Ganorbifates A and B from *Ganoderma orbiforme*, Determined by DFT Calculations of NMR data and ECD spectra.

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Experimental section

General experimental Procedures

Optical rotations (OR) were measured on an Autopol III automatic polarimeter. UV spectra were measured on a Thermo Scientific Evolution-300UV-visible spectrophotometer. Nuclear Magnetic Resonance (NMR) spectra were measured on Agilent 400 MR and Bruker Avance III 500 spectrometers with tetramethylsilane (TMS) as internal standard at room temperature. High-resolution (HR) ESIMS were recorded on an AB Sciex Triple TOF 4600 system. ECD spectra were obtained on a Chirascan spectrometer. Silica gel (300–400 mesh, Qingdao Marine Chemical Ltd., People's Republic of China), Sephadex LH-20 (Amersham Biosciences, Sweden) and RP-18 gel (20–45 μm, Fuji Silysia Chemical Ltd., Japan) were used for column chromatography (CC). Semipreparative HPLC was performed on a Waters 1525 liquid chromatography system equipped with Hypersil BDS C-18 column (4.6 mm × 250 mm, and 10.0 mm × 250 mm) and Chiralcel OD-H (4.6 mm × 150 mm). Fractions were monitored by TLC. Spots were visualized by heating silica gel plates immersed in vanillin/ H_2SO_4 in ethanol.

Fungal Material

Fruiting bodies of *Ganoderma orbiforme* were collected from BenTre province, VietNam in 2017 provided by Professor Hoang Xuan Nien, Thu Dau Mot University in January 2018 and identified by Dr. Do Huu Thu on the basis of morphological characteristics. And then, *G. orbiforme* was further confirmed by the sequence data of the ITS rDNA (GenBank accession number: KX421867) by Isaka in the National Center for Genetic Engineering and Biotechnology, National Science and Technology for Development Agency, Thailand.

DNA extraction, PCR amplification and sequencing of the *ITS-rDNA* region

Total genomic DNA was extracted using the plant/fungi DNA isolation Kit (Norgenbiotek, Canada). The nuclear gene (*ITS-rDNA*) was amplified through the following PCR cycling profile: an initial heating step at 95^{o}C for 3 min; followed by incubating for 40 cycles of 95^{o}C for 45s, 56^{o}C for 45s min and 72^{o}C for 45s, and completed by incubating at 72^{o}C for 10 min. All PCR reactions were performed in 25 μL volumes using Gene Amp PCR Systems 9700, including: 2 μL of genomic DNA (10 ng total), 12.5 μL Master Mix 2X, 1 μL of each 10 μM primer and 9.5 μL H_2O deionized. Two universal primers, forward primer (ITS1: 5'-TCC GTA GGT GAA CCT GCG G-3') and reverse primer (ITS-4: 5'-TCC TCC GCT TAT TGATAT GC- 3') were used for the amplification of the ITS regions of the fungus (White et al., 1990). Sequencing was performed in Macrogen Co. Ltd (Korea). Chromas Pro 2.1.6 software (Technelysium Pty Ltd., Tewantin, Australia) was used to edit the sequences. Aligned, combined sequences of ITS-rDNA yielded a total 555bp

positions is as follows:

GCTCATCCACTCTACACCTGTGCACTTATTGTGGGTTATAGATCGTGTGGAGCGAGCTCGT
TCGTTTGACGAGTTTGTGAAGCGCGTCTGTGCCTGCGTTTTTATCACAAACACTATAAAGTATT
AGAATGTGTATTGCGATGTAACGCATCTATATACAACTTTCAGCAACGGATCTCTTGGCTCTCG
CATCGATGAAGAACGCAGCGAAATGCGATAAGTAATGTGAATTGCAGAATTCAGTGAATCATC
GAATCTTTGAACGCACCTTGCGCTCCTTGGTATTCCGAGGAGCATGCCTGTTTGAGTGTCATGA
AACCTTCAACCTACAATCTCTATGCGGTTTTTGTAGGCTTGGACTTGGAGGCTTGTCGGTCTTTT
ATTGATCGGCTCCTCTCAAATGTATTAGCTTGGTTCCTTTGCGAATCGGCTGTCGGTGTGATAAT
GTCTACGCCGCGACCGTGACGCGTTTGGCGAGCTTCTAACCGTCCCGTTATTGGGACAACGCTT
ATGACCTCTGACCTCAAATCAGGTAGGACTACCCGCTGAACTTAA

Extraction and Isolation

G. orbiforme (3.3 kg) mushrooms were cut into small pieces and extracted with 95% EtOH under reflux three times. The combined ethanol extracts were filtered and concentrated under reduced pressure to give a dark brown residue of 223.0 g. The residue was suspended in H_2O and extracted with ethyl acetate (EA). The combined EA extract (162.7 g) was fractionated by CC (silica gel, diethyl ether/ethyl acetate (Et: EA) step gradients), step gradient elution 100:0, 90:10, 80:20, 60:40, 50:50, 30:70, then 0:100 to obtain nine fractions, Fr-1–Fr-9. By repeated column chromatography, HPLC separation, from fraction VII-3-6 (0.458 g) was further separated by reversed-phase HPLC (MeOH-H_2O, 80%) to afford seven fractions. Fraction VII-3-6-4 (0.289 g) was further separated by Chiralcel OD-H (4.6 mm × 150 mm) (n-hexan-EtOH, 98-2 %) to afford compounds **1** (3.8 mg) and **2** (3.3mg).

Compound **1**, white powder, $[\alpha]^{25}{}_{D}$ 36.53 (c 1.9, methanol); UV (methanol) λ_{max} nm (log ε): 272 (1.95), HRESIMS (*m/z* 551.2605 $[M + Na]^+$, cald for $C_{30}H_{40}O_8Na$, 551.2621)

Compound **2**, white powder, $[\alpha]^{25}{}_{D}$ -6.86 (c 2.9 ,methanol); UV (methanol) λ_{max} nm (log ε): 254 (1.42). HRESIMS (*m/z* 537.2822 $[M + Na]^+$, cald for $C_{30}H_{42}O_7Na$, 537.2828)

Computational Methods

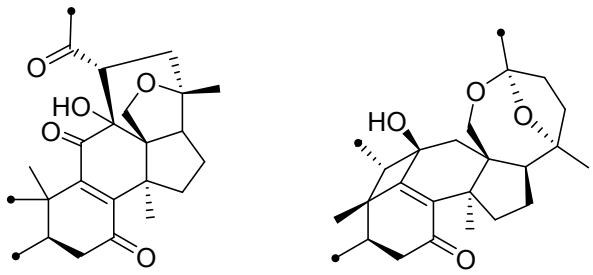
Molecular mechanics, Hartree-Fock (HF) and density functional theory (DFT) calculations were run with Spartan'18 (Wavefunction, Inc., Irvine CA, 2018), with standard parameters and convergence criteria. DFT and time-dependent (TD) DFT calculations were run with Gaussian16 with default grids and convergence criteria. [1] Extended conformational searches were run on full molecules **1** and **2** and on their epimers 12-*epi*-**1** and 11-*epi*-**2**. NMR calculations were run on full molecules **1** and **2**. ECD calculations were run on truncated models of **1** and **2** (trunc-**1** and trunc-**2**, see Chart). The truncation preserves the polycyclic core

while all substituents attached by flexible bonds are replaced by methyl groups.

Extended conformational searches were run with the Monte Carlo algorithm using Merck molecular force field (MMFF). All conformers thus obtained were analyzed for selected H-H distances, irrespective of their relative energy but with a maximum of 500 conformers for each compound. Selected H-H distances were measured on all conformers and analyzed through a cluster analysis visualized by histograms (see main text). For methyl groups, the distances were measured from the carbon atom.

For NMR calculations, the conformers obtained by a conformational search run with the Monte Carlo algorithm using Merck molecular force field (MMFF) were geometry-optimized at HF/3-21G level, screened by single-point calculations at ωB97X-D/6-31G(d) level, and geometry-optimized at the same level. Final energies and populations were estimated at the ωB97X-V/6-311+G(2df,2p) level, according to the procedure described by Hehre et al.[2] The procedure afforded 13 energy minima for **1**, and 30 for **2**, within the final energy threshold (10 kJ/mol at ωB97X-D/6-31G(d) level). ^{13}C-NMR chemical shifts were then calculated with the GIAO method at ωB97X-D/6-31G(d) level. Finally, an empirical correction was applied depending on the number of bonds to the carbon and on the bond lengths.[2] Calculated ^{13}C chemical shifts are reported in Table S1. The same procedure was applied to 4-*epi*-**1** and 4-*epi*-**2** (Table S2).

For ECD calculations, the same conformational search and geometry optimization procedure described above was applied to trunc-**1** and trunc-**2** models. This procedure resulted in 2 energy minima for trunc-**1**, and 1 for trunc-**2**, within the final energy threshold (10 kJ/mol at ωB97X-D/6-31G(d) level). The structures and coordinates are reported in the end of this Supporting Information. They were used as input structures for TDDFT calculations run at the B3LYP/def2-TZVP and CAM-B3LYP/def2-TZVP level, including 36 excited states (roots) in each case. For compound **2**, the inclusion of IEF-PCM solvent model for methanol was checked for consistency. Average ECD spectra were computed by weighting component CD spectra with Boltzmann factors at 300 K estimated from DFT internal energies. CD spectra were generated using the program SpecDis,[3] using dipole-length rotational strengths; the difference with dipole-velocity values was negligible in all cases. The plotting parameters for Figure 5 in the main text are the following: compound **1**, CAM-B3LYP/def2-TZVP, exponential bandwidth 0.35 eV, no wavelength shift, scaling factor 5; compound 2, B3LYP/def2-TZVP, exponential bandwidth 0.3 eV, wavelength shift –10 nm, scaling factor 3.



trunc-**1** trunc-**2**

Chart: truncated models of **1** and **2** used in ECD calculations. C-C bonds were cut at the atoms indicated by dots, and replaced (capped) by C-H bonds.

References

1) Frisch, M. J.; Trucks G.W.; Schlegel H. B.; et al. Gaussian 16, Revision A.03. Wallingford CT: Gaussian, Inc.; 2016.

2) Hehre, W.; Klunzinger, P.; Deppmeier, B.; Driessen, A.; Uchida, N.; Hashimoto, M.; Fukushi, E.; Takata, Y.; *J. Nat. Prod.* **2019**, *82*, 2299−2306

3) Bruhn, T.; Schaumlöffel, A.; Hemberger, Y.; Pescitelli, G. SpecDis Version 1.70; 2017. Berlin, Germany https://specdis-software.jimdo.com/.

S1. Computed NMR data

	Compound **1**, ^{13}C δ(ppm)			Compound **2**, ^{13}C δ(ppm)		
Carbon	Exp.	Calc.	Diff. Δ	Exp.	Calc.	Diff. Δ
1	32.9	31.7	-1.2	54.3	53.7	-0.6
2	29.4	31.0	1.6	31.3	34.0	2.7
3	173.4	176.5	3.1	171.6	173.2	1.6
4	57.5	55.8	-1.7	56.3	56.6	0.3
5	47.5	46.4	-1.1	42.5	43.0	0.5
6	37.3	38.1	0.8	36.9	37.9	1.0
7	198.5	203.3	4.8	198.7	199.8	1.1
8	154.7	157.6	2.9	133.0	133.7	0.7
9	148.5	147.9	-0.6	162.0	166.9	4.9
10	40.0	42.0	2.0	52.6	52.3	-0.3
11	203.3	209.4	6.1	81.7	80.8	-0.9
12	79.8	82.0	2.2	34.4	35.3	0.9
13	63.2	63.4	0.2	52.8	54.3	1.5
14	45.7	47.0	1.3	47.1	48.3	1.2
15	37.0	36.9	-0.1	30.5	31.4	0.9
16	21.3	22.6	1.3	25.6	27.2	1.6
17	44.6	45.2	0.6	51.7	53.0	1.3
18	75.2	75.3	0.1	64.8	66.5	1.7
19	21.3	20.9	-0.4	17.9	17.9	0.0
20	84.5	84.5	0.0	87.4	88.9	1.5
21	21.5	22.1	0.6	32.7	32.6	-0.1
22	42.0	42.0	0.0	34.6	36.2	1.6
23	46.0	46.0	0.0	33.8	36.1	2.3
24	218.4	222.3	3.9	111.3	112.2	0.9
25	37.4	37.4	0.0	31.0	33.1	2.1
26	7.5	8.4	0.9	8.6	9.5	0.9
28	57.4	53.2	-4.2	47.8	48.3	0.5
29	21.2	21.7	0.5	22.2	23.1	0.9
30	31.2	32.8	1.6	26.9	27.4	0.5
31	51.9	52.7	0.8	51.6	53.0	1.4
rmsd			2.1			1.5

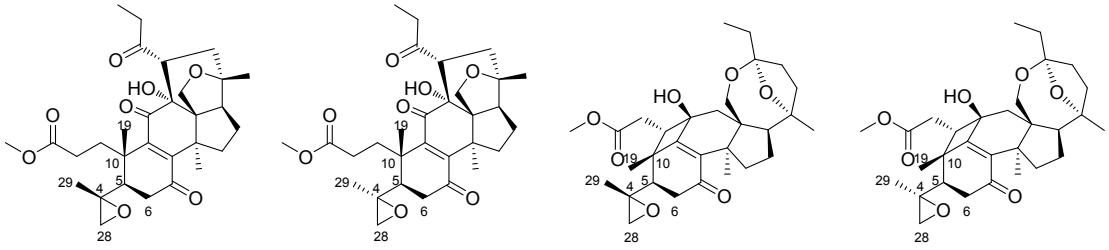
Table S1. ^{13}C chemical shifts computed for compounds **1** and **2** by the procedure explained in the Computational Section. The root-mean-square deviation (rmsd) is given by the formula $[(\Sigma\Delta^2)/n)]^{0.5}$ where Δ is the difference between calculated and experimental chemical shift, *n* the number of data employed, and Σ indicates the summation of Δ^2 values over *n* data.

	Compound 4-*epi*-**1**, ^{13}C δ(ppm)			Compound 4-*epi*-**2**, ^{13}C δ(ppm)		
Carbon	Exp.	Calc.	Diff. Δ	Exp.	Calc.	Diff. Δ
1	32.9	36.00	3.10	54.3	53.80	-0.50
2	29.4	30.50	1.10	31.3	33.80	2.50
3	173.4	175.60	2.20	171.6	137.20	-34.40
4	57.5	**53.30**	-4.20	56.3	**55.80**	-0.50
5	47.5	**50.40**	2.90	42.5	**45.10**	2.60
6	37.3	38.70	1.40	36.9	38.20	1.30
7	198.5	201.10	2.60	198.7	199.30	0.60
8	154.7	158.10	3.40	133.0	133.60	0.60
9	148.5	145.20	-3.30	162.0	166.50	4.50
10	40.0	40.40	0.40	52.6	52.90	0.30
11	203.3	210.50	7.20	81.7	81.10	-0.60
12	79.8	81.40	1.60	34.4	35.20	0.80
13	63.2	63.00	-0.20	52.8	54.20	1.40
14	45.7	46.60	0.90	47.1	48.30	1.20
15	37.0	38.10	1.10	30.5	31.40	0.90
16	21.3	22.90	1.60	25.6	27.20	1.60
17	44.6	44.60	0.00	51.7	53.00	1.30
18	75.2	77.00	1.80	64.8	66.50	1.70
19	21.3	**24.10**	2.80	17.9	**19.40**	1.50
20	84.5	84.60	0.10	87.4	88.80	1.40
21	21.5	22.10	0.60	32.7	32.60	-0.10
22	42.0	42.20	0.20	34.6	36.10	1.50
23	46.0	46.50	0.50	33.8	36.10	2.30
24	218.4	221.50	3.10	111.3	112.20	0.90
25	37.4	37.80	0.40	31.0	33.10	2.10
26	7.5	8.40	0.90	8.6	9.60	1.00
28	57.4	**53.30**	-4.10	47.8	**54.50**	6.70
29	21.2	**22.60**	1.40	22.2	**21.50**	-0.70
30	31.2	30.30	-0.90	26.9	27.40	0.50
31	51.9	57.90	6.00	51.6	52.70	1.10
rmsd			2.7			6.6

Table S2. ^{13}C chemical shifts computed for compounds 4-*epi*-**1** and 4-*epi*-**2**. For details see caption to Table S1. The values in bold are expected to be sensitive to the configuration at C-4.

Discussion about the relative configuration at C-4

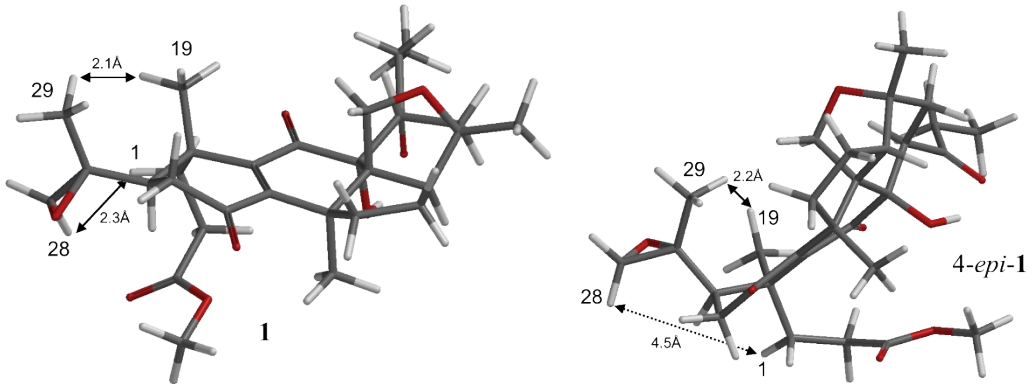
To assign the relative configuration at C-4 of compounds **1** and **2**, molecular modelling and NMR calculations data for compounds **1** (with 4*S* configuration), 4-*epi*-**1** (4*R*), **2** (4*S* configuration), and 4-*epi*-**2** (4*R*) were considered.



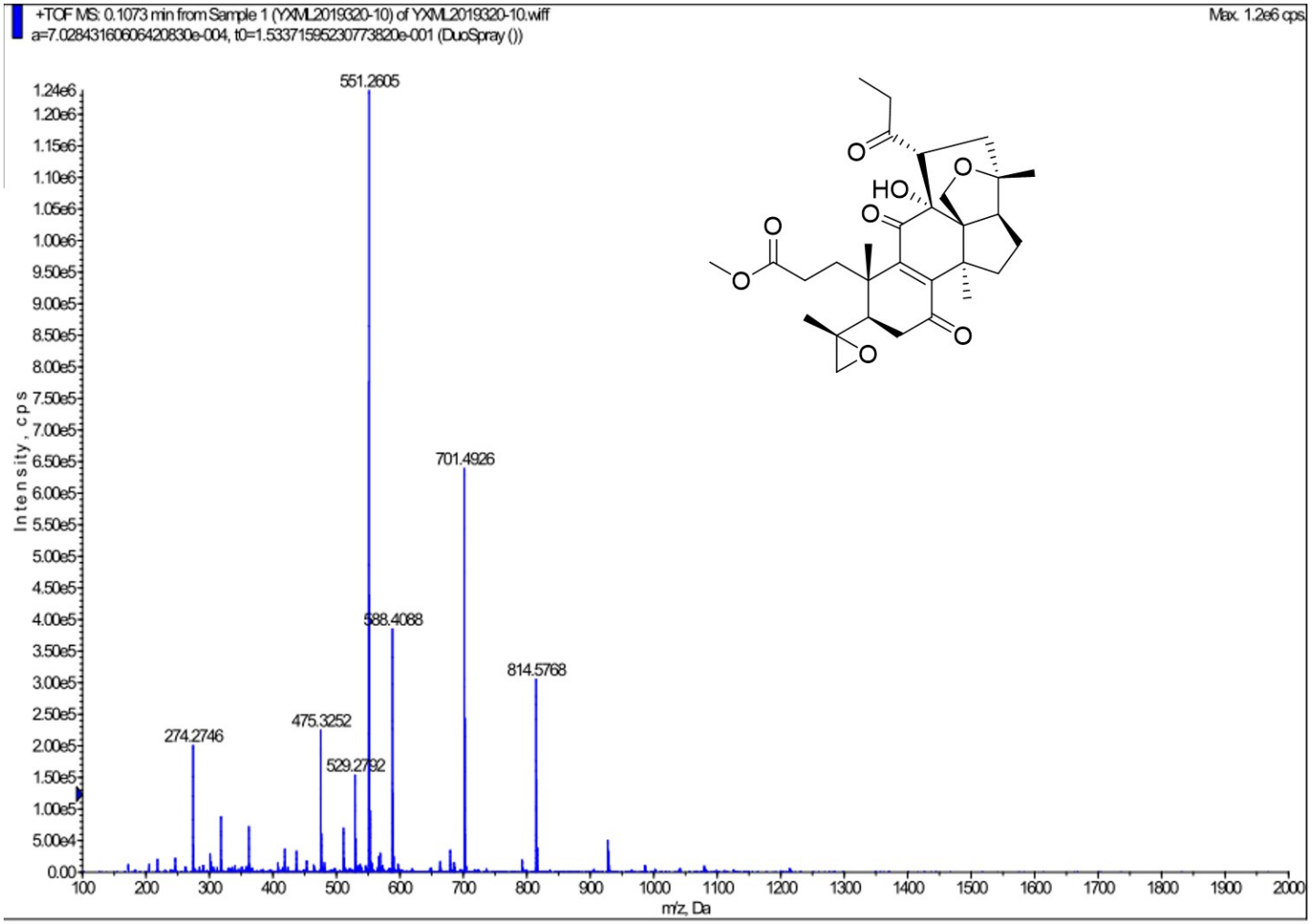
1 4-*epi*-**1** **2** 4-*epi*-**2**

Tables S1 and S2 show the comparison between experimental and calculated ^{13}C chemical shifts, using the procedure outlined in the Computational Section. The overall rms deviation is 2.1 ppm for **1** and 2.7 ppm for 4-*epi*-**1**. If we restrict the analysis to the signals more affected by configuration at C-4, namely those of C-4, C-5, C-19, C-28 and C-29, the rms deviation is similarly 2.1 ppm for **1** and 2.7 ppm for 4-*epi*-**1**. The situation is even more clear-cut for compound **2**. The overall rms deviation is 1.5 ppm for **2** and 6.6 ppm for 4-*epi*-**2**; for the restricted analysis, the rms deviation is 0.53 ppm for **2** and 3.3 ppm for 4-*epi*-**2**.

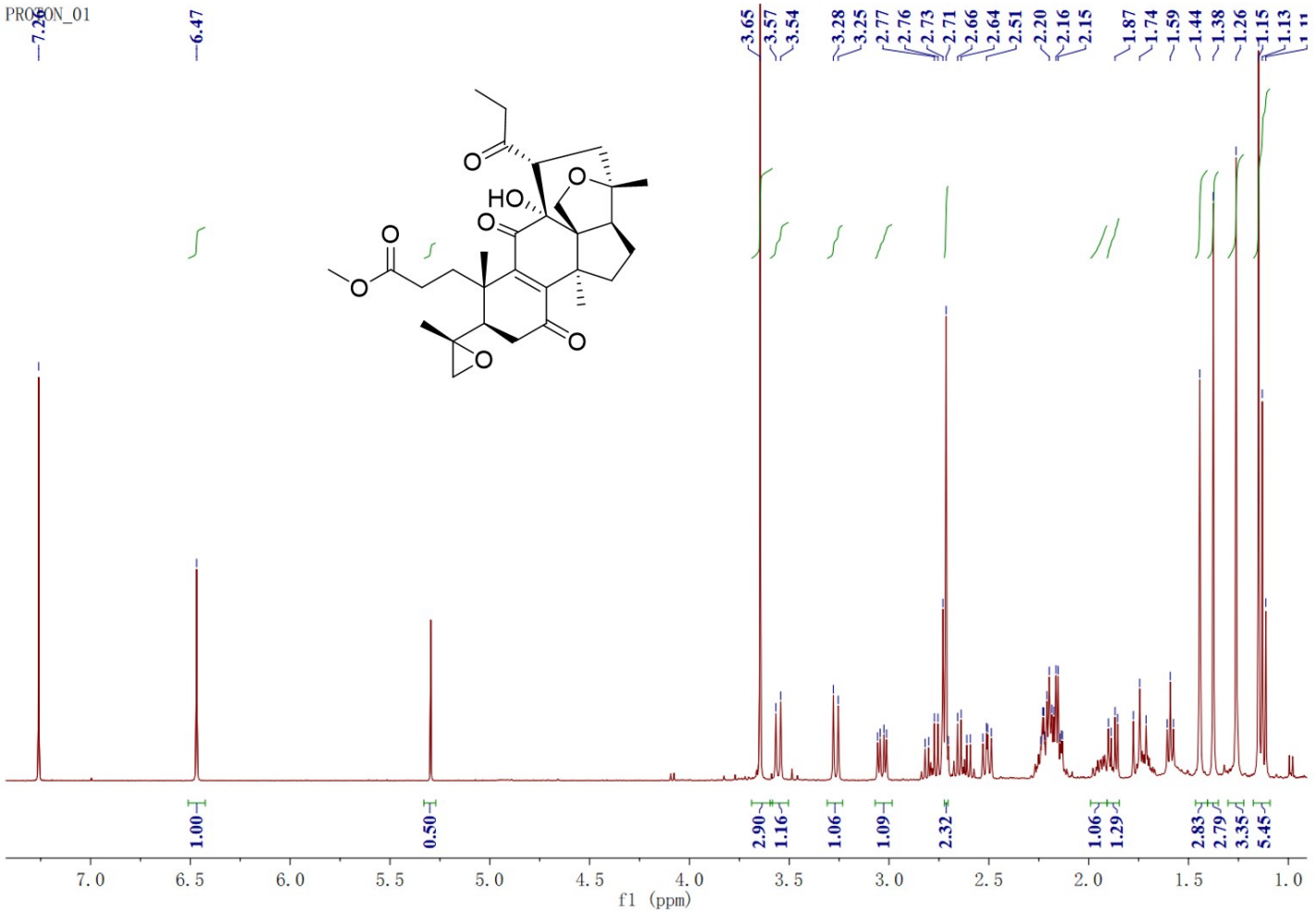
Further evidence in favor of the established assignment for **1** comes from analysis of NOE data helped by molecular modeling results. Although there is apparent free rotation around the C-4/C-5 bond, DFT-optimized geometries show a large preference for structures with the C-4/C-29 bond bisecting the C-6/C-5/C-10 angle, i.e. anti to the C-5H bond. Such preferential arrangement is found for an overall population of 72% at 300K, estimated using ωB97X-V/6-311+G(2df,2p) energies. It is in good agreement with the observed strong NOE correlation between Me-29 and Me-19, and between H-28 and H-1. The structure for the lowest-energy minimum (44% population) is shown below. Compound 4-*epi*-**1** showed even a stronger preference for a similar arrangement around the C-4/C-5 bond, with an overall population of 82% at 300K. In this case, however, H-28 would point far away from H-1 and make the observation of a NOE effect unfeasible (see lowest-energy minimum below, 40% population).



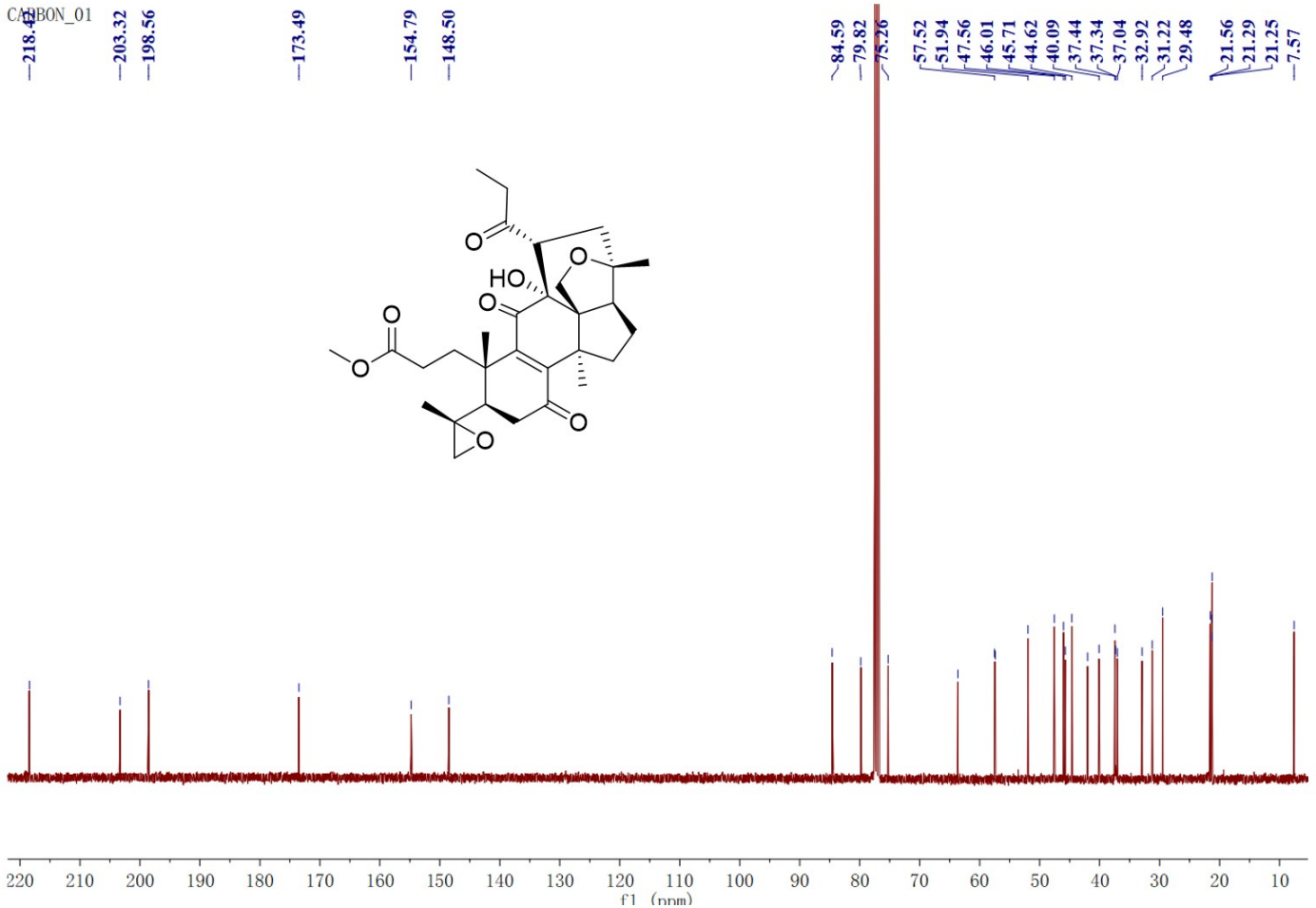
S2. HRESIMS of ganorbifate A (1)



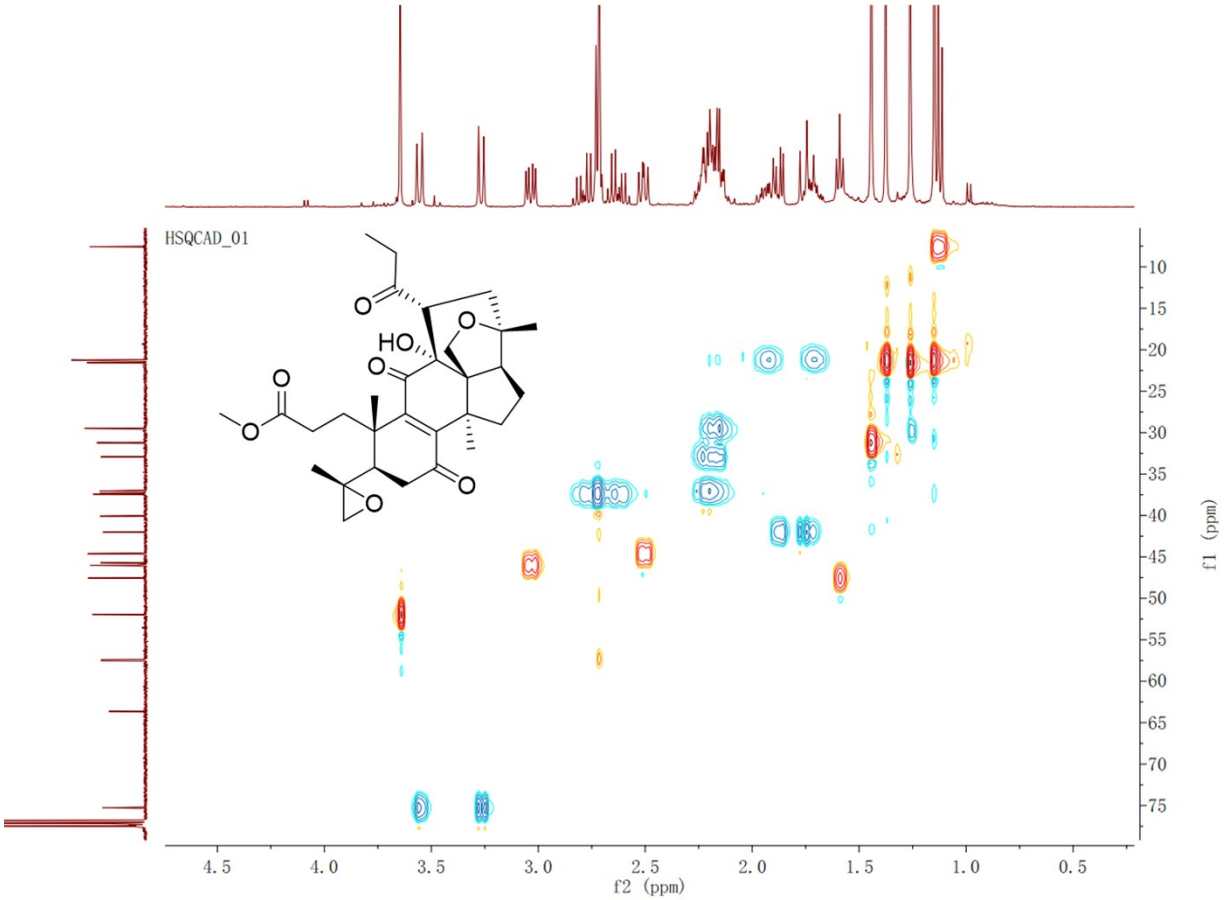
S3. ^{1}H NMR spectrum (500 MHz) of ganorbifate A (1) in $CDCl_3$.



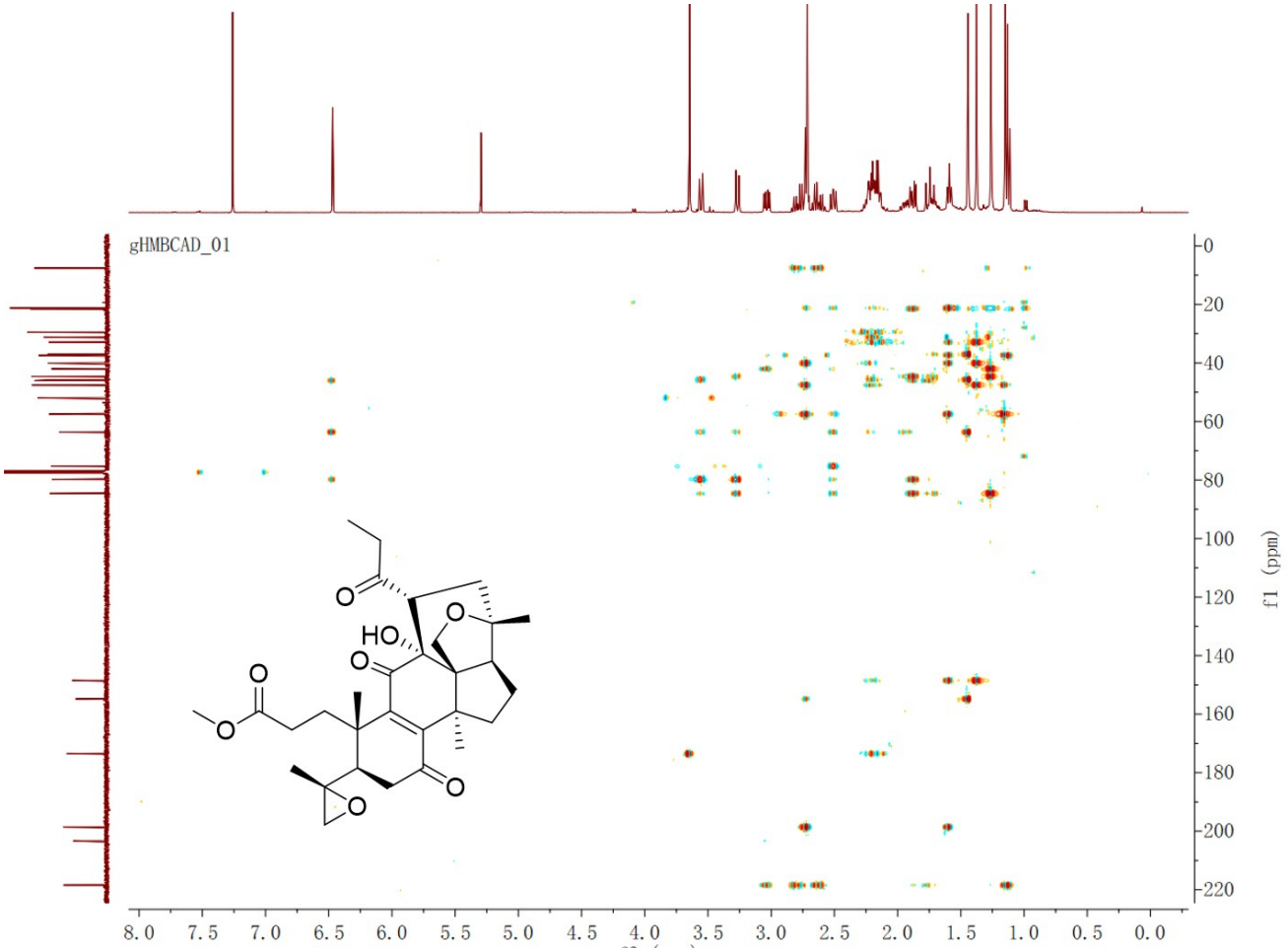
S4. ^{13}C NMR spectrum (125 MHz) of ganorbifate A (1) in $CDCl_3$.



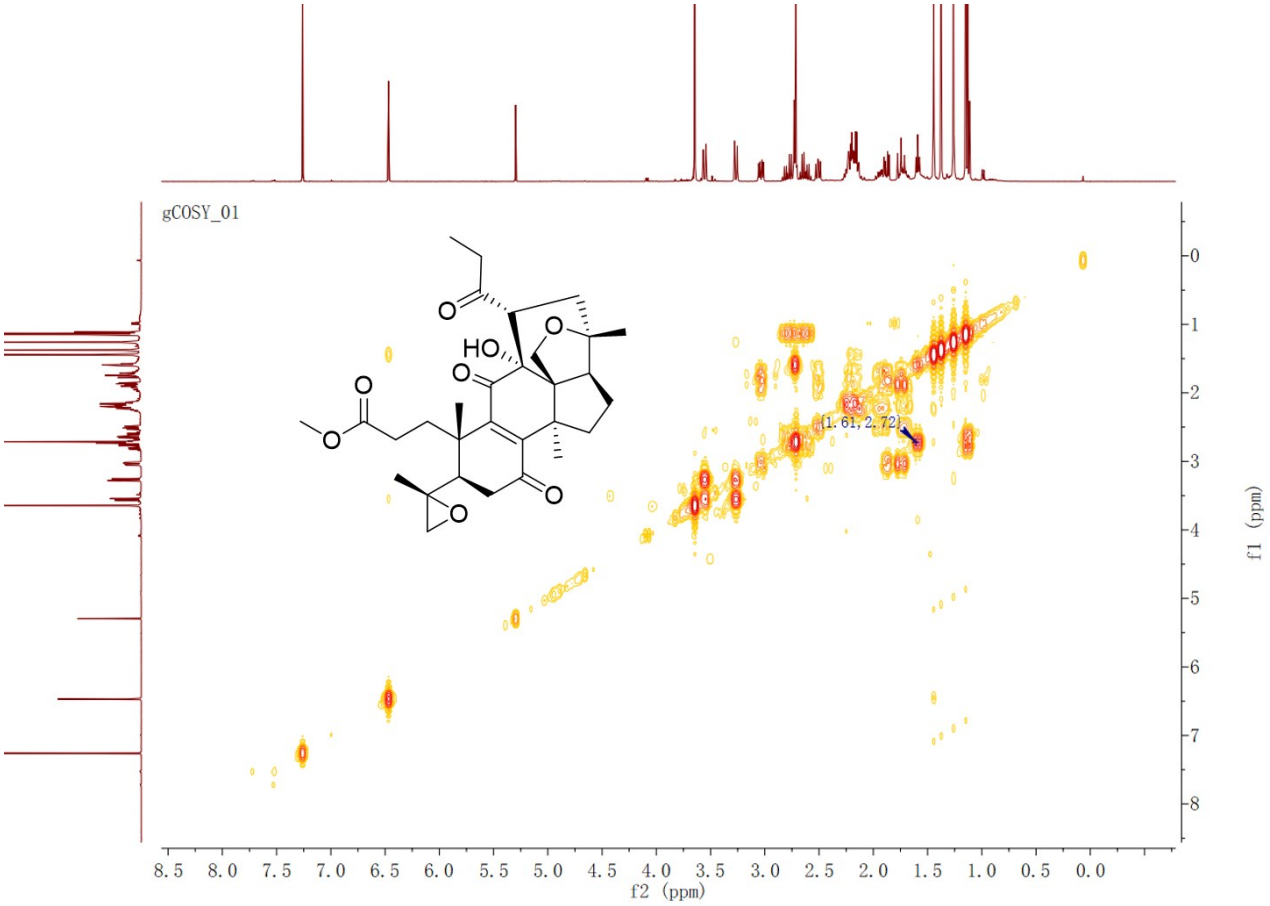
S5. HSQC spectrum (500 MHz) of ganorbifate A (1) in $CDCl_3$.



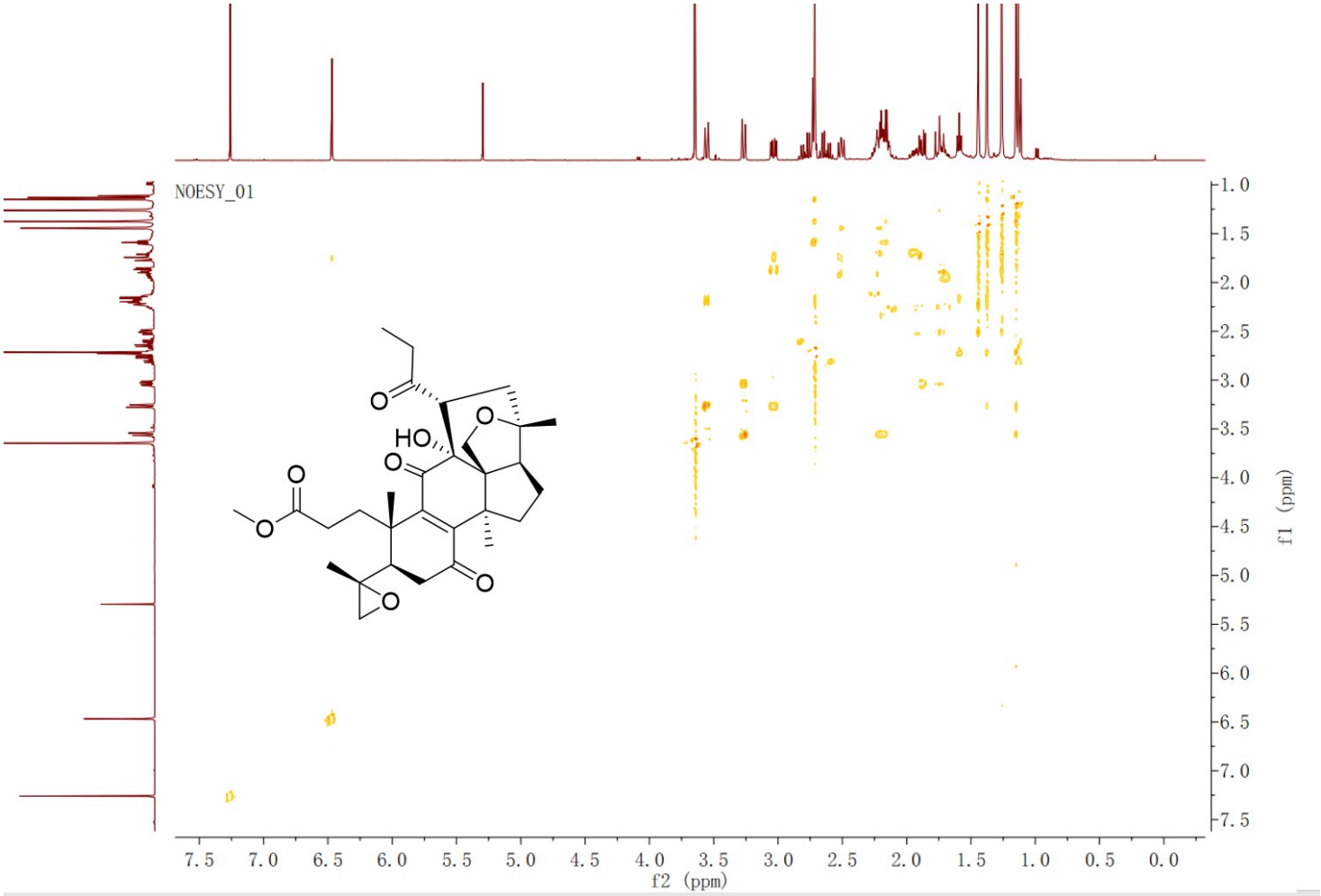
S6. HMBC spectrum (500 MHz) of ganorbifate A (1) in $CDCl_3$.



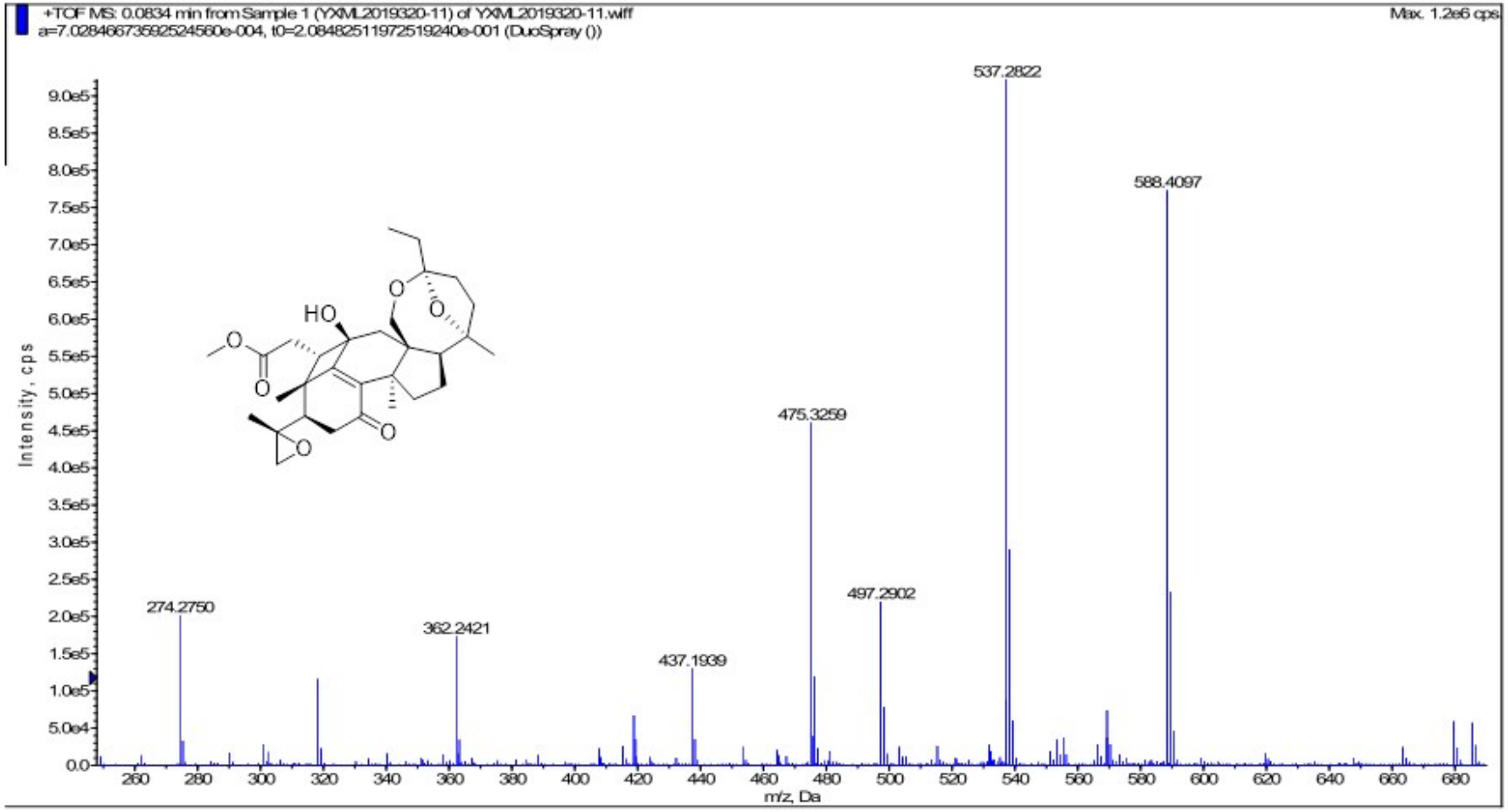
S7. ^{1}H–^{1}H COSY spectrum (500 MHz) of ganorbifate A (1) in $CDCl_3$.



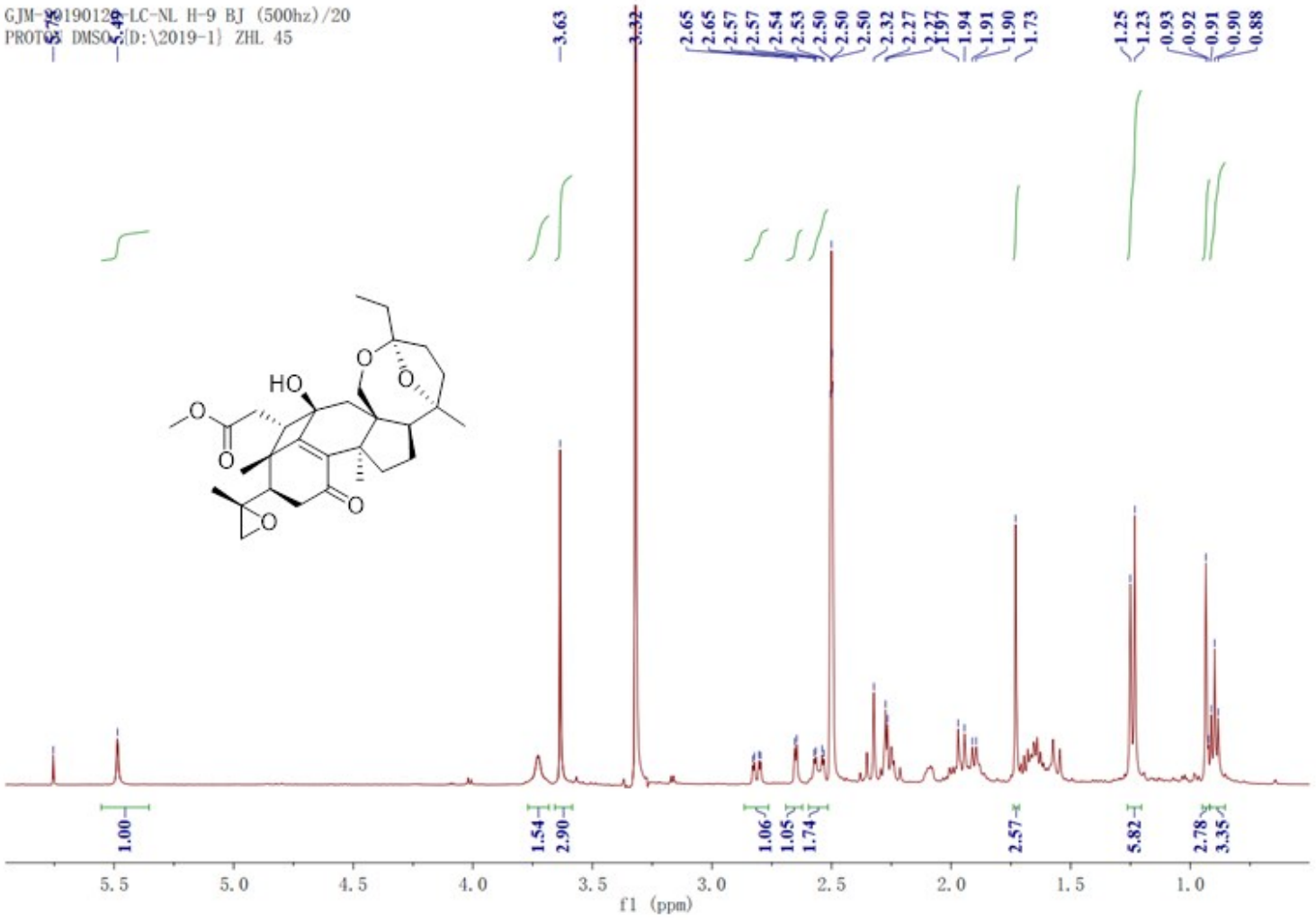
S8. NOESY spectrum (500 MHz) of ganorbifate A (1) in $CDCl_3$



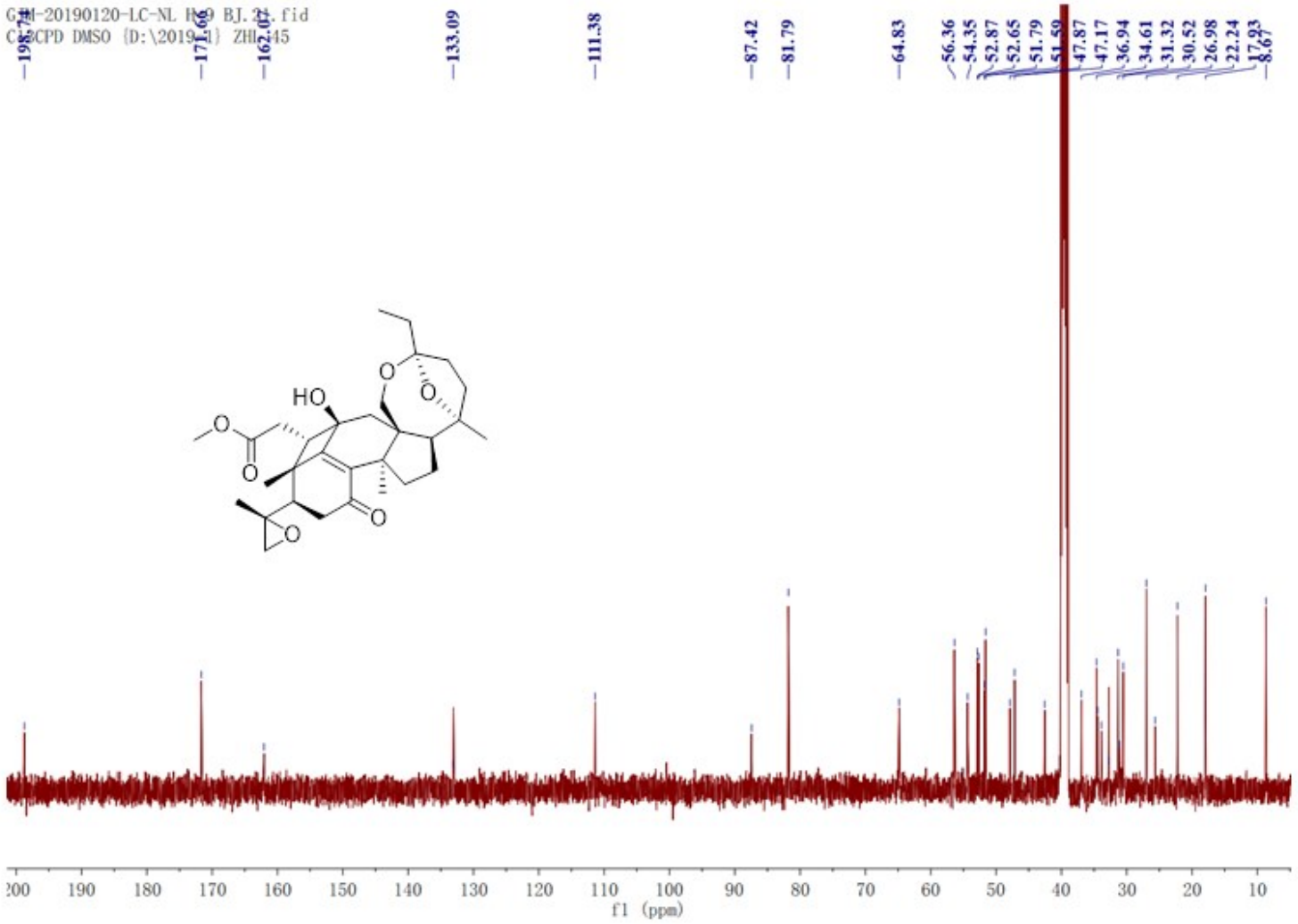
S9. HRESIMS of ganorbifate B (2)



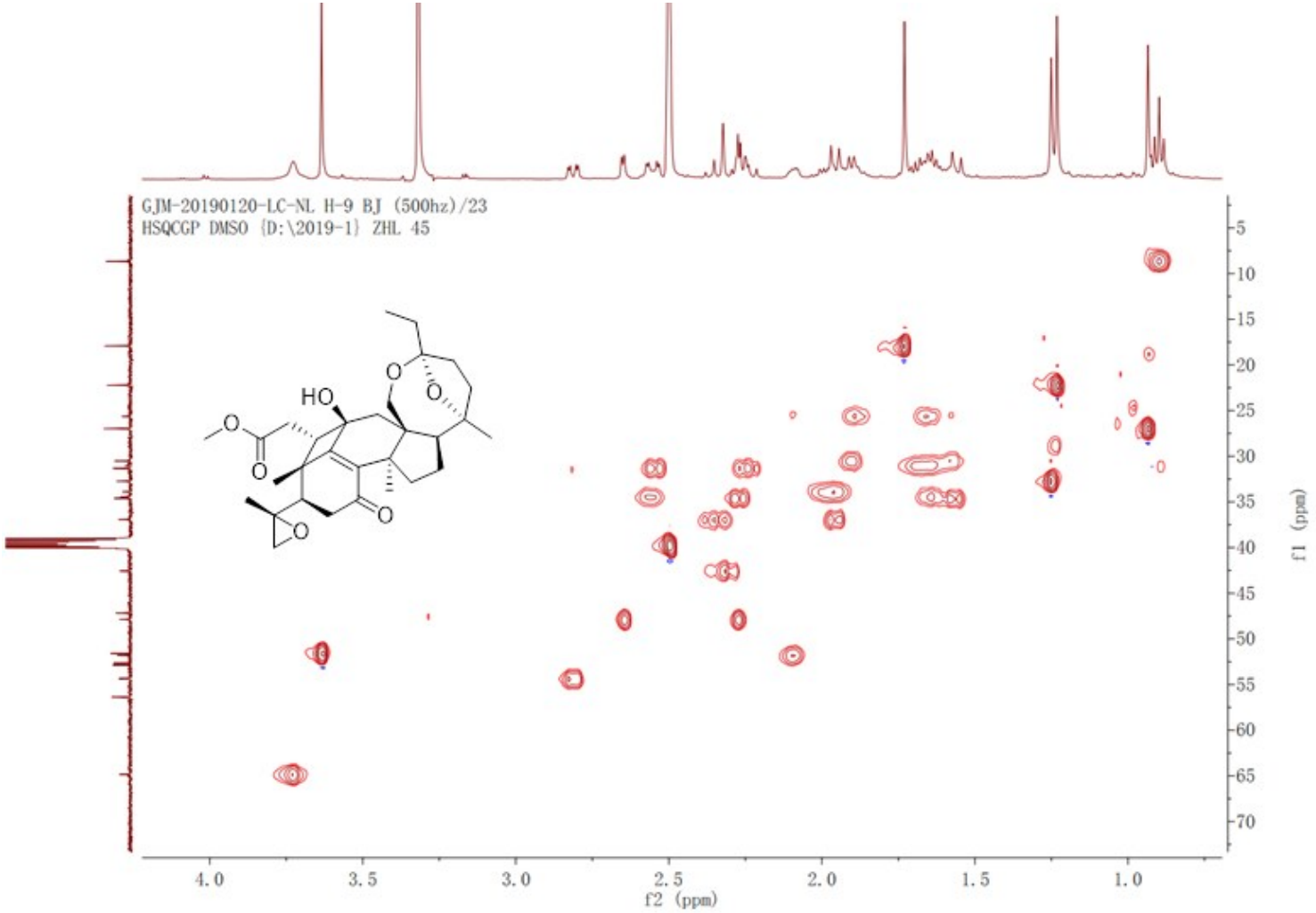
S10. ^{1}H NMR spectrum (500 MHz) of ganorbifate B (2) in $CDCl_3$



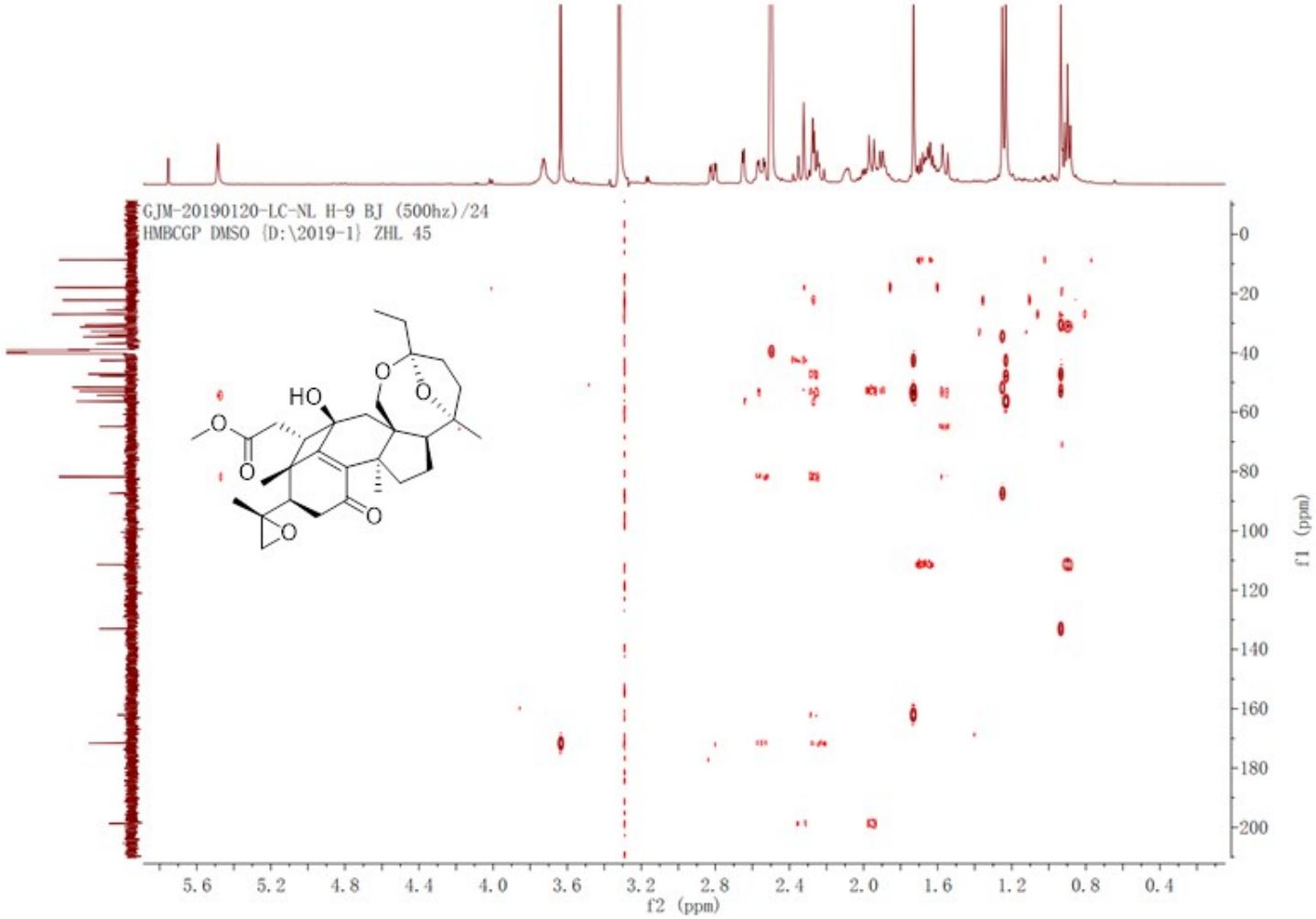
S11. ^{13}C NMR spectrum (125 MHz) of ganorbifate B (2) in $CDCl_3$



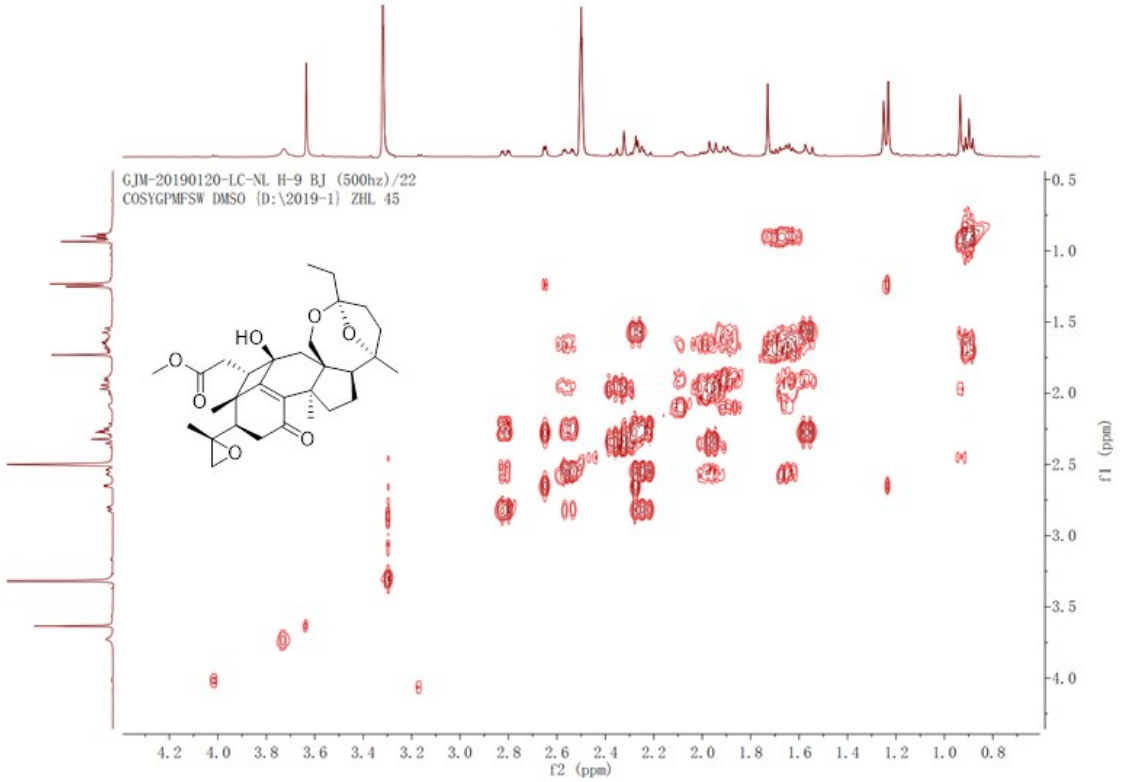
S12. HSQC spectrum (500 MHz) of ganorbifate B (2) in $CDCl_3$.



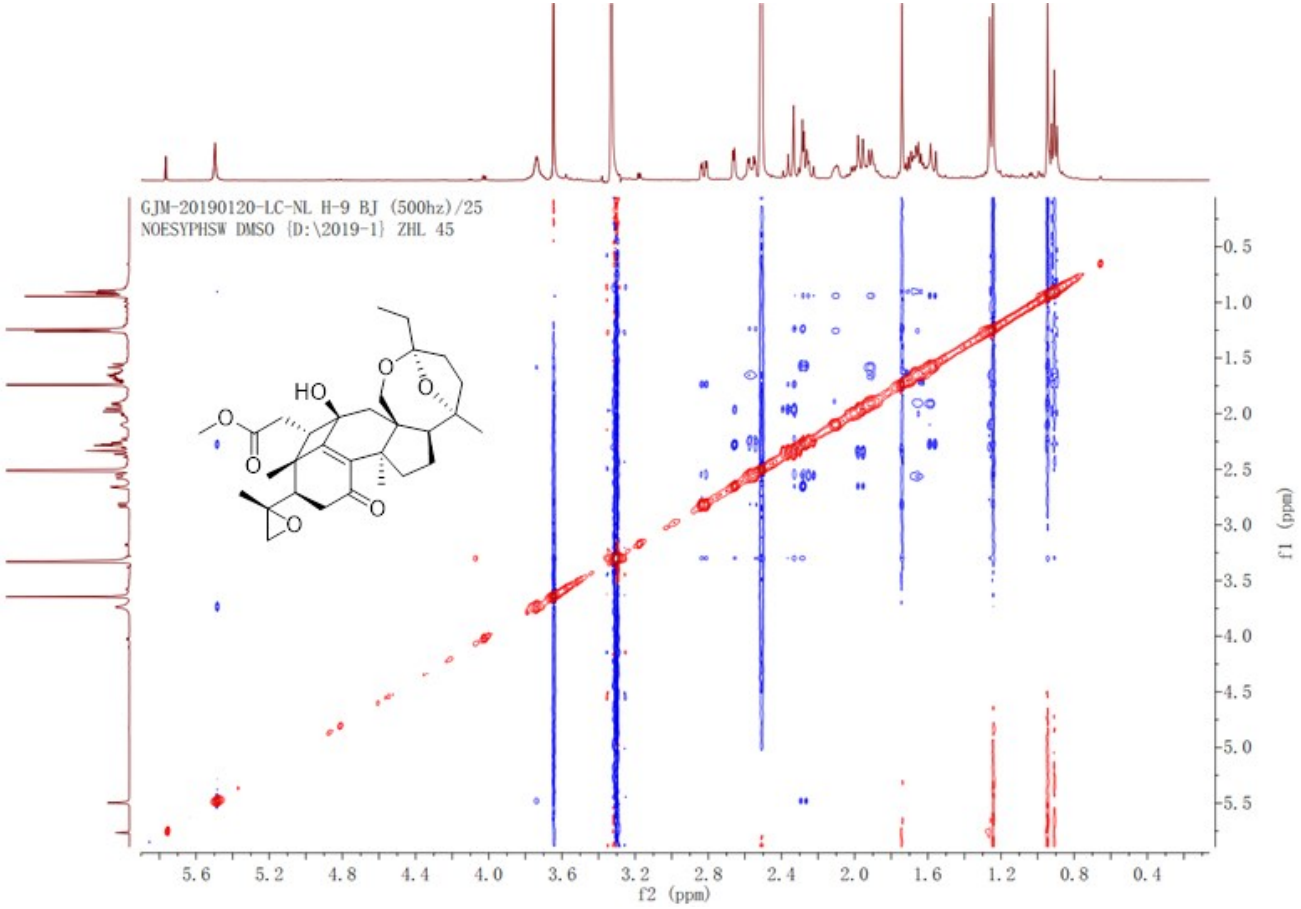
S13. HMBC spectrum (500 MHz) of ganorbifate B (2) in $CDCl_3$.



S14. ^{1}H–^{1}H COSY spectrum (500 MHz) of ganorbifate B (2) in $CDCl_3$.

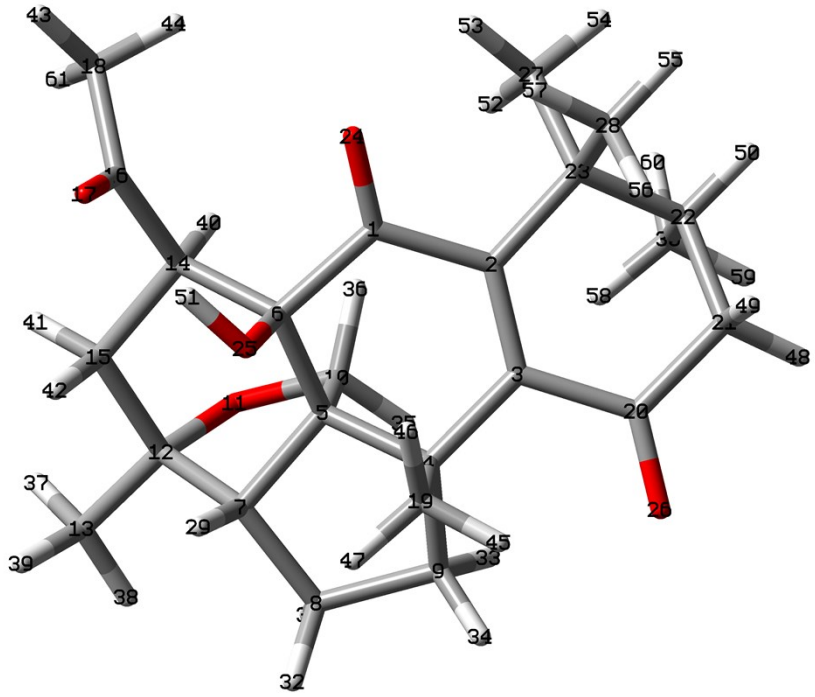


S15. NOESY spectrum (500 MHz) of ganorbifate B (2) in $CDCl_3$.



S16. Structures and coordinates for trunc-1 used for ECD calculations

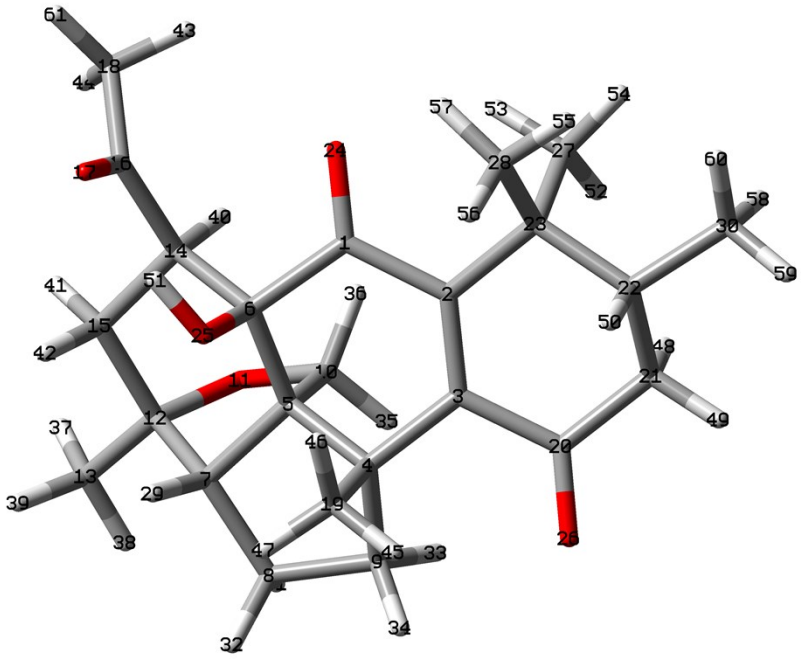
Conformer 1, DFT energy -1309.58409 au (ωB97X-V/6-311+G(2df,2p))



Tag	Symbol	X	Y	Z
1	C	-0.23091	1.337718	-0.46029
2	C	-1.53919	0.619209	-0.19284
3	C	-1.63625	-0.72099	-0.4142
4	C	-0.42366	-1.54672	-0.80008
5	C	0.784283	-0.88595	-0.13055
6	C	1.073492	0.522191	-0.61337
7	C	1.947676	-1.84548	-0.2791
8	C	1.262751	-3.21908	-0.06291
9	C	-0.27414	-3.00782	-0.27293
10	C	0.665189	-0.8619	1.424603
11	O	1.973062	-1.09808	1.928806
12	C	2.862372	-1.28721	0.817727
13	C	4.005011	-2.17904	1.261942
14	C	2.219949	1.128962	0.244912
15	C	3.375419	0.105595	0.361857
16	C	2.733276	2.452498	-0.30759
17	O	3.063593	2.568342	-1.47648
18	C	2.844612	3.597384	0.661139
19	C	-0.3709	-1.61755	-2.34388
20	C	-2.97227	-1.3996	-0.42373
21	C	-4.18174	-0.562	-0.09085

22	C	-3.83567	0.57372	0.870283
23	C	-2.72144	1.479101	0.271226
24	O	-0.17997	2.547073	-0.59771
25	O	1.430475	0.490982	-1.97393
26	O	-3.07401	-2.56716	-0.75009
27	C	-2.28545	2.490769	1.353091
28	C	-3.27501	2.272464	-0.93213
29	H	2.415366	-1.77069	-1.26318
30	C	-3.50327	-0.00132	2.255252
31	H	1.454678	-3.59165	0.948143
32	H	1.658068	-3.96493	-0.75717
33	H	-0.82341	-3.16795	0.657745
34	H	-0.68992	-3.71684	-0.98905
35	H	-0.00949	-1.63738	1.799851
36	H	0.288081	0.092731	1.811462
37	H	4.513621	-1.74201	2.126934
38	H	3.636841	-3.16889	1.544847
39	H	4.733587	-2.29426	0.452841
40	H	1.8488	1.317726	1.254835
41	H	4.105285	0.47568	1.091661
42	H	3.887205	0.015745	-0.60265
43	H	3.354946	4.44254	0.197397
44	H	1.829257	3.894677	0.948515
45	H	-1.23656	-2.19247	-2.68653
46	H	-0.38188	-0.63204	-2.80812
47	H	0.53544	-2.13209	-2.67775
48	H	-4.95207	-1.22462	0.314437
49	H	-4.57273	-0.17237	-1.03932
50	H	-4.72423	1.208648	0.982429
51	H	1.99201	1.271396	-2.14535
52	H	-1.68207	2.017941	2.135356
53	H	-1.7055	3.305612	0.922174
54	H	-3.17733	2.914603	1.82927
55	H	-4.13222	2.878999	-0.61728
56	H	-3.59936	1.616906	-1.74598
57	H	-2.50625	2.940039	-1.32671
58	H	-2.56175	-0.56309	2.250866
59	H	-4.29483	-0.68746	2.574107
60	H	-3.42124	0.780696	3.013797
61	H	3.367635	3.285783	1.571986

Conformer 2, DFT energy -1309.57979 au (ωB97X-V/6-311+G(2df,2p))

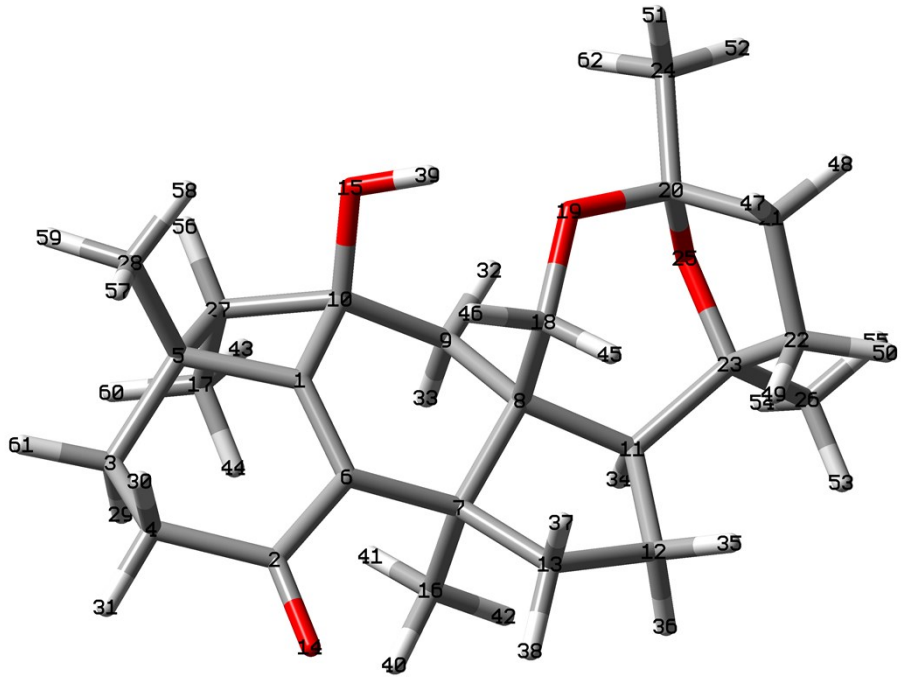


Tag	Symbol	X	Y	Z
1	C	0.301292	1.254024	0.11264
2	C	1.565908	0.411737	0.050477
3	C	1.488005	-0.94216	0.181614
4	C	0.215684	-1.63857	0.623932
5	C	-0.96803	-0.85098	0.062936
6	C	-1.03594	0.594666	0.5169
7	C	-2.20599	-1.67471	0.364761
8	C	-1.7008	-3.11885	0.10723
9	C	-0.13631	-3.07273	0.127851
10	C	-1.0254	-0.86352	-1.49532
11	O	-2.40388	-0.94691	-1.84029
12	C	-3.17548	-1.03502	-0.63306
13	C	-4.44735	-1.80494	-0.93023
14	C	-2.22352	1.296351	-0.19523
15	C	-3.48611	0.404356	-0.14053
16	C	-2.52316	2.68319	0.352687
17	O	-2.52782	2.918465	1.550857
18	C	-2.84642	3.748863	-0.65852
19	C	0.286462	-1.71994	2.17039
20	C	2.706314	-1.79585	0.012085
21	C	3.883513	-1.13729	-0.6444
22	C	4.110891	0.235977	-0.01139
23	C	2.88195	1.17453	-0.20329
24	O	0.298309	2.437932	-0.17816

25	O	-1.1674	0.654546	1.917963
26	O	2.724533	-2.95235	0.387585
27	C	2.864045	1.762385	-1.62958
28	C	3.012058	2.310881	0.835731
29	H	-2.5479	-1.53717	1.393066
30	C	5.437085	0.811774	-0.51647
31	H	-2.0527	-3.48422	-0.86238
32	H	-2.08558	-3.80611	0.864808
33	H	0.277153	-3.28431	-0.8612
34	H	0.284976	-3.82448	0.795008
35	H	-0.49838	-1.71921	-1.92555
36	H	-0.58701	0.036049	-1.94495
37	H	-5.00752	-1.31754	-1.73443
38	H	-4.2177	-2.82679	-1.24376
39	H	-5.08299	-1.84622	-0.03968
40	H	-1.97261	1.423417	-1.2502
41	H	-4.26121	0.844111	-0.77942
42	H	-3.87951	0.368832	0.881798
43	H	-1.92109	3.993736	-1.19228
44	H	-3.56542	3.379148	-1.39782
45	H	1.113979	-2.38557	2.432771
46	H	0.440458	-0.74612	2.630918
47	H	-0.63595	-2.14436	2.579051
48	H	3.683636	-1.03222	-1.72
49	H	4.754578	-1.78808	-0.53056
50	H	4.210669	0.077801	1.072844
51	H	-1.58962	1.512419	2.124084
52	H	2.879176	0.974186	-2.39117
53	H	1.972717	2.371072	-1.78247
54	H	3.736259	2.40399	-1.78838
55	H	4.006777	2.762182	0.778032
56	H	2.880874	1.918908	1.850858
57	H	2.276567	3.096388	0.670833
58	H	5.464325	0.849562	-1.61067
59	H	6.26259	0.171982	-0.18808
60	H	5.631286	1.819255	-0.13819
61	H	-3.23307	4.640929	-0.16388

S17. Structures and coordinates for trunc-2 used for ECD calculations

Conformer 1, DFT energy -1235.55923 au (ωB97X-V/6-311+G(2df,2p))

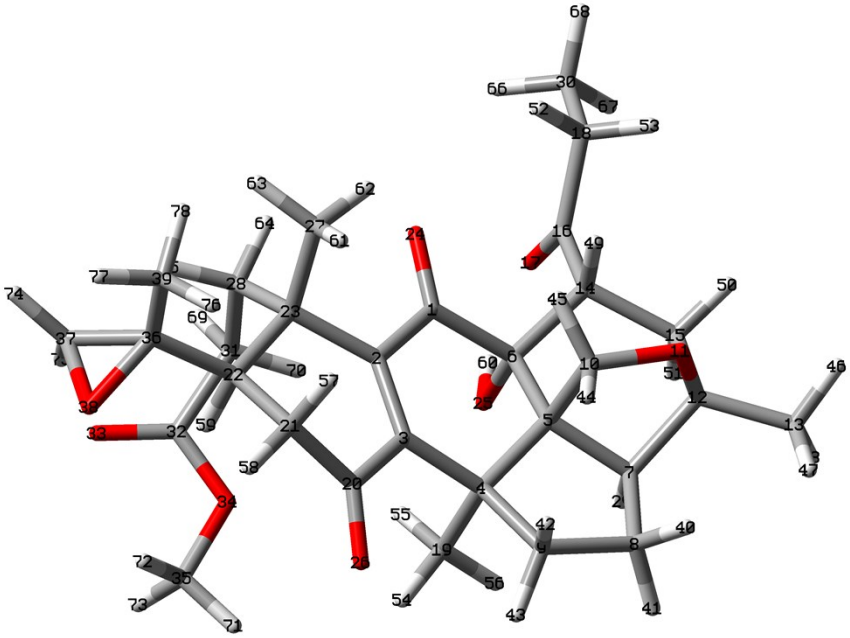


Tag	Symbol	X	Y	Z
1	C	-1.92831	-0.43811	-0.33029
2	C	-2.93212	1.685781	-0.87444
3	C	-4.36169	-0.17455	0.12431
4	C	-4.26384	0.935934	-0.93515
5	C	-3.21751	-1.17357	-0.08724
6	C	-1.75023	0.883256	-0.48553
7	C	-0.48462	1.516936	0.060139
8	C	0.627973	0.42702	0.230113
9	C	0.107371	-0.69819	1.161823
10	C	-1.06899	-1.40473	0.464173
11	C	1.827858	1.277388	0.72774
12	C	1.622905	2.675607	0.055964
13	C	0.270381	2.618771	-0.70164
14	O	-2.86616	2.878592	-1.11986
15	O	-0.64644	-2.55684	-0.24071
16	C	-0.92394	2.151613	1.410417
17	C	-2.71786	-1.23657	2.52158
18	C	0.996788	-0.1726	-1.15734
19	O	1.697237	-1.40893	-1.07378
20	C	3.026168	-1.41045	-0.55947
21	C	3.971396	-0.59251	-1.44911
22	C	3.913495	0.818911	-0.85079

23	C	3.235259	0.636416	0.542633
24	C	3.382414	-2.87434	-0.39952
25	O	3.110551	-0.78948	0.695084
26	C	4.159375	1.108251	1.659876
27	C	-2.43249	-1.80684	1.145958
28	C	-3.58958	-2.24062	-1.11981
29	H	-4.29152	0.285565	1.116777
30	H	-4.36527	0.509136	-1.94236
31	H	-5.05819	1.678876	-0.82419
32	H	0.892555	-1.41901	1.393745
33	H	-0.20441	-0.25675	2.112514
34	H	1.707093	1.390847	1.810967
35	H	2.442563	2.949975	-0.61165
36	H	1.594097	3.456985	0.820827
37	H	0.408804	2.35499	-1.75513
38	H	-0.26558	3.569479	-0.68444
39	H	0.245763	-2.38517	-0.59072
40	H	-1.64228	2.94762	1.195743
41	H	-1.41407	1.432167	2.068102
42	H	-0.09413	2.597474	1.964279
43	H	-2.0201	-1.65034	3.257254
44	H	-2.62535	-0.14631	2.551115
45	H	1.570915	0.538449	-1.75683
46	H	0.103436	-0.40873	-1.73605
47	H	3.668181	-0.6399	-2.49781
48	H	4.978505	-1.01136	-1.3696
49	H	3.366352	1.499907	-1.50255
50	H	4.912947	1.244869	-0.72781
51	H	3.353631	-3.37648	-1.36998
52	H	4.382923	-2.9691	0.028508
53	H	4.256607	2.199482	1.637238
54	H	3.758925	0.815542	2.635215
55	H	5.153943	0.66532	1.547435
56	H	-2.5166	-2.898	1.16453
57	H	-3.95488	-1.78268	-2.04607
58	H	-2.72904	-2.86733	-1.36011
59	H	-4.38806	-2.8763	-0.71956
60	H	-3.73432	-1.48857	2.842166
61	H	-5.33875	-0.66837	0.068304
62	H	2.662555	-3.35595	0.267838

S18. Coordinates of 1 used for NMR calculations

All conformers with population > 5% at 300K are listed. The structure refers to the lowest energy conformer.



Conformer 1, DFT energy -1769.17077 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.108668	-1.00784	0.30335
2	C	0.160319	0.017273	-0.81383
3	C	0.167153	1.345732	-0.51845
4	C	-0.07862	1.868284	0.881795
5	C	0.48616	0.847324	1.868495
6	C	-0.11895	-0.53815	1.754177
7	C	0.385166	1.48712	3.240424
8	C	0.769311	2.959634	2.934349
9	C	0.613077	3.167509	1.390282
10	C	2.035621	0.693315	1.772901
11	O	2.498984	0.516192	3.106857
12	C	1.376782	0.600384	3.998034
13	C	1.864395	1.118548	5.336726
14	C	0.59478	-1.49057	2.751705
15	C	0.745504	-0.81177	4.133214
16	C	-0.0889	-2.84164	2.888478
17	O	-1.30111	-2.93949	3.006359
18	C	0.806371	-4.05547	2.897721

19	C	-1.60448	2.122252	0.991885
20	C	0.302095	2.359955	-1.61069
21	C	0.847651	1.839913	-2.90732
22	C	0.032223	0.599376	-3.28973
23	C	0.200698	-0.55041	-2.24841
24	O	0.243328	-2.2026	0.095203
25	O	-1.50863	-0.4865	1.985613
26	O	-0.02063	3.519825	-1.44249
27	C	1.540927	-1.29033	-2.45029
28	C	-0.9494	-1.58788	-2.43488
29	H	-0.62019	1.404817	3.659905
30	C	0.074549	-5.35701	3.191081
31	C	-2.32884	-1.24479	-1.83214
32	C	-3.02447	-0.10917	-2.54084
33	O	-3.57722	-0.2023	-3.61406
34	O	-2.92214	1.046077	-1.86593
35	C	-3.40817	2.207831	-2.5426
36	C	0.246041	0.297929	-4.77769
37	C	-0.89458	-0.15162	-5.59177
38	O	-0.51008	1.217657	-5.57917
39	C	1.643352	0.088066	-5.32592
40	H	1.80088	3.160722	3.238861
41	H	0.132229	3.650767	3.491657
42	H	1.582683	3.337642	0.915245
43	H	0.007104	4.042798	1.15686
44	H	2.518271	1.574577	1.342464
45	H	2.341881	-0.16401	1.160662
46	H	2.647574	0.465658	5.734144
47	H	2.277056	2.125678	5.235433
48	H	1.039307	1.148516	6.055608
49	H	1.604602	-1.68514	2.383936
50	H	1.387563	-1.43534	4.766876
51	H	-0.23104	-0.735	4.624948
52	H	1.286099	-4.08018	1.910035
53	H	1.618049	-3.87353	3.616046
54	H	-1.85074	2.955735	0.327985
55	H	-2.19721	1.255505	0.710591
56	H	-1.87346	2.407177	2.013904
57	H	1.910162	1.596718	-2.77559
58	H	0.759042	2.618028	-3.6688
59	H	-1.01137	0.91649	-3.24341
60	H	-1.77112	-1.36641	2.324364
61	H	2.378071	-0.59332	-2.56245
62	H	1.748614	-1.9493	-1.60731

63	H	1.493497	-1.91571	-3.3464
64	H	-0.63665	-2.52988	-1.98497
65	H	-1.06726	-1.77358	-3.5069
66	H	-0.70904	-5.53333	2.449794
67	H	-0.40288	-5.32607	4.174644
68	H	0.770288	-6.20066	3.170096
69	H	-2.96717	-2.12497	-1.94865
70	H	-2.25349	-1.02258	-0.76461
71	H	-3.17603	3.044375	-1.88496
72	H	-2.89863	2.326298	-3.50363
73	H	-4.48391	2.130833	-2.71251
74	H	-0.69515	-0.67886	-6.52526
75	H	-1.85796	-0.36163	-5.132
76	H	2.339105	0.839308	-4.93882
77	H	1.611614	0.194378	-6.41304
78	H	2.042659	-0.89919	-5.08721

Conformer 2, DFT energy -1769.16991 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.109179	-1.03104	0.307021
2	C	0.223322	-0.03438	-0.83257
3	C	0.33455	1.296598	-0.56575
4	C	0.108729	1.864708	0.822028
5	C	0.579575	0.825952	1.83996
6	C	-0.11922	-0.5169	1.741687
7	C	0.495417	1.499052	3.196976
8	C	0.987516	2.934571	2.872132
9	C	0.882914	3.120601	1.321226
10	C	2.115408	0.561938	1.781586
11	O	2.536633	0.377885	3.128361
12	C	1.406106	0.561396	3.993504
13	C	1.903036	1.072741	5.331227
14	C	0.505839	-1.4941	2.773
15	C	0.673753	-0.79982	4.143918
16	C	-0.26839	-2.794	2.918156
17	O	-1.48774	-2.81254	2.988639
18	C	0.548221	-4.05918	3.00751
19	C	-1.39651	2.230031	0.897786
20	C	0.562039	2.279006	-1.67226
21	C	0.989006	1.698298	-2.99112
22	C	0.083755	0.502641	-3.2979
23	C	0.253318	-0.63724	-2.25177
24	O	0.203133	-2.23302	0.125065

25	O	-1.50583	-0.36172	1.942871
26	O	0.401715	3.473225	-1.50471
27	C	1.595584	-1.38547	-2.42032
28	C	-0.90995	-1.66014	-2.4461
29	H	-0.52186	1.494973	3.594878
30	C	-0.26926	-5.29752	3.34498
31	C	-2.28281	-1.3015	-1.8417
32	C	-2.95664	-0.14448	-2.53526
33	O	-3.41395	-0.17328	-3.65538
34	O	-2.95975	0.961559	-1.77035
35	C	-3.48753	2.13842	-2.3769
36	C	0.182303	0.162407	-4.79584
37	C	1.457906	-0.21392	-5.4193
38	O	0.433556	-1.18114	-5.20514
39	C	-0.85532	0.87393	-5.63511
40	H	2.022938	3.071203	3.198595
41	H	0.386612	3.679599	3.39955
42	H	1.872797	3.209321	0.86672
43	H	0.348727	4.032705	1.055504
44	H	2.667015	1.399593	1.346995
45	H	2.373856	-0.32616	1.191626
46	H	2.632086	0.37568	5.756504
47	H	2.386003	2.047069	5.219282
48	H	1.068781	1.173432	6.032966
49	H	1.508197	-1.76377	2.434041
50	H	1.257676	-1.45289	4.803706
51	H	-0.30481	-0.64386	4.61271
52	H	1.044355	-4.1611	2.032653
53	H	1.355508	-3.89389	3.734441
54	H	-1.56974	3.061716	0.208386
55	H	-2.04401	1.39961	0.627321
56	H	-1.66268	2.562602	1.905775
57	H	2.041114	1.390138	-2.93524
58	H	0.910133	2.477773	-3.75402
59	H	-0.93644	0.874953	-3.16133
60	H	-1.83742	-1.21755	2.28403
61	H	2.446986	-0.69578	-2.40424
62	H	1.728718	-2.10124	-1.60839
63	H	1.599289	-1.93599	-3.36236
64	H	-0.6102	-2.61207	-2.00822
65	H	-1.03136	-1.82867	-3.51914
66	H	-1.0474	-5.46169	2.59528
67	H	-0.76285	-5.18933	4.315159
68	H	0.372939	-6.18252	3.37977

69	H	-2.93453	-2.16924	-1.97835
70	H	-2.21967	-1.09594	-0.77082
71	H	-3.42582	2.913095	-1.61288
72	H	-2.88882	2.41877	-3.24906
73	H	-4.5215	1.9815	-2.69034
74	H	1.641066	0.043015	-6.4624
75	H	2.352253	-0.34258	-4.81052
76	H	-1.85709	0.540425	-5.34951
77	H	-0.70282	0.66508	-6.69695
78	H	-0.79766	1.958446	-5.48229

Conformer 3, DFT energy -1769.16907 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.547761	-0.5258	0.112808
2	C	0.598396	0.434531	-1.05186
3	C	0.66909	1.773048	-0.82043
4	C	0.322485	2.369181	0.532497
5	C	0.620725	1.34824	1.63745
6	C	-0.03069	-0.01436	1.440951
7	C	0.281092	2.055007	2.937791
8	C	0.839082	3.480731	2.67162
9	C	1.021897	3.628187	1.121454
10	C	2.142123	1.098519	1.884807
11	O	2.288644	0.93443	3.293562
12	C	1.014041	1.139202	3.919102
13	C	1.24278	1.689081	5.313569
14	C	0.36897	-0.95462	2.612803
15	C	0.252676	-0.21567	3.962204
16	C	-0.43648	-2.24416	2.596412
17	O	-1.6596	-2.20949	2.549406
18	C	0.317107	-3.54483	2.643439
19	C	-1.17667	2.763715	0.396475
20	C	0.914374	2.72493	-1.95246
21	C	0.923487	2.163366	-3.35325
22	C	0.10141	0.879324	-3.44158
23	C	0.628785	-0.19781	-2.45435
24	O	0.996355	-1.65375	0.02029
25	O	-1.42714	0.127004	1.315189
26	O	1.10794	3.906849	-1.7428
27	C	2.073012	-0.66353	-2.73731
28	C	-0.29522	-1.44567	-2.5169
29	H	-0.79292	2.065545	3.136388
30	C	-0.5767	-4.77092	2.527803

31	C	-1.69273	-1.26311	-1.90897
32	C	-2.11971	-2.42358	-1.029
33	O	-1.46344	-3.40741	-0.77831
34	O	-3.35047	-2.21248	-0.54431
35	C	-3.85635	-3.23542	0.319344
36	C	-0.09411	0.484707	-4.90486
37	C	-1.43972	0.110889	-5.3621
38	O	-0.94561	1.424291	-5.57437
39	C	1.085553	0.041678	-5.74362
40	H	1.79882	3.619665	3.178716
41	H	0.1592	4.242251	3.062236
42	H	2.075739	3.689989	0.844286
43	H	0.56073	4.54041	0.743362
44	H	2.764458	1.93432	1.558453
45	H	2.518218	0.203936	1.376349
46	H	1.873596	1.006719	5.891447
47	H	1.740778	2.661553	5.270166
48	H	0.288387	1.807157	5.83721
49	H	1.417116	-1.22704	2.488061
50	H	0.678638	-0.84774	4.74955
51	H	-0.79953	-0.0418	4.210722
52	H	1.045126	-3.50348	1.824684
53	H	0.909091	-3.54806	3.571263
54	H	-1.2496	3.562761	-0.347
55	H	-1.80525	1.929128	0.095341
56	H	-1.56579	3.156146	1.339713
57	H	1.969675	1.998828	-3.64229
58	H	0.526793	2.93053	-4.02399
59	H	-0.90765	1.13812	-3.08984
60	H	-1.8383	-0.67867	1.687755
61	H	2.769972	0.175431	-2.82304
62	H	2.40976	-1.30182	-1.91808
63	H	2.127845	-1.25093	-3.65573
64	H	0.193335	-2.27522	-2.00614
65	H	-0.38297	-1.74005	-3.5675
66	H	-1.10787	-4.75397	1.572346
67	H	-1.31718	-4.80035	3.33157
68	H	0.022633	-5.68403	2.57459
69	H	-1.75847	-0.37013	-1.2751
70	H	-2.46826	-1.12803	-2.6705
71	H	-4.87207	-2.92805	0.568137
72	H	-3.86433	-4.19931	-0.19582
73	H	-3.24399	-3.30395	1.22036
74	H	-1.5528	-0.49802	-6.2592

75	H	-2.25675	0.031079	-4.64524
76	H	1.979957	0.637399	-5.53502
77	H	0.833971	0.166129	-6.79983
78	H	1.326761	-1.01072	-5.57087

Conformer 4, DFT energy -1769.16888 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.36681	-0.66204	0.288745
2	C	0.49422	0.374555	-0.81261
3	C	0.476783	1.701778	-0.50767
4	C	0.04261	2.204078	0.855647
5	C	0.469479	1.177778	1.905168
6	C	-0.08431	-0.21942	1.693476
7	C	0.151399	1.798228	3.253387
8	C	0.548565	3.280753	3.024545
9	C	0.625453	3.507177	1.477245
10	C	2.01801	1.054125	2.042467
11	O	2.278629	0.864039	3.429283
12	C	1.034657	0.919828	4.143289
13	C	1.304849	1.430928	5.544684
14	C	0.495892	-1.16737	2.775994
15	C	0.416168	-0.50488	4.169989
16	C	-0.1595	-2.53846	2.790897
17	O	-1.36941	-2.67561	2.690265
18	C	0.759103	-3.72088	2.972047
19	C	-1.48779	2.431354	0.739264
20	C	0.746816	2.730354	-1.5653
21	C	1.256199	2.211377	-2.87979
22	C	0.436265	0.977395	-3.2636
23	C	0.635875	-0.18081	-2.24321
24	O	0.624072	-1.83849	0.097397
25	O	-1.49448	-0.19862	1.720981
26	O	0.561948	3.912972	-1.35422
27	C	2.011773	-0.86208	-2.3969
28	C	-0.46701	-1.24733	-2.49427
29	H	-0.90359	1.692739	3.515649
30	C	0.033151	-5.04398	3.163692
31	C	-1.86945	-0.84221	-2.02814
32	C	-2.95346	-1.57878	-2.77919
33	O	-2.90504	-1.88303	-3.95067
34	O	-4.01421	-1.82432	-2.0004
35	C	-5.11733	-2.45712	-2.64831
36	C	0.610629	0.677785	-4.75493

37	C	-0.55527	0.222834	-5.52741
38	O	-0.16721	1.590337	-5.54289
39	C	1.991943	0.442919	-5.33118
40	H	1.517667	3.495897	3.484706
41	H	-0.17891	3.953242	3.485576
42	H	1.651118	3.700201	1.15566
43	H	0.046856	4.375686	1.163684
44	H	2.54	1.951765	1.701998
45	H	2.431017	0.212982	1.472458
46	H	2.035938	0.790089	6.047553
47	H	1.703383	2.448926	5.516952
48	H	0.381216	1.43229	6.13317
49	H	1.555292	-1.32825	2.566807
50	H	0.964512	-1.12353	4.890055
51	H	-0.62555	-0.45036	4.505222
52	H	1.39654	-3.74052	2.077721
53	H	1.434447	-3.50166	3.810681
54	H	-1.6533	3.245961	0.028082
55	H	-2.01799	1.542171	0.404791
56	H	-1.90933	2.733118	1.702753
57	H	2.322087	1.970006	-2.77421
58	H	1.158483	3.001813	-3.62762
59	H	-0.61436	1.286254	-3.18763
60	H	-1.78316	-1.09328	1.995152
61	H	2.825881	-0.13422	-2.47214
62	H	2.209205	-1.5155	-1.54713
63	H	2.026139	-1.48537	-3.29494
64	H	-0.18684	-2.17869	-2.00092
65	H	-0.49381	-1.45376	-3.56626
66	H	-0.60908	-5.25935	2.306074
67	H	-0.60241	-5.01815	4.053422
68	H	0.751186	-5.86128	3.275366
69	H	-2.00966	-0.99011	-0.95385
70	H	-2.05527	0.22497	-2.21102
71	H	-5.87653	-2.58424	-1.87743
72	H	-5.49462	-1.83079	-3.46076
73	H	-4.81815	-3.42536	-3.05642
74	H	-0.39343	-0.3184	-6.45976
75	H	-1.49666	-0.00136	-5.02749
76	H	2.720008	1.158555	-4.9346
77	H	1.946286	0.577312	-6.41496
78	H	2.358549	-0.56495	-5.12417

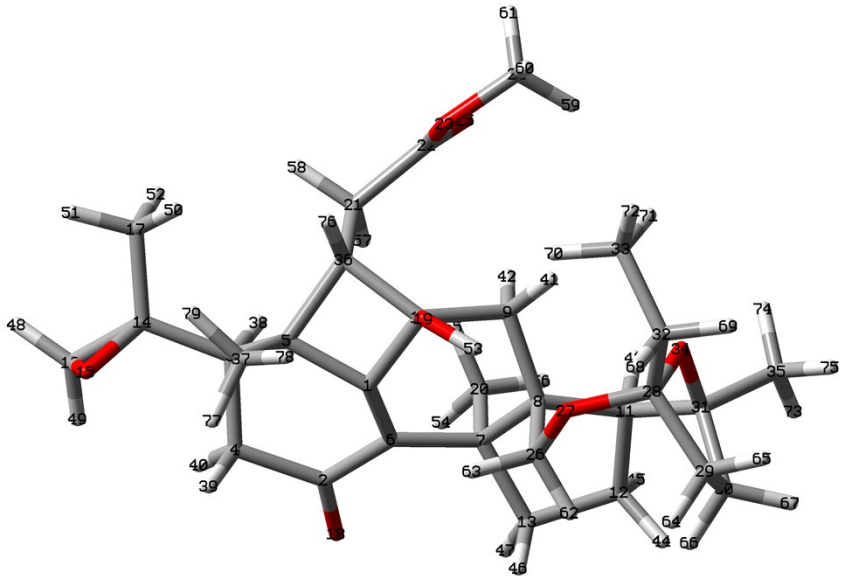
Conformer 5, DFT energy -1769.16880 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.032536	-1.05103	0.359324
2	C	0.05514	-0.01844	-0.75291
3	C	0.033143	1.308041	-0.45204
4	C	-0.20837	1.81533	0.95382
5	C	0.403608	0.805451	1.924321
6	C	-0.16707	-0.59602	1.820534
7	C	0.321775	1.439831	3.300572
8	C	0.657346	2.923022	2.991553
9	C	0.455992	3.132111	1.453524
10	C	1.953646	0.690568	1.78774
11	O	2.457641	0.526496	3.108166
12	C	1.358195	0.580254	4.028922
13	C	1.867302	1.109102	5.355492
14	C	0.594265	-1.53018	2.798656
15	C	0.769061	-0.84749	4.178073
16	C	-0.03886	-2.90068	2.982506
17	O	-1.24889	-3.06939	2.973722
18	C	0.902509	-4.05879	3.222866
19	C	-1.73851	2.02198	1.091238
20	C	0.137343	2.329749	-1.54023
21	C	0.703839	1.829551	-2.83564
22	C	-0.08023	0.571756	-3.2274
23	C	0.108714	-0.57851	-2.1903
24	O	0.164916	-2.24283	0.13487
25	O	-1.55073	-0.5826	2.090588
26	O	-0.2218	3.47874	-1.36899
27	C	1.464881	-1.28945	-2.39131
28	C	-1.01967	-1.63713	-2.3872
29	H	-0.66921	1.328267	3.746938
30	C	1.465752	-4.59915	1.899506
31	C	-2.40541	-1.32591	-1.7819
32	C	-3.12054	-0.19748	-2.48321
33	O	-3.666	-0.29222	-3.55993
34	O	-3.04338	0.954052	-1.79831
35	C	-3.54815	2.111805	-2.46815
36	C	0.149111	0.281759	-4.71537
37	C	-0.97853	-0.18084	-5.5399
38	O	-0.61625	1.194016	-5.51658
39	C	1.553518	0.095932	-5.25413
40	H	1.690657	3.15132	3.27039
41	H	0.016275	3.594212	3.568478

42	H	1.40804	3.333837	0.955867
43	H	-0.18153	3.989776	1.238802
44	H	2.402365	1.583055	1.343582
45	H	2.265076	-0.15954	1.167835
46	H	2.679214	0.477092	5.729491
47	H	2.249201	2.1283	5.245525
48	H	1.060977	1.115106	6.097011
49	H	1.600985	-1.70207	2.409273
50	H	1.446039	-1.45316	4.791689
51	H	-0.19357	-0.79587	4.699736
52	H	1.728203	-3.72962	3.86562
53	H	0.344888	-4.84219	3.742935
54	H	-2.0225	2.849073	0.43451
55	H	-2.30824	1.137362	0.817586
56	H	-1.99846	2.294795	2.119022
57	H	1.770731	1.609878	-2.69758
58	H	0.602028	2.608178	-3.59486
59	H	-1.13123	0.863941	-3.18582
60	H	-1.78612	-1.49462	2.356128
61	H	2.287682	-0.57465	-2.49431
62	H	1.682424	-1.95056	-1.55263
63	H	1.435303	-1.90932	-3.29183
64	H	-0.68867	-2.57714	-1.94628
65	H	-1.13429	-1.81332	-3.4612
66	H	2.028252	-3.83293	1.359503
67	H	0.656497	-4.93647	1.247451
68	H	2.132982	-5.44275	2.097104
69	H	-3.02679	-2.21699	-1.90765
70	H	-2.33507	-1.11204	-0.71241
71	H	-4.62728	2.028431	-2.61619
72	H	-3.30696	2.95168	-1.81805
73	H	-3.05913	2.229614	-3.43957
74	H	-0.76468	-0.69882	-6.47537
75	H	-1.94113	-0.40965	-5.08704
76	H	2.237417	0.849983	-4.85065
77	H	1.529474	0.216297	-6.34047
78	H	1.962314	-0.88994	-5.02506

S19. Coordinates of 2 used for NMR calculations

All conformers with population > 5% at 300K are listed. The structure refers to the lowest energy conformer.



Conformer 1, DFT energy -1695.11999 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.654441	0.850405	1.218534
2	C	0.597875	-0.03118	3.450298
3	C	-0.08255	2.402005	3.039167
4	C	0.700898	1.416705	3.927711
5	C	0.483027	2.295318	1.600155
6	C	0.518221	-0.23743	1.989176
7	C	-0.03876	-1.50471	1.372197
8	C	0.158294	-1.47792	-0.18206
9	C	-0.52241	-0.21123	-0.75899
10	C	0.215068	1.031412	-0.22091
11	C	-0.42085	-2.85947	-0.59151
12	C	-0.11473	-3.78927	0.628867
13	C	0.507433	-2.89485	1.732563
14	C	-0.1204	3.829456	3.579454
15	O	1.114358	4.351052	4.074552
16	C	0.063762	4.130065	5.006476
17	C	-0.94256	4.811783	2.77107
18	O	0.563445	-0.95088	4.249876
19	O	1.224461	1.472356	-1.10833
20	C	-1.53719	-1.50223	1.792468
21	C	-1.96946	2.274567	0.545958

22	C	-2.7635	1.927381	-0.69697
23	O	-2.15041	2.341703	-1.81411
24	C	-2.76423	1.948763	-3.03883
25	O	-3.81875	1.338401	-0.69062
26	C	1.670316	-1.45549	-0.53919
27	O	1.920601	-1.04188	-1.87966
28	C	1.532982	-1.90207	-2.95065
29	C	2.30177	-3.2285	-2.88811
30	C	1.401509	-4.1374	-2.04076
31	C	0.028134	-3.39989	-1.98029
32	C	1.736195	-1.09461	-4.22741
33	C	0.783848	0.09116	-4.3755
34	O	0.185584	-2.28052	-2.87
35	C	-1.07869	-4.26785	-2.56879
36	C	-0.46785	2.345359	0.317209
37	C	1.740533	3.149716	1.38785
38	H	-1.12542	2.055688	3.023335
39	H	1.757302	1.708483	3.968789
40	H	0.331488	1.41018	4.95502
41	H	-0.51186	-0.20822	-1.84856
42	H	-1.57272	-0.22161	-0.45827
43	H	-1.50662	-2.7354	-0.67117
44	H	0.544322	-4.62155	0.372223
45	H	-1.03949	-4.24779	0.990675
46	H	1.60169	-2.91398	1.697322
47	H	0.219774	-3.20122	2.74008
48	H	-0.39195	5.032898	5.413808
49	H	0.242791	3.343808	5.735743
50	H	-0.65152	4.812781	1.715874
51	H	-0.80338	5.823571	3.160488
52	H	-2.00684	4.559215	2.83339
53	H	1.606336	0.690069	-1.54495
54	H	-1.58594	-1.57999	2.881713
55	H	-2.05569	-0.58761	1.500605
56	H	-2.09855	-2.34231	1.379123
57	H	-2.24932	1.530028	1.295563
58	H	-2.34068	3.237375	0.915751
59	H	-2.88326	0.862121	-3.06909
60	H	-2.08668	2.279716	-3.82501
61	H	-3.74456	2.420375	-3.14946
62	H	2.14154	-2.42411	-0.35455
63	H	2.211235	-0.73197	0.072405
64	H	3.301653	-3.08767	-2.4713
65	H	2.410982	-3.62331	-3.90154

66	H	1.832206	-4.31084	-1.05465
67	H	1.277758	-5.12131	-2.50059
68	H	2.778324	-0.75967	-4.24636
69	H	1.597831	-1.77819	-5.07088
70	H	0.890139	0.812058	-3.56033
71	H	-0.25401	-0.256	-4.38979
72	H	0.980582	0.615488	-5.31571
73	H	-1.28382	-5.11877	-1.90946
74	H	-1.99998	-3.68819	-2.68303
75	H	-0.78497	-4.64891	-3.55207
76	H	-0.22671	3.178957	-0.34704
77	H	2.478816	2.957437	2.171667
78	H	2.186786	2.921276	0.419152
79	H	1.501994	4.216874	1.420223

Conformer 2, DFT energy -1695.11979 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.670715	0.61998	0.866209
2	C	0.631906	-0.22787	3.117964
3	C	-0.07039	2.170703	2.6445
4	C	0.745496	1.231287	3.557696
5	C	0.52825	2.078675	1.220528
6	C	0.520232	-0.45079	1.658934
7	C	-0.08706	-1.70994	1.073597
8	C	0.094557	-1.72104	-0.48229
9	C	-0.5516	-0.44524	-1.08356
10	C	0.227818	0.784272	-0.57621
11	C	-0.52949	-3.09274	-0.86104
12	C	-0.26688	-4.00334	0.383962
13	C	0.406691	-3.11308	1.459407
14	C	-0.27285	3.535268	3.308509
15	O	-0.17855	4.6972	2.48015
16	C	0.814006	4.506074	3.487476
17	C	-1.42161	3.570154	4.294048
18	O	0.6106	-1.13619	3.929961
19	O	1.245562	1.169827	-1.48201
20	C	-1.57964	-1.63981	1.508245
21	C	-1.92083	2.115583	0.122695
22	C	-2.47989	3.403999	0.683494
23	O	-2.06861	4.466054	-0.01265
24	C	-2.48011	5.735649	0.499379
25	O	-3.22854	3.470056	1.632426
26	C	1.606943	-1.75193	-0.83889

27	O	1.87734	-1.38526	-2.18772
28	C	1.481272	-2.2756	-3.2294
29	C	2.205945	-3.62255	-3.10243
30	C	1.259782	-4.47653	-2.24862
31	C	-0.08652	-3.68846	-2.23002
32	C	1.735883	-1.5313	-4.5344
33	C	0.84601	-0.30679	-4.74079
34	O	0.120212	-2.60529	-3.15307
35	C	-1.21754	-4.53499	-2.80311
36	C	-0.41157	2.13102	-0.06856
37	C	1.802171	2.89528	0.971792
38	H	-1.07638	1.734173	2.581953
39	H	1.80392	1.523139	3.551733
40	H	0.410758	1.275584	4.597342
41	H	-0.54405	-0.46909	-2.17368
42	H	-1.60095	-0.40429	-0.7784
43	H	-1.60967	-2.93345	-0.95481
44	H	0.343951	-4.87771	0.148429
45	H	-1.21308	-4.40073	0.762602
46	H	1.498495	-3.17978	1.41257
47	H	0.119837	-3.38406	2.477093
48	H	0.761896	5.204773	4.322095
49	H	1.816833	4.302177	3.12191
50	H	-1.27248	2.832678	5.090424
51	H	-2.36029	3.347901	3.780054
52	H	-1.50239	4.559933	4.752213
53	H	1.604856	0.364961	-1.89665
54	H	-1.62509	-1.73231	2.597255
55	H	-2.04581	-0.69013	1.239962
56	H	-2.1884	-2.44176	1.083266
57	H	-2.38573	1.949519	-0.85743
58	H	-2.25736	1.313261	0.782924
59	H	-3.56925	5.789788	0.55991
60	H	-2.09804	6.470658	-0.20799
61	H	-2.04176	5.888603	1.48746
62	H	2.046559	-2.72892	-0.62407
63	H	2.166062	-1.02894	-0.24346
64	H	3.199928	-3.49714	-2.6661
65	H	2.328996	-4.05362	-4.09968
66	H	1.667689	-4.64059	-1.25108
67	H	1.107754	-5.46652	-2.68708
68	H	2.794158	-1.24797	-4.55354
69	H	1.574115	-2.24255	-5.35141
70	H	0.982389	0.439058	-3.95354

71	H	-0.2079	-0.59927	-4.75207
72	H	1.077318	0.1702	-5.69803
73	H	-1.46042	-5.35646	-2.11998
74	H	-2.11537	-3.92629	-2.94717
75	H	-0.92754	-4.95746	-3.77013
76	H	-0.13738	2.950728	-0.73604
77	H	2.551627	2.711668	1.750082
78	H	2.23992	2.607627	0.014716
79	H	1.562581	3.96028	0.942132

Conformer 3, DFT energy -1695.11950 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.552143	0.857504	-0.66781
2	C	0.531734	3.117598	0.160271
3	C	-0.18865	2.628634	-2.22865
4	C	0.64051	3.5441	-1.30317
5	C	0.399402	1.200968	-2.12781
6	C	0.413324	1.661476	0.396708
7	C	-0.18441	1.090928	1.667312
8	C	-0.00808	-0.46501	1.688675
9	C	-0.67079	-1.07459	0.425221
10	C	0.09824	-0.58454	-0.81722
11	C	-0.62007	-0.83213	3.067838
12	C	-0.33475	0.414827	3.968896
13	C	0.326355	1.485272	3.062258
14	C	-0.39528	3.281502	-3.59797
15	O	-0.31461	2.441691	-4.75278
16	C	0.686627	3.443524	-4.57739
17	C	-1.53754	4.274664	-3.63496
18	O	0.520033	3.937267	1.06154
19	O	1.098176	-1.50646	-1.20412
20	C	-1.67528	1.532127	1.61062
21	C	-2.05855	0.123284	-2.13225
22	C	-2.62573	0.67901	-3.41919
23	O	-2.22806	-0.02668	-4.4802
24	C	-2.6459	0.480173	-5.74957
25	O	-3.36859	1.632499	-3.48492
26	C	1.505152	-0.82222	1.709766
27	O	1.77146	-2.17292	1.351099
28	C	1.371322	-3.21262	2.239289
29	C	2.096368	-3.10579	3.586482
30	C	1.164228	-2.23726	4.440666
31	C	-0.18504	-2.20621	3.658651

32	C	1.591631	-4.5073	1.470557
33	C	3.049706	-4.75431	1.092614
34	O	0.011267	-3.12766	2.570702
35	C	-1.31647	-2.77406	4.508037
36	C	-0.55126	-0.08023	-2.16097
37	C	1.664851	0.932647	-2.95161
38	H	-1.19197	2.577914	-1.78462
39	H	1.697485	3.526331	-1.60135
40	H	0.314029	4.586432	-1.35501
41	H	-0.66786	-2.16495	0.459789
42	H	-1.71948	-0.76582	0.394092
43	H	-1.70291	-0.91427	2.920961
44	H	0.292299	0.179996	4.831851
45	H	-1.27173	0.798317	4.383139
46	H	1.418904	1.440811	3.115757
47	H	0.041427	2.504228	3.330567
48	H	0.636096	4.271931	-5.28355
49	H	1.687908	3.072172	-4.37669
50	H	-2.47855	3.769765	-3.40051
51	H	-1.6223	4.722099	-4.62905
52	H	-1.37769	5.078079	-2.9071
53	H	1.435663	-1.94263	-0.40137
54	H	-1.714	2.622231	1.688658
55	H	-2.15588	1.253345	0.671515
56	H	-2.27504	1.121939	2.42652
57	H	-2.52959	-0.85191	-1.95465
58	H	-2.38208	0.791517	-1.33122
59	H	-3.73535	0.547165	-5.79611
60	H	-2.27379	-0.23412	-6.48315
61	H	-2.20342	1.464483	-5.91148
62	H	1.952413	-0.60192	2.682222
63	H	2.058825	-0.23431	0.976873
64	H	3.099513	-2.68896	3.469439
65	H	2.196216	-4.1091	4.011099
66	H	1.585413	-1.24387	4.596001
67	H	1.012651	-2.66774	5.434203
68	H	1.208434	-5.32402	2.09084
69	H	0.967443	-4.46535	0.570702
70	H	3.685289	-4.83507	1.981639
71	H	3.436739	-3.94059	0.473185
72	H	3.145686	-5.68752	0.529577
73	H	-1.55194	-2.09072	5.331558
74	H	-2.21742	-2.91132	3.902327
75	H	-1.03106	-3.74374	4.927783

76	H	-0.29006	-0.75577	-2.97826
77	H	2.421944	1.706746	-2.78205
78	H	2.096963	-0.02472	-2.65623
79	H	1.417287	0.893216	-4.0145

Conformer 4, DFT energy -1695.11939 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	-0.68869	-0.86991	1.185208
2	C	-0.5028	0.03267	3.400796
3	C	0.072834	-2.42869	2.990415
4	C	-0.63526	-1.4061	3.899909
5	C	-0.54682	-2.31611	1.573616
6	C	-0.48275	0.220901	1.936126
7	C	0.073278	1.467117	1.276245
8	C	-0.20881	1.428023	-0.26476
9	C	0.411948	0.140308	-0.86516
10	C	-0.3213	-1.07915	-0.27057
11	C	0.37357	2.793097	-0.72286
12	C	0.166021	3.740803	0.504822
13	C	-0.41899	2.874186	1.650102
14	C	0.082409	-3.85102	3.545506
15	O	-1.15174	-4.32756	4.085232
16	C	-0.06549	-4.13085	4.981037
17	C	0.846639	-4.86843	2.72293
18	O	-0.40023	0.958676	4.187201
19	O	-1.38025	-1.51188	-1.10079
20	C	1.591453	1.43732	1.615615
21	C	1.864386	-2.33173	0.462594
22	C	2.586273	-2.2021	-0.86003
23	O	3.600618	-1.32205	-0.77874
24	C	4.318775	-1.11415	-1.99474
25	O	2.303916	-2.80187	-1.86837
26	C	-1.74022	1.434219	-0.53093
27	O	-2.08279	1.016342	-1.84803
28	C	-1.75494	1.869293	-2.94332
29	C	-2.48724	3.213307	-2.82736
30	C	-1.50549	4.108292	-2.0597
31	C	-0.15124	3.3342	-2.0854
32	C	-2.07107	1.071855	-4.20278
33	C	-1.17423	-0.14654	-4.41581
34	O	-0.39576	2.2159	-2.95538
35	C	0.937092	4.168439	-2.75222
36	C	0.358949	-2.3989	0.261429

37	C	-1.83573	-3.13507	1.418208
38	H	1.126158	-2.12123	2.927793
39	H	-1.699	-1.65955	3.991298
40	H	-0.21979	-1.40223	4.909982
41	H	0.337391	0.124198	-1.95258
42	H	1.477734	0.125604	-0.6251
43	H	1.449472	2.64428	-0.86989
44	H	-0.48023	4.591842	0.278745
45	H	1.123259	4.173223	0.81002
46	H	-1.51263	2.921991	1.673878
47	H	-0.06978	3.18235	2.63745
48	H	0.375619	-5.04336	5.383478
49	H	-0.19721	-3.33173	5.706684
50	H	0.526696	-4.86903	1.676373
51	H	0.686086	-5.8717	3.125843
52	H	1.920344	-4.65189	2.752928
53	H	-1.77178	-0.72739	-1.52496
54	H	1.701096	1.518731	2.700329
55	H	2.076811	0.513293	1.299238
56	H	2.144585	2.265775	1.167832
57	H	2.160786	-1.50704	1.114597
58	H	2.217898	-3.25503	0.935205
59	H	4.760061	-2.04913	-2.34625
60	H	5.096078	-0.38937	-1.75464
61	H	3.652786	-0.72309	-2.76789
62	H	-2.17632	2.415349	-0.32649
63	H	-2.25669	0.728385	0.121034
64	H	-3.45445	3.095086	-2.33266
65	H	-2.66915	3.604936	-3.83191
66	H	-1.86084	4.307586	-1.04851
67	H	-1.38841	5.082115	-2.5432
68	H	-3.12408	0.773262	-4.15058
69	H	-1.96795	1.754104	-5.0535
70	H	-1.25445	-0.86837	-3.59945
71	H	-0.12721	0.158981	-4.49427
72	H	-1.44922	-0.65927	-5.34265
73	H	1.208889	5.018144	-2.11551
74	H	1.83226	3.562382	-2.92325
75	H	0.589115	4.550749	-3.71711
76	H	0.10511	-3.24098	-0.38811
77	H	-2.539	-2.90921	2.224913
78	H	-2.30897	-2.90762	0.462298
79	H	-1.6274	-4.20798	1.458531

Conformer 5, DFT energy -1695.11925 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.753846	-0.63807	1.216439
2	C	-0.14155	-0.50966	3.439103
3	C	2.316312	0.093426	3.032798
4	C	1.299758	-0.63733	3.930928
5	C	2.199622	-0.49707	1.604443
6	C	-0.33496	-0.4558	1.975701
7	C	-1.58726	0.108162	1.334924
8	C	-1.55145	-0.13608	-0.21167
9	C	-0.27164	0.50941	-0.80072
10	C	0.954932	-0.23148	-0.23074
11	C	-2.92139	0.448806	-0.65189
12	C	-3.86371	0.207949	0.574167
13	C	-2.99026	-0.40097	1.701836
14	C	3.740397	0.090055	3.58514
15	O	4.215753	-1.15695	4.097096
16	C	4.021717	-0.08915	5.016742
17	C	4.759461	0.86941	2.778342
18	O	-1.06556	-0.43774	4.231168
19	O	1.392602	-1.26374	-1.09523
20	C	-1.56233	1.617842	1.709745
21	C	2.233208	1.940746	0.543978
22	C	2.146948	2.72581	-0.74575
23	O	3.183526	2.450851	-1.55087
24	C	3.162157	3.097618	-2.82302
25	O	1.269075	3.505935	-1.03228
26	C	-1.552	-1.66115	-0.51171
27	O	-1.13491	-1.97554	-1.8368
28	C	-1.99356	-1.62772	-2.92213
29	C	-3.33339	-2.37001	-2.81818
30	C	-4.22977	-1.41086	-2.02338
31	C	-3.46413	-0.05109	-2.02311
32	C	-1.19768	-1.91077	-4.19065
33	C	0.007911	-0.99283	-4.38881
34	O	-2.34719	-0.27149	-2.90266
35	C	-4.30611	1.045885	-2.66498
36	C	2.279242	0.435707	0.310719
37	C	3.021544	-1.78001	1.417099
38	H	2.007199	1.147393	2.99315
39	H	1.562822	-1.69963	4.00468
40	H	1.294366	-0.23914	4.947462

41	H	-0.26392	0.457379	-1.88941
42	H	-0.25812	1.570292	-0.54389
43	H	-2.7793	1.52782	-0.77688
44	H	-4.71326	-0.43581	0.335706
45	H	-4.29795	1.155878	0.90425
46	H	-3.03199	-1.49503	1.698097
47	H	-3.29672	-0.07807	2.69843
48	H	4.93594	0.340752	5.427135
49	H	3.223216	-0.23569	5.739926
50	H	4.757861	0.573166	1.725181
51	H	5.762613	0.6963	3.176051
52	H	4.547032	1.942749	2.833158
53	H	0.60832	-1.66183	-1.51286
54	H	-1.64412	1.702497	2.796855
55	H	-0.63925	2.111416	1.403584
56	H	-2.39145	2.178997	1.273286
57	H	1.380679	2.237244	1.157731
58	H	3.143997	2.254632	1.06414
59	H	2.305999	2.753382	-3.40825
60	H	4.094634	2.816096	-3.30979
61	H	3.099726	4.181515	-2.70399
62	H	-2.53156	-2.10408	-0.31644
63	H	-0.84517	-2.19111	0.128062
64	H	-3.20791	-3.34809	-2.34705
65	H	-3.72822	-2.52984	-3.82523
66	H	-4.42012	-1.78979	-1.01924
67	H	-5.20701	-1.28872	-2.49846
68	H	-0.88517	-2.96038	-4.15902
69	H	-1.88391	-1.79999	-5.03702
70	H	0.728226	-1.07803	-3.57196
71	H	-0.31551	0.050209	-4.44891
72	H	0.524529	-1.24491	-5.31967
73	H	-5.15385	1.300917	-2.01922
74	H	-3.70462	1.946464	-2.82005
75	H	-4.69148	0.714894	-3.63442
76	H	3.120622	0.18261	-0.33947
77	H	2.798704	-2.50232	2.207308
78	H	2.790777	-2.2309	0.451394
79	H	4.094183	-1.57135	1.45988

Conformer 6, DFT energy -1695.11923 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.520359	0.885266	1.200356

2	C	0.465673	0.014959	3.437028
3	C	-0.19349	2.45088	3.020252
4	C	0.590411	1.4643	3.906615
5	C	0.355025	2.332224	1.575296
6	C	0.377339	-0.19715	1.977839
7	C	-0.17725	-1.46776	1.365168
8	C	0.039728	-1.44773	-0.18623
9	C	-0.64467	-0.19018	-0.77918
10	C	0.076688	1.060784	-0.23971
11	C	-0.52665	-2.8321	-0.60001
12	C	-0.23506	-3.75651	0.628238
13	C	0.366497	-2.85588	1.739001
14	C	-0.21855	3.881614	3.551906
15	O	1.024749	4.404696	4.023016
16	C	-0.0102	4.189708	4.974318
17	C	-1.0526	4.859443	2.749583
18	O	0.424825	-0.9005	4.241181
19	O	1.072574	1.508447	-1.13645
20	C	-1.6796	-1.46678	1.76841
21	C	-2.1098	2.279212	0.574837
22	C	-2.93772	1.919313	-0.63999
23	O	-2.42588	2.434172	-1.76631
24	C	-3.09977	2.067428	-2.96852
25	O	-3.94257	1.247809	-0.60788
26	C	1.559435	-1.41966	-0.51137
27	O	1.839904	-1.01505	-1.8464
28	C	1.477929	-1.87921	-2.92013
29	C	2.237147	-3.20967	-2.84678
30	C	1.316834	-4.11359	-2.01637
31	C	-0.05403	-3.37037	-1.98267
32	C	1.695734	-1.06154	-4.18499
33	C	3.146021	-0.63458	-4.39629
34	O	0.12651	-2.24972	-2.8685
35	C	-1.15289	-4.23156	-2.5949
36	C	-0.61546	2.36867	0.305394
37	C	1.610191	3.183855	1.3399
38	H	-1.23842	2.11173	3.019165
39	H	1.650756	1.745204	3.934846
40	H	0.230915	1.467861	4.937915
41	H	-0.61605	-0.19093	-1.86936
42	H	-1.69976	-0.21023	-0.49642
43	H	-1.6117	-2.71285	-0.69473
44	H	0.431136	-4.58715	0.385456
45	H	-1.16343	-4.21755	0.977227

46	H	1.461081	-2.87328	1.723441
47	H	0.062223	-3.1595	2.742361
48	H	-0.46073	5.093959	5.383946
49	H	0.182042	3.407519	5.704409
50	H	-0.7701	4.860322	1.691994
51	H	-0.91753	5.873159	3.136193
52	H	-2.11479	4.59973	2.820861
53	H	1.446505	0.728112	-1.58375
54	H	-1.74045	-1.52717	2.858851
55	H	-2.20336	-0.56234	1.454192
56	H	-2.22947	-2.31909	1.362139
57	H	-2.3554	1.534355	1.335515
58	H	-2.47839	3.240909	0.950784
59	H	-3.06739	0.982786	-3.10231
60	H	-2.55853	2.566264	-3.77106
61	H	-4.14237	2.394067	-2.94379
62	H	2.02922	-2.38558	-0.30907
63	H	2.081872	-0.68902	0.107091
64	H	3.232204	-3.08059	-2.4144
65	H	2.35837	-3.60015	-3.86154
66	H	1.728608	-4.28578	-1.02188
67	H	1.198742	-5.09836	-2.47659
68	H	1.342267	-1.6641	-5.02815
69	H	1.045849	-0.18133	-4.12186
70	H	3.808267	-1.50174	-4.49297
71	H	3.50156	-0.02974	-3.55823
72	H	3.24039	-0.04125	-5.30992
73	H	-1.37671	-5.08204	-1.9413
74	H	-2.06795	-3.64634	-2.72744
75	H	-0.84117	-4.61315	-3.57223
76	H	-0.39932	3.204294	-0.36484
77	H	2.358442	2.996864	2.11558
78	H	2.042467	2.947488	0.366717
79	H	1.372725	4.251413	1.367498

Conformer 7, DFT energy -1695.11902 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	-0.88994	0.618546	1.167278
2	C	0.027392	0.487938	3.38093
3	C	-2.44396	-0.06389	3.008572
4	C	-1.40483	0.660958	3.885403
5	C	-2.33476	0.507151	1.571313
6	C	0.20286	0.417217	1.916585

7	C	1.437576	-0.17332	1.26497
8	C	1.388907	0.06667	-0.28228
9	C	0.089949	-0.55532	-0.85609
10	C	-1.11657	0.209579	-0.27631
11	C	2.740988	-0.54557	-0.73656
12	C	3.704258	-0.30751	0.47341
13	C	2.853752	0.312943	1.61315
14	C	-3.86179	-0.03705	3.574125
15	O	-4.31947	1.220254	4.076199
16	C	-4.12795	0.161309	5.006305
17	C	-4.89381	-0.81539	2.783342
18	O	0.958539	0.397799	4.163374
19	O	-1.54151	1.241551	-1.14111
20	C	1.394516	-1.68061	1.647069
21	C	-2.38848	-1.93755	0.539103
22	C	-2.26121	-2.70373	-0.75852
23	O	-1.40976	-3.73817	-0.63366
24	C	-1.20147	-4.49842	-1.82391
25	O	-2.8395	-2.4377	-1.78359
26	C	1.41472	1.591571	-0.58507
27	O	0.989902	1.908975	-1.90522
28	C	1.816615	1.534088	-3.0033
29	C	3.177581	2.2393	-2.94395
30	C	4.064017	1.268017	-2.15369
31	C	3.265998	-0.07193	-2.12451
32	C	0.983558	1.806598	-4.24727
33	C	0.608421	3.275622	-4.42245
34	O	2.134749	0.168146	-2.98111
35	C	4.066347	-1.19473	-2.7751
36	C	-2.43897	-0.43898	0.289385
37	C	-3.13837	1.800577	1.378371
38	H	-2.15046	-1.12256	2.979241
39	H	-1.64107	1.730728	3.938992
40	H	-1.40002	0.28295	4.909649
41	H	0.067266	-0.51066	-1.94539
42	H	0.066852	-1.61402	-0.5868
43	H	2.578737	-1.62404	-0.84446
44	H	4.55404	0.329658	0.219129
45	H	4.137745	-1.25735	0.799327
46	H	2.913067	1.406073	1.61137
47	H	3.167771	-0.01662	2.605261
48	H	-5.04242	-0.25453	5.430471
49	H	-3.32144	0.308063	5.720524
50	H	-4.90082	-0.52467	1.728184

51	H	-5.89253	-0.63606	3.190375
52	H	-4.6846	-1.88963	2.841672
53	H	-0.75938	1.583622	-1.60966
54	H	1.466245	-1.75974	2.735487
55	H	0.470192	-2.16992	1.335868
56	H	2.224905	-2.24998	1.222455
57	H	-1.56943	-2.22213	1.203265
58	H	-3.31674	-2.2661	1.02034
59	H	-2.14504	-4.91018	-2.18951
60	H	-0.51569	-5.29808	-1.54572
61	H	-0.76276	-3.8688	-2.60255
62	H	2.40503	2.016128	-0.40243
63	H	0.722512	2.134839	0.059099
64	H	3.096097	3.228877	-2.48833
65	H	3.549916	2.36801	-3.96444
66	H	4.27905	1.654471	-1.15754
67	H	5.03048	1.11797	-2.64231
68	H	1.556747	1.447792	-5.10823
69	H	0.080888	1.188836	-4.18036
70	H	1.498888	3.90675	-4.52168
71	H	0.031293	3.636907	-3.56696
72	H	0.00323	3.410062	-5.32405
73	H	4.921899	-1.46585	-2.14631
74	H	3.439357	-2.0814	-2.9092
75	H	4.437496	-0.8821	-3.7561
76	H	-3.28257	-0.1952	-0.36167
77	H	-2.89893	2.526918	2.160091
78	H	-2.9106	2.2385	0.406107
79	H	-4.2135	1.607535	1.431623

Conformer 8, DFT energy -1695.11895 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
1	C	0.651889	0.708099	0.912775
2	C	0.604288	-0.11724	3.173312
3	C	-0.08802	2.277768	2.676178
4	C	0.725414	1.345529	3.598966
5	C	0.510676	2.170051	1.253399
6	C	0.495034	-0.35412	1.716607
7	C	-0.11083	-1.61946	1.142547
8	C	0.078301	-1.64408	-0.41175
9	C	-0.56518	-0.37438	-1.02856
10	C	0.212076	0.860498	-0.53322
11	C	-0.54543	-3.01669	-0.78287

12	C	-0.27581	-3.92069	0.465234
13	C	0.382507	-3.01929	1.542369
14	C	-0.28768	3.6495	3.326035
15	O	-0.19214	4.80224	2.485
16	C	0.80054	4.62062	3.493949
17	C	-1.43637	3.696916	4.311331
18	O	0.576141	-1.01729	3.99372
19	O	1.223156	1.237227	-1.44695
20	C	-1.60448	-1.54783	1.571669
21	C	-1.93792	2.196184	0.1562
22	C	-2.49745	3.489117	0.705798
23	O	-2.08667	4.545118	0.000232
24	C	-2.49669	5.819154	0.5015
25	O	-3.24568	3.56326	1.654323
26	C	1.594882	-1.68411	-0.75424
27	O	1.883174	-1.32447	-2.10038
28	C	1.471114	-2.20008	-3.14875
29	C	2.182448	-3.55376	-3.03812
30	C	1.23288	-4.4035	-2.18394
31	C	-0.10753	-3.60624	-2.15657
32	C	1.718235	-1.39952	-4.42295
33	C	1.20066	-2.06055	-5.69624
34	O	0.107779	-2.51281	-3.06669
35	C	-1.24405	-4.43674	-2.74152
36	C	-0.42886	2.210739	-0.03573
37	C	1.785734	2.982055	0.99462
38	H	-1.09495	1.842788	2.617812
39	H	1.785679	1.633025	3.587668
40	H	0.392428	1.402287	4.639195
41	H	-0.55189	-0.41062	-2.11872
42	H	-1.61636	-0.33197	-0.72969
43	H	-1.62637	-2.85947	-0.87085
44	H	0.348046	-4.78711	0.234728
45	H	-1.21841	-4.3296	0.840504
46	H	1.474845	-3.08341	1.509854
47	H	0.084022	-3.28433	2.558284
48	H	0.749733	5.328264	4.321068
49	H	1.802789	4.411347	3.130002
50	H	-1.2871	2.969381	5.117141
51	H	-2.37569	3.468268	3.800551
52	H	-1.51692	4.692484	4.756319
53	H	1.571576	0.429294	-1.86541
54	H	-1.65276	-1.62269	2.661469
55	H	-2.0742	-0.60524	1.286801

56	H	-2.20812	-2.35933	1.158915
57	H	-2.40324	2.021473	-0.82226
58	H	-2.27389	1.39931	0.823291
59	H	-3.58596	5.874102	0.563674
60	H	-2.11588	6.547799	-0.21362
61	H	-2.05727	5.980573	1.487158
62	H	2.025563	-2.66354	-0.53137
63	H	2.152076	-0.96122	-0.15723
64	H	3.178669	-3.43704	-2.60467
65	H	2.299376	-3.98469	-4.03541
66	H	1.643408	-4.57262	-1.18837
67	H	1.071812	-5.39118	-2.62429
68	H	1.229519	-0.42818	-4.28549
69	H	2.794132	-1.20529	-4.49191
70	H	0.134319	-2.28357	-5.60764
71	H	1.726895	-2.9948	-5.91982
72	H	1.344072	-1.39286	-6.55106
73	H	-1.49433	-5.26513	-2.06938
74	H	-2.1371	-3.8194	-2.87897
75	H	-0.95525	-4.84881	-3.71367
76	H	-0.15497	3.024932	-0.71005
77	H	2.535204	2.806235	1.774751
78	H	2.222505	2.682221	0.040765
79	H	1.547856	4.047095	0.952643

Conformer 9, DFT energy -1695.11893 au (ωB97X-V/6-311+G(2df,2p))

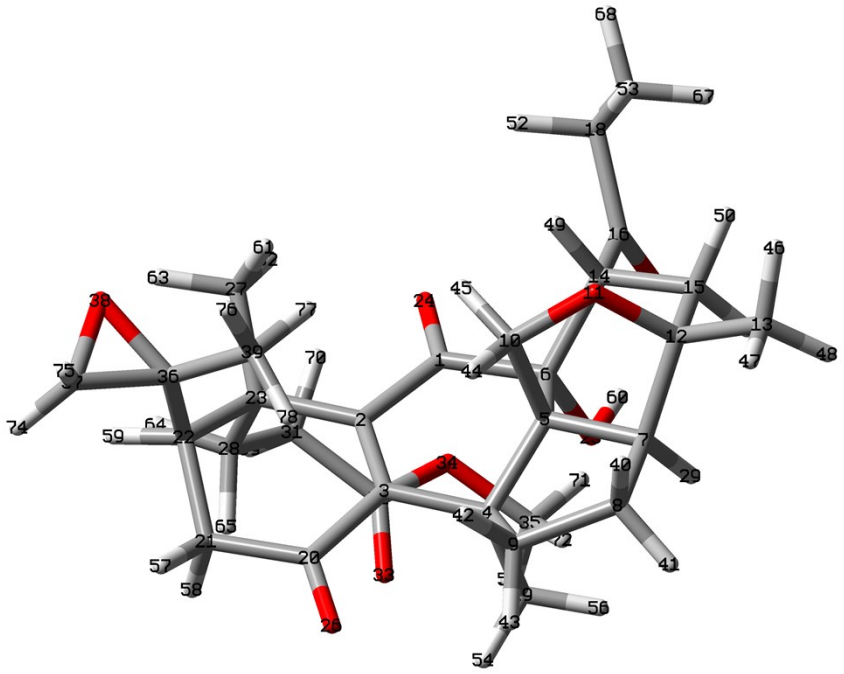
Tag	Symbol	X	Y	Z
1	C	0.802005	-0.53428	1.203467
2	C	-0.09055	-0.44396	3.429711
3	C	2.368135	0.154408	3.034739
4	C	1.350158	-0.59298	3.917166
5	C	2.248079	-0.402	1.593038
6	C	-0.2853	-0.36292	1.967975
7	C	-1.53944	0.209093	1.337989
8	C	-1.50385	-0.01619	-0.21145
9	C	-0.22695	0.642859	-0.79319
10	C	1.003389	-0.10203	-0.23779
11	C	-2.87414	0.57034	-0.64507
12	C	-3.8174	0.303048	0.574715
13	C	-2.94075	-0.30979	1.698438
14	C	3.793234	0.134943	3.583119
15	O	4.266502	-1.12408	4.066493
16	C	4.078076	-0.07673	5.009794

17	C	4.811565	0.929729	2.790899
18	O	-1.01372	-0.38013	4.22381
19	O	1.441182	-1.1109	-1.12558
20	C	-1.52009	1.713239	1.733018
21	C	2.267307	2.058737	0.593643
22	C	2.133037	2.886232	-0.66536
23	O	3.082677	2.57695	-1.56003
24	C	3.005864	3.275589	-2.80149
25	O	1.287332	3.728859	-0.85582
26	C	-1.50115	-1.53888	-0.52641
27	O	-1.08626	-1.83814	-1.85439
28	C	-1.93476	-1.47206	-2.93927
29	C	-3.27901	-2.2074	-2.86949
30	C	-4.17509	-1.26238	-2.05845
31	C	-3.4067	0.09491	-2.02935
32	C	-1.11096	-1.71728	-4.19513
33	C	-0.70473	-3.17604	-4.38572
34	O	-2.28148	-0.11448	-2.90305
35	C	-4.24055	1.204208	-2.66046
36	C	2.32296	0.561033	0.321185
37	C	3.069006	-1.68035	1.372662
38	H	2.061997	1.209827	3.020773
39	H	1.60638	-1.6587	3.96313
40	H	1.349385	-0.22002	4.943427
41	H	-0.21971	0.606911	-1.88335
42	H	-0.22054	1.700017	-0.52039
43	H	-2.73603	1.652292	-0.7475
44	H	-4.65812	-0.34829	0.32608
45	H	-4.26448	1.241727	0.914255
46	H	-2.97707	-1.40397	1.687012
47	H	-3.25022	0.004125	2.697033
48	H	4.994092	0.342108	5.427146
49	H	3.281466	-0.237	5.732155
50	H	4.799438	0.664114	1.72948
51	H	5.816045	0.73707	3.175653
52	H	4.608228	2.002604	2.878396
53	H	0.657883	-1.47127	-1.57906
54	H	-1.59118	1.781959	2.822699
55	H	-0.60412	2.219764	1.423357
56	H	-2.35942	2.273724	1.313295
57	H	1.431269	2.3312	1.241323
58	H	3.188709	2.371081	1.097909
59	H	2.042115	3.090972	-3.28404
60	H	3.818795	2.881535	-3.40978

61	H	3.127449	4.350293	-2.64669
62	H	-2.47956	-1.98648	-0.33457
63	H	-0.79058	-2.07347	0.104692
64	H	-3.17073	-3.19936	-2.42464
65	H	-3.66192	-2.33398	-3.88643
66	H	-4.36687	-1.66152	-1.06248
67	H	-5.15187	-1.13013	-2.53161
68	H	-1.70192	-1.36505	-5.04678
69	H	-0.22172	-1.07974	-4.13366
70	H	-1.58162	-3.82634	-4.47882
71	H	-0.10995	-3.53016	-3.53966
72	H	-0.10784	-3.29072	-5.29523
73	H	-5.09289	1.451188	-2.01748
74	H	-3.63575	2.105868	-2.79641
75	H	-4.61887	0.889928	-3.63831
76	H	3.165464	0.32851	-0.33517
77	H	2.851199	-2.41977	2.148251
78	H	2.833501	-2.10959	0.398354
79	H	4.141901	-1.47244	1.413283

S18. Coordinates of 4-*epi*-**1 used for NMR calculations**

All conformers with population > 5% at 300K are listed. The structure refers to the lowest energy conformer.



Conformer 1, DFT energy -1769.17175 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	-0.7615	0.116438	0.486819
C	2	0.563371	0.740016	0.889152
C	3	1.729764	0.183637	0.453332
C	4	1.762807	-1.05078	-0.4294
C	5	0.49569	-1.04397	-1.28566
C	6	-0.78983	-1.07953	-0.49064
C	7	0.652075	-2.16465	-2.29527
C	8	2.152684	-2.04856	-2.66809
C	9	2.844778	-1.20823	-1.54276
C	10	0.416938	0.170115	-2.26101
O	11	-0.15814	-0.32131	-3.46529
C	12	-0.40544	-1.72668	-3.31264
C	13	-0.33797	-2.37756	-4.68024
C	14	-1.9996	-0.96303	-1.4595
C	15	-1.80407	-1.91419	-2.66484
C	16	-3.33506	-1.22414	-0.77774
O	17	-3.50741	-2.19792	-0.06036
C	18	-4.44637	-0.24743	-1.06316
C	19	1.919455	-2.26892	0.514763

C	20	3.054425	0.684288	0.942566
C	21	3.077689	1.877304	1.859377
C	22	1.858464	2.786306	1.714826
C	23	0.519749	1.984153	1.801844
O	24	-1.82855	0.506474	0.926982
O	25	-0.86124	-2.2719	0.256744
O	26	4.085656	0.116729	0.635797
C	27	-0.62031	2.962611	1.440531
C	28	0.370035	1.587824	3.304925
H	29	0.409693	-3.1394	-1.8665
C	30	-5.78509	-0.64723	-0.45997
C	31	-0.79329	0.68743	3.719657
C	32	-0.49274	-0.78505	3.53806
O	33	0.618788	-1.2657	3.508305
O	34	-1.61372	-1.50826	3.469561
C	35	-1.43218	-2.92203	3.368095
C	36	2.038815	3.716099	0.509948
C	37	2.857985	4.915421	0.737924
O	38	1.442473	5.006507	0.657892
C	39	1.969935	3.168594	-0.89821
H	40	2.272737	-1.55195	-3.63583
H	41	2.608797	-3.03756	-2.75846
H	42	3.186121	-0.24406	-1.92795
H	43	3.731728	-1.70385	-1.14995
H	44	1.399256	0.596334	-2.48096
H	45	-0.20095	0.987806	-1.86933
H	46	-1.06046	-1.91311	-5.35841
H	47	0.659374	-2.26554	-5.11369
H	48	-0.56906	-3.44499	-4.60495
H	49	-2.03879	0.053871	-1.85664
H	50	-2.57873	-1.70419	-3.41231
H	51	-1.92655	-2.95527	-2.34392
H	52	-4.10335	0.719528	-0.67191
H	53	-4.51211	-0.11854	-2.15228
H	54	2.924451	-2.23305	0.944529
H	55	1.194973	-2.2658	1.325842
H	56	1.817287	-3.20615	-0.04073
H	57	4.01233	2.41814	1.68277
H	58	3.144036	1.477646	2.877948
H	59	1.845523	3.466153	2.574987
H	60	-1.81105	-2.46565	0.387209
H	61	-0.67078	3.156727	0.364909
H	62	-1.59345	2.592052	1.753617
H	63	-0.43051	3.921352	1.930676

H	64	0.283824	2.530984	3.857236
H	65	1.28347	1.095557	3.649252
H	66	-5.70311	-0.7461	0.625435
H	67	-6.12277	-1.60969	-0.85413
H	68	-6.54628	0.105349	-0.68442
H	69	-0.96969	0.821207	4.795116
H	70	-1.72963	0.929375	3.216369
H	71	-2.43378	-3.33349	3.243939
H	72	-0.80785	-3.16198	2.50586
H	73	-0.96707	-3.31214	4.277529
H	74	3.283909	5.101361	1.724274
H	75	3.403729	5.362092	-0.09243
H	76	2.136611	3.976442	-1.61507
H	77	0.990989	2.731077	-1.10313
H	78	2.728058	2.396562	-1.06678

Conformer 2, DFT energy -1769.17061 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	-0.74163	0.1213	0.504504
C	2	0.577102	0.771398	0.855505
C	3	1.745127	0.268862	0.359805
C	4	1.782509	-0.95438	-0.53373
C	5	0.471839	-1.0039	-1.32079
C	6	-0.76967	-1.08691	-0.45918
C	7	0.629445	-2.12447	-2.33175
C	8	2.10178	-1.93642	-2.78434
C	9	2.809962	-1.05456	-1.70128
C	10	0.284701	0.195601	-2.30062
O	11	-0.31701	-0.33548	-3.47573
C	12	-0.49712	-1.74703	-3.29582
C	13	-0.47143	-2.41169	-4.65839
C	14	-2.02989	-1.03712	-1.36749
C	15	-1.85155	-1.98927	-2.5746
C	16	-3.31797	-1.34741	-0.61907
O	17	-3.41042	-2.30693	0.131473
C	18	-4.48837	-0.43286	-0.88078
C	19	2.044366	-2.17377	0.387382
C	20	3.079206	0.80213	0.804109
C	21	3.115154	2.033392	1.672942
C	22	1.829395	2.850759	1.575538
C	23	0.560241	1.978726	1.816552
O	24	-1.80131	0.504047	0.972745
O	25	-0.74859	-2.2707	0.304333

O	26	4.103539	0.216388	0.517766
C	27	-0.66383	2.916541	1.67943
C	28	0.612015	1.500313	3.299578
H	29	0.457873	-3.10699	-1.88685
C	30	-5.78076	-0.8794	-0.214
C	31	-0.48205	0.537919	3.767596
C	32	-0.12089	-0.91622	3.547406
O	33	1.008713	-1.34826	3.485034
O	34	-1.21307	-1.68414	3.491162
C	35	-0.97594	-3.08861	3.371669
C	36	1.901749	3.67186	0.275569
C	37	1.113797	3.403882	-0.93144
O	38	2.465314	2.97837	-0.8524
C	39	2.462198	5.063639	0.468142
H	40	2.145802	-1.44333	-3.75972
H	41	2.599869	-2.90268	-2.89236
H	42	3.075913	-0.07189	-2.09801
H	43	3.740803	-1.50307	-1.3565
H	44	1.227453	0.682223	-2.56276
H	45	-0.3695	0.972592	-1.88876
H	46	-1.24405	-1.98437	-5.3052
H	47	0.498456	-2.26597	-5.1414
H	48	-0.6556	-3.48646	-4.56062
H	49	-2.13532	-0.02764	-1.77101
H	50	-2.67182	-1.82215	-3.28303
H	51	-1.90962	-3.03139	-2.24027
H	52	-4.17614	0.555931	-0.51775
H	53	-4.60371	-0.32529	-1.96856
H	54	3.072297	-2.10474	0.750936
H	55	1.377689	-2.20531	1.245019
H	56	1.938975	-3.1092	-0.17039
H	57	3.992032	2.616766	1.377201
H	58	3.3017	1.699662	2.698872
H	59	1.835506	3.586532	2.389114
H	60	-1.67909	-2.49262	0.506685
H	61	-0.94417	3.114783	0.644593
H	62	-1.54796	2.52149	2.17515
H	63	-0.41306	3.877372	2.145144
H	64	0.575734	2.403193	3.921517
H	65	1.565105	1.006902	3.503352
H	66	-5.64208	-0.96857	0.866273
H	67	-6.10228	-1.85508	-0.58962
H	68	-6.57943	-0.15589	-0.40126
H	69	-0.60991	0.64543	4.852529

H	70	-1.45638	0.734021	3.318474
H	71	-1.96402	-3.54366	3.301631
H	72	-0.39356	-3.29899	2.473328
H	73	-0.44376	-3.45993	4.250711
H	74	0.383978	2.601162	-0.94103
H	75	0.918215	4.213566	-1.63474
H	76	2.638607	5.54562	-0.49694
H	77	3.413681	5.025072	1.010278
H	78	1.765119	5.677301	1.049137

Conformer 3, DFT energy -1769.17060 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	-0.83022	-0.17295	0.611562
C	2	0.445407	0.616848	0.839394
C	3	1.598472	0.230206	0.223704
C	4	1.638302	-0.91048	-0.77436
C	5	0.265811	-0.96869	-1.44726
C	6	-0.88137	-1.2474	-0.49934
C	7	0.389288	-1.94596	-2.5996
C	8	1.79974	-1.61258	-3.15063
C	9	2.559491	-0.82387	-2.03208
C	10	-0.07438	0.326702	-2.24756
O	11	-0.76824	-0.09528	-3.41444
C	12	-0.84413	-1.52864	-3.40743
C	13	-0.91002	-2.01344	-4.84216
C	14	-2.22253	-1.16136	-1.28117
C	15	-2.10814	-1.94684	-2.60941
C	16	-3.41494	-1.64749	-0.47082
O	17	-3.38836	-2.71288	0.126834
C	18	-4.64526	-0.77595	-0.48369
C	19	2.062111	-2.18564	-0.00835
C	20	2.91543	0.822385	0.62459
C	21	2.904384	1.785988	1.77417
C	22	1.664058	2.683668	1.773096
C	23	0.328776	1.868858	1.730055
O	24	-1.82896	-0.00734	1.290059
O	25	-0.72595	-2.52359	0.080668
O	26	3.948624	0.47761	0.084215
C	27	-0.79851	2.769891	1.16191
C	28	-0.12955	1.55284	3.187378
H	29	0.312984	-2.98356	-2.26702
C	30	-5.84016	-1.3893	0.230758
C	31	0.796574	0.781276	4.139976

C	32	1.051415	-0.64237	3.702408
O	33	2.098334	-1.06675	3.264152
O	34	-0.05222	-1.38118	3.855488
C	35	0.009631	-2.74011	3.412557
C	36	1.847544	3.773298	0.709356
C	37	2.557984	4.986563	1.137294
O	38	1.146187	4.990109	0.975863
C	39	1.928372	3.403131	-0.75798
H	40	1.726058	-1.00219	-4.0561
H	41	2.336522	-2.5246	-3.42382
H	42	2.747449	0.208404	-2.33617
H	43	3.537542	-1.25565	-1.82195
H	44	0.822062	0.877928	-2.54474
H	45	-0.70099	1.027251	-1.68104
H	46	-1.76293	-1.56006	-5.35696
H	47	0.000179	-1.74381	-5.38471
H	48	-1.0252	-3.10197	-4.87071
H	49	-2.415	-0.11789	-1.54128
H	50	-2.99906	-1.74669	-3.21556
H	51	-2.07976	-3.02263	-2.40628
H	52	-4.34857	0.176078	-0.02271
H	53	-4.87574	-0.53734	-1.532
H	54	3.103169	-2.06408	0.30314
H	55	1.459288	-2.36218	0.878343
H	56	1.993986	-3.06717	-0.65325
H	57	3.826976	2.37261	1.745838
H	58	2.943819	1.152469	2.665328
H	59	1.642347	3.233378	2.721946
H	60	-1.62393	-2.84823	0.298003
H	61	-0.68261	2.954062	0.090081
H	62	-1.7744	2.310905	1.324427
H	63	-0.77678	3.741658	1.66115
H	64	-1.07954	1.021006	3.135906
H	65	-0.33418	2.522627	3.655885
H	66	-5.60615	-1.57402	1.282632
H	67	-6.11613	-2.34719	-0.2195
H	68	-6.70348	-0.71913	0.178267
H	69	1.756435	1.280149	4.284488
H	70	0.296384	0.744663	5.113345
H	71	-0.13158	-2.77745	2.33006
H	72	0.967874	-3.18706	3.681519
H	73	-0.81204	-3.25198	3.913773
H	74	2.912942	5.073834	2.164337
H	75	3.113242	5.572662	0.405345

H	76	1.954629	4.316785	-1.35718
H	77	1.067593	2.812659	-1.07993
H	78	2.833588	2.826439	-0.9721

Conformer 4, DFT energy -1769.17054 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	-1.10579	0.008251	0.108184
C	2	0.224166	0.707366	0.3279
C	3	1.373761	0.131303	-0.11603
C	4	1.417255	-1.26801	-0.69438
C	5	0.092952	-1.5067	-1.41735
C	6	-1.13275	-1.39483	-0.53284
C	7	0.243597	-2.82646	-2.14991
C	8	1.707689	-2.74267	-2.65979
C	9	2.428449	-1.6338	-1.82088
C	10	-0.11633	-0.55939	-2.63896
O	11	-0.75623	-1.34047	-3.64132
C	12	-0.9059	-2.68178	-3.15188
C	13	-0.89799	-3.62812	-4.3361
C	14	-2.40536	-1.56948	-1.40474
C	15	-2.23934	-2.77301	-2.3606
C	16	-3.68052	-1.70295	-0.58722
O	17	-3.74187	-2.43033	0.392037
C	18	-4.87841	-0.92422	-1.07193
C	19	1.712813	-2.23534	0.479457
C	20	2.676489	0.837735	0.059847
C	21	2.578226	2.325701	0.22895
C	22	1.596723	2.613066	1.369001
C	23	0.16319	2.049962	1.084088
O	24	-2.16839	0.51508	0.423491
O	25	-1.07666	-2.35119	0.499722
O	26	3.736439	0.240457	0.058577
C	27	-0.64035	3.064656	0.243686
C	28	-0.57097	1.8441	2.448276
H	29	0.088129	-3.68338	-1.49131
C	30	-6.16235	-1.23659	-0.31774
C	31	-0.22118	0.57316	3.248969
C	32	1.19724	0.570484	3.764324
O	33	1.619814	1.285754	4.645039
O	34	1.973428	-0.29544	3.090218
C	35	3.357301	-0.29441	3.436658
C	36	1.683157	4.101244	1.756178
C	37	2.195329	4.423326	3.098746

O	38	0.807631	4.534978	2.798142
C	39	1.888602	5.136169	0.665768
H	40	1.731988	-2.48519	-3.72307
H	41	2.211852	-3.70644	-2.5535
H	42	2.689091	-0.77484	-2.44487
H	43	3.36605	-1.99102	-1.39421
H	44	0.827047	-0.17448	-3.03535
H	45	-0.73629	0.313721	-2.40107
H	46	-1.69255	-3.36127	-5.03964
H	47	0.057865	-3.58	-4.86443
H	48	-1.06183	-4.65743	-4.00126
H	49	-2.52418	-0.68331	-2.03118
H	50	-3.0786	-2.78466	-3.06593
H	51	-2.26962	-3.71026	-1.79366
H	52	-4.60525	0.13571	-0.97504
H	53	-4.9859	-1.1043	-2.15133
H	54	2.730011	-2.03524	0.825615
H	55	1.022223	-2.11294	1.309386
H	56	1.662717	-3.27507	0.141332
H	57	2.227577	2.770132	-0.71181
H	58	3.574995	2.718922	0.445557
H	59	1.982409	2.066588	2.230626
H	60	-2.00054	-2.53647	0.764633
H	61	-0.13456	3.283577	-0.70417
H	62	-1.6336	2.678142	0.018188
H	63	-0.75952	3.998515	0.799895
H	64	-1.64456	1.814835	2.259774
H	65	-0.36727	2.719361	3.067434
H	66	-6.04762	-1.0154	0.746577
H	67	-6.42347	-2.29498	-0.4088
H	68	-6.99096	-0.63993	-0.71022
H	69	-0.87393	0.55171	4.126764
H	70	-0.40561	-0.33505	2.66913
H	71	3.822279	-1.0334	2.786345
H	72	3.796147	0.690867	3.254101
H	73	3.490772	-0.55645	4.48867
H	74	2.447055	3.619546	3.788794
H	75	2.706353	5.371208	3.265148
H	76	2.869813	5.027664	0.192738
H	77	1.831398	6.13289	1.109316
H	78	1.126258	5.070516	-0.11476

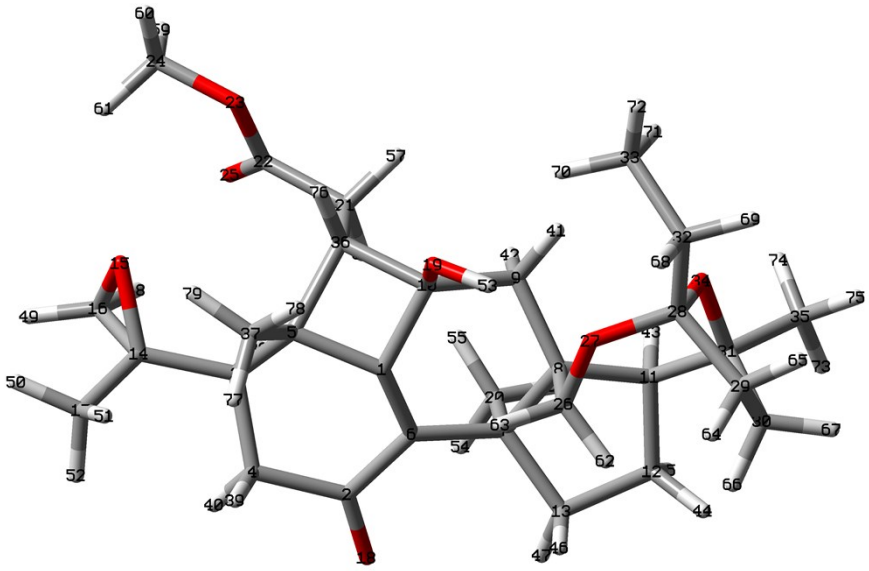
Conformer 5, DFT energy -1769.16976 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	-0.81333	-0.0075	0.532876
C	2	0.510472	0.631041	0.911624
C	3	1.675418	0.065341	0.486056
C	4	1.697926	-1.18169	-0.37992
C	5	0.44091	-1.15844	-1.25161
C	6	-0.85797	-1.17857	-0.47504
C	7	0.592503	-2.27961	-2.26141
C	8	2.099709	-2.19275	-2.61236
C	9	2.791678	-1.36633	-1.47706
C	10	0.39679	0.05887	-2.22423
O	11	-0.16451	-0.41842	-3.43966
C	12	-0.44031	-1.81849	-3.29424
C	13	-0.36488	-2.4686	-4.66182
C	14	-2.04718	-1.02399	-1.46296
C	15	-1.85208	-1.97749	-2.66914
C	16	-3.41333	-1.26379	-0.83518
O	17	-3.61155	-2.17745	-0.04882
C	18	-4.54009	-0.36206	-1.28202
C	19	1.815243	-2.3938	0.576007
C	20	2.998537	0.570306	0.971004
C	21	3.022972	1.789659	1.855792
C	22	1.801138	2.694408	1.699875
C	23	0.463222	1.890244	1.802712
O	24	-1.86729	0.345042	1.031022
O	25	-0.97251	-2.38453	0.244972
O	26	4.0296	-0.01173	0.688522
C	27	-0.68192	2.852837	1.417303
C	28	0.323027	1.526402	3.316007
H	29	0.324372	-3.25019	-1.83831
C	30	-4.4488	1.032358	-0.64534
C	31	-0.85886	0.674536	3.7775
C	32	-0.62593	-0.80831	3.590043
O	33	0.463505	-1.3296	3.495099
O	34	-1.77446	-1.48923	3.587606
C	35	-1.65198	-2.90553	3.450293
C	36	1.979112	3.611075	0.484901
C	37	2.774688	4.828468	0.705614
O	38	1.35912	4.89234	0.610245
C	39	1.932588	3.044919	-0.91613
H	40	2.243987	-1.69856	-3.57805
H	41	2.537419	-3.19049	-2.6964

H	42	3.16171	-0.41101	-1.85855
H	43	3.660647	-1.88209	-1.06946
H	44	1.38928	0.470454	-2.42623
H	45	-0.21493	0.884484	-1.83943
H	46	-1.06724	-1.98865	-5.35063
H	47	0.641341	-2.37653	-5.0795
H	48	-0.61888	-3.5313	-4.59162
H	49	-2.05291	-0.00773	-1.86341
H	50	-2.60912	-1.75032	-3.42828
H	51	-2.00063	-3.01532	-2.35215
H	52	-4.50129	-0.26706	-2.37539
H	53	-5.48161	-0.84488	-1.00877
H	54	2.809408	-2.36806	1.031725
H	55	1.0696	-2.3767	1.367973
H	56	1.715311	-3.33321	0.023321
H	57	3.954657	2.329019	1.656437
H	58	3.100951	1.418457	2.884905
H	59	1.788742	3.38562	2.550922
H	60	-1.9302	-2.5249	0.392968
H	61	-0.71803	3.035257	0.338647
H	62	-1.65533	2.474103	1.719377
H	63	-0.50946	3.819604	1.897996
H	64	0.275303	2.482444	3.850357
H	65	1.227825	1.01355	3.652561
H	66	-3.5137	1.53722	-0.90522
H	67	-4.49404	0.962917	0.443911
H	68	-5.279	1.652931	-0.99457
H	69	-0.98864	0.821234	4.858115
H	70	-1.80274	0.951615	3.308534
H	71	-2.67176	-3.27765	3.36123
H	72	-1.07435	-3.14827	2.556453
H	73	-1.1637	-3.3329	4.329843
H	74	3.186634	5.035225	1.69333
H	75	3.320533	5.27304	-0.12575
H	76	2.113816	3.841409	-1.6426
H	77	0.954969	2.610078	-1.13094
H	78	2.689883	2.267231	-1.06145

S19. Coordinates of 4-*epi*-**2 used for NMR calculations**

All conformers with population > 5% at 300K are listed. The structure refers to the lowest energy conformer.



Conformer 1, DFT energy -1695.12167 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	1.207861	0.315468	0.004672
C	2	2.851898	-1.3888	-0.43172
C	3	3.061572	0.067692	1.658155
C	4	3.785991	-0.57195	0.457071
C	5	1.951017	1.001067	1.120371
C	6	1.479018	-0.86136	-0.58081
C	7	0.328196	-1.72693	-1.05381
C	8	-0.95251	-0.85009	-1.26298
C	9	-1.29367	-0.12558	0.064439
C	10	-0.15481	0.862189	0.389741
C	11	-1.9659	-1.8997	-1.79681
C	12	-1.08723	-2.93539	-2.57357
C	13	0.390814	-2.51197	-2.37397
C	14	4.051935	0.705797	2.63445
O	15	3.422857	1.362949	3.73836
C	16	4.14815	0.160596	3.995862
C	17	5.276433	1.417362	2.093089
O	18	3.229407	-2.41599	-0.96853
O	19	-0.44469	2.163348	-0.08618
C	20	0.158327	-2.78819	0.071457
C	21	0.135873	0.016466	2.841288

C	22	0.729955	0.226076	4.21511
O	23	0.492993	1.459115	4.670499
C	24	1.077491	1.771065	5.933978
O	25	1.295139	-0.63373	4.853542
C	26	-0.70682	0.20504	-2.37719
O	27	-1.65451	1.267947	-2.36419
C	28	-3.00108	0.988227	-2.74427
C	29	-3.06883	0.507728	-4.20047
C	30	-2.9641	-1.01926	-4.09361
C	31	-3.186	-1.33391	-2.58188
C	32	-3.79073	2.258177	-2.44982
C	33	-3.89757	2.600101	-0.96473
O	34	-3.5513	-0.06847	-2.0043
C	35	-4.38221	-2.25965	-2.39062
C	36	0.50756	1.067387	1.806253
C	37	2.438142	2.415179	0.78596
H	38	2.564985	-0.74684	2.199541
H	39	4.249497	0.206038	-0.16493
H	40	4.587251	-1.2429	0.780724
H	41	-2.24209	0.407715	-0.00387
H	42	-1.41199	-0.87405	0.852407
H	43	-2.39638	-2.39695	-0.92034
H	44	-1.34488	-2.99922	-3.63294
H	45	-1.24929	-3.93954	-2.17136
H	46	0.744403	-1.88245	-3.19708
H	47	1.072096	-3.36238	-2.31361
H	48	3.532087	-0.6835	4.296548
H	49	5.072964	0.29755	4.55647
H	50	5.800657	1.9097	2.916575
H	51	5.024131	2.178026	1.351765
H	52	5.962766	0.702741	1.627435
H	53	-0.92942	2.076228	-0.92642
H	54	1.056193	-3.41203	0.091579
H	55	0.049556	-2.33581	1.058111
H	56	-0.69838	-3.44731	-0.08732
H	57	-0.95519	0.034729	2.962056
H	58	0.410384	-0.99417	2.530384
H	59	0.744014	1.065197	6.697717
H	60	0.742182	2.780277	6.17204
H	61	2.165014	1.740058	5.851277
H	62	-0.68043	-0.25905	-3.36621
H	63	0.256796	0.69948	-2.24763
H	64	-2.2791	0.961685	-4.80374
H	65	-4.03063	0.805157	-4.62667

H	66	-2.00279	-1.37588	-4.46382
H	67	-3.73012	-1.51641	-4.69479
H	68	-3.31749	3.077794	-3.00201
H	69	-4.7945	2.121638	-2.86626
H	70	-2.91791	2.756812	-0.50637
H	71	-4.40025	1.793358	-0.42362
H	72	-4.48111	3.516014	-0.83035
H	73	-4.14958	-3.26206	-2.76694
H	74	-4.63879	-2.33805	-1.3297
H	75	-5.25413	-1.8764	-2.92974
H	76	0.27999	2.063842	2.191337
H	77	3.270061	2.386803	0.073656
H	78	1.631988	2.993787	0.333843
H	79	2.768794	2.92234	1.697429

Conformer 2, DFT energy -1695.12140 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	1.174496	0.27684	0.112091
C	2	2.829925	-1.41777	-0.32152
C	3	3.033651	0.045466	1.763469
C	4	3.760111	-0.59239	0.563298
C	5	1.914371	0.968241	1.225955
C	6	1.453404	-0.89989	-0.47003
C	7	0.308811	-1.77413	-0.94247
C	8	-0.97523	-0.90368	-1.15324
C	9	-1.32247	-0.18087	0.173354
C	10	-0.19256	0.816061	0.498753
C	11	-1.98412	-1.95675	-1.68561
C	12	-1.10163	-2.98393	-2.46889
C	13	0.375753	-2.55922	-2.26283
C	14	4.020593	0.693401	2.736561
O	15	3.389154	1.34271	3.84321
C	16	4.127606	0.14799	4.09723
C	17	5.235726	1.417486	2.19093
O	18	3.213684	-2.4446	-0.85584
O	19	-0.50125	2.112514	0.027156
C	20	0.144435	-2.8366	0.181987
C	21	0.110595	-0.0322	2.948931
C	22	0.708124	0.178295	4.32133
O	23	0.461792	1.408357	4.781801
C	24	1.045168	1.719715	6.045001
O	25	1.284019	-0.67867	4.954718
C	26	-0.7289	0.148042	-2.27123

O	27	-1.6765	1.20917	-2.26387
C	28	-3.02578	0.929859	-2.62826
C	29	-3.12258	0.447624	-4.08123
C	30	-3.00698	-1.07823	-3.97219
C	31	-3.21262	-1.39095	-2.45805
C	32	-3.80367	2.195148	-2.29682
C	33	-3.35658	3.415364	-3.09717
O	34	-3.5689	-0.12327	-1.87788
C	35	-4.40803	-2.31421	-2.25282
C	36	0.472118	1.022696	1.914722
C	37	2.387045	2.385715	0.887228
H	38	2.544926	-0.77162	2.308114
H	39	4.218151	0.185862	-0.06124
H	40	4.565353	-1.25718	0.887759
H	41	-2.27426	0.34718	0.103857
H	42	-1.43863	-0.93031	0.960668
H	43	-2.40609	-2.45997	-0.80851
H	44	-1.3561	-3.03959	-3.52947
H	45	-1.26313	-3.99159	-2.07543
H	46	0.733029	-1.93036	-3.0847
H	47	1.056853	-3.40953	-2.19982
H	48	3.522347	-0.70347	4.397782
H	49	5.053267	0.294002	4.654182
H	50	5.759398	1.913207	3.012713
H	51	4.972363	2.177017	1.452302
H	52	5.926359	0.710365	1.720355
H	53	-1.01238	2.019092	-0.79744
H	54	1.047642	-3.45204	0.205789
H	55	0.026979	-2.38608	1.168307
H	56	-0.70493	-3.50376	0.018757
H	57	-0.98014	-0.0208	3.073265
H	58	0.38976	-1.04031	2.634679
H	59	0.730444	0.999056	6.803069
H	60	0.687691	2.71984	6.292722
H	61	2.133452	1.712747	5.958284
H	62	-0.70207	-0.3194	-3.25885
H	63	0.233168	0.644778	-2.14157
H	64	-2.35124	0.902682	-4.70679
H	65	-4.09729	0.739973	-4.4826
H	66	-2.04579	-1.42752	-4.34954
H	67	-3.77362	-1.58241	-4.56663
H	68	-4.86285	1.98246	-2.47401
H	69	-3.68666	2.380244	-1.22321
H	70	-3.4992	3.261419	-4.17299

H	71	-2.2984	3.630952	-2.92369
H	72	-3.9371	4.296902	-2.80739
H	73	-4.18108	-3.31727	-2.63057
H	74	-4.65285	-2.39112	-1.18925
H	75	-5.28517	-1.93051	-2.78269
H	76	0.238532	2.016876	2.301553
H	77	3.21592	2.363385	0.171816
H	78	1.573833	2.955718	0.436996
H	79	2.716727	2.897741	1.795683

Conformer 3, DFT energy -1695.12089 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	1.58891	0.289963	0.122165
C	2	3.178213	-1.47591	-0.26382
C	3	3.450202	0.042428	1.761226
C	4	4.148063	-0.64376	0.571768
C	5	2.371277	0.995118	1.199476
C	6	1.814194	-0.91838	-0.4121
C	7	0.627491	-1.76569	-0.82456
C	8	-0.62799	-0.85826	-1.05669
C	9	-0.92148	-0.05709	0.236164
C	10	0.254818	0.904886	0.495214
C	11	-1.68324	-1.9013	-1.51309
C	12	-0.85443	-2.99338	-2.26636
C	13	0.641416	-2.61556	-2.10524
C	14	4.418744	0.691506	2.74495
O	15	5.642152	-0.0151	2.953384
C	16	5.704752	1.250519	2.308489
C	17	3.796541	1.205098	4.024412
O	18	3.517442	-2.53037	-0.77007
O	19	0.016685	2.189313	-0.05009
C	20	0.444332	-2.7631	0.355865
C	21	0.578603	0.193938	3.004471
C	22	-0.90103	0.156538	3.32716
O	23	-1.49115	1.340693	3.11683
C	24	-2.90596	1.362101	3.292314
O	25	-1.4883	-0.8224	3.723478
C	26	-0.37609	0.130336	-2.228
O	27	-1.28819	1.224472	-2.24211
C	28	-2.65802	0.973299	-2.55724
C	29	-2.79963	0.431412	-3.98601
C	30	-2.73417	-1.09234	-3.81402
C	31	-2.91148	-1.33246	-2.28288

C	32	-3.39245	2.281147	-2.2852
C	33	-3.44098	2.674279	-0.80828
O	34	-3.21436	-0.03013	-1.75135
C	35	-4.13075	-2.20483	-2.00572
C	36	0.940517	1.162786	1.890341
C	37	2.943563	2.358036	0.790685
H	38	2.94353	-0.75569	2.322166
H	39	4.59541	0.104486	-0.0978
H	40	4.952871	-1.29955	0.91119
H	41	-1.8515	0.505562	0.160448
H	42	-1.05384	-0.76792	1.054662
H	43	-2.09849	-2.34722	-0.60248
H	44	-1.13036	-3.08251	-3.31918
H	45	-1.04608	-3.97694	-1.8283
H	46	1.005749	-2.03993	-2.96235
H	47	1.292608	-3.48629	-2.01183
H	48	5.995219	1.22375	1.25996
H	49	6.16284	2.049571	2.890808
H	50	4.557761	1.656111	4.666589
H	51	3.337545	0.375986	4.575667
H	52	3.022583	1.953906	3.820581
H	53	-0.49349	2.078359	-0.87379
H	54	1.33803	-3.38996	0.414061
H	55	0.325417	-2.26249	1.31799
H	56	-0.41331	-3.42613	0.224357
H	57	0.864356	-0.836	2.778676
H	58	1.108419	0.464665	3.924553
H	59	-3.38118	0.664736	2.596649
H	60	-3.21135	2.384382	3.073211
H	61	-3.17405	1.088175	4.315912
H	62	-0.39147	-0.38088	-3.19374
H	63	0.606502	0.597253	-2.14561
H	64	-2.02306	0.833455	-4.64103
H	65	-3.76966	0.738555	-4.38599
H	66	-1.7961	-1.49255	-4.19859
H	67	-3.53364	-1.5932	-4.36622
H	68	-2.90704	3.064673	-2.87839
H	69	-4.41347	2.1686	-2.6668
H	70	-2.44234	2.809848	-0.38382
H	71	-3.95568	1.90251	-0.22706
H	72	-3.9882	3.613779	-0.68691
H	73	-3.94692	-3.23112	-2.34242
H	74	-4.34984	-2.22588	-0.93373
H	75	-5.00837	-1.81519	-2.53122

H	76	0.74759	2.190352	2.207709
H	77	3.813832	2.237583	0.13631
H	78	2.189627	2.939333	0.258262
H	79	3.261328	2.926018	1.671936

Conformer 4, DFT energy -1695.12088 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	1.269595	0.341991	0.081959
C	2	2.927711	-1.35268	-0.34111
C	3	3.121122	0.114106	1.742263
C	4	3.853557	-0.52519	0.546259
C	5	2.003972	1.035568	1.197984
C	6	1.551646	-0.83601	-0.49643
C	7	0.409785	-1.71174	-0.97267
C	8	-0.87399	-0.84259	-1.19116
C	9	-1.2273	-0.117	0.132352
C	10	-0.09934	0.88101	0.46118
C	11	-1.87928	-1.89823	-1.72573
C	12	-0.99228	-2.925	-2.50437
C	13	0.483844	-2.4991	-2.29132
C	14	4.103369	0.764209	2.71863
O	15	3.466338	1.416558	3.820375
C	16	4.203241	0.222315	4.081132
C	17	5.321453	1.486716	2.177486
O	18	3.314374	-2.37967	-0.87242
O	19	-0.40634	2.176668	-0.01293
C	20	0.241134	-2.77264	0.152672
C	21	0.192014	0.037882	2.914193
C	22	0.782678	0.251326	4.289008
O	23	0.534306	1.482524	4.745228
C	24	1.113429	1.798581	6.009566
O	25	1.355158	-0.60416	4.927231
C	26	-0.62332	0.206621	-2.31107
O	27	-1.56879	1.270258	-2.31082
C	28	-2.9193	0.988202	-2.67431
C	29	-3.00088	0.504831	-4.12752
C	30	-2.89601	-1.02174	-4.01668
C	31	-3.10517	-1.33312	-2.50269
C	32	-3.6755	2.268332	-2.33519
C	33	-5.18961	2.165722	-2.48876
O	34	-3.45844	-0.06493	-1.92337
C	35	-4.30392	-2.25214	-2.29888
C	36	0.558443	1.090707	1.879674

C	37	2.477787	2.452946	0.859583
H	38	2.630345	-0.70236	2.286027
H	39	4.313414	0.252903	-0.07775
H	40	4.658365	-1.18881	0.875194
H	41	-2.17866	0.410996	0.057804
H	42	-1.34681	-0.86498	0.920704
H	43	-2.30394	-2.40114	-0.84966
H	44	-1.24135	-2.98084	-3.56628
H	45	-1.15504	-3.9328	-2.11157
H	46	0.844957	-1.87142	-3.11247
H	47	1.165193	-3.34893	-2.22312
H	48	3.595986	-0.62809	4.381052
H	49	5.126106	0.369557	4.642377
H	50	5.840283	1.985367	3.000676
H	51	5.062393	2.243664	1.434653
H	52	6.01498	0.777984	1.713397
H	53	-0.90546	2.083917	-0.8444
H	54	1.146298	-3.38538	0.18317
H	55	0.115862	-2.32072	1.137682
H	56	-0.60525	-3.44303	-0.01509
H	57	-0.89919	0.049639	3.033317
H	58	0.472571	-0.97074	2.603524
H	59	0.794634	1.082006	6.76978
H	60	0.757707	2.800111	6.252246
H	61	2.201738	1.789216	5.926259
H	62	-0.59289	-0.26437	-3.29703
H	63	0.339233	0.702239	-2.17956
H	64	-2.21259	0.957124	-4.73399
H	65	-3.96236	0.798913	-4.55479
H	66	-1.93718	-1.37897	-4.39276
H	67	-3.66648	-1.52108	-4.61034
H	68	-3.42463	2.518025	-1.29811
H	69	-3.27146	3.071357	-2.96117
H	70	-5.57969	1.337249	-1.89253
H	71	-5.48891	2.006963	-3.52996
H	72	-5.66588	3.090164	-2.14981
H	73	-4.08128	-3.25566	-2.67817
H	74	-4.54939	-2.32979	-1.23534
H	75	-5.17918	-1.86338	-2.82863
H	76	0.322501	2.08562	2.263437
H	77	3.310349	2.430051	0.148185
H	78	1.666409	3.02185	0.404541
H	79	2.802812	2.966444	1.769163

Conformer 5, DFT energy -1695.12078 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	1.56532	0.37903	0.093545
C	2	3.196099	-1.33983	-0.33956
C	3	3.374799	0.081662	1.757757
C	4	4.134426	-0.54936	0.576494
C	5	2.330613	1.066532	1.193225
C	6	1.820845	-0.80904	-0.47386
C	7	0.6521	-1.6825	-0.88708
C	8	-0.63274	-0.80771	-1.08423
C	9	-0.93317	-0.0381	0.226587
C	10	0.217026	0.953201	0.487625
C	11	-1.66452	-1.87113	-1.54778
C	12	-0.81618	-2.93199	-2.32327
C	13	0.669888	-2.51216	-2.18072
C	14	4.288566	0.653107	2.839462
O	15	3.569019	1.31214	3.889926
C	16	4.206908	0.075513	4.188659
C	17	5.582496	1.327073	2.436723
O	18	3.57082	-2.35757	-0.89447
O	19	-0.05604	2.238936	-0.03742
C	20	0.513987	-2.70049	0.282085
C	21	0.56907	0.248097	3.008608
C	22	-0.8983	0.214185	3.377752
O	23	-1.51522	1.374262	3.110265
C	24	-2.92284	1.388967	3.333754
O	25	-1.46144	-0.7477	3.847236
C	26	-0.41909	0.208607	-2.23898
O	27	-1.36202	1.275997	-2.2287
C	28	-2.726	0.992007	-2.53748
C	29	-2.86306	0.470549	-3.97434
C	30	-2.74966	-1.05302	-3.82842
C	31	-2.91224	-1.32401	-2.30085
C	32	-3.4943	2.273573	-2.23571
C	33	-3.54552	2.634165	-0.75126
O	34	-3.24777	-0.0406	-1.74521
C	35	-4.10471	-2.23536	-2.03409
C	36	0.902192	1.208635	1.88128
C	37	2.89325	2.445146	0.838836
H	38	2.814942	-0.73695	2.223843
H	39	4.637704	0.222912	-0.02026
H	40	4.906635	-1.24689	0.914129
H	41	-1.88166	0.495952	0.172275

H	42	-1.03073	-0.76276	1.039228
H	43	-2.06237	-2.33948	-0.64072
H	44	-1.10614	-3.02027	-3.37262
H	45	-0.97181	-3.92441	-1.89057
H	46	1.002717	-1.91307	-3.03457
H	47	1.348115	-3.36457	-2.11199
H	48	3.534186	-0.76059	4.380292
H	49	5.06131	0.145743	4.861361
H	50	6.062626	1.75805	3.319323
H	51	5.417337	2.129737	1.714465
H	52	6.269613	0.602348	1.988149
H	53	-0.57423	2.128791	-0.85491
H	54	1.412129	-3.32446	0.300582
H	55	0.428986	-2.21173	1.254336
H	56	-0.34582	-3.36532	0.171986
H	57	0.835286	-0.78762	2.781256
H	58	1.150307	0.531974	3.894417
H	59	-3.40859	0.611393	2.737832
H	60	-3.25947	2.37643	3.017769
H	61	-3.14841	1.222879	4.390445
H	62	-0.4246	-0.28485	-3.21416
H	63	0.549599	0.702828	-2.15213
H	64	-2.10446	0.906979	-4.62826
H	65	-3.84537	0.753765	-4.36163
H	66	-1.80152	-1.41798	-4.22352
H	67	-3.53619	-1.56879	-4.38578
H	68	-3.03224	3.081124	-2.8135
H	69	-4.51299	2.142493	-2.61483
H	70	-2.54836	2.776875	-0.32717
H	71	-4.04482	1.84179	-0.18633
H	72	-4.10798	3.561978	-0.60868
H	73	-3.89363	-3.24976	-2.39007
H	74	-4.31737	-2.28143	-0.96177
H	75	-4.99561	-1.86182	-2.54821
H	76	0.703809	2.23346	2.200731
H	77	3.754417	2.365696	0.166192
H	78	2.128415	3.040691	0.337842
H	79	3.203598	2.968049	1.74887

Conformer 6, DFT energy -1695.12039 au (ωB97X-V/6-311+G(2df,2p))

Tag	Symbol	X	Y	Z
C	1	1.587053	0.367254	0.057905
C	2	3.128807	-1.45517	-0.25121

C	3	3.466439	0.16247	1.684173
C	4	4.130024	-0.60038	0.52187
C	5	2.3982	1.107962	1.089013
C	6	1.777833	-0.87163	-0.4171
C	7	0.566156	-1.70675	-0.78032
C	8	-0.66851	-0.77844	-1.04431
C	9	-0.93121	0.08925	0.213081
C	10	0.272379	1.030847	0.415631
C	11	-1.75258	-1.81356	-1.4464
C	12	-0.95703	-2.95959	-2.15501
C	13	0.549114	-2.61282	-2.02198
C	14	4.464736	0.84245	2.616221
O	15	5.681715	0.127458	2.834692
C	16	5.748541	1.359182	2.127503
C	17	3.878967	1.428237	3.881523
O	18	3.433767	-2.54926	-0.69275
O	19	0.063377	2.295127	-0.18357
C	20	0.367383	-2.6484	0.442352
C	21	0.622423	0.400649	2.93946
C	22	-0.82761	0.567975	3.335267
O	23	-1.3936	-0.61461	3.634954
C	24	-2.78049	-0.55363	3.968677
O	25	-1.41883	1.619807	3.378536
C	26	-0.40047	0.148942	-2.26196
O	27	-1.28454	1.263633	-2.32073
C	28	-2.6612	1.033032	-2.62007
C	29	-2.82207	0.42664	-4.02086
C	30	-2.8007	-1.08804	-3.77623
C	31	-2.972	-1.24939	-2.23421
C	32	-3.36209	2.37072	-2.41432
C	33	-3.38596	2.851817	-0.96443
O	34	-3.23827	0.083317	-1.76434
C	35	-4.21039	-2.07684	-1.90829
C	36	0.982216	1.330076	1.791308
C	37	2.990425	2.437491	0.606744
H	38	2.953279	-0.59411	2.294663
H	39	4.581416	0.101363	-0.19268
H	40	4.925268	-1.25437	0.883884
H	41	-1.84741	0.672007	0.121761
H	42	-1.06923	-0.57721	1.067798
H	43	-2.17164	-2.20739	-0.51344
H	44	-1.24308	-3.08939	-3.20093
H	45	-1.17006	-3.91774	-1.67224
H	46	0.919896	-2.08472	-2.90646

H	47	1.179346	-3.49451	-1.89425
H	48	6.015607	1.277955	1.075341
H	49	6.230523	2.178852	2.66024
H	50	4.659215	1.903782	4.480925
H	51	3.427334	0.63359	4.4856
H	52	3.107717	2.173197	3.658855
H	53	-0.46444	2.159549	-0.99131
H	54	1.255252	-3.28149	0.531156
H	55	0.248492	-2.10448	1.381276
H	56	-0.49715	-3.30898	0.333706
H	57	0.81107	-0.64903	2.705599
H	58	1.231314	0.644059	3.817518
H	59	-2.94959	0.140795	4.795068
H	60	-3.0596	-1.56873	4.25197
H	61	-3.36137	-0.22341	3.10191
H	62	-0.43572	-0.40622	-3.20328
H	63	0.593849	0.594109	-2.20598
H	64	-2.03563	0.77413	-4.69487
H	65	-3.78342	0.742653	-4.43434
H	66	-1.87946	-1.53467	-4.14963
H	67	-3.6203	-1.58989	-4.29765
H	68	-2.86782	3.106036	-3.05842
H	69	-4.3889	2.258102	-2.77789
H	70	-2.38182	2.987752	-0.55477
H	71	-3.91319	2.13245	-0.3314
H	72	-3.90819	3.811187	-0.89556
H	73	-4.05527	-3.12238	-2.19662
H	74	-4.42143	-2.04036	-0.8351
H	75	-5.08205	-1.69058	-2.44529
H	76	0.804962	2.367422	2.083832
H	77	3.845352	2.268807	-0.05616
H	78	2.2392	3.008808	0.061711
H	79	3.335681	3.037251	1.454634