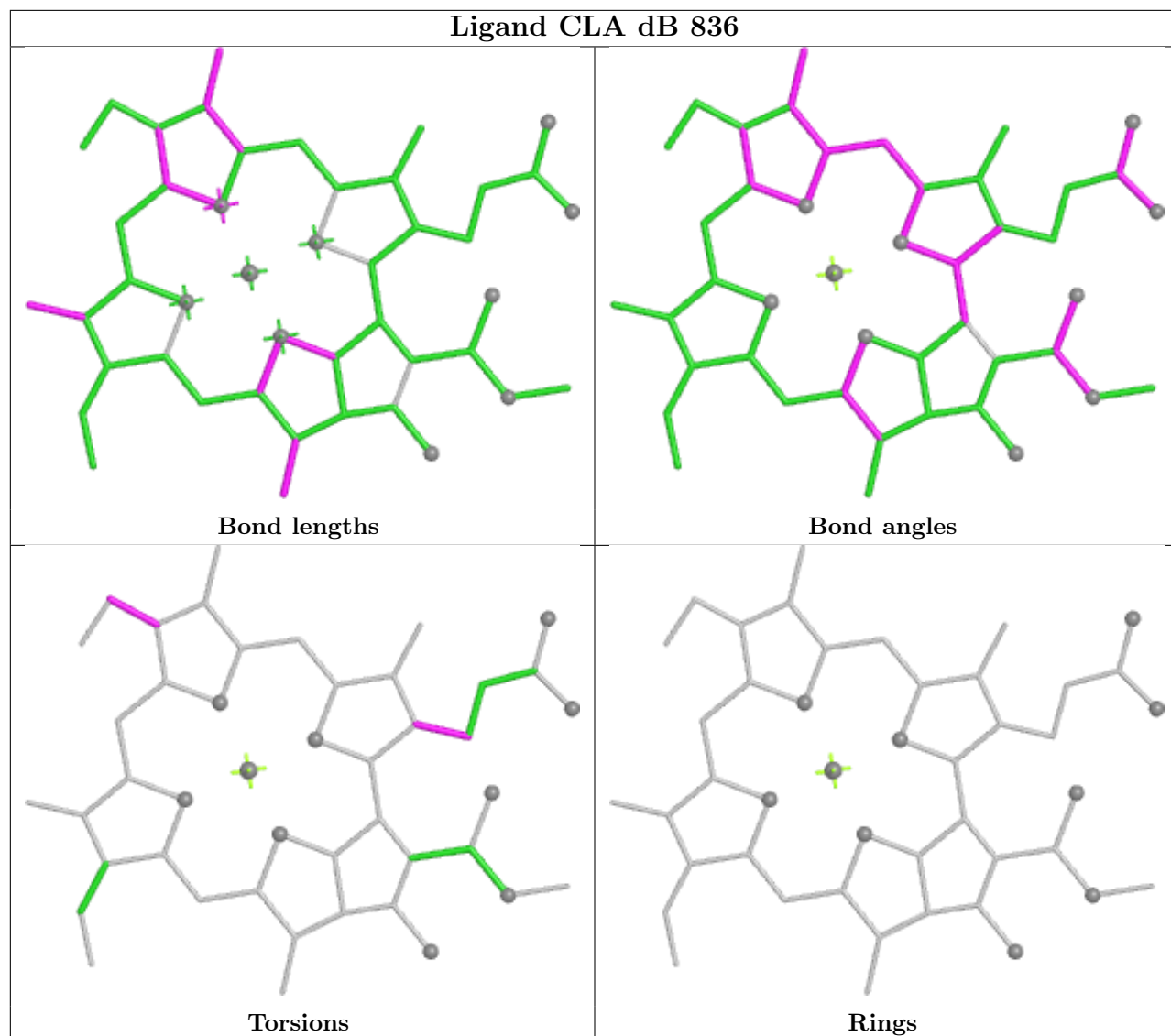
Ligand BCR aA 848

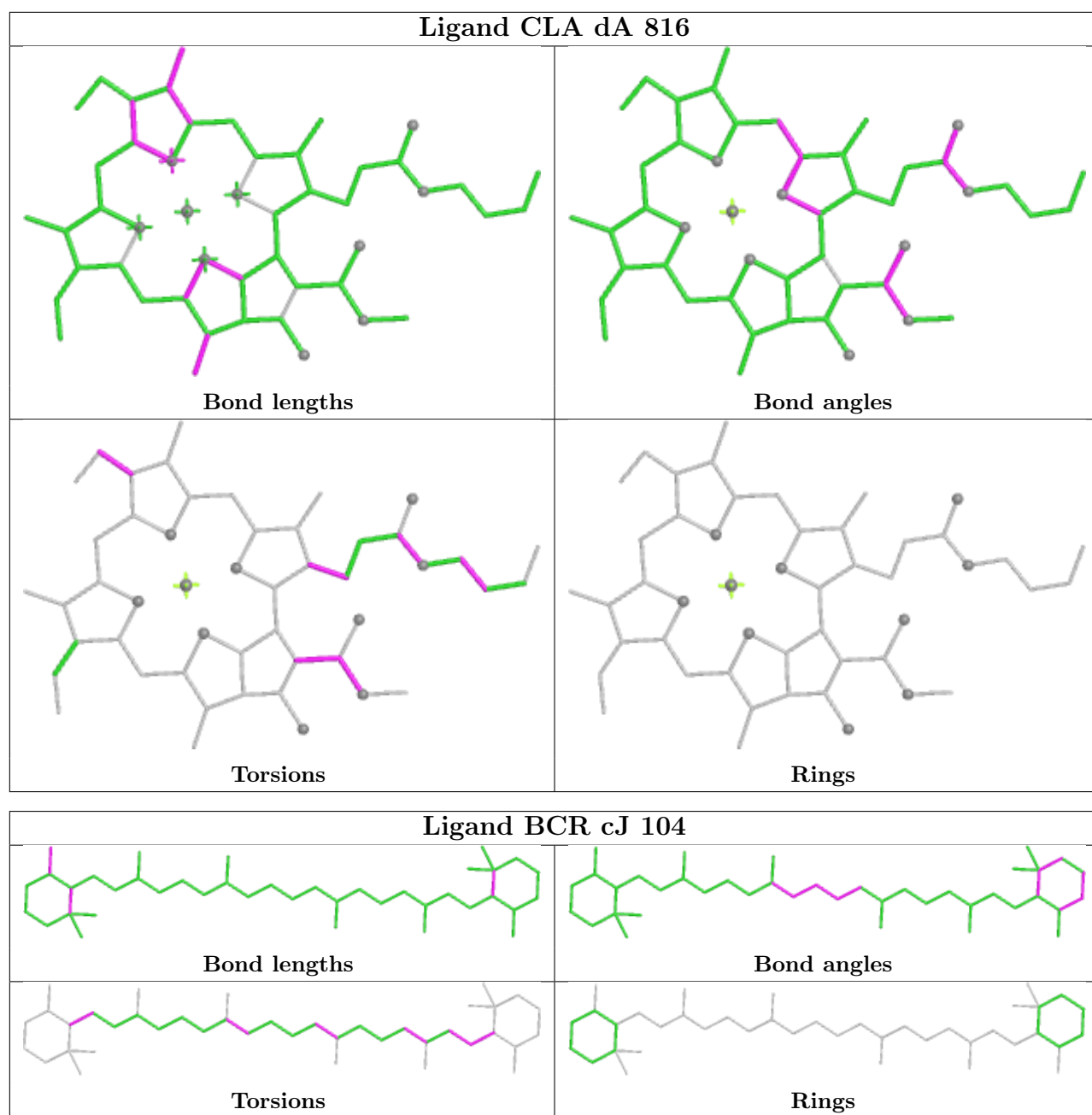


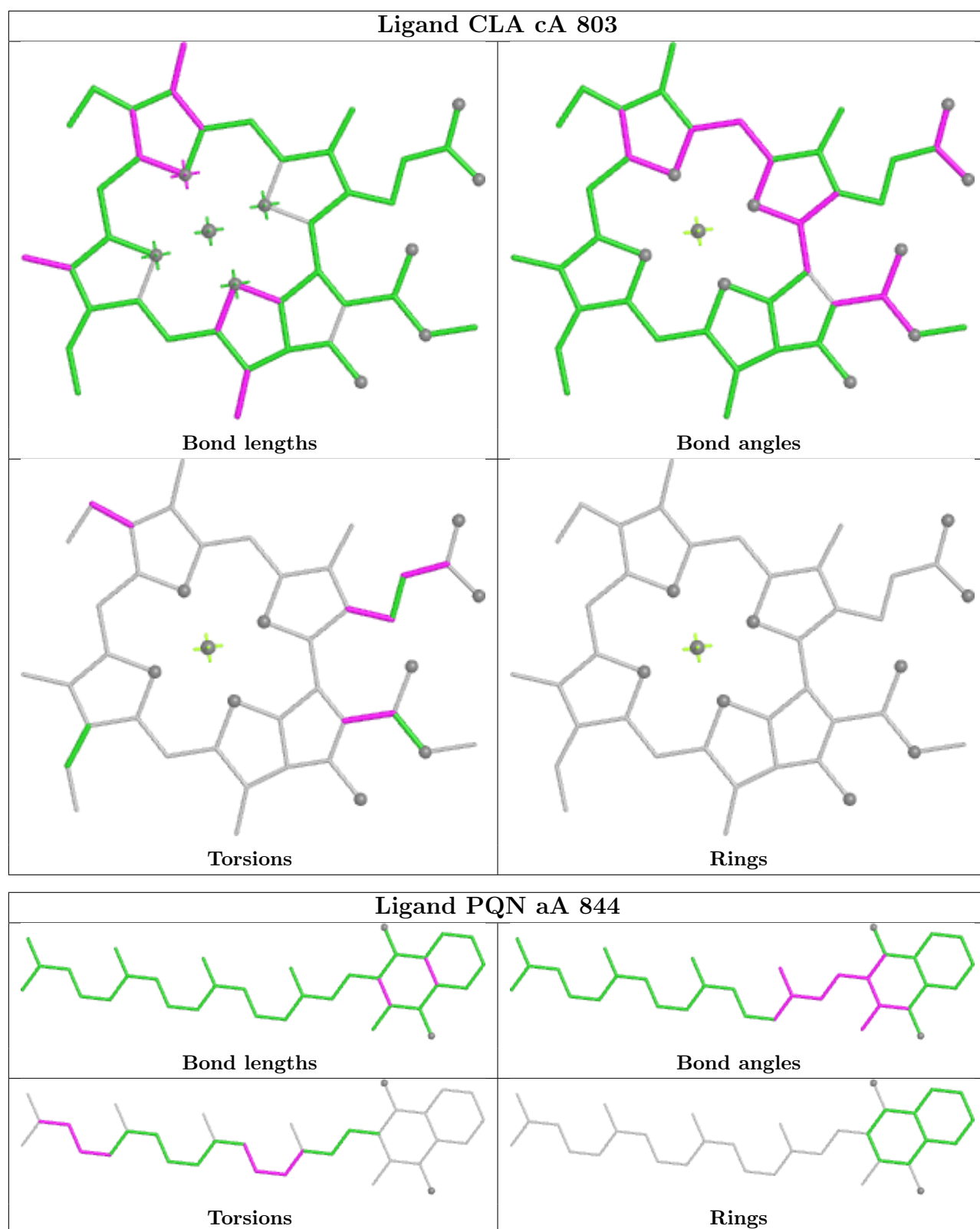


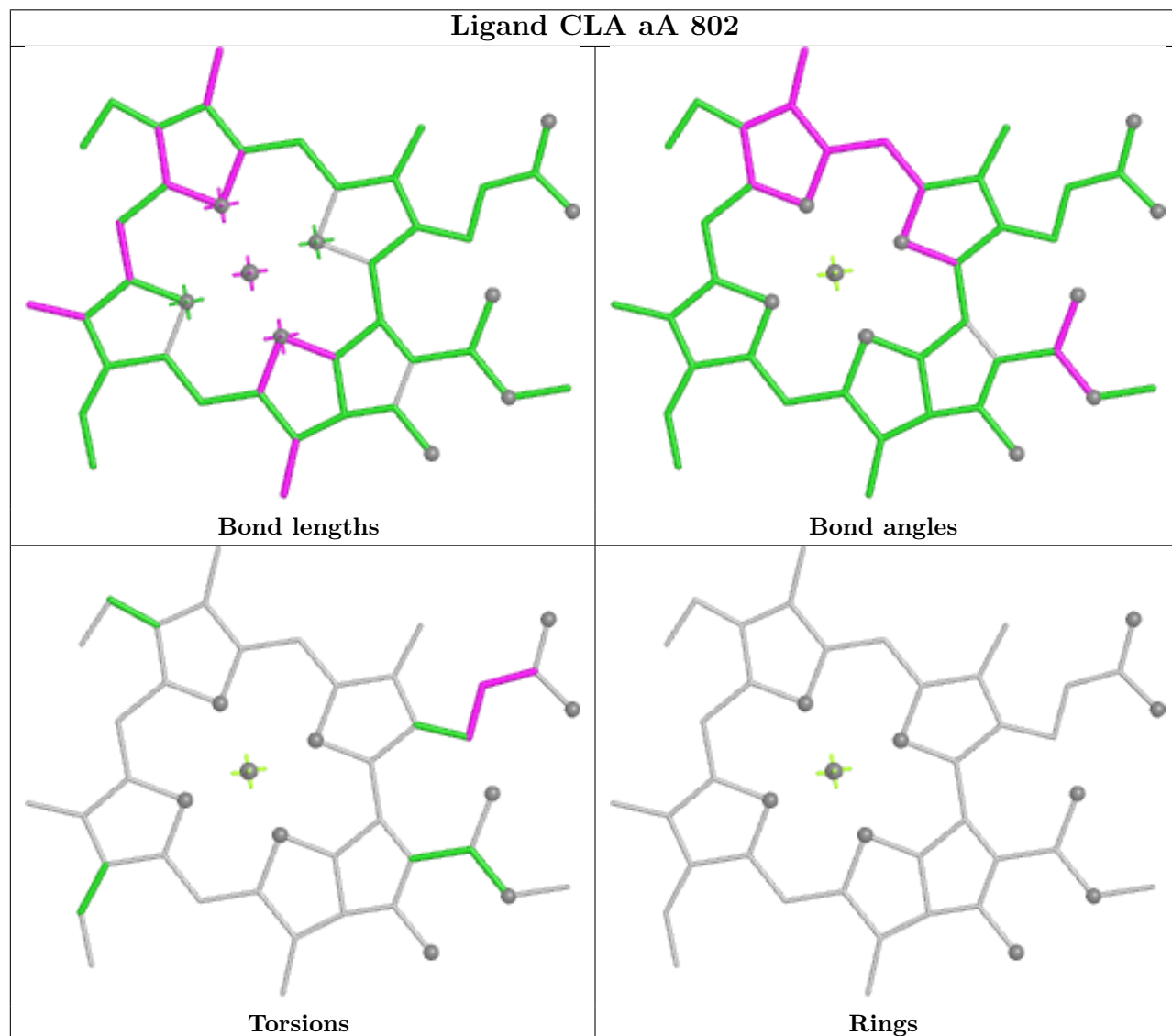
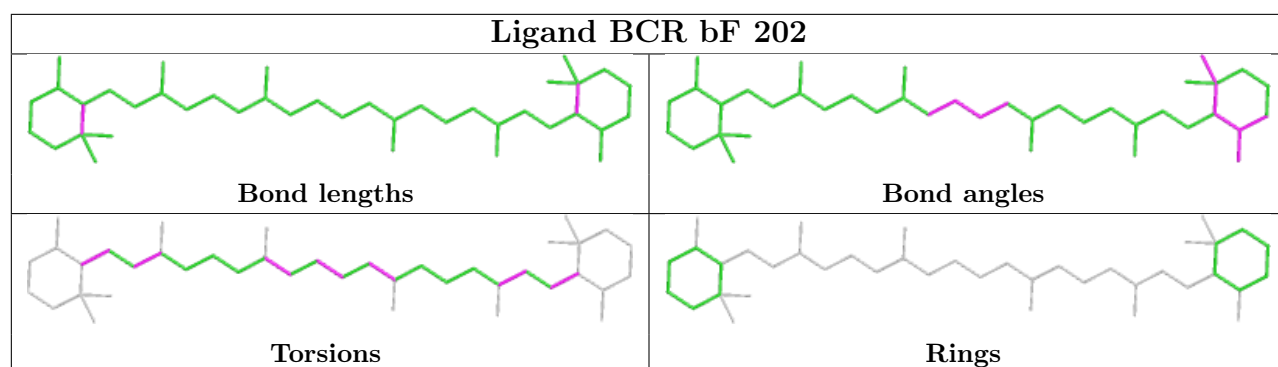


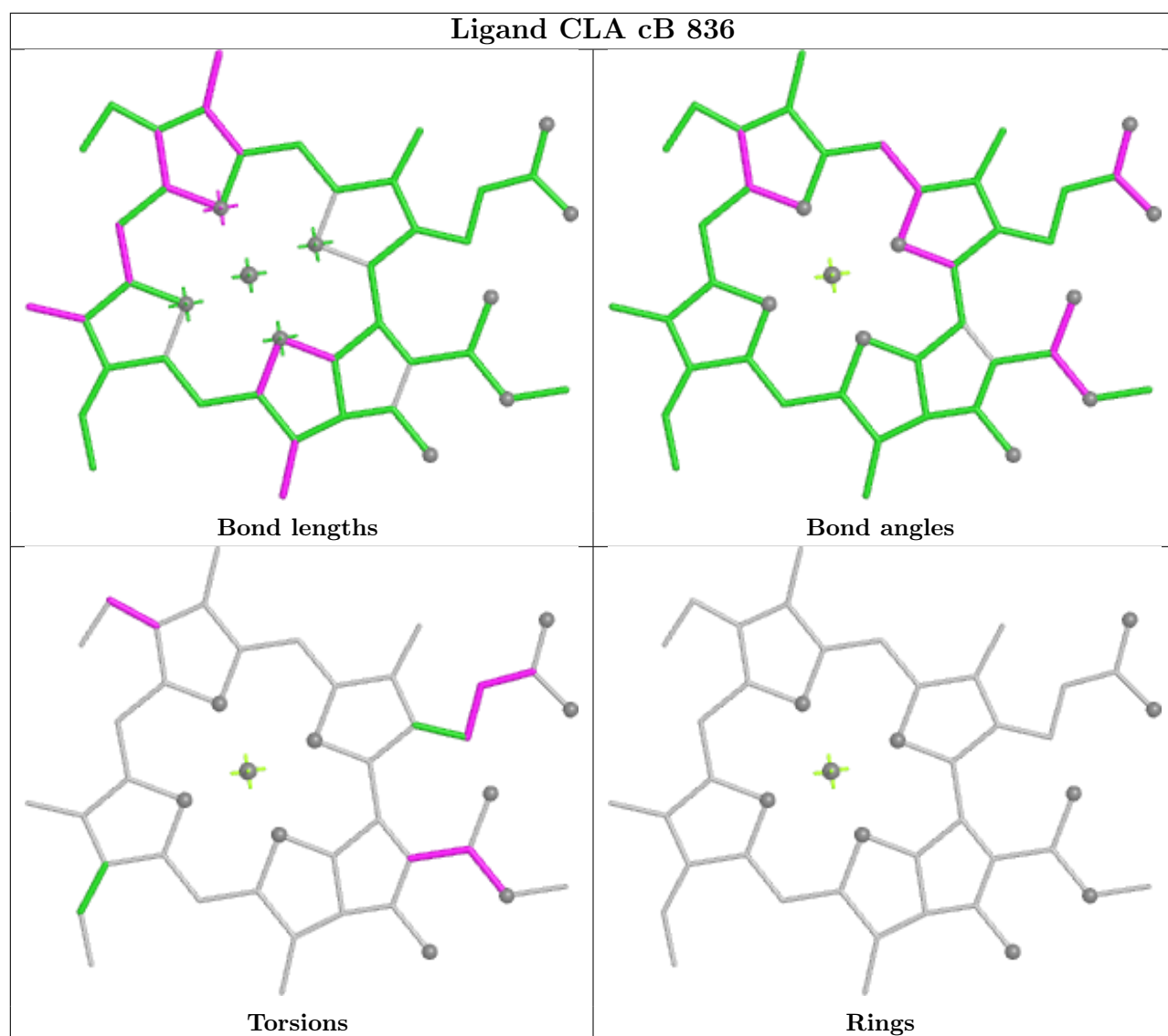
Ligand CLA dB 836



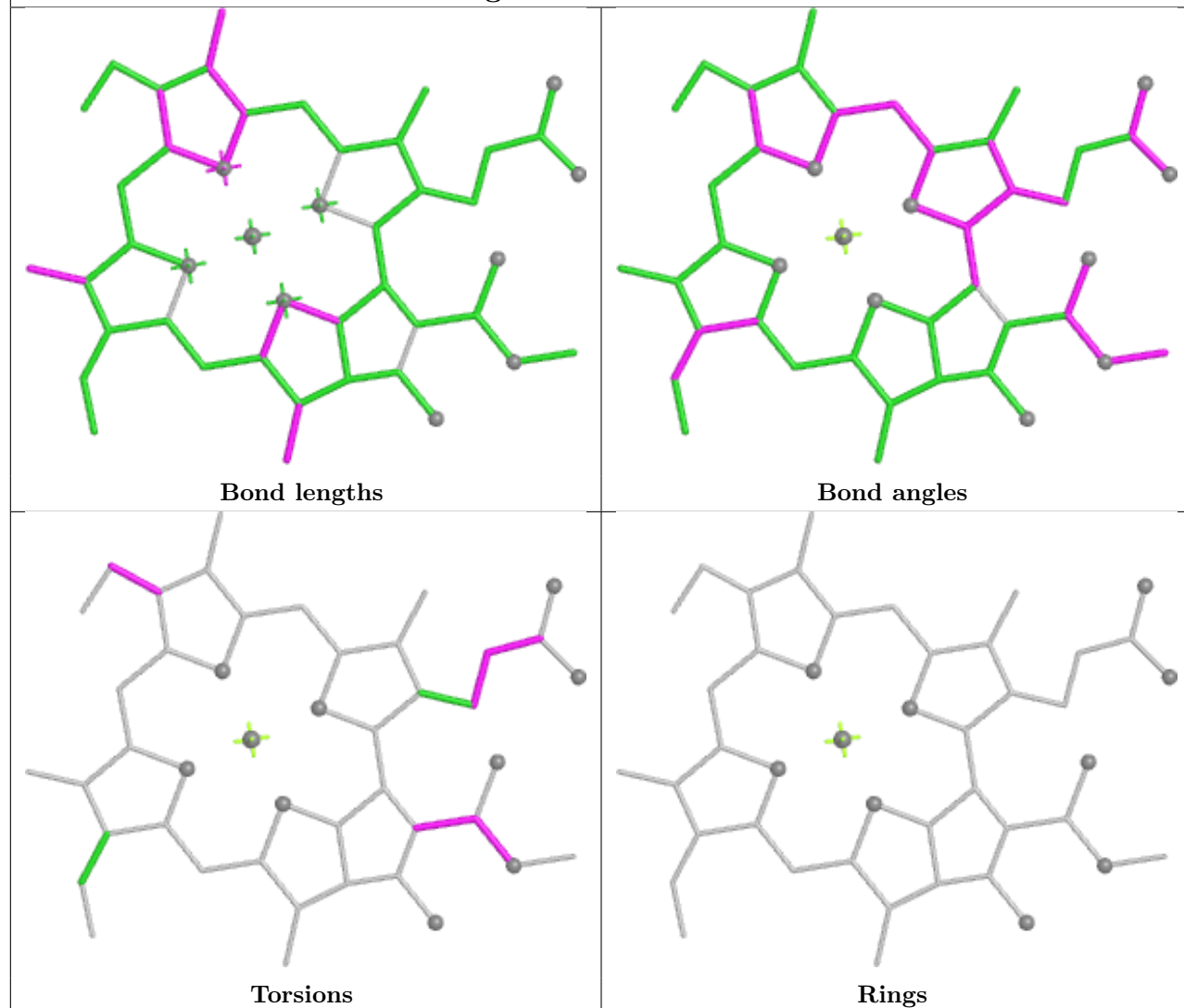




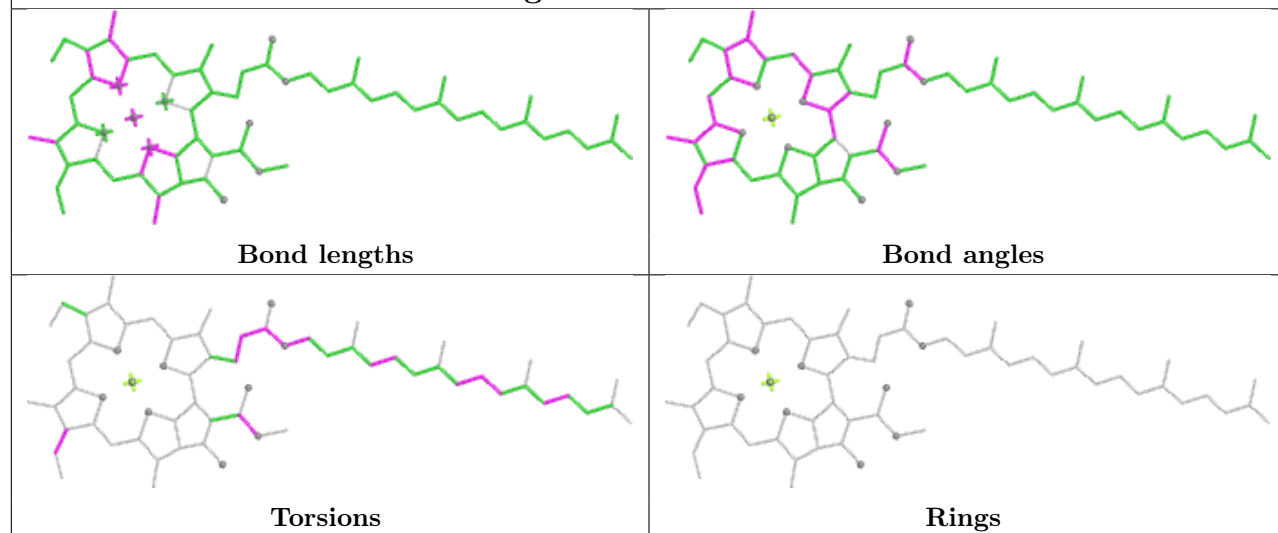


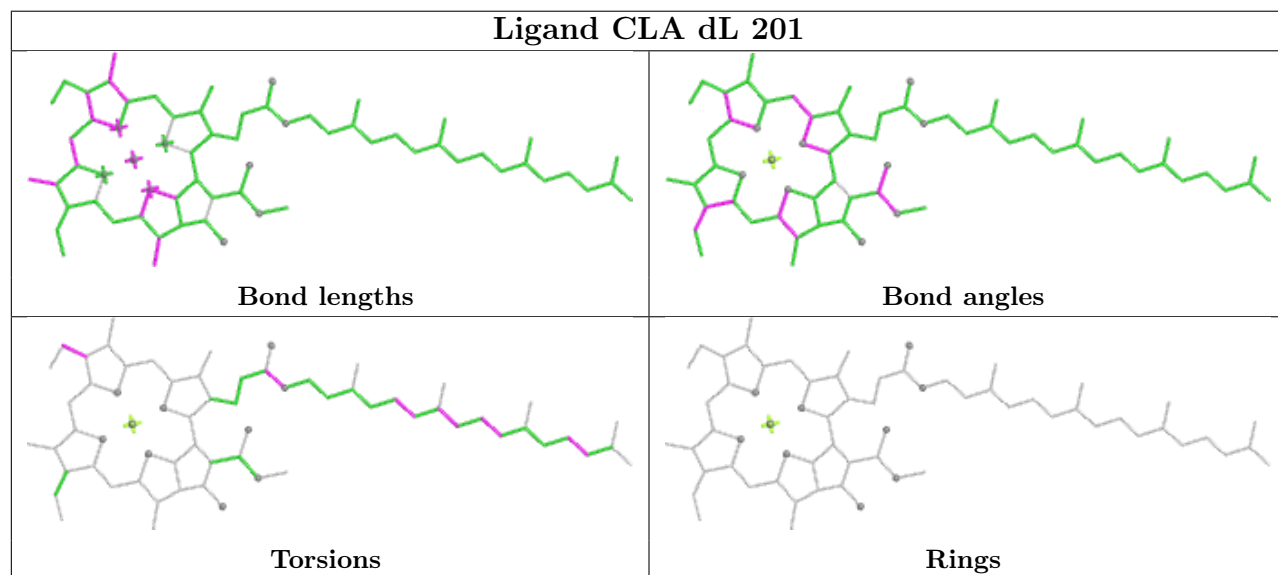
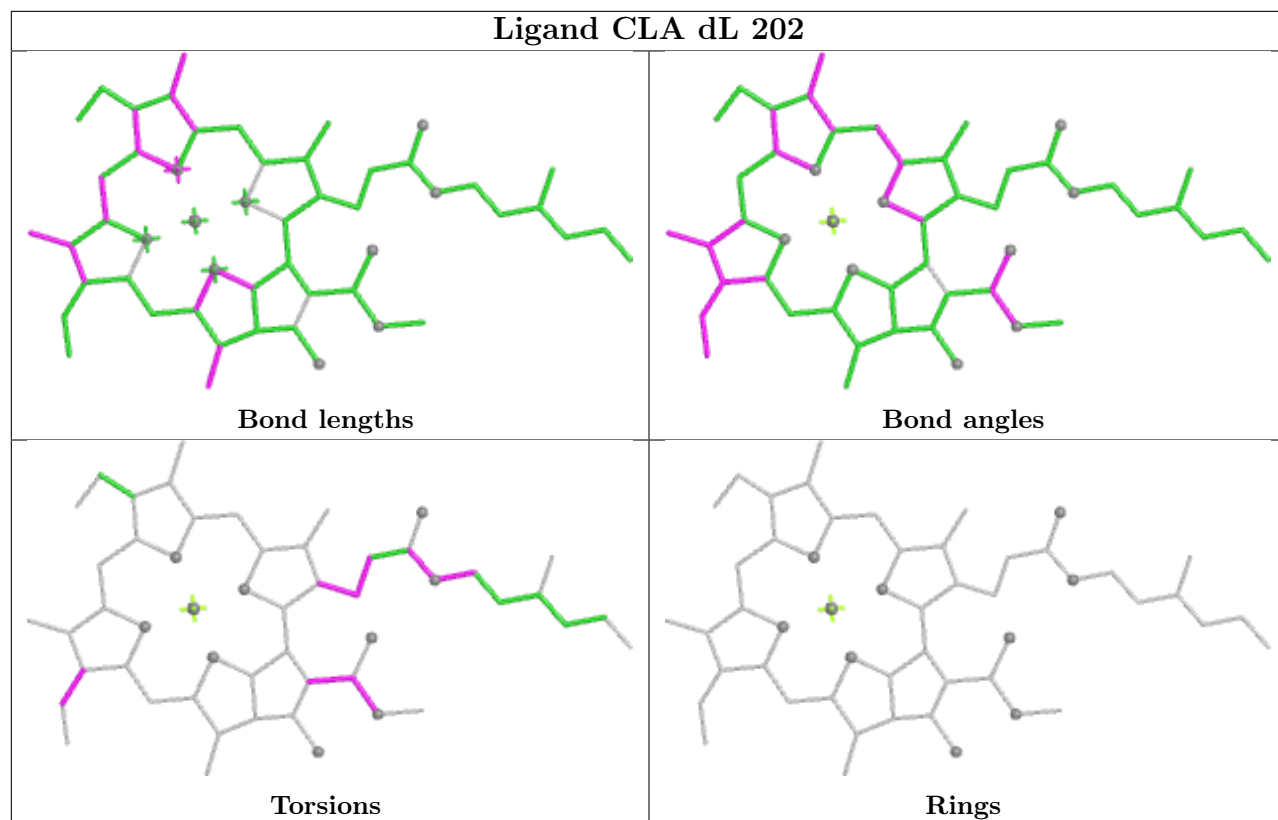


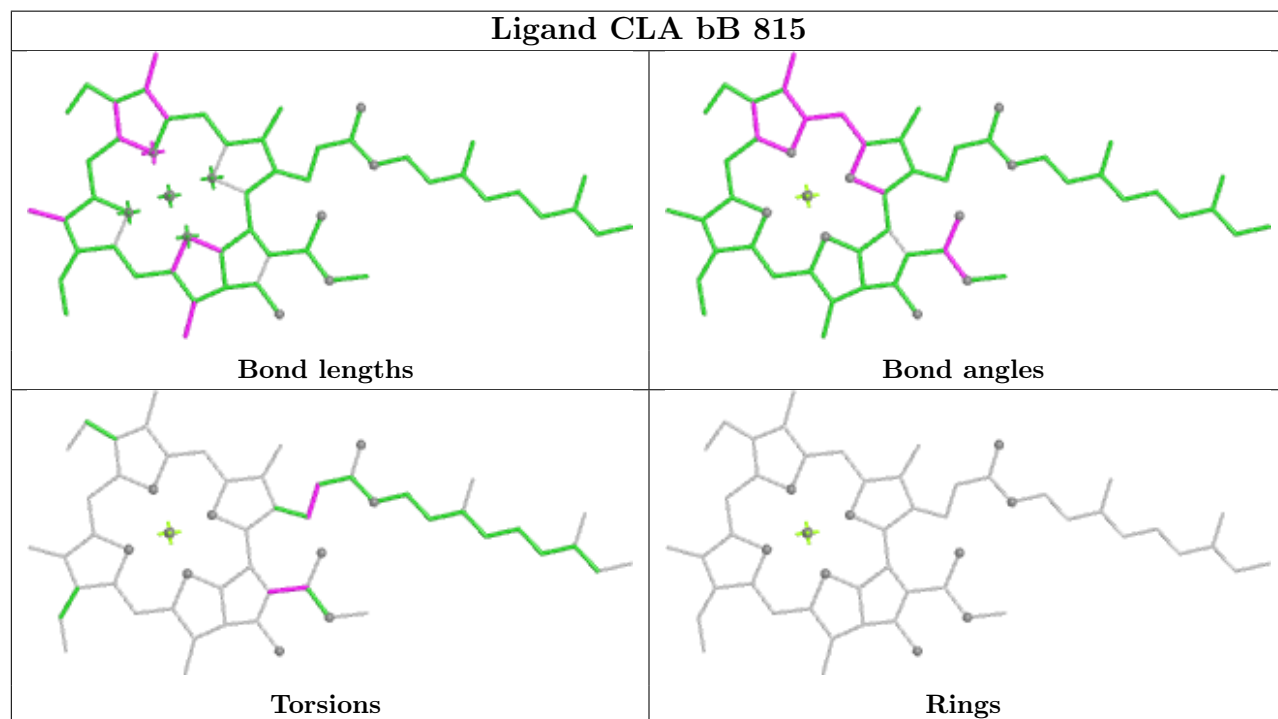
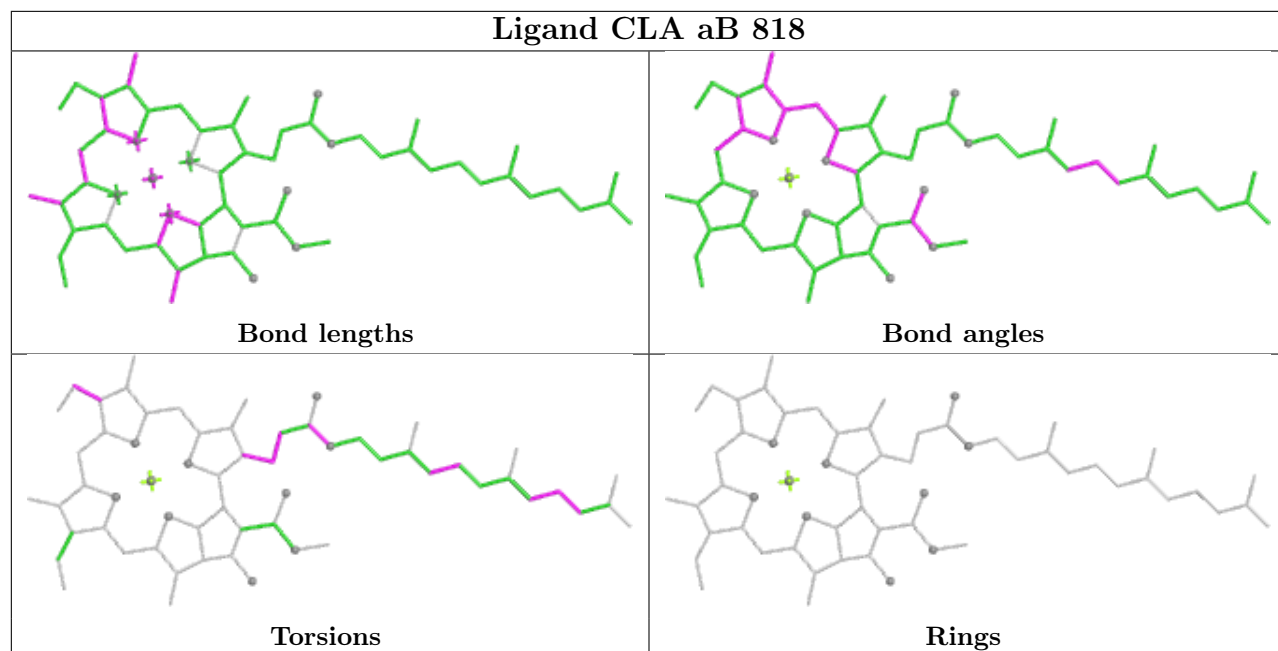
Ligand CLA cA 813



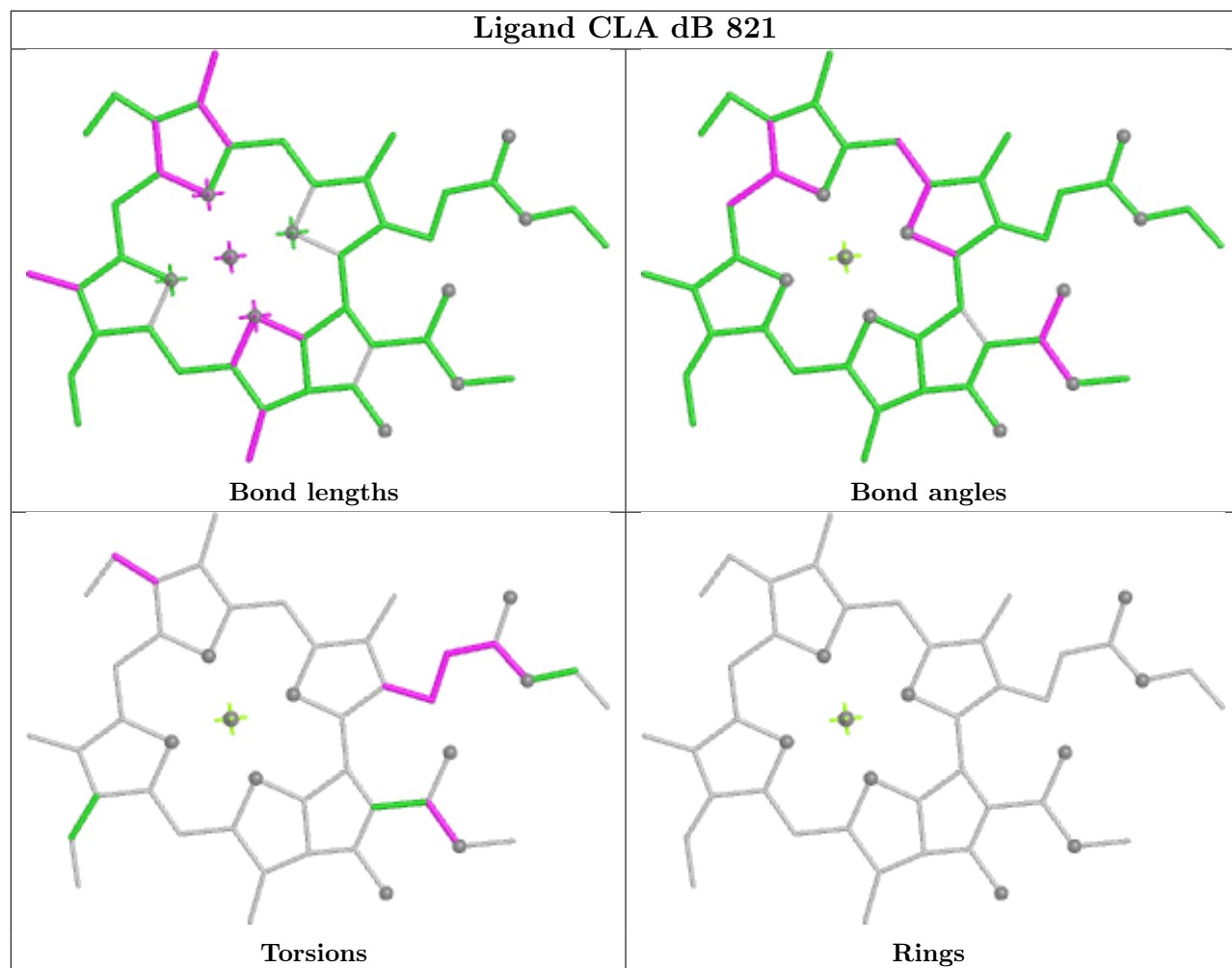
Ligand CLA cB 804

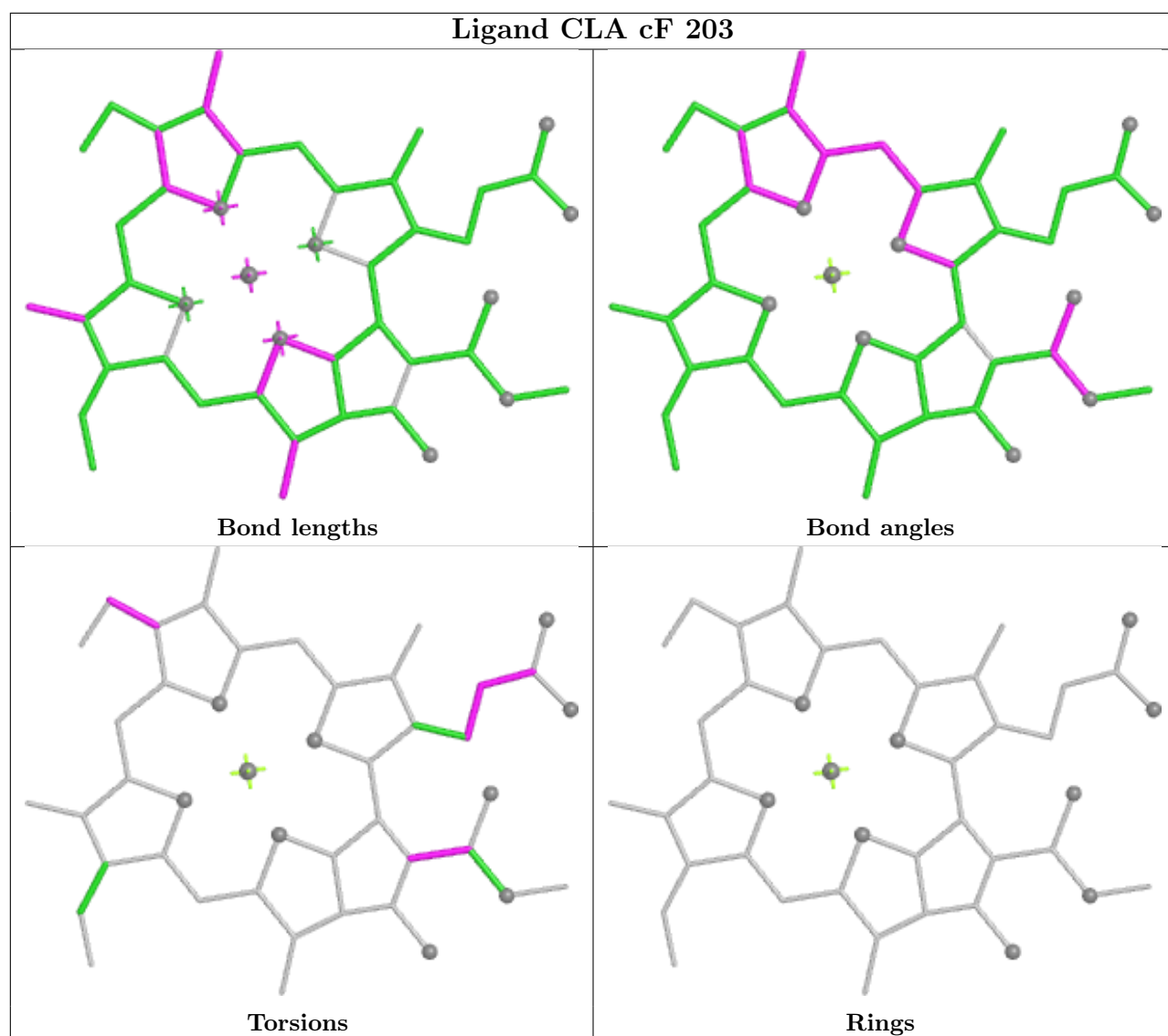


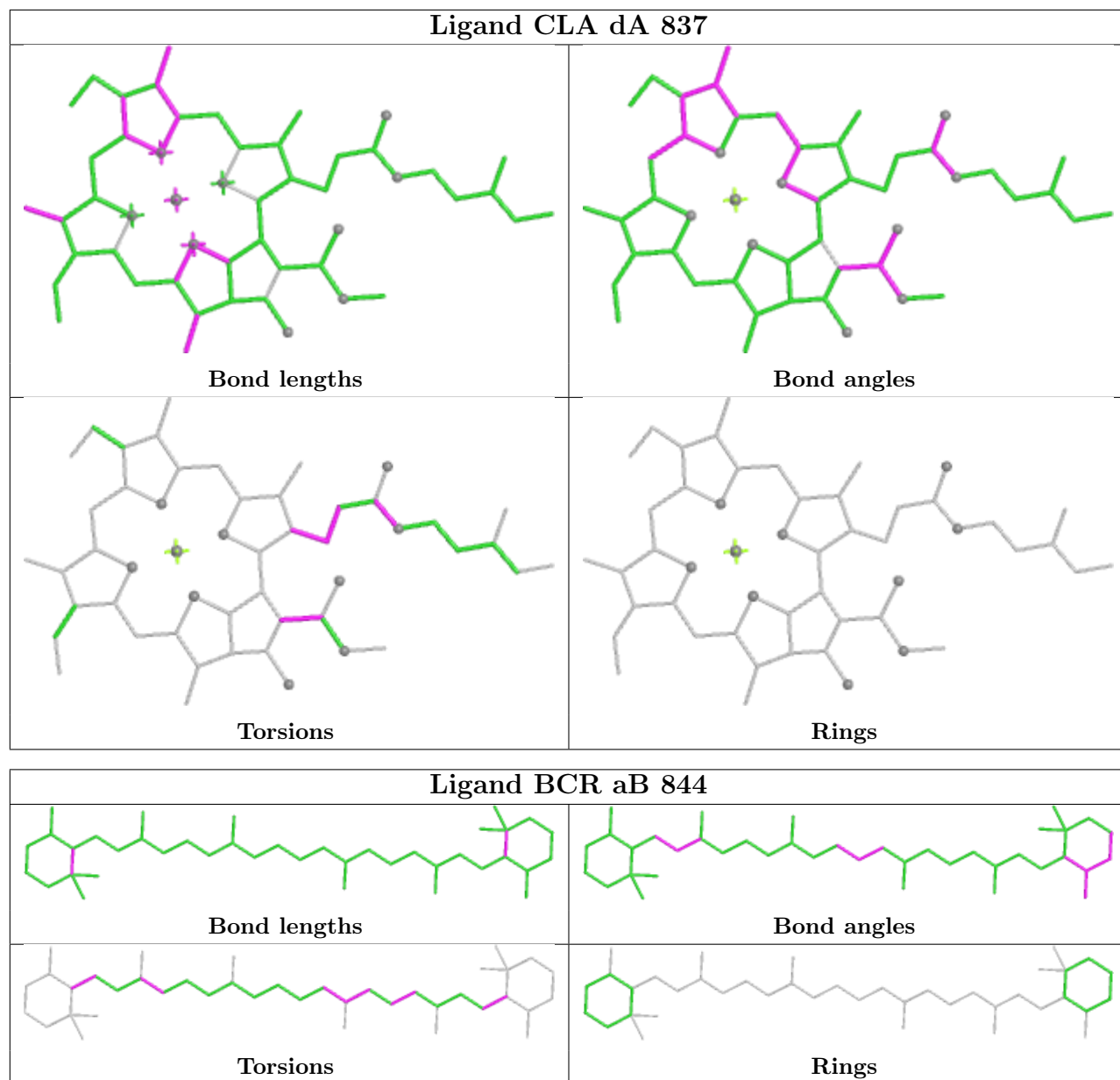


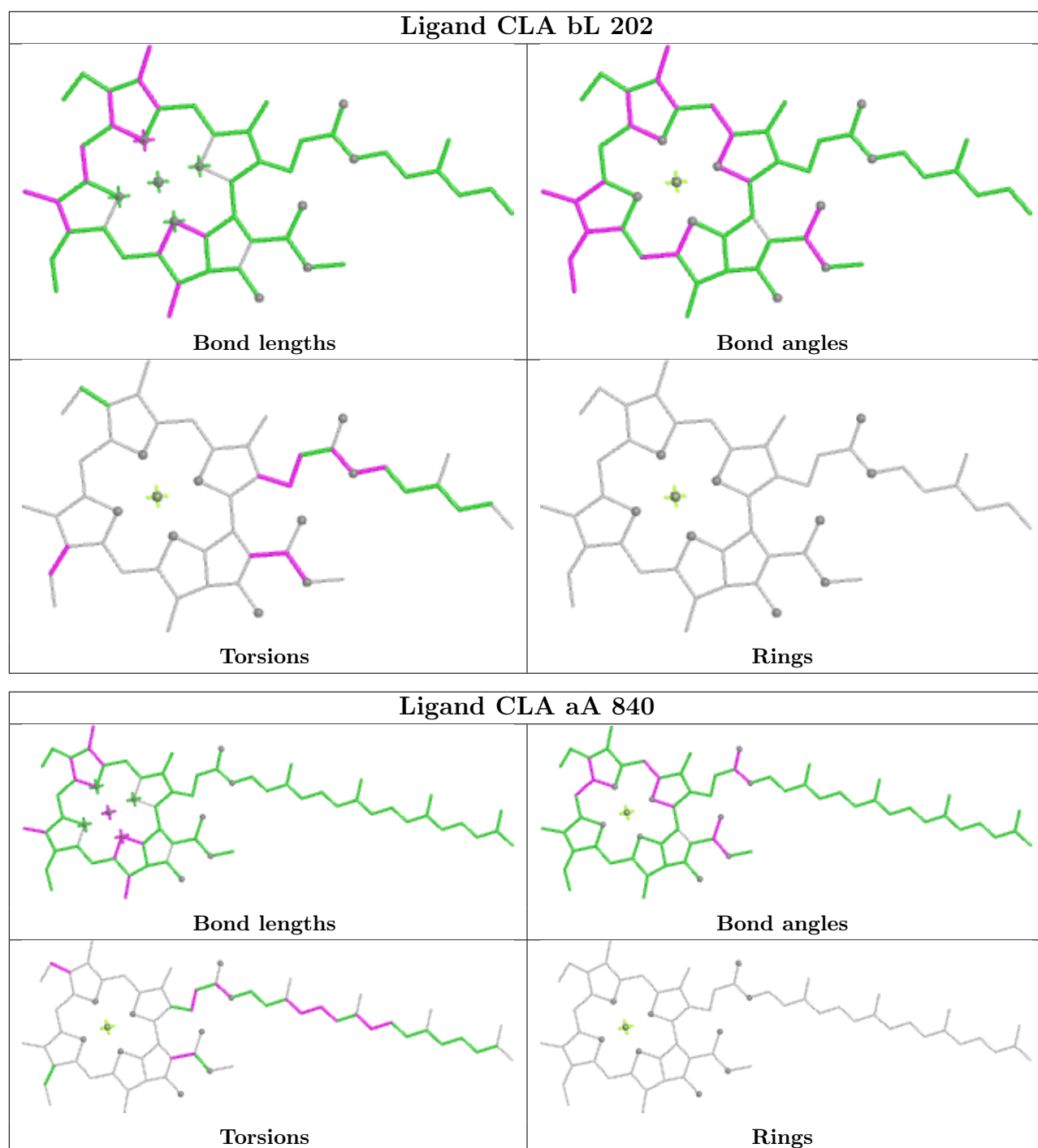


Ligand CLA dB 821

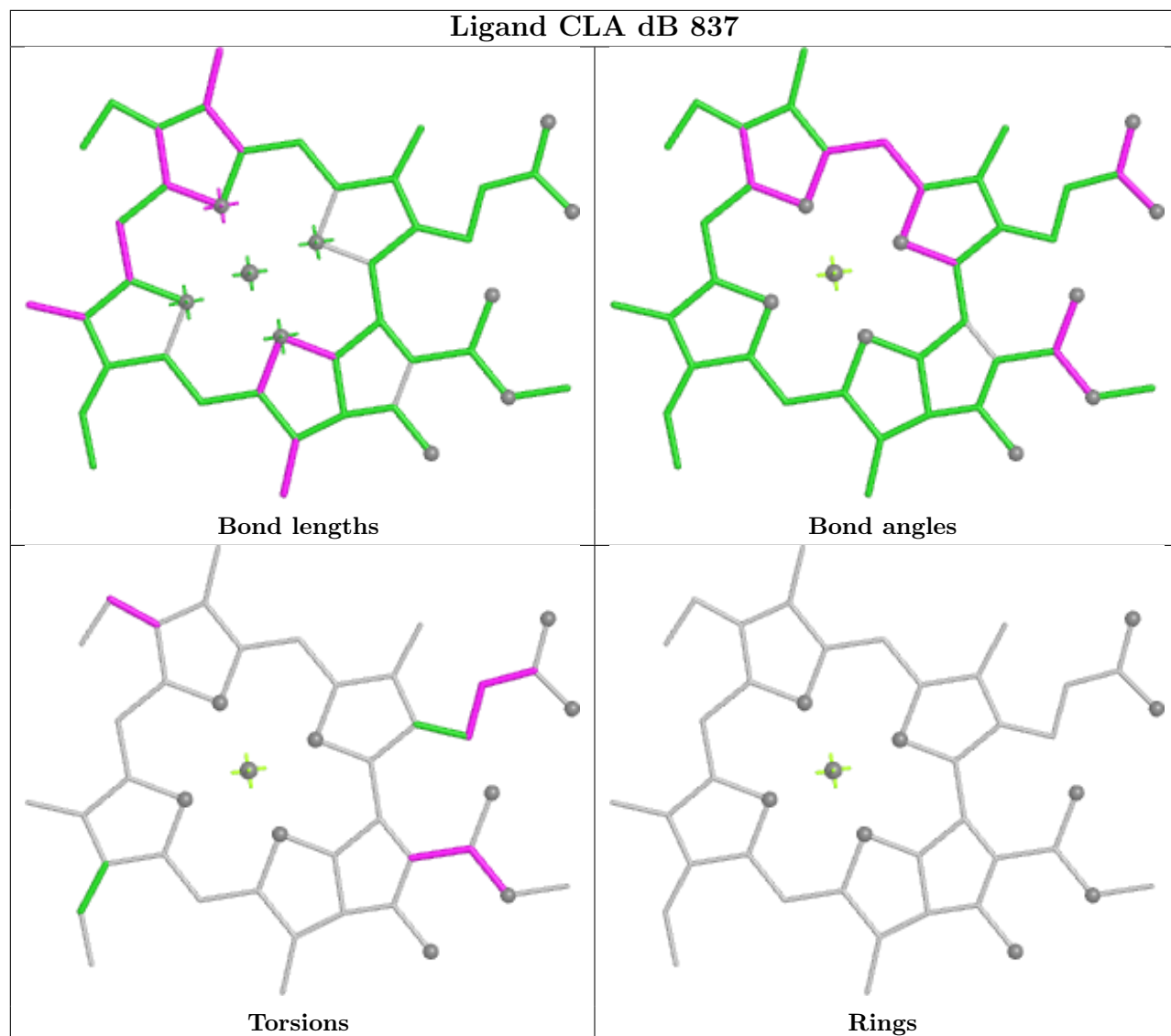


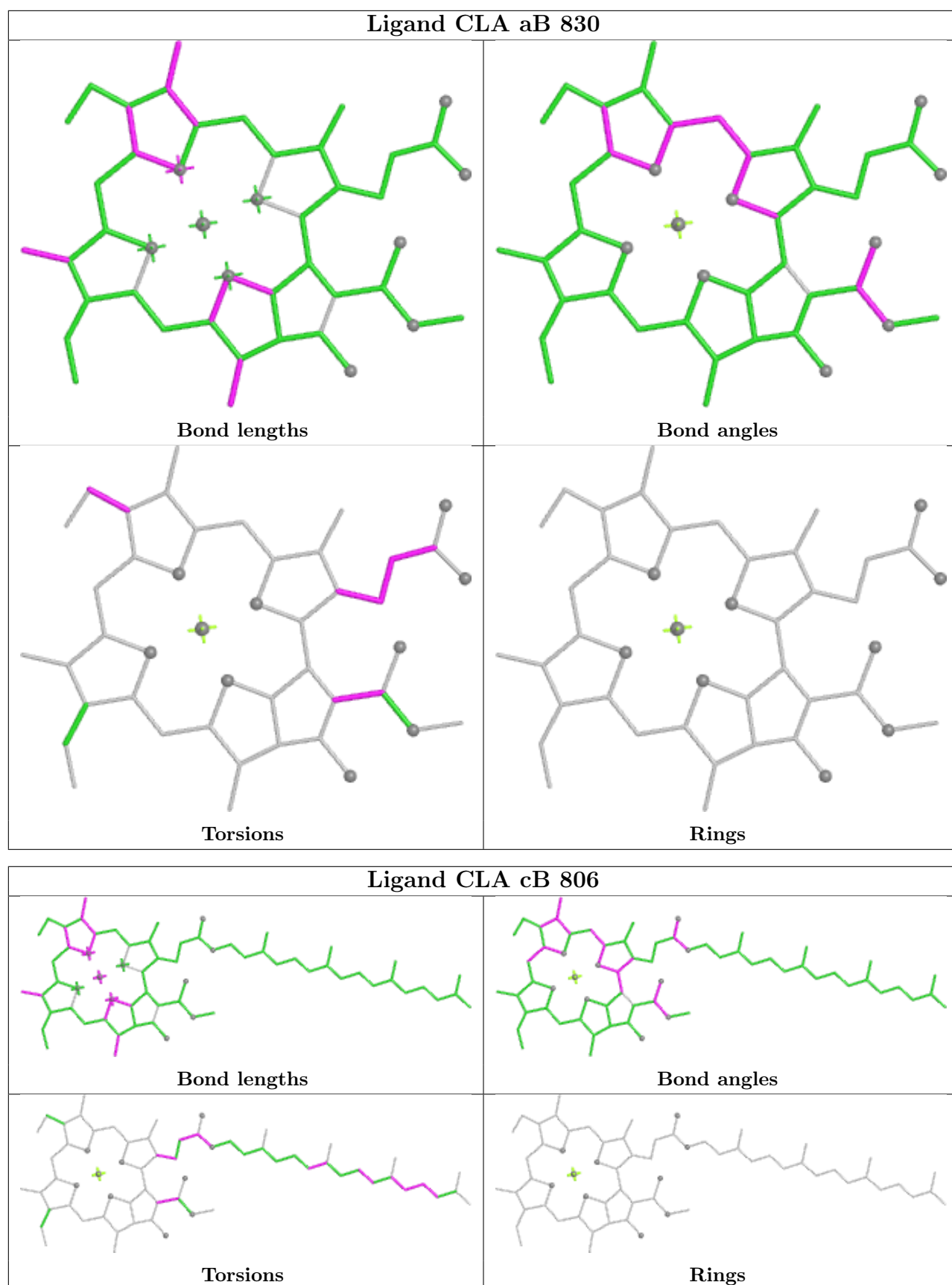


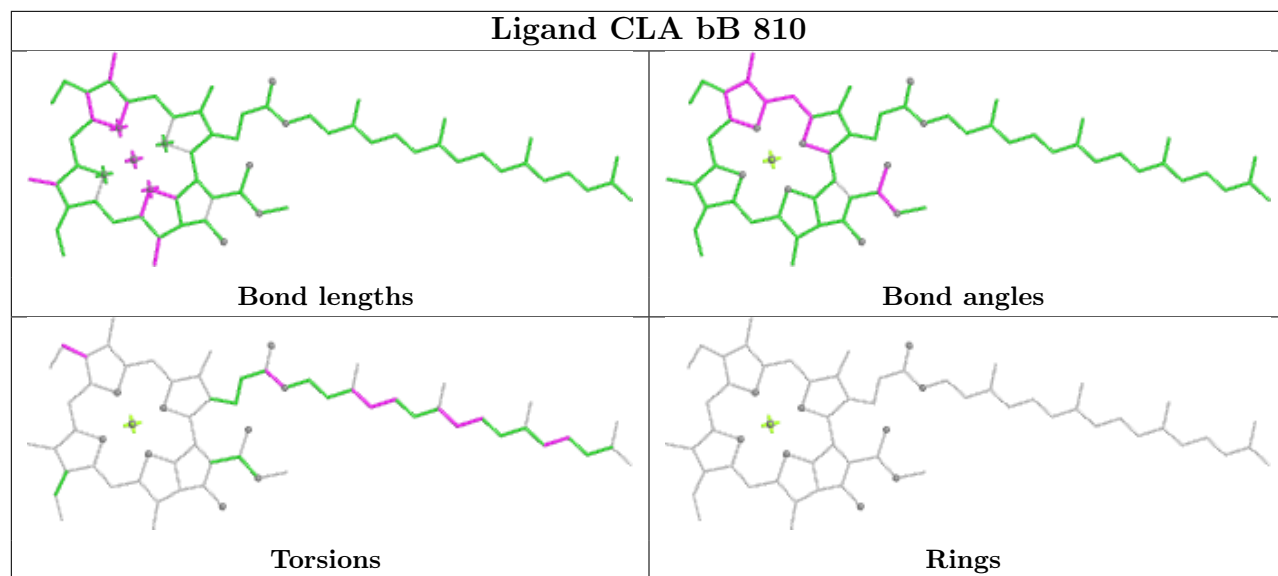


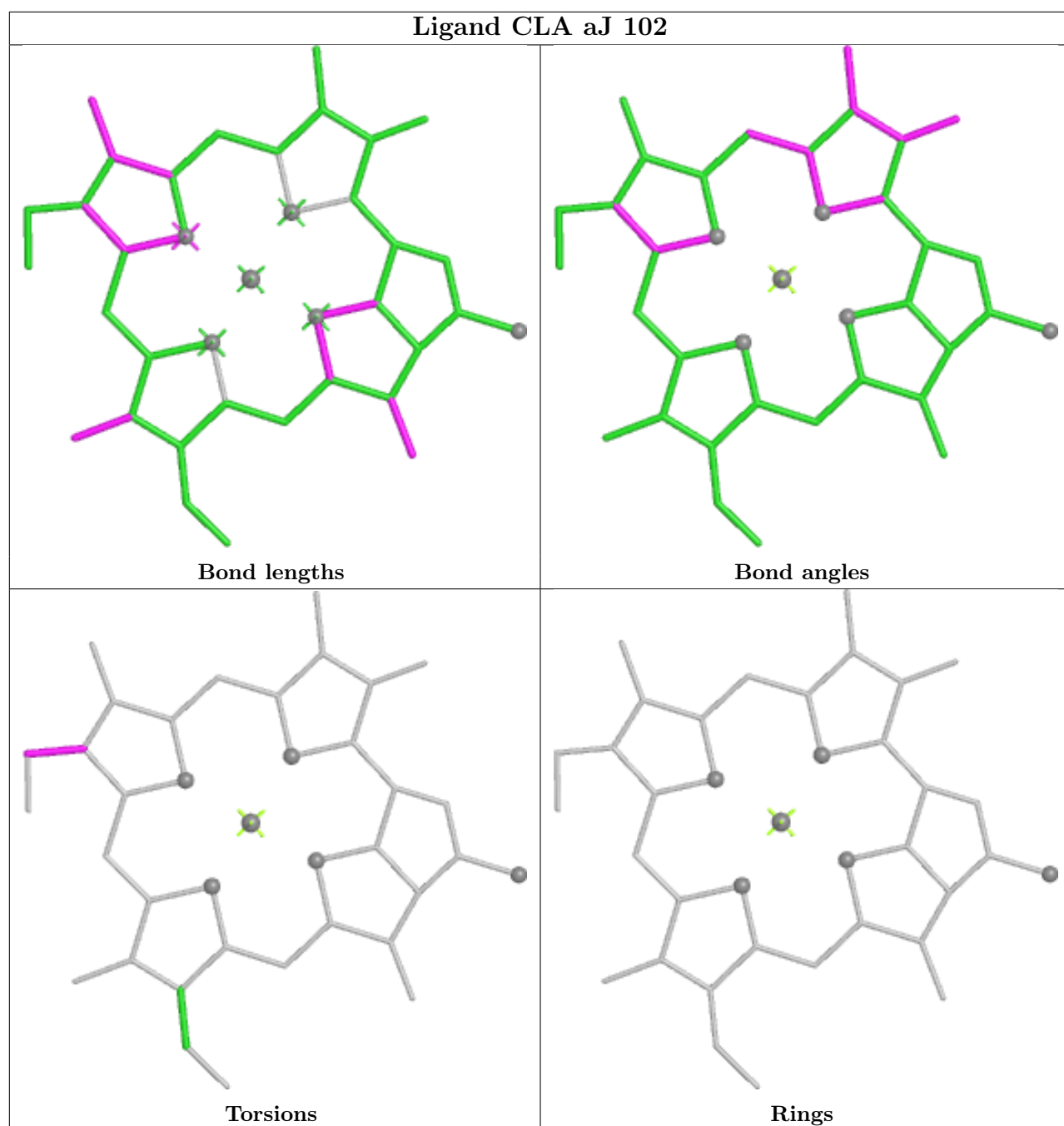


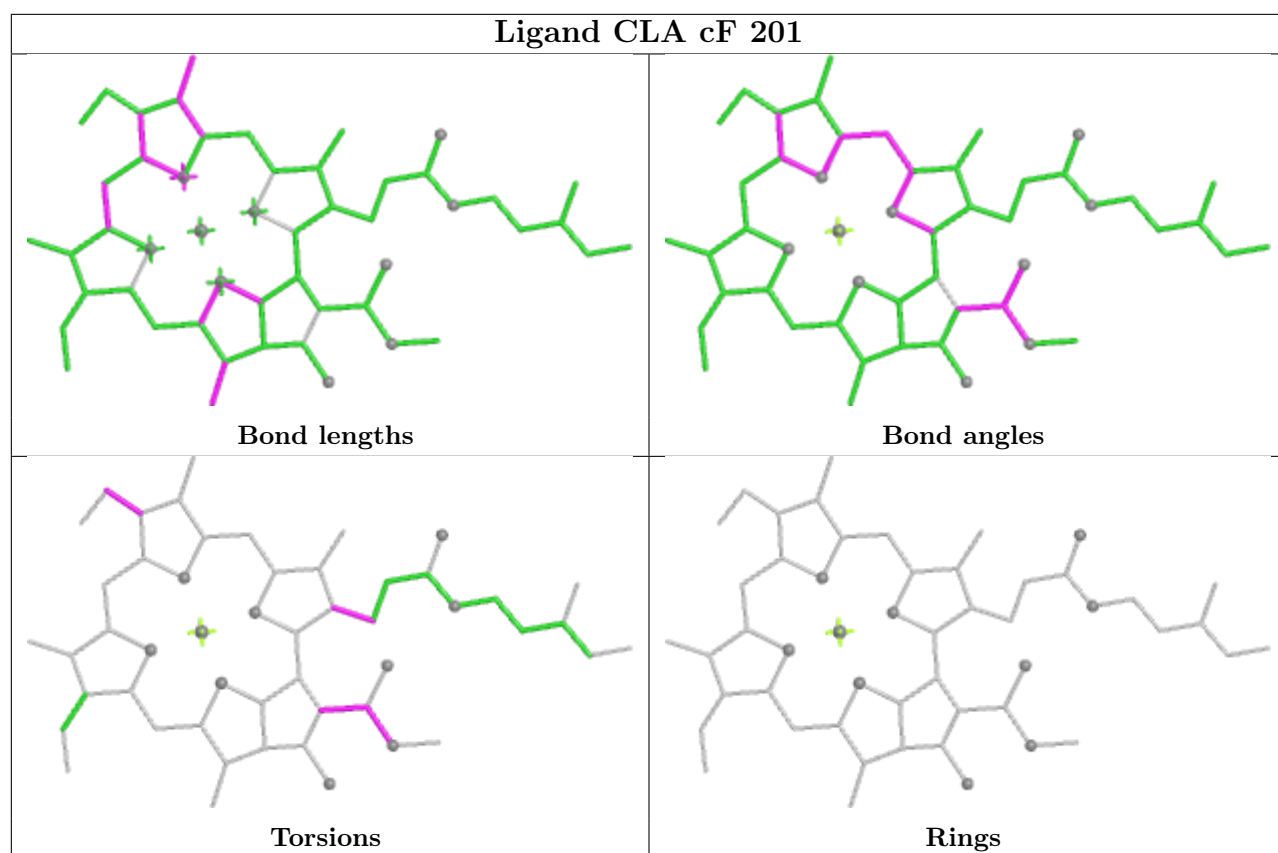
Ligand CLA dB 837

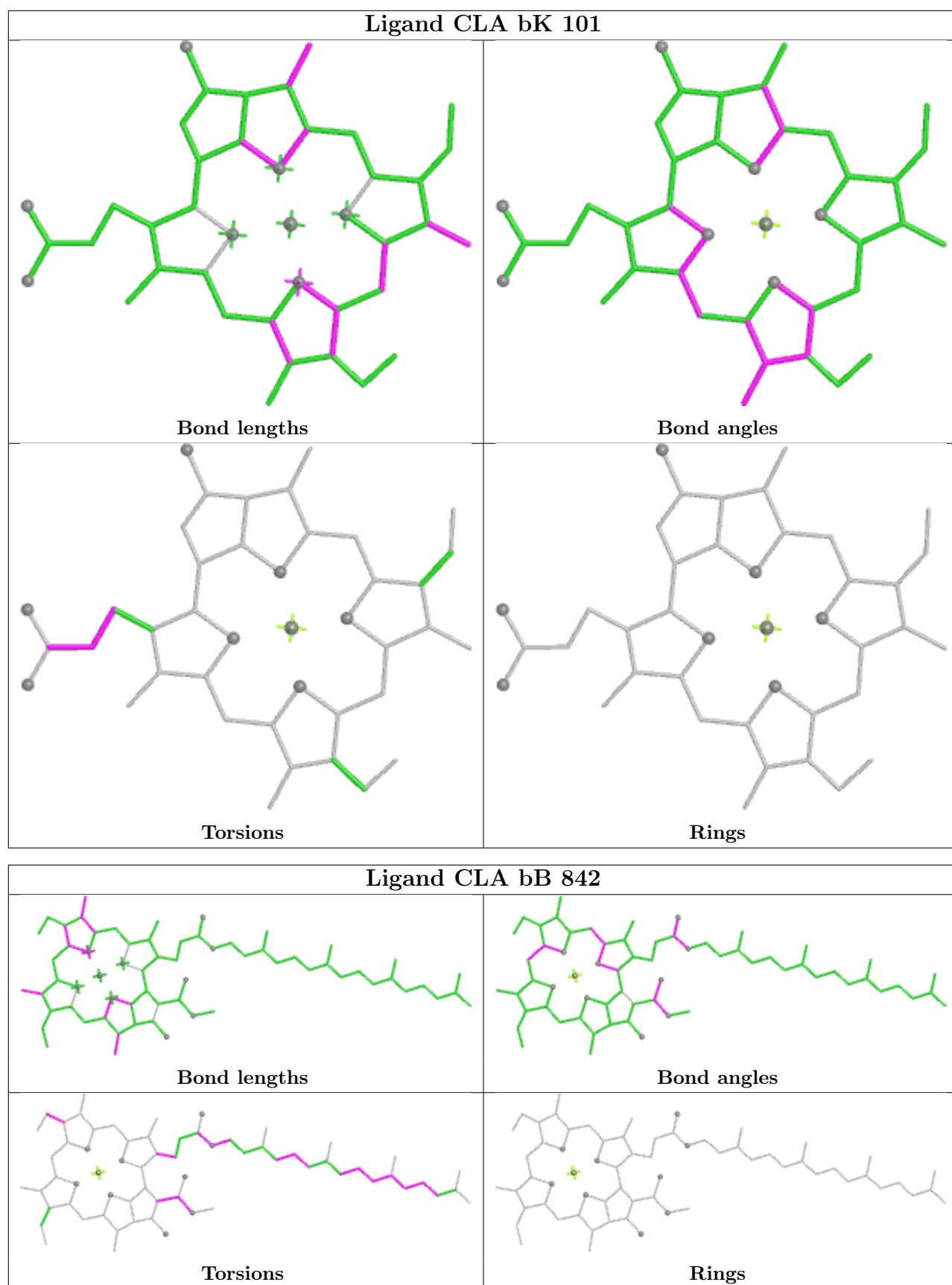


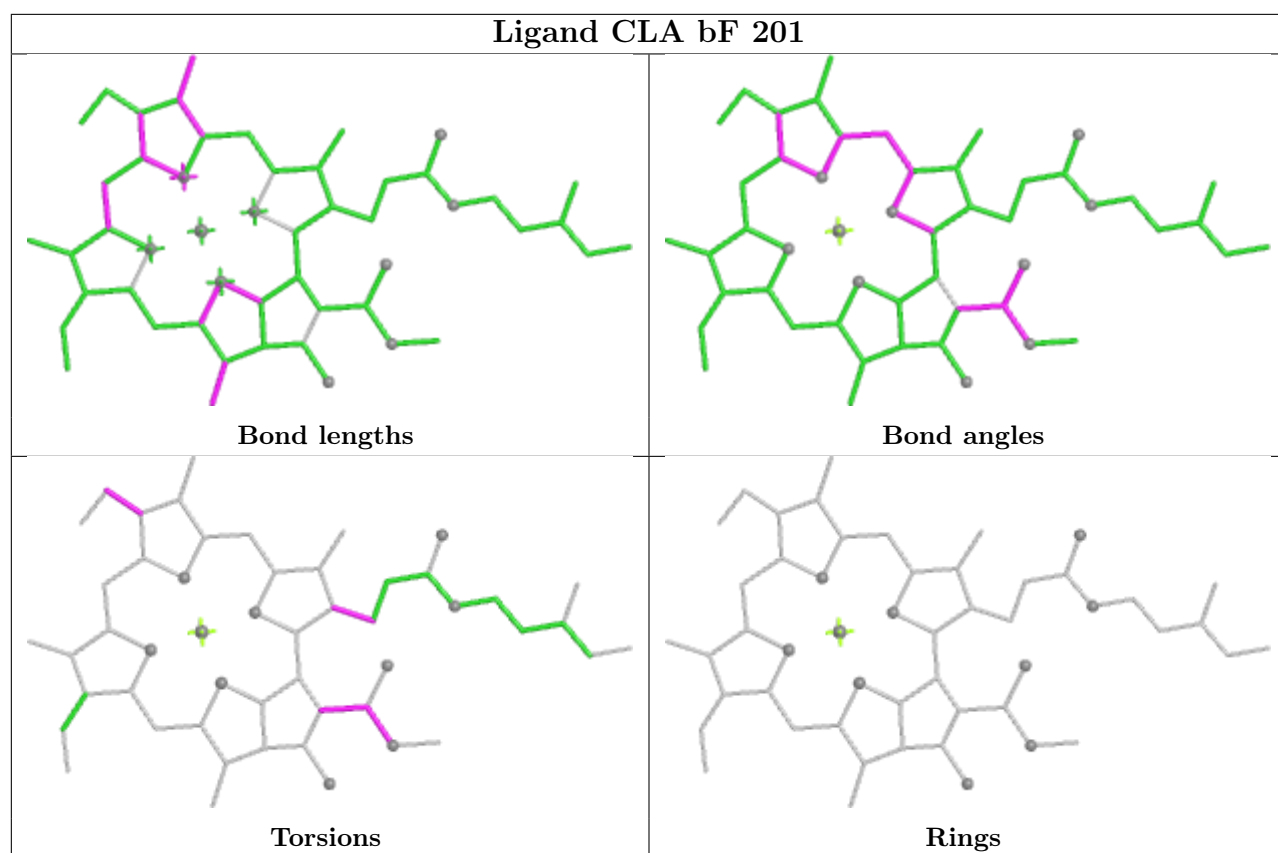




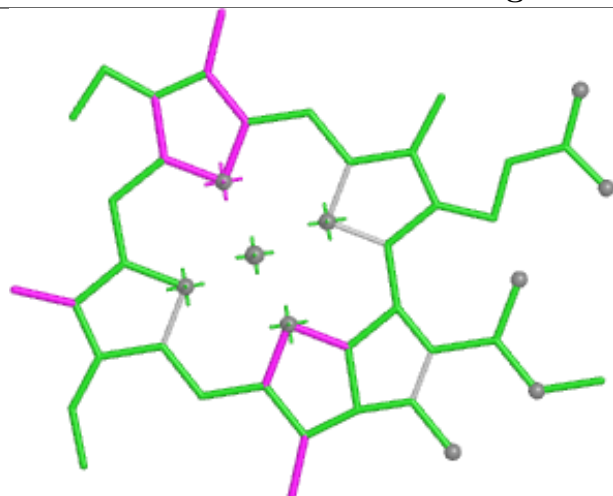




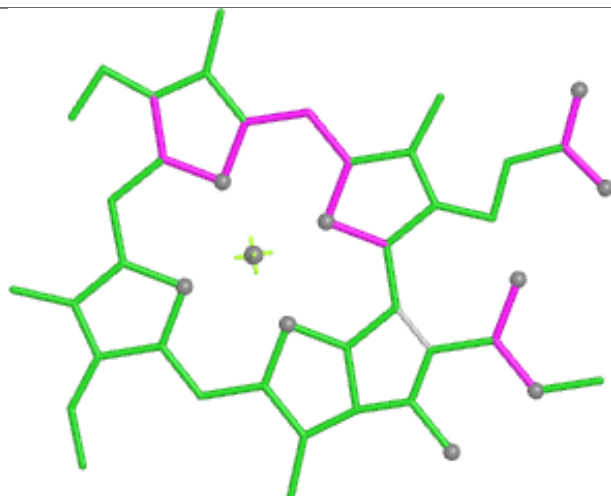




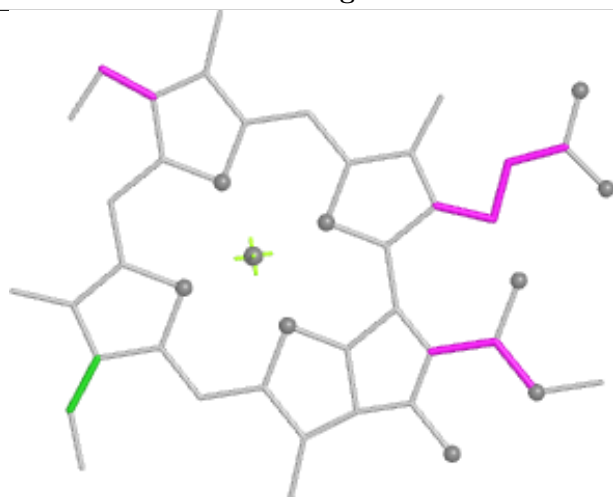
Ligand CLA cB 812



Bond lengths



Bond angles

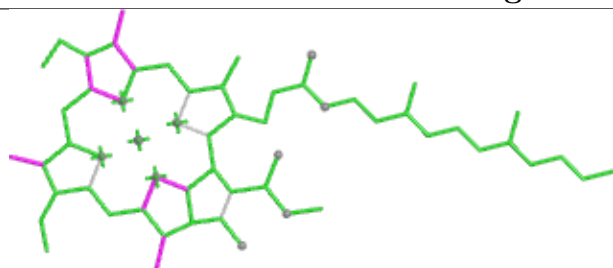


Torsions

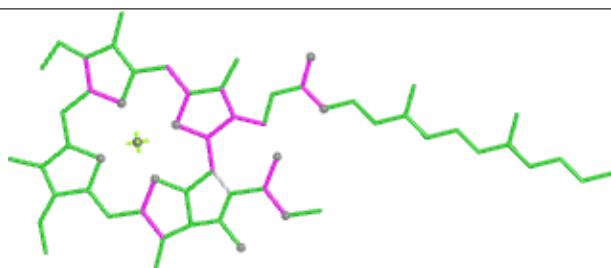


Rings

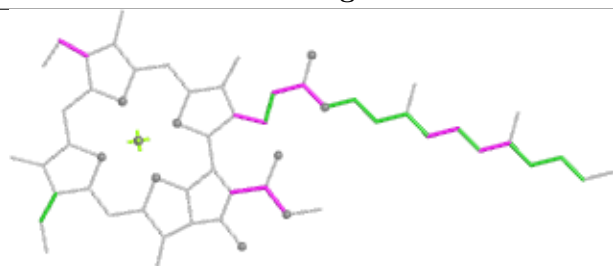
Ligand CLA bB 834



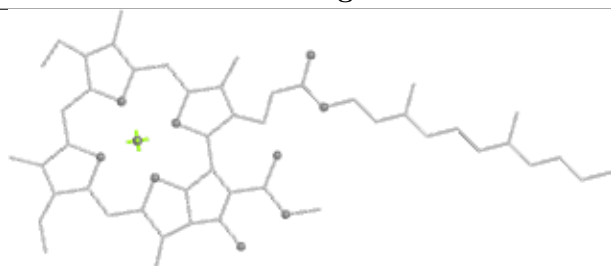
Bond lengths



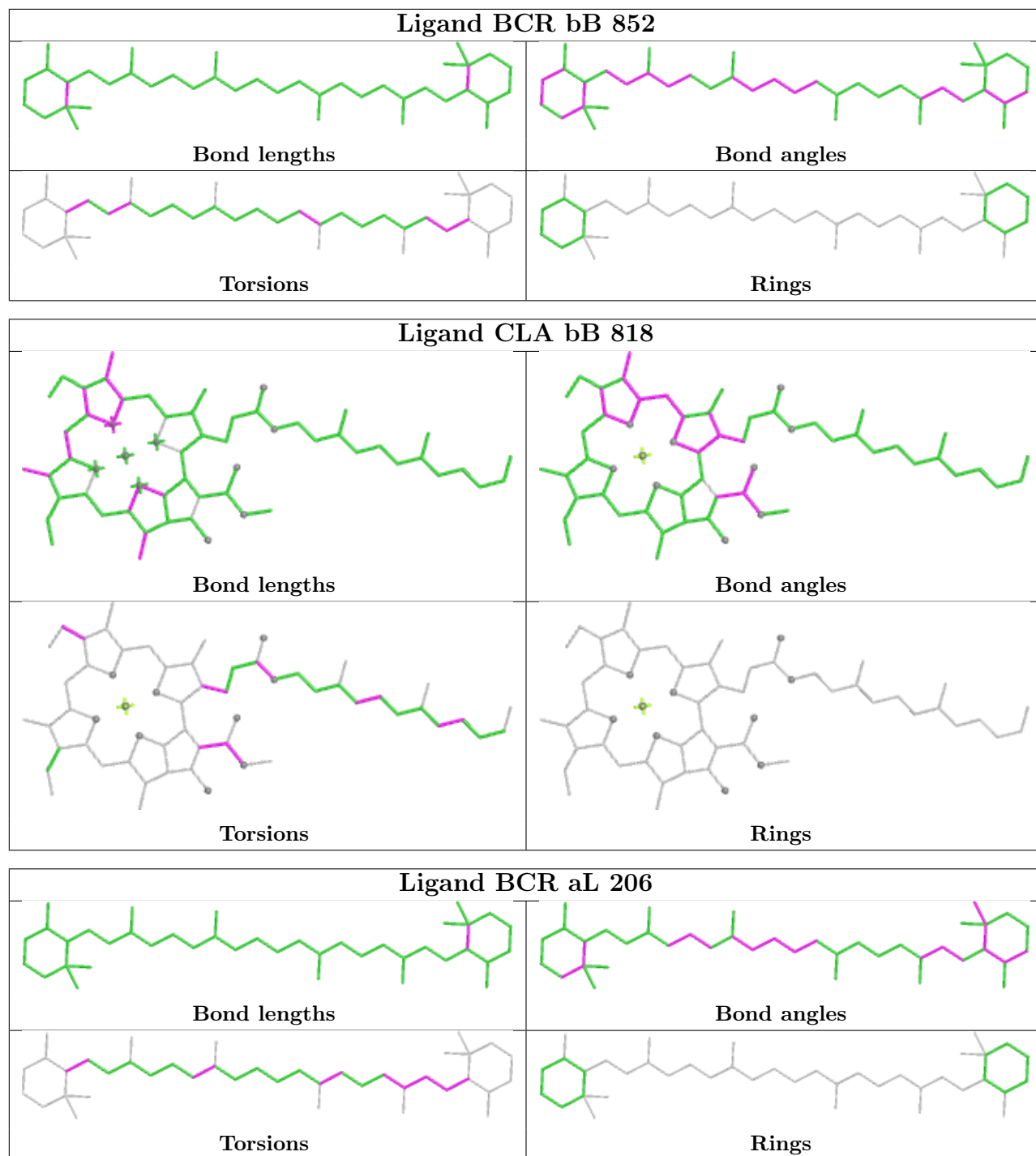
Bond angles



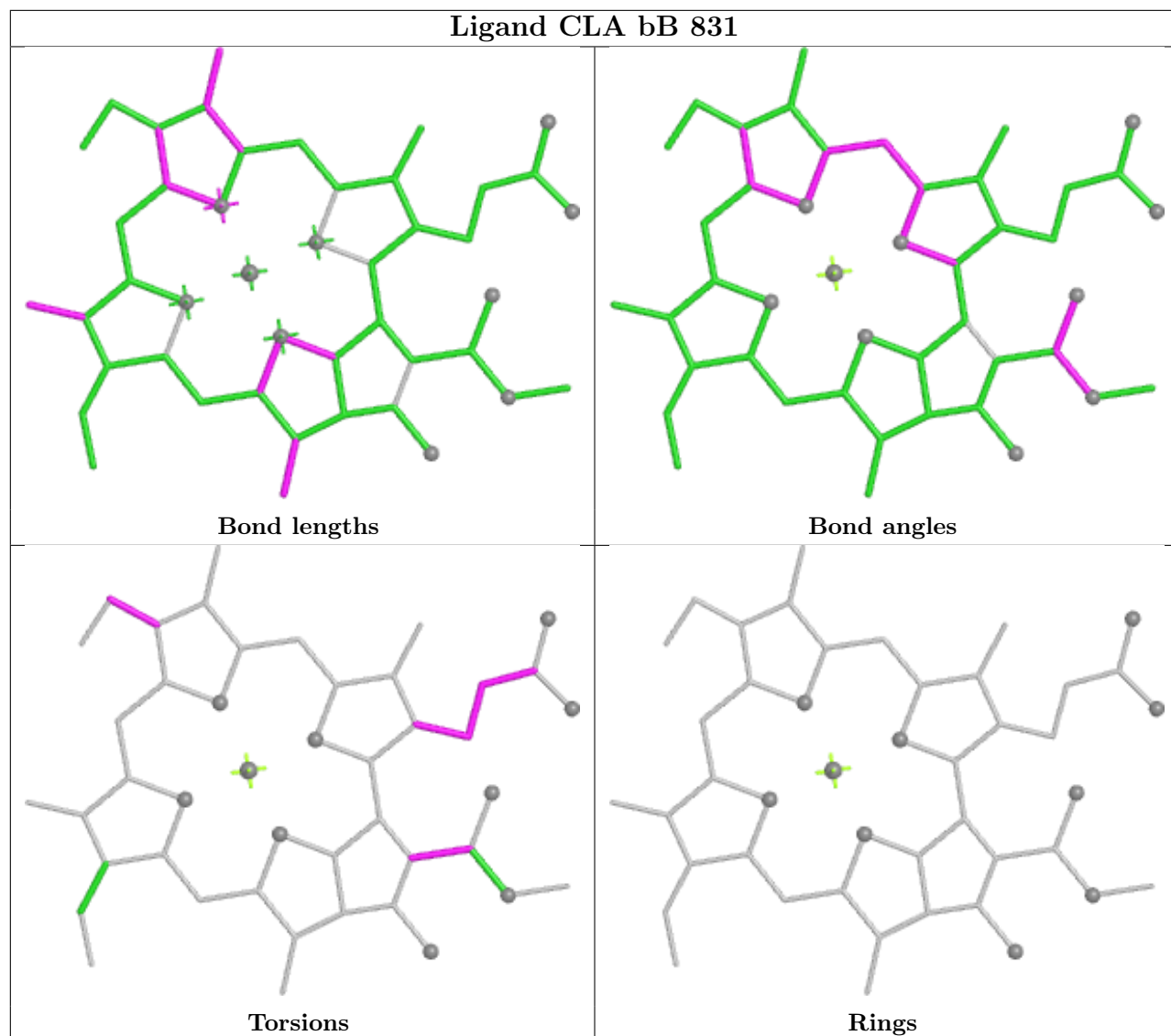
Torsions



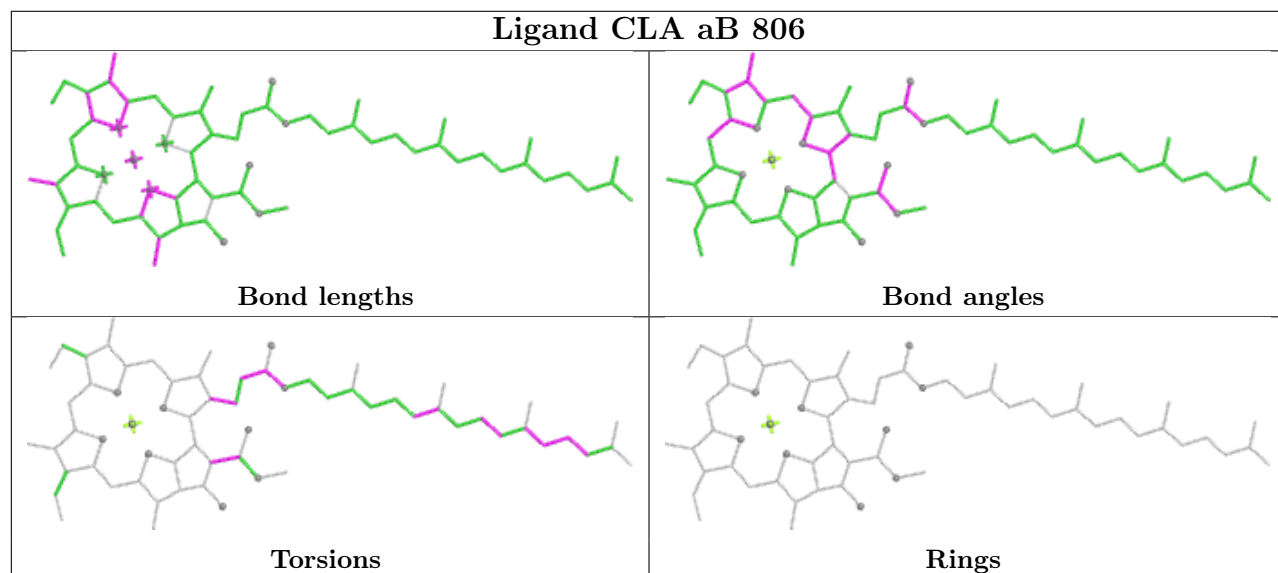
Rings

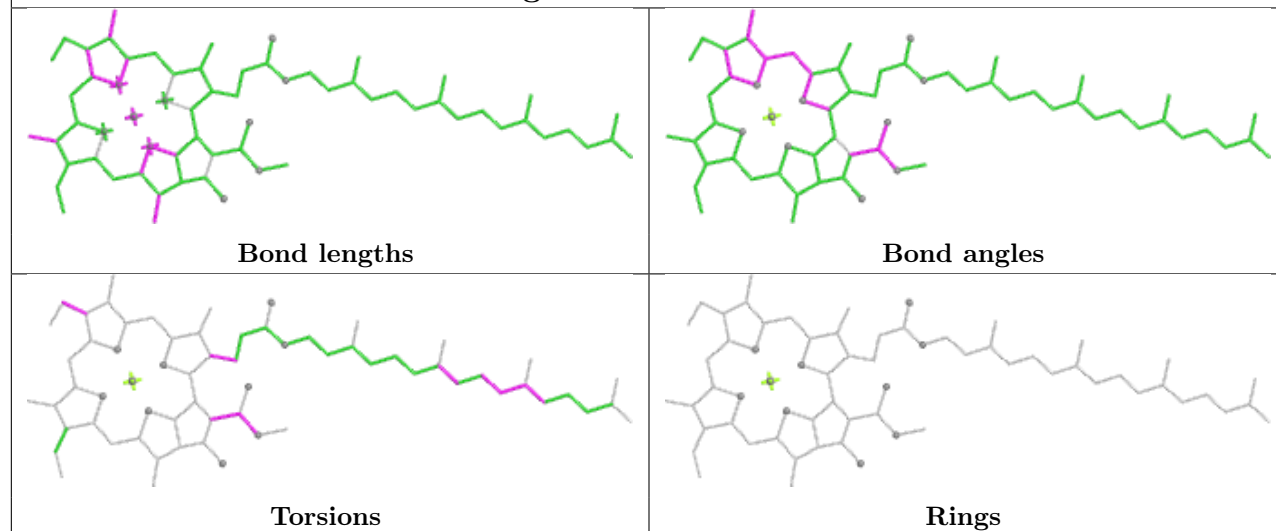
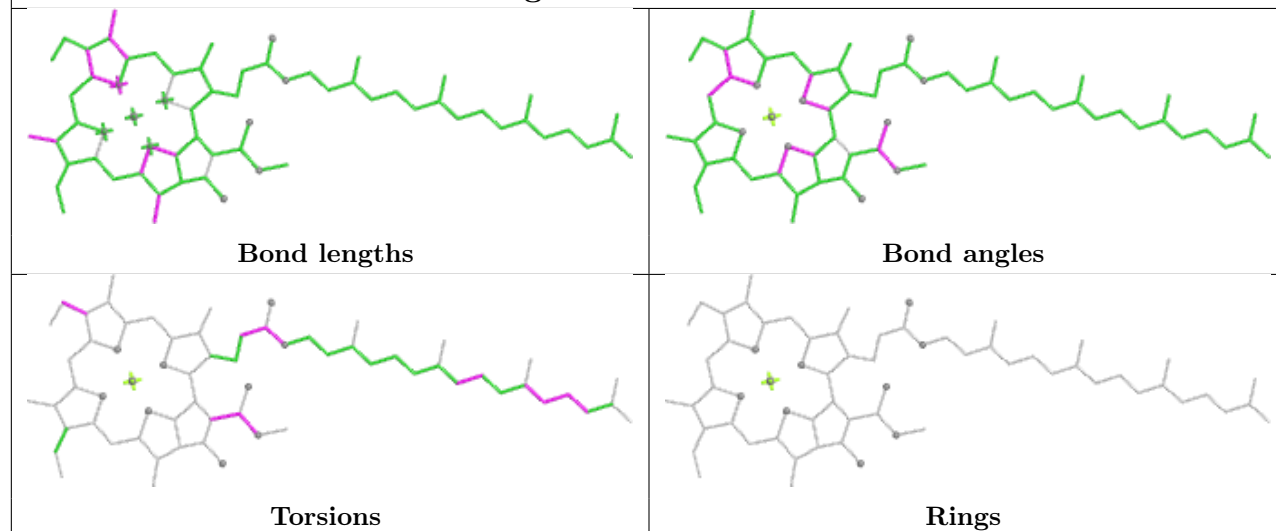


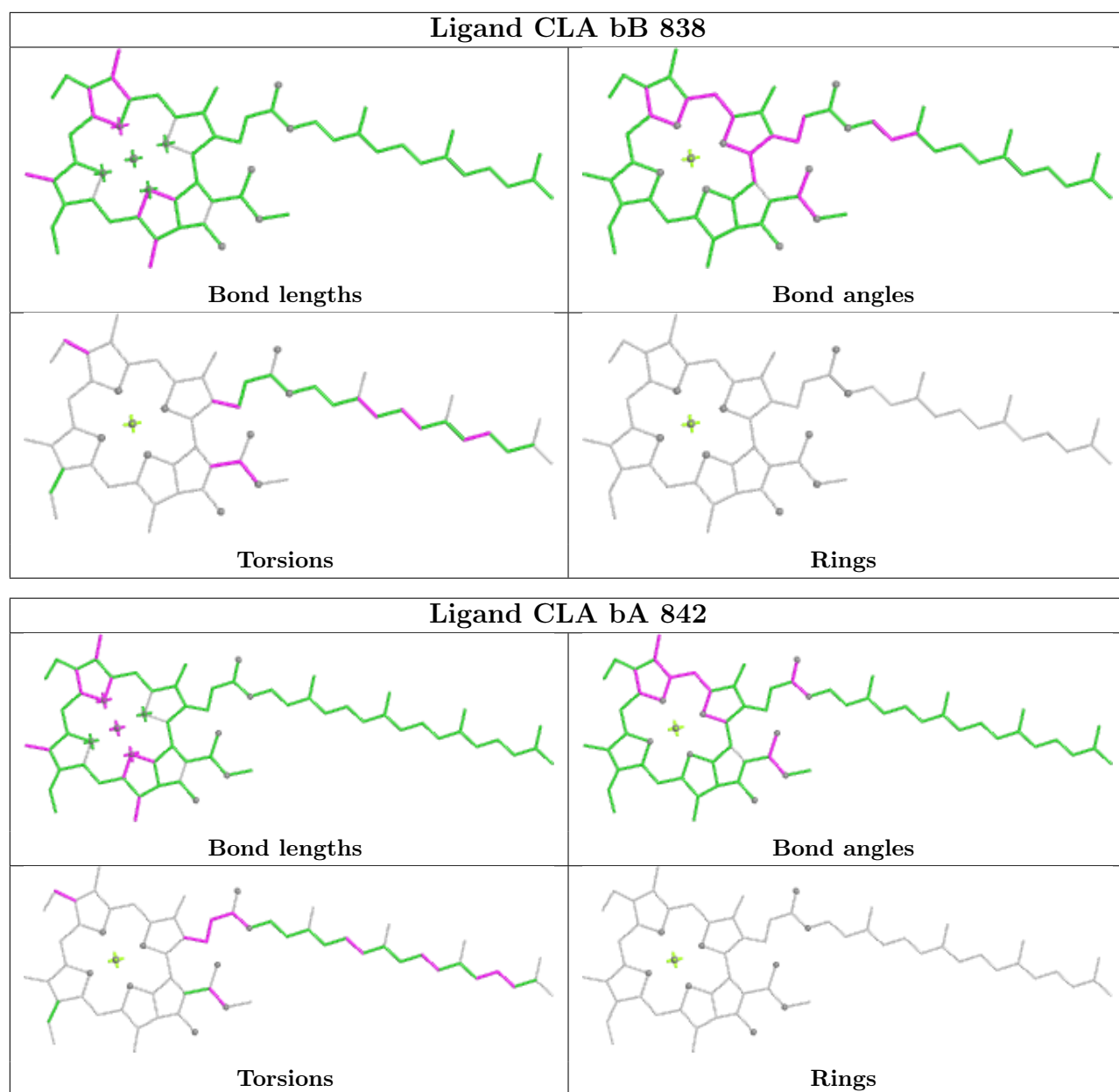
Ligand CLA bB 831

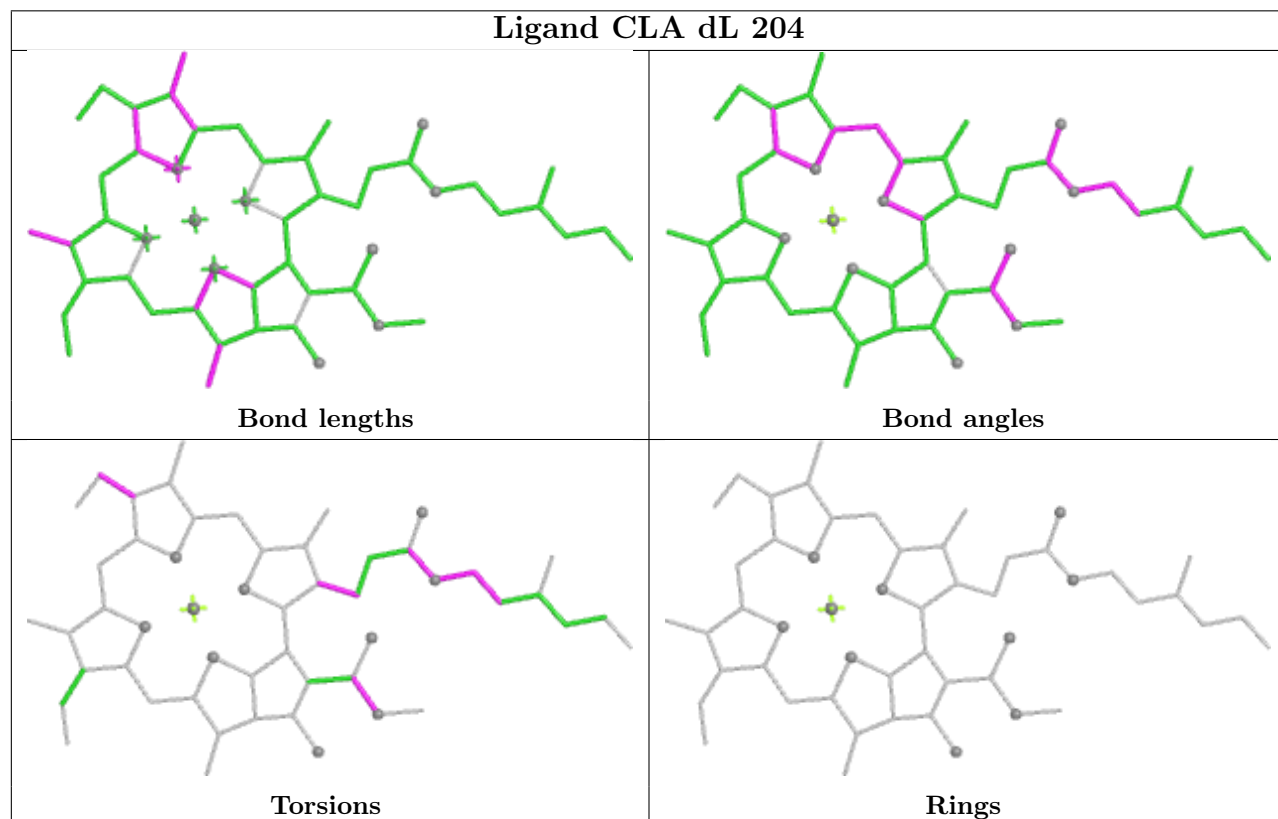
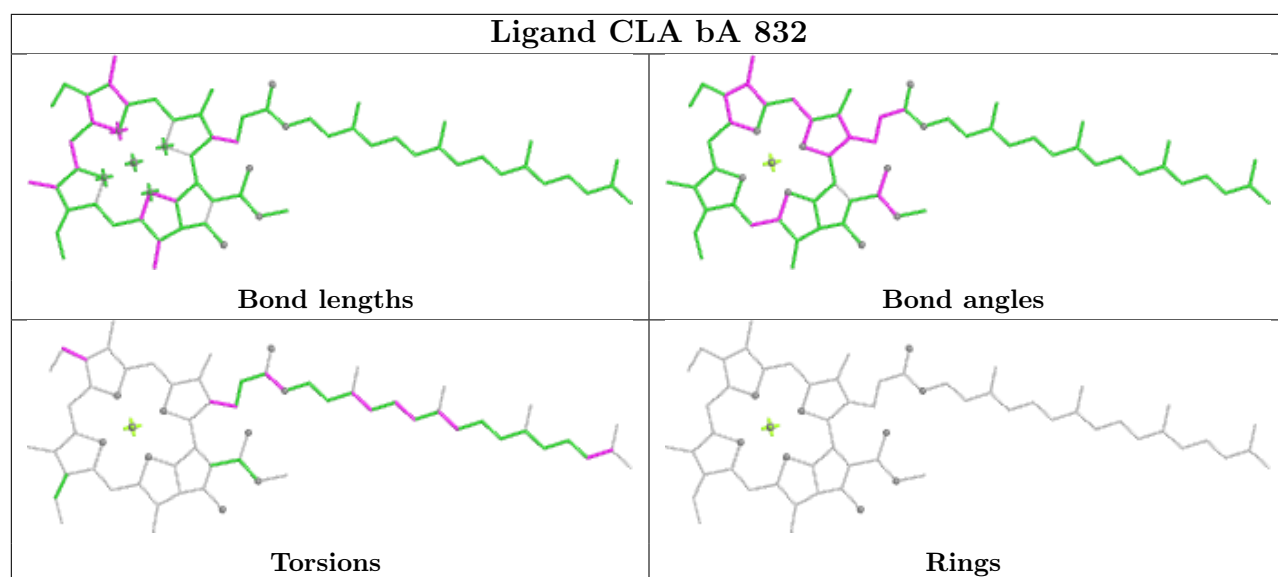


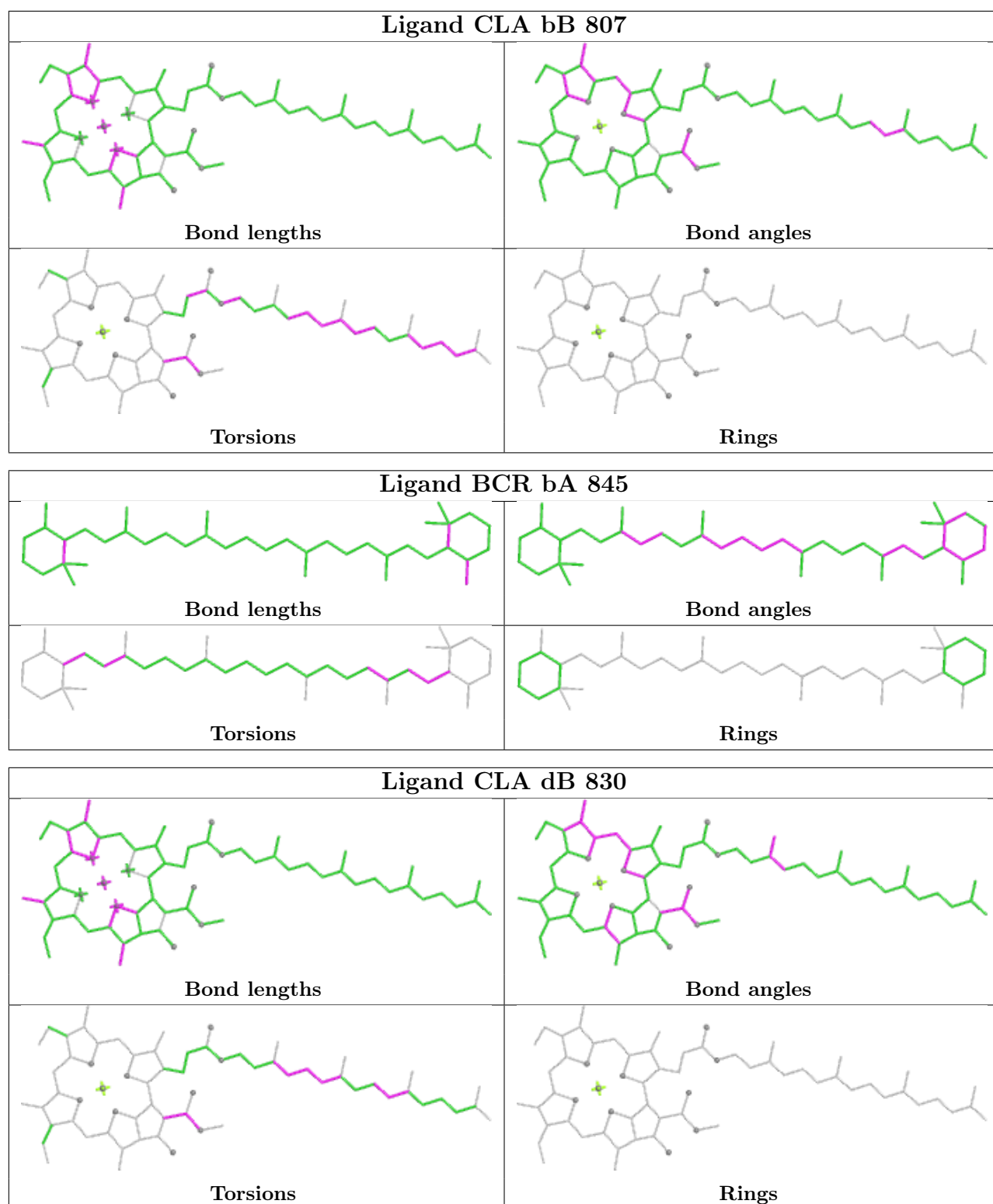
Ligand CLA aB 806

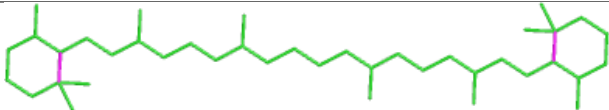
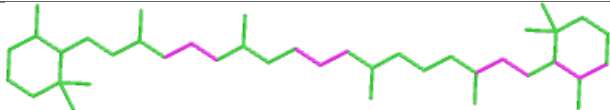
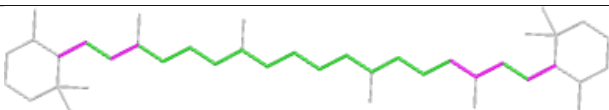
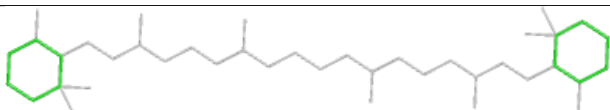
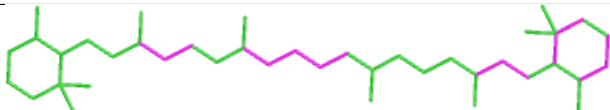
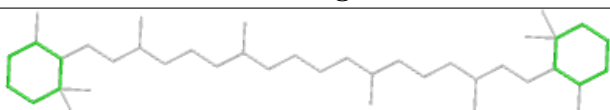
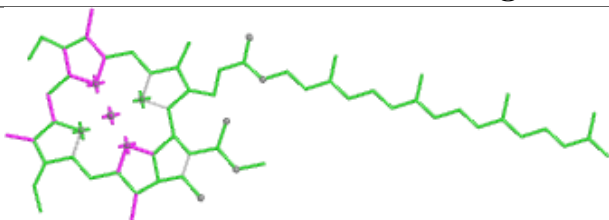
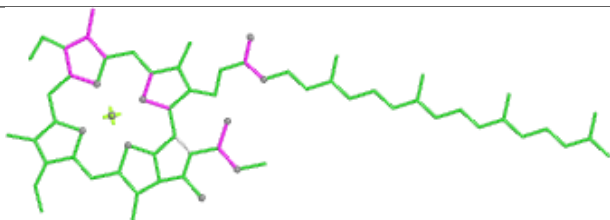
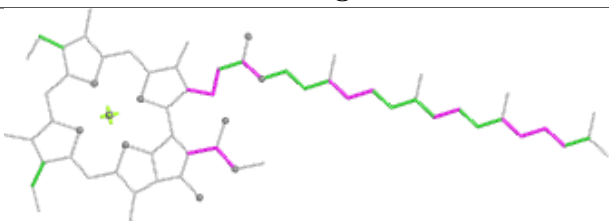
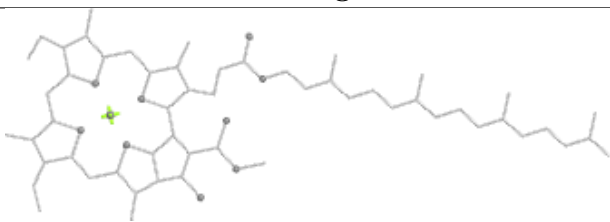


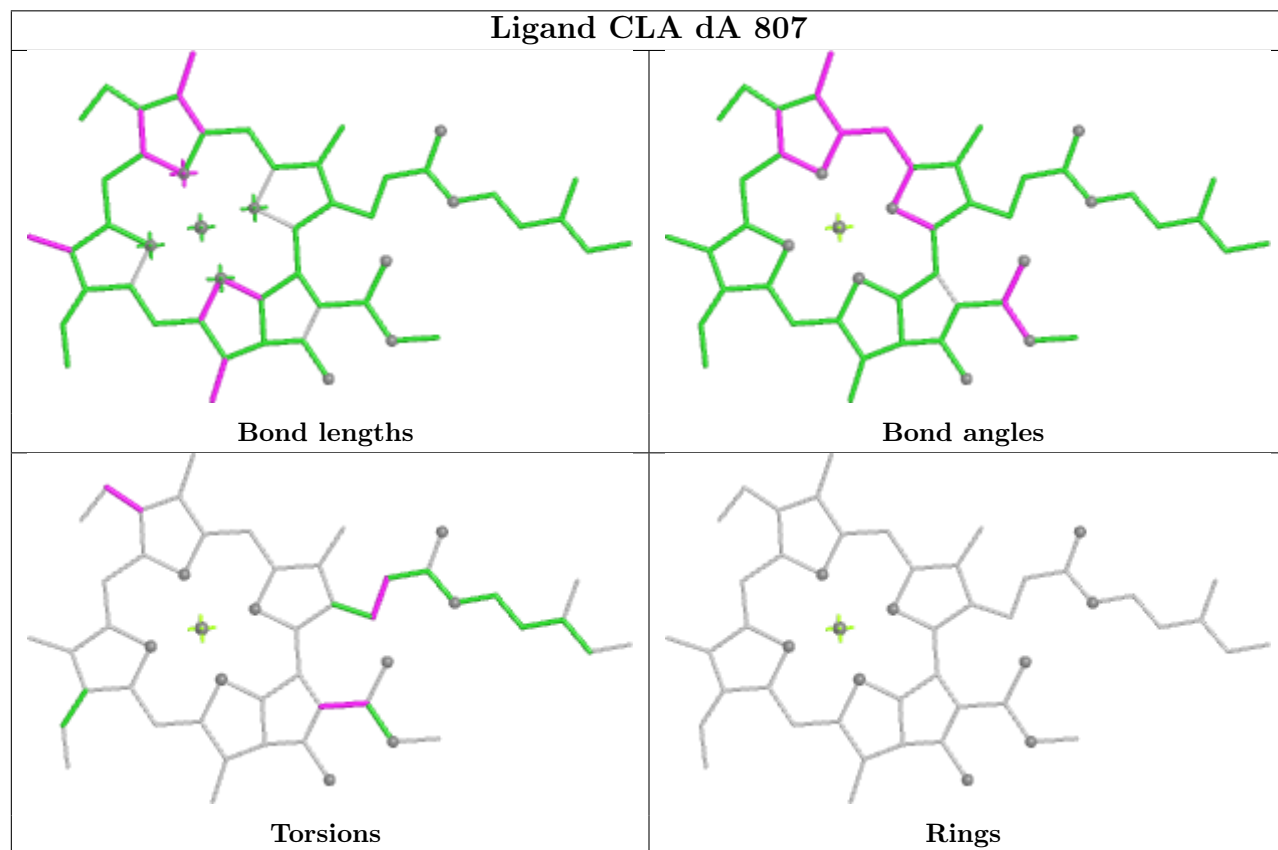
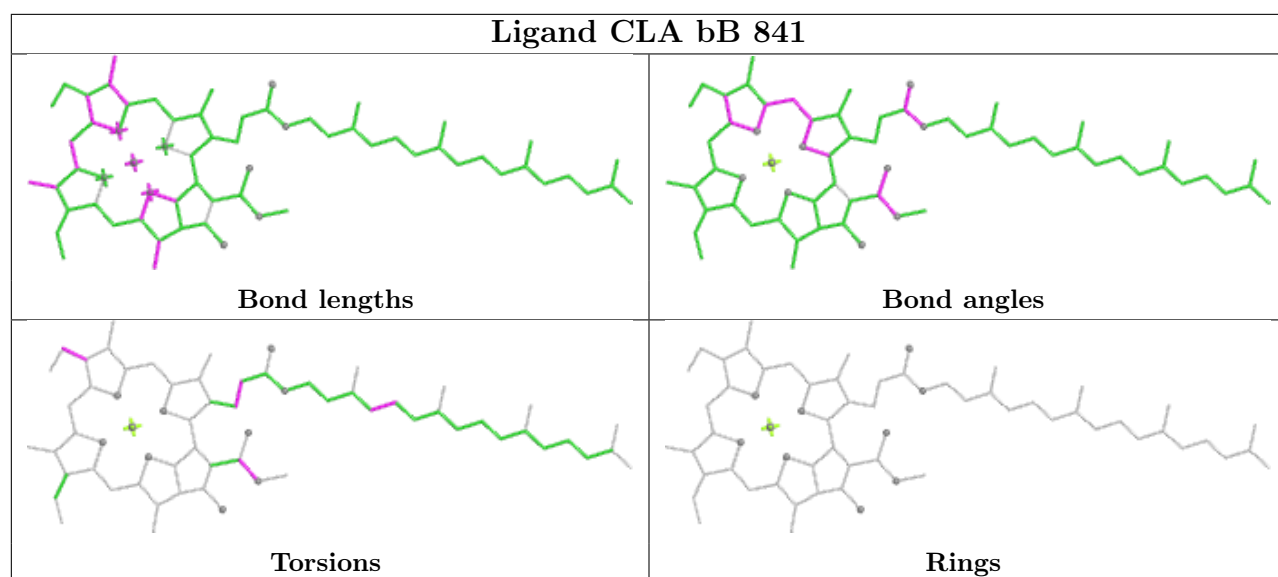
Ligand CLA aA 830**Ligand CLA cB 802**



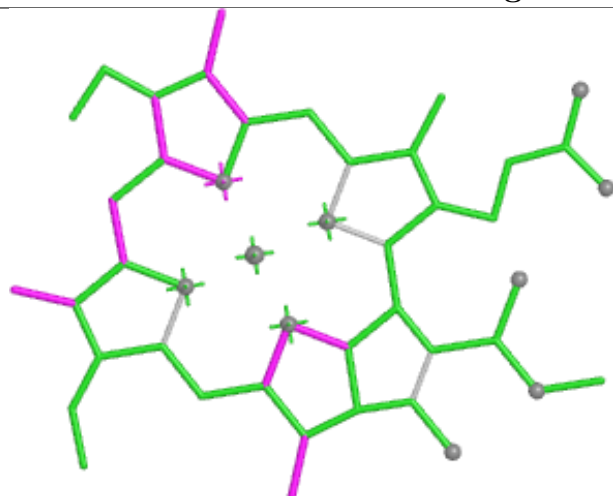




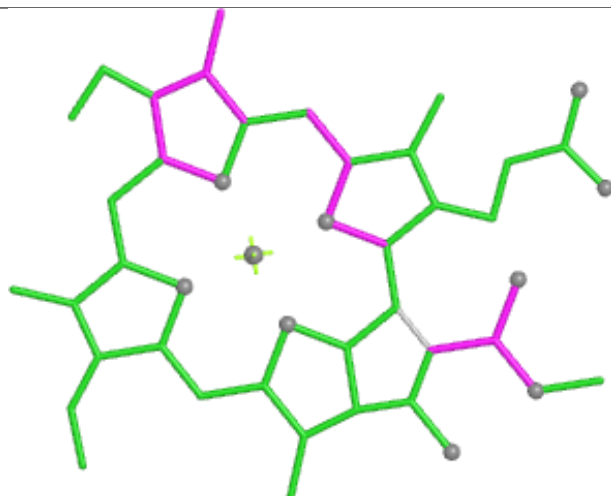
Ligand BCR dB 849	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR bB 844	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA dB 803	
	
Bond lengths	Bond angles
	
Torsions	Rings



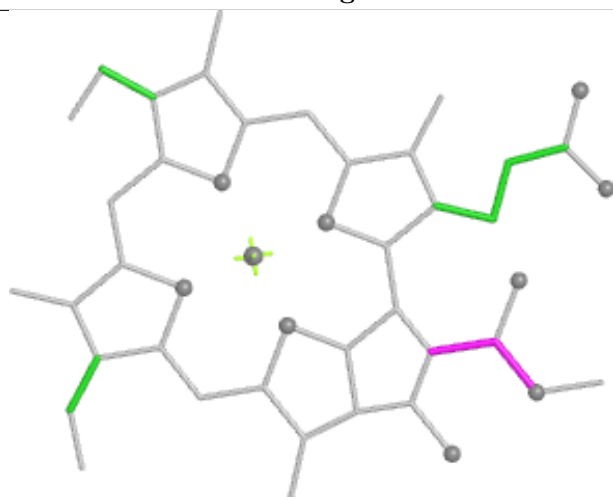
Ligand CLA dB 835



Bond lengths



Bond angles

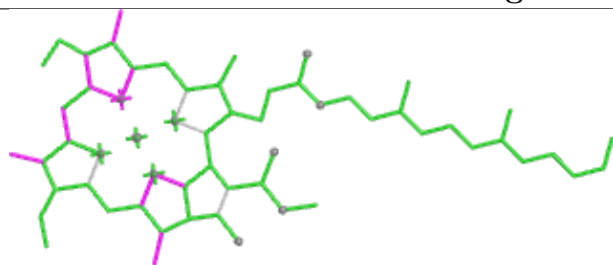


Torsions

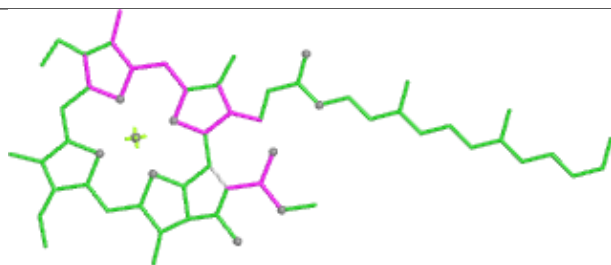


Rings

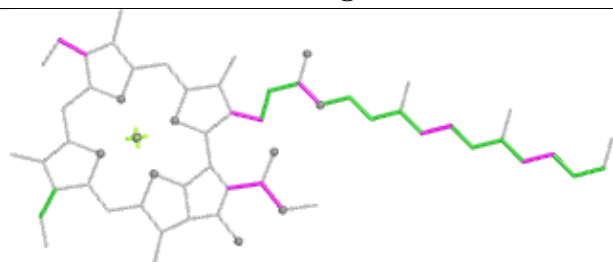
Ligand CLA aB 817



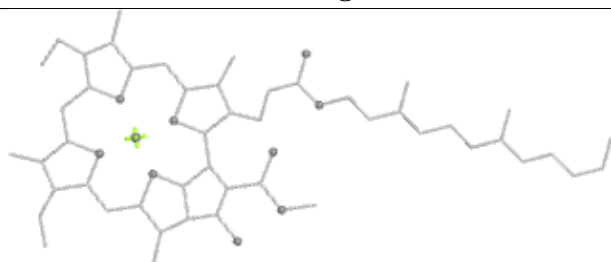
Bond lengths



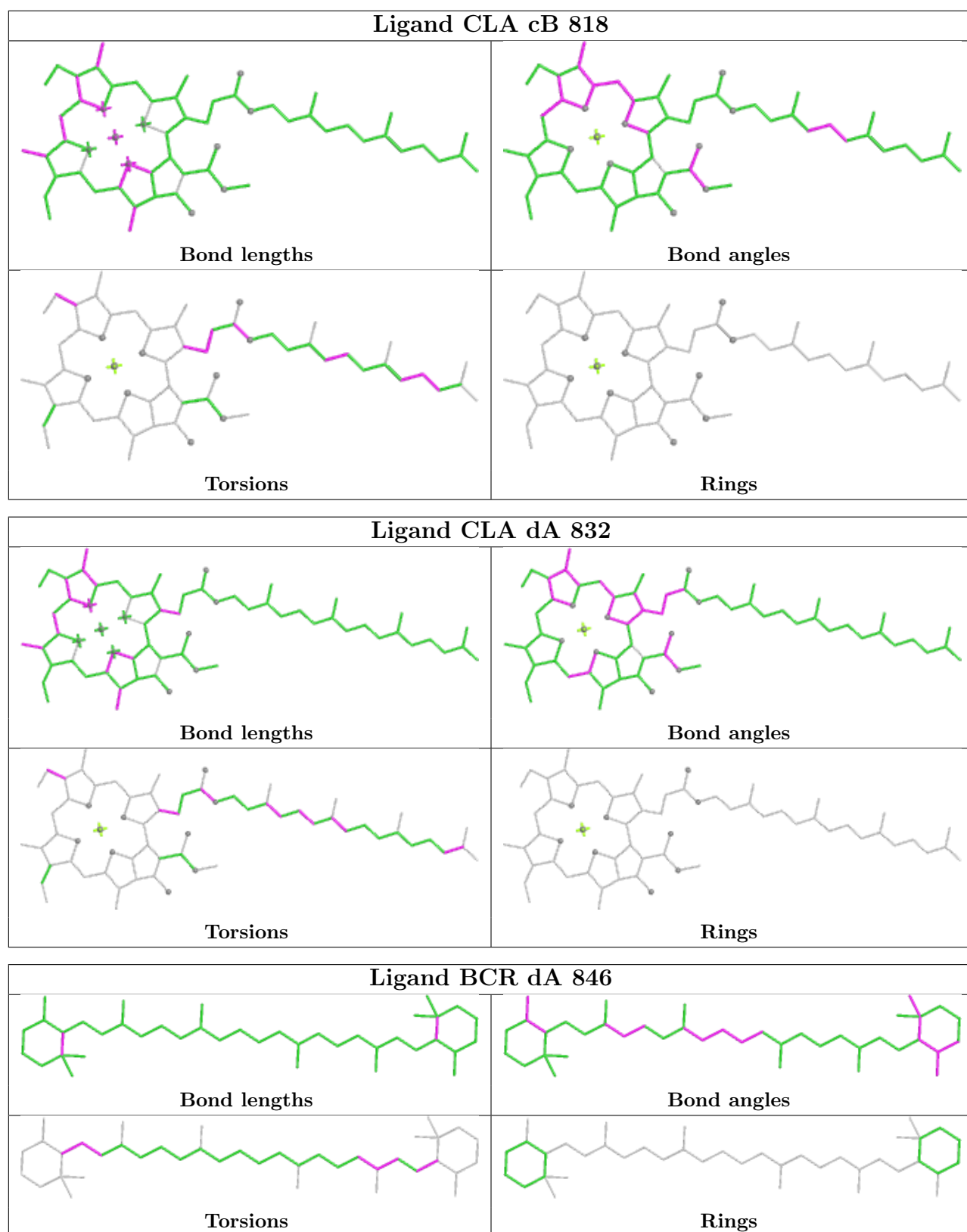
Bond angles

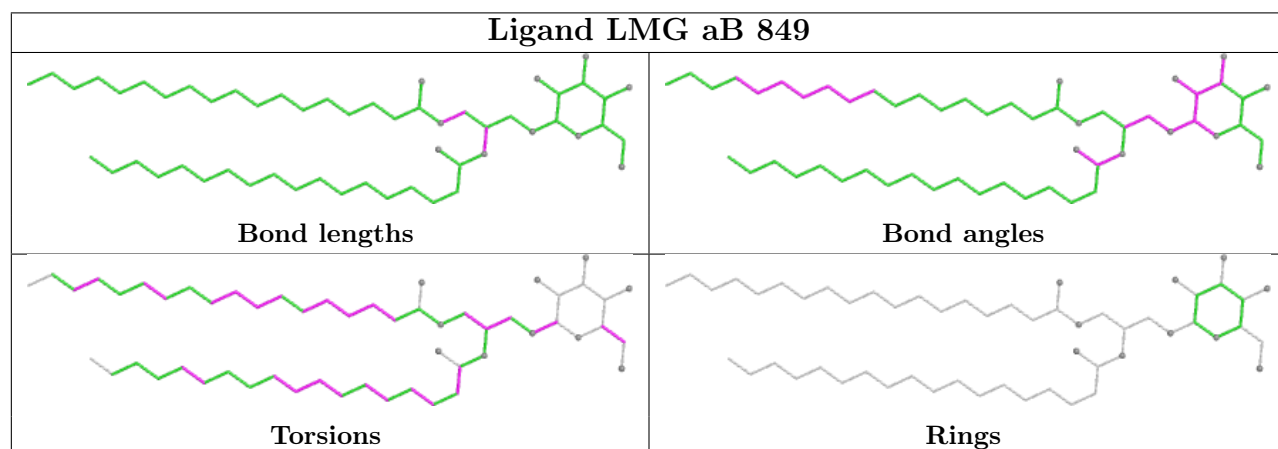
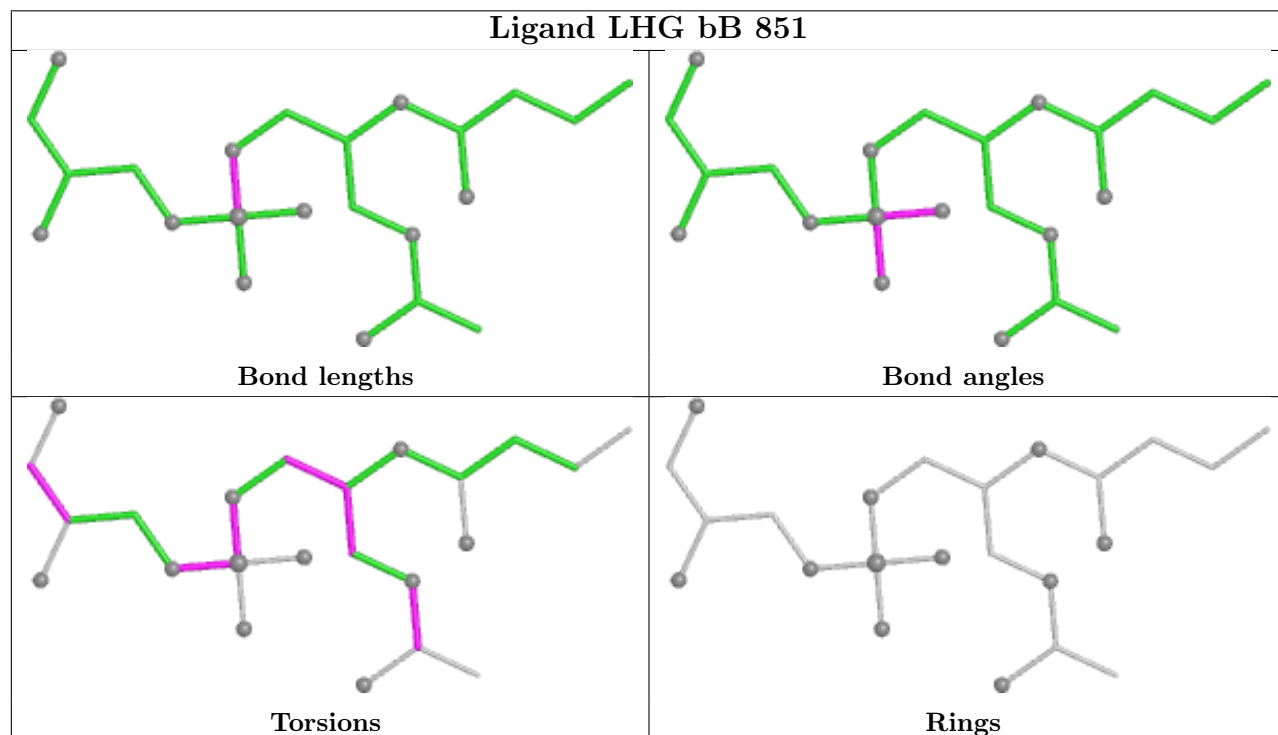
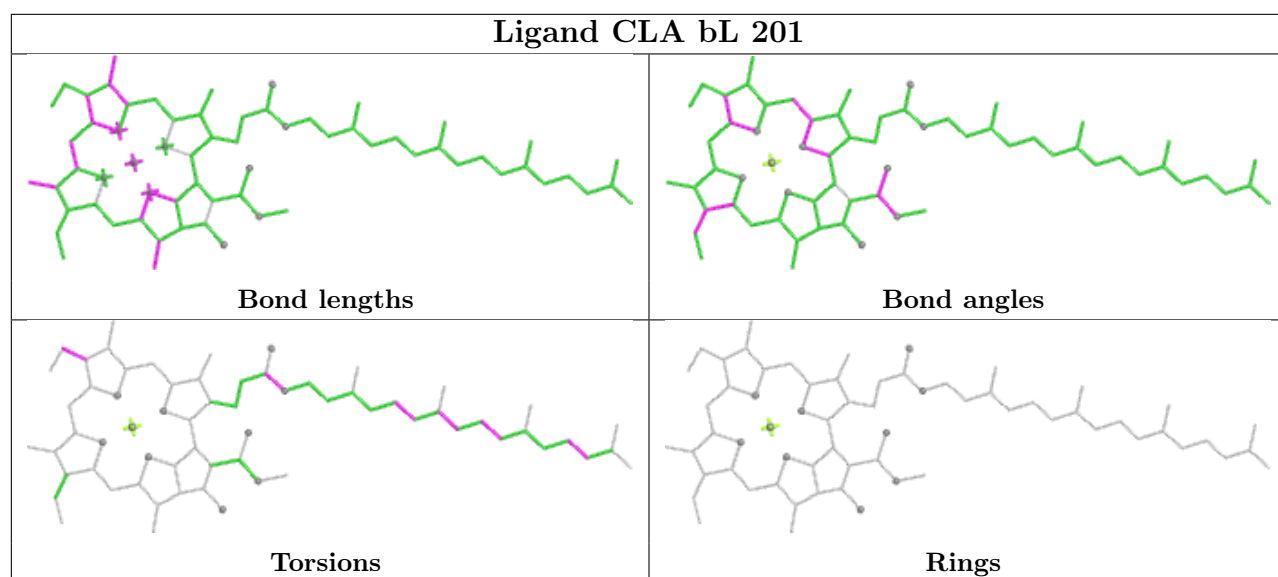


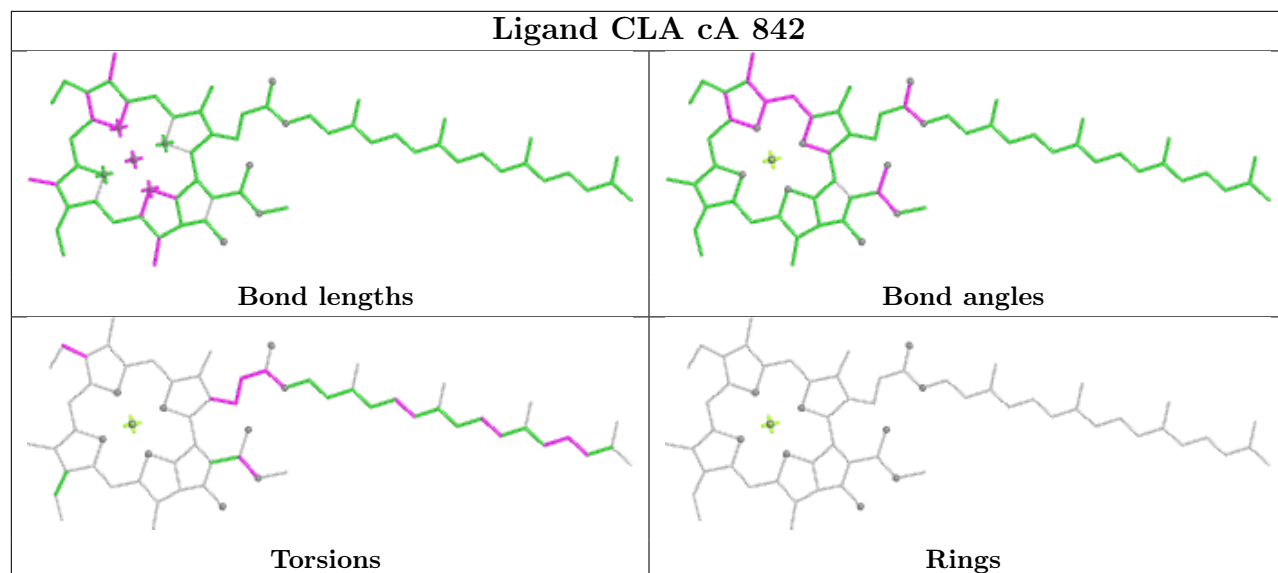
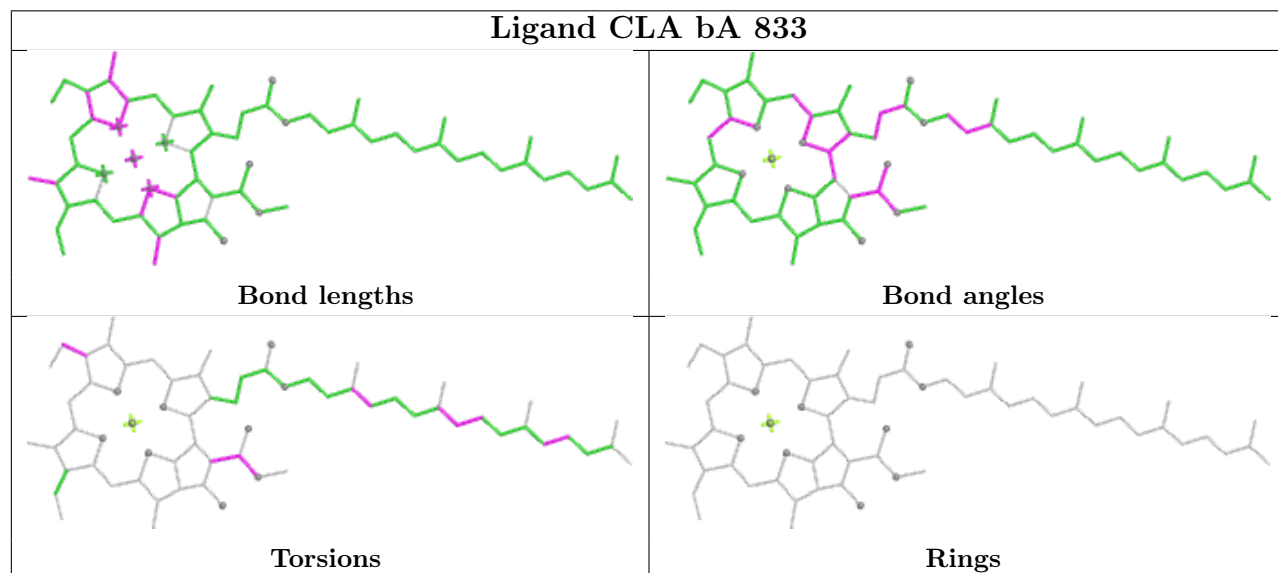
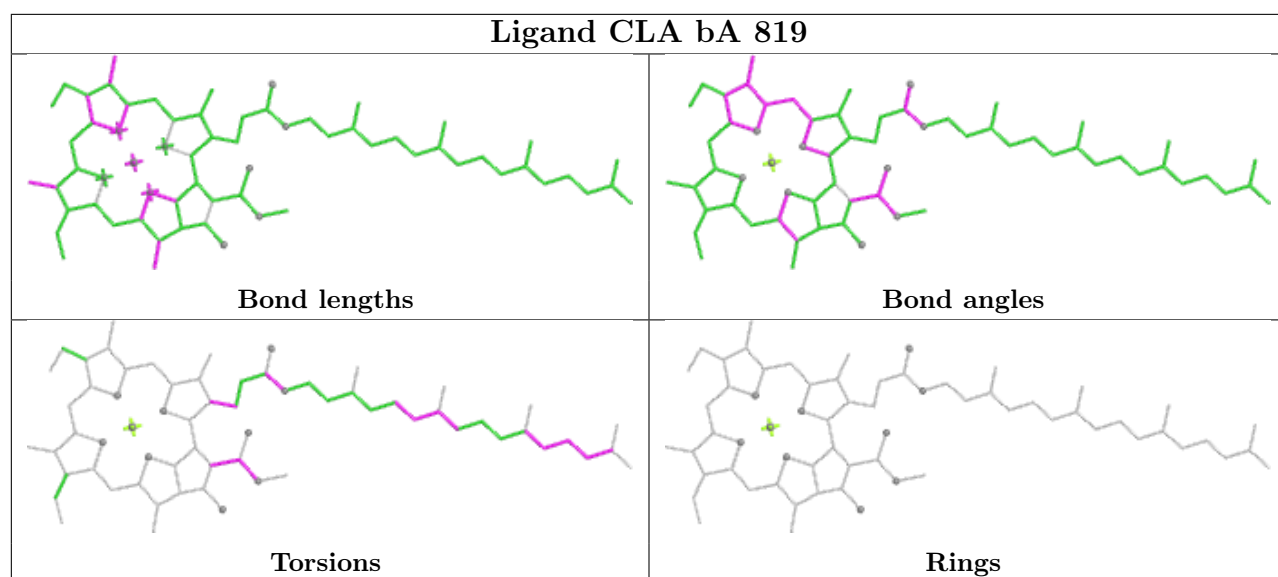
Torsions

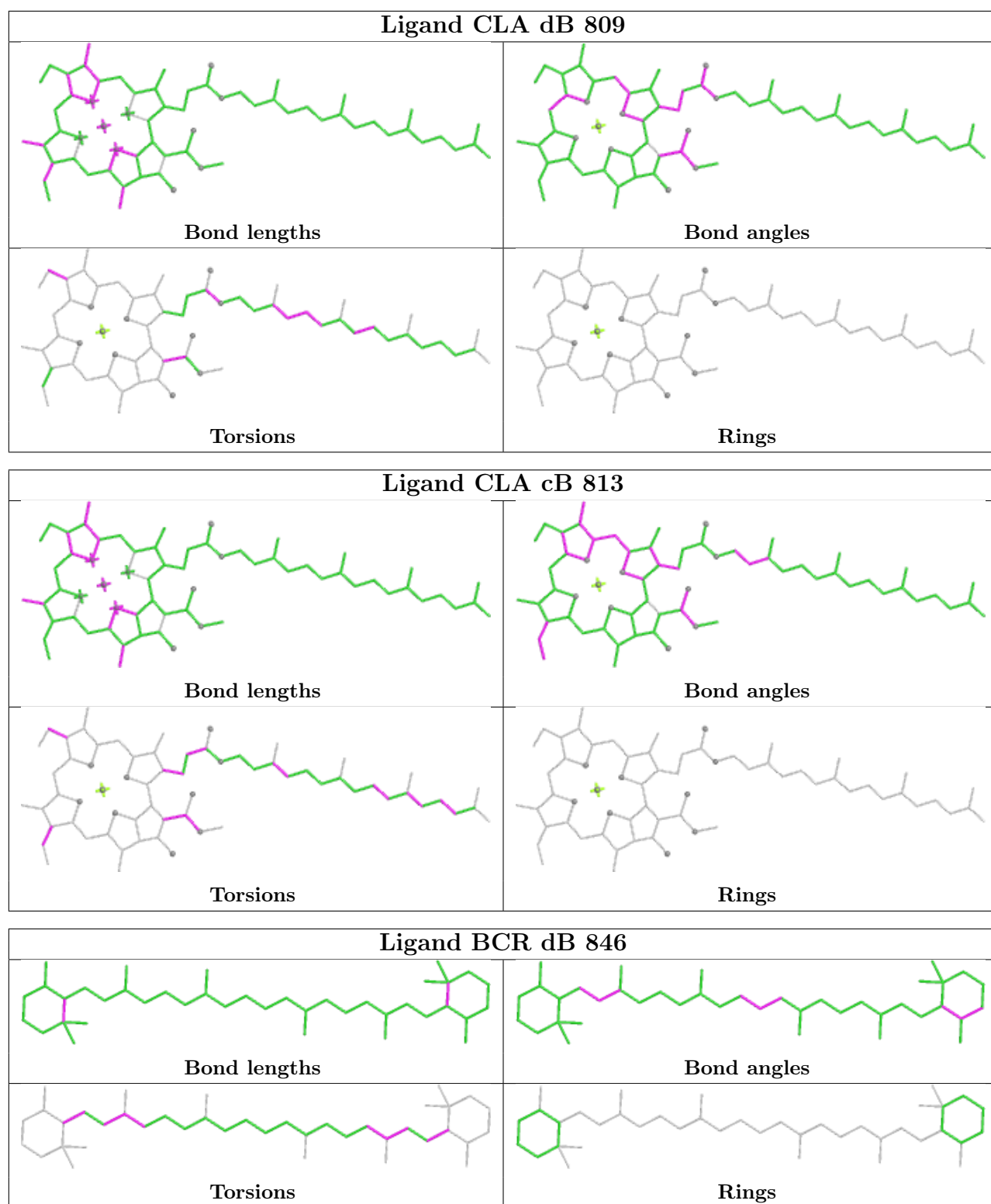


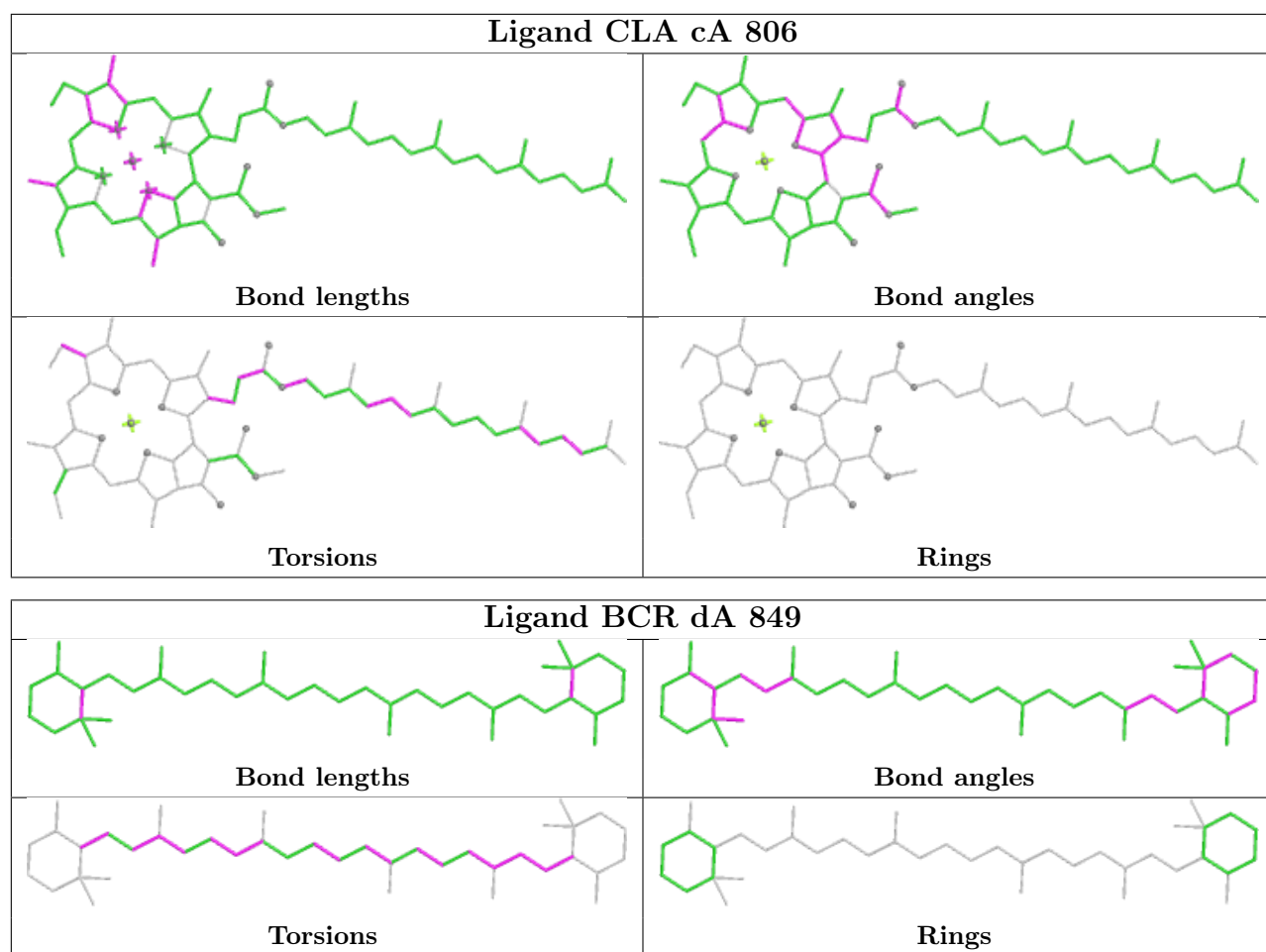
Rings

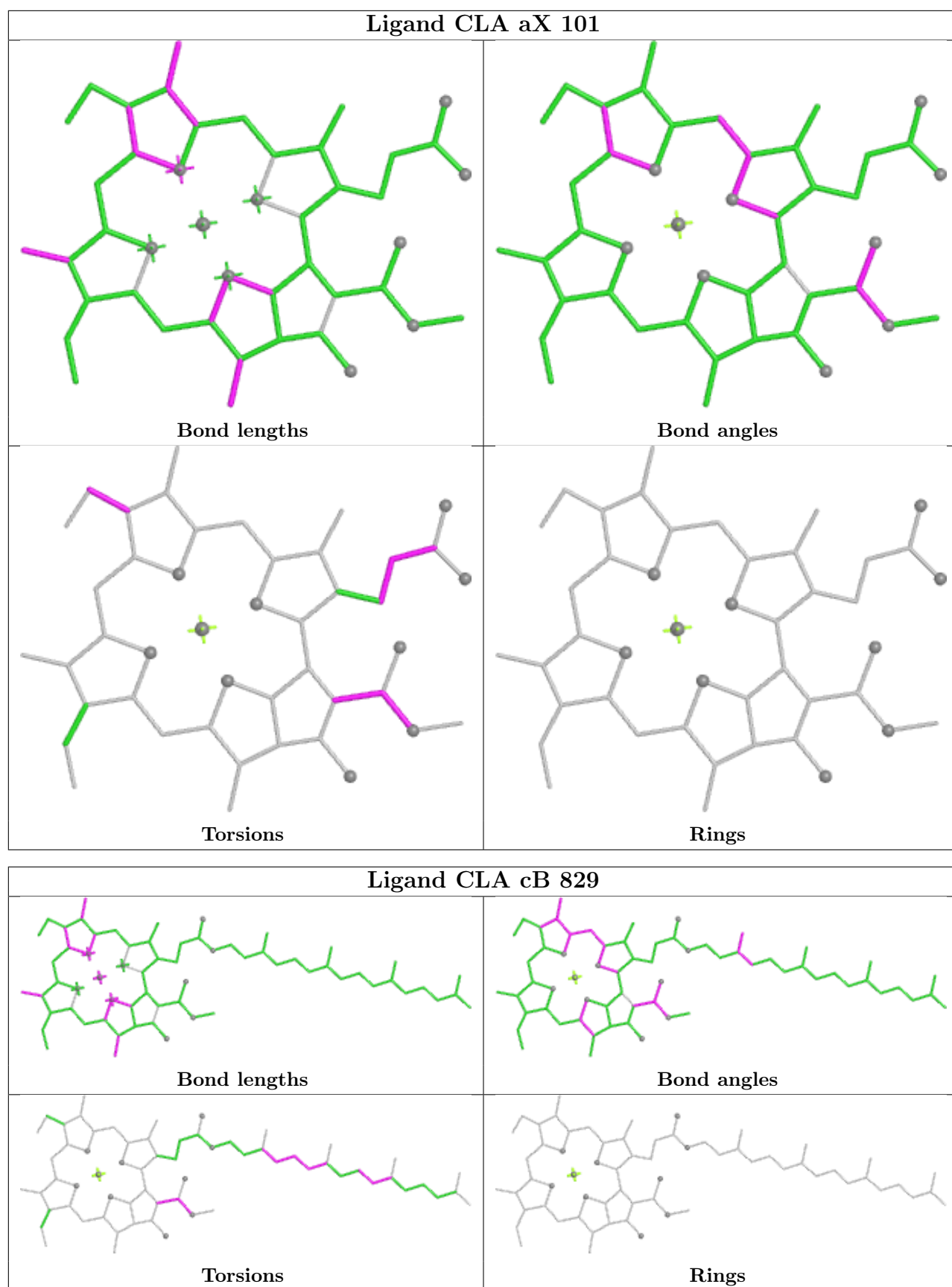


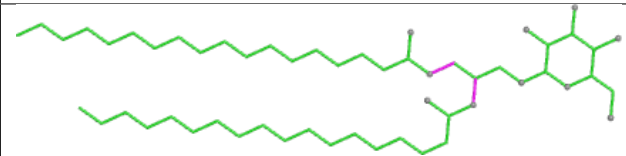
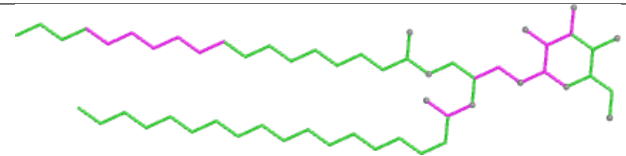
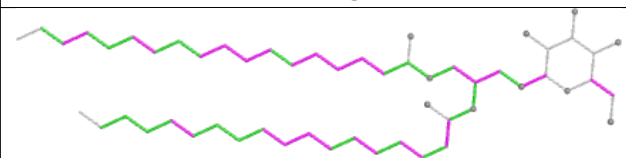
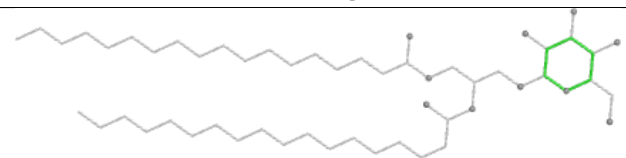


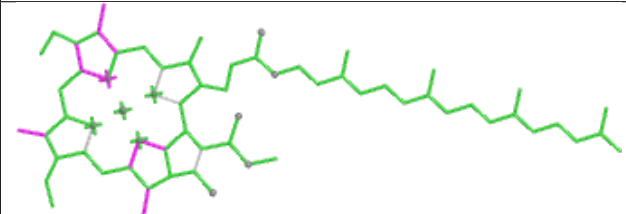
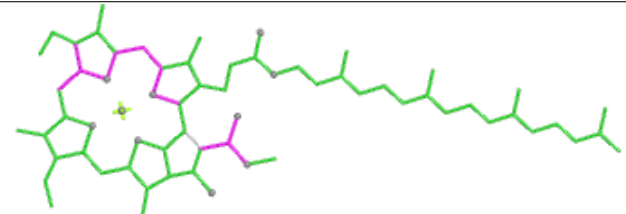
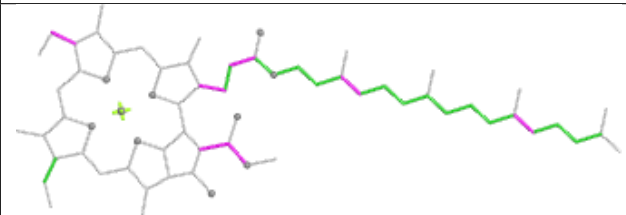
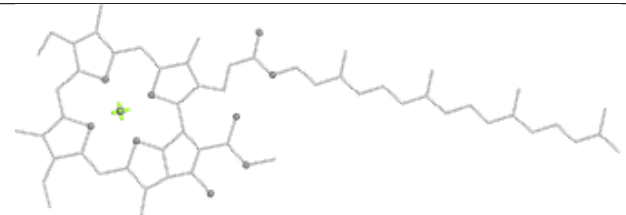


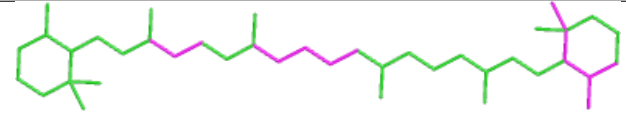
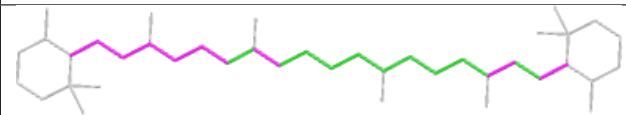
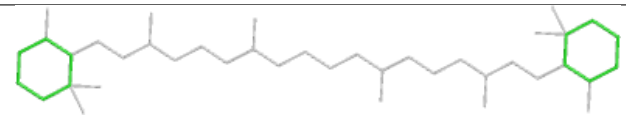




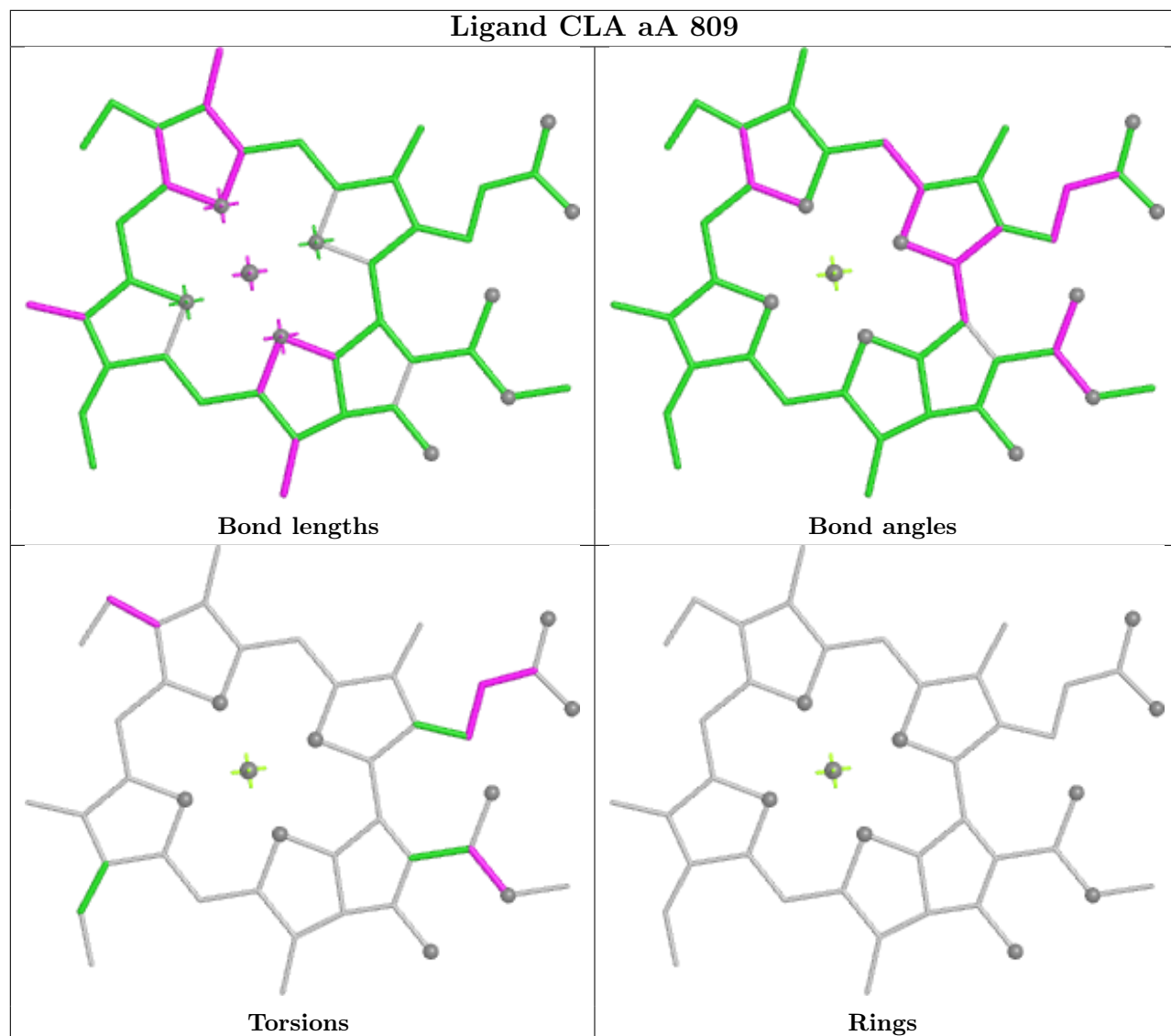


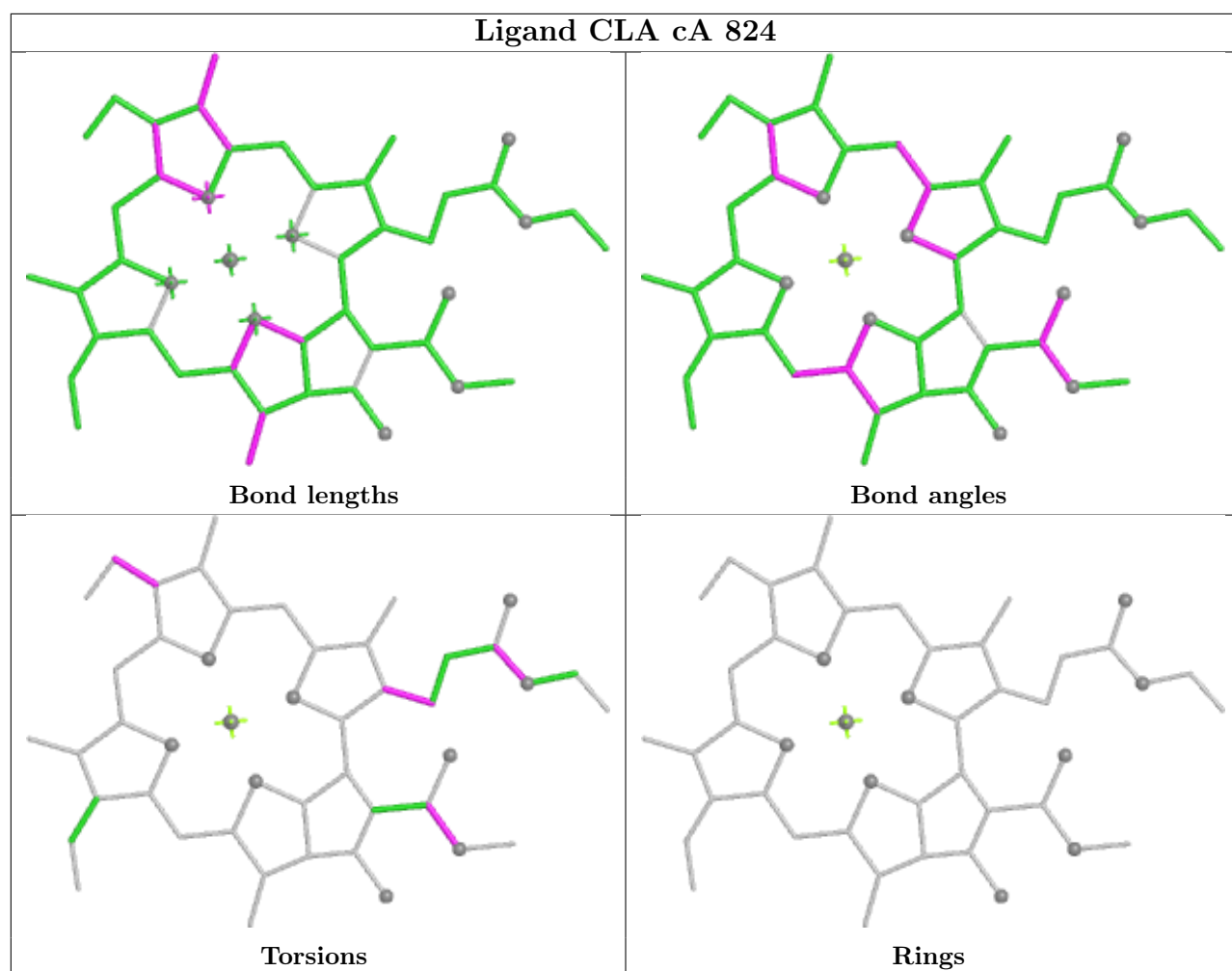
Ligand LMG dB 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

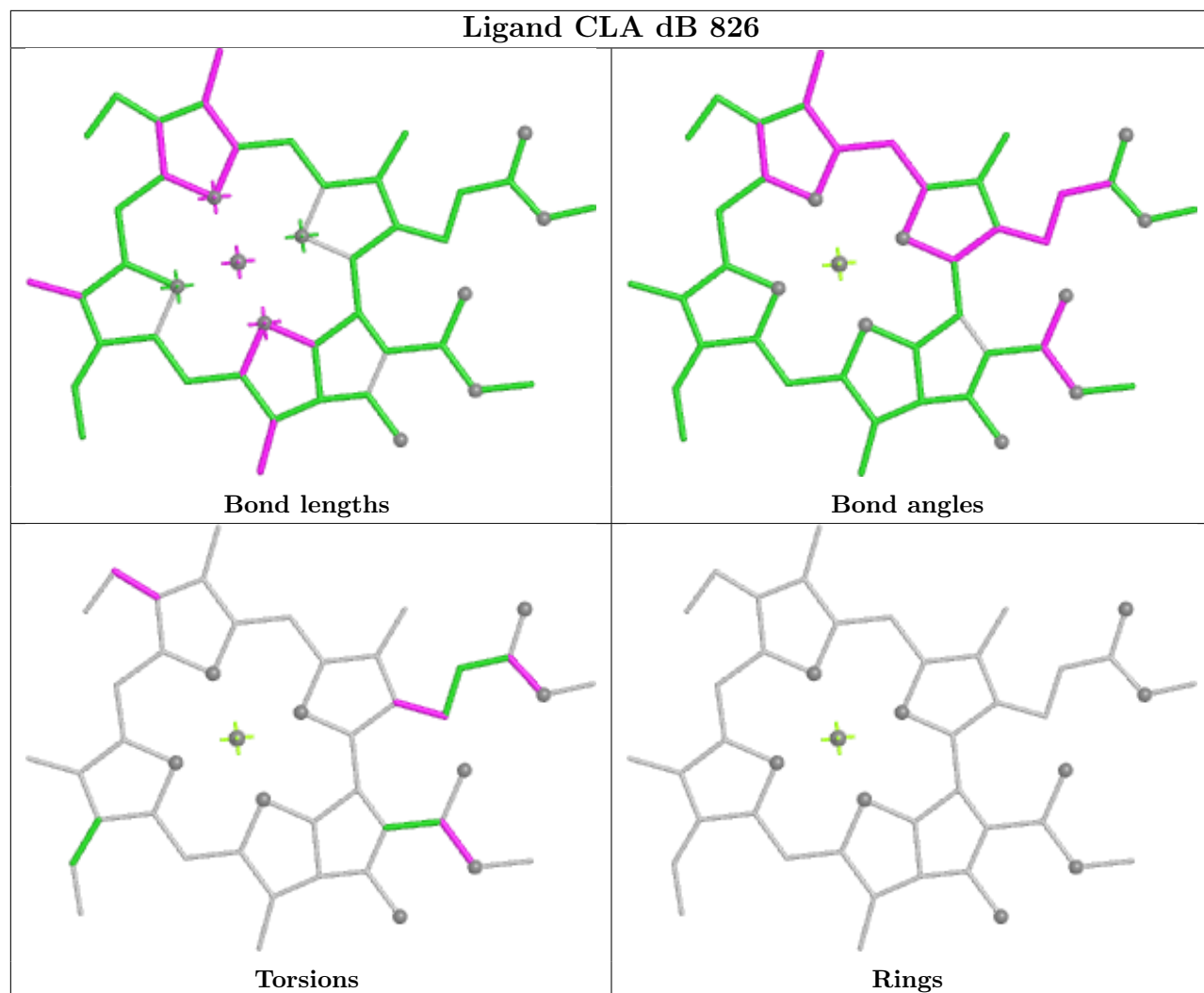
Ligand CLA bA 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR cF 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

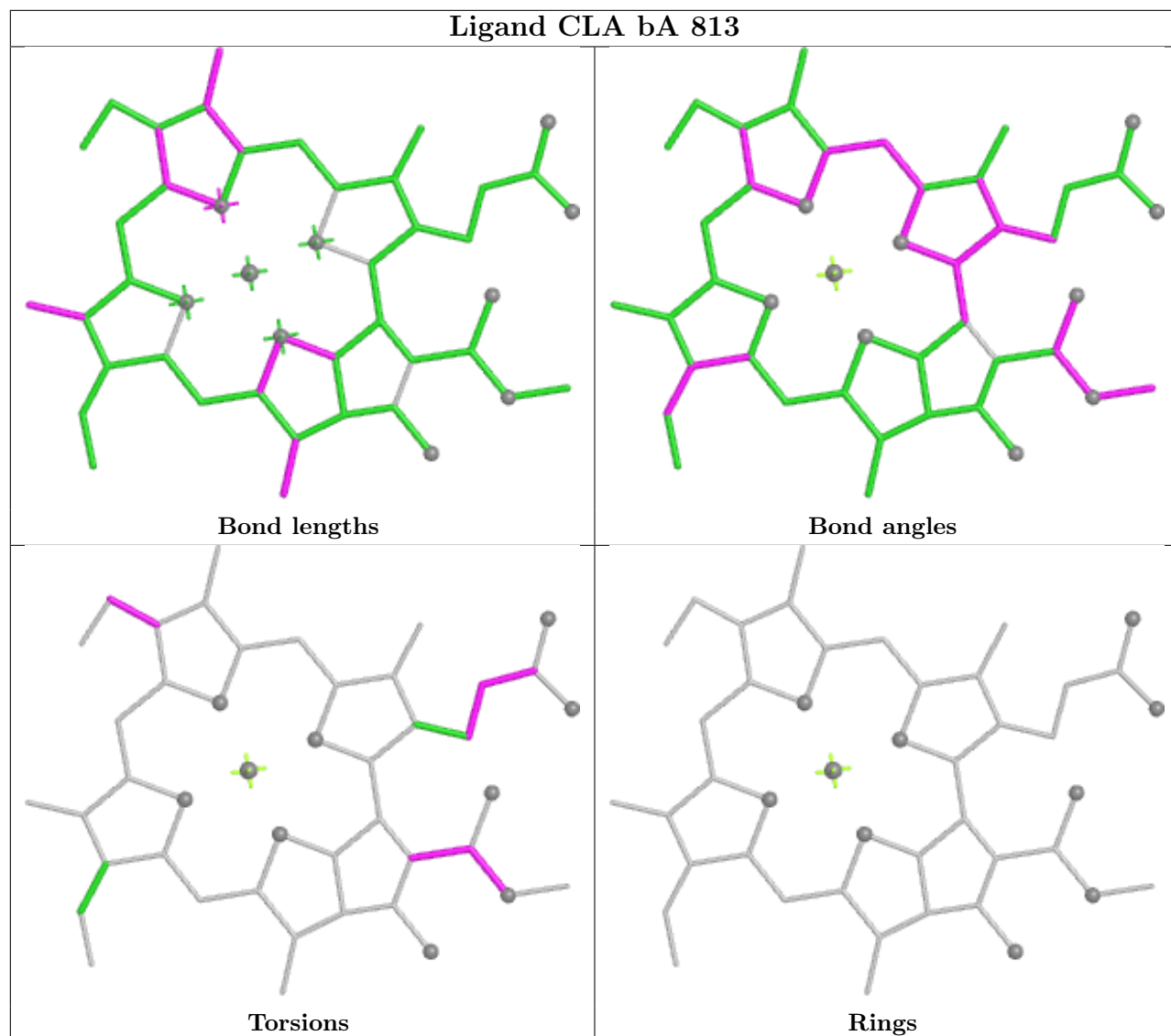
Ligand CLA aA 809



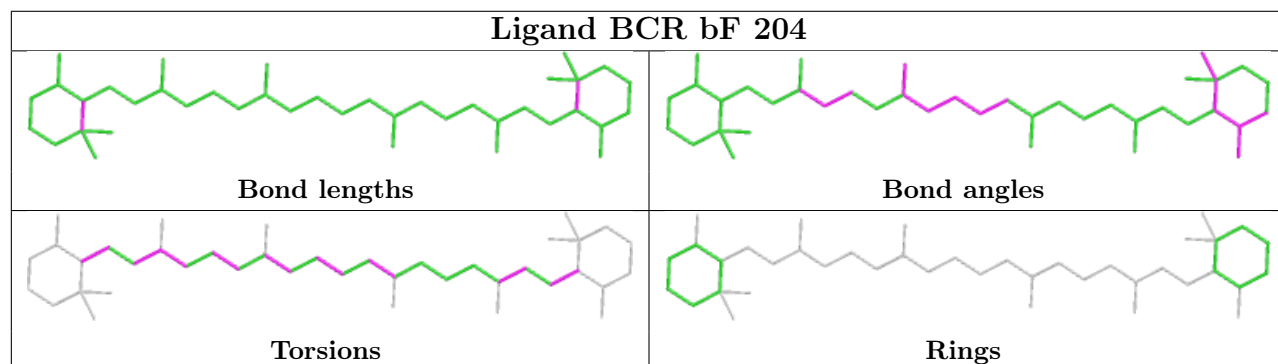


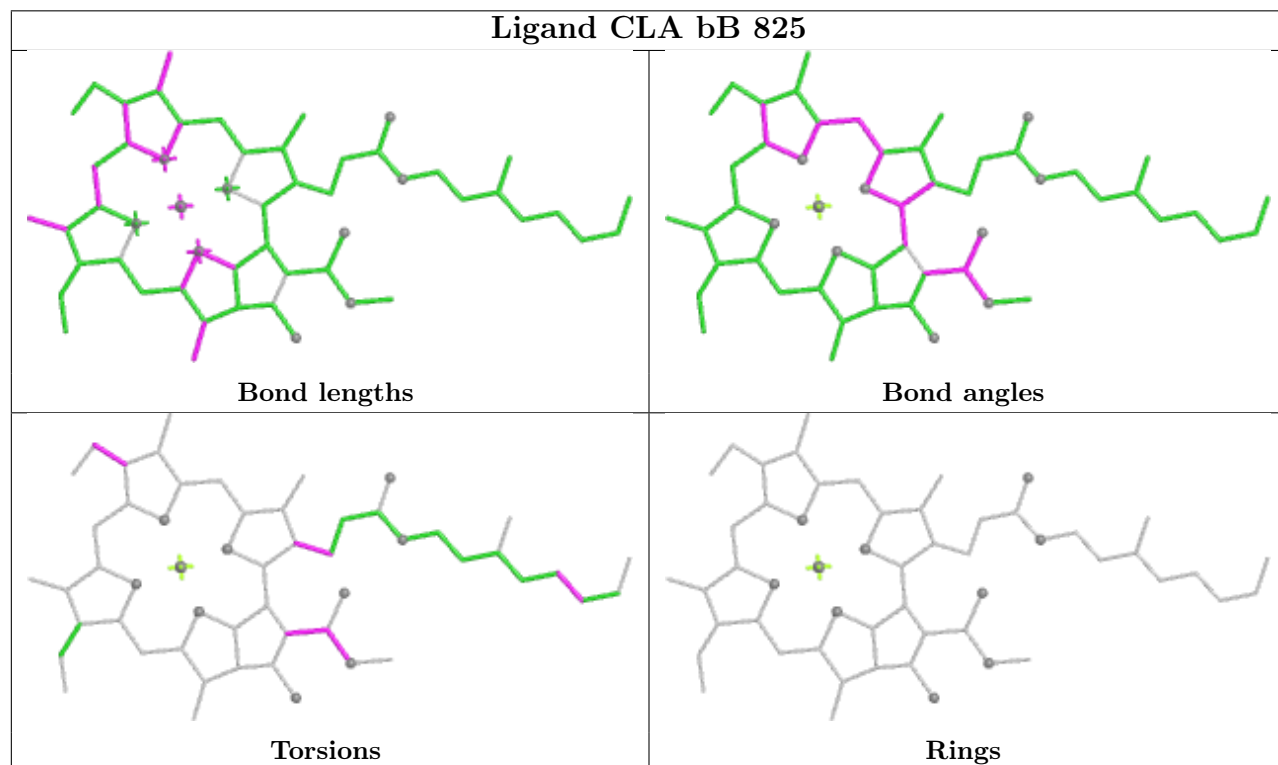
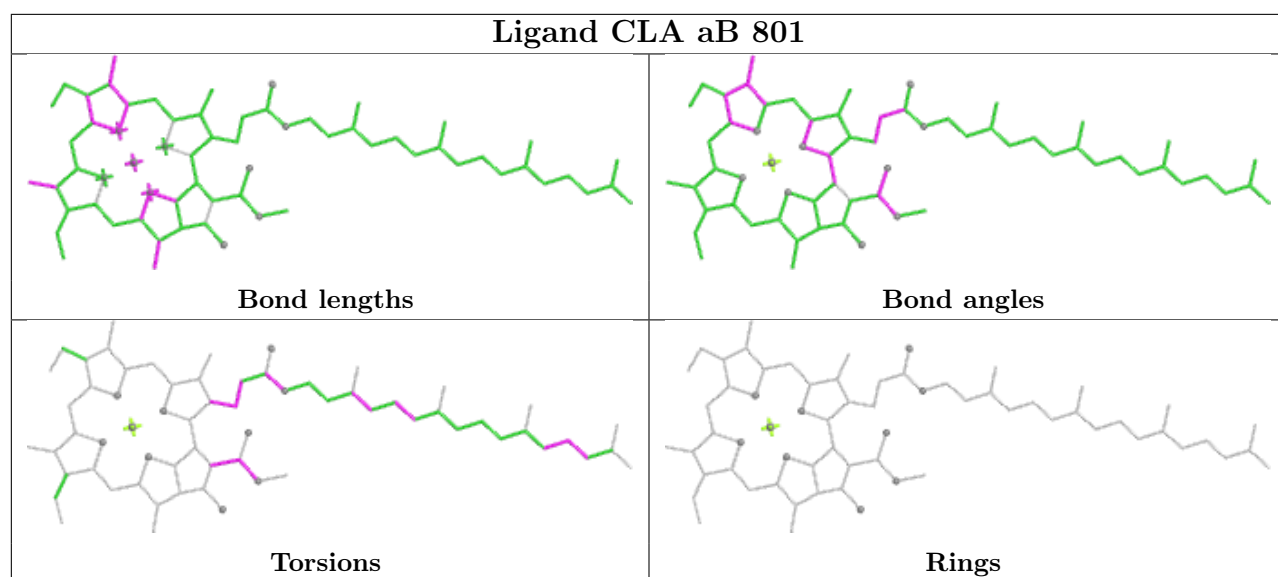


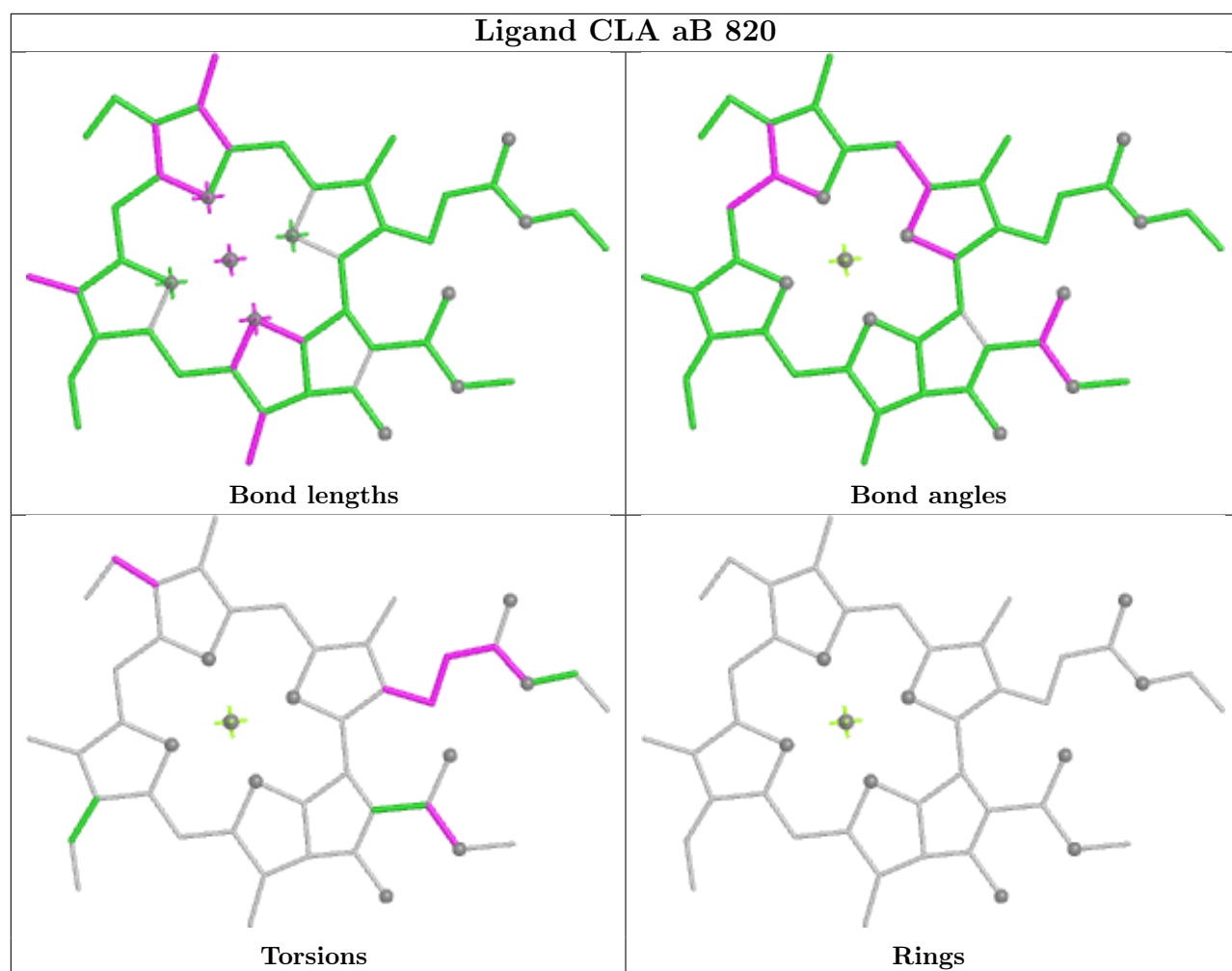
Ligand CLA bA 813

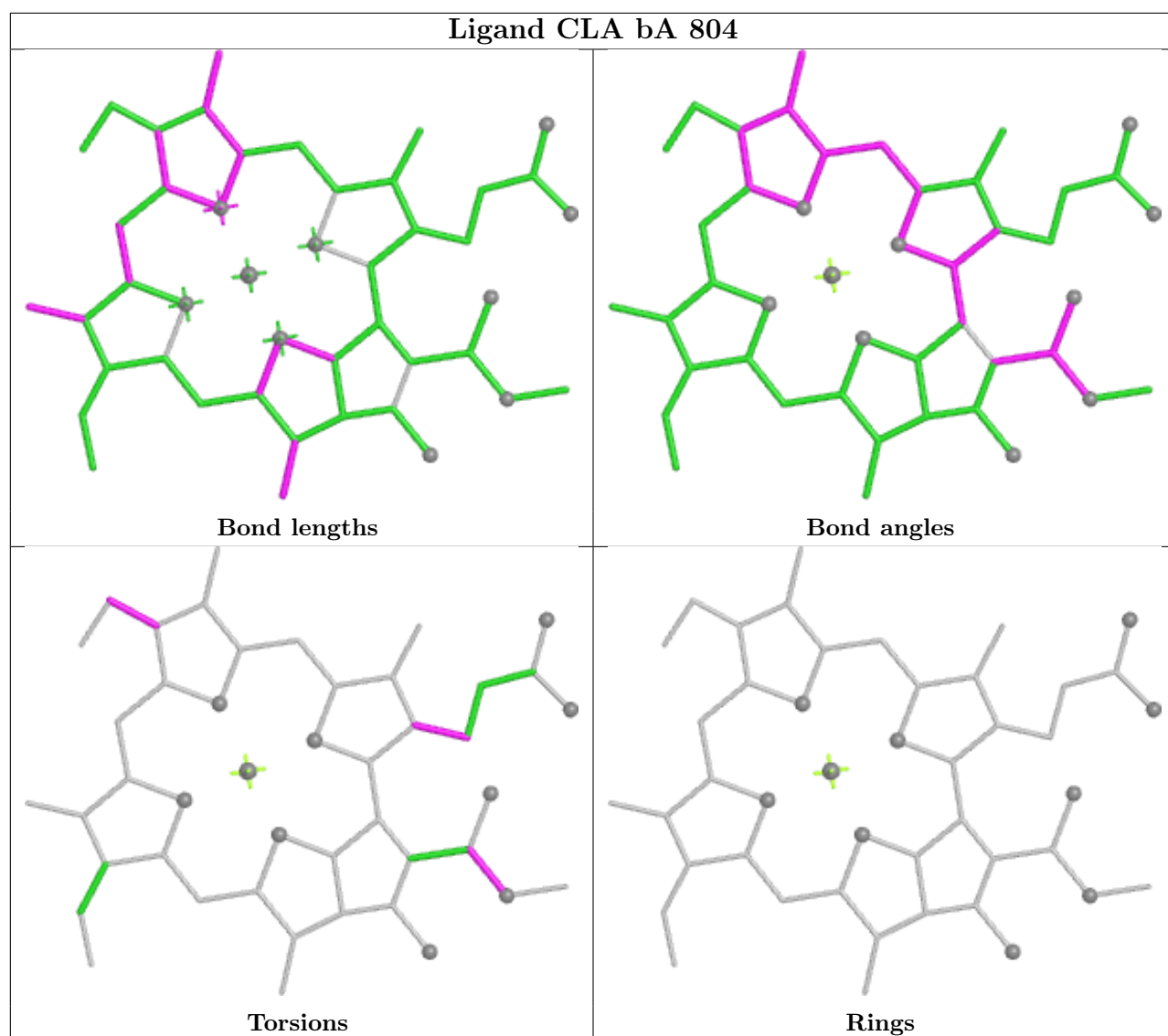


Ligand BCR bF 204

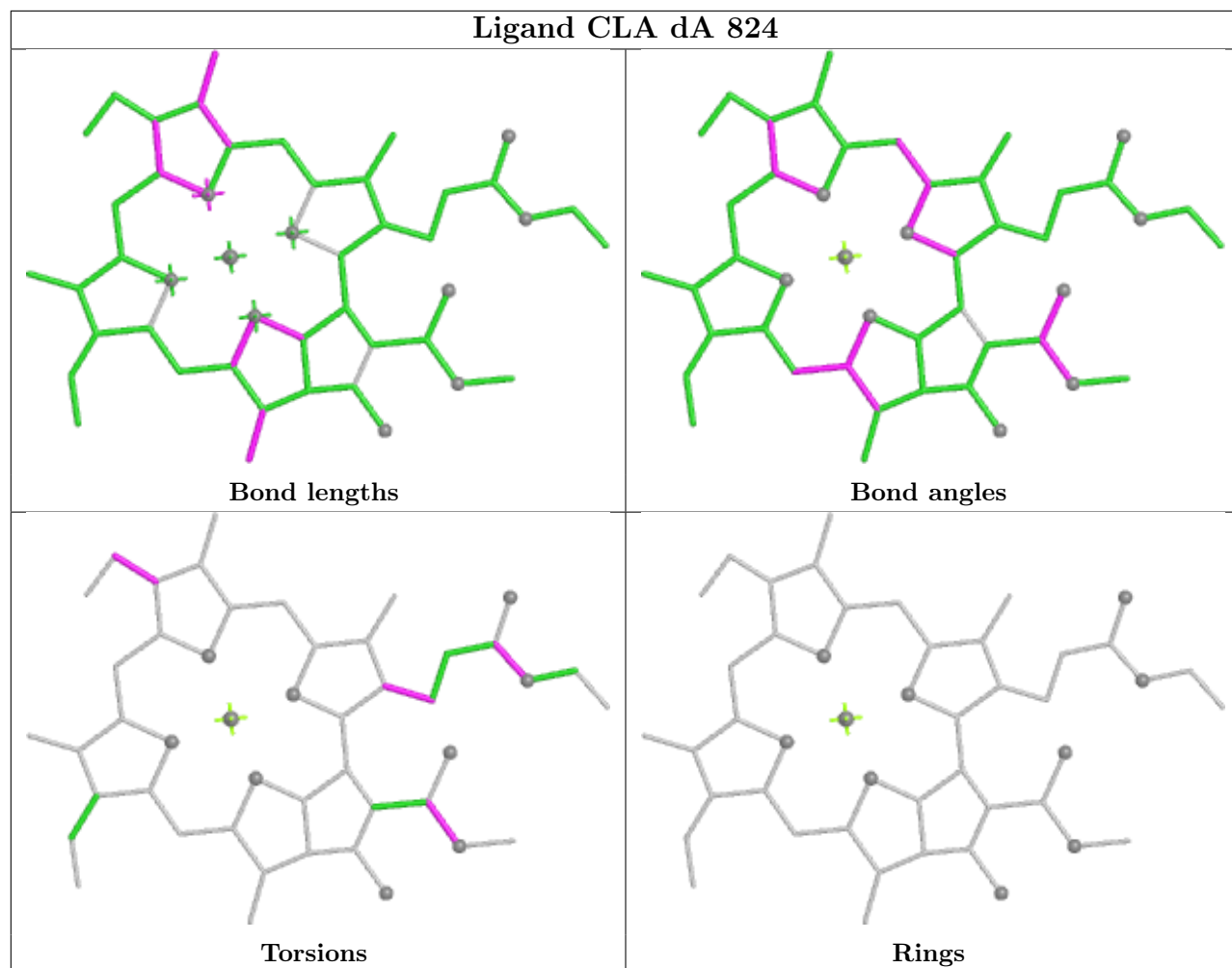


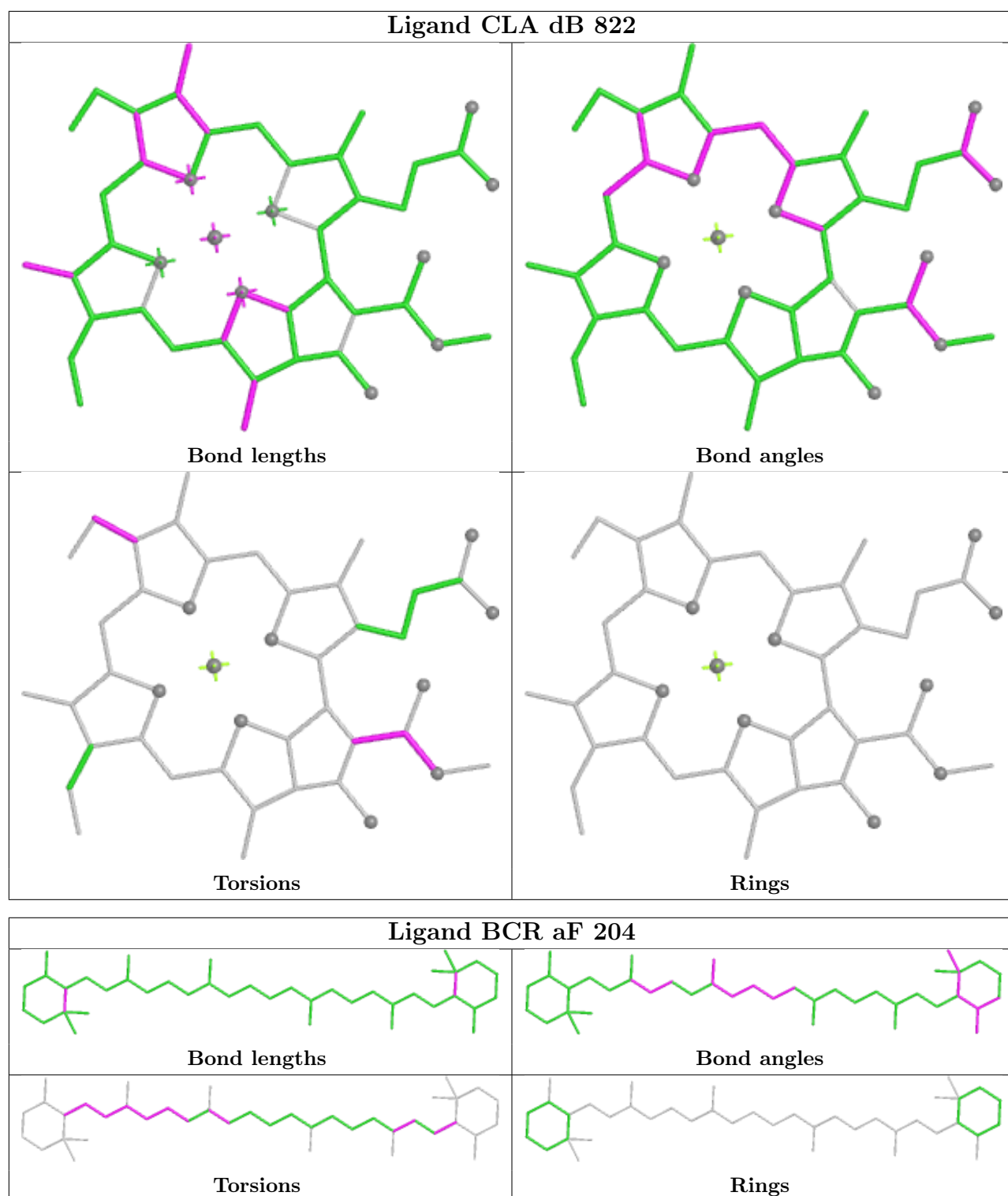




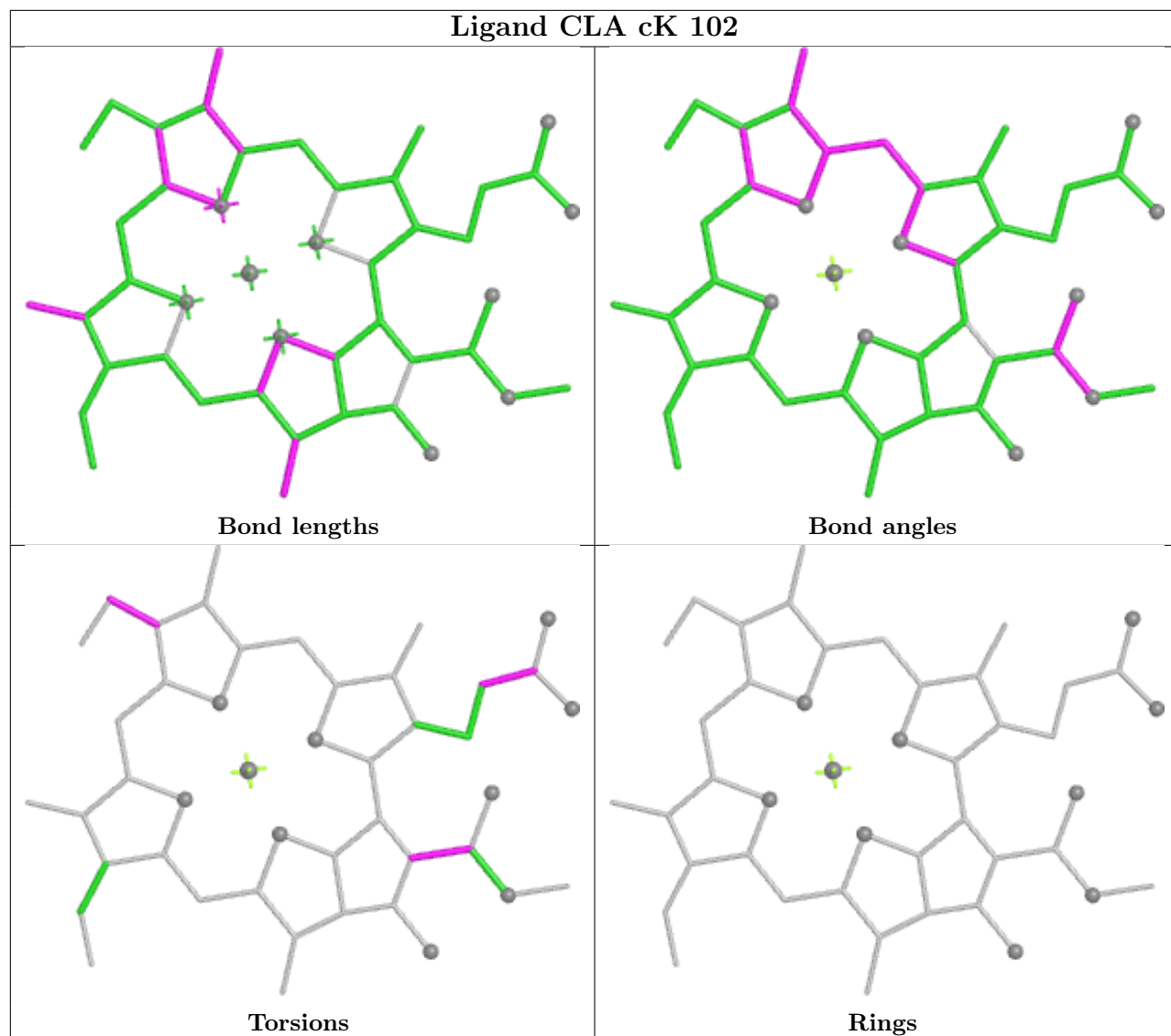


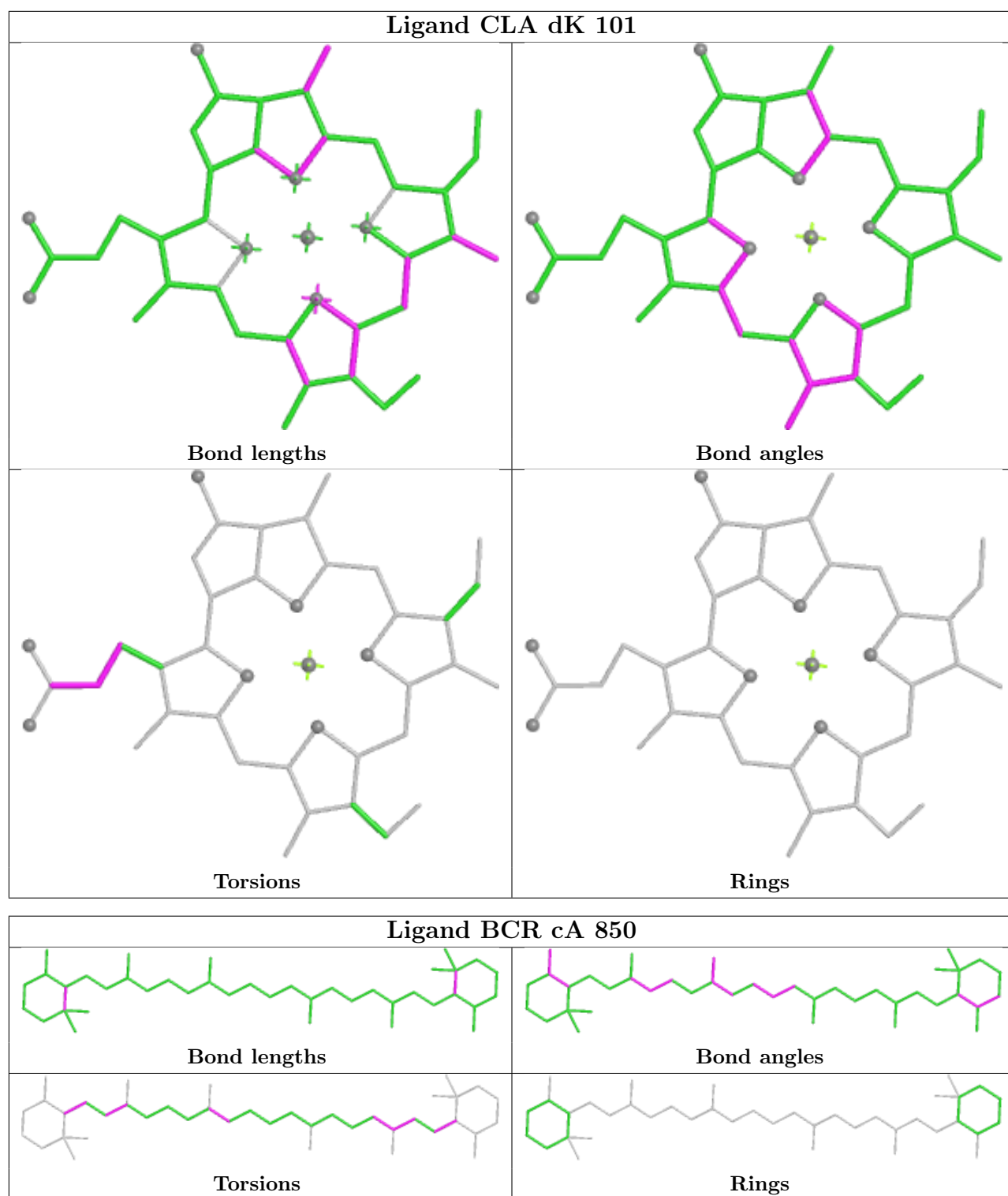
Ligand CLA dA 824

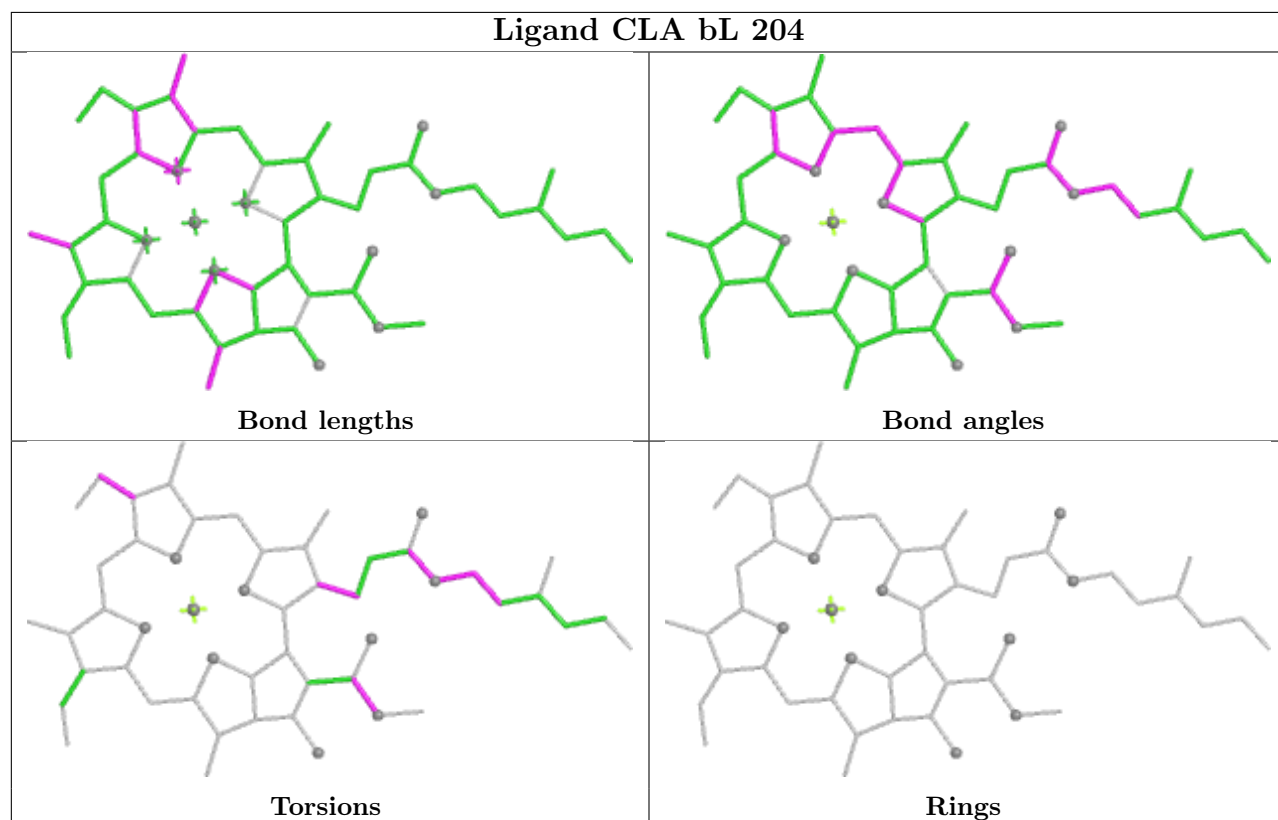
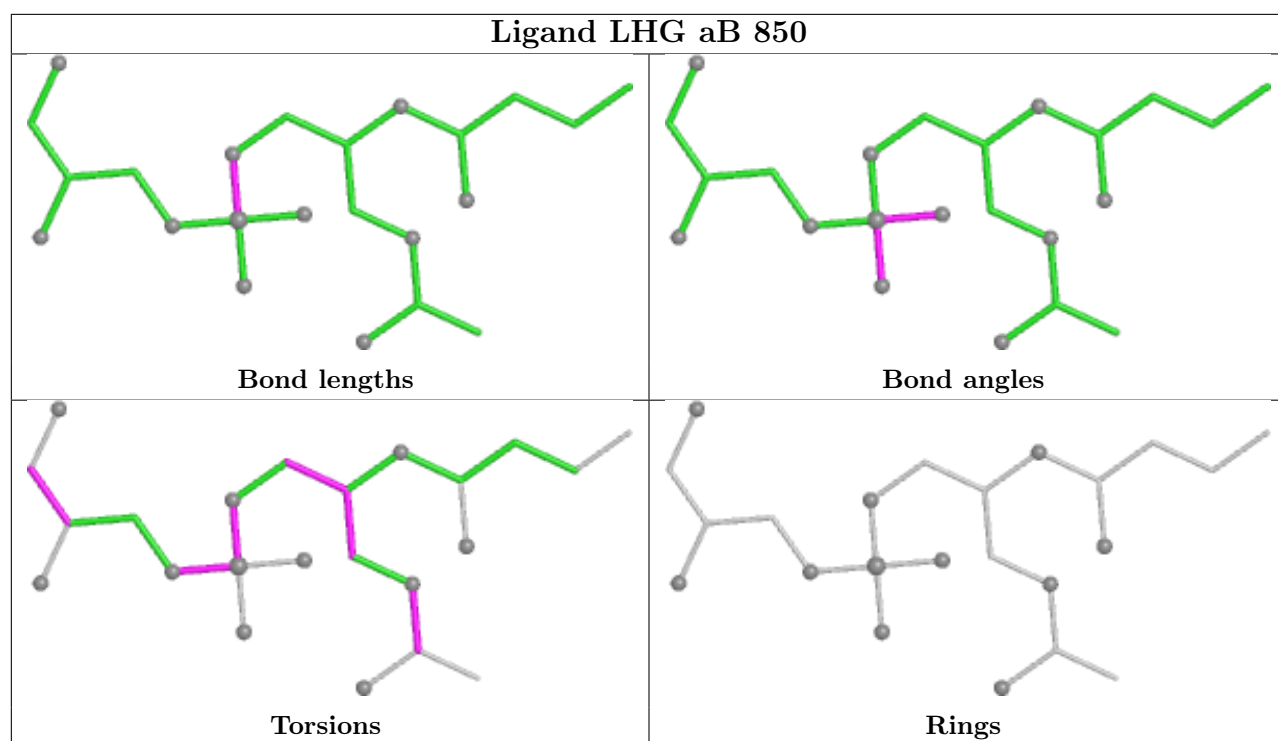


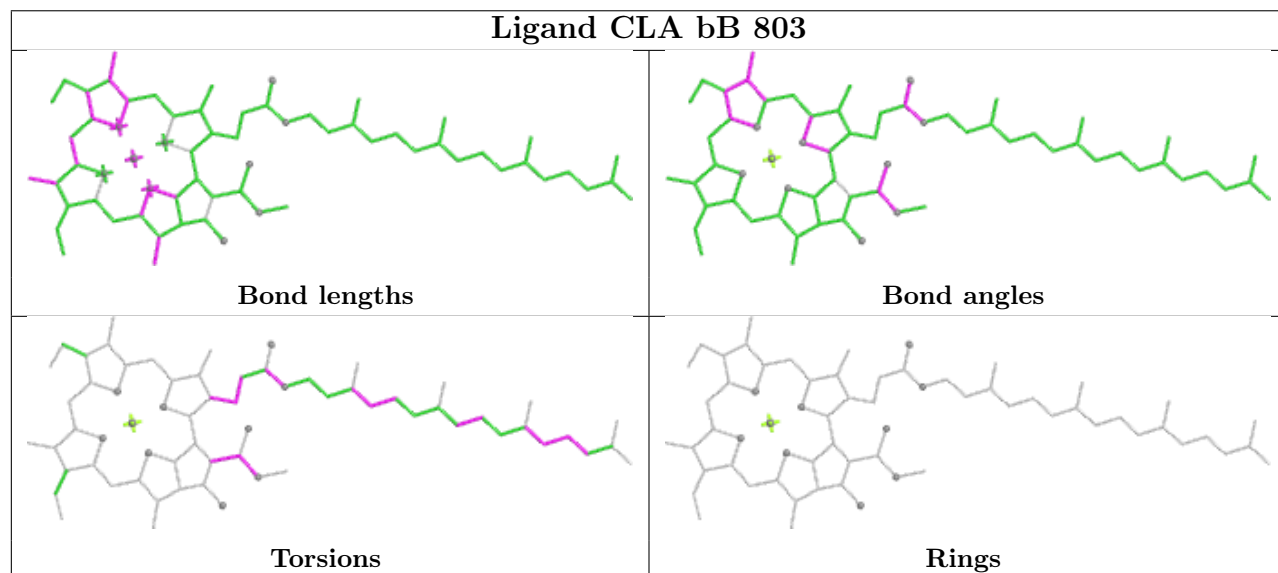
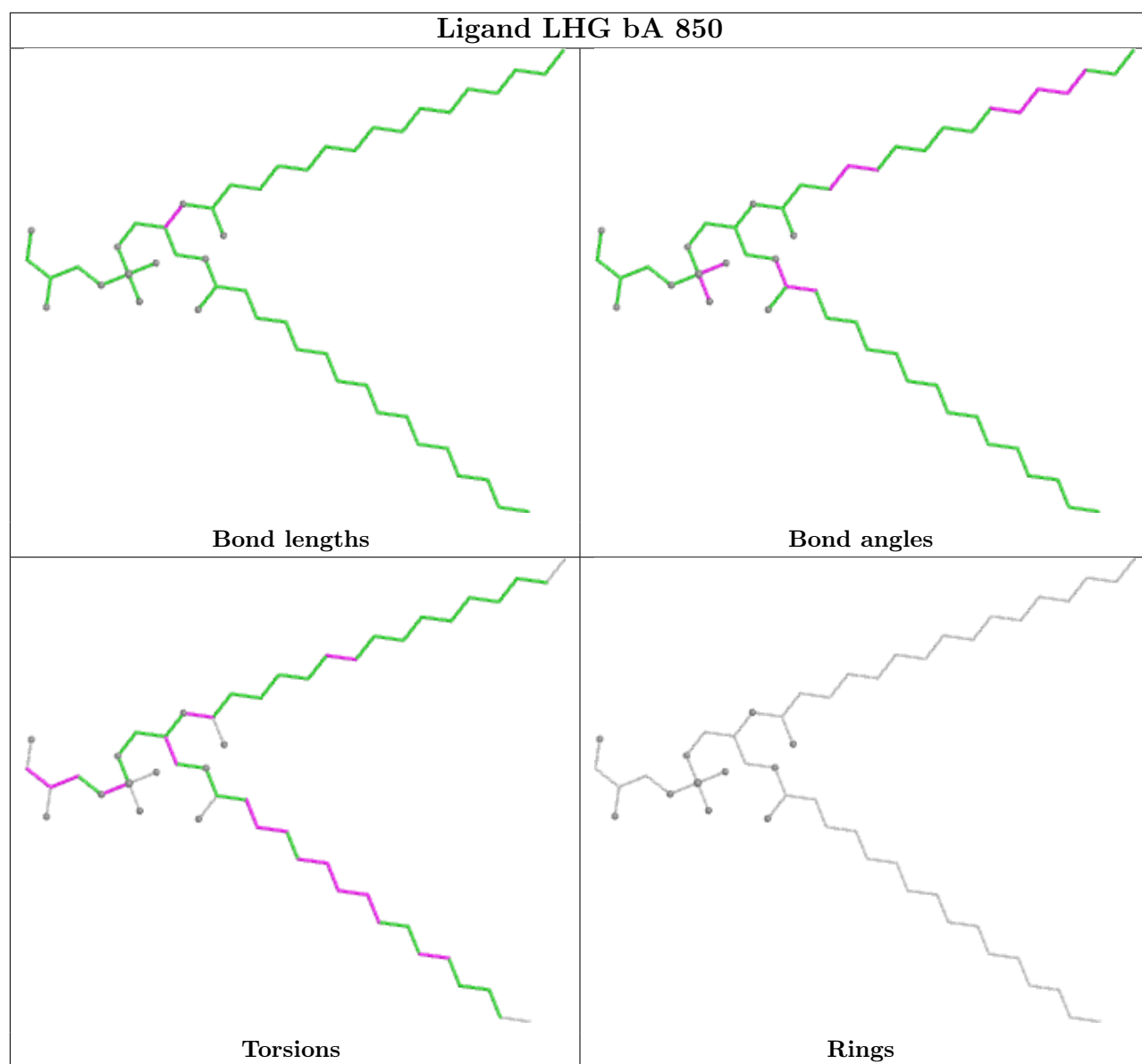


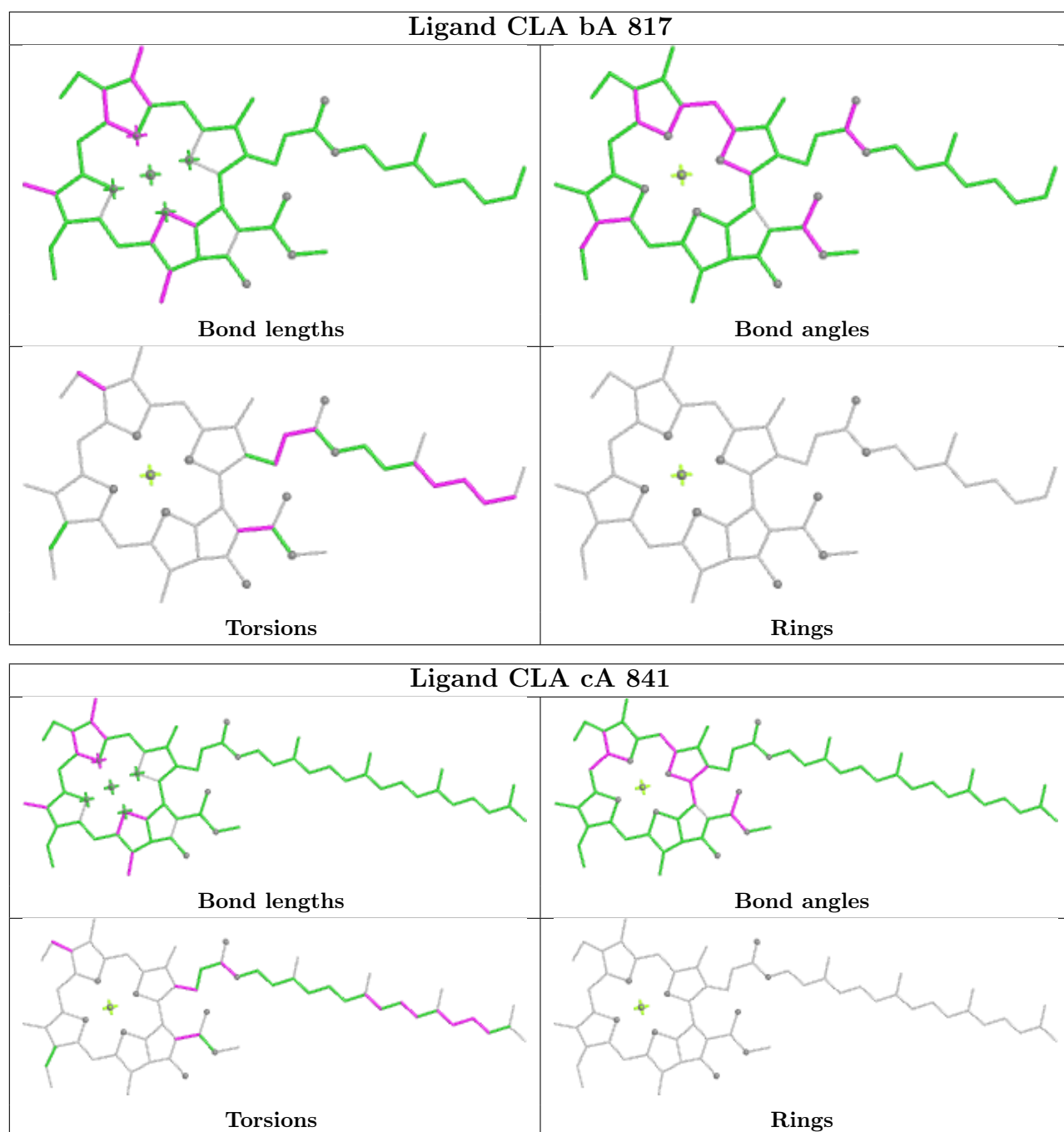
Ligand CLA cK 102

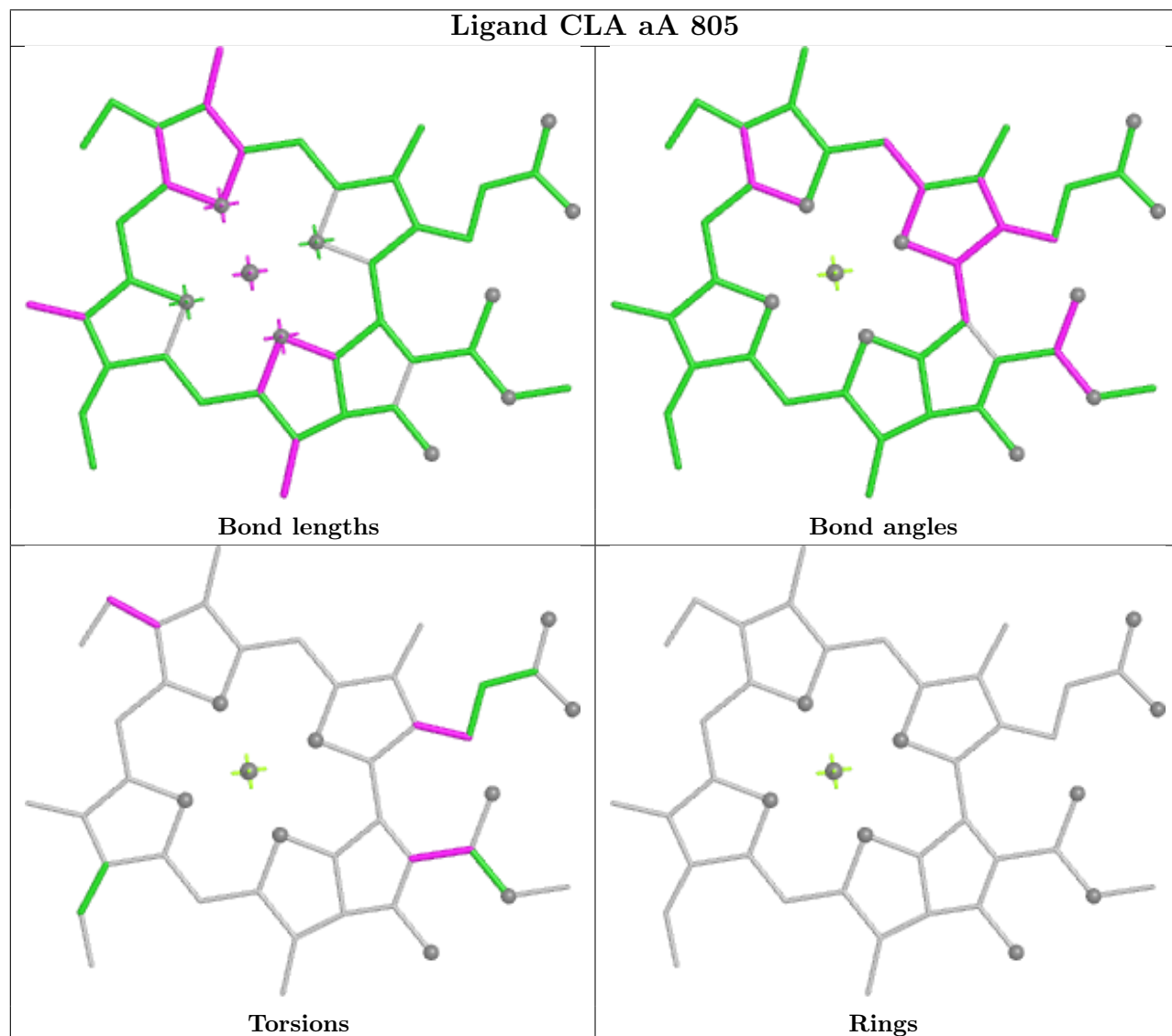
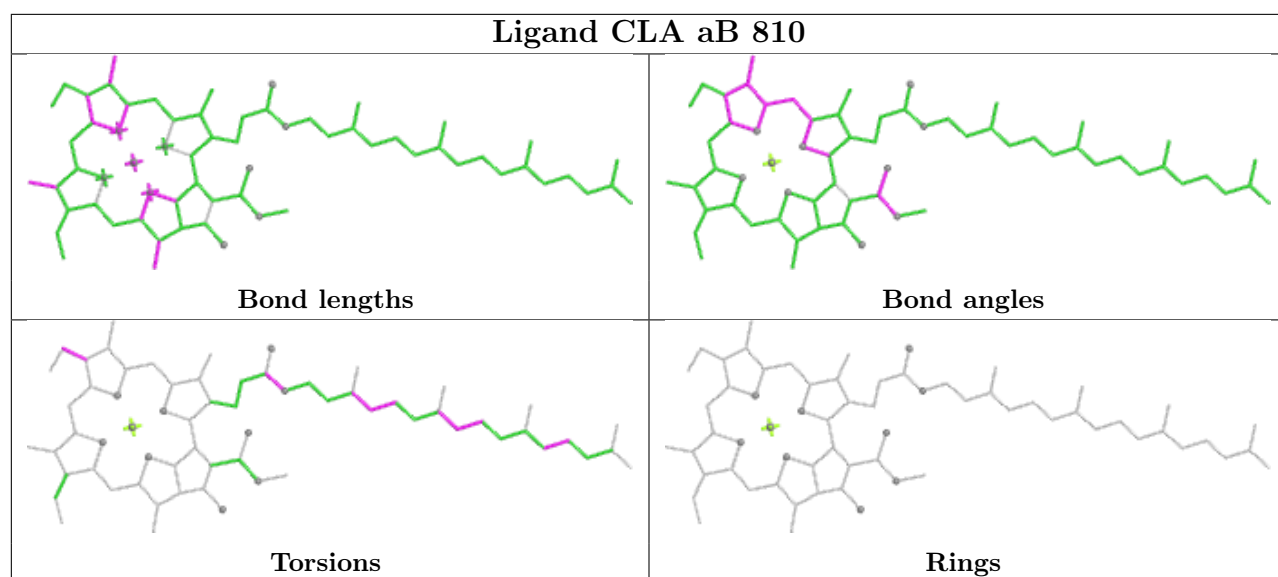




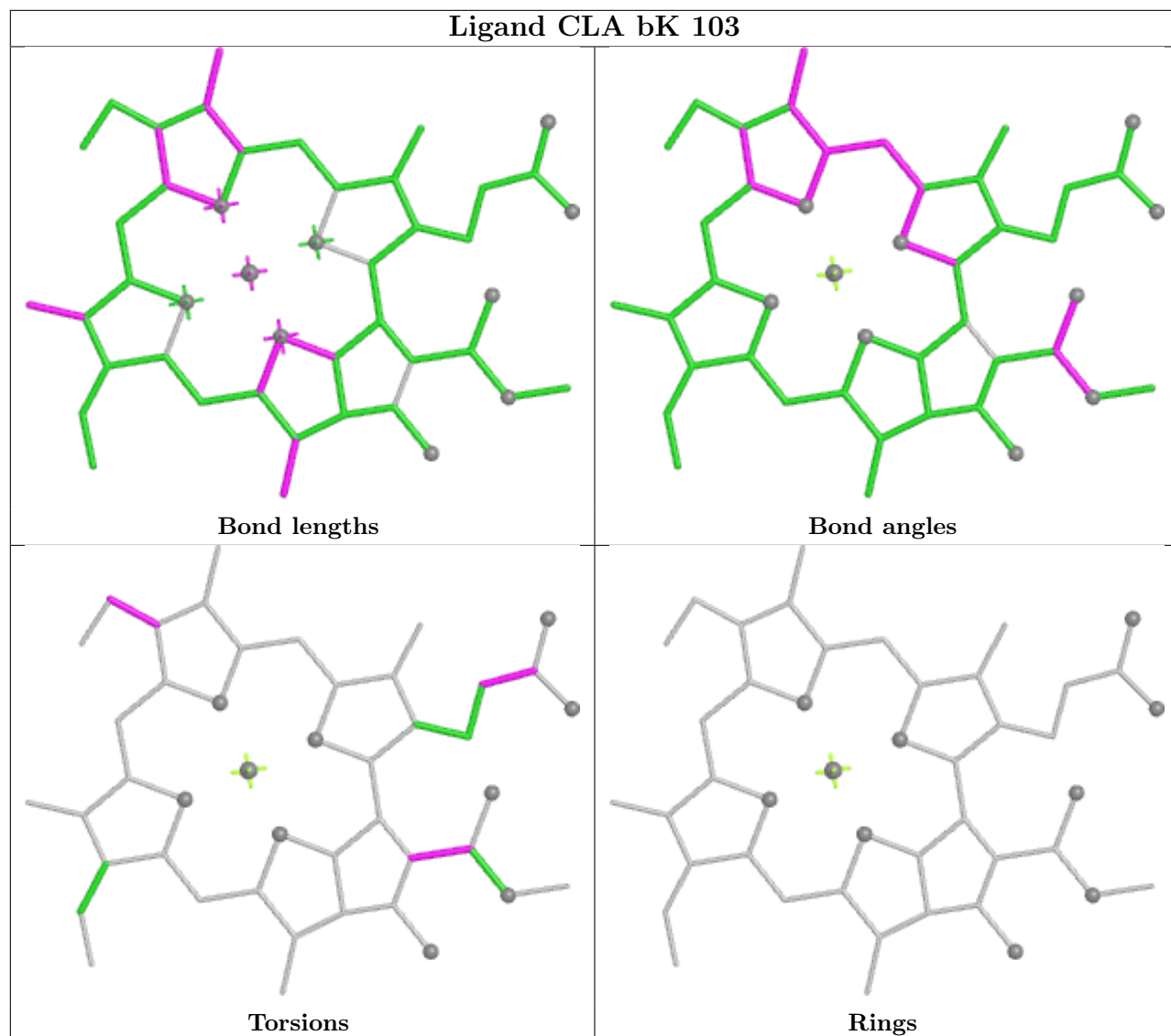




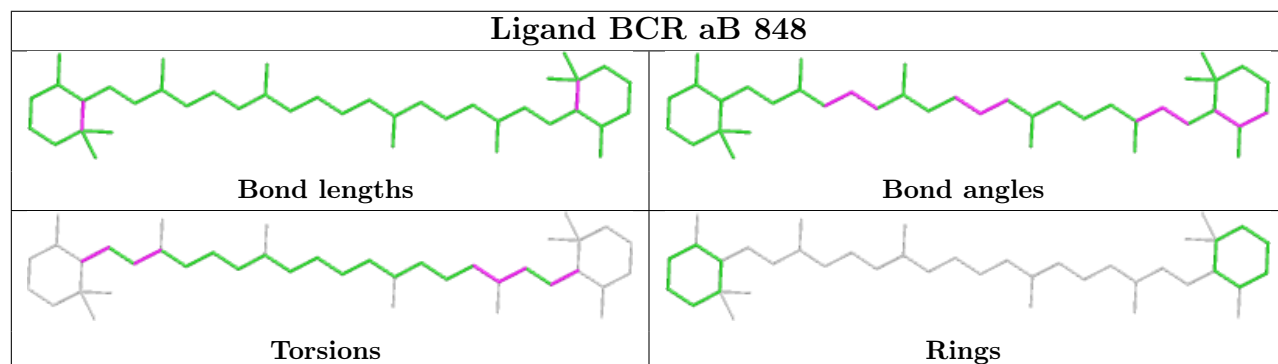


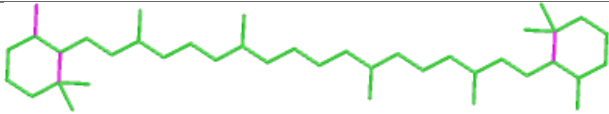
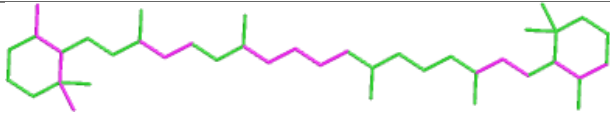
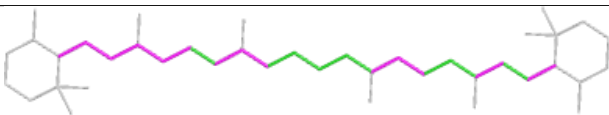
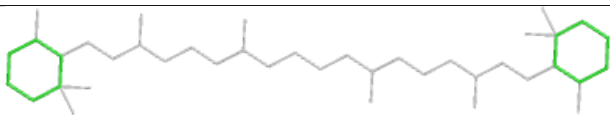


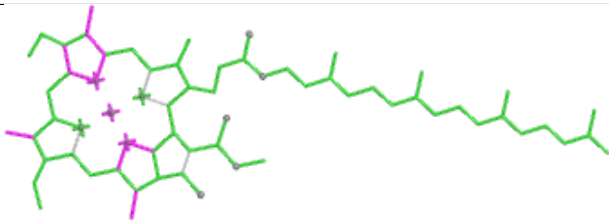
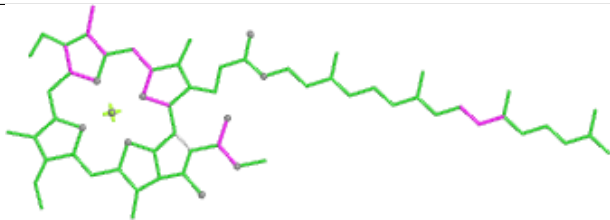
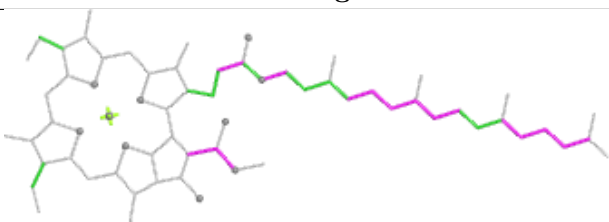
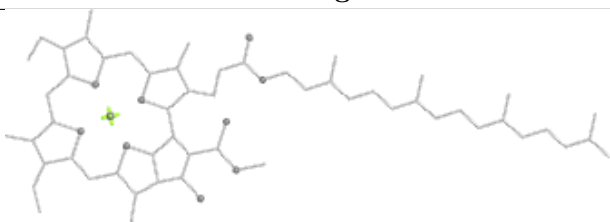
Ligand CLA bK 103

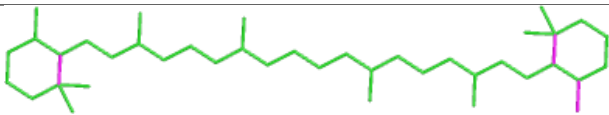
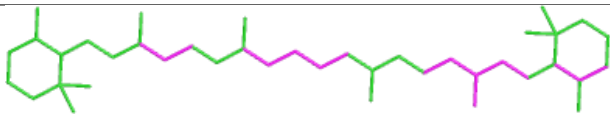
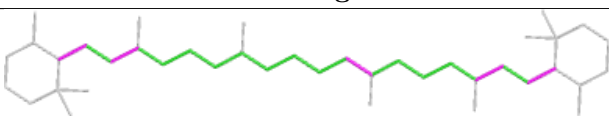
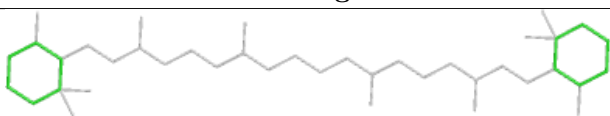


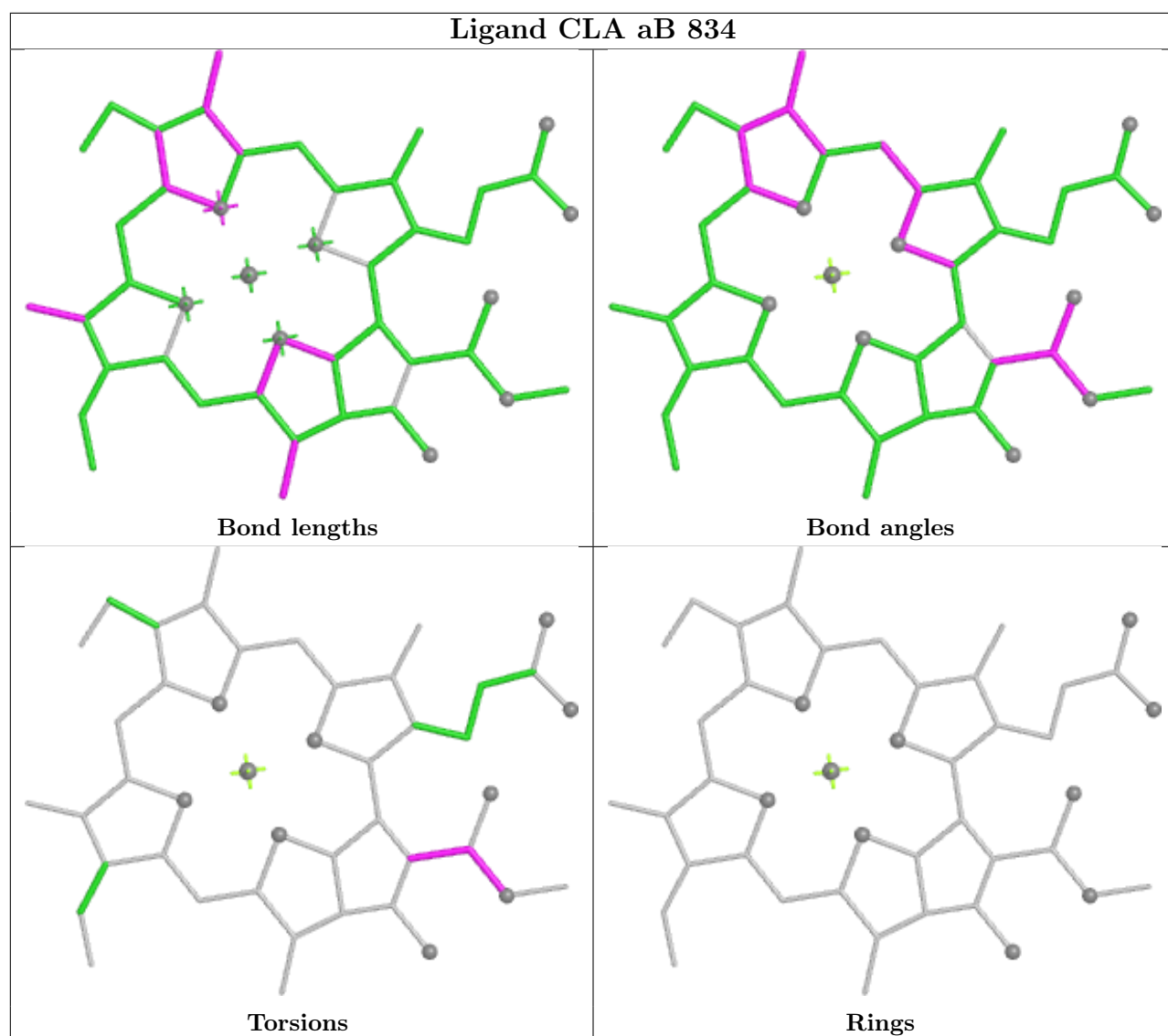
Ligand BCR aB 848

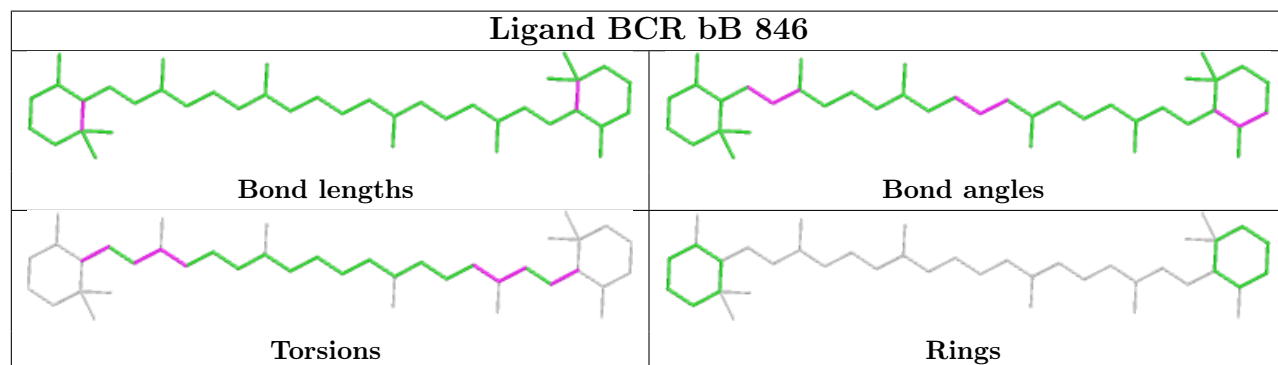
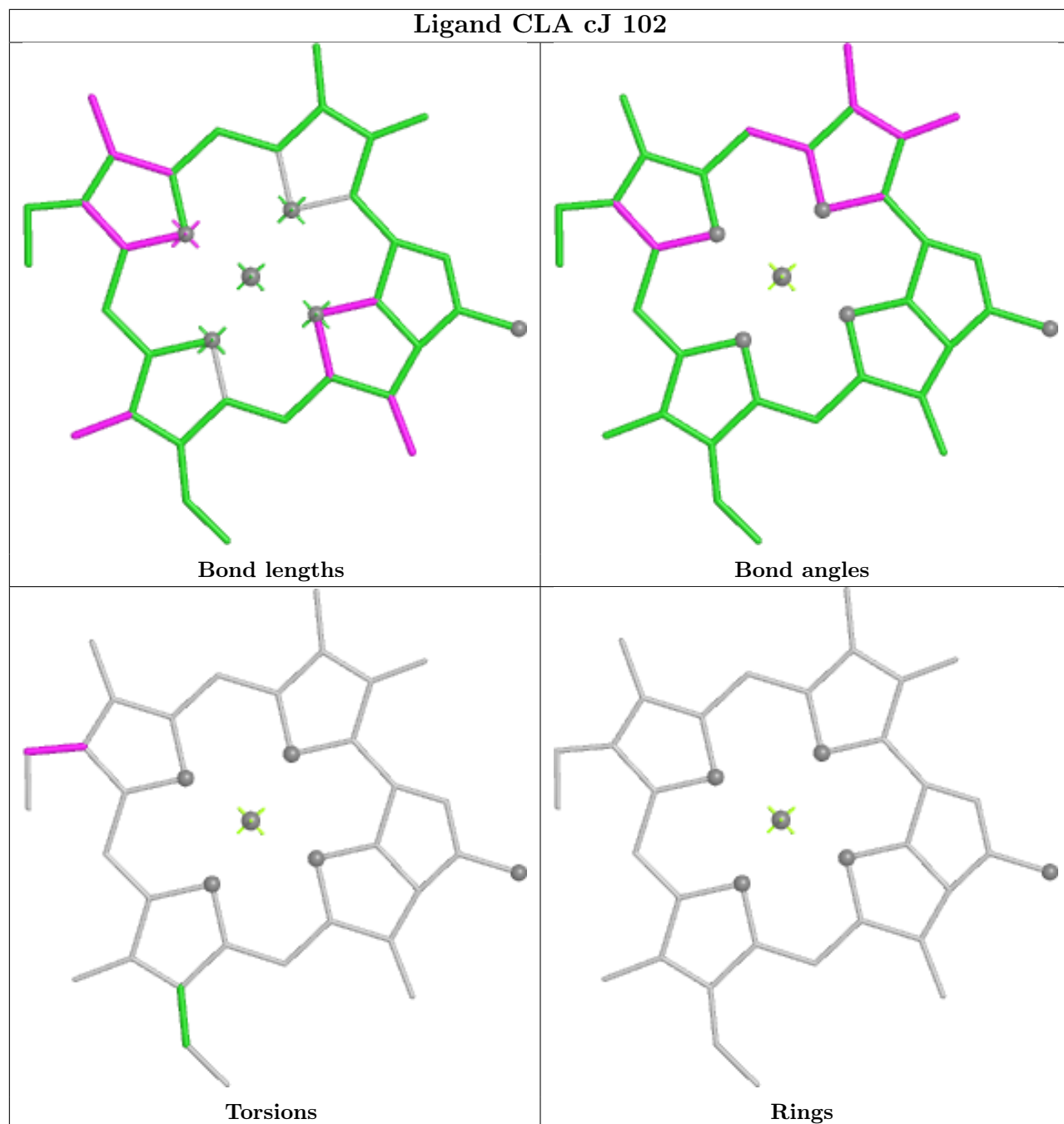


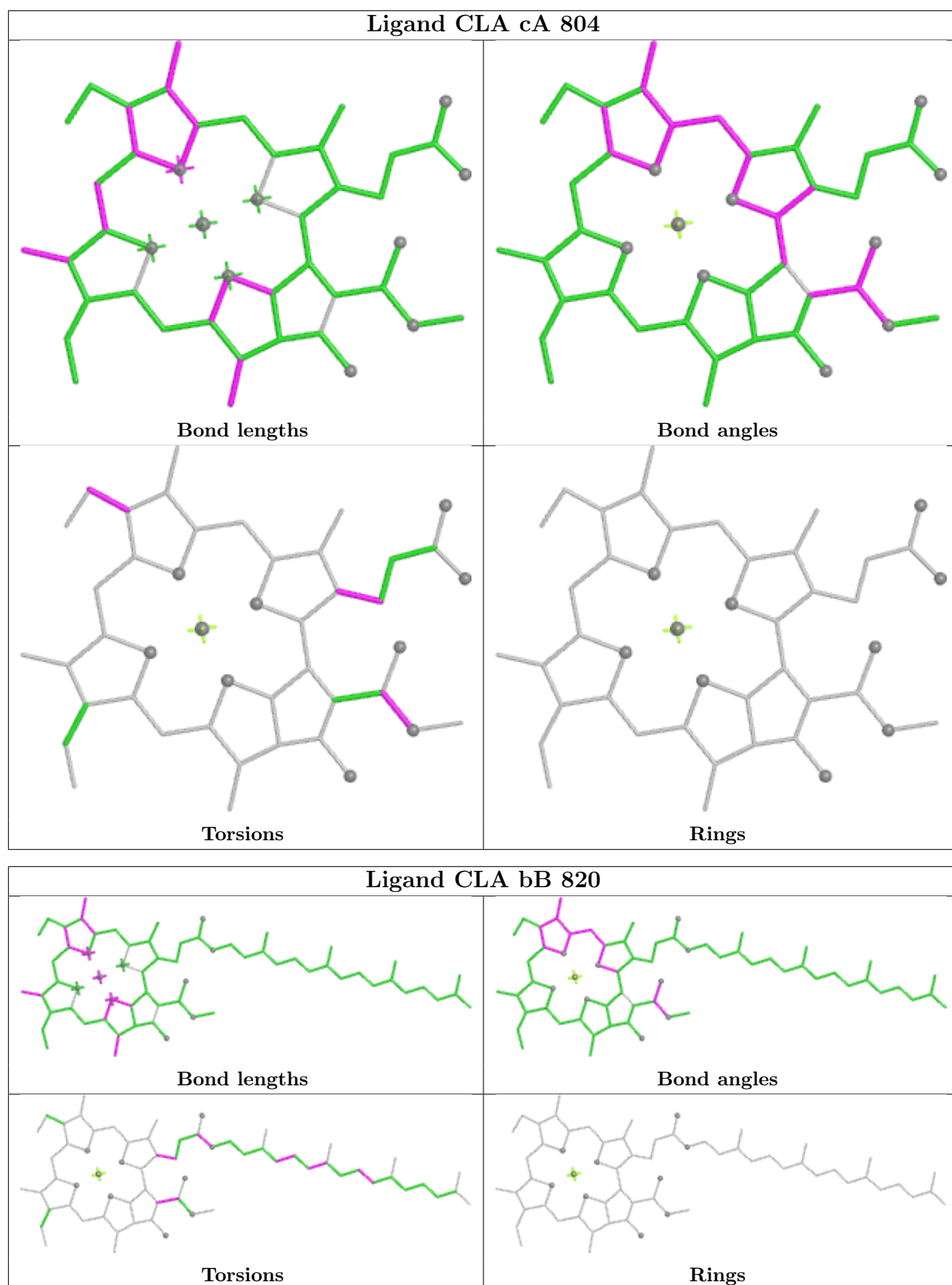
Ligand BCR bJ 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

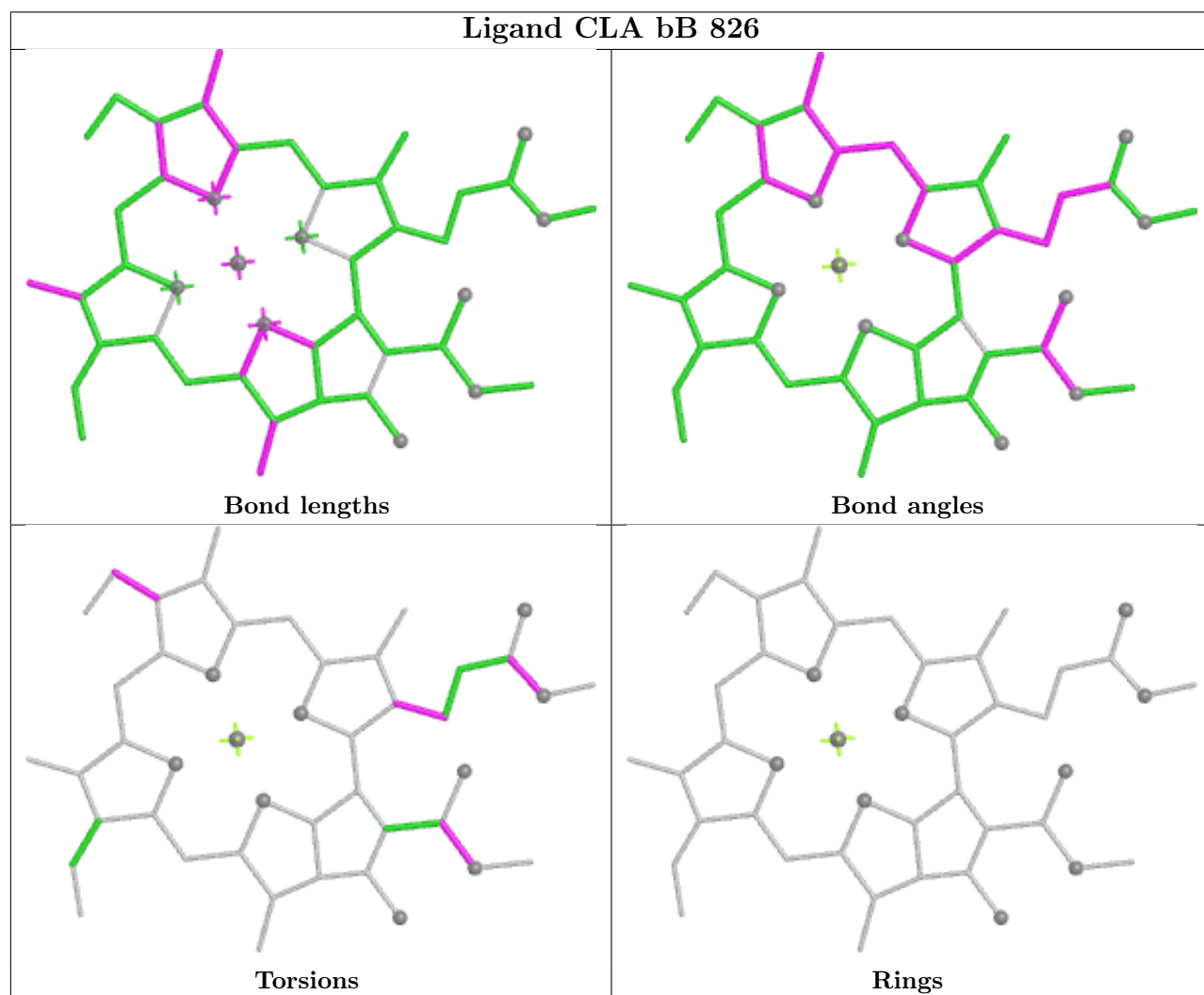
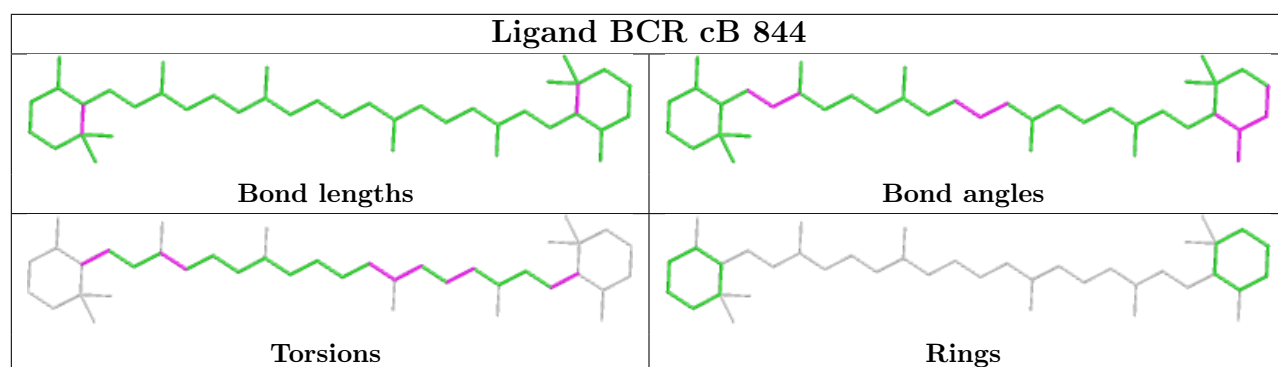
Ligand CLA cB 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

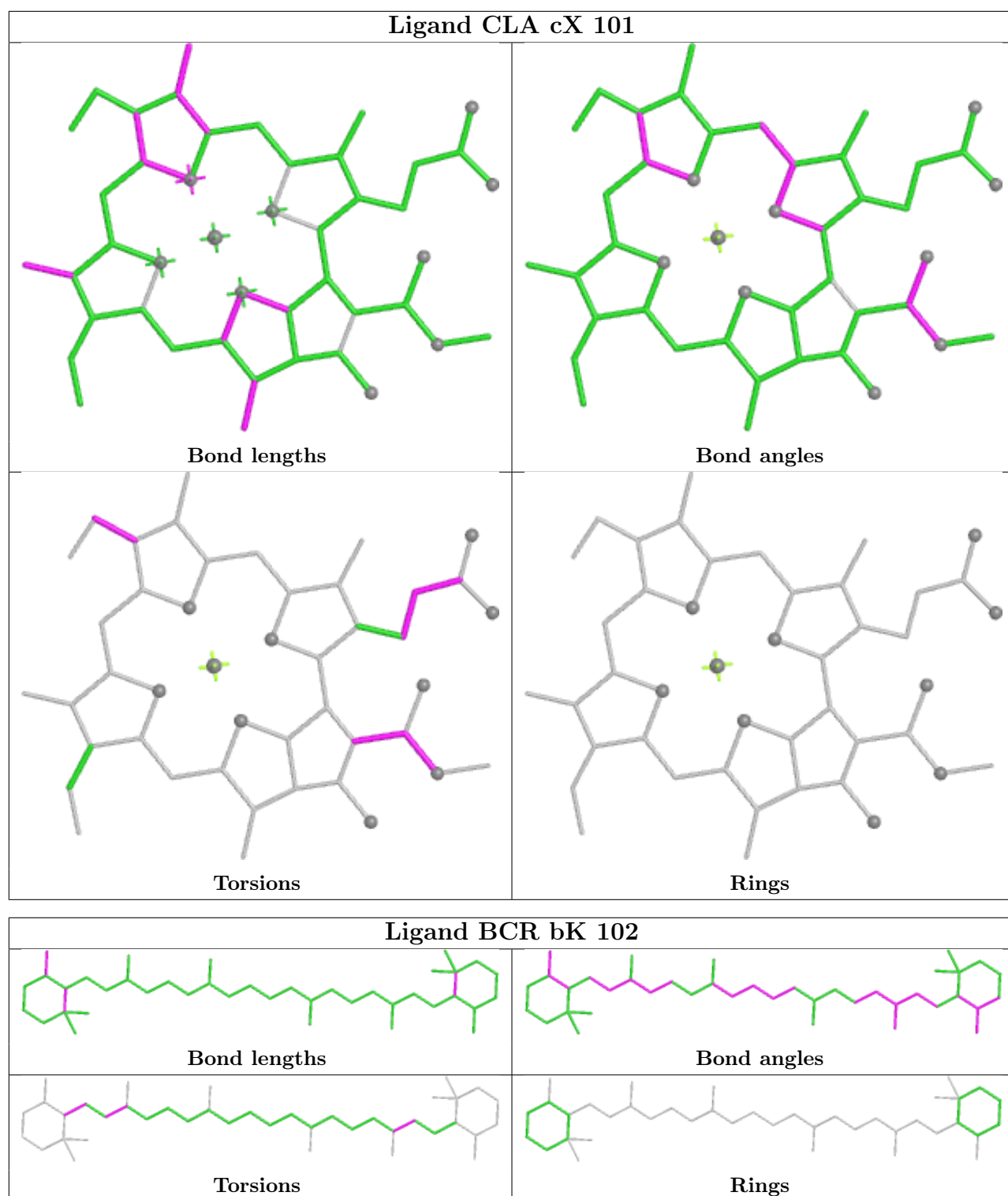
Ligand BCR dL 207	
	
Bond lengths	Bond angles
	
Torsions	Rings

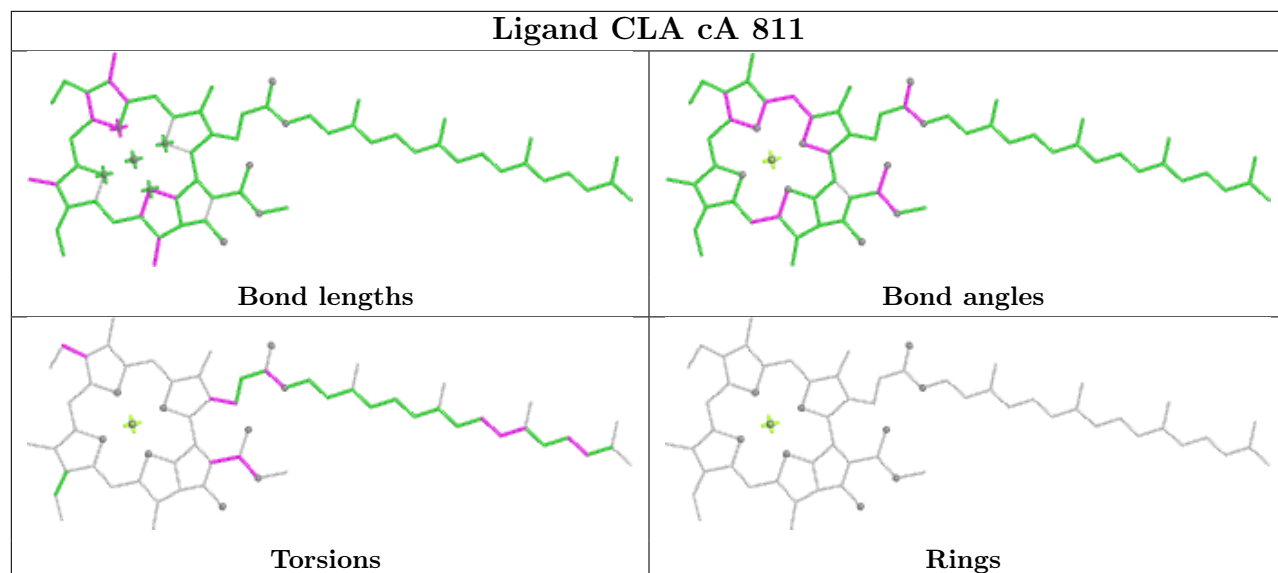
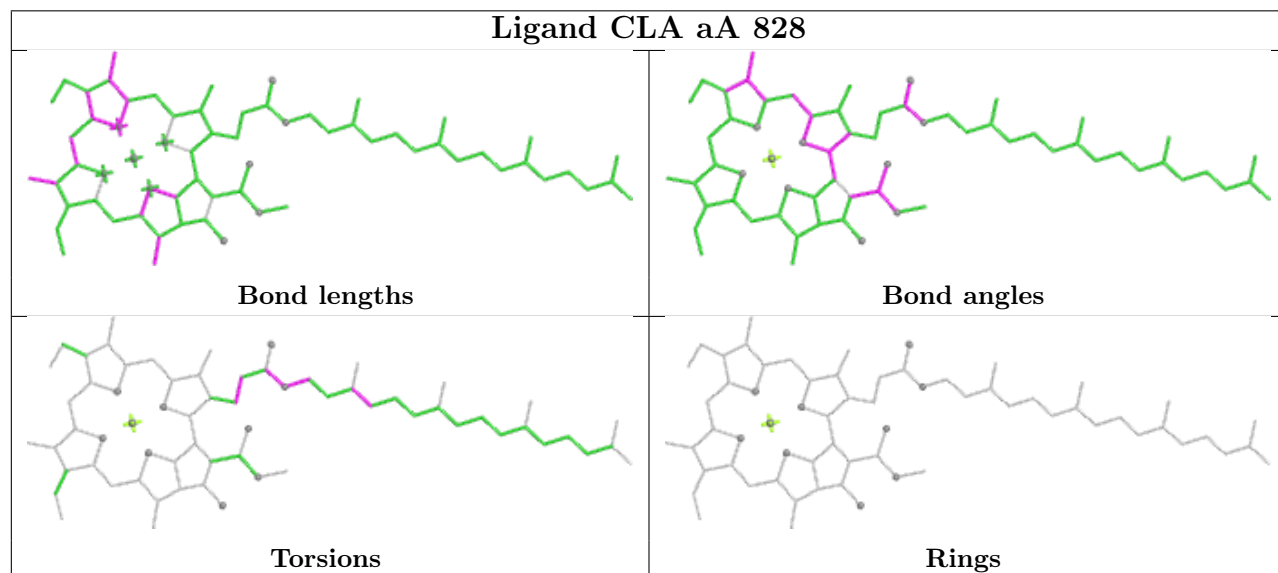
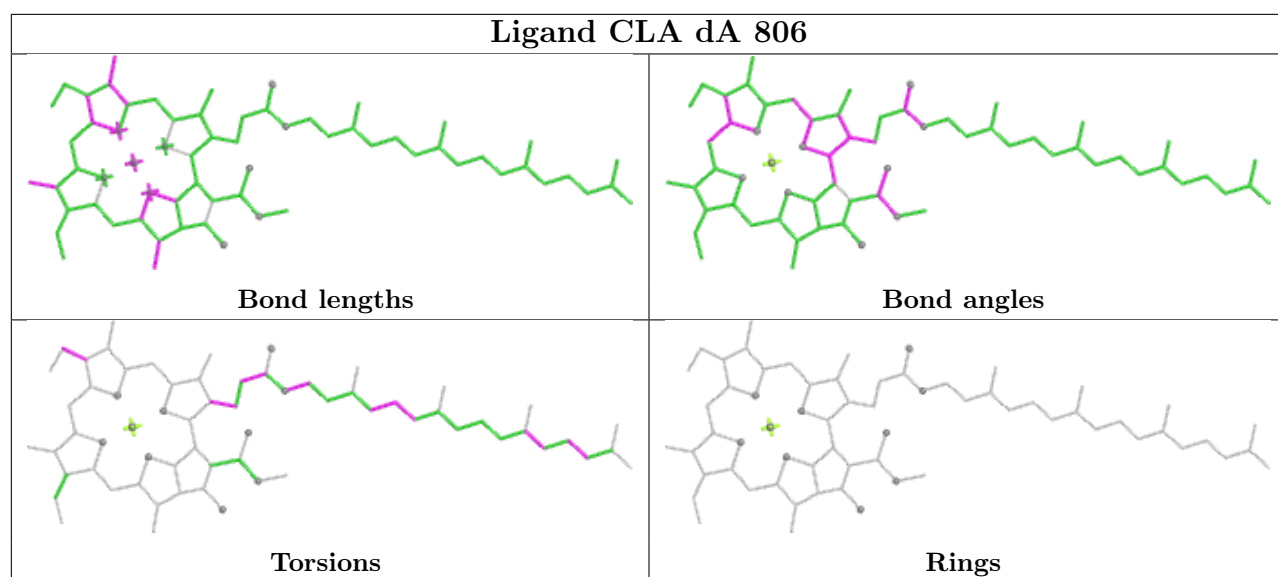


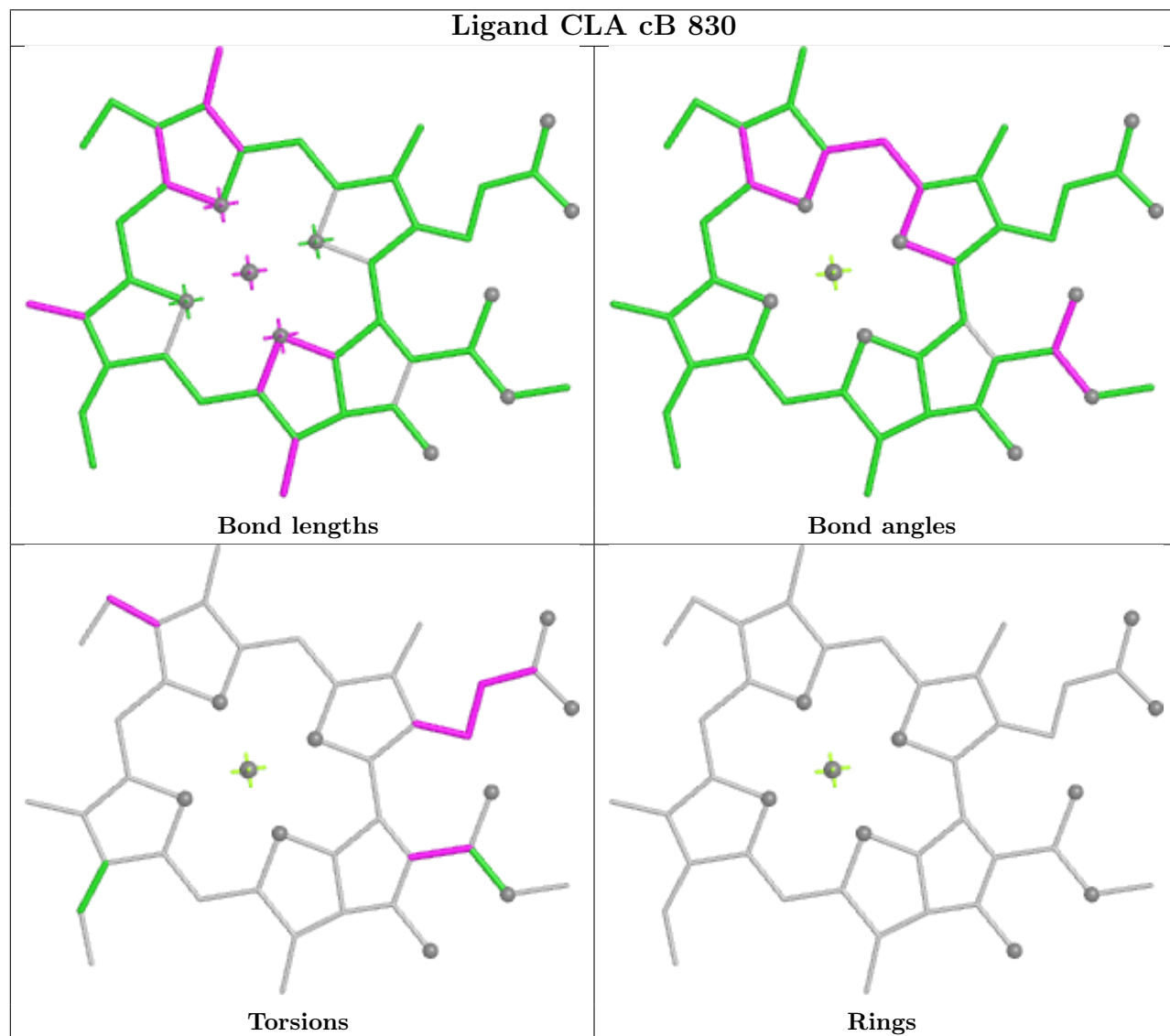
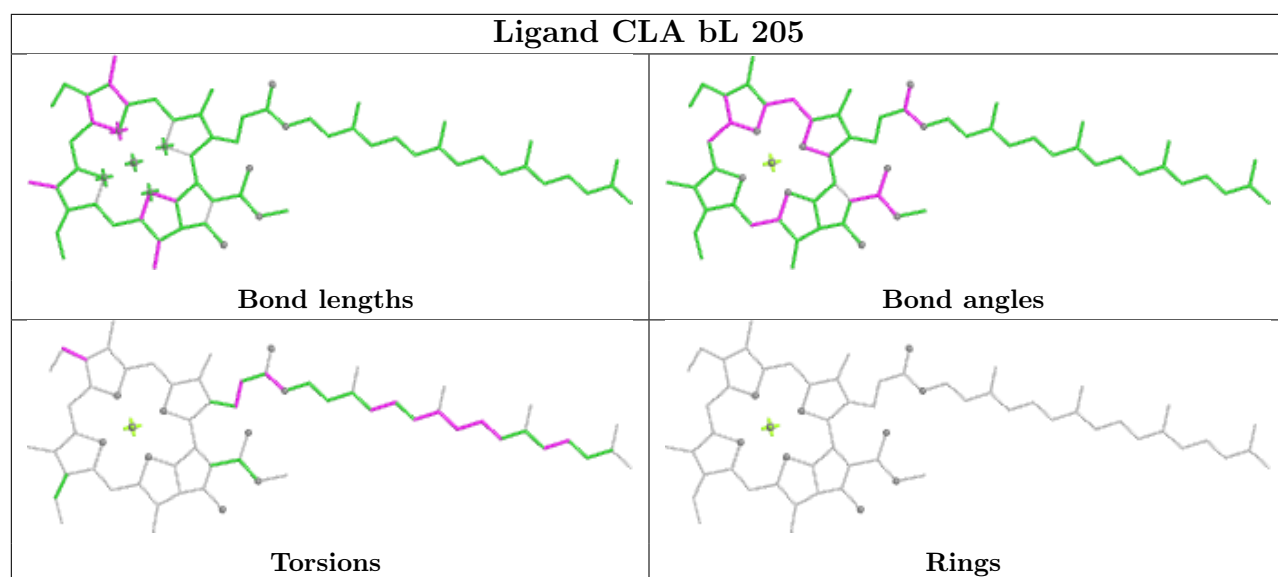


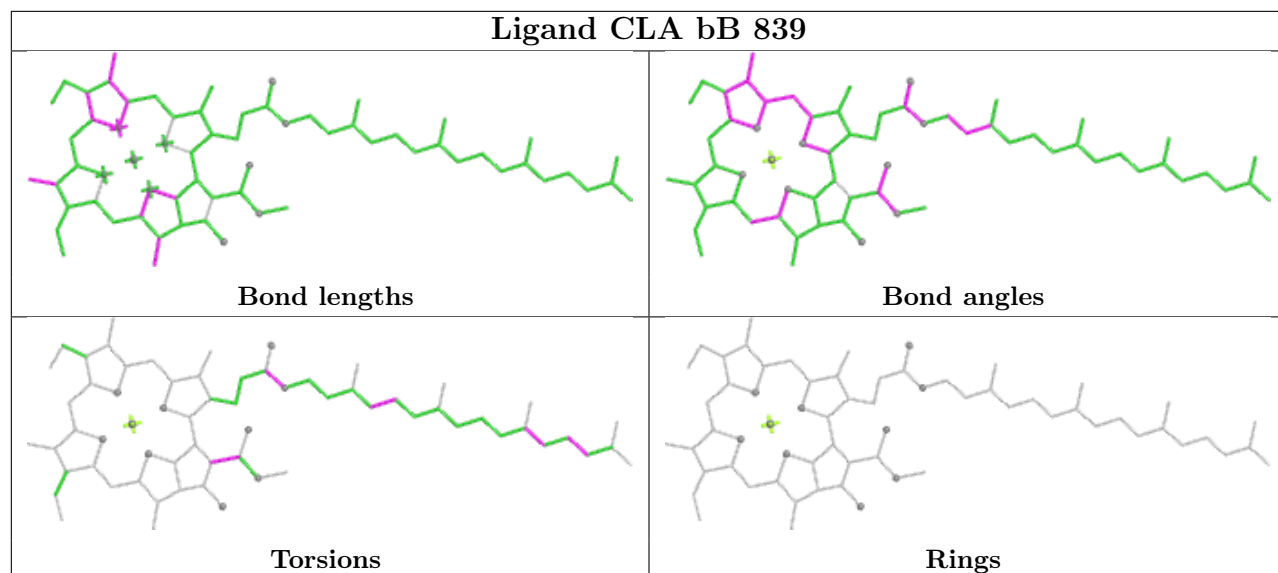
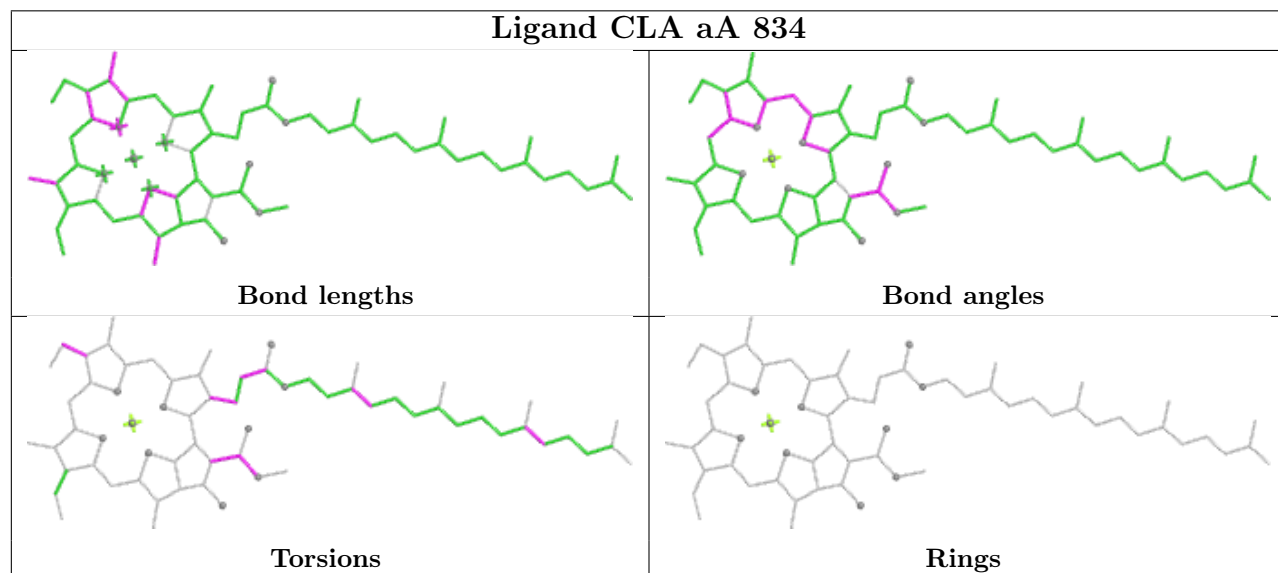
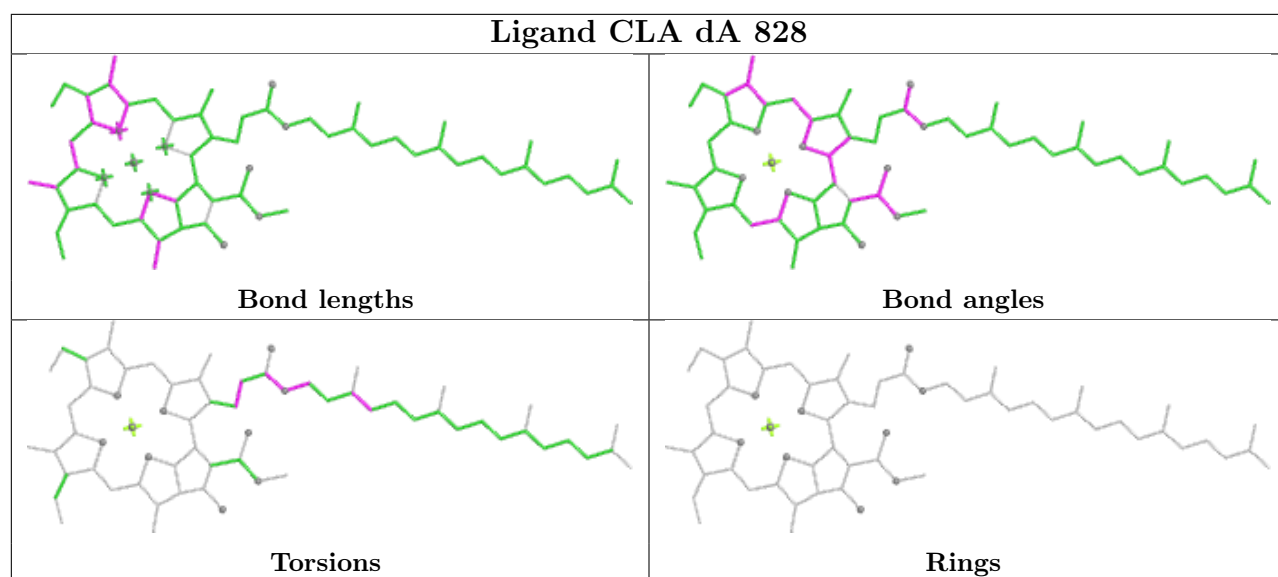


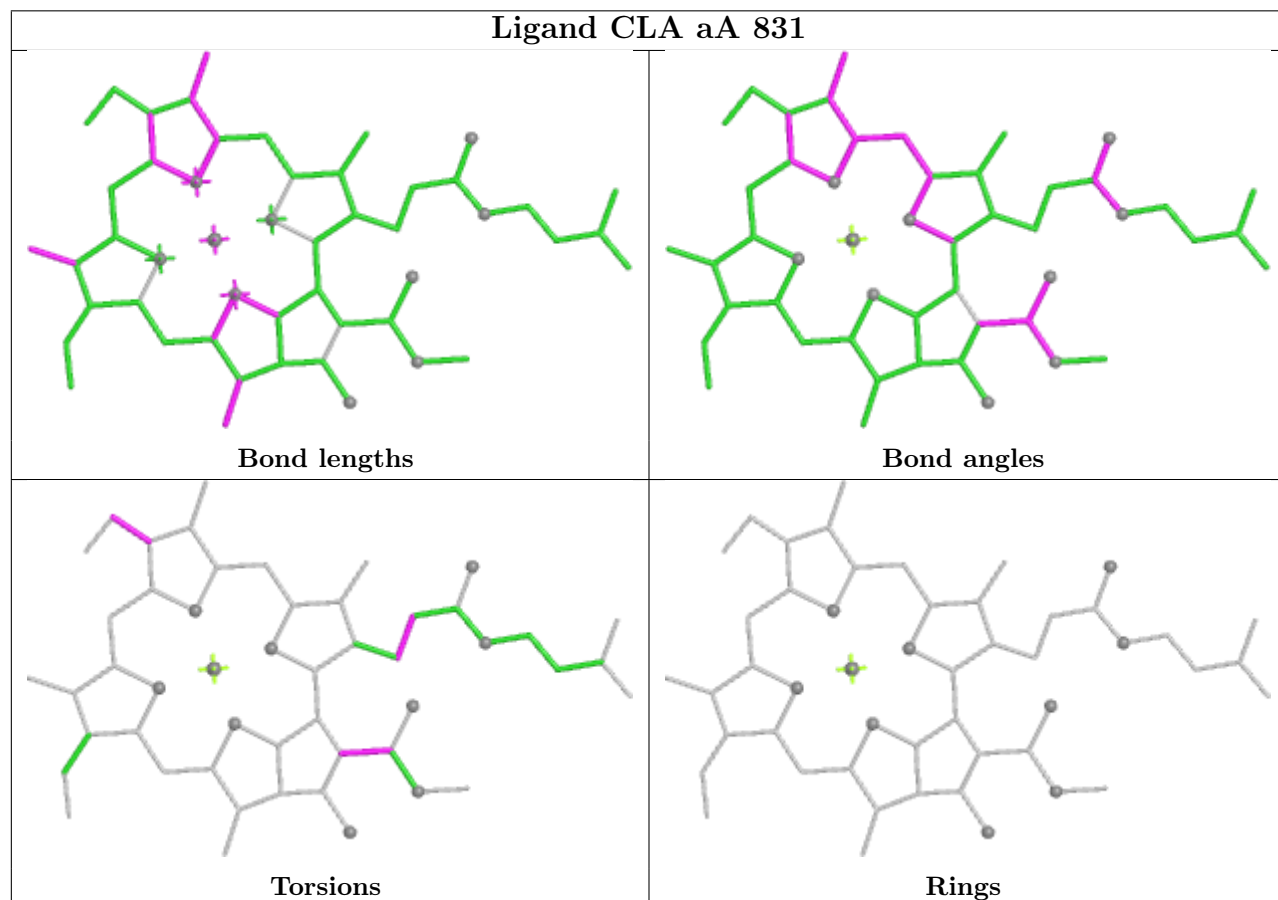
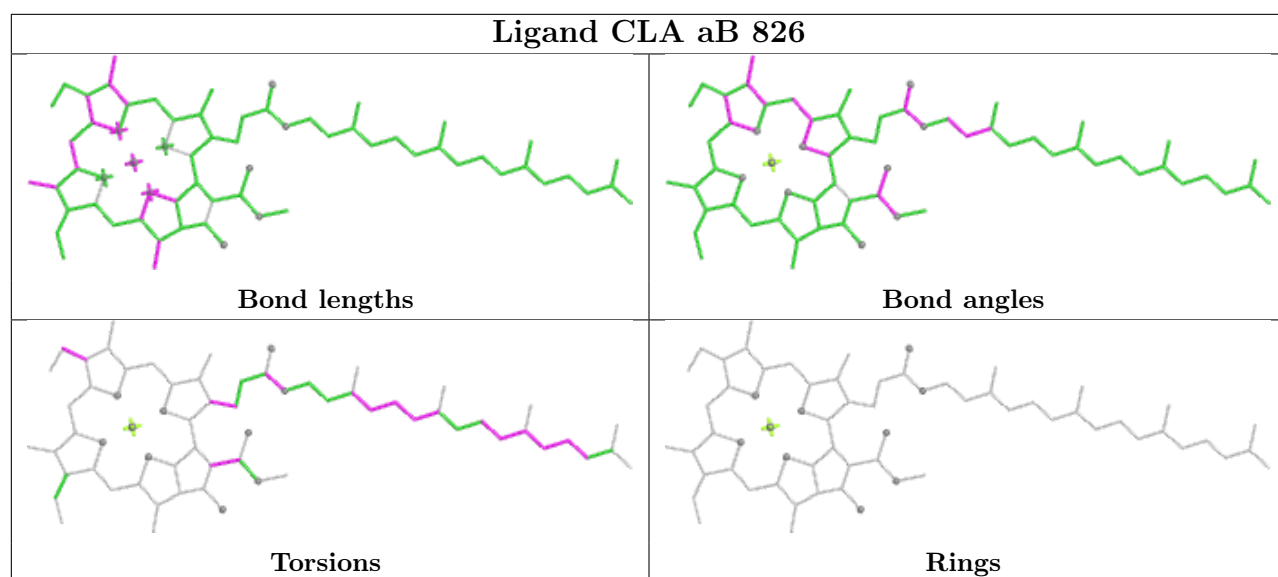


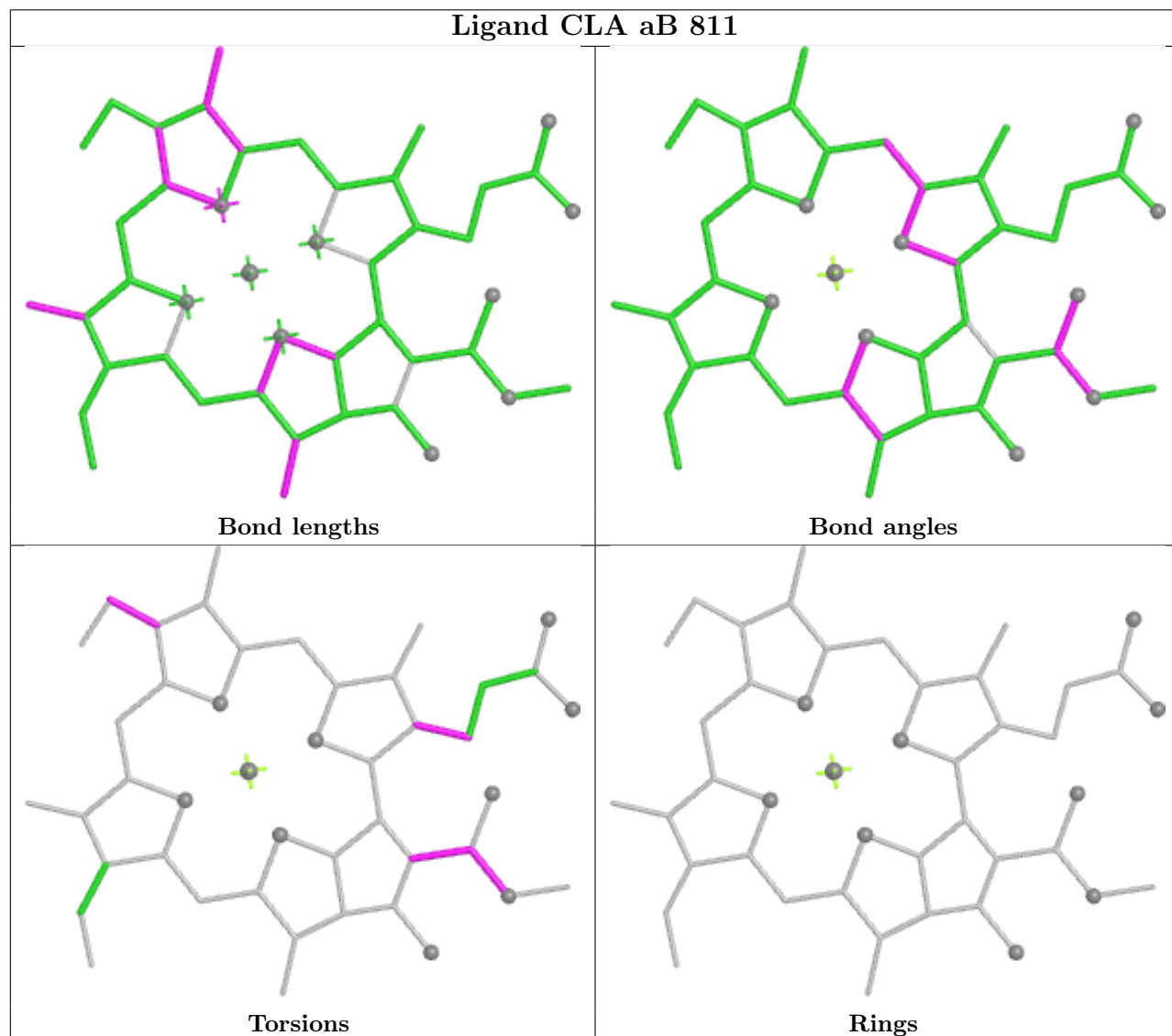
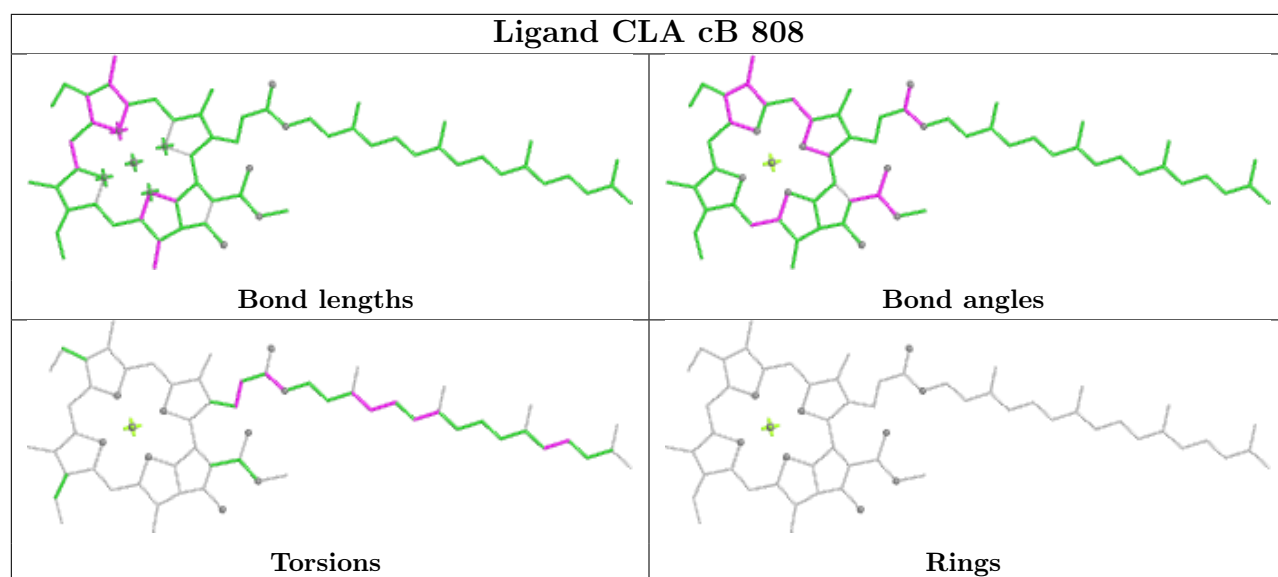


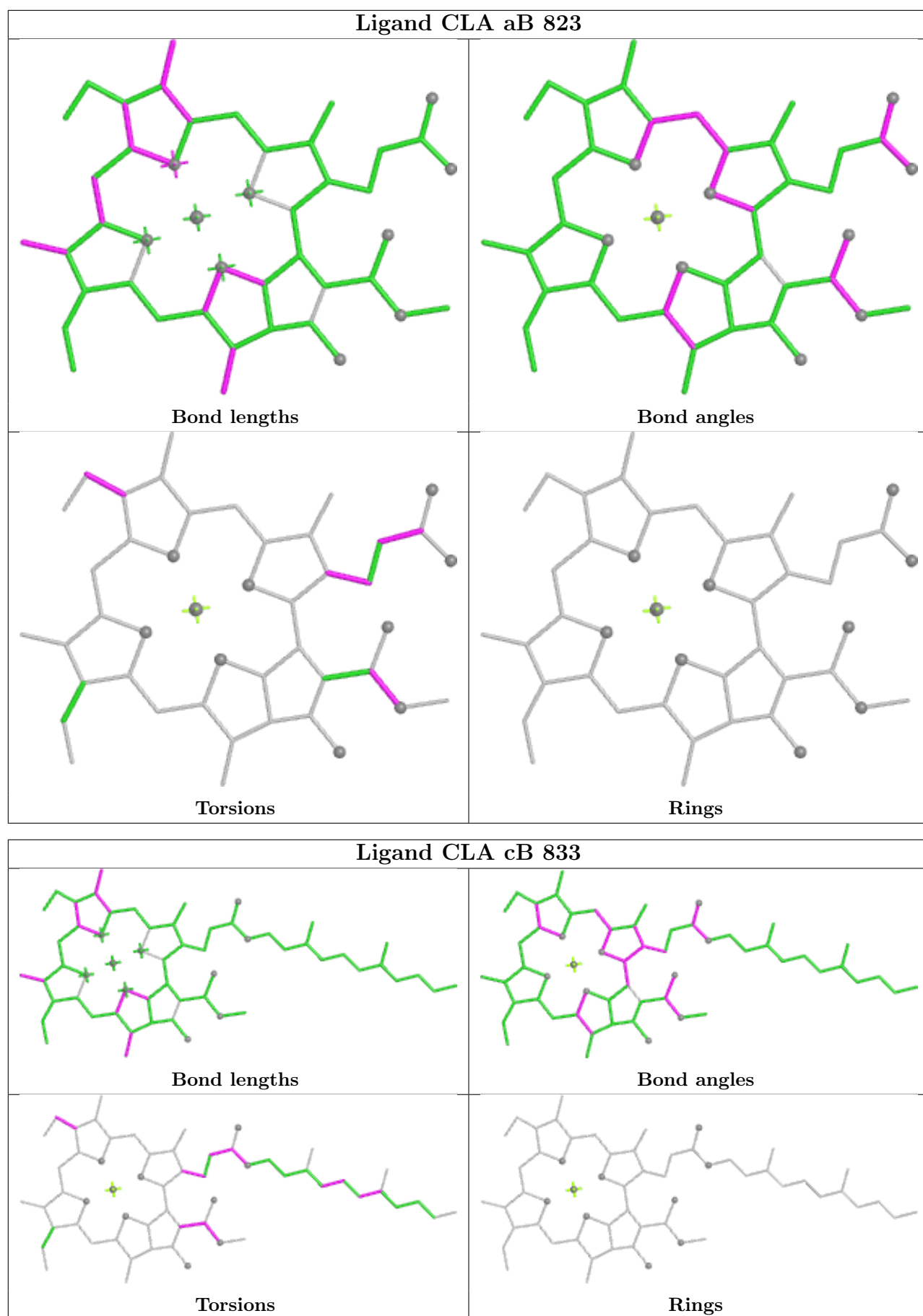




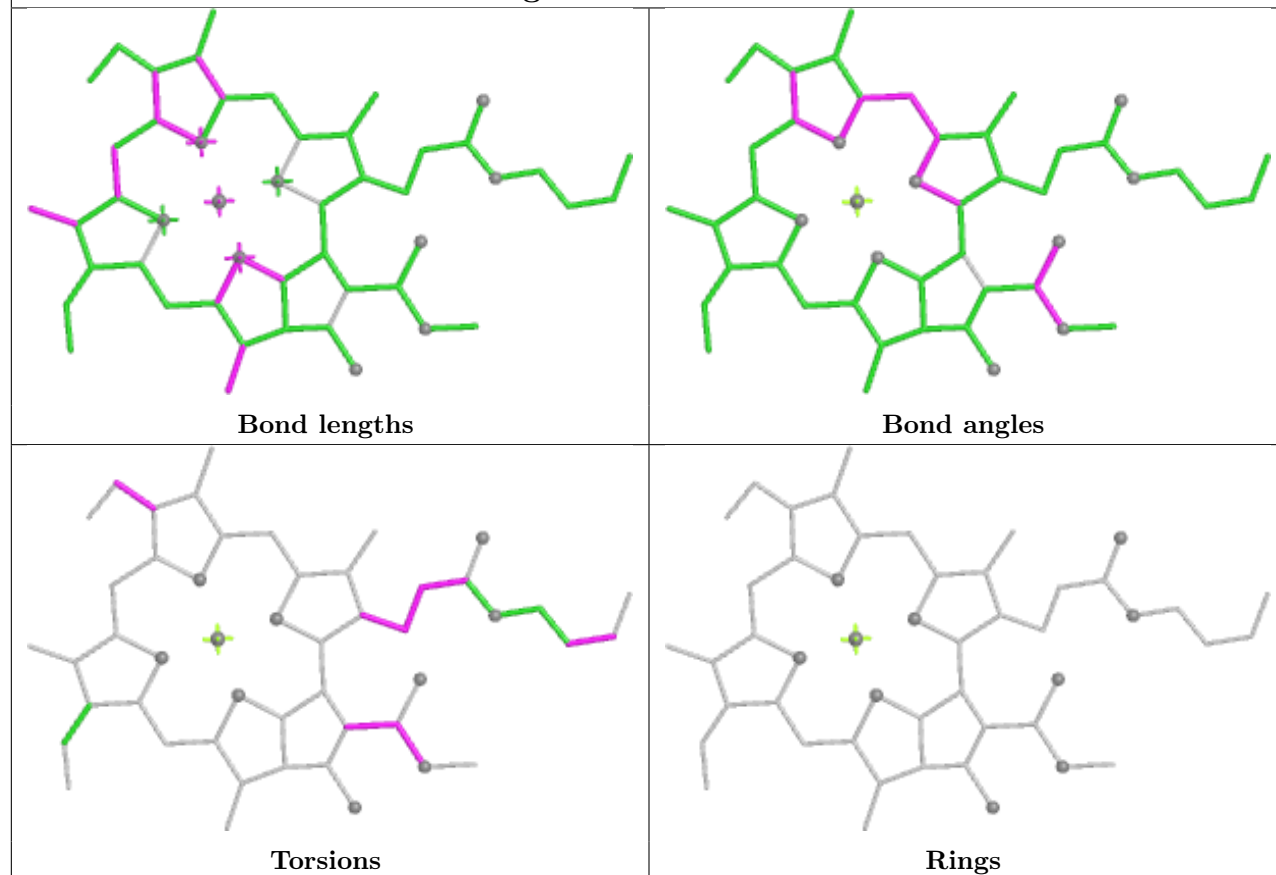




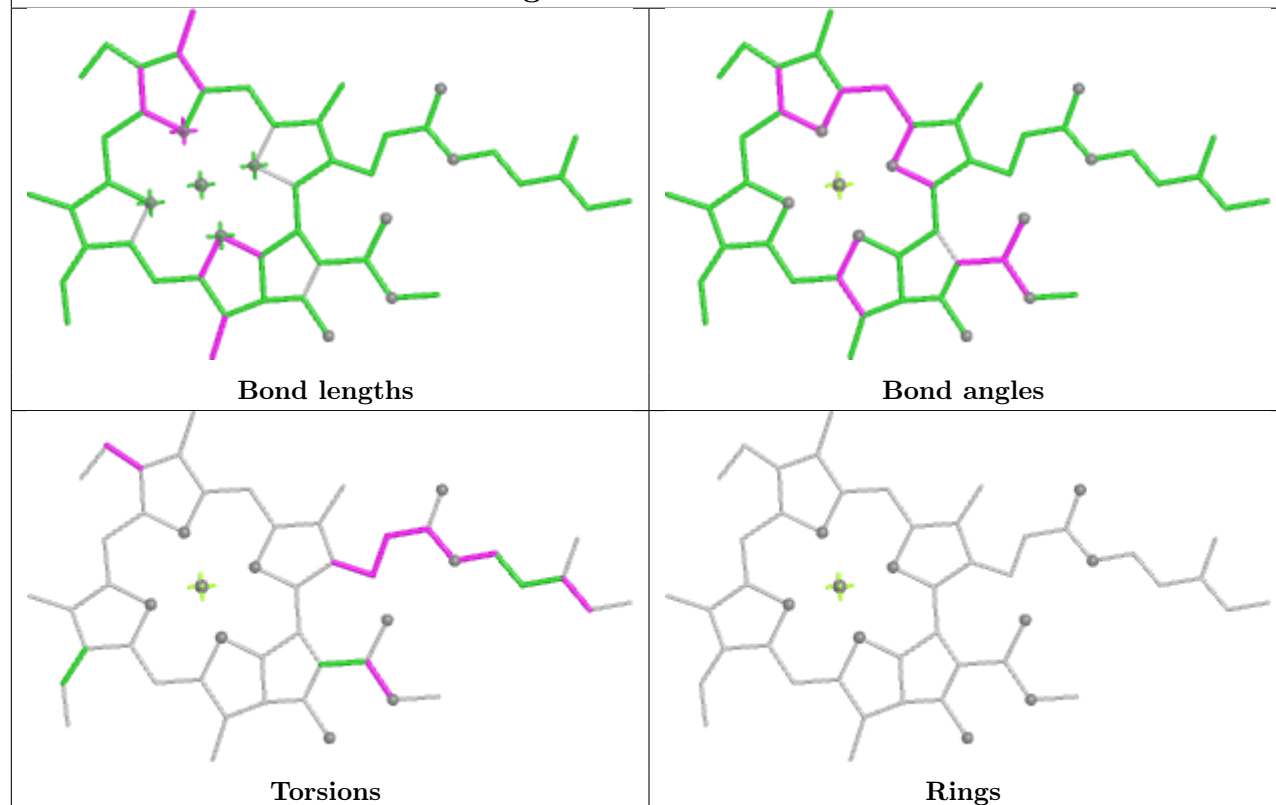




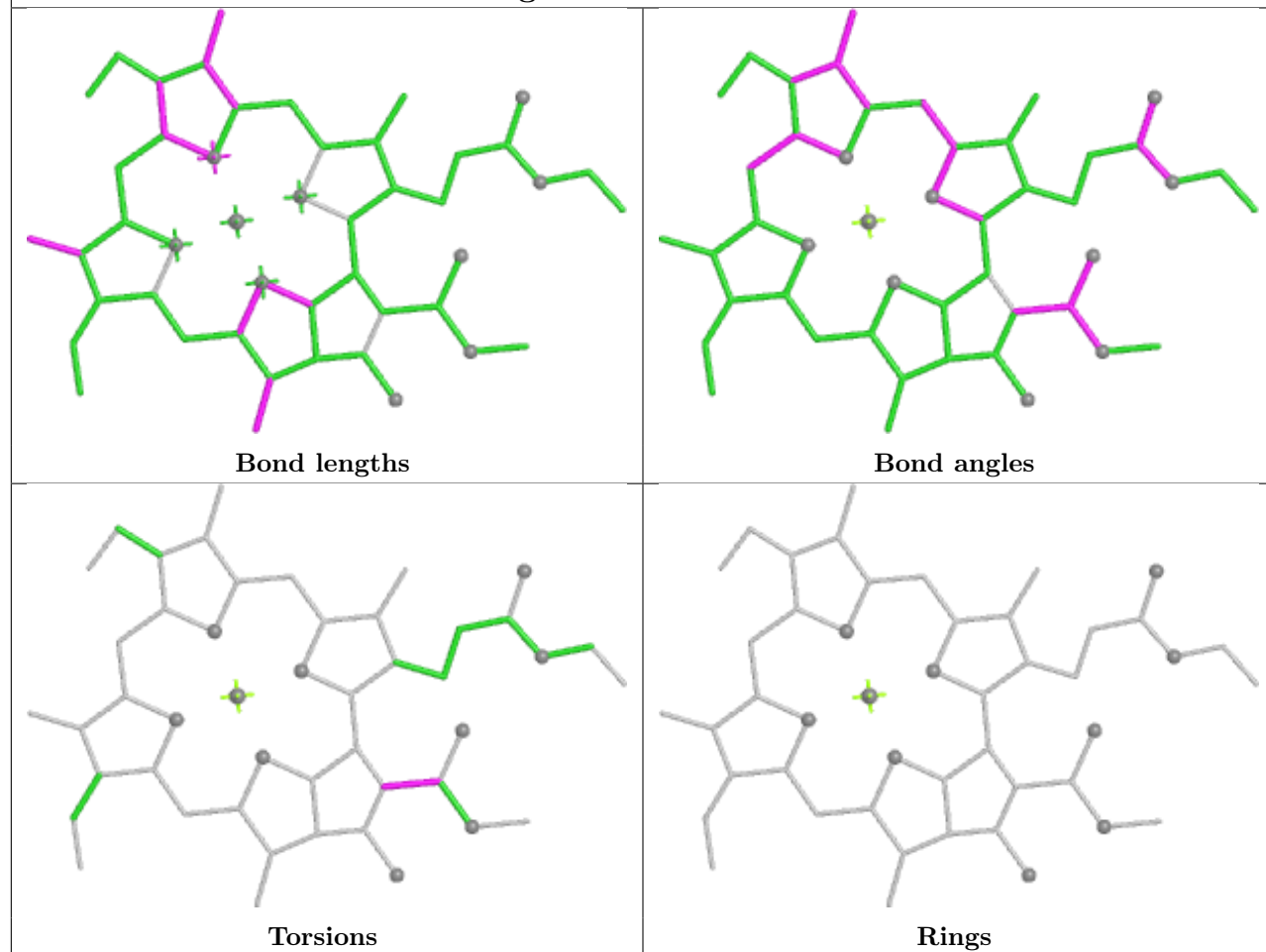
Ligand CLA aA 822



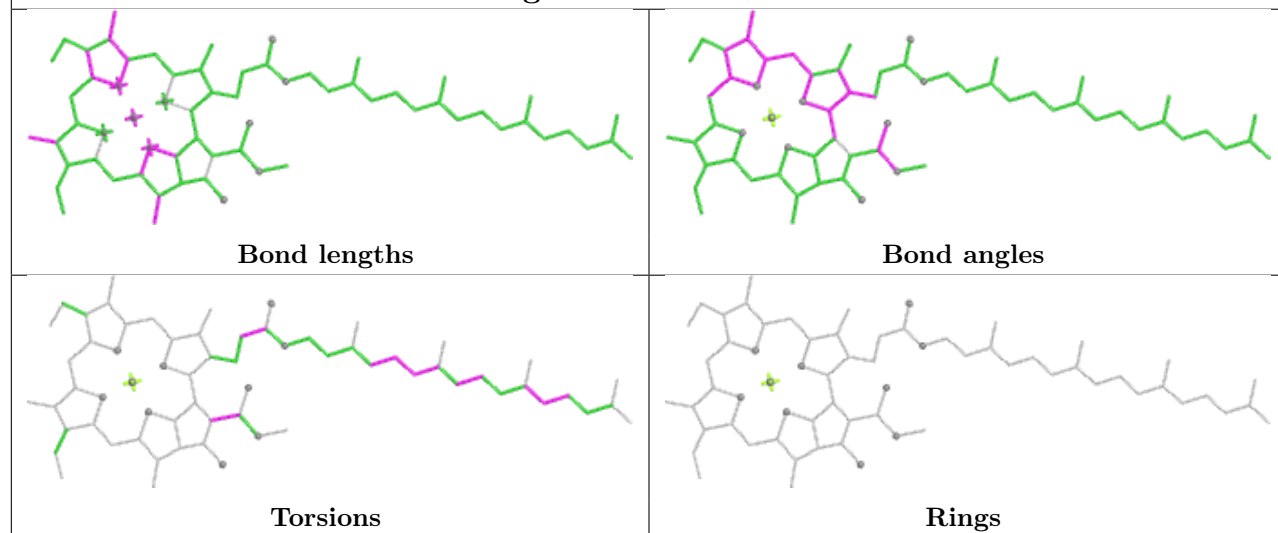
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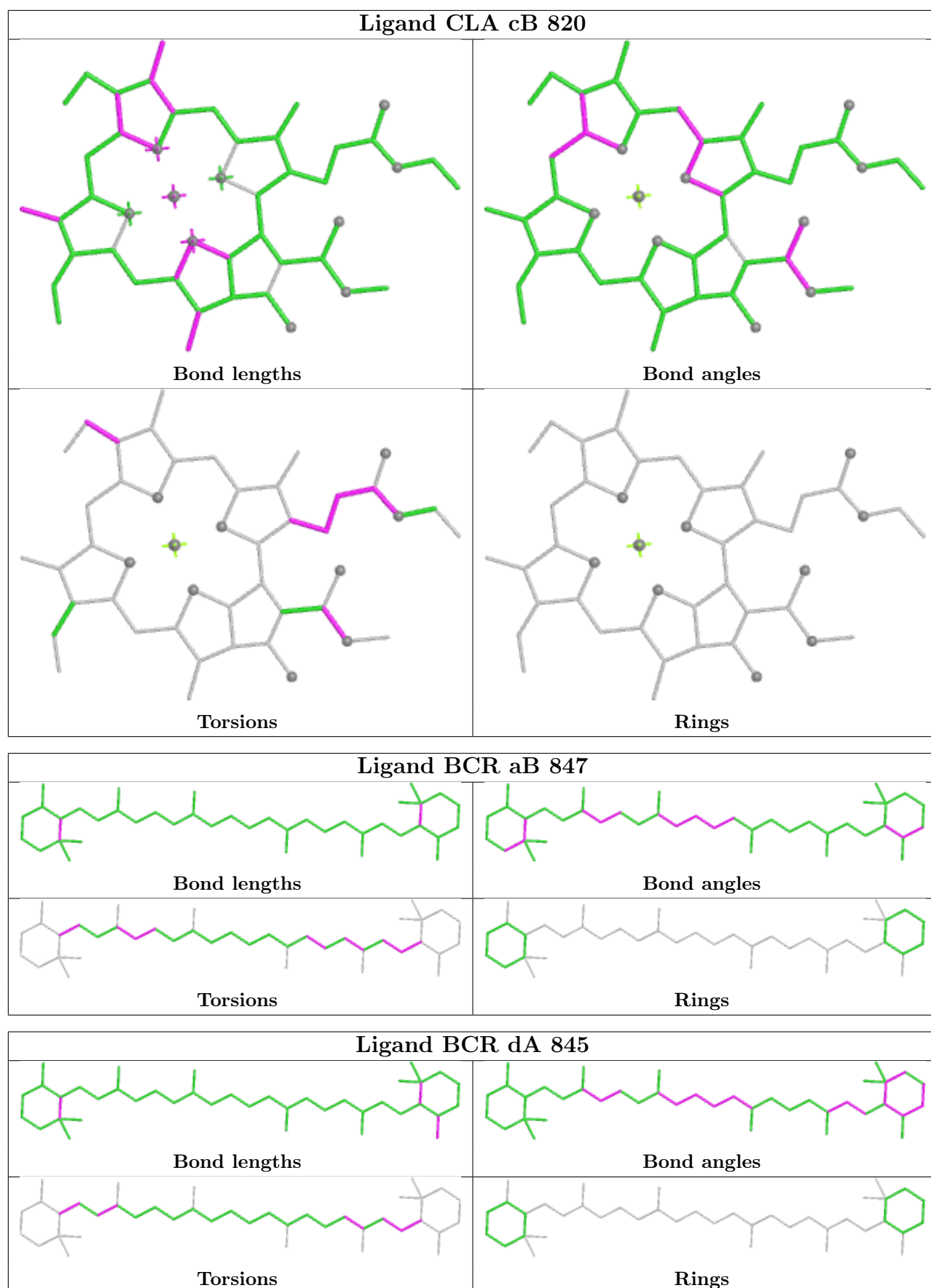


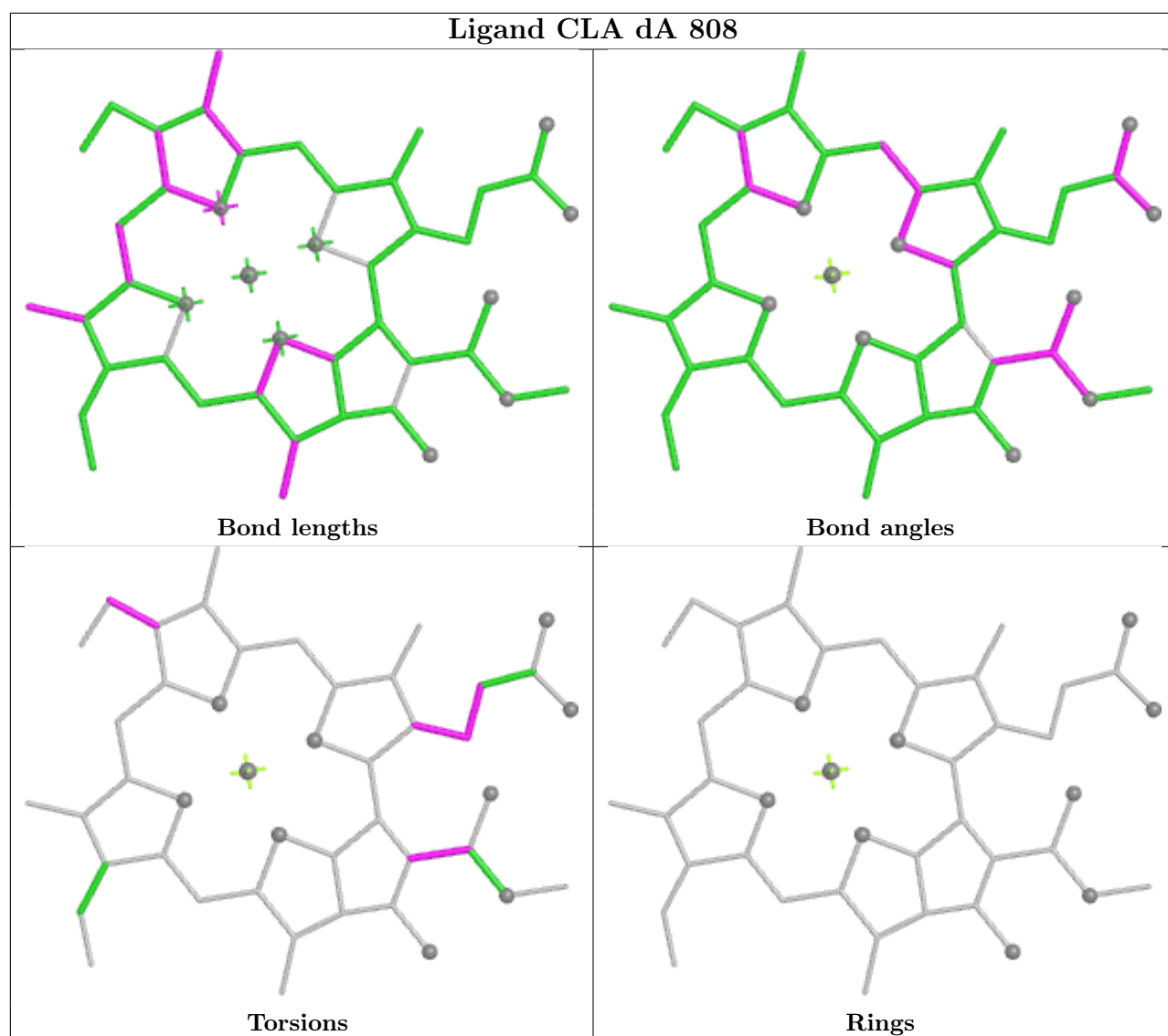
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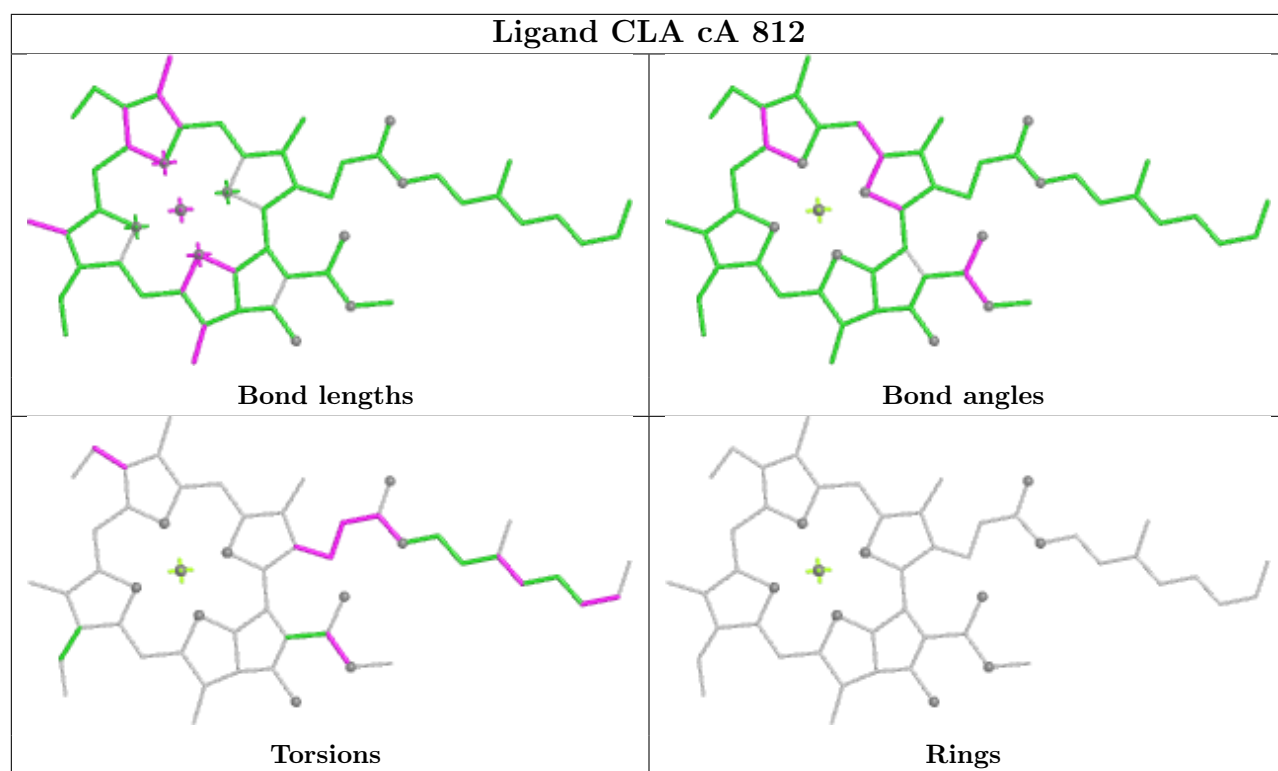


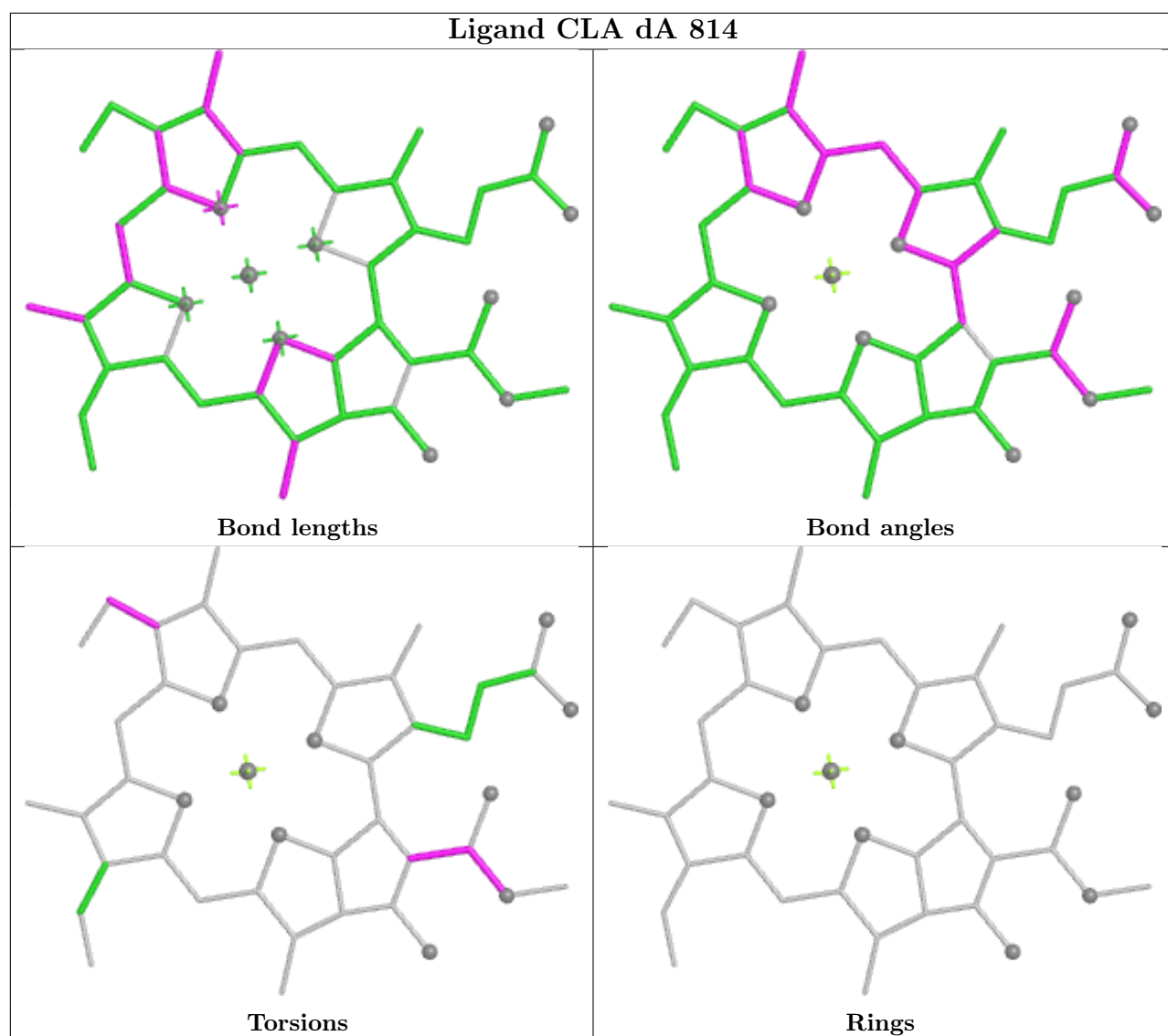
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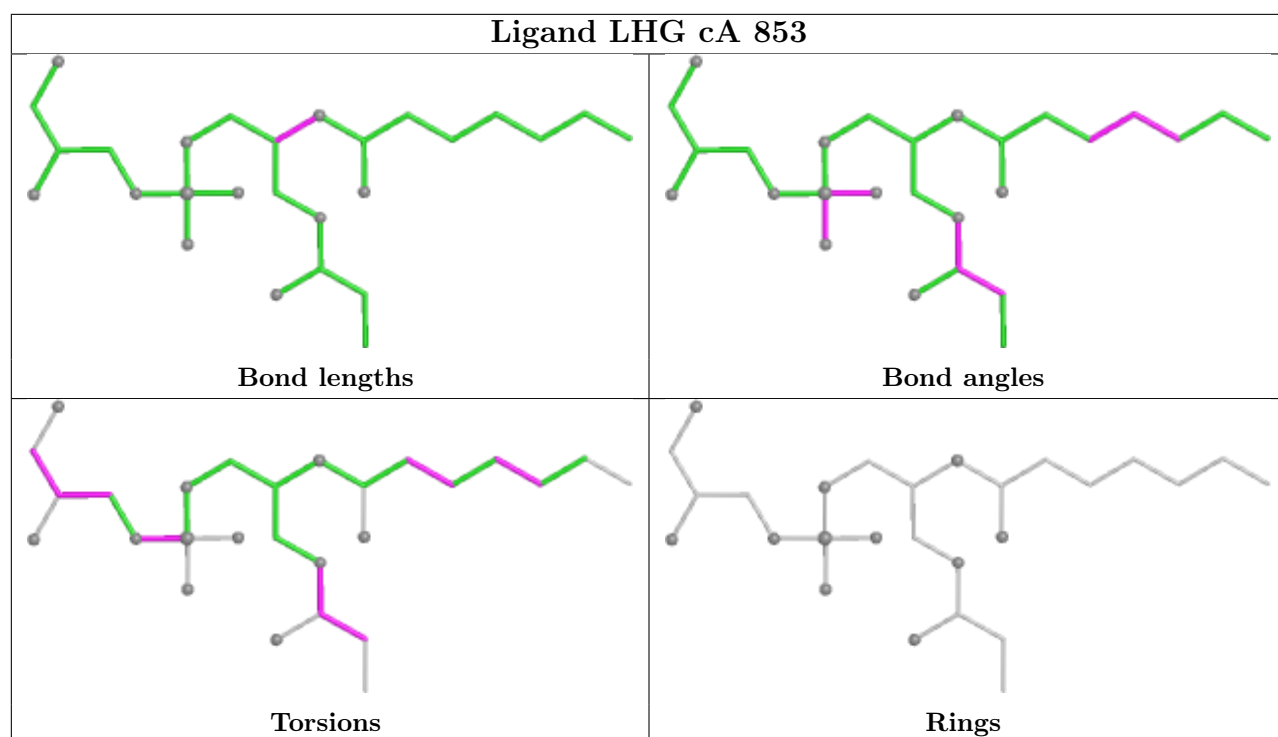




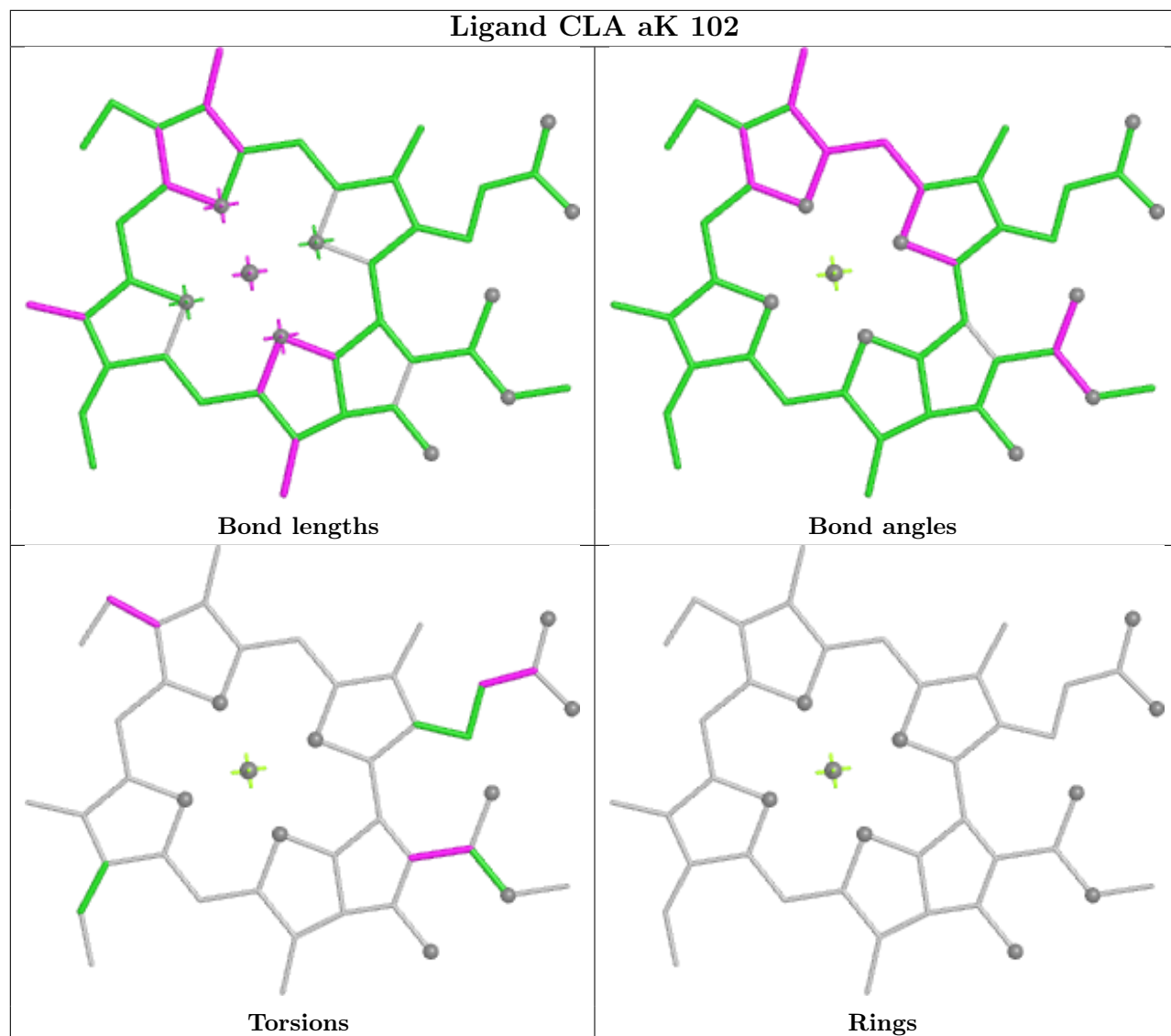




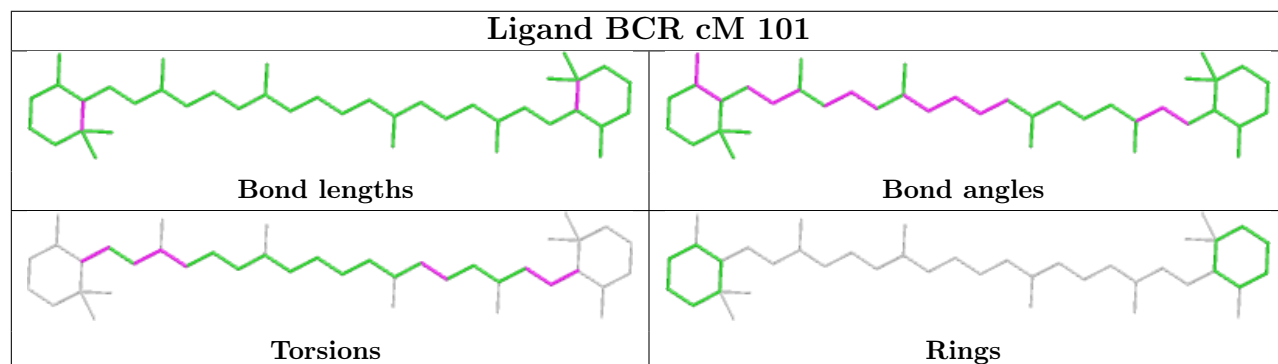


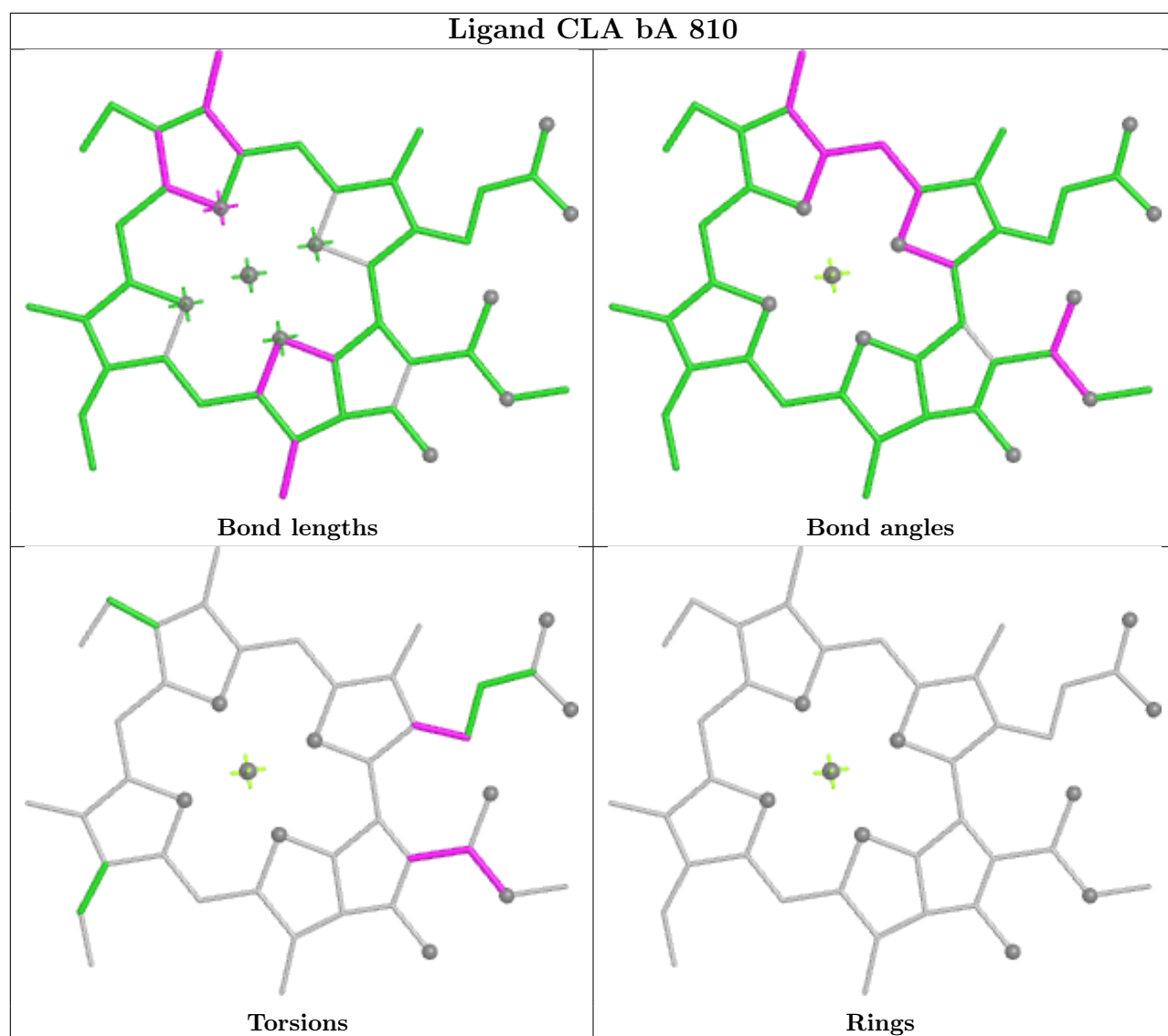


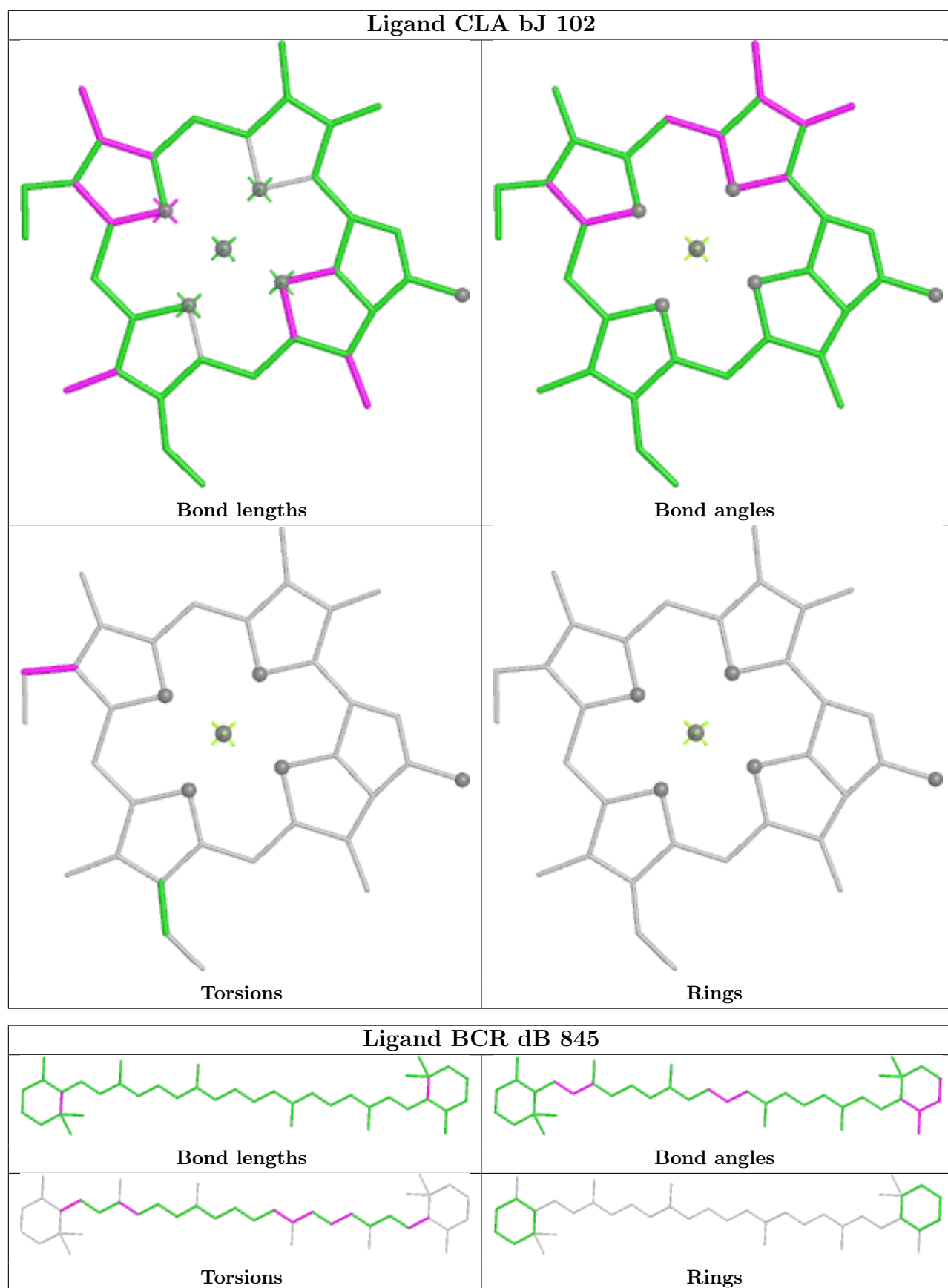
Ligand CLA aK 102

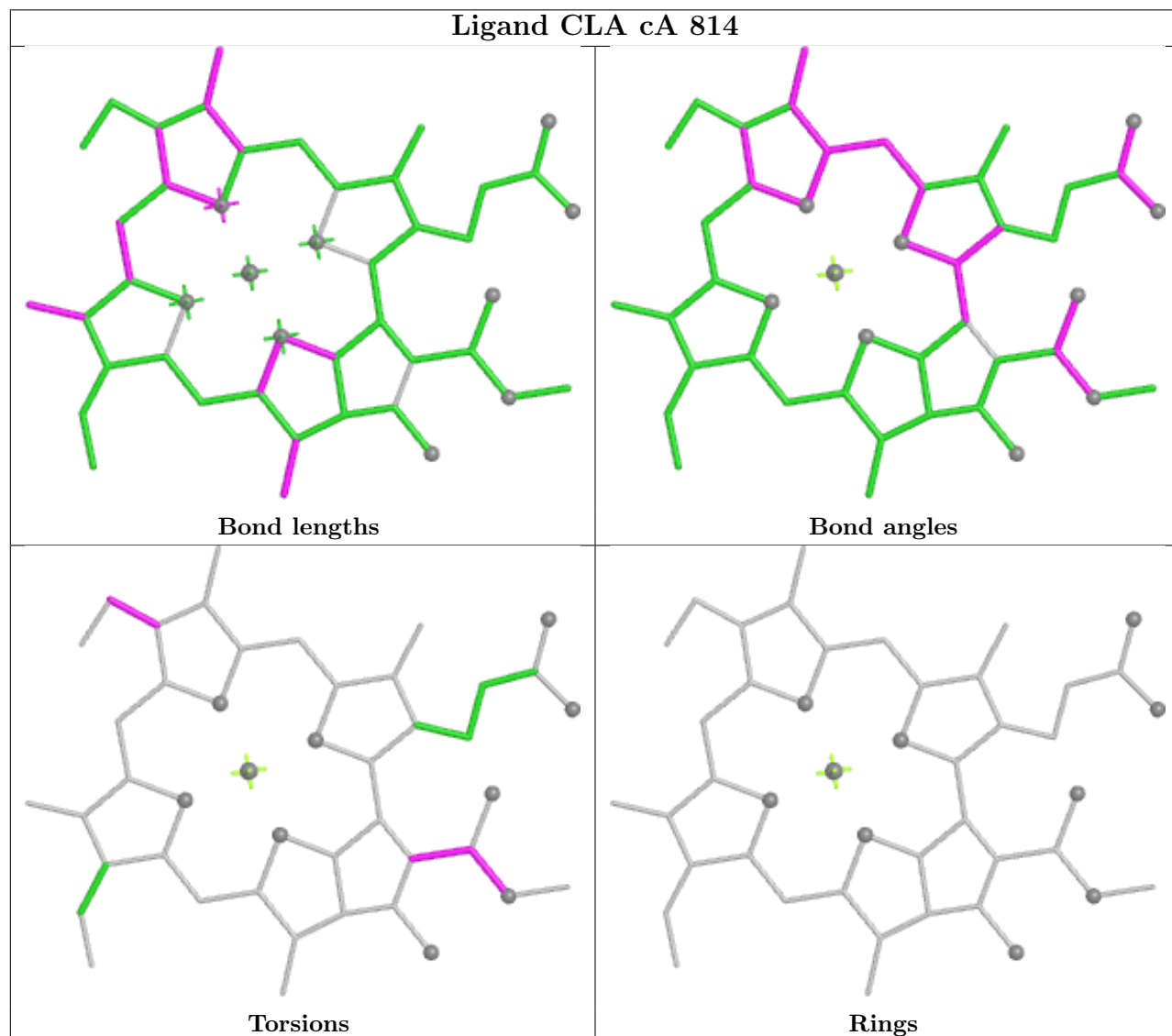
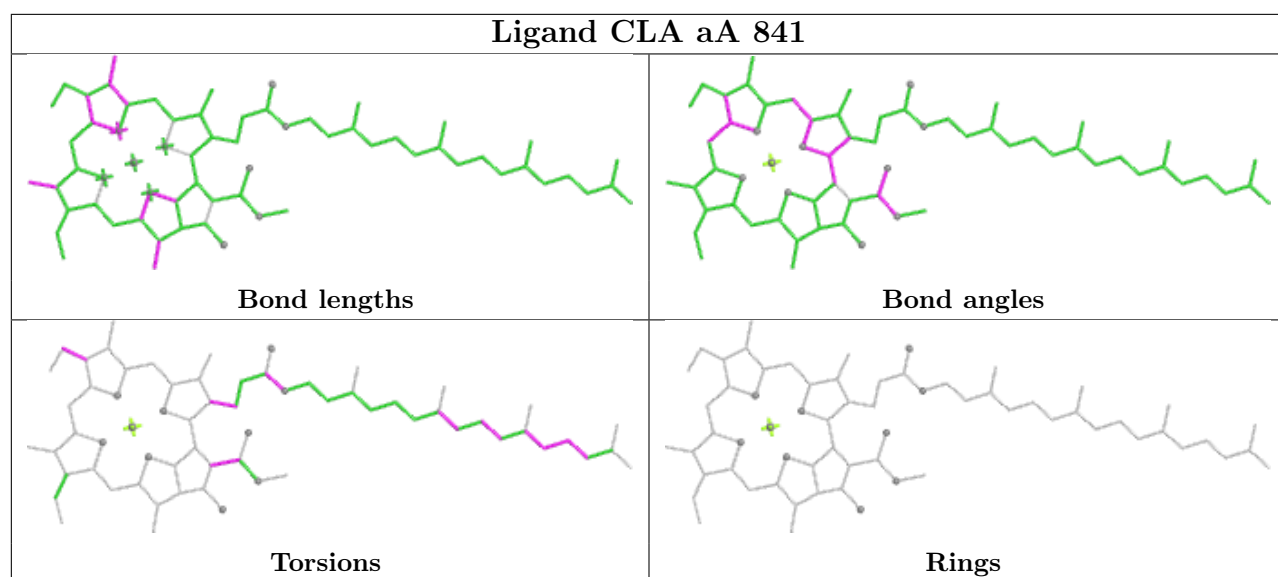


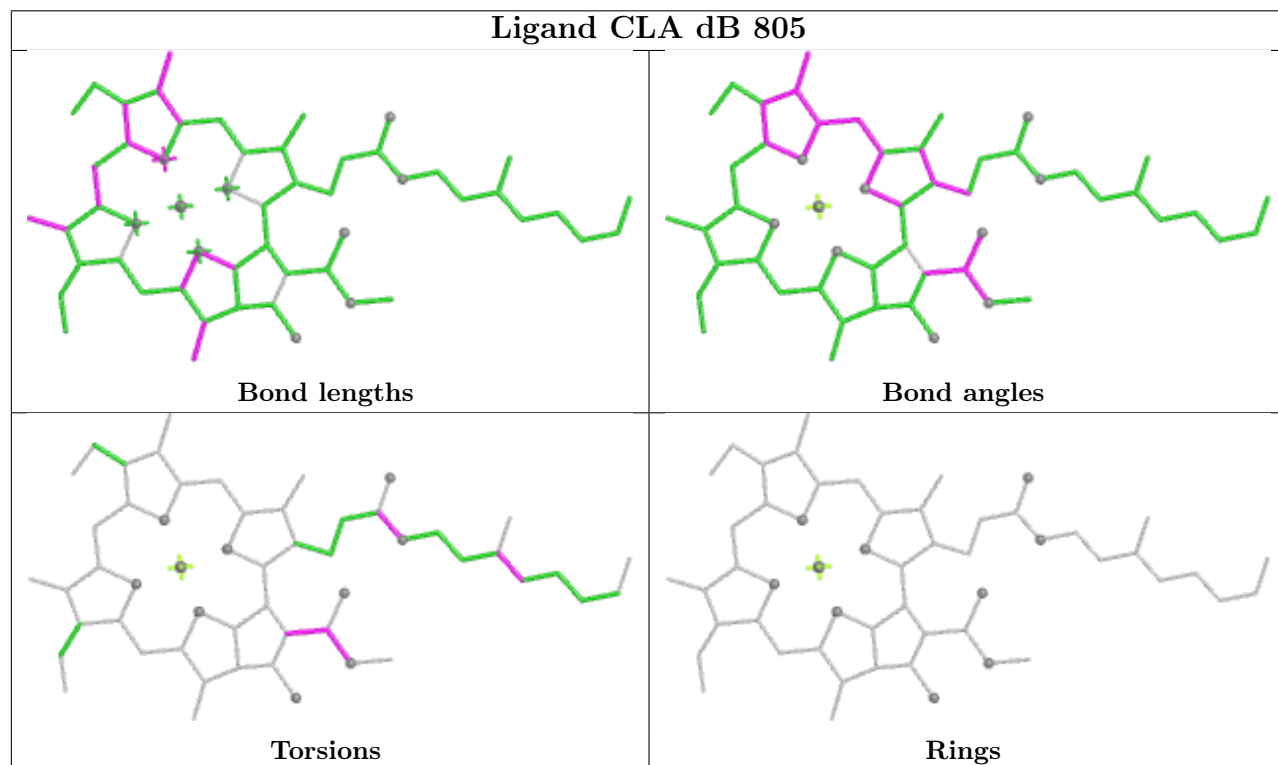
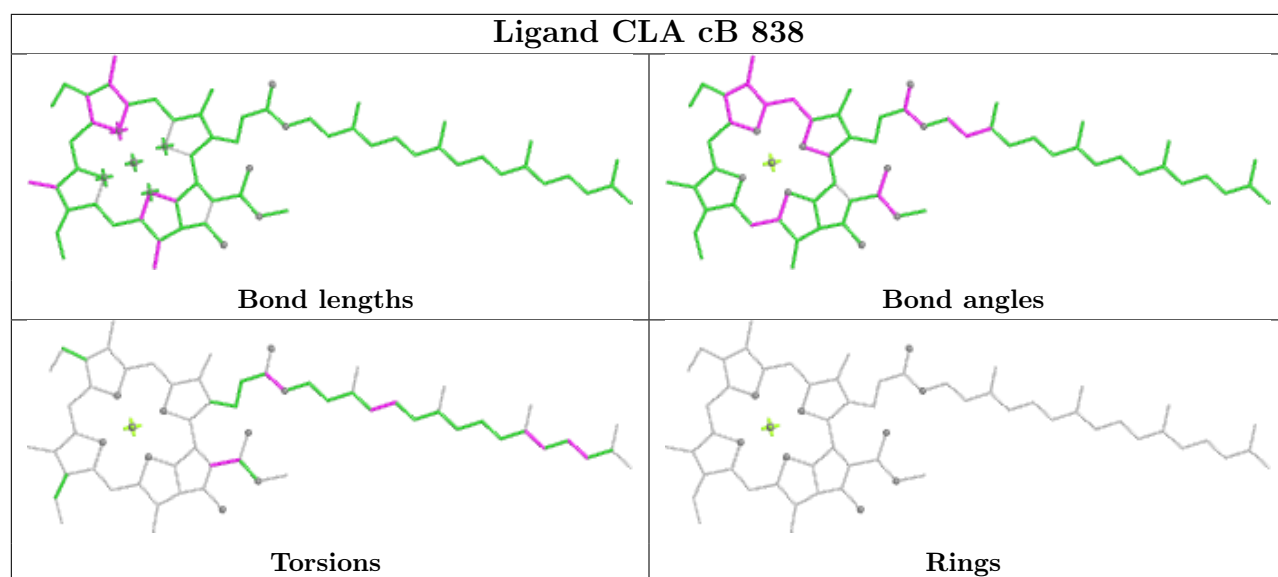
Ligand BCR cM 101



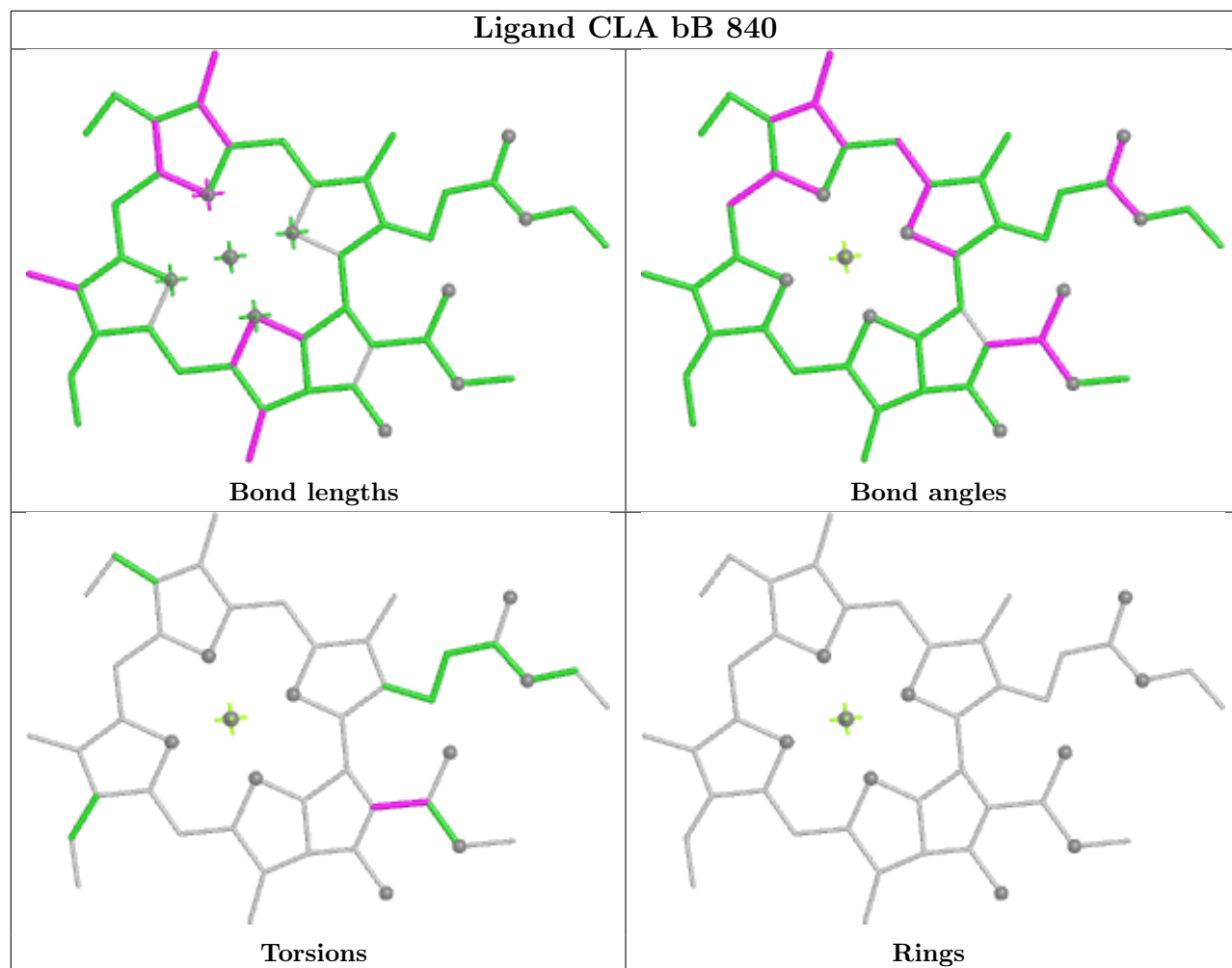


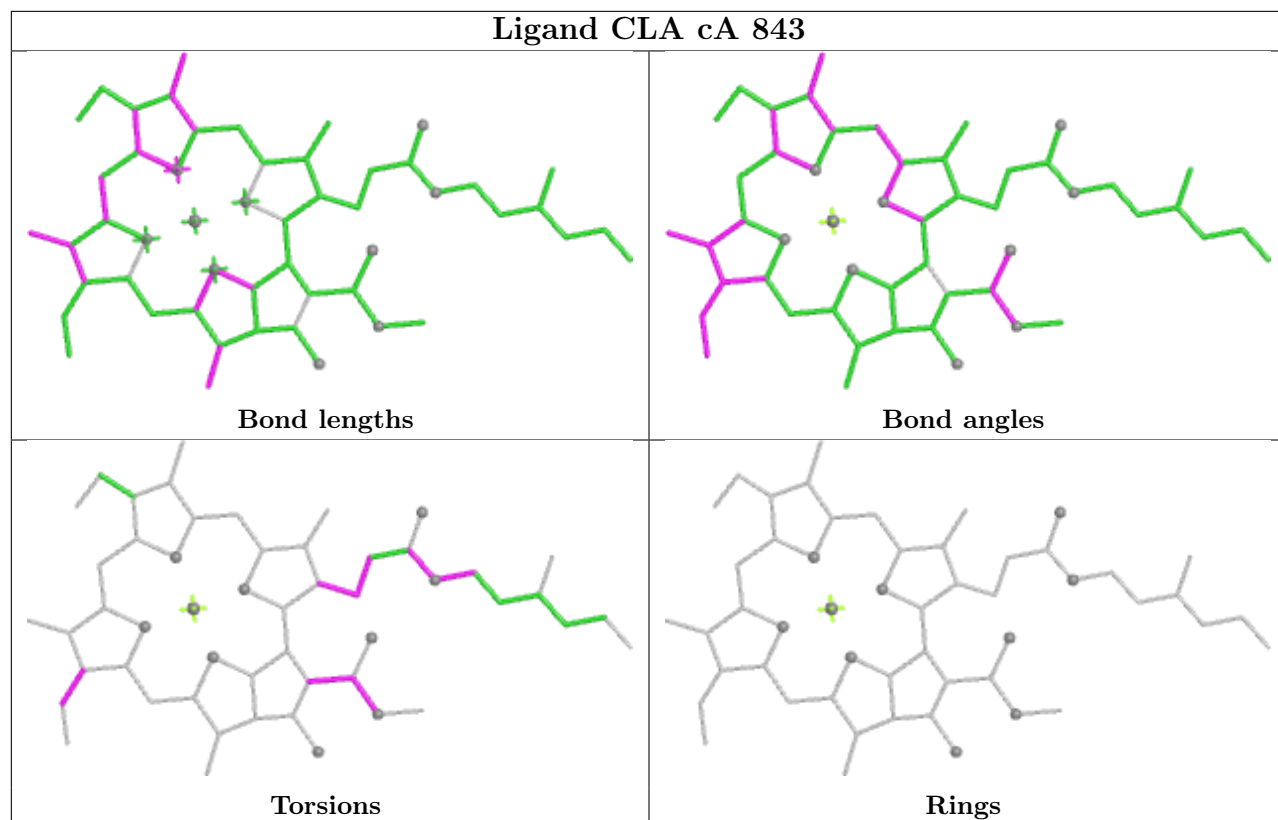




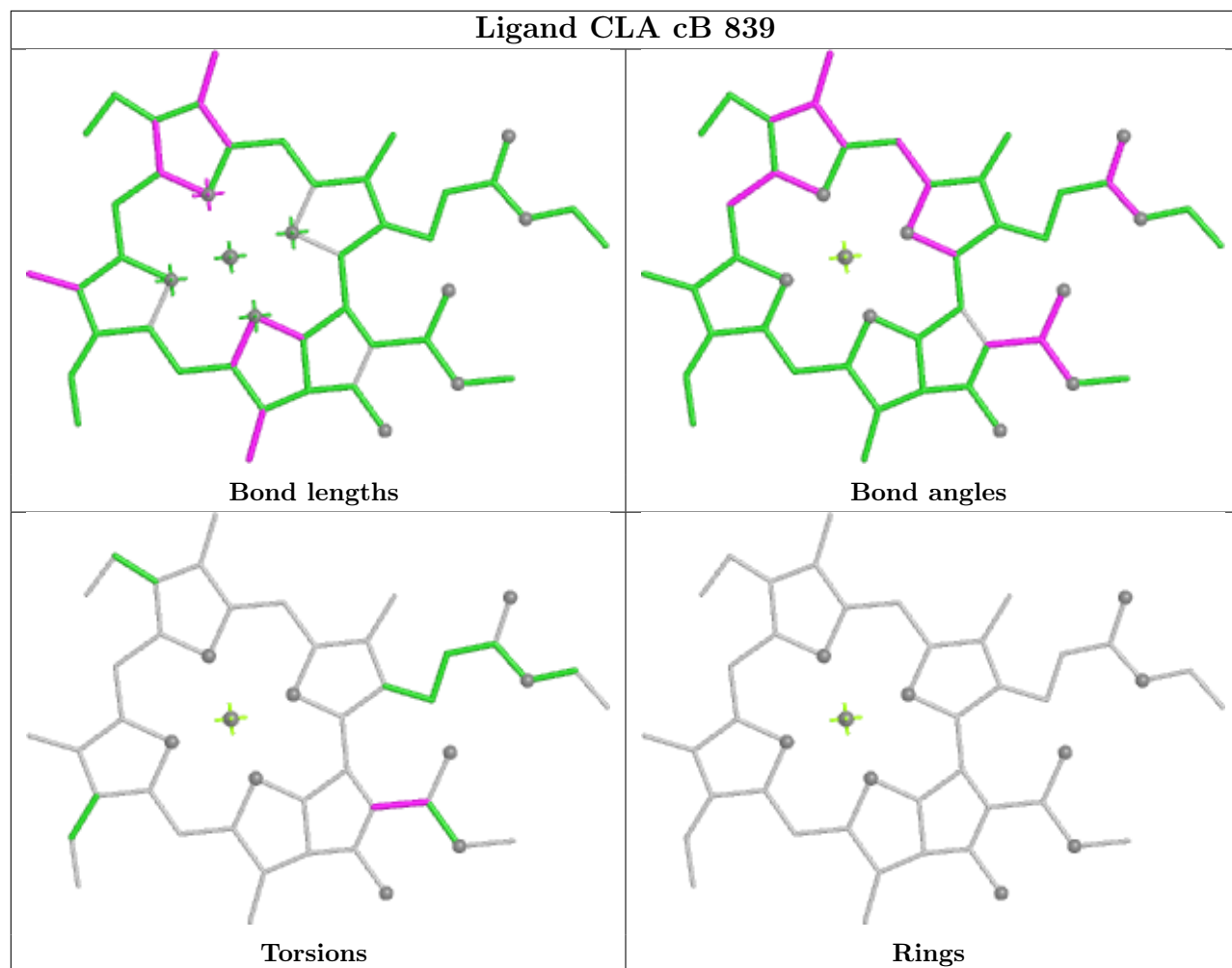


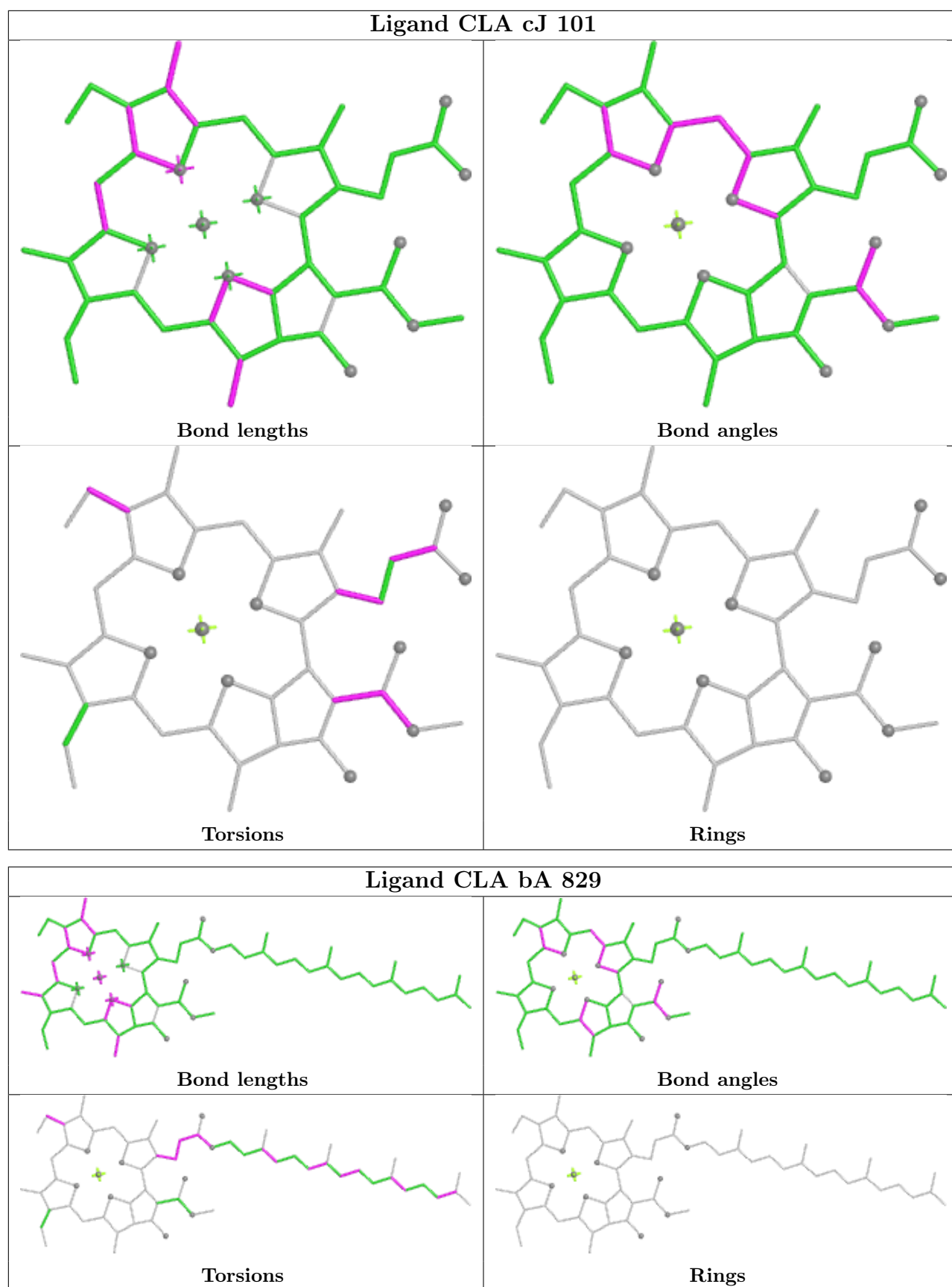
Ligand CLA bB 840

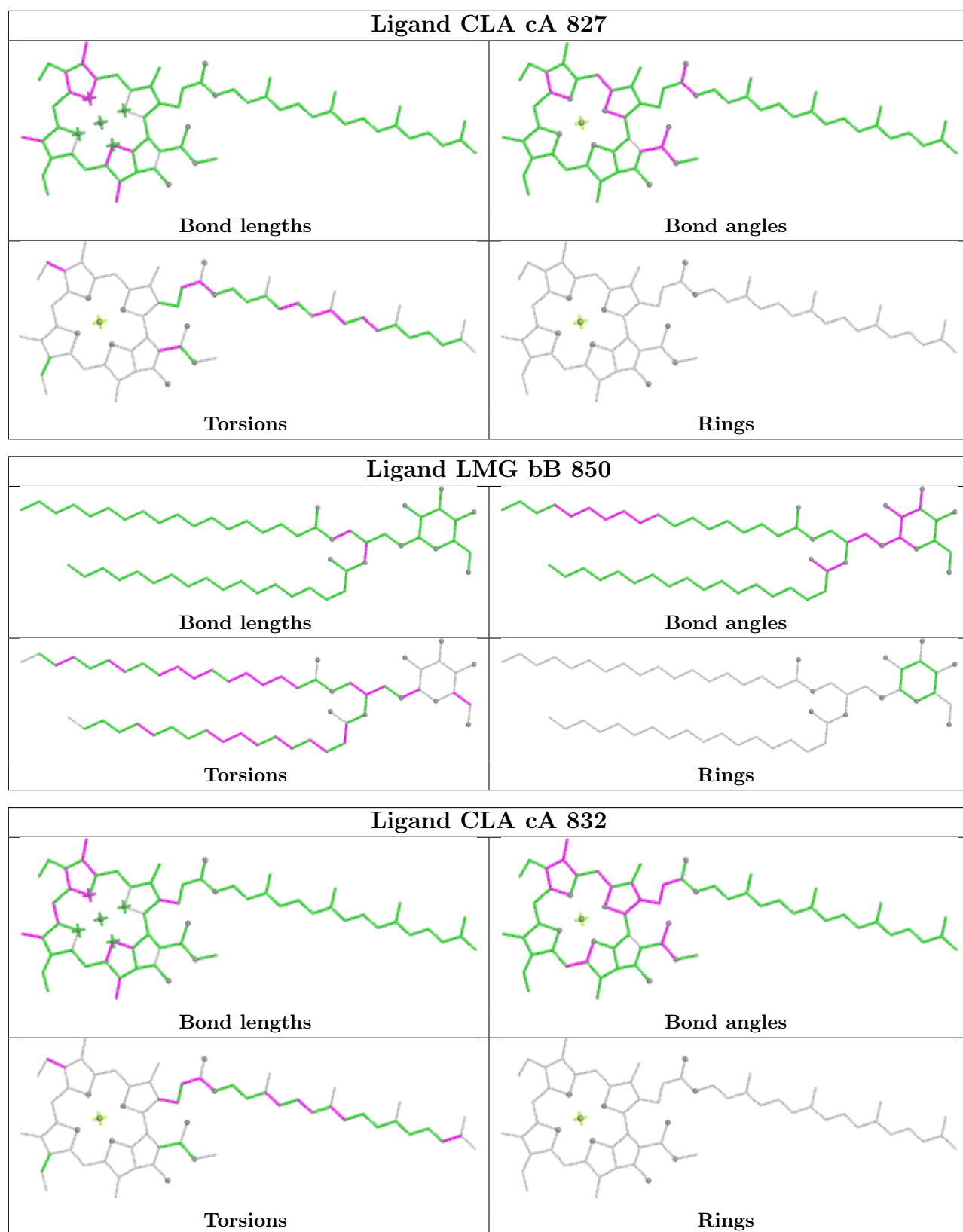


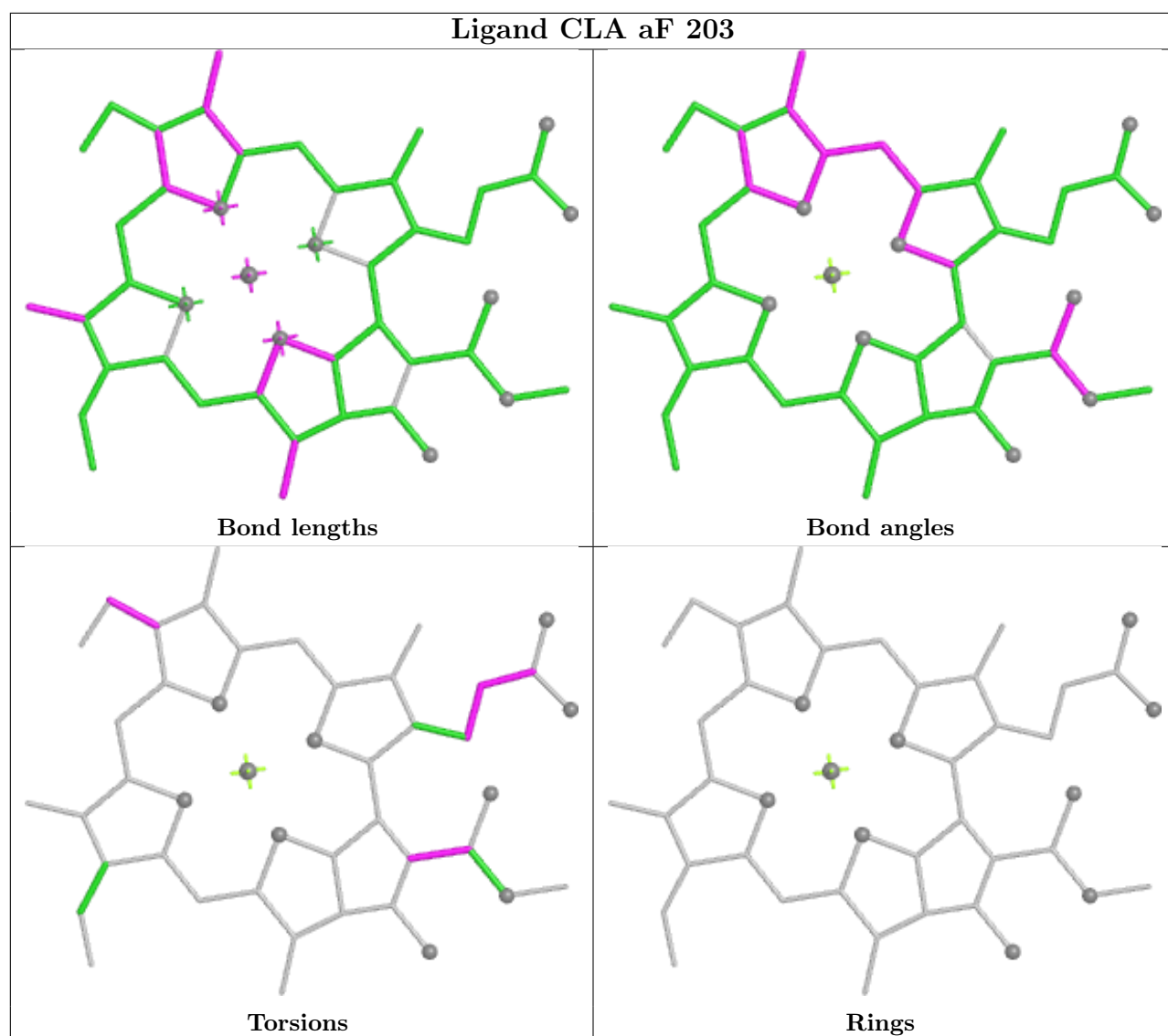


Ligand CLA cB 839

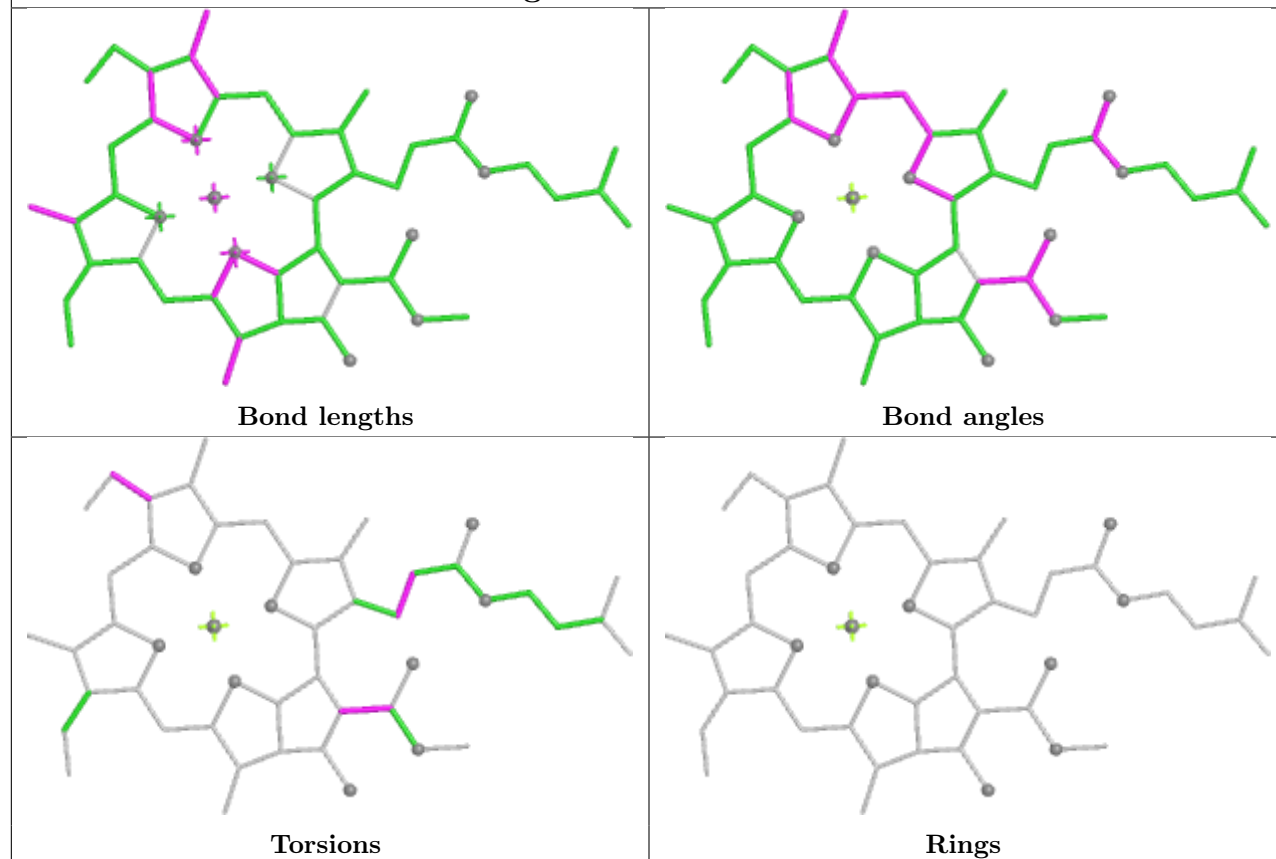




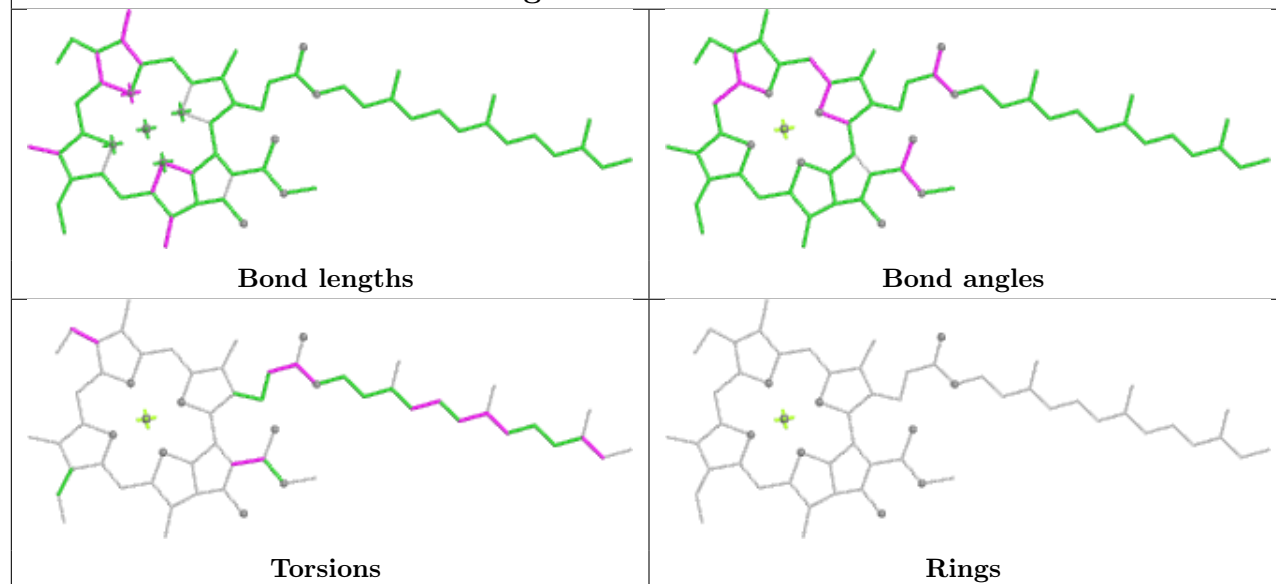


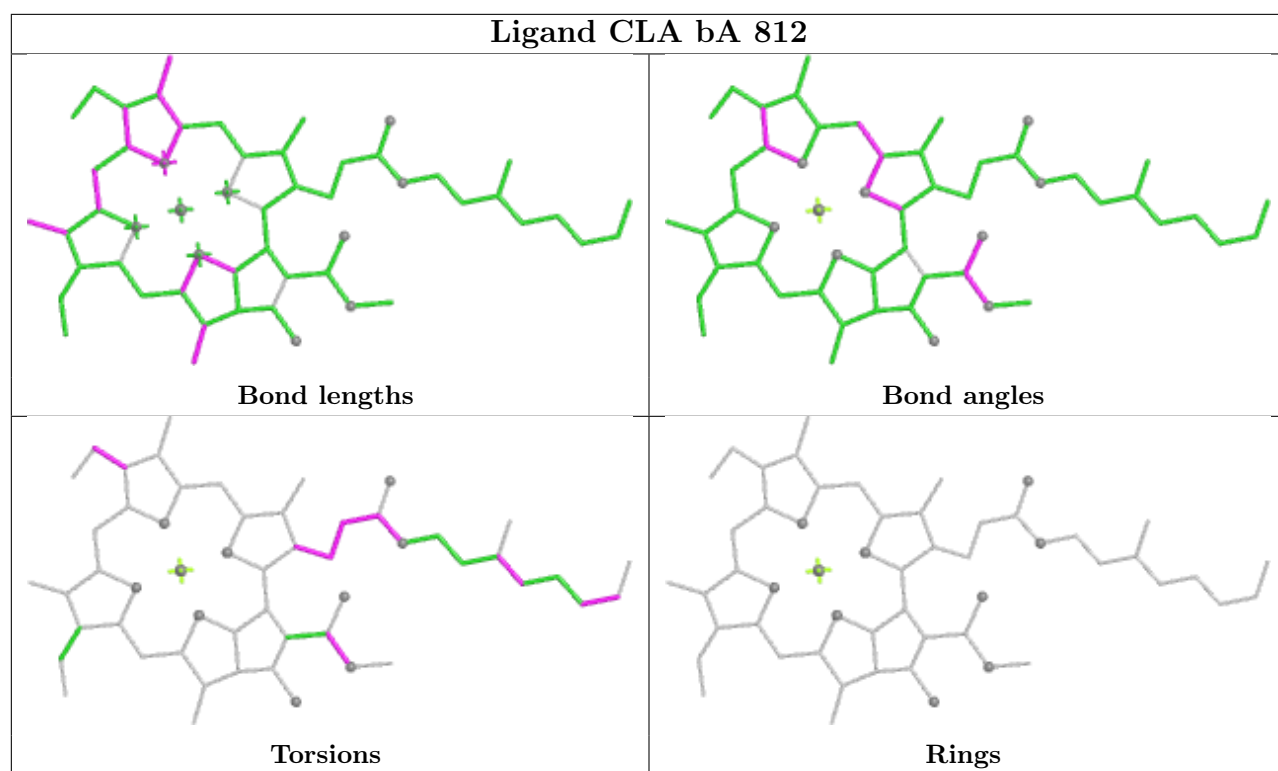


Ligand CLA cA 831

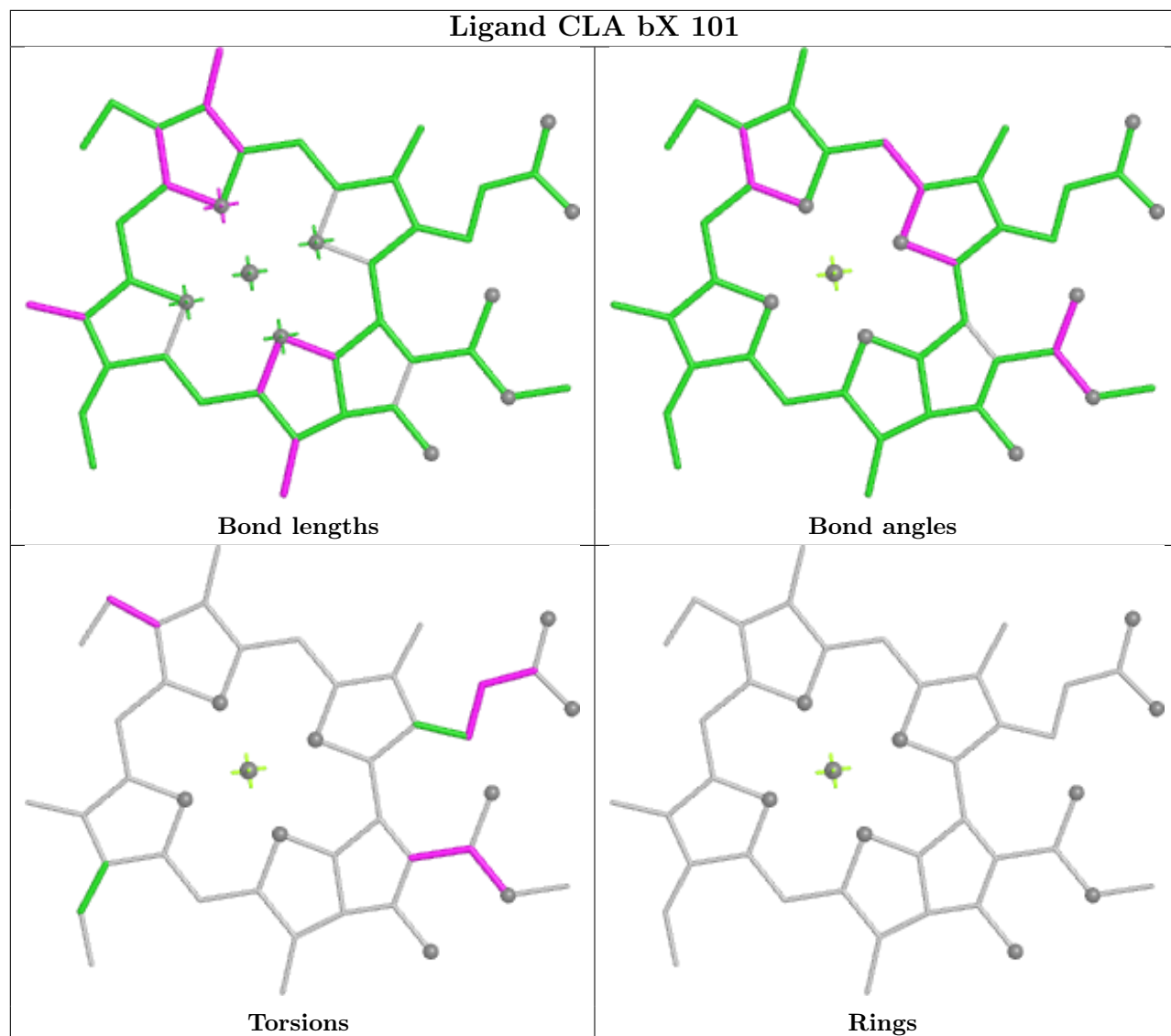


Ligand CLA cA 820

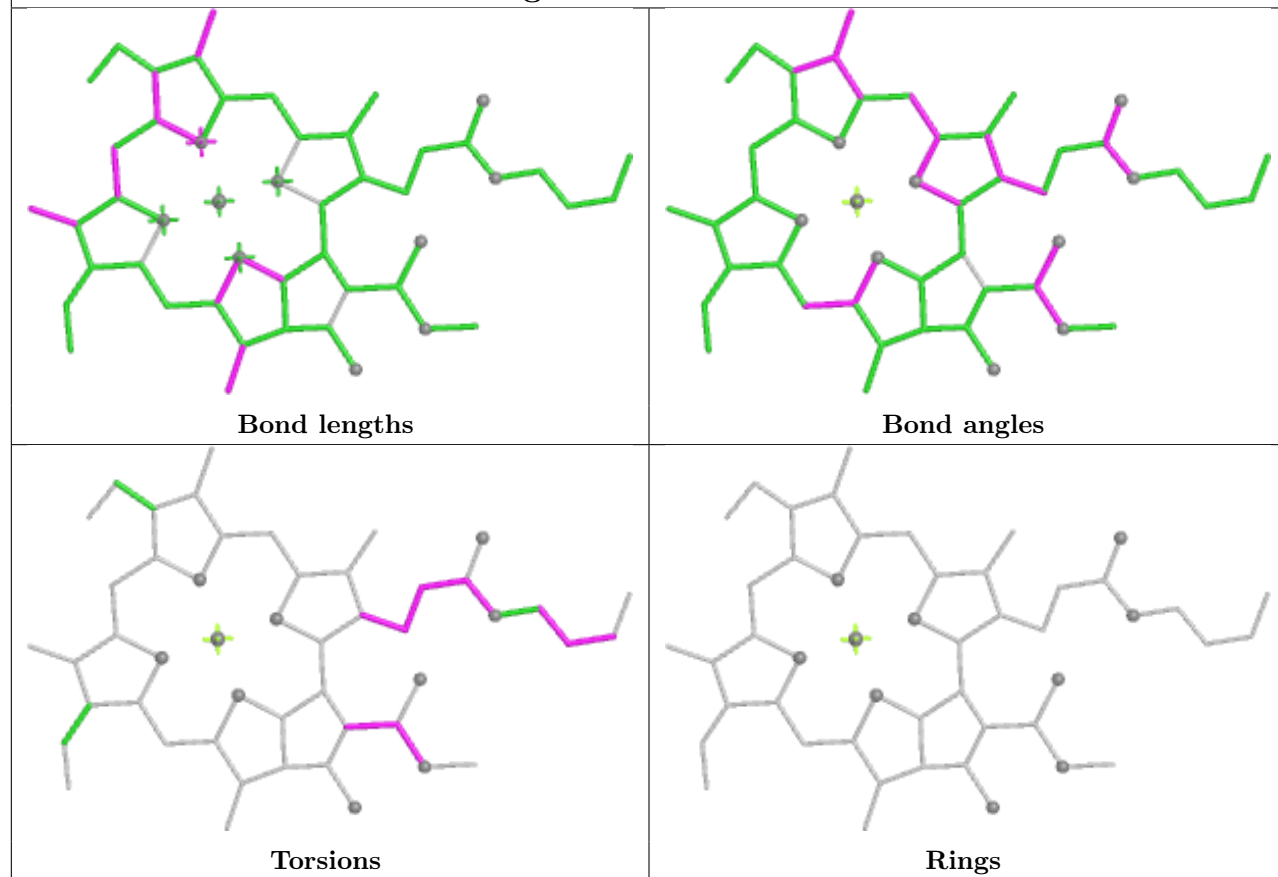




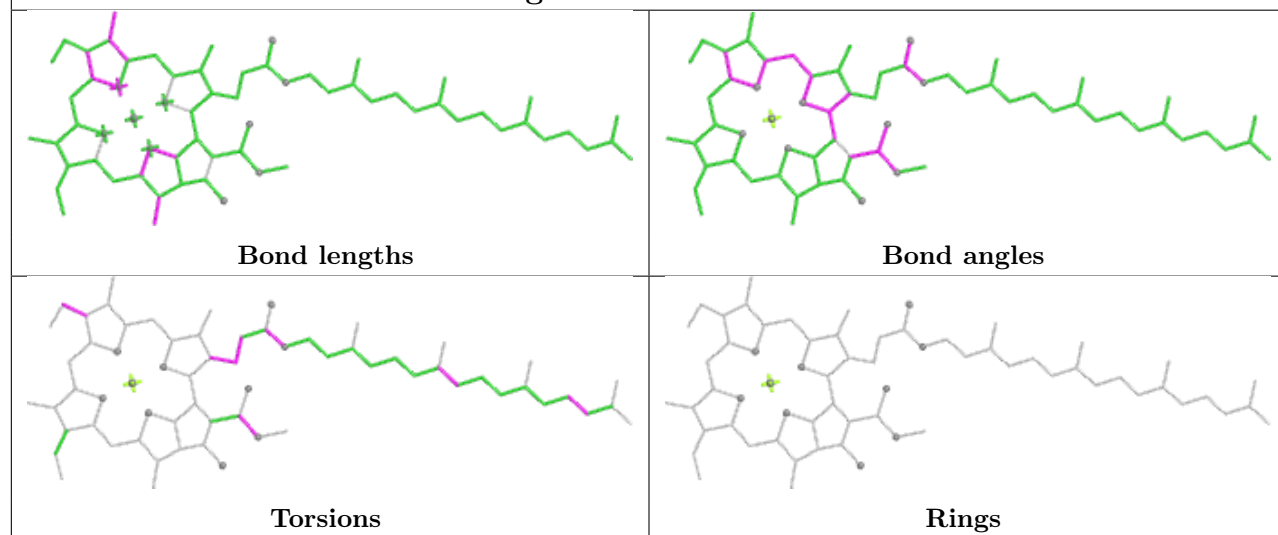
Ligand CLA bX 101

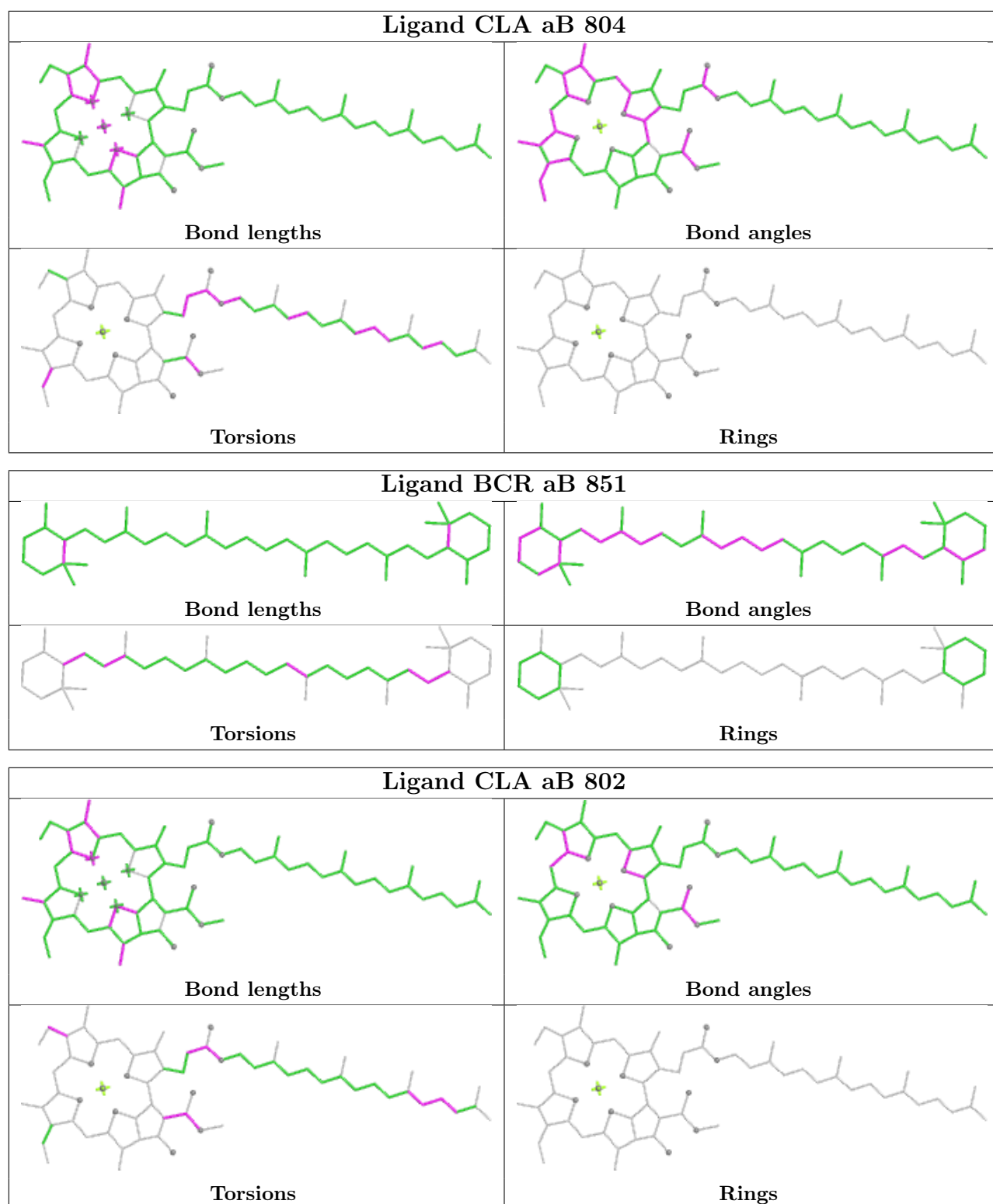


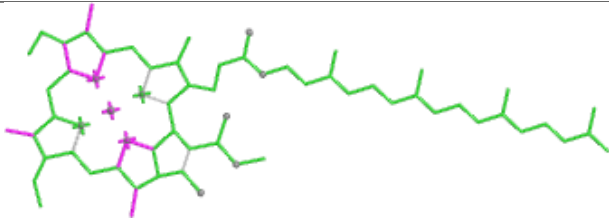
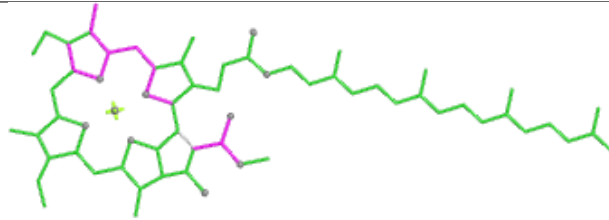
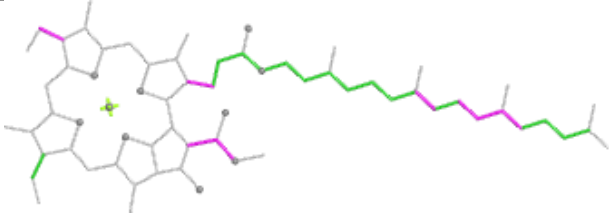
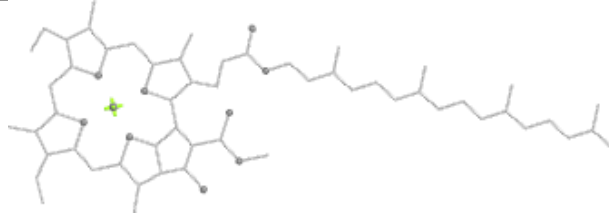
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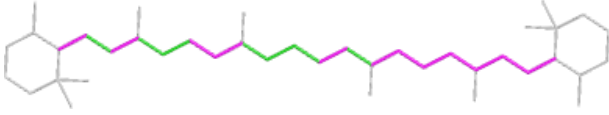
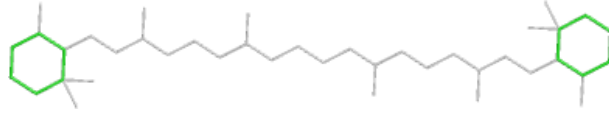


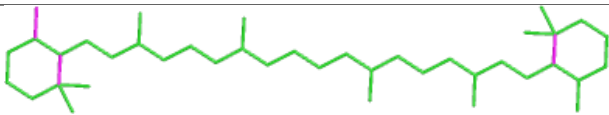
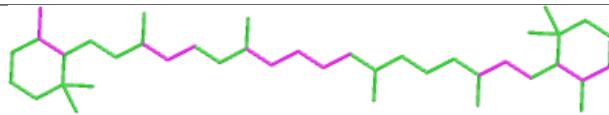
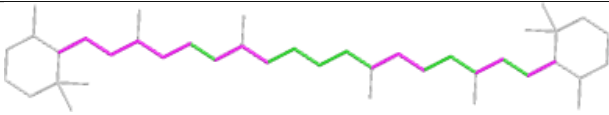
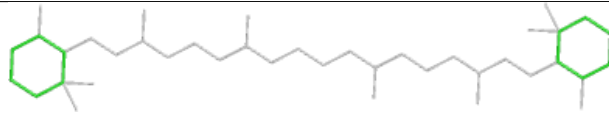
Ligand CLA aL 202

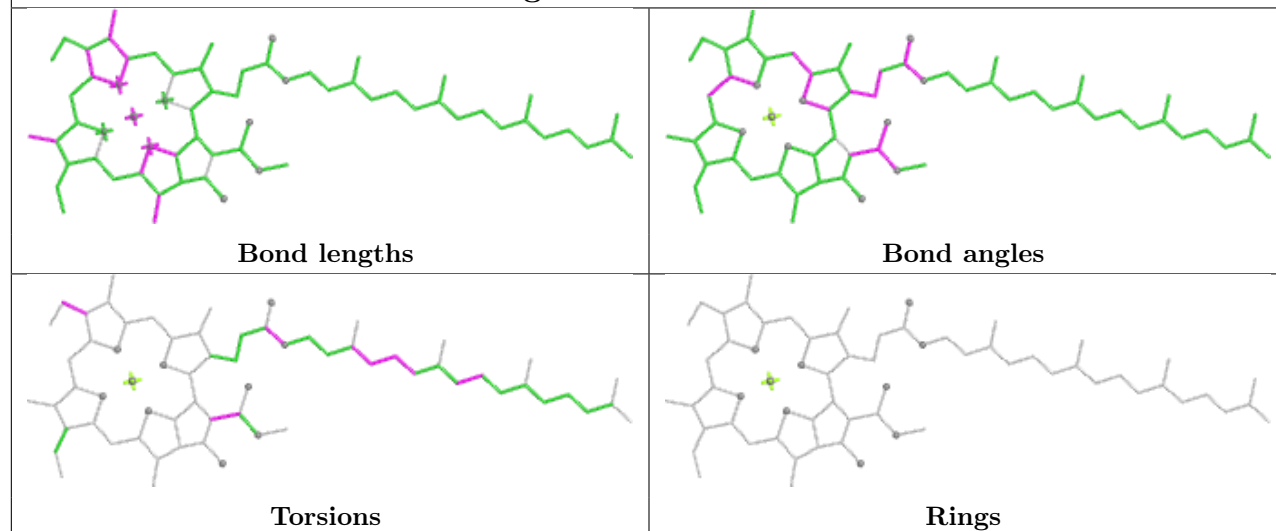
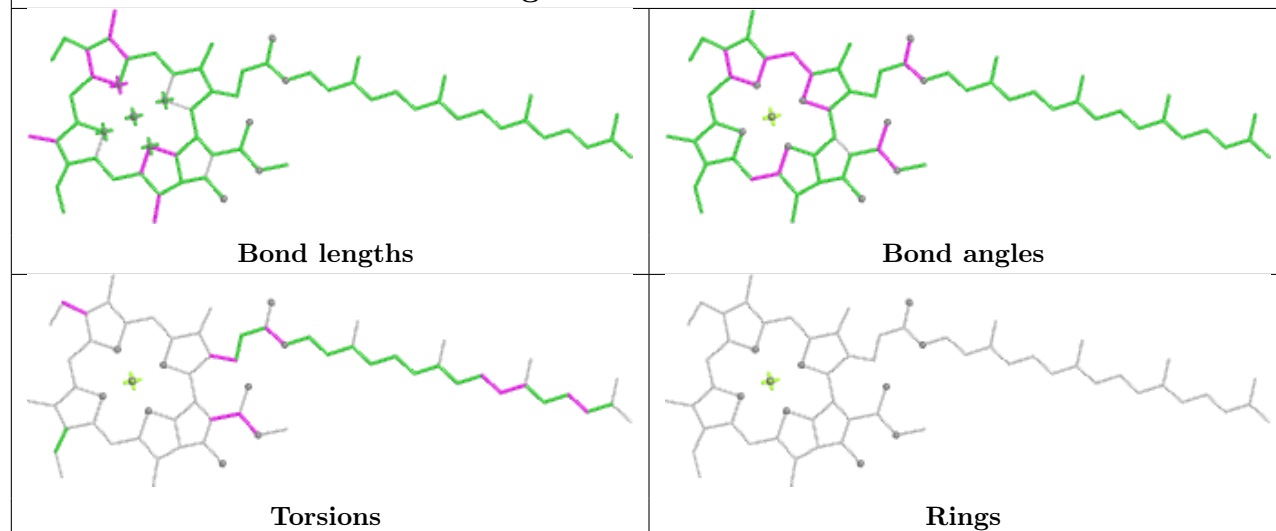


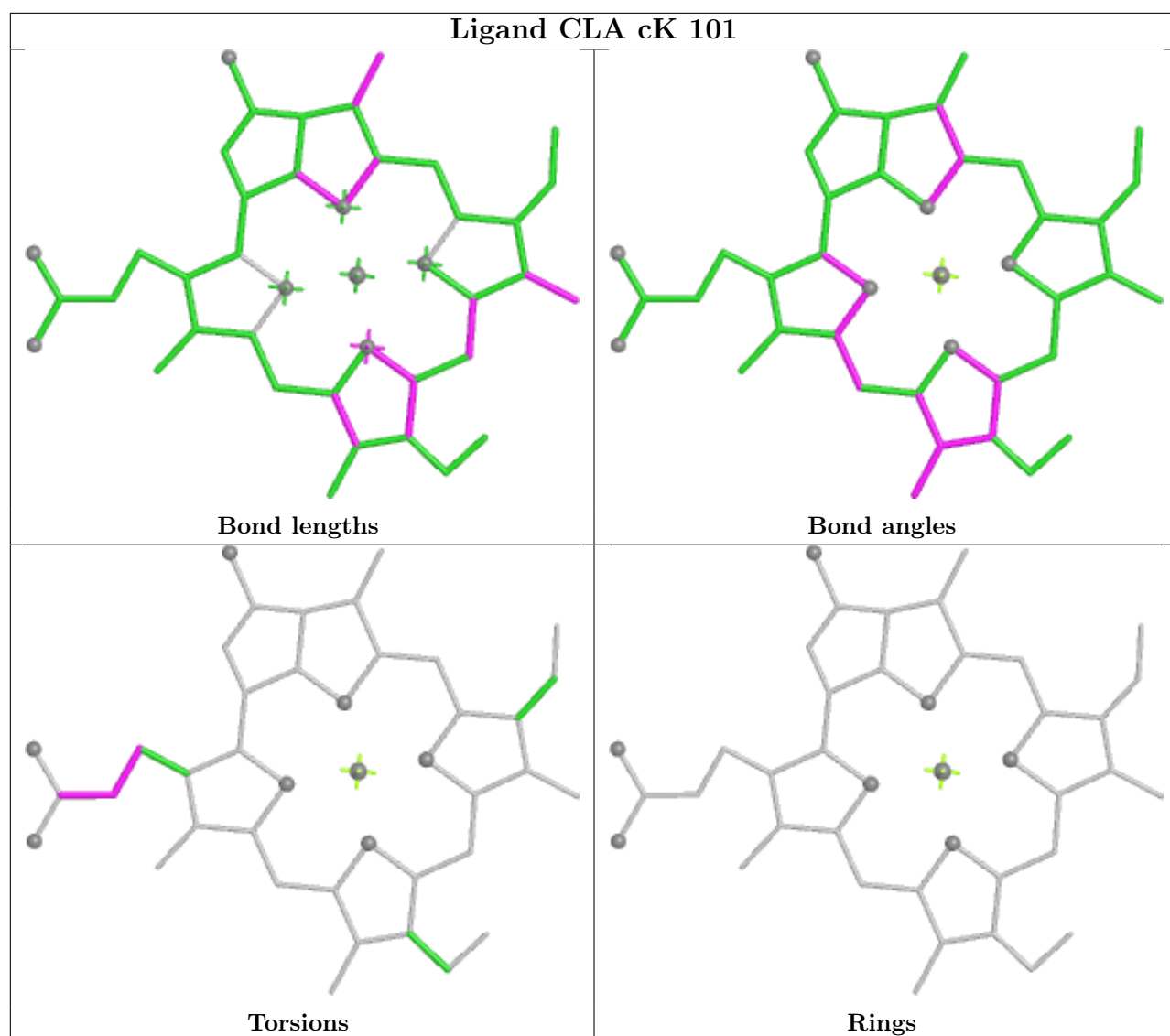


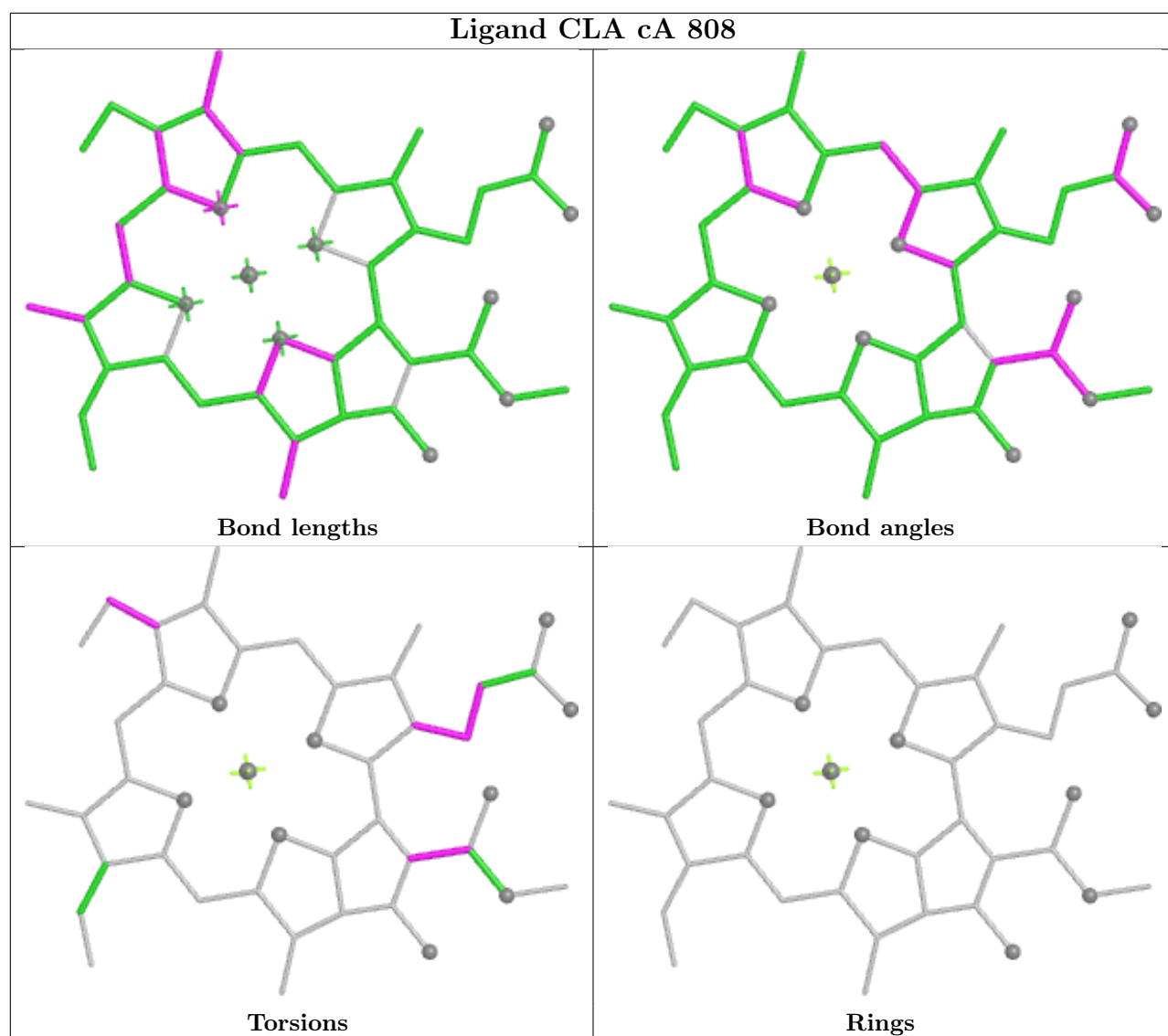
Ligand CLA bA 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR bB 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

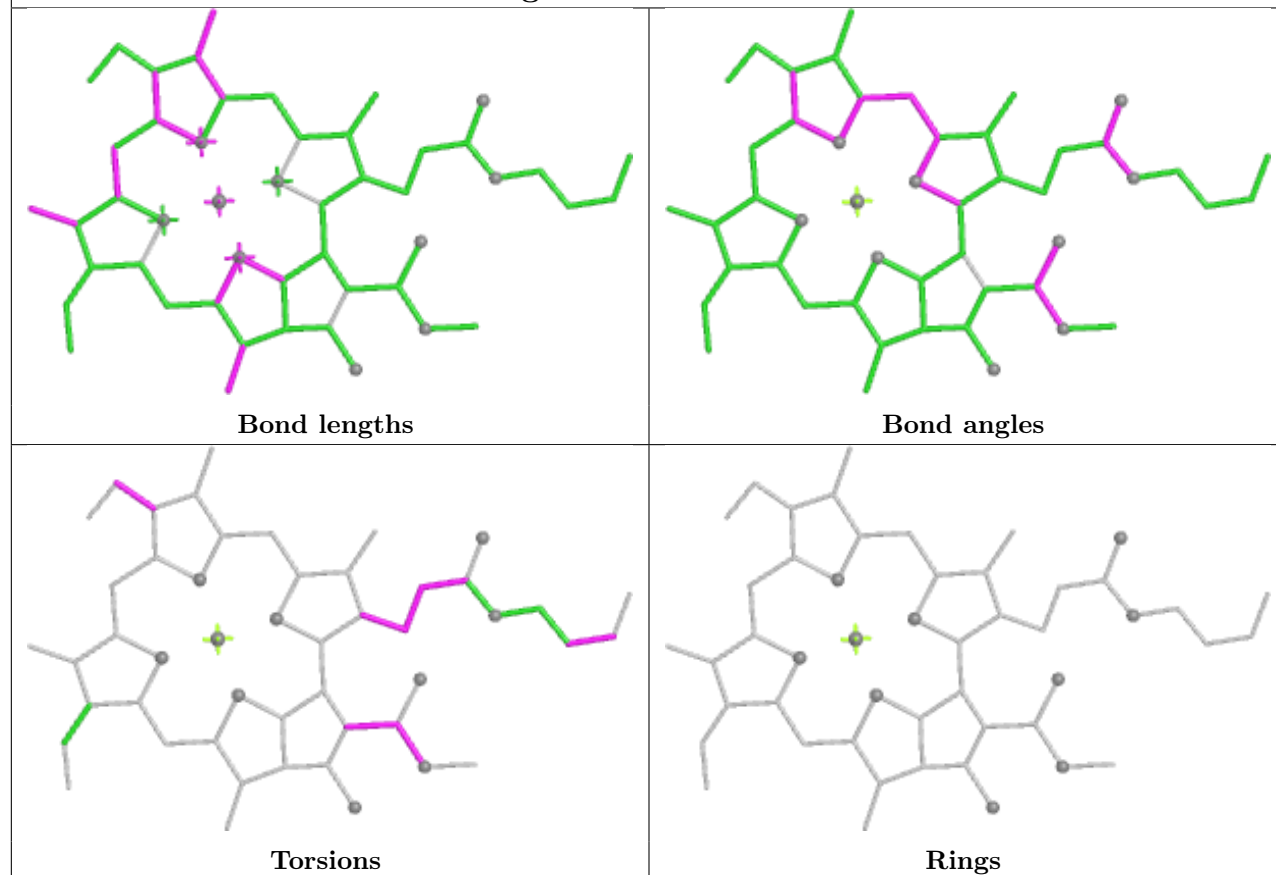
Ligand BCR aJ 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aB 809**Ligand CLA bA 811**

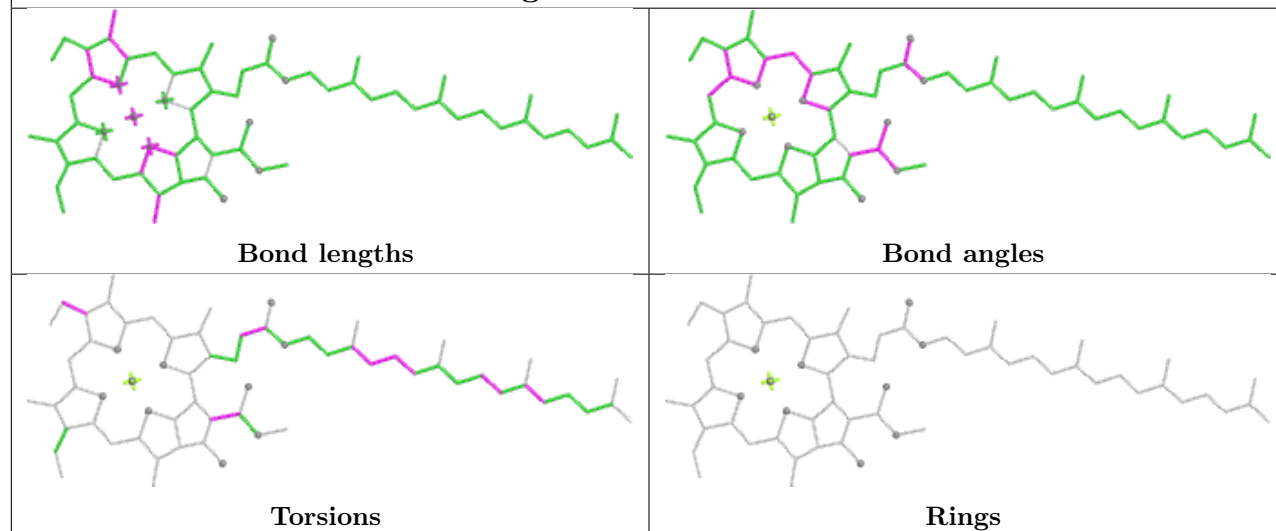


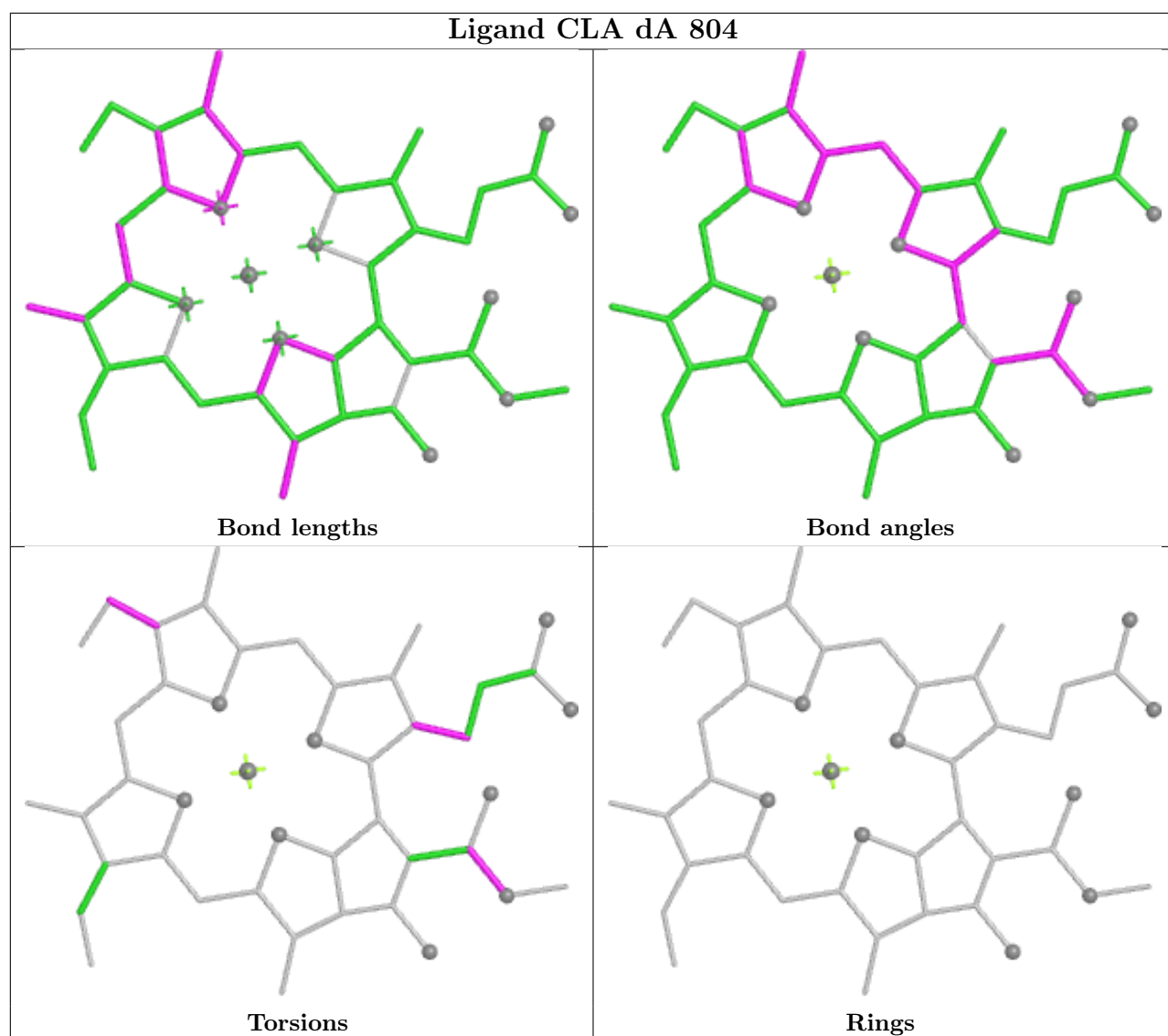


Ligand CLA dA 822

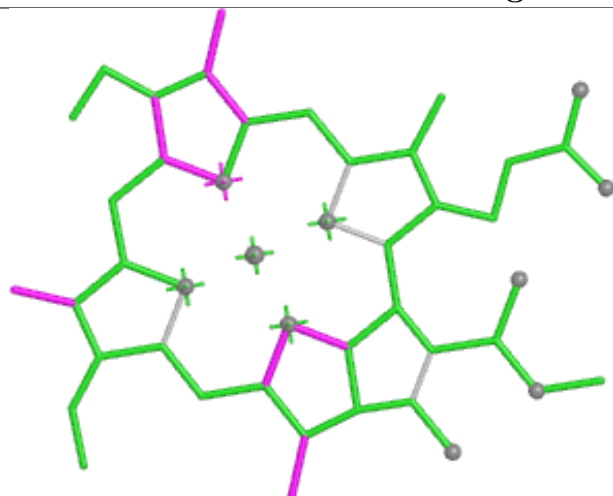


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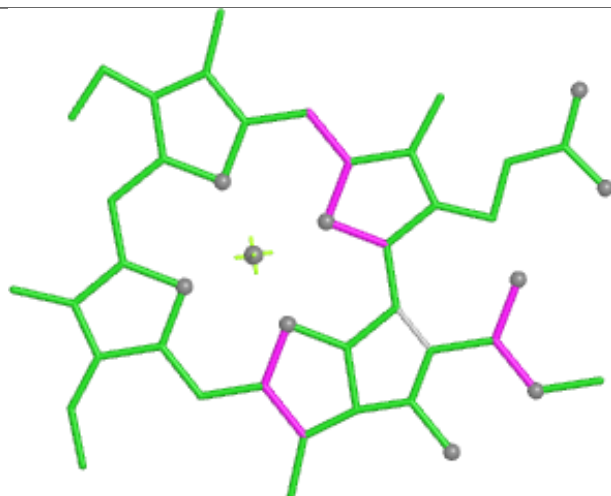




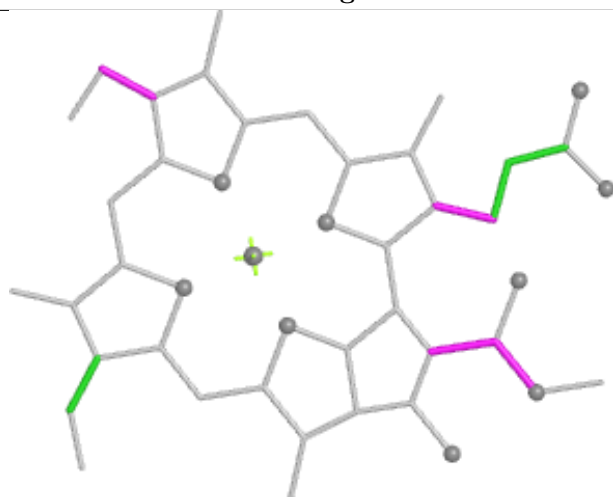
Ligand CLA cB 811



Bond lengths



Bond angles

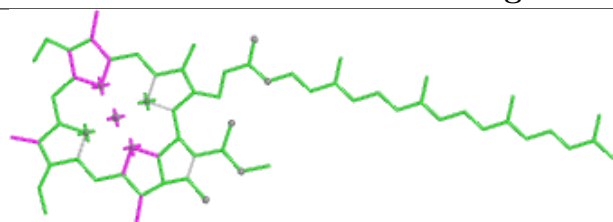


Torsions

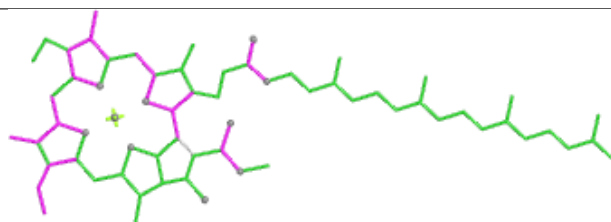


Rings

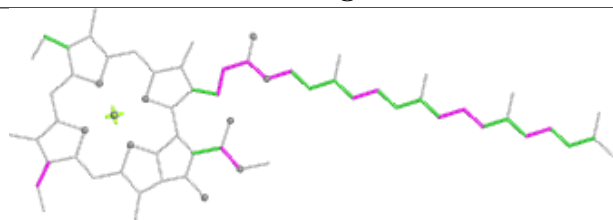
Ligand CLA dB 804



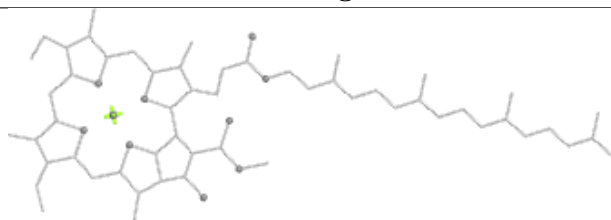
Bond lengths



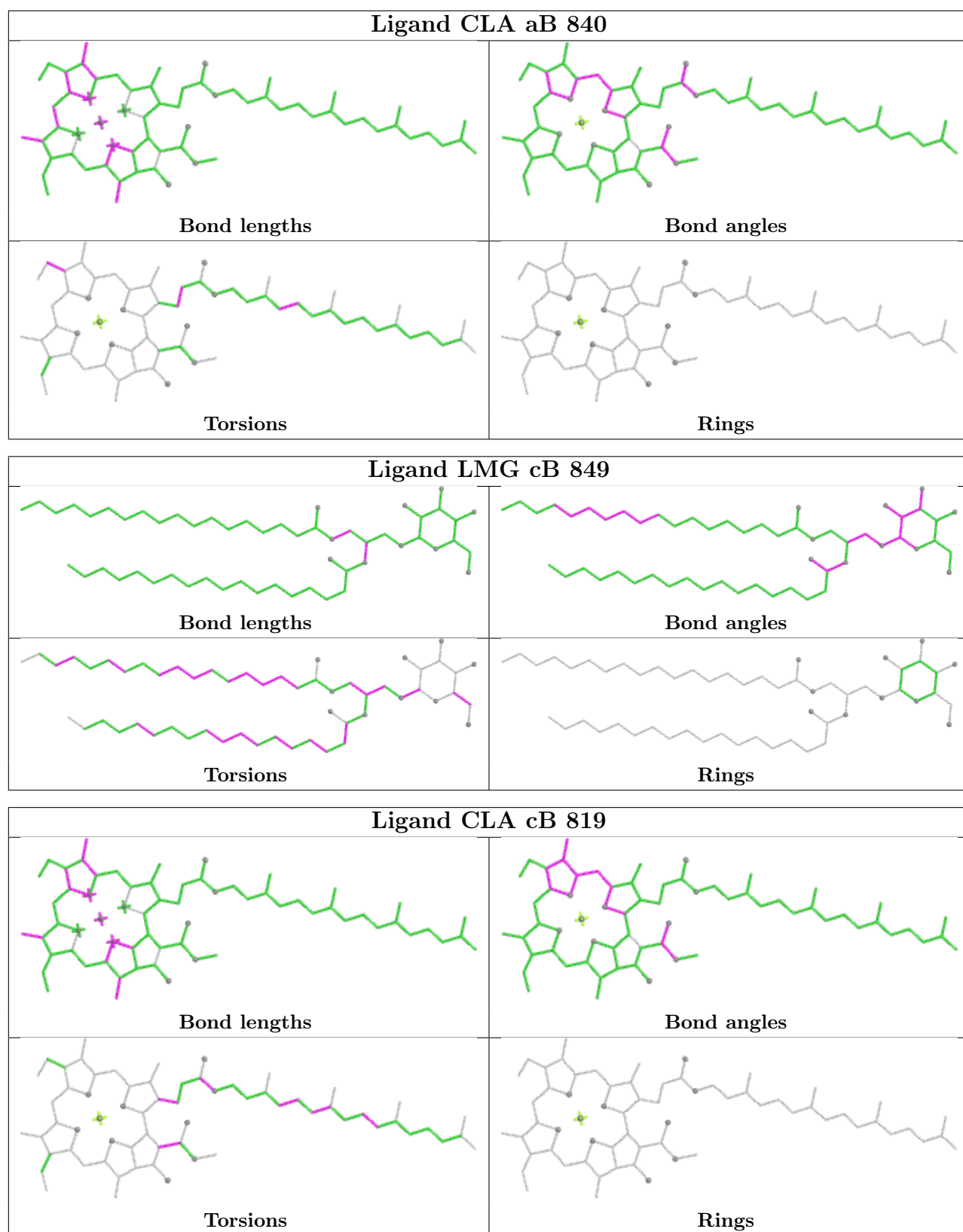
Bond angles

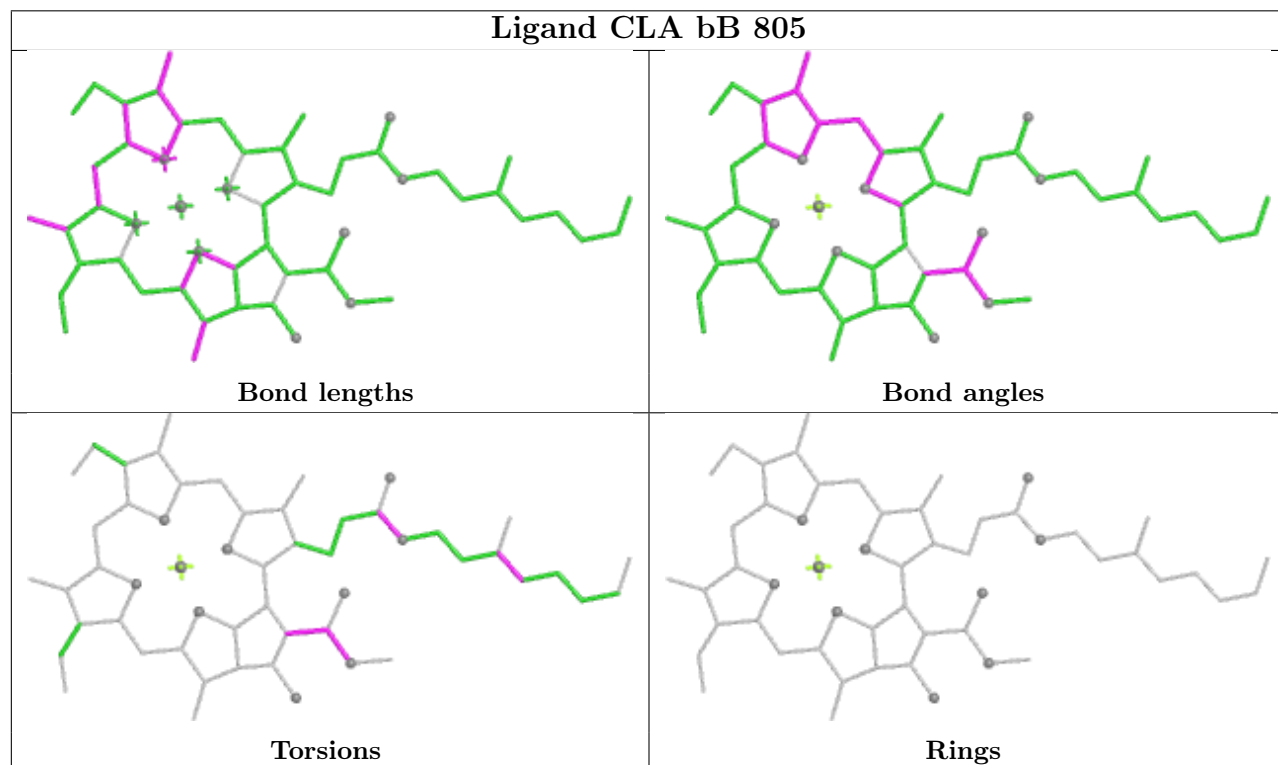
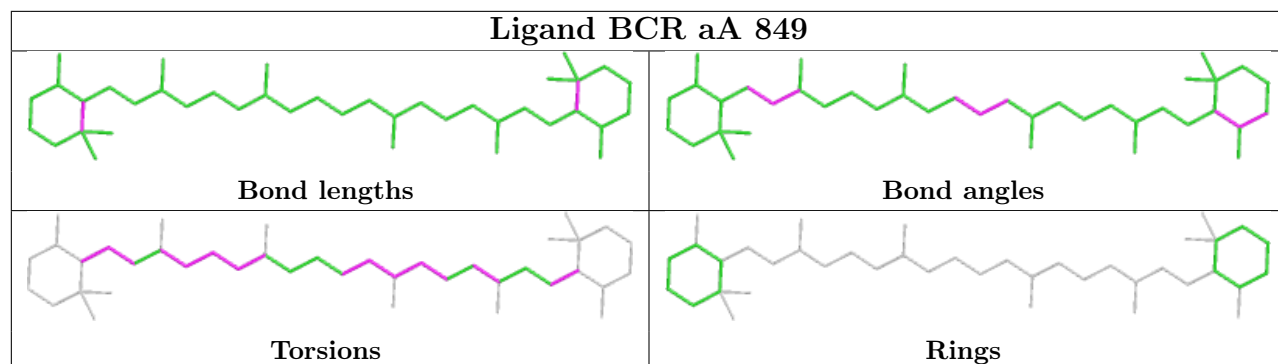


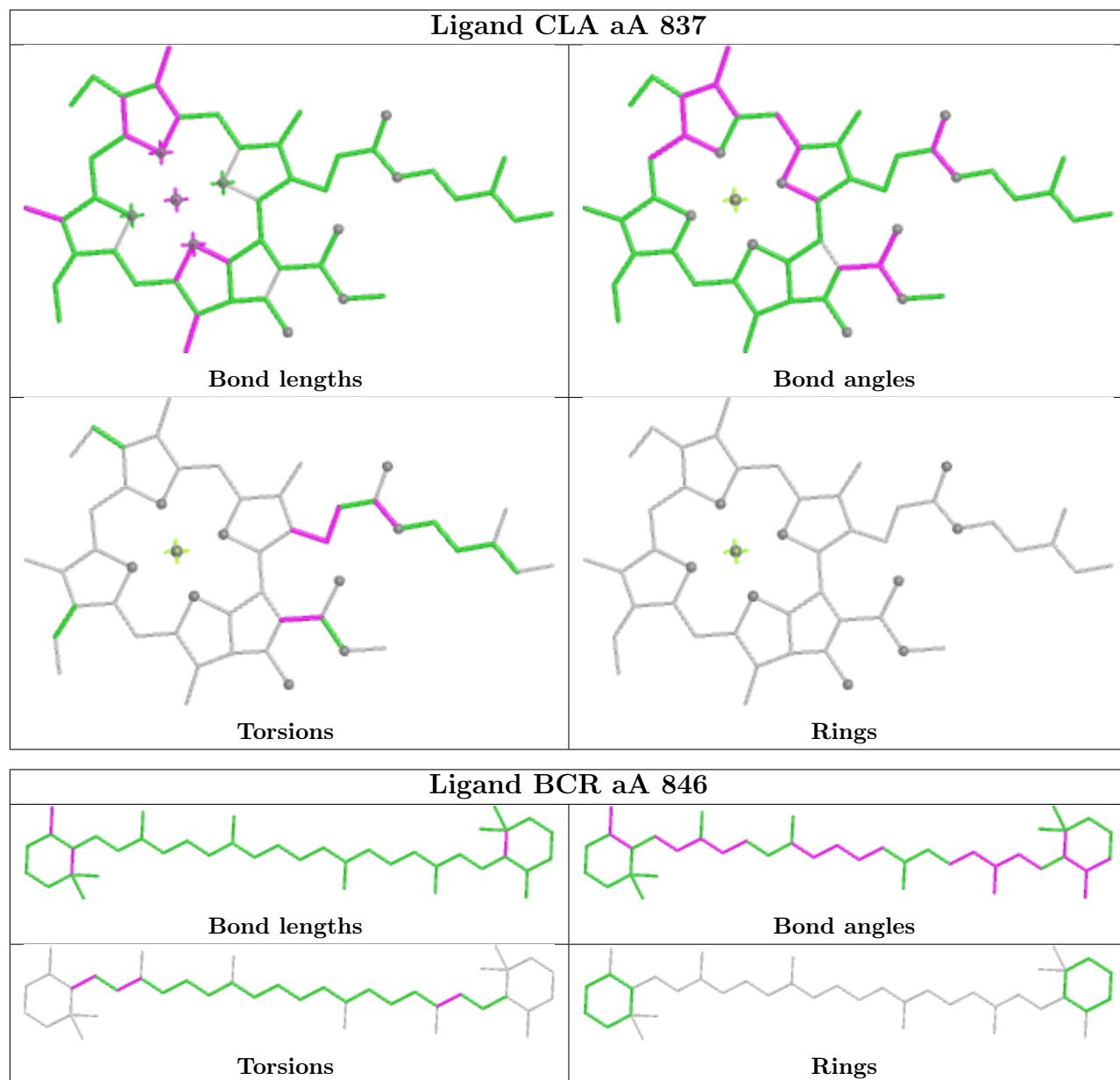
Torsions

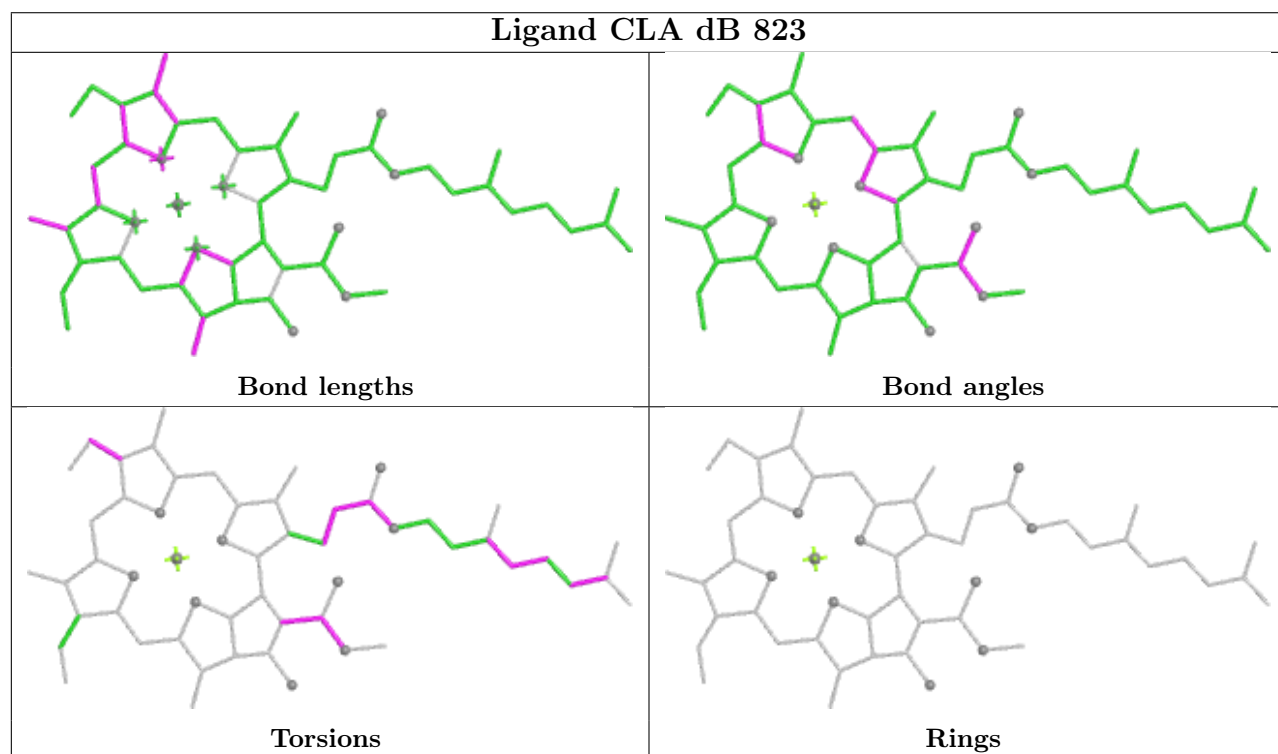
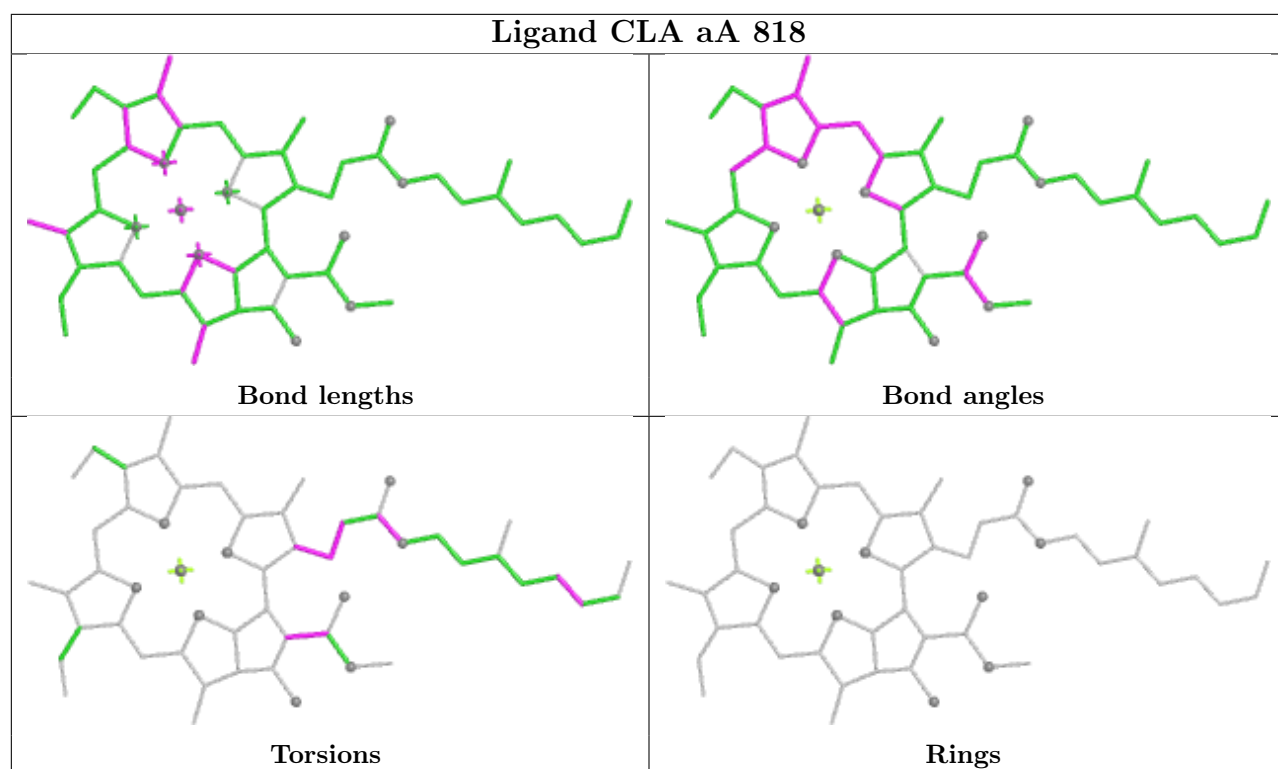


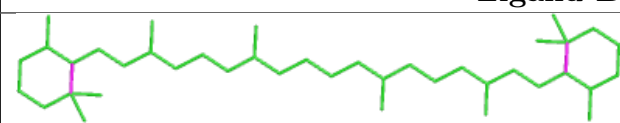
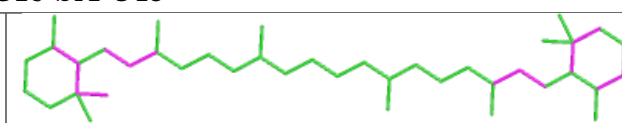
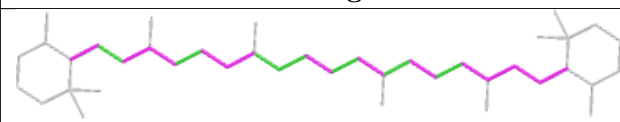
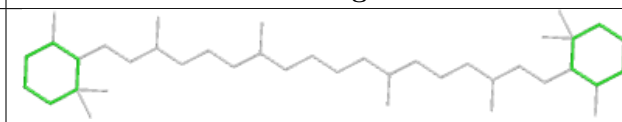
Rings

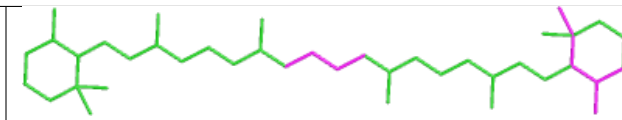
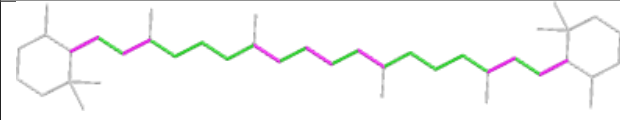
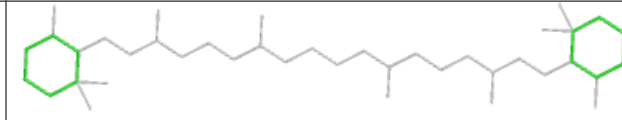


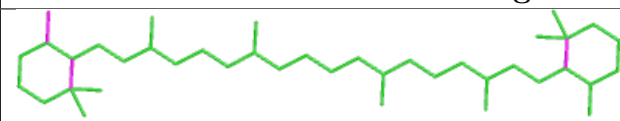
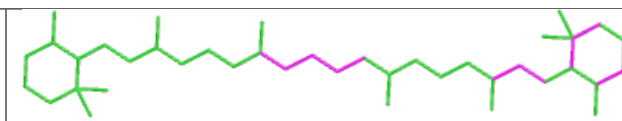
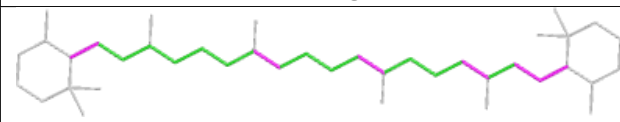
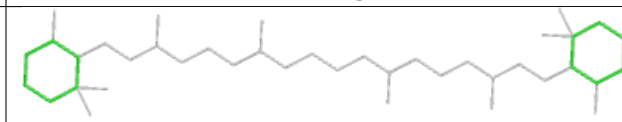


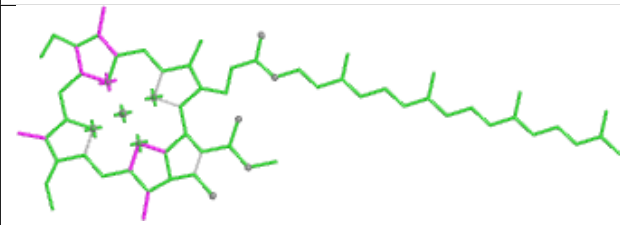
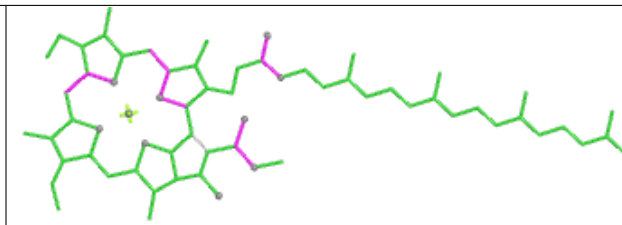
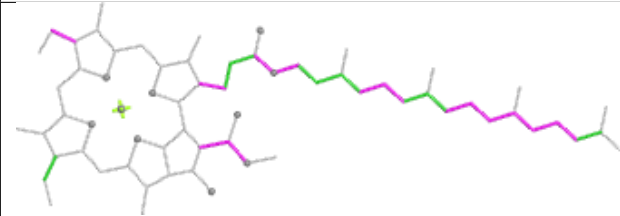
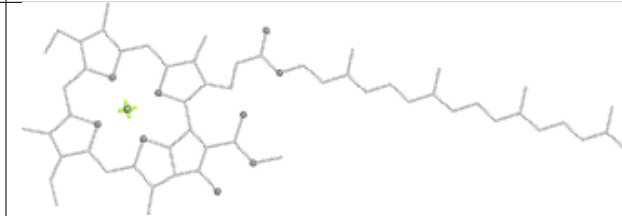


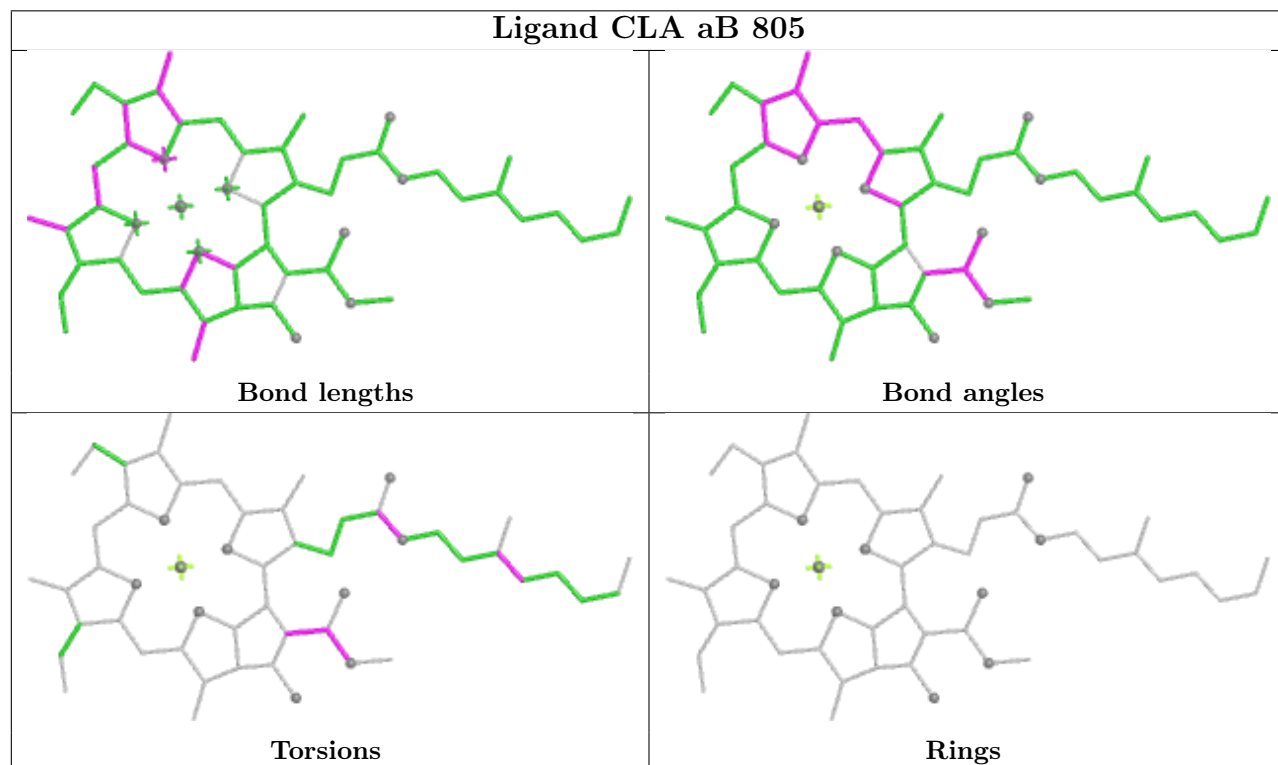
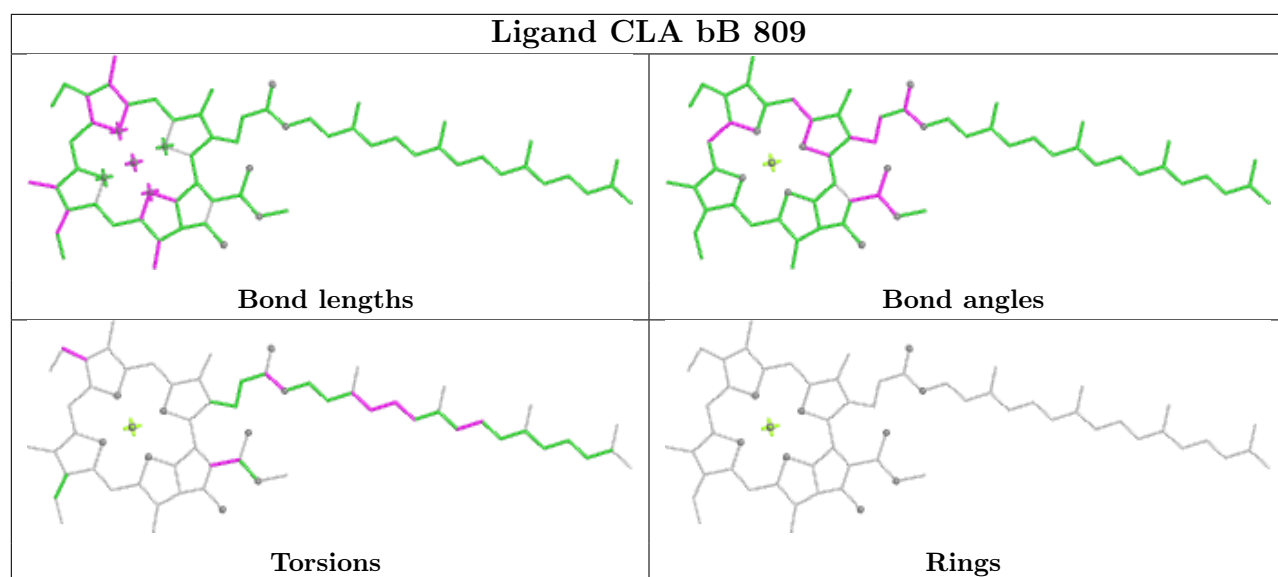


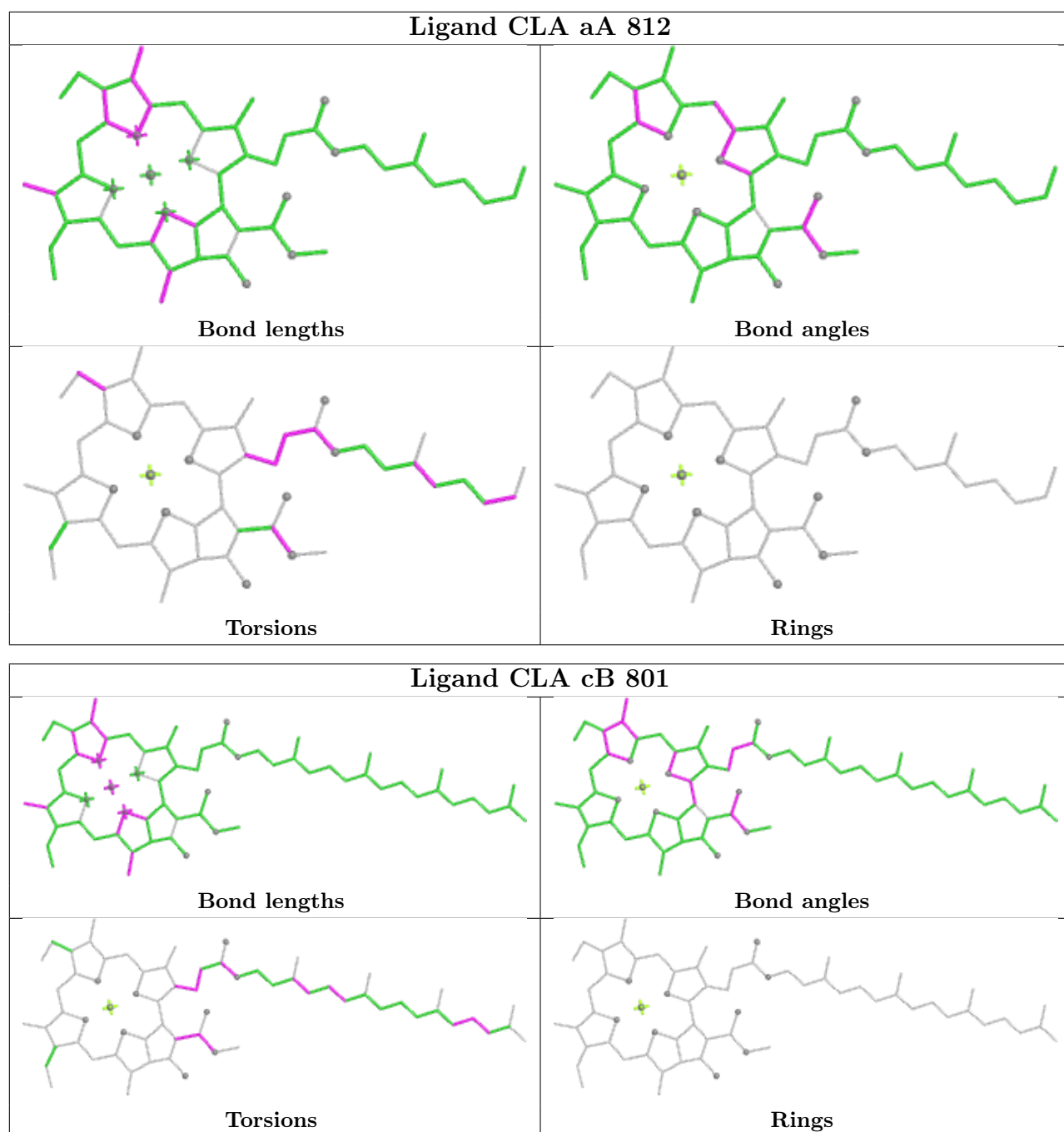
Ligand BCR bA 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

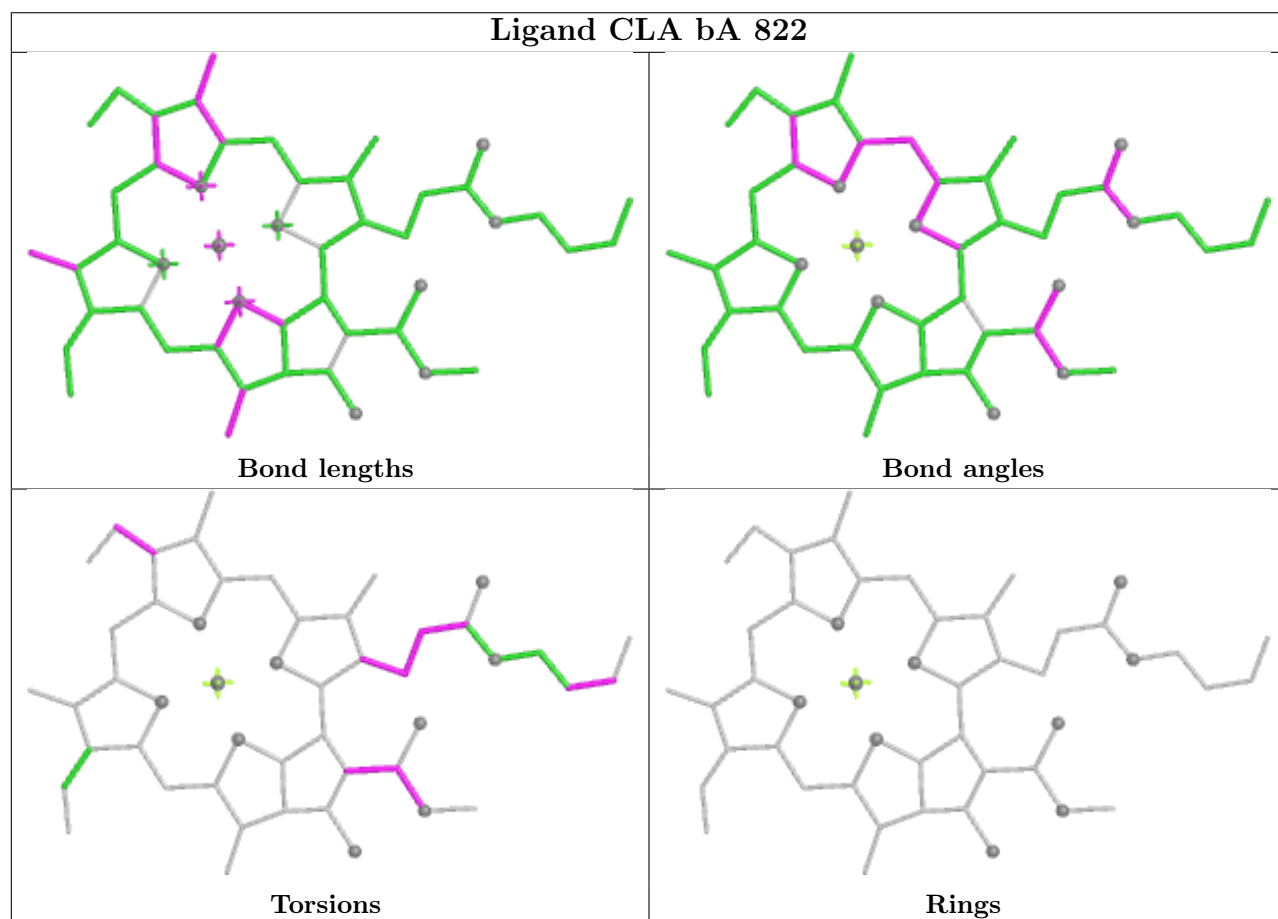
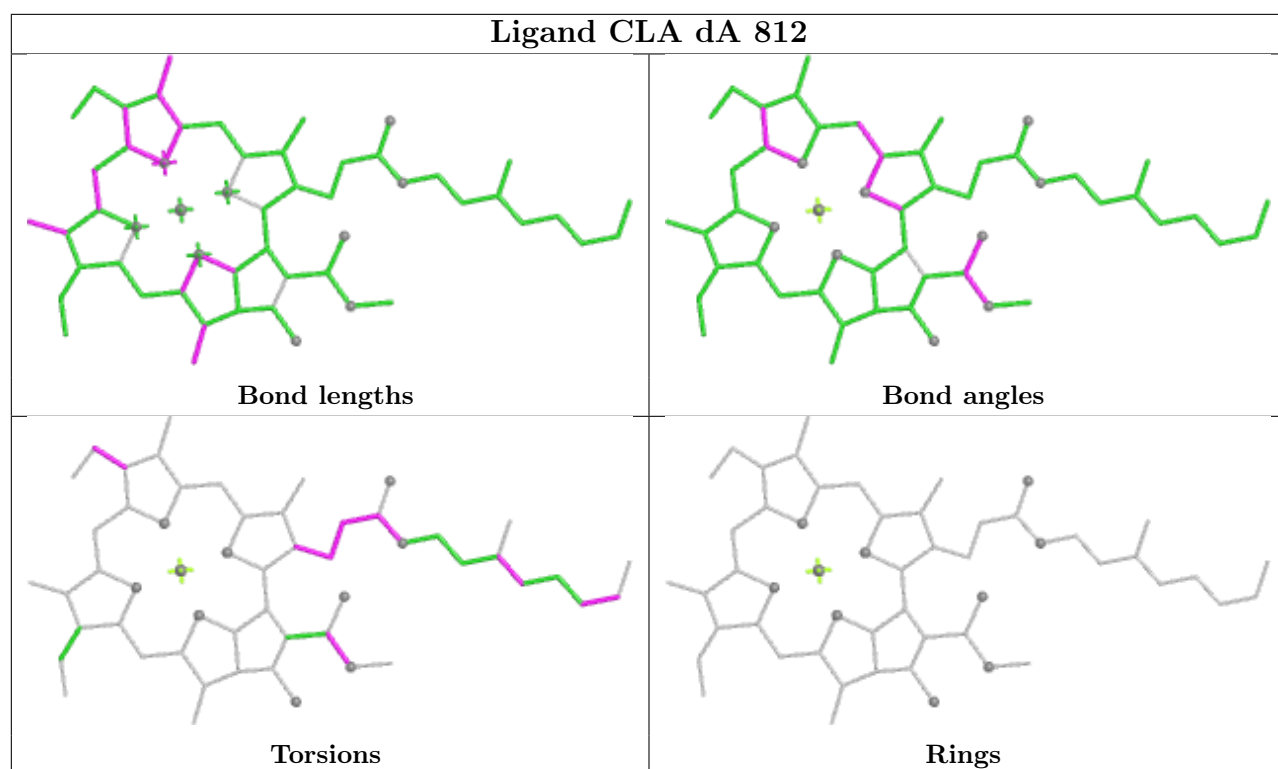
Ligand BCR aF 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR bJ 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

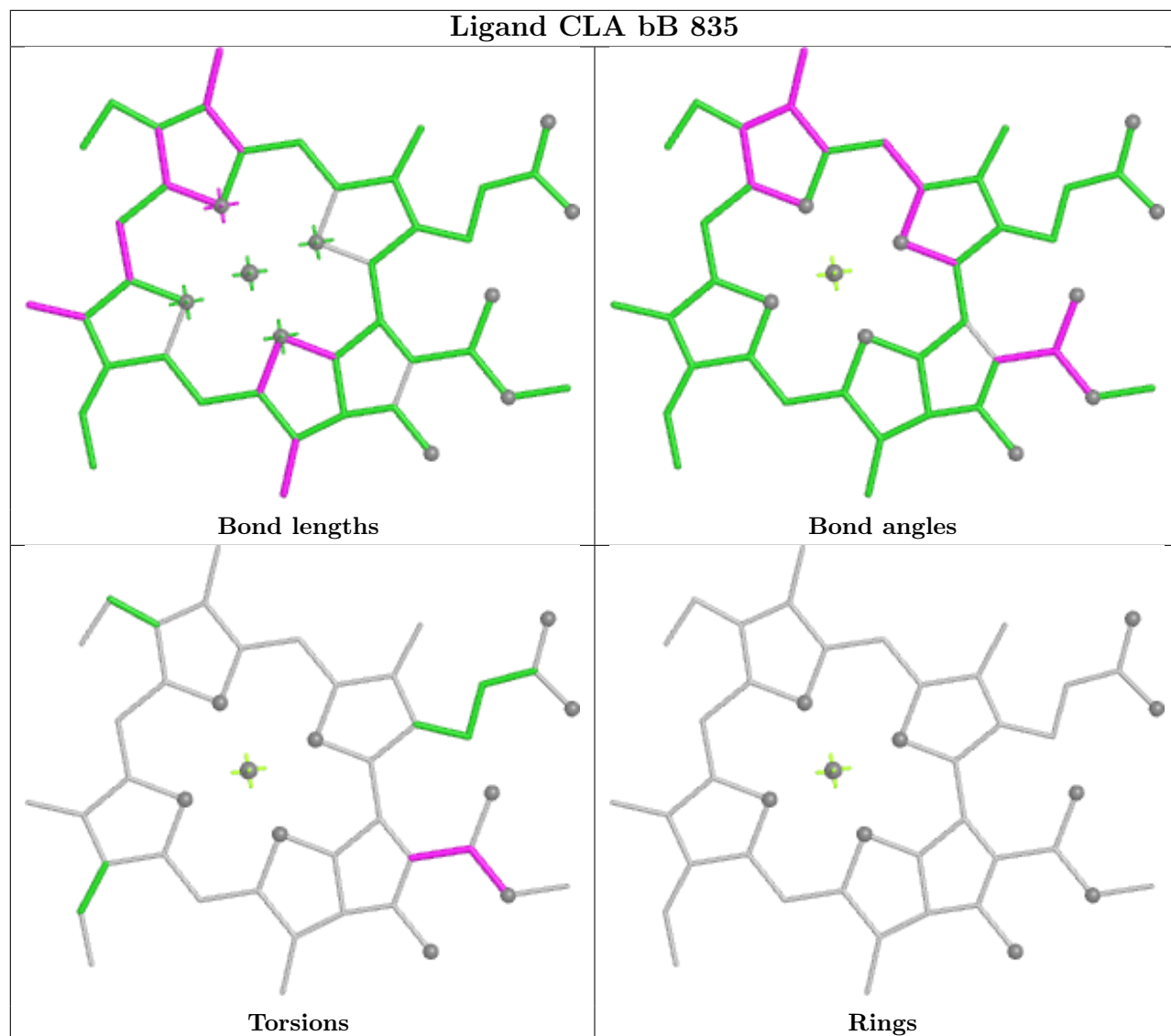
Ligand CLA cB 841	
	
Bond lengths	Bond angles
	
Torsions	Rings



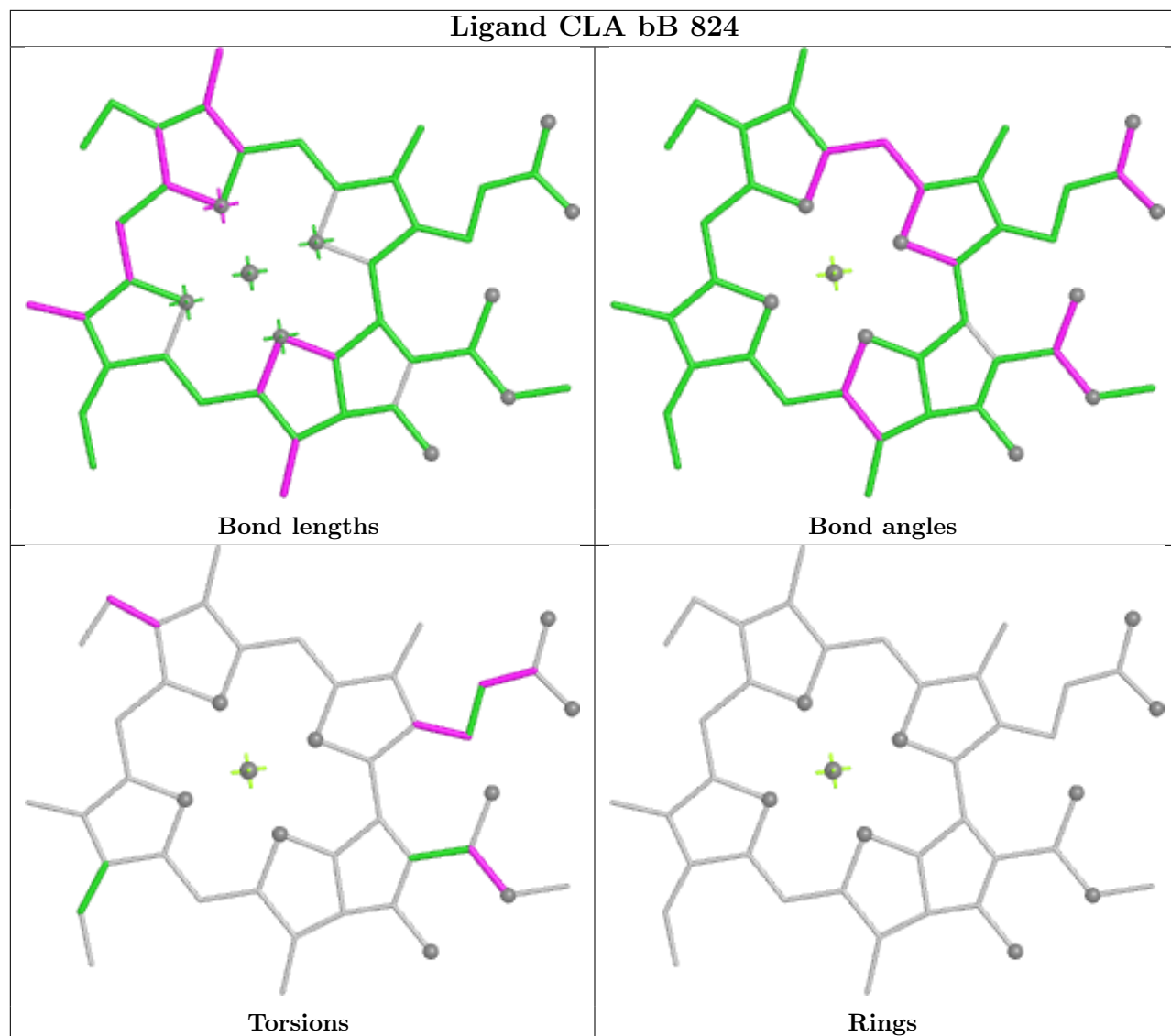




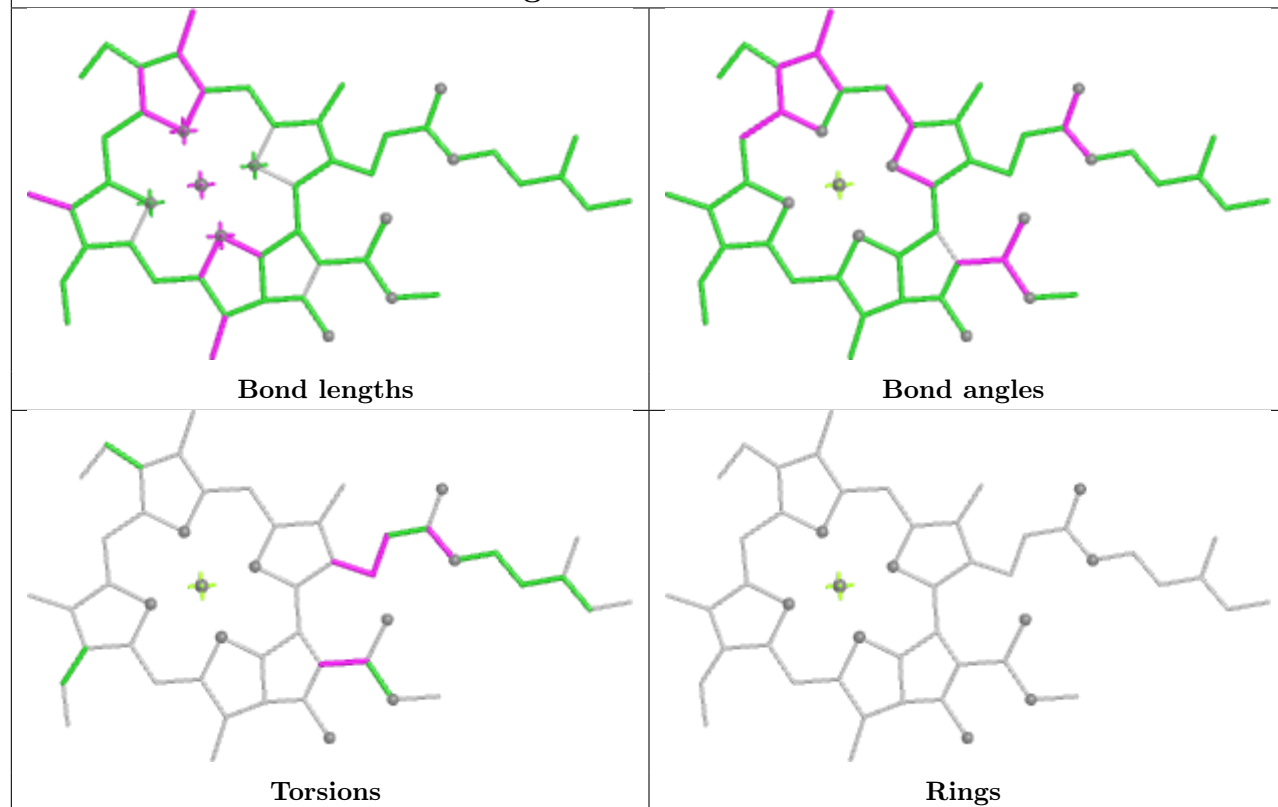
Ligand CLA bB 835



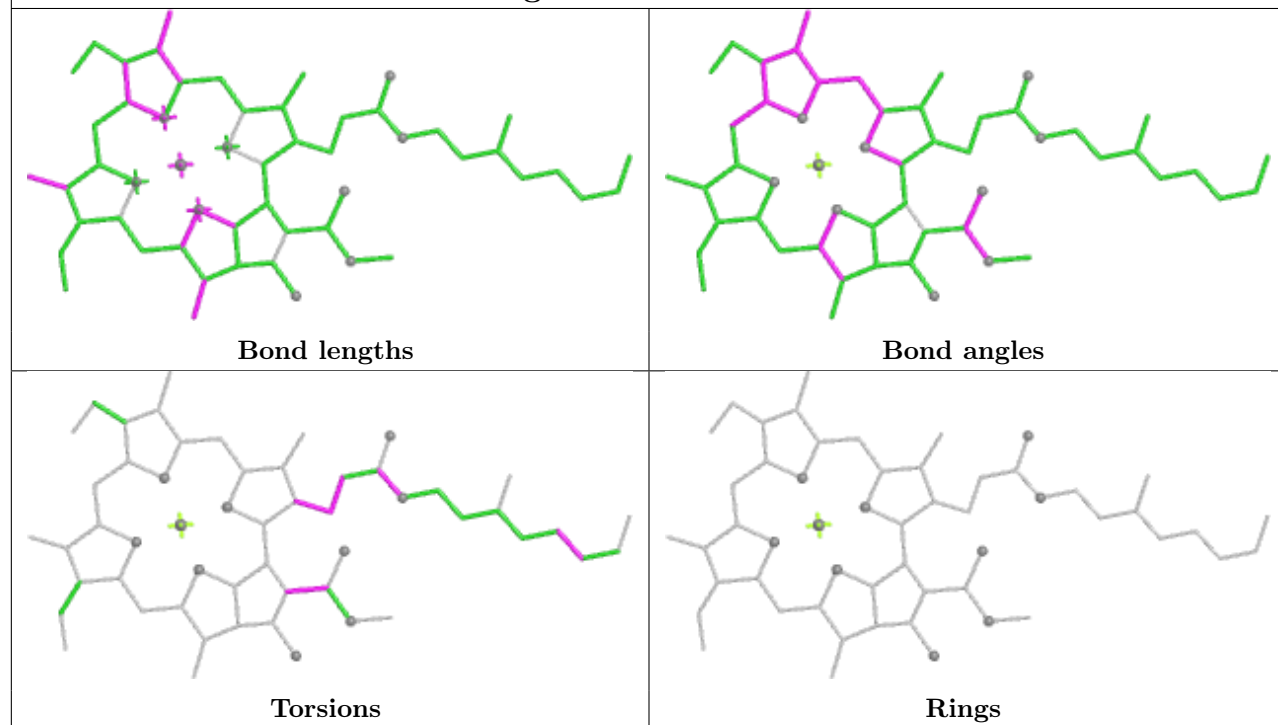
Ligand CLA bB 824



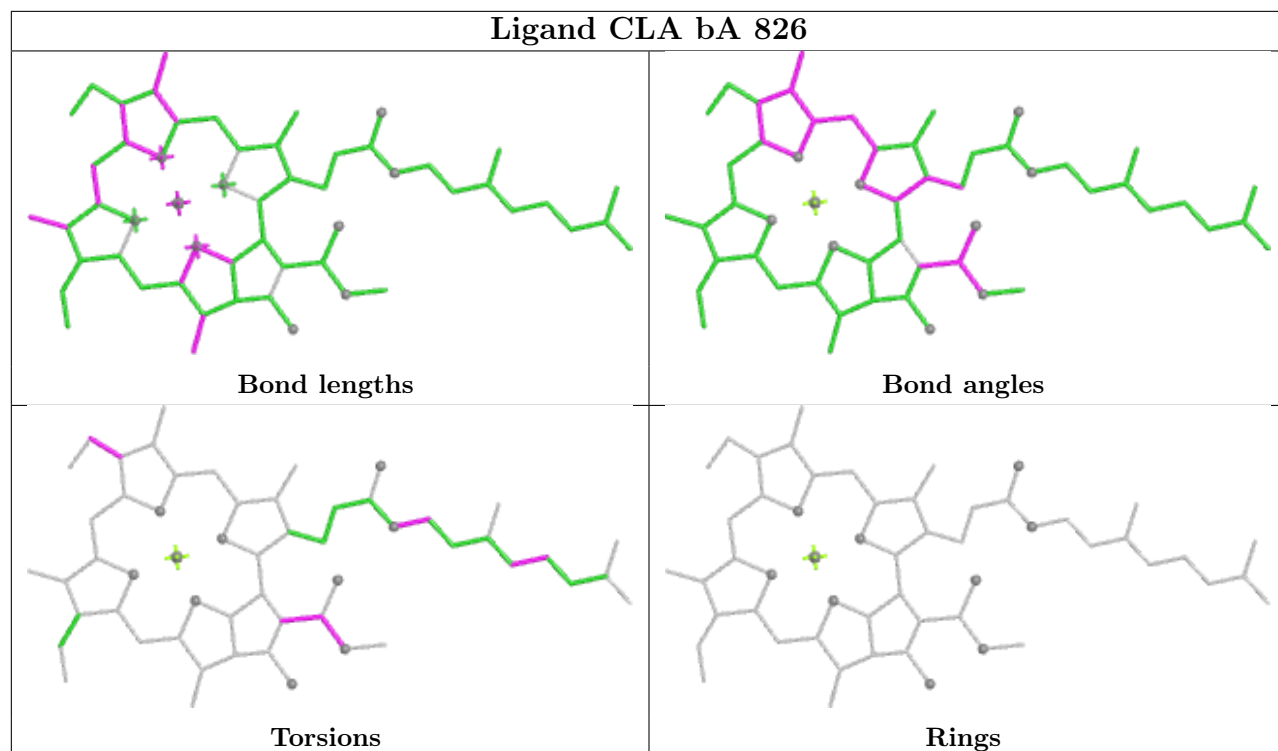
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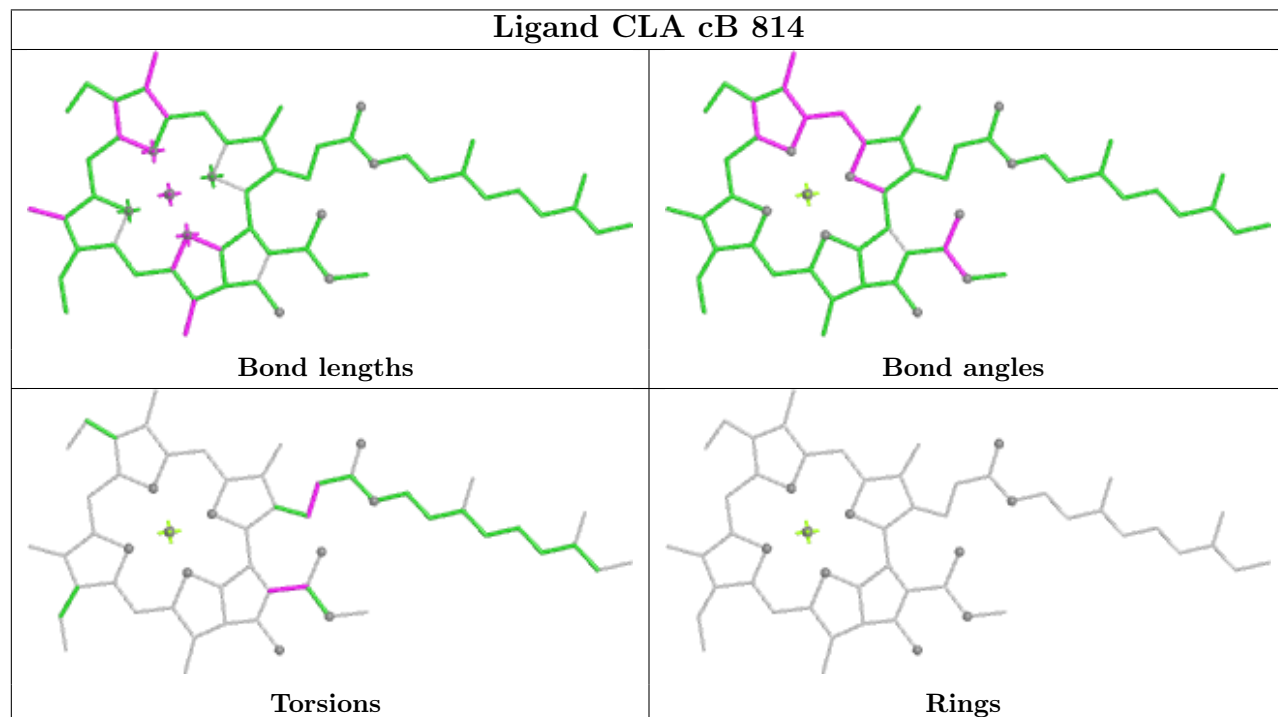
Ligand CLA cA 818



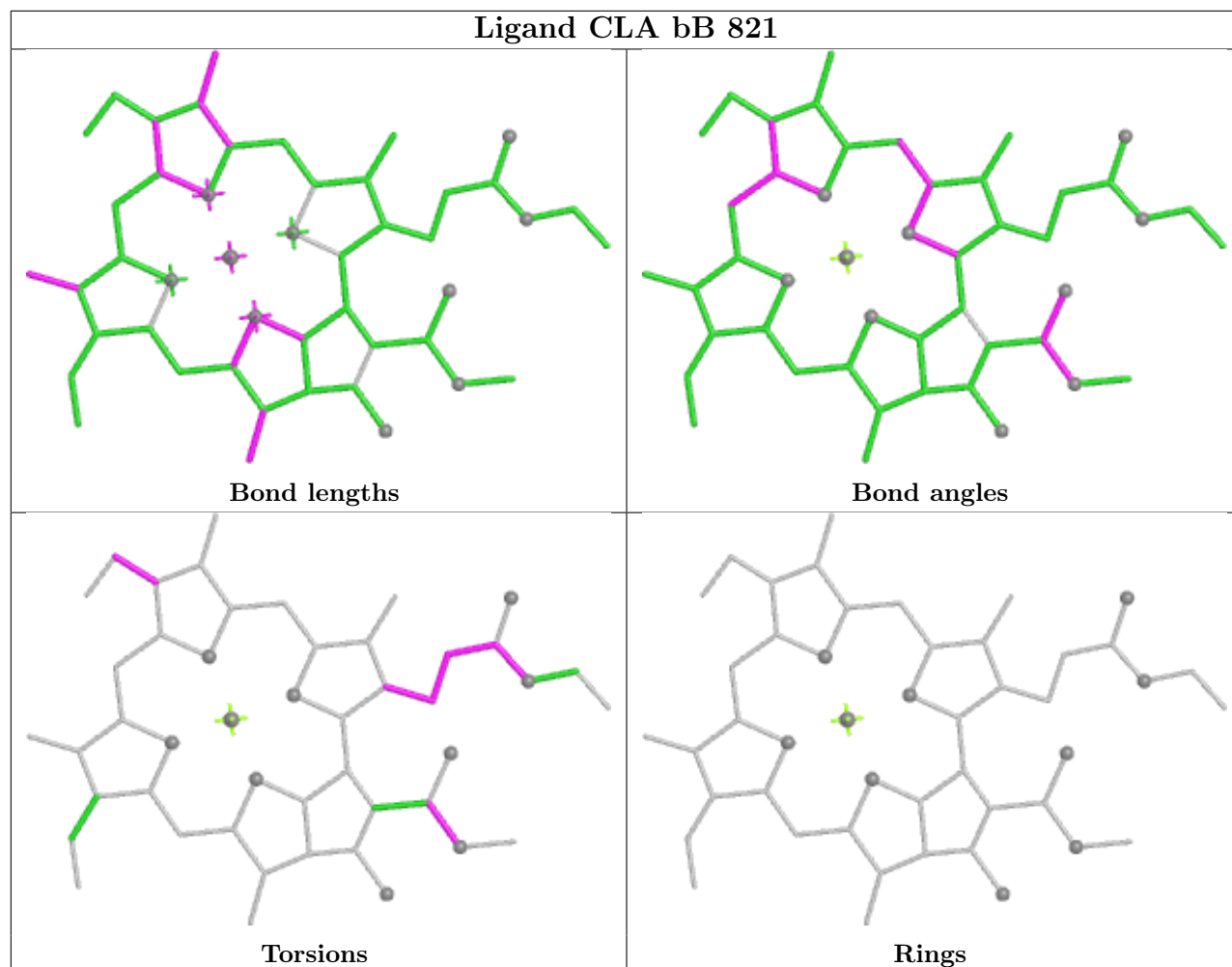
Ligand CLA bA 826



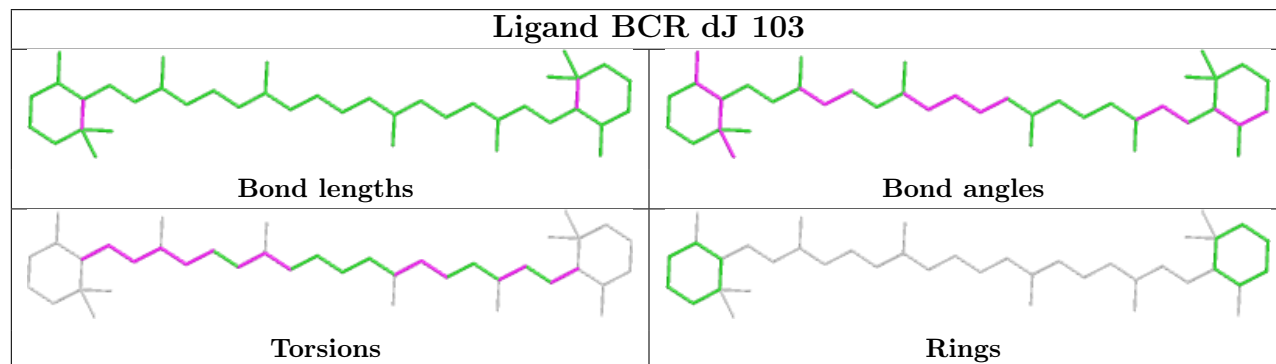
Ligand CLA cB 814

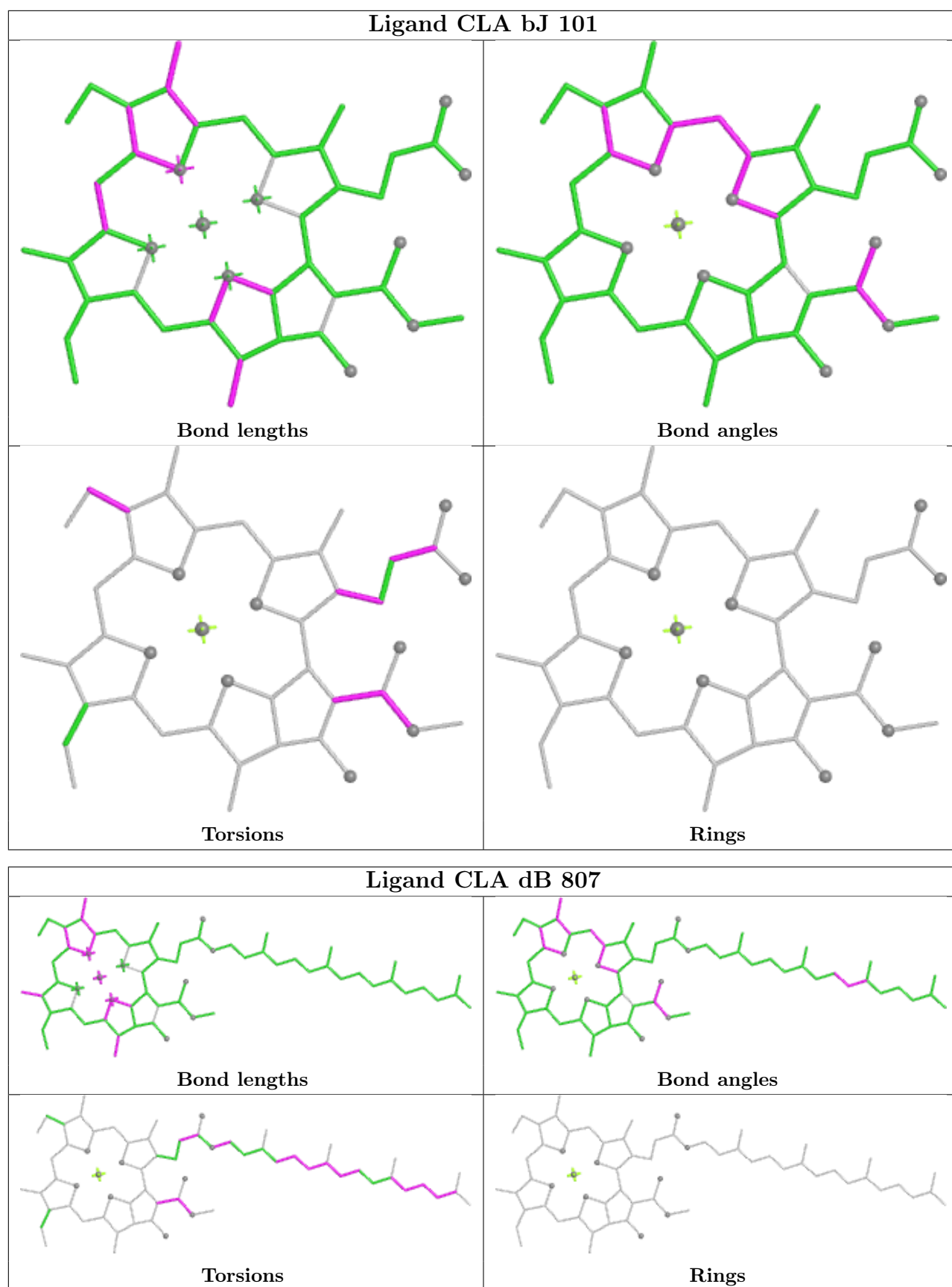


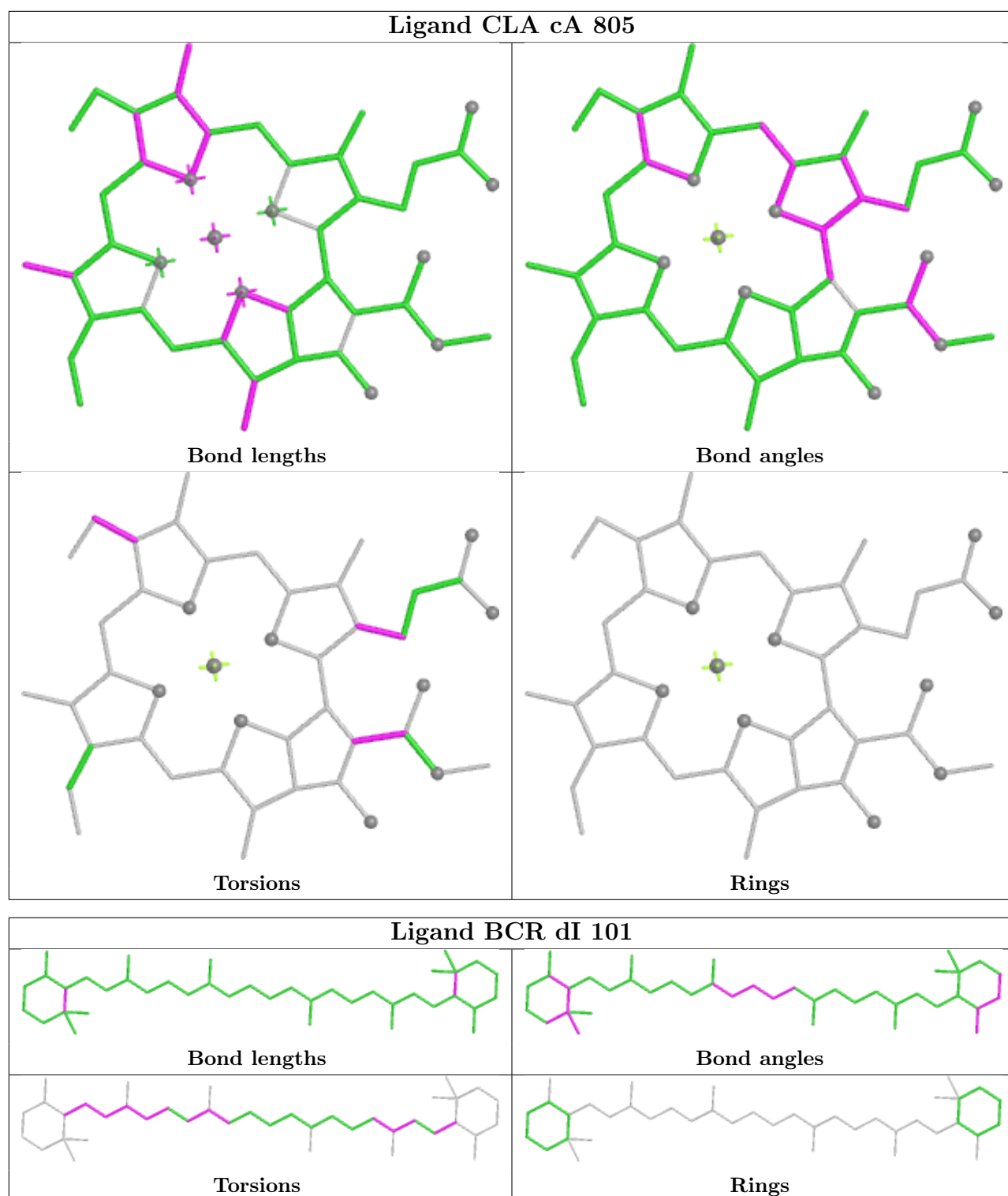
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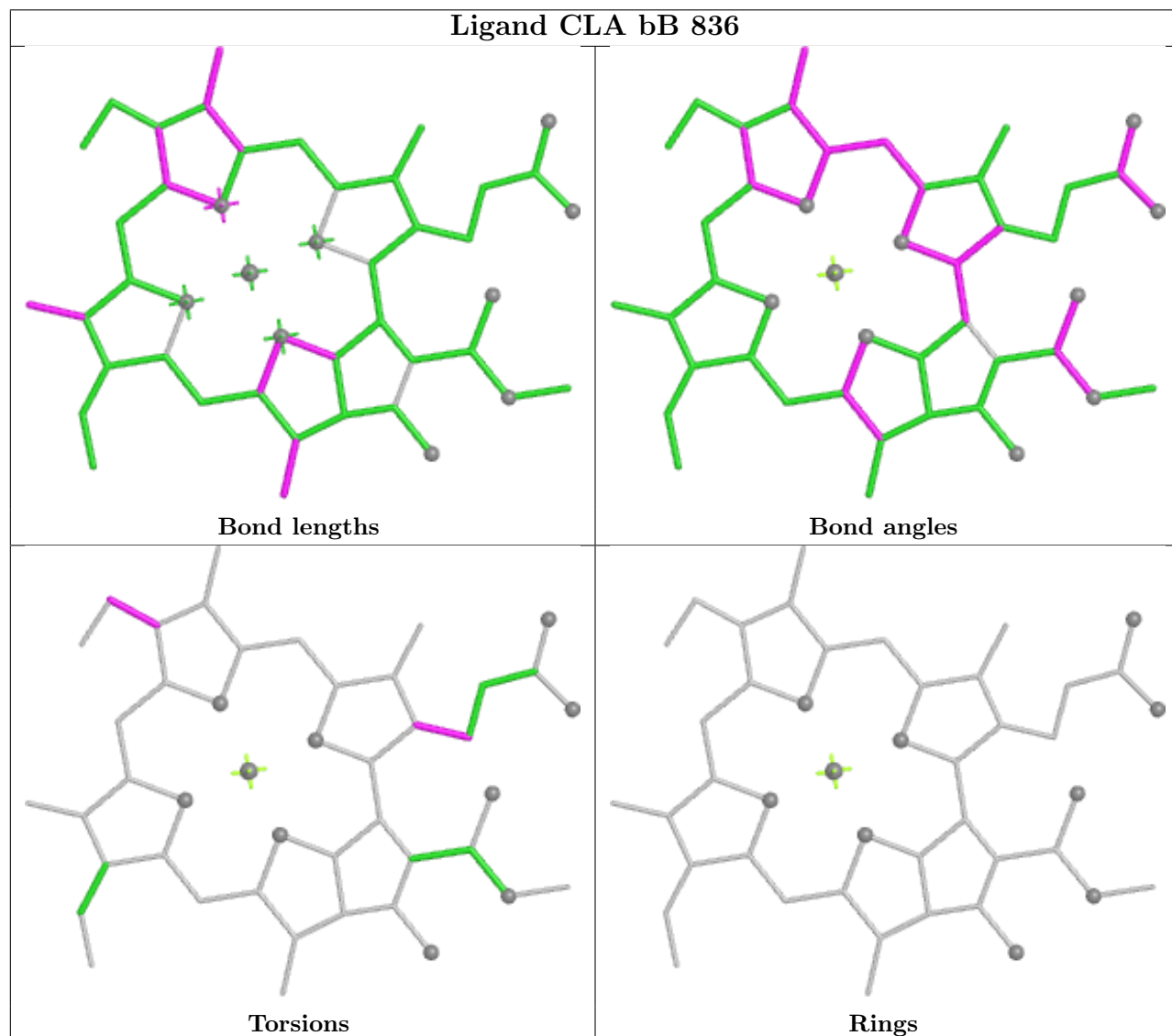
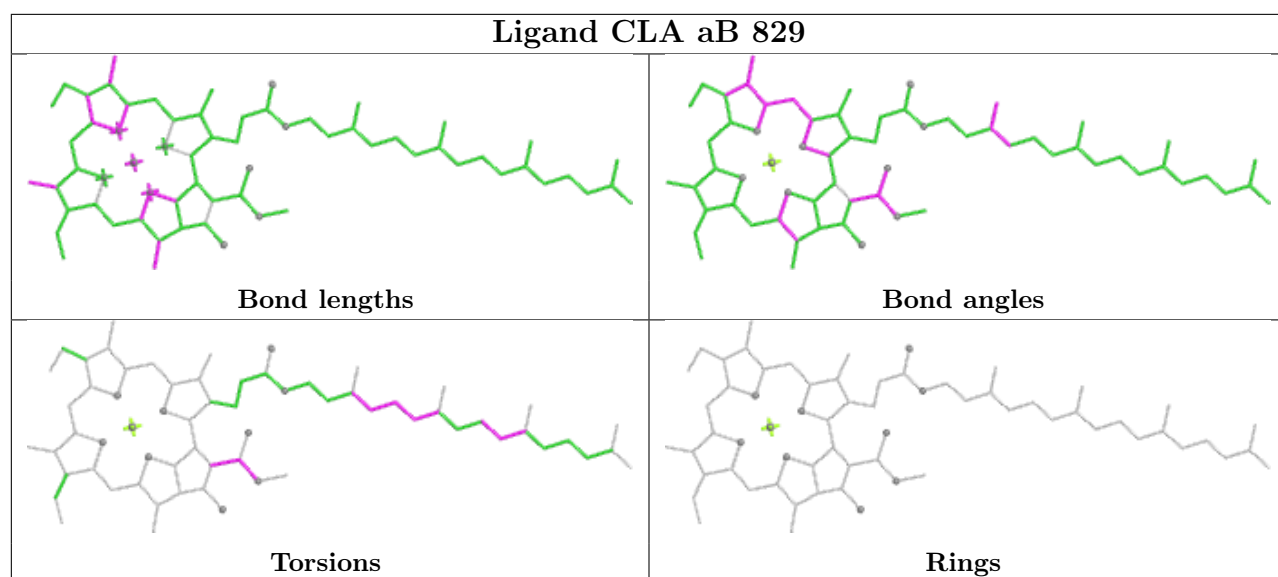


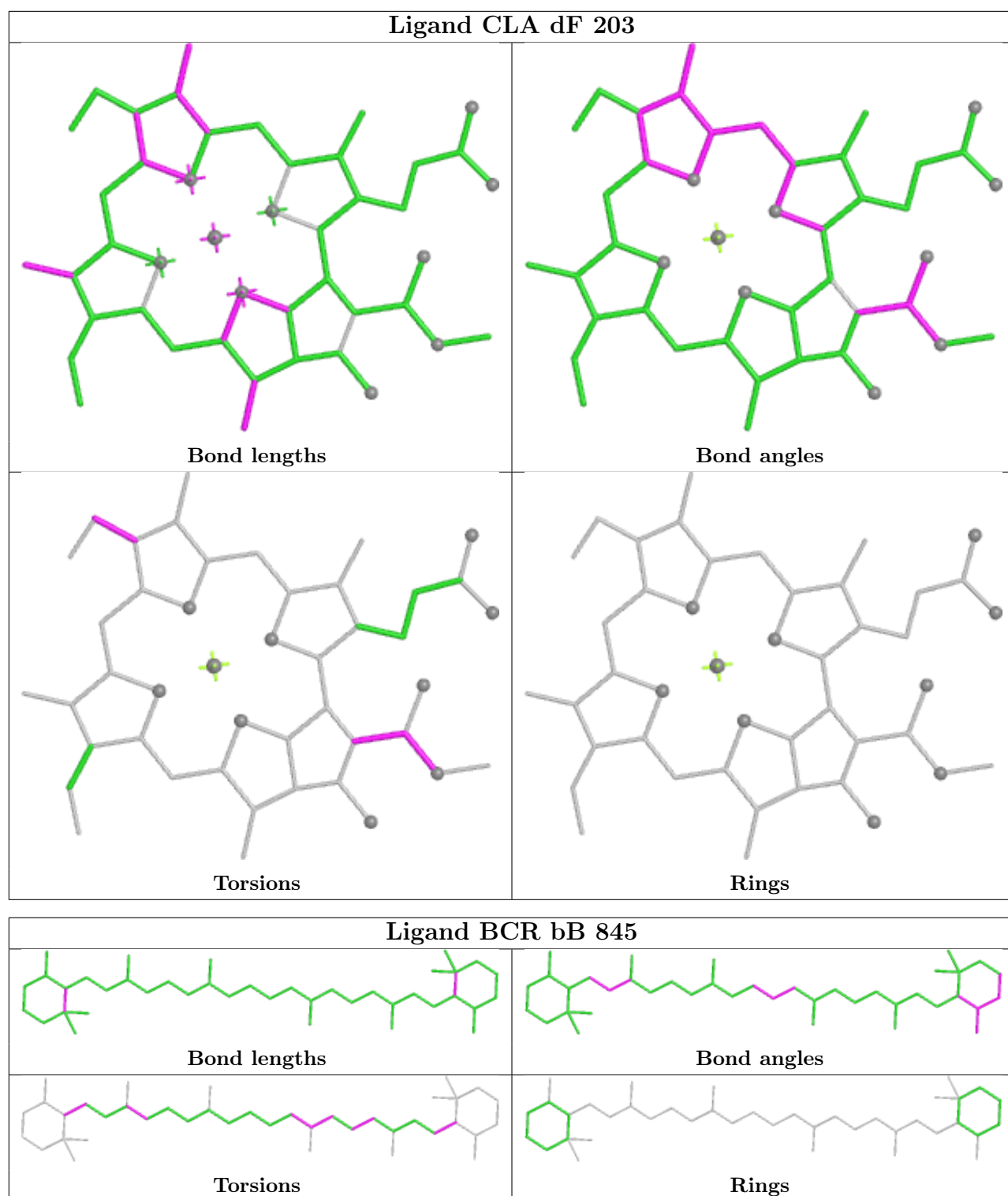
Ligand BCR dJ 103

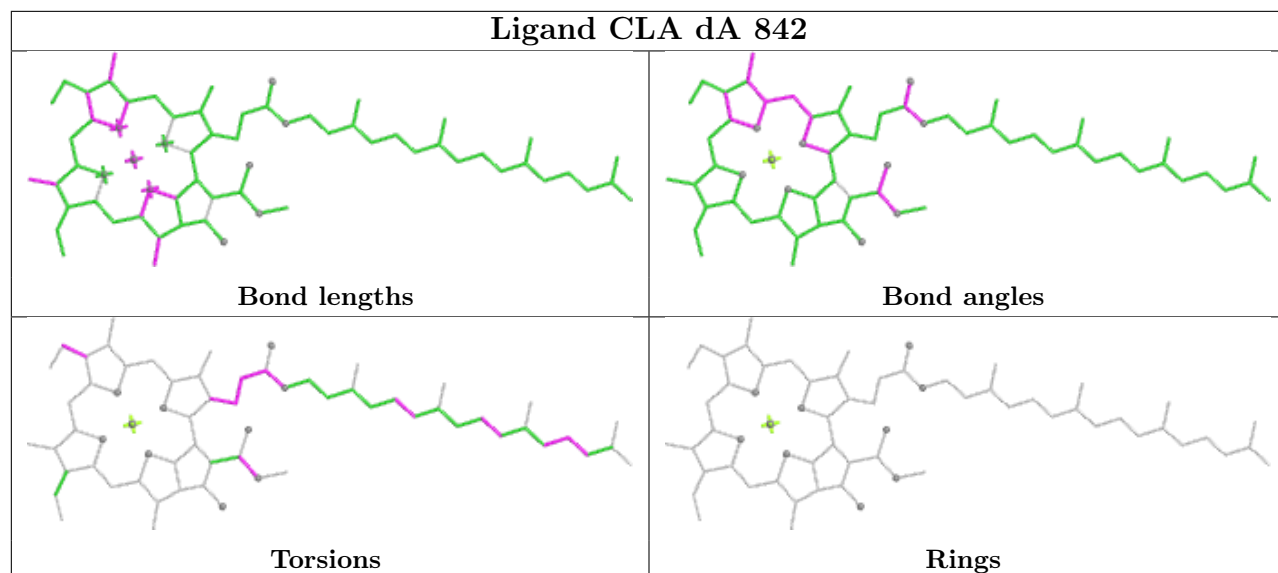
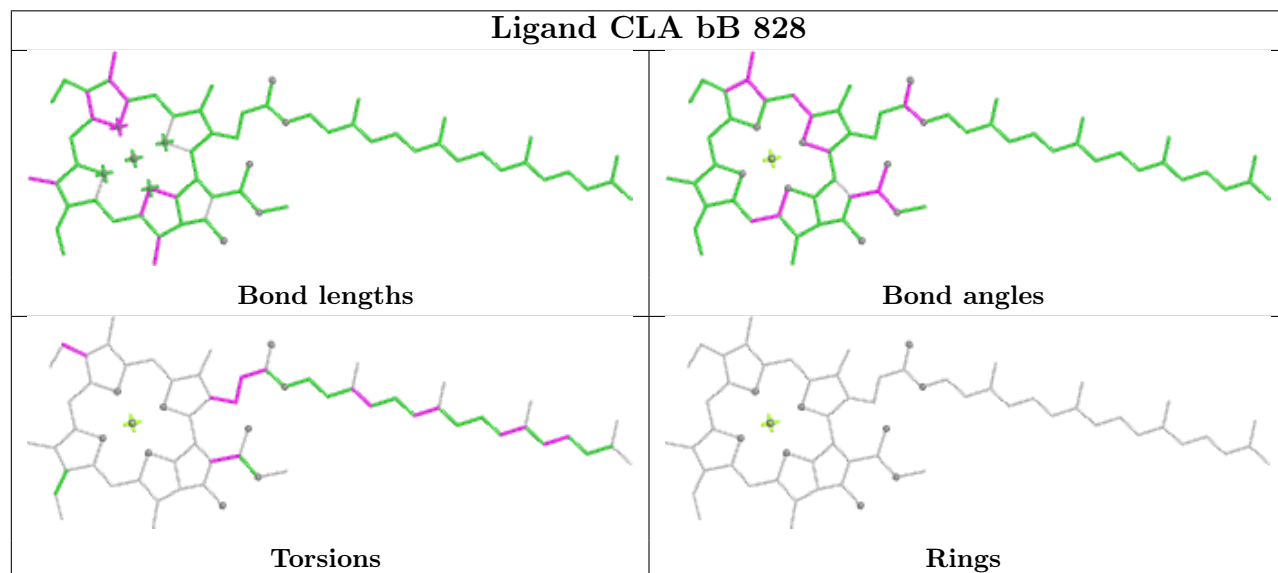
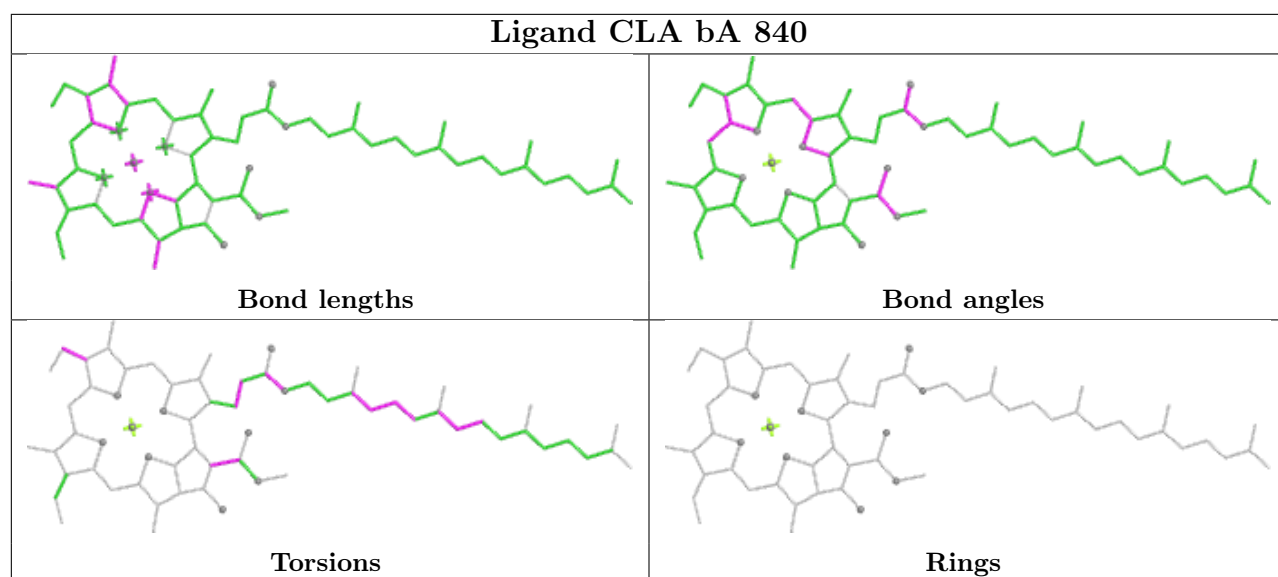


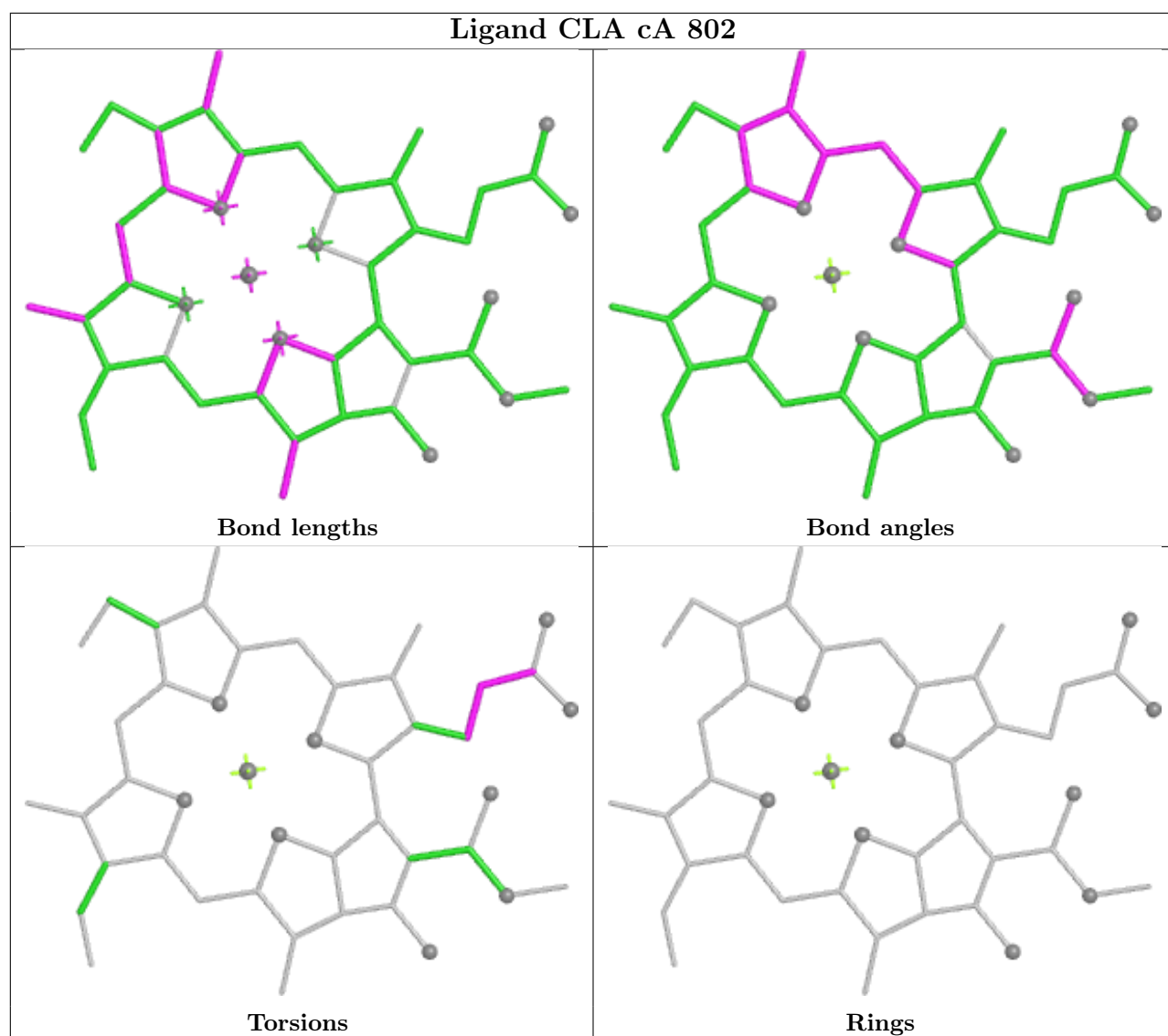


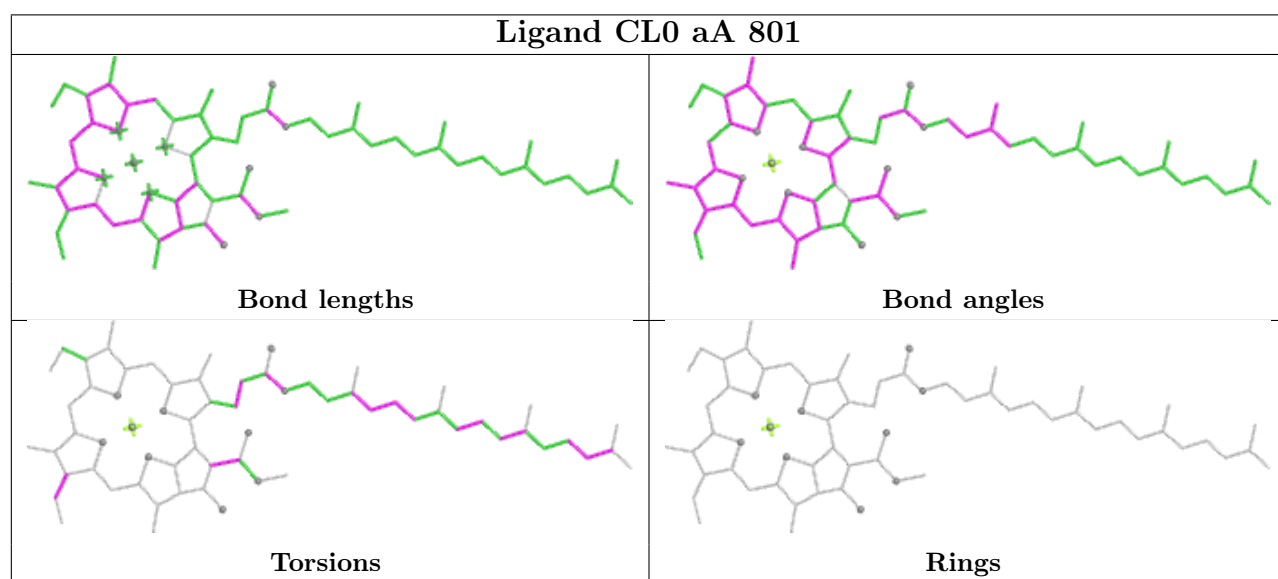
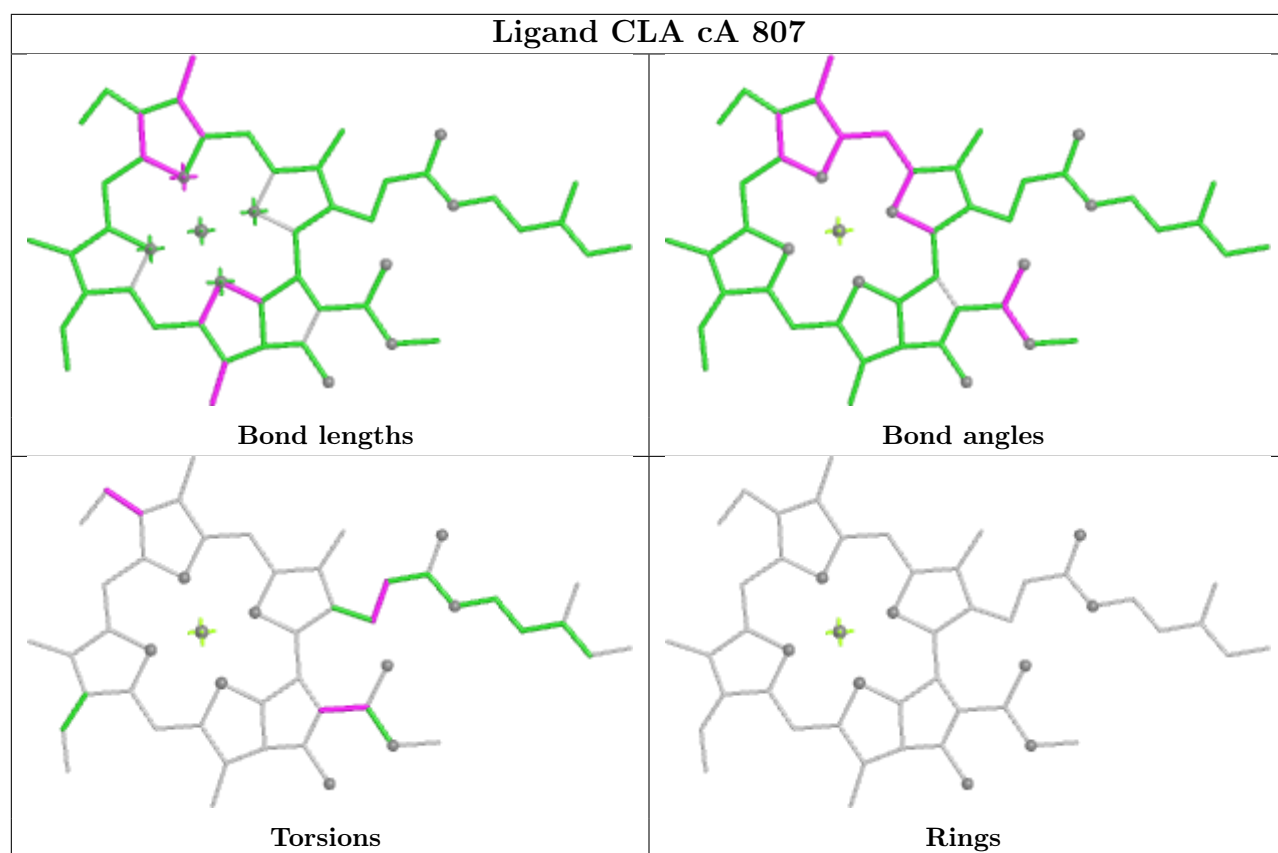


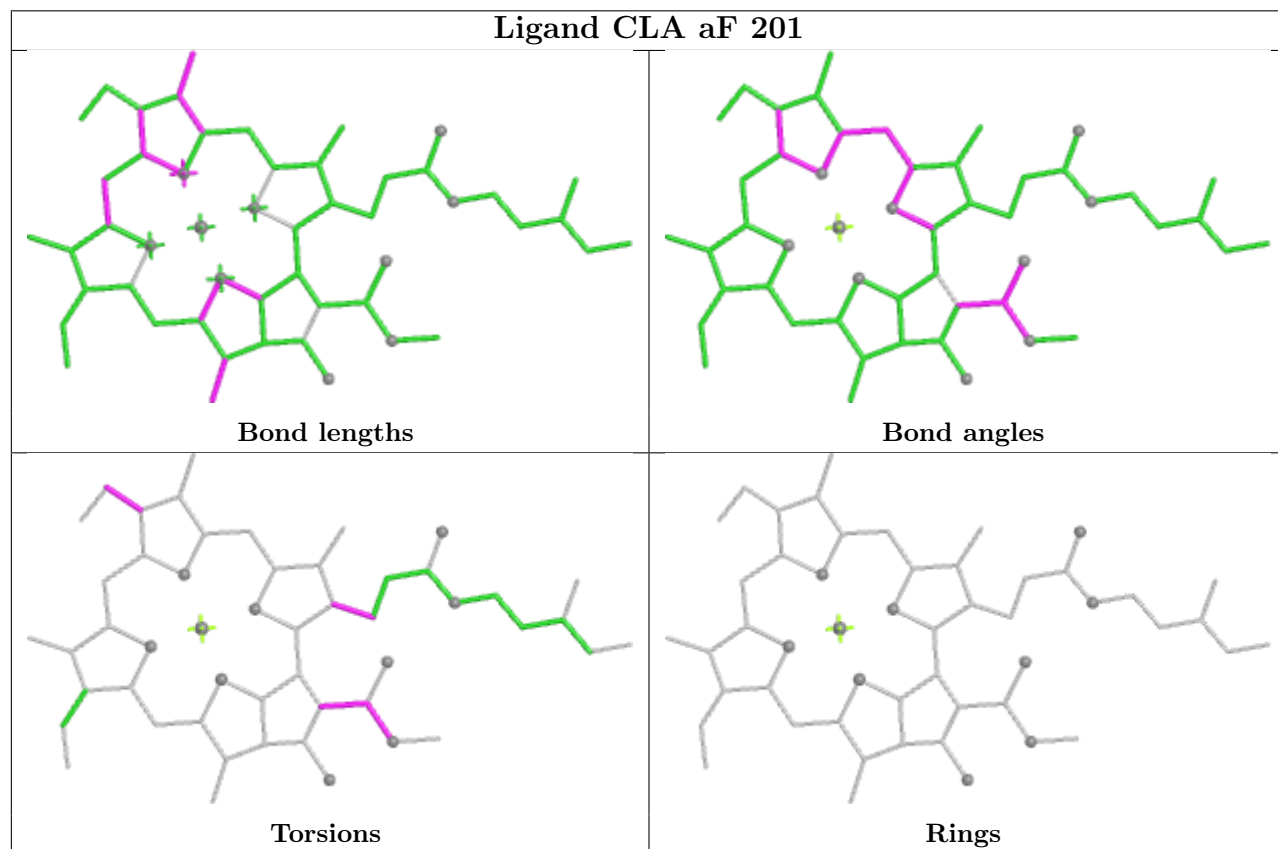
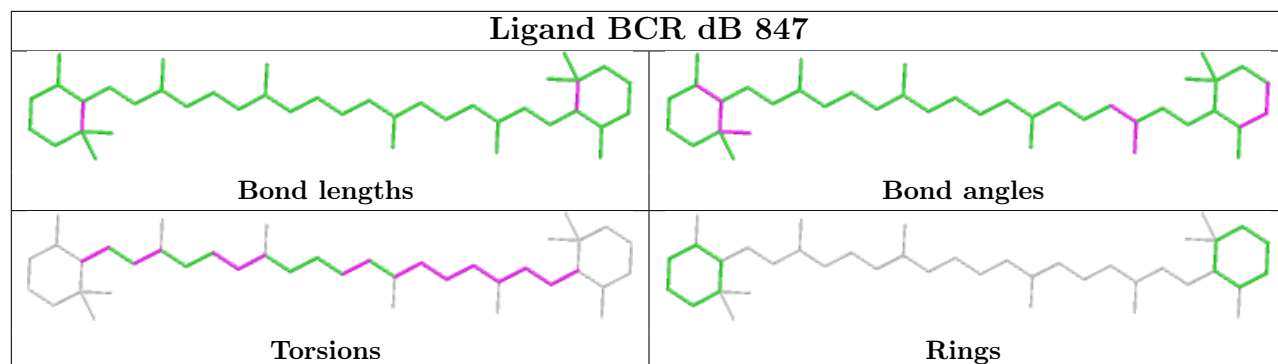


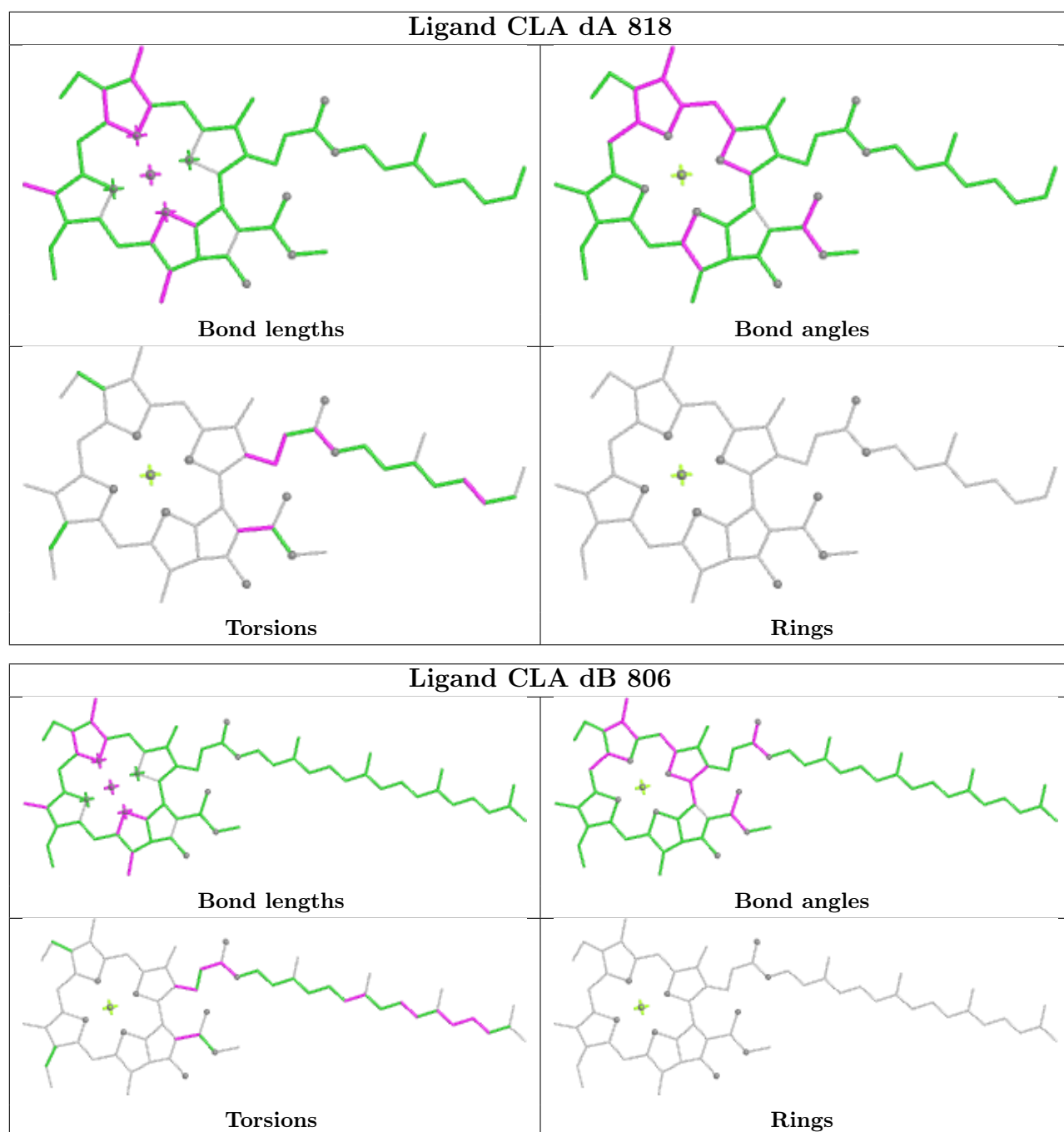


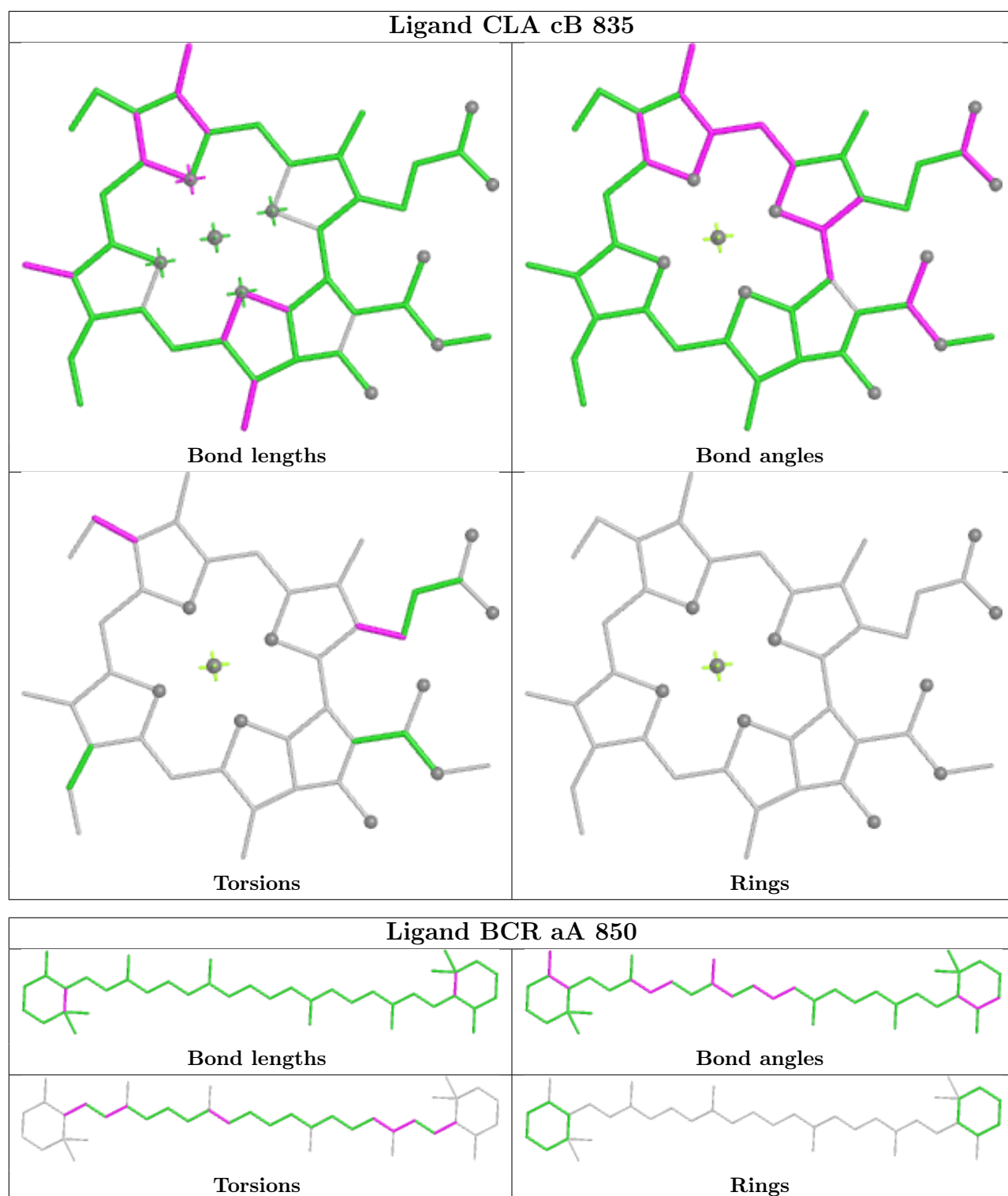


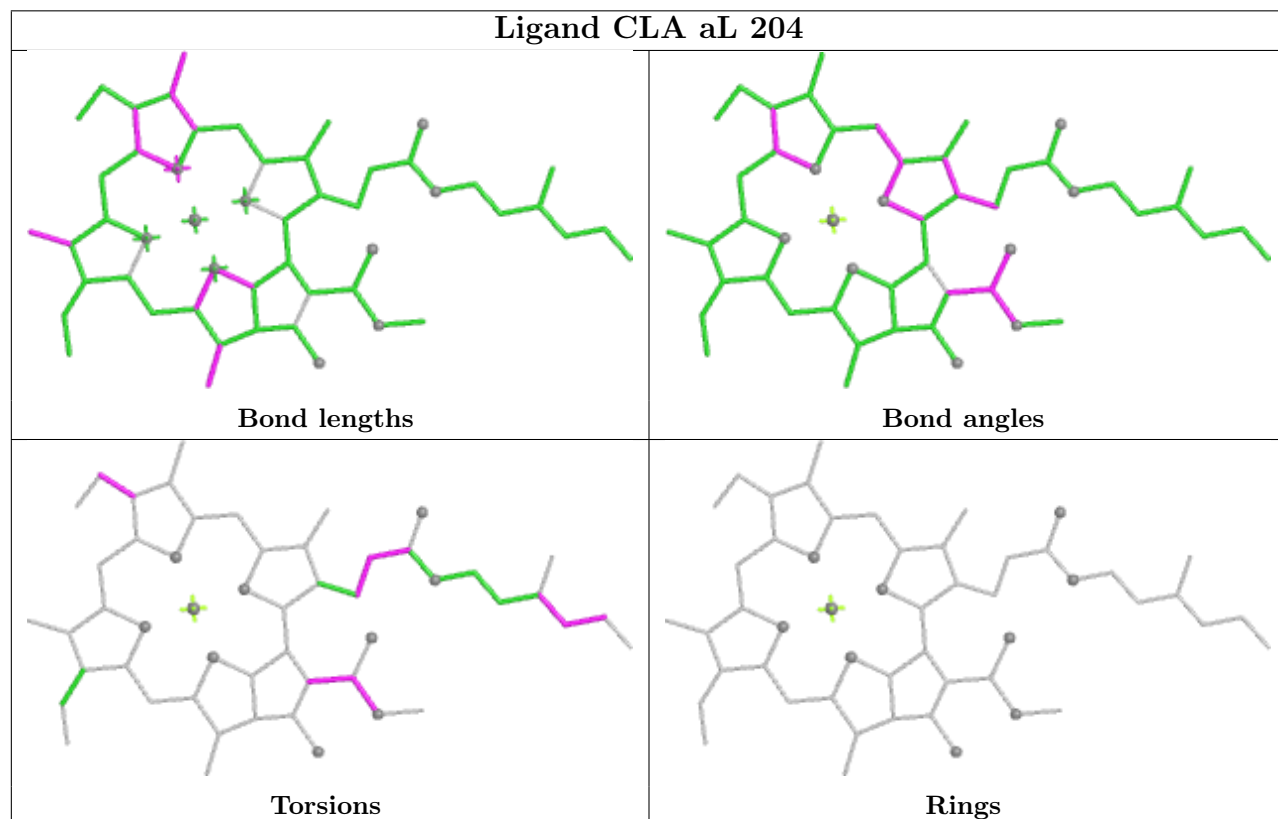
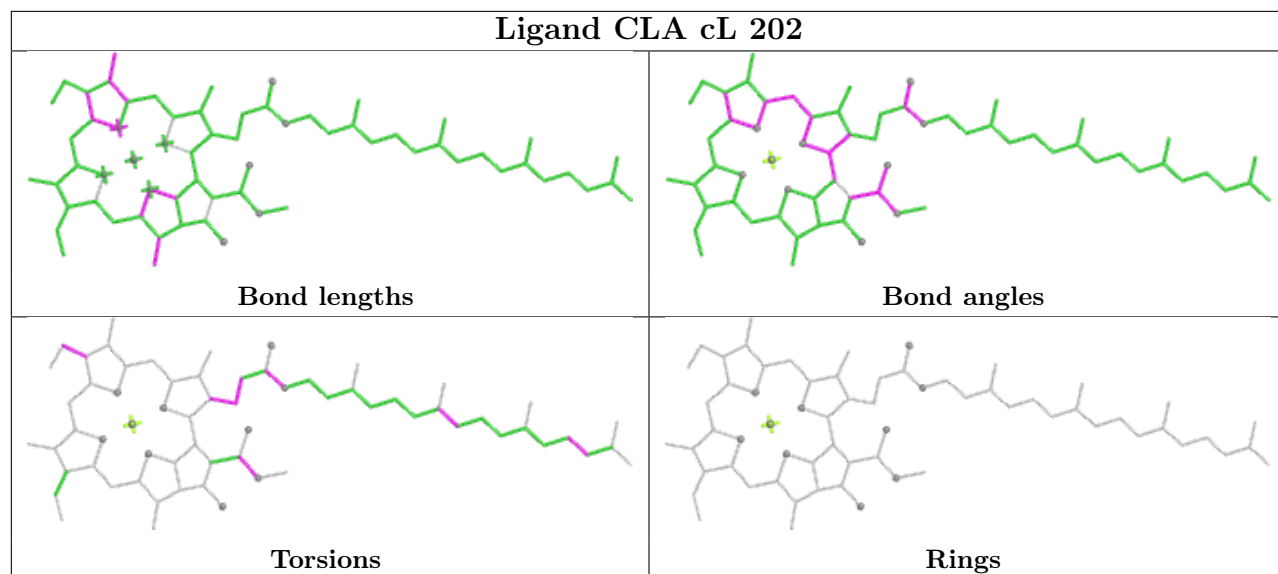


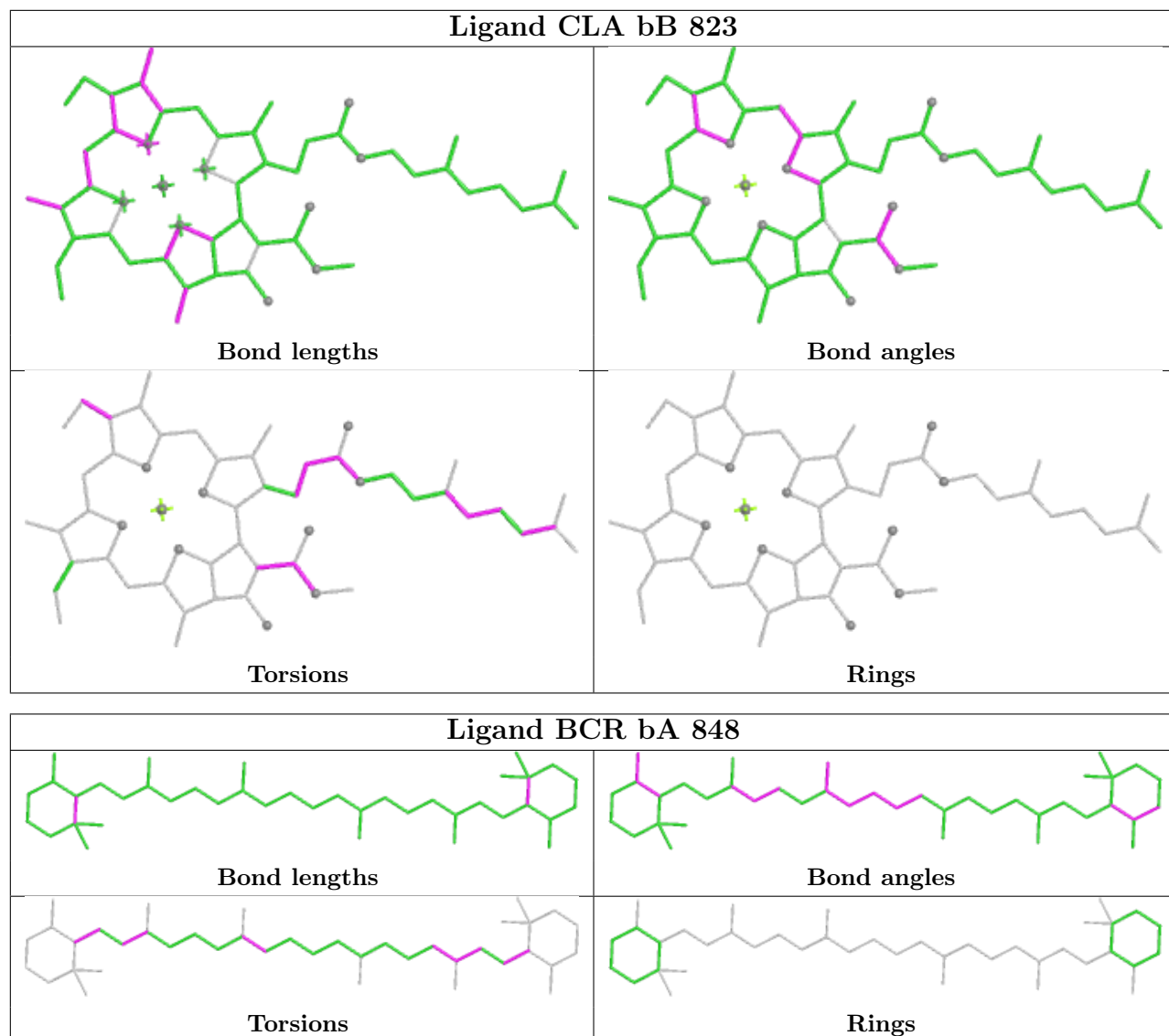


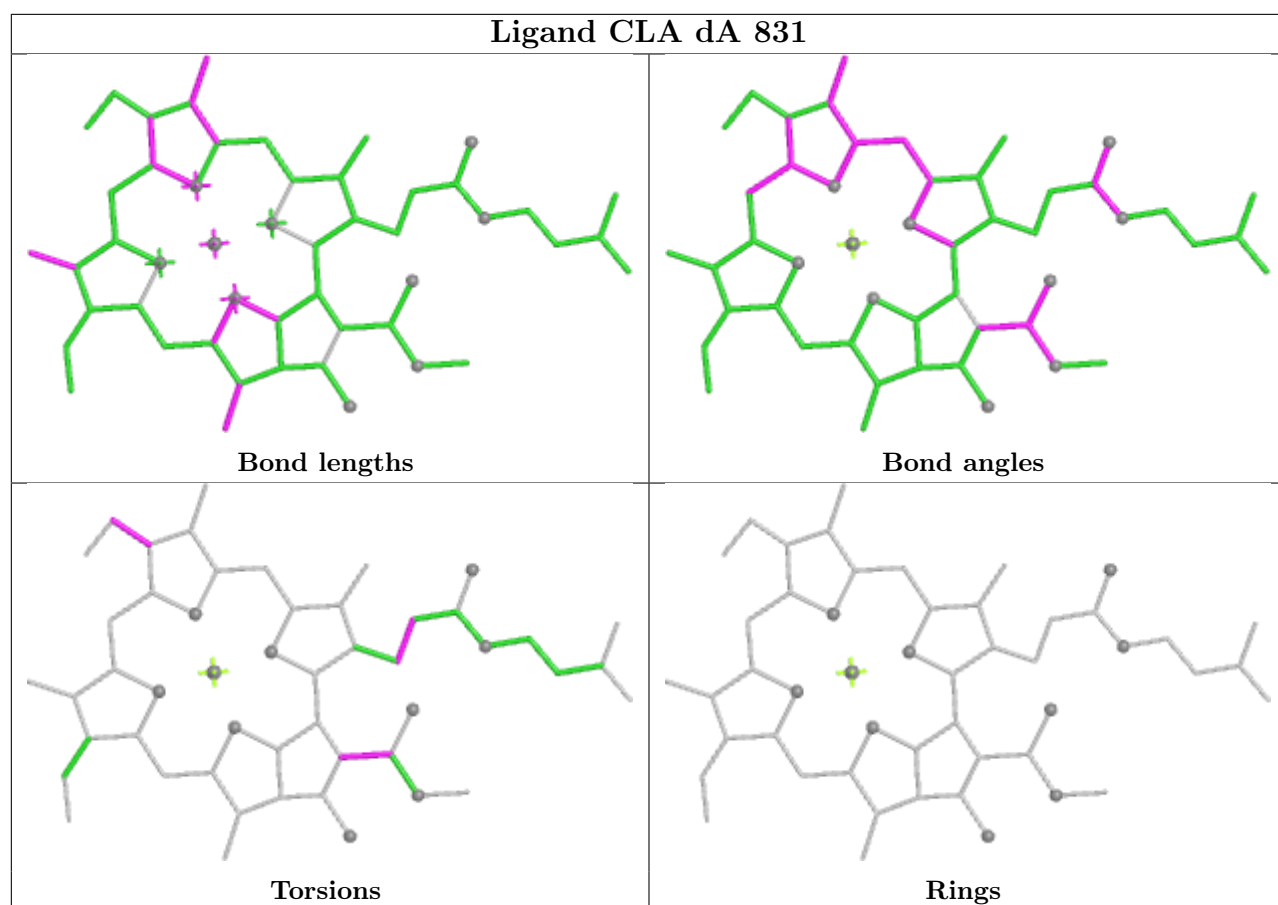


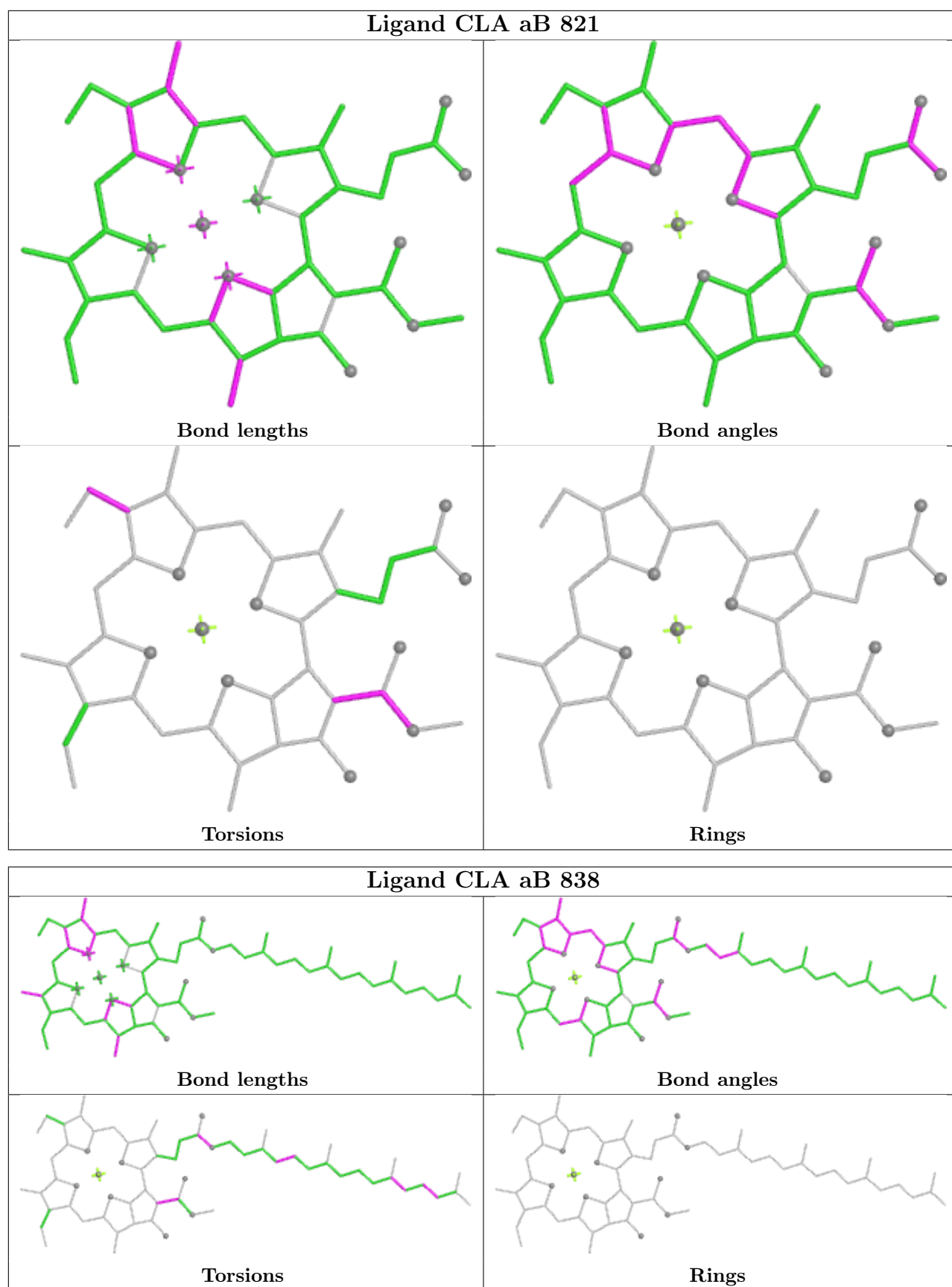


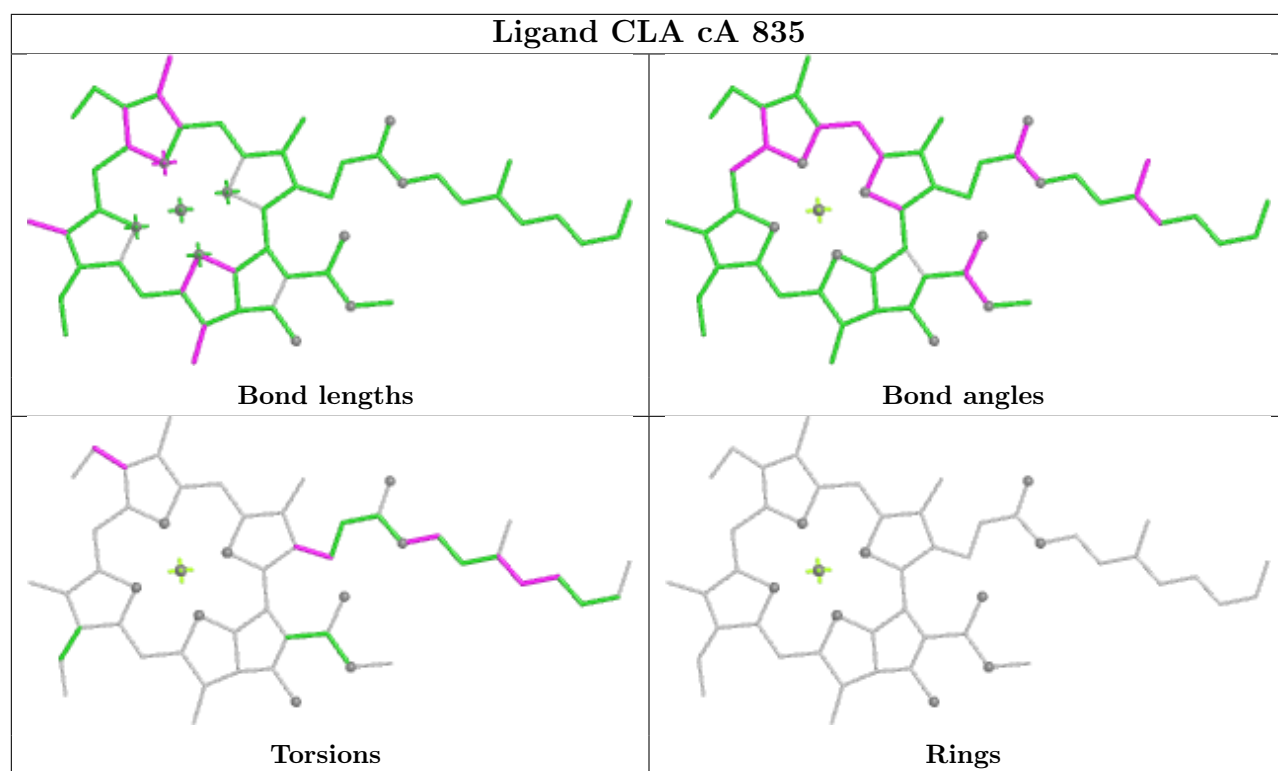




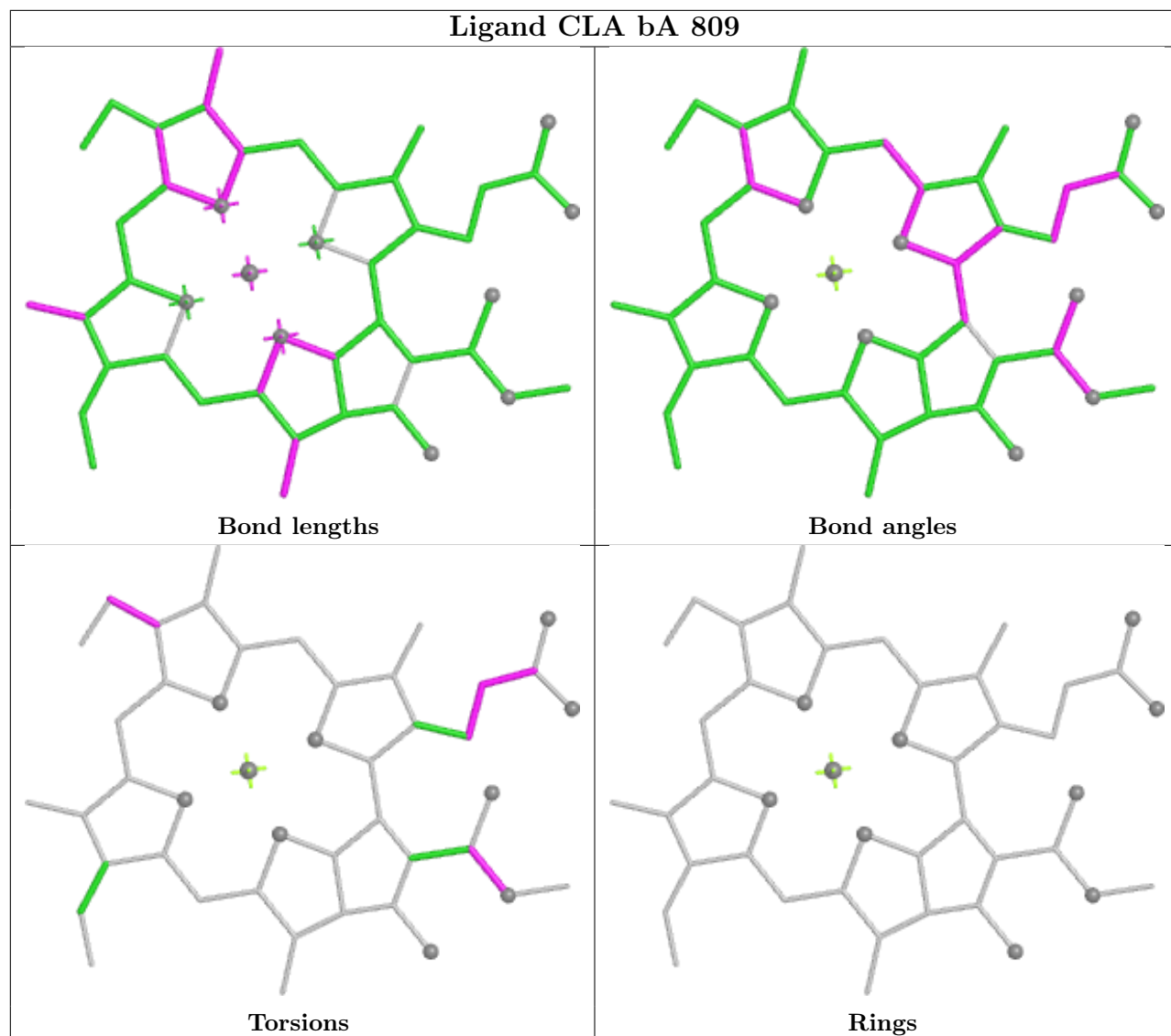




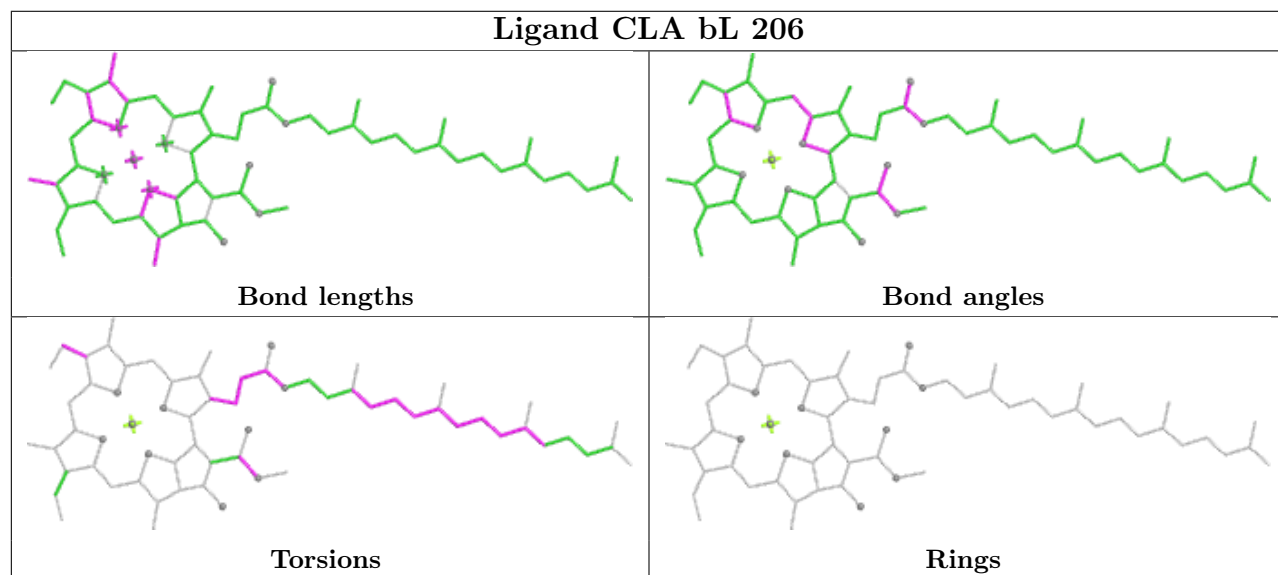




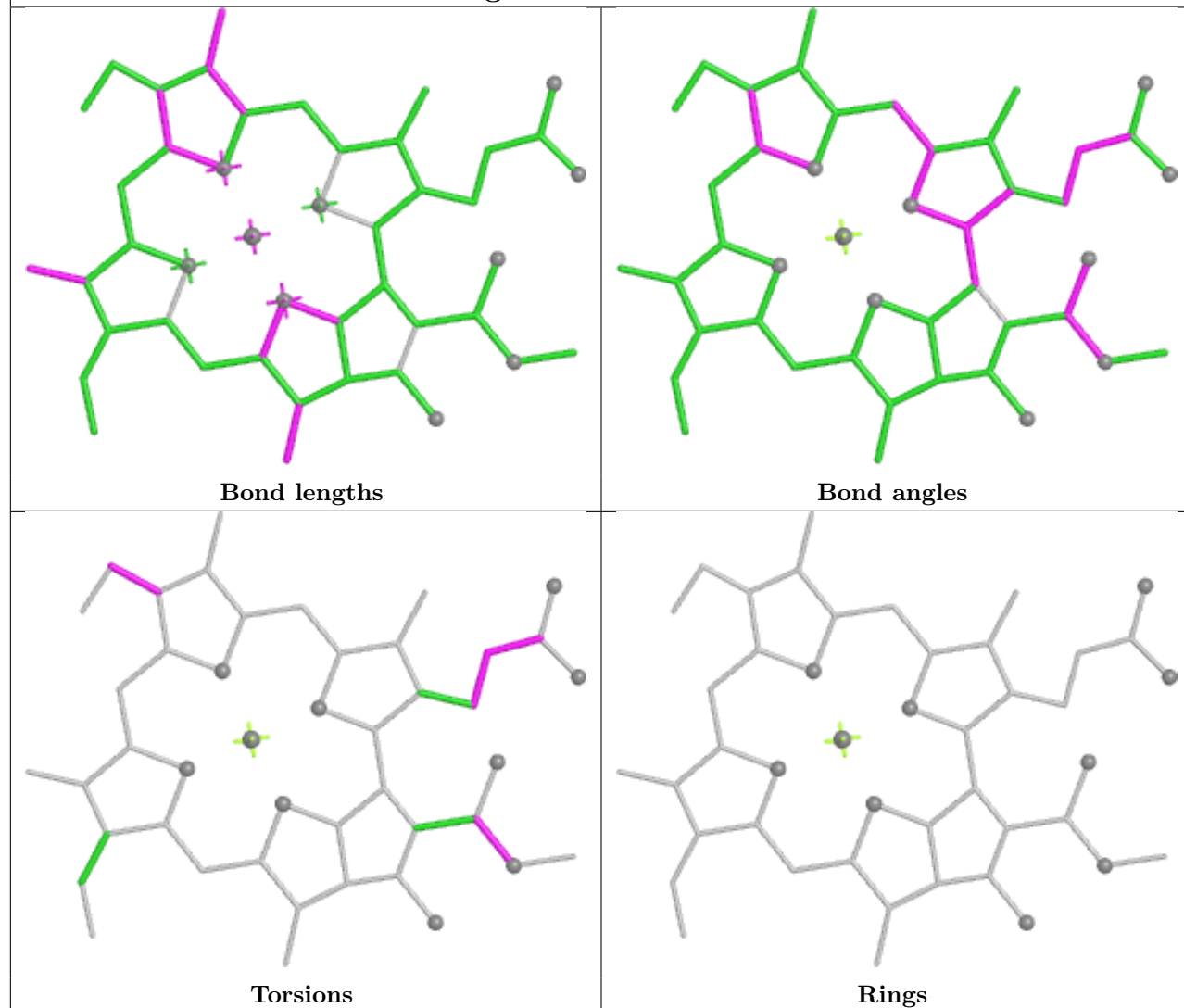
Ligand CLA bA 809



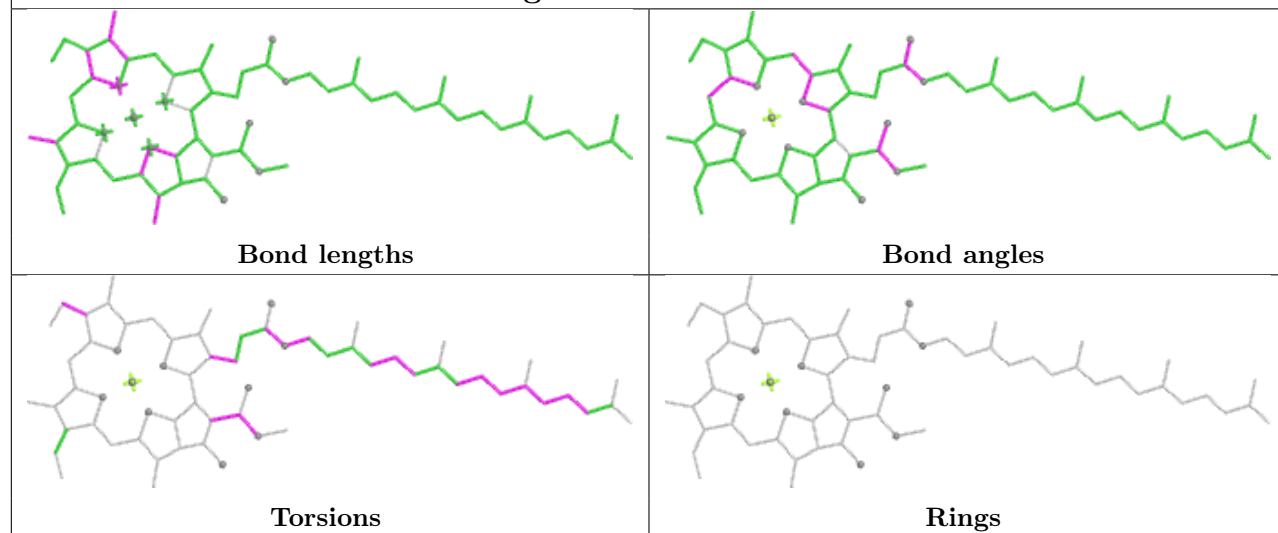
Ligand CLA bL 206

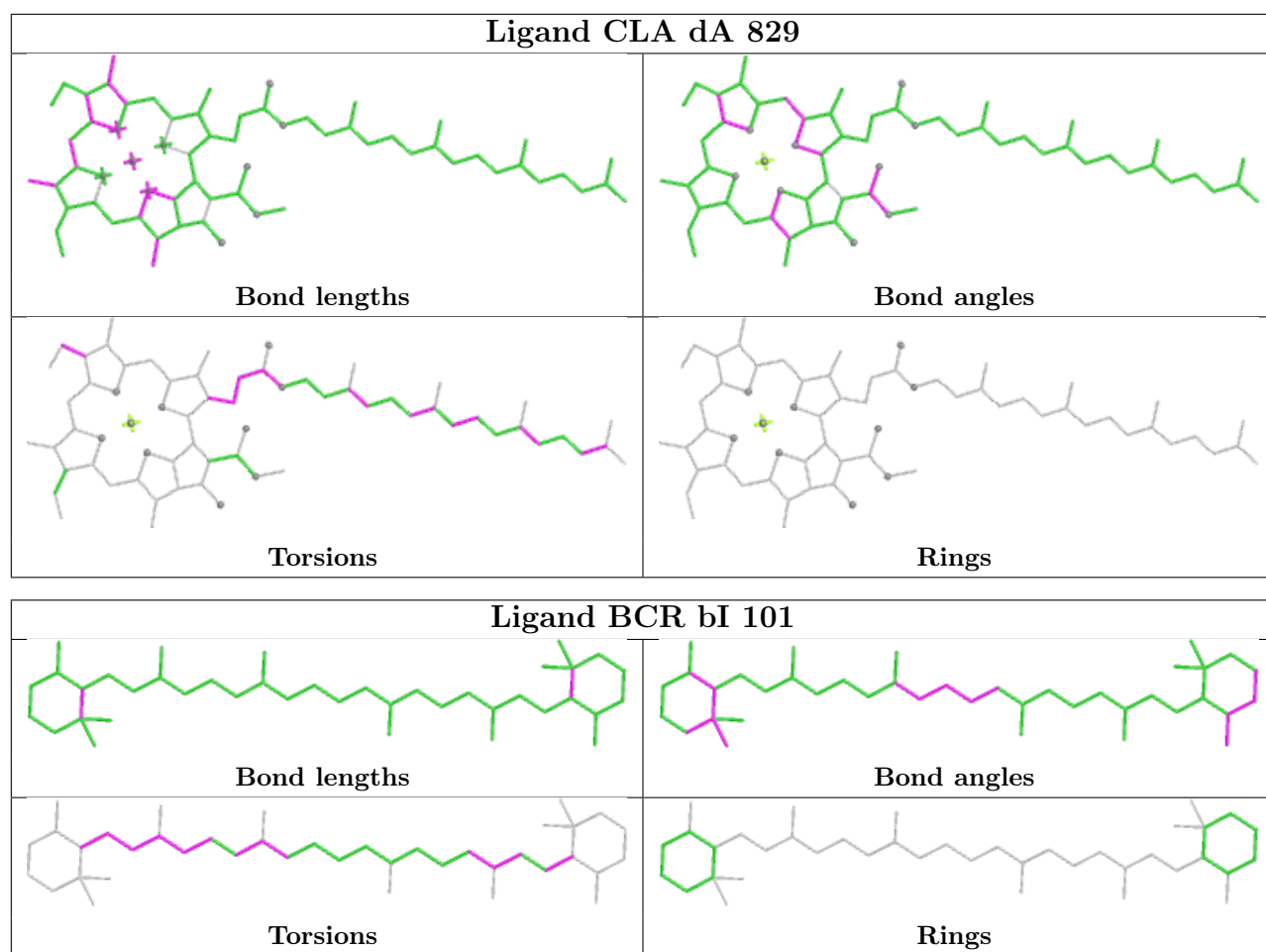


Ligand CLA cA 809

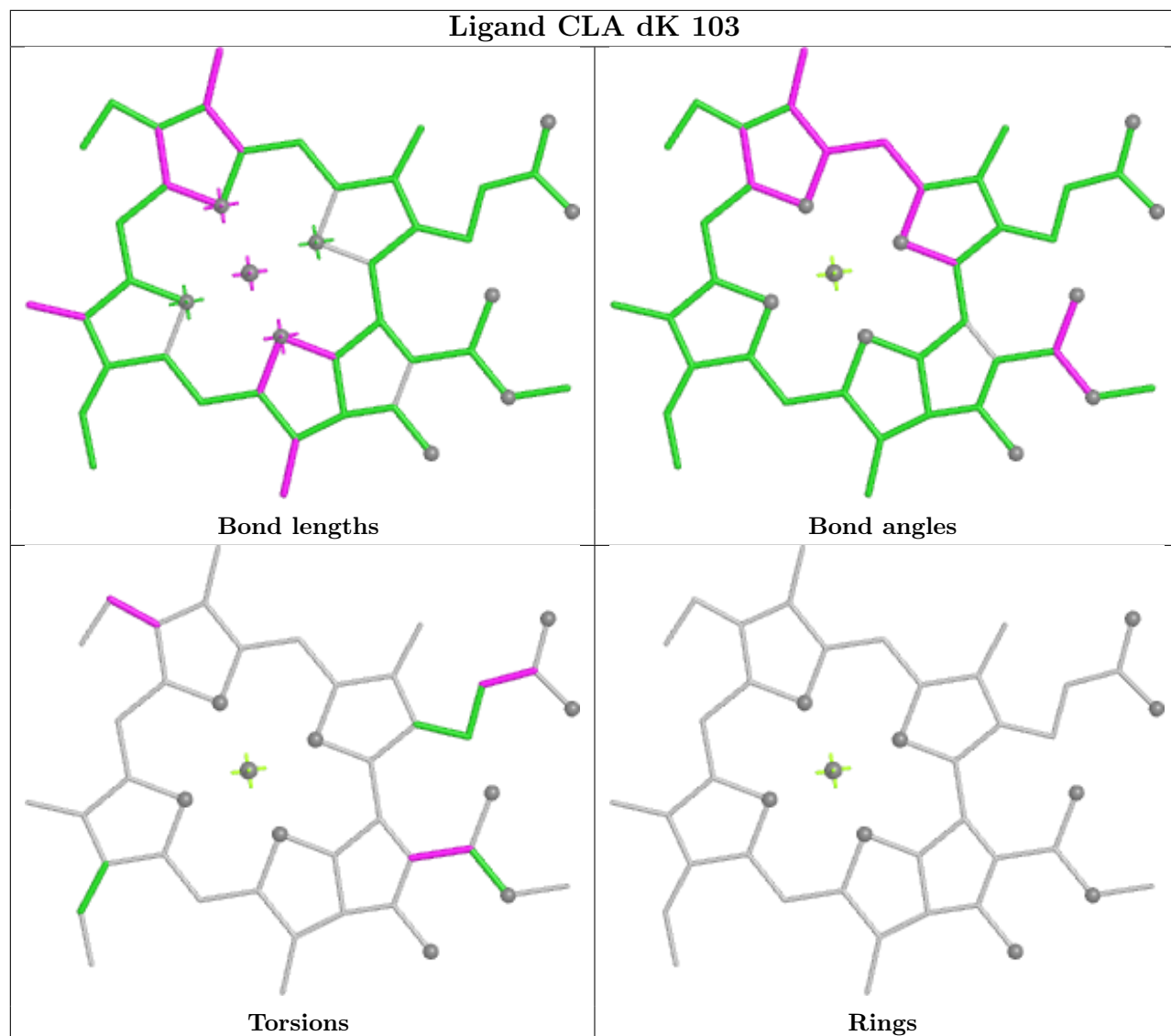


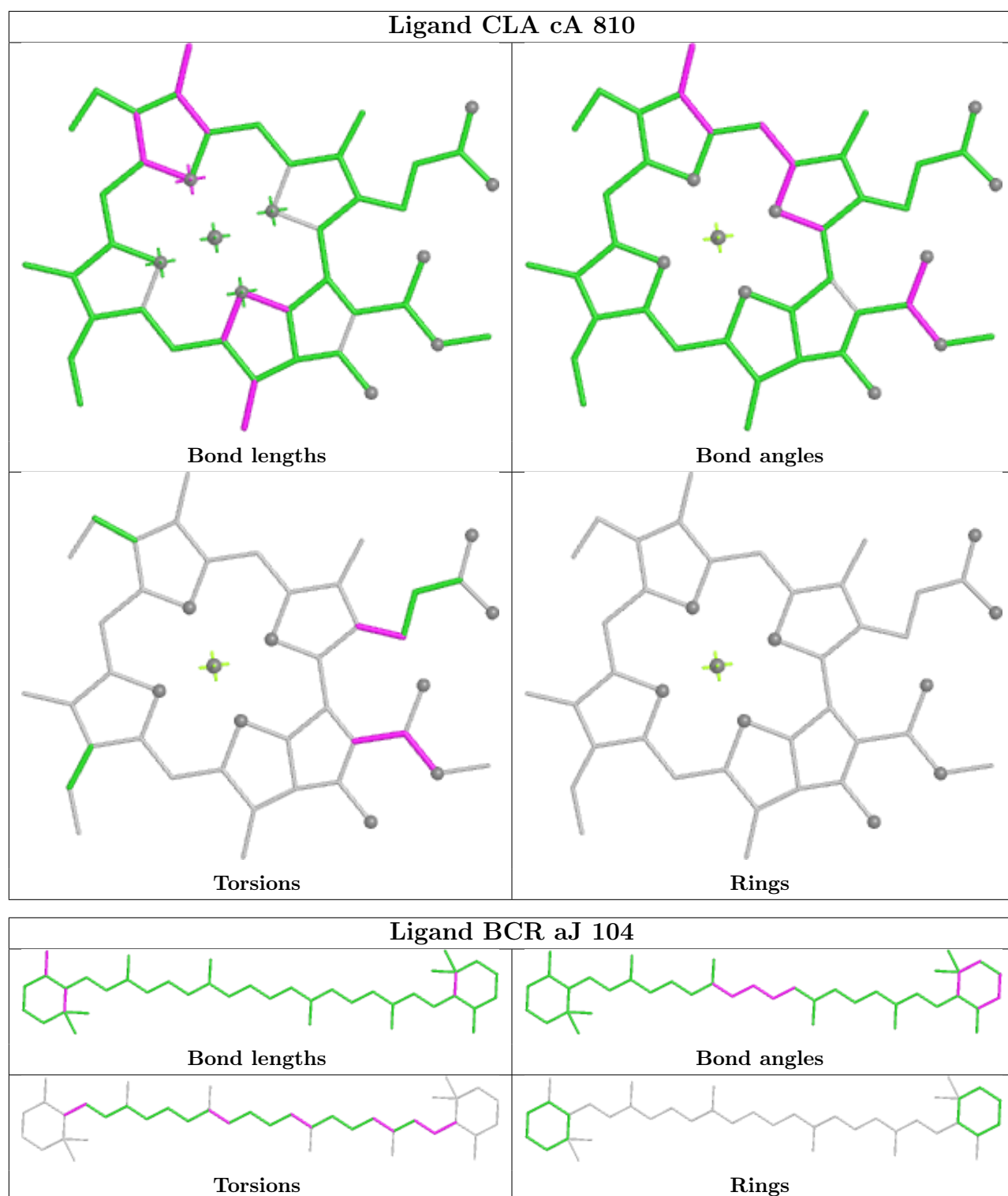
Ligand CLA aB 841

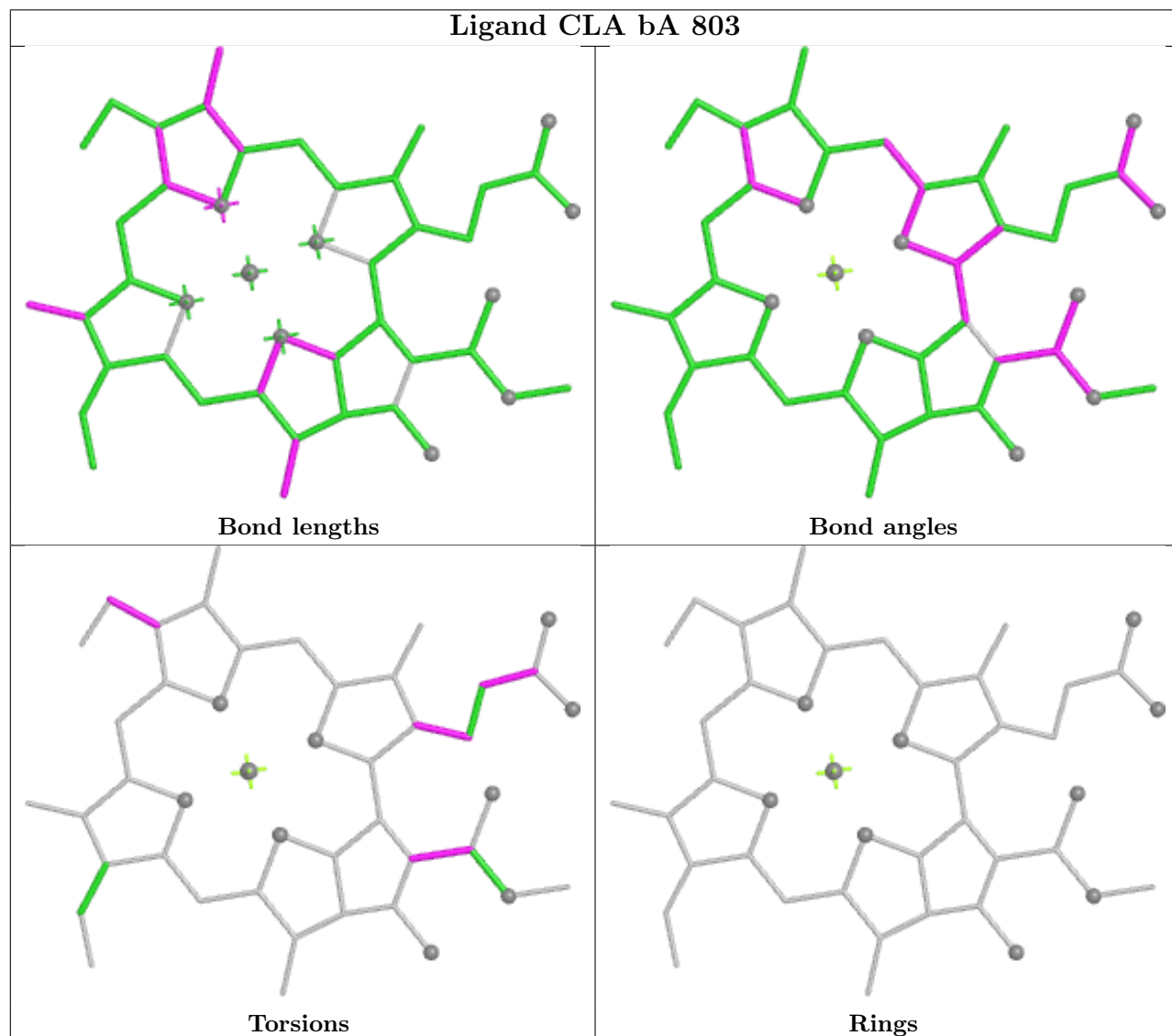
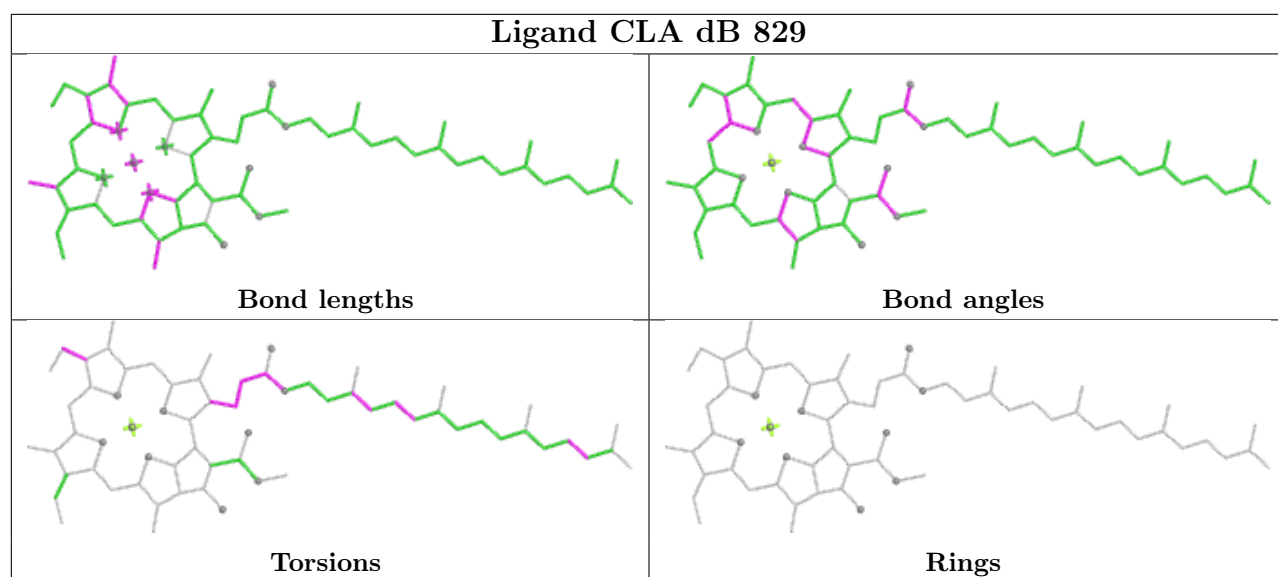


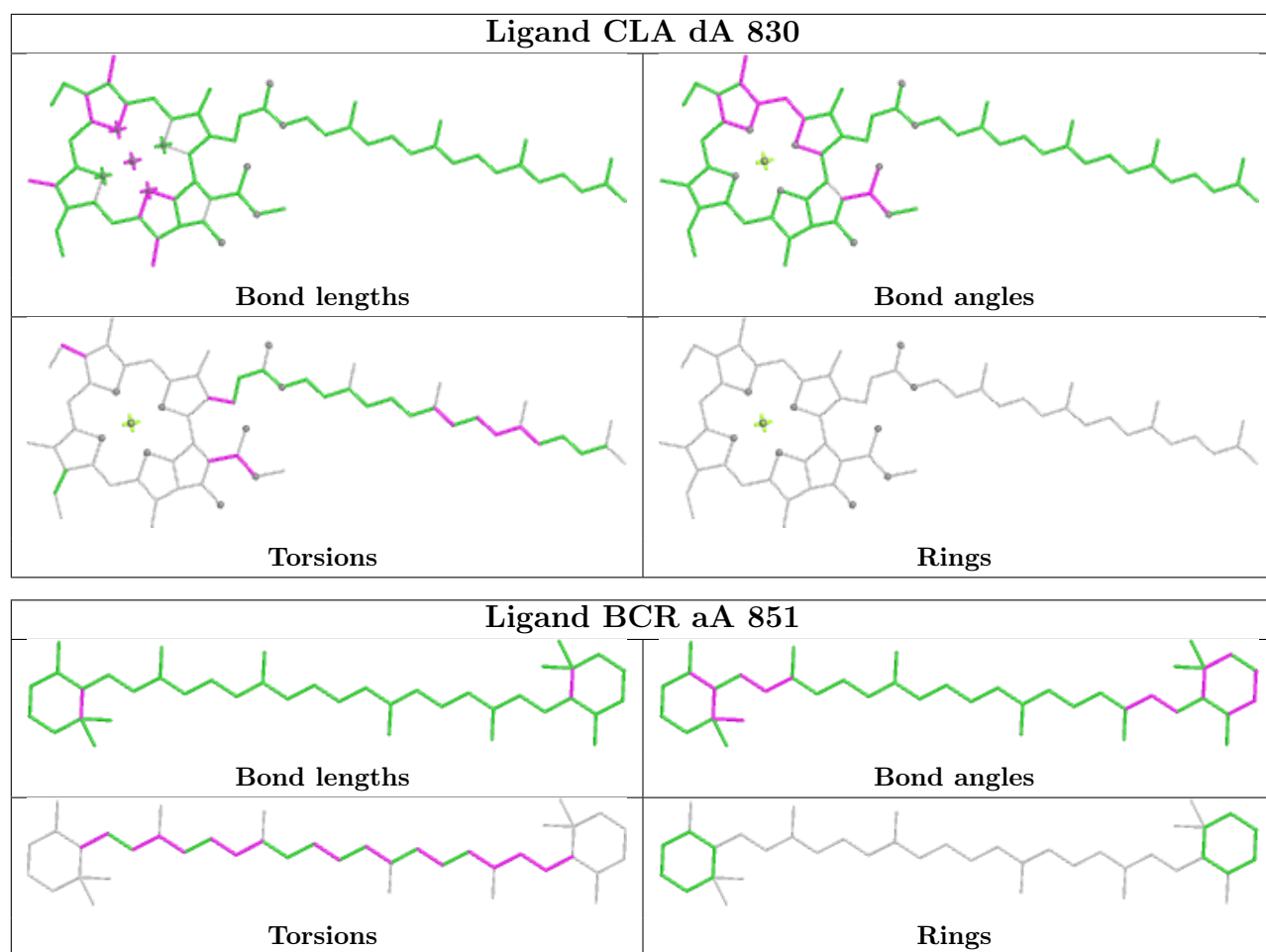


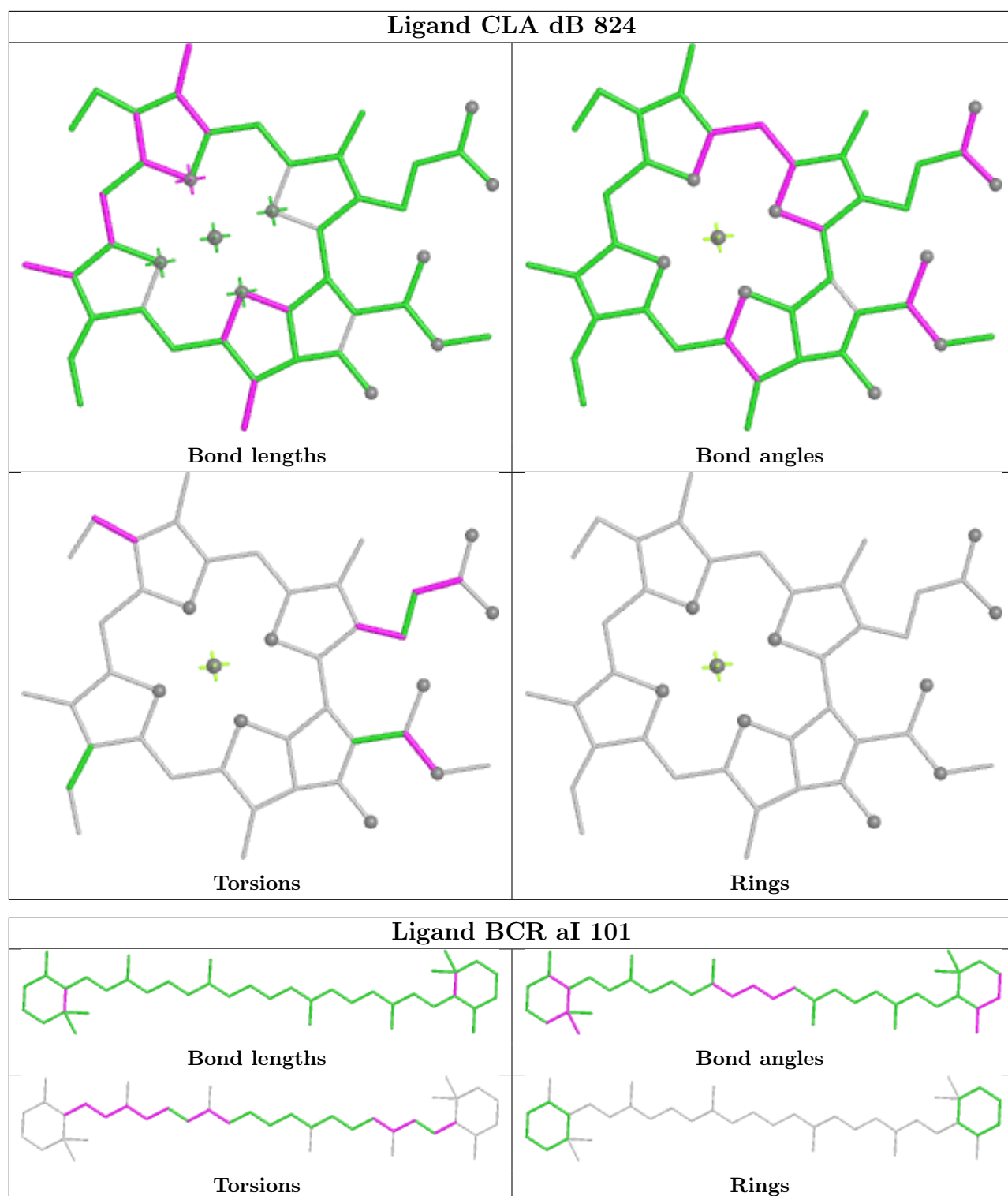
Ligand CLA dK 103

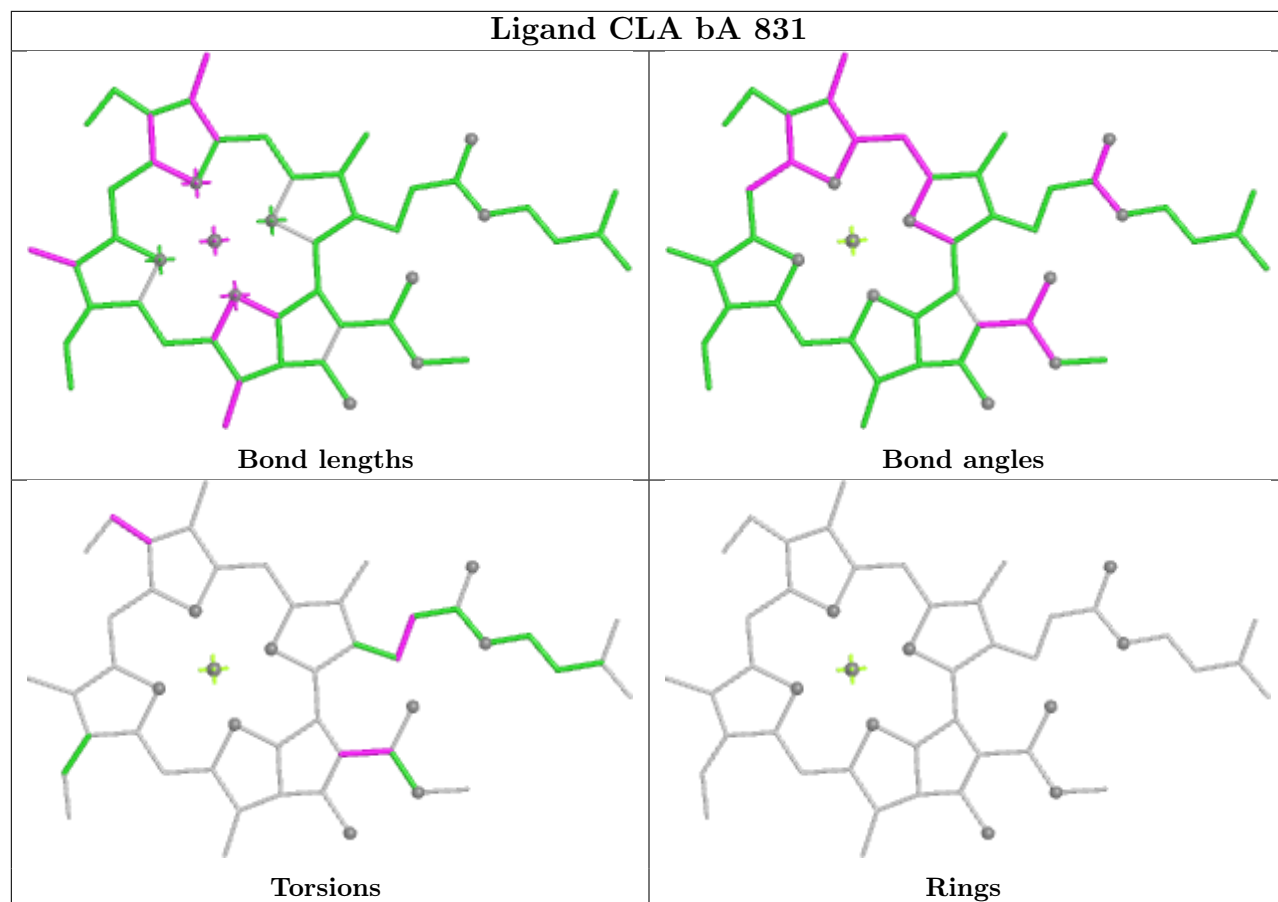


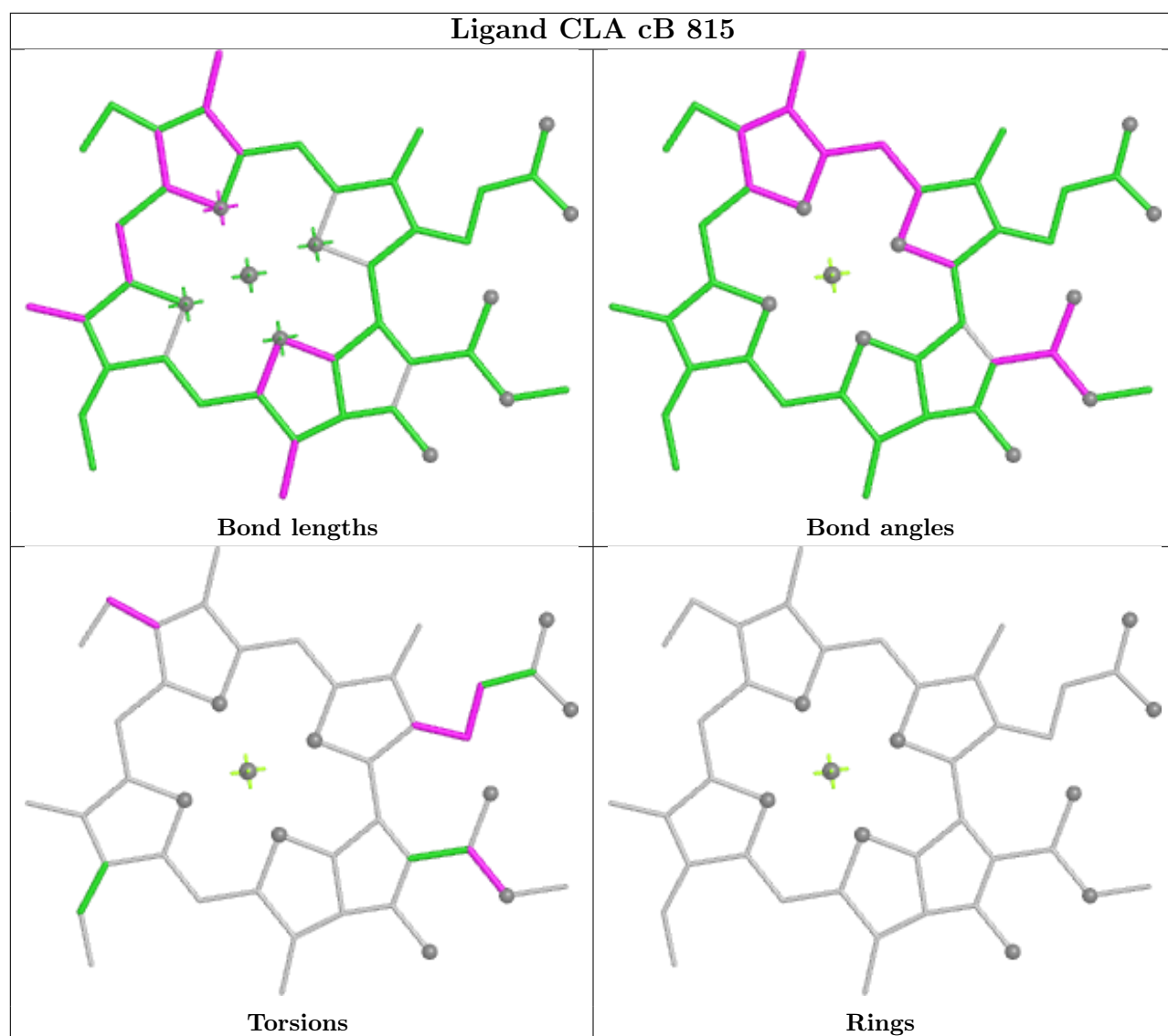




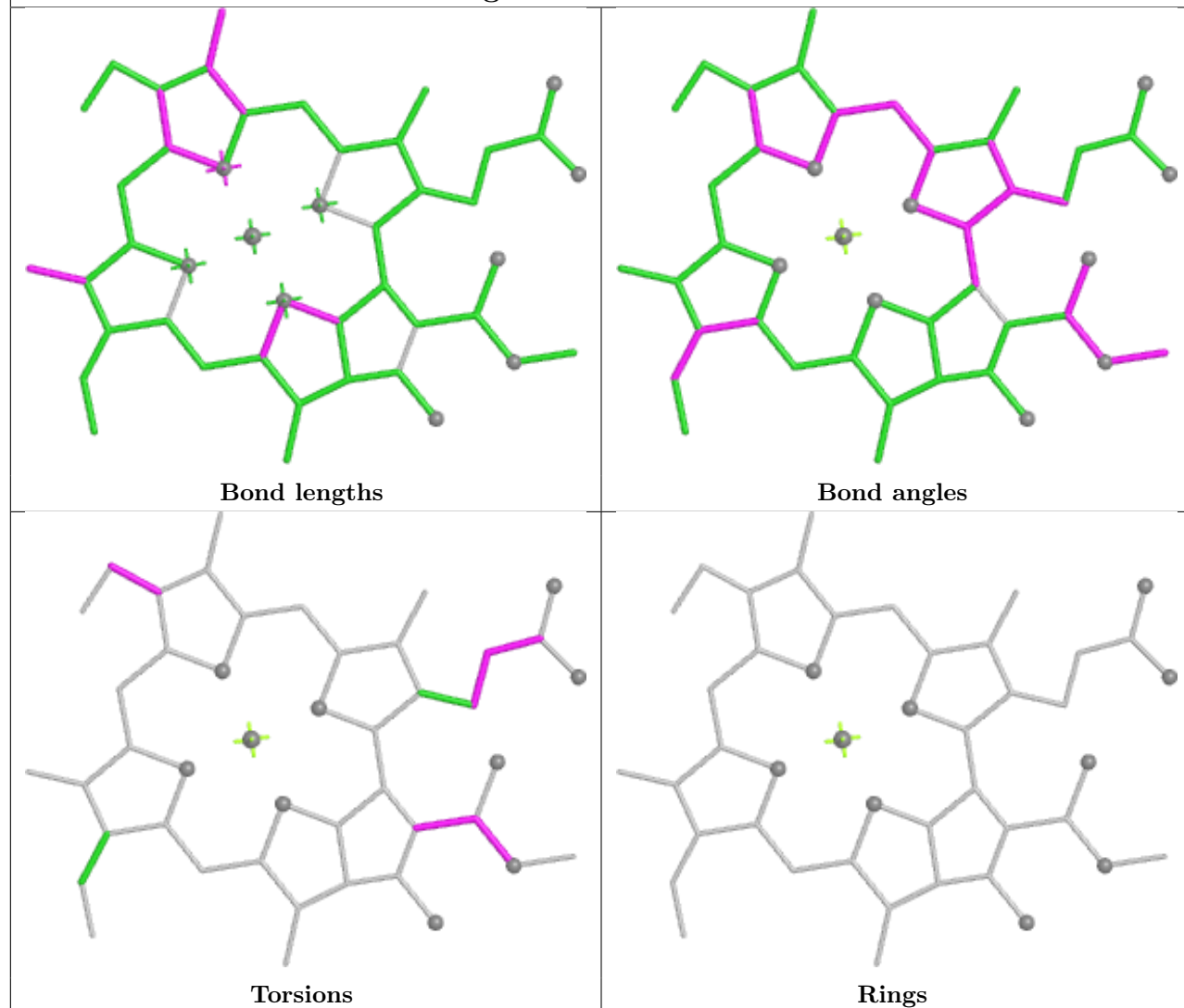




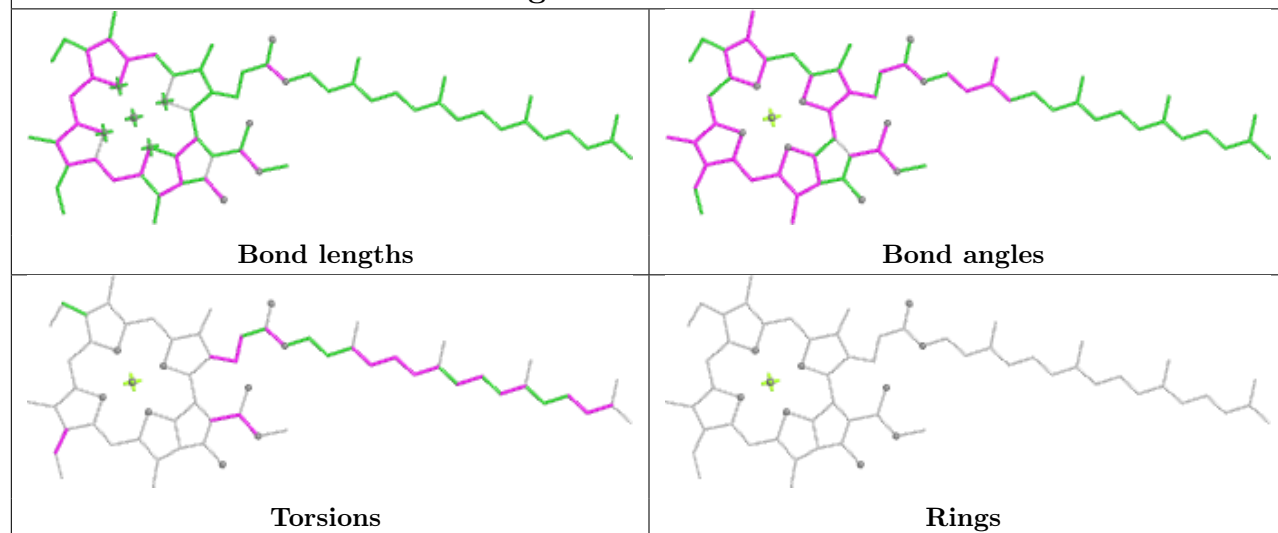




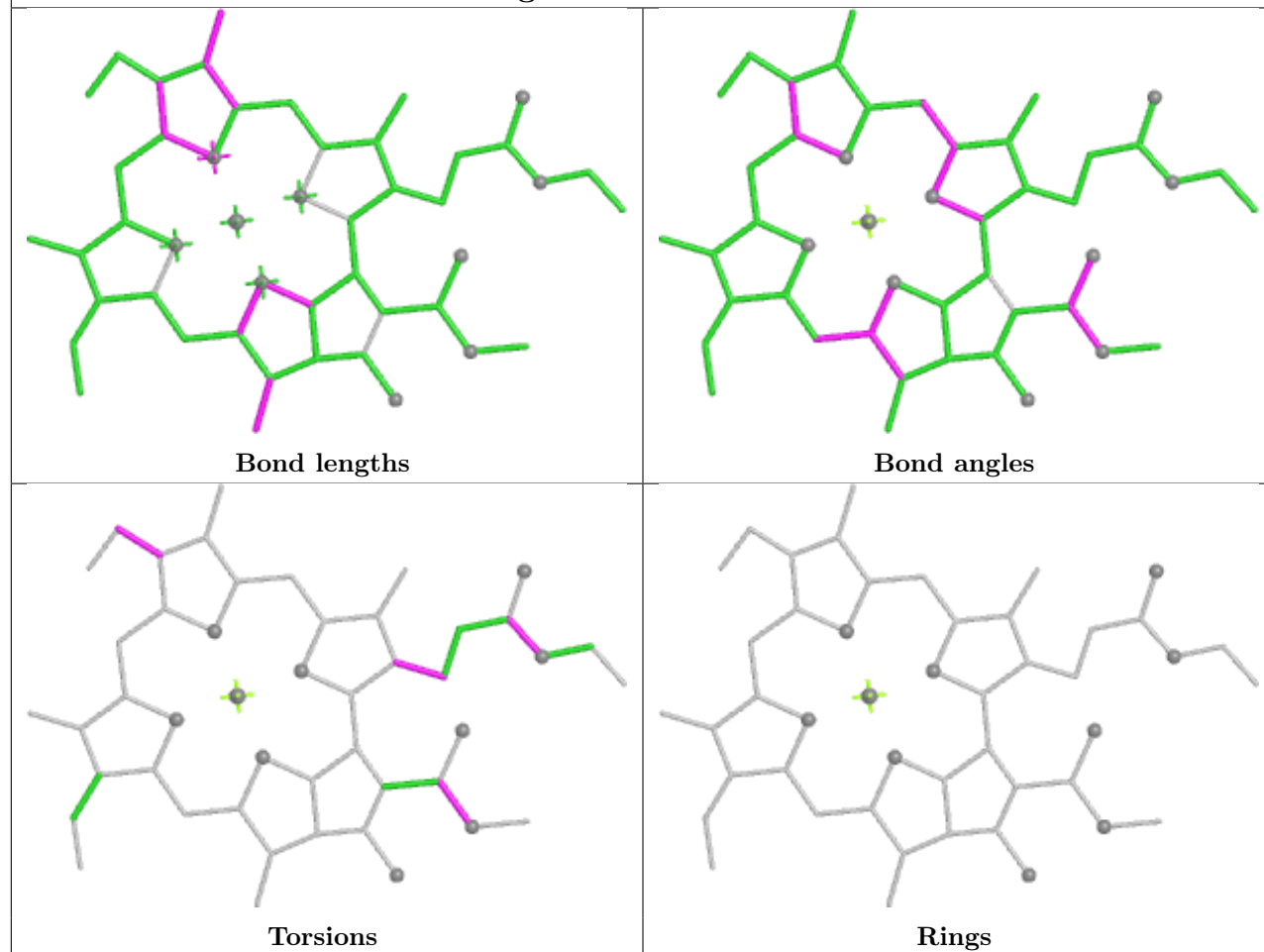
Ligand CLA dA 813



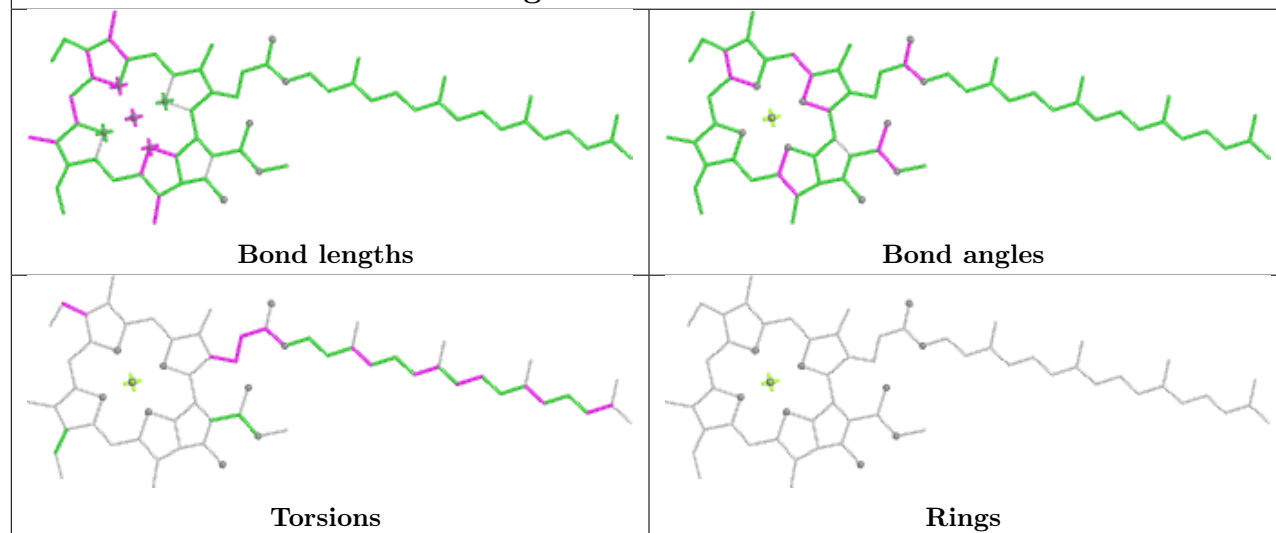
Ligand CL0 cA 801

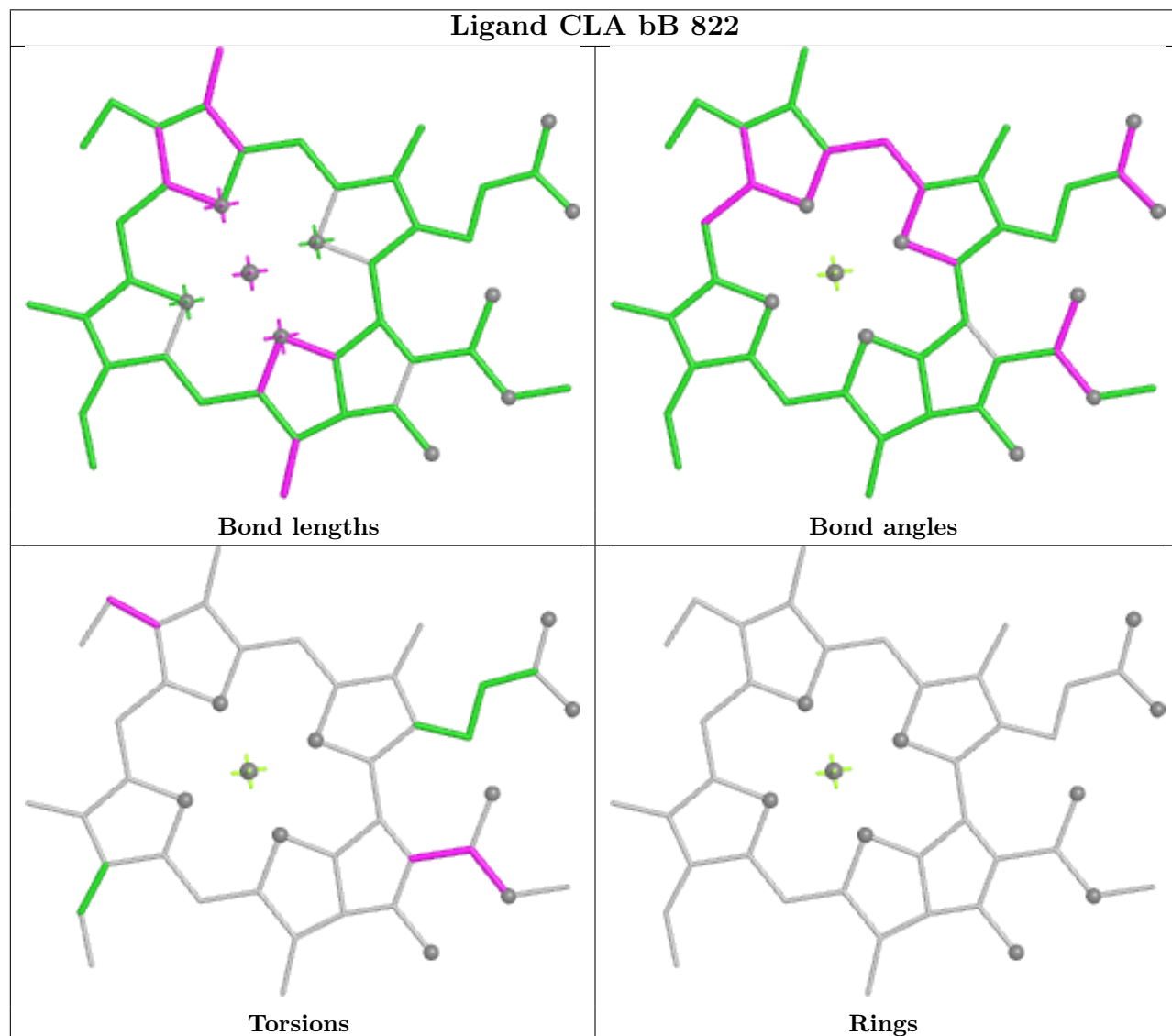
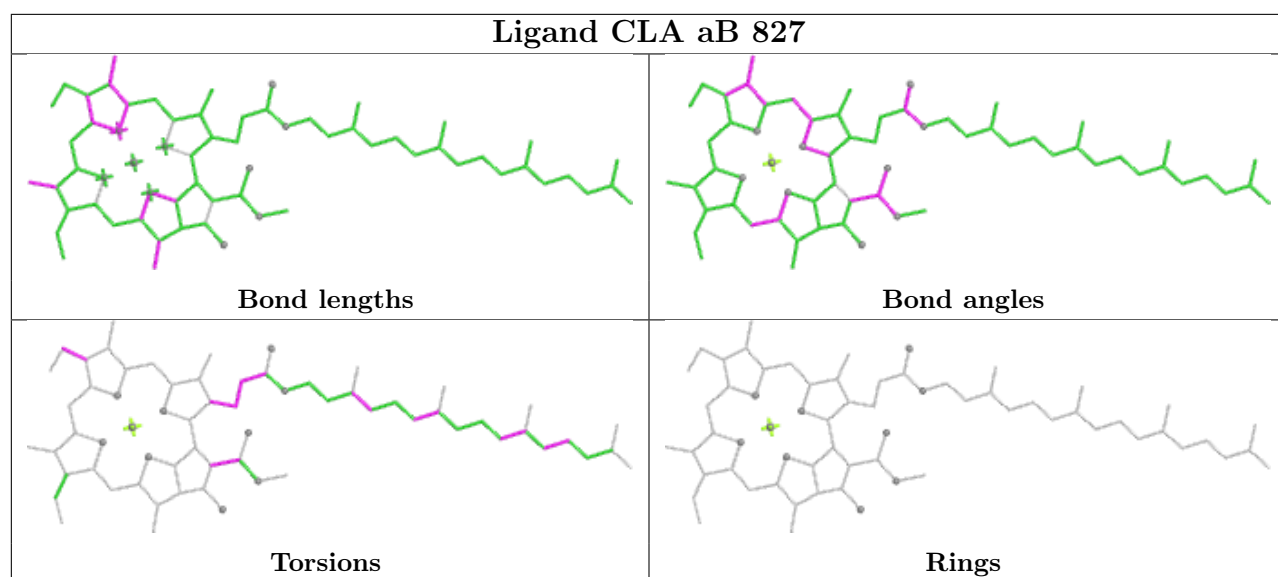


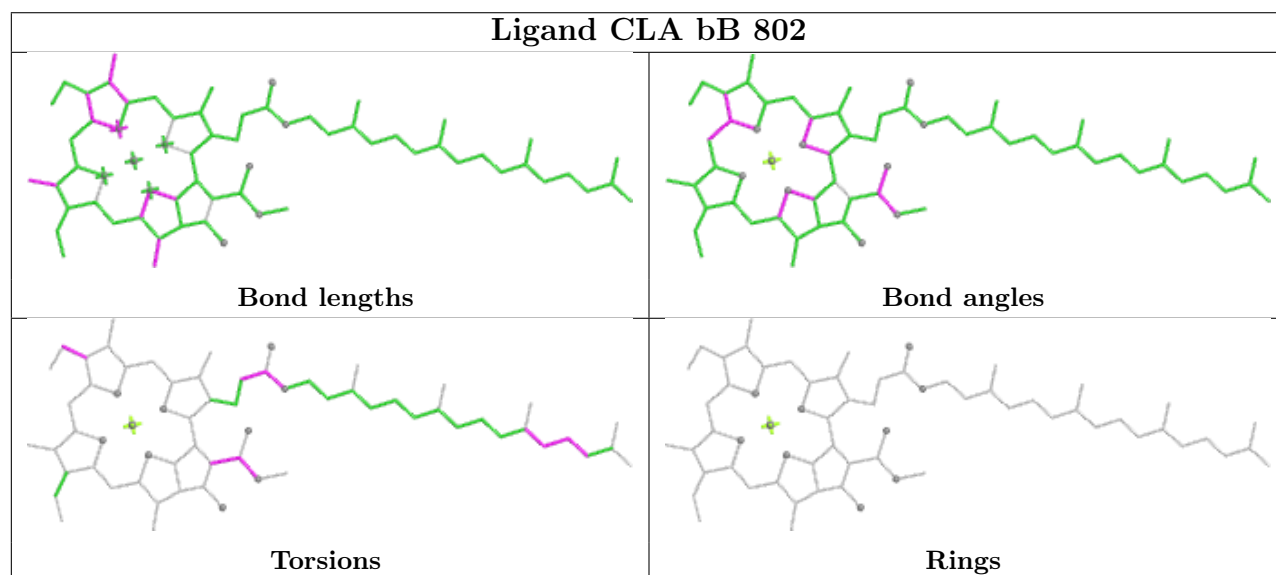
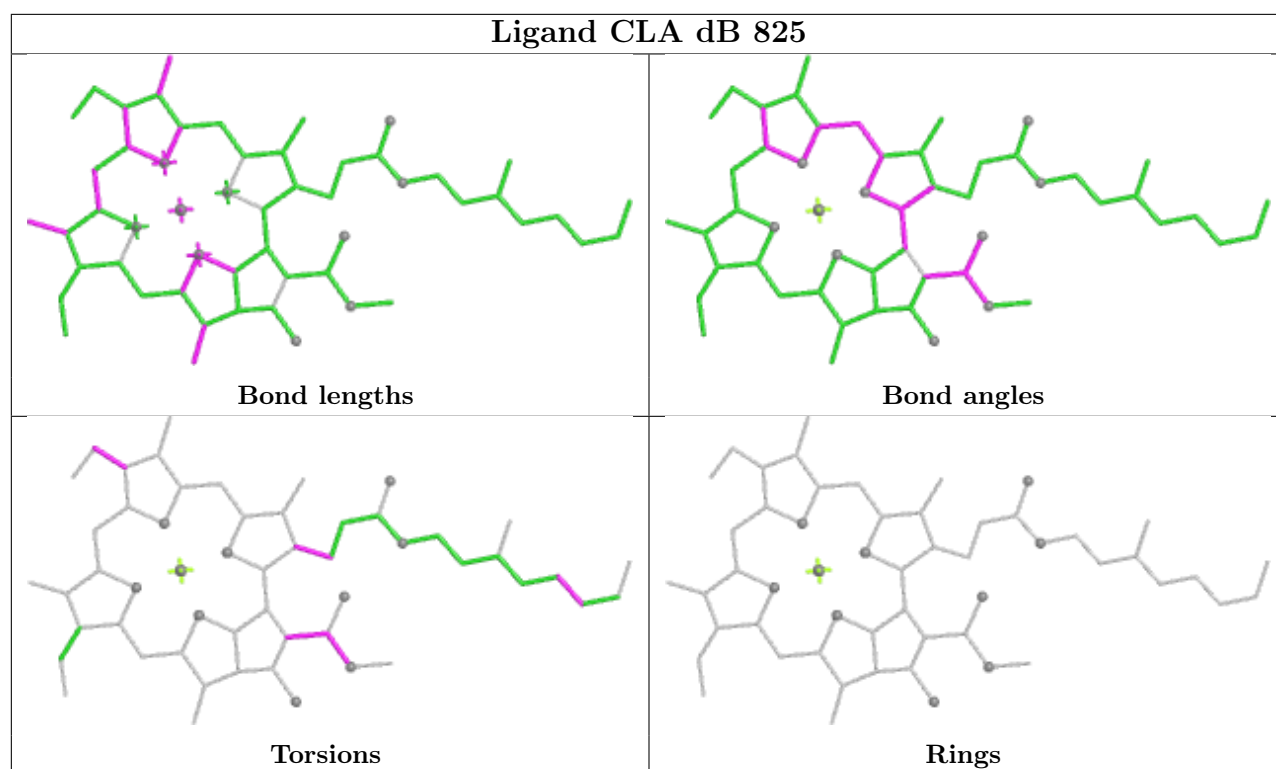
Ligand CLA aA 824

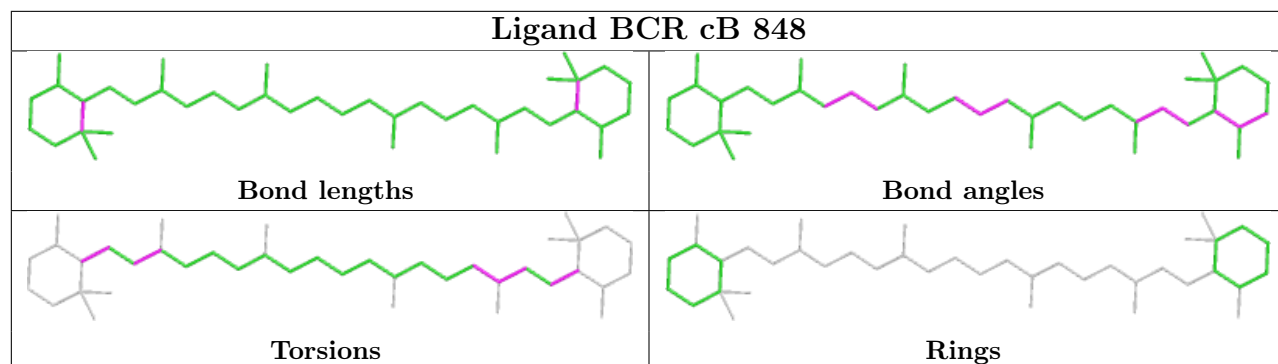
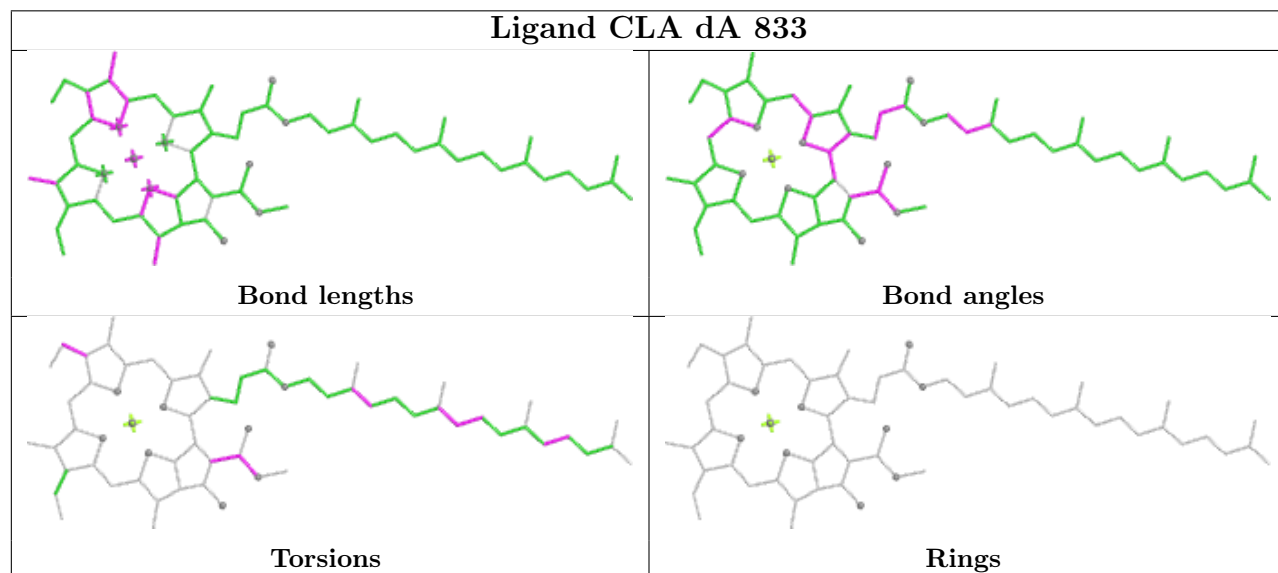
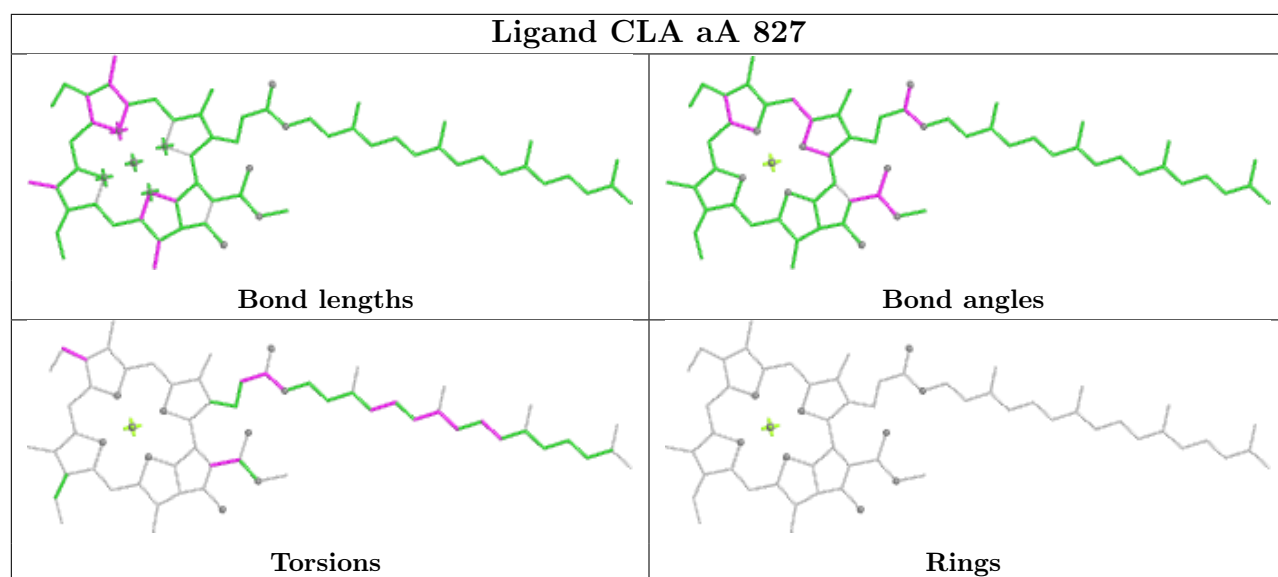


Ligand CLA cA 829

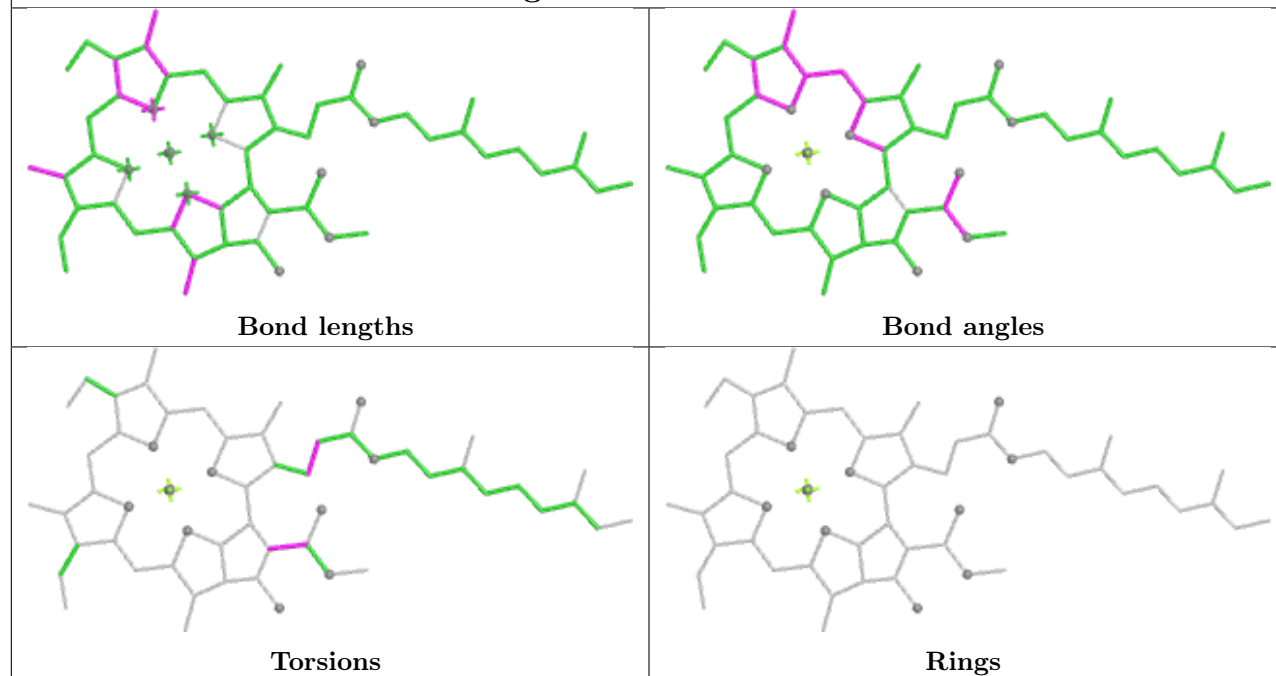




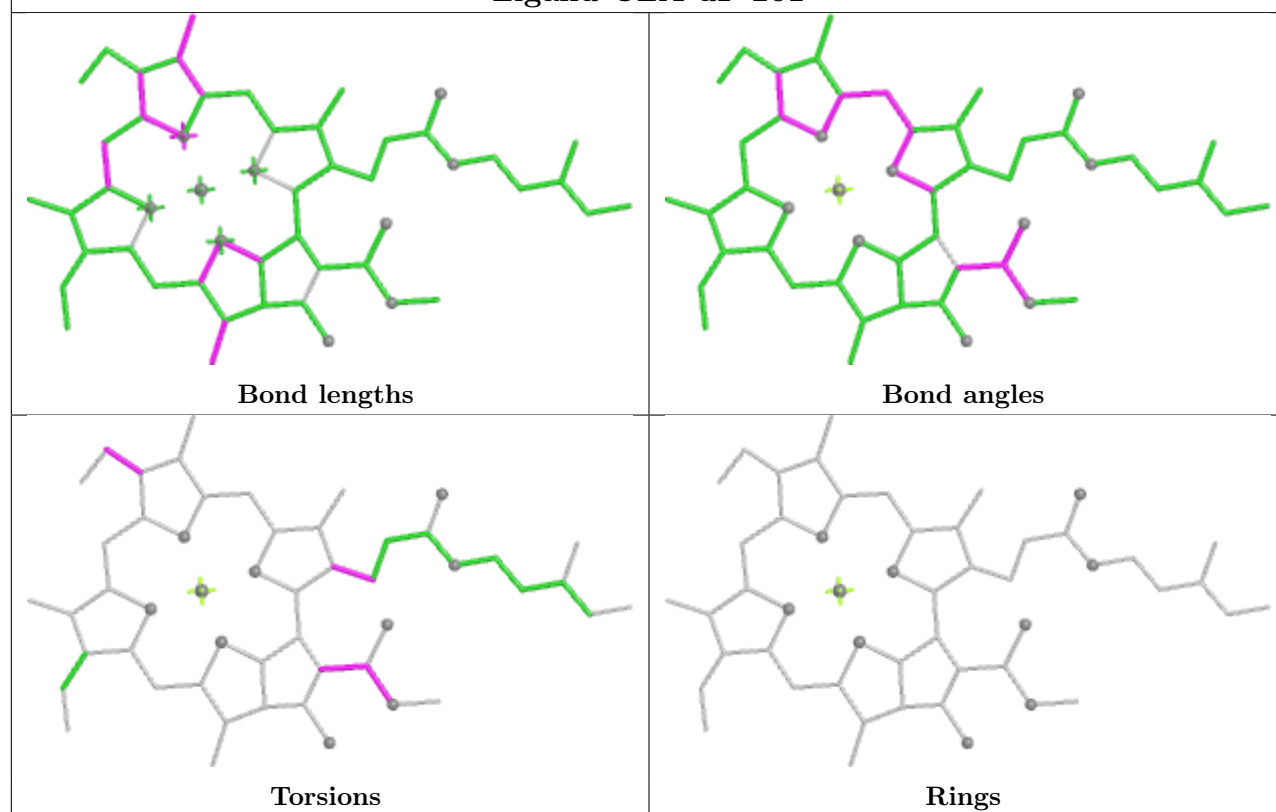


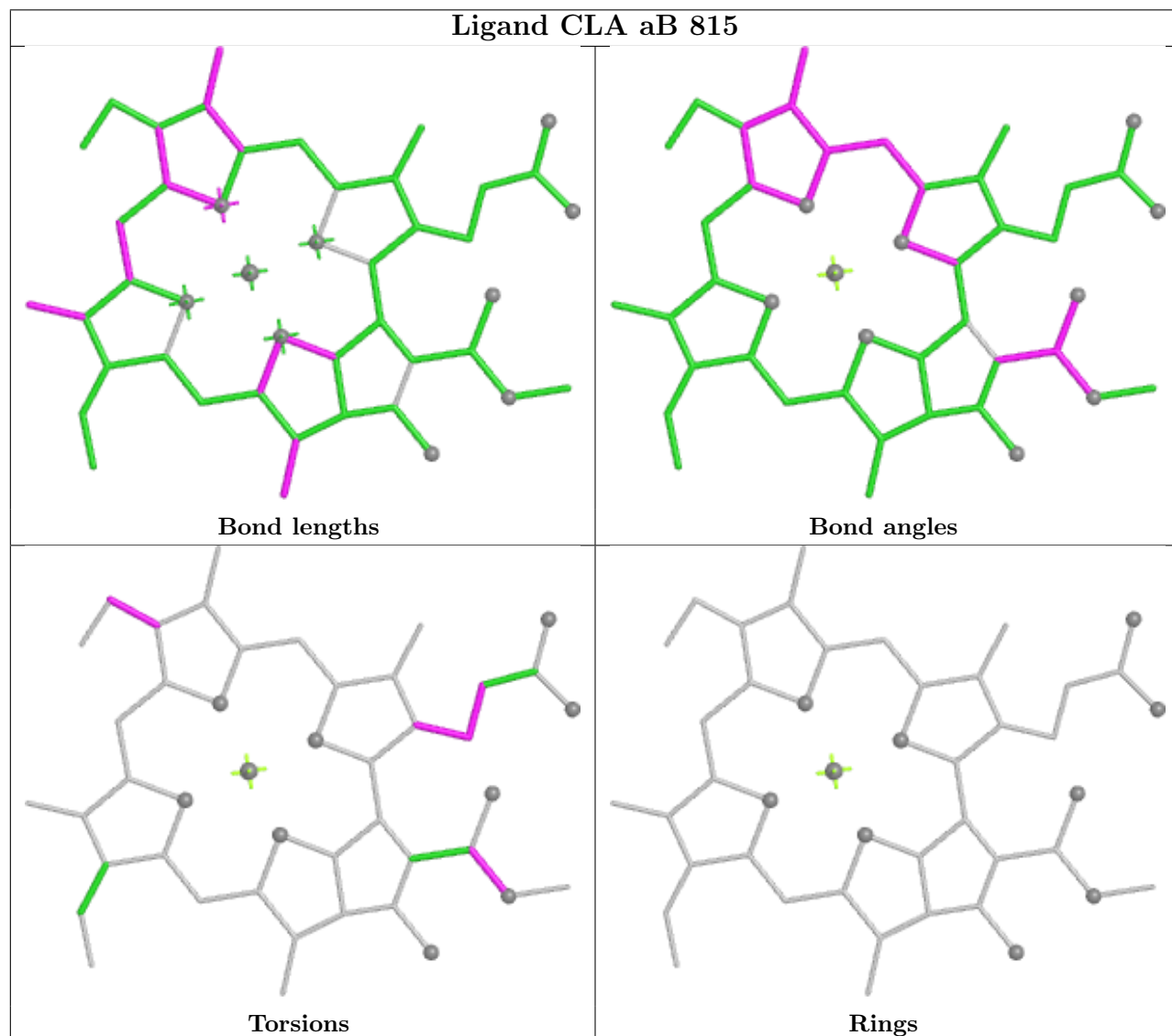
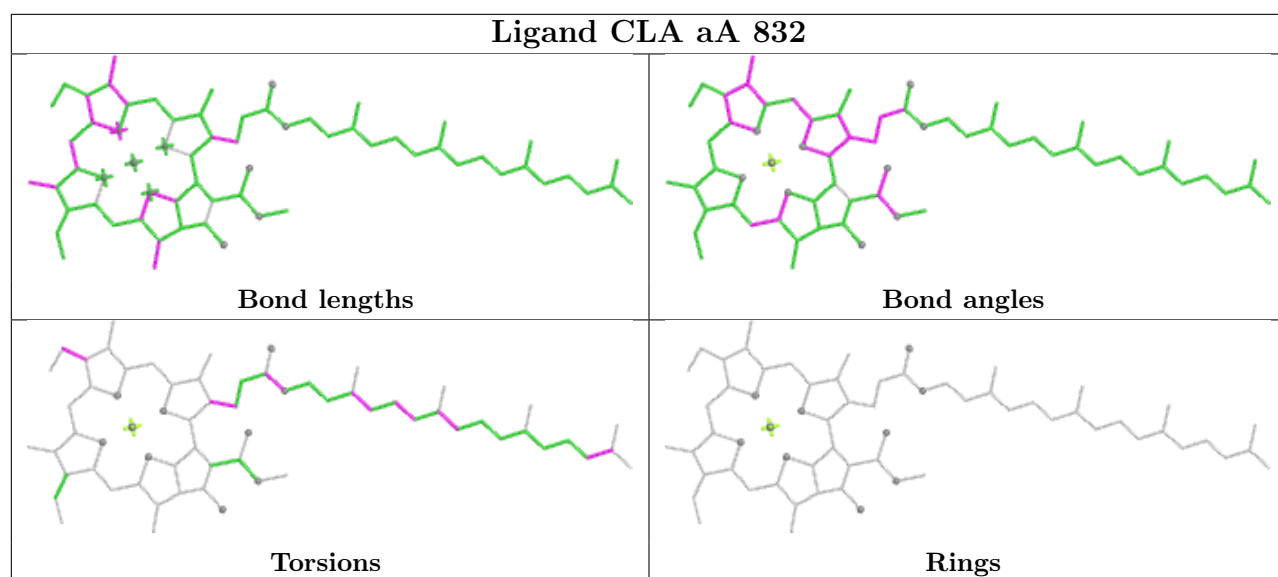


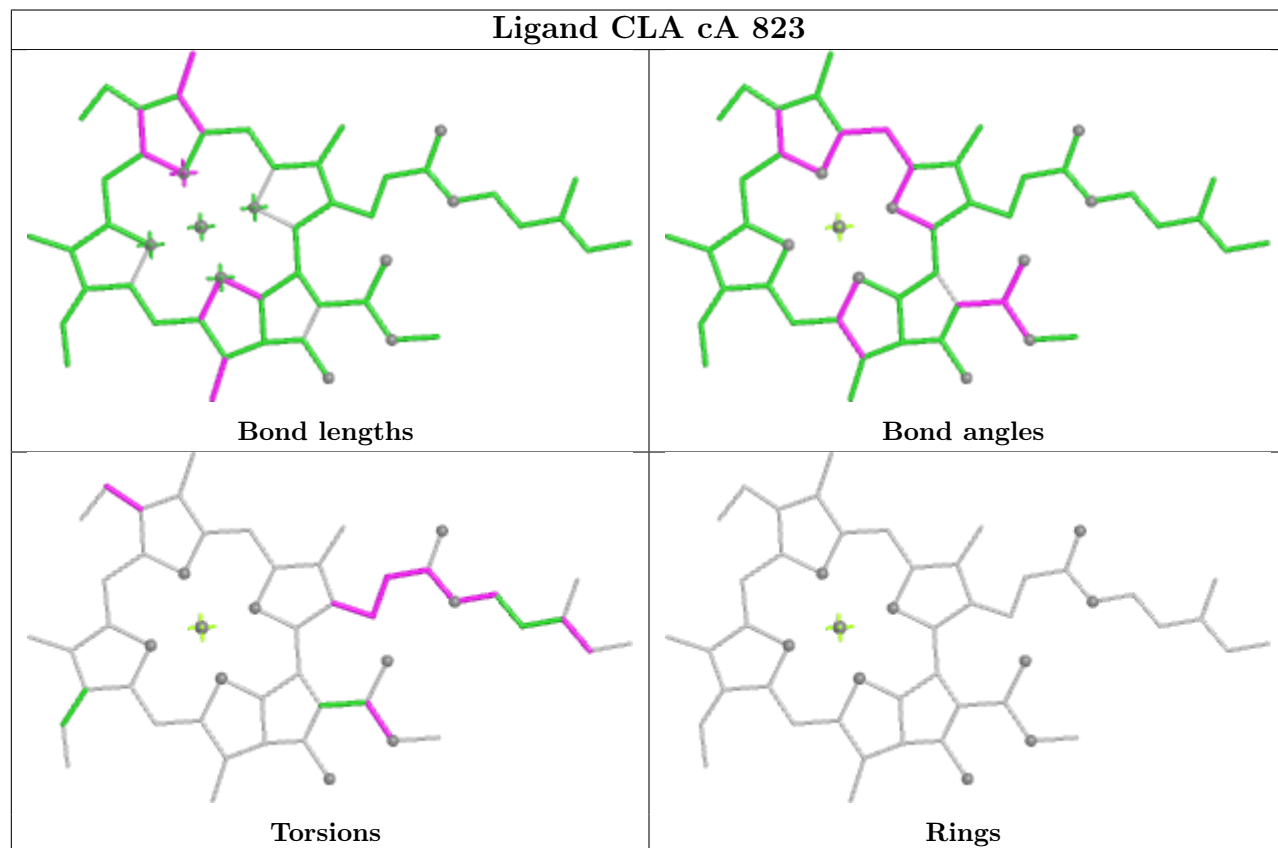
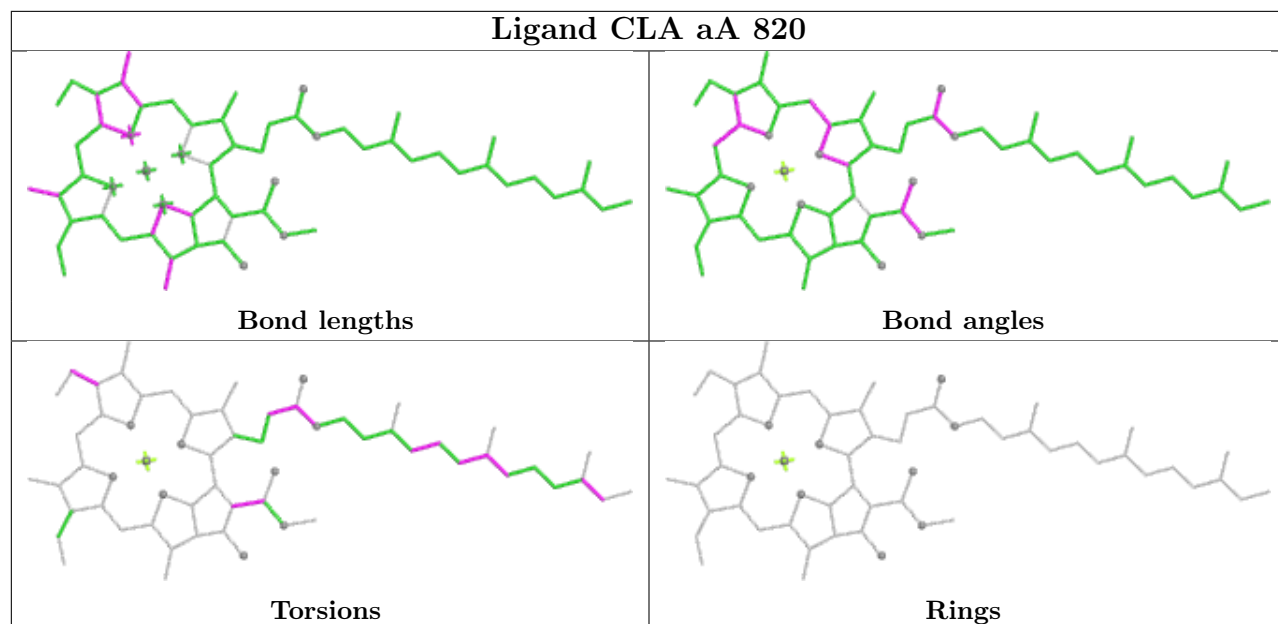
Ligand CLA aB 814



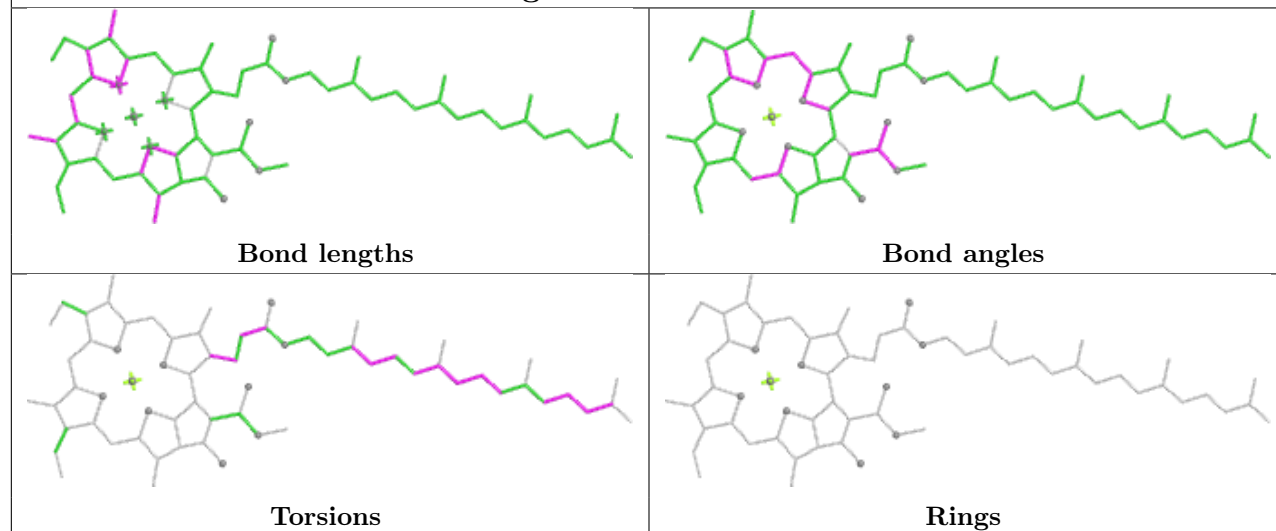
Ligand CLA dF 201



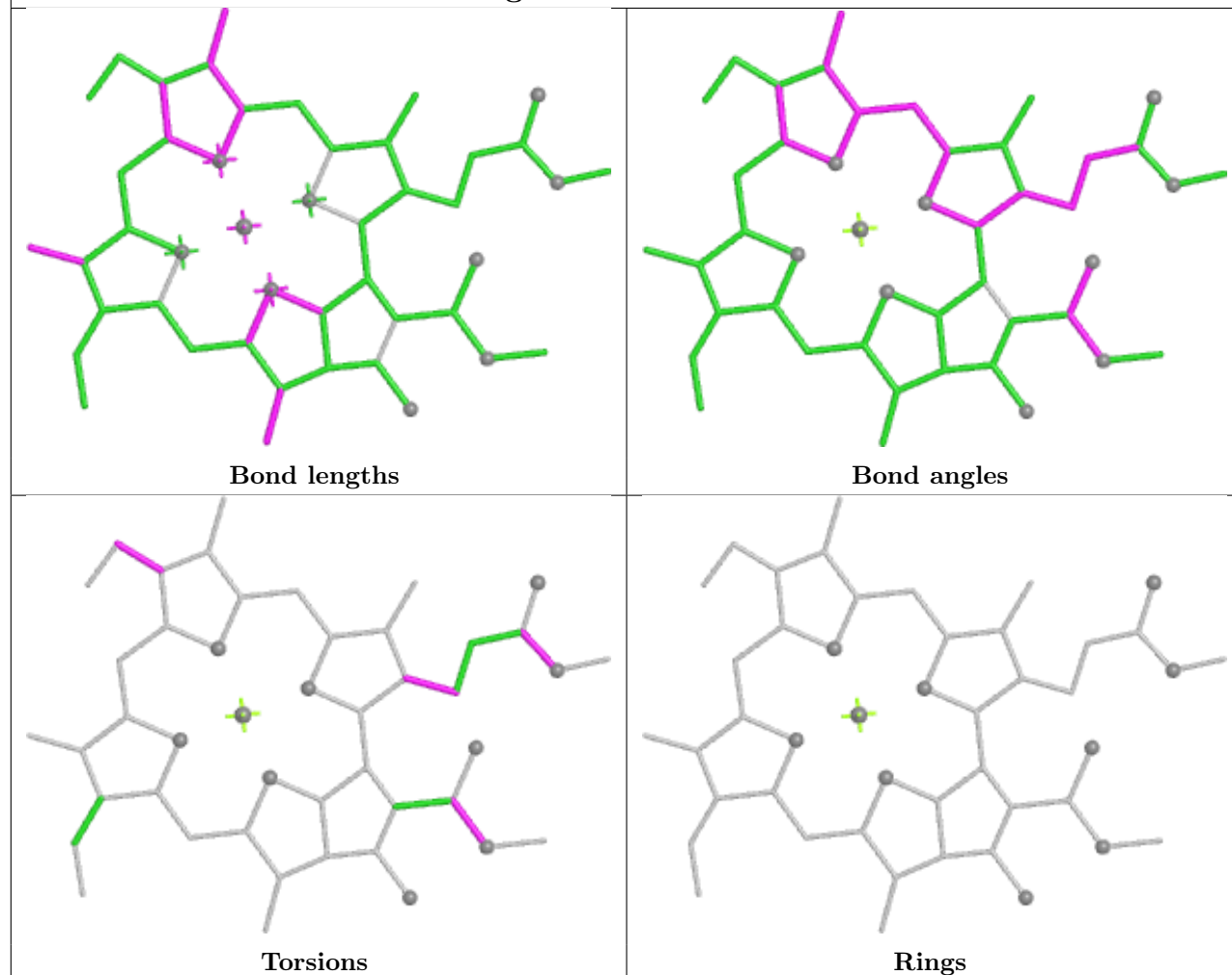


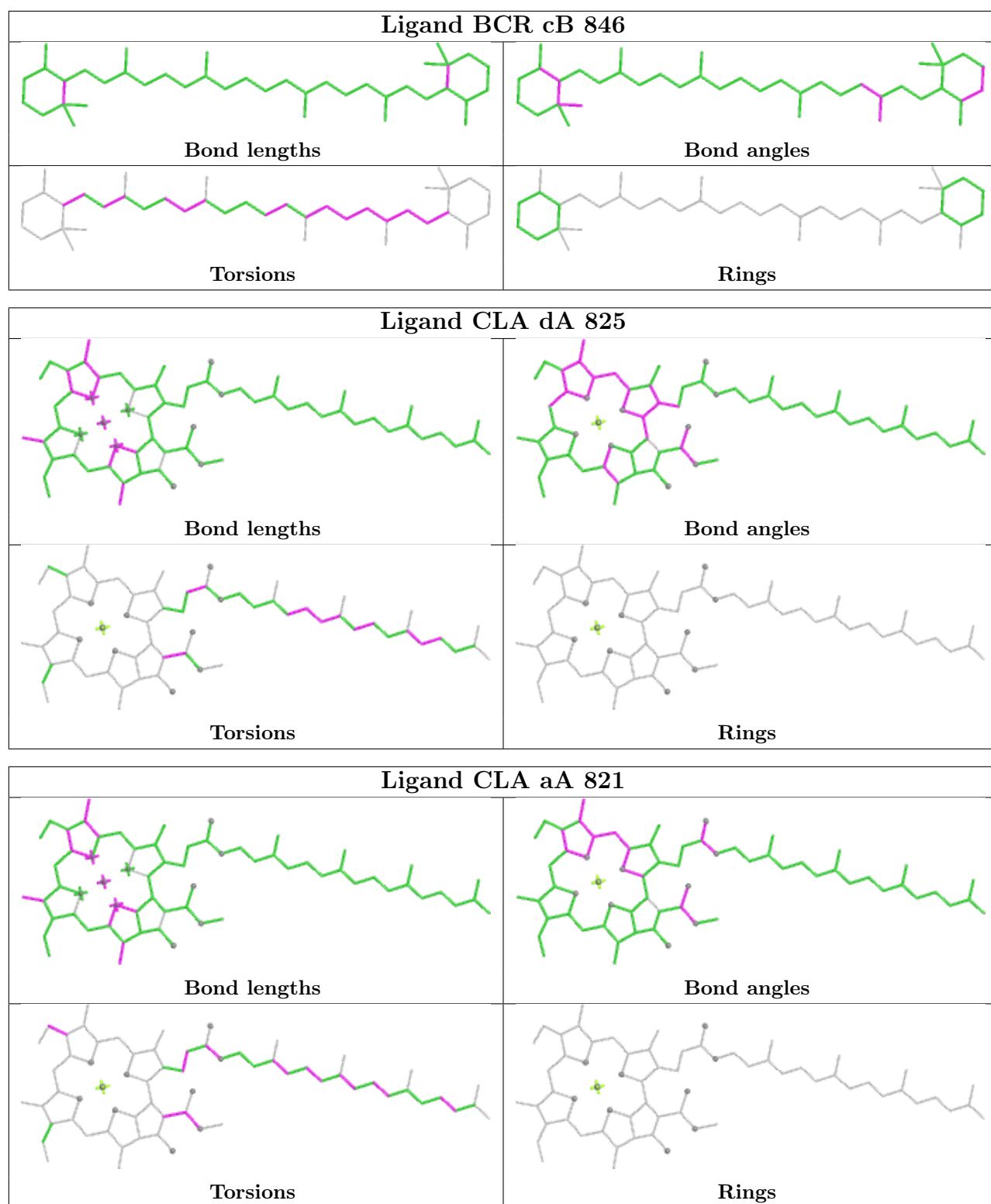


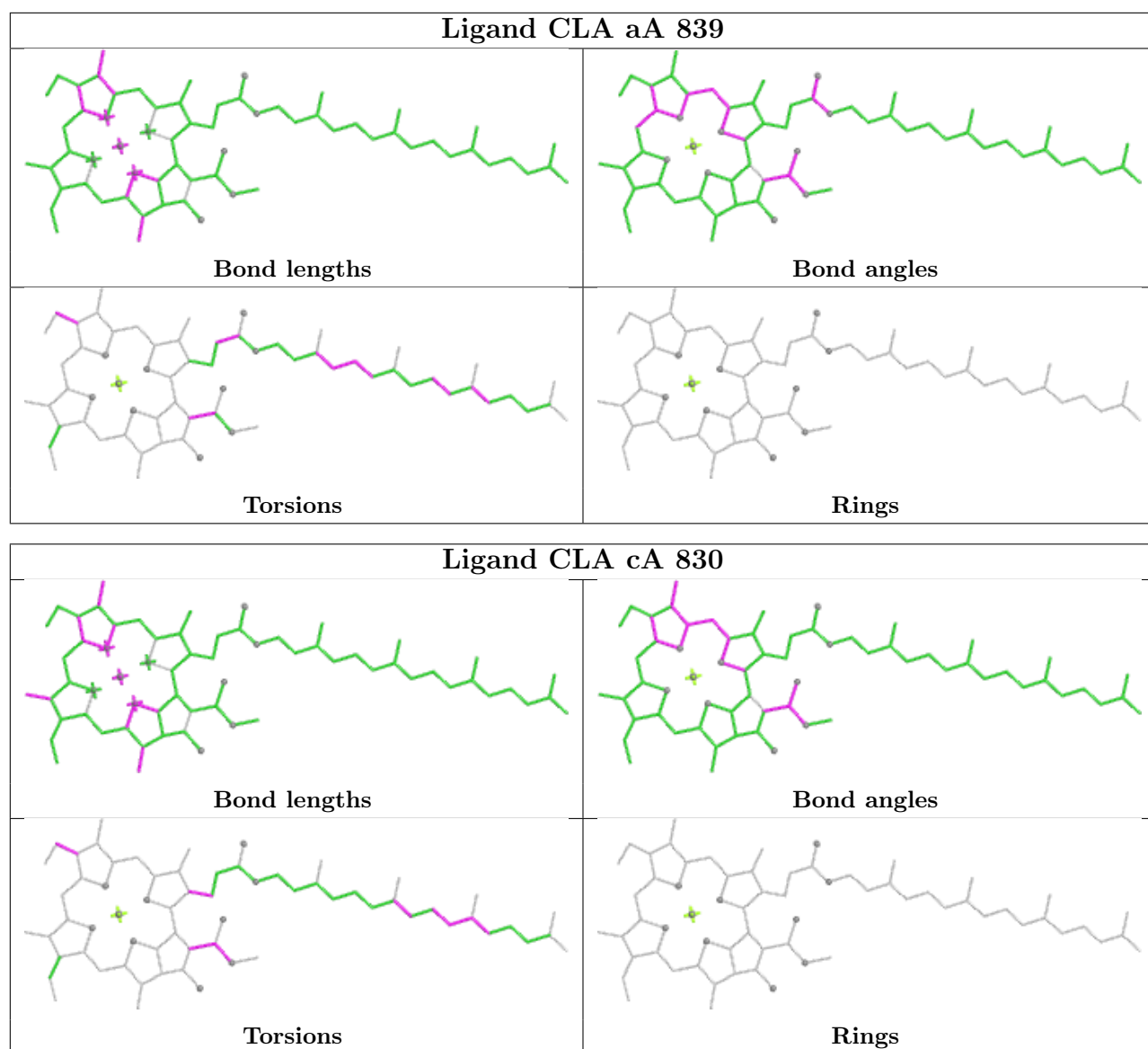
Ligand CLA dB 833

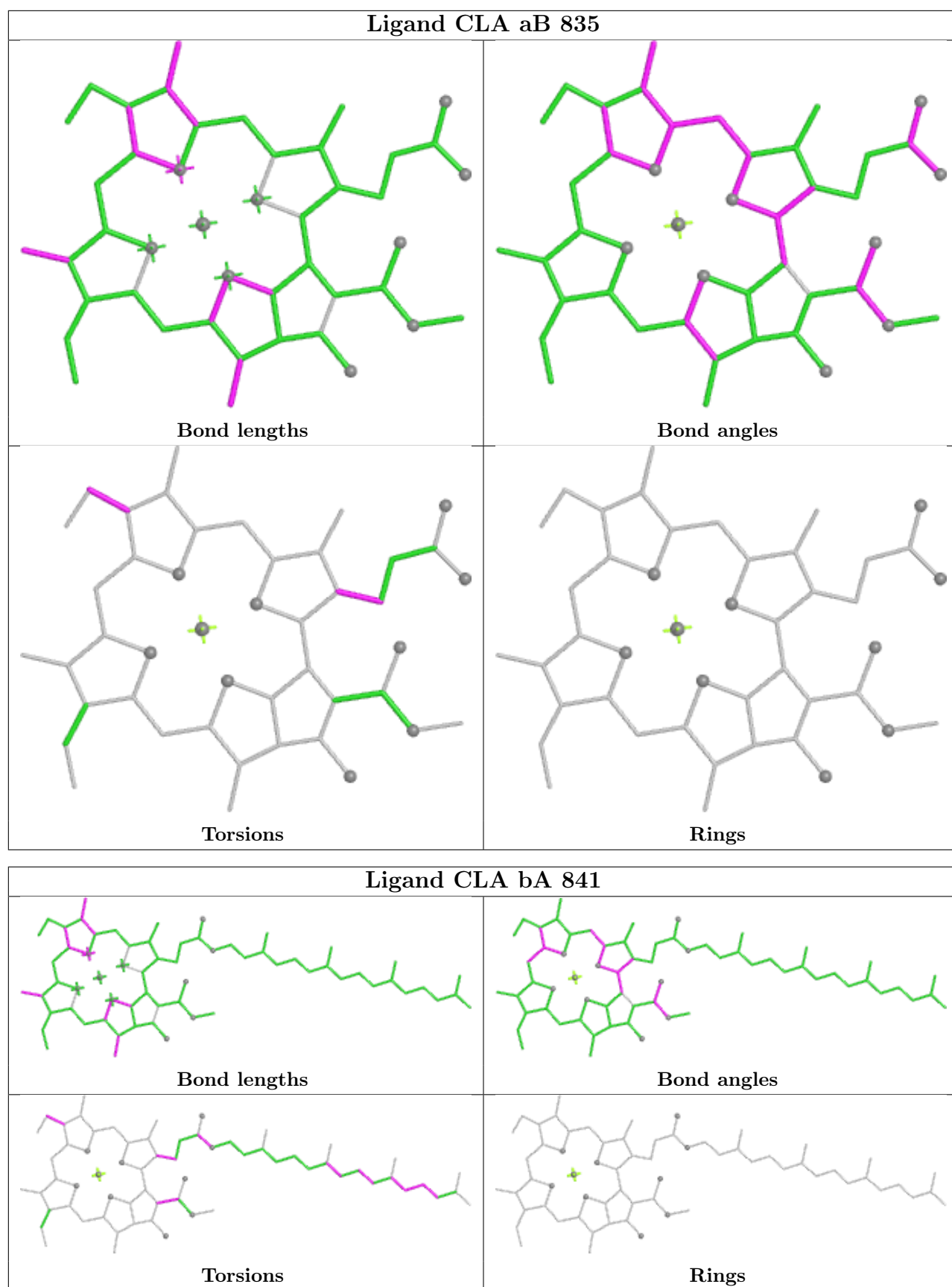


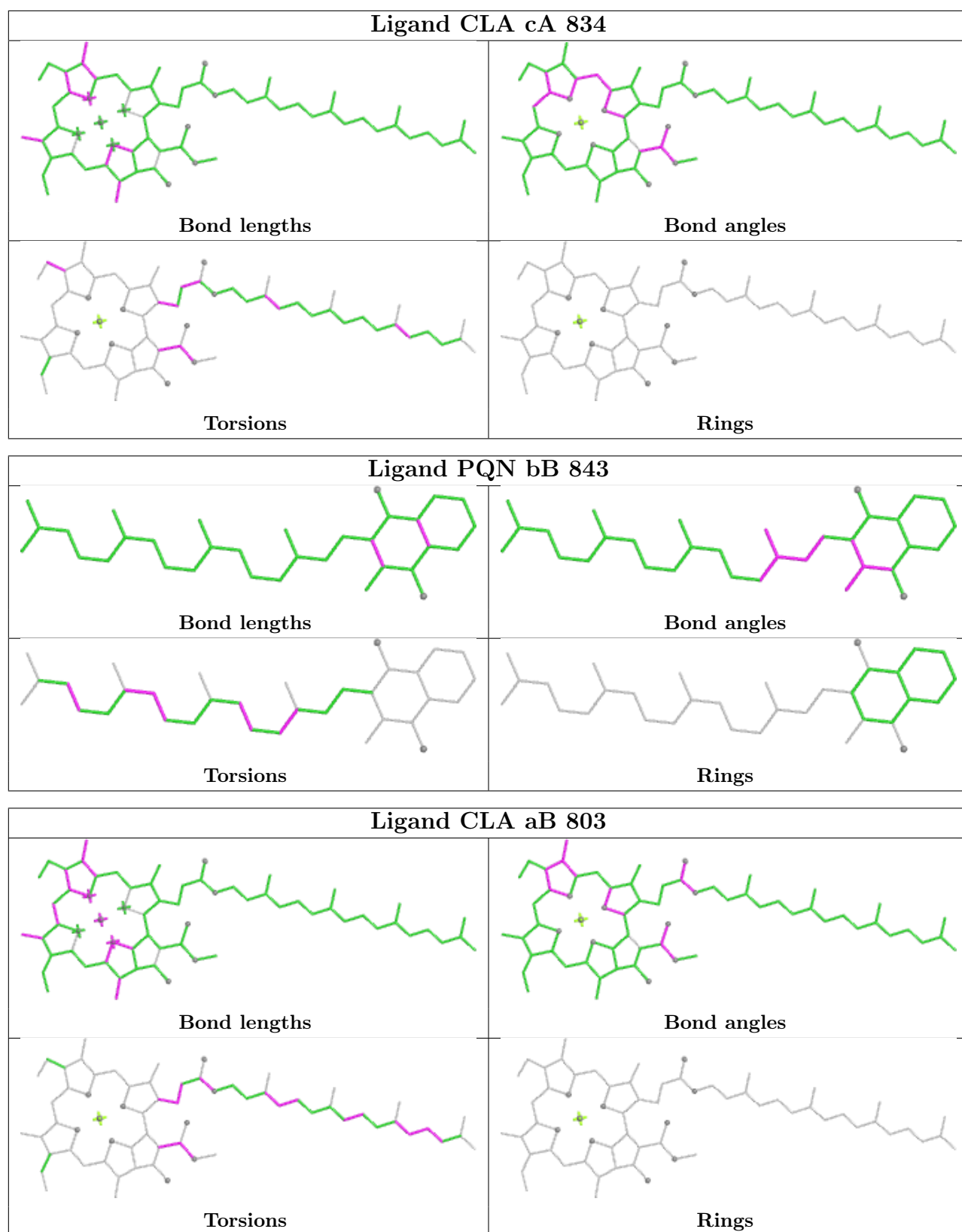
Ligand CLA aB 825

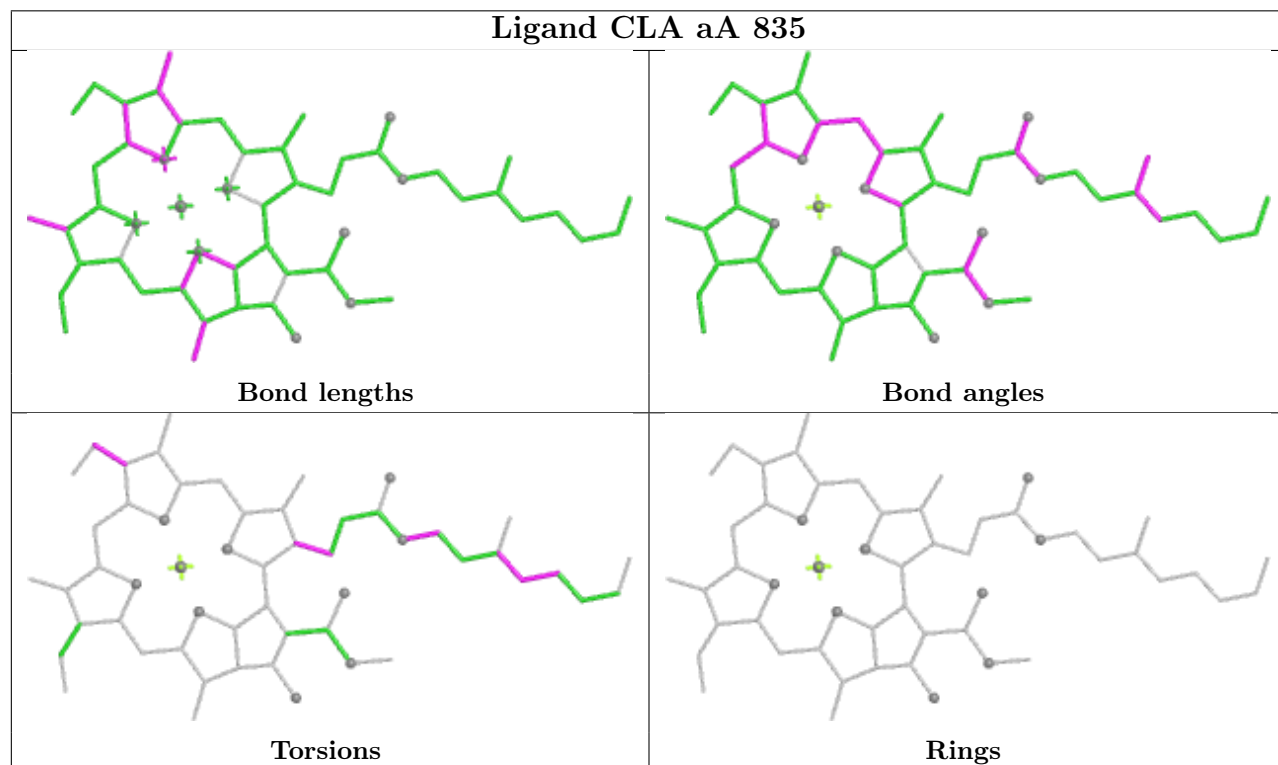
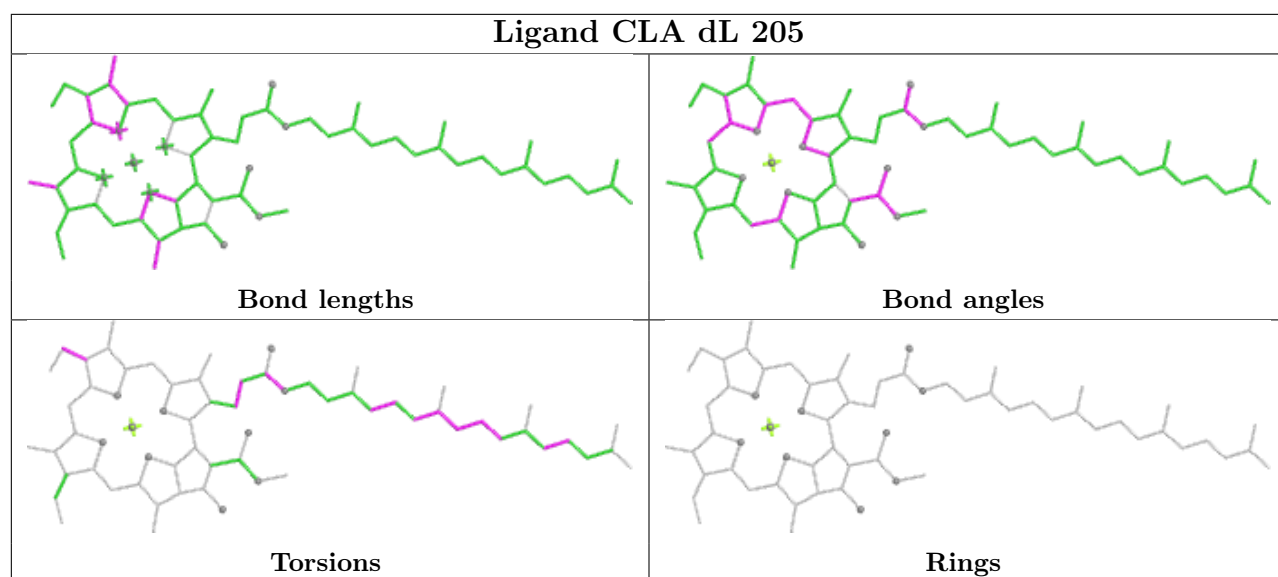




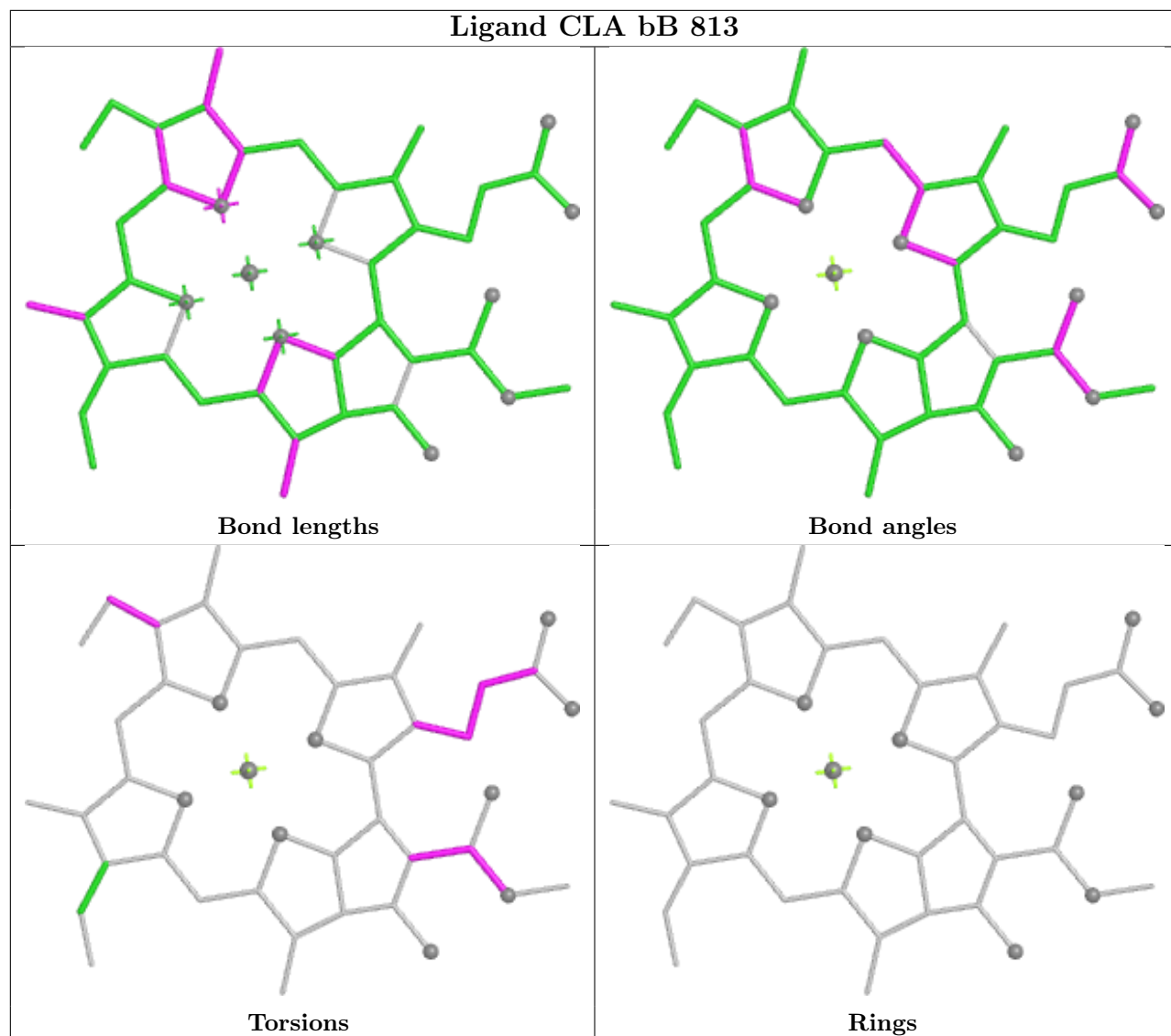




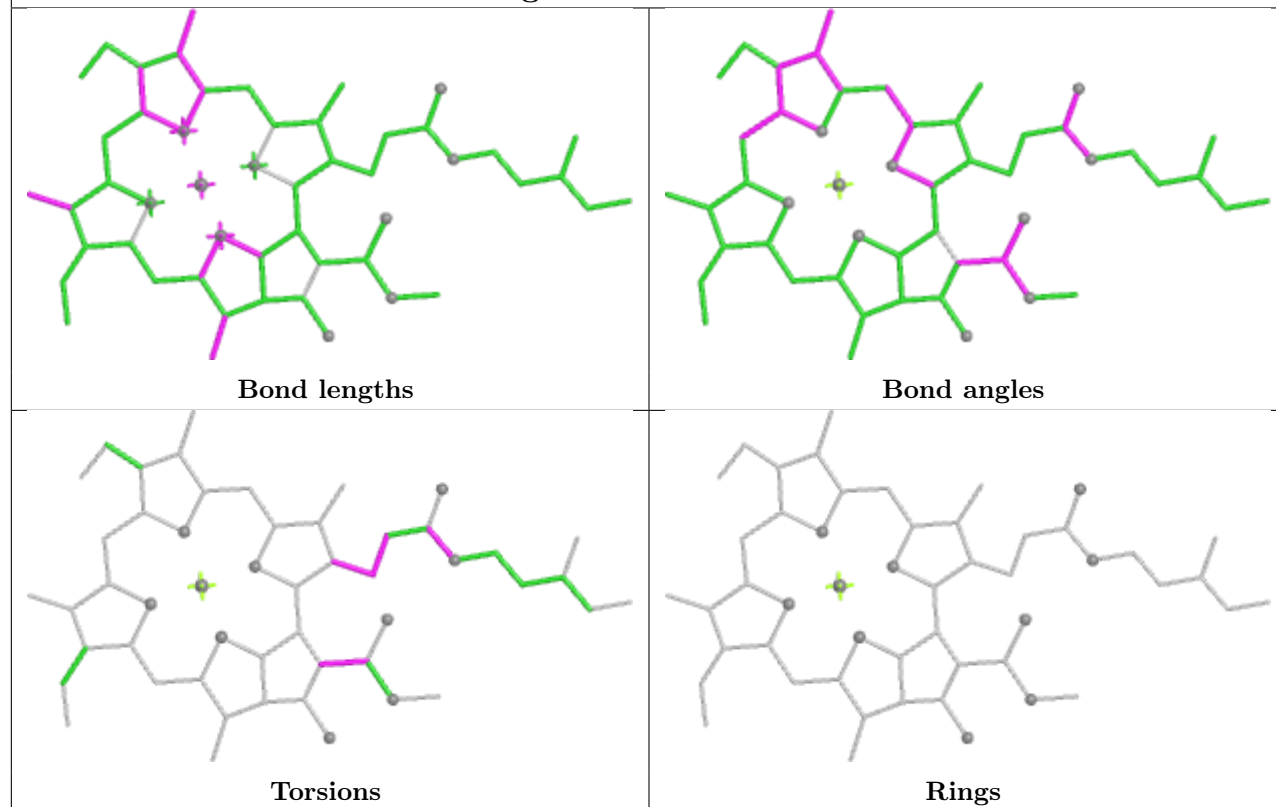




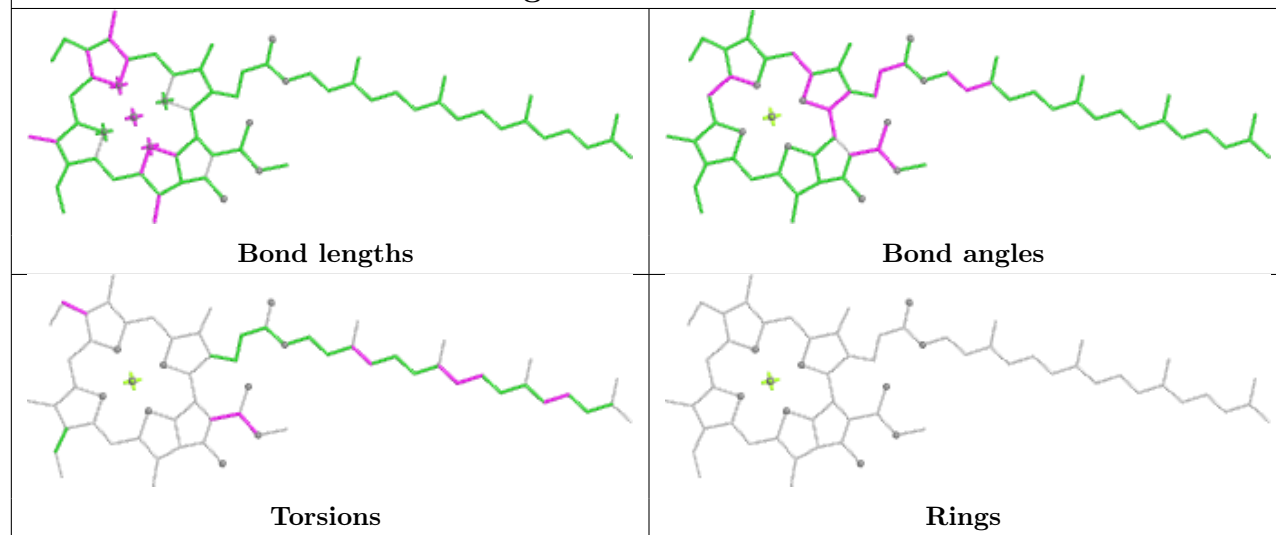
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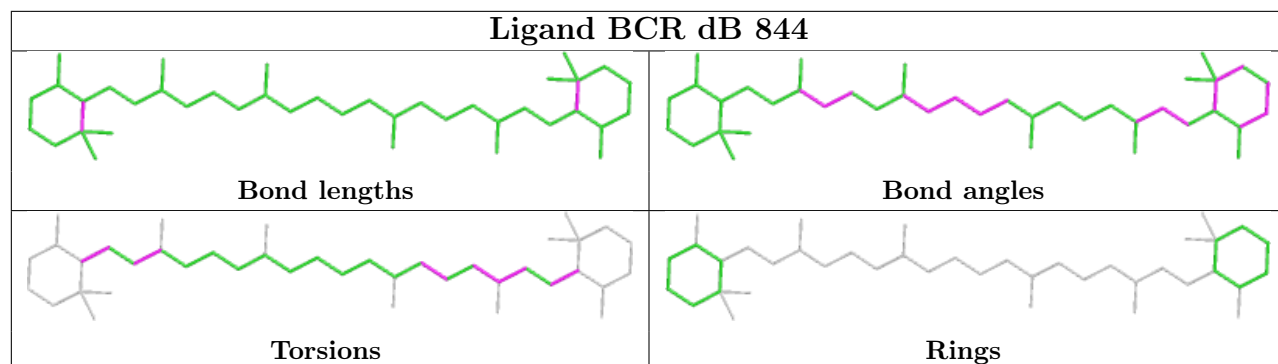
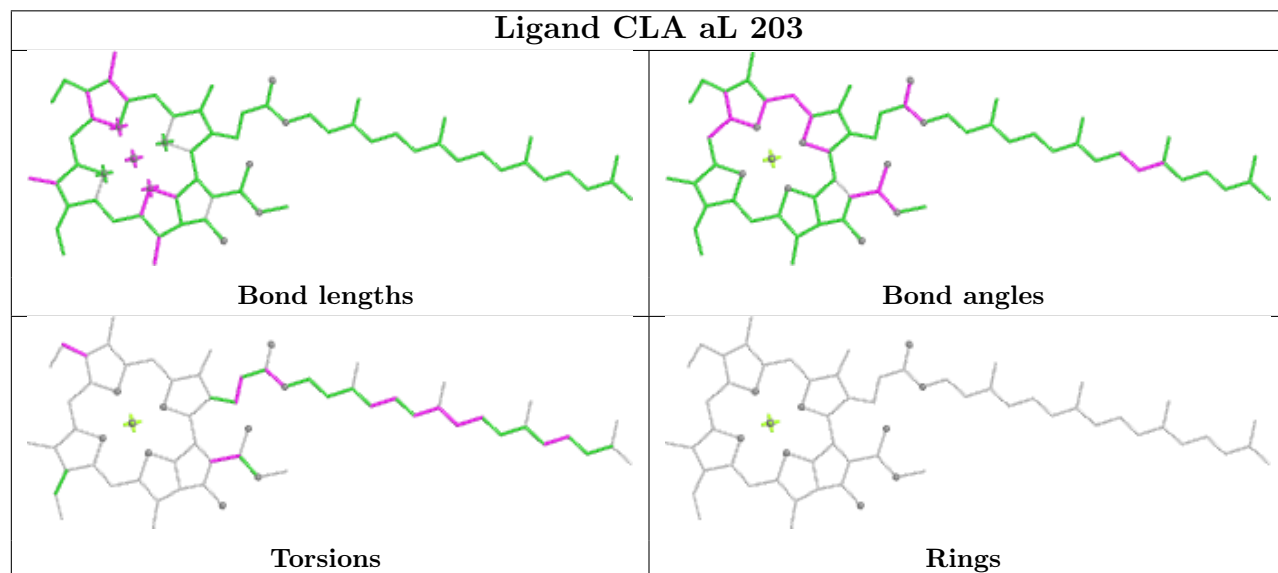
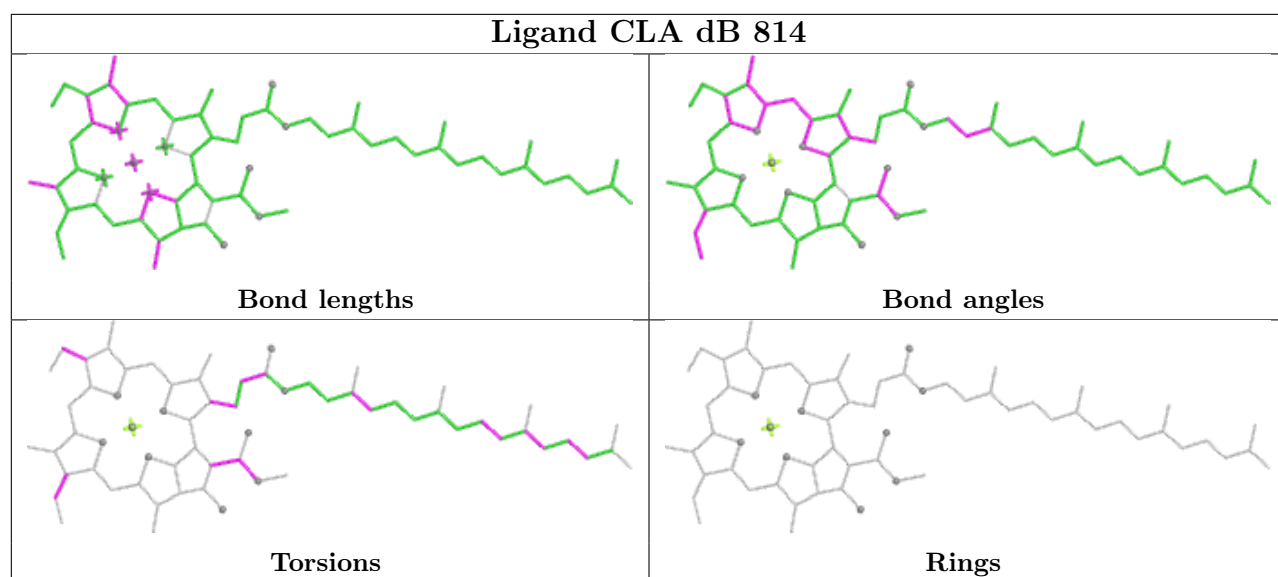


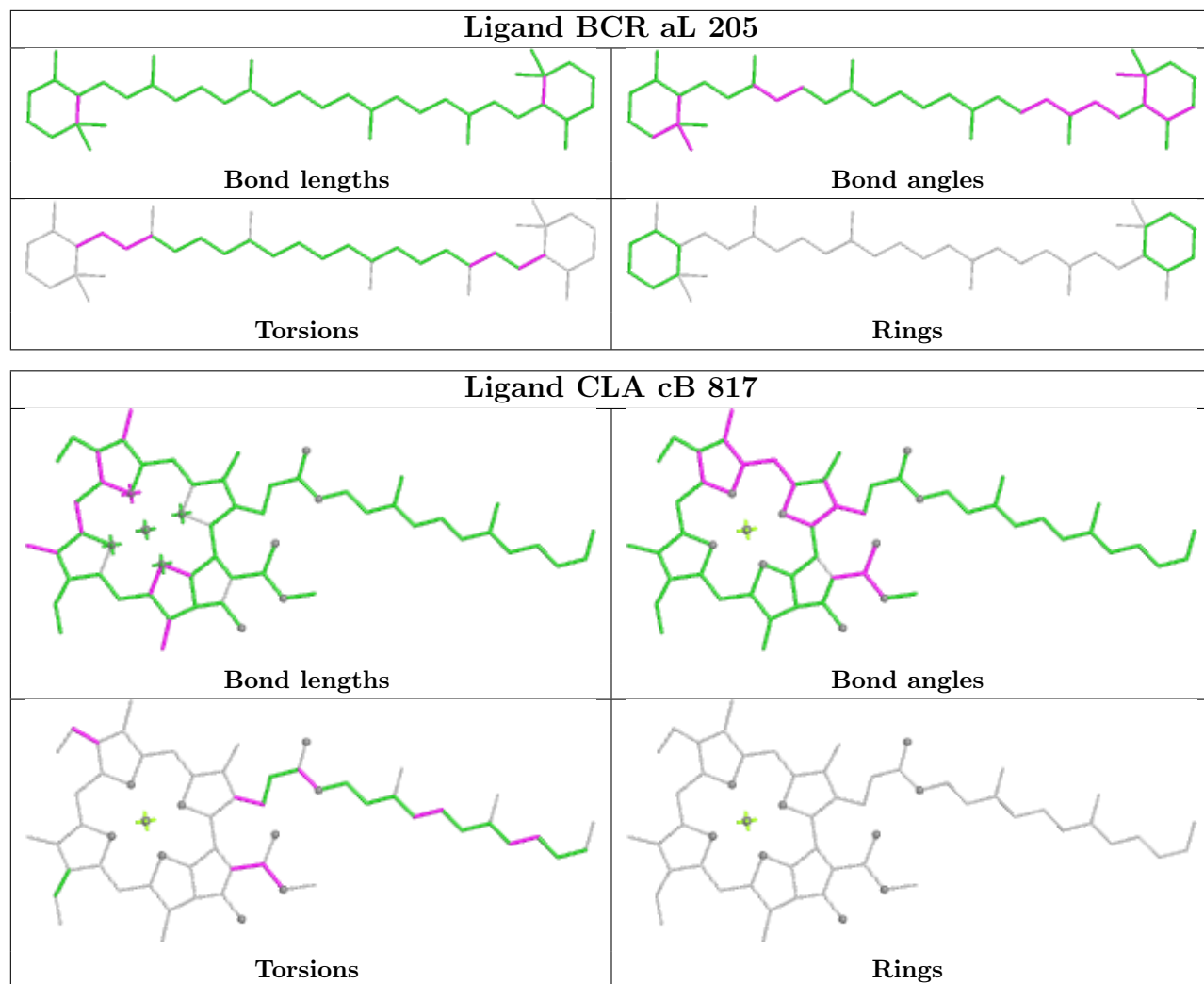
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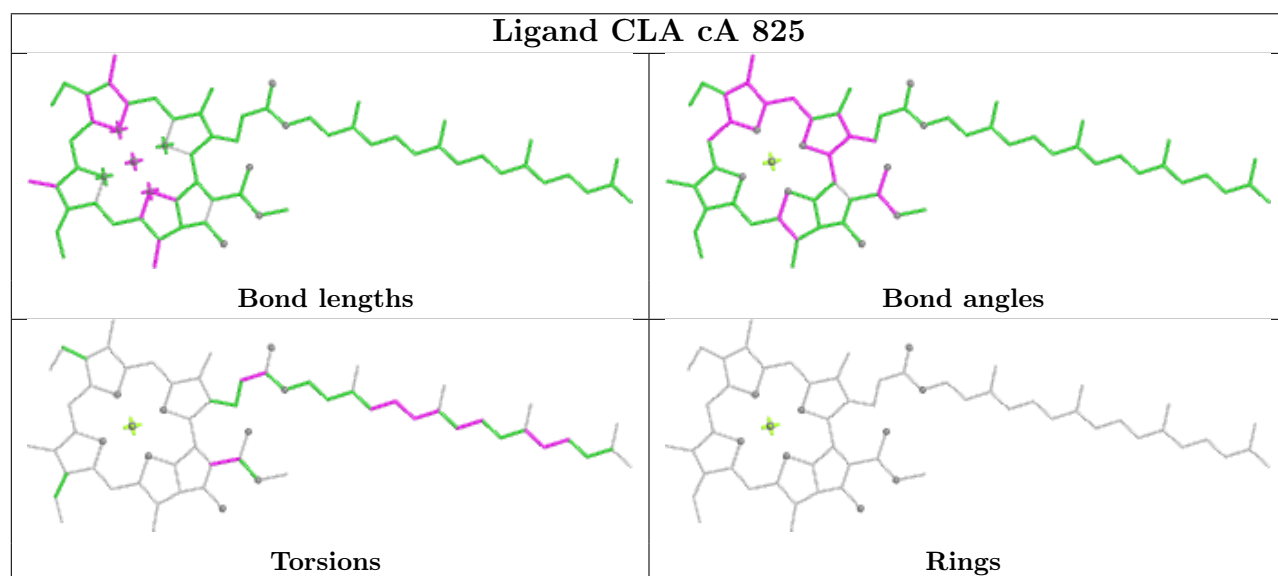
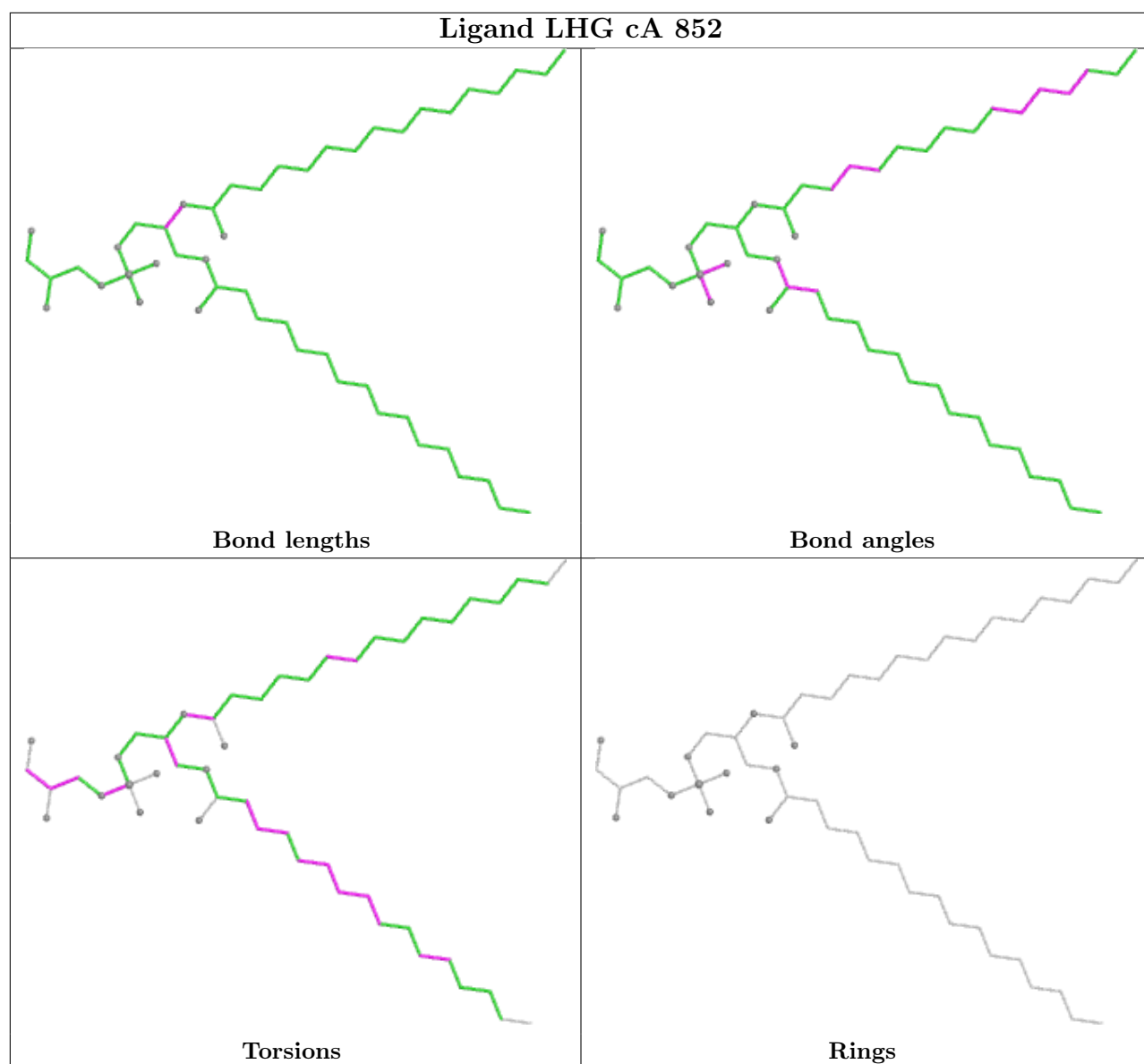


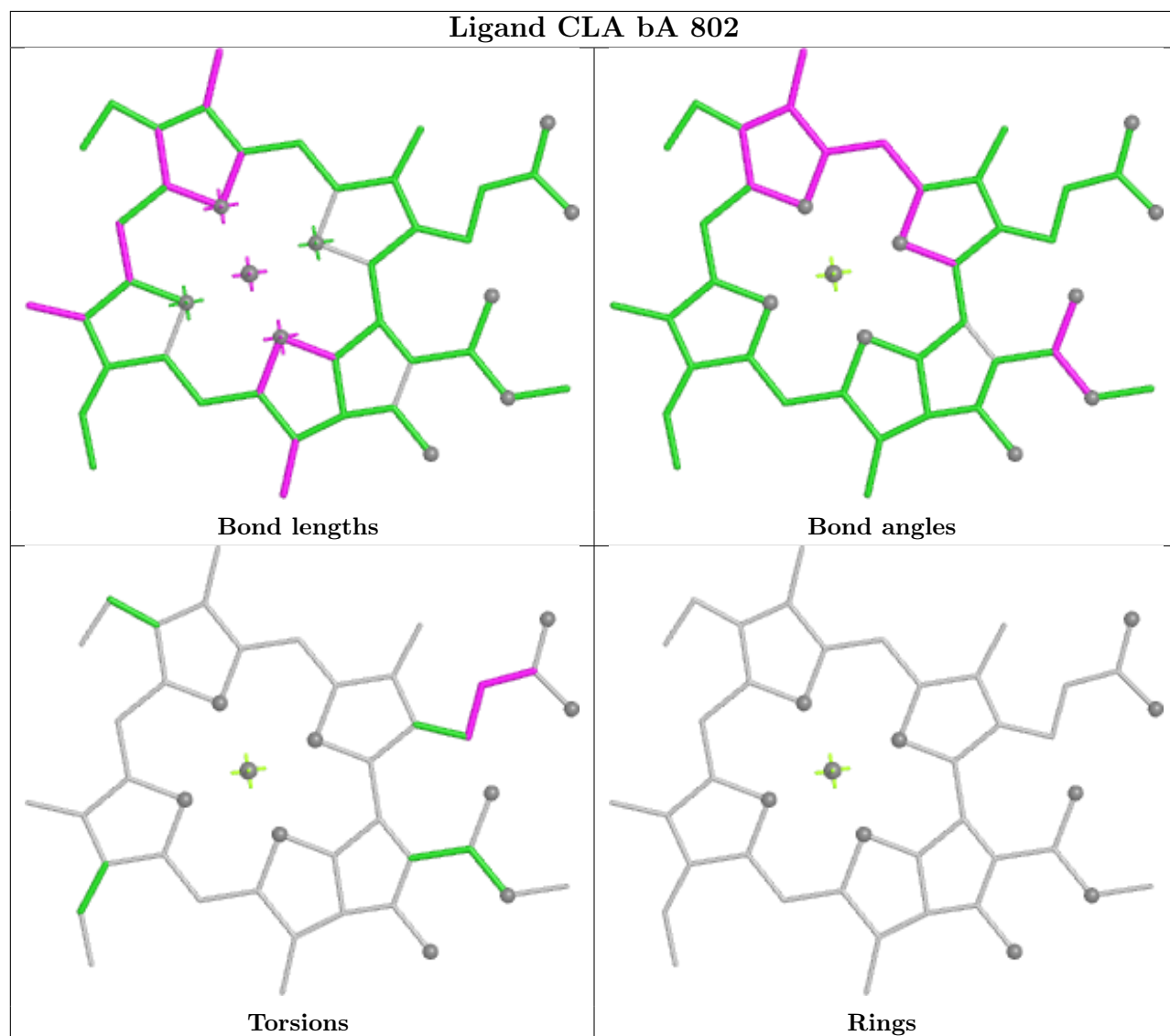
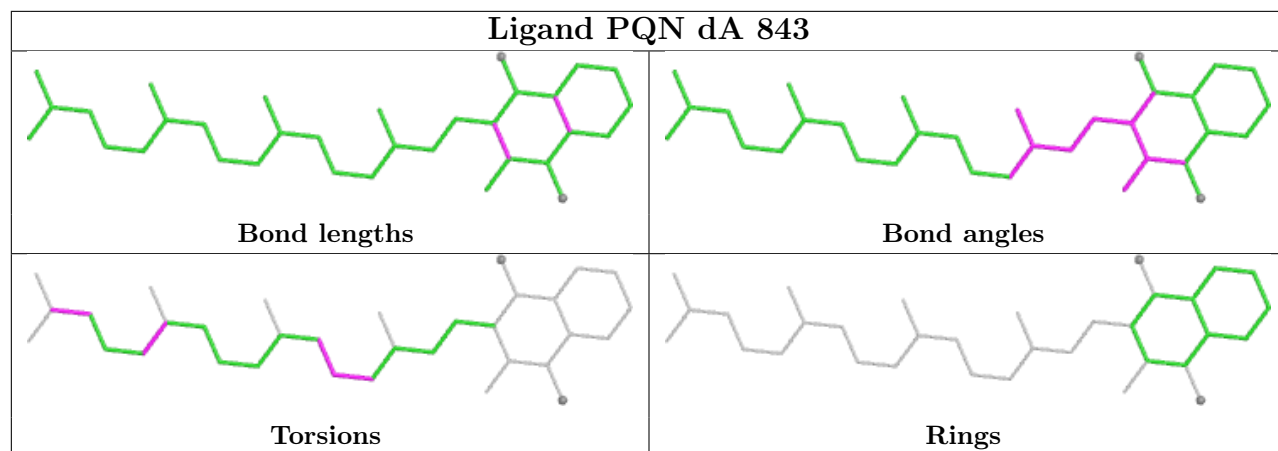
Ligand CLA cA 833

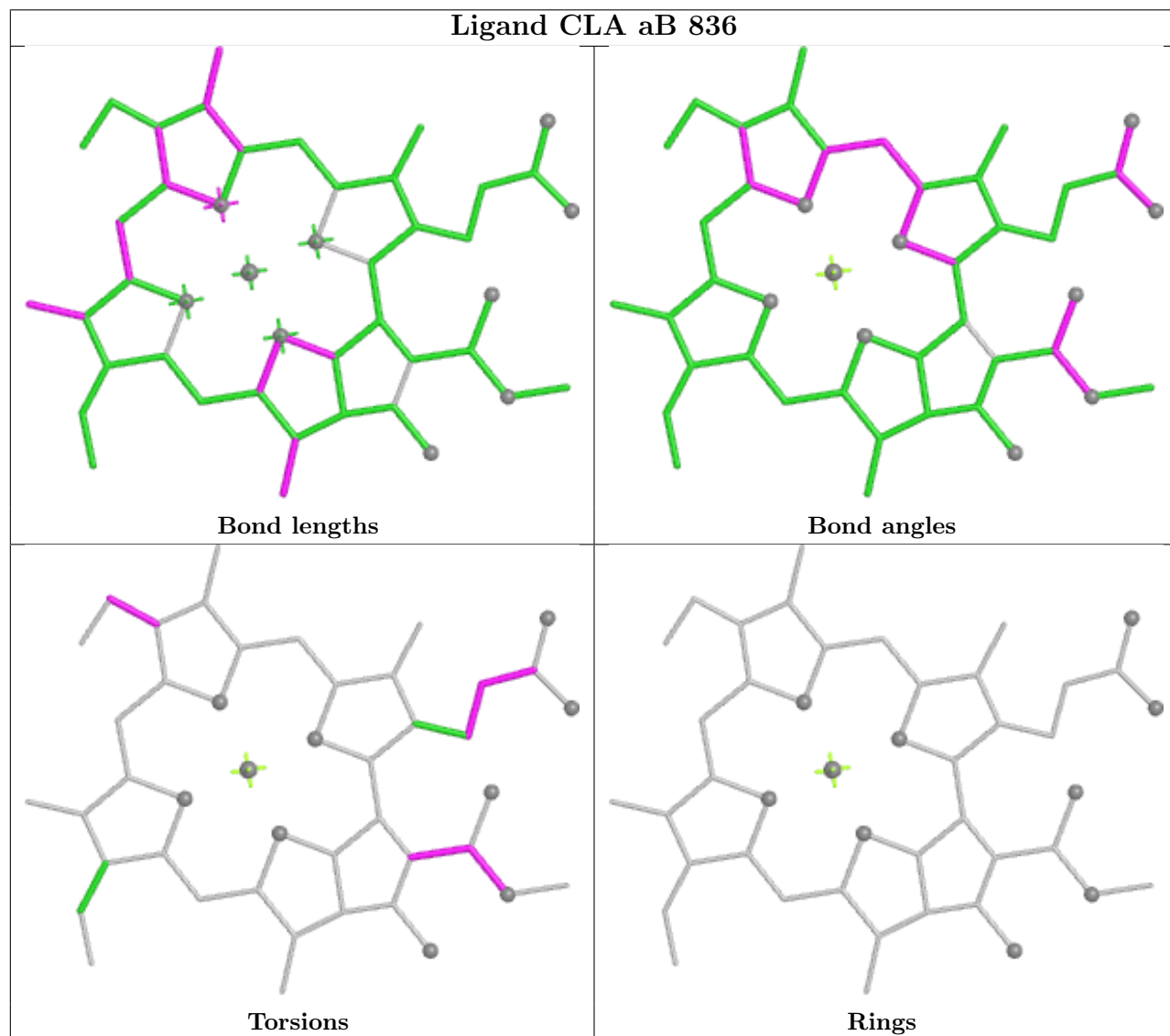
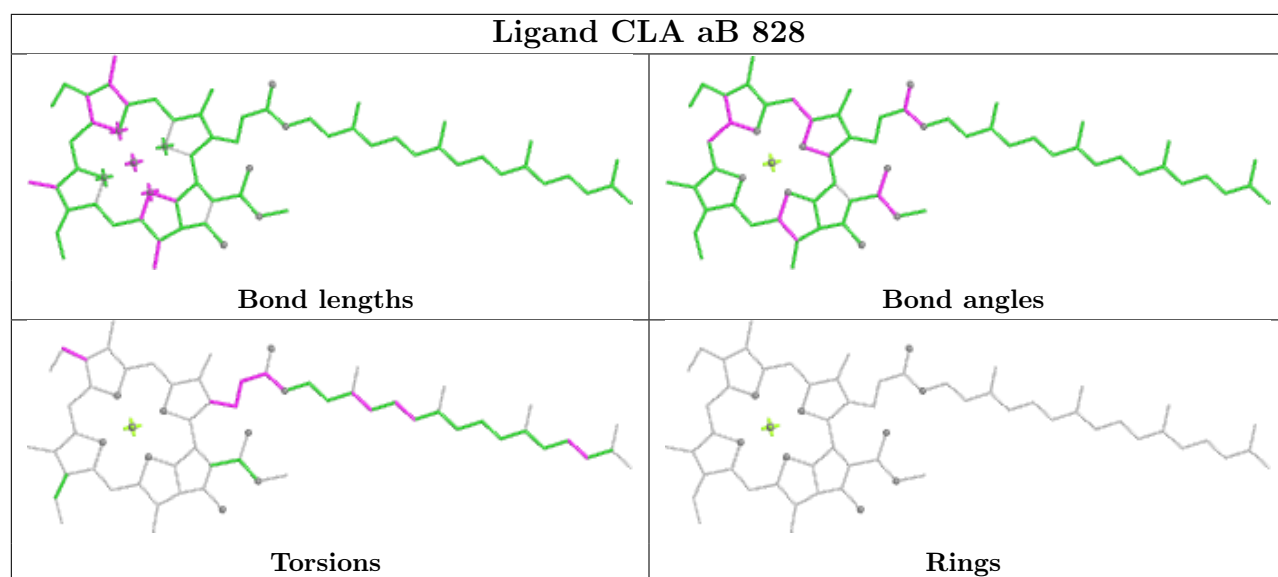


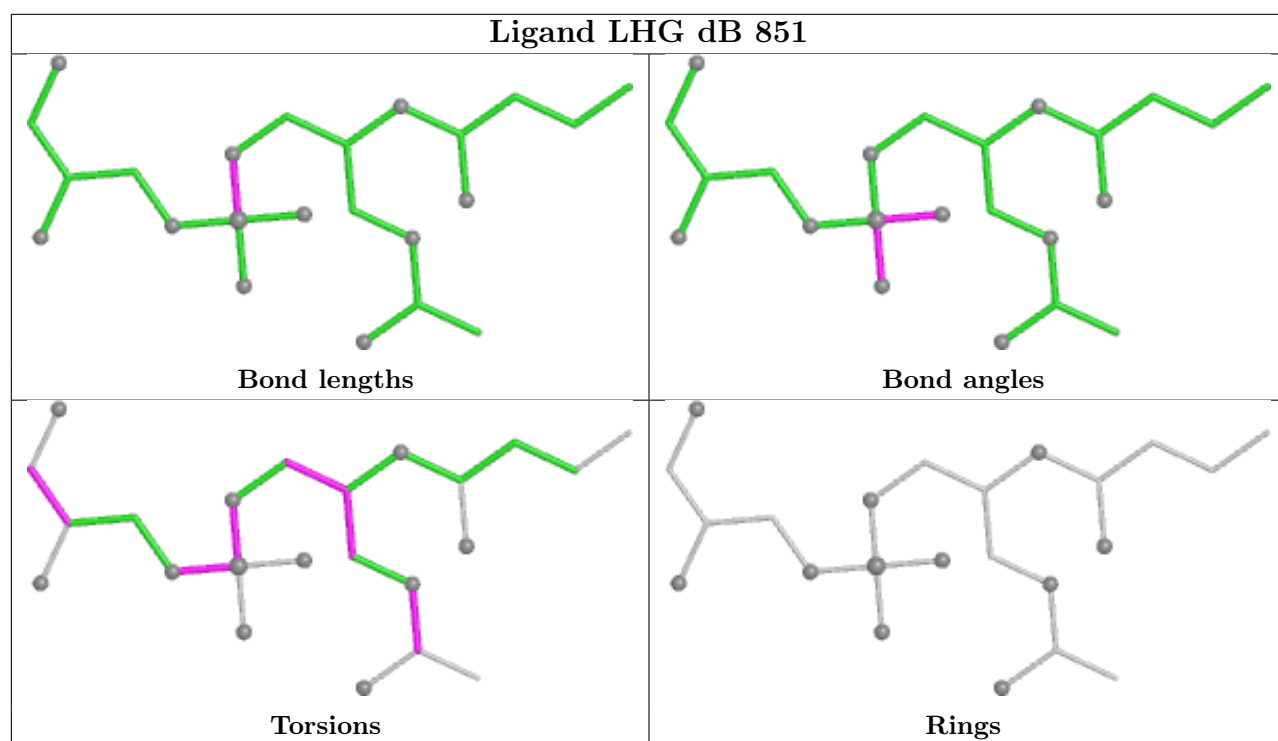


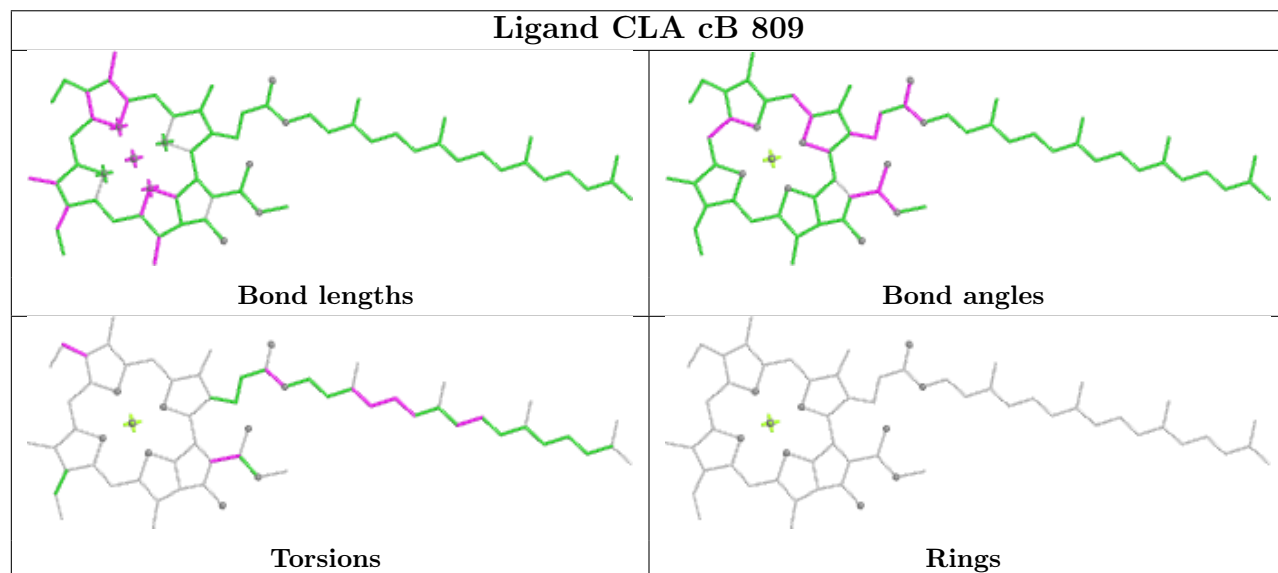
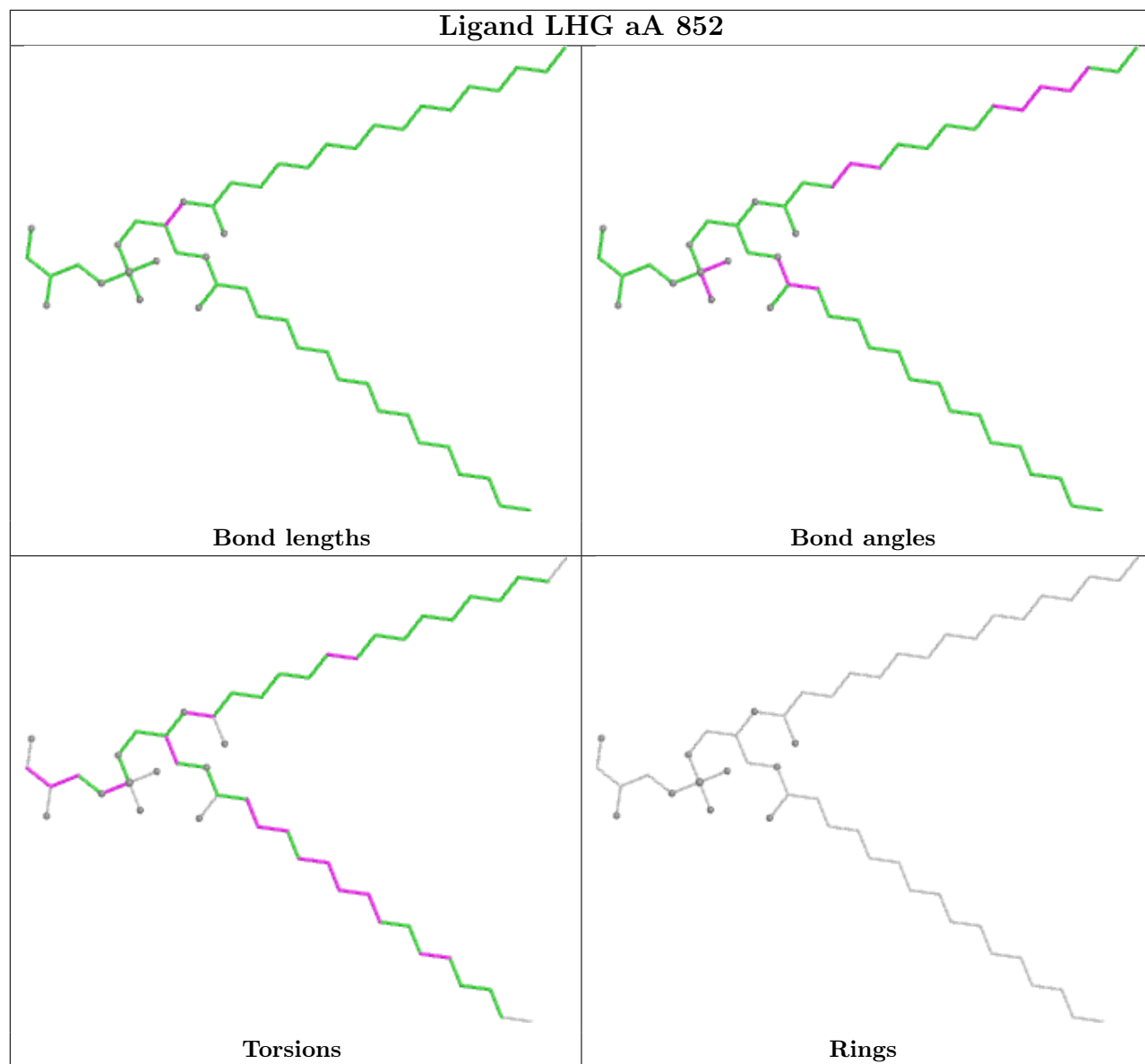




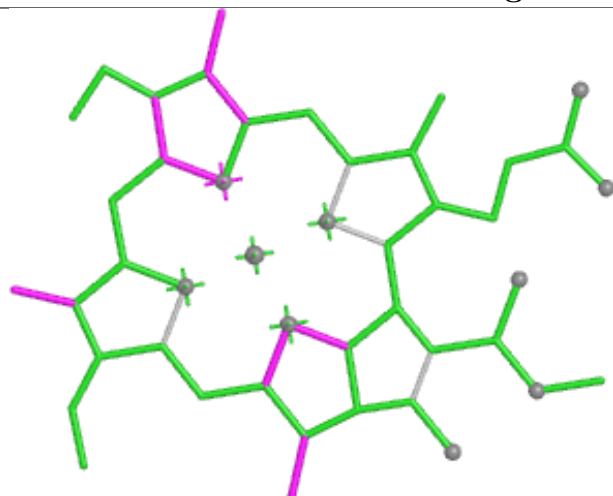




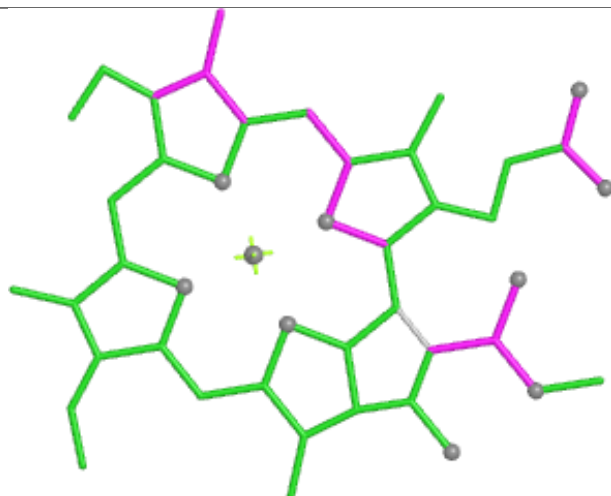




Ligand CLA aA 836



Bond lengths



Bond angles

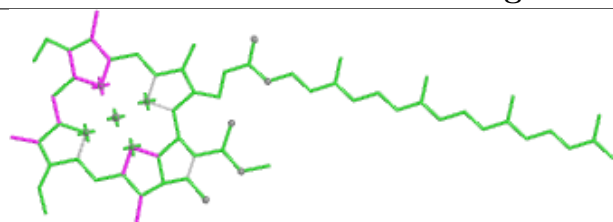


Torsions

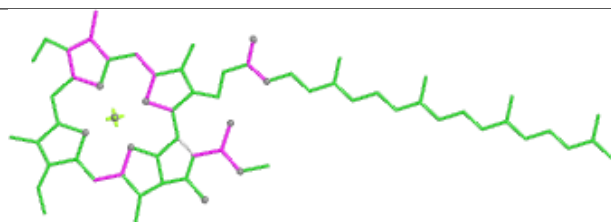


Rings

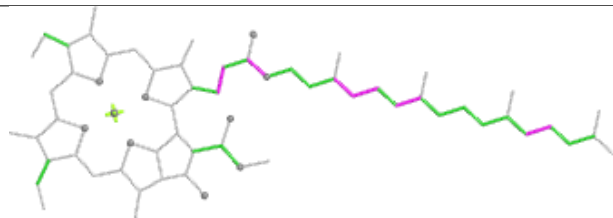
Ligand CLA dB 808



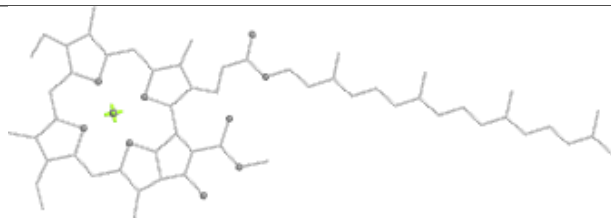
Bond lengths



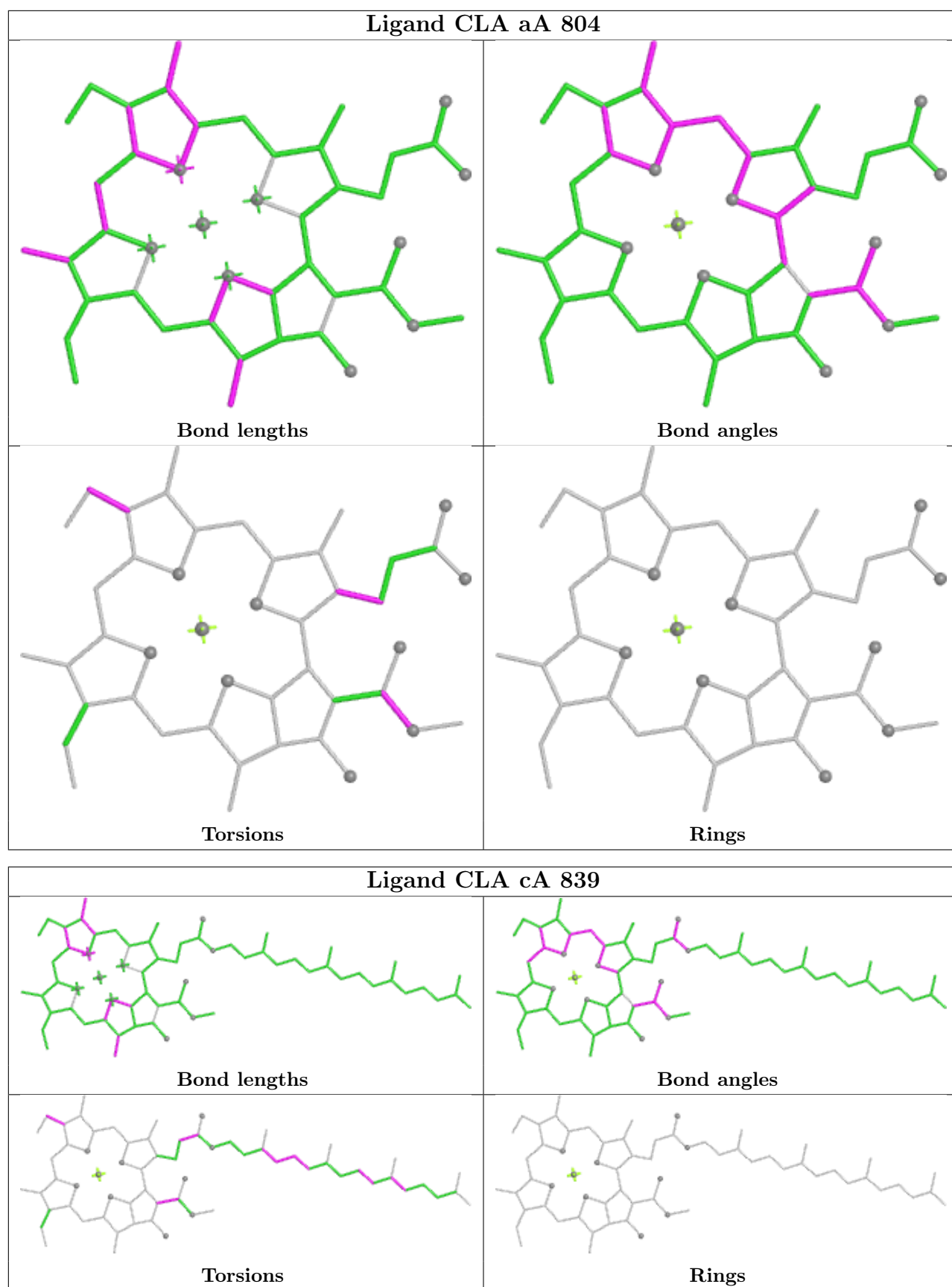
Bond angles



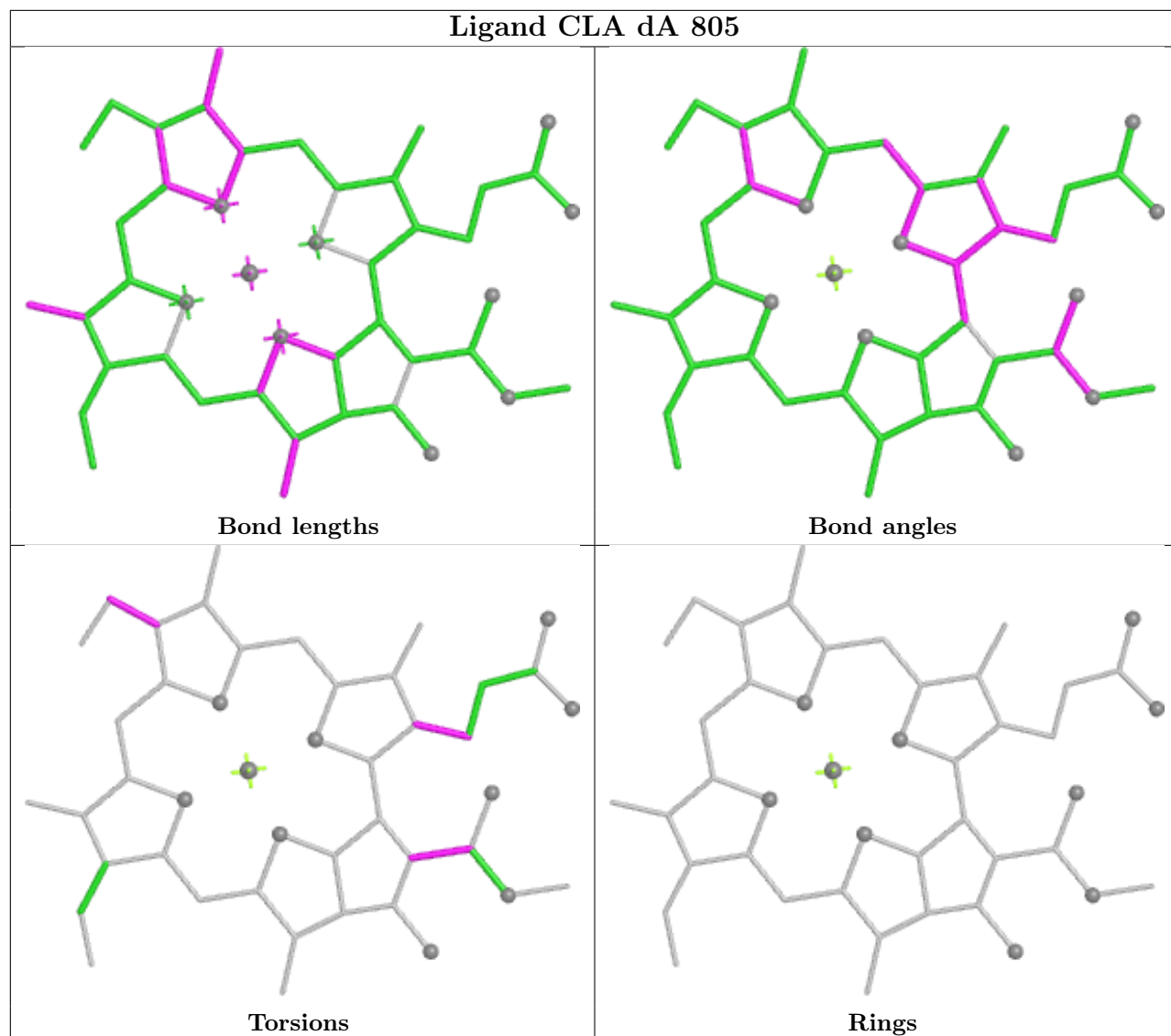
Torsions



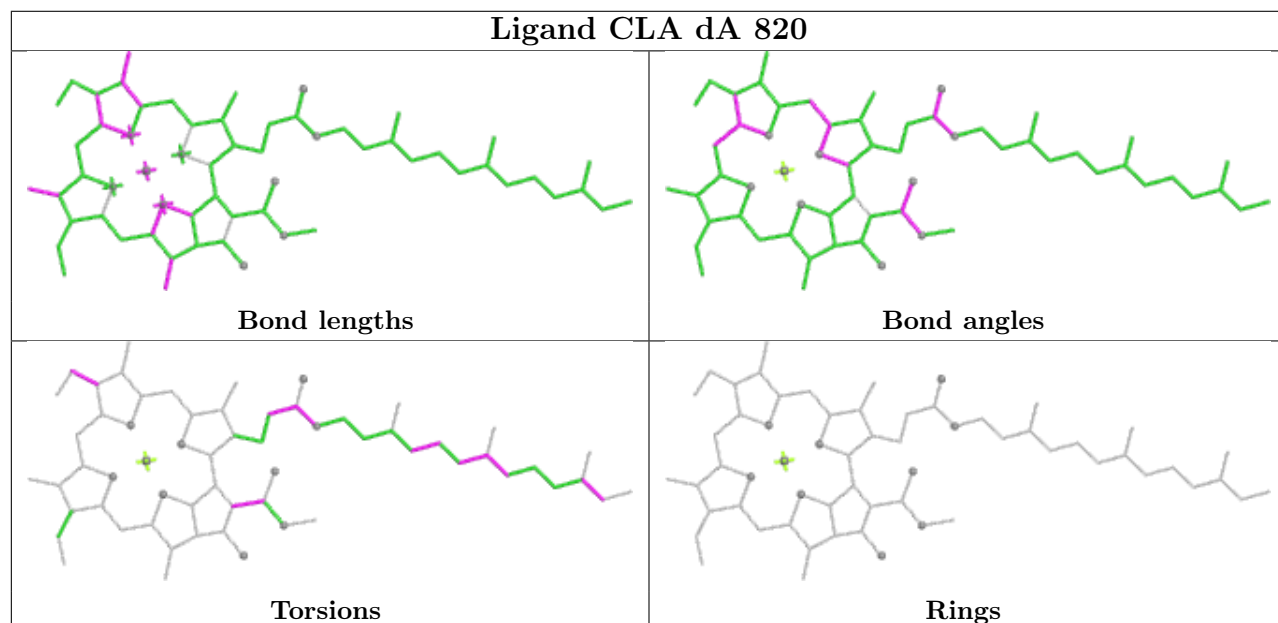
Rings

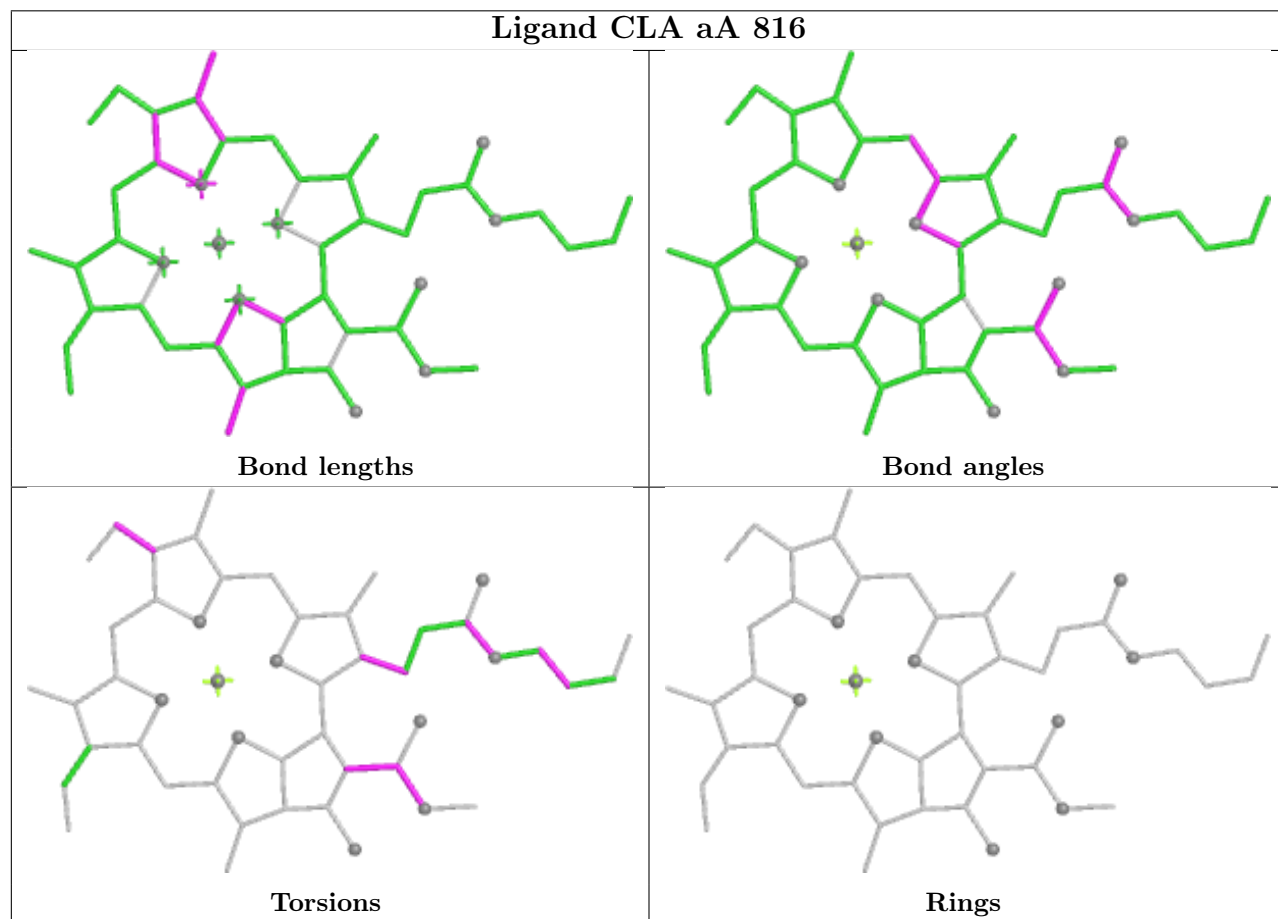
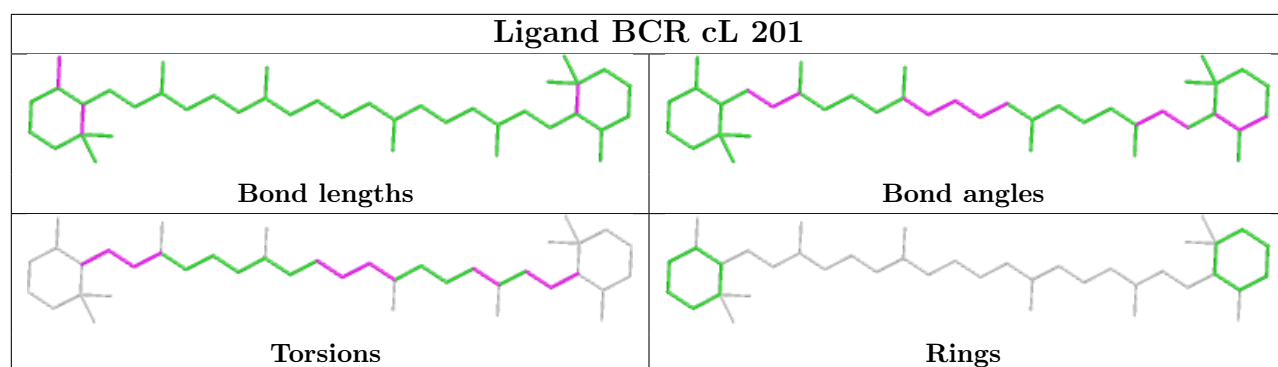


Ligand CLA dA 805

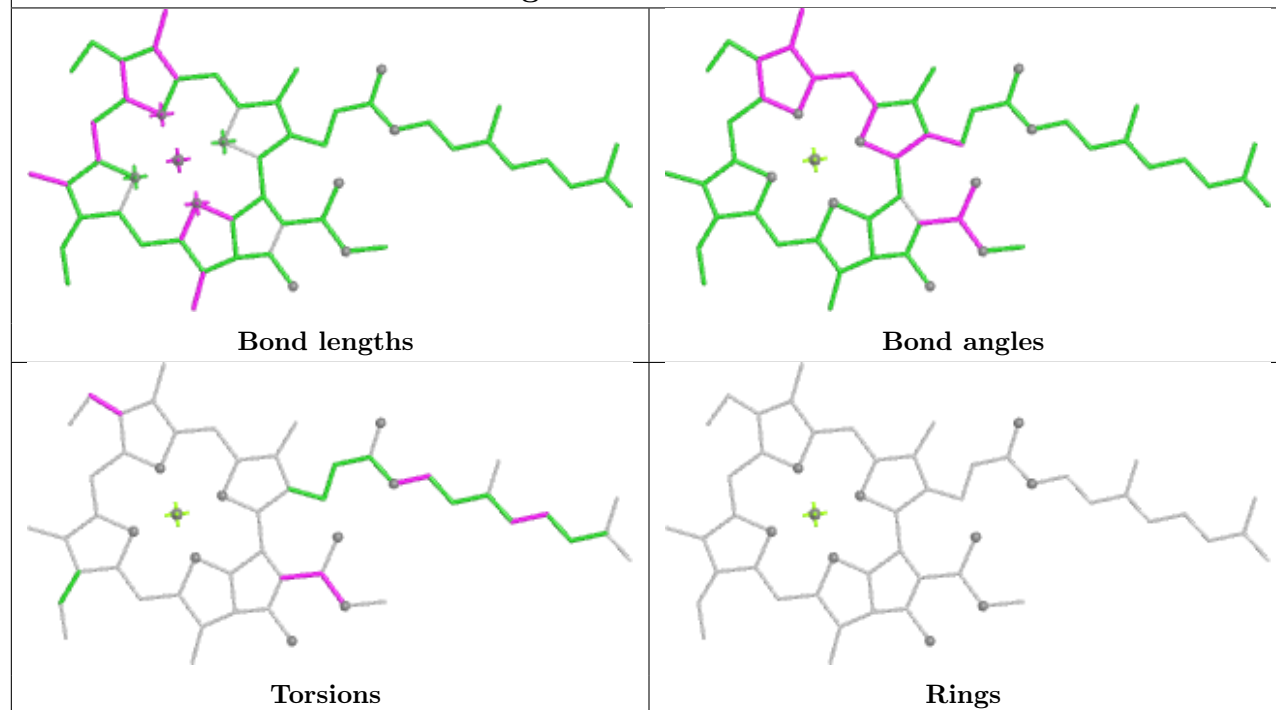


Ligand CLA dA 820

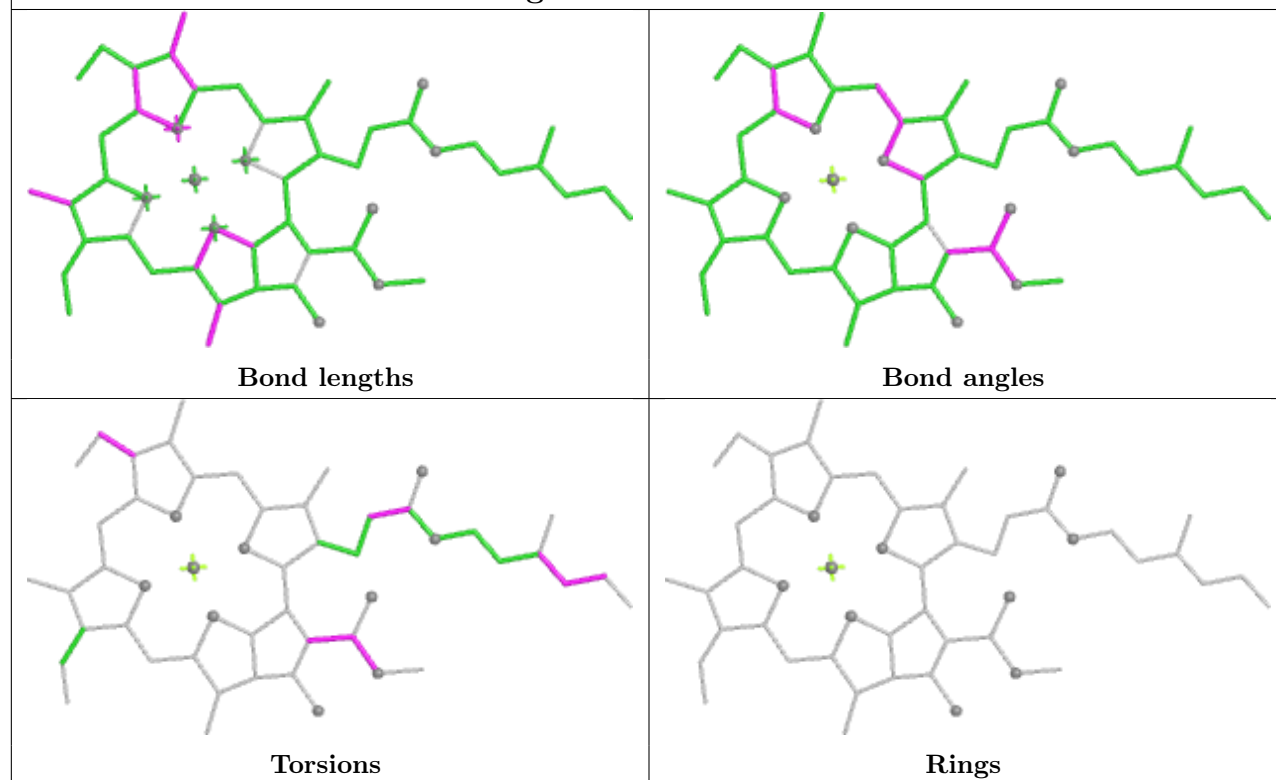


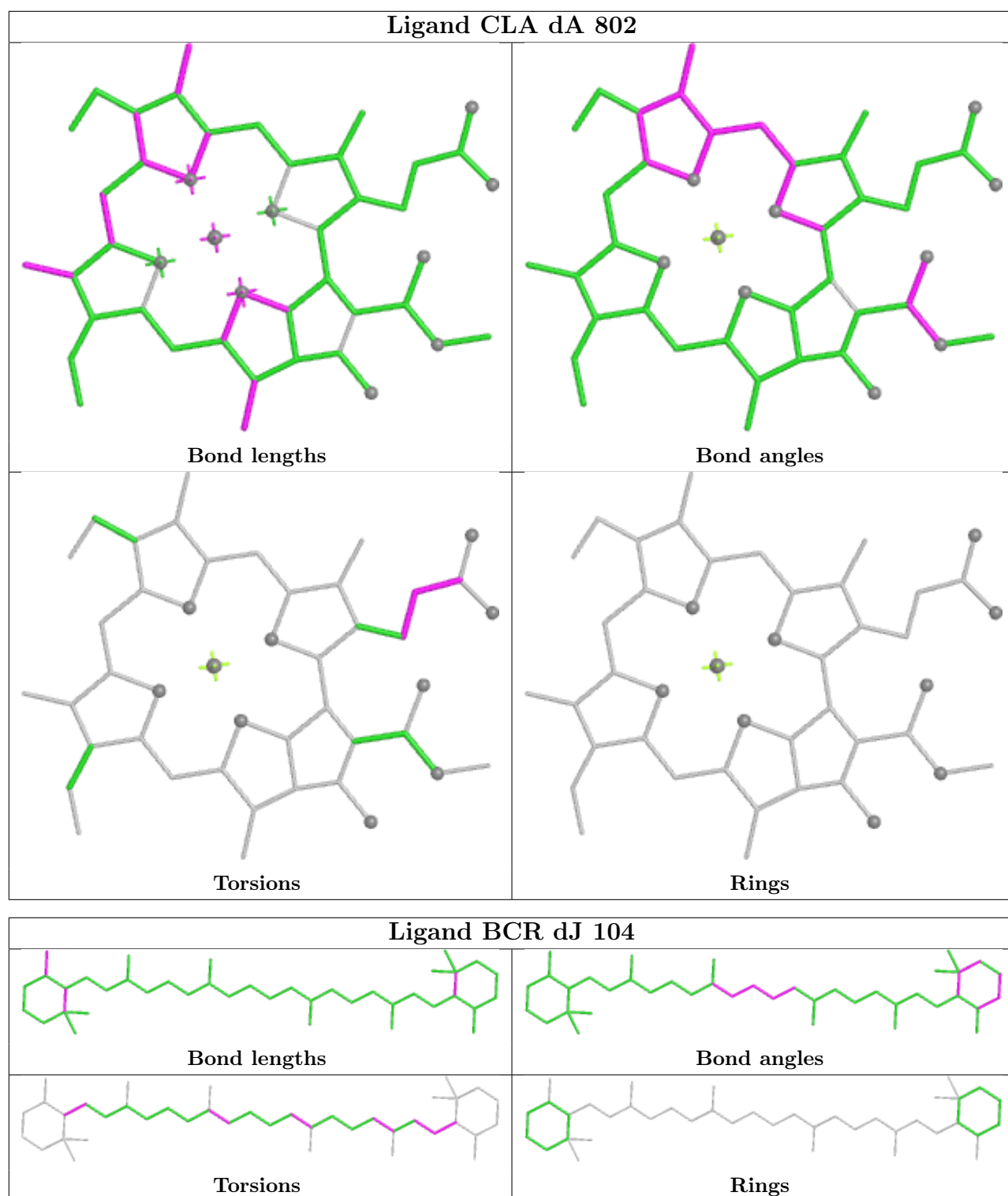


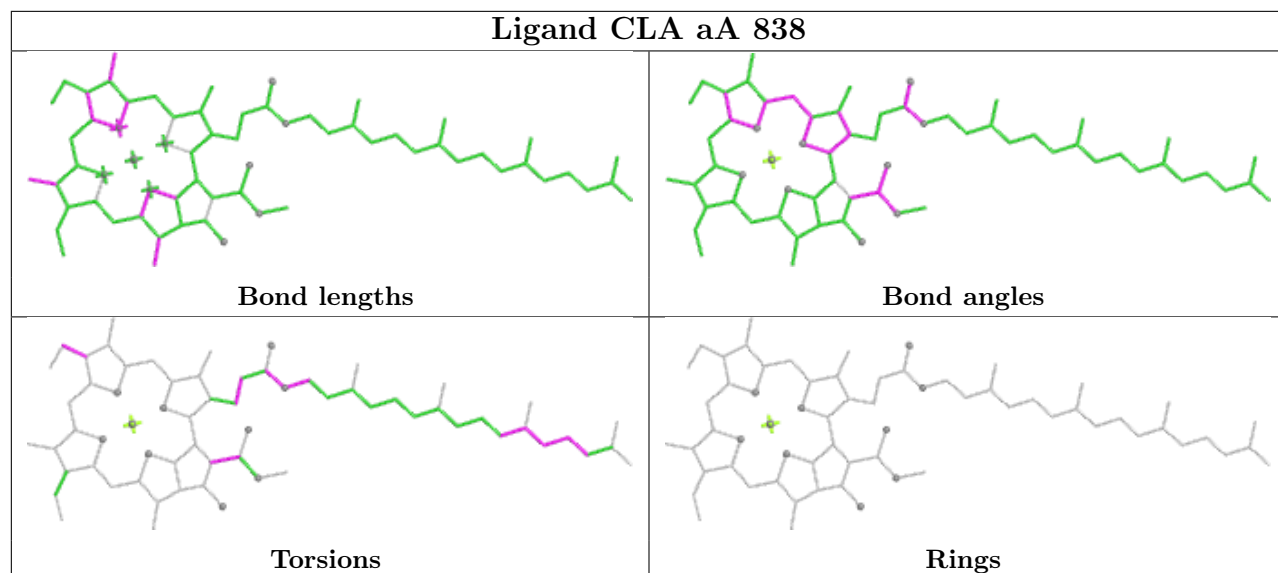
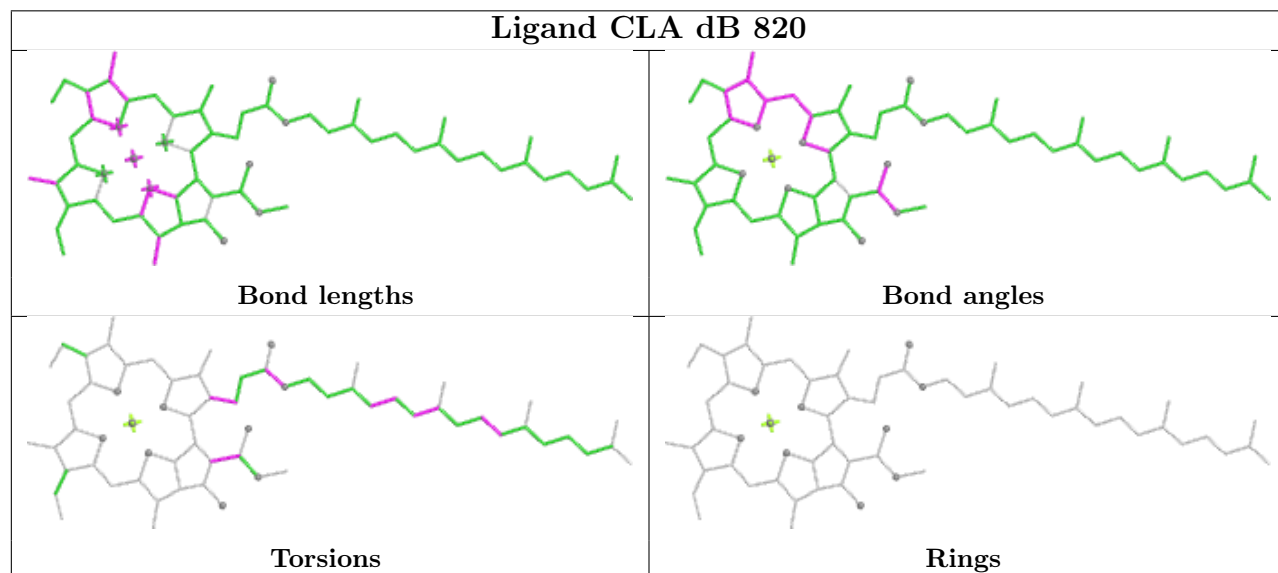
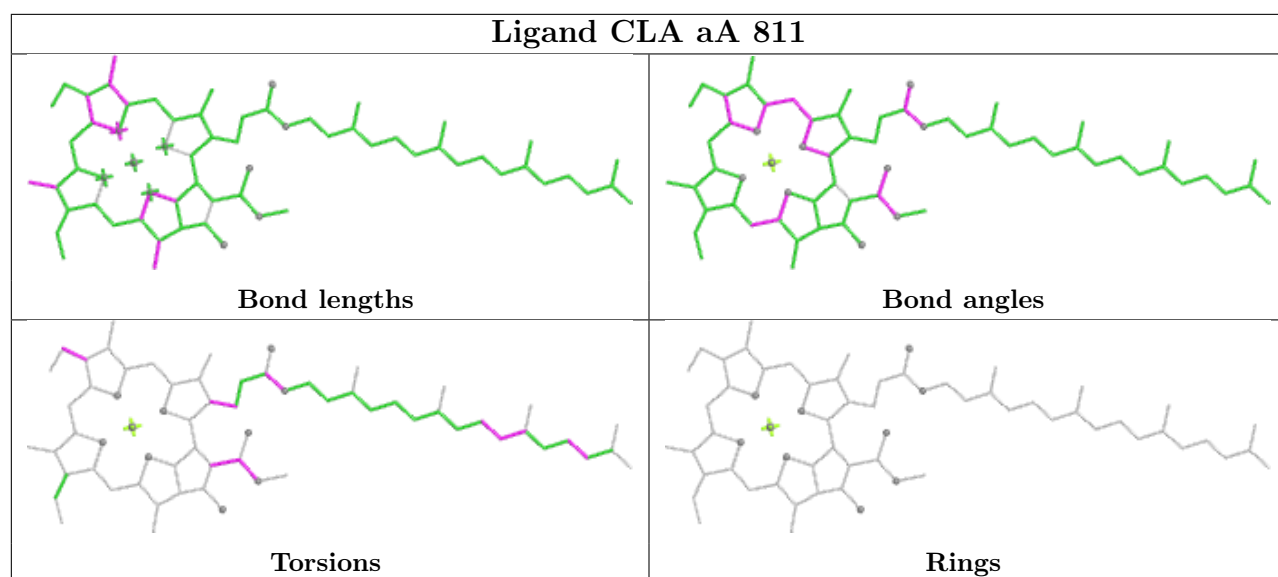
Ligand CLA dA 826

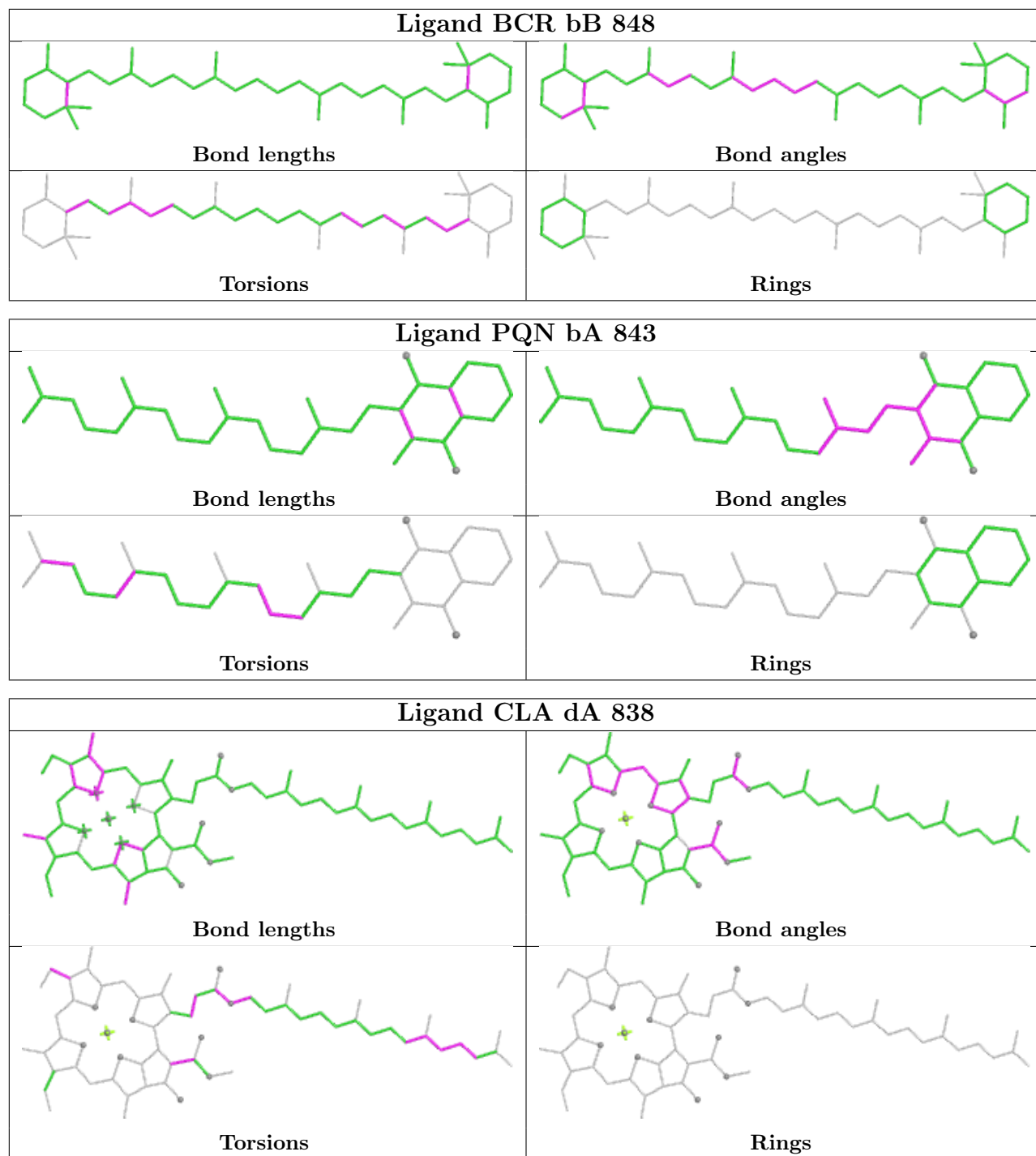


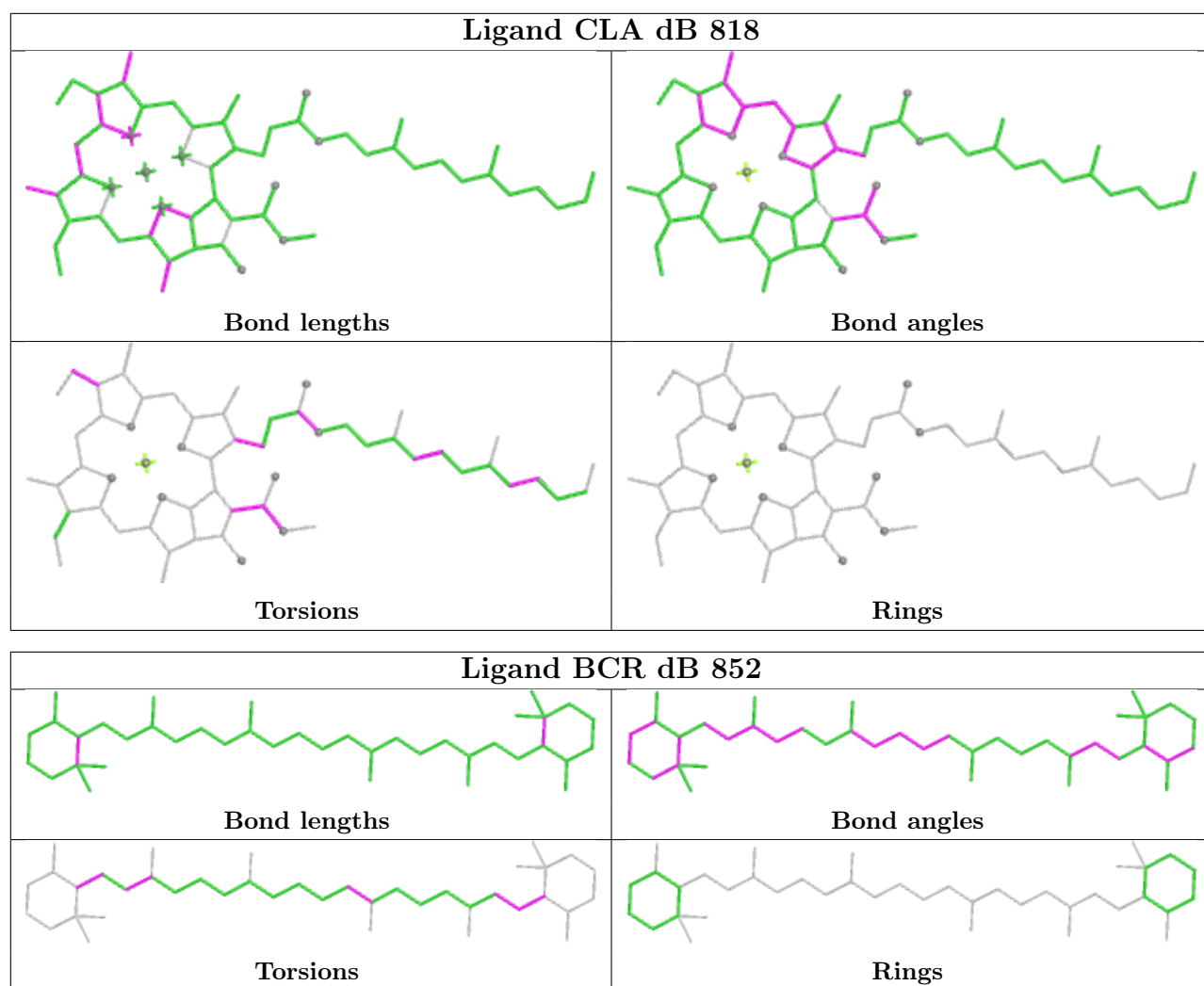
Ligand CLA cL 204

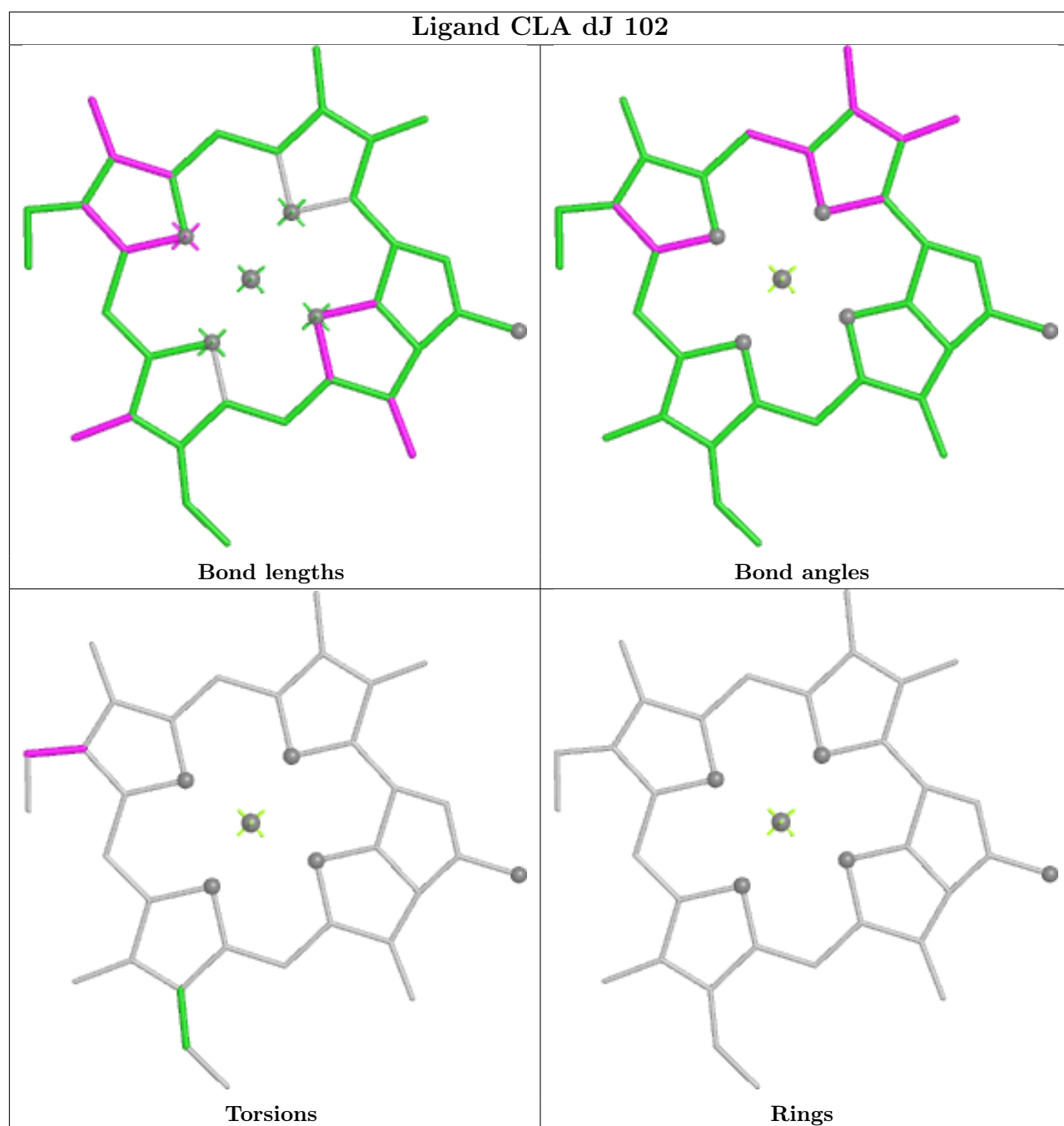


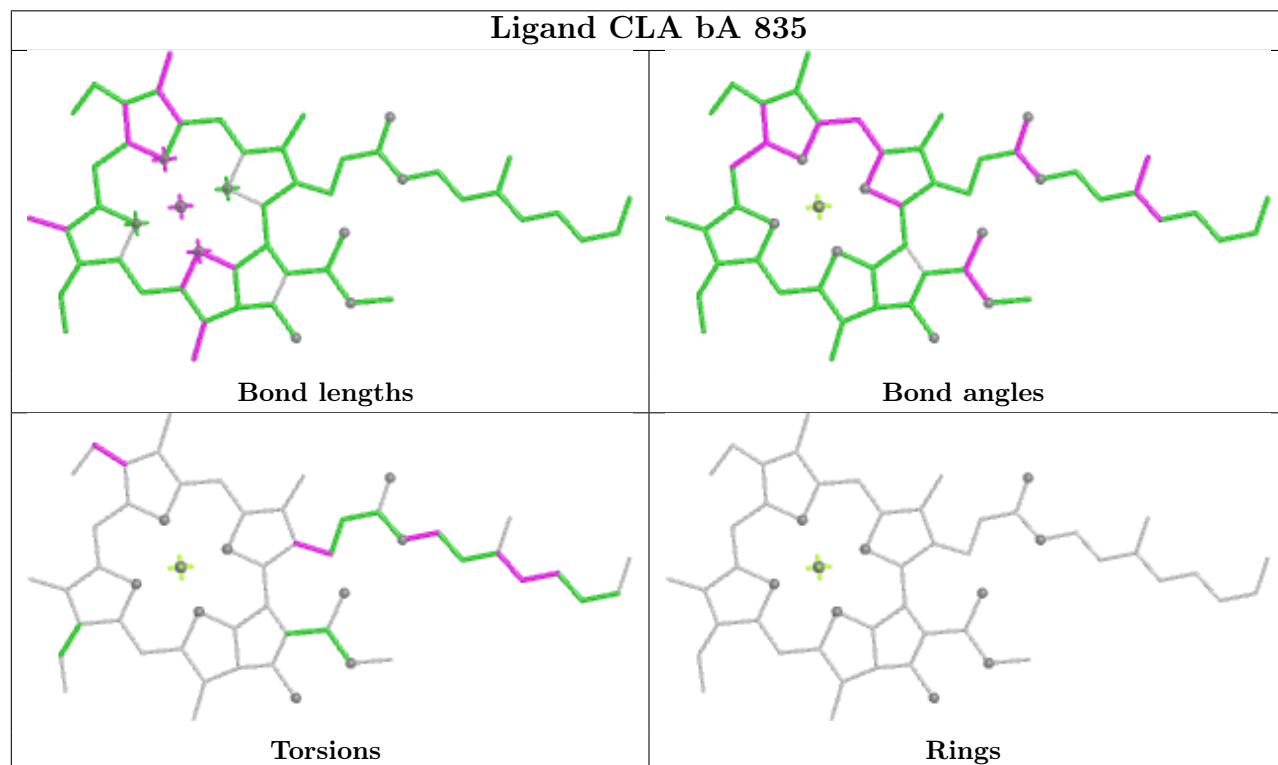
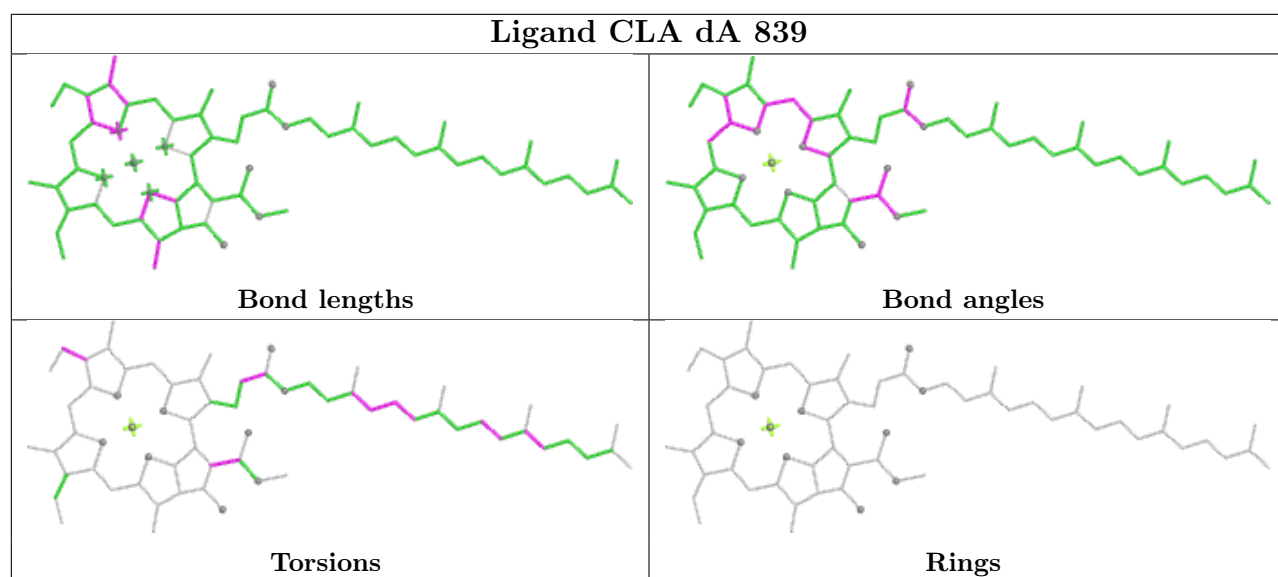




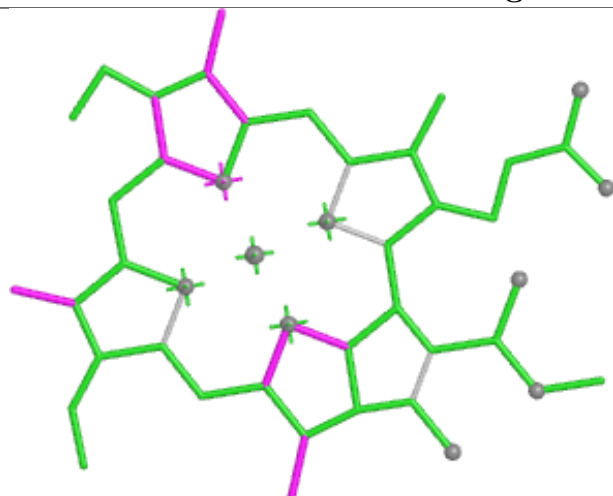




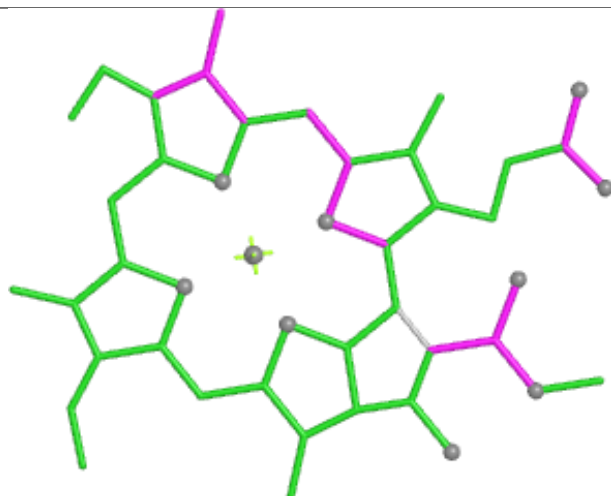




Ligand CLA cA 836



Bond lengths



Bond angles

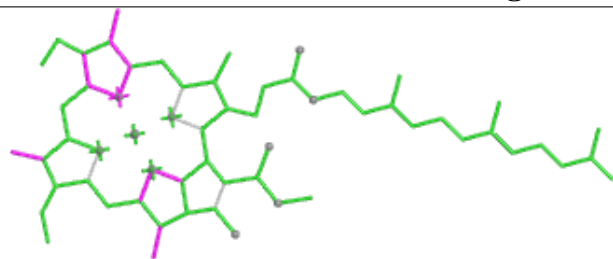


Torsions

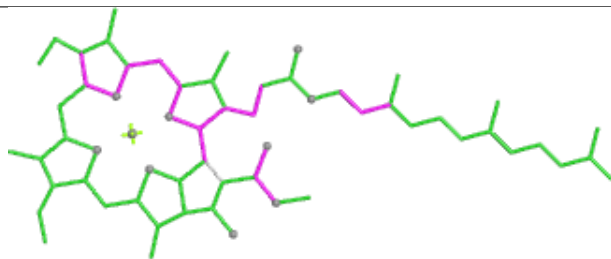


Rings

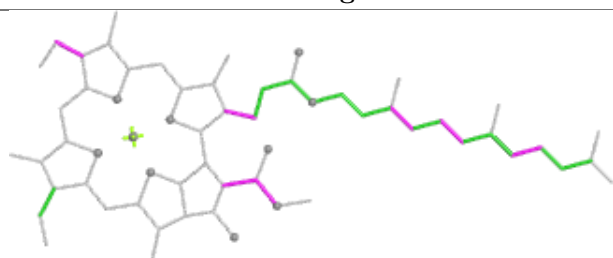
Ligand CLA aB 837



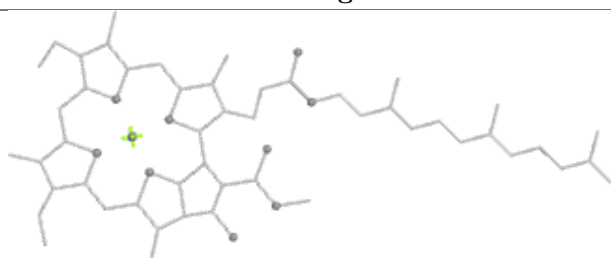
Bond lengths



Bond angles

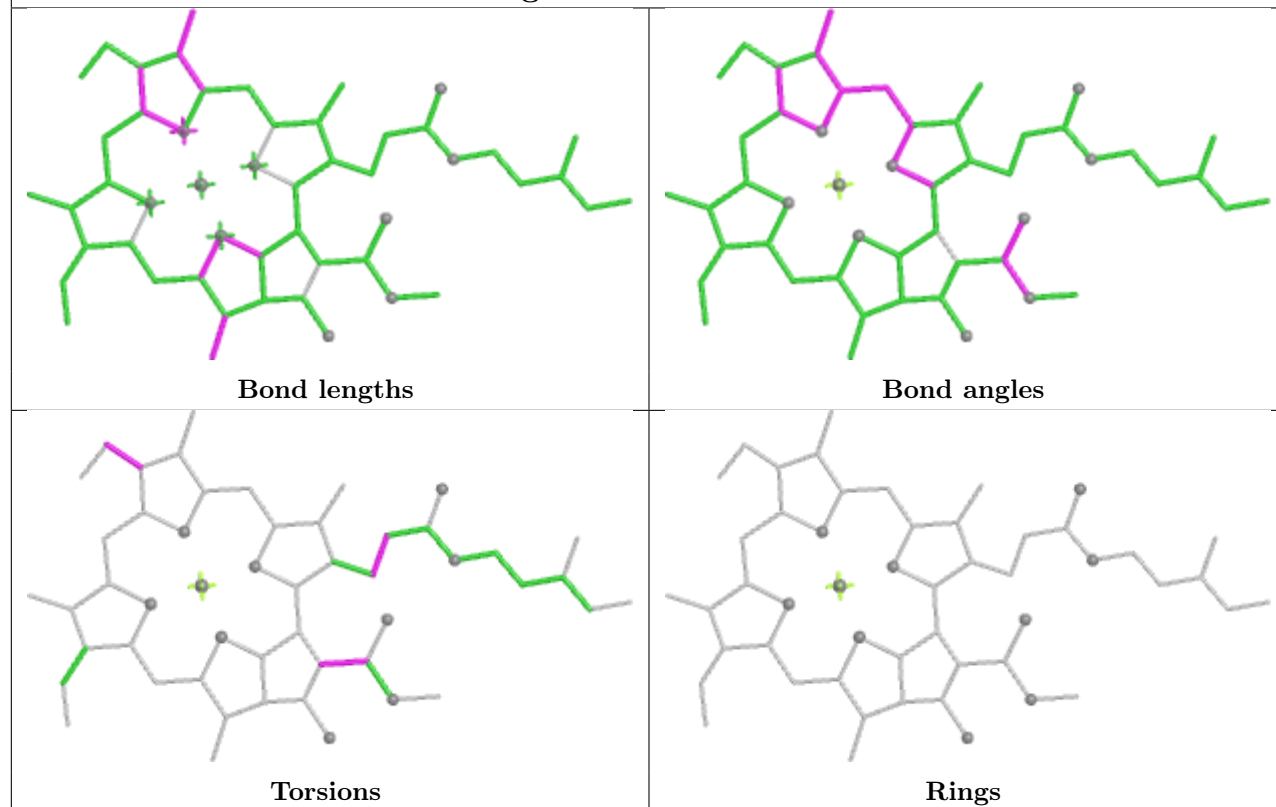


Torsions

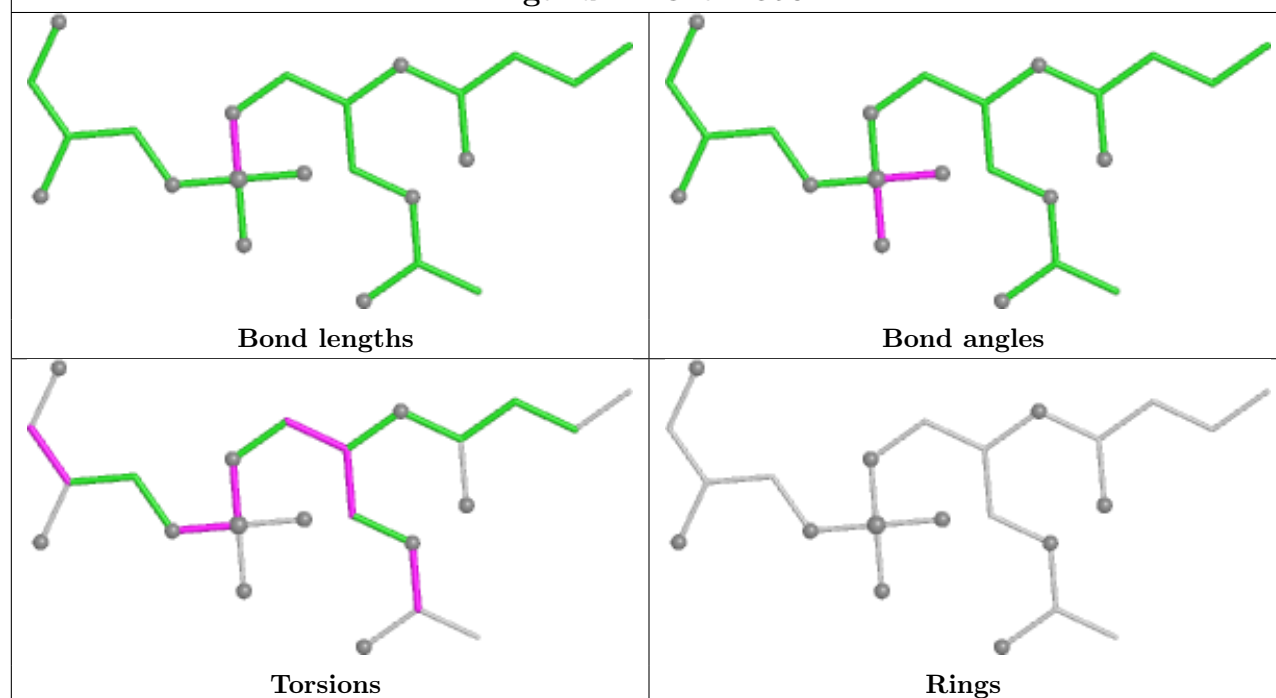


Rings

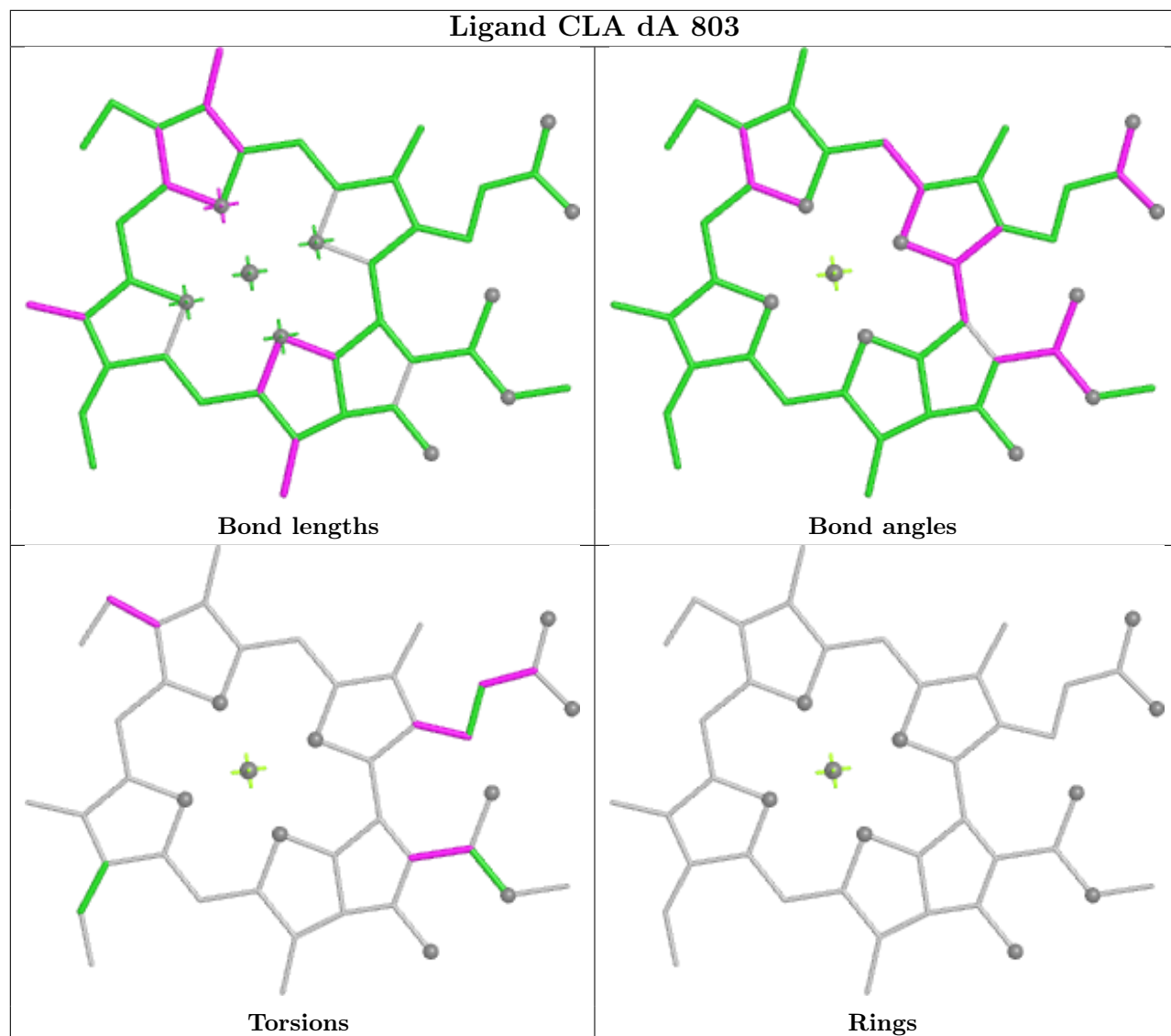
Ligand CLA bA 807



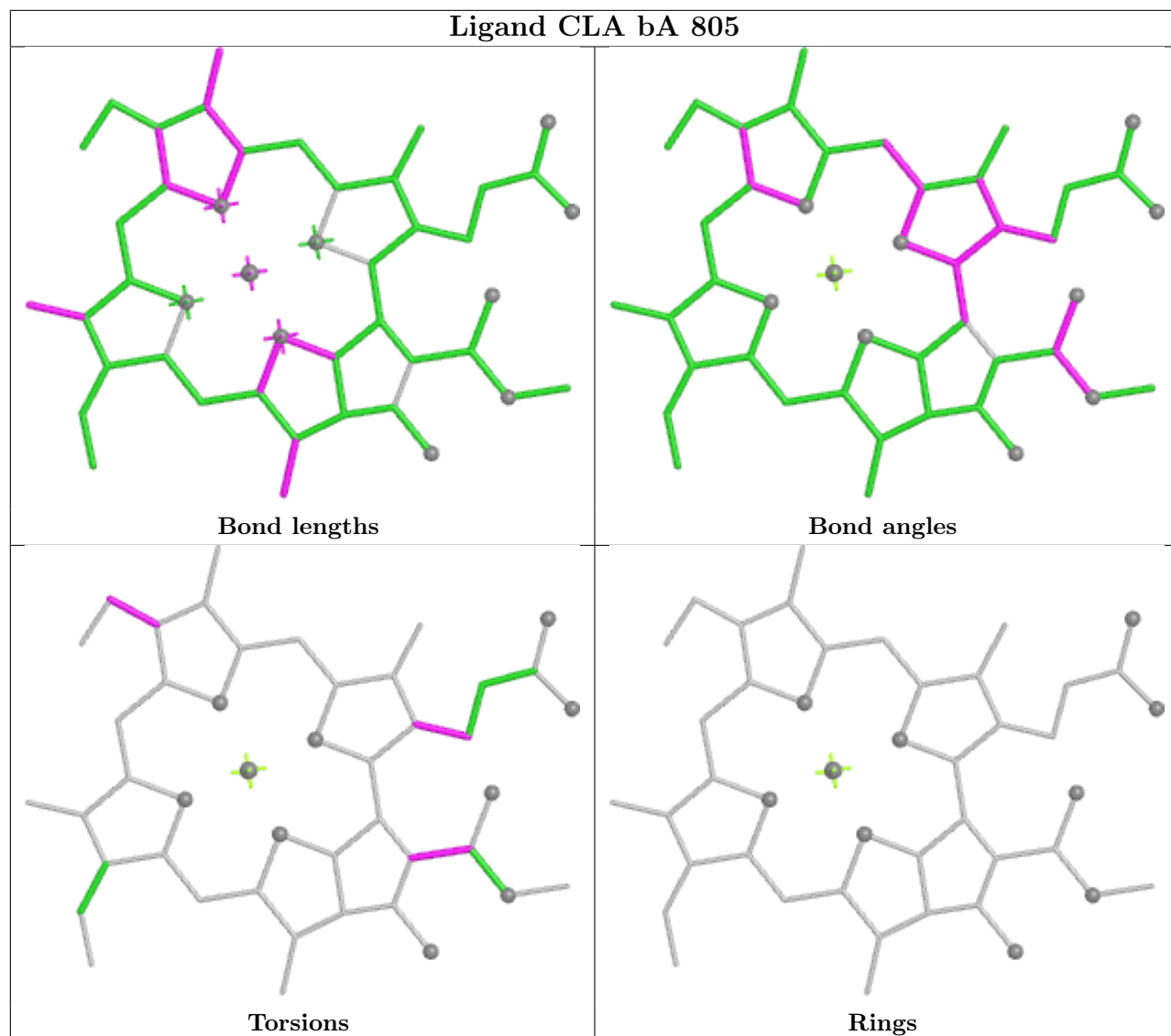
Ligand LHG cB 850



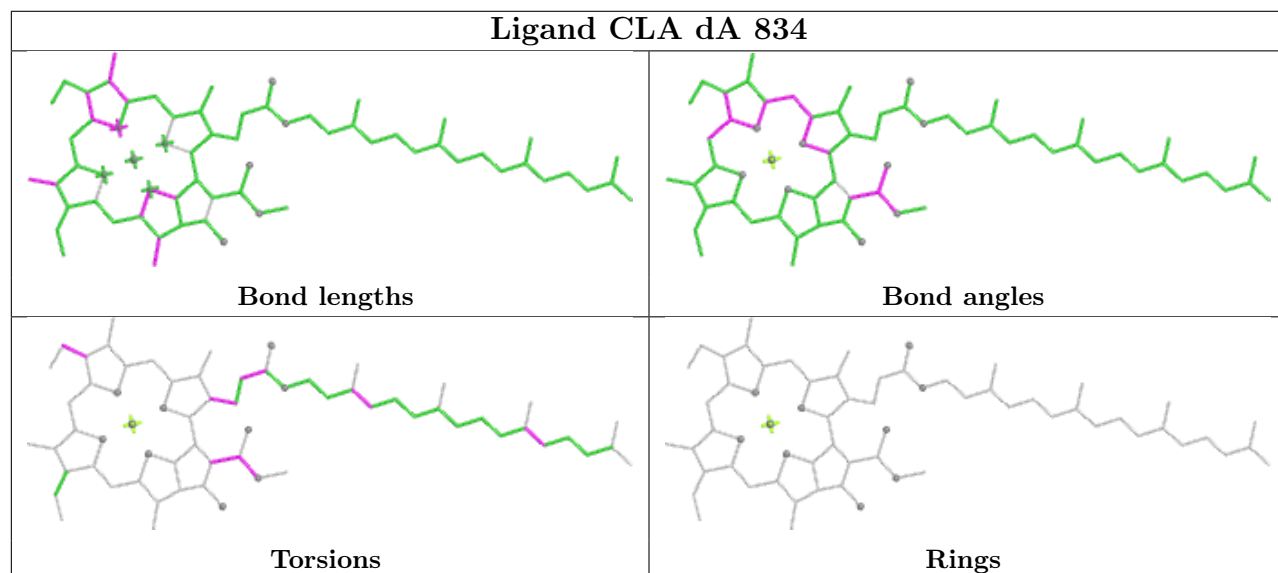
Ligand CLA dA 803

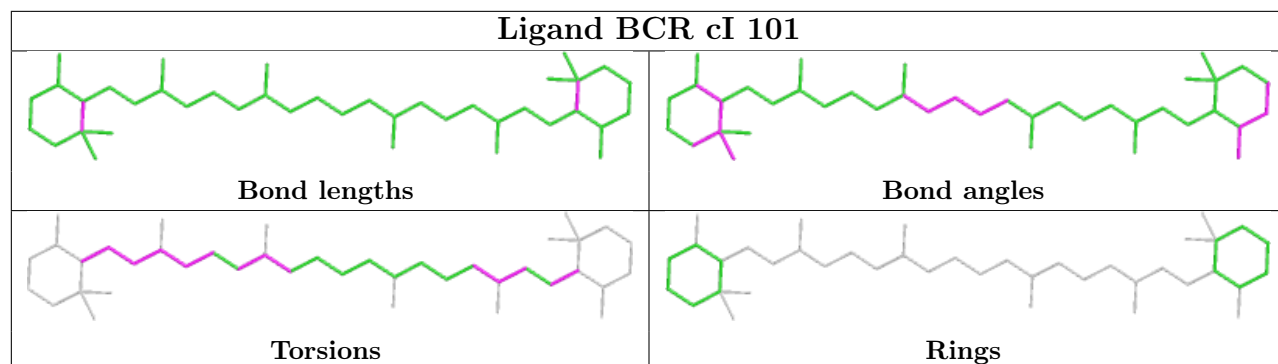
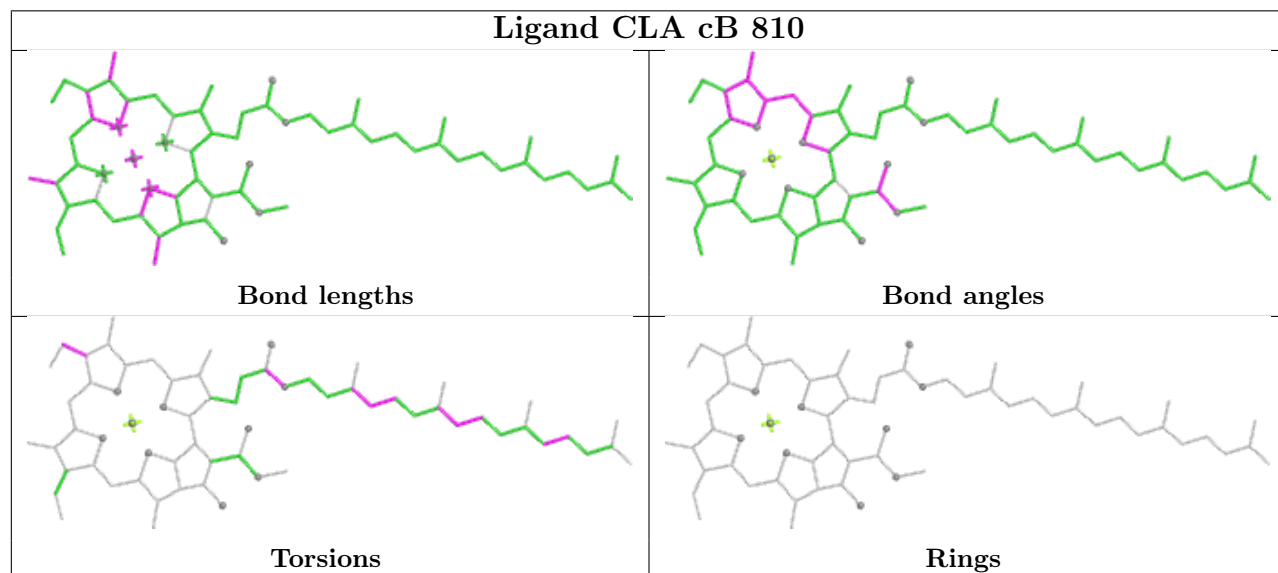
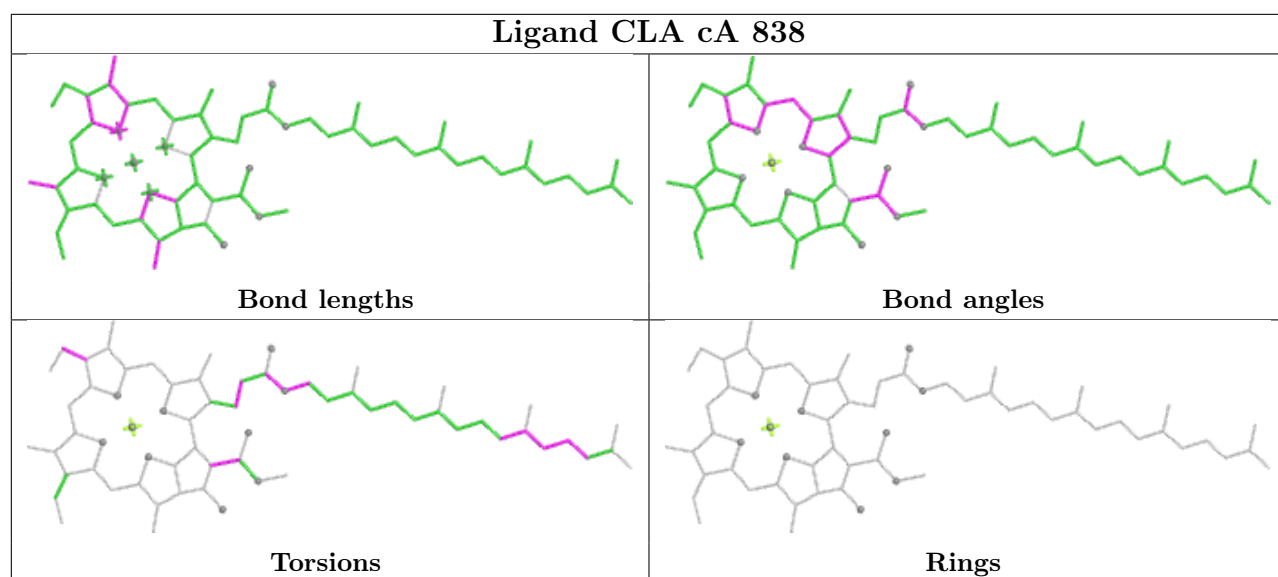


Ligand CLA bA 805

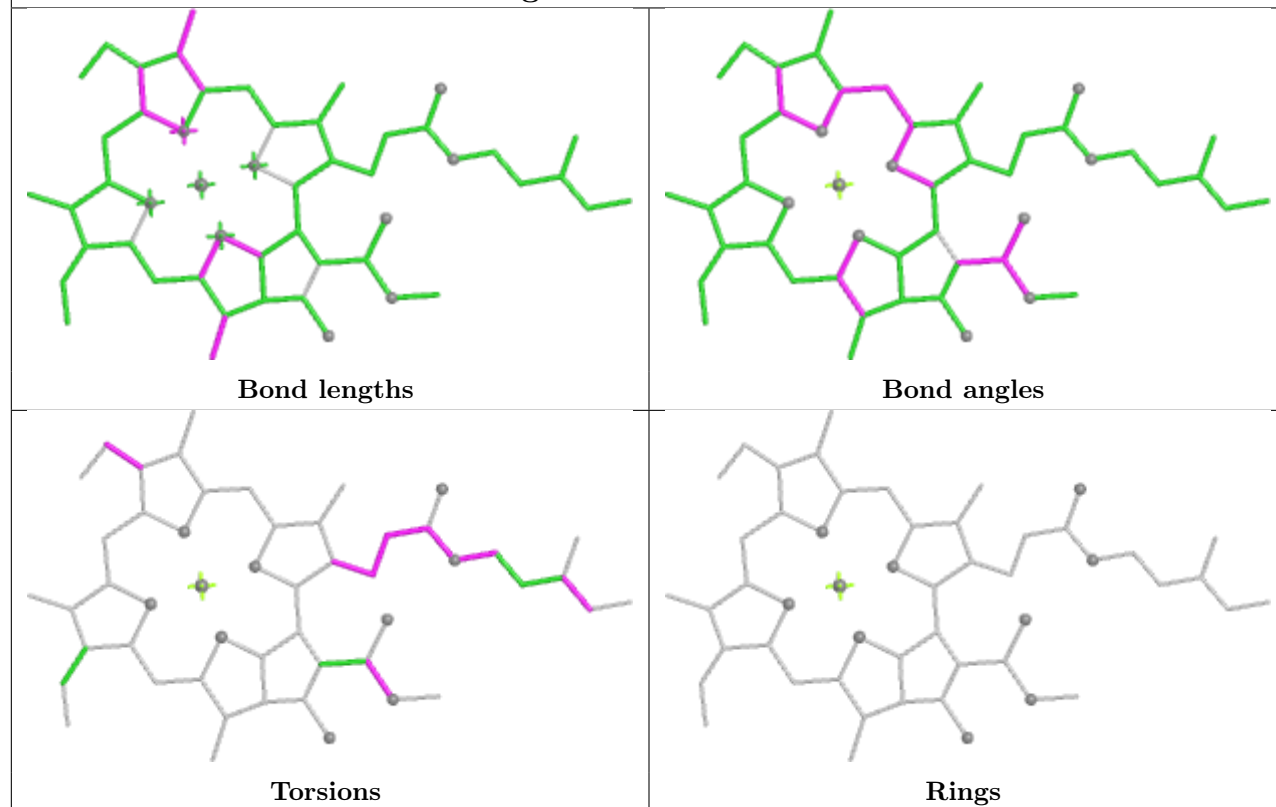


Ligand CLA dA 834

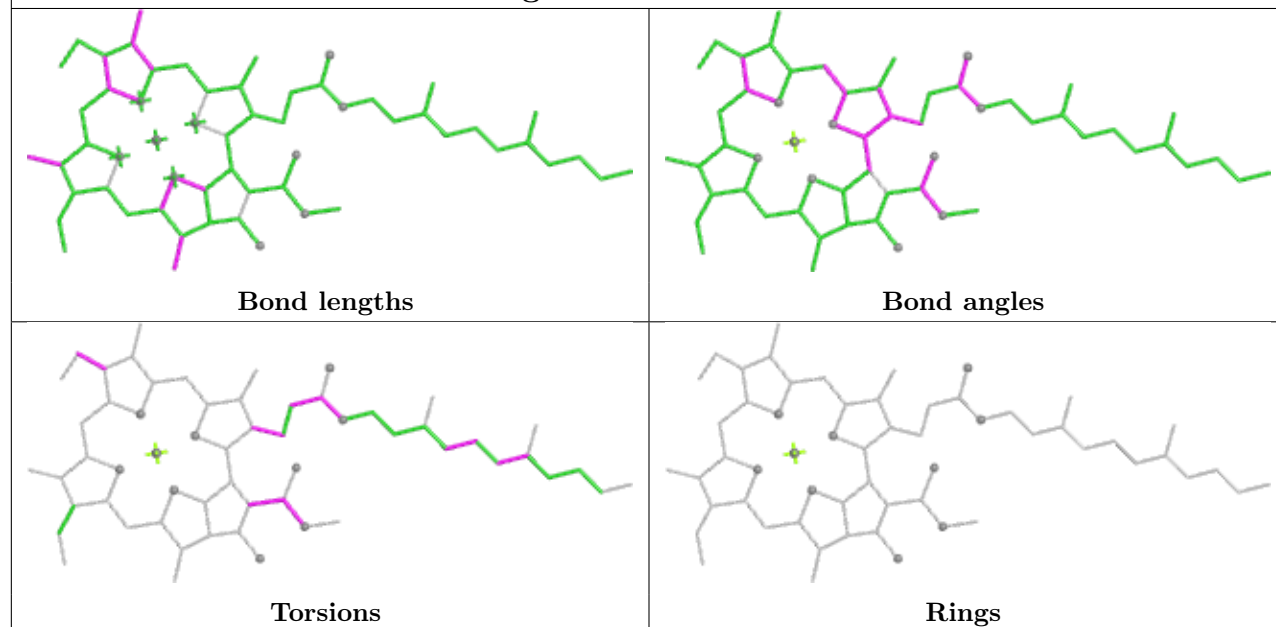




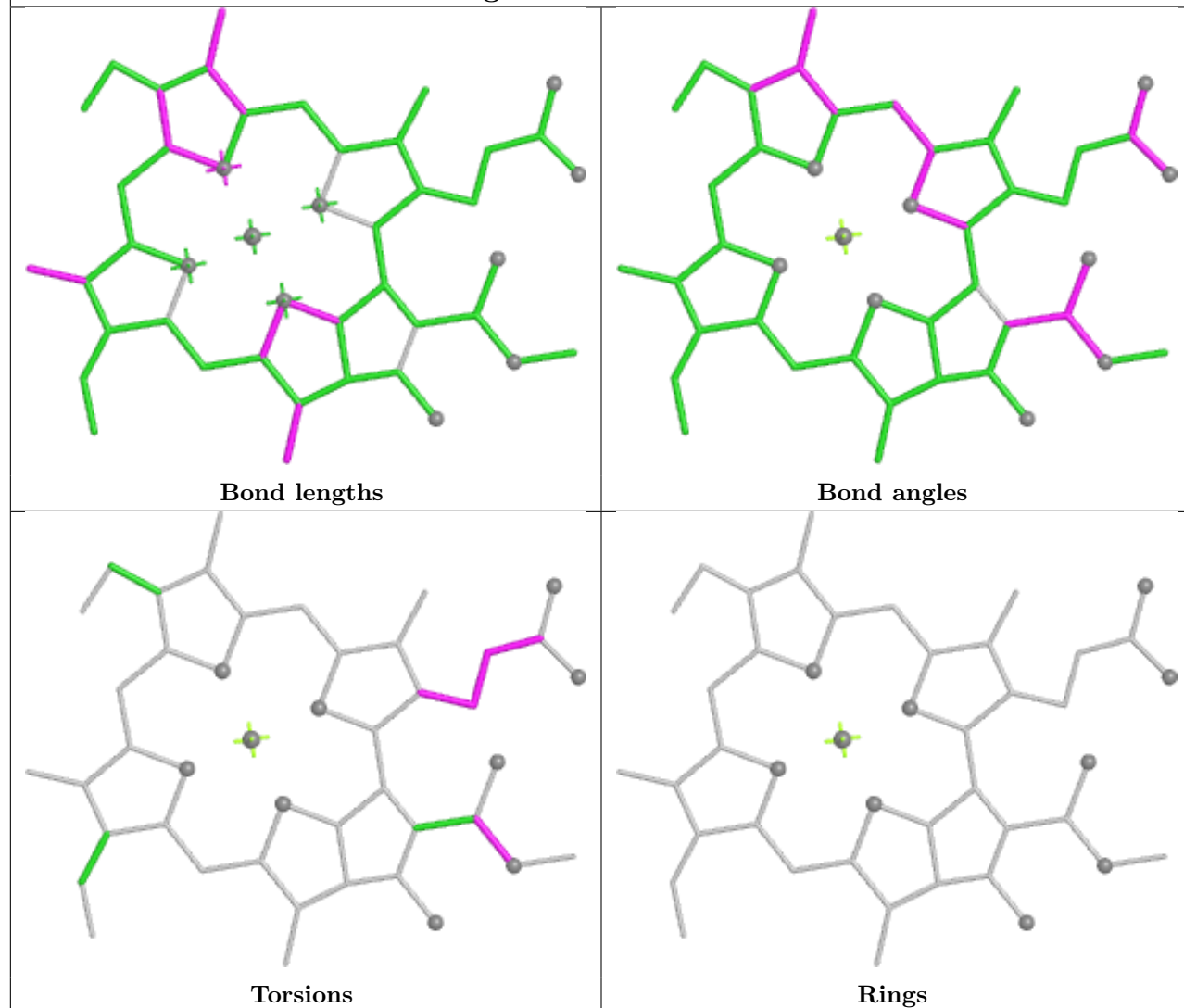
Ligand CLA bA 823



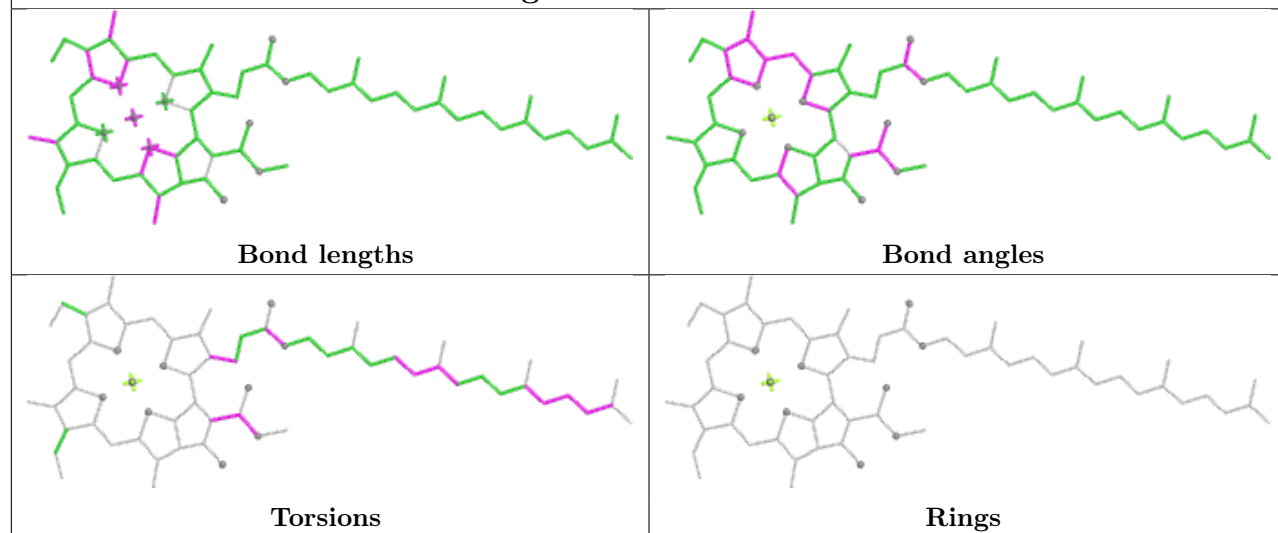
Ligand CLA dB 834

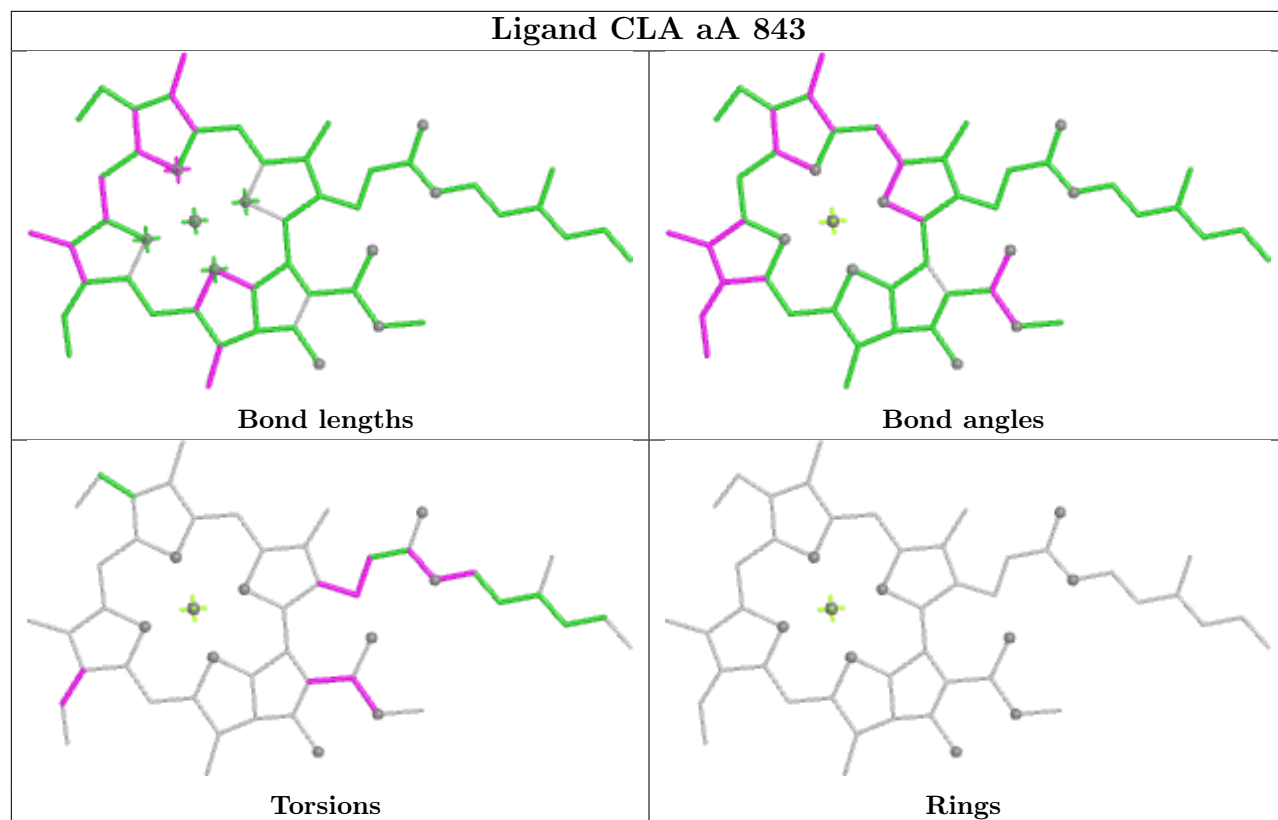


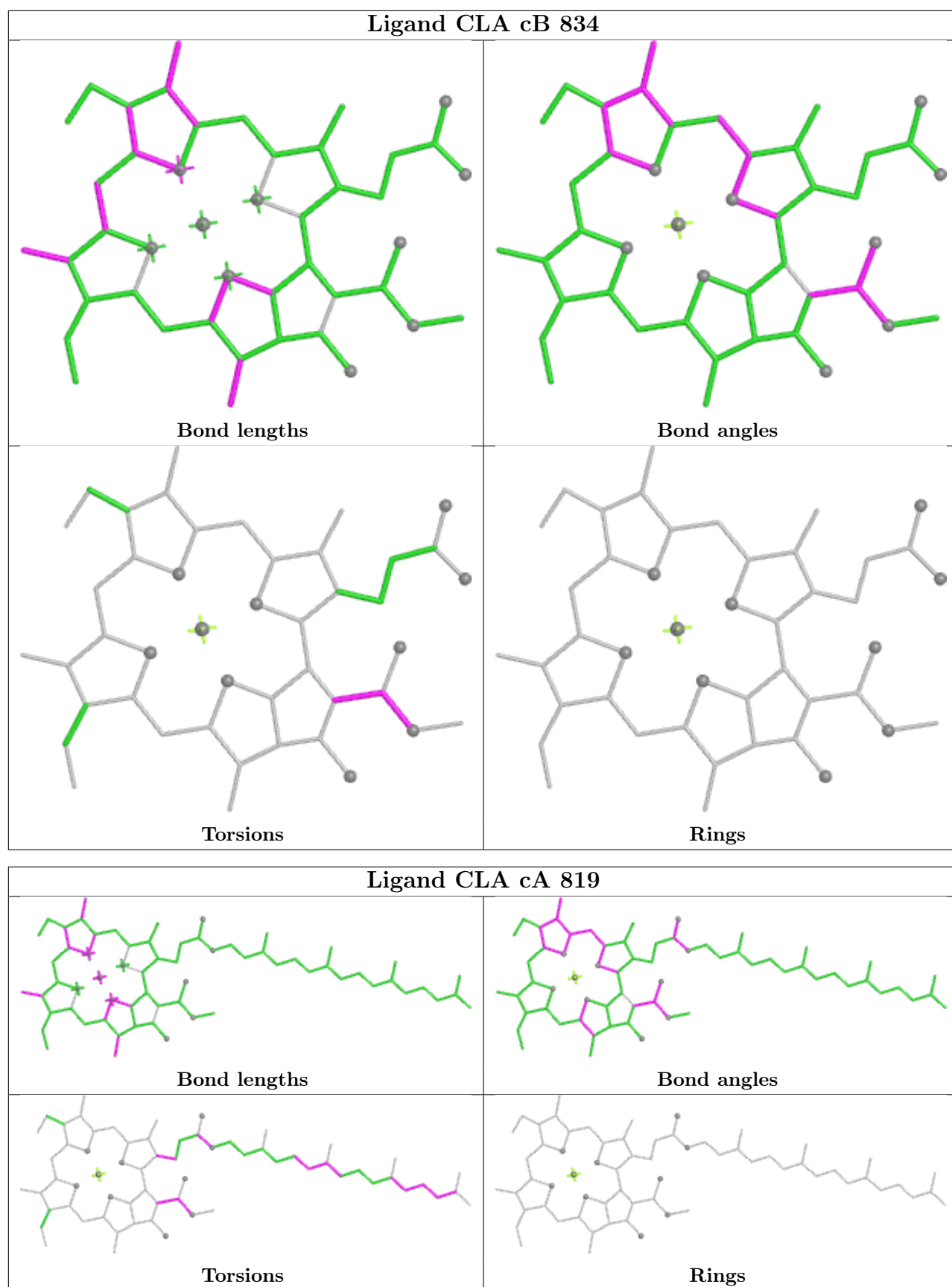
Ligand CLA bA 836

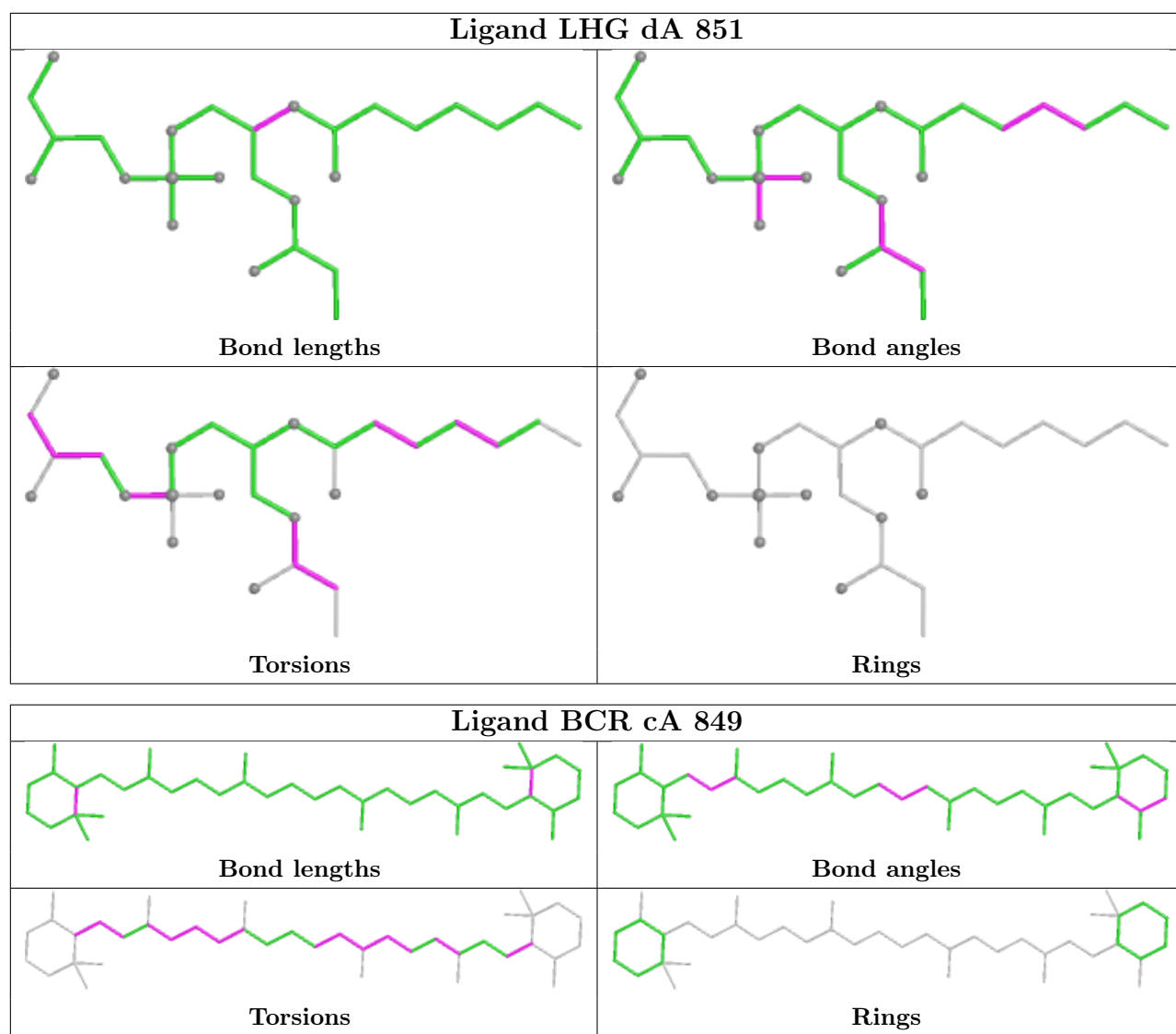


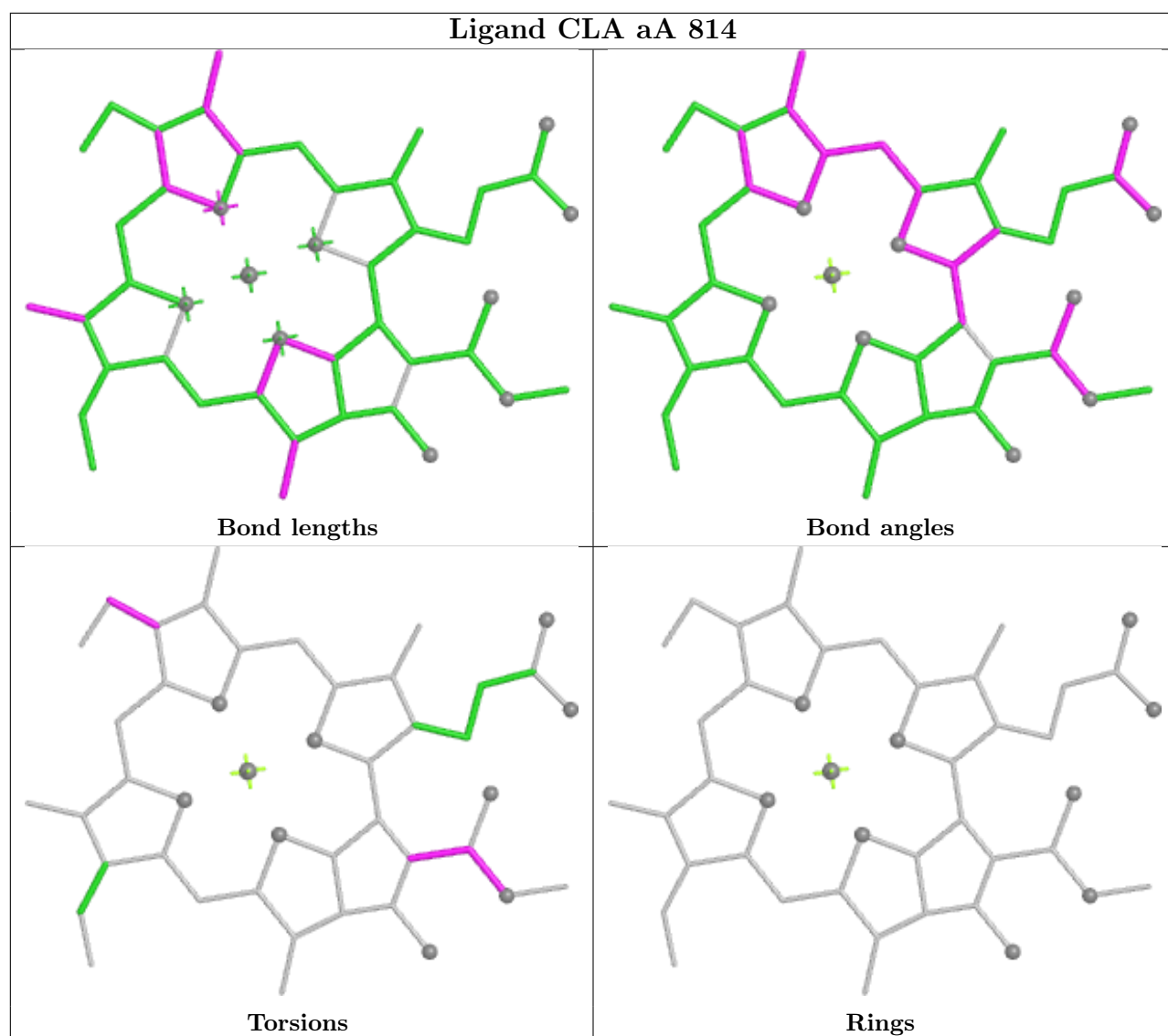
Ligand CLA dA 819



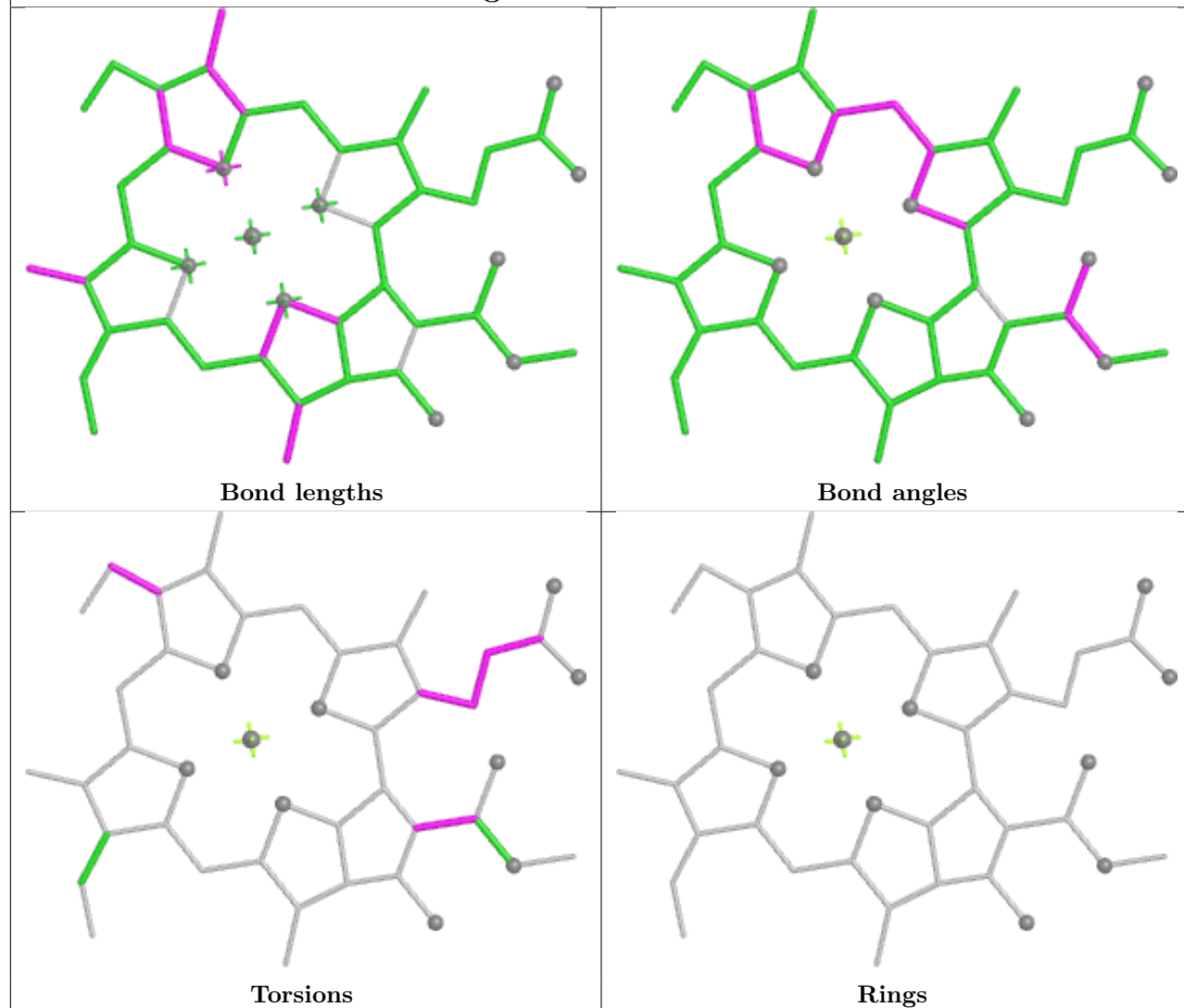




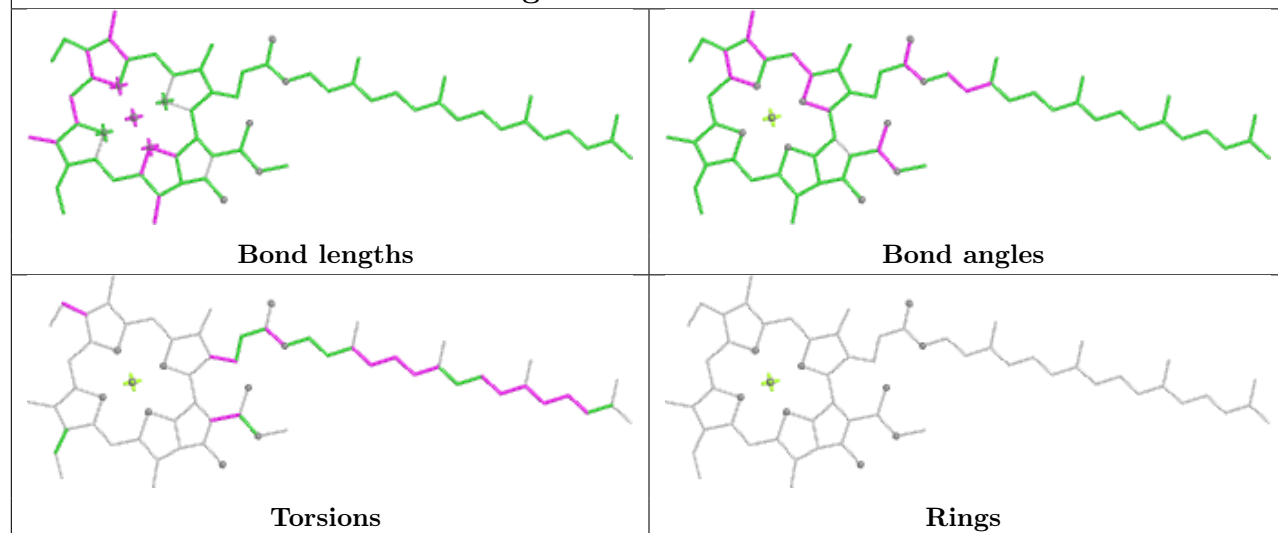


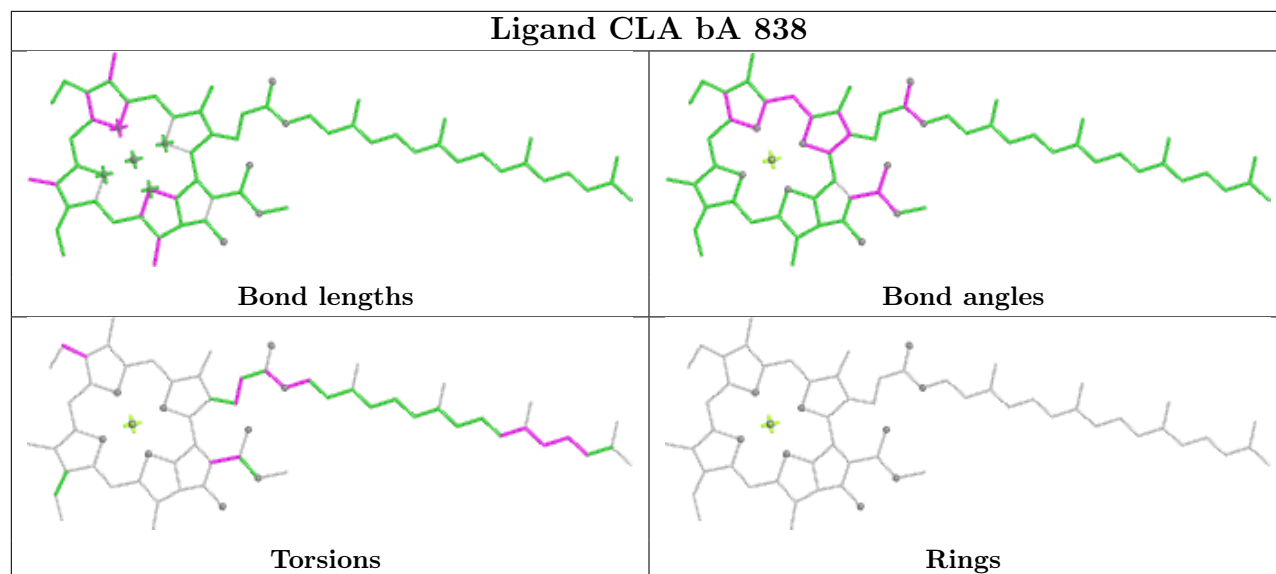
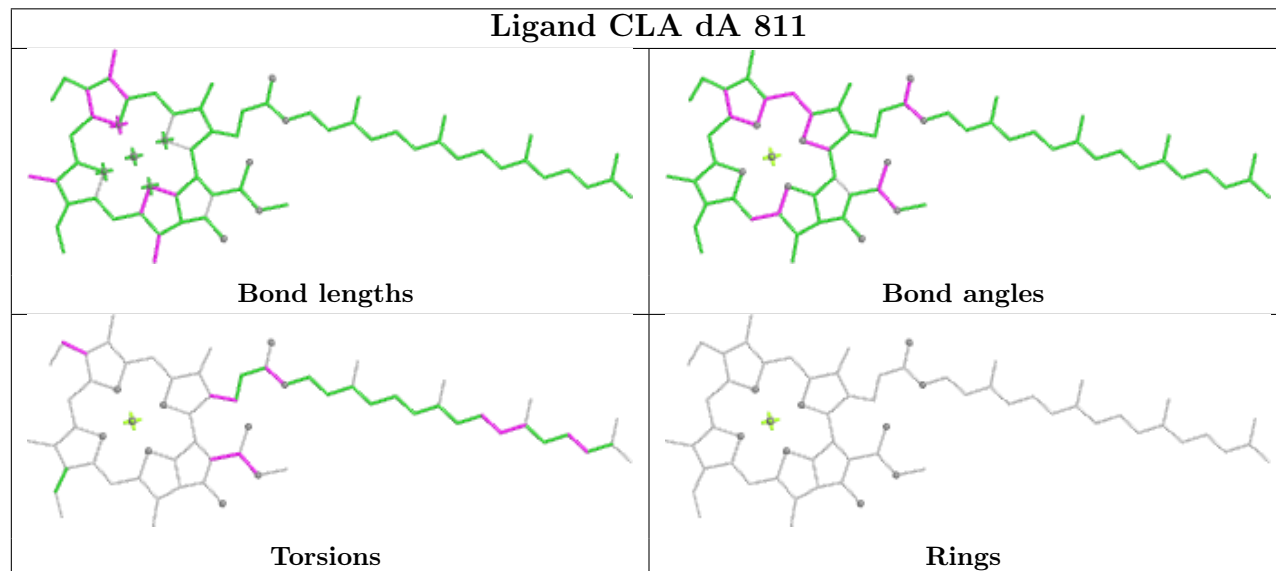


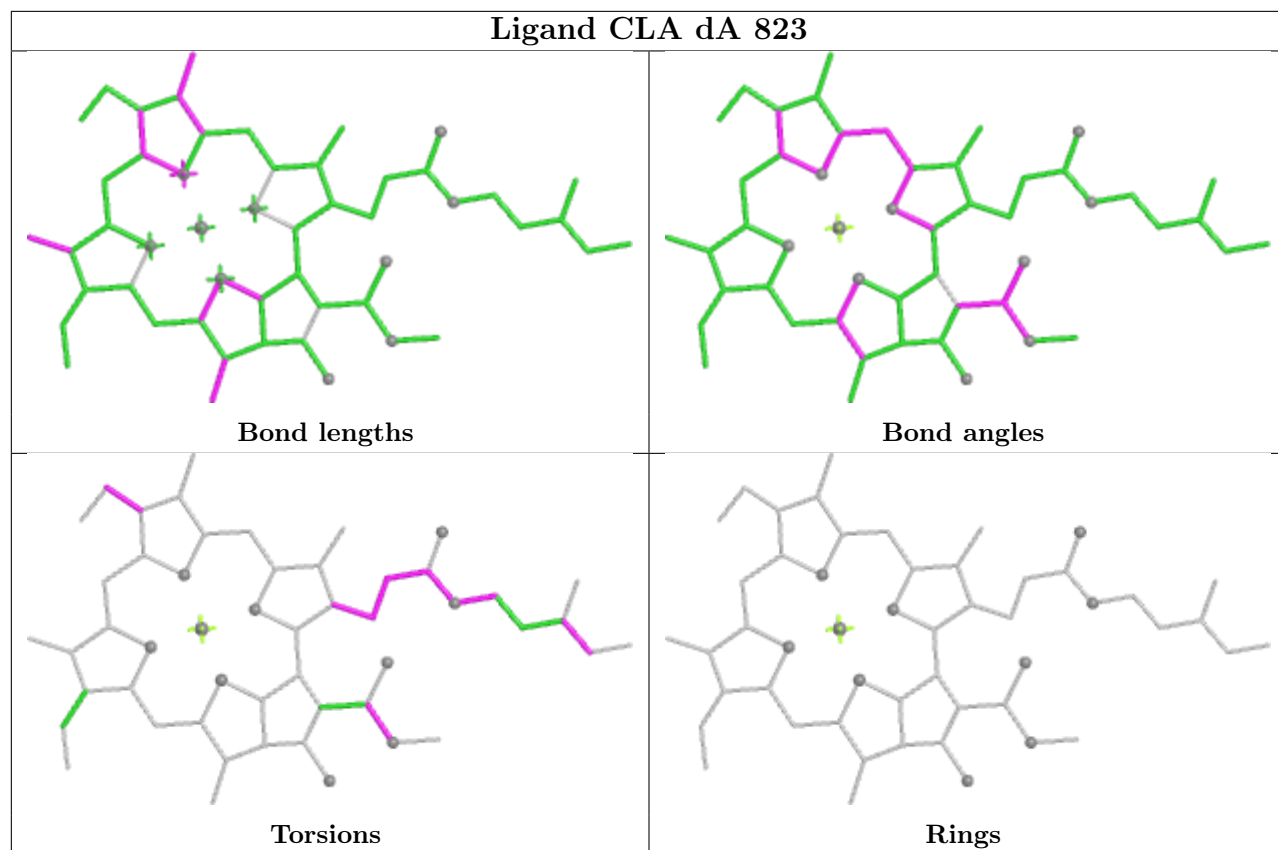
Ligand CLA dB 831



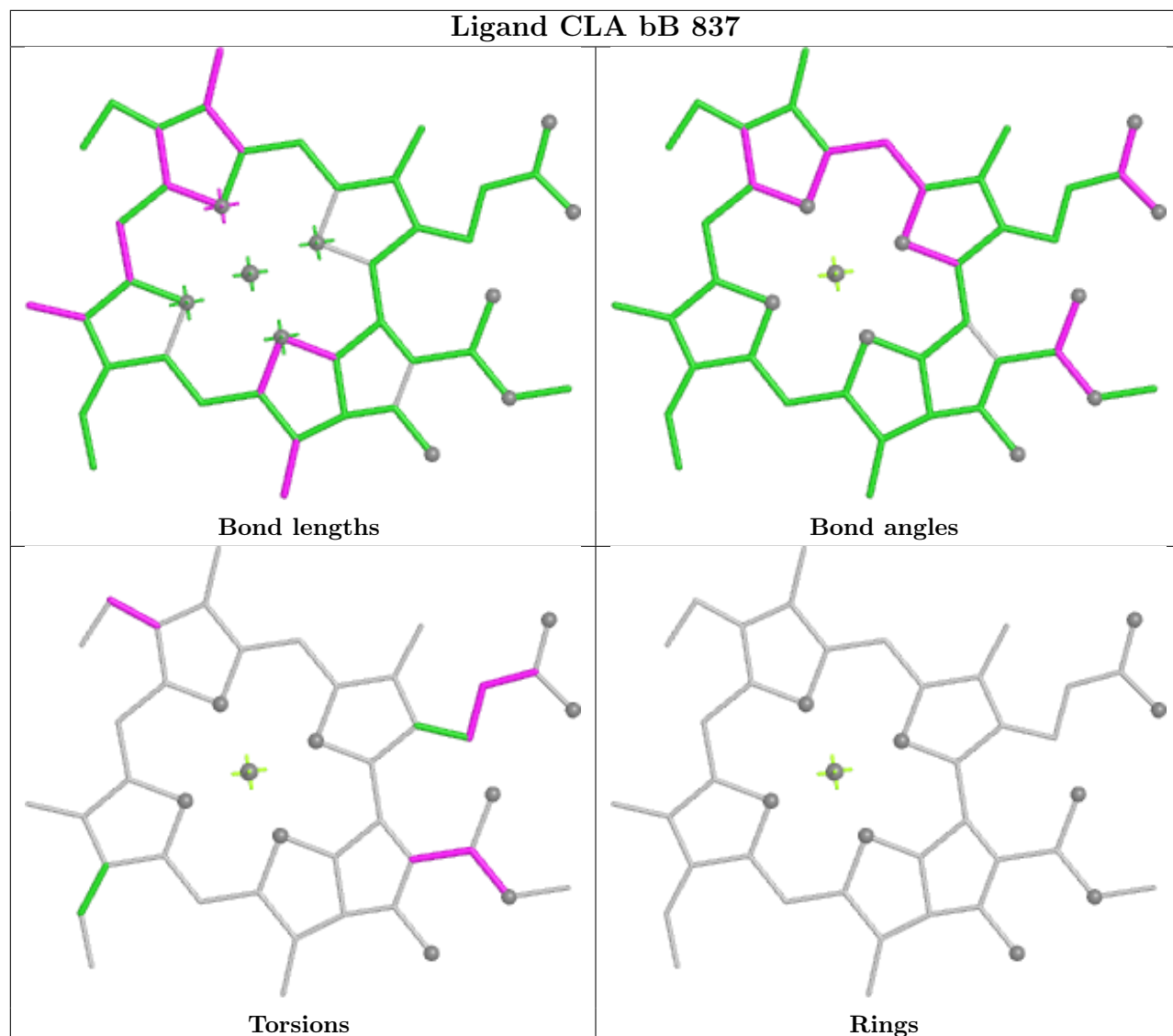
Ligand CLA bB 827



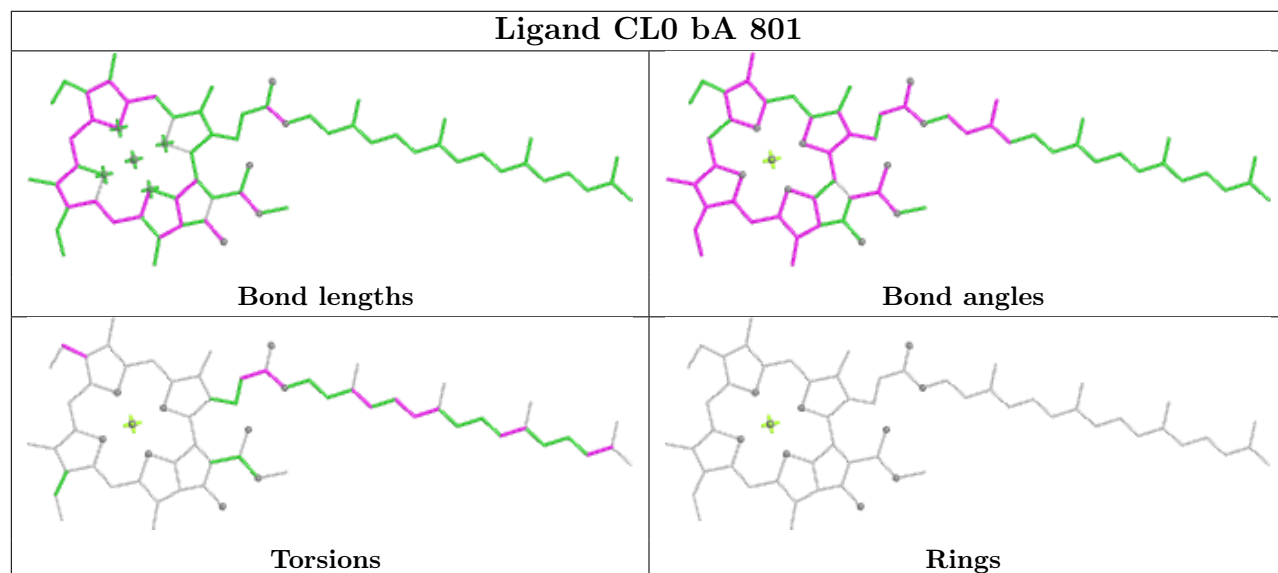
Ligand CLA bA 838**Ligand CLA dA 811**



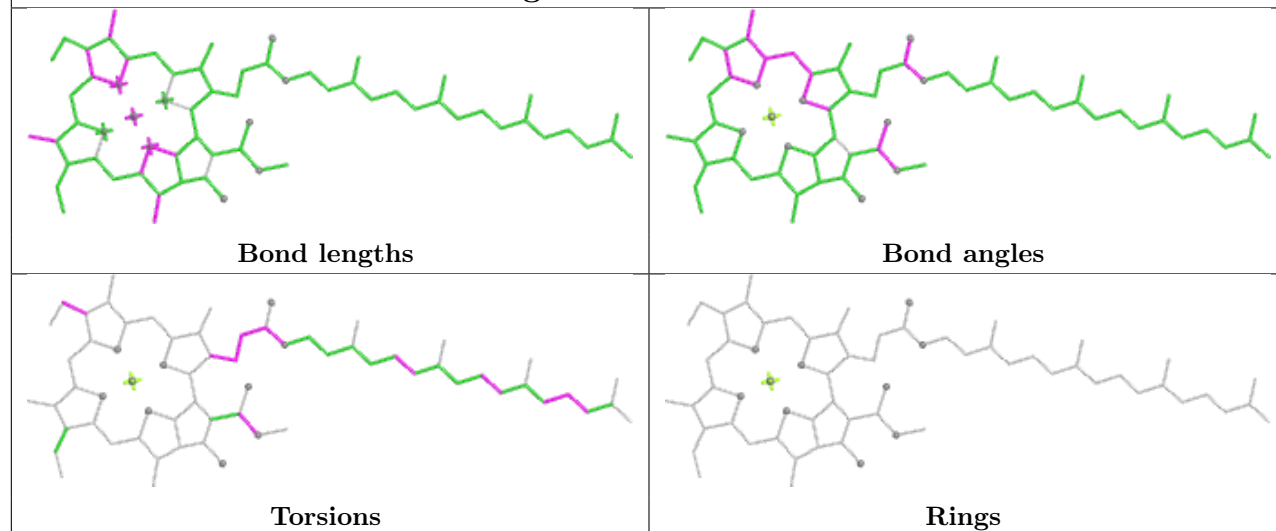
Ligand CLA bB 837



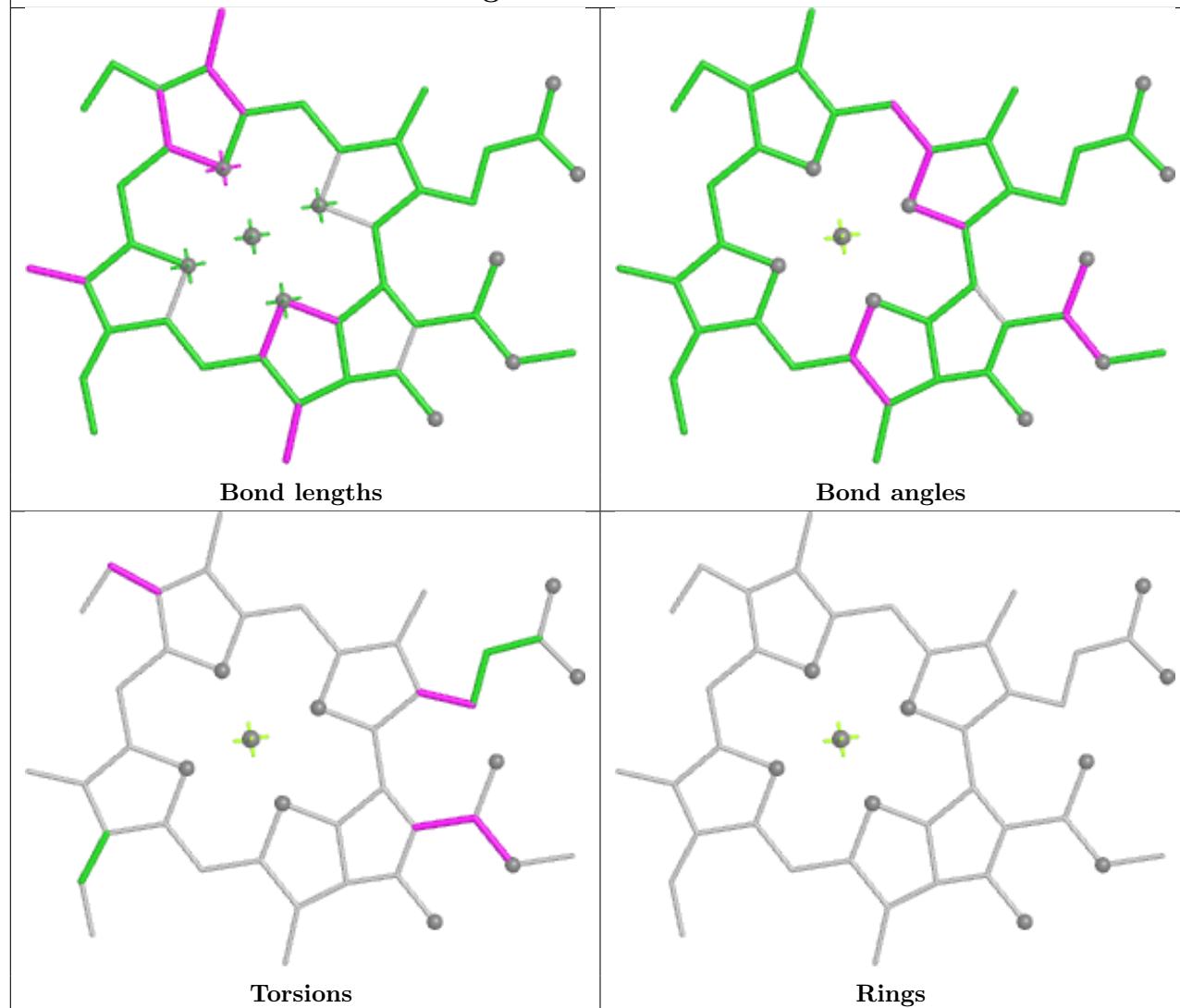
Ligand CL0 bA 801

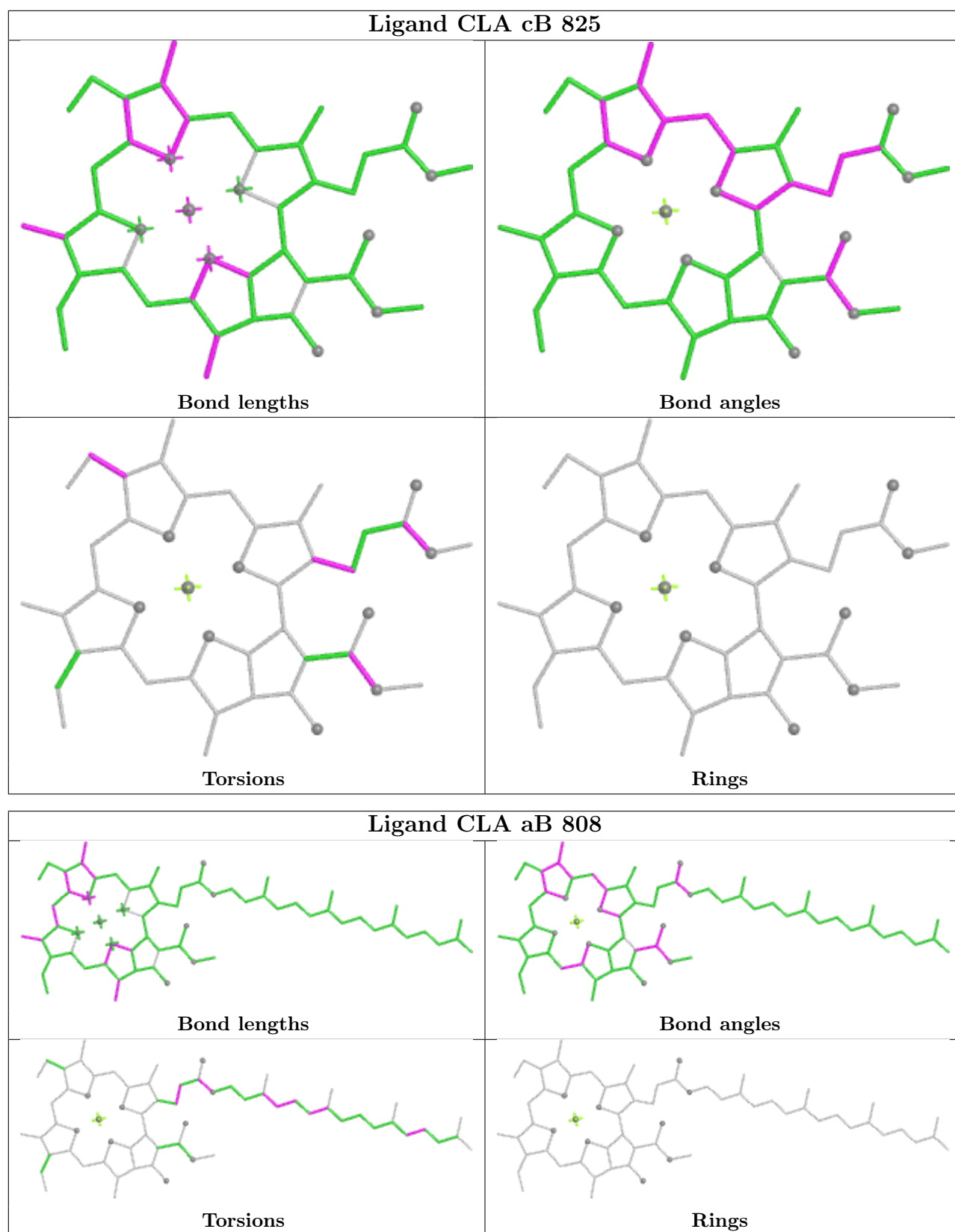


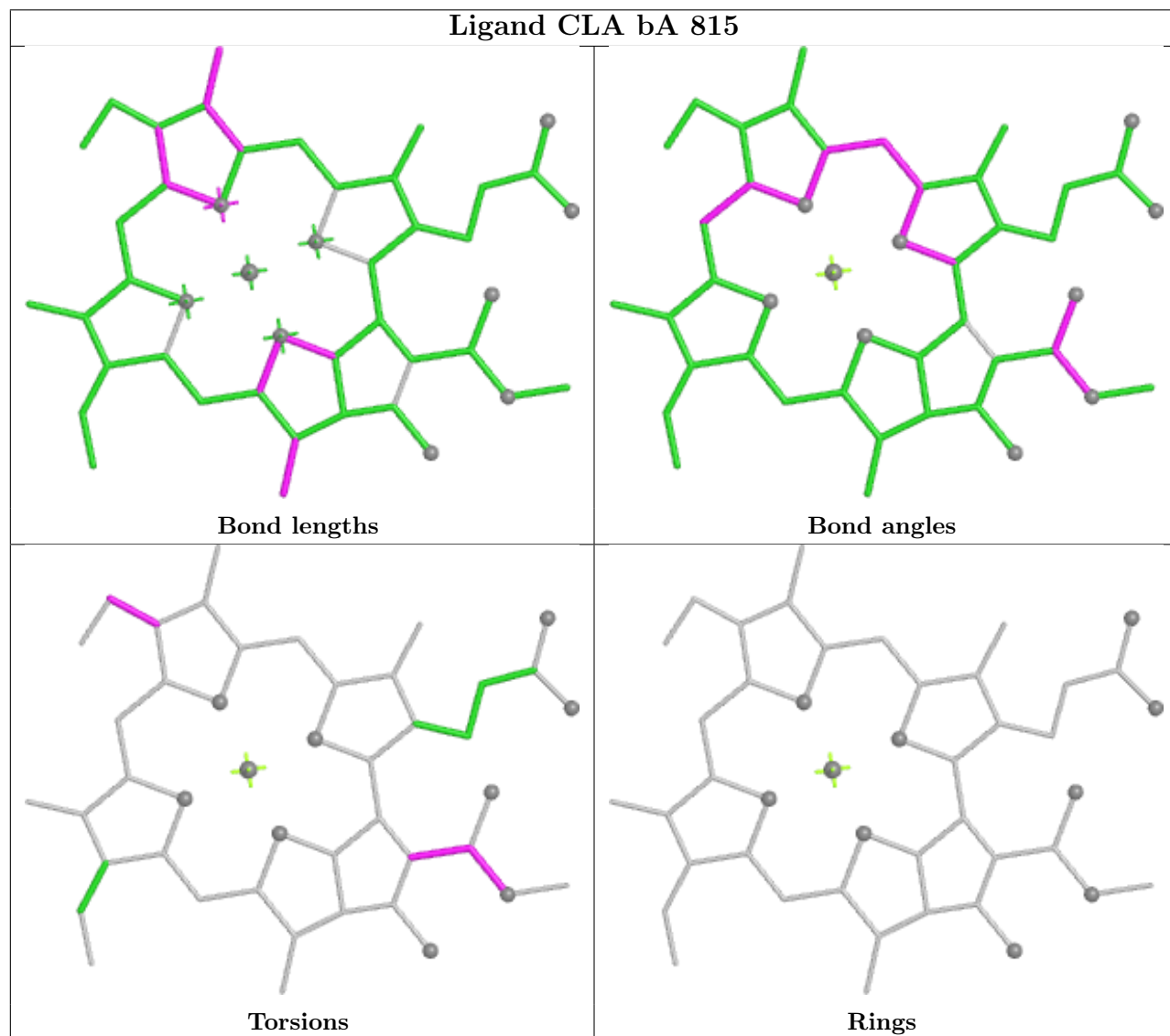
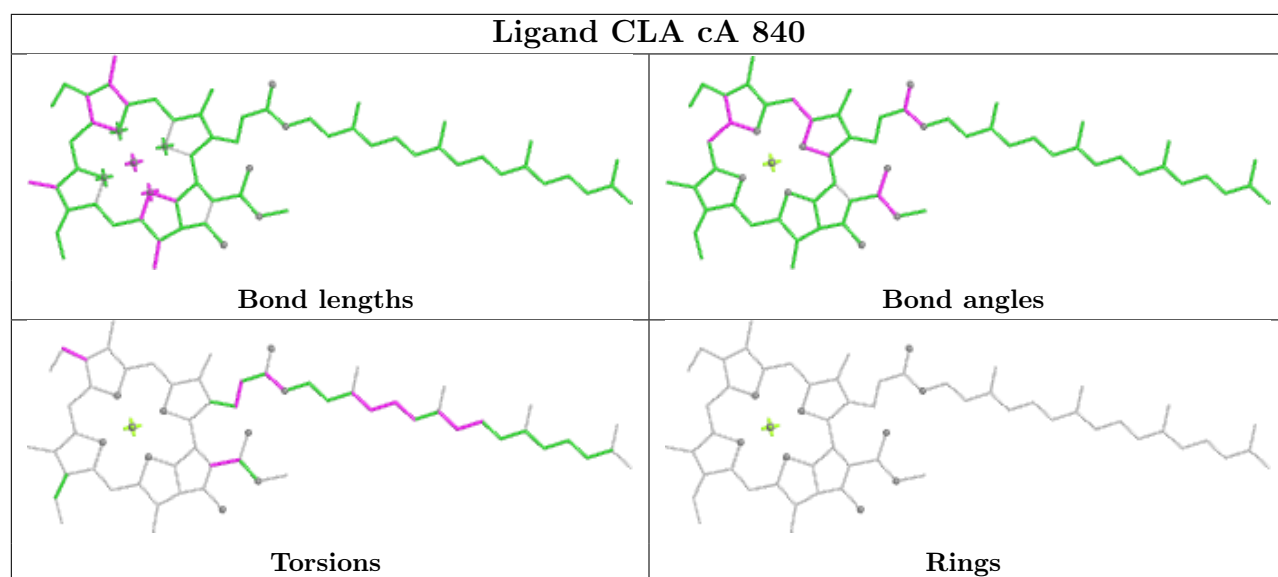
Ligand CLA aA 842

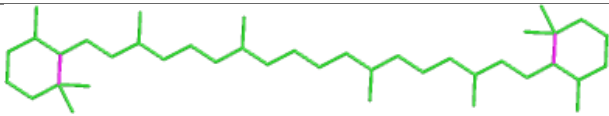
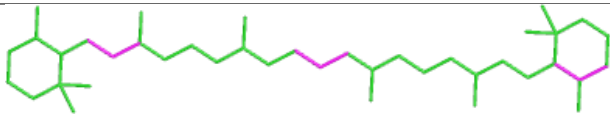
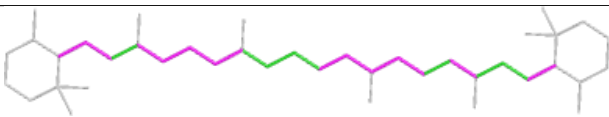
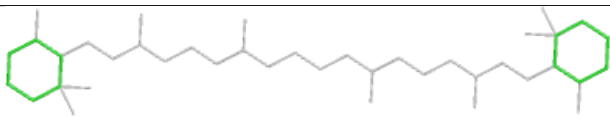


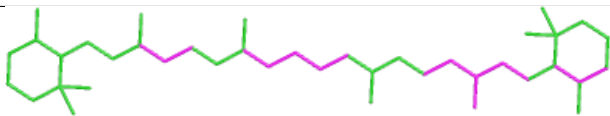
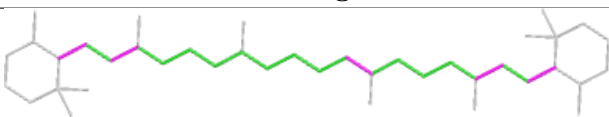
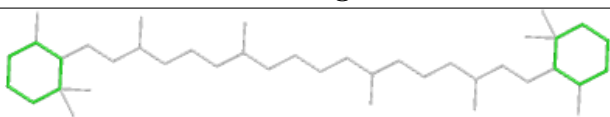
Ligand CLA dB 812



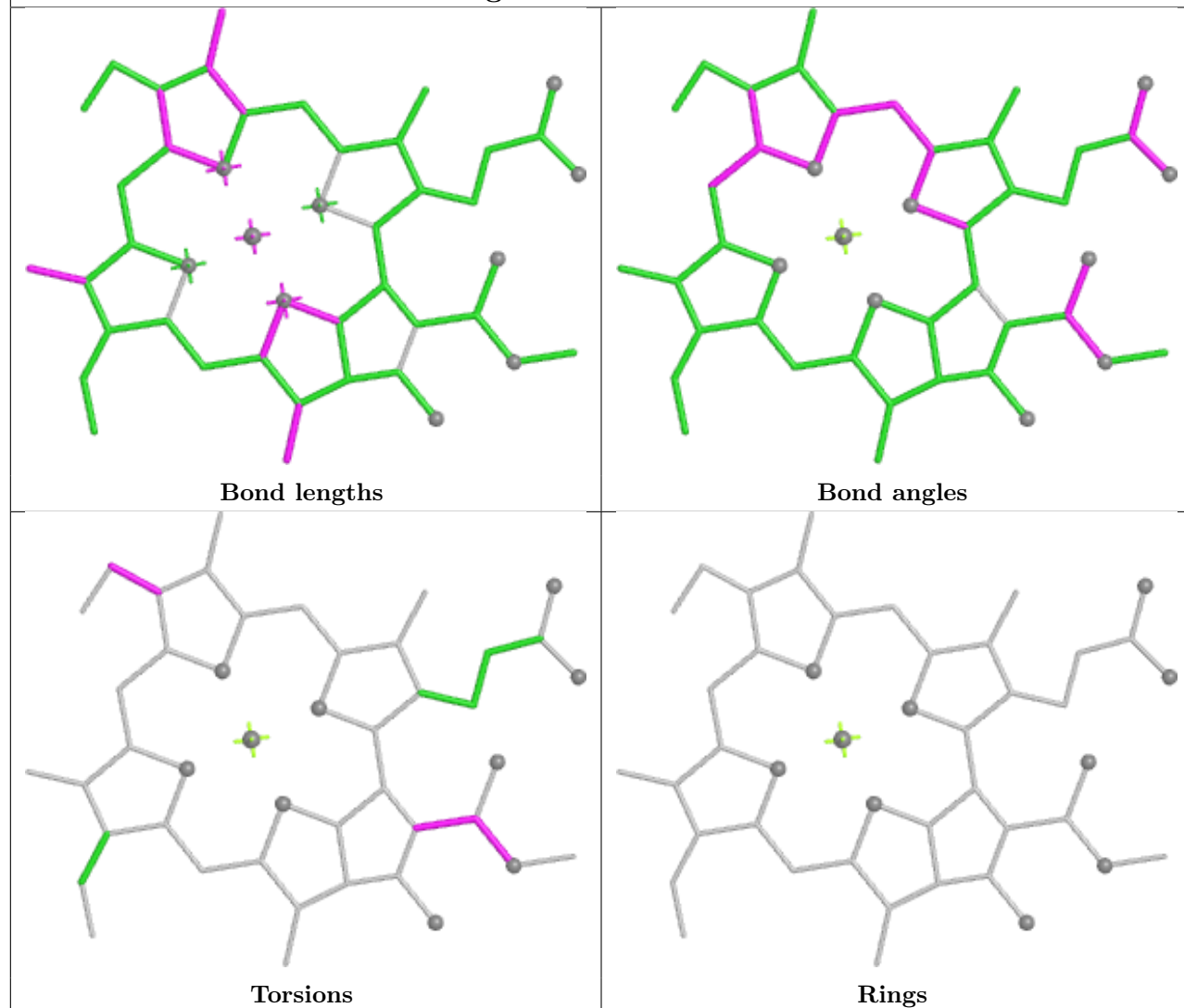




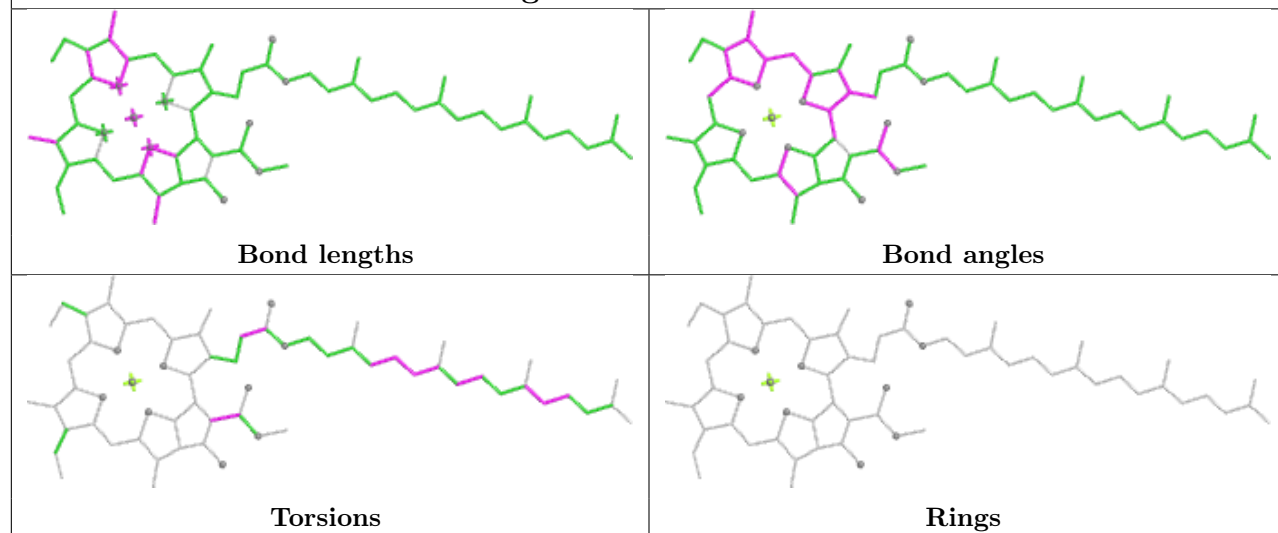
Ligand BCR dA 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

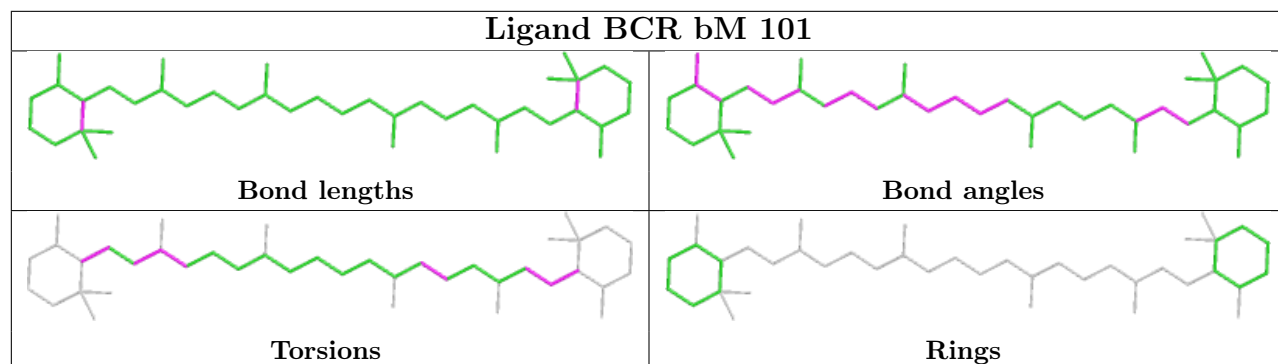
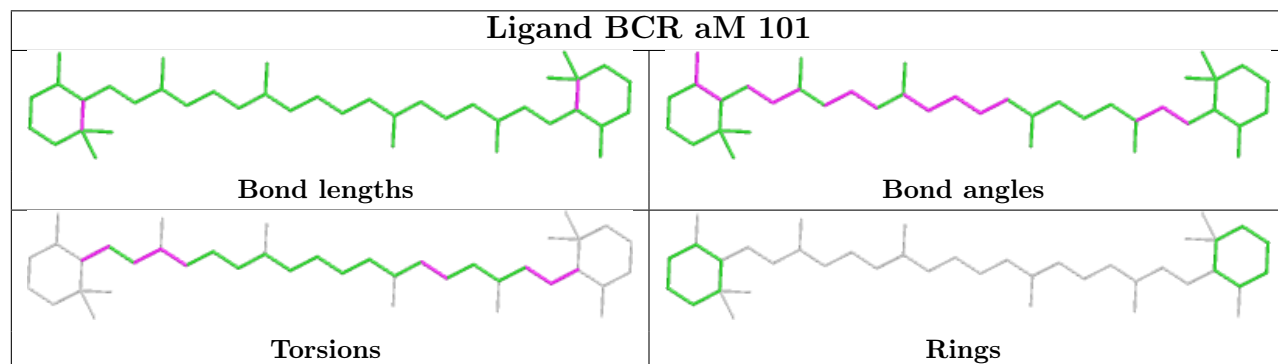
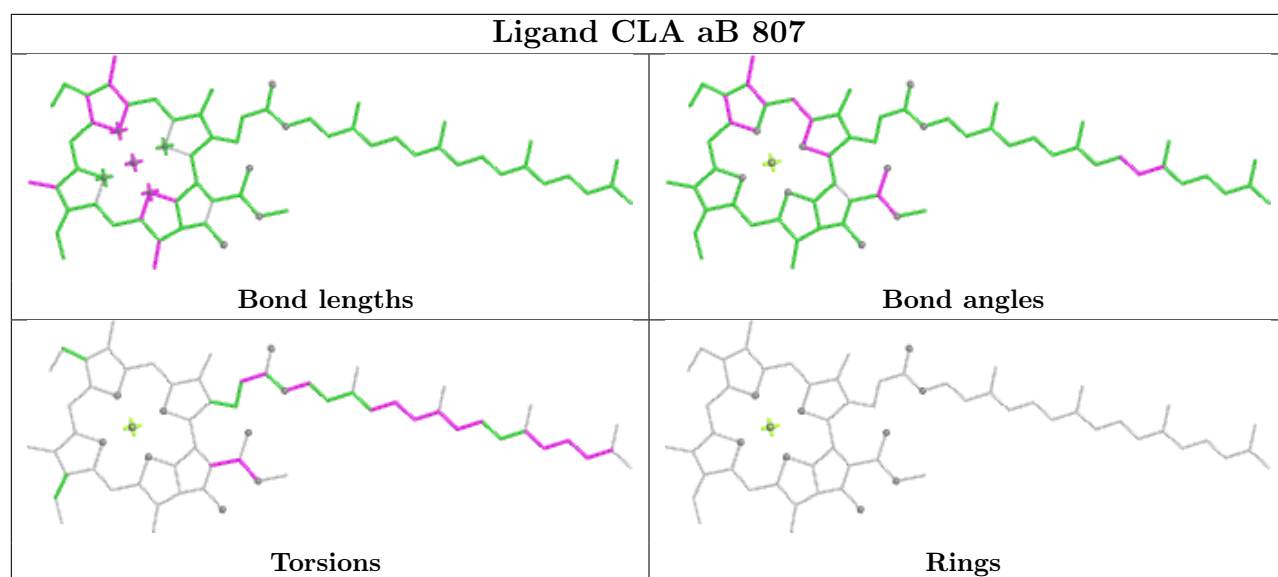
Ligand BCR bL 207	
	
Bond lengths	Bond angles
	
Torsions	Rings

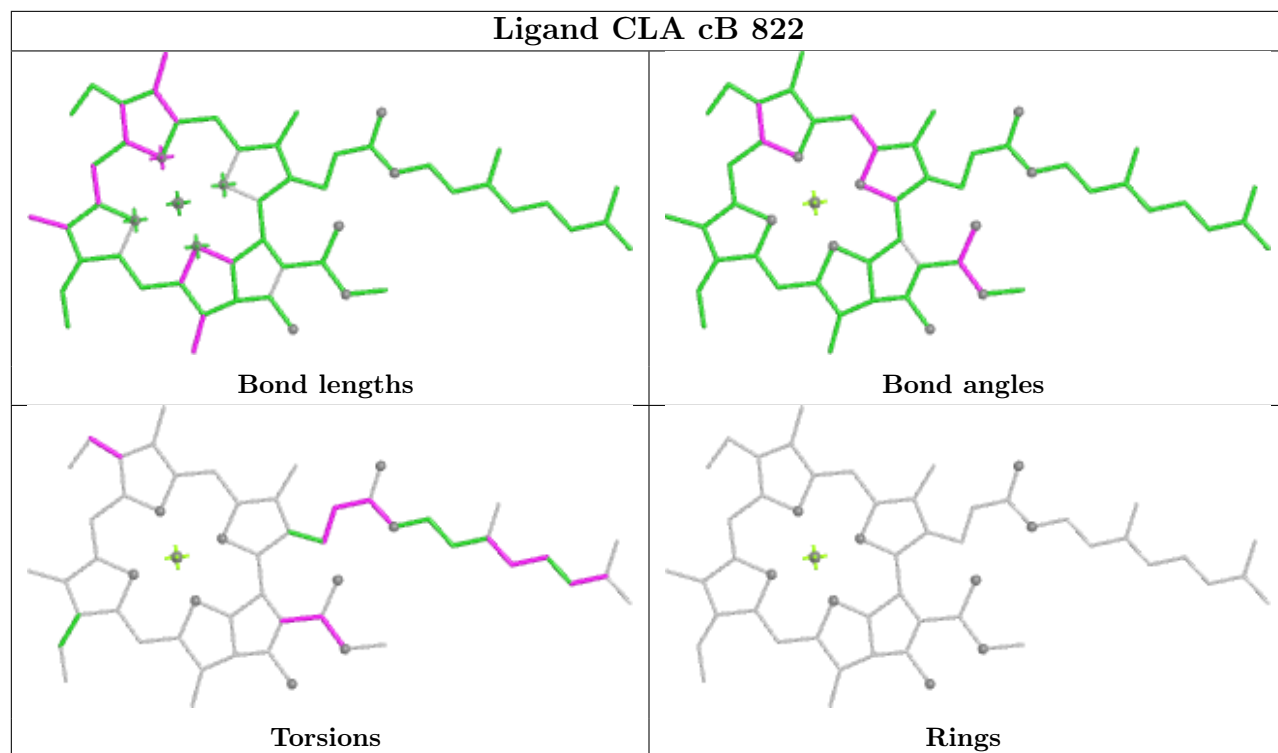
Ligand CLA cB 821

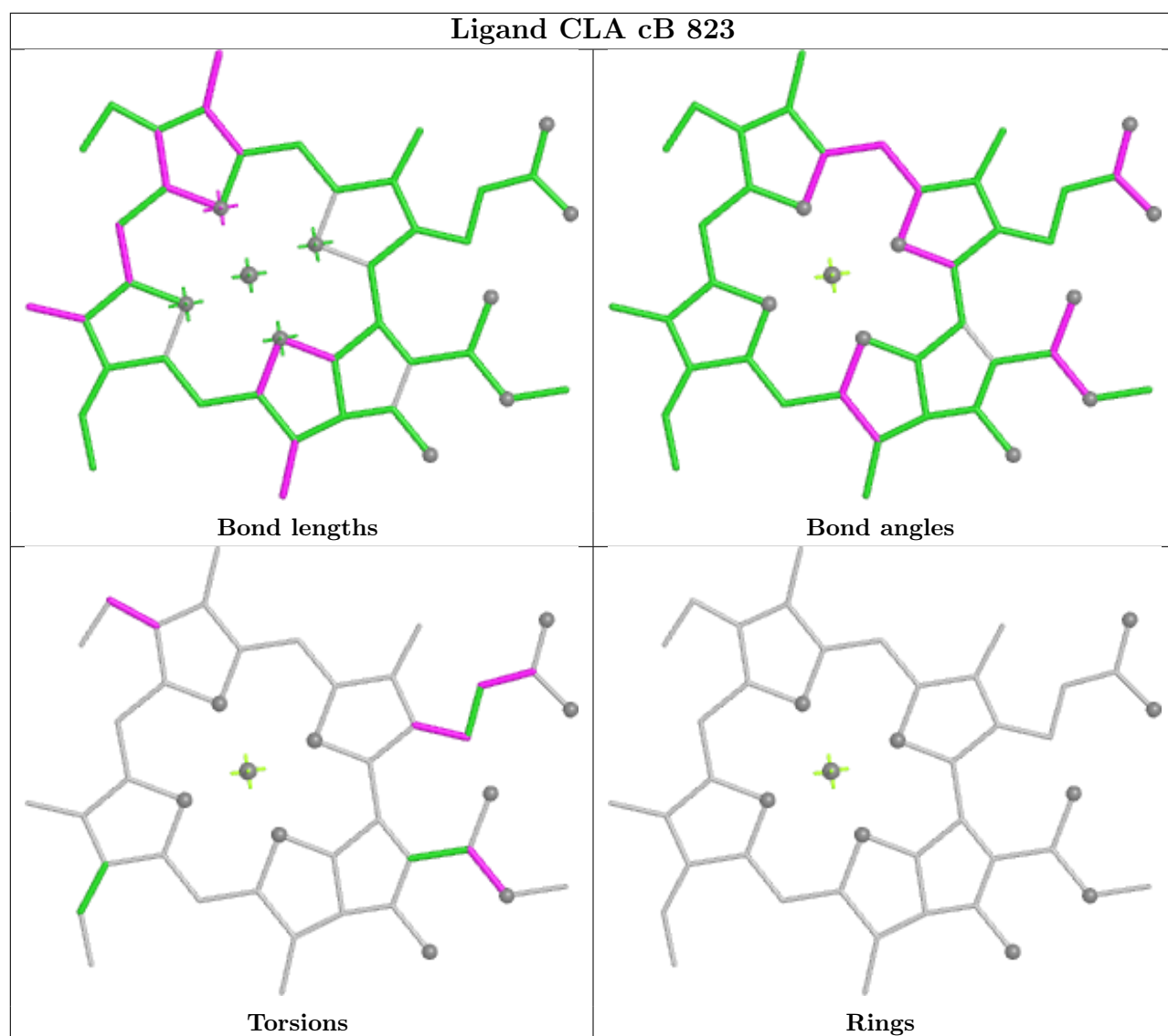


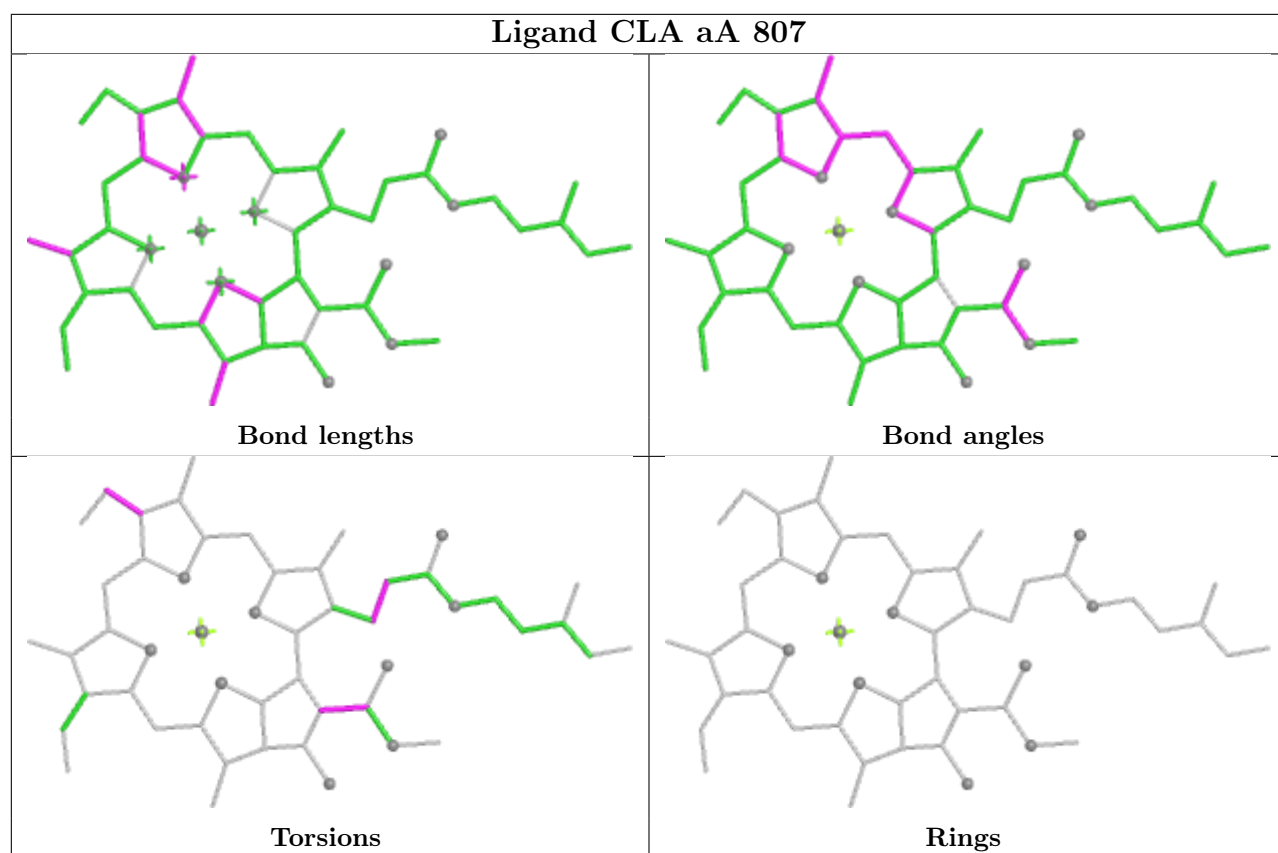
Ligand CLA bA 825



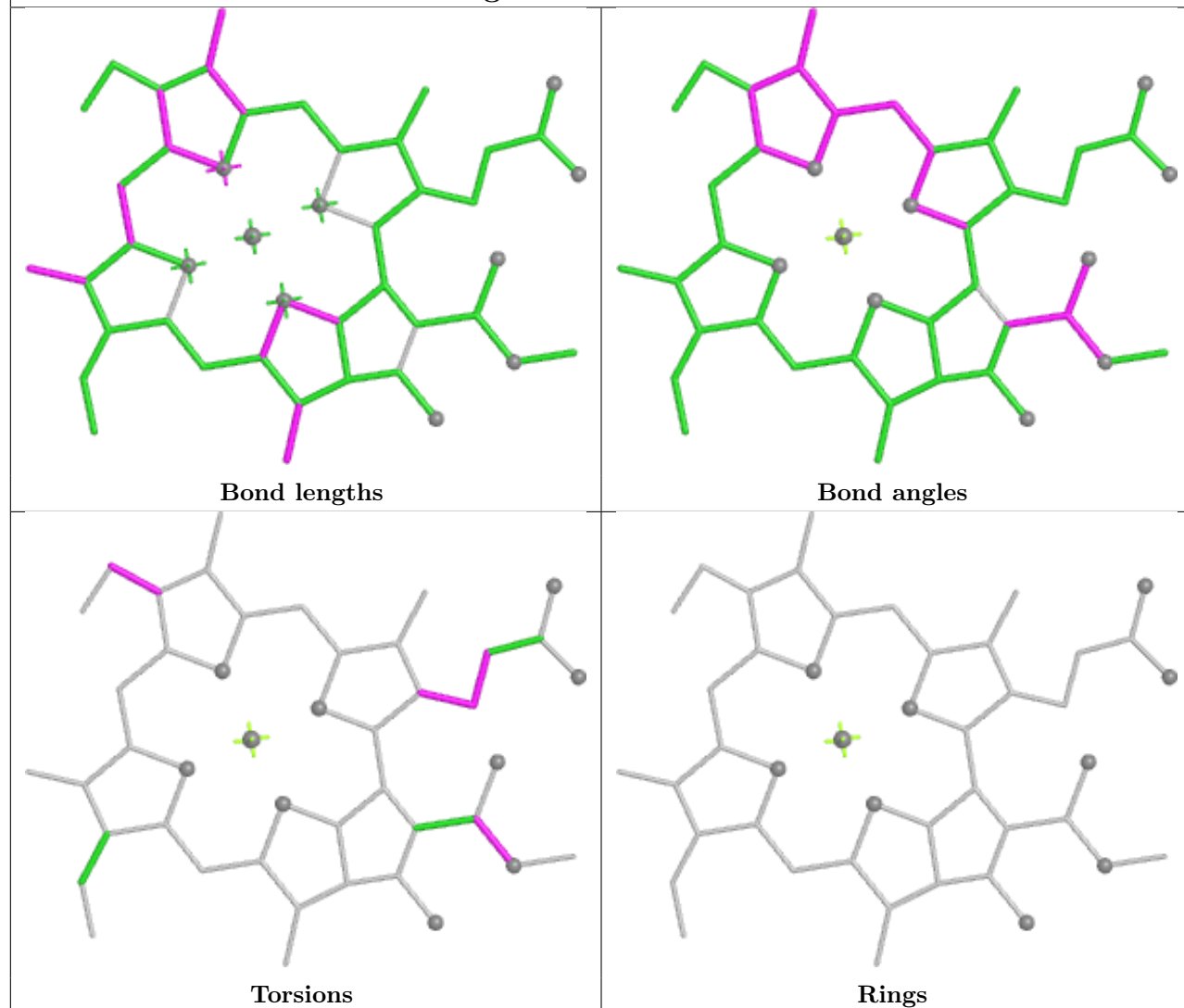




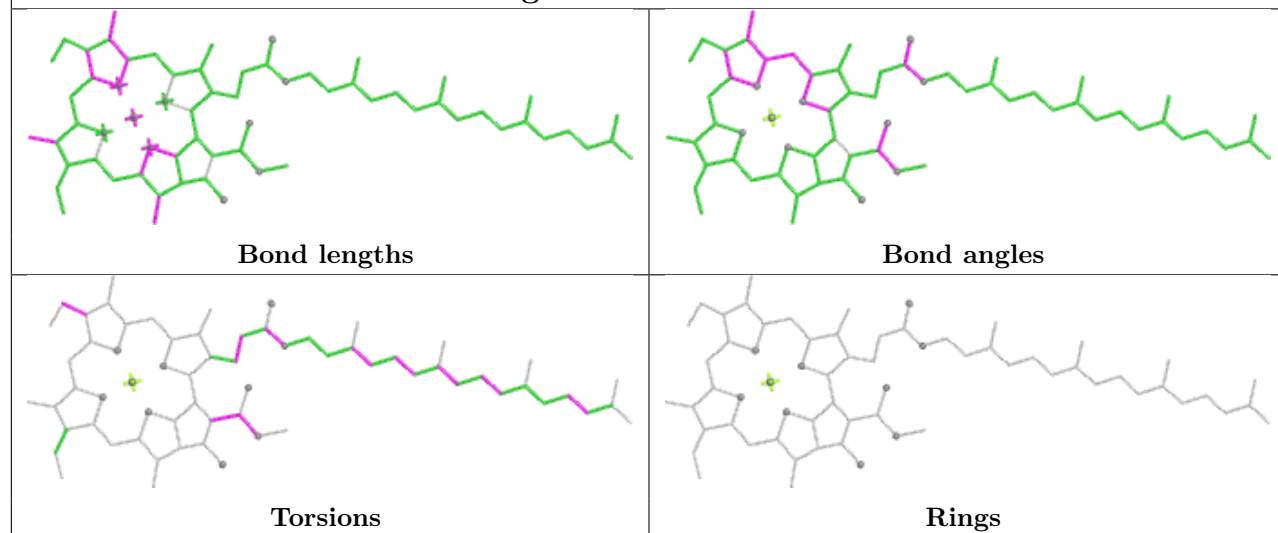


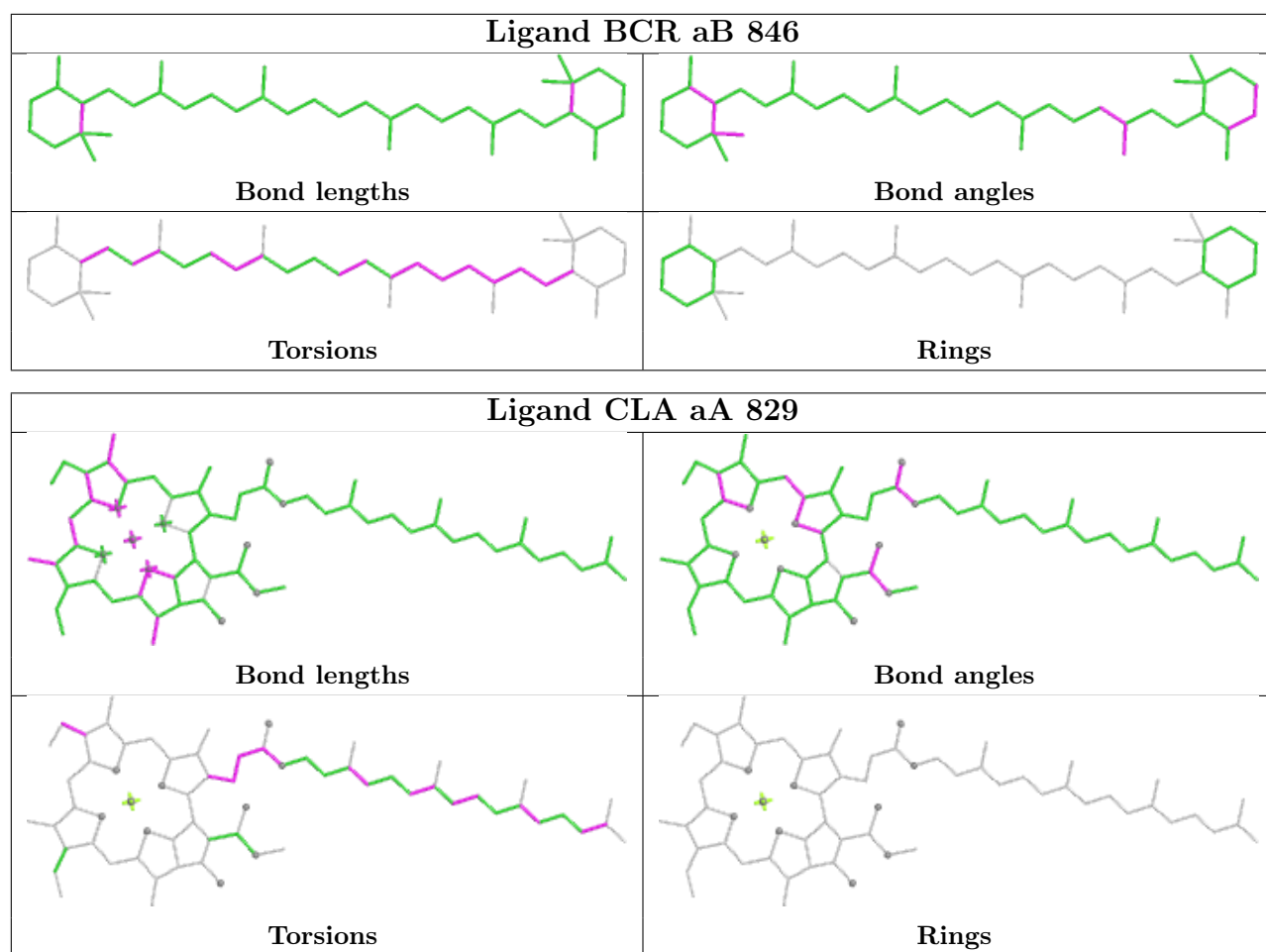


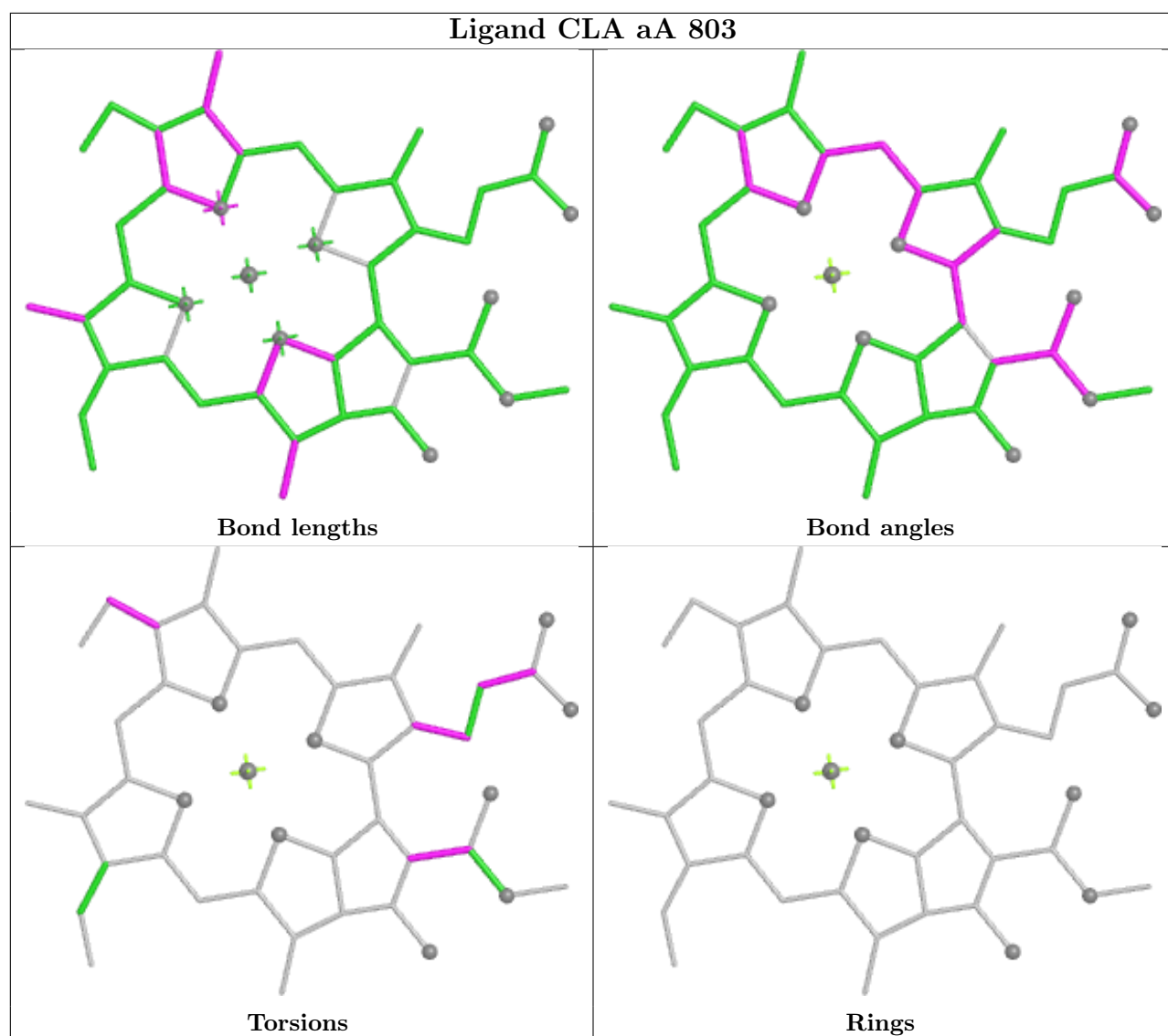
Ligand CLA dB 816



Ligand CLA bA 821







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

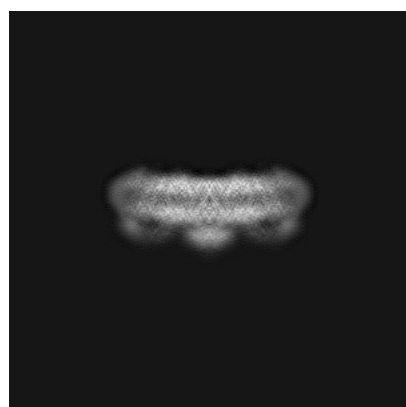
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9807. These allow visual inspection of the internal detail of the map and identification of artifacts.

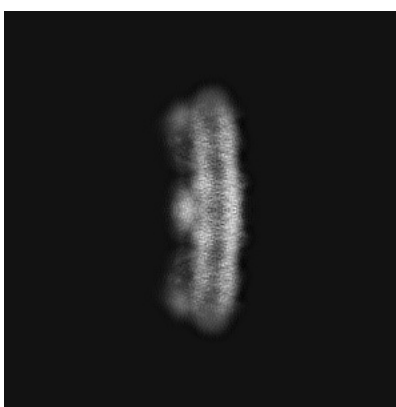
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

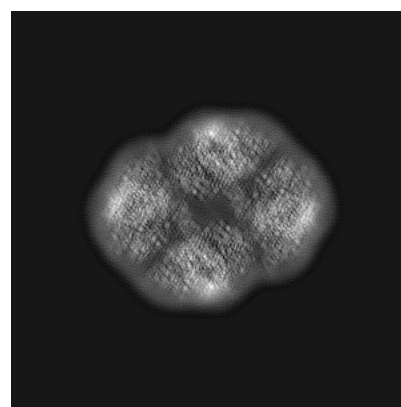
6.1.1 Primary map



X



Y

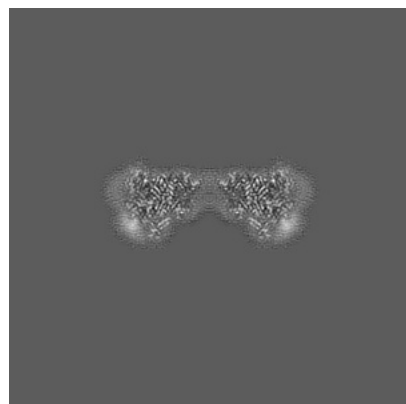


Z

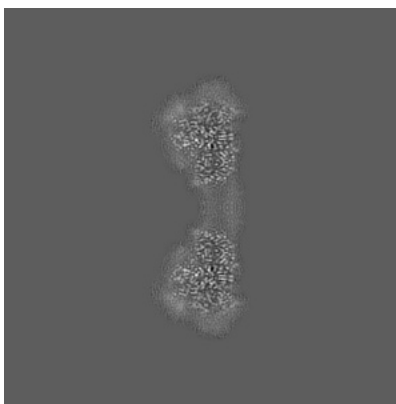
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

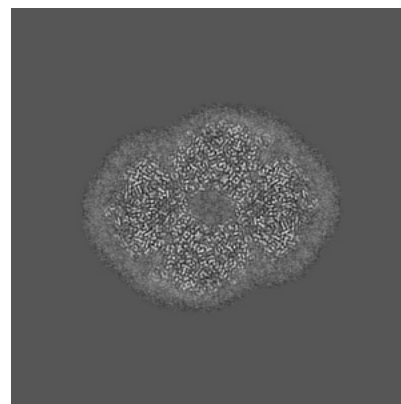
6.2.1 Primary map



X Index: 220



Y Index: 220

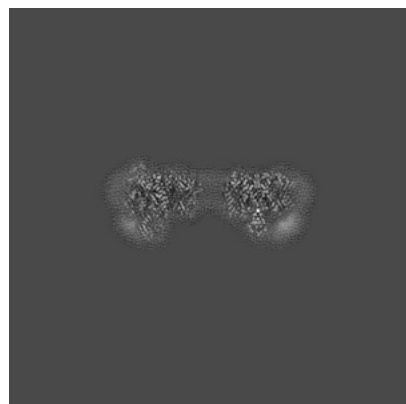


Z Index: 220

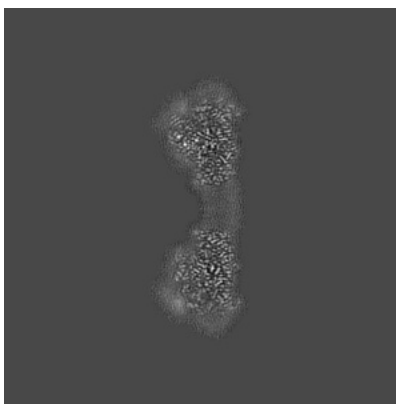
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

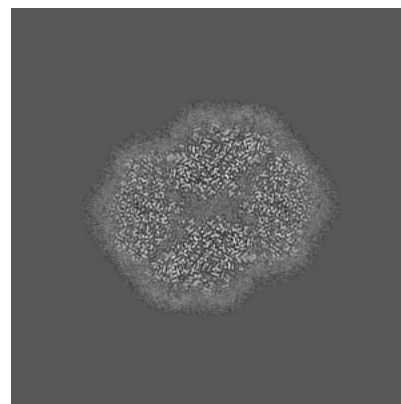
6.3.1 Primary map



X Index: 226



Y Index: 222

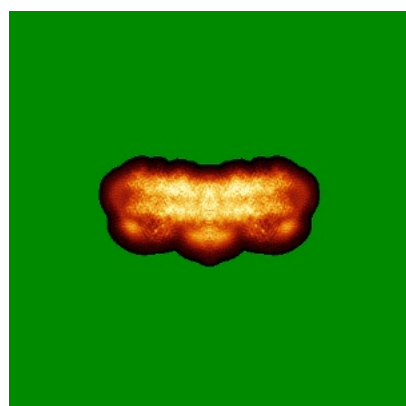


Z Index: 245

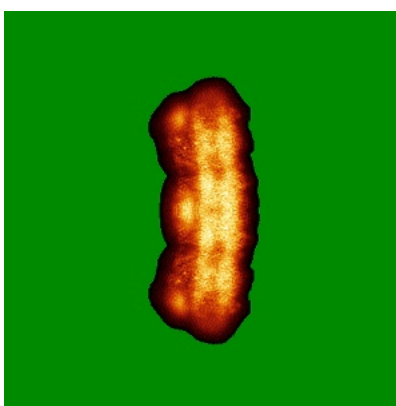
The images above show the largest variance slices of the map in three orthogonal directions.

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

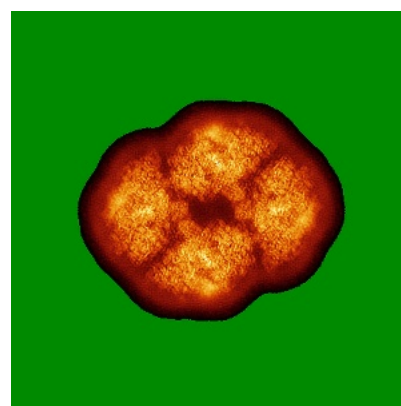
6.4.1 Primary map



X



Y

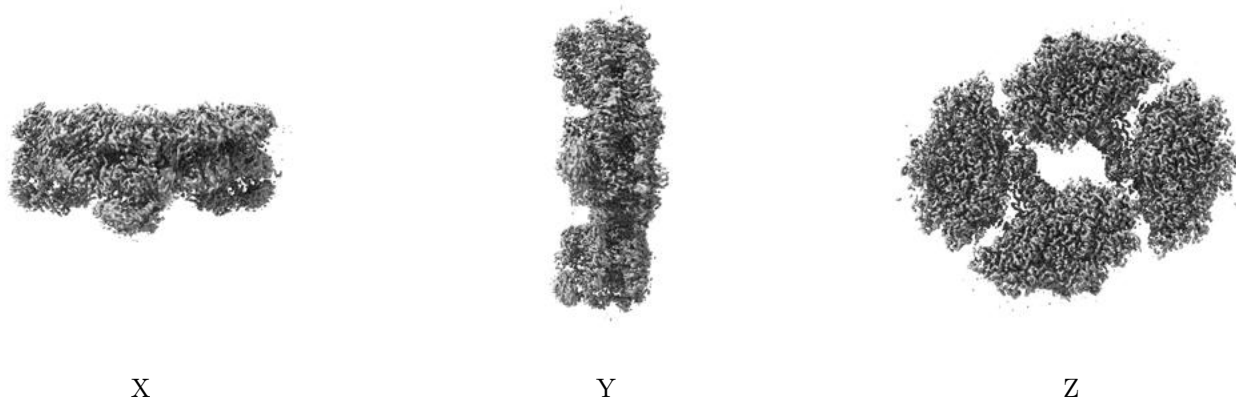


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

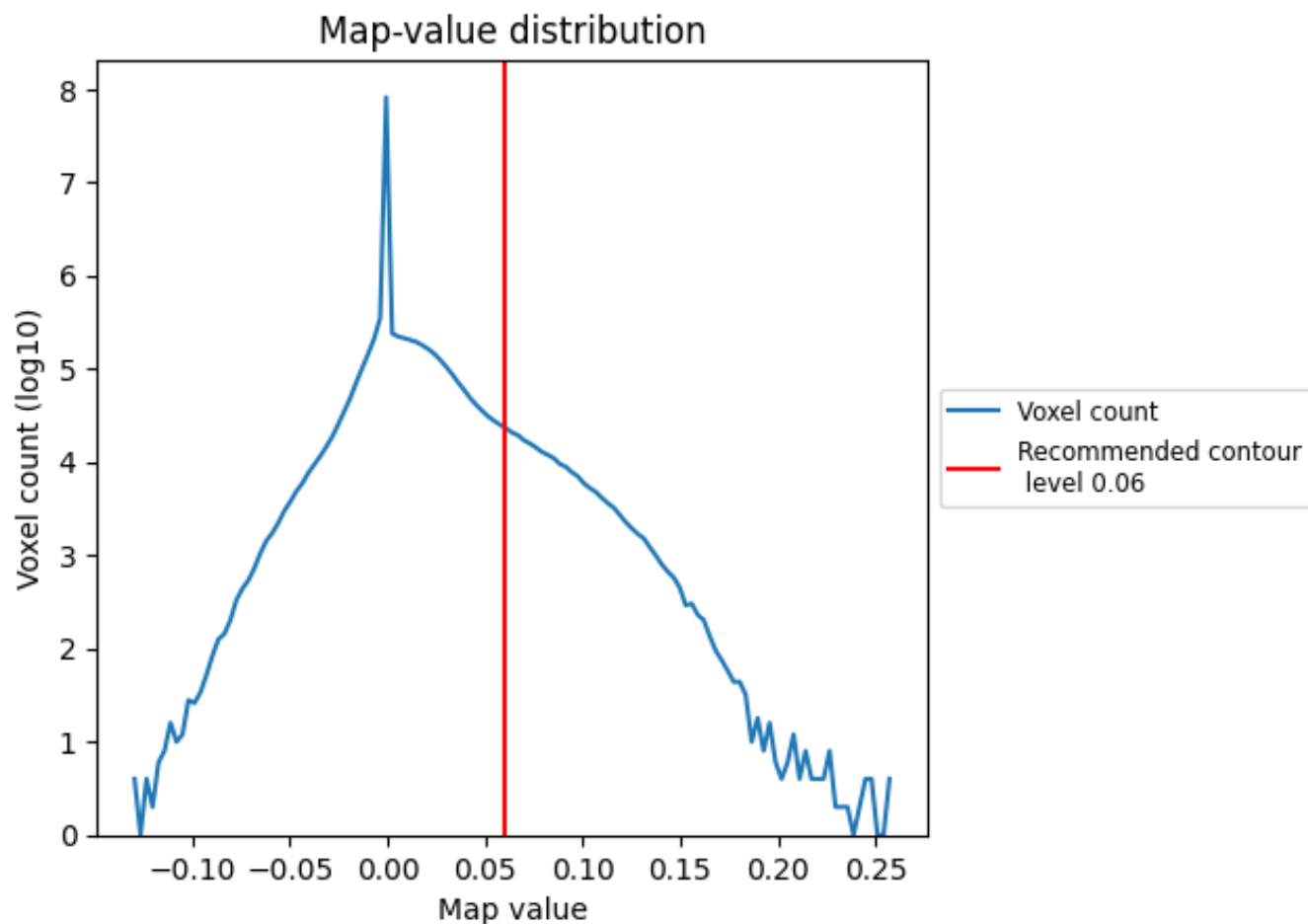
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

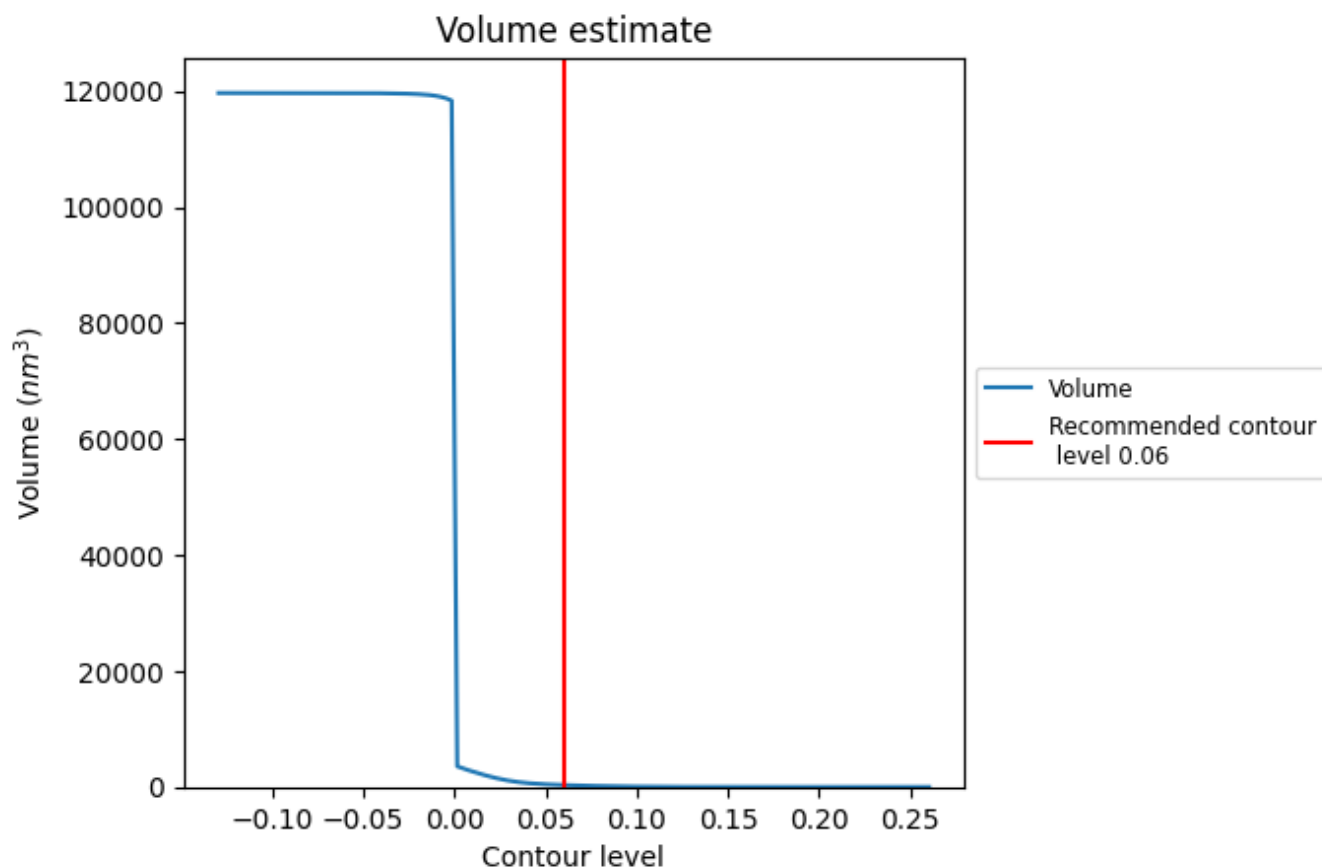
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

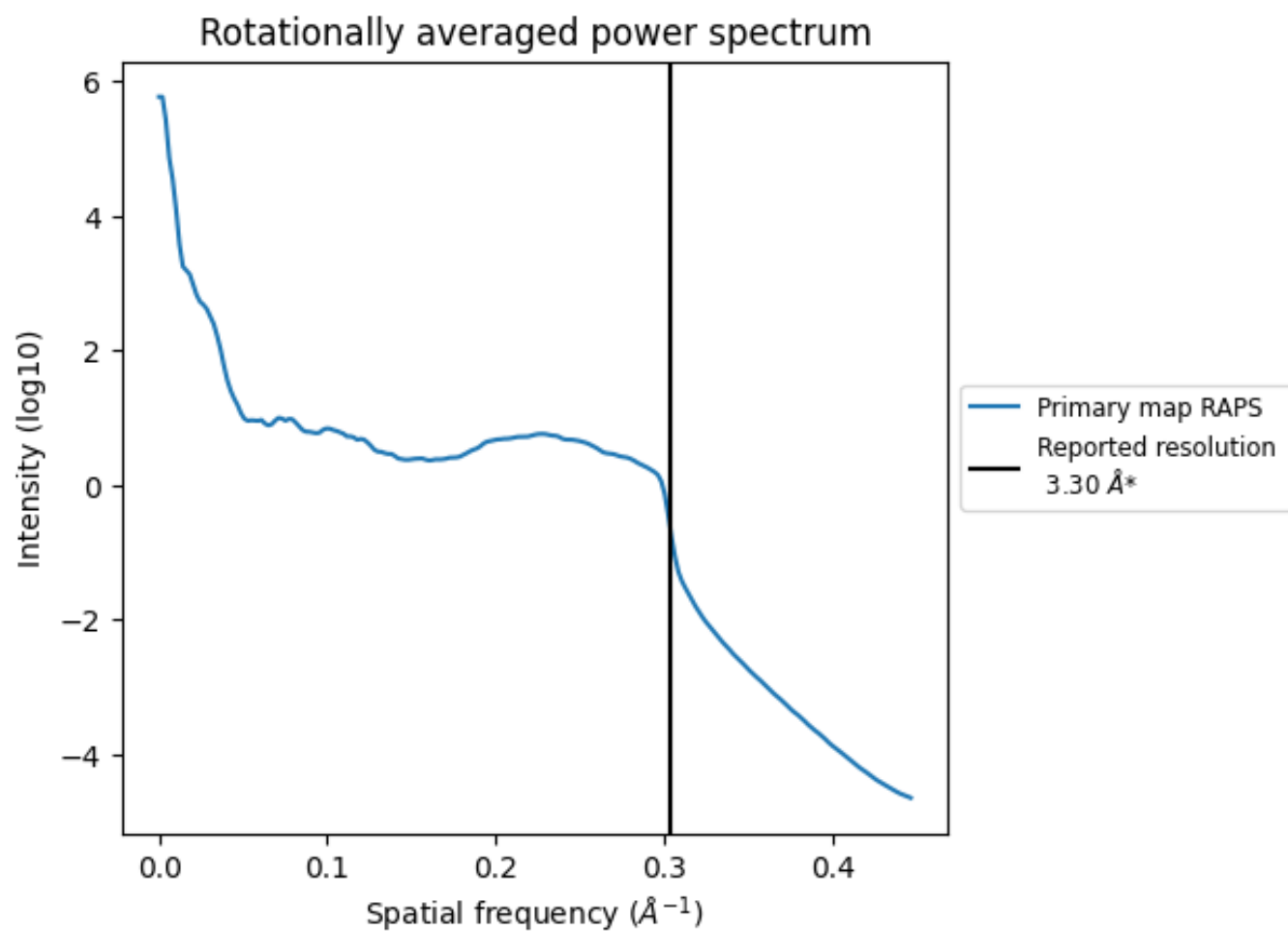
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 322 nm^3 ; this corresponds to an approximate mass of 291 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 ⓘ

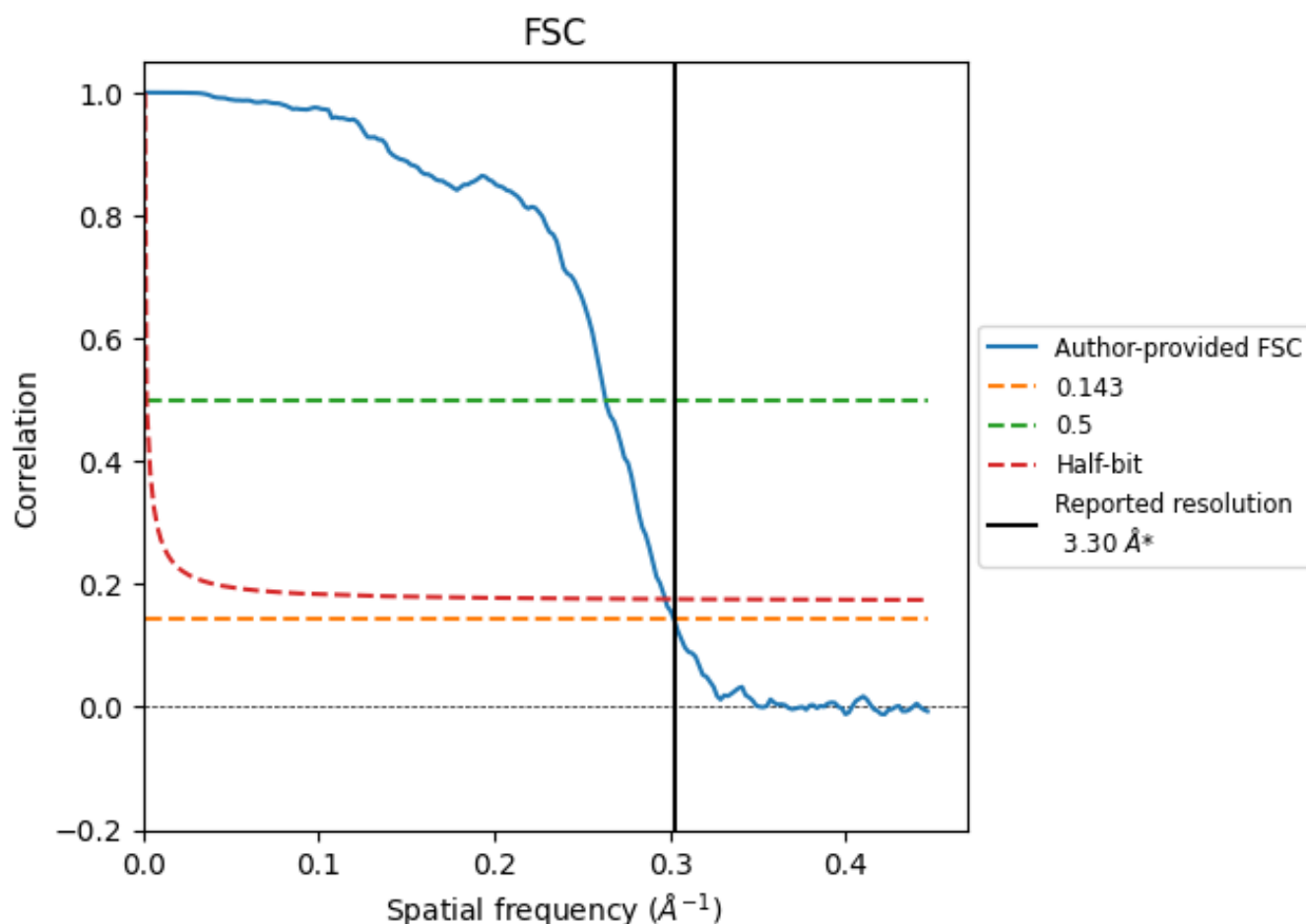


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

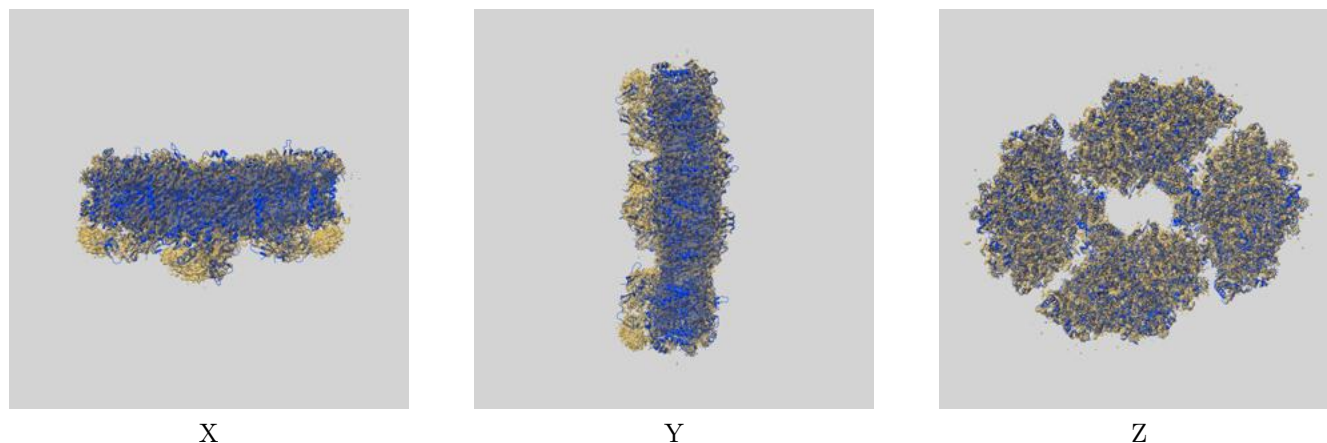
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.80	3.37
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

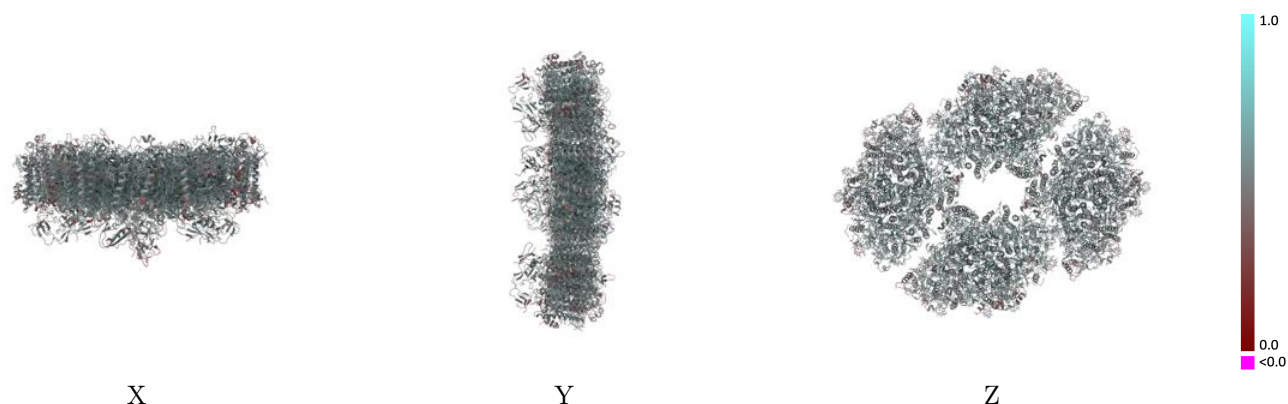
This section contains information regarding the fit between EMDB map EMD-9807 and PDB model 6JEO. Per-residue inclusion information can be found in section [3](#) on page [38](#).

9.1 Map-model overlay [i](#)



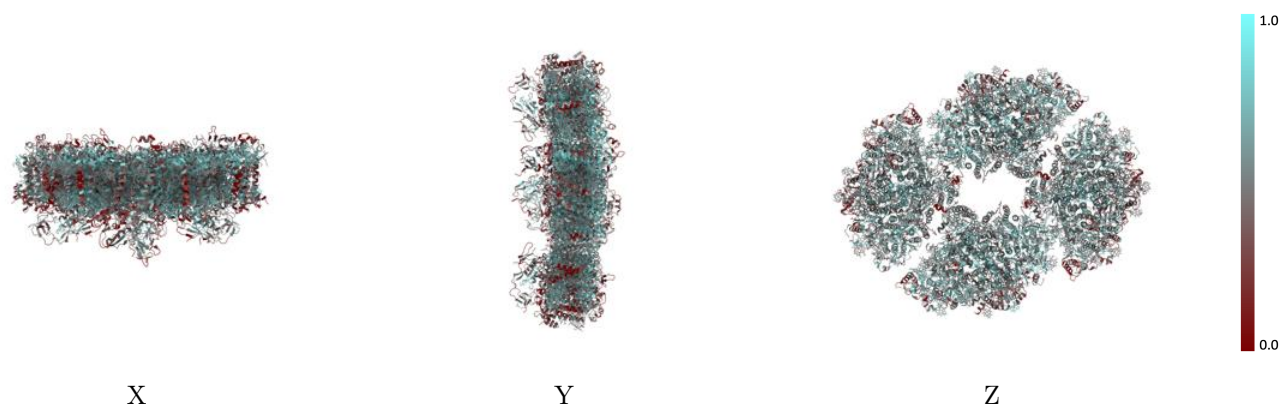
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



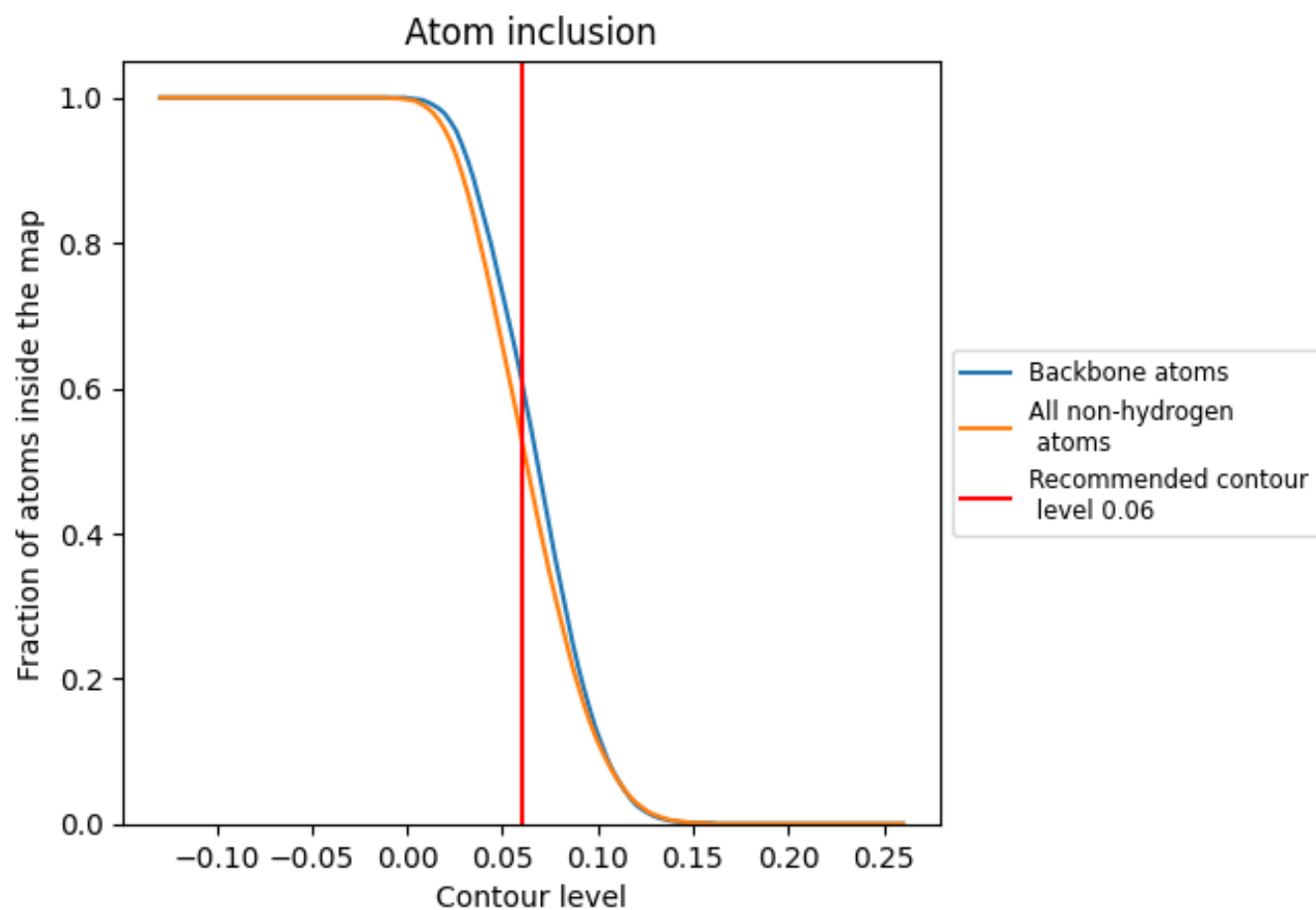
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 53% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5320	 0.5160
aA	 0.5500	 0.5240
aB	 0.5840	 0.5350
aC	 0.5340	 0.5000
aD	 0.3480	 0.4530
aE	 0.3640	 0.4150
aF	 0.3390	 0.4610
aI	 0.4840	 0.5240
aJ	 0.3320	 0.4990
aK	 0.1720	 0.3790
aL	 0.5000	 0.5250
aM	 0.4480	 0.5030
aX	 0.2630	 0.4440
bA	 0.5940	 0.5280
bB	 0.6000	 0.5390
bC	 0.5720	 0.5060
bD	 0.3780	 0.4650
bE	 0.3980	 0.4320
bF	 0.3780	 0.4630
bI	 0.3980	 0.5150
bJ	 0.3900	 0.4860
bK	 0.3060	 0.4020
bL	 0.4760	 0.5040
bM	 0.4440	 0.4930
bX	 0.4060	 0.4720
cA	 0.5500	 0.5250
cB	 0.5810	 0.5360
cC	 0.5420	 0.5000
cD	 0.3410	 0.4580
cE	 0.3580	 0.4210
cF	 0.3400	 0.4590
cI	 0.4740	 0.5250
cJ	 0.3300	 0.5000
cK	 0.1680	 0.3800
cL	 0.5000	 0.5250



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Chain	Atom inclusion	Q-score
cM	 0.4300	 0.4980
cX	 0.2590	 0.4400
dA	 0.5920	 0.5270
dB	 0.5970	 0.5390
dC	 0.5740	 0.5010
dD	 0.3720	 0.4640
dE	 0.3890	 0.4270
dF	 0.3780	 0.4600
dI	 0.3810	 0.5140
dJ	 0.4040	 0.4890
dK	 0.3050	 0.3920
dL	 0.4750	 0.5020
dM	 0.4330	 0.4980
dX	 0.3920	 0.4780