

Supporting Information

Herpotriquinones A and B, Two Dimeric Naphthoquinone-Epoxycyclohexenone Adducts with Anti-Neuroinflammatory Activity from the Isopod-Associated Fungus *Herpotrichia* sp. SF09

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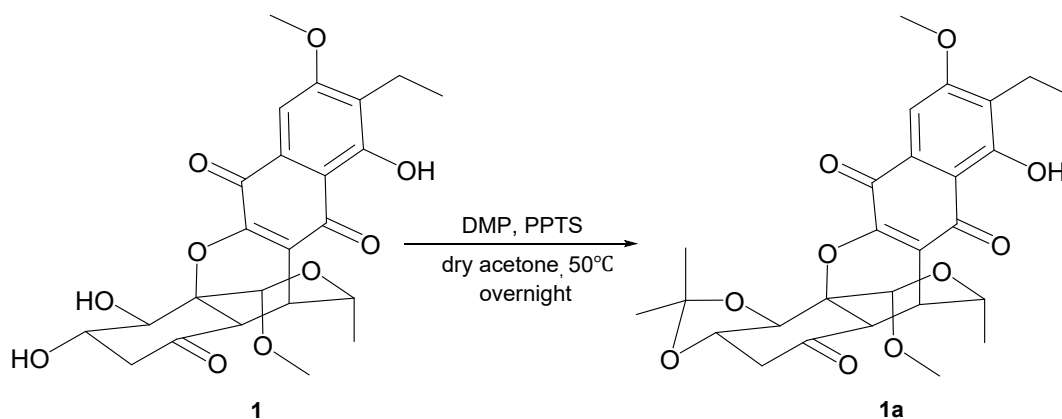
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Experimental Section

Preparation of acetonide derivative of **1**

Compound **1** (8.0 mg) in dry acetone (2.0 mL) was treated with 2,2-dimethoxypropane (DMP) (100 μ L) and catalytic amount pyridinium *p*-toluenesulfonate (PPTS) (1.0 mg) at room temperature then heated at 50 $^{\circ}$ C overnight. The solvent was evaporated under vacuum, the residue was purified by a silica gel chromatographic column (PE/EtOAc=2:1) to obtain the product as a yellow oil and crystallized in acetone/ EtOAc (v/v=1:1) as a red crystal; HR-ESI-MS: m/z 537.1728 [M + Na]⁺ (calcd. for C₂₇H₃₀O₁₀Na, 537.1731).



Computational details

The conformer rotamer ensemble sampling tool (crest)^{2,3} was utilized to generate candidate conformers and DFT calculations were performed using the Gaussian 16 program.⁴ The conformers within an energy window of 10 kcal/mol were optimized at B3LYP/6-31G(d) level of theory with Grimme's D3 dispersion correction ("EmpiricalDispersion=GD3" key words in input files). Frequency analysis of all optimized conformations was undertaken at the same level of theory to ensure they were true local minima on the potential energy surface. Then, energies of all optimized conformations were evaluated by M062X/6-311+G(2d,p) with D3 dispersion correction. Gibbs free energies of each conformers were calculated by adding "Thermal correction to Gibbs Free Energy" obtained by frequency analysis to electronic energies obtained at M062X/6-311+G(2d,p). Room-temperature (298.15 K) equilibrium

populations were calculated according to Boltzmann distribution law. Those conformers accounting for over 2% population were subjected to subsequent calculations.

NMR shielding constants were calculated with the GIAO method at mPW1PW91-SCRF/6-31+G(d,p) level with IEFPCM solvent model in acetone solvent. The shielding constants obtained were converted into chemical shifts by referencing to TMS at 0 ppm ($\delta_{\text{cal}} = \sigma_{\text{TMS}} - \sigma_{\text{cal}}$), where the σ_{TMS} was the shielding constant of TMS calculated at the same level.⁵ The DP4+ probabilities of each possible candidate were calculated with the EXCEL spreadsheet provided by Sarotti *et al.*⁶ For each possible candidate, the parameters a and b of the linear regression $\delta_{\text{cal}} = a\delta_{\text{exp}} + b$; the correlation coefficient, R^2 ; the mean absolute error (MAE) defined as $\sum_n |\delta_{\text{cal}} - \delta_{\text{exp}}|/n$; the corrected mean absolute error, CMAE, defined as $\sum_n |\delta_{\text{corr}} - \delta_{\text{exp}}|/n$, where $\delta_{\text{corr}} = (\delta_{\text{cal}} - b)/a$, were calculated.

Time-dependent density-functional theory (TDDFT) ECD calculations were run at PBE1PBE/6-311G(d) level of theory in MeOH with IEFPCM solvent model, respectively. For each conformer, 36 excited states were calculated.⁷ The calculated ECD curves were generated using Multiwfn 3.6 software.⁸

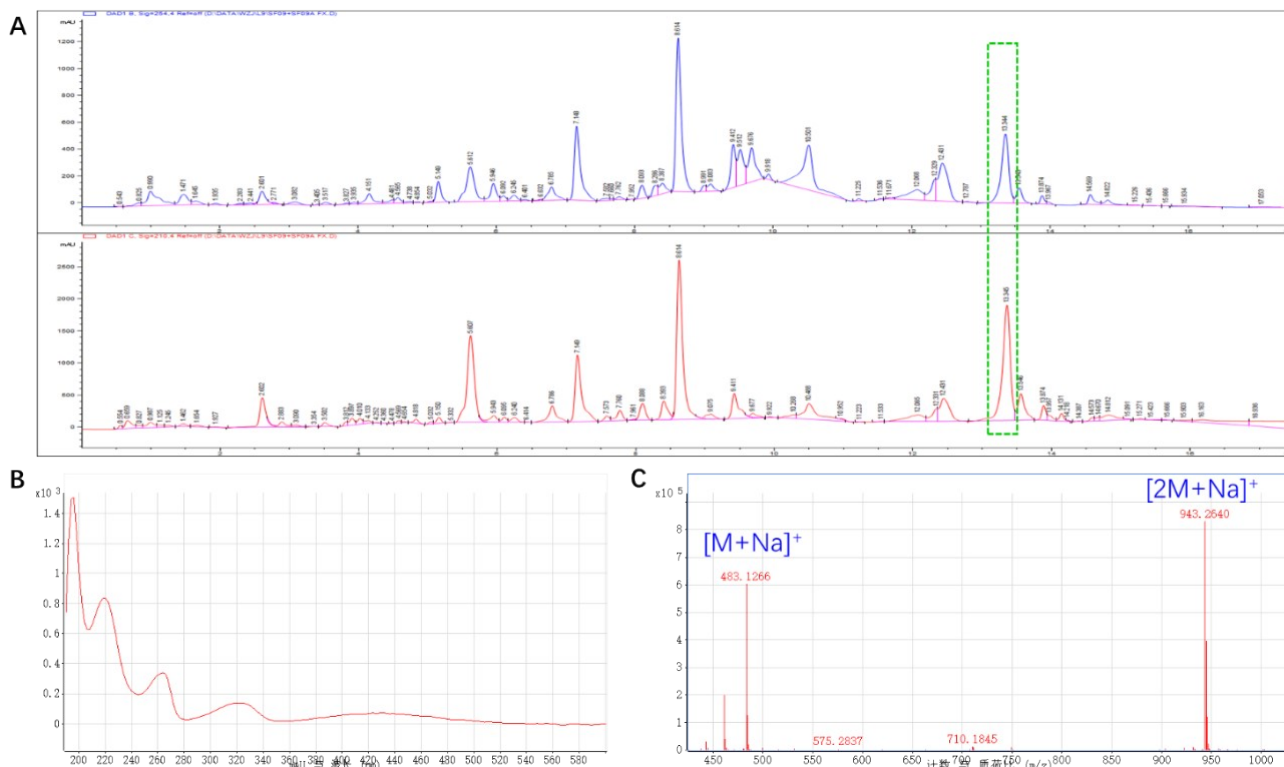


Figure S1. (A) HPLC-UV chromatogram of $CH_2Cl_2/MeOH$ (v/v = 100:8) fraction from *Herpotrichia* sp. extract; (B) UV spectrum for a compound at R_t 13.34 min; (C) HRESIMS spectrum for the peak at R_t 13.34 min.

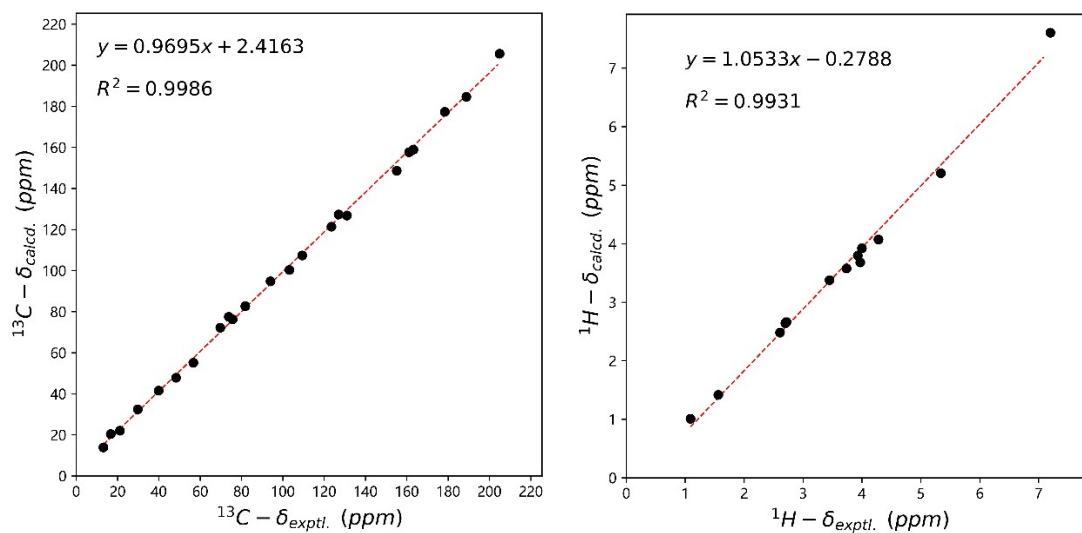


Figure S2. Linear regression analysis between the exptl. and calcd. ^{13}C and 1H NMR data of **2**.

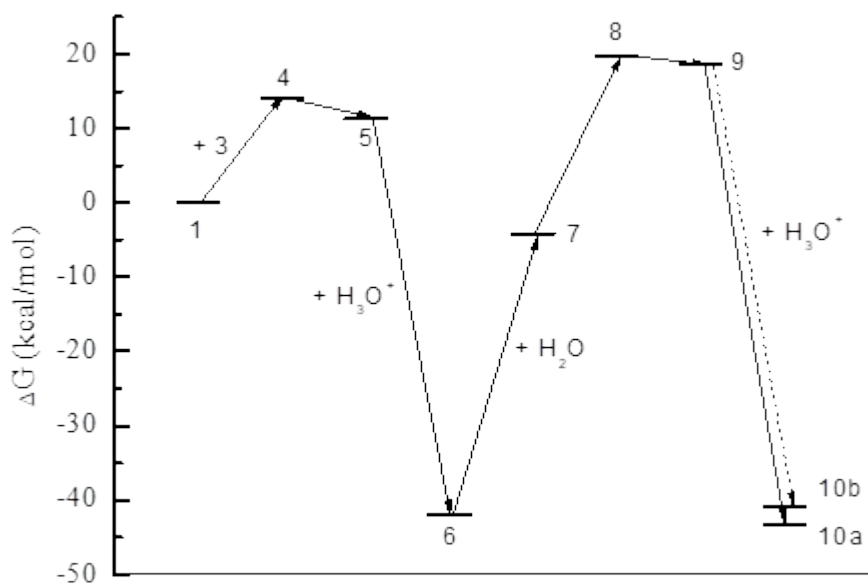


Figure S3. The schematic reaction mechanisms and free energy profiles of the reaction pathways from **VI** and **IX** to **XI** through intermediate **Xa** and **Xd**. The Gibbs Free Energies of the optimized structures were obtained from the thermal correction to Gibbs Free Energy in frequency analysis and the single point energy. Solvation effect was incorporated in single-point energy calculations using the PCM model with water as the solvent.

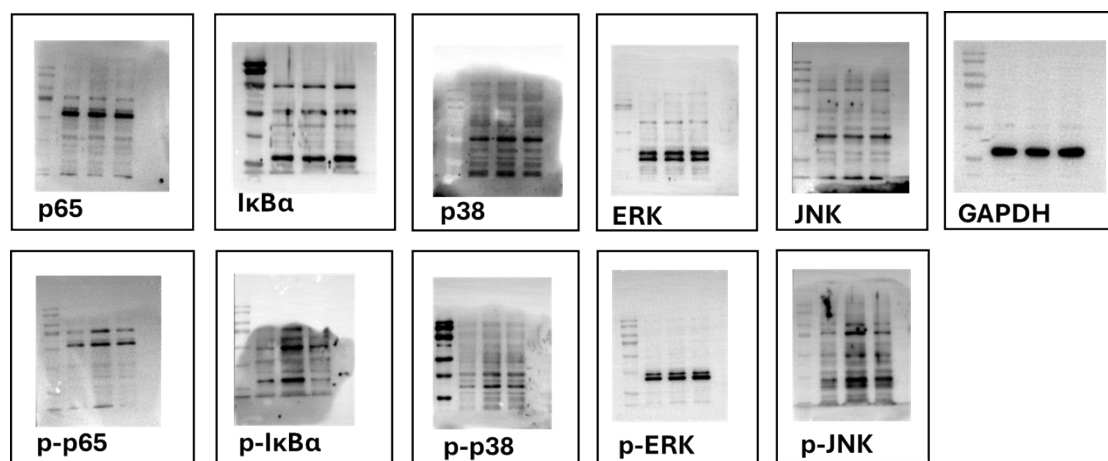


Figure S4. The raw images for all Western blotting.

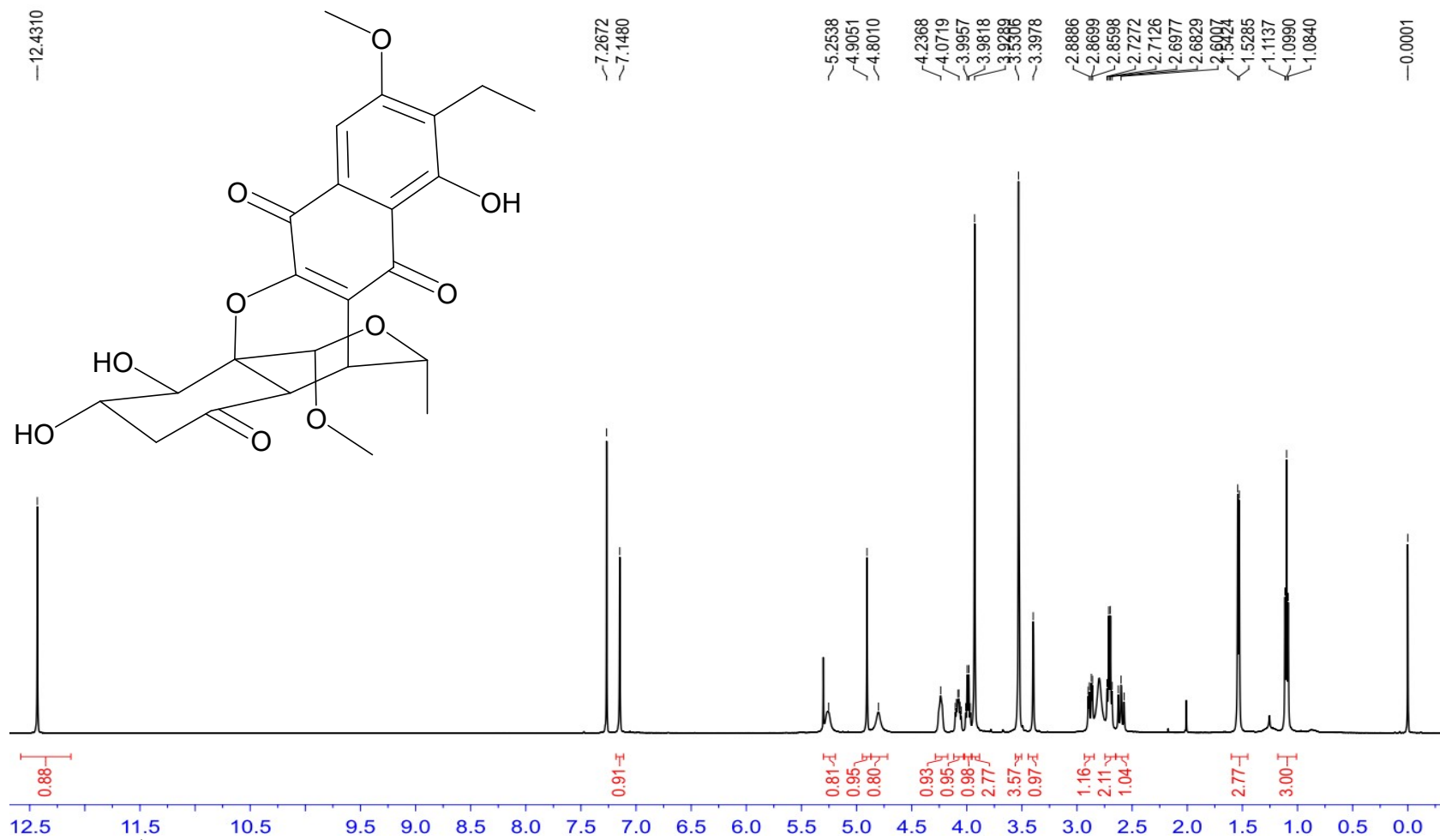


Figure S5. ¹H NMR spectrum of herpotriquinone A (**1**) in CDCl₃ (500 MHz).

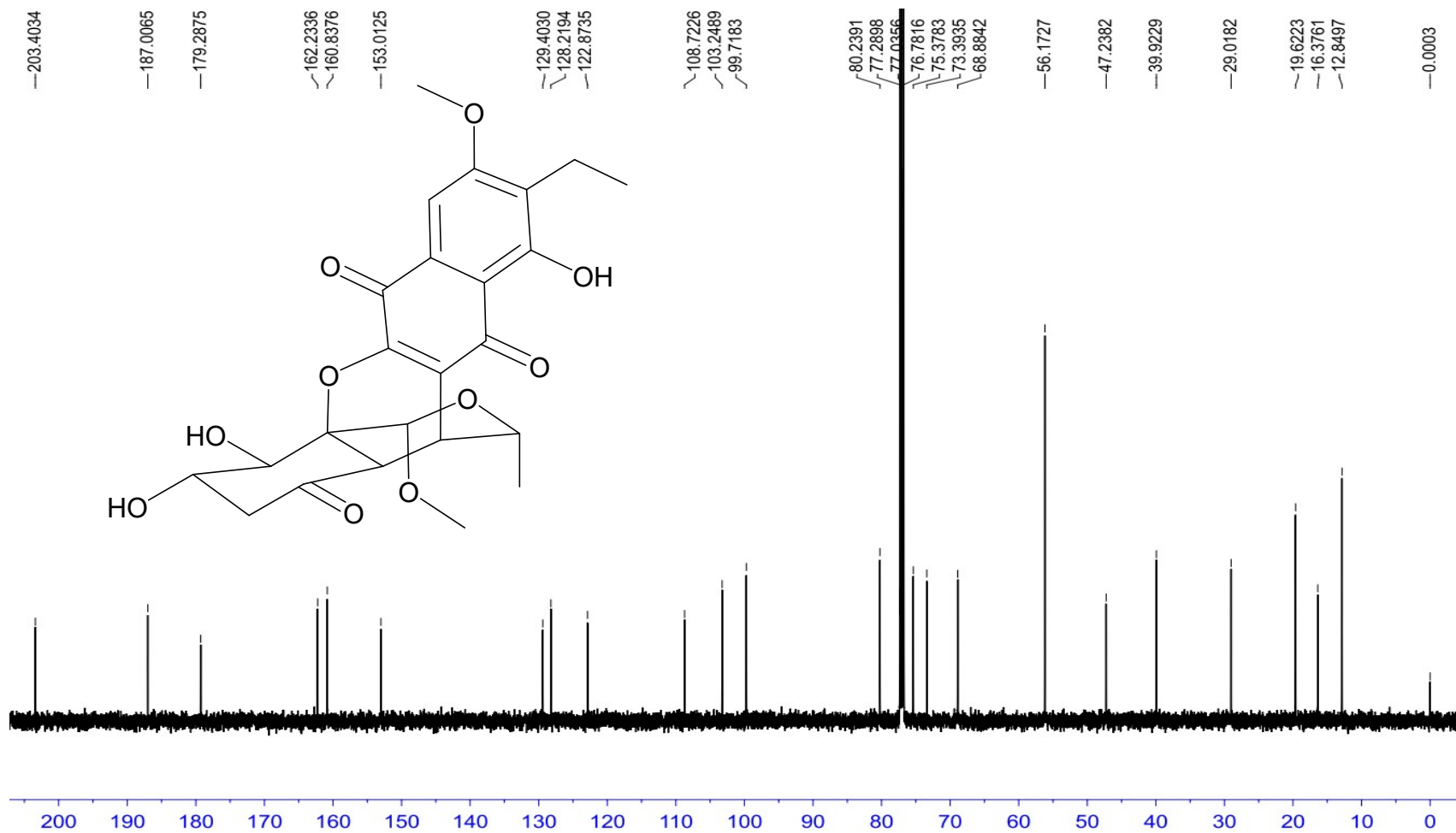


Figure S6. ^{13}C NMR spectrum of herpotriquinone A (**1**) in CDCl_3 (125 MHz).

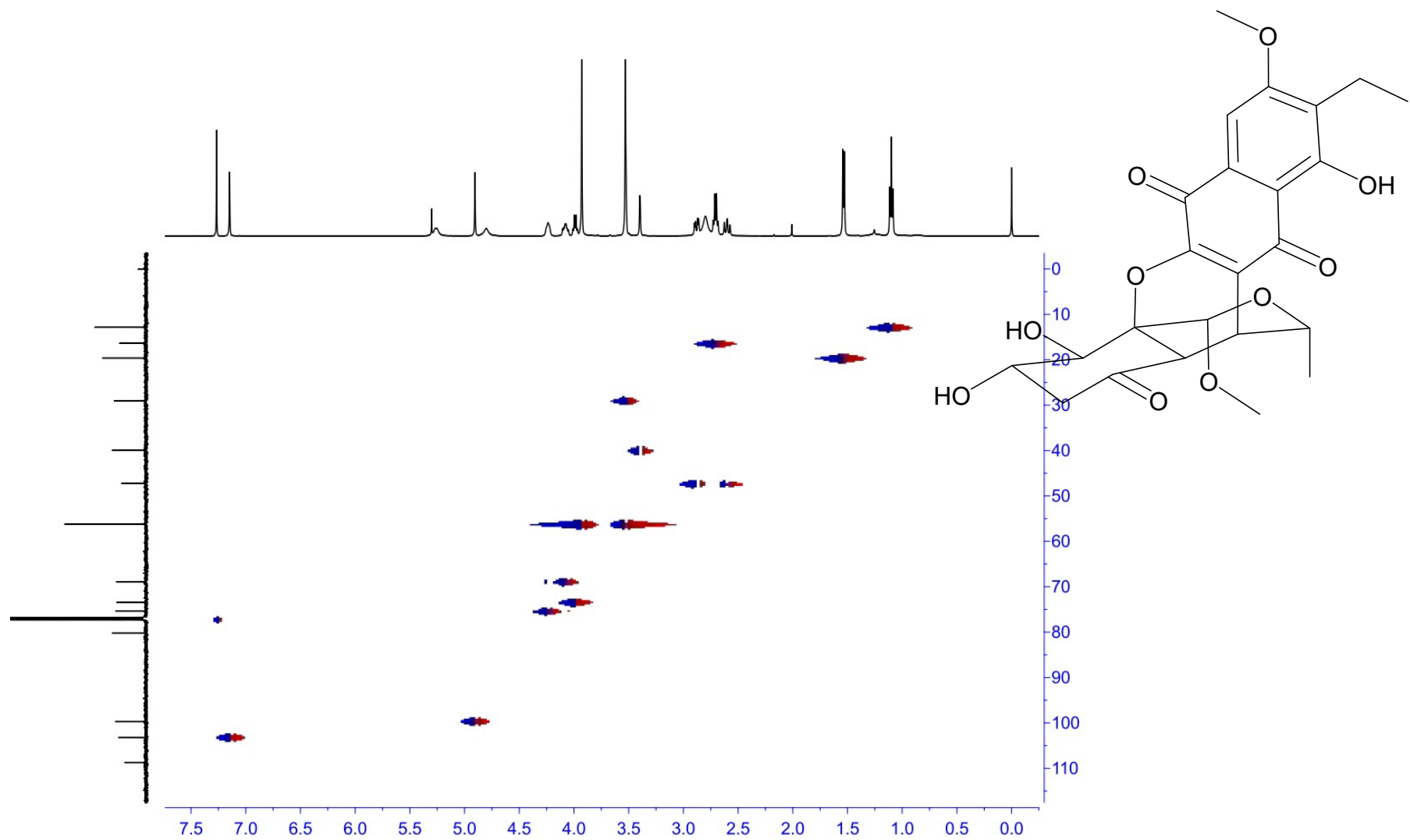


Figure S7. HMBC spectrum of herpotriquinone A (**1**) in CDCl₃.

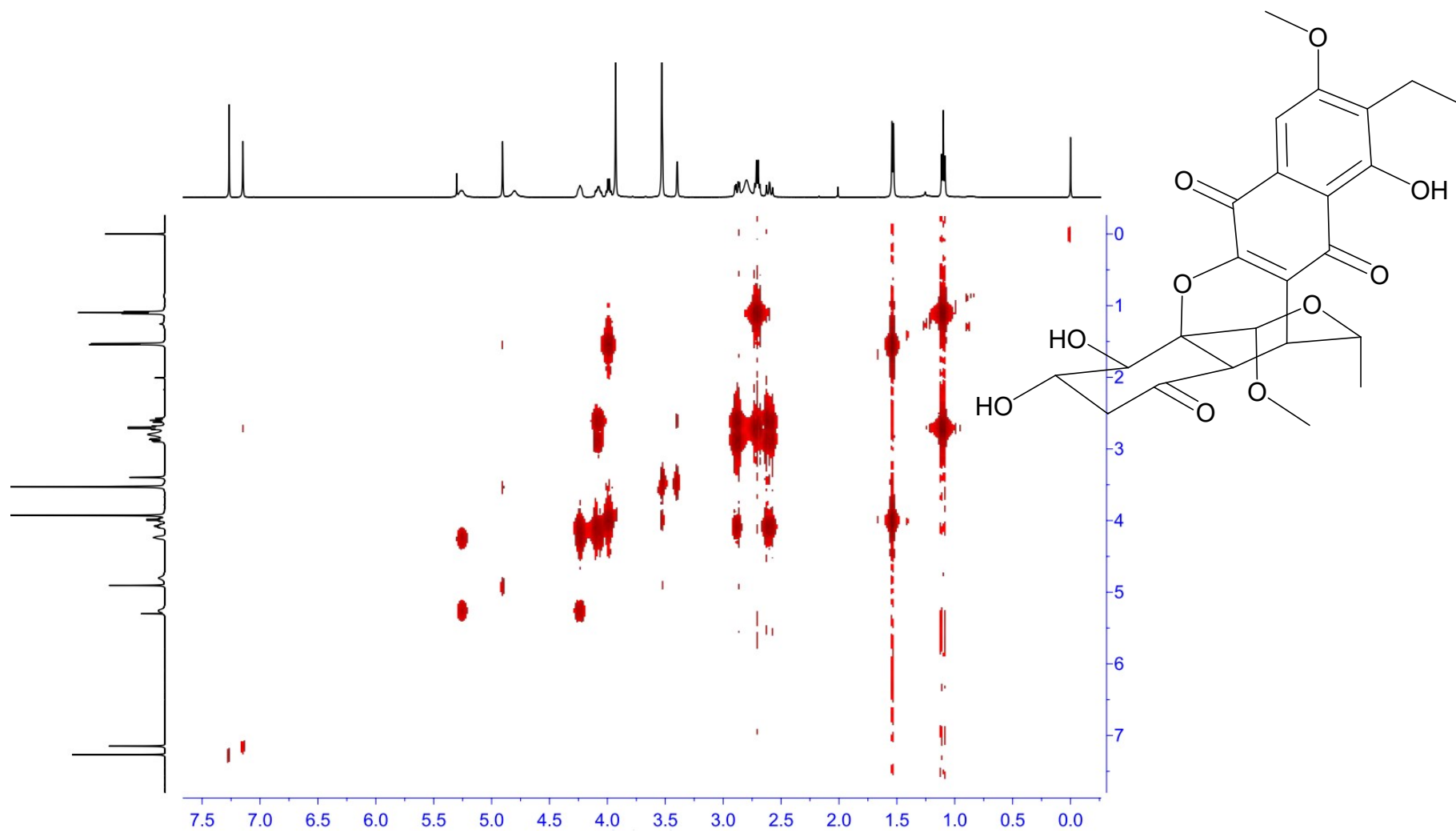
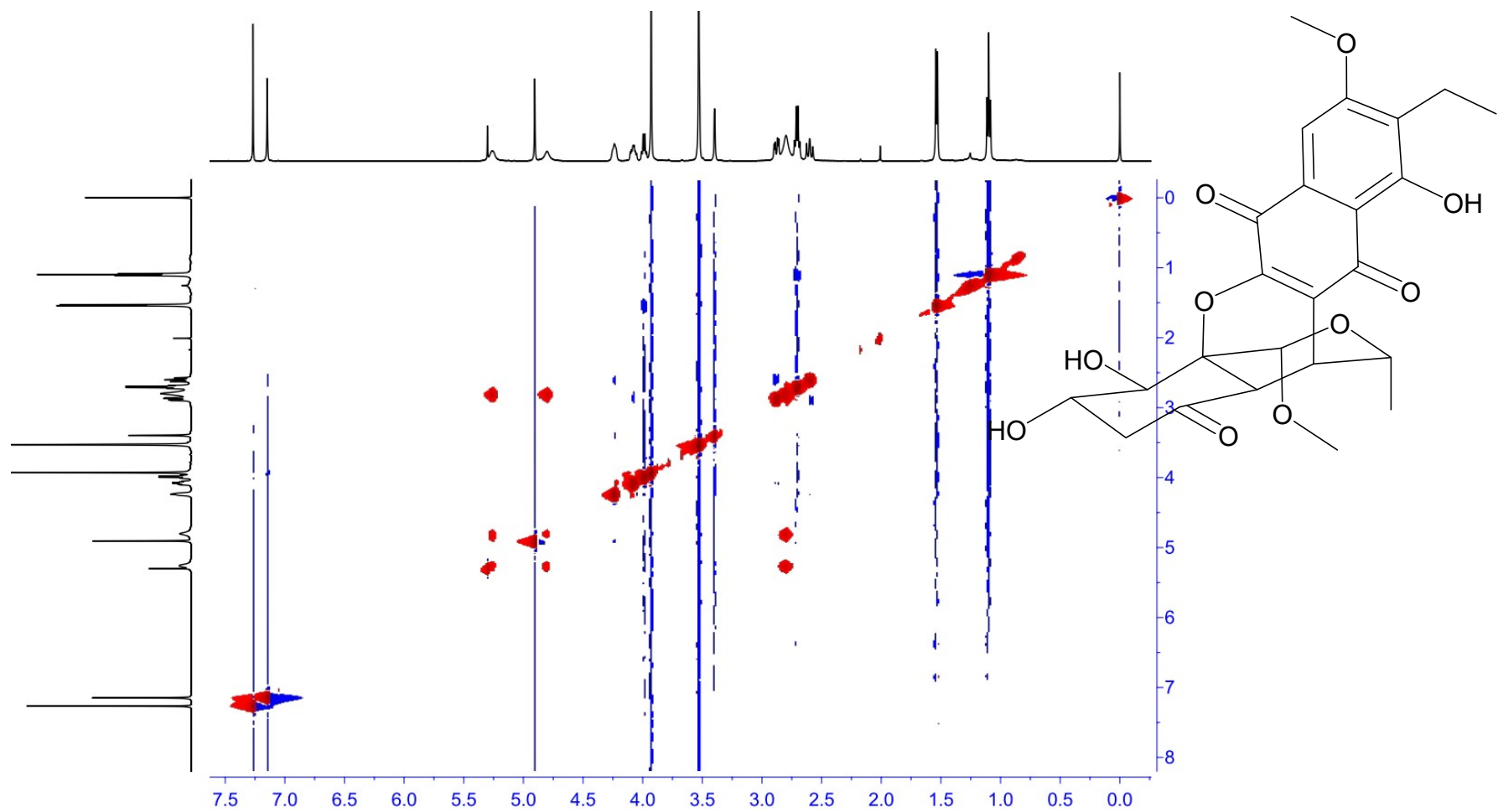


Figure S8. ^1H - ^1H COSY spectrum of herpotriquinone A (**1**) in CDCl_3 .



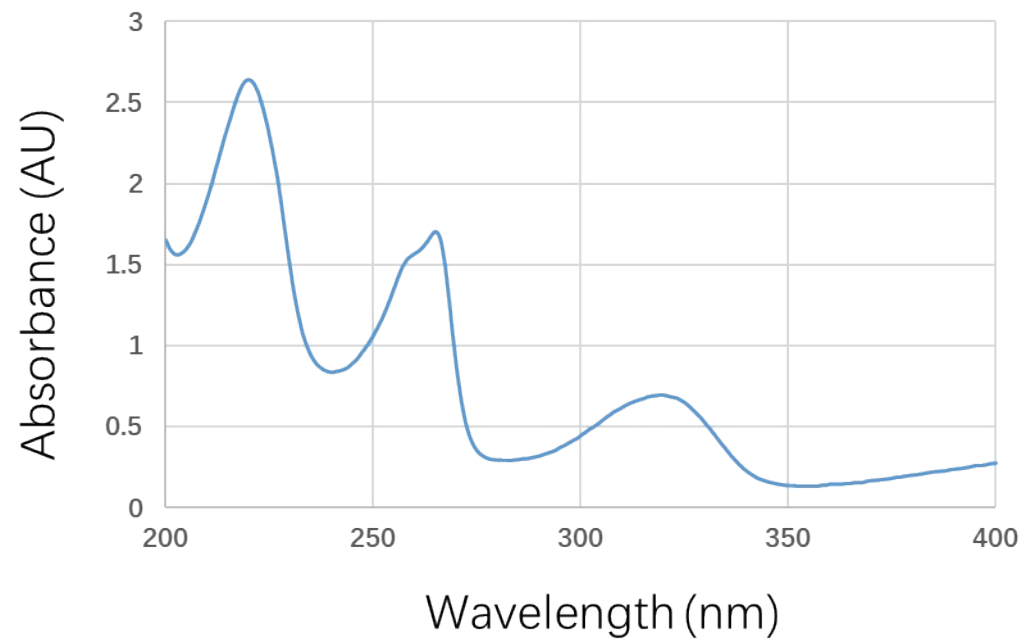


Figure S11. UV spectrum of herpotriquinone A (**1**) in methanol.

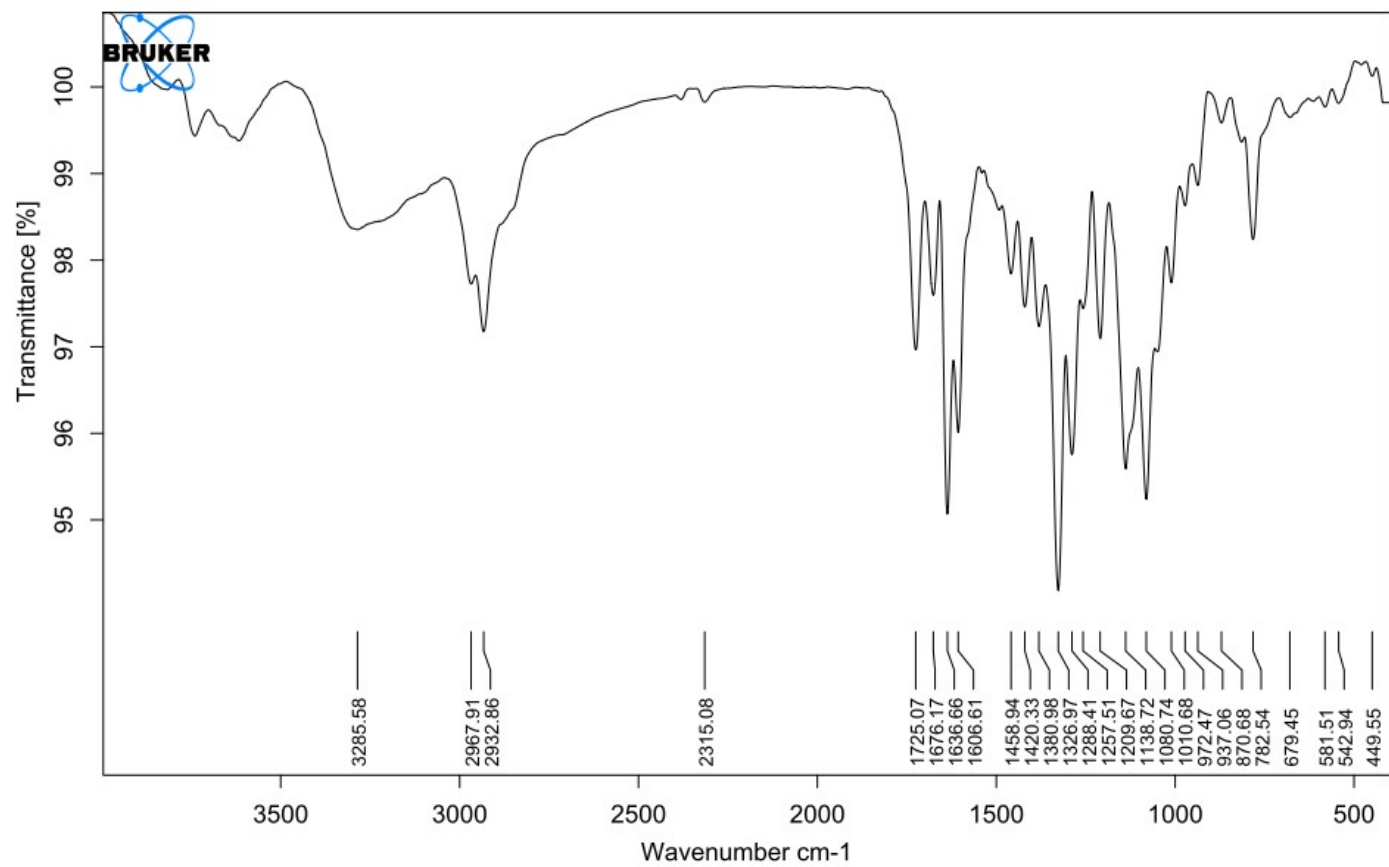


Figure S12. IR spectrum of herpotriquinone A (1).

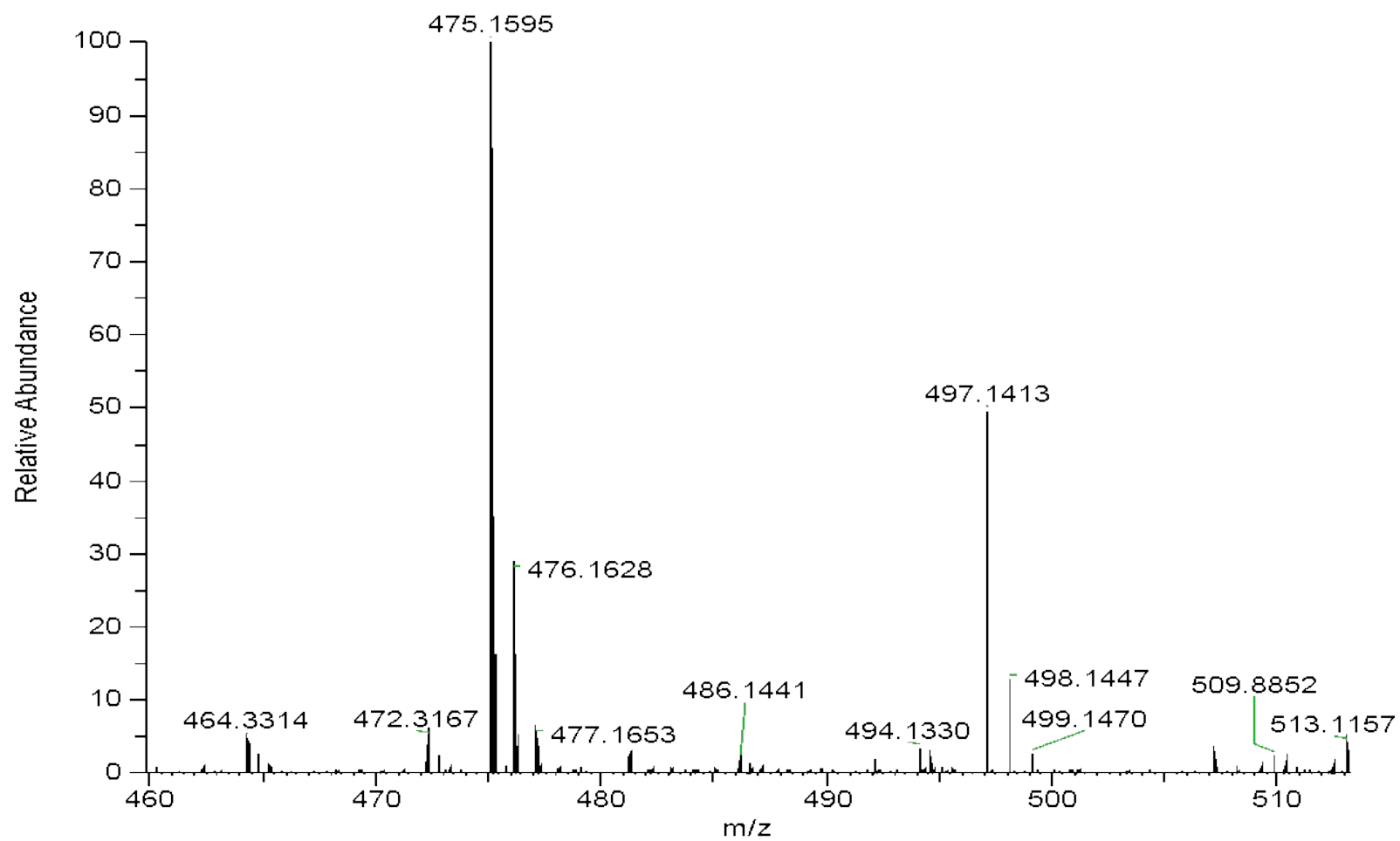


Figure S13. HRESIMS spectrum of herpotriquinone A (1).

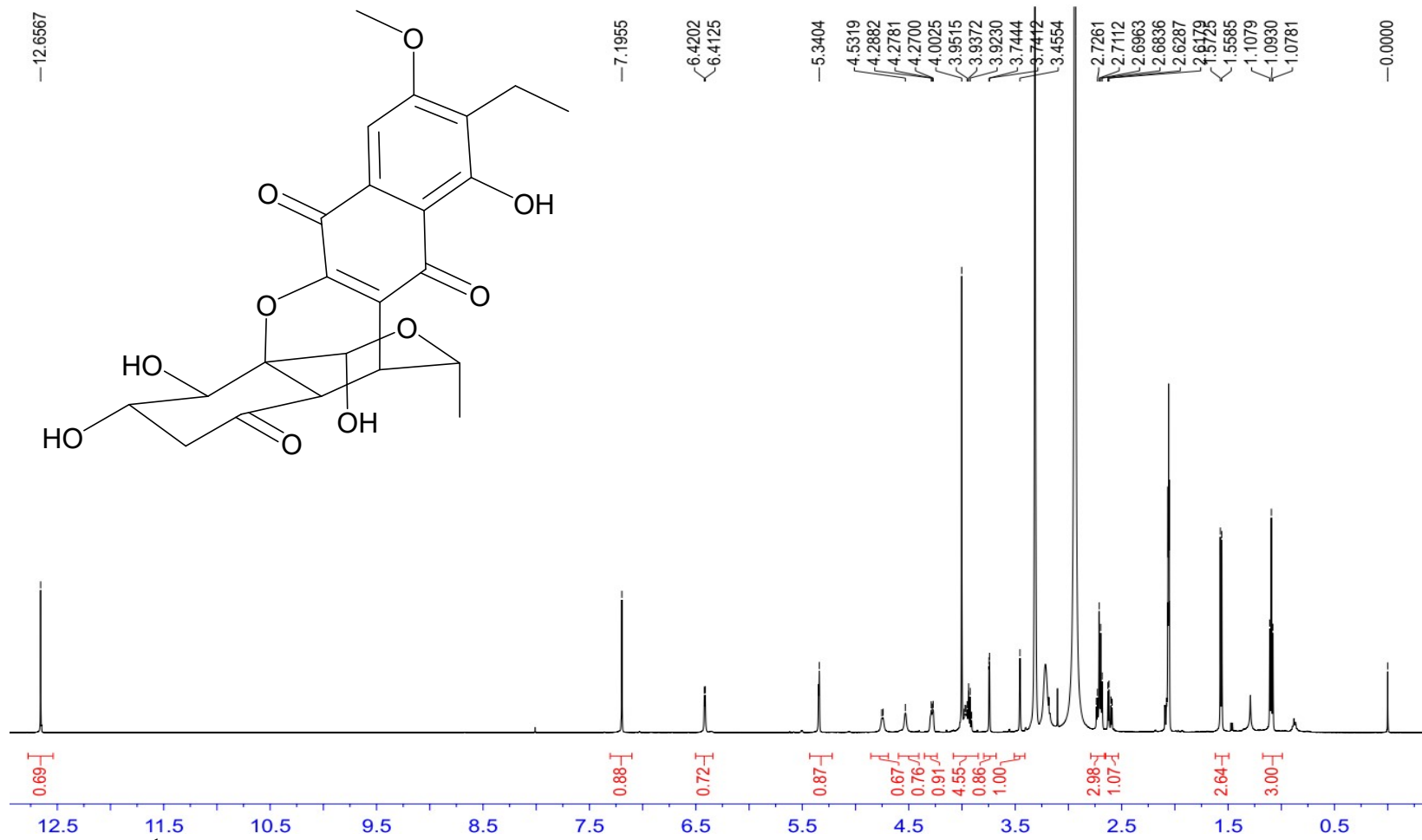


Figure S14. ¹H NMR spectrum of herpotriquinone B (2) in acetone-*d*₆ (500 MHz).

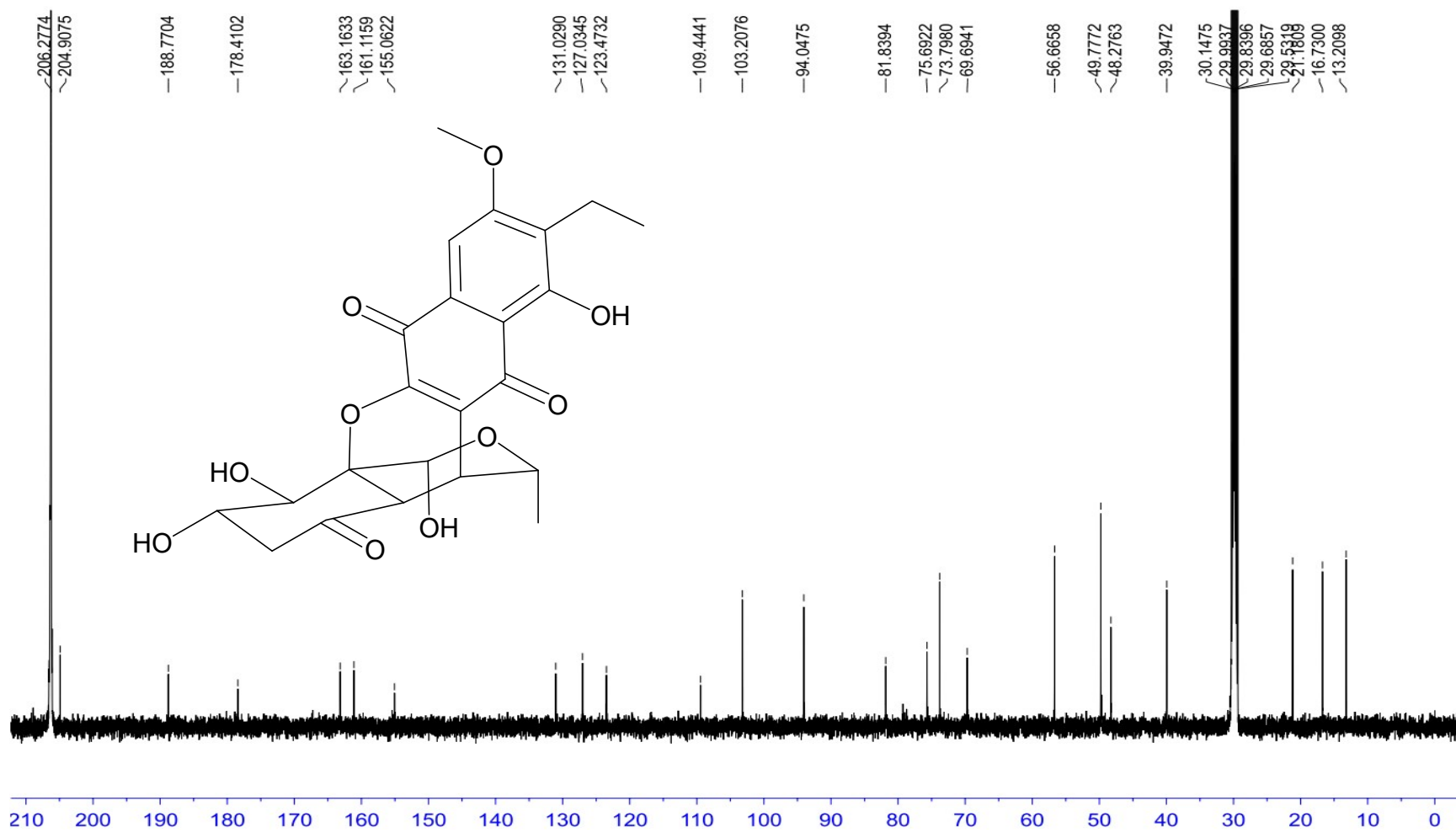


Figure S15. ^{13}C NMR spectrum of herpotriquinone B (**2**) in acetone- d_6 (125 MHz).

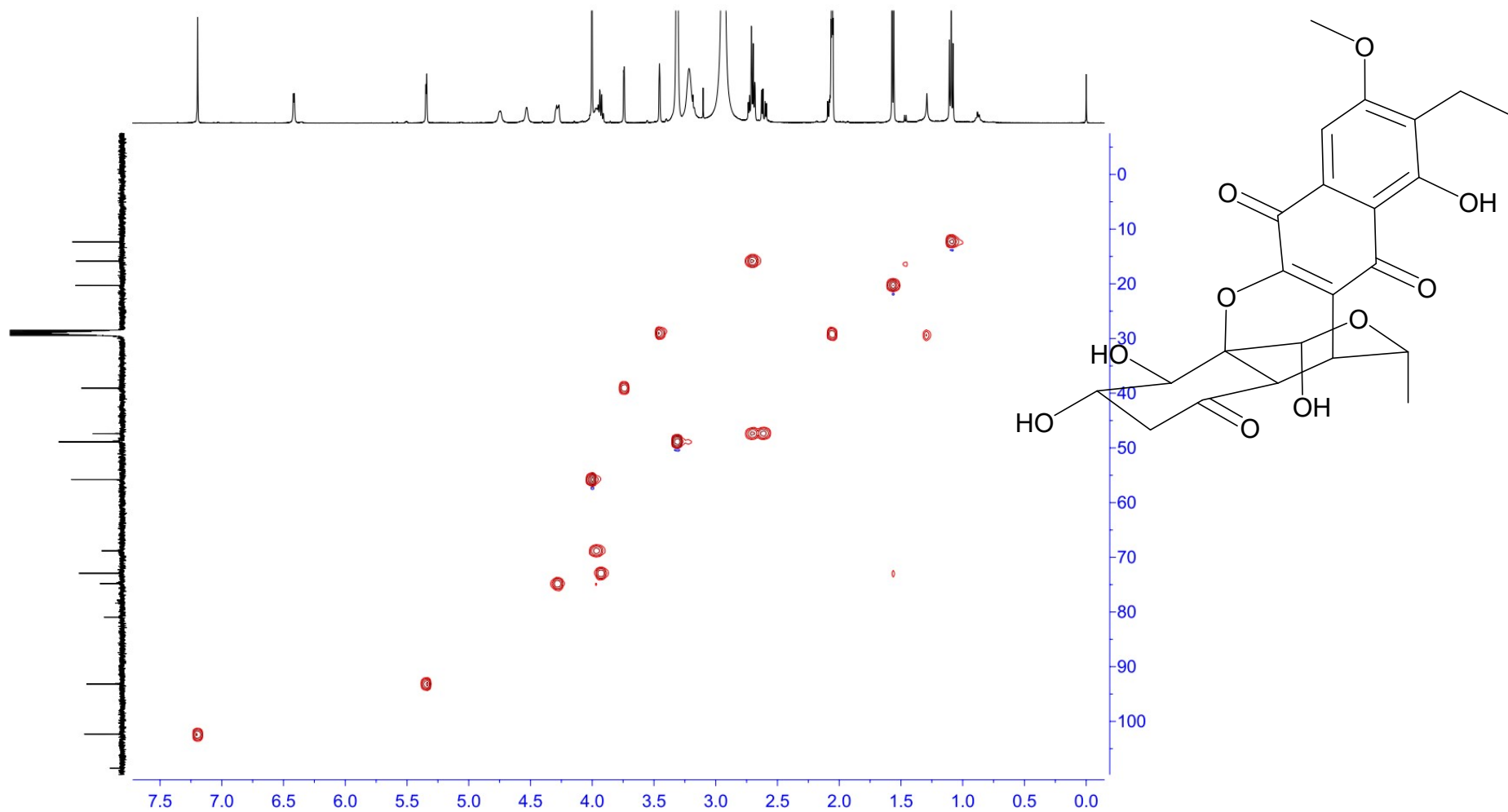


Figure S16. HMQC spectrum of herpotriquinone B (2) in acetone- d_6 .

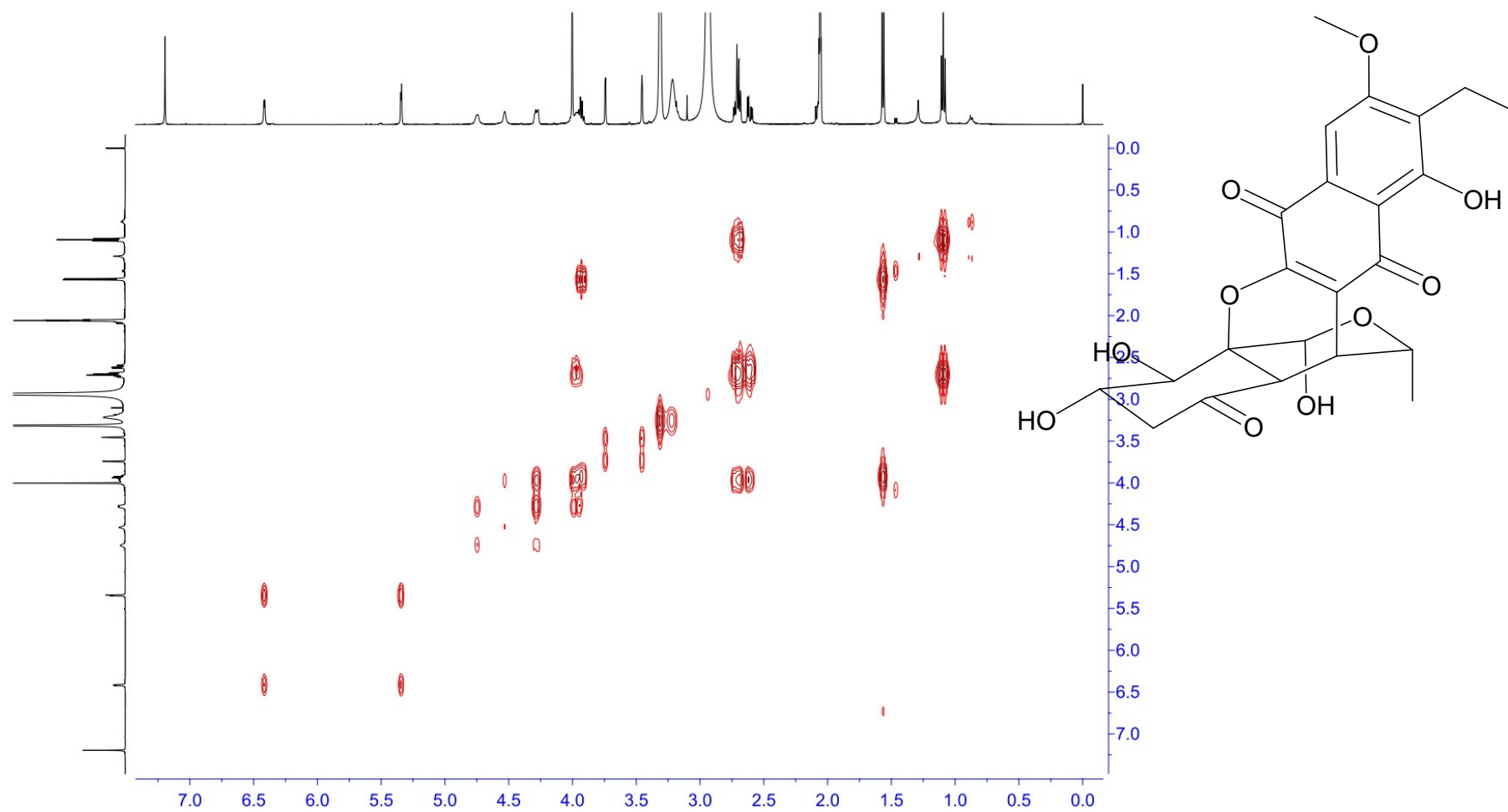


Figure S17. ^1H - ^1H COSY spectrum of herpotriquinone B (2) in acetone- d_6 .

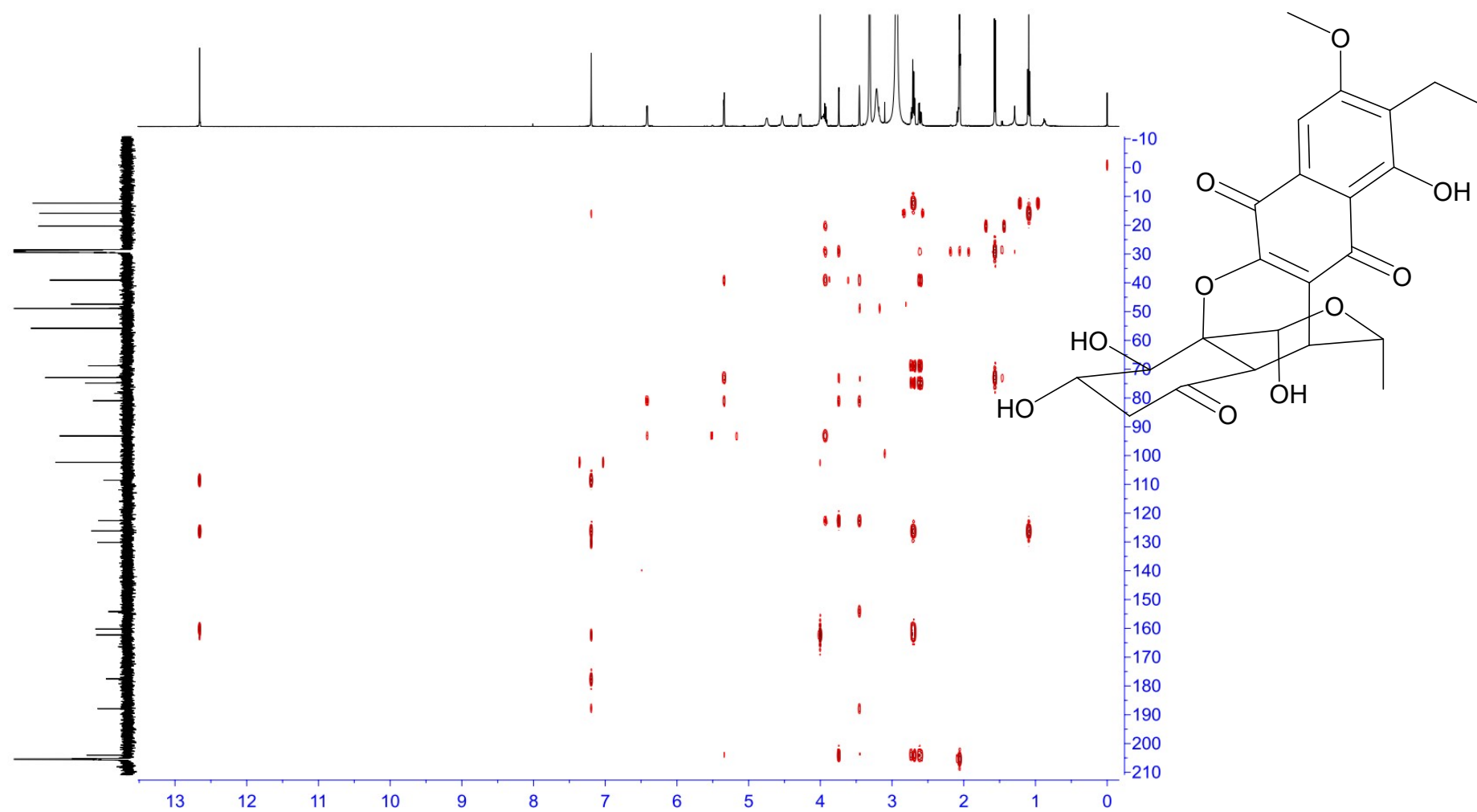


Figure S18. HMBC spectrum of herpotriquinone B (2) in acetone- d_6 .

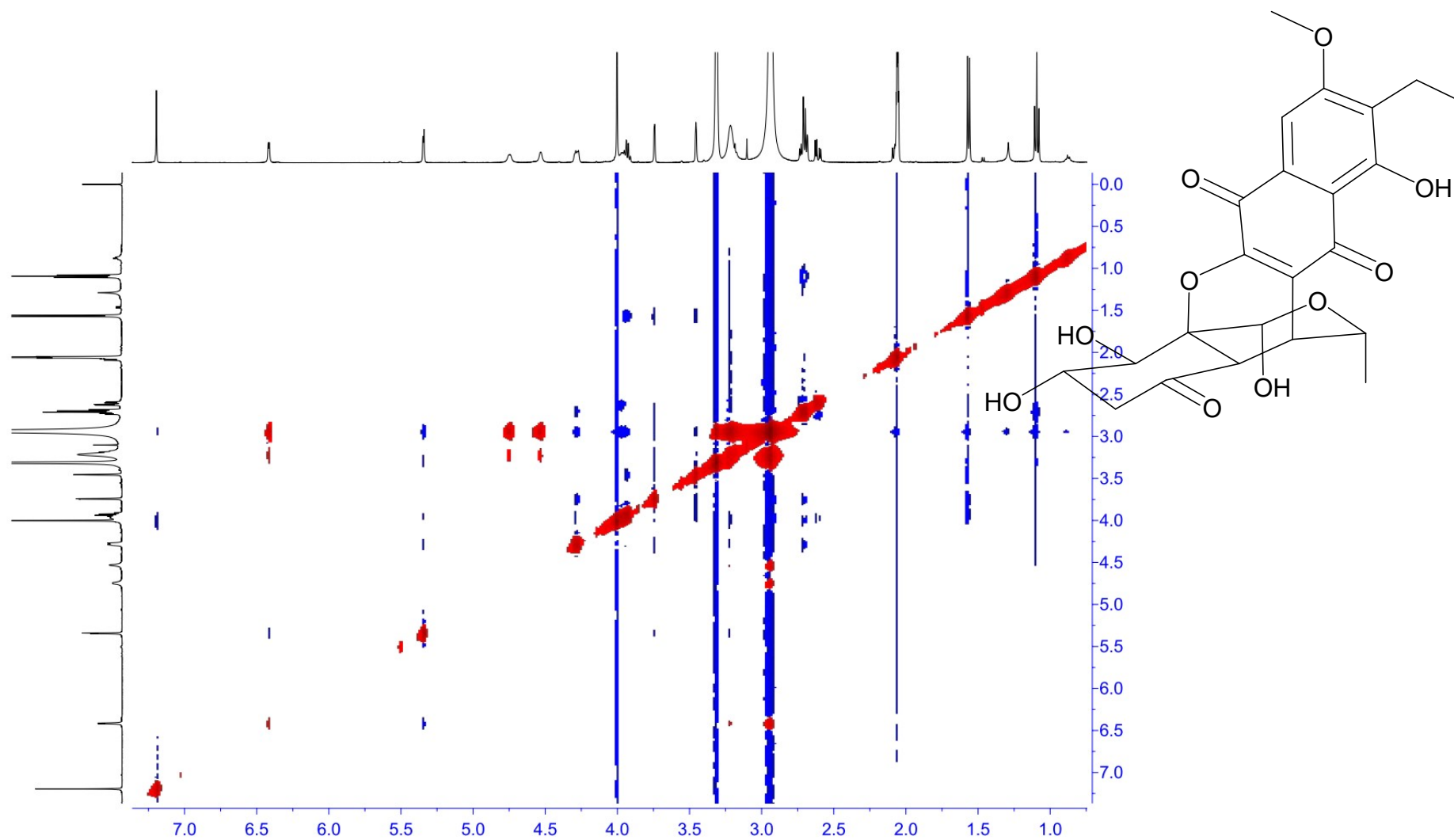


Figure S19. NOESY spectrum of herpotriquinone B (**2**) in acetone- d_6 .

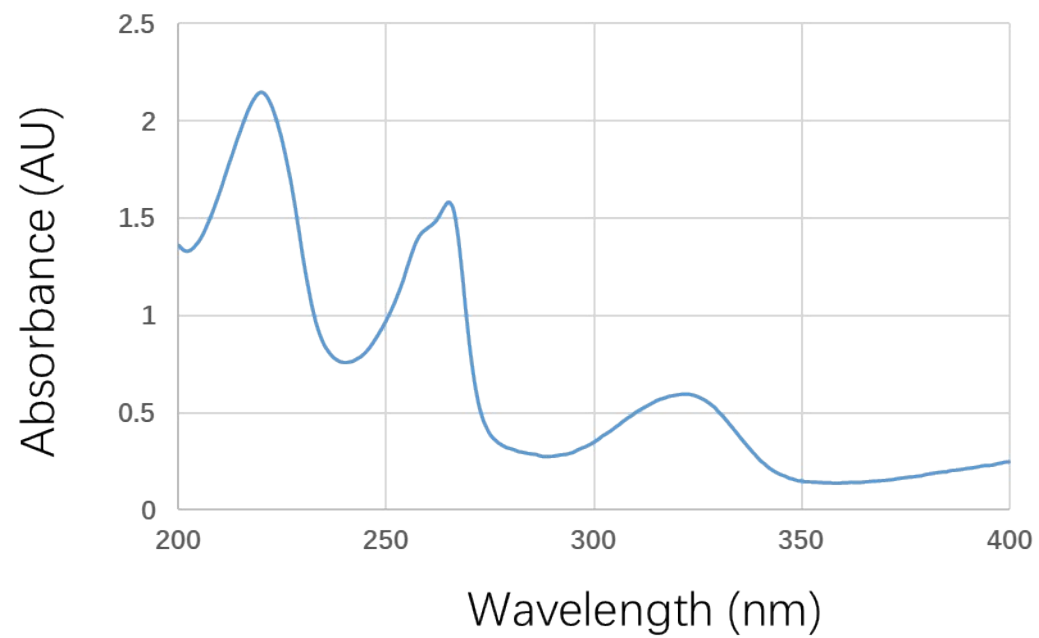


Figure S20. UV spectrum of herpotriquinone B (**2**) in methanol.

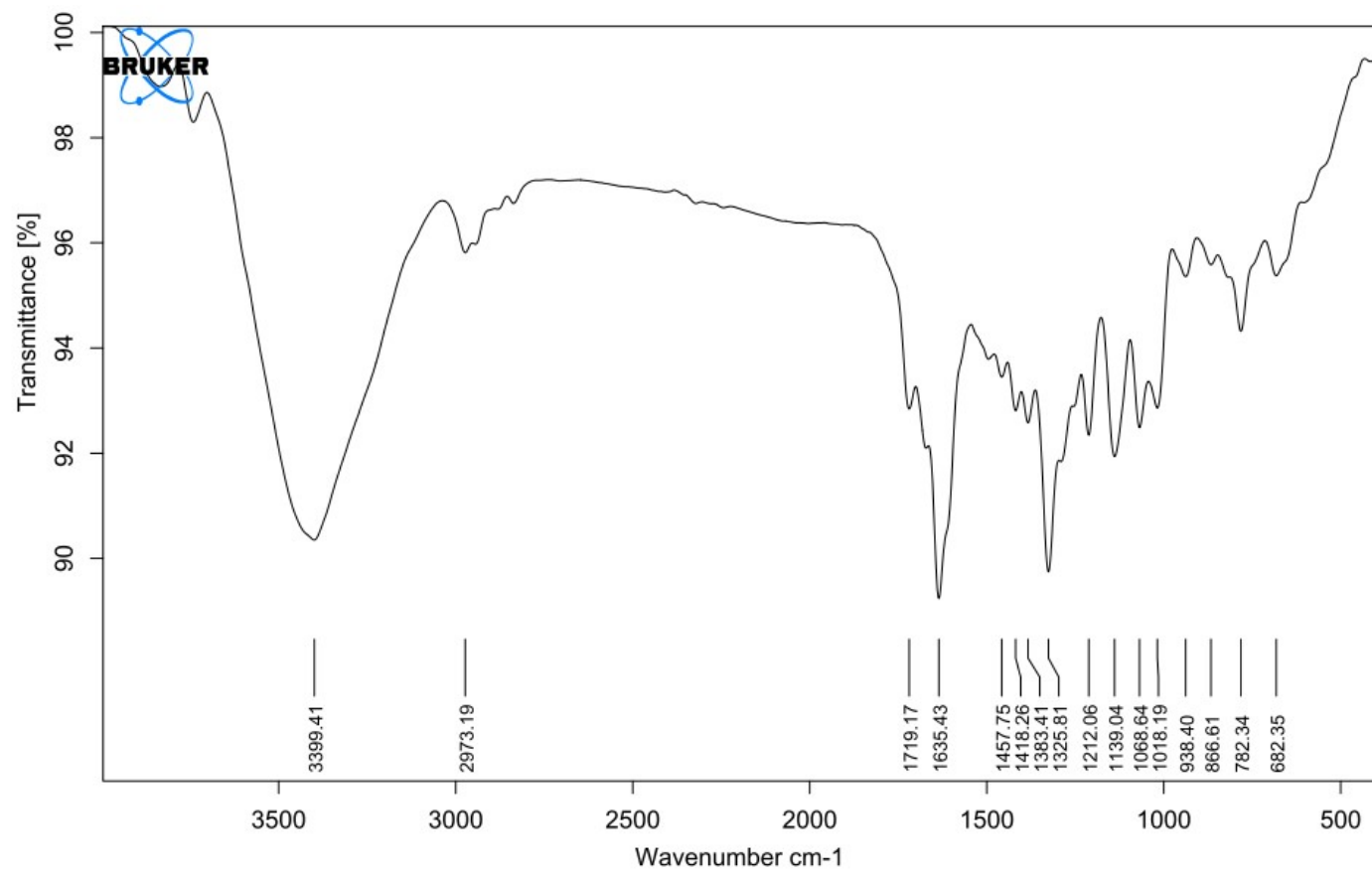


Figure S21. IR spectrum of herpotriquinone B (2).

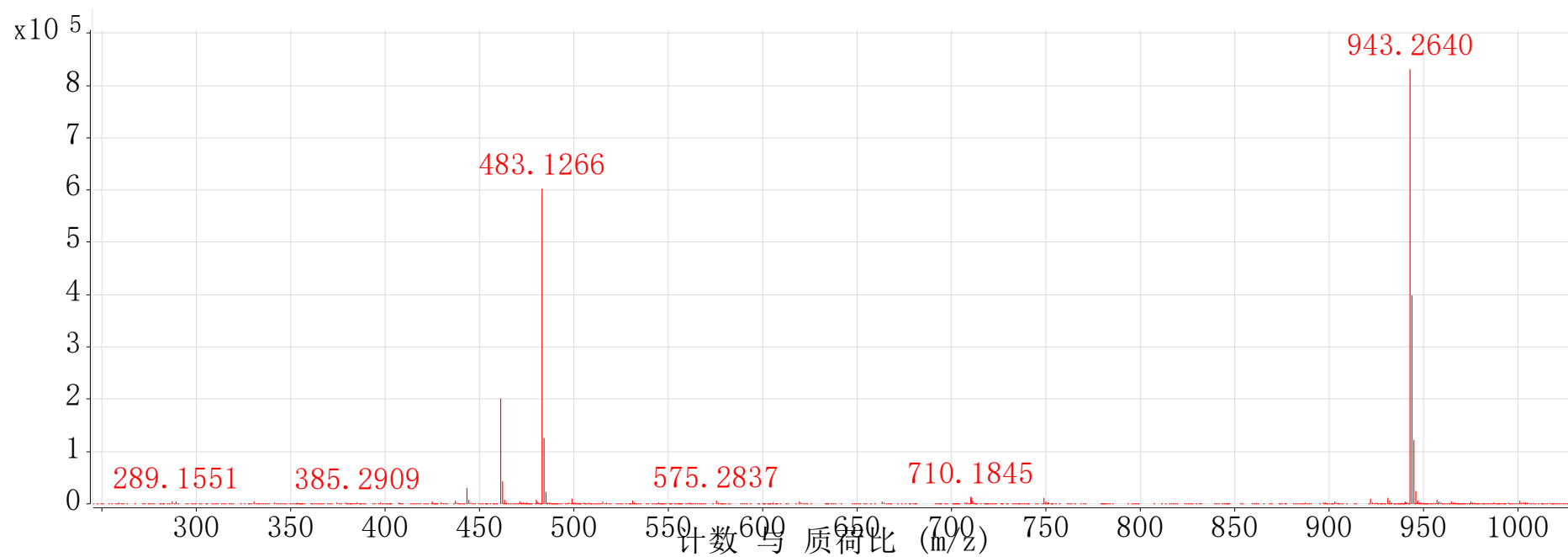


Figure S22. HRESIMS spectrum of herpotriquinone B (2).

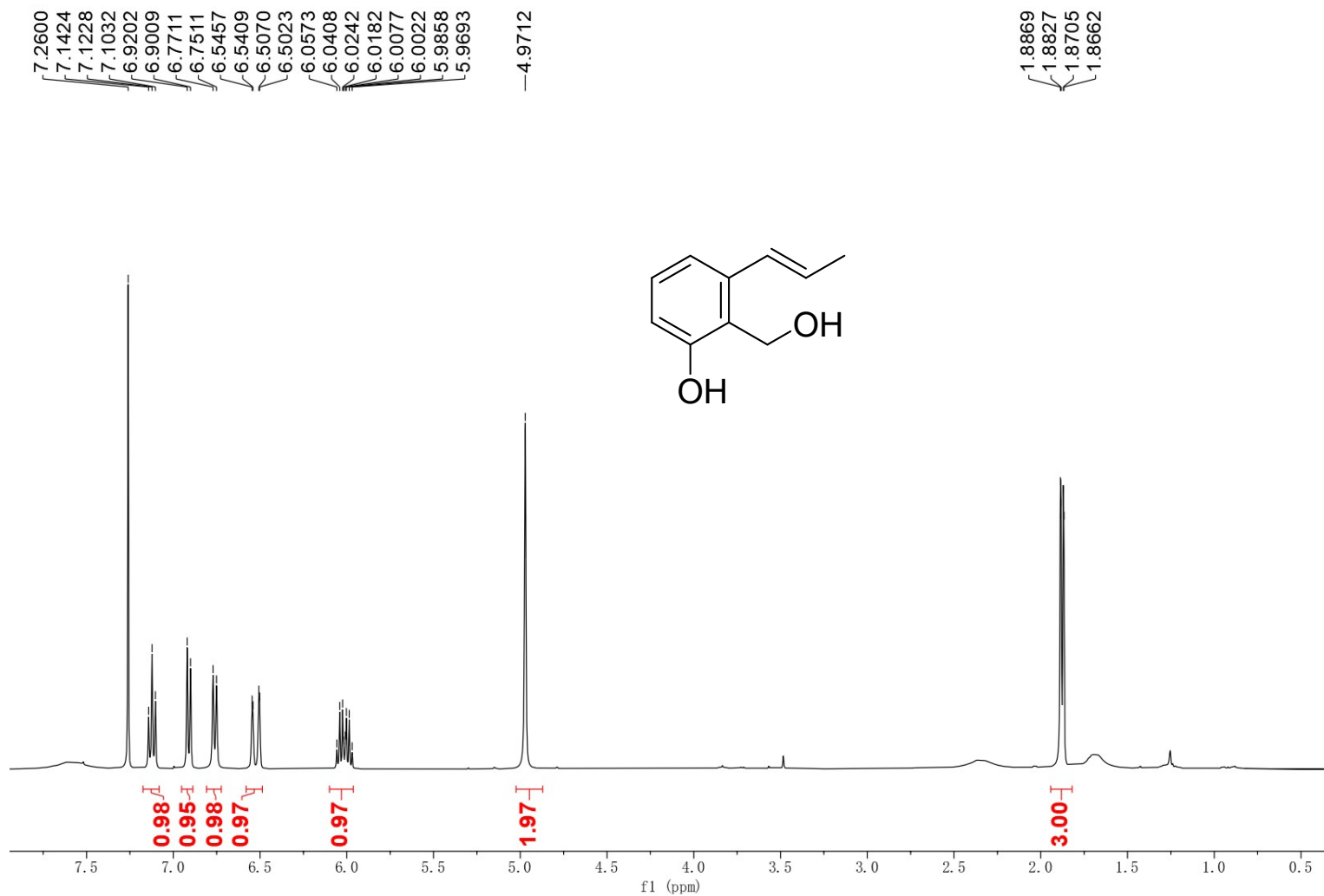


Figure S23. ¹H NMR spectrum of RKB 3564S (3) in CDCl₃ (400 MHz).

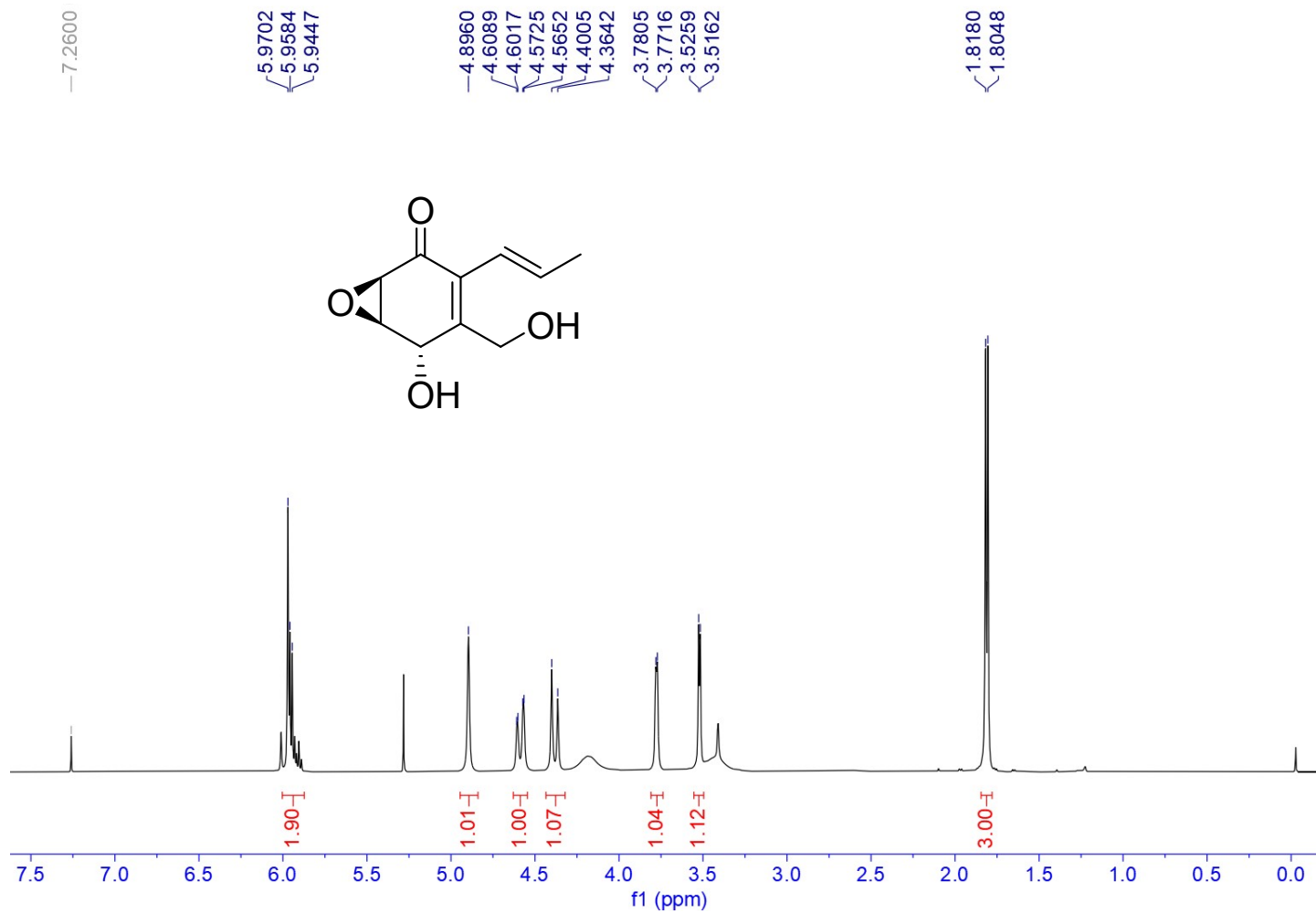


Figure S24. ^1H NMR spectrum of epoxycyclohexenone (**4**) in CDCl_3 (500 MHz).

Table S1. ^1H , ^{13}C , NOESY and HMBC NMR data for **1** in acetone- d_6 .

position	δ_{C}	δ_{H} (mult, J , Hz)	NOESY	HMBC
1	12.8	1.10 (t, 7.3)		C3
2	16.4	2.71 (q, 7.3)		C4
3	128.2			
4	160.8			
5	108.7			
6	187.0			
7	122.9			
8	153.0			
9	179.3			
10	129.4			
11	103.2	7.15 (s)		C3, C5, C9
12	162.2			
13	56.2	3.93 (s)		C12
14	19.6	1.54 (d, 7.0)	H16, H17	C16
15	73.4	3.99 (q, 7.0)		C7, C17
16	29.0	3.53 (br s)	H14	C6, C8, C22
17	39.9	3.40 (br s)	H19, H22	
18	203.4			
19a	47.2	2.88 (14.4, 5.1)	H17, H21	C17, C21
19b		2.60 (14.4, 12.5)		
20	68.9	4.07 (m)	H19	C21
21	75.4	4.24 (br s)	H19, H23	
22	80.2			
23	99.7	4.91 (s)	H21	C15, C17
24	56.2	3.53 (s)		C23
4-OH		12.43 (s)		C3, C5
20-OH		4.80 (br s)		
21-OH		5.25 (br s)		

Table S2. ^1H , ^{13}C , NOESY and HMBC NMR data for **2** in CDCl_3 .

position	δ_{C}	δ_{H} (mult, J , Hz)	NOESY	HMBC
1	13.2	1.09 (t, 7.5)		C3
2	16.7	2.70 (q, 7.5)		C4
3	127.0			
4	161.1			
5	109.4			
6	188.8			
7	123.5			
8	155.1			
9	178.4			
10	131.0			
11	103.2	7.20 (s)		C3, C5, C9
12	163.2			
13	56.7	4.00 (s)		C12
14	21.2	1.56 (d, 7.0)	H16, H17	C16
15	73.8	3.93 (qd, 7.0, 1.0)		C7, C23
16	29.8	3.45 (br s)	H14	C6, C8, C18
17	39.9	3.74 (d, 1.6)	H19, H21	C7, C15
18	204.9			
19a	48.3	2.72 (14.2, 5.1)	H17, H21	C17, C21
19b		2.61 (14.2, 5.4)		
20	69.7	3.97 (m)		
21	75.7	4.28 dd (9.1, 4.1)	H19, H23	
22	81.8			
23	94.0	5.34 (d, 3.9)	H21	
4-OH		12.66 (s)		C3, C5
20-OH		4.53 (br s)		
21-OH		4.75 (br d, 5.7)		
23-OH		6.42 (d, 3.9)		C22

Table S3. Experimental and calculated ^{13}C NMR chemical shifts of **2**.

No.	$\delta_{\text{exptl.}}$	$\delta_{\text{calcd.}}$
1	13.2	13.9
2	16.7	20.4
3	127.0	127.3
4	161.1	157.6
5	109.4	107.4
6	188.8	184.6
7	123.5	121.4
8	155.1	148.7
9	178.4	177.3
10	131.0	126.8
11	103.2	100.3
12	163.2	159.0
13	56.7	55.1
14	21.2	22.0
15	73.8	77.5
16	29.8	32.5

17	39.9	41.5
18	204.9	205.6
19	48.3	47.8
20	69.7	72.2
21	75.7	76.3
22	81.8	82.7
23	94.0	94.8

Table S4. Experimental and calculated ¹H NMR chemical shifts of **2**.

No.	$\delta_{\text{exptl.}}$	$\delta_{\text{calcd.}}$
1	1.09	1.01
2	2.7	2.64
11	7.2	7.61
13	4.0	3.92
14	1.56	1.42
15	3.93	3.8
16	3.45	3.38
17	3.74	3.58
19a	2.72	2.66
19b	2.61	2.48
20	3.97	3.68
21	4.28	4.07
23	5.34	5.2

Table S5. Comparison of key parameters of **2** in NMR computation.

atom_type	parameters	2
¹³ C	R^2	0.9986
	MAE	2.2
	CMAE	1.8
¹ H	R^2	0.9931
	MAE	0.15
	CMAE	0.1
¹³ C	formula	$y = 0.9695x + 2.4163$
¹ H	formula	$y = 1.0533x - 0.2788$

Table S6. Primer sequences of genes

Gene	Forward primer (5'→3')	Reverse primer (5'→3')
<i>β-actin</i>	TCGTCCACCGCAAAYGCTTCTA	CCGTCACCTTCACCGTTCCAGT
<i>jnk</i>	CAAACCTCTGCCAGGTCATT	GCCGAAATCCAAAATCTTCA
<i>il-1β</i>	TGGACTTCGCAGCACAAAATG	GTTCACTTCACGCTCTTGGATG
<i>tgf-β</i>	CCCAAGGAACCAGAAGTAGAAG	GGATCTTCTATGGTGTGCTGAA
<i>il-10</i>	TCACGTCATGAACGAGATCC	CCTCTTGCATTTACCATATCC

Table S7. Anti-neuroinflammatory activity of **1** and **2** (IC₅₀ in μM).

compound	IC ₅₀ (μM)	survival rate (%) ^a
1	5.17 \pm 0.35	106.1 \pm 9.5
2	7.52 \pm 0.81	97.5 \pm 9.2
dexamethasone ^b	7.98 \pm 0.79	103.9 \pm 8.3

^aSurvival rate (%) of BV-2 microglial cells at 20 μM was expressed as the mean \pm SD from three independent experiments; ^bpositive control.

Table S8. Conformational analysis of the B3LYP/6-31G(d) optimized conformers of **2** in the gas phase (T=298.15 K)

Conformer	E ^a (Hartree)	C ^b (Hartree)	G ^c (kcal/mol)	ΔG^d (kcal/mol)	Population ^e
M9-4-2-1-1	-1643.042408	0.387467	-1030765.975408	0.0	50.81%
M9-4-2-1-2	-1643.042209	0.387299	-1030765.956176	0.019233	49.19%

^aElectronic energy obtained at M062X/6-311+G(2d,p) level of theory; ^bThermal correction to Gibbs free energy obtained at B3LYP/6-31G(d) level of theory; ^cGibbs free energy (E + C); ^dThe relative Gibbs free energy; ^eThe Boltzmann distribution of each conformer.

Table S9. Atomic coordinates (\AA) of **2** obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	-6.428645	0.671850	1.656827	O	-1.063662	2.665798	0.579757
C	-5.965100	0.924333	0.211498	O	1.561554	0.460174	2.811191
C	-4.589114	0.366004	-0.042276	O	4.515702	-2.982313	1.643544
C	-3.446896	1.159062	0.182797	O	3.944491	-2.358687	-1.055756
C	-2.144736	0.640564	-0.020830	H	3.663928	1.310889	0.811543
C	-0.966874	1.472897	0.220188	H	1.362687	2.450177	1.059367
C	0.364412	0.891656	0.018406	H	4.898649	-0.945140	0.031891
C	0.494150	-0.370965	-0.446452	H	-2.964043	-2.511162	-1.001497
C	-0.665232	-1.277095	-0.691099	H	-4.954987	-3.105751	-2.034470
C	-2.009837	-0.693979	-0.456241	H	-4.873122	-3.638376	-0.328016
C	-3.122593	-1.492632	-0.673282	H	-6.458756	-3.406315	-1.117666
C	-4.405245	-0.961618	-0.454478	H	-5.950709	2.000118	0.016806
C	-5.435255	-3.035350	-1.051113	H	-6.672353	0.464744	-0.484807
C	3.051085	3.553829	-0.786258	H	-6.464985	-0.401612	1.869356
C	2.006836	2.461203	-1.008675	H	-5.742480	1.141595	2.368749
C	1.589712	1.719140	0.281397	H	-7.429111	1.087582	1.820309
C	2.712001	0.772858	0.724350	H	-2.736546	2.827250	0.695240
C	2.464674	0.110022	2.080224	H	2.547364	-2.506429	1.185590
C	3.445293	-0.994435	2.431977	H	4.444000	-0.555678	2.570049
C	3.531859	-2.023738	1.302694	H	3.145799	-1.464853	3.370870
C	3.892966	-1.366159	-0.035747	H	3.281251	-0.194704	-2.530585
C	2.908241	-0.250383	-0.398830	H	1.110743	2.925281	-1.428874
C	3.304818	0.501616	-1.687010	H	4.876355	1.470408	-2.260365
O	-3.639737	2.419689	0.600653	H	3.962064	3.176052	-0.317486
O	1.680590	-0.968274	-0.678282	H	3.323379	4.001009	-1.747546

O	-0.484824	-2.431910	-1.054996	H	2.626907	4.339881	-0.152106
O	-5.544117	-1.683512	-0.623205	H	4.665000	-3.497494	0.831128
O	2.392997	1.512733	-2.030665	H	3.020289	-2.617178	-1.227087
O	4.611951	0.988506	-1.460842	-	-	-	-

Table S10. Atomic coordinates (Å) of **2** obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	-6.606086	1.379310	-0.537692	O	-1.083944	2.565160	0.869087
C	-5.956865	0.719923	0.691613	O	1.762081	0.344387	2.838209
C	-4.580568	0.189869	0.385288	O	4.746771	-2.930321	1.320074
C	-3.448129	1.009136	0.559746	O	3.944220	-2.232059	-1.301371
C	-2.148001	0.533022	0.261776	H	3.685530	1.350679	0.730729
C	-0.979315	1.388516	0.461017	H	1.374246	2.399500	1.191078
C	0.351177	0.852232	0.156734	H	4.929758	-0.825219	-0.232909
C	0.484282	-0.386672	-0.367378	H	-2.950025	-2.588200	-0.824469
C	-0.665101	-1.313576	-0.579686	H	-4.810643	-3.784733	-0.105150
C	-2.007091	-0.777541	-0.239513	H	-6.429242	-3.551411	-0.824990
C	-3.112140	-1.592746	-0.433192	H	-4.967226	-3.187081	-1.784665
C	-4.392771	-1.102845	-0.124564	H	-6.587626	-0.102508	1.040790
C	-5.410429	-3.164409	-0.781858	H	-5.880139	1.452820	1.499399
C	2.893602	3.626250	-0.728242	H	-6.707458	0.658203	-1.355440
C	1.864545	2.513307	-0.916512	H	-7.603504	1.759531	-0.290701
C	1.566654	1.707781	0.369032	H	-5.998176	2.218543	-0.890594
C	2.746936	0.784183	0.689772	H	-2.750453	2.679098	1.083352
C	2.622273	0.059431	2.031149	H	2.732396	-2.519304	1.032016
C	3.665477	-1.018150	2.265518	H	4.655389	-0.546520	2.346914
C	3.703814	-2.001036	1.093053	H	3.454588	-1.534374	3.204461
C	3.936920	-1.280579	-0.241454	H	3.093997	-0.041200	-2.635763
C	2.890899	-0.189448	-0.485199	H	0.927221	2.966822	-1.249029
C	3.162202	0.623775	-1.769601	H	4.655536	1.662186	-2.424945
O	-3.648328	2.254152	1.018831	H	3.077910	4.120886	-1.687173
O	1.669175	-0.939590	-0.698417	H	2.499955	4.372169	-0.029223
O	-0.479467	-2.446054	-1.005698	H	3.847859	3.255683	-0.348688
O	-5.526105	-1.832546	-0.296919	H	4.852220	-3.408490	0.478702
O	2.196017	1.615799	-2.001548	H	3.018735	-2.516806	-1.413840
O	4.467761	1.144987	-1.625838	-	-	-	-

Table S11. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer **2-1** at the PBE1PBE/6-311G(d) level of theory in MeOH with IEFPCM solvent model.

<i>Num</i> ^a	<i>Transition</i> _b	<i>CI-coeff</i> ^c	<i>ΔE (eV)</i> ^d	<i>λ (nm)</i> ^e	<i>f</i> ^f	<i>R_{vel}</i> ^g	<i>R_{len}</i> ^h
1	121->122	0.68711	2.6599	466.13	0.0244	-7.4433	-7.6011
2	120->122	0.68815	2.9726	417.09	0.1535	-9.877	-8.8881
3	116->122	0.48185	3.0916	401.04	0.0013	-4.1891	-4.5016
	117->122	-0.43271					
4	114->122	0.47372	3.5014	354.10	0.0023	0.219	-0.0313
	115->122	0.32943					

	119->122	0.32109					
5	114->122	-0.28176	3.5451	349.73	0.0136	3.6132	3.7327
	119->122	0.58509					
6	118->122	0.64721	3.7427	331.27	0.1072	22.5506	24.7011
7	116->122	0.46318	3.9836	311.24	0.0498	-3.2972	-3.5113
	117->122	0.49561					
8	114->122	-0.33996	4.2884	289.11	0.0042	-1.6648	-2.1308
	115->122	0.59545					
9	118->123	0.27581	4.4035	281.56	0.0001	-3.7817	-5.1019
	119->123	0.47055					
	119->124	0.24491					
10	113->122	0.67844	4.7515	260.94	0.0085	-1.7445	-1.5418
11	112->122	0.68287	4.8425	256.03	0.0032	-3.4611	-3.7026
12	111->122	0.67963	4.9785	249.04	0.0062	1.3305	1.1924
13	121->123	0.51623	5.0275	246.61	0.2615	14.9016	14.3701
	121->124	-0.27686					
14	110->122	0.3789	5.1513	240.68	0.0166	10.5904	9.6757
	121->123	0.40281					
15	110->122	-0.31317	5.2139	237.80	0.1369	-25.6337	-26.8434
	121->124	0.52623					
16	110->122	-0.41189	5.2952	234.14	0.0238	4.1786	5.5539
	120->123	0.43823					
	120->124	-0.25816					
17	109->122	0.64805	5.3755	230.65	0.0003	0.3974	0.3291
18	120->123	0.44603	5.4390	227.95	0.0292	-0.2542	-0.4137
	120->124	0.47599					
19	105->122	0.22835	5.5467	223.53	0.0030	-6.9989	-6.9708
	108->122	0.62995					
20	107->122	0.64011	5.6167	220.74	0.0119	-7.2125	-7.5824
21	118->123	0.44326	5.6846	218.11	0.0205	-4.5284	-4.7349
	119->123	-0.38358					
22	118->124	-0.22765	5.7216	216.69	0.5563	-23.0874	-23.6571
	120->124	-0.27879					
	120->125	0.42852					
	121->125	0.29135					
23	105->122	-0.23302	5.7670	214.99	0.0024	3.5658	3.7798
	116->123	0.30767					
	116->124	-0.3082					
	117->123	-0.2622					
24	117->124	0.32007	5.8116	213.34	0.0015	6.1767	6.2571
	105->122	0.53141					
	116->123	0.27247					
	117->123	0.37968					
	118->123	0.35785					
25	120->125	-0.24387	5.8743	211.06	0.0246	1.0197	1.5944
	120->125	-0.36108					
	121->125	0.49616					
	118->124	0.22621					
26	119->123	-0.25665	6.0225	205.87	0.0052	-1.511	-1.55
	119->124	0.57006					
	118->124	0.55268					
27	119->124	-0.24091	6.0463	205.06	0.0448	4.4689	3.3909
	118->124	0.55268					
28	103->122	0.23097	6.0832	203.81	0.0019	4.5856	4.1975
	104->122	-0.38537					
	106->122	0.40493					

30	104->122	0.44059	6.1446	201.78	0.0012	-0.0022	0.1928
	106->122	0.47588					
31	104->122	-0.24154	6.1750	200.78	0.0004	-2.6109	-2.5432
	114->124	-0.27446					
	116->123	0.3383					
32	114->123	-0.27064	6.2192	199.36	0.0003	-2.2611	-2.767
	114->124	0.23993					
	116->123	0.25839					
	116->124	0.32632					
	117->124	-0.23538					
33	103->122	0.61919	6.2674	197.82	0.0153	-7.5845	-8.1084
34	102->122	0.58117	6.3298	195.87	0.0008	0.7708	1.3071
35	102->122	-0.31853	6.3613	194.90	0.0015	1.913	2.3325
	116->125	0.3646					
	117->125	-0.35503					
	118->125	0.23647					
36	101->122	0.35493	6.4296	192.83	0.0189	-0.5843	-0.6076
	118->125	-0.26568					
	119->125	0.46395					

^aNumber of the excited states; ^bOnly transitions with contribution over 10.0% were listed; ^cConfiguration-interaction coefficient; ^dExcitation energy; ^eWavelength; ^fOscillator strength; ^gRotatory strength in velocity form (10^{-40} cgs); ^hRotatory strength in length form (10^{-40} cgs).

Table S12. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer **2-2** at the PBE1PBE/6-311G(d) level of theory in MeOH with IEFPCM solvent model.

<i>Num^a</i>	<i>Transition_b</i>	<i>CI-coeff^c</i>	<i>ΔE (eV)^d</i>	<i>λ (nm)^e</i>	<i>f^f</i>	<i>R_{vel}^g</i>	<i>R_{len}^h</i>
1	121->122	0.68663	2.6604	466.04	0.0246	-3.5571	-4.2761
2	120->122	0.68823	2.9742	416.87	0.1546	10.0062	9.7151
3	116->122	0.47565	3.0914	401.06	0.0002	-8.217	-8.8199
	117->122	0.44279					
4	114->122	0.46367	3.5004	354.20	0.0045	0.1583	-0.242
	115->122	0.32848					
	119->122	0.33551					
5	114->122	-0.29329	3.5456	349.68	0.0118	3.1307	3.2414
	119->122	0.58053					
6	118->122	0.65173	3.7422	331.31	0.1075	13.6964	14.7275
7	116->122	-0.47292	3.9861	311.04	0.0495	-6.9681	-7.435
	117->122	0.48608					
8	114->122	-0.34329	4.2884	289.12	0.0042	-1.2711	-1.7693
	115->122	0.5933					
9	118->123	0.26878	4.4029	281.60	0.0001	-3.5782	-4.7897
	119->123	0.4746					
	119->124	0.24828					
10	113->122	0.67632	4.7522	260.90	0.0085	-1.6468	-1.5172
11	112->122	0.68145	4.8422	256.05	0.0032	-3.3963	-3.6721
12	111->122	0.67923	4.9762	249.15	0.0062	1.3888	1.273
13	121->123	0.50861	5.0299	246.49	0.2646	20.4777	22.0686
	121->124	-0.28275					
14	110->122	0.3763	5.1526	240.62	0.0166	14.1345	14.1192

	121->123	0.41124					
15	110->122	-0.31778	5.2143	237.78	0.1363	-25.9367	-27.1071
	121->124	0.52488					
16	110->122	-0.40924	5.2962	234.10	0.0214	-5.6349	-5.6522
	120->123	0.43042					
	120->124	-0.26445					
17	109->122	0.65196	5.3775	230.56	0.0015	4.0493	4.177
18	120->123	0.45265	5.4429	227.79	0.0273	-0.3792	-0.496
	120->124	0.47027					
19	105->122	-0.2309	5.5447	223.61	0.0039	-7.6146	-7.6964
	108->122	0.62939					
20	107->122	0.64642	5.6188	220.66	0.0041	4.949	5.354
21	118->123	0.44719	5.6879	217.98	0.0288	-3.671	-3.8091
	119->123	-0.37215					
22	118->124	-0.24536	5.7176	216.85	0.5383	10.8819	11.261
	120->124	-0.26781					
	120->125	0.41944					
	121->125	0.28627					
23	116->123	-0.28089	5.7692	214.91	0.0188	-6.013	-6.1149
	116->124	0.30578					
	117->123	-0.29469					
	117->124	0.33307					
24	105->122	0.5358	5.8123	213.31	0.0034	-3.3428	-3.6316
	108->122	0.22367					
25	116->123	-0.27981	5.8767	210.98	0.0280	-1.5892	-0.4702
	117->123	0.3654					
	118->123	-0.35528					
	120->125	0.25266					
26	120->125	-0.35684	5.9118	209.72	0.2361	10.0891	9.1014
	121->125	0.49238					
27	118->124	0.28713	6.0198	205.96	0.0055	-0.5177	-0.4576
	119->123	-0.24446					
	119->124	0.53916					
28	118->124	0.50894	6.0421	205.20	0.0391	17.5551	18.0128
	119->124	-0.30825					
29	104->122	0.41924	6.0847	203.76	0.0013	-5.8544	-5.8334
	106->122	-0.39633					
30	103->122	0.24765	6.1483	201.66	0.0044	-1.601	-1.4882
	104->122	0.37338					
	106->122	0.48731					
31	104->122	-0.24476	6.1795	200.64	0.0006	-4.1105	-4.08
	114->124	-0.27655					
	116->123	0.33439					
	117->123	0.22369					
32	114->123	-0.26238	6.2199	199.33	0.0010	-4.2474	-4.9206
	114->124	0.23328					
	116->123	0.25895					
	116->124	0.31813					
	117->124	0.23798					
33	103->122	0.61016	6.2716	197.69	0.0192	2.6491	2.6794
34	102->122	0.6383	6.3161	196.30	0.0016	1.725	1.5928
35	116->125	0.40813	6.3509	195.22	0.0003	0.3713	1.2326
	117->125	0.38972					
	118->125	0.31193					
36	101->122	0.34846	6.4320	192.76	0.0109	-1.2113	-1.2832

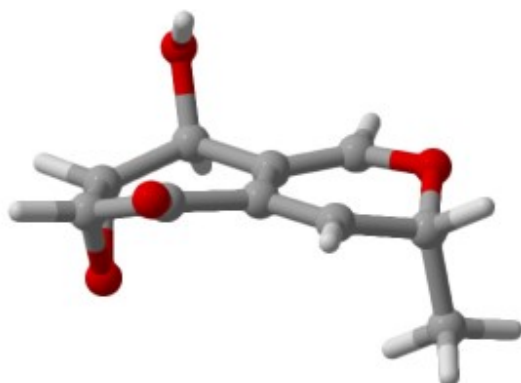
	119->125	0.56026				
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^aNumber of the excited states; ^bOnly transitions with contribution over 10.0% were listed; ^cConfiguration-interaction coefficient; ^dExcitation energy; ^eWavelength; ^fOscillator strength; ^gRotatory strength in velocity form (10^{-40} cgs); ^hRotatory strength in length form (10^{-40} cgs).

Table S13. Gibbs free energies of the species in the processes from VI and IX to XI through intermediates Xa to Xd.

	E	Thermal correction to Gibbs Free Energy	G (hartree)	ΔG (hartree)	ΔG (kcal/mol)
1# VI	-688.144691	0.148769	-687.995922	0.00	0.00
2# IXa	-879.061875	0.188848	-878.873027		
3# IXa_lostH	-878.602390	0.173367	-878.429023		
4# Xa_1_TS11	-1566.753005	0.350424	-1566.402581	0.022364	14.03
5# Xa_1_TS11_I1	-1566.759252	0.352418	-1566.406834	0.018111	11.36
6# Xb_addH_1	-1567.234347	0.365264	-1566.869083	-0.066905	-41.98
7# Xb_addH_lostH_1	-1566.782049	0.350423	-1566.431626	-0.006681	-4.19
8# Xc_addH_lostH_TS_31	-1566.744447	0.351023	-1566.393424	0.031521	19.78
9# Xc_addH_lostH_P_1	-1566.747137	0.352041	-1566.395096	0.029849	18.73
10a# XI_addH_lostH_P_1_P_R1	-1567.238797	0.367665	-1566.871132	-0.068954	-43.27
10b# XI_addH_lostH_P_1_P_S1	-1567.236629	0.369460	-1566.867169	-0.064991	-40.78

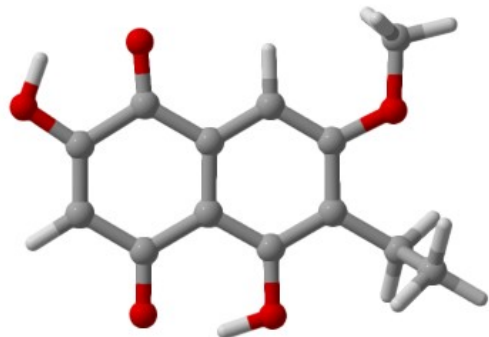
1#



C	-2.33196800	-0.45113100	0.61500300
C	-1.27763500	-1.46128700	0.19975500
C	0.07563300	-0.82586100	-0.00755100
C	0.22068800	0.59969400	-0.31988300

C	-0.98080000	1.46894500	-0.45161700
C	-2.20651300	0.98202700	0.26215700
H	1.15812200	-2.67708500	-0.07588900
C	1.17704600	-1.59329800	-0.13562800
C	1.44741200	1.12204000	-0.50378600
C	2.66427700	0.28923400	-0.22090700
H	1.56538200	2.16488300	-0.77871300
O	-0.99079000	2.52097300	-1.07049500
O	-1.96638700	0.50061400	1.60385100
O	-1.75557200	-2.17053400	-0.95180500
H	-1.61232300	-1.59801700	-1.71842700
H	-1.21339600	-2.22548000	0.98167500
H	-3.33714300	-0.86222100	0.70683400
H	-3.09262700	1.59993800	0.13496200
O	2.40448300	-1.12681600	-0.44847900
C	3.15993200	0.48262200	1.21381700
H	3.44071400	1.52781300	1.37583800
H	2.36864600	0.22528100	1.92303700
H	4.03127000	-0.15079800	1.40205100
H	3.46904300	0.52388500	-0.92410400

2#



C	-3.23730100	0.27563400	0.11083700
C	-2.06989900	1.21617800	0.07615800
C	-0.72316700	0.64191800	-0.03278800
C	-0.57547800	-0.75799200	-0.10087500
C	-1.74421700	-1.64835800	-0.06041200
C	-3.07723900	-1.06527000	0.04606100
H	0.20919900	2.55535700	-0.00347100
C	0.37810600	1.48904300	-0.06413200
C	0.72817500	-1.29542500	-0.20523600
H	-3.92110100	-1.74424700	0.07221600
C	1.85876200	-0.45245700	-0.25375900
C	1.66402800	0.93409500	-0.16627900
O	-1.60662100	-2.88910700	-0.11512200
O	-2.31932200	2.42112800	0.14180900

O	-4.41938100	0.88716700	0.21028600
H	-4.20555600	1.84483400	0.23653900
O	0.93120200	-2.61704700	-0.26128200
H	0.02570000	-3.03562400	-0.22235000
O	2.79716800	1.68453600	-0.18730200
C	2.67548900	3.10023000	-0.12618600
H	3.69366500	3.48725300	-0.16539800
H	2.10411500	3.49018500	-0.97648700
H	2.19959000	3.42108400	0.80768000
C	3.23957600	-1.04468100	-0.34389600
H	3.88468900	-0.36237300	-0.90315400
H	3.18078100	-1.98606200	-0.89537600
C	3.84513500	-1.30274100	1.04684500
H	3.92483000	-0.37015100	1.61290600
H	3.22161700	-1.99923000	1.61428300
H	4.84628500	-1.73548000	0.95746400

3#

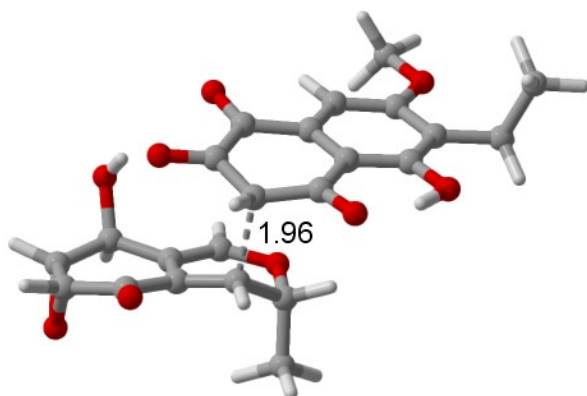


C	-3.33733700	0.38592700	0.12203900
C	-2.09348700	1.31126400	0.08733400
C	-0.74277900	0.68213400	-0.02681400
C	-0.62688100	-0.70993500	-0.09848300
C	-1.82763400	-1.59234500	-0.06037000
C	-3.09747800	-1.01213000	0.04406600
H	0.22636800	2.57433000	0.00939300
C	0.38464900	1.50618500	-0.05659400
C	0.66423500	-1.28274000	-0.20464900
H	-3.95578300	-1.67636200	0.06843000
C	1.81234100	-0.46622600	-0.25189800
C	1.64869600	0.92412900	-0.16126100
O	-1.62877700	-2.85913600	-0.12759300
O	-2.21746300	2.52730000	0.15211600
O	-4.44891900	0.93170000	0.21580700
O	0.81195900	-2.61393800	-0.26226300
H	-0.17599800	-2.95327200	-0.21915400
O	2.81826500	1.65693500	-0.18268300

C	2.70315300	3.06295500	-0.11921500
H	3.72237900	3.45458700	-0.15697500
H	2.12897900	3.46494000	-0.96451700
H	2.22345400	3.39223700	0.81201700
C	3.17539300	-1.10035700	-0.34916100
H	3.85618100	-0.42564600	-0.87672800
H	3.08544100	-2.02118400	-0.93295000
C	3.75610600	-1.43898700	1.03341400
H	3.86183500	-0.53258500	1.63808900
H	3.09028300	-2.12796300	1.56086500
H	4.74246600	-1.91121900	0.94799600

4#

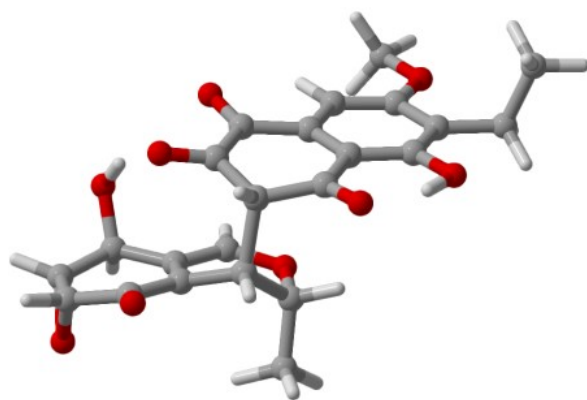
Imaginary frequency : -437.2350 cm⁻¹



C	4.77768700	1.38609300	0.22587600
C	3.37491100	1.78617100	0.65251400
C	2.47904000	0.58085700	0.89727500
C	2.77834600	-0.70685100	0.32171900
C	3.97634200	-0.98233400	-0.41951100
C	5.06899600	0.04894100	-0.31290400
H	0.90952400	1.74980800	1.79051400
C	1.26407300	0.77724100	1.47037000
C	1.69430100	-1.61850600	0.26669900
C	0.75387100	-1.55441900	1.45839300
H	1.94557900	-2.63071400	-0.03770500
O	4.16079600	-1.99374100	-1.11514500
O	5.46884000	0.42874400	1.03209300
O	2.84945300	2.70333500	-0.29723300
H	2.47970800	2.17743400	-1.03924700
H	3.46974300	2.35553200	1.58749200
H	5.38014600	2.23042400	-0.11383800
H	5.89368200	-0.09679700	-1.00941700
O	0.34298300	-0.20144500	1.73912000
C	1.40704300	-2.15238600	2.70615400
H	1.66144600	-3.20363500	2.53502400
H	2.32465400	-1.61025500	2.94653500

H	0.71823500	-2.08938000	3.55455800
H	-0.17665400	-2.08991000	1.25290700
C	0.88806000	0.26860900	-1.56753400
C	-0.19209400	1.25004400	-1.19020800
C	-1.48215900	0.68983200	-0.67472200
C	-1.71757000	-0.69623100	-0.66582500
C	-0.68332100	-1.64140900	-1.11082700
C	0.67167800	-1.14858300	-1.33771200
H	-2.22679800	2.63294200	-0.28863300
C	-2.45654700	1.57716500	-0.23989700
C	-2.97073300	-1.17530900	-0.21427300
H	1.27496100	-1.78232300	-1.98274800
C	-3.95719100	-0.29224700	0.26090800
C	-3.68019300	1.08131300	0.22872000
O	-0.94386900	-2.86967400	-1.19840600
O	-0.05859800	2.45637300	-1.38116400
O	1.98036200	0.67845000	-2.00590800
O	-3.24661800	-2.49240700	-0.22370800
H	-2.42490300	-2.92022900	-0.61763100
O	-4.69085600	1.89196900	0.67652800
C	-4.45246000	3.28849200	0.70750200
H	-5.35960300	3.73937400	1.11418900
H	-3.60037300	3.53920900	1.35086700
H	-4.26575400	3.69022800	-0.29601900
C	-5.28535300	-0.82079700	0.73695800
H	-5.66672900	-0.17258300	1.53122900
H	-5.13237000	-1.81795500	1.15870200
C	-6.31899800	-0.90299200	-0.39800000
H	-6.49587400	0.08741900	-0.82861500
H	-5.95870500	-1.56281300	-1.19264000
H	-7.27624300	-1.29477800	-0.03497300

5#

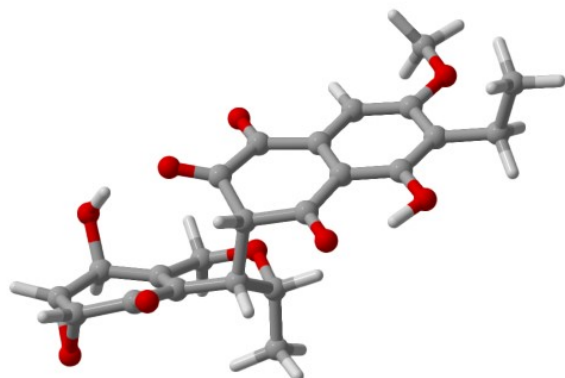


C	4.75008200	1.43326300	0.26678900
C	3.31847400	1.79978300	0.62273900
C	2.43585900	0.57118800	0.79208200

C	2.78598000	-0.67505400	0.22414700
C	4.03669500	-0.95799500	-0.39644100
C	5.10296000	0.09539400	-0.23150800
H	0.77749800	1.68632300	1.63037000
C	1.16912500	0.72885800	1.31079600
C	1.64614100	-1.60362000	0.07722600
C	0.83013200	-1.62521200	1.37799600
H	1.98726200	-2.61118500	-0.16233800
O	4.29001600	-1.98309400	-1.05638600
O	5.42095000	0.50702200	1.12590800
O	2.81714400	2.72562000	-0.33018500
H	2.45034000	2.21515600	-1.08275300
H	3.35294300	2.34619200	1.57556600
H	5.34552900	2.29082900	-0.05159200
H	5.96899200	-0.04004200	-0.87852000
O	0.34310300	-0.30321000	1.68083300
C	1.63299800	-2.16937800	2.55637600
H	1.92183200	-3.20853000	2.36571700
H	2.54188000	-1.58285100	2.70568200
H	1.02755200	-2.13453500	3.46726600
H	-0.07392700	-2.22922000	1.25981900
C	0.87060800	0.32079100	-1.50298200
C	-0.20065300	1.27904600	-1.11423900
C	-1.47761100	0.68863900	-0.60420300
C	-1.71290100	-0.70358100	-0.60934200
C	-0.67840900	-1.64084600	-1.02759500
C	0.72725200	-1.14511400	-1.20965300
H	-2.24718600	2.61975000	-0.23079400
C	-2.46997500	1.56245400	-0.18241900
C	-2.97960100	-1.19022500	-0.18883300
H	1.19166100	-1.68970400	-2.03497000
C	-3.97507500	-0.31879600	0.27837600
C	-3.69731600	1.05700600	0.26264900
O	-0.91866900	-2.86121900	-1.15811200
O	-0.10824500	2.49357000	-1.32827800
O	1.91458000	0.70478600	-2.05467100
O	-3.25450200	-2.50748100	-0.22262600
H	-2.43466000	-2.93504700	-0.60598400
O	-4.71667300	1.85892900	0.69920300
C	-4.48855300	3.25816300	0.73855400
H	-5.40478400	3.70011900	1.13422000
H	-3.64729300	3.51127000	1.39453800
H	-4.29050500	3.66359000	-0.26087700
C	-5.31311300	-0.85075500	0.72274300
H	-5.69985400	-0.22100200	1.52938900
H	-5.17303700	-1.85917900	1.12138000
C	-6.33439500	-0.89484200	-0.42537100
H	-6.49811800	0.10790600	-0.83179900

H	-5.97096300	-1.53647200	-1.23349000
H	-7.29901600	-1.28773900	-0.08364400

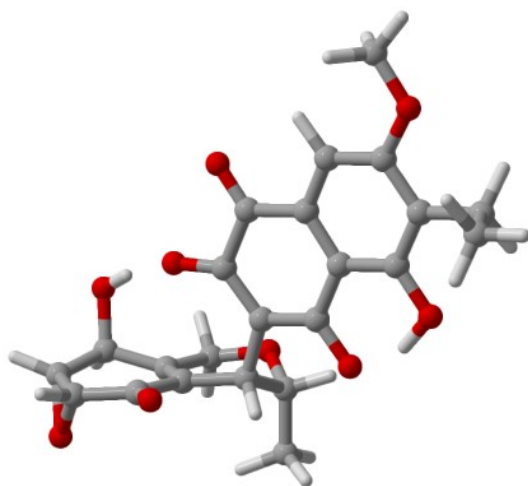
6#



C	5.45121300	0.59576700	-0.32875200
C	4.32666800	1.45757400	0.20699000
C	3.11935800	0.66927600	0.65410000
C	2.86982700	-0.59652200	0.26351800
C	3.81304200	-1.35040900	-0.58677700
C	5.20098600	-0.80473200	-0.72229000
H	2.50271900	1.68461400	2.42654700
C	2.09933500	1.46456900	1.42400400
C	1.51172600	-1.20521100	0.49436700
C	0.86086800	-0.57237100	1.72613400
H	1.59623500	-2.28871700	0.60863800
O	3.47594100	-2.36516300	-1.18383900
O	5.86720400	-0.47128700	0.51523800
O	3.92867500	2.42781100	-0.75616600
H	3.29672000	2.00699900	-1.36412900
H	4.72353800	2.03045800	1.05618400
H	6.24695800	1.14814500	-0.82764700
H	5.81748300	-1.29810400	-1.46996800
O	0.82318900	0.84842400	1.52149900
C	1.53104200	-0.96871800	3.03900400
H	1.38692400	-2.03789200	3.21895100
H	2.60635700	-0.77398600	3.02734400
H	1.08015700	-0.41588900	3.86716800
H	-0.19412000	-0.85303700	1.77882000
C	0.65246600	0.44963100	-1.24313900
C	-0.51839900	1.36379100	-0.85252100
C	-1.78676000	0.70233500	-0.46488400
C	-1.88940200	-0.70967800	-0.38246900
C	-0.74540700	-1.58487300	-0.58163800
C	0.63189900	-0.99793500	-0.81140800
H	-2.75398000	2.58059800	-0.31503000

C	-2.88690400	1.51101200	-0.22876600
C	-3.15534300	-1.27676300	-0.05446000
H	1.13279200	-1.59241400	-1.58039500
C	-4.27236600	-0.46512900	0.20472400
C	-4.12073600	0.92749400	0.10034200
O	-0.84112000	-2.82342700	-0.51375700
O	-0.38123500	2.57202600	-0.91792400
O	1.59521400	0.91431600	-1.85922900
O	-3.31844500	-2.60243700	0.02523400
H	-2.42949500	-3.00763000	-0.17081700
O	-5.24162300	1.65139900	0.33474000
C	-5.16467100	3.07241100	0.26665400
H	-6.16674300	3.43304300	0.49760200
H	-4.45416200	3.46827600	1.00056800
H	-4.87695200	3.40775800	-0.73579600
C	-5.60410000	-1.08557600	0.53482400
H	-6.14743700	-0.42243800	1.21267900
H	-5.43017400	-2.03148900	1.05329200
C	-6.44925900	-1.33940100	-0.72524400
H	-6.64653900	-0.40248800	-1.25415400
H	-5.92912000	-2.01775500	-1.40732100
H	-7.41013600	-1.79152700	-0.46105200
H	1.93608300	2.42092100	0.91827900

7#

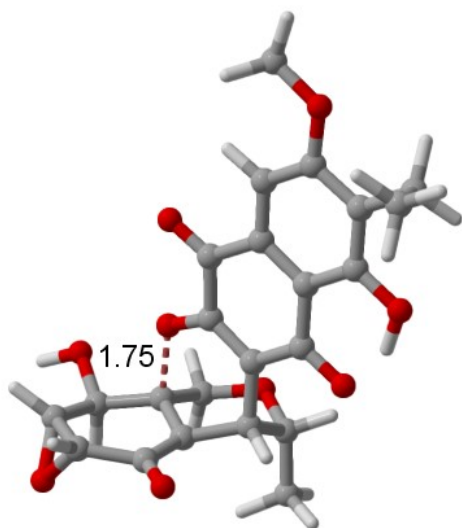


C	5.16933500	1.38682100	-0.86114000
C	4.72047200	1.07446300	0.54889000
C	3.77557300	-0.09743600	0.63997900
C	2.95014100	-0.44098800	-0.36518500
C	3.13586300	0.08477900	-1.72924400
C	4.36619400	0.90854900	-1.99386900
H	4.45250500	-1.26441300	2.28067600
C	3.57862400	-0.62955700	2.03131300

C	1. 71729400	-1. 26270500	-0. 10464000
C	1. 93207900	-2. 13072000	1. 15170000
H	1. 55335100	-1. 94028400	-0. 94923200
O	2. 34651400	-0. 12840600	-2. 64119400
O	5. 63590000	0. 29404800	-1. 65326600
O	4. 05585800	2. 20903000	1. 09478000
H	3. 12045100	2. 15643900	0. 78287500
H	5. 61173700	0. 90247300	1. 17037100
H	5. 72654000	2. 31837700	-0. 96554000
H	4. 35450100	1. 44286800	-2. 94186300
O	2. 36935300	-1. 32004600	2. 25273500
C	2. 87824200	-3. 30535200	0. 89751000
H	2. 41918400	-3. 99890400	0. 18658500
H	3. 83217800	-2. 97323600	0. 47513500
H	3. 07664900	-3. 84212300	1. 83074000
H	0. 96446300	-2. 51852300	1. 47047100
C	0. 48230400	1. 01432800	0. 17128800
C	-0. 87826500	1. 73813400	0. 31908700
C	-2. 13660100	0. 95085600	0. 21284500
C	-2. 06234600	-0. 42973200	0. 01372400
C	-0. 75226000	-1. 11514400	-0. 09159800
C	0. 46622700	-0. 39479800	0. 01122800
H	-3. 34808000	2. 67853500	0. 46561500
C	-3. 36212000	1. 60747200	0. 31595100
C	-3. 26616800	-1. 16862100	-0. 08427600
C	-4. 51545600	-0. 52750400	0. 03039900
C	-4. 53968500	0. 86286000	0. 21504500
O	-0. 76360300	-2. 38217700	-0. 26756000
O	-0. 90529500	2. 94423200	0. 51715400
O	1. 47726200	1. 77787200	0. 19703900
O	-3. 24337800	-2. 49566200	-0. 28665600
H	-2. 24218100	-2. 71038000	-0. 31924600
O	-5. 79434100	1. 42421200	0. 28704300
C	-5. 87328900	2. 82033800	0. 49678100
H	-6. 93763400	3. 06239100	0. 53083500
H	-5. 40310500	3. 11743900	1. 44311900
H	-5. 39991500	3. 38204100	-0. 31881000
C	-5. 78390200	-1. 33086200	-0. 09376200
H	-6. 56946800	-0. 86503600	0. 50827200
H	-5. 59865200	-2. 33288400	0. 30346500
C	-6. 25495400	-1. 44666700	-1. 55264200
H	-6. 45465000	-0. 45550600	-1. 97179000
H	-5. 48359300	-1. 92740400	-2. 16096500
H	-7. 17263200	-2. 04201100	-1. 62790200
H	3. 58838800	0. 21421700	2. 73028200

8#

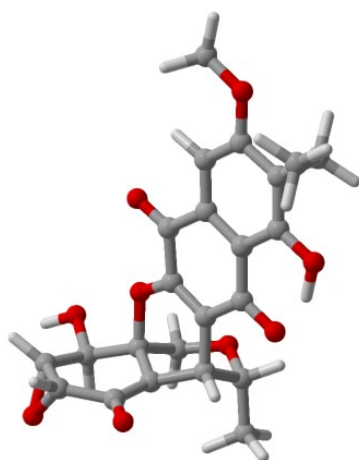
Imaginary frequency : -283.9031 cm⁻¹



C	-4.20551700	1.77031700	1.31484900
C	-4.21692200	1.37876500	-0.15631100
C	-3.15682300	0.34974700	-0.51061800
C	-2.85931200	-0.65136800	0.45459700
C	-2.98305400	-0.45044000	1.85146200
C	-3.66567700	0.82946800	2.30157400
H	-4.36701000	-0.53476800	-2.01744600
C	-3.33530900	-0.14647900	-1.94609500
C	-1.77727600	-1.57659000	-0.05749600
C	-2.16795200	-2.18122900	-1.41428500
H	-1.58683000	-2.37555400	0.66150200
O	-2.53134100	-1.19856500	2.74361500
O	-5.09848000	0.99996600	2.13166500
O	-4.10920300	2.50679600	-1.02293100
H	-4.89660600	3.04428100	-0.87022400
H	-5.17771000	0.86514900	-0.32235500
H	-4.19110700	2.84497200	1.51086300
H	-3.29379900	1.19430700	3.25912600
O	-2.40003600	-1.12192400	-2.36150000
C	-3.36454300	-3.12448500	-1.31029900
H	-4.19069800	-2.64034200	-0.78166600
H	-3.70043500	-3.43111100	-2.30622700
H	-3.08614300	-4.01833000	-0.74252700
H	-1.31066500	-2.71968500	-1.83126100
C	-0.61640800	0.62892900	-0.46598200
C	0.62084000	1.49886300	-0.44526700
C	1.94169800	0.82196800	-0.29491900
C	1.99686900	-0.56157000	-0.09390800
C	0.75625000	-1.36247500	-0.03260900
C	-0.52511900	-0.72940600	-0.18746600
H	2.99125400	2.65737600	-0.49015400
C	3.10006800	1.59138500	-0.34398600
C	3.25968600	-1.18122400	0.05050600

C	4.44616300	-0.42421000	-0.01324500
C	4.34102900	0.96182300	-0.19568600
O	0.84944000	-2.61117200	0.13913800
O	0.54323200	2.71497800	-0.56383100
O	-1.70452100	1.29429300	-0.72339300
O	3.35731300	-2.50543900	0.25294100
H	2.39625500	-2.82570500	0.25118400
O	5.53381300	1.64244700	-0.21732800
C	5.48789900	3.04296700	-0.41690800
H	6.52502900	3.38372400	-0.40587800
H	5.03092800	3.30149900	-1.38053100
H	4.93128800	3.54895900	0.38193000
C	5.78166900	-1.09904600	0.16221300
H	6.53661400	-0.56479900	-0.42185400
H	5.70915800	-2.11827500	-0.22712500
C	6.21423000	-1.15007500	1.63667900
H	6.30238200	-0.13911000	2.04630600
H	5.47565200	-1.69708100	2.22950200
H	7.18289500	-1.65093500	1.74799200
H	-3.23711700	0.69058200	-2.63895200

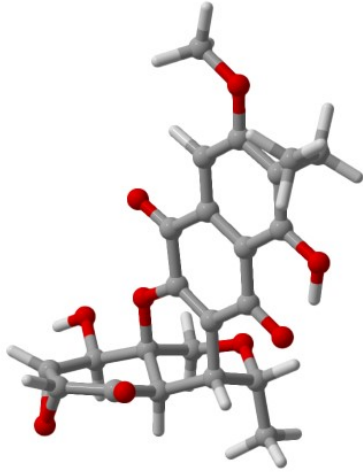
9#



C	-4.13355800	1.78963500	1.32105000
C	-4.14652100	1.41223900	-0.15398300
C	-3.04444400	0.42295200	-0.52149200
C	-2.85567900	-0.65979100	0.44725300
C	-3.02140300	-0.49913900	1.83477300
C	-3.65209600	0.80590900	2.29612300
H	-4.31914800	-0.48486800	-1.97895600
C	-3.28576300	-0.10337300	-1.94829700
C	-1.78983100	-1.59914100	-0.06325000
C	-2.16972100	-2.17634400	-1.43757600
H	-1.61938300	-2.40641600	0.65178600
O	-2.64491000	-1.29457900	2.72952300

O	-5.07412800	1.05947100	2.12184800
O	-4.06909100	2.55139400	-1.01166800
H	-4.83763900	3.09946600	-0.80869100
H	-5.08890700	0.86889600	-0.31809200
H	-4.06082800	2.85990100	1.52963600
H	-3.27067400	1.13995400	3.26150900
O	-2.36587400	-1.09500600	-2.36903500
C	-3.38692600	-3.09434000	-1.36115400
H	-4.19856600	-2.60462600	-0.81588200
H	-3.72947700	-3.36402700	-2.36543900
H	-3.12835200	-4.01023400	-0.81961600
H	-1.31872400	-2.72541900	-1.85501900
C	-0.61722600	0.58424900	-0.42894900
C	0.59114200	1.46601200	-0.44573400
C	1.91888000	0.80053900	-0.29568500
C	1.99422000	-0.58408600	-0.09628200
C	0.76660000	-1.39835300	-0.03010000
C	-0.52716600	-0.76744900	-0.17782200
H	2.94513100	2.64761400	-0.48978900
C	3.06712700	1.58317700	-0.34286500
C	3.26501100	-1.18628000	0.05178100
C	4.44165500	-0.41457000	-0.01018500
C	4.31692500	0.96974900	-0.19240800
O	0.86124400	-2.64235900	0.14014600
O	0.50201100	2.68035700	-0.59151800
O	-1.74156500	1.25106500	-0.64010000
O	3.38088800	-2.50939500	0.25404000
H	2.43084200	-2.84766700	0.25312000
O	5.49871200	1.66644400	-0.21274300
C	5.43521200	3.06718700	-0.41121100
H	6.46799400	3.42039200	-0.39834000
H	4.97656100	3.32020200	-1.37529300
H	4.87135300	3.56473600	0.38759800
C	5.78651100	-1.07029300	0.16653500
H	6.53288600	-0.52784700	-0.42093000
H	5.72832700	-2.09186000	-0.21888500
C	6.22199600	-1.10860700	1.64054700
H	6.29615800	-0.09475700	2.04564900
H	5.49288300	-1.66379300	2.23749200
H	7.19802500	-1.59468400	1.75194000
H	-3.19643900	0.71660200	-2.66415600

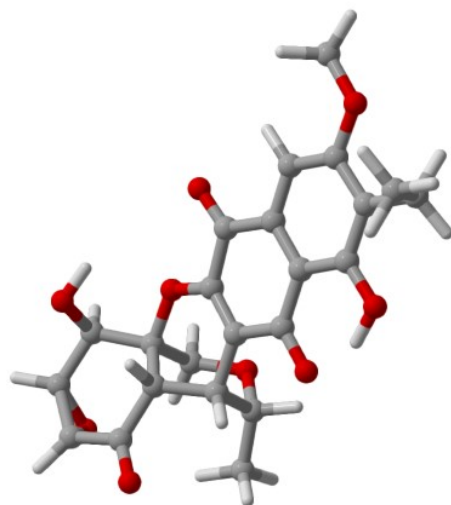
10a#



C	-4.17985700	1.82921700	1.22696100
C	-4.19499600	1.35235200	-0.22336100
C	-3.06190100	0.36918100	-0.53512100
C	-2.93044300	-0.72383100	0.54113100
C	-2.64088900	-0.11042800	1.91170100
C	-3.44390700	1.10094500	2.28181200
H	-4.31487900	-0.68981200	-1.91979100
C	-3.29510100	-0.27338200	-1.91548900
C	-1.79871200	-1.65136600	0.08075000
C	-2.14718500	-2.28620700	-1.28691900
H	-1.60971400	-2.43781400	0.81273700
O	-1.79468600	-0.54760700	2.66452400
O	-4.87222400	0.96538000	2.12726700
O	-4.10717200	2.42305800	-1.14377100
H	-4.93471100	2.91929800	-1.10813900
H	-5.13579000	0.79403700	-0.34883700
H	-4.35486700	2.89603400	1.37080500
H	-3.11381700	1.60820400	3.18590600
O	-2.33557300	-1.24942000	-2.25842100
C	-3.31732800	-3.26649000	-1.24131000
H	-4.24740000	-2.80586900	-0.89624000
H	-3.49482700	-3.67351700	-2.23988700
H	-3.08452600	-4.09445100	-0.56526700
H	-1.25939000	-2.82019000	-1.63528900
C	-0.67374700	0.50319700	-0.38609500
C	0.51311400	1.40546000	-0.51093900
C	1.84468800	0.76620100	-0.33843700
C	1.94762000	-0.60922500	-0.05375300
C	0.75122500	-1.43420200	0.08561500
C	-0.56289500	-0.80957400	-0.06717000
H	2.84397600	2.60746000	-0.67794000
C	2.97766100	1.55601400	-0.46378100
C	3.23409700	-1.18156900	0.09642800
C	4.39625800	-0.39801400	-0.03997300
C	4.24540100	0.97082800	-0.30487200

O	0.82390400	-2.66183300	0.32085900
O	0.37334700	2.59833400	-0.73753800
O	-1.84536300	1.14992100	-0.55920400
O	3.38423500	-2.48454300	0.37397800
H	2.46530800	-2.86486300	0.41916000
O	5.40377300	1.67753800	-0.39598800
C	5.32960000	3.06763500	-0.68611800
H	6.36099200	3.41917700	-0.71824100
H	4.85150800	3.24992900	-1.65544500
H	4.78336300	3.61092500	0.09351500
C	5.75674400	-1.01621100	0.14673700
H	6.47311400	-0.50408500	-0.50087600
H	5.71039400	-2.06356800	-0.16144400
C	6.23197900	-0.93256200	1.60722900
H	6.29791000	0.10968500	1.93274800
H	5.53589400	-1.45652000	2.26832200
H	7.22020900	-1.38944900	1.72043000
H	-3.23707000	0.50584900	-2.67613100
H	-3.88616500	-1.25490800	0.61608300

10b#



C	-5.05634400	1.43262800	0.72541000
C	-3.72426900	1.96867200	0.23856000
C	-2.79526400	0.85661700	-0.28924400
C	-2.69519100	-0.31949500	0.68460900
C	-4.01293300	-0.88756900	1.18606000
C	-5.19233100	0.04945500	1.21846400
H	-4.17303200	0.03945100	-1.73001400
C	-3.13659900	0.39012500	-1.71142000
C	-1.69707800	-1.31859700	0.08468200
C	-2.12113900	-1.75178100	-1.34546100
H	-1.59548000	-2.20277700	0.71553600
O	-4.09783800	-2.00494200	1.65513300

O	-5.69115100	0.44457400	-0.08266300
O	-3.14561300	2.60886700	1.36086700
H	-2.25997100	2.88954200	1.08227000
H	-3.90402000	2.68746500	-0.57691600
H	-5.71886000	2.19052200	1.14081400
H	-5.96339100	-0.21374400	1.93908800
O	-2.22859200	-0.59116900	-2.18053300
C	-3.36913100	-2.62837500	-1.41759300
H	-4.27432600	-2.10605200	-1.10160200
H	-3.51573400	-2.95827200	-2.44927500
H	-3.25679000	-3.50565700	-0.77577600
H	-1.28083800	-2.30813500	-1.76971500
C	-0.38424700	0.75731200	-0.20572900
C	0.86894700	1.57207700	-0.22171600
C	2.14402000	0.81581000	-0.15295700
C	2.13419400	-0.58623200	-0.01048800
C	0.87536600	-1.32261100	0.07631200
C	-0.38713400	-0.58325300	0.00328400
H	3.28960300	2.59522400	-0.32215900
C	3.33701400	1.51956600	-0.22206500
C	3.37080100	-1.27328500	0.05253200
C	4.59270900	-0.57733700	-0.03424900
C	4.55401400	0.81921500	-0.15556500
O	0.85055400	-2.56754500	0.20110100
O	0.81348900	2.79366500	-0.27335100
O	-1.49294300	1.51107500	-0.34772800
O	3.41759700	-2.60449800	0.19817500
H	2.47225400	-2.91421900	0.22891300
O	5.76515400	1.43373000	-0.20354400
C	5.80504400	2.84797000	-0.35113300
H	6.86195200	3.11351300	-0.37438100
H	5.32790900	3.16668800	-1.28494100
H	5.32095100	3.35225100	0.49302600
C	5.89885100	-1.32143500	0.05406200
H	6.64553700	-0.80372100	-0.55344200
H	5.75983900	-2.32272300	-0.36076200
C	6.40164400	-1.43270500	1.50358500
H	6.56011500	-0.44006900	1.93501600
H	5.67478400	-1.96592000	2.12280600
H	7.34959400	-1.97826800	1.54365000
H	-3.04180000	1.23923900	-2.39310700
H	-2.26922000	0.09497700	1.61168100

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