Characterization of Leptazolines A-D, Polar Oxazolines from the Cyanobacterium Leptolyngbya sp., Reveals a Glitch with the "Willoughby-Hoye" Scripts for Calculating NMR Chemical Shifts

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EXPERIMENTAL SECTION

General experimental procedures. Optical rotations were measured on a JASCO DIP-370 polarimeter at 589 nm using a sample cell of path length 0.1 dm. UV spectra were obtained on a Varian Cary 50 Bio UV-Visible spectrophotometer. IR spectra of the compounds, as thin films on CaF_2 discs, were recorded using a Shimadzu IRAffinity-1 Fourier Transform spectrophotometer. NMR spectra were acquired on a Varian Inova 500 MHz spectrometer operating at 500 (^{1}H) or 125 (^{13}C) MHz using the residual solvent signals as internal references (CD_3OD δ_H 3.30, δ_C 49.0; DMSO-d_6 δ_H 2.50, δ_C 39.5; $CDCl_3$ δ_H 7.26, δ_C 77.0). Samples were placed in 3-mm Shigemi NMR tubes as necessary. HRMS data were obtained from an Agilent 6545 LC/QTOF instruments using electrospray ionization in positive and negative modes. Samples were purified using a combination of chromatographic techniques, including high performance liquid chromatography. Purity of the compounds was assessed from their UV absorptions at the appropriate wavelengths, or from their ^{1}H NMR spectra. Percent yields of natural products were based on the amount of freeze-dried biological material or crude extract from the culture broth.

Biological material. The strain O-2-5 (*Leptolyngbya* sp.) was obtained from the Patterson culture collection housed at the University of Hawaii at Manoa. This strain was originally collected from the Blaisdell Center in Honolulu in 1996 and it was identified as *Lyngbya limnetica* by Dr. Gregory Patterson based on its unbranched, long fine trichomes and very small cells. Subsequent 16S sRNA phylogenetic studies revised the identification to *Leptolyngbya* sp. Strain O-2-5 is an unbranched cyanobacterium with long fine straight trichomes and much smaller cells that clustered like a hairball.

Cultivation. The strain was cultured in 11 L BG-11 media with MOPS buffer, under continuous illumination and aeration (3-4 L air/min; no CO_2 added) for 30 days. Cells were filtered off from the suspension and the media was extracted using 25 g of HP-20 resin. The cells were freeze-dried to obtain 5.61 g of dry biomass from the initial harvest.

Extraction, purification and isolation of metabolites. For the initial screening, 570 mg of freeze-dried cells were extracted using 50 mL of 4:1 methanol and dichloromethane (3 times) to yield 111.4 mg of crude extract. The crude extract was fractionated on a C8 column (diameter 2.2 cm, height 1.2 cm) and each fraction was collected by eluting with an increasing concentration of methanol in water (15 mL total volume), followed by isopropanol (with 0.1% TFA). At the same time, HP-20 resin that had been soaked overnight in the media was separated from the medium and re-suspended in 100 mL of organic solvent (methanol) for 2 h. The solution was filtered off

to get rid of the resin and the solvent was removed *in vacuo* to yield 25 mg of the crude media extract. After screening all C8 fractions and the crude media extract at a test concentration of 50 µg/mL, the media extract was found to exhibit activity against PANC-1 cell lines.

The media extract was purified by RP-HPLC (Phenomenex Luna C18, 250 x 10 mm, 5 µm particle size, 100 Å) eluting with MeCN/H_2O (with 0.1% formic acid) at 2.75 mL/min using the following gradient: 25% MeCN for 5 min, then a linear gradient to 70% MeCN over 30 min, and another gradient to 100% MeCN over 5 min, then a 10 min wash with MeCN. HPLC fractions were tested again in the PANC-1 assay at a test concentration of 20 µg/mL in order to identify compounds responsible for the growth inhibition. Due to the lack of sufficient material for structure elucidation, the culture was regrown several times in an effort to isolate sufficient quantities of the new natural products. There was considerable variability in the composition of the metabolites from the various growths and, as a result, material was combined from several extracts, based on LC-MS analysis, to allow for purification and isolation of the compounds of interest.

Like fractions (combined mass of 4.3 mg) showing LC-MS signals at ca. *m*/*z* 300 $[M+H]^+$ were combined and purified by RP-HPLC (Phenomenex Luna C18, 250 x 10 mm, 5 µm particle size, 100 Å) eluting with MeCN/H_2O at 2.75 mL/min using the following gradient: 25% MeCN for 5 min then a linear gradient to 45% MeCN over 20 min and then increasing to 100% MeCN over 5 min before a 10 min wash with MeCN, which yielded compounds **5** (t_R 6.6 min, 0.8 mg, 1.1% yield, >99% purity by LC-UV detection at 315 nm) and **1** (t_R 15.5 min, 1.0 mg, 1.4% yield, >99% purity by LC-UV detection at 315 nm).

Similarly, like fractions (3.9 mg) showing LC-MS signals at ca. *m*/*z* 389 $[M+H]^+$ were purified by RP-HPLC (Phenomenex Luna C18, 250 x 10 mm, 5 µm particle size, 100 Å) eluting with MeOH/H_2O at 2.75 mL/min using the following gradient: 45-85% MeOH over 20 min and then increasing to 100% MeOH over 5 min before a 10 min wash with MeOH, which yielded compounds **6** (t_R 6.9 min, 1.0 mg, 0.55% yield, 90% purity by LC-UV detection at 315 nm) and **2** (t_R 19.3 min, 1.0 mg, 0.55% yield, 96% purity by LC-UV detection at 315 nm).

From another harvest, purification of two fractions (1.8 mg and 9.1 mg) using the conditions described above led to the isolation of compound **3** (t_R 18.5 min, 0.3 mg, 0.19% yield, >95% purity by ^1H NMR) and compound **4** (t_R 14.5 min, 0.2 mg, 0.13% yield, isolated with other unidentified impurities). Further analysis and biological evaluation of these compounds was not possible because of the lack of sufficient material.

Leptazoline A (**1**): white, amorphous solid; $[\alpha]_D^{22}$ +47 (*c* 0.2, CH_3OH); UV (CH_3OH) λ_{max} (log ε) 317 (3.45), 263 (3.25), 251 (3.58), 210 (4.36) nm; IR (CaF_2 disc) ν_{max} 3600-2500 (br), 3381, 3206, 2986, 2920, 1694, 1682, 1639, 1574, 1246, 1101 cm^{-1}; ^1H NMR (500 MHz, DMSO-d_6) see Table 1; ^1H NMR (500 MHz, CD_3OD) δ 7.58 (d, *J* = 2.7 Hz, 1H), 7.34 (dd, *J* = 8.9, 2.7 Hz, 1H), 6.93 (d, *J* = 8.9 Hz, 1H), 4.79 (p, *J* = 6.4 Hz, 1H), 4.10 (ddd, *J* = 7.8, 5.5, 3.4 Hz, 1H), 3.99 (dd, *J* = 6.7, 3.4 Hz, 1H), 2.57 – 2.46 (m, 2H), 1.45 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) see Table 1; ^{13}C NMR (125 MHz, CD_3OD) δ 178.2, 165.7, 159.9, 134.1, 128.3, 124.2, 119.3, 113.2, 79.2, 77.5, 70.4, 41.1, 21.0; HRESIMS *m*/*z* 300.0630 $[M+H]^+$ (calcd for $C_{13}H_{15}ClNO_5$, 300.0633).

Leptazoline B (**2**): off-white, amorphous solid; $[\alpha]_D^{22}$ +44 (*c* 0.2, CH_3OH); UV (CH_3OH) λ_{max} (log ε) 315 (3.60), 262 (3.46), 251 (3.77), 210 (4.55) nm; IR (CaF_2 disc) ν_{max} 3476, 3277, 2926, 1676, 1661, 1643, 1556, 1229, 1069 cm^{-1}; ^1H NMR (500 MHz, CD_3OD) see Table S4; ^{13}C NMR (125 MHz, CD_3OD) see Table S4; HRESIMS *m*/*z* 389.1111 $[M+H]^+$ (calcd for $C_{16}H_{22}ClN_2O_7$, 389.1110).

Leptazoline C (**3**): white, amorphous solid; ^1H NMR (500 MHz, CD_3OD) δ 7.65 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.37 (ddd, *J* = 8.3, 7.6, 1.7 Hz, 1H), 6.94 (d, *J* = 8.3 Hz, 1H), 6.87 (t, *J* = 7.6 Hz, 1H), 4.78 (p, *J* = 6.3 Hz, 1H), 4.08 (ddd, *J* = 6.7, 6.3, 3.7 Hz,1H), 3.98 (dd, *J* = 6.7, 3.7 Hz, 1H), 2.47 (m, 2H), 1.46 (d, *J* = 6.3 Hz, 3H).; HRESIMS *m*/*z* 266.1019 $[M+H]^+$ (calcd for $C_{13}H_{16}NO_5$, 266.1023).

Leptazoline D (**4**): off-white, amorphous solid; ^1H NMR (500 MHz, CD_3OD) δ 7.63 (d, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 1H), 6.92 (d, *J* = 8.3 Hz, 1H), 6.86 (t, *J* = 7.5 Hz, 1H), 4.79 (p, *J* = 6.5 Hz, 1H), 4.24 (dd, *J* = 6.9, 3.2 Hz, 1H), 4.19 (d, *J* = 7.4 Hz, 1H), 3.96 (p, *J* = 5.7 Hz, 1H), 3.74 (dd, *J* = 7.6, 3.3 Hz, 1H), 3.69-3.58 (m, 4H), 1.46 (d, *J* = 6.2 Hz, 3H); HRESIMS *m*/*z* 355.1496 $[M+H]^+$ (calcd for $C_{16}H_{23}N_2O_7$, 355.1500).

Compound **5**: ^1H NMR (500 MHz, CD_3OD) δ 7.76 (d, *J* = 3.0 Hz, 1H), 7.01 (dd, *J* = 8.8, 3.0 Hz, 1H), 6.62 (d, *J* = 8.8 Hz, 1H), 4.27 (ddd, *J* = 7.3, 5.6, 3.4 Hz, 1H), 4.10 (m, 1H), 3.97 (t, *J* = 3.6 Hz, 1H), 2.41 – 2.33 (m, 2H), 1.20 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, CD_3OD) δ 180.7, 180.4, 171.1, 133.0, 130.0, 124.7, 121.0, 118.1, 71.9, 70.3, 59.0, 42.9, 20.6; HRESIMS *m*/*z* 318.0737 $[M+H]^+$ (calcd for $C_{13}H_{17}ClNO_6$, 318.0739).

Compound **6**: ^1H NMR (600 MHz, CD_3OD) δ 7.93 (d, *J* = 2.7 Hz, 1H), 7.36 (dd, *J* = 8.8, 2.7 Hz, 1H), 6.93 (d, *J* = 8.7 Hz, 1H), 4.29 (dd, *J* = 4.3, 2.5 Hz, 1H), 4.13 (qd, *J* = 6.3, 4.3 Hz, 1H), 4.06 (dd, *J* = 7.2, 2.5 Hz, 1H), 3.97 (d, *J* = 7.0 Hz, 1H); 3.97 (m, 1H), 3.68 – 3.60 (m, 4H), 1.23 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (150 MHz, CD_3OD) δ 173.9 (extrapolated from HMBC data), 169.1, 158.5, 134.2, 130.2, 125.2, 119.8, 119.8, 74.6, 73.1, 69.7, 61.9, 61.8, 56.1, 54.0, 20.6; HRESIMS *m*/*z* 407.1224 $[M+H]^+$ (calcd for $C_{16}H_{24}ClN_2O_8$, 407.1216).

Acetylation of compound 1. The reaction was carried out in an N_2 atmosphere using balloons. To 0.5 mg (1.7 µmol) of compound **1** in a reaction vial were added a drop of pyridine, 5 µL of acetic anhydride, and 0.5 mL dry CH_2Cl_2. The mixture was stirred at room temperature for 1 h. An additional 0.5 mL CH_2Cl_2 was added to the vial and the contents were washed sequentially with aq. $NaHCO_3$ (1 mL) and brine (1 mL). The organic layer was then dried over anhydrous $MgSO_4$ and filtered. Upon removal of the solvent by evaporation under a stream of N_2, 0.6 mg of crude solid was obtained. The residue was purified by RP-HPLC (Phenomenex Luna C18, 150 x 4.6 mm, 5 µm particle size, 100 Å) eluting with CH_3OH in H_2O at 0.7 mL/min using a linear gradient from 50% CH_3OH in H_2O to 100% CH_3OH over 20 min, which yielded compound **7** (t_R 6.4 min, 0.1 mg, 0.3 µmol, 17% yield, isolated with unidentified impurities) and compound **8** (t_R 7.8 min, 0.3 mg, 0.9 µmol, 52% yield).

3-Acetyl-**1** (**7**): ^{1}H NMR (500 MHz, CD_3OD) δ 7.57 (d, *J* = 2.7 Hz, 1H), 7.36 (dd, *J* = 8.9, 2.7 Hz, 1H), 6.94 (d, *J* = 8.9 Hz, 1H), 5.44 (td, *J* = 7.0, 3.8 Hz, 1H), 4.67 (p, *J* = 6.3 Hz, 1H), 4.23 (dd, *J* = 6.3, 3.8 Hz, 1H), 2.60-2.52 (m, 2H), 1.98 (s, 3H), 1.44 (d, *J* = 6.3 Hz, 3H); HRESIMS *m*/*z* 342.0743 $[M+H]^+$ (calcd for $C_{15}H_{16}ClNO_6$, 342.0739).

9-Acetyl-**1** (**8**): ^{1}H NMR (500 MHz, CD_3OD) δ 7.57 (d, *J* = 2.6 Hz, 1H), 7.33 (dd, *J* = 8.9, 2.7 Hz, 1H), 6.92 (d, *J* = 9.0 Hz, 1H), 4.79 (m, 1H), 4.05 (m, 1H), 3.98 (dd, *J* = 6.8, 3.5 Hz, 1H), 2.45 (m, 2H), 1.88 (s, 3H), 1.45 (d, *J* = 6.3 Hz, 3H).

NMR shift Calculations. Conformers of all diastereomers of **1** and **2** within 5 kcal/mol of the lowest energy conformer were searched using the Monte Carlo multiple minimum (MCMM) method and the OPLS-2005 force field in MacroModel[1] (Schrodinger Inc.). Each conformer within 5 kcal/mol of the lowest energy conformer was optimized in Gaussian09 at the M06-2X[2]/6-31+G level and the geometries of all conformers with similar energies were checked for redundancy. NMR shielding tensors of all unique conformers within the energy window were computed using the gauge-independent atomic orbital (GIAO) method at the B3LYP[3-6]/6-311+G[7, 8] level and ^{1}H and ^{13}C chemical shifts were obtained after applying appropriate scaling factors (^{1}H: intercept = 31.9477, slope = -1.0767; ^{13}C: intercept = 181.2412, slope = -1.0522). Statistical comparisons of the computed shifts with the experimental data were carried out using the spreadsheet provided by Sarotti.[9]

The new scripts were tested using Python V3 (Windows 10 using Anaconda 1.9.6 running Python 3.7.1; Python 3.6.5 on Mac Mavericks; Python 3.7.1 on Mac Mojave) and Python V2 (Python 2.7.10 on Mac El Capitan 10.11.6; Python 2.7.16 on Mac Mojave).

Growth inhibitory assay. Human pancreatic carcinoma (PANC-1) cell lines were maintained in DMEM media supplemented with 10% premium fetal bovine serum and 50 U/mL penicillin and 50 µg/mL streptomycin. One day before treatment, cancer cells were seeded at 5,000 cells per well into a 96-well tissue culture plate. Twenty-four hours post seeding, the serially diluted compounds were added to the cells for the growth inhibition assay, and incubated at 37 ^{o}C with 5% CO_2 for 72 h. Then, 40 µL MTS dye (Cell Titer aqueous One Solution Cell Proliferation Assay) was added to each well and incubated with 5% CO_2 at 37 ^{o}C for 90 minutes. Cell viability data were collected with a Modulus Microplate Reader and GI_{50} curves were generated using GraphPad Prism 5. For GI_{50} determination, samples were tested in triplicate at each concentration and the results were averaged. Three consecutive biological replicates were collected and average GI_{50} values were calculated.

Table S1. NMR Spectroscopic Data of Compound 1 in MeOH-d_4

C/H#	δ_C, type	δ_H (J in Hz)	COSY	HMBC[a]
1	178.2, C			
2	41.1, CH_2	2.54, dd (14.7, 5.1)	3	1, 3, 4
		2.50, dd (14.7, 6.7)	3	
3	70.4, CH	4.10, ddd (7.8, 5.5, 3.4)	2, 4	1,2, 5
4	77.5, CH	3.99, dd (6.7, 3.4)	3, 5	2, 3, 5, 7, 8
5	79.2, CH	4.79, p (6.4)	4, 6	3, 7
6	21.0, CH_3	1.45, d (6.3)		4, 5
7	165.7, C			
8	113.2, C			
9	159.9, C			
10	119.3, CH	6.93, d (8.9)	11	7, 8, 9, 12
11	134.1, CH	7.34, dd (8.9, 2.7)	10, 11	9, 12, 13
12	124.2, C			
13	128.3, CH	7.58, d (2.7)	11	7, 9, 11, 12
NH		12.28, brs		

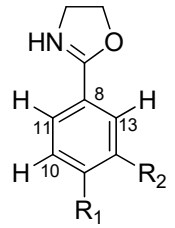
[a] HMBC correlations, optimized for 7 Hz, are from proton(s) stated to the indicated carbon

Table S2. Comparison of Calculated and Experimental Chemical Shifts for Aromatic Substitutions

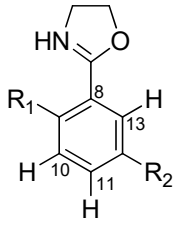
Pos [a]	Exp. [a]	A [b]	B [b]	C [b]	D [b]	E [b]	F [b]
8	113.2, C	129.6	127.3	110.7	127.4	121.0	111.0
9 (OH)	159.9, C	158.4	151.6	155.7	154.8	156.8	158.3
10	119.3, CH	117.9	128.4	118.5	132.1	130.4	129.8
11	134.1, CH	127.5	122.7	131.8	119.0	114.6	121.0
	124.2, C	120.8	122.6	125.0	126.2	136.2	138.6
13	128.3, CH	129.3	115.4	128.9	116.4	116.7	116.6
MAE		5.1	9.6	1.9	10.2	10.9	8.9

[a] Numbered for **A-F** as below with C9 as C-OH and C12 as C-Cl always, C13 corresponding to the carbon bearing the proton that gives rise to the doublet observed in the ^{1}H NMR spectrum with a meta coupling to H-13, which defines the position of C13.

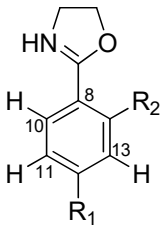
[b] ^{13}C NMR Chemical shifts calculated using ACD Labs Prediction V12



A R_1 = OH R_2 = Cl
B R_1 = Cl R_2 = OH



C R_1 = OH R_2 = Cl
D R_1 = Cl R_2 = OH



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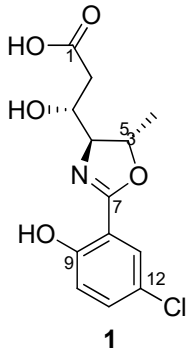
F R_1 = Cl R_2 = OH



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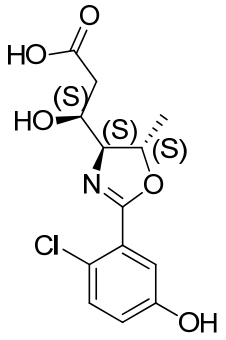
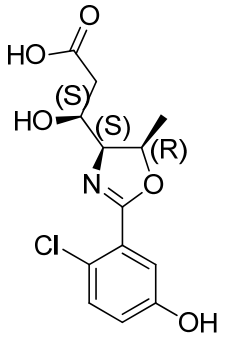
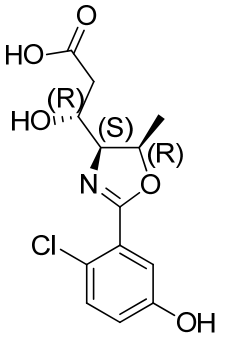


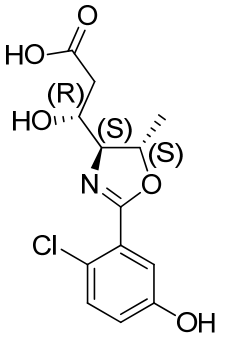
(3*S**,4*S**,5*S**)-**1a**



(3*S**,4*S**,5*R**)-**1b**



(3*R**,4*S**,5*R**)-**1c**



(3*R**,4*S**,5*S**)-**1d**

The four diastereomers of compound 1

Table S3. Experimental and Computed Chemical Shifts of Compound 1

Nuclei	Position	Experimental δ		Computed δ			
		1		**1a**	**1b**	**1c**	**1d**
H	2a	2.53		2.55	2.88	2.86	2.76
	2b	2.53		2.55	2.92	2.85	2.82
	3	4.10		4.46	4.15	4.31	3.96
	4	3.99		4.03	4.43	4.40	3.96
	5	4.79		4.70	4.96	4.97	4.70
	6	1.45		1.42	1.42	1.53	1.45
	10	6.93		6.90	6.88	6.91	6.90
	11	7.34		7.34	7.33	7.35	7.35
	13	7.58		7.64	7.64	7.68	7.66
			MAE (all)	**0.07**	0.17	0.18	0.10
			MAE (H3-H5)	0.16	0.22	0.27	**0.09**
C	1	178.2		172.0	173.2	172.1	172.0
	2	41.1		34.9	37.7	40.0	38.0
	3	70.4		68.0	68.4	66.1	69.5
	4	77.5		76.4	70.5	70.3	76.4
	5	79.2		74.9	78.4	78.5	77.9
	6	21.0		19.4	13.3	14.7	18.9
	7	165.7		162.7	162.5	163.3	163.2
	8	113.2		109.6	109.8	109.7	109.5
	9	159.9		156.6	156.5	156.4	156.5
	10	119.3		115.6	115.5	115.5	115.5
	11	134.1		131.6	131.6	131.7	131.7
	12	124.2		126.6	126.6	126.6	126.6
	13	128.3		125.7	125.6	125.8	125.8
			MAE (all)	3.3	3.6	3.6	**2.7**
			MAE (C3-C5)	2.6	3.3	4.1	**1.1**
Probabilities	sDP4+	H		**0.916**	0.001	0.000	0.083
		C		0.003	0.000	0.000	**0.997**
		all		0.033	0.000	0.000	**0.967**

Key:

1a = (3*S**,4*S**,5*S**)-**1**; **1b** = (3*S**,4*S**,5*R**)-**1**;

1c = (3*R**,4*S**,5*R**)-**1**; **1d** = (3*R**,4*S**,5*S**)-**1**

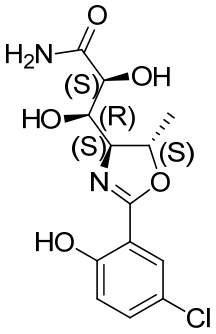
Table S4. NMR Spectroscopic Data of Compound 2 in CD_3OD

Pos.	δ_C, type	δ_H (J in Hz)	COSY	HMBC[a]	ROESY
1	175.6, C				
2	73.5, CH	4.18, d (7.4)	3	1, 3, 4	4, 3
3	74.2, CH	3.75, dd (7.5, 3.3)	2, 4	1, 2, 5	2, 4, 5
4	74.3, CH	4.26, dd (6.7, 3.2)	3, 5	6, 7, 2, 3, 8	2, 3, 6
5	79.3, CH	4.81, p (6.3)	4, 6	3, 7	3, 6
6	20.8, CH_3	1.46, d (6.3)	5	5, 4	4, 5
7	165.8, C				
8	113.2, C				
9	160.0, C				
10	119.3, CH	6.93, d (8.8)	11	7, 8, 9, 12	11
11	134.2, CH	7.34, dd (8.8, 2.7)	10, 13	9, 12, 13	10, 13
12	124.2, C				
13	128.3, CH	7.58, d (2.6)	11	7, 9, 11, 12	11
1’	54.0, CH	3.96, p (5.5)	2’, 3’	2’, 3’, 1	2’, 3’
2’/3’	61.7, CH_2	3.69-3.56, m	1’	1’, 2’	1’, 2’

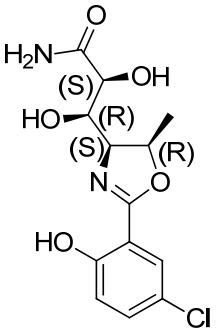
Table S5. Computed Chemical Shifts of a Truncated Version of 2

Nuclei	Pos.	Experimental δ		Computed δ							
		2		**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**
H	2	4.18		4.04	4.33	4.38	4.24	4.62	4.66	4.06	4.22
	3	3.75		3.94	4.34	4.13	3.85	4.50	4.90	4.12	3.38
	4	4.26		4.28	4.36	4.21	4.24	4.05	4.17	4.60	4.52
	5	4.81		4.84	5.12	4.76	4.63	5.07	4.96	4.87	4.68
	6	1.46		1.55	1.41	1.63	1.43	1.55	1.43	1.41	1.37
	10	6.93		6.90	6.91	6.90	6.90	6.90	6.92	6.91	6.91
	11	7.34		7.34	7.34	7.33	7.35	7.34	7.35	7.36	7.35
	13	7.58		7.64	7.68	7.59	7.65	7.62	7.67	7.67	7.67
			MAE (all)	0.07	0.17	0.11	**0.06**	0.23	0.25	0.13	0.13
			MAE (H2-H5)	0.10	0.29	0.17	**0.09**	0.41	0.47	0.22	0.20
C	1	175.		169.6	169.5	172.1	171.	169.8	169.9	171.6	170.1
	2	73.5		71.7	72.9	74.8	72.2	74.2	74.1	72.3	73.2
	3	74.2		74.3	74.6	68.4	73.7	71.6	73.8	70.6	75.4
	4	74.3		72.9	68.6	68.2	72.2	73.9	67.7	67.9	71.9
	5	79.3		75.4	78.8	78.5	77.8	75.9	80.1	77.1	78.1
	6	20.8		18.6	15.9	12.6	18.4	18.4	16.6	13.1	18.9
	7	165.		162.7	163.2	163.3	163.	162.9	163.8	163.4	163.6
	8	113.		109.6	110.0	109.7	109.	109.5	110.1	109.6	109.5
	9	160.		156.6	156.7	156.9	156.	156.8	156.7	156.6	156.7
	10	119.		115.5	115.5	115.6	115.7	115.6	115.6	115.7	115.7
	11	134.		131.6	131.6	131.5	131.	131.6	131.7	131.9	131.8
	12	124.		126.5	126.6	126.4	126.	126.4	126.6	126.7	126.6
	13	128.		125.7	125.6	125.6	125.	125.6	125.6	125.8	125.8
			MAE (all)	2.8	3.0	3.5	**2.5**	2.8	2.9	3.5	**2.5**
			MAE (C2-C5)	1.8	1.8	3.5	1.4	1.8	2.1	3.4	**1.3**
Probabilities sDP4+		H		0.349	0.003	0.030	**0.59**	0.000	0.001	0.009	0.012
		C		0.019	0.003	0.000	0.46	0.023	0.005	0.000	**0.481**
		all		0.022	0.000	0.000	**0.95**	0.000	0.000	0.000	0.021

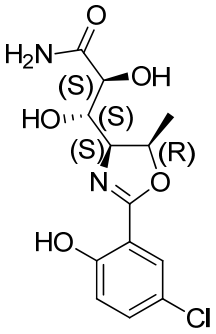
Key: **2a** = (2*S**,3*R**,4*S**,5*S**)-**2a**; 2b = (2*S**,3*R**,4*S**,5*R**)-**2a**; 2c = (2*S**,3*S**,4*S**,5*R**)-**2a**; 2d = (2*S**,3*S**,4*S**,5*S**)-**2a**; 2e = (2*R**,3*R**,4*S**,5*S**)-**2a**; 2f = (2*R**,3*R**,4*S**,5*R**)-**2a**; 2g = (2*R**,3*S**,4*S**,5*R**)-**2a**; 2h = (2*R**,3*S**,4*S**,5*S**)-**2a**



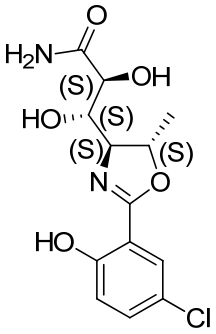
(2*S**,3*R**,4*S**,5*S**)-**2a**



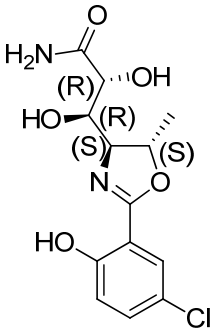
(2*S**,3*R**,4*S**,5*R**)-**2b**



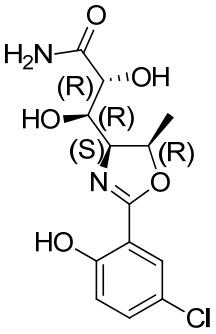
(2*S**,3*S**,4*S**,5*R**)-**2c**



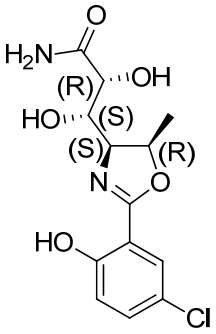
(2*S**,3*S**,4*S**,5*S**)-**2d**



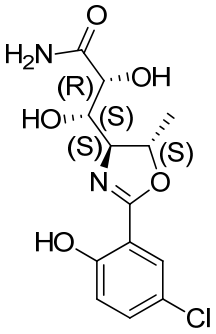
(2*R**,3*R**,4*S**,5*S**)-**2e**



(2*R**,3*R**,4*S**,5*R**)-**2f**



(2*R**,3*S**,4*S**,5*R**)-**2g**



(2*R**,3*S**,4*S**,5*S**)-**2h**

Figure S1. ^{1}H NMR Spectrum of Compound 1 in CD_3OD (500 MHz)

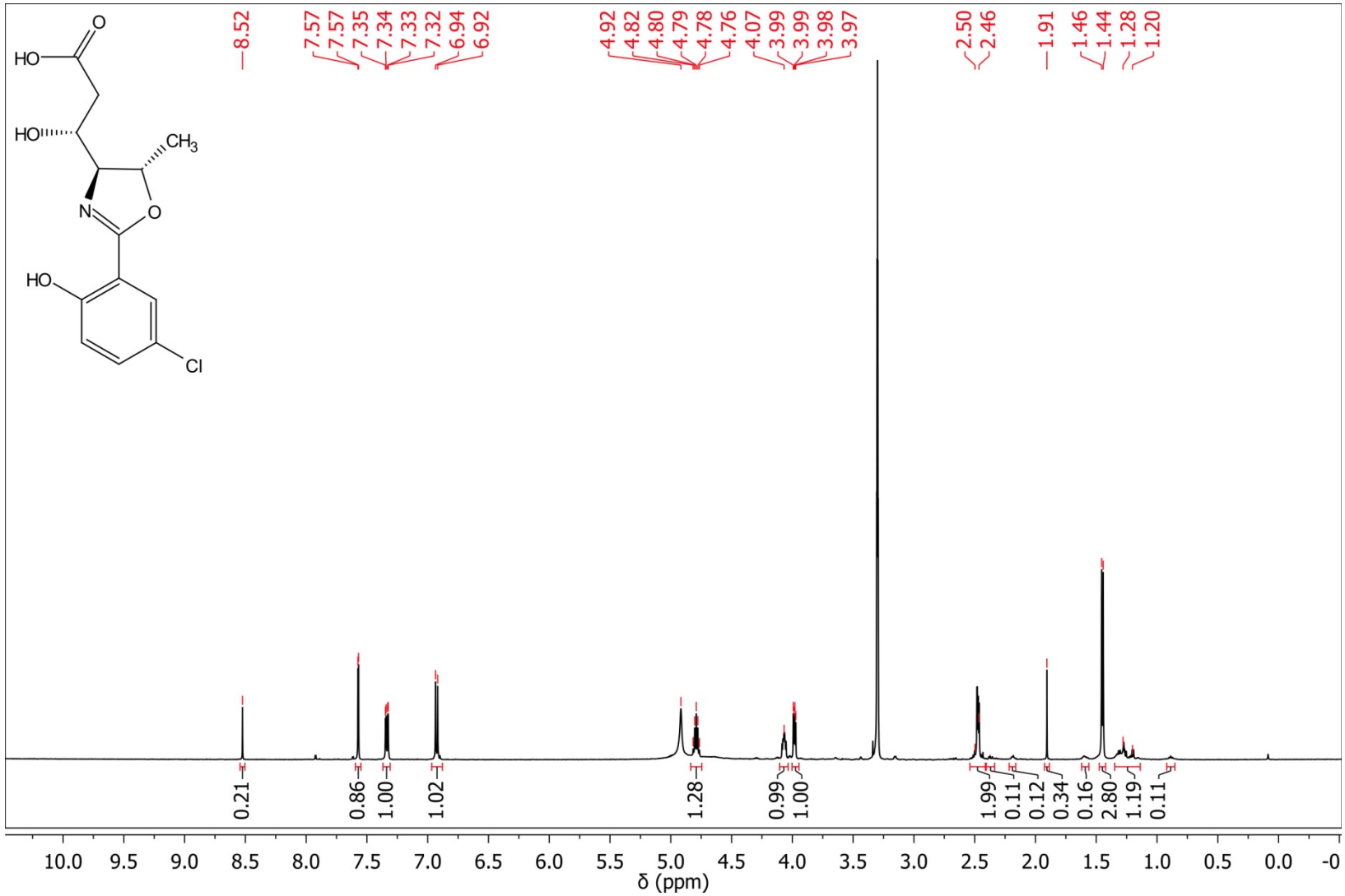


Figure S2. ^{1}H NMR Spectrum of Compound 1 in DMSO-d_6 (500 MHz)

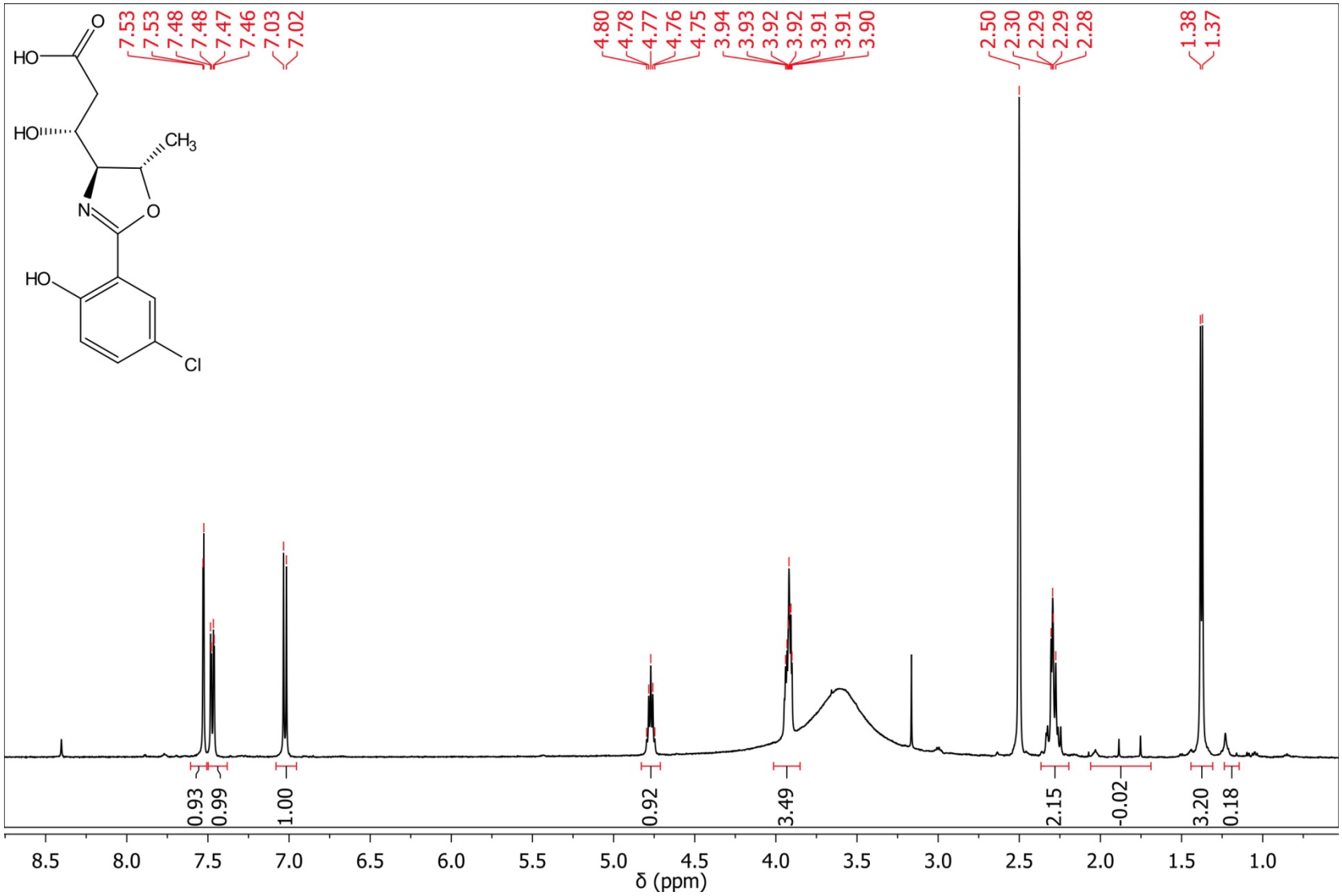


Figure S3. ^{13}C NMR Spectrum of Compound 1 in CD_3OD (125 MHz)

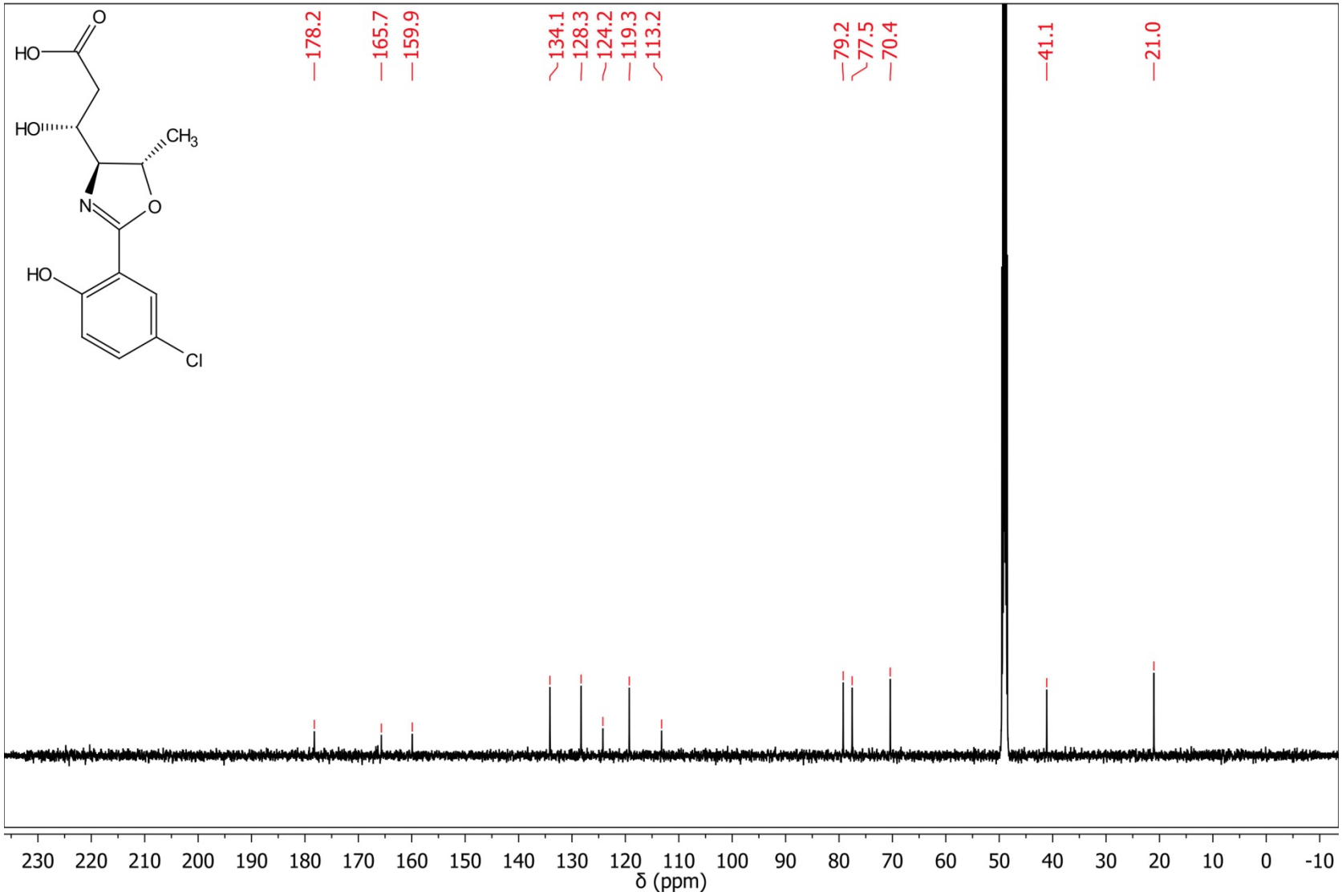


Figure S4. ^{13}C NMR Spectrum of Compound 1 in DMSO-d_6 (125 MHz)

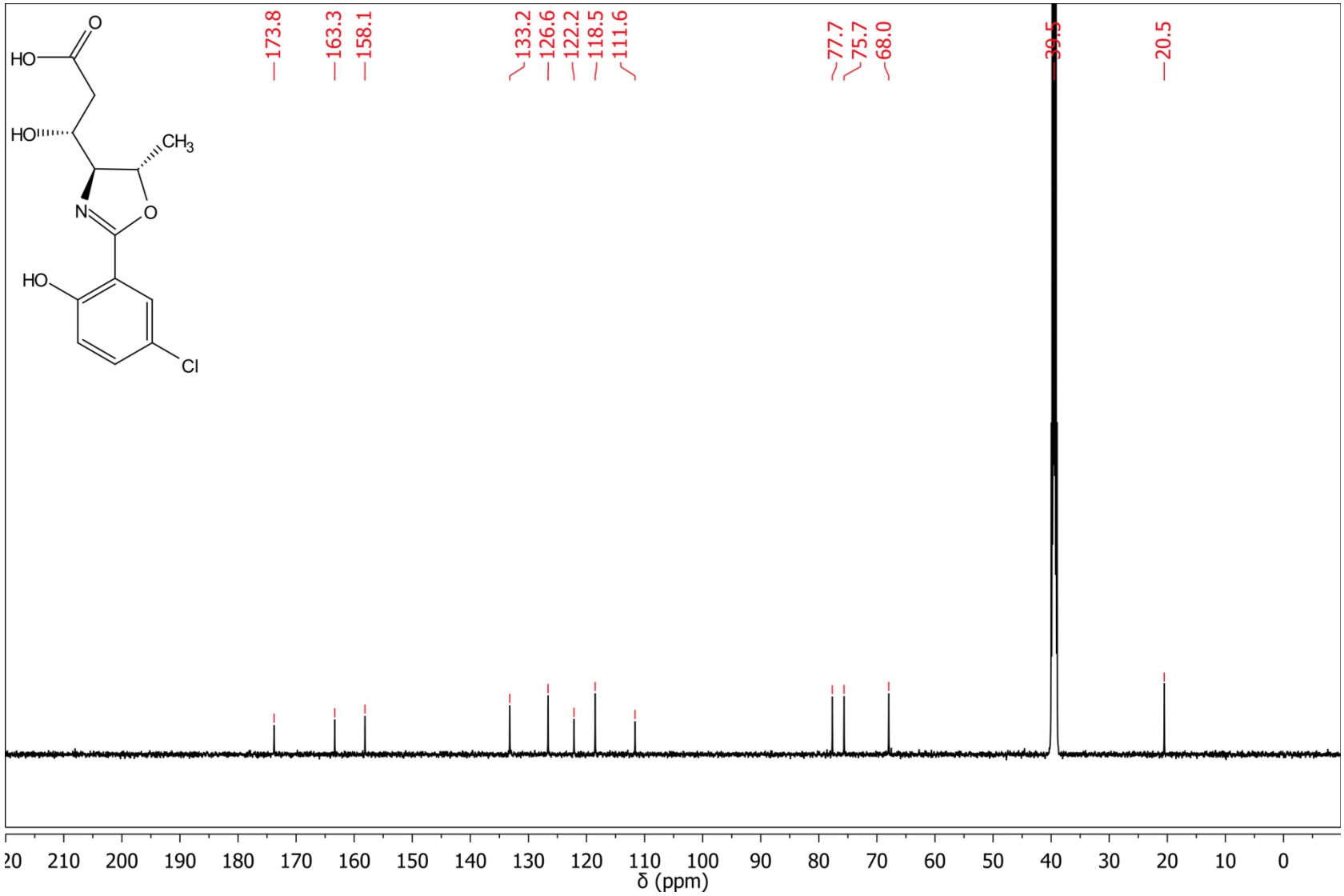


Figure S5. COSY Spectrum of Compound 1 in CD_3OD (500 MHz)

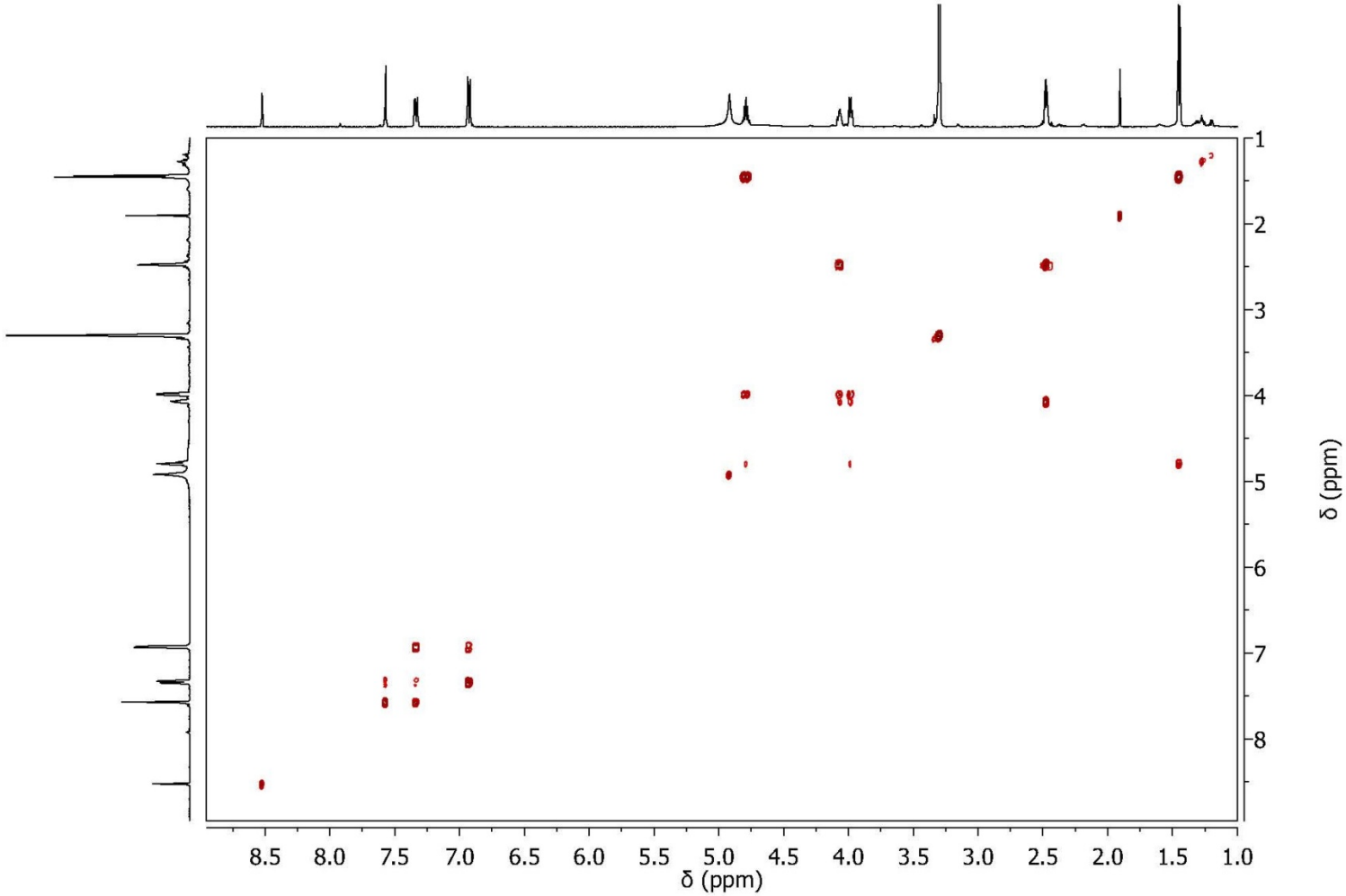


Figure S6. COSY Spectrum of Compound 1 in DMSO-d_6 (500 MHz)

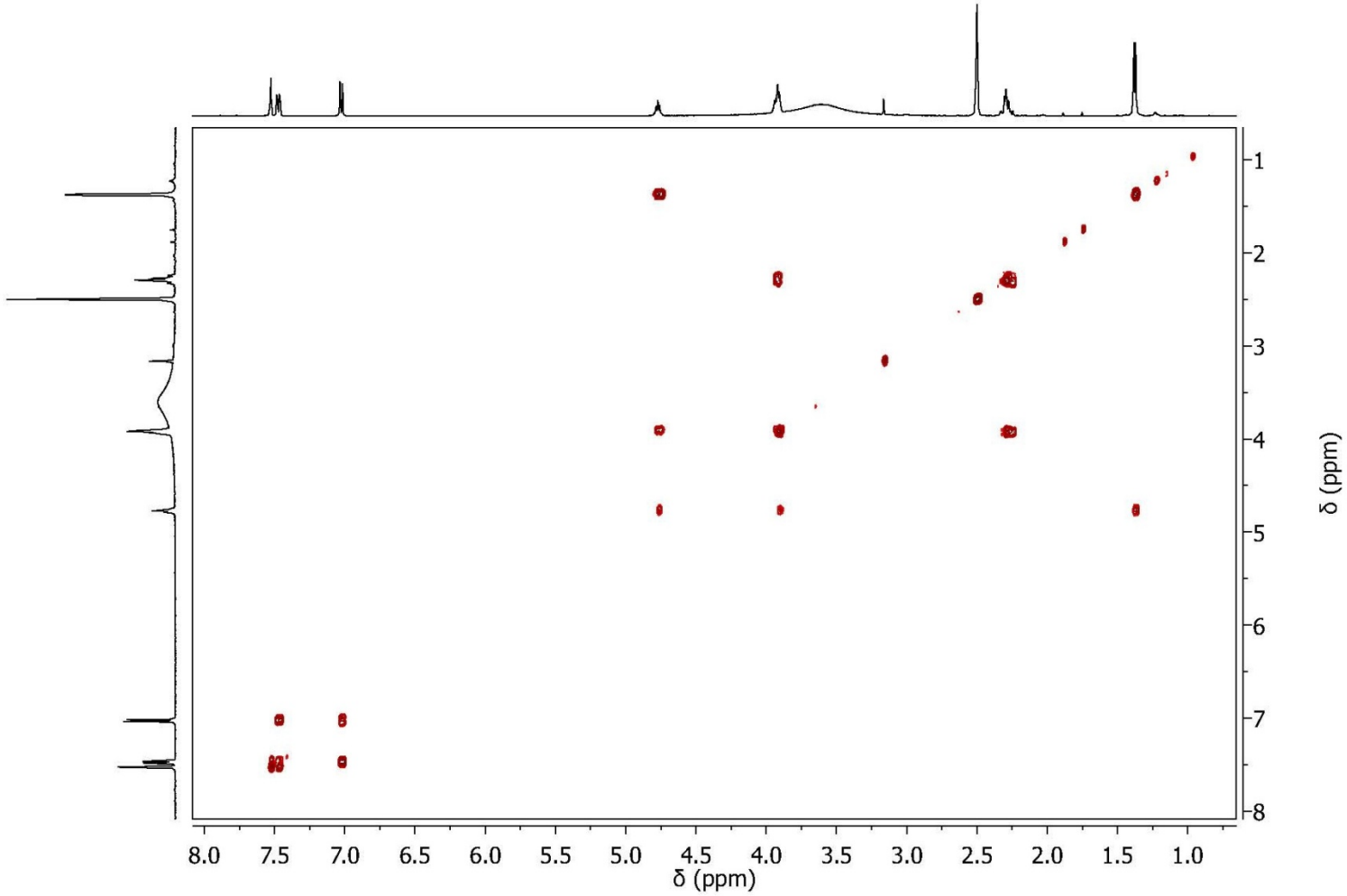


Figure S7. HSQC Spectrum of Compound 1 in CD_3OD (500 MHz)

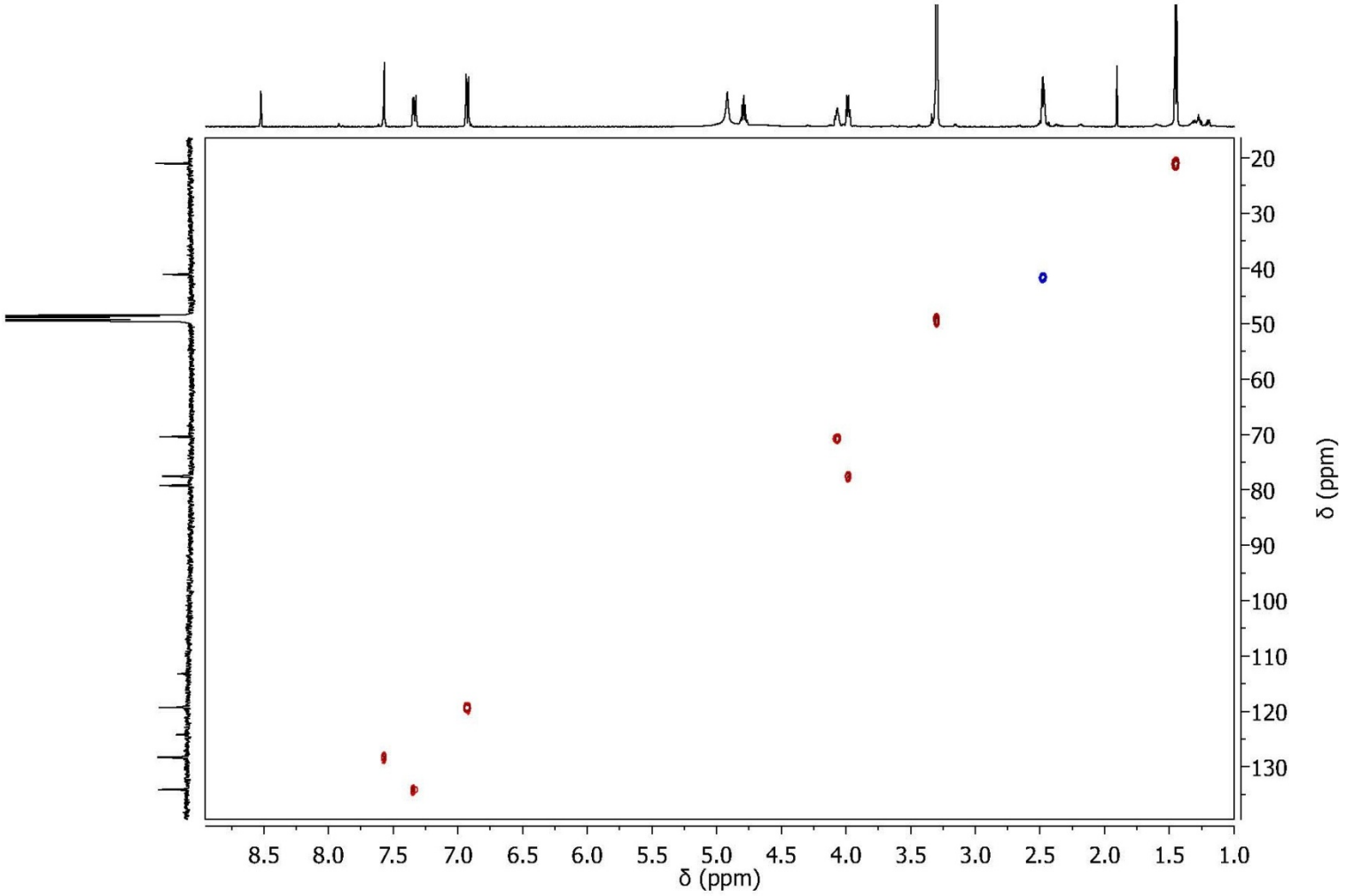


Figure S8. HSQC Spectrum of Compound 1 in DMSO-d_6 (500 MHz)

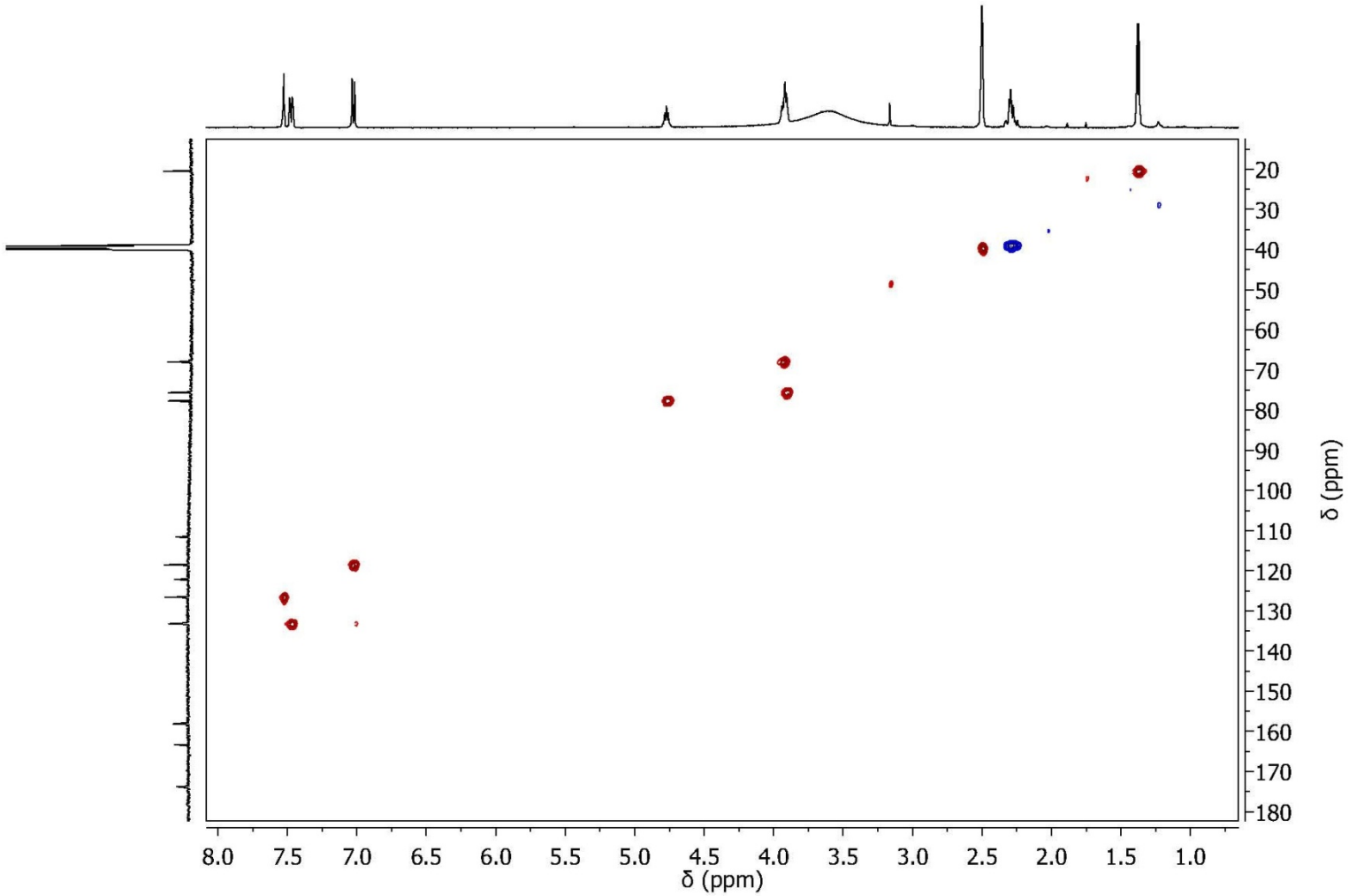


Figure S9. HMBC Spectrum of Compound 1 in CD_3OD (500 MHz)

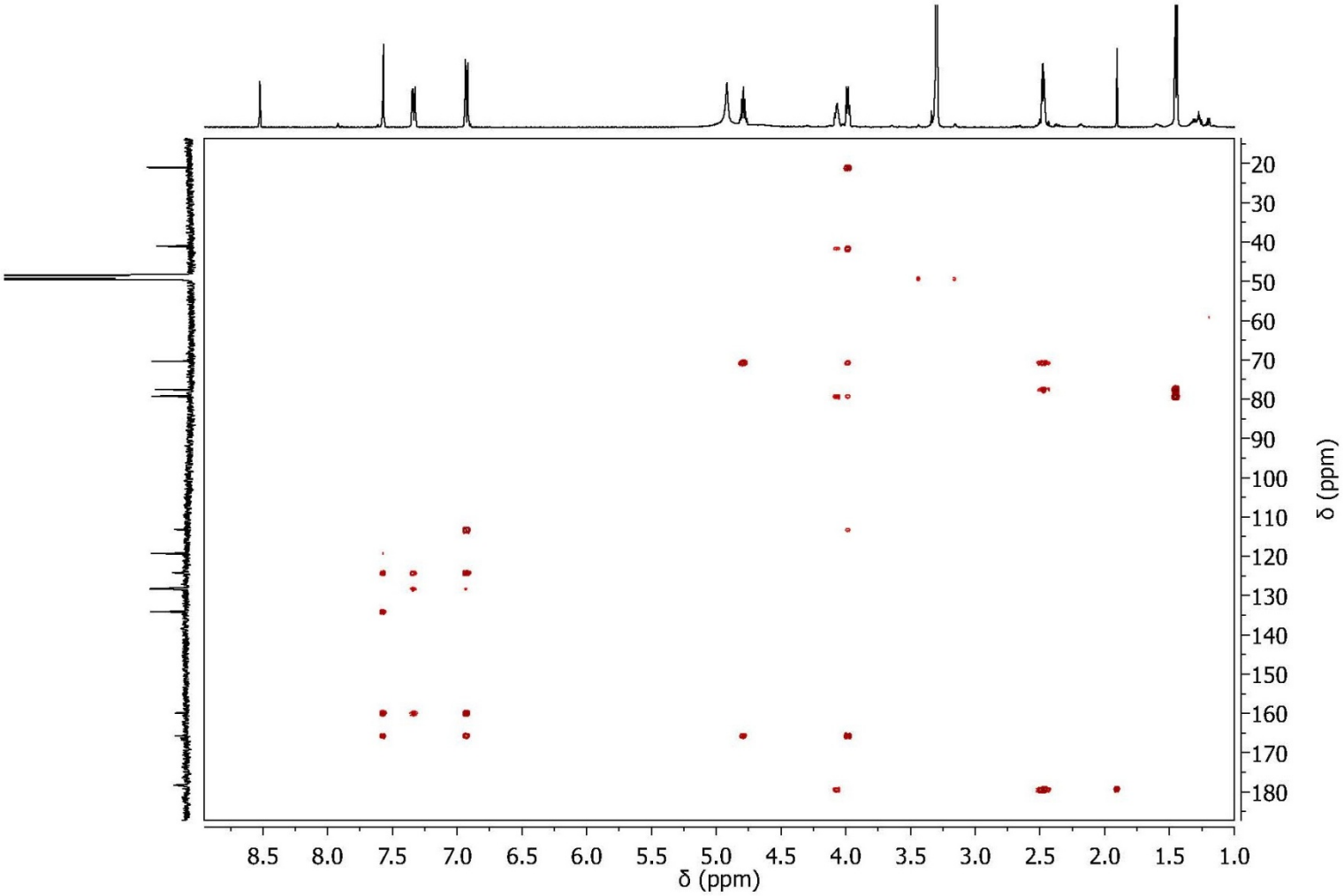


Figure S10. HMBC Spectrum of Compound 1 in DMSO-d_6 (500 MHz)

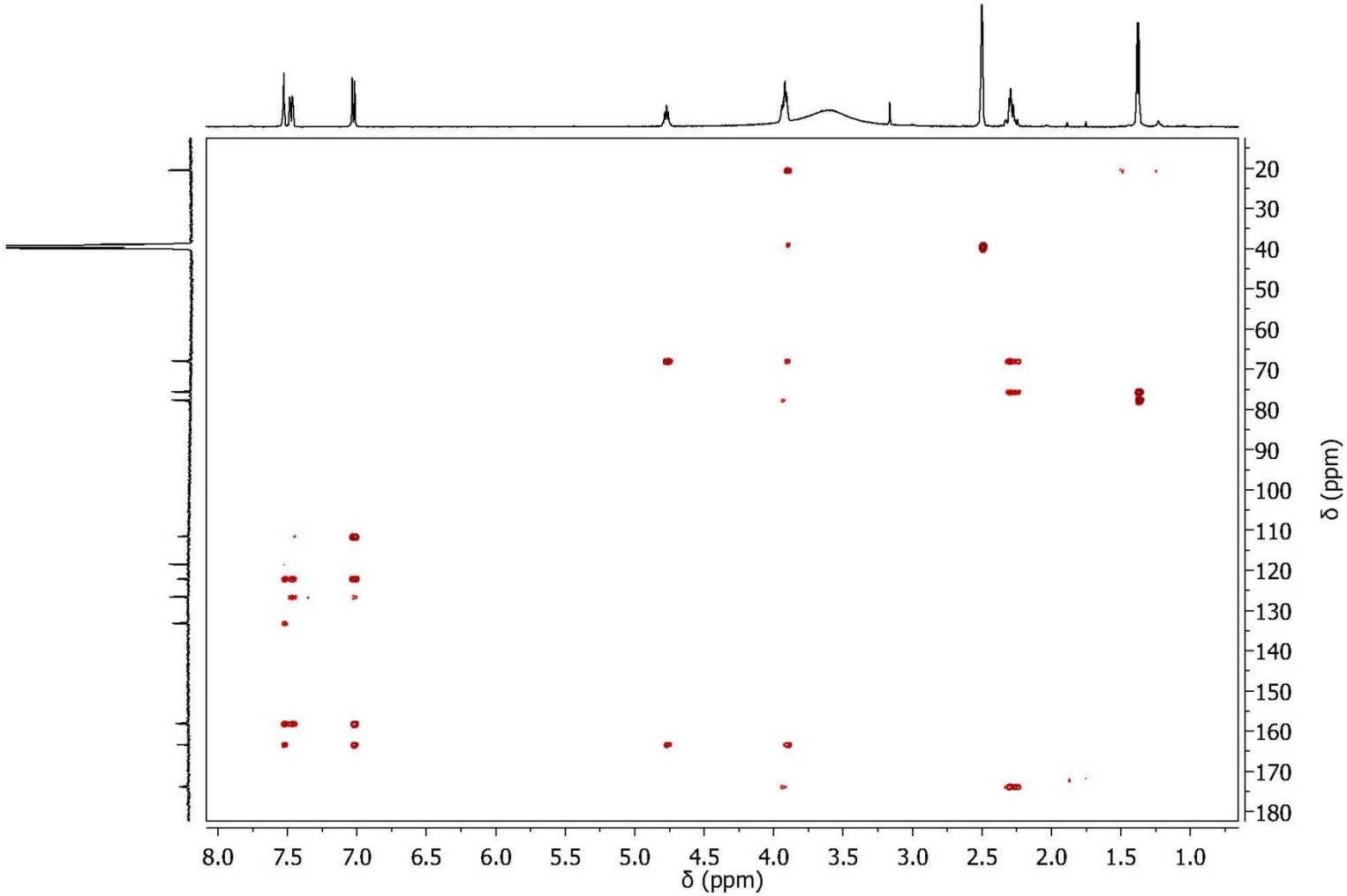


Figure S11. ^{15}N HMBC Spectrum of Compound 1 in DMSO-d_6 (500 MHz)

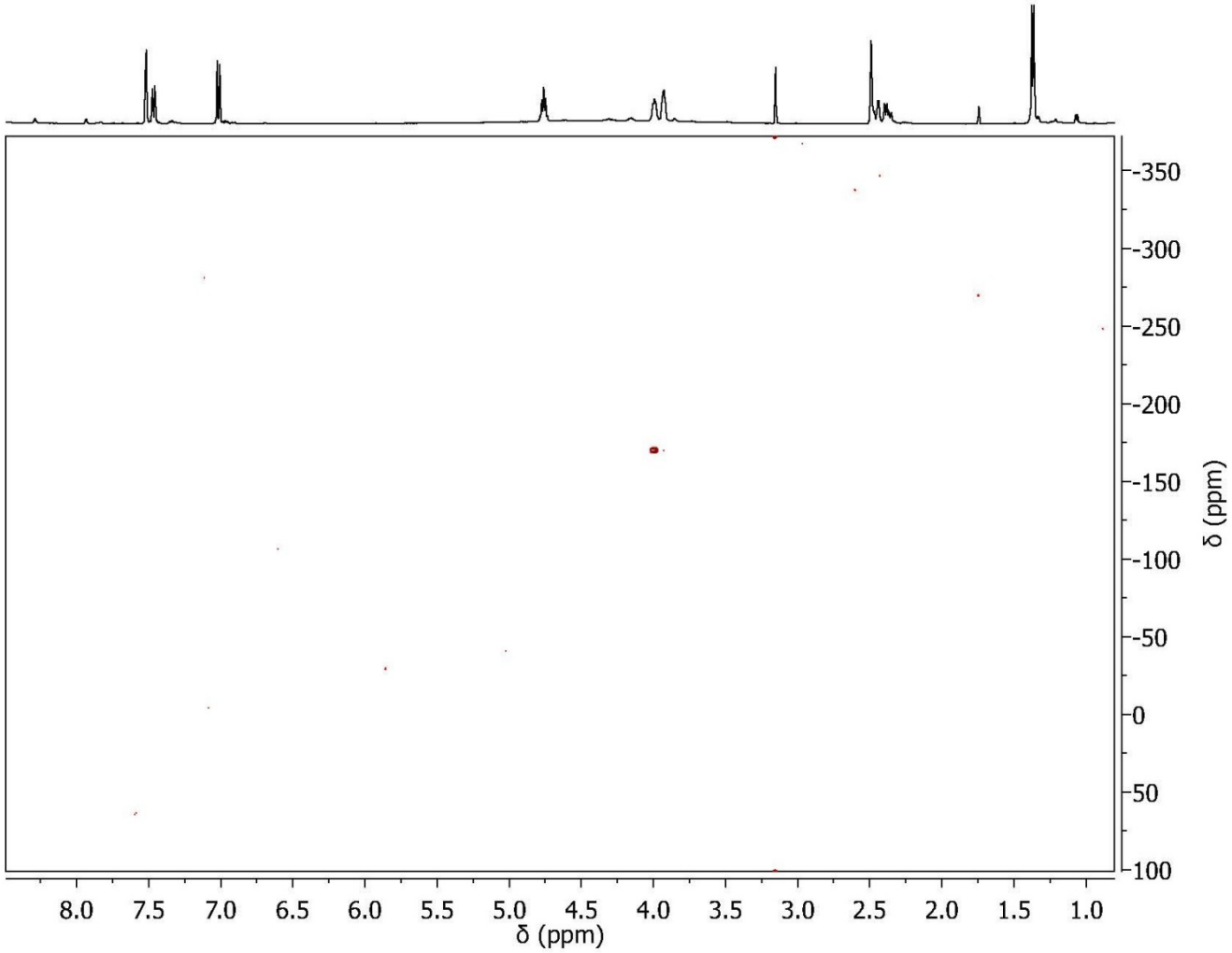


Figure S12. CIGAR Spectrum of Compound 1 in CD_3OD (500 MHz)

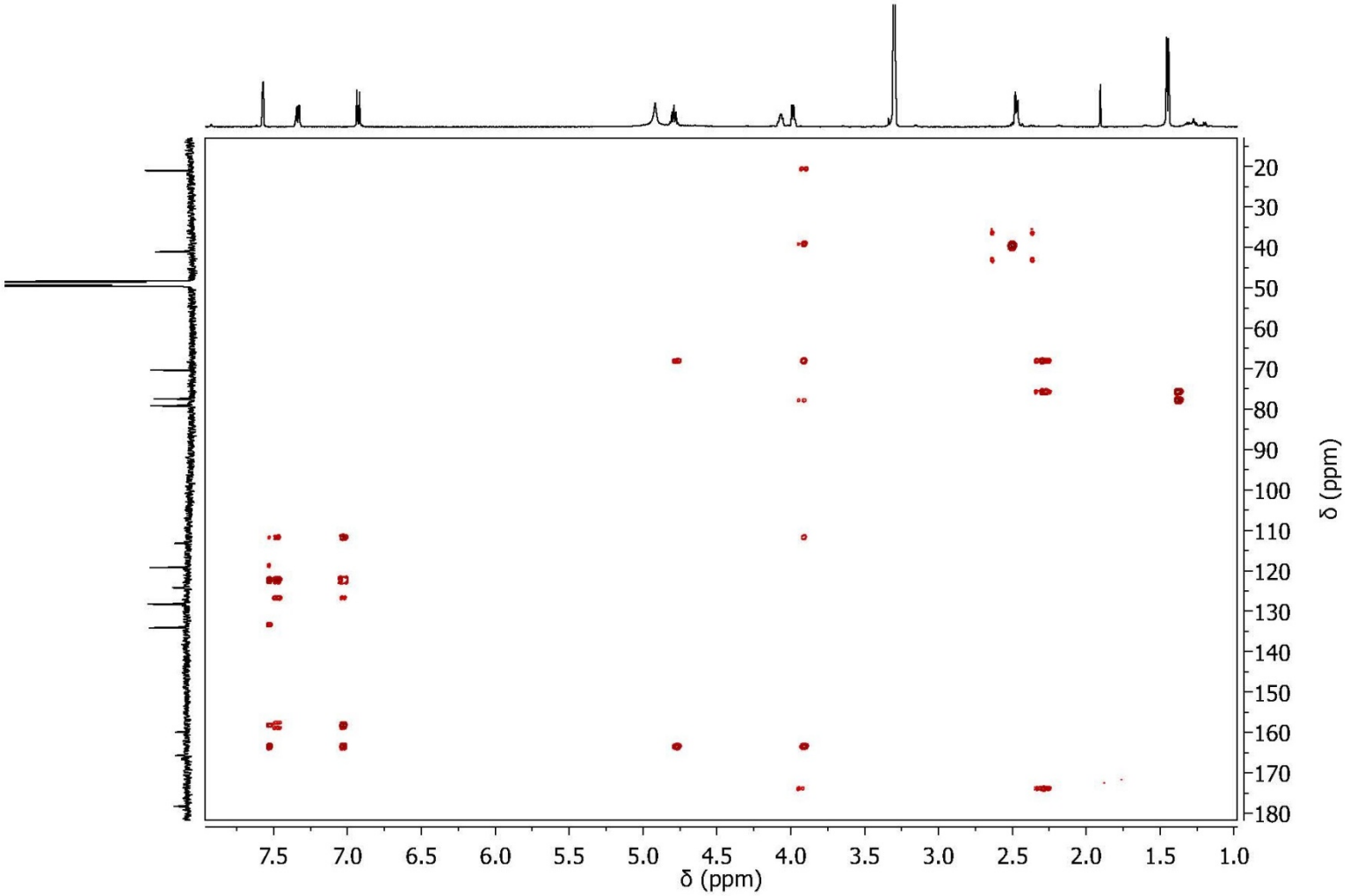


Figure S13. IR Spectrum of Compound 1 (CaF_2 disc)

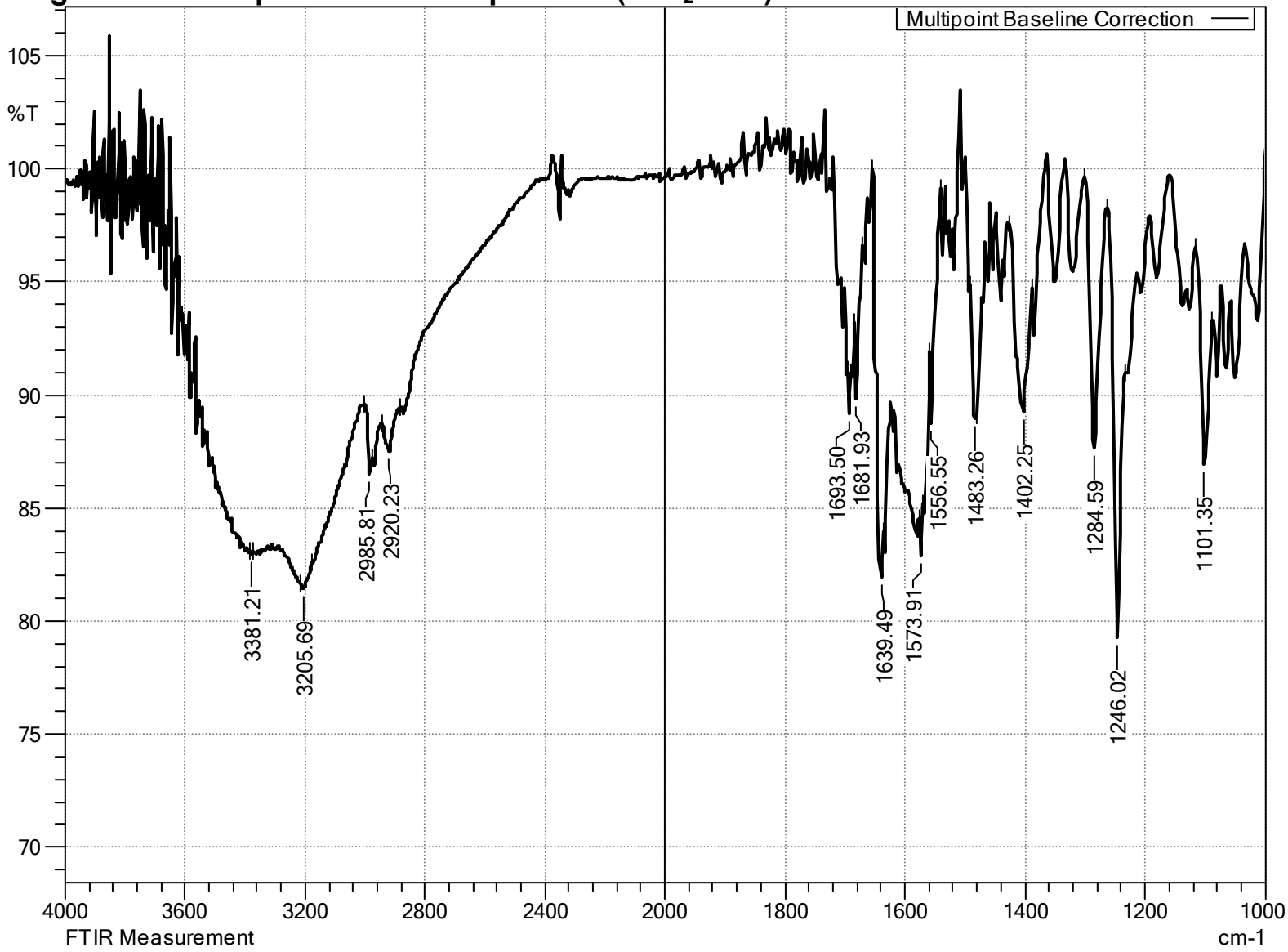
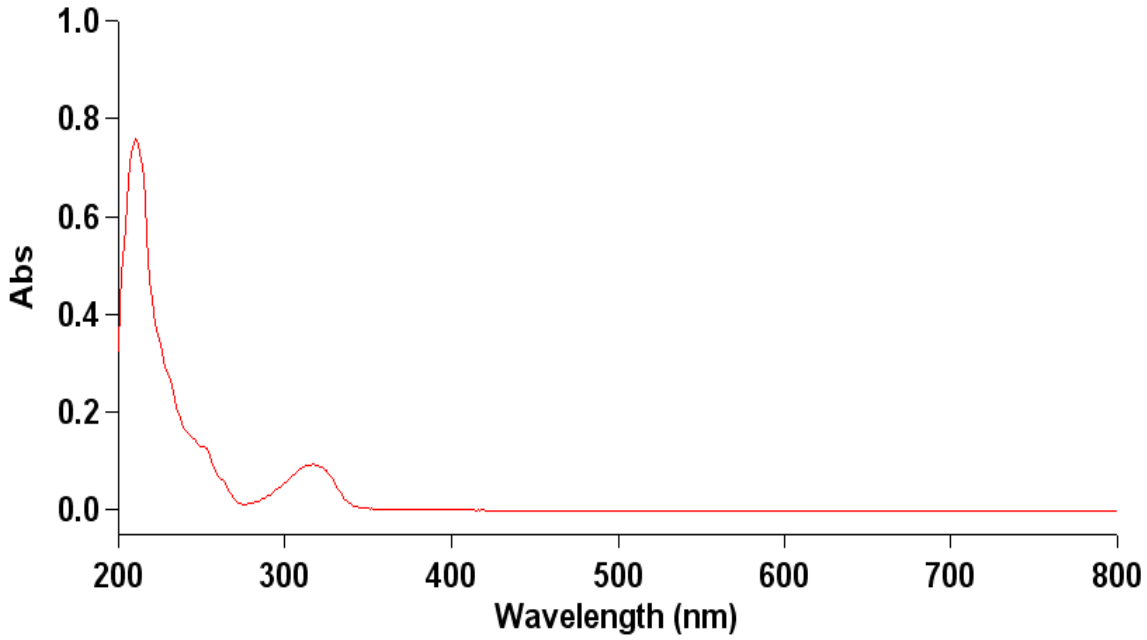


Figure S14. UV-Vis Spectrum of Compound 1 in CH_3OH



Range 799.9nm to 199.9nm

Conc: 10 µg/mL, which equals 3.337 x 10^{-5} mol/L
MW: 299.71 g/mol

ε = A / (c. l), where c is in mol/L and l is in cm

Wavelength (nm)	Abs	molar absorptivity (ε)	log ε
317.0	0.093	2787	3.45
210.0	0.758	22718	4.36
251.1	0.128	3836	3.58
263.0	0.059	1768	3.25

Figure S15. ^{1}H NMR Spectrum of Compound 2 in CD_3OD (500 MHz)

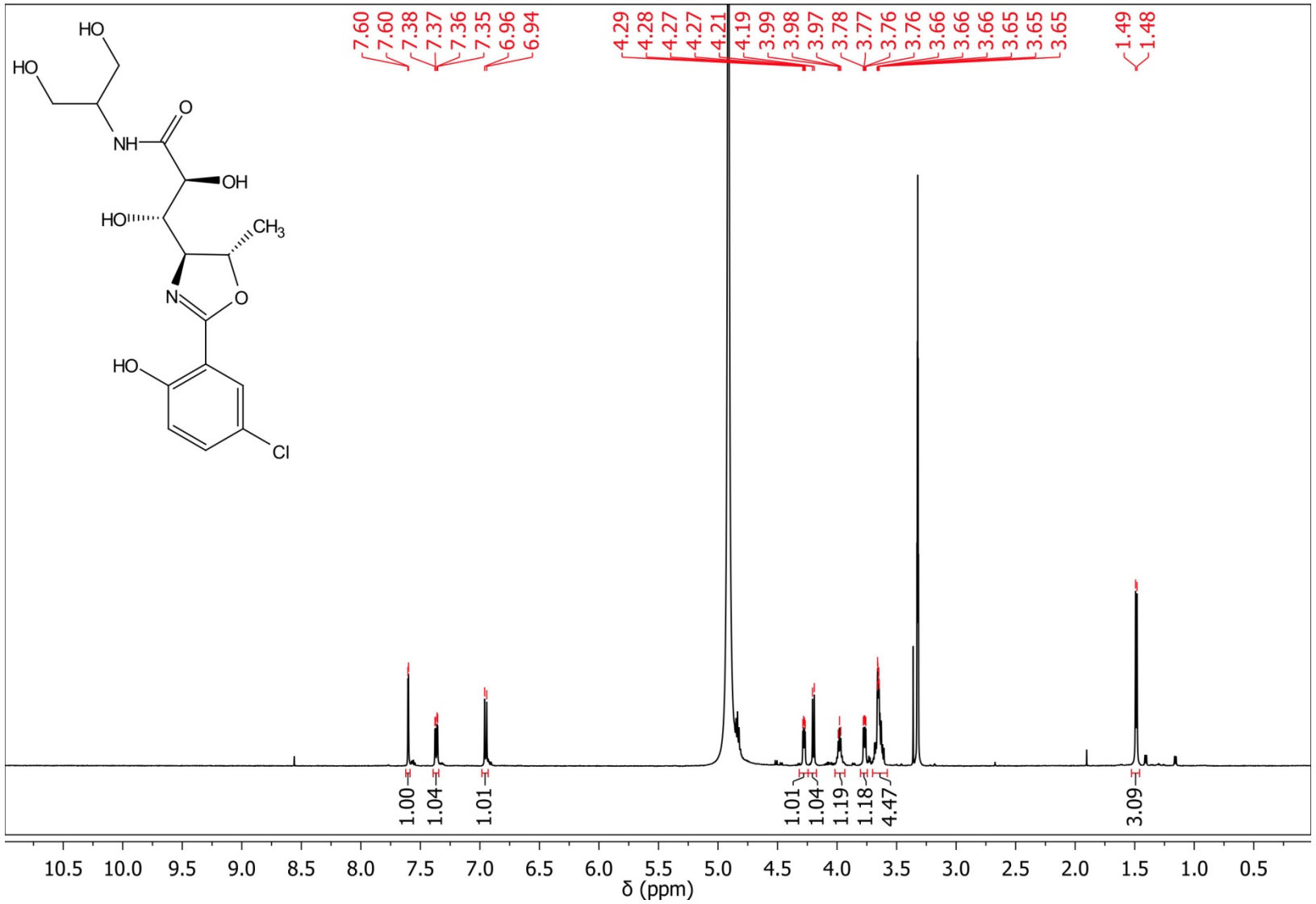


Figure S16. ^{13}C NMR Spectrum of Compound 2 in CD_3OD (125 MHz)

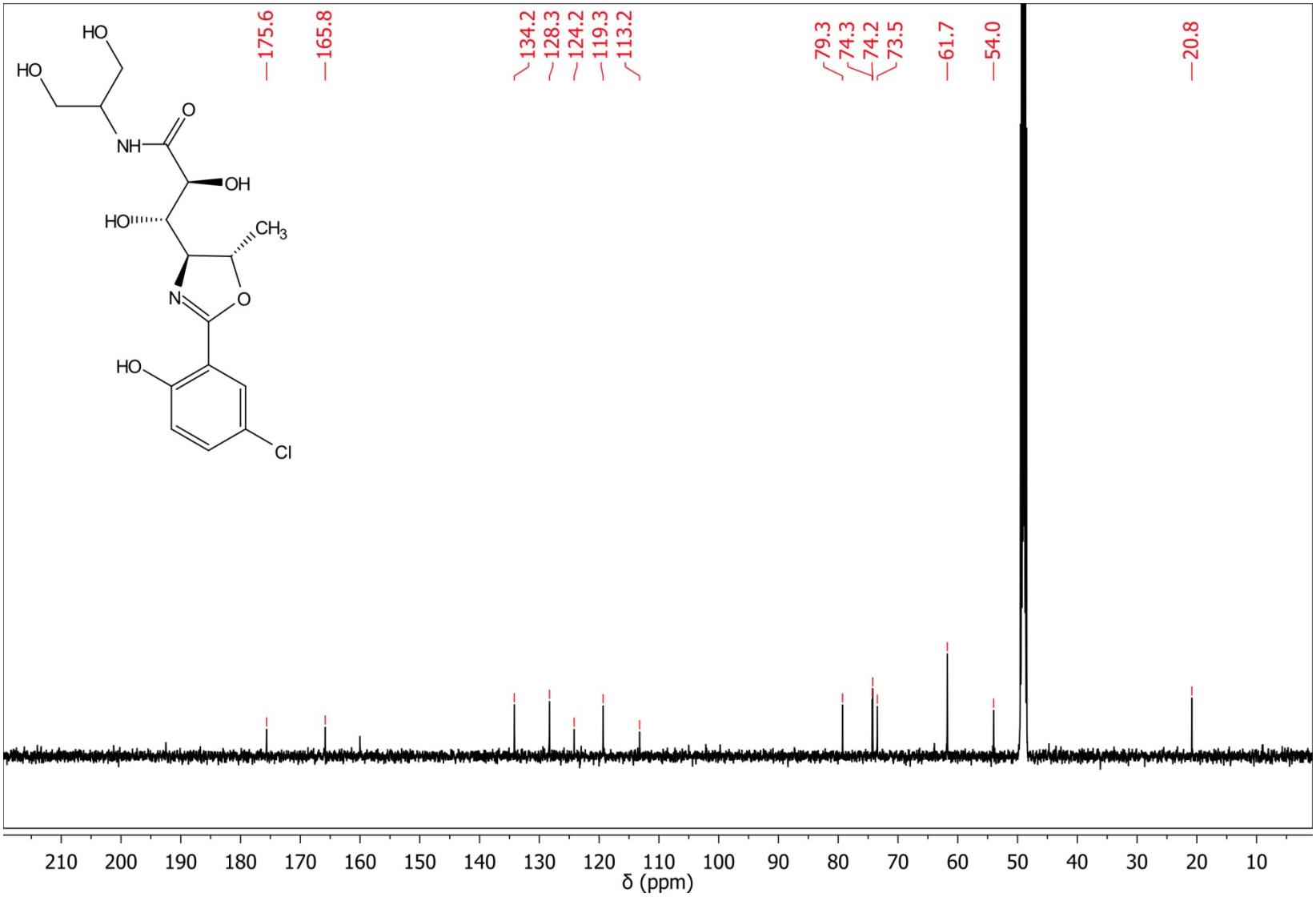


Figure S17. COSY Spectrum of Compound 2 in CD_3OD (500 MHz)

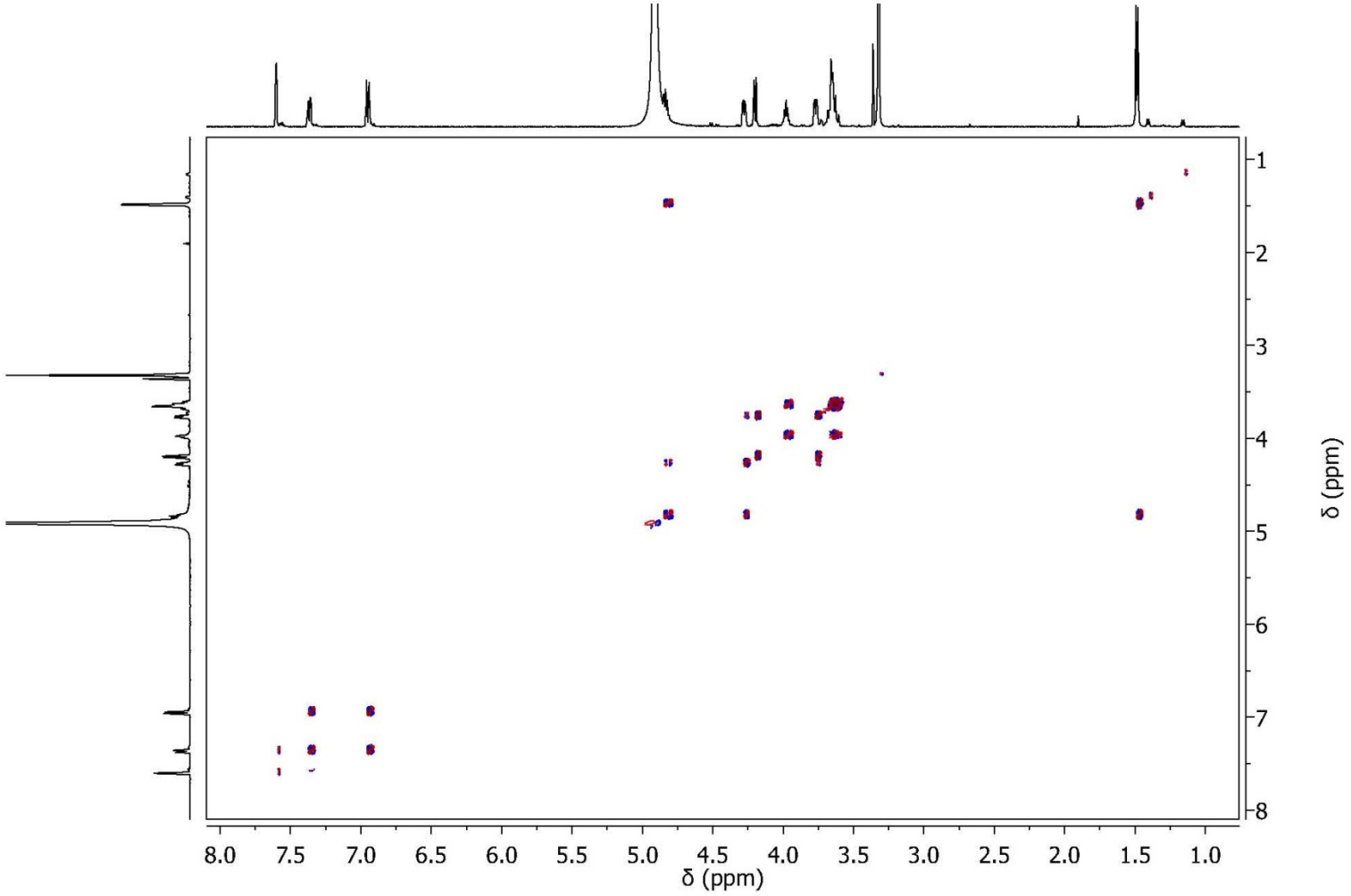


Figure S18. HSQC Spectrum of Compound 2 in CD_3OD (500 MHz)

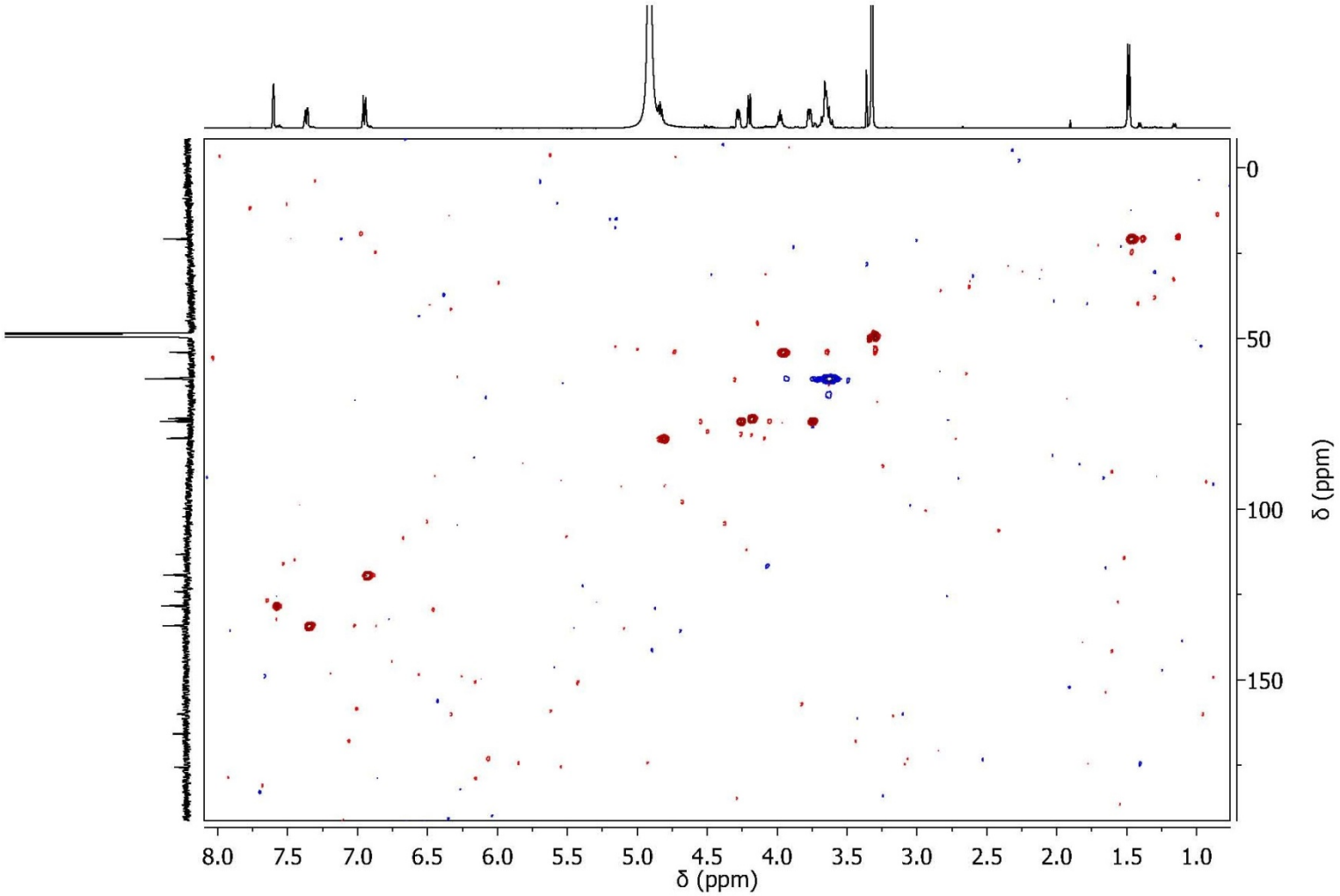


Figure S19. HMBC Spectrum of Compound 2 in CD_3OD (500 MHz)

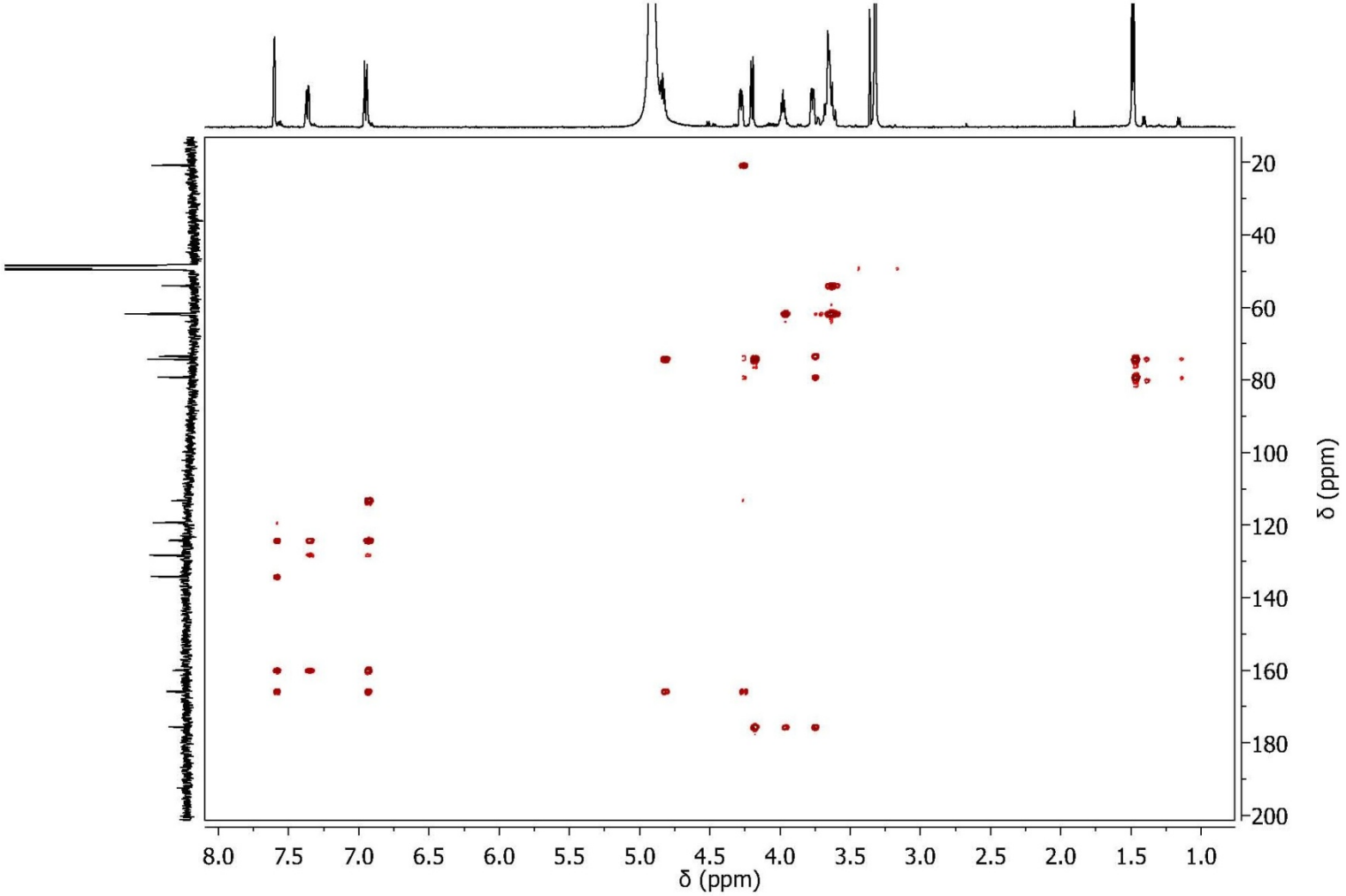


Figure S20. ^{15}N HMBC Spectrum of Compound 2 in CD_3OD (500 MHz)

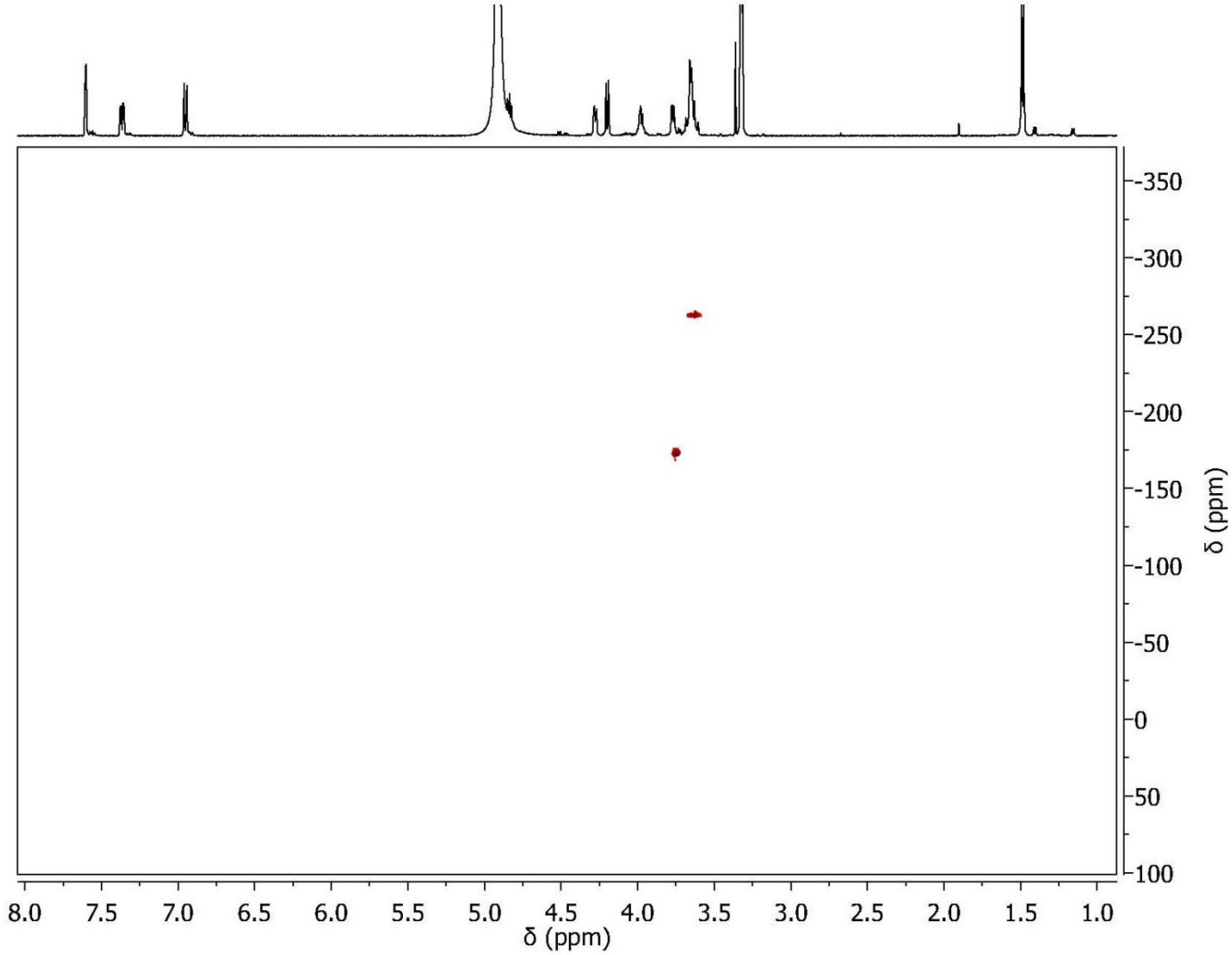


Figure S21. ROESY Spectrum of Compound 2 in CD_3OD (500 MHz)

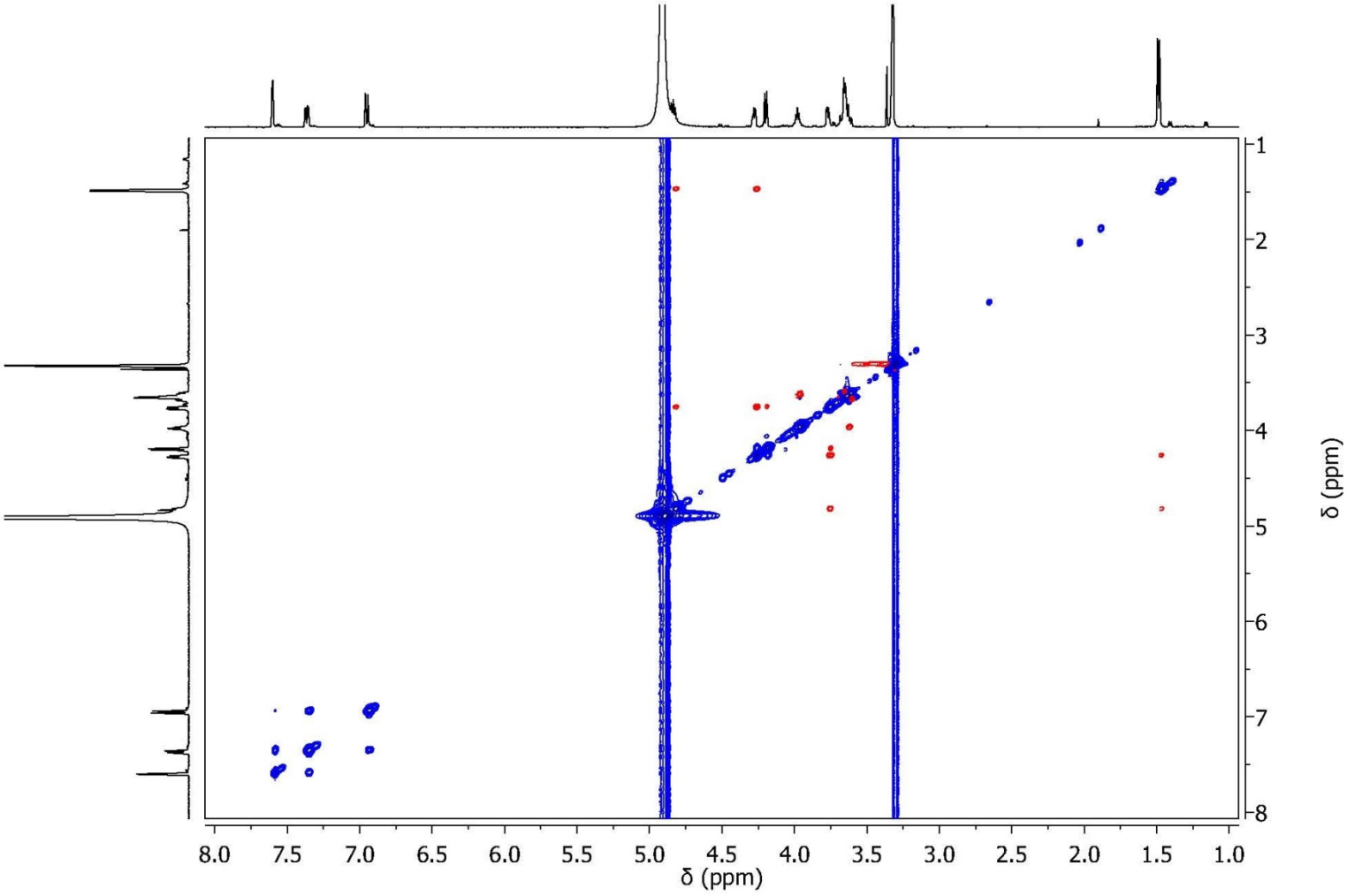


Figure S22. IR Spectrum of Compound 2 (CaF_2 disc)

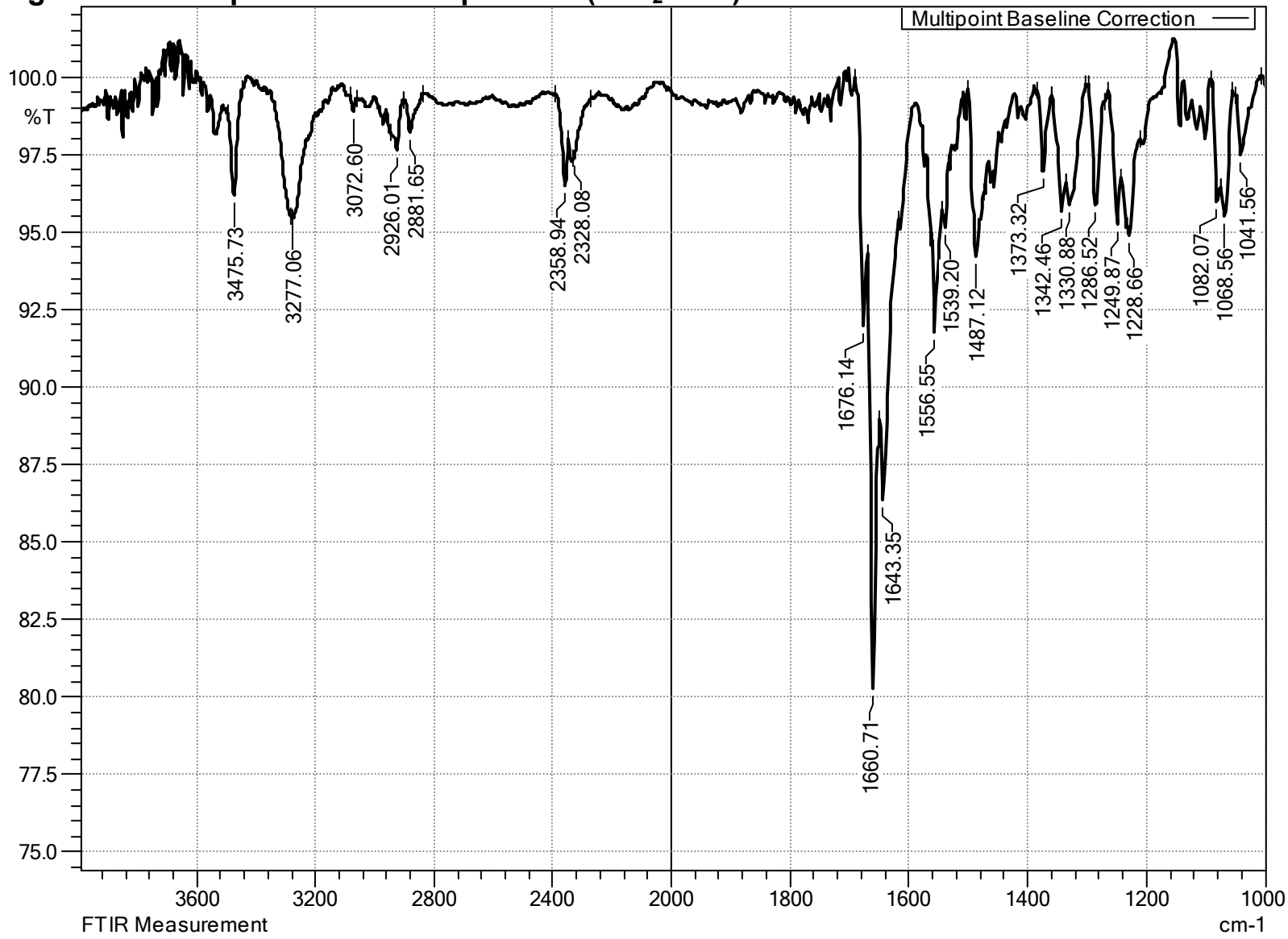
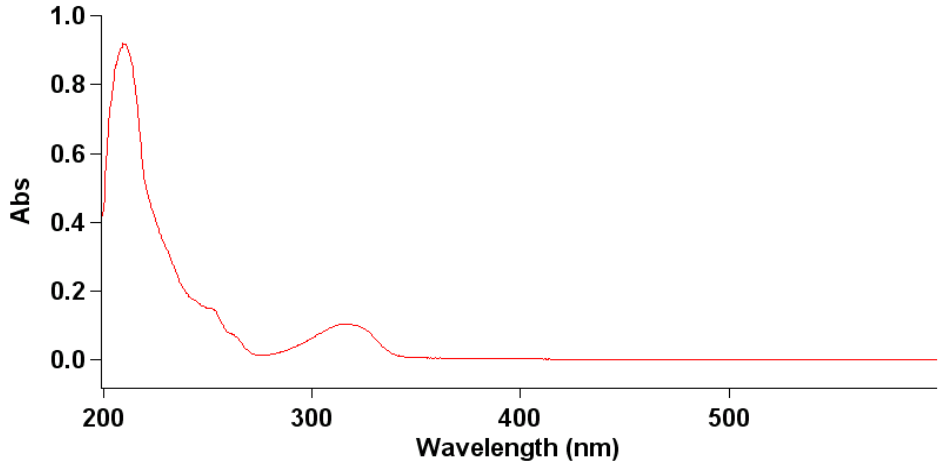


Figure S23. UV-Vis Spectrum of Compound 2 in CH_3OH



Peak Threshold 0.0100
Range 799.9nm to 199.9nm

Conc: 10 µg/mL, which equals 2.572 x 10^{-5} mol/L
MW: 388.80 g/mol

Pathlength = 1 cm

ε = A / (c.l), where c is in mol/L and l is in cm

Wavelength (nm)	Abs	molar absorptivity (ε)	log ε
314.9	0.103	4005	3.60
209.5	0.921	35808	4.55
251.0	0.150	5832	3.77
261.5	0.075	2916	3.46

Figure S24. ^{1}H NMR Spectrum of Compound 3 in CD_3OD (500 MHz)

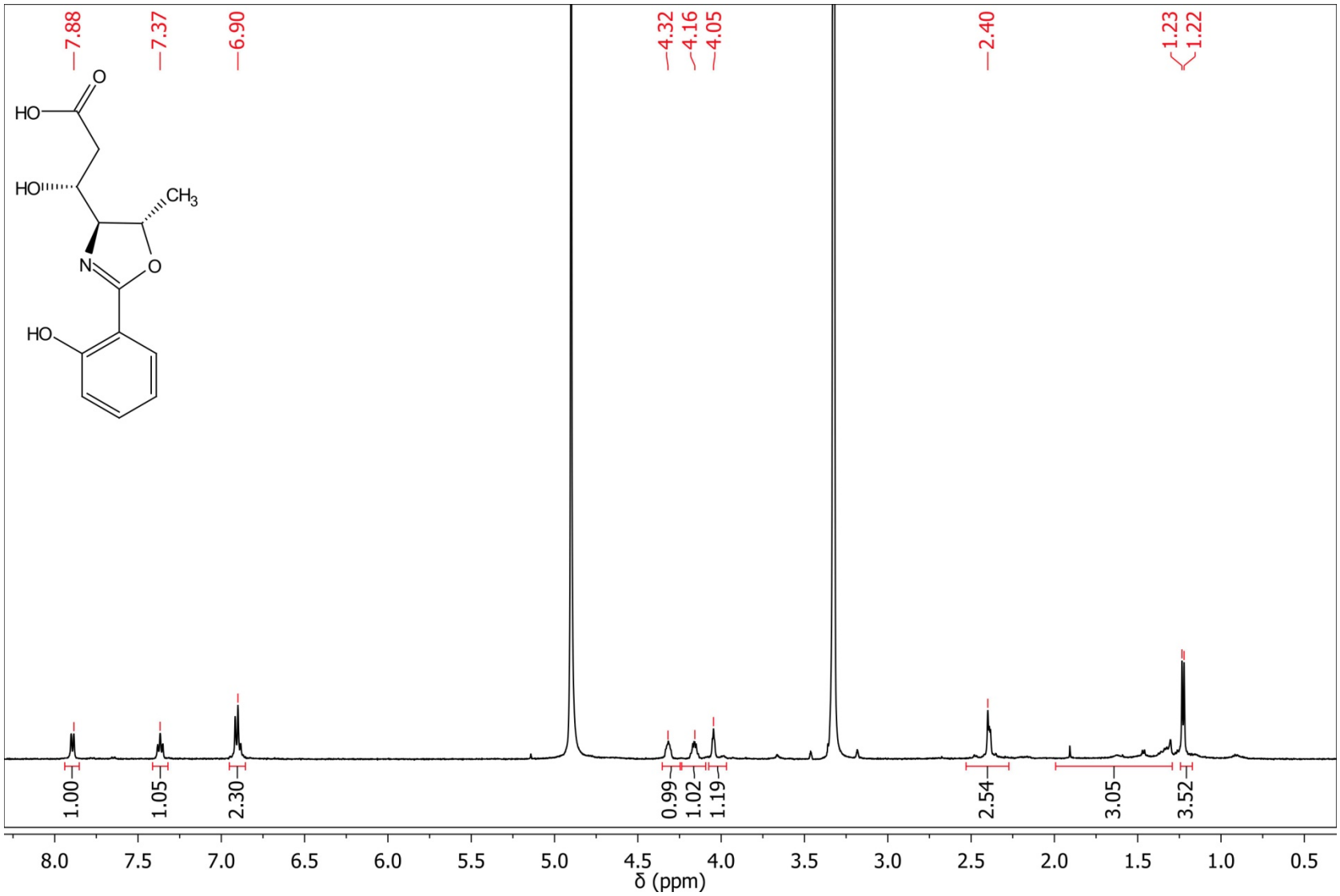


Figure S25. ^{1}H NMR Spectrum of Compound 4 in CD_3OD (500 MHz)

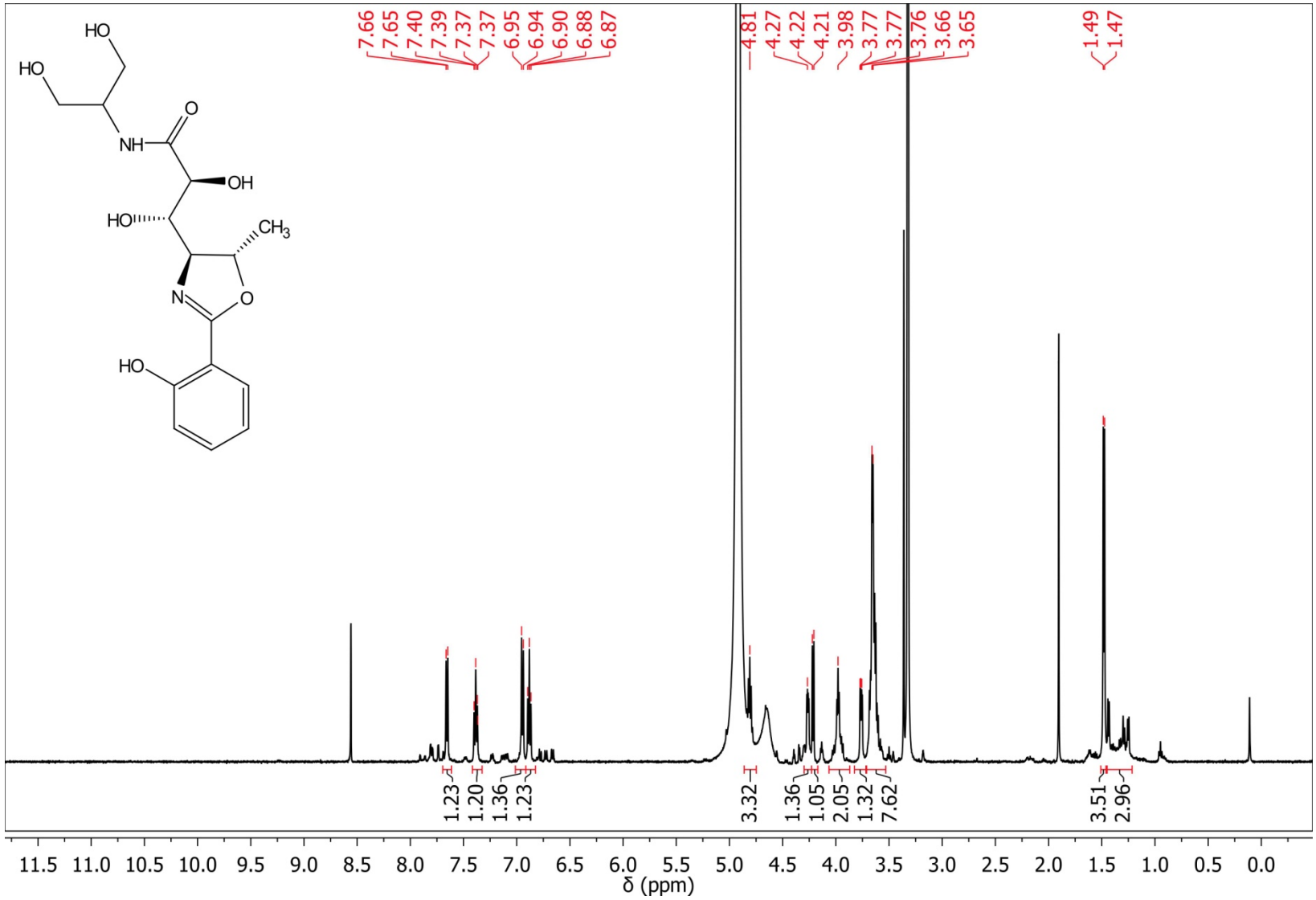


Figure S26. ^{1}H NMR Spectrum of Compound 5 in CD_3OD (500 MHz)

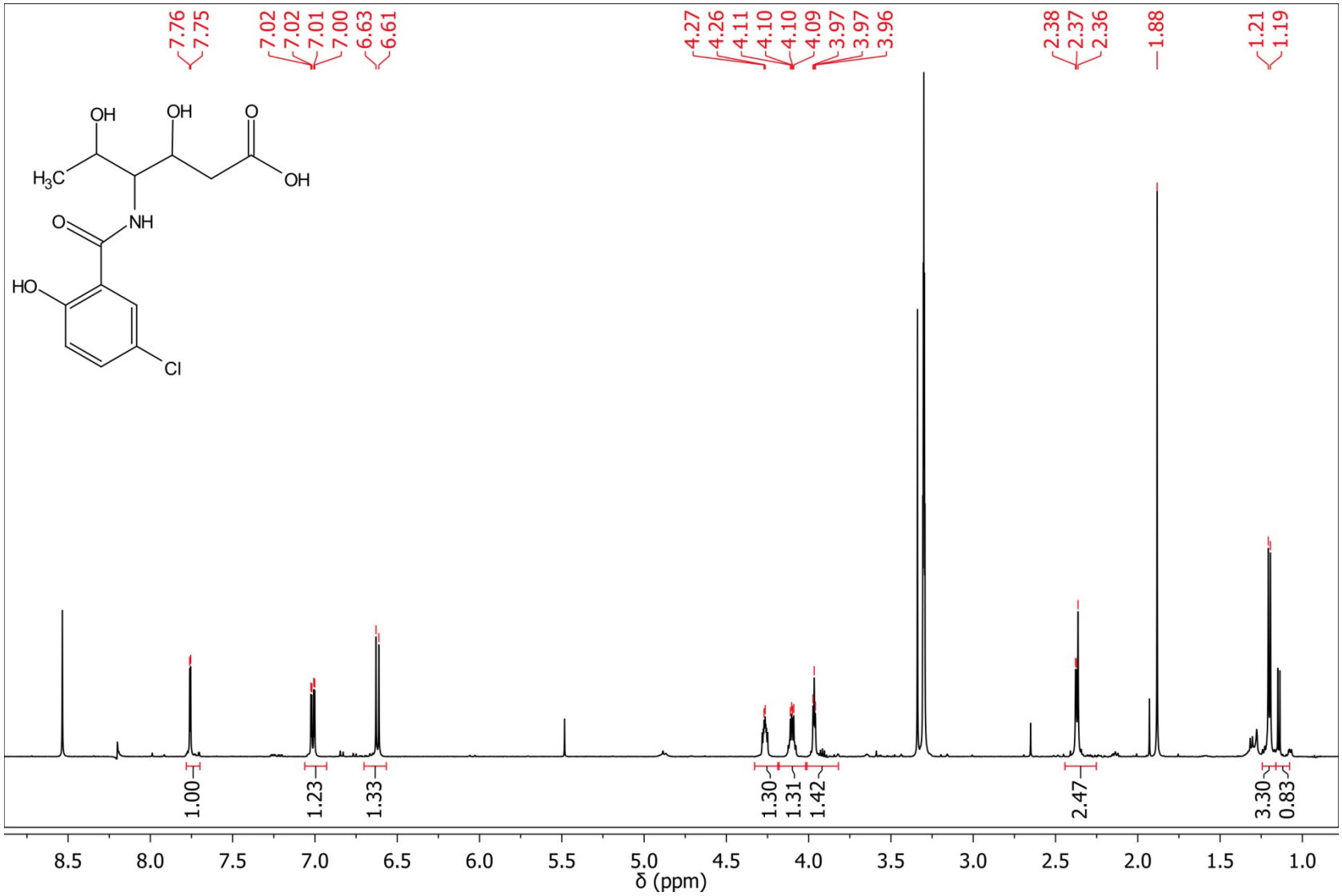


Figure S27. ^{13}C NMR Spectrum of Compound 5 in CD_3OD (125 MHz)

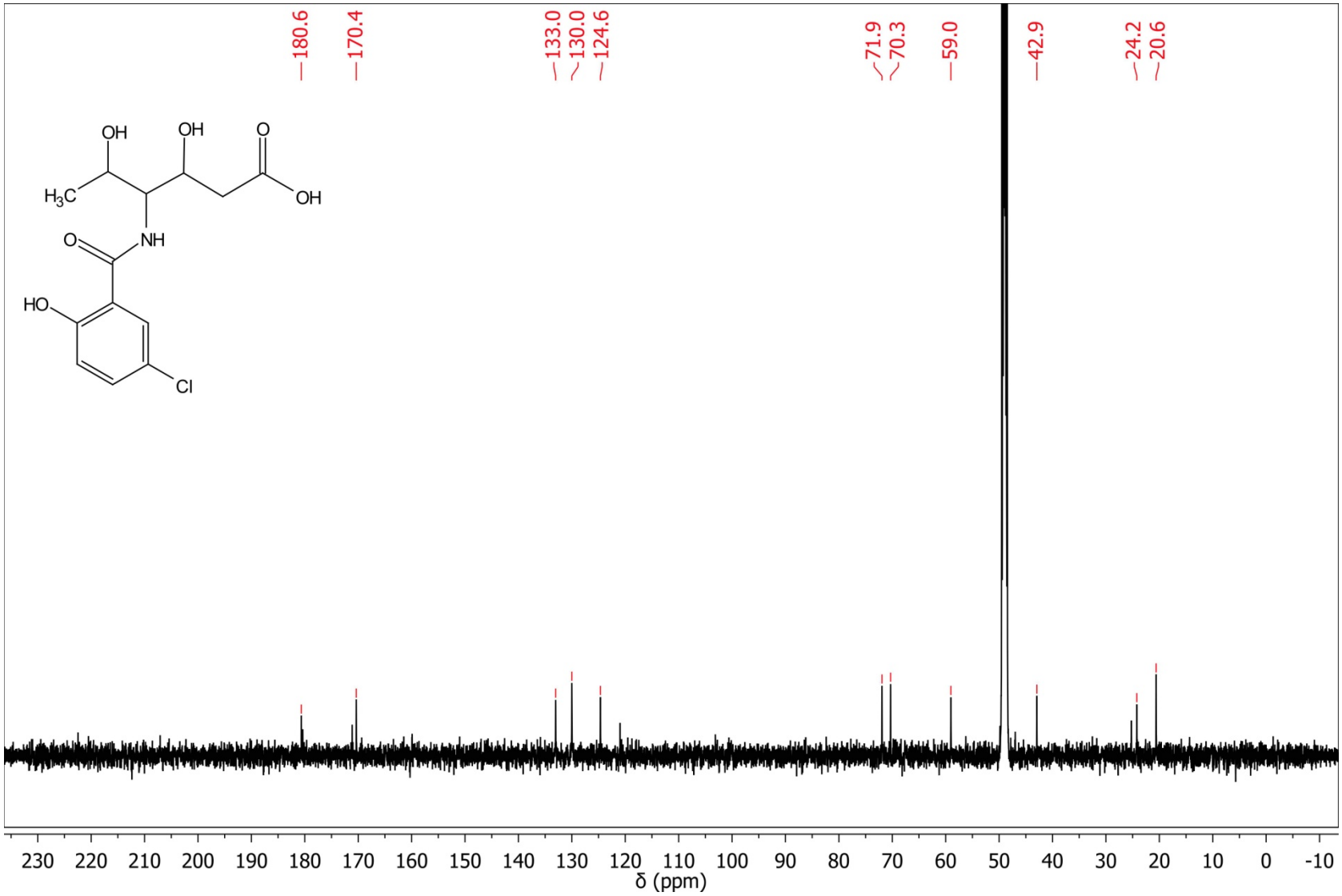


Figure S28. COSY Spectrum of Compound 5 in CD_3OD (500 MHz)

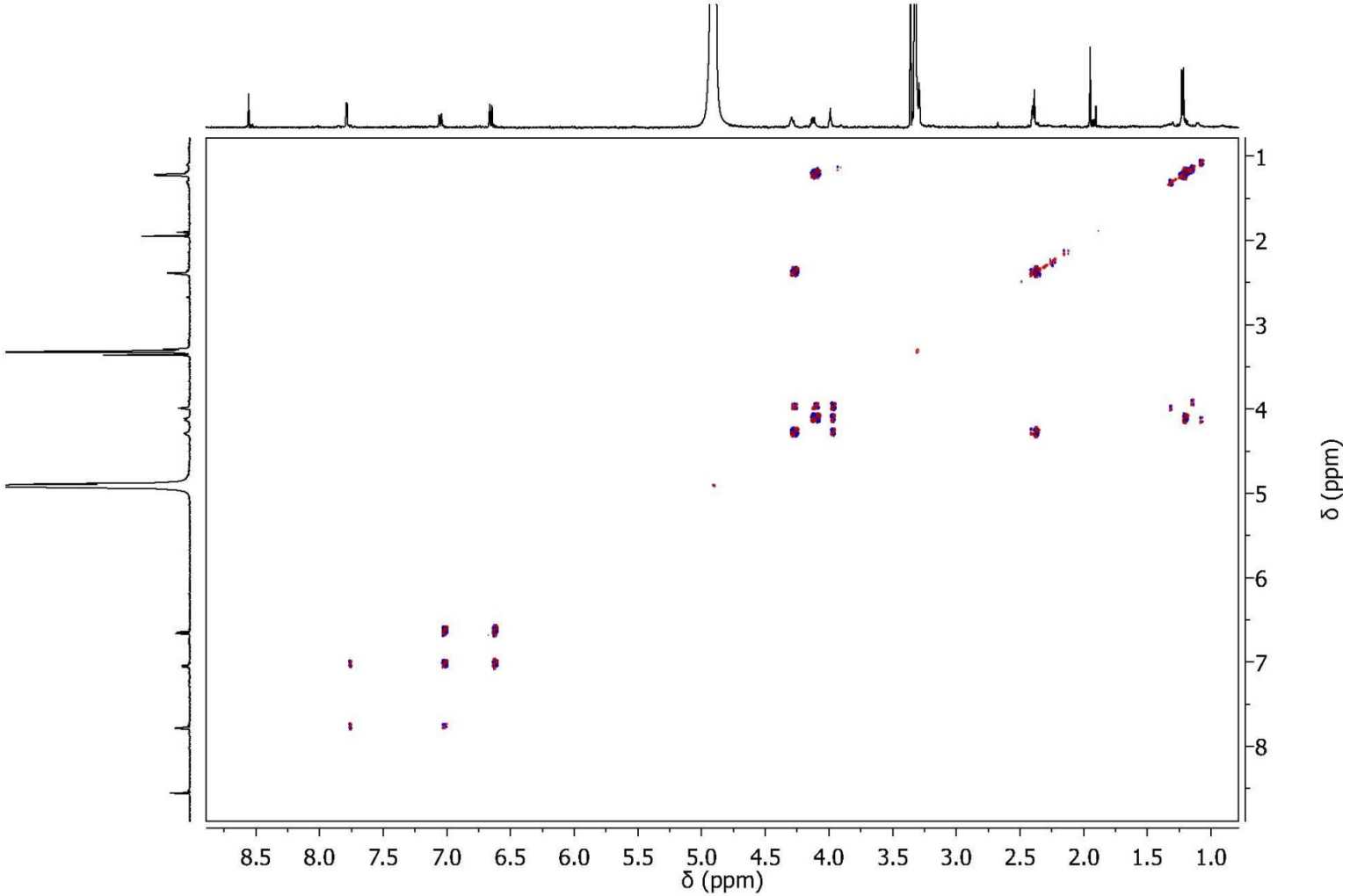


Figure S29. HSQC Spectrum of Compound 5 in CD_3OD (500 MHz)

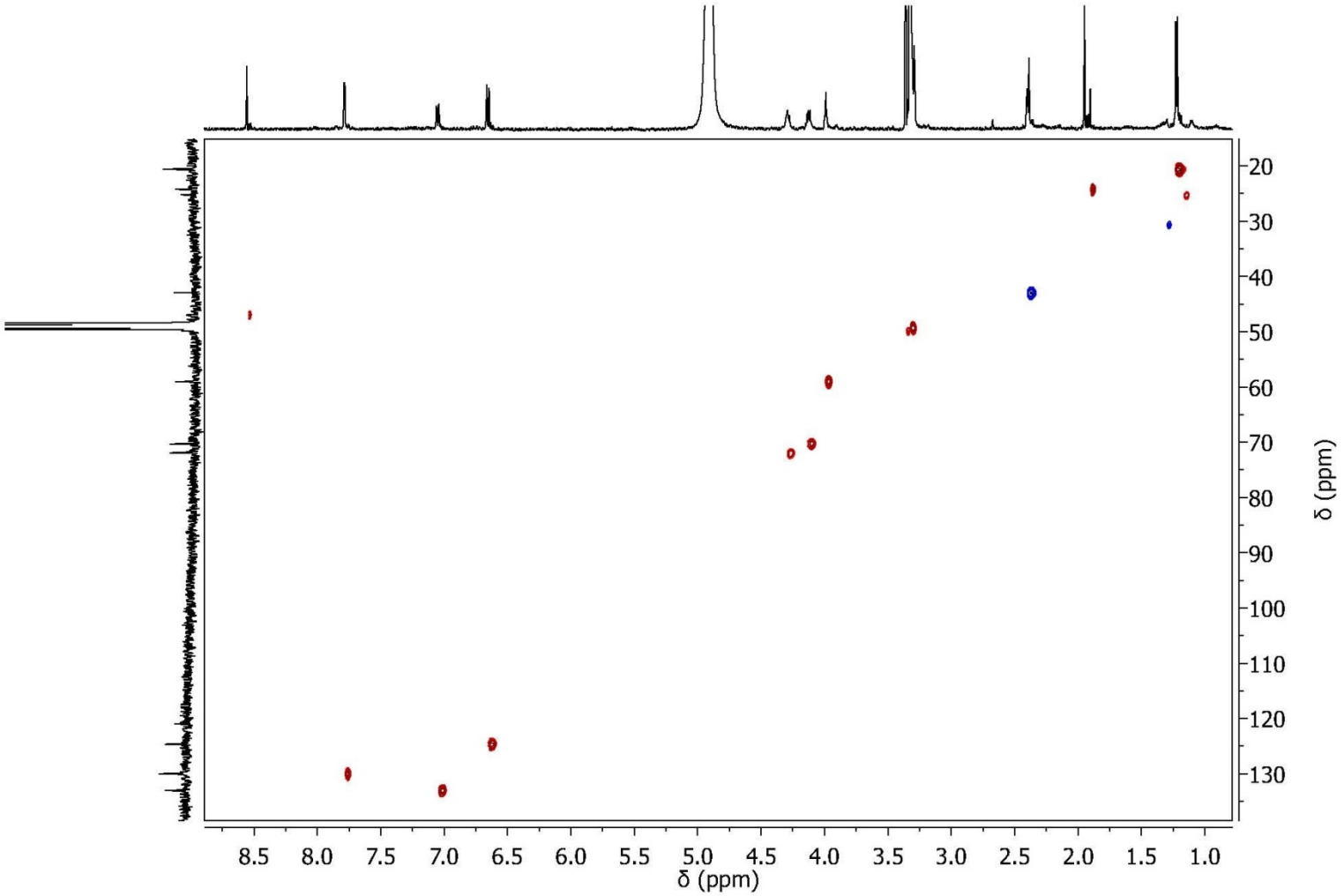


Figure S30. HMBC Spectrum of Compound 5 in CD_3OD (500 MHz)

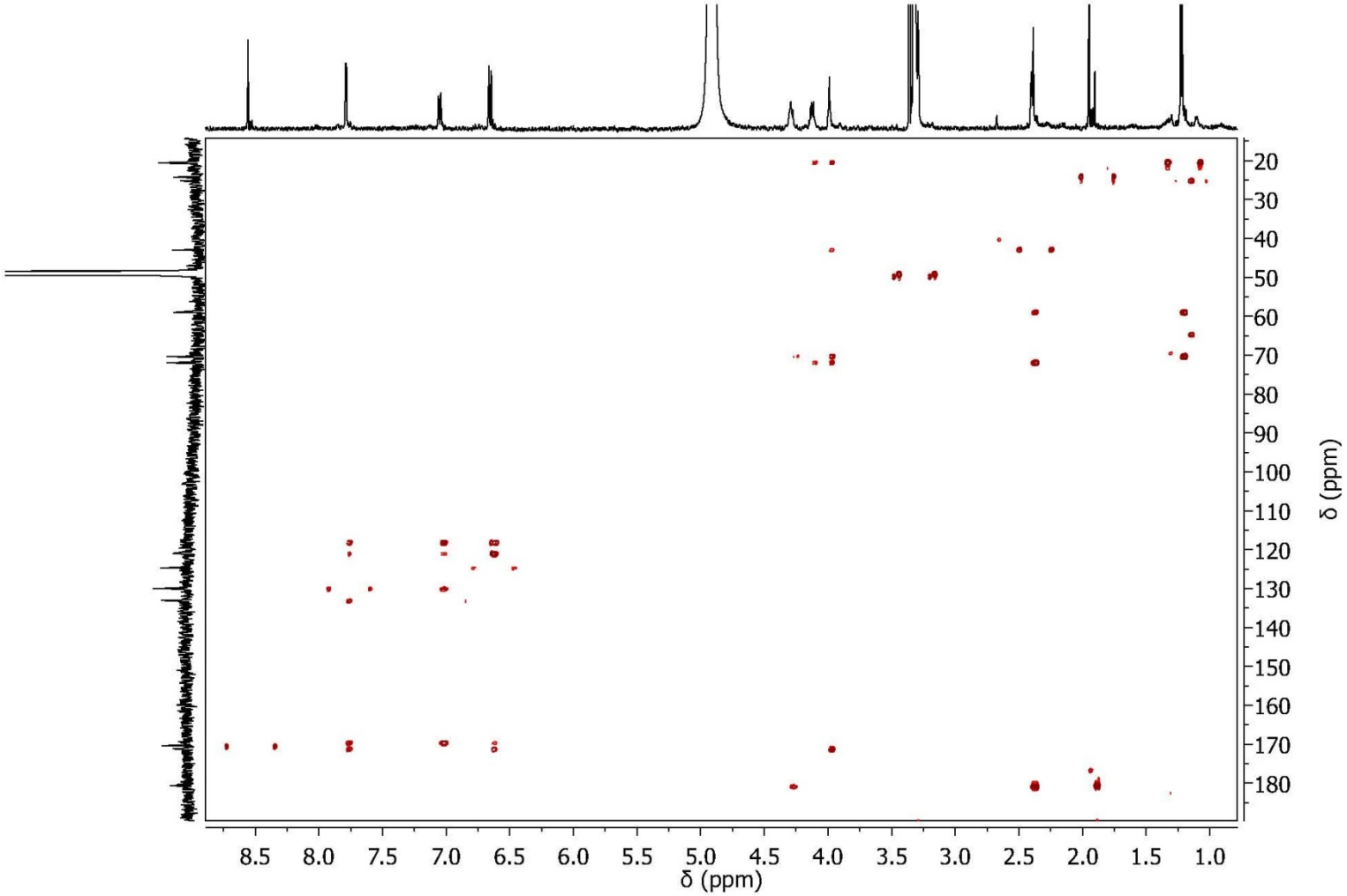


Figure S31. ^{1}H NMR Spectrum of Compound 6 in CD_3OD (500 MHz)

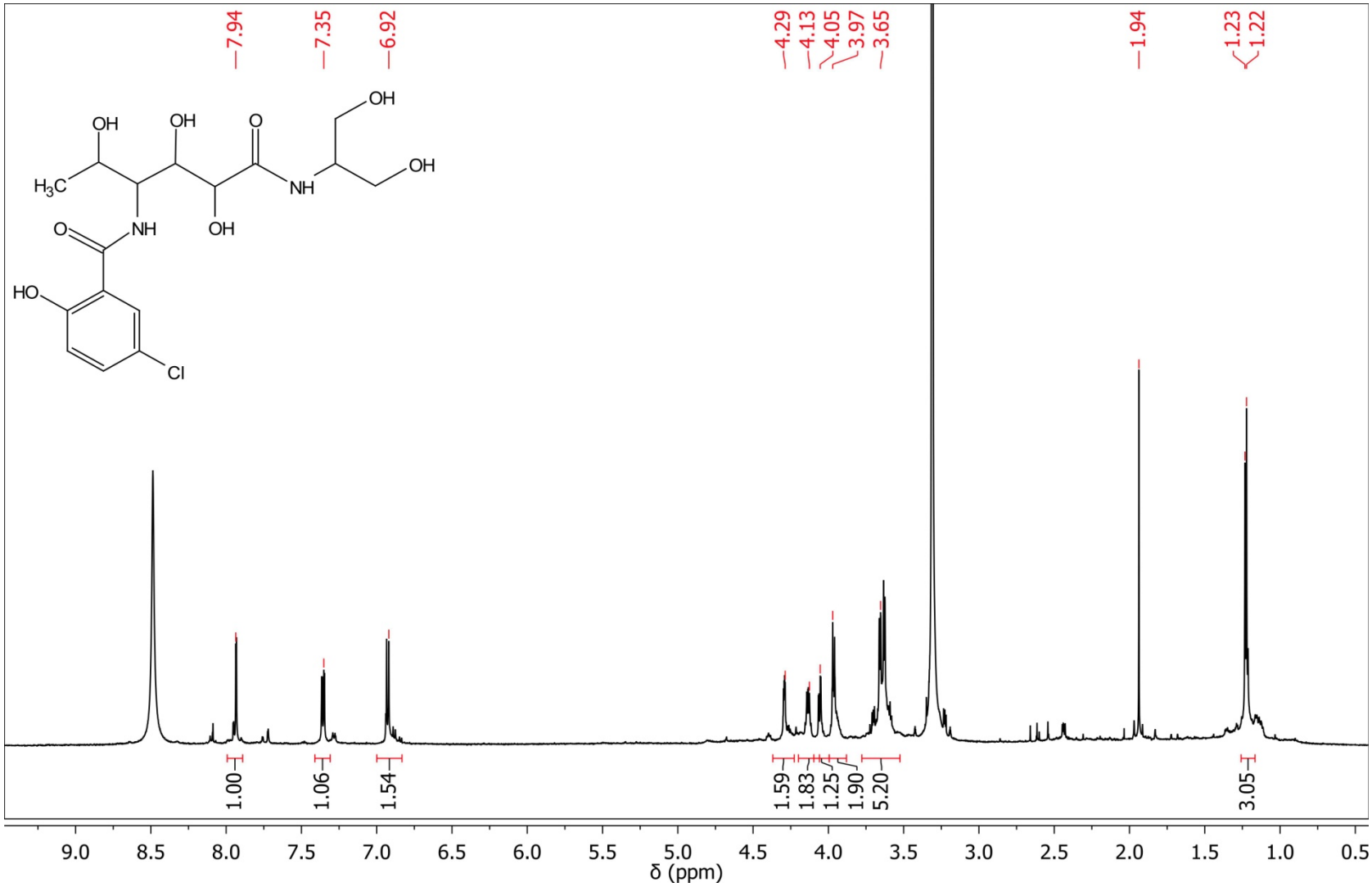


Figure S32. ^{13}C NMR Spectrum of Compound 6 in CD_3OD (125 MHz)

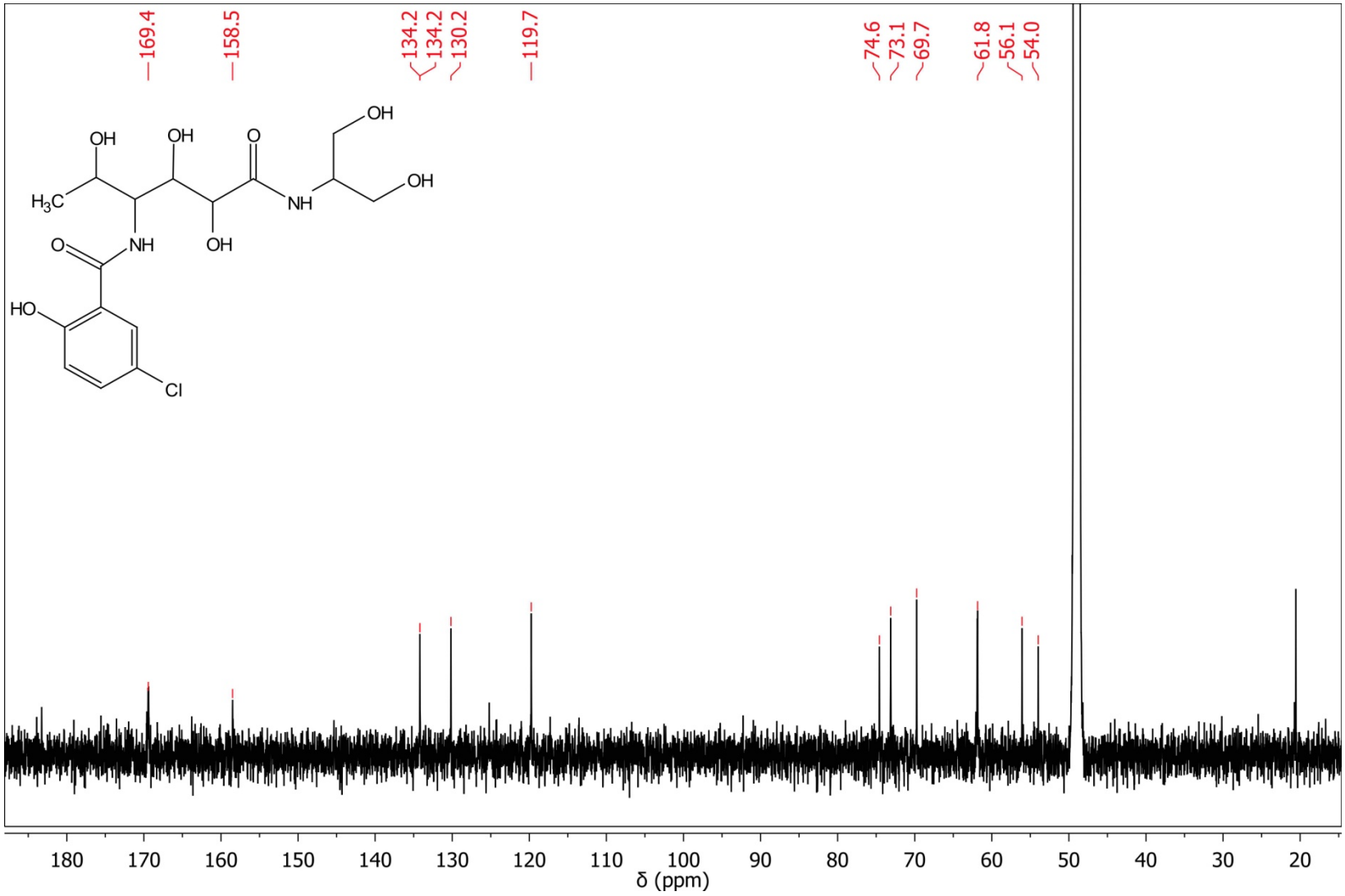


Figure S33. COSY Spectrum of Compound 6 in CD_3OD (500 MHz)

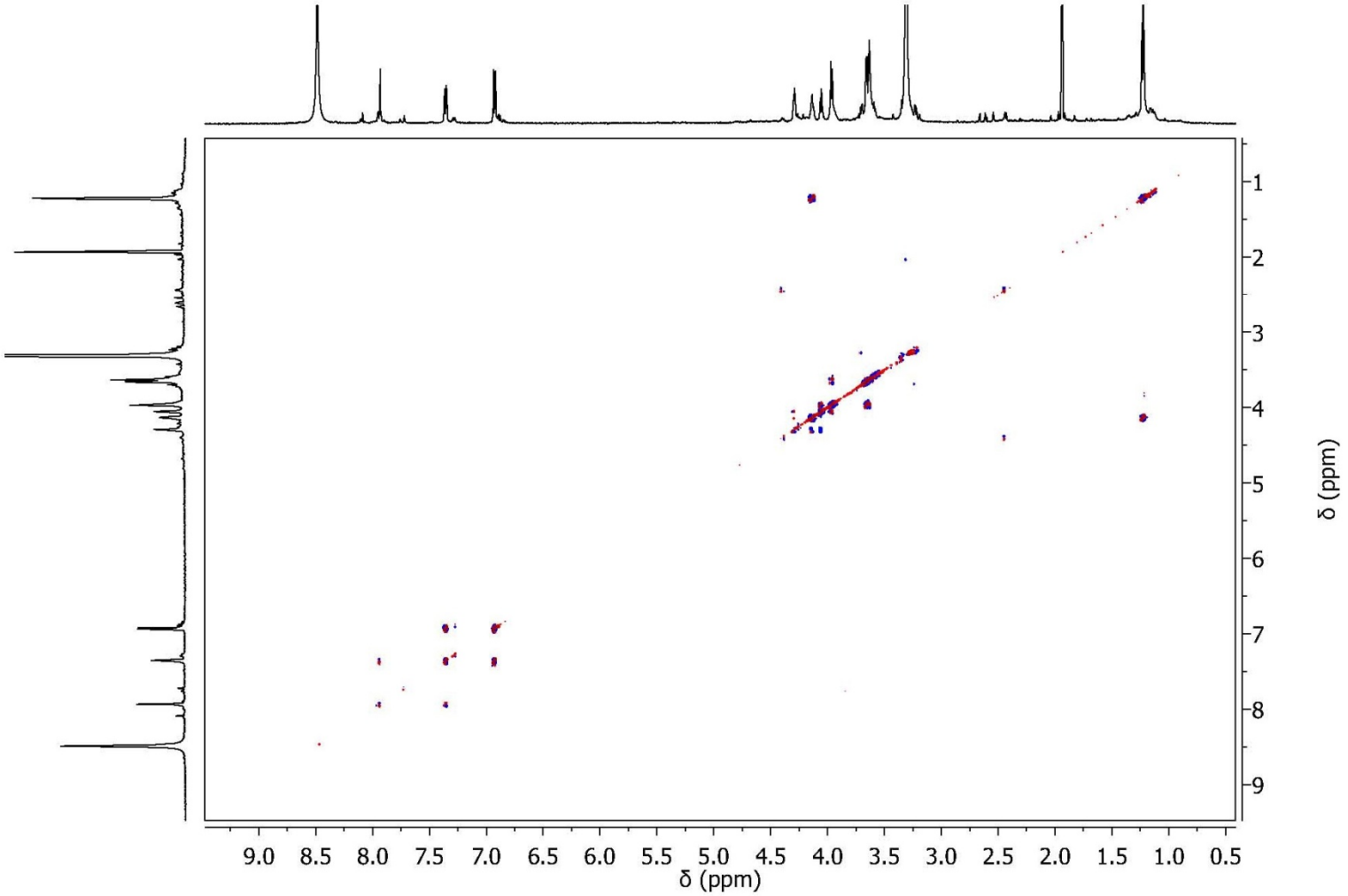


Figure S34. HSQC Spectrum of Compound 6 in CD_3OD (500 MHz)

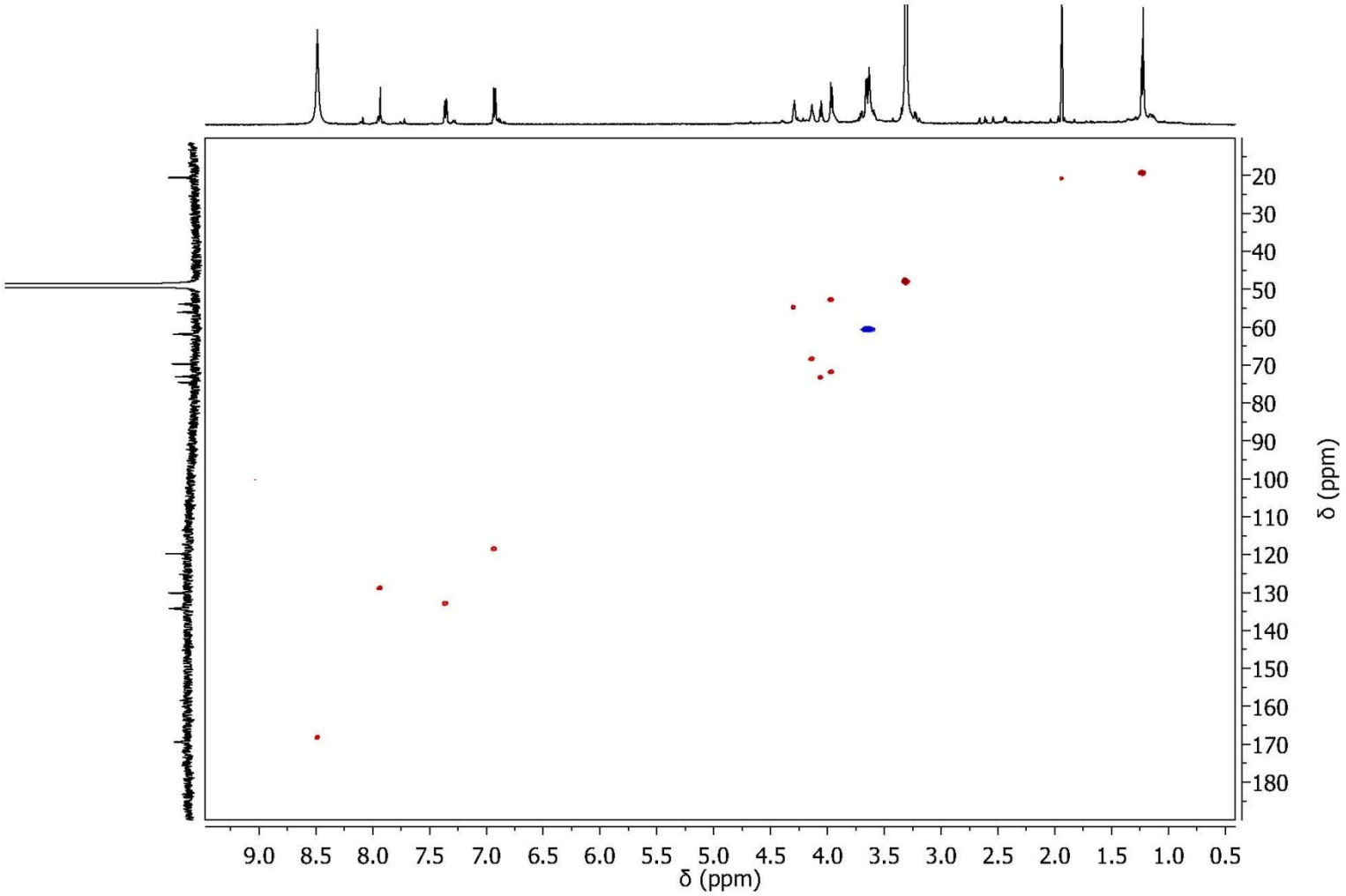


Figure S35. HMBC Spectrum of Compound 6 in CD_3OD (500 MHz)

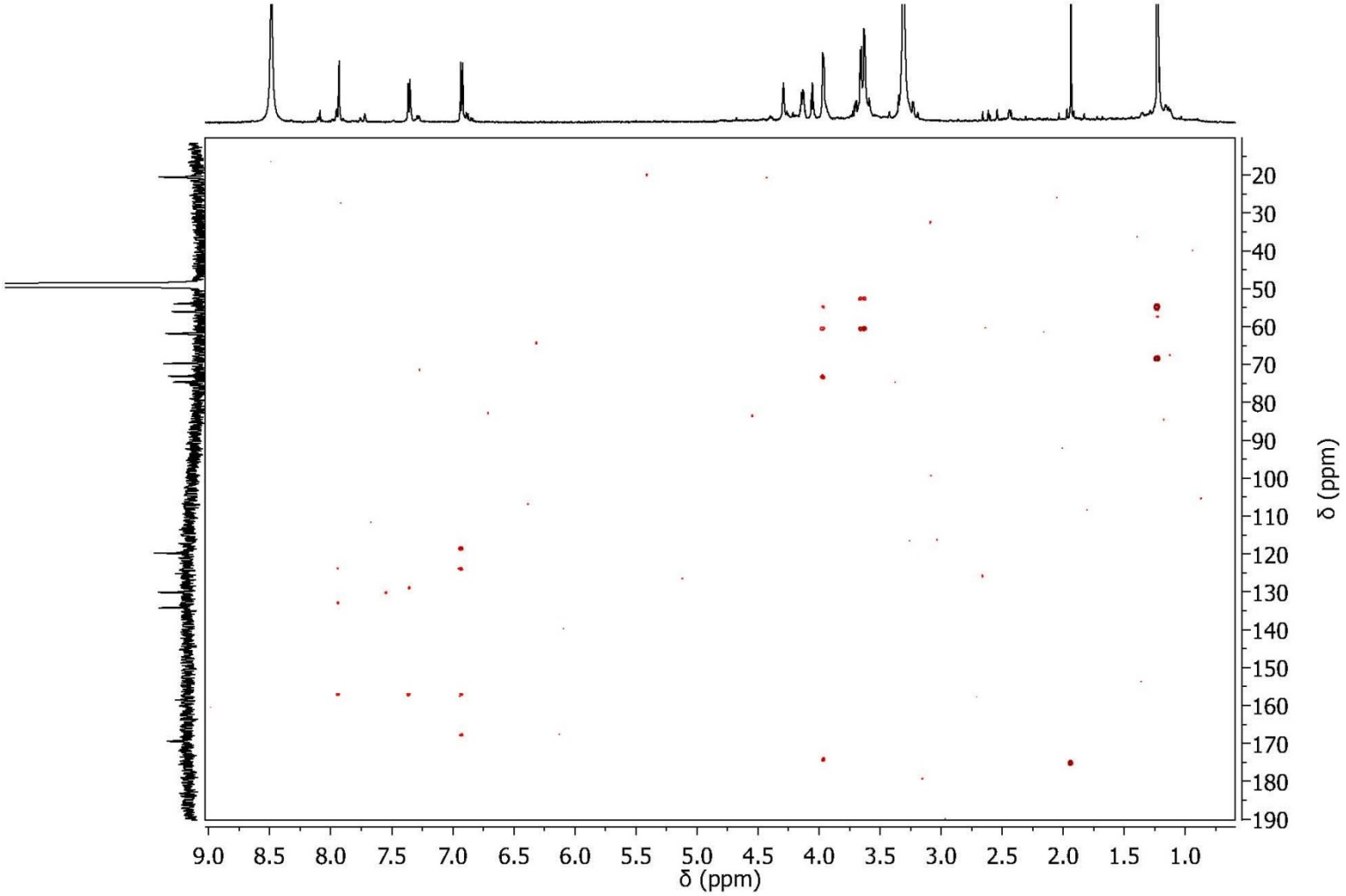


Figure S36. ^{1}H NMR Spectrum of Compound 7 in CD_3OD (500 MHz)

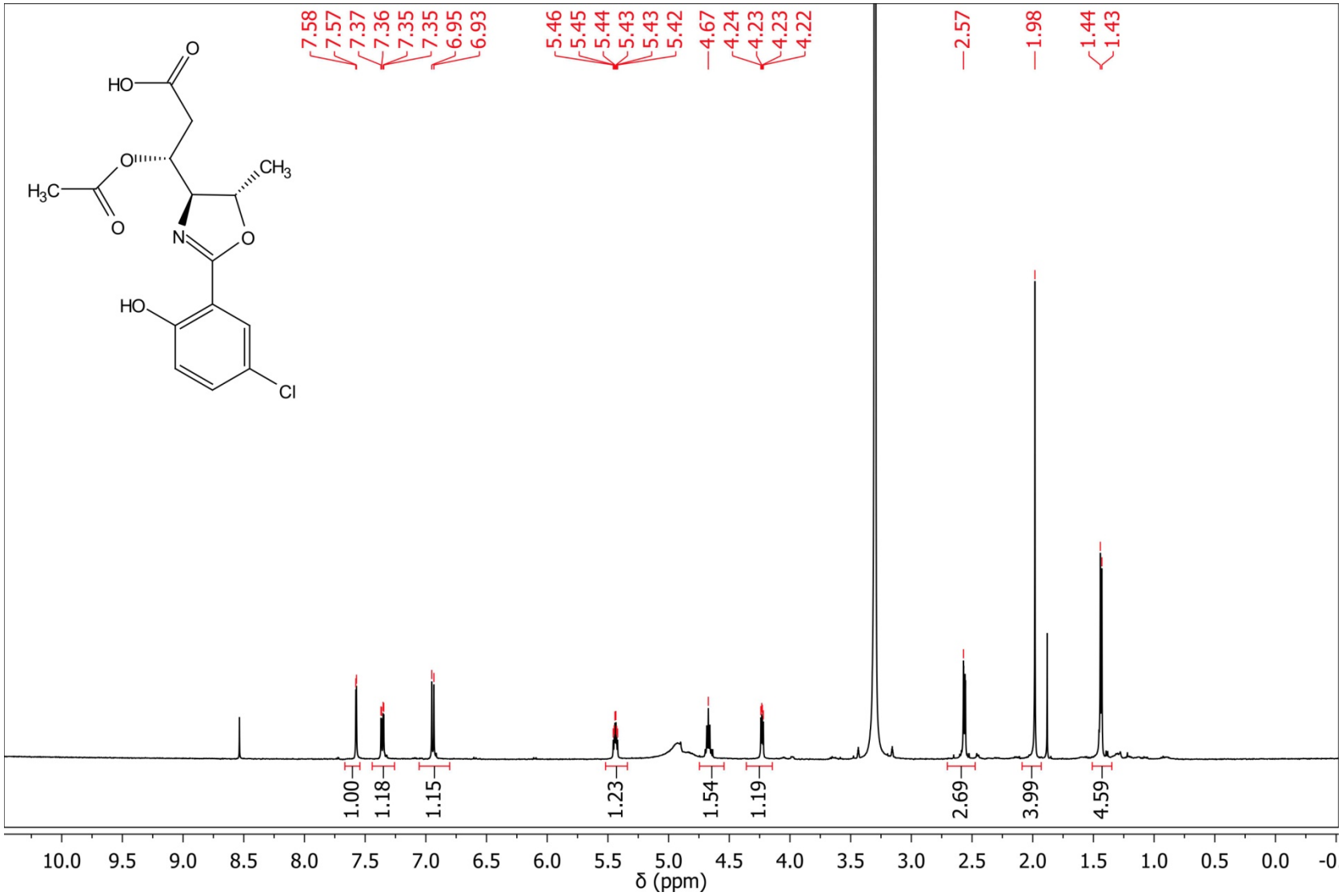


Figure S37. ^{1}H NMR Spectrum of Compound 8 in CD_3OD (500 MHz)

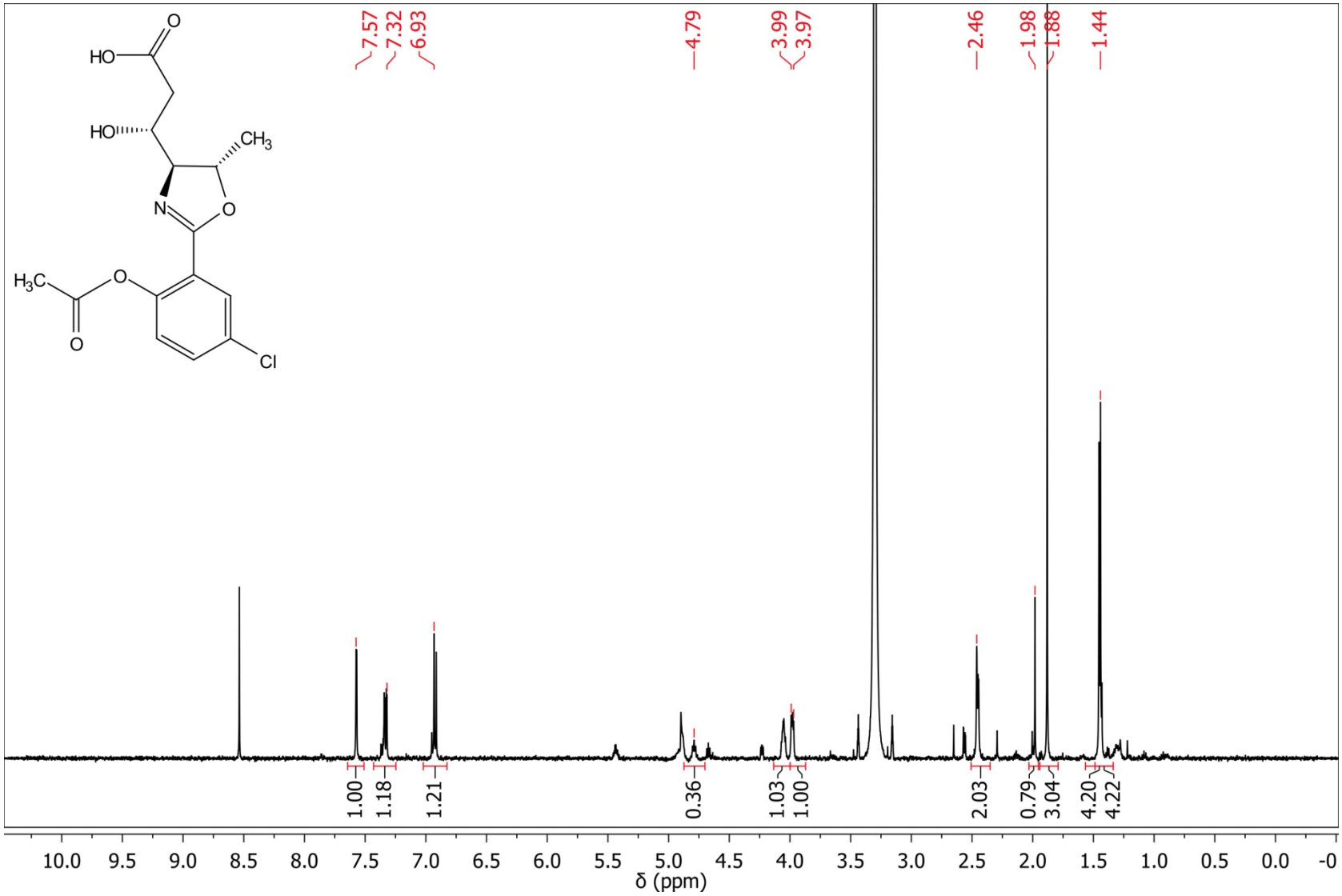


Figure S38. Growth Inhibition Curves for 2

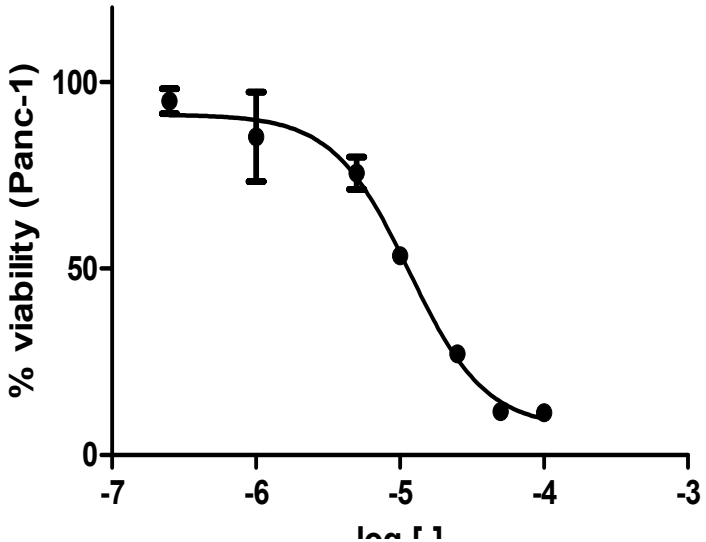


Figure S39. Micrographs of the Cyanobacterium O-2-5

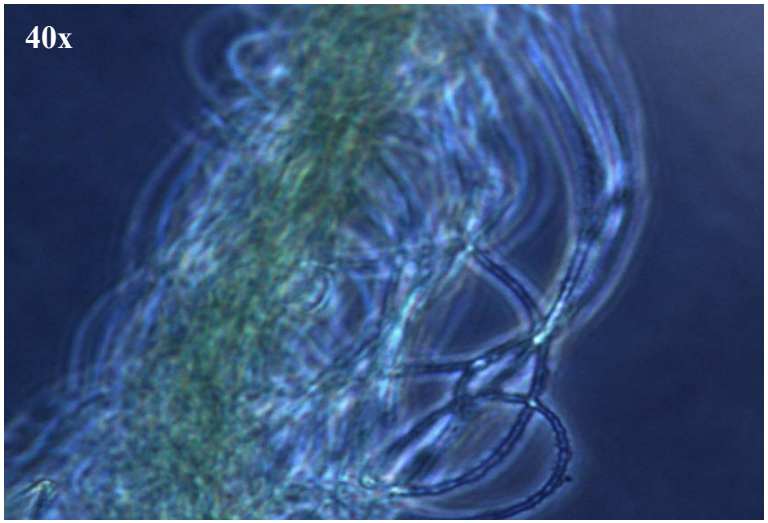
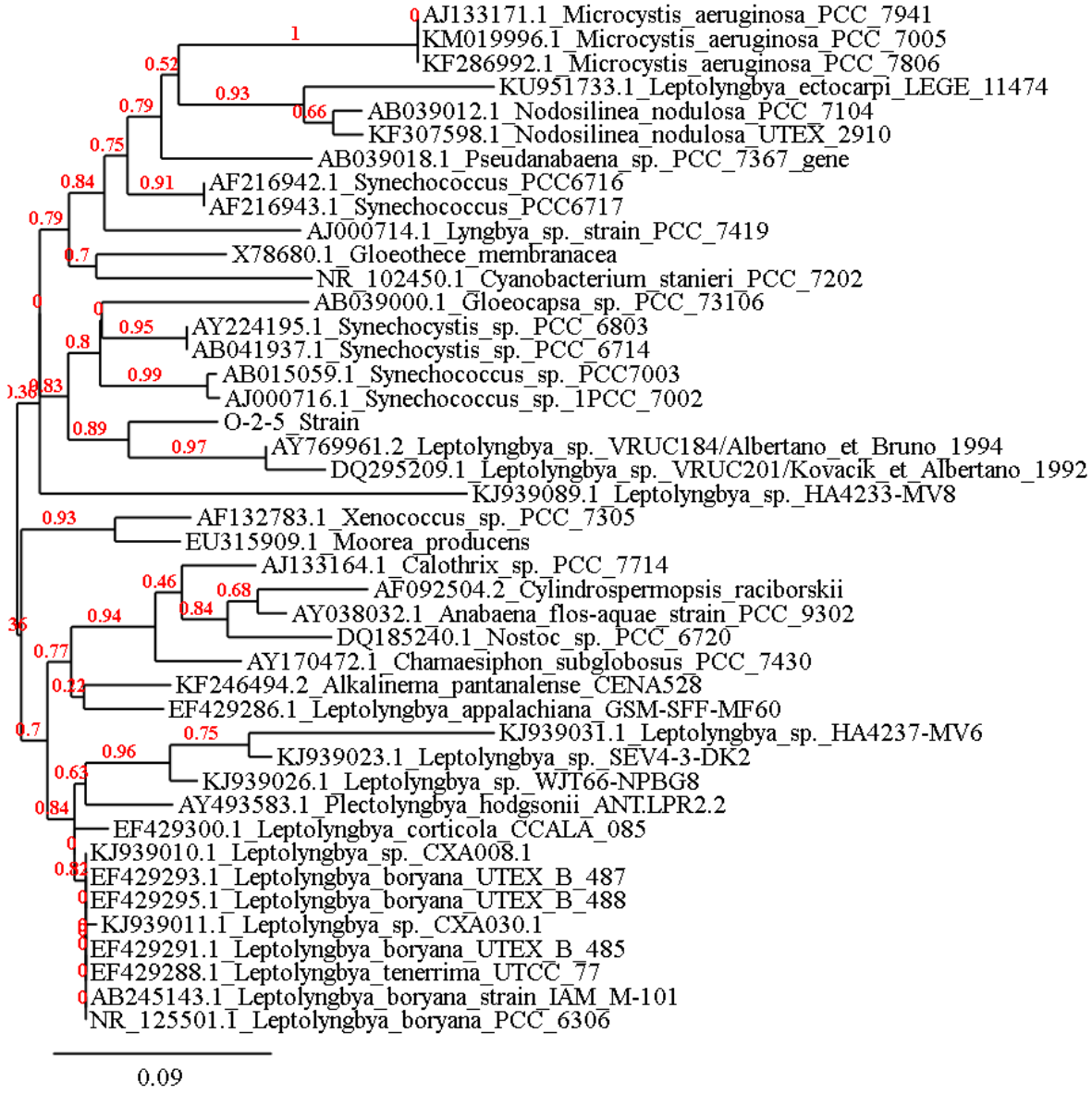


Figure S40. 16S sRNA Sequence of the Cyanobacterium O-2-5

CGGACGGGGNNAGTAACGCGTGAGGATCTGCCTACAGGACTGGGACAACGACTGGAAACGGTCGCTAAAACCGGNATGTGCCGAGAGGTGAAATATTTATAGCCTGT
AGATGAGCTCGCGTCTGATTAGCTAGTTGGTGAGGTAATGGCTCACCAAGGCGACGATCAGTAGCTGGTCTGAGAGGACGATCAGCCACACTGGGACTGAGACACGG
CCCAGACTCCTACGGGAGGCAGCAGTGGGGAATTTTCCGCAATGGGCGCAAGCCTGACGGAGCAATACCGCGTGAGGGAGGAAGGTCTGTGGATTGTAAACCTCTTT
TGATAGGGAAGAACACAATGACGGTACCTATCGAATCAGCATCGGCTAACTCCGTGCCAGCAGCCGCGGTAATACGGAGGATGCAAGCGTTATCCGGAATTATTGGGC
GTAAAGCGTCCGTAGGTGGTTAATCAAGTCTATTGTCAAAGCCTGGGGCTTAACCCTGGAGAGGCGGTGGAAACTGGTTAACTTGAGTGCGGTAGGGGCAGAGGGAAT
TCCCAGTGTAGCGGTGAAATGCGTAGATATTGGGAAGAACACCGGTGGCGAAAGCGCTCTGCTGGGCCTGCACTGACACTGAGGGACGAAAGCTAGGGGAGCGAATG
GGATTAGATACCCCCAGTAGTCA

Figure S41. 16S sRNA Phylogenetic Analysis of Strain O-2-5



Dereeper A., Audic S., Claverie J.M., Blanc G. BMC Evol Biol. 2010 Jan 12;10:8.

Dereeper A.*, Guignon V.*, Blanc G., Audic S., Buffet S., Chevenet F., Dufayard J.F., Guindon S., Lefort V., Lescot M., Claverie J.M., Gascuel O. Nucleic Acids Res. 2008 Jul 1;36(Web Server issue):W465-9. Epub 2008 Apr 19.

Table S6. Boltzmann Distribution of Conformers of (3*S**,4*S**,5*S**)-1a

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #24	-874980.3599	0.00	1.000	0.676	0
conformer #1	-874979.5567	0.80	0.257	0.174	0
conformer #18	-874978.7867	1.57	0.070	0.047	0
conformer #27	-874978.6989	1.66	0.060	0.041	0
conformer #6	-874978.3431	2.02	0.033	0.022	0
conformer #23	-874978.1573	2.20	0.024	0.016	0
conformer #22	-874977.6459	2.71	0.010	0.007	0
conformer #10	-874977.4206	2.94	0.007	0.005	0
conformer #4	-874977.1144	3.25	0.004	0.003	0
conformer #16	-874977.0435	3.32	0.004	0.002	0
conformer #3	-874976.9676	3.39	0.003	0.002	0
conformer #12	-874976.8396	3.52	0.003	0.002	0
conformer #5	-874976.6977	3.66	0.002	0.001	0
conformer #19	-874976.4034	3.96	0.001	0.001	0
conformer #2	-874975.7126	4.65	0.000	0.000	0
conformer #11	-874975.1516	5.21	0.000	0.000	0
conformer #13	-874974.9733	5.39	0.000	0.000	0
conformer #26	-874974.7782	5.58	0.000	0.000	0
conformer #21	-874973.3343	7.03	0.000	0.000	0
conformer #20	-874973.3136	7.05	0.000	0.000	0
conformer #8	-874972.8906	7.47	0.000	0.000	0
conformer #7	-874972.8812	7.48	0.000	0.000	0
conformer #9	-874972.8279	7.53	0.000	0.000	0
conformer #17	-874972.3485	8.01	0.000	0.000	0
conformer #15	-874972.3428	8.02	0.000	0.000	0
conformer #28	-874970.8236	9.54	0.000	0.000	0

Table S7. Boltzmann Distribution of Conformers of (3*S**,4*S**,5*R**)-1b

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #7	-874977.05	0.00	1.000	0.518	0
conformer #18	-874976.75	0.30	0.602	0.312	0
conformer #4	-874975.83	1.22	0.127	0.066	0
conformer #12	-874975.5	1.55	0.073	0.038	0
conformer #8	-874975.47	1.57	0.070	0.036	0
conformer #16	-874974.94	2.11	0.028	0.015	0
conformer #1	-874974.68	2.37	0.018	0.009	0
conformer #9	-874973.98	3.07	0.006	0.003	0
conformer #5	-874973.43	3.61	0.002	0.001	0
conformer #17	-874972.73	4.32	0.001	0.000	0
conformer #13	-874972.51	4.53	0.000	0.000	0
conformer #11	-874972.49	4.55	0.000	0.000	0
conformer #6	-874972.39	4.66	0.000	0.000	0
conformer #15	-874971.72	5.33	0.000	0.000	0
conformer #2	-874970.93	6.12	0.000	0.000	0
conformer #3	-874970.07	6.98	0.000	0.000	0
conformer #10	-874968.92	8.12	0.000	0.000	0
conformer #19	-874968.47	8.58	0.000	0.000	0
conformer #14	-874967.85	9.19	0.000	0.000	0

Table S8. Boltzmann Distribution of Conformers of (3*R**,4*S**,5*R**)-1c

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #1	-874977.46	0.25	0.658	0.261	0
conformer #10	-874975.12	2.59	0.013	0.005	0
conformer #11	-874973.38	4.33	0.001	0.000	0
conformer #13	-874971.33	6.38	0.000	0.000	0
conformer #14	-874976.55	1.15	0.143	0.057	0
conformer #15	-874973.79	3.92	0.001	0.001	0
conformer #17	-874970.8	6.90	0.000	0.000	0
conformer #18	-874974.79	2.91	0.007	0.003	0
conformer #19	-874976.61	1.10	0.156	0.062	0
conformer #2	-874973.9	3.81	0.002	0.001	0
conformer #20	-874973	4.70	0.000	0.000	0
conformer #22	-874971.41	6.30	0.000	0.000	0
conformer #23	-874973.82	3.89	0.001	0.001	0
conformer #24	-874976.6	1.10	0.155	0.061	0
conformer #25	-874976.09	1.61	0.065	0.026	0
conformer #26	-874967.85	9.86	0.000	0.000	0
conformer #27	-874977.7	0.00	1.000	0.397	0
conformer #28	-874967.36	10.35	0.000	0.000	0
conformer #29	-874972.41	5.29	0.000	0.000	0
conformer #3	-874973.51	4.20	0.001	0.000	0
conformer #4	-874970	7.71	0.000	0.000	0
conformer #5	-874973.81	3.89	0.001	0.001	0
conformer #6	-874970.22	7.48	0.000	0.000	0
conformer #7	-874973.64	4.06	0.001	0.000	0
conformer #8	-874977.02	0.68	0.315	0.125	0
conformer #9	-874970.01	7.69	0.000	0.000	0

Table S9. Boltzmann Distribution of Conformers of (3*R**,4*S**,5*S**)-1d

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #32	-874980.28	0	1	0.495	0
conformer #1	-874979.64	0.65	0.335	0.165	0
conformer #18	-874979.35	0.94	0.205	0.102	0
conformer #34	-874979.19	1.09	0.158	0.078	0
conformer #10	-874978.99	1.3	0.112	0.055	0
conformer #21	-874978.42	1.86	0.043	0.021	0
conformer #27	-874978.34	1.95	0.037	0.018	0
conformer #13	-874978.16	2.13	0.027	0.013	0
conformer #29	-874978.12	2.16	0.026	0.013	0
conformer #12	-874978.11	2.18	0.025	0.013	0
conformer #19	-874977.98	2.31	0.02	0.010	0
conformer #7	-874977.63	2.65	0.011	0.006	0
conformer #2	-874977.49	2.79	0.009	0.004	0
conformer #4	-874977.18	3.1	0.005	0.003	0
conformer #9	-874976.76	3.52	0.003	0.001	0
conformer #20	-874976.73	3.55	0.002	0.001	0
conformer #26	-874975.91	4.37	0.001	0	0
conformer #5	-874975.41	4.88	0	0	0
conformer #15	-874975.18	5.1	0	0	0
conformer #8	-874974.13	6.15	0	0	0
conformer #16	-874974.09	6.19	0	0	0
conformer #17	-874974.09	6.19	0	0	0
conformer #31	-874973.97	6.31	0	0	0
conformer #30	-874973.67	6.61	0	0	0
conformer #6	-874973.67	6.62	0	0	0
conformer #3	-874973.58	6.7	0	0	0
conformer #11	-874973.54	6.75	0	0	0
conformer #22	-874973.18	7.1	0	0	0
conformer #33	-874973.01	7.27	0	0	0
conformer #14	-874971.94	8.34	0	0	0
conformer #24	-874971.75	8.54	0	0	0
conformer #23	-874971.13	9.15	0	0	0
conformer #25	-874970.95	9.34	0	0	0
conformer #35	-874970.36	9.93	0	0	0

Table S10. Boltzmann Distribution of Conformers of (2*S**,3*R**,4*S**,*5S**)-2a

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #1	-909695.77	0.00	1.000	0.992	0
conformer #5	-909692.8	2.97	0.007	0.007	0
conformer #7	-909691.85	3.93	0.001	0.001	0
conformer #2	-909691.39	4.39	0.001	0.001	0
conformer #6	-909689.09	6.69	0.000	0.000	0
conformer #3	-909689.02	6.76	0.000	0.000	0
conformer #4	-909687.67	8.10	0.000	0.000	0

Table S11. Boltzmann Distribution of Conformers of (2*S**,3*R**,4*S**,5*R**)-2b

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #1	-909691.49	0.00	1.000	0.999	0
conformer #2	-909687.19	4.29	0.001	0.001	0
conformer #3	-909685.22	6.26	0.000	0.000	0
conformer #4	-909684.56	6.93	0.000	0.000	0

Table S12. Boltzmann Distribution of Conformers of (2*S**,3*S**,4*S**,5*R**)-2c

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #10	-909693.2	0.00	1.000	0.915	0
conformer #2	-909691.21	1.99	0.035	0.032	0
conformer #1	-909690.97	2.23	0.023	0.021	0
conformer #5	-909690.76	2.44	0.016	0.015	0
conformer #11	-909690.74	2.46	0.016	0.014	0
conformer #12	-909689.8	3.40	0.003	0.003	0
conformer #3	-909687.93	5.27	0.000	0.000	0
conformer #4	-909687.25	5.95	0.000	0.000	0
conformer #8	-909685.23	7.96	0.000	0.000	0
conformer #6	-909685.22	7.98	0.000	0.000	0
conformer #7	-909684.91	8.29	0.000	0.000	0
conformer #9	-909684.74	8.46	0.000	0.000	0

Table S13. Boltzmann Distribution of Conformers of (2*S**,3*S**,4*S**,5*S**)-2d

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #1	-909694	0	1.000	0.380	0
conformer #3	-909694	0.08	0.874	0.332	0
conformer #7	-909694	0.19	0.730	0.277	0
conformer #8	-909692	2.2	0.024	0.009	0
conformer #2	-909691	3.33	0.004	0.001	0
conformer #4	-909690	4.12	0.001	0.000	0
conformer #5	-909688	5.65	0.000	0.000	0
conformer #6	-909688	5.84	0.000	0.000	0

Table S14. Boltzmann Distribution of Conformers of (2*R**,3*R**,4*S**,5*S**)-2e

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #1	-909695.54	0.00	1.000	0.951	0
conformer #8	-909693.76	1.78	0.050	0.047	0
conformer #2	-909691.72	3.81	0.002	0.002	0
conformer #5	-909691.14	4.40	0.001	0.001	0
conformer #4	-909689.35	6.19	0.000	0.000	0
conformer #3	-909687.31	8.23	0.000	0.000	0
conformer #6	-909686.69	8.85	0.000	0.000	0

Table S15. Boltzmann Distribution of Conformers of (2*R**,3*R**,4*S**,5*R**)-2f

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #1	-909690.66	0.00	1.000	0.996	0
conformer #6	-909687.06	3.60	0.002	0.002	0
conformer #2	-909686.87	3.78	0.002	0.002	0
conformer #5	-909683.96	6.69	0.000	0.000	0
conformer #4	-909683.36	7.30	0.000	0.000	0
conformer #3	-909683.15	7.50	0.000	0.000	0

Table S16. Boltzmann Distribution of Conformers of (2*R**,3*S**,4*S**,5*R**)-2g

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #7	-909692.71	0.00	1.000	0.542	0
conformer #3	-909692.53	0.18	0.736	0.399	0
conformer #2	-909691.39	1.32	0.107	0.058	0
conformer #8	-909688.66	4.05	0.001	0.001	0
conformer #1	-909688.56	4.15	0.001	0.000	0
conformer #4	-909688.08	4.63	0.000	0.000	0
conformer #9	-909685.73	6.98	0.000	0.000	0
conformer #5	-909685.39	7.32	0.000	0.000	0
conformer #6	-909684.9	7.81	0.000	0.000	0

Table S17. Boltzmann Distribution of Conformers of (2*R**,3*S**,4*S**,5*S**)-2h

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
conformer #3	-909695.07	0.00	1.000	0.946	0
conformer #1	-909693.37	1.70	0.056	0.053	0
conformer #4	-909690.98	4.09	0.001	0.001	0
conformer #2	-909689.69	5.38	0.000	0.000	0
conformer #6	-909688.72	6.35	0.000	0.000	0
conformer #5	-909687.24	7.83	0.000	0.000	0

XYZ Coordinates of Conformers for the Diastereomers of 1

1d NMR Conformer 35
Energy: -875532.0543687

O	-1.77742	2.87577	-0.37603
C	-2.45820	1.71700	-0.24738
C	-1.87626	0.46775	0.04053
C	-0.42955	0.27817	0.23301
N	0.18135	-0.83708	0.30543
C	1.59455	-0.53107	0.56929
C	2.48345	-1.41655	-0.30975
O	2.14144	-2.77401	-0.09987
C	3.96482	-1.31068	0.03750
C	4.66925	-0.10935	-0.55502
O	5.86769	0.19599	-0.03804
O	4.23162	0.55880	-1.46389
C	1.71149	0.98782	0.32635
C	2.49367	1.76148	1.36350
O	0.31732	1.40833	0.36059
C	-2.69441	-0.66898	0.13769
C	-4.05822	-0.56120	-0.04674
Cl	-5.06447	-1.98550	0.08104
C	-4.64647	0.67354	-0.33260
C	-3.84621	1.79842	-0.43059
H	-0.82745	2.74435	-0.21073
H	1.80870	-0.78172	1.62133
H	2.33132	-1.13633	-1.36233
H	1.17842	-2.85842	-0.20793
H	4.46994	-2.19955	-0.36282
H	4.10691	-1.33468	1.12560
H	6.13751	-0.40407	0.68480
H	2.07145	1.19717	-0.68647
H	3.54118	1.44382	1.35902
H	2.46646	2.83291	1.15283
H	2.08223	1.58095	2.36046
H	-2.23435	-1.62650	0.36209
H	-5.72069	0.74830	-0.47492
H	-4.27775	2.76966	-0.65339

1d NMR Conformer 34
Energy: -875540.5706700

O	1.32006	-2.53201	-0.87853
C	2.22205	-1.63670	-0.44488
C	1.89915	-0.28661	-0.19625
C	0.52926	0.17875	-0.41128
N	-0.43683	-0.56705	-0.80702
C	-1.63678	0.26961	-0.88335
C	-2.71541	-0.28062	0.05500
O	-3.02848	-1.61931	-0.27238
C	-4.01374	0.50765	-0.07754
C	-5.09915	-0.06970	0.79821
O	-4.72027	-0.16094	2.07792
O	-6.19692	-0.40365	0.40977
C	-1.13895	1.68586	-0.49996
C	-1.25658	2.70941	-1.60910
O	0.26554	1.47665	-0.18608
C	2.88558	0.60275	0.25151
C	4.17528	0.14553	0.44947
Cl	5.40874	1.25203	1.00824
C	4.50907	-1.18982	0.20833
C	3.53692	-2.07192	-0.23625
H	0.44521	-2.07895	-0.98609
H	-2.02884	0.24291	-1.90998
H	-2.34539	-0.21393	1.08984
H	-2.22803	-2.16169	-0.16714
H	-4.36922	0.48478	-1.11077
H	-3.85750	1.55078	0.22330
H	-5.45735	-0.53719	2.60277
H	-1.60376	2.04773	0.42500
H	-2.31285	2.87886	-1.84093
H	-0.80829	3.65983	-1.31138
H	-0.75691	2.34546	-2.51190
H	2.62807	1.64072	0.43918
H	5.52731	-1.53262	0.36878
H	3.77692	-3.11293	-0.43068

1d NMR Conformer 33
Energy: -875534.3141370

O	-2.47070	-2.79681	0.20188
C	-2.74146	-1.47878	0.08933
C	-1.77304	-0.46743	-0.05461
C	-0.32530	-0.73420	-0.09867
N	0.59739	0.14408	-0.08488
C	1.87287	-0.57343	-0.17707
C	2.80504	-0.15023	0.96453
O	2.18543	-0.36002	2.21793
C	3.25494	1.30296	0.82142
C	4.22199	1.51054	-0.32322
O	4.54556	2.77884	-0.61312
O	4.72121	0.61206	-0.96105
C	1.50150	-2.07117	-0.11664
C	2.04113	-2.90605	-1.25571

O	0.04815	-2.04003	-0.17706
C	-2.18375	0.87086	-0.15438
C	-3.52602	1.19086	-0.11128
Cl	-4.02228	2.86206	-0.24141
C	-4.49519	0.19474	0.03140
C	-4.09807	-1.12726	0.13064
H	-1.51404	-2.96509	0.14179
H	2.35434	-0.32924	-1.13341
H	3.68715	-0.80049	0.95096
H	1.36325	0.16148	2.25137
H	3.76084	1.61392	1.74391
H	2.38481	1.95891	0.68898
H	4.08737	3.42783	-0.04503
H	1.76152	-2.50071	0.85745
H	3.13511	-2.89945	-1.22072
H	1.69924	-3.94112	-1.18281
H	1.72106	-2.48976	-2.21530
H	-1.42879	1.64276	-0.26774
H	-5.54888	0.45707	0.06249
H	-4.83113	-1.92045	0.24301

1d NMR Conformer 32
Energy: -875541.1477590

O	0.71302	-2.22897	-1.16243
C	1.77551	-1.57128	-0.66957
C	1.71159	-0.22738	-0.24742
C	0.44577	0.49907	-0.34599
N	-0.64877	-0.00924	-0.78516
C	-1.67476	1.03289	-0.72111
C	-2.82887	0.59758	0.18868
O	-2.37128	0.36845	1.50720
C	-3.55062	-0.62400	-0.36798
C	-4.81717	-0.91788	0.39639
O	-5.11799	-2.22032	0.40021
O	-5.51025	-0.08109	0.93137
C	-0.92530	2.27523	-0.17720
C	-0.88746	3.45020	-1.13046
O	0.42780	1.78528	0.03692
C	2.85473	0.40760	0.25536
C	4.04439	-0.29307	0.33476
Cl	5.47282	0.49704	0.95929
C	4.12064	-1.62476	-0.07961
C	2.99239	-2.25653	-0.57774
H	-0.06571	-1.61289	-1.17052
H	-2.07176	1.21688	-1.72924
H	-3.53925	1.42840	0.27031
H	-1.73995	-0.37425	1.50076
H	-2.89964	-1.50292	-0.35766
H	-3.84140	-0.44721	-1.41263
H	-5.96711	-2.35022	0.87464
H	-1.30674	2.56675	0.80717
H	-1.90350	3.82370	-1.29070
H	-0.27916	4.26176	-0.72381
H	-0.47173	3.14200	-2.09487
H	2.79728	1.44336	0.57688
H	5.06272	-2.16205	-0.01139
H	3.03410	-3.29108	-0.90553

1d NMR Conformer 31
Energy: -875536.1637149

O	1.62140	2.74626	0.09491
C	2.39053	1.64892	0.01725
C	1.86503	0.34332	0.08445
C	0.42779	0.15270	0.27330
N	-0.42637	1.10668	0.37142
C	-1.73256	0.49429	0.63140
C	-2.79634	1.11583	-0.27444
O	-2.88298	2.50126	-0.00463
C	-4.19144	0.56088	-0.00451
C	-4.49995	-0.74404	-0.70058
O	-5.53819	-1.44096	-0.22313
O	-3.91338	-1.15370	-1.67414
C	-1.48368	-1.01656	0.41282
C	-2.01758	-1.91759	1.50374
O	-0.02925	-1.10567	0.37357
C	2.71688	-0.76509	-0.01592
C	4.07472	-0.56707	-0.17719
Cl	5.14199	-1.94769	-0.30395
C	4.61035	0.72173	-0.24002
C	3.77122	1.81936	-0.14264
H	0.67632	2.46537	0.20357
H	-2.01928	0.70965	1.67316
H	-2.52024	0.93332	-1.32352
H	-2.02635	2.91050	-0.22004
H	-4.92189	1.28840	-0.38288
H	-4.36906	0.47136	1.07534
H	-5.95027	-1.03269	0.56297
H	-1.83521	-1.33894	-0.57317
H	-3.10998	-1.84187	1.54891
H	-1.75912	-2.96141	1.31224
H	-1.61475	-1.61831	2.47553
H	2.30232	-1.76753	0.03621
H	5.68065	0.85908	-0.36689
H	4.16699	2.82947	-0.19273

1d NMR Conformer 30
Energy: -875533.9523276

O	-2.26888	2.83677	-0.47727

C	-2.72458	1.58237	-0.27119
C	-1.91285	0.45647	-0.03581
C	-0.44191	0.51273	0.01668
N	0.33890	-0.46573	0.24911
C	1.71222	0.04953	0.19005
C	2.46781	-0.70756	-0.90904
O	2.46378	-2.09356	-0.63476
C	3.93364	-0.29972	-1.08575
C	4.81492	-0.72709	0.06318
O	4.58704	-0.01492	1.17606
O	5.64949	-1.60205	0.00638
C	1.56463	1.56628	-0.07425
C	2.07645	2.44141	1.04966
O	0.12538	1.72945	-0.20471
C	-2.51433	-0.79571	0.16640
C	-3.88853	-0.92144	0.13215
Cl	-4.62157	-2.48820	0.38583
C	-4.70305	0.18921	-0.10175
C	-4.11799	1.42734	-0.30064
H	-1.29705	2.86852	-0.43892
H	2.20355	-0.13925	1.15047
H	1.95273	-0.49906	-1.86118
H	1.54092	-2.37545	-0.50854
H	4.01163	0.78631	-1.20924
H	4.32272	-0.78118	-1.98433
H	5.17858	-0.33715	1.88937
H	1.98937	1.86847	-1.03882
H	3.15660	2.30019	1.15034
H	1.87177	3.49622	0.85220
H	1.60130	2.15390	1.99277
H	-1.87930	-1.65717	0.34907
H	-5.78357	0.07989	-0.12631
H	-4.72812	2.30686	-0.48338

1d NMR Conformer 29
Energy: -875538.6179295

O	0.19678	-2.13016	-0.88969
C	1.30296	-1.44878	-0.55284
C	1.28934	-0.07428	-0.23922
C	0.02554	0.66192	-0.28447
N	-1.10451	0.13345	-0.58915
C	-2.12847	1.17191	-0.47579
C	-3.14993	0.80109	0.60772
O	-2.54227	0.71896	1.87832
C	-3.94856	-0.46118	0.23548
C	-3.12824	-1.71605	0.08250
O	-2.46511	-2.02686	1.20878
O	-3.06982	-2.39939	-0.91422
C	-1.33003	2.45498	-0.13326
C	-1.37170	3.52626	-1.19956
O	0.04113	1.97018	0.00466
C	2.47586	0.57874	0.11925
C	3.65962	-0.13303	0.15690
Cl	5.14316	0.67706	0.60871
C	3.69022	-1.49285	-0.16055
C	2.51856	-2.14245	-0.51223
H	-0.57264	-1.49995	-0.88388
H	-2.65786	1.27540	-1.43383
H	-3.87208	1.62342	0.68122
H	-2.03181	-0.10557	1.93836
H	-4.48074	-0.29926	-0.70482
H	-4.68325	-0.64118	1.02830
H	-1.93878	-2.84234	1.06176
H	-1.61763	2.84588	0.84728
H	-2.39554	3.89927	-1.30461
H	-0.72285	4.36411	-0.93380
H	-1.04959	3.11615	-2.16165
H	2.45301	1.63698	0.36307
H	4.63028	-2.03669	-0.12782
H	2.52076	-3.19993	-0.76001

1d NMR Conformer 27
Energy: -875537.4782029

O	0.25228	-2.25334	-0.41234
C	1.38019	-1.54413	-0.25357
C	1.39599	-0.13947	-0.13163
C	0.14012	0.60495	-0.18521
N	-1.01483	0.07006	-0.34999
C	-1.99393	1.15742	-0.38557
C	-3.17930	0.87159	0.53472
O	-2.78321	0.47592	1.84539
C	-4.09918	-0.21663	-0.03258
C	-3.44420	-1.57457	-0.20123
O	-2.89313	-2.10714	0.89538
O	-3.44343	-2.19689	-1.23969
C	-1.17667	2.41597	-0.00496
C	-1.34964	3.59446	-0.93420
O	0.19707	1.94347	-0.05781
C	2.60940	0.54028	0.04109
C	3.79027	-0.17578	0.08607
Cl	5.30645	0.66996	0.29567
C	3.79082	-1.56791	-0.03581
C	2.59300	-2.24346	-0.20382
H	-0.52070	-1.63725	-0.42938
H	-2.39134	1.25381	-1.40714
H	-3.77347	1.79371	0.61036
H	-1.83012	0.61093	1.99400
H	-4.49207	0.09275	-1.00307

H	-4.94318	-0.33635	0.65723
H	-2.87845	-1.44456	1.61456
H	-1.36208	2.71050	1.03743
H	-2.38980	3.93321	-0.90250
H	-0.70695	4.42430	-0.63309
H	-1.10578	3.30552	-1.96029
H	2.61002	1.62202	0.13541
H	4.72796	-2.11589	0.00177
H	2.57239	-3.32491	-0.29907

1d NMR Conformer 26
Energy: -875536.3307767

O	2.31241	2.70798	0.92234
C	2.75886	1.47600	0.59685
C	1.96957	0.44773	0.04700
C	0.53370	0.59281	-0.24699
N	-0.22542	-0.30117	-0.74261
C	-1.56766	0.27869	-0.84993
C	-2.55408	-0.57747	-0.05105
O	-2.52116	-1.91588	-0.50495
C	-3.98420	-0.09724	-0.22904
C	-4.93768	-0.84737	0.67131
O	-6.15359	-0.96524	0.12871
O	-4.66196	-1.26920	1.77299
C	-1.42706	1.72809	-0.32483
C	-1.73999	2.80231	-1.34419
O	-0.02226	1.80154	0.03691
C	2.56081	-0.79177	-0.24595
C	3.90219	-1.00031	0.00390
Cl	4.62082	-2.55080	-0.36508
C	4.69442	0.01324	0.54902
C	4.11949	1.23785	0.84000
H	1.36442	2.80243	0.72643
H	-1.87733	0.26330	-1.90523
H	-2.27886	-0.52632	1.01430
H	-1.60548	-2.23696	-0.43845
H	-4.29592	-0.21154	-1.27164
H	-4.07839	0.96473	0.03381
H	-6.74504	-1.41904	0.76638
H	-1.98860	1.88355	0.60478
H	-2.79773	2.74804	-1.62047
H	-1.53747	3.79677	-0.94026
H	-1.13808	2.65172	-2.24520
H	1.94319	-1.57738	-0.67025
H	5.74932	-0.15949	0.74176
H	4.71222	2.04285	1.26402

1d NMR Conformer 25
Energy: -875530.1720976

O	1.90767	2.91130	-0.11593
C	2.57816	1.74310	-0.00765
C	1.87325	0.52894	-0.08375
C	0.40915	0.43142	-0.26248
N	-0.19014	-0.61855	-0.67688
C	-1.62105	-0.29693	-0.72321
C	-2.43087	-1.43950	-0.10376
O	-2.08570	-2.65749	-0.73915
C	-3.93352	-1.27889	-0.30480
C	-4.60163	-0.32956	0.65707
O	-5.76935	0.11599	0.18197
O	-4.17122	-0.01330	1.74595
C	-1.72755	1.06213	-0.00185
C	-2.57017	2.10507	-0.70314
O	-0.34578	1.50562	0.05177
C	2.58059	-0.67819	0.00100
C	3.95379	-0.67638	0.16724
Cl	4.81228	-2.19544	0.28371
C	4.66097	0.52175	0.24889
C	3.96958	1.72013	0.15835
H	2.52876	3.66169	-0.07825
H	-1.92113	-0.21173	-1.78068
H	-2.20460	-1.48891	0.97197
H	-1.11511	-2.71876	-0.75064
H	-4.40481	-2.25734	-0.14583
H	-4.16584	-0.98370	-1.33346
H	-6.19258	0.68717	0.85824
H	-2.04817	0.92919	1.03783
H	-3.61065	1.76924	-0.76566
H	-2.55023	3.05293	-0.16060
H	-2.20012	2.26732	-1.71951
H	2.02987	-1.61138	-0.06122
H	5.73900	0.51769	0.38088
H	4.50873	2.66339	0.21363

1d NMR Conformer 24
Energy: -875534.0879638

O	-1.89752	2.46138	-1.37490
C	-2.59790	1.40563	-0.90597
C	-1.93856	0.43789	-0.12848
C	-0.51028	0.52518	0.23646
N	0.23229	-0.48642	0.47812
C	1.54774	0.03555	0.85649
C	2.60682	-0.53781	-0.08416
O	2.55525	-1.96026	-0.05541
C	4.01777	-0.14457	0.33973
C	5.11860	-0.61963	-0.59479
O	4.96587	-1.82448	-1.14877
O	6.11442	0.03255	-0.81769

C	1.40476	1.57468	0.77677
C	1.64592	2.29597	2.08638
O	0.02549	1.75577	0.37502
C	-2.64804	-0.68132	0.32331
C	-3.99071	-0.82559	0.01803
Cl	-4.86376	-2.22321	0.60078
C	-4.65581	0.13362	-0.74278
C	-3.95611	1.24015	-1.20210
H	-2.46847	3.03221	-1.92143
H	1.78889	-0.29664	1.87746
H	2.40007	-0.17821	-1.10514
H	1.66978	-2.25210	-0.34041
H	4.21830	-0.57661	1.33008
H	4.11887	0.94052	0.42079
H	4.10889	-2.22405	-0.87837
H	2.01901	2.00237	-0.02650
H	2.68904	2.16832	2.39275
H	1.44103	3.36420	1.98592
H	1.00141	1.88105	2.86717
H	-2.13033	-1.42570	0.92057
H	-5.71019	0.01561	-0.97586
H	-4.46152	1.99034	-1.80637

1d NMR Conformer 23
Energy: -875530.5521173

O	-1.55308	2.66258	-0.79243
C	-2.39940	1.65435	-0.48598
C	-1.86519	0.43767	-0.03150
C	-0.41674	0.22412	0.15979
N	0.18475	-0.88179	-0.05507
C	1.57629	-0.69147	0.37287
C	2.52828	-1.26330	-0.68196
O	2.18693	-2.61351	-0.94266
C	3.98066	-1.28518	-0.21960
C	4.70026	0.03330	-0.34595
O	5.76509	0.09621	0.46020
O	4.39225	0.93252	-1.09831
C	1.69307	0.82785	0.61956
C	2.37430	1.22322	1.91156
O	0.30576	1.25449	0.64951
C	-2.72186	-0.63393	0.23873
C	-4.08970	-0.48732	0.07544
Cl	-5.14877	-1.83288	0.42534
C	-4.63089	0.71976	-0.36048
C	-3.78388	1.78293	-0.64208
H	-2.04761	3.42754	-1.13810
H	1.73169	-1.26008	1.30452
H	2.44126	-0.66116	-1.59870
H	1.23230	-2.64666	-1.12575
H	4.52812	-1.99431	-0.85366
H	4.06542	-1.65366	0.80816
H	6.23084	0.94588	0.30935
H	2.15390	1.33148	-0.23842
H	3.41525	0.88281	1.90738
H	2.37138	2.30817	2.03941
H	1.86600	0.76167	2.76303
H	-2.30022	-1.57354	0.58317
H	-5.70493	0.82708	-0.48230
H	-4.19433	2.72591	-0.99614

1d NMR Conformer 22
Energy: -875532.5550836

O	2.22889	-2.65677	-0.74571
C	2.68063	-1.42096	-0.43764
C	1.76459	-0.45238	0.00564
C	0.32157	-0.72354	0.17473
N	-0.59521	0.14960	0.00329
C	-1.86583	-0.50233	0.33797
C	-2.83896	-0.40507	-0.84391
O	-2.25727	-0.95471	-2.01191
C	-3.29653	1.02978	-1.09387
C	-4.21895	1.55396	-0.02448
O	-4.46624	2.85920	-0.17493
O	-4.70190	0.89231	0.86963
C	-1.48662	-1.96156	0.67621
C	-1.92437	-2.42678	2.04773
O	-0.03770	-1.95164	0.60354
C	2.21408	0.84319	0.28242
C	3.55340	1.16205	0.13410
Cl	4.09999	2.78273	0.49583
C	4.47126	0.20594	-0.29492
C	4.03018	-1.07798	-0.58159
H	2.95933	-3.21029	-1.07784
H	-2.31548	-0.00071	1.20563
H	-3.71358	-1.02841	-0.62502
H	-1.44888	-0.45365	-2.22239
H	-3.84337	1.07585	-2.04308
H	-2.43690	1.70375	-1.18461
H	-5.08592	3.14984	0.52738
H	-1.83382	-2.64734	-0.10581
H	-3.01760	-2.42178	2.10324
H	-1.57140	-3.44115	2.24933
H	-1.53365	-1.75424	2.81741
H	1.49899	1.58797	0.61875
H	5.52071	0.46364	-0.40598
H	4.73535	-1.83021	-0.92848

1d NMR Conformer 21
Energy: -875537.2831227

O	0.26303	-2.13781	-1.00866
C	1.34018	-1.45631	-0.58702
C	1.28899	-0.09215	-0.25262
C	0.02167	0.63232	-0.30465
N	-1.11244	0.10320	-0.59868
C	-2.11576	1.16438	-0.52993
C	-3.22928	0.80239	0.45912
O	-2.75768	0.77595	1.79064
C	-3.90576	-0.51352	0.05294
C	-3.04344	-1.71360	0.33934
O	-2.70522	-2.39412	-0.75306
O	-2.67461	-2.04304	1.45021
C	-1.31548	2.42499	-0.12522
C	-1.35794	3.55097	-1.13163
O	0.05276	1.94201	-0.01754
C	2.45176	0.58209	0.13463
C	3.64710	-0.10704	0.19577
Cl	5.10394	0.72755	0.67897
C	3.70818	-1.46493	-0.12012
C	2.55914	-2.13274	-0.50932
H	-0.49491	-1.50864	-1.05765
H	-2.58056	1.29548	-1.51739
H	-3.99319	1.58693	0.41439
H	-2.40191	-0.10527	1.99161
H	-4.16085	-0.49441	-1.00988
H	-4.82770	-0.63122	0.63032
H	-2.16328	-3.16660	-0.49598
H	-1.60494	2.76792	0.87150
H	-2.38216	3.92679	-1.22303
H	-0.71485	4.37522	-0.81474
H	-1.02771	3.19781	-2.11276
H	2.40478	1.63702	0.38937
H	4.65653	-1.99110	-0.06639
H	2.58850	-3.18578	-0.77138

1d NMR Conformer 20
Energy: -875538.7888003

O	0.59304	-2.40651	-0.53628
C	1.68663	-1.65175	-0.34558
C	1.62535	-0.25538	-0.15443
C	0.32409	0.41303	-0.15837
N	-0.79644	-0.18809	-0.33895
C	-1.85611	0.81733	-0.21957
C	-2.73145	0.51313	1.00346
O	-1.95377	0.51641	2.18467
C	-3.48715	-0.80684	0.86269
C	-4.57848	-0.76241	-0.18404
O	-5.19739	-1.92056	-0.45419
O	-4.92652	0.24364	-0.75910
C	-1.09174	2.15708	-0.08775
C	-1.22541	3.06614	-1.29103
O	0.29729	1.73994	0.03893
C	2.80134	0.48180	0.03833
C	4.02048	-0.17043	0.04066
Cl	5.49082	0.74675	0.27749
C	4.09654	-1.55319	-0.14605
C	2.93575	-2.28594	-0.33755
H	-0.20564	-1.81632	-0.52624
H	-2.48459	0.80634	-1.11754
H	-3.45297	1.33047	1.11416
H	-1.29912	-0.20357	2.13825
H	-3.95847	-1.05075	1.82301
H	-2.79140	-1.62331	0.62877
H	-4.83668	-2.67269	0.05439
H	-1.34352	2.67411	0.84301
H	-2.26491	3.39376	-1.38721
H	-0.58984	3.94819	-1.18509
H	-0.94301	2.53086	-2.20296
H	2.74379	1.55635	0.18320
H	5.06290	-2.04938	-0.14169
H	2.97415	-3.36097	-0.48556

1d NMR Conformer 19
Energy: -875538.5023172

O	-1.25901	2.57279	-0.66481
C	-2.18671	1.63897	-0.40081
C	-1.86019	0.29704	-0.11448
C	-0.45709	-0.11773	-0.10374
N	0.53324	0.66487	-0.33402
C	1.76208	-0.12621	-0.20238
C	2.60488	0.45316	0.94130
O	2.92906	1.80264	0.67798
C	3.93155	-0.27403	1.18862
C	4.94427	-0.04724	0.09213
O	4.62690	-0.69543	-1.03817
O	5.94326	0.62720	0.20131
C	1.25754	-1.56761	0.04960
C	1.57081	-2.52923	-1.07680
O	-0.18560	-1.40609	0.16260
C	-2.87446	-0.63215	0.15390
C	-4.19475	-0.22258	0.13790
Cl	-5.46333	-1.37864	0.47514
C	-4.53265	1.10338	-0.14486
C	-3.53306	2.02487	-0.41271
H	-0.36176	2.15149	-0.62370
H	2.33392	-0.06018	-1.13368

H	2.00801	0.36965	1.86420
H	2.10334	2.30818	0.58151
H	3.75892	-1.35032	1.29666
H	4.36826	0.10506	2.11372
H	5.31004	-0.50913	-1.71706
H	1.58945	-1.96528	1.01546
H	2.65569	-2.64338	-1.16080
H	1.12173	-3.50782	-0.89288
H	1.19065	-2.13281	-2.02358
H	-2.61401	-1.66347	0.37205
H	-5.57538	1.40806	-0.15376
H	-3.77498	3.06001	-0.63463

1d NMR Conformer 18
Energy: -875540.8857989

O	-1.37394	2.53874	-0.86935
C	-2.26045	1.62744	-0.43665
C	-1.91482	0.28204	-0.19301
C	-0.53821	-0.15914	-0.41532
N	0.41373	0.60234	-0.81475
C	1.62786	-0.21366	-0.89243
C	2.69347	0.35227	0.05167
O	2.96075	1.70602	-0.25605
C	4.01231	-0.38631	-0.09632
C	5.01697	0.05149	0.94303
O	6.27369	-0.05207	0.49967
O	4.73915	0.42463	2.06125
C	1.15235	-1.63993	-0.51561
C	1.27492	-2.65366	-1.63341
O	-0.25201	-1.45281	-0.19104
C	-2.88491	-0.62419	0.25584
C	-4.18148	-0.18880	0.45885
Cl	-5.39448	-1.31763	1.01717
C	-4.53770	1.14125	0.22170
C	-3.58147	2.04046	-0.22326
H	-0.49102	2.10074	-0.97619
H	2.02113	-0.17685	-1.91850
H	2.33173	0.25830	1.08739
H	2.14862	2.22312	-0.11755
H	4.42609	-0.22368	-1.09599
H	3.87719	-1.46829	0.03538
H	6.88856	0.20221	1.22068
H	1.62911	-2.00173	0.40364
H	2.33111	-2.80739	-1.87630
H	0.84168	-3.61222	-1.33926
H	0.76235	-2.28912	-2.52885
H	-2.60989	-1.65842	0.43978
H	-5.56114	1.46721	0.38525
H	-3.83961	3.07781	-0.41432

1d NMR Conformer 17
Energy: -875537.6474234

O	2.56356	2.58170	0.90310
C	2.79767	1.30066	0.54755
C	1.84055	0.42834	-0.00410
C	0.44514	0.81844	-0.26044
N	-0.49700	0.03543	-0.61510
C	-1.69553	0.86027	-0.78487
C	-2.86061	0.27269	0.01208
O	-2.52647	0.18318	1.39556
C	-3.28355	-1.09363	-0.53389
C	-4.49757	-1.69523	0.15310
O	-4.64238	-1.45243	1.45903
O	-5.30570	-2.38480	-0.42828
C	-1.28879	2.27203	-0.30423
C	-1.56204	3.38643	-1.28824
O	0.14579	2.13523	-0.10795
C	2.20906	-0.88790	-0.32448
C	3.49987	-1.32089	-0.10009
Cl	3.94617	-2.96073	-0.50834
C	4.45784	-0.46326	0.44741
C	4.10191	0.83490	0.76649
H	1.64705	2.84153	0.70626
H	-1.97766	0.87231	-1.84792
H	-3.70601	0.97166	-0.03492
H	-1.68416	-0.30545	1.48783
H	-2.44955	-1.79841	-0.41697
H	-3.51132	-1.03060	-1.60085
H	-3.91409	-0.87924	1.78770
H	-1.71699	2.49032	0.68092
H	-2.64124	3.47154	-1.44949
H	-1.19436	4.34257	-0.90906
H	-1.08109	3.17231	-2.24691
H	1.46320	-1.55098	-0.75194
H	5.47142	-0.81420	0.61887
H	4.82669	1.52090	1.19459

1d NMR Conformer 16
Energy: -875534.1286201

O	-2.28894	2.83355	-0.47044
C	-2.74202	1.57845	-0.26352
C	-1.92814	0.45367	-0.03143
C	-0.45699	0.51163	0.01474
N	0.32866	-0.47780	0.17014
C	1.69877	0.04907	0.15822
C	2.49362	-0.66749	-0.93847
O	2.50146	-2.06108	-0.70437
C	3.95695	-0.22835	-1.04185

C	4.73860	-0.59056	0.19850
O	5.61815	-1.57293	-0.00832
O	4.59507	-0.05041	1.27621
C	1.54722	1.57103	-0.06857
C	2.12878	2.42877	1.03319
O	0.10321	1.74456	-0.11478
C	-2.52721	-0.80064	0.16695
C	-3.90097	-0.92863	0.13372
Cl	-4.63111	-2.49756	0.38546
C	-4.71828	0.18111	-0.09637
C	-4.13550	1.42057	-0.29247
H	-1.31752	2.86795	-0.42637
H	2.16902	-0.16197	1.12599
H	2.00897	-0.44027	-1.90188
H	1.58085	-2.35316	-0.58601
H	4.01412	0.85743	-1.17071
H	4.40688	-0.70764	-1.91316
H	6.08371	-1.76443	0.83362
H	1.91876	1.88003	-1.05357
H	3.20829	2.25932	1.08732
H	1.93970	3.48885	0.84936
H	1.69005	2.14672	1.99505
H	-1.88990	-1.66089	0.34722
H	-5.79854	0.07004	-0.11975
H	-4.74674	2.29972	-0.47325

1d NMR Conformer 15
Energy: -875534.9461645

O	-2.35877	-2.83392	0.20278
C	-2.63854	-1.51739	0.09874
C	-1.68070	-0.49787	-0.05802
C	-0.23077	-0.74834	-0.12817
N	0.67410	0.13576	-0.28299
C	1.96377	-0.55868	-0.23226
C	2.74969	-0.11204	1.00887
O	2.03482	-0.41748	2.18940
C	3.10035	1.37985	0.96707
C	3.92589	1.77307	-0.23099
O	4.94984	0.93357	-0.43594
O	3.71552	2.73606	-0.93581
C	1.60960	-2.06384	-0.19961
C	1.93382	-2.80735	-1.47808
O	0.16741	-2.04312	-0.01446
C	-2.10536	0.83724	-0.15397
C	-3.44920	1.14597	-0.09445
Cl	-3.96058	2.81390	-0.21537
C	-4.40848	0.14184	0.06159
C	-3.99794	-1.17608	0.15664
H	-1.40075	-2.99489	0.15171
H	2.54850	-0.31708	-1.13067
H	3.67165	-0.70241	1.05560
H	1.20853	0.09837	2.20211
H	3.67815	1.62173	1.86646
H	2.19165	1.98634	0.96190
H	5.46172	1.23650	-1.21566
H	2.02700	-2.56094	0.68097
H	3.01830	-2.83104	-1.62110
H	1.56592	-3.83511	-1.43675
H	1.48029	-2.30049	-2.33561
H	-1.35751	1.61499	-0.27461
H	-5.46387	0.39455	0.10770
H	-4.72187	-1.97631	0.27816

1d NMR Conformer 14
Energy: -875533.0743414

O	-2.05570	2.72625	-0.76424
C	-2.67631	1.57362	-0.42902
C	-1.89615	0.46497	-0.06128
C	-0.42202	0.50997	0.00671
N	0.34078	-0.47864	-0.26299
C	1.70935	-0.03938	0.02108
C	2.59848	-0.31500	-1.19096
O	2.56717	-1.69897	-1.51909
C	4.06081	0.05525	-0.94683
C	4.69557	-0.65185	0.23916
O	4.46697	-1.96382	0.34476
O	5.39958	-0.08733	1.04747
C	1.58336	1.45920	0.37253
C	2.21987	1.86100	1.68521
O	0.14793	1.65359	0.44174
C	-2.52112	-0.74992	0.24100
C	-3.90172	-0.85097	0.19282
Cl	-4.66968	-2.37124	0.58623
C	-4.68583	0.24563	-0.15851
C	-4.06978	1.44993	-0.47037
H	-2.70693	3.39845	-1.03468
H	2.09192	-0.61914	0.87697
H	2.22351	0.27658	-2.03850
H	1.63977	-1.99906	-1.53246
H	4.16899	1.13115	-0.79060
H	4.63755	-0.21083	-1.84102
H	3.82271	-2.25461	-0.33749
H	1.94243	2.09388	-0.44937
H	3.30144	1.69626	1.63612
H	2.03757	2.91610	1.90086
H	1.81398	1.25477	2.50023
H	-1.90978	-1.60295	0.51936
H	-5.76799	0.15897	-0.19067

H	-4.67074	2.30963	-0.75803

1d NMR Conformer 13
Energy: -875538.6297079

O	-1.27262	2.58949	-0.61267
C	-2.20087	1.64951	-0.37113
C	-1.87326	0.30442	-0.10245
C	-0.46926	-0.10666	-0.08266
N	0.52287	0.68370	-0.27395
C	1.74911	-0.11410	-0.17034
C	2.62883	0.45550	0.94850
O	2.96788	1.79935	0.67188
C	3.94793	-0.29861	1.14362
C	4.84303	-0.18060	-0.06702
O	5.89290	0.61699	0.13647
O	4.64119	-0.74985	-1.12014
C	1.24553	-1.55399	0.09673
C	1.61757	-2.54750	-0.98208
O	-0.20099	-1.40348	0.14461
C	-2.88748	-0.63192	0.13911
C	-4.20914	-0.22641	0.11441
Cl	-5.47712	-1.39205	0.41682
C	-4.54770	1.10298	-0.15028
C	-3.54787	2.03185	-0.39159
H	-0.37533	2.16993	-0.57123
H	2.29908	-0.05343	-1.11638
H	2.06015	0.38361	1.88967
H	2.14687	2.31158	0.57012
H	3.74917	-1.36167	1.31221
H	4.45693	0.10785	2.01927
H	6.42323	0.65980	-0.68787
H	1.54178	-1.91593	1.08879
H	2.70722	-2.63369	-1.02945
H	1.18646	-3.52994	-0.77635
H	1.25843	-2.19447	-1.95378
H	-2.62642	-1.66584	0.34388
H	-5.59116	1.40499	-0.16678
H	-3.79096	3.06941	-0.60045

1d NMR Conformer 12
Energy: -875542.2180768

O	0.69343	-2.28938	-0.99481
C	1.77229	-1.60543	-0.58150
C	1.72245	-0.24237	-0.22598
C	0.45525	0.48015	-0.32008
N	-0.65286	-0.05136	-0.69546
C	-1.66614	1.00491	-0.69271
C	-2.86897	0.58612	0.15227
O	-2.46567	0.29208	1.48731
C	-3.60744	-0.60270	-0.46942
C	-4.87637	-1.00130	0.26474
O	-4.87840	-0.86774	1.59363
O	-5.85247	-1.43884	-0.30241
C	-0.92837	2.24315	-0.12867
C	-0.98252	3.46954	-1.01129
O	0.44925	1.78667	-0.01502
C	2.88237	0.41762	0.20297
C	4.07437	-0.27858	0.27322
Cl	5.52511	0.54128	0.80226
C	4.13856	-1.62983	-0.07759
C	2.99404	-2.28540	-0.50173
H	-0.08854	-1.68100	-1.00158
H	-2.01215	1.18290	-1.72100
H	-3.54902	1.44343	0.24047
H	-1.75518	-0.38012	1.46556
H	-2.94116	-1.47584	-0.47979
H	-3.88379	-0.38930	-1.50510
H	-4.02030	-0.50381	1.90540
H	-1.26365	2.46667	0.89037
H	-2.01946	3.80716	-1.10461
H	-0.39191	4.28275	-0.58373
H	-0.59974	3.23592	-2.00895
H	2.83445	1.46829	0.47297
H	5.08377	-2.16181	-0.01715
H	3.02362	-3.33508	-0.77813

1d NMR Conformer 11
Energy: -875533.2600968

O	-1.61356	2.84928	-0.56321
C	-2.31500	1.71129	-0.37460
C	-1.76404	0.47530	0.01317
C	-0.32800	0.27010	0.26407
N	0.22551	-0.82590	0.60382
C	1.66901	-0.57607	0.69578
C	2.38534	-1.43707	-0.35704
O	1.96568	-2.78162	-0.24933
C	3.90439	-1.47119	-0.16048
C	4.58163	-0.15112	-0.42069
O	4.52088	0.20203	-1.71027
O	5.11311	0.53560	0.42572
C	1.81918	0.95356	0.50027
C	2.22403	1.70102	1.75291
O	0.47408	1.35597	0.11559
C	-2.60810	-0.63558	0.17482
C	-3.96490	-0.51587	-0.04550
Cl	-5.00269	-1.90736	0.16492
C	-4.52243	0.70579	-0.43288
C	-3.69754	1.80458	-0.59409

H	-0.66717	2.71446	-0.38343
H	2.02370	-0.88473	1.68915
H	2.14679	-1.03764	-1.35632
H	0.99351	-2.79064	-0.21250
H	4.30851	-2.20967	-0.86009
H	4.13485	-1.78354	0.86072
H	4.96810	1.06705	-1.82931
H	2.45720	1.21776	-0.34894
H	3.24243	1.41369	2.02882
H	2.19681	2.78037	1.58666
H	1.54751	1.44879	2.57542
H	-2.17190	-1.58327	0.47536
H	-5.59171	0.78964	-0.60438
H	-4.10411	2.76579	-0.89398

1d NMR Conformer 10
Energy: -875539.6733314

O	0.66625	-2.47141	-0.31789
C	1.73471	-1.66395	-0.21341
C	1.62670	-0.26134	-0.12127
C	0.30514	0.36663	-0.13174
N	-0.80521	-0.27513	-0.20634
C	-1.88724	0.70877	-0.15934
C	-2.79161	0.44691	1.05101
O	-2.04056	0.49509	2.24663
C	-3.53716	-0.88685	0.93095
C	-4.42749	-0.97249	-0.28067
O	-5.14556	0.14490	-0.45339
O	-4.50376	-1.92272	-1.02605
C	-1.16234	2.07449	-0.07103
C	-1.43344	3.00567	-1.23273
O	0.24606	1.70551	-0.06177
C	2.78002	0.52758	-0.01651
C	4.02246	-0.07867	-0.00441
Cl	5.46267	0.90289	0.12762
C	4.14274	-1.46679	-0.09693
C	3.00518	-2.25050	-0.20137
H	-0.15662	-1.91573	-0.32278
H	-2.48583	0.64230	-1.08034
H	-3.51548	1.26549	1.12578
H	-1.40995	-0.24774	2.25749
H	-4.16765	-1.01219	1.81913
H	-2.83179	-1.72157	0.88741
H	-5.71805	0.04053	-1.24343
H	-1.35951	2.56194	0.89020
H	-2.49257	3.28206	-1.24114
H	-0.83732	3.91762	-1.14833
H	-1.19421	2.50944	-2.17848
H	2.68831	1.60740	0.05535
H	5.12642	-1.92876	-0.08661
H	3.07992	-3.33155	-0.27483

1d NMR Conformer 9
Energy: -875537.6349924

O	1.59354	2.73708	0.42169
C	2.33334	1.63869	0.20189
C	1.77972	0.34343	0.13964
C	0.33964	0.16373	0.31942
N	-0.49335	1.11844	0.52654
C	-1.83313	0.52600	0.61149
C	-2.69238	1.04569	-0.55319
O	-2.64686	2.45637	-0.60452
C	-4.17693	0.70454	-0.38505
C	-4.47869	-0.76803	-0.47563
O	-4.28313	-1.24739	-1.70926
O	-4.84213	-1.46096	0.45045
C	-1.56288	-1.00143	0.59460
C	-1.80703	-1.68225	1.92479
O	-0.14578	-1.08638	0.26885
C	2.60604	-0.76543	-0.08916
C	3.96516	-0.57834	-0.25665
Cl	4.99898	-1.95931	-0.54453
C	4.52727	0.69972	-0.19905
C	3.71425	1.79815	0.02947
H	0.64598	2.46895	0.53043
H	-2.30605	0.83667	1.55328
H	-2.31144	0.61171	-1.49195
H	-1.71551	2.73406	-0.64882
H	-4.72225	1.21830	-1.18275
H	-4.52883	1.07161	0.58200
H	-4.48497	-2.20764	-1.71876
H	-2.08030	-1.51826	-0.21952
H	-2.87530	-1.64729	2.15571
H	-1.48844	-2.72646	1.88805
H	-1.25392	-1.16785	2.71702
H	2.17094	-1.75936	-0.13262
H	5.59768	0.82866	-0.33271
H	4.13170	2.79941	0.07869

1d NMR Conformer 8
Energy: -875537.2548032

O	-2.29425	2.72922	-0.91122
C	-2.74464	1.49563	-0.59796
C	-1.95975	0.45962	-0.05684
C	-0.52458	0.59835	0.24078
N	0.23743	-0.31390	0.69962
C	1.57369	0.26942	0.84073
C	2.57336	-0.55884	0.03272

O	2.54711	-1.91012	0.47567
C	4.00306	-0.06426	0.22513
C	5.04368	-0.78967	-0.61290
O	4.88056	-2.10421	-0.77909
O	6.00344	-0.22803	-1.09253
C	1.43592	1.73187	0.35292
C	1.76229	2.77964	1.39509
O	0.02763	1.81857	0.00764
C	-2.55490	-0.78122	0.22318
C	-3.89621	-0.98284	-0.03147
Cl	-4.62182	-2.53310	0.32244
C	-4.68408	0.03869	-0.56867
C	-4.10551	1.26431	-0.84668
H	-1.34843	2.82363	-0.70612
H	1.87431	0.22594	1.89812
H	2.29158	-0.50822	-1.03144
H	1.65107	-2.27133	0.34533
H	4.27942	-0.19494	1.28055
H	4.08968	0.99812	-0.01592
H	4.05816	-2.41225	-0.33864
H	1.98921	1.90852	-0.57800
H	2.82215	2.71592	1.66084
H	1.56000	3.78379	1.01588
H	1.16723	2.61041	2.29728
H	-1.94126	-1.57264	0.64226
H	-5.73912	-0.12968	-0.76477
H	-4.69493	2.07506	-1.26427

1d NMR Conformer 7
Energy: -875541.7962210

O	1.34959	2.53915	0.84044
C	2.23991	1.62930	0.41333
C	1.90309	0.27980	0.17848
C	0.53017	-0.17029	0.40294
N	-0.43037	0.58658	0.79265
C	-1.63413	-0.24182	0.88089
C	-2.70571	0.30003	-0.06701
O	-2.97594	1.66498	0.23031
C	-4.02446	-0.44910	0.10062
C	-5.11725	-0.03394	-0.87044
O	-5.20793	1.26600	-1.15767
O	-5.90095	-0.82239	-1.35055
C	-1.14490	-1.66804	0.51869
C	-1.25612	-2.66967	1.64819
O	0.25665	-1.46816	0.19141
C	2.87964	-0.62340	-0.26311
C	4.17313	-0.18106	-0.46828
Cl	5.39387	-1.30570	-1.01807
C	4.52074	1.15311	-0.24035
C	3.55869	2.04918	0.19765
H	0.46952	2.09964	0.95351
H	-2.03033	-0.19697	1.90546
H	-2.34002	0.20767	-1.10233
H	-2.18244	2.20187	0.04963
H	-4.39991	-0.26589	1.11709
H	-3.88790	-1.52656	-0.01846
H	-4.49555	1.76996	-0.70481
H	-1.61803	-2.04514	-0.39597
H	-2.31065	-2.83400	1.89100
H	-0.81036	-3.62557	1.36482
H	-0.74923	-2.28843	2.53980
H	2.61135	-1.66069	-0.43950
H	5.54228	1.48425	-0.40513
H	3.81000	3.08932	0.38241

1d NMR Conformer 6
Energy: -875533.7052959

O	-1.75805	2.87849	-0.36725
C	-2.44553	1.72304	-0.24396
C	-1.87139	0.46954	0.04081
C	-0.42631	0.26997	0.23641
N	0.17565	-0.84942	0.31622
C	1.59039	-0.55297	0.58127
C	2.47866	-1.44086	-0.29446
O	2.14287	-2.79860	-0.07565
C	3.95941	-1.32046	0.04756
C	4.65138	-0.12395	-0.55449
O	5.79445	0.15577	0.07924
O	4.25676	0.50909	-1.51087
C	1.71978	0.96394	0.33440
C	2.50434	1.73274	1.37354
O	0.32930	1.39561	0.35915
C	-2.69659	-0.66264	0.13280
C	-4.05936	-0.54627	-0.05364
Cl	-5.07416	-1.96521	0.06699
C	-4.63996	0.69289	-0.33618
C	-3.83282	1.81324	-0.42901
H	-0.80881	2.74090	-0.20312
H	1.80204	-0.80271	1.63385
H	2.31912	-1.16829	-1.34834
H	1.18065	-2.88898	-0.18468
H	4.47296	-2.20465	-0.35119
H	4.11976	-1.33035	1.13109
H	6.23601	0.90657	-0.37254
H	2.08654	1.16729	-0.67778
H	3.54513	1.39331	1.38577
H	2.49949	2.80284	1.15456

H	2.07778	1.56756	2.36681
H	-2.24244	-1.62354	0.35476
H	-5.71347	0.77448	-0.47998
H	-4.25819	2.78783	-0.64904

1d NMR Conformer 5

Energy: -875535.6156983

O	-2.48564	-2.78040	0.18536
C	-2.72093	-1.45491	0.08488
C	-1.72791	-0.46749	-0.05680
C	-0.28658	-0.76790	-0.11180
N	0.64557	0.07376	-0.32653
C	1.91393	-0.65732	-0.23531
C	2.72235	-0.15009	0.96718
O	1.99493	-0.33672	2.16708
C	3.13980	1.31001	0.81288
C	4.18160	1.52112	-0.25518
O	4.41611	2.81896	-0.47437
O	4.76513	0.63706	-0.84639
C	1.51066	-2.14351	-0.09340
C	1.80973	-2.98826	-1.31374
O	0.06968	-2.06454	0.08977
C	-2.10713	0.88072	-0.15829
C	-3.44098	1.23335	-0.11687
Cl	-3.89586	2.91732	-0.24215
C	-4.43475	0.26132	0.02517
C	-4.06903	-1.06954	0.12440
H	-1.53173	-2.97053	0.16262
H	2.50099	-0.49533	-1.14717
H	3.61824	-0.77489	1.05916
H	1.19006	0.21094	2.13715
H	3.56580	1.66618	1.75824
H	2.27357	1.94391	0.59249
H	5.11434	2.90640	-1.15745
H	1.91305	-2.58907	0.82111
H	2.89280	-3.05404	-1.45438
H	1.41186	-3.99912	-1.19793
H	1.37024	-2.53177	-2.20620
H	-1.33256	1.63360	-0.26778
H	-5.48175	0.54866	0.05766
H	-4.82047	-1.84571	0.23442

1d NMR Conformer 4

Energy: -875538.2946366

O	1.66007	2.74958	0.20747
C	2.41196	1.64569	0.08085
C	1.87218	0.34401	0.10274
C	0.43256	0.15310	0.27232
N	-0.42157	1.10645	0.37452
C	-1.73669	0.49541	0.58646
C	-2.77293	1.10158	-0.36673
O	-2.79856	2.50962	-0.21693
C	-4.18907	0.63353	-0.04664
C	-4.56621	-0.70828	-0.62030
O	-5.58649	-1.25906	0.04242
O	-4.03975	-1.24038	-1.57367
C	-1.47814	-1.01811	0.39266
C	-1.99520	-1.89390	1.51159
O	-0.02516	-1.10689	0.33214
C	2.71266	-0.76856	-0.03266
C	4.07220	-0.57938	-0.18784
Cl	5.12467	-1.96631	-0.35640
C	4.62097	0.70499	-0.21284
C	3.79325	1.80734	-0.07881
H	0.71535	2.47653	0.32390
H	-2.06083	0.72113	1.61406
H	-2.51117	0.82541	-1.39956
H	-1.89987	2.85416	-0.35329
H	-4.88890	1.35748	-0.48294
H	-4.37439	0.63611	1.03306
H	-5.83075	-2.10439	-0.38880
H	-1.84028	-1.36604	-0.57946
H	-3.08766	-1.81944	1.56283
H	-1.73104	-2.94040	1.34477
H	-1.58473	-1.56742	2.47116
H	2.28812	-1.76788	-0.01358
H	5.69217	0.83514	-0.33628
H	4.19944	2.81415	-0.09510

1d NMR Conformer 3

Energy: -875536.0724311

O	2.18889	2.88115	0.39550
C	2.67947	1.63816	0.20579
C	1.89968	0.48095	0.01952
C	0.42813	0.48954	0.01026
N	-0.32869	-0.53538	0.00851
C	-1.70872	-0.04664	-0.04269
C	-2.53061	-0.70457	1.06595
O	-2.49334	-2.11966	0.93513
C	-4.00167	-0.29195	1.03136
C	-4.70827	-0.59331	-0.28005
O	-4.50389	-1.80401	-0.80598
O	-5.44569	0.19518	-0.82979
C	-1.60272	1.48864	0.09602
C	-2.32793	2.28098	-0.96834
O	-0.17087	1.71109	-0.01379
C	2.53557	-0.75855	-0.15762
C	3.91332	-0.84039	-0.14977

Cl	4.69031	-2.39007	-0.37635
C	4.69700	0.30179	0.03426
C	4.07756	1.52652	0.21024
H	1.21711	2.88864	0.35155
H	-2.14103	-0.32847	-1.01668
H	-2.10575	-0.40880	2.03601
H	-1.56976	-2.40445	0.80584
H	-4.11342	0.77602	1.23291
H	-4.52884	-0.83600	1.82472
H	-3.83112	-2.29510	-0.28520
H	-1.88821	1.81888	1.10395
H	-3.40333	2.08648	-0.90038
H	-2.15967	3.35263	-0.84151
H	-1.98351	1.97866	-1.96139
H	1.92406	-1.64382	-0.30288
H	5.78065	0.22770	0.03730
H	4.66288	2.42945	0.35605

1d NMR Conformer 2
Energy: -875540.2859564

O	-1.31055	2.63154	-0.42394
C	-2.21812	1.65329	-0.27425
C	-1.86352	0.30384	-0.06914
C	-0.45202	-0.07431	-0.01855
N	0.52747	0.74970	-0.11800
C	1.76197	-0.03351	-0.05452
C	2.69432	0.52942	1.01962
O	3.01137	1.88770	0.74807
C	4.02064	-0.22701	1.09257
C	4.80462	-0.24900	-0.20975
O	4.91746	0.91099	-0.86321
O	5.33061	-1.24858	-0.64680
C	1.28745	-1.47657	0.24064
C	1.80280	-2.52622	-0.71820
O	-0.15869	-1.37712	0.12964
C	-2.85982	-0.67104	0.08055
C	-4.19015	-0.29936	0.02646
Cl	-5.43463	-1.51313	0.21370
C	-4.55582	1.03403	-0.17709
C	-3.57418	2.00062	-0.32646
H	-0.40301	2.24042	-0.37108
H	2.26718	0.03009	-1.03165
H	2.18998	0.45083	1.99350
H	2.19128	2.39632	0.61160
H	3.86391	-1.26264	1.40340
H	4.64852	0.25614	1.85095
H	4.38134	1.60788	-0.42700
H	1.49269	-1.75591	1.28283
H	2.89349	-2.58771	-0.64348
H	1.38156	-3.50656	-0.48519
H	1.54011	-2.25817	-1.74563
H	-2.57750	-1.70758	0.23815
H	-5.60601	1.30912	-0.21807
H	-3.83792	3.04175	-0.48656

1d NMR Conformer 1
Energy: -875540.4403551

O	0.67749	-2.46249	-0.32923
C	1.75968	-1.67429	-0.22970
C	1.67338	-0.27139	-0.11485
C	0.35951	0.37262	-0.10503
N	-0.75611	-0.25827	-0.18140
C	-1.82814	0.73999	-0.14491
C	-2.78956	0.44689	1.01332
O	-2.08297	0.39330	2.23691
C	-3.58640	-0.83605	0.78859
C	-4.60830	-0.71424	-0.31223
O	-5.18554	-1.88712	-0.58831
O	-4.89980	0.31496	-0.88318
C	-1.08977	2.08815	0.02498
C	-1.37737	3.10644	-1.05525
O	0.31673	1.71132	-0.02261
C	2.83890	0.49973	-0.01230
C	4.07206	-0.12510	-0.02524
Cl	5.52886	0.83406	0.10313
C	4.17248	-1.51372	-0.14033
C	3.02234	-2.27982	-0.24183
H	-0.13437	-1.89007	-0.31313
H	-2.38738	0.71085	-1.08912
H	-3.48413	1.28996	1.10397
H	-1.46421	-0.35860	2.21100
H	-4.12676	-1.09200	1.70744
H	-2.92224	-1.67919	0.56378
H	-5.85531	-1.75657	-1.29213
H	-1.26167	2.50198	1.02467
H	-2.43687	3.37971	-1.02391
H	-0.78198	4.01076	-0.90951
H	-1.15510	2.68680	-2.04086
H	2.76274	1.57929	0.07637
H	5.14964	-1.98847	-0.14985
H	3.07976	-3.36046	-0.33210

1c NMR Conformer 29
Energy: -875533.1911586

O	2.51552	2.83640	0.04728
C	2.89786	1.54172	0.05239
C	2.03668	0.44700	-0.14820
C	0.59038	0.58828	-0.37848

N	-0.26079	-0.35704	-0.42911
C	-1.54909	0.26288	-0.77264
C	-2.68861	-0.44742	-0.04313
O	-2.62891	-1.83868	-0.29510
C	-4.05166	0.01467	-0.54931
C	-5.17276	-0.71320	0.15081
O	-5.09148	-0.59926	1.48184
O	-6.05812	-1.32456	-0.40548
C	-1.33571	1.75963	-0.45355
C	-1.72282	2.22253	0.94128
O	0.11732	1.85601	-0.55848
C	2.55904	-0.85657	-0.11756
C	3.90492	-1.05985	0.10860
Cl	4.54265	-2.68757	0.13943
C	4.76891	0.02026	0.31032
C	4.26188	1.30710	0.28064
H	1.56147	2.91928	-0.12417
H	-1.70632	0.12440	-1.85318
H	-2.60790	-0.26093	1.03651
H	-1.73715	-2.15021	-0.06270
H	-4.13986	-0.18066	-1.62057
H	-4.18356	1.08841	-0.37343
H	-5.83787	-1.08556	1.89022
H	-1.74990	2.41234	-1.22481
H	-2.80660	2.19498	1.08371
H	-1.25495	1.59223	1.70369
H	-1.38879	3.25236	1.08658
H	1.88583	-1.69311	-0.27747
H	5.82686	-0.15119	0.48659
H	4.91043	2.16430	0.43488

1c NMR Conformer 28
Energy: -875525.8315958

O	2.01561	2.88970	-0.50027
C	2.64476	1.70824	-0.32055
C	1.88509	0.53505	-0.17227
C	0.40788	0.50467	-0.17652
N	-0.28673	-0.55309	-0.36167
C	-1.69907	-0.13060	-0.35616
C	-2.58141	-1.22726	0.28952
O	-1.97300	-2.49970	0.14522
C	-3.94760	-1.36201	-0.37612
C	-4.84181	-0.16118	-0.24177
O	-6.02718	-0.35371	-0.82893
O	-4.56481	0.85374	0.36310
C	-1.64409	1.26231	0.31337
C	-1.83631	1.30999	1.81826
O	-0.25868	1.65293	0.04395
C	2.54591	-0.69222	-0.01793
C	3.92741	-0.74604	0.00211
Cl	4.73000	-2.28734	0.20742
C	4.68993	0.41272	-0.13630
C	4.04396	1.62844	-0.29870
H	2.66714	3.60714	-0.61043
H	-2.00411	-0.01758	-1.40858
H	-2.71732	-1.01211	1.35741
H	-1.01271	-2.35635	0.07574
H	-4.47528	-2.22275	0.05003
H	-3.81648	-1.57931	-1.44309
H	-6.58198	0.44486	-0.69735
H	-2.27751	1.99040	-0.19125
H	-2.88085	1.12686	2.07393
H	-1.20452	0.56655	2.31611
H	-1.55405	2.30138	2.18043
H	1.95238	-1.59454	0.09039
H	5.77482	0.36427	-0.11871
H	4.62413	2.54143	-0.41529

1c NMR Conformer 27
Energy: -875537.7357265

O	0.70578	-2.42462	-0.31249
C	1.80729	-1.67212	-0.15983
C	1.78468	-0.26322	-0.22270
C	0.51989	0.42816	-0.47376
N	-0.60903	-0.16082	-0.63387
C	-1.61195	0.87654	-0.90029
C	-2.86370	0.62484	-0.04912
O	-2.54765	0.45526	1.31849
C	-3.62775	-0.58857	-0.57485
C	-4.94147	-0.76506	0.14456
O	-5.27353	-2.05201	0.29224
O	-5.64545	0.14335	0.52742
C	-0.84611	2.21076	-0.66199
C	-1.18282	3.01920	0.57700
O	0.54103	1.76718	-0.55309
C	2.96801	0.46794	-0.05269
C	4.15557	-0.20186	0.17615
Cl	5.63485	0.70674	0.38561
C	4.19222	-1.59692	0.24043
C	3.02456	-2.32387	0.07298
H	-0.06893	-1.82531	-0.47354
H	-1.90764	0.81057	-1.95593
H	-3.52052	1.50006	-0.09688
H	-1.90944	-0.27630	1.40118
H	-3.02681	-1.49754	-0.47836
H	-3.86308	-0.46079	-1.63971
H	-6.15131	-2.10606	0.72674
H	-0.89349	2.84206	-1.55272

H	-2.21831	3.36833	0.53187
H	-1.06213	2.41940	1.48020
H	-0.52821	3.89265	0.62577
H	2.94125	1.55234	-0.10341
H	5.13400	-2.10774	0.42084
H	3.03324	-3.40880	0.11973

1c NMR Conformer 26
Energy: -875526.0295562

O	1.88507	2.78279	0.30299
C	2.58866	1.64315	0.12214
C	1.89233	0.44064	-0.08892
C	0.41995	0.36865	-0.15387
N	-0.27542	-0.61876	0.26347
C	-1.66278	-0.34495	-0.16058
C	-2.66405	-0.91724	0.86483
O	-2.12968	-2.08313	1.47088
C	-3.97063	-1.39101	0.23617
C	-4.80936	-0.32607	-0.41255
O	-5.92235	-0.83519	-0.95187
O	-4.53982	0.85567	-0.45560
C	-1.64521	1.18076	-0.40971
C	-1.95198	2.06905	0.78404
O	-0.23778	1.38601	-0.74496
C	2.60592	-0.75524	-0.22625
C	3.99006	-0.75007	-0.16971
Cl	4.86713	-2.25165	-0.35283
C	4.69078	0.43767	0.02565
C	3.98720	1.62539	0.17361
H	2.48727	3.52904	0.47824
H	-1.81315	-0.87125	-1.11728
H	-2.87391	-0.16438	1.63671
H	-1.17423	-1.94476	1.58354
H	-4.58257	-1.87443	1.00604
H	-3.75555	-2.16312	-0.51241
H	-6.44024	-0.10875	-1.35876
H	-2.22523	1.46977	-1.28502
H	-3.01333	2.02708	1.03026
H	-1.36272	1.76414	1.65535
H	-1.68625	3.09924	0.53532
H	2.05827	-1.67950	-0.38372
H	5.77623	0.43540	0.06530
H	4.52334	2.55721	0.33973

1c NMR Conformer 25
Energy: -875537.3319242

O	-1.28181	2.61046	0.06918
C	-2.24416	1.67326	0.07308
C	-1.97568	0.30402	-0.12579
C	-0.60177	-0.13430	-0.36380
N	0.42277	0.63776	-0.36380
C	1.56876	-0.19103	-0.76464
C	2.83466	0.22518	-0.01818
O	3.07745	1.60655	-0.21207
C	4.06245	-0.49460	-0.56508
C	5.31763	-0.06366	0.15373
O	5.21468	-0.21041	1.47956
O	6.31797	0.35243	-0.38739
C	1.05526	-1.62961	-0.53030
C	1.34583	-2.23502	0.83386
O	-0.38813	-1.44011	-0.62201
C	-3.02172	-0.62887	-0.10593
C	-4.31697	-0.19490	0.10824
Cl	-5.62493	-1.35442	0.13439
C	-4.59699	1.15989	0.30408
C	-3.56529	2.08512	0.28515
H	-0.40874	2.17422	-0.09155
H	1.74325	-0.02044	-1.83801
H	2.71980	0.01201	1.05308
H	2.32707	2.10862	0.14881
H	4.19071	-0.27067	-1.62669
H	3.95937	-1.57932	-0.44539
H	6.05193	0.07770	1.89849
H	1.33837	-2.30740	-1.33843
H	2.41242	-2.43860	0.96286
H	1.01910	-1.56383	1.63416
H	0.80651	-3.17993	0.93023
H	-2.80558	-1.68194	-0.25844
H	-5.62011	1.48417	0.47156
H	-3.76286	3.14205	0.43650

1c NMR Conformer 24
Energy: -875535.1879502

O	0.22305	-2.24548	-0.11522
C	1.36306	-1.53644	-0.05738
C	1.39054	-0.13472	-0.19740
C	0.14182	0.59301	-0.41862
N	-1.01198	0.03350	-0.45303
C	-1.99711	1.07705	-0.74001
C	-3.20393	0.94686	0.20168
O	-2.81779	0.92314	1.55720
C	-4.08287	-0.26027	-0.18007
C	-3.38058	-1.59340	-0.12622
O	-2.95571	-1.89406	1.11280
O	-3.20190	-2.32944	-1.07061
C	-1.17906	2.39716	-0.66286
C	-1.40446	3.31366	0.52582
O	0.20077	1.91947	-0.61026

C	2.60605	0.55782	-0.13036
C	3.77832	-0.14573	0.07627
Cl	5.29889	0.71205	0.16617
C	3.76602	-1.53572	0.21549
C	2.56450	-2.22365	0.14772
H	-0.52448	-1.61137	-0.28003
H	-2.35660	0.93442	-1.76853
H	-3.83813	1.83243	0.08236
H	-2.30457	0.11620	1.72399
H	-4.47014	-0.13257	-1.19315
H	-4.92664	-0.29304	0.51661
H	-2.52288	-2.77216	1.10516
H	-1.27263	2.95890	-1.59501
H	-2.43733	3.67404	0.54010
H	-1.21217	2.79065	1.46325
H	-0.74155	4.17822	0.44549
H	2.61717	1.63824	-0.23910
H	4.69629	-2.07233	0.37661
H	2.53511	-3.30376	0.25296

1c NMR Conformer 23
Energy: -875534.1505766

O	-1.30622	2.67494	-0.33752
C	-2.20099	1.68239	-0.21303
C	-1.83360	0.32190	-0.16895
C	-0.42174	-0.05146	-0.24711
N	0.54732	0.78328	-0.35112
C	1.80220	0.01484	-0.32054
C	2.57906	0.44809	0.93840
O	2.76027	1.85280	0.90653
C	3.98689	-0.14729	1.09143
C	4.79652	-0.07417	-0.17924
O	4.51091	-1.08940	-1.01046
O	5.60367	0.78576	-0.45099
C	1.31923	-1.45909	-0.43429
C	1.86633	-2.51520	0.50201
O	-0.11691	-1.35586	-0.19581
C	-2.81681	-0.66900	-0.04732
C	-4.14649	-0.30169	0.03413
Cl	-5.37605	-1.53617	0.18858
C	-4.52512	1.04271	-0.00398
C	-3.55616	2.02536	-0.12739
H	-0.40039	2.28010	-0.40050
H	2.39779	0.28974	-1.19715
H	1.99642	0.16446	1.82912
H	1.89799	2.27372	0.75167
H	3.93120	-1.18647	1.41669
H	4.50194	0.43642	1.85641
H	5.03936	-0.99316	-1.83083
H	1.43096	-1.78817	-1.47295
H	2.90853	-2.72933	0.25724
H	1.78717	-2.20635	1.54804
H	1.28956	-3.43396	0.37203
H	-2.52452	-1.71433	-0.01677
H	-5.57506	1.31317	0.06173
H	-3.82895	3.07579	-0.16133

1c NMR Conformer 22
Energy: -875531.3672521

O	2.29316	2.85026	-0.34222
C	2.73074	1.57707	-0.24372
C	1.90026	0.44564	-0.13658
C	0.43095	0.51941	-0.10888
N	-0.36965	-0.44574	0.10967
C	-1.72640	0.09550	-0.07804
C	-2.68511	-0.56733	0.91136
O	-2.63875	-1.97109	0.74147
C	-4.15552	-0.15910	0.75728
C	-4.78708	-0.69730	-0.50466
O	-4.35078	-0.06555	-1.60331
O	-5.60734	-1.58712	-0.54293
C	-1.53044	1.62154	0.03412
C	-1.67172	2.22885	1.42043
O	-0.12827	1.74187	-0.35411
C	2.48140	-0.82910	-0.03941
C	3.85447	-0.96939	-0.04536
Cl	4.56290	-2.56367	0.07236
C	4.68805	0.14737	-0.14926
C	4.12284	1.40657	-0.24781
H	1.32091	2.88728	-0.35031
H	-2.04619	-0.16592	-1.09419
H	-2.37331	-0.30247	1.93222
H	-1.70863	-2.25088	0.79699
H	-4.25125	0.93119	0.75765
H	-4.71988	-0.56381	1.59897
H	-4.78385	-0.45743	-2.39135
H	-2.11276	2.16943	-0.70992
H	-2.70815	2.19735	1.76604
H	-1.04649	1.69563	2.14317
H	-1.35698	3.27454	1.39189
H	1.83143	-1.69530	0.03805
H	5.76747	0.02642	-0.15486
H	4.74705	2.29127	-0.33029

1c NMR Conformer 20
Energy: -875533.5458207

O	2.47614	2.85105	0.07368
C	2.88647	1.56492	0.06518

C	2.04836	0.45321	-0.14224
C	0.59862	0.56409	-0.36739
N	-0.23213	-0.39852	-0.42515
C	-1.53324	0.19621	-0.76636
C	-2.65923	-0.53820	-0.04000
O	-2.57661	-1.92621	-0.30856
C	-4.02594	-0.09240	-0.53293
C	-5.14008	-0.64577	0.32374
O	-6.27541	-0.79627	-0.36558
O	-5.04627	-0.89637	1.50537
C	-1.34997	1.69638	-0.44282
C	-1.75490	2.14562	0.95147
O	0.09976	1.82316	-0.54287
C	2.59921	-0.83850	-0.12565
C	3.95008	-1.01501	0.09565
Cl	4.62186	-2.62926	0.11071
C	4.79070	0.08152	0.30506
C	4.25558	1.35757	0.28784
H	1.52215	2.91548	-0.10539
H	-1.68717	0.05877	-1.84768
H	-2.57977	-0.36412	1.04171
H	-1.69150	-2.23160	-0.04540
H	-4.16976	-0.40897	-1.57024
H	-4.12408	1.00060	-0.50970
H	-6.97719	-1.11452	0.24122
H	-1.77485	2.34303	-1.21344
H	-2.83875	2.09174	1.08655
H	-1.27786	1.52251	1.71406
H	-1.44564	3.18224	1.10325
H	1.94382	-1.68810	-0.29133
H	5.85269	-0.06781	0.47718
H	4.88628	2.22697	0.44761

1c NMR Conformer 19
Energy: -875534.5226898

O	0.21957	-2.18406	0.27664
C	1.37312	-1.50964	0.15835
C	1.42812	-0.12664	-0.12087
C	0.17848	0.60012	-0.35463
N	-0.97986	0.05509	-0.41365
C	-1.95055	1.11677	-0.72138
C	-3.20597	0.99397	0.15713
O	-2.89130	0.93119	1.52787
C	-4.09988	-0.17856	-0.27951
C	-3.44967	-1.52790	-0.10109
O	-3.62510	-2.32923	-1.15457
O	-2.88119	-1.88713	0.91078
C	-1.12589	2.42822	-0.56506
C	-1.34063	3.24467	0.69521
O	0.24885	1.92700	-0.54979
C	2.66562	0.52980	-0.18628
C	3.82945	-0.18922	0.01017
Cl	5.37679	0.62703	-0.08590
C	3.79282	-1.56006	0.27763
C	2.57253	-2.21132	0.35171
H	-0.54043	-1.55448	0.15708
H	-2.26382	0.99912	-1.76897
H	-3.79766	1.90776	0.02555
H	-2.40926	0.09908	1.68963
H	-4.42399	-0.05225	-1.31477
H	-4.99129	-0.18073	0.35989
H	-3.22472	-3.20816	-0.95861
H	-1.20949	3.05330	-1.45781
H	-2.35285	3.65715	0.71217
H	-1.20741	2.62619	1.58503
H	-0.63084	4.07515	0.71297
H	2.69460	1.59376	-0.40090
H	4.71806	-2.10998	0.42974
H	2.52059	-3.27450	0.56933

1c NMR Conformer 18
Energy: -875535.4580679

O	-1.22830	2.63801	0.16582
C	-2.16588	1.68367	0.04933
C	-1.85126	0.31223	-0.04706
C	-0.45149	-0.10913	-0.03494
N	0.55146	0.67802	0.10339
C	1.75593	-0.15090	-0.06936
C	2.87243	0.33462	0.85502
O	3.15659	1.69429	0.58498
C	4.19899	-0.42043	0.70263
C	4.89333	-0.13326	-0.60774
O	4.28479	-0.72171	-1.64697
O	5.89482	0.53633	-0.72770
C	1.22158	-1.58332	0.15115
C	1.27170	-2.11762	1.57375
O	-0.18623	-1.42151	-0.19650
C	-2.87452	-0.63833	-0.16270
C	-4.19242	-0.22092	-0.18343
Cl	-5.47089	-1.40550	-0.32806
C	-4.51868	1.13461	-0.09094
C	-3.50957	2.07800	0.02426
H	-0.33460	2.21256	0.16742
H	2.09139	-0.03097	-1.10658
H	2.54205	0.21903	1.89730
H	2.34154	2.21124	0.70544
H	4.03596	-1.49967	0.78084

H	4.87219	-0.10514	1.50135
H	4.76876	-0.49811	-2.47038
H	1.64548	-2.29349	-0.56226
H	2.29890	-2.30264	1.89790
H	0.80787	-1.41155	2.26956
H	0.72538	-3.06209	1.62221
H	-2.62223	-1.69188	-0.23500
H	-5.55940	1.44545	-0.10915
H	-3.74260	3.13601	0.09777

1c NMR Conformer 17
Energy: -875529.6753109

O	-2.05681	-2.66696	0.66516
C	-2.57989	-1.44898	0.39913
C	-1.73991	-0.43950	-0.10025
C	-0.30313	-0.64115	-0.38548
N	0.57388	0.28600	-0.30846
C	1.86561	-0.33330	-0.63939
C	2.73930	-0.36391	0.62571
O	2.07458	-1.01324	1.69439
C	3.17010	1.04108	1.04457
C	4.18259	1.65657	0.11408
O	4.42095	2.93853	0.41139
O	4.74316	1.07610	-0.79190
C	1.47481	-1.71521	-1.21884
C	2.27819	-2.92567	-0.79369
O	0.09452	-1.86462	-0.79118
C	-2.26412	0.83786	-0.33179
C	-3.60194	1.09853	-0.08709
Cl	-4.24024	2.69744	-0.39456
C	-4.44604	0.10165	0.39611
C	-3.92927	-1.16314	0.63902
H	-2.74126	-3.25941	1.02645
H	2.38630	0.26134	-1.39680
H	3.63413	-0.96074	0.42040
H	1.25468	-0.52696	1.89188
H	3.62852	0.99616	2.03957
H	2.30530	1.70993	1.12047
H	5.10048	3.28789	-0.20322
H	1.44389	-1.64957	-2.31337
H	3.30668	-2.83012	-1.15467
H	2.28676	-3.02203	0.29377
H	1.84877	-3.82909	-1.23326
H	-1.60678	1.61383	-0.71153
H	-5.49514	0.31103	0.58372
H	-4.57433	-1.94801	1.02804

1c NMR Conformer 15
Energy: -875534.1408816

O	-1.30672	2.66233	-0.30209
C	-2.21334	1.67769	-0.19343
C	-1.85498	0.31581	-0.15816
C	-0.44516	-0.05904	-0.24574
N	0.51633	0.77860	-0.38314
C	1.77364	0.01395	-0.36284
C	2.56821	0.47456	0.87746
O	2.80400	1.87108	0.77953
C	3.94889	-0.15959	1.07557
C	4.74796	-0.24228	-0.20241
O	5.82451	0.54723	-0.20663
O	4.44859	-0.95674	-1.13863
C	1.29137	-1.46081	-0.45571
C	1.86173	-2.50797	0.47527
O	-0.13898	-1.36370	-0.19027
C	-2.84262	-0.67080	-0.04002
C	-4.17069	-0.29587	0.04473
Cl	-5.40723	-1.52393	0.19164
C	-4.54158	1.05141	0.01530
C	-3.56615	2.02963	-0.10302
H	-0.40427	2.26084	-0.35519
H	2.35464	0.27835	-1.25038
H	1.97163	0.26294	1.77829
H	1.96026	2.31468	0.59455
H	3.85383	-1.17471	1.46402
H	4.48220	0.44011	1.81536
H	6.29746	0.43786	-1.05760
H	1.38208	-1.79771	-1.49361
H	2.90060	-2.71306	0.20859
H	1.80173	-2.19296	1.52053
H	1.29154	-3.43307	0.36341
H	-2.55634	-1.71775	-0.01741
H	-5.58952	1.32750	0.08385
H	-3.83207	3.08181	-0.12771

1c NMR Conformer 14
Energy: -875537.7637636

O	-1.35382	2.62646	0.01411
C	-2.29233	1.66662	0.04022
C	-1.99245	0.30043	-0.14126
C	-0.60904	-0.10684	-0.38027
N	0.39689	0.68875	-0.39336
C	1.56459	-0.11689	-0.77862
C	2.81088	0.32954	-0.01620
O	3.02255	1.71728	-0.20459
C	4.05880	-0.35909	-0.54390
C	5.25217	-0.12255	0.35124
O	6.40464	-0.19469	-0.32198
O	5.19480	0.07589	1.54498

C	1.07984	-1.56737	-0.54068
C	1.39564	-2.17148	0.81800
O	-0.36779	-1.41095	-0.62069
C	-3.01533	-0.65674	-0.09858
C	-4.31870	-0.25063	0.12037
Cl	-5.59754	-1.44233	0.17763
C	-4.63064	1.09976	0.29866
C	-3.62201	2.04951	0.25753
H	-0.47069	2.20804	-0.14630
H	1.74759	0.05366	-1.85041
H	2.69103	0.11350	1.05369
H	2.26682	2.19961	0.17174
H	4.28245	-0.00027	-1.55314
H	3.92366	-1.44630	-0.60996
H	7.14918	-0.07966	0.30622
H	1.36862	-2.23733	-1.35337
H	2.46886	-2.34273	0.93932
H	1.05437	-1.51438	1.62376
H	0.88485	-3.13217	0.91234
H	-2.77412	-1.70629	-0.23702
H	-5.66019	1.40154	0.46907
H	-3.84407	3.10357	0.39430

1c NMR Conformer 13
Energy: -875531.6743992

O	2.33325	2.83921	-0.36673
C	2.75527	1.56175	-0.25534
C	1.91078	0.44102	-0.14575
C	0.44235	0.53349	-0.12391
N	-0.37116	-0.42008	0.09848
C	-1.72089	0.13789	-0.09066
C	-2.68676	-0.50335	0.90508
O	-2.64887	-1.91016	0.75689
C	-4.15014	-0.08730	0.71867
C	-4.70727	-0.59827	-0.58883
O	-5.60874	-1.56838	-0.42573
O	-4.38237	-0.17665	-1.67999
C	-1.50527	1.66201	0.01028
C	-1.64175	2.28172	1.39159
O	-0.10051	1.76163	-0.37658
C	2.47602	-0.83995	-0.03735
C	3.84733	-0.99643	-0.03463
Cl	4.53650	-2.59800	0.09743
C	4.69472	0.10975	-0.14030
C	4.14530	1.37495	-0.24996
H	1.36129	2.88684	-0.37892
H	-2.05066	-0.12645	-1.10355
H	-2.38353	-0.22510	1.92479
H	-1.71919	-2.19332	0.80274
H	-4.23830	1.00320	0.71154
H	-4.73896	-0.48374	1.54773
H	-5.92408	-1.85981	-1.30762
H	-2.07850	2.21238	-0.73897
H	-2.67947	2.26466	1.73476
H	-1.02478	1.74631	2.11991
H	-1.31481	3.32346	1.35623
H	1.81537	-1.69784	0.04206
H	5.77263	-0.02451	-0.13847
H	4.78046	2.25168	-0.33421

1c NMR Conformer 11
Energy: -875532.4154000

O	2.35257	2.84812	-0.30986
C	2.65071	1.53602	-0.19968
C	1.70612	0.49235	-0.20069
C	0.25549	0.71467	-0.32554
N	-0.62855	-0.18875	-0.49367
C	-1.93404	0.48462	-0.45302
C	-2.66823	0.07455	0.83450
O	-1.89715	0.36610	1.98338
C	-3.04906	-1.41123	0.81713
C	-3.97686	-1.79388	-0.30741
O	-4.96364	-0.90323	-0.47576
O	-3.87269	-2.79312	-0.98506
C	-1.58724	1.98930	-0.57282
C	-2.32676	2.97366	0.30574
O	-0.17035	2.00300	-0.23835
C	2.14678	-0.83626	-0.09067
C	3.49418	-1.11503	0.01957
Cl	4.02647	-2.77478	0.16043
C	4.44013	-0.08665	0.02300
C	4.01368	1.22532	-0.08672
H	1.39058	2.98442	-0.36265
H	-2.54016	0.17454	-1.31244
H	-3.57951	0.67448	0.92413
H	-1.07817	-0.16021	1.95683
H	-3.55874	-1.64301	1.75969
H	-2.15597	-2.03665	0.74354
H	-5.54685	-1.20549	-1.20402
H	-1.64929	2.29217	-1.62464
H	-3.38622	2.98274	0.03304
H	-2.22859	2.70275	1.35850
H	-1.93122	3.98031	0.15119
H	1.40885	-1.63268	-0.09275
H	5.49809	-0.31606	0.11154
H	4.72768	2.04349	-0.08859

1c NMR Conformer 10

Energy: -875535.7417336

O	-1.22394	2.63673	0.18896
C	-2.16525	1.68723	0.06920
C	-1.85755	0.31642	-0.05056
C	-0.46111	-0.11619	-0.04697
N	0.54850	0.65875	0.11483
C	1.74672	-0.17665	-0.07360
C	2.86743	0.27520	0.86189
O	3.16190	1.64121	0.63309
C	4.18377	-0.48467	0.66716
C	4.78927	-0.20401	-0.68773
O	5.90115	0.52991	-0.62156
O	4.32393	-0.60123	-1.73599
C	1.19988	-1.60742	0.11227
C	1.24211	-2.17297	1.52257
O	-0.20718	-1.42630	-0.23669
C	-2.88583	-0.62709	-0.17759
C	-4.20129	-0.20342	-0.18459
Cl	-5.48644	-1.37963	-0.34150
C	-4.52098	1.15150	-0.06721
C	-3.50706	2.08767	0.05838
H	-0.33166	2.20858	0.16532
H	2.08825	-0.03849	-1.10707
H	2.54425	0.12903	1.90270
H	2.34176	2.15549	0.72494
H	4.01478	-1.56326	0.73445
H	4.88130	-0.18703	1.45203
H	6.23765	0.67967	-1.53036
H	1.62035	-2.30495	-0.61537
H	2.26755	-2.37297	1.84430
H	0.78327	-1.47781	2.23252
H	0.68829	-3.11393	1.55006
H	-2.63885	-1.68057	-0.26758
H	-5.56038	1.46689	-0.07516
H	-3.73412	3.14564	0.14909

1c NMR Conformer 9

Energy: -875529.8919460

O	1.84815	2.92772	-0.02161
C	2.48416	1.73716	-0.01260
C	1.85224	0.48478	-0.12985
C	0.39664	0.32338	-0.27018
N	-0.24489	-0.77604	-0.24377
C	-1.65260	-0.45078	-0.52869
C	-2.56225	-1.38354	0.28588
O	-2.09298	-2.71215	0.16100
C	-4.00834	-1.44128	-0.22562
C	-4.78394	-0.17189	0.00602
O	-4.67852	0.68805	-1.01495
O	-5.41616	0.07552	1.01047
C	-1.73087	1.07400	-0.27209
C	-2.13531	1.51371	1.12500
O	-0.33342	1.45761	-0.45903
C	2.62905	-0.68490	-0.10257
C	3.99938	-0.60582	0.04140
Cl	4.95360	-2.07050	0.07320
C	4.63664	0.63230	0.15965
C	3.87826	1.78931	0.13147
H	0.89015	2.81308	-0.14619
H	-1.83222	-0.66123	-1.59428
H	-2.55299	-1.08273	1.34411
H	-1.13098	-2.70170	0.30436
H	-4.51450	-2.24041	0.31972
H	-3.99277	-1.68329	-1.29203
H	-5.19346	1.49846	-0.80944
H	-2.30167	1.59326	-1.04142
H	-3.18511	1.29141	1.33114
H	-1.52038	1.01502	1.88091
H	-1.99354	2.59305	1.21774
H	2.13153	-1.64515	-0.19811
H	5.71593	0.68421	0.27032
H	4.34807	2.76418	0.22119

1c NMR Conformer 8

Energy: -875536.2261395

O	0.69984	-2.41818	0.51421
C	1.76688	-1.63275	0.28940
C	1.65079	-0.27234	-0.05663
C	0.32409	0.32471	-0.20178
N	-0.77670	-0.30642	-0.01045
C	-1.86888	0.62165	-0.31296
C	-2.94117	0.54669	0.78174
O	-2.38622	0.72233	2.06724
C	-3.69353	-0.79145	0.72060
C	-4.40198	-1.02026	-0.58751
O	-5.09004	0.06026	-0.97777
O	-4.35383	-2.03786	-1.24217
C	-1.15712	1.99079	-0.52329
C	-1.31146	3.05739	0.54579
O	0.24963	1.60950	-0.58300
C	2.79962	0.49997	-0.27311
C	4.04694	-0.08318	-0.14622
Cl	5.48158	0.87707	-0.41579
C	4.17541	-1.43204	0.19247
C	3.04110	-2.19865	0.40733
H	-0.12418	-1.88052	0.39868
H	-2.32967	0.31297	-1.26303
H	-3.65674	1.36312	0.64416

H	-1.71403	0.03263	2.21242
H	-4.44357	-0.79303	1.51952
H	-3.00820	-1.62732	0.88415
H	-5.53383	-0.13173	-1.82985
H	-1.40355	2.40157	-1.50558
H	-2.35916	3.35812	0.63536
H	-0.97696	2.68860	1.51651
H	-0.72496	3.93575	0.26570
H	2.70141	1.54799	-0.54007
H	5.16228	-1.87646	0.28775
H	3.12209	-3.24854	0.67261

1c NMR Conformer 7
Energy: -875533.8523904

O	-1.54680	2.72468	0.01597
C	-2.34725	1.64639	0.01405
C	-1.85509	0.33009	-0.10279
C	-0.41716	0.10520	-0.24164
N	0.47624	1.02523	-0.20944
C	1.76423	0.37757	-0.51068
C	2.89008	1.03866	0.29917
O	2.79040	2.44517	0.18080
C	4.29594	0.72118	-0.23010
C	4.72033	-0.70890	-0.02488
O	4.38925	-1.49571	-1.05615
O	5.27840	-1.12556	0.96736
C	1.45598	-1.12160	-0.26469
C	1.75042	-1.65874	1.12620
O	0.00656	-1.15624	-0.43603
C	-2.74113	-0.75589	-0.09695
C	-4.09906	-0.52622	0.02378
Cl	-5.20626	-1.87984	0.03208
C	-4.60069	0.77287	0.13914
C	-3.72795	1.84973	0.13324
H	-0.60757	2.42793	-0.07626
H	1.97950	0.54851	-1.57649
H	2.81318	0.74540	1.35636
H	1.89531	2.71256	0.45020
H	4.99795	1.35361	0.31687
H	4.33350	0.97429	-1.29348
H	4.68085	-2.41459	-0.86943
H	1.87738	-1.75917	-1.04130
H	2.82356	-1.70992	1.32478
H	1.28569	-1.02791	1.89070
H	1.34025	-2.66740	1.21289
H	-2.35238	-1.76561	-0.18715
H	-5.67060	0.93570	0.23295
H	-4.09815	2.86669	0.22148

1c NMR Conformer 6
Energy: -875529.9378044

O	1.84601	2.92454	-0.05353
C	2.48455	1.73541	-0.02731
C	1.85368	0.48195	-0.13633
C	0.39842	0.32158	-0.27967
N	-0.24430	-0.77740	-0.24553
C	-1.64826	-0.45076	-0.54378
C	-2.57078	-1.38123	0.25693
O	-2.10586	-2.71149	0.13807
C	-4.00614	-1.42222	-0.28273
C	-4.72551	-0.10608	-0.15825
O	-5.35988	0.02366	1.01205
O	-4.71195	0.76778	-0.99971
C	-1.72837	1.07093	-0.28243
C	-2.11715	1.50188	1.12192
O	-0.33085	1.45497	-0.48062
C	2.62997	-0.68727	-0.09524
C	3.99935	-0.60566	0.05543
Cl	4.95497	-2.06845	0.10499
C	4.63537	0.63393	0.16674
C	3.87745	1.79066	0.12428
H	0.88936	2.80395	-0.18473
H	-1.81665	-0.65509	-1.61252
H	-2.57443	-1.08038	1.31513
H	-1.14717	-2.70490	0.30199
H	-4.54962	-2.19055	0.27165
H	-3.97073	-1.69496	-1.34079
H	-5.80032	0.89943	1.04561
H	-2.31016	1.59347	-1.04138
H	-3.16422	1.27715	1.33775
H	-1.49398	0.99831	1.86798
H	-1.97631	2.58083	1.21966
H	2.13384	-1.64881	-0.18465
H	5.71407	0.68610	0.28302
H	4.34659	2.76638	0.20775

1c NMR Conformer 5
Energy: -875534.0240582

O	-1.55562	2.72650	0.03545
C	-2.35183	1.64650	0.02949
C	-1.85871	0.33259	-0.10437
C	-0.42191	0.10492	-0.24914
N	0.47278	1.02488	-0.21093
C	1.75825	0.37683	-0.52054
C	2.89373	1.02819	0.28505
O	2.79846	2.43665	0.19792
C	4.28601	0.71425	-0.28268
C	4.65543	-0.74225	-0.20540

O	5.25460	-1.06107	0.94646
O	4.42354	-1.55697	-1.07401
C	1.45066	-1.11949	-0.27371
C	1.73726	-1.65215	1.12018
O	-0.00206	-1.15544	-0.44854
C	-2.74328	-0.75452	-0.10803
C	-4.09990	-0.52777	0.02238
Cl	-5.20650	-1.88301	0.01831
C	-4.60338	0.76868	0.15813
C	-3.73215	1.84602	0.16057
H	-0.61848	2.43169	-0.08321
H	1.96469	0.54828	-1.58762
H	2.83397	0.71346	1.33739
H	1.90820	2.70372	0.48075
H	5.01198	1.30684	0.27767
H	4.30442	1.01648	-1.33298
H	5.47102	-2.01723	0.94473
H	1.87615	-1.75934	-1.04597
H	2.80867	-1.69423	1.32955
H	1.26073	-1.02358	1.87894
H	1.33519	-2.66407	1.20475
H	-2.35338	-1.76243	-0.21216
H	-5.67282	0.92745	0.26021
H	-4.10175	2.86172	0.26333

1c NMR Conformer 4
Energy: -875529.4905031

O	2.00817	2.91215	-0.11369
C	2.58838	1.69280	-0.10736
C	1.88841	0.47275	-0.14841
C	0.41926	0.39235	-0.18110
N	-0.27515	-0.66861	-0.05976
C	-1.67963	-0.27474	-0.27539
C	-2.62331	-1.14669	0.58608
O	-2.05562	-2.42646	0.79377
C	-3.96246	-1.42870	-0.08945
C	-4.82587	-0.22144	-0.32844
O	-6.00700	-0.55033	-0.86026
O	-4.50801	0.92531	-0.08847
C	-1.66037	1.24984	-0.02492
C	-1.88296	1.72011	1.40063
O	-0.26111	1.55512	-0.36304
C	2.60436	-0.73611	-0.13941
C	3.98271	-0.72301	-0.08530
Cl	4.86457	-2.23308	-0.07712
C	4.68897	0.48379	-0.03923
C	3.99050	1.67764	-0.05098
H	1.04049	2.83380	-0.17622
H	-1.90531	-0.46476	-1.33547
H	-2.79564	-0.65858	1.55434
H	-1.09226	-2.32383	0.84819
H	-4.53011	-2.13701	0.52328
H	-3.79143	-1.92473	-1.05257
H	-6.52902	0.26399	-1.00836
H	-2.27845	1.79818	-0.73368
H	-2.92932	1.59646	1.68235
H	-1.25216	1.16224	2.10019
H	-1.62704	2.77991	1.47185
H	2.05319	-1.67051	-0.17690
H	5.77386	0.48030	0.00236
H	4.51220	2.62926	-0.01683

1c NMR Conformer 3
Energy: -875533.3646963

O	-1.44764	2.67149	-0.06852
C	-2.30574	1.63847	-0.08407
C	-1.87758	0.29680	-0.10067
C	-0.44610	-0.00217	-0.12231
N	0.47743	0.88963	-0.08288
C	1.75447	0.17598	-0.27386
C	2.89578	0.84803	0.52627
O	2.65204	2.23262	0.68101
C	4.24226	0.78815	-0.18857
C	4.80614	-0.59398	-0.36354
O	5.99930	-0.57417	-0.96494
O	4.26072	-1.62050	-0.01391
C	1.37821	-1.28407	0.07530
C	1.53606	-1.71309	1.52226
O	-0.06495	-1.28424	-0.21181
C	-2.81765	-0.74380	-0.11501
C	-4.16610	-0.44046	-0.11117
Cl	-5.34412	-1.73513	-0.13163
C	-4.60687	0.88625	-0.09343
C	-3.67970	1.91649	-0.08019
H	-0.52238	2.32161	-0.08876
H	1.99636	0.24077	-1.34536
H	2.98676	0.37561	1.51285
H	1.72937	2.35307	0.95239
H	4.97339	1.38455	0.36733
H	4.15368	1.25519	-1.17719
H	6.32298	-1.49230	-1.06464
H	1.82714	-2.00362	-0.60644
H	2.59166	-1.84275	1.76552
H	1.09474	-0.97660	2.20157
H	1.02476	-2.66732	1.66725
H	-2.47631	-1.77404	-0.12979
H	-5.67061	1.10410	-0.09069
H	-3.99816	2.95429	-0.06695

1c NMR Conformer 2
Energy: -875532.5727857

O	-2.50030	-2.75622	-0.52402
C	-2.76470	-1.44514	-0.34124
C	-1.79013	-0.43830	-0.21118
C	-0.34164	-0.70138	-0.25780
N	0.57957	0.14504	-0.02196
C	1.85698	-0.54205	-0.25735
C	2.86307	-0.16158	0.83749
O	2.30545	-0.30926	2.12797
C	3.36216	1.27103	0.64455
C	4.29188	1.42662	-0.53050
O	4.60784	2.70650	-0.75313
O	4.72843	0.51439	-1.20079
C	1.48132	-2.04147	-0.38204
C	1.73730	-2.94354	0.81080
O	0.03849	-1.96384	-0.59688
C	-2.19618	0.89245	-0.02188
C	-3.53855	1.20786	0.03774
Cl	-4.02835	2.87042	0.26917
C	-4.51424	0.21548	-0.08958
C	-4.12207	-1.09804	-0.27748
H	-1.54177	-2.91551	-0.57390
H	2.26002	-0.19414	-1.21722
H	3.72020	-0.84194	0.79168
H	1.47211	0.19372	2.15785
H	3.91093	1.58355	1.54037
H	2.52181	1.96544	0.52720
H	5.22837	2.75519	-1.51061
H	1.90225	-2.47498	-1.29205
H	2.81034	-3.00778	1.01194
H	1.24530	-2.55885	1.70557
H	1.36812	-3.94864	0.59256
H	-1.43632	1.66204	0.07267
H	-5.56807	0.47457	-0.04317
H	-4.85874	-1.88932	-0.37947

1b NMR Conformer 19
Energy: -875526.2154182

O	-0.83770	-2.75189	-0.25299
C	-1.63405	-1.66181	-0.19974
C	-1.21474	-0.34505	-0.46269
C	0.16780	0.00317	-0.82778
N	0.64824	1.18095	-0.91608
C	2.09204	1.01896	-1.15644
C	2.89682	1.41398	0.10728
O	3.15284	2.80994	0.08772
C	2.23519	1.07875	1.45973
C	2.09340	-0.39093	1.76932
O	0.82247	-0.77638	1.93247
O	3.03158	-1.15095	1.90222
C	2.19852	-0.42787	-1.67379
C	3.43246	-1.24716	-1.37597
O	1.01470	-1.03475	-1.08706
C	-2.13725	0.70798	-0.34936
C	-3.44655	0.45060	0.00643
Cl	-4.58536	1.77234	0.13377
C	-3.87584	-0.85408	0.26543
C	-2.96946	-1.89581	0.16263
H	0.06034	-2.51789	-0.54060
H	2.41996	1.70814	-1.94116
H	3.88235	0.93769	0.05724
H	2.30838	3.28509	-0.00231
H	1.26308	1.57067	1.52414
H	2.89568	1.49270	2.22738
H	0.80479	-1.73173	2.15201
H	2.01301	-0.41254	-2.75501
H	3.61190	-1.34401	-0.30438
H	3.33170	-2.24440	-1.80997
H	4.30089	-0.76659	-1.83693
H	-1.79937	1.72038	-0.54744
H	-4.90736	-1.04688	0.54448
H	-3.27308	-2.91908	0.36190

1b NMR Conformer 18
Energy: -875536.3383759

O	-0.40391	2.25349	-0.40999
C	-1.49449	1.48353	-0.25604
C	-1.43548	0.07554	-0.22870
C	-0.14195	-0.58955	-0.37830
N	0.97779	0.02364	-0.50170
C	2.00743	-0.99895	-0.71690
C	3.28193	-0.69037	0.06231
O	4.21252	-1.67763	-0.34145
C	3.78681	0.72308	-0.25763
C	2.99845	1.77584	0.48232
O	2.60013	2.78361	-0.30273
O	2.78213	1.74981	1.67504
C	1.28818	-2.32357	-0.35620
C	1.55943	-2.88212	1.02682
O	-0.11986	-1.93316	-0.41692
C	-2.60679	-0.67566	-0.06243
C	-3.81876	-0.02489	0.07582
Cl	-5.28308	-0.95924	0.28338
C	-3.89205	1.36991	0.05282
C	-2.73572	2.11576	-0.11240

H	0.39148	1.67235	-0.51646
H	2.28189	-0.99592	-1.78259
H	3.09230	-0.75183	1.14166
H	4.97939	-1.66561	0.25660
H	3.77164	0.91424	-1.33396
H	4.82298	0.80761	0.09132
H	2.14396	3.45501	0.24916
H	1.43256	-3.08528	-1.12440
H	1.33422	-2.13904	1.79858
H	0.93283	-3.76053	1.19687
H	2.60890	-3.17630	1.11102
H	-2.55025	-1.75986	-0.04313
H	-4.85262	1.86552	0.16333
H	-2.77138	3.20096	-0.13406

1b NMR Conformer 17
Energy: -875533.1031127

O	-2.49119	-2.80743	-0.51710
C	-2.75258	-1.49890	-0.31198
C	-1.77519	-0.49718	-0.16227
C	-0.32770	-0.76421	-0.20599
N	0.59772	0.07523	0.03836
C	1.86637	-0.61974	-0.22045
C	2.93564	-0.25606	0.81180
O	4.12744	-0.97971	0.55890
C	3.17730	1.25155	0.89605
C	3.73553	1.84971	-0.37000
O	3.64625	3.17974	-0.38613
O	4.23988	1.21386	-1.27641
C	1.47985	-2.11758	-0.25996
C	1.64825	-2.89477	1.03192
O	0.05162	-2.02791	-0.55368
C	-2.17798	0.83105	0.05010
C	-3.51962	1.14953	0.11354
Cl	-4.00405	2.80917	0.37681
C	-4.49791	0.16262	-0.03301
C	-4.10890	-1.14855	-0.24431
H	-1.53248	-2.96795	-0.56377
H	2.22646	-0.30871	-1.21168
H	2.59205	-0.57916	1.80045
H	4.49864	-0.66224	-0.28187
H	3.90560	1.45644	1.69042
H	2.25389	1.77427	1.15823
H	4.05707	3.52003	-1.20978
H	1.93933	-2.63917	-1.10107
H	1.11916	-2.40219	1.85403
H	1.24115	-3.90135	0.91145
H	2.70841	-2.96959	1.28531
H	-1.41574	1.59616	0.16105
H	-5.55118	0.42331	0.01704
H	-4.84790	-1.93556	-0.36140

1b NMR Conformer 16
Energy: -875533.5766502

O	0.37681	-2.17228	-1.28810
C	1.35293	-1.36412	-0.84711
C	1.14005	-0.00507	-0.52389
C	-0.19709	0.57429	-0.66125
N	-1.22131	-0.04802	-1.12274
C	-2.38209	0.84165	-0.95957
C	-3.34192	0.31135	0.13271
O	-4.22210	-0.66383	-0.38459
C	-2.59511	-0.17485	1.38520
C	-1.82885	-1.46143	1.17520
O	-0.62523	-1.43718	1.75549
O	-2.27478	-2.45591	0.63303
C	-1.71953	2.21278	-0.67980
C	-2.33694	3.13476	0.34808
O	-0.37937	1.84130	-0.24820
C	2.20125	0.78007	-0.05158
C	3.45532	0.21497	0.09238
Cl	4.78101	1.19449	0.68037
C	3.68282	-1.12749	-0.22556
C	2.63629	-1.90900	-0.69185
H	-0.46517	-1.65288	-1.35784
H	-2.95327	0.87934	-1.89136
H	-3.98653	1.14253	0.43474
H	-3.74114	-1.50181	-0.47910
H	-3.31565	-0.36262	2.19011
H	-1.89762	0.58951	1.74017
H	-0.20007	-2.31285	1.64000
H	-1.58775	2.73949	-1.63184
H	-2.41935	2.65680	1.32742
H	-1.72389	4.03230	0.45252
H	-3.33418	3.44107	0.02042
H	2.02730	1.82232	0.19639
H	4.67443	-1.55332	-0.10584
H	2.78958	-2.95426	-0.94186

1b NMR Conformer 15
Energy: -875531.4802164

O	-1.76959	2.71659	-1.15485
C	-2.27598	1.53861	-0.73249
C	-1.59814	0.61677	0.08762
C	-0.23290	0.83491	0.59140
N	0.38652	0.10524	1.43348
C	1.75601	0.63785	1.51749
C	2.73498	-0.33194	0.83306

O	2.94527	-1.47346	1.64379
C	2.27974	-0.76804	-0.56647
C	3.33192	-1.61673	-1.23243
O	4.49984	-0.97103	-1.34445
O	3.16650	-2.75018	-1.62700
C	1.63361	2.04809	0.90498
C	2.77559	2.60851	0.08648
O	0.43993	1.90867	0.08259
C	-2.23962	-0.57532	0.46238
C	-3.52359	-0.83852	0.03031
Cl	-4.30940	-2.32732	0.50231
C	-4.20568	0.07006	-0.78367
C	-3.58049	1.24657	-1.15697
H	-0.86208	2.84497	-0.82771
H	2.06827	0.70531	2.56440
H	3.71275	0.15686	0.76415
H	2.08877	-1.91219	1.79540
H	2.08264	0.10111	-1.20459
H	1.36345	-1.35902	-0.49804
H	5.15240	-1.56098	-1.77677
H	1.36708	2.75290	1.70219
H	3.04345	1.96473	-0.75397
H	2.50510	3.59231	-0.30365
H	3.65407	2.72831	0.72693
H	-1.70608	-1.27923	1.09384
H	-5.21580	-0.14721	-1.11898
H	-4.08805	1.97024	-1.78775

1b NMR Conformer 14
Energy: -875524.3062771

O	0.65697	-2.55447	0.25932
C	1.58690	-1.58205	0.15201
C	1.31928	-0.21279	0.32840
C	-0.01901	0.28958	0.69289
N	-0.49279	1.43656	0.40064
C	-1.89036	1.43407	0.86897
C	-2.84112	1.45278	-0.34638
O	-2.97580	2.78762	-0.79851
C	-2.40030	0.59051	-1.54958
C	-2.48144	-0.89715	-1.34769
O	-3.73400	-1.35591	-1.42410
O	-1.53240	-1.62286	-1.11100
C	-1.94372	0.23023	1.82871
C	-3.19791	-0.61142	1.89684
O	-0.80859	-0.56403	1.39389
C	2.35087	0.72467	0.16681
C	3.63293	0.29801	-0.13466
Cl	4.91469	1.47628	-0.31964
C	3.91900	-1.06021	-0.28605
C	2.89633	-1.98767	-0.14598
H	-0.24411	-2.18863	0.21351
H	-2.10220	2.35623	1.42034
H	-3.84077	1.14462	-0.01654
H	-2.08639	3.15303	-0.95223
H	-1.36975	0.84359	-1.80688
H	-3.06299	0.85713	-2.37668
H	-3.73479	-2.32697	-1.27661
H	-1.68085	0.58681	2.83210
H	-3.48481	-1.01555	0.92496
H	-3.05165	-1.44311	2.58912
H	-4.02386	0.00038	2.27194
H	2.12775	1.77919	0.29703
H	4.92922	-1.38492	-0.51638
H	3.08684	-3.04857	-0.27680

1b NMR Conformer 13
Energy: -875531.5614789

O	-0.72983	2.79207	0.06184
C	-1.60798	1.77688	0.03626
C	-1.26047	0.48228	-0.39690
C	0.10946	0.21315	-0.82107
N	1.03113	1.10604	-0.89793
C	2.27610	0.40874	-1.24404
C	3.29748	0.48826	-0.08090
O	4.08608	1.65885	-0.22542
C	2.68804	0.50880	1.33547
C	1.96957	-0.74388	1.76472
O	2.81958	-1.74076	2.05180
O	0.76773	-0.86352	1.85721
C	1.76317	-0.97461	-1.71896
C	2.54603	-2.21689	-1.36831
O	0.42847	-1.05018	-1.14821
C	-2.21590	-0.54050	-0.40312
C	-3.50347	-0.26889	0.01851
Cl	-4.70356	-1.54242	0.00532
C	-3.86311	1.00836	0.45511
C	-2.91847	2.02232	0.46379
H	0.14279	2.46340	-0.27995
H	2.76205	0.91524	-2.08366
H	4.00215	-0.34564	-0.16925
H	3.50374	2.43909	-0.22811
H	1.98321	1.33960	1.41308
H	3.51950	0.67403	2.02600
H	2.30676	-2.52659	2.33692
H	1.61722	-0.92680	-2.80478
H	2.67983	-2.32927	-0.29114
H	2.02668	-3.09860	-1.75008
H	3.53211	-2.17250	-1.83988

H	-1.93560	-1.53459	-0.73813
H	-4.87965	1.20339	0.78405
H	-3.17731	3.02214	0.79882

1b NMR Conformer 12
Energy: -875536.1029845

O	-1.30696	2.63310	-0.05248
C	-2.26406	1.69227	-0.02531
C	-1.98650	0.31749	-0.17247
C	-0.60698	-0.11966	-0.38083
N	0.40855	0.66414	-0.41518
C	1.56826	-0.17168	-0.76039
C	2.83700	0.35863	-0.08971
O	2.74368	0.38747	1.32070
C	4.06184	-0.46353	-0.45047
C	5.34316	0.23616	-0.06305
O	6.34742	-0.62988	0.11354
O	5.48050	1.43416	0.04303
C	1.07096	-1.60358	-0.44792
C	1.32958	-2.17696	0.93535
O	-0.37805	-1.43240	-0.56974
C	-3.02668	-0.62041	-0.12542
C	-4.32574	-0.18665	0.06285
Cl	-5.62732	-1.35388	0.12215
C	-4.61596	1.17236	0.20724
C	-3.58986	2.10273	0.16254
H	-0.42817	2.19206	-0.18666
H	1.72512	-0.08229	-1.84665
H	2.98315	1.37818	-0.47476
H	2.05227	1.02272	1.57358
H	4.10408	-0.62506	-1.53546
H	4.04265	-1.44891	0.02268
H	7.16599	-0.13184	0.32057
H	1.36646	-2.30831	-1.22865
H	0.97153	-1.49615	1.71044
H	0.80395	-3.13124	1.02172
H	2.39405	-2.34682	1.10592
H	-2.80201	-1.67679	-0.23788
H	-5.64248	1.49554	0.35506
H	-3.79468	3.16319	0.27487

1b NMR Conformer 11
Energy: -875530.9938087

O	-0.67131	2.80958	-0.13129
C	-1.54892	1.79333	-0.11117
C	-1.19012	0.47344	-0.45033
C	0.19342	0.18197	-0.81399
N	1.11765	1.06818	-0.92076
C	2.37046	0.34091	-1.17668
C	3.31637	0.41959	0.04737
O	4.15074	1.56002	-0.07017
C	2.62831	0.48551	1.42453
C	1.85397	-0.74650	1.82279
O	0.55019	-0.51219	1.99523
O	2.33989	-1.85596	1.90958
C	1.85646	-1.03979	-1.64189
C	2.64917	-2.28403	-1.32024
O	0.53204	-1.10212	-1.04192
C	-2.14406	-0.55105	-0.40786
C	-3.44132	-0.25556	-0.03193
Cl	-4.63628	-1.53288	0.02456
C	-3.81401	1.04838	0.30628
C	-2.87116	2.06415	0.26609
H	0.21228	2.46159	-0.41741
H	2.91465	0.81660	-1.99834
H	3.99573	-0.43934	0.01931
H	3.59446	2.35479	-0.14892
H	1.98047	1.36365	1.46816
H	3.42978	0.59864	2.16023
H	0.09827	-1.35559	2.21049
H	1.68226	-0.98168	-2.72348
H	2.78601	-2.41488	-0.24626
H	2.13656	-3.16129	-1.72103
H	3.63067	-2.21888	-1.79976
H	-1.85468	-1.56458	-0.66819
H	-4.83796	1.26220	0.59823
H	-3.13911	3.08383	0.52545

1b NMR Conformer 10
Energy: -875527.0749117

O	1.96988	2.71349	-0.15979
C	2.63889	1.53884	-0.14225
C	1.89803	0.34546	-0.15615
C	0.42380	0.33836	-0.22744
N	-0.33752	-0.44232	0.43531
C	-1.69849	-0.18889	-0.07119
C	-2.72852	-0.38716	1.04000
O	-2.49611	0.45510	2.15376
C	-4.16055	-0.13053	0.58712
C	-4.68241	-1.17018	-0.37208
O	-5.86653	-0.81776	-0.88376
O	-4.12915	-2.21293	-0.64884
C	-1.57388	1.18779	-0.76436
C	-1.83428	2.44027	0.05825
O	-0.15695	1.19006	-1.10468
C	2.56095	-0.88252	-0.07644
C	3.94524	-0.91876	-0.00586
Cl	4.76430	-2.46126	0.08201

C	4.69056	0.25728	-0.00822
C	4.03442	1.48027	-0.07218
H	2.59322	3.46107	-0.10704
H	-1.91022	-0.95124	-0.83513
H	-2.64880	-1.44032	1.34533
H	-1.59198	0.28965	2.47191
H	-4.28291	0.85693	0.13101
H	-4.81582	-0.14464	1.46646
H	-6.18254	-1.53079	-1.47823
H	-2.12434	1.21488	-1.70815
H	-1.21409	2.44665	0.95702
H	-1.58594	3.31457	-0.54871
H	-2.87860	2.50990	0.36830
H	1.97885	-1.79939	-0.07870
H	5.77476	0.21995	0.04447
H	4.60616	2.40551	-0.05854

1b NMR Conformer 9
Energy: -875533.0536399

O	0.35946	-2.26052	-0.77817
C	1.41494	-1.48294	-0.50861
C	1.32961	-0.08474	-0.37908
C	0.04319	0.58392	-0.53073
N	-1.06847	0.00048	-0.80397
C	-2.07635	1.06110	-0.93027
C	-3.45961	0.66405	-0.38481
O	-4.17496	-0.09209	-1.34811
C	-3.46055	-0.04097	0.98246
C	-2.67153	-1.32388	1.00774
O	-1.78333	-1.37319	1.99880
O	-2.87381	-2.26835	0.27400
C	-1.36291	2.30653	-0.33372
C	-1.67489	2.70104	1.09610
O	0.04318	1.92116	-0.38414
C	2.47506	0.66583	-0.09873
C	3.68679	0.02534	0.05365
Cl	5.12189	0.96397	0.40392
C	3.78607	-1.36027	-0.06688
C	2.65532	-2.10526	-0.34725
H	-0.43201	-1.67993	-0.91187
H	-2.24470	1.23289	-2.00168
H	-4.03941	1.58746	-0.26541
H	-3.76230	-0.96967	-1.44297
H	-4.50012	-0.30754	1.20280
H	-3.10574	0.61678	1.77543
H	-1.33250	-2.24811	1.97900
H	-1.47351	3.16334	-1.00152
H	-1.39087	1.90613	1.79072
H	-1.10211	3.59562	1.35222
H	-2.73967	2.92727	1.21603
H	2.39714	1.74539	0.00005
H	4.74844	-1.84964	0.05752
H	2.70948	-3.18551	-0.44751

1b NMR Conformer 8
Energy: -875535.9737803

O	0.99435	-2.29555	-1.45234
C	1.86350	-1.49596	-0.81478
C	1.57255	-0.15265	-0.49769
C	0.27205	0.40518	-0.86300
N	-0.63732	-0.22794	-1.51307
C	-1.82960	0.63427	-1.52235
C	-2.90644	0.05754	-0.58658
O	-3.53731	-1.06123	-1.18121
C	-2.36447	-0.32550	0.79729
C	-3.47863	-0.78487	1.70219
O	-4.42123	0.15405	1.85393
O	-3.53500	-1.86758	2.24237
C	-1.24981	2.01581	-1.14806
C	-2.06953	2.95762	-0.29361
O	-0.01255	1.66038	-0.46424
C	2.51933	0.63536	0.17161
C	3.73901	0.08499	0.51764
Cl	4.92486	1.06430	1.35098
C	4.04064	-1.24474	0.21111
C	3.10767	-2.02697	-0.45050
H	0.16684	-1.78191	-1.64142
H	-2.26842	0.66387	-2.52447
H	-3.69846	0.80585	-0.47569
H	-2.86926	-1.74902	-1.35431
H	-1.86137	0.52560	1.27097
H	-1.64574	-1.14368	0.70821
H	-5.12410	-0.18867	2.44529
H	-0.94548	2.52390	-2.07146
H	-2.35477	2.51473	0.66314
H	-1.49794	3.86718	-0.09635
H	-2.97903	3.23864	-0.83231
H	2.28580	1.66875	0.40963
H	5.00389	-1.66116	0.49200
H	3.32307	-3.06257	-0.69615

1b NMR Conformer 7
Energy: -875537.6477371

O	0.67220	-2.35646	0.57768
C	1.76218	-1.60808	0.34479
C	1.68891	-0.24525	-0.01146
C	0.37990	0.39258	-0.14549
N	-0.73926	-0.19779	0.06768

C	-1.79554	0.76406	-0.27064
C	-2.95891	0.71571	0.72250
O	-3.93127	1.68662	0.37968
C	-3.55884	-0.68527	0.85345
C	-4.18642	-1.19513	-0.41872
O	-4.38414	-2.51248	-0.39742
O	-4.50825	-0.49601	-1.36094
C	-1.04241	2.11675	-0.33798
C	-1.08901	2.97935	0.90923
O	0.33920	1.68081	-0.53023
C	2.86125	0.48737	-0.24003
C	4.08878	-0.13655	-0.11477
Cl	5.55461	0.77536	-0.39785
C	4.17687	-1.48602	0.23644
C	3.01946	-2.21398	0.46393
H	-0.13475	-1.79251	0.44974
H	-2.18360	0.50818	-1.26672
H	-2.58714	0.99733	1.71336
H	-4.34173	1.41781	-0.45966
H	-4.35185	-0.66551	1.61119
H	-2.80549	-1.40110	1.19272
H	-4.83054	-2.78532	-1.22752
H	-1.31530	2.68987	-1.22558
H	-0.74121	2.41887	1.78293
H	-0.44105	3.84851	0.77624
H	-2.11080	3.32182	1.08937
H	2.79388	1.53627	-0.51258
H	5.14957	-1.96036	0.33043
H	3.06702	-3.26361	0.73794

1b NMR Conformer 6

Energy: -875531.8549964

O	1.74742	2.68882	1.21888
C	2.25558	1.52397	0.76301
C	1.57833	0.62638	-0.08411
C	0.21413	0.86101	-0.58286
N	-0.39707	0.16917	-1.46173
C	-1.77007	0.69671	-1.52730
C	-2.73906	-0.32025	-0.90199
O	-2.91339	-1.42315	-1.77516
C	-2.29287	-0.81255	0.47365
C	-3.40572	-1.53327	1.19531
O	-2.93618	-2.40239	2.09743
O	-4.58909	-1.34263	1.01854
C	-1.66265	2.07269	-0.83853
C	-2.81188	2.56875	0.01078
O	-0.46791	1.90390	-0.02358
C	2.21969	-0.55392	-0.49343
C	3.50388	-0.82926	-0.06903
Cl	4.28934	-2.30425	-0.58211
C	4.18574	0.05585	0.77055
C	3.56026	1.22089	1.17832
H	0.83740	2.82142	0.90038
H	-2.07486	0.81760	-2.57143
H	-3.72878	0.14114	-0.81940
H	-2.04238	-1.82308	-1.94671
H	-1.97333	0.01256	1.12390
H	-1.43189	-1.48169	0.37983
H	-3.69161	-2.81439	2.56703
H	-1.40600	2.82481	-1.59462
H	-3.06884	1.87175	0.81164
H	-2.55557	3.53131	0.45911
H	-3.69300	2.71285	-0.62081
H	1.68661	-1.23949	-1.14516
H	5.19590	-0.17087	1.09933
H	4.06801	1.92585	1.82974

1b NMR Conformer 5

Energy: -875532.1193787

O	0.30974	-2.26000	-0.85247
C	1.35812	-1.46937	-0.56576
C	1.24716	-0.06605	-0.45924
C	-0.05606	0.56376	-0.66585
N	-1.11692	-0.07345	-0.99482
C	-2.21020	0.90007	-1.06588
C	-3.47990	0.32715	-0.40809
O	-3.93866	-0.74980	-1.20443
C	-3.38787	-0.09843	1.07419
C	-2.21403	-0.98399	1.42008
O	-2.31091	-2.20114	0.86461
O	-1.28835	-0.65806	2.13444
C	-1.57482	2.22464	-0.54883
C	-1.98678	2.76634	0.80683
O	-0.15707	1.88905	-0.47567
C	2.37104	0.70822	-0.14230
C	3.59023	0.08615	0.05816
Cl	4.99708	1.05068	0.44827
C	3.71732	-1.30167	-0.04762
C	2.60599	-2.07218	-0.35673
H	-0.48655	-1.68659	-1.00502
H	-2.47991	1.02667	-2.12130
H	-4.26529	1.08955	-0.46870
H	-3.24559	-1.43143	-1.23611
H	-4.30634	-0.65496	1.28365
H	-3.35353	0.76756	1.73240
H	-1.51651	-2.72414	1.10402
H	-1.66799	2.99995	-1.31272
H	-1.70716	2.07157	1.60208

H	-1.47616	3.71543	0.98432
H	-3.06519	2.94880	0.83910
H	2.27358	1.78607	-0.05738
H	4.68266	-1.77241	0.11384
H	2.68266	-3.15188	-0.44055

1b NMR Conformer 4
Energy: -875536.3348995

O	0.99527	-2.22236	-1.58625
C	1.85511	-1.44777	-0.90640
C	1.55196	-0.12283	-0.52957
C	0.24753	0.43812	-0.87411
N	-0.65259	-0.17713	-1.55294
C	-1.85441	0.67221	-1.53168
C	-2.92314	0.03647	-0.62788
O	-3.52424	-1.06892	-1.28008
C	-2.38285	-0.39240	0.73534
C	-3.49757	-0.68575	1.71040
O	-3.10700	-1.52091	2.67907
O	-4.61002	-0.20810	1.66108
C	-1.29269	2.04126	-1.09082
C	-2.12823	2.92365	-0.18999
O	-0.05091	1.67235	-0.42268
C	2.48860	0.64121	0.18032
C	3.71069	0.08466	0.50818
Cl	4.88423	1.03283	1.39313
C	4.02445	-1.22752	0.14307
C	3.10121	-1.98582	-0.55926
H	0.16630	-1.70483	-1.75889
H	-2.28646	0.74160	-2.53454
H	-3.73328	0.75952	-0.48614
H	-2.83132	-1.71429	-1.50678
H	-1.75468	0.38285	1.19409
H	-1.75097	-1.28068	0.63451
H	-3.84687	-1.64741	3.30993
H	-0.99510	2.59934	-1.98702
H	-1.57135	3.82918	0.06042
H	-3.04045	3.21985	-0.71563
H	-2.40939	2.42257	0.73919
H	2.24545	1.66065	0.46430
H	4.98939	-1.64886	0.41019
H	3.32615	-3.00724	-0.85110

1b NMR Conformer 3
Energy: -875529.5350123

O	2.02031	2.86157	-0.28372
C	2.56333	1.62655	-0.23234
C	1.82998	0.42679	-0.16350
C	0.35952	0.37870	-0.13201
N	-0.35802	-0.65656	0.05785
C	-1.75205	-0.21923	-0.11584
C	-2.68299	-1.04312	0.77491
O	-2.35398	-0.94973	2.14405
C	-4.15609	-0.63800	0.64746
C	-4.60879	-0.73421	-0.78764
O	-4.66451	0.46075	-1.38808
O	-4.85891	-1.77352	-1.35874
C	-1.68476	1.31448	0.05661
C	-1.85729	1.89454	1.45034
O	-0.29739	1.55661	-0.34033
C	2.51526	-0.79774	-0.11060
C	3.89531	-0.82319	-0.12233
Cl	4.73359	-2.35621	-0.05320
C	4.63279	0.36174	-0.19087
C	3.96465	1.57243	-0.24566
H	1.04839	2.81412	-0.28754
H	-2.03019	-0.43854	-1.15971
H	-2.58500	-2.08478	0.43401
H	-1.44307	-1.27183	2.26088
H	-4.30934	0.37568	1.02224
H	-4.75223	-1.33266	1.24381
H	-4.93079	0.33833	-2.32475
H	-2.31395	1.82896	-0.67233
H	-1.17618	1.41636	2.15757
H	-1.64588	2.96640	1.41425
H	-2.87504	1.75318	1.81758
H	1.93928	-1.71678	-0.06151
H	5.71847	0.33113	-0.20250
H	4.51323	2.50803	-0.29929

1b NMR Conformer 2
Energy: -875530.6456162

O	2.15605	2.83575	-0.45389
C	2.66328	1.59111	-0.32591
C	1.89448	0.41818	-0.20524
C	0.42270	0.41450	-0.19357
N	-0.32763	-0.58362	0.05374
C	-1.70810	-0.11901	-0.16017
C	-2.66715	-0.84500	0.78341
O	-2.33996	-0.64920	2.14610
C	-4.11945	-0.41694	0.61245
C	-4.72657	-0.86672	-0.69259
O	-5.93865	-0.33523	-0.88106
O	-4.21016	-1.62876	-1.48161
C	-1.59335	1.42152	-0.09155
C	-1.76488	2.10500	1.25500
O	-0.19619	1.59613	-0.48753
C	2.54296	-0.82033	-0.07340

C	3.92177	-0.88475	-0.05850
Cl	4.71509	-2.43432	0.10602
C	4.69430	0.27357	-0.17681
C	4.06246	1.49764	-0.30966
H	1.18347	2.81379	-0.47771
H	-1.99494	-0.40592	-1.18215
H	-2.59168	-1.91172	0.52932
H	-1.43446	-0.97434	2.28951
H	-4.25011	0.66624	0.70231
H	-4.71452	-0.86405	1.41776
H	-6.30735	-0.67227	-1.72504
H	-2.19597	1.90644	-0.86310
H	-1.09535	1.66923	1.99950
H	-1.53639	3.16810	1.14274
H	-2.78638	2.00469	1.62605
H	1.93994	-1.71886	0.01502
H	5.77867	0.21200	-0.16637
H	4.63857	2.41336	-0.40321

1b NMR Conformer 1
Energy: -875535.0092543

O	-1.32989	2.66524	0.14670
C	-2.22849	1.67525	0.02483
C	-1.85813	0.32002	-0.10264
C	-0.44120	-0.03975	-0.11715
N	0.52410	0.79531	0.01177
C	1.76480	0.02840	-0.17596
C	2.88836	0.60410	0.68731
O	2.57389	0.59508	2.06632
C	4.20780	-0.14128	0.52904
C	4.85018	0.06125	-0.82028
O	5.92718	-0.71515	-0.97359
O	4.46799	0.83542	-1.67136
C	1.30516	-1.43499	0.03818
C	1.39238	-2.02739	1.43520
O	-0.11683	-1.33507	-0.29167
C	-2.84170	-0.67096	-0.22174
C	-4.17624	-0.30939	-0.21549
Cl	-5.40677	-1.54318	-0.36615
C	-4.55785	1.02906	-0.09136
C	-3.58801	2.01219	0.02793
H	-0.41827	2.27471	0.12133
H	2.07416	0.15524	-1.22311
H	3.03634	1.63728	0.34226
H	1.76971	1.12565	2.20007
H	4.10608	-1.21666	0.70684
H	4.91247	0.22806	1.28352
H	6.32751	-0.53683	-1.85084
H	1.74781	-2.10494	-0.70264
H	0.87392	-1.39453	2.15836
H	0.92849	-3.01687	1.42543
H	2.42839	-2.12909	1.76338
H	-2.54601	-1.71134	-0.31823
H	-5.61101	1.29546	-0.08852
H	-3.86456	3.05768	0.12580

1a NMR Conformer 28
Energy: -875532.9115592

O	1.17358	1.50477	2.30294
C	1.99484	0.79476	1.49960
C	1.54367	0.40433	0.22725
C	0.20918	0.74557	-0.30507
N	-0.40787	0.05502	-1.18708
C	-1.69581	0.71892	-1.40916
C	-2.82491	-0.18375	-0.89963
O	-2.85581	-1.38737	-1.66596
C	-2.69802	-0.51487	0.59324
C	-3.85632	-1.32975	1.14105
O	-4.35146	-2.28186	0.34691
O	-4.31184	-1.16498	2.25186
C	-1.56496	2.07079	-0.67758
C	-1.32550	3.24258	-1.60881
O	-0.38508	1.87234	0.14441
C	2.37720	-0.36966	-0.59012
C	3.63931	-0.73228	-0.15402
Cl	4.67166	-1.68504	-1.19508
C	4.10035	-0.34273	1.10215
C	3.27508	0.41377	1.92106
H	1.60240	1.67495	3.16131
H	-1.85982	0.86282	-2.48424
H	-3.78257	0.31567	-1.09276
H	-1.94918	-1.74811	-1.71347
H	-2.62338	0.38890	1.20292
H	-1.78075	-1.09892	0.74925
H	-3.89303	-2.26809	-0.52358
H	-2.39892	2.27377	0.00255
H	-2.21574	3.41621	-2.22044
H	-1.10876	4.14905	-1.03973
H	-0.48217	3.02950	-2.27322
H	2.01874	-0.67072	-1.56954
H	5.09265	-0.62947	1.43756
H	3.61764	0.71567	2.90828

1a NMR Conformer 27
Energy: -875539.1679980

O	-0.91774	-1.32992	2.34509
C	-1.80496	-0.97180	1.40332
C	-1.53444	0.01868	0.43629

C	-0.23479	0.68796	0.43496
N	0.70274	0.46384	1.28294
C	1.86051	1.26038	0.86416
C	2.98286	0.34267	0.35862
O	3.49170	-0.44876	1.41488
C	2.53940	-0.54565	-0.81024
C	3.66373	-1.44971	-1.24847
O	4.75426	-0.76175	-1.60586
O	3.60784	-2.65967	-1.28365
C	1.28144	2.21439	-0.20437
C	1.02471	3.61808	0.30517
O	0.00731	1.59188	-0.53246
C	-2.50268	0.35250	-0.52080
C	-3.72272	-0.29736	-0.50992
Cl	-4.93332	0.11812	-1.70137
C	-4.00375	-1.28215	0.44098
C	-3.04951	-1.61457	1.38952
H	-0.09538	-0.78789	2.23376
H	2.25818	1.81753	1.72049
H	3.81520	0.97708	0.03315
H	2.76607	-0.98165	1.78740
H	2.23950	0.06793	-1.66849
H	1.69751	-1.17890	-0.51792
H	5.45570	-1.39127	-1.87515
H	1.87112	2.22928	-1.12675
H	1.97640	4.10708	0.53214
H	0.49689	4.20924	-0.44638
H	0.42305	3.58395	1.21906
H	-2.28568	1.11748	-1.26013
H	-4.96765	-1.78330	0.43522
H	-3.24948	-2.37643	2.13701

1a NMR Conformer 26
Energy: -875534.8899899

O	1.81485	2.36033	1.68582
C	2.28125	1.27196	1.03736
C	1.56226	0.53261	0.07907
C	0.18974	0.86306	-0.33729
N	-0.46899	0.30401	-1.27321
C	-1.81410	0.89311	-1.25608
C	-2.83685	-0.15999	-0.80925
O	-2.93332	-1.18925	-1.77613
C	-2.51354	-0.74901	0.56228
C	-3.64138	-1.61552	1.06770
O	-3.20503	-2.59655	1.86515
O	-4.81454	-1.44225	0.81849
C	-1.69438	2.11294	-0.31836
C	-1.59471	3.43767	-1.04677
O	-0.43731	1.84955	0.36532
C	2.16606	-0.58048	-0.52823
C	3.45325	-0.94481	-0.18882
Cl	4.18959	-2.33534	-0.95114
C	4.17627	-0.21738	0.76036
C	3.58799	0.88032	1.36348
H	0.89892	2.55950	1.42581
H	-2.09102	1.20324	-2.27061
H	-3.82508	0.31268	-0.77297
H	-2.04098	-1.54536	-1.93474
H	-2.36420	0.03936	1.31275
H	-1.59170	-1.33745	0.52445
H	-3.97603	-3.10210	2.19945
H	-2.47168	2.13987	0.45237
H	-2.54196	3.65015	-1.55059
H	-1.38064	4.24951	-0.34803
H	-0.80114	3.39548	-1.79949
H	1.60102	-1.14436	-1.26409
H	5.18843	-0.51246	1.02157
H	4.12753	1.46307	2.10407

1a NMR Conformer 24
Energy: -875540.9871794

O	-1.37033	-2.54378	0.95963
C	-2.25452	-1.64016	0.50702
C	-1.90591	-0.29965	0.23974
C	-0.52812	0.14211	0.45525
N	0.41700	-0.61600	0.87749
C	1.63441	0.19392	0.94639
C	2.72329	-0.43212	0.06788
O	2.31942	-0.46702	-1.28915
C	4.01545	0.36446	0.12343
C	5.14797	-0.36793	-0.55677
O	6.05994	0.47132	-1.05754
O	5.25091	-1.57280	-0.62498
C	1.18287	1.60100	0.47854
C	1.35957	2.69419	1.51000
O	-0.23440	1.42690	0.19997
C	-2.87257	0.59990	-0.22877
C	-4.16955	0.16327	-0.42690
Cl	-5.37943	1.28395	-1.00881
C	-4.52890	-1.16184	-0.16762
C	-3.57559	-2.05485	0.29608
H	-0.48768	-2.10147	1.06557
H	1.99558	0.21401	1.98466
H	2.91245	-1.44916	0.43594
H	1.63401	-1.14838	-1.39769
H	4.31944	0.52621	1.16609
H	3.89437	1.34699	-0.34344
H	6.79228	-0.05043	-1.44943

H	1.64545	1.86904	-0.47715
H	2.42560	2.83385	1.71601
H	0.94973	3.64073	1.15029
H	0.85859	2.41961	2.44321
H	-2.59464	1.62985	-0.43142
H	-5.55238	-1.48861	-0.32865
H	-3.83612	-3.08825	0.50433

1a NMR Conformer 23
Energy: -875537.8587497

O	0.36522	-1.98446	-1.44924
C	1.39031	-1.29308	-0.93037
C	1.24686	-0.00605	-0.37161
C	-0.06851	0.63088	-0.35184
N	-1.15152	0.08314	-0.77103
C	-2.23166	1.06059	-0.59584
C	-3.44474	0.46912	0.13758
O	-4.27377	-0.25689	-0.74328
C	-3.06163	-0.36112	1.37500
C	-2.36143	-1.65604	1.04106
O	-1.19676	-1.79795	1.67874
O	-2.80259	-2.50184	0.28982
C	-1.55671	2.24287	0.13836
C	-1.73448	3.58645	-0.52909
O	-0.14572	1.88024	0.13757
C	2.36034	0.65940	0.15850
C	3.59747	0.04693	0.12567
Cl	4.99058	0.87594	0.78745
C	3.75696	-1.22480	-0.42925
C	2.65927	-1.88630	-0.95314
H	-0.46296	-1.44432	-1.37148
H	-2.58770	1.37525	-1.58705
H	-4.05374	1.31467	0.48356
H	-3.84101	-1.09999	-0.96315
H	-3.98385	-0.63396	1.89972
H	-2.44235	0.21819	2.06363
H	-0.80266	-2.66279	1.43214
H	-1.86109	2.29208	1.19141
H	-2.79773	3.84654	-0.54149
H	-1.19382	4.36608	0.01182
H	-1.37229	3.54646	-1.56020
H	2.23834	1.64913	0.58837
H	4.73843	-1.69020	-0.44678
H	2.76006	-2.87593	-1.38890

1a NMR Conformer 22
Energy: -875536.7003924

O	0.32419	-2.03871	-1.41694
C	1.34462	-1.31598	-0.92517
C	1.18287	-0.00762	-0.42611
C	-0.14014	0.60907	-0.42617
N	-1.18918	0.05959	-0.91980
C	-2.30875	0.97282	-0.69647
C	-3.47504	0.24867	-0.01011
O	-4.02375	-0.72038	-0.88111
C	-3.14499	-0.34833	1.37281
C	-2.01185	-1.34576	1.38662
O	-2.26808	-2.41768	0.62285
O	-0.97743	-1.21402	2.00588
C	-1.68678	2.15069	0.09174
C	-1.86440	3.50323	-0.55998
O	-0.27125	1.82221	0.13616
C	2.28171	0.69186	0.08768
C	3.52780	0.09242	0.09418
Cl	4.90204	0.96347	0.73259
C	3.70517	-1.20010	-0.40522
C	2.61809	-1.89713	-0.91065
H	-0.50097	-1.49197	-1.37228
H	-2.68763	1.31327	-1.66904
H	-4.27030	0.98519	0.15690
H	-3.33912	-1.37436	-1.09378
H	-4.05198	-0.85587	1.71433
H	-2.89959	0.43583	2.09165
H	-1.49303	-3.01389	0.63882
H	-2.02935	2.17547	1.13247
H	-2.92931	3.75090	-0.60155
H	-1.35013	4.27993	0.00958
H	-1.46999	3.48733	-1.57965
H	2.14583	1.69627	0.47675
H	4.69079	-1.65513	-0.39387
H	2.73523	-2.90362	-1.29949

1a NMR Conformer 21
Energy: -875532.0460919

O	1.93393	2.74350	0.33577
C	2.61295	1.58511	0.17973
C	1.89228	0.39905	-0.03894
C	0.41838	0.35873	-0.13574
N	-0.30063	-0.62165	0.25423
C	-1.68790	-0.29030	-0.08726
C	-2.56612	-0.40093	1.16491
O	-2.10705	0.47411	2.17926
C	-4.01573	-0.01691	0.90175
C	-4.72903	-0.96241	-0.03032
O	-5.88479	-0.45086	-0.46643
O	-4.33413	-2.06451	-0.34608
C	-1.61806	1.13593	-0.68126
C	-2.20486	1.27060	-2.07024

O	-0.19456	1.40634	-0.72637
C	2.58056	-0.81384	-0.15398
C	3.96303	-0.84048	-0.06893
Cl	4.80816	-2.36313	-0.22761
C	4.68783	0.33102	0.13597
C	4.00910	1.53545	0.26263
H	2.55025	3.47729	0.51464
H	-2.05479	-1.01501	-0.82667
H	-2.52446	-1.44331	1.50845
H	-1.19971	0.21588	2.41716
H	-4.09731	1.00433	0.51299
H	-4.56392	-0.02367	1.85178
H	-6.32960	-1.11021	-1.04050
H	-2.04877	1.87387	0.00615
H	-3.28130	1.06951	-2.03728
H	-2.05617	2.27869	-2.46420
H	-1.73989	0.54984	-2.74940
H	2.01501	-1.72627	-0.31655
H	5.77178	0.30330	0.19895
H	4.56280	2.45576	0.43507

1a NMR Conformer 20
Energy: -875532.9183363

O	1.22187	3.02937	0.89811
C	1.78104	1.87623	0.47275
C	1.07665	0.80982	-0.11209
C	-0.37722	0.82135	-0.31855
N	-1.04830	-0.05713	-0.95407
C	-2.45730	0.30769	-0.82803
C	-3.22011	-0.75960	-0.05082
O	-3.41425	-1.93910	-0.83157
C	-2.53561	-1.16831	1.26221
C	-1.23022	-1.93820	1.14706
O	-1.22603	-2.96736	0.29381
O	-0.28117	-1.75007	1.87192
C	-2.46130	1.68386	-0.11802
C	-2.90874	2.83969	-0.98443
O	-1.06283	1.85943	0.23743
C	1.77022	-0.34081	-0.51626
C	3.13554	-0.41613	-0.34700
Cl	3.99281	-1.85459	-0.84791
C	3.84797	0.64040	0.22855
C	3.16947	1.77412	0.63306
H	0.25678	3.01722	0.77667
H	-2.91268	0.38117	-1.82713
H	-4.20521	-0.34565	0.21352
H	-3.22901	-1.77281	-1.77404
H	-3.23612	-1.82042	1.79888
H	-2.35308	-0.29542	1.89358
H	-2.03192	-2.92252	-0.26099
H	-3.02432	1.66340	0.82195
H	-3.96184	2.70905	-1.25208
H	-2.80102	3.78792	-0.45306
H	-2.31589	2.87435	-1.90335
H	1.21057	-1.16347	-0.95135
H	4.92380	0.56719	0.35764
H	3.69727	2.60899	1.08443

1a NMR Conformer 19
Energy: -875538.4063521

O	-1.35854	2.66171	-0.51406
C	-2.24063	1.66675	-0.32500
C	-1.84896	0.32324	-0.15413
C	-0.42810	-0.02289	-0.18127
N	0.52017	0.82303	-0.35890
C	1.78559	0.08936	-0.30146
C	2.65861	0.66250	0.82451
O	2.00391	0.53221	2.07339
C	3.98807	-0.06501	0.96994
C	4.92861	0.15231	-0.19555
O	6.06265	-0.56120	-0.18382
O	4.72510	0.92671	-1.10078
C	1.35891	-1.38355	-0.07325
C	1.76937	-2.33162	-1.17972
O	-0.09240	-1.31237	-0.01535
C	-2.81483	-0.67255	0.04148
C	-4.15372	-0.32772	0.06549
Cl	-5.36178	-1.56838	0.30461
C	-4.55553	0.99969	-0.10139
C	-3.60294	1.98750	-0.29529
H	-0.44235	2.27973	-0.51036
H	2.31863	0.21170	-1.25254
H	2.85064	1.71863	0.59379
H	1.22927	1.12054	2.08305
H	3.83546	-1.14235	1.11954
H	4.48935	0.30066	1.87479
H	6.12967	-1.16280	0.58305
H	1.68005	-1.74781	0.90883
H	2.86186	-2.39522	-1.22496
H	1.37159	-3.33381	-1.00360
H	1.40476	-1.96674	-2.14474
H	-2.50427	-1.70506	0.17129
H	-5.61146	1.25451	-0.07894
H	-3.89655	3.02471	-0.42641

1a NMR Conformer 18
Energy: -875539.4893456

O	-0.94284	-0.84408	2.58021

C	-1.81617	-0.67097	1.57560
C	-1.52653	0.11054	0.43720
C	-0.22162	0.76011	0.32516
N	0.70665	0.68876	1.20890
C	1.87396	1.39349	0.66683
C	2.99800	0.39407	0.36221
O	3.49658	-0.16675	1.56218
C	2.56232	-0.70674	-0.60121
C	3.73711	-1.53190	-1.06757
O	3.37505	-2.77502	-1.40258
O	4.87535	-1.12851	-1.16323
C	1.31365	2.13293	-0.56841
C	1.06817	3.60986	-0.33467
O	0.03559	1.47144	-0.78865
C	-2.48112	0.25672	-0.57870
C	-3.70637	-0.37194	-0.45663
Cl	-4.90019	-0.19315	-1.72173
C	-4.00631	-1.14984	0.66494
C	-3.06585	-1.29622	1.67218
H	-0.11359	-0.34075	2.37358
H	2.25911	2.10051	1.41079
H	3.83567	0.94645	-0.07865
H	2.76195	-0.59810	2.03428
H	2.09324	-0.29092	-1.50373
H	1.82339	-1.36388	-0.13162
H	4.16077	-3.25671	-1.73835
H	1.91217	1.96847	-1.47063
H	2.02343	4.12330	-0.19278
H	0.55421	4.05456	-1.18966
H	0.45773	3.75350	0.56258
H	-2.24953	0.86133	-1.45037
H	-4.97419	-1.63671	0.74506
H	-3.28088	-1.89592	2.55158

1a NMR Conformer 17
Energy: -875529.6416011

O	0.75506	-2.63312	0.24569
C	1.62388	-1.60556	0.15846
C	1.26780	-0.25812	0.33031
C	-0.10688	0.14697	0.65265
N	-0.62459	1.29221	0.44469
C	-2.03955	1.19056	0.81281
C	-2.93959	1.40138	-0.42343
O	-3.03877	2.77781	-0.72809
C	-2.46357	0.63889	-1.67636
C	-2.40635	-0.85973	-1.52667
O	-3.62626	-1.40393	-1.42025
O	-1.39086	-1.52129	-1.51211
C	-2.17503	-0.19162	1.49548
C	-2.36788	-0.11585	2.99544
O	-0.88839	-0.81251	1.22202
C	2.23426	0.74439	0.16698
C	3.53500	0.40042	-0.13987
Cl	4.74031	1.65229	-0.33154
C	3.90667	-0.93847	-0.29471
C	2.95273	-1.92961	-0.14768
H	-0.14269	-2.30233	0.43466
H	-2.29826	1.99206	1.51516
H	-3.95473	1.08202	-0.16109
H	-2.15885	3.11052	-0.97891
H	-1.46564	0.97998	-1.95963
H	-3.16339	0.86881	-2.48591
H	-3.53643	-2.37644	-1.34522
H	-2.94188	-0.82288	1.03529
H	-3.33902	0.33485	3.22041
H	-2.33320	-1.11278	3.44026
H	-1.58374	0.50275	3.44298
H	1.94289	1.78253	0.29463
H	4.93500	-1.19472	-0.53253
H	3.21163	-2.97651	-0.27524

1a NMR Conformer 16
Energy: -875537.0329284

O	0.29409	-1.89469	-1.61881
C	1.29640	-1.21355	-1.04487
C	1.12515	0.04678	-0.43944
C	-0.20013	0.65829	-0.40680
N	-1.25346	0.14606	-0.93607
C	-2.38214	1.00598	-0.58612
C	-3.36594	0.29191	0.35420
O	-4.13428	-0.69688	-0.31665
C	-2.65469	-0.40309	1.52070
C	-1.78546	-1.60527	1.18655
O	-2.24983	-2.47526	0.28748
O	-0.71574	-1.80523	1.71347
C	-1.72215	2.23732	0.08867
C	-1.78505	3.50893	-0.72777
O	-0.33468	1.82958	0.23913
C	2.21687	0.70215	0.14573
C	3.46235	0.10636	0.11765
Cl	4.82845	0.91955	0.84708
C	3.64804	-1.14031	-0.48423
C	2.57088	-1.79234	-1.05909
H	-0.54333	-1.38056	-1.52199
H	-2.92451	1.29608	-1.49710
H	-4.03743	1.05491	0.77734
H	-4.58758	-0.31604	-1.09048
H	-3.41387	-0.75495	2.22969

H	-2.01678	0.30997	2.05069
H	-3.07564	-2.13258	-0.11313
H	-2.11230	2.40536	1.10013
H	-2.82669	3.82980	-0.82717
H	-1.21835	4.30774	-0.24395
H	-1.37594	3.33350	-1.72755
H	2.07347	1.67110	0.61510
H	4.63480	-1.59496	-0.49793
H	2.69353	-2.76335	-1.52980

1a NMR Conformer 15
Energy: -875530.3261512

O	-0.56225	2.50937	0.26632
C	-1.53691	1.58319	0.15154
C	-1.32431	0.19416	0.20034
C	0.01097	-0.37681	0.44686
N	0.48821	-1.43634	-0.07619
C	1.87827	-1.53589	0.38935
C	2.82883	-1.31284	-0.80004
O	2.71599	-2.39401	-1.70264
C	2.58924	0.00583	-1.56472
C	2.95515	1.25797	-0.81316
O	4.26244	1.32981	-0.55553
O	2.17389	2.12519	-0.47073
C	1.97852	-0.49690	1.52652
C	1.91387	-1.11013	2.91182
O	0.79386	0.31389	1.31584
C	-2.39670	-0.68523	0.00571
C	-3.66985	-0.18367	-0.19831
Cl	-5.00732	-1.28745	-0.42473
C	-3.90106	1.19238	-0.21884
C	-2.83696	2.06460	-0.04954
H	0.33415	2.12732	0.24078
H	2.07590	-2.54712	0.76426
H	3.85930	-1.33213	-0.42605
H	1.77955	-2.49038	-1.95274
H	1.54361	0.08122	-1.87371
H	3.21951	-0.03582	-2.45875
H	4.45317	2.16052	-0.06829
H	2.84556	0.16555	1.43822
H	2.81269	-1.70652	3.09251
H	1.84945	-0.33141	3.67484
H	1.03912	-1.76294	2.99381
H	-2.21540	-1.75576	0.03505
H	-4.90547	1.57537	-0.37437
H	-2.98981	3.13922	-0.08303

1a NMR Conformer 13
Energy: -875537.3230574

O	2.16999	2.58614	1.10527
C	2.67560	1.40738	0.68104
C	1.94175	0.40990	0.01053
C	0.51060	0.53880	-0.31022
N	-0.23511	-0.37714	-0.78810
C	-1.57278	0.19339	-0.94743
C	-2.58693	-0.67388	-0.19710
O	-2.27838	-0.70310	1.19609
C	-4.00766	-0.13698	-0.32887
C	-5.07394	-1.02769	0.28622
O	-4.77191	-1.60919	1.45023
O	-6.15982	-1.19916	-0.21902
C	-1.46593	1.64116	-0.40758
C	-1.83516	2.71864	-1.40422
O	-0.05792	1.75128	-0.07475
C	2.58259	-0.77807	-0.37176
C	3.92208	-0.96568	-0.09254
Cl	4.70931	-2.44717	-0.57840
C	4.65796	0.01745	0.57267
C	4.03301	1.19231	0.95368
H	1.23220	2.67549	0.86343
H	-1.84506	0.18424	-2.01290
H	-2.52872	-1.69017	-0.61106
H	-1.46240	-1.21951	1.33356
H	-4.26550	0.00364	-1.38143
H	-4.08228	0.84037	0.16884
H	-3.85433	-1.38327	1.72195
H	-2.01195	1.76169	0.53497
H	-2.89614	2.63401	-1.66001
H	-1.65898	3.71349	-0.98836
H	-1.24702	2.60509	-2.31976
H	2.00979	-1.54085	-0.89003
H	5.71103	-0.14069	0.78774
H	4.58408	1.97014	1.47354

1a NMR Conformer 12
Energy: -875536.3395430

O	0.82234	2.83078	-0.18473
C	1.67291	1.79301	-0.14019
C	1.28158	0.50275	0.27404
C	-0.10719	0.26238	0.66343
N	-1.02450	1.16083	0.67341
C	-2.28129	0.49705	1.02952
C	-3.29622	0.59500	-0.12359
O	-3.83671	1.90106	-0.17505
C	-2.72366	0.23931	-1.50645
C	-2.26992	-1.18748	-1.67503
O	-3.26711	-2.06162	-1.47545
O	-1.14592	-1.52881	-1.97182

C	-1.84524	-0.93302	1.43403
C	-1.92847	-1.18975	2.92517
O	-0.45132	-0.98518	1.02430
C	2.21456	-0.54262	0.29972
C	3.52039	-0.29850	-0.08279
Cl	4.68742	-1.60127	-0.05269
C	3.92307	0.97472	-0.49462
C	3.00320	2.01107	-0.52200
H	-0.07140	2.52367	0.11697
H	-2.74012	1.01145	1.88287
H	-4.13701	-0.06933	0.10846
H	-3.11267	2.53764	-0.31255
H	-1.87764	0.89016	-1.73945
H	-3.52092	0.41983	-2.23525
H	-2.92834	-2.97165	-1.61347
H	-2.36900	-1.71361	0.87454
H	-2.97487	-1.17199	3.24343
H	-1.50295	-2.16445	3.17354
H	-1.38395	-0.41274	3.47088
H	1.90213	-1.53270	0.61739
H	4.95332	1.14876	-0.79177
H	3.29631	3.00737	-0.83913

1a NMR Conformer 11

Energy: -875534.4199727

O	2.07125	2.83566	0.34769
C	2.59942	1.60618	0.16683
C	1.85361	0.43122	-0.04420
C	0.38144	0.40379	-0.09319
N	-0.34407	-0.64061	-0.16736
C	-1.73946	-0.19708	-0.19021
C	-2.50881	-0.86469	0.95741
O	-1.96515	-0.49601	2.20938
C	-3.97874	-0.44259	0.98735
C	-4.70016	-0.76836	-0.29569
O	-4.61294	-2.06650	-0.60574
O	-5.29381	0.03569	-0.98204
C	-1.68004	1.34620	-0.08468
C	-2.31589	2.08453	-1.24192
O	-0.24885	1.60780	-0.06478
C	2.52551	-0.79048	-0.20961
C	3.90452	-0.83721	-0.16680
Cl	4.72646	-2.36616	-0.37585
C	4.65424	0.32334	0.04109
C	3.99934	1.53126	0.20600
H	1.10025	2.81289	0.28774
H	-2.19341	-0.51115	-1.14272
H	-2.44542	-1.95123	0.81360
H	-1.07017	-0.87127	2.28053
H	-4.07190	0.63108	1.17029
H	-4.47025	-0.97485	1.80856
H	-5.09413	-2.23041	-1.44451
H	-2.06351	1.69693	0.87937
H	-3.39033	1.87439	-1.25648
H	-2.17021	3.16318	-1.14796
H	-1.88323	1.74630	-2.18851
H	1.94069	-1.69060	-0.37192
H	5.73900	0.27582	0.07225
H	4.55742	2.44813	0.37040

1a NMR Conformer 10

Energy: -875538.4664362

O	-1.63677	2.77205	-0.41770
C	-2.36160	1.66223	-0.20852
C	-1.79608	0.37032	-0.19987
C	-0.35973	0.20992	-0.42492
N	0.44872	1.18474	-0.63772
C	1.78696	0.61930	-0.81512
C	2.75670	1.28918	0.16738
O	2.37315	1.06413	1.51451
C	4.20718	0.82154	0.01061
C	4.52585	-0.58892	0.48308
O	4.12627	-0.92039	1.71447
O	5.15807	-1.37893	-0.18355
C	1.58504	-0.90484	-0.61820
C	2.00134	-1.75212	-1.80029
O	0.14807	-1.03102	-0.41434
C	-2.60444	-0.75293	0.02528
C	-3.95961	-0.58328	0.23801
Cl	-4.97340	-1.98083	0.51856
C	-4.53505	0.69083	0.23270
C	-3.73892	1.80312	0.01035
H	-0.68915	2.51406	-0.55908
H	2.13960	0.84297	-1.83153
H	2.73594	2.36547	-0.04625
H	1.48621	1.43035	1.67944
H	4.84772	1.49383	0.59459
H	4.51164	0.89533	-1.03528
H	3.52893	-0.23377	2.07569
H	2.04100	-1.26205	0.31011
H	3.08291	-1.66853	-1.94671
H	1.75690	-2.80267	-1.62937
H	1.49568	-1.40959	-2.70765
H	-2.15917	-1.74314	0.02957
H	-5.60168	0.80443	0.40232
H	-4.16582	2.80133	0.00249

1a NMR Conformer 9

Energy: -875533.1444907

O	1.18911	2.86067	0.33748
C	1.91651	1.72639	0.25937
C	1.43302	0.48819	-0.20233
C	0.04865	0.27823	-0.65798
N	-0.42837	-0.80528	-1.12701
C	-1.85650	-0.57432	-1.37614
C	-2.69233	-1.48810	-0.46138
O	-2.40456	-2.83707	-0.77771
C	-2.47187	-1.23420	1.03621
C	-3.36873	-0.17778	1.63667
O	-2.93064	0.22332	2.83417
O	-4.39006	0.24476	1.13415
C	-2.05151	0.94489	-1.17685
C	-2.21532	1.71809	-2.46914
O	-0.79699	1.33965	-0.54741
C	2.29698	-0.62023	-0.23956
C	3.60600	-0.49341	0.17621
Cl	4.66874	-1.88160	0.12977
C	4.09767	0.73216	0.63913
C	3.25353	1.82718	0.67642
H	0.27920	2.71569	0.02828
H	-2.08663	-0.86061	-2.40903
H	-3.75190	-1.33302	-0.69202
H	-1.44138	-2.96126	-0.72878
H	-1.42897	-0.99916	1.27319
H	-2.70389	-2.16282	1.57194
H	-3.56546	0.86837	3.20783
H	-2.84769	1.18658	-0.47013
H	-3.15890	1.43651	-2.94556
H	-2.22761	2.79362	-2.28132
H	-1.39628	1.48454	-3.15600
H	1.91186	-1.56964	-0.59819
H	5.12965	0.82068	0.96429
H	3.60650	2.79147	1.02919

1a NMR Conformer 8
Energy: -875532.9436877

O	1.53524	2.87466	0.47143
C	2.21096	1.71218	0.35014
C	1.65740	0.50683	-0.11932
C	0.25043	0.37310	-0.52905
N	-0.35264	-0.71435	-0.80372
C	-1.70406	-0.34059	-1.24510
C	-2.73992	-1.34464	-0.72377
O	-2.39198	-2.63316	-1.19670
C	-2.88311	-1.35278	0.80174
C	-3.91231	-0.37958	1.32176
O	-3.96969	-0.38099	2.65685
O	-4.62377	0.32182	0.63251
C	-1.85759	1.12371	-0.80289
C	-2.55296	2.03426	-1.78567
O	-0.46590	1.52785	-0.63797
C	2.46317	-0.64131	-0.19324
C	3.78673	-0.58445	0.19115
Cl	4.77991	-2.02014	0.09289
C	4.34822	0.60832	0.65826
C	3.56023	1.74252	0.73424
H	0.61262	2.77154	0.18101
H	-1.72749	-0.40878	-2.34271
H	-3.71258	-1.10730	-1.16708
H	-1.46766	-2.80691	-0.94844
H	-1.92912	-1.16325	1.30872
H	-3.20637	-2.35187	1.11497
H	-4.66120	0.24792	2.94819
H	-2.31089	1.20950	0.19002
H	-3.59181	1.70926	-1.89672
H	-2.55305	3.06684	-1.43021
H	-2.06228	1.99034	-2.76145
H	2.02481	-1.56478	-0.55853
H	5.39179	0.64169	0.95617
H	3.96885	2.68182	1.09447

1a NMR Conformer 7
Energy: -875536.1302623

O	1.80333	2.41382	1.58722
C	2.27570	1.29742	0.99406
C	1.56731	0.51456	0.06360
C	0.19961	0.82399	-0.38072
N	-0.46940	0.17989	-1.25426
C	-1.79928	0.79381	-1.30682
C	-2.83831	-0.19139	-0.75794
O	-2.90268	-1.34213	-1.59816
C	-2.55508	-0.61137	0.69060
C	-3.63884	-1.48855	1.29296
O	-4.19885	-2.39271	0.48637
O	-3.98933	-1.40359	2.44927
C	-1.66332	2.10094	-0.49715
C	-1.54081	3.34331	-1.35464
O	-0.40914	1.88903	0.21058
C	2.17631	-0.62618	-0.48544
C	3.45788	-0.97458	-0.11397
Cl	4.20463	-2.39510	-0.80679
C	4.17032	-0.20558	0.81144
C	3.57734	0.91875	1.35571
H	0.90107	2.61925	1.28817
H	-2.06872	1.00070	-2.34943
H	-3.82761	0.27849	-0.82438
H	-1.99626	-1.67827	-1.73948

H	-2.43994	0.25453	1.34757
H	-1.61537	-1.17961	0.72076
H	-3.82684	-2.31521	-0.42077
H	-2.44049	2.21778	0.26478
H	-2.48383	3.52182	-1.87942
H	-1.31302	4.21613	-0.73913
H	-0.74763	3.21282	-2.09731
H	1.62013	-1.22180	-1.20261
H	5.17842	-0.48986	1.09820
H	4.10765	1.53454	2.07594

1a NMR Conformer 6

Energy: -875541.9519124

O	1.34615	-2.48285	-1.12897
C	2.23105	-1.60661	-0.62561
C	1.88377	-0.28551	-0.27659
C	0.50766	0.17286	-0.46369
N	-0.44051	-0.55264	-0.93537
C	-1.65356	0.26406	-0.95319
C	-2.74641	-0.42147	-0.12930
O	-2.32723	-0.56575	1.22707
C	-4.03811	0.39032	-0.11941
C	-5.20710	-0.30083	0.56103
O	-4.93188	-0.98944	1.67034
O	-6.34696	-0.21093	0.16511
C	-1.20203	1.63391	-0.38437
C	-1.38441	2.80006	-1.33156
O	0.21557	1.43881	-0.12628
C	2.85179	0.58273	0.24603
C	4.14853	0.13415	0.41567
Cl	5.35933	1.21338	1.06732
C	4.50618	-1.17221	0.07305
C	3.55187	-2.03363	-0.44407
H	0.46298	-2.03917	-1.20488
H	-2.01598	0.35758	-1.98689
H	-2.92725	-1.41163	-0.57068
H	-1.64498	-1.26048	1.28699
H	-4.34864	0.62914	-1.13934
H	-3.87234	1.33766	0.41342
H	-3.96542	-0.97524	1.84977
H	-1.66035	1.83311	0.59079
H	-2.45114	2.95605	-1.52207
H	-0.97142	3.71670	-0.90429
H	-0.88776	2.59487	-2.28469
H	2.57569	1.59866	0.51227
H	5.52955	-1.50932	0.21245
H	3.81127	-3.05251	-0.71585

1a NMR Conformer 5

Energy: -875540.4842305

O	0.87845	-1.22604	-2.41802
C	1.77398	-0.91673	-1.46690
C	1.51768	0.02911	-0.45327
C	0.22464	0.70844	-0.40982
N	-0.72553	0.52611	-1.25523
C	-1.86953	1.31638	-0.79117
C	-2.99004	0.38607	-0.31183
O	-3.52874	-0.34179	-1.41320
C	-2.53355	-0.57960	0.78959
C	-3.65713	-1.41904	1.37240
O	-4.58841	-1.85613	0.52133
O	-3.71799	-1.71497	2.54502
C	-1.27287	2.21680	0.31352
C	-1.01491	3.64058	-0.13496
O	0.00157	1.57347	0.59601
C	2.49510	0.31155	0.51132
C	3.71006	-0.34503	0.46080
Cl	4.93228	0.00608	1.66090
C	3.97730	-1.28601	-0.53743
C	3.01424	-1.56708	-1.49309
H	0.06051	-0.68707	-2.27799
H	-2.27275	1.91384	-1.61731
H	-3.81418	1.01088	0.05523
H	-2.79953	-0.76489	-1.90687
H	-2.06334	-0.05122	1.62289
H	-1.78860	-1.27053	0.37106
H	-4.41274	-1.51579	-0.38393
H	-1.85197	2.19227	1.24233
H	-1.96636	4.14479	-0.32702
H	-0.47466	4.19315	0.63662
H	-0.42447	3.64538	-1.05660
H	2.28880	1.04235	1.28735
H	4.93747	-1.79355	-0.56175
H	3.20288	-2.29470	-2.27667

1a NMR Conformer 4

Energy: -875537.4695997

O	-1.21641	2.74001	0.05042
C	-2.04766	1.68707	0.11029
C	-1.63433	0.37152	-0.18370
C	-0.25013	0.12276	-0.58477
N	0.65578	1.02721	-0.67641
C	1.86503	0.36991	-1.18795
C	3.11748	0.88028	-0.46578
O	3.24274	2.27023	-0.70535
C	3.13456	0.58653	1.03765
C	3.77047	-0.73392	1.39603
O	3.67828	-0.98968	2.70402

O	4.32111	-1.48114	0.61472
C	1.54624	-1.13314	-1.05732
C	1.94163	-1.98116	-2.24299
O	0.09808	-1.13868	-0.89679
C	-2.54608	-0.68945	-0.09536
C	-3.85240	-0.43494	0.27910
Cl	-4.99334	-1.75597	0.38854
C	-4.27639	0.86421	0.57104
C	-3.37752	1.91574	0.48605
H	-0.31866	2.42403	-0.22402
H	1.98008	0.64622	-2.24650
H	3.99546	0.41562	-0.92607
H	2.43100	2.71355	-0.40262
H	2.13243	0.63214	1.48120
H	3.72975	1.36172	1.53419
H	4.12554	-1.84070	2.89603
H	1.94858	-1.55899	-0.13268
H	3.03069	-1.96430	-2.34768
H	1.62505	-3.01709	-2.10378
H	1.49227	-1.58877	-3.15937
H	-2.21839	-1.69927	-0.32273
H	-5.30652	1.04638	0.86365
H	-3.68692	2.93215	0.71021

1a NMR Conformer 3
Energy: -875536.8972170

O	0.95211	2.81309	-0.61343
C	1.74971	1.75166	-0.41884
C	1.29652	0.55511	0.17387
C	-0.09665	0.44790	0.60132
N	-0.96044	1.39584	0.52029
C	-2.25041	0.82820	0.93482
C	-3.17491	0.67034	-0.28855
O	-3.55353	1.95140	-0.75468
C	-2.56999	-0.14813	-1.43734
C	-2.64213	-1.64535	-1.26143
O	-1.72857	-2.27918	-2.00019
O	-3.45526	-2.23061	-0.57742
C	-1.84770	-0.48090	1.64327
C	-1.74007	-0.34387	3.14885
O	-0.51663	-0.73068	1.09840
C	2.17567	-0.52240	0.35024
C	3.48888	-0.40192	-0.06251
Cl	4.59254	-1.74070	0.16090
C	3.95177	0.77682	-0.65341
C	3.08591	1.84402	-0.82890
H	0.04625	2.59964	-0.26950
H	-2.75213	1.51158	1.62886
H	-4.09785	0.18403	0.04548
H	-2.75294	2.44641	-1.00365
H	-1.53850	0.14486	-1.65735
H	-3.15408	0.07060	-2.34005
H	-1.84979	-3.24697	-1.89810
H	-2.47131	-1.33155	1.36557
H	-2.73429	-0.18335	3.57571
H	-1.31320	-1.24919	3.58581
H	-1.10719	0.51081	3.40919
H	1.81700	-1.43824	0.81035
H	4.98732	0.85312	-0.97264
H	3.42610	2.76813	-1.28658

1a NMR Conformer 2
Energy: -875535.3620966

O	2.11814	2.83510	0.33416
C	2.63890	1.60035	0.16896
C	1.88843	0.42993	-0.05049
C	0.41698	0.41021	-0.12735
N	-0.31211	-0.62761	-0.23874
C	-1.70712	-0.17845	-0.26572
C	-2.47790	-0.84785	0.87981
O	-1.92378	-0.48551	2.13165
C	-3.94157	-0.43222	0.92838
C	-4.74879	-0.93157	-0.24252
O	-5.97138	-0.39165	-0.26554
O	-4.36592	-1.73617	-1.06483
C	-1.63808	1.36383	-0.15114
C	-2.22238	2.10872	-1.33180
O	-0.20825	1.61710	-0.07990
C	2.55513	-0.79703	-0.19879
C	3.93259	-0.85353	-0.13106
Cl	4.74668	-2.38978	-0.31860
C	4.68712	0.30243	0.08500
C	4.03751	1.51520	0.23290
H	1.14798	2.81979	0.26307
H	-2.16344	-0.48816	-1.21465
H	-2.41592	-1.93391	0.73007
H	-1.02305	-0.84881	2.18717
H	-4.05277	0.65598	1.00170
H	-4.39740	-0.84278	1.83726
H	-6.47118	-0.76256	-1.02361
H	-2.05433	1.71805	0.79789
H	-3.29921	1.91651	-1.38803
H	-2.06942	3.18593	-1.23378
H	-1.76137	1.76441	-2.26234
H	1.96641	-1.69346	-0.36731
H	5.77073	0.24815	0.13571
H	4.59872	2.42917	0.40282

1a NMR Conformer 1
Energy: -875540.0004709

O	-1.36216	2.65966	-0.51579
C	-2.24392	1.66362	-0.33142
C	-1.85159	0.32083	-0.15149
C	-0.42919	-0.02025	-0.16147
N	0.51856	0.82841	-0.32784
C	1.78464	0.09594	-0.26489
C	2.66979	0.68505	0.84156
O	2.03024	0.58018	2.10087
C	3.99755	-0.04627	0.97812
C	4.90581	0.13326	-0.21159
O	5.94609	-0.70426	-0.17053
O	4.74430	0.94369	-1.09820
C	1.36100	-1.37302	-0.00978
C	1.80800	-2.34853	-1.07720
O	-0.09161	-1.30890	0.00963
C	-2.81797	-0.67597	0.03622
C	-4.15764	-0.33321	0.04362
Cl	-5.36626	-1.57542	0.27310
C	-4.56004	0.99294	-0.13194
C	-3.60725	1.98207	-0.31789
H	-0.44505	2.27974	-0.50461
H	2.30939	0.20266	-1.22317
H	2.86050	1.73683	0.59019
H	1.24919	1.16064	2.10398
H	3.85498	-1.11676	1.16589
H	4.52960	0.34599	1.85323
H	6.52781	-0.53146	-0.94170
H	1.66030	-1.70588	0.99028
H	2.90196	-2.40157	-1.09079
H	1.41664	-3.34978	-0.88240
H	1.46583	-2.01578	-2.06186
H	-2.50670	-1.70731	0.17327
H	-5.61667	1.24607	-0.12278
H	-3.90140	3.01826	-0.45622

XYZ Coordinates of Conformers for the Diastereomers of 2

2h NMR Conformer 6
Energy: -910280.4668546

O	2.28958	-2.58848	-0.96823
C	2.79355	-1.38311	-0.62051
C	1.94367	-0.44237	-0.01587
C	0.52455	-0.71908	0.28941
N	-0.40247	0.15914	0.24195
C	-1.64118	-0.51288	0.64965
C	-2.64642	-0.49571	-0.50424
O	-2.09365	-1.09270	-1.66401
C	-3.15965	0.91181	-0.87445
O	-3.95208	0.83400	-2.04035
C	-3.99721	1.50271	0.25567
N	-5.32514	1.47201	0.06592
O	-3.45832	1.93868	1.27346
C	-1.20473	-1.94986	1.02869
C	-1.36721	-2.27587	2.49870
O	0.20576	-1.96639	0.69104
C	2.43615	0.82774	0.30289
C	3.75860	1.14666	0.04068
Cl	4.36228	2.73365	0.45869
C	4.61353	0.21729	-0.54675
C	4.12575	-1.03977	-0.87715
H	2.97225	-3.12909	-1.40648
H	-2.07862	0.01280	1.50538
H	-3.51109	-1.11824	-0.23533
H	-1.24499	-0.65563	-1.86711
H	-2.29869	1.57897	-1.02290
H	-3.53788	0.19056	-2.64117
H	-5.70576	1.15617	-0.81715
H	-5.93781	1.85515	0.77606
H	-1.68757	-2.70139	0.39526
H	-2.42972	-2.27002	2.76051
H	-0.95741	-3.26232	2.72777
H	-0.85415	-1.52688	3.10995
H	1.76973	1.55079	0.76328
H	5.64976	0.47319	-0.74789
H	4.77979	-1.77008	-1.34852

2h NMR Conformer 5
Energy: -910277.1685581

O	-1.66669	2.40852	-1.39733
C	-2.50795	1.47628	-0.89804
C	-1.98274	0.43232	-0.11800
C	-0.54783	0.31272	0.21313
N	0.04574	-0.79907	0.42948
C	1.45905	-0.47844	0.68963
C	2.27204	-0.96786	-0.52211
O	1.85684	-2.26156	-0.92133
C	3.77650	-1.13583	-0.27155
O	4.40735	-1.57371	-1.45599
C	4.43414	0.16048	0.18283
N	5.03084	0.87539	-0.78275
O	4.35879	0.51323	1.35963
C	1.45800	1.05430	0.88755
C	1.50752	1.48022	2.34126
O	0.16984	1.44584	0.33420
C	-2.83895	-0.56542	0.36243
C	-4.19459	-0.51277	0.08468
Cl	-5.25090	-1.76114	0.70362
C	-4.72738	0.52471	-0.67725
C	-3.88140	1.51009	-1.16656
H	-2.15720	3.05483	-1.93760
H	1.79842	-0.99978	1.59344
H	2.13054	-0.25411	-1.35296
H	0.88415	-2.27505	-0.94192
H	3.90644	-1.86278	0.54273
H	3.88740	-2.31100	-1.81973
H	5.12864	0.48792	-1.71336
H	5.50417	1.73928	-0.54404
H	2.21638	1.56981	0.29217
H	2.48194	1.21812	2.75803
H	1.35651	2.55873	2.42876
H	0.72276	0.96769	2.90768
H	-2.42380	-1.37201	0.95896
H	-5.79204	0.56092	-0.88906
H	-4.28241	2.31913	-1.77316

2h NMR Conformer 4
Energy: -910283.6187217

O	2.75416	2.71254	0.49383
C	2.96134	1.39650	0.27530
C	1.95661	0.45891	-0.03032
C	0.52998	0.80638	-0.14715
N	-0.41544	0.00258	-0.43913
C	-1.66385	0.77191	-0.39629
C	-2.56123	0.24765	0.72859
O	-1.89229	0.29975	1.97609
C	-3.07919	-1.18835	0.50266
O	-3.75651	-1.63540	1.65726
C	-4.03683	-1.23777	-0.68442
N	-5.33882	-1.31808	-0.37117

O	-3.60880	-1.17076	-1.83713
C	-1.22412	2.23800	-0.16139
C	-1.43806	3.14659	-1.35324
O	0.20289	2.10473	0.08448
C	2.30807	-0.88496	-0.23749
C	3.62611	-1.28238	-0.14026
Cl	4.04650	-2.95956	-0.40051
C	4.63114	-0.36060	0.16470
C	4.29297	0.96541	0.36908
H	1.81200	2.93954	0.40922
H	-2.19272	0.66281	-1.34877
H	-3.42811	0.91489	0.83199
H	-1.05269	-0.19316	1.90604
H	-2.22931	-1.84288	0.26214
H	-3.27404	-1.30763	2.43587
H	-5.62395	-1.42893	0.59369
H	-6.02728	-1.35953	-1.11335
H	-1.65664	2.65550	0.75285
H	-2.51040	3.25435	-1.54160
H	-1.01553	4.13735	-1.17076
H	-0.96953	2.71696	-2.24415
H	1.52464	-1.59845	-0.47408
H	5.66564	-0.68300	0.23991
H	5.05401	1.70259	0.60688

2h NMR Conformer 3
Energy: -910288.3351582

O	0.84052	-2.34378	-0.78551
C	1.92354	-1.60830	-0.48963
C	1.85360	-0.23051	-0.19492
C	0.55412	0.44037	-0.20423
N	-0.55842	-0.14243	-0.47399
C	-1.62135	0.85711	-0.33562
C	-2.55912	0.47290	0.81169
O	-1.84412	0.32683	2.02537
C	-3.37203	-0.81357	0.56072
O	-4.10508	-1.14145	1.72050
C	-4.34207	-0.63203	-0.60335
N	-5.62656	-0.45467	-0.26062
O	-3.93059	-0.62299	-1.76384
C	-0.86197	2.18022	-0.06111
C	-0.94498	3.18246	-1.19276
O	0.51975	1.74938	0.08943
C	3.01919	0.48635	0.10736
C	4.23720	-0.16761	0.11473
Cl	5.69400	0.72308	0.49395
C	4.32227	-1.53195	-0.17535
C	3.17187	-2.24431	-0.47536
H	0.04011	-1.75675	-0.76449
H	-2.19857	0.91102	-1.26423
H	-3.26441	1.29796	0.98247
H	-1.13386	-0.33107	1.90008
H	-2.68333	-1.62527	0.28330
H	-3.54496	-0.96152	2.49514
H	-5.91004	-0.52949	0.70823
H	-6.32307	-0.33508	-0.98672
H	-1.15193	2.62370	0.89628
H	-1.97929	3.52070	-1.30634
H	-0.31408	4.05094	-0.99081
H	-0.62491	2.71963	-2.13148
H	2.95432	1.54658	0.33239
H	5.28769	-2.02988	-0.16545
H	3.21780	-3.30482	-0.70398

2h NMR Conformer 2
Energy: -910280.5262358

O	-2.00227	2.78249	-0.89497
C	-2.62324	1.62476	-0.58521
C	-1.99172	0.49020	-0.04140
C	-0.55150	0.43148	0.25820
N	0.05830	-0.53616	0.82187
C	1.49117	-0.19478	0.83055
C	2.19462	-1.12426	-0.17459
O	1.75014	-2.45919	-0.02146
C	3.71603	-1.23779	-0.00447
O	4.23585	-2.10996	-0.98441
C	4.41466	0.10983	-0.12582
N	4.94389	0.38157	-1.32753
O	4.42853	0.88615	0.82961
C	1.52281	1.30467	0.45622
C	1.68804	2.22738	1.64560
O	0.19206	1.50616	-0.10925
C	-2.75484	-0.65426	0.24162
C	-4.11113	-0.66614	-0.01318
Cl	-5.04720	-2.09919	0.34372
C	-4.74778	0.45393	-0.55467
C	-4.00294	1.58571	-0.83525
H	-1.05024	2.73332	-0.70101
H	1.90278	-0.36244	1.83338
H	1.97859	-0.76820	-1.19743
H	0.77767	-2.46019	0.00182
H	3.91651	-1.61115	1.01002
H	3.67911	-2.90749	-1.00469
H	5.44055	1.25386	-1.46844
H	4.96620	-0.33294	-2.04504
H	2.22802	1.54126	-0.34388
H	2.69018	2.09697	2.05833
H	1.55708	3.26940	1.34437

H	0.94642	1.98491	2.41384
H	-2.25722	-1.52301	0.66158
H	-5.81558	0.43450	-0.75276
H	-4.47250	2.47011	-1.25542

2h NMR Conformer 1
Energy: -910284.8126212

O	1.72199	2.61552	0.82874
C	2.49652	1.59663	0.42415
C	1.99242	0.29897	0.19672
C	0.56822	0.03509	0.39730
N	-0.28511	0.91474	0.78261
C	-1.60738	0.26950	0.77655
C	-2.41534	0.84683	-0.40018
O	-2.29725	2.25557	-0.45992
C	-3.93238	0.62845	-0.31061
O	-4.55470	1.16545	-1.45687
C	-4.29866	-0.84506	-0.19429
N	-4.65104	-1.44612	-1.33989
O	-4.21701	-1.41704	0.89269
C	-1.26349	-1.23346	0.64120
C	-1.30100	-1.98845	1.95387
O	0.11614	-1.20589	0.16361
C	2.85071	-0.72799	-0.21865
C	4.19307	-0.45748	-0.40874
Cl	5.26717	-1.73583	-0.92964
C	4.70617	0.82391	-0.19004
C	3.86125	1.84159	0.22395
H	0.79202	2.28625	0.93656
H	-2.12675	0.47864	1.71921
H	-2.04843	0.39516	-1.33826
H	-1.35893	2.49143	-0.55817
H	-4.29033	1.11876	0.60616
H	-4.19073	2.05502	-1.60765
H	-4.92626	-2.42164	-1.32737
H	-4.77456	-0.89852	-2.18302
H	-1.84049	-1.74134	-0.13536
H	-2.33318	-2.04216	2.30485
H	-0.91176	-3.00066	1.82265
H	-0.69173	-1.47011	2.70175
H	2.45332	-1.72426	-0.38734
H	5.76375	1.01880	-0.34360
H	4.24133	2.84324	0.40096

2g NMR Conformer 9
Energy: -910277.6763514

O	2.58024	2.72019	0.11982
C	2.98859	1.43319	0.06968
C	2.03535	0.42385	-0.14918
C	0.60073	0.70129	-0.36030
N	-0.34418	-0.07789	0.00419
C	-1.58476	0.51221	-0.52301
C	-2.70562	0.38414	0.50971
O	-2.27506	0.75443	1.80601
C	-3.26903	-1.05726	0.58315
O	-4.09784	-1.18264	1.71653
C	-4.08547	-1.38590	-0.66406
N	-5.41715	-1.32394	-0.51137
O	-3.52896	-1.64813	-1.73138
C	-1.17449	1.94690	-0.94010
C	-1.49126	3.07854	0.02150
O	0.27217	1.82266	-1.03457
C	2.43907	-0.91612	-0.15406
C	3.77105	-1.24276	0.03977
Cl	4.25983	-2.92139	0.01677
C	4.72590	-0.24975	0.24564
C	4.32928	1.08044	0.26304
H	3.33420	3.30823	0.30960
H	-1.88382	-0.05754	-1.41052
H	-3.53488	1.05928	0.25940
H	-1.39175	0.36669	1.95313
H	-2.43042	-1.76772	0.62328
H	-3.70512	-0.64767	2.42833
H	-6.01823	-1.53637	-1.29874
H	-5.81602	-1.16980	0.40603
H	-1.53391	2.18125	-1.94489
H	-2.57287	3.19757	0.13130
H	-1.06439	2.88393	1.00741
H	-1.07860	4.01117	-0.37038
H	1.69455	-1.68885	-0.31964
H	5.76935	-0.51251	0.39378
H	5.06367	1.86421	0.43524

2g NMR Conformer 8
Energy: -910282.0096996

O	2.71425	2.84354	-0.03438
C	3.10647	1.55227	0.00478
C	2.24912	0.44446	-0.13490
C	0.79702	0.56650	-0.33635
N	-0.04997	-0.38394	-0.32436
C	-1.34792	0.21289	-0.67304
C	-2.46394	-0.44804	0.13189
O	-2.40840	-1.85482	-0.02632
C	-3.85067	-0.04751	-0.37938
O	-4.09075	-0.56362	-1.66711
C	-4.91551	-0.46721	0.64310
N	-5.95037	-1.16267	0.15124
O	-4.79758	-0.14018	1.82362

C	-1.13516	1.72717	-0.44858
C	-1.51843	2.27327	0.91646
O	0.31518	1.82129	-0.57330
C	2.78245	-0.85315	-0.07303
C	4.13544	-1.03956	0.12608
Cl	4.78538	-2.66128	0.19487
C	4.99522	0.05280	0.26837
C	4.47719	1.33458	0.20691
H	1.75799	2.91436	-0.19855
H	-1.53362	0.01039	-1.73773
H	-2.38425	-0.17956	1.19179
H	-1.49120	-2.14643	0.11701
H	-3.92086	1.04591	-0.45092
H	-3.69149	-1.45195	-1.71431
H	-6.70701	-1.43725	0.76663
H	-6.00698	-1.36315	-0.83910
H	-1.55870	2.32845	-1.25576
H	-2.60114	2.23784	1.06719
H	-1.03830	1.69760	1.71385
H	-1.19709	3.31435	0.99496
H	2.11219	-1.69960	-0.18726
H	6.05882	-0.10417	0.42298
H	5.12324	2.20072	0.31432

2g NMR Conformer 7
Energy: -910286.0306359

O	-1.53639	2.62064	0.19428
C	-2.48393	1.67028	0.14798
C	-2.19255	0.31121	-0.09056
C	-0.80797	-0.10183	-0.31286
N	0.20837	0.67933	-0.26242
C	1.37322	-0.12336	-0.66227
C	2.60463	0.26262	0.15290
O	2.83651	1.65723	0.06148
C	3.87701	-0.38084	-0.40653
O	4.19784	0.13530	-1.67692
C	5.01667	-0.22660	0.60998
N	6.16157	0.27634	0.12756
O	4.85125	-0.57988	1.77704
C	0.86628	-1.57708	-0.50796
C	1.14714	-2.25371	0.82350
O	-0.57697	-1.39562	-0.61055
C	-3.22632	-0.63474	-0.12531
C	-4.53138	-0.22450	0.07447
Cl	-5.82414	-1.40161	0.02971
C	-4.83458	1.11898	0.31039
C	-3.81537	2.05749	0.34573
H	-0.65328	2.20329	0.03722
H	1.58409	0.09645	-1.71855
H	2.48426	-0.03783	1.20010
H	2.02756	2.13304	0.31686
H	3.72777	-1.46188	-0.52639
H	3.98969	1.08763	-1.67897
H	6.96488	0.36699	0.73844
H	6.24689	0.50442	-0.85468
H	1.16480	-2.20700	-1.34858
H	2.21668	-2.43840	0.95857
H	0.79373	-1.63586	1.65490
H	0.62682	-3.21333	0.85714
H	-2.99215	-1.67890	-0.30909
H	-5.86560	1.42416	0.46493
H	-4.03031	3.10622	0.52750

2g NMR Conformer 6
Energy: -910274.8529101

O	-2.38309	-2.86866	-0.54789
C	-2.94829	-1.66920	-0.28718
C	-2.12492	-0.53685	-0.16764
C	-0.65261	-0.58470	-0.28270
N	0.06948	0.40297	-0.64935
C	1.46217	-0.07904	-0.65760
C	2.37663	1.05054	-0.16362
O	1.98857	2.27367	-0.76663
C	3.85283	0.91306	-0.56710
O	4.57193	2.04603	-0.13084
C	4.49791	-0.33561	0.01807
N	5.27055	-0.13971	1.09712
O	4.26362	-1.44001	-0.47257
C	1.39185	-1.39053	0.16190
C	1.71606	-1.29087	1.64337
O	-0.02288	-1.72869	0.05365
C	-2.70857	0.71571	0.05886
C	-4.08252	0.83364	0.17991
Cl	-4.79071	2.40466	0.47738
C	-4.90713	-0.28427	0.07330
C	-4.33577	-1.52650	-0.16237
H	-3.06893	-3.55581	-0.63513
H	1.73299	-0.30021	-1.70080
H	2.31443	1.14459	0.93134
H	1.02001	2.34360	-0.70899
H	3.89585	0.81185	-1.66136
H	4.05821	2.83780	-0.36608
H	5.48071	0.80127	1.40701
H	5.74729	-0.92890	1.51840
H	1.95162	-2.19537	-0.31120
H	2.77637	-1.08231	1.80595
H	1.12327	-0.50345	2.12020
H	1.47766	-2.24185	2.12539

H	-2.06604	1.58660	0.14443
H	-5.98425	-0.18492	0.17090
H	-4.96835	-2.40620	-0.25877

2g NMR Conformer 5
Energy: -910275.1128057

O	-1.95578	2.68450	-0.69295
C	-2.73265	1.61388	-0.41390
C	-2.11491	0.43526	0.03650
C	-0.65736	0.34192	0.24967
N	0.05611	-0.67657	-0.03902
C	1.41003	-0.38756	0.47222
C	2.43757	-0.96023	-0.51221
O	2.04293	-2.26402	-0.90658
C	3.84254	-1.18013	0.06912
O	4.66967	-1.77782	-0.90518
C	4.48934	0.11775	0.53315
N	5.39930	0.64422	-0.30033
O	4.14079	0.63807	1.59280
C	1.38266	1.14241	0.70998
C	1.88525	2.02013	-0.42429
O	-0.04791	1.38751	0.84335
C	-2.88845	-0.70411	0.27757
C	-4.26139	-0.66161	0.09043
Cl	-5.22060	-2.08841	0.40813
C	-4.88623	0.50535	-0.34165
C	-4.11941	1.63539	-0.59552
H	-2.49738	3.42010	-1.03303
H	1.52601	-0.91679	1.43009
H	2.51752	-0.31565	-1.40089
H	1.09826	-2.23571	-1.13753
H	3.74451	-1.82271	0.95626
H	4.17642	-2.51103	-1.31109
H	5.88308	1.49491	-0.03616
H	5.69409	0.12956	-1.12122
H	1.84509	1.41445	1.65685
H	2.96559	1.92071	-0.55648
H	1.38616	1.76400	-1.36444
H	1.66215	3.06397	-0.19192
H	-2.40049	-1.61225	0.61901
H	-5.96283	0.53143	-0.48300
H	-4.59565	2.54792	-0.94725

2g NMR Conformer 4
Energy: -910280.9544106

O	2.81288	2.75620	-0.34711
C	3.03965	1.43068	-0.23130
C	2.03815	0.44264	-0.18237
C	0.59969	0.74556	-0.25456
N	-0.35287	-0.08470	-0.09263
C	-1.59791	0.65381	-0.35452
C	-2.68229	0.22763	0.63584
O	-2.20045	0.19197	1.96536
C	-3.26973	-1.16474	0.29701
O	-4.07822	-1.60647	1.36363
C	-4.11731	-1.10530	-0.97112
N	-5.44410	-1.08443	-0.77485
O	-3.58636	-1.04441	-2.08103
C	-1.17745	2.14438	-0.32819
C	-1.41087	2.92443	0.95201
O	0.26290	2.03379	-0.53910
C	2.40614	-0.90677	-0.05678
C	3.73832	-1.25929	0.02127
Cl	4.18117	-2.94394	0.17394
C	4.74052	-0.28652	-0.02590
C	4.38579	1.04506	-0.15134
H	1.86090	2.94352	-0.41963
H	-1.94294	0.38970	-1.36075
H	-3.50701	0.95298	0.63028
H	-1.33057	-0.25046	1.96333
H	-2.44342	-1.86528	0.10663
H	-3.65250	-1.32817	2.19311
H	-6.06458	-1.04870	-1.57497
H	-5.82206	-1.19934	0.15706
H	-1.57472	2.68133	-1.19226
H	-2.48200	3.01019	1.15450
H	-0.94061	2.42968	1.80413
H	-0.99971	3.93107	0.84430
H	1.62525	-1.66049	-0.02642
H	5.78620	-0.57448	0.03289
H	5.14424	1.82116	-0.19113

2g NMR Conformer 3
Energy: -910285.8626516

O	0.88901	-2.48451	-0.32624
C	1.95836	-1.68474	-0.19176
C	1.86991	-0.27756	-0.24170
C	0.56639	0.35313	-0.44538
N	-0.53168	-0.29423	-0.60983
C	-1.61322	0.69680	-0.69114
C	-2.50311	0.57552	0.55167
O	-1.75082	0.66925	1.74815
C	-3.32573	-0.73204	0.59133
O	-4.00287	-0.82656	1.82512
C	-4.35255	-0.77092	-0.53766
N	-5.61510	-0.49814	-0.17631
O	-4.00328	-1.00755	-1.69460
C	-0.85257	2.04230	-0.83860

C	-1.32043	3.22753	-0.02328
O	0.50784	1.69358	-0.45056
C	3.02190	0.50729	-0.09728
C	4.24428	-0.10841	0.09739
Cl	5.68460	0.86685	0.27879
C	4.34732	-1.50116	0.15014
C	3.21072	-2.28101	0.00596
H	0.08472	-1.92017	-0.47140
H	-2.22741	0.50426	-1.57382
H	-3.20766	1.41695	0.57934
H	-1.04580	-0.00542	1.73539
H	-2.64931	-1.58678	0.44296
H	-3.41081	-0.49331	2.52180
H	-5.84869	-0.37182	0.80052
H	-6.34714	-0.51346	-0.87664
H	-0.79926	2.30732	-1.90064
H	-2.32345	3.52295	-0.34493
H	-1.34138	2.98400	1.04068
H	-0.65111	4.07512	-0.18741
H	2.94302	1.58939	-0.14019
H	5.31614	-1.96845	0.30242
H	3.27079	-3.36457	0.04247

2g NMR Conformer 2
Energy: -910282.4639662

O	-1.68539	2.69726	-0.08495
C	-2.53569	1.65905	-0.03778
C	-2.10716	0.31794	-0.12089
C	-0.68292	0.02326	-0.27575
N	0.24693	0.90733	-0.29112
C	1.50672	0.19986	-0.57944
C	2.64496	0.82879	0.23743
O	2.57299	2.24259	0.16009
C	4.05774	0.53218	-0.29194
O	5.01003	1.20144	0.50298
C	4.38181	-0.95543	-0.29941
N	5.16996	-1.38419	0.69750
O	3.89730	-1.68794	-1.16185
C	1.13925	-1.28319	-0.30739
C	1.45953	-1.82594	1.07469
O	-0.31741	-1.25909	-0.43030
C	-3.04192	-0.72462	-0.06427
C	-4.38530	-0.42786	0.07351
Cl	-5.55420	-1.72696	0.14640
C	-4.82416	0.89612	0.15589
C	-3.90298	1.93033	0.09948
H	-0.76299	2.34966	-0.18662
H	1.73468	0.34330	-1.64569
H	2.58462	0.51266	1.28937
H	1.71662	2.53403	0.51648
H	4.10196	0.87156	-1.33743
H	4.70631	2.11678	0.62996
H	5.44570	-2.35922	0.72965
H	5.59457	-0.71810	1.33148
H	1.51230	-1.94078	-1.08968
H	2.53770	-1.91751	1.22635
H	1.04643	-1.17779	1.85442
H	1.01554	-2.81853	1.17933
H	-2.70203	-1.75379	-0.12886
H	-5.88341	1.11153	0.26363
H	-4.22423	2.96572	0.16149

2g NMR Conformer 1
Energy: -910278.4650366

O	-2.26982	-2.92309	0.09256
C	-2.82923	-1.69476	0.06142
C	-2.12141	-0.49169	-0.12095
C	-0.66085	-0.43257	-0.29155
N	0.05070	0.62320	-0.31767
C	1.43305	0.19639	-0.60022
C	2.39475	1.08378	0.20341
O	1.98923	2.43809	0.10526
C	3.83930	1.11268	-0.32009
O	4.60321	2.01563	0.44787
C	4.50107	-0.25760	-0.27103
N	5.35156	-0.45730	0.74666
O	4.21123	-1.11327	-1.10735
C	1.41408	-1.32387	-0.30468
C	1.82763	-1.75825	1.09052
O	-0.01243	-1.61763	-0.44522
C	-2.82098	0.72571	-0.12950
C	-4.19035	0.74164	0.04292
Cl	-5.04680	2.26615	0.02739
C	-4.90274	-0.44647	0.22633
C	-4.22040	-1.65044	0.23372
H	-1.31026	-2.87387	-0.06091
H	1.62456	0.36916	-1.66965
H	2.40530	0.77832	1.26079
H	1.03483	2.48394	0.28802
H	3.80920	1.41483	-1.37720
H	4.09297	2.83770	0.54542
H	5.84415	-1.34056	0.81750
H	5.60218	0.31070	1.35749
H	1.93166	-1.89491	-1.07254
H	2.89677	-1.60170	1.25254
H	1.26970	-1.20552	1.85329
H	1.61894	-2.82391	1.21162
H	-2.26490	1.64678	-0.27493

H	-5.98052	-0.42371	0.35943
H	-4.74962	-2.58822	0.37394

2f NMR Conformer 6
Energy: -910278.5257231

O	0.61664	-2.27642	-1.16799
C	1.61556	-1.48994	-0.73437
C	1.46173	-0.10353	-0.52823
C	0.16635	0.52685	-0.78038
N	-0.86508	-0.08871	-1.22898
C	-1.96659	0.87703	-1.27530
C	-3.21690	0.30111	-0.58759
O	-3.56908	-0.89291	-1.27292
C	-3.21367	0.00618	0.93539
O	-4.35016	-0.77245	1.24249
C	-1.92536	-0.65593	1.43250
N	-1.91443	-1.99994	1.42230
O	-0.96955	0.03486	1.78360
C	-1.32399	2.21622	-0.80634
C	-1.89658	2.94244	0.39447
O	0.04780	1.83326	-0.50702
C	2.54071	0.66218	-0.06817
C	3.75600	0.04986	0.17796
Cl	5.10356	1.00569	0.75337
C	3.92368	-1.32209	-0.02428
C	2.85769	-2.08410	-0.47717
H	-0.19242	-1.71996	-1.29735
H	-2.28002	0.98512	-2.32061
H	-4.05279	0.99071	-0.75900
H	-2.77435	-1.44968	-1.36861
H	-3.29922	0.94464	1.48749
H	-4.61041	-1.26145	0.44162
H	-2.77227	-2.52027	1.28656
H	-1.09524	-2.48938	1.76498
H	-1.26777	2.89548	-1.66199
H	-2.96692	3.12538	0.25566
H	-1.73202	2.35700	1.30037
H	-1.40092	3.90952	0.50726
H	2.41189	1.72819	0.09198
H	4.88500	-1.78757	0.17389
H	2.96645	-3.15234	-0.63898

2f NMR Conformer 5
Energy: -910273.3693083

O	2.12290	2.74035	-0.28112
C	2.79031	1.56656	-0.21837
C	2.05074	0.37388	-0.14767
C	0.57543	0.35571	-0.17854
N	-0.16056	-0.42635	0.51300
C	-1.53221	-0.20141	0.01422
C	-2.56029	-0.51685	1.09887
O	-2.50346	0.36166	2.20451
C	-4.00989	-0.48484	0.60462
O	-4.41374	0.80732	0.20571
C	-4.18333	-1.45335	-0.56131
N	-4.61215	-0.91300	-1.71136
O	-3.91278	-2.64543	-0.41623
C	-1.44384	1.19569	-0.63384
C	-1.62970	2.42434	0.24127
O	-0.04100	1.19130	-1.04578
C	2.71943	-0.84779	-0.02202
C	4.10483	-0.88013	0.01265
Cl	4.92906	-2.41545	0.15857
C	4.84792	0.29437	-0.07315
C	4.18765	1.51143	-0.18434
H	2.74910	3.48738	-0.28482
H	-1.69475	-0.93807	-0.79008
H	-2.35649	-1.54887	1.41742
H	-1.61275	0.31704	2.59239
H	-4.64628	-0.85608	1.42012
H	-4.51489	1.35825	1.00041
H	-4.85315	0.06900	-1.75825
H	-4.75796	-1.51006	-2.51713
H	-2.04533	1.25922	-1.54302
H	-2.66409	2.52096	0.56635
H	-0.98772	2.37225	1.12438
H	-1.34840	3.30660	-0.33951
H	2.13891	-1.76350	0.03966
H	5.93327	0.26046	-0.04918
H	4.75769	2.43637	-0.23702

2f NMR Conformer 4
Energy: -910274.5525904

O	0.55163	2.25509	-0.02002
C	1.66471	1.49778	0.03749
C	1.65252	0.09505	0.14313
C	0.39068	-0.64680	0.29084
N	-0.67261	-0.22130	0.85113
C	-1.61637	-1.34636	0.82515
C	-3.07841	-0.90648	0.71072
O	-3.43767	-0.22596	1.90622
C	-3.56953	-0.04949	-0.48231
O	-4.93287	0.25068	-0.27154
C	-2.74211	1.22051	-0.69272
N	-3.17336	2.31924	-0.05651
O	-1.72010	1.19707	-1.38546
C	-1.00780	-2.33950	-0.19260
C	-1.52261	-2.30328	-1.61880

O	0.38176	-1.90912	-0.20568
C	2.85919	-0.61637	0.12898
C	4.06048	0.06792	0.06078
Cl	5.56423	-0.82627	0.06154
C	4.08807	1.46078	-0.00806
C	2.89361	2.16556	-0.02615
H	-0.24002	1.71723	-0.21980
H	-1.57509	-1.81477	1.81958
H	-3.69998	-1.81150	0.69326
H	-2.77119	0.46127	2.09400
H	-3.49973	-0.61485	-1.41325
H	-5.09833	0.28538	0.68783
H	-4.08584	2.33712	0.38296
H	-2.68854	3.19857	-0.20374
H	-1.02062	-3.35856	0.20060
H	-2.55688	-2.65913	-1.66129
H	-1.46725	-1.28758	-2.02142
H	-0.91202	-2.96479	-2.23802
H	2.84191	-1.70050	0.18944
H	5.03704	1.98660	-0.06004
H	2.88989	3.24858	-0.10537

2f NMR Conformer 3
Energy: -910272.8050330

O	0.97159	2.41830	1.07421
C	1.81869	1.45779	0.64638
C	1.45023	0.43009	-0.23993
C	0.10405	0.36305	-0.83884
N	-0.56024	-0.70292	-1.05154
C	-1.86014	-0.28913	-1.59675
C	-2.98804	-0.89912	-0.74281
O	-2.79016	-2.30526	-0.72579
C	-3.22474	-0.42277	0.71792
O	-4.06187	-1.35726	1.36154
C	-1.94593	-0.17608	1.52124
N	-1.50831	-1.19242	2.27195
O	-1.37585	0.91836	1.45296
C	-1.73160	1.24603	-1.80051
C	-2.79046	2.17691	-1.24318
O	-0.45093	1.54588	-1.18261
C	2.37901	-0.55851	-0.58602
C	3.66878	-0.49659	-0.08654
Cl	4.82963	-1.72426	-0.53931
C	4.05815	0.53792	0.76411
C	3.13157	1.50332	1.13005
H	0.04684	2.13112	0.96262
H	-1.99318	-0.76670	-2.57453
H	-3.94168	-0.74198	-1.26147
H	-1.84480	-2.47948	-0.55939
H	-3.75030	0.53541	0.70096
H	-3.95012	-2.21771	0.91851
H	-0.67760	-1.07031	2.84093
H	-2.07800	-2.01978	2.40056
H	-1.59878	1.43742	-2.87037
H	-3.78478	1.86355	-1.57711
H	-2.75238	2.18825	-0.15322
H	-2.61753	3.19212	-1.60798
H	2.07984	-1.35357	-1.26287
H	5.07477	0.57995	1.14430
H	3.40403	2.30399	1.81126

2f NMR Conformer 2
Energy: -910277.0598735

O	2.26487	2.81909	-0.57945
C	2.79719	1.59176	-0.39547
C	2.05033	0.41430	-0.20166
C	0.57937	0.39013	-0.16459
N	-0.15173	-0.59503	0.17852
C	-1.53973	-0.16636	-0.07674
C	-2.51035	-0.89811	0.84923
O	-2.35973	-0.55280	2.21070
C	-3.97939	-0.65429	0.49657
O	-4.34061	0.70610	0.61242
C	-4.25997	-1.13660	-0.92547
N	-4.78632	-0.22642	-1.75751
O	-3.98976	-2.29336	-1.24806
C	-1.44630	1.37365	-0.07551
C	-1.53948	2.11652	1.24581
O	-0.06436	1.53180	-0.54620
C	2.72126	-0.80512	-0.01740
C	4.10122	-0.84634	-0.02121
Cl	4.92250	-2.37366	0.20473
C	4.85203	0.31694	-0.20897
C	4.19766	1.52250	-0.39444
H	1.29276	2.77370	-0.60086
H	-1.78263	-0.49095	-1.10205
H	-2.32102	-1.97009	0.70059
H	-1.46193	-0.79463	2.49609
H	-4.58887	-1.27777	1.16515
H	-4.51532	0.90836	1.54690
H	-5.01082	-0.49397	-2.70880
H	-5.01860	0.69996	-1.42240
H	-2.09082	1.82066	-0.83429
H	-2.54796	2.05932	1.65092
H	-0.84710	1.69491	1.97914
H	-1.27921	3.16485	1.07565
H	2.13470	-1.70759	0.12526
H	5.93735	0.27362	-0.21197

H	4.75702	2.44132	-0.54295

2f NMR Conformer 1
Energy: -910281.4362375

O	-1.53179	2.67751	0.30052
C	-2.41361	1.68193	0.11778
C	-2.02006	0.33885	-0.05961
C	-0.59735	0.00335	-0.06263
N	0.35043	0.84629	0.13568
C	1.60321	0.10637	-0.09777
C	2.75265	0.70804	0.71078
O	2.60662	0.55188	2.10657
C	4.11809	0.11701	0.35070
O	4.19957	-1.26157	0.64308
C	4.40997	0.34226	-1.13109
N	4.68813	-0.75763	-1.84541
O	4.36550	1.47927	-1.60055
C	1.16786	-1.36364	0.09211
C	1.17877	-1.95878	1.48904
O	-0.24294	-1.27243	-0.30468
C	-2.98554	-0.66080	-0.23851
C	-4.32547	-0.31929	-0.24287
Cl	-5.53426	-1.56452	-0.46258
C	-4.72999	1.00726	-0.07224
C	-3.77798	1.99897	0.10639
H	-0.61431	2.29926	0.28271
H	1.85828	0.25321	-1.15990
H	2.78671	1.77307	0.44243
H	1.80662	1.02380	2.39494
H	4.87893	0.67941	0.90957
H	4.33917	-1.37217	1.59878
H	4.74198	-1.66197	-1.39380
H	4.90754	-0.66792	-2.83073
H	1.65605	-2.02343	-0.62741
H	2.19832	-2.08863	1.84732
H	0.64337	-1.31465	2.19131
H	0.68187	-2.93178	1.45386
H	-2.67141	-1.69164	-0.37168
H	-5.78700	1.25787	-0.07908
H	-4.07268	3.03526	0.24171

2e NMR Conformer 8
Energy: -910285.0601109

O	1.74858	2.63731	0.91050
C	2.51439	1.62131	0.48240
C	2.00025	0.32936	0.24503
C	0.57628	0.07141	0.46235
N	-0.25896	0.94698	0.89231
C	-1.59203	0.32089	0.87969
C	-2.39635	0.99521	-0.24146
O	-1.98656	0.53102	-1.51863
C	-3.92314	0.84077	-0.19260
O	-4.49578	1.52004	-1.28732
C	-4.38485	-0.61618	-0.10758
N	-5.02962	-1.09914	-1.17904
O	-4.15690	-1.26992	0.91125
C	-1.27297	-1.17886	0.66737
C	-1.31610	-1.99265	1.94494
O	0.10786	-1.15483	0.19154
C	2.84623	-0.69532	-0.19866
C	4.18765	-0.42933	-0.40386
Cl	5.24650	-1.70647	-0.95909
C	4.71109	0.84563	-0.17419
C	3.87738	1.86202	0.26612
H	0.81733	2.30756	1.02175
H	-2.09304	0.48761	1.83989
H	-2.21007	2.07520	-0.16143
H	-1.17994	0.99855	-1.79583
H	-4.28221	1.31795	0.72694
H	-3.87892	1.45477	-2.03879
H	-5.39802	-2.04300	-1.15262
H	-5.27898	-0.48711	-1.94529
H	-1.86085	-1.62997	-0.13219
H	-2.34605	-2.04290	2.30183
H	-0.94710	-3.00522	1.76502
H	-0.69068	-1.52224	2.71120
H	2.44052	-1.68668	-0.37628
H	5.76748	1.03696	-0.33986
H	4.26558	2.85911	0.45117

2e NMR Conformer 6
Energy: -910278.3681241

O	-0.53437	-2.33205	-0.17642
C	-1.63153	-1.55658	-0.05198
C	-1.58581	-0.15511	0.02340
C	-0.29922	0.57163	0.07844
N	0.64353	0.36253	0.90806
C	1.66283	1.38417	0.62676
C	3.08644	0.82923	0.68735
O	3.29323	0.20052	1.93908
C	3.57725	-0.11692	-0.43437
O	4.87861	-0.55230	-0.11175
C	2.63349	-1.29111	-0.67586
N	2.95898	-2.44714	-0.09337
O	1.60852	-1.13235	-1.35609
C	1.21283	2.04653	-0.69242
C	1.22774	3.55910	-0.67957

O	-0.14919	1.56453	-0.82885
C	-2.77300	0.58312	0.08174
C	-3.99053	-0.07709	0.12006
Cl	-5.47140	0.84941	0.21566
C	-4.05037	-1.46965	0.08919
C	-2.87407	-2.19991	-0.00383
H	0.23027	-1.83303	-0.54615
H	1.61640	2.11789	1.44623
H	3.78086	1.67951	0.66280
H	2.53035	-0.37569	2.13184
H	3.62785	0.43327	-1.38076
H	4.97400	-0.54861	0.85813
H	2.38731	-3.27118	-0.25090
H	3.85842	-2.55525	0.36089
H	1.76268	1.65423	-1.55576
H	2.25560	3.91361	-0.55375
H	0.83730	3.96126	-1.61695
H	0.62381	3.93696	0.15030
H	-2.73083	1.66840	0.11880
H	-5.01060	-1.97611	0.12320
H	-2.89786	-3.28426	-0.05816

2e NMR Conformer 5
Energy: -910283.0069564

O	0.67138	-1.97386	-1.69662
C	1.65465	-1.31065	-1.06632
C	1.46588	-0.04193	-0.48001
C	0.15059	0.59356	-0.54269
N	-0.87565	0.07978	-1.11586
C	-1.98221	1.02538	-0.94876
C	-3.24752	0.31760	-0.45203
O	-3.54921	-0.76430	-1.31589
C	-3.28127	-0.17705	1.01538
O	-4.43663	-0.96593	1.19518
C	-2.01063	-0.91772	1.44261
N	-2.01623	-2.25015	1.26362
O	-1.05110	-0.29042	1.88969
C	-1.39982	2.14668	-0.05223
C	-1.53434	3.53878	-0.62942
O	0.00705	1.79357	0.03758
C	2.53010	0.59855	0.16833
C	3.76514	-0.02077	0.22515
Cl	5.09642	0.77751	1.03173
C	3.96703	-1.27671	-0.35258
C	2.91619	-1.91500	-0.99272
H	-0.15278	-1.42442	-1.66449
H	-2.24059	1.42568	-1.93978
H	-4.09039	1.01400	-0.54738
H	-2.73900	-1.28489	-1.46703
H	-3.35708	0.68807	1.68288
H	-4.67446	-1.36086	0.33719
H	-2.87862	-2.73633	1.05114
H	-1.21341	-2.79111	1.56535
H	-1.78725	2.10093	0.97028
H	-2.59414	3.80078	-0.70587
H	-1.04144	4.27441	0.00992
H	-1.09128	3.57960	-1.62866
H	2.37405	1.57330	0.62036
H	4.94367	-1.74919	-0.29848
H	3.05212	-2.89190	-1.44690

2e NMR Conformer 4
Energy: -910278.6131351

O	2.12289	-2.75057	-0.29761
C	2.79998	-1.58833	-0.16028
C	2.07495	-0.40180	0.03869
C	0.60057	-0.36940	0.13804
N	-0.12553	0.58652	-0.29745
C	-1.51127	0.27130	0.07750
C	-2.39576	0.37371	-1.17046
O	-2.08145	-0.63605	-2.11138
C	-3.89193	0.22714	-0.89020
O	-4.21655	-1.03703	-0.35153
C	-4.36644	1.31974	0.06323
N	-5.07000	0.90291	1.12637
O	-4.09960	2.49874	-0.16858
C	-1.43175	-1.13011	0.73143
C	-2.00242	-1.21043	2.13012
O	-0.00067	-1.38830	0.78196
C	2.75781	0.81542	0.13362
C	4.14059	0.84568	0.04898
Cl	4.97990	2.37380	0.18483
C	4.86973	-0.32615	-0.13657
C	4.19567	-1.53543	-0.24414
H	2.74036	-3.48598	-0.46536
H	-1.85489	1.02656	0.80093
H	-2.23831	1.37119	-1.60029
H	-1.16200	-0.51544	-2.40593
H	-4.42300	0.39096	-1.83965
H	-4.04318	-1.71707	-1.02515
H	-5.29092	-0.07791	1.24366
H	-5.43897	1.58678	1.77694
H	-1.85983	-1.89708	0.08137
H	-3.07924	-1.02766	2.08871
H	-1.83133	-2.19848	2.56442
H	-1.53915	-0.45566	2.77303
H	2.18883	1.72835	0.28103
H	5.95360	-0.29521	-0.19942

H	4.75307	-2.45617	-0.40165

2e NMR Conformer 3
Energy: -910278.0638698

O	0.93549	-1.24238	2.28509
C	1.81041	-0.78236	1.36662
C	1.46329	0.11817	0.34442
C	0.11070	0.70289	0.25462
N	-0.58818	0.79361	-0.80652
C	-1.84708	1.44538	-0.42379
C	-3.03582	0.62404	-0.94124
O	-2.83716	0.34835	-2.31599
C	-3.39580	-0.69659	-0.20620
O	-4.31119	-1.41697	-0.99833
C	-2.18486	-1.54992	0.17222
N	-1.81426	-2.49138	-0.69813
O	-1.60309	-1.33465	1.24398
C	-1.73721	1.67262	1.10534
C	-1.85040	3.12405	1.52159
O	-0.40042	1.19131	1.40435
C	2.41375	0.49353	-0.61143
C	3.70866	0.01060	-0.51906
Cl	4.89715	0.49561	-1.70736
C	4.07900	-0.84976	0.51391
C	3.12915	-1.24591	1.44480
H	0.00987	-1.17108	1.96932
H	-1.90711	2.40914	-0.94887
H	-3.94081	1.24162	-0.88619
H	-1.90437	0.09524	-2.44690
H	-3.88459	-0.44996	0.74295
H	-4.17661	-1.15930	-1.92836
H	-1.02731	-3.09384	-0.48071
H	-2.39231	-2.70674	-1.50187
H	-2.42616	1.04207	1.67538
H	-2.85439	3.49328	1.29080
H	-1.67753	3.23598	2.59426
H	-1.12130	3.73211	0.97787
H	2.12895	1.17852	-1.40501
H	5.09935	-1.21630	0.58022
H	3.38808	-1.93746	2.24110

2e NMR Conformer 2
Energy: -910281.8465346

O	2.27098	2.85291	0.20035
C	2.81040	1.62012	0.08754
C	2.07477	0.43066	-0.07131
C	0.60285	0.39220	-0.13305
N	-0.11754	-0.65803	-0.12843
C	-1.51795	-0.22490	-0.22577
C	-2.31508	-0.88429	0.90599
O	-1.89881	-0.40784	2.17130
C	-3.82198	-0.63060	0.83915
O	-4.14400	0.73978	0.95365
C	-4.39937	-1.17947	-0.46278
N	-5.18233	-0.33885	-1.15523
O	-4.13905	-2.32939	-0.81564
C	-1.46431	1.32216	-0.18713
C	-2.12057	2.01011	-1.36255
O	-0.03012	1.59065	-0.21298
C	2.75658	-0.79285	-0.16684
C	4.13537	-0.82744	-0.10639
Cl	4.96951	-2.35934	-0.23214
C	4.87519	0.34727	0.05085
C	4.21018	1.55723	0.14639
H	1.30154	2.81800	0.12279
H	-1.92495	-0.58107	-1.18420
H	-2.16043	-1.96757	0.82436
H	-0.97421	-0.67232	2.31907
H	-4.28815	-1.20647	1.65229
H	-3.94545	1.03415	1.85922
H	-5.62292	-0.66085	-2.00928
H	-5.39419	0.58212	-0.79246
H	-1.82893	1.71109	0.76570
H	-3.19392	1.80475	-1.33925
H	-1.97065	3.09146	-1.31721
H	-1.70756	1.63214	-2.30266
H	2.17901	-1.70382	-0.29029
H	5.95977	0.30989	0.09611
H	4.76009	2.48545	0.26980

2e NMR Conformer 1
Energy: -910286.5401736

O	-1.54798	2.69731	-0.34859
C	-2.42991	1.69191	-0.23525
C	-2.03636	0.34131	-0.12953
C	-0.61215	0.00516	-0.14450
N	0.33050	0.87068	-0.24218
C	1.60368	0.14106	-0.24034
C	2.51319	0.71873	0.85129
O	2.00005	0.45488	2.14250
C	3.93050	0.14336	0.83666
O	3.94629	-1.24974	1.06739
C	4.61309	0.44444	-0.49504
N	5.18431	-0.60220	-1.10876
O	4.61409	1.59174	-0.94045
C	1.18989	-1.34074	-0.04829
C	1.66230	-2.27114	-1.14260
O	-0.26923	-1.28762	-0.05905

C	-3.00229	-0.66695	-0.01328
C	-4.34273	-0.32734	-0.00296
Cl	-5.55190	-1.58308	0.14250
C	-4.74756	1.00598	-0.10642
C	-3.79506	2.00636	-0.22187
H	-0.63011	2.31612	-0.34729
H	2.09298	0.29249	-1.21395
H	2.59446	1.79856	0.67331
H	1.16680	0.94323	2.25994
H	4.50839	0.67121	1.60938
H	3.70541	-1.41846	1.99451
H	5.68158	-0.45614	-1.97973
H	5.18471	-1.51568	-0.67248
H	1.47090	-1.70596	0.94118
H	2.75449	-2.31548	-1.12382
H	1.26815	-3.27923	-0.99425
H	1.33898	-1.90280	-2.12100
H	-2.68904	-1.70354	0.06695
H	-5.80492	1.25493	-0.09651
H	-4.08950	3.04833	-0.30378

3d NMR Conformer 8
Energy: -910285.2429233

O	2.54647	2.86213	0.17125
C	2.76195	1.53395	0.07503
C	1.75638	0.56006	-0.07348
C	0.32278	0.88363	-0.14085
N	-0.62214	0.05932	-0.37844
C	-1.88525	0.80052	-0.26687
C	-2.68255	0.29911	0.94810
O	-1.98637	0.55725	2.14798
C	-3.03973	-1.19349	0.84848
O	-1.90483	-2.02899	0.94388
C	-3.88409	-1.45423	-0.40142
N	-3.49277	-2.48556	-1.16433
O	-4.85417	-0.73810	-0.65240
C	-1.46059	2.28071	-0.13130
C	-1.72651	3.12038	-1.36258
O	-0.02204	2.17686	0.07044
C	2.11639	-0.79421	-0.17056
C	3.44418	-1.16617	-0.11831
Cl	3.87599	-2.85568	-0.23806
C	4.45040	-0.20751	0.03064
C	4.10393	1.12845	0.12550
H	1.59681	3.07068	0.14386
H	-2.48535	0.64606	-1.17316
H	-3.61733	0.86748	0.99506
H	-1.26297	-0.08822	2.23936
H	-3.67792	-1.43656	1.70738
H	-1.20226	-1.66022	0.37301
H	-2.72532	-3.07699	-0.87099
H	-4.03734	-2.73632	-1.98157
H	-1.86495	2.73908	0.77529
H	-2.80597	3.20989	-1.51604
H	-1.30700	4.12263	-1.24928
H	-1.28694	2.64725	-2.24627
H	1.33424	-1.53877	-0.28613
H	5.49283	-0.51004	0.07180
H	4.86583	1.89358	0.24054

3d NMR Conformer 7
Energy: -910285.9607376

O	0.47679	-2.18586	-0.65342
C	1.60746	-1.51951	-0.37361
C	1.63956	-0.12630	-0.14709
C	0.39493	0.63585	-0.22286
N	-0.75028	0.10545	-0.45467
C	-1.74097	1.18131	-0.47734
C	-2.84612	0.91834	0.54883
O	-2.30475	0.56795	1.80715
C	-3.90282	-0.11911	0.11120
O	-4.76323	-0.39103	1.19460
C	-3.27857	-1.39861	-0.45475
N	-3.05963	-2.38311	0.43755
O	-2.97009	-1.47003	-1.64212
C	-0.92081	2.45500	-0.14380
C	-0.99962	3.54365	-1.19053
O	0.44716	1.96590	-0.05655
C	2.85112	0.51615	0.13979
C	4.01595	-0.22586	0.20104
Cl	5.53076	0.57018	0.56222
C	4.00116	-1.60568	-0.02085
C	2.80486	-2.24448	-0.30655
H	-0.27875	-1.53794	-0.67506
H	-2.19089	1.24272	-1.47775
H	-3.39350	1.85552	0.71622
H	-1.66192	-0.15695	1.68972
H	-4.49213	0.31258	-0.70572
H	-4.29542	-0.18414	2.02346
H	-3.49594	-2.34757	1.35084
H	-2.69567	-3.27094	0.10923
H	-1.17401	2.83528	0.85222
H	-2.02899	3.90891	-1.25821
H	-0.35040	4.38282	-0.93135
H	-0.70369	3.15061	-2.16761
H	2.86311	1.58852	0.31045
H	4.92594	-2.17333	0.03052
H	2.77459	-3.31545	-0.48309

3d NMR Conformer 6
Energy: -910278.7782392

O	-2.15196	2.60263	-1.01327
C	-2.82949	1.49505	-0.63740
C	-2.11816	0.42672	-0.06625
C	-0.65997	0.46762	0.17207
N	0.10712	-0.55073	0.10760
C	1.46443	-0.07836	0.42323
C	2.32382	-0.29832	-0.82345
O	2.36823	-1.67436	-1.15696
C	3.78853	0.14619	-0.74957
O	4.41276	-0.09441	-1.99320
C	4.53960	-0.50703	0.41624
N	5.57644	-1.28971	0.08466
O	4.19087	-0.28125	1.57588
C	1.27961	1.40336	0.82374
C	1.53521	1.67439	2.29146
O	-0.11989	1.65317	0.52414
C	-2.79803	-0.74603	0.27987
C	-4.16499	-0.84357	0.07612
Cl	-5.00112	-2.31209	0.52638
C	-4.88169	0.21457	-0.47734
C	-4.20986	1.37607	-0.83424
H	-2.75696	3.25067	-1.41843
H	1.87649	-0.66677	1.24810
H	1.87136	0.27670	-1.64924
H	1.45633	-1.98919	-1.28320
H	3.83035	1.22646	-0.56539
H	4.02863	-0.90456	-2.37462
H	6.13574	-1.71069	0.81719
H	5.86865	-1.37114	-0.88045
H	1.85522	2.08662	0.18892
H	2.58459	1.46361	2.51342
H	1.30793	2.71319	2.54206
H	0.91048	1.01654	2.90445
H	-2.23962	-1.56971	0.71422
H	-5.95359	0.13149	-0.63148
H	-4.75556	2.20509	-1.27940

3d NMR Conformer 5
Energy: -910278.3188646

O	-1.80537	2.66886	-0.92423
C	-2.58417	1.62431	-0.56647
C	-1.97939	0.46571	-0.05028
C	-0.52240	0.32724	0.14985
N	0.09667	-0.79123	0.13029
C	1.51982	-0.49166	0.34542
C	2.26848	-0.77964	-0.96948
O	1.84783	-2.01540	-1.51670
C	3.78497	-0.94829	-0.79209
O	4.07561	-2.02645	0.06799
C	4.42240	0.32481	-0.25391
N	4.90109	0.25386	0.99757
O	4.43800	1.34404	-0.94393
C	1.52421	0.99100	0.78510
C	1.69159	1.17922	2.28063
O	0.19325	1.43959	0.40978
C	-2.77672	-0.63690	0.28065
C	-4.14990	-0.57955	0.11464
Cl	-5.12947	-1.96301	0.54374
C	-4.76062	0.56789	-0.38667
C	-3.97481	1.65981	-0.72630
H	-2.34918	3.38774	-1.29531
H	1.91808	-1.14457	1.13242
H	2.08334	0.04411	-1.67635
H	0.88672	-2.09274	-1.38548
H	4.21304	-1.11482	-1.79081
H	3.54808	-2.79114	-0.22345
H	5.36695	1.06061	1.39804
H	4.91905	-0.63326	1.48640
H	2.22862	1.60656	0.21924
H	2.69399	0.86393	2.58205
H	1.55438	2.22806	2.55346
H	0.95535	0.57399	2.81964
H	-2.30068	-1.52970	0.67407
H	-5.83870	0.60716	-0.51281
H	-4.43760	2.55788	-1.12958

3d NMR Conformer 4
Energy: -910281.9093796

O	2.45736	2.76430	0.77934
C	2.91459	1.53274	0.46725
C	2.11121	0.45587	0.04711
C	0.64874	0.54579	-0.10416
N	-0.11559	-0.36172	-0.56711
C	-1.49397	0.14433	-0.46447
C	-2.22003	-0.72255	0.56840
O	-2.26780	-2.06850	0.12928
C	-3.67338	-0.35200	0.89021
O	-4.18874	-1.26232	1.83678
C	-4.54391	-0.25617	-0.36726
N	-5.55827	-1.12786	-0.45269
O	-4.29894	0.60324	-1.21555
C	-1.33866	1.63013	-0.07379
C	-1.60676	2.58934	-1.21367
O	0.06852	1.70824	0.29954
C	2.71353	-0.77634	-0.25357

C	4.08023	-0.92982	-0.13664
Cl	4.81378	-2.47219	-0.51181
C	4.88691	0.13200	0.28082
C	4.30088	1.34981	0.57809
H	1.48978	2.81209	0.68915
H	-1.99525	0.04112	-1.43044
H	-1.66708	-0.65390	1.52037
H	-1.35760	-2.38704	0.00066
H	-3.69886	0.64477	1.34594
H	-3.78963	-2.13501	1.66837
H	-6.19162	-1.07875	-1.24220
H	-5.76077	-1.75455	0.31548
H	-1.90425	1.90177	0.82267
H	-2.65987	2.51302	-1.49500
H	-1.38008	3.61694	-0.92005
H	-0.99099	2.32202	-2.07866
H	2.08415	-1.59978	-0.57679
H	5.96140	0.00113	0.37086
H	4.90407	2.19190	0.90397

3d NMR Conformer 3

Energy: -910286.4325369

O	-1.52692	2.49632	-0.97925
C	-2.42725	1.59118	-0.56382
C	-2.07143	0.27875	-0.18890
C	-0.66748	-0.12893	-0.24310
N	0.29474	0.63166	-0.62043
C	1.54131	-0.13341	-0.46818
C	2.36121	0.52423	0.64594
O	2.71550	1.84826	0.28733
C	3.68548	-0.15420	1.02066
O	4.31247	0.58678	2.04320
C	4.59672	-0.36841	-0.19305
N	5.77252	0.27416	-0.16994
O	4.23533	-1.11418	-1.10478
C	1.05635	-1.56798	-0.15396
C	1.20878	-2.52686	-1.31549
O	-0.36230	-1.38301	0.12906
C	-3.05595	-0.62478	0.23267
C	-4.37677	-0.21860	0.28076
Cl	-5.60818	-1.34443	0.80608
C	-4.74391	1.07865	-0.08622
C	-3.77326	1.97483	-0.50580
H	-0.62736	2.07707	-0.97237
H	2.11117	-0.10142	-1.40022
H	1.74814	0.53088	1.56247
H	1.90759	2.38369	0.20458
H	3.48002	-1.15476	1.41862
H	4.11846	1.53025	1.89606
H	6.05025	0.80491	0.64556
H	6.43230	0.13172	-0.92583
H	1.49572	-1.97512	0.76186
H	2.27287	-2.65562	-1.52801
H	0.76159	-3.49523	-1.07994
H	0.71940	-2.11619	-2.20474
H	-2.77230	-1.63351	0.51719
H	-5.78643	1.38078	-0.04304
H	-4.03861	2.98682	-0.79661

3d NMR Conformer 2

Energy: -910281.6744275

O	-2.00071	2.88089	-0.51868
C	-2.62404	1.69875	-0.33002
C	-1.98269	0.48995	0.00007
C	-0.52779	0.36956	0.18742
N	0.09932	-0.68474	0.53440
C	1.53348	-0.35789	0.52137
C	2.18754	-1.12366	-0.64383
O	1.75940	-2.47187	-0.64857
C	3.71640	-1.22301	-0.53295
O	4.09408	-1.88449	0.65245
C	4.36761	0.15185	-0.58341
N	4.96073	0.55859	0.54928
O	4.29234	0.83041	-1.60761
C	1.57148	1.18303	0.38965
C	1.84440	1.90138	1.69580
O	0.21057	1.48807	-0.03366
C	-2.75050	-0.67357	0.17155
C	-4.12104	-0.63143	0.01672
Cl	-5.06233	-2.08883	0.23271
C	-4.76802	0.56307	-0.31197
C	-4.01858	1.71343	-0.48235
H	-1.03947	2.79707	-0.39563
H	1.99019	-0.68740	1.46280
H	1.93050	-0.62622	-1.59199
H	0.80754	-2.49286	-0.44925
H	4.06979	-1.76882	-1.41938
H	3.58999	-2.71552	0.70687
H	5.04980	-0.07650	1.33367
H	5.44415	1.44994	0.56434
H	2.22354	1.53328	-0.41408
H	2.86661	1.69125	2.02115
H	1.72912	2.98078	1.57377
H	1.15080	1.55410	2.46833
H	-2.24525	-1.59983	0.42734
H	-5.84731	0.58610	-0.43204
H	-4.49565	2.65496	-0.73743

3d NMR Conformer 1
Energy: -910285.9174081

O	1.70198	2.70761	0.50047
C	2.48649	1.64420	0.26237
C	1.98187	0.33220	0.14982
C	0.54546	0.09557	0.28795
N	-0.32782	1.01242	0.50276
C	-1.64882	0.36678	0.49754
C	-2.41133	0.82304	-0.75968
O	-2.35429	2.23063	-0.88996
C	-3.91669	0.52327	-0.70517
O	-4.51738	1.14203	0.40915
C	-4.18938	-0.97425	-0.66765
N	-4.73687	-1.44036	0.46493
O	-3.87447	-1.67959	-1.62587
C	-1.30747	-1.14336	0.54266
C	-1.46592	-1.75881	1.91864
O	0.10476	-1.16802	0.18368
C	2.85258	-0.73892	-0.09316
C	4.20731	-0.49828	-0.22641
Cl	5.29534	-1.83265	-0.53271
C	4.72111	0.79682	-0.11926
C	3.86392	1.85835	0.12435
H	0.76344	2.40264	0.58086
H	-2.21243	0.67641	1.38576
H	-1.98164	0.32701	-1.64372
H	-1.43325	2.52128	-0.77700
H	-4.35096	0.89393	-1.64460
H	-4.27818	2.08569	0.39919
H	-5.03724	-0.79793	1.18843
H	-4.97483	-2.42381	0.53335
H	-1.82320	-1.72476	-0.22511
H	-2.52327	-1.76870	2.19619
H	-1.08990	-2.78426	1.92627
H	-0.91315	-1.17200	2.65946
H	2.45483	-1.74582	-0.17543
H	5.78847	0.96827	-0.22586
H	4.24390	2.87170	0.21276

2c NMR Conformer 12
Energy: -910282.6158925

O	2.50636	2.89227	-0.18065
C	2.75235	1.56684	-0.13103
C	1.77268	0.55963	-0.21835
C	0.33782	0.84207	-0.37733
N	-0.57949	-0.02368	-0.57788
C	-1.86298	0.69488	-0.52862
C	-2.59411	0.31722	0.77289
O	-1.82546	0.64440	1.91135
C	-2.98068	-1.17186	0.80862
O	-1.85589	-2.02225	0.89160
C	-3.90938	-1.50928	-0.36007
N	-3.57824	-2.59731	-1.07091
O	-4.88728	-0.79928	-0.59788
C	-1.45589	2.18107	-0.65411
C	-2.17386	3.20136	0.19998
O	-0.04388	2.13972	-0.29312
C	2.16206	-0.78860	-0.15880
C	3.49340	-1.12215	-0.01589
Cl	3.96153	-2.80453	0.06105
C	4.47408	-0.13005	0.07179
C	4.09865	1.20024	0.01368
H	1.55426	3.07198	-0.26827
H	-2.49082	0.40486	-1.37859
H	-3.51928	0.89880	0.83345
H	-1.11650	-0.01480	2.01484
H	-3.56404	-1.33613	1.72346
H	-1.17036	-1.69343	0.27693
H	-4.17706	-2.89813	-1.83129
H	-2.79710	-3.17505	-0.78653
H	-1.48367	2.47484	-1.71003
H	-3.22838	3.23895	-0.08910
H	-2.09935	2.94328	1.25762
H	-1.74469	4.19257	0.03618
H	1.39954	-1.55901	-0.22607
H	5.51945	-0.40247	0.18521
H	4.84040	1.99063	0.07879

2c NMR Conformer 11
Energy: -910282.8631250

O	-0.49098	-2.22616	-0.19488
C	-1.64027	-1.53360	-0.15364
C	-1.68720	-0.14352	0.08625
C	-0.44149	0.58131	0.32636
N	0.72260	0.04503	0.27476
C	1.68369	1.06956	0.70027
C	2.94988	1.00587	-0.15595
O	2.66182	0.84500	-1.53050
C	3.94081	-0.09269	0.29986
O	4.97258	-0.20836	-0.65221
C	3.25219	-1.43622	0.56433
N	3.19865	-2.28229	-0.48229
O	2.75228	-1.67544	1.66152
C	0.86082	2.38373	0.63297
C	1.02778	3.24838	-0.60274
O	-0.51108	1.88319	0.65098
C	-2.91720	0.52665	0.12191
C	-4.08479	-0.18464	-0.08294

Cl	-5.62327	0.64593	-0.03604
C	-4.05481	-1.56122	-0.32220
C	-2.84016	-2.22798	-0.35623
H	0.26295	-1.60363	-0.01781
H	1.96618	0.86119	1.74081
H	3.49709	1.95297	-0.07404
H	1.97908	0.15534	-1.63280
H	4.37934	0.21149	1.25680
H	4.63117	0.09424	-1.51285
H	2.80714	-3.20774	-0.34480
H	3.77489	-2.11897	-1.29897
H	0.98577	2.97277	1.54401
H	2.04187	3.65432	-0.65181
H	0.84376	2.67171	-1.51157
H	0.32551	4.08374	-0.55540
H	-2.94065	1.59555	0.31184
H	-4.98210	-2.10504	-0.47866
H	-2.79773	-3.29766	-0.53799

2c NMR Conformer 10
Energy: -910283.9806001

O	0.58069	-2.34020	-0.09146
C	1.69748	-1.59643	-0.08477
C	1.68372	-0.19379	-0.24546
C	0.40133	0.48733	-0.41861
N	-0.71086	-0.12558	-0.59844
C	-1.77096	0.88409	-0.53958
C	-2.55632	0.72473	0.77452
O	-1.70644	0.81300	1.89509
C	-3.36515	-0.58707	0.85076
O	-2.47202	-1.66924	1.03436
C	-4.22921	-0.74169	-0.39874
N	-3.93007	-1.78233	-1.18856
O	-5.11288	0.08257	-0.63702
C	-0.99057	2.21702	-0.68269
C	-1.40755	3.39032	0.17571
O	0.37471	1.82936	-0.35256
C	2.88004	0.53358	-0.21308
C	4.07740	-0.13434	-0.03136
Cl	5.57504	0.76964	0.00627
C	4.10882	-1.52217	0.12614
C	2.92579	-2.24469	0.10159
H	-0.20321	-1.74371	-0.24241
H	-2.46119	0.76512	-1.38179
H	-3.27330	1.54973	0.84502
H	-1.21011	-0.02348	1.95154
H	-4.04682	-0.49851	1.70568
H	-2.84737	-2.29471	1.67678
H	-4.44904	-1.92868	-2.04661
H	-3.17089	-2.40476	-0.94045
H	-0.97158	2.50589	-1.74038
H	-2.42151	3.70058	-0.09389
H	-1.38126	3.12483	1.23406
H	-0.73828	4.23539	-0.00153
H	2.85510	1.61268	-0.33270
H	5.05798	-2.03094	0.26870
H	2.93089	-3.32334	0.22660

2c NMR Conformer 9
Energy: -910276.0839582

O	-2.39795	-2.83733	-0.51627
C	-2.96888	-1.62320	-0.35194
C	-2.14155	-0.51007	-0.12882
C	-0.67067	-0.60653	-0.02842
N	0.14138	0.31372	-0.37887
C	1.48983	-0.23577	-0.14618
C	2.42087	0.88163	0.31149
O	2.46028	1.90177	-0.67395
C	3.89003	0.50195	0.54268
O	4.61836	1.65379	0.90576
C	4.50296	-0.22332	-0.66144
N	5.49052	0.42024	-1.29908
O	4.09220	-1.34096	-0.97717
C	1.23818	-1.40924	0.81889
C	1.30467	-1.09383	2.30540
O	-0.14751	-1.73385	0.51170
C	-2.71533	0.76027	-0.00685
C	-4.08976	0.91342	-0.08708
Cl	-4.79149	2.50616	0.08407
C	-4.92003	-0.18541	-0.29521
C	-4.35491	-1.44611	-0.43015
H	-3.07768	-3.51365	-0.69116
H	1.86264	-0.61570	-1.10406
H	2.04985	1.29865	1.26018
H	1.55372	2.22303	-0.82065
H	3.96071	-0.20766	1.37422
H	4.22703	2.41946	0.44825
H	5.96045	-0.03286	-2.07413
H	5.84569	1.29722	-0.94077
H	1.84329	-2.28129	0.56366
H	2.32765	-0.88110	2.62599
H	0.67520	-0.23160	2.54735
H	0.94444	-1.95480	2.87293
H	-2.06883	1.61663	0.15955
H	-5.99694	-0.05765	-0.35429
H	-4.99060	-2.31124	-0.60556

2c NMR Conformer 8

Energy: -910276.3824394

O	-2.31546	2.73187	-0.25968
C	-2.93658	1.53797	-0.13483
C	-2.15101	0.39491	0.08752
C	-0.68259	0.46579	0.21848
N	0.13779	-0.36891	-0.28935
C	1.46578	0.01762	0.22571
C	2.51006	-0.23672	-0.85591
O	2.49173	-1.60873	-1.21784
C	3.97319	0.05192	-0.49341
O	4.79983	-0.30896	-1.57788
C	4.39786	-0.62225	0.81667
N	5.34868	-1.56162	0.71647
O	3.88233	-0.27405	1.87990
C	1.25597	1.46619	0.70866
C	1.51919	2.56935	-0.30442
O	-0.17433	1.46465	0.97828
C	-2.76040	-0.86083	0.16074
C	-4.13677	-0.97052	0.03418
Cl	-4.89014	-2.54512	0.13880
C	-4.92662	0.15767	-0.17126
C	-4.32314	1.40600	-0.25903
H	-2.96277	3.43576	-0.44857
H	1.69440	-0.63016	1.07981
H	2.27640	0.38060	-1.73676
H	1.59498	-1.83490	-1.51968
H	4.10476	1.12593	-0.32210
H	4.39823	-1.07638	-2.02340
H	5.69851	-2.00712	1.55668
H	5.79694	-1.74405	-0.17201
H	1.76709	1.65455	1.65449
H	2.58492	2.66353	-0.52817
H	0.97786	2.37634	-1.23580
H	1.17060	3.52097	0.10283
H	-2.14391	-1.73993	0.32412
H	-6.00434	0.06266	-0.26704
H	-4.92899	2.29214	-0.43468

3c NMR Conformer 7

Energy: -910275.0332187

O	-2.13551	-2.88017	-0.61517
C	-2.77623	-1.71426	-0.38154
C	-2.02818	-0.54486	-0.15907
C	-0.55190	-0.50042	-0.14009
N	0.13477	0.57151	-0.25782
C	1.54525	0.15344	-0.26104
C	2.42304	1.21391	0.42037
O	1.95589	2.51265	0.10208
C	3.87369	1.20163	-0.09720
O	3.91788	1.55404	-1.46019
C	4.50678	-0.16895	0.09641
N	4.72818	-0.87373	-1.02364
O	4.74607	-0.58093	1.23170
C	1.49225	-1.25829	0.36530
C	1.63458	-1.34305	1.87570
O	0.12809	-1.65459	0.03459
C	-2.70059	0.66760	0.04783
C	-4.08293	0.71120	0.04713
Cl	-4.89869	2.23427	0.31716
C	-4.83357	-0.44413	-0.16427
C	-4.17599	-1.64559	-0.37936
H	-2.77988	-3.59442	-0.77323
H	1.85992	0.08057	-1.31351
H	2.43356	1.07091	1.50796
H	0.98479	2.47870	0.05021
H	4.45187	1.90995	0.51241
H	3.33681	2.32522	-1.58422
H	4.56074	-0.45516	-1.93051
H	5.16393	-1.78671	-0.95969
H	2.15801	-1.96215	-0.13900
H	2.66013	-1.12321	2.17953
H	0.95242	-0.64171	2.36789
H	1.38203	-2.35580	2.19866
H	-2.11684	1.56755	0.21357
H	-5.91896	-0.40410	-0.16276
H	-4.74812	-2.55418	-0.55401

3c NMR Conformer 6

Energy: -910275.3522132

O	-2.03060	2.81103	-0.27358
C	-2.73560	1.66948	-0.11087
C	-2.03712	0.46290	0.06517
C	-0.56436	0.39710	0.11562
N	0.13938	-0.55104	-0.37142
C	1.52181	-0.28845	0.06815
C	2.52590	-0.75371	-0.99574
O	2.08429	-1.95989	-1.59260
C	3.89776	-1.11432	-0.39540
O	3.78760	-2.21351	0.47898
C	4.49229	0.07227	0.34979
N	4.54779	-0.04521	1.68520
O	4.85002	1.07263	-0.27234
C	1.49206	1.21390	0.43194
C	1.80328	2.19537	-0.68543
O	0.08553	1.37871	0.77774
C	-2.74672	-0.73695	0.18180
C	-4.13178	-0.73111	0.14117
Cl	-5.00611	-2.23671	0.30161

C	-4.83491	0.46035	-0.01917
C	-4.13422	1.65236	-0.14807
H	-2.63145	3.56265	-0.42986
H	1.69066	-0.88587	0.97744
H	2.66741	0.01891	-1.76174
H	1.11538	-1.92089	-1.67171
H	4.57658	-1.34073	-1.22944
H	3.23127	-2.88318	0.04283
H	4.95114	0.70488	2.23488
H	4.28941	-0.91707	2.13097
H	2.06901	1.43446	1.33256
H	2.86486	2.16714	-0.93952
H	1.20906	1.96667	-1.57637
H	1.54627	3.20325	-0.35128
H	-2.19721	-1.66444	0.31225
H	-5.92074	0.45794	-0.04670
H	-4.67291	2.58706	-0.28741

3c NMR Conformer 5
Energy: -910282.9111357

O	-1.53016	2.64777	-0.38855
C	-2.44505	1.67693	-0.23467
C	-2.10241	0.31030	-0.17318
C	-0.69783	-0.08706	-0.28131
N	0.27886	0.73166	-0.41861
C	1.52126	-0.05658	-0.46522
C	2.43412	0.48139	0.64794
O	2.71028	1.84715	0.37341
C	3.82310	-0.16539	0.81017
O	4.61649	0.62410	1.66576
C	4.50032	-0.44286	-0.53603
N	5.64375	0.21469	-0.77048
O	3.99097	-1.24897	-1.31713
C	1.02893	-1.53328	-0.40987
C	1.53934	-2.45583	0.67810
O	-0.41392	-1.39604	-0.23277
C	-3.10134	-0.65922	-0.01426
C	-4.42318	-0.26537	0.08445
Cl	-5.67176	-1.47421	0.28287
C	-4.77736	1.08487	0.02573
C	-3.79226	2.04705	-0.13370
H	-0.63210	2.23094	-0.44832
H	2.02129	0.13548	-1.41746
H	1.91893	0.39430	1.61674
H	1.88377	2.35652	0.42942
H	3.71270	-1.14202	1.28740
H	4.35304	1.55398	1.54671
H	6.05260	0.79784	-0.05141
H	6.15822	0.03283	-1.62446
H	1.17521	-1.99748	-1.38890
H	2.57022	-2.74377	0.46387
H	1.48051	-1.99082	1.66685
H	0.92820	-3.36160	0.68898
H	-2.82803	-1.70912	0.02993
H	-5.82081	1.37683	0.10391
H	-4.04710	3.10142	-0.18311

3c NMR Conformer 4
Energy: -910279.7764122

O	2.56546	2.86163	-0.16323
C	2.99336	1.58165	-0.13123
C	2.15435	0.45136	-0.11696
C	0.68485	0.53298	-0.12551
N	-0.12649	-0.44166	-0.01302
C	-1.47383	0.12688	-0.20007
C	-2.46140	-0.62587	0.68619
O	-2.44904	-2.00119	0.34032
C	-3.93599	-0.20983	0.58815
O	-4.71265	-1.04638	1.41564
C	-4.43989	-0.18307	-0.85984
N	-5.39901	-1.06624	-1.16845
O	-3.97324	0.63528	-1.65386
C	-1.27514	1.63324	0.05276
C	-1.45139	2.11765	1.48232
O	0.13979	1.77541	-0.28158
C	2.72636	-0.83073	-0.08504
C	4.09833	-0.97987	-0.06338
Cl	4.79446	-2.58363	-0.02627
C	4.94032	0.13538	-0.07507
C	4.38422	1.40208	-0.10950
H	1.59360	2.90554	-0.18684
H	-1.76176	-0.03749	-1.24456
H	-2.16818	-0.50580	1.74034
H	-1.54636	-2.34312	0.46234
H	-4.05482	0.81602	0.95394
H	-4.30504	-1.93134	1.42375
H	-5.79843	-1.06266	-2.09979
H	-5.80294	-1.65531	-0.45177
H	-1.83693	2.24139	-0.65797
H	-2.49930	2.07535	1.78957
H	-0.85851	1.51147	2.17433
H	-1.12010	3.15591	1.55746
H	2.06998	-1.69553	-0.07940
H	6.01891	0.00775	-0.05952
H	5.01502	2.28592	-0.12019

3c NMR Conformer 3
Energy: -910278.5124450

O	2.16423	2.93589	-0.25344
C	2.73500	1.71436	-0.18603
C	2.03093	0.49647	-0.12766
C	0.56266	0.41056	-0.12549
N	-0.13231	-0.64411	0.04238
C	-1.53524	-0.24858	-0.16824
C	-2.47275	-1.07597	0.72339
O	-2.01545	-2.41253	0.81000
C	-3.88708	-1.20247	0.12557
O	-3.85402	-1.92818	-1.08075
C	-4.49324	0.17154	-0.12325
N	-4.65249	0.51617	-1.41002
O	-4.76538	0.90424	0.82808
C	-1.50806	1.28271	0.04012
C	-1.70791	1.78603	1.45855
O	-0.12345	1.56839	-0.33710
C	2.74542	-0.71071	-0.05858
C	4.12538	-0.70191	-0.04445
Cl	5.00031	-2.21301	0.04449
C	4.83412	0.50123	-0.10180
C	4.13735	1.69464	-0.17238
H	1.19374	2.86831	-0.26986
H	-1.77986	-0.47352	-1.21775
H	-2.54841	-0.63426	1.72466
H	-1.04315	-2.40210	0.84091
H	-4.52123	-1.70299	0.87061
H	-3.29723	-2.71398	-0.93897
H	-5.07170	1.41081	-1.63724
H	-4.46003	-0.15362	-2.14485
H	-2.14242	1.81320	-0.67278
H	-2.74797	1.65863	1.76487
H	-1.05569	1.24957	2.15566
H	-1.46026	2.84958	1.49799
H	2.19207	-1.64396	-0.01840
H	5.92024	0.49772	-0.09259
H	4.66345	2.64349	-0.21788

3c NMR Conformer 2
Energy: -910284.0294580

O	-1.50098	2.65239	-0.02119
C	-2.43305	1.68599	-0.05221
C	-2.10761	0.31394	-0.07394
C	-0.70352	-0.09337	-0.07781
N	0.29418	0.71049	-0.01521
C	1.50031	-0.11866	-0.18650
C	2.64307	0.43959	0.65534
O	2.93334	1.76813	0.25158
C	3.98454	-0.30171	0.55654
O	4.94118	0.35740	1.35398
C	4.44993	-0.47926	-0.89422
N	5.58529	0.14746	-1.23105
O	3.79617	-1.18420	-1.66441
C	0.99134	-1.53725	0.14151
C	1.08679	-1.97692	1.59363
O	-0.42908	-1.40988	-0.17157
C	-3.12375	-0.65061	-0.10305
C	-4.44588	-0.24618	-0.11197
Cl	-5.71685	-1.44733	-0.15067
C	-4.78305	1.10964	-0.09241
C	-3.78079	2.06689	-0.06317
H	-0.60383	2.23253	-0.02025
H	1.79457	-0.06347	-1.24028
H	2.35374	0.42912	1.71687
H	2.16577	2.33391	0.44408
H	3.87403	-1.31806	0.94990
H	4.75496	1.31334	1.32584
H	6.12703	0.63857	-0.53165
H	5.96242	0.02596	-2.16381
H	1.40723	-2.28189	-0.53921
H	2.12372	-2.14325	1.89559
H	0.64490	-1.22635	2.25653
H	0.54301	-2.91546	1.72157
H	-2.86271	-1.70441	-0.11915
H	-5.82703	1.40984	-0.10040
H	-4.02267	3.12534	-0.04785

3c NMR Conformer 1
Energy: -910282.3190304

O	-1.61460	2.69650	0.07303
C	-2.46119	1.65610	0.00662
C	-2.02348	0.31714	-0.05990
C	-0.59131	0.02398	-0.07428
N	0.33930	0.90017	0.04392
C	1.60941	0.18799	-0.17218
C	2.73926	0.78095	0.68376
O	2.62994	2.19006	0.75148
C	4.12583	0.55151	0.05348
O	4.23643	1.23011	-1.17600
C	4.38399	-0.93376	-0.16038
N	4.42352	-1.34310	-1.43719
O	4.50234	-1.68181	0.81017
C	1.21430	-1.28749	0.08350
C	1.33440	-1.79061	1.51134
O	-0.21015	-1.25501	-0.24482
C	-2.95776	-0.72586	-0.12503
C	-4.30854	-0.43122	-0.12417
Cl	-5.47658	-1.73030	-0.20435
C	-4.75585	0.89107	-0.06099

C	-3.83564	1.92547	0.00300
H	-0.68612	2.35676	0.06678
H	1.87934	0.32281	-1.23043
H	2.73264	0.34924	1.69199
H	1.70546	2.42712	0.93608
H	4.87900	0.90722	0.77024
H	3.91167	2.13875	-1.04772
H	4.37354	-0.66927	-2.19161
H	4.61275	-2.31799	-1.64105
H	1.68455	-1.97087	-0.62652
H	2.38311	-1.91180	1.78924
H	0.85174	-1.09720	2.20824
H	0.83725	-2.76048	1.58713
H	-2.61135	-1.75362	-0.17521
H	-5.82087	1.10497	-0.06208
H	-4.16295	2.95962	0.05240

2b NMR Conformer 4
Energy: -910273.8160951

O	-0.98543	2.60042	-0.06458
C	-1.87408	1.58466	-0.07509
C	-1.56970	0.26838	0.31557
C	-0.24274	-0.10363	0.83894
N	0.33845	-1.22480	0.66648
C	1.66660	-1.10169	1.28381
C	2.77535	-1.28216	0.22798
O	3.02409	-2.67133	0.04890
C	2.52650	-0.70639	-1.18937
O	3.59565	-1.09788	-2.02606
C	2.43706	0.81320	-1.23198
N	3.58134	1.45026	-1.51280
O	1.37744	1.39378	-0.98486
C	1.58447	0.21549	2.09782
C	2.75073	1.17988	2.08044
O	0.38975	0.84430	1.57206
C	-2.54597	-0.73054	0.21700
C	-3.81651	-0.41197	-0.22939
Cl	-5.03391	-1.66402	-0.33599
C	-4.14185	0.89641	-0.58800
C	-3.17024	1.88306	-0.51384
H	-0.07236	2.26597	0.00046
H	1.82669	-1.93144	1.98122
H	3.71836	-0.86982	0.60872
H	2.17812	-3.12208	-0.13269
H	1.56633	-1.09209	-1.55744
H	3.79949	-2.02816	-1.82776
H	3.58336	2.46182	-1.58385
H	4.39493	0.92234	-1.80594
H	1.34807	-0.04483	3.13632
H	3.62825	0.70020	2.52414
H	3.00172	1.51190	1.07210
H	2.50774	2.05880	2.68239
H	-2.29529	-1.74550	0.51118
H	-5.14416	1.13648	-0.93071
H	-3.39303	2.90412	-0.80900

2b NMR Conformer 3
Energy: -910274.7785503

O	2.29664	2.72959	-0.03413
C	2.91328	1.52728	-0.04591
C	2.12955	0.36417	-0.13645
C	0.65786	0.39864	-0.24819
N	-0.13053	-0.45829	0.27634
C	-1.47106	-0.12243	-0.23689
C	-2.52545	-0.48066	0.80688
O	-2.31262	0.16403	2.04976
C	-3.97384	-0.14178	0.43079
O	-4.84262	-0.60196	1.44253
C	-4.36264	-0.78394	-0.89675
N	-5.12460	-1.88316	-0.80701
O	-3.95701	-0.30434	-1.95558
C	-1.31924	1.33473	-0.72229
C	-1.60361	2.45933	0.26085
O	0.11048	1.37366	-1.00839
C	2.74918	-0.88942	-0.09916
C	4.12740	-0.98103	0.01152
Cl	4.88715	-2.55579	0.04447
C	4.91424	0.16530	0.09025
C	4.30339	1.41223	0.06445
H	2.94995	3.44517	0.07172
H	-1.65745	-0.75995	-1.11201
H	-2.47439	-1.57273	0.94591
H	-1.45537	-0.12771	2.40568
H	-4.07742	0.94261	0.29331
H	-4.46066	-0.35392	2.30228
H	-5.42784	-2.35105	-1.65318
H	-5.47121	-2.18990	0.09356
H	-1.84203	1.48947	-1.66795
H	-2.66433	2.51434	0.51286
H	-1.04106	2.31645	1.18600
H	-1.30299	3.40580	-0.19552
H	2.13502	-1.78252	-0.16456
H	5.99421	0.08578	0.17431
H	4.90654	2.31447	0.13812

2b NMR Conformer 2
Energy: -910278.2625519

O	2.47120	2.84107	-0.09183

C	2.93599	1.57350	-0.10581
C	2.12827	0.42202	-0.16159
C	0.65754	0.46771	-0.19935
N	-0.12962	-0.52809	-0.10016
C	-1.48704	0.00645	-0.30311
C	-2.48096	-0.81048	0.52003
O	-2.17180	-0.82034	1.90126
C	-3.94456	-0.35537	0.44828
O	-4.75173	-1.25906	1.17005
C	-4.42894	-0.28595	-0.99577
N	-5.21371	-1.29646	-1.39405
O	-4.07270	0.64502	-1.71857
C	-1.33289	1.52148	-0.04892
C	-1.53723	2.04738	1.36169
O	0.08579	1.69504	-0.36688
C	2.73345	-0.84484	-0.16597
C	4.10807	-0.95874	-0.11201
Cl	4.84593	-2.54421	-0.11945
C	4.91923	0.17756	-0.05459
C	4.33006	1.42996	-0.05261
H	1.50036	2.85620	-0.15944
H	-1.74510	-0.14170	-1.36016
H	-2.44304	-1.83853	0.12554
H	-1.31699	-1.26827	2.02546
H	-4.03868	0.65995	0.85557
H	-4.31687	-1.43566	2.02250
H	-5.57648	-1.30413	-2.34030
H	-5.51147	-2.00210	-0.73167
H	-1.89607	2.10209	-0.78132
H	-2.58177	1.96737	1.66805
H	-0.93178	1.48767	2.07773
H	-1.24918	3.10151	1.39018
H	2.10069	-1.72583	-0.21307
H	6.00004	0.07745	-0.01395
H	4.93683	2.32944	-0.00874

2b NMR Conformer 1
Energy: -910282.6440677

O	-1.50370	2.67398	-0.23517
C	-2.42332	1.69630	-0.19688
C	-2.07994	0.32901	-0.14921
C	-0.66990	-0.05852	-0.15455
N	0.31234	0.76688	-0.15224
C	1.53257	-0.04486	-0.28908
C	2.68332	0.61945	0.46488
O	2.40750	0.80571	1.84042
C	4.02212	-0.13085	0.43050
O	5.01520	0.65222	1.05441
C	4.44796	-0.43879	-1.00105
N	5.41362	0.34425	-1.50097
O	3.89173	-1.34233	-1.62568
C	1.05896	-1.46333	0.10452
C	1.18750	-1.89747	1.55469
O	-0.37379	-1.37078	-0.18183
C	-3.08307	-0.64820	-0.10516
C	-4.41058	-0.26130	-0.11014
Cl	-5.66570	-1.47839	-0.05096
C	-4.76574	1.08912	-0.15995
C	-3.77621	2.05899	-0.20358
H	-0.60062	2.26372	-0.22495
H	1.80514	-0.05196	-1.35242
H	2.85004	1.59683	-0.01567
H	1.69051	1.45649	1.93401
H	3.91614	-1.09929	0.93698
H	4.65334	0.98503	1.89411
H	5.74943	0.18253	-2.44340
H	5.86696	1.03306	-0.91328
H	1.47115	-2.21137	-0.57469
H	2.23328	-2.01950	1.84274
H	0.73597	-1.16195	2.22358
H	0.68009	-2.85754	1.67801
H	-2.80783	-1.69788	-0.06735
H	-5.81367	1.37534	-0.16382
H	-4.03207	3.11358	-0.24212

2a NMR Conformer 7
Energy: -910283.8128669

O	-0.93656	2.69158	-0.57097
C	-1.85030	1.74502	-0.30139
C	-1.56560	0.36614	-0.38526
C	-0.22454	-0.06874	-0.77395
N	0.73945	0.72971	-1.05504
C	1.91074	-0.09540	-1.35300
C	3.13099	0.31224	-0.52015
O	3.75258	1.45863	-1.08051
C	2.87544	0.62075	0.97111
O	4.09929	0.98704	1.57346
C	2.30125	-0.56469	1.73954
N	3.21234	-1.36886	2.31298
O	1.08841	-0.76580	1.77048
C	1.41343	-1.55329	-1.16992
C	1.54453	-2.40578	-2.41424
O	0.01009	-1.38765	-0.84598
C	-2.55722	-0.57669	-0.08541
C	-3.81662	-0.14468	0.28865
Cl	-5.05706	-1.31959	0.66594
C	-4.11414	1.21765	0.37262
C	-3.13475	2.15391	0.07917

H	-0.08439	2.24636	-0.81925
H	2.20650	0.06826	-2.39884
H	3.88149	-0.48798	-0.58370
H	3.08727	2.16536	-1.17756
H	2.13519	1.43012	1.03856
H	4.55814	1.59742	0.97020
H	4.18491	-1.08822	2.34644
H	2.89944	-2.15939	2.86479
H	1.87737	-2.04783	-0.31016
H	2.60327	-2.52983	-2.66178
H	1.10693	-3.39399	-2.25612
H	1.04238	-1.92337	-3.25805
H	-2.32672	-1.63582	-0.14808
H	-5.10867	1.53954	0.66814
H	-3.34533	3.21739	0.14048

2a NMR Conformer 6
Energy: -910278.4652751

O	-0.95442	2.57185	0.27716
C	-1.86240	1.58800	0.10795
C	-1.57112	0.21879	0.24031
C	-0.23208	-0.24686	0.64485
N	0.38334	-1.25903	0.17759
C	1.69010	-1.29313	0.84290
C	2.82945	-1.27288	-0.18120
O	2.96983	-2.54851	-0.78594
C	2.71118	-0.24438	-1.33038
O	3.83609	-0.38136	-2.17350
C	2.65947	1.20225	-0.85400
N	3.84345	1.81614	-0.74623
O	1.58442	1.73497	-0.56420
C	1.66418	-0.11663	1.85145
C	1.75053	-0.55447	3.29933
O	0.37106	0.48615	1.61163
C	-2.56368	-0.73487	-0.01255
C	-3.84041	-0.32458	-0.35615
Cl	-5.08213	-1.52118	-0.65110
C	-4.15233	1.03112	-0.45974
C	-3.16362	1.97710	-0.23315
H	-0.04288	2.22499	0.28433
H	1.79883	-2.24564	1.37962
H	3.77533	-1.08933	0.34706
H	2.10053	-2.82974	-1.12778
H	1.77492	-0.43211	-1.87354
H	3.98170	-1.33213	-2.32203
H	4.68066	1.36515	-1.09622
H	3.87816	2.78724	-0.45628
H	2.41972	0.64601	1.63312
H	2.72750	-1.01017	3.48686
H	1.62896	0.29824	3.97108
H	0.97285	-1.29297	3.51649
H	-2.32226	-1.78966	0.08248
H	-5.15898	1.34152	-0.72452
H	-3.37774	3.03730	-0.33031

2a NMR Conformer 5
Energy: -910284.8141272

O	-1.05716	-0.82763	2.57982
C	-1.91291	-0.65398	1.55970
C	-1.62019	0.16448	0.44876
C	-0.32642	0.83826	0.37694
N	0.56614	0.80392	1.29813
C	1.75672	1.47013	0.75532
C	2.84915	0.43880	0.44266
O	3.20125	-0.27964	1.61279
C	2.50506	-0.56132	-0.67507
O	1.48891	-1.47385	-0.32688
C	3.79589	-1.26720	-1.11974
N	3.72715	-2.60393	-1.20385
O	4.80015	-0.61127	-1.39585
C	1.21154	2.22936	-0.46968
C	0.89776	3.68580	-0.18993
O	-0.03112	1.52246	-0.74492
C	-2.55469	0.30969	-0.58532
C	-3.76405	-0.35597	-0.50776
Cl	-4.93461	-0.17526	-1.79447
C	-4.06631	-1.17250	0.58525
C	-3.14459	-1.31906	1.61007
H	-0.24389	-0.28717	2.40854
H	2.16523	2.16232	1.50112
H	3.74095	0.98425	0.11382
H	2.43012	-0.34305	2.20318
H	2.14990	-0.01988	-1.56171
H	1.61552	-1.75733	0.59702
H	2.85758	-3.08569	-1.01614
H	4.53090	-3.12411	-1.53545
H	1.84084	2.12226	-1.35827
H	1.82657	4.23494	-0.01170
H	0.38154	4.13617	-1.04040
H	0.26416	3.77321	0.69837
H	-2.31994	0.94190	-1.43626
H	-5.02101	-1.68885	0.62966
H	-3.36119	-1.94896	2.46763

2a NMR Conformer 4
Energy: -910280.6986064

O	-1.64024	2.56750	-1.44848
C	-2.25526	1.47698	-0.94422

C	-1.68083	0.57557	-0.02814
C	-0.31419	0.71529	0.50019
N	0.24068	-0.04703	1.35761
C	1.61530	0.43180	1.52982
C	2.59662	-0.63356	1.02977
O	2.46426	-1.81741	1.78896
C	2.42421	-0.94387	-0.49710
O	1.93234	-2.23739	-0.73617
C	3.73543	-0.66453	-1.23485
N	4.18534	-1.64577	-2.02764
O	4.29464	0.42438	-1.08856
C	1.67876	1.76629	0.75414
C	1.71428	2.99341	1.64069
O	0.42341	1.75120	0.01436
C	-2.43153	-0.52304	0.42140
C	-3.72110	-0.71585	-0.03030
Cl	-4.64309	-2.08706	0.54091
C	-4.30114	0.17248	-0.94007
C	-3.56767	1.25675	-1.38811
H	-0.73543	2.65456	-1.10211
H	1.81661	0.58642	2.59739
H	3.61279	-0.26336	1.19940
H	1.51836	-1.96462	1.97518
H	1.70153	-0.24606	-0.94164
H	2.22288	-2.81158	-0.00492
H	3.65265	-2.50075	-2.12755
H	5.02914	-1.50682	-2.57111
H	2.48328	1.77905	0.01169
H	2.65859	3.01753	2.19234
H	1.63579	3.90502	1.04411
H	0.89006	2.96534	2.36021
H	-1.97739	-1.21192	1.12699
H	-5.31660	0.01192	-1.29067
H	-3.99423	1.96229	-2.09481

2a NMR Conformer 3
Energy: -910279.1517391

O	2.10240	-2.71592	-0.32927
C	2.79157	-1.55629	-0.23474
C	2.08883	-0.37114	0.03804
C	0.62841	-0.33588	0.26552
N	-0.12898	0.62833	-0.09010
C	-1.48546	0.28751	0.35717
C	-2.38883	0.18877	-0.87487
O	-1.94449	-0.84091	-1.74331
C	-3.85302	-0.16508	-0.57427
O	-4.56906	-0.29161	-1.78299
C	-4.51025	0.91049	0.28531
N	-5.31667	1.75899	-0.36875
O	-4.26594	0.97592	1.49002
C	-1.32177	-1.04205	1.13291
C	-1.61533	-0.92473	2.61353
O	0.08073	-1.36603	0.94200
C	2.78037	0.84379	0.08813
C	4.15120	0.87302	-0.11220
Cl	5.00215	2.39863	-0.02970
C	4.85962	-0.29769	-0.37014
C	4.17559	-1.50434	-0.43390
H	2.70308	-3.45190	-0.54762
H	-1.86581	1.08033	1.01044
H	-2.37080	1.15719	-1.39765
H	-1.11308	-0.56265	-2.16505
H	-3.89292	-1.10084	0.00254
H	-4.01621	-0.79463	-2.40551
H	-5.79012	2.49299	0.14485
H	-5.52036	1.61390	-1.34979
H	-1.88805	-1.85908	0.67470
H	-2.66671	-0.65446	2.74721
H	-1.41180	-1.86581	3.12991
H	-0.99726	-0.13623	3.05518
H	2.22833	1.75590	0.29350
H	5.93457	-0.26806	-0.52270
H	4.71527	-2.42435	-0.64755

2a NMR Conformer 2
Energy: -910282.4184279

O	2.42356	2.74750	0.66725
C	2.88888	1.51373	0.37628
C	2.09052	0.41929	-0.00666
C	0.62483	0.49176	-0.14194
N	-0.13729	-0.44729	-0.54090
C	-1.51390	0.06036	-0.48578
C	-2.29845	-0.77899	0.52698
O	-1.74295	-0.64959	1.82566
C	-3.77166	-0.37947	0.69782
O	-4.37721	-1.20931	1.66376
C	-4.53333	-0.50416	-0.61759
N	-5.31281	-1.58851	-0.73406
O	-4.38936	0.34517	-1.49713
C	-1.37572	1.55301	-0.10063
C	-1.74667	2.51036	-1.21232
O	0.04548	1.67505	0.19082
C	2.70138	-0.81344	-0.28663
C	4.07122	-0.95059	-0.18596
Cl	4.81476	-2.49387	-0.53762
C	4.87293	0.12870	0.19416
C	4.27841	1.34723	0.47125
H	1.45480	2.78483	0.58325

H	-1.98053	-0.04630	-1.47056
H	-2.26573	-1.83029	0.20353
H	-0.90733	-1.14612	1.86660
H	-3.83096	0.67704	0.99811
H	-3.77020	-1.27721	2.42134
H	-5.85421	-1.72513	-1.57971
H	-5.43157	-2.21712	0.05070
H	-1.89351	1.79212	0.83264
H	-2.80929	2.38888	-1.44036
H	-1.55242	3.54526	-0.92093
H	-1.16952	2.27903	-2.11342
H	2.07601	-1.65013	-0.58244
H	5.95001	0.01116	0.27072
H	4.87746	2.20294	0.76800
H	-0.90390	2.24568	-2.09417
H	2.76076	1.61953	0.42141
H	5.76505	-1.40310	-0.14723
H	4.00029	-3.03049	-0.81045

2a NMR Conformer 1
Energy: -910287.1231174

O	1.48323	-2.54792	-0.93627
C	2.39307	-1.63152	-0.56947
C	2.04498	-0.31038	-0.21801
C	0.63917	0.09506	-0.24990
N	-0.32609	-0.67586	-0.59655
C	-1.56942	0.09181	-0.47216
C	-2.46058	-0.58435	0.57378
O	-1.83262	-0.58505	1.84518
C	-3.81166	0.10805	0.80945
O	-4.52217	-0.57223	1.81860
C	-4.64993	0.12833	-0.46518
N	-5.64867	-0.76436	-0.51410
O	-4.37419	0.91231	-1.37350
C	-1.09662	1.51510	-0.08157
C	-1.35456	2.55847	-1.14676
O	0.34008	1.35530	0.10041
C	3.03856	0.60434	0.15463
C	4.36128	0.20163	0.17572
Cl	5.60391	1.34231	0.63884
C	4.72105	-1.10380	-0.16864
C	3.74097	-2.01181	-0.53815
H	0.58349	-2.12703	-0.91907
H	-2.09241	0.10126	-1.43382
H	-2.65763	-1.61664	0.24723
H	-1.12283	-1.25045	1.85261
H	-3.63972	1.15742	1.09203
H	-3.90202	-0.76753	2.54226
H	-5.85656	-1.34109	0.29165
H	-6.25045	-0.79487	-1.32884
H	-1.48816	1.82418	0.89206
H	-2.43415	2.65513	-1.29291
H	-0.93746	3.52546	-0.85648

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