Supporting Information

Structurally diverse brefeldin A derivatives as potent and selective acetylcholinesterase inhibitors from an endophytic fungus *Penicillium brefeldianum* F4a

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List of Supporting Information

and (2*E*, 4*R*, 5*S*, 7*R*, 8*R*, 9*R*, 10*E*, 15*R*)-**2b**.

Table S7. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 8*S*, 9*S*, 10*E*, 15*R*)-**2a**] in ECD calculation.

Table S8. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*R*, 8*R*, 9*R*, 10*E*, 15*R*)-**2b**] in ECD calculation.

Table S9. The Information of conformations of (2*E*, 4*S*, 5*R*, 7*R*, 9*S*, 10*E*, 12*R*, 15*R*)-**3a**, (2*E*, 4*S*, 5*R*, 7*S*, 9*S*, 10*E*, 12*S*, 15*R*)-**3b**, (2*E*, 4*S*, 5*R*, 7*R*, 9*S*, 10*E*, 12*S*, 15*R*)-**3c**, and (2*E*, 4*S*, 5*R*, 7*S*, 9*S*, 10*E*, 12*R*, 15*R*)-**3d**.

Table S10. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*R*, 9*S*, 10*E*, 12*R*, 15*R*)-**3a**] in NMR calculation.

Table S11. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 9*S*, 10*E*, 12*S*, 15*R*)-**3b**] in NMR calculation.

Table S12. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*R*, 9*S*, 10*E*, 12*S*, 15*R*)-**3c**] in NMR calculation.

Table S13. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 9*S*, 10*E*, 12*R*, 15*R*)-**3d**] in NMR calculation.

Table S14. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*R*, 9*S*, 10*E*, 12*S*, 15*R*)-**3c**] in ECD calculation.

Table S15. The Information of conformations of (2*E*, 4*R*, 5*S*, 7*S*, 9*S*, 10*E*, 15*S*)-**4a** and (2*E*, 4*R*, 5*S*, 7*R*, 9*S*, 10*E*, 15*S*)-**4b**.

Table S16. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*S*, 9*S*, 10*E*, 15*S*)-**4a**] in NMR calculation.

Table S17. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*R*, 9*S*, 10*E*, 15*S*)-**4b**] in NMR calculation.

Table S18. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*S*, 9*S*, 10*E*, 15*S*)-**4a**] in ECD calculation.

Table S19. The Information of conformations of (2*E*, 4*R*, 5*S*, 7*R*, 9*S*, 10*E*, 15*R*)-**5a**, (2*E*, 4*R*, 5*S*, 7*S*, 9*R*, 10*E*, 15*R*)-**5b**, (2*E*, 4*R*, 5*R*, 7*R*, 9*S*, 10*E*, 15*R*)-**5c**, and (2*E*, 4*R*, 5*R*, 7*S*, 9*R*, 10*E*, 15*R*)-**5d**.

Table S20. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*R*, 9*S*, 10*E*, 15*R*)-**5a**] in NMR calculation.

Table S21. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*S*, 9*R*, 10*E*, 15*R*)-**5b**] in NMR calculation.

Table S22. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*R*, 7*R*, 9*S*, 10*E*, 15*R*)-**5c**] in NMR calculation.

Table S23. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*R*, 7*S*, 9*R*, 10*E*, 15*R*)-**5d**] in NMR calculation.

Table S24. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*R*, 9*S*, 10*E*, 15*R*)-**5a**] in ECD calculation.

Table S25. The Information of conformations of (2*E*, 4*S*, 5*R*, 7*S*, 9*R*, 10*E*, 15*S*)-**6a** and (2*E*, 4*S*, 5*R*, 7*R*, 9*R*, 10*E*, 15*S*)-**6b.**

Table S26. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 9*R*, 10*E*, 15*S*)-**6a**] in NMR calculation.

Table S27. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*R*, 9*R*, 10*E*,

15*S*)-**6b**] in NMR calculation.

Table S28. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 9*R*, 10*E*, 15*S*)-**6a**] in ECD calculation.

Table S29. The Information of conformations of (2*E*, 4*S*, 5*R*, 7*S*, 9*R*, 10*E*, 15*S*)-**7a.**

Table S30. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 9*R*, 10*E*, 15*S*)-**7a**] in ECD calculation.

Table S31. The Information of conformations of (2*Z*, 4*R*, 5*S*, 9*S*, 10*E*, 15*S*)-**8a** and (2*Z*, 4*S*, 5*R*, 9*R*, 10*E*, 15*S*)-**8b**.

Table S32. The coordinate for the lowest-energy conformer [(2*Z*, 4*R*, 5*S*, 9*S*, 10*E*, 15*S*)-**8a**] in ECD calculation.

Table S33. The coordinate for the lowest-energy conformer [(2*Z*, 4*S*, 5*R*, 9*R*, 10*E*, 15*S*)-**8b**] in ECD calculation.

Table S34. The Information of conformations of (2*Z*, 4*S*, 5*S*, 9*S*, 10*E*, 15*S*)-**9a** and (2*Z*, 4*R*, 5*R*, 9*R*, 10*E*, 15*S*)-**9b**.

Table S35. The coordinate for the lowest-energy conformer [(2*Z*, 4*S*, 5*S*, 9*S*, 10*E*, 15*S*)-**9a**] in ECD calculation.

Table S36. The coordinate for the lowest-energy conformer [(2*Z*, 4*R*, 5*R*, 9*R*, 10*E*, 15*S*)-**9b**] in ECD calculation.

Figure S1. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **1**

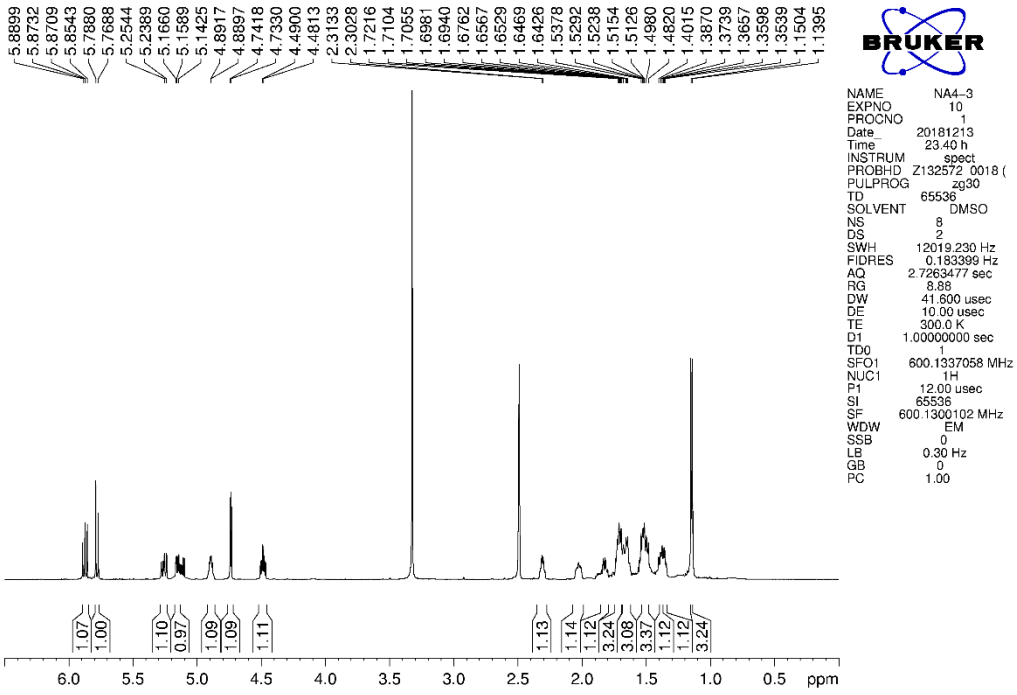


Figure S2. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **1**

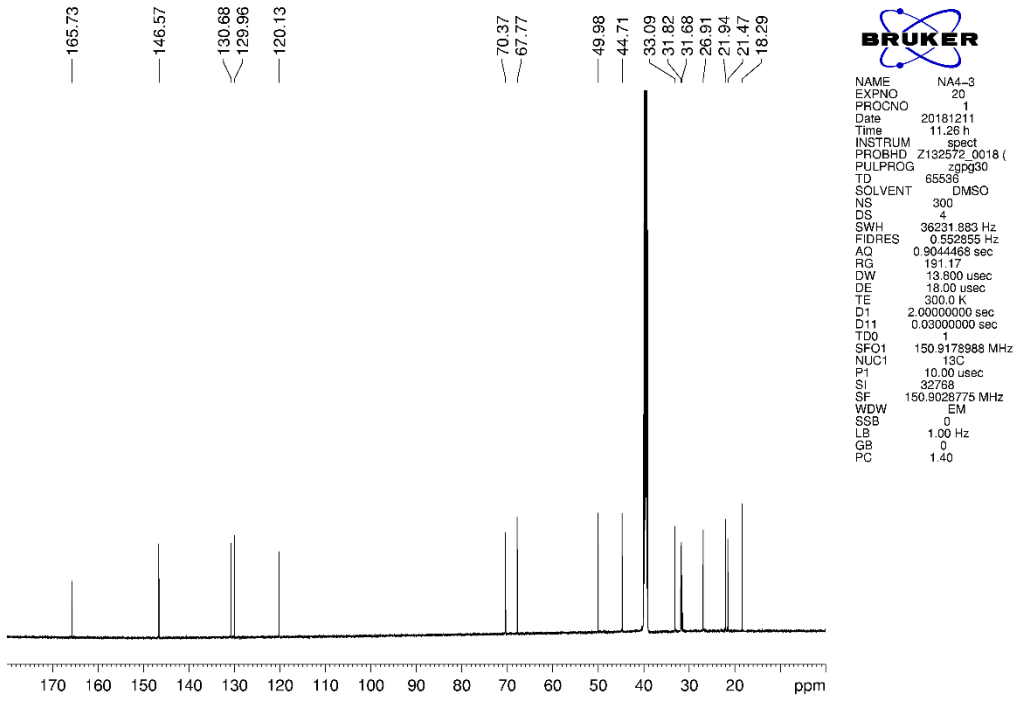


Figure S3. HSQC spectrum of **1**

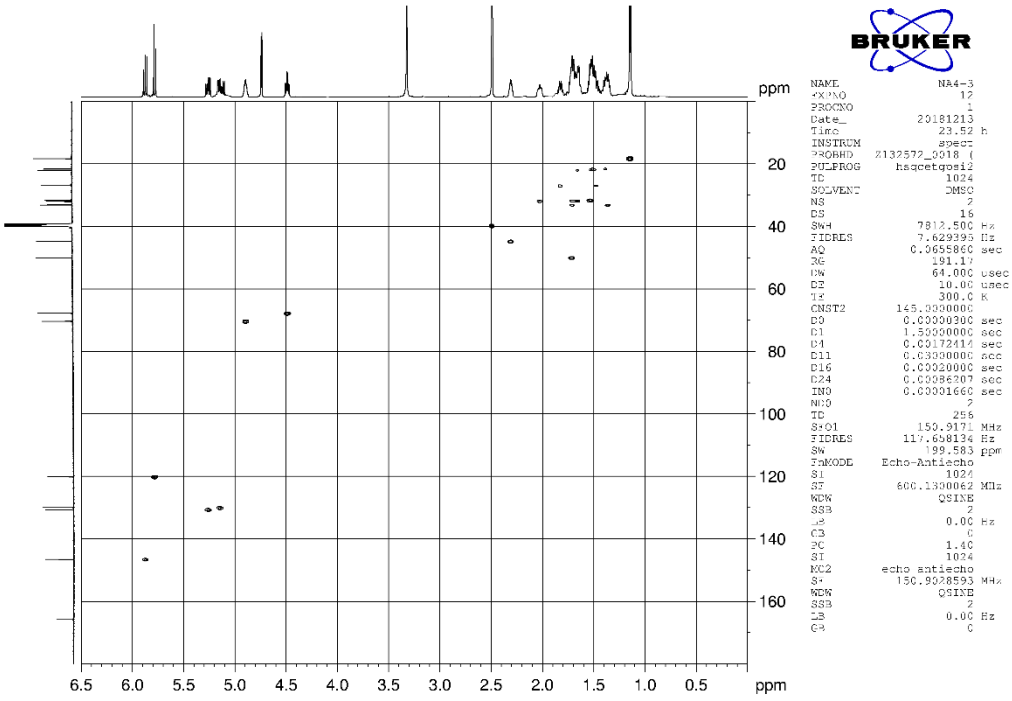


Figure S4. ^{1}H-^{13}C HMBC spectrum of **1**

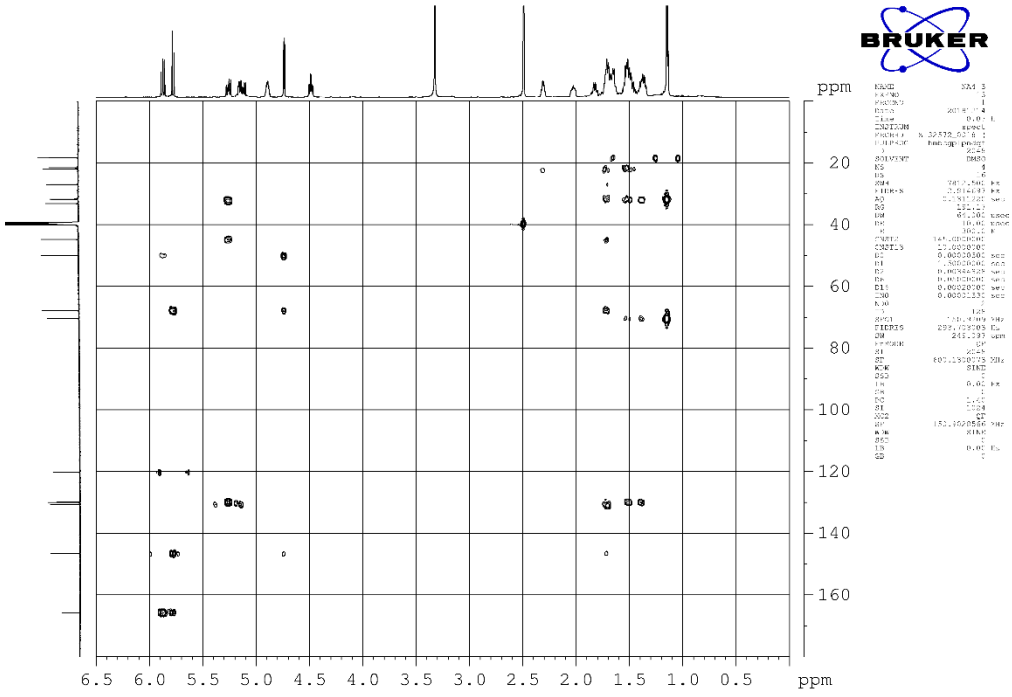


Figure S5. ^{1}H-^{1}H COSY spectrum of **1**

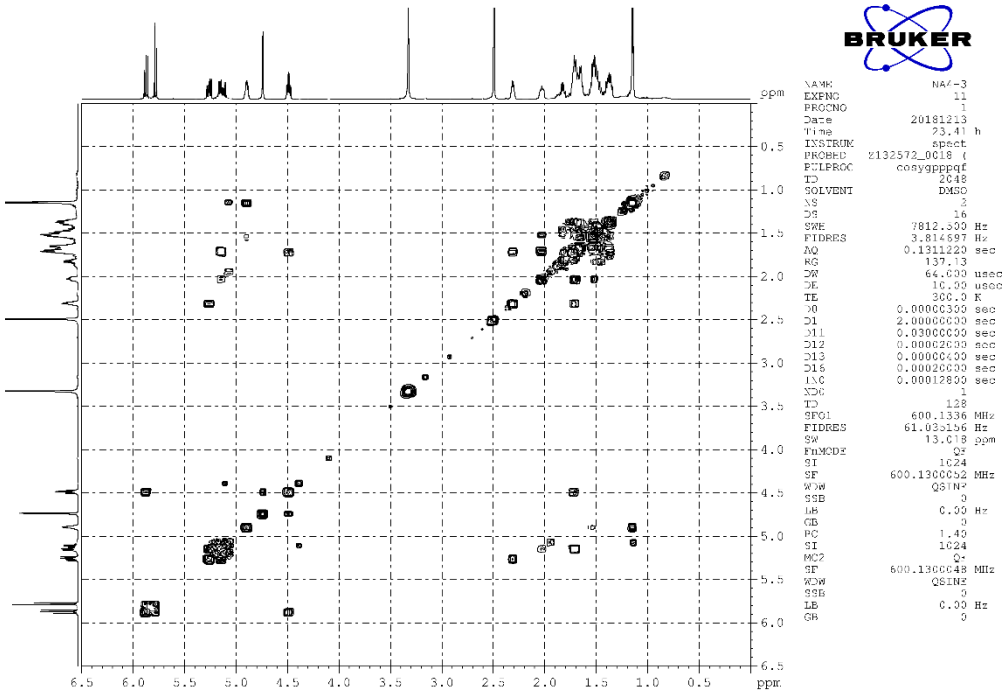


Figure S6. NOESY spectrum of **1**

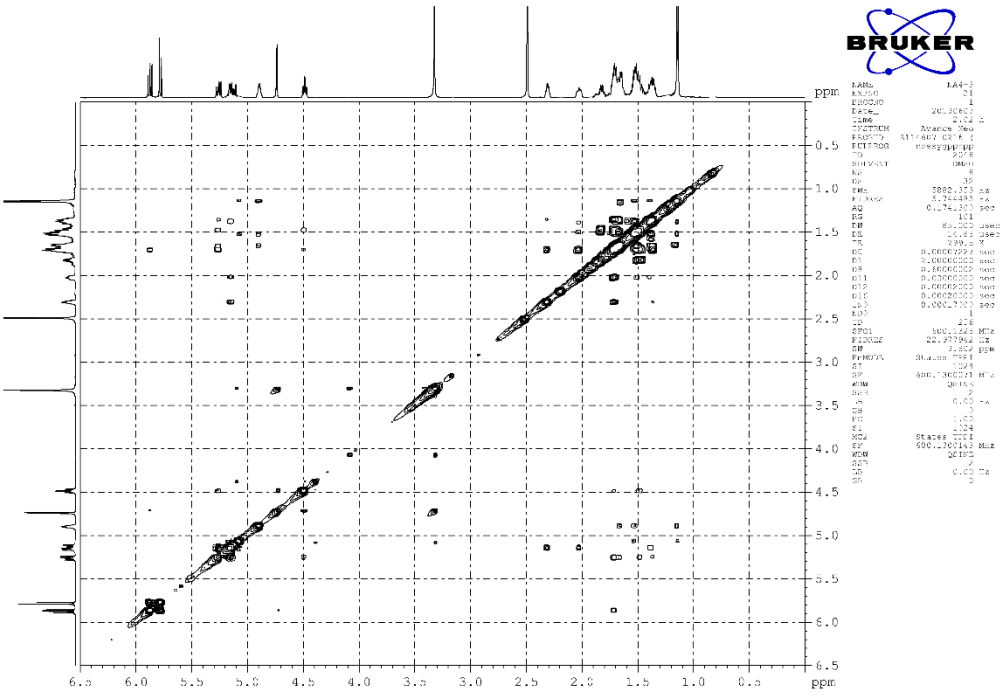


Figure S7. HRESIMS spectrum of **1**

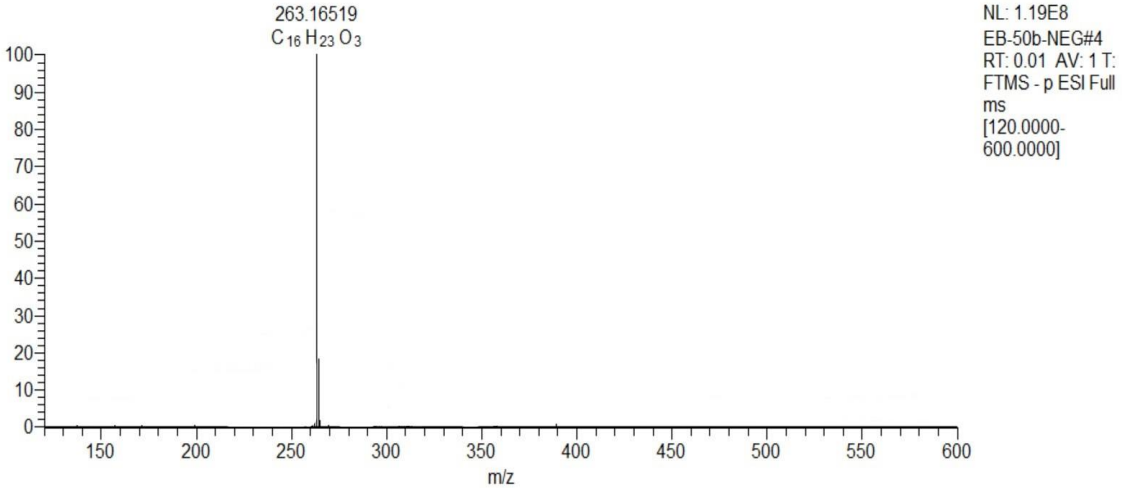


Figure S8. IR spectrum of **1**

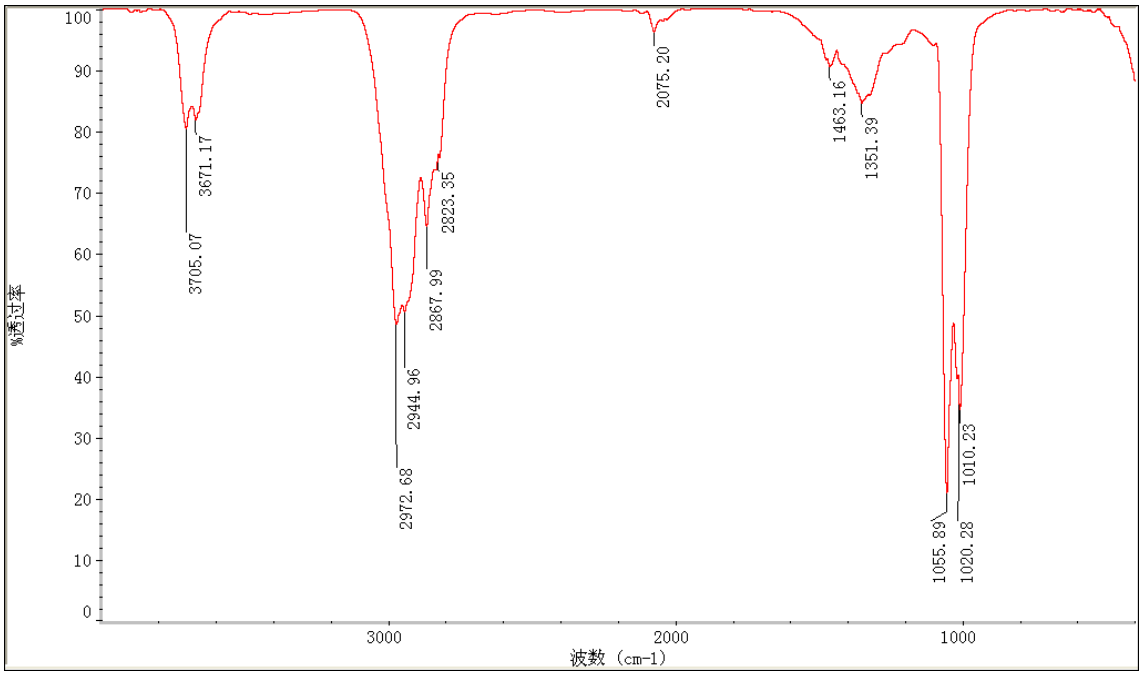


Figure S9. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **2**

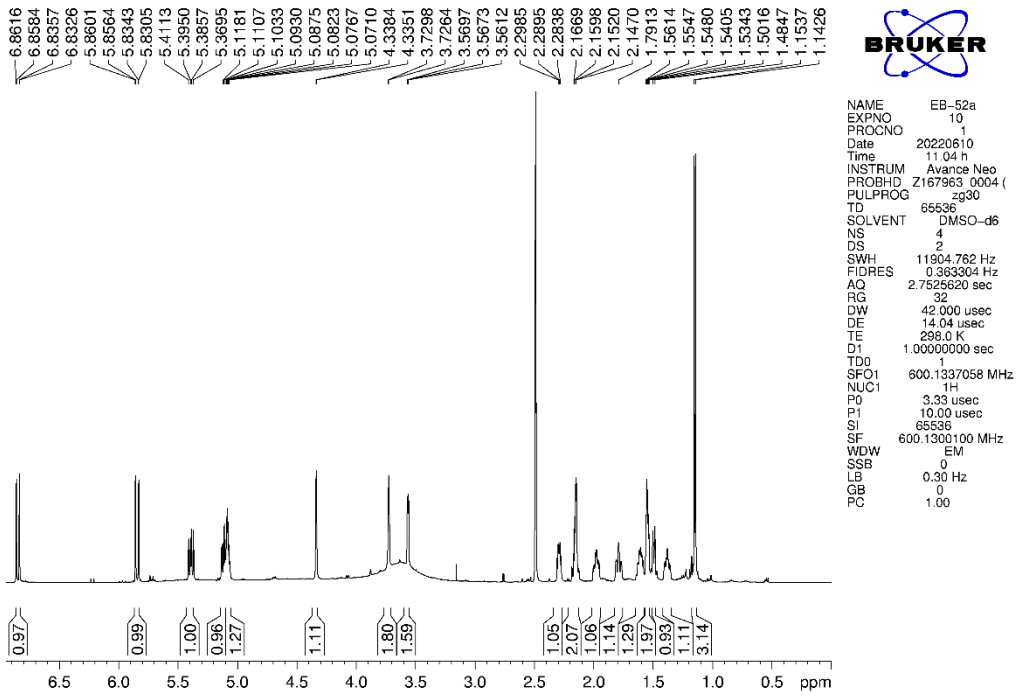


Figure S10. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **2**

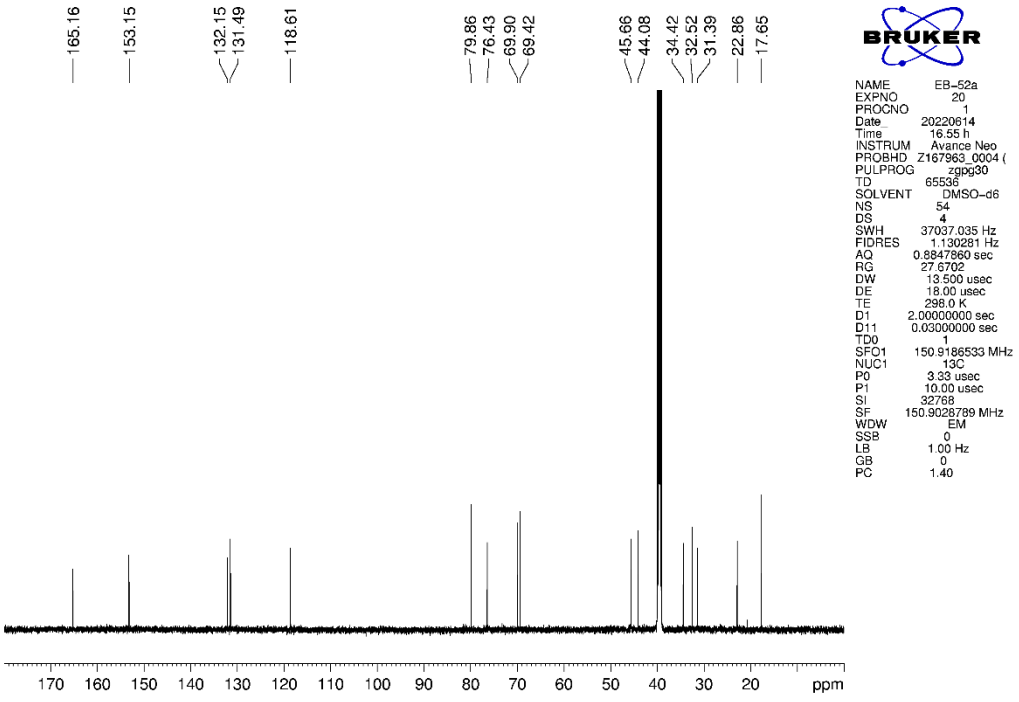


Figure S11. HSQC spectrum of **2**

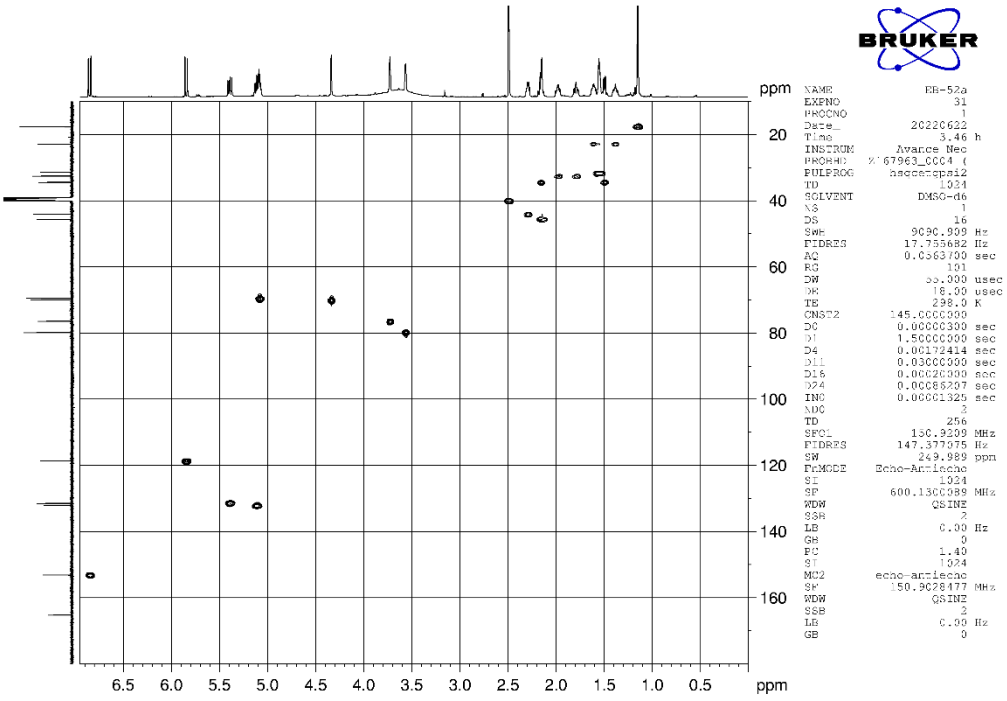


Figure S12. ^{1}H-^{13}C HMBC spectrum of **2**

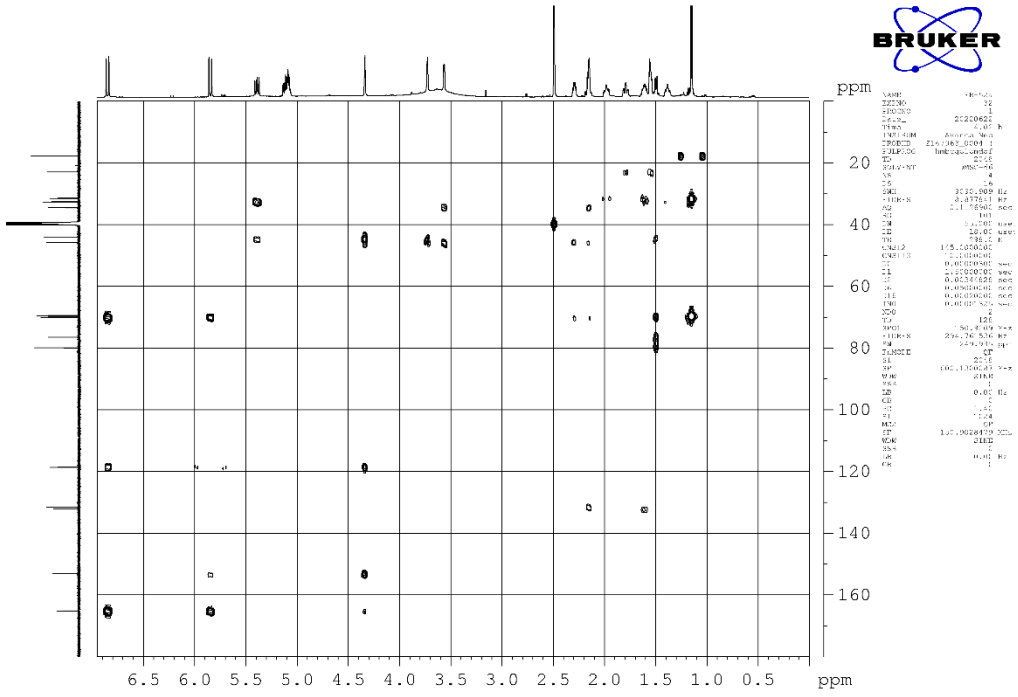


Figure S13. ^{1}H-^{1}H COSY spectrum of **2**

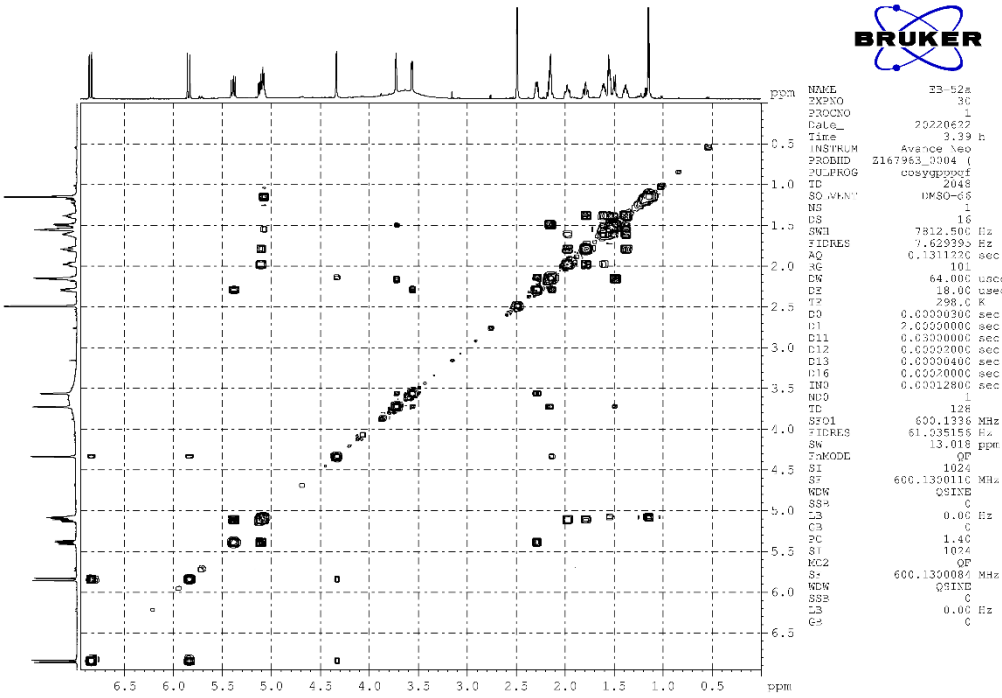


Figure S14. NOESY spectrum of **2**

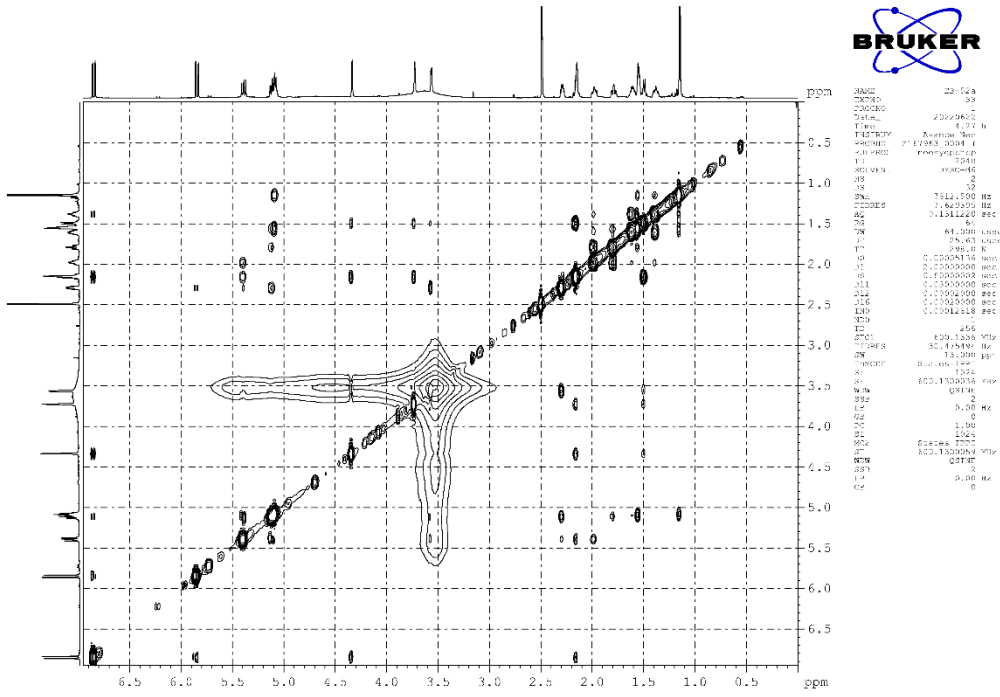


Figure S15. HRESIMS spectrum of **2**

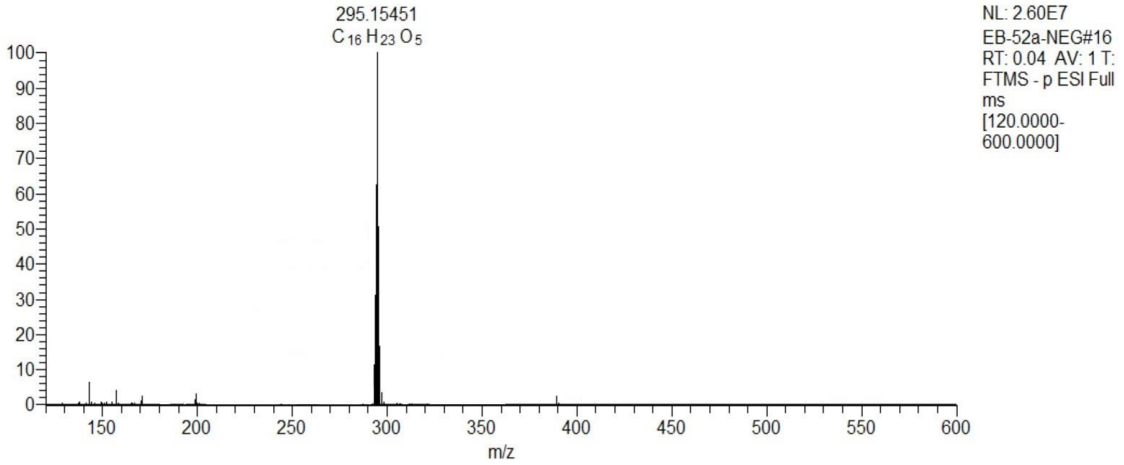


Figure S16. IR spectrum of **2**

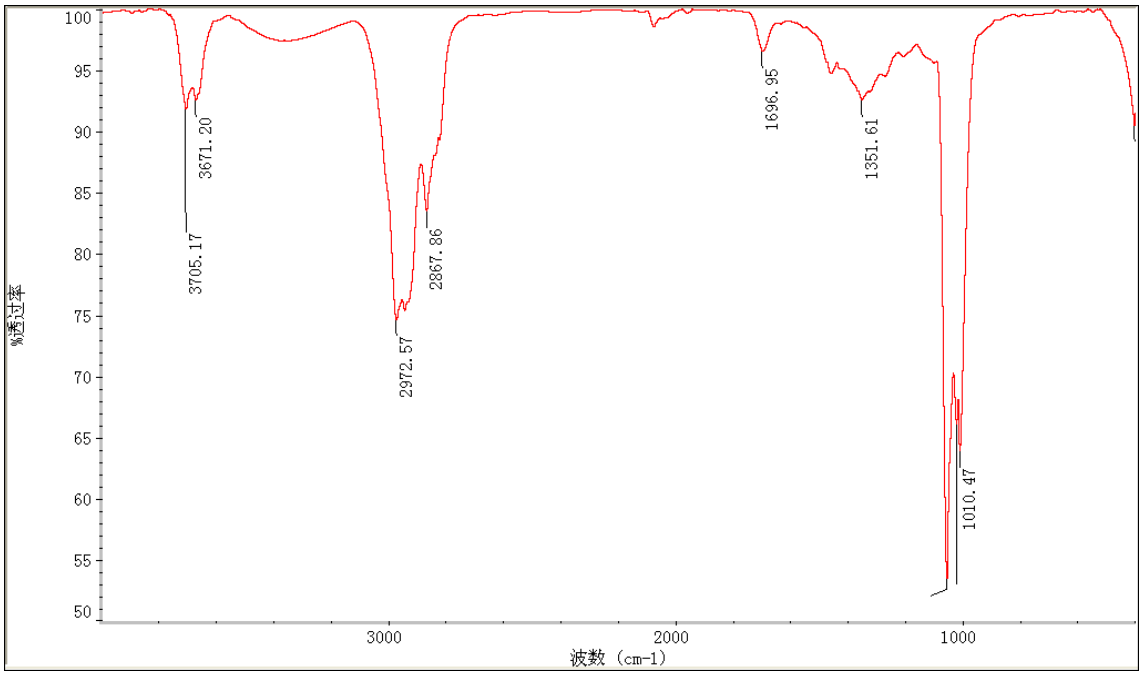


Figure S17. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **3**

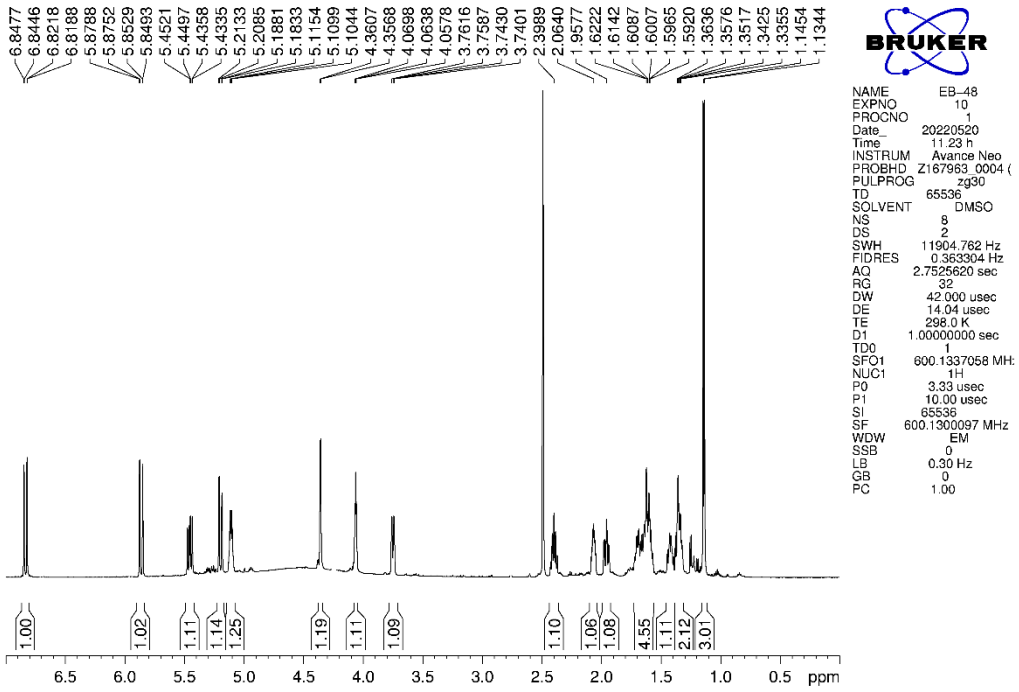


Figure S18. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **3**

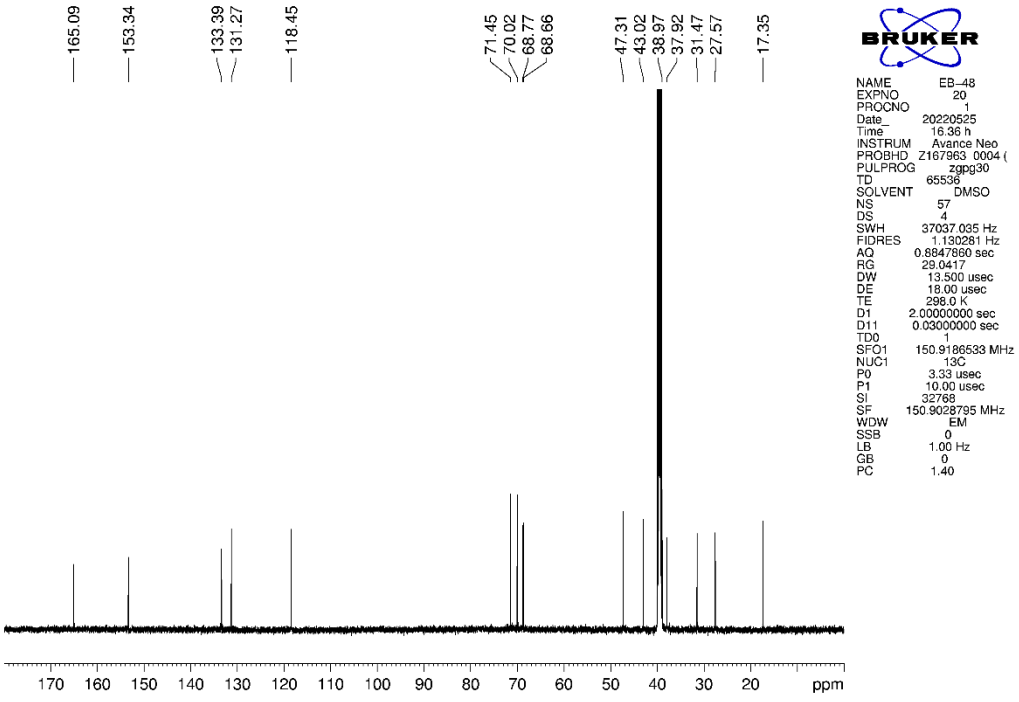


Figure S19. HSQC spectrum of **3**

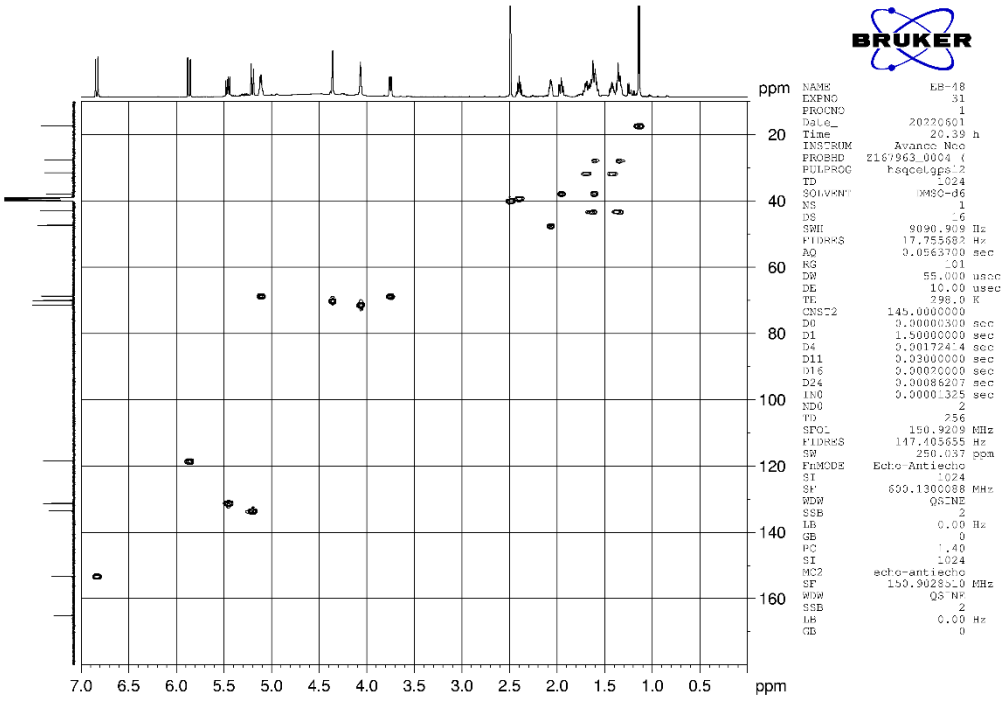


Figure S20. ^{1}H-^{13}C HMBC spectrum of **3**

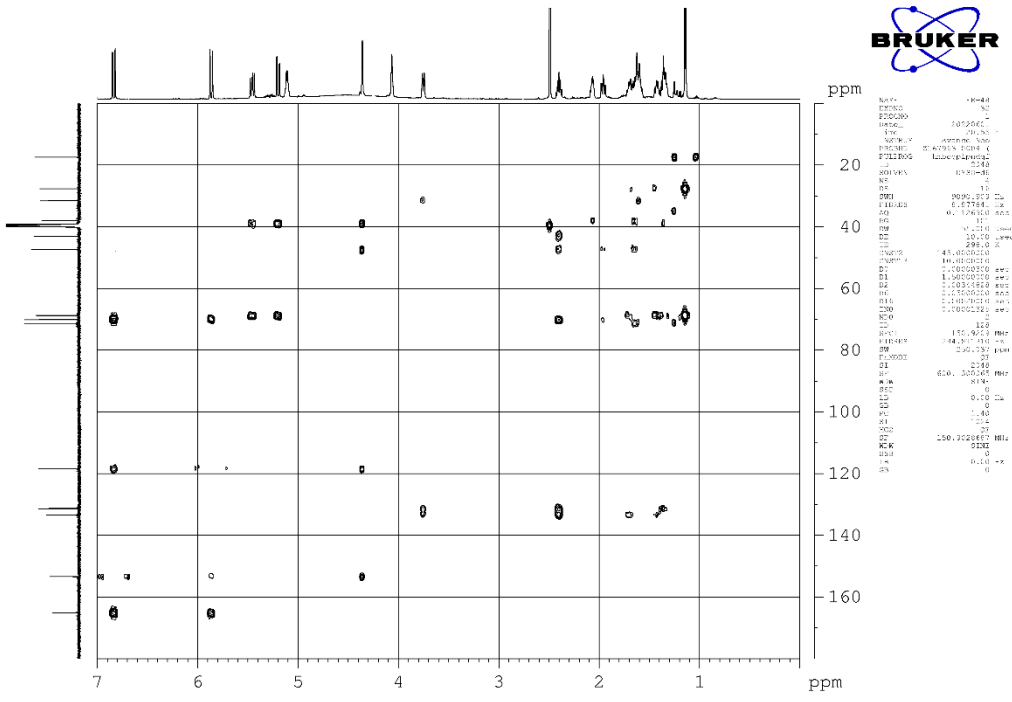


Figure S21. ^{1}H-^{1}H COSY spectrum of **3**

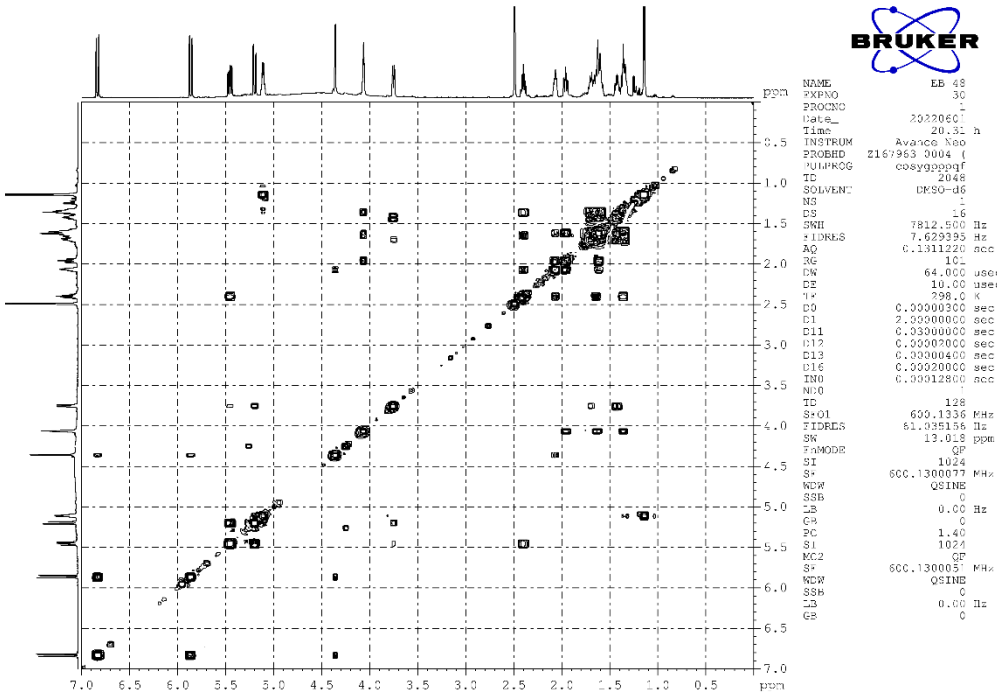


Figure S22. NOESY spectrum of **3**

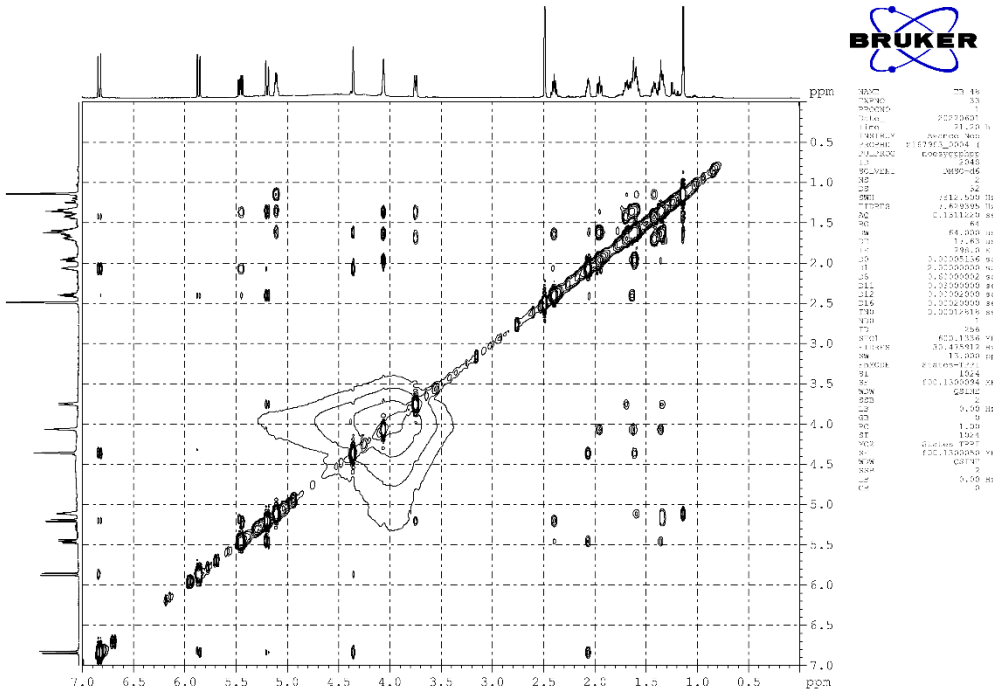


Figure S23. HRESIMS spectrum of **3**

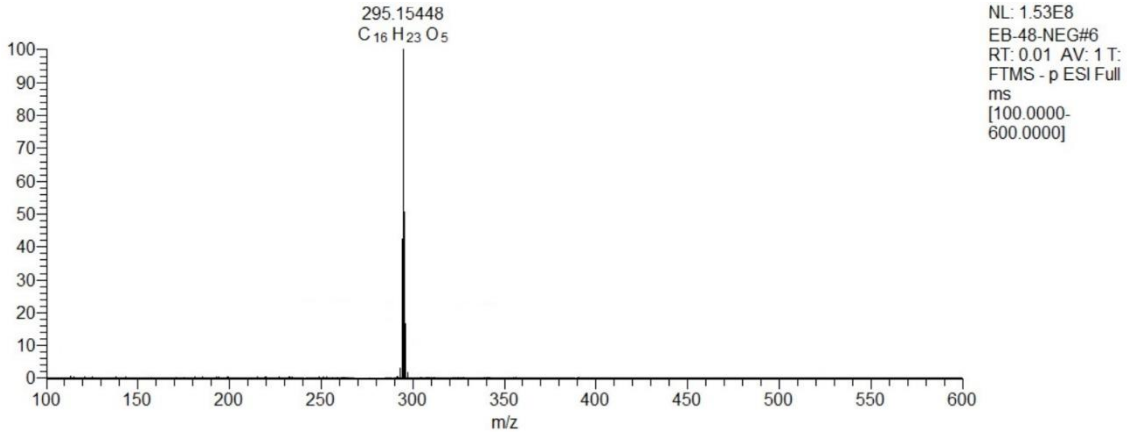


Figure S24. IR spectrum of **3**

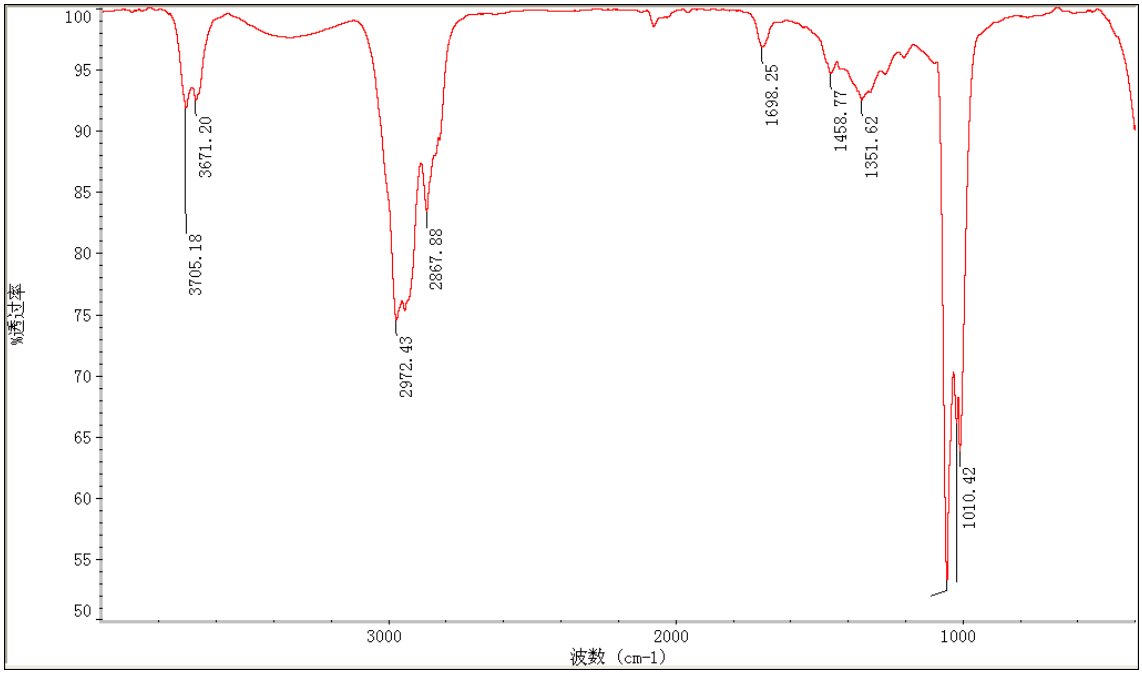


Figure S25. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **4**

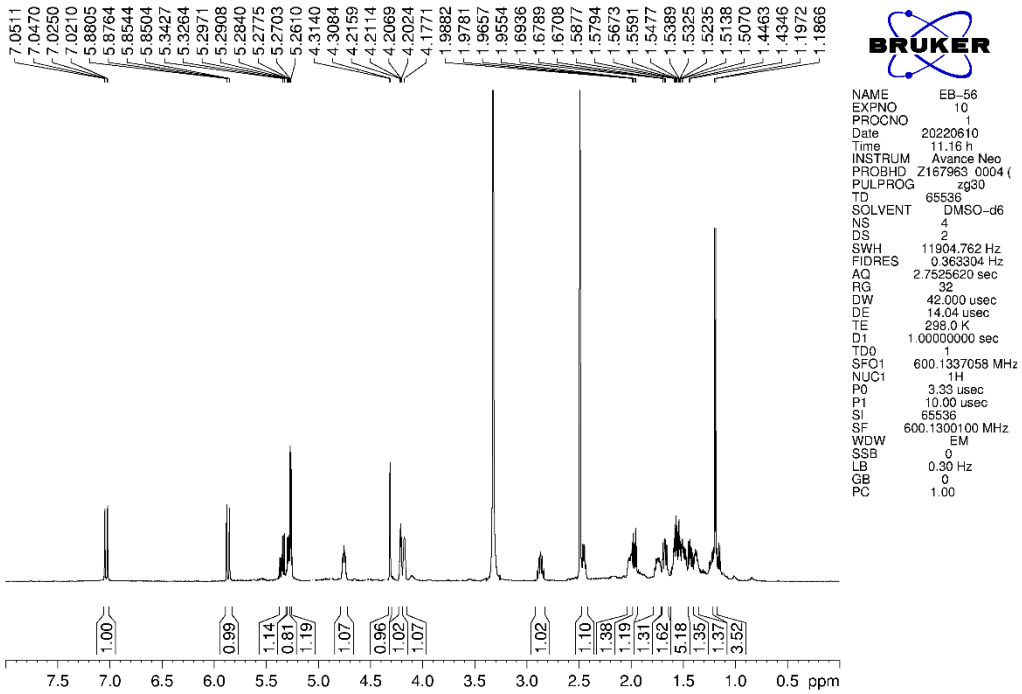


Figure S26. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **4**

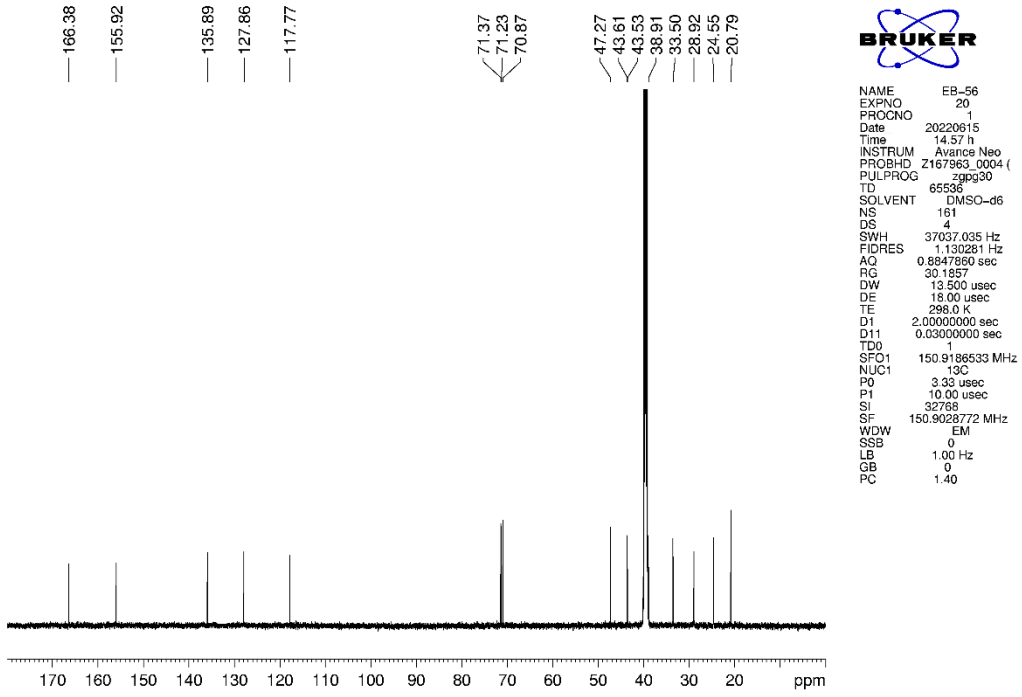


Figure S27. HSQC spectrum of **4**

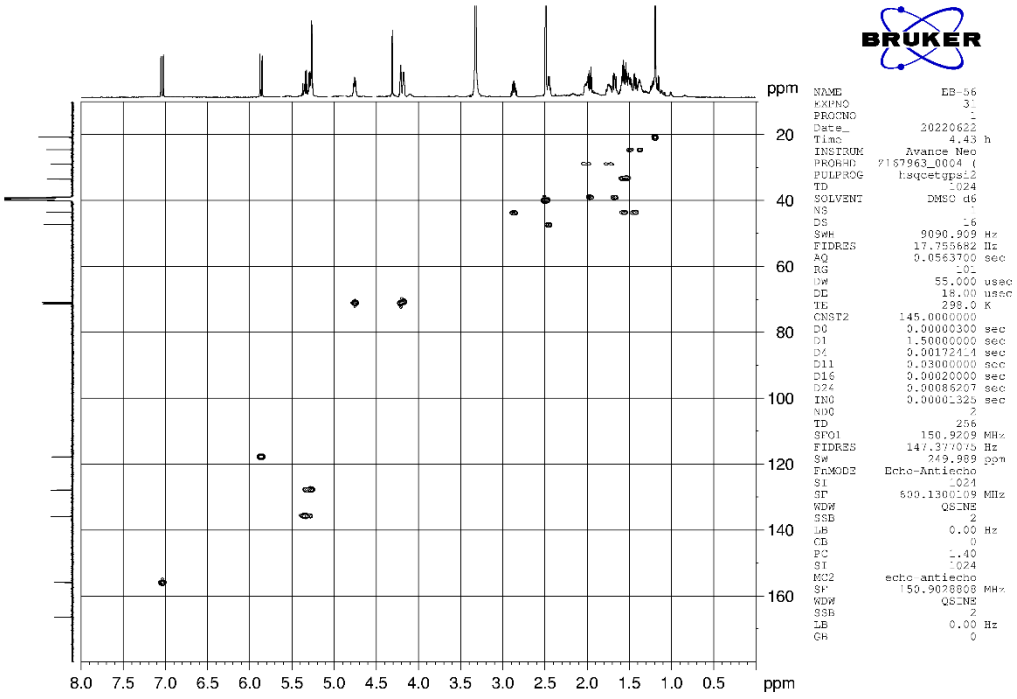


Figure S28. ^{1}H-^{13}C HMBC spectrum of **4**

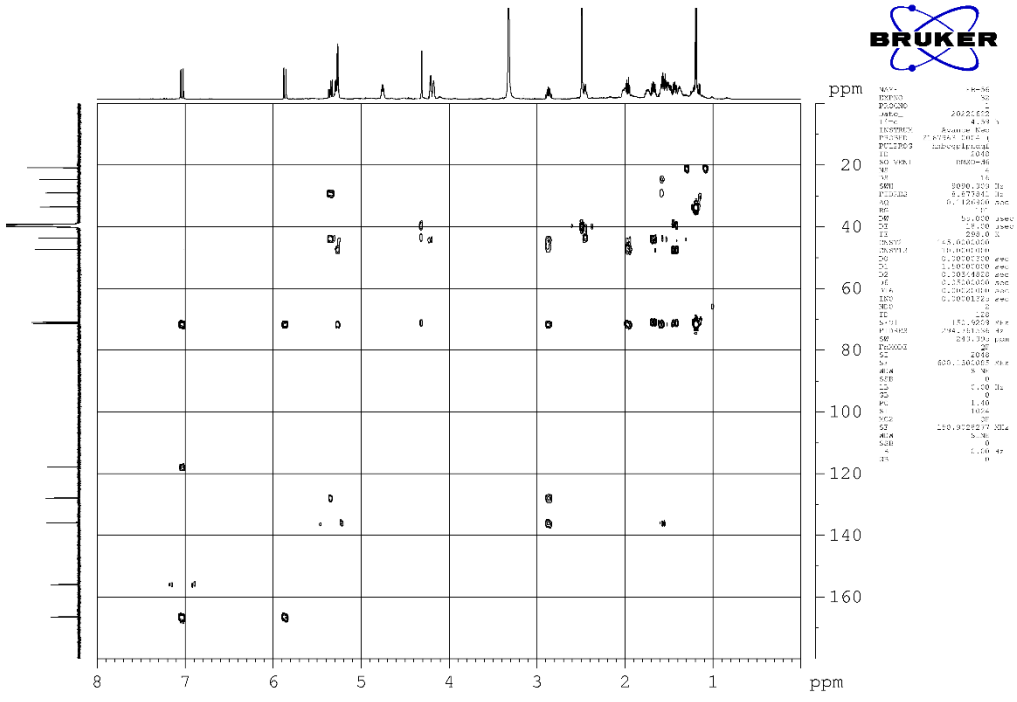


Figure S29. ^{1}H-^{1}H COSY spectrum of **4**

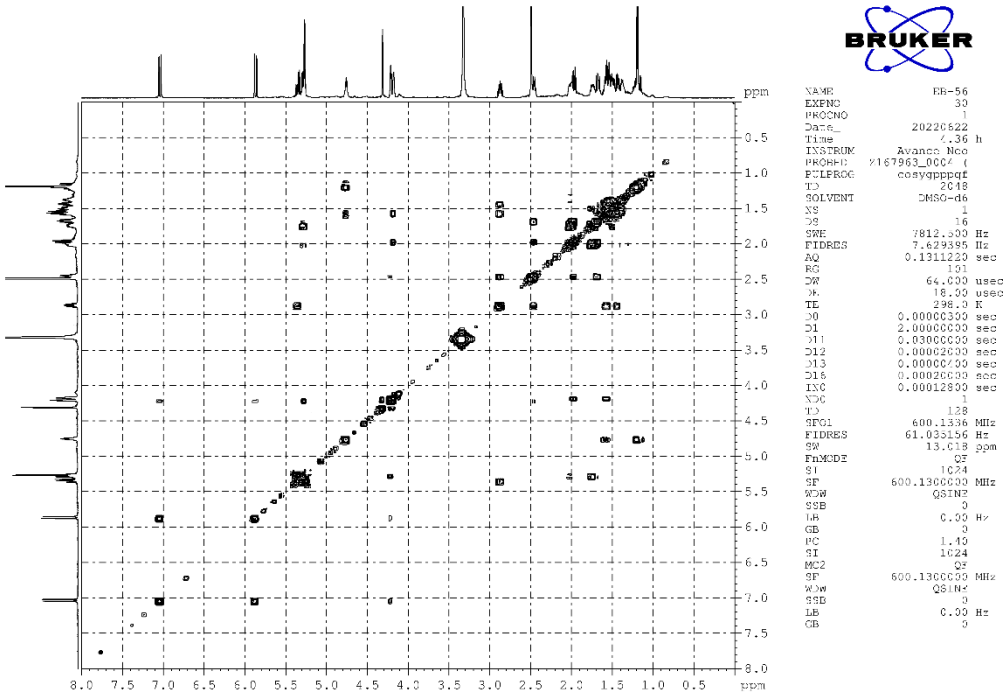


Figure S30. NOESY spectrum of **4**

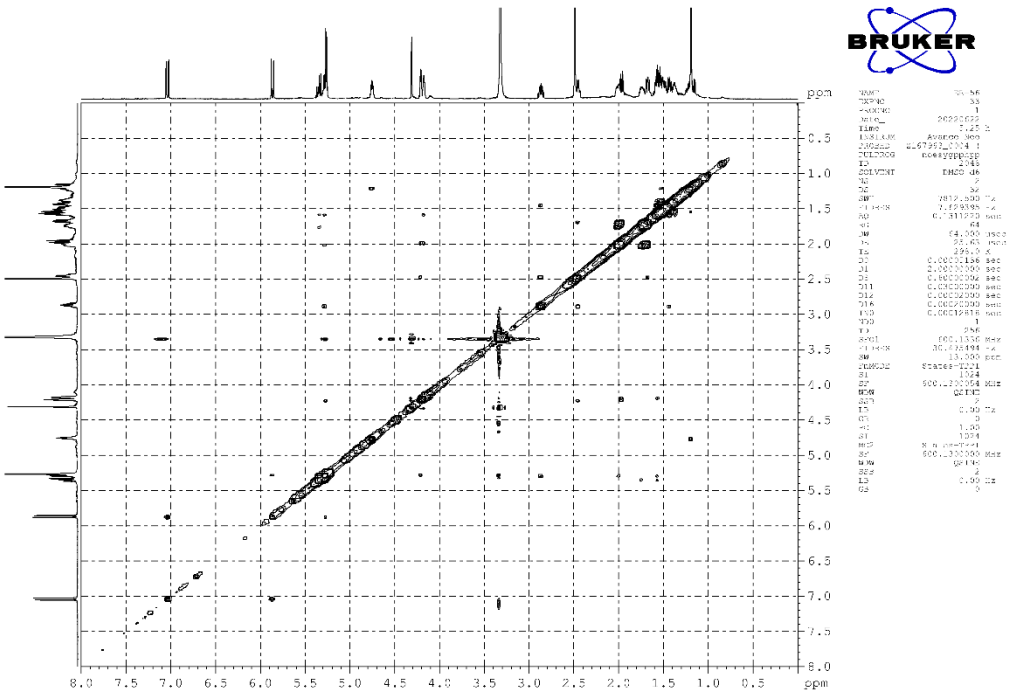


Figure S31. HRESIMS spectrum of **4**

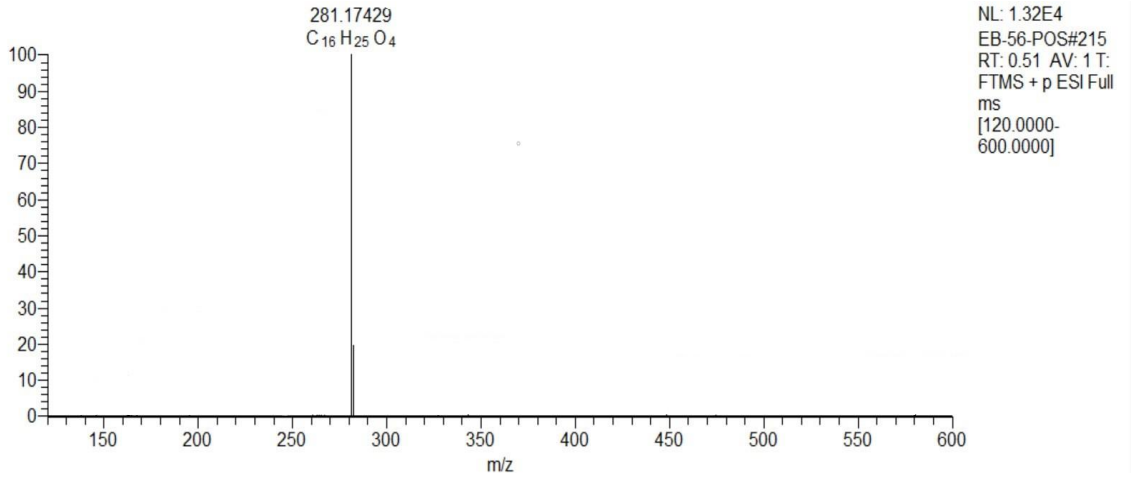


Figure S32. IR spectrum of **4**

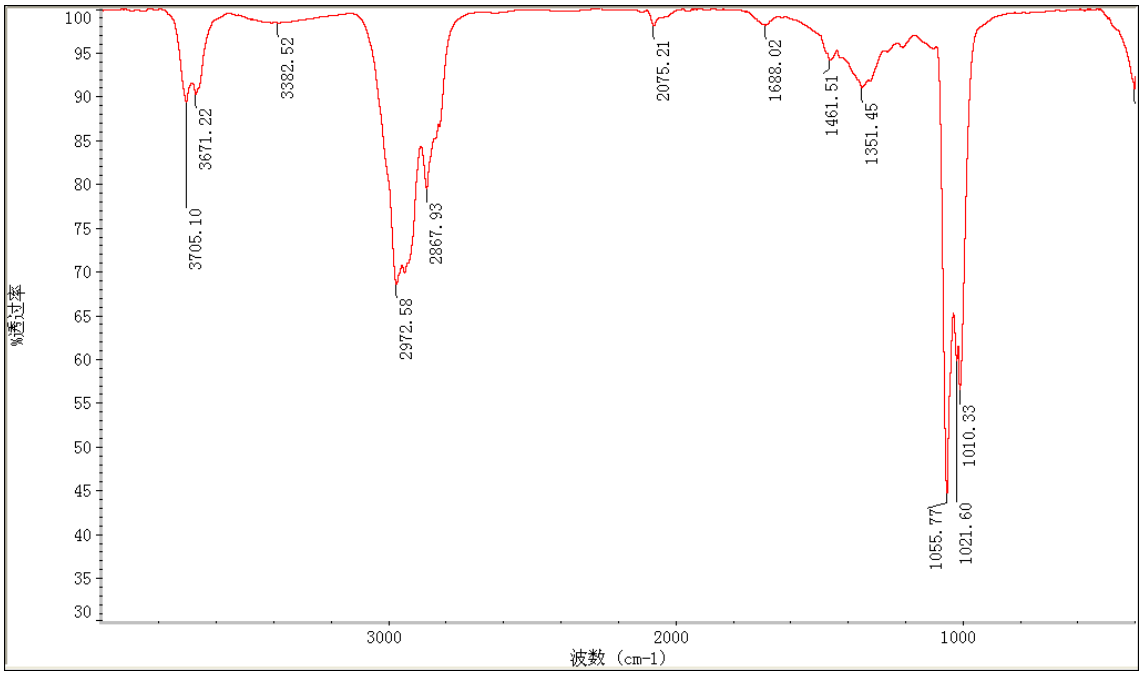


Figure S33. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **5**

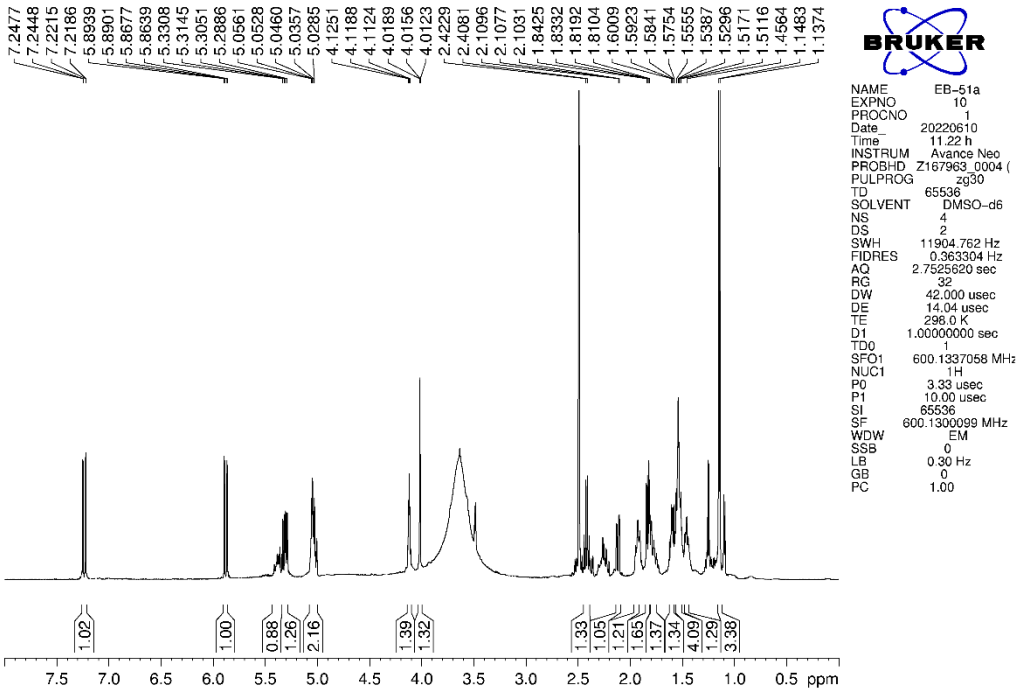


Figure S34. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **5**

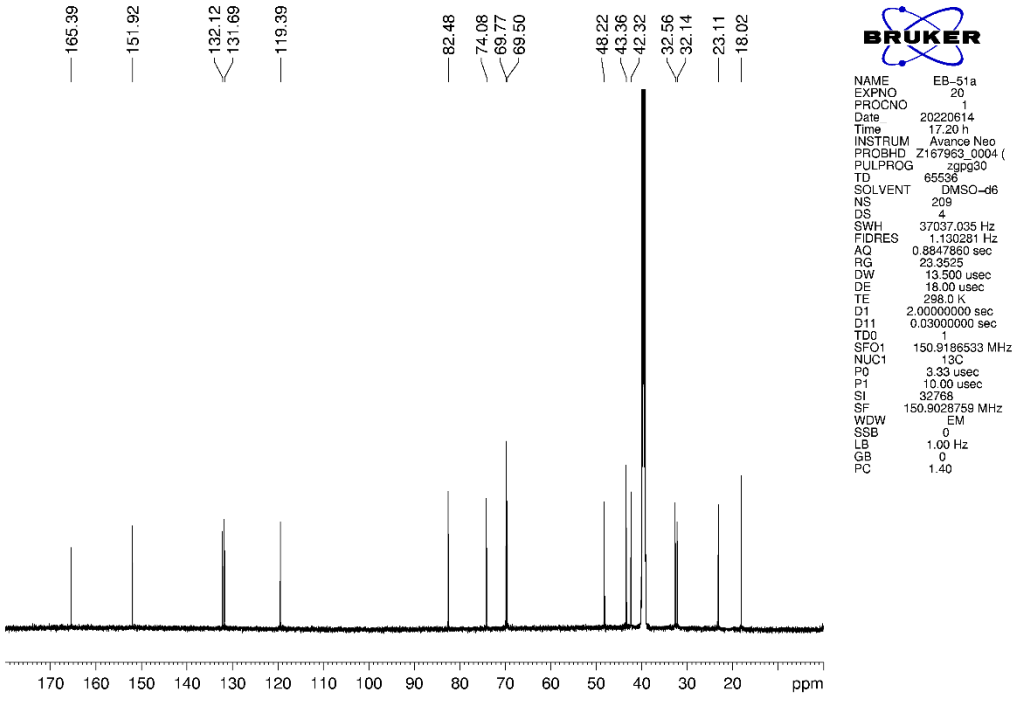


Figure S35. HSQC spectrum of **5**

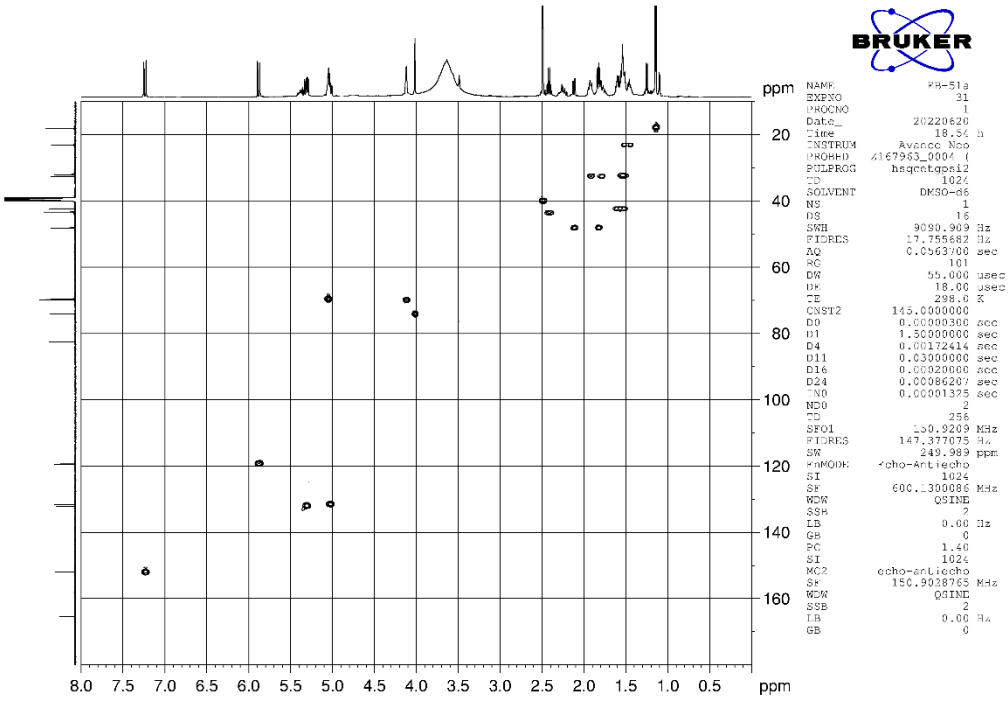


Figure S36. ^{1}H-^{13}C HMBC spectrum of **5**

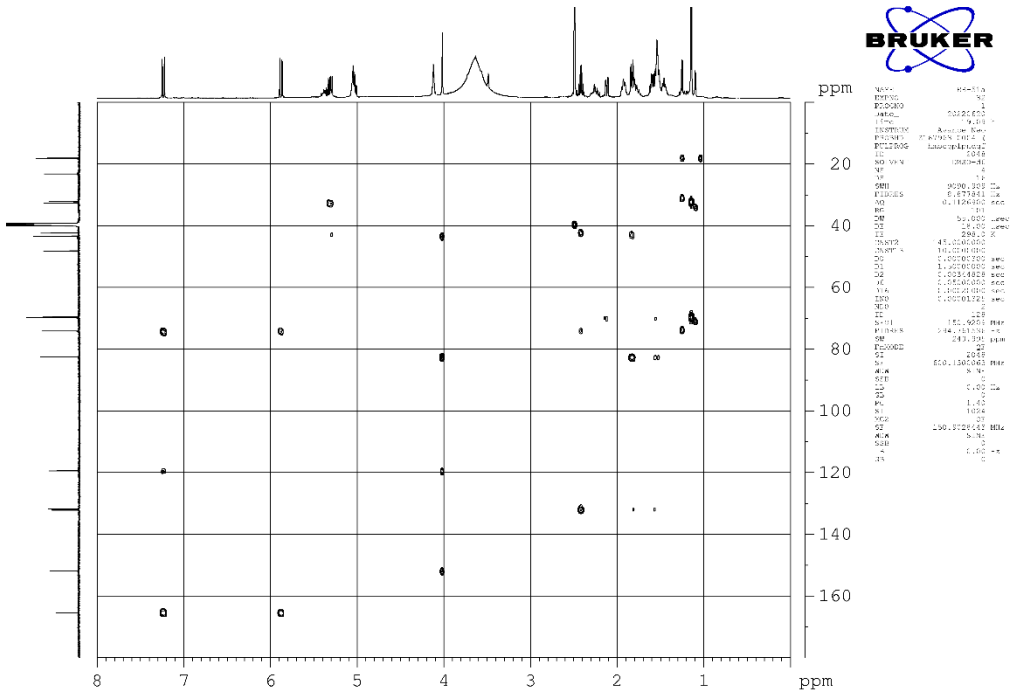


Figure S37. ^{1}H-^{1}H COSY spectrum of **5**

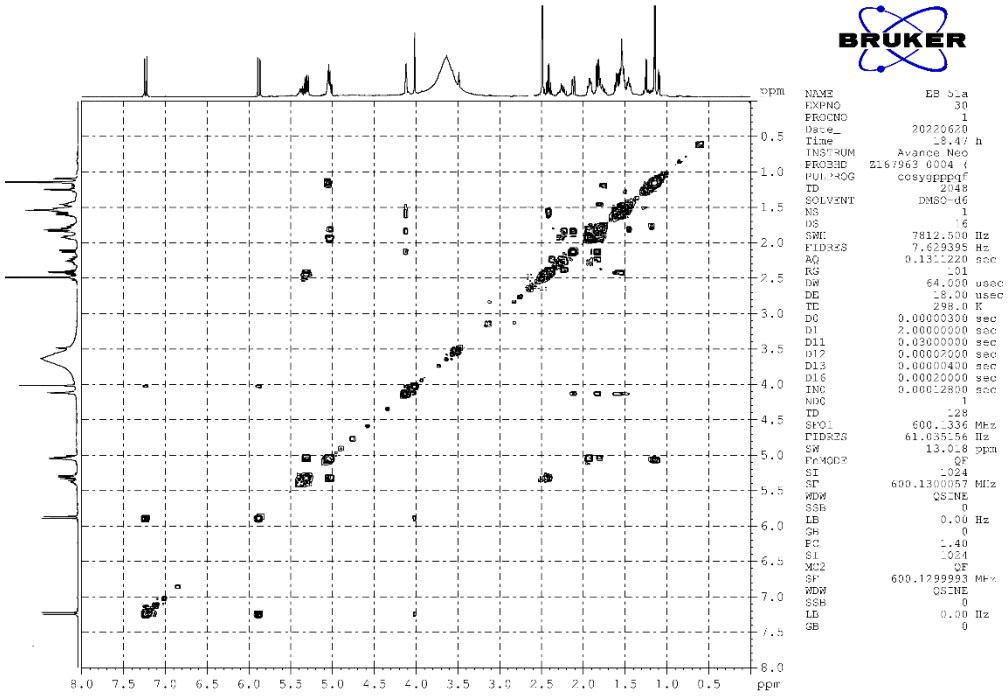


Figure S38. NOESY spectrum of **5**

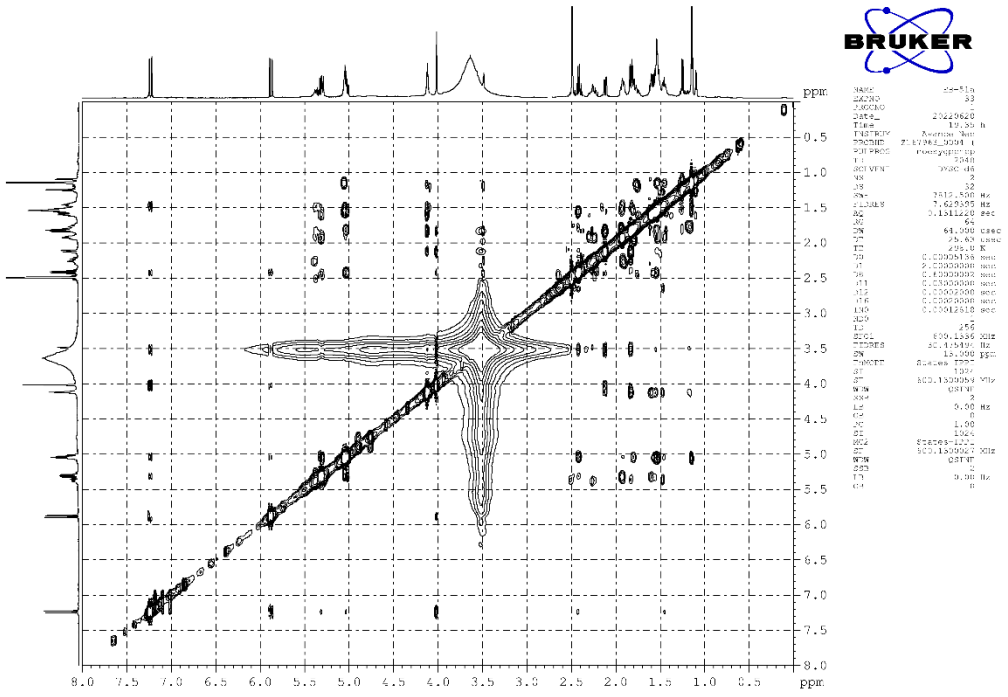


Figure S39. HRESIMS spectrum of **5**

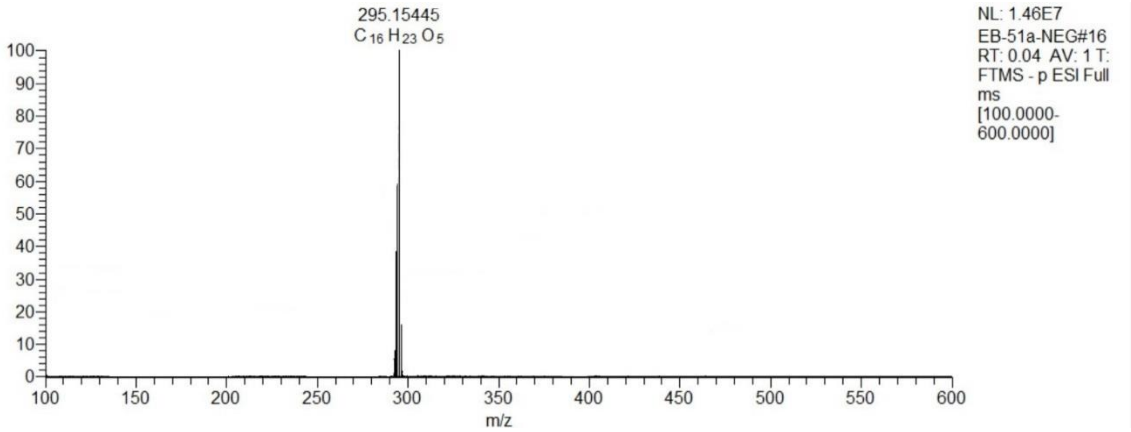


Figure S40. IR spectrum of **5**

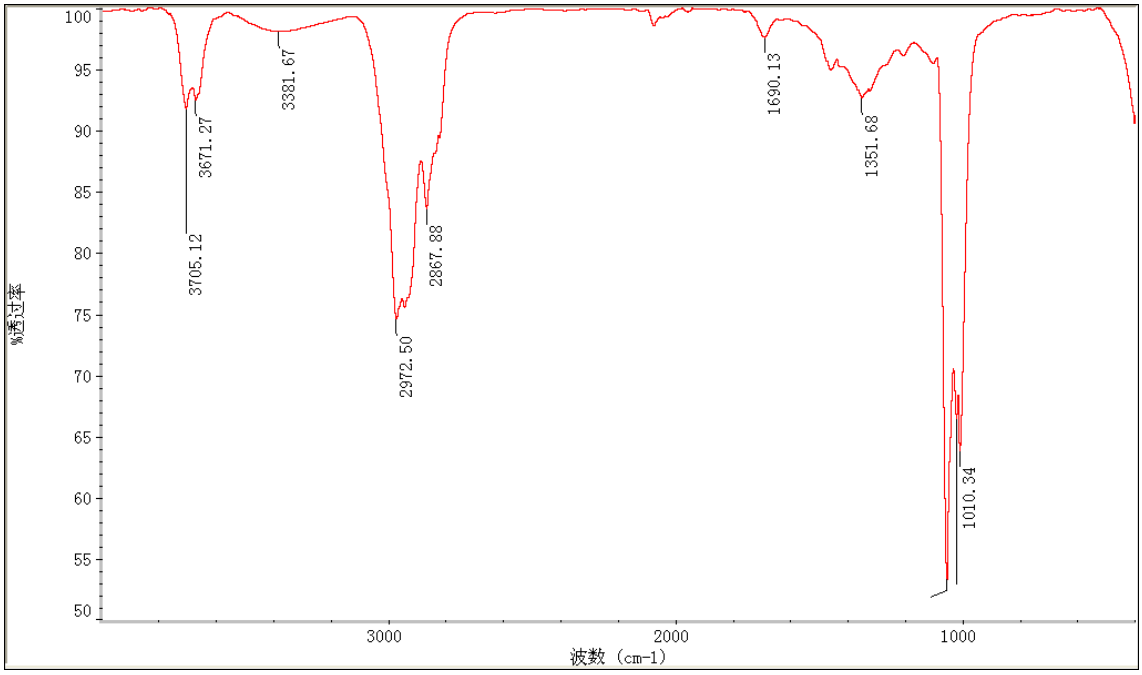


Figure S41. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **6**

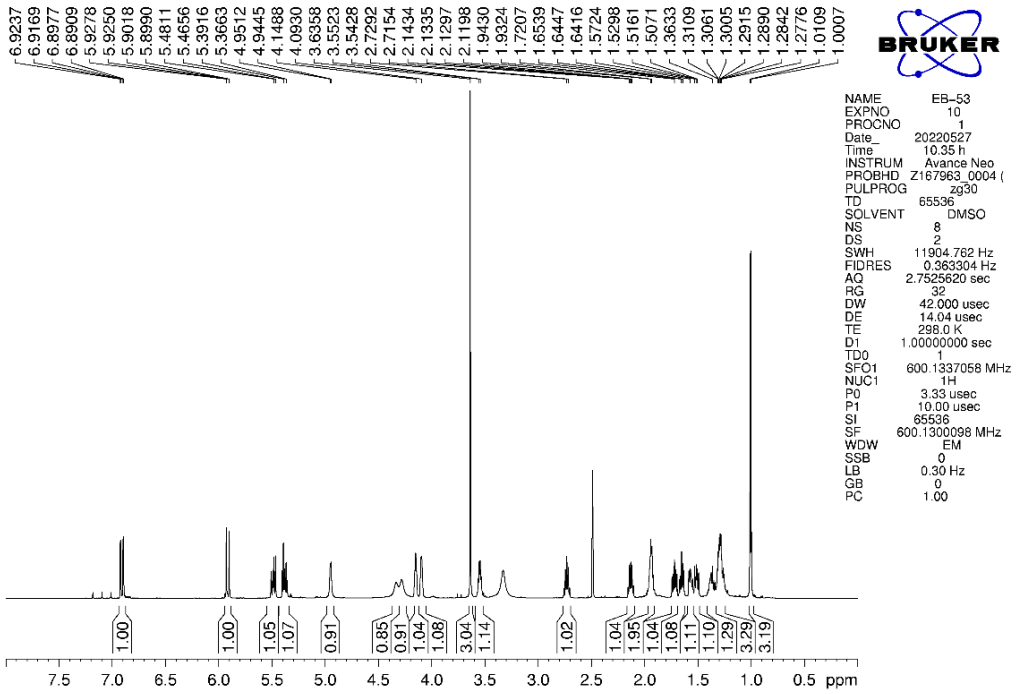


Figure S42. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **6**

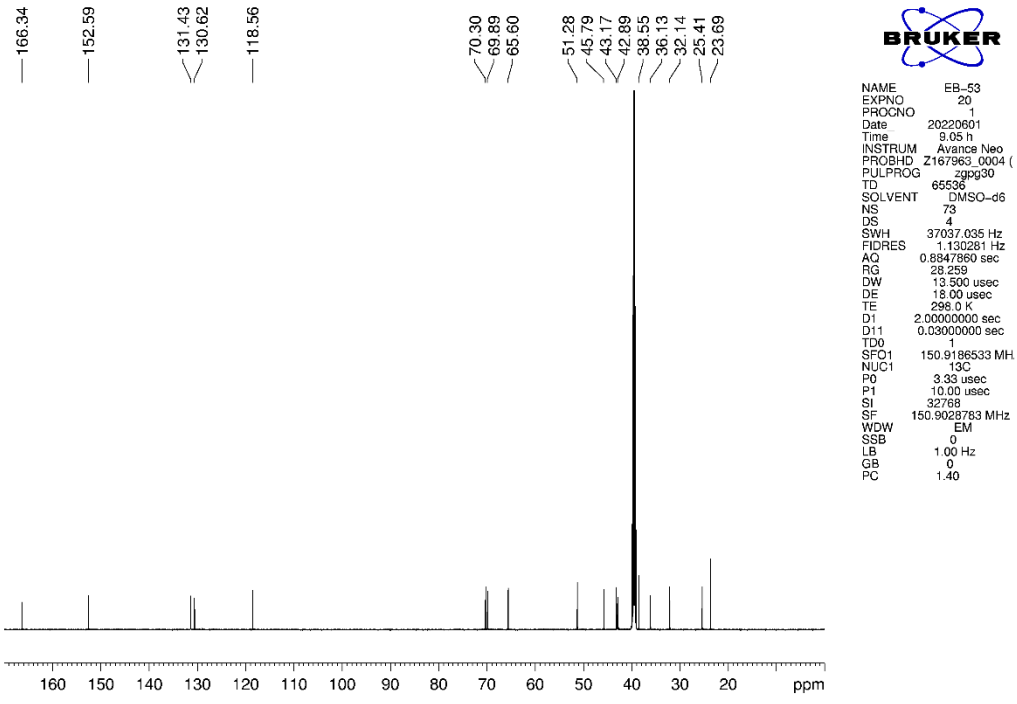


Figure S43. HSQC spectrum of **6**

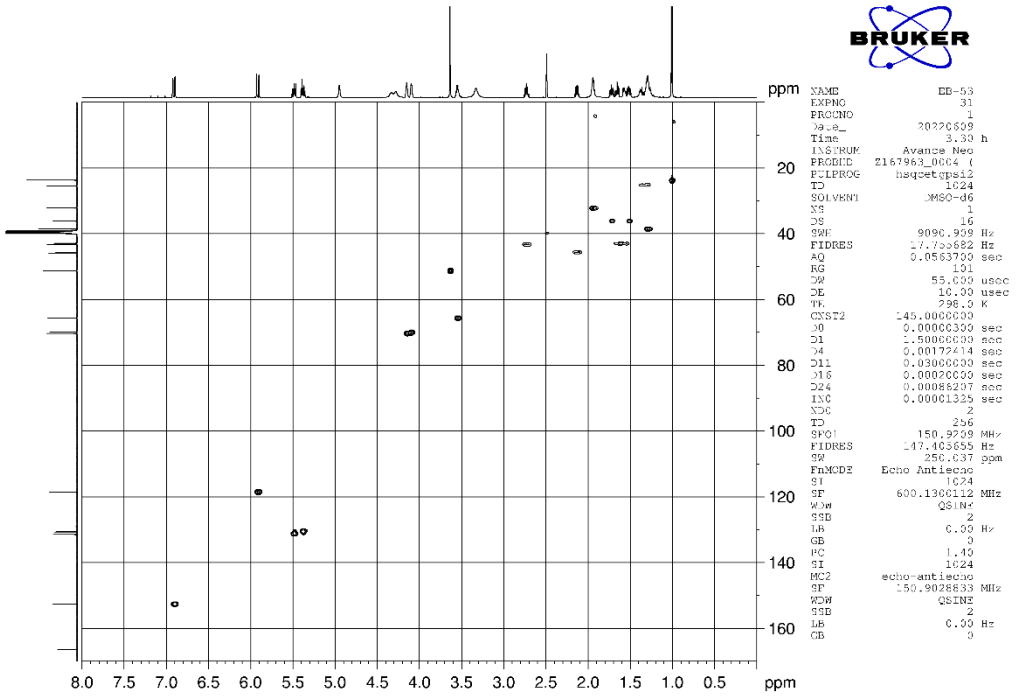


Figure S44. ^{1}H-^{13}C HMBC spectrum of **6**

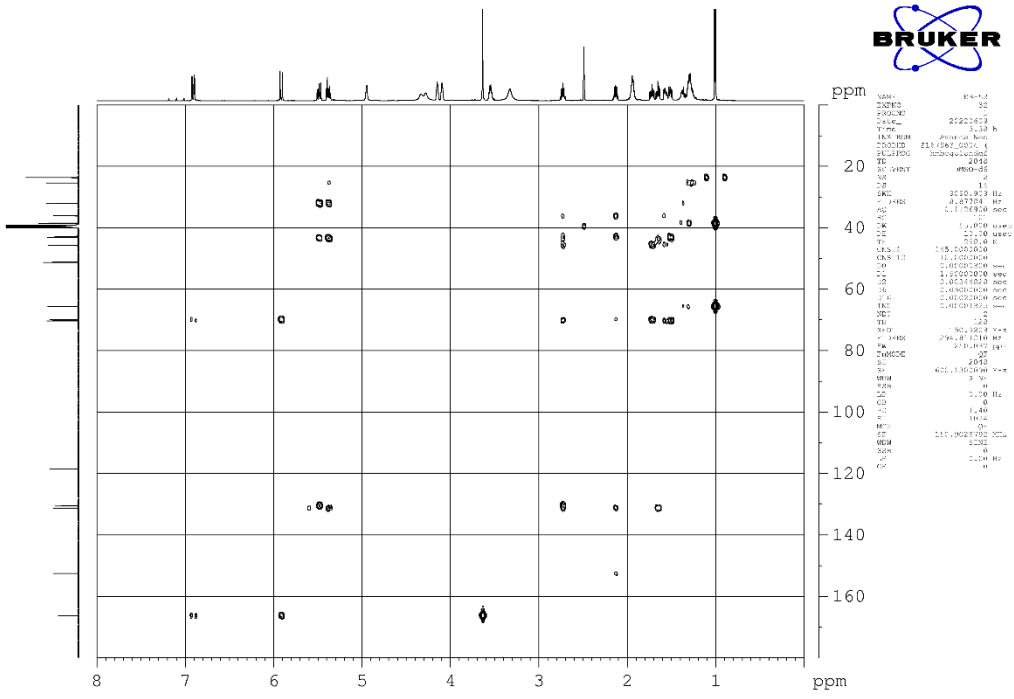


Figure S45. ^{1}H-^{1}H COSY spectrum of **6**

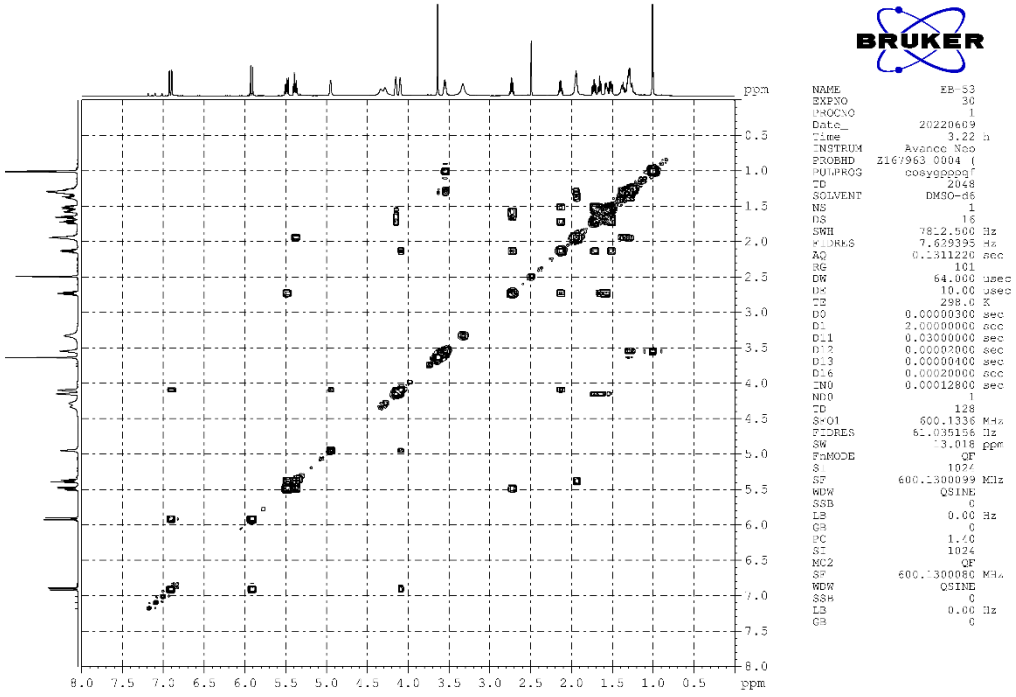


Figure S46. NOESY spectrum of **6**

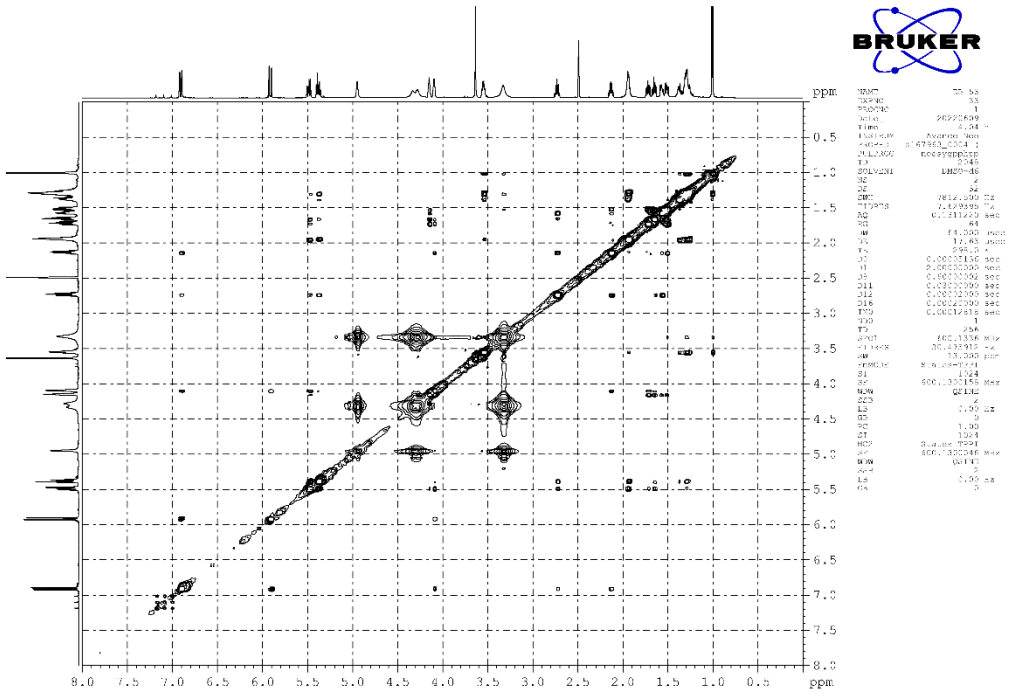


Figure S47. HRESIMS spectrum of **6**

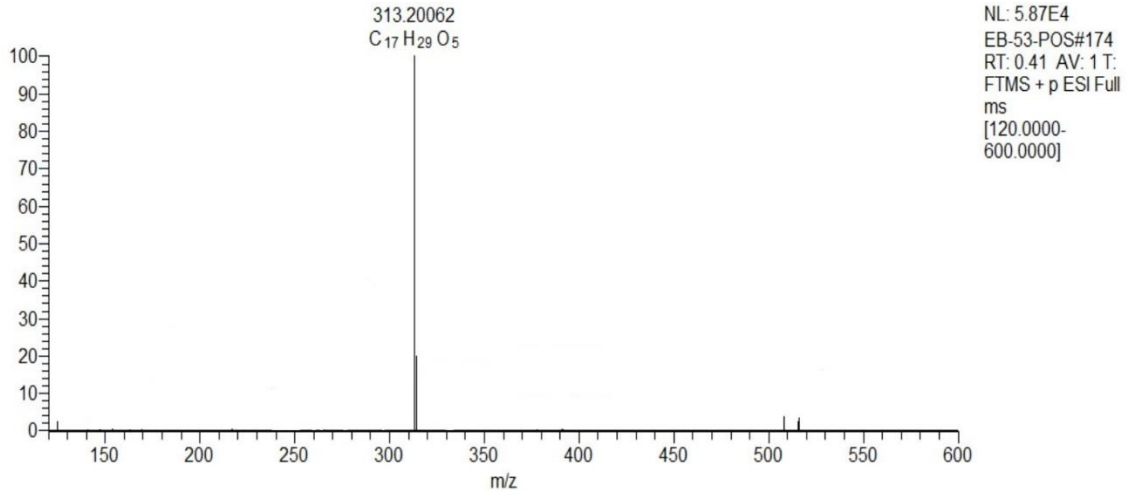


Figure S48. IR spectrum of **6**

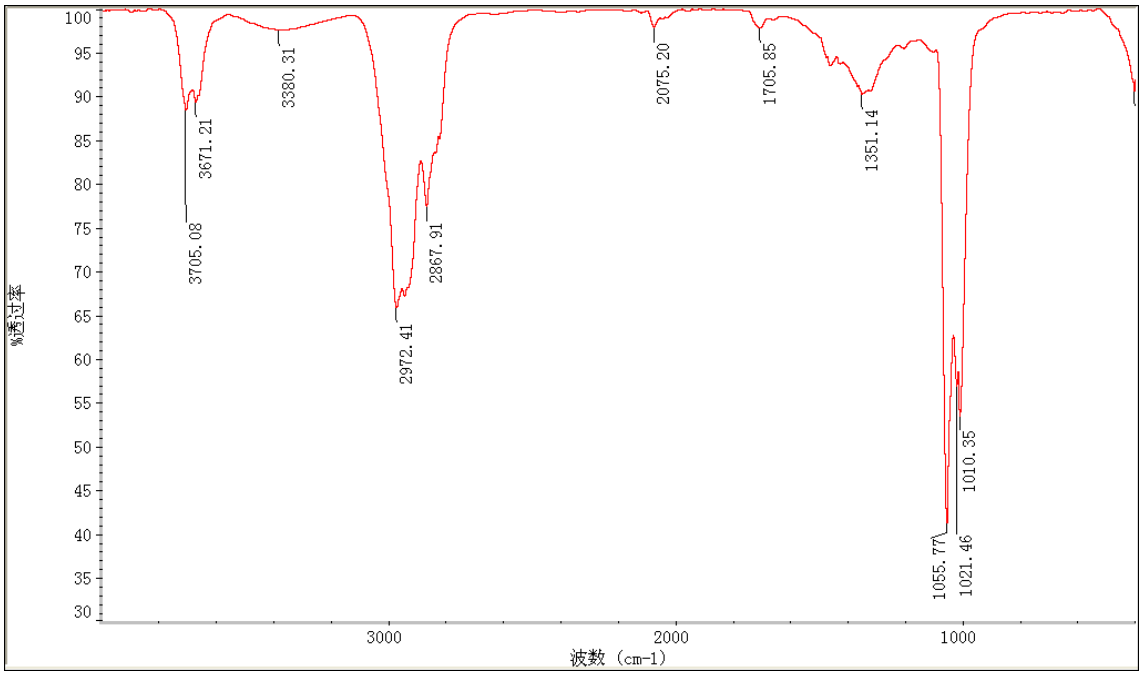


Figure S49. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **7**

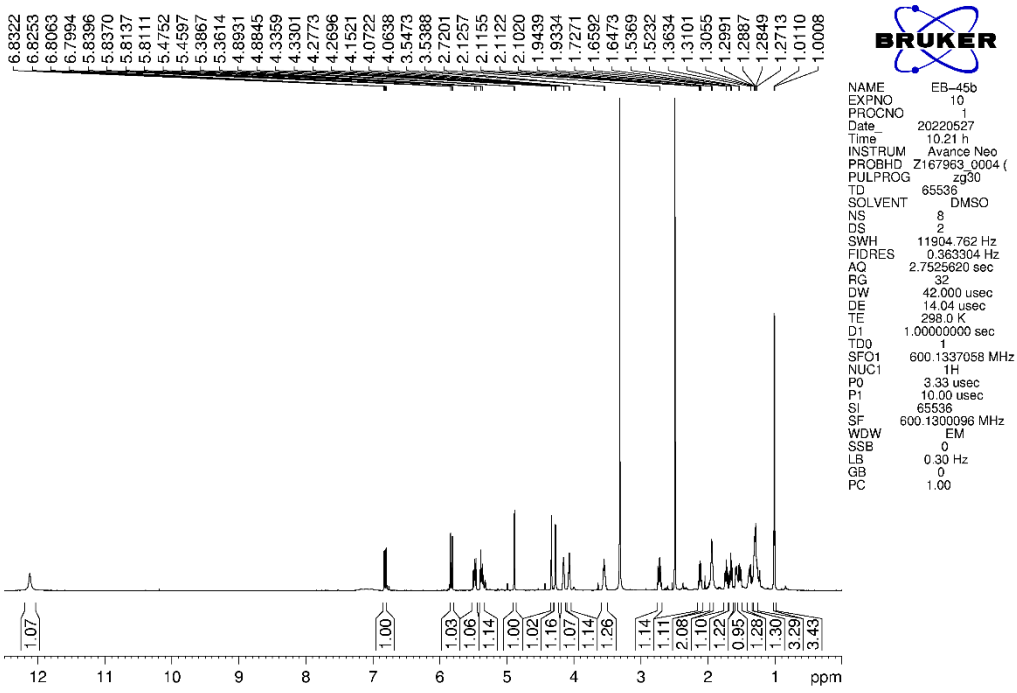


Figure S50. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **7**

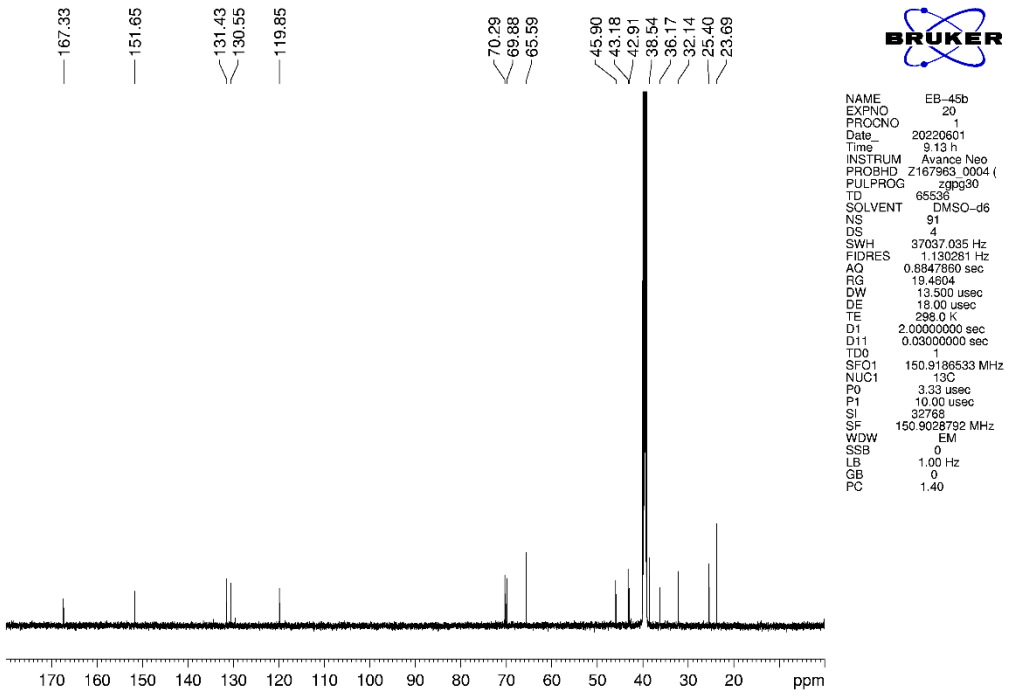


Figure S51. HSQC spectrum of **7**

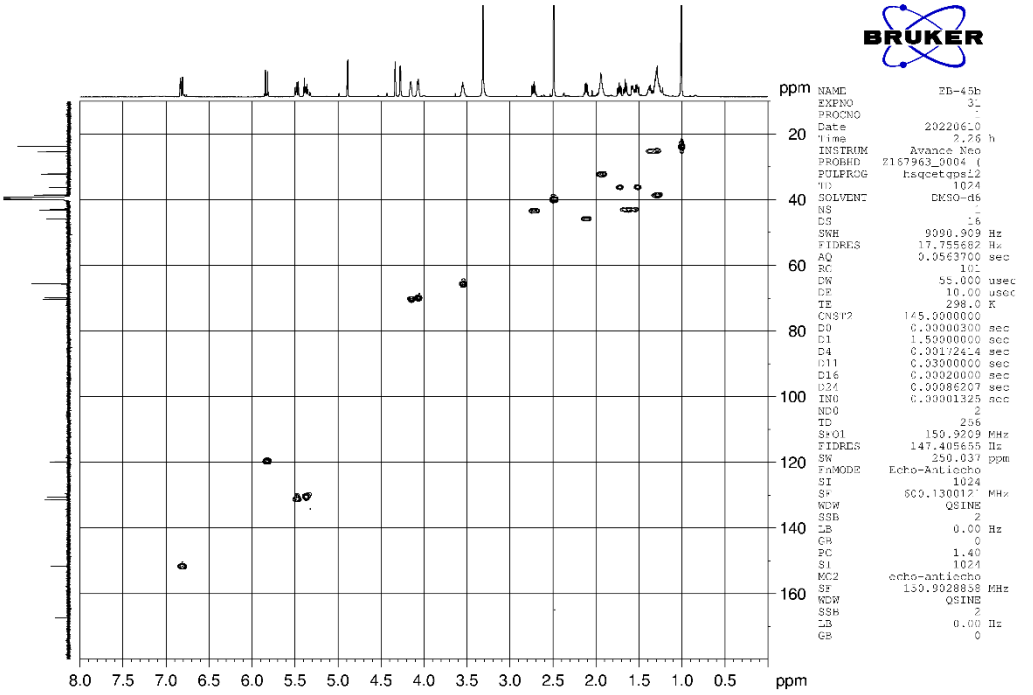


Figure S52. ^{1}H-^{13}C HMBC spectrum of **7**

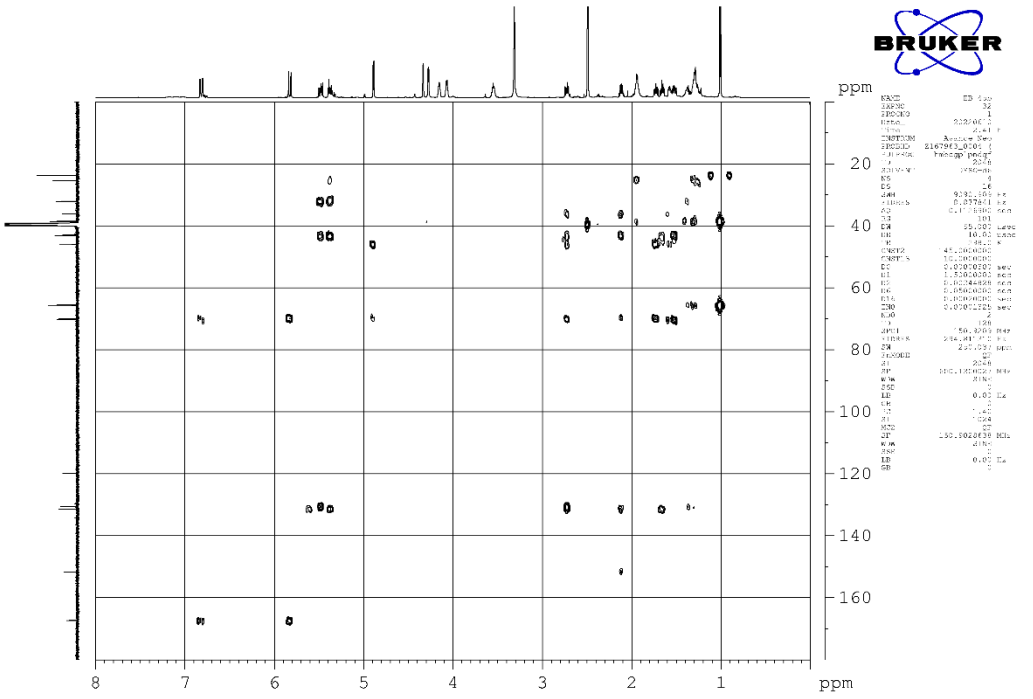


Figure S53. ^{1}H-^{1}H COSY spectrum of **7**

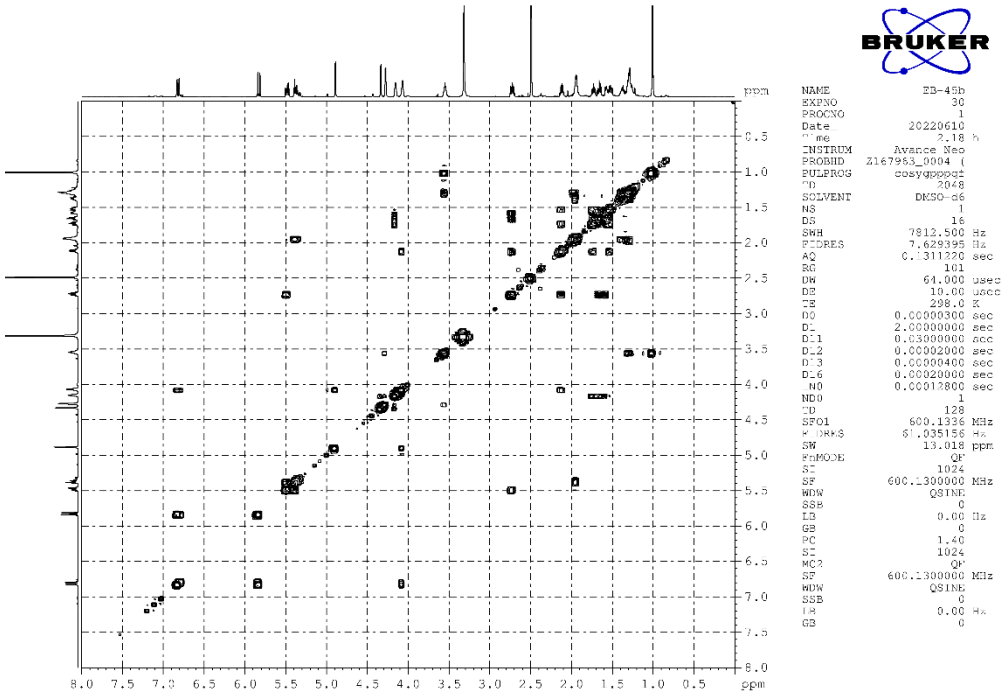


Figure S54. NOESY spectrum of **7**

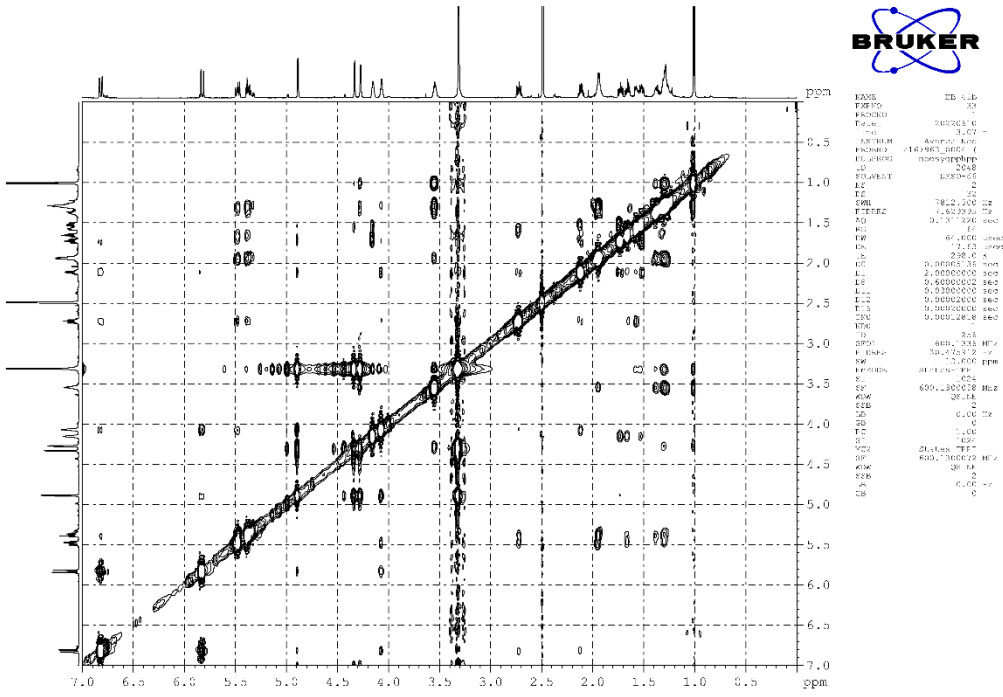


Figure S55. HRESIMS spectrum of **7**

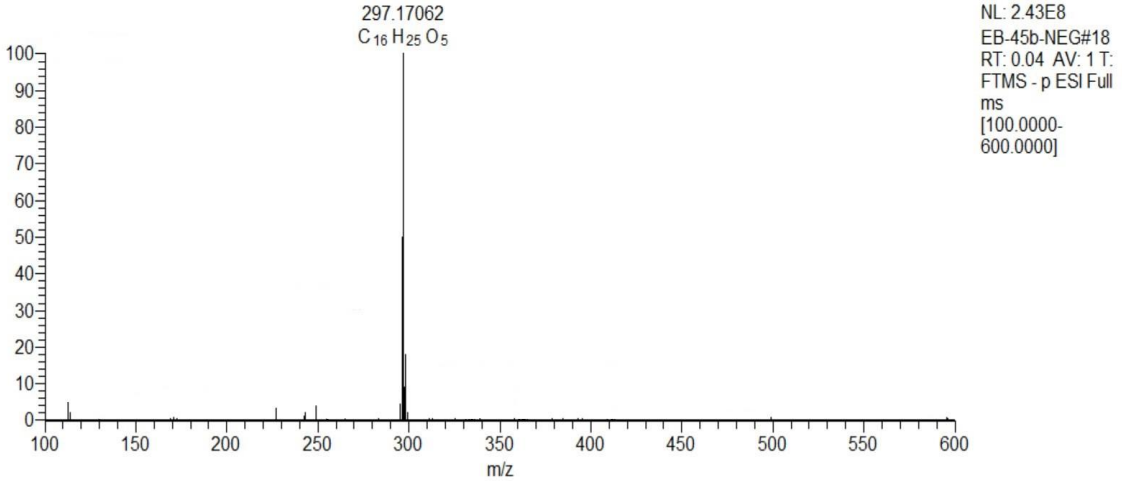


Figure S56. IR spectrum of **7**

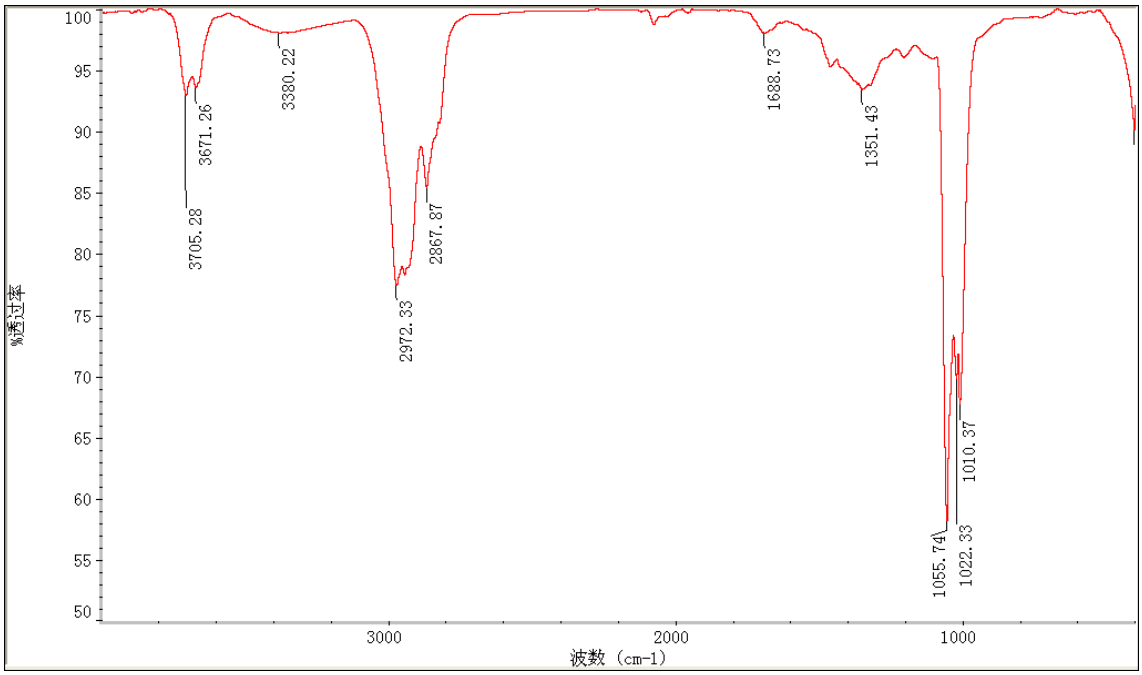


Figure S57. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **8**

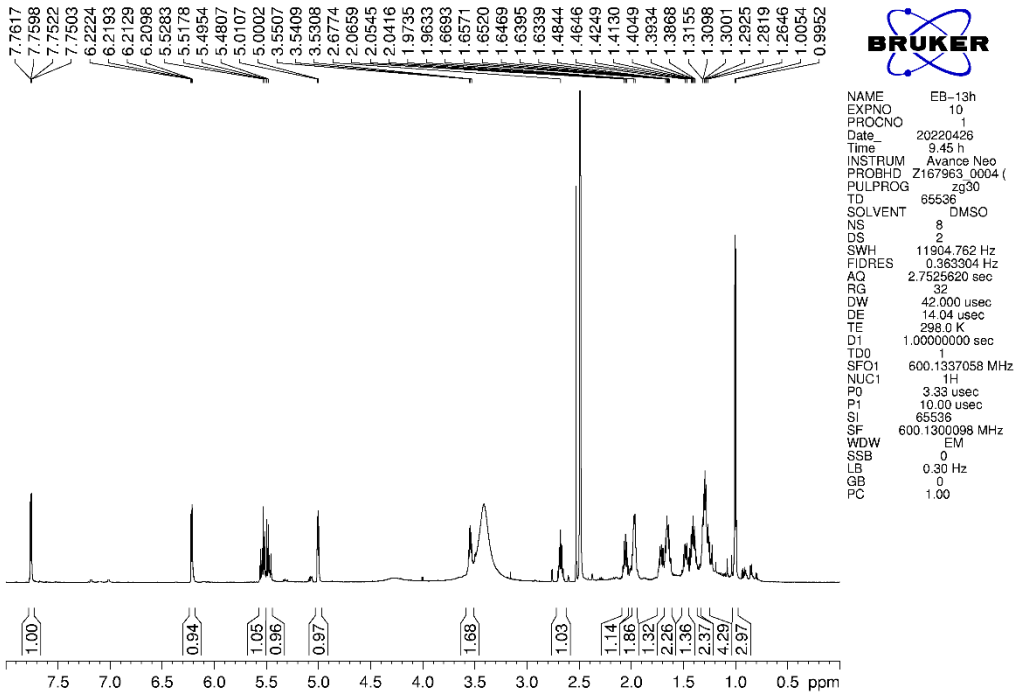


Figure S58. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **8**

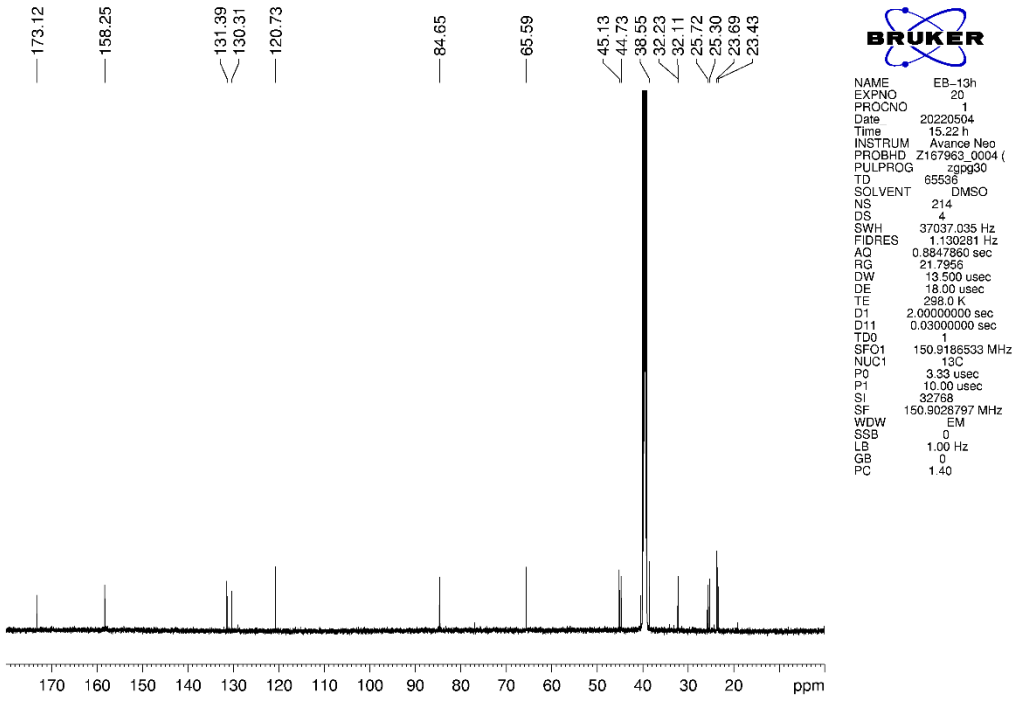


Figure S59. HSQC spectrum of **8**

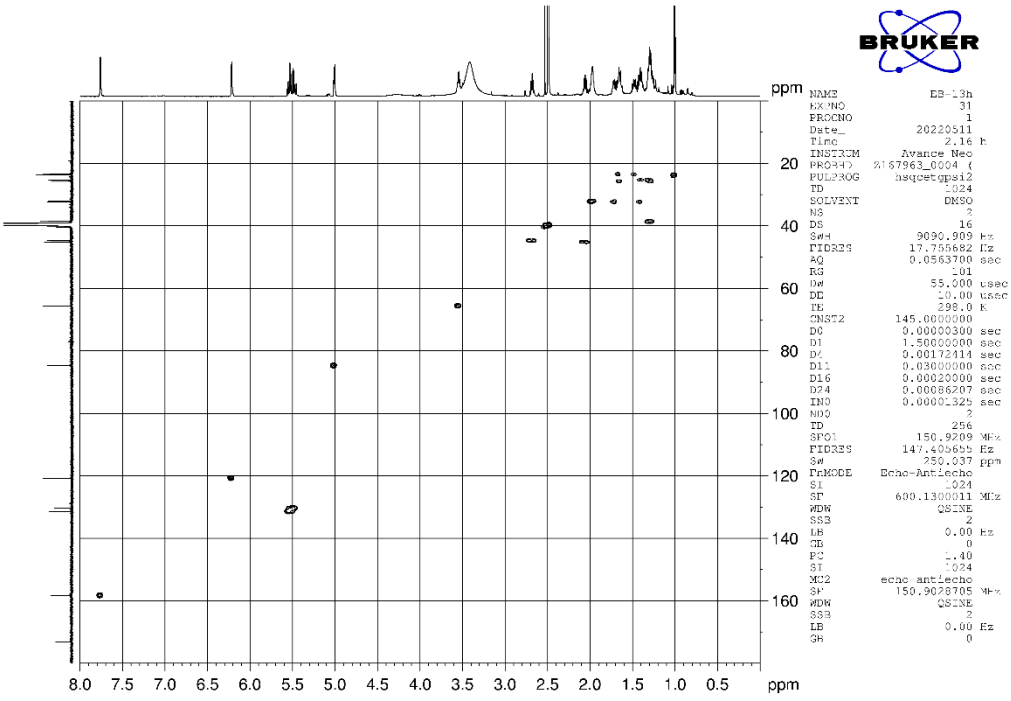


Figure S60. ^{1}H-^{13}C HMBC spectrum of **8**

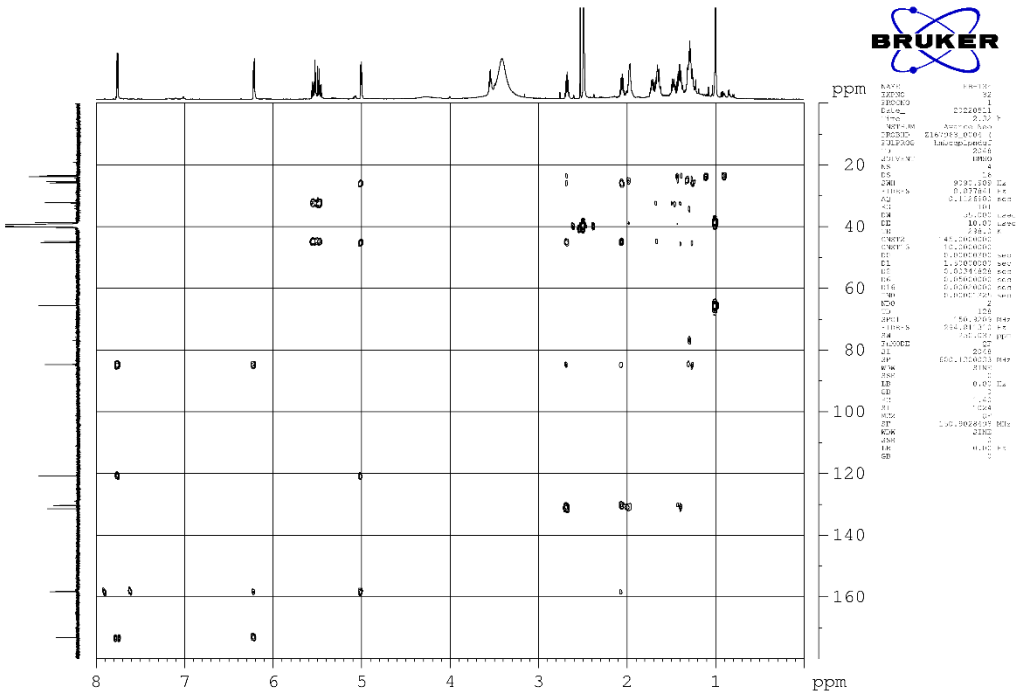


Figure S61. ^{1}H-^{1}H COSY spectrum of **8**

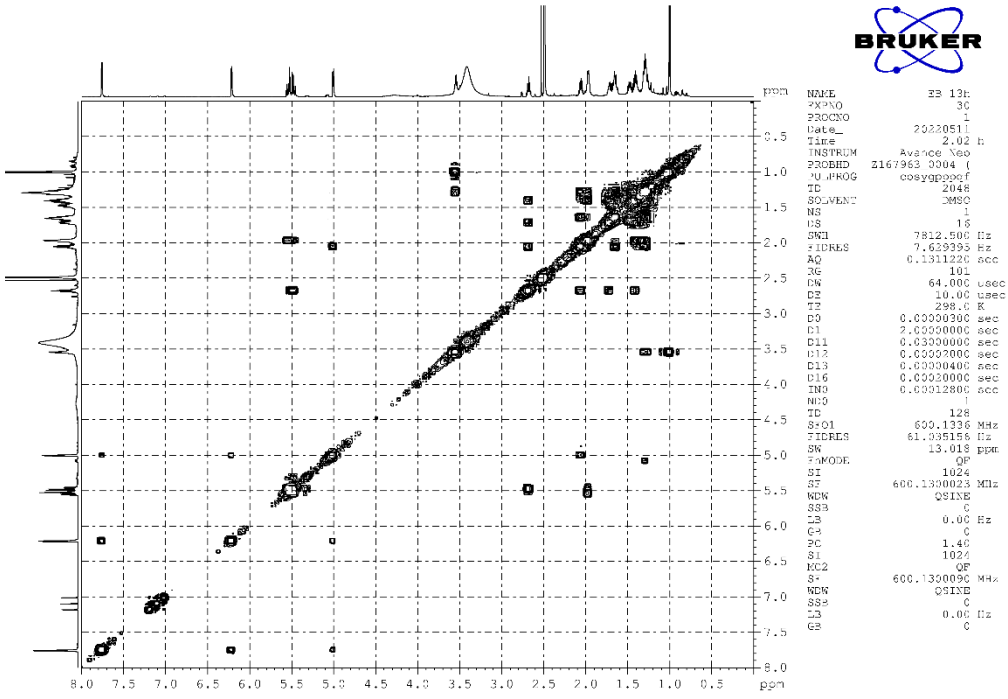


Figure S62. NOESY spectrum of **8**

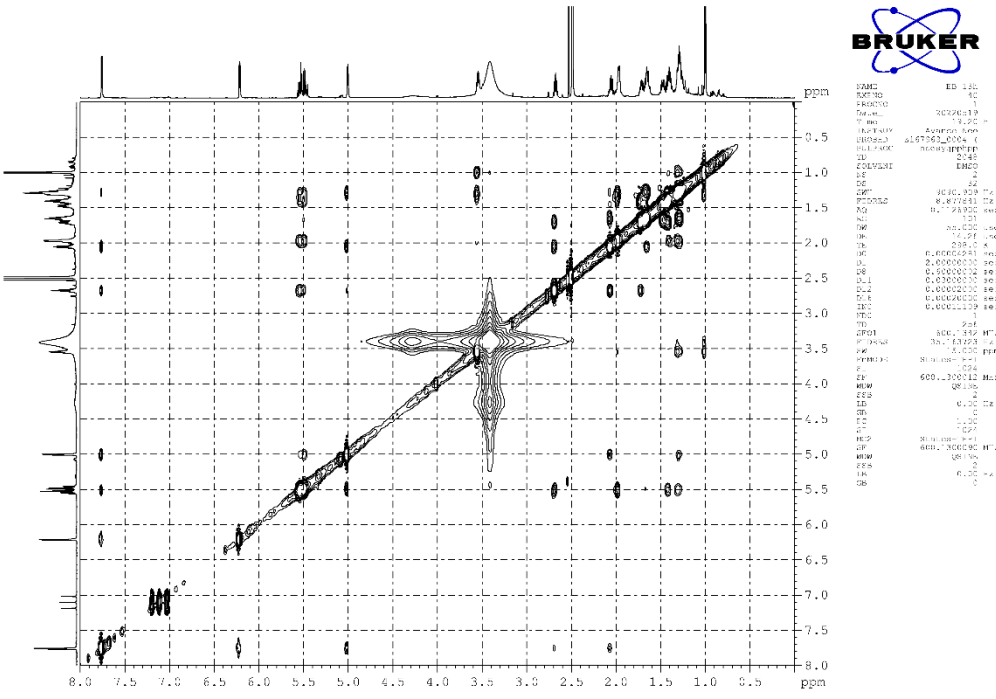


Figure S63. HRESIMS spectrum of **8**

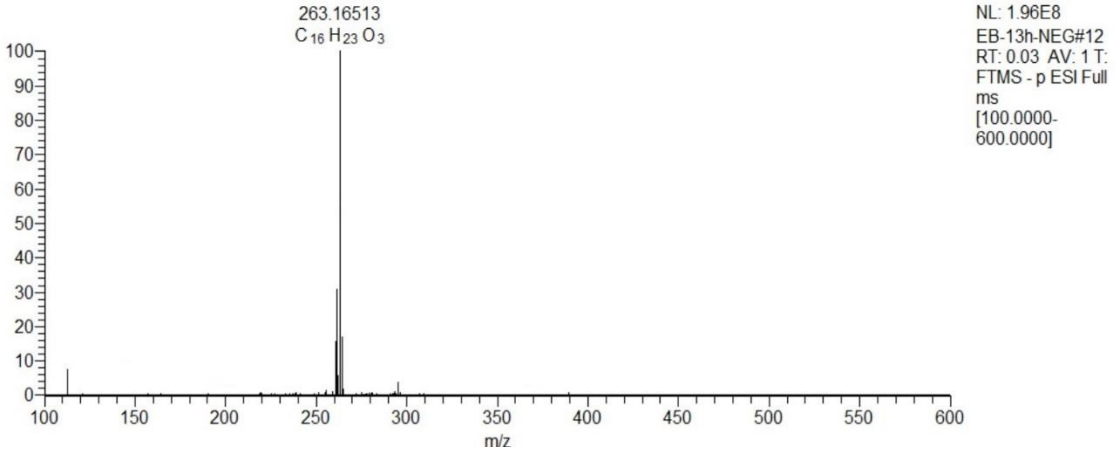


Figure S64. IR spectrum of **8**

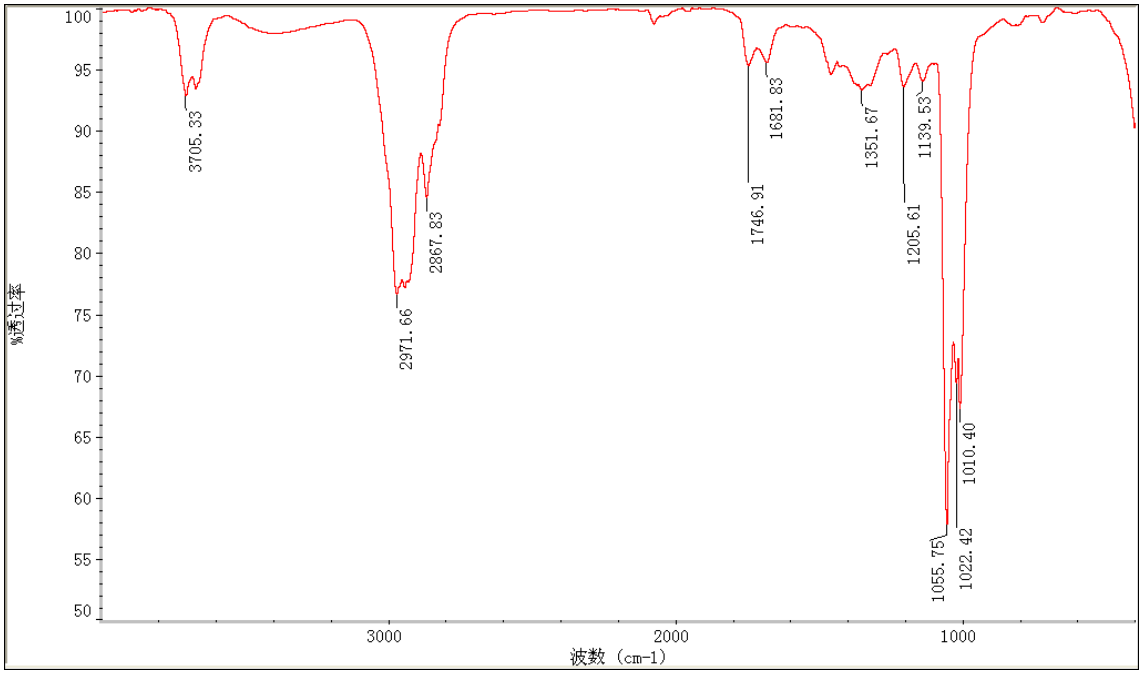


Figure S65. ^{1}H NMR (600 MHz, DMSO-d_6) spectrum of **9**

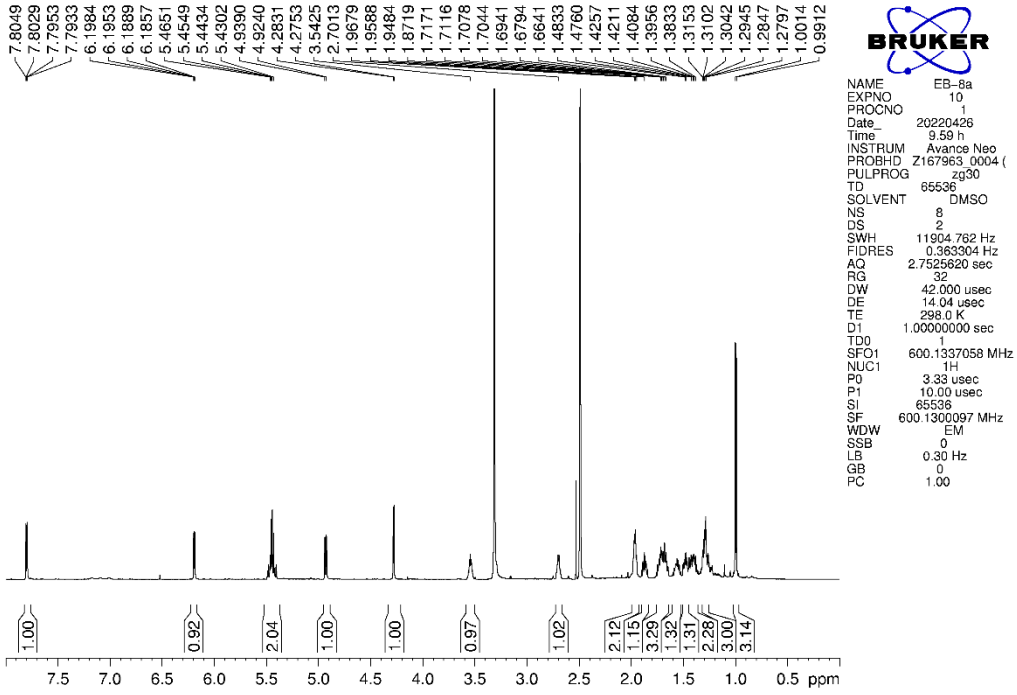


Figure S66. ^{13}C NMR (150 MHz, DMSO-d_6) spectrum of **9**

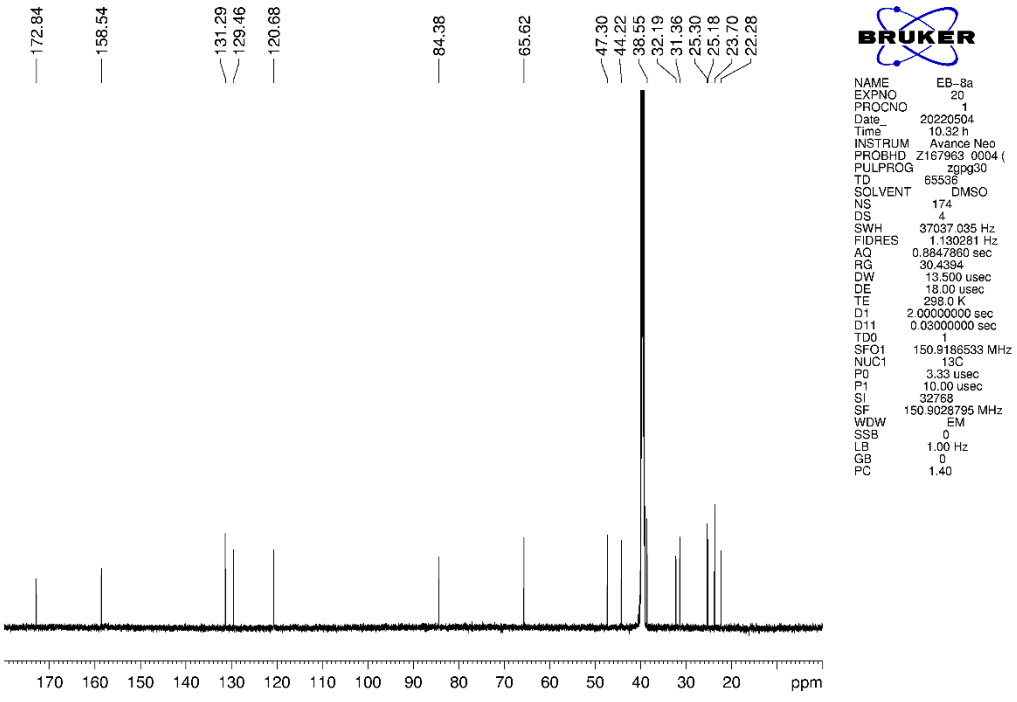


Figure S67. HSQC spectrum of **9**

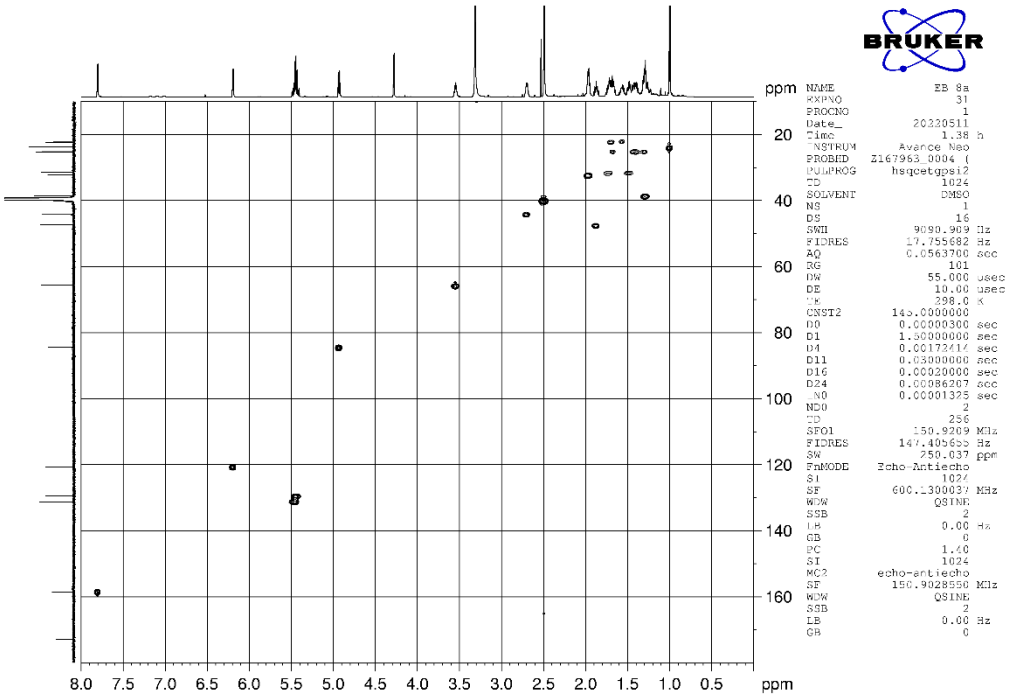


Figure S68. ^{1}H-^{13}C HMBC spectrum of **9**

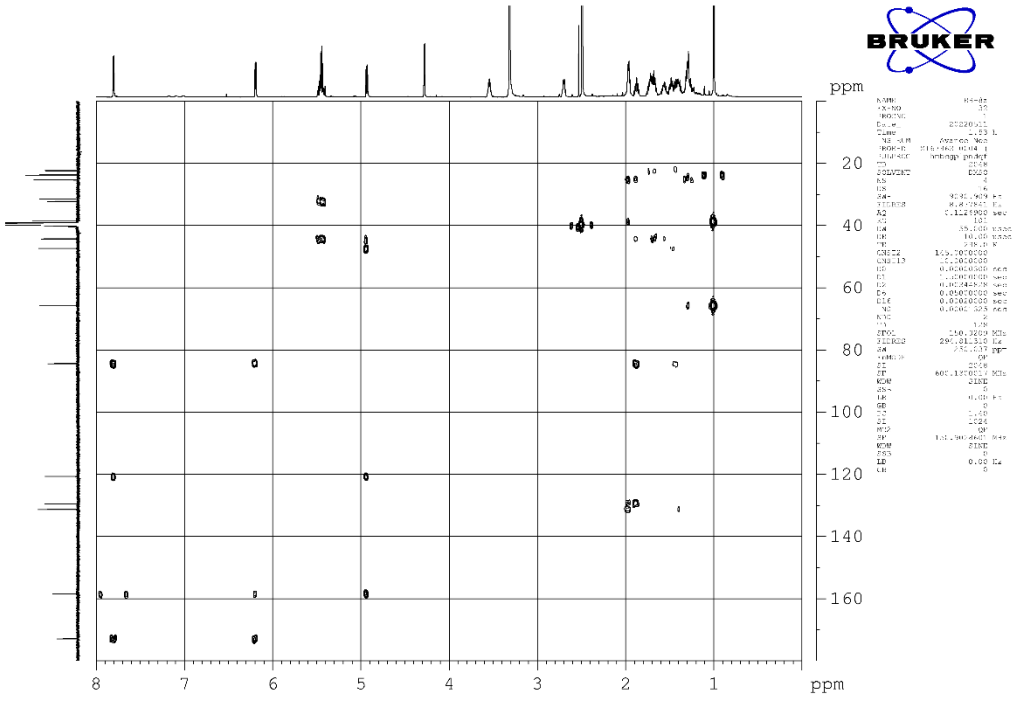


Figure S69. ^{1}H-^{1}H COSY spectrum of **9**

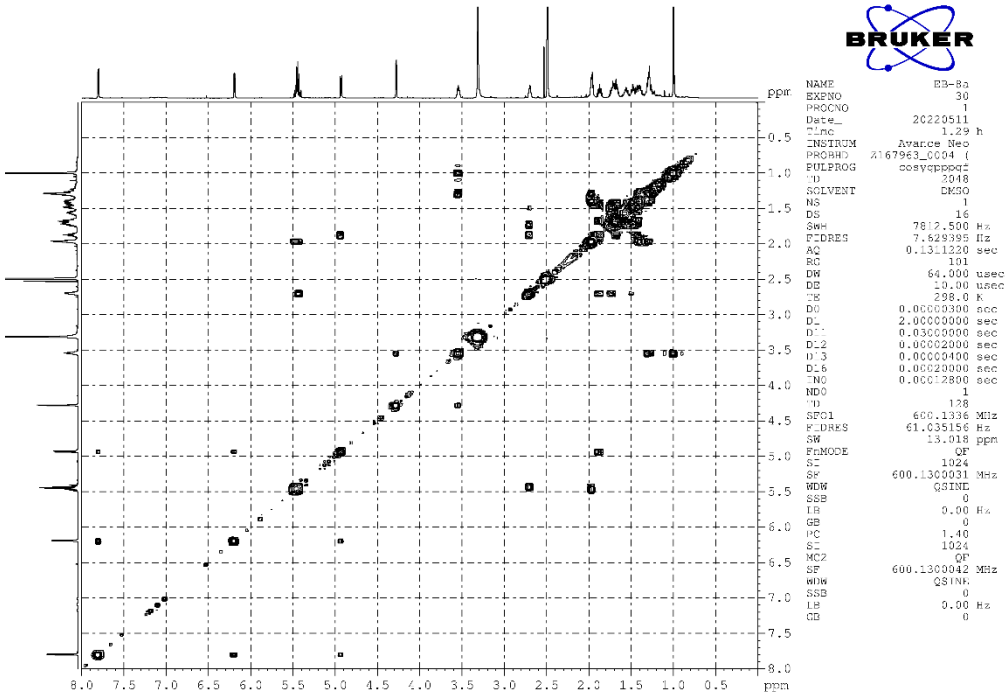


Figure S70. NOESY spectrum of **9**

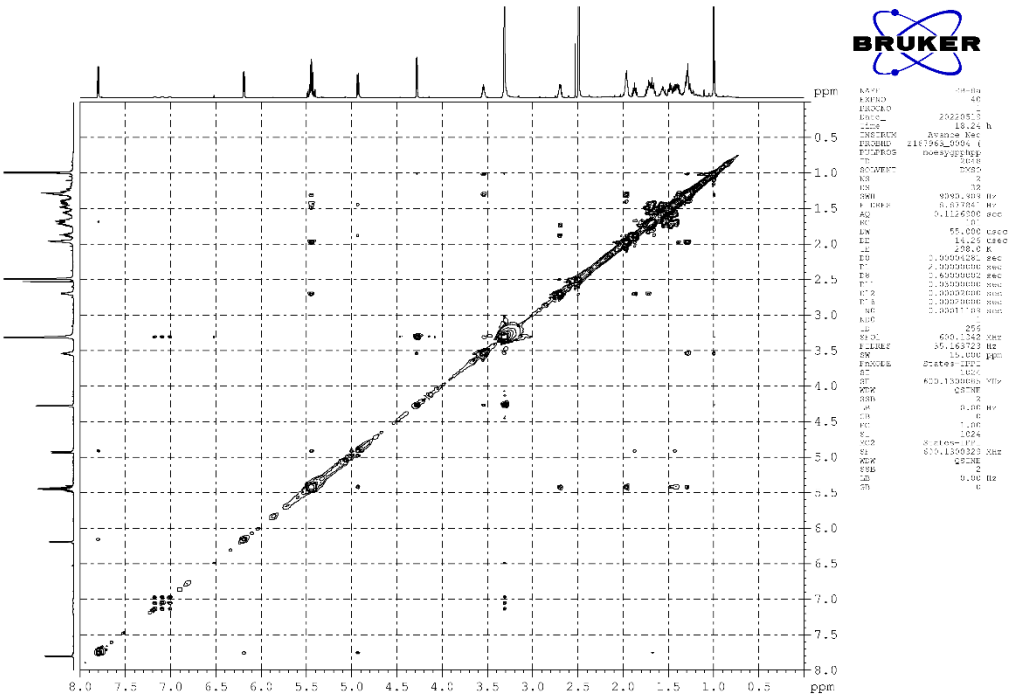


Figure S71. HRESIMS spectrum of **9**

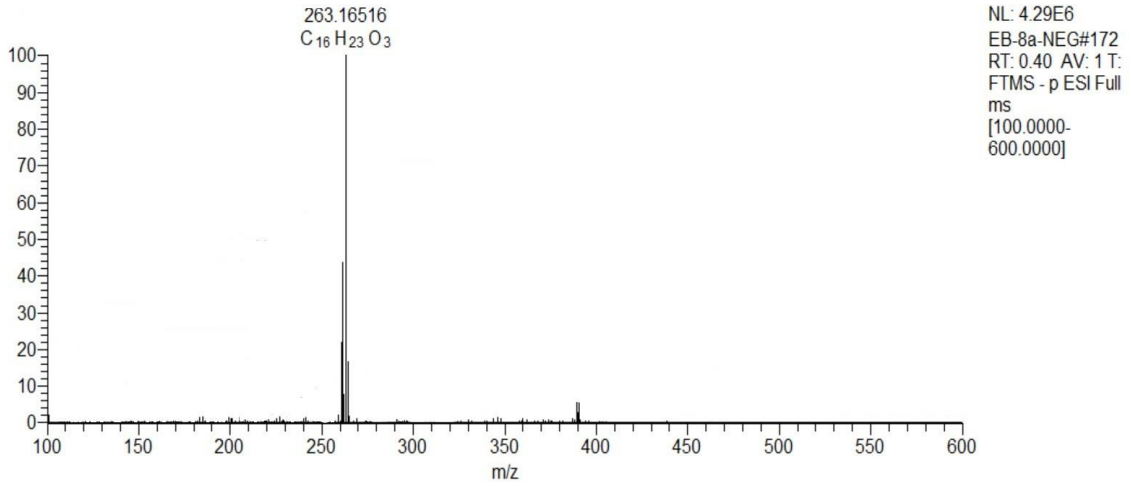


Figure S72. IR spectrum of **9**

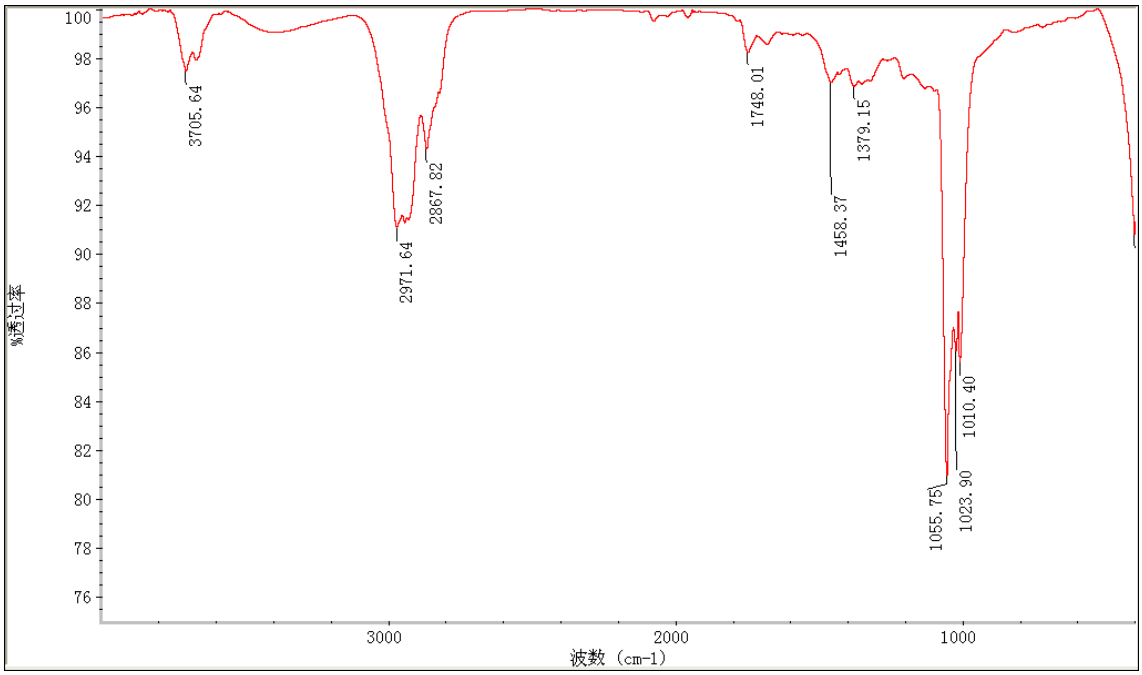
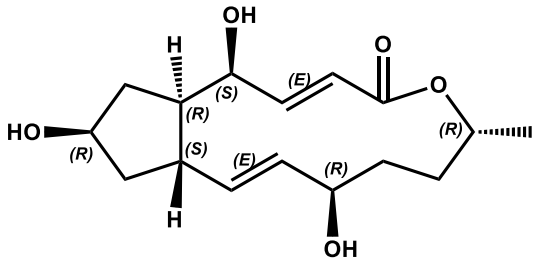
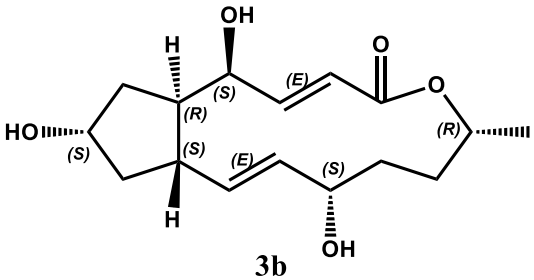


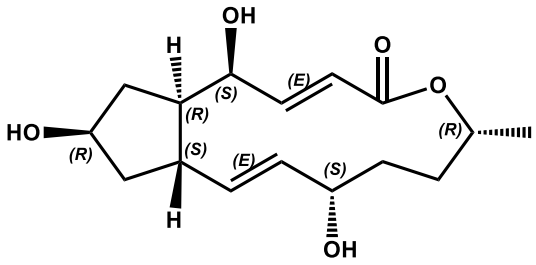
Figure S73. Detailed DP4+ probabilities of all isomers for compound **3**



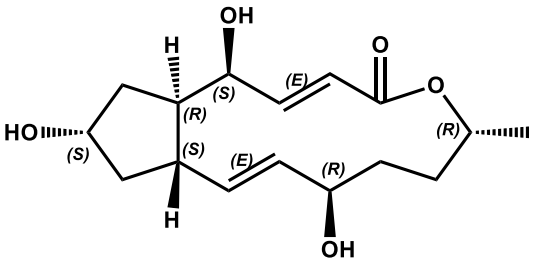
3a



3b



3c

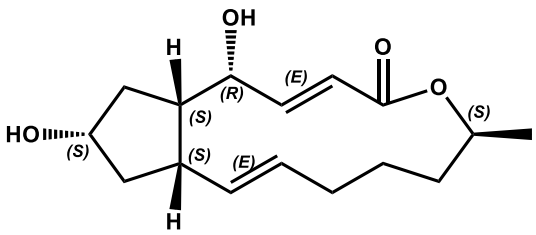


3d

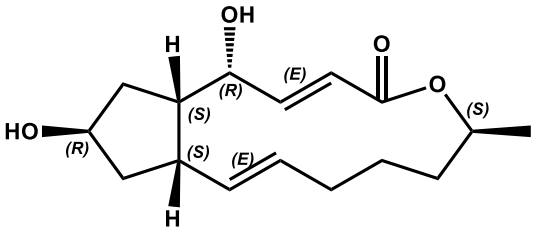
Functional	Solvent?	Basis Set	Type of Data
B3LYP	PCM	6-311+G(d,p)	Unscaled Shifts

		DP4+	3.39%	0.00%	96.61%	0.00%	-
Nuclei	sp2?	Experimental	3a	3b	3c	3d	Isomer 5
C	x	165.10	174.90	175.58	172.07	175.25	
C	x	153.30	162.78	164.58	166.04	164.98	
C	x	133.40	140.21	137.68	144.66	136.45	
C	x	131.30	141.02	147.45	139.83	150.72	
C	x	118.50	127.27	128.26	124.06	128.15	
C		71.50	80.21	80.47	81.11	81.53	
C		70.00	79.75	77.79	78.39	77.98	
C		68.80	79.20	81.05	78.02	80.94	
C		68.70	77.89	76.82	77.72	77.38	
C		43.00	49.65	47.67	48.87	46.22	
C		47.30	54.11	50.36	53.49	59.30	
C		39.00	45.11	43.25	45.45	46.48	
C		37.90	43.47	43.14	42.06	43.29	
C		31.50	34.50	32.05	37.39	32.90	
C		27.60	29.49	30.84	30.66	27.66	
C		17.40	18.25	18.23	21.58	18.45	

Figure S74. Detailed DP4+ probabilities of all isomers for compound **4**



4a

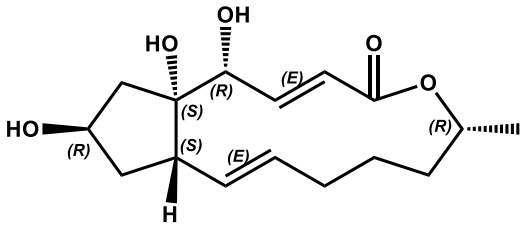


4b

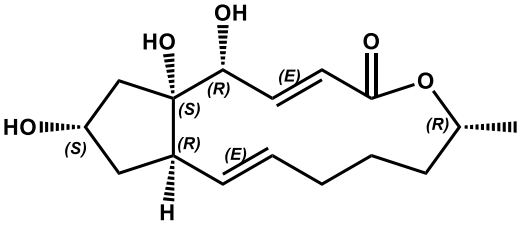
Functional	Solvent?	Basis Set	Type of Data
B3LYP	PCM	6-311+G(d,p)	Unscaled Shifts

		DP4+	100.00%	0.00%	–	–	–
Nuclei	sp2?	Experimental	4a	4b	Isomer 3	Isomer 4	Isomer 5
C	x	166.4	174.0	174.5			
C	x	155.9	167.3	155.5			
C	x	135.9	146.0	142.9			
C	x	117.8	125.2	134.5			
C	x	127.9	138.1	134.2			
C		71.4	79.8	79.5			
C		70.9	81.0	79.3			
C		71.2	78.0	77.8			
C		47.3	59.6	50.9			
C		43.6	55.7	44.8			
C		43.5	49.6	41.9			
C		38.9	46.05	38.9			
C		28.9	31.15	38.2			
C		33.5	40.41	36.3			
C		24.5	30.14	28.4			
C		20.8	22.24	20.6			

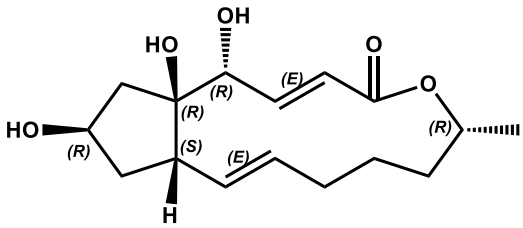
Figure S75. Detailed DP4+ probabilities of all isomers for compound **5**



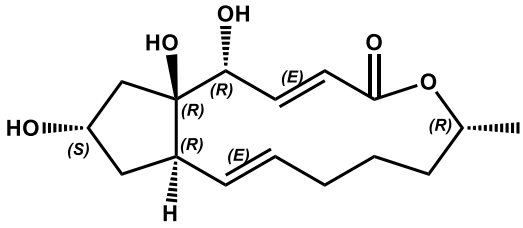
5a



5b



5c

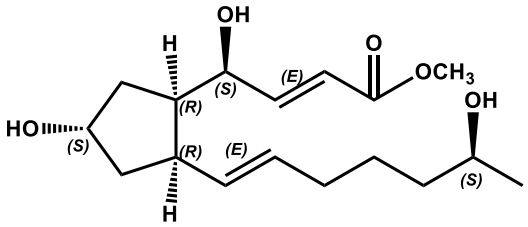


5d

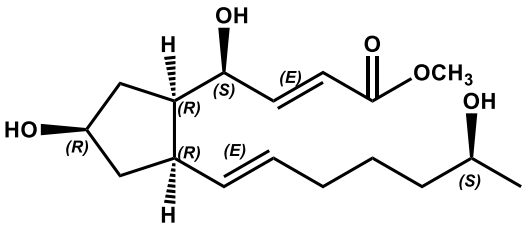
Functional	Solvent?	Basis Set	Type of Data
B3LYP	PCM	6-311+G(d,p)	Unscaled Shifts

		DP4+	100.00%	0.00%	0.00%	0.00%	-
Nuclei	sp2?	Experimental	5a	5b	5c	5d	Isomer 5
C	x	165.40	176.37	172.80	174.32	170.95	
C	x	151.90	161.49	159.30	161.59	162.48	
C	x	132.10	137.20	141.60	140.11	138.19	
C	x	131.70	143.64	140.40	137.48	145.61	
C	x	119.40	128.45	130.00	125.54	128.84	
C		82.50	89.07	94.30	94.67	91.36	
C		69.80	76.89	80.90	80.14	78.98	
C		74.10	81.82	81.40	79.65	84.91	
C		69.50	75.12	78.70	79.51	78.50	
C		43.40	49.54	61.40	58.70	49.74	
C		42.30	42.16	48.90	41.73	48.05	
C		48.20	56.32	51.40	44.70	52.08	
C		32.10	37.52	36.20	36.43	36.46	
C		32.60	35.08	31.80	35.72	37.99	
C		23.10	29.30	31.20	31.68	32.13	
C		18.00	21.62	23.00	22.23	22.14	

Figure S76. Detailed DP4+ probabilities of all isomers for compound **6**



6a



6b

Functional	Solvent?	Basis Set	Type of Data
B3LYP	PCM	6-311+G(d,p)	Unscaled Shifts

		DP4+	99.97%	0.03%	–	–	–
Nuclei	sp2?	Experimental	6a	6b	Isomer 3	Isomer 4	Isomer 5
C	x	166.3	176.58	177.99			
C	x	152.6	169.30	166.47			
C	x	131.4	141.63	136.91			
C	x	130.6	142.73	136.24			
C	x	118.6	123.42	123.55			
C		69.9	78.98	81.31			
C		70.3	79.65	80.44			
C		65.6	72.83	74.47			
C		45.8	55.44	56.56			
C		51.3	55.50	55.37			
C		43.2	46.60	52.02			
C		36.1	42.24	45.54			
C		38.5	39.84	44.13			
C		42.9	43.94	44.52			
C		32.1	36.58	36.77			
C		25.4	29.05	27.41			
C		23.7	20.91	24.64			

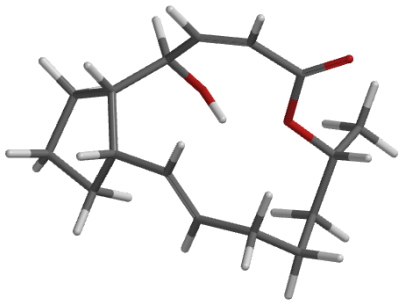
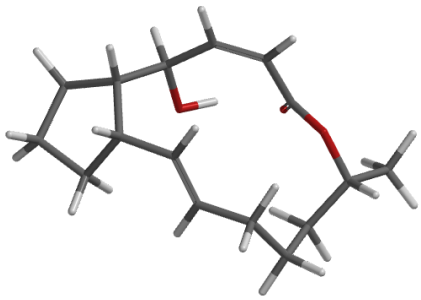
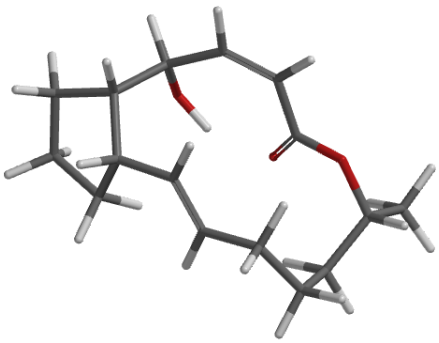
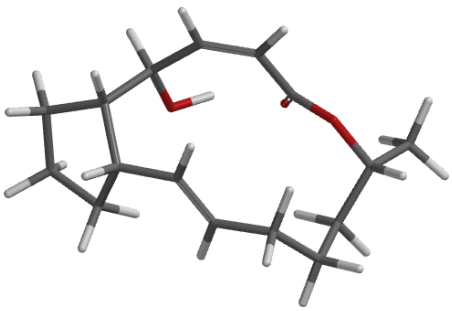
Table S1 ^{1}H and ^{13}C NMR Data for brefeldin A, **1**, and **4** in DMSO-d_6 (600/150 MHz, δ in ppm)

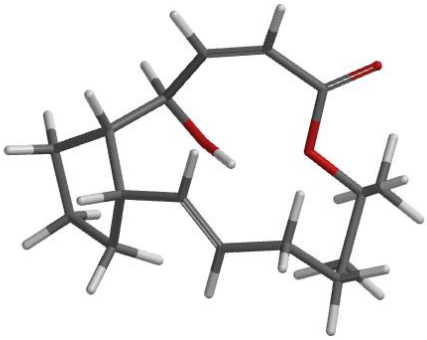
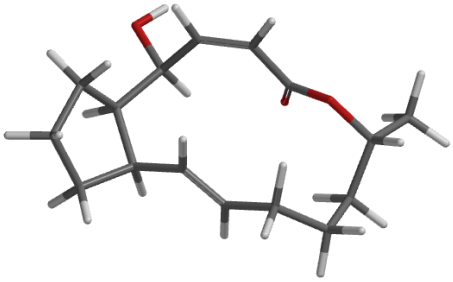
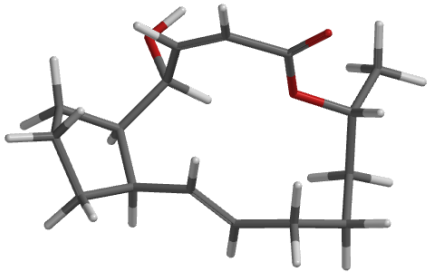
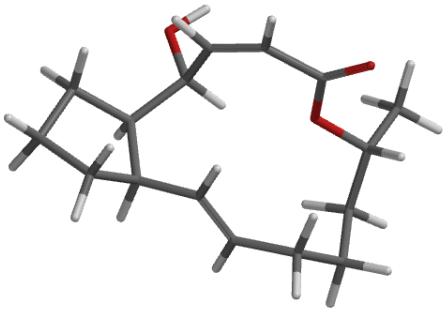
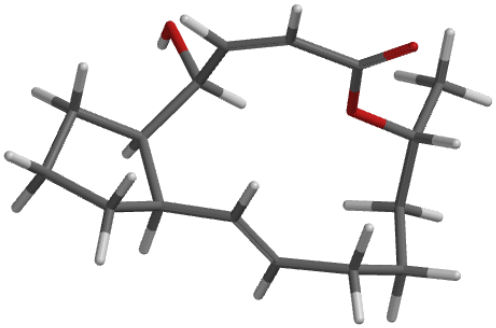
NO.	**brefeldin A**		**1**		**4**	
	δ_C, type	**δ_H, mult (*J*/Hz)**	**δ_C, type**	**δ_H, mult (*J*/Hz)**	**δ_C, type**	**δ_H, mult (*J*/Hz)**
1	165.7, C		165.7, C		166.4, C	
2	116.3, CH	5.70, dd (15.5, 1.6)	120.1, CH	5.78, d (11.4)	117.8, CH	5.86, dd (15.7, 2.5)
3	154.4, CH	7.34, dd (15.5, 2.9)	146.6, CH	5.87, dd (11.4, 10.0)	155.9, CH	7.03, dd (15.7, 2.5)
4	74.3, CH	3.92, q (2.2)	67.8, CH	4.48, m	71.4, CH	4.21, m (2.7)
5	51.7, CH	1.70, m	50.0, CH	1.71, m	47.3, CH	2.45, m
6	40.9, CH_2	1.79, m	26.9, CH_2	1.83, m	38.9, CH_2	1.96, m
		1.60, m		1.52, m		1.68, m
7	70.5, CH	4.04, m	21.9, CH_2	1.65, m	70.9, CH	4.18, m
8	43.1, CH_2	1.91, m	33.1, CH_2	1.71, m	43.5, CH_2	1.56, m
		1.29, m		1.36, m		1.43, m
9	43.3, CH_2	2.31, m	44.7, CH	2.31, m	43.6, CH	2.87, m
10	137.2, CH	5.20, dd (15.1, 9.7)	130.7, CH	5.26, dd (15.4, 9.4)	135.9, CH	5.35, dd (15.6, 9.7)
11	129.2, CH	5.66, m	130.0, CH	5.14, m	127.9, CH	5.29, m
12	31.5, CH_2	1.96, m	31.8, CH_2	2.03, m	28.9, CH_2	2.01, m
		1.79, m		1.71, m		1.74, m
13	26.5, CH_2	1.70, m	21.5, CH_2	1.52, m	24.5, CH_2	1.48, m
		0.74, m		1.39, m		1.38, m
14	33.4, CH_2	1.63, m	31.7, CH_2	1.65, m	33.5, CH_2	1.54, m
		1.48, m		1.52, m		
15	70.9, CH	4.70, m	70.4, CH	4.89, m	71.2, CH	4.75, m
16	20.7, CH_3	1.18, d (6.2)	18.3, CH_3	1.15, d (6.5)	20.8, CH_3	1.19, d (6.4)

Table S2 ^{1}H and ^{13}C NMR Data for 4-*epi*-15-*epi*-brefeldin A and **2**–**3** in DMSO-d_6 (600/150 MHz, δ in ppm)

NO.	**4-*epi*-15-*epi*-brefeldin A**		**2**		**3**	
	δ_C, type	**δ_H, mult (*J*/Hz)**	**δ_C, type**	**δ_H, mult (*J*/Hz)**	**δ_C, type**	**δ_H, mult (*J*/Hz)**
1	165.2, C		165.2, C		165.1, C	
2	118.6, CH	5.86, dd (15.5, 2.3)	118.6, CH	5.84, dd (15.5, 2.2)	118.5, CH	5.86, dd (15.5, 2.2)
3	153.3, CH	6.86, dd (15.5, 2.0)	153.2, CH	6.84, dd (15.5, 1.9)	153.3, CH	6.83, dd (15.5, 1.9)
4	70.0, CH	4.35, q (2.2)	69.9, CH	4.34, q (2.0)	70.0, CH	4.36, q (2.3)
5	47.3, CH	2.06, m	45.7, CH	2.15, m	47.3, CH	2.07, m
6	38.0, CH_2	1.94, m	34.4, CH_2	2.15, m	37.9, CH_2	1.96, m
		1.60, m		1.49, m		1.61, m
7	71.4, CH	4.04, m	76.4, CH	3.73, m	71.5, CH	4.06, m
8	43.0, CH_2	1.60, m	79.9, CH	3.57, m	43.0, CH_2	1.64, m
		1.34, m				1.36, m
9	39.5, CH_2	2.37, m	44.1, CH	2.29, m	39.0, CH	2.40, m
10	135.7, CH	5.19, dd (15.0, 9.5)	131.5, CH	5.39, dd (15.4, 9.8)	131.3, CH	5.45, dd (15.1, 9.5)
11	130.8, CH	5.08, m	132.1, CH	5.12, m	133.4, CH	5.19, dd (15.1, 2.9)
12	32.0, CH_2	1.94, m	32.5, CH_2	1.98, m	68.8, CH	3.75, m
		1.74, m		1.79, m		
13	22.8, CH_2	1.60, m	22.9, CH_2	1.61, m	31.5, CH_2	1.70, m
		1.34, m		1.38, m		1.41, m
14	31.2, CH_2	1.54, m	31.4, CH_2	1.55, m	27.6, CH_2	1.59, m
						1.34, m
15	69.3, CH	5.08, m	69.4, CH	5.08, m	68.7, CH	5.11, m
16	17.6, CH_3	1.14, d (6.1)	17.7, CH_3	1.14, d (6.7)	17.4, CH_3	1.13, d (6.6)

Table S3. The Information of conformations of (2*Z*, 4*R*, 5*S*, 9*S*, 10*E*, 15*R*)-**1a** and (2*Z*, 4*S*, 5*R*, 9*R*, 10*E*, 15*R*)-**1b**

Label	Conformers	Calculated energy (kJ/mol)	Boltzmann distribution
1a-Conf.1		0	0.50
1a-Conf.2		2.81	0.161
1a-Conf.3		3.70	0.113
1a-Conf.4		4.48	0.082

1a-Conf.5		4.73	0.074
1b-Conf.1		0	0.258
1b-Conf.2		0.21	0.238
1b-Conf.3		0.59	0.203
1b-Conf.4		2.73	0.086

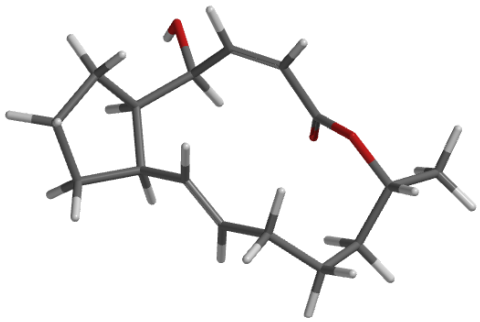
1b-Conf.5		3.19	0.071

Table S4. The coordinate for the lowest-energy conformer [(2*Z*, 4*R*, 5*S*, 9*S*, 10*E*, 15*R*)-**1a**] in ECD calculation

1a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.60231	-0.88016	-0.22621
2	6	0	-2.36618	0.584279	-0.77891
3	6	0	-3.65602	-0.71105	0.904631
4	6	0	-4.22838	0.705671	0.748075
5	6	0	-3.01929	1.512337	0.260685
6	6	0	-0.96572	0.924578	-1.20616
7	6	0	-0.2424	1.986188	-0.84759
8	8	0	-0.67467	-0.96982	1.329062
9	6	0	-1.3686	-1.66617	0.311331
10	6	0	1.948846	-1.56744	-0.62583
11	6	0	0.75493	-2.27887	-1.13848
12	6	0	-0.54227	-2.28067	-0.78994
13	6	0	1.155996	2.257361	-1.33588
14	6	0	2.152642	2.653236	-0.22693
15	6	0	2.307299	1.694654	0.964867
16	6	0	2.831749	0.291348	0.665775
17	8	0	1.697383	-0.47033	0.11743
18	8	0	3.073813	-1.9283	-0.90919
19	6	0	3.355253	-0.42352	1.905851
20	1	0	-3.02897	-1.48603	-1.03081
21	1	0	-2.98644	0.642653	-1.68465
22	1	0	-4.41979	-1.49193	0.870659
23	1	0	-3.15044	-0.78571	1.871763
24	1	0	-4.658	1.09135	1.676069
25	1	0	-5.0179	0.721035	-0.01175
26	1	0	-2.33155	1.684202	1.095325
27	1	0	-3.28586	2.486001	-0.15858
28	1	0	-0.5183	0.225272	-1.90953

29	1	0	-0.65933	2.718847	-0.15792
30	1	0	0.028529	-0.45018	0.914161
31	1	0	-1.80485	-2.54391	0.812171
32	1	0	1.040697	-2.9345	-1.95419
33	1	0	-1.1635	-2.92844	-1.40693
34	1	0	1.522804	1.387239	-1.88772
35	1	0	1.135585	3.088036	-2.05444
36	1	0	3.135299	2.808482	-0.68693
37	1	0	1.851929	3.627069	0.176417
38	1	0	1.36044	1.600299	1.507605
39	1	0	3.011212	2.151788	1.66769
40	1	0	3.600721	0.313811	-0.10886
41	1	0	3.673177	-1.43837	1.664518
42	1	0	2.583357	-0.46757	2.678723
43	1	0	4.215566	0.117477	2.307056

1a-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.817673	-0.6001	0.52347
2	6	0	2.34034	0.900386	0.603264
3	6	0	4.013543	-0.57284	-0.4799
4	6	0	4.213525	0.898715	-0.89812
5	6	0	2.829848	1.533476	-0.70766
6	6	0	0.918889	1.171758	1.017457
7	6	0	0.033649	1.961348	0.405532
8	8	0	1.249469	-1.23865	-1.18516
9	6	0	1.764414	-1.64431	0.068346
10	6	0	-1.4929	-1.40175	0.202443
11	6	0	-0.55869	-1.88547	1.244096
12	6	0	0.775556	-1.96087	1.159752
13	6	0	-1.33399	2.294666	0.950673
14	6	0	-2.45365	2.400621	-0.10346
15	6	0	-2.82652	1.130881	-0.88749
16	6	0	-3.47721	0.006202	-0.07142
17	8	0	-2.48567	-0.70508	0.761233
18	8	0	-1.39498	-1.61235	-0.99762
19	6	0	-4.31704	-0.9657	-0.89417
20	1	0	3.165325	-0.91613	1.510711
21	1	0	2.96334	1.333028	1.401761
22	1	0	4.91602	-1.00619	-0.04233
23	1	0	3.759417	-1.17132	-1.3575
24	1	0	4.592666	0.992498	-1.91884
25	1	0	4.935932	1.389645	-0.23684

26	1	0	2.16589	1.248685	-1.52798
27	1	0	2.864473	2.625156	-0.65736
28	1	0	0.621595	0.716699	1.960516
29	1	0	0.30443	2.447282	-0.53093
30	1	0	0.352587	-1.5962	-1.29879
31	1	0	2.33059	-2.58737	-0.05363
32	1	0	-1.03046	-2.1152	2.193158
33	1	0	1.281348	-2.31073	2.057753
34	1	0	-1.60483	1.575353	1.728791
35	1	0	-1.2806	3.273972	1.446805
36	1	0	-3.35478	2.781942	0.391206
37	1	0	-2.16561	3.167074	-0.8326
38	1	0	-1.96511	0.733848	-1.42816
39	1	0	-3.55678	1.41776	-1.65179
40	1	0	-4.11174	0.446593	0.700244
41	1	0	-4.65336	-1.79889	-0.2724
42	1	0	-3.76284	-1.3598	-1.74454
43	1	0	-5.20265	-0.4412	-1.26171

1a-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.84018	-0.22879	-0.6932
2	6	0	-2.14145	1.148728	-0.46244
3	6	0	-4.11428	-0.07644	0.171416
4	6	0	-3.71853	0.798414	1.390793
5	6	0	-2.3597	1.452468	1.032834
6	6	0	-0.75206	1.336309	-1.00817
7	6	0	0.270825	1.948516	-0.40811
8	8	0	-1.71184	-1.59355	1.054507
9	6	0	-2.06636	-1.53173	-0.31627
10	6	0	1.224925	-1.29841	-0.20674
11	6	0	0.355481	-1.78065	-1.30083
12	6	0	-0.98452	-1.84145	-1.32195
13	6	0	1.621708	2.175422	-1.04549
14	6	0	2.80689	2.197257	-0.06019
15	6	0	3.01176	0.972296	0.847254
16	6	0	3.447717	-0.32773	0.16443
17	8	0	2.40068	-0.90492	-0.70269
18	8	0	0.936934	-1.24323	0.981328
19	6	0	3.984842	-1.38253	1.126569
20	1	0	-3.11103	-0.33121	-1.74961
21	1	0	-2.78034	1.849123	-1.0241
22	1	0	-4.88162	0.432064	-0.41959

23	1	0	-4.52864	-1.04309	0.467756
24	1	0	-3.62214	0.189058	2.290409
25	1	0	-4.48514	1.551258	1.591764
26	1	0	-1.55805	1.001864	1.620418
27	1	0	-2.34923	2.527345	1.231049
28	1	0	-0.6029	0.972893	-2.02419
29	1	0	0.142752	2.341226	0.599371
30	1	0	-0.75436	-1.43122	1.147464
31	1	0	-2.80831	-2.32942	-0.46878
32	1	0	0.891125	-2.02052	-2.21202
33	1	0	-1.40969	-2.14831	-2.27561
34	1	0	1.78547	1.429615	-1.82888
35	1	0	1.617995	3.149999	-1.55288
36	1	0	3.726141	2.378214	-0.62958
37	1	0	2.685692	3.066647	0.596697
38	1	0	2.124658	0.783579	1.453141
39	1	0	3.815991	1.216905	1.55001
40	1	0	4.218553	-0.09864	-0.57415
41	1	0	4.211748	-2.30624	0.589258
42	1	0	3.271532	-1.60058	1.920851
43	1	0	4.911062	-1.01703	1.576526

1a-Conf.4

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	2.817673	-0.6001	0.52347
2	6	0	2.34034	0.900386	0.603264
3	6	0	4.013543	-0.57284	-0.4799
4	6	0	4.213525	0.898715	-0.89812
5	6	0	2.829848	1.533476	-0.70766
6	6	0	0.918889	1.171758	1.017457
7	6	0	0.033649	1.961348	0.405532
8	8	0	1.24947	-1.23865	-1.18516
9	6	0	1.764414	-1.64431	0.068346
10	6	0	-1.4929	-1.40175	0.202442
11	6	0	-0.55869	-1.88547	1.244096
12	6	0	0.775556	-1.96087	1.159751
13	6	0	-1.33399	2.294666	0.950673
14	6	0	-2.45365	2.400621	-0.10346
15	6	0	-2.82652	1.130881	-0.88749
16	6	0	-3.47721	0.006202	-0.07142
17	8	0	-2.48567	-0.70508	0.761233
18	8	0	-1.39498	-1.61235	-0.99762
19	6	0	-4.31704	-0.9657	-0.89417

20	1	0	3.165325	-0.91613	1.510711
21	1	0	2.96334	1.333028	1.401761
22	1	0	4.91602	-1.00619	-0.04233
23	1	0	3.759417	-1.17132	-1.3575
24	1	0	4.592666	0.992498	-1.91884
25	1	0	4.935932	1.389645	-0.23684
26	1	0	2.16589	1.248685	-1.52798
27	1	0	2.864473	2.625156	-0.65736
28	1	0	0.621595	0.716699	1.960516
29	1	0	0.30443	2.447282	-0.53093
30	1	0	0.352587	-1.5962	-1.29879
31	1	0	2.330591	-2.58737	-0.05363
32	1	0	-1.03046	-2.1152	2.193158
33	1	0	1.281348	-2.31073	2.057753
34	1	0	-1.60483	1.575353	1.728791
35	1	0	-1.2806	3.273972	1.446805
36	1	0	-3.35478	2.781942	0.391205
37	1	0	-2.16561	3.167074	-0.8326
38	1	0	-1.96511	0.733848	-1.42816
39	1	0	-3.55678	1.41776	-1.65179
40	1	0	-4.11174	0.446593	0.700244
41	1	0	-4.65336	-1.79889	-0.2724
42	1	0	-3.76284	-1.3598	-1.74454
43	1	0	-5.20265	-0.4412	-1.26171

1a-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.64644	-0.70674	-0.35716
2	6	0	-2.30859	0.793774	-0.72756
3	6	0	-3.69717	-0.60386	0.785451
4	6	0	-4.15884	0.8609	0.814996
5	6	0	-2.88901	1.627578	0.428855
6	6	0	-0.89346	1.102985	-1.14426
7	6	0	-0.08946	2.029602	-0.61687
8	8	0	-0.67887	-1.03505	1.10885
9	6	0	-1.46586	-1.61362	0.076411
10	6	0	1.763045	-1.87676	-0.33649
11	6	0	0.650425	-2.31309	-1.22858
12	6	0	-0.66922	-2.17862	-1.07321
13	6	0	1.266239	2.411418	-1.14933
14	6	0	2.41181	2.50045	-0.1061
15	6	0	3.367765	1.29566	-0.01974
16	6	0	2.896023	0.011738	0.66204

17	8	0	1.801189	-0.54599	-0.13991
18	8	0	2.594521	-2.65122	0.086655
19	6	0	2.42727	0.169304	2.102921
20	1	0	-3.10235	-1.18361	-1.2295
21	1	0	-2.92988	1.011152	-1.60762
22	1	0	-4.51782	-1.31254	0.650046
23	1	0	-3.21	-0.84315	1.735599
24	1	0	-4.56169	1.156516	1.786885
25	1	0	-4.94106	1.034506	0.067468
26	1	0	-2.19675	1.637033	1.277376
27	1	0	-3.07541	2.664954	0.139601
28	1	0	-0.52684	0.535832	-1.99821
29	1	0	-0.43674	2.618327	0.230833
30	1	0	-0.1868	-0.30009	0.715483
31	1	0	-1.93159	-2.49352	0.542357
32	1	0	1.013247	-2.88819	-2.07537
33	1	0	-1.29446	-2.6325	-1.8395
34	1	0	1.550299	1.738165	-1.9637
35	1	0	1.161205	3.406876	-1.60069
36	1	0	3.03466	3.361671	-0.3655
37	1	0	1.996684	2.729218	0.881251
38	1	0	4.26272	1.610234	0.529353
39	1	0	3.70853	1.035942	-1.02807
40	1	0	3.708665	-0.71446	0.628439
41	1	0	2.145882	-0.79924	2.520028
42	1	0	1.569543	0.840475	2.180334
43	1	0	3.238048	0.580099	2.710131

Table S5. The coordinate for the lowest-energy conformer [(2*Z*, 4*S*, 5*R*, 9*R*, 10*E*, 15*R*)-**1b**] in ECD calculation

1b-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.623394	-0.35739	-0.53872
2	6	0	2.093459	1.121102	-0.57736
3	6	0	3.735735	-0.35733	0.522949
4	6	0	4.449251	0.972217	0.247422
5	6	0	3.292238	1.959924	-0.00618
6	6	0	0.833049	1.403922	0.19527
7	6	0	-0.24659	2.02344	-0.28614
8	8	0	2.294685	-2.68543	-0.86766
9	6	0	1.584125	-1.4869	-0.47895

10	6	0	-1.42464	-1.30911	0.293848
11	6	0	-0.31765	-1.67921	1.215445
12	6	0	0.974193	-1.73638	0.876117
13	6	0	-1.45786	2.408375	0.526641
14	6	0	-2.79872	2.324956	-0.22774
15	6	0	-3.22676	0.951206	-0.76901
16	6	0	-3.56408	-0.11177	0.283335
17	8	0	-2.36542	-0.62644	0.968817
18	8	0	-1.48589	-1.58842	-0.88668
19	6	0	-4.42829	-1.2553	-0.24018
20	1	0	3.118644	-0.52011	-1.50347
21	1	0	1.910732	1.393689	-1.62053
22	1	0	4.389406	-1.2285	0.443445
23	1	0	3.314874	-0.3482	1.534764
24	1	0	5.099407	1.291189	1.065708
25	1	0	5.072921	0.874031	-0.64768
26	1	0	3.568798	2.772228	-0.682
27	1	0	2.990653	2.423167	0.937946
28	1	0	0.845933	1.128601	1.249174
29	1	0	-0.25548	2.321098	-1.33592
30	1	0	1.648681	-3.39939	-0.91586
31	1	0	0.80029	-1.27974	-1.20834
32	1	0	-0.61216	-1.84652	2.245712
33	1	0	1.68678	-2.00906	1.649971
34	1	0	-1.49134	1.808035	1.440083
35	1	0	-1.34351	3.45197	0.851281
36	1	0	-3.58789	2.707649	0.430165
37	1	0	-2.75622	3.015876	-1.07805
38	1	0	-4.13901	1.09803	-1.35743
39	1	0	-2.481	0.552647	-1.45888
40	1	0	-4.08766	0.366973	1.113886
41	1	0	-4.56112	-2.01548	0.533459
42	1	0	-3.98899	-1.72149	-1.12128
43	1	0	-5.41489	-0.86507	-0.50247

1b-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.340875	-0.18393	-0.82855
2	6	0	2.122112	1.250761	-0.18817
3	6	0	3.712139	-0.67705	-0.29992
4	6	0	4.442523	0.597779	0.148756
5	6	0	3.319581	1.431074	0.776946
6	6	0	0.788683	1.487974	0.454723

7	6	0	-0.14132	2.346159	0.036224
8	8	0	1.544557	-2.27933	-1.602
9	6	0	1.177971	-1.19138	-0.72015
10	6	0	-1.55997	-1.4106	1.116883
11	6	0	-0.18622	-1.91746	1.360586
12	6	0	0.938521	-1.80323	0.637991
13	6	0	-1.48847	2.522049	0.681902
14	6	0	-2.67651	2.437839	-0.29864
15	6	0	-2.82767	1.143722	-1.1155
16	6	0	-3.03621	-0.14677	-0.31909
17	8	0	-1.70116	-0.65767	0.015875
18	8	0	-2.47319	-1.67103	1.878161
19	6	0	-3.78122	-1.2215	-1.10211
20	1	0	2.430775	-0.03308	-1.90855
21	1	0	2.233695	1.975588	-1.00088
22	1	0	4.259425	-1.24772	-1.05242
23	1	0	3.585933	-1.33062	0.567892
24	1	0	5.265789	0.394363	0.838249
25	1	0	4.860312	1.124059	-0.71721
26	1	0	3.575949	2.484301	0.915914
27	1	0	3.065242	1.022264	1.762331
28	1	0	0.572679	0.885532	1.334678
29	1	0	0.05907	2.961473	-0.84222
30	1	0	0.803606	-2.89569	-1.62363
31	1	0	0.269876	-0.71462	-1.084
32	1	0	-0.14248	-2.47687	2.28895
33	1	0	1.808595	-2.31058	1.045892
34	1	0	-1.60529	1.788193	1.485675
35	1	0	-1.5389	3.509477	1.160271
36	1	0	-3.59963	2.606067	0.26804
37	1	0	-2.60221	3.270664	-1.00761
38	1	0	-3.69631	1.267795	-1.77007
39	1	0	-1.96625	1.000067	-1.77524
40	1	0	-3.55251	0.050499	0.622248
41	1	0	-3.26874	-1.43696	-2.04361
42	1	0	-4.79376	-0.87986	-1.33054
43	1	0	-3.85537	-2.14279	-0.52181

1b-Conf.3

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	2.340875	-0.18393	-0.82855
2	6	0	2.122112	1.250761	-0.18817
3	6	0	3.712139	-0.67705	-0.29992

4	6	0	4.442523	0.597779	0.148756
5	6	0	3.319581	1.431074	0.776946
6	6	0	0.788682	1.487974	0.454722
7	6	0	-0.14132	2.346161	0.036225
8	8	0	1.544557	-2.27933	-1.602
9	6	0	1.177971	-1.19138	-0.72015
10	6	0	-1.55997	-1.4106	1.116882
11	6	0	-0.18622	-1.91746	1.360586
12	6	0	0.938521	-1.80323	0.637992
13	6	0	-1.48846	2.52205	0.681903
14	6	0	-2.67651	2.43784	-0.29864
15	6	0	-2.82767	1.143723	-1.1155
16	6	0	-3.03621	-0.14677	-0.31909
17	8	0	-1.70116	-0.65767	0.015876
18	8	0	-2.47319	-1.67104	1.878158
19	6	0	-3.78122	-1.2215	-1.10211
20	1	0	2.430775	-0.03308	-1.90855
21	1	0	2.233695	1.975587	-1.00088
22	1	0	4.259425	-1.24772	-1.05242
23	1	0	3.585933	-1.33062	0.567892
24	1	0	5.265788	0.394363	0.83825
25	1	0	4.860312	1.124059	-0.71721
26	1	0	3.575948	2.484301	0.915914
27	1	0	3.065241	1.022264	1.762331
28	1	0	0.572678	0.885531	1.334676
29	1	0	0.059071	2.961476	-0.84222
30	1	0	0.803605	-2.89569	-1.62363
31	1	0	0.269875	-0.71462	-1.084
32	1	0	-0.14249	-2.47687	2.288951
33	1	0	1.808595	-2.31058	1.045892
34	1	0	-1.60529	1.788193	1.485676
35	1	0	-1.5389	3.509478	1.160272
36	1	0	-3.59963	2.606067	0.268042
37	1	0	-2.60221	3.270665	-1.00761
38	1	0	-3.69631	1.267796	-1.77007
39	1	0	-1.96625	1.000068	-1.77524
40	1	0	-3.55251	0.050499	0.622248
41	1	0	-3.85537	-2.14279	-0.52181
42	1	0	-3.26874	-1.43695	-2.04361
43	1	0	-4.79376	-0.87986	-1.33055

1b-Conf.4

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

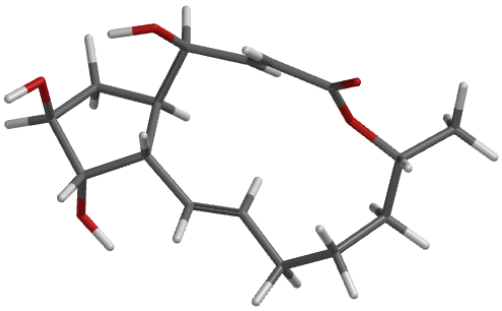
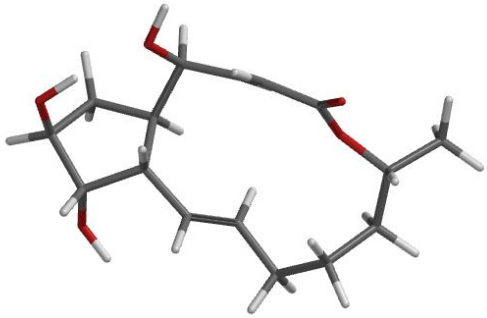
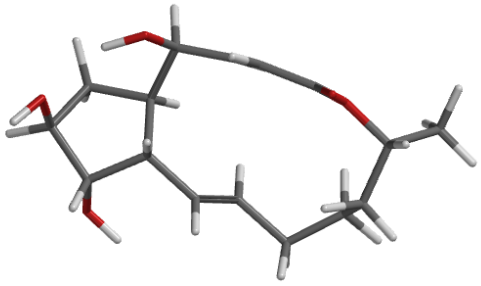
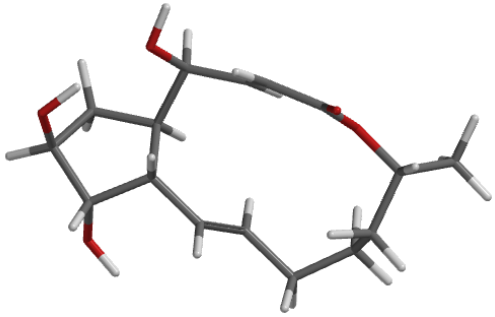
1	6	0	2.623394	-0.35739	-0.53871
2	6	0	2.093457	1.121097	-0.57737
3	6	0	3.735725	-0.35732	0.522964
4	6	0	4.449247	0.97222	0.247426
5	6	0	3.292241	1.959928	-0.00621
6	6	0	0.833054	1.40392	0.195271
7	6	0	-0.24659	2.023433	-0.28614
8	8	0	2.294693	-2.68543	-0.86765
9	6	0	1.584128	-1.4869	-0.47895
10	6	0	-1.42464	-1.3091	0.293845
11	6	0	-0.31766	-1.67921	1.215443
12	6	0	0.974191	-1.73638	0.876118
13	6	0	-1.45786	2.408369	0.526651
14	6	0	-2.79872	2.324957	-0.22772
15	6	0	-3.22677	0.951212	-0.769
16	6	0	-3.56408	-0.11177	0.283331
17	8	0	-2.36543	-0.62644	0.968815
18	8	0	-1.48589	-1.58841	-0.88669
19	6	0	-4.42828	-1.2553	-0.2402
20	1	0	3.118654	-0.52011	-1.50346
21	1	0	1.910718	1.393671	-1.62054
22	1	0	4.389396	-1.22849	0.443478
23	1	0	3.314854	-0.34817	1.534774
24	1	0	5.099391	1.291203	1.065717
25	1	0	5.072931	0.874017	-0.64767
26	1	0	3.56881	2.772206	-0.68206
27	1	0	2.990655	2.423205	0.937898
28	1	0	0.845947	1.128606	1.249176
29	1	0	-0.25548	2.321083	-1.33591
30	1	0	1.648687	-3.3994	-0.91587
31	1	0	0.800296	-1.27975	-1.20834
32	1	0	-0.61217	-1.84652	2.245711
33	1	0	1.686775	-2.00906	1.649974
34	1	0	-1.49134	1.808025	1.440091
35	1	0	-1.3435	3.451962	0.851295
36	1	0	-3.58789	2.707647	0.430184
37	1	0	-2.75622	3.015883	-1.07803
38	1	0	-4.13901	1.098042	-1.35743
39	1	0	-2.481	0.552657	-1.45888
40	1	0	-4.08767	0.366966	1.113883
41	1	0	-5.41489	-0.86507	-0.50248
42	1	0	-4.56112	-2.01549	0.533439
43	1	0	-3.98898	-1.72148	-1.12129

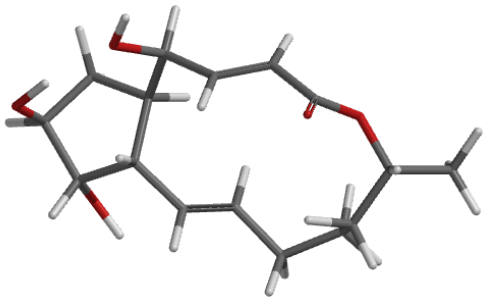
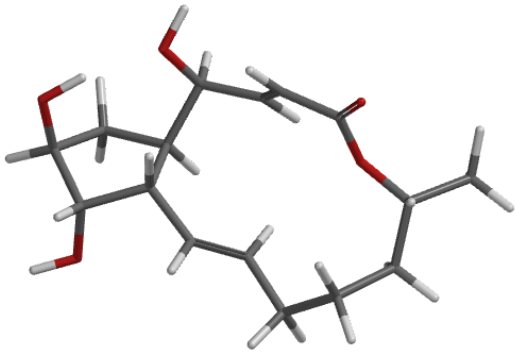
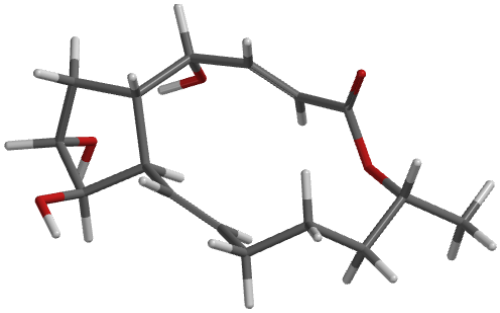
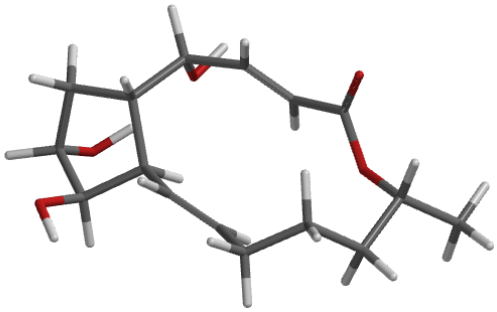
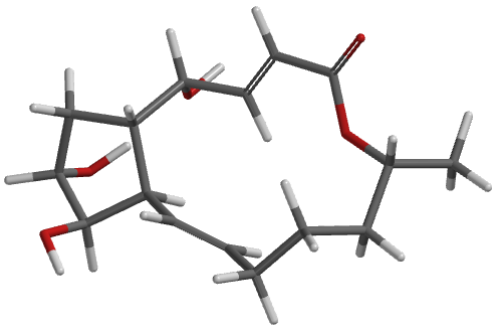
1b-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.340875	-0.18393	-0.82855
2	6	0	2.122112	1.250761	-0.18817
3	6	0	3.712139	-0.67705	-0.29992
4	6	0	4.442523	0.597779	0.148756
5	6	0	3.319581	1.431074	0.776946
6	6	0	0.788683	1.487974	0.454723
7	6	0	-0.14132	2.346159	0.036224
8	8	0	1.544557	-2.27933	-1.602
9	6	0	1.177971	-1.19138	-0.72015
10	6	0	-1.55997	-1.4106	1.116883
11	6	0	-0.18622	-1.91746	1.360586
12	6	0	0.938521	-1.80323	0.637991
13	6	0	-1.48847	2.522049	0.681902
14	6	0	-2.67651	2.437839	-0.29864
15	6	0	-2.82767	1.143722	-1.1155
16	6	0	-3.03621	-0.14677	-0.31909
17	8	0	-1.70116	-0.65767	0.015875
18	8	0	-2.47319	-1.67103	1.878162
19	6	0	-3.78122	-1.2215	-1.10211
20	1	0	2.430775	-0.03308	-1.90855
21	1	0	2.233695	1.975587	-1.00088
22	1	0	4.259425	-1.24772	-1.05242
23	1	0	3.585933	-1.33062	0.567892
24	1	0	5.265789	0.394364	0.838249
25	1	0	4.860312	1.124059	-0.71721
26	1	0	3.575949	2.484301	0.915913
27	1	0	3.065242	1.022264	1.762331
28	1	0	0.572679	0.885532	1.334678
29	1	0	0.05907	2.961473	-0.84222
30	1	0	0.803606	-2.89569	-1.62363
31	1	0	0.269876	-0.71462	-1.084
32	1	0	-0.14248	-2.47687	2.28895
33	1	0	1.808595	-2.31058	1.045892
34	1	0	-1.60529	1.788192	1.485675
35	1	0	-1.5389	3.509477	1.160271
36	1	0	-3.59963	2.606067	0.26804
37	1	0	-2.60221	3.270664	-1.00761
38	1	0	-3.69631	1.267795	-1.77007
39	1	0	-1.96625	1.000067	-1.77524
40	1	0	-3.55251	0.050499	0.622248
41	1	0	-3.85537	-2.14279	-0.52181
42	1	0	-3.26874	-1.43696	-2.04361

43	1	0	-4.79376	-0.87986	-1.33054

Table S6. The Information of conformations of (2*E*, 4*S*, 5*R*, 7*S*, 8*S*, 9*S*, 10*E*, 15*R*)-**2a** and (2*E*, 4*R*, 5*S*, 7*R*, 8*R*, 9*R*, 10*E*, 15*R*)-**2b**

Label	**Conformers**	**Calculated energy (kJ/mol)**	**Boltzmann distribution**
2a-Conf.1		0	0.539
2a-Conf.2		2.57	0.191
2a-Conf.3		3.63	0.125
2a-Conf.4		4.64	0.083

2a-Conf.5		7.79	0.023
2a-Conf.6		8.60	0.017
2b-Conf.1		0	0.368
2b-Conf.2		0.41	0.312
2b-Conf.3		1.26	0.221

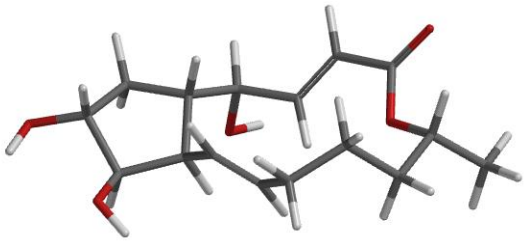
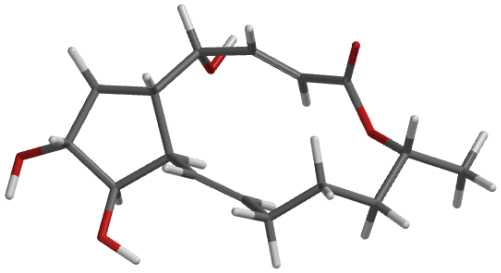
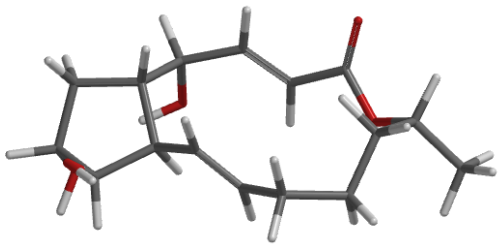
2b-Conf.4		6.15	0.031
2b-Conf.5		6.23	0.030
2b-Conf.6		8.20	0.013

Table S7. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 8*S*, 9*S*, 10*E*, 15*R*)-**2a**] in ECD calculation

2a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.87064	-0.3115	0.919539
2	6	0	-1.84486	0.509998	-0.40664
3	6	0	-0.73817	1.503258	-0.65565
4	6	0	0.308665	1.816617	0.11169
5	6	0	0.206769	-1.61129	0.568908
6	6	0	-1.27042	-1.73879	0.747048
7	6	0	1.407843	2.754302	-0.31969
8	6	0	2.713832	2.032141	-0.73398
9	6	0	2.327921	-1.54967	-0.6841
10	6	0	0.921824	-1.96668	-0.5011
11	6	0	-3.36291	-0.3386	1.365145
12	6	0	-4.16231	0.101814	0.14361
13	6	0	-3.25107	1.153034	-0.50223
14	6	0	3.555727	1.446209	0.426779
15	6	0	3.990591	-0.00696	0.220805
16	8	0	2.778833	-0.81144	0.351619

17	8	0	-1.84392	-2.47027	-0.32622
18	8	0	2.978581	-1.79132	-1.68227
19	6	0	4.993662	-0.49979	1.252936
20	1	0	-1.28526	0.182445	1.696562
21	1	0	-1.80234	-0.20868	-1.23286
22	8	0	-3.36873	2.33311	0.291777
23	8	0	-4.3001	-1.05423	-0.70278
24	1	0	-0.80806	1.989187	-1.63069
25	1	0	0.431987	1.341074	1.080814
26	1	0	0.712383	-1.10288	1.382283
27	1	0	-1.45181	-2.26854	1.696647
28	1	0	1.056611	3.343857	-1.17227
29	1	0	1.633675	3.464477	0.485119
30	1	0	3.329301	2.743798	-1.29214
31	1	0	2.452031	1.242606	-1.44495
32	1	0	0.475219	-2.48585	-1.33915
33	1	0	-3.69014	-1.31739	1.723027
34	1	0	-3.52268	0.380176	2.168946
35	1	0	-5.1471	0.509399	0.388443
36	1	0	-3.53042	1.365958	-1.54302
37	1	0	4.45534	2.051523	0.572281
38	1	0	3.001716	1.491234	1.370403
39	1	0	4.379922	-0.15945	-0.78706
40	1	0	-2.7496	-2.14871	-0.47907
41	1	0	5.921474	0.072566	1.177422
42	1	0	4.597998	-0.38363	2.265557
43	1	0	5.226978	-1.55417	1.09007
44	1	0	-2.54294	2.825731	0.20475
45	1	0	-4.66041	-0.78618	-1.5565

2a-Conf.2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-1.8983	-0.2931	0.931423
2	6	0	-1.83946	0.518986	-0.40196
3	6	0	-0.71972	1.499912	-0.63885
4	6	0	0.315686	1.818906	0.141705
5	6	0	0.202021	-1.5826	0.590685
6	6	0	-1.27349	-1.70369	0.801187
7	6	0	1.417833	2.757382	-0.2832
8	6	0	2.719039	2.039037	-0.71877
9	6	0	2.305681	-1.54364	-0.6918
10	6	0	0.897021	-1.94851	-0.48797
11	6	0	-3.4072	-0.35661	1.314571

12	6	0	-4.1701	0.10528	0.066549
13	6	0	-3.23667	1.176664	-0.51471
14	6	0	3.572059	1.435061	0.424615
15	6	0	3.993426	-0.0186	0.197041
16	8	0	2.776118	-0.81413	0.33899
17	8	0	-1.94748	-2.39133	-0.25983
18	8	0	2.937177	-1.79024	-1.70026
19	6	0	5.008188	-0.53098	1.207774
20	1	0	-1.35026	0.223491	1.720727
21	1	0	-1.79574	-0.19994	-1.22874
22	8	0	-3.35455	2.333633	0.316642
23	8	0	-4.38014	-0.95015	-0.87174
24	1	0	-0.77412	1.980918	-1.61741
25	1	0	0.425567	1.352245	1.116917
26	1	0	0.723694	-1.06984	1.391276
27	1	0	-1.45252	-2.22663	1.750128
28	1	0	1.063346	3.36015	-1.12516
29	1	0	1.651204	3.455856	0.529509
30	1	0	3.330304	2.757871	-1.27237
31	1	0	2.449464	1.260379	-1.43886
32	1	0	0.439228	-2.46713	-1.32116
33	1	0	-3.72529	-1.35274	1.629478
34	1	0	-3.60615	0.334419	2.134472
35	1	0	-5.15125	0.524492	0.299762
36	1	0	-3.4918	1.418073	-1.55347
37	1	0	4.478097	2.031987	0.564408
38	1	0	3.031092	1.473645	1.376023
39	1	0	4.364879	-0.16395	-0.81858
40	1	0	-1.80007	-3.33914	-0.16969
41	1	0	5.939349	0.034552	1.123168
42	1	0	4.629705	-0.42216	2.227705
43	1	0	5.230144	-1.5854	1.030045
44	1	0	-2.53963	2.842761	0.224864
45	1	0	-3.63438	-1.56717	-0.79317

2a-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.89084	-0.17046	0.959198
2	6	0	-1.70687	0.463412	-0.45626
3	6	0	-0.54342	1.396943	-0.69093
4	6	0	0.248395	1.958051	0.22561
5	6	0	0.169533	-1.54427	0.827172
6	6	0	-1.31177	-1.61092	1.0421

7	6	0	1.44485	2.831262	-0.03669
8	6	0	2.764155	2.135753	0.387054
9	6	0	2.226921	-1.80723	-0.52348
10	6	0	0.836312	-2.1413	-0.16397
11	6	0	-3.41817	-0.10806	1.254397
12	6	0	-4.08034	0.183092	-0.08896
13	6	0	-3.07613	1.118001	-0.77673
14	6	0	3.336047	1.180425	-0.68384
15	6	0	3.929501	-0.13783	-0.16761
16	8	0	2.819654	-0.94902	0.338649
17	8	0	-1.90919	-2.51873	0.126746
18	8	0	2.756821	-2.2134	-1.54019
19	6	0	4.950153	-0.01009	0.950822
20	1	0	-1.36907	0.410875	1.719524
21	1	0	-1.60185	-0.35685	-1.17398
22	8	0	-3.22444	2.396392	-0.16375
23	8	0	-4.17542	-1.07242	-0.78628
24	1	0	-0.35061	1.616894	-1.74109
25	1	0	0.08078	1.740497	1.278598
26	1	0	0.706366	-0.88543	1.501014
27	1	0	-1.49403	-1.96143	2.070811
28	1	0	1.490804	3.120742	-1.09163
29	1	0	1.338658	3.755438	0.542912
30	1	0	2.575282	1.58995	1.316269
31	1	0	3.508754	2.898803	0.629451
32	1	0	0.332913	-2.80651	-0.85348
33	1	0	-3.81223	-1.02354	1.700963
34	1	0	-3.62984	0.714631	1.937432
35	1	0	-5.0696	0.64056	0.000014
36	1	0	-3.24845	1.190828	-1.85902
37	1	0	2.554365	0.917358	-1.40398
38	1	0	4.113074	1.694687	-1.25922
39	1	0	4.366826	-0.68004	-1.00574
40	1	0	-2.73771	-2.13865	-0.2142
41	1	0	5.793425	0.597706	0.612488
42	1	0	4.521744	0.461012	1.837866
43	1	0	5.329265	-0.99448	1.233367
44	1	0	-2.37193	2.846948	-0.22585
45	1	0	-4.43631	-0.91325	-1.70126

2a-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.90982	-0.15128	0.962172

2	6	0	-1.70597	0.475909	-0.45505
3	6	0	-0.53295	1.398592	-0.6812
4	6	0	0.258089	1.954787	0.23907
5	6	0	0.165831	-1.52354	0.833343
6	6	0	-1.31367	-1.57547	1.069938
7	6	0	1.457284	2.826122	-0.01857
8	6	0	2.776151	2.125323	0.397617
9	6	0	2.209027	-1.79873	-0.5359
10	6	0	0.816044	-2.12119	-0.16735
11	6	0	-3.44519	-0.1279	1.21593
12	6	0	-4.08271	0.178577	-0.14578
13	6	0	-3.06746	1.14016	-0.78249
14	6	0	3.34432	1.177081	-0.68169
15	6	0	3.929868	-0.14877	-0.17696
16	8	0	2.813847	-0.95407	0.328126
17	8	0	-1.99907	-2.41422	0.131214
18	8	0	2.724779	-2.20446	-1.5592
19	6	0	4.954154	-0.0374	0.939623
20	1	0	-1.41505	0.447515	1.72688
21	1	0	-1.60545	-0.34454	-1.174
22	8	0	-3.21657	2.403342	-0.13248
23	8	0	-4.25041	-0.98926	-0.94995
24	1	0	-0.33588	1.621476	-1.73005
25	1	0	0.086661	1.735789	1.291229
26	1	0	0.715301	-0.86888	1.501107
27	1	0	-1.5048	-1.93379	2.089861
28	1	0	1.502335	3.122693	-1.0716
29	1	0	1.354669	3.746838	0.567153
30	1	0	2.587999	1.572775	1.322983
31	1	0	3.522667	2.885104	0.644367
32	1	0	0.306851	-2.77741	-0.86219
33	1	0	-3.82459	-1.06344	1.631727
34	1	0	-3.68794	0.674415	1.913686
35	1	0	-5.06418	0.65	-0.05786
36	1	0	-3.2252	1.238113	-1.8631
37	1	0	2.562161	0.924971	-1.40522
38	1	0	4.125043	1.691945	-1.25143
39	1	0	4.359554	-0.68954	-1.01996
40	1	0	-1.89306	-3.33679	0.387108
41	1	0	5.801895	0.564765	0.602555
42	1	0	4.532141	0.432476	1.830341
43	1	0	5.325119	-1.0268	1.215308
44	1	0	-2.37195	2.866558	-0.20298
45	1	0	-3.55289	-1.61846	-0.70382

2a-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.86213	-0.35824	0.772689
2	6	0	-1.78541	0.497682	-0.53726
3	6	0	-0.54594	1.324809	-0.79266
4	6	0	0.323562	1.782807	0.112641
5	6	0	-0.15293	-1.985	-0.07598
6	6	0	-1.51386	-1.84725	0.544077
7	6	0	1.519339	2.659133	-0.1549
8	6	0	2.853826	2.006999	0.282724
9	6	0	2.249445	-1.7122	-0.17499
10	6	0	1.003439	-1.95128	0.587607
11	6	0	-3.30685	-0.16423	1.318532
12	6	0	-4.10621	0.45169	0.162205
13	6	0	-3.07307	1.370597	-0.50729
14	6	0	3.432575	1.021475	-0.75423
15	6	0	4.127126	-0.21611	-0.1696
16	8	0	3.116253	-0.98725	0.56436
17	8	0	-2.52068	-2.39965	-0.32143
18	8	0	2.438828	-2.0242	-1.33192
19	6	0	5.254998	0.063313	0.808071
20	1	0	-1.14594	0.001842	1.510564
21	1	0	-1.91467	-0.1743	-1.39143
22	8	0	-2.92666	2.51691	0.329869
23	8	0	-4.59398	-0.52239	-0.75868
24	1	0	-0.40133	1.612147	-1.83392
25	1	0	0.199928	1.50193	1.15731
26	1	0	-0.12942	-1.98753	-1.16216
27	1	0	-1.54686	-2.35271	1.515931
28	1	0	1.561021	2.938888	-1.21293
29	1	0	1.393295	3.589974	0.411402
30	1	0	2.683705	1.489731	1.231877
31	1	0	3.584462	2.793691	0.488985
32	1	0	1.053991	-1.88669	1.669015
33	1	0	-3.7612	-1.0923	1.670522
34	1	0	-3.28807	0.53972	2.151607
35	1	0	-4.96853	1.027708	0.506199
36	1	0	-3.38697	1.663133	-1.51623
37	1	0	2.635811	0.664012	-1.41312
38	1	0	4.149533	1.536274	-1.40218
39	1	0	4.484466	-0.8435	-0.98681
40	1	0	-2.42619	-3.35758	-0.35575

41	1	0	4.90909	0.640967	1.667783
42	1	0	5.68431	-0.87268	1.171609
43	1	0	6.043424	0.630154	0.306706
44	1	0	-2.04724	2.882832	0.166226
45	1	0	-3.98422	-1.27827	-0.73863

2a-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.02837	-0.40752	1.019048
2	6	0	-1.75444	0.625611	-0.13333
3	6	0	-0.6121	1.575085	0.113311
4	6	0	0.448524	1.702543	-0.68602
5	6	0	0.09679	-1.62685	0.599759
6	6	0	-1.38488	-1.78652	0.744526
7	6	0	1.567277	2.699798	-0.5426
8	6	0	2.994751	2.146553	-0.76625
9	6	0	2.244291	-1.57599	-0.61731
10	6	0	0.828438	-1.97189	-0.46122
11	6	0	-3.5743	-0.48586	1.162943
12	6	0	-4.13256	0.178911	-0.10267
13	6	0	-3.11886	1.311397	-0.35843
14	6	0	3.668341	1.440688	0.438874
15	6	0	3.930019	-0.05593	0.268785
16	8	0	2.630938	-0.71446	0.34209
17	8	0	-1.99742	-2.34651	-0.42519
18	8	0	2.951847	-1.9421	-1.53562
19	6	0	4.820918	-0.64807	1.352583
20	1	0	-1.58876	-0.04222	1.950103
21	1	0	-1.54267	0.06701	-1.04906
22	8	0	-3.26953	2.351113	0.614785
23	8	0	-4.1961	-0.71395	-1.21568
24	1	0	-0.69455	2.200626	0.999749
25	1	0	0.508216	1.065313	-1.56891
26	1	0	0.580524	-1.11224	1.422643
27	1	0	-1.59866	-2.42619	1.611009
28	1	0	1.407219	3.480404	-1.2991
29	1	0	1.505587	3.203463	0.428354
30	1	0	3.627074	2.987827	-1.06284
31	1	0	2.979743	1.473601	-1.63119
32	1	0	0.400999	-2.49619	-1.30686
33	1	0	-3.94519	-1.50654	1.276347
34	1	0	-3.88954	0.087155	2.036034
35	1	0	-5.14219	0.575715	0.039362

36	1	0	-3.20892	1.713104	-1.37395
37	1	0	4.636102	1.912117	0.634304
38	1	0	3.07254	1.579655	1.347426
39	1	0	4.349482	-0.26544	-0.7166
40	1	0	-1.90112	-3.30461	-0.41182
41	1	0	5.812522	-0.19025	1.31664
42	1	0	4.394762	-0.47296	2.344103
43	1	0	4.936418	-1.72469	1.209318
44	1	0	-4.12743	2.765822	0.472516
45	1	0	-3.49317	-1.37495	-1.1027

Table S8. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*R*, 8*R*, 9*R*, 10*E*, 15*R*)-**2b**] in ECD calculation

2b-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.2233	-0.48201	-0.8974
2	6	0	-1.72434	0.599719	0.127227
3	6	0	-0.66938	1.535075	-0.39887
4	6	0	0.526397	1.72711	0.163547
5	6	0	-0.14581	-1.84781	-0.9578
6	6	0	-1.60759	-1.88784	-0.63001
7	6	0	1.602195	2.6356	-0.3649
8	6	0	-4.0955	0.22886	0.516554
9	6	0	2.2062	-1.46397	-0.45919
10	6	0	0.836718	-1.84197	-0.05659
11	6	0	-3.7765	-0.4723	-0.79944
12	6	0	2.906741	1.903695	-0.76002
13	6	0	-3.01764	1.316515	0.604093
14	6	0	3.750041	1.359715	0.423496
15	6	0	4.076349	-0.13476	0.357961
16	8	0	2.827947	-0.86656	0.580681
17	8	0	-1.79453	-2.34082	0.702875
18	8	0	2.689152	-1.589	-1.56684
19	6	0	5.052973	-0.59098	1.431087
20	1	0	-1.92873	-0.20134	-1.91151
21	1	0	-1.31812	0.081921	0.999319
22	8	0	-3.44058	2.35909	-0.27628
23	1	0	3.519467	2.603019	-1.33608
24	1	0	-0.9156	2.07461	-1.31355
25	1	0	0.771448	1.162632	1.061901
26	1	0	0.099638	-1.70534	-2.00683

27	1	0	-2.09743	-2.58361	-1.32973
28	1	0	1.845845	3.394624	0.390631
29	1	0	1.221234	3.17454	-1.23825
30	8	0	-3.93135	-0.74525	1.563762
31	1	0	-5.10212	0.65402	0.554127
32	1	0	0.623865	-1.92526	1.000834
33	1	0	-4.19629	0.113613	-1.61808
34	1	0	-4.22233	-1.46892	-0.83994
35	1	0	2.655884	1.091485	-1.44754
36	1	0	-2.9052	1.704594	1.624335
37	1	0	3.244771	1.547121	1.377272
38	1	0	4.700605	1.898993	0.474118
39	1	0	4.443059	-0.40572	-0.63281
40	1	0	-2.58055	-1.9055	1.079068
41	1	0	4.673052	-0.35446	2.42864
42	1	0	5.216796	-1.66888	1.368873
43	1	0	6.014671	-0.08921	1.300167
44	1	0	-2.78423	3.063256	-0.23765
45	1	0	-3.97018	-0.30373	2.42049

2b-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.25506	-0.45623	-0.90437
2	6	0	-1.71664	0.608972	0.11999
3	6	0	-0.65276	1.527756	-0.4164
4	6	0	0.544485	1.719586	0.142809
5	6	0	-0.15805	-1.82102	-0.99343
6	6	0	-1.62886	-1.85684	-0.70022
7	6	0	1.620504	2.625435	-0.38965
8	6	0	-4.06837	0.250053	0.602247
9	6	0	2.188505	-1.46084	-0.45376
10	6	0	0.805525	-1.81964	-0.07279
11	6	0	-3.80165	-0.47043	-0.72614
12	6	0	2.931083	1.897092	-0.77021
13	6	0	-2.99167	1.343955	0.613636
14	6	0	3.761376	1.352824	0.422458
15	6	0	4.060761	-0.14772	0.379567
16	8	0	2.795288	-0.85651	0.58842
17	8	0	-1.91444	-2.26996	0.642691
18	8	0	2.687131	-1.60816	-1.5509
19	6	0	5.010567	-0.60953	1.473988
20	1	0	-2.00567	-0.1494	-1.92271
21	1	0	-1.31127	0.083102	0.988253

22	8	0	-3.42905	2.361522	-0.29358
23	1	0	3.548762	2.599943	-1.33656
24	1	0	-0.89879	2.064021	-1.33321
25	1	0	0.78987	1.160416	1.044345
26	1	0	0.110219	-1.68273	-2.03754
27	1	0	-2.11728	-2.54192	-1.40499
28	1	0	1.857198	3.392897	0.359686
29	1	0	1.242549	3.154858	-1.27016
30	8	0	-3.93542	-0.60814	1.734385
31	1	0	-5.06637	0.691001	0.651609
32	1	0	0.579268	-1.89529	0.983149
33	1	0	-4.26775	0.092688	-1.53636
34	1	0	-4.22578	-1.4769	-0.72859
35	1	0	2.691774	1.085964	-1.46334
36	1	0	-2.85301	1.757421	1.618458
37	1	0	3.259432	1.565969	1.372593
38	1	0	4.723184	1.872397	0.466032
39	1	0	4.438507	-0.43628	-0.60194
40	1	0	-1.73875	-3.21355	0.729766
41	1	0	4.61757	-0.35636	2.46228
42	1	0	5.157499	-1.69053	1.425143
43	1	0	5.982592	-0.12511	1.354752
44	1	0	-2.77862	3.071762	-0.27632
45	1	0	-3.2618	-1.27509	1.521133

2b-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.01381	-0.62998	-0.73528
2	6	0	-1.85276	0.644277	0.175455
3	6	0	-0.81793	1.617448	-0.31771
4	6	0	0.270598	1.998644	0.354937
5	6	0	0.198063	-1.58839	-0.03899
6	6	0	-1.26653	-1.86544	-0.19031
7	6	0	1.343974	2.907396	-0.18444
8	6	0	-4.18552	-0.01856	0.245768
9	6	0	2.576216	-1.59913	-0.71225
10	6	0	1.176461	-2.0793	-0.80404
11	6	0	-3.54689	-0.86808	-0.86109
12	6	0	2.635028	2.157508	-0.59081
13	6	0	-3.28744	1.227141	0.275562
14	6	0	3.448219	1.556404	0.579715
15	6	0	3.944037	0.134144	0.316603
16	8	0	2.734446	-0.68535	0.262239

17	8	0	-1.84123	-2.17901	1.095175
18	8	0	3.45998	-1.95784	-1.46454
19	6	0	4.862642	-0.41351	1.398495
20	1	0	-1.5908	-0.42907	-1.72187
21	1	0	-1.58152	0.322587	1.184784
22	8	0	-3.64315	2.017203	-0.86413
23	1	0	3.271699	2.846517	-1.15411
24	1	0	-0.97377	2.004172	-1.32497
25	1	0	0.430321	1.596446	1.354516
26	1	0	0.456063	-0.87931	0.737675
27	1	0	-1.43234	-2.70121	-0.87921
28	1	0	1.59402	3.672048	0.561589
29	1	0	0.960633	3.435568	-1.06321
30	8	0	-4.1905	-0.67373	1.513057
31	1	0	-5.21866	0.258054	0.024033
32	1	0	0.993501	-2.80061	-1.5932
33	1	0	-3.89238	-0.5079	-1.83146
34	1	0	-3.82952	-1.91931	-0.77257
35	1	0	2.350873	1.364495	-1.2887
36	1	0	-3.42755	1.797963	1.199529
37	1	0	2.85156	1.530862	1.497284
38	1	0	4.316307	2.185989	0.796145
39	1	0	4.42979	0.063893	-0.6587
40	1	0	-1.49531	-3.02469	1.400866
41	1	0	4.367971	-0.39217	2.373155
42	1	0	5.150306	-1.44287	1.175064
43	1	0	5.77151	0.190399	1.458715
44	1	0	-3.14496	2.840321	-0.82251
45	1	0	-3.42036	-1.26581	1.542961

2b-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.91243	-0.95498	-0.38732
2	6	0	-1.82701	0.407144	0.396938
3	6	0	-0.91071	1.405981	-0.25853
4	6	0	0.190798	1.916516	0.296633
5	6	0	0.408506	-1.68027	0.199423
6	6	0	-1.03541	-2.08535	0.18477
7	6	0	1.156188	2.843109	-0.3962
8	6	0	-4.09011	0.044074	-0.51632
9	6	0	2.726102	-1.55476	-0.6524
10	6	0	1.367876	-2.14516	-0.60558
11	6	0	-3.41042	-1.31458	-0.43857

12	6	0	2.473636	2.152205	-0.82121
13	6	0	-3.3151	0.888355	0.492453
14	6	0	3.406109	1.735519	0.339911
15	6	0	4.015791	0.343955	0.165729
16	8	0	2.887344	-0.58063	0.262248
17	8	0	-1.48745	-2.35447	1.519445
18	8	0	3.573928	-1.88375	-1.45807
19	6	0	5.042108	-0.02339	1.226657
20	1	0	-1.56306	-0.78292	-1.41039
21	1	0	-1.46699	0.213377	1.409361
22	8	0	-3.54708	2.265213	0.206966
23	1	0	3.015774	2.823574	-1.49416
24	1	0	-1.17192	1.701322	-1.27423
25	1	0	0.446213	1.616157	1.31208
26	1	0	0.660947	-0.9031	0.910496
27	1	0	-1.17335	-2.97439	-0.44432
28	1	0	1.39167	3.692879	0.256964
29	1	0	0.678528	3.255401	-1.29064
30	8	0	-5.48289	-0.05185	-0.23549
31	1	0	-3.93751	0.483857	-1.51347
32	1	0	1.187353	-2.92909	-1.33329
33	1	0	-3.65803	-1.9646	-1.28027
34	1	0	-3.71578	-1.81499	0.48441
35	1	0	2.20799	1.272865	-1.4152
36	1	0	-3.7042	0.647343	1.490099
37	1	0	2.868361	1.741101	1.293509
38	1	0	4.221894	2.457114	0.443934
39	1	0	4.448509	0.229124	-0.82995
40	1	0	-0.97054	-3.09062	1.864677
41	1	0	4.605633	0.042043	2.226836
42	1	0	5.409064	-1.04017	1.071852
43	1	0	5.894207	0.659128	1.176126
44	1	0	-3.10448	2.793343	0.880326
45	1	0	-5.83662	0.8449	-0.25395

2b-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.143878	-0.899	0.605746
2	6	0	1.705748	0.335876	-0.26194
3	6	0	0.756992	1.274839	0.435811
4	6	0	-0.43668	1.638933	-0.0387
5	6	0	-0.06468	-2.05851	0.677661
6	6	0	1.378331	-2.2027	0.286909

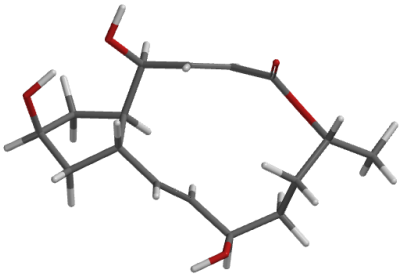
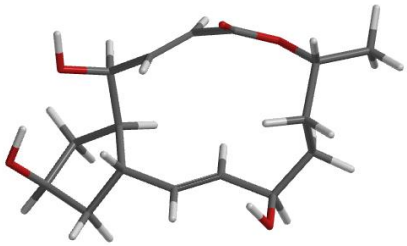
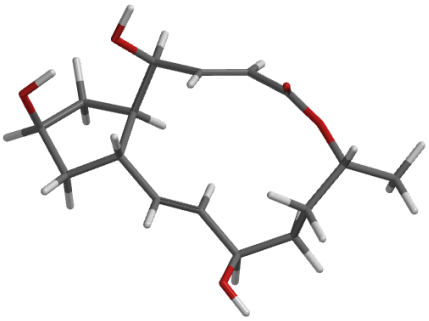
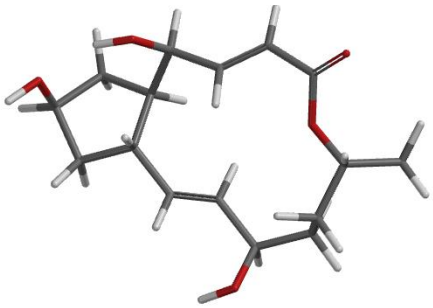
7	6	0	-1.40434	2.560565	0.653297
8	6	0	4.1245	0.407584	0.236977
9	6	0	-2.39331	-1.44525	0.315143
10	6	0	-1.07303	-1.89085	-0.17778
11	6	0	3.666293	-1.03267	0.404317
12	6	0	-2.75687	1.904574	1.017973
13	6	0	3.059222	1.017176	-0.67102
14	6	0	-3.68761	1.586086	-0.18196
15	6	0	-4.15297	0.130711	-0.27648
16	8	0	-2.98451	-0.68076	-0.62679
17	8	0	1.558233	-2.49101	-1.09729
18	8	0	-2.85353	-1.65717	1.418592
19	6	0	-5.19479	-0.10529	-1.35898
20	1	0	1.953575	-0.66863	1.659102
21	1	0	1.222126	-0.02735	-1.16995
22	8	0	3.109053	2.435615	-0.54146
23	1	0	-3.28149	2.57945	1.700426
24	1	0	1.090632	1.678868	1.391202
25	1	0	-0.76388	1.221559	-0.98976
26	1	0	-0.26161	-1.99219	1.744634
27	1	0	1.826976	-3.00056	0.896757
28	1	0	-1.6029	3.431425	0.013934
29	1	0	-0.94181	2.945	1.568059
30	8	0	5.443996	0.475341	-0.29549
31	1	0	4.082451	0.929548	1.204699
32	1	0	-0.90992	-1.88495	-1.2481
33	1	0	4.15782	-1.5431	1.23513
34	1	0	3.881645	-1.58521	-0.51478
35	1	0	-2.55927	0.995546	1.591831
36	1	0	3.303308	0.732645	-1.70304
37	1	0	-3.19957	1.840263	-1.12917
38	1	0	-4.58364	2.211506	-0.12676
39	1	0	-4.51839	-0.22082	0.689064
40	1	0	1.195017	-3.36629	-1.27149
41	1	0	-4.82005	0.2135	-2.33532
42	1	0	-5.45737	-1.16373	-1.4164
43	1	0	-6.10158	0.461704	-1.13545
44	1	0	2.42404	2.814323	-1.10356
45	1	0	5.653779	1.408868	-0.4134

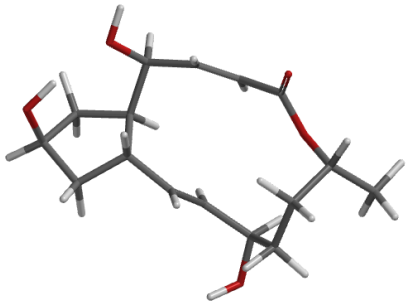
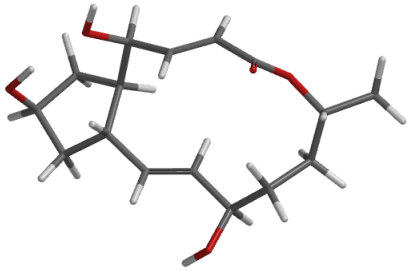
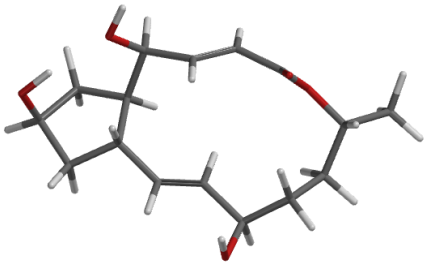
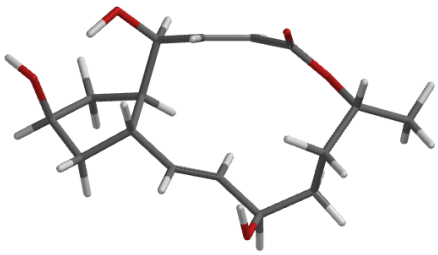
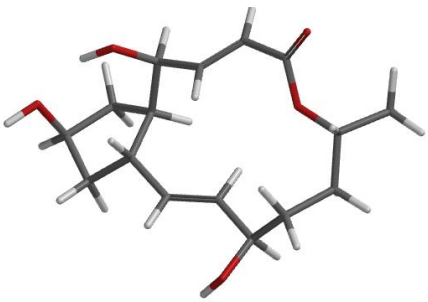
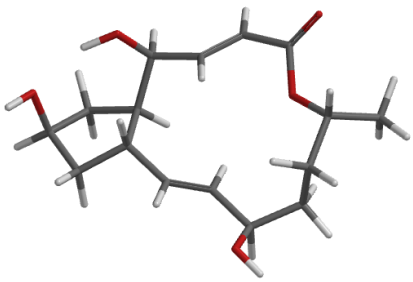
2b-Conf.6

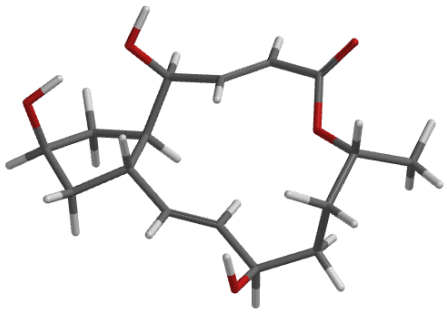
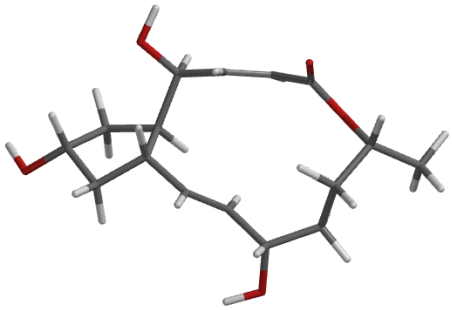
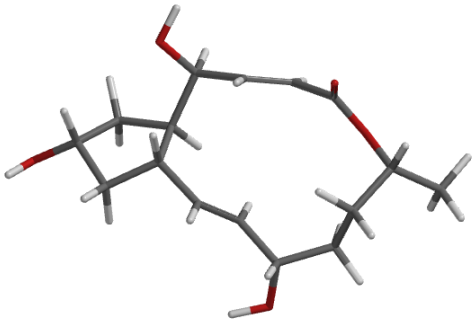
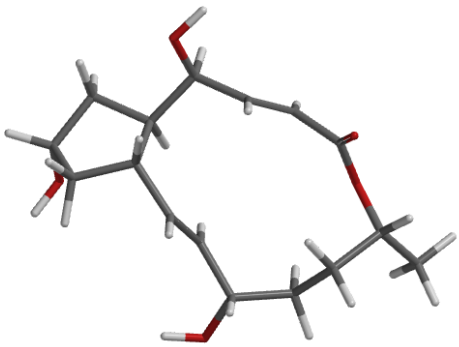
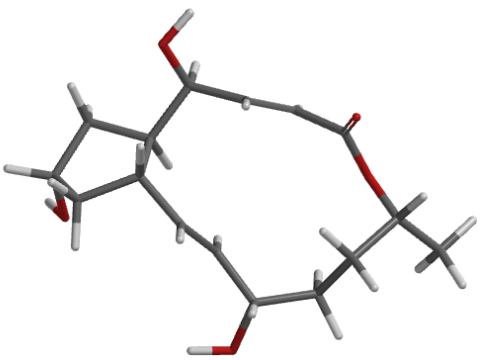
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.18298	-0.6095	-0.83727

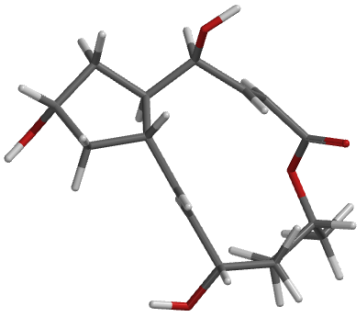
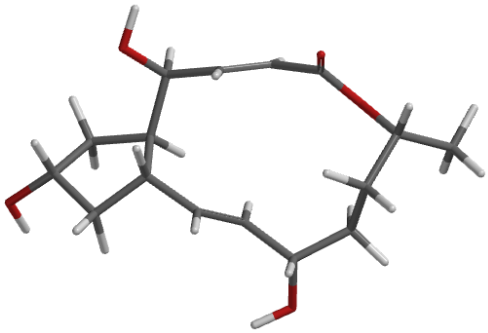
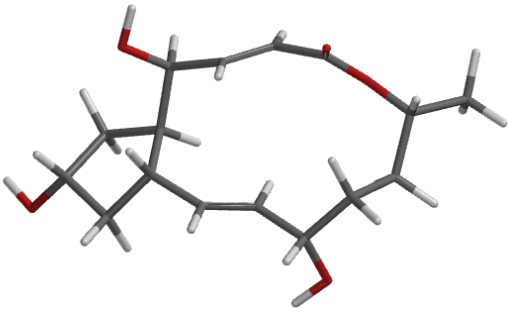
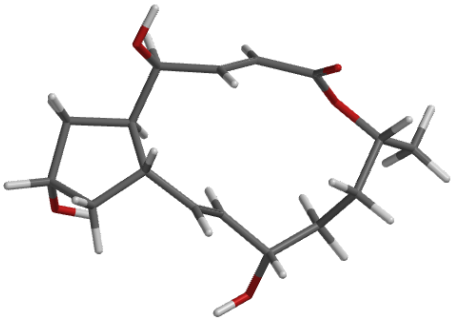
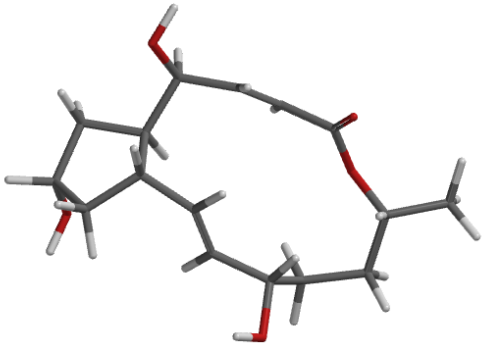
2	6	0	-1.70428	0.59255	0.047635
3	6	0	-0.55684	1.410026	-0.48873
4	6	0	0.477207	1.796879	0.262322
5	6	0	-0.18275	-2.05667	-0.63983
6	6	0	-1.64132	-1.97789	-0.3192
7	6	0	1.629926	2.678181	-0.13554
8	6	0	-4.10504	0.370884	0.324385
9	6	0	2.178546	-1.6603	-0.30816
10	6	0	0.823181	-1.90681	0.223359
11	6	0	-3.73783	-0.53692	-0.84366
12	6	0	3.007673	2.128735	0.304092
13	6	0	-2.99059	1.423647	0.308104
14	6	0	3.61257	1.057445	-0.63561
15	6	0	4.085138	-0.243	0.029493
16	8	0	2.909686	-0.93391	0.567221
17	8	0	-1.85543	-2.17921	1.070013
18	8	0	2.571609	-1.97768	-1.41337
19	6	0	5.066879	-0.08101	1.177368
20	1	0	-1.81854	-0.49454	-1.86065
21	1	0	-1.40282	0.195693	1.019599
22	8	0	-3.3059	2.319998	-0.75796
23	1	0	2.899265	1.72755	1.316274
24	1	0	-0.60455	1.7079	-1.53576
25	1	0	0.498039	1.469168	1.302553
26	1	0	0.054412	-2.12905	-1.69794
27	1	0	-2.16029	-2.76157	-0.89347
28	1	0	1.490503	3.651266	0.354083
29	1	0	1.616097	2.87134	-1.21366
30	8	0	-4.03683	-0.43125	1.518097
31	1	0	-5.09523	0.825634	0.232796
32	1	0	0.65072	-1.77276	1.282906
33	1	0	-4.08299	-0.07264	-1.76825
34	1	0	-4.22009	-1.51361	-0.75978
35	1	0	3.704966	2.966368	0.388101
36	1	0	-2.9248	1.970379	1.257499
37	1	0	4.469592	1.476024	-1.173
38	1	0	2.88604	0.780102	-1.40491
39	1	0	4.515131	-0.88817	-0.73697
40	1	0	-2.66247	-1.70137	1.331965
41	1	0	4.643212	0.504819	1.995496
42	1	0	5.356047	-1.05837	1.569428
43	1	0	5.967451	0.426009	0.821839
44	1	0	-2.60411	2.978791	-0.80393
45	1	0	-4.11767	0.139941	2.291183

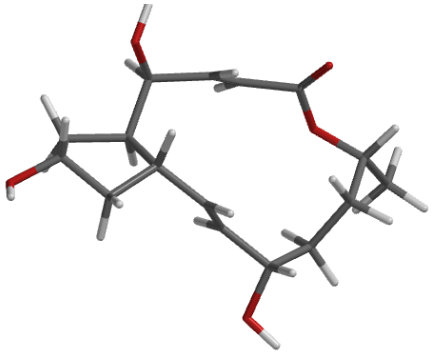
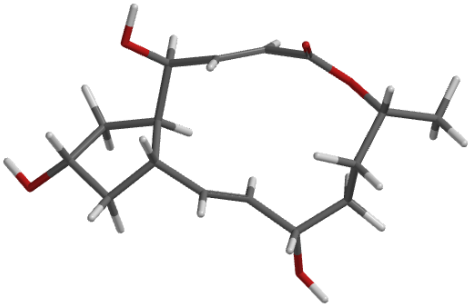
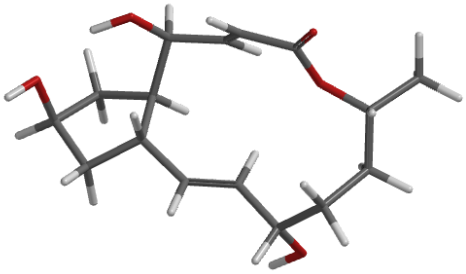
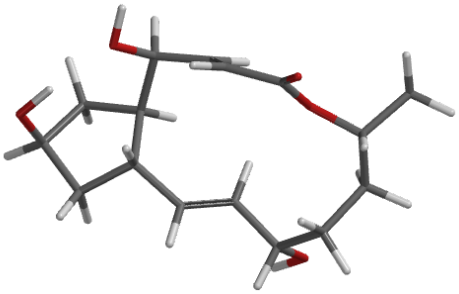
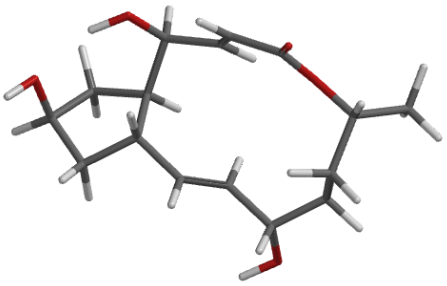
Table S9. The Information of conformations of (2*E*, 4*S*, 5*R*, 7*R*, 9*S*, 10*E*, 12*R*, 15*R*)-**3a**, (2*E*, 4*S*, 5*R*, 7*S*, 9*S*, 10*E*, 12*S*, 15*R*)-**3b**, (2*E*, 4*S*, 5*R*, 7*R*, 9*S*, 10*E*, 12*S*, 15*R*)-**3c**, and (2*E*, 4*S*, 5*R*, 7*S*, 9*S*, 10*E*, 12*R*, 15*R*)-**3d**

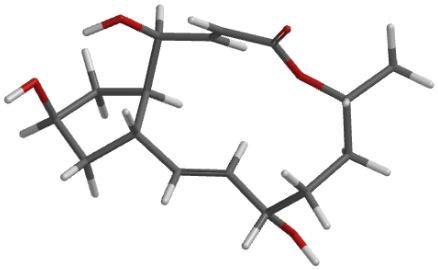
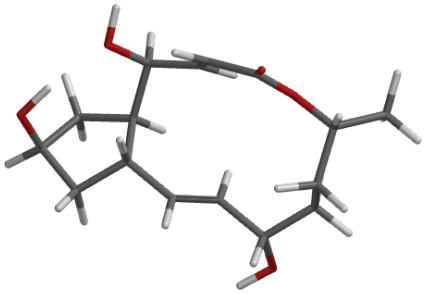
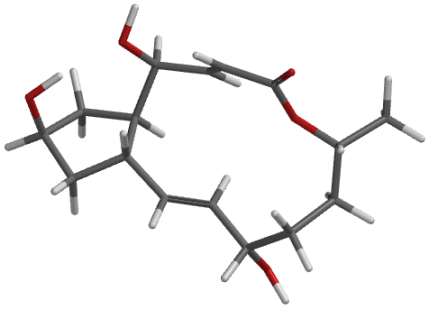
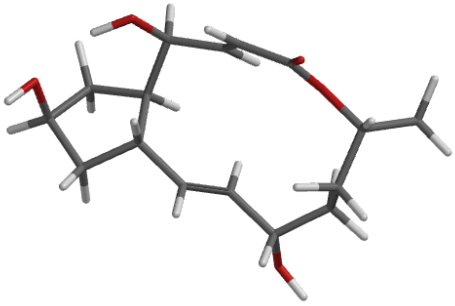
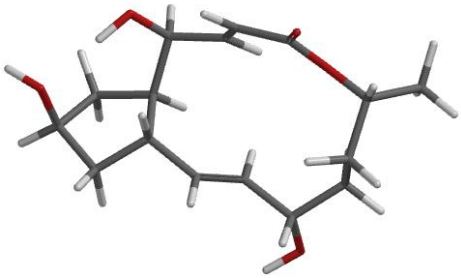
Label	**Conformers**	**Calculated energy (kJ/mol)**	**Boltzmann distribution**
3a-Conf.1		0	0.492
3a-Conf.2		2.06	0.214
3a-Conf.3		4.72	0.073
3a-Conf.4		6.62	0.034

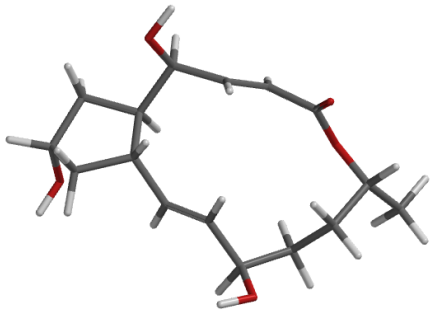
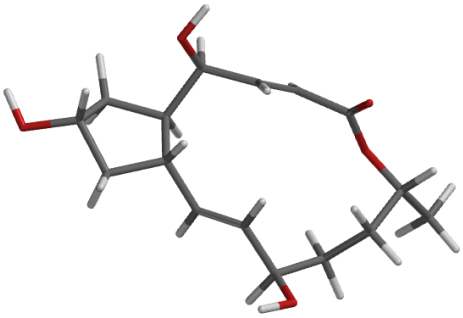
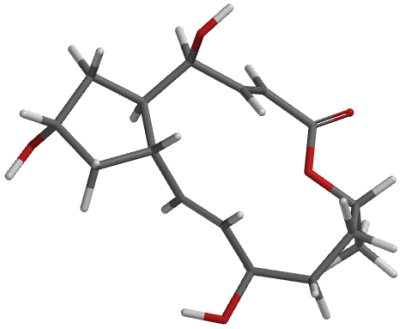
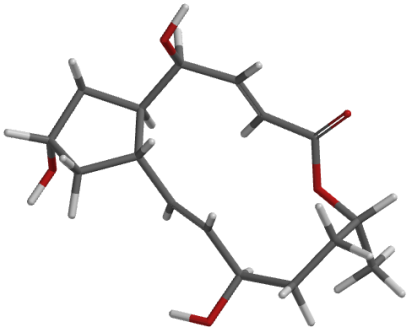
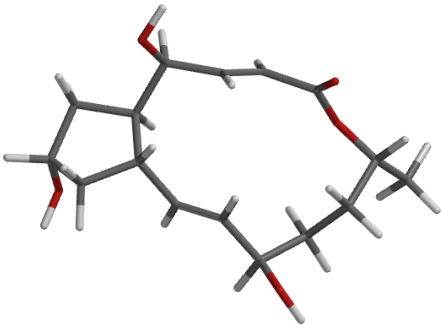
3a-Conf.5		7.14	0.028
3a-Conf.6		7.58	0.023
3a-Conf.7		7.62	0.023
3a-Conf.8		7.88	0.021
3a-Conf.9		7.93	0.020
3a-Conf.10		8.15	0.018

3a-Conf.11		8.19	0.018
3b-Conf.1		0	0.302
3b-Conf.2		0.96	0.205
3b-Conf.3		1.97	0.137
3b-Conf.4		2.93	0.092

3b-Conf.5		3.93	0.062
3b-Conf.6		4.43	0.051
3b-Conf.7		4.78	0.044
3b-Conf.8		5.80	0.029
3b-Conf.9		7.31	0.016

3b-Conf.10		8.19	0.011
3b-Conf.11		8.24	0.011
3c-Conf.1		0	0.514
3c-Conf.2		3.38	0.131
3c-Conf.3		3.74	0.114

3c-Conf.4		3.81	0.111
3c-Conf.5		5.79	0.050
3c-Conf.6		7.64	0.024
3c-Conf.7		8.24	0.018
3c-Conf.8		9.27	0.012

3d-Conf.1		0	0.380
3d-Conf.2		0.34	0.331
3d-Conf.3		3.19	0.105
3d-Conf.4		4.70	0.057
3d-Conf.5		5.79	0.037

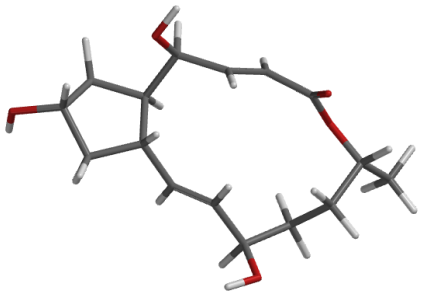
3d-Conf.6		5.95	0.034

Table S10. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*R*, 9*S*, 10*E*, 12*R*, 15*R*)-**3a**] in NMR calculation

3a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.14137	-0.22532	0.827815
2	6	0	-1.90899	0.747937	-0.37769
3	6	0	-0.59364	1.488892	-0.45792
4	6	0	0.361477	1.582316	0.466149
5	6	0	-0.61112	-1.94234	-0.17742
6	6	0	-1.94996	-1.71739	0.463553
7	6	0	1.616992	2.423531	0.378639
8	6	0	2.903357	1.606673	0.596763
9	6	0	1.801789	-1.92589	-0.3003
10	6	0	0.546904	-2.09288	0.466505
11	6	0	-3.57728	0.079438	1.347041
12	6	0	-4.26914	0.870315	0.225817
13	6	0	-3.12204	1.718152	-0.33814
14	6	0	3.307838	0.708043	-0.59057
15	6	0	3.846641	-0.67409	-0.19679
16	8	0	2.764335	-1.39537	0.484199
17	8	0	-4.84613	0.018389	-0.76896
18	8	0	-3.00228	-2.08499	-0.44551
19	8	0	1.933294	-2.13505	-1.48821
20	6	0	5.034756	-0.67279	0.749036
21	1	0	-1.42444	-0.02433	1.623968
22	1	0	-2.00957	0.168982	-1.30274
23	8	0	1.751486	3.13109	-0.85546
24	1	0	-0.4522	2.032291	-1.39104
25	1	0	0.264991	1.056806	1.41301
26	1	0	-0.5912	-1.85399	-1.26006
27	1	0	-2.04083	-2.30353	1.385128
28	1	0	1.566192	3.147027	1.207533
29	1	0	2.747762	1.001909	1.494196

30	1	0	3.712281	2.304941	0.827648
31	1	0	0.616183	-2.13121	1.547986
32	1	0	-4.13649	-0.81995	1.612174
33	1	0	-3.51532	0.705879	2.240781
34	1	0	-5.0857	1.490733	0.603322
35	1	0	-2.91292	2.547803	0.346216
36	1	0	-3.36155	2.13723	-1.31789
37	1	0	2.452352	0.552985	-1.2522
38	1	0	4.069744	1.204737	-1.1979
39	1	0	4.089184	-1.23144	-1.10196
40	1	0	-4.29813	-0.78164	-0.82018
41	1	0	-2.99982	-3.04001	-0.57118
42	1	0	5.346226	-1.69573	0.970638
43	1	0	5.874258	-0.15216	0.281631
44	1	0	4.801451	-0.17223	1.691068
45	1	0	1.004554	3.734745	-0.93353

3a-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.14849	-0.23617	0.822381
2	6	0	-1.95313	0.778569	-0.35475
3	6	0	-0.66302	1.56244	-0.41852
4	6	0	0.37331	1.529633	0.41862
5	6	0	-0.58929	-1.90664	-0.22317
6	6	0	-1.93372	-1.71388	0.416041
7	6	0	1.605707	2.407335	0.340863
8	6	0	2.912706	1.622795	0.596212
9	6	0	1.825896	-1.8951	-0.31893
10	6	0	0.561641	-2.08819	0.425802
11	6	0	-3.58454	0.022017	1.367819
12	6	0	-4.30875	0.828017	0.278539
13	6	0	-3.18886	1.71632	-0.27563
14	6	0	3.363758	0.715393	-0.56949
15	6	0	3.881703	-0.66903	-0.15317
16	8	0	2.776298	-1.38442	0.493786
17	8	0	-4.88078	-0.00857	-0.73211
18	8	0	-2.97675	-2.06969	-0.50837
19	8	0	1.974684	-2.06861	-1.51048
20	6	0	5.038413	-0.66819	0.830285
21	1	0	-1.42654	-0.03959	1.61551
22	1	0	-2.04515	0.22663	-1.29775
23	8	0	1.67049	3.19258	-0.8521
24	1	0	-0.61854	2.263483	-1.2507

25	1	0	0.370816	0.855097	1.270225
26	1	0	-0.55936	-1.76929	-1.30048
27	1	0	-2.02073	-2.3264	1.320661
28	1	0	1.525344	3.1494	1.144371
29	1	0	2.760886	1.028219	1.501636
30	1	0	3.699067	2.34608	0.826375
31	1	0	0.618453	-2.17621	1.505199
32	1	0	-4.12029	-0.89679	1.614556
33	1	0	-3.5249	0.624176	2.278239
34	1	0	-5.13346	1.419022	0.684271
35	1	0	-2.99236	2.533471	0.427466
36	1	0	-3.44941	2.154597	-1.24152
37	1	0	2.538329	0.543976	-1.26794
38	1	0	4.150881	1.204733	-1.15015
39	1	0	4.151438	-1.22871	-1.0492
40	1	0	-4.31473	-0.79336	-0.81465
41	1	0	-2.96948	-3.0225	-0.64979
42	1	0	5.895317	-0.15478	0.38728
43	1	0	4.777298	-0.16154	1.761596
44	1	0	5.336336	-1.69181	1.066493
45	1	0	1.679205	2.58983	-1.6049

3a-Conf.3

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.1478	-0.22767	0.822382
2	6	0	-1.93817	0.770469	-0.36646
3	6	0	-0.63879	1.538898	-0.43841
4	6	0	0.374036	1.536327	0.427213
5	6	0	-0.6042	-1.91876	-0.20885
6	6	0	-1.94514	-1.71174	0.433172
7	6	0	1.607838	2.401052	0.354195
8	6	0	2.912672	1.610243	0.600551
9	6	0	1.810684	-1.90691	-0.31546
10	6	0	0.549668	-2.08883	0.437673
11	6	0	-3.58229	0.051371	1.360877
12	6	0	-4.29549	0.851125	0.25971
13	6	0	-3.16506	1.721479	-0.30218
14	6	0	3.349116	0.709258	-0.57406
15	6	0	3.866769	-0.67772	-0.1703
16	8	0	2.766189	-1.39193	0.487585
17	8	0	-4.87302	0.007751	-0.74225
18	8	0	-2.9941	-2.07198	-0.48286
19	8	0	1.952735	-2.09442	-1.50574

20	6	0	5.035472	-0.68755	0.799318
21	1	0	-1.42602	-0.03029	1.615292
22	1	0	-2.03489	0.207335	-1.30231
23	8	0	1.62915	3.096668	-0.89466
24	1	0	-0.55899	2.195451	-1.30206
25	1	0	0.346686	0.902484	1.308892
26	1	0	-0.57901	-1.80026	-1.28849
27	1	0	-2.03266	-2.31334	1.345096
28	1	0	1.526499	3.133547	1.173285
29	1	0	2.762914	1.015283	1.506384
30	1	0	3.706578	2.326097	0.836013
31	1	0	0.611456	-2.15759	1.518197
32	1	0	-4.12786	-0.85884	1.617713
33	1	0	-3.51882	0.664402	2.263801
34	1	0	-5.11562	1.455041	0.655737
35	1	0	-2.96205	2.545002	0.391565
36	1	0	-3.41892	2.150795	-1.27388
37	1	0	2.513272	0.564462	-1.26258
38	1	0	4.133632	1.199891	-1.15749
39	1	0	4.123296	-1.23581	-1.07129
40	1	0	-4.31389	-0.78298	-0.81407
41	1	0	-2.98906	-3.02568	-0.61807
42	1	0	5.331823	-1.71342	1.027974
43	1	0	5.889555	-0.17613	0.348459
44	1	0	4.788197	-0.18356	1.735965
45	1	0	2.360405	3.723021	-0.86704

3a-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.217	-0.50585	0.828481
2	6	0	-2.00735	0.846088	0.042933
3	6	0	-0.82097	1.651632	0.498187
4	6	0	0.243774	1.946124	-0.24972
5	6	0	-0.29414	-1.68933	-0.20141
6	6	0	-1.77665	-1.75015	0.009299
7	6	0	1.456217	2.710517	0.226622
8	6	0	2.670093	1.814112	0.547718
9	6	0	2.069177	-2.31508	-0.01895
10	6	0	0.621289	-2.58106	0.18501
11	6	0	-3.72268	-0.53823	1.220434
12	6	0	-4.40435	0.487003	0.318694
13	6	0	-3.35606	1.594046	0.195009
14	6	0	3.278594	1.043612	-0.65059

15	6	0	3.60102	-0.4241	-0.34375
16	8	0	2.306948	-0.99249	0.014941
17	8	0	-4.64017	-0.17085	-0.9478
18	8	0	-2.39335	-1.81488	-1.27985
19	8	0	2.91871	-3.16593	-0.18696
20	6	0	4.619956	-0.63529	0.769732
21	1	0	-1.61089	-0.5052	1.738128
22	1	0	-1.87441	0.601202	-1.01335
23	8	0	1.801921	3.758235	-0.69887
24	1	0	-0.85224	1.998246	1.532465
25	1	0	0.27543	1.600937	-1.283
26	1	0	0.056114	-0.78952	-0.69141
27	1	0	-2.03678	-2.64681	0.588816
28	1	0	1.192506	3.23736	1.147503
29	1	0	2.345562	1.10686	1.3145
30	1	0	3.432759	2.450474	1.005747
31	1	0	0.365521	-3.53843	0.626482
32	1	0	-4.17548	-1.52739	1.117597
33	1	0	-3.84464	-0.23114	2.261591
34	1	0	-5.35877	0.842227	0.717791
35	1	0	-3.36369	2.185997	1.116863
36	1	0	-3.55279	2.279089	-0.63428
37	1	0	2.59271	1.043365	-1.50331
38	1	0	4.195761	1.529117	-0.99463
39	1	0	3.941091	-0.92744	-1.25249
40	1	0	-4.87258	0.493517	-1.60703
41	1	0	-3.2394	-1.3299	-1.24916
42	1	0	4.792203	-1.69949	0.930365
43	1	0	5.568285	-0.16985	0.488207
44	1	0	4.282937	-0.18904	1.707798
45	1	0	2.022762	3.34885	-1.54319

3a-Conf.5

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	2.166204	-0.04645	-0.82559
2	6	0	1.697242	0.664041	0.492744
3	6	0	0.264942	1.153868	0.545454
4	6	0	-0.5228	1.421044	-0.49577
5	6	0	0.789652	-2.06685	-0.22954
6	6	0	2.130684	-1.59137	-0.73029
7	6	0	-1.95979	1.88189	-0.49448
8	6	0	-2.79022	1.712706	0.786502
9	6	0	-1.62458	-2.04651	-0.08598

10	6	0	-0.37336	-1.94025	-0.87051
11	6	0	3.586991	0.511485	-1.12498
12	6	0	4.053583	1.181194	0.17681
13	6	0	2.751865	1.776616	0.731725
14	6	0	-3.05242	0.291588	1.325153
15	6	0	-3.61064	-0.77124	0.364799
16	8	0	-2.54692	-1.17913	-0.56192
17	8	0	4.64389	0.24675	1.087212
18	8	0	3.167006	-1.9944	0.180985
19	8	0	-1.77985	-2.72231	0.909566
20	6	0	-4.80322	-0.35155	-0.47716
21	1	0	1.50315	0.211268	-1.65009
22	1	0	1.813463	-0.05093	1.314262
23	8	0	-2.01966	3.263009	-0.92419
24	1	0	-0.13064	1.275028	1.552266
25	1	0	-0.12596	1.317685	-1.50243
26	1	0	0.775054	-2.40915	0.801749
27	1	0	2.342513	-1.99824	-1.72606
28	1	0	-2.46201	1.345643	-1.30249
29	1	0	-3.74603	2.203844	0.58027
30	1	0	-2.32509	2.294405	1.591286
31	1	0	-0.44679	-1.5376	-1.87405
32	1	0	4.288356	-0.25605	-1.4574
33	1	0	3.523749	1.266084	-1.91346
34	1	0	4.809294	1.95038	-0.00126
35	1	0	2.486943	2.672256	0.159224
36	1	0	2.842896	2.057932	1.783187
37	1	0	-2.14495	-0.11939	1.773851
38	1	0	-3.77314	0.381563	2.145476
39	1	0	-3.86951	-1.65163	0.953671
40	1	0	4.227196	-0.61636	0.931876
41	1	0	3.294101	-2.94748	0.125488
42	1	0	-5.13977	-1.18518	-1.0969
43	1	0	-5.62746	-0.05834	0.177832
44	1	0	-4.57071	0.490881	-1.13097
45	1	0	-1.48535	3.770782	-0.30196

3a-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.09552	-0.41525	0.781424
2	6	0	-2.05578	0.768953	-0.2386
3	6	0	-0.80111	1.598955	-0.3472
4	6	0	0.344961	1.509101	0.328966

5	6	0	-0.49661	-1.8218	-0.53752
6	6	0	-1.84251	-1.79464	0.127834
7	6	0	1.541868	2.410805	0.099332
8	6	0	2.752537	1.663663	-0.50241
9	6	0	1.936101	-1.7144	-0.49782
10	6	0	0.63941	-2.10478	0.099819
11	6	0	-3.49278	-0.33611	1.465468
12	6	0	-4.33787	0.597474	0.585678
13	6	0	-3.30521	1.623535	0.103567
14	6	0	3.647401	0.918299	0.520294
15	6	0	3.963899	-0.54136	0.178681
16	8	0	2.765485	-1.32486	0.491117
17	8	0	-4.9555	-0.09523	-0.50467
18	8	0	-2.89415	-2.02361	-0.82505
19	8	0	2.194713	-1.6592	-1.68151
20	6	0	5.095538	-1.12589	1.008965
21	1	0	-1.31895	-0.29237	1.537863
22	1	0	-2.23941	0.353261	-1.23667
23	8	0	1.252952	3.48581	-0.80079
24	1	0	-0.86924	2.375291	-1.10749
25	1	0	0.489604	0.746419	1.089359
26	1	0	-0.45774	-1.45625	-1.55976
27	1	0	-1.88885	-2.5536	0.917253
28	1	0	1.850828	2.828409	1.069912
29	1	0	3.350999	2.421871	-1.01261
30	1	0	2.393204	0.980767	-1.27587
31	1	0	0.650447	-2.41256	1.14004
32	1	0	-3.96576	-1.31295	1.586003
33	1	0	-3.38757	0.103935	2.460569
34	1	0	-5.15149	1.066765	1.143812
35	1	0	-3.07222	2.318103	0.91856
36	1	0	-3.66614	2.205132	-0.74767
37	1	0	4.597216	1.450672	0.620703
38	1	0	3.192116	0.924238	1.516374
39	1	0	4.168473	-0.65975	-0.88606
40	1	0	-4.35829	-0.81322	-0.77119
41	1	0	-2.86686	-2.94107	-1.11737
42	1	0	5.236202	-2.18329	0.775692
43	1	0	6.02764	-0.59873	0.792823
44	1	0	4.884149	-1.03019	2.077328
45	1	0	0.527645	3.996588	-0.42332

3a-Conf.7

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-2.07542	-0.44386	0.761084
2	6	0	-2.08784	0.803737	-0.18287
3	6	0	-0.85512	1.668389	-0.27418
4	6	0	0.344971	1.509496	0.285001
5	6	0	-0.46944	-1.77042	-0.63682
6	6	0	-1.81941	-1.77873	0.020678
7	6	0	1.526248	2.429612	0.045204
8	6	0	2.772387	1.663363	-0.46189
9	6	0	1.965786	-1.69375	-0.54944
10	6	0	0.65426	-2.11714	-0.00857
11	6	0	-3.45528	-0.43456	1.485814
12	6	0	-4.34225	0.531554	0.686931
13	6	0	-3.34298	1.607308	0.246033
14	6	0	3.585809	0.903737	0.616717
15	6	0	3.9589	-0.5403	0.260176
16	8	0	2.766023	-1.36236	0.48415
17	8	0	-4.97083	-0.1068	-0.43004
18	8	0	-2.86806	-1.94716	-0.94815
19	8	0	2.256239	-1.56768	-1.71998
20	6	0	5.053284	-1.11946	1.141968
21	1	0	-1.28056	-0.35007	1.502735
22	1	0	-2.29024	0.447187	-1.20028
23	8	0	1.210743	3.501631	-0.8479
24	1	0	-0.99649	2.542587	-0.90744
25	1	0	0.550045	0.662175	0.933215
26	1	0	-0.41646	-1.3282	-1.62761
27	1	0	-1.86892	-2.58518	0.761257
28	1	0	1.787421	2.930306	0.985189
29	1	0	3.417519	2.409106	-0.93257
30	1	0	2.455836	0.980747	-1.25581
31	1	0	0.643876	-2.50262	1.005567
32	1	0	-3.90557	-1.42671	1.560045
33	1	0	-3.33095	-0.05277	2.50255
34	1	0	-5.1518	0.94633	1.292008
35	1	0	-3.10218	2.253493	1.097909
36	1	0	-3.73767	2.234788	-0.55629
37	1	0	4.511157	1.450633	0.816993
38	1	0	3.043702	0.870745	1.567872
39	1	0	4.228391	-0.62676	-0.79331
40	1	0	-4.3616	-0.78851	-0.75805
41	1	0	-2.84848	-2.84935	-1.28535
42	1	0	5.229337	-2.16853	0.895646
43	1	0	5.984508	-0.56896	0.990109

44	1	0	4.779465	-1.05086	2.198146
45	1	0	1.023195	3.115523	-1.71221

3a-Conf.8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.12602	-0.25244	0.806592
2	6	0	-1.93515	0.765802	-0.36848
3	6	0	-0.65128	1.56181	-0.42559
4	6	0	0.385337	1.529589	0.41074
5	6	0	-0.60307	-1.9435	-0.23439
6	6	0	-1.95991	-1.73717	0.378335
7	6	0	1.615774	2.409692	0.332559
8	6	0	2.92347	1.626764	0.587773
9	6	0	1.814732	-1.90076	-0.30679
10	6	0	0.546306	-2.076	0.430597
11	6	0	-3.5335	0.047785	1.400178
12	6	0	-4.2751	0.840154	0.317792
13	6	0	-3.1783	1.698496	-0.29924
14	6	0	3.369056	0.708355	-0.57167
15	6	0	3.873964	-0.67812	-0.14513
16	8	0	2.762584	-1.37811	0.504926
17	8	0	-4.77763	-0.04325	-0.71654
18	8	0	-2.94426	-2.17534	-0.55833
19	8	0	1.976746	-2.09677	-1.49373
20	6	0	5.030903	-0.68021	0.838399
21	1	0	-1.37829	-0.08389	1.581737
22	1	0	-2.01285	0.213989	-1.31261
23	8	0	1.67876	3.194144	-0.86097
24	1	0	-0.61018	2.266039	-1.25523
25	1	0	0.386651	0.851471	1.259305
26	1	0	-0.56808	-1.86782	-1.31749
27	1	0	-2.04684	-2.34388	1.289962
28	1	0	1.5346	3.151925	1.135838
29	1	0	2.775571	1.040385	1.499148
30	1	0	3.710706	2.352171	0.808096
31	1	0	0.59484	-2.10879	1.513572
32	1	0	-4.07681	-0.85178	1.699568
33	1	0	-3.43138	0.675483	2.289737
34	1	0	-5.1045	1.431937	0.71233
35	1	0	-2.97759	2.542112	0.368081
36	1	0	-3.4655	2.098724	-1.27348
37	1	0	2.543273	0.539119	-1.27043
38	1	0	4.161134	1.187563	-1.15408

39	1	0	4.140014	-1.24558	-1.03737
40	1	0	-5.59404	-0.44277	-0.39415
41	1	0	-3.61223	-1.47662	-0.68264
42	1	0	5.32039	-1.70478	1.081055
43	1	0	5.892169	-0.17658	0.392557
44	1	0	4.774002	-0.16597	1.766763
45	1	0	1.691983	2.590655	-1.61316

3a-Conf.9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.07514	-0.43181	0.761018
2	6	0	-2.04725	0.759795	-0.24918
3	6	0	-0.79993	1.602755	-0.34941
4	6	0	0.35042	1.504407	0.317807
5	6	0	-0.5054	-1.85771	-0.55417
6	6	0	-1.86855	-1.8139	0.075728
7	6	0	1.546068	2.408455	0.094098
8	6	0	2.757398	1.664349	-0.51099
9	6	0	1.924983	-1.7196	-0.48197
10	6	0	0.62476	-2.09626	0.112262
11	6	0	-3.44063	-0.32515	1.501782
12	6	0	-4.308	0.58991	0.641321
13	6	0	-3.30526	1.605339	0.093128
14	6	0	3.658684	0.922142	0.508746
15	6	0	3.955788	-0.5448	0.181738
16	8	0	2.74997	-1.31001	0.504906
17	8	0	-4.86346	-0.23837	-0.40632
18	8	0	-2.83472	-2.0946	-0.93418
19	8	0	2.196131	-1.68952	-1.66438
20	6	0	5.084376	-1.13327	1.013871
21	1	0	-1.27268	-0.33515	1.4935
22	1	0	-2.22153	0.344266	-1.24852
23	8	0	1.256642	3.488868	-0.79936
24	1	0	-0.87529	2.389766	-1.09794
25	1	0	0.500692	0.729509	1.064364
26	1	0	-0.45318	-1.54491	-1.59324
27	1	0	-1.92917	-2.57482	0.866985
28	1	0	1.854731	2.820357	1.067159
29	1	0	3.351194	2.424841	-1.02315
30	1	0	2.398659	0.979575	-1.28321
31	1	0	0.624315	-2.35529	1.165787
32	1	0	-3.92053	-1.2922	1.669656
33	1	0	-3.29621	0.140372	2.47945

34	1	0	-5.1262	1.054226	1.199246
35	1	0	-3.0735	2.329199	0.881411
36	1	0	-3.68787	2.164271	-0.76549
37	1	0	4.615531	1.445353	0.588676
38	1	0	3.217452	0.94648	1.510889
39	1	0	4.15599	-0.67598	-0.88235
40	1	0	-5.2373	0.32875	-1.09087
41	1	0	-3.62329	-1.54034	-0.78902
42	1	0	5.213438	-2.19411	0.789562
43	1	0	6.021377	-0.61782	0.790558
44	1	0	4.877198	-1.02627	2.082023
45	1	0	0.535692	4.001024	-0.41551

3a-Conf.10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.11703	-0.37275	0.777765
2	6	0	-2.03741	0.804587	-0.25269
3	6	0	-0.84924	1.734501	-0.22383
4	6	0	0.256699	1.656281	0.5158
5	6	0	-0.248	-1.69927	-0.15154
6	6	0	-1.71295	-1.74107	0.159367
7	6	0	1.412089	2.634473	0.467764
8	6	0	2.79457	1.945763	0.522206
9	6	0	2.131647	-2.23868	0.017381
10	6	0	0.700893	-2.51337	0.315535
11	6	0	-3.58075	-0.36208	1.311096
12	6	0	-4.37833	0.471019	0.311678
13	6	0	-3.38574	1.557758	-0.10059
14	6	0	3.202534	1.141631	-0.73882
15	6	0	3.5817	-0.32087	-0.47788
16	8	0	2.349795	-0.91176	0.032512
17	8	0	-4.70019	-0.40738	-0.79149
18	8	0	-2.41653	-2.03509	-1.05099
19	8	0	2.979052	-3.07824	-0.20489
20	6	0	4.740631	-0.52486	0.490512
21	1	0	-1.43967	-0.19821	1.616189
22	1	0	-2.05204	0.354864	-1.25239
23	8	0	1.31833	3.566055	-0.61353
24	1	0	-0.92797	2.561491	-0.92819
25	1	0	0.38616	0.851045	1.232769
26	1	0	0.058038	-0.86831	-0.77741
27	1	0	-1.91384	-2.52436	0.903188
28	1	0	1.349606	3.262683	1.364766

29	1	0	2.793578	1.298105	1.403006
30	1	0	3.535191	2.726037	0.714237
31	1	0	0.483611	-3.40524	0.893922
32	1	0	-4.00474	-1.36198	1.430568
33	1	0	-3.61769	0.126328	2.287422
34	1	0	-5.30586	0.871932	0.730367
35	1	0	-3.32199	2.298753	0.703433
36	1	0	-3.68215	2.085064	-1.01188
37	1	0	2.387225	1.129818	-1.46975
38	1	0	4.049833	1.622047	-1.23522
39	1	0	3.810311	-0.81433	-1.42647
40	1	0	-5.02191	0.123237	-1.5297
41	1	0	-3.28228	-1.58681	-1.02544
42	1	0	4.953191	-1.58712	0.607996
43	1	0	5.63434	-0.03364	0.096572
44	1	0	4.521198	-0.1018	1.472937
45	1	0	1.296303	3.063358	-1.4364

3a-Conf.11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.14288	-0.35037	0.798963
2	6	0	-2.04213	0.810591	-0.25091
3	6	0	-0.84511	1.729078	-0.22672
4	6	0	0.253568	1.658138	0.524734
5	6	0	-0.24386	-1.67684	-0.11254
6	6	0	-1.70079	-1.71699	0.232426
7	6	0	1.412377	2.632573	0.474281
8	6	0	2.793591	1.940507	0.526696
9	6	0	2.134432	-2.23541	0.009022
10	6	0	0.705984	-2.50244	0.332417
11	6	0	-3.62926	-0.35921	1.268559
12	6	0	-4.39932	0.483846	0.240969
13	6	0	-3.38356	1.575606	-0.11547
14	6	0	3.200549	1.144077	-0.73956
15	6	0	3.585544	-0.31798	-0.48611
16	8	0	2.358433	-0.9112	0.034786
17	8	0	-4.78942	-0.2816	-0.90421
18	8	0	-2.50229	-1.97282	-0.94147
19	8	0	2.97015	-3.07885	-0.23804
20	6	0	4.751223	-0.52416	0.47321
21	1	0	-1.49837	-0.14542	1.656201
22	1	0	-2.05724	0.351146	-1.24676
23	8	0	1.320438	3.563982	-0.60713

24	1	0	-0.91348	2.546372	-0.9433
25	1	0	0.373348	0.863976	1.255986
26	1	0	0.055528	-0.84404	-0.7383
27	1	0	-1.8952	-2.49345	0.980512
28	1	0	1.352621	3.261137	1.371181
29	1	0	2.790306	1.286929	1.403081
30	1	0	3.535823	2.717821	0.724313
31	1	0	0.49246	-3.39189	0.915951
32	1	0	-4.0441	-1.36605	1.354515
33	1	0	-3.70498	0.112448	2.251597
34	1	0	-5.32181	0.898855	0.653377
35	1	0	-3.3233	2.300405	0.704471
36	1	0	-3.6562	2.113615	-1.02629
37	1	0	2.382416	1.131802	-1.46736
38	1	0	4.044012	1.629877	-1.23718
39	1	0	3.805977	-0.80968	-1.4374
40	1	0	-4.08706	-0.93081	-1.07459
41	1	0	-2.33991	-2.87468	-1.23956
42	1	0	4.963616	-1.58686	0.588398
43	1	0	5.642676	-0.0342	0.072788
44	1	0	4.53966	-0.10132	1.457428
45	1	0	1.302503	3.061785	-1.43035

Table S11. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 9*S*, 10*E*, 12*S*, 15*R*)-**3b**] in NMR calculation

3b-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.225117	-0.61027	-0.45276
2	6	0	2.053751	0.114699	0.921191
3	6	0	0.836544	1.000196	1.088573
4	6	0	-0.06198	1.37489	0.177035
5	6	0	0.373466	-2.22515	0.030255
6	6	0	1.783391	-2.09106	-0.46953
7	6	0	-1.18338	2.352101	0.41864
8	6	0	-2.54248	1.860682	-0.09713
9	6	0	-2.01949	-1.88354	0.008922
10	6	0	-0.73426	-2.07673	-0.69782
11	6	0	3.708537	-0.42193	-0.8314
12	6	0	4.077089	0.937663	-0.23628
13	6	0	3.379113	0.927619	1.124136
14	6	0	-3.21229	0.798046	0.798808

15	6	0	-3.87612	-0.36295	0.044682
16	8	0	-2.82846	-1.06809	-0.70156
17	8	0	3.519613	2.021648	-0.99821
18	8	0	2.681272	-2.83352	0.36345
19	8	0	-2.28661	-2.30614	1.114806
20	6	0	-4.93847	0.034608	-0.96452
21	1	0	1.618285	-0.103	-1.20356
22	1	0	2.009001	-0.64023	1.712367
23	8	0	-0.91676	3.570069	-0.31119
24	1	0	0.719941	1.389537	2.100862
25	1	0	0.009014	1.029013	-0.85107
26	1	0	0.271953	-2.34512	1.105786
27	1	0	1.85204	-2.44699	-1.50604
28	1	0	-1.25436	2.577631	1.492035
29	1	0	-2.39161	1.472438	-1.10862
30	1	0	-3.18823	2.737482	-0.19209
31	1	0	-0.71142	-1.89265	-1.76637
32	1	0	3.880114	-0.4722	-1.91092
33	1	0	4.315811	-1.1987	-0.3596
34	1	0	5.161227	1.071954	-0.14278
35	1	0	4.021803	0.426158	1.851847
36	1	0	3.202191	1.943874	1.480836
37	1	0	-2.47637	0.360867	1.479839
38	1	0	-3.97166	1.262907	1.435113
39	1	0	-4.28968	-1.06544	0.768968
40	1	0	3.882543	1.968643	-1.88925
41	1	0	2.4328	-3.76313	0.316751
42	1	0	-4.53583	0.697862	-1.73292
43	1	0	-5.3492	-0.85106	-1.45378
44	1	0	-5.75326	0.553908	-0.454
45	1	0	-0.01885	3.841155	-0.08862

3b-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.093998	-0.4103	-0.64966
2	6	0	1.923803	0.386018	0.689515
3	6	0	0.676483	1.219272	0.870524
4	6	0	-0.28224	1.48757	-0.01762
5	6	0	0.381007	-2.09913	0.060378
6	6	0	1.751999	-1.91425	-0.5256
7	6	0	-1.4475	2.414471	0.217311
8	6	0	-2.79564	1.806843	-0.19288
9	6	0	-2.02784	-1.88949	0.141426

10	6	0	-0.7681	-2.06121	-0.61588
11	6	0	3.560439	-0.17695	-1.0983
12	6	0	4.28304	0.382036	0.127154
13	6	0	3.211041	1.241709	0.804887
14	6	0	-3.35397	0.771615	0.805696
15	6	0	-3.97117	-0.47989	0.165765
16	8	0	-2.91324	-1.16949	-0.58062
17	8	0	5.444697	1.103113	-0.28597
18	8	0	2.744593	-2.5233	0.307571
19	8	0	-2.21885	-2.24884	1.284601
20	6	0	-5.10125	-0.22375	-0.81594
21	1	0	1.420958	-0.01495	-1.41066
22	1	0	1.954916	-0.33457	1.515029
23	8	0	-1.29369	3.591598	-0.60546
24	1	0	0.590119	1.668622	1.860679
25	1	0	-0.24478	1.071522	-1.02157
26	1	0	0.339899	-2.15483	1.144889
27	1	0	1.792192	-2.34718	-1.53352
28	1	0	-1.47977	2.709502	1.275496
29	1	0	-2.6671	1.356905	-1.18149
30	1	0	-3.49995	2.633725	-0.31451
31	1	0	-0.80846	-1.94929	-1.69389
32	1	0	3.597209	0.585952	-1.88222
33	1	0	4.032419	-1.08062	-1.48605
34	1	0	4.570029	-0.44146	0.793241
35	1	0	3.452752	1.503119	1.83849
36	1	0	3.105037	2.17108	0.234352
37	1	0	-2.56265	0.433655	1.481133
38	1	0	-4.11513	1.232622	1.442514
39	1	0	-4.30539	-1.15333	0.955513
40	1	0	5.921903	1.371584	0.506417
41	1	0	2.582131	-3.47275	0.323683
42	1	0	-4.7789	0.407021	-1.64706
43	1	0	-5.47214	-1.16685	-1.22278
44	1	0	-5.92633	0.276889	-0.30334
45	1	0	-0.41174	3.941594	-0.43603

3b-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.094	-0.41029	-0.64966
2	6	0	1.923802	0.386022	0.689514
3	6	0	0.676486	1.219283	0.870516
4	6	0	-0.28225	1.487551	-0.01761

5	6	0	0.381011	-2.09913	0.060374
6	6	0	1.752004	-1.91425	-0.52561
7	6	0	-1.44751	2.414464	0.217309
8	6	0	-2.79565	1.806848	-0.19287
9	6	0	-2.02784	-1.88949	0.141424
10	6	0	-0.76809	-2.06121	-0.61588
11	6	0	3.56044	-0.17694	-1.0983
12	6	0	4.283043	0.382037	0.127156
13	6	0	3.211044	1.241706	0.804896
14	6	0	-3.35398	0.771614	0.805703
15	6	0	-3.97117	-0.47989	0.165769
16	8	0	-2.91324	-1.16948	-0.58062
17	8	0	5.444698	1.10312	-0.28597
18	8	0	2.744596	-2.52329	0.307573
19	8	0	-2.21884	-2.24884	1.284598
20	6	0	-5.10125	-0.22376	-0.81594
21	1	0	1.420959	-0.01495	-1.41066
22	1	0	1.954905	-0.33457	1.515029
23	8	0	-1.29369	3.591583	-0.60547
24	1	0	0.590141	1.668667	1.860658
25	1	0	-0.24481	1.07147	-1.02155
26	1	0	0.339903	-2.15484	1.144884
27	1	0	1.7922	-2.34717	-1.53352
28	1	0	-1.47977	2.709508	1.27549
29	1	0	-2.66713	1.35692	-1.18149
30	1	0	-3.49996	2.633736	-0.31448
31	1	0	-0.80846	-1.94927	-1.6939
32	1	0	3.597209	0.585965	-1.88222
33	1	0	4.03242	-1.08061	-1.48605
34	1	0	4.570034	-0.44146	0.793239
35	1	0	3.452754	1.503107	1.838501
36	1	0	3.105045	2.171083	0.234369
37	1	0	-2.56266	0.433658	1.481144
38	1	0	-4.11515	1.232617	1.442518
39	1	0	-4.30539	-1.15334	0.955515
40	1	0	5.92195	1.371512	0.506422
41	1	0	2.582172	-3.47275	0.323636
42	1	0	-5.47214	-1.16686	-1.22277
43	1	0	-5.92634	0.276873	-0.30333
44	1	0	-4.77891	0.407015	-1.64705
45	1	0	-0.41173	3.941558	-0.43607

3b-Conf.4

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	2.225117	-0.61027	-0.45276
2	6	0	2.053751	0.114699	0.921191
3	6	0	0.836544	1.000195	1.088573
4	6	0	-0.06198	1.37489	0.177035
5	6	0	0.373466	-2.22515	0.030255
6	6	0	1.783391	-2.09106	-0.46953
7	6	0	-1.18338	2.352101	0.41864
8	6	0	-2.54248	1.860682	-0.09713
9	6	0	-2.01949	-1.88354	0.008922
10	6	0	-0.73426	-2.07673	-0.69782
11	6	0	3.708537	-0.42193	-0.8314
12	6	0	4.077089	0.937663	-0.23628
13	6	0	3.379113	0.927619	1.124136
14	6	0	-3.21229	0.798046	0.798808
15	6	0	-3.87612	-0.36295	0.044682
16	8	0	-2.82846	-1.06809	-0.70156
17	8	0	3.519613	2.021648	-0.99821
18	8	0	2.681272	-2.83352	0.36345
19	8	0	-2.28661	-2.30614	1.114806
20	6	0	-4.93847	0.034608	-0.96452
21	1	0	1.618285	-0.103	-1.20356
22	1	0	2.009002	-0.64023	1.712367
23	8	0	-0.91676	3.570069	-0.31119
24	1	0	0.719941	1.389537	2.100862
25	1	0	0.009014	1.029013	-0.85107
26	1	0	0.271953	-2.34512	1.105786
27	1	0	1.85204	-2.44699	-1.50604
28	1	0	-1.25436	2.57763	1.492035
29	1	0	-2.39161	1.472438	-1.10862
30	1	0	-3.18823	2.737482	-0.19209
31	1	0	-0.71142	-1.89265	-1.76637
32	1	0	3.880114	-0.4722	-1.91092
33	1	0	4.315811	-1.1987	-0.3596
34	1	0	5.161227	1.071954	-0.14278
35	1	0	4.021803	0.426159	1.851847
36	1	0	3.202191	1.943875	1.480836
37	1	0	-2.47637	0.360868	1.479839
38	1	0	-3.97166	1.262907	1.435113
39	1	0	-4.28968	-1.06544	0.768968
40	1	0	3.882543	1.968643	-1.88925
41	1	0	2.4328	-3.76313	0.316752
42	1	0	-5.3492	-0.85106	-1.45378
43	1	0	-5.75326	0.553908	-0.454

44	1	0	-4.53583	0.697861	-1.73292
45	1	0	-0.01885	3.841155	-0.08862

3b-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.11645	-0.49511	0.570671
2	6	0	-2.08876	0.513013	-0.62497
3	6	0	-0.85516	1.350325	-0.85291
4	6	0	0.291568	1.408352	-0.17079
5	6	0	-0.37654	-1.99869	-0.42115
6	6	0	-1.75655	-1.94551	0.170009
7	6	0	1.418538	2.329644	-0.57001
8	6	0	2.7498	1.630564	-0.90576
9	6	0	2.041413	-1.73535	-0.28923
10	6	0	0.736676	-2.10295	0.30464
11	6	0	-3.54489	-0.39636	1.173388
12	6	0	-4.37159	0.404703	0.166629
13	6	0	-3.35391	1.382568	-0.42745
14	6	0	3.592771	1.128451	0.29611
15	6	0	3.972254	-0.3547	0.266437
16	8	0	2.784759	-1.12234	0.65281
17	8	0	-5.47213	1.023585	0.834107
18	8	0	-2.7443	-2.40199	-0.75865
19	8	0	2.3669	-1.8713	-1.45012
20	6	0	5.063134	-0.71829	1.261875
21	1	0	-1.38715	-0.1985	1.326591
22	1	0	-2.25119	-0.06423	-1.54378
23	8	0	1.698346	3.285581	0.471366
24	1	0	-0.94404	2.001731	-1.72406
25	1	0	0.461134	0.792509	0.707868
26	1	0	-0.30041	-1.80595	-1.48794
27	1	0	-1.7894	-2.55485	1.082675
28	1	0	1.102395	2.86471	-1.47574
29	1	0	3.349321	2.348585	-1.47246
30	1	0	2.530128	0.810684	-1.59409
31	1	0	0.705771	-2.23158	1.381545
32	1	0	-3.52185	0.169514	2.10972
33	1	0	-3.98061	-1.37405	1.384386
34	1	0	-4.74059	-0.26266	-0.62298
35	1	0	-3.69304	1.852737	-1.35438
36	1	0	-3.16374	2.173617	0.306793
37	1	0	4.523753	1.700314	0.33902
38	1	0	3.077526	1.329257	1.239026

39	1	0	4.253297	-0.66815	-0.73992
40	1	0	-6.01803	1.452473	0.166409
41	1	0	-2.57936	-3.33381	-0.93904
42	1	0	5.250756	-1.79401	1.250783
43	1	0	5.991616	-0.20441	1.002346
44	1	0	4.777708	-0.42497	2.275697
45	1	0	0.863454	3.708604	0.70052

3b-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.202447	-0.60761	-0.48232
2	6	0	2.03068	0.087672	0.911124
3	6	0	0.84606	1.02119	1.059393
4	6	0	-0.06592	1.376691	0.151587
5	6	0	0.399369	-2.26262	0.003759
6	6	0	1.804591	-2.10052	-0.50623
7	6	0	-1.17608	2.370179	0.383518
8	6	0	-2.54258	1.862776	-0.09562
9	6	0	-1.99311	-1.89986	0.015274
10	6	0	-0.71499	-2.08362	-0.7074
11	6	0	3.668011	-0.35298	-0.89858
12	6	0	4.032175	0.971391	-0.21996
13	6	0	3.382621	0.835825	1.162655
14	6	0	-3.18054	0.796841	0.819708
15	6	0	-3.84756	-0.37459	0.084192
16	8	0	-2.80687	-1.07353	-0.67743
17	8	0	3.543287	2.113166	-0.94362
18	8	0	2.728179	-2.81862	0.316677
19	8	0	-2.25016	-2.33676	1.117792
20	6	0	-4.93289	0.007747	-0.90649
21	1	0	1.551835	-0.12307	-1.21245
22	1	0	1.92821	-0.67825	1.685252
23	8	0	-0.91999	3.563164	-0.38739
24	1	0	0.757327	1.452199	2.057176
25	1	0	-0.03327	0.983349	-0.86139
26	1	0	0.307926	-2.41859	1.075545
27	1	0	1.874458	-2.44863	-1.54512
28	1	0	-1.22818	2.626878	1.45068
29	1	0	-2.41078	1.470995	-1.10835
30	1	0	-3.19889	2.732633	-0.18019
31	1	0	-0.70179	-1.86621	-1.76981
32	1	0	3.79944	-0.30998	-1.98212
33	1	0	4.307266	-1.14736	-0.50502

34	1	0	5.111575	1.121722	-0.15966
35	1	0	4.028043	0.229525	1.803808
36	1	0	3.251769	1.806422	1.645466
37	1	0	-2.42559	0.37062	1.486896
38	1	0	-3.93122	1.256113	1.470077
39	1	0	-4.2405	-1.07704	0.819743
40	1	0	2.581533	2.126435	-0.88014
41	1	0	2.517793	-3.75683	0.256508
42	1	0	-5.34477	-0.8844	-1.38276
43	1	0	-5.74236	0.522457	-0.38302
44	1	0	-4.55154	0.670195	-1.68631
45	1	0	-0.03755	3.87043	-0.15074

3b-Conf.7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.25309	-0.61513	0.407879
2	6	0	-2.24376	0.292217	-0.86082
3	6	0	-1.01964	1.140295	-1.11841
4	6	0	0.098873	1.295583	-0.4055
5	6	0	-0.41986	-2.13251	-0.35491
6	6	0	-1.8274	-2.08018	0.166058
7	6	0	1.212243	2.212777	-0.8498
8	6	0	2.579573	1.534398	-1.0584
9	6	0	1.978717	-1.77346	-0.14606
10	6	0	0.662205	-2.13675	0.423595
11	6	0	-3.68293	-0.49669	0.970527
12	6	0	-4.07839	0.948102	0.665576
13	6	0	-3.53839	1.17214	-0.74786
14	6	0	3.384788	1.192221	0.223042
15	6	0	3.82834	-0.26714	0.358013
16	8	0	2.656937	-1.04881	0.765461
17	8	0	-3.40136	1.874711	1.532035
18	8	0	-2.74813	-2.66503	-0.76029
19	8	0	2.360702	-2.00109	-1.27502
20	6	0	4.882622	-0.4791	1.433499
21	1	0	-1.56329	-0.20606	1.148543
22	1	0	-2.36531	-0.35195	-1.738
23	8	0	1.414133	3.277631	0.100371
24	1	0	-1.0901	1.705466	-2.04935
25	1	0	0.250516	0.773621	0.535013
26	1	0	-0.30248	-2.02693	-1.43015
27	1	0	-1.88286	-2.60217	1.130703
28	1	0	0.918454	2.643386	-1.81668

29	1	0	3.17924	2.211905	-1.67293
30	1	0	2.417827	0.640089	-1.66494
31	1	0	0.587176	-2.17382	1.505353
32	1	0	-3.74094	-0.737	2.036448
33	1	0	-4.35218	-1.17711	0.436367
34	1	0	-5.161	1.109271	0.726183
35	1	0	-4.28451	0.846042	-1.47633
36	1	0	-3.3446	2.231912	-0.92317
37	1	0	4.286565	1.81003	0.250394
38	1	0	2.816213	1.457709	1.11803
39	1	0	4.172442	-0.66364	-0.59816
40	1	0	-3.66368	1.673196	2.437142
41	1	0	-2.52514	-3.59749	-0.85393
42	1	0	4.535821	-0.09844	2.397956
43	1	0	5.113943	-1.54087	1.541293
44	1	0	5.801187	0.047644	1.164733
45	1	0	0.554992	3.685127	0.256492

3b-Conf.8

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	2.202447	-0.60761	-0.48232
2	6	0	2.03068	0.087672	0.911124
3	6	0	0.84606	1.02119	1.059393
4	6	0	-0.06592	1.37669	0.151587
5	6	0	0.399369	-2.26262	0.003759
6	6	0	1.804591	-2.10052	-0.50623
7	6	0	-1.17608	2.370178	0.383518
8	6	0	-2.54258	1.862776	-0.09561
9	6	0	-1.99311	-1.89986	0.015274
10	6	0	-0.71499	-2.08362	-0.7074
11	6	0	3.668011	-0.35298	-0.89858
12	6	0	4.032175	0.971391	-0.21996
13	6	0	3.382622	0.835825	1.162654
14	6	0	-3.18054	0.79684	0.819708
15	6	0	-3.84756	-0.37459	0.084192
16	8	0	-2.80687	-1.07353	-0.67743
17	8	0	3.543287	2.113166	-0.94363
18	8	0	2.728179	-2.81862	0.316678
19	8	0	-2.25016	-2.33676	1.117792
20	6	0	-4.93289	0.007747	-0.90649
21	1	0	1.551835	-0.12307	-1.21245
22	1	0	1.92821	-0.67825	1.685252
23	8	0	-0.91999	3.563164	-0.38739

24	1	0	0.757327	1.4522	2.057176
25	1	0	-0.03327	0.983348	-0.86139
26	1	0	0.307926	-2.41859	1.075545
27	1	0	1.874458	-2.44863	-1.54512
28	1	0	-1.22818	2.626877	1.450681
29	1	0	-2.41078	1.470995	-1.10835
30	1	0	-3.19889	2.732633	-0.18019
31	1	0	-0.70179	-1.86621	-1.76981
32	1	0	3.79944	-0.30998	-1.98212
33	1	0	4.307266	-1.14736	-0.50502
34	1	0	5.111575	1.121722	-0.15966
35	1	0	4.028044	0.229526	1.803807
36	1	0	3.251769	1.806422	1.645465
37	1	0	-2.42559	0.37062	1.486896
38	1	0	-3.93122	1.256113	1.470077
39	1	0	-4.2405	-1.07704	0.819742
40	1	0	2.581533	2.126433	-0.88015
41	1	0	2.517793	-3.75683	0.256509
42	1	0	-4.55154	0.670195	-1.68631
43	1	0	-5.34477	-0.8844	-1.38276
44	1	0	-5.74236	0.522457	-0.38302
45	1	0	-0.03755	3.870429	-0.15074

3b-Conf.9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.247853	-0.63434	-0.43498
2	6	0	2.092799	0.39559	0.741179
3	6	0	0.666835	0.822862	0.984659
4	6	0	-0.00093	1.814105	0.390424
5	6	0	0.365159	-2.14641	0.278588
6	6	0	1.805146	-2.08881	-0.15692
7	6	0	-1.49384	1.974584	0.52011
8	6	0	-2.18071	1.757931	-0.84005
9	6	0	-2.01192	-1.71188	0.100174
10	6	0	-0.70299	-2.02952	-0.51405
11	6	0	3.735261	-0.5277	-0.86695
12	6	0	4.313004	0.708976	-0.15064
13	6	0	3.085687	1.492419	0.330934
14	6	0	-3.63338	1.256512	-0.80217
15	6	0	-3.82559	-0.14634	-0.20674
16	8	0	-2.77319	-1.00247	-0.76248
17	8	0	5.152501	1.432934	-1.05451
18	8	0	2.661279	-2.62752	0.854513

19	8	0	-2.3303	-1.94927	1.247256
20	6	0	-5.18226	-0.75538	-0.52434
21	1	0	1.611884	-0.27825	-1.25036
22	1	0	2.468651	-0.08506	1.651596
23	8	0	-1.87469	3.289731	0.967479
24	1	0	0.104439	0.191012	1.668901
25	1	0	0.490278	2.495494	-0.30207
26	1	0	0.209205	-2.17459	1.353722
27	1	0	1.933061	-2.64772	-1.09366
28	1	0	-1.85403	1.232662	1.244487
29	1	0	-1.58864	1.052107	-1.4248
30	1	0	-2.14536	2.71439	-1.37119
31	1	0	-0.62387	-1.94711	-1.5924
32	1	0	3.81668	-0.37762	-1.94616
33	1	0	4.289022	-1.4307	-0.60939
34	1	0	4.903993	0.392307	0.718595
35	1	0	3.309966	2.190413	1.141714
36	1	0	2.696671	2.067018	-0.51653
37	1	0	-4.26061	1.945145	-0.22648
38	1	0	-4.02165	1.25979	-1.82646
39	1	0	-3.67722	-0.1307	0.872831
40	1	0	5.554883	2.15778	-0.56363
41	1	0	2.491742	-3.57349	0.919139
42	1	0	-5.28903	-1.73297	-0.04985
43	1	0	-5.97889	-0.10501	-0.15351
44	1	0	-5.30847	-0.87254	-1.60377
45	1	0	-1.49828	3.414812	1.84583

3b-Conf.10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.090588	-0.40208	-0.65245
2	6	0	1.910769	0.381985	0.693097
3	6	0	0.66373	1.216954	0.872779
4	6	0	-0.27143	1.517783	-0.02758
5	6	0	0.39456	-2.11132	0.046027
6	6	0	1.763389	-1.91036	-0.53952
7	6	0	-1.44337	2.433658	0.208065
8	6	0	-2.78718	1.793632	-0.19379
9	6	0	-2.01381	-1.91066	0.134109
10	6	0	-0.75576	-2.07014	-0.62796
11	6	0	3.55482	-0.15141	-1.09781
12	6	0	4.273136	0.394319	0.135925
13	6	0	3.196015	1.239405	0.823856

14	6	0	-3.32466	0.754175	0.812154
15	6	0	-3.9521	-0.49641	0.180409
16	8	0	-2.90352	-1.18584	-0.57845
17	8	0	5.431445	1.127195	-0.26595
18	8	0	2.761827	-2.51695	0.288273
19	8	0	-2.20046	-2.28111	1.274474
20	6	0	-5.09484	-0.23972	-0.78624
21	1	0	1.41391	-0.00912	-1.41131
22	1	0	1.936915	-0.34563	1.512279
23	8	0	-1.19458	3.596416	-0.60904
24	1	0	0.562825	1.642925	1.871581
25	1	0	-0.21488	1.128769	-1.04132
26	1	0	0.355303	-2.18104	1.129791
27	1	0	1.806849	-2.33517	-1.55077
28	1	0	-1.47589	2.728198	1.26617
29	1	0	-2.65451	1.343142	-1.18162
30	1	0	-3.52145	2.597038	-0.31552
31	1	0	-0.79862	-1.9443	-1.70431
32	1	0	3.585595	0.623527	-1.87013
33	1	0	4.033303	-1.04568	-1.49931
34	1	0	4.563896	-0.43677	0.790793
35	1	0	3.434735	1.486416	1.861712
36	1	0	3.087969	2.176802	0.267109
37	1	0	-2.51864	0.416305	1.470215
38	1	0	-4.07324	1.212725	1.465441
39	1	0	-4.27662	-1.16935	0.974575
40	1	0	5.904024	1.39074	0.530876
41	1	0	2.608292	-3.46799	0.296416
42	1	0	-5.47412	-1.18301	-1.18479
43	1	0	-5.91135	0.264836	-0.26376
44	1	0	-4.7823	0.387343	-1.62394
45	1	0	-1.97286	4.162658	-0.55118

3b-Conf.11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.225319	-0.60416	-0.4537
2	6	0	2.045331	0.117041	0.921383
3	6	0	0.828183	1.004206	1.086785
4	6	0	-0.04476	1.410648	0.166266
5	6	0	0.379485	-2.22939	0.021043
6	6	0	1.789158	-2.08676	-0.47563
7	6	0	-1.17766	2.372686	0.408935
8	6	0	-2.53189	1.843101	-0.10383

9	6	0	-2.01392	-1.90376	0.001092
10	6	0	-0.7285	-2.08565	-0.70756
11	6	0	3.71068	-0.41394	-0.82392
12	6	0	4.078077	0.942439	-0.22154
13	6	0	3.368916	0.931314	1.133379
14	6	0	-3.18351	0.777708	0.802244
15	6	0	-3.86422	-0.37901	0.056534
16	8	0	-2.82856	-1.08745	-0.70283
17	8	0	3.531875	2.030087	-0.98578
18	8	0	2.687873	-2.82862	0.357341
19	8	0	-2.27727	-2.33376	1.104953
20	6	0	-4.93777	0.02431	-0.93831
21	1	0	1.620213	-0.09814	-1.2068
22	1	0	1.997934	-0.64044	1.7097
23	8	0	-0.82306	3.574199	-0.30753
24	1	0	0.695124	1.370623	2.105305
25	1	0	0.047802	1.090728	-0.86837
26	1	0	0.277234	-2.35413	1.095921
27	1	0	1.861953	-2.43925	-1.513
28	1	0	-1.25111	2.594271	1.482726
29	1	0	-2.37197	1.448918	-1.1116
30	1	0	-3.21079	2.696113	-0.20864
31	1	0	-0.70662	-1.89709	-1.77529
32	1	0	3.887867	-0.45961	-1.90277
33	1	0	4.314775	-1.19343	-0.35265
34	1	0	5.161885	1.072485	-0.11799
35	1	0	4.00645	0.430968	1.866414
36	1	0	3.18796	1.947613	1.487862
37	1	0	-2.4328	0.337943	1.465205
38	1	0	-3.92781	1.241706	1.456701
39	1	0	-4.27159	-1.08003	0.785628
40	1	0	3.903029	1.977479	-1.87339
41	1	0	2.443081	-3.75898	0.306683
42	1	0	-4.5413	0.683431	-1.71341
43	1	0	-5.3612	-0.85935	-1.42025
44	1	0	-5.74194	0.549922	-0.41748
45	1	0	-1.57262	4.177825	-0.24872

Table S12. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*R*, 9*S*, 10*E*, 12*S*, 15*R*)-**3c**] in NMR calculation

3c-Conf.1

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-2.27225	-0.09025	1.04076
2	6	0	-1.87688	0.794092	-0.19699
3	6	0	-0.65726	1.647974	0.022494
4	6	0	0.462619	1.588402	-0.69932
5	6	0	-0.36829	-1.62382	0.695253
6	6	0	-1.85479	-1.57678	0.866589
7	6	0	1.66034	2.497588	-0.54811
8	6	0	3.039049	1.835377	-0.798
9	6	0	1.728755	-1.94093	-0.56816
10	6	0	0.28227	-2.13686	-0.35148
11	6	0	-3.80264	0.102198	1.238412
12	6	0	-4.30659	0.702933	-0.07193
13	6	0	-3.15564	1.612602	-0.50476
14	6	0	3.64582	0.948575	0.316007
15	6	0	3.615856	-0.56105	0.080354
16	8	0	2.231593	-0.9829	0.238104
17	8	0	-4.48192	-0.40434	-0.98674
18	8	0	-2.5085	-2.23551	-0.20902
19	8	0	2.37889	-2.52667	-1.41281
20	6	0	4.481282	-1.34113	1.062661
21	1	0	-1.74765	0.270818	1.928953
22	1	0	-1.68599	0.128309	-1.04224
23	8	0	1.642958	3.244635	0.671853
24	1	0	-0.72683	2.374476	0.831581
25	1	0	0.529245	0.873785	-1.51657
26	1	0	0.200207	-1.12127	1.470448
27	1	0	-2.11205	-2.08807	1.808418
28	1	0	1.567726	3.265146	-1.32714
29	1	0	3.731538	2.661356	-0.97963
30	1	0	2.984203	1.276005	-1.73847
31	1	0	-0.24075	-2.6729	-1.13297
32	1	0	-3.98995	0.80912	2.049645
33	1	0	-4.3282	-0.8236	1.483437
34	1	0	-5.25807	1.231686	0.034049
35	1	0	-3.18354	2.524157	0.102353
36	1	0	-3.22052	1.916394	-1.55337
37	1	0	4.698263	1.221944	0.432941
38	1	0	3.181917	1.155346	1.286393
39	1	0	3.915411	-0.79447	-0.94322
40	1	0	-4.56991	-0.06029	-1.8833
41	1	0	-3.22969	-1.67259	-0.54543
42	1	0	4.399236	-2.41384	0.876326
43	1	0	5.530121	-1.05507	0.951964

44	1	0	4.174323	-1.14071	2.092684
45	1	0	1.546868	2.619055	1.399317

3c-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.16021	0.024338	0.936017
2	6	0	-1.97425	0.72278	-0.45237
3	6	0	-0.74274	1.558997	-0.69021
4	6	0	0.388261	1.635004	0.014298
5	6	0	-0.29526	-1.59542	0.692093
6	6	0	-1.76739	-1.47573	0.921446
7	6	0	1.563494	2.477869	-0.41218
8	6	0	2.813822	1.6895	-0.84361
9	6	0	1.760649	-1.93125	-0.62389
10	6	0	0.313755	-2.11562	-0.37513
11	6	0	-3.65677	0.23379	1.313261
12	6	0	-4.35956	0.661461	0.016877
13	6	0	-3.28815	1.515946	-0.67053
14	6	0	3.580762	0.93117	0.268704
15	6	0	3.668819	-0.58214	0.07011
16	8	0	2.318829	-1.09688	0.274575
17	8	0	-4.74832	-0.45898	-0.78525
18	8	0	-2.55085	-2.13504	-0.08067
19	8	0	2.354587	-2.42253	-1.56334
20	6	0	4.601946	-1.27557	1.052706
21	1	0	-1.52951	0.504404	1.687059
22	1	0	-1.95795	-0.06388	-1.21747
23	8	0	1.979073	3.358973	0.648865
24	1	0	-0.79646	2.144889	-1.60938
25	1	0	0.520146	1.075984	0.934952
26	1	0	0.313414	-1.12204	1.454379
27	1	0	-2.01247	-1.88614	1.90961
28	1	0	1.252472	3.075176	-1.28032
29	1	0	3.490363	2.413072	-1.30776
30	1	0	2.512388	1.002437	-1.63979
31	1	0	-0.23165	-2.62121	-1.16234
32	1	0	-3.73876	1.03763	2.049376
33	1	0	-4.11588	-0.6573	1.747191
34	1	0	-5.27497	1.225579	0.208752
35	1	0	-3.22627	2.491429	-0.17449
36	1	0	-3.50911	1.684642	-1.72687
37	1	0	4.605054	1.310249	0.322547
38	1	0	3.135794	1.13018	1.24737

39	1	0	3.958977	-0.82257	-0.95423
40	1	0	-4.07245	-1.1472	-0.67268
41	1	0	-2.54971	-3.08376	0.087162
42	1	0	4.299341	-1.07267	2.083452
43	1	0	4.594666	-2.35603	0.893554
44	1	0	5.625113	-0.91689	0.915864
45	1	0	1.19782	3.838892	0.945096

3c-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.12563	0.139506	0.911355
2	6	0	-1.85601	0.630443	-0.54727
3	6	0	-0.59396	1.413163	-0.81021
4	6	0	0.352863	1.758639	0.062592
5	6	0	-0.2815	-1.51894	0.903632
6	6	0	-1.75549	-1.35804	1.120372
7	6	0	1.620729	2.50218	-0.25626
8	6	0	2.872149	1.71691	0.167669
9	6	0	1.702468	-2.15913	-0.43179
10	6	0	0.282361	-2.26545	-0.0494
11	6	0	-3.6278	0.440916	1.186619
12	6	0	-4.2565	0.676832	-0.18441
13	6	0	-3.1459	1.388703	-0.95843
14	6	0	3.289802	0.601285	-0.81542
15	6	0	3.646652	-0.75389	-0.18782
16	8	0	2.416255	-1.32686	0.361162
17	8	0	-4.53684	-0.63135	-0.73423
18	8	0	-2.48109	-2.24705	0.283903
19	8	0	2.162119	-2.71474	-1.4115
20	6	0	4.672727	-0.71265	0.932278
21	1	0	-1.52558	0.704377	1.625888
22	1	0	-1.80245	-0.25897	-1.18619
23	8	0	1.664343	3.73401	0.493433
24	1	0	-0.45302	1.690618	-1.85535
25	1	0	0.256824	1.50713	1.11604
26	1	0	0.351645	-0.90386	1.533436
27	1	0	-1.97487	-1.59005	2.17529
28	1	0	1.669088	2.723519	-1.33142
29	1	0	2.684093	1.308259	1.164552
30	1	0	3.683115	2.441486	0.278046
31	1	0	-0.31908	-2.89376	-0.69342
32	1	0	-3.7212	1.352827	1.780488
33	1	0	-4.13783	-0.3571	1.731016

34	1	0	-5.18566	1.251816	-0.139
35	1	0	-3.09939	2.431516	-0.62752
36	1	0	-3.31243	1.391717	-2.03921
37	1	0	2.489802	0.415971	-1.53952
38	1	0	4.15331	0.930085	-1.40228
39	1	0	3.988309	-1.42436	-0.9759
40	1	0	-4.729	-0.54291	-1.67518
41	1	0	-3.25438	-1.78483	-0.08812
42	1	0	4.881593	-1.72211	1.292743
43	1	0	5.605986	-0.28106	0.561399
44	1	0	4.328208	-0.111	1.775956
45	1	0	0.842845	4.205717	0.314985

3c-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.14018	0.011987	0.92718
2	6	0	-1.97362	0.714251	-0.45926
3	6	0	-0.75277	1.565111	-0.7021
4	6	0	0.369641	1.659558	0.011426
5	6	0	-0.30298	-1.61804	0.680597
6	6	0	-1.77793	-1.5047	0.882753
7	6	0	1.549249	2.488874	-0.42034
8	6	0	2.784488	1.667698	-0.86008
9	6	0	1.768608	-1.95261	-0.61152
10	6	0	0.322703	-2.14439	-0.37499
11	6	0	-3.61653	0.264407	1.351645
12	6	0	-4.34719	0.670948	0.075614
13	6	0	-3.29873	1.492991	-0.67431
14	6	0	3.559951	0.931624	0.260831
15	6	0	3.661829	-0.5834	0.082582
16	8	0	2.316061	-1.1058	0.284772
17	8	0	-4.66749	-0.55511	-0.62243
18	8	0	-2.47682	-2.229	-0.11665
19	8	0	2.376966	-2.44618	-1.54139
20	6	0	4.594666	-1.25416	1.081324
21	1	0	-1.48205	0.467749	1.669524
22	1	0	-1.95016	-0.07594	-1.21962
23	8	0	1.873265	3.363577	0.676927
24	1	0	-0.80672	2.13831	-1.62898
25	1	0	0.495423	1.113257	0.940393
26	1	0	0.29353	-1.13751	1.447933
27	1	0	-2.02147	-1.91165	1.877876
28	1	0	1.240292	3.089663	-1.28614

29	1	0	3.465449	2.363079	-1.36328
30	1	0	2.459154	0.963935	-1.63266
31	1	0	-0.21626	-2.6605	-1.15891
32	1	0	-3.66231	1.09156	2.063652
33	1	0	-4.08362	-0.6014	1.826985
34	1	0	-5.2712	1.223807	0.266593
35	1	0	-3.23851	2.485619	-0.21528
36	1	0	-3.54178	1.633436	-1.73141
37	1	0	4.580421	1.321431	0.312496
38	1	0	3.110271	1.138954	1.235999
39	1	0	3.962069	-0.83479	-0.93616
40	1	0	-4.93865	-0.34112	-1.52276
41	1	0	-3.31424	-1.76969	-0.31319
42	1	0	4.282857	-1.03911	2.106903
43	1	0	4.597424	-2.33683	0.937883
44	1	0	5.615794	-0.88882	0.946626
45	1	0	2.641166	3.885842	0.417562

3c-Conf.5

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.14214	0.160146	0.915686
2	6	0	-1.85754	0.646604	-0.54242
3	6	0	-0.585	1.41324	-0.79923
4	6	0	0.357305	1.761708	0.077601
5	6	0	-0.27734	-1.49598	0.905901
6	6	0	-1.74661	-1.31974	1.146843
7	6	0	1.63046	2.496947	-0.24034
8	6	0	2.877986	1.702704	0.17926
9	6	0	1.687776	-2.14905	-0.4487
10	6	0	0.267734	-2.24282	-0.05666
11	6	0	-3.65928	0.413976	1.155272
12	6	0	-4.26437	0.668161	-0.23349
13	6	0	-3.13673	1.419491	-0.95378
14	6	0	3.292657	0.595189	-0.81416
15	6	0	3.646416	-0.76609	-0.19876
16	8	0	2.414296	-1.33711	0.35059
17	8	0	-4.60782	-0.54931	-0.90526
18	8	0	-2.54959	-2.13338	0.282506
19	8	0	2.131207	-2.69794	-1.43873
20	6	0	4.675347	-0.73832	0.918858
21	1	0	-1.56779	0.748171	1.632841
22	1	0	-1.81466	-0.24071	-1.1859
23	8	0	1.683396	3.727072	0.511373

24	1	0	-0.43424	1.682742	-1.84509
25	1	0	0.25361	1.519895	1.132836
26	1	0	0.369341	-0.88716	1.527872
27	1	0	-1.97325	-1.56073	2.193671
28	1	0	1.678994	2.720008	-1.31512
29	1	0	2.686958	1.285089	1.17183
30	1	0	3.691652	2.422922	0.297585
31	1	0	-0.33961	-2.862	-0.70499
32	1	0	-3.78785	1.306696	1.772627
33	1	0	-4.15589	-0.41392	1.665504
34	1	0	-5.18373	1.256184	-0.1846
35	1	0	-3.09001	2.450172	-0.58452
36	1	0	-3.28504	1.450083	-2.03543
37	1	0	2.492027	0.418334	-1.53966
38	1	0	4.156762	0.926858	-1.39841
39	1	0	3.981826	-1.43254	-0.99287
40	1	0	-3.97453	-1.22839	-0.62167
41	1	0	-2.56724	-3.03693	0.615858
42	1	0	4.336529	-0.14005	1.767183
43	1	0	4.879536	-1.75121	1.272164
44	1	0	5.609871	-0.3096	0.548015
45	1	0	0.864721	4.204353	0.334969

3c-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.16386	0.041074	0.937132
2	6	0	-1.96647	0.723556	-0.45724
3	6	0	-0.73311	1.558111	-0.69299
4	6	0	0.376411	1.666768	0.038543
5	6	0	-0.30224	-1.58419	0.706337
6	6	0	-1.77327	-1.45937	0.94057
7	6	0	1.561025	2.493232	-0.3871
8	6	0	2.789478	1.674328	-0.8504
9	6	0	1.745116	-1.94918	-0.61523
10	6	0	0.299414	-2.12538	-0.35468
11	6	0	-3.66238	0.257581	1.302113
12	6	0	-4.35556	0.673024	-0.00353
13	6	0	-3.27738	1.516946	-0.69349
14	6	0	3.574605	0.917053	0.249248
15	6	0	3.660271	-0.59599	0.049378
16	8	0	2.31226	-1.1072	0.270306
17	8	0	-4.74248	-0.45501	-0.79587
18	8	0	-2.56076	-2.13094	-0.05044

19	8	0	2.331362	-2.45295	-1.55285
20	6	0	4.604926	-1.28944	1.020866
21	1	0	-1.53749	0.527374	1.687695
22	1	0	-1.94584	-0.07111	-1.21377
23	8	0	1.896787	3.347527	0.722285
24	1	0	-0.7695	2.115279	-1.63045
25	1	0	0.48703	1.139972	0.980791
26	1	0	0.311415	-1.09751	1.456108
27	1	0	-2.01524	-1.85701	1.934706
28	1	0	1.250923	3.109915	-1.24118
29	1	0	3.467928	2.375818	-1.34842
30	1	0	2.454323	0.984876	-1.63162
31	1	0	-0.25211	-2.64336	-1.12943
32	1	0	-3.74755	1.069352	2.029112
33	1	0	-4.12643	-0.62788	1.742247
34	1	0	-5.27046	1.241978	0.176297
35	1	0	-3.2163	2.497885	-0.20835
36	1	0	-3.49106	1.673986	-1.75314
37	1	0	4.599258	1.296896	0.290456
38	1	0	3.141521	1.115344	1.233749
39	1	0	3.937999	-0.83692	-0.97827
40	1	0	-4.07081	-1.14475	-0.66871
41	1	0	-2.56597	-3.07659	0.133609
42	1	0	4.315532	-1.08482	2.055042
43	1	0	4.593937	-2.37003	0.86301
44	1	0	5.626822	-0.9325	0.870619
45	1	0	2.662864	3.873533	0.465404

3c-Conf.7

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.12453	0.164083	0.906184
2	6	0	-1.8392	0.630738	-0.55755
3	6	0	-0.57623	1.414445	-0.81764
4	6	0	0.34289	1.79872	0.066348
5	6	0	-0.2881	-1.50252	0.92248
6	6	0	-1.76001	-1.32999	1.144615
7	6	0	1.619884	2.528627	-0.24102
8	6	0	2.856661	1.697962	0.166339
9	6	0	1.683436	-2.1944	-0.4032
10	6	0	0.265945	-2.28395	-0.00826
11	6	0	-3.62787	0.474496	1.162866
12	6	0	-4.24369	0.68797	-0.21767
13	6	0	-3.12448	1.383089	-0.99433

14	6	0	3.24122	0.586911	-0.83484
15	6	0	3.619627	-0.76875	-0.22115
16	8	0	2.405473	-1.34204	0.36139
17	8	0	-4.52292	-0.62894	-0.74705
18	8	0	-2.49565	-2.23513	0.33431
19	8	0	2.13487	-2.77894	-1.36962
20	6	0	4.678743	-0.72721	0.867769
21	1	0	-1.52936	0.738197	1.617208
22	1	0	-1.77802	-0.26832	-1.18187
23	8	0	1.56963	3.746881	0.525959
24	1	0	-0.41552	1.66219	-1.8671
25	1	0	0.222515	1.578961	1.124216
26	1	0	0.352635	-0.86816	1.524736
27	1	0	-1.97385	-1.53808	2.205554
28	1	0	1.67119	2.766368	-1.31235
29	1	0	2.660312	1.280734	1.158057
30	1	0	3.70045	2.386042	0.284641
31	1	0	-0.34225	-2.93174	-0.62609
32	1	0	-3.72349	1.397281	1.739275
33	1	0	-4.14503	-0.31217	1.71685
34	1	0	-5.17163	1.266049	-0.19071
35	1	0	-3.07863	2.431604	-0.68213
36	1	0	-3.28122	1.366803	-2.07643
37	1	0	2.415769	0.403581	-1.53027
38	1	0	4.083273	0.918945	-1.45037
39	1	0	3.93883	-1.43792	-1.01962
40	1	0	-4.70599	-0.55666	-1.69113
41	1	0	-3.25477	-1.7721	-0.06478
42	1	0	4.356897	-0.12995	1.723456
43	1	0	4.902249	-1.73699	1.21832
44	1	0	5.598872	-0.29055	0.470852
45	1	0	2.419675	4.189795	0.423989

3c-Conf.8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.12631	0.15249	0.912019
2	6	0	-1.8487	0.636055	-0.54838
3	6	0	-0.58621	1.419526	-0.80784
4	6	0	0.359001	1.764564	0.066801
5	6	0	-0.2824	-1.50827	0.907721
6	6	0	-1.75562	-1.34247	1.129183
7	6	0	1.630012	2.503268	-0.25098
8	6	0	2.877814	1.709637	0.168465

9	6	0	1.695821	-2.16575	-0.42693
10	6	0	0.276244	-2.26437	-0.04077
11	6	0	-3.63086	0.451767	1.175917
12	6	0	-4.24938	0.675525	-0.20822
13	6	0	-3.13875	1.386462	-0.97391
14	6	0	3.287295	0.59504	-0.81908
15	6	0	3.64327	-0.76229	-0.19563
16	8	0	2.413982	-1.331	0.359684
17	8	0	-4.4924	-0.59343	-0.86778
18	8	0	-2.49258	-2.23555	0.304929
19	8	0	2.151661	-2.7291	-1.40389
20	6	0	4.676401	-0.72612	0.918156
21	1	0	-1.53083	0.722512	1.626216
22	1	0	-1.78633	-0.25536	-1.18427
23	8	0	1.681112	3.732179	0.502738
24	1	0	-0.44241	1.695596	-1.85291
25	1	0	0.260708	1.514153	1.120317
26	1	0	0.355054	-0.89041	1.530471
27	1	0	-1.97138	-1.57011	2.185229
28	1	0	1.678195	2.727859	-1.32544
29	1	0	2.689083	1.298444	1.16416
30	1	0	3.692978	2.429293	0.279923
31	1	0	-0.32931	-2.89607	-0.67765
32	1	0	-3.72798	1.369771	1.761686
33	1	0	-4.13865	-0.34117	1.730621
34	1	0	-5.18044	1.246325	-0.17856
35	1	0	-3.09742	2.4299	-0.64663
36	1	0	-3.30476	1.373639	-2.05285
37	1	0	2.482939	0.413265	-1.5392
38	1	0	4.148634	0.922558	-1.40981
39	1	0	3.977716	-1.43297	-0.98659
40	1	0	-5.31722	-0.95351	-0.52168
41	1	0	-3.21334	-1.75014	-0.13606
42	1	0	4.339308	-0.12409	1.764556
43	1	0	4.883703	-1.73672	1.276301
44	1	0	5.60898	-0.29764	0.542027
45	1	0	0.862777	4.209708	0.325534

Table S13. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 9*S*, 10*E*, 12*R*, 15*R*)-**3d**] in NMR calculation

3d-Conf.1

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-2.21692	-0.53619	0.705468
2	6	0	-1.91828	0.667313	-0.27716
3	6	0	-0.74642	1.499224	0.16869
4	6	0	0.426821	1.627269	-0.45354
5	6	0	-0.4701	-1.98063	-0.40654
6	6	0	-1.87923	-1.92681	0.119516
7	6	0	1.578961	2.442113	0.083222
8	6	0	2.74289	1.599686	0.628273
9	6	0	1.948187	-1.85276	-0.31001
10	6	0	0.637468	-2.12539	0.322289
11	6	0	-3.71121	-0.41085	1.086908
12	6	0	-4.33818	0.449098	-0.0091
13	6	0	-3.23912	1.472089	-0.3207
14	6	0	3.486679	0.748596	-0.42271
15	6	0	3.971264	-0.61354	0.095156
16	8	0	2.811801	-1.35739	0.600154
17	8	0	-5.55666	1.024745	0.46709
18	8	0	-2.81224	-2.20424	-0.93033
19	8	0	2.199733	-1.96654	-1.492
20	6	0	4.966235	-0.55399	1.241261
21	1	0	-1.59508	-0.43324	1.59762
22	1	0	-1.71535	0.267483	-1.2736
23	8	0	2.122576	3.300417	-0.93642
24	1	0	-0.89291	2.026628	1.113374
25	1	0	0.597737	1.116104	-1.3992
26	1	0	-0.36395	-1.79496	-1.47209
27	1	0	-2.00287	-2.65776	0.929502
28	1	0	1.205497	3.053662	0.915937
29	1	0	2.328624	0.954575	1.407019
30	1	0	3.443047	2.280387	1.121836
31	1	0	0.617047	-2.25998	1.398245
32	1	0	-4.20332	-1.3788	1.19487
33	1	0	-3.81475	0.1289	2.033787
34	1	0	-4.53532	-0.16893	-0.8929
35	1	0	-3.38237	1.987671	-1.27381
36	1	0	-3.25184	2.226882	0.474083
37	1	0	2.845999	0.561786	-1.28637
38	1	0	4.355371	1.289999	-0.80717
39	1	0	4.387219	-1.18315	-0.73727
40	1	0	-5.96714	1.493167	-0.26757
41	1	0	-2.67355	-3.11134	-1.22387
42	1	0	5.868414	-0.02949	0.917366
43	1	0	4.552519	-0.02733	2.10402

44	1	0	5.248431	-1.56127	1.554771
45	1	0	1.392519	3.811669	-1.30277

3d-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.33187	-0.64213	0.458287
2	6	0	-2.037	0.466739	-0.62589
3	6	0	-0.93582	1.393891	-0.17777
4	6	0	0.277044	1.50083	-0.7233
5	6	0	-0.48823	-2.13092	-0.37688
6	6	0	-1.93139	-2.07555	0.047137
7	6	0	1.359972	2.409498	-0.19484
8	6	0	2.511757	1.672131	0.506032
9	6	0	1.910592	-1.88678	-0.13709
10	6	0	0.571027	-2.15335	0.433451
11	6	0	-3.83366	-0.51289	0.799308
12	6	0	-4.187	0.938972	0.469838
13	6	0	-3.39429	1.206487	-0.80814
14	6	0	3.356098	0.755918	-0.40511
15	6	0	3.85484	-0.52755	0.274979
16	8	0	2.692676	-1.27156	0.774029
17	8	0	-3.70318	1.84862	1.473744
18	8	0	-2.78113	-2.48435	-1.03002
19	8	0	2.245892	-2.1013	-1.28392
20	6	0	4.765252	-0.31431	1.471831
21	1	0	-1.74262	-0.41185	1.349324
22	1	0	-1.74632	0.000867	-1.56955
23	8	0	1.945064	3.187773	-1.25569
24	1	0	-1.18117	2.005166	0.690522
25	1	0	0.535096	0.899353	-1.59341
26	1	0	-0.31648	-2.04805	-1.44678
27	1	0	-2.09173	-2.72586	0.917597
28	1	0	0.907644	3.082476	0.546489
29	1	0	2.06756	1.087699	1.315498
30	1	0	3.151885	2.425463	0.975163
31	1	0	0.481339	-2.1774	1.513954
32	1	0	-4.41831	-1.17756	0.158474
33	1	0	-4.05278	-0.77286	1.839123
34	1	0	-5.26487	1.08365	0.330772
35	1	0	-3.93732	0.780187	-1.65588
36	1	0	-3.27464	2.276113	-0.9933
37	1	0	2.782667	0.457699	-1.2845
38	1	0	4.228184	1.294641	-0.78583

39	1	0	4.349264	-1.15473	-0.46851
40	1	0	-4.11221	1.604882	2.311532
41	1	0	-2.59143	-3.40766	-1.22886
42	1	0	5.665752	0.218727	1.157273
43	1	0	4.272671	0.271745	2.250768
44	1	0	5.065192	-1.27329	1.89953
45	1	0	1.224079	3.621139	-1.72573

3d-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.426011	-0.7107	-0.14477
2	6	0	2.009504	0.638847	0.528162
3	6	0	0.752845	1.225609	-0.05234
4	6	0	-0.31702	1.656516	0.618913
5	6	0	0.255638	-1.83397	0.310989
6	6	0	1.74396	-1.9732	0.414836
7	6	0	-1.54327	2.208075	-0.07268
8	6	0	-2.85947	2.080637	0.716776
9	6	0	-2.01659	-2.1557	-0.55048
10	6	0	-0.57063	-2.48857	-0.50988
11	6	0	3.959616	-0.7234	-0.03493
12	6	0	4.34714	0.717617	-0.35109
13	6	0	3.265451	1.560003	0.355164
14	6	0	-3.34865	0.696474	1.186325
15	6	0	-3.56052	-0.40107	0.137524
16	8	0	-2.22154	-0.87199	-0.20154
17	8	0	4.282682	0.859085	-1.78069
18	8	0	2.137104	-2.11304	1.788696
19	8	0	-2.89874	-2.93343	-0.85366
20	6	0	-4.31605	0.016087	-1.11739
21	1	0	2.164848	-0.65906	-1.20635
22	1	0	1.85643	0.457617	1.595299
23	8	0	-1.36428	3.602512	-0.42146
24	1	0	0.728304	1.274585	-1.14246
25	1	0	-0.32573	1.623113	1.708199
26	1	0	-0.16615	-1.07233	0.953714
27	1	0	2.093069	-2.83827	-0.1639
28	1	0	-1.64159	1.712812	-1.0407
29	1	0	-3.63242	2.555404	0.105284
30	1	0	-2.76151	2.705814	1.613714
31	1	0	-0.24738	-3.30227	-1.15032
32	1	0	4.25787	-0.97319	0.986411
33	1	0	4.435526	-1.43201	-0.71682

34	1	0	5.355794	0.967716	-0.00328
35	1	0	3.619386	1.893842	1.333946
36	1	0	3.037543	2.45795	-0.22512
37	1	0	-2.67079	0.29166	1.94373
38	1	0	-4.30932	0.848888	1.689863
39	1	0	-4.08122	-1.23924	0.607308
40	1	0	4.443113	1.785098	-1.99181
41	1	0	1.738076	-2.92127	2.129129
42	1	0	-5.30157	0.402899	-0.8441
43	1	0	-3.78315	0.79425	-1.66735
44	1	0	-4.45508	-0.84305	-1.77464
45	1	0	-1.20381	4.084435	0.398781

3d-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.32667	-0.58055	0.681439
2	6	0	-1.79934	0.572872	-0.25678
3	6	0	-0.50074	1.171163	0.205812
4	6	0	0.581926	1.421292	-0.53216
5	6	0	-0.57735	-2.25387	-0.11358
6	6	0	-2.04476	-1.99674	0.145255
7	6	0	1.839611	2.029796	0.051059
8	6	0	3.11621	1.779517	-0.76974
9	6	0	1.82044	-1.92754	0.136666
10	6	0	0.44039	-1.88466	0.665103
11	6	0	-3.84217	-0.31527	0.878079
12	6	0	-4.22034	0.727304	-0.1743
13	6	0	-2.96077	1.593391	-0.28029
14	6	0	3.538903	0.33183	-1.07796
15	6	0	3.834137	-0.61273	0.097149
16	8	0	2.574811	-0.98648	0.745418
17	8	0	-5.39082	1.431282	0.244117
18	8	0	-2.78882	-2.15451	-1.07009
19	8	0	2.213927	-2.63081	-0.77131
20	6	0	4.734661	-0.05161	1.183907
21	1	0	-1.82392	-0.50843	1.64889
22	1	0	-1.67228	0.172881	-1.26672
23	8	0	1.695059	3.456636	0.246786
24	1	0	-0.46325	1.417349	1.268711
25	1	0	0.577835	1.193118	-1.59744
26	1	0	-0.34635	-2.71701	-1.06979
27	1	0	-2.41282	-2.71466	0.891994
28	1	0	1.971474	1.644486	1.064156

29	1	0	3.927992	2.304297	-0.25789
30	1	0	2.989557	2.289257	-1.73372
31	1	0	0.300619	-1.36887	1.606454
32	1	0	-4.44114	-1.22348	0.797725
33	1	0	-4.02761	0.12484	1.862647
34	1	0	-4.40578	0.230947	-1.13544
35	1	0	-2.93839	2.227701	-1.17027
36	1	0	-2.91876	2.24496	0.600556
37	1	0	2.796118	-0.15429	-1.71621
38	1	0	4.455053	0.379763	-1.67706
39	1	0	4.266343	-1.52867	-0.30808
40	1	0	-5.64965	2.022551	-0.47076
41	1	0	-2.81524	-3.09182	-1.29004
42	1	0	5.692627	0.246841	0.750979
43	1	0	4.291048	0.820395	1.668644
44	1	0	4.924796	-0.80943	1.946682
45	1	0	1.483596	3.843083	-0.61143

3d-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.21679	-0.54151	0.697608
2	6	0	-1.91199	0.668599	-0.27358
3	6	0	-0.73197	1.489188	0.171939
4	6	0	0.413245	1.666967	-0.48681
5	6	0	-0.47528	-1.98613	-0.4189
6	6	0	-1.8869	-1.92836	0.099574
7	6	0	1.577028	2.460836	0.050959
8	6	0	2.71032	1.586371	0.627961
9	6	0	1.942396	-1.87012	-0.30396
10	6	0	0.62618	-2.14072	0.317104
11	6	0	-3.71013	-0.41212	1.082316
12	6	0	-4.33277	0.468625	0.000571
13	6	0	-3.22589	1.486252	-0.29994
14	6	0	3.464132	0.732983	-0.41241
15	6	0	3.956116	-0.62221	0.115907
16	8	0	2.798112	-1.37323	0.613181
17	8	0	-5.54498	1.047673	0.488901
18	8	0	-2.8168	-2.18852	-0.95743
19	8	0	2.204415	-1.98587	-1.48331
20	6	0	4.940298	-0.5503	1.270437
21	1	0	-1.59409	-0.44997	1.590463
22	1	0	-1.72003	0.278381	-1.2761
23	8	0	2.050759	3.288971	-1.02668

24	1	0	-0.85252	1.970053	1.144617
25	1	0	0.557678	1.206204	-1.46207
26	1	0	-0.36114	-1.79341	-1.48234
27	1	0	-2.01966	-2.66671	0.901386
28	1	0	1.208368	3.096133	0.86729
29	1	0	2.263118	0.943071	1.39061
30	1	0	3.413017	2.243606	1.152601
31	1	0	0.597068	-2.28107	1.392151
32	1	0	-4.20855	-1.37832	1.176183
33	1	0	-3.80941	0.113765	2.037388
34	1	0	-4.53826	-0.13472	-0.8915
35	1	0	-3.36718	2.017122	-1.2449
36	1	0	-3.22863	2.229502	0.505767
37	1	0	2.825991	0.536449	-1.2759
38	1	0	4.330693	1.276616	-0.79913
39	1	0	4.384051	-1.19159	-0.71062
40	1	0	-5.95176	1.533336	-0.23654
41	1	0	-2.68494	-3.09445	-1.25756
42	1	0	5.840027	-0.01731	0.953605
43	1	0	4.513495	-0.02655	2.128545
44	1	0	5.229865	-1.55417	1.588068
45	1	0	2.812838	3.781669	-0.70202

3d-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.33299	-0.63719	0.452205
2	6	0	-2.03237	0.476725	-0.62446
3	6	0	-0.92322	1.394912	-0.17692
4	6	0	0.26987	1.530772	-0.75598
5	6	0	-0.49896	-2.13463	-0.38651
6	6	0	-1.94337	-2.07072	0.031649
7	6	0	1.365008	2.420877	-0.22694
8	6	0	2.488259	1.655529	0.504118
9	6	0	1.899467	-1.9033	-0.13089
10	6	0	0.555324	-2.16495	0.430081
11	6	0	-3.83334	-0.50081	0.796692
12	6	0	-4.17647	0.95642	0.481373
13	6	0	-3.38469	1.229482	-0.79591
14	6	0	3.338889	0.735858	-0.39611
15	6	0	3.838847	-0.5421	0.292867
16	8	0	2.676214	-1.2885	0.785716
17	8	0	-3.68355	1.8528	1.492788
18	8	0	-2.79272	-2.46429	-1.05138

19	8	0	2.243218	-2.12006	-1.27466
20	6	0	4.739899	-0.32116	1.495302
21	1	0	-1.74114	-0.41674	1.344057
22	1	0	-1.75024	0.015863	-1.57321
23	8	0	1.881688	3.161462	-1.34866
24	1	0	-1.14933	1.978467	0.715212
25	1	0	0.507138	0.961834	-1.65306
26	1	0	-0.32131	-2.04965	-1.45527
27	1	0	-2.11238	-2.72614	0.896679
28	1	0	0.918954	3.115746	0.497147
29	1	0	2.015535	1.072208	1.298803
30	1	0	3.131163	2.390303	1.00218
31	1	0	0.458577	-2.19047	1.509965
32	1	0	-4.42355	-1.15529	0.150404
33	1	0	-4.05279	-0.76913	1.834354
34	1	0	-5.25351	1.110634	0.34611
35	1	0	-3.93334	0.815699	-1.64626
36	1	0	-3.25643	2.299714	-0.97127
37	1	0	2.767353	0.43098	-1.27456
38	1	0	4.211023	1.273529	-0.77883
39	1	0	4.341235	-1.16963	-0.44501
40	1	0	-4.09349	1.6046	2.328813
41	1	0	-2.61115	-3.38805	-1.25555
42	1	0	5.638858	0.217724	1.186323
43	1	0	4.237968	0.261853	2.270501
44	1	0	5.043551	-1.27775	1.925698
45	1	0	2.607469	3.708111	-1.02704

Table S14. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*R*, 9*S*, 10*E*, 12*S*, 15*R*)-**3c**] in ECD calculation

3c-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.27219	-0.09053	1.0406
2	6	0	-1.8771	0.794004	-0.19709
3	6	0	-0.65748	1.647943	0.022198
4	6	0	0.462541	1.588016	-0.69934
5	6	0	-0.36813	-1.62397	0.695071
6	6	0	-1.8547	-1.57704	0.866034
7	6	0	1.660163	2.49736	-0.54824
8	6	0	3.038952	1.83531	-0.7982
9	6	0	1.729048	-1.94075	-0.5682

10	6	0	0.282549	-2.13682	-0.35165
11	6	0	-3.80251	0.101942	1.238729
12	6	0	-4.30687	0.702915	-0.07135
13	6	0	-3.15595	1.612513	-0.5045
14	6	0	3.645995	0.948788	0.315879
15	6	0	3.615926	-0.56092	0.080672
16	8	0	2.231729	-0.98265	0.238425
17	8	0	-4.48277	-0.40423	-0.98607
18	8	0	-2.50773	-2.23532	-0.21009
19	8	0	2.379353	-2.52602	-1.41289
20	6	0	4.481323	-1.34077	1.063205
21	1	0	-1.74735	0.270398	1.928741
22	1	0	-1.68635	0.128212	-1.04235
23	8	0	1.642756	3.24439	0.671659
24	1	0	-0.72712	2.374983	0.830808
25	1	0	0.529316	0.872999	-1.51623
26	1	0	0.200278	-1.12147	1.470367
27	1	0	-2.11226	-2.08865	1.807646
28	1	0	1.567355	3.264916	-1.32725
29	1	0	3.731265	2.661394	-0.98001
30	1	0	2.984116	1.275723	-1.73855
31	1	0	-0.24041	-2.67286	-1.13316
32	1	0	-3.98963	0.808695	2.050178
33	1	0	-4.32807	-0.82388	1.483659
34	1	0	-5.25824	1.231817	0.035148
35	1	0	-3.18362	2.52412	0.102564
36	1	0	-3.22106	1.916435	-1.55307
37	1	0	4.698457	1.222238	0.432537
38	1	0	3.182328	1.155892	1.286316
39	1	0	3.915579	-0.79467	-0.9428
40	1	0	-4.57136	-0.06024	-1.88257
41	1	0	-3.2304	-1.67357	-0.54505
42	1	0	4.399322	-2.4135	0.877012
43	1	0	5.530187	-1.05474	0.952582
44	1	0	4.174262	-1.14022	2.093179
45	1	0	1.54728	2.61868	1.399066

3c-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.16025	0.02413	0.93609
2	6	0	-1.97429	0.722634	-0.45227
3	6	0	-0.74272	1.558756	-0.69007
4	6	0	0.388457	1.634456	0.014181

5	6	0	-0.29526	-1.59567	0.691986
6	6	0	-1.76738	-1.47592	0.921451
7	6	0	1.563689	2.477379	-0.4122
8	6	0	2.814076	1.689145	-0.84368
9	6	0	1.760586	-1.93051	-0.62449
10	6	0	0.313599	-2.11478	-0.37581
11	6	0	-3.6568	0.2336	1.313412
12	6	0	-4.35967	0.661619	0.017131
13	6	0	-3.28811	1.515977	-0.67026
14	6	0	3.581137	0.931014	0.268687
15	6	0	3.668936	-0.58236	0.070483
16	8	0	2.318886	-1.09692	0.274779
17	8	0	-4.749	-0.45839	-0.78502
18	8	0	-2.55105	-2.13496	-0.08057
19	8	0	2.354355	-2.42109	-1.56427
20	6	0	4.601744	-1.27572	1.05344
21	1	0	-1.52946	0.504185	1.68709
22	1	0	-1.95811	-0.06399	-1.21739
23	8	0	1.979217	3.35831	0.648935
24	1	0	-0.79655	2.144862	-1.6091
25	1	0	0.520562	1.075051	0.93457
26	1	0	0.313578	-1.12314	1.454693
27	1	0	-2.01245	-1.88638	1.909655
28	1	0	1.252661	3.07474	-1.28032
29	1	0	3.490482	2.412856	-1.30779
30	1	0	2.512736	1.001993	-1.63981
31	1	0	-0.23187	-2.61921	-1.16372
32	1	0	-3.73873	1.03724	2.049775
33	1	0	-4.11602	-0.65756	1.747063
34	1	0	-5.27485	1.22601	0.209279
35	1	0	-3.22601	2.491461	-0.17422
36	1	0	-3.5092	1.684682	-1.72656
37	1	0	4.605479	1.310014	0.322216
38	1	0	3.136457	1.130515	1.24738
39	1	0	3.959271	-0.82314	-0.95372
40	1	0	-4.07309	-1.14665	-0.67349
41	1	0	-2.54694	-3.08409	0.084824
42	1	0	4.298909	-1.07263	2.084084
43	1	0	4.594384	-2.3562	0.894439
44	1	0	5.625003	-0.9172	0.916832
45	1	0	1.19802	3.838402	0.944979

3c-Conf.3

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-2.12558	0.139239	0.911347
2	6	0	-1.85602	0.630281	-0.54724
3	6	0	-0.59395	1.412951	-0.81023
4	6	0	0.35289	1.758508	0.06252
5	6	0	-0.28151	-1.51923	0.903529
6	6	0	-1.75555	-1.35839	1.120075
7	6	0	1.620723	2.502112	-0.25635
8	6	0	2.872217	1.717008	0.167637
9	6	0	1.702571	-2.15899	-0.43192
10	6	0	0.282425	-2.26546	-0.04965
11	6	0	-3.62767	0.440866	1.186805
12	6	0	-4.25655	0.67706	-0.18411
13	6	0	-3.14586	1.388709	-0.95826
14	6	0	3.290014	0.601324	-0.81533
15	6	0	3.646642	-0.75386	-0.18758
16	8	0	2.416203	-1.32664	0.361257
17	8	0	-4.5374	-0.63094	-0.73388
18	8	0	-2.48081	-2.24712	0.283145
19	8	0	2.162383	-2.71432	-1.41162
20	6	0	4.672617	-0.71262	0.932633
21	1	0	-1.52537	0.703967	1.62588
22	1	0	-1.80257	-0.25915	-1.18613
23	8	0	1.664206	3.733954	0.493228
24	1	0	-0.45296	1.69027	-1.85541
25	1	0	0.256892	1.507032	1.115979
26	1	0	0.351604	-0.90429	1.533509
27	1	0	-1.97518	-1.59068	2.174901
28	1	0	1.669086	2.723332	-1.33155
29	1	0	2.684201	1.308442	1.164556
30	1	0	3.683027	2.441756	0.278001
31	1	0	-0.31894	-2.89369	-0.69379
32	1	0	-3.72088	1.3527	1.780844
33	1	0	-4.1378	-0.35715	1.731104
34	1	0	-5.18552	1.252364	-0.13842
35	1	0	-3.09913	2.431543	-0.62741
36	1	0	-3.31248	1.391779	-2.03904
37	1	0	2.490139	0.415961	-1.53955
38	1	0	4.153627	0.93007	-1.40207
39	1	0	3.988319	-1.4244	-0.97559
40	1	0	-4.73034	-0.54243	-1.67465
41	1	0	-3.2549	-1.7854	-0.08767
42	1	0	4.881256	-1.72206	1.293243
43	1	0	5.606011	-0.28121	0.561849

44	1	0	4.328091	-0.11084	1.776215
45	1	0	0.842633	4.205524	0.31484

3c-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.14011	0.011698	0.927175
2	6	0	-1.97355	0.714067	-0.45921
3	6	0	-0.75257	1.56472	-0.70211
4	6	0	0.369958	1.658854	0.011224
5	6	0	-0.30309	-1.6184	0.680376
6	6	0	-1.77807	-1.50507	0.882444
7	6	0	1.54948	2.488311	-0.42042
8	6	0	2.784929	1.66739	-0.86011
9	6	0	1.768384	-1.95186	-0.61217
10	6	0	0.322506	-2.14388	-0.37566
11	6	0	-3.61634	0.264385	1.351871
12	6	0	-4.3471	0.671426	0.076043
13	6	0	-3.29846	1.493229	-0.67391
14	6	0	3.560397	0.931409	0.260873
15	6	0	3.661748	-0.58374	0.083119
16	8	0	2.315918	-1.10573	0.284992
17	8	0	-4.668	-0.55433	-0.62209
18	8	0	-2.47673	-2.22896	-0.11728
19	8	0	2.376724	-2.44441	-1.54246
20	6	0	4.594072	-1.25444	1.082401
21	1	0	-1.48179	0.46734	1.669448
22	1	0	-1.95039	-0.07615	-1.21954
23	8	0	1.873264	3.362917	0.676925
24	1	0	-0.8066	2.138166	-1.62883
25	1	0	0.495894	1.112329	0.940018
26	1	0	0.293448	-1.1384	1.448029
27	1	0	-2.02181	-1.91228	1.877439
28	1	0	1.240441	3.089088	-1.28622
29	1	0	3.465802	2.362993	-1.36319
30	1	0	2.459917	0.963611	-1.6328
31	1	0	-0.21654	-2.65938	-1.1599
32	1	0	-3.66187	1.091355	2.064123
33	1	0	-4.08366	-0.60144	1.826962
34	1	0	-5.27086	1.224625	0.267391
35	1	0	-3.2378	2.485808	-0.21483
36	1	0	-3.54165	1.633919	-1.73097
37	1	0	4.581036	1.320878	0.3122
38	1	0	3.110977	1.139359	1.236027

39	1	0	3.962315	-0.83554	-0.93542
40	1	0	-4.93946	-0.34017	-1.52226
41	1	0	-3.31474	-1.77045	-0.3128
42	1	0	4.281909	-1.03907	2.107807
43	1	0	4.596558	-2.33715	0.939223
44	1	0	5.615381	-0.88946	0.948036
45	1	0	2.64099	3.885436	0.417626

3c-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.14215	0.160006	0.915696
2	6	0	-1.85751	0.646343	-0.54243
3	6	0	-0.58493	1.412906	-0.79922
4	6	0	0.357426	1.761375	0.077556
5	6	0	-0.27732	-1.49618	0.905976
6	6	0	-1.74659	-1.31985	1.146979
7	6	0	1.630484	2.496832	-0.24031
8	6	0	2.878194	1.702849	0.179204
9	6	0	1.68783	-2.14882	-0.44892
10	6	0	0.267665	-2.24247	-0.05702
11	6	0	-3.65929	0.413919	1.155295
12	6	0	-4.26442	0.668279	-0.23346
13	6	0	-3.13662	1.419351	-0.95383
14	6	0	3.292997	0.595318	-0.81414
15	6	0	3.646406	-0.76605	-0.19869
16	8	0	2.414169	-1.33673	0.350538
17	8	0	-4.60847	-0.54885	-0.90519
18	8	0	-2.54979	-2.13335	0.28283
19	8	0	2.131383	-2.69773	-1.43873
20	6	0	4.675298	-0.73848	0.918981
21	1	0	-1.56774	0.748099	1.63277
22	1	0	-1.81471	-0.24101	-1.18586
23	8	0	1.683187	3.726841	0.511472
24	1	0	-0.43418	1.682383	-1.84509
25	1	0	0.253818	1.519512	1.132792
26	1	0	0.3695	-0.88787	1.528295
27	1	0	-1.97321	-1.56069	2.193889
28	1	0	1.678985	2.719916	-1.3151
29	1	0	2.687338	1.2853	1.171831
30	1	0	3.691632	2.423327	0.297467
31	1	0	-0.33967	-2.86106	-0.70593
32	1	0	-3.78781	1.306555	1.772808
33	1	0	-4.15602	-0.41401	1.665354

34	1	0	-5.18355	1.256643	-0.18443
35	1	0	-3.08969	2.450101	-0.58474
36	1	0	-3.28504	1.449742	-2.03546
37	1	0	2.492532	0.418514	-1.53984
38	1	0	4.157265	0.926907	-1.39822
39	1	0	3.981667	-1.43259	-0.9928
40	1	0	-3.97503	-1.22809	-0.62253
41	1	0	-2.565	-3.0376	0.61436
42	1	0	4.336629	-0.14004	1.767245
43	1	0	4.879116	-1.75141	1.272391
44	1	0	5.610015	-0.3101	0.548207
45	1	0	0.86442	4.203961	0.335151

3c-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.16386	0.041072	0.937166
2	6	0	-1.96632	0.723238	-0.45734
3	6	0	-0.73282	1.55758	-0.69305
4	6	0	0.376709	1.666032	0.038467
5	6	0	-0.30233	-1.58435	0.706538
6	6	0	-1.77333	-1.45937	0.940943
7	6	0	1.561259	2.492717	-0.38684
8	6	0	2.789917	1.674201	-0.85039
9	6	0	1.74477	-1.94839	-0.61582
10	6	0	0.299052	-2.12454	-0.35512
11	6	0	-3.66238	0.257811	1.302074
12	6	0	-4.3555	0.673354	-0.00362
13	6	0	-3.27705	1.516884	-0.69369
14	6	0	3.5752	0.9168	0.249072
15	6	0	3.660264	-0.59633	0.049503
16	8	0	2.312178	-1.10712	0.270413
17	8	0	-4.74304	-0.45443	-0.79575
18	8	0	-2.56108	-2.13093	-0.04976
19	8	0	2.330737	-2.45142	-1.55387
20	6	0	4.604633	-1.28991	1.021198
21	1	0	-1.53743	0.527542	1.687588
22	1	0	-1.94583	-0.07158	-1.2137
23	8	0	1.896858	3.346545	0.72289
24	1	0	-0.76921	2.114924	-1.6304
25	1	0	0.487352	1.139121	0.980635
26	1	0	0.311563	-1.09847	1.456653
27	1	0	-2.01526	-1.85679	1.935238
28	1	0	1.251062	3.109658	-1.24071

29	1	0	3.468221	2.376041	-1.34817
30	1	0	2.455036	0.984911	-1.63187
31	1	0	-0.25265	-2.64141	-1.13047
32	1	0	-3.74744	1.069573	2.029112
33	1	0	-4.12665	-0.62758	1.742109
34	1	0	-5.27015	1.2427	0.176268
35	1	0	-3.21565	2.497914	-0.20876
36	1	0	-3.49079	1.673708	-1.75335
37	1	0	4.600049	1.296229	0.289793
38	1	0	3.142589	1.115618	1.233674
39	1	0	3.938009	-0.83759	-0.97806
40	1	0	-4.07137	-1.14424	-0.66939
41	1	0	-2.56344	-3.07698	0.132207
42	1	0	4.315164	-1.0851	2.055319
43	1	0	4.593348	-2.3705	0.86344
44	1	0	5.626676	-0.93332	0.871068
45	1	0	2.662199	3.873534	0.465897

3c-Conf.7

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.12441	0.163706	0.906073
2	6	0	-1.83913	0.630425	-0.55763
3	6	0	-0.57618	1.414171	-0.81772
4	6	0	0.342933	1.798435	0.066237
5	6	0	-0.28809	-1.50294	0.922449
6	6	0	-1.76009	-1.33049	1.144185
7	6	0	1.619668	2.528793	-0.24105
8	6	0	2.856763	1.698395	0.165938
9	6	0	1.683704	-2.19448	-0.40297
10	6	0	0.266172	-2.2843	-0.00818
11	6	0	-3.62761	0.474519	1.163021
12	6	0	-4.24368	0.688285	-0.21737
13	6	0	-3.12435	1.382972	-0.99428
14	6	0	3.241151	0.587088	-0.83503
15	6	0	3.619449	-0.76852	-0.22106
16	8	0	2.405395	-1.34152	0.36157
17	8	0	-4.52371	-0.62843	-0.74657
18	8	0	-2.49517	-2.23527	0.333182
19	8	0	2.135508	-2.77896	-1.36913
20	6	0	4.6787	-0.72684	0.867757
21	1	0	-1.52901	0.737658	1.617057
22	1	0	-1.77805	-0.26868	-1.18187
23	8	0	1.569077	3.746734	0.526257

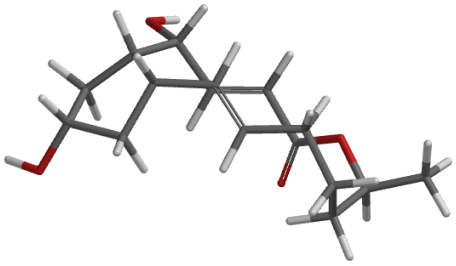
24	1	0	-0.41559	1.66215	-1.86714
25	1	0	0.222682	1.578572	1.124085
26	1	0	0.352529	-0.8685	1.524746
27	1	0	-1.97436	-1.53892	2.205001
28	1	0	1.670733	2.766776	-1.31236
29	1	0	2.6609	1.281451	1.157863
30	1	0	3.70051	2.386659	0.283758
31	1	0	-0.3418	-2.9323	-0.62597
32	1	0	-3.72288	1.397274	1.73956
33	1	0	-4.14495	-0.31206	1.71696
34	1	0	-5.17134	1.266844	-0.19006
35	1	0	-3.07812	2.431542	-0.68231
36	1	0	-3.28122	1.366626	-2.07639
37	1	0	2.415581	0.403621	-1.53028
38	1	0	4.083135	0.91891	-1.45079
39	1	0	3.938537	-1.43785	-1.01944
40	1	0	-4.70774	-0.55612	-1.69043
41	1	0	-3.25551	-1.77286	-0.06415
42	1	0	4.357001	-0.12939	1.723375
43	1	0	4.902032	-1.73658	1.218515
44	1	0	5.59892	-0.29043	0.470728
45	1	0	2.419125	4.189726	0.424835

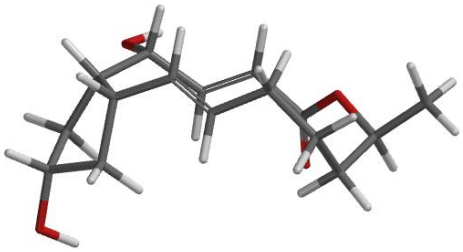
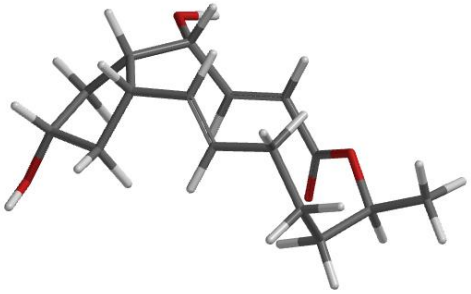
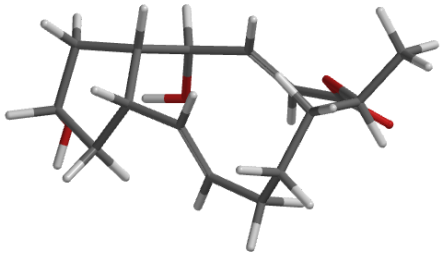
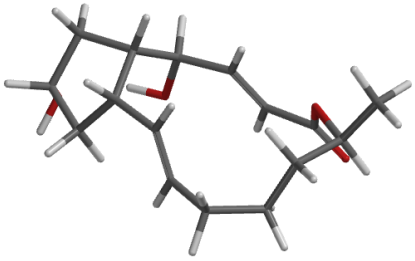
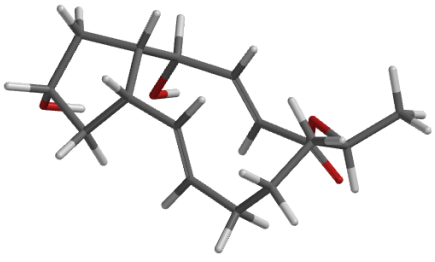
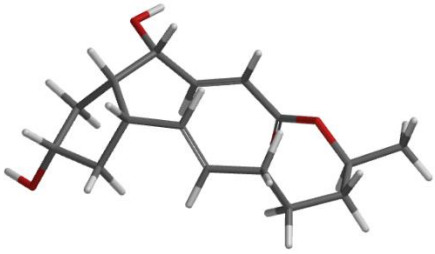
3c-Conf.8

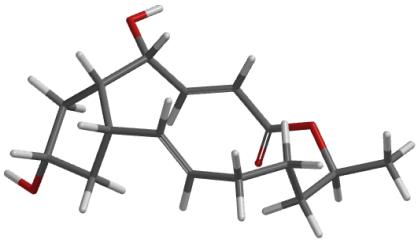
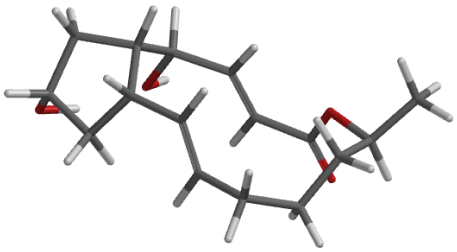
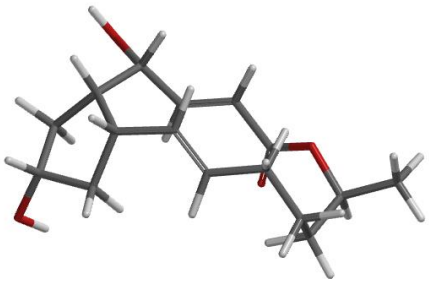
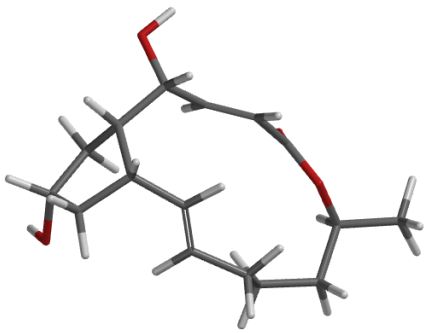
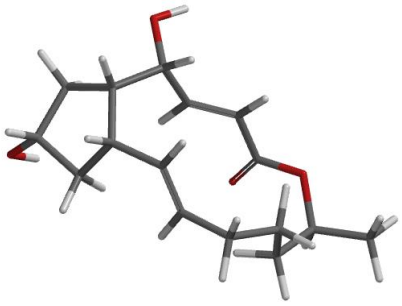
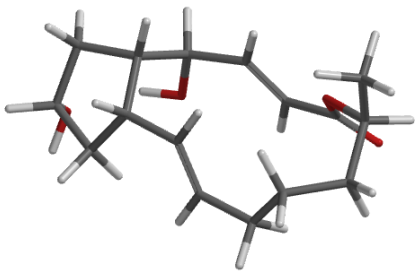
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.12653	0.152624	0.912083
2	6	0	-1.84863	0.636115	-0.5483
3	6	0	-0.58609	1.419549	-0.8076
4	6	0	0.359021	1.764734	0.067084
5	6	0	-0.28232	-1.50794	0.907844
6	6	0	-1.75554	-1.3422	1.129661
7	6	0	1.630086	2.503399	-0.25063
8	6	0	2.877877	1.709588	0.168469
9	6	0	1.695643	-2.16591	-0.42684
10	6	0	0.276082	-2.26443	-0.04043
11	6	0	-3.63125	0.451534	1.175505
12	6	0	-4.24934	0.675447	-0.20885
13	6	0	-3.13853	1.386634	-0.97403
14	6	0	3.287077	0.595116	-0.81932
15	6	0	3.64295	-0.76236	-0.19609
16	8	0	2.413813	-1.33072	0.359561
17	8	0	-4.49186	-0.59325	-0.86883
18	8	0	-2.4928	-2.23573	0.306318

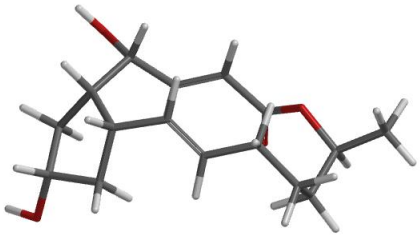
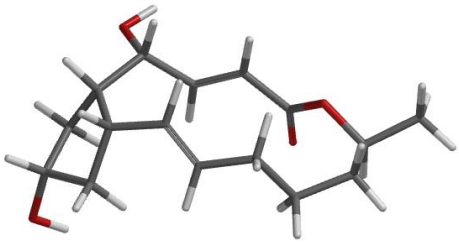
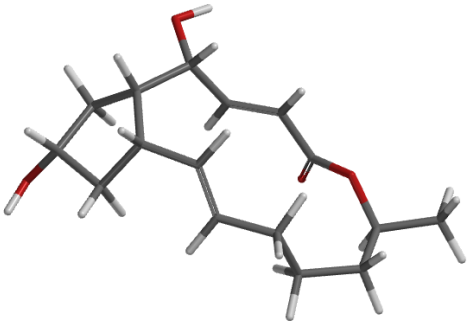
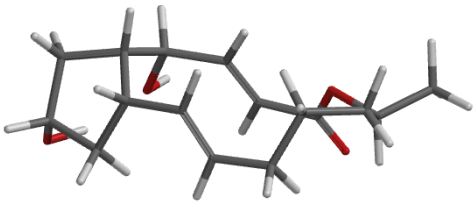
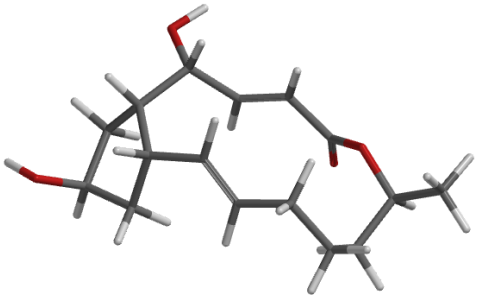
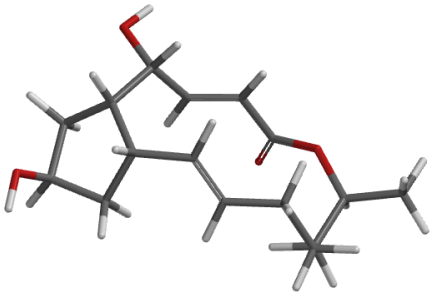
19	8	0	2.151473	-2.72945	-1.40356
20	6	0	4.676558	-0.72648	0.917288
21	1	0	-1.53136	0.722997	1.626296
22	1	0	-1.78618	-0.2553	-1.18416
23	8	0	1.681342	3.73208	0.503314
24	1	0	-0.4421	1.695387	-1.85271
25	1	0	0.260673	1.514425	1.12062
26	1	0	0.355375	-0.88977	1.53006
27	1	0	-1.97095	-1.56947	2.185865
28	1	0	1.678192	2.728148	-1.32508
29	1	0	2.68926	1.298231	1.164112
30	1	0	3.693025	2.429245	0.279997
31	1	0	-0.32957	-2.89653	-0.67681
32	1	0	-3.72888	1.369355	1.761507
33	1	0	-4.13898	-0.34172	1.729833
34	1	0	-5.18047	1.246223	-0.17941
35	1	0	-3.09728	2.430016	-0.64651
36	1	0	-3.3043	1.373992	-2.05299
37	1	0	2.482545	0.41345	-1.53928
38	1	0	4.148301	0.922653	-1.41023
39	1	0	3.97692	-1.43307	-0.98724
40	1	0	-5.31634	-0.95406	-0.52273
41	1	0	-3.21191	-1.7502	-0.1371
42	1	0	4.33998	-0.12436	1.763832
43	1	0	4.883626	-1.73714	1.275369
44	1	0	5.609173	-0.29831	0.540857
45	1	0	0.863069	4.209732	0.326275

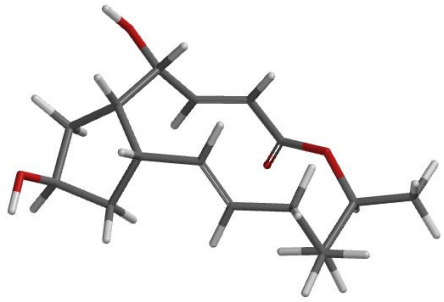
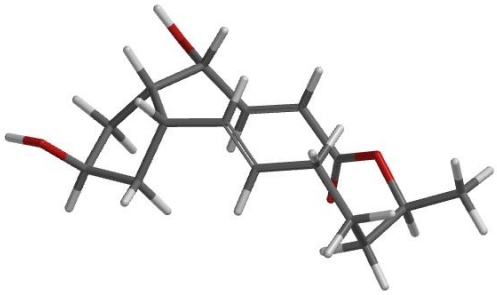
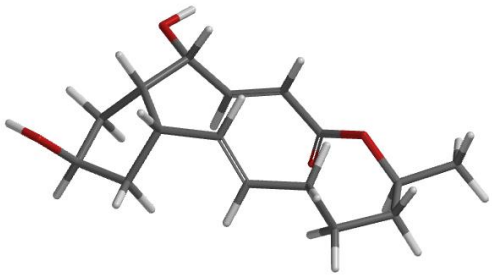
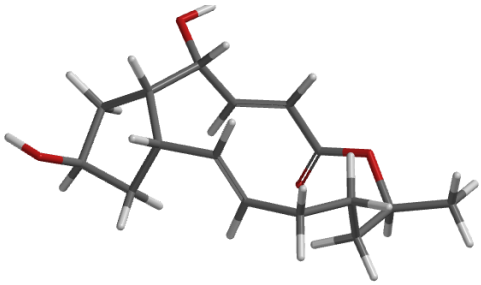
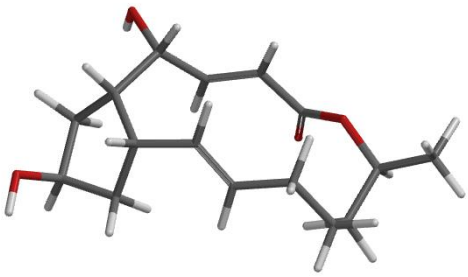
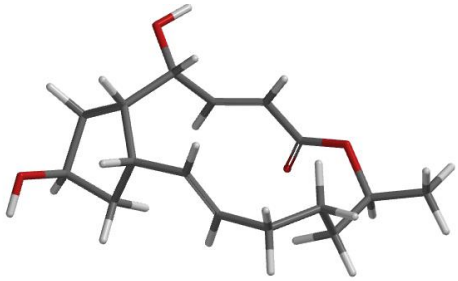
Table S15. The Information of conformations of (2*E*, 4*R**, 5*S**, 7*S**, 9*S**, 10*E*, 15*S**)-**4a** and (2*E*, 4*R**, 5*S**, 7*R**, 9*S**, 10*E*, 15*S**)-**4b**

Label	**Conformers**	**Calculated energy (kJ/mol)**	**Boltzmann distribution**
4a-Conf.1		0	0.307

4a-Conf.2		1.69	0.155
4a-Conf.3		2.29	0.122
4a-Conf.4		4.32	0.054
4a-Conf.5		5.33	0.036
4a-Conf.6		5.40	0.035
4a-Conf.7		5.41	0.035

4a-Conf.8		5.69	0.031
4a-Conf.9		5.90	0.028
4a-Conf.10		6.40	0.023
4a-Conf.11		6.47	0.023
4a-Conf.12		6.99	0.018
4a-Conf.13		7.16	0.017

4a-Conf.14		7.27	0.016
4a-Conf.15		7.41	0.015
4a-Conf.16		7.85	0.013
4a-Conf.17		7.96	0.012
4b-Conf.1		0	0.408
4b-Conf.2		2.30	0.161

4b-Conf.3		3.35	0.105
4b-Conf.4		4.01	0.081
4b-Conf.5		5.25	0.049
4b-Conf.6		6.07	0.035
4b-Conf.7		6.30	0.032
4b-Conf.8		7.82	0.017

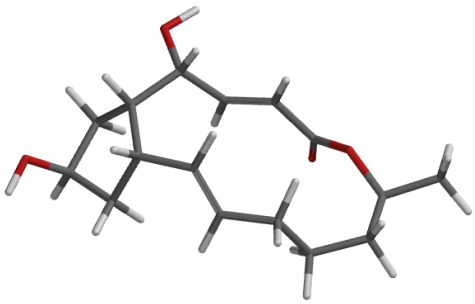
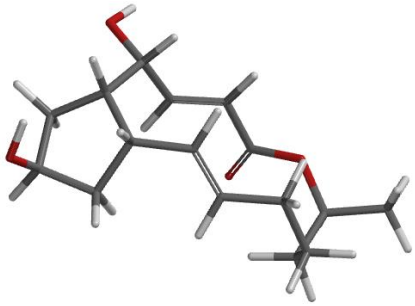
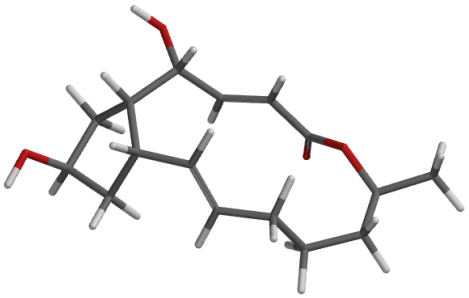
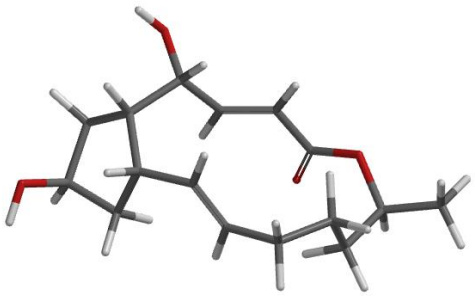
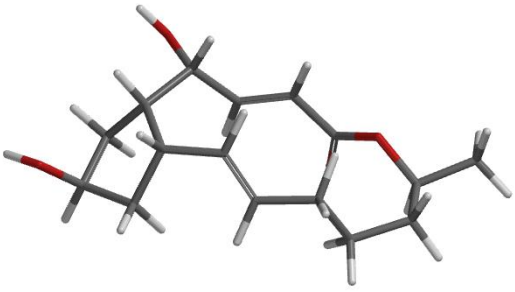
4b-Conf.9		8.00	0.016
4b-Conf.10		8.27	0.015
4b-Conf.11		8.45	0.013
4b-Conf.12		8.54	0.013
4b-Conf.13		9.00	0.011

Table S16. The coordinate for the lowest-energy conformer [(2*E*, 4*R**, 5*S**, 7*S**, 9*S**, 10*E*, 15*S**)-**4a**] in NMR calculation

4a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.75119	0.391179	-1.01397
2	6	0	-1.77112	1.526979	-0.55003
3	6	0	-0.36678	1.518671	-1.11031
4	6	0	0.731904	1.928095	-0.47211
5	6	0	-1.10105	-1.43994	-0.28119
6	6	0	-2.15461	-1.02344	-1.26537
7	6	0	2.133461	1.907439	-1.03976
8	6	0	3.253113	1.847066	0.022588
9	6	0	1.282709	-1.62607	0.298872
10	6	0	0.165748	-1.60678	-0.66586
11	6	0	-3.84922	0.454842	0.07019
12	6	0	-3.16906	0.843421	1.395565
13	6	0	-1.85791	1.547796	0.998637
14	6	0	3.247208	0.68091	1.028989
15	6	0	3.518187	-0.73974	0.512341
16	8	0	2.399202	-1.18164	-0.31827
17	8	0	-3.25975	-1.94211	-1.28284
18	8	0	1.216298	-1.90102	1.479329
19	6	0	4.769159	-0.8988	-0.33551
20	1	0	-3.18821	0.671739	-1.97631
21	1	0	-2.25373	2.445833	-0.9109
22	8	0	-2.81919	-0.30006	2.201023
23	1	0	-0.26726	1.159695	-2.13444
24	1	0	0.639925	2.311092	0.54281
25	1	0	-1.38304	-1.4819	0.766283
26	1	0	-1.69329	-1.00417	-2.26045
27	1	0	2.228312	1.078405	-1.7463
28	1	0	2.303636	2.824231	-1.62046
29	1	0	4.218365	1.88246	-0.49269
30	1	0	3.203212	2.769575	0.613305
31	1	0	0.446659	-1.50935	-1.70868
32	1	0	-4.41945	-0.4706	0.153615
33	1	0	-4.55236	1.247737	-0.20451
34	1	0	-3.8196	1.495797	1.987757
35	1	0	-1.80783	2.566172	1.388737
36	1	0	-1.02902	0.991557	1.441808
37	1	0	2.299923	0.662172	1.576122
38	1	0	4.018846	0.884381	1.780579
39	1	0	3.563412	-1.40982	1.372742
40	1	0	-2.91436	-2.80033	-1.55311

41	1	0	4.911985	-1.94658	-0.60794
42	1	0	5.644754	-0.56839	0.228765
43	1	0	4.709291	-0.31032	-1.25344
44	1	0	-3.63604	-0.76048	2.424385

4a-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.684166	0.407608	-0.8538
2	6	0	1.927546	-0.98676	-1.0399
3	6	0	0.460209	-0.96538	-1.39542
4	6	0	-0.50349	-1.7319	-0.87964
5	6	0	0.735305	1.77674	0.061259
6	6	0	1.864011	1.713488	-0.92528
7	6	0	-1.94059	-1.73734	-1.34927
8	6	0	-2.98546	-2.07741	-0.26498
9	6	0	-1.62841	1.567906	0.643253
10	6	0	-0.54142	1.879761	-0.30871
11	6	0	3.495263	0.254519	0.453051
12	6	0	3.65764	-1.25809	0.640124
13	6	0	2.293736	-1.80542	0.212399
14	6	0	-3.11895	-1.13559	0.945582
15	6	0	-3.66442	0.282106	0.713799
16	8	0	-2.68034	1.065351	-0.03557
17	8	0	2.808754	2.773292	-0.69432
18	8	0	-1.56732	1.646812	1.852589
19	6	0	-4.96497	0.366492	-0.06711
20	1	0	3.394965	0.498179	-1.67988
21	1	0	2.428865	-1.45927	-1.89469
22	8	0	4.080301	-1.6534	1.943449
23	1	0	0.191657	-0.29013	-2.20655
24	1	0	-0.26069	-2.4378	-0.08669
25	1	0	0.973362	1.64822	1.113122
26	1	0	1.449962	1.80996	-1.93653
27	1	0	-2.1748	-0.78101	-1.82393
28	1	0	-2.04853	-2.50191	-2.13116
29	1	0	-3.96011	-2.18489	-0.75179
30	1	0	-2.7468	-3.07155	0.131403
31	1	0	-0.8216	1.96847	-1.35217
32	1	0	2.935202	0.640861	1.312551
33	1	0	4.446833	0.78578	0.421745
34	1	0	4.436484	-1.63657	-0.02967
35	1	0	2.304295	-2.88239	0.032389
36	1	0	1.575753	-1.60804	1.018407

37	1	0	-2.15755	-1.04548	1.46066
38	1	0	-3.79695	-1.60893	1.665193
39	1	0	-3.78247	0.763375	1.685936
40	1	0	2.335689	3.607922	-0.78819
41	1	0	-5.30032	1.403623	-0.13297
42	1	0	-5.74006	-0.21287	0.440615
43	1	0	-4.85281	-0.02325	-1.08083
44	1	0	3.417357	-1.34317	2.571709

4a-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.64966	0.352464	-1.15083
2	6	0	-1.71237	1.4584	-0.55858
3	6	0	-0.25477	1.460679	-0.94573
4	6	0	0.769339	1.938627	-0.23599
5	6	0	-0.97774	-1.42831	-0.24999
6	6	0	-2.20271	-1.16922	-1.07728
7	6	0	2.188507	2.019624	-0.75057
8	6	0	3.294388	1.863789	0.313058
9	6	0	1.40115	-1.63127	0.183708
10	6	0	0.244074	-1.64609	-0.73566
11	6	0	-3.93608	0.656042	-0.35466
12	6	0	-3.46393	0.867929	1.087058
13	6	0	-2.05825	1.509208	0.954423
14	6	0	3.340496	0.559821	1.128125
15	6	0	3.631509	-0.75629	0.391175
16	8	0	2.486609	-1.13442	-0.44187
17	8	0	-3.25245	-2.03455	-0.62718
18	8	0	1.375659	-1.94019	1.358458
19	6	0	4.837972	-0.73654	-0.53222
20	1	0	-2.81477	0.563601	-2.21002
21	1	0	-2.12663	2.378796	-0.99543
22	8	0	-3.41537	-0.44319	1.697424
23	1	0	-0.04875	1.093445	-1.9508
24	1	0	0.593939	2.334148	0.764136
25	1	0	-1.11092	-1.38509	0.826777
26	1	0	-1.99885	-1.48764	-2.1015
27	1	0	2.32291	1.288586	-1.5525
28	1	0	2.338812	3.006722	-1.20987
29	1	0	4.261162	2.024573	-0.17521
30	1	0	3.190763	2.683728	1.033846
31	1	0	0.451646	-1.64422	-1.80013
32	1	0	-4.7032	-0.11339	-0.42668

33	1	0	-4.36471	1.589981	-0.72898
34	1	0	-4.15363	1.491407	1.66281
35	1	0	-2.05213	2.534362	1.33101
36	1	0	-1.33173	0.94632	1.546738
37	1	0	2.408841	0.431498	1.685322
38	1	0	4.126867	0.665753	1.88459
39	1	0	3.749237	-1.54172	1.140022
40	1	0	-3.43091	-1.77911	0.293684
41	1	0	4.713652	-0.01403	-1.34138
42	1	0	4.994232	-1.72337	-0.97283
43	1	0	5.733221	-0.46794	0.03403
44	1	0	-3.01617	-0.37084	2.571547

4a-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.154143	-0.15353	1.291075
2	6	0	1.791505	1.214111	0.623464
3	6	0	0.342431	1.467612	0.288344
4	6	0	-0.1743	1.635253	-0.92789
5	6	0	0.180548	-1.5115	0.542624
6	6	0	1.674769	-1.47166	0.603607
7	6	0	-1.61473	1.843486	-1.32775
8	6	0	-2.66821	2.320322	-0.3065
9	6	0	-1.98599	-1.58965	-0.62575
10	6	0	-0.54881	-1.89905	-0.50811
11	6	0	3.692227	-0.03984	1.348442
12	6	0	4.117711	0.655848	0.039918
13	6	0	2.8427	1.361474	-0.49634
14	6	0	-3.22861	1.36045	0.76723
15	6	0	-3.63334	-0.04564	0.303821
16	8	0	-2.42532	-0.85583	0.41611
17	8	0	2.186468	-1.71778	-0.69812
18	8	0	-2.6702	-1.87424	-1.59143
19	6	0	-4.71856	-0.68125	1.162067
20	1	0	1.739622	-0.19535	2.3031
21	1	0	2.053174	1.951857	1.395934
22	8	0	4.596533	-0.37762	-0.85443
23	1	0	-0.31531	1.513243	1.153503
24	1	0	0.497633	1.574647	-1.78264
25	1	0	-0.33103	-1.12532	1.416492
26	1	0	2.005975	-2.27338	1.288447
27	1	0	-1.61219	2.586885	-2.13491
28	1	0	-1.9626	0.925705	-1.82226

29	1	0	-2.28386	3.209354	0.206129
30	1	0	-3.52174	2.667095	-0.89979
31	1	0	-0.08859	-2.30575	-1.39888
32	1	0	4.208795	-0.99508	1.469211
33	1	0	3.969909	0.589188	2.197565
34	1	0	4.934504	1.361578	0.210141
35	1	0	3.022819	2.406086	-0.75864
36	1	0	2.515263	0.839051	-1.39774
37	1	0	-4.11272	1.845194	1.194329
38	1	0	-2.52654	1.234139	1.596082
39	1	0	-3.93979	-0.05295	-0.74401
40	1	0	3.122519	-1.45201	-0.7485
41	1	0	-5.64671	-0.1104	1.078823
42	1	0	-4.41847	-0.70118	2.213407
43	1	0	-4.91431	-1.70513	0.836204
44	1	0	4.762829	0.017568	-1.71861

4a-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.086954	-0.14615	1.16807
2	6	0	1.949785	1.211091	0.404385
3	6	0	0.676108	1.488087	-0.34623
4	6	0	-0.20655	2.437024	-0.02075
5	6	0	0.048797	-1.4378	0.452664
6	6	0	1.547008	-1.43046	0.478012
7	6	0	-1.45952	2.780764	-0.8081
8	6	0	-2.47162	1.627227	-0.96451
9	6	0	-2.16791	-1.66987	-0.60619
10	6	0	-0.71253	-1.90387	-0.54223
11	6	0	3.60667	-0.19036	1.436469
12	6	0	4.282926	0.36291	0.174513
13	6	0	3.224495	1.283965	-0.48556
14	6	0	-3.24108	1.283824	0.323524
15	6	0	-3.79842	-0.14335	0.35671
16	8	0	-2.64122	-1.02916	0.486241
17	8	0	2.031372	-1.6633	-0.83529
18	8	0	-2.8517	-1.95714	-1.56977
19	6	0	-4.71476	-0.41762	1.537481
20	1	0	1.547137	-0.0833	2.11786
21	1	0	2.046401	1.980429	1.179211
22	8	0	4.623884	-0.77182	-0.66067
23	1	0	0.507471	0.879557	-1.23262
24	1	0	-0.00877	3.037199	0.866298

25	1	0	-0.43723	-1.00068	1.317224
26	1	0	1.853868	-2.25869	1.143564
27	1	0	-1.95518	3.637073	-0.3398
28	1	0	-1.16719	3.114864	-1.81037
29	1	0	-3.18984	1.886001	-1.74985
30	1	0	-1.92999	0.75145	-1.32886
31	1	0	-0.27846	-2.35603	-1.42456
32	1	0	3.988149	-1.18293	1.688147
33	1	0	3.83518	0.471535	2.276068
34	1	0	5.20675	0.896465	0.410487
35	1	0	3.578938	2.312353	-0.58264
36	1	0	3.007777	0.915918	-1.49176
37	1	0	-4.0701	1.987898	0.453403
38	1	0	-2.58986	1.398884	1.196989
39	1	0	-4.30106	-0.39227	-0.57974
40	1	0	2.999745	-1.54184	-0.83726
41	1	0	-5.03611	-1.46134	1.540879
42	1	0	-5.60314	0.215696	1.477568
43	1	0	-4.20497	-0.2076	2.481697
44	1	0	4.999673	-0.44175	-1.48553

4a-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.174672	-0.11843	1.305091
2	6	0	1.779916	1.229686	0.610073
3	6	0	0.321148	1.479443	0.310581
4	6	0	-0.21291	1.653449	-0.89771
5	6	0	0.19293	-1.48414	0.557474
6	6	0	1.684148	-1.46074	0.691304
7	6	0	-1.65367	1.879692	-1.28469
8	6	0	-2.70373	2.32102	-0.24573
9	6	0	-1.94401	-1.57096	-0.65939
10	6	0	-0.50625	-1.87532	-0.51108
11	6	0	3.71299	-0.00918	1.300138
12	6	0	4.101216	0.693834	-0.03157
13	6	0	2.791045	1.355694	-0.54231
14	6	0	-3.25796	1.319325	0.792541
15	6	0	-3.63454	-0.07785	0.280596
16	8	0	-2.41488	-0.8729	0.390646
17	8	0	2.34484	-1.73439	-0.55434
18	8	0	-2.59806	-1.83761	-1.64991
19	6	0	-4.72221	-0.75564	1.10232
20	1	0	1.787551	-0.1243	2.328418

21	1	0	2.062571	1.983652	1.359744
22	8	0	4.668792	-0.20098	-0.99033
23	1	0	-0.3205	1.529702	1.187904
24	1	0	0.44843	1.589367	-1.76027
25	1	0	-0.34727	-1.08543	1.408493
26	1	0	1.980085	-2.22849	1.420852
27	1	0	-1.65057	2.650645	-2.06584
28	1	0	-2.00528	0.981101	-1.81053
29	1	0	-2.31986	3.191439	0.298124
30	1	0	-3.5592	2.687356	-0.82411
31	1	0	-0.03355	-2.28608	-1.39447
32	1	0	4.22318	-0.97007	1.39267
33	1	0	4.02334	0.610341	2.146276
34	1	0	4.877075	1.440498	0.146747
35	1	0	2.937521	2.393258	-0.85151
36	1	0	2.454949	0.795878	-1.4183
37	1	0	-4.15272	1.775224	1.228733
38	1	0	-2.55904	1.177199	1.621463
39	1	0	-3.9229	-0.06012	-0.77217
40	1	0	2.314563	-2.68386	-0.71563
41	1	0	-5.65785	-0.19706	1.020174
42	1	0	-4.43844	-0.80075	2.157353
43	1	0	-4.89649	-1.77262	0.744309
44	1	0	4.012191	-0.90907	-1.08289

4a-Conf.7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.84279	0.092115	-1.04647
2	6	0	-2.10859	1.424058	-0.64853
3	6	0	-0.67255	1.561507	-1.09965
4	6	0	0.311061	2.167899	-0.43274
5	6	0	-0.87275	-1.36344	-0.17602
6	6	0	-1.98646	-1.20244	-1.17356
7	6	0	1.767637	2.14023	-0.82475
8	6	0	2.690449	1.865398	0.395167
9	6	0	1.535263	-1.35049	0.359324
10	6	0	0.396803	-1.47379	-0.57432
11	6	0	-3.98826	0.028982	-0.01346
12	6	0	-3.45278	0.622083	1.29736
13	6	0	-2.3351	1.59531	0.880461
14	6	0	3.952609	1.030373	0.08533
15	6	0	3.801381	-0.46391	0.390828
16	8	0	2.629987	-0.95865	-0.33188

17	8	0	-2.9	-2.31148	-1.10192
18	8	0	1.497067	-1.50012	1.563119
19	6	0	4.996098	-1.30053	-0.03961
20	1	0	-3.27803	0.216559	-2.04164
21	1	0	-2.68978	2.207602	-1.15245
22	8	0	-2.8585	-0.37388	2.154498
23	1	0	-0.43137	1.094494	-2.05356
24	1	0	0.0911	2.660015	0.513122
25	1	0	-1.13242	-1.31891	0.877035
26	1	0	-1.53331	-1.18519	-2.17219
27	1	0	1.914865	1.370865	-1.58709
28	1	0	2.069085	3.091912	-1.28089
29	1	0	2.987741	2.823022	0.831538
30	1	0	2.1156	1.355014	1.174686
31	1	0	0.650943	-1.47062	-1.62886
32	1	0	-4.39186	-0.9752	0.116654
33	1	0	-4.8045	0.665414	-0.37155
34	1	0	-4.24939	1.126925	1.854462
35	1	0	-2.58683	2.627961	1.129761
36	1	0	-1.43631	1.336732	1.44328
37	1	0	4.793968	1.385164	0.689255
38	1	0	4.247356	1.1599	-0.96219
39	1	0	3.603661	-0.60395	1.454308
40	1	0	-2.39891	-3.10774	-1.3118
41	1	0	5.153782	-1.22369	-1.11858
42	1	0	4.845163	-2.35147	0.216484
43	1	0	5.899416	-0.95065	0.466365
44	1	0	-3.54046	-1.0212	2.367131

4a-Conf.8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.7207	0.441563	-0.98255
2	6	0	-1.95894	1.580816	-0.22042
3	6	0	-0.59733	2.004164	-0.71912
4	6	0	0.48107	2.207124	0.042125
5	6	0	-0.91372	-1.33167	-0.47595
6	6	0	-1.89974	-0.78013	-1.46746
7	6	0	1.835094	2.670562	-0.4361
8	6	0	2.889952	1.542389	-0.54844
9	6	0	1.428263	-1.65242	0.22945
10	6	0	0.376499	-1.46922	-0.79183
11	6	0	-3.85291	0.104614	0.013645
12	6	0	-3.29891	0.317894	1.438824

13	6	0	-2.04405	1.196422	1.273715
14	6	0	3.165195	0.768194	0.757725
15	6	0	3.624612	-0.6858	0.544606
16	8	0	2.630442	-1.33658	-0.31033
17	8	0	-2.85972	-1.7824	-1.8502
18	8	0	1.261862	-1.9323	1.397987
19	6	0	4.961781	-0.84439	-0.15801
20	1	0	-3.1569	0.851378	-1.89795
21	1	0	-2.61236	2.45461	-0.35902
22	8	0	-2.88821	-0.90756	2.075587
23	1	0	-0.5327	2.211147	-1.78795
24	1	0	0.403838	2.014298	1.108779
25	1	0	-1.27023	-1.54751	0.526566
26	1	0	-1.34015	-0.46424	-2.35648
27	1	0	1.737956	3.140519	-1.4202
28	1	0	2.20778	3.444494	0.246814
29	1	0	2.542921	0.841126	-1.31059
30	1	0	3.821054	1.976698	-0.92589
31	1	0	0.73086	-1.23314	-1.78913
32	1	0	-4.25219	-0.90062	-0.12423
33	1	0	-4.67551	0.806955	-0.1525
34	1	0	-4.04983	0.800892	2.072848
35	1	0	-2.06749	2.079216	1.915789
36	1	0	-1.18074	0.600369	1.577403
37	1	0	2.260157	0.728263	1.369341
38	1	0	3.91864	1.28264	1.363222
39	1	0	3.636435	-1.20713	1.503287
40	1	0	-2.37002	-2.51136	-2.24757
41	1	0	5.203168	-1.90166	-0.28668
42	1	0	5.75005	-0.38176	0.44072
43	1	0	4.951804	-0.36983	-1.1416
44	1	0	-3.66863	-1.46535	2.169308

4a-Conf.9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.273221	-0.12928	1.326054
2	6	0	1.937377	1.246066	0.664881
3	6	0	0.511095	1.7295	0.596771
4	6	0	-0.17125	2.089632	-0.49181
5	6	0	0.156747	-1.3661	0.589818
6	6	0	1.644801	-1.43504	0.757873
7	6	0	-1.53653	2.734792	-0.50642
8	6	0	-2.70036	1.781834	-0.89646

9	6	0	-1.9502	-1.5644	-0.69941
10	6	0	-0.50676	-1.78339	-0.49218
11	6	0	3.809601	-0.13953	1.172464
12	6	0	4.113507	0.53757	-0.20024
13	6	0	2.791245	1.245082	-0.61084
14	6	0	-3.4683	1.197086	0.314533
15	6	0	-3.81349	-0.28833	0.203357
16	8	0	-2.54757	-1.00359	0.368896
17	8	0	2.292853	-1.83348	-0.46212
18	8	0	-2.51802	-1.8158	-1.7457
19	6	0	-4.75923	-0.78244	1.286114
20	1	0	1.979761	-0.10647	2.379748
21	1	0	2.421081	1.959048	1.351299
22	8	0	4.579993	-0.37931	-1.18945
23	1	0	0.045927	1.88938	1.570411
24	1	0	0.277435	1.930941	-1.47143
25	1	0	-0.39533	-0.94131	1.420726
26	1	0	1.856419	-2.19641	1.522622
27	1	0	-1.7468	3.183036	0.470124
28	1	0	-1.50563	3.562787	-1.22307
29	1	0	-3.40915	2.320186	-1.53175
30	1	0	-2.30151	0.97623	-1.51877
31	1	0	0.008344	-2.20855	-1.34394
32	1	0	4.249355	-1.13724	1.213529
33	1	0	4.250012	0.44911	1.981572
34	1	0	4.921088	1.263705	-0.08878
35	1	0	2.959587	2.250792	-1.00285
36	1	0	2.314731	0.657163	-1.40023
37	1	0	-4.39471	1.7594	0.467785
38	1	0	-2.87984	1.317498	1.23006
39	1	0	-4.20425	-0.53349	-0.78512
40	1	0	2.202428	-2.78745	-0.56031
41	1	0	-4.9172	-1.85944	1.197729
42	1	0	-5.7271	-0.28413	1.192602
43	1	0	-4.35692	-0.57043	2.280495
44	1	0	3.905366	-1.07527	-1.2125

4a-Conf.10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.678846	0.391422	-0.85718
2	6	0	1.90368	-0.99527	-1.03466
3	6	0	0.439322	-0.9592	-1.40067
4	6	0	-0.53196	-1.72007	-0.89077

5	6	0	0.75938	1.79447	0.064794
6	6	0	1.884212	1.722912	-0.92235
7	6	0	-1.96739	-1.71629	-1.36501
8	6	0	-3.01554	-2.05527	-0.28356
9	6	0	-1.60241	1.558605	0.650454
10	6	0	-0.51807	1.875128	-0.30395
11	6	0	3.500039	0.229756	0.442924
12	6	0	3.6284	-1.28429	0.645576
13	6	0	2.251369	-1.80534	0.228041
14	6	0	-3.13549	-1.12424	0.936588
15	6	0	-3.65811	0.303806	0.718
16	8	0	-2.66306	1.076003	-0.02829
17	8	0	2.761819	2.826406	-0.64433
18	8	0	-1.53392	1.622891	1.860229
19	6	0	-4.95917	0.415742	-0.05874
20	1	0	3.383036	0.459983	-1.69381
21	1	0	2.405288	-1.48332	-1.88054
22	8	0	4.047383	-1.67423	1.951386
23	1	0	0.181272	-0.28145	-2.21302
24	1	0	-0.29683	-2.42764	-0.09704
25	1	0	1.000202	1.674249	1.116943
26	1	0	1.469183	1.833539	-1.93141
27	1	0	-2.1956	-0.75666	-1.83593
28	1	0	-2.0777	-2.47695	-2.15035
29	1	0	-3.99194	-2.1462	-0.77023
30	1	0	-2.78816	-3.0561	0.102528
31	1	0	-0.80196	1.96044	-1.34636
32	1	0	2.957139	0.639793	1.302325
33	1	0	4.465442	0.735343	0.401346
34	1	0	4.395753	-1.68749	-0.02299
35	1	0	2.237182	-2.88451	0.062141
36	1	0	1.538611	-1.5806	1.031526
37	1	0	-2.17284	-1.05385	1.452339
38	1	0	-3.82096	-1.59421	1.6513
39	1	0	-3.76529	0.779481	1.694168
40	1	0	3.520117	2.753897	-1.23592
41	1	0	-4.85683	0.029373	-1.07481
42	1	0	-5.27617	1.459029	-0.11799
43	1	0	-5.74295	-0.1525	0.448239
44	1	0	3.393508	-1.34348	2.578712

4a-Conf.11

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	2.671445	0.807794	-0.3911
2	6	0	2.429063	-0.46002	-1.28094
3	6	0	0.977133	-0.85716	-1.40174
4	6	0	0.298447	-1.80212	-0.74811
5	6	0	0.443771	1.942555	0.128491
6	6	0	1.754363	2.034251	-0.59909
7	6	0	-1.18018	-2.0214	-0.94517
8	6	0	-2.00953	-1.97956	0.362694
9	6	0	-1.91975	1.406772	0.388648
10	6	0	-0.74947	1.772267	-0.44253
11	6	0	2.741891	0.231881	1.033362
12	6	0	3.496431	-1.10544	0.883604
13	6	0	3.361233	-1.49449	-0.60772
14	6	0	-3.48897	-1.59753	0.128752
15	6	0	-3.80513	-0.11285	0.357357
16	8	0	-2.79694	0.687091	-0.34468
17	8	0	2.501043	3.160284	-0.10024
18	8	0	-2.04325	1.639673	1.573091
19	6	0	-5.1734	0.306225	-0.15488
20	1	0	3.668193	1.177972	-0.65886
21	1	0	2.782711	-0.24099	-2.29399
22	8	0	2.942752	-2.15629	1.690372
23	1	0	0.419333	-0.25876	-2.11995
24	1	0	0.801036	-2.42476	-0.01012
25	1	0	0.502976	1.961195	1.212935
26	1	0	1.576049	2.158259	-1.67505
27	1	0	-1.55448	-1.25827	-1.6321
28	1	0	-1.35891	-2.99099	-1.4291
29	1	0	-1.95563	-2.95693	0.85072
30	1	0	-1.55747	-1.27287	1.065728
31	1	0	-0.8713	1.712408	-1.51756
32	1	0	1.738431	0.000369	1.401016
33	1	0	3.213411	0.914399	1.743533
34	1	0	4.553177	-0.98066	1.146534
35	1	0	4.342351	-1.45918	-1.08689
36	1	0	2.99388	-2.51762	-0.69778
37	1	0	-4.13846	-2.15736	0.809211
38	1	0	-3.78858	-1.88205	-0.8864
39	1	0	-3.70963	0.123646	1.417122
40	1	0	1.962144	3.94954	-0.22761
41	1	0	-5.36401	1.359263	0.063079
42	1	0	-5.95116	-0.29036	0.328583
43	1	0	-5.24522	0.154024	-1.23495
44	1	0	3.028189	-1.89349	2.613676

4a-Conf.12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.646	-0.16218	-1.05551
2	6	0	-2.03066	1.255547	-0.70228
3	6	0	-0.64196	1.598591	-1.18405
4	6	0	0.344764	2.098512	-0.43547
5	6	0	-0.6527	-1.54087	-0.22447
6	6	0	-1.66747	-1.32674	-1.31287
7	6	0	1.696955	2.543022	-0.94335
8	6	0	2.831526	1.504571	-0.77855
9	6	0	1.654598	-1.5717	0.600458
10	6	0	0.64791	-1.70157	-0.47518
11	6	0	-3.62932	-0.46129	0.110776
12	6	0	-3.69125	0.811544	0.973697
13	6	0	-2.30484	1.436573	0.797706
14	6	0	3.104009	1.05671	0.6711
15	6	0	3.725127	-0.34659	0.790835
16	8	0	2.856694	-1.27099	0.056551
17	8	0	-2.49325	-2.49558	-1.47154
18	8	0	1.438932	-1.61031	1.793194
19	6	0	5.112333	-0.49663	0.191391
20	1	0	-3.207	-0.06806	-1.98859
21	1	0	-2.69349	1.964199	-1.21904
22	8	0	-4.0869	0.584432	2.325145
23	1	0	-0.4818	1.495946	-2.25794
24	1	0	0.179911	2.210782	0.633358
25	1	0	-0.98879	-1.51617	0.807892
26	1	0	-1.13083	-1.13265	-2.24922
27	1	0	1.622713	2.788371	-2.00781
28	1	0	1.97898	3.469534	-0.42812
29	1	0	2.569076	0.629887	-1.37776
30	1	0	3.744574	1.919379	-1.21738
31	1	0	1.02847	-1.71154	-1.49028
32	1	0	-3.25082	-1.2795	0.731664
33	1	0	-4.61349	-0.77181	-0.24277
34	1	0	-4.4477	1.497072	0.579891
35	1	0	-2.26945	2.480698	1.115712
36	1	0	-1.5787	0.878037	1.401687
37	1	0	2.169857	1.043437	1.23932
38	1	0	3.760787	1.769077	1.181242
39	1	0	3.731243	-0.65325	1.838044
40	1	0	-1.91073	-3.23475	-1.68023

41	1	0	5.469147	-1.5222	0.307486
42	1	0	5.808954	0.170104	0.705121
43	1	0	5.116888	-0.24779	-0.87204
44	1	0	-3.44982	-0.02419	2.717616

4a-Conf.13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.200111	-0.18124	1.280614
2	6	0	1.932763	1.237236	0.678176
3	6	0	0.496895	1.523097	0.336575
4	6	0	-0.01615	1.792143	-0.86272
5	6	0	0.118492	-1.41167	0.515224
6	6	0	1.619231	-1.42122	0.532374
7	6	0	-1.47706	1.849885	-1.24
8	6	0	-2.5394	1.922926	-0.11774
9	6	0	-2.09495	-1.54384	-0.59835
10	6	0	-0.63992	-1.77065	-0.52596
11	6	0	3.74243	-0.18377	1.335254
12	6	0	4.217236	0.543451	0.062559
13	6	0	3.004804	1.385442	-0.42088
14	6	0	-3.80243	1.072827	-0.41377
15	6	0	-3.88881	-0.24512	0.384115
16	8	0	-2.57034	-0.86614	0.467609
17	8	0	2.08196	-1.61032	-0.79668
18	8	0	-2.78233	-1.86677	-1.54974
19	6	0	-4.34443	-0.0596	1.82347
20	1	0	1.785953	-0.23895	2.292157
21	1	0	2.209542	1.924761	1.490586
22	8	0	4.597138	-0.4766	-0.89282
23	1	0	-0.1723	1.448414	1.190426
24	1	0	0.658617	1.869569	-1.71367
25	1	0	-0.36232	-1.06746	1.424042
26	1	0	1.925717	-2.28137	1.15597
27	1	0	-1.6331	2.680064	-1.93954
28	1	0	-1.65738	0.951892	-1.84782
29	1	0	-2.11222	1.593265	0.829542
30	1	0	-2.8252	2.967299	0.029423
31	1	0	-0.1937	-2.14099	-1.43952
32	1	0	4.188199	-1.17891	1.406471
33	1	0	4.066047	0.380957	2.212905
34	1	0	5.094138	1.164807	0.260251
35	1	0	3.269877	2.429484	-0.60022
36	1	0	2.64549	0.963683	-1.36229

37	1	0	-3.84897	0.843395	-1.48173
38	1	0	-4.7109	1.638065	-0.18599
39	1	0	-4.55235	-0.93988	-0.13302
40	1	0	3.03619	-1.41903	-0.84811
41	1	0	-5.36204	0.337263	1.840825
42	1	0	-3.69458	0.636684	2.359805
43	1	0	-4.33723	-1.01486	2.352639
44	1	0	4.798241	-0.0489	-1.73377

4a-Conf.14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.7438	0.410773	-1.00037
2	6	0	-1.7478	1.531428	-0.53073
3	6	0	-0.34967	1.521609	-1.10656
4	6	0	0.755991	1.919049	-0.47282
5	6	0	-1.12771	-1.45691	-0.2992
6	6	0	-2.17226	-1.01909	-1.27988
7	6	0	2.154138	1.895725	-1.0485
8	6	0	3.278253	1.828266	0.008954
9	6	0	1.257322	-1.60963	0.296206
10	6	0	0.145198	-1.58672	-0.67466
11	6	0	-3.832	0.472657	0.093095
12	6	0	-3.13754	0.841988	1.417725
13	6	0	-1.81521	1.522953	1.01825
14	6	0	3.262197	0.668074	1.022226
15	6	0	3.50751	-0.75901	0.511442
16	8	0	2.3814	-1.18301	-0.31869
17	8	0	-3.21712	-2.00387	-1.28424
18	8	0	1.182292	-1.87749	1.47779
19	6	0	4.75591	-0.94359	-0.33514
20	1	0	-3.18229	0.715011	-1.95674
21	1	0	-2.2272	2.460608	-0.86883
22	8	0	-2.8066	-0.3109	2.216941
23	1	0	-0.26168	1.173212	-2.13531
24	1	0	0.672816	2.291289	0.546809
25	1	0	-1.41673	-1.52625	0.744839
26	1	0	-1.70708	-0.99109	-2.27234
27	1	0	2.242588	1.067917	-1.75728
28	1	0	2.324871	2.813157	-1.62793
29	1	0	4.2415	1.849349	-0.51083
30	1	0	3.241841	2.754456	0.594853
31	1	0	0.433552	-1.46702	-1.71267
32	1	0	-4.40398	-0.45267	0.176639

33	1	0	-4.53647	1.269346	-0.16596
34	1	0	-3.77308	1.504669	2.014635
35	1	0	-1.73498	2.531294	1.428749
36	1	0	-0.99423	0.937008	1.437328
37	1	0	2.318463	0.666778	1.575697
38	1	0	4.041877	0.864046	1.767482
39	1	0	3.540059	-1.42677	1.374298
40	1	0	-3.87497	-1.73192	-1.9351
41	1	0	4.878907	-1.9944	-0.60557
42	1	0	5.637158	-0.62893	0.229336
43	1	0	4.708042	-0.35566	-1.25417
44	1	0	-3.63205	-0.74678	2.457293

4a-Conf.15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.680058	0.669005	-0.71661
2	6	0	2.251414	-0.8138	-1.12192
3	6	0	0.774976	-1.0409	-1.33192
4	6	0	-0.02453	-1.94006	-0.75487
5	6	0	0.454352	1.700582	0.053761
6	6	0	1.65145	1.809588	-0.84876
7	6	0	-1.51048	-2.01119	-0.99842
8	6	0	-2.3397	-2.01552	0.311256
9	6	0	-1.91485	1.311603	0.524174
10	6	0	-0.80535	1.674814	-0.38537
11	6	0	3.332729	0.530699	0.669616
12	6	0	3.996245	-0.84833	0.606907
13	6	0	2.918913	-1.71556	-0.05804
14	6	0	-3.77969	-1.48164	0.139371
15	6	0	-3.95239	-0.00408	0.51381
16	8	0	-2.92597	0.769646	-0.18919
17	8	0	2.382155	3.011912	-0.53983
18	8	0	-1.89792	1.404409	1.734083
19	6	0	-5.30672	0.569509	0.130415
20	1	0	3.473328	0.960494	-1.41249
21	1	0	2.728419	-1.00449	-2.09045
22	8	0	4.467136	-1.34866	1.856036
23	1	0	0.323069	-0.38046	-2.06953
24	1	0	0.374957	-2.64471	-0.02845
25	1	0	0.641173	1.605034	1.119278
26	1	0	1.308472	1.851858	-1.8901
27	1	0	-1.80839	-1.16276	-1.6192
28	1	0	-1.76365	-2.91633	-1.56623

29	1	0	-2.37205	-3.03572	0.704361
30	1	0	-1.82467	-1.4221	1.073563
31	1	0	-1.04106	1.73313	-1.442
32	1	0	2.579758	0.513667	1.467074
33	1	0	4.033684	1.3365	0.889013
34	1	0	4.888597	-0.79856	-0.02514
35	1	0	3.314357	-2.64412	-0.47444
36	1	0	2.196338	-1.98523	0.720042
37	1	0	-4.46949	-2.04293	0.77759
38	1	0	-4.11679	-1.63762	-0.89169
39	1	0	-3.77208	0.128607	1.580807
40	1	0	1.784058	3.756528	-0.67133
41	1	0	-5.45836	0.513464	-0.95071
42	1	0	-5.38822	1.613407	0.440804
43	1	0	-6.10341	0.003095	0.619227
44	1	0	3.710117	-1.40759	2.450862

4a-Conf.16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.218954	-0.16787	1.294085
2	6	0	1.912985	1.240241	0.679861
3	6	0	0.466931	1.518687	0.37296
4	6	0	-0.05656	1.822301	-0.81392
5	6	0	0.135152	-1.40439	0.515859
6	6	0	1.635017	-1.43099	0.602862
7	6	0	-1.51745	1.900584	-1.18614
8	6	0	-2.58261	1.92899	-0.06408
9	6	0	-2.05042	-1.51437	-0.64964
10	6	0	-0.59428	-1.73948	-0.55225
11	6	0	3.760977	-0.16406	1.290998
12	6	0	4.199961	0.594045	0.006963
13	6	0	2.943841	1.387113	-0.4513
14	6	0	-3.82946	1.064616	-0.38494
15	6	0	-3.88291	-0.2866	0.357493
16	8	0	-2.54725	-0.87423	0.426829
17	8	0	2.246639	-1.64249	-0.67913
18	8	0	-2.71459	-1.81472	-1.6238
19	6	0	-4.35208	-0.17261	1.799943
20	1	0	1.831221	-0.20716	2.31662
21	1	0	2.20748	1.935854	1.479711
22	8	0	4.695627	-0.27642	-1.01236
23	1	0	-0.19232	1.421074	1.232409
24	1	0	0.613643	1.922755	-1.66591

25	1	0	-0.37467	-1.07057	1.413085
26	1	0	1.913799	-2.26362	1.265577
27	1	0	-1.66887	2.761389	-1.84879
28	1	0	-1.70149	1.032085	-1.83414
29	1	0	-2.15232	1.588018	0.878098
30	1	0	-2.8891	2.964171	0.104332
31	1	0	-0.13674	-2.09104	-1.46868
32	1	0	4.204663	-1.16142	1.321856
33	1	0	4.111335	0.37814	2.17384
34	1	0	5.031892	1.2647	0.228919
35	1	0	3.167509	2.432871	-0.67479
36	1	0	2.574137	0.925852	-1.37036
37	1	0	-3.88034	0.880379	-1.46141
38	1	0	-4.74731	1.600715	-0.12623
39	1	0	-4.52215	-0.97925	-0.19191
40	1	0	2.160813	-2.57412	-0.91028
41	1	0	-5.38185	0.190935	1.825637
42	1	0	-3.72788	0.522451	2.367417
43	1	0	-4.31779	-1.14714	2.291521
44	1	0	3.984672	-0.92152	-1.15133

4a-Conf.17

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.218954	-0.16787	1.294085
2	6	0	1.912985	1.240241	0.679862
3	6	0	0.46693	1.518687	0.372961
4	6	0	-0.05656	1.822301	-0.81392
5	6	0	0.135152	-1.40439	0.515859
6	6	0	1.635018	-1.43099	0.602862
7	6	0	-1.51745	1.900585	-1.18614
8	6	0	-2.58261	1.92899	-0.06408
9	6	0	-2.05041	-1.51437	-0.64964
10	6	0	-0.59428	-1.73948	-0.55225
11	6	0	3.760977	-0.16406	1.290998
12	6	0	4.199961	0.594046	0.006963
13	6	0	2.94384	1.387113	-0.4513
14	6	0	-3.82946	1.064616	-0.38494
15	6	0	-3.88291	-0.2866	0.357494
16	8	0	-2.54725	-0.87423	0.426829
17	8	0	2.24664	-1.64249	-0.67913
18	8	0	-2.71459	-1.81472	-1.6238
19	6	0	-4.35208	-0.17261	1.799943
20	1	0	1.83122	-0.20716	2.31662

21	1	0	2.20748	1.935854	1.479711
22	8	0	4.695628	-0.27642	-1.01236
23	1	0	-0.19233	1.421074	1.23241
24	1	0	0.613643	1.922755	-1.66591
25	1	0	-0.37467	-1.07057	1.413085
26	1	0	1.9138	-2.26362	1.265577
27	1	0	-1.66887	2.761391	-1.84879
28	1	0	-1.70149	1.032088	-1.83414
29	1	0	-2.15232	1.588019	0.878098
30	1	0	-2.8891	2.964171	0.104332
31	1	0	-0.13674	-2.09104	-1.46868
32	1	0	4.204663	-1.16142	1.321855
33	1	0	4.111334	0.37814	2.17384
34	1	0	5.031891	1.264701	0.22892
35	1	0	3.167508	2.432871	-0.67479
36	1	0	2.574136	0.925852	-1.37036
37	1	0	-3.88034	0.880379	-1.46141
38	1	0	-4.74731	1.600714	-0.12623
39	1	0	-4.52215	-0.97925	-0.19191
40	1	0	2.160813	-2.57412	-0.91028
41	1	0	-4.31779	-1.14714	2.291521
42	1	0	-5.38185	0.190934	1.825638
43	1	0	-3.72788	0.52245	2.367417
44	1	0	3.984672	-0.92152	-1.15133

Table S17. The coordinate for the lowest-energy conformer [(2*E*, 4*R**, 5*S**, 7*R**, 9*S**, 10*E*, 15*S**)-**4b**] in NMR calculation

4b-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.669908	0.404439	-0.58842
2	6	0	1.962175	-1.0187	-0.6906
3	6	0	0.515054	-1.07682	-1.11661
4	6	0	-0.4534	-1.82943	-0.58848
5	6	0	0.641403	1.828021	0.021836
6	6	0	1.841618	1.676014	-0.86635
7	6	0	-1.85983	-1.92451	-1.13452
8	6	0	-2.96117	-2.15997	-0.07864
9	6	0	-1.7531	1.617702	0.459112
10	6	0	-0.60709	1.847143	-0.44611
11	6	0	3.370206	0.405568	0.79292
12	6	0	3.579648	-1.07311	1.127564

13	6	0	2.28261	-1.7151	0.651493
14	6	0	-3.19027	-1.07845	0.992599
15	6	0	-3.75465	0.280329	0.547964
16	8	0	-2.73906	0.999593	-0.22349
17	8	0	2.753292	2.775074	-0.68825
18	8	0	-1.78306	1.846217	1.65048
19	6	0	-4.99558	0.221869	-0.32692
20	1	0	3.450457	0.425857	-1.35255
21	1	0	2.52072	-1.54896	-1.47048
22	8	0	4.650736	-1.64835	0.360216
23	1	0	0.268556	-0.48373	-1.99601
24	1	0	-0.23695	-2.45891	0.273361
25	1	0	0.804171	1.836648	1.095719
26	1	0	1.503221	1.650869	-1.90971
27	1	0	-2.08182	-1.03651	-1.73198
28	1	0	-1.90782	-2.77819	-1.825
29	1	0	-3.90201	-2.35479	-0.60337
30	1	0	-2.72507	-3.0897	0.452606
31	1	0	-0.8125	1.799341	-1.50941
32	1	0	2.730745	0.847831	1.562967
33	1	0	4.303668	0.972141	0.78782
34	1	0	3.760525	-1.23664	2.196397
35	1	0	1.49976	-1.50491	1.386705
36	1	0	2.372171	-2.79941	0.55762
37	1	0	-2.26471	-0.89328	1.54653
38	1	0	-3.90002	-1.47823	1.726145
39	1	0	-3.95695	0.873021	1.441478
40	1	0	2.277715	3.58393	-0.90914
41	1	0	-5.79104	-0.31728	0.193423
42	1	0	-4.7972	-0.28626	-1.27264
43	1	0	-5.35166	1.230591	-0.54617
44	1	0	5.455614	-1.1637	0.573072

4b-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.67489	0.40745	-0.60301
2	6	0	1.961672	-1.01408	-0.68315
3	6	0	0.51959	-1.0746	-1.12495
4	6	0	-0.45462	-1.82031	-0.59752
5	6	0	0.646495	1.822936	0.028341
6	6	0	1.840823	1.678421	-0.86883
7	6	0	-1.85851	-1.91482	-1.15046
8	6	0	-2.96339	-2.15772	-0.09987

9	6	0	-1.74729	1.60931	0.472369
10	6	0	-0.60402	1.846057	-0.43407
11	6	0	3.400914	0.416733	0.766898
12	6	0	3.580416	-1.05302	1.133046
13	6	0	2.263943	-1.68175	0.675777
14	6	0	-3.19161	-1.08715	0.982592
15	6	0	-3.75296	0.277334	0.552135
16	8	0	-2.73696	1.001279	-0.21402
17	8	0	2.750428	2.77952	-0.69441
18	8	0	-1.77305	1.824704	1.666331
19	6	0	-4.99539	0.23043	-0.32129
20	1	0	3.43959	0.425924	-1.38303
21	1	0	2.529642	-1.56296	-1.44329
22	8	0	4.699752	-1.54918	0.379234
23	1	0	0.281914	-0.48768	-2.011
24	1	0	-0.24555	-2.44145	0.272128
25	1	0	0.814863	1.822096	1.101425
26	1	0	1.493931	1.655964	-1.90941
27	1	0	-2.07926	-1.02348	-1.74343
28	1	0	-1.9031	-2.76427	-1.8463
29	1	0	-3.9035	-2.3441	-0.62895
30	1	0	-2.73135	-3.0937	0.422129
31	1	0	-0.81324	1.807605	-1.49704
32	1	0	2.788819	0.893928	1.536931
33	1	0	4.353537	0.946092	0.73232
34	1	0	3.762566	-1.19684	2.204452
35	1	0	1.485076	-1.43465	1.40521
36	1	0	2.317707	-2.77208	0.610799
37	1	0	-2.26629	-0.90966	1.539369
38	1	0	-3.90281	-1.49333	1.711194
39	1	0	-3.95232	0.861787	1.451746
40	1	0	2.270451	3.587498	-0.90891
41	1	0	-5.79126	-0.31213	0.194842
42	1	0	-4.79947	-0.2687	-1.27229
43	1	0	-5.34952	1.24207	-0.53
44	1	0	4.752418	-2.49991	0.52604

4b-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.668169	0.39595	-0.60211
2	6	0	1.941121	-1.02028	-0.67851
3	6	0	0.501253	-1.0704	-1.12806
4	6	0	-0.47848	-1.81203	-0.6052

5	6	0	0.666093	1.848545	0.022321
6	6	0	1.858034	1.690747	-0.87217
7	6	0	-1.88057	-1.90066	-1.16325
8	6	0	-2.98903	-2.14177	-0.11599
9	6	0	-1.72441	1.60281	0.475229
10	6	0	-0.58469	1.839837	-0.43653
11	6	0	3.396921	0.400887	0.766588
12	6	0	3.555316	-1.0692	1.140757
13	6	0	2.230907	-1.68235	0.685594
14	6	0	-3.20545	-1.07862	0.976225
15	6	0	-3.74733	0.296713	0.556752
16	8	0	-2.72305	1.008831	-0.20953
17	8	0	2.69648	2.840109	-0.66538
18	8	0	-1.74177	1.811146	1.670562
19	6	0	-4.99387	0.274316	-0.31175
20	1	0	3.433322	0.3912	-1.38507
21	1	0	2.508611	-1.57868	-1.43196
22	8	0	4.668286	-1.5839	0.390038
23	1	0	0.271833	-0.48209	-2.0152
24	1	0	-0.27544	-2.43381	0.265396
25	1	0	0.836449	1.867633	1.094843
26	1	0	1.511752	1.676271	-1.91287
27	1	0	-2.09616	-1.00698	-1.75447
28	1	0	-1.92626	-2.74821	-1.8613
29	1	0	-3.93071	-2.31292	-0.64745
30	1	0	-2.7674	-3.08491	0.397546
31	1	0	-0.79735	1.787068	-1.49784
32	1	0	2.792148	0.892376	1.53321
33	1	0	4.358739	0.914094	0.73179
34	1	0	3.735038	-1.20964	2.212934
35	1	0	1.45381	-1.41965	1.411442
36	1	0	2.269898	-2.77372	0.628038
37	1	0	-2.27877	-0.91848	1.535945
38	1	0	-3.92318	-1.48196	1.69999
39	1	0	-3.93372	0.878997	1.460551
40	1	0	3.503054	2.709849	-1.17787
41	1	0	-5.7956	-0.25988	0.204054
42	1	0	-4.80927	-0.22123	-1.26688
43	1	0	-5.33378	1.292475	-0.51224
44	1	0	4.709408	-2.53431	0.542561

4b-Conf.4

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	2.663404	0.39373	-0.58829
2	6	0	1.94197	-1.02447	-0.68617
3	6	0	0.497193	-1.07259	-1.12053
4	6	0	-0.47679	-1.82106	-0.59674
5	6	0	0.660662	1.853504	0.015732
6	6	0	1.858322	1.688721	-0.87002
7	6	0	-1.88146	-1.91048	-1.14775
8	6	0	-2.98613	-2.14456	-0.09504
9	6	0	-1.73043	1.611388	0.462504
10	6	0	-0.5882	1.841149	-0.44815
11	6	0	3.36735	0.391074	0.791453
12	6	0	3.554304	-1.08858	1.135401
13	6	0	2.24861	-1.71443	0.66204
14	6	0	-3.2032	-1.07063	0.986313
15	6	0	-3.74878	0.299071	0.552854
16	8	0	-2.72538	1.006991	-0.21858
17	8	0	2.697863	2.836961	-0.6604
18	8	0	-1.75199	1.832856	1.655392
19	6	0	-4.99399	0.264523	-0.31722
20	1	0	3.444085	0.391762	-1.3559
21	1	0	2.500733	-1.56488	-1.45884
22	8	0	4.617327	-1.68375	0.372243
23	1	0	0.259027	-0.47854	-2.00141
24	1	0	-0.26635	-2.45072	0.266435
25	1	0	0.825574	1.881847	1.088868
26	1	0	1.520185	1.671309	-1.91339
27	1	0	-2.09857	-1.02008	-1.74332
28	1	0	-1.93052	-2.76216	-1.84061
29	1	0	-3.92872	-2.32404	-0.62214
30	1	0	-2.76026	-3.08172	0.427523
31	1	0	-0.79734	1.779215	-1.50964
32	1	0	2.73585	0.849512	1.558448
33	1	0	4.311238	0.940629	0.784838
34	1	0	3.73195	-1.24796	2.205287
35	1	0	1.467105	-1.48651	1.393361
36	1	0	2.322256	-2.80066	0.576983
37	1	0	-2.276	-0.90251	1.542903
38	1	0	-3.91902	-1.46792	1.71529
39	1	0	-3.93834	0.889391	1.45073
40	1	0	3.503869	2.707511	-1.17398
41	1	0	-5.795	-0.26666	0.202826
42	1	0	-4.80674	-0.24007	-1.26708
43	1	0	-5.3364	1.279697	-0.52832
44	1	0	5.431738	-1.21915	0.593426

4b-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.671546	0.558829	-0.49901
2	6	0	2.254278	-0.94664	-0.79618
3	6	0	0.788964	-1.1849	-1.0637
4	6	0	-0.05394	-2.02236	-0.45588
5	6	0	0.416373	1.67271	0.037925
6	6	0	1.668433	1.691068	-0.79342
7	6	0	-1.52446	-2.10051	-0.77927
8	6	0	-2.42992	-1.97562	0.472467
9	6	0	-1.98197	1.350078	0.395244
10	6	0	-0.81494	1.619929	-0.47369
11	6	0	3.231322	0.535941	0.937289
12	6	0	3.885412	-0.84424	1.043533
13	6	0	2.857654	-1.758	0.380019
14	6	0	-3.85106	-1.45376	0.163403
15	6	0	-4.03195	0.0543	0.380752
16	8	0	-2.95538	0.752409	-0.32626
17	8	0	2.395025	2.910519	-0.54453
18	8	0	-2.0371	1.553612	1.590397
19	6	0	-5.35308	0.592394	-0.14385
20	1	0	3.51508	0.778402	-1.15772
21	1	0	2.780034	-1.22461	-1.71642
22	8	0	5.097799	-0.91938	0.27496
23	1	0	0.385464	-0.59083	-1.88164
24	1	0	0.292138	-2.66368	0.351905
25	1	0	0.535465	1.670992	1.11742
26	1	0	1.39073	1.644895	-1.85405
27	1	0	-1.77205	-1.30901	-1.49072
28	1	0	-1.75866	-3.05103	-1.27682
29	1	0	-2.49715	-2.95337	0.958232
30	1	0	-1.95459	-1.31483	1.20441
31	1	0	-0.98579	1.585836	-1.54382
32	1	0	2.431857	0.601158	1.682601
33	1	0	3.927379	1.354986	1.129437
34	1	0	4.087497	-1.13336	2.081345
35	1	0	2.088969	-1.98956	1.121201
36	1	0	3.302729	-2.70181	0.058676
37	1	0	-4.58352	-1.94718	0.810151
38	1	0	-4.12778	-1.70823	-0.86609
39	1	0	-3.91923	0.290146	1.439232
40	1	0	1.814437	3.645608	-0.77246

41	1	0	-6.18521	0.080601	0.346156
42	1	0	-5.43614	0.430232	-1.22168
43	1	0	-5.44311	1.662206	0.056362
44	1	0	5.712698	-0.27015	0.633921

4b-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.6382	-0.36333	-0.82388
2	6	0	-2.081	1.07933	-0.50156
3	6	0	-0.74556	1.499099	-1.06539
4	6	0	0.258288	2.04669	-0.3749
5	6	0	-0.54167	-1.6367	-0.09034
6	6	0	-1.61501	-1.47604	-1.13083
7	6	0	1.554839	2.558155	-0.95844
8	6	0	2.750474	1.583519	-0.84151
9	6	0	1.80339	-1.53249	0.621614
10	6	0	0.7529	-1.71961	-0.40229
11	6	0	-3.53789	-0.71604	0.399155
12	6	0	-3.59424	0.53528	1.28994
13	6	0	-2.2647	1.231331	1.019599
14	6	0	3.119545	1.168669	0.596868
15	6	0	3.816036	-0.20053	0.698009
16	8	0	2.960495	-1.17603	0.016788
17	8	0	-2.38541	-2.68665	-1.25465
18	8	0	1.650072	-1.57446	1.823829
19	6	0	5.176501	-0.28578	0.028794
20	1	0	-3.25353	-0.30307	-1.72473
21	1	0	-2.81789	1.751899	-0.95708
22	8	0	-4.63243	1.442951	0.881765
23	1	0	-0.64511	1.408948	-2.14776
24	1	0	0.153151	2.146668	0.702581
25	1	0	-0.83227	-1.63565	0.956291
26	1	0	-1.13241	-1.25455	-2.09034
27	1	0	1.412153	2.784959	-2.02008
28	1	0	1.812974	3.505298	-0.46856
29	1	0	2.505299	0.688581	-1.41773
30	1	0	3.617171	2.039865	-1.3304
31	1	0	1.083757	-1.70478	-1.4346
32	1	0	-3.10775	-1.54662	0.963869
33	1	0	-4.53782	-1.03601	0.097409
34	1	0	-3.72732	0.279327	2.347298
35	1	0	-1.46779	0.719423	1.56845
36	1	0	-2.28072	2.273668	1.345119

37	1	0	2.218411	1.116944	1.214111
38	1	0	3.765742	1.919072	1.064232
39	1	0	3.890781	-0.49452	1.746244
40	1	0	-1.77548	-3.39435	-1.49198
41	1	0	5.589086	-1.292	0.128378
42	1	0	5.865019	0.41704	0.503941
43	1	0	5.112593	-0.04165	-1.03374
44	1	0	-5.47212	0.975707	0.948128

4b-Conf.7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.672446	0.403295	-0.60777
2	6	0	1.955736	-1.01845	-0.68128
3	6	0	0.513796	-1.07565	-1.12339
4	6	0	-0.46169	-1.81947	-0.59577
5	6	0	0.647772	1.832104	0.019384
6	6	0	1.845374	1.685166	-0.87504
7	6	0	-1.86575	-1.91192	-1.14851
8	6	0	-2.9709	-2.15215	-0.09758
9	6	0	-1.74379	1.609507	0.468404
10	6	0	-0.60284	1.84602	-0.44151
11	6	0	3.40242	0.41144	0.76176
12	6	0	3.576367	-1.05872	1.132553
13	6	0	2.256444	-1.68258	0.679208
14	6	0	-3.19629	-1.08066	0.984565
15	6	0	-3.75418	0.284946	0.553587
16	8	0	-2.73728	1.005236	-0.21518
17	8	0	2.696647	2.843706	-0.80386
18	8	0	-1.76445	1.822758	1.662832
19	6	0	-4.998	0.240886	-0.31797
20	1	0	3.436408	0.416731	-1.38839
21	1	0	2.523093	-1.56987	-1.4399
22	8	0	4.692297	-1.55851	0.378094
23	1	0	0.277641	-0.48854	-2.00973
24	1	0	-0.2535	-2.44087	0.273916
25	1	0	0.808503	1.832198	1.094712
26	1	0	1.502785	1.670712	-1.91203
27	1	0	-2.08503	-1.02069	-1.74214
28	1	0	-1.91166	-2.76189	-1.84357
29	1	0	-3.91153	-2.33652	-0.62642
30	1	0	-2.74083	-3.08847	0.424644
31	1	0	-0.81426	1.801483	-1.50363
32	1	0	2.794768	0.887416	1.537926

33	1	0	4.363282	0.928424	0.727181
34	1	0	3.760135	-1.19835	2.203966
35	1	0	1.479556	-1.43003	1.408852
36	1	0	2.306418	-2.77323	0.618355
37	1	0	-2.27046	-0.9054	1.54114
38	1	0	-3.90841	-1.4848	1.713416
39	1	0	-3.9504	0.871027	1.452825
40	1	0	3.036743	2.915843	0.095507
41	1	0	-5.79491	-0.29847	0.19991
42	1	0	-4.80503	-0.26002	-1.26864
43	1	0	-5.34916	1.253395	-0.52744
44	1	0	4.746641	-2.50822	0.530628

4b-Conf.8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.63869	-0.3661	-0.82857
2	6	0	-2.08168	1.075332	-0.50244
3	6	0	-0.75011	1.499416	-1.07171
4	6	0	0.258378	2.040935	-0.38318
5	6	0	-0.54458	-1.63876	-0.08446
6	6	0	-1.61451	-1.47997	-1.12869
7	6	0	1.55326	2.553251	-0.96906
8	6	0	2.750558	1.580859	-0.84868
9	6	0	1.800971	-1.52732	0.629354
10	6	0	0.75081	-1.718	-0.39412
11	6	0	-3.54922	-0.71683	0.387564
12	6	0	-3.5962	0.521814	1.286685
13	6	0	-2.25964	1.218205	1.019264
14	6	0	3.121374	1.172898	0.59139
15	6	0	3.815564	-0.19696	0.698952
16	8	0	2.958315	-1.17433	0.022818
17	8	0	-2.38493	-2.69048	-1.25306
18	8	0	1.647596	-1.56403	1.83169
19	6	0	5.175589	-0.28773	0.029532
20	1	0	-3.2474	-0.30539	-1.73393
21	1	0	-2.82352	1.74806	-0.95025
22	8	0	-4.70483	1.327675	0.848632
23	1	0	-0.65604	1.41581	-2.15516
24	1	0	0.159296	2.133061	0.69558
25	1	0	-0.83842	-1.63915	0.961294
26	1	0	-1.12836	-1.26048	-2.08687
27	1	0	1.40978	2.776354	-2.03135
28	1	0	1.809956	3.502388	-0.48218

29	1	0	2.506273	0.683081	-1.42082
30	1	0	3.616212	2.036361	-1.34014
31	1	0	1.082323	-1.70276	-1.42621
32	1	0	-3.13765	-1.56093	0.943924
33	1	0	-4.55685	-1.0025	0.082343
34	1	0	-3.72866	0.260357	2.342531
35	1	0	-1.46274	0.698972	1.563008
36	1	0	-2.25894	2.260011	1.352146
37	1	0	2.221415	1.126046	1.21064
38	1	0	3.769729	1.924601	1.053622
39	1	0	3.890294	-0.48583	1.748621
40	1	0	-1.7741	-3.39937	-1.48438
41	1	0	5.865594	0.416115	0.500972
42	1	0	5.111598	-0.04859	-1.03415
43	1	0	5.586415	-1.2942	0.133694
44	1	0	-4.69667	2.141015	1.365445

4b-Conf.9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.680502	0.565943	-0.5156
2	6	0	2.250882	-0.945	-0.77079
3	6	0	0.790468	-1.18086	-1.06336
4	6	0	-0.05934	-2.01591	-0.46183
5	6	0	0.422898	1.664488	0.049166
6	6	0	1.666402	1.692705	-0.79482
7	6	0	-1.52685	-2.0966	-0.79802
8	6	0	-2.44069	-1.98412	0.449137
9	6	0	-1.97592	1.338547	0.412341
10	6	0	-0.81143	1.619903	-0.45607
11	6	0	3.285212	0.573665	0.905211
12	6	0	3.894632	-0.81719	1.049832
13	6	0	2.818613	-1.72217	0.442616
14	6	0	-3.85783	-1.45173	0.139642
15	6	0	-4.03317	0.053531	0.379148
16	8	0	-2.95357	0.757572	-0.31702
17	8	0	2.387633	2.916796	-0.55424
18	8	0	-2.02655	1.520702	1.611105
19	6	0	-5.35157	0.604466	-0.13909
20	1	0	3.500524	0.775236	-1.20616
21	1	0	2.797338	-1.25843	-1.66732
22	8	0	5.110905	-0.8312	0.284183
23	1	0	0.399265	-0.59048	-1.88998
24	1	0	0.279124	-2.65124	0.354018

25	1	0	0.549973	1.647545	1.127661
26	1	0	1.375666	1.645959	-1.8519
27	1	0	-1.77154	-1.30037	-1.50524
28	1	0	-1.75458	-3.04388	-1.30459
29	1	0	-2.51499	-2.9679	0.921481
30	1	0	-1.96723	-1.33524	1.1928
31	1	0	-0.9867	1.60066	-1.5259
32	1	0	2.513501	0.697047	1.670723
33	1	0	4.022103	1.365448	1.042809
34	1	0	4.111091	-1.07461	2.093217
35	1	0	2.042114	-1.87318	1.19842
36	1	0	3.202908	-2.70921	0.171225
37	1	0	-4.59607	-1.95186	0.774548
38	1	0	-4.12989	-1.68873	-0.89522
39	1	0	-3.92059	0.273454	1.44109
40	1	0	1.799474	3.647636	-0.7763
41	1	0	-6.18638	0.090268	0.343778
42	1	0	-5.43466	0.456625	-1.21899
43	1	0	-5.43671	1.672017	0.074841
44	1	0	5.442008	-1.7357	0.277627

4b-Conf.10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.671663	0.409583	-0.60115
2	6	0	1.962026	-1.01482	-0.69592
3	6	0	0.516136	-1.07203	-1.12817
4	6	0	-0.45288	-1.82509	-0.60215
5	6	0	0.641985	1.824382	0.026298
6	6	0	1.837112	1.680088	-0.86994
7	6	0	-1.85916	-1.91711	-1.1487
8	6	0	-2.95997	-2.16005	-0.09389
9	6	0	-1.75122	1.612986	0.470564
10	6	0	-0.60813	1.848283	-0.43687
11	6	0	3.386405	0.414137	0.775365
12	6	0	3.578189	-1.06272	1.136256
13	6	0	2.2743	-1.70197	0.653298
14	6	0	-3.18669	-1.08768	0.987036
15	6	0	-3.75237	0.274716	0.555423
16	8	0	-2.73913	0.999748	-0.21361
17	8	0	2.747083	2.779938	-0.69512
18	8	0	-1.77716	1.833	1.663492
19	6	0	-4.99621	0.223569	-0.31569
20	1	0	3.439528	0.439787	-1.37976

21	1	0	2.513374	-1.55265	-1.47878
22	8	0	4.741189	-1.63877	0.519483
23	1	0	0.273114	-0.47746	-2.00727
24	1	0	-0.23733	-2.4558	0.258839
25	1	0	0.809365	1.824524	1.099423
26	1	0	1.49196	1.656156	-1.91093
27	1	0	-2.08152	-1.02558	-1.74068
28	1	0	-1.90631	-2.76643	-1.84447
29	1	0	-3.90134	-2.34896	-0.61973
30	1	0	-2.7247	-3.09468	0.428982
31	1	0	-0.8175	1.809439	-1.49977
32	1	0	2.757884	0.880303	1.539481
33	1	0	4.332423	0.955937	0.755819
34	1	0	3.738089	-1.20817	2.205828
35	1	0	1.484956	-1.47671	1.377858
36	1	0	2.354656	-2.78792	0.571695
37	1	0	-2.25993	-0.90708	1.540455
38	1	0	-3.89464	-1.49383	1.718767
39	1	0	-3.95142	0.860133	1.454403
40	1	0	2.268649	3.588387	-0.9113
41	1	0	-5.78985	-0.32006	0.20273
42	1	0	-4.80093	-0.27652	-1.2663
43	1	0	-5.35308	1.234056	-0.52522
44	1	0	4.671535	-1.52575	-0.4347

4b-Conf.11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.677985	0.557373	-0.52334
2	6	0	2.228179	-0.95342	-0.75647
3	6	0	0.769429	-1.17758	-1.06434
4	6	0	-0.08641	-2.01151	-0.46996
5	6	0	0.439993	1.688626	0.051651
6	6	0	1.678757	1.708904	-0.79703
7	6	0	-1.55185	-2.09177	-0.81451
8	6	0	-2.47055	-1.98693	0.43026
9	6	0	-1.95429	1.330535	0.421758
10	6	0	-0.79322	1.619606	-0.44952
11	6	0	3.306068	0.574168	0.888306
12	6	0	3.875744	-0.83058	1.056609
13	6	0	2.769443	-1.71586	0.477143
14	6	0	-3.87893	-1.43034	0.124852
15	6	0	-4.02987	0.074962	0.379473
16	8	0	-2.93988	0.768339	-0.31087

17	8	0	2.319497	2.970832	-0.53369
18	8	0	-1.99735	1.496445	1.623121
19	6	0	-5.33951	0.652559	-0.13207
20	1	0	3.493064	0.737669	-1.23183
21	1	0	2.783592	-1.29078	-1.6386
22	8	0	5.083333	-0.89503	0.279828
23	1	0	0.388698	-0.58578	-1.8947
24	1	0	0.246181	-2.64649	0.348665
25	1	0	0.570248	1.680253	1.1298
26	1	0	1.379193	1.668533	-1.85172
27	1	0	-1.79387	-1.29216	-1.51879
28	1	0	-1.7761	-3.03651	-1.32721
29	1	0	-2.56011	-2.97694	0.886579
30	1	0	-1.99192	-1.35624	1.186205
31	1	0	-0.97213	1.597018	-1.51836
32	1	0	2.549674	0.73993	1.660853
33	1	0	4.070458	1.343781	1.001594
34	1	0	4.094889	-1.07209	2.103153
35	1	0	1.988043	-1.81849	1.236203
36	1	0	3.11948	-2.72265	0.23324
37	1	0	-4.62502	-1.92501	0.754845
38	1	0	-4.15436	-1.6528	-0.91232
39	1	0	-3.91288	0.282262	1.443459
40	1	0	3.15987	2.975137	-1.00699
41	1	0	-6.18218	0.148268	0.347567
42	1	0	-5.42642	0.515504	-1.21311
43	1	0	-5.40641	1.719487	0.091222
44	1	0	5.387434	-1.80899	0.286147

4b-Conf.12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.63507	-0.35925	-0.82445
2	6	0	-2.06401	1.078466	-0.50128
3	6	0	-0.73208	1.491951	-1.07722
4	6	0	0.280447	2.032561	-0.39397
5	6	0	-0.55944	-1.65486	-0.08128
6	6	0	-1.62682	-1.49742	-1.12608
7	6	0	1.57485	2.539476	-0.9855
8	6	0	2.770817	1.566015	-0.86122
9	6	0	1.782107	-1.51584	0.637797
10	6	0	0.735792	-1.7273	-0.38675
11	6	0	-3.55037	-0.6978	0.391168
12	6	0	-3.57847	0.540065	1.292506

13	6	0	-2.23492	1.221271	1.021027
14	6	0	3.142125	1.165441	0.581123
15	6	0	3.815658	-0.21376	0.698002
16	8	0	2.943643	-1.18336	0.029621
17	8	0	-2.31824	-2.7564	-1.21315
18	8	0	1.621828	-1.52474	1.839709
19	6	0	5.173495	-0.32981	0.027923
20	1	0	-3.2434	-0.28203	-1.73141
21	1	0	-2.8025	1.757471	-0.94516
22	8	0	-4.67914	1.359219	0.859609
23	1	0	-0.64237	1.40361	-2.16061
24	1	0	0.184754	2.12893	0.684715
25	1	0	-0.85395	-1.6388	0.963995
26	1	0	-1.13713	-1.28753	-2.08442
27	1	0	1.429662	2.756574	-2.0488
28	1	0	1.833636	3.491101	-0.50459
29	1	0	2.523986	0.665718	-1.42823
30	1	0	3.636712	2.017134	-1.35618
31	1	0	1.070977	-1.73029	-1.41745
32	1	0	-3.14997	-1.54981	0.9439
33	1	0	-4.56345	-0.96732	0.088345
34	1	0	-3.71013	0.278258	2.348277
35	1	0	-1.44166	0.693179	1.561339
36	1	0	-2.22197	2.26271	1.354698
37	1	0	2.244768	1.137862	1.205001
38	1	0	3.804196	1.91104	1.033587
39	1	0	3.887005	-0.49608	1.749663
40	1	0	-3.05252	-2.64304	-1.82864
41	1	0	5.874623	0.366418	0.494211
42	1	0	5.112319	-0.09674	-1.03731
43	1	0	5.568864	-1.34178	0.138359
44	1	0	-4.66183	2.170391	1.379568

4b-Conf.13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.67155	0.551038	-0.51003
2	6	0	2.230267	-0.95618	-0.77551
3	6	0	0.76725	-1.18065	-1.06419
4	6	0	-0.08339	-2.01811	-0.46737
5	6	0	0.435494	1.694776	0.041569
6	6	0	1.680872	1.706157	-0.79761
7	6	0	-1.55131	-2.09472	-0.80208
8	6	0	-2.46313	-1.98122	0.446719

9	6	0	-1.95843	1.340433	0.408775
10	6	0	-0.79556	1.619352	-0.4638
11	6	0	3.263316	0.545367	0.915006
12	6	0	3.867646	-0.85439	1.052585
13	6	0	2.798768	-1.7476	0.429601
14	6	0	-3.87443	-1.43138	0.142466
15	6	0	-4.02845	0.076066	0.382216
16	8	0	-2.9412	0.764974	-0.31722
17	8	0	2.324902	2.965834	-0.53091
18	8	0	-2.00436	1.523858	1.607461
19	6	0	-5.34069	0.645445	-0.13177
20	1	0	3.50667	0.737897	-1.19337
21	1	0	2.769693	-1.26663	-1.67722
22	8	0	5.064588	-0.99583	0.26926
23	1	0	0.377063	-0.58394	-1.8865
24	1	0	0.25504	-2.66041	0.34296
25	1	0	0.559745	1.699271	1.120417
26	1	0	1.391222	1.664287	-1.85503
27	1	0	-1.79492	-1.29741	-1.50837
28	1	0	-1.78153	-3.04103	-1.30922
29	1	0	-2.54771	-2.96726	0.912511
30	1	0	-1.98226	-1.34225	1.194299
31	1	0	-0.97151	1.584036	-1.53276
32	1	0	2.482747	0.66565	1.673128
33	1	0	3.995438	1.340521	1.071558
34	1	0	4.074531	-1.12039	2.095527
35	1	0	2.021505	-1.91339	1.179898
36	1	0	3.199222	-2.72284	0.145332
37	1	0	-4.61628	-1.92149	0.78099
38	1	0	-4.15398	-1.6655	-0.89104
39	1	0	-3.90949	0.294324	1.44378
40	1	0	3.163922	2.970141	-1.00656
41	1	0	-6.18096	0.143134	0.354132
42	1	0	-5.42949	0.498527	-1.21134
43	1	0	-5.41012	1.714124	0.082197
44	1	0	5.711331	-0.3663	0.606559

Table S18. The coordinate for the lowest-energy conformer [(2*E*, 4*R**, 5*S**, 7*R**, 9*S**, 10*E*, 15*S**)-**4a**] in ECD calculation

4a-Conf.1

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-2.75113	0.390158	-1.01451
2	6	0	-1.77185	1.526712	-0.55077
3	6	0	-0.36715	1.518557	-1.11011
4	6	0	0.731125	1.928262	-0.47143
5	6	0	-1.09999	-1.4399	-0.27987
6	6	0	-2.15387	-1.02449	-1.26421
7	6	0	2.132858	1.908202	-1.03866
8	6	0	3.252285	1.847949	0.023924
9	6	0	1.284098	-1.62691	0.298992
10	6	0	0.16652	-1.60755	-0.66509
11	6	0	-3.85004	0.454446	0.068666
12	6	0	-3.17083	0.843709	1.394299
13	6	0	-1.85997	1.548947	0.997831
14	6	0	3.247056	0.681032	1.029434
15	6	0	3.518873	-0.73906	0.511629
16	8	0	2.399946	-1.18112	-0.31878
17	8	0	-3.25865	-1.94356	-1.28086
18	8	0	1.218844	-1.90292	1.479113
19	6	0	4.769664	-0.89662	-0.3368
20	1	0	-3.18753	0.66972	-1.97743
21	1	0	-2.25449	2.445076	-0.91289
22	8	0	-2.82043	-0.29934	2.199904
23	1	0	-0.26701	1.159659	-2.13422
24	1	0	0.638618	2.311176	0.543471
25	1	0	-1.38147	-1.48091	0.767791
26	1	0	-1.69254	-1.00599	-2.25936
27	1	0	2.228201	1.079342	-1.74533
28	1	0	2.302797	2.825204	-1.61909
29	1	0	4.217631	1.884449	-0.49112
30	1	0	3.201575	2.770029	0.615256
31	1	0	0.446905	-1.51083	-1.70814
32	1	0	-4.42034	-0.47096	0.151962
33	1	0	-4.55292	1.247246	-0.20706
34	1	0	-3.82209	1.495784	1.986103
35	1	0	-1.81125	2.56779	1.386908
36	1	0	-1.03103	0.993956	1.442424
37	1	0	2.299773	0.661189	1.576516
38	1	0	4.01851	0.884431	1.781246
39	1	0	3.564889	-1.40967	1.371578
40	1	0	-2.91252	-2.80249	-1.54785
41	1	0	4.913151	-1.94412	-0.60996
42	1	0	5.645281	-0.56591	0.227278
43	1	0	4.708958	-0.30766	-1.25437
44	1	0	-3.63674	-0.7617	2.421183

4a-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.684026	0.408163	-0.85311
2	6	0	1.927868	-0.98635	-1.04023
3	6	0	0.460403	-0.9652	-1.39522
4	6	0	-0.50306	-1.73202	-0.87947
5	6	0	0.734867	1.77736	0.06117
6	6	0	1.863785	1.713965	-0.92508
7	6	0	-1.9402	-1.73764	-1.34896
8	6	0	-2.98497	-2.07777	-0.2646
9	6	0	-1.62884	1.567971	0.642991
10	6	0	-0.54183	1.879811	-0.30901
11	6	0	3.494141	0.254917	0.454275
12	6	0	3.658052	-1.25769	0.639947
13	6	0	2.294789	-1.80597	0.211256
14	6	0	-3.1187	-1.13573	0.945772
15	6	0	-3.66445	0.281817	0.713672
16	8	0	-2.68065	1.065026	-0.03594
17	8	0	2.808477	2.773722	-0.6942
18	8	0	-1.56785	1.647038	1.852229
19	6	0	-4.96512	0.365764	-0.06711
20	1	0	3.395571	0.499073	-1.67853
21	1	0	2.428974	-1.45796	-1.89564
22	8	0	4.080786	-1.65397	1.942842
23	1	0	0.191479	-0.28983	-2.20613
24	1	0	-0.25999	-2.43813	-0.08679
25	1	0	0.972737	1.649562	1.113152
26	1	0	1.449917	1.810111	-1.93649
27	1	0	-2.17457	-0.78133	-1.82359
28	1	0	-2.04805	-2.50223	-2.13083
29	1	0	-3.9596	-2.18559	-0.75141
30	1	0	-2.7461	-3.0718	0.131946
31	1	0	-0.82197	1.967941	-1.35254
32	1	0	2.932838	0.639823	1.313631
33	1	0	4.445035	0.787413	0.424304
34	1	0	4.437455	-1.63468	-0.03005
35	1	0	2.306465	-2.88274	0.030153
36	1	0	1.576447	-1.61021	1.017343
37	1	0	-2.15736	-1.04525	1.460878
38	1	0	-3.79659	-1.6091	1.665495
39	1	0	-3.78245	0.763269	1.68573
40	1	0	2.335076	3.608355	-0.78617

41	1	0	-5.3006	1.40283	-0.13327
42	1	0	-5.74013	-0.21354	0.440836
43	1	0	-4.85301	-0.02422	-1.08074
44	1	0	3.417695	-1.34469	2.57138

4a-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.64987	0.352897	-1.15051
2	6	0	-1.71225	1.45864	-0.5584
3	6	0	-0.25476	1.460875	-0.94602
4	6	0	0.769608	1.938497	-0.23647
5	6	0	-0.97824	-1.42836	-0.25035
6	6	0	-2.20305	-1.16893	-1.07777
7	6	0	2.188694	2.0192	-0.75134
8	6	0	3.294692	1.8635	0.312195
9	6	0	1.400539	-1.63079	0.184047
10	6	0	0.243746	-1.64573	-0.73573
11	6	0	-3.93592	0.656213	-0.35364
12	6	0	-3.46308	0.867747	1.087925
13	6	0	-2.05747	1.509124	0.954771
14	6	0	3.340472	0.559875	1.127856
15	6	0	3.631085	-0.75666	0.391469
16	8	0	2.486409	-1.13465	-0.44165
17	8	0	-3.25293	-2.03436	-0.62877
18	8	0	1.374653	-1.93885	1.35892
19	6	0	4.837858	-0.7377	-0.5316
20	1	0	-2.81559	0.564432	-2.20955
21	1	0	-2.12655	2.379219	-0.99485
22	8	0	-3.41414	-0.44345	1.697872
23	1	0	-0.04905	1.093812	-1.95122
24	1	0	0.594531	2.333834	0.763791
25	1	0	-1.11158	-1.38565	0.826408
26	1	0	-1.99887	-1.48666	-2.10216
27	1	0	2.322847	1.287838	-1.55301
28	1	0	2.339016	3.006138	-1.21098
29	1	0	4.261451	2.023784	-0.1763
30	1	0	3.19145	2.683836	1.032607
31	1	0	0.451708	-1.64368	-1.80013
32	1	0	-4.70295	-0.11332	-0.42548
33	1	0	-4.36486	1.590211	-0.7275
34	1	0	-4.15258	1.491093	1.664114
35	1	0	-2.0511	2.534214	1.331584
36	1	0	-1.33064	0.946044	1.546541

37	1	0	2.408787	0.431993	1.685097
38	1	0	4.126847	0.665944	1.884316
39	1	0	3.748334	-1.54178	1.14075
40	1	0	-3.43129	-1.7803	0.292438
41	1	0	4.713987	-0.01549	-1.34109
42	1	0	4.993821	-1.72475	-0.97183
43	1	0	5.733104	-0.46924	0.034748
44	1	0	-3.01511	-0.37129	2.57207

4a-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.154065	-0.15366	1.29109
2	6	0	1.791577	1.214122	0.623665
3	6	0	0.342571	1.467952	0.288424
4	6	0	-0.17419	1.634073	-0.92797
5	6	0	0.18037	-1.51146	0.542462
6	6	0	1.67462	-1.4716	0.603274
7	6	0	-1.61446	1.842517	-1.32815
8	6	0	-2.66798	2.320074	-0.30728
9	6	0	-1.98622	-1.58947	-0.62574
10	6	0	-0.54899	-1.89883	-0.50828
11	6	0	3.692169	-0.04015	1.348546
12	6	0	4.117786	0.65576	0.040158
13	6	0	2.84277	1.361305	-0.49617
14	6	0	-3.22862	1.360784	0.766827
15	6	0	-3.63334	-0.04555	0.304094
16	8	0	-2.42537	-0.85556	0.416393
17	8	0	2.186052	-1.71706	-0.69856
18	8	0	-2.67062	-1.87384	-1.59121
19	6	0	-4.71834	-0.68081	1.162901
20	1	0	1.739517	-0.19562	2.303124
21	1	0	2.053395	1.951834	1.396143
22	8	0	4.59702	-0.37746	-0.85414
23	1	0	-0.31509	1.515055	1.153576
24	1	0	0.497621	1.571824	-1.78268
25	1	0	-0.33121	-1.12535	1.416366
26	1	0	2.006005	-2.27357	1.287771
27	1	0	-1.61155	2.585572	-2.13564
28	1	0	-1.96242	0.924624	-1.82234
29	1	0	-2.28355	3.20933	0.204906
30	1	0	-3.52137	2.666692	-0.90087
31	1	0	-0.08881	-2.30538	-1.39913
32	1	0	4.208657	-0.99548	1.469013

33	1	0	3.969994	0.588595	2.197847
34	1	0	4.934429	1.361629	0.210751
35	1	0	3.02278	2.4059	-0.75866
36	1	0	2.515162	0.838632	-1.39734
37	1	0	-4.11274	1.845824	1.193608
38	1	0	-2.52664	1.234822	1.595819
39	1	0	-3.94012	-0.05334	-0.74365
40	1	0	3.122506	-1.45287	-0.74846
41	1	0	-5.6466	-0.1101	1.079629
42	1	0	-4.418	-0.70026	2.214184
43	1	0	-4.91404	-1.70485	0.837547
44	1	0	4.762559	0.017598	-1.71851

4a-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.086962	-0.14607	1.168182
2	6	0	1.949462	1.211	0.404278
3	6	0	0.675474	1.487778	-0.34587
4	6	0	-0.20651	2.437426	-0.02072
5	6	0	0.048899	-1.43787	0.452791
6	6	0	1.547137	-1.4305	0.47823
7	6	0	-1.45984	2.781149	-0.80751
8	6	0	-2.47168	1.627438	-0.96428
9	6	0	-2.16763	-1.66991	-0.60634
10	6	0	-0.71222	-1.90392	-0.54223
11	6	0	3.606735	-0.18999	1.436339
12	6	0	4.282717	0.363259	0.17418
13	6	0	3.223773	1.283506	-0.48624
14	6	0	-3.24122	1.283663	0.323617
15	6	0	-3.79817	-0.1437	0.356518
16	8	0	-2.64088	-1.02906	0.486213
17	8	0	2.031465	-1.6632	-0.83502
18	8	0	-2.8514	-1.95702	-1.56985
19	6	0	-4.71478	-0.4183	1.537026
20	1	0	1.547235	-0.08316	2.118036
21	1	0	2.046441	1.980606	1.178828
22	8	0	4.624468	-0.77152	-0.66048
23	1	0	0.50609	0.878406	-1.23152
24	1	0	-0.00779	3.038396	0.865592
25	1	0	-0.4373	-1.00068	1.317216
26	1	0	1.854102	-2.25871	1.143783
27	1	0	-1.95559	3.637102	-0.33862
28	1	0	-1.16785	3.115953	-1.80965

29	1	0	-3.18984	1.886192	-1.74968
30	1	0	-1.92994	0.751795	-1.32872
31	1	0	-0.27799	-2.35604	-1.42449
32	1	0	3.988485	-1.18249	1.687917
33	1	0	3.835346	0.471944	2.275893
34	1	0	5.206195	0.897484	0.410144
35	1	0	3.577811	2.311934	-0.58446
36	1	0	3.006546	0.91441	-1.49194
37	1	0	-4.07039	1.987575	0.453553
38	1	0	-2.59004	1.398694	1.197122
39	1	0	-4.30051	-0.39266	-0.58009
40	1	0	2.999917	-1.54292	-0.83678
41	1	0	-5.0358	-1.46211	1.540215
42	1	0	-5.60336	0.214755	1.476989
43	1	0	-4.2053	-0.20829	2.481411
44	1	0	4.999658	-0.44159	-1.48564

4a-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.174662	-0.11841	1.305149
2	6	0	1.779795	1.229621	0.610009
3	6	0	0.320993	1.479531	0.310746
4	6	0	-0.21322	1.653077	-0.89751
5	6	0	0.192973	-1.48424	0.557367
6	6	0	1.684168	-1.46082	0.691534
7	6	0	-1.65393	1.879646	-1.28444
8	6	0	-2.70393	2.320937	-0.24542
9	6	0	-1.94387	-1.5706	-0.65981
10	6	0	-0.50601	-1.87478	-0.51151
11	6	0	3.712992	-0.00915	1.300051
12	6	0	4.101114	0.693999	-0.03169
13	6	0	2.790724	1.355316	-0.54257
14	6	0	-3.25825	1.319103	0.792685
15	6	0	-3.63453	-0.07813	0.280619
16	8	0	-2.41479	-0.87288	0.390598
17	8	0	2.345337	-1.73466	-0.55372
18	8	0	-2.59782	-1.83692	-1.65033
19	6	0	-4.72209	-0.75621	1.102275
20	1	0	1.787611	-0.12423	2.328534
21	1	0	2.062679	1.983703	1.359508
22	8	0	4.669321	-0.2004	-0.99024
23	1	0	-0.32051	1.530437	1.188157
24	1	0	0.447957	1.588349	-1.76013

25	1	0	-0.34746	-1.08606	1.408501
26	1	0	1.979941	-2.22839	1.421398
27	1	0	-1.65066	2.650788	-2.06541
28	1	0	-2.00565	0.981249	-1.81051
29	1	0	-2.31998	3.191258	0.298545
30	1	0	-3.55936	2.687453	-0.82374
31	1	0	-0.03323	-2.28468	-1.39524
32	1	0	4.223255	-0.97003	1.392312
33	1	0	4.023486	0.61021	2.146267
34	1	0	4.876587	1.441022	0.146814
35	1	0	2.936904	2.392751	-0.85232
36	1	0	2.454625	0.79498	-1.41821
37	1	0	-4.15311	1.774879	1.228826
38	1	0	-2.5594	1.177	1.621683
39	1	0	-3.92292	-0.06041	-0.77215
40	1	0	2.312708	-2.68382	-0.71627
41	1	0	-5.65787	-0.19782	1.020246
42	1	0	-4.4383	-0.80145	2.1573
43	1	0	-4.89617	-1.77314	0.744088
44	1	0	4.012903	-0.90848	-1.08364

4a-Conf.7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.84244	0.092438	-1.04712
2	6	0	-2.10844	1.424178	-0.64833
3	6	0	-0.6723	1.561926	-1.09892
4	6	0	0.311101	2.167972	-0.43144
5	6	0	-0.87238	-1.36282	-0.17532
6	6	0	-1.98623	-1.2024	-1.17282
7	6	0	1.767734	2.140655	-0.82318
8	6	0	2.690358	1.865039	0.396683
9	6	0	1.535886	-1.35068	0.359283
10	6	0	0.397016	-1.47368	-0.57395
11	6	0	-3.98908	0.029858	-0.01542
12	6	0	-3.45409	0.621597	1.296213
13	6	0	-2.33568	1.594646	0.880654
14	6	0	3.952792	1.030676	0.086197
15	6	0	3.801805	-0.46397	0.390133
16	8	0	2.630238	-0.95808	-0.33248
17	8	0	-2.89989	-2.31123	-1.10026
18	8	0	1.498538	-1.50119	1.562851
19	6	0	4.996472	-1.29998	-0.04171
20	1	0	-3.2765	0.21686	-2.04282

21	1	0	-2.6895	2.207925	-1.15213
22	8	0	-2.86064	-0.3753	2.152618
23	1	0	-0.43085	1.095454	-2.05304
24	1	0	0.090882	2.659398	0.514711
25	1	0	-1.13173	-1.31781	0.877794
26	1	0	-1.53306	-1.18605	-2.17152
27	1	0	1.915153	1.371758	-1.58595
28	1	0	2.069173	3.092654	-1.27869
29	1	0	2.987283	2.822368	0.833974
30	1	0	2.115525	1.353757	1.175604
31	1	0	0.650869	-1.47086	-1.62858
32	1	0	-4.39388	-0.97399	0.113523
33	1	0	-4.80423	0.667444	-0.37399
34	1	0	-4.25075	1.126421	1.853316
35	1	0	-2.5871	2.627266	1.130432
36	1	0	-1.43738	1.335261	1.44386
37	1	0	4.793992	1.385083	0.69059
38	1	0	4.247645	1.161372	-0.96116
39	1	0	3.604568	-0.60514	1.45356
40	1	0	-2.39832	-3.10805	-1.30674
41	1	0	5.153524	-1.22214	-1.1207
42	1	0	4.845838	-2.35118	0.213481
43	1	0	5.900054	-0.95046	0.464067
44	1	0	-3.54233	-1.02367	2.362816

4a-Conf.8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.72063	0.441172	-0.98289
2	6	0	-1.95938	1.580781	-0.22082
3	6	0	-0.59769	2.004313	-0.71913
4	6	0	0.48061	2.20701	0.042298
5	6	0	-0.91335	-1.33179	-0.47506
6	6	0	-1.8993	-0.78065	-1.4669
7	6	0	1.834614	2.670797	-0.43562
8	6	0	2.889698	1.542859	-0.54816
9	6	0	1.428958	-1.65278	0.229726
10	6	0	0.376783	-1.46957	-0.7912
11	6	0	-3.85325	0.10441	0.012869
12	6	0	-3.29975	0.317976	1.438209
13	6	0	-2.04496	1.196695	1.273363
14	6	0	3.165119	0.768427	0.757811
15	6	0	3.624873	-0.68542	0.544278
16	8	0	2.630869	-1.33614	-0.31064

17	8	0	-2.85911	-1.78301	-1.84964
18	8	0	1.26327	-1.93308	1.398116
19	6	0	4.962072	-0.84351	-0.15843
20	1	0	-3.15651	0.850508	-1.89867
21	1	0	-2.6129	2.454445	-0.35989
22	8	0	-2.8889	-0.90718	2.07514
23	1	0	-0.53293	2.211802	-1.78786
24	1	0	0.403281	2.013703	1.108851
25	1	0	-1.26971	-1.54735	0.527582
26	1	0	-1.33946	-0.46495	-2.35588
27	1	0	1.737496	3.141081	-1.41957
28	1	0	2.207049	3.444624	0.247558
29	1	0	2.54282	0.841623	-1.31041
30	1	0	3.820703	1.977444	-0.92557
31	1	0	0.730939	-1.23363	-1.78862
32	1	0	-4.2523	-0.90089	-0.12514
33	1	0	-4.67584	0.806659	-0.1538
34	1	0	-4.05095	0.800992	2.071944
35	1	0	-2.06871	2.079616	1.915257
36	1	0	-1.18179	0.600728	1.577497
37	1	0	2.260067	0.728001	1.369365
38	1	0	3.918365	1.282963	1.363503
39	1	0	3.63685	-1.20693	1.502868
40	1	0	-2.36906	-2.51347	-2.24376
41	1	0	5.20365	-1.90069	-0.2874
42	1	0	5.750326	-0.38086	0.44032
43	1	0	4.951916	-0.36877	-1.14194
44	1	0	-3.6689	-1.4657	2.167902

4a-Conf.9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.273452	-0.12911	1.326166
2	6	0	1.937041	1.246	0.6648
3	6	0	0.510666	1.729276	0.597152
4	6	0	-0.17208	2.089022	-0.49126
5	6	0	0.157147	-1.36623	0.589958
6	6	0	1.645161	-1.43511	0.758368
7	6	0	-1.53715	2.73459	-0.50559
8	6	0	-2.70135	1.782282	-0.89603
9	6	0	-1.94954	-1.56395	-0.69983
10	6	0	-0.50604	-1.78282	-0.49247
11	6	0	3.809797	-0.13904	1.172133
12	6	0	4.113157	0.538088	-0.20076

13	6	0	2.790415	1.244783	-0.61124
14	6	0	-3.46912	1.196712	0.314699
15	6	0	-3.81323	-0.28894	0.203129
16	8	0	-2.54695	-1.00335	0.368694
17	8	0	2.293647	-1.83382	-0.46122
18	8	0	-2.51725	-1.81517	-1.74608
19	6	0	-4.75889	-0.78391	1.285585
20	1	0	1.980261	-0.10621	2.37996
21	1	0	2.420925	1.959257	1.350835
22	8	0	4.580266	-0.37842	-1.18978
23	1	0	0.045913	1.889669	1.570924
24	1	0	0.276179	1.92985	-1.47099
25	1	0	-0.39526	-0.94207	1.420965
26	1	0	1.856723	-2.19621	1.523463
27	1	0	-1.74721	3.182633	0.471098
28	1	0	-1.5059	3.562844	-1.22195
29	1	0	-3.41015	2.321408	-1.53064
30	1	0	-2.303	0.977083	-1.51916
31	1	0	0.009214	-2.20705	-1.34459
32	1	0	4.249816	-1.13663	1.212946
33	1	0	4.250378	0.449635	1.981139
34	1	0	4.920264	1.264767	-0.08935
35	1	0	2.958163	2.250364	-1.00382
36	1	0	2.313842	0.656271	-1.40013
37	1	0	-4.39596	1.758344	0.467955
38	1	0	-2.88088	1.317309	1.230348
39	1	0	-4.20363	-0.53413	-0.78549
40	1	0	2.200327	-2.78734	-0.56093
41	1	0	-4.91611	-1.861	1.196899
42	1	0	-5.7271	-0.28626	1.192038
43	1	0	-4.35693	-0.57193	2.280113
44	1	0	3.905859	-1.0745	-1.21353

4a-Conf.10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.678761	0.391628	-0.85677
2	6	0	1.903697	-0.99507	-1.03485
3	6	0	0.439336	-0.95893	-1.40081
4	6	0	-0.53195	-1.71988	-0.89109
5	6	0	0.759447	1.795025	0.064882
6	6	0	1.884266	1.723217	-0.92224
7	6	0	-1.96737	-1.71593	-1.36532
8	6	0	-3.01553	-2.05516	-0.28395

9	6	0	-1.60225	1.558356	0.650639
10	6	0	-0.51802	1.875029	-0.30386
11	6	0	3.499372	0.229751	0.443665
12	6	0	3.628245	-1.28435	0.645639
13	6	0	2.251451	-1.80562	0.227527
14	6	0	-3.13542	-1.12438	0.936407
15	6	0	-3.65792	0.303776	0.718112
16	8	0	-2.66306	1.075928	-0.02825
17	8	0	2.762005	2.82656	-0.64455
18	8	0	-1.53366	1.622162	1.860344
19	6	0	-4.9592	0.415924	-0.05827
20	1	0	3.383396	0.460243	-1.69308
21	1	0	2.405286	-1.4828	-1.88094
22	8	0	4.047181	-1.67487	1.951164
23	1	0	0.181255	-0.28103	-2.21303
24	1	0	-0.29682	-2.42763	-0.09753
25	1	0	1.000309	1.675583	1.117094
26	1	0	1.469158	1.833589	-1.93134
27	1	0	-2.19558	-0.75614	-1.83591
28	1	0	-2.07767	-2.47635	-2.15089
29	1	0	-3.99193	-2.14595	-0.77065
30	1	0	-2.7882	-3.0561	0.101879
31	1	0	-0.802	1.95998	-1.34627
32	1	0	2.955828	0.63925	1.30292
33	1	0	4.464556	0.735804	0.402972
34	1	0	4.395834	-1.68695	-0.02304
35	1	0	2.237607	-2.88472	0.061179
36	1	0	1.538441	-1.58146	1.030951
37	1	0	-2.17279	-1.0541	1.452172
38	1	0	-3.82087	-1.59449	1.651057
39	1	0	-3.76477	0.779275	1.694408
40	1	0	3.520665	2.753411	-1.23556
41	1	0	-4.85719	0.029571	-1.07439
42	1	0	-5.27599	1.459272	-0.11748
43	1	0	-5.743	-0.15215	0.448881
44	1	0	3.393209	-1.34471	2.578669

4a-Conf.11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.671436	0.807871	-0.39082
2	6	0	2.429237	-0.45969	-1.28101
3	6	0	0.977362	-0.85704	-1.40184
4	6	0	0.298755	-1.8017	-0.74772

5	6	0	0.443793	1.942699	0.128805
6	6	0	1.754423	2.034392	-0.59868
7	6	0	-1.17983	-2.02121	-0.94473
8	6	0	-2.00916	-1.97918	0.363132
9	6	0	-1.91975	1.406729	0.388685
10	6	0	-0.74935	1.772258	-0.44235
11	6	0	2.741497	0.23158	1.033516
12	6	0	3.49592	-1.10583	0.883589
13	6	0	3.36153	-1.49417	-0.60799
14	6	0	-3.48868	-1.59751	0.129082
15	6	0	-3.80509	-0.11273	0.356946
16	8	0	-2.79685	0.687066	-0.34498
17	8	0	2.501261	3.16025	-0.09984
18	8	0	-2.04343	1.639465	1.573046
19	6	0	-5.17324	0.305934	-0.15597
20	1	0	3.668241	1.178191	-0.65818
21	1	0	2.782904	-0.24044	-2.29402
22	8	0	2.941547	-2.15702	1.689333
23	1	0	0.419536	-0.25902	-2.12037
24	1	0	0.801371	-2.42385	-0.00936
25	1	0	0.502836	1.961475	1.213253
26	1	0	1.576101	2.158404	-1.67469
27	1	0	-1.55427	-1.2583	-1.63183
28	1	0	-1.35838	-2.99094	-1.42845
29	1	0	-1.95505	-2.95641	0.851417
30	1	0	-1.55724	-1.27225	1.065982
31	1	0	-0.87103	1.712223	-1.51738
32	1	0	1.737902	0.000088	1.400817
33	1	0	3.212898	0.914004	1.74386
34	1	0	4.552564	-0.98139	1.147199
35	1	0	4.342843	-1.45819	-1.08673
36	1	0	2.994636	-2.51739	-0.69871
37	1	0	-4.13804	-2.15714	0.80985
38	1	0	-3.78829	-1.88261	-0.88592
39	1	0	-3.71002	0.124214	1.416654
40	1	0	1.961799	3.94938	-0.22548
41	1	0	-5.36415	1.358979	0.06167
42	1	0	-5.95114	-0.29068	0.32723
43	1	0	-5.24453	0.153528	-1.23605
44	1	0	3.02517	-1.89429	2.612806

4a-Conf.12

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-2.64615	-0.16182	-1.05553
2	6	0	-2.03019	1.255609	-0.70222
3	6	0	-0.64156	1.598452	-1.18438
4	6	0	0.345392	2.09809	-0.43594
5	6	0	-0.65333	-1.54114	-0.22467
6	6	0	-1.6681	-1.32681	-1.31299
7	6	0	1.697522	2.542628	-0.94389
8	6	0	2.832225	1.50437	-0.77871
9	6	0	1.653923	-1.57143	0.600472
10	6	0	0.647323	-1.7014	-0.4753
11	6	0	-3.62945	-0.46065	0.110862
12	6	0	-3.69046	0.81203	0.974138
13	6	0	-2.30374	1.436305	0.797901
14	6	0	3.104412	1.056548	0.671029
15	6	0	3.724787	-0.3471	0.790929
16	8	0	2.856124	-1.27099	0.05649
17	8	0	-2.49442	-2.49517	-1.47159
18	8	0	1.438072	-1.60959	1.793106
19	6	0	5.112086	-0.49782	0.191839
20	1	0	-3.20722	-0.06752	-1.98855
21	1	0	-2.693	1.964644	-1.21851
22	8	0	-4.08605	0.585097	2.32553
23	1	0	-0.48172	1.496099	-2.25835
24	1	0	0.180725	2.210127	0.632935
25	1	0	-0.98944	-1.51687	0.807687
26	1	0	-1.13142	-1.13285	-2.24939
27	1	0	1.623299	2.787741	-2.00841
28	1	0	1.979349	3.469339	-0.4289
29	1	0	2.570068	0.629591	-1.3779
30	1	0	3.745318	1.919278	-1.21737
31	1	0	1.028009	-1.71106	-1.49036
32	1	0	-3.2514	-1.27937	0.731343
33	1	0	-4.61383	-0.77057	-0.24258
34	1	0	-4.44657	1.498088	0.580571
35	1	0	-2.26762	2.480272	1.116319
36	1	0	-1.57763	0.877127	1.401366
37	1	0	2.170242	1.043739	1.239207
38	1	0	3.761485	1.768666	1.181161
39	1	0	3.730449	-0.65371	1.838158
40	1	0	-1.91217	-3.23509	-1.67827
41	1	0	5.468325	-1.52358	0.307993
42	1	0	5.808965	0.168543	0.705722
43	1	0	5.117031	-0.24903	-0.87161
44	1	0	-3.44918	-0.02366	2.718096

4a-Conf.13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.200063	-0.18115	1.280655
2	6	0	1.933004	1.237359	0.678143
3	6	0	0.497201	1.523534	0.336542
4	6	0	-0.01588	1.791209	-0.86301
5	6	0	0.118243	-1.41137	0.515217
6	6	0	1.619009	-1.42097	0.532266
7	6	0	-1.47674	1.848896	-1.24033
8	6	0	-2.53907	1.922606	-0.11815
9	6	0	-2.09522	-1.54364	-0.59819
10	6	0	-0.64015	-1.77038	-0.52592
11	6	0	3.742391	-0.184	1.335342
12	6	0	4.217387	0.543197	0.062665
13	6	0	3.004965	1.38504	-0.42105
14	6	0	-3.8023	1.072734	-0.41398
15	6	0	-3.88888	-0.245	0.384286
16	8	0	-2.5706	-0.86609	0.468119
17	8	0	2.081525	-1.60961	-0.7968
18	8	0	-2.78272	-1.86618	-1.54949
19	6	0	-4.34471	-0.05899	1.823522
20	1	0	1.785854	-0.23876	2.29221
21	1	0	2.21007	1.924988	1.490393
22	8	0	4.597705	-0.47682	-0.89247
23	1	0	-0.17191	1.450063	1.190578
24	1	0	0.658828	1.867222	-1.71412
25	1	0	-0.36259	-1.06705	1.423988
26	1	0	1.925561	-2.2813	1.155622
27	1	0	-1.63272	2.678705	-1.94035
28	1	0	-1.65706	0.950581	-1.84765
29	1	0	-2.11196	1.592976	0.829185
30	1	0	-2.82451	2.967115	0.028807
31	1	0	-0.19396	-2.14068	-1.4395
32	1	0	4.187992	-1.17922	1.406403
33	1	0	4.06619	0.38055	2.213063
34	1	0	5.094165	1.164702	0.26063
35	1	0	3.269975	2.429025	-0.60091
36	1	0	2.645415	0.962747	-1.36212
37	1	0	-3.84883	0.842876	-1.48184
38	1	0	-4.71067	1.638257	-0.18642
39	1	0	-4.55243	-0.93979	-0.1328
40	1	0	3.036053	-1.42008	-0.84789

41	1	0	-5.36234	0.337883	1.840675
42	1	0	-3.69493	0.637487	2.359718
43	1	0	-4.33753	-1.01405	2.353023
44	1	0	4.798227	-0.04929	-1.73363

4a-Conf.14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.74354	0.410684	-1.00067
2	6	0	-1.74768	1.531368	-0.53085
3	6	0	-0.34947	1.521747	-1.10645
4	6	0	0.756045	1.919048	-0.47241
5	6	0	-1.12771	-1.45709	-0.2985
6	6	0	-2.17213	-1.01942	-1.27939
7	6	0	2.154268	1.896113	-1.04788
8	6	0	3.278249	1.828425	0.009699
9	6	0	1.257566	-1.6099	0.296465
10	6	0	0.145145	-1.58687	-0.67408
11	6	0	-3.83221	0.473039	0.092306
12	6	0	-3.13808	0.842215	1.417193
13	6	0	-1.81536	1.522713	1.018101
14	6	0	3.26232	0.667757	1.022424
15	6	0	3.507614	-0.75909	0.510918
16	8	0	2.381439	-1.18284	-0.31901
17	8	0	-3.21721	-2.00391	-1.2836
18	8	0	1.183183	-1.87785	1.477914
19	6	0	4.755843	-0.94315	-0.33606
20	1	0	-3.18159	0.714738	-1.95735
21	1	0	-2.22707	2.460564	-0.86898
22	8	0	-2.8077	-0.3106	2.216442
23	1	0	-0.26128	1.173748	-2.13533
24	1	0	0.672658	2.290825	0.547363
25	1	0	-1.41668	-1.52649	0.745541
26	1	0	-1.70674	-0.99188	-2.2718
27	1	0	2.24295	1.068521	-1.75688
28	1	0	2.32491	2.813773	-1.62698
29	1	0	4.241554	1.849974	-0.50998
30	1	0	3.241578	2.754368	0.595983
31	1	0	0.433316	-1.46731	-1.71216
32	1	0	-4.40439	-0.45218	0.175643
33	1	0	-4.53636	1.26992	-0.1671
34	1	0	-3.77362	1.505246	2.013788
35	1	0	-1.73476	2.530963	1.428764
36	1	0	-0.99479	0.936274	1.437231

37	1	0	2.318643	0.666055	1.575959
38	1	0	4.042011	0.86347	1.76775
39	1	0	3.540466	-1.42714	1.373539
40	1	0	-3.87447	-1.7325	-1.93524
41	1	0	4.878853	-1.99383	-0.607
42	1	0	5.637264	-0.62864	0.228247
43	1	0	4.707634	-0.3549	-1.25487
44	1	0	-3.63308	-0.74758	2.454911

4a-Conf.15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.680002	0.668912	-0.71665
2	6	0	2.25129	-0.81388	-1.12195
3	6	0	0.77485	-1.04097	-1.33192
4	6	0	-0.02465	-1.94012	-0.75488
5	6	0	0.454455	1.700813	0.053707
6	6	0	1.651543	1.809643	-0.84881
7	6	0	-1.5106	-2.01124	-0.99838
8	6	0	-2.33977	-2.01552	0.311337
9	6	0	-1.91472	1.311608	0.524165
10	6	0	-0.80522	1.674737	-0.38545
11	6	0	3.33256	0.530625	0.669613
12	6	0	3.99611	-0.84839	0.606985
13	6	0	2.918767	-1.71561	-0.05801
14	6	0	-3.77973	-1.48154	0.139508
15	6	0	-3.95226	-0.0039	0.513797
16	8	0	-2.92589	0.769621	-0.18932
17	8	0	2.382551	3.011734	-0.54005
18	8	0	-1.89777	1.404375	1.733981
19	6	0	-5.30658	0.569736	0.130439
20	1	0	3.473358	0.960398	-1.41244
21	1	0	2.728277	-1.0047	-2.09048
22	8	0	4.466976	-1.34871	1.856021
23	1	0	0.322878	-0.38054	-2.0695
24	1	0	0.37488	-2.6448	-0.02853
25	1	0	0.641188	1.605709	1.119271
26	1	0	1.308486	1.851834	-1.89018
27	1	0	-1.80855	-1.1628	-1.61913
28	1	0	-1.76376	-2.91637	-1.56621
29	1	0	-2.37217	-3.03572	0.704454
30	1	0	-1.82469	-1.42211	1.073608
31	1	0	-1.04092	1.732693	-1.44211
32	1	0	2.579443	0.513566	1.466952

33	1	0	4.033335	1.336524	0.889102
34	1	0	4.88849	-0.79862	-0.02503
35	1	0	3.314131	-2.64426	-0.47428
36	1	0	2.19614	-1.98518	0.720067
37	1	0	-4.46953	-2.04274	0.77783
38	1	0	-4.11692	-1.63761	-0.89151
39	1	0	-3.77186	0.128887	1.580778
40	1	0	1.784002	3.756388	-0.66915
41	1	0	-5.45822	0.513757	-0.9507
42	1	0	-5.38802	1.61363	0.440841
43	1	0	-6.10335	0.003378	0.619221
44	1	0	3.71011	-1.407	2.451077

4a-Conf.16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.218941	-0.16805	1.294075
2	6	0	1.913038	1.240095	0.679903
3	6	0	0.466991	1.518738	0.373166
4	6	0	-0.05655	1.821961	-0.81376
5	6	0	0.135086	-1.40452	0.515732
6	6	0	1.634966	-1.4311	0.60277
7	6	0	-1.51741	1.900433	-1.18598
8	6	0	-2.58256	1.928833	-0.06392
9	6	0	-2.05053	-1.514	-0.64989
10	6	0	-0.59432	-1.73895	-0.55256
11	6	0	3.76097	-0.16434	1.291007
12	6	0	4.200048	0.594024	0.007079
13	6	0	2.943782	1.386773	-0.45136
14	6	0	-3.82947	1.064562	-0.38487
15	6	0	-3.88299	-0.28672	0.357489
16	8	0	-2.54739	-0.8743	0.426993
17	8	0	2.246828	-1.64241	-0.67906
18	8	0	-2.71465	-1.81392	-1.62407
19	6	0	-4.35243	-0.17281	1.799864
20	1	0	1.831128	-0.20741	2.316609
21	1	0	2.207732	1.93569	1.479722
22	8	0	4.696356	-0.27603	-1.01207
23	1	0	-0.19218	1.421625	1.232748
24	1	0	0.613632	1.921859	-1.66582
25	1	0	-0.3748	-1.07131	1.413158
26	1	0	1.913739	-2.26377	1.26554
27	1	0	-1.66873	2.761325	-1.84854
28	1	0	-1.70151	1.032024	-1.83405

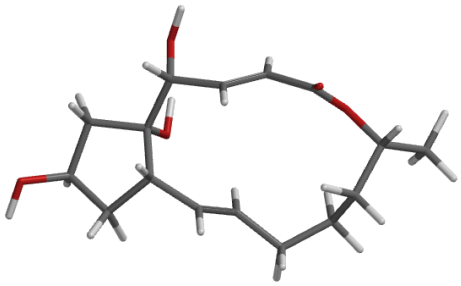
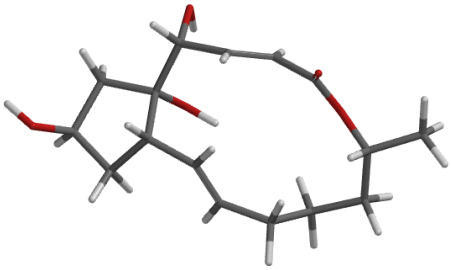
29	1	0	-2.15225	1.587679	0.878186
30	1	0	-2.88892	2.964029	0.104659
31	1	0	-0.13678	-2.08959	-1.46935
32	1	0	4.204662	-1.16171	1.321536
33	1	0	4.1114	0.377566	2.174013
34	1	0	5.031686	1.264924	0.2294
35	1	0	3.16727	2.432486	-0.67522
36	1	0	2.574034	0.925156	-1.3702
37	1	0	-3.88031	0.880283	-1.46132
38	1	0	-4.7473	1.600726	-0.12619
39	1	0	-4.5221	-0.97932	-0.19212
40	1	0	2.158346	-2.57335	-0.91187
41	1	0	-5.38228	0.190555	1.825434
42	1	0	-3.72846	0.522369	2.36746
43	1	0	-4.31803	-1.14732	2.291463
44	1	0	3.985442	-0.92086	-1.15215

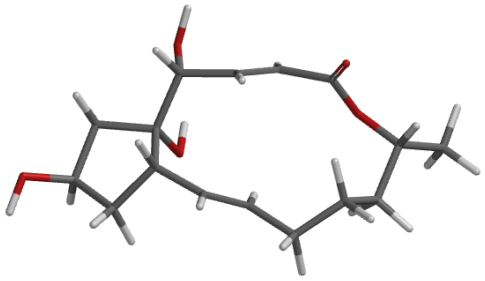
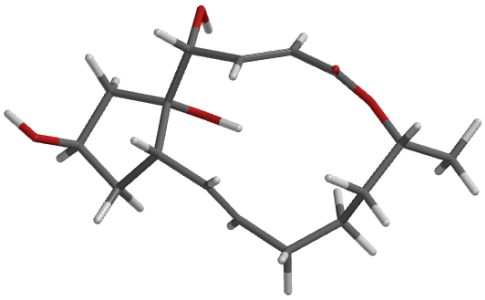
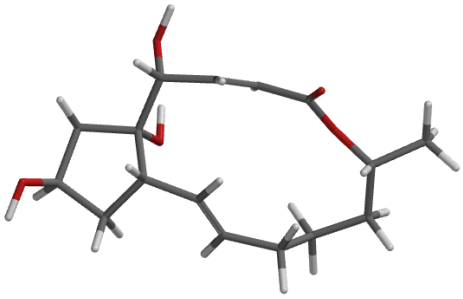
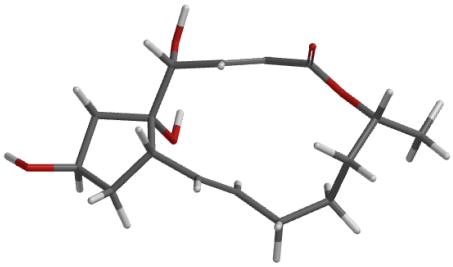
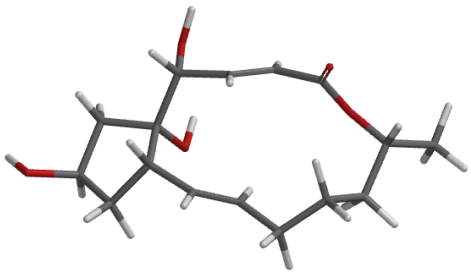
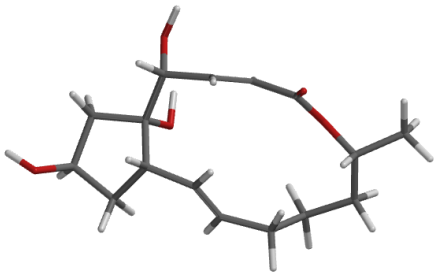
4a-Conf.17

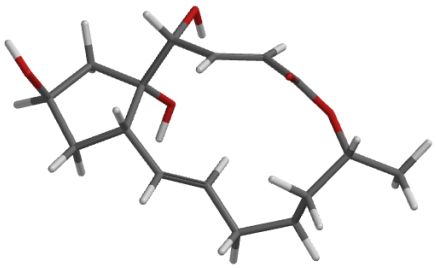
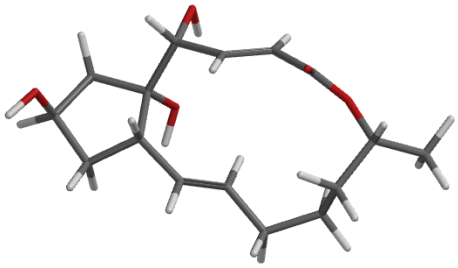
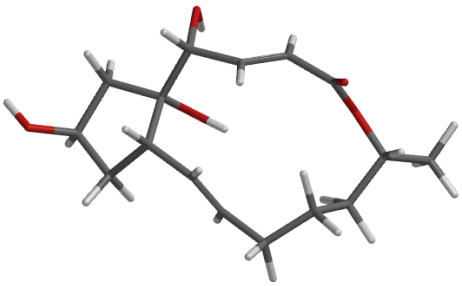
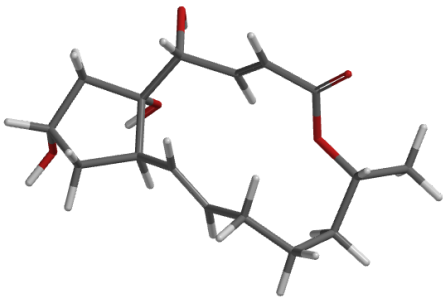
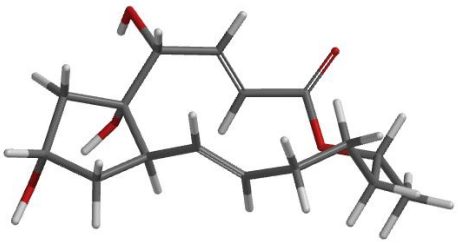
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.21894	-0.16805	1.294075
2	6	0	1.913037	1.240094	0.679903
3	6	0	0.46699	1.518738	0.373167
4	6	0	-0.05655	1.821962	-0.81376
5	6	0	0.135087	-1.40452	0.515731
6	6	0	1.634966	-1.43111	0.60277
7	6	0	-1.51741	1.900434	-1.18598
8	6	0	-2.58256	1.928833	-0.06392
9	6	0	-2.05053	-1.514	-0.64989
10	6	0	-0.59432	-1.73895	-0.55256
11	6	0	3.76097	-0.16434	1.291007
12	6	0	4.200047	0.594025	0.007079
13	6	0	2.943781	1.386773	-0.45136
14	6	0	-3.82947	1.064561	-0.38487
15	6	0	-3.88298	-0.28672	0.357489
16	8	0	-2.54739	-0.8743	0.426993
17	8	0	2.246829	-1.64241	-0.67906
18	8	0	-2.71465	-1.81392	-1.62407
19	6	0	-4.35243	-0.17281	1.799864
20	1	0	1.831128	-0.20741	2.316609
21	1	0	2.207731	1.935689	1.479722
22	8	0	4.696357	-0.27603	-1.01207
23	1	0	-0.19219	1.421624	1.232749
24	1	0	0.613631	1.921859	-1.66582

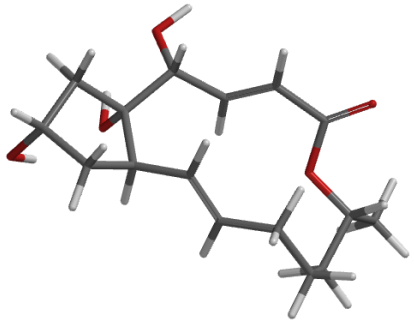
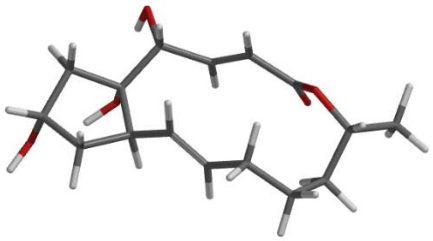
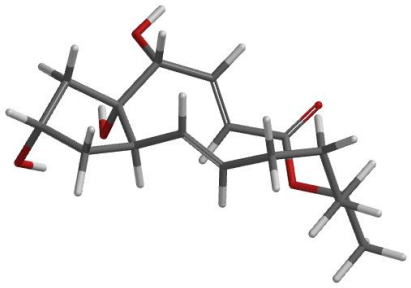
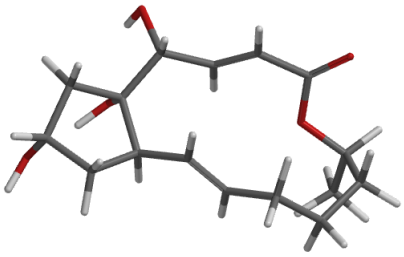
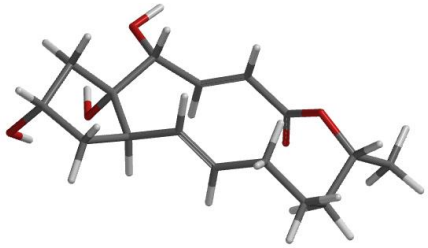
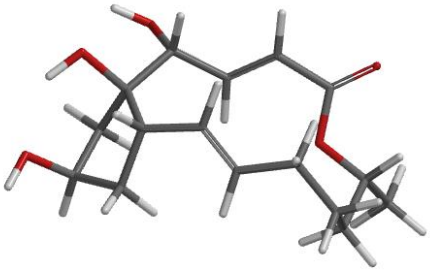
25	1	0	-0.3748	-1.07132	1.413158
26	1	0	1.91374	-2.26378	1.26554
27	1	0	-1.66873	2.761328	-1.84853
28	1	0	-1.70151	1.032027	-1.83405
29	1	0	-2.15225	1.587679	0.878186
30	1	0	-2.88892	2.964029	0.10466
31	1	0	-0.13678	-2.08959	-1.46935
32	1	0	4.204662	-1.16171	1.321535
33	1	0	4.1114	0.377566	2.174014
34	1	0	5.031685	1.264926	0.2294
35	1	0	3.167268	2.432486	-0.67522
36	1	0	2.574033	0.925156	-1.3702
37	1	0	-3.88031	0.880282	-1.46132
38	1	0	-4.7473	1.600724	-0.12619
39	1	0	-4.5221	-0.97932	-0.19212
40	1	0	2.158346	-2.57335	-0.91187
41	1	0	-4.31803	-1.14732	2.291463
42	1	0	-5.38228	0.190554	1.825434
43	1	0	-3.72846	0.522368	2.36746
44	1	0	3.985443	-0.92085	-1.15215

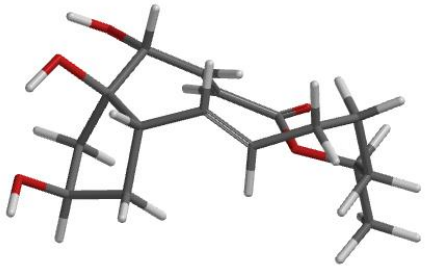
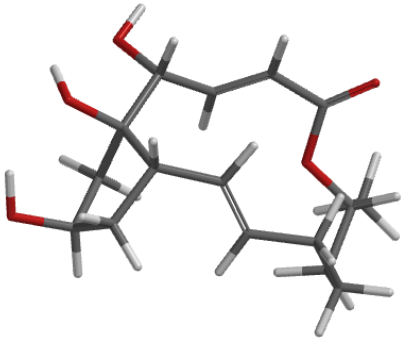
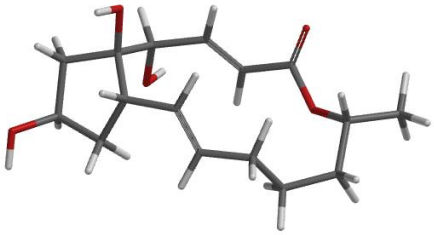
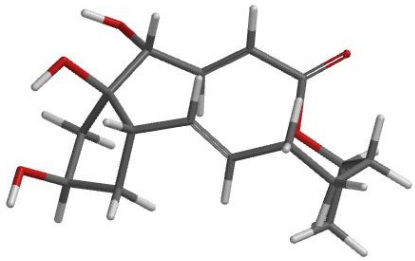
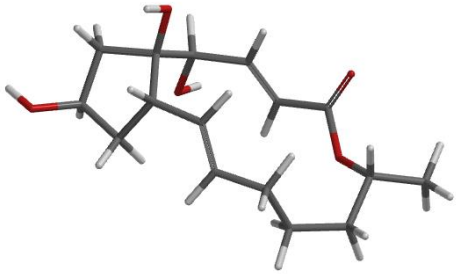
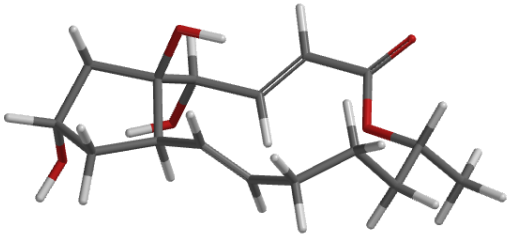
Table S19. The Information of conformations of (2*E*, 4*R*, 5*S*, 7*R*, 9*S*, 10*E*, 15*R*)-**5a**, (2*E*, 4*R*, 5*S*, 7*S*, 9*R*, 10*E*, 15*R*)-**5b**, (2*E*, 4*R*, 5*R*, 7*R*, 9*S*, 10*E*, 15*R*)-**5c**, and (2*E*, 4*R*, 5*R*, 7*S*, 9*R*, 10*E*, 15*R*)-**5d**

Label	**Conformers**	**Calculated energy (kJ/mol)**	**Boltzmann distribution**
5a-Conf.1		0	0.181
5a-Conf.2		0.18	0.168

5a-Conf.3		0.18	0.168
5a-Conf.4		1.39	0.103
5a-Conf.5		1.90	0.084
5a-Conf.6		1.90	0.084
5a-Conf.7		1.99	0.081
5a-Conf.8		4.59	0.028

5a-Conf.9		4.72	0.027
5a-Conf.10		5.70	0.018
5a-Conf.11		6.04	0.016
5b-Conf.1		0	0.602
5b-Conf.2		3.16	0.168

5b-Conf.3		4.81	0.087
5b-Conf.4		6.85	0.038
5b-Conf.5		6.87	0.038
5b-Conf.6		8.02	0.024
5b-Conf.7		8.68	0.018
5c-Conf.1		0	0.772

5c-Conf.2		5.47	0.058
5c-Conf.3		7.27	0.041
5c-Conf.4		8.18	0.028
5c-Conf.5		8.68	0.023
5c-Conf.6		9.76	0.015
5d-Conf.1		0	0.852

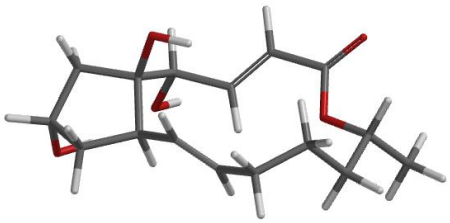
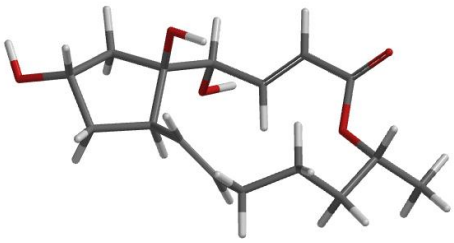
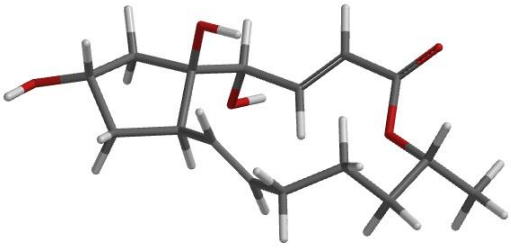
5d-Conf.2		5.35	0.099
5d-Conf.3		9.91	0.016
5d-Conf.4		11.03	0.010

Table S20. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*R*, 9*S*, 10*E*, 15*R*)-**5a**] in NMR calculation

5a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.137789	-0.32314	-0.52042
2	6	0	1.897358	0.859831	0.473701
3	6	0	0.588793	1.622078	0.531443
4	6	0	-0.34283	1.801634	-0.4078
5	6	0	0.326109	-1.66844	0.649121
6	6	0	1.699982	-1.70917	0.056177
7	6	0	-1.55968	2.682569	-0.28658
8	6	0	-2.88657	1.946097	-0.59296
9	6	0	-2.08098	-1.52101	0.662341
10	6	0	-0.81485	-1.89561	-0.00325
11	6	0	3.682932	-0.31201	-0.78048
12	6	0	4.278584	0.810233	0.072966
13	6	0	3.11383	1.788032	0.239539
14	6	0	-3.46215	1.164374	0.608557
15	6	0	-4.05412	-0.21295	0.28034
16	8	0	-2.97248	-1.0591	-0.23923

17	8	0	4.667204	0.232717	1.331425
18	8	0	1.812663	-2.60857	-1.05011
19	8	0	-2.27315	-1.52911	1.861241
20	6	0	-5.15205	-0.22185	-0.76855
21	8	0	1.436186	-0.10638	-1.74283
22	1	0	2.05864	0.430848	1.469329
23	1	0	0.455472	2.145426	1.479983
24	1	0	-0.22864	1.293088	-1.35833
25	1	0	0.266652	-1.33631	1.681074
26	1	0	2.416322	-1.98	0.841082
27	1	0	-1.60353	3.151184	0.703211
28	1	0	-1.45507	3.500012	-1.01224
29	1	0	-2.70791	1.264813	-1.43048
30	1	0	-3.62613	2.671538	-0.94311
31	1	0	-0.84205	-2.16334	-1.05195
32	1	0	4.161854	-1.26694	-0.55954
33	1	0	3.838944	-0.09279	-1.8381
34	1	0	5.149361	1.272433	-0.40482
35	1	0	2.975848	2.363488	-0.68171
36	1	0	3.268913	2.497189	1.057297
37	1	0	-2.68361	1.009845	1.360613
38	1	0	-4.24268	1.753093	1.101705
39	1	0	-4.41165	-0.67412	1.20192
40	1	0	4.96915	0.948422	1.902105
41	1	0	1.471303	-3.46994	-0.78559
42	1	0	-5.99596	0.378899	-0.4204
43	1	0	-4.80503	0.190367	-1.71832
44	1	0	-5.50503	-1.24054	-0.94268
45	1	0	1.478445	-0.94727	-2.21995

5a-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.139556	-0.43584	-0.38634
2	6	0	1.971518	0.703399	0.684107
3	6	0	0.558474	1.206276	0.854686
4	6	0	-0.1049	2.078335	0.086678
5	6	0	0.268836	-1.79057	0.630245
6	6	0	1.639434	-1.86841	0.020466
7	6	0	-1.58276	2.343346	0.233433
8	6	0	-2.37176	1.861017	-1.01442
9	6	0	-2.11454	-1.36251	0.616056
10	6	0	-0.88565	-1.8688	-0.03707
11	6	0	3.651365	-0.42332	-0.7311

12	6	0	4.25032	0.844869	-0.07928
13	6	0	3.038888	1.719512	0.236943
14	6	0	-3.81016	1.379655	-0.75924
15	6	0	-3.94219	0.144816	0.143797
16	8	0	-2.949	-0.83558	-0.30728
17	8	0	4.885326	0.54995	1.175498
18	8	0	1.694831	-2.70292	-1.12926
19	8	0	-2.3098	-1.31434	1.813025
20	6	0	-5.3222	-0.49246	0.095127
21	8	0	1.449864	-0.08381	-1.59513
22	1	0	2.30495	0.283632	1.638124
23	1	0	-0.00045	0.749859	1.667764
24	1	0	0.398673	2.589071	-0.73291
25	1	0	0.231715	-1.51939	1.68106
26	1	0	2.335618	-2.28295	0.754701
27	1	0	-1.93913	1.832086	1.132124
28	1	0	-1.77265	3.411675	0.386298
29	1	0	-1.82926	1.038086	-1.48607
30	1	0	-2.40215	2.665915	-1.75469
31	1	0	-0.93092	-2.09891	-1.09434
32	1	0	4.158471	-1.31872	-0.36657
33	1	0	3.760767	-0.39969	-1.81649
34	1	0	4.96394	1.344152	-0.74275
35	1	0	2.718258	2.240889	-0.66804
36	1	0	3.264168	2.463383	1.002845
37	1	0	-4.40894	2.177057	-0.3046
38	1	0	-4.27168	1.156704	-1.72758
39	1	0	-3.69084	0.392128	1.174816
40	1	0	5.615135	-0.05452	1.002325
41	1	0	1.451507	-2.13163	-1.87294
42	1	0	-6.08107	0.236714	0.390772
43	1	0	-5.55188	-0.83769	-0.91627
44	1	0	-5.37973	-1.34276	0.777754
45	1	0	0.580214	0.262669	-1.3447

5a-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.124258	-0.41326	-0.46811
2	6	0	2.037193	0.923948	0.326814
3	6	0	0.788531	1.774866	0.363409
4	6	0	-0.37069	1.693893	-0.29504
5	6	0	0.276143	-1.46475	0.919905
6	6	0	1.646989	-1.65708	0.347219

7	6	0	-1.49742	2.677401	-0.09529
8	6	0	-2.79579	2.06661	0.485907
9	6	0	-2.14306	-1.28765	0.798132
10	6	0	-0.85351	-1.81961	0.307419
11	6	0	3.643293	-0.56105	-0.82473
12	6	0	4.368171	0.651241	-0.2349
13	6	0	3.274468	1.717683	-0.15769
14	6	0	-3.6822	1.286961	-0.52176
15	6	0	-4.09258	-0.12391	-0.0873
16	8	0	-2.92396	-0.9927	-0.26017
17	8	0	4.833531	0.277144	1.073494
18	8	0	1.714347	-2.73901	-0.58534
19	8	0	-2.43251	-1.06445	1.955403
20	6	0	-5.20256	-0.72259	-0.93665
21	8	0	1.348709	-0.32198	-1.66287
22	1	0	2.262572	0.657664	1.367797
23	1	0	0.900544	2.609018	1.059489
24	1	0	-0.52848	0.886931	-1.00085
25	1	0	0.21632	-0.90535	1.848288
26	1	0	2.363573	-1.80941	1.163661
27	1	0	-1.15528	3.471714	0.576406
28	1	0	-1.7389	3.162247	-1.05107
29	1	0	-3.38945	2.883322	0.907054
30	1	0	-2.53107	1.425363	1.329909
31	1	0	-0.84736	-2.31301	-0.65623
32	1	0	4.079839	-1.49129	-0.4599
33	1	0	3.732255	-0.55219	-1.91239
34	1	0	5.217408	0.963832	-0.85208
35	1	0	3.088378	2.131934	-1.15415
36	1	0	3.533946	2.54596	0.507212
37	1	0	-4.59896	1.853214	-0.71143
38	1	0	-3.17843	1.194564	-1.49
39	1	0	-4.36487	-0.14352	0.968894
40	1	0	5.226245	1.058053	1.479599
41	1	0	1.372875	-3.53408	-0.16126
42	1	0	-6.11796	-0.13782	-0.82025
43	1	0	-4.92572	-0.72369	-1.99436
44	1	0	-5.40957	-1.75017	-0.63054
45	1	0	1.343726	-1.21164	-2.0421

5a-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.063939	-0.37628	-0.45348

2	6	0	1.897525	0.794364	0.582648
3	6	0	0.537201	1.452307	0.707769
4	6	0	-0.12076	2.128943	-0.2412
5	6	0	0.292415	-1.73969	0.706864
6	6	0	1.659122	-1.791	0.085595
7	6	0	-1.4671	2.792857	-0.07588
8	6	0	-2.65671	1.927638	-0.58776
9	6	0	-2.12459	-1.56284	0.674216
10	6	0	-0.84839	-1.99475	0.062826
11	6	0	3.558976	-0.33629	-0.87089
12	6	0	4.214844	0.80466	-0.07464
13	6	0	3.055652	1.750353	0.21915
14	6	0	-3.37226	1.166422	0.547749
15	6	0	-4.01618	-0.17118	0.159903
16	8	0	-2.95198	-1.08253	-0.2787
17	8	0	4.717388	0.353258	1.193763
18	8	0	1.749064	-2.7253	-0.98237
19	8	0	-2.36899	-1.53855	1.862175
20	6	0	-5.02085	-0.11135	-0.97692
21	8	0	1.305425	-0.15545	-1.65124
22	1	0	2.149423	0.367714	1.557126
23	1	0	0.077188	1.386173	1.691868
24	1	0	0.321996	2.224856	-1.23124
25	1	0	0.237971	-1.35054	1.719491
26	1	0	2.38956	-2.09276	0.841702
27	1	0	-1.6315	3.047601	0.976023
28	1	0	-1.4503	3.738664	-0.62588
29	1	0	-2.2834	1.218105	-1.33152
30	1	0	-3.37467	2.567514	-1.10742
31	1	0	-0.86797	-2.34094	-0.96336
32	1	0	4.062314	-1.29064	-0.706
33	1	0	3.604381	-0.12219	-1.94067
34	1	0	5.019157	1.286344	-0.64089
35	1	0	2.809696	2.325009	-0.67798
36	1	0	3.289151	2.452408	1.021754
37	1	0	-2.66838	0.960282	1.358036
38	1	0	-4.15129	1.80059	0.984346
39	1	0	-4.47507	-0.61078	1.046898
40	1	0	5.392888	-0.31191	1.023094
41	1	0	1.467035	-2.24276	-1.77341
42	1	0	-5.84625	0.550748	-0.70399
43	1	0	-4.56496	0.266585	-1.89444
44	1	0	-5.42918	-1.10398	-1.17796
45	1	0	0.397902	0.057323	-1.3903

5a-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.14207	0.479596	-0.35291
2	6	0	-1.97215	-0.71005	0.650811
3	6	0	-0.56222	-1.20056	0.86541
4	6	0	0.109407	-2.10139	0.146925
5	6	0	-0.2277	1.796323	0.668335
6	6	0	-1.62233	1.874679	0.124974
7	6	0	1.586916	-2.35563	0.308577
8	6	0	2.36211	-1.92266	-0.96587
9	6	0	2.149018	1.359469	0.57348
10	6	0	0.894746	1.832637	-0.0538
11	6	0	-3.67704	0.510457	-0.61776
12	6	0	-4.2367	-0.85801	-0.17772
13	6	0	-2.9974	-1.71867	0.103471
14	6	0	3.805396	-1.43679	-0.75179
15	6	0	3.954662	-0.17226	0.105892
16	8	0	2.947844	0.788985	-0.35445
17	8	0	-5.0001	-0.62982	1.021089
18	8	0	-1.72812	2.702558	-1.03907
19	8	0	2.392819	1.372783	1.762812
20	6	0	5.331572	0.466041	0.005695
21	8	0	-1.44819	0.128315	-1.54741
22	1	0	-2.36239	-0.35085	1.610255
23	1	0	-0.02188	-0.7146	1.674468
24	1	0	-0.37943	-2.62038	-0.6755
25	1	0	-0.14529	1.581795	1.729225
26	1	0	-2.2941	2.238513	0.910944
27	1	0	1.94343	-1.8013	1.181951
28	1	0	1.788995	-3.41472	0.508244
29	1	0	1.808637	-1.12029	-1.45842
30	1	0	2.381366	-2.75721	-1.67373
31	1	0	0.88823	1.987893	-1.12482
32	1	0	-4.17493	1.290971	-0.03915
33	1	0	-3.86221	0.707396	-1.6742
34	1	0	-4.88392	-1.30448	-0.93963
35	1	0	-2.63541	-2.15617	-0.83045
36	1	0	-3.20592	-2.53342	0.801365
37	1	0	4.411529	-2.21875	-0.27995
38	1	0	4.251597	-1.24779	-1.7347
39	1	0	3.727515	-0.38591	1.149997
40	1	0	-5.33108	-1.48344	1.322307

41	1	0	-1.32747	3.557291	-0.84543
42	1	0	6.098735	-0.25129	0.308973
43	1	0	5.538361	0.777243	-1.02161
44	1	0	5.401568	1.338955	0.65793
45	1	0	-1.46729	0.918809	-2.10409

5a-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.128456	-0.29613	-0.5325
2	6	0	1.879368	0.870991	0.480869
3	6	0	0.572311	1.635766	0.534588
4	6	0	-0.35607	1.820962	-0.40668
5	6	0	0.349482	-1.67571	0.640685
6	6	0	1.721992	-1.69244	0.042147
7	6	0	-1.5798	2.691222	-0.2795
8	6	0	-2.89946	1.940615	-0.58356
9	6	0	-2.05893	-1.53542	0.653422
10	6	0	-0.79054	-1.89484	-0.01623
11	6	0	3.668354	-0.25492	-0.81172
12	6	0	4.262765	0.826704	0.101495
13	6	0	3.104693	1.799595	0.290648
14	6	0	-3.45915	1.145404	0.616482
15	6	0	-4.04022	-0.23542	0.283369
16	8	0	-2.95276	-1.06929	-0.24385
17	8	0	4.599647	0.312332	1.401049
18	8	0	1.844647	-2.5868	-1.06722
19	8	0	-2.25144	-1.55761	1.852039
20	6	0	-5.14175	-0.24894	-0.7617
21	8	0	1.407707	-0.08718	-1.74468
22	1	0	2.019897	0.42231	1.470686
23	1	0	0.433235	2.150261	1.487159
24	1	0	-0.23741	1.321046	-1.36104
25	1	0	0.288265	-1.36363	1.678714
26	1	0	2.448125	-1.95103	0.822257
27	1	0	-1.6256	3.15599	0.711995
28	1	0	-1.48622	3.511712	-1.0031
29	1	0	-2.71654	1.26593	-1.42548
30	1	0	-3.64957	2.658793	-0.92612
31	1	0	-0.81608	-2.14316	-1.06965
32	1	0	4.152824	-1.22418	-0.67442
33	1	0	3.804548	0.03651	-1.85574
34	1	0	5.142552	1.3017	-0.34655
35	1	0	2.98074	2.407991	-0.61009

36	1	0	3.263054	2.469913	1.138068
37	1	0	-2.67399	0.993345	1.36219
38	1	0	-4.2418	1.723395	1.118916
39	1	0	-4.39033	-0.70433	1.203812
40	1	0	5.261384	-0.37746	1.281448
41	1	0	1.506948	-3.45102	-0.8074
42	1	0	-5.98948	0.343107	-0.40794
43	1	0	-4.80167	0.170363	-1.71085
44	1	0	-5.48678	-1.26978	-0.93908
45	1	0	1.462559	-0.92409	-2.22752

5a-Conf.7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.121677	-0.38413	-0.49303
2	6	0	2.021385	0.93997	0.325741
3	6	0	0.775867	1.796182	0.341541
4	6	0	-0.38631	1.700018	-0.30948
5	6	0	0.302324	-1.46489	0.905354
6	6	0	1.669253	-1.64084	0.317533
7	6	0	-1.51875	2.677972	-0.11636
8	6	0	-2.80767	2.06156	0.480455
9	6	0	-2.11888	-1.29468	0.799833
10	6	0	-0.83022	-1.81806	0.297252
11	6	0	3.638317	-0.50582	-0.8638
12	6	0	4.361792	0.66622	-0.18617
13	6	0	3.281421	1.737004	-0.09394
14	6	0	-3.69633	1.266816	-0.51352
15	6	0	-4.08577	-0.1467	-0.06854
16	8	0	-2.90993	-1.00339	-0.25189
17	8	0	4.757923	0.349823	1.159295
18	8	0	1.738049	-2.71583	-0.62248
19	8	0	-2.40033	-1.07466	1.959612
20	6	0	-5.19931	-0.7609	-0.90213
21	8	0	1.334308	-0.29583	-1.67959
22	1	0	2.208099	0.651824	1.368322
23	1	0	0.887817	2.640802	1.024956
24	1	0	-0.54414	0.881654	-1.0018
25	1	0	0.246521	-0.91529	1.839802
26	1	0	2.39731	-1.78927	1.124642
27	1	0	-1.17955	3.483355	0.543521
28	1	0	-1.77068	3.148741	-1.07642
29	1	0	-3.40438	2.876692	0.900262
30	1	0	-2.53055	1.428917	1.327157

31	1	0	-0.82881	-2.30284	-0.67078
32	1	0	4.066939	-1.47141	-0.58815
33	1	0	3.720573	-0.40633	-1.94861
34	1	0	5.234879	0.995457	-0.76014
35	1	0	3.12982	2.195483	-1.07582
36	1	0	3.539477	2.524673	0.616893
37	1	0	-4.62175	1.821546	-0.69502
38	1	0	-3.20273	1.176147	-1.48715
39	1	0	-4.34518	-0.16494	0.990884
40	1	0	5.365839	-0.39638	1.118722
41	1	0	1.406002	-3.51644	-0.20136
42	1	0	-6.11964	-0.18572	-0.77712
43	1	0	-4.93514	-0.76337	-1.96308
44	1	0	-5.39137	-1.78941	-0.58946
45	1	0	1.337758	-1.18321	-2.06424

5a-Conf.8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.1401	0.477265	-0.34994
2	6	0	-1.97077	-0.70983	0.656407
3	6	0	-0.56026	-1.19942	0.870793
4	6	0	0.111046	-2.10293	0.155466
5	6	0	-0.22724	1.798518	0.66828
6	6	0	-1.62298	1.873616	0.127052
7	6	0	1.589114	-2.3548	0.316401
8	6	0	2.362114	-1.92536	-0.96057
9	6	0	2.149683	1.362854	0.569481
10	6	0	0.893665	1.833554	-0.05635
11	6	0	-3.67468	0.504517	-0.62052
12	6	0	-4.23267	-0.8727	-0.17755
13	6	0	-2.99489	-1.72258	0.112059
14	6	0	3.805224	-1.43726	-0.75051
15	6	0	3.954975	-0.16958	0.102501
16	8	0	2.94604	0.789132	-0.35851
17	8	0	-4.97042	-0.77812	1.053287
18	8	0	-1.73222	2.700946	-1.037
19	8	0	2.396503	1.380607	1.758137
20	6	0	5.330954	0.469874	-0.00354
21	8	0	-1.44335	0.125186	-1.5423
22	1	0	-2.35903	-0.34852	1.615854
23	1	0	-0.01908	-0.70984	1.677087
24	1	0	-0.37816	-2.62616	-0.66405
25	1	0	-0.1425	1.587202	1.729638

26	1	0	-2.29415	2.236141	0.914262
27	1	0	1.945901	-1.7967	1.187292
28	1	0	1.792873	-3.41287	0.519731
29	1	0	1.807074	-1.12526	-1.45501
30	1	0	2.38117	-2.76232	-1.66563
31	1	0	0.884885	1.985598	-1.12781
32	1	0	-4.1677	1.297906	-0.05345
33	1	0	-3.85285	0.694441	-1.68021
34	1	0	-4.86969	-1.32035	-0.94743
35	1	0	-2.62937	-2.16754	-0.81585
36	1	0	-3.21768	-2.52521	0.817127
37	1	0	4.412975	-2.21696	-0.27701
38	1	0	4.249539	-1.25129	-1.73489
39	1	0	3.730747	-0.37986	1.147946
40	1	0	-5.7275	-0.20266	0.898865
41	1	0	-1.33177	3.556083	-0.84458
42	1	0	6.099684	-0.2456	0.300164
43	1	0	5.534628	0.777665	-1.03252
44	1	0	5.401743	1.345167	0.645426
45	1	0	-1.46349	0.914499	-2.10067

5a-Conf.9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.163944	-0.23702	-0.57141
2	6	0	1.880224	0.892383	0.485861
3	6	0	0.616329	1.724178	0.443923
4	6	0	-0.39742	1.716718	-0.42486
5	6	0	0.349979	-1.6227	0.541672
6	6	0	1.712416	-1.6579	-0.09195
7	6	0	-1.59255	2.635791	-0.39526
8	6	0	-2.93266	1.89697	-0.6136
9	6	0	-2.04979	-1.53884	0.672454
10	6	0	-0.81086	-1.92109	-0.04106
11	6	0	3.70494	-0.19576	-0.79495
12	6	0	4.281825	0.735306	0.27788
13	6	0	3.166545	1.75637	0.479204
14	6	0	-3.45233	1.143286	0.630609
15	6	0	-4.04625	-0.24642	0.359422
16	8	0	-2.98542	-1.09726	-0.19527
17	8	0	4.471445	0.061518	1.532363
18	8	0	1.807394	-2.5732	-1.17296
19	8	0	-2.18758	-1.52179	1.878714
20	6	0	-5.19425	-0.28444	-0.63397

21	8	0	1.474932	-0.08263	-1.82357
22	1	0	1.891155	0.38936	1.460295
23	1	0	0.569996	2.438488	1.268162
24	1	0	-0.37667	1.015341	-1.2507
25	1	0	0.31564	-1.23994	1.557194
26	1	0	2.430119	-1.98022	0.668715
27	1	0	-1.61673	3.213098	0.536114
28	1	0	-1.48133	3.365334	-1.20886
29	1	0	-2.79433	1.194517	-1.44133
30	1	0	-3.6855	2.616329	-0.94748
31	1	0	-0.88231	-2.25498	-1.06891
32	1	0	4.153397	-1.19124	-0.78472
33	1	0	3.909307	0.231848	-1.7818
34	1	0	5.22234	1.195615	-0.04309
35	1	0	3.15699	2.459221	-0.35978
36	1	0	3.292911	2.329616	1.399736
37	1	0	-2.64246	1.0137	1.353523
38	1	0	-4.2179	1.737561	1.140117
39	1	0	-4.35511	-0.69041	1.306528
40	1	0	5.118261	-0.63956	1.397027
41	1	0	1.571284	-2.06333	-1.96193
42	1	0	-4.89764	0.108653	-1.60865
43	1	0	-5.54824	-1.30877	-0.76838
44	1	0	-6.02426	0.318767	-0.25774
45	1	0	1.844301	0.666925	-2.30214

5a-Conf.10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.167236	-0.25845	-0.56465
2	6	0	1.891172	0.8836	0.47973
3	6	0	0.623495	1.709774	0.44401
4	6	0	-0.38501	1.711721	-0.43092
5	6	0	0.335865	-1.61921	0.553073
6	6	0	1.698012	-1.67175	-0.07893
7	6	0	-1.57835	2.6331	-0.40019
8	6	0	-2.92096	1.899794	-0.62295
9	6	0	-2.06349	-1.52812	0.683373
10	6	0	-0.82589	-1.92302	-0.02496
11	6	0	3.71088	-0.23654	-0.78184
12	6	0	4.29247	0.7268	0.251331
13	6	0	3.171737	1.752949	0.438947
14	6	0	-3.45256	1.15678	0.62259
15	6	0	-4.05407	-0.23057	0.356197

16	8	0	-2.99658	-1.09104	-0.18946
17	8	0	4.529849	-0.02553	1.45179
18	8	0	1.783726	-2.59253	-1.156
19	8	0	-2.20245	-1.49862	1.88932
20	6	0	-5.19783	-0.26645	-0.64214
21	8	0	1.484921	-0.10267	-1.82093
22	1	0	1.920516	0.393242	1.460551
23	1	0	0.572926	2.41665	1.274385
24	1	0	-0.3596	1.018454	-1.26354
25	1	0	0.303741	-1.22025	1.562463
26	1	0	2.411334	-1.99902	0.683615
27	1	0	-1.60244	3.20774	0.532838
28	1	0	-1.46304	3.364836	-1.21127
29	1	0	-2.78139	1.191702	-1.44564
30	1	0	-3.66788	2.621148	-0.96572
31	1	0	-0.89778	-2.27169	-1.04787
32	1	0	4.157458	-1.22895	-0.71129
33	1	0	3.924678	0.142097	-1.78529
34	1	0	5.227042	1.182771	-0.09239
35	1	0	3.149587	2.43526	-0.41788
36	1	0	3.297577	2.35901	1.340086
37	1	0	-2.64774	1.026135	1.350859
38	1	0	-4.21703	1.759113	1.124211
39	1	0	-4.36997	-0.66747	1.304334
40	1	0	4.814426	0.591135	2.135609
41	1	0	1.554977	-2.08238	-1.94705
42	1	0	-6.0258	0.343697	-0.27267
43	1	0	-4.89426	0.120057	-1.61733
44	1	0	-5.5575	-1.28923	-0.77324
45	1	0	1.878213	0.626569	-2.31157

5a-Conf.11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.057086	-0.50489	-0.39627
2	6	0	1.907378	0.787665	0.481832
3	6	0	0.511614	1.362938	0.571327
4	6	0	-0.02964	2.298575	-0.21605
5	6	0	0.257475	-1.71895	0.891135
6	6	0	1.619886	-1.85416	0.274031
7	6	0	-1.40491	2.920198	-0.04554
8	6	0	-2.51939	2.016293	0.523717
9	6	0	-2.15143	-1.41176	0.775444
10	6	0	-0.88752	-1.9821	0.258289

11	6	0	3.55527	-0.53815	-0.80303
12	6	0	4.192454	0.760241	-0.26815
13	6	0	3.007283	1.703545	-0.08702
14	6	0	-3.33206	1.277819	-0.56262
15	6	0	-3.96694	-0.04884	-0.11838
16	8	0	-2.93672	-1.08348	-0.27063
17	8	0	4.777716	0.572966	1.030753
18	8	0	1.684448	-2.87944	-0.70965
19	8	0	-2.41098	-1.17153	1.936161
20	6	0	-5.13943	-0.48448	-0.98134
21	8	0	1.307906	-0.37417	-1.61437
22	1	0	2.217438	0.50842	1.494102
23	1	0	-0.09319	0.965771	1.380186
24	1	0	0.572587	2.733034	-1.01089
25	1	0	0.214213	-1.24964	1.86964
26	1	0	2.348672	-2.1044	1.049855
27	1	0	-1.28335	3.796396	0.604413
28	1	0	-1.72693	3.328116	-1.00966
29	1	0	-3.20919	2.628169	1.112574
30	1	0	-2.09459	1.301056	1.22857
31	1	0	-0.90669	-2.41173	-0.73538
32	1	0	4.069206	-1.41986	-0.41573
33	1	0	3.613106	-0.57548	-1.89236
34	1	0	4.945226	1.15832	-0.95663
35	1	0	2.71476	2.102854	-1.06131
36	1	0	3.244367	2.540968	0.571442
37	1	0	-4.12284	1.940905	-0.9275
38	1	0	-2.69828	1.050849	-1.42649
39	1	0	-4.25521	-0.01889	0.933564
40	1	0	5.473655	-0.08798	0.948085
41	1	0	1.389983	-2.46426	-1.53379
42	1	0	-5.96035	0.229218	-0.8806
43	1	0	-4.85047	-0.53177	-2.03472
44	1	0	-5.4988	-1.46884	-0.67432
45	1	0	0.454977	0.030135	-1.39548

Table S21. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*S*, 9*R*, 10*E*, 15*R*)-**5b**] in NMR calculation

5b-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.32589	-0.51739	0.160658

2	6	0	-1.85046	0.986161	-0.06072
3	6	0	-0.57911	1.212548	-0.82808
4	6	0	0.481754	1.869238	-0.35166
5	6	0	0.0128	-1.49422	-0.0619
6	6	0	-1.44681	-1.66364	-0.39729
7	6	0	1.780687	2.072202	-1.09618
8	6	0	2.98959	2.468976	-0.22492
9	6	0	2.41775	-1.46513	-0.6727
10	6	0	1.003572	-1.83127	-0.89247
11	6	0	-3.75806	-0.5672	-0.42234
12	6	0	-4.28285	0.849533	-0.23089
13	6	0	-3.08803	1.700861	-0.66656
14	6	0	3.419722	1.534949	0.922905
15	6	0	3.814484	0.107068	0.538601
16	8	0	2.561603	-0.62423	0.368136
17	8	0	-4.5519	0.990379	1.182492
18	8	0	-1.94836	-2.90841	0.106952
19	8	0	3.328817	-1.81322	-1.39968
20	6	0	4.650371	-0.59935	1.597678
21	8	0	-2.36722	-0.77793	1.580644
22	1	0	-1.691	1.370871	0.948735
23	1	0	-0.53819	0.804522	-1.83777
24	1	0	0.424258	2.283567	0.654705
25	1	0	0.249132	-1.04874	0.897049
26	1	0	-1.55765	-1.70972	-1.48299
27	1	0	2.007396	1.174215	-1.68076
28	1	0	1.651553	2.873102	-1.83604
29	1	0	2.784689	3.451425	0.216376
30	1	0	3.847432	2.614268	-0.89126
31	1	0	0.809679	-2.30657	-1.84873
32	1	0	-4.37032	-1.32427	0.068677
33	1	0	-3.72533	-0.7924	-1.49187
34	1	0	-5.19254	1.058455	-0.80198
35	1	0	-3.03596	1.700595	-1.76061
36	1	0	-3.16105	2.742684	-0.34343
37	1	0	2.637541	1.470851	1.686809
38	1	0	4.284482	1.996636	1.410926
39	1	0	4.337171	0.086868	-0.42008
40	1	0	-4.69582	1.923378	1.376998
41	1	0	-2.18174	-2.72358	1.02926
42	1	0	4.853373	-1.63031	1.3006
43	1	0	5.606027	-0.08541	1.727516
44	1	0	4.128964	-0.60842	2.558717
45	1	0	-3.09275	-0.23475	1.925944

5b-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.281262	0.43938	-0.03119
2	6	0	1.631327	-1.00648	0.137862
3	6	0	0.542484	-1.44103	-0.8095
4	6	0	-0.66273	-1.85623	-0.41332
5	6	0	0.177715	1.768134	-0.82197
6	6	0	1.633241	1.424052	-1.02124
7	6	0	-1.77941	-2.32005	-1.30875
8	6	0	-3.02516	-1.40035	-1.31274
9	6	0	-2.06384	1.540308	0.103361
10	6	0	-0.59122	1.454025	0.219911
11	6	0	3.749775	0.149499	-0.42374
12	6	0	4.087408	-1.1318	0.328387
13	6	0	2.842124	-1.98781	0.095715
14	6	0	-3.80497	-1.31667	0.026184
15	6	0	-3.96338	0.100021	0.586479
16	8	0	-2.61504	0.584604	0.884467
17	8	0	4.239725	-0.76394	1.719607
18	8	0	2.402951	2.636484	-1.06131
19	8	0	-2.69071	2.266585	-0.63923
20	6	0	-4.77125	0.164884	1.872664
21	8	0	2.259975	1.125881	1.237343
22	1	0	1.209778	-1.00794	1.144986
23	1	0	0.788545	-1.45204	-1.87199
24	1	0	-0.8824	-1.83498	0.65301
25	1	0	-0.28171	2.271197	-1.66933
26	1	0	1.720945	0.995652	-2.02437
27	1	0	-1.40955	-2.40678	-2.33561
28	1	0	-2.0957	-3.32638	-1.00309
29	1	0	-3.69984	-1.76218	-2.09402
30	1	0	-2.71501	-0.40098	-1.63023
31	1	0	-0.19976	0.931747	1.080458
32	1	0	4.408024	0.981473	-0.17425
33	1	0	3.82686	-0.03928	-1.49861
34	1	0	5.006084	-1.61073	-0.02333
35	1	0	2.918346	-2.4488	-0.89453
36	1	0	2.738354	-2.79971	0.820387
37	1	0	-3.32083	-1.92916	0.794147
38	1	0	-4.80965	-1.73003	-0.10328
39	1	0	-4.39115	0.76585	-0.16437
40	1	0	4.256762	-1.56888	2.249632

41	1	0	2.495708	2.900453	-0.13524
42	1	0	-4.31698	-0.45746	2.648237
43	1	0	-4.82864	1.191704	2.240022
44	1	0	-5.78809	-0.19344	1.694511
45	1	0	2.89446	0.654533	1.801152

5b-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.325892	0.500974	0.165674
2	6	0	1.859335	-0.99556	-0.06294
3	6	0	0.582632	-1.22143	-0.82204
4	6	0	-0.47483	-1.87861	-0.33922
5	6	0	-0.00764	1.489142	-0.06653
6	6	0	1.448089	1.644288	-0.39902
7	6	0	-1.77408	-2.09045	-1.08075
8	6	0	-2.98289	-2.47839	-0.20544
9	6	0	-2.41085	1.458851	-0.68544
10	6	0	-0.99287	1.819725	-0.90642
11	6	0	3.765563	0.564052	-0.39918
12	6	0	4.294818	-0.85984	-0.21332
13	6	0	3.097893	-1.70182	-0.67548
14	6	0	-3.41487	-1.53187	0.931452
15	6	0	-3.8087	-0.1083	0.531347
16	8	0	-2.55325	0.619069	0.353867
17	8	0	4.643181	-1.12012	1.153958
18	8	0	1.998651	2.834246	0.20431
19	8	0	-3.31908	1.812175	-1.41199
20	6	0	-4.64405	0.610959	1.581981
21	8	0	2.367174	0.647585	1.603865
22	1	0	1.708516	-1.38335	0.946985
23	1	0	0.537399	-0.81854	-1.83355
24	1	0	-0.41325	-2.28956	0.668255
25	1	0	-0.24354	1.055728	0.89748
26	1	0	1.571678	1.695109	-1.48632
27	1	0	-2.00144	-1.19974	-1.67613
28	1	0	-1.64399	-2.89998	-1.81094
29	1	0	-2.77721	-3.45539	0.247311
30	1	0	-3.84012	-2.63229	-0.87061
31	1	0	-0.79476	2.28226	-1.86801
32	1	0	4.369631	1.320107	0.104894
33	1	0	3.739062	0.802794	-1.46685
34	1	0	5.194789	-1.05928	-0.79837
35	1	0	3.043855	-1.68471	-1.76976

36	1	0	3.173467	-2.74345	-0.35782
37	1	0	-2.63409	-1.45954	1.696064
38	1	0	-4.28065	-1.98778	1.422951
39	1	0	-4.32971	-0.09735	-0.42846
40	1	0	3.998401	-0.6483	1.70093
41	1	0	1.404902	3.57034	0.018968
42	1	0	-4.84566	1.638913	1.273851
43	1	0	-5.60037	0.099486	1.716241
44	1	0	-4.12341	0.629149	2.543266
45	1	0	2.512537	1.591349	1.769375

5b-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.39879	-0.50053	0.008972
2	6	0	-1.76027	0.948559	0.156693
3	6	0	-0.47932	1.265176	-0.56905
4	6	0	0.567971	1.885798	-0.02167
5	6	0	-0.21373	-1.76821	-0.05632
6	6	0	-1.57338	-1.61921	-0.67421
7	6	0	1.8208	2.294078	-0.7621
8	6	0	3.092818	2.408078	0.10308
9	6	0	2.197386	-1.40353	-0.01469
10	6	0	0.921217	-1.60523	-0.73521
11	6	0	-3.74289	-0.26191	-0.71646
12	6	0	-4.19572	1.100499	-0.20525
13	6	0	-2.90567	1.919425	-0.26734
14	6	0	3.652517	1.136871	0.767377
15	6	0	4.161882	0.047983	-0.18843
16	8	0	3.034274	-0.68146	-0.78694
17	8	0	-4.64435	0.899957	1.155368
18	8	0	-2.30667	-2.84689	-0.58648
19	8	0	2.423434	-1.74499	1.128228
20	6	0	5.203466	-0.88908	0.415537
21	8	0	-2.65579	-1.03038	1.328168
22	1	0	-1.57211	1.065046	1.225945
23	1	0	-0.44506	1.014139	-1.62921
24	1	0	0.520697	2.15391	1.034618
25	1	0	-0.17839	-1.92398	1.017903
26	1	0	-1.47114	-1.39529	-1.73816
27	1	0	1.98666	1.615999	-1.60425
28	1	0	1.65763	3.287389	-1.20212
29	1	0	2.89812	3.136863	0.898975
30	1	0	3.882489	2.847956	-0.51718

31	1	0	0.922115	-1.39702	-1.79914
32	1	0	-4.46115	-1.05772	-0.51841
33	1	0	-3.58534	-0.20141	-1.79727
34	1	0	-5.00701	1.53664	-0.79571
35	1	0	-2.7541	2.250339	-1.30006
36	1	0	-2.93538	2.816007	0.357189
37	1	0	2.926013	0.698298	1.455901
38	1	0	4.504401	1.439935	1.385371
39	1	0	4.596879	0.52412	-1.07
40	1	0	-4.74864	1.761728	1.574419
41	1	0	-2.67102	-2.85323	0.311161
42	1	0	5.437926	-1.69526	-0.28397
43	1	0	6.121705	-0.32529	0.600456
44	1	0	4.859574	-1.32527	1.351764
45	1	0	-3.38182	-0.49631	1.689567

5b-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.285091	0.417245	-0.03512
2	6	0	1.627938	-1.011	0.143358
3	6	0	0.538014	-1.43816	-0.80632
4	6	0	-0.66722	-1.85168	-0.40934
5	6	0	0.180299	1.747409	-0.833
6	6	0	1.639845	1.414128	-1.0131
7	6	0	-1.78257	-2.32061	-1.30339
8	6	0	-3.03096	-1.40476	-1.30773
9	6	0	-2.06042	1.537839	0.089692
10	6	0	-0.58593	1.470632	0.220809
11	6	0	3.753235	0.124184	-0.42499
12	6	0	4.088428	-1.15542	0.347043
13	6	0	2.83125	-2.00322	0.115094
14	6	0	-3.80394	-1.31485	0.034742
15	6	0	-3.95828	0.103319	0.591902
16	8	0	-2.60751	0.591164	0.880835
17	8	0	4.329648	-0.89525	1.735918
18	8	0	2.446488	2.606927	-0.89519
19	8	0	-2.68397	2.246182	-0.67208
20	6	0	-4.75603	0.17183	1.883963
21	8	0	2.272605	1.005369	1.292565
22	1	0	1.202314	-0.9998	1.148721
23	1	0	0.786157	-1.45369	-1.86807
24	1	0	-0.88723	-1.82685	0.656782
25	1	0	-0.29359	2.196154	-1.70381

26	1	0	1.75046	1.004339	-2.02535
27	1	0	-1.41328	-2.40848	-2.33031
28	1	0	-2.09539	-3.32715	-0.99508
29	1	0	-3.70833	-1.77426	-2.08297
30	1	0	-2.72612	-0.40659	-1.63389
31	1	0	-0.19241	0.993552	1.106715
32	1	0	4.415056	0.957769	-0.18776
33	1	0	3.821379	-0.07179	-1.50015
34	1	0	4.988718	-1.64766	-0.02585
35	1	0	2.896622	-2.47709	-0.87017
36	1	0	2.72463	-2.79592	0.85784
37	1	0	-3.31827	-1.92673	0.802148
38	1	0	-4.81033	-1.7257	-0.08876
39	1	0	-4.39072	0.767057	-0.15787
40	1	0	3.677685	-0.23026	2.004125
41	1	0	2.032751	3.312565	-1.40515
42	1	0	-4.29648	-0.44908	2.65747
43	1	0	-4.81048	1.199466	2.249311
44	1	0	-5.77418	-0.18646	1.713739
45	1	0	2.570344	1.920095	1.180248

5b-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.337436	0.477968	0.104998
2	6	0	1.754844	-0.99507	-0.03013
3	6	0	0.477681	-1.20964	-0.79829
4	6	0	-0.59835	-1.8211	-0.29637
5	6	0	0.05453	1.554978	-0.0353
6	6	0	1.499552	1.653656	-0.44789
7	6	0	-1.85283	-2.17659	-1.05558
8	6	0	-3.1714	-2.2323	-0.23974
9	6	0	-2.37454	1.623718	-0.51077
10	6	0	-0.96302	1.927419	-0.81469
11	6	0	3.736522	0.411732	-0.54611
12	6	0	4.197028	-1.01603	-0.2786
13	6	0	2.940189	-1.82999	-0.59485
14	6	0	-4.0797	-0.98312	-0.23736
15	6	0	-3.80278	0.152274	0.756673
16	8	0	-2.49454	0.744364	0.502843
17	8	0	4.535526	-1.0757	1.126339
18	8	0	2.08623	2.884937	-0.00744
19	8	0	-3.31411	2.057904	-1.14998
20	6	0	-3.80366	-0.25609	2.221086

21	8	0	2.469875	0.786694	1.510844
22	1	0	1.566991	-1.30899	0.998604
23	1	0	0.467584	-0.88289	-1.83803
24	1	0	-0.56459	-2.15401	0.741529
25	1	0	-0.15051	1.122906	0.936979
26	1	0	1.558172	1.663245	-1.53857
27	1	0	-1.96871	-1.51673	-1.92248
28	1	0	-1.70009	-3.1816	-1.47137
29	1	0	-2.95198	-2.55083	0.784811
30	1	0	-3.77568	-3.03755	-0.6674
31	1	0	-0.80261	2.394998	-1.78083
32	1	0	4.411063	1.167006	-0.14153
33	1	0	3.658341	0.562299	-1.62655
34	1	0	5.063223	-1.31364	-0.87714
35	1	0	2.852371	-1.92947	-1.68198
36	1	0	2.967319	-2.84013	-0.17764
37	1	0	-5.10374	-1.31091	-0.02477
38	1	0	-4.10898	-0.55469	-1.244
39	1	0	-4.54938	0.931281	0.589506
40	1	0	4.644353	-1.99997	1.37716
41	1	0	2.359274	2.712475	0.906437
42	1	0	-3.64748	0.617586	2.857276
43	1	0	-4.76587	-0.70338	2.481858
44	1	0	-3.01658	-0.98173	2.435911
45	1	0	3.184668	0.218159	1.838785

5b-Conf.7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.40135	-0.48084	0.010703
2	6	0	-1.76806	0.958297	0.172218
3	6	0	-0.48964	1.273786	-0.55865
4	6	0	0.564984	1.88287	-0.01282
5	6	0	-0.21454	-1.7494	-0.04755
6	6	0	-1.56555	-1.59139	-0.67099
7	6	0	1.812371	2.294648	-0.76086
8	6	0	3.089573	2.411388	0.09604
9	6	0	2.198611	-1.40163	-0.01104
10	6	0	0.921029	-1.60973	-0.73085
11	6	0	-3.74428	-0.24743	-0.71701
12	6	0	-4.21121	1.111861	-0.18624
13	6	0	-2.91638	1.933647	-0.2356
14	6	0	3.654314	1.142418	0.760345
15	6	0	4.160709	0.05155	-0.19448

16	8	0	3.030206	-0.68074	-0.78712
17	8	0	-4.75101	1.012294	1.137622
18	8	0	-2.36037	-2.78122	-0.50059
19	8	0	2.423612	-1.73896	1.132667
20	6	0	5.203395	-0.88484	0.408067
21	8	0	-2.67343	-0.91304	1.367666
22	1	0	-1.57447	1.061263	1.241957
23	1	0	-0.4655	1.036796	-1.62235
24	1	0	0.528511	2.138248	1.046944
25	1	0	-0.18453	-1.87958	1.0297
26	1	0	-1.46212	-1.36056	-1.73676
27	1	0	1.974517	1.617508	-1.60454
28	1	0	1.643813	3.287459	-1.19971
29	1	0	2.899391	3.141829	0.891406
30	1	0	3.875	2.850297	-0.53014
31	1	0	0.924162	-1.42812	-1.79948
32	1	0	-4.45733	-1.05206	-0.53296
33	1	0	-3.5758	-0.17884	-1.79668
34	1	0	-4.99961	1.553835	-0.79866
35	1	0	-2.75511	2.285683	-1.26018
36	1	0	-2.95775	2.809543	0.414285
37	1	0	2.932478	0.705033	1.45449
38	1	0	4.509341	1.448007	1.372636
39	1	0	4.591602	0.524703	-1.07948
40	1	0	-4.18514	0.386923	1.615091
41	1	0	-1.83402	-3.53906	-0.77887
42	1	0	5.435034	-1.69293	-0.29008
43	1	0	6.122461	-0.32097	0.588121
44	1	0	4.862838	-1.31807	1.346884
45	1	0	-2.96375	-1.83483	1.298617

Table S22. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*R*, 7*R*, 9*S*, 10*E*, 15*R*)-**5c**] in NMR calculation

5c-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.330835	0.560039	-0.16029
2	6	0	2.019726	-0.68543	-1.07306
3	6	0	0.551873	-0.89317	-1.38305
4	6	0	-0.30731	-1.78843	-0.88867
5	6	0	0.01266	1.61503	0.016717
6	6	0	1.45445	1.830508	-0.32422

7	6	0	-1.73812	-1.91865	-1.36013
8	6	0	-2.76034	-2.45503	-0.33721
9	6	0	-2.40379	1.566095	-0.47454
10	6	0	-1.01989	2.033086	-0.71892
11	6	0	2.346981	-0.05352	1.252181
12	6	0	3.144285	-1.34379	1.067201
13	6	0	2.718883	-1.86275	-0.32653
14	6	0	-3.08415	-1.61889	0.914558
15	6	0	-3.62253	-0.20447	0.671556
16	8	0	-2.44426	0.640059	0.49876
17	8	0	4.54435	-0.97028	1.104903
18	8	0	1.970252	2.846	0.544205
19	8	0	-3.36528	1.913195	-1.13213
20	6	0	-4.44813	0.343136	1.828089
21	8	0	3.647204	1.060948	-0.48157
22	1	0	2.521017	-0.49016	-2.02471
23	1	0	0.166606	-0.20532	-2.13241
24	1	0	0.014543	-2.51374	-0.14337
25	1	0	-0.19496	1.040931	0.910756
26	1	0	1.54329	2.159087	-1.36875
27	1	0	-2.07514	-0.96805	-1.78584
28	1	0	-1.75168	-2.62967	-2.19785
29	1	0	-3.69758	-2.63395	-0.87666
30	1	0	-2.42061	-3.44047	0.002685
31	1	0	-0.89191	2.634121	-1.61271
32	1	0	1.333522	-0.30887	1.568488
33	1	0	2.785765	0.608892	1.998524
34	1	0	2.955518	-2.07356	1.858537
35	1	0	2.052402	-2.71889	-0.22347
36	1	0	3.593218	-2.21368	-0.87921
37	1	0	-2.20808	-1.53327	1.565936
38	1	0	-3.83745	-2.17038	1.486565
39	1	0	-4.20087	-0.15301	-0.25361
40	1	0	5.071593	-1.73847	0.856627
41	1	0	2.932064	2.77346	0.447042
42	1	0	-5.35158	-0.2571	1.961052
43	1	0	-3.87507	0.31649	2.758892
44	1	0	-4.74805	1.374595	1.6316
45	1	0	4.292713	0.478988	-0.04365

5c-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.329392	0.408256	-0.34886

2	6	0	2.052206	-1.17015	-0.39031
3	6	0	0.808149	-1.66461	-1.09448
4	6	0	-0.2318	-2.31683	-0.56699
5	6	0	-0.04675	1.259438	-0.54371
6	6	0	1.336819	1.347033	-1.08082
7	6	0	-1.46349	-2.72758	-1.34049
8	6	0	-2.63717	-1.72114	-1.23399
9	6	0	-2.30423	1.882968	0.110024
10	6	0	-0.91173	2.237369	-0.26117
11	6	0	2.476824	0.72948	1.154732
12	6	0	3.075318	-0.54289	1.741114
13	6	0	2.237281	-1.63583	1.073383
14	6	0	-3.2549	-1.5586	0.173639
15	6	0	-3.65559	-0.11855	0.507376
16	8	0	-2.38882	0.607137	0.540535
17	8	0	4.456234	-0.57937	1.313784
18	8	0	1.813445	2.684033	-1.04565
19	8	0	-3.25625	2.628998	0.001652
20	6	0	-4.36988	0.028622	1.842566
21	8	0	3.573352	0.683354	-1.02398
22	1	0	2.894532	-1.54604	-0.9788
23	1	0	0.78504	-1.45942	-2.16528
24	1	0	-0.23949	-2.54068	0.496547
25	1	0	-0.3974	0.246817	-0.41756
26	1	0	1.297136	0.995346	-2.1263
27	1	0	-1.20713	-2.83331	-2.39938
28	1	0	-1.80118	-3.7126	-0.99725
29	1	0	-2.27554	-0.75194	-1.58798
30	1	0	-3.41802	-2.02952	-1.93637
31	1	0	-0.69213	3.289832	-0.38854
32	1	0	1.497437	0.903768	1.608185
33	1	0	3.092721	1.613829	1.320537
34	1	0	3.030248	-0.58065	2.8335
35	1	0	1.278373	-1.68315	1.596501
36	1	0	2.694401	-2.62639	1.141271
37	1	0	-2.55016	-1.88162	0.946546
38	1	0	-4.13753	-2.19702	0.275028
39	1	0	-4.26199	0.316369	-0.29173
40	1	0	4.812226	-1.45574	1.499062
41	1	0	2.759073	2.617387	-1.23867
42	1	0	-5.31435	-0.5213	1.824958
43	1	0	-3.75414	-0.36806	2.654256
44	1	0	-4.58673	1.078318	2.046644
45	1	0	4.268239	0.310667	-0.45807

5c-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.332157	0.541899	-0.15696
2	6	0	2.029421	-0.69361	-1.07066
3	6	0	0.560366	-0.89588	-1.38055
4	6	0	-0.29763	-1.79306	-0.88859
5	6	0	0.013576	1.603296	0.019019
6	6	0	1.457679	1.807972	-0.32006
7	6	0	-1.72833	-1.92218	-1.36046
8	6	0	-2.7523	-2.45578	-0.33779
9	6	0	-2.40227	1.567139	-0.47558
10	6	0	-1.01565	2.028291	-0.71893
11	6	0	2.353049	-0.0677	1.256513
12	6	0	3.164023	-1.3598	1.069616
13	6	0	2.734963	-1.86996	-0.33149
14	6	0	-3.07787	-1.6178	0.912338
15	6	0	-3.62176	-0.20541	0.668244
16	8	0	-2.44642	0.645204	0.50087
17	8	0	4.573953	-1.12346	1.157137
18	8	0	2.064755	2.765479	0.575095
19	8	0	-3.36015	1.913408	-1.13831
20	6	0	-4.4538	0.337444	1.822272
21	8	0	3.678584	0.95036	-0.50611
22	1	0	2.528426	-0.49216	-2.02272
23	1	0	0.174856	-0.20663	-2.12855
24	1	0	0.026282	-2.5199	-0.14579
25	1	0	-0.19658	1.03283	0.914537
26	1	0	1.560213	2.159567	-1.35281
27	1	0	-2.06372	-0.97192	-1.78826
28	1	0	-1.74182	-2.63461	-2.19693
29	1	0	-3.68877	-2.63535	-0.87832
30	1	0	-2.41347	-3.44068	0.004404
31	1	0	-0.88315	2.624088	-1.6157
32	1	0	1.337825	-0.3188	1.575324
33	1	0	2.792585	0.59894	1.999171
34	1	0	2.947809	-2.09204	1.848687
35	1	0	2.074439	-2.73311	-0.24543
36	1	0	3.621153	-2.20252	-0.87436
37	1	0	-2.20172	-1.52825	1.563009
38	1	0	-3.82881	-2.17094	1.485808
39	1	0	-4.19651	-0.1552	-0.25916
40	1	0	4.74321	-0.39891	0.536473

41	1	0	1.729615	3.64024	0.348835
42	1	0	-5.35501	-0.26697	1.951235
43	1	0	-3.88402	0.312083	2.755085
44	1	0	-4.75756	1.367789	1.625913
45	1	0	3.815142	1.7953	-0.05159

5c-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.45716	-0.80136	-0.41082
2	6	0	-2.05551	0.700934	-0.61669
3	6	0	-0.62005	0.986105	-0.95157
4	6	0	0.157922	1.939701	-0.43652
5	6	0	-0.15193	-1.83359	-0.03086
6	6	0	-1.5463	-1.68316	0.502927
7	6	0	1.621612	2.104853	-0.76333
8	6	0	2.494376	2.099452	0.517197
9	6	0	2.244044	-1.42476	-0.07036
10	6	0	0.962549	-1.56092	0.649814
11	6	0	-3.87735	-0.69415	0.216695
12	6	0	-4.06955	0.754074	0.706986
13	6	0	-2.68408	1.414038	0.584245
14	6	0	3.940926	1.602931	0.351355
15	6	0	4.08308	0.140919	-0.10235
16	8	0	3.085463	-0.63387	0.635788
17	8	0	-5.02382	1.372483	-0.17637
18	8	0	-1.58605	-1.17025	1.828556
19	8	0	2.492626	-1.85385	-1.17882
20	6	0	5.46478	-0.43986	0.155109
21	8	0	-2.444	-1.5238	-1.64622
22	1	0	-2.65574	0.99154	-1.49425
23	1	0	-0.19674	0.337644	-1.71691
24	1	0	-0.24229	2.614077	0.319289
25	1	0	-0.07945	-2.13276	-1.07078
26	1	0	-2.02635	-2.67224	0.465741
27	1	0	1.919778	1.299757	-1.44171
28	1	0	1.79539	3.042507	-1.30628
29	1	0	2.522616	3.111299	0.933875
30	1	0	2.011423	1.473779	1.27092
31	1	0	0.93077	-1.20786	1.67219
32	1	0	-4.00785	-1.41385	1.024699
33	1	0	-4.62688	-0.91097	-0.54751
34	1	0	-4.44812	0.79261	1.733382
35	1	0	-2.09722	1.224466	1.485185

36	1	0	-2.76538	2.495666	0.448964
37	1	0	4.454183	1.723593	1.311971
38	1	0	4.48371	2.222692	-0.37161
39	1	0	3.83854	0.039445	-1.15993
40	1	0	-5.14419	2.282543	0.117218
41	1	0	-1.35163	-1.88035	2.435126
42	1	0	6.223932	0.161932	-0.35175
43	1	0	5.687057	-0.44307	1.225437
44	1	0	5.530761	-1.46304	-0.22041
45	1	0	-2.99415	-1.04646	-2.27744

5c-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.322686	0.583605	-0.14979
2	6	0	2.143696	-0.62458	-1.14112
3	6	0	0.695287	-0.93148	-1.4407
4	6	0	-0.08922	-1.87946	-0.92255
5	6	0	-0.07871	1.511727	0.026766
6	6	0	1.36168	1.795991	-0.28557
7	6	0	-1.56397	-1.98507	-1.21289
8	6	0	-2.43742	-2.08737	0.068613
9	6	0	-2.50273	1.485739	-0.5172
10	6	0	-1.10116	1.908855	-0.73518
11	6	0	2.328129	-0.109	1.224464
12	6	0	3.232802	-1.3224	1.004157
13	6	0	2.940061	-1.77108	-0.4495
14	6	0	-3.79961	-1.35786	-0.04666
15	6	0	-3.8856	-0.04485	0.753283
16	8	0	-2.64838	0.715844	0.576082
17	8	0	4.593652	-0.84826	1.158376
18	8	0	1.796898	2.811659	0.626498
19	8	0	-3.40667	1.760387	-1.28214
20	6	0	-4.03822	-0.24172	2.253402
21	8	0	3.611813	1.192212	-0.38798
22	1	0	2.625734	-0.33161	-2.07717
23	1	0	0.238134	-0.24329	-2.14751
24	1	0	0.309782	-2.60339	-0.2141
25	1	0	-0.28514	0.953026	0.93194
26	1	0	1.446291	2.166126	-1.31652
27	1	0	-1.86428	-1.11446	-1.80341
28	1	0	-1.76582	-2.86022	-1.84337
29	1	0	-2.59998	-3.14185	0.304957
30	1	0	-1.87889	-1.67187	0.910728

31	1	0	-0.9475	2.484094	-1.64192
32	1	0	1.324649	-0.45443	1.481056
33	1	0	2.68546	0.538599	2.02531
34	1	0	3.053872	-2.11885	1.730612
35	1	0	2.381713	-2.70716	-0.46121
36	1	0	3.879445	-1.96187	-0.97322
37	1	0	-4.61418	-1.99688	0.306717
38	1	0	-4.01691	-1.14463	-1.09707
39	1	0	-4.70491	0.563789	0.368833
40	1	0	5.194047	-1.55767	0.901535
41	1	0	2.76401	2.789922	0.557971
42	1	0	-4.9832	-0.74744	2.46466
43	1	0	-3.2252	-0.84681	2.662058
44	1	0	-4.04133	0.722435	2.766054
45	1	0	4.27935	0.643291	0.059172

5c-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.46102	-0.81279	-0.17106
2	6	0	-2.10243	0.66675	-0.60282
3	6	0	-0.65196	0.983509	-0.82627
4	6	0	0.090589	1.945869	-0.27256
5	6	0	-0.11303	-1.7986	0.065552
6	6	0	-1.42984	-1.54656	0.746945
7	6	0	1.554617	2.135764	-0.58646
8	6	0	2.461861	1.992183	0.659885
9	6	0	2.290361	-1.46585	-0.16988
10	6	0	1.074496	-1.62846	0.65214
11	6	0	-3.81177	-0.66065	0.591312
12	6	0	-4.2468	0.804666	0.450019
13	6	0	-2.92082	1.559248	0.341341
14	6	0	3.913364	1.564347	0.377044
15	6	0	4.078215	0.163368	-0.2355
16	8	0	3.196618	-0.7293	0.517247
17	8	0	-4.95669	1.033828	-0.78001
18	8	0	-1.27606	-0.89141	1.999392
19	8	0	2.434724	-1.81216	-1.32357
20	6	0	5.504194	-0.35982	-0.16772
21	8	0	-2.55894	-1.67308	-1.31087
22	1	0	-2.58561	0.757519	-1.58405
23	1	0	-0.17256	0.353717	-1.57372
24	1	0	-0.34392	2.618969	0.465288
25	1	0	-0.15965	-2.04803	-0.98831

26	1	0	-1.89627	-2.51264	0.974656
27	1	0	1.838394	1.406064	-1.35047
28	1	0	1.721459	3.124078	-1.03278
29	1	0	2.481209	2.942949	1.201833
30	1	0	2.021044	1.262099	1.342348
31	1	0	1.156794	-1.35203	1.695233
32	1	0	-3.66362	-0.88862	1.648682
33	1	0	-4.55473	-1.35941	0.198866
34	1	0	-4.85534	1.141067	1.295883
35	1	0	-2.46207	1.632381	1.331337
36	1	0	-3.05981	2.571001	-0.04489
37	1	0	4.471292	1.598095	1.319333
38	1	0	4.399974	2.276359	-0.29959
39	1	0	3.733434	0.148094	-1.27028
40	1	0	-5.76503	0.510458	-0.75452
41	1	0	-0.75899	-0.08921	1.849401
42	1	0	6.178784	0.324006	-0.68966
43	1	0	5.834427	-0.4421	0.871115
44	1	0	5.578371	-1.34192	-0.63893
45	1	0	-3.23515	-1.31379	-1.89628

Table S23. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*R*, 7*S*, 9*R*, 10*E*, 15*R*)-**5d**] in NMR calculation

5d-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.12209	-0.41244	-0.64004
2	6	0	-1.89456	0.939169	0.156056
3	6	0	-0.79219	1.79862	-0.39846
4	6	0	0.353308	2.077606	0.228413
5	6	0	-0.03132	-1.49348	0.232366
6	6	0	-1.51658	-1.64734	0.11768
7	6	0	1.483655	2.885363	-0.35123
8	6	0	-4.27888	0.45493	0.171211
9	6	0	2.319437	-1.6816	-0.52774
10	6	0	0.884253	-2.05052	-0.56684
11	6	0	-3.65874	-0.54155	-0.80089
12	6	0	2.729246	2.036879	-0.70141
13	6	0	-3.28414	1.617545	0.163832
14	6	0	3.497924	1.460284	0.51203
15	6	0	3.853858	-0.01965	0.370949
16	8	0	2.573327	-0.72555	0.38393

17	8	0	-2.03637	-1.79873	1.434669
18	8	0	3.153319	-2.15644	-1.27272
19	6	0	4.724018	-0.55947	1.495895
20	8	0	-1.58858	-0.38223	-1.96258
21	1	0	-1.64503	0.670085	1.184767
22	1	0	3.40844	2.654593	-1.29641
23	1	0	-0.96066	2.205194	-1.39489
24	1	0	0.512845	1.666998	1.224317
25	1	0	0.299539	-0.809	1.004447
26	1	0	-1.76125	-2.52494	-0.49545
27	1	0	1.778265	3.671462	0.355724
28	1	0	1.138027	3.389392	-1.25924
29	8	0	-4.32783	-0.20437	1.457672
30	1	0	-5.29108	0.753196	-0.11463
31	1	0	0.623131	-2.76832	-1.33678
32	1	0	-3.90379	-0.25307	-1.82469
33	1	0	-4.0289	-1.55627	-0.6403
34	1	0	2.405831	1.22261	-1.35686
35	1	0	-3.43304	2.199824	-0.7519
36	1	0	-3.41665	2.29797	1.009355
37	1	0	2.915522	1.572972	1.432226
38	1	0	4.425667	2.018549	0.667681
39	1	0	4.324363	-0.21602	-0.59437
40	1	0	-2.88923	-1.33131	1.513822
41	1	0	5.6876	-0.04386	1.50396
42	1	0	4.242308	-0.40765	2.465434
43	1	0	4.90898	-1.62721	1.361384
44	1	0	-0.6296	-0.28419	-1.8983
45	1	0	-4.50544	0.451484	2.14198

5d-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.146534	-0.40348	0.651241
2	6	0	1.897394	0.940024	-0.15194
3	6	0	0.786293	1.790333	0.400143
4	6	0	-0.35635	2.073513	-0.23039
5	6	0	0.028643	-1.48046	-0.1982
6	6	0	1.510214	-1.64097	-0.05708
7	6	0	-1.48555	2.885697	0.345477
8	6	0	4.282649	0.472373	-0.23569
9	6	0	-2.33101	-1.67964	0.531427
10	6	0	-0.89463	-2.04702	0.584338
11	6	0	3.686584	-0.54593	0.745516

12	6	0	-2.73661	2.044222	0.692501
13	6	0	3.27886	1.631418	-0.16488
14	6	0	-3.50046	1.463388	-0.52204
15	6	0	-3.85696	-0.01583	-0.37718
16	8	0	-2.57514	-0.72146	-0.37897
17	8	0	2.1281	-1.74723	-1.3486
18	8	0	-3.17023	-2.1588	1.266898
19	6	0	-4.71998	-0.56121	-1.50474
20	8	0	1.653037	-0.35222	1.988704
21	1	0	1.65082	0.664717	-1.18049
22	1	0	-3.4168	2.668231	1.279708
23	1	0	0.951503	2.197963	1.396948
24	1	0	-0.51292	1.667186	-1.2286
25	1	0	-0.29213	-0.78581	-0.96523
26	1	0	1.753345	-2.51463	0.556771
27	1	0	-1.77389	3.672855	-0.36291
28	1	0	-1.14072	3.388789	1.254314
29	8	0	4.407311	-0.05422	-1.56113
30	1	0	5.287538	0.782046	0.059242
31	1	0	-0.64026	-2.76801	1.353504
32	1	0	3.970066	-0.2829	1.767192
33	1	0	4.037465	-1.56028	0.547422
34	1	0	-2.42075	1.232572	1.354803
35	1	0	3.431851	2.189137	0.766279
36	1	0	3.392622	2.327699	-0.99842
37	1	0	-2.91498	1.573396	-1.44056
38	1	0	-4.42801	2.020418	-0.68293
39	1	0	-4.33262	-0.20863	0.586325
40	1	0	1.893326	-2.59405	-1.74376
41	1	0	-5.68345	-0.04562	-1.52065
42	1	0	-4.2326	-0.41366	-2.47206
43	1	0	-4.90587	-1.62825	-1.36624
44	1	0	0.699354	-0.2022	1.953496
45	1	0	3.668811	-0.66817	-1.70046

5d-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.09181	-0.63345	-0.25178
2	6	0	-1.88877	0.74436	0.503208
3	6	0	-0.86658	1.646341	-0.14076
4	6	0	0.305099	2.000241	0.393283
5	6	0	0.182894	-1.53865	0.340334
6	6	0	-1.28926	-1.81398	0.373786

7	6	0	1.324295	2.88473	-0.27554
8	6	0	-4.20849	0.524213	-0.33832
9	6	0	2.46111	-1.58204	-0.62939
10	6	0	1.055798	-2.04477	-0.5361
11	6	0	-3.60219	-0.8766	-0.20493
12	6	0	2.586268	2.128366	-0.75343
13	6	0	-3.30911	1.38501	0.553706
14	6	0	3.508376	1.602824	0.37294
15	6	0	3.964128	0.15789	0.171392
16	8	0	2.749314	-0.64743	0.293513
17	8	0	-1.73767	-1.97484	1.722026
18	8	0	3.238944	-1.97294	-1.47649
19	6	0	4.975869	-0.32444	1.19964
20	8	0	-1.74958	-0.54111	-1.6379
21	1	0	-1.56346	0.514015	1.519323
22	1	0	3.159353	2.795127	-1.40455
23	1	0	-1.13671	2.048721	-1.1169
24	1	0	0.569316	1.608989	1.374584
25	1	0	0.535209	-0.82184	1.072403
26	1	0	-1.52697	-2.70281	-0.22323
27	1	0	1.629164	3.683354	0.41276
28	1	0	0.863192	3.372164	-1.14042
29	8	0	-5.56112	0.62568	0.109726
30	1	0	-4.13809	0.85617	-1.38092
31	1	0	0.769733	-2.77915	-1.28101
32	1	0	-3.91453	-1.57086	-0.98863
33	1	0	-3.88227	-1.28911	0.766843
34	1	0	2.257833	1.296572	-1.38388
35	1	0	-3.30409	2.433896	0.250183
36	1	0	-3.7079	1.340206	1.571426
37	1	0	3.007131	1.657586	1.34472
38	1	0	4.399216	2.232626	0.452597
39	1	0	4.353607	0.009287	-0.83739
40	1	0	-1.28706	-2.73964	2.096784
41	1	0	5.892623	0.266081	1.127874
42	1	0	4.577568	-0.22273	2.212599
43	1	0	5.230067	-1.3725	1.02818
44	1	0	-0.8298	-0.25428	-1.70309
45	1	0	-6.11799	0.163012	-0.52556

5d-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.09185	-0.63185	-0.25319

2	6	0	-1.88998	0.746033	0.50059
3	6	0	-0.86611	1.647311	-0.14132
4	6	0	0.303621	2.003064	0.395879
5	6	0	0.184192	-1.53587	0.337348
6	6	0	-1.288	-1.81156	0.371726
7	6	0	1.324434	2.88671	-0.27176
8	6	0	-4.2143	0.508327	-0.34194
9	6	0	2.462821	-1.58075	-0.63067
10	6	0	1.05732	-2.0433	-0.53799
11	6	0	-3.60104	-0.8811	-0.20651
12	6	0	2.58561	2.128731	-0.74932
13	6	0	-3.31268	1.384047	0.546726
14	6	0	3.507251	1.602555	0.377066
15	6	0	3.96518	0.15862	0.173118
16	8	0	2.751389	-0.6484	0.294344
17	8	0	-1.73477	-1.97238	1.720605
18	8	0	3.240289	-1.96986	-1.47889
19	6	0	4.977672	-0.32407	1.200436
20	8	0	-1.7502	-0.53912	-1.63946
21	1	0	-1.56779	0.516729	1.517962
22	1	0	3.159482	2.794437	-1.40084
23	1	0	-1.13308	2.047591	-1.1192
24	1	0	0.565035	1.613685	1.378688
25	1	0	0.536423	-0.81846	1.068849
26	1	0	-1.52583	-2.70081	-0.22464
27	1	0	1.629862	3.684741	0.41695
28	1	0	0.864563	3.374935	-1.13686
29	8	0	-5.5821	0.475005	0.069563
30	1	0	-4.15072	0.838211	-1.38566
31	1	0	0.771406	-2.77798	-1.28267
32	1	0	-3.91185	-1.57683	-0.98839
33	1	0	-3.87825	-1.29483	0.76586
34	1	0	2.256023	1.297029	-1.37927
35	1	0	-3.30762	2.430776	0.233347
36	1	0	-3.71008	1.346869	1.565064
37	1	0	3.004799	1.654466	1.348374
38	1	0	4.396989	2.233633	0.458954
39	1	0	4.354623	0.01207	-0.83598
40	1	0	-1.28672	-2.73952	2.093637
41	1	0	5.89371	0.267652	1.129444
42	1	0	4.579411	-0.22444	2.213619
43	1	0	5.233076	-1.37156	1.02729
44	1	0	-0.83054	-0.25209	-1.70476
45	1	0	-5.96477	1.340434	-0.1102

Table S24. The coordinate for the lowest-energy conformer [(2*E*, 4*R*, 5*S*, 7*R*, 9*S*, 10*E*, 15*R*)-**5a**] in ECD calculation

5a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.1381	-0.32329	-0.52035
2	6	0	1.897476	0.859705	0.473649
3	6	0	0.588912	1.621959	0.531072
4	6	0	-0.34291	1.800677	-0.40809
5	6	0	0.325895	-1.66842	0.648854
6	6	0	1.699814	-1.70925	0.056059
7	6	0	-1.55949	2.68205	-0.28737
8	6	0	-2.88664	1.945876	-0.59324
9	6	0	-2.08113	-1.52064	0.66226
10	6	0	-0.81507	-1.89503	-0.00366
11	6	0	3.683373	-0.31248	-0.77976
12	6	0	4.278762	0.810184	0.073323
13	6	0	3.113874	1.787935	0.239288
14	6	0	-3.46211	1.164577	0.608606
15	6	0	-4.05428	-0.21277	0.280773
16	8	0	-2.97297	-1.05891	-0.23918
17	8	0	4.667163	0.23319	1.332067
18	8	0	1.812449	-2.6086	-1.05033
19	8	0	-2.273	-1.52876	1.861132
20	6	0	-5.15268	-0.2217	-0.76765
21	8	0	1.437104	-0.10619	-1.74295
22	1	0	2.058764	0.430859	1.469352
23	1	0	0.455856	2.146173	1.479176
24	1	0	-0.22902	1.291215	-1.35815
25	1	0	0.266283	-1.33681	1.680969
26	1	0	2.416066	-1.98031	0.840985
27	1	0	-1.60314	3.151341	0.702117
28	1	0	-1.45458	3.499002	-1.01356
29	1	0	-2.70833	1.26429	-1.43057
30	1	0	-3.62609	2.671439	-0.94342
31	1	0	-0.84239	-2.16204	-1.05255
32	1	0	4.162159	-1.26728	-0.55801
33	1	0	3.839801	-0.0939	-1.83746
34	1	0	5.149618	1.272218	-0.40452
35	1	0	2.975796	2.362924	-0.68223
36	1	0	3.268693	2.49751	1.056753

37	1	0	-2.68342	1.010045	1.360507
38	1	0	-4.24243	1.753539	1.10183
39	1	0	-4.41139	-0.67381	1.202595
40	1	0	4.96951	0.949027	1.902344
41	1	0	1.46994	-3.46961	-0.78616
42	1	0	-5.99649	0.379062	-0.41921
43	1	0	-4.80603	0.190419	-1.71759
44	1	0	-5.50571	-1.24041	-0.9416
45	1	0	1.479217	-0.94706	-2.22011

5a-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.139337	-0.43554	-0.38653
2	6	0	1.971476	0.703551	0.684147
3	6	0	0.558448	1.206456	0.854742
4	6	0	-0.10498	2.078375	0.086627
5	6	0	0.269138	-1.79048	0.630348
6	6	0	1.639666	-1.86823	0.020402
7	6	0	-1.58288	2.343213	0.23329
8	6	0	-2.37178	1.860656	-1.01454
9	6	0	-2.11415	-1.36223	0.616417
10	6	0	-0.88543	-1.86888	-0.03676
11	6	0	3.650988	-0.4227	-0.73198
12	6	0	4.250217	0.844846	-0.07924
13	6	0	3.03898	1.719644	0.237286
14	6	0	-3.81017	1.379209	-0.7594
15	6	0	-3.94211	0.144395	0.143727
16	8	0	-2.94894	-0.83592	-0.30718
17	8	0	4.884779	0.548912	1.175467
18	8	0	1.695203	-2.70277	-1.12919
19	8	0	-2.30903	-1.31305	1.813323
20	6	0	-5.32209	-0.49296	0.095054
21	8	0	1.449061	-0.08354	-1.59498
22	1	0	2.304886	0.283626	1.638098
23	1	0	-0.00051	0.750098	1.667827
24	1	0	0.398623	2.589088	-0.73296
25	1	0	0.232011	-1.519	1.681093
26	1	0	2.336045	-2.28252	0.754621
27	1	0	-1.93919	1.83194	1.131991
28	1	0	-1.77292	3.411528	0.386114
29	1	0	-1.82924	1.037628	-1.486
30	1	0	-2.40215	2.665409	-1.75499
31	1	0	-0.93089	-2.09957	-1.09389

32	1	0	4.158196	-1.31854	-0.36868
33	1	0	3.759757	-0.39799	-1.81741
34	1	0	4.964119	1.344396	-0.74225
35	1	0	2.71843	2.241356	-0.66755
36	1	0	3.264435	2.463172	1.003452
37	1	0	-4.40904	2.176637	-0.3049
38	1	0	-4.2716	1.156133	-1.72775
39	1	0	-3.6909	0.391792	1.174766
40	1	0	5.614387	-0.05574	1.002144
41	1	0	1.451754	-2.13162	-1.87291
42	1	0	-6.08109	0.236171	0.390491
43	1	0	-5.55162	-0.83846	-0.91629
44	1	0	-5.37955	-1.34312	0.777857
45	1	0	0.57946	0.262632	-1.34396

5a-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.124116	-0.41444	-0.46662
2	6	0	2.037922	0.923294	0.327241
3	6	0	0.789051	1.773801	0.36548
4	6	0	-0.36981	1.694068	-0.29368
5	6	0	0.274775	-1.46487	0.920906
6	6	0	1.645921	-1.65759	0.349103
7	6	0	-1.49639	2.677532	-0.09291
8	6	0	-2.79521	2.066397	0.486859
9	6	0	-2.14434	-1.28763	0.797728
10	6	0	-0.85452	-1.81963	0.307713
11	6	0	3.643154	-0.56343	-0.82297
12	6	0	4.36814	0.651182	-0.23782
13	6	0	3.273787	1.716971	-0.16094
14	6	0	-3.68108	1.287919	-0.52218
15	6	0	-4.09265	-0.12298	-0.08884
16	8	0	-2.92442	-0.99224	-0.26121
17	8	0	4.836602	0.280839	1.07053
18	8	0	1.713547	-2.74003	-0.58297
19	8	0	-2.4346	-1.06473	1.954752
20	6	0	-5.20227	-0.72056	-0.93945
21	8	0	1.348848	-0.32298	-1.66148
22	1	0	2.265738	0.658016	1.367963
23	1	0	0.90082	2.606789	1.062991
24	1	0	-0.52732	0.888311	-1.00095
25	1	0	0.214348	-0.9054	1.849204
26	1	0	2.362037	-1.80981	1.165993

27	1	0	-1.15428	3.470768	0.580074
28	1	0	-1.7372	3.16386	-1.04812
29	1	0	-3.389	2.882795	0.908469
30	1	0	-2.53116	1.42427	1.330379
31	1	0	-0.8478	-2.3128	-0.65604
32	1	0	4.080004	-1.49199	-0.45427
33	1	0	3.732026	-0.55913	-1.91066
34	1	0	5.215844	0.96287	-0.85758
35	1	0	3.08541	2.129054	-1.15785
36	1	0	3.533821	2.546848	0.501782
37	1	0	-4.5973	1.854855	-0.71254
38	1	0	-3.17632	1.195672	-1.48992
39	1	0	-4.36581	-0.14299	0.967125
40	1	0	5.230235	1.062906	1.473458
41	1	0	1.370861	-3.53455	-0.15888
42	1	0	-6.11745	-0.13533	-0.82362
43	1	0	-4.92448	-0.72139	-1.99691
44	1	0	-5.41016	-1.74817	-0.63402
45	1	0	1.343766	-1.2126	-2.04076

5a-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.063453	-0.37569	-0.45382
2	6	0	1.897127	0.794575	0.582851
3	6	0	0.536857	1.452581	0.707952
4	6	0	-0.12102	2.129226	-0.24106
5	6	0	0.293155	-1.7398	0.707052
6	6	0	1.659749	-1.79065	0.085434
7	6	0	-1.46746	2.792957	-0.0759
8	6	0	-2.6568	1.927403	-0.58786
9	6	0	-2.12384	-1.56282	0.674538
10	6	0	-0.8477	-1.99498	0.063185
11	6	0	3.558168	-0.33482	-0.87228
12	6	0	4.214388	0.804802	-0.07453
13	6	0	3.055502	1.750587	0.2202
14	6	0	-3.37229	1.166029	0.547588
15	6	0	-4.01569	-0.17184	0.159764
16	8	0	-2.95125	-1.08282	-0.2787
17	8	0	4.716424	0.351622	1.193387
18	8	0	1.749986	-2.72497	-0.98238
19	8	0	-2.36821	-1.53778	1.86242
20	6	0	-5.02037	-0.11244	-0.97709
21	8	0	1.30398	-0.15516	-1.65101

22	1	0	2.148754	0.367431	1.557178
23	1	0	0.076766	1.386429	1.692014
24	1	0	0.321913	2.225139	-1.23102
25	1	0	0.238682	-1.35061	1.719664
26	1	0	2.390599	-2.09184	0.841384
27	1	0	-1.63201	3.047726	0.975968
28	1	0	-1.45079	3.738765	-0.62592
29	1	0	-2.28318	1.21788	-1.33149
30	1	0	-3.37485	2.56702	-1.10773
31	1	0	-0.86741	-2.34153	-0.96288
32	1	0	4.061624	-1.28951	-0.70965
33	1	0	3.602617	-0.11871	-1.9417
34	1	0	5.01899	1.286945	-0.64003
35	1	0	2.80969	2.326173	-0.67638
36	1	0	3.28927	2.451753	1.023487
37	1	0	-2.66848	0.960118	1.357995
38	1	0	-4.15154	1.800016	0.984073
39	1	0	-4.47439	-0.6115	1.046835
40	1	0	5.391858	-0.31342	1.02204
41	1	0	1.467476	-2.24271	-1.77341
42	1	0	-5.84612	0.54928	-0.70426
43	1	0	-4.5646	0.265623	-1.89463
44	1	0	-5.42821	-1.10527	-1.17816
45	1	0	0.396513	0.056911	-1.38926

5a-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.14192	0.479084	-0.35337
2	6	0	-1.97243	-0.7099	0.651186
3	6	0	-0.56263	-1.20078	0.865845
4	6	0	0.109057	-2.1005	0.146085
5	6	0	-0.2278	1.795883	0.668092
6	6	0	-1.62218	1.874271	0.124124
7	6	0	1.586499	-2.35513	0.30743
8	6	0	2.361527	-1.92108	-0.96674
9	6	0	2.148918	1.358867	0.574215
10	6	0	0.894918	1.832097	-0.0536
11	6	0	-3.67681	0.510041	-0.61893
12	6	0	-4.23703	-0.85758	-0.17707
13	6	0	-2.99805	-1.71854	0.104521
14	6	0	3.805069	-1.43607	-0.7524
15	6	0	3.954831	-0.1722	0.106201
16	8	0	2.948738	0.789776	-0.35381

17	8	0	-4.99962	-0.62752	1.021866
18	8	0	-1.7273	2.701753	-1.04028
19	8	0	2.391753	1.370957	1.763688
20	6	0	5.332092	0.465475	0.006859
21	8	0	-1.4475	0.126948	-1.54719
22	1	0	-2.36258	-0.35003	1.610408
23	1	0	-0.02248	-0.71599	1.675737
24	1	0	-0.37967	-2.61795	-0.67736
25	1	0	-0.1457	1.581355	1.72901
26	1	0	-2.29432	2.238489	0.909632
27	1	0	1.943158	-1.80164	1.181272
28	1	0	1.788436	-3.41445	0.506142
29	1	0	1.808169	-1.118	-1.45827
30	1	0	2.380273	-2.7549	-1.6755
31	1	0	0.888857	1.987186	-1.12463
32	1	0	-4.17487	1.291587	-0.04187
33	1	0	-3.86135	0.705308	-1.67579
34	1	0	-4.8849	-1.3045	-0.93818
35	1	0	-2.63622	-2.15667	-0.82916
36	1	0	-3.20669	-2.5328	0.802965
37	1	0	4.410889	-2.21868	-0.28119
38	1	0	4.251312	-1.24648	-1.73518
39	1	0	3.727313	-0.3864	1.150125
40	1	0	-5.33047	-1.48062	1.324642
41	1	0	-1.32643	3.55639	-0.84675
42	1	0	6.098877	-0.25241	0.309819
43	1	0	5.539298	0.777399	-1.02015
44	1	0	5.402249	1.337845	0.659796
45	1	0	-1.4662	0.917005	-2.10446

5a-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.128521	-0.29572	-0.53277
2	6	0	1.8791	0.871125	0.480854
3	6	0	0.572128	1.636044	0.534129
4	6	0	-0.35638	1.820547	-0.40711
5	6	0	0.349725	-1.67582	0.640193
6	6	0	1.722285	-1.69213	0.041794
7	6	0	-1.57999	2.69101	-0.2803
8	6	0	-2.89974	1.940317	-0.58367
9	6	0	-2.05865	-1.53542	0.653084
10	6	0	-0.79026	-1.89417	-0.01703
11	6	0	3.668451	-0.2542	-0.81181

12	6	0	4.262631	0.82669	0.102393
13	6	0	3.104627	1.799644	0.291603
14	6	0	-3.45886	1.145294	0.616749
15	6	0	-4.04001	-0.23559	0.28399
16	8	0	-2.95284	-1.06922	-0.24389
17	8	0	4.598714	0.311335	1.401739
18	8	0	1.845317	-2.58658	-1.06756
19	8	0	-2.25084	-1.55816	1.851657
20	6	0	-5.14221	-0.24921	-0.76039
21	8	0	1.407939	-0.08685	-1.74496
22	1	0	2.019089	0.422144	1.470622
23	1	0	0.433235	2.151223	1.486356
24	1	0	-0.23793	1.319917	-1.36111
25	1	0	0.288267	-1.36476	1.678514
26	1	0	2.448443	-1.95055	0.821959
27	1	0	-1.62559	3.156438	0.710897
28	1	0	-1.48641	3.511031	-1.00444
29	1	0	-2.71709	1.265405	-1.42546
30	1	0	-3.65002	2.658398	-0.92612
31	1	0	-0.81589	-2.14123	-1.07074
32	1	0	4.152907	-1.2236	-0.67537
33	1	0	3.804628	0.03814	-1.85558
34	1	0	5.142728	1.301893	-0.34488
35	1	0	2.981028	2.408522	-0.60885
36	1	0	3.262816	2.469417	1.139473
37	1	0	-2.67331	0.993245	1.362053
38	1	0	-4.24124	1.723351	1.119565
39	1	0	-4.38945	-0.70452	1.204685
40	1	0	5.260932	-0.37796	1.282068
41	1	0	1.5052	-3.45007	-0.80851
42	1	0	-5.98983	0.342723	-0.40616
43	1	0	-4.80274	0.170102	-1.70976
44	1	0	-5.4872	-1.27009	-0.93761
45	1	0	1.462817	-0.9238	-2.22772

5a-Conf.7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.121403	-0.38397	-0.49312
2	6	0	2.021365	0.940098	0.325758
3	6	0	0.775867	1.7963	0.341866
4	6	0	-0.38619	1.700433	-0.30937
5	6	0	0.302353	-1.46486	0.905563
6	6	0	1.669368	-1.64055	0.317856

7	6	0	-1.51869	2.678187	-0.11573
8	6	0	-2.80749	2.061311	0.480867
9	6	0	-2.11888	-1.29484	0.79969
10	6	0	-0.83004	-1.81787	0.297099
11	6	0	3.637929	-0.50557	-0.86445
12	6	0	4.361627	0.666112	-0.18647
13	6	0	3.281432	1.737047	-0.09393
14	6	0	-3.69599	1.26684	-0.51346
15	6	0	-4.0855	-0.14678	-0.06879
16	8	0	-2.90976	-1.00338	-0.25223
17	8	0	4.757604	0.349171	1.15889
18	8	0	1.738524	-2.71592	-0.62179
19	8	0	-2.40058	-1.07526	1.95939
20	6	0	-5.19902	-0.76076	-0.9026
21	8	0	1.33362	-0.29594	-1.67932
22	1	0	2.208252	0.651824	1.368276
23	1	0	0.887689	2.640509	1.025809
24	1	0	-0.54385	0.882517	-1.00225
25	1	0	0.246209	-0.91556	1.840159
26	1	0	2.397515	-1.78848	1.125004
27	1	0	-1.17954	3.483273	0.544542
28	1	0	-1.77065	3.149422	-1.07556
29	1	0	-3.40435	2.87614	0.901075
30	1	0	-2.53022	1.428348	1.327269
31	1	0	-0.82846	-2.30207	-0.67122
32	1	0	4.066541	-1.47138	-0.5895
33	1	0	3.719726	-0.4055	-1.94925
34	1	0	5.234795	0.995432	-0.76031
35	1	0	3.12969	2.195736	-1.07569
36	1	0	3.539759	2.524468	0.617068
37	1	0	-4.62134	1.821663	-0.69511
38	1	0	-3.20214	1.176275	-1.48698
39	1	0	-4.34499	-0.1652	0.99062
40	1	0	5.366348	-0.39631	1.118002
41	1	0	1.404659	-3.51593	-0.201
42	1	0	-6.11934	-0.18553	-0.77769
43	1	0	-4.93468	-0.76319	-1.9635
44	1	0	-5.3912	-1.78929	-0.59008
45	1	0	1.337029	-1.18335	-2.06384

5a-Conf.8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.13989	0.476799	-0.35031

2	6	0	-1.97113	-0.70966	0.65687
3	6	0	-0.56075	-1.19962	0.871363
4	6	0	0.110635	-2.10201	0.154755
5	6	0	-0.22718	1.79807	0.668042
6	6	0	-1.62273	1.873209	0.126373
7	6	0	1.588625	-2.3543	0.31544
8	6	0	2.361499	-1.92395	-0.96129
9	6	0	2.149745	1.362307	0.57006
10	6	0	0.893923	1.83297	-0.05625
11	6	0	-3.67439	0.504222	-0.62164
12	6	0	-4.23303	-0.87222	-0.17708
13	6	0	-2.99564	-1.7224	0.113212
14	6	0	3.804886	-1.43674	-0.75102
15	6	0	3.955194	-0.16962	0.102744
16	8	0	2.946969	0.789792	-0.35801
17	8	0	-4.97043	-0.77587	1.053783
18	8	0	-1.73149	2.700324	-1.0379
19	8	0	2.39572	1.379079	1.758832
20	6	0	5.331527	0.46919	-0.00259
21	8	0	-1.44264	0.123909	-1.542
22	1	0	-2.3593	-0.34768	1.616099
23	1	0	-0.0198	-0.71126	1.678554
24	1	0	-0.37844	-2.6237	-0.6658
25	1	0	-0.14263	1.586816	1.72943
26	1	0	-2.29415	2.236033	0.913271
27	1	0	1.945567	-1.79696	1.186754
28	1	0	1.792192	-3.41259	0.517931
29	1	0	1.806622	-1.12316	-1.45481
30	1	0	2.38001	-2.76025	-1.66716
31	1	0	0.885524	1.984749	-1.12775
32	1	0	-4.16745	1.298592	-0.05597
33	1	0	-3.85188	0.69275	-1.68169
34	1	0	-4.8704	-1.32042	-0.94638
35	1	0	-2.6302	-2.1681	-0.81438
36	1	0	-3.21877	-2.52439	0.818879
37	1	0	4.41229	-2.21706	-0.27805
38	1	0	4.249254	-1.25033	-1.73529
39	1	0	3.730635	-0.38031	1.148048
40	1	0	-5.72761	-0.20074	0.898747
41	1	0	-1.32998	3.555021	-0.84581
42	1	0	6.099885	-0.24681	0.300846
43	1	0	5.535565	0.777571	-1.03133
44	1	0	5.402523	1.344021	0.646966
45	1	0	-1.46227	0.912849	-2.10088

5a-Conf.9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.164084	-0.23674	-0.57147
2	6	0	1.88038	0.892576	0.485892
3	6	0	0.616848	1.724888	0.443236
4	6	0	-0.39753	1.716089	-0.42478
5	6	0	0.349737	-1.62248	0.541041
6	6	0	1.712207	-1.65763	-0.09252
7	6	0	-1.59247	2.635462	-0.39585
8	6	0	-2.93271	1.896736	-0.6136
9	6	0	-2.04992	-1.53889	0.672261
10	6	0	-0.8111	-1.92088	-0.04161
11	6	0	3.705114	-0.19574	-0.79476
12	6	0	4.282043	0.734645	0.278627
13	6	0	3.167058	1.756038	0.479978
14	6	0	-3.45204	1.143244	0.630855
15	6	0	-4.04624	-0.24642	0.359849
16	8	0	-2.98583	-1.09722	-0.19535
17	8	0	4.4709	0.060346	1.532855
18	8	0	1.807471	-2.57271	-1.17364
19	8	0	-2.18752	-1.52194	1.878451
20	6	0	-5.19474	-0.28424	-0.633
21	8	0	1.475522	-0.0818	-1.82385
22	1	0	1.890589	0.389455	1.460271
23	1	0	0.571196	2.440523	1.266352
24	1	0	-0.37765	1.013181	-1.24934
25	1	0	0.315308	-1.23989	1.55663
26	1	0	2.429747	-1.98021	0.668202
27	1	0	-1.61646	3.213474	0.535092
28	1	0	-1.48114	3.364412	-1.20998
29	1	0	-2.79467	1.194074	-1.4412
30	1	0	-3.68557	2.616122	-0.94742
31	1	0	-0.88271	-2.2548	-1.06944
32	1	0	4.153207	-1.1914	-0.7851
33	1	0	3.909564	0.232274	-1.78144
34	1	0	5.222835	1.194821	-0.04182
35	1	0	3.158059	2.459247	-0.35874
36	1	0	3.293407	2.328874	1.400752
37	1	0	-2.6419	1.013444	1.353419
38	1	0	-4.21726	1.737707	1.140693
39	1	0	-4.35467	-0.69036	1.307123
40	1	0	5.117819	-0.64065	1.397701

41	1	0	1.570625	-2.06311	-1.96252
42	1	0	-4.89853	0.108846	-1.60781
43	1	0	-5.54882	-1.30854	-0.76736
44	1	0	-6.02458	0.31898	-0.25639
45	1	0	1.842921	0.67001	-2.30037

5a-Conf.10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.167378	-0.25762	-0.56508
2	6	0	1.890867	0.883903	0.479834
3	6	0	0.623654	1.710737	0.443058
4	6	0	-0.38545	1.711105	-0.43116
5	6	0	0.336182	-1.61914	0.552049
6	6	0	1.698259	-1.67124	-0.08019
7	6	0	-1.57866	2.632693	-0.40134
8	6	0	-2.92133	1.899228	-0.62312
9	6	0	-2.06306	-1.5282	0.683195
10	6	0	-0.82569	-1.9227	-0.02583
11	6	0	3.711011	-0.23537	-0.78194
12	6	0	4.292353	0.72612	0.253044
13	6	0	3.171962	1.7526	0.441161
14	6	0	-3.45218	1.156511	0.62291
15	6	0	-4.05379	-0.23094	0.357055
16	8	0	-2.99673	-1.09124	-0.1893
17	8	0	4.528294	-0.028	1.452546
18	8	0	1.784119	-2.59142	-1.15769
19	8	0	-2.2015	-1.49869	1.889113
20	6	0	-5.19833	-0.26696	-0.6404
21	8	0	1.485419	-0.1012	-1.82149
22	1	0	1.918775	0.392875	1.460347
23	1	0	0.573686	2.419132	1.272171
24	1	0	-0.36083	1.016121	-1.26237
25	1	0	0.304086	-1.22085	1.561704
26	1	0	2.411705	-1.99883	0.682102
27	1	0	-1.60255	3.208375	0.531059
28	1	0	-1.46341	3.363543	-1.21323
29	1	0	-2.7821	1.190816	-1.44559
30	1	0	-3.66847	2.620428	-0.96579
31	1	0	-0.89793	-2.27099	-1.04883
32	1	0	4.157521	-1.22792	-0.71324
33	1	0	3.924866	0.145205	-1.78467
34	1	0	5.227462	1.182066	-0.08934
35	1	0	3.150886	2.436132	-0.41473

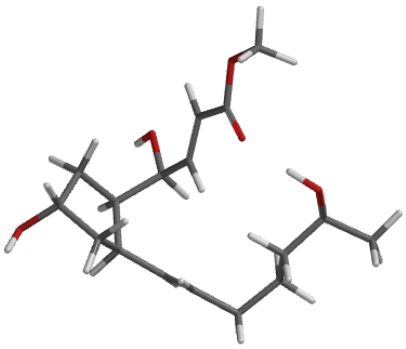
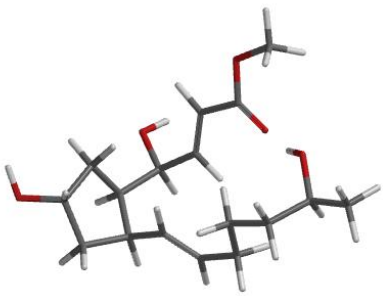
36	1	0	3.297373	2.357478	1.343175
37	1	0	-2.64688	1.025885	1.350645
38	1	0	-4.21628	1.758982	1.124957
39	1	0	-4.36891	-0.66771	1.305512
40	1	0	4.813289	0.587338	2.137356
41	1	0	1.554635	-2.08125	-1.94845
42	1	0	-6.02613	0.343127	-0.27041
43	1	0	-4.89551	0.119439	-1.61587
44	1	0	-5.55796	-1.28979	-0.77118
45	1	0	1.87678	0.630345	-2.31022

5a-Conf.11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.057024	-0.50451	-0.39661
2	6	0	1.907215	0.787814	0.48187
3	6	0	0.511436	1.363113	0.571194
4	6	0	-0.02999	2.298172	-0.21675
5	6	0	0.257951	-1.7188	0.890969
6	6	0	1.620255	-1.85394	0.273623
7	6	0	-1.40521	2.919971	-0.04631
8	6	0	-2.51973	2.016343	0.523335
9	6	0	-2.15088	-1.41156	0.775734
10	6	0	-0.88715	-1.98224	0.258475
11	6	0	3.555103	-0.53738	-0.80376
12	6	0	4.192399	0.760376	-0.26758
13	6	0	3.007376	1.703839	-0.08627
14	6	0	-3.33256	1.277473	-0.56264
15	6	0	-3.96681	-0.0494	-0.11803
16	8	0	-2.93638	-1.08363	-0.27047
17	8	0	4.776904	0.571881	1.031433
18	8	0	1.684917	-2.8791	-0.71005
19	8	0	-2.4101	-1.17056	1.936275
20	6	0	-5.1395	-0.48552	-0.98051
21	8	0	1.307572	-0.37375	-1.61452
22	1	0	2.217027	0.508291	1.494138
23	1	0	-0.09326	0.966481	1.380405
24	1	0	0.572146	2.732122	-1.01195
25	1	0	0.214677	-1.24917	1.86932
26	1	0	2.349233	-2.10404	1.049336
27	1	0	-1.28348	3.796329	0.603389
28	1	0	-1.7273	3.327661	-1.01052
29	1	0	-3.20942	2.628501	1.112021
30	1	0	-2.09501	1.301358	1.228479

31	1	0	-0.90653	-2.41247	-0.73493
32	1	0	4.068984	-1.41964	-0.41764
33	1	0	3.612569	-0.57347	-1.89314
34	1	0	4.945595	1.158864	-0.9554
35	1	0	2.715166	2.103665	-1.06045
36	1	0	3.244453	2.540831	0.572727
37	1	0	-4.12366	1.940274	-0.92738
38	1	0	-2.69903	1.050604	-1.42673
39	1	0	-4.25472	-0.01937	0.934022
40	1	0	5.47257	-0.08931	0.948661
41	1	0	1.390388	-2.46393	-1.53416
42	1	0	-5.96069	0.227841	-0.87958
43	1	0	-4.8509	-0.53288	-2.034
44	1	0	-5.49834	-1.47	-0.67327
45	1	0	0.454585	0.030188	-1.39523

Table S25. The Information of conformations of (2*E*, 4*S*, 5*R*, 7*S*, 9*R*, 10*E*, 15*S*)-**6a** and (2*E*, 4*S*, 5*R*, 7*R*, 9*R*, 10*E*, 15*S*)-**6b**

Label	**Conformers**	**Calculated energy (kJ/mol)**	**Boltzmann distribution**
6a-Conf.1		0	0.920
6a-Conf.2		9.25	0.022

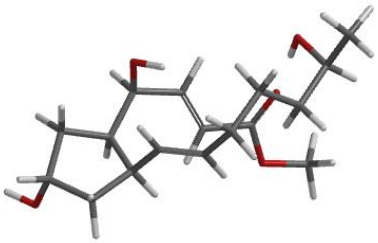
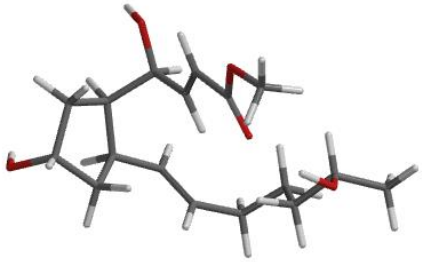
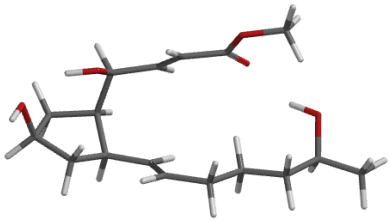
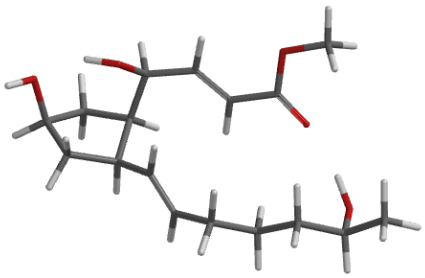
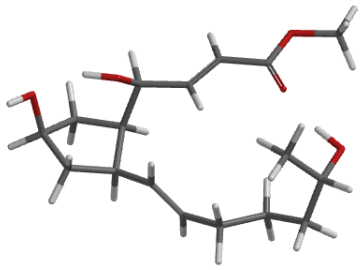
6a-Conf.3		9.60	0.019
6a-Conf.4		10.12	0.016
6b-Conf.1		0	0.410
6a-Conf.2		0.24	0.372
6b-Conf.3		4.74	0.060

Table S26. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 9*R*, 10*E*, 15*S*)-**6a**] in NMR calculation

6a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.928063	0.020042	0.870617
2	6	0	2.679184	-1.29095	0.03228
3	6	0	1.566895	-2.19054	0.501866
4	6	0	0.501198	-2.57776	-0.2022
5	6	0	0.554269	0.97713	0.728475
6	6	0	1.699642	0.609309	1.61416
7	6	0	-0.5979	-3.46905	0.316801
8	6	0	-1.88169	-2.70818	0.722767
9	6	0	-1.24326	2.355185	-0.16808
10	6	0	-0.0679	2.158958	0.700221
11	6	0	3.552415	1.026529	-0.13807
12	6	0	3.734757	0.272213	-1.46086
13	6	0	2.645027	-0.80475	-1.42635
14	8	0	2.078866	1.758054	2.3704
15	8	0	5.049386	-0.31162	-1.44183
16	8	0	-1.66783	1.549513	-0.98185
17	6	0	-2.52254	-1.89398	-0.4084
18	6	0	-3.70647	-1.01908	0.032296
19	6	0	-4.97335	-1.80842	0.332515
20	1	0	3.64488	-0.21407	1.663224
21	1	0	3.609043	-1.86209	0.136204
22	8	0	-4.04313	-0.07343	-0.99426
23	8	0	-1.82105	3.545693	0.048356
24	6	0	-3.01134	3.832231	-0.71847
25	1	0	1.679009	-2.56976	1.518407
26	1	0	0.384429	-2.21828	-1.22188
27	1	0	0.180713	0.181038	0.09529
28	1	0	1.320759	-0.17101	2.292326
29	1	0	-0.2366	-4.02521	1.187818
30	1	0	-0.85529	-4.21137	-0.44878
31	1	0	-1.63496	-2.03497	1.552721
32	1	0	-2.60024	-3.43553	1.115725
33	1	0	0.236394	2.984274	1.329368
34	1	0	4.508442	1.426357	0.202917
35	1	0	2.881888	1.875711	-0.28887
36	1	0	3.640762	0.934155	-2.32883
37	1	0	1.681512	-0.34966	-1.67933
38	1	0	2.827258	-1.60741	-2.14653
39	1	0	2.761898	1.488939	2.994159
40	1	0	5.144559	-0.84204	-2.24077
41	1	0	-2.85028	-2.55718	-1.21906
42	1	0	-1.77364	-1.22109	-0.83692
43	1	0	-3.4075	-0.47205	0.939231
44	1	0	-4.81268	-2.52907	1.137513

45	1	0	-5.77795	-1.1331	0.633515
46	1	0	-5.2976	-2.35277	-0.55982
47	1	0	-3.2689	0.496193	-1.12193
48	1	0	-2.7713	3.890639	-1.7806
49	1	0	-3.76085	3.057633	-0.55476
50	1	0	-3.36565	4.79274	-0.35431

6a-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.827651	0.090774	0.801321
2	6	0	2.565247	-1.43606	0.622699
3	6	0	1.187409	-1.77939	0.122718
4	6	0	0.354587	-2.63119	0.72318
5	6	0	0.485446	1.16506	0.968553
6	6	0	1.816449	0.918769	1.62802
7	6	0	-1.06732	-2.93702	0.325187
8	6	0	-1.6263	-2.08848	-0.82227
9	6	0	-1.24015	2.504365	-0.15688
10	6	0	0.084366	2.339547	0.472872
11	6	0	3.128974	0.6037	-0.62176
12	6	0	3.737466	-0.60491	-1.38882
13	6	0	3.669865	-1.79302	-0.40141
14	8	0	2.495852	2.138461	1.941477
15	8	0	5.052812	-0.375	-1.90223
16	8	0	-2.09202	1.643512	-0.29837
17	6	0	-3.15374	-2.12256	-0.97425
18	6	0	-3.94229	-1.70514	0.282711
19	6	0	-5.399	-1.37967	-0.04939
20	1	0	3.750539	0.162685	1.387116
21	1	0	2.73196	-1.95914	1.568996
22	8	0	-3.32685	-0.62575	0.997437
23	8	0	-1.40899	3.765527	-0.58649
24	6	0	-2.66467	4.064617	-1.23229
25	1	0	0.868898	-1.27676	-0.78785
26	1	0	0.69828	-3.13532	1.626777
27	1	0	-0.1912	0.318904	0.922645
28	1	0	1.618448	0.355524	2.552617
29	1	0	-1.68278	-2.787	1.219236
30	1	0	-1.16155	-4.00578	0.087541
31	1	0	-1.17127	-2.39827	-1.76952
32	1	0	-1.32963	-1.04799	-0.67111
33	1	0	0.720079	3.215273	0.502077
34	1	0	3.823454	1.445682	-0.62204

35	1	0	2.216328	0.944809	-1.1169
36	1	0	3.14469	-0.81631	-2.28051
37	1	0	3.497583	-2.74874	-0.90014
38	1	0	4.630698	-1.86278	0.121536
39	1	0	1.94369	2.639132	2.55312
40	1	0	5.633255	-0.20139	-1.15194
41	1	0	-3.49156	-3.12405	-1.26596
42	1	0	-3.42744	-1.45441	-1.80065
43	1	0	-3.93135	-2.53627	0.995135
44	1	0	-5.9488	-1.12367	0.859581
45	1	0	-5.8949	-2.23205	-0.5242
46	1	0	-5.45423	-0.52841	-0.73592
47	1	0	-3.0518	0.073439	0.385658
48	1	0	-2.79641	3.437089	-2.11405
49	1	0	-2.60192	5.112184	-1.5146
50	1	0	-3.49345	3.903273	-0.54235

6a-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.53324	0.247228	0.58495
2	6	0	-2.32006	-0.465	-0.80186
3	6	0	-1.39318	-1.65616	-0.78209
4	6	0	-0.17477	-1.68711	-1.33048
5	6	0	-0.10223	0.901654	1.079888
6	6	0	-1.36504	0.245128	1.587987
7	6	0	0.771863	-2.8553	-1.27996
8	6	0	2.011931	-2.60207	-0.39186
9	6	0	1.286327	2.60485	-0.00042
10	6	0	-0.01898	2.048119	0.398199
11	6	0	-3.83469	-0.35969	1.127439
12	6	0	-4.72485	-0.43614	-0.11664
13	6	0	-3.76721	-0.87544	-1.23442
14	8	0	-1.07786	-1.04944	2.125068
15	8	0	-5.2327	0.861773	-0.475
16	8	0	2.380153	2.093025	0.181135
17	6	0	2.966054	-1.52986	-0.93329
18	6	0	4.02689	-1.04045	0.069457
19	6	0	4.904267	-2.14853	0.640163
20	1	0	-2.74681	1.296591	0.358928
21	1	0	-1.90639	0.261576	-1.50388
22	8	0	3.419571	-0.36779	1.183307
23	8	0	1.138671	3.786908	-0.616
24	6	0	2.34713	4.44007	-1.06118

25	1	0	-1.77388	-2.56027	-0.30349
26	1	0	0.183689	-0.79009	-1.83234
27	1	0	0.817245	0.386502	1.344675
28	1	0	-1.69512	0.823731	2.459342
29	1	0	1.108392	-3.0982	-2.29633
30	1	0	0.240428	-3.73554	-0.90421
31	1	0	2.549355	-3.54893	-0.27885
32	1	0	1.677803	-2.31123	0.609032
33	1	0	-0.89087	2.623257	0.111324
34	1	0	-4.28543	0.23515	1.927665
35	1	0	-3.65322	-1.36445	1.521496
36	1	0	-5.56043	-1.1335	0.007454
37	1	0	-3.82869	-1.95818	-1.36853
38	1	0	-4.06037	-0.41515	-2.17956
39	1	0	-0.77069	-1.59997	1.39387
40	1	0	-5.7821	1.171223	0.253911
41	1	0	2.398414	-0.64925	-1.2518
42	1	0	3.475668	-1.90714	-1.82858
43	1	0	4.674225	-0.32927	-0.46301
44	1	0	4.314125	-2.8441	1.242035
45	1	0	5.678148	-1.71978	1.281346
46	1	0	5.391795	-2.71196	-0.15989
47	1	0	3.048817	0.46915	0.857641
48	1	0	3.003327	4.640115	-0.21394
49	1	0	2.020168	5.369453	-1.51965
50	1	0	2.868284	3.816618	-1.78806

6a-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.926168	-0.04264	0.88942
2	6	0	2.655198	-1.3276	0.019563
3	6	0	1.53905	-2.22724	0.483317
4	6	0	0.468102	-2.59537	-0.22256
5	6	0	0.565672	0.953205	0.751339
6	6	0	1.70149	0.554832	1.635678
7	6	0	-0.63983	-3.47934	0.289274
8	6	0	-1.91391	-2.70633	0.703141
9	6	0	-1.19587	2.374234	-0.14735
10	6	0	-0.02621	2.150386	0.722514
11	6	0	3.57851	0.974276	-0.09126
12	6	0	3.686194	0.279911	-1.46571
13	6	0	2.599772	-0.80248	-1.42546
14	8	0	2.095507	1.68558	2.410018

15	8	0	4.991714	-0.26793	-1.71023
16	8	0	-1.6441	1.574449	-0.95405
17	6	0	-2.54253	-1.87072	-0.41929
18	6	0	-3.71763	-0.98766	0.028712
19	6	0	-4.99535	-1.76558	0.312401
20	1	0	3.628615	-0.30934	1.684669
21	1	0	3.573276	-1.92616	0.106813
22	8	0	-4.03824	-0.02433	-0.98622
23	8	0	-1.73745	3.583422	0.057892
24	6	0	-2.91716	3.899059	-0.71386
25	1	0	1.652903	-2.61947	1.494471
26	1	0	0.352649	-2.2232	-1.23767
27	1	0	0.169478	0.167051	0.11985
28	1	0	1.308377	-0.2302	2.299851
29	1	0	-0.28435	-4.04796	1.154532
30	1	0	-0.90651	-4.21066	-0.48357
31	1	0	-1.65902	-2.0461	1.540993
32	1	0	-2.64224	-3.42871	1.087053
33	1	0	0.29906	2.969189	1.349625
34	1	0	4.564182	1.305389	0.240608
35	1	0	2.95512	1.867926	-0.17268
36	1	0	3.53451	0.98183	-2.28671
37	1	0	1.628012	-0.34667	-1.64051
38	1	0	2.776183	-1.57979	-2.17187
39	1	0	2.767447	1.39638	3.036918
40	1	0	5.215367	-0.86073	-0.98437
41	1	0	-2.87529	-2.51988	-1.2392
42	1	0	-1.78502	-1.2009	-0.83737
43	1	0	-3.4161	-0.45689	0.944444
44	1	0	-4.84701	-2.49997	1.107308
45	1	0	-5.79282	-1.08479	0.619984
46	1	0	-5.32251	-2.29262	-0.58922
47	1	0	-3.25729	0.538345	-1.10256
48	1	0	-2.6747	3.935403	-1.7764
49	1	0	-3.69197	3.151882	-0.54078
50	1	0	-3.23974	4.875425	-0.36264

Table S27. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*R*, 9*R*, 10*E*, 15*S*)-**6b**] in NMR calculation

6b-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.887412	0.01424	1.251847
2	6	0	2.495441	-1.35474	0.616128
3	6	0	1.041944	-1.54903	0.286278
4	6	0	0.525533	-2.02917	-0.84545
5	6	0	0.902011	1.529677	0.744824
6	6	0	2.374776	1.312954	0.56576
7	6	0	-0.9417	-2.22119	-1.13991
8	6	0	-1.91476	-1.76204	-0.05022
9	6	0	-1.35245	2.199643	0.067418
10	6	0	0.085774	2.02519	-0.1898
11	6	0	4.427741	-0.09334	1.24428
12	6	0	4.801989	-0.79436	-0.07309
13	6	0	3.533439	-1.57735	-0.50622
14	8	0	2.689226	1.438143	-0.81145
15	8	0	5.158268	0.242155	-1.02132
16	8	0	-1.95967	1.785559	1.043741
17	6	0	-3.38628	-1.9436	-0.43819
18	6	0	-4.37389	-1.35389	0.577937
19	6	0	-5.81474	-1.74338	0.274338
20	1	0	2.521784	0.065802	2.28236
21	1	0	2.726464	-2.08221	1.408738
22	8	0	-4.34097	0.082935	0.589028
23	8	0	-1.94647	2.868262	-0.93461
24	6	0	-3.37003	3.088935	-0.8161
25	1	0	0.36719	-1.29549	1.100316
26	1	0	1.193375	-2.30557	-1.65899
27	1	0	0.495251	1.29846	1.725202
28	1	0	2.859687	2.129601	1.133811
29	1	0	-1.1741	-1.69011	-2.07367
30	1	0	-1.11983	-3.28141	-1.3692
31	1	0	-1.72186	-2.3164	0.876111
32	1	0	-1.72136	-0.70946	0.176235
33	1	0	0.452829	2.297036	-1.17002
34	1	0	4.742349	-0.72058	2.082177
35	1	0	4.944411	0.86457	1.340382
36	1	0	5.667958	-1.4488	0.051395
37	1	0	3.740784	-2.63719	-0.66789
38	1	0	3.169258	-1.16168	-1.44867
39	1	0	3.627146	1.207309	-0.94819
40	1	0	5.329368	-0.17173	-1.87575
41	1	0	-3.58135	-1.47427	-1.41046
42	1	0	-3.59993	-3.01299	-0.55288
43	1	0	-4.11089	-1.72491	1.57973
44	1	0	-5.94083	-2.82805	0.311134

45	1	0	-6.10135	-1.39523	-0.72271
46	1	0	-6.49169	-1.29101	1.002759
47	1	0	-3.47719	0.404504	0.884716
48	1	0	-3.89392	2.136668	-0.73596
49	1	0	-3.58458	3.700935	0.060942
50	1	0	-3.65537	3.614498	-1.72376

6b-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.735036	0.120961	0.980736
2	6	0	2.468491	-1.2994	0.38145
3	6	0	1.220817	-1.45799	-0.43552
4	6	0	0.223875	-2.29614	-0.14803
5	6	0	1.020249	1.78194	-0.07614
6	6	0	2.452365	1.340259	0.06901
7	6	0	-1.08822	-2.35496	-0.87992
8	6	0	-2.27057	-2.05296	0.066066
9	6	0	-1.3881	2.009121	0.45408
10	6	0	-0.02174	1.518302	0.716325
11	6	0	4.227155	0.007377	1.369703
12	6	0	4.905578	-0.78953	0.247078
13	6	0	3.785514	-1.6709	-0.36107
14	8	0	2.941864	1.194773	-1.26589
15	8	0	5.428668	0.16775	-0.70904
16	8	0	-2.37304	1.580125	1.033054
17	6	0	-3.54925	-1.63839	-0.66681
18	6	0	-4.74136	-1.36754	0.261389
19	6	0	-5.94442	-0.80877	-0.49971
20	1	0	2.134941	0.259022	1.884035
21	1	0	2.384931	-1.96613	1.246887
22	8	0	-4.39288	-0.51168	1.358483
23	8	0	-1.45548	2.962426	-0.487
24	6	0	-2.77179	3.452588	-0.81779
25	1	0	1.137658	-0.81237	-1.30756
26	1	0	0.31414	-2.94066	0.727557
27	1	0	0.867184	2.425163	-0.93773
28	1	0	2.96125	2.197508	0.545395
29	1	0	-1.07407	-1.62715	-1.69887
30	1	0	-1.23809	-3.34141	-1.33762
31	1	0	-2.4681	-2.93003	0.694287
32	1	0	-1.98455	-1.24711	0.746194
33	1	0	0.047507	0.861593	1.57407
34	1	0	4.306454	-0.56325	2.298988

35	1	0	4.721922	0.968308	1.530292
36	1	0	5.743726	-1.38183	0.621834
37	1	0	4.002414	-2.73622	-0.25614
38	1	0	3.699894	-1.45901	-1.42941
39	1	0	3.892957	0.98253	-1.21088
40	1	0	5.844244	-0.32082	-1.42953
41	1	0	-3.3462	-0.73133	-1.25257
42	1	0	-3.84295	-2.41084	-1.38763
43	1	0	-5.03434	-2.31173	0.735122
44	1	0	-6.27507	-1.49983	-1.28124
45	1	0	-5.68878	0.144963	-0.97294
46	1	0	-6.77876	-0.63755	0.184689
47	1	0	-3.85121	0.223559	1.03563
48	1	0	-3.38413	2.649975	-1.22998
49	1	0	-3.25644	3.865364	0.067101
50	1	0	-2.61143	4.228271	-1.56196

6b-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.67416	0.557157	-0.75704
2	6	0	-2.48018	-0.99282	-0.83429
3	6	0	-1.19732	-1.54754	-0.28519
4	6	0	-0.22606	-2.09646	-1.01731
5	6	0	-0.66144	1.393961	0.55946
6	6	0	-2.15931	1.278624	0.524911
7	6	0	1.086365	-2.60273	-0.48659
8	6	0	2.283735	-1.83467	-1.08654
9	6	0	1.536137	2.291248	-0.00496
10	6	0	0.065065	2.315384	-0.07967
11	6	0	-4.20135	0.690162	-0.95115
12	6	0	-4.83631	-0.47696	-0.18612
13	6	0	-3.75998	-1.59113	-0.1788
14	8	0	-2.54253	0.64863	1.744565
15	8	0	-5.14148	-0.00242	1.149738
16	8	0	2.200807	1.476717	0.6162
17	6	0	3.675403	-2.30684	-0.62082
18	6	0	4.278695	-1.58753	0.601893
19	6	0	3.488133	-1.73691	1.901758
20	1	0	-2.15143	1.032045	-1.59151
21	1	0	-2.51405	-1.23164	-1.90288
22	8	0	4.533135	-0.20377	0.319098
23	8	0	2.080472	3.286166	-0.72128
24	6	0	3.522899	3.357267	-0.73843

25	1	0	-1.07829	-1.48617	0.79504
26	1	0	-0.35707	-2.15857	-2.09865
27	1	0	-0.14404	0.654738	1.161222
28	1	0	-2.57587	2.296425	0.480494
29	1	0	1.089831	-2.53706	0.604592
30	1	0	1.201349	-3.66569	-0.73882
31	1	0	2.227987	-1.93059	-2.17652
32	1	0	2.168682	-0.76671	-0.8773
33	1	0	-0.38135	3.097339	-0.68344
34	1	0	-4.431	0.5752	-2.01417
35	1	0	-4.61156	1.65013	-0.62858
36	1	0	-5.77085	-0.80426	-0.64798
37	1	0	-4.09363	-2.47959	-0.71923
38	1	0	-3.56051	-1.89453	0.85206
39	1	0	-3.50631	0.494968	1.716174
40	1	0	-5.51426	-0.73533	1.654122
41	1	0	3.656876	-3.38544	-0.42112
42	1	0	4.387908	-2.15908	-1.43874
43	1	0	5.272248	-2.02211	0.757877
44	1	0	3.321357	-2.78959	2.146144
45	1	0	2.515457	-1.24254	1.832021
46	1	0	4.038984	-1.27537	2.725365
47	1	0	3.712936	0.3006	0.434069
48	1	0	3.905485	3.519464	0.269635
49	1	0	3.943394	2.437138	-1.14497
50	1	0	3.762522	4.202334	-1.37816

Table S28. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 9*R*, 10*E*, 15*S*)-**6a**] in ECD calculation

6a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.928597	0.01967	0.870405
2	6	0	2.679008	-1.29131	0.032228
3	6	0	1.56654	-2.19057	0.502074
4	6	0	0.50035	-2.57712	-0.2016
5	6	0	0.555032	0.977166	0.728787
6	6	0	1.700623	0.609458	1.614244
7	6	0	-0.59887	-3.46818	0.317487
8	6	0	-1.88265	-2.70713	0.723181
9	6	0	-1.24253	2.354741	-0.16796
10	6	0	-0.067	2.159038	0.700299

11	6	0	3.552992	1.025888	-0.13852
12	6	0	3.73484	0.271347	-1.46122
13	6	0	2.644628	-0.80514	-1.42642
14	8	0	2.080252	1.758421	2.369868
15	8	0	5.049156	-0.31305	-1.44215
16	8	0	-1.66695	1.54868	-0.98135
17	6	0	-2.52342	-1.89314	-0.40819
18	6	0	-3.70733	-1.01804	0.032247
19	6	0	-4.97435	-1.8072	0.332413
20	1	0	3.645697	-0.21465	1.66273
21	1	0	3.608729	-1.86272	0.135842
22	8	0	-4.04384	-0.07257	-0.99431
23	8	0	-1.82063	3.545206	0.048127
24	6	0	-3.01108	3.830932	-0.71868
25	1	0	1.678993	-2.57025	1.51842
26	1	0	0.383263	-2.21723	-1.22109
27	1	0	0.181174	0.180971	0.09592
28	1	0	1.321791	-0.17055	2.292849
29	1	0	-0.23765	-4.02429	1.188577
30	1	0	-0.85625	-4.2106	-0.448
31	1	0	-1.63594	-2.03376	1.553024
32	1	0	-2.60125	-3.43436	1.116288
33	1	0	0.237484	2.984576	1.329062
34	1	0	4.50924	1.425438	0.202132
35	1	0	2.882662	1.875242	-0.28916
36	1	0	3.641025	0.933274	-2.32923
37	1	0	1.681234	-0.34968	-1.67918
38	1	0	2.82632	-1.608	-2.14653
39	1	0	2.764676	1.489936	2.992338
40	1	0	5.144292	-0.84321	-2.24125
41	1	0	-2.85117	-2.55645	-1.21873
42	1	0	-1.7745	-1.22035	-0.83683
43	1	0	-3.40835	-0.47104	0.939257
44	1	0	-4.81386	-2.52799	1.137334
45	1	0	-5.77881	-1.13172	0.633391
46	1	0	-5.29868	-2.35125	-0.56006
47	1	0	-3.26917	0.496176	-1.12301
48	1	0	-2.7711	3.88939	-1.78083
49	1	0	-3.7601	3.055845	-0.55503
50	1	0	-3.36598	4.791252	-0.35457

6a-Conf.2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	2.826806	0.091772	0.801661
2	6	0	2.565926	-1.43522	0.62237
3	6	0	1.188543	-1.77953	0.121874
4	6	0	0.356185	-2.63205	0.7219
5	6	0	0.48361	1.164235	0.968244
6	6	0	1.814435	0.918376	1.628292
7	6	0	-1.0655	-2.93859	0.323712
8	6	0	-1.62496	-2.08986	-0.82339
9	6	0	-1.24196	2.503467	-0.15733
10	6	0	0.082431	2.338744	0.472698
11	6	0	3.128203	0.605529	-0.62112
12	6	0	3.737985	-0.60228	-1.38847
13	6	0	3.671211	-1.79078	-0.40146
14	8	0	2.492805	2.138265	1.943127
15	8	0	5.053151	-0.37106	-1.90152
16	8	0	-2.09344	1.642472	-0.2998
17	6	0	-3.15248	-2.12362	-0.97454
18	6	0	-3.9401	-1.70606	0.283024
19	6	0	-5.39674	-1.37936	-0.04823
20	1	0	3.749348	0.164465	1.387918
21	1	0	2.732758	-1.95853	1.568527
22	8	0	-3.32343	-0.62772	0.997932
23	8	0	-1.41117	3.764948	-0.58604
24	6	0	-2.66683	4.063877	-1.23181
25	1	0	0.869861	-1.27684	-0.78858
26	1	0	0.700076	-3.13623	1.625394
27	1	0	-0.1929	0.317981	0.922088
28	1	0	1.616231	0.354264	2.552344
29	1	0	-1.68104	-2.78925	1.217788
30	1	0	-1.15899	-4.00731	0.085604
31	1	0	-1.17043	-2.39955	-1.7709
32	1	0	-1.32821	-1.04941	-0.67218
33	1	0	0.717989	3.214564	0.502184
34	1	0	3.821864	1.448168	-0.62081
35	1	0	2.215464	0.946112	-1.11642
36	1	0	3.145593	-0.81391	-2.28035
37	1	0	3.500152	-2.74652	-0.90052
38	1	0	4.631981	-1.85968	0.121754
39	1	0	1.939468	2.638453	2.554058
40	1	0	5.633233	-0.19689	-1.15112
41	1	0	-3.49073	-3.12499	-1.26621
42	1	0	-3.42644	-1.4553	-1.80071
43	1	0	-3.92949	-2.53753	0.995059
44	1	0	-5.94578	-1.12316	0.861128

45	1	0	-5.89361	-2.23115	-0.52309
46	1	0	-5.45167	-0.5278	-0.73441
47	1	0	-3.05035	0.072714	0.386691
48	1	0	-2.79848	3.436442	-2.11365
49	1	0	-2.60428	5.111514	-1.51392
50	1	0	-3.49559	3.902173	-0.54195

6a-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.53303	0.247193	0.584928
2	6	0	-2.31989	-0.46511	-0.80182
3	6	0	-1.39317	-1.65641	-0.78187
4	6	0	-0.17477	-1.68763	-1.33025
5	6	0	-0.10202	0.901734	1.079705
6	6	0	-1.36476	0.245092	1.58792
7	6	0	0.771818	-2.85584	-1.27952
8	6	0	2.01201	-2.60241	-0.39166
9	6	0	1.286056	2.605147	-0.00089
10	6	0	-0.01907	2.048183	0.397951
11	6	0	-3.83437	-0.35991	1.127488
12	6	0	-4.72465	-0.43638	-0.11654
13	6	0	-3.76704	-0.87538	-1.23449
14	8	0	-1.07762	-1.04944	2.124803
15	8	0	-5.23267	0.861418	-0.47478
16	8	0	2.379916	2.093006	0.1792
17	6	0	2.966145	-1.53036	-0.93341
18	6	0	4.026842	-1.04052	0.06937
19	6	0	4.904172	-2.14844	0.640521
20	1	0	-2.7468	1.296521	0.35883
21	1	0	-1.90605	0.261306	-1.5039
22	8	0	3.419399	-0.36769	1.182806
23	8	0	1.138118	3.787978	-0.61516
24	6	0	2.346447	4.441278	-1.06023
25	1	0	-1.77397	-2.56035	-0.30304
26	1	0	0.183776	-0.79072	-1.83225
27	1	0	0.817544	0.386722	1.344517
28	1	0	-1.69475	0.823639	2.459358
29	1	0	1.108143	-3.09907	-2.29589
30	1	0	0.240363	-3.73598	-0.90352
31	1	0	2.549467	-3.54925	-0.27849
32	1	0	1.678132	-2.31136	0.60925
33	1	0	-0.89108	2.623283	0.111273
34	1	0	-4.28514	0.234821	1.927811

35	1	0	-3.65265	-1.36459	1.521633
36	1	0	-5.56008	-1.13397	0.007537
37	1	0	-3.82854	-1.95805	-1.36914
38	1	0	-4.06028	-0.4146	-2.17936
39	1	0	-0.76853	-1.59927	1.393903
40	1	0	-5.78272	1.170444	0.253805
41	1	0	2.398533	-0.64984	-1.25219
42	1	0	3.475831	-1.90794	-1.82855
43	1	0	4.674266	-0.32957	-0.46334
44	1	0	4.313957	-2.84358	1.24282
45	1	0	5.678019	-1.71942	1.281536
46	1	0	5.391646	-2.71233	-0.15927
47	1	0	3.049575	0.469675	0.85717
48	1	0	3.00337	4.639862	-0.2132
49	1	0	2.019526	5.371422	-1.51723
50	1	0	2.866968	3.818633	-1.78829

6a-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.926772	-0.0426	0.889175
2	6	0	2.655292	-1.32769	0.019609
3	6	0	1.538983	-2.22703	0.483641
4	6	0	0.467588	-2.59454	-0.22186
5	6	0	0.566384	0.953306	0.751483
6	6	0	1.702407	0.55519	1.635691
7	6	0	-0.64044	-3.4783	0.290068
8	6	0	-1.91455	-2.70516	0.703612
9	6	0	-1.19551	2.373506	-0.14735
10	6	0	-0.02565	2.150381	0.722536
11	6	0	3.578894	0.974098	-0.09189
12	6	0	3.68654	0.279263	-1.46609
13	6	0	2.599822	-0.80282	-1.42552
14	8	0	2.096634	1.686188	2.409477
15	8	0	4.991894	-0.26895	-1.71026
16	8	0	-1.64331	1.573289	-0.95376
17	6	0	-2.54321	-1.86994	-0.4191
18	6	0	-3.71836	-0.98674	0.028572
19	6	0	-4.99608	-1.7646	0.312504
20	1	0	3.629503	-0.30925	1.684249
21	1	0	3.573215	-1.92654	0.106774
22	8	0	-4.03904	-0.02385	-0.98653
23	8	0	-1.73777	3.582456	0.057709
24	6	0	-2.91777	3.897016	-0.71399

25	1	0	1.653125	-2.61968	1.494615
26	1	0	0.351864	-2.22203	-1.2368
27	1	0	0.170164	0.16706	0.120136
28	1	0	1.309409	-0.22961	2.300249
29	1	0	-0.28504	-4.04684	1.155424
30	1	0	-0.90705	-4.20975	-0.48268
31	1	0	-1.65973	-2.04465	1.541285
32	1	0	-2.64285	-3.42745	1.08777
33	1	0	0.299541	2.969393	1.349414
34	1	0	4.564551	1.305533	0.239684
35	1	0	2.955339	1.867612	-0.17343
36	1	0	3.535132	0.980935	-2.28734
37	1	0	1.628161	-0.34679	-1.64051
38	1	0	2.775943	-1.58032	-2.17178
39	1	0	2.769032	1.397415	3.036044
40	1	0	5.214904	-0.86224	-0.98463
41	1	0	-2.87595	-2.51936	-1.2388
42	1	0	-1.78576	-1.20022	-0.83744
43	1	0	-3.4168	-0.45579	0.944242
44	1	0	-4.8478	-2.4988	1.107616
45	1	0	-5.79352	-1.08366	0.619816
46	1	0	-5.32324	-2.29174	-0.58904
47	1	0	-3.25769	0.537943	-1.1042
48	1	0	-2.67532	3.933832	-1.77653
49	1	0	-3.69178	3.148939	-0.54123
50	1	0	-3.24138	4.872967	-0.36254

Table S29. The Information of conformations of (2*E*, 4*S*, 5*R*, 7*S*, 9*R*, 10*E*, 15*S*)-**7a**

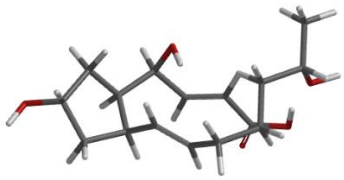
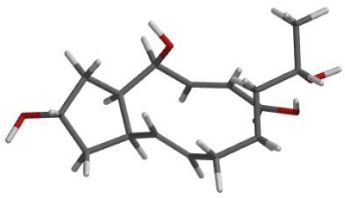
Label	**Conformers**	**Calculated energy (kJ/mol)**	**Boltzmann distribution**
7a-Conf.1		0	0.500
7a-Conf.2		0.02	0.495

Table S30. The coordinate for the lowest-energy conformer [(2*E*, 4*S*, 5*R*, 7*S*, 9*R*, 10*E*, 15*S*)-**7a**] in ECD calculation

7a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.53739	0.48001	0.572157
2	6	0	-2.35289	-0.26355	-0.79384
3	6	0	-1.21738	-1.26142	-0.87359
4	6	0	-0.14039	-1.11466	-1.65065
5	6	0	-0.45006	1.886531	0.510791
6	6	0	-1.27563	0.932816	1.333846
7	6	0	0.963623	-2.11219	-1.86888
8	6	0	2.361556	-1.61004	-1.43775
9	6	0	0.867088	1.793183	0.325246
10	6	0	-3.48922	-0.42879	1.362704
11	6	0	-4.53451	-0.81746	0.3191
12	6	0	-3.72963	-0.98352	-0.99326
13	8	0	-0.51336	-0.14767	1.868047
14	8	0	-5.46693	0.274703	0.243051
15	6	0	2.631796	-1.79502	0.059734
16	6	0	3.95695	-1.21976	0.550816
17	6	0	4.306944	-1.67968	1.961895
18	1	0	-3.09252	1.396589	0.34413
19	1	0	-2.19179	0.47781	-1.58
20	8	0	3.847478	0.229373	0.525288
21	6	0	1.593952	2.71776	-0.57796
22	8	0	1.125089	3.725647	-1.0649
23	8	0	2.857629	2.356045	-0.87548
24	1	0	-1.33972	-2.1892	-0.31246
25	1	0	-0.04159	-0.18942	-2.2185
26	1	0	-0.99224	2.695242	0.026546
27	1	0	-1.62725	1.48775	2.213526
28	1	0	0.998757	-2.3391	-2.94138
29	1	0	0.733522	-3.05405	-1.35883
30	1	0	2.47054	-0.55717	-1.71741
31	1	0	3.12532	-2.1585	-1.99897
32	1	0	1.438023	1.004451	0.798246
33	1	0	-3.94569	0.065409	2.223422
34	1	0	-2.96356	-1.31834	1.721005
35	1	0	-5.07091	-1.73468	0.585208
36	1	0	-3.57784	-2.04312	-1.21459

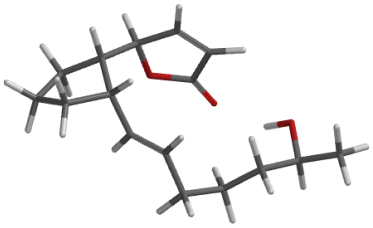
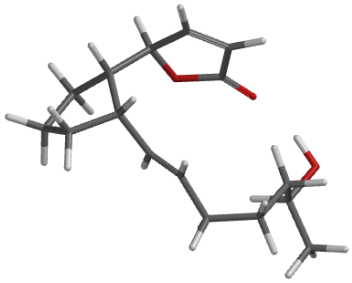
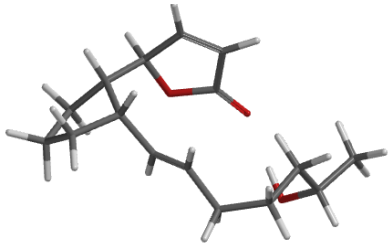
37	1	0	-4.28396	-0.55962	-1.83398
38	1	0	-0.27844	-0.7207	1.125872
39	1	0	-6.08463	0.083988	-0.47101
40	1	0	2.627742	-2.86634	0.286743
41	1	0	1.830885	-1.35	0.659593
42	1	0	4.758869	-1.5128	-0.13848
43	1	0	5.237022	-1.21684	2.304968
44	1	0	4.44586	-2.76342	1.986347
45	1	0	3.509836	-1.41373	2.661467
46	1	0	4.657857	0.598524	0.895673
47	1	0	3.127823	1.527232	-0.41743

7a-Conf.2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.53732	0.479965	0.572091
2	6	0	-2.35297	-0.2637	-0.79388
3	6	0	-1.21738	-1.26146	-0.87379
4	6	0	-0.14049	-1.11453	-1.65096
5	6	0	-0.44993	1.886491	0.510669
6	6	0	-1.27554	0.93284	1.333733
7	6	0	0.963675	-2.11189	-1.86928
8	6	0	2.361504	-1.60962	-1.43793
9	6	0	0.867263	1.793237	0.325336
10	6	0	-3.48912	-0.42873	1.362785
11	6	0	-4.53451	-0.81737	0.31929
12	6	0	-3.72971	-0.98375	-0.99307
13	8	0	-0.51331	-0.14762	1.868072
14	8	0	-5.46677	0.274929	0.243183
15	6	0	2.631729	-1.79513	0.059488
16	6	0	3.956716	-1.21982	0.550918
17	6	0	4.306503	-1.68027	1.961864
18	1	0	-3.09244	1.396528	0.344007
19	1	0	-2.19202	0.477619	-1.58012
20	8	0	3.846986	0.229345	0.525912
21	6	0	1.594186	2.717764	-0.57788
22	8	0	1.125375	3.725629	-1.06489
23	8	0	2.857845	2.355964	-0.87535
24	1	0	-1.33954	-2.18927	-0.31268
25	1	0	-0.04186	-0.18928	-2.21882
26	1	0	-0.99211	2.695095	0.026246
27	1	0	-1.62721	1.487801	2.213373
28	1	0	0.99891	-2.33861	-2.94181
29	1	0	0.733676	-3.05386	-1.35939

30	1	0	2.470298	-0.55664	-1.71725
31	1	0	3.125382	-2.15775	-1.99931
32	1	0	1.438203	1.004608	0.798509
33	1	0	-3.94548	0.065546	2.223527
34	1	0	-2.96348	-1.31827	1.721106
35	1	0	-5.07108	-1.73445	0.585554
36	1	0	-3.57791	-2.0434	-1.21412
37	1	0	-4.28405	-0.56015	-1.83393
38	1	0	-0.27834	-0.7207	1.125952
39	1	0	-6.08336	0.085179	-0.47209
40	1	0	2.627881	-2.86655	0.28599
41	1	0	1.830698	-1.35052	0.659489
42	1	0	4.758797	-1.51241	-0.13837
43	1	0	5.23626	-1.21725	2.305548
44	1	0	4.44592	-2.76397	1.985776
45	1	0	3.509049	-1.41513	2.661353
46	1	0	4.657114	0.598473	0.89687
47	1	0	3.128018	1.527218	-0.41721

Table S31. The Information of conformations of (2*Z*, 4*R*, 5*S*, 9*S*, 10*E*, 15*S*)-**8a**

Label	**Conformers**	**Calculated energy (kJ/mol)**	**Boltzmann distribution**
8a-Conf.1		0	0.377
8a-Conf.2		1.72	0.189
8a-Conf.3		2.29	0.150

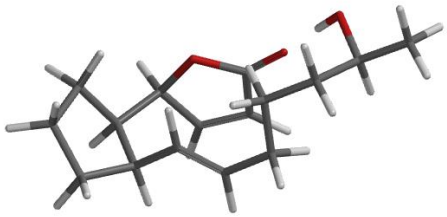
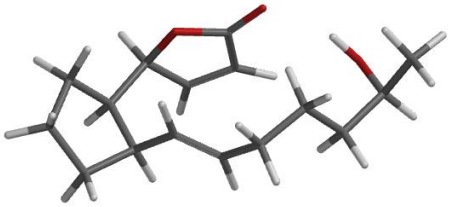
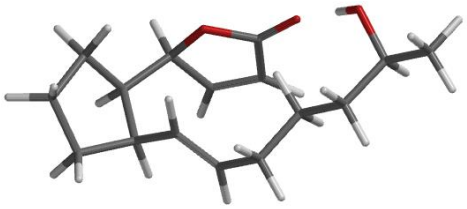
8b-Conf.1		0	0.339
8b-Conf.2		1.76	0.166
8b-Conf.3		3.08	0.098

Table S32. The coordinate for the lowest-energy conformer [(2*Z*, 4*R*, 5*S*, 9*S*, 10*E*, 15*S*)-**8a**] in ECD calculation

8a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.852254	-0.62533	0.496852
2	6	0	2.28057	0.772403	0.872905
3	6	0	3.85201	-0.34751	-0.64791
4	6	0	4.382977	1.088004	-0.38014
5	6	0	3.58539	1.613171	0.840356
6	6	0	1.252499	1.340896	-0.07234
7	6	0	0.065463	1.825838	0.297019
8	6	0	0.861377	-2.04235	1.288547
9	6	0	1.89145	-1.78755	0.229963
10	6	0	-0.35695	-2.01787	0.747945
11	6	0	-0.21341	-1.74333	-0.69112
12	8	0	1.105831	-1.60046	-0.97647
13	8	0	-1.06499	-1.64061	-1.5512
14	6	0	-0.9354	2.461328	-0.63406
15	6	0	-2.15997	1.57615	-0.95256
16	6	0	-3.0604	1.262919	0.250624
17	6	0	-4.11291	0.180469	-0.031
18	6	0	-5.1931	0.128904	1.041757

19	8	0	-3.5315	-1.13224	-0.0764
20	1	0	3.428835	-0.95429	1.371054
21	1	0	1.855513	0.75473	1.880711
22	1	0	2.491391	-2.69077	0.065987
23	1	0	4.649603	-1.09369	-0.66607
24	1	0	3.341353	-0.39939	-1.612
25	1	0	4.220436	1.724138	-1.25314
26	1	0	5.456518	1.093631	-0.18117
27	1	0	4.14527	1.429455	1.762623
28	1	0	3.384427	2.685056	0.788131
29	1	0	1.537534	1.406465	-1.122
30	1	0	-0.21643	1.761093	1.347268
31	1	0	1.122137	-2.2194	2.323128
32	1	0	-1.32042	-2.15082	1.214833
33	1	0	-0.43793	2.715135	-1.57582
34	1	0	-1.28442	3.406852	-0.19844
35	1	0	-1.79768	0.64848	-1.4031
36	1	0	-2.76233	2.079045	-1.71836
37	1	0	-3.56915	2.182733	0.563003
38	1	0	-2.46509	0.924788	1.105796
39	1	0	-4.58964	0.396375	-0.99965
40	1	0	-5.89998	-0.67661	0.828682
41	1	0	-5.74491	1.071014	1.084964
42	1	0	-4.74728	-0.05751	2.023609
43	1	0	-2.82359	-1.16684	-0.73853

8a-Conf.2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.93547	-0.39725	-0.51876
2	6	0	-2.11672	0.891687	-0.83218
3	6	0	-3.9309	0.028476	0.583132
4	6	0	-4.19282	1.53968	0.330174
5	6	0	-3.2544	1.943628	-0.8367
6	6	0	-1.0557	1.232122	0.183112
7	6	0	0.251168	1.317709	-0.06715
8	6	0	-1.18941	-2.09923	-1.28045
9	6	0	-2.18415	-1.70368	-0.23067
10	6	0	0.025254	-2.18879	-0.73996
11	6	0	-0.08569	-1.86668	0.693097
12	8	0	-1.39209	-1.62844	0.983246
13	8	0	0.779762	-1.79618	1.541305
14	6	0	1.304038	1.612254	0.974098
15	6	0	2.58997	2.259987	0.434498

16	6	0	3.448888	1.409035	-0.51832
17	6	0	3.983056	0.076297	0.043424
18	6	0	5.268459	-0.35289	-0.65884
19	8	0	3.040701	-0.99651	-0.14214
20	1	0	-3.5128	-0.61332	-1.42661
21	1	0	-1.64775	0.815222	-1.81748
22	1	0	-2.92032	-2.49979	-0.07288
23	1	0	-4.84471	-0.56849	0.541612
24	1	0	-3.48809	-0.12932	1.569022
25	1	0	-3.96949	2.12123	1.227513
26	1	0	-5.23775	1.734791	0.080662
27	1	0	-3.79047	1.8815	-1.78865
28	1	0	-2.87506	2.96331	-0.74176
29	1	0	-1.40259	1.418558	1.199446
30	1	0	0.602171	1.115211	-1.07771
31	1	0	-1.46748	-2.25898	-2.31338
32	1	0	0.969015	-2.41639	-1.21006
33	1	0	1.561449	0.681722	1.492974
34	1	0	0.875464	2.262417	1.744427
35	1	0	3.21147	2.54669	1.291166
36	1	0	2.33041	3.194735	-0.0767
37	1	0	4.303683	2.024706	-0.81966
38	1	0	2.902418	1.175972	-1.43869
39	1	0	4.191044	0.192671	1.115519
40	1	0	5.616089	-1.30891	-0.26064
41	1	0	6.058882	0.389795	-0.52442
42	1	0	5.090033	-0.47407	-1.7321
43	1	0	2.463953	-1.09445	0.628084

8a-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.895544	-0.47388	0.155068
2	6	0	2.253999	0.839385	0.683076
3	6	0	3.497612	-0.0963	-1.21898
4	6	0	3.845627	1.413734	-1.10837
5	6	0	3.371044	1.849343	0.299507
6	6	0	0.939042	1.236957	0.05531
7	6	0	-0.06549	1.817508	0.714989
8	6	0	1.485652	-2.18592	1.45471
9	6	0	2.073931	-1.76412	0.142852
10	6	0	0.168699	-2.34912	1.325897
11	6	0	-0.19998	-2.02593	-0.0618
12	8	0	0.924612	-1.68279	-0.73983

13	8	0	-1.29044	-2.03497	-0.59448
14	6	0	-1.30039	2.410433	0.086363
15	6	0	-2.60746	2.155654	0.863008
16	6	0	-3.1725	0.726566	0.81993
17	6	0	-3.82052	0.310121	-0.51107
18	6	0	-4.6492	-0.9692	-0.3716
19	8	0	-2.86172	0.171095	-1.57096
20	1	0	3.728804	-0.69519	0.833985
21	1	0	2.128313	0.802791	1.769376
22	1	0	2.708437	-2.56645	-0.25298
23	1	0	4.370017	-0.71281	-1.44729
24	1	0	2.76658	-0.27003	-2.0118
25	1	0	3.32575	1.981961	-1.88313
26	1	0	4.913305	1.598223	-1.24273
27	1	0	4.191488	1.755792	1.018284
28	1	0	3.021306	2.882759	0.331785
29	1	0	0.851931	1.116165	-1.02303
30	1	0	0.025039	1.945237	1.795571
31	1	0	2.087234	-2.33374	2.341165
32	1	0	-0.55423	-2.65221	2.067518
33	1	0	-1.40257	2.059317	-0.94233
34	1	0	-1.15867	3.499701	0.040598
35	1	0	-3.37553	2.843159	0.48857
36	1	0	-2.44348	2.434436	1.911255
37	1	0	-3.93879	0.642956	1.599513
38	1	0	-2.39482	-0.00251	1.0756
39	1	0	-4.47992	1.121097	-0.84135
40	1	0	-5.08385	-1.24088	-1.33691
41	1	0	-5.46179	-0.84066	0.349165
42	1	0	-4.0175	-1.79699	-0.03603
43	1	0	-2.28042	-0.57016	-1.33606

Table S33. The coordinate for the lowest-energy conformer [(2*Z*, 4*S*, 5*R*, 9*R*, 10*E*, 15*S*)-**8b**] in ECD calculation

8b-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.011918	0.252187	-0.23028
2	6	0	2.461055	-0.82636	0.749448
3	6	0	3.178767	-0.48683	-1.57885
4	6	0	3.435205	-1.97268	-1.20386
5	6	0	3.329707	-2.04327	0.340061

6	6	0	0.990056	-1.10733	0.587023
7	6	0	0.094048	-1.07171	1.573612
8	6	0	2.086271	2.34408	0.941197
9	6	0	2.283282	1.59663	-0.34274
10	6	0	0.790748	2.603517	1.118349
11	6	0	0.047656	2.032263	-0.01711
12	8	0	0.936273	1.45981	-0.87005
13	8	0	-1.14656	2.031178	-0.23074
14	6	0	-1.39331	-1.28285	1.446093
15	6	0	-1.90958	-1.61414	0.040934
16	6	0	-3.43553	-1.52637	-0.10056
17	6	0	-3.98508	-0.09026	-0.15667
18	6	0	-5.50007	-0.07295	-0.32609
19	8	0	-3.42251	0.629459	-1.26371
20	1	0	4.011882	0.516082	0.136276
21	1	0	2.655251	-0.54072	1.787594
22	1	0	2.830371	2.221032	-1.059
23	1	0	3.993672	-0.05519	-2.16425
24	1	0	2.268996	-0.38888	-2.17522
25	1	0	2.688728	-2.6179	-1.67274
26	1	0	4.411752	-2.31765	-1.54964
27	1	0	4.321979	-1.93585	0.789448
28	1	0	2.910577	-2.98714	0.694972
29	1	0	0.659785	-1.34559	-0.4201
30	1	0	0.439696	-0.8269	2.578349
31	1	0	2.90931	2.614419	1.588587
32	1	0	0.305724	3.12116	1.931629
33	1	0	-1.70616	-2.07225	2.143547
34	1	0	-1.88446	-0.3735	1.817022
35	1	0	-1.46137	-0.93457	-0.68968
36	1	0	-1.57591	-2.61998	-0.23593
37	1	0	-3.73969	-2.02824	-1.02657
38	1	0	-3.92194	-2.06228	0.724043
39	1	0	-3.73188	0.434107	0.774304
40	1	0	-5.99417	-0.60648	0.490148
41	1	0	-5.77885	-0.55332	-1.26924
42	1	0	-5.87008	0.954831	-0.34406
43	1	0	-2.59173	1.037715	-0.97682

8b-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.89688	-0.607	0.336813
2	6	0	-2.34354	0.772449	0.797396

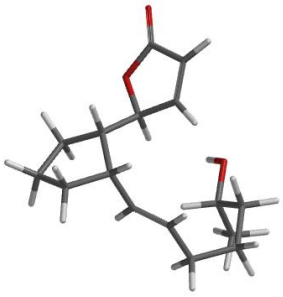
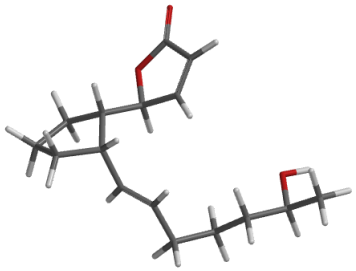
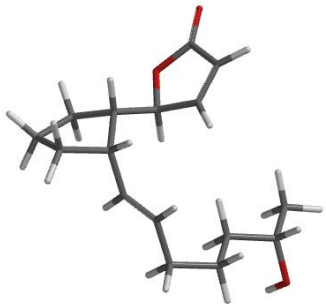
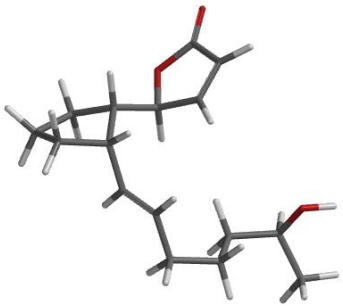
3	6	0	-3.77666	-0.29067	-0.89373
4	6	0	-4.29727	1.154507	-0.65703
5	6	0	-3.62562	1.635729	0.653662
6	6	0	-1.21841	1.344774	-0.02763
7	6	0	-0.0647	1.795944	0.468538
8	6	0	-1.01593	-2.07011	1.292148
9	6	0	-1.93208	-1.77994	0.141783
10	6	0	0.250354	-2.05412	0.875823
11	6	0	0.254666	-1.75269	-0.56504
12	8	0	-1.02816	-1.58325	-0.97694
13	8	0	1.188852	-1.6499	-1.3343
14	6	0	1.028036	2.44565	-0.34148
15	6	0	2.270195	1.557692	-0.57756
16	6	0	3.050081	1.205326	0.698331
17	6	0	4.087731	0.077723	0.549639
18	6	0	5.086832	0.29327	-0.5887
19	8	0	3.467471	-1.21432	0.448922
20	1	0	-3.56067	-0.94272	1.143812
21	1	0	-2.02155	0.725868	1.84193
22	1	0	-2.52578	-2.67006	-0.09888
23	1	0	-4.58652	-1.01646	-0.99676
24	1	0	-3.17927	-0.34425	-1.80645
25	1	0	-4.02106	1.800886	-1.49325
26	1	0	-5.38577	1.187933	-0.57854
27	1	0	-4.2812	1.437352	1.507233
28	1	0	-3.40568	2.705196	0.651386
29	1	0	-1.40072	1.446723	-1.09715
30	1	0	0.112634	1.695005	1.538613
31	1	0	-1.38094	-2.26135	2.292075
32	1	0	1.160854	-2.20867	1.433414
33	1	0	0.623845	2.738499	-1.31597
34	1	0	1.344273	3.371061	0.157758
35	1	0	1.941626	0.645996	-1.08362
36	1	0	2.93318	2.079498	-1.27562
37	1	0	3.562773	2.102988	1.065543
38	1	0	2.359767	0.896335	1.489336
39	1	0	4.64707	0.026447	1.489234
40	1	0	4.58785	0.289426	-1.56183
41	1	0	5.830292	-0.50729	-0.58744
42	1	0	5.608538	1.248911	-0.47835
43	1	0	2.870239	-1.23886	-0.31577

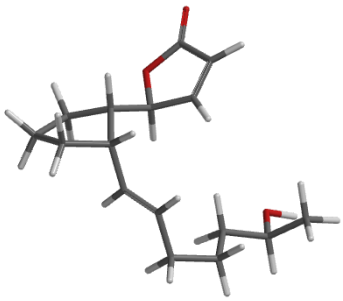
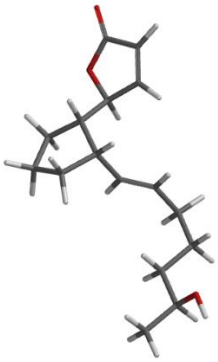
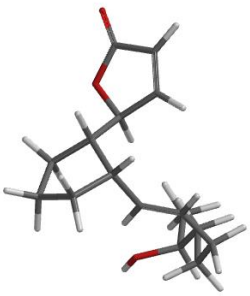
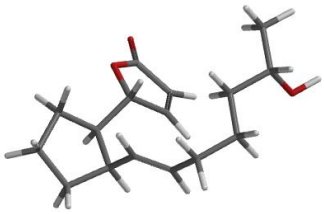
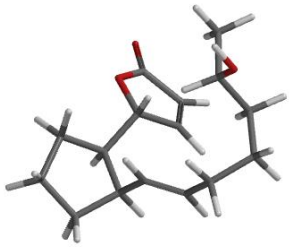
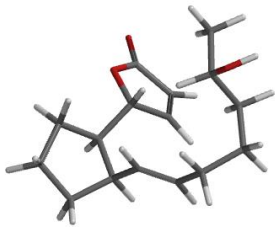
8b-Conf.3

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.02183	-0.63092	0.20314
2	6	0	-2.59891	0.785235	0.695703
3	6	0	-3.72493	-0.39436	-1.15728
4	6	0	-4.2533	1.06517	-1.10491
5	6	0	-3.84824	1.607383	0.285044
6	6	0	-1.33659	1.317615	0.069931
7	6	0	-0.32311	1.859078	0.747015
8	6	0	-1.19488	-1.99645	1.418632
9	6	0	-1.98549	-1.76059	0.16748
10	6	0	0.109206	-1.96648	1.141366
11	6	0	0.26851	-1.68881	-0.29601
12	8	0	-0.96617	-1.55566	-0.84706
13	8	0	1.276101	-1.57917	-0.96453
14	6	0	0.974292	2.309596	0.133968
15	6	0	2.171852	1.496078	0.685179
16	6	0	3.288916	1.271932	-0.33874
17	6	0	4.34155	0.249597	0.110794
18	6	0	5.416355	0.02994	-0.95461
19	8	0	3.741135	-0.9995	0.487327
20	1	0	-3.77725	-0.98312	0.916289
21	1	0	-2.47645	0.790415	1.782885
22	1	0	-2.50959	-2.6824	-0.11334
23	1	0	-4.52468	-1.12212	-1.31236
24	1	0	-3.01474	-0.52042	-1.97674
25	1	0	-3.79559	1.662276	-1.89724
26	1	0	-5.33364	1.116576	-1.25447
27	1	0	-4.6473	1.417721	1.009124
28	1	0	-3.65414	2.681929	0.284691
29	1	0	-1.26042	1.25235	-1.0144
30	1	0	-0.38941	1.920825	1.834042
31	1	0	-1.66201	-2.17845	2.376878
32	1	0	0.948158	-2.10849	1.805229
33	1	0	0.91345	2.183234	-0.95215
34	1	0	1.140345	3.378389	0.316127
35	1	0	2.575463	1.981431	1.581107
36	1	0	1.812087	0.517065	1.006216
37	1	0	2.844355	0.910076	-1.27529
38	1	0	3.790133	2.21718	-0.57719
39	1	0	4.823354	0.614221	1.025598
40	1	0	4.966471	-0.33409	-1.88411
41	1	0	6.141401	-0.71251	-0.61261
42	1	0	5.950871	0.959268	-1.17416
43	1	0	3.030142	-1.21091	-0.14029

Table S34. The Information of conformations of (2*Z*, 4*S*, 5*S*, 9*S*, 10*E*, 15*S*)-**9a** and (2*Z*, 4*R*, 5*R*, 9*R*, 10*E*, 15*S*)-**9b**

Label	Conformers	Calculated energy (kJ/mol)	Boltzmann distribution
9a-Conf.1		0	0.118
9a-Conf.2		0.10	0.114
9a-Conf.3		0.56	0.094
9a-Conf.4		0.57	0.094

9a-Conf.5		0.84	0.084
9a-Conf.6		1.50	0.065
9a-Conf.7		1.62	0.062
9b-Conf.1		0	0.591
9b-Conf.2		4.71	0.089
9b-Conf.3		6.21	0.048

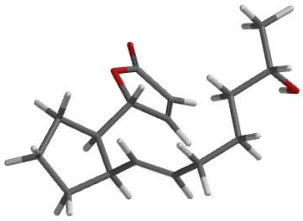
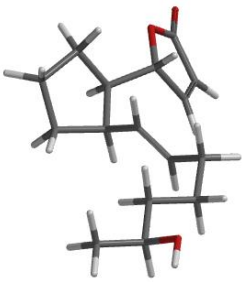
9b-Conf.4		6.27	0.047
9b-Conf.5		7.08	0.034

Table S35. The coordinate for the lowest-energy conformer [(2*Z*, 4*S*, 5*S*, 9*S*, 10*E*, 15*S*)-**9a**] in ECD calculation

9a-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.96328	0.891038	0.045467
2	6	0	-1.06649	1.980789	-0.61342
3	6	0	-2.17537	1.388883	1.4934
4	6	0	-2.09407	2.938994	1.413733
5	6	0	-1.72025	3.269236	-0.05278
6	6	0	0.389299	1.8815	-0.23502
7	6	0	1.403514	1.785333	-1.0967
8	6	0	-1.35273	-1.09947	-1.44139
9	6	0	-1.43525	-0.54203	-0.05092
10	6	0	-2.13316	-2.17486	-1.5441
11	6	0	-2.78016	-2.41283	-0.23828
12	8	0	-2.35332	-1.44211	0.62492
13	8	0	-3.55157	-3.2764	0.101703
14	6	0	2.858382	1.714929	-0.72033
15	6	0	3.559917	0.421653	-1.19326
16	6	0	2.933235	-0.88006	-0.66904
17	6	0	2.950874	-1.07006	0.853609
18	6	0	4.346805	-1.31271	1.423448
19	8	0	2.057447	-2.13455	1.230371
20	1	0	-2.92688	0.913244	-0.4767
21	1	0	-1.14975	1.945176	-1.70336
22	1	0	-0.47081	-0.63425	0.460412
23	1	0	-1.39051	0.994728	2.145866

24	1	0	-3.12573	1.03739	1.896916
25	1	0	-3.03799	3.410135	1.695032
26	1	0	-1.33584	3.31717	2.10327
27	1	0	-2.62347	3.484197	-0.63195
28	1	0	-1.06266	4.136704	-0.14007
29	1	0	0.618495	1.920018	0.83012
30	1	0	1.184486	1.747955	-2.16485
31	1	0	-0.73685	-0.65826	-2.21235
32	1	0	-2.30639	-2.80616	-2.40245
33	1	0	3.387939	2.563429	-1.1716
34	1	0	2.961581	1.830703	0.36303
35	1	0	3.540413	0.392631	-2.28846
36	1	0	4.616964	0.475084	-0.91228
37	1	0	1.889052	-0.93051	-0.99084
38	1	0	3.444427	-1.73537	-1.12982
39	1	0	2.518707	-0.18952	1.335522
40	1	0	4.292728	-1.46083	2.504353
41	1	0	4.794307	-2.20661	0.975279
42	1	0	5.012376	-0.46802	1.226502
43	1	0	2.357357	-2.93662	0.786041

9a-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.46908	-0.47596	0.321442
2	6	0	-1.49845	-1.57533	0.842903
3	6	0	-3.4028	-1.21571	-0.66526
4	6	0	-3.45674	-2.6863	-0.16504
5	6	0	-2.47582	-2.76259	1.030805
6	6	0	-0.38058	-1.90405	-0.11402
7	6	0	0.918218	-1.86312	0.1903
8	6	0	-0.96349	1.566341	0.681199
9	6	0	-1.79431	0.76141	-0.27422
10	6	0	-1.45672	2.800607	0.778091
11	6	0	-2.63386	2.907728	-0.10661
12	8	0	-2.80938	1.69794	-0.72069
13	8	0	-3.36476	3.843988	-0.31961
14	6	0	2.038435	-2.20914	-0.75288
15	6	0	2.996696	-1.03814	-1.05768
16	6	0	3.829684	-0.57527	0.142882
17	6	0	4.770823	0.584934	-0.17427
18	6	0	5.680897	0.941778	0.999206
19	8	0	3.94294	1.705548	-0.53341
20	1	0	-3.0607	-0.13701	1.179533

21	1	0	-1.06081	-1.27994	1.800862
22	1	0	-1.20748	0.481612	-1.15578
23	1	0	-2.99198	-1.16912	-1.67823
24	1	0	-4.38721	-0.74758	-0.70306
25	1	0	-4.46583	-2.97758	0.133361
26	1	0	-3.15401	-3.37097	-0.96065
27	1	0	-3.0179	-2.6226	1.971051
28	1	0	-1.9545	-3.72012	1.094225
29	1	0	-0.66943	-2.21891	-1.11723
30	1	0	1.20376	-1.5586	1.196816
31	1	0	-0.09895	1.161536	1.188057
32	1	0	-1.10301	3.625877	1.377328
33	1	0	2.625158	-3.03636	-0.33008
34	1	0	1.613862	-2.57582	-1.69296
35	1	0	3.677826	-1.35156	-1.8579
36	1	0	2.423651	-0.19246	-1.44818
37	1	0	3.177092	-0.25909	0.964639
38	1	0	4.428486	-1.41354	0.517391
39	1	0	5.394398	0.307652	-1.03725
40	1	0	5.084899	1.215199	1.874704
41	1	0	6.324147	1.789936	0.745558
42	1	0	6.326839	0.1001	1.265198
43	1	0	4.523873	2.426449	-0.7988

9a-Conf.3

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.41124	-0.46877	0.081171
2	6	0	-1.6709	-1.68977	0.701152
3	6	0	-3.02763	-1.01052	-1.22966
4	6	0	-3.26796	-2.52587	-0.9808
5	6	0	-2.69837	-2.81813	0.428805
6	6	0	-0.33334	-1.98328	0.069192
7	6	0	0.815067	-2.10653	0.737201
8	6	0	-1.04896	1.413743	1.157841
9	6	0	-1.55602	0.78524	-0.10641
10	6	0	-1.51335	2.658862	1.260291
11	6	0	-2.34835	2.948322	0.077129
12	8	0	-2.35552	1.832895	-0.71472
13	8	0	-2.9485	3.950434	-0.22538
14	6	0	2.145578	-2.47104	0.137021
15	6	0	3.272707	-1.46411	0.437982
16	6	0	3.070675	-0.09045	-0.20774
17	6	0	4.240697	0.873784	0.016359

18	6	0	3.972123	2.263302	-0.55849
19	8	0	5.471101	0.33848	-0.50312
20	1	0	-3.2237	-0.20421	0.767846
21	1	0	-1.52649	-1.55037	1.776414
22	1	0	-0.72896	0.576386	-0.79338
23	1	0	-2.33392	-0.86184	-2.06256
24	1	0	-3.9433	-0.47562	-1.48477
25	1	0	-4.32681	-2.7854	-1.041
26	1	0	-2.75416	-3.12232	-1.73831
27	1	0	-3.49408	-2.7537	1.177294
28	1	0	-2.25186	-3.81129	0.510948
29	1	0	-0.32579	-2.14158	-1.00948
30	1	0	0.810494	-1.95421	1.817818
31	1	0	-0.40342	0.892927	1.850881
32	1	0	-1.34553	3.381713	2.044285
33	1	0	2.451983	-3.44737	0.535137
34	1	0	2.040551	-2.59615	-0.94666
35	1	0	3.367875	-1.34406	1.524753
36	1	0	4.221657	-1.88064	0.08917
37	1	0	2.921255	-0.21133	-1.29014
38	1	0	2.157192	0.374389	0.17835
39	1	0	4.42469	0.962094	1.092315
40	1	0	4.831705	2.916292	-0.39093
41	1	0	3.790896	2.205159	-1.63742
42	1	0	3.093923	2.719663	-0.09324
43	1	0	5.364841	0.248262	-1.45785

9a-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.364	-0.41099	0.137305
2	6	0	-1.6372	-1.62637	0.78373
3	6	0	-3.0856	-0.99818	-1.09897
4	6	0	-3.35996	-2.48859	-0.75388
5	6	0	-2.71949	-2.72502	0.635271
6	6	0	-0.34887	-2.00476	0.096632
7	6	0	0.837016	-2.09435	0.701186
8	6	0	-0.83113	1.45616	0.999828
9	6	0	-1.47323	0.791548	-0.18196
10	6	0	-1.23714	2.723073	1.079857
11	6	0	-2.16106	2.993125	-0.03961
12	8	0	-2.279	1.844458	-0.77315
13	8	0	-2.74665	4.004872	-0.33887
14	6	0	2.131875	-2.5029	0.054231

15	6	0	3.231584	-1.42366	0.147625
16	6	0	2.952721	-0.20245	-0.7373
17	6	0	3.864577	1.003361	-0.49733
18	6	0	5.352658	0.725282	-0.70817
19	8	0	3.609986	1.453587	0.84635
20	1	0	-3.11792	-0.06973	0.855905
21	1	0	-1.42522	-1.43156	1.838892
22	1	0	-0.71886	0.512529	-0.9254
23	1	0	-2.44457	-0.91914	-1.98207
24	1	0	-3.99776	-0.44359	-1.32294
25	1	0	-4.42824	-2.71369	-0.74032
26	1	0	-2.90993	-3.14217	-1.50483
27	1	0	-3.46736	-2.58768	1.422359
28	1	0	-2.3063	-3.72948	0.749203
29	1	0	-0.41103	-2.24463	-0.96513
30	1	0	0.899812	-1.85722	1.764473
31	1	0	-0.13983	0.944316	1.654239
32	1	0	-0.97062	3.474384	1.807694
33	1	0	2.501349	-3.40915	0.550845
34	1	0	1.958127	-2.76867	-0.99464
35	1	0	3.330459	-1.10068	1.188892
36	1	0	4.187899	-1.8761	-0.13213
37	1	0	3.026609	-0.48687	-1.79341
38	1	0	1.923385	0.133172	-0.57654
39	1	0	3.558099	1.792746	-1.19817
40	1	0	5.936153	1.639636	-0.56262
41	1	0	5.717969	-0.02458	-0.00263
42	1	0	5.542009	0.368831	-1.72503
43	1	0	4.164578	2.224274	1.008033

9a-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.38834	-0.38096	0.153712
2	6	0	-1.66379	-1.62213	0.75168
3	6	0	-3.12816	-0.92363	-1.09126
4	6	0	-3.425	-2.41732	-0.78108
5	6	0	-2.76103	-2.70482	0.587662
6	6	0	-0.39334	-1.9978	0.030668
7	6	0	0.794251	-2.16587	0.614938
8	6	0	-0.8407	1.444948	1.064938
9	6	0	-1.48844	0.82161	-0.13579
10	6	0	-1.22942	2.714607	1.179104
11	6	0	-2.14896	3.026804	0.066829

12	8	0	-2.2828	1.899501	-0.69651
13	8	0	-2.72144	4.053738	-0.20469
14	6	0	2.054043	-2.61558	-0.07345
15	6	0	3.257683	-1.67448	0.132183
16	6	0	3.088686	-0.30445	-0.53214
17	6	0	4.326043	0.589668	-0.46206
18	6	0	4.689917	1.03497	0.953249
19	8	0	4.032134	1.730279	-1.2884
20	1	0	-3.13148	-0.05715	0.891417
21	1	0	-1.43214	-1.46323	1.80875
22	1	0	-0.7374	0.555118	-0.88722
23	1	0	-2.49135	-0.83343	-1.97639
24	1	0	-4.03221	-0.34841	-1.29518
25	1	0	-4.49724	-2.62084	-0.75001
26	1	0	-3.00512	-3.05888	-1.55928
27	1	0	-3.49245	-2.58592	1.392951
28	1	0	-2.35609	-3.7163	0.661288
29	1	0	-0.47396	-2.1781	-1.04148
30	1	0	0.878964	-1.9911	1.688702
31	1	0	-0.16423	0.903001	1.710542
32	1	0	-0.956	3.441602	1.928746
33	1	0	2.331013	-3.60319	0.31814
34	1	0	1.864232	-2.74707	-1.14453
35	1	0	3.432029	-1.55543	1.207344
36	1	0	4.151391	-2.16337	-0.27238
37	1	0	2.846396	-0.44449	-1.59187
38	1	0	2.245494	0.235265	-0.08676
39	1	0	5.177661	0.043486	-0.89429
40	1	0	5.55481	1.705217	0.933204
41	1	0	3.851935	1.571168	1.408526
42	1	0	4.947654	0.184328	1.589265
43	1	0	4.804305	2.306258	-1.27782

9a-Conf.6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.181868	0.963726	0.305819
2	6	0	0.686603	0.895573	0.73682
3	6	0	2.251325	2.162804	-0.66731
4	6	0	1.121503	3.129802	-0.21636
5	6	0	0.369442	2.400426	0.924918
6	6	0	-0.21035	0.249082	-0.2883
7	6	0	-0.97659	-0.8205	-0.06654
8	6	0	2.81253	-1.49239	0.68087

9	6	0	2.754687	-0.33316	-0.26928
10	6	0	4.076463	-1.88518	0.836791
11	6	0	4.941681	-1.0288	0.001228
12	8	0	4.141688	-0.12588	-0.64383
13	8	0	6.13826	-1.04705	-0.1539
14	6	0	-1.87614	-1.48105	-1.07496
15	6	0	-3.34509	-1.59666	-0.62252
16	6	0	-4.06798	-0.25048	-0.51205
17	6	0	-5.52226	-0.36865	-0.06254
18	6	0	-6.25166	0.973455	-0.07542
19	8	0	-5.50676	-0.92454	1.264472
20	1	0	2.764148	1.203161	1.203151
21	1	0	0.582465	0.35597	1.682464
22	1	0	2.215306	-0.60862	-1.18195
23	1	0	2.080679	1.823824	-1.69367
24	1	0	3.237045	2.629303	-0.64998
25	1	0	1.518852	4.08833	0.123503
26	1	0	0.449	3.345836	-1.04977
27	1	0	0.758451	2.720756	1.896246
28	1	0	-0.70436	2.599038	0.922267
29	1	0	-0.23349	0.708384	-1.27676
30	1	0	-0.96272	-1.27789	0.924089
31	1	0	1.930762	-1.91483	1.141522
32	1	0	4.46652	-2.68395	1.449224
33	1	0	-1.82159	-0.94295	-2.02822
34	1	0	-1.50164	-2.49516	-1.26642
35	1	0	-3.88046	-2.23263	-1.33724
36	1	0	-3.39073	-2.1091	0.343316
37	1	0	-3.54305	0.401684	0.195515
38	1	0	-4.04802	0.256478	-1.48373
39	1	0	-6.04397	-1.06417	-0.73669
40	1	0	-5.7488	1.686046	0.584766
41	1	0	-6.28213	1.393821	-1.08479
42	1	0	-7.28354	0.857252	0.269946
43	1	0	-6.42054	-1.06874	1.532328

9a-Conf.7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.646779	1.045825	-0.4155
2	6	0	0.714237	2.047036	0.327199
3	6	0	1.158202	1.082774	-1.88143
4	6	0	0.596527	2.516669	-2.09177
5	6	0	0.654729	3.203028	-0.70336

6	6	0	-0.65565	1.489284	0.622983
7	6	0	-1.20375	1.42631	1.837895
8	6	0	2.270253	-0.4463	1.571329
9	6	0	1.70391	-0.35973	0.185057
10	6	0	3.356554	-1.21825	1.567419
11	6	0	3.582826	-1.70496	0.19192
12	8	0	2.595962	-1.19052	-0.60339
13	8	0	4.444544	-2.42751	-0.24587
14	6	0	-2.58704	0.933974	2.190311
15	6	0	-3.40475	0.305035	1.05414
16	6	0	-2.93014	-1.09847	0.647488
17	6	0	-3.48378	-1.56631	-0.69581
18	6	0	-3.1314	-3.01935	-1.00525
19	8	0	-2.93326	-0.68687	-1.69579
20	1	0	2.66196	1.457367	-0.37124
21	1	0	1.171005	2.382316	1.262932
22	1	0	0.71396	-0.82615	0.141746
23	1	0	0.372171	0.336698	-2.03302
24	1	0	1.963885	0.83939	-2.57512
25	1	0	1.175225	3.074466	-2.83086
26	1	0	-0.43004	2.473524	-2.46278
27	1	0	1.568805	3.798132	-0.61563
28	1	0	-0.18939	3.872006	-0.52327
29	1	0	-1.22359	1.135153	-0.23451
30	1	0	-0.61887	1.784223	2.685912
31	1	0	1.82443	0.058411	2.416719
32	1	0	4.001552	-1.48356	2.391365
33	1	0	-2.5014	0.218841	3.020342
34	1	0	-3.14535	1.781549	2.610216
35	1	0	-4.45204	0.24419	1.369427
36	1	0	-3.38711	0.961693	0.180032
37	1	0	-1.83747	-1.12866	0.584802
38	1	0	-3.22067	-1.82013	1.418571
39	1	0	-4.5783	-1.45724	-0.68942
40	1	0	-2.04621	-3.15618	-1.00511
41	1	0	-3.56834	-3.69428	-0.26365
42	1	0	-3.51279	-3.31023	-1.98875
43	1	0	-3.32446	-0.92178	-2.54408

Table S36. The coordinate for the lowest-energy conformer [(2*Z*, 4*R*, 5*R*, 9*R*, 10*E*, 15*S*)-**9b**] in ECD calculation

9b-Conf.1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.34908	-0.31862	-0.1327
2	6	0	-1.7061	-1.60233	-0.73489
3	6	0	-3.09122	-0.80929	1.132337
4	6	0	-3.46692	-2.29034	0.847638
5	6	0	-2.85404	-2.62383	-0.53431
6	6	0	-0.43897	-2.03685	-0.04147
7	6	0	0.73248	-2.23335	-0.64885
8	6	0	-0.71424	1.406461	-1.09011
9	6	0	-1.37925	0.835519	0.127273
10	6	0	-1.0341	2.694074	-1.21661
11	6	0	-1.91984	3.071102	-0.09712
12	8	0	-2.10486	1.963073	0.683796
13	8	0	-2.43093	4.131613	0.1677
14	6	0	1.995563	-2.71932	0.007735
15	6	0	3.193371	-1.76402	-0.1654
16	6	0	3.055439	-0.45167	0.612509
17	6	0	4.200028	0.529633	0.371688
18	6	0	4.111473	1.766704	1.263028
19	8	0	4.143436	0.900628	-1.01781
20	1	0	-3.08839	0.039898	-0.85811
21	1	0	-1.49174	-1.46379	-1.79842
22	1	0	-0.63354	0.537219	0.872131
23	1	0	-3.96217	-0.1878	1.344328
24	1	0	-2.43475	-0.7394	2.004884
25	1	0	-3.05635	-2.94263	1.621971
26	1	0	-4.54796	-2.44355	0.847945
27	1	0	-3.59849	-2.47305	-1.3221
28	1	0	-2.50531	-3.65608	-0.6081
29	1	0	-0.50808	-2.23014	1.029289
30	1	0	0.803379	-2.04407	-1.72115
31	1	0	-0.07507	0.820899	-1.73557
32	1	0	-0.73077	3.394993	-1.97948
33	1	0	2.267885	-3.68665	-0.434
34	1	0	1.814086	-2.90273	1.072923
35	1	0	3.328835	-1.53966	-1.228
36	1	0	4.103474	-2.27984	0.162166
37	1	0	3.001503	-0.66679	1.685908
38	1	0	2.118762	0.049287	0.342686
39	1	0	5.153377	0.016632	0.567502
40	1	0	4.933046	2.457223	1.049563
41	1	0	4.170467	1.493023	2.320381
42	1	0	3.168713	2.294001	1.090755

43	1	0	4.900231	1.467376	-1.20146

9b-Conf.2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.120971	0.822629	0.037372
2	6	0	1.221489	1.916934	-0.60857
3	6	0	2.398513	1.341983	1.467112
4	6	0	2.330511	2.891592	1.366102
5	6	0	1.917664	3.202632	-0.09339
6	6	0	-0.22423	1.853079	-0.18382
7	6	0	-1.2637	1.805598	-1.01922
8	6	0	1.397016	-1.181	-1.38224
9	6	0	1.551629	-0.59602	-0.00954
10	6	0	2.136248	-2.28487	-1.48807
11	6	0	2.823801	-2.51556	-0.20182
12	8	0	2.46244	-1.51109	0.653659
13	8	0	3.57774	-3.39715	0.130337
14	6	0	-2.71319	1.815526	-0.6169
15	6	0	-3.53621	0.642091	-1.18773
16	6	0	-3.12295	-0.75367	-0.69907
17	6	0	-3.32724	-1.00183	0.795059
18	6	0	-2.90767	-2.41091	1.209338
19	8	0	-4.7226	-0.78411	1.070258
20	1	0	3.063789	0.811468	-0.52155
21	1	0	1.268216	1.862841	-1.69997
22	1	0	0.604014	-0.63774	0.538125
23	1	0	3.361125	0.986328	1.836651
24	1	0	1.637624	0.967593	2.158499
25	1	0	1.595131	3.287321	2.070451
26	1	0	3.28626	3.35763	1.613984
27	1	0	2.806513	3.387304	-0.7045
28	1	0	1.275236	4.081675	-0.17711
29	1	0	-0.42131	1.887171	0.887841
30	1	0	-1.07073	1.775768	-2.09287
31	1	0	0.76603	-0.73623	-2.13878
32	1	0	2.255383	-2.94122	-2.33676
33	1	0	-3.17026	2.744771	-0.98193
34	1	0	-2.79441	1.844261	0.474341
35	1	0	-3.46518	0.663694	-2.28144
36	1	0	-4.58891	0.803031	-0.94111
37	1	0	-2.06937	-0.93627	-0.93477
38	1	0	-3.70271	-1.50631	-1.24673
39	1	0	-2.73264	-0.27611	1.366776

40	1	0	-3.0762	-2.56689	2.27914
41	1	0	-1.84511	-2.57784	1.01051
42	1	0	-3.48732	-3.15773	0.659116
43	1	0	-4.85171	-0.87492	2.020361

9b-Conf.3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.140249	0.809595	0.046595
2	6	0	1.249691	1.909143	-0.60281
3	6	0	2.410938	1.324202	1.479311
4	6	0	2.34962	2.874293	1.381876
5	6	0	1.947269	3.190768	-0.07942
6	6	0	-0.19968	1.851412	-0.1897
7	6	0	-1.23207	1.80587	-1.03404
8	6	0	1.41187	-1.18558	-1.38285
9	6	0	1.566306	-0.60694	-0.0074
10	6	0	2.148305	-2.29092	-1.49254
11	6	0	2.833403	-2.52919	-0.2063
12	8	0	2.4735	-1.52758	0.653128
13	8	0	3.584415	-3.41432	0.122934
14	6	0	-2.68509	1.824964	-0.64493
15	6	0	-3.50455	0.643608	-1.20518
16	6	0	-3.11023	-0.73955	-0.66912
17	6	0	-3.40817	-0.96281	0.819221
18	6	0	-2.98526	-2.3531	1.290018
19	8	0	-4.79435	-0.72198	1.119
20	1	0	3.086487	0.796076	-0.50647
21	1	0	1.304382	1.857483	-1.69397
22	1	0	0.618034	-0.64815	0.539192
23	1	0	3.369862	0.96383	1.853889
24	1	0	1.644294	0.951051	2.165008
25	1	0	1.611359	3.271051	2.08261
26	1	0	3.305558	3.336031	1.636966
27	1	0	2.840695	3.373928	-0.68427
28	1	0	1.308675	4.072454	-0.16477
29	1	0	-0.40577	1.890104	0.880106
30	1	0	-1.02991	1.771638	-2.10582
31	1	0	0.782937	-0.73603	-2.13826
32	1	0	2.266803	-2.94383	-2.34397
33	1	0	-3.13665	2.749428	-1.02817
34	1	0	-2.77545	1.870618	0.444951
35	1	0	-3.41149	0.638577	-2.29723
36	1	0	-4.56163	0.816997	-0.98426

37	1	0	-2.0429	-0.91718	-0.84018
38	1	0	-3.64555	-1.50893	-1.24146
39	1	0	-2.87696	-0.21403	1.413859
40	1	0	-3.22242	-2.48448	2.348269
41	1	0	-1.91062	-2.50418	1.154029
42	1	0	-3.50982	-3.12906	0.721819
43	1	0	-5.31402	-1.35688	0.611274

9b-Conf.4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.35769	-0.35386	-0.13387
2	6	0	-1.68198	-1.62009	-0.73699
3	6	0	-3.08435	-0.86504	1.131656
4	6	0	-3.43049	-2.35204	0.84054
5	6	0	-2.8054	-2.66957	-0.54002
6	6	0	-0.40778	-2.02685	-0.03978
7	6	0	0.769946	-2.20224	-0.64162
8	6	0	-0.78012	1.418088	-1.09787
9	6	0	-1.41807	0.825432	0.123602
10	6	0	-1.13548	2.697064	-1.21701
11	6	0	-2.02073	3.046385	-0.08789
12	8	0	-2.16889	1.931054	0.690327
13	8	0	-2.5576	4.091854	0.185226
14	6	0	2.034428	-2.67446	0.022678
15	6	0	3.230501	-1.71764	-0.15077
16	6	0	3.08238	-0.39158	0.60038
17	6	0	4.254965	0.571991	0.386067
18	6	0	4.130234	1.841996	1.225397
19	8	0	4.420337	0.896203	-1.00624
20	1	0	-3.10788	-0.01534	-0.85777
21	1	0	-1.46848	-1.47527	-1.79989
22	1	0	-0.65814	0.545156	0.861083
23	1	0	-3.967	-0.26272	1.350534
24	1	0	-2.42562	-0.7861	2.001731
25	1	0	-3.01198	-2.99918	1.614892
26	1	0	-4.50852	-2.52501	0.834821
27	1	0	-3.55084	-2.53693	-1.33009
28	1	0	-2.43098	-3.69281	-0.61319
29	1	0	-0.47744	-2.2226	1.030499
30	1	0	0.843544	-2.01205	-1.71361
31	1	0	-0.13416	0.850705	-1.75283
32	1	0	-0.85933	3.408184	-1.98077
33	1	0	2.313306	-3.64364	-0.41111

34	1	0	1.849412	-2.85199	1.088175
35	1	0	3.38178	-1.51221	-1.21538
36	1	0	4.13716	-2.22554	0.198084
37	1	0	2.98351	-0.58844	1.674918
38	1	0	2.157267	0.113278	0.293355
39	1	0	5.186521	0.060046	0.64963
40	1	0	4.972529	2.509658	1.030253
41	1	0	4.113616	1.607928	2.293514
42	1	0	3.205312	2.376867	0.982654
43	1	0	3.623454	1.35946	-1.29099

9b-Conf.5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.24229	0.974732	0.232241
2	6	0	-0.76897	0.954676	0.737873
3	6	0	-2.27276	2.092265	-0.83575
4	6	0	-1.16232	3.0965	-0.41971
5	6	0	-0.46829	2.472652	0.816342
6	6	0	0.181576	0.235931	-0.18611
7	6	0	0.944194	-0.80276	0.160552
8	6	0	-2.87427	-1.44973	0.771151
9	6	0	-2.78025	-0.36876	-0.2643
10	6	0	-4.14165	-1.84034	0.901972
11	6	0	-4.97331	-1.06066	-0.03625
12	8	0	-4.15009	-0.20496	-0.71581
13	8	0	-6.16172	-1.10141	-0.24155
14	6	0	1.904305	-1.52877	-0.74136
15	6	0	3.347295	-1.58586	-0.20234
16	6	0	4.037832	-0.22004	-0.13419
17	6	0	5.481548	-0.2835	0.358099
18	6	0	6.112045	1.099883	0.506206
19	8	0	6.215634	-1.07531	-0.59311
20	1	0	-2.86776	1.279014	1.079365
21	1	0	-0.70854	0.494483	1.728288
22	1	0	-2.1979	-0.70972	-1.12701
23	1	0	-3.25864	2.555073	-0.89443
24	1	0	-2.06154	1.673074	-1.82406
25	1	0	-0.44994	3.23665	-1.23612
26	1	0	-1.57126	4.081764	-0.18702
27	1	0	-0.9101	2.869552	1.73547
28	1	0	0.603182	2.680268	0.853312
29	1	0	0.251457	0.614226	-1.20625
30	1	0	0.882578	-1.17862	1.183275

31	1	0	-2.01158	-1.82634	1.302135
32	1	0	-4.55426	-2.59157	1.55823
33	1	0	1.898471	-1.0678	-1.73549
34	1	0	1.552308	-2.56034	-0.87247
35	1	0	3.937526	-2.24985	-0.83912
36	1	0	3.339551	-2.03949	0.79707
37	1	0	3.477478	0.449122	0.526766
38	1	0	4.035703	0.244283	-1.12877
39	1	0	5.497788	-0.78964	1.334823
40	1	0	7.15057	1.018705	0.841442
41	1	0	5.569413	1.701992	1.24067
42	1	0	6.102799	1.626323	-0.45254
43	1	0	7.113937	-1.17503	-0.26043