

Supplementary Material

Heterodimeric Diketopiperazine Alkaloids from *Penicillium expansum* MA147 and Their Cytotoxicity

Jing Li,^a Jing Wang,^b Xi Zhou,^b Xiao-Qian Wu,^b Yan Li,^b Yi-Yun Yuan,^b Wen-Yu Lu,^b
Ai-Lin Liang,^b Peng-Ju Xu,^b and Wen-Xuan Wang^{b*}

^a *Department of Pharmacy, National Clinical Research Center for Geriatric Disorder, Xiangya Hospital, Central South University, Changsha, Hunan 410008, PR China;*

^b *Xiangya School of Pharmaceutical Sciences, Central South University, Changsha, Hunan 410008, PR China.*

Table of contents

Fig. S1. ESI-MS spectrum of compound 1 .	5
Fig. S2. ¹ H NMR spectrum of compound 1 (600 MHz, CDCl ₃).	5
Fig. S3. ¹³ C NMR and DEPT spectrum of compound 1 (150 MHz, CDCl ₃).	6
Fig. S4. ¹ H- ¹ H COSY spectrum of compound 1 .	6
Fig. S5. HSQC spectrum of compound 1 .	7
Fig. S6. HMBC spectrum of compound 1 .	7
Fig. S7. Zoomed area of HMBC spectrum of compound 1 for the correlation between H-22 and C-23.	8
Fig. S8. ROESY spectrum of compound 1 .	8
Fig. S9. Zoomed area of ROESY spectrum of compound 1 for the correlation between H-21 and H-23.	9
Fig. S10. IR spectrum of compound 1 .	9
Fig. S11. UV spectrum of compound 1 (CH ₃ CN).	10
Fig. S12. ECD spectrum of compound 1 (CH ₃ CN).	10
Fig. S13. ESI-MS spectrum of compound 2 .	11
Fig. S14. ¹ H NMR spectrum of compound 2 (600 MHz, pyridine- <i>d</i> ₅).	11
Fig. S15. ¹³ C NMR and DEPT spectrum of compound 2 (150 MHz, pyridine- <i>d</i> ₅).	12
Fig. S16. ¹ H- ¹ H COSY spectrum of compound 2 .	12
Fig. S17. HSQC spectrum of compound 2 .	13
Fig. S18. HMBC spectrum of compound 2 .	13
Fig. S19. ROESY spectrum of compound 2 .	14
Fig. S20. Zoomed area of ROESY spectrum of compound 2 for the correlations between H-22/H-23 and H-21/H-23.	15
Fig. S21. Zoomed area of ROESY spectrum of compound 2 for the correlations between H-19/13-NH.	15
Fig. S22. IR spectrum of compound 2 .	16
Fig. S23. UV spectrum of compound 2 (CH ₃ CN).	16
Fig. S24. ECD spectrum of compound 2 (CH ₃ CN).	17
Fig. S25. ESI-MS spectrum of compound 3 .	18
Fig. S26. ¹ H NMR spectrum of compound 3 (500 MHz, methanol- <i>d</i> ₄).	18
Fig. S27. ¹³ C NMR spectrum of compound 3 (150 MHz, methanol- <i>d</i> ₄).	19
Fig. S28. DEPT spectrum of compound 3 (150 MHz, methanol- <i>d</i> ₄).	19
Fig. S29. ¹ H- ¹ H COSY spectrum of compound 3 in methanol- <i>d</i> ₄ .	20
Fig. S30. HSQC spectrum of compound 3 in methanol- <i>d</i> ₄ .	20
Fig. S31. HMBC spectrum of compound 3 in methanol- <i>d</i> ₄ .	21
Fig. S32. Zoomed area of HMBC spectrum of compound 3 for the correlations between H-23/C-21 and H-23/C-22 in methanol- <i>d</i> ₄ .	21
Fig. S33. ROESY spectrum of compound 3 in methanol- <i>d</i> ₄ .	22
Fig. S34. Zoomed area of ROESY spectrum of compound 3 for the correlations between H-23/H-22 and H-23/H-21 in methanol- <i>d</i> ₄ .	22
Fig. S35. ¹ H NMR spectrum of compound 3 (500 MHz, acetone- <i>d</i> ₆).	23

Fig. S36. ^{13}C NMR and DEPT spectrum of compound 3 (150 MHz, acetone- d_6).	23
Fig. S37. ^1H - ^1H COSY spectrum of compound 3 in acetone- d_6	24
Fig. S38. HSQC spectrum of compound 3 in acetone- d_6	24
Fig. S39. HMBC spectrum of compound 3 in acetone- d_6	25
Fig. S40. ROESY spectrum of compound 3 in acetone- d_6	25
Fig. S41. Zoomed area of ROESY spectrum of compound 3 for the correlations between H-19/13-NH.	26
Fig. S42. IR spectrum of compound 3	26
Fig. S43. UV spectrum of compound 3 (CH_3CN).	27
Fig. S44. ECD spectrum of compound 3 (CH_3CN).	27
Fig. S45. ESI-MS spectrum of compound 4	28
Fig. S46. ^1H NMR spectrum of compound 4 (600 MHz, methanol- d_4).	28
Fig. S47. ^{13}C NMR and DEPT spectrum of compound 4 (150 MHz, methanol- d_4). ..	29
Fig. S48. ^1H - ^1H COSY spectrum of compound 4	29
Fig. S49. HSQC spectrum of compound 4	30
Fig. S50. HMBC spectrum of compound 4	30
Fig. S51. ROESY spectrum of compound 4	31
Fig. S52. Zoomed area of ROESY spectrum of compound 4 for the correlations between H-23/H-21 and H-23/H-22.	31
Fig. S53. Zoomed area of ROESY spectrum of compound 4 for the correlations between H-13/H-2.	32
Fig. S54. IR spectrum of compound 4	32
Fig. S55. UV spectrum of compound 4 (CH_3CN).	33
Fig. S56. ECD spectrum of compound 4 (CH_3CN).	33
Fig. S57. ESI-MS spectrum of compound 5	34
Fig. S58. ^1H NMR spectrum of compound 5 (600 MHz, CDCl_3).	34
Fig. S59. ^{13}C NMR and DEPT spectrum of compound 5 (150 MHz, CDCl_3).	35
Fig. S60. ^1H - ^1H COSY spectrum of compound 5	35
Fig. S61. HSQC spectrum of compound 5	36
Fig. S62. HMBC spectrum of compound 5	36
Fig. S63. ROESY spectrum of compound 5	37
Fig. S64. IR spectrum of compound 5	37
Fig. S65. UV spectrum of compound 5 (CH_3CN).	38
Fig. S66. ECD spectrum of compound 5 (CH_3CN).	38
Table S1. ITS1 sequences of the fungal strain <i>Penicillium expansum</i> MA147	39
Fig. S67. Four possible relative configurations of compound 1	39
Table S2. The calculated ^{13}C NMR chemical shifts of structures 1a-d fitting to the experimental data of compound 1 following STS protocol.	40
Table S3. The calculated $^1\text{H}/^{13}\text{C}$ NMR chemical shifts (scaled) of structures 1a-d fitting to the experimental data of compound 1 at mPW1PW91/6-31G(d,p) level.	41
Fig. S68. Weighted ECD curve and the curves of conformers of structure 1a	43
Fig. S69. Weighted ECD curve and the curves of conformers of structure 1b	43
Fig. S70. Weighted ECD curve and the curves of conformers of the enantiomer of structure 1b	44

Fig. S71. Weighted ECD curve and the curves of conformers of structure 1c	44
Fig. S72. Weighted ECD curve of structure 1d	45
Fig. S73. Experimental ECD curve of compound 1 and weighted ECD curves of structures 1a–d	45
Fig. S74. ¹ H NMR spectrum of compound 6 (600 MHz, CD ₃ OD).	46
Fig. S75. ¹³ C NMR spectrum of compound 6 (150 MHz, CD ₃ OD).	46
Fig. S76. ¹ H NMR spectrum of compound 7 (600 MHz, CDCl ₃).	47
Fig. S77. ¹³ C NMR spectrum of compound 7 (150 MHz, CDCl ₃).	47
Fig. S78. ¹ H NMR spectrum of compound 8 (600 MHz, CDCl ₃).	48
Fig. S79. ¹³ C NMR spectrum of compound 8 (150 MHz, CDCl ₃).	48
Fig. S80. ¹ H NMR spectrum of compound 9 (600 MHz, DMSO- <i>d</i> ₆).	49
Fig. S81. ¹³ C NMR spectrum of compound 9 (150 MHz, DMSO- <i>d</i> ₆).	49
Fig. S82. ¹ H NMR spectrum of compound 10 (600 MHz, CD ₃ OD).	50
Fig. S83. ¹³ C NMR spectrum of compound 10 (150 MHz, CD ₃ OD).	50
Fig. S84. Raw image of Western blotting of ABCA1.	51
Fig. S85. Raw image of Western blotting of α -tubulin.	52
Fig. S86. LC-MS analysis of the raw EtOAc extraction of the strain MA147.	53
Fig. S87. LC-MS analysis of the raw EtOAc extraction of the strain MA147 and the standard sample of compound 4	54
Fig. S88. LC-MS analysis of the raw EtOAc extraction of the strain MA147 and the standard sample of compound 5	55
Table S4. ¹ H (600 MHz) and ¹³ C (150 MHz) NMR spectroscopic data of compound 3 in acetone- <i>d</i> ₆	56
Table S5. Coordinates and relative free energy of low-energy conformers of structures 1a–d for GIAO NMR calculations.	57
Table S6. Coordinates and relative free energy of low-energy conformers of structures 1a–d for ECD calculations.	83
Table S7. Coordinates and relative free energy of low-energy conformers of structures 13R/S-5	106

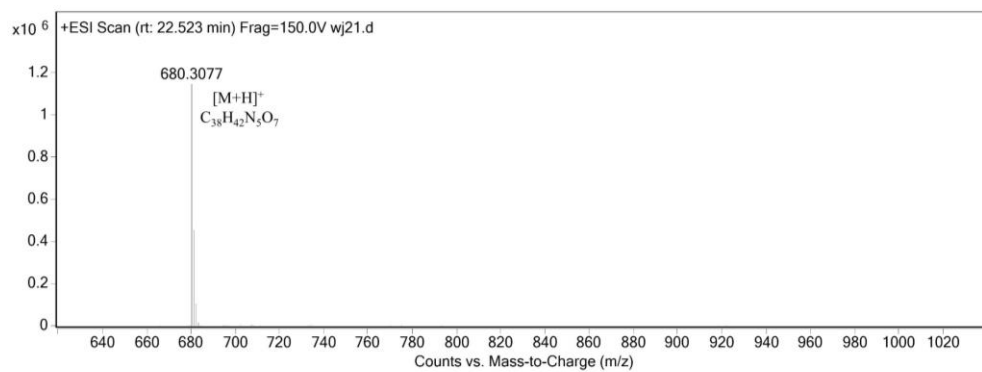


Fig. S1. ESI-MS spectrum of compound **1**.

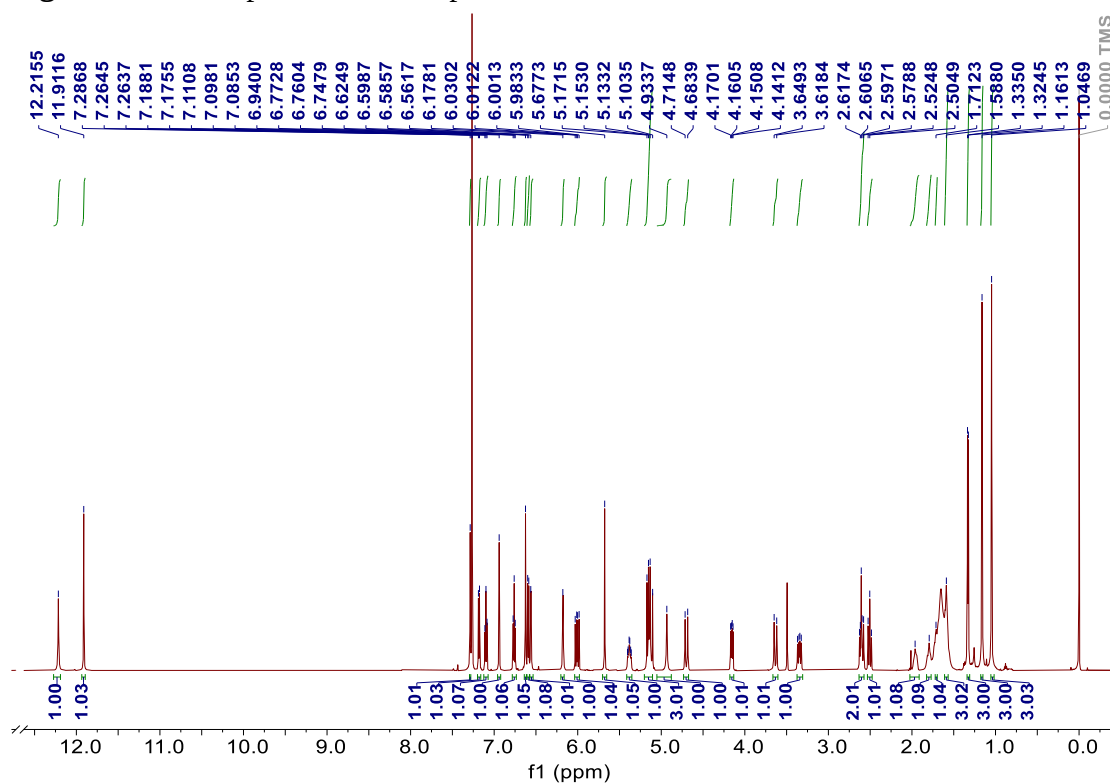


Fig. S2. 1H NMR spectrum of compound **1** (600 MHz, $CDCl_3$).

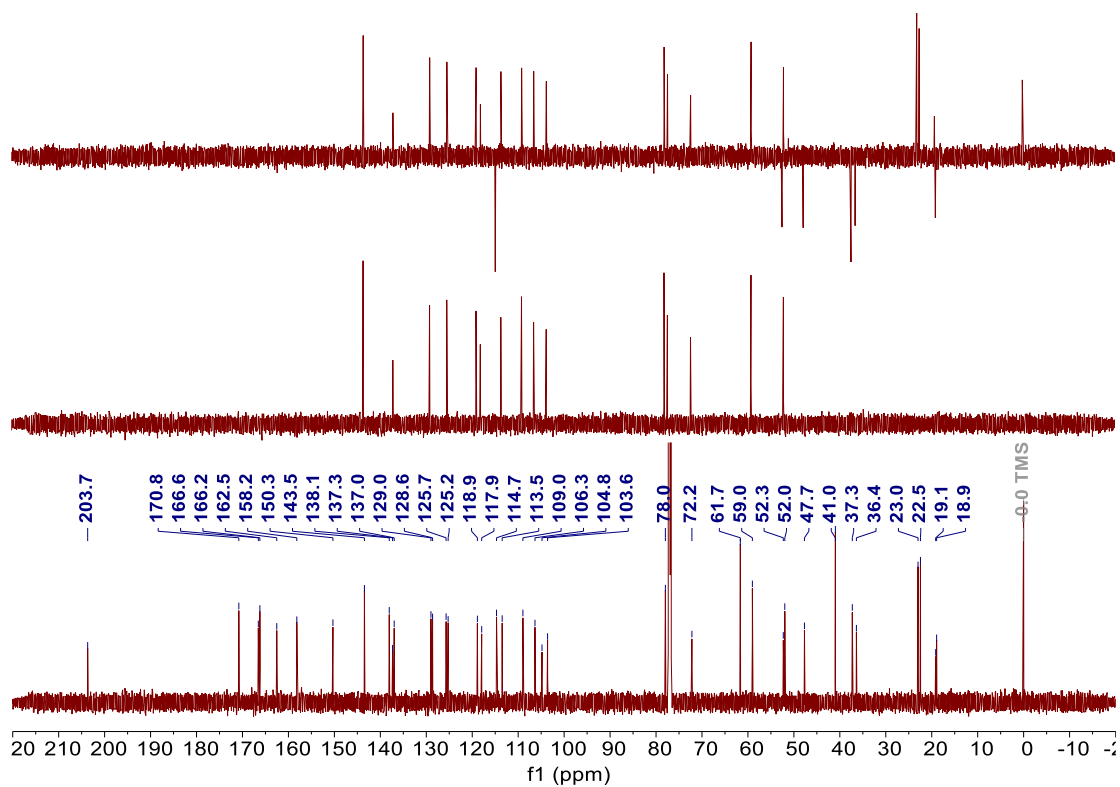


Fig. S3. ^{13}C NMR and DEPT spectrum of compound **1** (150 MHz, CDCl_3).

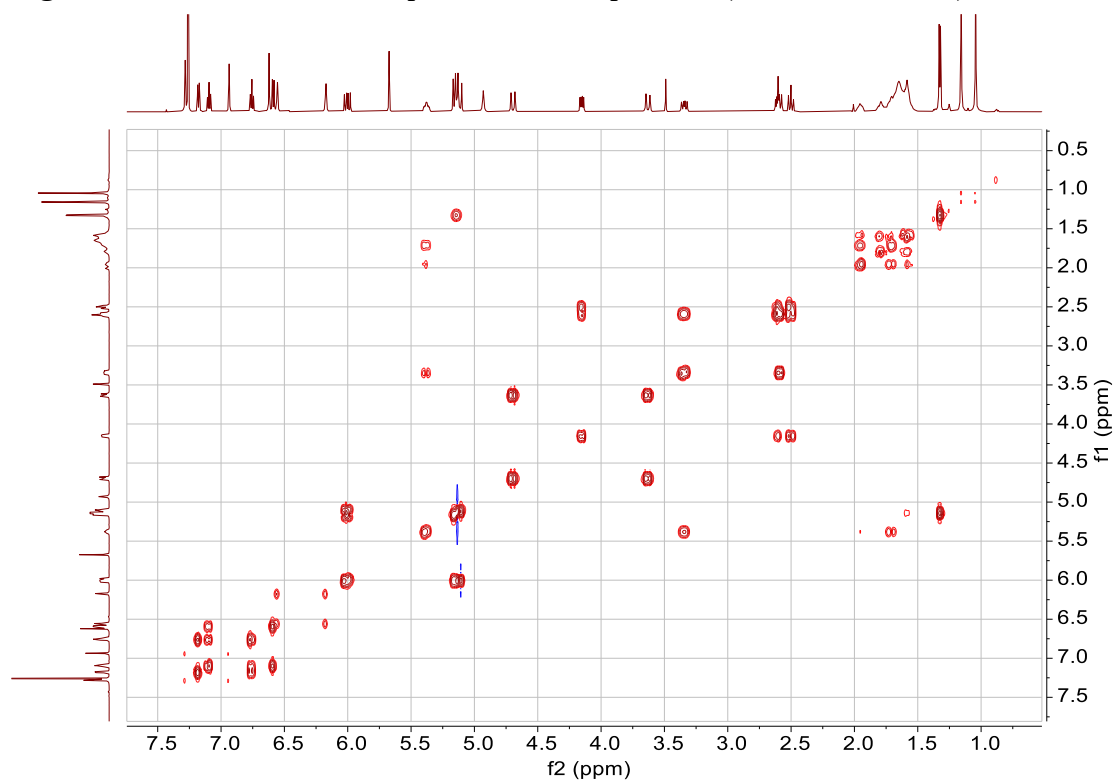


Fig. S4. ^1H - ^1H COSY spectrum of compound **1**.

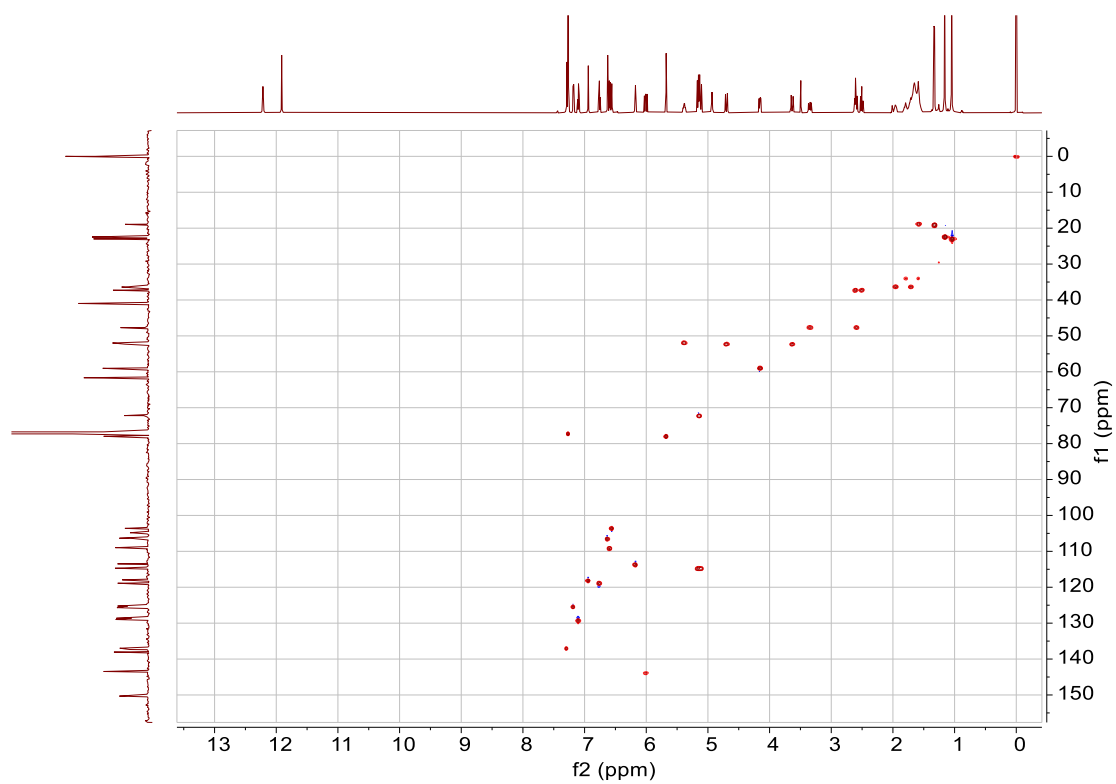


Fig. S5. HSQC spectrum of compound **1**.

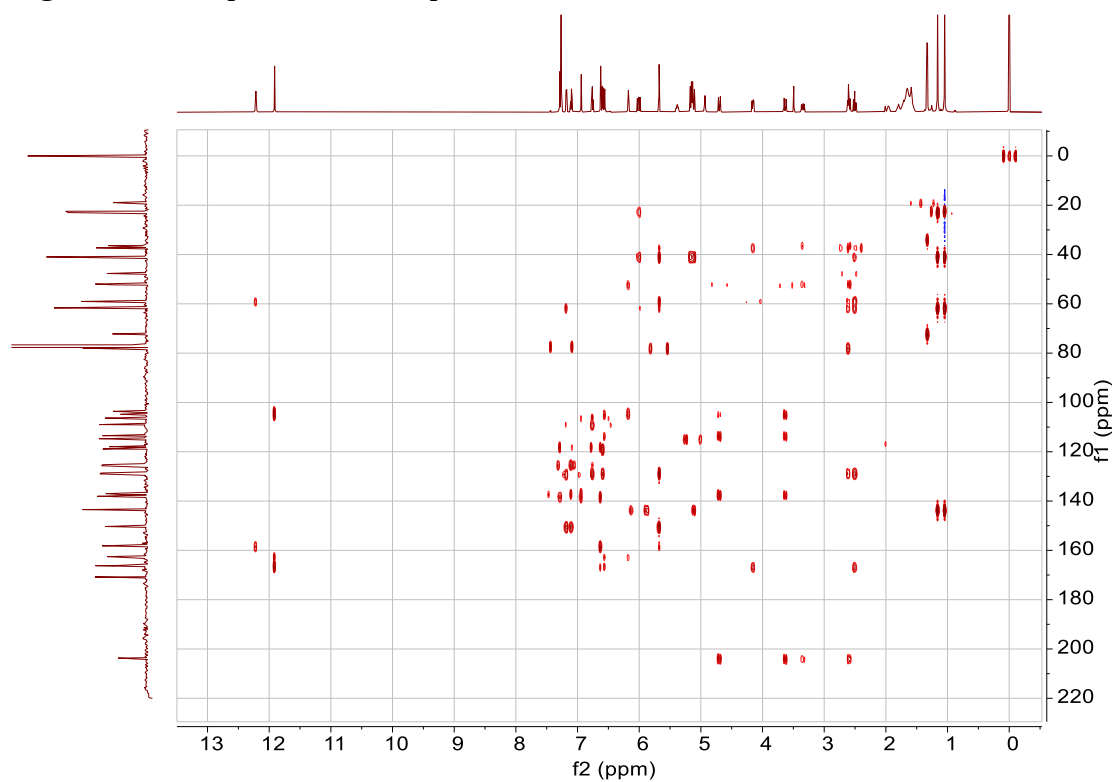


Fig. S6. HMBC spectrum of compound **1**.

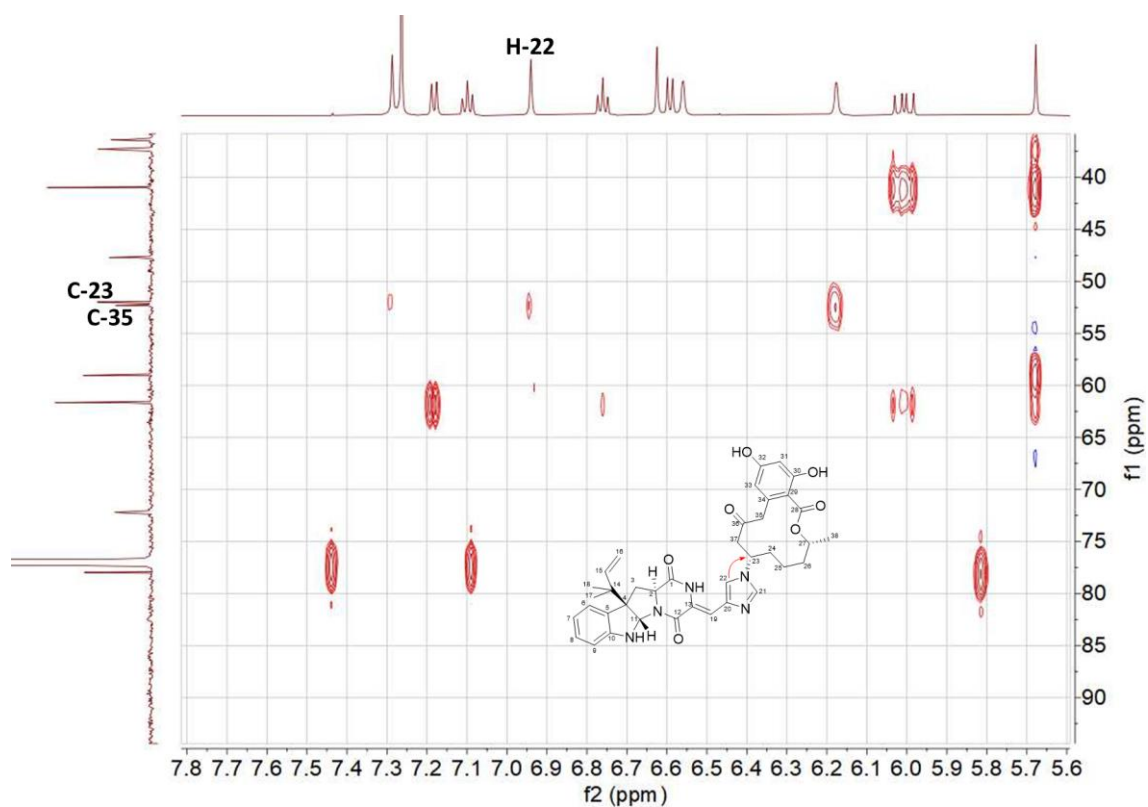


Fig. S7. Zoomed area of HMBC spectrum of compound **1** for the correlation between H-22 and C-23.

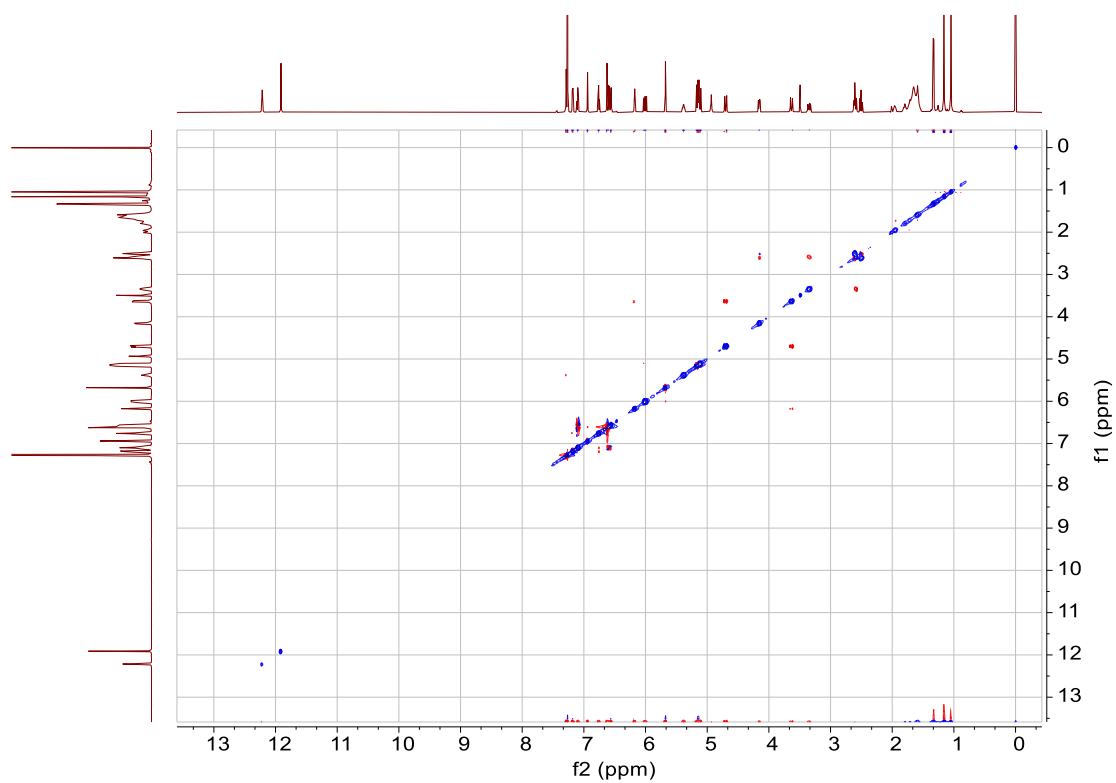


Fig. S8. ROESY spectrum of compound **1**.

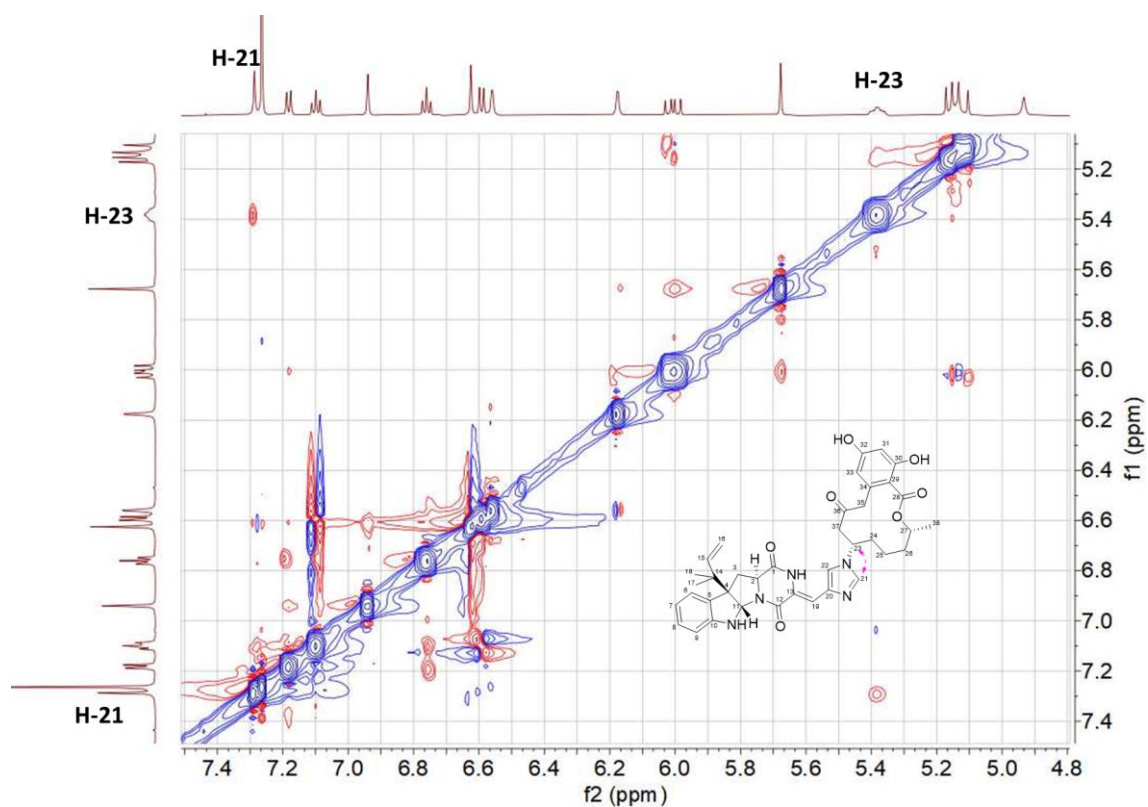


Fig. S9. Zoomed area of ROESY spectrum of compound **1** for the correlation between H-21 and H-23.

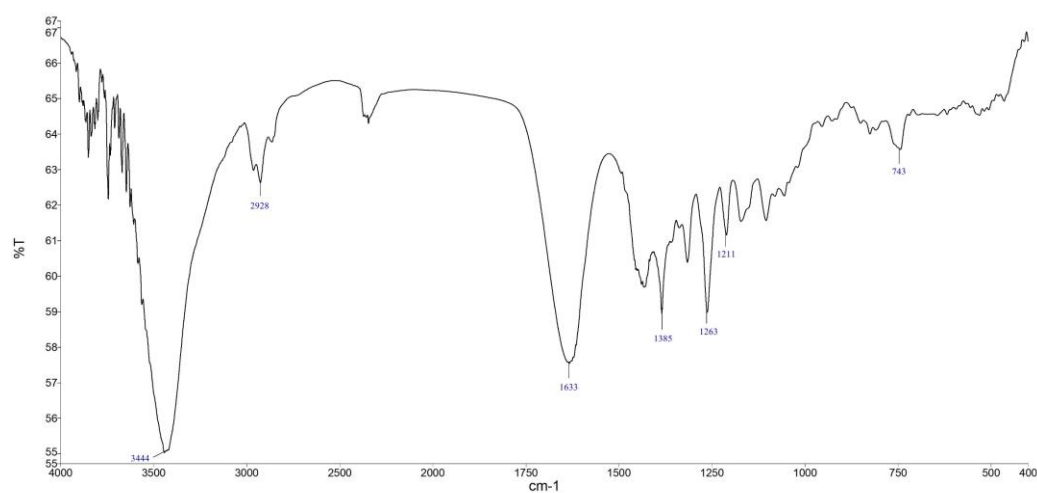


Fig. S10. IR spectrum of compound **1**.

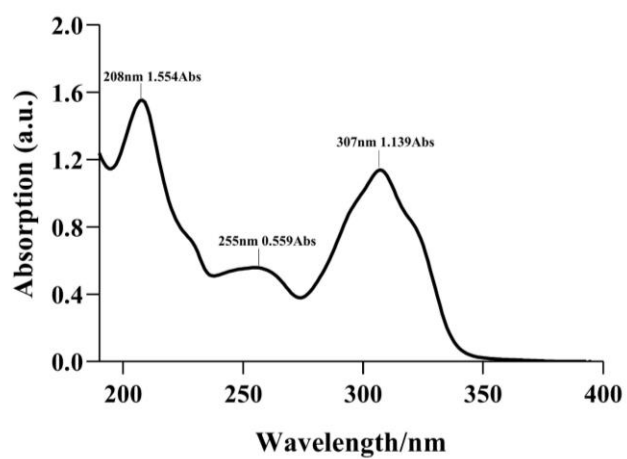


Fig. S11. UV spectrum of compound **1** (CH₃CN).

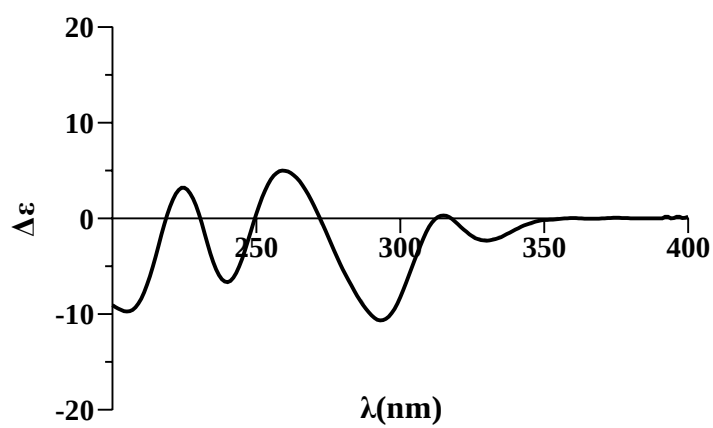


Fig. S12. ECD spectrum of compound **1** (CH₃CN).

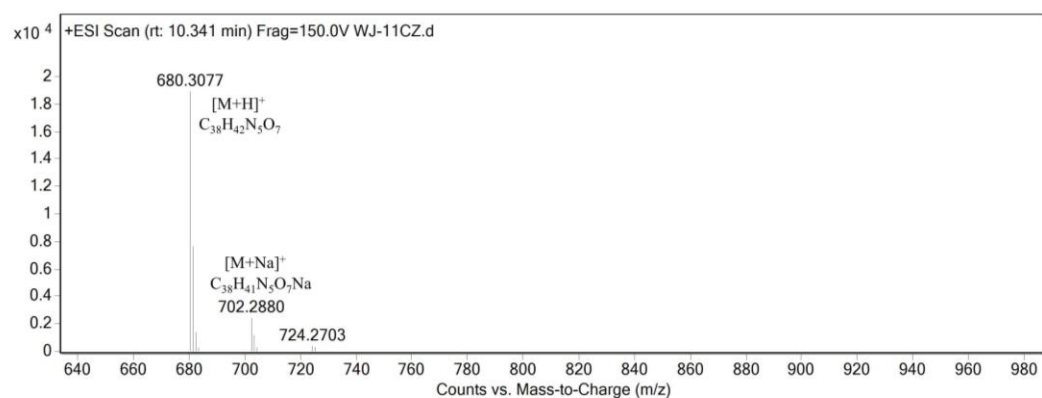


Fig. S13. ESI-MS spectrum of compound 2.

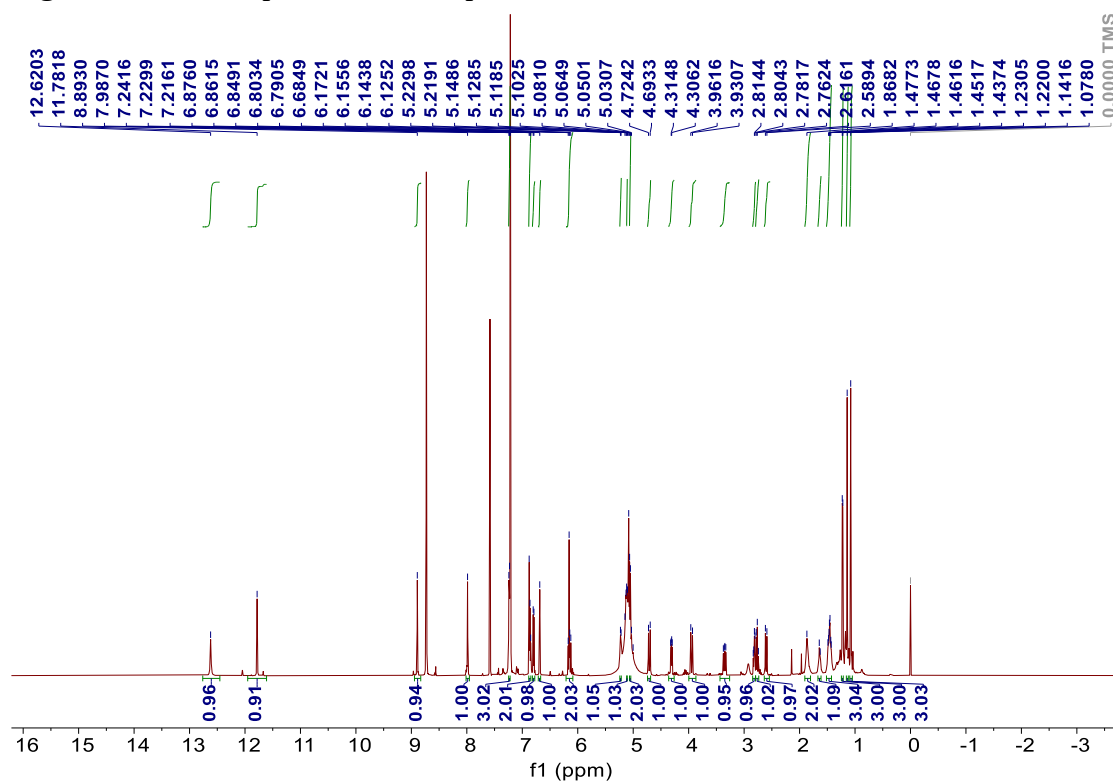


Fig. S14. 1H NMR spectrum of compound 2 (600 MHz, pyridine- d_5).

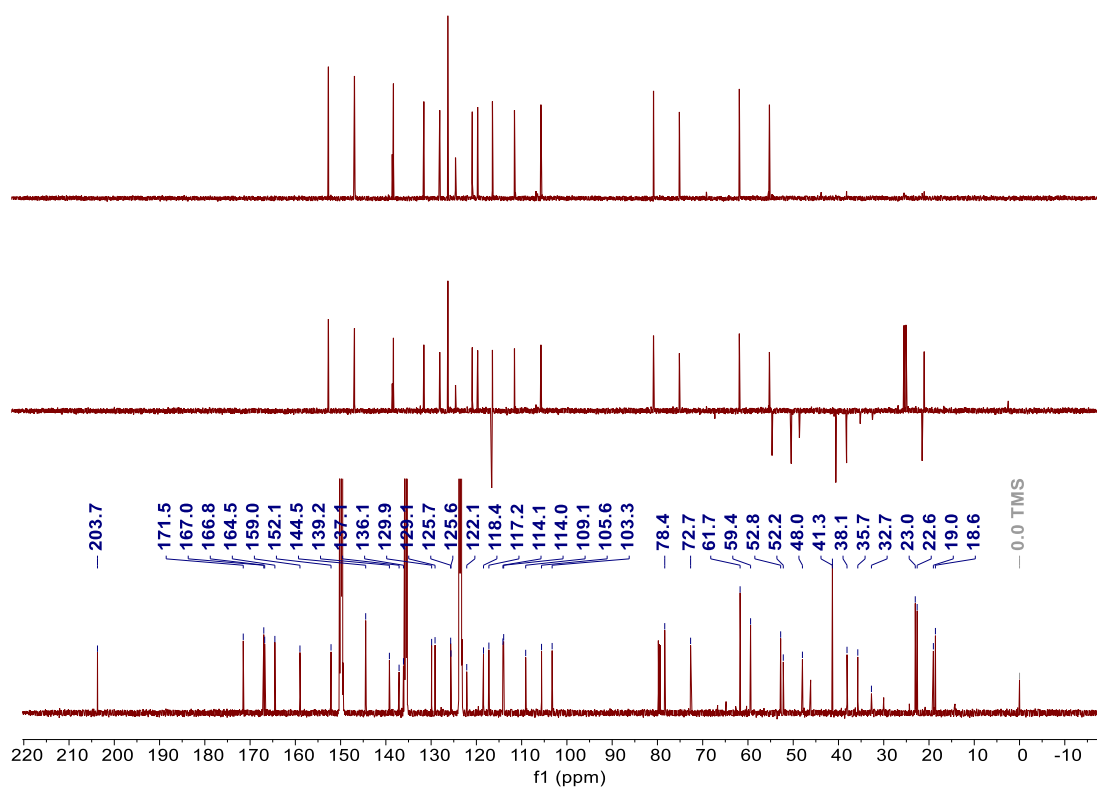


Fig. S15. ^{13}C NMR and DEPT spectrum of compound 2 (150 MHz, pyridine- d_5).

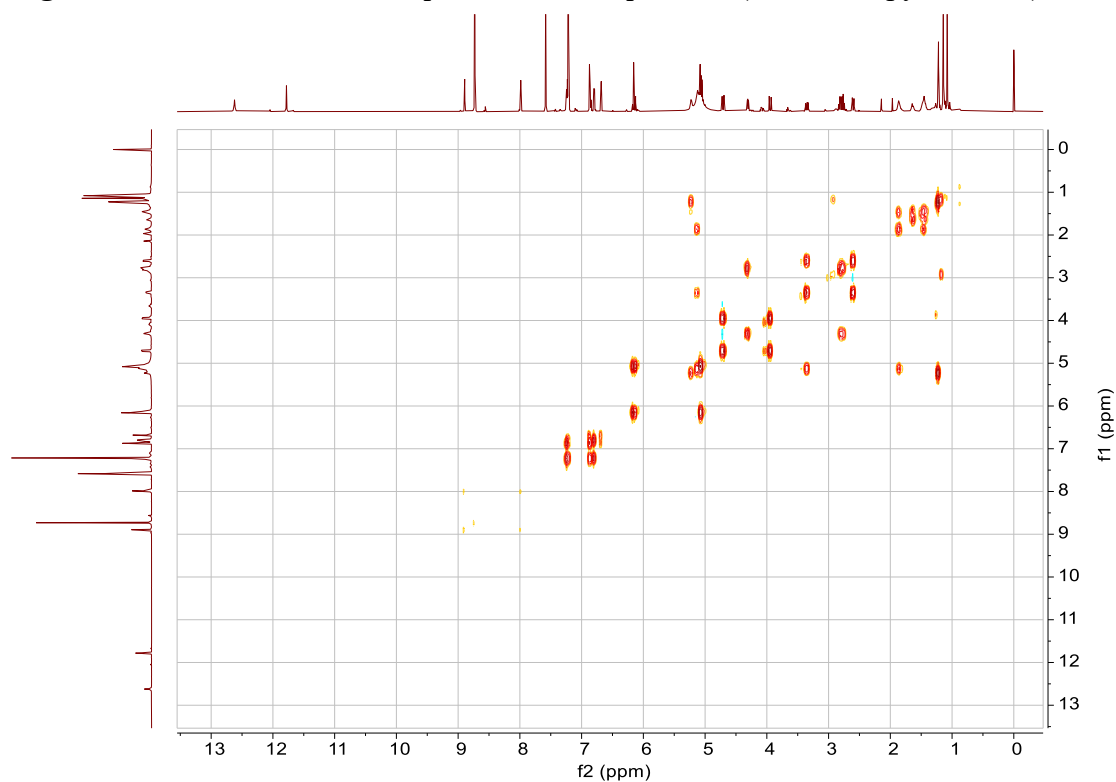


Fig. S16. ^1H - ^1H COSY spectrum of compound 2.

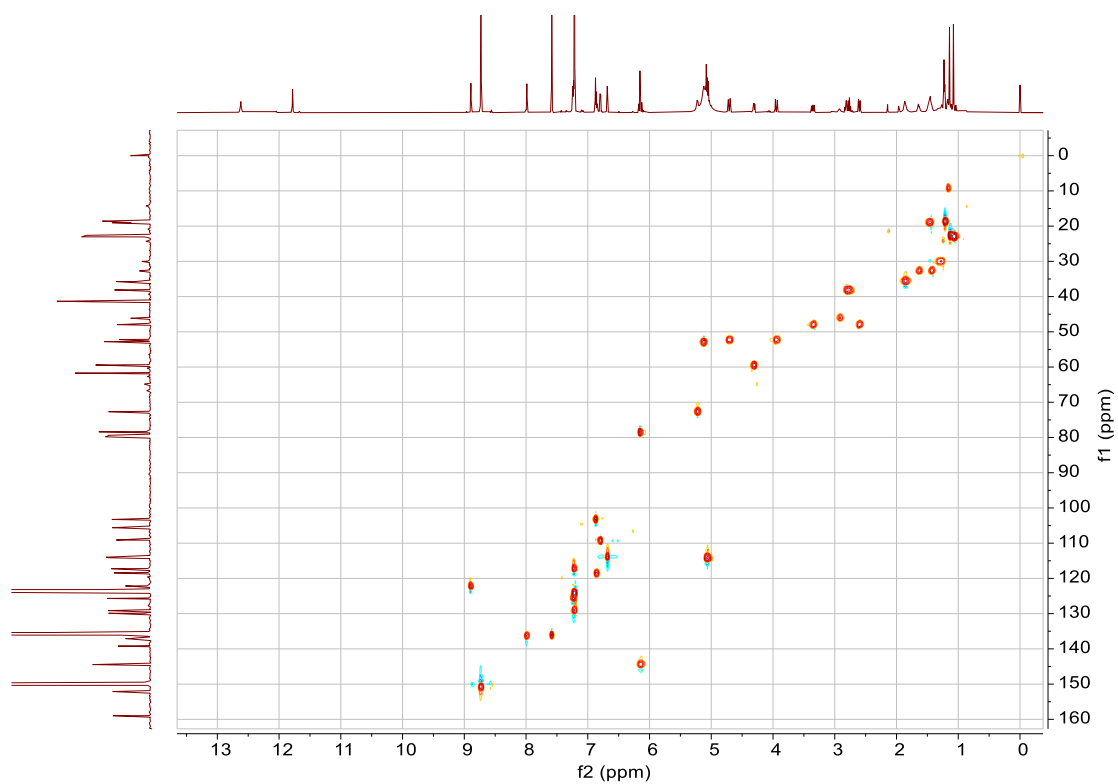


Fig. S17. HSQC spectrum of compound **2**.

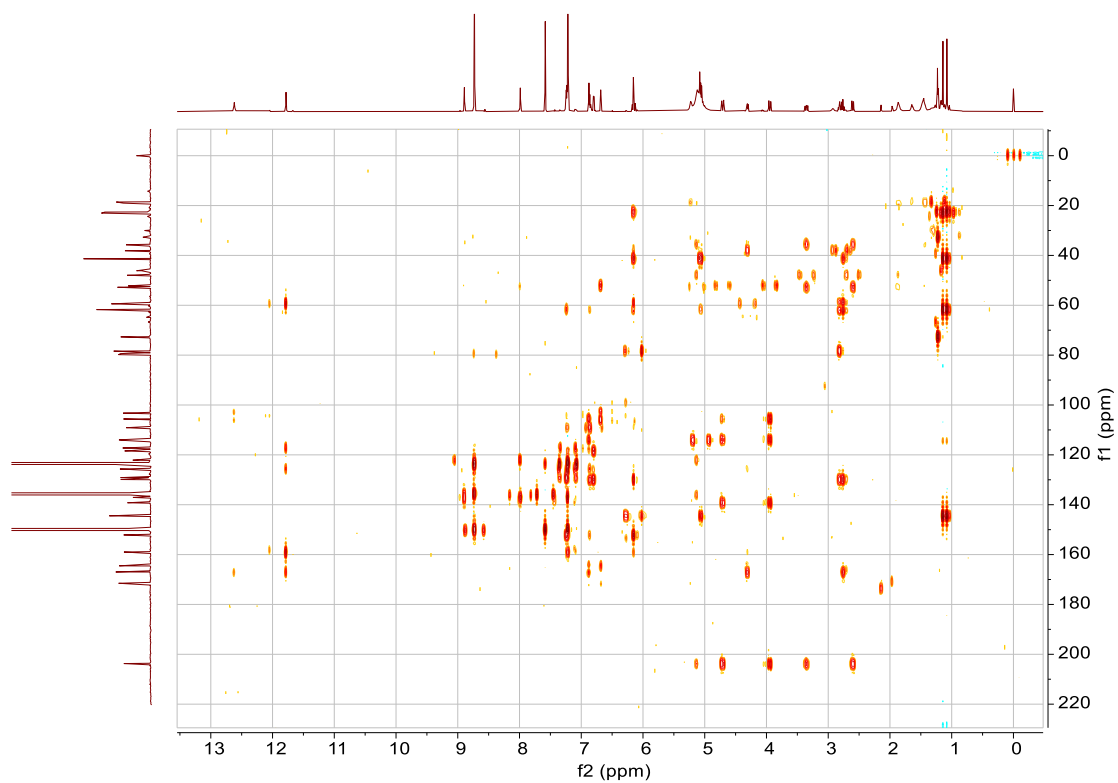


Fig. S18. HMBC spectrum of compound **2**.

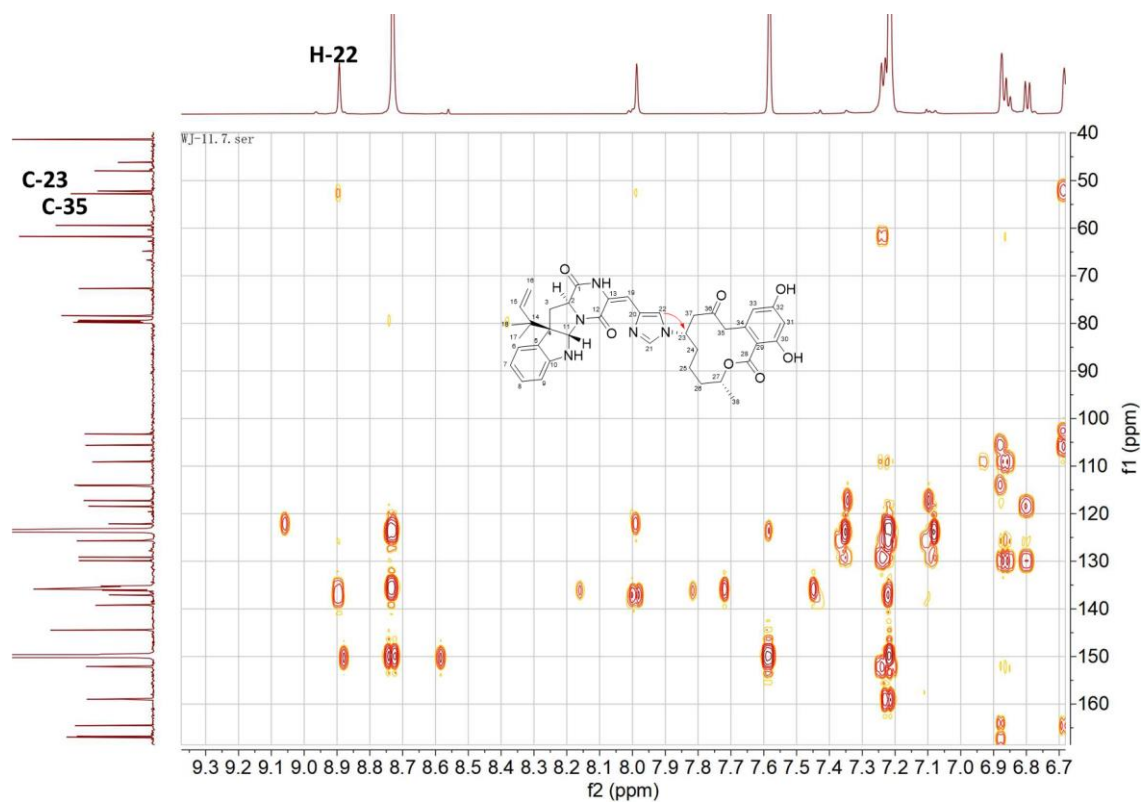


Fig. S19. Zoomed area of HMBC spectrum of compound **2** for the correlation between H-22 and C-23.

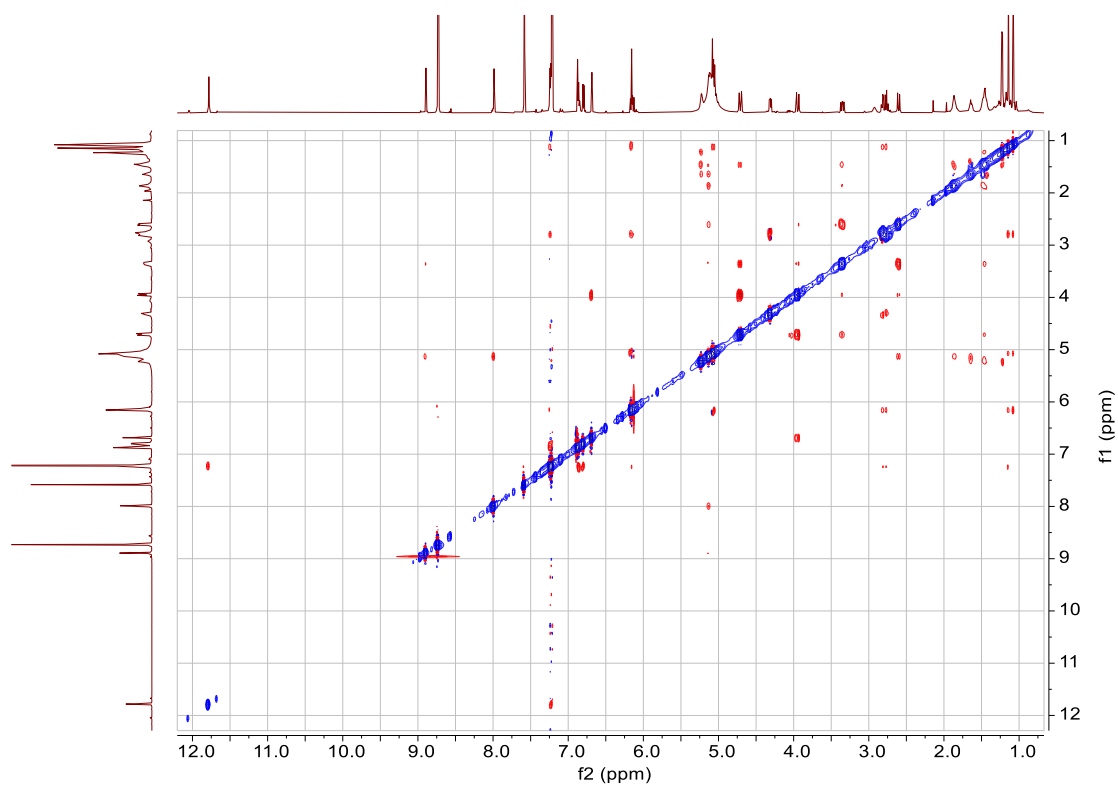


Fig. S19. ROESY spectrum of compound **2**.

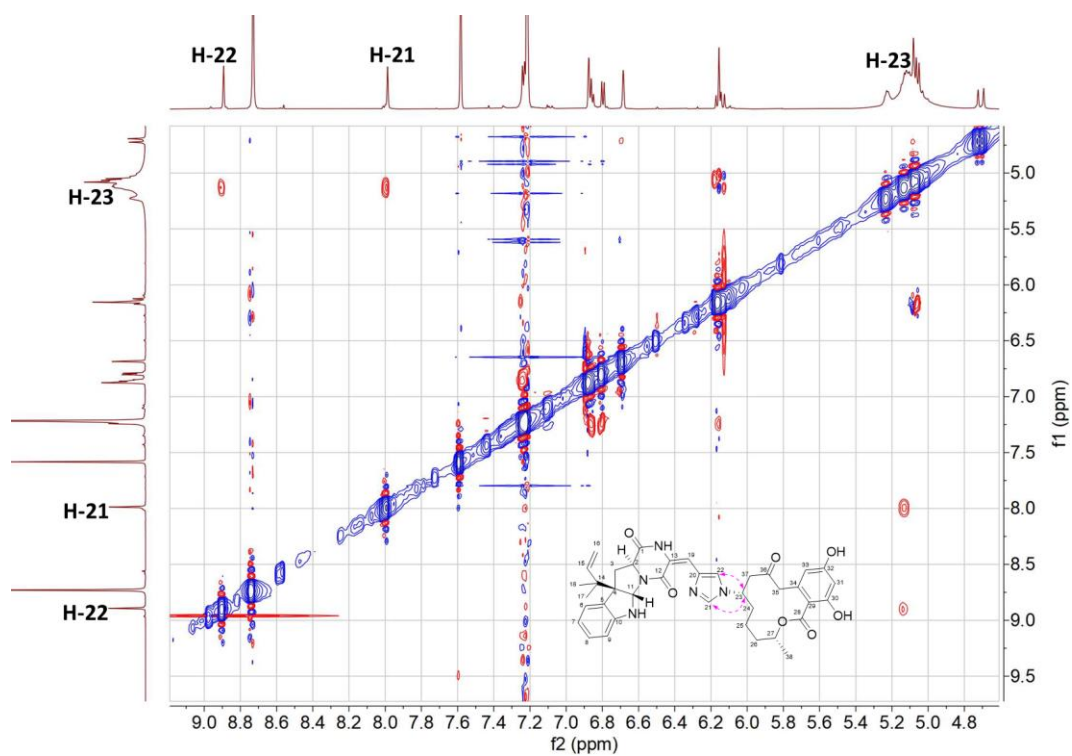


Fig. S20. Zoomed area of ROESY spectrum of compound 2 for the correlations between H-22/H-23 and H-21/H-23.

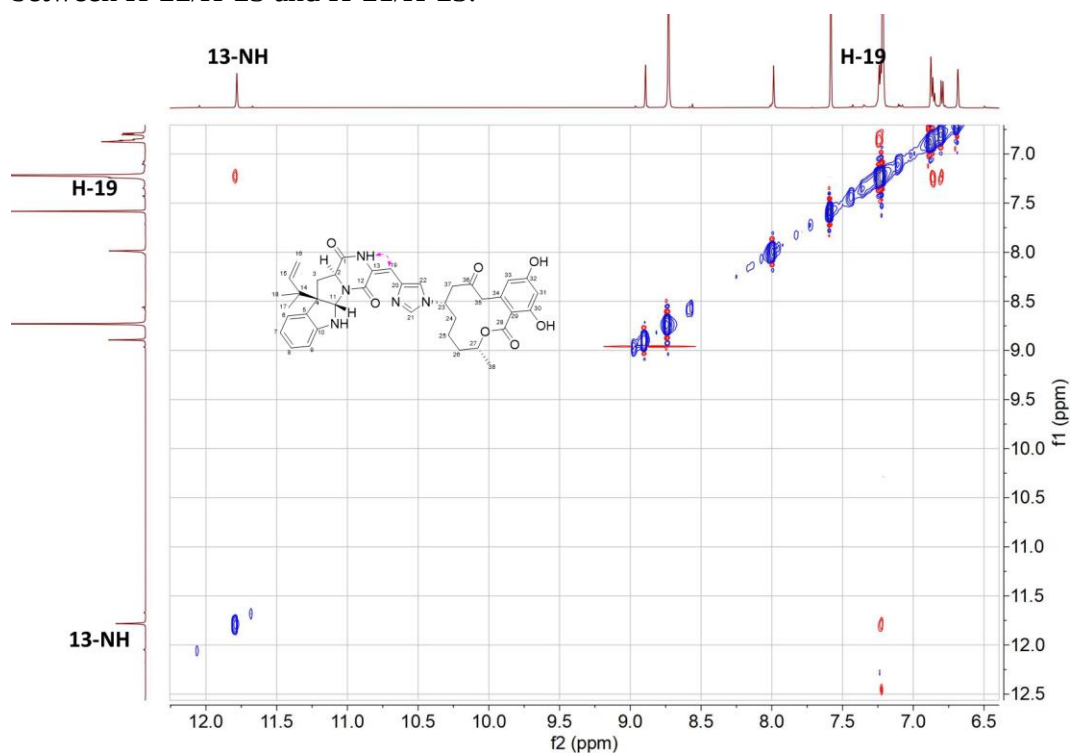


Fig. S21. Zoomed area of ROESY spectrum of compound 2 for the correlations between H-19/13-NH.

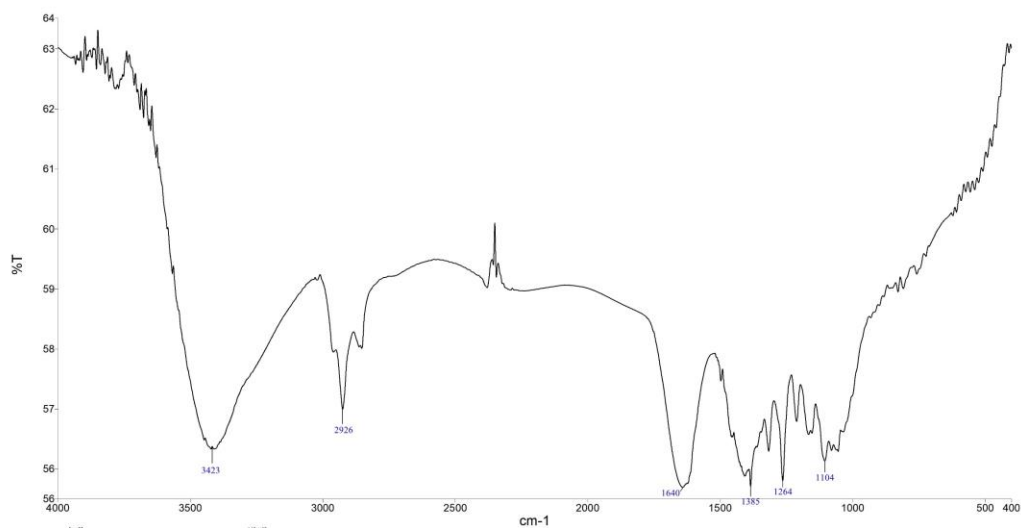


Fig. S22. IR spectrum of compound 2.

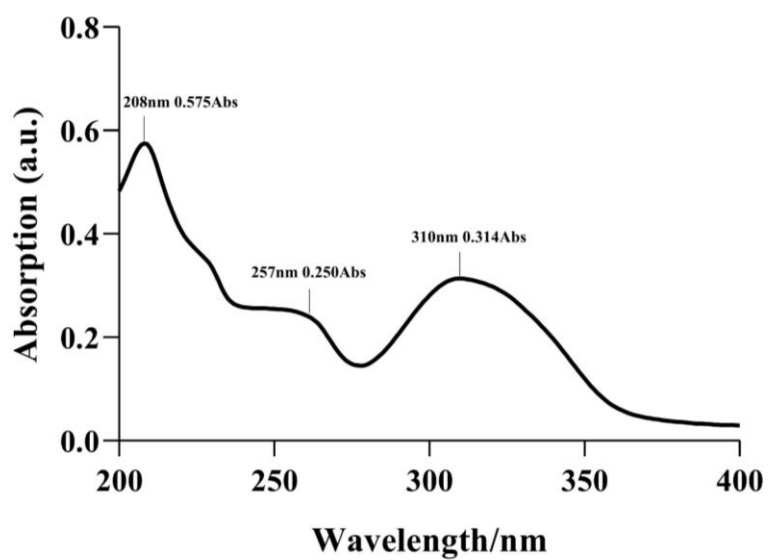


Fig. S23. UV spectrum of compound 2 (CH₃CN).

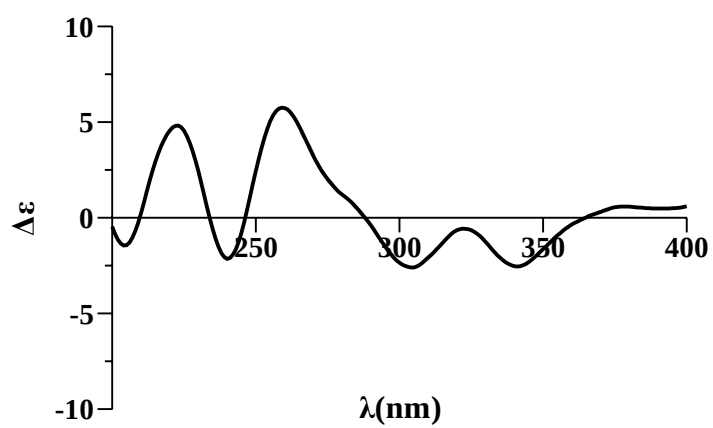


Fig. S24. ECD spectrum of compound 2 (CH₃CN).

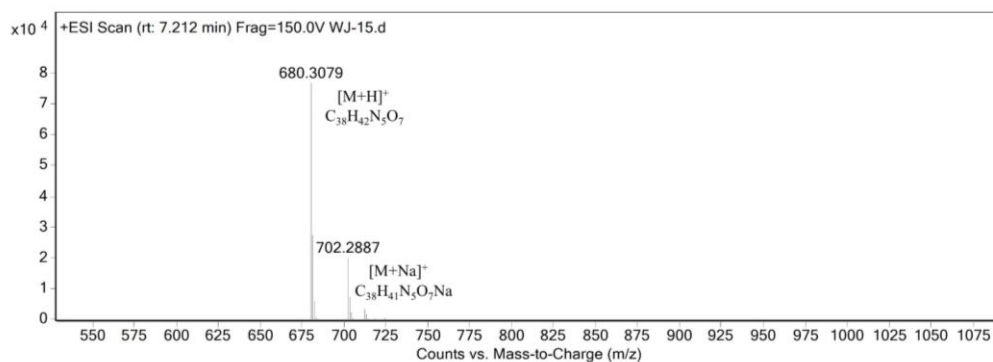


Fig. S25. ESI-MS spectrum of compound **3**.

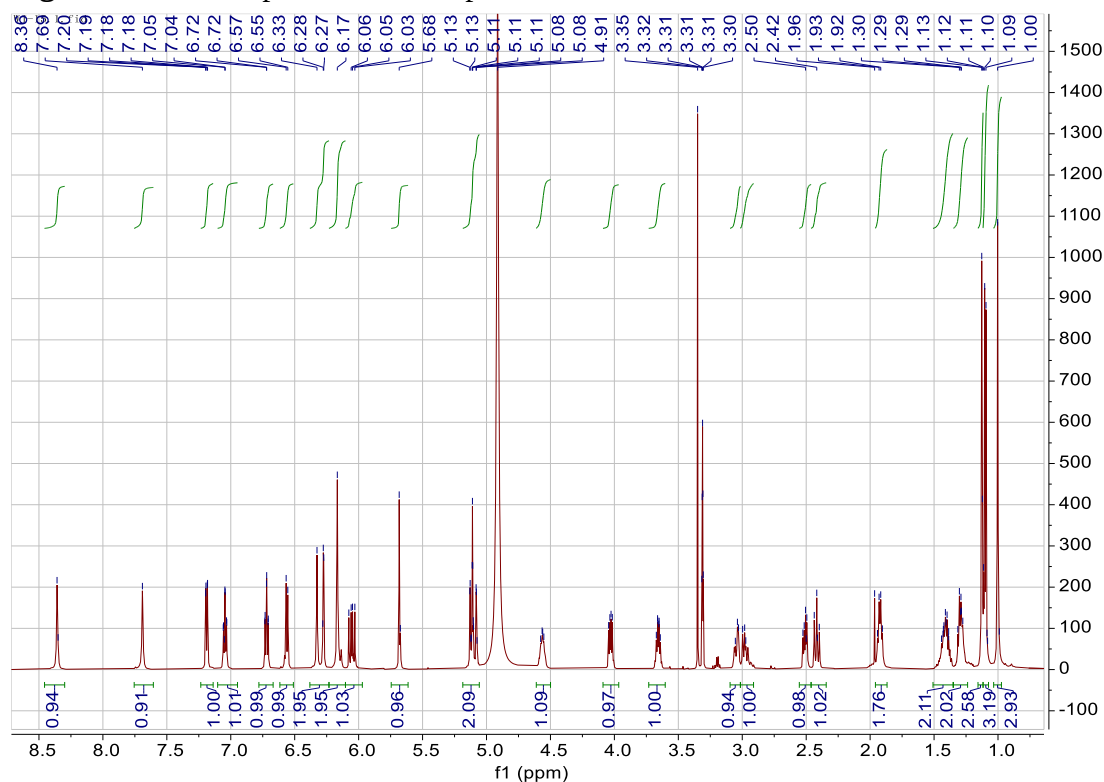


Fig. S26. 1H NMR spectrum of compound **3** (500 MHz, CH_3OH-d_4).

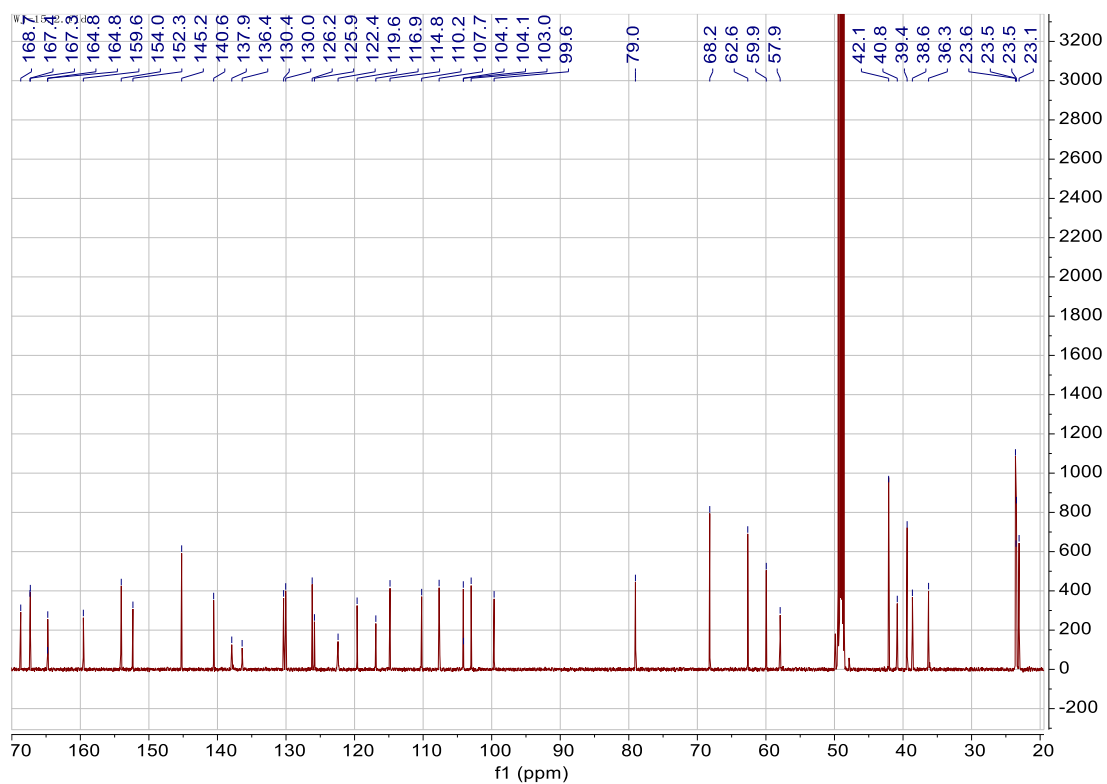


Fig. S27. ^{13}C NMR spectrum of compound **3** (150 MHz, methanol- d_4).

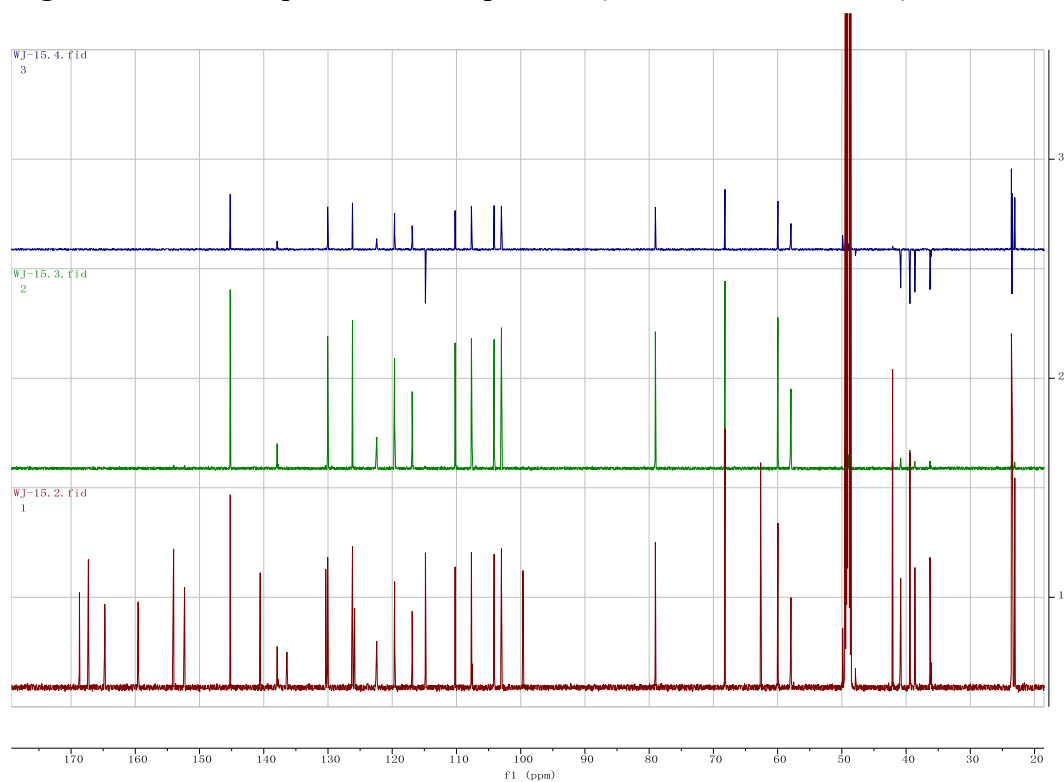


Fig. S28. DEPT spectrum of compound **3** (150 MHz, methanol- d_4).

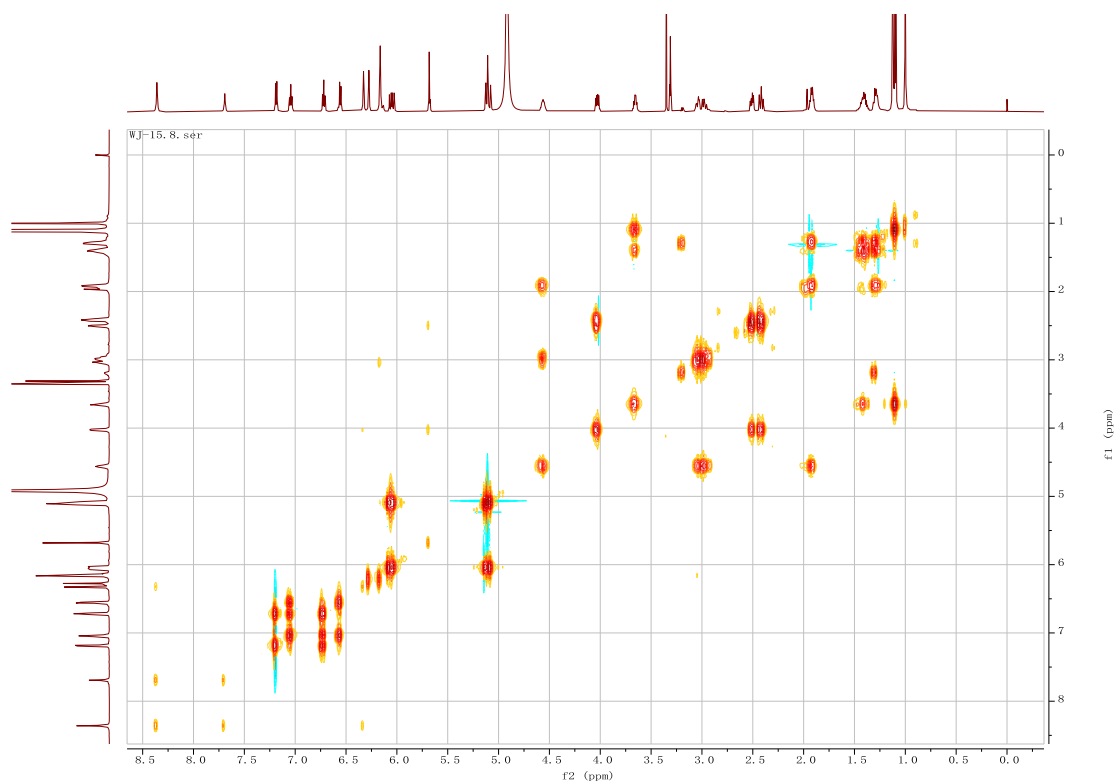


Fig. S29. ^1H - ^1H COSY spectrum of compound **3** in methanol- d_4 .

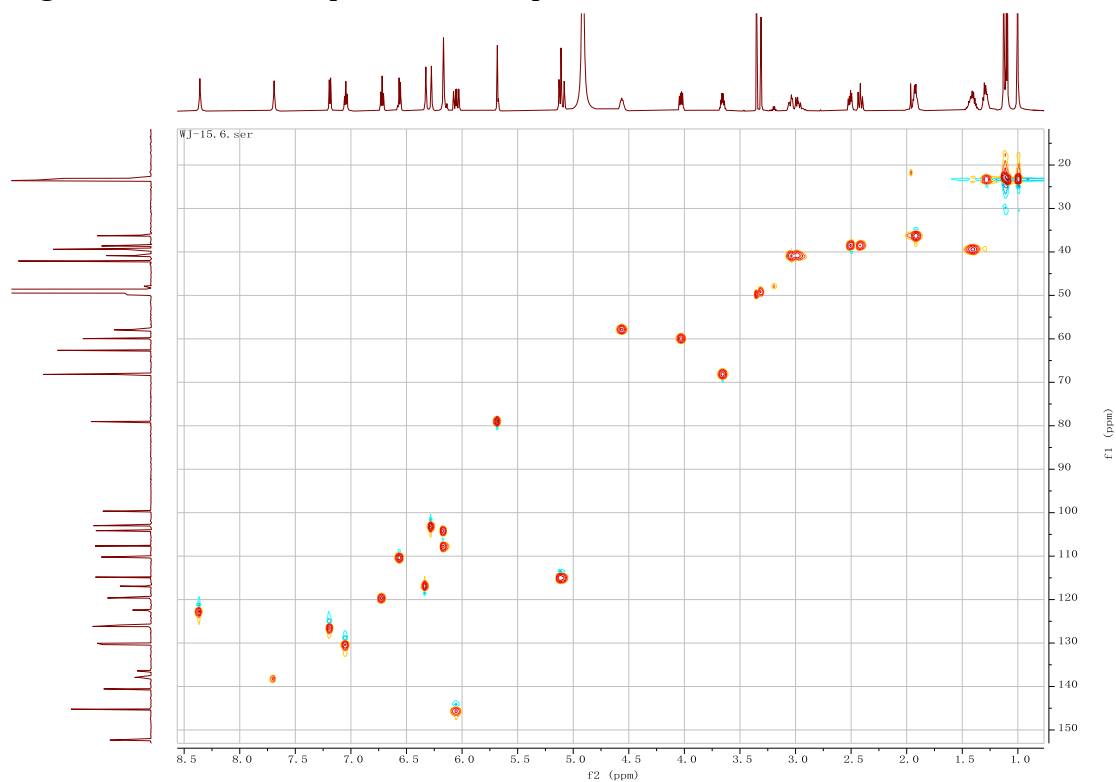


Fig. S30. HSQC spectrum of compound **3** in methanol- d_4 .

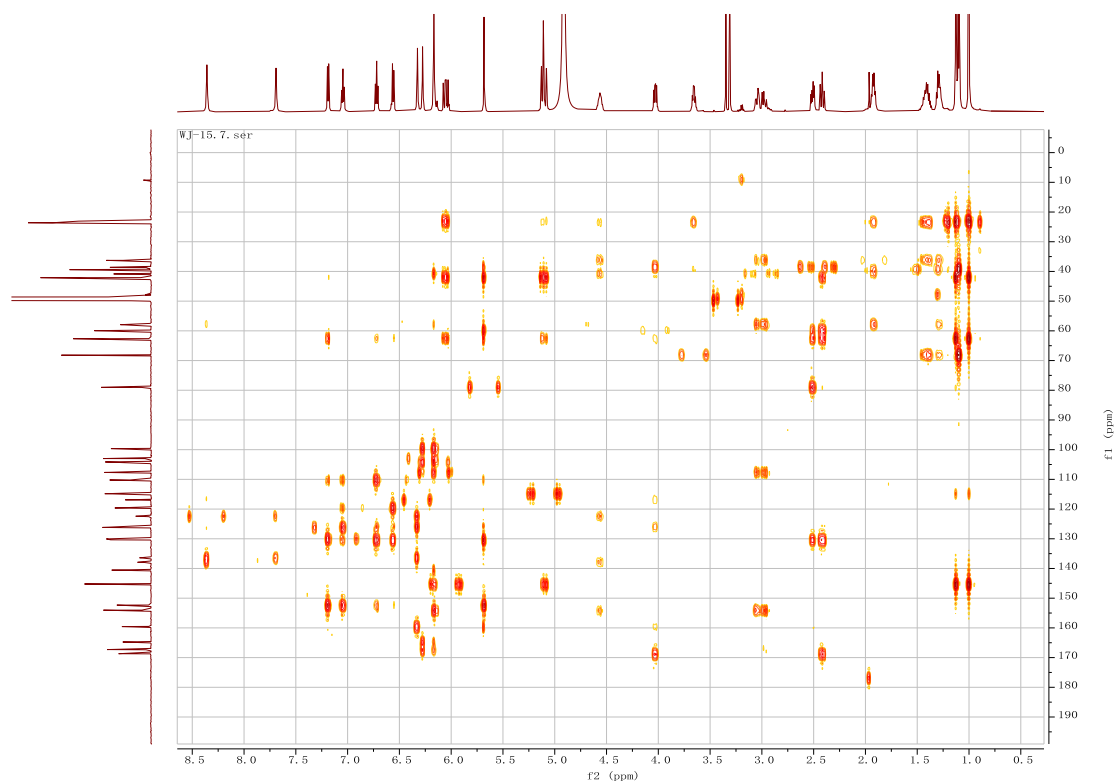


Fig. S31. HMBC spectrum of compound **3** in methanol- d_4 .

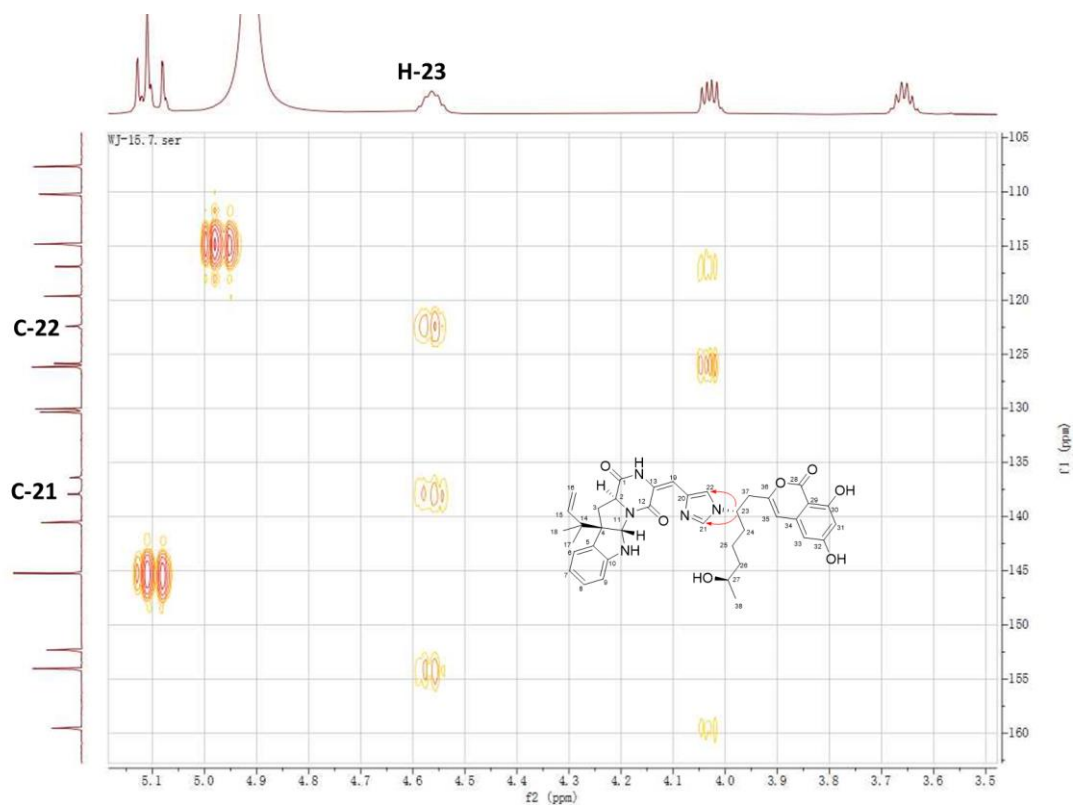


Fig. S32. Zoomed area of HMBC spectrum of compound **3** for the correlations between H-23/C-21 and H-23/C-22 in methanol- d_4 .

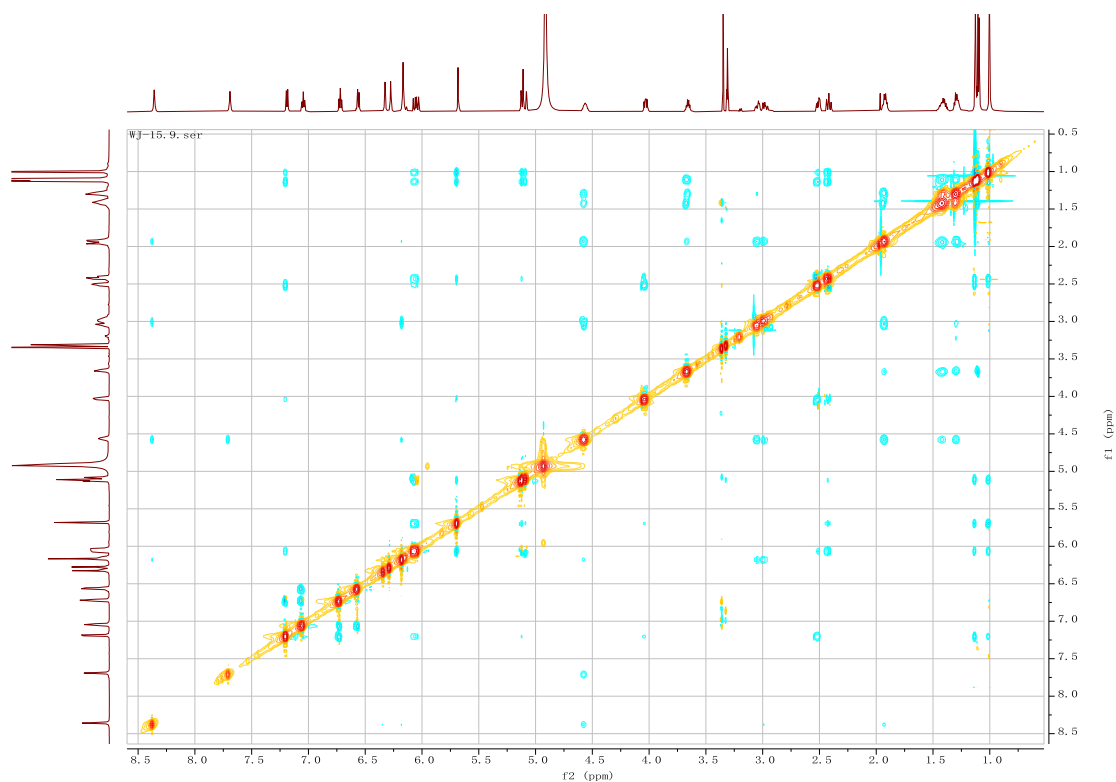


Fig. S33. ROESY spectrum of compound **3** in methanol- d_4 .

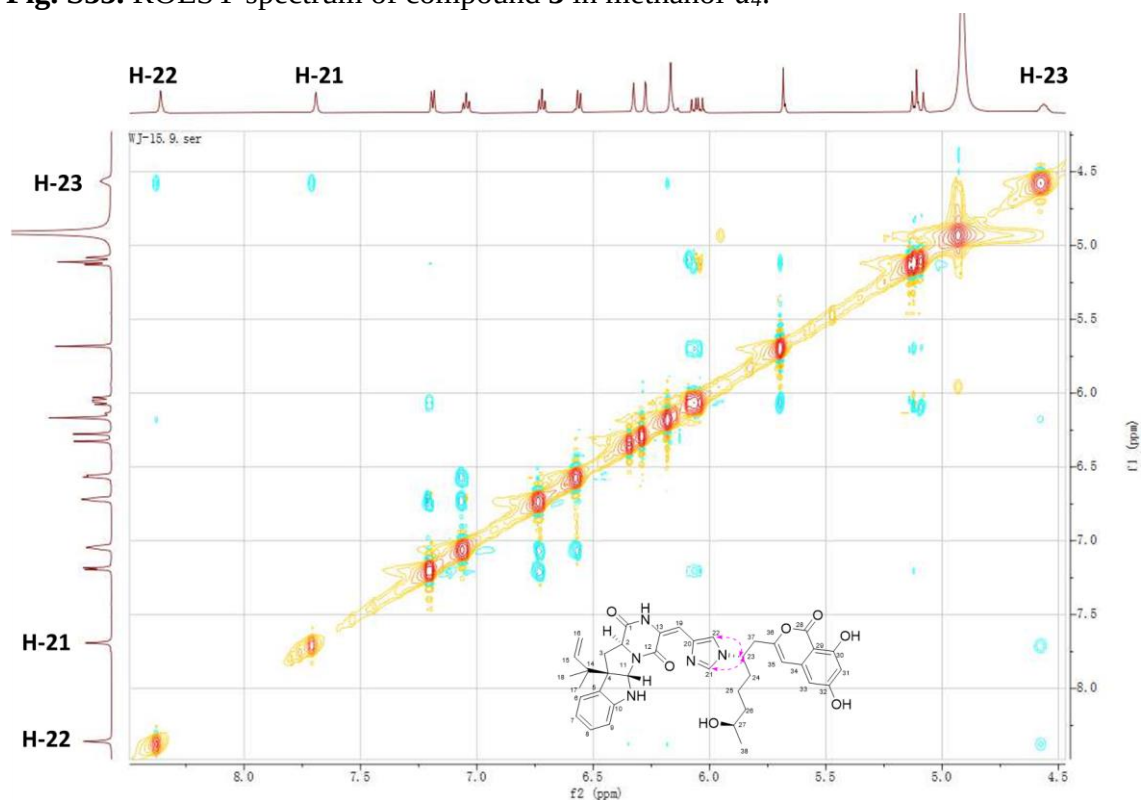


Fig. S34. Zoomed area of ROESY spectrum of compound **3** for the correlations between H-23/H-22 and H-23/H-21 in methanol- d_4 .

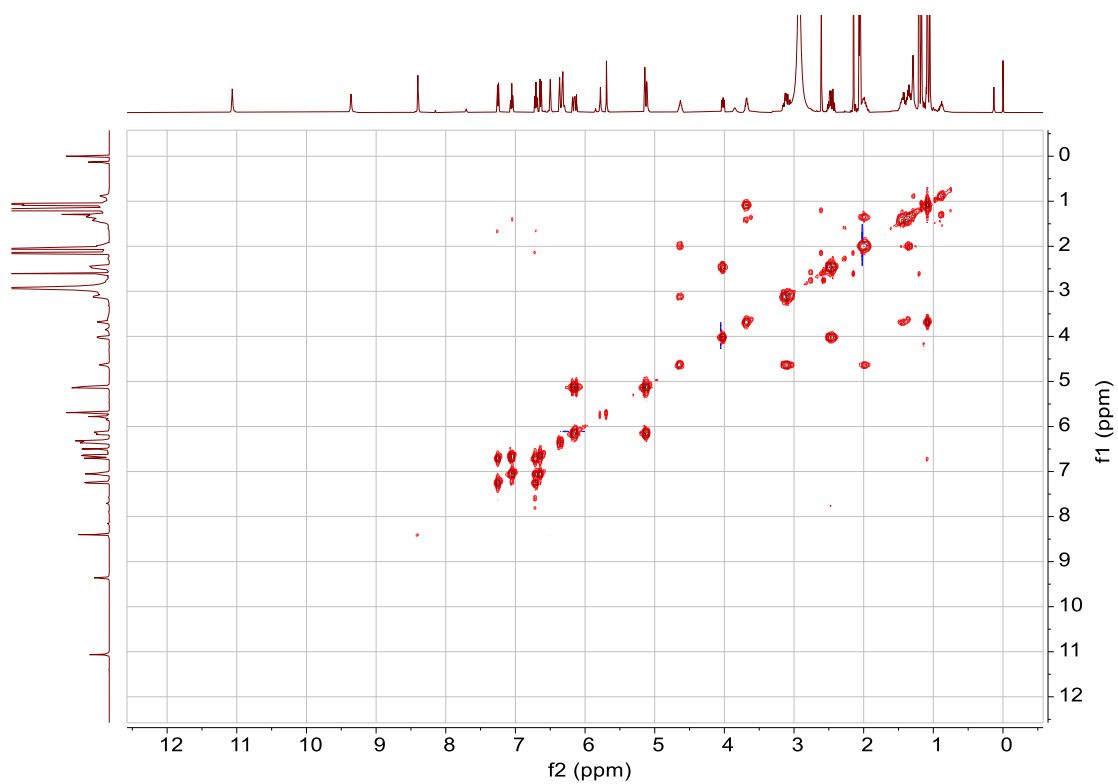


Fig. S37. ^1H - ^1H COSY spectrum of compound **3** in acetone- d_6 .

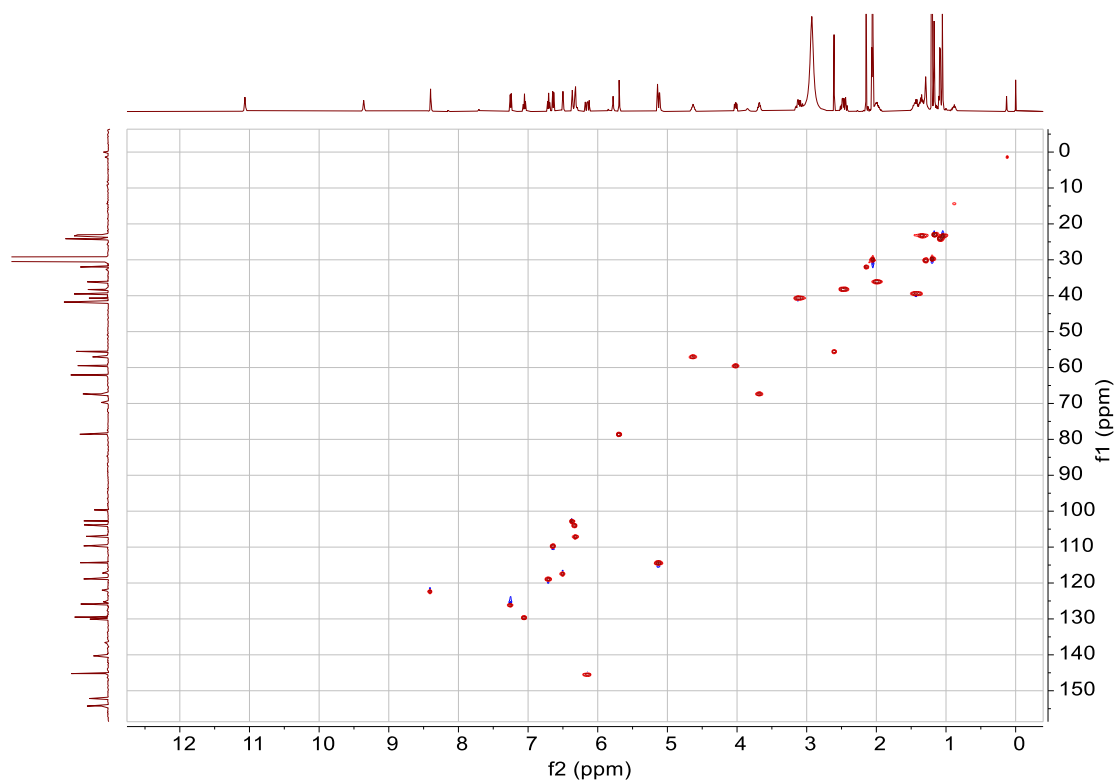


Fig. S38. HSQC spectrum of compound **3** in acetone- d_6 .

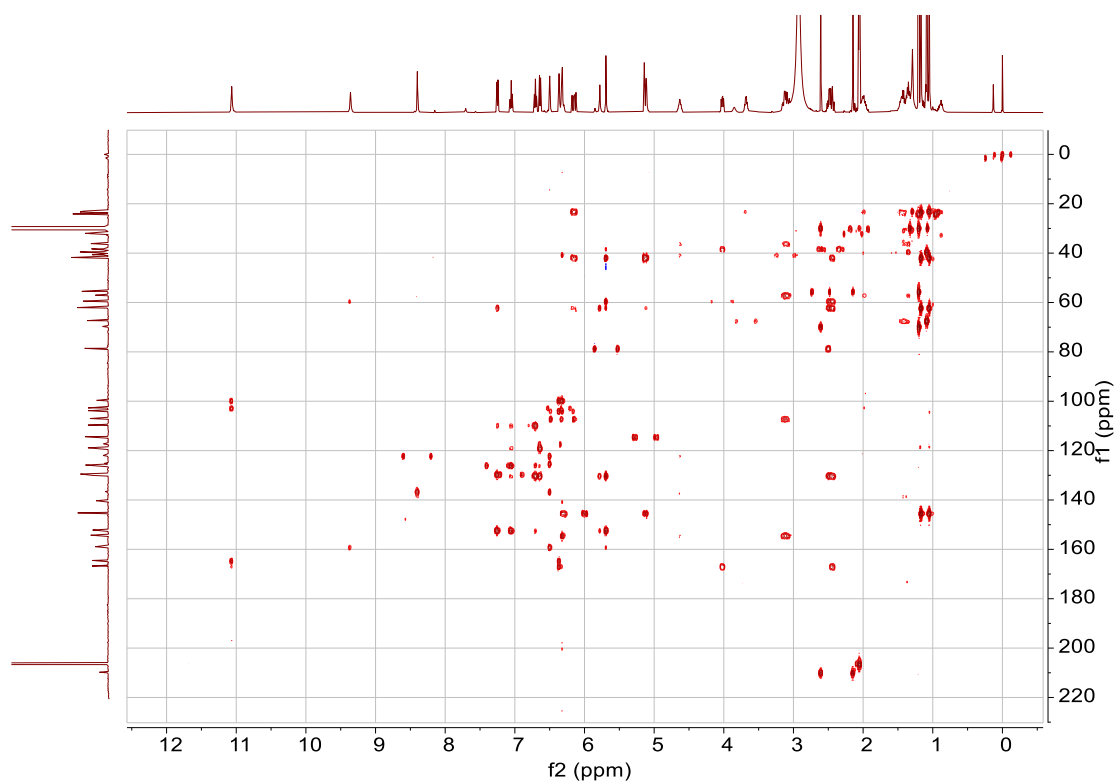


Fig. S39. HMBC spectrum of compound **3** in acetone- d_6 .

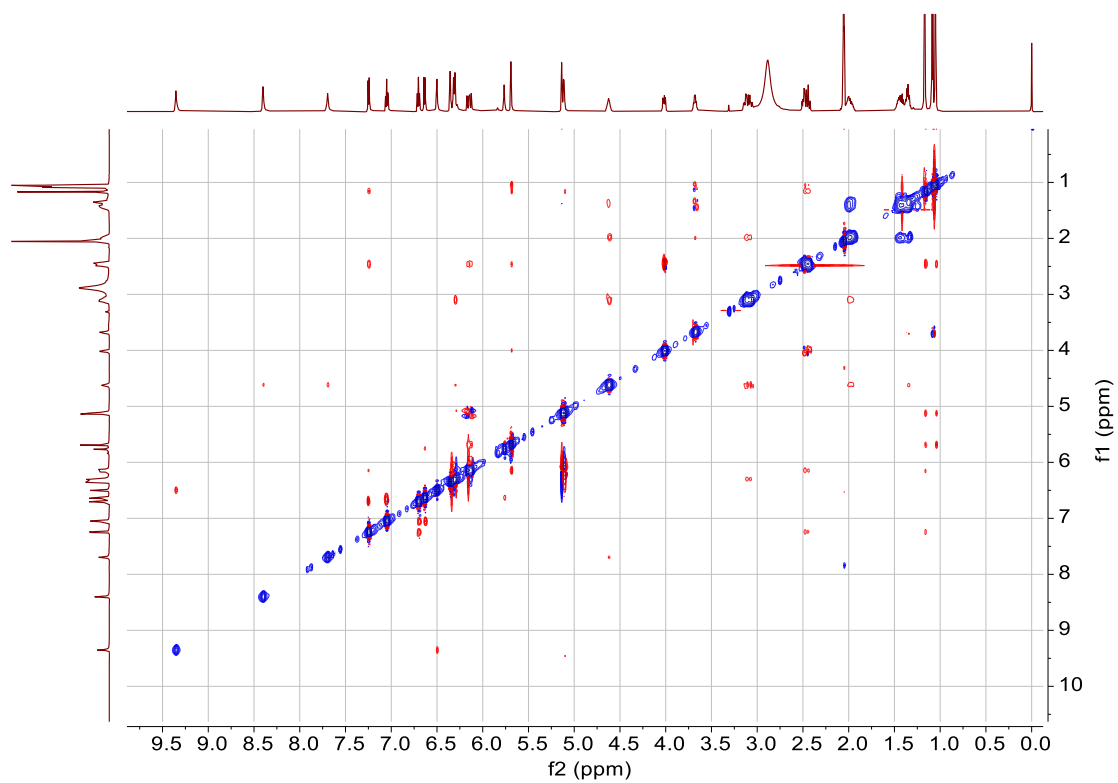


Fig. S40. ROESY spectrum of compound **3** in acetone- d_6 .

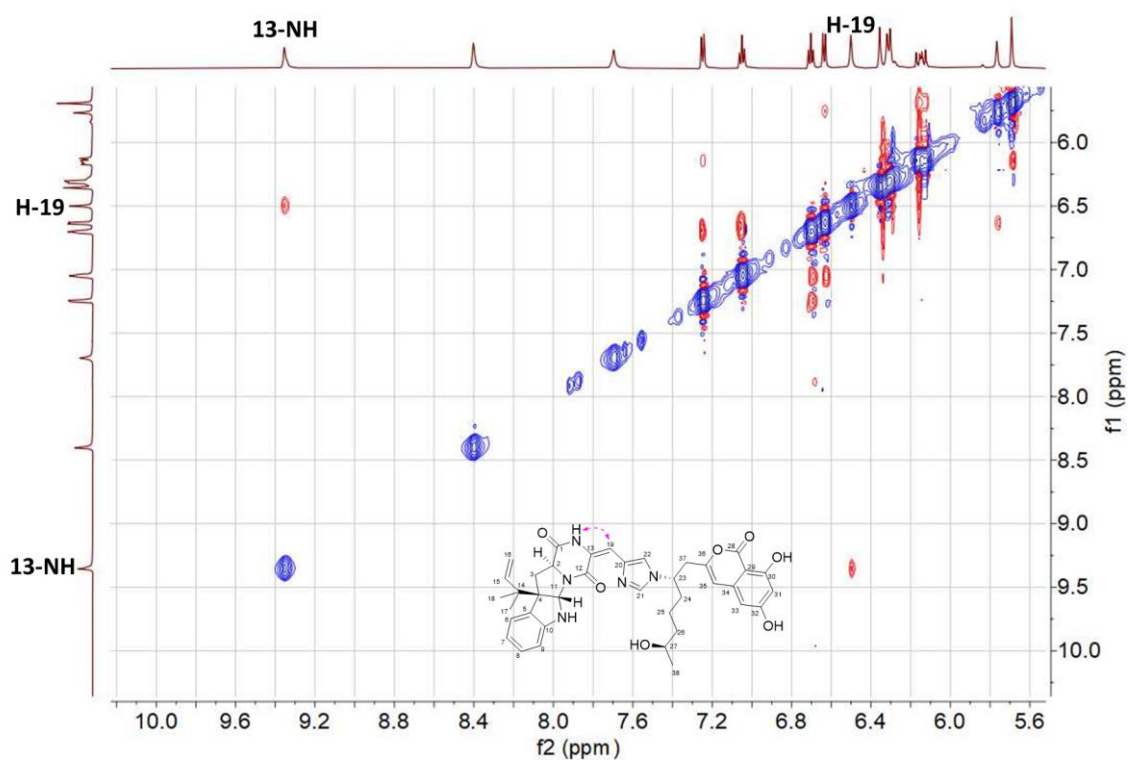


Fig. S41. Zoomed area of ROESY spectrum of compound **3** for the correlations between H-19/13-NH.

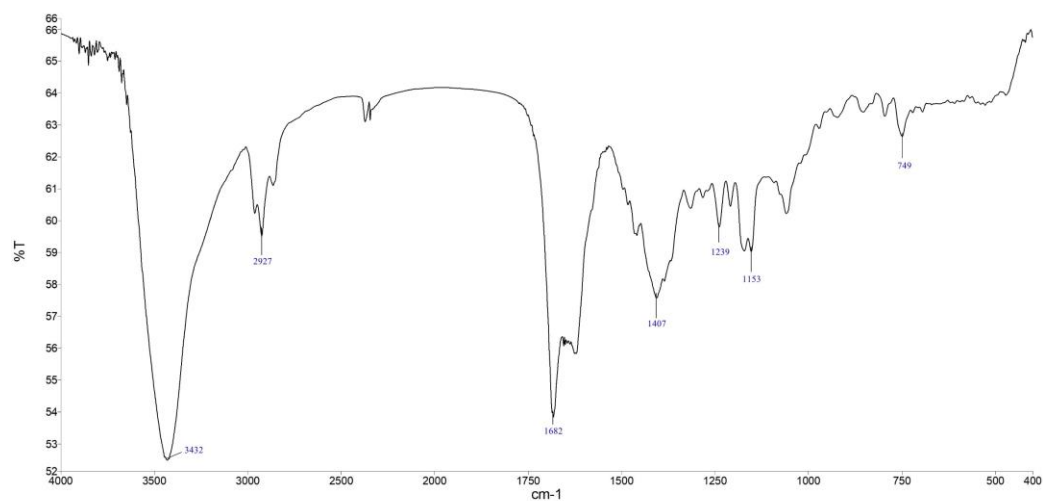


Fig. S42. IR spectrum of compound **3**.

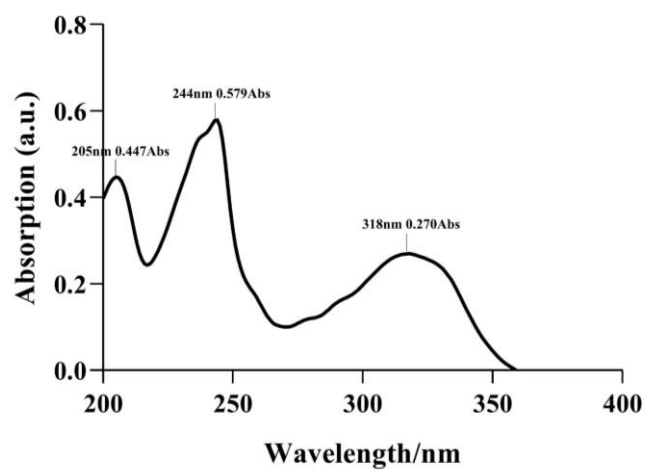


Fig. S43. UV spectrum of compound **3** (CH₃CN).

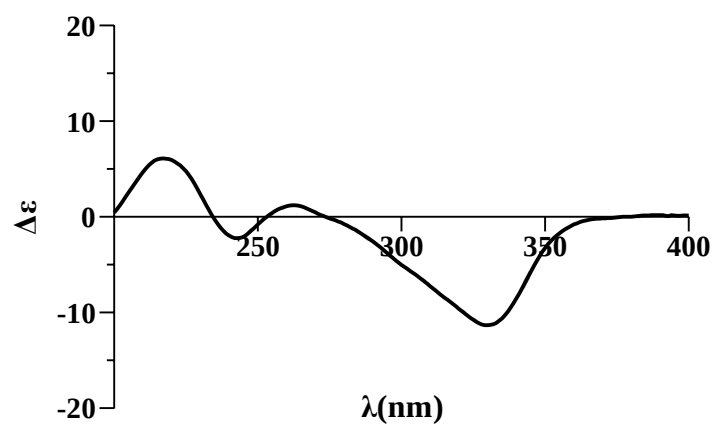


Fig. S44. ECD spectrum of compound **3** (CH₃CN).

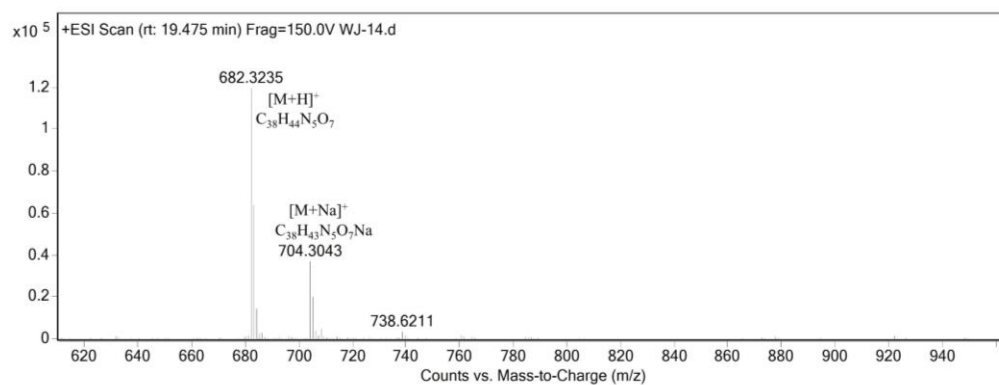


Fig. S45. ESI-MS spectrum of compound **4**.

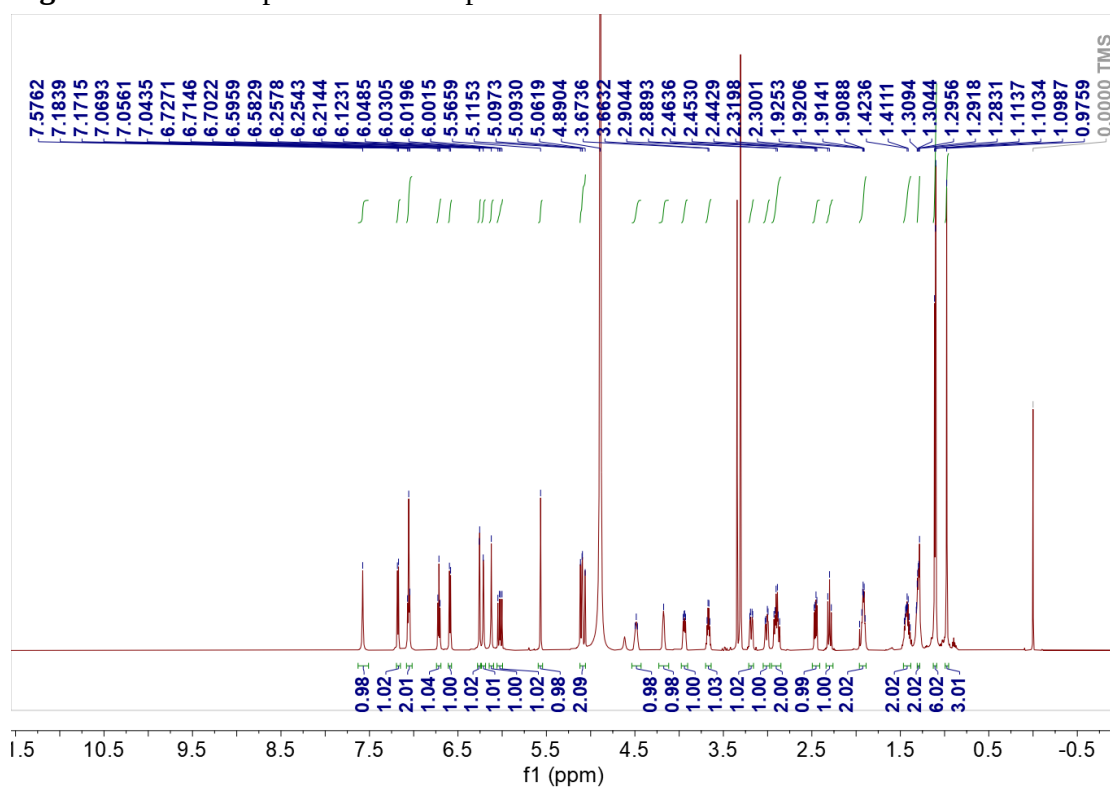


Fig. S46. 1H NMR spectrum of compound **4** (600 MHz, $methanol-d_4$).

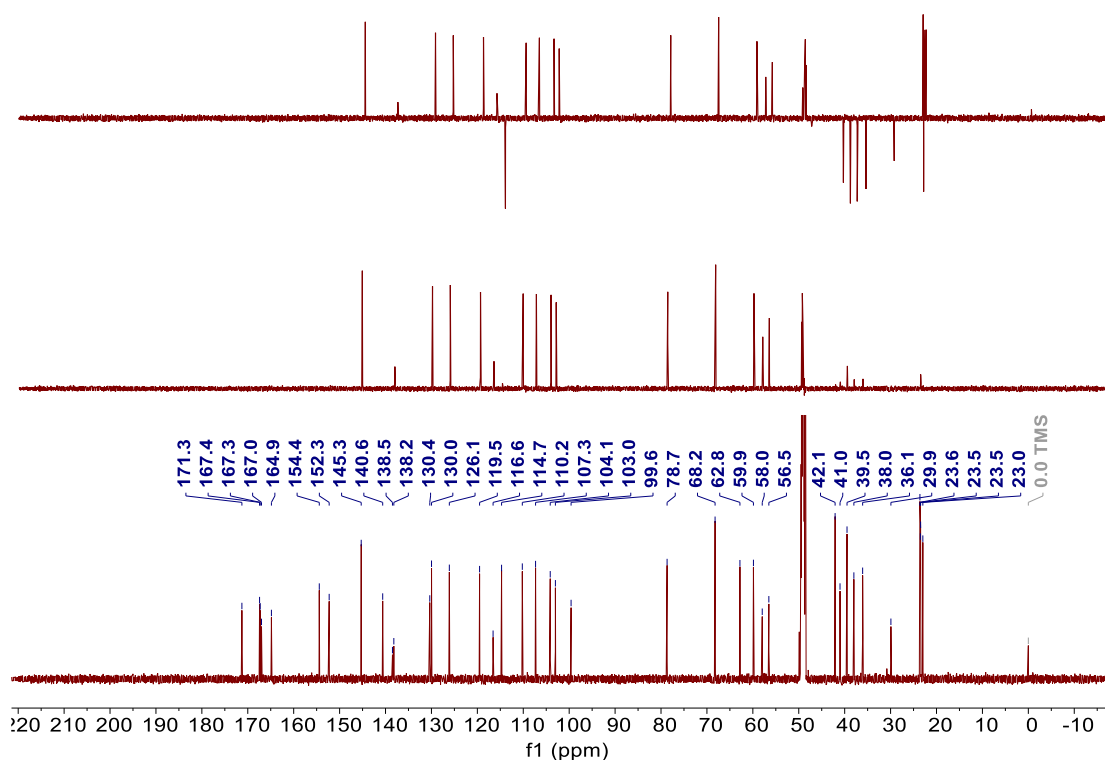


Fig. S47. ^{13}C NMR and DEPT spectrum of compound **4** (150 MHz, methanol- d_4).

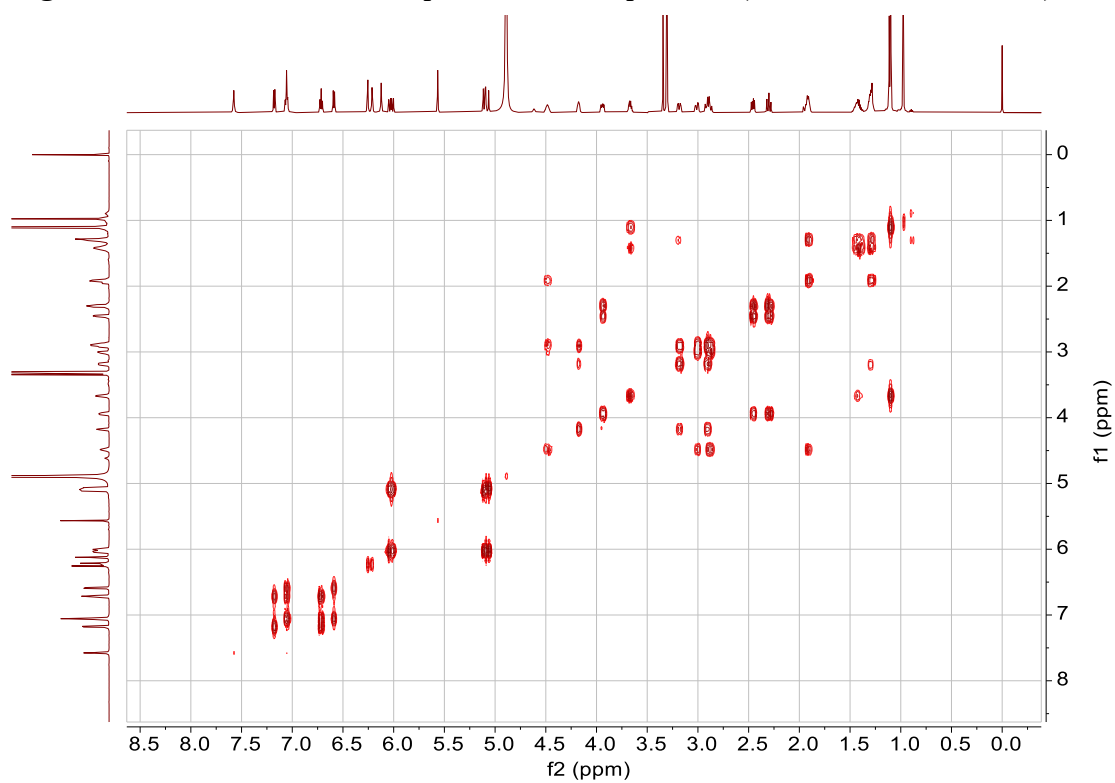


Fig. S48. ^1H - ^1H COSY spectrum of compound **4**.

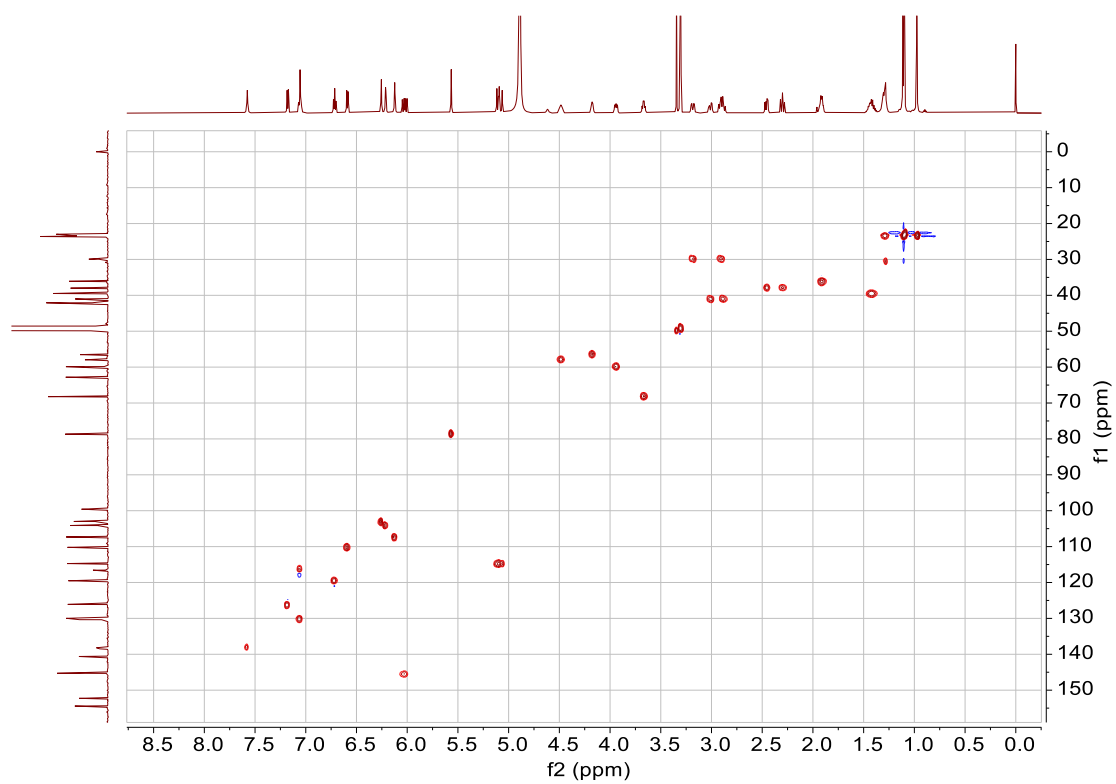


Fig. S49. HSQC spectrum of compound 4.

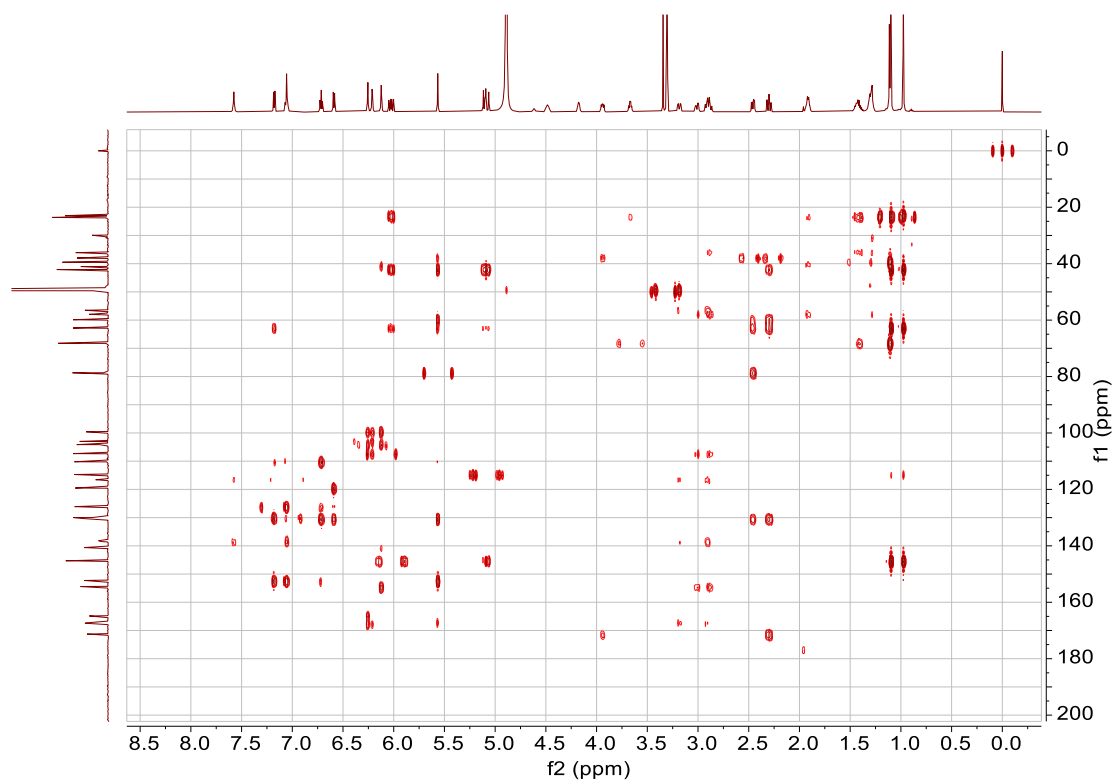


Fig. S50. HMBC spectrum of compound 4.

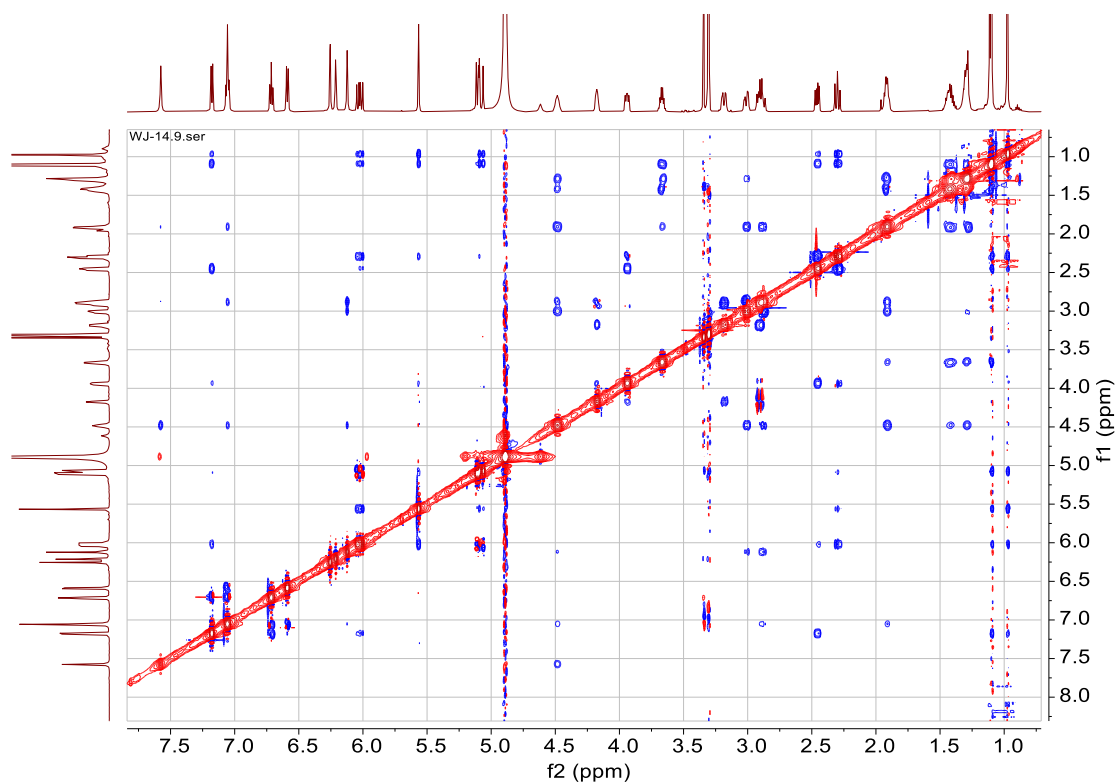


Fig. S51. ROESY spectrum of compound **4**.

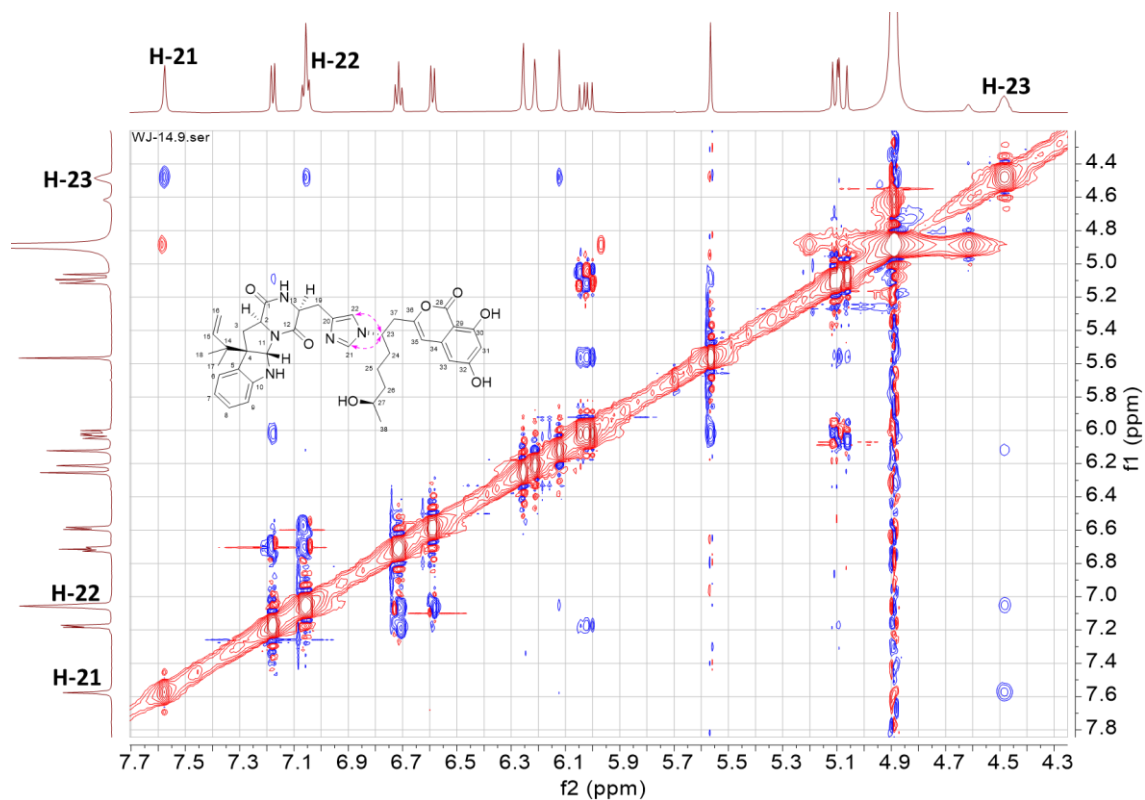


Fig. S52. Zoomed area of ROESY spectrum of compound **4** for the correlations between H-23/H-21 and H-23/H-22.

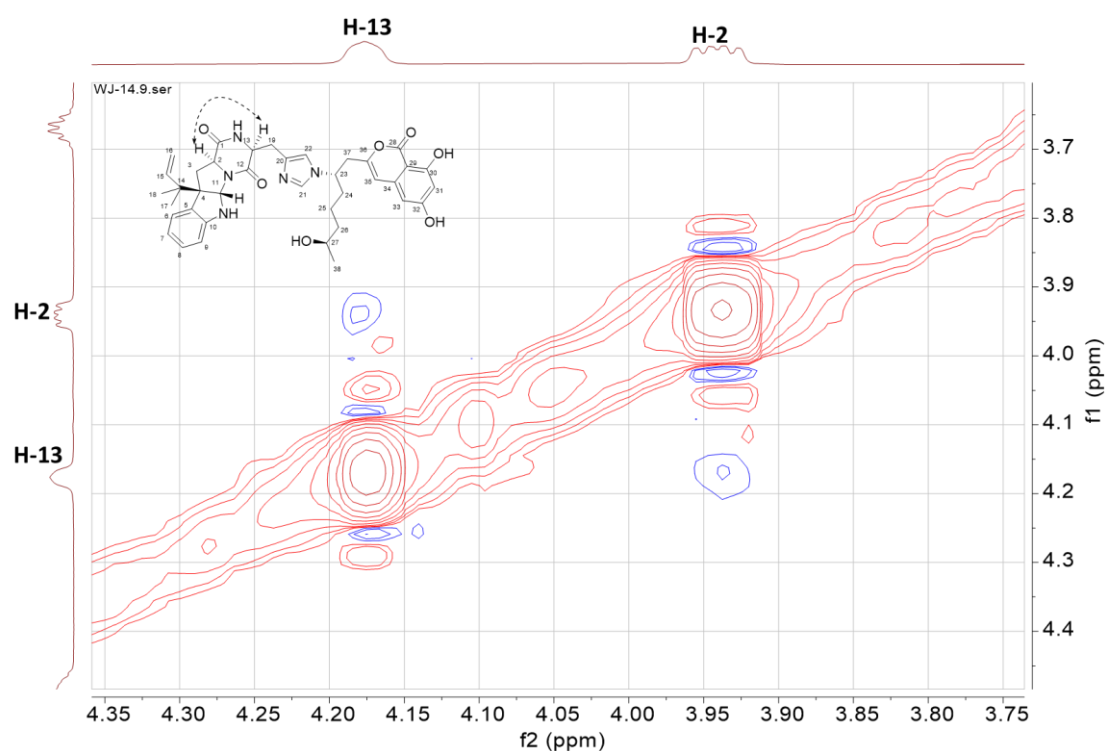


Fig. S53. Zoomed area of ROESY spectrum of compound **4** for the correlations between H-13/H-2.

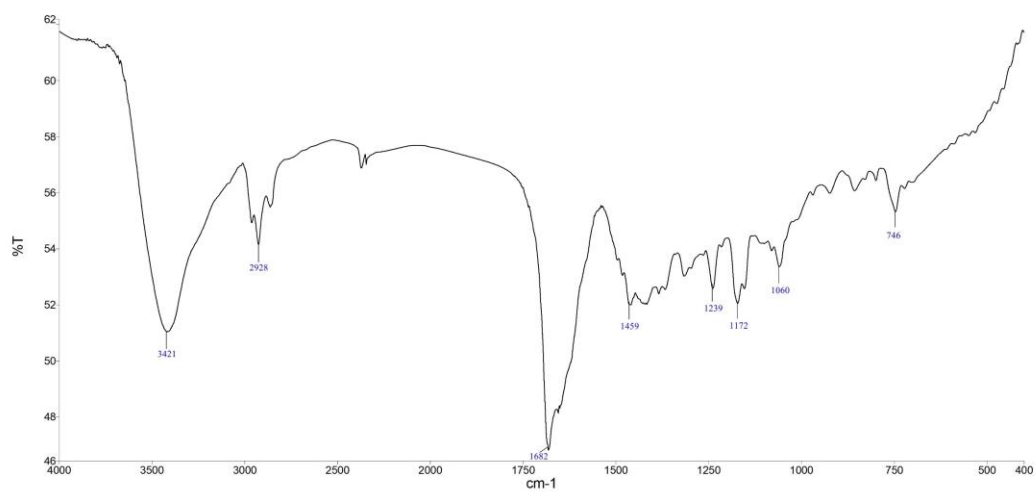


Fig. S54. IR spectrum of compound **4**.

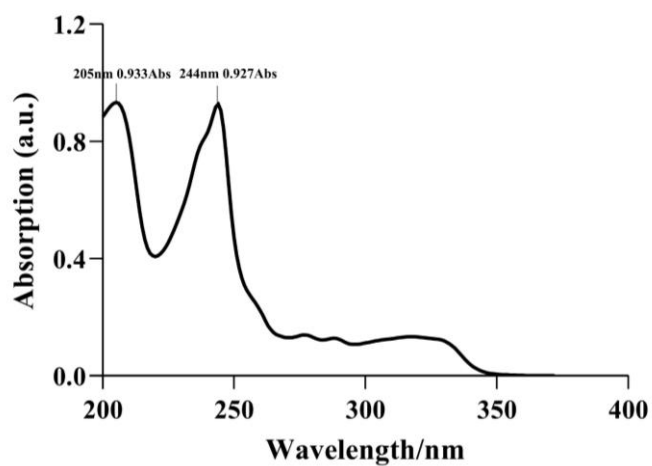


Fig. S55. UV spectrum of compound **4** (CH₃CN).

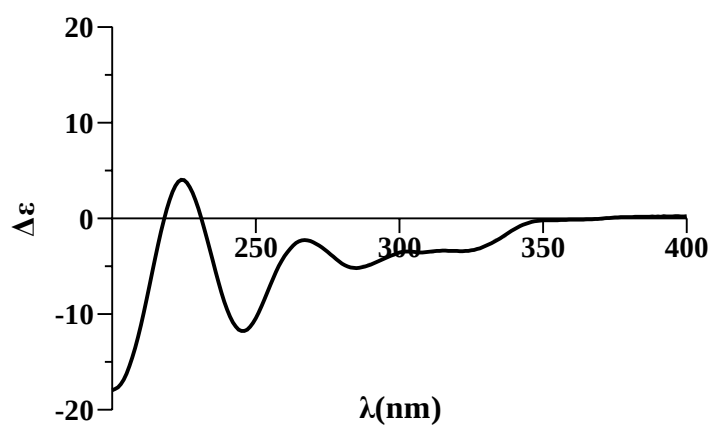


Fig. S56. ECD spectrum of compound **4** (CH₃CN).

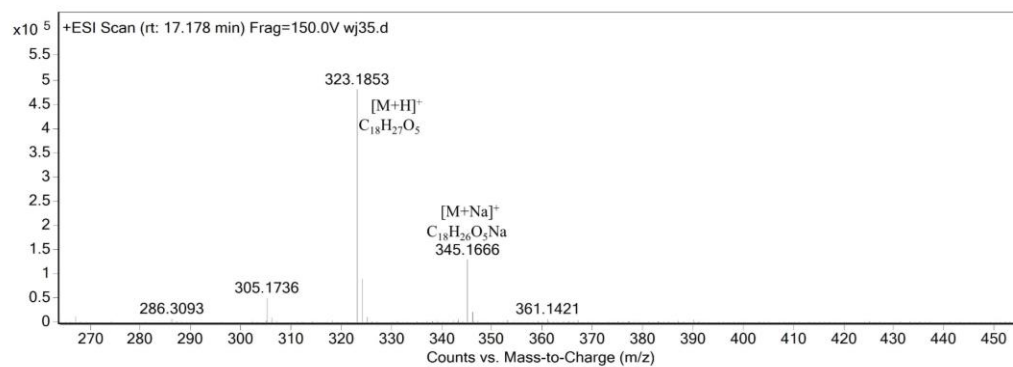


Fig. S57. ESI-MS spectrum of compound 5.

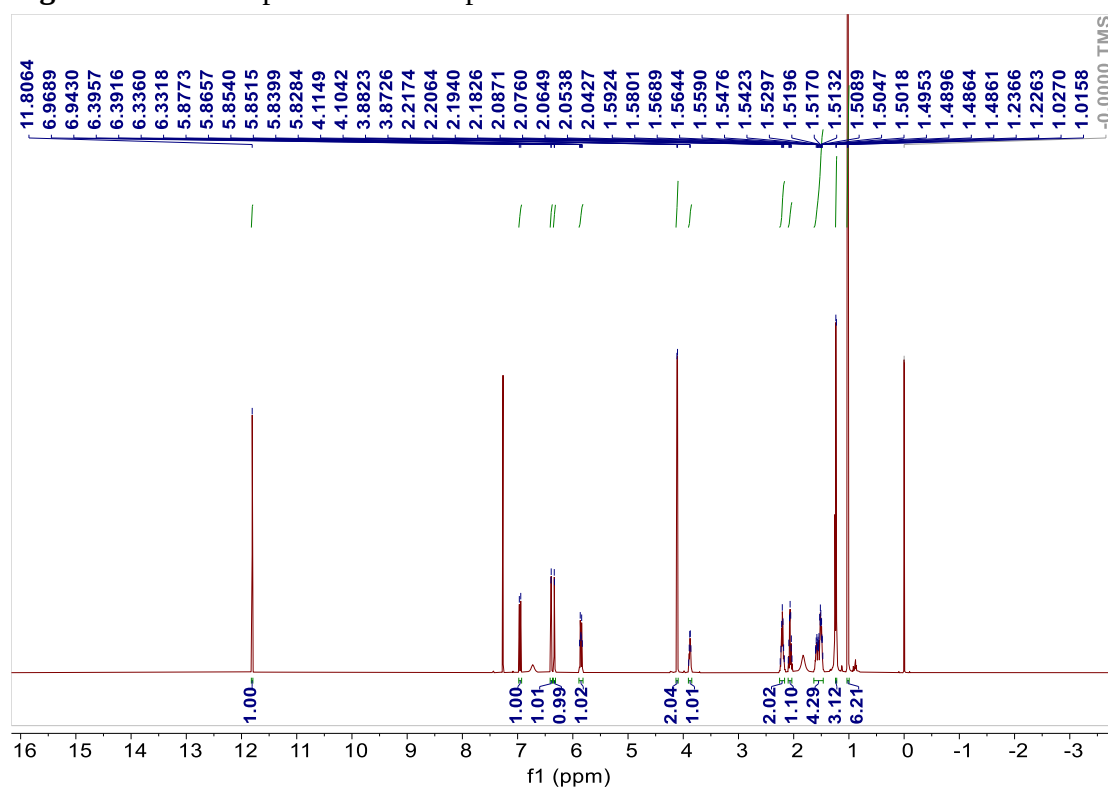


Fig. S58. 1H NMR spectrum of compound 5 (600 MHz, $CDCl_3$).

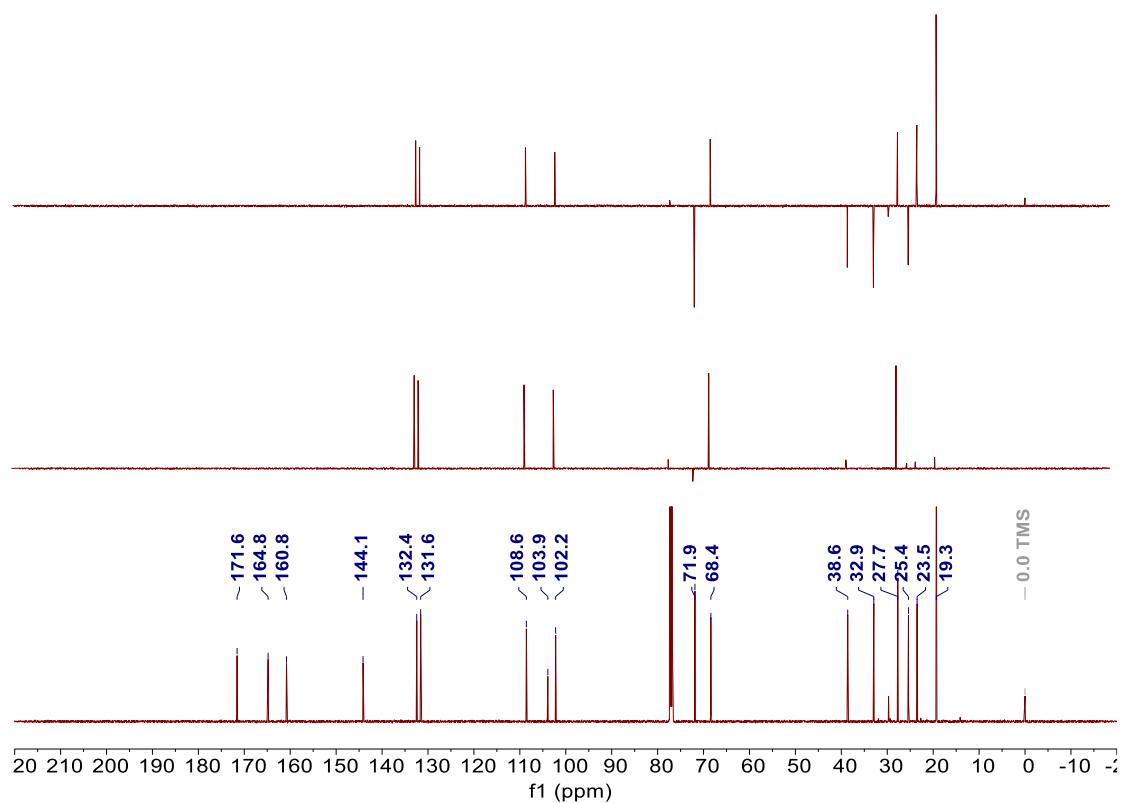


Fig. S59. ¹³C NMR and DEPT spectrum of compound 5 (150 MHz, CDCl₃).

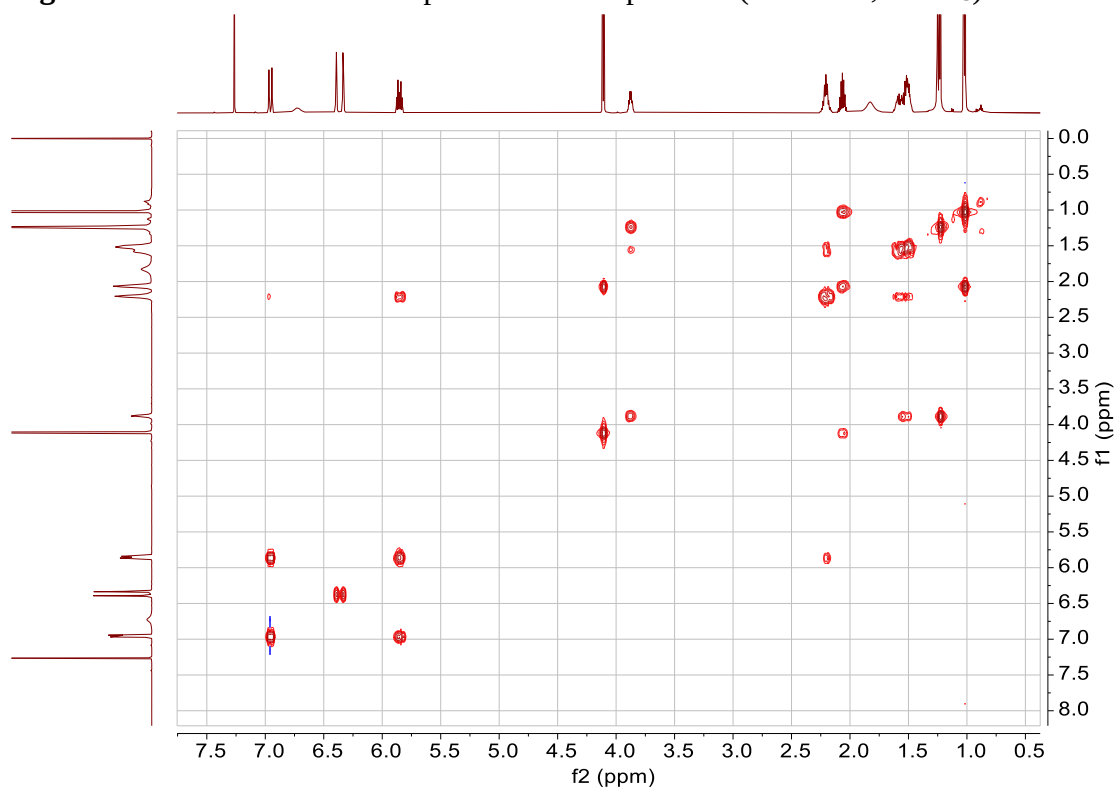


Fig. S60. ¹H-¹H COSY spectrum of compound 5.

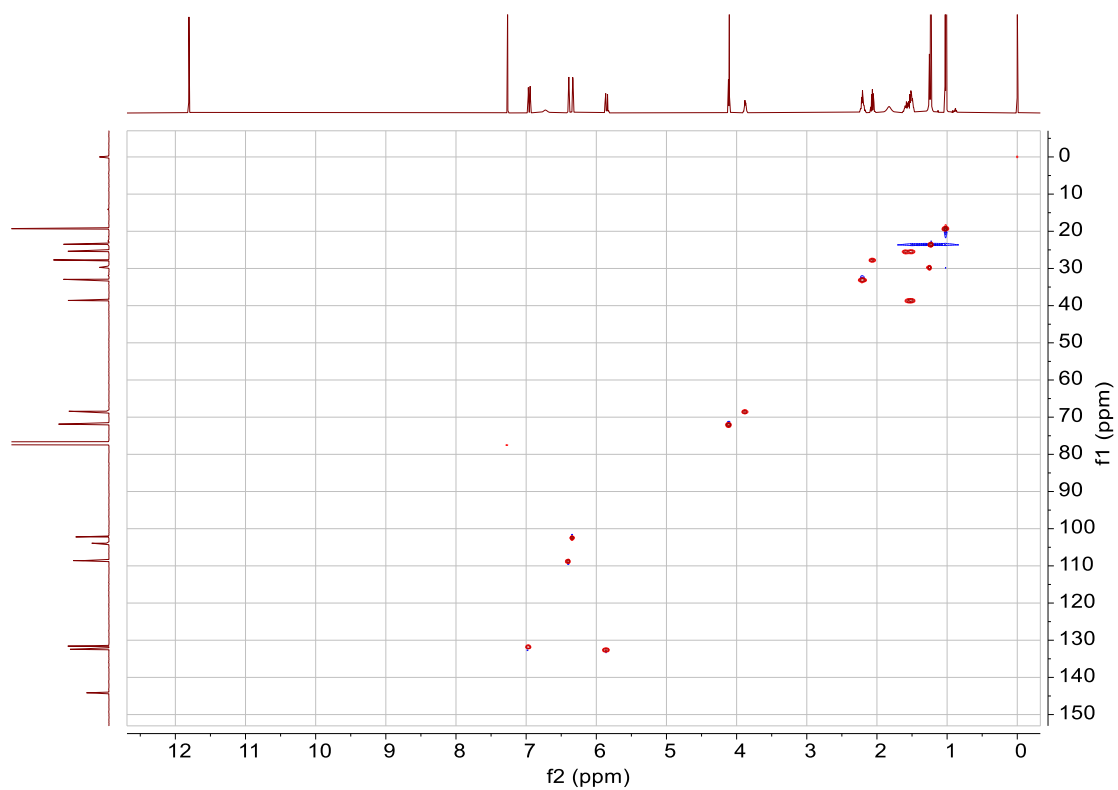


Fig. S61. HSQC spectrum of compound 5.

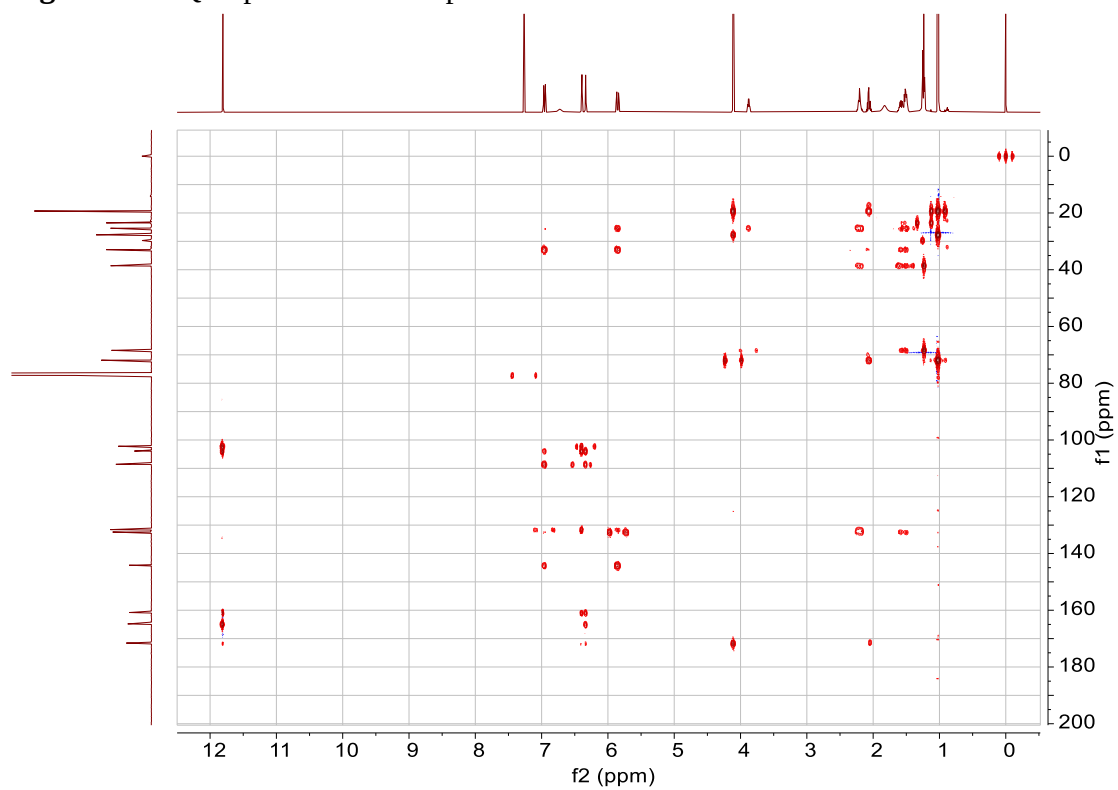


Fig. S62. HMBC spectrum of compound 5.

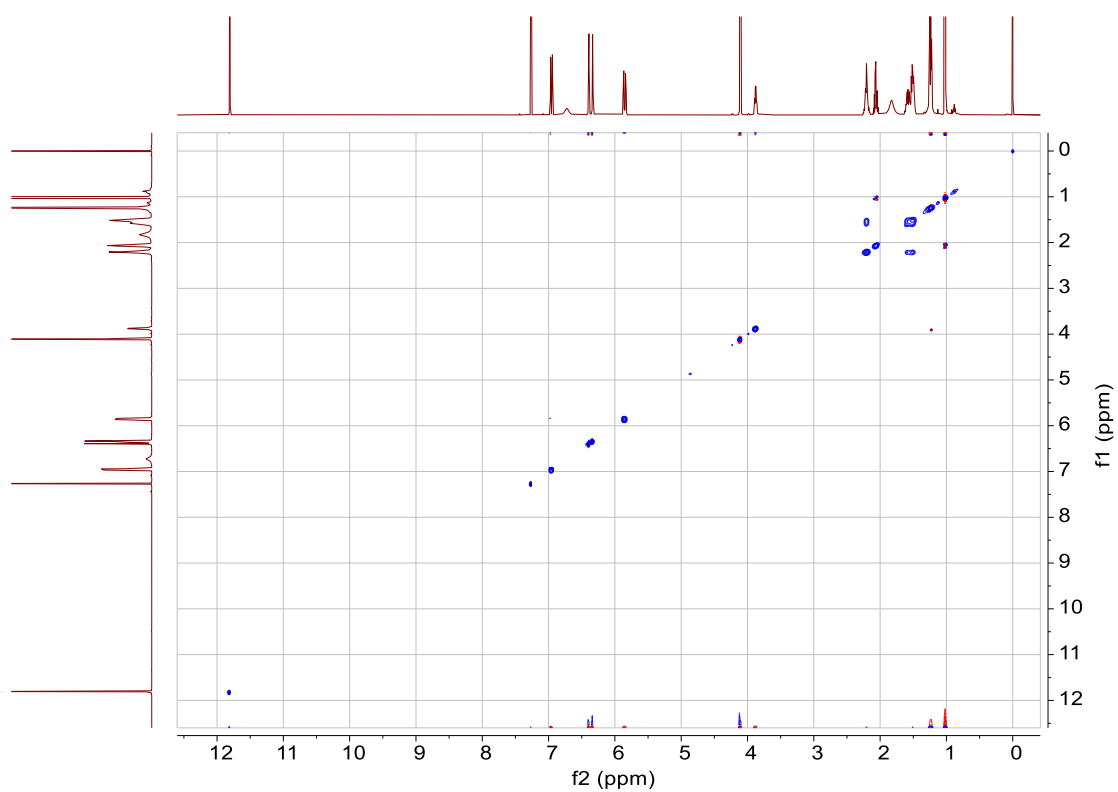


Fig. S63. ROESY spectrum of compound 5.

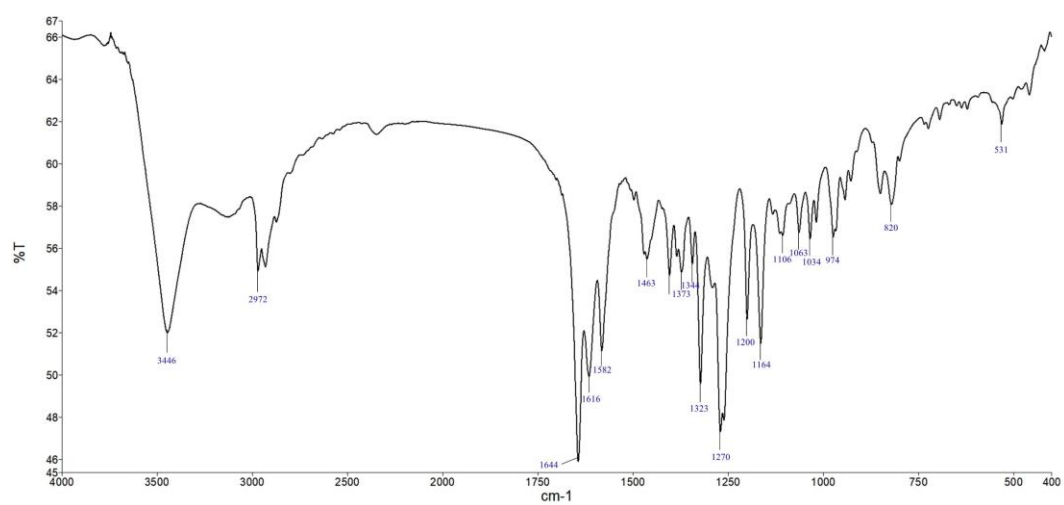


Fig. S64. IR spectrum of compound 5.

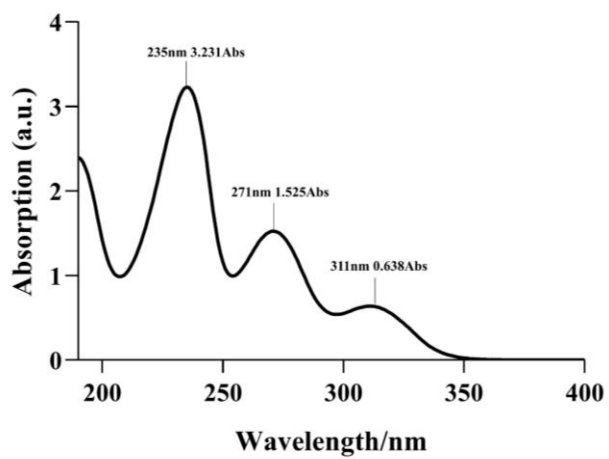


Fig. S65. UV spectrum of compound **5** (CH₃CN).

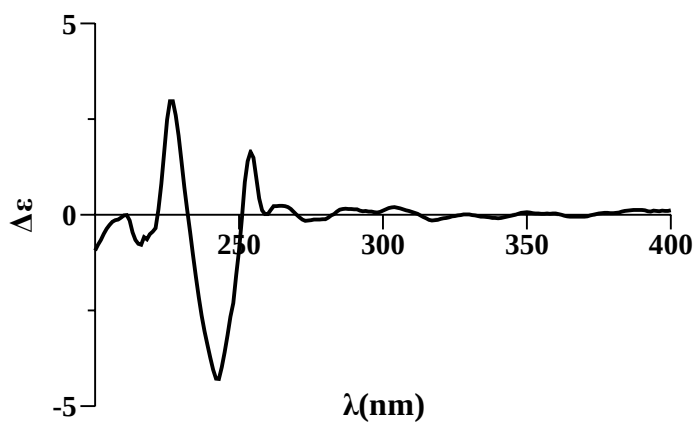


Fig. S66. ECD spectrum of compound **5** (CH₃CN).

Table S1. ITS1 sequences of the fungal strain *Penicillium expansum* MA147

ITS1	GCCTCCGTGAGGACTTTGGGTCACCTCCCACCCGTGTTTATTACCTCGTTGCTTCGGCG GGCCCCGCCTTAACTGGCCGCCGGGGGGCTCACGCCCCCGGGCCCGCGCCCGCCGAAGA CACCCCCGAACCTCTGCCTGAAGATTGTCGTCTGAGTGAAAATATAAATTATTAAAACTT TCAACAACGGATCTCTTGGTTCGGGCATCGATGAAGAACGCAGCGAAATGCGATACGTA ATGTGAATTGCAAATTCAGTGAATCATCGAGTCTTTGAACGCACATTGCGCCCCCTGGTA TTCCGGGGGGCATGCCTGTCCGAGCGTCATTGCTGCCCTCAAGCCCGGCTTGTGTGTTG GGCCCCGTCCTCCGATTCCGGGGGACGGGGCCGAAAGGCAGCGGCGGCACCGCGTCCG GTCTCGAGCGTATGGGGCTTTGTCACCCGCTCTGTAGGCCCGGCCGGCGCTTGCCGAT CAACCCAAATTTTATCCAGTTGACCTCGGATCAGGTAGGGATACCCGCTGAACTTAA GCATATCTAAAACCGGGAAGGAAAAAA
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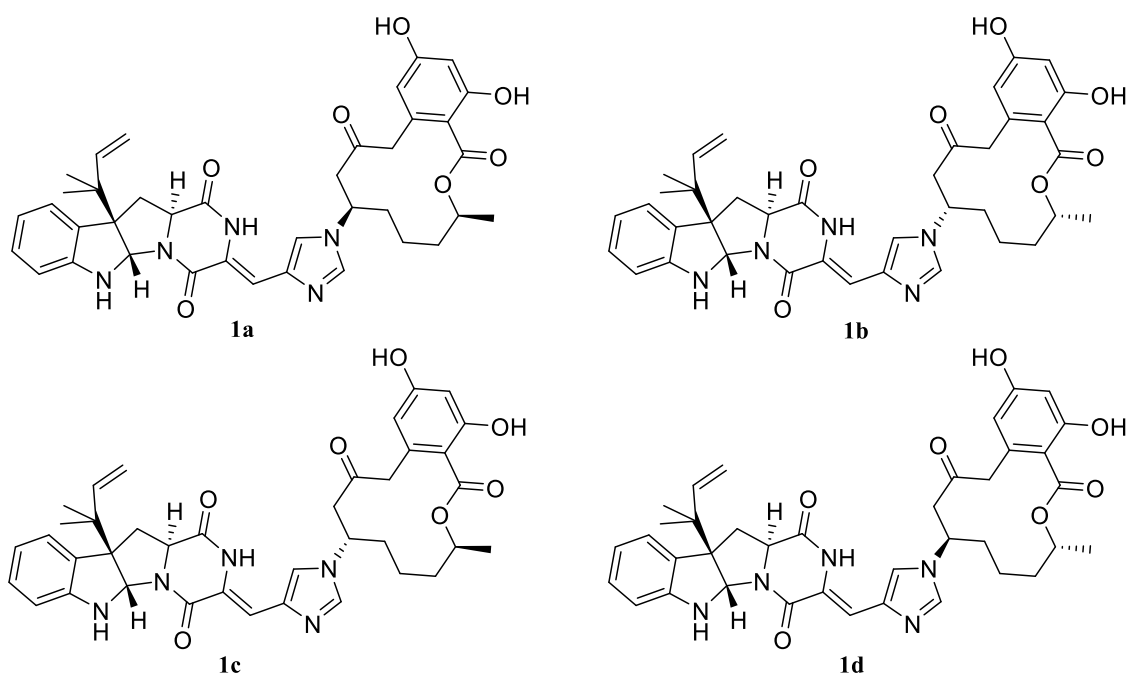


Fig. S67. Four possible relative configurations of compound 1.

Table S2. The calculated ^{13}C NMR chemical shifts of structures **1a–d** fitting to the experimental data of compound **1** following STS protocol.

no.	Exptl.	1a	dev	1b	dev	1c	dev	1d	dev
1	166.2	170.1	2.3	168.9	2.0	171.5	5.2	171.1	3.6
2	59.0	59.9	1.6	59.7	0.5	59.5	0.4	59.8	0.6
3	37.3	36.5	0.4	37.9	0.5	37.6	0.7	37.9	0.5
4	61.7	61.5	0.5	61.5	0.4	61.5	1.1	62.0	0.0
5	128.6	129.0	0.3	128.7	0.5	128.7	0.3	128.9	0.6
6	125.2	125.6	0.2	125.6	0.1	125.8	0.2	125.7	0.4
7	118.9	114.8	4.5	115.1	4.3	115.1	4.2	115.0	4.7
8	129.0	129.0	0.7	129.1	0.5	129.1	0.3	129.3	0.6
9	109.0	109.1	0.2	109.6	0.2	109.5	0.0	109.4	0.4
10	150.3	149.1	2.4	149.9	1.0	149.2	1.3	149.6	1.8
11	78.0	79.4	1.7	80.1	1.8	80.4	1.7	80.4	1.9
12	158.2	159.8	0.2	159.7	0.8	159.5	1.2	158.8	0.6
13	125.7	123.9	2.4	125.1	1.1	124.6	1.5	126.9	0.4
14	41.0	42.3	2.4	42.3	1.2	41.5	0.5	41.9	0.8
15	143.5	141.5	3.0	142.5	1.6	142.1	1.6	141.9	2.6
16	114.7	113.5	1.6	114.0	1.2	112.9	2.3	112.8	2.7
17	23.0	20.1	1.3	22.0	1.0	23.4	0.8	22.8	0.1
18	22.5	24.1	3.1	22.4	0.1	20.8	2.9	21.7	0.7
19	106.3	118.7	11.9	114.1	7.3	117.5	10.8	117.8	10.7
20	138.1	134.3	4.7	133.5	5.1	132.4	6.0	132.5	6.6
21	137.0	134.1	3.8	134.1	3.5	133.5	3.8	136.0	2.0
22	117.9	122.0	3.6	121.5	3.1	121.4	3.1	121.4	2.7
23	52.0	52.2	1.1	54.7	2.5	56.0	3.1	57.2	5.0
24	36.4	28.0	7.0	38.5	2.1	37.3	0.2	32.5	3.9
25	18.9	18.8	1.5	17.1	1.7	22.9	2.8	25.7	6.9
26	34.2	29.2	3.7	32.5	1.7	36.7	1.4	30.5	3.7
27	72.2	73.1	1.3	71.7	0.7	75.2	2.3	74.0	1.4
28	170.8	173.9	1.4	172.4	0.9	169.1	1.7	172.4	0.3
29	104.8	107.1	2.0	105.8	0.6	107.2	1.9	105.4	0.1
30	166.6	164.6	3.5	165.7	1.7	161.4	5.2	164.2	3.6
31	103.6	102.2	1.6	102.4	1.6	104.0	0.2	102.7	1.6
32	162.5	161.4	2.5	161.1	2.1	161.0	1.6	161.0	2.7
33	113.5	113.7	0.2	113.6	0.4	111.0	3.0	112.5	1.8
34	137.3	142.0	3.7	141.9	4.0	141.8	4.3	139.2	0.9
35	52.3	50.1	1.3	51.8	0.7	49.5	3.8	47.9	4.6
36	203.7	208.6	2.5	206.7	2.0	206.3	2.9	212.5	7.1
37	47.7	51.9	5.1	51.1	3.3	50.4	1.7	49.0	1.2
38	19.1	16.1	1.3	17.2	1.8	21.0	0.7	20.7	1.7
		MAE	2.4	MAE	1.7	MAE	2.3	MAE	2.4
		RMS	3.3	RMS	2.3	RMS	3.1	RMS	3.4
		P_{mean}	1.9%	P_{mean}	10.6%	P_{mean}	3.5%	P_{mean}	1.6%
		P_{rel}	0.0%	P_{rel}	100.0%	P_{rel}	0.0%	P_{rel}	0.0%

Table S3. The calculated $^1\text{H}/^{13}\text{C}$ NMR chemical shifts (scaled) of structures **1a–d** fitting to the experimental data of compound **1** at mPW1PW91/6-31G(d,p) level.

no.	Exptl.	1a	dev	1b	dev	1c	dev	1d	dev
^{13}C NMR chemical shifts									
1	166.2	166.99	0.59	163.90	2.50	168.36	1.96	166.97	0.57
2	59.0	61.87	2.67	61.55	2.35	59.99	0.79	61.02	1.82
3	37.3	38.10	0.70	38.06	0.66	36.41	0.99	37.99	0.59
4	61.7	65.22	3.42	64.85	3.05	63.47	1.67	64.35	2.55
5	128.6	128.23	0.57	129.18	0.38	128.31	0.49	127.80	1.00
6	125.2	124.56	0.84	124.78	0.62	124.65	0.75	124.17	1.23
7	118.9	116.66	2.34	116.76	2.24	116.64	2.36	116.21	2.79
8	129.0	128.51	0.59	128.62	0.48	128.68	0.42	128.27	0.83
9	109.0	106.58	2.52	106.69	2.41	106.57	2.53	105.98	3.12
10	150.3	149.37	1.13	150.65	0.15	150.51	0.01	149.25	1.25
11	78.0	81.31	3.21	82.61	4.51	81.32	3.22	81.15	3.05
12	158.2	156.21	2.09	157.06	1.24	156.83	1.47	155.46	2.84
13	125.7	124.86	0.94	127.76	1.96	125.09	0.71	126.26	0.46
14	41.0	45.38	4.28	44.86	3.76	43.55	2.45	44.69	3.59
15	143.5	143.26	0.34	144.41	0.81	144.28	0.68	143.12	0.48
16	114.7	113.79	1.01	115.06	0.26	114.52	0.28	113.38	1.42
17	23.0	21.88	1.22	22.98	0.12	20.67	2.43	20.80	2.30
18	22.5	22.15	0.45	18.80	3.80	17.88	4.72	21.35	1.25
19	106.3	115.64	9.14	105.14	1.36	114.37	7.87	114.51	8.01
20	138.1	133.84	3.66	136.57	0.93	133.59	3.91	133.43	4.07
21	137.0	132.95	4.15	133.63	3.47	133.50	3.60	135.62	1.48
22	117.9	120.86	2.76	122.04	3.94	119.32	1.22	118.38	0.28
23	52.0	54.63	2.53	56.97	4.87	56.28	4.18	59.54	7.44
24	36.4	34.82	1.68	38.95	2.45	35.89	0.61	33.37	3.13
25	18.9	18.45	0.65	18.30	0.80	21.09	1.99	23.95	4.85
26	34.2	32.74	1.46	33.43	0.77	35.26	1.06	31.04	3.16
27	72.2	72.75	0.45	71.26	1.04	75.85	3.55	74.86	2.56
28	170.8	170.28	0.62	170.58	0.32	168.41	2.49	169.93	0.97
29	104.8	105.76	0.76	105.84	0.84	107.44	2.44	105.11	0.11
30	166.6	164.82	1.88	166.77	0.07	162.52	4.18	164.86	1.84
31	103.6	100.55	3.15	100.45	3.25	101.79	1.91	99.98	3.72
32	162.5	161.43	1.27	160.67	2.03	162.33	0.37	161.33	1.37
33	113.5	109.01	4.59	109.01	4.59	109.36	4.24	110.75	2.85
34	137.3	139.48	1.28	140.37	2.17	140.58	2.38	138.54	0.34
35	52.3	46.76	5.64	47.33	5.07	48.03	4.37	46.58	5.82
36	203.7	212.70	8.90	209.84	6.04	210.56	6.76	214.89	11.09
37	47.7	51.65	3.85	48.60	0.80	49.13	1.33	47.80	0.00
38	19.1	17.65	1.65	17.44	1.86	18.61	0.69	18.73	0.57
		MAE	2.34	MAE	2.05	MAE	2.29	MAE	2.49
		RMS	3.13	RMS	2.61	RMS	2.90	RMS	3.42
^1H NMR chemical shifts									
2	4.16	4.19	0.03	3.97	0.19	4.18	0.02	4.12	0.04
3-1	2.5	2.07	0.43	2.32	0.18	2.08	0.42	2.17	0.33
3-2	2.61	2.31	0.30	2.40	0.21	2.20	0.41	2.31	0.30
6	7.18	8.00	0.82	7.55	0.37	8.55	1.37	7.88	0.70
7	6.76	7.45	0.69	7.00	0.24	7.90	1.14	7.29	0.53
8	7.1	7.95	0.85	7.43	0.33	8.42	1.32	7.79	0.69
9	6.59	7.15	0.56	6.73	0.14	7.57	0.98	7.03	0.44
11	5.68	5.92	0.24	5.47	0.21	6.00	0.32	5.75	0.07
15	6.01	7.14	1.13	6.77	0.76	7.55	1.54	6.84	0.83
16	5.14	5.63	0.49	5.55	0.41	6.02	0.88	5.55	0.41
17	1.05	0.40	0.65	1.07	0.02	0.33	0.72	0.57	0.48

18	1.16	0.70	0.46	0.82	0.34	0.22	0.94	0.73	0.43
19	6.62	7.56	0.94	6.39	0.23	7.84	1.22	7.39	0.77
21	7.29	8.30	1.01	7.88	0.59	8.77	1.48	8.05	0.76
22	6.94	7.02	0.08	6.39	0.55	6.66	0.28	6.90	0.04
23	5.38	4.72	0.66	4.60	0.78	4.30	1.08	4.17	1.21
24-1	1.71	1.46	0.25	1.46	0.25	1.08	0.63	1.22	0.49
24-2	1.96	1.78	0.18	1.78	0.18	1.53	0.43	2.09	0.13
25	1.59	1.50	0.09	1.76	0.17	1.28	0.31	1.56	0.03
26-1	1.59	1.23	0.36	1.69	0.10	1.10	0.49	1.43	0.16
26-2	1.79	1.59	0.20	1.85	0.06	1.48	0.31	1.50	0.29
27	5.14	6.24	1.10	6.32	1.18	6.17	1.03	5.80	0.66
31	6.56	6.65	0.09	6.61	0.05	7.25	0.69	6.64	0.08
33	6.18	7.73	1.55	6.56	0.38	7.57	1.39	8.01	1.83
35-1	3.63	3.09	0.54	3.14	0.49	2.95	0.68	3.04	0.59
35-2	4.7	4.68	0.02	4.87	0.17	5.87	1.17	5.32	0.62
37-1	3.35	3.14	0.21	3.40	0.05	3.13	0.22	3.33	0.02
37-2	2.6	1.74	0.86	2.45	0.15	1.39	1.21	2.12	0.48
38	1.33	0.92	0.41	1.39	0.06	0.72	0.61	1.06	0.27
10-NH	4.93	4.69	0.24	4.44	0.49	4.75	0.18	4.45	0.48
13-NH	12.22	7.61	4.61	10.84	1.38	8.13	4.09	8.55	3.67
30-OH	11.91	12.79	0.88	12.44	0.53	10.37	1.54	12.69	0.78
		MAE	0.65	MAE	0.35	MAE	0.91	MAE	0.58
		RMS	1.03	RMS	0.47	RMS	1.16	RMS	0.89
		sDP4+	0.0%	sDP4+	100.0%	sDP4+	0.0%	sDP4+	0.0%
		uDP4+	0.3%	uDP4+	93.4%	uDP4+	6.2%	uDP4+	0.2%
		DP4+	0.0%	DP4+	100.0%	DP4+	0.0%	DP4+	0.0%

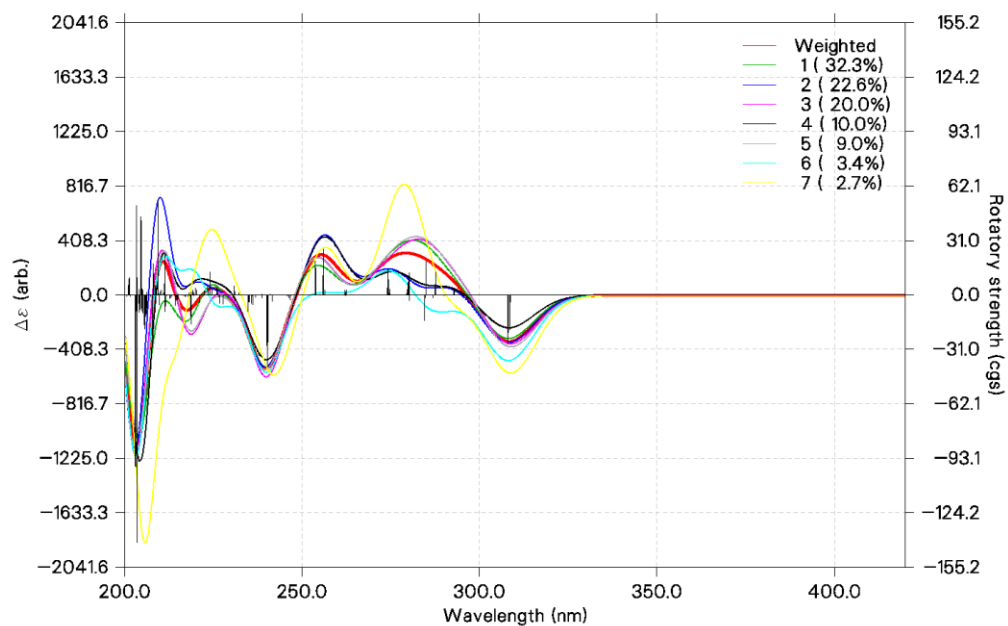


Fig. S68. Weighted ECD curve and the curves of conformers of structure **1a**.

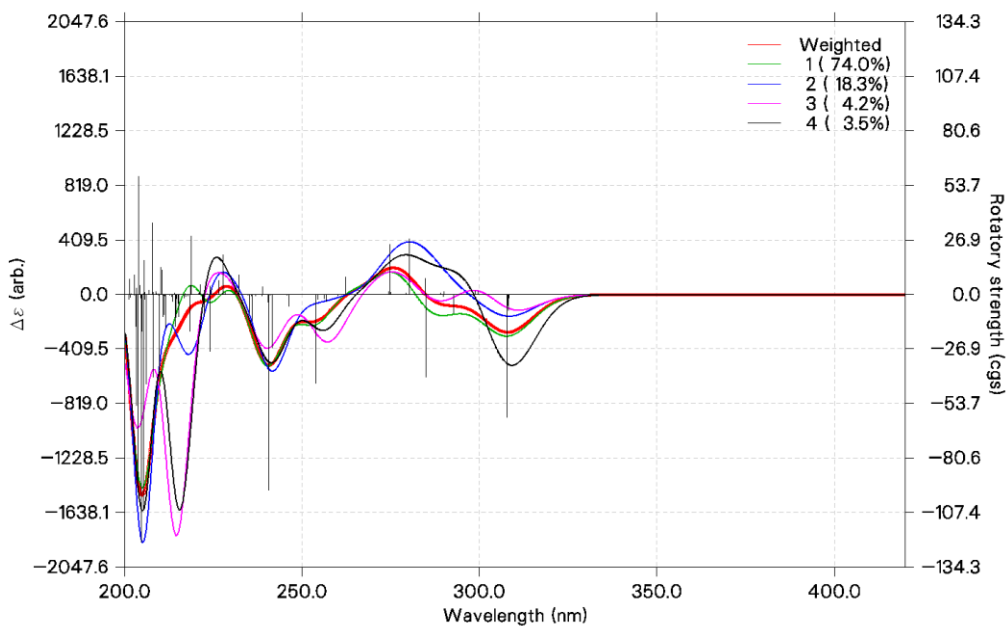


Fig. S69. Weighted ECD curve and the curves of conformers of structure **1b**.

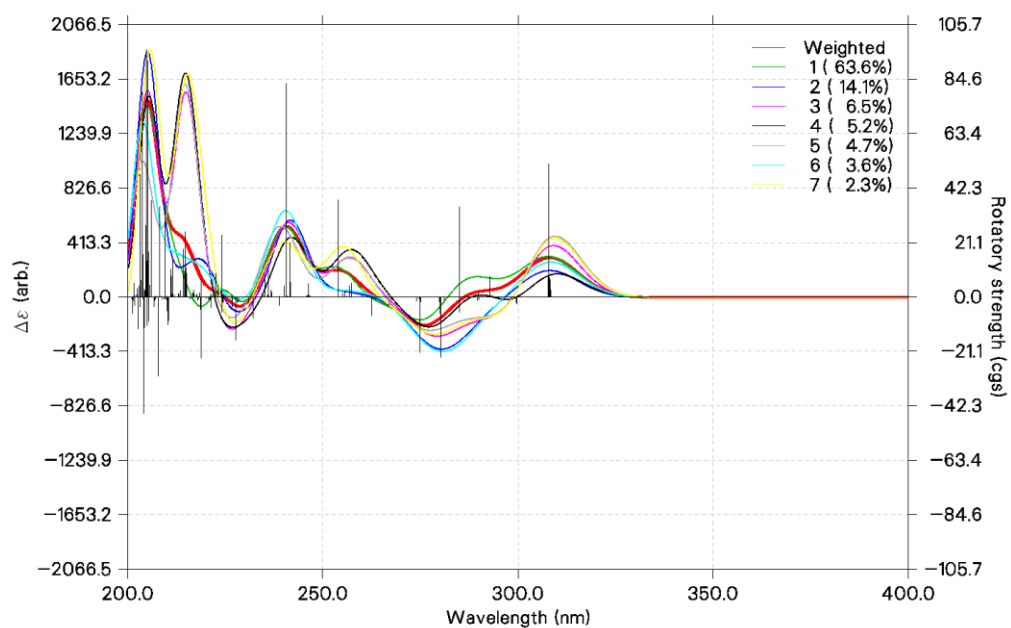


Fig. S70. Weighted ECD curve and the curves of conformers of the enantiomer of structure **1b**.

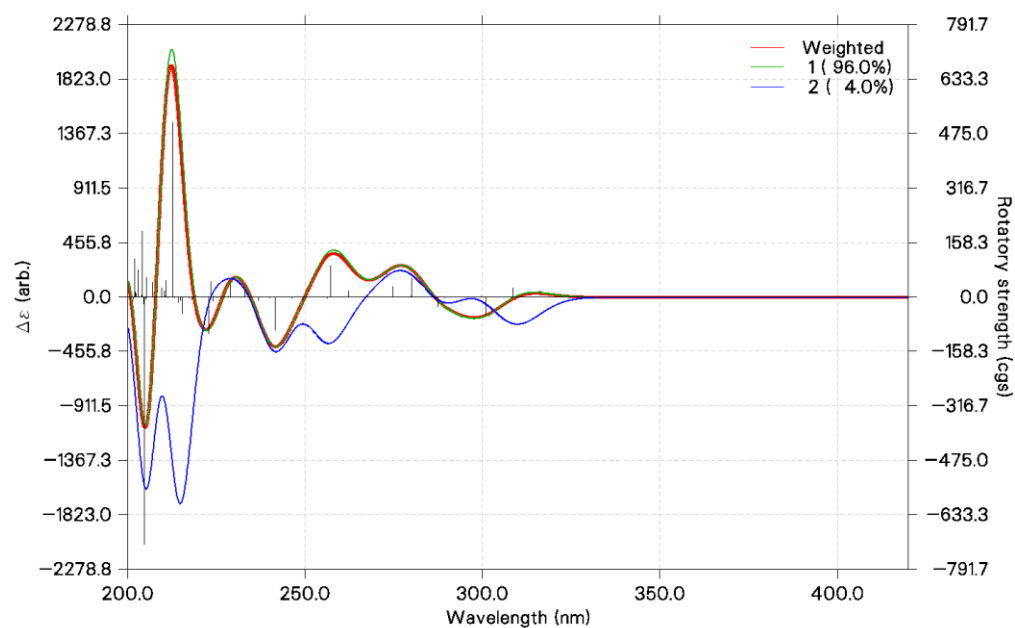


Fig. S71. Weighted ECD curve and the curves of conformers of structure **1c**.

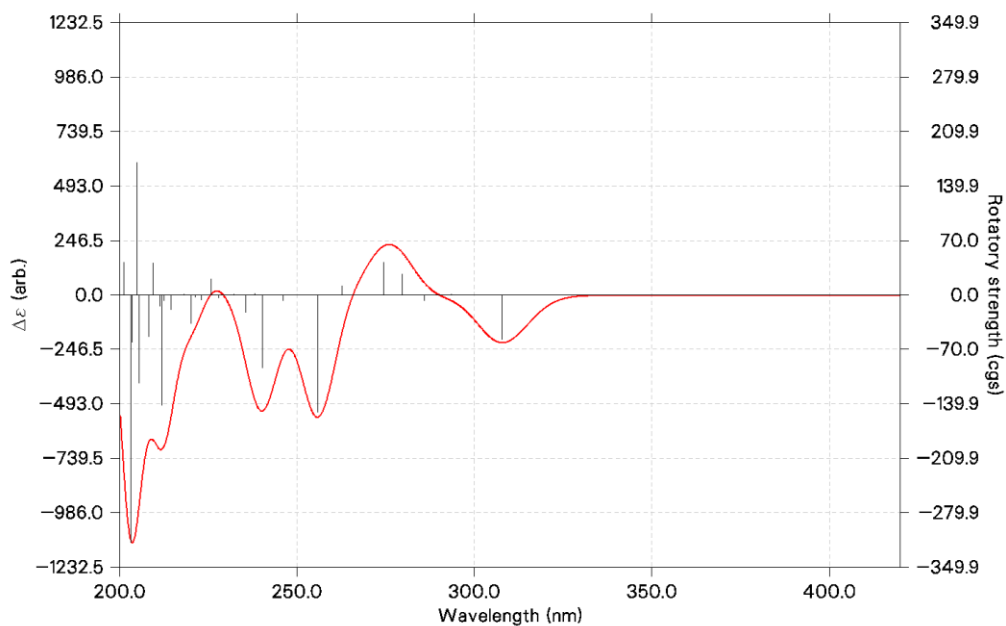


Fig. S72. Weighted ECD curve of structure **1d**.

Note: it had only one dominated conformer.

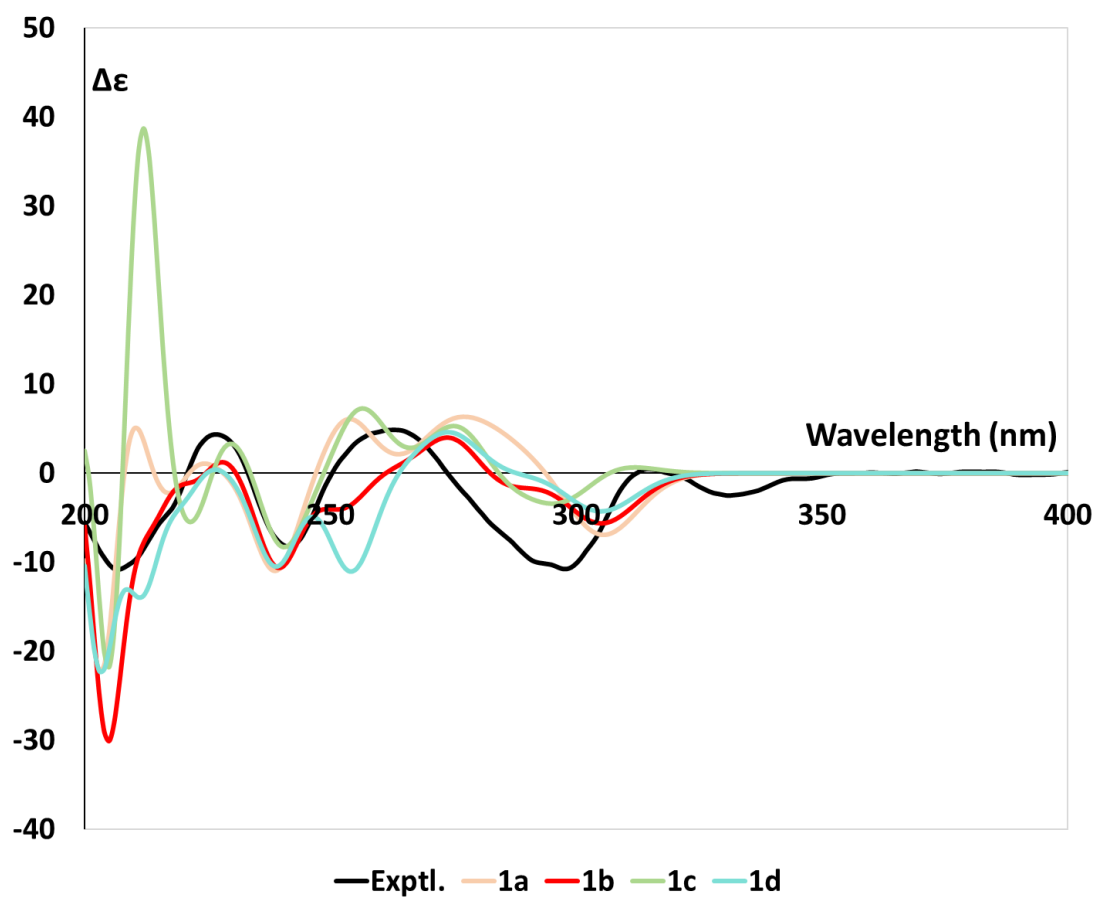


Fig. S73. Experimental ECD curve of compound **1** and weighted ECD curves of structures **1a–d**.

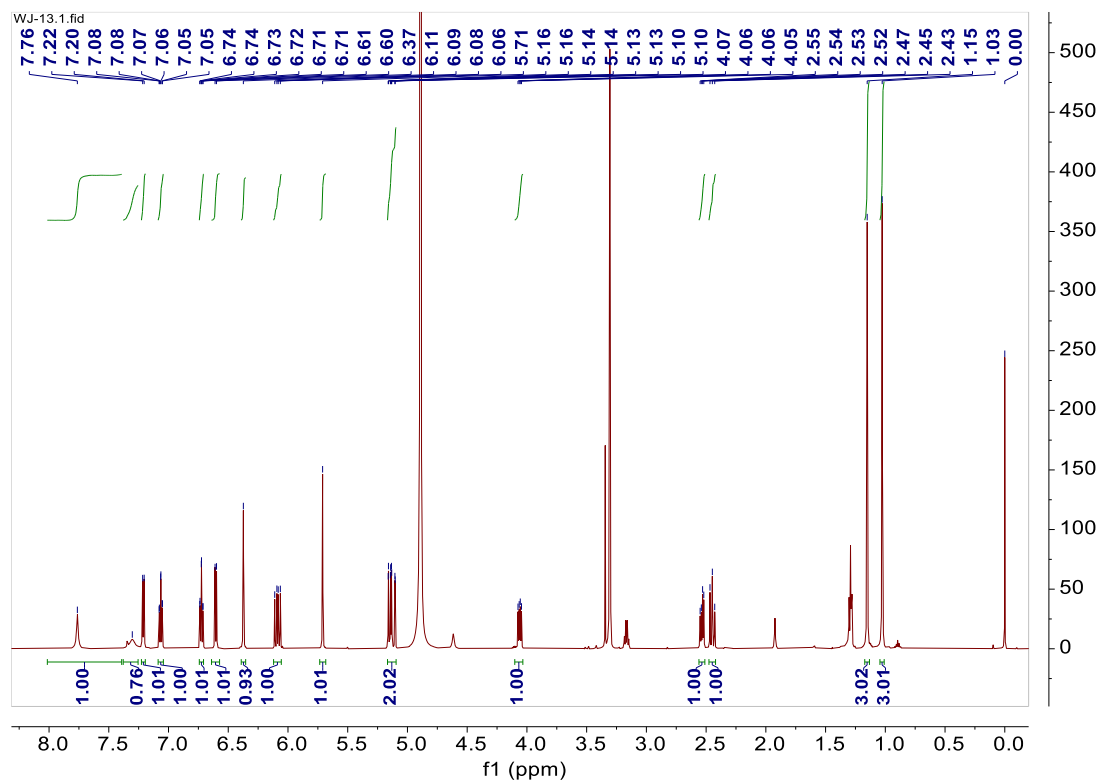


Fig. S74. ^1H NMR spectrum of compound **6** (600 MHz, CD_3OD).

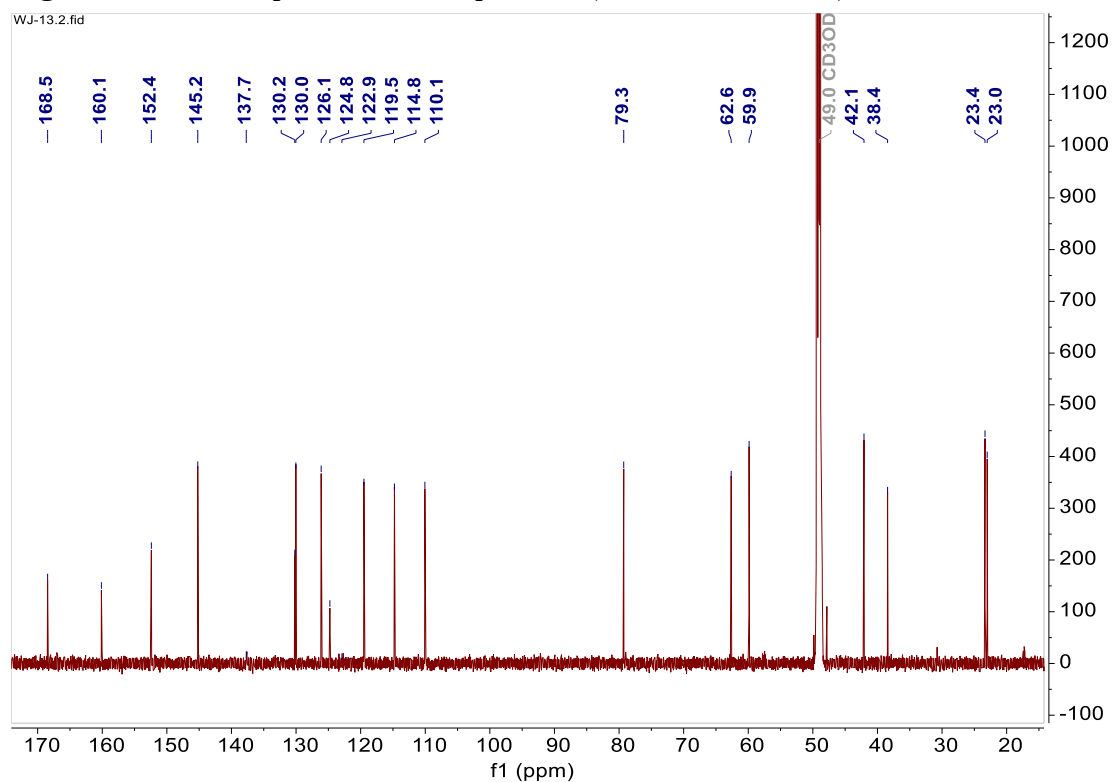


Fig. S75. ^{13}C NMR spectrum of compound **6** (150 MHz, CD_3OD).

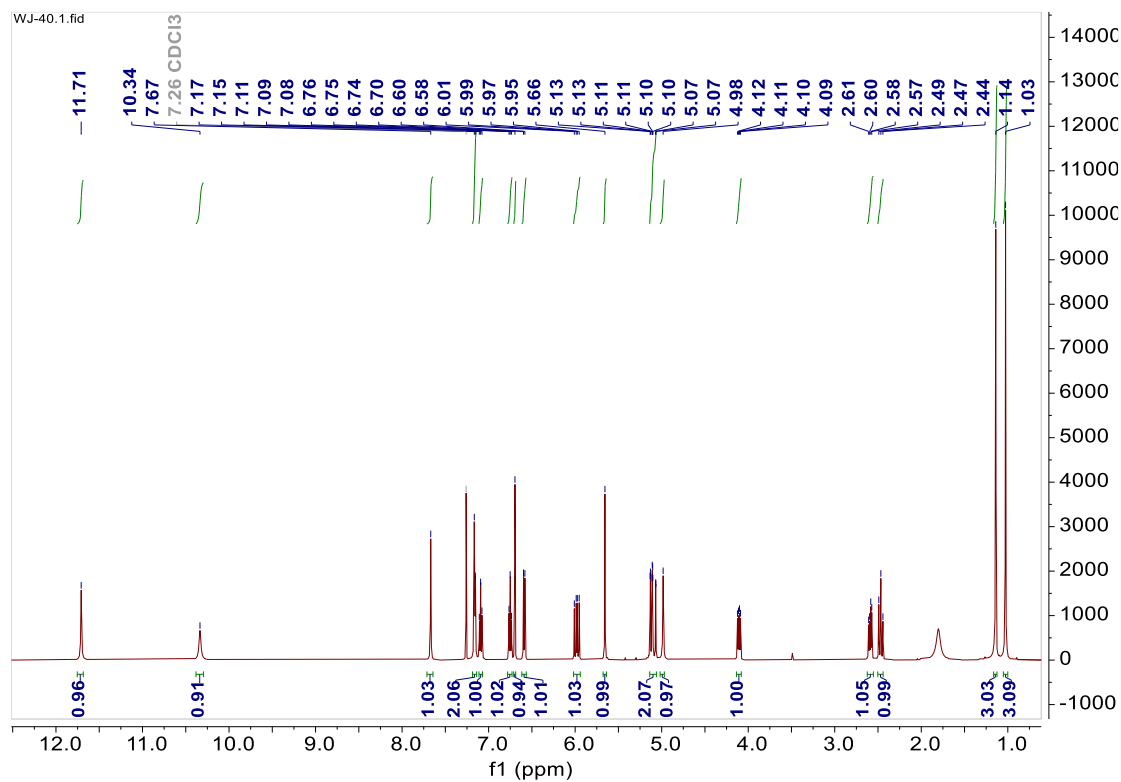


Fig. S76. ^1H NMR spectrum of compound **7** (600 MHz, CDCl_3).

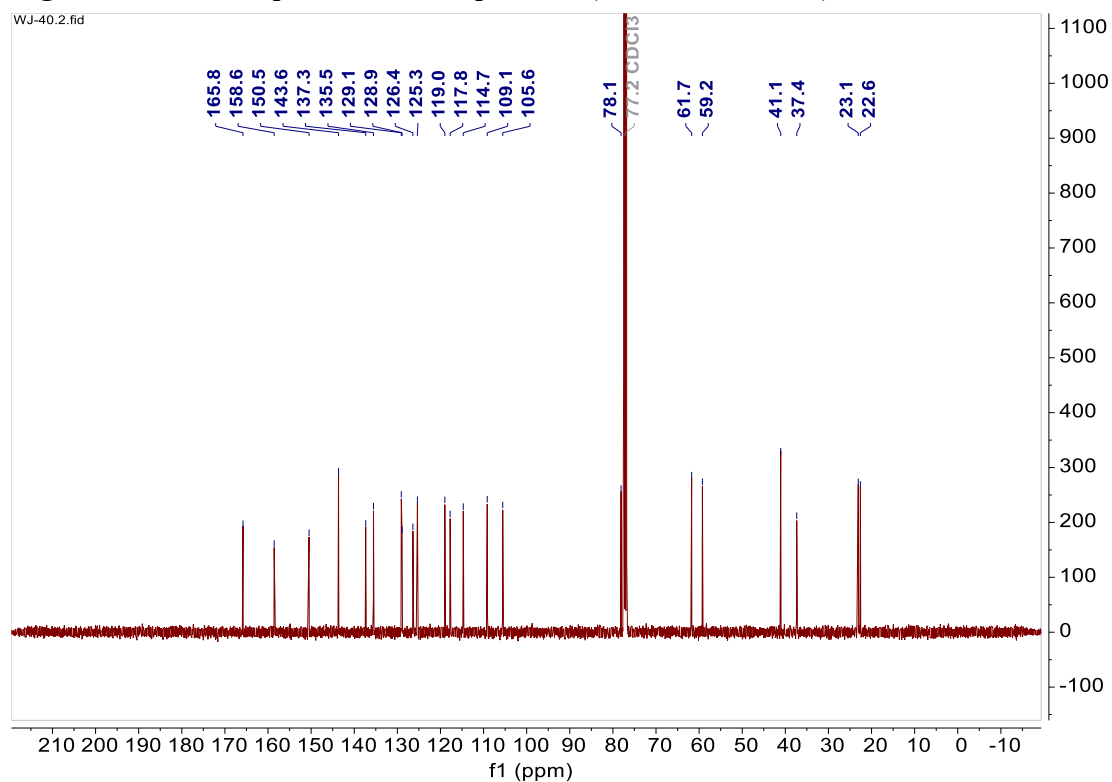


Fig. S77. ^{13}C NMR spectrum of compound **7** (150 MHz, CDCl_3).

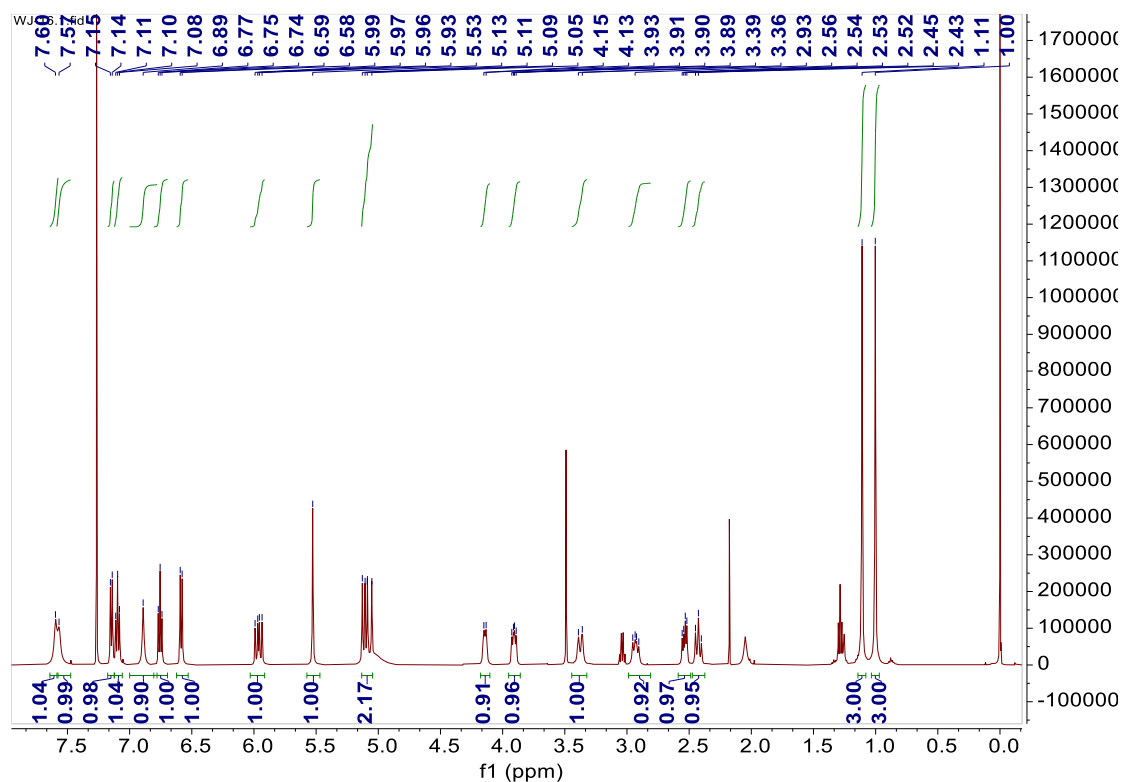


Fig. S78. ^1H NMR spectrum of compound **8** (600 MHz, CDCl_3).

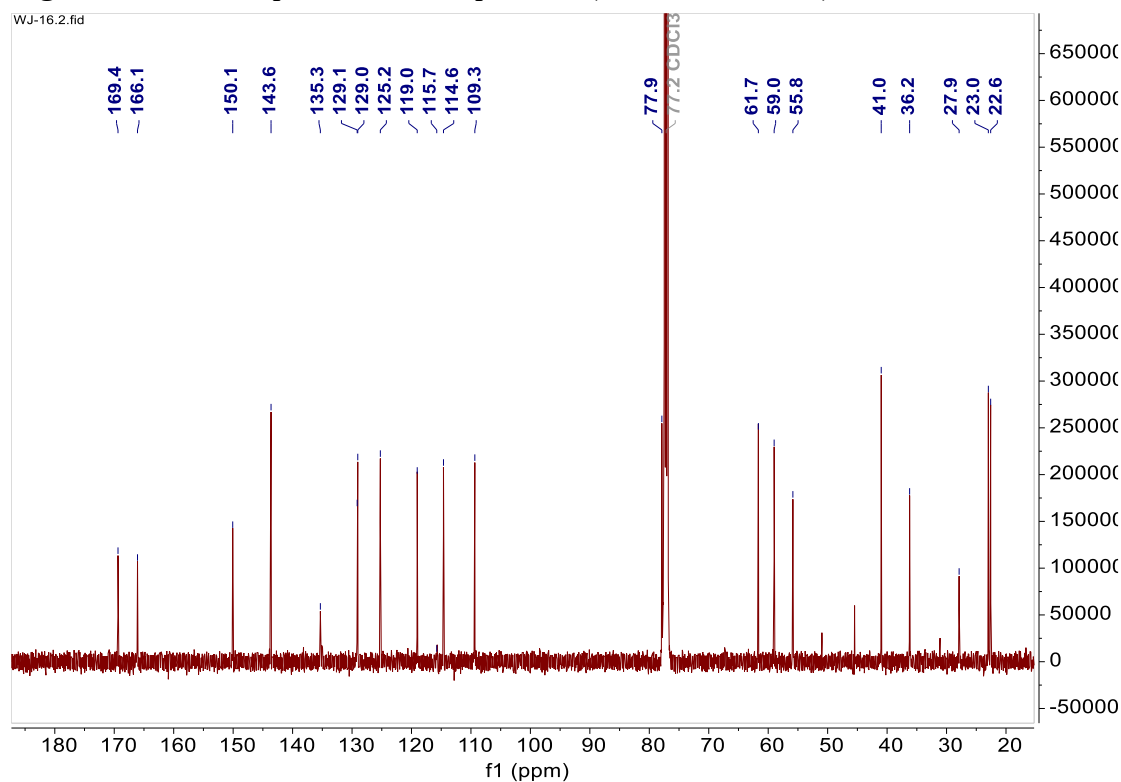


Fig. S79. ^{13}C NMR spectrum of compound **8** (150 MHz, CDCl_3).

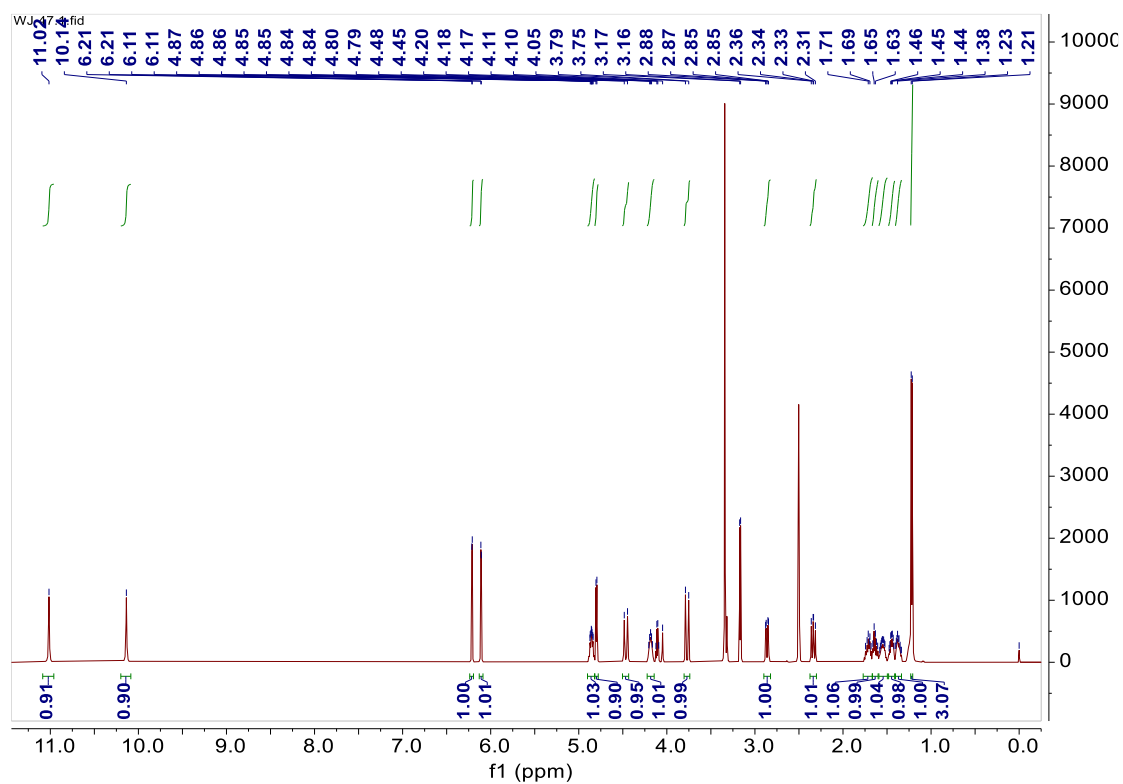


Fig. S80. ^1H NMR spectrum of compound **9** (600 MHz, $\text{DMSO}-d_6$).

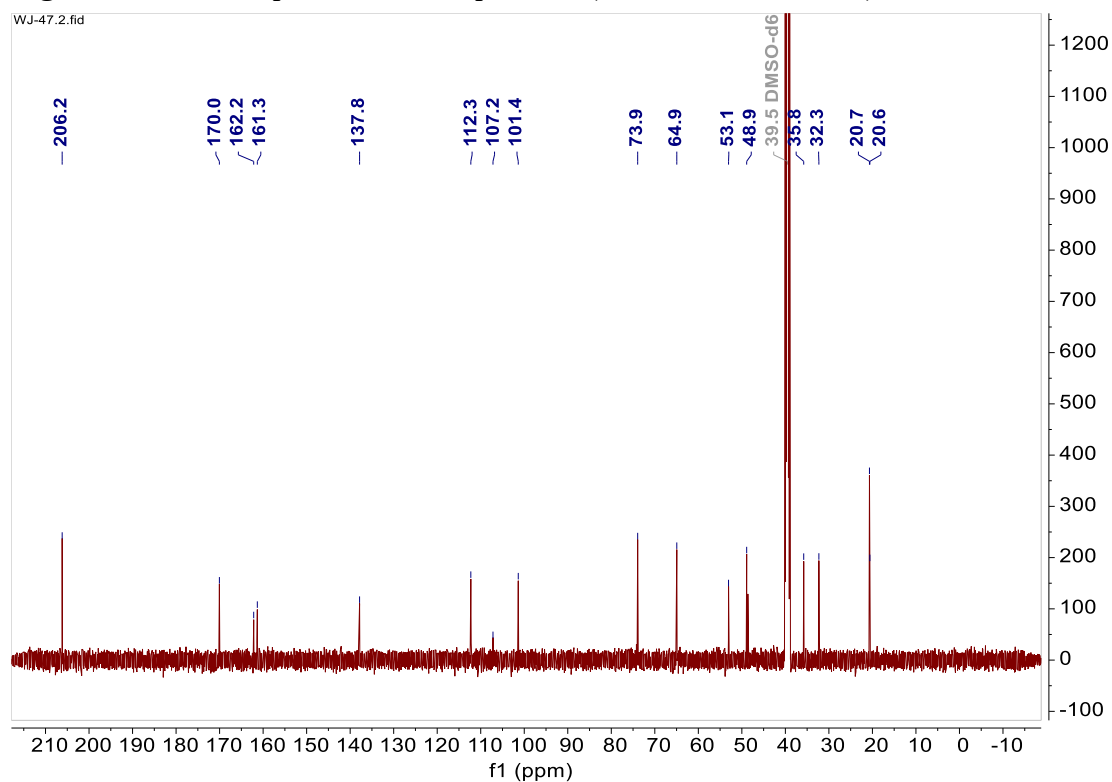


Fig. S81. ^{13}C NMR spectrum of compound **9** (150 MHz, $\text{DMSO}-d_6$).

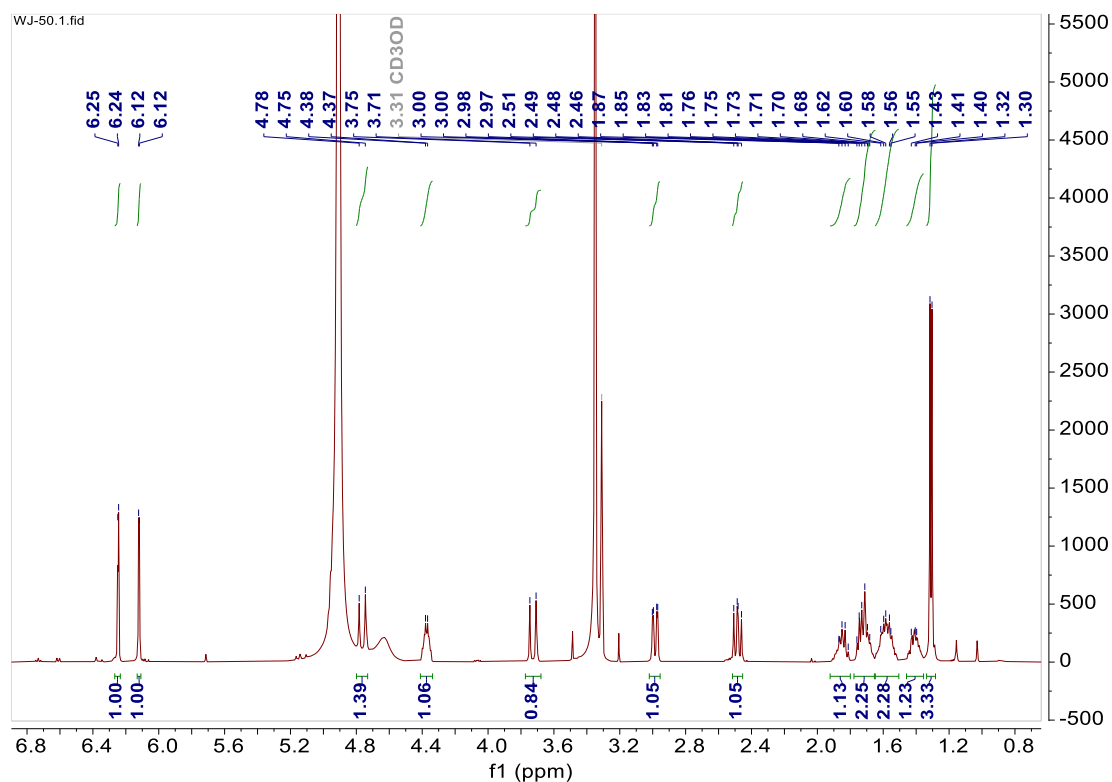


Fig. S82. ^1H NMR spectrum of compound **10** (600 MHz, CD_3OD).

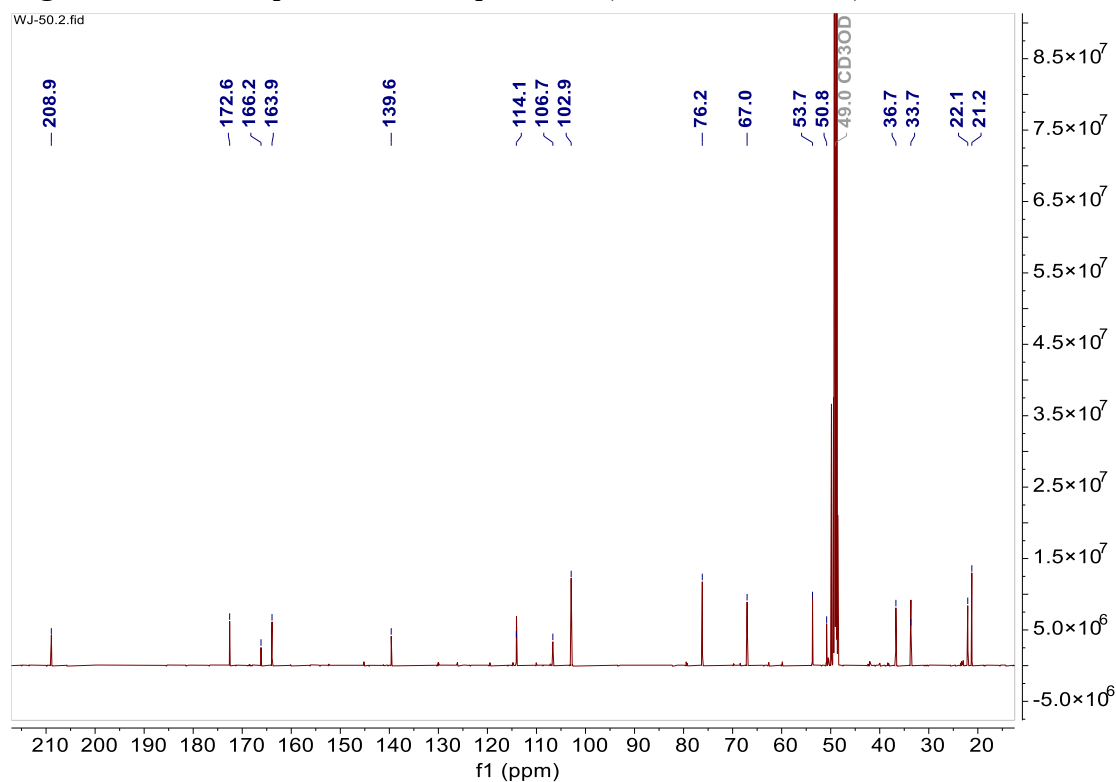


Fig. S83. ^{13}C NMR spectrum of compound **10** (150 MHz, CD_3OD).

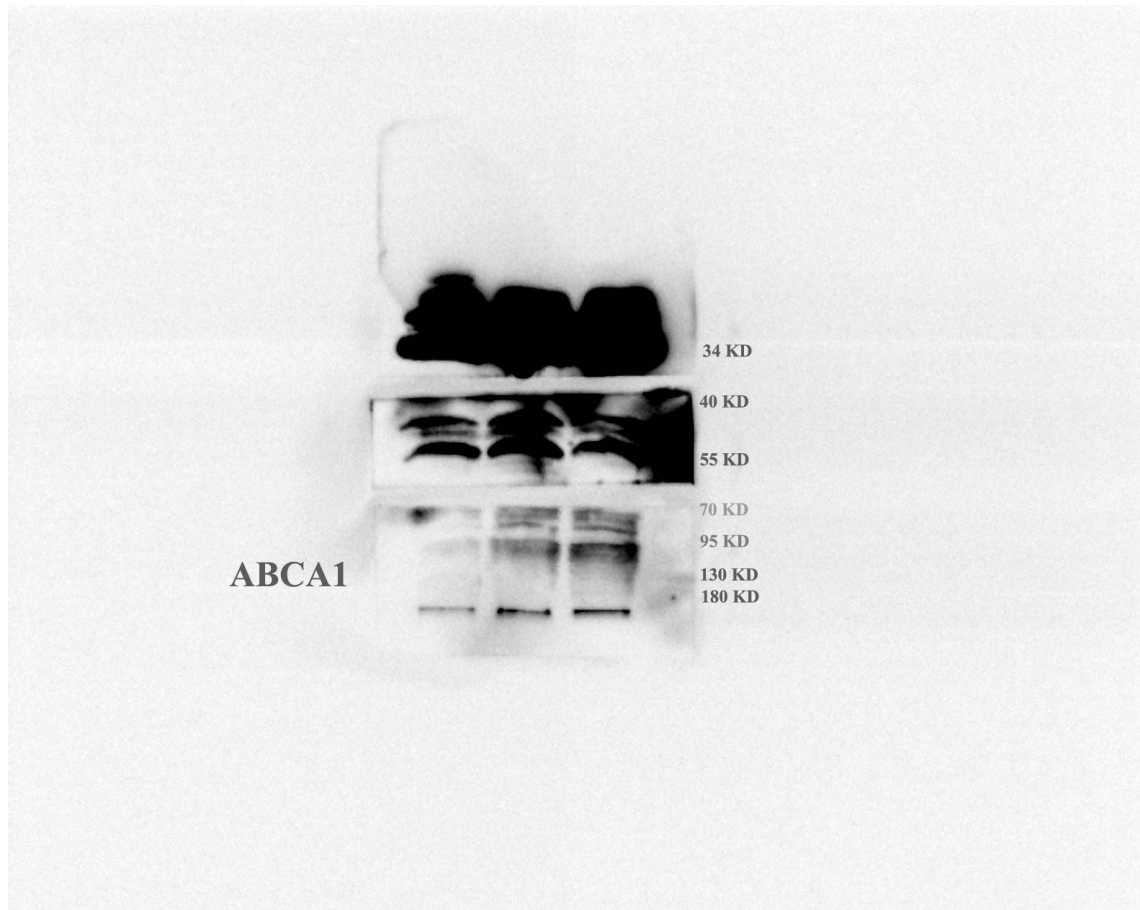


Fig. S84. Raw image of Western blotting of ABCA1.

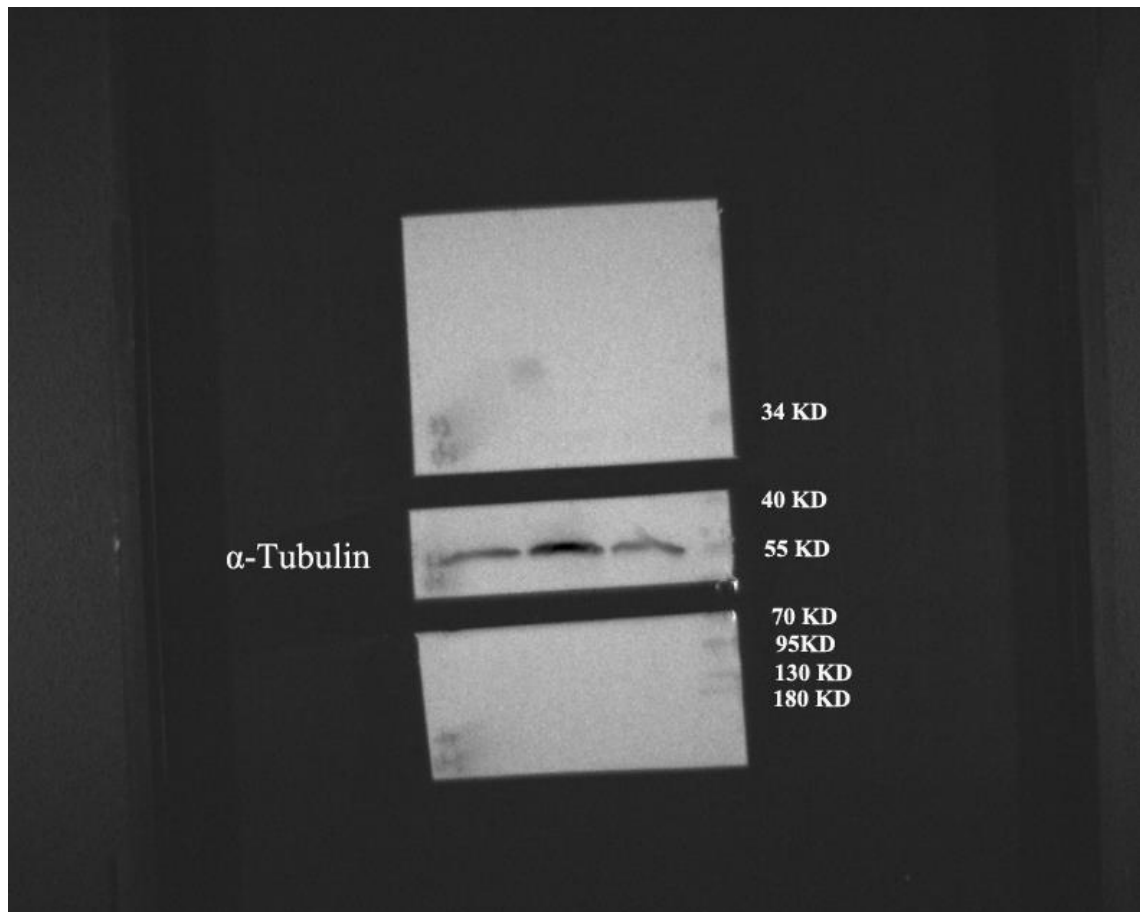


Fig. S85. Raw image of Western blotting of α -tubulin.

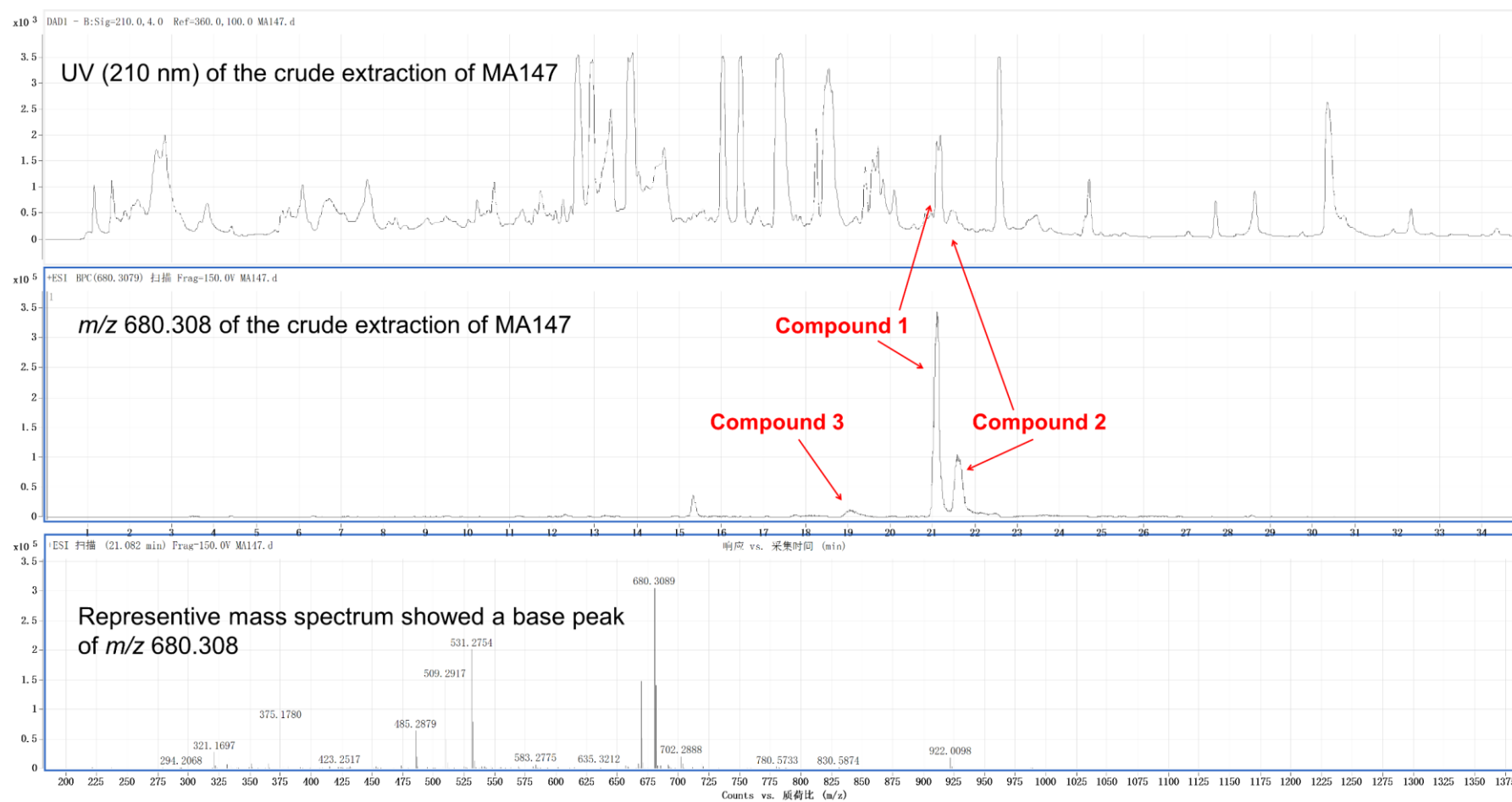


Fig. S86. LC-MS analysis of the raw EtOAc extraction of the strain MA147.
chromatogram condition: Supersil ODS2, 2.1×150 mm, $3 \mu\text{m}$, 5%–100% acetonitrile (0–30 min), flow rate: 0.2 mL/min.

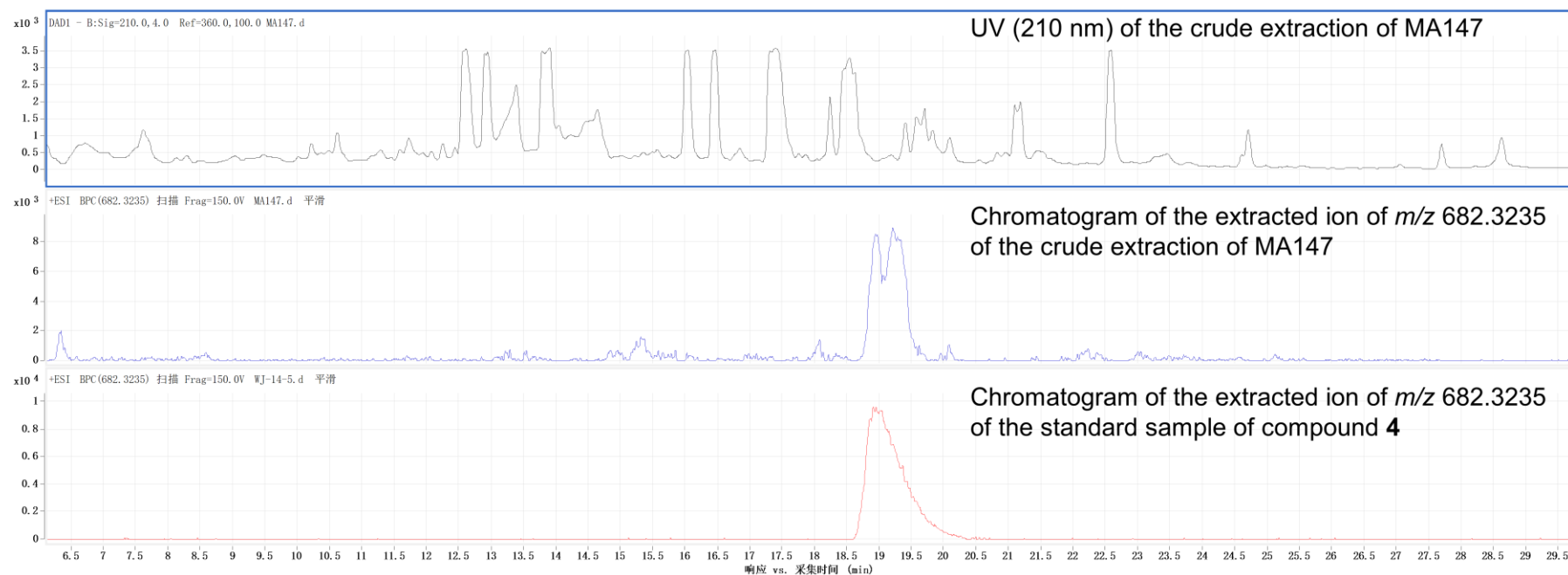


Fig. S87. LC-MS analysis of the raw EtOAc extraction of the strain MA147 and the standard sample of compound **4**.
chromatogram condition: Supersil ODS2, 2.1 × 150 mm, 3 μm, 5%–100% acetonitrile (0–30 min), flow rate: 0.2 mL/min.

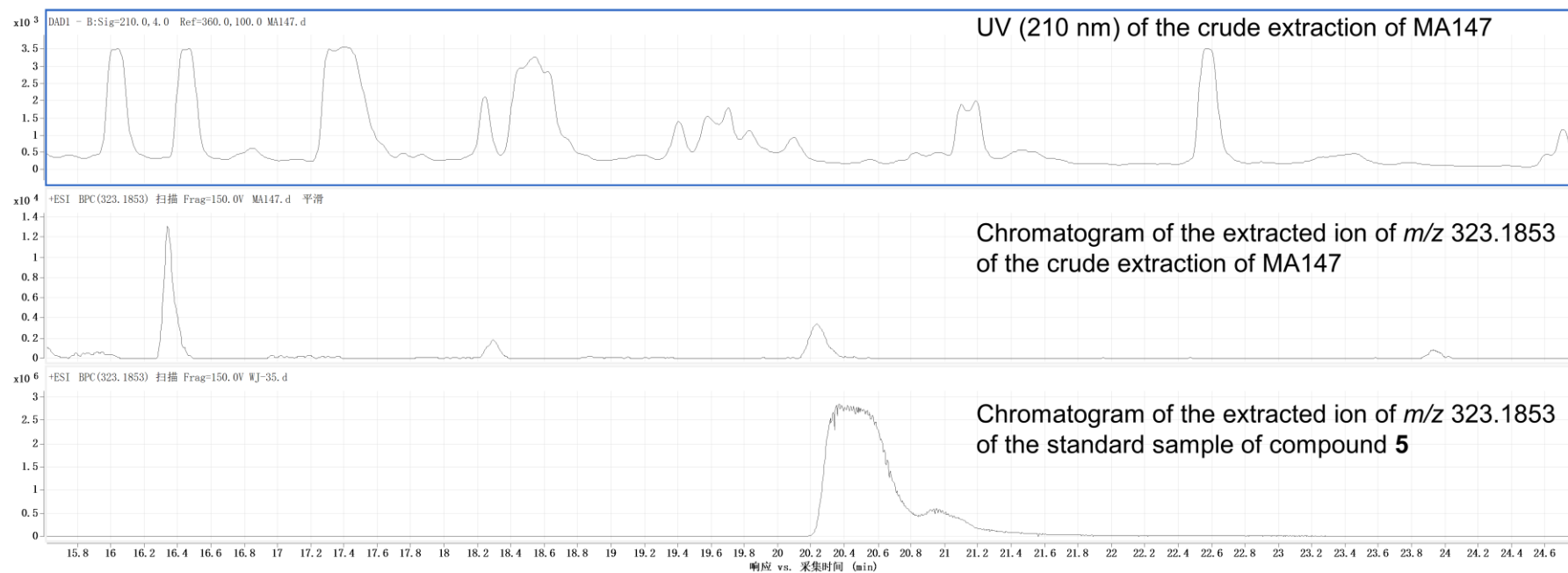


Fig. S88. LC-MS analysis of the raw EtOAc extraction of the strain MA147 and the standard sample of compound 5.
 chromatogram condition: Supersil ODS2, 2.1 × 150 mm, 3 μm, 5%–100% acetonitrile (0–30 min), flow rate: 0.2 mL/min.

Table S4. ^1H (600 MHz) and ^{13}C (150 MHz) NMR spectroscopic data of compound **3** in acetone- d_6

Position	3^c	
	δ_{H} (<i>J</i> in Hz)	δ_{C}
1	-	166.8
2	4.02, 1H, dd, 11.1, 5.9	59.5
3	2.47, 2H, m	38.3
4	-	62.1
5	-	130.1
6	7.25, 1H, d, 7.5	125.9
7	6.70, 1H, dd, 7.5	118.9
8	7.05, 1H, dd, 7.5	129.5
9	6.64, 1H, d, 7.5	109.7
10	-	152.2
11	5.69, 1H, s	78.6
12	-	158.9
13	-	125.2
14	-	41.8
15	6.15, 1H, dd, 17.7, 10.5	145.2
16	5.12, 2H, overlapped	114.4
17	1.05, 3H, s	23.4
18	1.17, 3H, s	23.0
19	6.50, 1H, s	117.3
20	-	136.6
21	7.71, 1H, s	137.1
22	8.40, 1H, s	122.0
23	4.63, 1H, m	57.0
24	1.99, 2H, m	36.1
25	1.35, 2H, m	23.3
26	1.43, 2H, m	39.5
27	3.68, 1H, m	67.3
28	-	166.7
29	-	99.6
30	-	164.5
31	6.36, 1H, s	102.7
32	-	166.7
33	6.32, 1H, s	103.8
34	-	140.3
35	6.30, 1H, s	107.0
36	-	154.3
37	3.11, 2H, overlapped	40.7
38	1.08, 3H, d, 6.2	24.1
10-NH	5.78, 1H, s	-
13-NH	9.36, 1H, s	-
30-OH	-	-
32-OH	11.06, 1H, s	-

Table S5. Coordinates and relative free energy of low-energy conformers of structures **1a–d** for GIAO NMR calculations.

1a-c4, $\Delta G = 0.0000$ kcal/mol, population = 40.20 %

C -1.555638 -0.615048 -0.717247
 C -2.921443 -0.344879 -0.126532
 C -4.024034 -1.310016 -0.562233
 C -5.334847 -0.520295 -0.312301
 C -5.693908 -0.513301 1.174618
 C -5.919776 -1.563781 2.048742
 C -6.218903 -1.294873 3.388426
 C -6.281994 0.021605 3.838362
 C -6.046277 1.090109 2.973348
 C -5.747970 0.806195 1.644190
 C -4.929107 0.988305 -0.516263
 C -2.718647 2.059943 -0.795831
 C -1.249856 1.821474 -0.928984
 C -6.536689 -0.975207 -1.245127
 C -6.778505 -2.460480 -1.047978
 C -7.897717 -3.053090 -0.647043
 C -7.791653 -0.143306 -0.939119
 C -6.193725 -0.785346 -2.743806
 C -0.411904 2.866203 -1.052808
 C 1.024091 2.851907 -1.217878
 C 2.921323 3.588510 -1.908539
 C 1.977414 1.937865 -0.812841
 C 4.479323 1.708166 -1.166298
 C 5.645745 2.706372 -1.205735
 C 7.022886 2.129010 -0.848167
 C 7.215368 1.714920 0.628327
 C 7.345118 0.228268 0.957957
 C 5.582028 -1.281665 1.626665
 C 4.230857 -1.813296 1.389176
 C 3.516249 -2.255188 2.545317
 C 2.174992 -2.606106 2.469588
 C 1.522180 -2.576093 1.247362
 C 2.227846 -2.243100 0.081908
 C 3.562493 -1.874232 0.135868
 C 4.277525 -1.692560 -1.198844
 C 3.719741 -0.565129 -2.075497
 C 4.589021 0.656979 -2.301794
 C 8.419091 -0.528285 0.193551

N -5.512096 1.702178 0.605464
 N -3.455564 0.958580 -0.519731
 N -0.823888 0.479177 -1.020977
 O -1.124226 -1.759632 -0.867160
 O -3.228203 3.168927 -0.952078
 H -2.797910 -0.389612 0.964217
 H -5.254289 1.435592 -1.451154
 O 2.622938 -0.658483 -2.588335
 O 6.232003 -1.545854 2.639474
 O 4.082877 -2.323226 3.765970
 O 0.217227 -2.920157 1.223437
 O 6.041479 -0.414667 0.710093
 N 3.185881 2.414161 -1.257077
 N 1.647546 3.890732 -1.889171
 H -6.396552 -2.112238 4.075710
 H -6.510495 0.223348 4.878149
 H -6.086992 2.112589 3.328654
 H -5.867433 -2.588549 1.705238
 H -5.144177 2.622049 0.798732
 H -3.893796 -1.546544 -1.617385
 H -3.987611 -2.239744 -0.000246
 H 0.092871 0.301340 -1.419223
 H -5.934111 -3.093892 -1.309824
 H -8.616085 -0.457892 -1.581022
 H -8.109569 -0.247148 0.098142
 H -7.611385 0.915089 -1.129009
 H -5.959264 0.253015 -2.982750
 H -7.058969 -1.071614 -3.343747
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 H -8.787588 -2.501070 -0.372100
 H -0.883102 3.839885 -1.094419
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 H 9.388860 -0.054751 0.358789
 H 8.224568 -0.543205 -0.879341
 H 5.040568 -2.114546 3.656679
 H -0.201791 -2.661369 0.376056
 H 1.730174 -2.309540 -0.876072
 H 1.652124 -2.906871 3.366994
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 H 6.410235 2.125944 1.243465
 H 8.133795 2.171661 1.005919
 H 7.751096 2.906663 -1.085893
 H 7.269205 1.301937 -1.516526

H 5.627903 0.336812 -2.377104
H 4.296859 1.123596 -3.243235
H 4.120848 -2.608593 -1.774338
H 5.343122 -1.564916 -1.058691
H 5.418169 3.525601 -0.518469
H 5.709206 3.141425 -2.206766
H 4.486166 1.204555 -0.200602
H 1.909769 1.038909 -0.224899
H 3.691476 4.184609 -2.367327

1a-c7, $\Delta G = 0.0138$ kcal/mol,
population = 39.27 %

C -1.583354 -0.647893 -0.707544
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C -4.063193 -1.297354 -0.512429
C -5.353307 -0.477447 -0.265438
C -5.678743 -0.414043 1.230537
C -5.859492 -1.426657 2.159481
C -6.123985 -1.103563 3.494236
C -6.192414 0.230394 3.887998
C -5.988425 1.261679 2.971751
C -5.722676 0.923644 1.648377
C -4.928807 1.016014 -0.524378
C -2.703704 2.042963 -0.847811
C -1.240271 1.777191 -0.987629
C -6.570860 -0.942426 -1.174656
C -6.920570 -2.377806 -0.826833
C -6.822072 -3.450494 -1.605453
C -7.820704 -0.083829 -0.873762
C -6.248919 -0.795864 -2.672386
C -0.386832 2.804380 -1.147181
C 1.047418 2.761244 -1.322917
C 2.951636 3.444535 -2.048271
C 1.988269 1.844171 -0.896387
C 4.483731 1.562966 -1.256628
C 5.666446 2.539447 -1.334780
C 7.033623 1.950421 -0.958450
C 7.221159 1.590817 0.532990
C 7.328418 0.116220 0.919753
C 5.545206 -1.346391 1.638549
C 4.186224 -1.866122 1.419873
C 3.467254 -2.260317 2.590455
C 2.120965 -2.594095 2.527732
C 1.466442 -2.593802 1.306030

C 2.174817 -2.308598 0.129613
C 3.514733 -1.957621 0.170017
C 4.230322 -1.829720 -1.170614
C 3.684377 -0.727428 -2.085858
C 4.569407 0.473863 -2.357918
C 8.392335 -0.684396 0.186833
N -5.499643 1.777470 0.572316
N -3.455306 0.962951 -0.531108
N -0.836984 0.426209 -1.046732
O -1.170042 -1.802380 -0.829166
O -3.197408 3.154845 -1.033057
H -2.805603 -0.360839 0.977883
H -5.250627 1.434249 -1.473389
O 2.585155 -0.824637 -2.592685
O 6.192974 -1.586689 2.658692
O 4.034888 -2.297277 3.812038
O 0.156606 -2.919407 1.294909
O 6.015596 -0.516039 0.693982
N 3.201326 2.286563 -1.362728
N 1.683107 3.768476 -2.029893
H -6.267013 -1.892559 4.221451
H -6.394719 0.474954 4.923933
H -6.023863 2.298070 3.284596
H -5.786475 -2.466790 1.867528
H -5.121207 2.700512 0.727167
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H -4.041050 -2.215767 0.068084
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H -6.039041 0.240218 -2.938057
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H -7.127390 -4.425278 -1.243904
H -6.443611 -3.411350 -2.619325
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H 8.199392 -0.736468 -0.885190
H 8.439446 -1.701201 0.577805
H 4.995212 -2.105641 3.694988
H -0.260204 -2.682188 0.440131
H 1.674522 -2.398236 -0.825080

H 1.595423 -2.858330 3.435016
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H 8.146481 2.047974 0.892778
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H 7.261730 1.093164 -1.594470
H 5.602895 0.135595 -2.429875
H 4.277385 0.913787 -3.312129
H 4.063422 -2.763449 -1.713980
H 5.297316 -1.708791 -1.035585
H 5.455100 3.386596 -0.676848
H 5.734692 2.937071 -2.350960
H 4.488393 1.091068 -0.275064
H 1.909682 0.965170 -0.280309
H 3.728374 4.013290 -2.530123

1a-c10, $\Delta G = 0.6633$ kcal/mol,
population = 13.10 %

C -1.520306 -0.659103 -0.760265
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C -3.975290 -1.406501 -0.606387
C -5.294071 -0.649171 -0.312303
C -5.615551 -0.668578 1.184631
C -5.755930 -1.729322 2.064899
C -6.035294 -1.478725 3.412189
C -6.160387 -0.168359 3.866161
C -5.999228 0.911418 2.998407
C -5.717678 0.645325 1.662417
C -4.923321 0.869291 -0.499570
C -2.733844 1.993711 -0.742869
C -1.260471 1.788429 -0.881533
C -6.506850 -1.119249 -1.224028
C -7.740574 -0.308010 -0.870436
C -8.918305 -0.765023 -0.460316
C -6.221081 -0.859748 -2.724315
C -6.746236 -2.626866 -1.050082
C -0.441908 2.852427 -0.962500
C 0.994996 2.870534 -1.119701
C 2.882165 3.666124 -1.771277
C 1.962819 1.960890 -0.740159
C 4.470234 1.789693 -1.083996
C 5.618018 2.809859 -1.076445
C 7.005825 2.245659 -0.739563
C 7.204517 1.766848 0.716178

C 7.354498 0.268447 0.977618
C 5.607565 -1.283575 1.589891
C 4.266262 -1.828185 1.327212
C 3.553583 -2.320930 2.464023
C 2.219496 -2.693655 2.368871
C 1.573024 -2.635854 1.144334
C 2.278336 -2.250899 -0.005131
C 3.605466 -1.858956 0.068720
C 4.320905 -1.615143 -1.255774
C 3.752655 -0.456762 -2.084634
C 4.608421 0.783488 -2.256412
C 8.436052 -0.439077 0.177737
N -5.528815 1.556558 0.626379
N -3.448272 0.870807 -0.497536
N -0.809154 0.458734 -1.024059
O -1.070039 -1.789462 -0.956023
O -3.265535 3.096414 -0.867832
H -2.752899 -0.511466 0.936304
H -5.253263 1.318957 -1.431515
O 2.657163 -0.539373 -2.602068
O 6.255497 -1.570034 2.598003
O 4.114653 -2.419146 3.685189
O 0.275014 -3.003981 1.101091
O 6.059585 -0.381544 0.703887
N 3.164733 2.474861 -1.159276
N 1.602845 3.943736 -1.750012
H -6.145792 -2.305317 4.102428
H -6.374065 0.019910 4.911546
H -6.079170 1.930140 3.357810
H -5.637993 -2.751487 1.727715
H -5.187379 2.485671 0.824805
H -3.856082 -1.606137 -1.670539
H -3.913658 -2.353413 -0.076347
H 0.110066 0.313212 -1.429926
H -7.628219 0.764956 -1.001155
H -7.074089 -1.204088 -3.311022
H -6.081386 0.198029 -2.949348
H -5.342798 -1.402391 -3.076225
H -5.859434 -3.198324 -1.327450
H -7.559364 -2.952466 -1.700739
H -7.015842 -2.886929 -0.027754
H -9.736857 -0.083349 -0.262540
H -9.118598 -1.817050 -0.300106
H -0.931148 3.818057 -0.970199

H 9.400297 0.038547 0.362289
 H 8.239346 -0.408600 -0.894427
 H 8.512644 -1.482939 0.483669
 H 5.069070 -2.190017 3.588372
 H -0.144328 -2.723529 0.260800
 H 1.786845 -2.294371 -0.967617
 H 1.697505 -3.033457 3.252743
 H 7.550269 0.133415 2.038592
 H 6.395383 2.139148 1.350503
 H 8.117819 2.217307 1.113391
 H 7.717522 3.049264 -0.937857
 H 7.272420 1.456123 -1.444479
 H 5.652529 0.481286 -2.330583
 H 4.320496 1.281019 -3.183290
 H 4.173603 -2.507420 -1.869639
 H 5.385037 -1.483237 -1.108752
 H 5.372427 3.595142 -0.356471
 H 5.676264 3.287509 -2.058193
 H 4.478029 1.250146 -0.137981
 H 1.908515 1.039315 -0.186677
 H 3.643803 4.292116 -2.203655

1a-c2, $\Delta G = 0.9990$ kcal/mol,
 population = 7.43 %

C -1.722670 0.456776 0.823247
 C -3.056501 0.228818 0.147449
 C -4.246097 0.935090 0.796970
 C -5.475604 0.114776 0.327924
 C -5.847733 0.464891 -1.114345
 C -6.184343 1.681238 -1.685086
 C -6.466717 1.746544 -3.053589
 C -6.403183 0.595384 -3.834872
 C -6.055291 -0.634894 -3.277222
 C -5.776139 -0.683294 -1.914965
 C -4.922511 -1.347239 0.135033
 C -2.615108 -2.236104 0.146414
 C -1.172482 -1.900176 0.342304
 C -6.705853 0.190099 1.329222
 C -7.090471 1.644842 1.527771
 C -8.265465 2.212772 1.280134
 C -7.879005 -0.645327 0.794190
 C -6.330274 -0.355965 2.729041
 C -0.237667 -2.852320 0.166923
 C 1.198458 -2.760323 0.296210

C 3.193894 -3.519735 0.568808
 C 2.055740 -1.679482 0.205078
 C 4.537801 -1.339491 0.456935
 C 5.780182 -2.002838 -0.143570
 C 5.852753 -2.139092 -1.670303
 C 5.699352 -0.868699 -2.528954
 C 6.522959 0.381762 -2.187711
 C 4.894270 1.932697 -1.320581
 C 3.958529 2.217917 -0.220925
 C 2.652139 2.645764 -0.605009
 C 1.611682 2.687850 0.318821
 C 1.858155 2.382886 1.649664
 C 3.164184 2.097624 2.069283
 C 4.200314 1.976634 1.160036
 C 5.556730 1.618112 1.723781
 C 5.854993 0.149874 2.064704
 C 4.783761 -0.921383 1.929202
 C 7.982888 0.166012 -1.841365
 N -5.442474 -1.792810 -1.143891
 N -3.458252 -1.177407 0.171527
 N -0.875357 -0.598422 0.802806
 O -1.426779 1.547849 1.311830
 O -3.013588 -3.390226 -0.004293
 H -2.937784 0.571645 -0.889489
 H -5.192987 -2.054291 0.914119
 O 6.962794 -0.131571 2.473353
 O 4.734693 2.378297 -2.458124
 O 2.339731 2.983410 -1.869022
 O 0.878932 2.354641 2.578725
 O 5.879179 1.062022 -1.041232
 N 3.324730 -2.173483 0.373468
 N 1.943606 -3.908827 0.513277
 H -6.730200 2.694574 -3.505036
 H -6.619640 0.653251 -4.894971
 H -5.996939 -1.526568 -3.889478
 H -6.230493 2.579473 -1.083265
 H -4.993985 -2.592760 -1.565293
 H -4.131882 0.901311 1.879474
 H -4.305401 1.977839 0.496129
 H 0.022826 -0.459972 1.250723
 H -6.308836 2.263678 1.962371
 H -7.597339 -1.694307 0.698149
 H -8.722555 -0.591595 1.484194
 H -8.215657 -0.298372 -0.182489

H -6.001920 -1.395692 2.689696
 H -7.210150 -0.315617 3.373087
 H -5.549578 0.230069 3.214671
 H -8.430272 3.261476 1.497114
 H -9.100524 1.670796 0.854603
 H -0.621290 -3.837273 -0.066908
 H 8.120296 -0.448976 -0.953258
 H 8.477893 1.123436 -1.675693
 H 8.478093 -0.329944 -2.678550
 H 3.168780 2.916725 -2.402396
 H 0.007378 2.212736 2.145160
 H 3.340175 1.935670 3.125179
 H 0.623469 2.969073 -0.019219
 H 6.452575 1.066798 -3.028839
 H 4.649693 -0.565570 -2.571481
 H 5.957971 -1.141452 -3.556401
 H 5.097272 -2.851144 -2.014463
 H 6.816577 -2.603637 -1.895857
 H 5.109616 -1.786671 2.507713
 H 3.846743 -0.550428 2.346527
 H 5.679586 2.145023 2.674739
 H 6.372006 1.950623 1.086030
 H 5.916874 -2.991021 0.303402
 H 6.634481 -1.422458 0.201160
 H 4.298765 -0.449027 -0.113990
 H 1.890529 -0.639975 -0.021021
 H 4.037851 -4.166834 0.739906

1b-c19, ΔG = 0.0000 kcal/mol,
 population = 98.10 %

C 2.924160 2.171184 0.117712
 C 4.063630 1.221950 0.432324
 C 5.359609 1.459837 -0.343380
 C 6.112923 0.109748 -0.225771
 C 6.752755 -0.036592 1.156412
 C 7.649129 0.779532 1.827405
 C 8.070950 0.433618 3.115592
 C 7.580591 -0.719758 3.722587
 C 6.660492 -1.540595 3.070726
 C 6.248781 -1.182340 1.790328
 C 4.971885 -0.968026 -0.132941
 C 2.524640 -0.730465 0.100234
 C 1.392203 0.238524 0.157498
 C 7.113360 -0.176909 -1.427452

C 6.350036 -0.186399 -2.740938
 C 6.160490 -1.215285 -3.561032
 C 8.163314 0.951426 -1.530633
 C 7.854824 -1.503999 -1.199584
 C 0.125508 -0.220749 0.228945
 C -1.077892 0.569550 0.232951
 C -2.353220 2.307333 0.176520
 C -2.378055 0.115968 0.322583
 C -4.648467 1.230977 0.428100
 C -5.044740 1.840624 1.783595
 C -6.525917 1.741342 2.179697
 C -7.078909 0.325503 2.458403
 C -7.911632 -0.375152 1.380104
 C -6.777901 -1.999468 -0.022723
 C -5.850145 -2.256660 -1.138577
 C -5.242760 -3.553068 -1.170682
 C -4.264735 -3.869638 -2.105858
 C -3.901678 -2.934229 -3.057971
 C -4.525502 -1.684206 -3.094812
 C -5.486298 -1.333843 -2.159327
 C -6.130532 0.031443 -2.367123
 C -5.173950 1.198601 -2.077893
 C -5.320614 1.943892 -0.763731
 C -9.096959 0.411717 0.848541
 N 5.362983 -1.851790 0.953454
 N 3.758914 -0.176995 0.130031
 N 1.691613 1.605667 0.050275
 O 3.108196 3.375665 -0.002981
 O 2.355500 -1.946793 -0.007850
 H 4.254493 1.334642 1.508159
 H 4.811875 -1.535331 -1.045830
 O -4.340913 1.529356 -2.894830
 O -7.235581 -2.900705 0.682155
 O -5.561319 -4.525520 -0.297810
 O -2.948395 -3.289144 -3.955674
 O -7.053327 -0.711275 0.229095
 N -3.181451 1.227367 0.283844
 N -1.090694 1.954454 0.139712
 H 8.771793 1.068603 3.642428
 H 7.907059 -0.980753 4.722268
 H 6.267440 -2.427075 3.553535
 H 8.018196 1.690325 1.372723
 H 4.642857 -2.442782 1.341810
 H 5.115718 1.694765 -1.378641

H 5.927475 2.290786 0.067304
 H 0.883078 2.226477 -0.031198
 H 5.951011 0.776569 -3.047270
 H 8.786253 0.995385 -0.637338
 H 8.818781 0.761366 -2.382660
 H 7.702108 1.929312 -1.680925
 H 8.425226 -1.465593 -0.271774
 H 8.553758 -1.686185 -2.017688
 H 7.177277 -2.355697 -1.138281
 H 5.615660 -1.089053 -4.489062
 H 6.532814 -2.210564 -3.352803
 H 0.013948 -1.295884 0.270986
 H -8.792992 1.326300 0.338708
 H -9.752928 0.686546 1.676573
 H -9.671253 -0.195502 0.147984
 H -6.300472 -4.185482 0.262773
 H -2.759755 -2.553663 -4.552840
 H -4.262516 -0.978301 -3.873004
 H -3.812584 -4.851521 -2.091339
 H -8.260227 -1.317745 1.793764
 H -7.740477 0.380009 3.327402
 H -6.265543 -0.343803 2.753368
 H -7.150490 2.261944 1.451077
 H -6.627365 2.322411 3.098922
 H -4.900249 2.942030 -0.888842
 H -6.381746 2.048233 -0.540467
 H -7.039249 0.136059 -1.788727
 H -6.382185 0.116198 -3.425414
 H -4.756977 2.895916 1.789683
 H -4.438885 1.351207 2.551396
 H -4.936747 0.184211 0.421296
 H -2.782672 -0.878385 0.401574
 H -2.716140 3.320418 0.124431

1b-c4, $\Delta G = 2.4774$ kcal/mol,
 population = 1.49 %

C 1.972270 0.402273 -0.664075
 C 3.411377 0.296253 -0.224195
 C 4.279506 -0.676565 -1.025057
 C 5.477574 -0.958579 -0.085167
 C 6.470245 0.206972 -0.090662
 C 7.146529 0.814106 -1.137369
 C 7.986742 1.902355 -0.881721
 C 8.131999 2.380761 0.418060

C 7.440107 1.798698 1.479492
 C 6.606007 0.718360 1.208125
 C 4.878915 -0.819117 1.366551
 C 2.651504 -0.080199 2.135454
 C 1.281105 0.332521 1.704445
 C 6.141175 -2.377978 -0.350358
 C 5.114866 -3.474017 -0.117249
 C 4.619616 -4.326202 -1.009107
 C 6.708003 -2.440512 -1.776849
 C 7.299706 -2.621464 0.642163
 C 0.343594 0.560245 2.641584
 C -1.063058 0.872183 2.507499
 C -2.952499 1.662842 3.165868
 C -1.997844 0.527881 1.548154
 C -4.497748 0.910392 1.279209
 C -5.585086 0.507180 2.292474
 C -6.936976 0.023144 1.741299
 C -6.929898 -1.364291 1.055770
 C -7.162855 -1.396519 -0.455757
 C -5.045446 -1.291759 -1.633197
 C -3.928219 -0.439575 -2.059569
 C -2.677243 -1.084142 -2.283466
 C -1.520409 -0.346618 -2.525151
 C -1.590699 1.037557 -2.602296
 C -2.827867 1.684144 -2.464290
 C -3.981781 0.979925 -2.176728
 C -5.255230 1.786689 -2.044927
 C -5.754934 2.166525 -0.647205
 C -4.772654 2.235931 0.515844
 C -8.477440 -0.803483 -0.929629
 N 5.836876 -0.016471 2.103991
 N 3.571115 -0.175931 1.147221
 N 1.038283 0.403998 0.315169
 O 1.689993 0.534698 -1.856662
 O 2.915940 -0.367396 3.302102
 H 3.816930 1.312811 -0.319885
 H 4.698427 -1.752746 1.890393
 O -6.907287 2.521882 -0.513003
 O -5.014932 -2.523309 -1.690293
 O -2.536807 -2.420788 -2.249433
 O -0.506891 1.808825 -2.816082
 O -6.084757 -0.634022 -1.108165
 N -3.200481 1.030227 1.980936
 N -1.693748 1.578859 3.518940

H 8.517794 2.376321 -1.697292
 H 8.781980 3.226104 0.609881
 H 7.540080 2.184961 2.486574
 H 7.023117 0.465726 -2.154840
 H 5.516467 0.403539 2.963926
 H 3.720638 -1.592150 -1.219770
 H 4.585076 -0.249460 -1.976632
 H 0.089839 0.588451 0.014395
 H 4.785248 -3.582855 0.912737
 H 7.131402 -3.428584 -1.963886
 H 5.950185 -2.253821 -2.539218
 H 7.508282 -1.713627 -1.905125
 H 7.758544 -3.590680 0.438567
 H 6.956949 -2.623516 1.677680
 H 8.067489 -1.853205 0.540755
 H 3.908578 -5.087260 -0.710523
 H 4.894742 -4.309115 -2.056362
 H 0.704773 0.515039 3.661298
 H -9.305263 -1.338606 -0.460537
 H -8.573364 -0.911308 -2.010788
 H -8.562813 0.254154 -0.682004
 H -3.433466 -2.804104 -2.081931
 H 0.316171 1.306119 -2.612690
 H -2.855489 2.760458 -2.573537
 H -0.586840 -0.871831 -2.675144
 H -7.077694 -2.425570 -0.797518
 H -7.716012 -1.986755 1.491205
 H -5.993095 -1.888381 1.267955
 H -7.366608 0.779016 1.086531
 H -7.606658 -0.026642 2.602314
 H -3.818842 2.592333 0.122830
 H -5.155611 2.980156 1.216018
 H -6.092399 1.318348 -2.556559
 H -5.089273 2.750785 -2.537242
 H -5.776866 1.360814 2.948087
 H -5.165474 -0.280424 2.924470
 H -4.352984 0.106986 0.562867
 H -1.938120 -0.074701 0.657309
 H -3.724106 2.158732 3.731080

1b-c12, $\Delta G = 3.2417$ kcal/mol,
 population = 0.41 %

C 1.888248 0.136834 -0.716724
 C 3.331004 0.127759 -0.274252

C 4.207762 -0.963943 -0.888654
 C 5.414069 -1.055055 0.081985
 C 6.384004 0.106810 -0.141501
 C 7.070645 0.497239 -1.279402
 C 7.897277 1.624628 -1.233713
 C 8.021889 2.350816 -0.051819
 C 7.328522 1.977264 1.099345
 C 6.508974 0.854501 1.037537
 C 4.815578 -0.663371 1.486405
 C 2.592787 0.217467 2.116765
 C 1.224627 0.561401 1.621791
 C 6.125343 -2.475182 0.077158
 C 6.558951 -2.802505 -1.340104
 C 7.790075 -3.048056 -1.774378
 C 7.310695 -2.478690 1.055089
 C 5.150549 -3.599654 0.505552
 C 0.305974 1.004426 2.498347
 C -1.095397 1.314743 2.313160
 C -2.958297 2.274565 2.799475
 C -2.051386 0.787342 1.464465
 C -4.546702 1.153359 1.146266
 C -5.627922 1.012017 2.233911
 C -6.990620 0.432216 1.817890
 C -7.000207 -1.073355 1.461515
 C -7.253939 -1.441768 -0.001191
 C -5.155090 -1.632693 -1.203234
 C -4.036911 -0.912684 -1.825902
 C -2.797534 -1.609134 -1.921479
 C -1.637533 -0.959997 -2.337841
 C -1.694294 0.374124 -2.716706
 C -2.921898 1.052869 -2.707462
 C -4.077900 0.446393 -2.253152
 C -5.339887 1.281097 -2.283419
 C -5.807456 1.973180 -0.999152
 C -4.804302 2.278862 0.106497
 C -8.566998 -0.949972 -0.582910
 N 5.756474 0.281329 2.058767
 N 3.497128 -0.090887 1.158564
 N 0.964251 0.342552 0.250778
 O 1.594661 0.015842 -1.907501
 O 2.866416 0.165900 3.314996
 H 3.726186 1.114404 -0.552600
 H 4.654587 -1.491041 2.170988
 O -6.951708 2.371144 -0.930908

O -5.139805 -2.846932 -0.988046
 O -2.671250 -2.907387 -1.595125
 O -0.606022 1.063264 -3.111850
 O -6.176013 -0.859530 -0.818446
 N -3.237123 1.399223 1.788816
 N -1.695973 2.242457 3.148926
 H 8.436421 1.934194 -2.120005
 H 8.660961 3.225354 -0.023680
 H 7.420569 2.550430 2.013878
 H 6.974436 -0.062226 -2.200594
 H 5.425006 0.845498 2.827244
 H 3.647458 -1.897898 -0.917601
 H 4.507319 -0.714666 -1.903176
 H 0.012899 0.464396 -0.071565
 H 5.743945 -2.876934 -2.056330
 H 7.795482 -3.456241 1.052813
 H 8.057237 -1.728387 0.795684
 H 6.975474 -2.277752 2.073043
 H 5.686992 -4.549813 0.509791
 H 4.307240 -3.709136 -0.176385
 H 4.758552 -3.441995 1.511354
 H 7.970399 -3.304483 -2.811577
 H 8.659374 -3.000843 -1.130770
 H 0.680615 1.165637 3.501369
 H -8.631633 0.137761 -0.582882
 H -9.395522 -1.348164 0.005773
 H -8.681019 -1.300165 -1.609593
 H -3.568715 -3.230723 -1.332488
 H 0.214445 0.609625 -2.809186
 H -2.939389 2.079103 -3.050723
 H -0.712695 -1.519073 -2.383008
 H -7.185092 -2.522303 -0.104312
 H -7.782060 -1.577201 2.035886
 H -6.062115 -1.542546 1.772504
 H -7.420817 1.025955 1.013506
 H -7.651432 0.584611 2.673677
 H -3.848808 2.512572 -0.365744
 H -5.158279 3.170391 0.626387
 H -6.192264 0.722822 -2.662474
 H -5.173551 2.107148 -2.982985
 H -5.801691 1.995949 2.677836
 H -5.211858 0.383478 3.026235
 H -4.428252 0.205952 0.629025
 H -2.017244 0.001687 0.728351

H -3.710886 2.903119 3.245963

1c-c5, $\Delta G = 0.0000$ kcal/mol,
 population = 57.17 %

C 1.705347 0.614608 -0.614804
 C 3.160646 0.639840 -0.209716
 C 4.147058 0.107597 -1.250064
 C 5.401928 -0.257029 -0.415951
 C 6.192355 0.999360 -0.043585
 C 6.733265 1.996169 -0.839834
 C 7.403942 3.069906 -0.245091
 C 7.515092 3.140001 1.141358
 C 6.957457 2.157096 1.958568
 C 6.291611 1.096243 1.352311
 C 4.834257 -0.667350 0.990925
 C 2.565784 -0.467411 1.955324
 C 1.144127 -0.096703 1.680071
 C 6.289662 -1.404691 -1.065112
 C 5.460338 -2.668218 -1.223237
 C 5.635447 -3.834407 -0.609685
 C 6.746051 -0.989668 -2.481398
 C 7.542647 -1.659645 -0.211738
 C 0.240539 -0.168929 2.673671
 C -1.181255 0.099493 2.641433
 C -3.064098 0.756485 3.446573
 C -2.119939 -0.056476 1.640901
 C -4.591839 0.460175 1.425556
 C -5.768831 0.035671 2.323503
 C -7.128202 -0.168575 1.627568
 C -7.367641 -1.539257 0.944899
 C -7.491365 -1.540441 -0.578440
 C -5.729975 -0.247439 -1.723984
 C -4.309388 -0.326926 -2.139689
 C -3.742059 -1.554075 -2.579878
 C -2.413780 -1.628911 -2.975338
 C -1.598827 -0.509434 -2.886175
 C -2.132770 0.709123 -2.445935
 C -3.470241 0.815794 -2.091156
 C -3.934108 2.181121 -1.603828
 C -3.720114 2.373855 -0.097863
 C -4.793999 1.894497 0.871235
 C -8.082114 -2.827971 -1.127880
 N 5.681033 0.004450 1.960476

N 3.440337 -0.187254 0.961662
 N 0.825415 0.272425 0.355011
 O 1.349352 0.944184 -1.747138
 O 2.912416 -1.026335 2.995294
 H 3.385431 1.692835 0.009561
 H 4.816424 -1.738167 1.175218
 O -2.722679 2.928090 0.314780
 O -6.457751 0.716864 -1.815782
 O -4.443321 -2.710952 -2.670181
 O -0.302082 -0.642453 -3.236846
 O -6.142124 -1.417005 -1.155044
 N -3.318338 0.363779 2.162514
 N -1.806020 0.595813 3.773848
 H 7.828783 3.849725 -0.864144
 H 8.032341 3.975925 1.596982
 H 7.031041 2.223903 3.037168
 H 6.632491 1.962233 -1.917351
 H 5.325982 0.078041 2.902475
 H 3.716160 -0.768080 -1.733266
 H 4.358285 0.847726 -2.017615
 H -0.149482 0.415872 0.125306
 H 4.658193 -2.603852 -1.953470
 H 5.901585 -0.792370 -3.144308
 H 7.375872 -0.100797 -2.449044
 H 7.332822 -1.796309 -2.924725
 H 8.147985 -2.445876 -0.665840
 H 7.299932 -1.963899 0.806467
 H 8.153296 -0.758988 -0.152977
 H 4.988902 -4.676078 -0.827780
 H 6.416103 -4.003917 0.121356
 H 0.646547 -0.425144 3.644039
 H -7.509856 -3.697492 -0.797154
 H -8.099985 -2.812559 -2.218380
 H -9.107966 -2.941938 -0.774748
 H -5.272226 -2.611047 -2.171168
 H 0.242869 0.067559 -2.832659
 H -1.492506 1.580298 -2.393278
 H -2.010931 -2.575459 -3.308358
 H -8.066033 -0.681233 -0.920229
 H -8.304785 -1.953044 1.324108
 H -6.590381 -2.256335 1.225242
 H -7.319712 0.637431 0.916222
 H -7.887384 -0.048557 2.402178
 H -4.799490 2.587992 1.714180

H -5.764190 1.938188 0.379696
 H -4.979543 2.342199 -1.848905
 H -3.329896 2.941835 -2.095340
 H -5.896647 0.795573 3.098498
 H -5.487959 -0.887061 2.837505
 H -4.496840 -0.248650 0.604404
 H -2.064550 -0.475692 0.650836
 H -3.829891 1.143623 4.097745

1c-c10, $\Delta G = 0.5591$ kcal/mol,
 population = 22.23 %

C 1.689128 0.680004 -0.534928
 C 3.149968 0.666610 -0.153109
 C 4.083876 -0.031683 -1.143446
 C 5.340032 -0.358861 -0.298987
 C 6.201140 0.892553 -0.100190
 C 6.765945 1.756655 -1.025209
 C 7.499120 2.862373 -0.582996
 C 7.648225 3.099506 0.781159
 C 7.065943 2.254928 1.725424
 C 6.337790 1.160084 1.269326
 C 4.791614 -0.563449 1.163738
 C 2.533378 -0.235833 2.106696
 C 1.113909 0.113192 1.798416
 C 6.140843 -1.620230 -0.842238
 C 6.643084 -1.314572 -2.241449
 C 6.283138 -1.898755 -3.379701
 C 7.382455 -1.884911 0.039629
 C 5.271966 -2.890161 -0.828382
 C 0.196919 0.072680 2.781833
 C -1.229632 0.307379 2.713043
 C -3.143165 0.946445 3.457272
 C -2.146524 0.079552 1.705539
 C -4.630691 0.513356 1.432252
 C -5.809938 0.114432 2.339312
 C -7.150529 -0.174115 1.636774
 C -7.337126 -1.591981 1.039163
 C -7.444725 -1.688918 -0.482320
 C -5.710178 -0.413500 -1.687359
 C -4.283093 -0.475052 -2.083014
 C -3.675599 -1.708561 -2.444229
 C -2.340807 -1.767179 -2.819562
 C -1.559470 -0.621064 -2.785428
 C -2.133336 0.604933 -2.423794

C -3.477789 0.692656 -2.091740
 C -3.987046 2.069076 -1.687416
 C -3.787136 2.351988 -0.193729
 C -4.858180 1.909284 0.795479
 C -7.989852 -3.024280 -0.959736
 N 5.689804 0.186909 2.022695
 N 3.415931 -0.037621 1.099397
 N 0.805438 0.423081 0.456942
 O 1.333448 0.966557 -1.679167
 O 2.873543 -0.718079 3.186406
 H 3.435434 1.723083 -0.057533
 H 4.732367 -1.593966 1.500458
 O -2.800878 2.944226 0.192259
 O -6.465891 0.519905 -1.846889
 O -4.342495 -2.888799 -2.474175
 O -0.254665 -0.737016 -3.111727
 O -6.092971 -1.558216 -1.051312
 N -3.364930 0.488413 2.188875
 N -1.886952 0.837131 3.811321
 H 7.943558 3.537413 -1.303169
 H 8.214593 3.959504 1.118143
 H 7.168288 2.452020 2.785547
 H 6.637667 1.593368 -2.087854
 H 5.362459 0.398708 2.953719
 H 3.605736 -0.938496 -1.510928
 H 4.312946 0.597399 -1.999117
 H -0.164991 0.595760 0.226049
 H 7.406222 -0.543591 -2.283690
 H 8.054838 -1.026753 0.054048
 H 7.099969 -2.111829 1.068603
 H 7.935036 -2.739816 -0.354328
 H 4.384739 -2.814331 -1.456053
 H 4.947577 -3.142754 0.181057
 H 5.858707 -3.732937 -1.197095
 H 6.733807 -1.602502 -4.319511
 H 5.540615 -2.685329 -3.430030
 H 0.591270 -0.129635 3.769479
 H -7.393388 -3.854318 -0.574783
 H -7.998436 -3.072762 -2.049472
 H -9.014784 -3.150107 -0.607875
 H -5.179753 -2.784175 -1.990342
 H 0.264679 0.010030 -2.743231
 H -1.518510 1.495692 -2.412996
 H -1.906495 -2.719172 -3.092084

H -8.040955 -0.869564 -0.880531
 H -8.262933 -2.014204 1.436321
 H -6.538234 -2.262443 1.368925
 H -7.351318 0.579161 0.872193
 H -7.926973 -0.027246 2.389364
 H -4.882402 2.649179 1.597705
 H -5.826453 1.905017 0.298116
 H -5.034974 2.183633 -1.947023
 H -3.402716 2.818542 -2.218723
 H -5.972278 0.919822 3.060114
 H -5.512052 -0.764007 2.917599
 H -4.510966 -0.238054 0.653293
 H -2.061406 -0.380795 0.735801
 H -3.930920 1.339060 4.078249

1c-c16, $\Delta G = 1.2657$ kcal/mol,
 population = 6.74 %

C 1.636163 0.545121 -0.599433
 C 3.092510 0.591941 -0.203787
 C 4.065962 -0.056433 -1.188323
 C 5.330333 -0.329114 -0.333071
 C 6.129422 0.957494 -0.117565
 C 6.693879 1.827458 -1.035707
 C 7.373471 2.963029 -0.582682
 C 7.473598 3.217424 0.782970
 C 6.901072 2.357105 1.719683
 C 6.228047 1.231861 1.253321
 C 4.773849 -0.569847 1.121810
 C 2.493981 -0.337488 2.047029
 C 1.068363 -0.014895 1.735395
 C 6.214792 -1.531324 -0.874175
 C 6.587649 -1.255290 -2.319480
 C 7.806896 -1.152081 -2.836621
 C 7.455109 -1.722116 0.012089
 C 5.421000 -2.861644 -0.878097
 C 0.156389 -0.045246 2.723038
 C -1.267995 0.207538 2.669719
 C -3.148155 0.908399 3.442140
 C -2.209759 -0.006415 1.682244
 C -4.685231 0.516037 1.440245
 C -5.858837 0.211550 2.388234
 C -7.292893 0.300468 1.839571
 C -7.747454 -0.681459 0.738285
 C -7.682809 -0.159119 -0.700488

C -5.658431 -1.257218 -1.548732
 C -4.256799 -1.094902 -1.970401
 C -3.555109 -2.295212 -2.319054
 C -2.211545 -2.273621 -2.670911
 C -1.518567 -1.075706 -2.677527
 C -2.186550 0.120069 -2.369797
 C -3.531665 0.132790 -2.033732
 C -4.116995 1.521366 -1.787173
 C -3.803710 2.084195 -0.391075
 C -4.810088 1.886256 0.731171
 C -8.655813 -0.829506 -1.662201
 N 5.617611 0.225234 1.995059
 N 3.374137 -0.114410 1.043238
 N 0.755071 0.273389 0.390345
 O 1.279084 0.795950 -1.751867
 O 2.841538 -0.810686 3.128156
 H 3.331959 1.658680 -0.094686
 H 4.764818 -1.604012 1.453182
 O -2.775079 2.698494 -0.199263
 O -6.213611 -2.356896 -1.481278
 O -4.141569 -3.504295 -2.316359
 O -0.211972 -1.102276 -3.007744
 O -6.296657 -0.135092 -1.206460
 N -3.408866 0.441668 2.183061
 N -1.889815 0.767238 3.773552
 H 7.817374 3.646119 -1.295675
 H 7.997677 4.100969 1.127583
 H 6.972577 2.563521 2.780626
 H 6.615329 1.635412 -2.097667
 H 5.269222 0.413158 2.923396
 H 3.629964 -0.982045 -1.562974
 H 4.270478 0.591722 -2.036458
 H -0.219559 0.403321 0.150064
 H 5.740359 -1.177995 -2.997020
 H 8.079166 -0.829226 0.039882
 H 7.167829 -1.962254 1.036214
 H 8.059909 -2.548787 -0.363928
 H 4.552495 -2.831073 -1.536523
 H 5.082755 -3.140631 0.120791
 H 6.070626 -3.661094 -1.237946
 H 7.945633 -0.986488 -3.898425
 H 8.706148 -1.222342 -2.237708
 H 0.557623 -0.236815 3.710124
 H -8.609770 -1.913788 -1.610766

H -8.457662 -0.516551 -2.688645
 H -9.666256 -0.505399 -1.404701
 H -5.074925 -3.373615 -2.010549
 H 0.247177 -0.288499 -2.704390
 H -1.644454 1.055040 -2.429195
 H -1.713576 -3.201077 -2.917504
 H -7.906869 0.908399 -0.692231
 H -8.801087 -0.908847 0.918211
 H -7.222976 -1.636255 0.811406
 H -7.509989 1.324972 1.523009
 H -7.934640 0.133688 2.707944
 H -4.662203 2.682099 1.462670
 H -5.813412 1.971793 0.319130
 H -5.185362 1.536424 -1.962756
 H -3.636126 2.204449 -2.486668
 H -5.813358 0.903365 3.231881
 H -5.692263 -0.787956 2.799654
 H -4.627788 -0.270669 0.692729
 H -2.154756 -0.475627 0.714540
 H -3.907078 1.333021 4.076567

1c-c23, $\Delta G = 1.4232$ kcal/mol,
 population = 5.16 %

C 1.595359 0.822760 -0.307308
 C 3.067455 0.742531 0.020011
 C 3.944282 0.053322 -1.026710
 C 5.219566 -0.337587 -0.240150
 C 6.127193 0.874974 -0.017965
 C 6.686237 1.764124 -0.922527
 C 7.468736 2.825978 -0.457860
 C 7.673366 2.995041 0.909181
 C 7.097667 2.125573 1.834923
 C 6.319475 1.075726 1.356614
 C 4.712030 -0.588258 1.230247
 C 2.500904 -0.226969 2.265181
 C 1.082045 0.170869 2.019865
 C 5.960268 -1.594650 -0.868340
 C 5.031679 -2.797212 -0.852297
 C 4.548978 -3.466078 -1.894703
 C 6.431383 -1.274695 -2.295263
 C 7.200002 -1.966192 -0.024309
 C 0.195169 0.105450 3.030041
 C -1.226964 0.368760 3.000870
 C -3.127082 0.996513 3.790896

C -2.150178 0.223514 1.984875
 C -4.599471 0.769868 1.719921
 C -5.864164 0.481828 2.542747
 C -7.033734 0.041487 1.644755
 C -6.912103 -1.423808 1.170264
 C -6.986830 -1.691918 -0.329894
 C -5.619639 -1.042436 -2.246913
 C -4.285574 -0.558962 -2.665308
 C -3.598108 -1.372572 -3.601111
 C -2.241832 -1.188795 -3.838140
 C -1.566772 -0.157560 -3.197936
 C -2.268986 0.756684 -2.398200
 C -3.615316 0.565014 -2.129964
 C -4.407282 1.660682 -1.432953
 C -3.804224 2.267722 -0.166660
 C -4.655336 2.183896 1.081965
 C -6.948307 -3.189902 -0.607403
 N 5.664926 0.090904 2.089098
 N 3.354412 -0.014046 1.236527
 N 0.738296 0.547239 0.704544
 O 1.209570 1.182965 -1.418551
 O 2.862860 -0.760903 3.313219
 H 3.392856 1.784463 0.142944
 H 4.626696 -1.629376 1.526441
 O -2.714987 2.802674 -0.164005
 O -6.422512 -1.544114 -3.023993
 O -4.204347 -2.391844 -4.256804
 O -0.239105 -0.039085 -3.422988
 O -5.815145 -1.010503 -0.917888
 N -3.358856 0.624203 2.497105
 N -1.871563 0.839823 4.133512
 H 7.908071 3.520266 -1.162694
 H 8.278063 3.821195 1.263767
 H 7.242689 2.270712 2.898578
 H 6.514276 1.656290 -1.985886
 H 5.374451 0.272631 3.038470
 H 3.437878 -0.836382 -1.401874
 H 4.155151 0.709845 -1.867017
 H -0.231863 0.763900 0.513735
 H 4.771864 -3.163529 0.137484
 H 7.167535 -0.472710 -2.286085
 H 6.910434 -2.152177 -2.732267
 H 5.612443 -0.980440 -2.953309
 H 7.712023 -2.815558 -0.480301

H 6.933679 -2.244832 0.996003
 H 7.901792 -1.132451 0.024629
 H 3.914831 -4.332480 -1.749170
 H 4.758956 -3.190868 -2.920719
 H 0.611321 -0.150911 3.995760
 H -7.786600 -3.665273 -0.095059
 H -6.024046 -3.623672 -0.219758
 H -7.028087 -3.411371 -1.667671
 H -5.167661 -2.320718 -4.108072
 H 0.182996 0.537589 -2.752971
 H -1.762702 1.632054 -2.015802
 H -1.719088 -1.854885 -4.510811
 H -7.876944 -1.240491 -0.772614
 H -7.705034 -2.017487 1.629267
 H -5.974417 -1.857971 1.529431
 H -7.116970 0.713049 0.786144
 H -7.962378 0.165103 2.203901
 H -4.316417 2.923639 1.807055
 H -5.690220 2.406318 0.816059
 H -5.420185 1.327451 -1.231396
 H -4.488305 2.496747 -2.137330
 H -6.142799 1.370643 3.114245
 H -5.654011 -0.308817 3.266876
 H -4.536415 0.018492 0.932718
 H -2.077113 -0.181060 0.989803
 H -3.908718 1.365561 4.434769

1c-c22, $\Delta G = 1.5104$ kcal/mol,
 population = 4.45 %

C 1.597224 0.881294 -0.307251
 C 3.071147 0.778999 0.006482
 C 3.937045 0.138848 -1.080424
 C 5.214448 -0.301034 -0.319787
 C 6.128161 0.896635 -0.052565
 C 6.692510 1.815343 -0.923116
 C 7.487667 2.849533 -0.418707
 C 7.698977 2.960070 0.953332
 C 7.120013 2.058085 1.845611
 C 6.329603 1.035933 1.328722
 C 4.716314 -0.617499 1.137378
 C 2.517174 -0.281686 2.211271
 C 1.099480 0.138612 1.995736
 C 5.955509 -1.541077 -0.982767
 C 5.013160 -2.732483 -1.037752

C 5.127591 -3.886884 -0.388565
 C 6.345051 -1.212946 -2.440856
 C 7.237795 -1.875873 -0.204495
 C 0.220422 0.039137 3.009786
 C -1.200923 0.309462 2.999617
 C -3.094665 0.916736 3.820046
 C -2.130979 0.194599 1.986161
 C -4.581957 0.746896 1.753813
 C -5.840849 0.431448 2.575465
 C -7.012034 0.008655 1.671191
 C -6.884037 -1.442635 1.156771
 C -6.963848 -1.670811 -0.349708
 C -5.609710 -0.962694 -2.255227
 C -4.280993 -0.459280 -2.667513
 C -3.593526 -1.242602 -3.628872
 C -2.240017 -1.042825 -3.869011
 C -1.568526 -0.024077 -3.205587
 C -2.272155 0.863318 -2.377662
 C -3.615374 0.654696 -2.106262
 C -4.409397 1.724984 -1.373258
 C -3.801407 2.298597 -0.093610
 C -4.646121 2.177930 1.156252
 C -6.918377 -3.160613 -0.667414
 N 5.674240 0.023254 2.020995
 N 3.360284 -0.040902 1.180404
 N 0.746819 0.569877 0.699466
 O 1.205159 1.286460 -1.400843
 O 2.884465 -0.855919 3.235636
 H 3.403471 1.811587 0.179493
 H 4.635079 -1.676669 1.366139
 O -2.713239 2.835529 -0.081284
 O -6.413280 -1.448651 -3.041492
 O -4.196476 -2.248327 -4.308043
 O -0.242778 0.110085 -3.434762
 O -5.798750 -0.967309 -0.924917
 N -3.335697 0.581794 2.517796
 N -1.836959 0.748763 4.149541
 H 7.931273 3.568013 -1.096084
 H 8.312708 3.765449 1.338874
 H 7.272615 2.157617 2.913442
 H 6.515840 1.751625 -1.989474
 H 5.390936 0.162044 2.979641
 H 3.407292 -0.714320 -1.501739
 H 4.151025 0.836489 -1.886043

H -0.223757 0.799423 0.526140
 H 4.174169 -2.624792 -1.719949
 H 7.049184 -0.382333 -2.484769
 H 6.827584 -2.081489 -2.892761
 H 5.475308 -0.963273 -3.051193
 H 7.040487 -2.129469 0.837329
 H 7.923441 -1.028823 -0.215424
 H 7.744428 -2.723429 -0.669054
 H 4.398852 -4.675790 -0.531956
 H 5.936690 -4.098424 0.299310
 H 0.642277 -0.257805 3.961334
 H -7.751265 -3.654378 -0.163727
 H -5.989681 -3.599350 -0.296257
 H -7.002376 -3.354131 -1.732794
 H -5.159408 -2.187985 -4.152202
 H 0.177989 0.673534 -2.752847
 H -1.769616 1.731383 -1.974351
 H -1.716935 -1.686867 -4.562577
 H -7.858484 -1.212645 -0.776060
 H -7.671910 -2.052817 1.602609
 H -5.942649 -1.881254 1.500534
 H -7.102719 0.702798 0.831503
 H -7.938880 0.111708 2.237423
 H -4.306078 2.898689 1.899681
 H -5.683177 2.403716 0.901634
 H -5.419145 1.380289 -1.175006
 H -4.499656 2.580689 -2.052488
 H -6.121065 1.303813 3.171037
 H -5.623406 -0.376631 3.277838
 H -4.522344 0.018647 0.944928
 H -2.064571 -0.181768 0.979613
 H -3.871311 1.268288 4.479568

1c-c11, $\Delta G = 1.7614$ kcal/mol,
 population = 2.91 %

C 1.665612 0.617323 -0.608846
 C 3.119061 0.687613 -0.203959
 C 4.116421 0.129539 -1.219792
 C 5.377669 -0.175511 -0.374764
 C 6.153281 1.104937 -0.054492
 C 6.672394 2.080379 -0.891293
 C 7.321702 3.190871 -0.342612
 C 7.433969 3.320110 1.039434
 C 6.895809 2.361221 1.896876

C 6.250209 1.263777 1.335490
 C 4.816495 -0.533370 1.053045
 C 2.539459 -0.365431 1.995370
 C 1.109854 -0.044011 1.701639
 C 6.267436 -1.331448 -1.003982
 C 5.454399 -2.612227 -1.092401
 C 5.104842 -3.280184 -2.187150
 C 6.789063 -0.907693 -2.385557
 C 7.483749 -1.628133 -0.098721
 C 0.202539 -0.113809 2.691363
 C -1.224014 0.130100 2.649000
 C -3.108115 0.800457 3.438494
 C -2.166440 -0.075003 1.660742
 C -4.647350 0.425031 1.435002
 C -5.811825 0.063295 2.374345
 C -7.250364 0.148775 1.836152
 C -7.694168 -0.789965 0.693769
 C -7.640608 -0.204273 -0.720817
 C -5.610019 -1.245218 -1.625994
 C -4.211412 -1.049999 -2.043125
 C -3.495893 -2.227113 -2.439504
 C -2.152339 -2.175808 -2.788191
 C -1.473000 -0.970625 -2.744063
 C -2.155041 0.203852 -2.388860
 C -3.500977 0.187720 -2.056373
 C -4.103524 1.558882 -1.759159
 C -3.800035 2.071829 -0.342141
 C -4.802700 1.814440 0.771527
 C -8.612574 -0.839780 -1.707052
 N 5.655001 0.190856 1.990733
 N 3.414674 -0.080851 1.003244
 N 0.789713 0.284555 0.367347
 O 1.303826 0.903140 -1.751513
 O 2.894586 -0.889092 3.050714
 H 3.323231 1.753255 -0.030758
 H 4.811131 -1.590089 1.302961
 O -2.781500 2.695060 -0.126477
 O -6.154480 -2.352177 -1.606805
 O -4.069111 -3.441660 -2.486645
 O -0.165908 -0.968867 -3.072373
 O -6.257239 -0.145979 -1.230815
 N -3.368118 0.352885 2.172459
 N -1.847363 0.664992 3.764088
 H 7.729472 3.952968 -0.994367

H 7.935526 4.183845 1.459302
 H 6.967688 2.473922 2.971729
 H 6.569931 2.001535 -1.966138
 H 5.300033 0.300833 2.929267
 H 3.718884 -0.785211 -1.659902
 H 4.311067 0.839653 -2.019419
 H -0.187476 0.399334 0.130166
 H 5.164262 -3.038495 -0.135665
 H 7.448247 -0.045497 -2.300494
 H 7.369418 -1.719415 -2.826929
 H 5.985502 -0.657107 -3.079778
 H 8.100743 -0.737699 0.029824
 H 8.098662 -2.405791 -0.555431
 H 7.182686 -1.976714 0.889908
 H 4.544272 -4.204519 -2.114446
 H 5.355734 -2.947367 -3.186573
 H 0.609200 -0.335655 3.669865
 H -8.420695 -0.481130 -2.719619
 H -9.624398 -0.534768 -1.432053
 H -8.558767 -1.924972 -1.703021
 H -5.003956 -3.333551 -2.176624
 H 0.283911 -0.162065 -2.737558
 H -1.623238 1.146435 -2.408140
 H -1.643216 -3.086303 -3.072335
 H -7.873738 0.859848 -0.664476
 H -8.743991 -1.039397 0.866392
 H -7.156889 -1.739978 0.723348
 H -7.489091 1.182581 1.569029
 H -7.883586 -0.070013 2.699301
 H -4.672764 2.588990 1.528720
 H -5.807705 1.890506 0.362399
 H -5.171574 1.568530 -1.937571
 H -3.628654 2.273261 -2.430945
 H -5.774391 0.721770 3.244739
 H -5.625760 -0.948384 2.745497
 H -4.574360 -0.335289 0.661723
 H -2.109719 -0.527217 0.685151
 H -3.868954 1.208488 4.081569

1c-c19, $\Delta G = 2.7039$ kcal/mol,
 population = 0.59 %

C 1.766529 -0.199510 -0.849340
 C 3.235495 0.051385 -0.608485
 C 4.087290 -1.195834 -0.367296

C 5.351428 -0.650723 0.340435	O -4.538312 -3.217994 1.254010
C 6.303124 0.015273 -0.656446	O -0.371993 -3.027237 -0.831529
C 6.893111 -0.476462 -1.810575	O -6.146783 -1.228338 0.701666
C 7.715558 0.355117 -2.577246	N -3.212302 2.322578 0.368541
C 7.929674 1.674829 -2.187641	N -1.730349 3.864302 0.971674
C 7.324476 2.193743 -1.043827	H 8.179199 -0.027166 -3.477650
C 6.506640 1.354403 -0.293177	H 8.565886 2.315385 -2.786677
C 4.841732 0.610219 1.137031	H 7.478092 3.225761 -0.753079
C 2.638312 1.719933 1.173359	H 6.716119 -1.493852 -2.135488
C 1.229507 1.664806 0.681474	H 5.543381 2.600550 1.080466
C 6.043143 -1.738824 1.269670	H 3.550729 -1.883916 0.286509
C 5.069938 -2.182687 2.348985	H 4.316462 -1.709986 -1.297169
C 4.558172 -3.395610 2.532999	H -0.059512 0.556893 -0.520896
C 6.518860 -2.930809 0.425899	H 4.800790 -1.413634 3.068178
C 7.270198 -1.133278 1.987041	H 6.959838 -3.690421 1.073214
C 0.329749 2.550120 1.148871	H 5.707716 -3.400042 -0.132790
C -1.086687 2.640795 0.872255	H 7.286322 -2.620389 -0.281177
C -2.980150 3.639797 0.649616	H 8.000065 -0.761032 1.266860
C -2.007913 1.678867 0.506257	H 7.753160 -1.899708 2.596029
C -4.448669 1.702176 -0.139937	H 6.993599 -0.309027 2.645805
C -5.694349 2.114026 0.667324	H 3.892167 -3.594063 3.364267
C -5.822721 1.354963 2.010735	H 4.775273 -4.231849 1.880192
C -7.078245 0.474779 2.163706	H 0.731626 3.317093 1.798278
C -7.386079 -0.506410 1.030776	H -8.669200 -2.177767 0.545177
C -5.738225 -1.288241 -0.602544	H -9.385989 -0.995779 1.645802
C -4.346319 -1.783560 -0.717149	H -8.161287 -2.121569 2.245317
C -3.813834 -2.695688 0.233837	H -5.350871 -2.694845 1.364950
C -2.497515 -3.128766 0.153730	H 0.198573 -2.387072 -1.308803
C -1.659144 -2.620390 -0.827822	H -1.503133 -1.343732 -2.550303
C -2.160664 -1.718018 -1.775979	H -2.120215 -3.823274 0.891571
C -3.486284 -1.308707 -1.744209	H -7.674719 0.026873 0.128079
C -3.910472 -0.317525 -2.823898	H -7.964643 1.109617 2.261418
C -3.594233 1.148971 -2.486326	H -6.992949 -0.078941 3.103289
C -4.601501 1.941503 -1.663525	H -5.820374 2.062892 2.841231
C -8.462193 -1.516796 1.387455	H -4.939845 0.728934 2.157713
N 5.819867 1.650970 0.879083	H -4.475062 3.001029 -1.888219
N 3.502259 0.864897 0.576028	H -5.607375 1.636465 -1.951908
N 0.903072 0.629586 -0.218540	H -4.969598 -0.418165 -3.039515
O 1.388627 -1.076545 -1.627591	H -3.342026 -0.542451 -3.725177
O 2.984325 2.455542 2.097082	H -6.564724 1.916955 0.040990
H 3.590808 0.573076 -1.507587	H -5.694734 3.192612 0.829632
H 4.724301 0.472661 2.207592	H -4.295634 0.639832 0.025824
O -2.571827 1.665133 -2.886489	H -1.941928 0.610075 0.392967
O -6.443568 -0.908696 -1.511455	H -3.754510 4.387713 0.607167

1c-c18, $\Delta G = 2.7454$ kcal/mol,
population = 0.55 %

C 1.624417 0.598070 -0.623755
C 3.080400 0.616012 -0.221665
C 4.064291 0.097611 -1.270893
C 5.323226 -0.270145 -0.445816
C 6.103221 0.986249 -0.048248
C 6.627821 2.006734 -0.824693
C 7.288265 3.075309 -0.209975
C 7.406339 3.116541 1.176887
C 6.863931 2.109666 1.974697
C 6.207576 1.055336 1.347960
C 4.757529 -0.706646 0.957373
C 2.487277 -0.537891 1.921116
C 1.065220 -0.162903 1.654918
C 6.224600 -1.382414 -1.134141
C 7.397247 -1.705840 -0.225388
C 8.690991 -1.595296 -0.504810
C 5.439900 -2.703027 -1.333622
C 6.689871 -0.905136 -2.518350
C 0.162424 -0.258161 2.646599
C -1.257244 0.025214 2.627625
C -3.117364 0.702921 3.466066
C -2.211394 -0.103596 1.637669
C -4.679955 0.469595 1.458417
C -5.848618 0.110872 2.393184
C -7.285303 0.245219 1.860606
C -7.752224 -0.659516 0.699942
C -7.693744 -0.044807 -0.702004
C -5.678534 -1.090456 -1.635662
C -4.280023 -0.903724 -2.058370
C -3.586275 -2.079040 -2.496673
C -2.246162 -2.037248 -2.859826
C -1.548699 -0.843987 -2.789638
C -2.208771 0.329330 -2.392075
C -3.550727 0.323025 -2.043228
C -4.127724 1.692917 -1.694490
C -3.798550 2.155338 -0.265487
C -4.797430 1.887354 0.848754
C -8.674805 -0.648653 -1.699052
N 5.606419 -0.053710 1.936476
N 3.362820 -0.227916 0.936943
N 0.745612 0.240459 0.340915

O 1.265302 0.944006 -1.750476
O 2.834826 -1.123235 2.946031
H 3.307787 1.665249 0.011849
H 4.735270 -1.777275 1.139096
O -2.763621 2.747455 -0.040647
O -6.236205 -2.190915 -1.636269
O -4.177304 -3.283525 -2.572381
O -0.245232 -0.851388 -3.133592
O -6.310688 0.008027 -1.214508
N -3.397711 0.329003 2.180628
N -1.858542 0.517719 3.773893
H 7.700332 3.873517 -0.814123
H 7.916435 3.948227 1.648098
H 6.941626 2.153540 3.054179
H 6.521141 1.996103 -1.901988
H 5.252168 0.001442 2.880140
H 3.637687 -0.776889 -1.760605
H 4.269391 0.846400 -2.031441
H -0.229896 0.389058 0.116130
H 7.118753 -2.093729 0.750834
H 4.590183 -2.577909 -2.005961
H 6.103231 -3.444190 -1.782026
H 5.074105 -3.122609 -0.395850
H 5.837632 -0.681803 -3.161720
H 7.270077 -1.689513 -3.007115
H 7.316886 -0.016988 -2.460876
H 9.440051 -1.883100 0.223161
H 9.058777 -1.215890 -1.449869
H 0.568685 -0.539857 3.609771
H -8.481001 -0.271635 -2.704569
H -9.682512 -0.337887 -1.415654
H -8.632994 -1.734203 -1.717104
H -5.106693 -3.171805 -2.247678
H 0.219800 -0.062862 -2.777240
H -1.663279 1.264232 -2.390005
H -1.754265 -2.946799 -3.175571
H -7.914032 1.020559 -0.623140
H -8.806092 -0.892433 0.871263
H -7.233064 -1.619991 0.706709
H -7.497317 1.289739 1.613598
H -7.923300 0.025677 2.719953
H -4.637249 2.628711 1.633012
H -5.803354 2.009745 0.452483
H -5.197514 1.724093 -1.858640

H -3.650198 2.421377 -2.349069
H -5.792475 0.744889 3.280614
H -5.686566 -0.914912 2.735984
H -4.637520 -0.262803 0.656742
H -2.173584 -0.506459 0.639712
H -3.862773 1.096178 4.135766

1c-c21, $\Delta G = 3.3842$ kcal/mol,
population = 0.19 %

C 1.715393 0.441410 -0.487075
C 3.179825 0.524919 -0.128501
C 4.141192 -0.207086 -1.065389
C 5.421662 -0.390458 -0.209542
C 6.213383 0.916362 -0.129398
C 6.748547 1.704630 -1.134876
C 7.419412 2.886008 -0.801983
C 7.541029 3.266824 0.532171
C 6.998129 2.489731 1.555275
C 6.332176 1.318428 1.208047
C 4.891687 -0.496747 1.270692
C 2.631323 -0.183688 2.216047
C 1.197109 0.085682 1.902656
C 6.306138 -1.634571 -0.646539
C 6.670460 -1.489671 -2.112973
C 7.887099 -1.428186 -2.642710
C 7.552260 -1.739735 0.245995
C 5.516845 -2.961552 -0.523693
C 0.290587 0.103751 2.897244
C -1.140698 0.289408 2.811229
C -3.082049 0.913098 3.496643
C -2.035120 0.006424 1.796637
C -4.507828 0.405902 1.441496
C -5.712000 -0.178440 2.228124
C -6.465429 -1.317375 1.498469
C -7.730703 -0.985426 0.688697
C -7.643073 0.111101 -0.374766
C -5.899794 -0.888655 -1.798187
C -4.487165 -0.790761 -2.201609
C -3.886380 -1.984829 -2.710441
C -2.521351 -2.057348 -2.957972
C -1.717367 -0.952197 -2.728810
C -2.294115 0.255037 -2.302705
C -3.652558 0.353913 -2.043844
C -4.145796 1.754077 -1.680992

C -3.802500 2.188648 -0.248641
C -4.755609 1.829552 0.880444
C -8.809300 0.117691 -1.351297
N 5.744656 0.380329 2.051610
N 3.488238 -0.057614 1.175108
N 0.858662 0.260228 0.544311
O 1.329567 0.594894 -1.646797
O 3.006762 -0.543018 3.331393
H 3.416608 1.597882 -0.125829
H 4.895072 -1.495382 1.697526
O -2.788558 2.818890 -0.028736
O -6.614936 -1.858163 -2.059013
O -4.595446 -3.102536 -2.949975
O -0.396030 -1.077098 -2.961796
O -6.338566 0.130019 -1.056540
N -3.268737 0.405751 2.242232
N -1.830096 0.843953 3.877574
H 7.839606 3.506139 -1.583583
H 8.058272 4.185181 0.783452
H 7.085223 2.794594 2.591040
H 6.652272 1.414352 -2.173020
H 5.406663 0.653655 2.962518
H 3.707587 -1.166039 -1.346562
H 4.326717 0.361611 -1.972802
H -0.119075 0.386553 0.318473
H 5.820304 -1.476393 -2.791131
H 8.181400 -0.852536 0.176837
H 7.271542 -1.868128 1.291636
H 8.150609 -2.604651 -0.044840
H 4.646800 -2.996354 -1.179698
H 5.181535 -3.146944 0.497731
H 6.168606 -3.788863 -0.808819
H 8.020809 -1.357693 -3.715675
H 8.788941 -1.439855 -2.043746
H 0.695627 0.000805 3.895599
H -8.905294 -0.834673 -1.867812
H -8.689462 0.913508 -2.087985
H -9.729965 0.310269 -0.796378
H -5.537486 -2.906107 -2.720129
H 0.120071 -0.338323 -2.570708
H -1.668213 1.133664 -2.207847
H -2.094885 -2.983558 -3.317643
H -7.615558 1.079735 0.124665
H -8.523113 -0.668540 1.374349

H -8.076077 -1.910418 0.223377
H -6.779205 -2.043675 2.251505
H -5.757848 -1.856817 0.863038
H -4.628291 2.558348 1.681585
H -5.776846 1.887461 0.516869
H -5.213153 1.849918 -1.846100
H -3.627121 2.458553 -2.330715
H -6.399559 0.620917 2.516792
H -5.324086 -0.592538 3.158759
H -4.295590 -0.266018 0.613561
H -1.930036 -0.490217 0.847096
H -3.891929 1.313042 4.085326

1d-c19, $\Delta G = 0.0000$ kcal/mol,
population = 27.07 %

C -1.478675 -0.112262 -0.920329
C -2.955470 -0.141545 -0.603995
C -3.590250 1.207339 -0.261491
C -4.896136 0.822593 0.482887
C -5.975182 0.378924 -0.506566
C -6.546992 1.053495 -1.572666
C -7.518347 0.416105 -2.351538
C -7.900036 -0.890865 -2.058454
C -7.325471 -1.587599 -0.995501
C -6.360143 -0.940163 -0.230394
C -4.559702 -0.550599 1.179823
C -2.554338 -1.984885 1.047356
C -1.176160 -2.120563 0.483210
C -5.397739 1.933338 1.499916
C -5.579733 3.241672 0.751285
C -6.689621 3.963062 0.639995
C -6.695788 1.478993 2.184492
C -4.345155 2.208726 2.602902
C -0.423175 -3.175156 0.845396
C 0.957474 -3.435142 0.489238
C 2.658601 -4.590700 -0.123031
C 2.008336 -2.553716 0.363143
C 4.422700 -2.812729 -0.427119
C 5.038467 -1.920494 0.660502
C 6.566463 -1.804745 0.544303
C 7.163521 -0.700577 1.435826
C 7.323270 0.669835 0.774589
C 5.616730 2.266647 0.131907

C 4.273404 2.483592 -0.430664
C 3.597237 3.663133 0.006659
C 2.253636 3.873087 -0.280731
C 1.565660 2.945545 -1.044219
C 2.240755 1.847980 -1.596638
C 3.568008 1.594177 -1.295079
C 4.242936 0.436952 -2.018911
C 3.540337 -0.923649 -1.971305
C 4.401504 -2.175965 -1.847112
C 8.411232 0.741216 -0.286265
N -5.684926 -1.419884 0.887718
N -3.289548 -0.960754 0.556471
N -0.721764 -1.091592 -0.371562
O -1.013763 0.725416 -1.693182
O -2.975276 -2.721717 1.938396
H -3.433978 -0.553489 -1.502975
H -4.397880 -0.502076 2.252731
O 2.336754 -1.034475 -2.087601
O 6.298349 3.170613 0.619469
O 4.200758 4.610029 0.753078
O 0.248490 3.151445 -1.268978
O 6.029022 0.994009 0.160885
N 3.090053 -3.295948 -0.039787
N 1.395866 -4.717609 0.201124
H -7.969236 0.938967 -3.185414
H -8.650324 -1.380675 -2.667727
H -7.618334 -2.607090 -0.776102
H -6.250133 2.067623 -1.805971
H -5.543697 -2.411205 1.013582
H -2.913413 1.767822 0.382659
H -3.779938 1.799284 -1.153076
H 0.229580 -1.148610 -0.723459
H -4.672223 3.632329 0.296851
H -6.537149 0.558612 2.747438
H -7.036767 2.241438 2.886613
H -7.494397 1.297310 1.465564
H -4.113360 1.314153 3.182794
H -4.743502 2.952286 3.294961
H -3.412480 2.607935 2.203931
H -6.686446 4.904943 0.104319
H -7.635803 3.652735 1.065043
H -0.924576 -3.920039 1.450339
H 8.458740 1.739853 -0.720826
H 8.242678 0.021293 -1.088460

H 9.379111 0.525062 0.169870
 H 5.148950 4.352521 0.843593
 H -0.177121 2.326127 -1.579586
 H 1.705450 1.187294 -2.260681
 H 1.756569 4.750804 0.108928
 H 7.516014 1.420089 1.539370
 H 8.158917 -0.995461 1.776784
 H 6.553656 -0.589412 2.336291
 H 6.860854 -1.634055 -0.493610
 H 7.003907 -2.767373 0.821369
 H 3.996986 -2.915520 -2.539641
 H 5.429345 -1.963705 -2.141104
 H 5.273959 0.323047 -1.714717
 H 4.263544 0.682436 -3.089575
 H 4.793471 -2.354005 1.633177
 H 4.585657 -0.928640 0.638402
 H 5.031557 -3.715155 -0.512186
 H 2.077849 -1.499480 0.558994
 H 3.319399 -5.392031 -0.415437

1d-c21, $\Delta G = 0.2466$ kcal/mol,
 population = 17.85 %

C -1.516301 -0.122069 -0.900238
 C -2.998870 -0.149272 -0.612197
 C -3.634014 1.194681 -0.249351
 C -4.951843 0.797101 0.461908
 C -6.009949 0.369342 -0.560352
 C -6.532626 1.041760 -1.653729
 C -7.486962 0.415119 -2.461514
 C -7.897950 -0.884125 -2.174376
 C -7.363774 -1.584704 -1.093510
 C -6.413931 -0.947889 -0.300472
 C -4.633678 -0.588582 1.139592
 C -2.636312 -2.031293 1.006591
 C -1.248141 -2.160732 0.466762
 C -5.455304 1.891921 1.497902
 C -5.737643 3.181986 0.749298
 C -5.097113 4.341584 0.857795
 C -6.783615 1.440633 2.146827
 C -4.431989 2.118100 2.625071
 C -0.505514 -3.224527 0.823542
 C 0.879998 -3.485692 0.488896
 C 2.585584 -4.645143 -0.103455
 C 1.937322 -2.608461 0.386926

C 4.364545 -2.875834 -0.362568
 C 4.970646 -2.004235 0.747027
 C 6.501376 -1.901644 0.657008
 C 7.094794 -0.817536 1.575164
 C 7.277070 0.561495 0.938151
 C 5.596166 2.182631 0.288990
 C 4.262682 2.418703 -0.288903
 C 3.590561 3.597794 0.155696
 C 2.252442 3.822316 -0.145490
 C 1.566419 2.910455 -0.929461
 C 2.239686 1.814718 -1.488197
 C 3.561178 1.546590 -1.174028
 C 4.238412 0.395902 -1.906567
 C 3.523873 -0.959153 -1.897606
 C 4.372053 -2.220575 -1.774097
 C 8.382866 0.640113 -0.103555
 N -5.764616 -1.443099 0.825667
 N -3.360385 -0.996989 0.520618
 N -0.774388 -1.117196 -0.358829
 O -1.032376 0.728081 -1.647209
 O -3.075935 -2.782553 1.876533
 H -3.461457 -0.536640 -1.530172
 H -4.481039 -0.558928 2.214142
 O 2.322577 -1.058095 -2.044291
 O 6.279584 3.074199 0.796530
 O 4.192186 4.529685 0.922296
 O 0.254300 3.130917 -1.167440
 O 5.995715 0.905762 0.308921
 N 3.021923 -3.353264 -0.003432
 N 1.317083 -4.768111 0.198333
 H -7.898893 0.939209 -3.314435
 H -8.635239 -1.366188 -2.805183
 H -7.672003 -2.601632 -0.883572
 H -6.202626 2.043701 -1.897807
 H -5.633146 -2.437136 0.941222
 H -2.969826 1.740989 0.419079
 H -3.808809 1.811689 -1.126496
 H 0.182315 -1.172243 -0.695716
 H -6.586481 3.131497 0.074136
 H -7.126550 2.204114 2.847484
 H -7.564764 1.292548 1.400705
 H -6.660665 0.507039 2.697981
 H -3.461902 2.460519 2.266469
 H -4.272186 1.212102 3.209401

H -4.811371 2.877911 3.310044
 H -5.410671 5.202033 0.278639
 H -4.249149 4.488940 1.515059
 H -1.021083 -3.978518 1.404774
 H 8.221944 -0.066298 -0.919260
 H 9.341453 0.409451 0.364912
 H 8.445114 1.644777 -0.522006
 H 5.136986 4.263120 1.021463
 H -0.175549 2.314526 -1.495365
 H 1.707893 1.167706 -2.168360
 H 1.757426 4.698826 0.249460
 H 7.463438 1.298182 1.717610
 H 8.082019 -1.127195 1.926608
 H 6.472057 -0.714797 2.467785
 H 6.813988 -1.717694 -0.373287
 H 6.925046 -2.872792 0.925703
 H 3.973336 -2.947693 -2.482904
 H 5.406451 -2.012983 -2.047807
 H 5.262531 0.267216 -1.585450
 H 4.281247 0.661110 -2.971868
 H 4.705983 -2.448908 1.709474
 H 4.527272 -1.007994 0.731531
 H 4.966675 -3.782624 -0.450098
 H 2.009569 -1.556258 0.592527
 H 3.247425 -5.447322 -0.390914

1d-c2, ΔG = 0.3859 kcal/mol,
 population = 14.10 %

C -1.580822 0.031847 -0.827540
 C -3.076221 -0.047990 -0.631446
 C -3.773572 1.271290 -0.293708
 C -5.116926 0.824071 0.338708
 C -6.102879 0.376785 -0.742222
 C -6.589939 1.046933 -1.853013
 C -7.480714 0.400758 -2.716361
 C -7.863850 -0.914301 -2.464883
 C -7.365858 -1.611134 -1.364302
 C -6.479077 -0.955456 -0.515357
 C -4.791475 -0.554419 1.022120
 C -2.753153 -1.948872 0.970881
 C -1.334850 -2.030648 0.505880
 C -5.721875 1.875672 1.365072
 C -4.739201 2.108613 2.500571
 C -4.899436 1.807461 3.785321

C -5.933789 3.239622 0.671345
 C -7.081577 1.387296 1.890233
 C -0.577942 -3.076421 0.884942
 C 0.833063 -3.287358 0.634856
 C 2.614734 -4.397094 0.186550
 C 1.866848 -2.376318 0.590941
 C 4.355830 -2.571638 0.058962
 C 4.777770 -1.593876 1.176561
 C 6.267399 -1.648776 1.568948
 C 7.341417 -1.187096 0.569872
 C 7.458934 0.316567 0.354398
 C 5.759843 2.014280 0.088535
 C 4.384468 2.330064 -0.321285
 C 3.770094 3.448641 0.323066
 C 2.415608 3.715939 0.165777
 C 1.646138 2.905729 -0.653892
 C 2.248190 1.869772 -1.381511
 C 3.590377 1.569519 -1.225130
 C 4.142193 0.470586 -2.125752
 C 3.569621 -0.919531 -1.819412
 C 4.506462 -2.046793 -1.397283
 C 8.579710 0.700870 -0.598216
 N -5.876148 -1.441157 0.639831
 N -3.475448 -0.920617 0.469057
 N -0.845001 -0.957453 -0.271153
 O -1.078983 0.920478 -1.517436
 O -3.219619 -2.731325 1.798137
 H -3.469834 -0.438123 -1.580102
 H -4.697580 -0.510590 2.103816
 O 2.385985 -1.140386 -1.977275
 O 6.476458 2.799324 0.713854
 O 4.451703 4.275504 1.139148
 O 0.325152 3.167549 -0.752541
 O 6.172465 0.770841 -0.188793
 N 2.999611 -3.090683 0.297503
 N 1.331873 -4.558222 0.396881
 H -7.864400 0.921876 -3.584139
 H -8.550747 -1.411769 -3.139143
 H -7.653027 -2.639441 -1.181820
 H -6.280341 2.061627 -2.069692
 H -5.723273 -2.431660 0.758447
 H -3.160706 1.827383 0.414438
 H -3.916026 1.888460 -1.177027
 H 0.129032 -0.984564 -0.555669

H -3.819930 2.613955 2.217022
 H -5.003791 3.645423 0.268967
 H -6.657706 3.162600 -0.139684
 H -6.321911 3.958807 1.394962
 H -7.790569 1.281571 1.069426
 H -7.490722 2.112943 2.595153
 H -7.013287 0.424318 2.396739
 H -4.130742 2.049528 4.509531
 H -5.786159 1.319012 4.169638
 H -1.099918 -3.857934 1.422452
 H 8.442769 0.224712 -1.571315
 H 9.538127 0.375225 -0.189499
 H 8.619552 1.780887 -0.735914
 H 5.391003 3.969206 1.147261
 H -0.145082 2.412952 -1.165056
 H 1.649040 1.296450 -2.074560
 H 1.971976 4.545389 0.699102
 H 7.595152 0.819482 1.312065
 H 7.236535 -1.686880 -0.396138
 H 8.311604 -1.508681 0.959527
 H 6.496735 -2.681626 1.849391
 H 6.383161 -1.062687 2.485945
 H 4.295918 -2.881937 -2.069770
 H 5.541436 -1.751274 -1.547784
 H 5.223013 0.447913 -2.118762
 H 3.813555 0.692733 -3.144507
 H 4.216626 -1.872218 2.070753
 H 4.478694 -0.576453 0.928258
 H 5.000242 -3.450893 0.124054
 H 1.895514 -1.318540 0.781407
 H 3.321366 -5.180693 -0.039551

1d-c25, $\Delta G = 0.4675$ kcal/mol,
 population = 12.29 %

C -1.479274 -0.137787 -0.960251
 C -2.959493 -0.144647 -0.659326
 C -3.575640 1.216263 -0.325106
 C -4.895967 0.850751 0.403074
 C -5.966704 0.431298 -0.609263
 C -6.490594 1.105661 -1.700775
 C -7.453183 0.484422 -2.503173
 C -7.871560 -0.811539 -2.211522
 C -7.337913 -1.514197 -1.131913
 C -6.379030 -0.883104 -0.344250

C -4.596128 -0.530373 1.098175
 C -2.602277 -1.985462 1.005748
 C -1.214974 -2.134345 0.466961
 C -5.374956 1.951854 1.442192
 C -6.656311 1.474694 2.102201
 C -6.891124 1.317164 3.400445
 C -4.284117 2.255391 2.484267
 C -5.700813 3.273462 0.709226
 C -0.474258 -3.189475 0.851204
 C 0.913000 -3.453916 0.522279
 C 2.622654 -4.609139 -0.065836
 C 1.970716 -2.576293 0.435276
 C 4.401313 -2.835700 -0.302121
 C 4.979506 -1.922994 0.789110
 C 6.510205 -1.804325 0.718405
 C 7.076598 -0.681598 1.606835
 C 7.254505 0.676552 0.925515
 C 5.577674 2.264295 0.191117
 C 4.252803 2.473107 -0.415977
 C 3.569705 3.665419 -0.027789
 C 2.234394 3.870403 -0.354793
 C 1.563580 2.924118 -1.110620
 C 2.250225 1.812289 -1.618726
 C 3.568514 1.563976 -1.276548
 C 4.261215 0.389472 -1.953402
 C 3.558155 -0.969828 -1.890180
 C 4.419299 -2.218367 -1.730387
 C 8.370465 0.729905 -0.107085
 N -5.729137 -1.377176 0.778007
 N -3.320357 -0.957653 0.498031
 N -0.738925 -1.116955 -0.389760
 O -0.997119 0.684103 -1.739655
 O -3.043722 -2.715210 1.892482
 H -3.434501 -0.549962 -1.563100
 H -4.461452 -0.484550 2.174970
 O 2.356278 -1.083849 -2.019805
 O 6.252570 3.177810 0.670010
 O 4.157236 4.630084 0.708816
 O 0.252407 3.125208 -1.372311
 O 5.977347 0.989677 0.271819
 N 3.058872 -3.318646 0.049901
 N 1.351484 -4.734099 0.225073
 H -7.866349 1.010242 -3.354393
 H -8.615434 -1.289451 -2.837801

H -7.652744 -2.528355 -0.918469
 H -6.156843 2.105442 -1.948236
 H -5.628054 -2.370120 0.924141
 H -2.896609 1.764536 0.325771
 H -3.744814 1.811250 -1.218853
 H 0.217642 -1.185695 -0.725819
 H -7.463548 1.264620 1.406013
 H -3.942575 1.368810 3.019901
 H -3.415977 2.730172 2.028664
 H -4.672387 2.955913 3.224759
 H -6.552216 3.168148 0.038180
 H -4.845263 3.631127 0.132300
 H -5.952630 4.040914 1.443088
 H -7.861692 0.984547 3.748679
 H -6.145183 1.502776 4.163019
 H -0.989938 -3.927667 1.452382
 H 9.326187 0.522994 0.377987
 H 8.428579 1.720621 -0.558040
 H 8.223055 -0.004353 -0.900407
 H 5.101641 4.372299 0.831053
 H -0.168014 2.290356 -1.664015
 H 1.730535 1.136080 -2.279481
 H 1.729539 4.758597 -0.000482
 H 7.426921 1.440179 1.681980
 H 8.061426 -0.967392 1.984334
 H 6.438524 -0.554918 2.485423
 H 6.836393 -1.652234 -0.312882
 H 6.941358 -2.760092 1.027275
 H 4.034927 -2.967199 -2.424444
 H 5.454078 -2.007041 -1.999406
 H 5.284109 0.283232 -1.620010
 H 4.310371 0.607638 -3.029149
 H 4.705505 -2.340094 1.761204
 H 4.525368 -0.932908 0.735105
 H 5.017262 -3.735989 -0.353275
 H 2.039689 -1.524587 0.645209
 H 3.284734 -5.409068 -0.359003

1d-c9, ΔG = 0.5792 kcal/mol,
 population = 10.17 %

C -1.570867 0.008125 -0.764117
 C -3.062089 -0.092629 -0.546211
 C -3.765682 1.207641 -0.155000
 C -5.095441 0.730925 0.485945

C -6.100546 0.318163 -0.590868
 C -6.632972 1.041374 -1.645403
 C -7.533231 0.424650 -2.520463
 C -7.883883 -0.910198 -2.333577
 C -7.347848 -1.655210 -1.283378
 C -6.452730 -1.027939 -0.422018
 C -4.748581 -0.673862 1.111015
 C -2.694490 -2.040593 0.988817
 C -1.284230 -2.094397 0.497362
 C -5.692653 1.754967 1.541792
 C -5.878563 3.103411 0.869796
 C -7.003207 3.799658 0.747361
 C -7.009470 1.215007 2.120183
 C -4.713047 1.989619 2.718846
 C -0.512942 -3.146255 0.827891
 C 0.894087 -3.340098 0.545153
 C 2.673213 -4.426176 0.032991
 C 1.921510 -2.421552 0.505327
 C 4.401370 -2.586950 -0.076743
 C 4.839581 -1.642372 1.062895
 C 6.336653 -1.702265 1.425023
 C 7.389674 -1.209525 0.418492
 C 7.498779 0.299862 0.242503
 C 5.787634 1.996622 0.066934
 C 4.401408 2.317895 -0.300036
 C 3.795465 3.408886 0.397496
 C 2.436258 3.672865 0.280357
 C 1.652949 2.887542 -0.550467
 C 2.244032 1.881508 -1.327257
 C 3.591131 1.584386 -1.211648
 C 4.127837 0.520741 -2.162448
 C 3.571527 -0.882675 -1.888417
 C 4.522811 -2.016035 -1.518120
 C 8.598672 0.714431 -0.721635
 N -5.824740 -1.557529 0.701142
 N -3.433212 -1.001710 0.533821
 N -0.817115 -0.991747 -0.251977
 O -1.088261 0.923829 -1.431598
 O -3.141121 -2.853784 1.797163
 H -3.468525 -0.457457 -1.499521
 H -4.645621 -0.690536 2.192044
 O 2.386610 -1.107234 -2.031107
 O 6.514375 2.764529 0.701717
 O 4.490724 4.210654 1.226991

O 0.328759 3.144649 -0.610432
 O 6.200361 0.765527 -0.261283
 N 3.052351 -3.120481 0.170788
 N 1.395773 -4.601000 0.263964
 H -7.952805 0.985523 -3.345920
 H -8.578577 -1.383797 -3.017069
 H -7.615439 -2.695895 -1.146927
 H -6.359444 2.077250 -1.797563
 H -5.654313 -2.549785 0.771620
 H -3.146813 1.747524 0.561029
 H -3.928457 1.850291 -1.016176
 H 0.151773 -1.000743 -0.554157
 H -4.962069 3.548475 0.489294
 H -6.849257 0.264954 2.631028
 H -7.415224 1.917631 2.849752
 H -7.760467 1.056037 1.346624
 H -3.774333 2.443044 2.399468
 H -4.482166 1.066219 3.251811
 H -5.174592 2.673042 3.433209
 H -7.001950 4.774405 0.274138
 H -7.959544 3.436941 1.102429
 H -1.019555 -3.948829 1.348794
 H 8.441902 0.267338 -1.705453
 H 9.566006 0.378799 -0.343177
 H 8.633993 1.798147 -0.827871
 H 5.431876 3.911172 1.202321
 H -0.146533 2.404238 -1.042073
 H 1.632606 1.329530 -2.026937
 H 2.000205 4.480115 0.852590
 H 7.653094 0.776258 1.210878
 H 7.267246 -1.683325 -0.558447
 H 8.368141 -1.538433 0.780324
 H 6.574459 -2.741786 1.671899
 H 6.468360 -1.141557 2.355589
 H 4.304886 -2.830869 -2.212708
 H 5.553177 -1.709430 -1.677302
 H 5.208618 0.506267 -2.182927
 H 3.772280 0.774645 -3.164504
 H 4.296834 -1.951366 1.958356
 H 4.530984 -0.619335 0.851949
 H 5.050718 -3.464618 -0.051230
 H 1.947997 -1.368967 0.722812
 H 3.380004 -5.199093 -0.226776

1d-c32, $\Delta G = 0.8245$ kcal/mol,
 population = 6.72 %

C -1.475584 -0.081539 -0.900220
 C -2.957870 -0.124015 -0.610734
 C -3.615198 1.219278 -0.288418
 C -4.927614 0.820525 0.433852
 C -5.975145 0.328034 -0.568835
 C -6.510678 0.941114 -1.690079
 C -7.455620 0.262241 -2.466049
 C -7.845373 -1.028523 -2.118264
 C -7.298081 -1.669822 -1.007538
 C -6.357117 -0.982027 -0.247919
 C -4.577106 -0.530188 1.164107
 C -2.569026 -1.960869 1.050072
 C -1.186641 -2.096234 0.496712
 C -5.472256 1.942660 1.416716
 C -6.728913 1.435164 2.101842
 C -7.936958 1.986993 2.088050
 C -4.450760 2.257252 2.538501
 C -5.728944 3.246003 0.644932
 C -0.439743 -3.155510 0.857318
 C 0.941076 -3.422281 0.507453
 C 2.635781 -4.590977 -0.097384
 C 1.999692 -2.548990 0.386920
 C 4.418360 -2.829741 -0.385548
 C 5.036748 -1.953797 0.713661
 C 6.566398 -1.851225 0.607518
 C 7.168392 -0.765829 1.518497
 C 7.340623 0.613312 0.878916
 C 5.648941 2.228384 0.242344
 C 4.310591 2.459811 -0.326479
 C 3.638366 3.637760 0.121108
 C 2.297909 3.859046 -0.172212
 C 1.609741 2.945372 -0.951986
 C 2.281986 1.850548 -1.513447
 C 3.605692 1.585024 -1.206290
 C 4.280054 0.433750 -1.940788
 C 3.566289 -0.921851 -1.925204
 C 4.415066 -2.182786 -1.800789
 C 8.436619 0.694728 -0.172845
 N -5.695674 -1.415741 0.897608
 N -3.303423 -0.942007 0.547819
 N -0.723222 -1.061717 -0.346373
 O -1.002084 0.764836 -1.658107

O -2.995172 -2.693992 1.941886
 H -3.414937 -0.546010 -1.516133
 H -4.412823 -0.452923 2.234997
 O 2.364510 -1.021772 -2.067058
 O 6.333048 3.122619 0.744150
 O 4.242337 4.571881 0.883083
 O 0.295650 3.162631 -1.183368
 O 6.052659 0.952899 0.260499
 N 3.077346 -3.300039 -0.011046
 N 1.370593 -4.707898 0.220299
 H -7.877413 0.739669 -3.341314
 H -8.575940 -1.550823 -2.724412
 H -7.590031 -2.680618 -0.749866
 H -6.198308 1.935668 -1.982484
 H -5.542806 -2.401371 1.052723
 H -2.958575 1.793842 0.363977
 H -3.796321 1.802927 -1.187147
 H 0.232997 -1.113873 -0.684811
 H -6.591508 0.527851 2.684080
 H -4.219946 1.388018 3.155333
 H -3.515062 2.653154 2.142282
 H -4.872654 3.017474 3.197606
 H -6.059825 4.026178 1.332356
 H -6.496021 3.131237 -0.119124
 H -4.816548 3.601843 0.164381
 H -8.754648 1.539919 2.640666
 H -8.166681 2.888168 1.533809
 H -0.948174 -3.901863 1.454554
 H 8.491008 1.698997 -0.593356
 H 8.270993 -0.013595 -0.985967
 H 9.400362 0.468642 0.287195
 H 5.188451 4.307890 0.976638
 H -0.133208 2.345184 -1.510059
 H 1.747950 1.202114 -2.190501
 H 1.803340 4.734762 0.225043
 H 7.531431 1.351320 1.656035
 H 8.160138 -1.073590 1.858697
 H 6.555643 -0.664106 2.418133
 H 6.868546 -1.668210 -0.426069
 H 6.993145 -2.821916 0.873077
 H 4.010398 -2.913715 -2.502235
 H 5.447373 -1.977120 -2.083722
 H 5.306063 0.306596 -1.625192
 H 4.316537 0.697236 -3.006720

H 4.782296 -2.394652 1.680625
 H 4.593049 -0.957707 0.698820
 H 5.016577 -3.739243 -0.473132
 H 2.077974 -1.495746 0.585144
 H 3.291349 -5.397102 -0.387855

1d-c35, $\Delta G = 0.9155$ kcal/mol,
 population = 5.76 %

C -1.531885 0.055290 -0.713573
 C -3.024197 -0.040219 -0.501628
 C -3.724240 1.256931 -0.092607
 C -5.054379 0.773779 0.537132
 C -6.052080 0.367207 -0.551963
 C -6.549895 1.080274 -1.631001
 C -7.443968 0.466769 -2.514298
 C -7.819442 -0.859545 -2.316018
 C -7.308881 -1.599500 -1.250093
 C -6.418812 -0.975261 -0.381223
 C -4.713873 -0.636138 1.150829
 C -2.669886 -2.013697 1.005776
 C -1.259196 -2.068216 0.516033
 C -5.640527 1.791291 1.607857
 C -5.937414 3.110788 0.918587
 C -5.343953 4.283089 1.118920
 C -6.977562 1.260429 2.173583
 C -4.674380 1.988265 2.789752
 C -0.494689 -3.129592 0.831695
 C 0.910974 -3.329458 0.546726
 C 2.681553 -4.423107 0.021061
 C 1.945207 -2.418107 0.515597
 C 4.423176 -2.596317 -0.072155
 C 4.871018 -1.666405 1.075771
 C 6.367931 -1.743050 1.435536
 C 7.424069 -1.252768 0.431035
 C 7.547411 0.256866 0.266578
 C 5.852114 1.971660 0.112658
 C 4.467295 2.308717 -0.245011
 C 3.874378 3.398413 0.465539
 C 2.516957 3.674923 0.357887
 C 1.722492 2.903793 -0.475721
 C 2.301020 1.899964 -1.264982
 C 3.646216 1.590786 -1.159413
 C 4.170340 0.533811 -2.124726
 C 3.603423 -0.868178 -1.866212

C 4.546466 -2.012394 -1.508209
 C 8.646775 0.668081 -0.699562
 N -5.800411 -1.509156 0.744739
 N -3.404016 -0.966999 0.561718
 N -0.784753 -0.956994 -0.215443
 O -1.042140 0.977427 -1.366626
 O -3.121394 -2.834121 1.804313
 H -3.428282 -0.388038 -1.462242
 H -4.603454 -0.660900 2.230608
 O 2.416938 -1.082462 -2.011500
 O 6.589076 2.727413 0.750253
 O 4.580818 4.186655 1.298599
 O 0.400609 3.173299 -0.525983
 O 6.251417 0.739317 -0.227285
 N 3.070515 -3.121888 0.172408
 N 1.403129 -4.590960 0.251493
 H -7.836279 1.022389 -3.356437
 H -8.509415 -1.331432 -3.005330
 H -7.588413 -2.636432 -1.109373
 H -6.245924 2.104530 -1.806495
 H -5.637172 -2.502940 0.812610
 H -3.109410 1.787770 0.632920
 H -3.885908 1.916447 -0.940814
 H 0.184235 -0.967320 -0.516986
 H -6.754342 3.069664 0.204509
 H -6.843030 0.305297 2.683662
 H -7.378496 1.974724 2.895032
 H -7.720270 1.122597 1.387336
 H -3.701886 2.380076 2.493274
 H -4.508915 1.057023 3.331239
 H -5.108451 2.696777 3.496829
 H -5.662829 5.164063 0.574569
 H -4.530567 4.420639 1.820556
 H -1.006931 -3.936678 1.339959
 H 8.692943 1.752226 -0.797024
 H 8.480217 0.230789 -1.686185
 H 9.612421 0.319138 -0.328910
 H 5.519181 3.879294 1.266348
 H -0.084345 2.442283 -0.962915
 H 1.681532 1.360171 -1.967105
 H 2.090733 4.480759 0.939433
 H 7.711049 0.723848 1.238002
 H 7.295287 -1.717587 -0.549384
 H 8.399967 -1.593967 0.788406

H 6.596325 -2.786499 1.674491
 H 6.506082 -1.190400 2.370003
 H 4.321339 -2.818878 -2.210242
 H 5.578844 -1.711966 -1.666266
 H 5.250910 0.510356 -2.148734
 H 3.813839 0.803067 -3.122412
 H 4.326435 -1.978703 1.968978
 H 4.571671 -0.638692 0.874692
 H 5.065668 -3.479256 -0.056390
 H 1.980032 -1.368165 0.744433
 H 3.382333 -5.198298 -0.248142

1d-c18, $\Delta G = 1.2136$ kcal/mol,
 population = 3.48 %

C -1.546056 0.045230 -0.775118
 C -3.038441 -0.035312 -0.557203
 C -3.734101 1.287254 -0.227472
 C -5.069452 0.844929 0.425821
 C -6.065017 0.390951 -0.646218
 C -6.560217 1.055332 -1.756983
 C -7.448554 0.401614 -2.617084
 C -7.821549 -0.915855 -2.362569
 C -7.314727 -1.607820 -1.263321
 C -6.429114 -0.944397 -0.418390
 C -4.737455 -0.532089 1.113476
 C -2.688551 -1.913199 1.067072
 C -1.276443 -1.997566 0.584381
 C -5.655871 1.901738 1.455405
 C -6.932619 1.340245 2.055618
 C -7.217694 1.166978 3.341774
 C -4.628719 2.255470 2.545345
 C -6.030581 3.211514 0.724033
 C -0.512522 -3.037234 0.966302
 C 0.893877 -3.253163 0.696143
 C 2.665719 -4.373852 0.236207
 C 1.927960 -2.344689 0.616843
 C 4.407469 -2.554645 0.046328
 C 4.851812 -1.563224 1.142959
 C 6.348286 -1.617481 1.508443
 C 7.404503 -1.172537 0.483185
 C 7.520634 0.327658 0.244019
 C 5.818699 2.023696 -0.012470
 C 4.436449 2.336418 -0.401034
 C 3.834516 3.462585 0.241979

C 2.477781 3.729805 0.105478
 C 1.693299 2.912202 -0.692393
 C 2.281433 1.867702 -1.419107
 C 3.625725 1.566999 -1.282304
 C 4.159848 0.456386 -2.179234
 C 3.592312 -0.928938 -1.843047
 C 4.535090 -2.050561 -1.419388
 C 8.625388 0.696506 -0.733107
 N -5.815993 -1.423371 0.730959
 N -3.419546 -0.892619 0.561647
 N -0.800234 -0.934449 -0.214656
 O -1.055920 0.925176 -1.484054
 O -3.142512 -2.686277 1.909839
 H -3.444294 -0.440258 -1.494473
 H -4.650430 -0.497066 2.195578
 O 2.406200 -1.151398 -1.978506
 O 6.546990 2.814967 0.591121
 O 4.531005 4.297347 1.037146
 O 0.371224 3.175078 -0.771125
 O 6.225723 0.776843 -0.283263
 N 3.054177 -3.066176 0.315759
 N 1.386750 -4.528990 0.472647
 H -7.839151 0.919207 -3.483863
 H -8.507437 -1.418935 -3.033721
 H -7.592983 -2.638189 -1.078651
 H -6.260005 2.072327 -1.975486
 H -5.674118 -2.412642 0.868510
 H -3.114702 1.851713 0.467307
 H -3.887398 1.893569 -1.116474
 H 0.169488 -0.963982 -0.512990
 H -7.690955 1.078560 1.322790
 H -3.774229 2.789283 2.130961
 H -5.088043 2.919620 3.278502
 H -4.254699 1.382934 3.082486
 H -6.847465 3.065063 0.018613
 H -5.175902 3.625893 0.184929
 H -6.355175 3.953426 1.455543
 H -8.180122 0.772078 3.644588
 H -6.522203 1.399746 4.138487
 H -1.025696 -3.811557 1.522387
 H 8.664766 1.774479 -0.886155
 H 8.470748 0.207598 -1.697177
 H 9.590141 0.374448 -0.336625
 H 5.470074 3.990279 1.032017

H -0.107410 2.417002 -1.167058
 H 1.669811 1.288022 -2.095822
 H 2.044346 4.565365 0.637657
 H 7.674200 0.843879 1.191903
 H 7.280570 -1.686302 -0.473194
 H 8.381149 -1.490506 0.859381
 H 6.579711 -2.647360 1.798001
 H 6.483015 -1.019842 2.415310
 H 4.313476 -2.894987 -2.076525
 H 5.567765 -1.758094 -1.590123
 H 5.240622 0.433296 -2.192776
 H 3.811587 0.665427 -3.194186
 H 4.306352 -1.828129 2.050821
 H 4.550912 -0.548366 0.886446
 H 5.050281 -3.435021 0.112194
 H 1.961840 -1.283637 0.787341
 H 3.367214 -5.162657 0.012319

1d-c20, $\Delta G = 1.3981$ kcal/mol,
 population = 2.55 %

C -1.550768 0.014708 -0.763294
 C -3.042020 -0.073898 -0.540559
 C -3.743026 1.241595 -0.196354
 C -5.073608 0.788285 0.456407
 C -6.069033 0.316488 -0.606803
 C -6.570559 0.964775 -1.723888
 C -7.464785 0.298837 -2.568159
 C -7.837319 -1.014175 -2.292098
 C -7.323561 -1.689618 -1.185606
 C -6.433185 -1.013971 -0.357014
 C -4.724137 -0.584095 1.146736
 C -2.676246 -1.961668 1.069124
 C -1.266833 -2.037929 0.578396
 C -5.679099 1.858701 1.461218
 C -6.948732 1.299099 2.077838
 C -8.168879 1.821791 2.031254
 C -4.706260 2.148336 2.631599
 C -5.935984 3.186691 0.732573
 C -0.496865 -3.076899 0.950145
 C 0.909446 -3.284182 0.673108
 C 2.685346 -4.392697 0.199583
 C 1.938400 -2.369785 0.595218
 C 4.416200 -2.562758 0.011830
 C 4.860171 -1.573366 1.110484

C 6.358338 -1.621848 1.469763
 C 7.408423 -1.171446 0.440549
 C 7.519243 0.329622 0.204359
 C 5.811191 2.021802 -0.036185
 C 4.425339 2.331487 -0.414075
 C 3.824035 3.453000 0.237533
 C 2.465319 3.715607 0.112115
 C 1.678042 2.897828 -0.682770
 C 2.264644 1.858294 -1.417793
 C 3.611069 1.562374 -1.292282
 C 4.143119 0.457840 -2.197919
 C 3.583346 -0.931250 -1.864464
 C 4.533282 -2.051104 -1.452117
 C 8.616603 0.703526 -0.779138
 N -5.810566 -1.480606 0.797169
 N -3.416281 -0.944171 0.570309
 N -0.798656 -0.967120 -0.215095
 O -1.067302 0.902616 -1.466738
 O -3.121727 -2.738046 1.913570
 H -3.449433 -0.470759 -1.480469
 H -4.606194 -0.547418 2.225802
 O 2.397221 -1.157795 -1.993108
 O 6.541340 2.813444 0.564663
 O 4.523324 4.287474 1.030579
 O 0.354309 3.155769 -0.750498
 O 6.219794 0.776849 -0.313331
 N 3.067175 -3.083422 0.285500
 N 1.408137 -4.556035 0.440018
 H -7.859992 0.803564 -3.440488
 H -8.527639 -1.526743 -2.951389
 H -7.601154 -2.716923 -0.983617
 H -6.269609 1.977331 -1.961193
 H -5.644500 -2.468479 0.921063
 H -3.125776 1.804945 0.502604
 H -3.902082 1.854216 -1.079789
 H 0.169645 -0.990650 -0.518619
 H -6.811746 0.377547 2.637378
 H -3.767925 2.583612 2.285617
 H -5.169953 2.868680 3.307179
 H -4.474516 1.258642 3.217930
 H -6.675353 3.087954 -0.060478
 H -5.015627 3.578083 0.296828
 H -6.304587 3.932687 1.438623
 H -8.996788 1.338182 2.535779

H -8.398396 2.734283 1.495611
 H -1.004019 -3.857147 1.503450
 H 8.456481 0.216848 -1.743443
 H 9.584699 0.382497 -0.390064
 H 8.652651 1.781981 -0.929537
 H 5.463455 3.983943 1.017428
 H -0.123921 2.398015 -1.147384
 H 1.650141 1.278779 -2.092020
 H 2.032715 4.547563 0.650569
 H 7.677685 0.843937 1.152462
 H 7.281322 -1.683175 -0.516477
 H 8.387765 -1.487553 0.811270
 H 6.595191 -2.651091 1.757136
 H 6.494339 -1.024649 2.376730
 H 4.311186 -2.893135 -2.112142
 H 5.563717 -1.753553 -1.627480
 H 5.223833 0.439070 -2.219095
 H 3.787052 0.670249 -3.209463
 H 4.319632 -1.844048 2.019576
 H 4.553528 -0.559010 0.858815
 H 5.064289 -3.439763 0.070550
 H 1.967307 -1.309612 0.771767
 H 3.390105 -5.176414 -0.031798

Table S6. Coordinates and relative free energy of low-energy conformers of structures **1a–d** for ECD calculations. **1a-c11**, $\Delta G = 0.0000$ kcal/mol, population = 32.33 %

C 3.940421 -1.859808 -0.111507
 C 5.220168 -1.063349 -0.193037
 C 6.422724 -1.684334 0.515433
 C 7.383216 -0.486972 0.677991
 C 8.026475 -0.130515 -0.655209
 C 8.737144 -0.916422 -1.548179
 C 9.209994 -0.349752 -2.738118
 C 8.952015 0.990227 -3.024782
 C 8.211321 1.786346 -2.149542
 C 7.745993 1.205686 -0.972223
 C 6.441477 0.751314 0.879443
 C 3.995667 0.961360 0.633423
 C 2.733601 0.233022 0.344685
 C 8.433812 -0.660974 1.842430

C 9.210118 0.630912 1.989147
 C 10.503275 0.822148 1.739448
 C 7.734262 -0.920690 3.194426
 C 9.351978 -1.851947 1.552499
 C 1.552226 0.892254 0.395873
 C 0.247750 0.328750 0.200469
 C -1.298024 -1.128968 -0.168486
 C -0.957845 1.010025 0.228140
 C -3.375560 0.291619 -0.093913
 C -3.720200 1.240303 -1.244020
 C -3.571967 0.597287 -2.621451
 C -4.586523 -0.510792 -2.928676
 C -6.063725 -0.123228 -2.959899
 C -7.883922 -0.334727 -1.410544
 C -8.409840 -0.359085 -0.039670
 C -9.835274 -0.328513 0.099432
 C -10.442757 -0.295898 1.350581
 C -9.655290 -0.334572 2.489335
 C -8.262216 -0.415445 2.387321
 C -7.637482 -0.427454 1.150157
 C -6.137028 -0.514278 1.183838
 C -5.442532 0.836710 1.229334
 C -3.925159 0.799575 1.250959
 C -6.356337 1.213031 -3.615240
 N 7.005121 1.803675 0.042317
 N 5.129692 0.256141 0.429803
 N 2.808506 -1.146004 0.110041
 O 3.932829 -3.076480 -0.296080
 O 4.013239 2.120093 1.072583
 H 5.441623 -0.956316 -1.270503
 H 6.338171 1.101760 1.910091
 O -6.055374 1.887194 1.273908
 O -8.619980 -0.493263 -2.397743
 O -10.661551 -0.318200 -0.960406
 O -10.287359 -0.309729 3.687955
 O -6.572836 -0.112075 -1.560882
 N -1.926953 0.071321 -0.008793
 N 0.008713 -1.017873 -0.051170
 H 9.769276 -0.958904 -3.441763
 H 9.318007 1.422387 -3.952526
 H 7.989264 2.823200 -2.386604
 H 8.916051 -1.968293 -1.343129
 H 6.388576 2.570954 -0.190932
 H 6.104434 -2.079606 1.484715

H 6.864042 -2.494535 -0.067569
 H 1.911563 -1.635229 0.051174
 H 8.624950 1.473941 2.360092
 H 7.242132 -1.897188 3.211800
 H 8.489422 -0.918086 3.987345
 H 6.994049 -0.153179 3.440294
 H 10.042603 -1.996635 2.389922
 H 9.945672 -1.706838 0.647631
 H 8.766182 -2.769632 1.437731
 H 10.957694 1.796446 1.898379
 H 11.151309 0.030829 1.372943
 H 1.604675 1.953211 0.618210
 H -5.926408 1.216428 -4.622575
 H -5.915119 2.040130 -3.052128
 H -7.432721 1.377367 -3.698322
 H -10.073339 -0.409030 -1.761952
 H -9.637061 -0.348563 4.404091
 H -7.663381 -0.475825 3.292926
 H -11.524910 -0.259408 1.420409
 H -6.614389 -0.916852 -3.473024
 H -4.467913 -1.361628 -2.246049
 H -4.362192 -0.901397 -3.929431
 H -2.562917 0.174117 -2.719678
 H -3.646517 1.378360 -3.386631
 H -3.556357 1.810027 1.454557
 H -3.595830 0.123574 2.050015
 H -5.732391 -1.101574 0.356347
 H -5.825511 -1.037111 2.098980
 H -3.084984 2.131574 -1.167463
 H -4.748272 1.588839 -1.103002
 H -3.793702 -0.700358 -0.292504
 H -1.181626 2.053967 0.394894
 H -1.849058 -2.040612 -0.368483

1a-c1, $\Delta G = 0.2130$ kcal/mol,
 population = 22.56 %

C 3.926911 -0.270666 -1.586603
 C 5.231085 0.095930 -0.919836
 C 6.415639 -0.798279 -1.279751
 C 7.419328 -0.532791 -0.134491
 C 8.104304 0.811869 -0.326096
 C 8.846153 1.290547 -1.393431
 C 9.361546 2.591566 -1.342116
 C 9.118601 3.396014 -0.228953

C 8.358795 2.932234 0.846481
 C 7.853872 1.635631 0.778989
 C 6.522892 -0.227882 1.117794
 C 4.082209 0.073032 1.307737
 C 2.794443 0.068032 0.568657
 C 8.441032 -1.708983 0.105888
 C 9.221874 -1.935492 -1.169261
 C 10.542733 -1.882661 -1.321002
 C 9.353610 -1.374179 1.290175
 C 7.709786 -3.035208 0.412526
 C 1.634985 0.267349 1.238369
 C 0.311075 0.230030 0.687877
 C -1.287902 0.003607 -0.745260
 C -0.871177 0.489533 1.359420
 C -3.310385 0.450816 0.748799
 C -3.805266 -0.846482 1.418534
 C -3.545275 -2.166125 0.684108
 C -4.423290 -2.532278 -0.519305
 C -5.911857 -2.688444 -0.239184
 C -7.742806 -1.201765 0.239598
 C -8.467632 0.030167 -0.080455
 C -9.818282 0.124418 0.378131
 C -10.609194 1.231952 0.083622
 C -10.072802 2.271475 -0.656991
 C -8.744738 2.218796 -1.103897
 C -7.947389 1.121809 -0.829943
 C -6.519558 1.182139 -1.297412
 C -5.529776 1.224917 -0.146224
 C -4.096601 0.883626 -0.485536
 C -6.598230 -3.559523 -1.278129
 N 7.110897 0.954970 1.739267
 N 5.190128 -0.002029 0.537926
 N 2.822692 -0.227920 -0.800670
 O 3.877673 -0.538322 -2.786930
 O 4.142819 0.099118 2.545217
 H 5.445859 1.136987 -1.222221
 H 6.444997 -1.038644 1.847329
 O -5.858345 1.577934 0.971853
 O -8.229083 -2.095834 0.950605
 O -10.398763 -0.845963 1.103290
 O -10.874537 3.331891 -0.918704
 O -6.524779 -1.340312 -0.302078
 N -1.874121 0.354915 0.437374
 N 0.023919 -0.073752 -0.637544

H 9.944010 2.975903 -2.174066
 H 9.516418 4.407099 -0.198793
 H 8.158135 3.566430 1.705635
 H 9.023285 0.667573 -2.265260
 H 6.507187 1.484553 2.354346
 H 6.085949 -1.841535 -1.292365
 H 6.830669 -0.548756 -2.257806
 H 1.909674 -0.359378 -1.244288
 H 8.611034 -2.203220 -2.033605
 H 10.079228 -2.178840 1.445437
 H 9.903033 -0.441394 1.128077
 H 8.768838 -1.271721 2.209319
 H 8.455205 -3.795933 0.665816
 H 7.141669 -3.405915 -0.444926
 H 7.028639 -2.938809 1.264060
 H 10.996669 -2.092596 -2.285860
 H 11.214173 -1.625726 -0.506452
 H 1.723471 0.464012 2.302138
 H -6.393688 -3.177715 -2.284376
 H -7.679230 -3.592570 -1.121165
 H -6.209769 -4.580117 -1.208438
 H -9.698352 -1.547405 1.227794
 H -10.391076 3.992955 -1.434842
 H -8.336994 3.056010 -1.664499
 H -11.633417 1.269526 0.439723
 H -6.076056 -3.078416 0.770878
 H -4.079283 -3.509968 -0.878948
 H -4.291645 -1.849431 -1.366112
 H -3.658445 -2.969636 1.423614
 H -2.494238 -2.204041 0.367783
 H -4.082305 0.140817 -1.284678
 H -3.654919 1.800135 -0.907673
 H -6.359087 2.107896 -1.867613
 H -6.264580 0.356637 -1.966734
 H -4.871531 -0.724121 1.636487
 H -3.301573 -0.904212 2.391516
 H -3.401313 1.253289 1.489568
 H -1.067831 0.763689 2.386556
 H -1.853244 -0.180680 -1.649527

1a-c2, $\Delta G = 0.2837$ kcal/mol,
 population = 20.01 %

C 4.123648 -0.153003 -1.922014
 C 5.291363 0.225439 -1.043070

C 6.574518 -0.562383 -1.298660
C 7.386757 -0.344333 -0.001915
C 7.997213 1.048958 0.016788
C 8.847320 1.661650 -0.888850
C 9.258373 2.980641 -0.659885
C 8.804231 3.668334 0.465287
C 7.934047 3.068641 1.377663
C 7.535941 1.755768 1.135231
C 6.304455 -0.204506 1.127219
C 3.845850 -0.077364 0.983328
C 2.678032 -0.107364 0.067073
C 8.444554 -1.476719 0.291450
C 9.405523 -1.550977 -0.874026
C 10.725066 -1.383913 -0.836114
C 9.161844 -1.188253 1.614133
C 7.771851 -2.863799 0.394063
C 1.424119 -0.078055 0.576863
C 0.196967 -0.177645 -0.158056
C -1.163932 -0.413994 -1.818858
C -1.085056 -0.136257 0.363862
C -3.402838 -0.321995 -0.626920
C -3.939965 -1.688387 -1.060819
C -3.708511 -2.783650 -0.021166
C -4.523187 -2.632086 1.269226
C -6.045240 -2.676982 1.150022
C -7.770286 -1.009093 1.107124
C -8.258136 0.326798 0.741623
C -9.666279 0.552557 0.877010
C -10.246906 1.761545 0.507438
C -9.441876 2.785885 0.036967
C -8.056257 2.615319 -0.055849
C -7.461973 1.410414 0.284979
C -5.967801 1.358447 0.129552
C -5.510919 0.902055 -1.245990
C -4.009204 0.824616 -1.454864
C -6.575752 -3.711429 0.175815
N 6.713851 0.951233 1.917390
N 5.052875 -0.009524 0.379522
N 2.920695 -0.257188 -1.304846
O 4.262760 -0.305005 -3.135504
O 3.732375 -0.159079 2.214738
H 5.472947 1.300687 -1.222148
H 6.183697 -1.080310 1.770675
O -6.292131 0.638443 -2.141088

O -8.487222 -1.827971 1.704511
O -10.503001 -0.386074 1.351329
O -10.046296 3.949086 -0.307009
O -6.520728 -1.325334 0.746977
N -1.934565 -0.287288 -0.698159
N 0.121362 -0.351573 -1.535384
H 9.924609 3.469827 -1.364120
H 9.121804 4.694251 0.633150
H 7.569057 3.612269 2.244751
H 9.188938 1.128556 -1.771250
H 5.998922 1.385314 2.486048
H 6.323551 -1.617467 -1.444354
H 7.104231 -0.201743 -2.182179
H 2.093361 -0.410248 -1.887494
H 8.941296 -1.801856 -1.829952
H 8.452179 -1.201975 2.446726
H 9.917672 -1.956223 1.806774
H 9.656610 -0.211929 1.602877
H 6.987727 -2.881624 1.157610
H 8.529588 -3.601455 0.677423
H 7.337990 -3.187368 -0.555839
H 11.321055 -1.486560 -1.739034
H 11.254834 -1.133865 0.078913
H 1.347543 0.011655 1.655757
H -6.172536 -4.693374 0.445843
H -6.271650 -3.487941 -0.850577
H -7.665851 -3.762116 0.217833
H -9.923419 -1.152621 1.622103
H -9.384434 4.583900 -0.616657
H -7.438300 3.442097 -0.397776
H -11.319011 1.894502 0.608163
H -6.461205 -2.856576 2.145524
H -4.247771 -1.718937 1.811970
H -4.253888 -3.462692 1.934061
H -2.643650 -2.812973 0.247472
H -3.929905 -3.755579 -0.476576
H -3.820211 0.668054 -2.521678
H -3.555063 1.772250 -1.138712
H -5.486911 0.742801 0.893581
H -5.554692 2.368709 0.258501
H -3.474517 -1.963465 -2.015331
H -5.010734 -1.586354 -1.263955
H -3.633264 -0.152068 0.429257
H -1.445957 -0.021093 1.376304

H -1.588262 -0.545379 -2.806650

1a-c3, ΔG = 0.6943 kcal/mol,
population = 10.00 %

C 3.954018 -0.123966 -1.585971

C 5.261627 0.215779 -0.912392

C 6.426713 -0.710812 -1.256348

C 7.425612 -0.461558 -0.105664

C 8.137626 0.870765 -0.305204

C 8.862236 1.348572 -1.385756

C 9.397877 2.641208 -1.338611

C 9.187272 3.444435 -0.218205

C 8.434967 2.988568 0.865221

C 7.909040 1.700177 0.801151

C 6.530917 -0.126169 1.139090

C 4.096313 0.221484 1.308952

C 2.812490 0.225358 0.563271

C 8.402879 -1.674654 0.147170

C 9.240308 -1.879577 -1.096251

C 9.194645 -2.913341 -1.933669

C 9.368742 -1.337794 1.300904

C 7.635687 -2.950130 0.521936

C 1.650352 0.418276 1.230313

C 0.327863 0.378232 0.676859

C -1.267772 0.159102 -0.761114

C -0.858206 0.602713 1.354263

C -3.296453 0.522960 0.747547

C -3.745696 -0.791518 1.416585

C -3.438584 -2.100009 0.680573

C -4.295301 -2.491684 -0.530172

C -5.777955 -2.707847 -0.261162

C -7.664710 -1.301719 0.241728

C -8.435273 -0.091850 -0.054977

C -9.784285 -0.051893 0.416567

C -10.616182 1.031361 0.145714

C -10.124130 2.098946 -0.585733

C -8.799693 2.098735 -1.046427

C -7.961315 1.027167 -0.794913

C -6.541584 1.143826 -1.276780

C -5.544153 1.222500 -0.134198

C -4.102314 0.930400 -0.482509

C -6.427158 -3.581058 -1.322051

N 7.151610 1.038465 1.762357

N 5.209132 0.135233 0.547119

N 2.845481 -0.061043 -0.807668

O 3.907090 -0.388682 -2.787144

O 4.149633 0.247784 2.546799

H 5.504575 1.247976 -1.223287

H 6.422280 -0.930587 1.870898

O -5.876755 1.564748 0.986051

O -8.117552 -2.227469 0.934187

O -10.323371 -1.052553 1.132270

O -10.965791 3.133539 -0.824794

O -6.440864 -1.382704 -0.297896

N -1.859286 0.472088 0.429558

N 0.045305 0.101468 -0.655410

H 9.968355 3.020643 -2.180935

H 9.600903 4.449168 -0.190623

H 8.251097 3.624158 1.727085

H 9.005196 0.737371 -2.272805

H 6.563703 1.584557 2.378310

H 6.074403 -1.746414 -1.267924

H 6.861400 -0.481743 -2.230665

H 1.933564 -0.180387 -1.257035

H 9.967166 -1.089929 -1.287931

H 10.071033 -2.165903 1.443251

H 9.945795 -0.432304 1.086624

H 8.824338 -1.187791 2.238926

H 8.352125 -3.760817 0.690050

H 6.941606 -3.280348 -0.254290

H 7.070474 -2.816847 1.448234

H 9.860283 -2.957901 -2.791574

H 8.505708 -3.743077 -1.801940

H 1.735185 0.605398 2.296066

H -6.233643 -3.169879 -2.318839

H -7.506768 -3.658299 -1.170654

H -6.000972 -4.587688 -1.272885

H -9.598176 -1.732240 1.236284

H -10.514277 3.816325 -1.341651

H -8.427405 2.956527 -1.600645

H -11.637642 1.027823 0.511550

H -5.931264 -3.126138 0.739257

H -3.912562 -3.453969 -0.892530

H -4.183863 -1.800544 -1.373157

H -3.530517 -2.908822 1.417277

H -2.384715 -2.102798 0.371417

H -4.066273 0.188931 -1.282123

H -3.694061 1.861804 -0.905755

H -6.422951 2.076893 -1.845363
H -6.261637 0.330945 -1.951456
H -4.815738 -0.707729 1.633766
H -3.240919 -0.832996 2.389786
H -3.409979 1.321001 1.490065
H -1.058981 0.847662 2.387954
H -1.830435 -0.010790 -1.669836

1a-cl6, $\Delta G = 0.7579$ kcal/mol,
population = 8.98 %

C 4.109966 -0.148048 -2.032560
C 5.290033 0.211596 -1.162194
C 6.566294 -0.580235 -1.443020
C 7.391198 -0.380791 -0.153244
C 7.983669 1.021133 -0.106386
C 8.776784 1.692122 -1.023509
C 9.176344 3.007098 -0.755764
C 8.764661 3.637228 0.418087
C 7.941957 2.984598 1.337683
C 7.552469 1.677661 1.054536
C 6.322189 -0.277399 0.989932
C 3.865714 -0.117046 0.875580
C 2.687234 -0.122402 -0.027149
C 8.461812 -1.512300 0.100477
C 9.108642 -1.271296 1.447913
C 10.381000 -0.958393 1.681337
C 7.801133 -2.906977 0.162678
C 9.488654 -1.530807 -1.034824
C 1.439698 -0.094372 0.498038
C 0.203349 -0.174177 -0.223740
C -1.178884 -0.372016 -1.871879
C -1.071944 -0.138432 0.314700
C -3.402234 -0.301811 -0.649746
C -3.942421 -1.664196 -1.092740
C -3.696082 -2.771039 -0.068682
C -4.495745 -2.636628 1.232906
C -6.019022 -2.683832 1.130806
C -7.747703 -1.019456 1.129605
C -8.239992 0.321672 0.791381
C -9.646224 0.545209 0.948610
C -10.231708 1.759636 0.605607
C -9.432865 2.791207 0.140530
C -8.048579 2.622234 0.026712
C -7.449815 1.412346 0.341021

C -5.957925 1.362864 0.164187
C -5.520575 0.926240 -1.224142
C -4.021941 0.853183 -1.455696
C -6.557890 -3.708260 0.150472
N 6.755688 0.836665 1.825297
N 5.066550 -0.036835 0.261088
N 2.912801 -0.250769 -1.404167
O 4.235007 -0.284017 -3.249541
O 3.766209 -0.227404 2.106064
H 5.476348 1.287437 -1.331708
H 6.195043 -1.177657 1.597502
O -6.314390 0.674374 -2.111519
O -8.457087 -1.848447 1.721883
O -10.476719 -0.400442 1.420088
O -10.041728 3.959589 -0.176997
O -6.501888 -1.328890 0.750314
N -1.935044 -0.264320 -0.739611
N 0.110137 -0.320177 -1.603248
H 9.798985 3.538420 -1.469201
H 9.074040 4.660070 0.616830
H 7.601328 3.485784 2.239566
H 9.075797 1.216736 -1.953620
H 6.051863 1.247476 2.424647
H 6.309235 -1.632305 -1.598203
H 7.087319 -0.211394 -2.328180
H 2.077160 -0.387760 -1.978990
H 8.440937 -1.395148 2.302191
H 7.401819 -3.206729 -0.810246
H 8.559651 -3.643129 0.448469
H 6.994438 -2.959601 0.900190
H 10.194583 -2.353718 -0.880580
H 10.061916 -0.602908 -1.092226
H 8.992696 -1.689799 -1.997606
H 10.739865 -0.826338 2.698584
H 11.104919 -0.823179 0.882435
H 1.375952 -0.023617 1.579168
H -6.148209 -4.691917 0.404044
H -6.266669 -3.471457 -0.876681
H -7.647237 -3.763083 0.204549
H -9.893733 -1.170316 1.673303
H -9.384216 4.599199 -0.485930
H -7.435273 3.454349 -0.310587
H -11.302366 1.890678 0.722769
H -6.422902 -2.876928 2.128779

H -4.216104 -1.729011 1.782736
H -4.216520 -3.474267 1.884675
H -2.628064 -2.800802 0.187052
H -3.920435 -3.738074 -0.532996
H -3.848231 0.709581 -2.526890
H -3.564693 1.797862 -1.135076
H -5.466990 0.734714 0.911565
H -5.542576 2.370830 0.302985
H -3.487903 -1.926994 -2.055956
H -5.015829 -1.562051 -1.281573
H -3.618928 -0.144352 0.411260
H -1.419678 -0.041812 1.333677
H -1.615597 -0.482437 -2.856850

1a-c25, $\Delta G = 1.3256$ kcal/mol,
population = 3.44 %

C 4.252777 1.502317 -1.503831
C 5.360544 0.875717 -0.691523
C 6.636030 0.559897 -1.470568
C 7.353570 -0.470631 -0.568855
C 8.001574 0.221992 0.619997
C 8.933997 1.245805 0.655485
C 9.363137 1.740014 1.893429
C 8.845018 1.210219 3.075033
C 7.892698 0.189676 3.053585
C 7.477136 -0.290578 1.813650
C 6.193655 -1.252137 0.144031
C 3.757130 -0.876798 0.113301
C 2.662271 -0.031355 -0.425094
C 8.349531 -1.416521 -1.343007
C 9.394087 -0.560332 -2.023567
C 10.711954 -0.611978 -1.847137
C 8.973087 -2.424955 -0.372381
C 7.628062 -2.202149 -2.460922
C 1.375286 -0.344776 -0.145848
C 0.203923 0.323912 -0.632288
C -1.038835 1.717977 -1.709347
C -1.109269 0.011316 -0.322262
C -3.348043 1.049945 -0.974698
C -3.818882 1.752173 0.305236
C -3.608140 0.989856 1.617616
C -4.545851 1.511614 2.721989
C -5.754624 0.635966 3.025391
C -7.779412 0.148942 1.826583

C -8.433094 -0.391780 0.628589
C -9.858673 -0.281748 0.569684
C -10.575623 -0.725055 -0.536438
C -9.900596 -1.334106 -1.582283
C -8.514154 -1.514878 -1.526009
C -7.779635 -1.052821 -0.445362
C -6.296611 -1.289931 -0.508635
C -5.534700 -0.173819 -1.194687
C -4.023418 -0.308809 -1.200252
C -5.416946 -0.697776 3.668261
N 6.575764 -1.318102 1.551289
N 5.008235 -0.422658 -0.120063
N 3.003619 1.023981 -1.281226
O 4.480005 2.430098 -2.280051
O 3.547196 -1.948322 0.699382
H 5.588935 1.593441 0.116999
H 5.999466 -2.256131 -0.242331
O -6.087117 0.760748 -1.745172
O -8.417176 0.434846 2.851748
O -10.578326 0.263763 1.566252
O -10.637086 -1.759644 -2.637486
O -6.458234 0.350775 1.752018
N -1.885513 0.902831 -1.014856
N 0.224041 1.402257 -1.509247
H 10.093701 2.542450 1.931778
H 9.177580 1.603546 4.032221
H 7.478897 -0.210304 3.975215
H 9.326735 1.667080 -0.265373
H 5.828564 -1.491029 2.210969
H 6.367304 0.128565 -2.439484
H 7.241816 1.452080 -1.638068
H 2.218499 1.498039 -1.735031
H 8.996703 0.144952 -2.756256
H 8.202379 -3.071383 0.058147
H 9.685983 -3.063679 -0.903240
H 9.500262 -1.927905 0.448074
H 7.258593 -1.551585 -3.258157
H 6.787484 -2.786316 -2.072497
H 8.338616 -2.902243 -2.912239
H 11.371102 0.039850 -2.414331
H 11.179655 -1.288274 -1.136995
H 1.221489 -1.199740 0.504863
H -4.923923 -0.521984 4.629486
H -4.747015 -1.287575 3.034811

H -6.326146 -1.279043 3.849639
 H -9.933870 0.433845 2.306161
 H -10.058865 -2.168597 -3.297223
 H -8.008302 -2.026264 -2.341500
 H -11.654341 -0.610546 -0.558786
 H -6.444350 1.194080 3.663222
 H -4.892803 2.520565 2.466244
 H -4.008554 1.605292 3.672983
 H -2.564548 1.086983 1.935333
 H -3.780580 -0.082589 1.471234
 H -3.711111 -1.052738 -0.462656
 H -3.739189 -0.696648 -2.188665
 H -6.091859 -2.194553 -1.100901
 H -5.842784 -1.464738 0.469800
 H -4.887134 1.953867 0.172382
 H -3.326508 2.730948 0.364494
 H -3.599917 1.698106 -1.821036
 H -1.519110 -0.757605 0.315387
 H -1.406901 2.516984 -2.342274

1a-c12, $\Delta G = 1.4753$ kcal/mol,
 population = 2.67 %

C 3.940867 -2.106090 0.242926
 C 4.900416 -0.993393 -0.106144
 C 6.240038 -1.030452 0.627874
 C 6.765471 0.414345 0.467912
 C 7.298381 0.633218 -0.940451
 C 8.263089 -0.060430 -1.653987
 C 8.557962 0.325861 -2.967101
 C 7.872755 1.389720 -3.552996
 C 6.879680 2.080499 -2.856707
 C 6.598735 1.683808 -1.551181
 C 5.478338 1.306989 0.437145
 C 3.092800 0.685584 0.337743
 C 2.129751 -0.443769 0.309026
 C 7.768518 0.866801 1.599498
 C 7.093103 0.746956 2.950375
 C 6.729234 1.743858 3.754708
 C 8.993589 -0.065306 1.621039
 C 8.249592 2.297566 1.331482
 C 0.799854 -0.190771 0.299839
 C -0.258258 -1.157138 0.339705
 C -1.269383 -3.058953 0.439928
 C -1.617524 -0.889436 0.334465

C -3.690426 -2.380688 0.369239
 C -4.204350 -2.490933 -1.076731
 C -3.963887 -1.247583 -1.939878
 C -4.771492 -1.206416 -3.241055
 C -6.285492 -1.096720 -3.071367
 C -6.894188 -0.278335 -0.854028
 C -6.771000 0.861789 0.061548
 C -6.637806 2.203379 -0.393764
 C -6.539854 3.260396 0.505597
 C -6.531684 2.999912 1.866836
 C -6.614571 1.685199 2.343241
 C -6.743313 0.621869 1.464918
 C -6.833754 -0.759493 2.073997
 C -5.824699 -1.814804 1.633874
 C -4.446930 -1.346565 1.204643
 C -7.005211 -0.774239 -4.363227
 N 5.675266 2.237419 -0.670161
 N 4.393240 0.338036 0.222975
 N 2.640449 -1.746938 0.382720
 O 4.321250 -3.273091 0.334368
 O 2.739900 1.862755 0.499138
 H 5.072362 -1.072081 -1.195162
 H 5.282945 1.847093 1.368955
 O -6.080411 -2.998265 1.765105
 O -7.240689 -1.399363 -0.518841
 O -6.624545 2.554610 -1.697983
 O -6.427804 4.061236 2.702342
 O -6.551633 0.014586 -2.138761
 N -2.244370 -2.104587 0.402907
 N -0.062493 -2.531828 0.407014
 H 9.313445 -0.211921 -3.531888
 H 8.101889 1.679735 -4.575144
 H 6.330607 2.893921 -3.323044
 H 8.779283 -0.909160 -1.213646
 H 4.842275 2.670601 -1.046786
 H 6.065343 -1.285321 1.677314
 H 6.920539 -1.766738 0.196675
 H 1.946031 -2.489412 0.499263
 H 6.926127 -0.273468 3.296861
 H 9.555752 0.011172 0.686329
 H 9.658714 0.227650 2.440320
 H 8.706066 -1.110622 1.775553
 H 8.765831 2.345748 0.367734
 H 8.953042 2.604017 2.112532

H 7.426904 3.018177 1.310678
 H 6.269309 1.535870 4.717133
 H 6.873596 2.788978 3.494418
 H 0.511689 0.855453 0.277191
 H -6.652764 0.177735 -4.774513
 H -8.086003 -0.717556 -4.204797
 H -6.802521 -1.561865 -5.095677
 H -6.594991 1.741446 -2.239979
 H -6.436049 3.760631 3.622392
 H -6.577725 1.502196 3.414032
 H -6.459178 4.276394 0.133223
 H -6.698501 -1.999968 -2.616373
 H -4.582927 -2.111201 -3.834526
 H -4.427761 -0.353868 -3.841403
 H -2.900028 -1.191934 -2.200021
 H -4.176857 -0.332638 -1.372479
 H -4.507503 -0.373093 0.710652
 H -3.910681 -1.165778 2.150025
 H -7.825661 -1.195736 1.927272
 H -6.685895 -0.660555 3.158775
 H -5.274213 -2.714692 -1.005778
 H -3.729965 -3.360194 -1.549118
 H -3.815830 -3.356797 0.850463
 H -2.153576 0.047344 0.291613
 H -1.505731 -4.115057 0.499566

1b-c10, $\Delta G = 0.0000$ kcal/mol,
 population = 74.04 %

C 5.550843 1.641458 -0.134844
 C 6.801905 1.702383 0.707631
 C 8.000083 0.941434 0.142830
 C 8.911058 0.754387 1.375116
 C 9.623716 2.059864 1.705722
 C 10.422341 2.871274 0.915499
 C 10.940785 4.057137 1.449308
 C 10.639129 4.423636 2.760525
 C 9.812199 3.632326 3.558942
 C 9.305257 2.455632 3.011926
 C 7.926432 0.646266 2.592180
 C 5.480131 0.933277 2.696400
 C 4.252370 1.209598 1.907818
 C 9.878315 -0.487339 1.253477
 C 10.781530 -0.269257 0.059299

C 10.772586 -0.945561 -1.087250
 C 10.776356 -0.573852 2.503324
 C 9.098206 -1.803840 1.132950
 C 3.042004 1.148153 2.511279
 C 1.762084 1.308500 1.884129
 C 0.276999 1.619288 0.351358
 C 0.526625 1.242690 2.506314
 C -1.863568 1.446753 1.669083
 C -2.369202 0.080792 2.140387
 C -2.337900 -0.983243 1.044750
 C -3.338303 -0.764607 -0.096235
 C -4.823717 -0.766411 0.259802
 C -6.463432 0.949391 0.610393
 C -6.843583 2.292604 1.065581
 C -8.247313 2.569757 1.138486
 C -8.723560 3.791888 1.601804
 C -7.822374 4.779281 1.964158
 C -6.444586 4.556931 1.858870
 C -5.950531 3.338987 1.418880
 C -4.452406 3.232404 1.354384
 C -3.816942 2.707980 2.630838
 C -2.304803 2.579230 2.613130
 C -5.232521 -1.814085 1.277844
 N 8.485832 1.512820 3.624836
 N 6.645927 1.113015 2.037069
 N 4.388259 1.436053 0.532476
 O 5.594247 1.822795 -1.351385
 O 5.443942 0.520226 3.864193
 H 7.053832 2.774342 0.799992
 H 7.777000 -0.361322 2.987813
 O -4.468159 2.432196 3.621377
 O -7.291776 0.165072 0.119729
 O -9.177741 1.670450 0.776619
 O -8.330514 5.957941 2.399854
 O -5.184298 0.586978 0.764836
 N -0.403327 1.442946 1.520753
 N 1.580270 1.545077 0.525776
 H 11.569181 4.696145 0.836382
 H 11.040152 5.348587 3.166783
 H 9.558800 3.931667 4.572249
 H 10.637119 2.605833 -0.116112
 H 7.846069 1.821326 4.345381
 H 7.664196 -0.018832 -0.259855
 H 8.500820 1.494576 -0.653415

H 3.513198 1.491575 0.004555
 H 11.521961 0.520342 0.189399
 H 11.377794 0.332985 2.623881
 H 10.176614 -0.714394 3.408513
 H 11.457133 -1.426394 2.407998
 H 9.807887 -2.629069 1.015071
 H 8.419133 -1.828207 0.277258
 H 8.514039 -2.003261 2.035252
 H 11.481190 -0.704830 -1.875244
 H 10.071401 -1.751825 -1.284833
 H 3.047540 0.935480 3.575501
 H -4.765690 -1.632374 2.249858
 H -4.910989 -2.798892 0.922255
 H -6.316975 -1.829616 1.404774
 H -8.670819 0.889410 0.415325
 H -7.611695 6.569425 2.614711
 H -5.753453 5.354759 2.119812
 H -9.793372 3.964586 1.655787
 H -5.394911 -0.903565 -0.662798
 H -3.206765 -1.581929 -0.816846
 H -3.119094 0.155573 -0.652484
 H -2.517516 -1.963806 1.500225
 H -1.329054 -1.032611 0.612514
 H -1.869051 3.524404 2.265455
 H -1.964237 2.376020 3.633607
 H -4.023826 4.232392 1.199631
 H -4.111078 2.630339 0.508804
 H -3.391415 0.203588 2.511423
 H -1.769419 -0.239121 3.001505
 H -2.243877 1.656327 0.663929
 H 0.259061 1.076004 3.539875
 H -0.235529 1.794424 -0.587407

1b-c6, ΔG = 0.8285 kcal/mol,
 population = 18.26 %

C 4.399900 0.969825 -1.801578
 C 5.482118 0.630934 -0.804415
 C 6.751492 0.027185 -1.404081
 C 7.422476 -0.653270 -0.188983
 C 8.085734 0.383763 0.704319
 C 9.035191 1.348698 0.407768
 C 9.473205 2.215381 1.416572
 C 8.943309 2.114830 2.702600
 C 7.965991 1.166630 3.009559

C 7.541172 0.312198 1.994613
 C 6.232477 -1.109497 0.721866
 C 3.813013 -0.665240 0.544027
 C 2.751946 -0.014548 -0.265348
 C 8.369492 -1.859232 -0.564350
 C 7.582069 -2.898369 -1.336400
 C 7.232233 -4.112973 -0.917552
 C 9.502713 -1.374851 -1.487196
 C 8.992727 -2.450037 0.705722
 C 1.454709 -0.152862 0.096023
 C 0.308970 0.343145 -0.608902
 C -0.881985 1.305202 -2.126790
 C -1.014953 0.205088 -0.225767
 C -3.222095 0.901261 -1.299695
 C -3.839793 -0.433810 -1.734634
 C -3.734313 -1.593660 -0.738562
 C -4.793395 -2.673303 -1.028680
 C -5.989770 -2.687056 -0.086442
 C -7.859559 -1.209775 0.219997
 C -8.366007 0.124152 0.562700
 C -9.781993 0.309369 0.489991
 C -10.367410 1.543533 0.760709
 C -9.565647 2.602032 1.157968
 C -8.183354 2.435568 1.296850
 C -7.580624 1.224032 1.005617
 C -6.087749 1.175094 1.175398
 C -5.324370 1.554136 -0.077329
 C -3.813723 1.445144 0.007676
 C -5.663478 -3.121107 1.331544
 N 6.604084 -0.712530 2.076232
 N 5.080212 -0.378517 0.174030
 N 3.132659 0.652563 -1.437293
 O 4.662736 1.550297 -2.854629
 O 3.561411 -1.453524 1.466745
 H 5.728363 1.577493 -0.289722
 H 6.016091 -2.181499 0.675521
 O -5.871858 1.960062 -1.085932
 O -8.610028 -2.193995 0.125793
 O -10.620633 -0.683908 0.148245
 O -10.067053 3.826875 1.449109
 O -6.545937 -1.314957 -0.015257
 N -1.757594 0.823508 -1.196851
 N 0.368653 1.040129 -1.810217
 H 10.218078 2.972968 1.192513

H 9.283261 2.794995 3.479253
 H 7.537766 1.106016 4.006333
 H 9.428982 1.450581 -0.599755
 H 5.850242 -0.631952 2.745917
 H 6.472260 -0.700132 -2.171974
 H 7.391453 0.787106 -1.855630
 H 2.365894 0.968622 -2.036679
 H 7.310842 -2.612629 -2.353111
 H 10.117513 -2.230176 -1.787205
 H 9.112518 -0.903022 -2.395134
 H 10.149499 -0.660751 -0.969906
 H 9.652500 -3.283025 0.441858
 H 8.239499 -2.819397 1.407526
 H 9.589448 -1.690746 1.220782
 H 6.682450 -4.784485 -1.571636
 H 7.476819 -4.483454 0.074359
 H 1.269466 -0.715316 1.005635
 H -6.559852 -3.097017 1.958920
 H -4.904824 -2.473737 1.782299
 H -5.282036 -4.146882 1.316306
 H -10.056797 -1.503647 0.083304
 H -11.026892 3.830512 1.323101
 H -7.585825 3.274062 1.641451
 H -11.445670 1.647799 0.678100
 H -6.763975 -3.333693 -0.506210
 H -4.354492 -3.675209 -0.956396
 H -5.153446 -2.570122 -2.059868
 H -3.856745 -1.229557 0.288059
 H -2.731387 -2.030826 -0.787206
 H -3.429619 2.459892 0.184314
 H -3.526498 0.841496 0.872882
 H -5.721526 0.204900 1.520625
 H -5.779601 1.902783 1.941002
 H -3.390220 -0.727410 -2.691526
 H -4.896173 -0.231933 -1.941296
 H -3.420593 1.631282 -2.091891
 H -1.452993 -0.271052 0.638822
 H -1.220544 1.840319 -3.006259

1b-c13, $\Delta G = 1.6944$ kcal/mol,
 population = 4.23 %

C 3.427490 -1.550914 1.405805
 C 4.541142 -0.976418 0.564619
 C 5.735563 -0.447762 1.357246

C 6.450575 0.475571 0.344713
 C 7.227438 -0.347684 -0.671075
 C 8.228610 -1.285970 -0.480958
 C 8.780770 -1.935394 -1.591984
 C 8.314771 -1.645024 -2.874100
 C 7.294240 -0.714811 -3.078998
 C 6.757391 -0.076904 -1.962902
 C 5.296656 1.043659 -0.557817
 C 2.884633 0.536171 -0.562630
 C 1.809145 -0.266533 0.072375
 C 7.326419 1.603505 1.014697
 C 8.355267 0.944127 1.905677
 C 9.678697 1.045958 1.812587
 C 7.970518 2.474964 -0.067742
 C 6.474420 2.512480 1.927921
 C 0.517067 -0.036017 -0.260356
 C -0.639983 -0.657774 0.315062
 C -1.848880 -1.928812 1.576491
 C -1.962341 -0.398417 -0.002805
 C -4.182402 -1.252350 0.838392
 C -4.718326 -2.666192 0.621243
 C -4.328690 -3.318547 -0.708674
 C -4.650615 -2.537798 -1.991832
 C -6.099907 -2.106439 -2.219536
 C -6.030410 0.260895 -1.756797
 C -6.093414 1.343710 -0.765601
 C -5.626776 2.630142 -1.197893
 C -5.588182 3.720456 -0.335627
 C -6.017633 3.568746 0.972317
 C -6.491768 2.332232 1.423039
 C -6.531866 1.227224 0.585330
 C -7.080552 -0.021035 1.242330
 C -6.191525 -0.668391 2.302614
 C -4.682811 -0.636429 2.158682
 C -7.148531 -3.157111 -1.924401
 N 5.771957 0.904783 -1.930514
 N 4.146953 0.187265 -0.227170
 N 2.167402 -1.179015 1.072544
 O 3.665326 -2.350590 2.311057
 O 2.647220 1.493174 -1.313047
 H 4.871319 -1.791261 -0.104222
 H 5.011633 2.080901 -0.361616
 O -6.709243 -1.224325 3.256310
 O -5.622805 0.439842 -2.914927

O -5.196984 2.854661 -2.449682
 O -5.962694 4.656013 1.777268
 O -6.404283 -0.954187 -1.341636
 N -2.714191 -1.211502 0.801526
 N -0.593861 -1.625698 1.312426
 H 9.566465 -2.671878 -1.452690
 H 8.743199 -2.158022 -3.731293
 H 6.922015 -0.501902 -4.077361
 H 8.581440 -1.521443 0.518775
 H 5.065491 0.911201 -2.654673
 H 5.369489 0.112658 2.222609
 H 6.381028 -1.255215 1.707689
 H 1.388030 -1.624558 1.564456
 H 7.935588 0.354084 2.722847
 H 8.595284 3.245934 0.394431
 H 8.595480 1.885793 -0.746220
 H 7.202541 2.979669 -0.661806
 H 7.111866 3.312095 2.319155
 H 6.061406 1.973989 2.785019
 H 5.650280 2.981986 1.382026
 H 10.323581 0.544645 2.529444
 H 10.165544 1.617241 1.026996
 H 0.345363 0.715735 -1.024045
 H -8.145320 -2.780896 -2.171502
 H -7.140962 -3.466166 -0.875857
 H -6.949014 -4.037902 -2.543032
 H -5.269769 1.978736 -2.925265
 H -6.287129 4.432708 2.661630
 H -6.841016 2.236876 2.449116
 H -5.224380 4.676305 -0.697777
 H -6.204589 -1.759064 -3.250732
 H -4.380089 -3.173590 -2.844670
 H -4.011794 -1.648884 -2.074021
 H -4.812643 -4.301798 -0.749942
 H -3.248436 -3.515008 -0.709284
 H -4.353380 0.410330 2.202609
 H -4.259153 -1.173716 3.012841
 H -7.319887 -0.802694 0.519793
 H -8.015684 0.231333 1.752648
 H -5.809564 -2.612012 0.701764
 H -4.391492 -3.308869 1.449320
 H -4.497200 -0.612139 0.014391
 H -2.413376 0.280415 -0.713694
 H -2.183688 -2.651358 2.310569

1b-c9, $\Delta G = 1.8105$ kcal/mol,

population = 3.47 %

C 2.985180 0.386618 -1.510916
 C 4.337232 0.498683 -0.848684
 C 5.500862 -0.088002 -1.647861
 C 6.597235 -0.280865 -0.575852
 C 7.235617 1.053249 -0.219916
 C 7.842710 2.001826 -1.027557
 C 8.334065 3.180692 -0.453729
 C 8.196010 3.400821 0.916415
 C 7.561515 2.467760 1.738129
 C 7.078363 1.300257 1.151480
 C 5.815040 -0.594871 0.744418
 C 3.396009 -0.575167 1.214400
 C 2.045737 -0.358134 0.636232
 C 7.647502 -1.408907 -0.919142
 C 6.925925 -2.723657 -1.134954
 C 6.954963 -3.793396 -0.342301
 C 8.373711 -1.071731 -2.234163
 C 8.689749 -1.512269 0.200281
 C 0.949361 -0.602347 1.391806
 C -0.419150 -0.523736 0.970903
 C -2.139972 -0.234929 -0.295662
 C -1.534998 -0.790694 1.746898
 C -4.033496 -0.783890 1.265902
 C -4.319766 -2.231871 1.673407
 C -4.191590 -3.268151 0.543960
 C -5.489501 -3.614304 -0.208434
 C -5.890851 -2.725213 -1.374326
 C -6.117980 -0.332361 -1.599362
 C -6.311315 0.976565 -0.958885
 C -6.111855 2.126927 -1.793725
 C -6.232751 3.420381 -1.297492
 C -6.561707 3.609580 0.034374
 C -6.772269 2.511226 0.874131
 C -6.650757 1.210949 0.405294
 C -6.927883 0.157699 1.461159
 C -5.948589 0.179882 2.631377
 C -4.460252 0.223007 2.342549
 C -7.090627 -3.266210 -2.130190
 N 6.437650 0.233181 1.772450
 N 4.430606 -0.217427 0.422934
 N 1.956251 0.006424 -0.713205

O 2.832123 0.679234 -2.696565
 O 3.570200 -1.092353 2.327167
 H 4.507403 1.578191 -0.685086
 H 5.825432 -1.650015 1.035223
 O -6.360070 0.151180 3.778227
 O -5.819548 -0.454837 -2.797167
 O -5.794268 2.023277 -3.093796
 O -6.672329 4.884534 0.476294
 O -6.239990 -1.405162 -0.812528
 N -2.616980 -0.602644 0.928980
 N -0.824420 -0.176227 -0.313020
 H 8.812415 3.928007 -1.079555
 H 8.573946 4.321093 1.354235
 H 7.433953 2.652571 2.801227
 H 7.925614 1.848107 -2.099967
 H 5.888990 0.410608 2.603482
 H 5.188847 -1.041306 -2.084579
 H 5.821592 0.578304 -2.450569
 H 1.011559 0.021572 -1.106447
 H 6.353459 -2.791769 -2.060595
 H 9.056375 -1.888722 -2.491210
 H 7.671937 -0.943307 -3.064997
 H 8.966551 -0.159009 -2.129341
 H 9.423630 -2.285703 -0.048710
 H 8.242490 -1.764269 1.165982
 H 9.219136 -0.560853 0.311572
 H 6.410804 -4.694446 -0.612528
 H 7.513031 -3.817018 0.589883
 H 1.134083 -0.910449 2.415939
 H -7.936098 -3.408115 -1.448606
 H -6.835654 -4.234229 -2.572413
 H -7.388990 -2.587962 -2.933099
 H -5.735417 1.043906 -3.284618
 H -6.907682 4.890948 1.415335
 H -7.045028 2.679783 1.913923
 H -6.071018 4.264618 -1.959478
 H -5.039106 -2.573481 -2.046741
 H -6.329308 -3.681544 0.497035
 H -5.373468 -4.614903 -0.643393
 H -3.823270 -4.198838 0.988944
 H -3.418855 -2.954194 -0.172454
 H -4.220662 1.237008 1.992299
 H -3.927613 0.048888 3.282884
 H -6.926665 -0.853676 1.054006

H -7.921116 0.335349 1.885114
 H -5.331083 -2.279216 2.096502
 H -3.642854 -2.488683 2.497579
 H -4.564750 -0.553261 0.343851
 H -1.625658 -1.088933 2.781589
 H -2.803185 -0.026387 -1.127932

1b-enantiomer-c3, ΔG = 0.0000

kcal/mol, population = 63.64 %

H 1.736234 -0.295801 2.087037
 H 1.241308 0.422611 -2.040145
 H 3.744353 -0.156241 0.835997
 H 3.269659 1.736746 -1.503610
 H 4.891574 1.294993 -1.012479
 H 5.611917 -1.129831 0.992273
 H 5.525329 -2.732450 0.302608
 H 3.465053 -0.879153 -2.132880
 H 3.370401 -2.026056 -0.763422
 H 2.828249 2.532172 0.884692
 H 4.016431 3.463121 -0.003653
 H 4.618409 1.346029 2.151203
 H 4.705459 3.083731 2.313814
 H 6.893953 2.405963 2.160810
 H 11.294933 -2.462569 -0.151584
 H 7.255745 -3.854934 -0.616032
 H 9.114648 -5.069575 -1.108130
 H 10.170817 0.613085 1.085548
 H 7.815906 3.330795 0.092721
 H 6.408942 4.299466 0.573647
 H 6.265113 3.131442 -0.752726
 H -1.547323 0.563649 -2.075406
 H -8.569595 3.251691 2.787822
 H -9.977992 2.203712 3.379693
 H -7.016664 3.505625 -0.533924
 H -6.916995 3.328157 1.223603
 H -8.307969 4.129433 0.490505
 H -9.957571 2.927621 -0.903635
 H -8.678203 2.215136 -1.905352
 H -9.879106 1.168160 -1.119727
 H -10.019983 0.978686 1.314693
 H -2.012344 0.008079 1.495655
 H -7.000472 0.004248 2.153956
 H -6.163983 1.518214 1.762196

H -6.345449 -0.315523 -2.845788
 H -9.135773 -1.107699 1.614907
 H -8.057579 -2.425824 -3.075615
 H -9.538600 -3.845426 -1.672244
 H -10.067508 -3.196700 0.659303
 N -0.079734 -0.046306 0.974080
 N 1.903771 0.055609 -0.021079
 O 6.684061 0.913899 0.734636
 O 9.833147 -4.457320 -0.894446
 O 10.678090 -0.167985 0.724849
 O 8.791345 1.337516 1.379260
 O 5.969155 -0.933993 -2.120432
 H -6.275923 1.864550 -1.484657
 H -5.552641 -1.273880 0.699980
 O -3.943585 0.980999 -2.363244
 O -4.093375 -0.322486 2.852014
 N -2.887552 0.064155 0.968040
 N -5.145358 0.388546 -0.535895
 N -6.985113 -0.008482 -2.124537
 C 6.731428 3.314521 0.219291
 C 3.805797 -1.081132 -1.112219
 C 5.317964 -1.209021 -1.129655
 C 5.953539 -1.732417 0.147168
 C 7.451714 -1.838391 0.083131
 C 7.946423 -3.056549 -0.355565
 C 9.324374 -3.278447 -0.460073
 C 10.225007 -2.290370 -0.098318
 C 9.748047 -1.067953 0.363508
 C 8.344221 -0.791243 0.435655
 C 7.963460 0.552300 0.889301
 C 6.322933 2.267661 1.238281
 C 4.837454 2.265712 1.594077
 C 3.837197 2.482886 0.452679
 C 3.869180 1.417825 -0.641960
 C 3.364032 0.052190 -0.169388
 C 0.973776 0.256006 -1.006558
 C 1.223546 -0.120685 1.148350
 C -0.261643 0.190240 -0.384307
 C -1.541630 0.350994 -1.011174
 C -7.598303 3.304610 0.369659
 C -9.277274 2.074788 -0.999688
 C -9.270448 2.444971 2.590914
 C -9.280070 1.768845 1.444265
 C -8.378071 1.987945 0.249331

C -2.751884 0.290288 -0.407397
 C -3.979660 0.567483 -1.195602
 C -6.425664 0.856422 -1.090525
 C -7.804342 -0.952331 -1.513010
 C -8.311085 -2.128299 -2.061803
 C -9.137767 -2.921020 -1.264556
 C -9.439327 -2.556626 0.047269
 C -8.921086 -1.371468 0.582842
 C -8.122725 -0.558631 -0.206177
 C -7.410458 0.746593 0.126253
 C -6.499613 0.558314 1.358438
 C -5.301248 -0.201854 0.793067
 C -4.050111 -0.141025 1.635478

1b-enantiomer-c9, $\Delta G = 0.8927$

kcal/mol, population = 14.08 %
 H 1.210351 -1.913684 2.963879
 H 1.461167 0.383254 -0.565534
 H 3.407426 -1.702090 2.040301
 H 4.920690 0.132315 1.999489
 H 3.429525 0.616107 2.785755
 H 5.716626 -1.746325 -2.031764
 H 5.708662 -0.084204 -1.484581
 H 3.505674 -0.727648 -0.868738
 H 3.379800 -2.385050 -0.283542
 H 2.794418 2.048771 0.966946
 H 3.900204 1.291894 -0.159169
 H 5.233287 2.452472 2.261817
 H 4.455116 3.643118 1.235128
 H 6.854961 3.276572 0.751054
 H 11.401950 -1.735189 -0.835827
 H 7.484571 -3.174618 -1.864574
 H 9.397538 -4.378706 -2.046265
 H 10.103544 1.403440 0.016318
 H 5.385954 4.236162 -1.010685
 H 4.966651 2.603822 -1.575827
 H 6.635206 3.197685 -1.723691
 H -1.263411 0.841674 -0.925079
 H -7.591280 4.473672 0.019046
 H -6.799058 4.744854 1.671308
 H -9.603318 1.654089 -1.224755
 H -8.281151 2.821726 -1.367350
 H -9.714371 3.221799 -0.403001
 H -9.138067 0.793653 2.380812

H -10.167661 2.111241 1.793693
 H -10.159991 0.559004 0.943707
 H -7.357867 2.531455 2.383777
 H -2.369780 -0.982822 2.031590
 H -7.393238 -0.861606 1.801491
 H -6.504066 0.630823 2.174307
 H -5.821740 0.720163 -2.735849
 H -9.401129 -1.525634 0.501807
 H -7.457920 -1.010864 -4.066503
 H -9.176908 -2.747682 -3.611775
 H -10.136916 -3.009927 -1.343695
 N -0.372491 -1.042399 1.809849
 N 1.755486 -0.806982 1.210550
 O 6.587948 1.298199 0.134526
 O 10.073273 -3.765054 -1.724059
 O 10.644635 0.576908 -0.115264
 O 8.672878 2.132723 0.038434
 O 5.844826 -2.022816 0.986101
 H -6.043359 2.206881 -0.623443
 H -5.702044 -1.571661 0.226675
 O -3.561190 1.565459 -1.383203
 O -4.666906 -1.625759 2.800310
 N -3.134234 -0.650836 1.437860
 N -5.078417 0.408511 -0.160801
 N -6.584297 0.767515 -2.072842
 C 5.742428 3.204400 -1.090732
 C 3.787514 -1.391924 -0.047427
 C 5.296173 -1.537176 0.014075
 C 6.053917 -1.086403 -1.218583
 C 7.546984 -1.182968 -1.074909
 C 8.116262 -2.384228 -1.466202
 C 9.495844 -2.594280 -1.360330
 C 10.328206 -1.589892 -0.892633
 C 9.778136 -0.367541 -0.521570
 C 8.365553 -0.140940 -0.562490
 C 7.896632 1.177315 -0.119254
 C 6.064256 2.675637 0.295560
 C 4.871438 2.629079 1.241299
 C 3.787343 1.593270 0.888557
 C 3.868684 0.371521 1.810429
 C 3.218468 -0.919460 1.297559
 C 1.018086 -0.133573 0.272748
 C 0.876047 -1.331286 2.113324
 C -0.307362 -0.285314 0.645683

C -1.451028 0.238633 -0.042375
 C -9.030954 2.413674 -0.683360
 C -9.532240 1.276117 1.480228
 C -7.331375 4.078797 0.997498
 C -7.642415 2.841101 1.377784
 C -8.403573 1.804902 0.576037
 C -2.750046 0.070404 0.299655
 C -3.811629 0.735975 -0.497000
 C -6.237610 1.132737 -0.703106
 C -7.503196 -0.275923 -2.033083
 C -7.897986 -1.108471 -3.077856
 C -8.860349 -2.083828 -2.811472
 C -9.404405 -2.231860 -1.536053
 C -8.996555 -1.386421 -0.496963
 C -8.062936 -0.394791 -0.752766
 C -7.430441 0.627921 0.178578
 C -6.761813 -0.077019 1.381028
 C -5.475934 -0.640381 0.777245
 C -4.400731 -1.000342 1.774139

1b-enantiomer-c5, $\Delta G = 1.3512$
 kcal/mol, population = 6.49 %

H 2.702606 -0.273908 1.244072
 H 1.648075 1.286209 -2.531302
 H 4.519455 0.430930 -0.104999
 H 3.828406 2.397689 -2.342597
 H 5.421764 2.159987 -1.662944
 H 7.862040 -0.658780 -2.067103
 H 7.214204 0.699020 -1.168938
 H 3.803704 -0.152893 -3.022195
 H 4.247513 -1.320320 -1.751751
 H 2.962593 3.269023 -0.216740
 H 4.370943 4.166496 -0.744316
 H 4.201934 2.127143 1.545377
 H 4.420842 3.857845 1.653917
 H 6.491401 2.884642 2.169473
 H 6.173767 -4.095477 2.271030
 H 6.900081 -2.867546 -1.782366
 H 6.651040 -5.019510 -1.104767
 H 6.146087 -0.769932 3.359707
 H 6.796674 3.669928 -0.783876
 H 8.068627 3.619270 0.455556
 H 6.748935 4.798914 0.581926
 H -1.126998 1.164325 -2.236836

H -7.538362 3.948239 -0.203262
 H -6.344911 4.654157 1.025209
 H -9.412173 2.415454 0.264503
 H -9.294039 0.719471 -0.240352
 H -8.276108 1.944494 -1.013251
 H -7.664622 0.732485 3.115649
 H -9.036798 1.754080 2.652450
 H -8.990515 0.061367 2.137191
 H -6.263385 2.592349 2.236975
 H -1.101326 -0.253766 1.120191
 H -5.936954 -0.858240 2.299999
 H -5.244708 0.770997 2.153231
 H -5.936958 -0.087247 -2.685124
 H -8.100014 -1.969763 1.800314
 H -7.567628 -2.222381 -3.155747
 H -8.798231 -3.996091 -1.924006
 H -9.057311 -3.876321 0.536374
 N 0.749072 0.033918 0.413717
 N 2.581214 0.551105 -0.731128
 O 6.541136 1.451331 0.660349
 O 6.508888 -4.929431 -0.151391
 O 6.137389 -1.763099 3.245689
 O 6.250810 0.677678 2.745219
 O 6.159731 0.046779 -3.707474
 H -5.831425 1.782572 -0.889500
 H -4.631736 -1.667315 0.432325
 O -3.564181 1.377671 -2.173295
 O -2.964404 -1.110657 2.557794
 N -2.036809 -0.166674 0.713828
 N -4.482945 0.251416 -0.434994
 N -6.488977 0.016926 -1.844077
 C 6.999642 3.775493 0.285085
 C 4.416500 -0.302519 -2.127930
 C 5.868473 -0.177976 -2.545020
 C 6.985401 -0.311786 -1.510463
 C 6.729242 -1.268565 -0.366453
 C 6.728963 -2.604493 -0.740331
 C 6.521819 -3.621314 0.197580
 C 6.327828 -3.314305 1.534006
 C 6.331619 -1.983119 1.935818
 C 6.523478 -0.913500 0.998195
 C 6.440485 0.449659 1.540250
 C 6.185910 2.812359 1.122350
 C 4.668640 2.982476 1.039867

C 4.049996 3.194986 -0.349322
 C 4.355383 2.138710 -1.414825
 C 4.009759 0.700624 -1.031650
 C 1.524210 0.868776 -1.542408
 C 2.065566 0.053137 0.429939
 C 0.383599 0.545964 -0.826576
 C -0.972738 0.714367 -1.261424
 C -8.719223 1.633447 -0.062541
 C -8.376600 0.949226 2.312418
 C -6.929691 3.803611 0.685209
 C -6.888877 2.648018 1.345532
 C -7.662542 1.386669 1.020365
 C -2.090480 0.388552 -0.570694
 C -3.424298 0.705395 -1.141968
 C -5.853118 0.701217 -0.722680
 C -7.182288 -1.085703 -1.356712
 C -7.704076 -2.156040 -2.079817
 C -8.389306 -3.149492 -1.378615
 C -8.538911 -3.083089 0.006305
 C -8.007679 -2.000559 0.718110
 C -7.349939 -0.991760 0.032455
 C -6.660719 0.262725 0.546857
 C -5.584304 -0.105227 1.592890
 C -4.429702 -0.624252 0.734913
 C -3.087834 -0.642287 1.426070

1b-enantiomer-c6, $\Delta G = 1.4875$

kcal/mol, population = 5.15 %
 H 2.122837 2.750027 -2.229994
 H 2.334832 -0.295186 0.681448
 H 4.424591 0.631413 0.003192
 H 4.332424 3.353279 -1.385585
 H 5.745206 2.638276 -0.646050
 H 7.941854 -0.191855 -1.742394
 H 7.246885 0.826589 -0.496329
 H 4.191851 1.249615 -2.984427
 H 4.277794 -0.349675 -2.204243
 H 3.184422 3.527861 0.774374
 H 4.750095 4.310687 0.827961
 H 3.943227 1.640179 2.112246
 H 4.314647 3.152515 2.905483
 H 6.136559 1.727812 3.289864
 H 5.138549 -4.665111 0.640592
 H 6.758032 -2.182657 -2.470834

H 6.199936 -4.373265 -2.715374
 H 5.193279 -2.001073 2.908313
 H 8.079167 2.761709 2.226015
 H 6.885845 4.015546 2.617100
 H 7.076268 3.469260 0.941294
 H -0.428260 -0.737744 0.961494
 H -6.552094 -4.154894 -0.970119
 H -5.570373 -4.071819 -2.538710
 H -8.737630 -3.067031 -0.534919
 H -8.798090 -1.681633 0.570878
 H -7.437155 -2.811764 0.643053
 H -9.027505 -1.554360 -2.509219
 H -9.168310 -0.187489 -1.394722
 H -7.996014 -0.131135 -2.732087
 H -6.138231 -1.769559 -2.856584
 H -1.452498 1.732283 -1.510723
 H -6.455388 1.458557 -1.622366
 H -5.472479 0.107667 -2.225034
 H -5.144473 -0.965766 2.605477
 H -8.609915 1.738811 -0.399010
 H -6.974715 0.380517 4.116228
 H -8.760545 2.093118 3.880440
 H -9.568620 2.773381 1.639958
 N 0.527116 1.694418 -1.273610
 N 2.644630 1.252459 -0.774989
 O 6.333658 0.951837 1.368481
 O 5.874852 -4.609187 -1.834549
 O 5.117404 -2.869812 2.419914
 O 5.551380 -0.464179 2.921520
 O 6.642317 1.287446 -3.228097
 H -5.138919 -2.005985 0.230064
 H -4.916416 1.870233 0.197667
 O -2.739836 -1.508516 1.213347
 O -3.723411 2.532325 -2.200144
 N -2.235549 1.275008 -1.035566
 N -4.226909 -0.124554 0.209505
 N -5.852553 -0.907578 1.885396
 C 7.083199 3.143930 1.984903
 C 4.612271 0.694497 -2.140053
 C 6.121254 0.721139 -2.282344
 C 7.006566 0.055722 -1.230032
 C 6.453768 -1.200345 -0.591590
 C 6.409476 -2.292368 -1.445960
 C 5.932865 -3.534361 -1.013345

C 5.504325 -3.704768 0.292593
 C 5.546696 -2.627764 1.171279
 C 6.016583 -1.336251 0.758001
 C 5.957790 -0.268490 1.765612
 C 6.032280 2.091245 2.264192
 C 4.583917 2.528945 2.043266
 C 4.264238 3.329091 0.771852
 C 4.654098 2.695924 -0.567104
 C 4.113081 1.288068 -0.809125
 C 1.887866 0.411952 -0.003962
 C 1.783788 2.001932 -1.524017
 C 0.567178 0.688719 -0.314042
 C -0.594309 0.050938 0.234677
 C -8.132145 -2.305108 -0.033333
 C -8.460758 -0.779545 -1.981978
 C -6.201991 -3.565747 -1.813458
 C -6.520409 -2.282790 -1.973647
 C -7.408859 -1.445610 -1.076101
 C -1.884794 0.310564 -0.082471
 C -2.968096 -0.509596 0.516519
 C -5.389459 -0.976458 0.503326
 C -6.826707 0.080239 1.979653
 C -7.346978 0.660387 3.134528
 C -8.346204 1.624248 2.991692
 C -8.804789 2.007167 1.731599
 C -8.270303 1.414833 0.580925
 C -7.297747 0.435641 0.707331
 C -6.538080 -0.343079 -0.355407
 C -5.819742 0.622690 -1.324404
 C -4.607598 1.086319 -0.516777
 C -3.491675 1.684418 -1.338121

1b-enantiomer-c14, $\Delta G = 1.5469$

kcal/mol, population = 4.66 %

H 2.765266 -0.282095 1.258043
 H 1.699032 1.364056 -2.477382
 H 4.582520 0.401569 -0.109127
 H 3.918629 2.348834 -2.371964
 H 5.513603 2.068718 -1.713965
 H 7.855828 -0.810344 -2.112497
 H 7.248102 0.576103 -1.229387
 H 3.789629 -0.213648 -2.999737
 H 4.222310 -1.369781 -1.715426
 H 3.117920 3.288817 -0.250026

H 4.546972 4.127406 -0.817030
 H 4.349371 2.135398 1.511857
 H 4.622739 3.860180 1.586737
 H 6.671051 2.834389 2.086381
 H 6.173430 -4.132144 2.316971
 H 6.836977 -2.993073 -1.772928
 H 6.562000 -5.126058 -1.050617
 H 6.252523 -0.788305 3.346052
 H 8.240898 3.495883 0.337631
 H 6.954996 4.713085 0.457909
 H 6.953525 3.556233 -0.885300
 H -1.072042 1.349670 -2.126324
 H -10.438396 0.944254 0.569776
 H -10.396785 1.962866 -0.976537
 H -7.847367 0.303810 3.098081
 H -9.084964 -0.191908 1.929215
 H -9.203330 1.380488 2.729468
 H -6.337780 3.075005 1.084236
 H -7.797179 3.305896 2.052648
 H -6.463994 2.346808 2.699193
 H -8.059546 2.426691 -0.688610
 H -1.046111 -0.168566 1.190867
 H -5.899752 -0.931124 2.277708
 H -5.251773 0.722763 2.288019
 H -5.834980 0.405595 -2.621156
 H -7.953143 -2.115721 1.557504
 H -7.372991 -1.716350 -3.383265
 H -8.527621 -3.686536 -2.400751
 H -8.806946 -3.891276 0.051815
 N 0.809258 0.099976 0.465531
 N 2.637900 0.574618 -0.703446
 O 6.654424 1.374988 0.601655
 O 6.436420 -5.016026 -0.097026
 O 6.215755 -1.782789 3.250239
 O 6.381295 0.645040 2.704393
 O 6.136446 -0.120025 -3.739643
 H -5.765187 2.017658 -0.623764
 H -4.535915 -1.543405 0.380709
 O -3.503714 1.654655 -1.999994
 O -2.917524 -1.072537 2.593344
 N -1.981210 -0.058869 0.789989
 N -4.424009 0.446173 -0.319066
 N -6.402347 0.382409 -1.783848
 C 7.174204 3.677593 0.178548

C 4.416679 -0.365746 -2.115767
 C 5.862812 -0.299819 -2.565136
 C 6.995317 -0.436229 -1.548444
 C 6.739753 -1.365956 -0.382078
 C 6.696832 -2.707617 -0.732109
 C 6.487073 -3.702718 0.228240
 C 6.329756 -3.367908 1.562858
 C 6.375375 -2.030478 1.940671
 C 6.574366 -0.982392 0.980363
 C 6.541202 0.391437 1.500232
 C 6.346677 2.753328 1.045645
 C 4.833805 2.967293 0.984309
 C 4.199825 3.175029 -0.398325
 C 4.451597 2.089181 -1.447899
 C 4.064868 0.671064 -1.031578
 C 1.578403 0.937468 -1.492012
 C 2.125774 0.076758 0.459372
 C 0.440157 0.641550 -0.761036
 C -0.916740 0.861765 -1.169391
 C -8.504384 0.656973 2.296664
 C -7.018323 2.583684 1.786675
 C -9.863878 1.553443 -0.122488
 C -8.567273 1.800762 0.047126
 C -7.689662 1.328440 1.187529
 C -2.033507 0.541934 -0.474577
 C -3.365410 0.918725 -1.012545
 C -5.791091 0.925389 -0.575856
 C -7.053487 -0.801323 -1.450081
 C -7.520171 -1.793163 -2.309469
 C -8.162563 -2.897882 -1.747963
 C -8.323599 -3.014156 -0.367713
 C -7.850905 -2.006105 0.481304
 C -7.237155 -0.889372 -0.063422
 C -6.616661 0.324033 0.614523
 C -5.553734 -0.110578 1.646785
 C -4.369899 -0.523911 0.773284
 C -3.035414 -0.561741 1.479860

1b-enantiomer-c17, ΔG = 1.6920
 kcal/mol, population = 3.65 %
 H 1.222175 -2.077860 2.867928
 H 1.479711 0.559547 -0.414214
 H 3.414212 -1.765880 1.996183
 H 4.958480 0.030043 2.054177

H 3.480774 0.512627 2.866594
H 5.678465 -1.644164 -2.095790
H 5.722484 -0.013192 -1.462921
H 3.503361 -0.628383 -0.852852
H 3.346184 -2.313895 -0.363372
H 2.889944 2.058922 1.125734
H 3.973722 1.328234 -0.038935
H 5.347504 2.313907 2.432526
H 4.595084 3.584573 1.485908
H 6.981341 3.180012 0.960608
H 11.372105 -1.853188 -0.950770
H 7.409000 -3.127057 -2.022705
H 9.287550 -4.378229 -2.270840
H 10.167851 1.270472 0.077167
H 6.738594 3.255446 -1.515418
H 5.538206 4.293760 -0.723388
H 5.049765 2.717574 -1.383067
H -1.246696 1.088921 -0.697705
H -8.406295 4.469831 0.237211
H -9.306688 4.289027 -1.370829
H -10.249981 0.433096 0.733593
H -10.315640 1.720093 1.945845
H -9.342809 0.269070 2.254267
H -8.511332 3.367960 2.201440
H -7.592206 2.004448 2.824221
H -6.884914 3.053772 1.581451
H -9.459191 1.905030 -1.096074
H -2.352629 -1.101357 1.999472
H -7.373780 -1.094985 1.673223
H -6.540689 0.348484 2.287028
H -5.765272 1.243526 -2.527073
H -9.308606 -1.627551 0.223507
H -7.276616 -0.347351 -4.152076
H -8.920466 -2.207060 -4.017368
H -9.923420 -2.850387 -1.846024
N -0.358023 -1.091208 1.807264
N 1.770443 -0.800337 1.236116
O 6.652077 1.252416 0.225460
O 9.981973 -3.796953 -1.929221
O 10.685346 0.438298 -0.105206
O 8.758443 2.034179 0.156961
O 5.829380 -2.074535 0.905359
H -6.067793 2.351308 -0.226180
H -5.626225 -1.510916 0.054176

O -3.554999 1.861193 -1.055013
O -4.645899 -1.894073 2.633430
N -3.116932 -0.711530 1.441636
N -5.062734 0.524062 -0.017870
N -6.539440 1.143748 -1.883771
C 5.853730 3.256160 -0.871435
C 3.778750 -1.345447 -0.074671
C 5.283884 -1.528837 -0.036266
C 6.041845 -1.037169 -1.253174
C 7.532800 -1.182453 -1.129268
C 8.065324 -2.376534 -1.588528
C 9.439159 -2.630544 -1.503255
C 10.302563 -1.675166 -0.991441
C 9.789698 -0.459356 -0.552497
C 8.383717 -0.192505 -0.568393
C 7.954890 1.110706 -0.047459
C 6.170096 2.631794 0.475734
C 4.983362 2.561113 1.427621
C 3.868444 1.577918 1.022972
C 3.913321 0.307422 1.879342
C 3.232051 -0.939122 1.301140
C 1.034951 -0.034504 0.370205
C 0.889585 -1.412249 2.080088
C -0.290975 -0.219442 0.726561
C -1.434733 0.377809 0.100454
C -9.662822 0.974884 1.479663
C -7.810229 2.576556 1.919230
C -8.886232 3.817130 -0.486786
C -8.964138 2.498253 -0.324726
C -8.451635 1.687401 0.846063
C -2.733875 0.155476 0.409520
C -3.799057 0.911582 -0.296889
C -6.231499 1.296748 -0.466014
C -7.407126 0.068112 -2.033512
C -7.735832 -0.612737 -3.203788
C -8.656215 -1.658433 -3.117036
C -9.224213 -2.021204 -1.895967
C -8.884187 -1.324917 -0.729858
C -7.992386 -0.266977 -0.804463
C -7.426274 0.623805 0.293868
C -6.760712 -0.237408 1.390455
C -5.445407 -0.665121 0.742387
C -4.379162 -1.132366 1.704265

1b-enantiomer-c2, ΔG = 1.9579	O 6.624045 -4.864211 -0.440413
kcal/mol, population = 2.33 %	O 5.722713 -1.948094 3.159617
H 2.802633 0.042363 1.099878	O 5.792819 0.519436 2.805825
H 1.663622 1.044349 -2.836994	O 6.417732 -0.232520 -3.748855
H 4.577818 0.545395 -0.361260	H -5.775040 1.662261 -1.153445
H 3.687037 2.439523 -2.563977	H -4.503156 -1.561446 0.622945
H 5.369273 2.233331 -2.135780	O -3.540334 1.068812 -2.419825
H 7.943372 -0.412409 -1.825813	O -2.837160 -0.640011 2.629570
H 6.953738 0.809663 -1.038690	N -1.947866 0.004345 0.643098
H 3.977221 -0.109557 -3.296868	N -4.415457 0.216262 -0.512306
H 4.241023 -1.276240 -1.980042	N -6.428453 -0.201182 -1.870579
H 3.432533 2.955610 0.096143	C 7.086022 3.303660 2.082255
H 3.848564 4.177710 -1.085116	C 4.493258 -0.270606 -2.345005
H 5.386000 4.626398 0.550769	C 5.986598 -0.242718 -2.608935
H 6.350452 3.664312 -0.558188	C 6.946014 -0.210815 -1.422742
H 5.031241 2.621370 1.998028	C 6.636005 -1.235725 -0.347954
H 5.972628 -4.214449 2.089885	C 6.741827 -2.547016 -0.783800
H 7.024550 -2.756248 -1.811956	C 6.501171 -3.620384 0.079209
H 6.436662 -5.526831 0.240137	C 6.159187 -3.394487 1.402006
H 5.678935 -0.963066 3.327319	C 6.054310 -2.086178 1.866800
H 6.832415 4.282597 2.500643	C 6.282455 -0.961537 1.007094
H 7.937490 3.426307 1.404392	C 6.098192 0.364403 1.613282
H 7.374894 2.642397 2.902629	C 5.889316 2.751962 1.329286
H -1.101905 0.876355 -2.492539	C 5.503111 3.615855 0.139759
H -7.285509 3.166229 3.091227	C 4.212293 3.255898 -0.618472
H -6.282920 4.422561 2.170829	C 4.352062 2.197304 -1.725809
H -9.372691 2.385936 -0.011109	C 4.056973 0.758401 -1.293418
H -9.145019 0.699450 -0.522068	C 1.562623 0.762724 -1.798596
H -8.134989 1.986089 -1.215053	C 2.147735 0.238486 0.258042
H -7.740963 0.841214 2.959912	C 0.439092 0.508951 -1.029088
H -9.081524 1.853298 2.393585	C -0.925848 0.582464 -1.462735
H -9.004728 0.155315 1.918603	C -8.626417 1.638834 -0.300686
H -6.399127 3.148492 0.154063	C -8.400210 1.044880 2.110005
H -1.005503 -0.006918 1.042330	C -6.820363 3.478072 2.160217
H -5.823666 -0.535845 2.363674	C -6.889946 2.754041 1.044987
H -5.199412 1.086384 1.978751	C -7.622393 1.442312 0.852371
H -5.881590 -0.381186 -2.702370	C -2.028072 0.349910 -0.711738
H -7.917078 -1.820101 1.999138	C -3.374228 0.562652 -1.300764
H -7.426771 -2.616623 -2.902546	C -5.793458 0.614885 -0.841448
H -8.566096 -4.288284 -1.457727	C -7.073760 -1.266260 -1.250967
H -8.800619 -3.898876 0.977432	C -7.555499 -2.433472 -1.839309
N 0.832105 0.181147 0.263892	C -8.188653 -3.368256 -1.018999
N 2.636616 0.586551 -0.967572	C -8.324829 -3.149923 0.351637
O 6.234121 1.416810 0.801433	C -7.835375 -1.970955 0.926307

C -7.231950 -1.018542 0.119718
C -6.585863 0.312224 0.479254
C -5.496280 0.120399 1.555419
C -4.331115 -0.479974 0.771137
C -2.982604 -0.362363 1.439362

1c-c1, ΔG = 0.0000 kcal/mol,
population = 96.02 %

C 3.245288 -0.501292 -1.413607
C 4.644049 -0.134151 -0.979577
C 5.704372 -1.205739 -1.228358
C 6.851893 -0.787419 -0.281815
C 7.609594 0.400318 -0.856121
C 8.231373 0.559856 -2.084345
C 8.846508 1.780011 -2.390184
C 8.815595 2.827746 -1.470283
C 8.168748 2.691544 -0.240816
C 7.562716 1.470956 0.048383
C 6.137665 -0.118214 0.941043
C 3.765943 0.460758 1.293034
C 2.403541 0.421480 0.704740
C 7.789577 -1.976618 0.161784
C 6.961677 -3.045109 0.846613
C 6.986098 -3.372652 2.137061
C 8.435885 -2.629101 -1.074093
C 8.903915 -1.453073 1.075513
C 1.348164 0.870047 1.424464
C -0.030348 0.847700 1.030427
C -1.800319 0.490013 -0.153792
C -1.106301 1.325703 1.760766
C -3.600681 1.448402 1.347541
C -4.129783 2.501507 0.364388
C -5.431547 3.148751 0.850065
C -6.347444 3.684208 -0.251121
C -6.707235 2.682322 -1.345161
C -6.794694 0.282259 -1.438750
C -6.928960 -1.012378 -0.759019
C -6.889606 -2.177933 -1.591786
C -7.007763 -3.458369 -1.060030
C -7.147935 -3.614834 0.308177
C -7.169544 -2.498173 1.152706
C -7.065981 -1.211995 0.644745
C -7.072104 -0.121917 1.689717

C -5.706199 0.296372 2.233139
C -4.467156 0.173199 1.366067
C -7.951682 3.090155 -2.109162
N 6.887490 1.105186 1.208293
N 4.767251 0.108232 0.457214
N 2.247960 -0.163798 -0.559132
O 3.033925 -1.025169 -2.507370
O 3.974251 0.754498 2.479117
H 4.904369 0.782507 -1.539534
H 6.088772 -0.748336 1.834794
O -5.616805 0.708470 3.377235
O -6.557317 0.372597 -2.653821
O -6.743125 -2.103665 -2.924284
O -7.256944 -4.877267 0.786025
O -6.930670 1.376976 -0.684780
N -2.216833 1.092313 0.998176
N -0.492585 0.323915 -0.171404
H 9.337350 1.912549 -3.349577
H 9.289133 3.774466 -1.717073
H 8.125907 3.517165 0.464262
H 8.231425 -0.243136 -2.816323
H 6.408240 1.820858 1.738590
H 5.294820 -2.183890 -0.959439
H 6.020100 -1.232539 -2.272770
H 1.281865 -0.293263 -0.871258
H 6.306273 -3.615826 0.188108
H 9.038668 -3.487214 -0.758261
H 7.683201 -2.986637 -1.784404
H 9.096949 -1.924286 -1.586237
H 8.513363 -0.979801 1.981027
H 9.510979 -0.713851 0.543734
H 9.556361 -2.279666 1.375323
H 6.359083 -4.176225 2.514051
H 7.621372 -2.864811 2.857757
H 1.575171 1.275797 2.405208
H -7.794274 4.084044 -2.541309
H -8.810270 3.143170 -1.431610
H -8.171565 2.390627 -2.918442
H -6.626274 -1.132660 -3.130791
H -7.348489 -4.859273 1.749566
H -7.271707 -2.643447 2.225262
H -6.982667 -4.317589 -1.722082
H -5.867256 2.543951 -2.032347
H -5.884246 4.540303 -0.758669

H -7.268835 4.054491 0.216057
H -5.191156 3.965530 1.541022
H -6.012498 2.435662 1.438428
H -3.885101 -0.641382 1.819783
H -4.713733 -0.134515 0.346793
H -7.649268 -0.457241 2.556281
H -7.550455 0.790676 1.324311
H -4.271282 2.010649 -0.606327
H -3.360346 3.269418 0.220874
H -3.559362 1.863312 2.361384
H -1.162882 1.797064 2.731813
H -2.487880 0.193301 -0.936753

1c-c2, $\Delta G = 1.8833$ kcal/mol,
population = 3.98 %

C 3.421687 0.009984 -2.221786
C 4.549091 0.230580 -1.243086
C 5.771073 -0.662403 -1.456296
C 6.504145 -0.579620 -0.098171
C 7.237228 0.747617 0.026497
C 8.181192 1.332653 -0.802521
C 8.689269 2.597206 -0.481349
C 8.232976 3.265466 0.654511
C 7.261661 2.701673 1.483412
C 6.767228 1.442614 1.149998
C 5.365046 -0.389460 0.961202
C 2.938007 -0.074119 0.656500
C 1.841216 0.036760 -0.338418
C 7.405941 -1.833754 0.226445
C 6.549135 -3.083221 0.233644
C 6.242715 -3.837817 1.287258
C 8.466796 -2.019996 -0.873673
C 8.121712 -1.630095 1.566259
C 0.558071 0.118061 0.085834
C -0.616102 0.156648 -0.736437
C -1.862993 0.155801 -2.500830
C -1.927839 0.240619 -0.301161
C -4.171135 0.308432 -1.454658
C -4.662491 1.498434 -2.278328
C -4.179400 2.867432 -1.793231
C -4.547223 3.252390 -0.351208
C -6.032833 3.129833 -0.006959
C -5.875729 1.143867 1.424184
C -6.026413 -0.316958 1.508212

C -5.538928 -0.937416 2.704641
C -5.604998 -2.315696 2.891607
C -6.147246 -3.110744 1.895582
C -6.624679 -2.538793 0.712127
C -6.570251 -1.170110 0.501983
C -7.118895 -0.734001 -0.839702
C -6.253636 -1.044215 -2.059510
C -4.741566 -1.033944 -1.951904
C -6.530788 4.115659 1.035459
N 5.821746 0.686997 1.835588
N 4.189142 -0.048838 0.146482
N 2.172260 -0.035228 -1.697749
O 3.637507 -0.071054 -3.431013
O 2.726778 -0.224773 1.868334
H 4.842172 1.290666 -1.349248
H 5.134829 -1.288858 1.540669
O -6.794121 -1.282291 -3.126216
O -5.303666 1.804382 2.304888
O -4.992844 -0.233460 3.708349
O -6.242360 -4.456618 2.007598
O -6.367919 1.721589 0.327866
N -2.703792 0.240138 -1.428560
N -0.600610 0.104469 -2.125828
H 9.430472 3.061354 -1.124888
H 8.626530 4.249954 0.893927
H 6.889944 3.234565 2.354315
H 8.515880 0.829741 -1.705549
H 5.109611 1.167634 2.369349
H 5.435312 -1.680109 -1.676807
H 6.392500 -0.312286 -2.282439
H 1.380330 -0.081900 -2.344611
H 6.180356 -3.398875 -0.742795
H 9.054991 -2.919153 -0.661623
H 8.010368 -2.139099 -1.861804
H 9.152526 -1.168559 -0.902212
H 8.770423 -0.750198 1.515519
H 8.745209 -2.501660 1.790696
H 7.422349 -1.487079 2.395354
H 5.633873 -4.730036 1.167823
H 6.580710 -3.604230 2.293297
H 0.409665 0.137261 1.160706
H -6.586660 5.102246 0.563375
H -5.867661 4.176382 1.899120
H -7.536205 3.844550 1.372242

H -4.982152 0.717575 3.397977
 H -5.886098 -4.742700 2.860984
 H -7.045866 -3.188331 -0.050112
 H -5.225156 -2.742125 3.815927
 H -6.629211 3.259440 -0.917468
 H -4.263669 4.301078 -0.201588
 H -3.958062 2.683319 0.376611
 H -4.597750 3.620623 -2.472844
 H -3.088435 2.930932 -1.898832
 H -4.437975 -1.821129 -1.248695
 H -4.339751 -1.271671 -2.941597
 H -7.328187 0.335973 -0.879419
 H -8.070096 -1.246204 -1.015712
 H -5.758948 1.474004 -2.273344
 H -4.366513 1.358611 -3.326281
 H -4.456514 0.439274 -0.411073
 H -2.356216 0.298866 0.690237
 H -2.221251 0.135187 -3.522758

1d-cl, $\Delta G = 0.0000$ kcal/mol,
 population = 100.00 %

C 3.982973 -0.208103 1.721865
 C 5.247799 -0.302030 0.903793
 C 6.424376 0.510908 1.441220
 C 7.362148 0.624194 0.217452
 C 8.104717 -0.685238 -0.001586
 C 8.932719 -1.394319 0.852967
 C 9.485771 -2.606755 0.422966
 C 9.192655 -3.096241 -0.849748
 C 8.346317 -2.400424 -1.714902
 C 7.806444 -1.195036 -1.271885
 C 6.399696 0.628391 -1.023873
 C 3.952324 0.348943 -1.144594
 C 2.713188 0.122529 -0.357830
 C 8.323103 1.873358 0.258757
 C 9.139238 1.807137 1.530135
 C 10.465020 1.751189 1.628499
 C 9.203193 1.895240 -0.995103
 C 7.528416 3.197149 0.315574
 C 1.510300 0.164539 -0.977934
 C 0.222214 0.045868 -0.358236
 C -1.280711 -0.179198 1.172153
 C -1.006675 0.102529 -0.994356

C -3.406891 -0.047138 -0.171255
 C -3.854129 -1.201877 -1.070539
 C -3.683973 -2.573244 -0.418350
 C -4.535693 -2.812877 0.833510
 C -6.042384 -2.847286 0.620900
 C -7.725692 -1.269512 -0.054107
 C -8.313326 0.071174 0.053033
 C -9.712933 0.177425 -0.222148
 C -10.397775 1.377547 -0.052064
 C -9.703871 2.502089 0.360295
 C -8.322678 2.443162 0.587575
 C -7.627328 1.254420 0.441433
 C -6.133699 1.341114 0.589164
 C -5.405332 1.369908 -0.747106
 C -3.890845 1.320218 -0.687160
 C -6.767552 -3.482525 1.795057
 N 6.979905 -0.319820 -1.969650
 N 5.108779 0.204904 -0.460066
 N 2.830290 -0.038228 1.028407
 O 4.008455 -0.331197 2.946274
 O 3.932712 0.692369 -2.334998
 H 5.517849 -1.373162 0.879815
 H 6.256909 1.600190 -1.503464
 O -5.994708 1.455950 -1.808753
 O -8.331174 -2.216584 -0.580086
 O -10.446334 -0.869319 -0.637665
 O -10.406530 3.650561 0.514377
 O -6.517495 -1.446418 0.495588
 N -1.948086 -0.041162 -0.009739
 N 0.024907 -0.133568 1.006642
 H 10.136524 -3.169557 1.085471
 H 9.619793 -4.041741 -1.173929
 H 8.107052 -2.791714 -2.699927
 H 9.149587 -1.018085 1.848458
 H 6.355427 -0.694918 -2.671534
 H 6.063604 1.491486 1.766251
 H 6.908011 0.017200 2.285999
 H 1.947675 -0.068204 1.546084
 H 8.551016 1.843051 2.449237
 H 9.885485 2.750603 -0.960253
 H 9.800086 0.982617 -1.088875
 H 8.586888 1.994588 -1.893949
 H 8.237849 4.031044 0.309712
 H 6.925593 3.285779 1.223422

H 6.871570 3.315649 -0.551958
H 10.947017 1.732874 2.602345
H 11.112646 1.713670 0.756908
H 1.529966 0.325386 -2.051021
H -6.481168 -4.535970 1.870621
H -7.851815 -3.430203 1.669909
H -6.489605 -2.979349 2.727505
H -9.803631 -1.624418 -0.748281
H -9.816663 4.360050 0.807099
H -7.790496 3.349144 0.866675
H -11.463800 1.419116 -0.249930
H -6.285153 -3.360710 -0.315402
H -4.306006 -2.092160 1.629387
H -4.265190 -3.795467 1.238696
H -2.628104 -2.721270 -0.153552
H -3.926422 -3.344731 -1.160002
H -3.501440 1.509176 -1.692569
H -3.532411 2.102618 -0.006047
H -5.721015 0.546726 1.214236
H -5.865738 2.283385 1.087321
H -3.290471 -1.158785 -2.011097
H -4.903951 -1.045892 -1.338837
H -3.797150 -0.194109 0.840800
H -1.262924 0.235756 -2.035617
H -1.803860 -0.310418 2.112257

Table S7. Coordinates and relative free energy of low-energy conformers of structures 13R/S-5.

13R-5-c40, $\Delta G = 0.0000$ kcal/mol, population = 19.56 %

C 1.513581 2.771974 1.363816
C 2.394433 1.685637 0.902626
C 3.631392 2.089863 0.299669
C 4.492959 1.145787 -0.275599
C 4.162198 -0.207303 -0.236927
C 2.978552 -0.629676 0.393618
C 2.086593 0.284028 0.960059
C 0.894857 -0.252875 1.655535
C 0.240036 -1.376459 1.312037
C -0.905523 -1.979837 2.074059
C -2.149894 -2.272656 1.216870
C -2.863205 -1.026410 0.689178

C -4.049428 -1.340227 -0.231835
C -4.794451 -0.083564 -0.679035
C -0.642403 3.451255 2.139925
C -1.328679 4.195417 0.991158
C -2.085410 3.243288 0.059141
C -2.250399 5.274439 1.573477
H 5.421134 1.496185 -0.732336
H 2.793576 -1.701120 0.468621
H 3.308854 3.894935 0.713238
H 5.747141 -0.768319 -1.152894
H 0.542525 0.307285 2.523591
H 0.545963 -1.922179 0.409627
H -1.171973 -1.333551 2.928206
H -0.561123 -2.938759 2.506319
H -1.381325 2.907193 2.747082
H -0.092574 4.151931 2.783389
H -0.535820 4.699054 0.411744
H -2.533025 3.795169 -0.782600
H -2.901464 2.729678 0.595802
H -1.419670 2.472363 -0.357780
H -3.050219 4.824840 2.186596
H -1.696793 5.984469 2.209042
H -2.732539 5.850055 0.767988
H -2.859517 -2.869606 1.816358
H -1.866125 -2.906907 0.360052
H -2.148290 -0.389413 0.134779
H -3.221527 -0.413630 1.535604
H -4.753663 -1.991027 0.317080
H -3.027574 -1.588537 -1.876158
H -4.117929 0.598425 -1.222746
H -5.625412 -0.349361 -1.350482
H -5.205541 0.467061 0.182054
O 0.266156 2.425723 1.681216
O 1.879724 3.951556 1.431151
O -3.646849 -2.122063 -1.355972
O 4.013667 3.368600 0.244453
O 4.954232 -1.164818 -0.762196

13R-5-c30, $\Delta G = 0.8245$ kcal/mol, population = 4.86 %

C 0.738265 1.530853 0.224081
C 2.084134 0.927800 0.143293
C 3.270342 1.698037 0.358782
C 4.526954 1.078501 0.397694

C 4.638233 -0.298261 0.210838
 C 3.490086 -1.070039 -0.039212
 C 2.224542 -0.485311 -0.073179
 C 1.062517 -1.345221 -0.381759
 C 0.871602 -2.589129 0.089402
 C -0.330532 -3.434443 -0.220417
 C -1.207007 -3.722310 1.019247
 C -1.782825 -2.501143 1.752649
 C -2.855019 -1.693158 1.004373
 C -3.530945 -0.664601 1.914951
 C -0.505416 3.595958 0.294335
 C -0.249584 5.090161 0.124238
 C 0.390403 5.413698 -1.231436
 C -1.563961 5.853980 0.328879
 H 5.406055 1.702547 0.571920
 H 3.611082 -2.134175 -0.242945
 H 2.354047 3.351163 0.496259
 H 6.542665 -0.315726 0.406615
 H 0.296711 -0.918067 -1.032252
 H 1.596199 -3.011836 0.798465
 H 0.006444 -4.406926 -0.625280
 H -0.935664 -2.944408 -0.996063
 H -1.173469 3.208213 -0.490540
 H -0.962429 3.371366 1.270443
 H 0.450613 5.395094 0.923766
 H -0.281263 5.131583 -2.060229
 H 1.340838 4.876342 -1.369973
 H 0.596422 6.492105 -1.317392
 H -1.396773 6.939320 0.251126
 H -2.308286 5.575063 -0.436105
 H -2.003598 5.650842 1.318546
 H -0.608965 -4.305573 1.742559
 H -2.035927 -4.385163 0.712601
 H -0.965970 -1.814164 2.039918
 H -2.229755 -2.851953 2.699029
 H -3.626549 -2.399300 0.645061
 H -1.664922 -0.428943 0.086235
 H -2.787366 0.045606 2.315833
 H -4.278755 -0.089584 1.347085
 H -4.035970 -1.144549 2.768534
 O 0.755068 2.891796 0.206697
 O -0.323106 0.939449 0.309494
 O -2.355984 -1.064557 -0.171556
 O 3.275457 3.025730 0.554855

O 5.822731 -0.941597 0.236645

13R-5-c42, $\Delta G = 0.8352$ kcal/mol,
population = 4.77 %

C 0.910679 1.157918 0.613194
 C 2.256008 0.553218 0.529675
 C 3.446243 1.321837 0.742648
 C 4.700452 0.702025 0.773732
 C 4.809577 -0.674186 0.579540
 C 3.659573 -1.444061 0.334625
 C 2.392322 -0.857685 0.310370
 C 1.228946 -1.718310 0.009543
 C 1.039738 -2.959896 0.487681
 C -0.163948 -3.806462 0.187603
 C -1.035569 -4.085900 1.432612
 C -1.608902 -2.859642 2.159418
 C -2.683000 -2.056502 1.408599
 C -3.356884 -1.022326 2.314283
 C -0.330650 3.224494 0.679057
 C -0.072309 4.717831 0.504999
 C 0.575774 5.035807 -0.848156
 C -1.387093 5.483706 0.699277
 H 5.589314 1.309792 0.945923
 H 3.762288 -2.510572 0.123685
 H 2.529511 2.974821 0.888489
 H 5.990519 -2.173622 0.463756
 H 0.460666 -1.293651 -0.639625
 H 1.766734 -3.379079 1.196461
 H 0.171093 -4.781603 -0.212360
 H -0.771924 -3.320782 -0.588495
 H -0.997641 2.835489 -0.106103
 H -0.789980 3.003361 1.654859
 H 0.623660 5.025131 1.307289
 H 1.527285 4.498371 -0.978489
 H 0.781734 6.113971 -0.937320
 H -0.090670 4.749913 -1.679851
 H -1.832751 5.284470 1.687040
 H -1.218244 6.568579 0.618763
 H -2.127239 5.202924 -0.069085
 H -0.434636 -4.663930 2.157717
 H -1.865457 -4.751035 1.133703
 H -0.791116 -2.170928 2.439826
 H -2.053332 -3.204052 3.109326
 H -3.455259 -2.764988 1.055556

H -1.495699 -0.797510 0.480306
H -3.860055 -1.497142 3.171810
H -2.612451 -0.309713 2.709263
H -4.105939 -0.450827 1.744519
O 0.929050 2.518380 0.595756
O -0.151142 0.567389 0.699370
O -2.186562 -1.435344 0.227573
O 3.450831 2.649330 0.943105
O 6.042756 -1.218056 0.614460

13R-5-c57, $\Delta G = 1.0505$ kcal/mol,
population = 3.32 %

C 0.328881 1.096728 0.768819
C 1.667848 0.522214 0.526422
C 2.829861 1.352571 0.420673
C 4.104871 0.787749 0.286786
C 4.255674 -0.596821 0.232421
C 3.127609 -1.430801 0.299519
C 1.844329 -0.904124 0.454161
C 0.701011 -1.842302 0.484896
C 0.737997 -3.083113 1.003827
C -0.391058 -4.082578 1.010667
C -1.775581 -3.560313 0.609978
C -2.420895 -2.639509 1.657060
C -3.513144 -1.723679 1.087276
C -4.233854 -0.931508 2.178890
C -0.992431 3.114306 0.778642
C -0.831764 4.588929 0.424215
C -0.423363 4.788257 -1.040570
C -2.131475 5.332664 0.757765
H 4.963460 1.459172 0.217260
H 3.274487 -2.505449 0.192376
H 1.864739 2.980693 0.528669
H 6.159749 -0.526656 0.046864
H -0.235067 -1.473818 0.069201
H 1.663645 -3.430539 1.479331
H -0.442327 -4.541020 2.016433
H -0.102527 -4.918542 0.343981
H -1.755873 2.629635 0.149767
H -1.283178 2.978595 1.831568
H -0.031276 4.994999 1.069807
H 0.518098 4.268237 -1.274044
H -0.282560 5.857407 -1.263624
H -1.200804 4.401110 -1.721172

H -2.971962 4.955688 0.150695
H -2.404374 5.221260 1.819417
H -2.025996 6.408405 0.548625
H -2.439962 -4.421650 0.424975
H -1.706217 -3.023537 -0.349952
H -1.652323 -1.993986 2.116158
H -2.843989 -3.245993 2.476675
H -4.257111 -2.348222 0.559001
H -2.278063 -0.323763 0.495342
H -3.518526 -0.307809 2.742135
H -4.989628 -0.266088 1.733379
H -4.738243 -1.599340 2.895860
O 0.269503 2.440345 0.561891
O -0.668771 0.493186 1.124679
O -2.987741 -0.852987 0.088835
O 2.797997 2.693939 0.459708
O 5.457329 -1.192263 0.093265

13R-5-c5, $\Delta G = 1.0599$ kcal/mol,
population = 3.26 %

C 0.627038 1.544210 1.098228
C 1.941078 0.902350 0.894895
C 3.167699 1.594014 1.151285
C 4.395221 0.920353 1.081987
C 4.437551 -0.431116 0.743824
C 3.248619 -1.121121 0.449092
C 2.010828 -0.483297 0.521426
C 0.803189 -1.254377 0.158941
C 0.572532 -2.535454 0.492463
C -0.674729 -3.290705 0.132522
C -1.519805 -3.686565 1.363517
C -2.026579 -2.536353 2.247574
C -3.088330 -1.611995 1.630563
C -3.704753 -0.677567 2.674997
C -0.501914 3.657480 1.478430
C -1.179994 4.080286 0.174038
C -2.469755 4.843050 0.501560
C -0.242509 4.900860 -0.718712
H 5.306656 1.484140 1.292592
H 3.315300 -2.160283 0.126385
H 2.333149 3.263286 1.470501
H 6.344498 -0.551480 0.866306
H 0.037553 -0.725198 -0.411695
H 1.299902 -3.065203 1.122357

H -0.393970 -4.221395 -0.394974
 H -1.284127 -2.689638 -0.556915
 H -1.177558 3.053732 2.098507
 H -0.169929 4.534993 2.052751
 H -1.456321 3.155053 -0.361331
 H -2.996528 5.129183 -0.422073
 H -2.253473 5.768577 1.062143
 H -3.160662 4.234894 1.107434
 H 0.039022 5.849022 -0.228956
 H 0.683320 4.350210 -0.945234
 H -0.730823 5.149063 -1.674298
 H -0.920083 -4.365998 1.995641
 H -2.382353 -4.283385 1.016491
 H -1.176739 -1.914100 2.583087
 H -2.458668 -2.976386 3.163117
 H -3.893339 -2.245073 1.213464
 H -1.872899 -0.291740 0.831237
 H -4.444441 -0.014412 2.200241
 H -4.206399 -1.239029 3.479438
 H -2.926726 -0.045438 3.136745
 O 0.708604 2.897315 1.246408
 O -0.454482 0.986839 1.153738
 O -2.597161 -0.864439 0.522645
 O 3.239689 2.891547 1.481881
 O 5.590870 -1.123850 0.658654

13R-5-c49, $\Delta G = 1.0693$ kcal/mol,
population = 3.21 %

C 1.856316 2.677675 -0.002254
 C 2.876234 1.626597 0.161833
 C 4.194528 1.943565 -0.308291
 C 5.219530 0.987339 -0.276465
 C 4.963763 -0.288112 0.220805
 C 3.684688 -0.614996 0.706255
 C 2.638924 0.309855 0.684520
 C 1.338261 -0.120896 1.246590
 C 0.802621 -1.343059 1.082598
 C -0.490703 -1.809615 1.688360
 C -1.550290 -2.224210 0.648954
 C -2.088913 -1.064956 -0.191504
 C -3.079163 -1.495663 -1.280916
 C -3.652663 -0.308128 -2.052481
 C -0.464709 3.299454 0.125588
 C -0.971275 3.898209 1.440342

C -1.595719 2.844905 2.363584
 C 0.097481 4.726725 2.164319
 H 6.208050 1.270031 -0.644918
 H 3.534897 -1.604224 1.138699
 H 3.671638 3.687792 -0.768196
 H 6.749763 -0.911910 -0.065344
 H 0.788045 0.614919 1.835142
 H 1.317329 -2.070863 0.441270
 H -0.899143 -1.027505 2.351351
 H -0.280090 -2.686233 2.328963
 H -0.113980 4.084819 -0.555349
 H -1.263099 2.723570 -0.365070
 H -1.776625 4.587088 1.123296
 H -0.840523 2.125106 2.719223
 H -2.388175 2.276559 1.850175
 H -2.042641 3.320455 3.250932
 H 0.536594 5.490003 1.503712
 H -0.335906 5.237948 3.038369
 H 0.917059 4.086953 2.531429
 H -2.389640 -2.712991 1.174300
 H -1.127239 -2.986602 -0.026816
 H -1.249468 -0.528755 -0.672842
 H -2.582477 -0.326246 0.465099
 H -3.912099 -2.039594 -0.800211
 H -1.756534 -2.017518 -2.618351
 H -4.343159 -0.657542 -2.835436
 H -4.200287 0.377236 -1.386182
 H -2.845489 0.267254 -2.538390
 O 0.607949 2.347606 0.329834
 O 2.122950 3.802178 -0.443961
 O -2.499037 -2.449561 -2.170201
 O 4.507403 3.143358 -0.803314
 O 5.909557 -1.248007 0.280743

13R-5-c1, $\Delta G = 1.1032$ kcal/mol,
population = 3.03 %

C 1.358062 2.031394 0.365747
 C 2.400417 1.008166 0.171021
 C 3.734328 1.391953 0.540544
 C 4.794928 0.478561 0.464461
 C 4.563847 -0.817372 0.010488
 C 3.271669 -1.208257 -0.382201
 C 2.187381 -0.331315 -0.306201
 C 0.871258 -0.831851 -0.763228

C 0.436041 -2.096953 -0.615226
 C -0.878929 -2.617563 -1.121896
 C -1.703256 -3.372416 -0.057788
 C -2.034748 -2.611797 1.234924
 C -2.962101 -1.396806 1.105786
 C -3.377348 -0.846993 2.471156
 C -0.952641 2.650393 0.324837
 C -1.153911 3.527187 -0.913803
 C -1.467558 2.698118 -2.164190
 C -2.260750 4.548399 -0.619183
 H 5.791871 0.813145 0.758733
 H 3.140683 -2.212089 -0.785837
 H 3.178066 3.134502 0.969259
 H 6.391052 -1.358272 0.186804
 H 0.216144 -0.113895 -1.258077
 H 1.061658 -2.818220 -0.072897
 H -0.678830 -3.328341 -1.946645
 H -1.465833 -1.790730 -1.546474
 H -1.851720 2.051944 0.525094
 H -0.714835 3.264888 1.203523
 H -0.215029 4.081851 -1.083928
 H -2.383197 2.099391 -2.021923
 H -0.647680 2.005447 -2.408831
 H -1.622611 3.352152 -3.036940
 H -2.019257 5.170046 0.258157
 H -2.406794 5.221823 -1.478080
 H -3.223003 4.045660 -0.421899
 H -1.153099 -4.288008 0.223418
 H -2.641518 -3.718401 -0.526081
 H -1.101159 -2.283718 1.730720
 H -2.508252 -3.319597 1.936486
 H -3.872111 -1.704949 0.560081
 H -1.476111 -0.215032 0.594395
 H -3.927355 -1.600805 3.056856
 H -2.491133 -0.543301 3.054213
 H -4.025059 0.034475 2.347254
 O 0.092514 1.658659 0.156940
 O 1.614810 3.187157 0.724602
 O -2.388534 -0.362748 0.301751
 O 4.031529 2.617264 0.978563
 O 5.544784 -1.736862 -0.094924

13R-5-c89, $\Delta G = 1.1496$ kcal/mol,
 population = 2.80 %

C 1.593432 2.068049 0.164841
 C 2.611972 1.016037 0.335287
 C 3.934197 1.328512 -0.132685
 C 4.955824 0.372044 -0.095086
 C 4.696759 -0.901229 0.406797
 C 3.416055 -1.223618 0.890182
 C 2.369984 -0.296162 0.861340
 C 1.067323 -0.724475 1.420284
 C 0.529645 -1.945564 1.254421
 C -0.766220 -2.409825 1.856400
 C -1.823258 -2.822844 0.813814
 C -2.357199 -1.663042 -0.028863
 C -3.344623 -2.092886 -1.121164
 C -3.914922 -0.904907 -1.894358
 C -0.727437 2.692077 0.283230
 C -1.237912 3.295866 1.594153
 C -1.866636 2.246408 2.518859
 C -0.170822 4.125858 2.318923
 H 5.949496 0.636410 -0.458253
 H 3.247640 -2.207981 1.331475
 H 3.414188 3.072639 -0.599507
 H 5.410565 -2.632526 0.795802
 H 0.517213 0.012472 2.007487
 H 1.043945 -2.674060 0.613462
 H -1.175260 -1.626958 2.518074
 H -0.558864 -3.286714 2.497675
 H -0.373655 3.474740 -0.399232
 H -1.524592 2.115121 -0.208168
 H -2.041472 3.984426 1.271935
 H -1.113466 1.526914 2.879395
 H -2.658079 1.677273 2.004760
 H -2.315892 2.725456 3.403140
 H 0.271610 4.886130 1.657070
 H -0.606801 4.640873 3.189452
 H 0.646668 3.486538 2.691454
 H -2.665079 -3.309878 1.336797
 H -1.399530 -3.586282 0.139652
 H -1.515394 -1.128508 -0.507939
 H -2.851629 -0.923199 0.625794
 H -4.179376 -2.636180 -0.642900
 H -2.019690 -2.615084 -2.456139
 H -4.602958 -1.253824 -2.679696
 H -4.464441 -0.219417 -1.229751
 H -3.105864 -0.329760 -2.377419

O 0.343822 1.740055 0.494392
O 1.862518 3.190588 -0.279445
O -2.762572 -3.047238 -2.008724
O 4.248688 2.527229 -0.630631
O 5.712082 -1.788994 0.427128

13R-5-c11, $\Delta G = 1.1628$ kcal/mol,
population = 2.74 %

C 0.689737 1.621361 0.733366
C 2.002940 0.977260 0.529323
C 3.233314 1.666149 0.786878
C 4.457360 0.990923 0.717498
C 4.496967 -0.360290 0.377244
C 3.307087 -1.046736 0.080028
C 2.068515 -0.406046 0.154476
C 0.860187 -1.176585 -0.206379
C 0.629136 -2.456734 0.130825
C -0.618901 -3.212785 -0.224509
C -1.463866 -3.600062 1.009571
C -1.972556 -2.443742 1.884192
C -3.032983 -1.523902 1.258180
C -3.655424 -0.585801 2.295737
C -0.434821 3.735391 1.121572
C -1.115690 4.164181 -0.179371
C -2.402741 4.928485 0.155153
C -0.179098 4.986150 -1.071750
H 5.377601 1.537231 0.926870
H 3.355308 -2.086874 -0.248794
H 2.399774 3.336454 1.106794
H 5.602368 -1.891059 0.075221
H 0.094496 -0.647974 -0.777311
H 1.356555 -2.984772 0.762157
H -0.339135 -4.147022 -0.746101
H -1.228210 -2.615447 -0.917237
H -1.110133 3.130914 1.741314
H -0.099563 4.610263 1.698049
H -1.395613 3.241452 -0.717197
H -2.182356 5.851903 0.717609
H -3.092342 4.319846 0.762037
H -2.932489 5.218276 -0.765600
H 0.744983 4.434507 -1.302913
H -0.669557 5.238976 -2.025039
H 0.105694 5.931916 -0.579249
H -0.863456 -4.273858 1.647022

H -2.325456 -4.200646 0.666726
H -1.123715 -1.818801 2.217209
H -2.406452 -2.877589 2.801852
H -3.835169 -2.159886 0.840108
H -1.814864 -0.206407 0.459229
H -4.393316 0.074771 1.814675
H -4.160543 -1.144762 3.099720
H -2.880236 0.048687 2.758990
O 0.773652 2.973630 0.883900
O -0.392754 1.065696 0.787472
O -2.537283 -0.780668 0.149295
O 3.305597 2.963742 1.118800
O 5.703216 -0.959908 0.322920

13R-5-c9, $\Delta G = 1.2186$ kcal/mol,
population = 2.49 %

C 0.888865 1.723564 0.349606
C 2.202324 1.069647 0.520466
C 3.392736 1.821276 0.787488
C 4.595817 1.172209 1.085233
C 4.656629 -0.220578 1.105409
C 3.512151 -0.979659 0.806795
C 2.292596 -0.361944 0.521151
C 1.135929 -1.217803 0.184125
C 0.825324 -2.374065 0.794479
C -0.371429 -3.215652 0.455893
C -1.400922 -3.293637 1.605399
C -2.006481 -1.963196 2.078065
C -2.943237 -1.246123 1.093292
C -3.689844 -0.088235 1.761134
C -0.228885 3.857250 0.060251
C -0.728707 4.314214 1.432542
C 0.328413 5.127884 2.188101
C -2.033704 5.100881 1.256461
H 5.484443 1.769075 1.293124
H 3.586272 -2.068235 0.762504
H 2.568122 3.503201 0.505182
H 5.761176 -1.758532 1.372421
H 0.479739 -0.862143 -0.612566
H 1.435286 -2.713591 1.642605
H -0.036763 -4.246473 0.235583
H -0.854900 -2.823683 -0.449945
H 0.049335 4.717725 -0.565888
H -0.989421 3.261671 -0.460920

H -0.954379 3.403804 2.015433
 H 0.563756 6.063358 1.651885
 H 1.265966 4.564004 2.309982
 H -0.032012 5.398776 3.192920
 H -1.870996 6.012843 0.656985
 H -2.807735 4.499453 0.753191
 H -2.433454 5.412558 2.233961
 H -0.919095 -3.778680 2.473414
 H -2.215940 -3.972668 1.296879
 H -1.202720 -1.261370 2.366472
 H -2.580063 -2.160246 3.000405
 H -3.689555 -1.978905 0.734402
 H -1.590563 -0.154727 0.177730
 H -2.977019 0.655832 2.156594
 H -4.338904 0.417327 1.029409
 H -4.315117 -0.436603 2.598804
 O 0.982769 3.069071 0.149395
 O -0.202130 1.183767 0.382595
 O -2.274598 -0.797225 -0.081158
 O 3.440920 3.163645 0.792606
 O 5.842449 -0.793425 1.393450

13R-5-c10, $\Delta G = 1.2625$ kcal/mol,
population = 2.32 %

C 0.987928 2.265394 0.572067
 C 2.027974 1.239133 0.377469
 C 3.365448 1.618405 0.746423
 C 4.421727 0.703376 0.669309
 C 4.186667 -0.591807 0.214092
 C 2.893241 -0.978231 -0.177793
 C 1.809682 -0.097198 -0.099627
 C 0.492515 -0.595601 -0.555357
 C 0.054351 -1.859422 -0.404380
 C -1.261326 -2.378525 -0.910628
 C -2.086885 -3.131266 0.153935
 C -2.418221 -2.368842 1.445616
 C -3.343081 -1.152193 1.314233
 C -3.759668 -0.600721 2.678507
 C -1.321424 2.889647 0.529822
 C -1.521068 3.764267 -0.710630
 C -1.835604 2.933198 -1.959483
 C -2.626590 4.787576 -0.418366
 H 5.424407 1.019679 0.958504
 H 2.742036 -1.978591 -0.587681

H 2.813169 3.363124 1.175093
 H 4.950821 -2.299478 -0.186218
 H -0.160852 0.122852 -1.051694
 H 0.677507 -2.580895 0.140626
 H -1.061849 -3.090318 -1.734657
 H -1.846836 -1.551266 -1.336230
 H -2.221836 2.293680 0.731495
 H -1.082034 3.505395 1.407190
 H -0.581355 4.317260 -0.881642
 H -1.990188 3.585823 -2.833364
 H -2.751742 2.335524 -1.816013
 H -1.016345 2.239420 -2.203051
 H -3.589659 4.286530 -0.220756
 H -2.384719 5.410448 0.457999
 H -2.771189 5.459684 -1.278535
 H -1.537901 -4.047191 0.436370
 H -3.025252 -3.476685 -0.314500
 H -1.484537 -2.042116 1.942164
 H -2.893799 -3.075144 2.147278
 H -4.252708 -1.458919 0.767099
 H -1.854557 0.027598 0.805954
 H -4.405548 0.281832 2.552849
 H -4.312093 -1.353150 3.263703
 H -2.873954 -0.298254 3.262949
 O -0.278479 1.895222 0.363716
 O 1.247582 3.420502 0.929763
 O -2.766098 -0.119811 0.510474
 O 3.664570 2.843805 1.184482
 O 5.236559 -1.435629 0.146302

13R-5-c128, $\Delta G = 1.2625$ kcal/mol,
population = 2.32 %

C 1.760454 2.521945 0.444005
 C 2.835140 1.550673 0.714621
 C 4.154312 1.925819 0.288396
 C 5.226572 1.032292 0.398677
 C 5.021209 -0.235782 0.937800
 C 3.744061 -0.613973 1.390319
 C 2.650310 0.250566 1.288853
 C 1.358508 -0.218890 1.838890
 C 0.869922 -1.463121 1.696470
 C -0.432307 -1.941808 2.276029
 C -1.560458 -2.092714 1.231230
 C -1.974971 -0.755704 0.613589

C -3.063414 -0.814697 -0.464258
 C -4.440182 -1.186134 0.068809
 C -0.580035 2.997122 0.342474
 C -0.918504 3.972017 1.473107
 C -2.056527 4.892224 1.011902
 C -1.268575 3.251647 2.779396
 H 6.217108 1.341381 0.063291
 H 3.614676 -1.587139 1.868342
 H 3.553936 3.623037 -0.251833
 H 5.817316 -1.907290 1.417878
 H 0.771172 0.510057 2.401955
 H 1.416854 -2.183989 1.074667
 H -0.765483 -1.247591 3.066533
 H -0.271546 -2.921513 2.759661
 H -0.323164 3.545687 -0.574080
 H -1.426797 2.326297 0.134725
 H -0.024033 4.595790 1.644313
 H -2.298138 5.632242 1.790764
 H -2.974470 4.316391 0.803463
 H -1.789480 5.443760 0.095923
 H -2.159274 2.612558 2.652829
 H -0.441247 2.613605 3.125768
 H -1.487420 3.978129 3.578001
 H -2.423557 -2.572461 1.722804
 H -1.234118 -2.786844 0.435176
 H -1.084262 -0.285582 0.163532
 H -2.312648 -0.066350 1.409264
 H -2.766267 -1.567917 -1.222900
 H -2.376234 0.654151 -1.561150
 H -5.177924 -1.191803 -0.748326
 H -4.433898 -2.183308 0.533578
 H -4.768084 -0.452416 0.823775
 O 0.513475 2.106966 0.668161
 O 1.978890 3.655475 -0.000681
 O -3.201169 0.462986 -1.093981
 O 4.417242 3.124233 -0.239563
 O 6.083709 -1.061889 1.027075

13R-5-c93, $\Delta G = 1.2820$ kcal/mol,
 population = 2.24 %

C 1.312058 2.496786 0.270574
 C 2.388631 1.528180 0.540658
 C 3.704418 1.907221 0.114015
 C 4.781567 1.016425 0.226776

C 4.580522 -0.251065 0.768225
 C 3.303664 -0.634070 1.218725
 C 2.208906 0.225622 1.116335
 C 0.917783 -0.246812 1.665991
 C 0.432253 -1.492114 1.523330
 C -0.868821 -1.974125 2.102952
 C -1.998151 -2.124075 1.059253
 C -2.416315 -0.786016 0.446339
 C -3.506773 -0.843848 -0.629524
 C -4.881909 -1.219022 -0.094840
 C -1.029143 2.970412 0.178687
 C -1.363266 3.945232 1.310730
 C -2.504359 4.864290 0.854900
 C -1.706323 3.224688 2.618799
 H 5.766059 1.343914 -0.114181
 H 3.193360 -1.609837 1.691956
 H 3.099950 3.600804 -0.430311
 H 6.412044 -0.777594 0.586642
 H 0.328595 0.480468 2.229367
 H 0.981691 -2.211466 0.902045
 H -1.202278 -1.282291 2.895462
 H -0.706268 -2.954735 2.584138
 H -0.776640 3.518998 -0.739059
 H -1.876360 2.299007 -0.025296
 H -0.468568 4.569886 1.477568
 H -2.742712 5.604370 1.634712
 H -3.422832 4.287587 0.651270
 H -2.242387 5.415739 -0.062598
 H -2.596568 2.584156 2.496380
 H -0.876450 2.588036 2.961610
 H -1.922733 3.951043 3.418190
 H -2.859665 -2.607031 1.550494
 H -1.671592 -2.815049 0.260544
 H -1.527307 -0.312951 -0.003990
 H -2.753698 -0.099616 1.244703
 H -3.209866 -1.594467 -1.390829
 H -2.823980 0.629413 -1.723168
 H -5.621232 -1.223586 -0.910557
 H -4.873107 -2.217479 0.367112
 H -5.209524 -0.487956 0.662820
 O 0.066290 2.081242 0.500153
 O 1.527589 3.629757 -0.177881
 O -3.647942 0.435345 -1.255488
 O 3.965337 3.104330 -0.416657

O 5.577080 -1.149054 0.908483

13R-5-c15, $\Delta G = 1.3228$ kcal/mol,
population = 2.09 %

C 1.095058 2.562514 0.220852
C 2.162308 1.554926 0.099733
C 3.457061 1.935728 0.580946
C 4.509417 1.009524 0.618424
C 4.301404 -0.295697 0.177602
C 3.045272 -0.683070 -0.325987
C 1.977475 0.213682 -0.374123
C 0.707046 -0.260700 -0.968197
C 0.132949 -1.447959 -0.711942
C -1.173631 -1.893068 -1.323889
C -2.416141 -1.314955 -0.614112
C -2.570878 -1.725153 0.851701
C -3.689378 -0.973499 1.585376
C -3.935727 -1.516166 2.991960
C -1.245907 3.056284 0.133363
C -1.504234 3.934594 -1.093367
C -1.767759 3.107820 -2.356376
C -2.668334 4.886449 -0.787727
H 5.480574 1.337826 0.995116
H 2.932438 -1.693983 -0.718255
H 2.867949 3.683907 0.939214
H 6.095878 -0.854308 0.538529
H 0.207784 0.421522 -1.661487
H 0.596652 -2.111838 0.027471
H -1.227376 -2.995313 -1.317944
H -1.209026 -1.581001 -2.381348
H -2.105420 2.400711 0.338209
H -1.046861 3.678440 1.017071
H -0.598695 4.545078 -1.255024
H -2.662925 2.473939 -2.234702
H -0.918461 2.449993 -2.596083
H -1.936630 3.764874 -3.224294
H -2.852910 5.561035 -1.638314
H -3.600315 4.326887 -0.597936
H -2.463523 5.509968 0.097560
H -3.318610 -1.620117 -1.173380
H -2.371649 -0.215396 -0.671354
H -1.626466 -1.545118 1.399029
H -2.761846 -2.810843 0.920514
H -4.621136 -1.069205 0.999937

H -2.634979 0.572044 2.150938

H -3.017175 -1.451129 3.601008

H -4.722720 -0.934015 3.495535

H -4.247129 -2.572393 2.965026

O -0.140139 2.142000 -0.046323

O 1.307166 3.726055 0.584056

O -3.436504 0.433271 1.624466

O 3.717656 3.168428 1.023840

O 5.274503 -1.229673 0.187592

13R-5-c54, $\Delta G = 1.3768$ kcal/mol,
population = 1.91 %

C 0.038075 0.961379 0.637893
C 1.398033 0.386000 0.607737
C 2.565667 1.216118 0.624398
C 3.845556 0.654590 0.716710
C 4.001428 -0.729233 0.770393
C 2.874701 -1.565928 0.714766
C 1.583425 -1.041378 0.642604
C 0.451008 -1.989863 0.557803
C 0.407653 -3.186716 1.171103
C -0.699212 -4.205272 1.068952
C -1.997022 -3.746131 0.394901
C -2.821964 -2.759330 1.235868
C -3.790175 -1.901831 0.409279
C -4.701292 -1.044208 1.288309
C -1.256700 3.000047 0.526802
C -1.000209 4.497159 0.669010
C -2.333363 5.250451 0.575183
C -0.252173 4.829622 1.966407
H 4.705669 1.327395 0.731189
H 3.033948 -2.643917 0.693946
H 1.601794 2.836403 0.440642
H 5.911717 -0.655420 0.865833
H -0.404020 -1.668810 -0.034535
H 1.243597 -3.478808 1.818937
H -0.919626 -4.582168 2.085715
H -0.294429 -5.085998 0.533207
H -1.821436 2.771882 -0.390632
H -1.822344 2.603493 1.383423
H -0.373335 4.805432 -0.187812
H -3.011069 4.963891 1.397207
H -2.850403 5.046403 -0.376105
H -2.169321 6.337016 0.642509

H 0.705604 4.291858 2.036443
 H -0.036836 5.907786 2.027464
 H -0.856331 4.555518 2.848039
 H -2.612714 -4.633412 0.168749
 H -1.765245 -3.285818 -0.579216
 H -2.150607 -2.072273 1.779561
 H -3.388936 -3.310009 2.006599
 H -4.422968 -2.573026 -0.200429
 H -2.473156 -0.525200 -0.045642
 H -4.103129 -0.373914 1.929286
 H -5.359804 -0.421056 0.663456
 H -5.331073 -1.666707 1.944107
 O 0.013463 2.310264 0.454630
 O -1.004601 0.355369 0.816735
 O -3.089622 -1.097915 -0.536322
 O 2.532497 2.557053 0.561711
 O 5.209310 -1.322504 0.849029

13R-5-c43, $\Delta G = 1.3805$ kcal/mol,
population = 1.90 %

C 1.401935 1.687017 0.328830
 C 2.468166 0.677994 0.205346
 C 3.766241 1.055305 0.686096
 C 4.815964 0.129306 0.718604
 C 4.606516 -1.174211 0.272462
 C 3.348955 -1.558429 -0.229303
 C 2.279961 -0.659455 -0.271305
 C 1.007938 -1.133194 -0.862292
 C 0.432341 -2.318864 -0.601723
 C -0.875980 -2.763446 -1.210339
 C -2.116460 -2.179206 -0.502057
 C -2.271522 -2.583203 0.965480
 C -3.389743 -1.827987 1.695897
 C -3.637768 -2.365814 3.104042
 C -0.938189 2.184420 0.240405
 C -1.194526 3.064356 -0.985563
 C -1.459349 2.239180 -2.249341
 C -2.356945 4.018072 -0.679279
 H 5.792645 0.439709 1.091415
 H 3.217628 -2.565382 -0.631118
 H 3.178596 2.803795 1.049366
 H 5.384799 -2.897447 -0.020808
 H 0.508748 -0.451769 -1.556381
 H 0.895623 -2.981342 0.139261

H -0.932331 -3.865496 -1.199419
 H -0.911465 -2.455965 -2.269115
 H -1.798768 1.529965 0.444226
 H -0.738439 2.805269 1.124853
 H -0.287824 3.673299 -1.146499
 H -2.355894 1.607105 -2.128470
 H -0.611352 1.579748 -2.489262
 H -1.626493 2.897248 -3.116817
 H -3.289946 3.460017 -0.490094
 H -2.151132 4.640465 0.206559
 H -2.540199 4.693718 -1.529305
 H -3.019925 -2.484464 -1.059615
 H -2.069279 -1.080014 -0.563933
 H -1.327097 -2.401433 1.512203
 H -2.463174 -3.668482 1.038675
 H -4.321121 -1.924638 1.110036
 H -2.334990 -0.281507 2.258362
 H -2.719461 -2.300460 3.713412
 H -4.424033 -1.780694 3.605289
 H -3.951000 -3.421567 3.080234
 O 0.166341 1.268606 0.060135
 O 1.615565 2.849214 0.694399
 O -3.135488 -0.421347 1.730623
 O 4.027238 2.287444 1.131848
 O 5.648158 -2.030050 0.320678

13R-5-c95, $\Delta G = 1.3824$ kcal/mol,
population = 1.89 %

C 1.229043 1.805279 -0.330452
 C 2.178256 0.752819 0.071202
 C 3.439534 1.195535 0.587003
 C 4.361737 0.278707 1.111433
 C 4.062388 -1.082241 1.112839
 C 2.847648 -1.542160 0.571392
 C 1.903249 -0.654808 0.052952
 C 0.677579 -1.226171 -0.549320
 C -0.020850 -2.256854 -0.043333
 C -1.268722 -2.815266 -0.676058
 C -2.573306 -2.206458 -0.119396
 C -2.829355 -2.468508 1.366181
 C -4.055763 -1.729269 1.917171
 C -4.385357 -2.129096 3.354248
 C -1.036204 2.351410 -0.945938
 C -2.084126 2.520485 0.156005

C -1.480457 3.060380 1.457295
 C -3.210878 3.423868 -0.362759
 H 5.308162 0.656589 1.504199
 H 2.675295 -2.617692 0.526451
 H 3.033441 2.986911 0.190696
 H 5.717689 -1.590123 1.928454
 H 0.324845 -0.762734 -1.474500
 H 0.291175 -2.689547 0.914801
 H -1.292150 -3.911148 -0.537987
 H -1.239814 -2.632595 -1.763189
 H -0.557505 3.309259 -1.191285
 H -1.497303 1.936550 -1.854636
 H -2.515660 1.525349 0.364995
 H -0.703852 2.387678 1.853601
 H -2.257381 3.160675 2.231855
 H -1.024580 4.053205 1.305151
 H -3.664182 3.021512 -1.283327
 H -4.009331 3.519173 0.389475
 H -2.838634 4.438459 -0.585679
 H -3.423131 -2.599881 -0.705338
 H -2.553311 -1.118238 -0.292398
 H -1.951984 -2.164083 1.966946
 H -2.956769 -3.552089 1.538297
 H -4.924217 -1.964514 1.276358
 H -3.166395 -0.050016 2.375288
 H -3.531659 -1.921832 4.022872
 H -5.253240 -1.559531 3.720482
 H -4.617382 -3.203337 3.428215
 O -0.019258 1.399506 -0.561926
 O 1.548244 2.996412 -0.418323
 O -3.906477 -0.312275 1.807725
 O 3.787375 2.485104 0.606912
 O 4.911270 -2.012293 1.596579

13R-5-c62, $\Delta G = 1.3843$ kcal/mol,
population = 1.89 %

C 0.294500 1.691689 0.438270
 C 1.666958 1.152460 0.353445
 C 2.803319 2.011193 0.198719
 C 4.104969 1.495584 0.240906
 C 4.311730 0.128004 0.411805
 C 3.213327 -0.739936 0.525052
 C 1.903119 -0.259453 0.507240
 C 0.800516 -1.241442 0.602445

C 0.845499 -2.375102 1.325845
 C -0.231003 -3.427398 1.408602
 C -1.591652 -3.069603 0.800242
 C -2.382398 -2.028681 1.608267
 C -3.439683 -1.280109 0.784984
 C -4.309851 -0.367495 1.650023
 C -1.074298 3.674469 0.237356
 C -0.858844 5.184598 0.215256
 C -2.220156 5.889566 0.157124
 C -0.024663 5.661900 1.410963
 H 4.940120 2.189404 0.123387
 H 3.407342 -1.810276 0.592853
 H 1.773261 3.579702 -0.060040
 H 6.220079 0.261619 0.347096
 H -0.108327 -1.001238 0.053556
 H 1.738656 -2.582109 1.928521
 H -0.359713 -3.709971 2.470722
 H 0.160812 -4.344916 0.927786
 H -1.700472 3.343003 -0.605685
 H -1.557729 3.348377 1.170589
 H -0.310870 5.424186 -0.714508
 H -2.801705 5.580077 -0.726019
 H -2.088551 6.981486 0.107433
 H -2.822366 5.666727 1.054240
 H 0.953156 5.158572 1.455295
 H 0.158470 6.746072 1.351280
 H -0.549559 5.459910 2.360224
 H -2.192555 -3.990430 0.708190
 H -1.451254 -2.699161 -0.228140
 H -1.694897 -1.275267 2.030260
 H -2.869615 -2.517750 2.469758
 H -4.093860 -2.023123 0.292369
 H -2.209367 0.082035 0.101302
 H -5.035029 0.175500 1.024172
 H -4.866123 -0.941498 2.408493
 H -3.687834 0.376546 2.176755
 O 0.209258 3.014722 0.128772
 O -0.709456 1.078588 0.758670
 O -2.841354 -0.551349 -0.283724
 O 2.719472 3.338545 0.013359
 O 5.541658 -0.422459 0.449257

13R-5-c104, $\Delta G = 1.4201$ kcal/mol,
population = 1.78 %

C 1.175988 1.777866 0.819955
 C 2.206995 0.725734 0.740556
 C 3.559327 1.147895 0.988476
 C 4.625578 0.246413 0.895987
 C 4.379166 -1.087317 0.577330
 C 3.064659 -1.529002 0.353907
 C 1.973870 -0.654569 0.416231
 C 0.626375 -1.215299 0.166030
 C 0.365685 -2.245874 -0.659913
 C -0.986316 -2.842813 -0.951902
 C -2.193273 -2.234126 -0.229576
 C -2.327684 -2.620228 1.249802
 C -3.300966 -1.723714 2.025425
 C -3.576568 -2.233065 3.438405
 C -1.131623 2.392697 0.607008
 C -1.327115 3.193056 -0.682931
 C -1.612452 2.287132 -1.885630
 C -2.444498 4.221989 -0.468542
 H 5.640258 0.596476 1.088155
 H 2.892537 -2.589006 0.158858
 H 3.001482 2.907719 1.343207
 H 5.138398 -2.818165 0.283105
 H -0.200057 -0.736008 0.684688
 H 1.190597 -2.696607 -1.225593
 H -0.936385 -3.931895 -0.754735
 H -1.144181 -2.774388 -2.044819
 H -2.020753 1.788169 0.839531
 H -0.915737 3.062890 1.450193
 H -0.388032 3.742657 -0.871662
 H -0.801957 1.559683 -2.044345
 H -1.718183 2.881988 -2.806871
 H -2.549677 1.722638 -1.740146
 H -3.405195 3.724861 -0.250404
 H -2.218633 4.900934 0.369623
 H -2.585316 4.837197 -1.370960
 H -3.111177 -2.545581 -0.756889
 H -2.153798 -1.136359 -0.317808
 H -1.345779 -2.577655 1.755311
 H -2.662620 -3.669157 1.329317
 H -4.255620 -1.680574 1.471663
 H -2.043489 -0.331837 2.593910
 H -4.039467 -3.232304 3.419181
 H -2.638978 -2.307814 4.016644
 H -4.253537 -1.546410 3.969423

O -0.066410 1.420313 0.500377
 O 1.427809 2.940400 1.161182
 O -2.847232 -0.366735 2.054383
 O 3.864343 2.408014 1.310389
 O 5.435031 -1.924968 0.512664

13R-5-c2, $\Delta G = 1.4426$ kcal/mol,
 population = 1.71 %

C 1.687029 1.789297 0.365246
 C 2.723503 0.759494 0.168867
 C 4.059009 1.132627 0.542537
 C 5.109100 0.205836 0.485042
 C 4.867345 -1.090244 0.036767
 C 3.576167 -1.466710 -0.372583
 C 2.501512 -0.576811 -0.311588
 C 1.188040 -1.054828 -0.798714
 C 0.735058 -2.316690 -0.680578
 C -0.574950 -2.813717 -1.222322
 C -1.423444 -3.586412 -0.190814
 C -1.765855 -2.855604 1.116072
 C -2.672385 -1.623423 1.004488
 C -3.106956 -1.108167 2.377572
 C -0.651705 2.369661 0.372104
 C -1.340585 2.650414 -0.964311
 C -2.547678 3.564675 -0.716441
 C -0.386184 3.242385 -2.006612
 H 6.107382 0.530844 0.785520
 H 3.439679 -2.468488 -0.779539
 H 3.523369 2.889750 0.935000
 H 6.685062 -1.652257 0.240663
 H 0.552519 -0.320666 -1.296091
 H 1.341439 -3.054249 -0.138341
 H -0.366351 -3.506307 -2.060373
 H -1.147243 -1.972055 -1.637764
 H -1.361465 1.907004 1.071140
 H -0.241479 3.285666 0.816414
 H -1.717159 1.681529 -1.336030
 H -2.231134 4.544328 -0.319414
 H -3.252392 3.119970 0.004766
 H -3.096821 3.746271 -1.653454
 H 0.457948 2.567412 -2.217538
 H -0.912602 3.418624 -2.958089
 H 0.027538 4.206391 -1.665820
 H -0.887587 -4.515082 0.074701

H -2.358267 -3.909583 -0.681768
H -0.836487 -2.555383 1.636718
H -2.261835 -3.574731 1.790039
H -3.576213 -1.902568 0.433340
H -1.155214 -0.457544 0.542603
H -2.228034 -0.838202 2.987690
H -3.736115 -0.211643 2.266843
H -3.682498 -1.869097 2.928571
O 0.416651 1.400450 0.219361
O 1.959724 2.954570 0.675774
O -2.070042 -0.573945 0.243771
O 4.367303 2.359201 0.969780
O 5.838403 -2.022030 -0.051320

13R-5-c39, $\Delta G = 1.4602$ kcal/mol,
population = 1.66 %

C 1.050331 1.313250 -0.358305
C 2.395082 0.702947 -0.349823
C 3.582585 1.503311 -0.428954
C 4.848145 0.923618 -0.296230
C 4.972645 -0.452502 -0.110379
C 3.826776 -1.263324 -0.069762
C 2.544996 -0.715534 -0.174339
C 1.387126 -1.635773 -0.150519
C 1.326713 -2.775547 0.562271
C 0.189184 -3.765128 0.573717
C -1.117911 -3.319933 -0.092032
C -1.887184 -2.250823 0.699334
C -2.861748 -1.429298 -0.155624
C -3.719794 -0.484610 0.686899
C -0.185984 3.368239 -0.725602
C -0.435471 3.996567 0.647213
C 0.709972 4.922815 1.071337
C -1.783926 4.727440 0.629431
H 5.732625 1.558877 -0.352255
H 3.944597 -2.345855 0.009398
H 2.649397 3.116718 -0.771097
H 6.175150 -1.921738 0.119712
H 0.525428 -1.340474 -0.746966
H 2.171038 -3.038031 1.211862
H -0.006727 -4.056665 1.622932
H 0.551539 -4.695707 0.094839
H -0.060836 4.141060 -1.498153
H -1.009176 2.701524 -1.013586

H -0.506003 3.168565 1.374286
H 1.677004 4.396851 1.075846
H 0.538690 5.317147 2.085258
H 0.796402 5.783662 0.386051
H -1.780200 5.553369 -0.102223
H -2.611325 4.048387 0.367785
H -2.003212 5.159829 1.617977
H -1.763743 -4.203578 -0.231656
H -0.907128 -2.939824 -1.104622
H -1.178810 -1.544948 1.166766
H -2.439363 -2.726864 1.528309
H -3.532062 -2.125086 -0.693351
H -1.513536 -0.140032 -0.753397
H -3.083341 0.214995 1.255429
H -4.384597 0.108086 0.039470
H -4.341663 -1.039056 1.408122
O 1.050020 2.613304 -0.768690
O 0.006834 0.771867 -0.036429
O -2.173472 -0.715868 -1.179720
O 3.573648 2.834219 -0.611707
O 6.216159 -0.961216 0.000203

13R-5-c23, $\Delta G = 1.4797$ kcal/mol,
population = 1.61 %

C 0.111928 1.873003 0.340684
C 1.457534 1.265539 0.351875
C 2.641183 2.067899 0.270456
C 3.910066 1.490603 0.406225
C 4.037257 0.115979 0.598598
C 2.892954 -0.697399 0.642502
C 1.612100 -0.153871 0.533805
C 0.455635 -1.076259 0.560422
C 0.397698 -2.212653 1.278645
C -0.736957 -3.205359 1.294957
C -2.043813 -2.769313 0.622866
C -2.818843 -1.696749 1.404083
C -3.790681 -0.881745 0.539731
C -4.653690 0.066669 1.372899
C -1.126286 3.927730 -0.024780
C -1.377206 4.553971 1.348765
C -0.232502 5.479990 1.775470
C -2.725639 5.284954 1.330497
H 4.784474 2.142005 0.346149
H 3.029981 -1.775089 0.730332

H 1.707242 3.679466 -0.075321
 H 5.949518 0.157941 0.666417
 H -0.406081 -0.785920 -0.038482
 H 1.242988 -2.469567 1.929142
 H -0.934441 -3.489579 2.345939
 H -0.370910 -4.138563 0.824039
 H -1.001419 4.701742 -0.796199
 H -1.948779 3.260722 -0.314059
 H -1.448376 3.724865 2.074519
 H -0.404288 5.871621 2.790345
 H -0.146905 6.342632 1.092356
 H 0.734994 4.954889 1.778638
 H -2.946028 5.716222 2.319297
 H -2.720747 6.111704 0.599808
 H -3.552837 4.606333 1.067053
 H -2.686502 -3.656043 0.488390
 H -1.831502 -2.396593 -0.392145
 H -2.114320 -0.987020 1.871481
 H -3.374571 -2.168827 2.232913
 H -4.457679 -1.581788 0.003413
 H -2.442818 0.406969 -0.060342
 H -5.316203 0.655030 0.719203
 H -5.278200 -0.484552 2.094356
 H -4.020655 0.770066 1.940582
 O 0.110350 3.174022 -0.068060
 O -0.931593 1.329929 0.659594
 O -3.099210 -0.173525 -0.485839
 O 2.632327 3.397634 0.082654
 O 5.233672 -0.492410 0.723627

13R-5-c73, $\Delta G = 1.5054$ kcal/mol,
 population = 1.54 %

C 0.565148 1.295536 0.496433
 C 1.923606 0.715767 0.468415
 C 3.096053 1.542337 0.491796
 C 4.371504 0.977331 0.589596
 C 4.522387 -0.407455 0.640365
 C 3.393557 -1.239955 0.575277
 C 2.102220 -0.710396 0.500186
 C 0.967668 -1.655362 0.409927
 C 0.918579 -2.853358 1.020815
 C -0.192355 -3.867171 0.914983
 C -1.488932 -3.400263 0.243980
 C -2.308595 -2.412911 1.089455

C -3.273659 -1.547945 0.266866
 C -4.179264 -0.688207 1.149475
 C -0.724413 3.336060 0.378126
 C -0.464638 4.833669 0.509651
 C -1.796658 5.588725 0.415855
 C 0.289100 5.173218 1.801912
 H 5.242655 1.632763 0.612185
 H 3.533841 -2.322173 0.546585
 H 2.135757 3.164990 0.303177
 H 5.749284 -1.869793 0.749640
 H 0.114732 -1.330091 -0.183121
 H 1.751412 -3.149962 1.670674
 H -0.413212 -4.247262 1.930422
 H 0.208653 -4.747265 0.375362
 H -1.292362 3.102779 -0.536020
 H -1.288155 2.945839 1.238928
 H 0.159652 5.134785 -0.351552
 H -2.317828 5.378757 -0.531861
 H -1.630104 6.675362 0.474630
 H -2.471539 5.309459 1.242690
 H -0.311850 4.905741 2.687772
 H 1.246326 4.634490 1.871500
 H 0.506215 6.251457 1.855186
 H -2.108568 -4.284206 0.015672
 H -1.256697 -2.937665 -0.728930
 H -1.633600 -1.731121 1.635425
 H -2.877488 -2.963923 1.858538
 H -3.910808 -2.214157 -0.343783
 H -1.950959 -0.176123 -0.185589
 H -3.576990 -0.021718 1.790535
 H -4.836133 -0.060868 0.527084
 H -4.810697 -1.309132 1.805204
 O 0.544140 2.643119 0.306619
 O -0.478908 0.692890 0.678783
 O -2.570439 -0.744726 -0.677304
 O 3.064677 2.883901 0.431099
 O 5.773709 -0.901558 0.725611

13R-5-c124, $\Delta G = 1.5154$ kcal/mol,
 population = 1.51 %

C 1.294448 2.449212 -0.039338
 C 2.236659 1.389847 0.362232
 C 3.501721 1.822491 0.882632
 C 4.415323 0.899692 1.405847

C 4.107013 -0.459576 1.402989
 C 2.890871 -0.909645 0.857335
 C 1.951778 -0.013531 0.338677
 C 0.724841 -0.576576 -0.268400
 C 0.018766 -1.604453 0.232854
 C -1.229578 -2.154589 -0.406020
 C -2.533120 -1.541705 0.148588
 C -2.795707 -1.808765 1.632120
 C -4.021024 -1.066530 2.181564
 C -4.357680 -1.470799 3.615742
 C -0.966807 3.009369 -0.657496
 C -2.018008 3.179806 0.441070
 C -1.416554 3.713064 1.746116
 C -3.138816 4.089787 -0.079045
 H 5.366947 1.253977 1.803462
 H 2.697145 -1.982811 0.799777
 H 3.107290 3.617748 0.488073
 H 4.696087 -2.223752 1.849777
 H 0.378047 -0.109078 -1.193738
 H 0.324017 -2.040736 1.191592
 H -1.258528 -3.250843 -0.272009
 H -1.195981 -1.968036 -1.492329
 H -0.482369 3.965621 -0.897754
 H -1.426417 2.599900 -1.569402
 H -2.454777 2.185990 0.645454
 H -2.195735 3.814568 2.518246
 H -0.955709 4.704297 1.598560
 H -0.644355 3.035705 2.143103
 H -3.590484 3.692274 -1.002518
 H -3.939590 4.186276 0.670562
 H -2.761281 5.103404 -0.297431
 H -3.382640 -1.928690 -0.442018
 H -2.507307 -0.452909 -0.019900
 H -1.919328 -1.510508 2.237411
 H -2.928384 -2.892493 1.799268
 H -4.888040 -1.295547 1.536563
 H -3.126778 0.607164 2.650308
 H -5.224577 -0.899125 3.981009
 H -4.594464 -2.544354 3.684424
 H -3.505685 -1.269812 4.288445
 O 0.043949 2.051186 -0.272559
 O 1.621286 3.638059 -0.125442
 O -3.865277 0.350197 2.078284
 O 3.856380 3.110686 0.905157

O 5.019745 -1.312779 1.912018

13R-5-c17, $\Delta G = 1.5261$ kcal/mol,
population = 1.48 %

C 0.685743 0.982419 1.101276
 C 1.976885 0.364583 0.742896
 C 3.185314 1.130478 0.707673
 C 4.423037 0.503503 0.512457
 C 4.486110 -0.875623 0.317758
 C 3.307696 -1.640140 0.297693
 C 2.060358 -1.052617 0.513613
 C 0.852919 -1.902337 0.424162
 C 0.796047 -3.204874 0.756340
 C -0.396776 -4.114946 0.607084
 C -1.728798 -3.452198 0.237485
 C -2.373138 -2.658617 1.386161
 C -3.327928 -1.551334 0.917264
 C -4.086017 -0.907243 2.078409
 C -0.506419 3.078641 1.350433
 C -1.512405 3.204643 0.203887
 C -2.726285 4.004551 0.694438
 C -0.883432 3.832732 -1.044465
 H 5.322739 1.122630 0.503966
 H 3.387345 -2.703072 0.069952
 H 2.312027 2.796327 0.934101
 H 6.390902 -0.905167 0.129195
 H -0.050955 -1.413453 0.063019
 H 1.689131 -3.683744 1.176799
 H -0.514185 -4.693184 1.543311
 H -0.138583 -4.877492 -0.153383
 H -0.959665 2.587084 2.221815
 H -0.128074 4.067502 1.648848
 H -1.858729 2.187318 -0.047483
 H -3.199807 3.531302 1.569775
 H -3.486461 4.079107 -0.098634
 H -2.438953 5.031250 0.978811
 H -0.547199 4.864137 -0.840944
 H -0.012561 3.255962 -1.391244
 H -1.612308 3.874141 -1.869155
 H -2.431269 -4.232606 -0.100922
 H -1.581407 -2.786561 -0.628284
 H -1.591755 -2.182959 2.004697
 H -2.914598 -3.348520 2.056407
 H -4.063448 -1.990238 0.218303

H -1.919095 -0.204868 0.710405
H -3.382248 -0.480323 2.813417
H -4.731636 -0.094457 1.711011
H -4.717971 -1.642065 2.602699
O 0.681729 2.338599 0.974036
O -0.309381 0.396836 1.492300
O -2.631676 -0.568665 0.153421
O 3.230124 2.461116 0.872669
O 5.648634 -1.527551 0.113570

13R-5-c34, $\Delta G = 1.5650$ kcal/mol,
population = 1.39 %

C 1.108103 1.979502 0.407202
C 2.397733 1.359416 0.045841
C 3.610343 2.122386 0.011818
C 4.844110 1.493393 -0.185395
C 4.903523 0.114566 -0.385000
C 3.723056 -0.646102 -0.408594
C 2.475682 -0.055180 -0.187933
C 1.266688 -0.902349 -0.277090
C 1.207036 -2.204856 0.055030
C 0.011946 -3.112143 -0.092695
C -1.319690 -2.446247 -0.458027
C -1.959594 -1.653254 0.693548
C -2.912788 -0.542837 0.228764
C -3.666110 0.101458 1.392901
C -0.080434 4.077187 0.658254
C -1.086817 4.205112 -0.487684
C -2.299032 5.007118 0.003531
C -0.457483 4.832268 -1.736337
H 5.753421 2.095168 -0.194169
H 3.782053 -1.710752 -0.642937
H 2.739273 3.789540 0.243177
H 6.032412 -1.395417 -0.708078
H 0.363482 -0.411095 -0.636688
H 2.098974 -2.686059 0.475426
H -0.104210 -3.691419 0.842999
H 0.266821 -3.874093 -0.854883
H -0.533858 3.585822 1.529648
H 0.299759 5.065244 0.956895
H -1.435014 3.188387 -0.738892
H -2.772483 4.535086 0.879556
H -3.059822 5.082387 -0.788888
H -2.009885 6.033556 0.286987

H -0.119275 5.863024 -1.532805
H 0.412162 4.254060 -2.083798
H -1.186837 4.875134 -2.560536
H -2.024361 -3.224910 -0.795850
H -1.173341 -1.779619 -1.323221
H -1.175792 -1.180437 1.311220
H -2.501091 -2.343171 1.363761
H -3.651160 -0.978719 -0.469049
H -1.500913 0.800138 0.020772
H -2.959188 0.525559 2.126509
H -4.310773 0.916350 1.028503
H -4.298408 -0.632549 1.917921
O 1.106271 3.335318 0.280568
O 0.112870 1.395077 0.799661
O -2.215656 0.439100 -0.535219
O 3.656459 3.452832 0.181394
O 6.117593 -0.438952 -0.579835

13R-5-c58, $\Delta G = 1.5732$ kcal/mol,
population = 1.37 %

C 1.090893 2.234600 0.433740
C 2.167879 1.241203 0.275143
C 3.477876 1.647951 0.700052
C 4.548703 0.745938 0.691384
C 4.351046 -0.562557 0.255612
C 3.083334 -0.975007 -0.193473
C 1.991308 -0.102485 -0.191228
C 0.708851 -0.613345 -0.725350
C 0.206858 -1.836072 -0.481569
C -1.093182 -2.347597 -1.036795
C -2.225444 -2.426945 0.010613
C -2.591370 -1.057169 0.588625
C -3.841264 -0.998300 1.473465
C -3.775060 -1.890618 2.711212
C -1.249900 2.721930 0.413475
C -1.537491 3.600811 -0.806701
C -1.833126 2.774562 -2.062933
C -2.693136 4.552953 -0.471201
H 5.532357 1.080075 1.023005
H 2.960903 -1.984884 -0.590349
H 2.871287 3.385597 1.081435
H 5.151024 -2.270126 -0.063540
H 0.136726 0.065859 -1.361128
H 0.735724 -2.504107 0.210984

H -0.935520 -3.356820 -1.457272
 H -1.419108 -1.702179 -1.870327
 H -2.108982 2.073054 0.639337
 H -1.027512 3.343560 1.291756
 H -0.635811 4.210364 -0.990617
 H -2.726777 2.142917 -1.920240
 H -0.991164 2.115028 -2.323186
 H -2.021315 3.432206 -2.926429
 H -3.619676 3.993396 -0.256371
 H -2.465018 5.177426 0.407742
 H -2.900226 5.226972 -1.317059
 H -1.926903 -3.117596 0.818547
 H -3.111545 -2.878819 -0.469776
 H -2.750386 -0.348208 -0.242358
 H -1.738278 -0.659266 1.166680
 H -4.714694 -1.301119 0.868662
 H -3.416817 0.638948 2.453417
 H -2.893045 -1.641031 3.327151
 H -4.676128 -1.749919 3.327860
 H -3.706626 -2.956067 2.442352
 O -0.150277 1.805164 0.206484
 O 1.301982 3.400331 0.790061
 O -4.111446 0.357973 1.839624
 O 3.732967 2.886311 1.130858
 O 5.412052 -1.395467 0.260942

13R-5-c21, $\Delta G = 1.5889$ kcal/mol,
population = 1.33 %

C 0.794028 2.458994 1.223277
 C 1.828553 1.427106 1.024116
 C 3.167182 1.794510 1.399927
 C 4.213749 0.867361 1.336327
 C 3.969404 -0.425458 0.878997
 C 2.677149 -0.796474 0.469055
 C 1.602411 0.096132 0.537305
 C 0.287934 -0.379433 0.050941
 C -0.167229 -1.640453 0.170517
 C -1.478176 -2.135990 -0.370211
 C -2.326801 -2.907564 0.661974
 C -2.668472 -2.175800 1.968520
 C -3.573598 -0.942663 1.856073
 C -4.008730 -0.426600 3.228657
 C -1.543243 3.046117 1.221596
 C -2.228693 3.326908 -0.116566

C -3.434303 4.244106 0.127557
 C -1.270505 3.915472 -1.157316
 H 5.217159 1.173343 1.633986
 H 2.521219 -1.792472 0.050378
 H 2.634235 3.551217 1.801757
 H 4.719526 -2.140963 0.485668
 H -0.346418 0.355689 -0.446402
 H 0.437476 -2.378540 0.714050
 H -1.270706 -2.828945 -1.208236
 H -2.049682 -1.293753 -0.785503
 H -2.255455 2.586125 1.919917
 H -1.131488 3.961537 1.665666
 H -2.606635 2.358456 -0.488042
 H -3.116523 5.223411 0.524461
 H -4.141747 3.801614 0.847450
 H -3.980729 4.426043 -0.810979
 H -0.427506 3.238230 -1.365484
 H -1.794231 4.091972 -2.110225
 H -0.855229 4.878847 -0.816601
 H -1.791491 -3.836470 0.927794
 H -3.261918 -3.230346 0.171384
 H -1.738835 -1.876325 2.489159
 H -3.165271 -2.894114 2.642743
 H -4.477241 -1.220856 1.284182
 H -2.055270 0.222472 1.396583
 H -3.130058 -0.157657 3.839580
 H -4.636632 0.470700 3.117137
 H -4.585772 -1.186697 3.779232
 O -0.476911 2.074156 1.071367
 O 1.069013 3.621746 1.539836
 O -2.969340 0.105883 1.095564
 O 3.476389 3.018918 1.834256
 O 5.010639 -1.280917 0.823336

13R-5-c28, $\Delta G = 1.5889$ kcal/mol,
population = 1.33 %

C 1.237761 1.726731 0.439584
 C 2.321482 0.735554 0.321502
 C 3.598696 1.118334 0.846263
 C 4.664664 0.207358 0.876011
 C 4.486832 -1.085074 0.387081
 C 3.247003 -1.475373 -0.153477
 C 2.167078 -0.593329 -0.196411
 C 0.912071 -1.074099 -0.818961

C 0.340366 -2.263820 -0.570191
 C -0.963807 -2.707367 -1.186659
 C -2.204485 -2.168983 -0.442101
 C -2.344093 -2.642249 1.006411
 C -3.443679 -1.910675 1.788222
 C -3.685040 -2.518929 3.168350
 C -1.125002 2.165191 0.227124
 C -1.650660 2.616958 -1.137421
 C -2.953373 3.401564 -0.933045
 C -0.620023 3.428021 -1.930043
 H 5.621689 0.536260 1.287075
 H 3.156341 -2.476384 -0.575783
 H 2.973288 2.842833 1.252257
 H 6.282972 -1.627701 0.763849
 H 0.418793 -0.392485 -1.517005
 H 0.798737 -2.926079 0.174101
 H -1.003932 -3.809933 -1.218408
 H -1.014270 -2.358583 -2.231865
 H -1.880568 1.553799 0.741761
 H -0.856270 3.025416 0.855600
 H -1.888197 1.703054 -1.711992
 H -2.773574 4.325313 -0.357141
 H -3.705513 2.806813 -0.389931
 H -3.389196 3.691950 -1.901600
 H -1.031840 3.727758 -2.906858
 H -0.332719 4.344544 -1.388118
 H 0.295931 2.847841 -2.122044
 H -3.110282 -2.455299 -1.005901
 H -2.166023 -1.067728 -0.451556
 H -1.391182 -2.497863 1.549314
 H -2.546855 -3.727650 1.029386
 H -4.382436 -1.962427 1.208510
 H -2.360931 -0.411364 2.422170
 H -2.759289 -2.500816 3.769567
 H -4.456361 -1.949458 3.709208
 H -4.015535 -3.566868 3.091665
 O 0.024682 1.299697 0.093828
 O 1.422702 2.875673 0.858260
 O -3.167588 -0.511413 1.894787
 O 3.829637 2.338584 1.337648
 O 5.474025 -2.004231 0.386526

13R-5-c25, $\Delta G = 1.6108$ kcal/mol,
 population = 1.29 %

C 1.798865 2.452166 0.618117
 C 2.878554 1.462171 0.460646
 C 4.184915 1.874792 0.884402
 C 5.260887 0.975587 0.876138
 C 5.068080 -0.334273 0.443247
 C 3.801154 -0.753024 -0.003525
 C 2.707966 0.114722 -0.003698
 C 1.426988 -0.399539 -0.538513
 C 0.927864 -1.623596 -0.295996
 C -0.370161 -2.137964 -0.853560
 C -1.505336 -2.217639 0.190659
 C -1.874871 -0.847786 0.766228
 C -3.129002 -0.789506 1.645083
 C -3.068681 -1.682293 2.882758
 C -0.542849 2.934093 0.595781
 C -0.829317 3.814439 -0.623580
 C -1.121164 2.989691 -1.881668
 C -1.986969 4.764431 -0.288940
 H 6.238385 1.329803 1.210211
 H 3.698074 -1.766386 -0.391845
 H 3.573399 3.610040 1.265141
 H 6.892248 -0.845298 0.717271
 H 0.853608 0.278220 -1.174791
 H 1.458272 -2.290813 0.396089
 H -0.210015 -3.147486 -1.272364
 H -0.695030 -1.494183 -1.688804
 H -1.401196 2.283243 0.818690
 H -0.323595 3.554746 1.475551
 H 0.071827 4.425591 -0.804716
 H -2.014615 2.357090 -1.742051
 H -0.278011 2.331198 -2.140687
 H -1.307793 3.648350 -2.744731
 H -2.913168 4.203286 -0.076821
 H -1.761466 5.387853 0.591426
 H -2.193288 5.439480 -1.134161
 H -1.208363 -2.907051 1.000222
 H -2.389481 -2.671142 -0.291859
 H -2.030456 -0.139342 -0.065834
 H -1.024801 -0.448958 1.348064
 H -3.999406 -1.092296 1.035911
 H -2.709610 0.847799 2.627276
 H -2.189584 -1.433121 3.503036
 H -3.972672 -1.541801 3.495160
 H -2.999017 -2.747615 2.613751

O 0.558984 2.019791 0.389730
O 2.006477 3.618798 0.974715
O -3.401431 0.566595 2.010424
O 4.437436 3.113482 1.314231
O 6.064536 -1.242650 0.407734

13R-5-c6, $\Delta G = 1.6478$ kcal/mol,
population = 1.21 %

C 1.335219 2.509563 -0.196125
C 2.337353 1.458942 0.058879
C 3.640584 1.915932 0.445925
C 4.634843 1.007071 0.832071
C 4.373343 -0.361545 0.798921
C 3.124309 -0.832999 0.359575
C 2.100470 0.044385 -0.006018
C 0.836755 -0.528240 -0.519057
C 0.330909 -1.731107 -0.188552
C -0.915850 -2.325398 -0.779498
C -1.889840 -2.907817 0.264463
C -2.381284 -1.956361 1.365520
C -3.246084 -0.770115 0.921086
C -3.853503 -0.030810 2.114693
C -0.979134 3.085401 -0.520234
C -1.753777 3.524045 0.724571
C -0.875768 4.211366 1.775439
C -2.918830 4.422270 0.287145
H 5.609454 1.397396 1.132745
H 2.988267 -1.910709 0.270988
H 3.174470 3.707803 0.124650
H 6.117251 -0.855845 1.417596
H 0.285043 0.080278 -1.237437
H 0.843040 -2.342681 0.565758
H -0.620610 -3.154747 -1.451054
H -1.423391 -1.575305 -1.402963
H -0.525375 3.944121 -1.033276
H -1.650779 2.556128 -1.210302
H -2.181708 2.609038 1.168445
H -0.407683 5.123862 1.371288
H -0.072187 3.549702 2.134127
H -1.480213 4.499189 2.650522
H -3.574529 3.913283 -0.437742
H -3.534809 4.708261 1.153883
H -2.552354 5.350978 -0.182682
H -1.399881 -3.766803 0.756539

H -2.761870 -3.325495 -0.268854
H -1.520608 -1.561320 1.938768
H -2.969920 -2.546362 2.088541
H -4.070176 -1.153241 0.292327
H -1.657626 0.295487 0.457172
H -4.508972 -0.692595 2.703205
H -3.061771 0.346512 2.784211
H -4.449550 0.827814 1.769623
O 0.057338 2.120934 -0.209442
O 1.641626 3.696150 -0.353146
O -2.533213 0.134987 0.074050
O 3.964919 3.211771 0.471937
O 5.293006 -1.286020 1.145080

13R-5-c59, $\Delta G = 1.6667$ kcal/mol,
population = 1.17 %

C 1.727057 2.612434 0.881599
C 2.809744 1.619582 0.762479
C 4.090075 1.999523 1.286857
C 5.152660 1.088054 1.315596
C 4.972822 -0.204120 0.826025
C 3.732241 -0.591521 0.285605
C 2.651872 0.293473 0.244407
C 1.396072 -0.186094 -0.377163
C 0.821524 -1.373939 -0.125642
C -0.484057 -1.815161 -0.740650
C -1.722888 -1.273722 0.004826
C -1.862477 -1.746050 1.453646
C -2.960543 -1.012310 2.235618
C -3.202538 -1.619796 3.615964
C -0.635237 3.053874 0.673129
C -1.160955 3.511331 -0.689476
C -2.461759 4.298086 -0.481121
C -0.129372 4.322958 -1.480305
H 6.115360 1.400339 1.721707
H 3.623498 -1.589770 -0.143966
H 3.466821 3.725557 1.693253
H 5.780866 -1.907638 0.502391
H 0.904307 0.495317 -1.076435
H 1.277699 -2.035629 0.620558
H -0.526469 -2.917653 -0.771734
H -0.534671 -1.466713 -1.785938
H -1.391426 2.441902 1.186120
H -0.364806 3.911513 1.304396

H -1.401015 2.599931 -1.266966
 H -3.214614 3.703230 0.060885
 H -2.897987 4.592638 -1.448234
 H -2.279267 5.219535 0.097613
 H 0.160324 5.237030 -0.935557
 H 0.785228 3.741589 -1.675138
 H -0.541509 4.626831 -2.455707
 H -2.629677 -1.558370 -0.558188
 H -1.682069 -0.172571 -0.005246
 H -0.909087 -1.603035 1.996067
 H -2.067115 -2.831089 1.477205
 H -3.899537 -1.062634 1.656169
 H -1.876170 0.485501 2.870499
 H -2.276542 -1.603226 4.216856
 H -3.972617 -1.048768 4.156947
 H -3.535001 -2.667135 3.539663
 O 0.513158 2.186990 0.536678
 O 1.913814 3.760774 1.300218
 O -2.682056 0.386487 2.341739
 O 4.321940 3.220314 1.777785
 O 6.025154 -1.046830 0.873397

13R-5-c38, $\Delta G = 1.7338$ kcal/mol,
population = 1.04 %

C 1.759160 2.106102 0.357749
 C 2.846730 1.123110 0.207004
 C 4.144387 1.535303 0.653858
 C 5.220364 0.635941 0.661989
 C 5.034221 -0.673546 0.224709
 C 3.774994 -1.091817 -0.244959
 C 2.683307 -0.222812 -0.263830
 C 1.410872 -0.732037 -0.825130
 C 0.885786 -1.942864 -0.572989
 C -0.403217 -2.447625 -1.159983
 C -1.560652 -2.541555 -0.142017
 C -1.944399 -1.184298 0.456049
 C -3.239510 -1.148257 1.276020
 C -3.237138 -2.074525 2.489905
 C -0.623449 2.490711 0.330016
 C -1.326981 2.841647 -0.981715
 C -2.693111 3.462488 -0.661074
 C -0.478618 3.747101 -1.880338
 H 6.192100 0.988666 1.013981
 H 3.677421 -2.105019 -0.635359

H 3.522603 3.267091 1.034334
 H 6.852571 -1.185513 0.532462
 H 0.866009 -0.057940 -1.490268
 H 1.386607 -2.605639 0.145132
 H -0.236682 -3.452396 -1.588335
 H -0.709521 -1.793407 -1.994218
 H -1.292803 1.889657 0.961480
 H -0.316789 3.392856 0.876846
 H -1.504020 1.889892 -1.515170
 H -3.311386 2.773826 -0.063162
 H -3.241959 3.697044 -1.586422
 H -2.580702 4.401623 -0.092650
 H -0.273831 4.713437 -1.389345
 H 0.488956 3.283653 -2.129185
 H -1.000168 3.954216 -2.828304
 H -1.284358 -3.248468 0.659713
 H -2.434609 -2.983054 -0.653472
 H -2.057983 -0.450368 -0.360384
 H -1.119173 -0.810941 1.088562
 H -4.077817 -1.435537 0.616525
 H -2.893257 0.458436 2.340426
 H -4.171009 -1.954426 3.060311
 H -3.149218 -3.131445 2.194788
 H -2.390699 -1.840397 3.159530
 O 0.532337 1.654279 0.103408
 O 1.953558 3.270111 0.727187
 O -3.536832 0.196716 1.665713
 O 4.387239 2.773252 1.092034
 O 6.030814 -1.582388 0.206842

13R-5-c72, $\Delta G = 1.8016$ kcal/mol,
population = 0.93 %

C 1.364071 1.842767 0.280729
 C 2.449074 0.856665 0.127466
 C 3.750691 1.263056 0.574500
 C 4.821680 0.361025 0.581073
 C 4.630575 -0.946990 0.140461
 C 3.370285 -1.358836 -0.330728
 C 2.279508 -0.485329 -0.345774
 C 1.005162 -0.991414 -0.905146
 C 0.478408 -2.201370 -0.651785
 C -0.813155 -2.703805 -1.234896
 C -1.966563 -2.797468 -0.212330
 C -2.346187 -1.440361 0.388696

C -3.637800 -1.403801 1.214095
 C -3.630721 -2.330077 2.427943
 C -1.018055 2.231993 0.257935
 C -1.726377 2.579942 -1.051968
 C -3.090802 3.202713 -0.727801
 C -0.880624 3.482273 -1.956177
 H 5.799753 0.693664 0.930306
 H 3.253161 -2.368328 -0.730403
 H 3.134093 2.997431 0.956665
 H 5.435066 -2.655084 -0.165192
 H 0.460197 -0.315901 -1.568678
 H 0.979209 -2.865004 0.065633
 H -0.649345 -3.708344 -1.664830
 H -1.121738 -2.048270 -2.067221
 H -1.685518 1.633592 0.893955
 H -0.707880 3.135223 0.800994
 H -1.906153 1.626864 -1.582136
 H -3.707532 2.515925 -0.126131
 H -3.642767 3.435694 -1.651704
 H -2.975475 4.142990 -0.161860
 H -0.673639 4.449929 -1.468703
 H 0.085840 3.017527 -2.206986
 H -1.405320 3.686935 -2.902950
 H -1.687773 -3.505581 0.587486
 H -2.843076 -3.237407 -0.720719
 H -2.462460 -0.705532 -0.426544
 H -1.517898 -1.068524 1.018111
 H -4.478983 -1.690711 0.558101
 H -3.286618 0.202541 2.277440
 H -4.562331 -2.209953 3.002033
 H -3.544027 -3.387025 2.132490
 H -2.781636 -2.096020 3.094256
 O 0.135806 1.393511 0.028665
 O 1.562116 3.005845 0.649972
 O -3.932805 -0.058691 1.605026
 O 3.996316 2.500627 1.013800
 O 5.690962 -1.780528 0.163600

13R-5-c32, $\Delta G = 1.8882$ kcal/mol,
 population = 0.80 %

C 1.354651 2.511684 0.249137
 C 2.354170 1.458155 0.504998
 C 3.660229 1.910769 0.895218
 C 4.649425 0.999990 1.281760

C 4.384234 -0.368097 1.245046
 C 3.135584 -0.835402 0.801540
 C 2.112513 0.046723 0.436863
 C 0.847647 -0.522662 -0.076229
 C 0.337968 -1.723561 0.255853
 C -0.910976 -2.314658 -0.333585
 C -1.884103 -2.895879 0.711876
 C -2.370296 -1.944672 1.815459
 C -3.233202 -0.755690 1.374718
 C -3.834967 -0.015765 2.570779
 C -0.958313 3.092906 -0.075696
 C -1.732461 3.535573 1.167967
 C -0.853374 4.223807 2.217320
 C -2.896053 4.434604 0.728289
 H 5.628345 1.369763 1.588524
 H 2.982451 -1.911522 0.700369
 H 3.198523 3.704492 0.573106
 H 5.071506 -2.127740 1.546759
 H 0.297752 0.087054 -0.794931
 H 0.847390 -2.335679 1.011639
 H -0.618605 -3.144021 -1.006364
 H -1.417938 -1.562909 -0.955473
 H -0.502114 3.949629 -0.589901
 H -1.630870 2.564156 -0.765286
 H -2.162020 2.622307 1.613854
 H -0.383899 5.134717 1.811182
 H -0.050772 3.561692 2.577361
 H -1.457296 4.514460 3.091831
 H -3.552704 3.924676 0.004923
 H -3.511390 4.723954 1.594369
 H -2.528148 5.361412 0.255847
 H -1.395301 -3.756914 1.201531
 H -2.758476 -3.310423 0.179999
 H -1.507197 -1.552573 2.387084
 H -2.958569 -2.534163 2.539189
 H -4.060162 -1.135993 0.748047
 H -1.644588 0.308719 0.908867
 H -4.490297 -0.676328 3.160807
 H -3.040190 0.358962 3.238155
 H -4.429845 0.844670 2.228232
 O 0.075692 2.126389 0.237323
 O 1.664385 3.696793 0.090113
 O -2.520358 0.148056 0.526222
 O 3.986034 3.206737 0.922734

O 5.371943 -1.209285 1.614772
13R-5-c101, $\Delta G = 1.9672$ kcal/mol,
population = 0.70 %

C 0.266236 1.221189 0.420026
C 1.616788 0.676892 0.169842
C 2.752521 1.535290 -0.004559
C 4.040350 1.005333 -0.130045
C 4.234916 -0.374927 -0.112133
C 3.135061 -1.238289 0.017783
C 1.836166 -0.743673 0.167175
C 0.725913 -1.716205 0.263254
C 0.808740 -2.922963 0.852757
C -0.283248 -3.960561 0.921356
C -1.684123 -3.514826 0.486474
C -2.369021 -2.560020 1.476636
C -3.480269 -1.707459 0.848516
C -4.231258 -0.876314 1.889707
C -1.107566 3.205587 0.439572
C -0.950235 4.711853 0.254629
C -0.018986 5.332687 1.305345
C -0.541508 5.083129 -1.177537
H 4.884608 1.684004 -0.254973
H 3.297388 -2.316561 -0.036235
H 1.729662 3.128849 0.004811
H 5.503593 -1.801499 -0.230573
H -0.224231 -1.404516 -0.166621
H 1.747265 -3.209701 1.343466
H -0.321090 -4.357754 1.953446
H 0.038496 -4.824700 0.307950
H -1.840214 2.786855 -0.267253
H -1.434451 2.954349 1.459490
H -1.965666 5.111571 0.429068
H -0.358456 5.102169 2.327891
H 0.011515 6.428163 1.198502
H 1.015061 4.963996 1.206145
H 0.467324 4.712048 -1.421188
H -1.241218 4.660496 -1.916381
H -0.532132 6.176478 -1.307150
H -2.314759 -4.409786 0.349478
H -1.628136 -3.032934 -0.502839
H -1.625832 -1.869323 1.911392
H -2.784815 -3.135637 2.321969
H -4.202262 -2.380285 0.349925

H -2.285554 -0.301205 0.191795
H -5.002283 -0.258692 1.403430
H -4.721513 -1.516908 2.640437
H -3.537177 -0.202158 2.420246
O 0.167682 2.559773 0.197451
O -0.710839 0.597316 0.797747
O -2.969617 -0.878658 -0.192513
O 2.673594 2.875455 -0.049141
O 5.495504 -0.832938 -0.248535

13R-5-c179, $\Delta G = 1.9723$ kcal/mol,
population = 0.70 %

C 0.625897 1.238234 0.838451
C 1.968649 0.634608 0.717285
C 3.163915 1.412279 0.851118
C 4.420150 0.795480 0.857333
C 4.524991 -0.587384 0.715766
C 3.367925 -1.367573 0.546918
C 2.099447 -0.783814 0.549321
C 0.929239 -1.659884 0.323805
C 0.758046 -2.876800 0.867753
C -0.456254 -3.736181 0.652660
C -1.388359 -3.790272 1.887839
C -1.925079 -2.429667 2.354315
C -2.880021 -1.703865 1.388126
C -4.276786 -2.312476 1.361836
C -0.627134 3.297817 0.888782
C -0.390706 4.785838 0.650355
C 0.190986 5.061347 -0.741514
C -1.702732 5.547346 0.879039
H 5.313520 1.410686 0.969411
H 3.464651 -2.441321 0.373775
H 2.248642 3.068771 0.967167
H 5.705164 -2.089708 0.618170
H 0.141050 -1.263535 -0.321233
H 1.504297 -3.256478 1.578194
H -0.139437 -4.768385 0.420085
H -1.013144 -3.374919 -0.227378
H -1.326944 2.876976 0.149929
H -1.038071 3.109832 1.892760
H 0.337783 5.127323 1.408702
H 0.379040 6.137784 -0.878593
H -0.509058 4.737954 -1.530773
H 1.142497 4.530426 -0.896327

H -2.100414 5.378060 1.892535
H -1.547775 6.630055 0.754077
H -2.474905 5.234698 0.155821
H -0.835850 -4.252992 2.724378
H -2.223051 -4.477386 1.665019
H -1.072617 -1.755148 2.537182
H -2.439671 -2.547738 3.324586
H -2.459626 -1.761708 0.364417
H -2.164634 0.091972 1.588700
H -4.249468 -3.374387 1.072887
H -4.741303 -2.237210 2.359265
H -4.917814 -1.776595 0.644478
O 0.633061 2.596432 0.771461
O -0.422002 0.636553 0.991080
O -3.019912 -0.337300 1.759407
O 3.172139 2.746808 0.996703
O 5.759816 -1.128327 0.725071

13R-5-c22, $\Delta G = 1.9974$ kcal/mol,
population = 0.67 %

C 1.520059 2.686696 0.768156
C 2.537080 1.648417 0.516968
C 3.886082 1.989174 0.875155
C 4.929934 1.065538 0.722752
C 4.665353 -0.202690 0.212902
C 3.355524 -0.555219 -0.156655
C 2.288293 0.333370 -0.009279
C 0.949913 -0.140378 -0.430610
C 0.506567 -1.402891 -0.283957
C -0.831019 -1.905497 -0.747392
C -1.616223 -2.676929 0.334283
C -1.889810 -1.943903 1.656293
C -2.824634 -0.729769 1.597696
C -3.180062 -0.213237 2.992441
C -0.798107 3.348529 0.710535
C -1.268485 4.003424 -0.590957
C -0.217103 4.927953 -1.217151
C -1.795586 2.976677 -1.602490
H 5.939199 1.371113 1.006991
H 3.194504 -1.539440 -0.596019
H 3.368144 3.708967 1.424202
H 6.486937 -0.783573 0.309829
H 0.287414 0.593128 -0.890675
H 1.144596 -2.137653 0.224877

H -0.668379 -2.601960 -1.592350
H -1.428867 -1.068305 -1.134894
H -1.617249 2.769361 1.156904
H -0.438960 4.097183 1.427396
H -2.121718 4.630997 -0.271013
H 0.134202 5.688199 -0.502615
H -0.635105 5.448819 -2.093365
H 0.661870 4.359066 -1.562713
H -2.296179 3.481001 -2.444108
H -0.971317 2.376245 -2.021599
H -2.510374 2.281171 -1.136474
H -1.059840 -3.600724 0.573248
H -2.574704 -3.009038 -0.101843
H -0.935354 -1.626170 2.118060
H -2.330982 -2.667927 2.362393
H -3.757322 -1.029202 1.086474
H -1.363937 0.462280 1.032716
H -2.270003 0.080327 3.542989
H -3.834384 0.668810 2.917079
H -3.702232 -0.982100 3.584010
O 0.253508 2.369709 0.490463
O 1.805673 3.801246 1.222320
O -2.293327 0.326605 0.793174
O 4.215558 3.183788 1.370941
O 5.625982 -1.132322 0.034569

13R-5-c157, $\Delta G = 1.9999$ kcal/mol,
population = 0.67 %

C 0.220003 1.646767 0.626516
C 1.563487 1.045606 0.505168
C 2.754603 1.826397 0.635879
C 4.014452 1.211967 0.642390
C 4.122798 -0.170693 0.505071
C 2.967361 -0.954928 0.340017
C 1.699349 -0.375044 0.340946
C 0.529991 -1.253238 0.118189
C 0.361213 -2.469904 0.663279
C -0.852567 -3.330814 0.450554
C -1.784133 -3.383801 1.686209
C -2.322100 -2.022945 2.150584
C -3.278941 -1.300024 1.184142
C -4.674645 -1.911124 1.159281
C -1.036000 3.704903 0.677996
C -0.802013 5.193414 0.439785

C -0.222346 5.470439 -0.952632
 C -2.114951 5.952661 0.670390
 H 4.897620 1.844587 0.753249
 H 3.083246 -2.026176 0.174100
 H 1.838122 3.481601 0.750094
 H 6.034531 -0.176177 0.608947
 H -0.259911 -0.858770 -0.525946
 H 1.109522 -2.848205 1.372228
 H -0.535055 -4.363156 0.219455
 H -1.410302 -2.971674 -0.429859
 H -1.736264 3.283367 -0.060045
 H -1.445400 3.516154 1.682461
 H -0.073085 5.535585 1.197408
 H -0.036522 6.547296 -1.089561
 H -0.922547 5.145964 -1.741287
 H 0.730032 4.941461 -1.108715
 H -2.511075 5.782182 1.684291
 H -1.961999 7.035682 0.545799
 H -2.887453 5.638958 -0.052004
 H -1.230644 -3.844323 2.523317
 H -2.618199 -4.072288 1.465151
 H -1.470050 -1.347259 2.330861
 H -2.835510 -2.139506 3.121670
 H -2.858988 -1.358188 0.160273
 H -2.566928 0.497442 1.381895
 H -4.645599 -2.973361 0.871765
 H -5.138886 -1.835254 2.156798
 H -5.316961 -1.377397 0.441481
 O 0.224947 3.005353 0.558916
 O -0.827026 1.043887 0.780254
 O -3.421179 0.066707 1.554063
 O 2.762401 3.160843 0.778409
 O 5.309617 -0.809939 0.500555

13R-5-c76, $\Delta G = 2.0112$ kcal/mol,
population = 0.65 %

C 0.443807 1.628274 0.281854
 C 1.796223 1.086993 0.037211
 C 2.928821 1.947735 -0.128987
 C 4.220682 1.420114 -0.248262
 C 4.418232 0.040645 -0.230713
 C 3.319370 -0.825604 -0.108933
 C 2.020397 -0.334984 0.032650
 C 0.910685 -1.309468 0.118741

C 0.992943 -2.519028 0.702370
 C -0.097194 -3.559142 0.761038
 C -1.497324 -3.114023 0.323099
 C -2.187521 -2.164577 1.314767
 C -3.297928 -1.311165 0.686335
 C -4.053710 -0.485432 1.728372
 C -0.933239 3.610379 0.302823
 C -0.780484 5.116775 0.115238
 C 0.146305 5.743108 1.166601
 C -0.370031 5.486505 -1.316809
 H 5.054660 2.115006 -0.366372
 H 3.500951 -1.898834 -0.164145
 H 1.905007 3.539853 -0.121049
 H 6.315428 0.166374 -0.447745
 H -0.037942 -0.997188 -0.314113
 H 1.930324 -2.806456 1.194738
 H -0.138277 -3.962003 1.790842
 H 0.228501 -4.419420 0.144275
 H -1.663317 3.188014 -0.404445
 H -1.261220 3.360119 1.322671
 H -1.797620 5.513427 0.286725
 H 1.181941 5.378067 1.070389
 H -0.194479 5.513463 2.188908
 H 0.173086 6.838474 1.057573
 H 0.640539 5.118272 -1.557523
 H -1.066750 5.059966 -2.056234
 H -0.364062 6.579615 -1.448662
 H -2.125890 -4.009510 0.180021
 H -1.438565 -2.627857 -0.663960
 H -1.447007 -1.474665 1.755327
 H -2.605525 -2.744499 2.156073
 H -4.017273 -1.983083 0.182699
 H -2.102933 0.099368 0.038968
 H -3.362537 0.187748 2.263931
 H -4.824123 0.132873 1.241981
 H -4.545396 -1.129839 2.474888
 O 0.344469 2.968086 0.064445
 O -0.534595 1.001923 0.651868
 O -2.785200 -0.477359 -0.349645
 O 2.849708 3.287481 -0.171966
 O 5.638069 -0.519901 -0.353012

13R-5-c53, $\Delta G = 2.0664$ kcal/mol,
population = 0.60 %

C 1.406634 2.522489 0.727280
 C 2.421674 1.482239 0.473403
 C 3.773675 1.817608 0.833346
 C 4.813429 0.893264 0.677599
 C 4.545895 -0.372048 0.161524
 C 3.235555 -0.719301 -0.209634
 C 2.168594 0.172121 -0.057274
 C 0.829489 -0.298800 -0.478684
 C 0.383559 -1.560413 -0.331529
 C -0.955378 -2.060216 -0.793944
 C -1.740953 -2.830642 0.288127
 C -2.012406 -2.097607 1.610561
 C -2.945194 -0.881863 1.552781
 C -3.299564 -0.365401 2.947785
 C -0.909387 3.191530 0.664520
 C -1.376106 3.847205 -0.637822
 C -0.319481 4.765466 -1.264388
 C -1.908044 2.822168 -1.648517
 H 5.827673 1.179045 0.958141
 H 3.055837 -1.698194 -0.658131
 H 3.258614 3.537008 1.388725
 H 5.266866 -2.068772 -0.346775
 H 0.168366 0.436257 -0.938151
 H 1.019646 -2.296498 0.177980
 H -0.794685 -2.756565 -1.639381
 H -1.551877 -1.221637 -1.180463
 H -1.730722 2.615009 1.110309
 H -0.548859 3.939486 1.381411
 H -2.226219 4.479527 -0.318918
 H 0.035424 5.524614 -0.550454
 H -0.734044 5.287590 -2.141492
 H 0.556614 4.191389 -1.608733
 H -2.626582 2.130815 -1.182071
 H -2.405781 3.328232 -2.490803
 H -1.086765 2.217075 -2.066839
 H -1.185972 -3.755478 0.526353
 H -2.700263 -3.160968 -0.147522
 H -1.057163 -1.781676 2.071982
 H -2.454409 -2.821200 2.316597
 H -3.878423 -1.179441 1.041477
 H -1.483342 0.309704 0.990270
 H -2.388966 -0.073543 3.498377
 H -3.952489 0.517727 2.872904
 H -3.822885 -1.133704 3.539084

O 0.139834 2.209828 0.445569
 O 1.694445 3.634247 1.185913
 O -2.412157 0.173889 0.748607
 O 4.104272 3.010464 1.333843
 O 5.578539 -1.227932 0.019903

13R-5-c134, $\Delta G = 2.1304$ kcal/mol,
 population = 0.53 %

C 1.622709 1.884164 -0.089659
 C 2.703843 0.902349 0.111628
 C 4.011155 1.291196 -0.336466
 C 5.083647 0.392213 -0.289805
 C 4.889208 -0.895903 0.204051
 C 3.622987 -1.290361 0.673905
 C 2.530439 -0.419473 0.637879
 C 1.250378 -0.909123 1.199066
 C 0.737144 -2.133123 0.987578
 C -0.559421 -2.625305 1.568990
 C -1.712217 -2.708962 0.543630
 C -2.100737 -1.342527 -0.025914
 C -3.244034 -1.335275 -1.047723
 C -4.607145 -1.655396 -0.449954
 C -0.750809 2.308581 -0.074094
 C -1.405278 2.776405 1.226798
 C -0.487760 3.676191 2.061170
 C -2.732774 3.469130 0.890875
 H 6.065652 0.712120 -0.639862
 H 3.501933 -2.282899 1.112858
 H 3.398465 3.006453 -0.800101
 H 5.693674 -2.586299 0.596387
 H 0.691123 -0.210650 1.825959
 H 1.254195 -2.819155 0.303697
 H -0.865725 -1.967796 2.400705
 H -0.403461 -3.630570 1.999129
 H -0.434957 3.159828 -0.692448
 H -1.454923 1.683860 -0.641636
 H -1.633482 1.870007 1.816892
 H -0.221533 4.592577 1.508330
 H 0.447620 3.164167 2.336063
 H -0.986051 3.978119 2.996124
 H -3.404719 2.801365 0.328009
 H -3.254674 3.778241 1.809806
 H -2.566368 4.373638 0.281123
 H -2.578219 -3.178884 1.039540

H -1.423773 -3.387359 -0.280126
H -1.214645 -0.899712 -0.510883
H -2.369516 -0.657077 0.798831
H -3.020149 -2.086554 -1.832468
H -2.567231 0.105820 -2.190323
H -4.621820 -2.660142 -0.002012
H -4.863928 -0.922505 0.332776
H -5.384815 -1.614234 -1.228013
O 0.389558 1.456091 0.177677
O 1.828349 3.029128 -0.508711
O -3.357571 -0.041930 -1.652976
O 4.261896 2.508564 -0.825908
O 5.951649 -1.726557 0.232147

13R-5-c96, $\Delta G = 2.1448$ kcal/mol,
population = 0.52 %

C 1.683763 1.669654 0.371366
C 2.767002 0.690299 0.570034
C 4.070329 1.083443 0.120374
C 5.147418 0.186475 0.165865
C 4.957651 -1.102065 0.659657
C 3.692566 -1.501316 1.129669
C 2.599233 -0.634733 1.095915
C 1.320518 -1.127359 1.658048
C 0.809553 -2.352162 1.446262
C -0.485556 -2.847327 2.028565
C -1.640006 -2.930097 1.004940
C -2.031857 -1.562788 0.439804
C -3.176563 -1.554782 -0.580402
C -4.538364 -1.878529 0.018384
C -0.690186 2.091136 0.395774
C -1.340784 2.556994 1.699303
C -0.421246 3.456715 2.531515
C -2.670035 3.248858 1.368656
H 6.122757 0.524977 -0.190278
H 3.590943 -2.496893 1.561980
H 3.453375 2.796328 -0.343493
H 6.781174 -1.624422 0.402244
H 0.760400 -0.430643 2.286192
H 1.327983 -3.036701 0.761992
H -0.791515 -2.192054 2.862204
H -0.327835 -3.853344 2.456293
H -0.377617 2.943333 -0.222935
H -1.395365 1.465908 -0.169894

H -1.566167 1.649789 2.289243
H -0.916563 3.757162 3.468527
H -0.157747 4.373956 1.978775
H 0.515526 2.945207 2.802603
H -3.343246 2.581176 0.807196
H -3.189177 3.556307 2.289707
H -2.506564 4.154308 0.759497
H -2.504455 -3.402841 1.500923
H -1.351809 -3.605697 0.178794
H -1.147222 -1.116957 -0.045033
H -2.300770 -0.880173 1.266870
H -2.952574 -2.303729 -1.367342
H -2.503673 -0.109909 -1.720497
H -5.317141 -1.836864 -0.758545
H -4.550764 -2.884310 0.464056
H -4.795329 -1.147867 0.803144
O 0.452160 1.240115 0.643256
O 1.886131 2.814921 -0.049412
O -3.293027 -0.260103 -1.182382
O 4.318650 2.300380 -0.370044
O 5.954849 -2.007384 0.732825

13R-5-c116, $\Delta G = 2.2044$ kcal/mol,
population = 0.47 %

C 0.711564 1.554320 -0.025703
C 1.989734 0.901582 0.315041
C 3.220880 1.631001 0.325941
C 4.441858 0.968356 0.508582
C 4.467220 -0.410670 0.710914
C 3.266913 -1.140177 0.751574
C 2.035039 -0.516330 0.551089
C 0.805006 -1.330899 0.661636
C 0.698525 -2.622205 0.300293
C -0.515158 -3.501644 0.463789
C -1.812211 -2.818362 0.914366
C -2.473384 -1.961066 -0.179995
C -3.358161 -0.811404 0.333597
C -4.505467 -1.261261 1.230056
C -0.421725 3.681417 -0.284602
C -1.396265 3.854864 0.882490
C -0.720236 4.486696 2.103975
C -2.599605 4.679159 0.406316
H 5.359550 1.560334 0.499573
H 3.316929 -2.203949 0.983860

H 2.395627 3.320600 0.092029
 H 6.372562 -0.493658 0.873263
 H -0.071390 -0.823857 1.063738
 H 1.563795 -3.114948 -0.160701
 H -0.249712 -4.300829 1.182921
 H -0.687283 -4.038991 -0.488368
 H -0.020576 4.653347 -0.607935
 H -0.908976 3.189413 -1.137076
 H -1.763687 2.851756 1.159557
 H 0.143758 3.892861 2.439137
 H -1.426771 4.561254 2.945631
 H -0.362274 5.505206 1.874312
 H -3.105898 4.204365 -0.449689
 H -3.339046 4.787936 1.214931
 H -2.291639 5.692713 0.097368
 H -1.607403 -2.194166 1.799502
 H -2.516598 -3.595870 1.252902
 H -3.074047 -2.603336 -0.848113
 H -1.693701 -1.509775 -0.816647
 H -3.798273 -0.317792 -0.557644
 H -1.874778 0.461167 0.491218
 H -5.158172 -1.975425 0.704246
 H -4.127068 -1.744155 2.144844
 H -5.112857 -0.394203 1.533417
 O 0.752113 2.911633 0.077933
 O -0.310311 0.994132 -0.384615
 O -2.589446 0.137896 1.068697
 O 3.303650 2.958079 0.148732
 O 5.613181 -1.094717 0.902567

13R-5-c182, $\Delta G = 2.2101$ kcal/mol,
population = 0.47 %

C 0.453197 1.477592 0.052514
 C 1.815881 0.910771 0.115604
 C 2.978690 1.739159 0.232601
 C 4.240506 1.174297 0.448015
 C 4.385345 -0.209525 0.534385
 C 3.266133 -1.045460 0.377039
 C 1.992031 -0.511915 0.172564
 C 0.868463 -1.452797 -0.027641
 C 0.667940 -2.578038 0.679157
 C -0.495021 -3.508596 0.478357
 C -1.540807 -3.429912 1.616326
 C -2.161871 -2.041159 1.827071

C -3.026993 -1.498080 0.674247
 C -4.404064 -2.146956 0.606000
 C -0.844880 3.505846 -0.131207
 C -0.604726 5.009932 -0.044134
 C -1.939967 5.746249 -0.212456
 C 0.097198 5.404646 1.261636
 H 5.107233 1.829485 0.540990
 H 3.400783 -2.129145 0.378892
 H 2.032227 3.357318 -0.045150
 H 5.597062 -1.667647 0.784467
 H 0.144957 -1.188933 -0.803101
 H 1.344692 -2.816293 1.510454
 H -0.127294 -4.548860 0.425083
 H -0.973902 -3.296879 -0.491538
 H -1.379945 3.233920 -1.054338
 H -1.434131 3.142637 0.724982
 H 0.047653 5.286737 -0.892554
 H -1.786720 6.835977 -0.180768
 H -2.642525 5.484361 0.596759
 H -2.422566 5.501134 -1.172049
 H 1.054346 4.876522 1.389203
 H 0.305367 6.485742 1.281078
 H -0.535374 5.167045 2.133889
 H -1.059089 -3.743271 2.559149
 H -2.327596 -4.179079 1.420220
 H -1.351998 -1.312747 1.996392
 H -2.772531 -2.043854 2.747505
 H -2.505359 -1.694918 -0.283445
 H -2.367794 0.330445 0.655781
 H -4.977693 -1.746970 -0.244718
 H -4.330826 -3.239119 0.489535
 H -4.968186 -1.934710 1.529586
 O 0.432104 2.824588 -0.134324
 O -0.588921 0.857132 0.165354
 O -3.226164 -0.096350 0.817181
 O 2.949080 3.079891 0.155580
 O 5.623148 -0.700028 0.744054

13R-5-c19, $\Delta G = 2.2220$ kcal/mol,
population = 0.46 %

C 1.113592 1.118294 0.538066
 C 2.402919 0.485528 0.196306
 C 3.619430 1.239133 0.164658
 C 4.851810 0.599298 -0.022732

C 4.902577 -0.780830 -0.213114
 C 3.717106 -1.534035 -0.234061
 C 2.474564 -0.933911 -0.024759
 C 1.260679 -1.775200 -0.106502
 C 1.193930 -3.074008 0.237934
 C -0.010607 -3.971879 0.108253
 C -1.345652 -3.292063 -0.217723
 C -1.941620 -2.495562 0.953718
 C -2.937371 -1.408580 0.524761
 C -3.633344 -0.755472 1.719282
 C -0.040214 3.259417 0.742702
 C -0.666596 3.893467 -0.500028
 C -1.138590 2.847229 -1.516074
 C -1.810050 4.818799 -0.062918
 H 5.757442 1.209740 -0.029076
 H 3.787488 -2.598929 -0.455508
 H 2.761943 2.913923 0.375938
 H 6.807585 -0.828803 -0.394576
 H 0.359162 -1.281412 -0.466206
 H 2.085185 -3.557612 0.656707
 H -0.109139 -4.559033 1.040890
 H 0.219337 -4.728261 -0.667346
 H -0.754550 2.608922 1.264227
 H 0.317729 4.032571 1.438184
 H 0.113023 4.514338 -0.977994
 H -0.302303 2.227128 -1.875174
 H -1.585095 3.337980 -2.395341
 H -1.895125 2.173379 -1.081507
 H -2.618516 4.248136 0.424692
 H -1.464369 5.588034 0.646486
 H -2.244468 5.334962 -0.932954
 H -2.068091 -4.062989 -0.535491
 H -1.219577 -2.624423 -1.085291
 H -1.136050 -2.001337 1.524542
 H -2.436806 -3.186193 1.658268
 H -3.707548 -1.868687 -0.121217
 H -1.559071 -0.049448 0.204241
 H -2.893198 -0.303718 2.401866
 H -4.314762 0.039637 1.378968
 H -4.218691 -1.490882 2.294461
 O 1.129224 2.474801 0.400208
 O 0.109834 0.541196 0.917504
 O -2.303725 -0.429899 -0.296433
 O 3.677532 2.569480 0.326981

O 6.059670 -1.444369 -0.410939

13R-5-c37, $\Delta G = 2.3067$ kcal/mol,
population = 0.40 %

C 0.814459 1.017166 0.677338
 C 2.100493 0.383095 0.323941
 C 3.320218 1.134931 0.284783
 C 4.547972 0.494250 0.087449
 C 4.595251 -0.885624 -0.107333
 C 3.408385 -1.636173 -0.123566
 C 2.166709 -1.033808 0.098768
 C 0.951666 -1.873852 0.027005
 C 0.885998 -3.172588 0.372206
 C -0.321664 -4.067974 0.254990
 C -1.660017 -3.384402 -0.048797
 C -2.236487 -2.590831 1.134228
 C -3.239966 -1.503576 0.724456
 C -3.912451 -0.850390 1.932341
 C -0.334665 3.159507 0.893470
 C -0.974745 3.791697 -0.343237
 C -1.459842 2.743929 -1.351527
 C -2.112024 4.719209 0.105195
 H 5.462331 1.088257 0.074548
 H 3.457633 -2.702709 -0.351456
 H 2.464783 2.810226 0.505695
 H 5.710499 -2.406438 -0.426872
 H 0.047504 -1.378466 -0.323653
 H 1.779961 -3.657965 0.783225
 H -0.407903 -4.659162 1.186217
 H -0.103996 -4.821093 -0.527320
 H -1.043620 2.510995 1.424747
 H 0.032283 3.933744 1.583004
 H -0.199965 4.410630 -0.831432
 H -0.628504 2.122218 -1.719243
 H -1.916206 3.233442 -2.226402
 H -2.211956 2.071890 -0.906609
 H -2.555224 5.234912 -0.760683
 H -2.915891 4.150229 0.602274
 H -1.757619 5.488903 0.809791
 H -2.388574 -4.152898 -0.358393
 H -1.545849 -2.713908 -0.915813
 H -1.421574 -2.097310 1.692268
 H -2.719323 -3.283230 1.845576
 H -4.022583 -1.963436 0.093424

H -1.867579 -0.145099 0.377493
H -4.486718 -1.585697 2.518738
H -3.158970 -0.399020 2.600431
H -4.600027 -0.054995 1.605376
O 0.830217 2.373217 0.539325
O -0.186261 0.440690 1.065627
O -2.622043 -0.525019 -0.108686
O 3.379468 2.465224 0.450421
O 5.804073 -1.450147 -0.303386

13R-5-c31, $\Delta G = 2.3099$ kcal/mol,
population = 0.39 %

C 0.721727 1.152414 0.605320
C 2.000644 0.543905 0.187884
C 3.203412 1.315762 0.104775
C 4.431537 0.698713 -0.167132
C 4.490809 -0.676181 -0.389616
C 3.316324 -1.446477 -0.359867
C 2.079376 -0.869432 -0.069062
C 0.874555 -1.727120 -0.102776
C 0.841809 -3.030958 0.227245
C -0.356047 -3.943526 0.144648
C -1.715614 -3.277828 -0.098605
C -2.258618 -2.507185 1.115240
C -3.290066 -1.427799 0.757340
C -3.923655 -0.796464 1.997346
C -0.454694 3.274365 0.896944
C -1.105813 3.924545 -0.324931
C -0.165191 4.926250 -1.007471
C -1.653432 2.889779 -1.316432
H 5.326257 1.323379 -0.210913
H 3.388279 -2.505494 -0.607566
H 2.338870 2.969377 0.425724
H 6.383603 -0.692336 -0.676580
H -0.049459 -1.241122 -0.412007
H 1.758966 -3.507475 0.595284
H -0.396977 -4.548249 1.070346
H -0.157385 -4.683037 -0.655499
H -1.148044 2.601042 1.415125
H -0.094213 4.037120 1.602644
H -1.962156 4.487289 0.091096
H 0.172756 5.705410 -0.304997
H -0.668837 5.426136 -1.849653
H 0.729038 4.419091 -1.405461

H -2.204116 3.389096 -2.129131
H -0.834699 2.315348 -1.781214
H -2.334405 2.172233 -0.833097
H -2.443355 -4.054360 -0.389640
H -1.645184 -2.595622 -0.961040
H -1.429852 -2.011000 1.650299
H -2.706669 -3.214936 1.834201
H -4.091182 -1.889958 0.151501
H -1.948273 -0.049242 0.375012
H -4.465073 -1.545177 2.597907
H -3.151162 -0.340927 2.640512
H -4.633804 -0.007350 1.705197
O 0.721897 2.512735 0.518216
O -0.261728 0.553596 1.003876
O -2.716685 -0.431779 -0.086776
O 3.253248 2.642991 0.294580
O 5.644014 -1.318127 -0.665544

13R-5-c147, $\Delta G = 2.3268$ kcal/mol,
population = 0.38 %

C 0.362540 1.488934 0.034302
C 1.638854 0.834455 0.380219
C 2.873942 1.561121 0.392789
C 4.090586 0.897608 0.583657
C 4.111830 -0.480629 0.794254
C 2.909841 -1.206818 0.832567
C 1.678509 -0.580438 0.621998
C 0.447336 -1.393368 0.728998
C 0.340279 -2.684651 0.367369
C -0.875073 -3.562340 0.527474
C -2.171875 -2.877020 0.975524
C -2.829816 -2.018884 -0.120114
C -3.713154 -0.867529 0.392168
C -4.860906 -1.315241 1.289117
C -0.766476 3.617395 -0.230149
C -1.741112 3.796580 0.936035
C -1.064123 4.430708 2.155797
C -2.942477 4.622014 0.456852
H 5.017075 1.472647 0.578856
H 2.938723 -2.271468 1.072553
H 2.050949 3.251188 0.149250
H 5.198613 -2.018609 1.130332
H -0.429637 -0.884818 1.128005
H 1.205742 -3.178706 -0.092021

H -0.612345 -4.362267 1.246755
 H -1.045758 -4.098827 -0.425401
 H -0.362858 4.587406 -0.556086
 H -1.254410 3.124003 -1.081429
 H -2.110830 2.795133 1.216122
 H -0.201676 3.835891 2.493182
 H -1.770842 4.509617 2.996897
 H -0.703646 5.447610 1.923012
 H -3.449842 4.145477 -0.397550
 H -3.681719 4.735297 1.265031
 H -2.632132 5.633774 0.144412
 H -1.967614 -2.253054 1.860957
 H -2.878010 -3.653387 1.313003
 H -3.430743 -2.660289 -0.788799
 H -2.048422 -1.569325 -0.755895
 H -4.152560 -0.374208 -0.499555
 H -2.228185 0.403367 0.548563
 H -5.514518 -2.029072 0.763992
 H -4.482815 -1.797875 2.204147
 H -5.467246 -0.447259 1.591903
 O 0.405350 2.845960 0.135384
 O -0.659380 0.929513 -0.325651
 O -2.943208 0.081540 1.126369
 O 2.958042 2.887679 0.209108
 O 5.310741 -1.067406 0.984822

13R-5-c184, $\Delta G = 2.3469$ kcal/mol,
population = 0.37 %

C 0.313103 1.378978 0.220486
 C 1.673285 0.812518 0.118768
 C 2.842093 1.635142 0.176772
 C 4.120027 1.061593 0.215436
 C 4.269150 -0.323695 0.182200
 C 3.136822 -1.151997 0.087647
 C 1.851683 -0.611913 0.056453
 C 0.710428 -1.541616 -0.091592
 C 0.580964 -2.714385 0.551620
 C -0.599668 -3.633619 0.406749
 C -1.545327 -3.608734 1.632296
 C -2.144688 -2.233550 1.959093
 C -3.097398 -1.635051 0.907568
 C -4.467651 -2.301558 0.895056
 C -1.003273 3.401429 0.258577
 C -0.788412 4.911913 0.250960

C 0.003820 5.391196 1.475581
 C -0.179280 5.408775 -1.067306
 H 4.984873 1.726446 0.265738
 H 3.283928 -2.228700 0.000847
 H 1.874167 3.261308 0.152494
 H 6.180100 -0.261951 0.260809
 H -0.088809 -1.227838 -0.767669
 H 1.338857 -3.006406 1.290516
 H -0.243034 -4.670257 0.272866
 H -1.159033 -3.375305 -0.507217
 H -1.641504 3.079524 -0.578394
 H -1.472251 3.066669 1.195844
 H -1.808974 5.328789 0.327954
 H 0.074280 6.489942 1.487364
 H 1.032351 4.994944 1.478327
 H -0.478491 5.072757 2.413648
 H -0.128977 6.508649 -1.081197
 H 0.845775 5.029564 -1.210206
 H -0.779380 5.086468 -1.933384
 H -0.986460 -3.964578 2.515607
 H -2.347355 -4.349480 1.468811
 H -1.322931 -1.512645 2.100981
 H -2.682407 -2.283774 2.922669
 H -2.643858 -1.762682 -0.095496
 H -2.459986 0.199301 0.965937
 H -4.966401 -2.161910 1.868785
 H -5.106511 -1.855553 0.116752
 H -4.389581 -3.381985 0.699110
 O 0.277756 2.735758 0.127129
 O -0.717178 0.750176 0.384475
 O -3.302116 -0.248533 1.153796
 O 2.809407 2.977052 0.208688
 O 5.475091 -0.924945 0.212459

13R-5-c52, $\Delta G = 2.3619$ kcal/mol,
population = 0.36 %

C 1.327792 2.220356 1.054507
 C 2.378245 1.201761 0.876040
 C 3.685878 1.541645 1.356069
 C 4.732211 0.608627 1.314626
 C 4.504773 -0.668124 0.806537
 C 3.232245 -1.019846 0.318483
 C 2.171219 -0.114164 0.342712
 C 0.878084 -0.565879 -0.221037

C 0.301937 -1.750143 0.044460
 C -1.032214 -2.175199 -0.519102
 C -2.235615 -1.613184 0.266875
 C -2.334701 -2.077906 1.721438
 C -3.391216 -1.318434 2.534815
 C -3.603083 -1.915816 3.924500
 C -1.019841 2.754699 0.930517
 C -1.513186 3.433810 -0.350015
 C -0.477165 4.386787 -0.959083
 C -2.031868 2.426325 -1.383569
 H 5.712879 0.908409 1.690422
 H 3.097363 -2.010925 -0.115168
 H 3.115553 3.261645 1.850122
 H 6.303251 -1.257950 1.090653
 H 0.363915 0.128590 -0.890294
 H 0.786074 -2.424624 0.760984
 H -1.090468 -3.277084 -0.543137
 H -1.116042 -1.831227 -1.563720
 H -1.804477 2.106247 1.347157
 H -0.721018 3.497956 1.680677
 H -2.373336 4.041594 -0.011392
 H -0.911335 4.936348 -1.809324
 H 0.399110 3.835079 -1.338052
 H -0.118908 5.122559 -0.222949
 H -2.803508 1.767372 -0.954290
 H -2.474844 2.946692 -2.247513
 H -1.216318 1.789181 -1.762482
 H -3.165757 -1.884027 -0.263970
 H -2.176624 -0.513264 0.252247
 H -1.361275 -1.949609 2.230974
 H -2.558649 -3.158770 1.757616
 H -4.349028 -1.350133 1.985570
 H -2.245367 0.157400 3.111745
 H -2.658063 -1.921626 4.495149
 H -4.340637 -1.324170 4.488186
 H -3.964025 -2.954671 3.861988
 O 0.097756 1.862991 0.689852
 O 1.556035 3.337146 1.535289
 O -3.079092 0.074320 2.625061
 O 3.967095 2.741639 1.869760
 O 5.470079 -1.607816 0.741226

13R-5-c48, $\Delta G = 2.3902$ kcal/mol,
 population = 0.34 %

C 0.931716 1.490634 0.989880
 C 2.208881 0.879833 0.569183
 C 3.416149 1.648478 0.486227
 C 4.639497 1.029743 0.208267
 C 4.693450 -0.344232 -0.023026
 C 3.516914 -1.110599 0.007223
 C 2.281043 -0.530554 0.306703
 C 1.075078 -1.386352 0.274957
 C 1.041298 -2.689995 0.605980
 C -0.157453 -3.601474 0.525344
 C -1.516330 -2.934703 0.281394
 C -2.058653 -2.162552 1.494602
 C -3.086844 -1.080520 1.135332
 C -3.721439 -0.448430 2.374403
 C -0.240137 3.614407 1.284307
 C -0.888981 4.267643 0.062831
 C 0.054562 5.267796 -0.617940
 C -1.438765 3.235564 -0.930276
 H 5.544350 1.636514 0.161986
 H 3.567128 -2.171014 -0.247165
 H 2.554774 3.302791 0.815670
 H 5.807516 -1.841368 -0.443125
 H 0.151292 -0.899074 -0.032982
 H 1.957998 -3.167284 0.974330
 H -0.198600 -4.204641 1.452020
 H 0.040475 -4.342396 -0.273659
 H -0.935307 2.942051 1.801308
 H 0.121737 4.375472 1.991086
 H -1.744118 4.832022 0.479114
 H 0.393716 6.045474 0.085576
 H -0.447198 5.769668 -1.460060
 H 0.947946 4.758933 -1.015613
 H -0.621357 2.659638 -1.395549
 H -2.121843 2.519161 -0.448239
 H -1.987804 3.737386 -1.742538
 H -2.244722 -3.710813 -0.009012
 H -1.445115 -2.253434 -0.581706
 H -1.229252 -1.668493 2.030653
 H -2.509338 -2.869102 2.213068
 H -3.887768 -1.540426 0.527540
 H -1.741458 0.295609 0.756971
 H -2.949121 0.004666 3.019482
 H -4.428945 0.342678 2.081270
 H -4.266030 -1.196189 2.973254

O 0.935027 2.850676 0.905250
O -0.052665 0.892928 1.387844
O -2.509282 -0.085415 0.292993
O 3.468086 2.975071 0.682839
O 5.896466 -0.887545 -0.298320

13R-5-c92, $\Delta G = 2.4523$ kcal/mol,
population = 0.31 %

C 1.515515 1.840164 0.964667
C 2.563125 0.818104 0.785663
C 3.874518 1.153076 1.264708
C 4.915207 0.216939 1.225248
C 4.682234 -1.060093 0.719582
C 3.408834 -1.406405 0.231005
C 2.349706 -0.495286 0.254388
C 1.055635 -0.943448 -0.309577
C 0.475458 -2.125628 -0.043157
C -0.859608 -2.546833 -0.607112
C -2.061521 -1.984132 0.180646
C -2.161205 -2.452002 1.634167
C -3.216604 -1.692669 2.449118
C -3.429497 -2.292795 3.837457
C -0.831502 2.378680 0.848519
C -1.327236 3.060152 -0.429820
C -0.291564 4.012337 -1.040706
C -1.850536 2.054805 -1.463121
H 5.901463 0.497847 1.596199
H 3.254184 -2.394803 -0.206924
H 3.309891 2.876786 1.755217
H 5.427582 -2.778659 0.334560
H 0.544293 -0.247861 -0.979783
H 0.956256 -2.800784 0.675033
H -0.919976 -3.648554 -0.633403
H -0.942986 -2.200355 -1.650907
H -1.616279 1.731382 1.266688
H -0.529078 3.120537 1.598631
H -2.185453 3.668846 -0.087943
H 0.582734 3.459849 -1.423071
H 0.070042 4.746539 -0.304659
H -0.727510 4.563693 -1.888871
H -2.622040 1.396598 -1.032461
H -2.295108 2.577022 -2.325120
H -1.037122 1.416816 -1.845203
H -2.992292 -2.251922 -0.350599

H -2.000326 -0.884310 0.168511
H -1.187638 -2.326282 2.144056
H -2.386847 -3.532594 1.667901
H -4.174387 -1.721778 1.899682
H -2.069569 -0.219651 3.030884
H -3.791906 -3.330994 3.772609
H -2.484562 -2.301200 4.408223
H -4.166281 -1.701352 4.402349
O 0.283636 1.484775 0.604188
O 1.747751 2.957023 1.442534
O -2.902394 -0.300618 2.542304
O 4.159046 2.354141 1.775339
O 5.713251 -1.929708 0.703525

13R-5-c142, $\Delta G = 2.6443$ kcal/mol,
population = 0.22 %

C 0.830380 1.784108 0.321928
C 1.921354 0.828081 0.585240
C 3.225186 1.209040 0.122137
C 4.319530 0.342288 0.256265
C 4.146649 -0.908973 0.842239
C 2.879759 -1.300521 1.312676
C 1.769430 -0.463073 1.195342
C 0.485076 -0.963944 1.737720
C 0.022486 -2.212940 1.556738
C -1.282787 -2.731219 2.092773
C -2.369341 -2.895404 1.006065
C -2.792990 -1.561259 0.388639
C -3.820481 -1.633490 -0.746478
C -5.211030 -2.055848 -0.292967
C -1.528594 2.259153 0.396001
C -2.031610 3.021942 1.624976
C -2.529876 2.086814 2.733799
C -1.012899 4.037554 2.157054
H 5.294205 0.674265 -0.107908
H 2.787280 -2.267941 1.806477
H 2.581967 2.859474 -0.501525
H 5.983593 -1.411252 0.653437
H -0.119755 -0.258987 2.311917
H 0.592493 -2.905189 0.923154
H -1.658163 -2.056040 2.880732
H -1.113829 -3.713754 2.567948
H -1.245620 2.952092 -0.406404
H -2.304057 1.572416 0.026693

H -2.903629 3.586323 1.244148
 H -2.977818 2.664082 3.558026
 H -1.703374 1.492330 3.156271
 H -3.293235 1.386219 2.359307
 H -0.126732 3.533056 2.576477
 H -0.667566 4.720238 1.365828
 H -1.457464 4.642763 2.963035
 H -3.238346 -3.402043 1.458574
 H -1.995861 -3.571161 0.214775
 H -1.895395 -1.055468 -0.005898
 H -3.194002 -0.897350 1.176118
 H -3.460549 -2.363652 -1.500424
 H -3.121144 -0.124675 -1.779997
 H -5.600739 -1.345382 0.454837
 H -5.904678 -2.070650 -1.147719
 H -5.197332 -3.060008 0.156452
 O -0.392872 1.407674 0.695166
 O 1.020501 2.874332 -0.231418
 O -3.963836 -0.349199 -1.361676
 O 3.460340 2.386745 -0.460949
 O 5.159951 -1.784851 1.000965

13R-5-c109, $\Delta G = 2.7887$ kcal/mol,
population = 0.18 %

C 1.138629 1.926770 1.123555
 C 2.431930 1.285542 0.817415
 C 3.669735 1.987051 0.957179
 C 4.887804 1.305053 0.854166
 C 4.905021 -0.064386 0.589548
 C 3.699680 -0.762382 0.392872
 C 2.469777 -0.111929 0.504970
 C 1.234925 -0.869015 0.208884
 C 0.975135 -2.135680 0.574072
 C -0.301208 -2.859724 0.240436
 C -1.299744 -2.942344 1.420884
 C -1.756527 -1.588246 1.983969
 C -2.548023 -0.675519 1.029030
 C -3.970737 -1.158512 0.777741
 C -0.006371 4.031689 1.450090
 C -1.056581 4.115391 0.339841
 C -2.252944 4.928760 0.851203
 C -0.479623 4.699905 -0.953553
 H 5.820313 1.856806 0.977516
 H 3.728114 -1.816022 0.107227

H 2.846025 3.677112 1.200619
 H 5.991473 -1.614311 0.312713
 H 0.470235 -0.329817 -0.358304
 H 1.695435 -2.671971 1.205735
 H -0.062973 -3.890188 -0.076413
 H -0.783833 -2.373409 -0.623037
 H -0.426001 3.571275 2.355739
 H 0.379021 5.030617 1.701190
 H -1.408668 3.088508 0.144354
 H -3.041806 4.979801 0.084692
 H -1.957961 5.963406 1.096247
 H -2.693333 4.478443 1.755430
 H 0.378323 4.113293 -1.315985
 H -1.241197 4.711602 -1.749173
 H -0.138143 5.738155 -0.799803
 H -0.832862 -3.518114 2.239222
 H -2.170109 -3.538530 1.095812
 H -0.867134 -1.025656 2.310965
 H -2.369772 -1.753719 2.887760
 H -2.021094 -0.638830 0.055026
 H -1.727432 0.982858 1.628545
 H -4.493823 -0.474482 0.091189
 H -3.982166 -2.165640 0.333706
 H -4.534841 -1.190582 1.724815
 O 1.175756 3.284508 1.063446
 O 0.114851 1.342016 1.428304
 O -2.636108 0.642697 1.561788
 O 3.750005 3.302319 1.212638
 O 6.105991 -0.670949 0.501271

13R-5-c115, $\Delta G = 2.8941$ kcal/mol,
population = 0.15 %

C 1.652515 2.514139 -0.262357
 C 2.726102 1.526837 -0.051910
 C 4.015704 1.862361 -0.578078
 C 5.073050 0.942421 -0.526975
 C 4.875036 -0.312149 0.045662
 C 3.623220 -0.653251 0.591875
 C 2.551303 0.238943 0.555422
 C 1.282397 -0.183241 1.191634
 C 0.702696 -1.383721 1.026772
 C -0.616348 -1.764046 1.654473
 C -1.841495 -1.264764 0.856733
 C -1.962013 -1.846656 -0.555245

C -2.962213 -1.127679 -1.477220
 C -4.385730 -1.067603 -0.938749
 C -0.713455 2.975698 -0.145030
 C -1.272335 3.523556 1.170202
 C -0.265994 4.400661 1.922439
 C -2.576191 4.278996 0.880656
 H 6.040135 1.235238 -0.941417
 H 3.516087 -1.621196 1.082043
 H 3.414024 3.560319 -1.111922
 H 6.671237 -0.894361 -0.265930
 H 0.784813 0.554904 1.826361
 H 1.166307 -2.106686 0.344926
 H -0.674942 -1.339281 2.670705
 H -0.672848 -2.860666 1.765800
 H -0.423708 3.789200 -0.824436
 H -1.457012 2.331007 -0.635869
 H -1.516306 2.652585 1.805650
 H -0.698959 4.762251 2.868729
 H 0.019794 5.281209 1.323082
 H 0.653483 3.848027 2.170539
 H -2.392358 5.157902 0.239430
 H -3.312816 3.637798 0.370217
 H -3.033486 4.638648 1.815480
 H -1.782226 -0.166306 0.784515
 H -2.752175 -1.493293 1.435810
 H -2.234676 -2.916150 -0.503672
 H -0.976980 -1.813302 -1.055118
 H -2.983085 -1.687669 -2.433761
 H -1.677282 0.197574 -2.135193
 H -4.434671 -0.481754 -0.007710
 H -5.049459 -0.588322 -1.674823
 H -4.768207 -2.079396 -0.733628
 O 0.428266 2.117373 0.079757
 O 1.855987 3.630997 -0.753022
 O -2.559469 0.220106 -1.738488
 O 4.266934 3.044327 -1.146858
 O 5.853593 -1.237161 0.124865

13R-5-c81, $\Delta G = 2.9123$ kcal/mol,
 population = 0.14 %

C 1.322741 2.234821 0.619838
 C 2.341697 1.201540 0.362018
 C 3.643363 1.681496 -0.001675
 C 4.650780 0.792892 -0.401375

C 4.402706 -0.578456 -0.405788
 C 3.156007 -1.073706 0.013808
 C 2.120483 -0.216356 0.392957
 C 0.862958 -0.818245 0.888528
 C 0.368687 -2.011357 0.508305
 C -0.864889 -2.654683 1.074914
 C -1.866162 -3.136748 0.004205
 C -2.384606 -2.074141 -0.977148
 C -3.224653 -0.916533 -0.412958
 C -4.481103 -1.356003 0.328197
 C -1.006776 2.790791 0.865687
 C -1.746413 3.198762 -0.410679
 C -2.946230 4.074931 -0.026253
 C -0.844897 3.892345 -1.437236
 H 5.623831 1.200321 -0.684320
 H 3.031577 -2.154581 0.077306
 H 3.154825 3.461350 0.354007
 H 6.153969 -1.038961 -1.027315
 H 0.312479 -0.246476 1.638482
 H 0.883089 -2.577982 -0.278866
 H -1.353948 -1.964943 1.778201
 H -0.554566 -3.542638 1.658656
 H -1.693341 2.264283 1.542157
 H -0.576059 3.662248 1.376374
 H -2.138283 2.269423 -0.859345
 H -3.618333 3.556668 0.676706
 H -3.534436 4.341158 -0.918233
 H -2.618356 5.014690 0.449934
 H -0.414860 4.821403 -1.028534
 H -0.012772 3.244589 -1.753456
 H -1.421046 4.153075 -2.339358
 H -2.713531 -3.625055 0.514272
 H -1.383226 -3.931480 -0.591840
 H -2.996389 -2.577128 -1.746301
 H -1.530602 -1.635043 -1.525240
 H -3.543541 -0.308146 -1.284491
 H -1.601403 0.071237 0.105776
 H -5.133675 -1.951909 -0.328421
 H -4.233089 -1.960128 1.214851
 H -5.046504 -0.474460 0.668138
 O 0.048494 1.832576 0.596634
 O 1.612479 3.421160 0.806088
 O -2.479769 -0.086759 0.481679
 O 3.954047 2.980939 0.005489

O 5.333247 -1.484644 -0.769977

13R-5-c107, $\Delta G = 2.9242$ kcal/mol,
population = 0.14 %

C 1.384347 2.515662 0.906122
C 2.445298 1.514981 0.686305
C 3.764548 1.876875 1.125994
C 4.829429 0.972922 1.028547
C 4.615917 -0.298293 0.501096
C 3.335219 -0.672515 0.055080
C 2.249832 0.204260 0.138764
C 0.948033 -0.280255 -0.374804
C 0.443124 -1.502140 -0.132995
C -0.882674 -1.994334 -0.642013
C -1.959635 -2.105151 0.459747
C -2.286762 -0.754416 1.101796
C -3.476741 -0.721282 2.066953
C -3.337757 -1.656408 3.266421
C -0.960566 3.053419 0.817895
C -1.453899 3.756992 -0.449886
C -0.405007 4.694064 -1.061478
C -2.008264 2.774113 -1.488690
H 5.820374 1.276257 1.367969
H 3.194457 -1.656087 -0.398087
H 3.174244 3.575515 1.669169
H 5.400325 -1.979821 0.037011
H 0.364079 0.417128 -0.978823
H 0.990306 -2.184778 0.530525
H -0.748827 -2.990397 -1.100665
H -1.247165 -1.322739 -1.438027
H -1.751822 2.410570 1.230300
H -0.652199 3.783028 1.577223
H -2.296197 4.379548 -0.093678
H -0.840526 5.266453 -1.895767
H 0.450814 4.127333 -1.464280
H -0.016076 5.408717 -0.320342
H -1.215013 2.115711 -1.878790
H -2.797796 2.136104 -1.060320
H -2.440141 3.315633 -2.345120
H -1.621953 -2.823524 1.227081
H -2.872269 -2.537922 0.012647
H -2.497402 -0.020773 0.304750
H -1.397521 -0.373523 1.635492
H -4.389444 -0.997954 1.509386

H -2.977521 0.876310 3.075433

H -4.196328 -1.532462 3.944284

H -3.294216 -2.712366 2.958021

H -2.416253 -1.432129 3.832284

O 0.148673 2.155691 0.559865

O 1.610281 3.626743 1.400722

O -3.711828 0.622801 2.496887

O 4.036695 3.074449 1.650819

O 5.671877 -1.133964 0.423186

13R-5-c102, $\Delta G = 3.1451$ kcal/mol,
population = 0.10 %

C 1.486279 2.777293 0.673754
C 2.401425 1.630424 0.811598
C 3.697294 1.784600 0.213329
C 4.612269 0.722421 0.191906
C 4.274080 -0.496184 0.775306
C 3.025868 -0.656855 1.401996
C 2.083427 0.373818 1.428952
C 0.817264 0.121818 2.152379
C 0.181032 -1.062932 2.185748
C -1.041992 -1.375243 3.000541
C -2.214655 -2.028547 2.238794
C -3.052748 -1.096408 1.353301
C -2.420737 -0.601656 0.048887
C -2.175532 -1.709165 -0.974165
C -0.680868 3.715134 0.834629
C -2.091204 3.339262 1.273287
C -2.174963 3.035492 2.773416
C -3.049100 4.473444 0.881228
H 5.584149 0.882506 -0.279753
H 2.823355 -1.601127 1.907108
H 3.334511 3.568742 -0.248372
H 5.944820 -1.329805 0.351504
H 0.387123 0.963374 2.698135
H 0.577091 -1.896113 1.590454
H -1.392204 -0.467568 3.521331
H -0.734775 -2.084284 3.793091
H -0.298602 4.576827 1.406095
H -0.655872 3.989535 -0.231181
H -2.389183 2.436715 0.711335
H -1.894780 3.919980 3.371373
H -1.507833 2.209173 3.059923
H -3.200597 2.750580 3.057084

H -3.027816 4.668270 -0.203252
 H -4.084325 4.218097 1.156030
 H -2.789903 5.413583 1.397838
 H -2.892474 -2.464181 2.991300
 H -1.838755 -2.885550 1.652384
 H -3.338922 -0.205905 1.939470
 H -3.998175 -1.602755 1.088096
 H -1.458263 -0.109759 0.278642
 H -2.949202 0.738519 -1.281011
 H -3.119979 -2.220315 -1.224219
 H -1.753456 -1.293003 -1.904155
 H -1.462715 -2.459851 -0.598856
 O 0.215218 2.595418 1.033125
 O 1.849006 3.868014 0.214509
 O -3.333298 0.370878 -0.473090
 O 4.090435 2.925844 -0.357118
 O 5.112496 -1.552841 0.794296

13R-5-c125, $\Delta G = 3.1758$ kcal/mol,
population = 0.09 %

C 0.445056 1.216069 -0.160281
 C 1.745858 0.560430 0.079295
 C 2.953478 1.306059 0.283858
 C 4.156098 0.652514 0.578464
 C 4.195153 -0.736019 0.685151
 C 3.025947 -1.490645 0.480931
 C 1.812668 -0.870599 0.180048
 C 0.630711 -1.739090 -0.027727
 C 0.259587 -2.727015 0.803631
 C -0.980919 -3.558504 0.633348
 C -2.082435 -3.211575 1.665241
 C -2.558693 -1.751180 1.639140
 C -3.337596 -1.317474 0.382959
 C -4.787845 -1.784304 0.394108
 C -0.685408 3.368993 -0.339104
 C -1.201898 3.962458 0.973766
 C -2.398300 4.873017 0.666170
 C -1.556013 2.892974 2.014572
 H 5.059014 1.245716 0.726753
 H 3.073125 -2.580559 0.528246
 H 2.125968 2.993500 0.047264
 H 5.278571 -2.275059 1.023099
 H 0.010049 -1.525616 -0.900515
 H 0.837812 -2.897958 1.721646

H -0.729446 -4.627591 0.751441
 H -1.368234 -3.439677 -0.391847
 H -0.387967 4.166448 -1.034748
 H -1.444193 2.738833 -0.821840
 H -0.391155 4.589804 1.387216
 H -2.748351 5.374436 1.581653
 H -3.243747 4.293081 0.258936
 H -2.139398 5.653809 -0.067170
 H -0.673444 2.300511 2.302444
 H -1.945289 3.365426 2.930389
 H -2.321351 2.194979 1.638493
 H -1.697562 -3.435009 2.675679
 H -2.934072 -3.897303 1.512459
 H -1.681050 -1.090921 1.727916
 H -3.186829 -1.551168 2.525478
 H -2.842133 -1.752622 -0.507491
 H -2.439959 0.379338 0.047770
 H -5.297426 -1.489133 -0.536370
 H -4.856700 -2.878460 0.493342
 H -5.325909 -1.325870 1.240555
 O 0.511609 2.577055 -0.142489
 O -0.616094 0.648848 -0.351226
 O -3.349597 0.102122 0.254993
 O 3.025142 2.643149 0.216152
 O 5.378585 -1.312628 0.974137

13R-5-c136, $\Delta G = 3.1852$ kcal/mol,
population = 0.09 %

C 0.879144 2.467769 0.551194
 C 1.905091 1.456067 0.236107
 C 3.262393 1.818285 0.533660
 C 4.313930 0.915436 0.320483
 C 4.046589 -0.354679 -0.183193
 C 2.726083 -0.730203 -0.487845
 C 1.653390 0.140674 -0.285385
 C 0.304715 -0.355277 -0.647001
 C -0.123733 -1.611791 -0.431093
 C -1.469376 -2.146821 -0.830802
 C -2.292060 -2.704084 0.351189
 C -2.582532 -1.704385 1.479516
 C -3.388280 -0.458685 1.089602
 C -4.820993 -0.756171 0.670361
 C -1.454250 3.057469 0.631840
 C -2.016701 3.769987 -0.601648

C -0.997880 4.700326 -1.271728
 C -2.640748 2.795900 -1.608711
 H 5.331061 1.235268 0.557118
 H 2.558829 -1.716105 -0.921339
 H 2.735385 3.514583 1.142826
 H 5.880757 -0.899789 -0.179040
 H -0.373565 0.355499 -1.120917
 H 0.531497 -2.315623 0.099033
 H -1.322112 -2.972772 -1.551474
 H -2.035732 -1.369132 -1.368659
 H -2.226940 2.432031 1.101162
 H -1.076567 3.781232 1.364894
 H -2.830217 4.398824 -0.193263
 H -1.476124 5.279335 -2.077649
 H -0.171555 4.128208 -1.725256
 H -0.560255 5.409715 -0.552967
 H -3.120527 3.343718 -2.435196
 H -1.877347 2.133915 -2.049104
 H -3.407565 2.161295 -1.136291
 H -1.749388 -3.561980 0.784997
 H -3.236316 -3.117264 -0.042180
 H -1.620529 -1.359655 1.901760
 H -3.114819 -2.217169 2.299938
 H -2.874940 0.044620 0.247937
 H -2.577297 0.540587 2.568124
 H -5.360301 -1.272754 1.481390
 H -5.353792 0.180896 0.445750
 H -4.852270 -1.389178 -0.228929
 O -0.385897 2.133234 0.298985
 O 1.160446 3.571489 1.034930
 O -3.464308 0.451037 2.192343
 O 3.591585 3.013575 1.028405
 O 5.014757 -1.264974 -0.414134

13R-5-c122, $\Delta G = 3.4877$ kcal/mol,
population = 0.05 %

C 0.979291 1.642707 -0.290526
 C 2.310488 1.043293 -0.073122
 C 3.481520 1.841401 0.131291
 C 4.712874 1.242006 0.430790
 C 4.813101 -0.143615 0.536430
 C 3.679900 -0.950198 0.326245
 C 2.442061 -0.385500 0.025648
 C 1.298231 -1.301795 -0.187469

C 0.983081 -2.325390 0.623782
 C -0.222636 -3.205516 0.449611
 C -1.318641 -2.940063 1.511200
 C -1.856890 -1.501463 1.542652
 C -2.683797 -1.062618 0.319428
 C -4.114358 -1.585701 0.350600
 C -0.242375 3.750935 -0.442199
 C -0.662413 4.343042 0.905444
 C -1.003556 3.270577 1.949415
 C 0.377481 5.338742 1.435933
 H 5.580542 1.888753 0.578044
 H 3.792713 -2.033421 0.375110
 H 2.588633 3.486410 -0.152929
 H 6.684342 -0.122968 0.936584
 H 0.654699 -1.095439 -1.045478
 H 1.582314 -2.493519 1.528660
 H 0.077495 -4.265618 0.529633
 H -0.634041 -3.072762 -0.564454
 H -0.031449 4.547458 -1.169747
 H -1.012155 3.085202 -0.851025
 H -1.588272 4.902884 0.676343
 H -1.728306 2.534328 1.569873
 H -1.429226 3.737161 2.851742
 H -0.100356 2.721122 2.263536
 H 0.564690 6.150109 0.713975
 H 0.038178 5.796351 2.378300
 H 1.337692 4.835413 1.635858
 H -0.905847 -3.179716 2.506771
 H -2.143108 -3.656442 1.349954
 H -1.005981 -0.807063 1.630643
 H -2.470485 -1.355464 2.449388
 H -2.194230 -1.451715 -0.595384
 H -1.860027 0.675949 0.016392
 H -4.139393 -2.684375 0.415474
 H -4.647906 -1.175309 1.224160
 H -4.658086 -1.281118 -0.557256
 O 0.998592 3.004548 -0.337871
 O -0.067692 1.032469 -0.413267
 O -2.753659 0.358485 0.234742
 O 3.495022 3.180991 0.061476
 O 5.971653 -0.769357 0.822578

13R-5-c148, $\Delta G = 3.6113$ kcal/mol,
population = 0.04 %

C 0.462720 1.857874 -0.622848
 C 1.793092 1.255362 -0.406589
 C 2.967981 2.050621 -0.199362
 C 4.195633 1.448664 0.099312
 C 4.293526 0.062244 0.200836
 C 3.158819 -0.740932 -0.012413
 C 1.920214 -0.171876 -0.311533
 C 0.775090 -1.086057 -0.525879
 C 0.457510 -2.109341 0.284947
 C -0.750222 -2.986531 0.110273
 C -1.844709 -2.720118 1.173197
 C -2.379562 -1.280318 1.207448
 C -3.206845 -0.837677 -0.014172
 C -4.638697 -1.357154 0.018083
 C -0.754394 3.968778 -0.771226
 C -1.170663 4.560810 0.577615
 C -1.513390 3.488266 1.620989
 C -0.126956 5.552836 1.107525
 H 5.072344 2.078973 0.251690
 H 3.252608 -1.828115 0.028399
 H 2.076915 3.697534 -0.482499
 H 5.443457 -1.429616 0.533551
 H 0.132301 -0.877709 -1.383932
 H 1.055553 -2.278940 1.190377
 H -0.452317 -4.047379 0.188609
 H -1.161988 -2.851347 -0.903302
 H -0.542501 4.765334 -1.498445
 H -1.526483 3.305337 -1.179426
 H -2.095202 5.123612 0.350461
 H -2.240828 2.754525 1.241716
 H -1.936403 3.955146 2.524408
 H -0.611327 2.935897 1.933268
 H 0.061561 6.364392 0.386126
 H -0.463421 6.010451 2.050903
 H 0.832044 5.046417 1.305388
 H -1.431675 -2.962413 2.168021
 H -2.670946 -3.434303 1.011395
 H -1.527015 -0.587957 1.295663
 H -2.991802 -1.134378 2.115097
 H -2.719394 -1.226759 -0.930136
 H -2.378903 0.899153 -0.315324
 H -4.666479 -2.455841 0.081604
 H -5.170095 -0.946485 0.892817
 H -5.182754 -1.050022 -0.888712

O 0.484907 3.219258 -0.669290
 O -0.585450 1.249582 -0.745370
 O -3.273182 0.583680 -0.096749
 O 2.982264 3.390775 -0.267094
 O 5.499959 -0.463337 0.491423

13R-5-c145, $\Delta G = 3.6778$ kcal/mol,
 population = 0.04 %

C 1.025843 1.498523 0.438700
 C 2.300340 0.841072 0.088677
 C 3.550472 1.532304 0.162438
 C 4.756269 0.839213 0.004450
 C 4.749609 -0.532006 -0.249542
 C 3.530396 -1.222054 -0.376317
 C 2.312416 -0.560424 -0.210708
 C 1.060523 -1.314830 -0.435069
 C 0.811965 -2.572483 -0.032897
 C -0.482514 -3.295173 -0.290295
 C -1.416398 -3.359432 0.942777
 C -1.841535 -1.996357 1.508553
 C -2.694042 -1.103882 0.587662
 C -4.131845 -1.586609 0.445284
 C -0.054550 3.649202 0.819816
 C -0.848816 4.199762 -0.366173
 C 0.002950 5.128465 -1.240807
 C -1.530386 3.102856 -1.195938
 H 5.697837 1.384692 0.075985
 H 3.536796 -2.279567 -0.649308
 H 2.754008 3.228079 0.440214
 H 5.807784 -2.091561 -0.574117
 H 0.273201 -0.781905 -0.976219
 H 1.557929 -3.100464 0.575546
 H -0.265091 -4.330395 -0.606870
 H -1.008499 -2.816800 -1.132572
 H -0.682725 3.029235 1.471621
 H 0.378692 4.469409 1.409632
 H -1.642202 4.808145 0.107130
 H -0.599839 5.564125 -2.053075
 H 0.838733 4.576816 -1.701185
 H 0.428592 5.958493 -0.653805
 H -0.788964 2.509230 -1.756502
 H -2.108167 2.408117 -0.567691
 H -2.213588 3.551302 -1.934514
 H -0.906311 -3.923044 1.743620

H -2.303243 -3.959590 0.674623
H -0.935190 -1.426015 1.769051
H -2.396251 -2.146171 2.452090
H -2.234279 -1.090139 -0.420233
H -1.831604 0.568068 1.084419
H -4.631874 -1.587272 1.428195
H -4.697313 -0.921510 -0.226066
H -4.175399 -2.606682 0.033959
O 1.088991 2.857231 0.398152
O 0.001172 0.924209 0.757822
O -2.742620 0.227491 1.095579
O 3.655836 2.848529 0.401596
O 5.939703 -1.148736 -0.394816

13S-5-c40, $\Delta G = 0.0000$ kcal/mol,
population = 19.51 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365

H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c30, $\Delta G = 0.8245$ kcal/mol,
population = 4.84 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054

H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c42, $\Delta G = 0.8352$ kcal/mol,
population = 4.76 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152

C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c57, $\Delta G = 1.0505$ kcal/mol,
population = 3.31 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049

C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690

O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c5, $\Delta G = 1.0599$ kcal/mol,
 population = 3.25 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886

H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c49, $\Delta G = 1.0693$ kcal/mol,
population = 3.20 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916

H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c1, $\Delta G = 1.1032$ kcal/mol,
population = 3.03 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874

H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c89, $\Delta G = 1.1496$ kcal/mol,
 population = 2.80 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207

C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c11, $\Delta G = 1.1628$ kcal/mol,
 population = 2.74 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341

C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c9, $\Delta G = 1.2186$ kcal/mol,

population = 2.49 %
 C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200

H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c126, $\Delta G = 1.2625$ kcal/mol,
population = 2.31 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270

H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c10, $\Delta G = 1.2625$ kcal/mol,
population = 2.31 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365

H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c91, $\Delta G = 1.2820$ kcal/mol,
 population = 2.24 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054

H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c15, $\Delta G = 1.3228$ kcal/mol,
 population = 2.09 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152

C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c54, $\Delta G = 1.3768$ kcal/mol,
 population = 1.91 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049

C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690

O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c43, $\Delta G = 1.3805$ kcal/mol,
population = 1.89 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886

H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c95, $\Delta G = 1.3824$ kcal/mol,
population = 1.89 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916

H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c62, $\Delta G = 1.3843$ kcal/mol,
population = 1.88 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874

H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c104, $\Delta G = 1.4201$ kcal/mol,
population = 1.77 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207

C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c2, $\Delta G = 1.4426$ kcal/mol,
population = 1.70 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341

C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c39, $\Delta G = 1.4602$ kcal/mol,

population = 1.65 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200

H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c23, $\Delta G = 1.4797$ kcal/mol,
population = 1.60 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270

H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c73, $\Delta G = 1.5054$ kcal/mol,
population = 1.53 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365

H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c124, $\Delta G = 1.5154$ kcal/mol,
population = 1.51 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054

H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c17, $\Delta G = 1.5261$ kcal/mol,
population = 1.48 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152

C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c34, $\Delta G = 1.5650$ kcal/mol,
population = 1.39 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049

C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690

O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c58, $\Delta G = 1.5732$ kcal/mol,
 population = 1.37 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886

H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c28, $\Delta G = 1.5889$ kcal/mol,
population = 1.33 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916

H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c21, $\Delta G = 1.5889$ kcal/mol,
population = 1.33 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874

H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c25, $\Delta G = 1.6108$ kcal/mol,
 population = 1.28 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207

C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c6, $\Delta G = 1.6478$ kcal/mol,
 population = 1.21 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341

C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c59, $\Delta G = 1.6667$ kcal/mol,

population = 1.17 %
 C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200

H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c38, $\Delta G = 1.7338$ kcal/mol,
population = 1.04 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270

H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c72, $\Delta G = 1.8016$ kcal/mol,
population = 0.93 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365

H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c32, $\Delta G = 1.8882$ kcal/mol,
 population = 0.80 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054

H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c101, $\Delta G = 1.9672$ kcal/mol,
 population = 0.70 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152

C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c179, $\Delta G = 1.9723$ kcal/mol,
 population = 0.70 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049

C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690

O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c22, $\Delta G = 1.9974$ kcal/mol,
population = 0.67 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886

H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c152, $\Delta G = 1.9999$ kcal/mol,
population = 0.66 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916

H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c76, $\Delta G = 2.0112$ kcal/mol,
population = 0.65 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874

H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c53, $\Delta G = 2.0664$ kcal/mol,
population = 0.59 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207

C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c134, $\Delta G = 2.1304$ kcal/mol,
population = 0.53 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341

C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c96, $\Delta G = 2.1448$ kcal/mol,

population = 0.52 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200

H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c116, $\Delta G = 2.2044$ kcal/mol,
population = 0.47 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270

H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c182, $\Delta G = 2.2101$ kcal/mol,
population = 0.47 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365

H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c19, $\Delta G = 2.2220$ kcal/mol,
population = 0.46 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054

H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c37, $\Delta G = 2.3067$ kcal/mol,
population = 0.40 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152

C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c31, $\Delta G = 2.3099$ kcal/mol,
population = 0.39 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049

C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690

O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c147, $\Delta G = 2.3268$ kcal/mol,
 population = 0.38 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886

H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c184, $\Delta G = 2.3469$ kcal/mol,
population = 0.37 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916

H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c52, $\Delta G = 2.3619$ kcal/mol,
population = 0.36 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874

H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c48, $\Delta G = 2.3902$ kcal/mol,
 population = 0.34 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207

C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c92, $\Delta G = 2.4523$ kcal/mol,
 population = 0.31 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341

C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c142, $\Delta G = 2.6443$ kcal/mol,

population = 0.22 %
 C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200

H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c97, $\Delta G = 2.6958$ kcal/mol,
population = 0.21 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270

H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c109, $\Delta G = 2.7887$ kcal/mol,
population = 0.18 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365

H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c115, $\Delta G = 2.8941$ kcal/mol,
population = 0.15 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054

H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c81, $\Delta G = 2.9123$ kcal/mol,
population = 0.14 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152

C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c107, $\Delta G = 2.9242$ kcal/mol,
 population = 0.14 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049

C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690

O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c102, $\Delta G = 3.1451$ kcal/mol,
population = 0.10 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886

H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c123, $\Delta G = 3.1758$ kcal/mol,
population = 0.09 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916

H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c136, $\Delta G = 3.1852$ kcal/mol,
population = 0.09 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874

H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c122, $\Delta G = 3.4877$ kcal/mol,
population = 0.05 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341
 C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207

C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c148, $\Delta G = 3.6113$ kcal/mol,
population = 0.04 %

C -1.231151 -1.795084 -0.679098
 C -2.112003 -0.708746 -0.217908
 C -3.348962 -1.112973 0.385049
 C -4.210529 -0.168896 0.960317
 C -3.879769 1.184193 0.921645
 C -2.696122 1.606567 0.291100
 C -1.804163 0.692863 -0.275341

C -0.612428 1.229766 -0.970817
 C 0.042394 2.353350 -0.627319
 C 1.187953 2.956728 -1.389342
 C 2.432323 3.249546 -0.532152
 C 3.145634 2.003301 -0.004460
 C 4.331858 2.317117 0.916553
 C 5.076881 1.060455 1.363753
 C 0.924832 -2.474365 -1.455207
 C 1.611109 -3.218526 -0.306440
 C 2.367839 -2.266397 0.625577
 C 2.532829 -4.297549 -0.888759
 H -5.138704 -0.519294 1.417054
 H -2.511146 2.678010 0.216096
 H -3.026424 -2.918044 -0.028520
 H -5.464711 1.745209 1.837612
 H -0.260095 0.669605 -1.838874
 H -0.263533 2.899070 0.275091
 H 1.454403 2.310441 -2.243488
 H 0.843552 3.915650 -1.821601
 H 1.663754 -1.930303 -2.062365
 H 0.375004 -3.175040 -2.098671
 H 0.818250 -3.722164 0.272974
 H 2.815455 -2.818278 1.467317
 H 3.183894 -1.752788 0.088916
 H 1.702100 -1.495472 1.042498
 H 3.332648 -3.847949 -1.501878
 H 1.979223 -5.007579 -1.524325
 H 3.014969 -4.873165 -0.083270
 H 3.141946 3.846497 -1.131640
 H 2.148555 3.883798 0.324666
 H 2.430720 1.366304 0.549939
 H 3.503956 1.390521 -0.850886
 H 5.036093 2.967917 0.367638
 H 3.310004 2.565428 2.560876
 H 4.400359 0.378465 1.907464
 H 5.907842 1.326251 2.035200
 H 5.487970 0.509830 0.502664
 O 0.016274 -1.448832 -0.996499
 O -1.597294 -2.974666 -0.746433
 O 3.929279 3.098953 2.040690
 O -3.731237 -2.391710 0.440265
 O -4.671802 2.141709 1.446914

13S-5-c113, $\Delta G = 3.6496$ kcal/mol,

population = 0.04 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270
H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200

H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.446914

13S-5-c145, $\Delta G = 3.6778$ kcal/mol,
population = 0.04 %

C -1.231151 -1.795084 -0.679098
C -2.112003 -0.708746 -0.217908
C -3.348962 -1.112973 0.385049
C -4.210529 -0.168896 0.960317
C -3.879769 1.184193 0.921645
C -2.696122 1.606567 0.291100
C -1.804163 0.692863 -0.275341
C -0.612428 1.229766 -0.970817
C 0.042394 2.353350 -0.627319
C 1.187953 2.956728 -1.389342
C 2.432323 3.249546 -0.532152
C 3.145634 2.003301 -0.004460
C 4.331858 2.317117 0.916553
C 5.076881 1.060455 1.363753
C 0.924832 -2.474365 -1.455207
C 1.611109 -3.218526 -0.306440
C 2.367839 -2.266397 0.625577
C 2.532829 -4.297549 -0.888759
H -5.138704 -0.519294 1.417054
H -2.511146 2.678010 0.216096
H -3.026424 -2.918044 -0.028520
H -5.464711 1.745209 1.837612
H -0.260095 0.669605 -1.838874
H -0.263533 2.899070 0.275091
H 1.454403 2.310441 -2.243488
H 0.843552 3.915650 -1.821601
H 1.663754 -1.930303 -2.062365
H 0.375004 -3.175040 -2.098671
H 0.818250 -3.722164 0.272974
H 2.815455 -2.818278 1.467317
H 3.183894 -1.752788 0.088916
H 1.702100 -1.495472 1.042498
H 3.332648 -3.847949 -1.501878
H 1.979223 -5.007579 -1.524325
H 3.014969 -4.873165 -0.083270

H 3.141946 3.846497 -1.131640
H 2.148555 3.883798 0.324666
H 2.430720 1.366304 0.549939
H 3.503956 1.390521 -0.850886
H 5.036093 2.967917 0.367638
H 3.310004 2.565428 2.560876
H 4.400359 0.378465 1.907464
H 5.907842 1.326251 2.035200
H 5.487970 0.509830 0.502664
O 0.016274 -1.448832 -0.996499
O -1.597294 -2.974666 -0.746433
O 3.929279 3.098953 2.040690
O -3.731237 -2.391710 0.440265
O -4.671802 2.141709 1.4469

