Supplementary Material for:

Interplay between conformational flexibility, intermolecular H-bonding and *3d*-metal cations extraction ability in a series of (thia)calix[4]arene lower rim disubstituted Schiff base derivatives

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1. Spectral characterization of the ligands 3-6

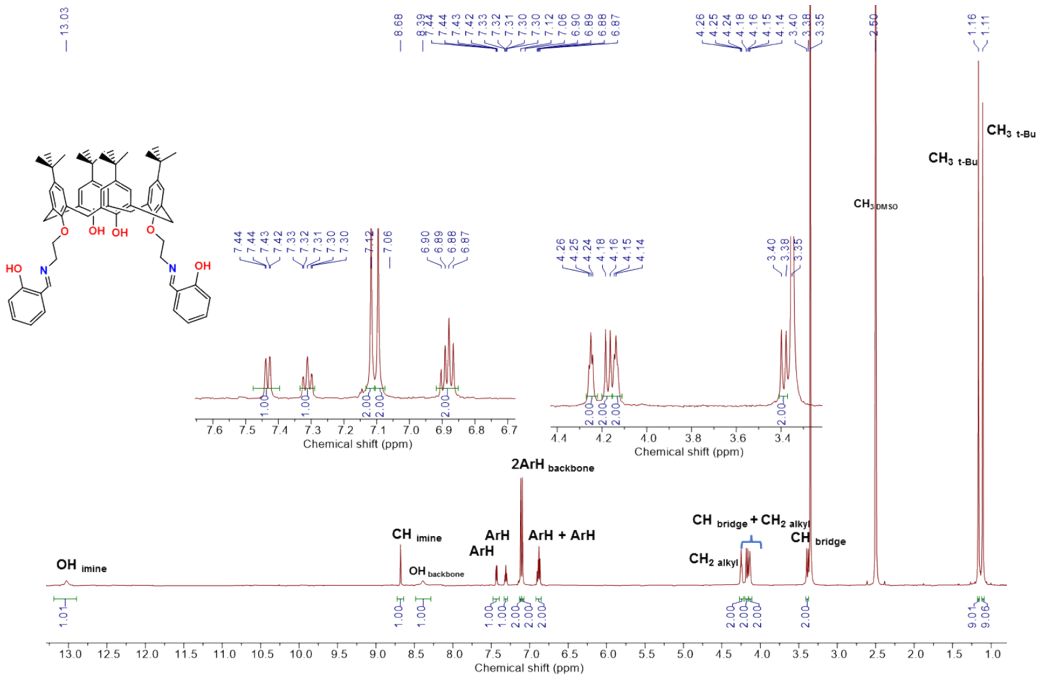


Figure S1. ^{1}H NMR spectrum for **3** ($CDCl_3$, 400 MHz, 25 °C).

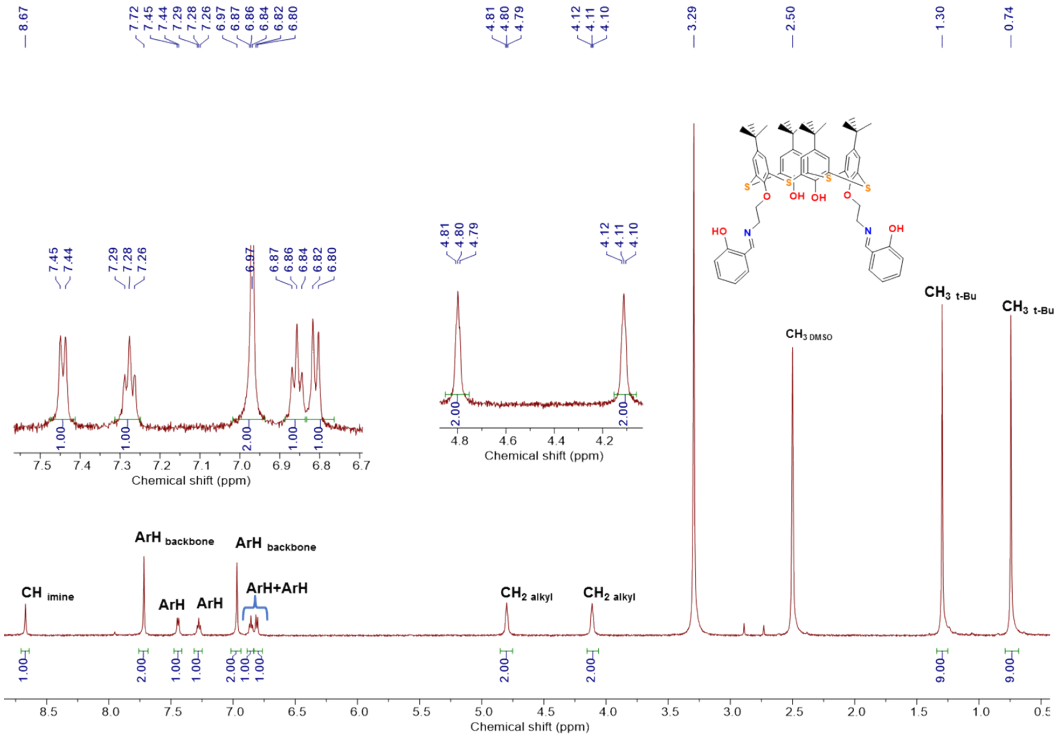


Figure S2. ^{1}H NMR spectrum for **4** ($CDCl_3$, 400 MHz, 25 °C).

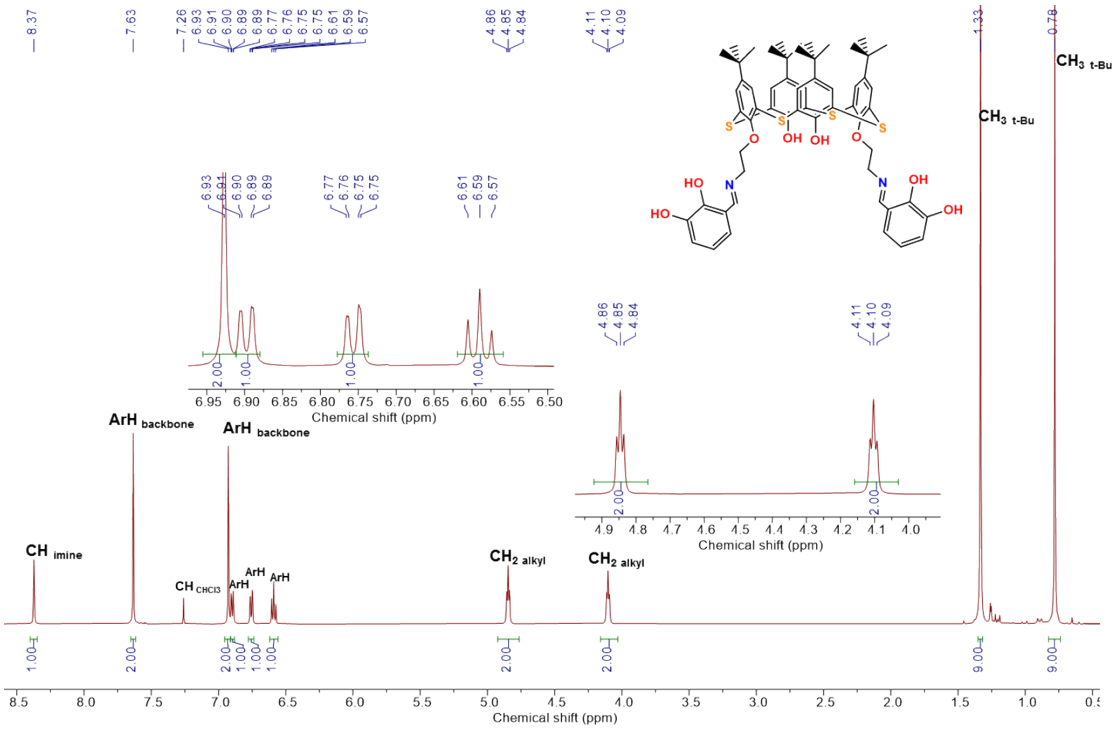


Figure S3. ^{1}H NMR spectrum for **6** ($CDCl_3$, 400 MHz, 25 °C).

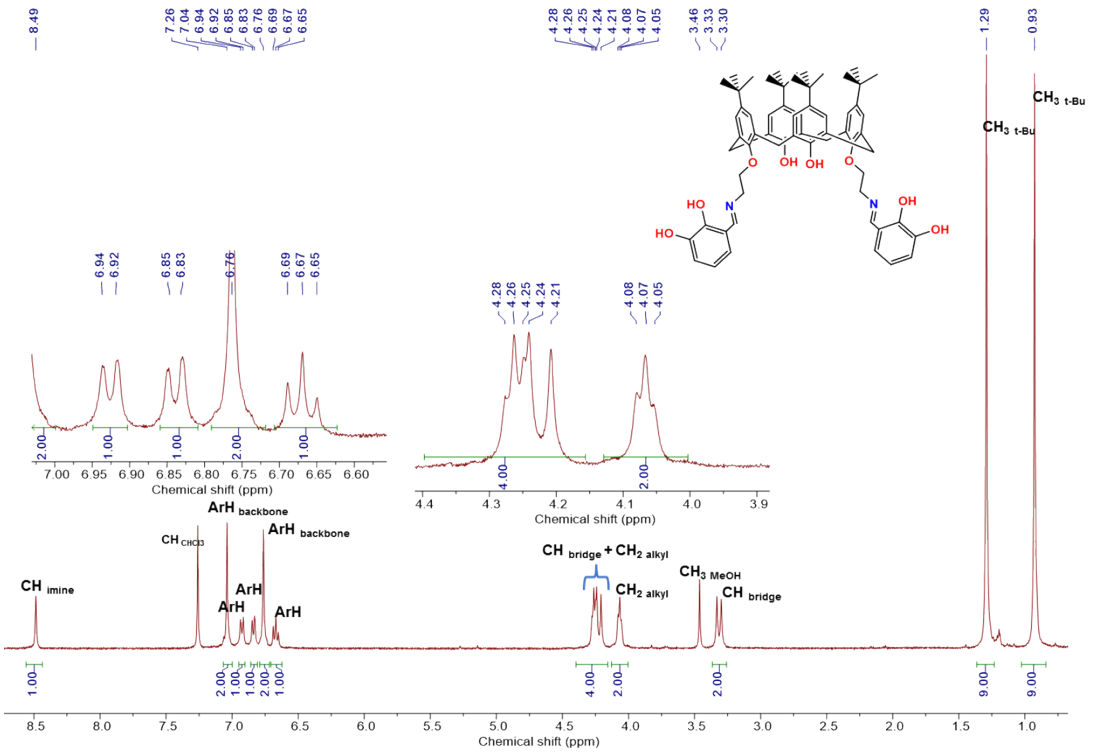


Figure S4. ^{1}H NMR spectrum for **5** ($CDCl_3$, 400 MHz, 25 °C).

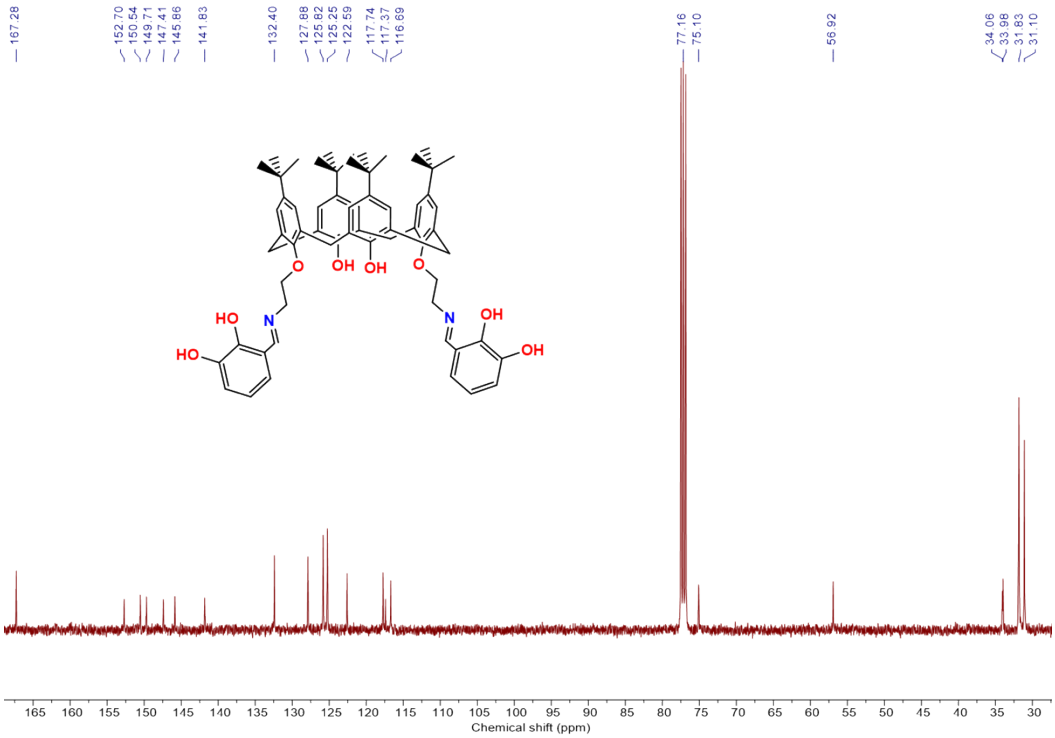


Figure S5. ^{13}C NMR spectrum for **5** ($CDCl_3$, 100 MHz, 25 °C).

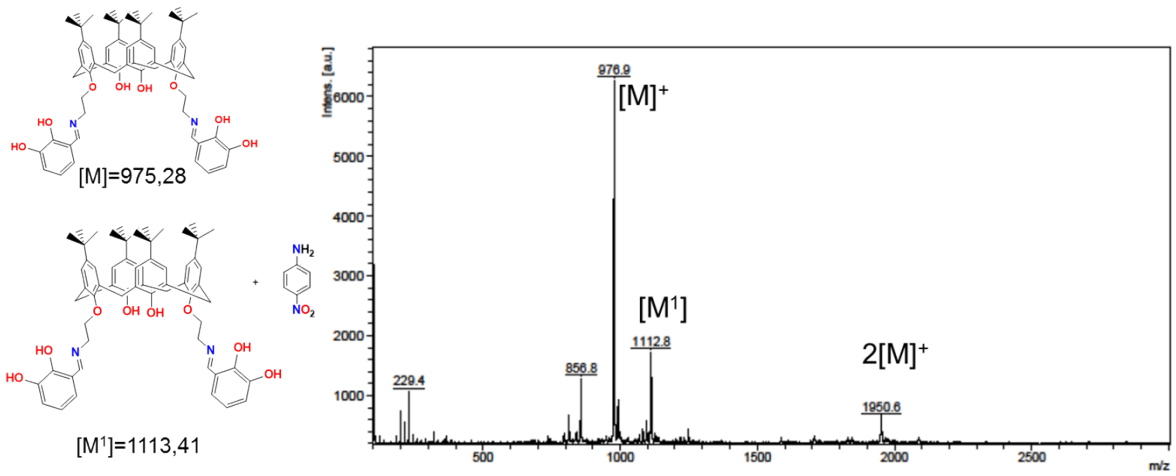


Figure S6. MALDI-MS spectrum for **5** (right) and the m/z_{teor} calculated for $[M]^+$ and $[M^1]^+$ (M^1=M+M_{PNA}).

2. Single Crystal X-ray diffraction data for 4-6

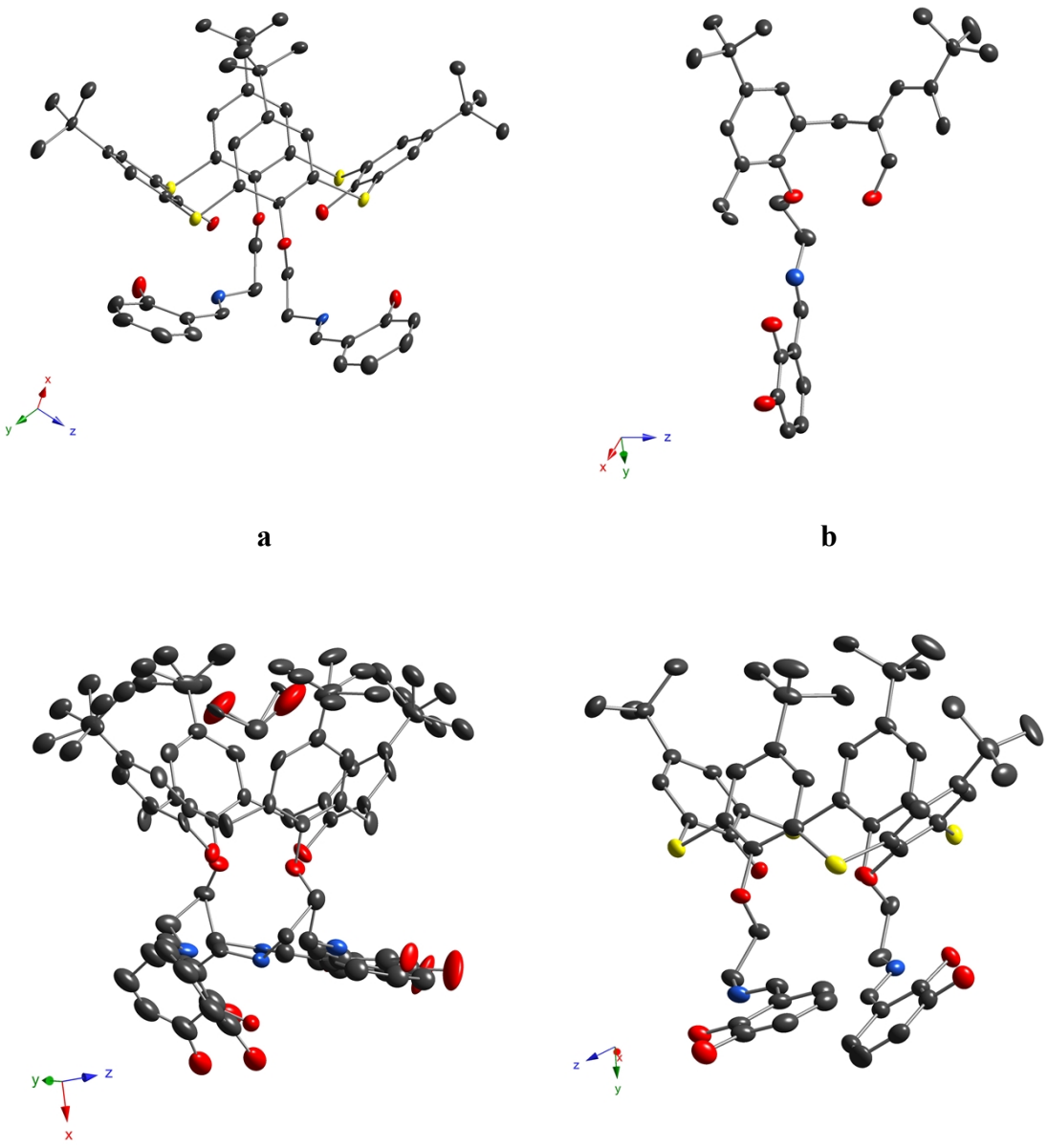
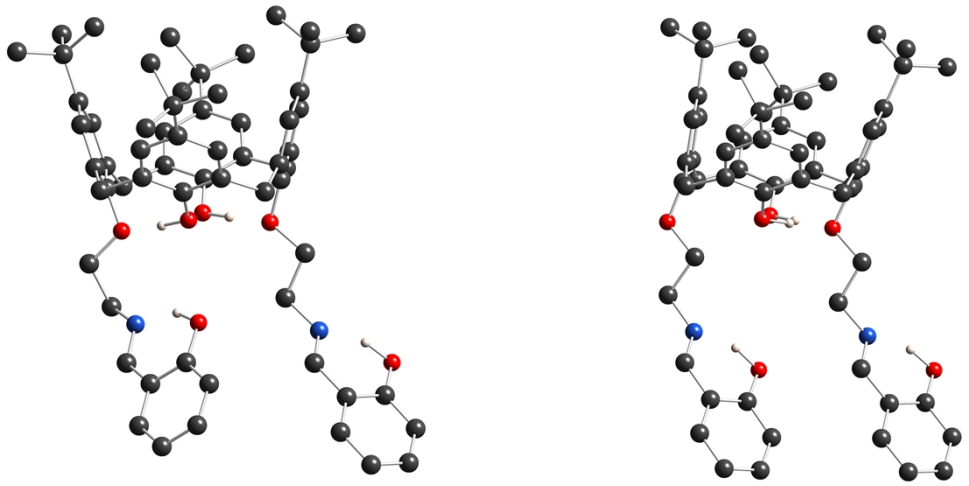


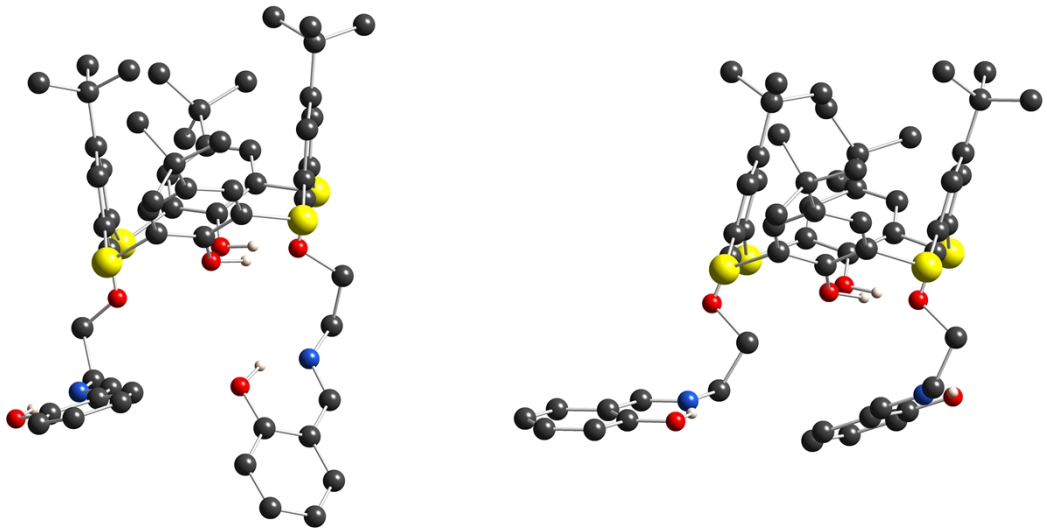
Figure S7. ORTEP views for asymetric parts of **4** (a), **5a** (b), **5b** (c) and **6** (d), showing thermal ellipsoids at the 50% probability level. The C-, O-, N- and S- atoms are represented by dark grey, red, blue and yellow ellipsoids. The H-atoms and solvate moleules are omitted for clarity.

3. DFT-optimized geometry of the ligands 4-6



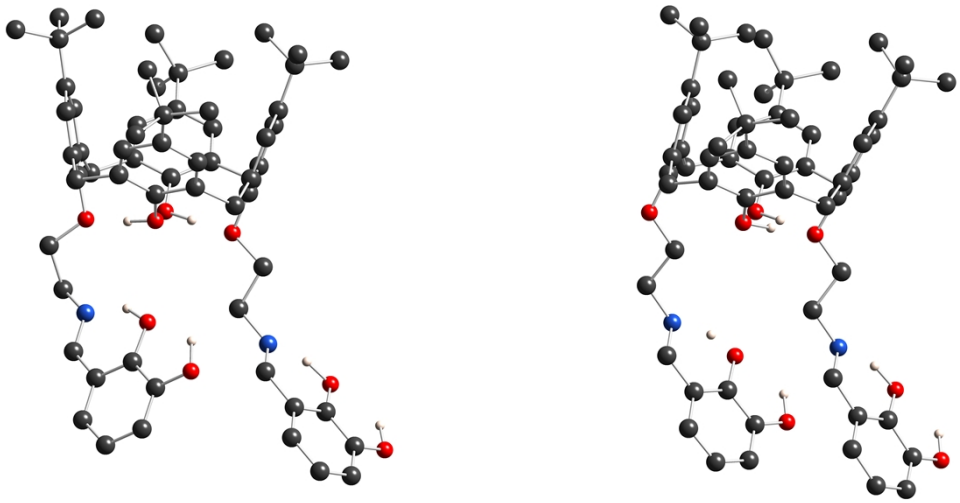
a **b**

Figure S8. For **3**, DFT-optimized geometry of *exo-exo* (a) and *endo-exo* (b) rotamers. The H-, C-, O-, and N- atoms are represented by pale rose, dark grey, red and blue spheres. H-atoms, which are not involved in intramolecular H-bonding, are omitted for clarity.



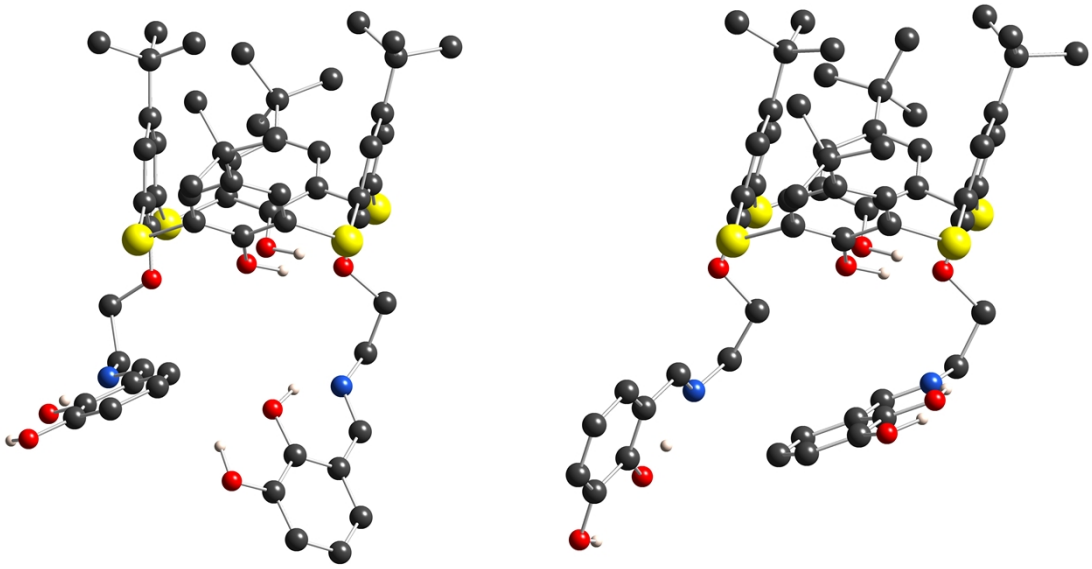
a **b**

Figure S9. For **4**, DFT-optimized geometry of *exo-exo* (a) and *endo-exo* (b) rotamers. The H-, C-, O-, N- and S-atoms are represented by pale rose, dark grey, red, blue and yellow spheres. H-atoms, which are not involved in intramolecular H-bonding, are omitted for clarity.



a **b**

Figure S10. For **5**, DFT-optimized geometry of *exo-exo* (a) and *endo-exo* (b) rotamers. The H-, C-, O-, and N- atoms are represented by pale rose, dark grey, red and blue spheres. H-atoms, which are not involved in intramolecular H-bonding, are omitted for clarity.



a **b**

Figure S11. For **6**, DFT-optimized geometry of *exo-exo* (a) and *endo-exo* (b) rotamers. The H-, C-, O-, N- and S-atoms are represented by pale rose, dark grey, red, blue and yellow spheres. H-atoms, which are not involved in intramolecular H-bonding, are omitted for clarity.

4. Solid state IR and Raman spectra for 3-6

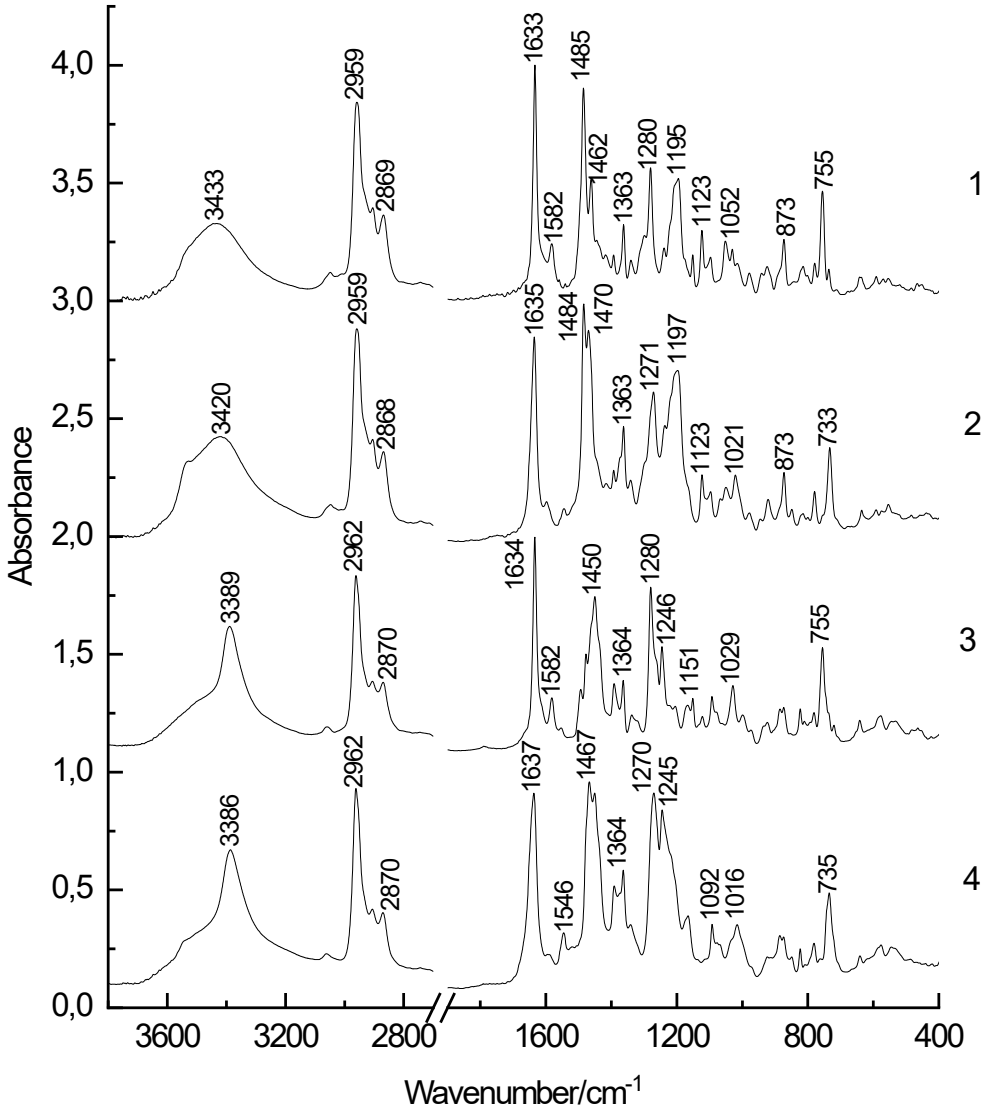


Figure S12. Comparison of experimentally obtained IR spectra for crystalline samples of calix[4]arenes **3** (1) and **5** (2), thiacalix[4]arenes **4** (3) and **6** (4).

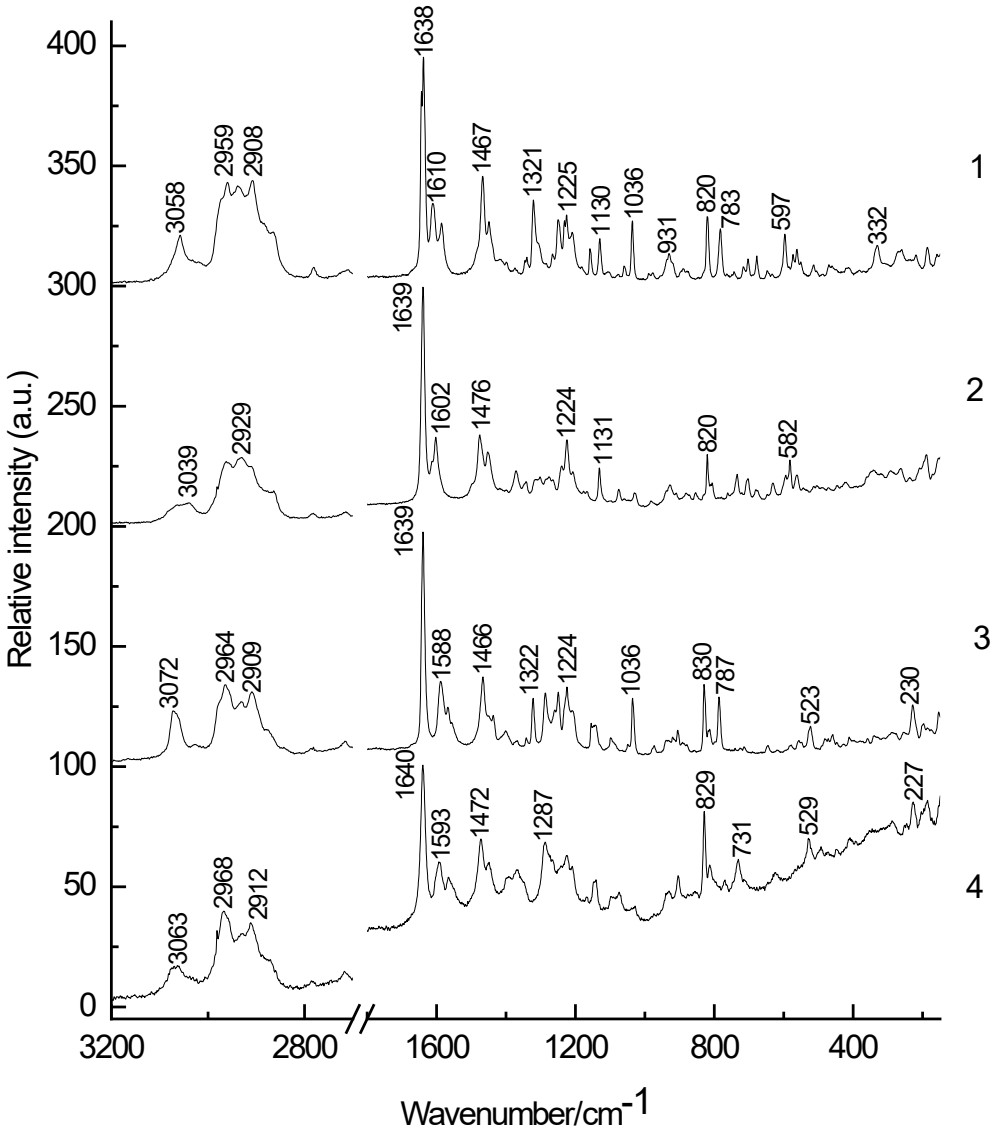


Figure S13. Comparison of experimentally obtained Raman spectra for crystalline samples of calix[4]arenes **3** (1) and **5** (2), thiacalix[4]arenes **4** (3) and **6** (4).

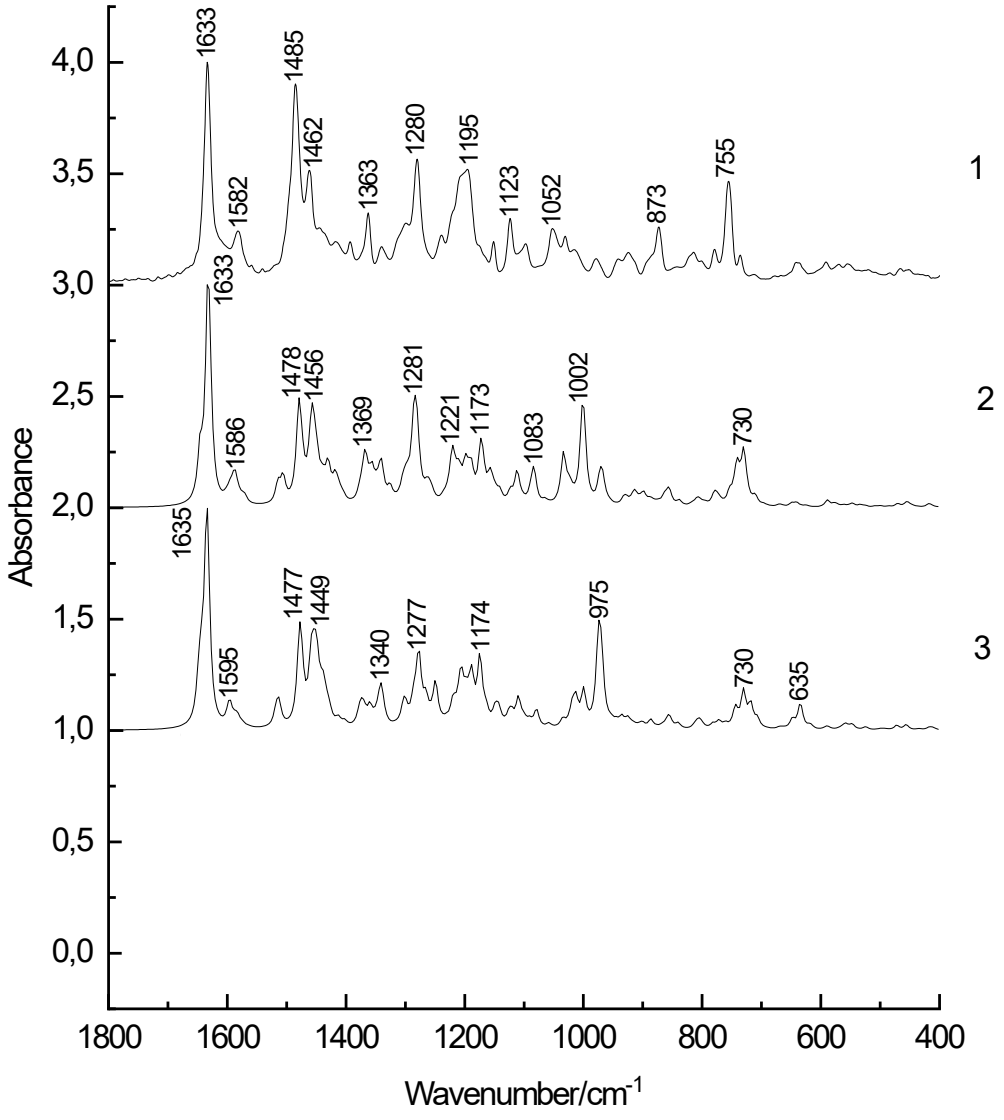


Figure S14. For **3**, comparison of experimentally obtained (1) and theoretically calculated IR spectra of *exo-exo* (2) and *endo-exo* (3) rotamers.

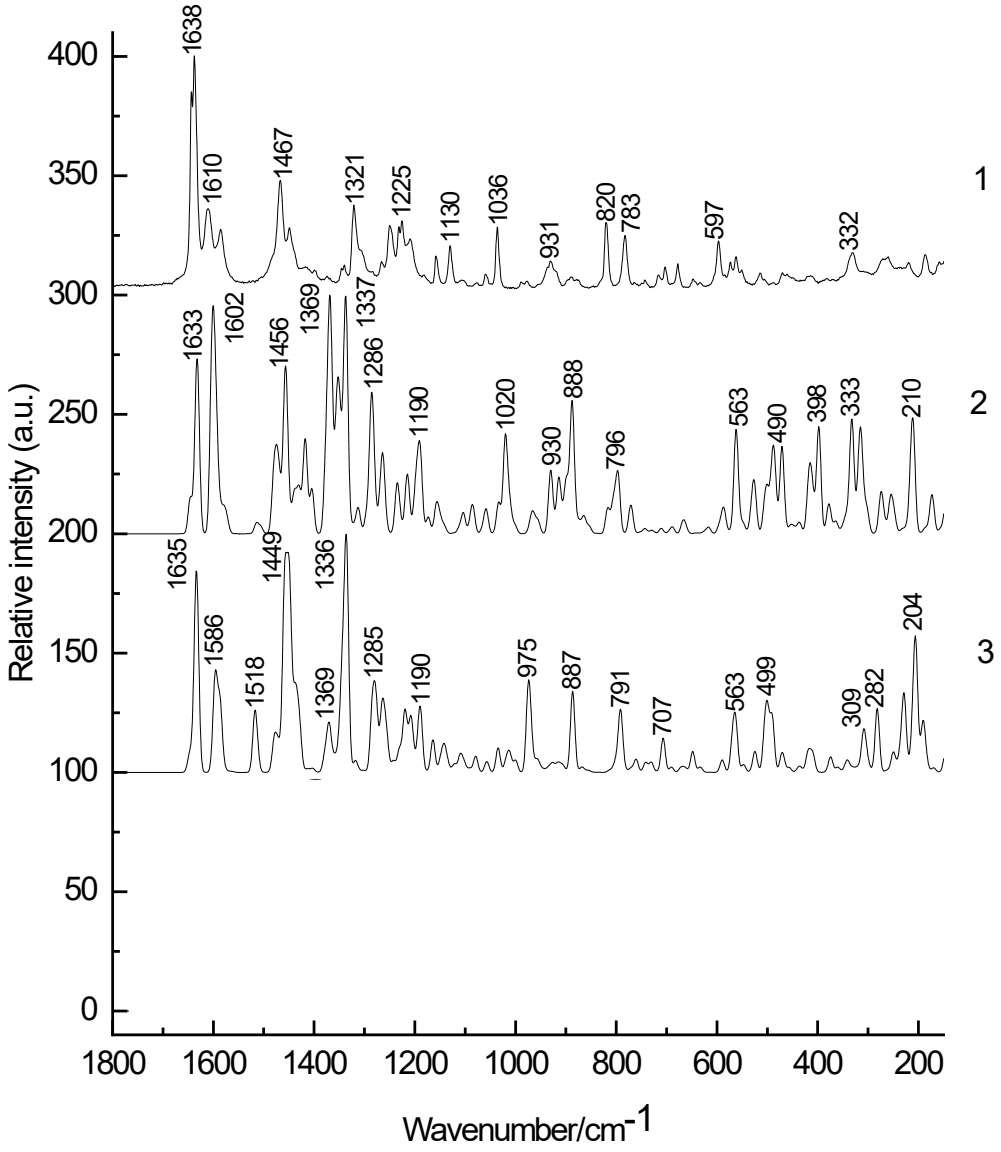


Figure S15. For **3**, comparison of experimentally obtained (1) and theoretically calculated Raman spectra of *exo-exo* (2) and *endo-exo* (3) rotamers.

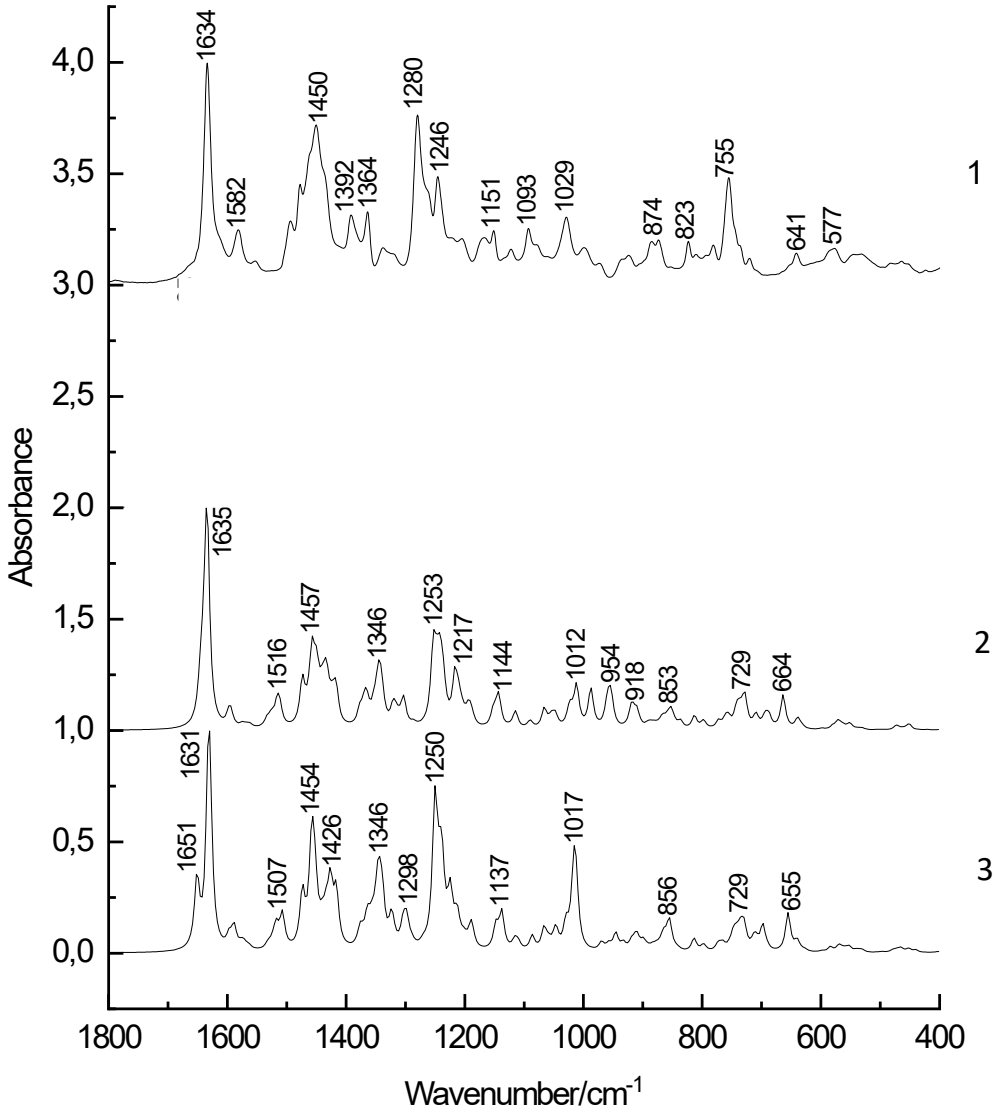


Figure S16. For **4**, comparison of experimentally obtained (1) and theoretically calculated IR spectra of *endo-exo* (2) and *exo-exo* (3) rotamers.

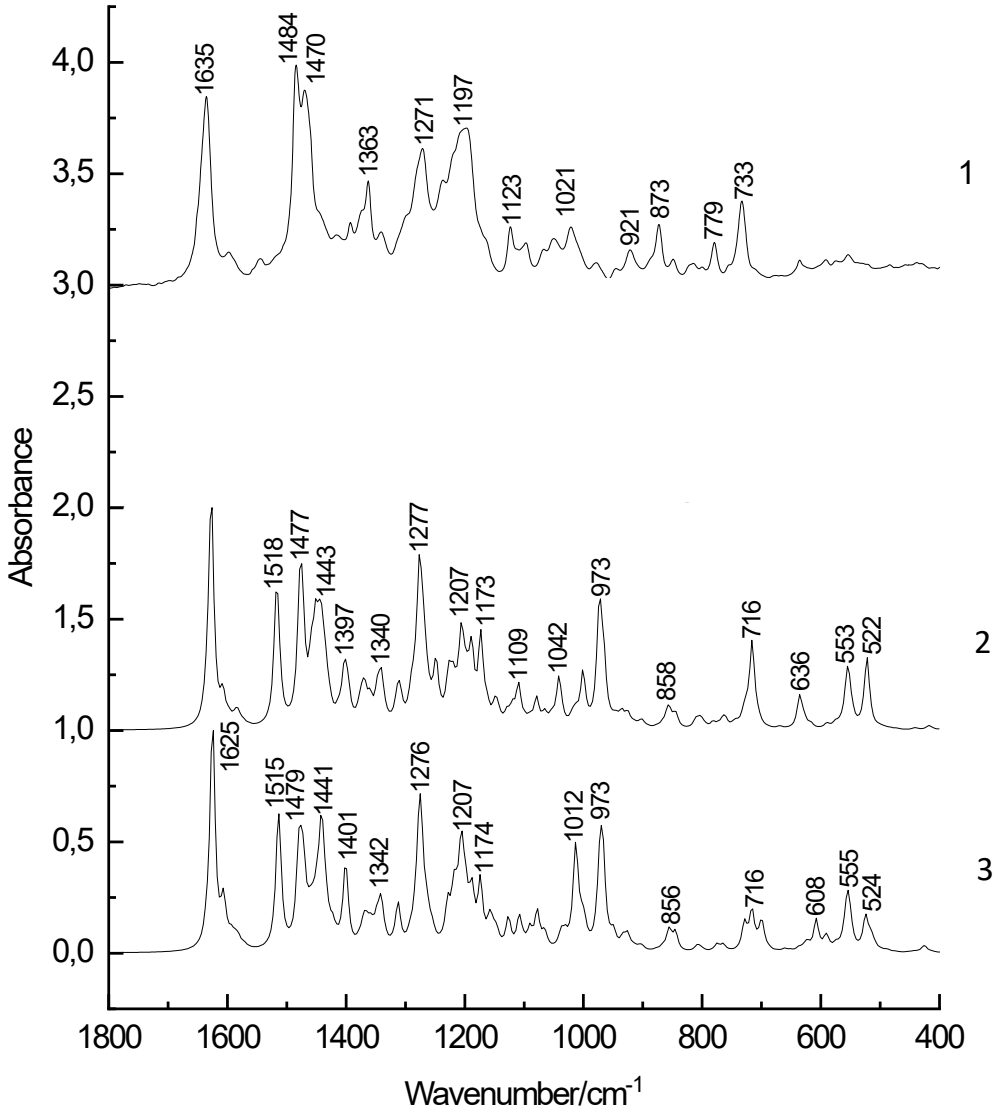


Figure S17. For **4**, comparison of experimentally obtained (1) and theoretically calculated Raman spectra of *endo-exo* (2) and *exo-exo* (3) rotamers.

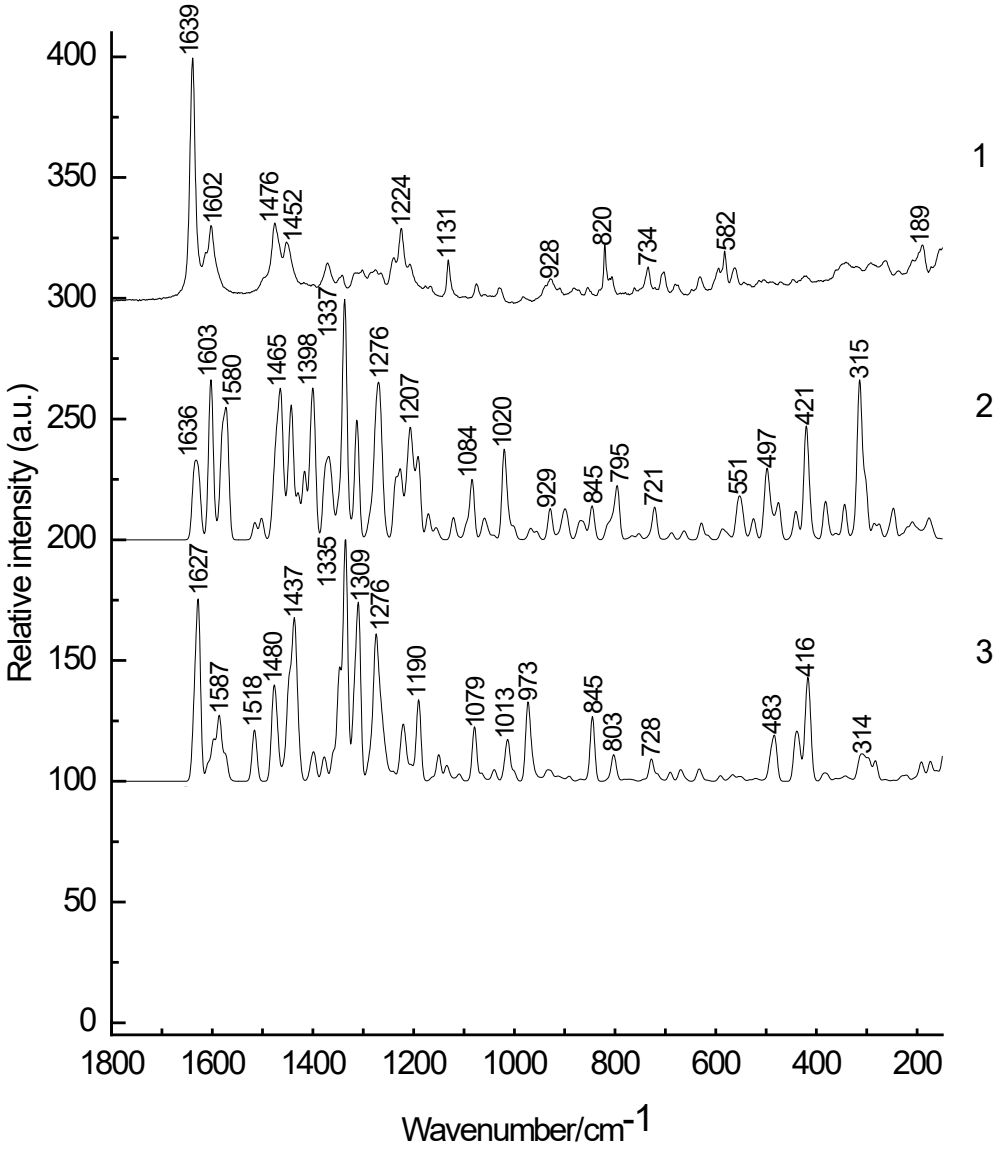


Figure S18. For **5**, comparison of experimentally obtained (1) and theoretically calculated IR spectra of *exo-exo* (2) and *endo-exo* (3) rotamers.

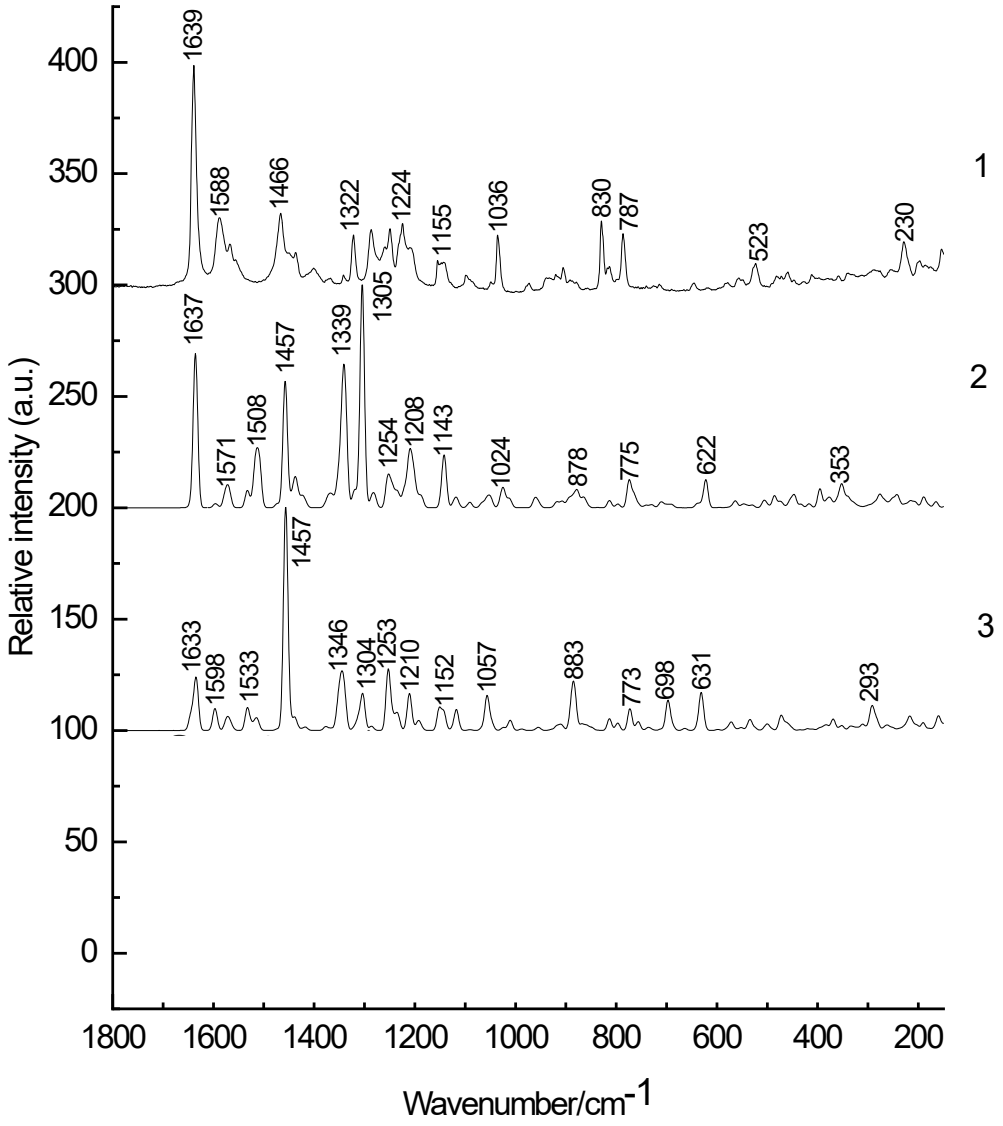


Figure S19. For **5**, comparison of experimentally obtained (1) and theoretically calculated Raman spectra of *exo-exo* (2) and *endo-exo* (3) rotamers.

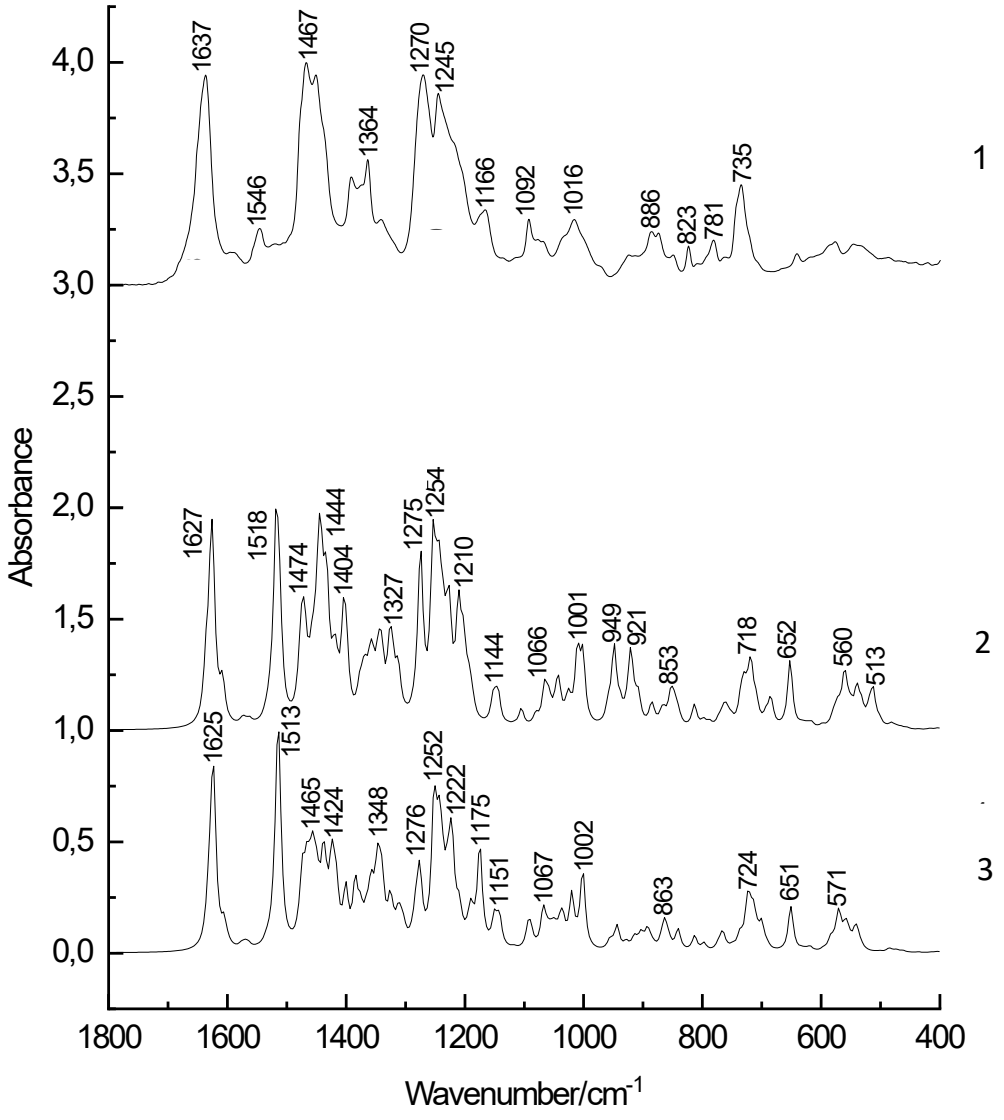


Figure S20. For **6**, comparison of experimentally obtained (1) and theoretically calculated IR spectra of *endo-exo* (2) and *exo-exo* (3) rotamers.

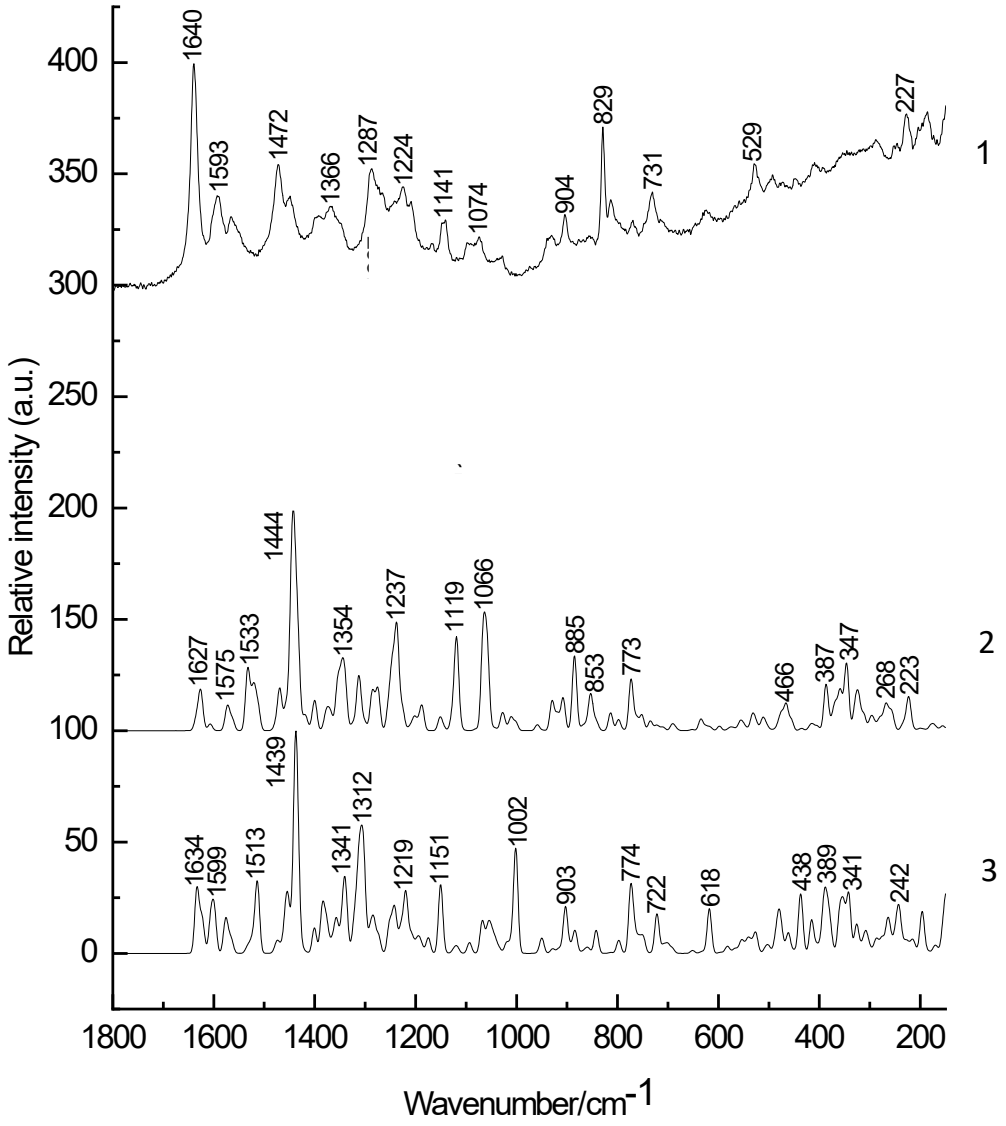
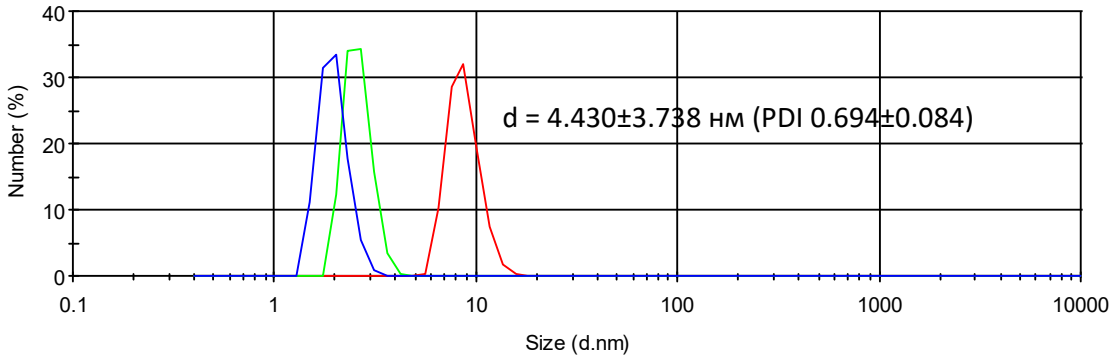
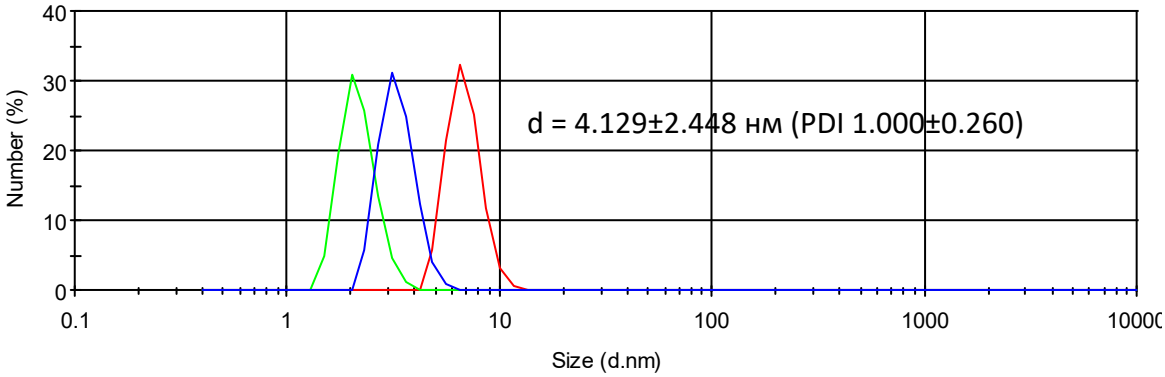


Figure S21. For **6**, comparison of experimentally obtained (1) and theoretically calculated Raman spectra of *exo-exo* (2) and *endo-exo* (3) rotamers.

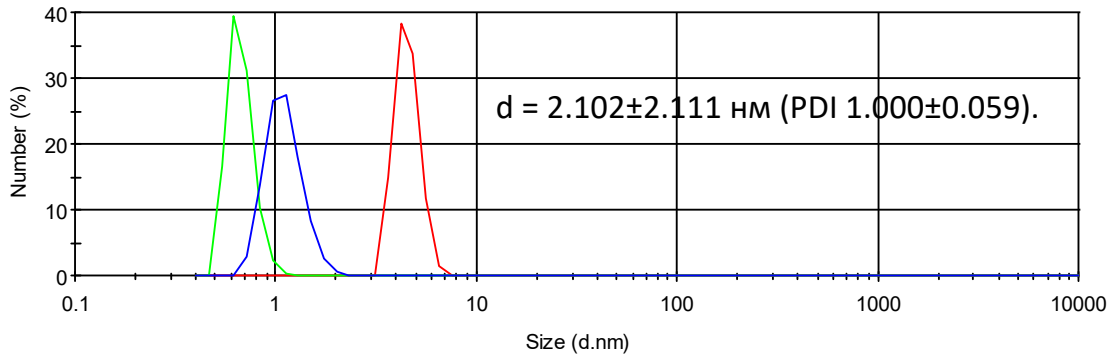
5. DLS study



a



b



c

Figure S21. DLS spectra, obtained by three consecutive measurements of the CH_2Cl_2 solutions (C = 4×10^{-3}M, 25 °C) of **3** (a), **4** (b) and **5** (c), showing the average hydrodynamic diameter (d, nm) of forming aggregates and polydispersity index (PDI).

6. Structural characteristics for ligands 3-6

Table S1. For **3-6**, a comparison of experimental and theoretical dihedral angles (°) of *exo-exo* and *endo-exo* rotamers.

System	Dihedral angles	Exp.	*exo-exo*	*endo-exo*
3	C(4)–C(3)–C(40)–C(43)	-80.6	-79.0	-79.8
	C(3)–C(40)–C(43)–C(49)	83.0	104.6	103.8
	C(46)–C(45)–C(64)–C(67)	-79.0	-95.7	-104.5
	C(45)–C(64)–C(67)–C(73)	80.0	67.0	53.1
	C(70)–C(69)–C(106)–C(109)	-84.5	-77.9	-54.5
	C(69)–C(106)–C(109)–C(115)	87.4	105.9	106.3
	C(112)–C(111)–C(130)–C(1)	-83.1	-96.9	-104.1
	C(111)–C(130)–C(1)–C(7)	76.7	67.4	78.9
4	C(14)–C(15)–S(16)–C(27)	-78.6	-102.3	-80.1
	C(15)–S(16)–C(27)–C(26)	107.3	60.5	112.2
	C(6)–C(7)–S(25)–C(8)	-108.6	-61.3	-113.8
	C(7)–S(25)–C(8)–C(9)	42.9	104.1	46.5
	C(11)–C(12)–S(29)–C(32)	-47.3	-104.5	-47.5
	C(12)–S(29)–C(32)–C(31)	121.8	76.5	116.1
	C(19)–C(24)–S(23)–C(22)	-115.5	-76.9	-112.1
	C(24)–S(23)–C(22)–C(17)	77.8	103.8	79.2
5	C(4)–C(3)–C(40)–C(43)	-80.6	-77.8	-79.8
	C(3)–C(40)–C(43)–C(49)	83.0	105.2	103.6
	C(46)–C(45)–C(64)–C(67)	-79.0	-96.5	-104.4
	C(45)–C(64)–C(67)–C(73)	80.0	66.2	53.0
	C(70)–C(69)–C(106)–C(109)	-84.5	-77.2	-54.3
	C(69)–C(106)–C(109)–C(115)	87.4	106.7	106.0
	C(112)–C(111)–C(130)–C(1)	-83.1	-97.6	-104.0
	C(111)–C(130)–C(1)–C(7)	76.7	66.3	79.0
6	C(11)–C(12)–S(29)–C(32)	-78.4	-62.8	-79.9
	C(12)–S(29)–C(32)–C(31)	98.1	115.7	112.2
	C(19)–C(24)–S(23)–C(22)	-103.0	-108.5	-115.0
	C(24)–S(23)–C(22)–C(17)	41.9	74.0	47.6
	C(14)–C(15)–S(16)–C(27)	-41.1	-80.4	-48.6
	C(15)–S(16)–C(27)–C(26)	107.0	113.6	115.0
	C(6)–C(7)–S(25)–C(8)	-107.6	-112.3	-111.8
	C(7)–S(25)–C(8)–C(9)	81.5	57.9	78.8

Table S2. For **3-6**, a comparison of experimental and theoretical bond distances (Å) and bond angles (°) of *exo-exo* and *endo-exo* rotamers.

Compound name		Exp.	*exo-exo*	*endo-exo*
3	*Bond distances*			
	C(2)–O(135)	1.389	1.399	1.389
	C(22)–C(25)	1.495	1.530	1.530
	C(22)–O(135)	1.435	1.441	1.439
	C(25)–N(133)	1.445	1.452	1.452
	C(28)–C(30)	1.417	1.448	1.450
	C(28)–N(133)	1.281	1.292	1.290
	C(30)–C(39)	1.355	1.429	1.430
	C(39)–O(136)	1.410	1.336	1.338
	C(44)–O(138)	1.376	1.356	1.361
	C(67)–C(73)	1.393	1.403	1.403
	C(64)–C(67)	1.521	1.524	1.523
	C(72)–C(75)	1.527	1.538	1.538
	C(75)–C(84)	1.503	1.546	1.539
	Angles			
	C(2)–O(135)–C(22)	112.7	115.6	120.9
	C(4)–C(6)–C(7)	117.5	123.0	117.5
	C(22)–C(25)–N(133)	110.3	110.0	109.3
	C(25)–C(22)–O(135)	107.5	106.7	106.2
	C(25)–N(133)–C(28)	118.5	118.9	120.2
	C(28)–C(30)–C(31)	121.4	120.5	120.8
	C(30)–C(28)–N(133)	123.8	121.7	121.4
	C(30)–C(39)–O(136)	121.8	121.5	121.4
	C(43)–C(49)–C(48)	122.7	109.5	122.6
	C(45)–C(44)–O(138)	117.8	116.6	116.5
	C(49)–C(48)–C(51)	121.8	123.2	123.1
	Dihedral angles			
	C(2)–O(135)–C(22)–C(25)	176.7	175.9	172.9
	C(3)–C(2)–O(135)–C(22)	93.0	97.5	94.4
	C(22)–C(25)–N(133)–C(28)	119.1	126.0	125.0
	C(25)–N(133)–C(28)–C(30)	178.0	179.6	178.8
	C(31)–C(30)–C(28)–N(133)	179.8	179.6	178.9
	C(43)–C(49)–C(48)–C(51)	175.9	178.9	178.8
	C(45)–C(64)–C(67)–C(68)	93.1	109.6	123.2
	C(46)–C(45)–C(64)–C(67)	79.0	95.7	104.5
	C(49)–C(43)–C(44)–O(138)	178.0	176.7	176.4
	C(49)–C(48)–C(51)–C(60)	118.4	119.6	119.6
	N(133)–C(25)–C(22)–O(135)	172.6	178.5	179.1
4	*Bond distances*			
	C(3)–O(20)	1.380	1.540	1.373
	C(5)–C(34)	1.533	1.540	1.537
	C(6)–C(7)	1.388	1.404	1.395
	C(7)–S(25)	1.779	1.430	1.796
	O(20)–C(49)	1.435	1.409	1.448
	C(34)–C(40)	1.530	1.397	1.539
	C(49)–C(101)	1.500	1.512	1.523
	C(101)–N(104)	1.464	1.528	1.451

	N(104)–C(106)	1.272	1.402	1.290
	C(106)–C(110)	1.461	1.512	1.449
	C(110)–C(112)	1.392	1.512	1.408
	O(108)–C(109)	1.345	1.512	1.335
	Angles			
	O(2)–C(18)–C(7)	117.9	115.9	120.2
	C(3)–O(20)–C(49)	116.3	108.1	116.2
	C(5)–C(6)–C(7)	122.4	117.8	122.8
	C(5)–C(34)–C(40)	112.0	117.4	112.1
	C(6)–C(5)–C(34)	120.1	123.2	120.1
	O(20)–C(49)–C(101)	106.0	119.0	106.9
	C(49)–C(101)–N(104)	111.2	119.1	112.1
	C(101)–N(104)–C(106)	118.7	113.9	119.4
	N(104)–C(106)–C(110)	122.6	122.5	112.1
	C(106)–C(110)–C(112)	120.7	113.3	120.6
	O(108)–C(109)–C(110)	122.0	126.0	121.6
	Dihedral angles			
	C(3)–C(8)–S(25)–C(7)	130.6	179.7	130.9
	C(3)–O(20)–C(49)–C(101)	173.1	121.2	178.5
	C(6)–C(5)–C(34)–C(40)	171.3	0.7	179.5
	C(6)–C(7)–S(25)–C(8)	121.8	179.7	116.1
	C(7)–C(6)–C(5)–C(34)	179.8	87.9	179.5
	C(8)–C(3)–O(20)–C(49)	85.6	106.0	92.4
	C(49)–C(101)– N(104)–C(106)	141.4	104.5	113.6
	O(108)–C(109)–C(110)–C(112)	179.0	176.7	180.0
	O(20)–C(49)–C(101)–N(104)	59.0	117.8	69.2
	N(104)–C(106)–C(110)–C(112)	177.9	62.0	179.4
5	*Bond distances*			
	C(2)–O(135)	1.378	1.400	1.388
	C(3)–C(40)	1.498	1.523	1.523
	C(22)–O(135)	1.452	1.441	1.443
	C(25)–N(133)	1.395	1.453	1.452
	C(28)–C(30)	1.396	1.447	1.451
	C(28)–N(133)	1.286	1.295	1.289
	C(30)–C(31)	1.421	1.414	1.413
	C(37)–O(38)	1.359	1.362	1.364
	C(72)–C(75)	1.527	1.538	1.539
	C(75)–C(76)	1.567	1.547	1.546
	C(44)–O(138)	1.360	1.357	1.366
	C(112)–C(114)	1.420	1.401	1.405
	Angles			
	C(2)–O(135)–C(22)	124.2	115.1	120.2
	C(22)–C(25)– N(133)	111.3	109.7	112.4
	C(25)–C(22)–O(135)	114.7	107.2	107.6

	C(25)–N(133)–C(28)	132.7	119.2	119.5
	C(28)–C(30)–C(31)	117.6	121.5	120.4
	C(30)–C(28)– N(133)	129.3	121.2	121.7
	C(30)–C(39)–O(136)	121.7	123.1	122.6
	C(43)–C(44)–O(138)	119.0	124.2	123.8
	C(43)–C(49)–C(48)	123.0	123.0	122.9
	C(48)–C(51)–C(56)	114.2	109.5	109.4
	C(49)–C(48)–C(51)	123.2	123.2	123.2
	Dihedral angles			
	C(1)–C(2)–O(135)–C(22)	71.9	87.1	89.4
	C(2)–O(135)–C(22)–C(25)	147.3	172.5	171.7
	C(22)–C(25)–N(133)–C(28)	149.9	116.7	126.2
	C(31)–C(30)–C(28)–N(133)	132.8	179.7	179.5
	C(45)–C(46)–C(48)–C(51)	175.9	179.7	178.8
	C(45)–C(64)–C(67)–C(73)	117.1	66.2	78.0
	C(46)–C(45)–C(44)–O(138)	175.6	175.9	177.8
	C(46)–C(45)–C(64)–C(67)	115.8	96.0	113.5
	C(46)–C(48)–C(51)–C(52)	132.8	179.4	120.5
	N(133)–C(25)–C(22)–O(135)	63.6	179.8	73.6
6	*Bond distances*			
	C(5)–C(34)	1.542	1.537	1.538
	C(6)–C(7)	1.410	1.396	1.398
	C(15)–S(16)	1.778	1.796	1.812
	C(30)–O(1)	1.369	1.389	1.389
	C(49)–C(101)	1.513	1.525	1.521
	C(49)–O(20)	1.450	1.457	1.457
	C(101)–N(104)	1.469	1.452	1.450
	C(106)–C(110)	1.426	1.445	1.445
	C(106)–N(104)	1.289	1.294	1.294
	Angles			
	C(5)–C(6)–C(7)	120.7	122.0	121.9
	C(5)–C(34)–C(40)	109.9	109.3	112.1
	C(6)–C(5)–C(34)	119.0	119.9	120.1
	C(7)–C(18)–O(2)	121.4	124.0	123.0
	C(3)–O(20)–C(49)	112.5	113.9	114.4
	C(49)–C(101)–N(104)	111.1	113.7	112.1
	C(101)–C(49)–O(20)	108.5	110.1	109.1
	C(101)–N(104)–C(106)	118.1	117.7	119.8
	C(106)–C(110)–C(112)	121.1	119.5	119.2
	C(110)–C(106)–N(104)	124.1	122.8	121.6
	C(110)–C(109)–O(108)	123.0	122.4	123.3
	Dihedral angles			
	C(6)–C(5)–C(34)–C(40)	167.1	179.4	179.6
	C(6)–C(7)–S(25)–C(8)	98.1	113.6	112.2

C(7)–C(6)–C(5)–C(34)	172.8	179.4	179.3
C(7)–S(25)–C(8)–C(3)	104.5	103.2	103.7
C(8)–C(3)–O(20)–C(49)	92.1	86.9	89.3
C(3)–O(20)–C(49)–C(101)	179.0	167.2	175.8
C(49)–C(101)–N(104)–C(106)	143.0	122.0	131.7
C(112)–C(110)–C(106)–N(104)	175.4	179.4	179.7
C(112)–C(110)–C(109)–O(108)	177.9	179.9	179.8
N(104)–C(101)–C(49)–O(20)	61.1	80.6	71.9

7. IR and Raman spectra charactiristics for ligands 3-6

Table S3. For **3**, a comparison of experimental and calculated wavenumbers ν (cm^{-1}), intensity I (km/mol) of the bands in the IR spectra and relative intensity J (a.u.) of the lines in the Raman spectra of *exo-exo* and *endo-exo* rotamers.

IR_{exp}	$Raman_{exp}$	*exo-exo*			*endo-exo*			Assignment
ν	ν	ν	I	J	ν	I	J	
3433 m		3408	875.3	12.0	3505	717.2	16.3	νO143−H144
		3366	910.4	1.2	3462	639.7	45.2	νO138−H119
		3140	10.3	5.7	3140	12.8	7.3	νC99−H100
		3139	11.0	10.9	3140	5.3	2.8	νC33−H34
		3132	2.8	2.9	3134	5.1	3.1	νC73−H74
		3132	6.0	8.1	3133	8.6	4.7	νC35−H38
		3132	7.4	1.1	3130	2.2	0.0	νC103−H104
		3131	3.1	4.3	3126	3.0	0.0	νC7−H8
		3114	7.9	0.4	3115	6.5	2.6	νC49−H50
		3114	6.2	0.4	3115	5.1	1.9	νC112−H113
		3113	3.0	1.4	3112	2.9	4.6	νC101−H102
		3110	5.0	20.1	3112	6.3	9.7	νC35−H36
		3101	9.4	0.5	3105	5.3	0.4	νC70−H71
		3100	8.0	0.3	3102	3.6	0.1	νC4−H5
		3098	6.3	0.2	3102	8.4	0.5	νC97−H98
		3097	3.3	13.7	3097	5.7	1.0	νC31−H32
		3087	18.5	8.0	3091	18.0	0.3	νC46−H47
		3086	13.1	6.6	3091	8.9	0.1	νC115−H116
		3065	3.0	4.5	3060	16.6	0.2	νC130−H131 ν_{as} CH_2
		3064	5.6	0.6	3056	4.5	0.0	νC64−H65 ν_{as} CH_2
		3056	27.6	0.3	3056	8.0	0.7	νC76−H77 ν_{as} CH_3
	3058 w	3056	11.0	1.8	3055	5.3	0.1	νC14−H16 ν_{as} CH_3
		3054	15.0	0.5	3055	37.2	1.5	νC10−H13 ν_{as} CH_3
		3053	28.7	0.6	3055	28.5	0.4	νC56−H59 ν_{as} CH_3
		3053	5.7	1.1	3054	20.3	1.4	νC118−H120 ν_{as} CH_3
		3053	35.0	0.5	3054	5.2	0.8	νC80−H81 ν_{as} CH_3
		3052	17.3	1.1	3053	14.8	0.0	νC122−H125 ν_{as} CH_3
		3051	17.4	0.3	3053	14.6	0.3	νC60−H63 ν_{as} CH_3
		3048	65.8	3.9	3052	16.5	0.2	νC84−H85 ν_{as} CH_3
		3048	21.9	1.5	3051	68.5	5.2	νC18−H21 ν_{as} CH_3
3049 w		3047	111.0	4.2	3049	23.9	2.4	νC14−H15 ν_{as} CH_3
		3047	18.8	1.6	3047	21.8	0.4	νC84−H86 ν_{as} CH_3
		3047	11.9	2.6	3047	70.7	3.1	νC52−H55 ν_{as} CH_2
		3046	20.0	3.2	3046	70.8	1.9	νC126−H127 ν_{as} CH_2
		3045	73.6	13.9	3045	21.7	2.7	νC52−H54 ν_{as} CH_3
		3045	82.3	5.1	3045	6.7	0.9	νC126−H127 ν_{as} CH_3
		3042	2.3	3.1	3045	57.5	2.1	νC76−H79 ν_{as} CH_2
		3042	2.4	2.5	3045	60.0	1.9	νC14−H16 ν_{s} CH_3
		3041	3.1	3.1	3043	2.6	0.1	νC10−H11 ν_{s} CH_3
		3041	2.0	1.5	3040	4.4	2.6	νC80−H83 ν_{as} CH_3
		3039	11.9	3.4	3040	3.7	1.9	νC56−H58 ν_{as} CH_3
		3039	6.2	3.6	3039	2.8	2.6	νC118−H120 ν_{as} CH_3
		3038	5.1	0.4	3039	5.0	1.3	νC60−H61 ν_{as} CH_3

		3038	3.8	0.4	3038	7.2	0.1	νC122−H123 ν_{as} CH_3
		3033	6.5	2.5	3038	5.1	0.3	νC40−H41 ν_{as} CH_2
		3032	5.9	2.4	3031	5.9	0.2	νC106−H107 ν_{as} CH_2
		3010	19.4	2.4	3030	5.3	0.9	νC22−H24 ν_s CH_2
		3002	17.5	0.8	3029	16.8	10.3	νC91−H93 ν_s CH_2
		2991	24.0	4.5	2998	35.2	0.5	νC88−H89 ν_s CH_2
		2990	22.8	2.7	2991	2.9	26.6	νC130−H132 ν_s CH_2
		2989	12.6	0.2	2987	8.0	3.0	νC64−H65 ν_s CH_2
		2986	25.6	33.9	2986	26.2	1.3	νC40−H42 ν_s CH_2
		2985	25.1	16.5	2984	23.1	1.5	νC106−H107 ν_s CH_2
		2984	1.8	1.8	2983	35.7	12.7	νC25−H27 ν_s CH_2
		2973	39.9	0.4	2982	15.2	2.6	νC76−H77 ν_s CH_3
		2973	23.6	3.6	2976	25.6	0.3	νC10−H11 ν_s CH_3
		2971	29.2	4.9	2974	18.1	4.2	νC52−H53 ν_s CH_3
		2971	33.4	2.0	2972	38.0	3.3	νC122−H123 ν_s CH_3
		2967	15.3	0.7	2972	41.3	3.1	νC80−H81 ν_s CH_3
		2966	28.1	1.9	2971	17.7	3.2	νC14−H15 ν_s CH_2
		2966	22.6	0.1	2969	16.2	2.4	νC18−H19 ν_s CH_3
		2965	13.2	1.0	2967	20.7	0.2	νC84−H85 ν_s CH_3
2959 s	2959 m	2964	27.7	5.4	2965	4.0	0.2	νC60−H61 ν_s CH_3
		2964	24.3	6.3	2965	27.4	0.4	νC118−H119 ν_s CH_2
		2963	25.5	4.1	2965	26.4	0.1	νC56−H58 ν_s CH_3
		2963	24.4	1.2	2964	42.7	2.2	νC118−H120 ν_s CH_3
		2960	15.6	7.9	2964	20.7	0.5	νC28−H29
		2951	37.9	0.6	2963	21.3	0.1	νC22−H23 ν_s CH_2
		2942	43.4	0.6	2961	21.5	4.7	νC88−H89 ν_s CH_2
	2939 m	2938	11.8	5.5	2945	34.5	0.4	νC25−H26 ν_s CH_2
		2931	34.6	32.3	2928	21.7	5.0	νC94−H95
2905 m	2908 m	2910	17.4	1.8	2925	32.5	0.1	νC91−H92 ν_s CH_2
2869 m	2781 w	2808	492.4	8.7	2762	751.2	1.2	νO141−H142
2360 vw	2710 w	2706	831.7	11.9	2609	703.7	25.4	νO136−H137
	1643 s	1646	112.2	18.6	1648	81.3	5.5	βO136−H137
1633 s	1638 s	1633	387.5	70.4	1643	101.4	5.7	νC94=N134
		1630	72.1	10.1	1635	484.1	66.2	νC28=N133
		1630	142.4	16.7	1632	69.5	32.7	βO141−H142
	1610 m	1602	4.3	87.7	1598	1.6	1.2	νC11−C14
		1602	4.9	6.6	1598	6.9	11.1	νC109−C115
		1596	23.7	59.7	1598	19.0	7.7	νC45−C46
		1591	17.8	4.3	1595	35.3	24.5	νC30−C31
		1591	8.6	5.9	1594	1.9	3.5	νC3−C4
1582 w	1586 m	1586	56.5	7.6	1587	15.1	29.3	νC69−C70
		1580	8.8	9.0	1582	15.3	1.0	νC46−C48
		1576	4.8	4.0	1581	4.0	1.9	νC43−C44
1560 vw		1573	6.9	4.6	1574	7.5	0.8	νC2−C3
1541 vw		1570	11.5	0.1	1564	1.9	0.5	νC1−C7
		1515	46.7	5.4	1518	34.4	25.2	νC33−C35
		1506	60.2	3.6	1513	42.2	2.8	νC99−C101
		1481	32.4	1.5	1513	11.9	3.9	βC22−H23 δ_s CH_2
		1480	80.1	22.0	1480	53.0	9.8	νC44−O138
1485 s		1478	120.7	6.5	1477	148.4	5.8	νC109−C110
		1474	19.6	6.1	1477	26.0	0.3	βC76−H77 δ_s CH_3
		1474	26.4	13.9	1474	38.4	0.2	βC10−H11 δ_s CH_3
		1471	1.2	11.4	1472	5.3	2.2	βC52−H53 δ_s CH_3

		1470	3.3	7.8	1471	1.0	6.6	βC126−H127 δ_s CH_3
	1467 m	1465	6.7	9.4	1470	6.4	3.2	βC88−H89 δ_s CH_2
		1461	34.9	0.9	1460	5.8	23.5	βC18−H19 δ_s CH_2
		1459	5.7	3.1	1459	49.7	0.2	βC84−H85 δ_s CH_3
		1458	24.3	2.8	1459	12.2	27.8	βC126−H128 δ_s CH_3
		1458	4.4	4.1	1458	6.1	1.0	βC18−H20 δ_s CH_3
		1457	13.2	0.9	1458	6.4	0.5	βC56−H57 δ_s CH_2
		1457	53.1	14.5	1457	47.7	35.5	νC105−O141
1462 m		1456	55.5	57.3	1457	19.8	0.8	νC31−C33
		1455	7.4	2.1	1455	8.5	0.1	βC88−H90 δ_s CH_2
		1454	3.7	0.4	1455	3.9	0.1	βC60−H61 δ_s CH_3
		1453	21.8	0.2	1453	62.1	6.3	βC122−H125 δ_s CH_3
		1452	23.7	4.0	1449	87.3	2.0	βC25−H27 δ_s CH_2
		1450	27.2	0.6	1449	28.5	79.0	νC2−C3
	1449 m	1448	36.8	6.0	1444	13.5	2.3	νC68−O140
1444 sh		1441	4.2	0.5	1442	13.4	0.2	βC52−H55 δ_s CH_3
		1441	2.0	0.3	1441	3.7	1.7	βC56−H59 δ_s CH_3
		1440	5.5	0.4	1441	0.3	0.2	βC10−H12 δ_s CH_3
		1440	11.7	1.1	1440	13.4	0.5	βC76−H78 δ_s CH_3
		1439	16.8	17.2	1439	1.6	7.4	βO136−H137
		1437	0.5	0.4	1439	5.4	14.4	βC118−H120 δ_s CH_3
		1437	0.4	0.2	1438	45.6	2.1	βC14−H17 δ_s CH_2
		1436	0.3	0.1	1438	0.9	0.3	βC76−H79 δ_s CH_2
		1436	0.4	0.3	1437	1.2	0.1	βC60−H63 δ_s CH_3
		1432	22.6	2.8	1436	0.8	0.7	νC101−C103
		1431	0.1	0.6	1435	0.7	0.1	βC18−H19 δ_s CH_3
		1431	3.4	0.4	1435	2.7	0.8	βC126−H129 δ_s CH_3
		1430	0.1	0.6	1433	25.6	18.4	βC84−H87 δ_s CH_3
		1430	5.1	2.7	1433	0.8	0.2	βC56−H58 δ_s CH_3
		1430	35.7	8.8	1432	0.3	0.1	βC100−H108 δ_s CH_3
		1428	19.2	7.7	1432	0.2	0.0	βC40−H42 δ_s CH_2
		1420	18.9	5.1	1431	0.4	0.2	βC130−H132 δ_s CH_2
		1418	8.3	6.5	1430	3.7	1.9	νC45−C46
1418 w		1418	25.1	30.3	1428	22.9	12.8	βC64−H65 δ_s CH_2
	1416 vw	1417	8.1	9.0	1414	10.1	1.1	νC43−C49
		1411	22.2	0.4	1412	8.3	0.5	βC91−H92 δ_s CH_2
		1405	11.2	4.9	1403	8.7	1.8	νC1−C130
1393 w	1400 vw	1404	1.7	18.6	1401	3.9	0.0	νC67−C73
		1377	6.6	9.6	1379	8.2	5.1	βC10−H13 δ_s CH_3
		1377	4.5	6.2	1377	12.3	0.4	βC76−H77 δ_s CH_3
		1376	5.3	17.5	1376	3.4	0.5	βC25−H26 wag CH_2
		1375	8.3	5.5	1375	5.9	2.7	βC126−H129 δ_s CH_3
	1374 vw	1375	1.5	0.3	1374	13.2	0.2	βC52−H55 δ_s CH_3
1363 m		1369	80.7	92.8	1374	16.4	3.4	βO138−H139
		1365	43.4	33.3	1369	30.8	18.7	βO143−H144
		1360	5.1	1.7	1360	43.1	6.2	βC91−H92 wag CH_2
		1356	59.7	23.6	1353	5.7	2.9	βC88−H89 wag CH_2
		1353	9.0	46.4	1350	6.9	5.5	νC30−C39
		1348	18.0	33.1	1345	6.3	4.7	νC96−C105
	1346 vw	1347	8.0	1.6	1344	16.3	30.1	νC28−C30
		1342	3.3	1.8	1344	3.2	4.4	νC75−C84
		1342	10.1	5.4	1343	11.1	0.6	νC9−C10
		1342	7.7	1.7	1341	0.2	0.3	βC10−H12 δ_s CH_3
		1341	10.4	3.7	1341	21.7	1.1	βC80−H83 δ_s CH_3
		1341	27.5	3.5	1340	3.6	1.6	νC75−C80

1340 w		1341	11.5	0.2	1340	28.5	0.0	νC51−C52
	1340 w	1340	8.7	1.0	1340	9.9	0.4	βC122−H124 δ_s CH_3
		1339	10.4	0.5	1339	13.9	0.1	βC56−H58 δ_s CH_3
		1338	5.5	14.4	1336	5.2	100.0	νC6−C7
		1337	1.6	100.0	1331	2.0	5.9	ν51−C52
	1321 m	1326	33.7	3.6	1318	2.4	4.9	βC91−H92 wag CH_2
		1319	2.6	2.9	1313	2.5	1.1	νC44−O138
	1308 sh	1312	4.4	13.1	1303	47.6	0.6	νC109−C110
		1304	40.7	0.4	1299	26.9	0.4	νC139−O136
1299 sh		1298	33.2	0.8	1287	33.6	1.0	νC105−O141
		1295	19.3	9.2	1285	20.1	22.9	βC22−H24 wag CH_2
1280 m		1286	142.5	61.4	1282	15.6	7.5	βC130−H131 wag CH_2
	1284 vw	1283	37.2	5.5	1278	69.2	0.7	νC48−C51
		1281	94.4	15.5	1277	70.6	21.9	νC72−C75
	1243 w	1280	47.4	0.8	1276	27.6	6.7	βC130−H132 wag CH_2
		1274	8.5	2.3	1266	46.4	8.7	βC25−H27 wag CH_2
		1271	1.5	2.3	1265	12.3	20.8	βC65−H65 wag CH_2
		1267	4.0	15.5	1258	4.4	14.0	βC91−H93 wag CH_2
	1266 w	1265	7.0	3.6	1257	1.7	0.1	βC22−H24 wag CH_2
		1263	6.4	26.7	1256	3.6	3.9	βC25−H26 wag CH_2
		1262	25.6	0.9	1255	0.4	1.4	βC106−H107
		1256	21.3	1.7	1249	103.0	1.4	νC48−C51
	1250 m	1253	3.4	0.2	1242	1.4	4.8	νC44−O138
1239 w		1237	4.0	6.3	1239	3.3	0.2	βC7−H8
		1235	6.2	14.9	1233	0.1	0.1	βC70−H71
	1232 m	1232	3.8	6.9	1231	6.2	3.2	βC31−H32
	1225 m	1228	9.7	2.4	1230	3.4	7.1	νC96−C97
		1221	104.7	1.2	1220	46.1	23.6	βC46−H47
		1217	20.7	4.6	1217	14.8	6.3	νC68−O140
		1215	9.0	25.4	1212	8.7	2.5	νC2−O135
		1213	11.1	1.2	1208	37.3	12.3	βO138−H139
		1210	6.8	0.5	1206	25.2	12.2	βC88−H89 ρ CH_2
1208 sh	1209 m	1209	47.6	1.4	1205	63.3	0.3	νC28−C30
		1202	13.0	1.3	1198	39.1	2.4	νC94−C96
		1199	32.2	6.8	1197	12.5	0.2	νC51−C52
1195 m		1198	40.3	15.4	1195	7.6	1.3	νC100−C109
		1194	6.9	3.4	1193	0.8	3.2	νC6−C9
		1193	6.7	4.0	1191	4.4	0.3	νC72−C75
		1190	13.5	25.0	1190	34.8	19.3	νC117−C126
		1189	34.2	5.6	1189	9.2	0.1	νC51−C56
		1189	3.2	0.4	1188	12.8	0.3	νC9−C10
		1189	6.5	2.2	1188	7.0	0.1	νC75−C80
		1188	9.1	2.4	1188	4.8	0.4	C51−C60
		1187	2.6	0.1	1188	39.0	6.4	νC114−C117
	1182 vw	1187	4.7	6.0	1187	7.3	1.9	βC22−H23 ρ CH_2
		1173	108.8	8.7	1174	165.2	0.4	νC2−O135
		1169	56.9	0.2	1164	32.0	15.1	νC68−O140
1151 w	1158 w	1158	48.6	11.5	1151	2.5	0.2	νC1−C7
		1154	22.8	5.4	1149	32.1	5.2	βC40−H42 ρ CH_2
		1149	12.3	4.8	1144	16.4	0.6	βC106−H107 ρ CH_2
		1148	5.8	1.1	1142	11.6	0.7	βC40−H41 ρ CH_2
		1142	7.2	2.2	1142	14.2	9.7	βC99−H100
		1141	19.1	1.6	1135	0.5	4.0	βC33−H34
1123 m	1130 m	1123	27.3	0.4	1126	24.3	0.7	νC25−N133

		1112	7.3	0.4	1121	26.0	3.4	βC101−H102
		1112	69.3	2.5	1110	68.5	7.8	βC112−H113
		1104	0.7	7.8	1104	3.9	2.0	βC37−H38
	1105 vw	1103	8.2	2.9	1102	6.8	2.1	βC115−H116
		1090	12.0	4.2	1099	9.0	0.3	βC4−H5
1097 w		1085	40.6	12.5	1091	15.4	1.8	νC88−C91
	1077 vw	1083	50.7	1.1	1080	44.5	7.5	νC91−N134
		1065	9.3	2.7	1058	9.4	1.0	νC94=N134
1052 w	1060 w	1058	1.4	12.5	1057	0.7	4.0	νC22−C25
	1036 m	1038	10.9	1.2	1035	1.0	0.4	νC25−N133
1031 w		1033	112.5	15.6	1035	18.5	11.0	νC88−O140
		1025	28.0	0.8	1020	22.7	0.4	νC99−C101
		1020	16.2	49.8	1019	20.6	3.7	νC33−C35
1016 w		1014	0.2	1.3	1015	0.4	1.6	νC9−C10
		1014	0.0	1.0	1015	0.1	0.0	νC117−C118
		1014	0.1	0.2	1013	1.9	0.1	βC60−H61 ρ CH_3
		1013	0.3	1.5	1013	0.3	0.1	βC80−H81 ρ CH_3
		1013	0.6	1.1	1013	6.2	0.3	βC14−H15 ρ CH_3
		1012	0.9	0.5	1013	51.7	2.2	βC118−H119 ρ CH_3
		1011	1.2	1.0	1012	0.4	0.1	βC84−H85 ρ CH_3
		1011	1.7	9.1	1011	0.7	5.1	βC52−H53 ρ CH_3
		1002	180.8	4.1	1011	1.2	0.2	νC22−O135
	989 vw	998	96.0	0.5	1000	85.4	5.6	νC22−C25
979 w	977 vw	973	28.3	0.6	975	192.3	36.8	γO141−H142
		971	36.1	2.5	971	10.4	0.3	γC94−H95
		968	6.1	0.4	970	125.1	9.6	νC64−C67
		967	37.4	5.9	968	3.8	3.1	νC1−C130
		963	0.9	5.2	960	0.6	0.6	γC28−H29
		960	1.8	0.5	960	0.5	0.0	γC99−H100
		957	0.4	0.1	958	2.9	4.4	γC35−H36
		956	2.0	1.2	953	8.1	1.5	νC3−C40
		955	1.2	5.2	952	2.0	0.7	γC97−H98
942 w	931 w	932	12.4	5.2	945	11.1	1.3	νC69−C106
		930	5.2	26.0	935	23.4	2.0	νC45−C64
		928	0.6	1.8	929	0.4	0.5	βC84−H87 ρ CH_3
		927	3.0	0.6	928	1.2	0.6	βC18−H19 ρ CH_3
924 w		927	5.1	1.3	927	2.1	1.8	βC14−H15 ρ CH_3
		925	0.2	0.0	927	0.1	0.0	βC118−H119 ρ CH_3
		925	0.3	0.0	927	0.6	0.2	βC56−H59 ρ CH_3
		922	1.0	0.2	925	18.2	1.2	βC60−H61 ρ CH_3
		920	0.3	0.4	920	0.6	0.0	γC31−H32
		919	3.0	0.1	919	2.0	0.7	γC103−H104
		916	6.2	7.7	918	1.0	0.5	νC75−C84
		916	1.9	2.4	916	2.2	1.1	νC9−C18
		914	3.3	1.0	915	2.2	1.0	νC51−C52
		913	14.7	13.5	914	1.8	1.2	νC88−C91
		913	6.6	5.8	913	0.2	0.1	νC40−C43
		907	0.9	0.9	911	0.6	0.1	νC9−C14
		907	2.4	1.0	908	1.4	1.5	νC75−C80
		905	4.0	0.3	906	1.2	1.4	νC117−C122
		904	0.3	2.6	905	1.6	0.2	νC117−C118
		904	1.6	0.6	904	1.9	0.1	νC51−C56
		902	2.3	3.5	901	5.6	0.5	βC40−H41 ρ CH_2
		899	24.4	23.4	900	5.4	0.1	βC64−H65 ρ CH_2

		894	2.9	0.2	891	0.9	0.1	βC130−H131 ρ CH_2
	889 vw	888	9.7	65.3	887	13.9	26.9	β_R
		884	5.4	5.8	886	7.7	11.4	β_R
		879	3.7	2.3	877	2.4	0.3	γC46−H47
	876 vw	874	3.9	5.3	875	1.1	0.1	γC112−H113
873 m		873	2.6	0.2	871	0.1	0.3	γC49−H50
		868	0.3	0.3	868	2.8	2.2	γC70−H71
		864	11.8	8.4	866	4.4	0.1	γC73−H74
		862	9.1	0.3	858	21.4	0.5	γC49−H50
		857	17.0	1.2	854	14.3	0.2	γC116−H115
		856	17.5	0.2	854	3.4	0.4	νC70−C72
		853	6.8	2.9	841	12.7	0.0	γC7−H8
		839	9.0	0.2	839	1.0	0.1	γC97−H98
		838	4.1	0.1	814	3.9	0.9	γC37−H38
	820 m	817	4.8	13.0	809	8.4	0.1	νC2−O135
814 w		810	9.3	1.2	808	3.6	0.0	νC110−O143
		807	4.8	8.2	804	16.8	2.3	βC25−H26 ρ CH_2
		805	8.5	5.7	800	5.7	1.1	βC22−H23 ρ CH_2
801 sh		801	1.8	5.5	797	0.6	4.7	γC67−C68
		796	5.2	27.6	791	0.3	27.4	β_R
		794	2.1	1.5	782	11.5	1.3	νC72−C75
779 w	783 m	781	13.3	0.1	773	8.3	0.1	γC44−O134
		777	22.6	0.1	772	3.7	0.2	νC110−O143
		774	2.6	2.3	770	7.1	1.7	β_R
	764 vw	771	9.4	13.4	761	11.1	6.0	β_R
755 m		754	27.1	0.8	747	3.6	0.1	β_R
		744	23.4	1.0	744	16.6	0.5	γC31−H32
	743 vw	743	14.4	1.4	744	27.0	0.1	γC99−H100
736 w		740	66.9	0.5	741	4.1	4.1	βC91−H92 ρ CH_2
		731	24.8	0.2	731	8.8	0.5	β_R
		730	75.7	1.1	731	20.0	2.9	γC103−H104
		729	21.6	0.5	730	61.5	1.3	γC101−H102
		725	16.5	0.3	718	56.7	0.4	β_R
712 vw	717 w	711	21.4	2.9	707	22.6	15.9	β_R
	703 w	696	4.2	0.7	691	0.9	2.4	β_R
		689	0.4	3.6	672	1.2	1.7	β_R
	678 w	670	4.1	0.5	669	3.7	0.8	β_R
		668	2.3	5.3	663	2.8	2.0	τC1−C7
		662	0.2	3.1	648	10.0	9.7	γC114−C117
	648 vw	649	8.8	0.1	648	13.7	0.0	β_R
642 w		641	9.5	0.4	635	58.3	0.6	β_R
	634 vw	632	1.1	0.2	633	6.7	1.9	τC3−C4
		625	3.8	1.1	619	5.1	0.0	τC110−C111
		617	0.3	3.3	617	6.2	0.1	τC109−C115
591 w	597 m	596	0.2	3.9	591	2.3	0.6	β_R
		589	16.0	4.9	590	5.6	4.9	β_R
		585	0.6	9.5	586	1.9	0.5	β_R
	573 w	577	6.9	0.5	570	0.6	0.6	τC111−C112
571 vw		573	3.7	1.0	569	1.6	13.3	β_R
		563	1.3	36.3	563	4.3	21.4	β_R
	562 w	561	2.7	18.1	560	1.2	0.4	β_R
555 w		557	1.2	3.7	558	11.1	0.1	β_R
	551 vw	551	1.7	0.8	550	3.8	0.1	τC97−C99
		549	1.4	3.6	548	3.0	1.8	β_R
		546	6.8	1.2	546	7.6	1.7	β_R
		535	2.0	1.4	533	0.3	0.2	τC103−C105

		533	3.2	1.3	526	2.4	3.7	β_R
		529	0.4	15.5	525	0.6	0.2	β_R
		525	3.2	16.2	524	4.7	6.3	β_R
	514 w	509	2.4	0.4	511	0.5	0.3	β_R
		506	0.4	6.7	505	0.2	16.2	β_R
		503	0.1	8.5	501	0.8	0.5	τC4−C6
		500	2.4	3.7	500	1.0	10.7	β_R
		499	0.7	11.7	499	0.8	12.6	β_R
		490	0.4	28.5	493	1.9	2.3	β_R
		485	2.1	26.5	490	1.1	22.8	β_R
		472	0.6	7.5	473	7.6	3.7	β_R
	470 vw	471	6.8	36.4	472	3.6	1.1	β_R
466 vw		467	1.2	3.6	469	0.2	5.6	β_R
		456	4.8	0.6	457	1.9	0.8	β_R
452 vw		454	8.3	3.5	456	11.0	1.4	τC96−C105
		447	3.7	3.1	439	0.9	1.6	β_R
		438	0.5	3.0	436	0.3	0.2	τC4−C6
		437	0.3	0.5	434	0.6	0.5	τC44−C45
		435	0.8	3.0	433	1.7	1.1	τC109−C110
		419	6.2	16.0	421	1.0	5.0	β_R
		415	2.6	7.3	418	4.2	4.7	τC9−C18
	414 vw	414	0.9	6.9	413	4.7	3.2	τC48−C51
		413	0.7	11.4	411	0.3	0.1	τC6−C9
		408	0.3	10.2	409	1.1	4.8	τC72−C75
		398	1.1	56.2	408	0.1	1.4	β_R
		382	2.2	0.2	380	5.4	0.1	β_R
		379	2.9	11.4	379	4.7	0.8	β_R
		375	0.3	5.4	374	0.5	6.8	τC9−C10
		372	2.2	0.1	362	0.6	0.3	τC75−C84
		364	1.4	6.2	361	0.2	1.3	τC51−C52
	332 vw	359	0.0	0.3	358	1.1	1.1	τC117−C126
		358	1.0	0.5	350	0.1	0.2	τC51−C56
		353	6.1	0.6	348	1.9	0.1	τC110−C111
		348	0.2	3.6	345	1.5	1.5	τC31−C33
		342	0.8	8.4	341	2.0	4.5	τC109−C115
		333	3.4	34.2	334	0.9	1.1	τC96−C105
		332	4.3	24.7	330	11.2	0.6	τC96−C94
		330	0.4	0.6	329	4.8	0.9	τC117−C126
		327	0.4	0.1	325	1.9	0.1	τC75−C84
		326	1.3	1.9	322	0.9	1.2	τC25−C32
		322	0.8	5.1	320	1.1	0.7	τC51−C52
		317	0.1	3.1	316	0.7	0.3	τC75−C84
		316	0.1	35.7	314	0.4	0.9	τC9−C18
		314	0.4	3.1	312	0.0	0.0	τC51−C52
		313	0.1	14.1	309	0.1	11.6	τC117−C126
		308	0.3	6.9	309	0.2	1.6	τC51−C60
		305	1.6	2.4	306	0.1	6.9	τC9−C10
		302	1.0	8.6	302	2.1	1.5	τC75−C76
		301	0.3	0.2	301	0.5	2.7	τC75−C80
		300	0.5	1.0	294	2.8	0.7	τC45−C64
		283	1.8	0.2	282	2.6	29.8	τC6−C7
		279	0.1	0.7	280	0.2	0.0	τC114−C117
	271 vw	274	0.3	20.2	273	0.4	0.1	τC94−C96
		268	0.7	5.2	266	0.5	0.1	τC117−C122
		262	0.4	0.4	264	0.6	0.1	τC9−C10
	260 vw	259	0.4	1.9	263	0.4	0.2	τC51−C60

	255	0.3	12.8	260	0.1	0.8	τC9−C14
	253	0.9	5.1	250	0.2	8.7	τC75−C76
	248	0.1	7.6	245	0.2	1.4	τC75−C80
	244	0.5	0.4	239	2.8	2.8	τC28−C30
	233	0.9	0.4	235	0.8	7.1	τC48−C51
	233	3.8	1.6	233	0.0	0.3	τC64−C67
	230	0.3	0.2	230	0.1	0.1	τC117−C118
	226	0.0	1.0	229	1.3	21.3	τC51−C60
	224	0.1	0.7	227	0.4	13.2	τC9−C14
	222	3.5	0.8	219	5.7	0.3	τC67−C68
219 vw	221	0.2	0.9	215	2.9	4.1	τC75−C80
	215	1.0	22.1	213	2.2	3.9	τC28−N133
	210	0.6	46.1	208	1.1	2.6	τC91−N134
	208	1.0	1.0	207	0.4	35.5	τC70−C72
	206	1.1	0.2	204	0.4	26.4	τC72−C73
	201	1.3	0.4	202	0.5	2.2	τC1−C130
	191	3.4	0.5	191	9.8	20.1	τC94−C96
	186	6.2	2.8	187	1.2	6.5	τC88−C91
	178	1.7	0.3	181	2.8	1.3	τC22−O135
	175	1.4	8.0	170	1.8	2.1	τC68−O140
	172	1.2	14.0	165	0.6	0.1	τC43−C44
	156	0.0	2.7	154	0.1	0.2	τC68−C69
	145	2.7	18.2	146	0.3	9.9	τC88−C91
	135	1.0	1.5	137	1.6	0.0	τC44−O138
	133	1.0	1.9	135	0.4	3.2	τC25−N133
	126	0.1	8.1	133	2.2	2.3	τC69−C70
121 m	123	0.5	1.9	123	1.1	5.4	τC47−C51
	116	2.0	1.2	121	0.0	1.8	τC94−N134
	108	0.5	2.6	113	0.2	0.5	τC110−C111
	105	2.1	0.3	112	0.2	0.1	τC91−N134
	104	0.6	1.5	106	0.4	3.0	τC44−C45
	99	1.5	0.6	102	1.1	0.5	τC44−C45

Abbreviations: ν: stretching; δ: deformation in plane; ρ: deformation out of plane; χ: torsion; as: antisymmetric; s: symmetric.

Table S4. For **4**, a comparison of experimental and calculated wavenumbers ν (cm^{-1}), intensity I (km/mol) of the bands in the IR spectra and relative intensity J (a.u.) of the lines in the Raman spectra of *exo-exo* and *endo-exo* rotamers.

IR_{exp}	$Raman_{exp}$	*exo-exo*			*endo-exo*			Assignment
ν	ν	ν	I	J	ν	I	J	
		3466	340.3	2.2	3446	420.7	4.6	νO2−H52
		3435	403.8	3.5	3429	248.9	1.4	νO1−H51
3389 m		3146	0.1	0.4	3146	0.1	0.7	νC14−H56
		3144	0.6	0.6	3145	0.6	1.0	νC9−H54
		3140	13.9	8.2	3142	7.1	3.0	νC131−H132
		3139	0.2	0.6	3141	0.2	1.8	νC31−H60
		3139	0.3	0.5	3141	0.2	2.6	νC113−H114
		3136	9.3	4.6	3139	13.0	4.2	νC26−H59
		3133	1.0	1.9	3135	5.3	3.6	νC135−H136
		3129	10.0	3.2	3132	8.0	1.8	νC113−H114
		3124	1.8	0.9	3126	1.6	0.2	νC17−H57
		3120	3.0	0.4	3125	2.4	2.9	νC11−H55
		3116	2.4	1.6	3117	2.7	3.0	νC19−H58
		3116	3.6	1.0	3116	2.8	2.2	νC6−H53
		3114	4.6	1.6	3113	4.8	1.1	νC133−H134
		3108	6.5	3.0	3110	5.3	0.4	νC115−H116
		3103	0.6	1.1	3101	4.4	0.8	νC112−H111
		3098	6.6	0.6	3096	5.1	0.3	νC130−H129
		3059	12.4	2.1	3064	10.4	0.6	νC49−H97 ν_{as} CH_2
		3057	22.0	1.5	3057	24.0	1.2	νC46−H88 ν_{as} CH_3
	3072 m	3056	29.8	2.0	3056	19.5	0.7	νC42−H77 ν_{as} CH_3
3059 w		3055	26.0	0.9	3056	26.0	0.5	νC37−H62 ν_{as} CH_3
		3055	12.7	0.9	3055	13.6	1.1	νC43−H80 ν_{as} CH_3
		3054	8.3	0.4	3054	24.2	0.8	νC46−H89 ν_{as} CH_3
		3054	24.5	1.0	3054	15.2	1.2	νC39−H68 ν_{as} CH_3
		3053	13.8	0.5	3053	18.5	1.2	νC41−H75 ν_{as} CH_3
		3052	71.1	4.5	3052	58.1	3.3	νC43−H81 ν_{as} CH_3
		3049	17.0	0.9	3050	20.8	0.5	νC47−H91 ν_{as} CH_3
		3048	78.6	2.0	3050	2.1	2.3	νC38−H65 ν_{as} CH_3
		3048	84.6	2.9	3049	67.7	1.8	νC47−H93 ν_{as} CH_3
		3048	13.7	1.1	3049	76.4	2.8	νC45−H85 ν_{as} CH_3
		3047	40.0	3.1	3048	10.8	0.2	νC40−H70 ν_{as} CH_3
		3046	14.1	1.1	3047	4.1	0.5	νC43−H79 ν_{as} CH_3
		3046	20.4	0.6	3047	39.1	0.5	νC38−H65 ν_{as} CH_3
		3046	47.1	0.7	3046	39.1	1.5	νC41−H73 ν_{as} CH_3
		3045	2.7	1.4	3046	47.0	1.9	νC46−H88 ν_{as} CH_3
		3042	3.2	0.3	3045	2.9	1.1	νC48−H94 ν_{as} CH_3
		3042	2.8	0.2	3043	2.8	0.4	νC38−H64 ν_{as} CH_3
		3041	1.6	0.7	3043	3.5	0.2	νC44−H82 ν_{s} CH_3
		3041	5.7	0.3	3041	2.3	0.2	νC39−H69 ν_{s} CH_3
		3040	3.4	0.3	3041	0.9	0.1	νC42−H76 ν_{as} CH_3
		3040	4.1	0.2	3041	8.5	0.1	νC43−H79 ν_{as} CH_3
		3028	13.0	0.4	3040	2.8	0.3	νC41−H73 ν_{as} CH_3
		3012	22.2	4.7	3031	10.0	0.6	νC50−H99 ν_{as} CH_2
		3002	5.9	4.2	2993	34.5	3.8	νC49−H98 ν_{as} CH_2

		3000	25.2	1.3	2983	29.4	4.6	νC101−H103 ν_{as} CH_2
		2991	10.8	0.8	2978	19.7	3.2	νC46−H88 ν_s CH_3
		2976	21.5	25.6	2978	13.7	3.7	νC119−H120 ν_s CH_2
		2973	20.6	78.3	2973	26.2	20.5	νC38−H64 ν_s CH_3
		2973	49.4	4.8	2973	37.7	9.0	νC44−H82 ν_s CH_3
		2972	18.8	6.5	2972	21.5	7.7	νC42−H76 ν_s CH_3
		2970	17.0	2.4	2971	18.2	1.6	νC46−H88 ν_s CH_3
		2969	22.5	2.3	2969	9.6	1.9	νC47−H91 ν_s CH_3
		2968	16.8	1.2	2968	19.9	0.8	νC38−H65 ν_s CH_3
		2966	21.7	0.8	2967	20.5	1.9	νC106−H105
		2966	19.2	2.9	2967	23.6	2.9	νC45−H85 ν_s CH_3
		2966	9.2	1.4	2966	17.5	0.5	νC39−H67 ν_s CH_3
		2966	53.8	7.6	2966	24.2	1.3	νC42−H76 ν_s CH_3
		2965	7.2	1.8	2965	22.9	0.8	νC40−H70 ν_s CH_3
		2965	17.3	10.2	2964	18.7	2.2	νC41−H74 ν_s CH_3
2962 s	2964 m	2947	34.0	17.5	2948	24.6	1.6	νC50−H100 ν_s CH_2
		2941	24.6	2.1	2944	27.5	2.7	νC124−H123
	2932 m	2930	33.7	2.6	2919	45.7	3.6	νC101−H103 ν_s CH_2
2906 m	2909 m	2907	10.1	9.8	2917	17.3	1.1	νC119−H121
2870 m								
	2782 vw	2832	561.9	38.3	2786	525.6	11.1	νO126−H125
	2716 vw	2616	617.0	14.4	2691	691.1	27.1	νO108−H107
		1651	150.5	11.8	1645	74.4	19.2	νC106=N104
1634 s	1639 s	1633	108.3	29.2	1641	66.8	8.8	νC124=N122
		1631	260.1	46.2	1635	301.4	39.1	νC127−C128
		1629	164.8	72.7	1633	252.0	40.6	νC106−C110
1582 m	1588 m	1597	27.2	1.6	1598	23.9	26.0	νC110−C112
		1589	49.3	9.7	1594	32.2	9.0	νC133−C135
		1577	6.5	26.4	1575	7.6	9.0	νC19−C24
		1575	5.6	13.9	1574	1.2	4.2	νC5−C6
	1567 w	1571	11.1	26.3	1569	5.2	13.3	νC11−C12
	1556 sh	1564	7.7	12.2	1562	8.3	3.5	νC14−C15
1554 vw		1532	9.5	7.7	1533	13.3	20.9	νC28−C31
		1529	3.6	25.9	1532	7.1	12.6	νC18−C27
		1523	10.5	8.4	1525	23.5	6.4	νC13−C14
1494 m		1519	13.6	3.1	1521	5.3	3.2	νC3−C12
1477 m		1517	37.1	10.6	1516	46.9	10.6	νC113−C115
		1507	74.8	22.5	1512	44.4	9.6	νC131−C133
		1475	5.2	2.0	1475	6.2	0.2	βC38−H65 δ_s CH_3
		1474	60.3	1.0	1474	53.6	0.7	βC41−H75 δ_s CH_3
		1473	25.7	0.5	1474	17.8	0.3	βC43−H79 δ_s CH_3
	1466 m	1472	27.8	1.0	1473	30.8	0.8	βC46−H89 δ_s CH_3
		1460	4.5	0.7	1465	17.3	2.9	βC38−H64 δ_s CH_3
		1459	5.8	1.2	1462	7.2	0.8	βC45−H85 δ_s CH_3
		1459	10.6	0.8	1459	6.3	0.5	βC40−H70 δ_s CH_3
		1459	6.5	0.8	1459	8.0	0.5	βC47−H91 δ_s CH_3
		1458	78.1	80.0	1459	14.3	1.7	νC127−C135
		1458	29.0	7.3	1457	64.1	100.0	βC41−H73 δ_s CH_3
		1457	44.5	36.2	1457	18.0	49.2	βC44−H84 δ_s CH_3
		1456	6.5	0.9	1456	36.6	81.0	νC109−O108
		1456	23.9	2.9	1456	10.6	86.0	βC48−H94 δ_s CH_3
		1455	28.7	23.7	1456	7.1	10.1	βC39−H67 δ_s CH_3
		1454	32.0	2.7	1455	1.3	1.7	βC41−H73 δ_s CH_3

1450 m	1449 sh	1453	17.4	13.8	1451	29.6	15.2	βC49−H97 δ_s CH_2
		1451	55.3	2.3	1449	83.7	4.8	βC50−H99 δ_s CH_2
		1443	6.8	1.6	1443	17.4	1.0	βC49−H98 δ_s CH_2
		1442	8.5	0.3	1442	6.8	1.8	βC38−H65 δ_s CH_3
		1440	13.5	5.8	1440	2.4	0.9	βC46−H90 δ_s CH_3
		1440	1.6	0.9	1440	13.8	0.3	νC115−C117
		1440	5.4	1.5	1440	14.4	5.9	βC41−H75 δ_s CH_3
		1439	8.6	2.1	1439	11.1	1.3	βC43−H81 δ_s CH_3
		1438	0.3	1.0	1438	4.6	0.8	βC37−H63 δ_s CH_3
	1437 w	1437	0.2	0.4	1438	12.7	6.1	βC41−H75 δ_s CH_3
		1437	0.2	1.1	1437	0.3	0.4	βC44−H84 δ_s CH_3
		1436	0.3	0.4	1437	0.4	0.8	νC128−C130
		1434	39.9	12.0	1437	0.5	0.5	βC46−H89 δ_s CH_3
		1433	0.1	0.0	1434	85.2	2.9	βC39−H67 δ_s CH_3
		1432	17.1	9.0	1433	1.0	0.0	βC41−H73 δ_s CH_3
		1432	0.1	0.1	1432	0.1	0.1	βC45−H85 δ_s CH_2
		1432	0.1	0.2	1432	0.2	0.1	βC39−H69 δ_s CH_3
		1431	0.1	0.1	1431	24.9	0.1	βC101−H102 δ_s CH_2
	1401 w	1426	127.4	21.0	1425	32.4	1.6	νC21−C22
1392 m		1417	28.8	3.0	1420	46.6	1.4	βC49−H97 δ_s CH_2
		1416	87.9	4.6	1416	57.6	3.7	βC119−H120 δ_s CH_2
		1380	2.0	0.4	1379	3.1	0.3	βC39−H67 δ_s CH_3
		1377	6.6	3.9	1378	1.2	2.2	βC47−H93 δ_s CH_3
		1377	1.9	1.6	1378	7.9	0.0	βC45−H85 δ_s CH_3
		1377	4.4	1.9	1377	9.5	2.4	βC40−H70 δ_s CH_3
		1375	21.7	4.4	1376	7.5	0.4	νC26−C27
		1374	8.9	2.7	1375	10.7	0.5	νC19−C24
		1367	8.0	5.2	1369	34.8	0.9	βC119−H120 wag CH_2
1364 m	1368 vw	1365	8.2	3.1	1367	20.2	0.7	νC10−C11
		1364	25.0	2.6	1365	19.4	1.8	νC13−C17
		1363	22.8	6.6	1363	16.6	0.2	βC101−H102 wag CH_2
		1357	39.6	7.1	1354	13.0	6.4	βC50−H100 wag CH_2
		1351	19.9	17.3	1354	18.1	13.0	νC109−C110
		1351	15.0	12.5	1350	9.9	16.0	νC127−C128
		1346	70.3	48.2	1349	7.8	11.9	βO1−H51
		1346	18.9	20.2	1346	71.5	40.7	βC39−H67 δ_s CH_3
		1345	35.4	4.1	1344	4.3	1.1	βC40−H70 δ_s CH_3
		1343	2.8	0.3	1344	6.7	1.2	βC48−H95 δ_s CH_3
	1342 vw	1343	5.8	2.5	1343	2.0	1.4	βC37−H63 δ_s CH_3
		1343	8.2	0.2	1343	23.3	4.4	βC43−H79 δ_s CH_3
		1341	4.3	1.3	1342	23.2	5.6	βC41−H73 δ_s CH_3
1338 w		1341	29.2	0.9	1340	6.2	6.7	βC47−H93 δ_s CH_3
		1339	35.9	3.3	1340	29.0	22.4	βC40−H72 δ_s CH_3
		1339	6.0	1.2	1339	7.6	11.5	βC43−H79 δ_s CH_3
1321 sh	1322 m	1338	30.5	1.0	1338	9.9	2.9	βC49−H98 wag CH_2
		1324	50.3	8.7	1321	43.9	3.2	βC101−H103 wag CH_2
		1321	23.7	8.0	1316	21.0	4.3	βC119−H120 wag CH_2
		1305	3.8	6.7	1311	9.5	15.4	νO126−C127
		1304	12.6	100.0	1304	39.7	33.8	νC15−C22
	1287 m	1303	35.9	3.0	1302	28.1	14.6	νC109−O108
1280 m		1298	55.6	37.8	1301	3.2	6.5	νC3−O20
1263 sh	1261 sh	1291	4.4	16.1	1287	5.9	3.0	νC18−O2
		1288	6.3	7.7	1286	2.2	3.5	νC31−C32
		1270	9.0	5.1	1253	152.7	79.9	βC6−H53
		1250	298.8	3.5	1251	27.7	9.7	βC119−H121 wag CH_2

1246 m	1249 m	1249	3.0	7.7	1247	71.6	5.5	βC101−H103 wag CH_2
		1245	43.2	8.6	1246	6.9	7.7	βC26−H59
		1242	30.4	10.5	1242	75.3	3.0	νC13−C36
		1239	134.8	0.7	1241	47.7	7.0	νC33−C39
		1238	8.6	0.3	1237	2.3	3.0	νC28−C35
		1236	16.9	3.7	1237	79.8	0.6	νC5−C34
1223 vw	1224 m	1235	15.6	18.7	1235	3.5	10.5	νC109−O108
		1229	11.4	39.6	1233	5.2	11.6	βC130−H129
	1210 sh	1224	108.1	6.9	1217	110.2	1.7	νC106−C110
1205 vw		1215	26.9	16.9	1212	25.6	25.5	νC49−O20
		1212	46.5	13.4	1210	37.8	31.0	βC119−H120 ρ CH_2
		1203	9.9	1.8	1204	20.4	1.3	νC21−O4
		1202	6.6	1.4	1202	1.2	0.9	νC109−C117
		1199	5.9	0.91	1199	0.5	0.6	νC124−C128
		1197	0.9	4.8	1197	1.9	0.3	C33−C37
		1194	3.6	9.4	1195	19.0	1.2	C36−C46
		1194	0.1	1.1	1194	0.1	2.2	νC35−C43
		1190	30.1	3.4	1193	24.5	9.0	νC34−C41
		1189	2.5	2.4	1189	4.3	0.9	νC33−C38
		1188	6.9	2.2	1189	7.3	0.5	νC35−C45
		1188	3.7	0.7	1189	8.0	1.5	νC34−C42
		1188	7.4	4.6	1188	3.3	0.6	νC36−C47
1167 w		1186	5.2	1.1	1186	2.3	0.3	νC10−C33
		1186	3.8	0.7	1186	0.8	1.0	νC36−C47
		1148	47.5	4.2	1152	38.2	31.8	βC31−H60
1151 w	1155 vw	1145	6.6	11.0	1144	66.4	8.6	βC26−H59
	1141 sh	1139	17.3	2.1	1142	8.6	13.7	βC135−H136
		1137	64.1	1.5	1141	8.8	5.7	βC117−H118
		1126	0.1	5.4	1126	2.0	2.4	νC9−C10
1122 w		1118	2.1	12.0	1118	1.6	22.0	νC14−C15
		1117	2.7	4.9	1117	1.5	6.8	νC19−C28
		1115	11.5	1.7	1115	11.1	1.1	νC5−C26
1093 w	1099 vw	1115	7.4	0.8	1114	27.6	0.1	νC112−C113
		1110	14.1	1.3	1114	0.4	2.6	νC130−C131
		1087	16.5	1.2	1092	4.8	0.6	νC101−N104
1079 sh		1086	15.9	1.1	1089	14.1	0.6	νC119−N122
		1066	45.8	2.9	1066	46.8	4.1	νC50−C119
		1060	7.9	4.3	1059	2.5	0.4	νC8−S25
		1059	4.2	6.0	1057	3.4	48.4	νC32−S29
		1057	4.5	1.7	1054	20.7	3.6	νC15−S16
	1049 sh	1048	28.2	1.6	1048	19.5	6.8	νC22−S23
		1045	20.6	2.0	1047	11.5	4.9	νC49−C101
	1036 m	1030	25.7	15.1	1025	6.9	1.4	νC50−O4
1029 m		1029	25.6	36.0	1025	23.9	2.4	νC113−C115
		1023	5.6	6.1	1021	28.2	0.9	νC130−C131
		1017	1.3	1.7	1016	0.1	0.1	νC49−O20
		1017	121.6	0.2	1014	0.2	0.2	βC39−H67 ρ CH_3
		1016	0.1	2.2	1014	1.1	0.1	βC46−H88 ρ CH_3
		1015	0.2	0.7	1014	0.1	0.2	βC42−H77 ρ CH_3
		1014	0.1	0.4	1012	93.8	4.4	βC43−H79 ρ CH_3
		1013	118.5	1.8	1011	0.2	1.2	βC38−H65 ρ CH_3
		1012	7.9	4.5	1010	5.6	3.1	βC47−H91 ρ CH_3
		1010	9.9	3.0	1010	0.6	5.6	βC40−H70 ρ CH_3

999 w		1009	0.5	2.8	1009	0.5	1.0	βC45−H87 ρ CH_2
975 vw	973 w	1009	0.5	4.2	988	96.7	2.3	βO108−H107
		970	17.6	14.9	961	22.3	0.6	βC106−H105
		964	0.7	0.1	959	33.2	0.2	γC131−H132
		958	12.1	0.5	958	9.2	0.5	γC115−H116
935 sh	937 sh	956	1.7	2.7	955	4.8	0.7	γC124−H123
		946	38.3	0.4	954	67.5	3.5	βO126−H125
		933	16.0	6.8	929	0.1	0.2	βC37−H63 ρ CH_3
		930	0.2	0.1	929	0.1	0.1	βC46−H89 ρ CH_3
		928	0.3	0.0	929	0.2	1.0	βC41−H75 ρ CH_3
924 w	920 w	927	0.1	0.0	928	0.1	0.2	βC43−H80 ρ CH_3
		927	0.1	0.1	920	19.1	0.7	γC112−H111
		920	4.3	3.2	918	27.7	2.4	γC130−H129
		920	2.6	1.6	918	1.4	0.1	νC33−C37
		919	0.4	0.2	918	2.7	1.5	νC36−C47
		918	8.8	0.5	918	2.0	1.0	νC34−C40
		917	2.2	0.8	917	5.8	0.7	νC35−C45
		917	2.1	0.6	911	18.9	3.2	βC49−H97 ρ CH_2
		911	31.0	2.9	910	16.8	0.8	βC50−H100 ρ CH_2
	905 w	909	1.7	1.6	909	3.7	2.4	νC36−C48
		907	1.2	1.8	907	0.8	0.5	νC33−C39
	891 sh	906	2.1	1.0	907	1.8	1.5	βC43−H81 ρ CH_3
		906	1.6	0.6	906	1.7	0.8	βC42−H78 ρ CH_3
		899	19.6	10.6	893	6.4	3.6	νC10−C11
885 w		893	5.1	8.3	889	0.9	0.4	νC124−C128
		889	0.9	2.7	888	6.7	4.3	γC11−H55
		887	0.9	0.3	888	0.6	28.8	γC26−H59
	877 sh	886	0.6	2.8	886	0.9	4.4	γC19−H58
874 w		884	1.7	7.7	883	1.2	47.8	γC31−H60
		883	6.3	5.4	882	6.5	1.4	γC11−H55
		877	3.7	3.2	878	1.0	0.9	γC14−H56
		876	6.8	1.4	877	5.5	1.6	νC131−C133
		868	11.3	12.6	869	11.7	6.3	νC49−C101
	858 vw	868	0.2	0.8	866	9.2	2.4	γC9−H54
		865	10.5	1.3	864	8.9	1.6	γC6−H53
		864	13.2	7.3	859	4.1	1.1	γC26−H59
		862	6.6	1.3	858	14.3	5.3	νC33−C39
	830 m	856	54.8	5.7	853	38.4	1.4	γC17−H57
823 w		854	12.4	9.8	848	10.1	3.5	νC36−C48
		844	4.1	0.1	837	10.0	0.2	γC135−H136
	813 w	839	2.1	0.2	837	7.5	0.2	γC112−H111
811 vw		814	11.0	13.6	813	7.0	15.8	νC34−C42
		813	17.7	13.5	813	24.9	1.9	νC30−O1
794 sh		799	8.1	1.2	799	11.0	2.6	νC21−O4
		797	7.3	19.4	797	9.4	8.7	νC49−O20
781 w	787 m	774	4.7	1.0	774	3.4	3.8	β_R
		773	2.3	2.0	773	6.4	24.4	β_R
		773	1.8	17.9	773	3.3	1.1	β_R
		772	8.0	3.2	771	5.5	3.8	β_R
		765	14.3	1.1	762	10.1	0.7	β_R
755 m		763	0.4	2.6	759	13.9	2.2	β_R
		755	6.4	4.0	756	2.0	6.3	β_R
		748	28.2	0.5	755	16.2	5.1	β_R
		745	5.8	1.0	743	23.2	0.3	β_R
736 sh		742	21.1	0.3	741	22.2	0.5	β_R

		737	17.6	1.2	736	17.4	2.7	γC18−O2
720 w	725 vw	736	18.8	1.6	736	15.4	1.4	γC3−O20
	715 vw	732	24.2	0.8	729	66.1	0.9	γC117−H118
		729	35.2	0.4	728	9.6	0.2	γC135−H136
		713	19.2	5.5	711	4.0	1.5	βO2−H52
		709	18.6	2.3	709	29.0	0.8	βO1−H51
		698	54.9	3.6	698	3.4	38.9	β_R
		694	1.6	2.6	694	26.2	9.0	β_R
		690	4.1	0.8	688	29.2	5.7	β_R
641 w	645 vw	655	84.7	6.7	664	83.7	3.1	β_R
		641	15.4	0.9	640	12.0	2.4	β_R
		640	7.3	3.2	638	14.8	1.3	β_R
	618 vw	634	2.3	14.5	634	2.7	2.6	β_R
		633	0.3	0.8	633	0.4	6.3	β_R
		628	2.4	29.3	631	3.8	47.3	β_R
		626	1.8	13.0	626	0.1	4.9	β_R
577 w	578 vw	598	2.8	0.7	598	3.0	1.6	β_R
		584	11.3	10.4	580	7.6	3.1	β_R
		571	9.4	0.9	572	17.5	12.1	β_R
		567	8.0	0.6	568	5.6	0.3	β_R
	557 vw	561	0.8	1.9	565	3.0	0.6	β_R
	549 sh	560	5.7	2.4	562	4.9	1.3	β_R
546 sh		553	4.5	4.0	553	7.9	1.4	β_R
		552	5.7	1.7	552	3.1	2.3	β_R
		551	1.6	0.9	550	5.4	0.7	β_R
532 w		541	3.9	7.9	539	2.7	2.8	β_R
	523 w	536	2.8	15.5	534	1.0	14.5	β_R
		531	4.5	13.3	530	4.0	0.6	β_R
		527	1.3	8.3	524	0.1	3.7	β_R
		507	0.4	6.6	507	0.4	1.3	β_R
		505	0.4	1.6	505	0.5	1.3	β_R
		499	1.2	3.6	500	0.4	8.6	β_R
483 vw	483 sh	496	0.8	1.4	498	0.4	0.2	β_R
		488	0.7	15.1	491	0.6	2.0	β_R
		479	4.4	2.5	475	2.2	0.6	β_R
		476	0.6	1.5	475	0.9	6.6	β_R
	473 vw	474	0.8	4.8	473	3.8	3.1	β_R
		472	0.8	1.7	472	1.0	2.0	βC127−O126
464 w		471	3.7	4.2	471	3.8	11.7	βC109−O128
453 sh	459 vw	465	6.0	0.7	465	1.3	0.3	β_R
		465	2.7	2.1	462	2.2	9.3	β_R
		455	1.3	15.3	456	1.3	3.6	β_R
		452	7.5	0.6	452	8.0	1.5	β_R
	427 vw	440	5.6	0.6	450	6.7	1.0	β_R
424 vw		435	0.2	3.3	436	0.6	0.6	γC30−O1
	412 w	434	0.0	0.9	434	0.0	0.5	γC18−O2
		426	0.6	14.5	420	1.3	2.6	β_R
		411	0.5	0.9	410	0.4	2.0	β_R
		403	1.6	7.3	397	0.6	3.2	β_R
		394	2.1	6.5	391	1.4	2.1	β_R
		386	1.3	4.7	387	0.1	1.3	νC24−S23
		384	2.7	5.3	385	3.0	2.5	νC15−S16
		383	1.1	13.4	382	3.9	0.6	νC27−S16
		382	2.3	28.1	381	2.4	4.8	νC32−S29
		378	0.7	0.7	376	0.8	0.3	νC8−S25
		374	1.6	2.4	372	0.5	1.8	τC124−C128

	373	1.0	2.7	369	1.1	15.5	β_R
359 vw	361	0.1	2.1	360	1.5	1.7	β_R
	360	1.5	12.5	358	0.1	0.3	τC28−C35
	354	0.1	0.6	354	0.1	0.6	β_R
	352	0.1	7.6	352	3.2	6.4	β_R
340 vw	349	0.7	5.0	348	0.3	0.2	β_R
	336	7.3	8.5	336	7.6	2.2	β_R
	334	3.1	19.3	335	5.5	3.4	β_R
	330	3.8	5.7	329	0.7	3.0	νC12−S29
	326	2.2	2.1	327	1.3	0.3	β_R
	324	1.0	0.6	324	0.9	0.6	τC33−C38
	321	0.9	0.7	322	0.2	0.6	τC5−C34
	319	2.4	0.6	320	6.0	2.7	νC22−S23
	314	0.3	0.1	312	0.5	1.8	νC27−S16
	314	1.1	0.5	312	0.1	0.4	τC35−C45
	312	0.1	0.1	311	0.7	5.2	τC34−C40
	312	0.1	0.4	310	1.8	1.5	τC36−C47
	304	0.3	0.6	302	0.3	2.4	νC7−S25
290 vw	303	0.5	6.4	299	4.4	0.6	β_R
	297	2.4	2.4	299	1.3	2.0	τC50−O4
	290	1.9	0.6	293	0.6	26.3	τC10−C33
	287	0.7	2.0	290	0.2	11.5	β_R
	283	0.3	1.5	283	0.1	13.8	τC13−C36
	277	0.5	1.8	280	0.0	0.7	β_R
	276	1.1	2.4	276	0.4	0.9	τC5−C34
	268	0.7	2.1	270	0.6	0.9	τC28−C35
	266	0.3	1.2	268	0.6	1.9	τC34−C41
	261	0.0	0.9	263	0.0	1.7	τC35−C44
	260	1.0	0.9	262	0.4	1.5	τC34−C42
	258	0.0	0.9	261	0.0	3.8	τC35−C43
254 vw	254	0.2	0.3	258	0.4	0.8	τC36−C46
	250	1.2	1.5	252	3.0	3.6	τC33−C39
	244	0.4	0.6	247	3.6	1.0	τC34−C41
	239	3.0	1.8	239	0.4	1.0	τO4−C50
	232	0.1	6.7	234	0.1	2.0	τO2−C18
230 w	229	0.1	7.7	230	0.0	1.4	τC34−C42
	227	0.0	0.5	229	0.2	0.5	τC33−C37
	226	0.4	1.5	227	0.9	1.8	τC36−C48
	224	0.0	2.9	226	0.4	1.1	τC35−C44
	217	0.2	3.9	219	2.7	2.9	τC110−C106
	213	0.7	9.5	217	0.9	7.3	τC124−C128
	209	1.8	1.7	214	1.8	11.0	τC12−S29
197 vw	208	1.6	1.8	210	0.6	3.3	τC28−C35
	203	2.3	9.7	203	0.3	5.2	τC109−C110
	198	2.2	6.3	203	1.8	0.4	τC15−S16
	191	0.5	1.3	203	0.9	5.4	τC119−N122
	187	1.2	6.2	191	0.4	1.2	τC13−C36
	182	2.1	13.9	179	2.1	2.8	τC24−S23
	169	5.1	7.0	170	4.1	1.3	τC32−S29
153 w	158	1.5	31.6	166	4.1	3.0	τC3−C12
	153	2.1	25.8	162	1.0	2.7	τC50−C119
	147	1.2	23.6	159	0.6	18.4	τC26−C27
	144	0.6	12.3	149	0.1	8.5	τC7−S25
	140	0.8	21.8	144	1.9	1.5	τC27−S16
	134	3.7	7.3	139	1.9	9.0	τC119−N122
	124	1.4	32.1	128	0.8	3.7	τC21−O4

122	0.4	3.9	119	0.1	3.5	τC6−C7
115	0.4	18.9	117	0.9	1.7	τC21−C22
108	0.4	10.8	111	0.9	33.2	τC30−C32
106	0.6	13.9	106	0.7	3.1	τC18−C27
100	0.8	6.9	102	0.8	8.7	τC18−C27

Abbreviations: ν: stretching; δ: deformation in plane; ρ: deformation out of plane; χ: torsion; as: antisymmetric; s: symmetric.

Table S5. For **5**, a comparison of Experimental and calculated wavenumbers ν (cm^{-1}), intensity I (km/mol) of the bands in the IR spectra and relative intensity J (a.u.) of the lines in the Raman spectra of *exo-exo* and *endo-exo* rotamers.

IR_{exp}	$Raman_{exp}$	*exo-exo*			*endo-exo*			Assignment
ν	ν	ν	I	J	ν	I	J	
		3613	66.7	0.8	3620	65.8	1.5	νO38−H145
		3611	80.4	42.9	3617	51.7	1.8	νO104−H146
3420 m		3413	988.2	1.0	3503	720.0	0.4	νO143−H144
		3395	721.5	2.0	3460	639.9	0.8	νO138−H139
		3140	8.0	3.2	3140	7.6	1.2	νC99−H100
		3138	8.5	1.0	3139	5.3	1.7	νC31−H32
		3132	2.9	1.2	3130	2.1	0.0	νC73−H74
		3131	2.6	0.9	3127	7.8	0.3	νC7−H8
		3125	6.1	0.7	3126	3.0	0.2	νC101−H102
		3123	5.1	0.8	3125	5.3	0.2	νC33−H34
		3114	7.3	0.1	3116	6.6	3.1	νC49−H50
		3114	6.2	0.0	3115	4.9	1.6	νC112−H113
		3112	0.1	0.7	3113	0.9	0.2	νC35−H36
		3111	2.2	0.1	3110	2.1	1.1	νC97−H98
		3101	9.2	3.6	3106	5.4	0.2	νC70−H71
		3100	7.8	0.8	3102	8.1	0.7	νC4−H5
		3088	19.1	0.1	3092	16.4	0.7	νC46−H47
		3087	11.5	1.6	3092	9.8	0.2	νC115−H116
		3064	5.7	0.1	3062	8.1	1.9	νC64−H65 ν_{as} CH_2
		3062	5.4	0.2	3060	16.8	0.1	νC131−H132 ν_{as} CH_2
		3056	28.5	0.1	3056	9.7	0.2	νC14−H16 ν_{as} CH_3
		3056	12.8	0.8	3055	0.7	0.1	νC76−H78 ν_{as} CH_3
		3054	14.9	0.0	3055	3.8	0.2	νC10−H12 ν_{as} CH_3
		3054	17.3	0.2	3055	37.8	2.0	νC118−H119 ν_{as} CH_3
		3054	26.4	0.1	3055	31.3	0.3	νC56−H57 ν_{as} CH_3
		3053	22.2	0.1	3055	21.1	1.1	νC80−H81 ν_{as} CH_3
		3052	19.5	0.0	3053	15.5	0.0	νC60−H61 ν_{as} CH_3
		3052	15.7	0.2	3053	14.0	0.2	νC122−H123 ν_{as} CH_3
		3049	44.5	1.2	3052	16.5	0.4	νC76−H77 ν_{as} CH_3
		3048	61.5	0.5	3051	69.2	4.8	νC14−H15 ν_{as} CH_3
		3048	90.2	0.3	3049	20.7	1.1	νC10−H11 ν_{as} CH_3
		3048	10.3	0.4	3047	23.4	0.2	νC84−H85 ν_{as} CH_3
3047 w		3047	15.6	0.5	3047	75.0	3.3	νC52−H53 ν_{as} CH_3
		3046	32.2	1.1	3047	74.6	1.1	νC126−H127 ν_{as} CH_3
		3046	77.0	2.3	3046	2.2	0.5	νC52−H54 ν_{as} CH_3
		3045	69.8	1.0	3045	20.5	2.1	νC122−H124 ν_{as} CH_3
		3042	2.2	0.3	3045	38.4	0.7	νC76−H79 ν_{as} CH_3
		3042	3.0	1.3	3045	73.5	1.3	νC14−H17 ν_{s} CH_3
		3041	2.7	0.6	3043	2.5	0.0	νC10−H13 ν_{s} CH_3
	3039 w	3041	2.6	0.1	3040	4.1	1.6	νC80−H83 ν_{as} CH_3
		3040	9.4	0.9	3040	3.7	1.2	νC56−H58 ν_{as} CH_3
		3039	6.1	0.6	3039	2.6	1.5	νC118−H121 ν_{as} CH_3
		3038	1.7	0.1	3039	3.1	0.3	νC122−H124 ν_{as} CH_3
		3038	8.0	0.0	3039	10.3	0.5	νC60−H61 ν_{as} CH_3
		3033	6.4	0.9	3039	4.7	0.7	νC40−H41 ν_{as} CH_2

		3033	5.8	0.3	3031	6.5	0.3	νC106−H107 ν_{as} CH_2
		3010	20.3	0.1	3030	4.7	0.4	νC22−H23 ν_s CH_2
		3002	19.0	0.5	3028	15.5	1.4	νC88−H89 ν_s CH_2
		2991	21.3	1.3	3003	30.4	0.1	νC91−H92 ν_s CH_2
		2990	22.1	0.1	2990	0.5	1.5	νC130−H131 ν_s CH_2
		2989	16.1	0.3	2990	18.1	0.5	νC64−H65 ν_s CH_2
		2986	21.6	3.0	2986	25.8	1.0	νC40−H42 ν_s CH_2
		2986	4.8	1.8	2985	23.9	0.6	νC25−H26 ν_s CH_2
		2986	24.7	2.2	2983	45.8	6.9	νC106−H108 ν_s CH_2
		2973	40.8	0.2	2982	6.6	2.0	νC14−H15 ν_s CH_3
		2973	19.0	0.4	2976	24.9	0.3	νC10−H11 ν_s CH_3
		2971	30.2	2.0	2974	18.6	0.3	νC52−H53 ν_s CH_3
		2971	20.7	0.3	2972	39.0	4.3	νC122−H123 ν_s CH_3
		2971	20.0	0.9	2972	40.0	2.9	νC28−H29 ν_s CH_2
		2967	6.2	0.1	2971	16.1	2.2	νC76−H79 ν_s CH_3
		2967	35.7	1.2	2970	16.1	1.2	νC14−H16 ν_s CH_3
		2966	33.5	0.3	2967	20.2	0.1	νC80−H81 ν_s CH_3
		2966	6.2	0.3	2965	2.1	0.3	νC18−H19 ν_s CH_3
		2964	27.4	0.3	2965	25.5	0.7	νC52−H54 ν_s CH_3
		2964	24.6	0.9	2965	26.6	0.9	νC126−H127 ν_s CH_3
		2964	27.1	0.2	2965	47.5	1.1	νC56−H57 ν_s CH_3
		2964	21.8	0.1	2964	19.6	1.0	νC118−H119 ν_s CH_3
	2962 m	2950	42.4	0.6	2964	18.9	1.0	νC22−H24 ν_s CH_2
		2946	57.1	1.9	2963	20.8	0.3	νC94−H95
2959 s		2943	21.9	0.6	2959	30.9	1.4	νC88−H89 ν_s CH_2
		2940	7.4	0.2	2931	39.4	0.1	νC25−H26 ν_s CH_2
2905 m	2929 m	2915	25.0	0.3	2924	25.8	0.9	νC91−H92 ν_s CH_2
2868 m	2782 vw	2656	602.6	100.0	2618	866.0	56.3	νO141−H142
	2714 vw	2516	999.9	17.3	2364	779.9	35.1	νO136−H137
		1636	24.5	9.4	1637	10.6	7.7	νC28=N133
		1629	263.3	6.7	1634	26.5	23.9	νC94=N134
1635 s	1639 s	1625	129.7	2.8	1627	389.6	71.5	νC30−C31
		1625	32.2	2.3	1626	59.4	1.0	νC96−C97
		1607	36.1	2.5	1609	16.9	6.0	νC31−C33
1598 w	1602 m	1603	22.3	15.7	1607	38.3	1.5	νC109−C110
		1602	6.5	7.3	1598	3.6	4.4	νC43−C44
		1600	15.8	1.5	1598	7.8	10.4	νC101−C103
		1591	16.0	0.6	1594	4.0	3.6	νC1−C2
		1591	6.3	1.1	1587	14.8	24.6	νC69−C70
		1580	5.0	15.1	1582	15.9	3.0	νC4−C6
		1576	4.9	0.2	1581	4.0	3.2	νC44−C45
		1573	6.5	8.4	1573	7.6	10.9	νC72−C73
		1570	9.4	11.2	1563	1.9	0.4	νC6−C7
1545 w		1515	161.7	2.7	1518	212.4	12.2	νC33−C35
1484 s		1502	105.2	3.4	1514	72.1	11.8	νC99−C101
		1481	40.7	0.7	1513	12.1	0.2	βC22−H23 δ_s CH_2
	1476 m	1480	57.9	0.1	1480	53.1	19.4	βC22−H24 δ_s CH_2
		1478	117.0	4.5	1477	144.5	1.1	βC118−H119 δ_s CH_3
		1474	17.3	0.5	1476	25.1	17.0	βC76−H77 δ_s CH_3
		1473	29.3	4.0	1474	12.2	1.2	βC10−H11 δ_s CH_3
1470 s		1473	45.2	2.3	1474	71.4	2.7	νC35−C37
		1471	2.6	1.9	1472	11.9	0.1	βC52−H53 δ_s CH_3
		1471	4.0	4.6	1472	42.8	1.8	βC126−H127 δ_s CH_3

		1465	15.1	12.2	1471	0.9	11.2	βC88−H90 δ_s CH_2
		1462	152.2	9.7	1470	6.2	1.6	νC96−C97
		1460	87.5	0.2	1460	7.6	1.6	βC10−H12 δ_s CH_3
		1459	23.4	0.2	1459	44.1	0.1	βC18−H19 δ_s CH_3
		1458	10.1	0.1	1459	11.0	3.2	βC84−H85 δ_s CH_3
		1458	11.0	0.1	1458	6.7	0.2	βC52−H53 δ_s CH_3
		1458	4.8	0.1	1458	5.5	0.1	βC18−H20 δ_s CH_3
		1456	13.9	1.0	1457	13.7	0.6	βC25−H26 δ_s CH_2
		1455	4.3	0.6	1455	11.6	0.7	βC88−H89 δ_s CH_2
	1452 m	1455	13.7	0.0	1455	3.9	0.1	βC56−H57 δ_s CH_3
		1453	18.5	0.1	1451	90.6	0.1	βC118−H121 δ_s CH_3
		1450	29.6	1.8	1450	38.8	0.4	βC10−H13 δ_s CH_3
1443 sh		1448	34.8	4.0	1449	20.9	32.9	βC80−H81 δ_s CH_3
		1443	76.5	15.9	1448	2.1	0.5	C37−C39
		1442	52.5	2.2	1443	129.7	16.4	C97−C99
		1441	5.3	0.3	1441	5.4	0.6	βC52−H54 δ_s CH_3
		1441	5.3	0.1	1441	0.2	0.1	βC84−H85 δ_s CH_3
		1439	13.9	0.7	1440	16.7	0.1	βC14−H17 δ_s CH_3
		1439	8.6	0.1	1439	1.5	2.5	βC10−H12 δ_s CH_3
		1437	0.3	0.1	1438	2.1	0.3	βC118−H119 δ_s CH_3
		1436	0.8	0.1	1437	49.3	41.2	βC56−H58 δ_s CH_3
		1436	0.1	0.1	1437	1.2	0.3	βC14−H16 δ_s CH_2
		1436	0.1	0.0	1436	1.3	0.4	βC76−H77 δ_s CH_3
		1432	0.2	0.1	1436	1.2	0.7	βC52−H53 δ_s CH_3
		1431	0.3	0.0	1435	2.1	0.3	βC118−H119 δ_s CH_3
		1431	0.0	0.2	1434	34.2	21.9	βC10−H11 δ_s CH_3
		1431	0.0	0.0	1433	0.8	0.2	βC80−H81 δ_s CH_3
		1430	19.1	3.6	1432	0.5	0.1	βC106−H107 δ_s CH_2
		1429	20.6	3.2	1432	0.3	0.0	βC40−H41 δ_s CH_2
		1419	13.3	0.1	1431	0.3	0.2	C111−C112
1416 w		1418	31.9	0.3	1430	3.6	1.3	βC64−H65 δ_s CH_2
		1417	6.0	9.1	1428	23.2	11.0	βC130−H131 δ_s CH_2
		1416	7.0	1.1	1413	9.9	0.1	νC43−C44
		1411	26.1	0.5	1412	8.6	0.1	βC91−H92 δ_s CH_2
1393 w		1405	11.1	1.8	1403	86.6	6.2	νC1−C2
		1404	1.9	6.7	1403	6.7	0.4	νC70−C72
		1401	90.4	8.7	1401	3.9	0.2	νC30−C31
		1398	95.4	12.7	1397	56.0	9.7	νC97−C99
		1377	5.5	3.3	1380	7.3	5.7	βC10−H11 δ_s CH_3
		1376	5.8	5.3	1377	5.2	1.6	βC84−H85 δ_s CH_3
1375 sh	1371 w	1375	8.7	0.6	1376	2.9	1.2	βC122−H123 δ_s CH_3
		1375	1.2	0.1	1375	4.3	2.4	βC52−H53 δ_s CH_3
1363 m		1371	7.3	0.9	1374	2.7	1.0	βC22−H23 wag CH_2
		1368	46.3	8.9	1374	26.9	0.2	βO138−H139
		1364	75.2	1.7	1369	56.3	0.2	νC46−C48
		1361	9.6	4.2	1360	41.4	12.4	βC91−H92 wag CH_2
		1354	45.2	0.4	1348	44.2	45.9	βC88−H89 wag CH_2
		1349	41.8	5.2	1347	2.7	0.5	βC22−H23 wag CH_2
		1342	2.9	1.5	1345	5.2	0.1	βC14−H17 δ_s CH_3
		1342	11.2	0.7	1344	9.9	1.2	βC84−H86 δ_s CH_3
		1341	4.4	2.0	1341	0.2	0.2	βC52−H54 δ_s CH_3
		1341	37.7	0.1	1341	21.4	0.2	βC60−H61 δ_s CH_3
1341 w	1342 w	1341	2.3	0.0	1341	4.4	0.5	βC10−H12 δ_s CH_3
		1341	13.5	0.1	1340	29.2	0.3	βC76−H77 δ_s CH_3
		1340	6.9	0.1	1340	9.3	0.9	βC122−H125 δ_s CH_3

		1340	11.1	0.3	1339	13.0	0.1	βC56−H58 δ_s CH_3
		1338	4.7	0.4	1335	5.1	100.0	νC2−C3
		1337	1.2	35.4	1331	1.6	8.6	νC67−C68
		1325	66.6	2.3	1318	2.7	31.2	βC91−H92 wag CH_2
	1316 w	1318	2.5	0.1	1314	40.3	6.9	βO138−H139
		1313	64.5	16.7	1313	3.5	0.5	βO38−H145
		1312	3.2	1.2	1309	45.4	69.7	βO104−H146
	1302 w	1310	25.6	1.6	1290	44.8	5.2	βO141−H142
		1294	26.2	0.5	1284	35.6	8.9	βC25−H27 wag CH_2
1298 sh		1286	125.4	3.2	1281	10.6	4.4	βC106−H107 wag CH_2
	1284 sh	1283	32.6	0.6	1277	65.3	0.6	βC40−H41 wag CH_2
		1281	98.4	0.3	1277	59.8	0.2	βC106−H108 wag CH_2
		1279	56.6	0.2	1276	33.5	1.5	βC64−H65 wag CH_2
	1276 w	1276	124.7	12.7	1276	101.7	45.5	νC30−C39
		1273	3.9	1.1	1271	98.6	22.6	βC130−H131 wag CH_2
1271 m		1272	16.6	2.2	1266	52.3	0.8	νC103−O104
	1265 w	1269	55.2	14.0	1265	8.8	21.8	νC94−C96
		1265	3.6	6.2	1259	6.1	1.9	βC106−H108 wag CH_2
		1264	11.8	0.8	1257	4.0	7.7	βC40−H42 wag CH_2
		1262	16.6	2.6	1257	4.8	0.5	βC88−H89 wag CH_2
		1261	13.8	1.2	1256	0.9	2.0	βC22−H24 wag CH_2
	1239 w	1256	24.4	0.3	1248	108.2	3.1	βC64−H65 wag CH_2
1237 sh		1253	4.0	0.3	1242	1.1	1.1	νC44−O138
		1237	1.8	1.1	1239	3.1	3.0	βC7−H8
		1236	8.9	7.6	1233	0.2	0.0	βC4−H5
		1228	44.6	4.5	1227	70.5	2.8	νC39−O136
	1224 m	1225	45.8	6.5	1224	19.5	9.0	νC105−O141
		1220	105.4	0.7	1220	52.8	15.2	βC46−H47
		1216	29.0	0.8	1216	13.6	5.5	νC68−O140
		1214	12.1	3.8	1211	11.0	1.8	βC49−H50
		1212	13.2	3.1	1207	65.2	0.5	βO138−H139
	1207 sh	1207	45.8	6.0	1206	50.0	2.7	βO38−H145
		1206	49.4	3.0	1204	51.2	3.4	βO104−H146
		1206	49.0	5.8	1198	36.2	0.2	βC88−H89 ρ CH_2
1197 m		1199	28.1	3.0	1197	11.4	0.9	νC40−C43
		1198	34.6	3.7	1195	7.9	0.2	νC114−C117
		1194	13.9	0.2	1193	1.6	2.2	νC9−C10
		1193	7.7	0.1	1193	1.4	2.8	νC75−C76
		1190	16.2	10.1	1190	1.7	0.2	νC117−C118
		1190	25.3	0.2	1190	42.0	30.1	C51−C52
		1189	18.2	1.0	1189	12.7	0.1	βC22−H23 ρ CH_2
		1188	6.8	0.2	1188	12.5	0.1	νC51−C56
		1188	3.3	0.2	1188	6.8	0.2	νC9−C14
		1188	6.2	0.1	1188	6.0	0.3	νC117−C122
		1188	3.2	0.2	1188	49.6	0.8	νC51−C60
		1173	114.3	2.2	1173	162.7	0.1	νC1−C130
		1169	44.1	2.3	1163	27.8	1.8	βC106−H107 ρ CH_2
	1177 vw	1157	49.7	1.0	1151	1.6	1.9	βC130−H131 ρ CH_2
		1155	22.0	0.9	1150	5.0	0.9	βC64−H65 ρ CH_2
	1167 vw	1151	2.1	0.3	1150	4.1	7.9	βC31−H32
		1150	4.5	0.1	1148	28.0	1.1	βC97−H98
		1149	13.6	0.0	1144	17.4	0.1	βC40−H42 ρ CH_2
	1131 w	1148	6.9	0.0	1135	0.7	6.3	βC106−H108 ρ CH_2
1123 m		1121	34.3	3.5	1129	22.3	1.7	βC26−H27 ρ CH_2
		1111	61.0	0.3	1120	30.4	1.1	βC112−H113

		1103	5.3	0.2	1109	75.8	3.1	βC115−H116
		1095	32.1	2.4	1099	8.4	0.1	νC91−N134
1097 w		1089	12.7	0.4	1090	13.1	0.3	νC4−C6
		1084	86.8	9.4	1079	52.1	24.0	νC2−C3
		1068	22.0	0.2	1068	4.8	0.1	βC88−H89 ρ CH_2
	1075 w	1067	6.1	0.1	1065	19.1	3.4	βC91−H92 ρ CH_2
1067 sh		1060	13.7	3.0	1054	5.6	0.2	βC88−H90 ρ CH_2
1050 w		1053	7.1	1.3	1053	11.7	0.5	νC2−O135
	1030 w	1044	17.0	0.3	1042	78.5	2.2	νC105−O141
1021 m		1040	3.6	0.5	1039	17.8	2.8	C28−C30
		1020	56.2	13.6	1036	2.3	0.4	C33−C35
		1019	70.2	0.3	1019	13.9	4.3	C94−C96
		1014	0.1	0.1	1015	0.1	0.0	βC118−H119 ρ CH_3
		1014	0.2	0.1	1015	0.8	0.1	βC14−H17 ρ CH_3
		1014	0.2	0.2	1014	3.1	2.2	βC56−H57 ρ CH_3
		1013	0.3	0.1	1013	0.1	0.0	βC76−H77 ρ CH_3
		1013	0.9	0.0	1013	1.6	1.4	βC18−H19 ρ CH_3
		1012	1.0	2.7	1013	16.0	9.9	βC52−H53 ρ CH_3
		1011	1.3	0.0	1012	0.2	1.0	βC18−H20 ρ CH_3
		1011	2.0	0.0	1011	0.9	2.3	βC84−H85 ρ CH_3
		1001	218.4	2.0	1011	1.1	0.3	νC2−O135
978 w	983 vw	995	89.1	0.0	1001	101.1	4.2	βO136−H137
		986	56.4	0.0	973	211.6	32.6	βO141−H142
		972	3.0	0.3	970	15.4	0.1	νC3−C40
		968	1.7	0.7	968	14.0	0.9	νC64−C67
947 sh		968	22.3	0.2	966	89.2	8.5	νC72−C75
	939 sh	966	1.8	0.8	957	3.2	2.3	βC28−H29
		956	2.1	0.3	950	1.3	0.3	νC40−C43
		955	0.6	1.0	949	6.8	0.8	βC94−H95
		932	19.9	0.1	944	11.2	0.7	νC114−C117
		930	0.8	0.0	935	23.9	4.1	γC31−H32
	928 w	929	0.2	1.0	930	0.1	0.2	βC99−H100
		929	1.1	3.1	928	2.1	0.2	βC101−H102
		927	0.2	0.1	928	0.6	0.9	βC18−H19 ρ CH_3
921 w		927	5.1	0.7	928	0.2	0.1	νC3−C4
		927	0.3	0.0	927	3.3	1.5	βC84−H85 ρ CH_3
		926	0.0	0.0	927	0.1	0.1	βC52−H53 ρ CH_3
		926	0.5	0.1	927	0.4	0.3	βC60−H62 ρ CH_3
		921	1.1	0.0	925	18.9	0.8	νC48−C51
		915	0.8	0.3	920	0.8	0.2	νC9−C18
		915	0.9	0.1	917	2.8	0.1	νC75−C84
		914	1.4	0.2	916	1.9	0.7	νC51−C52
	910 w	913	0.6	0.1	914	1.8	0.9	νC117−C122
		907	1.1	0.2	912	0.2	0.0	νC9−C14
		906	5.1	0.4	911	0.6	0.3	νC75−C76
		906	24.1	0.1	908	1.4	0.6	νC69−C70
		905	3.6	0.1	906	1.2	0.3	νC51−C60
		904	0.6	0.1	905	1.7	0.1	νC117−C126
		904	5.8	1.1	904	2.0	0.1	νC40−C43
		902	4.4	1.2	902	5.8	0.6	νC45−C64
	881 w	898	32.4	2.7	900	5.5	0.1	νC91−N134
873 m		894	4.3	1.4	891	2.2	2.2	νC1−C130
		876	3.2	0.1	877	2.4	0.0	γC46−H47
		874	10.9	0.6	875	1.0	0.0	γC7−H8

		873	1.7	0.0	871	0.1	0.3	γC4−H5
		870	0.3	2.2	868	2.6	0.4	γC112−H113
		868	0.2	0.0	866	4.6	0.3	γC49−H50
		862	0.7	2.3	859	4.4	0.0	γC115−H116
	854 w	862	2.0	0.0	858	22.7	0.2	γC31−H32
		859	3.5	0.0	857	2.1	0.1	γC101−H102
849 w		857	14.5	0.0	854	13.9	0.3	γC115−H116
		854	16.8	0.0	854	3.9	0.3	γC73−H74
		851	8.1	0.7	845	17.6	22.3	γC70−H71
	832 sh	845	16.4	4.9	844	10.2	6.4	νC37−O38
	820 m	841	15.9	0.3	814	2.8	0.8	νC103−O104
815 w		816	4.0	1.8	810	7.7	0.1	νC2−C3
		810	8.4	1.3	809	6.7	0.2	νC51−C52
801 sh	806 sh	805	12.1	1.6	803	14.4	9.2	νC9−C18
		801	1.8	1.6	800	5.4	3.1	νC2−O135
		800	0.3	0.1	796	2.2	0.0	νC44−O138
779 w		795	4.6	7.7	794	1.6	0.6	νC75−C84
		794	2.4	0.2	782	11.0	0.8	νC45−C64
	762 vw	778	2.1	0.1	773	5.6	0.7	νC43−C44
755 sh		773	25.3	0.1	766	2.9	0.4	γO138−H139
		767	10.4	0.1	765	10.4	0.0	νC39−O136
733 m	734 w	765	8.2	0.5	761	13.3	0.2	νC105−O141
		753	21.9	1.0	748	5.0	0.1	νC138−O139
		739	66.3	0.2	742	7.5	0.9	νC110−O141
	720 vw	731	41.6	0.5	731	8.2	0.7	β_R
		729	38.9	0.2	728	23.2	9.3	β_R
		725	21.1	0.2	724	9.7	0.0	β_R
		721	22.4	4.9	718	3.5	0.0	β_R
	703 w	720	38.6	0.0	716	55.1	2.5	γC31−H32
		717	33.2	0.1	716	105.8	0.6	γC99−H100
	680 w	708	15.9	0.1	705	12.0	0.6	β_R
	675 vw	695	5.8	0.2	690	0.8	4.0	β_R
		687	1.5	1.1	672	1.3	2.6	β_R
	649 vw	670	2.6	0.0	668	3.1	2.9	β_R
636 w		666	0.6	0.6	660	0.1	1.0	β_R
	631 w	661	0.2	1.0	636	60.5	1.1	γC48−C51
		632	0.0	0.0	633	0.7	3.7	γC114−C117
		629	3.6	2.6	629	9.0	0.9	β_R
		626	5.5	0.1	627	6.5	0.6	β_R
		616	3.4	0.2	617	3.2	0.1	β_R
591 w	594 w	616	0.6	0.5	617	5.0	0.3	γC3−C40
		595	0.1	0.0	591	2.1	1.4	β_R
		589	21.2	0.8	590	6.1	1.1	β_R
	582 w	586	1.1	0.9	586	1.3	0.1	β_R
		580	2.9	0.6	576	4.2	0.3	β_R
575 vw		576	14.7	0.4	575	4.9	0.4	γC103−O104
	562 w	573	12.6	0.0	570	0.5	0.3	γC105−O141
		572	4.2	0.1	566	4.4	2.6	β_R
554 w		568	105.2	0.1	558	12.5	0.2	γO104−H146
		557	10.8	1.6	557	24.1	0.3	β_R
	545 vw	557	1.7	2.7	555	30.0	1.0	β_R
		554	32.9	0.2	554	4.6	0.1	β_R
		551	9.6	4.1	553	54.1	0.2	β_R
		546	8.9	1.9	548	15.4	1.4	β_R
		541	31.7	0.2	533	0.4	0.6	τC103−C105

		534	3.1	0.2	526	5.7	0.1	γC2−O135
	514 vw	529	4.3	0.6	525	1.3	0.1	β_R
	504 w	525	10.6	2.1	523	49.3	0.3	νC72−C75
		523	42.4	0.8	522	83.4	0.2	γO38−H145
		521	5.3	0.1	519	1.8	0.8	β_R
		508	1.9	0.1	512	0.5	0.4	β_R
		503	2.9	0.1	503	1.4	0.4	β_R
484 vw		502	0.1	3.6	501	0.9	0.1	β_R
		499	0.3	2.7	500	0.5	0.0	β_R
		497	2.3	6.3	497	1.2	0.4	β_R
	471 vw	490	1.0	2.9	492	1.5	5.1	β_R
		487	0.9	0.1	489	0.4	6.3	β_R
		483	2.0	2.2	483	1.8	15.0	β_R
		475	3.8	5.4	480	0.1	2.7	β_R
	447 vw	472	1.2	0.1	472	1.6	0.0	β_R
438 w		449	2.1	0.4	442	3.2	16.4	β_R
		441	1.2	4.2	438	0.2	0.1	βC39−O136
		437	0.3	0.1	436	0.4	0.2	γC44−O138
	420 w	435	0.7	0.7	435	0.4	14.2	γC110−O143
		421	5.6	15.1	421	1.1	16.8	β_R
		416	0.3	3.7	418	6.1	6.6	β_R
		414	0.4	2.0	416	0.9	27.8	β_R
		413	1.8	1.0	412	0.4	4.7	β_R
		408	0.4	0.3	410	0.6	1.5	β_R
		402	0.8	0.3	408	0.1	0.9	β_R
		382	3.1	5.7	386	6.4	2.9	β_R
		380	2.1	0.0	380	6.5	0.3	β_R
		376	0.3	1.2	378	0.8	2.4	β_R
		372	3.3	0.1	364	0.8	0.5	τC72−C75
	361 sh	365	1.5	0.5	362	0.3	0.3	τC48−C51
		360	0.1	0.4	361	0.6	0.4	τC114−C117
		358	1.1	0.3	354	0.3	0.2	τC44−C45
	343 vw	354	0.8	0.0	353	1.5	0.7	β_R
		352	5.6	0.1	346	2.3	0.5	β_R
		344	4.9	4.8	344	2.9	0.1	β_R
		342	3.1	0.7	343	16.4	1.3	γC103−O104
		341	3.3	0.2	339	4.5	0.8	β_R
		330	1.4	0.1	332	0.2	0.9	τC117−C126
	320 vw	329	0.6	0.5	328	0.5	0.0	τC75−C84
		327	0.5	0.1	322	0.7	0.1	τC9−C18
		321	0.7	1.6	321	0.7	0.6	τC117−C122
		316	0.8	0.3	317	0.3	1.3	τC9−C14
		316	0.0	1.3	316	0.6	0.1	τC28−C30
		315	0.3	1.4	314	2.4	6.3	τC51−C52
		315	1.7	12.1	313	1.0	0.0	βC39−O136
		314	0.2	7.6	312	1.8	1.1	τC117−C126
		311	0.9	2.8	309	0.2	1.3	βC103−O104
		309	0.5	1.8	308	0.3	1.8	τC3−C40
		305	1.5	2.0	306	0.6	4.5	τC2−O135
	292 vw	302	0.6	2.2	302	1.5	3.4	τC51−C56
		301	0.3	4.3	301	0.6	1.3	τC75−C76
		300	0.5	0.3	295	2.0	8.2	τC117−C118
		286	0.1	2.4	284	0.1	2.5	τC25−N133
		284	0.7	0.0	283	0.4	2.7	τC94−N134
		283	0.8	0.1	282	2.3	3.6	τC30−C39
		280	0.0	0.0	281	0.1	0.4	τC117−C122

	275	0.2	2.3	273	0.1	0.2	τC51−C60
	268	0.6	0.1	266	0.4	0.3	βC68−O140
264 vw	262	0.3	0.2	264	0.6	0.1	τC52−C56
	261	0.3	0.1	263	0.4	0.0	τC6−C10
	255	0.4	1.4	262	0.2	0.4	τC9−C14
	252	0.4	0.2	249	0.0	0.2	τC75−C80
	247	0.2	4.5	246	0.3	0.3	τC91−N134
	244	0.3	0.2	239	2.7	0.0	τC68−O140
	234	0.9	0.1	235	0.5	0.0	τC44−C45
238 vw	231	1.0	0.3	233	0.0	0.7	τC51−C56
	230	2.6	0.5	230	0.1	1.1	τC28−C30
	228	0.9	0.0	229	0.7	0.1	τC117−C118
	223	1.4	0.0	227	0.4	0.6	τC9−C14
	220	1.6	1.5	220	4.9	2.4	τC9−C10
	220	0.1	0.3	210	0.2	0.1	τC75−C76
	210	0.7	2.5	207	0.4	0.7	τC22−O135
209 sh	204	0.6	0.5	203	0.0	0.6	τC25−N133
	200	0.9	1.3	198	3.7	1.0	τC94−N134
	193	1.2	1.0	192	0.5	7.7	τC94−C96
189 w	186	0.0	0.7	188	4.8	0.1	τC28−C30
	183	1.9	0.8	184	0.2	1.9	τC94−C96
	176	2.7	2.8	175	6.6	3.6	τC96−C105
	170	1.5	1.1	173	8.9	4.7	τC30−C39
	169	5.2	0.1	167	2.3	1.5	τC88−C91
	167	6.0	0.2	161	1.7	3.8	βC37−O38
	155	0.6	0.2	154	0.3	1.4	τC1−C7
	136	2.2	12.7	147	0.5	12.6	βC105−O141
	134	1.8	0.5	136	2.7	1.0	βC103−O104
	130	1.4	4.8	136	2.0	0.2	τC22−C25
	124	0.2	1.4	132	1.5	0.5	τC67−C68
	121	0.7	1.4	121	0.2	6.3	τC25−N133
	114	1.9	1.2	121	1.1	1.5	τC110−C111
	107	0.4	0.4	111	0.2	0.1	τC43−C44
	103	0.8	1.6	108	0.2	5.0	τC48−C49
	100	0.7	3.1	104	0.4	0.3	τC112−C114
	99	2.7	0.1	101	1.1	0.1	τC112−C114

Abbreviations: ν: stretching; δ: deformation in plane; ρ: deformation out of plane; χ: torsion; as: antisymmetric; s: symmetric.

Table S6. For **6**, a comparison of Experimental and calculated wavenumbers ν (cm^{-1}), intensity I (km/mol) of the bands in the IR spectra and relative intensity J (a.u.) of the lines in the Raman spectra of *exo-exo* and *endo-exo* rotamers.

IR_{exp}	$Raman_{exp}$	*exo-exo*			*endoo-exo*			Assignment
ν	ν	ν	I	J	ν	I	J	
		3595	58.0	0.9	3620	55.9	9.3	νO118−H137
		3572	521.7	1.4	3602	57.2	3.3	νO136−H138
		3462	314.7	10.4	3444	326.5	4.3	νO2−H52
		3431	408.6	3.4	3420	342.7	9.8	νO1−H51
3386 m		3146	0.1	6.2	3145	0.1	15.6	νC14−H56
		3143	0.5	0.4	3145	0.6	0.2	νC1−H54
		3139	0.1	2.1	3143	1.9	1.3	νC130−H129
		3139	5.0	0.0	3141	0.1	10.3	νC31−H60
		3138	0.3	2.4	3139	0.1	8.1	νC26−H59
		3138	11.2	0.1	3137	8.2	19.1	νC112−H111
		3126	4.6	1.0	3127	2.8	6.0	νC130−H129
		3124	1.9	0.3	3126	2.4	6.6	νC17−H57
		3123	7.3	4.4	3126	1.7	0.1	νC115−H116
		3119	3.2	3.2	3122	6.9	7.4	νC11−H55
		3118	1.2	0.3	3119	2.8	4.1	νC6−H53
		3116	2.1	5.7	3118	0.5	1.7	νC19−H58
		3116	3.4	10.4	3116	2.1	1.3	νC113−H114
		3110	2.1	0.7	3112	0.5	0.5	νC130−H129
		3058	14.1	0.7	3063	10.5	3.8	νC39−H67 ν_{as} CH_3
		3057	19.4	0.3	3057	19.1	0.3	νC42−H78 ν_{as} CH_3
		3056	29.9	1.0	3056	24.1	1.0	νC46−H89 ν_{as} CH_3
3062 w	3063 w	3056	25.7	0.2	3055	5.7	4.7	νC44−H84 ν_{as} CH_3
		3055	13.6	0.3	3055	41.5	4.2	νC37−H62 ν_{as} CH_3
		3054	14.4	7.8	3054	16.4	0.2	νC46−H89 ν_{as} CH_3
		3054	23.2	0.1	3053	23.9	1.8	νC43−H80 ν_{as} CH_3
		3053	11.3	0.1	3053	55.0	21.4	νC41−H75 ν_{as} CH_3
		3052	71.9	1.5	3052	20.8	1.0	νC39−H68 ν_{as} CH_3
		3049	15.7	0.4	3050	17.0	0.5	νC38−H64 ν_{as} CH_3
		3049	68.9	0.4	3050	3.2	4.5	νC38−H65 ν_{as} CH_3
		3049	101.2	0.5	3050	66.5	6.3	νC40−H72 ν_{as} CH_3
		3048	42.1	1.4	3049	70.1	2.6	νC45−H85 ν_{as} CH_3
		3048	14.3	0.1	3048	38.1	0.7	νC47−H92 ν_{as} CH_3
		3047	28.4	0.0	3048	8.6	17.8	νC45−H87 ν_{as} CH_2
		3046	2.7	0.8	3047	14.5	0.5	νC40−H71 ν_{as} CH_3
		3046	40.9	0.1	3047	38.0	6.9	νC39−H69 ν_{as} CH_3
		3045	1.8	1.1	3047	44.2	2.5	νC47−H91 ν_{as} CH_3
		3043	3.3	0.3	3045	2.7	2.4	νC48−H94 ν_{as} CH_3
		3043	2.7	0.8	3044	3.0	0.2	νC37−H61 ν_{s} CH_3
		3042	1.4	1.0	3043	6.3	0.2	νC42−H77 ν_{s} CH_3
		3041	5.1	1.5	3042	3.6	0.3	νC44−H82 ν_{as} CH_3
		3041	0.8	5.0	3041	5.5	1.4	νC43−H81 ν_{as} CH_3
		3041	4.9	1.2	3041	2.0	0.4	νC41−H73 ν_{as} CH_3
		3033	8.5	0.7	3040	2.3	0.5	νC50−H99 ν_{as} CH_2
		3028	13.7	4.0	3030	10.8	0.2	νC49−H97 ν_{as} CH_2
		3024	20.6	1.4	3015	2.4	4.5	νC119−H120 ν_{as} CH_2

		2994	28.3	0.6	2993	25.7	1.0	νC106−H105
		2991	12.5	2.9	2980	33.3	1.0	νC101−H102 ν_s CH_2
		2976	21.4	2.4	2979	19.0	1.3	νC39−H69 ν_s CH_3
	2981 w	2973	30.3	0.4	2978	14.4	2.6	νC46−H88 ν_s CH_3
		2973	42.5	0.7	2974	26.9	4.0	νC42−H76 ν_s CH_3
		2973	12.3	0.6	2974	33.1	16.9	νC45−H85 ν_s CH_3
		2970	18.4	1.1	2972	22.8	8.3	νC38−H65 ν_s CH_3
		2969	20.4	2.5	2971	17.2	19.7	νC124−H123
		2969	15.1	0.2	2968	18.5	6.2	νC46−H90 ν_s CH_3
		2967	21.3	0.1	2968	25.2	0.9	νC47−H91 ν_s CH_3
		2967	18.2	0.3	2967	22.6	0.8	νC37−H63 ν_s CH_3
		2966	24.2	0.6	2967	3.3	0.5	νC41−H74 ν_s CH_3
		2966	31.3	0.4	2966	19.4	0.5	νC44−H82 ν_s CH_3
		2966	15.8	0.3	2966	23.1	0.5	νC43−H79 ν_s CH_3
	2968 m	2966	15.7	1.7	2966	22.2	0.3	νC40−H70 ν_s CH_3
2962 s		2955	21.1	4.7	2965	16.1	0.9	νC50−H100 ν_s CH_2
		2942	34.5	0.4	2953	24.4	0.5	νC49−H98 ν_s CH_2
		2936	35.7	2.8	2953	21.3	1.6	νC101−H102 ν_s CH_2
2906 m	2912 m	2909	20.7	1.0	2917	25.3	1.0	νC119−H121 ν_s CH_2
2870 m		2749	620.2	4.0	2673	556.1	100.0	νO108−H107
2361 vw		2300	686.2	100.0	2345	980.6	19.8	νO126−H125
		1634	22.6	24.4	1636	74.5	5.4	νC106=N104
1637 s	1640 s	1631	53.4	2.4	1634	5.7	5.9	νC124=N122
		1625	273.5	8.1	1627	207.0	27.7	νC128−C130
		1622	105.7	7.3	1624	108.7	13.1	νC106−C110
1591 w	1593 m	1606	44.4	14.0	1609	41.4	1.6	νC133−C135
		1599	4.7	16.8	1607	17.6	5.0	νC115−C117
		1577	4.8	10.5	1575	6.3	7.5	νC6−C7
		1575	2.7	3.3	1574	0.8	5.9	νC19−C24
		1570	9.2	3.6	1571	5.3	13.1	νC3−C8
	1566 w	1565	8.2	4.5	1563	7.5	9.6	νC14−C15
1546 w		1534	7.2	1.6	1534	8.8	17.1	νC5−C6
		1530	5.6	2.1	1533	2.2	39.5	νC30−C32
		1523	9.6	5.1	1526	24.1	15.1	νC13−C17
		1519	15.7	1.0	1520	5.2	27.0	νC3−C12
		1516	187.4	5.7	1518	261.4	9.9	νC113−C115
		1513	278.8	24.6	1512	125.5	19.8	νC131−C133
		1478	21.4	1.8	1478	44.7	4.2	βC37−H62 δ_s CH_3
1467 s	1472 m	1474	13.9	0.2	1475	0.3	2.2	νC135−O136
		1473	48.3	3.3	1474	44.7	0.4	βC40−H71 δ_s CH_3
		1473	29.3	0.3	1473	24.8	0.3	βC43−H79 δ_s CH_3
		1472	24.3	0.5	1473	39.8	0.8	νC110−C112
		1465	117.4	2.2	1469	4.2	27.7	βC46−H88 δ_s CH_3
		1459	3.8	0.2	1469	62.1	10.5	βC38−H64 δ_s CH_3
		1459	9.7	1.5	1461	7.8	1.1	βC44−H82 δ_s CH_3
		1459	8.7	0.2	1459	6.9	0.3	βC41−H73 δ_s CH_3
		1459	6.2	0.1	1459	6.4	0.3	βC45−H85 δ_s CH_3
		1458	62.8	9.7	1459	13.7	0.2	βC40−H70 δ_s CH_3
		1457	10.9	0.3	1457	10.8	13.7	βC43−H79 δ_s CH_3
		1456	15.6	0.3	1456	20.0	0.6	βC38−H65 δ_s CH_3
		1455	10.6	0.3	1456	10.4	0.7	βC48−H94 δ_s CH_3
1451 s	1449 m	1453	30.7	9.2	1455	3.7	8.2	νC30−O1
		1453	21.6	6.9	1451	44.2	1.2	νO2−C18

		1449	74.4	3.3	1447	72.1	52.6	βC49−H97 δ_s CH_2
		1442	7.7	2.2	1444	96.2	56.0	βC50−H99 δ_s CH_2
		1441	8.5	2.9	1444	4.7	12.8	νC109−C110
		1439	3.8	0.6	1443	12.0	42.2	βC39−H67 δ_s CH_3
		1439	9.3	0.2	1442	63.9	4.6	βC38−H66 δ_s CH_3
		1439	60.4	46.6	1440	14.2	48.4	βC47−H93 δ_s CH_3
		1438	5.7	15.7	1439	1.9	2.0	βC43−H80 δ_s CH_3
		1438	45.4	3.3	1438	1.8	6.0	βC37−H63 δ_s CH_3
		1437	1.2	0.5	1438	25.7	32.0	βC39−H69 δ_s CH_3
		1437	0.3	0.5	1437	2.3	0.3	βC41−H75 δ_s CH_3
		1436	0.2	0.3	1436	0.1	0.3	βC43−H81 δ_s CH_3
		1436	0.3	0.1	1436	0.2	0.2	βC46−H90 δ_s CH_3
		1434	43.9	31.6	1433	140.5	62.7	βC37−H62 δ_s CH_3
		1433	0.1	0.3	1432	0.7	4.3	βC41−H75 δ_s CH_3
		1432	0.2	0.9	1432	0.1	0.0	βC44−H84 δ_s CH_3
		1432	0.1	0.8	1432	0.1	0.1	βC48−H95 δ_s CH_3
		1432	0.2	0.0	1431	27.2	3.0	βC119−H120 δ_s CH_2
		1424	129.3	1.9	1422	38.0	7.6	βC49−H98 δ_s CH_2
	1393 w	1420	47.6	0.1	1417	58.2	9.5	νC21−C22
1391 m		1416	71.0	0.3	1405	35.1	0.9	βC101−H102 δ_s CH_2
		1401	100.0	10.6	1404	93.1	5.6	νC112−C113
		1385	109.8	19.0	1399	73.8	25.1	νC12−C128
		1380	2.3	0.1	1381	3.2	3.4	βC39−H68 δ_s CH_3
		1377	3.4	0.6	1378	13.8	0.9	βC47−H91 δ_s CH_3
		1377	6.1	5.4	1377	3.5	1.3	βC44−H82 δ_s CH_3
		1377	4.7	4.7	1377	4.4	4.0	βC42−H78 δ_s CH_3
	1366 w	1376	28.2	0.4	1376	12.2	5.5	νC6−C7
1364 m		1375	12.1	1.3	1375	7.2	4.4	νC19−C24
		1367	19.4	2.5	1370	24.2	9.6	νC49−C101
		1366	7.3	1.2	1370	20.4	0.2	νC50−C119
		1365	14.8	0.7	1368	14.2	6.0	νC8−C9
		1360	47.1	4.8	1364	15.8	2.0	νC14−C15
		1356	61.8	10.2	1359	62.3	2.6	βC49−H97 wag CH_2
		1348	110.9	0.3	1354	37.6	41.9	βC50−H99 wag CH_2
		1347	6.5	6.9	1347	45.2	41.0	βC37−H63 δ_s CH_3
		1345	10.6	0.0	1346	7.6	0.6	βC40−H71 δ_s CH_3
1341 w		1343	3.4	0.2	1344	9.5	4.2	βC46−H90 δ_s CH_3
		1342	10.3	2.1	1343	8.1	0.3	βC42−H77 δ_s CH_3
		1342	9.7	0.4	1342	10.3	0.4	βC41−H74 δ_s CH_3
		1342	29.7	12.2	1342	9.5	1.2	βC43−H79 δ_s CH_3
		1341	11.8	0.1	1342	6.3	8.5	βC38−H66 δ_s CH_3
		1339	37.4	0.1	1340	42.0	29.6	βC47−H92 δ_s CH_3
		1339	14.4	1.7	1339	0.9	1.8	βO2−H52
		1338	13.5	15.6	1339	10.4	3.4	βO1−H51
		1326	78.0	2.8	1327	85.0	3.8	βC119−H121 wag CH_2
		1320	14.5	15.1	1321	60.3	4.4	βC101−H103 wag CH_2
		1312	55.0	35.2	1314	22.9	33.4	νC127−O126
		1305	23.9	20.6	1312	43.0	4.0	νC109−O108
		1305	9.9	6.0	1310	4.4	19.1	ν15−C21
	1287 m	1302	6.0	19.9	1301	3.2	8.2	νC3−C8
		1290	3.8	8.4	1287	5.0	28.0	νO2−C18
		1285	7.7	3.6	1282	8.3	14.6	νO1−C30
1270 s		1283	48.8	9.6	1275	165.6	10.5	βC106−H105
		1276	129.4	0.5	1274	74.9	27.3	νC135−O136
		1273	5.7	6.7	1268	6.1	0.4	βC49−H98 wag CH_2

1245 s		1252	248.7	11.2	1254	185.2	18.1	βC50−H100 wag CH_2
		1249	4.5	0.6	1252	49.5	4.3	βC19−H58
		1245	99.6	5.6	1247	63.2	43.8	βC31−H60
		1243	27.8	3.1	1244	90.0	13.2	νC10−C33
		1241	86.4	9.9	1241	50.6	9.3	νC13−C36
		1237	20.8	2.9	1237	1.7	83.6	νC5−C34
		1236	44.3	0.2	1236	73.9	4.3	νC28−C35
	1224 m	1229	90.3	10.5	1231	23.6	0.9	βC112−H111
	1209 vw	1222	169.3	0.6	1227	110.7	15.3	βO136−H138
		1219	23.2	24.1	1224	30.8	6.5	βC14−H56
		1210	56.1	4.9	1212	73.2	2.6	βO118−H137
		1206	11.4	3.9	1210	76.9	1.4	νC3−O20
		1200	1.8	0.9	1205	10.0	2.5	νC21−O4
		1198	0.9	0.1	1203	26.9	2.0	βC101−H102 ρ CH_2
		1198	1.9	2.4	1202	58.2	7.9	βC50−H100 ρ CH_2
		1194	7.2	2.5	1197	4.2	2.0	βC9−H54
		1193	0.1	1.4	1195	23.0	0.2	βC17−H57
		1191	43.4	0.7	1193	3.2	4.5	νC35−C44
		1189	4.8	0.2	1193	13.7	0.4	νC34−C41
		1189	1.2	0.8	1189	11.8	0.3	νC36−C47
		1189	5.3	0.6	1189	3.8	0.6	νC34−C40
		1188	6.8	0.2	1188	4.3	0.3	νC35−C44
		1186	4.3	0.1	1188	1.8	13.0	νC34−C42
1166 w	1168 vw	1185	3.4	0.6	1187	3.6	6.7	νC15−C21
		1175	197.6	6.5	1186	1.0	1.7	βC14−H56
		1151	43.5	26.8	1153	2.7	1.1	βC112−H111
		1150	4.5	0.3	1152	36.9	9.2	βC130−H129
	1148 sh	1148	11.1	1.6	1150	1.8	2.7	βC26−H59
	1141 w	1142	55.1	0.3	1144	44.1	2.7	βO1−H51
		1124	0.4	1.5	1127	1.5	14.2	νC8−S25
		1118	1.8	2.0	1119	0.2	82.8	νC12−S29
		1118	1.8	0.4	1117	1.9	1.4	C28−C35
		1115	0.5	0.3	1114	0.6	7.5	νC13−C36
1092 m	1099 sh	1093	38.2	4.4	1105	24.9	0.5	νC119−N122
1078 vw		1089	29.6	0.1	1081	15.3	1.7	νC101−N104
		1069	31.0	6.0	1066	44.2	87.4	νC49−C101
	1074 w	1067	47.7	7.9	1064	9.4	4.4	νC50−C119
1068 vw		1060	15.9	0.3	1061	9.1	0.5	νC50−O4
		1059	2.1	0.8	1059	1.1	39.8	νC49−O20
		1057	3.6	3.4	1058	19.0	26.3	νC131−C133
		1056	9.5	5.6	1056	5.2	11.3	νC7−S25
		1052	16.6	3.2	1047	15.9	1.0	νC32−S29
1034 sh	1028 w	1048	23.3	5.2	1045	10.3	0.7	νC15−S16
1016 m		1042	10.6	4.4	1042	49.7	1.6	νC3−O20
		1038	36.8	0.4	1029	11.9	12.1	νC50−O4
		1034	32.7	1.8	1025	30.2	7.1	νC106−C110
		1020	99.9	4.1	1016	0.1	0.3	νC135−O136
		1015	0.1	0.1	1015	0.2	0.5	βC39−H67 ρ CH_3
		1015	0.0	0.4	1014	0.0	0.1	βC47−H92 ρ CH_3
		1014	0.0	0.1	1014	0.0	0.5	βC41−H73 ρ CH_3
		1014	0.1	0.1	1012	0.3	1.7	βC43−H79 ρ CH_3
		1011	3.2	1.6	1011	33.3	8.0	βC38−H64 ρ CH_3
		1010	2.0	0.6	1010	60.2	1.9	βC47−H91 ρ CH_3
974 sh		1009	0.7	1.6	1010	5.1	0.1	βC40−H70 ρ CH_3

		1009	0.8	0.7	1009	0.6	0.3	βC45−H85 ρ CH_3
		1002	151.5	43.0	1001	94.0	7.9	βO126−H125
		956	17.7	0.4	959	4.1	4.6	βO108−H107
		950	4.7	6.2	958	20.6	1.0	γC106−H105
	930 vw	944	45.5	0.0	949	109.9	0.5	γC124−H123
		930	0.1	0.5	939	22.2	0.1	γC112−H111
		929	11.5	0.9	930	0.1	26.9	γC130−H129
		928	0.5	0.4	928	0.2	0.1	βC39−H68 ρ CH_3
925 sh		927	0.0	0.1	927	0.1	0.3	βC47−H92 ρ CH_3
		927	0.1	0.0	927	0.4	0.2	βC40−H72 ρ CH_3
		927	2.0	0.1	927	11.4	0.9	βC44−H84 ρ CH_3
		919	0.8	0.1	921	84.3	0.6	βC50−H99 ρ CH_2
		918	0.9	0.2	920	2.0	11.5	βC39−H68 ρ CH_3
		917	2.0	0.7	918	17.5	0.3	βC48−H94 ρ CH_3
		917	1.9	0.3	917	2.1	0.4	νC34−C40
		914	19.4	0.9	917	2.2	3.2	νC35−C43
		908	2.2	0.3	909	20.2	0.9	βC49−H97 ρ CH_2
	904 w	907	1.3	0.6	908	18.4	20.6	νC36−C48
		906	1.5	0.1	907	0.6	7.9	νC33−C39
		906	1.9	0.3	906	1.7	1.1	νC35−C44
		903	25.3	18.4	906	1.4	0.7	νC34−C41
		893	30.0	2.1	889	0.0	0.4	νC10−C33
		889	3.1	0.2	888	2.4	0.2	γC6−H53
886 w		889	11.0	0.6	887	3.1	4.9	γC31−H60
		888	0.5	0.3	886	4.8	10.3	νC50−C119
		886	0.7	0.4	885	17.0	51.6	νC24−S23
874 w		884	0.8	7.8	883	2.8	3.8	νC5−C34
		883	5.7	0.6	882	3.8	1.7	γC11−H55
		872	0.1	0.3	870	10.6	3.8	γC14−H56
		869	11.4	0.4	866	9.9	0.3	γC26−H59
		866	10.1	0.0	864	7.1	0.6	γC19−H58
		864	17.5	0.5	863	0.4	2.7	γC115−H116
	857 vw	863	5.4	0.1	858	1.7	0.6	γC133−H134
850 vw		863	19.9	0.6	857	0.1	4.2	γC9−H54
	829 m	858	2.1	1.7	853	43.6	31.4	γC130−H129
823 vw		857	11.9	0.1	847	24.0	0.9	νC13−C36
		857	3.8	0.0	845	4.1	4.5	νC49−O20
		842	9.2	8.6	842	1.9	2.2	νC127−O126
808 sh	813 w	841	32.4	1.1	840	13.5	3.5	νC109−O108
		814	12.9	0.2	814	14.0	11.8	νC30−O1
		813	16.4	0.2	813	18.8	5.3	νC18−O2
		798	2.6	3.6	798	10.0	10.6	νC21−O4
781 w		797	11.8	1.8	788	7.2	0.8	βO2−H52
		774	3.6	24.2	773	4.5	46.4	βO1−H51
	770 vw	773	7.0	2.2	771	6.3	2.8	νC7−S25
		767	15.9	5.6	766	4.9	0.3	νC8−S25
		765	13.7	2.1	765	6.7	0.2	νC24−S23
763 sh		764	7.3	0.4	762	12.0	10.1	νC32−S29
		763	0.2	1.2	760	9.0	1.4	νC12−S29
		757	2.1	5.6	757	8.5	0.6	νC22−S23
		749	7.2	6.4	751	8.9	14.4	β_R
		737	16.5	0.1	735	16.4	3.0	β_R
735 m		736	12.0	0.1	735	18.4	5.9	βO2−H52
	731 w	724	62.5	2.0	729	45.9	0.7	νC7−C18

		722	27.9	12.9	723	17.0	4.0	νC30−C32
		721	17.4	1.9	720	13.8	0.2	γC115−H116
		715	40.0	0.2	718	65.6	1.4	γC113−H114
		713	23.6	0.2	711	9.9	1.2	γC109−O108
		709	17.7	3.2	709	20.6	2.2	νC106−C110
		700	46.3	3.7	693	10.9	0.5	νC5−C34
		692	7.2	1.0	691	4.0	5.5	νC28−C35
		691	1.2	1.1	685	39.1	2.1	νC13−C36
641 vw		651	88.7	1.2	652	98.4	1.1	νC33−C37
		634	2.1	0.2	635	1.7	10.6	νC19−C28
		632	0.5	0.5	633	0.7	0.3	νC10−C11
	624 vw	629	2.3	0.1	630	3.8	0.3	νC10−C33
		626	1.2	0.2	625	0.1	3.6	νC9−C10
		620	5.5	0.4	623	3.9	0.3	νC124−C128
		618	3.0	18.0	617	7.2	3.3	νC106−C110
585 sh		596	3.8	0.4	598	4.0	4.2	γC8−S25
		584	15.8	1.1	581	7.0	1.0	γC30−O1
576 w		581	7.6	1.9	577	10.7	0.3	γC117−O118
		576	7.0	0.3	575	3.1	2.1	γC110−C106
		571	60.6	0.2	572	19.8	0.5	β_R
		568	14.1	1.6	569	3.5	1.2	β_R
		565	1.2	0.3	565	7.1	0.8	β_R
545 w		559	32.4	0.6	560	68.0	0.5	β_R
		556	17.5	2.0	557	5.1	8.1	β_R
		553	2.8	1.8	553	9.1	0.2	β_R
535 sh		552	7.4	2.0	549	16.2	4.9	β_R
	529 w	543	23.2	3.6	540	48.6	1.6	β_R
		540	27.0	2.1	534	4.8	1.9	β_R
		537	3.5	1.7	532	21.9	13.0	γC22−S23
		533	6.8	2.3	525	0.3	6.7	γC24−S23
		526	1.0	7.9	519	21.3	0.1	γC124−C128
	493 vw	521	0.2	0.4	513	50.1	9.6	γO118−H137
		507	0.6	1.7	508	1.1	2.2	νC34−C41
		505	0.4	0.4	507	0.2	2.6	νC34−C42
		500	1.3	2.7	505	0.5	0.8	β_R
		488	1.8	0.5	501	8.8	1.7	β_R
	472 vw	487	0.4	3.2	491	0.9	1.0	β_R
		485	5.6	3.1	482	6.0	4.0	β_R
		480	0.9	14.2	480	1.1	1.6	β_R
		475	1.2	1.0	475	0.2	13.4	β_R
	447 vw	473	2.0	3.5	474	2.9	1.0	β_R
		471	1.4	0.4	472	0.2	0.4	β_R
		465	1.2	0.5	466	1.8	23.5	β_R
		461	2.6	8.1	464	0.9	0.8	νC36−C47
	409 vw	451	0.4	1.2	456	2.3	10.2	β_R
		438	1.1	20.4	436	0.7	1.6	β_R
	393 sh	434	0.4	5.3	434	0.1	0.6	γC18−O2
		433	0.1	0.1	419	1.2	3.5	β_R
		415	1.0	14.0	413	0.8	4.9	β_R
		405	1.5	3.5	404	1.7	4.2	γC15−S16
		394	1.6	8.3	394	1.7	0.4	γC27−S16
		389	0.0	19.0	388	0.1	1.6	γC12−S29
		384	2.8	0.5	387	1.1	37.2	β_R
		384	1.4	3.1	384	4.1	5.2	γC7−S25
		381	3.1	10.3	382	1.5	2.1	β_R

	378	0.8	2.4	375	0.7	4.8	β_R
	376	2.0	2.5	373	0.6	4.4	β_R
	373	0.6	0.1	368	0.4	21.7	β_R
	361	0.4	6.4	360	0.5	15.2	β_R
	359	1.5	9.9	358	0.3	22.7	β_R
	354	0.2	0.2	355	0.1	0.7	β_R
	352	2.0	17.6	350	1.5	4.6	β_R
	349	0.5	0.2	347	6.2	37.9	β_R
	343	9.8	9.6	345	2.4	16.7	γC127−O126
	341	1.3	15.1	344	3.7	9.1	γC109−O108
	328	6.2	2.8	329	1.3	17.8	β_R
	326	1.8	8.9	327	1.1	5.1	β_R
	323	1.3	0.5	325	2.2	1.0	β_R
	320	1.6	0.3	322	0.4	25.1	γC30−O1
	317	2.6	1.1	321	0.3	3.0	βC35−C45
	317	3.4	0.7	317	0.2	0.5	τC33−C38
	315	0.3	0.0	312	3.5	13.0	τC33−C37
	312	0.1	0.2	312	0.7	0.3	τC35−C45
	311	0.5	1.7	311	2.0	0.6	τC36−C47
	311	0.1	1.3	310	0.1	1.3	τC34−C40
	308	1.8	5.0	302	3.1	0.3	β_R
	304	0.2	2.9	299	6.5	8.8	τC35−C43
	303	0.8	0.1	295	1.3	0.4	γC21−O4
	297	2.9	1.3	294	0.2	7.9	γC3−O20
288 vw	288	2.5	3.7	290	0.3	0.8	β_R
	286	1.4	0.9	286	0.2	2.7	τC124−C128
	286	0.4	0.9	283	0.0	0.4	τC106−C110
	283	0.3	0.8	282	0.5	2.4	τC10−C33
	279	0.1	1.5	280	1.2	4.0	γC117−O118
	276	0.8	0.6	277	3.2	5.7	τC49−C101
	275	0.8	4.6	270	0.2	9.1	τC5−C34
	267	0.5	0.3	268	0.6	12.9	τC22−S23
	265	0.3	10.8	265	2.8	0.1	τC12−S29
	261	0.8	5.4	264	1.3	7.1	τC33−C37
	258	0.3	0.3	260	1.4	0.9	τC34−C41
	256	0.0	0.0	258	0.1	9.1	τC35−C44
	254	0.1	2.7	257	0.1	2.6	τC35−C43
245 vw	247	0.7	8.5	254	0.5	6.7	τC36−C48
	242	2.0	15.7	241	3.7	0.5	τC36−C46
227 w	234	1.3	2.8	236	0.2	0.9	τC28−C35
	231	0.6	0.2	233	0.1	5.8	β_R
	228	0.2	3.0	228	0.3	0.9	τC33−C39
	225	0.0	0.3	226	0.5	3.0	τC34−C42
	223	0.1	1.8	225	0.1	3.0	τC36−C48
	223	0.4	0.0	223	0.9	17.6	τC34−C42
	216	0.2	4.0	222	3.4	8.7	τC106−C110
	212	0.1	2.2	217	1.2	1.4	γC106−N104
	202	2.0	1.1	215	1.0	0.8	γC124−N122
	196	3.4	16.7	209	0.3	0.5	γC27−S16
	191	0.5	0.2	201	0.3	2.1	γC15−S16
187 w	186	0.8	0.6	192	0.1	1.2	τC10−C33
	183	2.6	0.4	180	1.1	4.5	νC22−S23
	172	4.2	1.6	174	1.8	0.6	β_R
	171	3.3	0.7	172	0.3	3.9	τC30−C32
	167	0.5	1.5	169	3.5	0.4	τC109−C110
	155	1.9	8.8	167	1.3	1.0	τC15−S16

149	1.1	16.2	158	0.3	2.5	τC32−S29
145	0.3	7.5	154	0.4	2.7	τC8−S25
140	2.0	0.9	140	1.4	4.2	τC27−S16
139	0.3	10.7	138	2.9	25.0	τC21−O4
125	5.2	30.9	127	1.4	0.9	τC119−N122
121	2.4	42.2	120	2.5	7.5	τC3−O20
120	0.6	0.3	118	1.7	2.6	τC18−O2
114	0.4	9.1	115	1.0	25.5	τC33−C38
107	0.5	3.1	108	1.7	5.1	τC28−C35
104	0.6	0.4	104	1.0	6.3	τC24−S23

Abbreviations: ν: stretching; δ: deformation in plane; ρ: deformation out of plane; χ: torsion; as: antisymmetric; s: symmetric.

8. DFT-optimiezed coordinates of atoms for ligands 3-6.

Table S7. For **3** *exo-exo* rotamer, the optimized geometry in Cartesian coordinates, obtained by DFT- calculations.

Center Number	Atomic number	Coordinates (Angstroms)		
		X	Y	Z
1	6	3,44091	8,72556	4,84784
2	6	2,93869	8,37322	6,10771
3	6	3,53403	8,83414	7,29485
4	6	4,61187	9,71577	7,19417
5	1	5,07697	10,06456	8,12159
6	6	5,11822	10,14025	5,95593
7	6	4,52002	9,62047	4,80343
8	1	4,91327	9,88608	3,81977
9	6	6,3119	11,10946	5,90864
10	6	5,94761	12,41428	6,65339
11	1	6,80289	13,11098	6,63964
12	1	5,68488	12,22241	7,7054
13	1	5,08882	12,91141	6,17404
14	6	7,53002	10,44759	6,59497
15	1	8,39492	11,13237	6,57635
16	1	7,81051	9,51755	6,07493
17	1	7,31698	10,19618	7,64562
18	6	6,71281	11,47487	4,46771
19	1	7,56312	12,17581	4,49124
20	1	5,88641	11,96594	3,92836
21	1	7,02611	10,5868	3,89511
22	6	0,5609	8,02351	6,14133
23	1	0,45058	8,58754	5,19796
24	1	0,3795	8,71591	6,98492
25	6	-0,41857	6,84923	6,17917
26	1	-0,19687	6,16014	5,34109
27	1	-0,2625	6,30087	7,12702
28	6	-2,58503	6,88691	5,23218
29	1	-2,24645	6,13746	4,48997
30	6	-3,96161	7,32779	5,1428
31	6	-4,81393	6,81081	4,1472
32	1	-4,40876	6,06933	3,4502
33	6	-6,13531	7,22319	4,04873
34	1	-6,78768	6,81612	3,27357
35	6	-6,6239	8,17297	4,96232
36	1	-7,66379	8,50468	4,89302
37	6	-5,80987	8,70082	5,957
38	1	-6,18504	9,43853	6,67033
39	6	-4,46778	8,29159	6,0687
40	6	3,08064	8,32382	8,65714
41	1	3,11298	9,15779	9,37669
42	1	2,03124	7,98959	8,60267
43	6	3,9603	7,20234	9,19222
44	6	3,89059	5,89618	8,66547
45	6	4,77958	4,90451	9,14343
46	6	5,66295	5,22005	10,17452

47	1	6,32116	4,4256	10,54289
48	6	5,73768	6,50184	10,74426
49	6	4,87974	7,47185	10,21653
50	1	4,90082	8,48964	10,6152
51	6	6,73097	6,78568	11,88325
52	6	6,65785	8,24364	12,37208
53	1	5,6573	8,49101	12,76268
54	1	6,90425	8,95483	11,56673
55	1	7,38407	8,39541	13,18737
56	6	6,42169	5,86027	13,08276
57	1	5,40429	6,04452	13,46394
58	1	7,13806	6,04194	13,90233
59	1	6,49064	4,7976	12,80189
60	6	8,17237	6,51705	11,39026
61	1	8,89724	6,71027	12,19961
62	1	8,41979	7,17142	10,53873
63	1	8,30046	5,4727	11,06449
64	6	4,79591	3,5333	8,48696
65	1	5,21791	2,80408	9,19883
66	1	3,76657	3,23082	8,24984
67	6	5,63372	3,52525	7,21203
68	6	5,06405	3,40994	5,93665
69	6	5,83442	3,54333	4,76886
70	6	7,21145	3,72998	4,90544
71	1	7,80509	3,84454	3,99303
72	6	7,83737	3,80113	6,15938
73	6	7,02205	3,70707	7,29198
74	1	7,46074	3,80796	8,28689
75	6	9,35812	4,01596	6,24486
76	6	9,71902	5,36221	5,57382
77	1	9,21765	6,19851	6,08683
78	1	9,41508	5,38417	4,5157
79	1	10,80876	5,52824	5,61919
80	6	10,08316	2,86441	5,51096
81	1	9,7907	2,80983	4,45071
82	1	9,84948	1,89426	5,97879
83	1	11,17516	3,01503	5,5537
84	6	9,8636	4,0528	7,69867
85	1	9,41243	4,8828	8,26636
86	1	10,95598	4,19959	7,70209
87	1	9,64974	3,10926	8,22708
88	6	3,20476	1,90162	5,79504
89	1	3,69985	1,33738	6,60607
90	1	3,44467	1,40999	4,83244
91	6	1,69997	1,89531	6,04982
92	1	1,39645	0,84655	6,25363
93	1	1,51429	2,49224	6,96091
94	6	-0,00201	1,76242	4,41765
95	1	-0,199	0,72147	4,74821
96	6	-0,86028	2,28253	3,37236
97	6	-1,84794	1,46612	2,787
98	1	-1,93494	0,42875	3,12666
99	6	-2,69671	1,95536	1,80402

100	1	-3,45637	1,31155	1,35647
101	6	-2,56463	3,29188	1,39178
102	1	-3,22489	3,68658	0,61451
103	6	-1,60309	4,12513	1,9519
104	1	-1,48827	5,16245	1,62796
105	6	-0,73452	3,63932	2,94668
106	6	5,1887	3,57913	3,38943
107	1	5,82881	3,02714	2,68226
108	1	4,21639	3,05929	3,41239
109	6	5,00695	4,99434	2,86079
110	6	4,01783	5,85159	3,39216
111	6	3,91354	7,17487	2,91408
112	6	4,76177	7,60293	1,8885
113	1	4,63938	8,62657	1,52431
114	6	5,74093	6,77389	1,32553
115	6	5,83945	5,4752	1,84603
116	1	6,59087	4,78812	1,44169
117	6	6,68018	7,22747	0,19528
118	6	6,47359	6,32587	-1,04389
119	1	5,43714	6,40044	-1,41063
120	1	6,67478	5,26816	-0,81199
121	1	7,1533	6,63035	-1,85832
122	6	8,14873	7,11675	0,66768
123	1	8,3233	7,75599	1,5482
124	1	8,83533	7,4353	-0,13542
125	1	8,40815	6,08252	0,94348
126	6	6,42354	8,68591	-0,22586
127	1	6,58707	9,38505	0,61066
128	1	5,3969	8,82533	-0,60192
129	1	7,1184	8,96288	-1,03558
130	6	2,909	8,11963	3,5533
131	1	1,97949	7,56983	3,7562
132	1	2,68485	8,93247	2,8423
133	7	-1,78475	7,34026	6,14012
134	7	0,92967	2,47134	4,96095
135	8	1,8846	7,45972	6,21785
136	8	-3,69734	8,80724	7,03055
137	1	-2,77721	8,36091	6,91626
138	8	2,99999	5,50072	7,72217
139	1	2,543	6,2564	7,27096
140	8	3,67646	3,25987	5,80454
141	8	0,18029	4,45973	3,47621
142	1	0,71028	3,90467	4,15336
143	8	3,12782	5,48391	4,34516
144	1	3,32077	4,60148	4,74908

Table S8. For **3** *endo-exo* rotamer, the optimized geometry in Cartesian coordinates, obtained by DFT- calculations.

Center Number	Atomic number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-0,04947	-1,72933	-0,89585
2	8	-0,27331	1,67654	-0,59336
3	6	0,31603	-0,26092	2,10697
4	8	0,2037	0,32594	-3,90174
5	6	2,12761	4,9714	0,37975
6	6	1,52442	4,21352	1,3877
7	6	0,73355	3,08693	1,11436
8	6	0,80157	0,97146	2,56176
9	6	1,98739	0,96471	3,31025
10	6	2,68274	-0,21398	3,60237
11	6	2,16455	-1,41621	3,09525
12	6	0,99002	-1,47126	2,34037
13	6	4,06613	0,44869	-2,24047
14	6	3,27779	1,59815	-2,32238
15	6	1,94791	1,5706	-2,76371
16	6	1,13991	2,86426	-2,68796
17	6	3,43892	-0,76675	-2,54238
18	6	0,53241	2,70931	-0,22446
19	6	2,19099	-4,26419	0,56688
20	8	-0,85319	-0,28078	1,31052
21	6	1,39094	0,34814	-3,18187
22	6	2,11762	-0,84603	-2,98837
23	6	0,504	-2,80669	1,7808
24	6	1,21949	-3,25293	0,51214
25	6	0,10589	2,29534	2,25393
26	6	1,94093	4,53098	-0,94318
27	6	1,17665	3,41127	-1,26911
28	6	2,88265	-4,70488	-0,56525
29	6	1,49362	-2,22969	-3,16669
30	6	0,92552	-2,6646	-0,72974
31	6	2,5934	-4,05501	-1,77896
32	6	1,65029	-3,0336	-1,88566
33	6	3,96236	-0,23332	4,45631
34	6	2,97615	6,22226	0,66324
35	6	3,93066	-5,82961	-0,52401
36	6	5,5351	0,46866	-1,78784
37	6	5,11428	-0,88065	3,65391
38	6	3,69982	-1,06142	5,73613
39	6	4,40563	1,17956	4,87722
40	6	4,41187	6,00614	0,13027
41	6	2,34625	7,44284	-0,04708
42	6	3,06719	6,53747	2,16734
43	6	5,29779	-5,28074	-0,99519
44	6	4,11046	-6,40859	0,89104
45	6	3,49041	-6,97766	-1,46165
46	6	6,04502	1,89715	-1,52361
47	6	5,67868	-0,3463	-0,48155

48	6	6,42005	-0,16425	-2,88627
49	7	-4,46872	-0,78917	1,79743
50	7	-3,41936	-0,13513	-3,69265
51	6	-5,50074	-0,05413	1,54444
52	6	-4,3911	0,64855	-4,01714
53	6	-6,75519	-0,23811	2,24324
54	6	-5,69759	0,52909	-3,39895
55	6	-7,86368	0,58035	1,94623
56	6	-9,07209	0,41943	2,6084
57	6	-9,18559	-0,58031	3,59007
58	6	-8,11309	-1,4054	3,90459
59	6	-6,88119	-1,25294	3,24151
60	6	-5,91856	-0,45256	-2,38347
61	6	-7,19278	-0,54506	-1,79312
62	6	-8,21599	0,30635	-2,19463
63	6	-8,00774	1,27496	-3,19083
64	6	-6,75513	1,37663	-3,78101
65	8	-5,85958	-2,05474	3,55742
66	8	-4,94009	-1,27182	-1,98288
67	6	-2,08809	-0,45471	2,06049
68	6	-3,23909	-0,56845	1,0613
69	6	-1,05602	0,19403	-3,21976
70	6	-2,11558	0,02519	-4,31017
71	1	-0,36241	-1,35756	-0,03816
72	1	-0,52767	1,11076	0,17144
73	1	1,6499	4,50129	2,43492
74	1	2,36659	1,92545	3,66558
75	1	2,69191	-2,35616	3,28399
76	1	3,68421	2,56307	-2,01086
77	1	1,57051	3,62011	-3,36728
78	1	0,10984	2,67834	-3,02399
79	1	3,98239	-1,70605	-2,40134
80	1	2,38934	-4,72289	1,5392
81	1	0,66433	-3,57762	2,55164
82	1	-0,58409	-2,77059	1,60183
83	1	0,1418	2,91847	3,16217
84	1	-0,96248	2,12034	2,04135
85	1	2,42449	5,06943	-1,76532
86	1	1,99693	-2,76939	-3,98733
87	1	0,4367	-2,12423	-3,45039
88	1	3,13602	-4,33901	-2,68705
89	1	4,60954	-1,09441	6,35895
90	1	3,41491	-2,09784	5,49649
91	1	2,88818	-0,61434	6,33259
92	1	6,03022	-0,90808	4,26767
93	1	5,3272	-0,30587	2,73886
94	1	4,87713	-1,91358	3,35575
95	1	5,32781	1,10903	5,47635
96	1	4,62086	1,81536	4,00313
97	1	3,64338	1,67954	5,4968
98	1	5,02945	6,90039	0,32113
99	1	4,41819	5,81722	-0,95455
100	1	4,8867	5,14462	0,6272

101	1	2,95242	8,34678	0,13463
102	1	1,32655	7,62781	0,32755
103	1	2,28411	7,28924	-1,13575
104	1	3,67985	7,44147	2,31706
105	1	2,07308	6,72992	2,60293
106	1	3,54179	5,71494	2,72722
107	1	6,05828	-6,08	-0,97588
108	1	5,63717	-4,46361	-0,33793
109	1	5,24561	-4,89037	-2,0236
110	1	4,86523	-7,21151	0,86653
111	1	3,17227	-6,84153	1,2749
112	1	4,45992	-5,64233	1,6024
113	1	4,24063	-7,78678	-1,45498
114	1	2,52468	-7,39713	-1,1366
115	1	3,37568	-6,62998	-2,50021
116	1	7,1041	1,85902	-1,21957
117	1	5,4798	2,38845	-0,71497
118	1	5,97542	2,52468	-2,42714
119	1	6,72932	-0,34464	-0,14333
120	1	5,3654	-1,39306	-0,61919
121	1	5,05307	0,08927	0,31415
122	1	7,477	-0,1698	-2,56915
123	1	6,12255	-1,2036	-3,09555
124	1	6,343	0,40659	-3,8258
125	1	-5,46733	0,74202	0,77544
126	1	-4,26227	1,4429	-4,77967
127	1	-7,75152	1,34692	1,17264
128	1	-9,9241	1,0598	2,37141
129	1	-10,13409	-0,71506	4,11755
130	1	-8,19605	-2,18489	4,66564
131	1	-7,35208	-1,2995	-1,01897
132	1	-9,19898	0,21416	-1,72411
133	1	-8,82069	1,93609	-3,49791
134	1	-6,56906	2,12311	-4,56043
135	1	-5,0846	-1,76606	2,95119
136	1	-4,12325	-1,02929	-2,57078
137	1	-2,01863	-1,3673	2,67663
138	1	-2,23268	0,40927	2,73226
139	1	-3,28389	0,33916	0,42571
140	1	-3,05783	-1,43147	0,39494
141	1	-1,2729	1,08551	-2,60863
142	1	-1,05123	-0,68106	-2,55207
143	1	-2,08804	0,88926	-5,00473
144	1	-1,88003	-0,88464	-4,89163

Table S9. For **4** *exo-exo* rotamer, the optimized geometry in Cartesian coordinates, obtained by DFT- calculations.

Center Number	Atomic number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1,11379	0,2754	0,54935
2	8	1,45367	-2,19743	0,24407
3	6	1,52631	0,13578	2,73524
4	8	-1,07485	-1,7449	-2,20659
5	6	5,47829	-2,77084	-0,84766
6	6	4,41896	-2,89271	-1,7641
7	6	3,08719	-2,67701	-1,40968
8	6	2,89952	-0,15419	2,61475
9	6	3,8259	0,88983	2,60065
10	6	3,43225	2,23514	2,69807
11	6	2,06432	2,49775	2,83747
12	6	1,11157	1,47022	2,85959
13	6	1,84826	1,16131	-3,1281
14	6	2,17642	-0,19648	-3,1037
15	6	1,23199	-1,18455	-2,79175
16	16	3,45845	-1,87576	2,5799
17	6	0,51964	1,50037	-2,83582
18	6	2,74767	-2,34124	-0,07406
19	6	-2,12636	3,48568	-0,86131
20	8	0,5925	-0,88864	2,64005
21	6	-0,11058	-0,83898	-2,53981
22	6	-0,44396	0,53481	-2,5429
23	16	-2,13083	1,04907	-2,16315
24	6	-1,82019	2,12766	-0,76507
25	16	1,8021	-2,8942	-2,64451
26	6	5,14082	-2,39375	0,45504
27	6	3,80943	-2,17997	0,84202
28	6	-1,97372	4,38	0,21363
29	16	-0,63712	1,84765	3,12803
30	6	-1,34915	1,59344	0,46097
31	6	-1,46452	3,85349	1,40406
32	6	-1,1514	2,49227	1,53005
33	6	4,49594	3,34593	2,69086
34	6	6,92486	-3,02508	-1,30173
35	6	-2,346	5,86167	0,04142
36	6	2,86793	2,26276	-3,46116
37	6	5,42364	3,16326	3,91476
38	6	5,33068	3,25042	1,39316
39	6	3,86929	4,75019	2,75921
40	6	7,93437	-2,83053	-0,15625
41	6	7,28825	-2,04288	-2,43953
42	6	7,05108	-4,47696	-1,81813
43	6	-3,8473	5,9726	-0,31187
44	6	-1,50416	6,47708	-1,1004
45	6	-2,08938	6,67633	1,32185
46	6	4,27206	1,69323	-3,73297
47	6	2,40164	3,0293	-4,72026
48	6	2,96465	3,24354	-2,26952

49	6	0,28471	-1,53909	3,90502
50	6	-1,43519	-2,73768	-3,18241
51	1	-0,80477	0,05898	1,4632
52	1	1,3571	-1,91735	1,18812
53	1	4,61837	-3,15828	-2,80583
54	1	4,88322	0,62697	2,51731
55	1	1,7016	3,52148	2,9405
56	1	3,19759	-0,52319	-3,30487
57	1	0,20416	2,54671	-2,83353
58	1	-2,50014	3,84098	-1,82545
59	1	5,91108	-2,26671	1,21762
60	1	-1,30658	4,48999	2,27632
61	1	4,66931	5,50735	2,73236
62	1	3,19978	4,9376	1,90399
63	1	3,30065	4,89999	3,69134
64	1	6,10561	4,03496	1,38783
65	1	4,69312	3,38858	0,50558
66	1	5,83643	2,27669	1,30126
67	1	6,19982	3,94665	3,91933
68	1	4,85263	3,23705	4,85426
69	1	5,92982	2,18529	3,89935
70	1	8,95296	-3,02752	-0,52803
71	1	7,91421	-1,79959	0,2335
72	1	7,7422	-3,52444	0,67833
73	1	8,32178	-2,22185	-2,78117
74	1	6,62117	-2,16181	-3,30758
75	1	7,21369	-0,99913	-2,09366
76	1	6,37025	-4,66792	-2,66236
77	1	8,08098	-4,6704	-2,16287
78	1	6,81182	-5,19746	-1,01951
79	1	-4,12792	7,03002	-0,45422
80	1	-4,08657	5,43009	-1,23971
81	1	-4,46957	5,554	0,49528
82	1	-1,76912	7,53902	-1,2386
83	1	-1,67759	5,9598	-2,05691
84	1	-0,42827	6,41584	-0,86934
85	1	-2,37328	7,72741	1,15071
86	1	-1,02513	6,65934	1,60907
87	1	-2,68678	6,30161	2,16892
88	1	4,9644	2,51983	-3,96185
89	1	4,27189	1,0077	-4,59601
90	1	4,66823	1,15259	-2,85789
91	1	3,11669	3,83385	-4,96254
92	1	1,41156	3,48781	-4,57189
93	1	2,33541	2,35197	-5,58685
94	1	3,69292	4,04171	-2,49318
95	1	1,99491	3,71817	-2,05286
96	1	3,29275	2,7144	-1,3602
97	1	-0,3314	-0,85595	4,51535
98	1	1,23186	-1,75594	4,42773
99	1	-1,59993	-2,26225	-4,16686
100	1	-0,64338	-3,50298	-3,27242
101	6	-0,43903	-2,85504	3,64741

102	1	-0,35349	-3,45923	4,57589
103	1	0,10561	-3,39462	2,85103
104	7	-1,82565	-2,6891	3,25021
105	1	-2,45844	-3,90109	4,83338
106	6	-2,73157	-3,29125	3,94715
107	1	-2,78978	-2,01159	2,07358
108	8	-3,71874	-1,86338	1,67502
109	6	-4,58147	-2,51511	2,46627
110	6	-4,1387	-3,23175	3,61821
111	1	-4,72825	-4,44834	5,29985
112	6	-5,08479	-3,90112	4,42087
113	6	-6,43605	-3,87463	4,11039
114	1	-7,1605	-4,3962	4,73907
115	6	-6,85992	-3,17042	2,9704
116	1	-7,92224	-3,14686	2,71239
117	6	-5,95362	-2,50138	2,15689
118	1	-6,28355	-1,95807	1,26816
119	6	-2,72014	-3,40453	-2,69384
120	1	-2,56771	-3,70083	-1,63726
121	1	-2,872	-4,3193	-3,29196
122	7	-3,87952	-2,54169	-2,85602
123	1	-3,75162	-1,84337	-0,87879
124	1	-4,96963	-2,14253	-3,95553
125	6	-4,25638	-1,80689	-1,86066
126	8	-5,80626	-1,61207	-4,2547
127	6	-6,13256	-0,85392	-3,2043
128	6	-5,38713	-0,90673	-1,98693
129	1	-5,15016	-0,11362	-0,00119
130	6	-5,7546	-0,0727	-0,91321
131	6	-6,84045	0,78815	-1,01196
132	1	-7,11404	1,43382	-0,17468
133	6	-7,5789	0,82187	-2,20703
134	1	-8,43699	1,49467	-2,29484
135	6	-7,23553	0,01776	-3,28757
136	1	-7,8017	0,0447	-4,22191

Table S10. For **4** *endo-exo* rotamer, the optimized geometry in Cartesian coordinates, obtained by DFT- calculations.

Center Number	Atomic number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1,35312	-1,42661	-0,35518
2	8	1,46614	0,63233	-1,31772
3	6	-1,72311	1,41913	-2,22873
4	8	2,06189	-2,03665	1,43899
5	6	3,41032	4,32103	-0,76354
6	6	2,3739	4,19347	-1,69267
7	6	1,69728	2,97863	-1,8767
8	6	-1,09039	2,67469	-2,31178
9	6	-1,71801	3,80057	-1,77512
10	6	-2,96577	3,72381	-1,13501
11	6	-3,57946	2,46609	-1,06963
12	6	-2,98046	1,31967	-1,609
13	6	0,08987	1,3606	2,97447
14	6	1,32899	1,47322	2,33712
15	6	1,96397	0,36126	1,76795
16	16	3,5195	0,56517	0,87552
17	6	-0,50908	0,09346	3,00136
18	6	2,04643	1,83128	-1,13605
19	6	-3,47817	-2,05155	2,54827
20	8	-1,07489	0,27629	-2,67976
21	6	1,38574	-0,91595	1,85243
22	6	0,10575	-1,02058	2,42838
23	16	-0,77039	-2,59829	2,35257
24	6	-2,34315	-1,97951	1,73985
25	16	0,48202	2,84251	-3,1967
26	6	3,71456	3,18517	0,00843
27	6	3,05467	1,96579	-0,14816
28	6	-4,73578	-1,57335	2,13853
29	16	-3,87495	-0,25563	-1,63192
30	6	-2,43817	-1,42975	0,43665
31	6	-4,80277	-0,97451	0,87683
32	6	-3,68073	-0,89371	0,04001
33	6	-3,63641	5,00324	-0,60549
34	6	4,18537	5,63068	-0,54496
35	6	-5,94903	-1,6956	3,07499
36	6	-0,61708	2,55232	3,64165
37	6	-4,01922	5,89178	-1,81294
38	6	-2,6594	5,77732	0,30846
39	6	-4,91057	4,69703	0,20272
40	6	5,68682	5,38706	-0,82244
41	6	4,00318	6,10027	0,91714
42	6	3,69794	6,7545	-1,47689
43	6	-6,20273	-3,18821	3,38878
44	6	-7,22664	-1,11048	2,44692
45	6	-5,66432	-0,93561	4,39132
46	6	-2,04354	2,69679	3,06233
47	6	0,13368	3,87658	3,41157
48	6	-0,7064	2,29804	5,16428

49	6	-1,26596	-0,00706	-4,09572
50	6	1,88211	-2,4156	0,05281
51	1	-1,58481	-1,02526	-1,23026
52	1	0,76693	0,69975	-2,01473
53	1	2,06933	5,03896	-2,3117
54	1	-1,20677	4,76059	-1,87805
55	1	-4,55952	2,34899	-0,60492
56	1	1,82742	2,44013	2,25881
57	1	-1,49146	-0,04185	3,45904
58	1	-3,35272	-2,49232	3,54102
59	1	4,48896	3,23374	0,77873
60	1	-5,74072	-0,56121	0,50246
61	1	-3,13347	6,16704	-2,40713
62	1	-4,49723	6,82151	-1,46156
63	1	-4,72608	5,36853	-2,47682
64	1	-3,14499	6,69652	0,67581
65	1	-2,36677	5,16978	1,17884
66	1	-1,74324	6,07562	-0,22415
67	1	-5,33254	5,63928	0,58761
68	1	-4,69616	4,04489	1,06502
69	1	-5,68535	4,21774	-0,41725
70	1	5,84403	5,06503	-1,86435
71	1	6,10076	4,60979	-0,16138
72	1	6,25978	6,31482	-0,65552
73	1	2,93958	6,28559	1,13871
74	1	4,5612	7,03636	1,08789
75	1	4,37464	5,35136	1,63389
76	1	4,28619	7,66723	-1,28892
77	1	2,63727	6,9984	-1,30137
78	1	3,82515	6,48651	-2,53845
79	1	-6,42105	-3,7489	2,46583
80	1	-7,06337	-3,29272	4,07091
81	1	-5,32981	-3,65534	3,87097
82	1	-7,11931	-0,03465	2,23172
83	1	-8,0675	-1,22853	3,14945
84	1	-7,49467	-1,62973	1,51242
85	1	-5,48686	0,13416	4,19406
86	1	-4,78019	-1,33808	4,91009
87	1	-6,52541	-1,02321	5,07526
88	1	-2,55103	3,56189	3,52276
89	1	-2,00735	2,84799	1,97145
90	1	-2,65796	1,80395	3,25685
91	1	-0,41949	4,69983	3,89279
92	1	0,22598	4,1095	2,3381
93	1	1,1442	3,85278	3,85061
94	1	-1,25981	1,37169	5,38453
95	1	-1,22624	3,13466	5,66166
96	1	0,29984	2,20452	5,60335
97	1	-0,80313	0,80443	-4,68302
98	1	-2,34741	-0,05977	-4,30804
99	1	2,2323	-1,60156	-0,60207
100	1	0,81415	-2,61602	-0,13601
101	6	-0,5981	-1,33303	-4,4287

102	1	-0,56572	-1,39333	-5,53298
103	1	0,45078	-1,32373	-4,06507
104	7	-1,35156	-2,46434	-3,92483
105	1	0,31305	-3,27662	-2,94805
106	6	-0,76159	-3,36165	-3,20697
107	1	-2,86675	-3,08698	-3,9822
108	8	-3,53454	-3,82552	-3,7433
109	6	-2,85055	-4,7095	-3,01044
110	6	-1,46567	-4,52374	-2,70966
111	1	0,26427	-5,32803	-1,70218
112	6	-0,79496	-5,48644	-1,92902
113	6	-1,45238	-6,61018	-1,4515
114	1	-0,92212	-7,34766	-0,84598
115	6	-2,81331	-6,78521	-1,75581
116	1	-3,34117	-7,66777	-1,38384
117	6	-3,50483	-5,85512	-2,5213
118	1	-4,56311	-5,98482	-2,7596
119	6	2,69324	-3,68583	-0,16845
120	1	2,37784	-4,44799	0,57371
121	1	2,44363	-4,06326	-1,17752
122	7	4,1221	-3,43802	-0,11251
123	1	4,34351	-4,57189	1,63197
124	6	4,81431	-3,93806	0,85429
125	1	5,27147	-2,61275	-0,89949
126	8	6,25497	-2,32871	-1,0141
127	6	6,91053	-2,88834	0,00556
128	6	6,23957	-3,7022	0,97008
129	1	6,44583	-4,88702	2,75909
130	6	6,97681	-4,26882	2,02746
131	6	8,34276	-4,05409	2,14914
132	1	8,90335	-4,49876	2,97397
133	6	8,99461	-3,25435	1,19519
134	1	10,07068	-3,07836	1,28122
135	6	8,29621	-2,67922	0,14063
136	1	8,79744	-2,0552	-0,6032

Table S11. For **5** *exo-exo* rotamer, the optimized geometry in Cartesian coordinates, obtained by DFT- calculations.

Center Number	Atomic number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1,79496	2,58134	4,46652
2	6	-2,63082	2,88611	5,54921
3	6	-2,47964	2,25738	6,79706
4	6	-1,42626	1,35544	6,95902
5	1	-1,31966	0,86156	7,92999
6	6	-0,53235	1,0541	5,91998
7	6	-0,74877	1,67338	4,68456
8	1	-0,10689	1,43088	3,83489
9	6	0,60654	0,04776	6,15761
10	6	1,50615	0,55035	7,31015
11	1	2,31839	-0,17147	7,50043
12	1	0,93782	0,6743	8,24512
13	1	1,95943	1,5223	7,05659
14	6	9,6837E-4	-1,32399	6,53807
15	1	0,80566	-2,05642	6,72026
16	1	-0,63938	-1,7044	5,72602
17	1	-0,61245	-1,25832	7,45008
18	6	1,48709	-0,1458	4,90968
19	1	2,28915	-0,86695	5,13648
20	1	1,96263	0,79827	4,59736
21	1	0,90789	-0,54421	4,06086
22	6	-3,39928	5,15728	5,55495
23	1	-2,5468	5,42992	4,90724
24	1	-3,11905	5,37052	6,60396
25	6	-4,64412	5,95094	5,1511
26	1	-4,92593	5,68767	4,11281
27	1	-5,47802	5,65712	5,81439
28	6	-4,41172	8,13853	4,26682
29	1	-4,63382	7,73999	3,25815
30	6	-4,15004	9,55725	4,3724
31	6	-4,16571	10,3987	3,2363
32	1	-4,3791	9,95869	2,25783
33	6	-3,91023	11,75462	3,37349
34	1	-3,9201	12,40794	2,49835
35	6	-3,63539	12,30386	4,6392
36	1	-3,43372	13,37161	4,75789
37	6	-3,61525	11,49531	5,7704
38	8	-3,35235	12,00274	7,00701
39	6	-3,87193	10,11029	5,64464
40	6	-3,48517	2,47728	7,92027
41	1	-2,94394	2,52863	8,87877
42	1	-3,99055	3,44817	7,78637
43	6	-4,5123	1,35814	8,01428
44	6	-5,54636	1,22837	7,06489
45	6	-6,4282	0,12477	7,14279
46	6	-6,30068	-0,77657	8,19849
47	1	-7,01437	-1,60609	8,24917
48	6	-5,30329	-0,65948	9,18071

49	6	-4,41688	0,41369	9,04683
50	1	-3,61334	0,54818	9,77587
51	6	-5,21989	-1,68332	10,32487
52	6	-4,05412	-1,39017	11,28669
53	1	-4,15902	-0,40167	11,76283
54	1	-3,0815	-1,42767	10,76929
55	1	-4,03805	-2,14818	12,08677
56	6	-6,53409	-1,65577	11,13935
57	1	-6,69596	-0,66013	11,58295
58	1	-6,49574	-2,39777	11,95528
59	1	-7,40538	-1,89084	10,50802
60	6	-5,01261	-3,09949	9,73844
61	1	-4,95844	-3,84589	10,54946
62	1	-4,07609	-3,14717	9,1595
63	1	-5,84	-3,38694	9,07073
64	6	-7,45746	-0,09143	6,04549
65	1	-8,27045	-0,72292	6,44164
66	1	-7,88374	0,87719	5,74985
67	6	-6,84952	-0,77169	4,82275
68	6	-6,67094	-0,10621	3,6022
69	6	-5,99018	-0,7037	2,52796
70	6	-5,54214	-2,01736	2,68018
71	1	-5,002	-2,47364	1,84469
72	6	-5,73818	-2,74325	3,86498
73	6	-6,3844	-2,0911	4,92034
74	1	-6,51318	-2,60177	5,87702
75	6	-5,21089	-4,18403	3,97554
76	6	-3,67477	-4,17693	3,7924
77	1	-3,19356	-3,56669	4,57351
78	1	-3,3832	-3,76466	2,81391
79	1	-3,28024	-5,20492	3,86064
80	6	-5,85681	-5,0552	2,8737
81	1	-5,63064	-4,67133	1,86667
82	1	-6,95244	-5,08309	2,98933
83	1	-5,47586	-6,08864	2,93532
84	6	-5,52861	-4,82121	5,34061
85	1	-5,05968	-4,26617	6,16921
86	1	-5,13594	-5,85079	5,36365
87	1	-6,61442	-4,87227	5,52343
88	6	-8,44147	1,4061	3,02303
89	1	-9,09582	0,68856	3,54977
90	1	-8,52442	1,21856	1,93508
91	6	-8,89585	2,82023	3,36982
92	1	-9,99589	2,87009	3,22883
93	1	-8,67849	2,98556	4,44081
94	6	-8,92107	4,74961	2,00257
95	1	-10,02901	4,72626	2,03416
96	6	-8,30862	5,84966	1,28778
97	6	-9,08436	6,83515	0,63661
98	1	-10,17438	6,74644	0,65108
99	6	-8,46762	7,89971	-0,00358
100	1	-9,06688	8,66179	-0,50606
101	6	-7,06596	8,00962	-0,0113

102	1	-6,56914	8,84352	-0,51354
103	6	-6,28342	7,05178	0,6229
104	8	-4,92045	7,14156	0,64391
105	6	-6,89942	5,962	1,27703
106	6	-5,65988	0,07841	1,26297
107	1	-5,79785	-0,57966	0,38987
108	1	-6,36389	0,91881	1,14369
109	6	-4,22833	0,59325	1,24921
110	6	-3,82692	1,65959	2,0841
111	6	-2,47635	2,06696	2,09209
112	6	-1,56577	1,44394	1,2332
113	1	-0,53207	1,79993	1,24615
114	6	-1,93439	0,40035	0,37431
115	6	-3,2762	-0,00566	0,41913
116	1	-3,61394	-0,82215	-0,22839
117	6	-0,94805	-0,29231	-0,58101
118	6	-1,42948	-0,11537	-2,03988
119	1	-1,47321	0,95248	-2,30825
120	1	-2,43336	-0,54314	-2,18868
121	1	-0,7383	-0,62059	-2,73619
122	6	-0,8767	-1,80062	-0,24662
123	1	-0,52705	-1,95401	0,78716
124	1	-0,17708	-2,31224	-0,92963
125	1	-1,86096	-2,28453	-0,34691
126	6	0,47371	0,28829	-0,47241
127	1	0,88787	0,16231	0,54143
128	1	0,49537	1,36019	-0,7281
129	1	1,14041	-0,23796	-1,17493
130	6	-2,0297	3,14263	3,06799
131	1	-2,79701	3,92812	3,1152
132	1	-1,09263	3,59152	2,69796
133	7	-4,39028	7,3724	5,3104
134	7	-8,21466	3,84861	2,60184
135	8	-3,71084	3,76134	5,38215
136	8	-3,83636	9,37743	6,77366
137	1	-4,04909	8,40559	6,46299
138	8	-5,77755	2,1133	6,0626
139	1	-5,04025	2,7617	5,93317
140	8	-7,08506	1,22644	3,46823
141	8	-6,08053	5,07663	1,87796
142	1	-6,70034	4,36563	2,30075
143	8	-4,66848	2,34847	2,89376
144	1	-5,56996	1,94662	2,9612
145	1	-3,39975	11,23316	7,61511
146	1	-4,61117	6,30432	1,05433

Table S12. For **5** *endo-exo* rotamer, the optimized geometry in Cartesian coordinates, obtained by DFT- calculations.

Center Number	Atomic number	Coordinates (Angstroms)		
		X	Y	Z
1	6	2,50239	-1,13744	-2,84681
2	6	1,85912	0,06755	-3,20273
3	6	2,44949	1,29521	-2,85049
4	6	3,74271	1,30086	-2,31081
5	1	4,17644	2,26983	-2,05355
6	6	4,45851	0,12752	-2,06538
7	6	3,7893	-1,07902	-2,30624
8	1	4,26901	-2,02583	-2,04
9	6	5,88849	0,11863	-1,50123
10	6	6,81659	-0,65476	-2,46597
11	1	7,84521	-0,68111	-2,06729
12	1	6,84073	-0,17046	-3,45559
13	1	6,47928	-1,69375	-2,60493
14	6	6,45499	1,5393	-1,3247
15	1	7,48503	1,47864	-0,93631
16	1	5,8594	2,12948	-0,60937
17	1	6,48684	2,08358	-2,28268
18	6	5,88936	-0,57812	-0,12068
19	1	6,9104	-0,5954	0,29804
20	1	5,53039	-1,61697	-0,18959
21	1	5,23116	-0,04144	0,58152
22	6	-0,57512	-0,00879	-3,38735
23	1	-0,81655	0,94578	-2,89072
24	1	-0,6149	-0,80348	-2,62811
25	6	-1,59004	-0,29619	-4,49661
26	1	-1,59401	0,52474	-5,24121
27	1	-1,29742	-1,22771	-5,01246
28	6	-3,85349	0,35391	-4,11782
29	1	-3,72584	1,19691	-4,82461
30	6	-5,1322	0,22057	-3,45012
31	6	-6,20162	1,11148	-3,69491
32	1	-6,06568	1,91535	-4,42416
33	6	-7,40231	0,96151	-3,01629
34	1	-8,22965	1,64942	-3,20376
35	6	-7,56921	-0,07669	-2,08248
36	1	-8,50837	-0,19986	-1,53746
37	6	-6,53271	-0,96884	-1,82902
38	8	-6,66832	-1,9824	-0,93057
39	6	-5,30131	-0,8239	-2,50917
40	6	1,70449	2,62493	-2,94589
41	1	2,21921	3,29863	-3,65253
42	1	0,69316	2,45362	-3,34147
43	6	1,03229	3,20097	0,7813
44	6	0,91018	2,71745	-0,53271
45	6	1,66745	3,29209	-1,57929
46	6	2,46709	4,397	-1,28961
47	1	3,03893	4,83698	-2,11365
48	6	2,58077	4,94165	0,00246

49	6	1,86337	4,30632	1,02025
50	1	1,92739	4,67877	2,0461
51	6	3,47535	6,16872	0,24565
52	6	3,47334	6,6098	1,72057
53	1	2,46244	6,88935	2,05964
54	1	3,85834	5,81696	2,38273
55	1	4,12347	7,49165	1,84138
56	6	2,96914	7,35212	-0,61136
57	1	1,93682	7,62007	-0,33414
58	1	3,61045	8,23704	-0,45925
59	1	2,97851	7,10697	-1,68489
60	6	4,93185	5,83525	-0,15368
61	1	5,58309	6,71097	0,00902
62	1	5,3197	4,9983	0,44942
63	1	5,00725	5,55157	-1,215
64	6	0,27603	2,5474	1,93078
65	1	0,27819	3,2482	2,78129
66	1	-0,78127	2,40794	1,64798
67	6	0,86934	1,22403	2,40903
68	6	0,35339	-0,0201	2,02334
69	6	0,93973	-1,23506	2,41498
70	6	2,05271	-1,16788	3,2574
71	1	2,51161	-2,11106	3,56891
72	6	2,59491	0,04877	3,70044
73	6	1,98993	1,22816	3,25182
74	1	2,39266	2,19777	3,55299
75	6	3,80245	0,04543	4,65366
76	6	3,39992	-0,65421	5,97313
77	1	2,57044	-0,11924	6,46322
78	1	3,07933	-1,69334	5,79931
79	1	4,25677	-0,67467	6,66731
80	6	4,97609	-0,7223	4,00311
81	1	4,70835	-1,76575	3,77594
82	1	5,28679	-0,24128	3,06229
83	1	5,84067	-0,73673	4,68769
84	6	4,28635	1,4679	4,98873
85	1	3,50607	2,05545	5,49947
86	1	5,1542	1,40789	5,66515
87	1	4,60248	2,01336	4,08478
88	6	-2,05007	-0,07428	1,77764
89	1	-2,15938	-1,00681	2,35783
90	1	-2,12707	0,77979	2,47234
91	6	-3,1187	0,01159	0,68714
92	1	-2,99792	0,95514	0,11644
93	1	-2,99157	-0,82677	-0,02214
94	6	-5,30467	0,83821	1,09952
95	1	-5,07721	1,71169	0,45848
96	6	-6,62364	0,77309	1,68635
97	6	-7,5815	1,78981	1,46683
98	1	-7,31275	2,64282	0,83761
99	6	-8,84057	1,69482	2,0386
100	1	-9,58181	2,47919	1,87125
101	6	-9,17829	0,58695	2,83705

102	1	-10,16927	0,50045	3,29003
103	6	-8,25482	-0,42745	3,06392
104	8	-8,56082	-1,51088	3,82909
105	6	-6,9653	-0,34004	2,48981
106	6	0,43068	-2,5922	1,93333
107	1	0,48795	-3,29699	2,77846
108	1	-0,63613	-2,52322	1,66018
109	6	1,22175	-3,18137	0,77243
110	6	1,05278	-2,6954	-0,53492
111	6	1,84465	-3,19434	-1,59377
112	6	2,72689	-4,23994	-1,32372
113	1	3,32357	-4,62617	-2,15707
114	6	2,89105	-4,78977	-0,03915
115	6	2,13655	-4,22245	0,99218
116	1	2,23805	-4,60046	2,01294
117	6	3,87798	-5,94831	0,18212
118	6	3,92203	-6,40549	1,65146
119	1	2,93802	-6,76435	1,99488
120	1	4,2523	-5,59365	2,32014
121	1	4,63768	-7,23723	1,75628
122	6	5,30163	-5,50017	-0,22372
123	1	5,34624	-5,19998	-1,28231
124	1	6,01897	-6,32558	-0,07673
125	1	5,62959	-4,6433	0,38706
126	6	3,45566	-7,15645	-0,68568
127	1	3,43725	-6,89871	-1,75614
128	1	2,44897	-7,50515	-0,40414
129	1	4,16345	-7,99189	-0,5494
130	6	1,82383	-2,5037	-2,94895
131	1	0,79739	-2,38179	-3,32341
132	1	2,35941	-3,13744	-3,67668
133	7	-2,8947	-0,48062	-3,88595
134	7	-4,42741	-0,09116	1,30451
135	8	0,72332	0,04419	-4,00296
136	8	-4,3278	-1,70693	-2,21027
137	1	-3,52543	-1,42782	-2,83366
138	8	0,07631	1,69767	-0,87539
139	1	-0,25579	1,20822	-0,08792
140	8	-0,74583	-0,0512	1,13237
141	8	-6,11483	-1,35151	2,74872
142	1	-5,24983	-1,1074	2,23515
143	8	0,13739	-1,74079	-0,85599
144	1	-0,21777	-1,27665	-0,06207
145	1	-5,80987	-2,4586	-0,94764
146	1	-7,75631	-2,07328	3,81625

Table S13. For **6** *exo-exo* rotamer, the optimized geometry in Cartesian coordinates, obtained by DFT- calculations.

Center Number	Atomic number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-0,99247	0,24729	0,36456
2	8	1,56281	-2,21187	-0,31971
3	6	1,45127	-0,61504	2,67217
4	8	-0,663	-0,99745	-2,662
5	6	5,65038	-2,70227	-1,19986
6	6	4,67512	-2,53113	-2,19781
7	6	3,32412	-2,34195	-1,90635
8	6	1,0537	0,6641	3,0889
9	6	2,02265	1,62863	3,39664
10	6	3,39218	1,35709	3,30179
11	6	3,76843	0,06314	2,90371
12	6	2,82554	-0,9168	2,58971
13	6	2,41625	1,88809	-2,81272
14	6	2,68383	0,53943	-3,0633
15	6	1,67972	-0,43743	-3,02333
16	16	3,35748	-2,59566	2,17036
17	6	1,08613	2,23252	-2,53254
18	6	2,87528	-2,33877	-0,56134
19	6	-1,63517	3,79502	-0,22872
20	8	0,50881	-1,54844	2,26089
21	6	0,34225	-0,07896	-2,76451
22	6	0,06482	1,28155	-2,50267
23	16	-1,62336	1,80615	-2,14128
24	6	-1,01154	2,12968	1,88912
25	16	2,1487	-2,16748	-3,25296
26	6	5,20794	-2,65004	0,12496
27	6	3,85453	-2,47087	0,44674
28	6	-1,56345	4,35941	1,05722
29	16	-0,7046	1,04035	3,28636
30	6	-1,13378	1,56319	0,60307
31	6	-1,23094	3,49709	2,10601
32	6	-1,42127	2,43752	-0,47386
33	6	4,4718	2,39597	3,64808
34	6	7,12333	-2,91074	-1,58747
35	6	-1,83132	5,86012	1,2562
36	6	3,50292	2,97549	-2,84257
37	6	5,38426	2,61372	2,41909
38	6	3,86483	3,75306	4,04669
39	6	5,31802	1,87248	4,83194
40	6	8,02874	-3,07814	-0,35414
41	6	7,24861	-4,18269	-2,45751
42	6	7,62174	-1,68811	-2,39264
43	6	-3,27233	6,18529	0,79926
44	6	-0,82831	6,68096	0,41279
45	6	-1,68334	6,28452	2,72828
46	6	4,8944	2,3991	-3,1609
47	6	3,56838	3,66614	-1,46051
48	6	3,15153	4,02298	-3,92406

49	6	0,12499	-2,4958	3,29866
50	6	-1,09158	-1,65889	-3,86226
51	1	-0,80219	-0,21086	1,22051
52	1	1,389	-2,19193	0,65446
53	1	4,9592	-2,53563	-3,25359
54	1	1,67116	2,60916	3,72089
55	1	4,82417	-0,21054	2,83667
56	1	3,70046	0,207	-3,27802
57	1	0,81503	3,27184	-2,3306
58	1	-1,86995	4,42202	-1,09306
59	1	5,90989	-2,76108	0,95323
60	1	-1,14338	3,86618	3,12922
61	1	6,17168	3,34678	2,66122
62	1	4,80507	2,99827	1,56451
63	1	5,87674	1,68041	2,10458
64	1	6,10316	2,60412	5,08559
65	1	4,69026	1,71607	5,72388
66	1	5,81109	0,91791	4,59033
67	1	4,67696	4,46262	4,27251
68	1	3,26011	4,18317	3,23188
69	1	3,23464	3,67045	4,94713
70	1	9,06983	-3,23082	-0,68176
71	1	8,00895	-2,18412	0,29046
72	1	7,73582	-3,9523	0,24997
73	1	8,29916	-4,33734	-2,75636
74	1	6,64373	-4,10849	-3,37474
75	1	6,91245	-5,07178	-1,90019
76	1	8,67571	-1,82947	-2,686
77	1	7,03323	-1,53967	-3,31154
78	1	7,55049	-0,76796	-1,79029
79	1	-3,47675	7,2623	0,92254
80	1	-3,42956	5,92924	-0,26007
81	1	-4,00732	5,62215	1,39637
82	1	-1,01793	7,76004	0,54114
83	1	-0,91492	6,4497	-0,66034
84	1	0,20789	6,47204	0,72474
85	1	-1,88729	7,36357	2,82081
86	1	-2,39619	5,75224	3,3789
87	1	-0,66289	6,10325	3,10415
88	1	5,63568	3,21475	-3,1662
89	1	4,91783	1,91883	-4,15267
90	1	5,21119	1,65985	-2,40715
91	1	3,91604	4,81804	-3,94533
92	1	4,34077	4,4539	-1,46647
93	1	2,60763	4,13289	-1,19268
94	1	3,82097	2,93529	-0,67533
95	1	2,17607	4,49552	-3,72999
96	1	3,11006	3,55569	-4,92107
97	1	-0,47967	-1,96903	4,05736
98	1	1,04337	-2,89221	3,76373
99	1	-1,33455	-0,91508	-4,64409
100	1	-0,3053	-2,34023	-4,23632
101	6	-0,65318	-3,65658	2,68768

102	1	-0,54667	-4,51854	3,38002
103	1	-0,16227	-3,93635	1,73767
104	7	-2,05238	-3,35527	2,44058
105	1	-2,63511	-4,94594	3,66715
106	6	-2,93942	-4,10666	3,00863
107	1	-3,03874	-2,35274	1,58781
108	8	-3,98395	-2,06329	1,31092
109	6	-4,82246	-2,89494	1,95959
110	6	-4,35964	-3,92114	2,82072
111	1	-4,91076	-5,55123	4,13636
112	6	-5,28616	-4,76365	3,47668
113	6	-6,64558	-4,58553	3,27797
114	1	-7,36797	-5,23143	3,78169
115	6	-7,10394	-3,57241	2,42121
116	1	-8,17293	-3,42126	2,24966
117	6	-6,21504	-2,72763	1,75735
118	8	-6,69782	-1,76521	0,93513
119	6	-2,32937	-2,47873	-3,50172
120	1	-2,08598	-3,0767	-2,60301
121	1	-2,53328	-3,17442	-4,33241
122	7	-3,50832	-1,64806	-3,29178
123	1	-2,97348	-1,1906	-1,31247
124	6	-3,678	-1,06018	-2,14925
125	1	-4,73275	-1,19296	-4,09482
126	8	-5,63831	-0,65043	-4,17791
127	6	-5,75963	-0,04015	-2,98739
128	6	-4,82355	-0,19741	-1,93977
129	1	-4,27283	0,39637	0,06766
130	6	-5,02065	0,49963	-0,7235
131	6	-6,13254	1,31572	-0,5608
132	1	-6,28463	1,85544	0,37644
133	6	-7,07143	1,45908	-1,59876
134	1	-7,95182	2,09548	-1,47831
135	6	-6,8916	0,79176	-2,80444
136	8	-7,77609	0,91313	-3,8323
137	1	-5,95037	-1,26701	0,53506
138	1	-7,40928	0,34576	-4,54635

Table S14. For **6** *endo-exo* rotamer, the optimized geometry in Cartesian coordinates, obtained by DFT- calculations.

Center Number	Atomic number	Coordinates (Angstroms)		
		X	Y	Z
1	8	-1,43512	-2,02034	-1,1791
2	8	0,80272	0,74335	-0,45403
3	6	0,2848	-1,77101	1,94057
4	8	-1,03119	0,37227	-2,71299
5	6	1,22962	4,31696	1,72303
6	6	0,58386	4,3072	0,48297
7	6	0,40946	3,12261	-0,24635
8	6	-1,0191	-2,29592	1,9479
9	6	-2,0755	-1,58162	2,52847
10	6	-1,88257	-0,31682	3,09154
11	6	-0,59074	0,22354	3,03215
12	6	0,46783	-0,46914	2,44346
13	6	-4,28021	2,57591	-1,15155
14	6	-2,98823	3,11594	-1,193
15	6	-1,90712	2,41195	-1,74032
16	16	-0,28604	3,2035	-1,90395
17	6	-4,46076	1,29255	-1,69297
18	6	0,89596	1,89053	0,23798
19	6	-4,0126	-4,02374	0,46753
20	8	1,35636	-2,51476	1,51051
21	6	-2,10899	1,12142	-2,25842
22	6	-3,4015	0,56221	-2,23509
23	16	-3,70546	-1,05466	-2,99436
24	6	-2,77106	-3,44062	0,1861
25	16	-1,33875	-3,89527	1,17146
26	6	1,65807	3,07502	2,22471
27	6	1,49481	1,88027	1,52256
28	6	-5,17193	-3,71768	-0,25903
29	16	2,06943	0,34061	2,25077
30	6	-2,6465	-2,52163	-0,88123
31	6	-5,04723	-2,75944	-1,27549
32	6	-3,81998	-2,1653	-1,58284
33	6	-3,01223	0,47838	3,76672
34	6	1,45537	5,59818	2,54225
35	6	-6,53915	-4,35792	0,03451
36	6	-5,49026	3,35762	-0,61152
37	6	-2,68377	0,64727	5,2682
38	6	-4,37479	-0,22732	3,64188
39	6	-3,1255	1,87249	3,10711
40	6	0,73485	5,47341	3,90484
41	6	2,97105	5,79188	2,77872
42	6	0,91531	6,84741	1,82333
43	6	-6,46712	-5,37388	1,18857
44	6	-7,03996	-5,09462	-1,22929
45	6	-7,55223	-3,25569	0,42158
46	6	-6,26494	2,49762	0,41291
47	6	-5,07144	4,66809	0,07956
48	6	-6,42122	3,70128	-1,79859

49	6	1,60572	-2,50314	0,0779
50	6	-0,78779	0,4755	-4,14539
51	1	-1,50691	-1,36412	-1,91749
52	1	0,39178	0,92732	-1,33556
53	1	0,20593	5,2309	0,04178
54	1	-3,06472	-2,0408	2,52198
55	1	-0,39139	1,22099	3,43003
56	1	-2,79212	4,11799	-0,80864
57	1	-5,45247	0,83457	-1,71185
58	1	-4,04881	-4,7313	1,29789
59	1	2,1339	3,01242	3,20712
60	1	-5,91717	-2,45802	-1,86463
61	1	-3,47366	1,23334	5,76813
62	1	-2,61287	-0,3338	5,76471
63	1	-1,72581	1,17069	5,41353
64	1	-5,15131	0,38768	4,12547
65	1	-4,37024	-1,21038	4,14001
66	1	-4,66245	-0,37164	2,58752
67	1	-3,94696	2,44362	3,57265
68	1	-3,3287	1,77725	2,02827
69	1	-2,20039	2,45811	3,22418
70	1	0,89792	6,38397	4,50573
71	1	1,1091	4,61593	4,48576
72	1	-0,35032	5,34255	3,76286
73	1	3,14889	6,70122	3,37726
74	1	3,40953	4,93941	3,32059
75	1	3,50568	5,89632	1,82115
76	1	1,10791	7,73827	2,44274
77	1	1,41028	7,00219	0,85079
78	1	-0,17275	6,78461	1,65751
79	1	-7,46493	-5,81175	1,35309
80	1	-5,77234	-6,19883	0,96209
81	1	-6,15079	-4,89923	2,13165
82	1	-8,0265	-5,54962	-1,03833
83	1	-6,33982	-5,89491	-1,51796
84	1	-7,14382	-4,4092	-2,08515
85	1	-8,5397	-3,7022	0,6271
86	1	-7,67825	-2,51774	-0,38637
87	1	-7,2199	-2,71951	1,32524
88	1	-7,13664	3,06055	0,78553
89	1	-5,62821	2,23841	1,27298
90	1	-6,63849	1,56171	-0,03057
91	1	-5,96703	5,17193	0,4771
92	1	-4,38636	4,48076	0,92243
93	1	-4,58491	5,36526	-0,62158
94	1	-7,30348	4,25638	-1,43842
95	1	-5,89779	4,32655	-2,53966
96	1	-6,77567	2,79201	-2,3095
97	1	2,02486	-1,52238	-0,20837
98	1	0,65522	-2,65731	-0,45603
99	1	-1,65237	0,04938	-4,68304
100	1	-0,66528	1,53956	-4,41051
101	6	2,546	-3,64938	-0,2621

102	1	2,14603	-4,57895	0,1839
103	1	2,50249	-3,79901	-1,35777
104	7	3,95435	-3,53945	0,10054
105	1	3,72543	-1,84618	1,32479
106	6	4,3928	-2,60248	0,87924
107	1	5,24036	-4,31996	-0,24912
108	8	6,28493	-4,45554	-0,18804
109	6	6,69341	-3,46086	0,62044
110	6	5,80714	-2,51497	1,18792
111	1	5,63129	-0,76916	2,45503
112	6	6,32275	-1,49843	2,02367
113	6	7,68408	-1,4316	2,28191
114	1	8,08357	-0,64622	2,92737
115	6	8,56438	-2,37253	1,71642
116	1	9,63866	-2,32898	1,91401
117	6	8,07993	-3,38171	0,89192
118	8	8,90602	-4,3078	0,32838
119	6	0,47252	-0,30191	-4,49319
120	1	0,38849	-1,34141	-4,11313
121	1	0,5026	-0,35624	-5,59835
122	7	1,67164	0,36331	-4,02294
123	1	2,42529	-1,38314	-3,1445
124	6	2,56587	-0,30764	-3,37106
125	1	2,34703	1,83505	-4,07396
126	8	3,13699	2,45779	-3,84495
127	6	4,01131	1,68088	-3,17307
128	6	3,78779	0,30861	-2,90806
129	1	4,58425	-1,48389	-1,98091
130	6	4,76084	-0,42542	-2,19045
131	6	5,91915	0,19607	-1,75033
132	1	6,6623	-0,36845	-1,1834
133	6	6,13868	1,55898	-2,01766
134	1	7,04746	2,05934	-1,67367
135	6	5,19835	2,30202	-2,7234
136	8	5,38961	3,62418	-2,99106
137	1	8,31074	-4,89153	-0,1917
138	1	4,58934	3,90618	-3,48445