Supplementary Materials

Indole diterpene derivatives from the *Aspergillus flavus* GZWMJZ-288, an endophytic fungus from *Garcinia multiflora*

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Table S1. The X-ray single crystal experimental details.

Crystal data	**Compound 2 (CCDC 2222865)**
Chemical formula	$C_{28}H_{39}O_3N$
M_r	437.60
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	150
a, b, c (Å)	9.3756 (3), 10.4260 (4), 12.5667 (5)
α, β, γ (°)	90, 96.673 (2), 90
V (Å^3)	1220.07 (8)
Z	2
Radiation	CuKα (λ = 1.54178)
μ/mm^{-1}	0.595
Crystal size (mm^3)	0.2 × 0.15 × 0.1
Data collection	
Diffractometer	Bruker D8 goniometer with CCD area detector
Absorption correction	Multi-scan *SADABS*
T_{min}, T_{max}	0.898, 0.942
No. of measured, independent and observed [$I > 2\sigma$ (I)] reflections	10667, 4676, 4676
R_{int}	0.0407
Refinement	
R [$F^2 > 2\sigma$ (F^2)], $wR(F^2)$, S	0.0710, 0.1633
No. of data	4676
No. of parameters	296
No. of restraints	2
Largest diff. peak/hole (e Å^{-3})	0.48, -0.21
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -15 ≤ l ≤ 15
Flack parameter	0.06 (13)

A suitable crystal was selected and on a Bruker APEX-II CCD diffractometer. The crystal was kept at 150.00 K during data collection. Using Olex2, the structure was solved with the SHELXT structure solution program using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimisation.

Table S2. Geometric parameters (Å, º).

Atom - Atom	Length/Å	Atom - Atom	Length/Å
O001-C00F	1.431(4)	C00B-C00D	1.592(4)
O002-C00K	1.443(4)	C00B-C00K	1.560(4)
O003-C00V	1.426(4)	C00B-C00L	1.575(4)
N004-C005	1.368(4)	C00B-C00U	1.542(5)
N004-C00E	1.367(5)	C00C-C00E	1.369(5)
C005-C00I	1.403(4)	C00C-C00I	1.441(4)
C005-C00M	1.398(5)	C00D-C00F	1.557(4)
C006-C00A	1.528(4)	C00D-C00H	1.554(4)
C006-C00D	1.561(4)	C00F-C00O	1.525(4)
C006-C00J	1.566(4)	C00G-C00H	1.538(4)
C007-C008	1.522(4)	C00I-C00N	1.410(5)
C007-C00V	1.513(5)	C00J-C00S	1.541(5)
C007-C00W	1.527(5)	C00L-C00P	1.543(4)
C008-C00A	1.337(4)	C00L-C00Q	1.534(4)
C008-C00G	1.511(5)	C00M-C00R	1.381(6)
C009-C00J	1.529(5)	C00N-C00T	1.379(5)
C009-C00K	1.508(5)	C00O-C00Q	1.513(4)
C00A-C00C	1.489(4)	C00R-C00T	1.408(6)

Atom -Atom- Atom	Length/Å	Atom -Atom- Atom	Length/Å
C00E-N004-C005	108.9(3)	C00H-C00D-C006	106.9(2)
N004-C005-C00I	107.8(3)	C00H-C00D-C00B	113.6(2)
N004-C005-C00M	129.5(3)	C00H-C00D-C00F	106.6(2)
C00M-C005-C00I	122.7(3)	N004-C00E-C00C	110.5(3)
C00A-C006-C00D	112.4(2)	O001-C00F-C00D	109.5(2)
C00A-C006-C00J	109.9(2)	O001-C00F-C00O	109.5(2)
C00D-C006-C00J	117.0(3)	C00O-C00F-C00D	114.3(2)
C008-C007-C00W	111.3(3)	C008-C00G-C00H	115.3(3)
C00V-C007-C008	111.3(3)	C00G-C00H-C00D	111.9(2)
C00V-C007-C00W	111.7(3)	C005-C00I-C00C	107.3(3)
C00A-C008-C007	121.6(3)	C005-C00I-C00N	118.8(3)
C00A-C008-C00G	121.8(3)	C00N-C00I-C00C	133.9(3)
C00G-C008-C007	116.5(3)	C009-C00J-C006	110.7(3)
C00K-C009-C00J	111.6(3)	C009-C00J-C00S	110.3(3)
C008-C00A-C006	122.9(3)	C00S-C00J-C006	116.6(3)
C008-C00A-C00C	122.3(3)	O002-C00K-C009	111.3(2)
C00C-C00A-C006	114.7(3)	O002-C00K-C00B	114.1(3)
C00K-C00B-C00D	106.6(2)	C009-C00K-C00B	113.3(3)
C00K-C00B-C00L	111.9(2)	C00P-C00L-C00B	115.2(3)
C00L-C00B-C00D	109.2(2)	C00Q-C00L-C00B	111.6(2)
C00U-C00B-C00D	112.7(2)	C00Q-C00L-C00P	108.2(3)
C00U-C00B-C00K	107.2(3)	C00R-C00M-C005	117.2(3)
C00U-C00B-C00L	109.3(3)	C00T-C00N-C00I	118.9(3)
C00E-C00C-C00A	127.5(3)	C00Q-C00O-C00F	111.7(3)
C00E-C00C-C00I	105.6(3)	C00O-C00Q-C00L	110.9(3)
C00I-C00C-C00A	126.8(3)	C00M-C00R-C00T	121.4(3)
C006-C00D-C00B	110.9(2)	C00N-C00T-C00R	121.0(3)
C00F-C00D-C006	107.7(2)	O003-C00V-C007	109.7(3)

C00F-C00D-C00B	111.0(2)

Atom	-Atom-Atom-Atom	Length/Å	Atom	-Atom-Atom-Atom	Length/Å
O001	C00F-C00O-C00Q	70.1(3)	C00E	C00C-C00I-C00N	-178.7(3)
N004	C005-C00I-C00C	-0.4(3)	C00F	C00D-C00H-C00G	55.0(3)
N004	C005-C00I-C00N	178.6(3)	C00F	C00O-C00Q-C00L	56.6(4)
N004	C005-C00M-C00R	-177.1(3)	C00G	C008-C00A-C006	-1.2(5)
C005	N004-C00E-C00C	-0.6(4)	C00G	C008-C00A-C00C	-179.9(3)
C005	C00I-C00N-C00T	-0.9(5)	C00H	C00D-C00F-O001	51.5(3)
C005	C00M-C00R-C00T	-1.2(5)	C00H	C00D-C00F-C00O	174.8(3)
C006	C00A-C00C-C00E	92.7(4)	C00I	C005-C00M-C00R	0.7(5)
C006	C00A-C00C-C00I	-84.4(4)	C00I	C00C-C00E-N004	0.3(3)
C006	C00D-C00F-O001	165.9(2)	C00I	C00N-C00T-C00R	0.4(5)
C006	C00D-C00F-C00O	-70.9(3)	C00J	C006-C00A-C008	109.2(3)
C006	C00D-C00H-C00G	-59.9(3)	C00J	C006-C00A-C00C	-72.0(3)
C007	C008-C00A-C006	175.0(3)	C00J	C006-C00D-C00B	47.5(3)
C007	C008-C00A-C00C	-3.7(5)	C00J	C006-C00D-C00F	169.1(2)
C007	C008-C00G-C00H	177.2(3)	C00J	C006-C00D-C00H	-76.8(3)
C008	C007-C00V-O003	-166.3(3)	C00J	C009-C00K-O002	167.1(2)
C008	C00A-C00C-C00E	-88.5(4)	C00J	C009-C00K-C00B	-62.8(3)
C008	C00A-C00C-C00I	94.4(4)	C00K	C009-C00J-C006	50.3(4)
C008	C00G-C00H-C00D	38.2(4)	C00K	C009-C00J-C00S	-80.3(3)
C00A	C006-C00D-C00B	176.0(2)	C00K	C00B-C00D-C006	-52.5(3)
C00A	C006-C00D-C00F	-62.4(3)	C00K	C00B-C00D-C00F	-172.1(2)
C00A	C006-C00D-C00H	51.8(3)	C00K	C00B-C00D-C00H	67.8(3)
C00A	C006-C00J-C009	-174.8(2)	C00K	C00B-C00L-C00P	-61.7(4)
C00A	C006-C00J-C00S	-47.6(4)	C00K	C00B-C00L-C00Q	174.4(3)
C00A	C008-C00G-C00H	-6.5(4)	C00L	C00B-C00D-C006	68.5(3)
C00A	C00C-C00E-N004	-177.2(3)	C00L	C00B-C00D-C00F	-51.1(3)
C00A	C00C-C00I-C005	177.7(3)	C00L	C00B-C00D-C00H	-171.1(3)
C00A	C00C-C00I-C00N	-1.2(5)	C00L	C00B-C00K-O002	71.8(3)
C00B	C00D-C00F-O001	-72.6(3)	C00L	C00B-C00K-C009	-56.9(3)
C00B	C00D-C00F-C00O	50.7(3)	C00M	C005-C00I-C00C	-178.7(3)
C00B	C00D-C00H-C00G	177.5(3)	C00M	C005-C00I-C00N	0.4(5)
C00B	C00L-C00Q-C00O	-59.8(4)	C00M	C00R-C00T-C00N	0.7(6)
C00C	C00I-C00N-C00T	177.8(3)	C00P	C00L-C00Q-C00O	172.4(3)
C00D	C006-C00A-C008	-23.0(4)	C00U	C00B-C00D-C006	-169.8(3)
C00D	C006-C00A-C00C	155.8(3)	C00U	C00B-C00D-C00F	70.5(3)
C00D	C006-C00J-C009	-45.1(4)	C00U	C00B-C00D-C00H	-49.5(3)
C00D	C006-C00J-C00S	82.1(4)	C00U	C00B-C00K-O002	-48.0(3)
C00D	C00B-C00K-O002	-168.9(2)	C00U	C00B-C00K-C009	-176.7(3)
C00D	C00B-C00K-C009	62.4(3)	C00U	C00B-C00L-C00P	56.8(4)
C00D	C00B-C00L-C00P	-179.5(3)	C00U	C00B-C00L-C00Q	-67.1(3)
C00D	C00B-C00L-C00Q	56.6(4)	C00V	C007-C008-C00A	121.8(4)
C00D	C00F-C00O-C00Q	-53.2(4)	C00V	C007-C008-C00G	-61.8(4)
C00E	N004-C005-C00I	0.6(3)	C00W	C007-C008-C00A	-112.8(4)
C00E	N004-C005-C00M	178.7(3)	C00W	C007-C008-C00G	63.6(4)
C00E	C00C-C00I-C005	0.1(3)	C00W	C007-C00V-O003	68.6(4)

Table S3. Hydrogen Atom Coordinates and Isotropic Displacement Parameters.

Atom	*x*	*y*	*z*	U(eq)
H001	1358.98	1335.02	7097.79	76
H002	8280.04	2819.32	8887.46	79
H003	938.16	6788.82	2766.66	85
H004	2822.48	9601.31	7184.8	59
H006	3843.03	4849.67	8149.19	51
H007	1049.32	6340.24	5331.41	57
H00A	7736.55	4873.08	7952.94	59
H00B	6661	4674.86	8840.37	59
H00E	3918.81	7885.66	6266.57	59
H00F	1780.83	3298.36	7176.58	53
H00C	3036.38	3522.93	4648.09	59
H00D	1941.51	2914.46	5390.49	59
H00G	4968.69	3169.02	5870.12	55
H00H	4016.4	1915.08	5994.76	55
H00J	5569.8	6151.47	7720.81	57
H00K	6717.67	3055.7	7035.26	57
H00L	4993.69	3635.36	9404.64	57
H00M	734.03	9855.15	8551.97	65
H00N	550.15	5336.19	8160.62	61
H00I	2325.91	3779.17	8971.88	58
H00O	1391.84	2489.75	8898.81	58
H00P	6315.27	1205.56	9913.94	91
H00Q	5781.99	2111.85	10816.5	91
H00R	7026.1	2588.92	10140	91
H00S	3464.1	1248.45	9325.6	62
H00T	3382	2311.22	10237.5	62
H00U	-781.47	8611.11	9490.85	71
H00V	6875.97	6143.85	6314.71	86
H00W	5269.09	5871.42	5784.48	86
H00X	6396.2	4717.13	5966.15	86
H00Y	-887.19	6381.52	9281.24	70
H00Z	4570.44	594.89	8082.51	75
H	6284.12	710.47	8228.39	75
HA	5402.52	908.94	7071.29	75
H00	2579.76	6016.79	3937.12	75
HB	1558.07	4846.88	3511.42	75
H1	-189.15	3956.36	4592.16	106
HC	-1019.02	5288.07	4671.37	106
HD	-399.93	4543.89	5739.97	106

Table S4. ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR data of compounds **3**-**6.**

Position	3		4		5		6	
	δ_C	δ_H, (*J* in Hz)	δ_C	δ_H, (*J* in Hz)	δ_C	δ_H, (*J* in Hz)	δ_C	δ_H, (*J* in Hz)
2	122.0	6.91, d, (2.3)	123.5	7.06, d, (2.2)	138.5		121.4	6.89, d, (1.8)
3	116.6		118.3		118.8		119.5	

4	127.0		127.0		123.2		127.7	
5	118.4	7.41, d, (8.0)	117.4	7.35, d, (8.1)	121.8	8.03, d, (7.9)	119.7	7.44, d, (8.2)
6	118.5	7.09, td, (7.5, 0.9)	114.6	7.19, td, (7.4, 08)	119.6	7.29, td, (7.9, 1.1)	118.7	7.09, td, (7.5, 0.6)
7	120.8	7.19, td, (7.2, 0.8)	120.6	7.12, td, (7.5, 0.9)	124.5	7.40, td, (7.2, 0.8)	121.9	7.19, dt, (7.0, 0.7)
8	111.5	7.38, d, (7.8)	111.5	7.53, d, (7.8)	110.8	7.42, d, (7.5)	111.2	7.37, d, (8.2)
9	135.9		135.9		139.6		136.0	
10	125.5		33.9	3.66, dd, (12.5, 5.5)	34.7		125.6	
11	43.1	2.48, d, (6.2)	38.4	2.68, ddd, (5.2, 5.2, 0.8)	38.9	4.22, dd, (6.4, 1.3)	43.6	2.44, d, (4.8)
12	29.8	1.50-1.52, m	27.2	1.61-1.66, m	31.5	2.86-2.91, m	31.4	1.95-1.99, m
13	35.4	0.84-0.88, m 1.72-1.84, m	37.3	1.21, dddd, (12.5, 2.8, 2.8, 0.8) 1.74-1.83, m	35.4	2.40-2.43, m 1.73, dd, (12.4, 1.8)	25.8	1.63-1.65, m 1.15-1.18, m
14	69.4	4.48-4.81, m	69.5	4.66-4.69, m	72.3	4.26, dd, (12.8, 3.2)	27.7	1.55-1.58, m 1.19-1.22, m
15	42.9		42.6		43.8		38.6	
16	30.2	2.21-2.25, m	30.6	2.19-2.24, m	31.4	2.61-2.66, m	29.2	2.03-2.08, m
17	29.3	1.17-1.20, m 1.72-1.84, m	30.0	1.74-1.83, m 1.33-1.34, overlap	27.3	1.27-1.30, m 1.78-1.84, m	25.5	1.25-1.27, m 1.65-1.68, m
18	31.0	1.24-1.26, m 1.72-1.84, m	31.0	1.74-1.83, m 1.33-1.34, overlap	24.5	1.32-1.39, m 1.87-1.93, m	21.9	1.74-1.78, m 2.03-2.08, m
19	68.0	4.04, dd, (12.4, 3.5)	66.1	3.98, dd, (12.3, 2.7)	71.0	3.88, dd, (2.6, 2.6)	71.3	4.49, bs
20	44.0		45.4		44.0		42.5	
21	21.6	1.88-1.92, m 2.12-2.25, m	24.3	1.84-1.92, m 2.11-2.15, m	22.0	2.16-2.22, m 2.74-2.81, m	30.2	1.82-1.85, m 1.72-1.75, m
22	27.3	1.88-1.92, m 2.12-2.25, m	27.3	1.84-1.92, m 2.20-2.29, m	30.3	2.44-2.47, m 2.91-2.95, m	20.6	2.21-2.24, m 2.10-2.13, m
23	139.7		43.7	3.14-3.21, m	126.0		141.2	
24	30.4	2.56-2.61, m	149.9		135.1		31.1	2.56-2.64, m
25	21.7	1.01, d, (6.6)	111.1	4.85, dd, (2.7, 2.7) 4.80, d, (1.8)	109.3	7.08, s	22.0	0.83, d, (6.9)
26	20.0	0.95, d, (7.3)	22.4	1.51, s	20.7	2.38, s	20.9	0.97, d, (6.8)
27	19.2	0.83, d, (6.8)	19.4	1.30, d, (7.1)	19.2	0.67, d, (7.5)	18.2	1.09, d, (7.5)
28	19.4	1.15, d, (7.3)	18.2	1.05, d, (6.8)	19.6	1.25, d, (6.7)	15.9	0.76, d, (6.8)
29	13.3	1.28, s	13.5	1.27, s	13.2	1.41, s	18.2	1.00, s
NH		8.08, brs		7.95, s		8.06, s		8.05, brs

^{1}H (600 MHz) and ^{13}C (150 MHz) NMR data of **5**, **6** in Chloroform-d_3, and ^{1}HNMR **3**, **4** in Chloroform-d_3, ^{13}CNMR in DMSO-d_6.

Figure S1. HRESIMS spectrum of compound **1.**

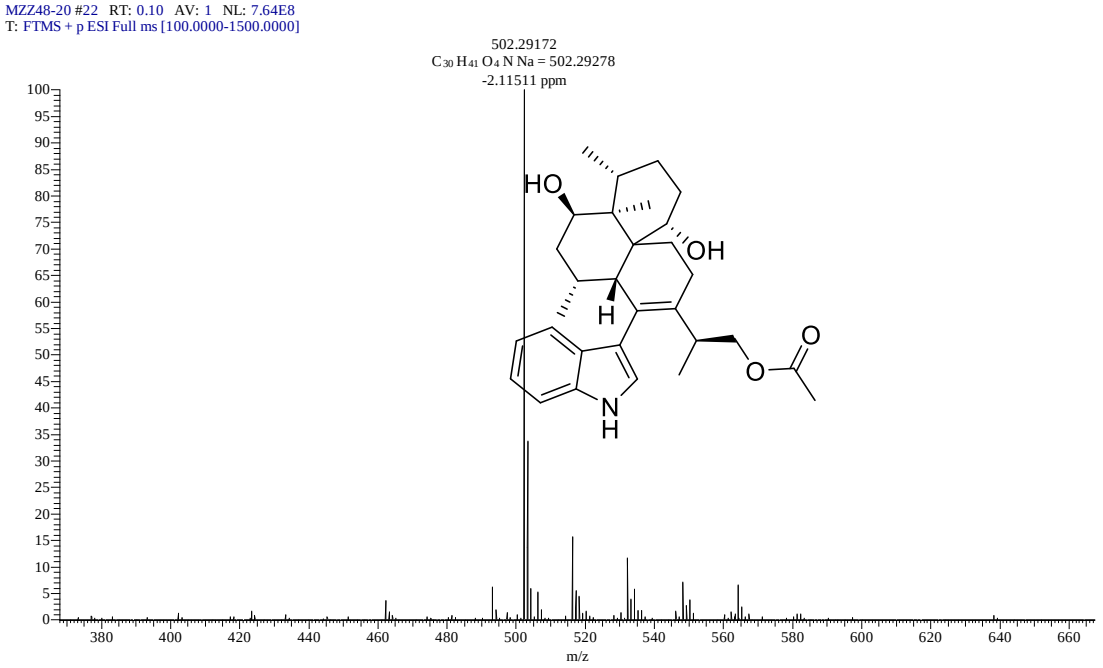


Figure S2. ^{1}H-NMR spectrum of compound **1** in DMSO-d$_6$ (600 MHz).

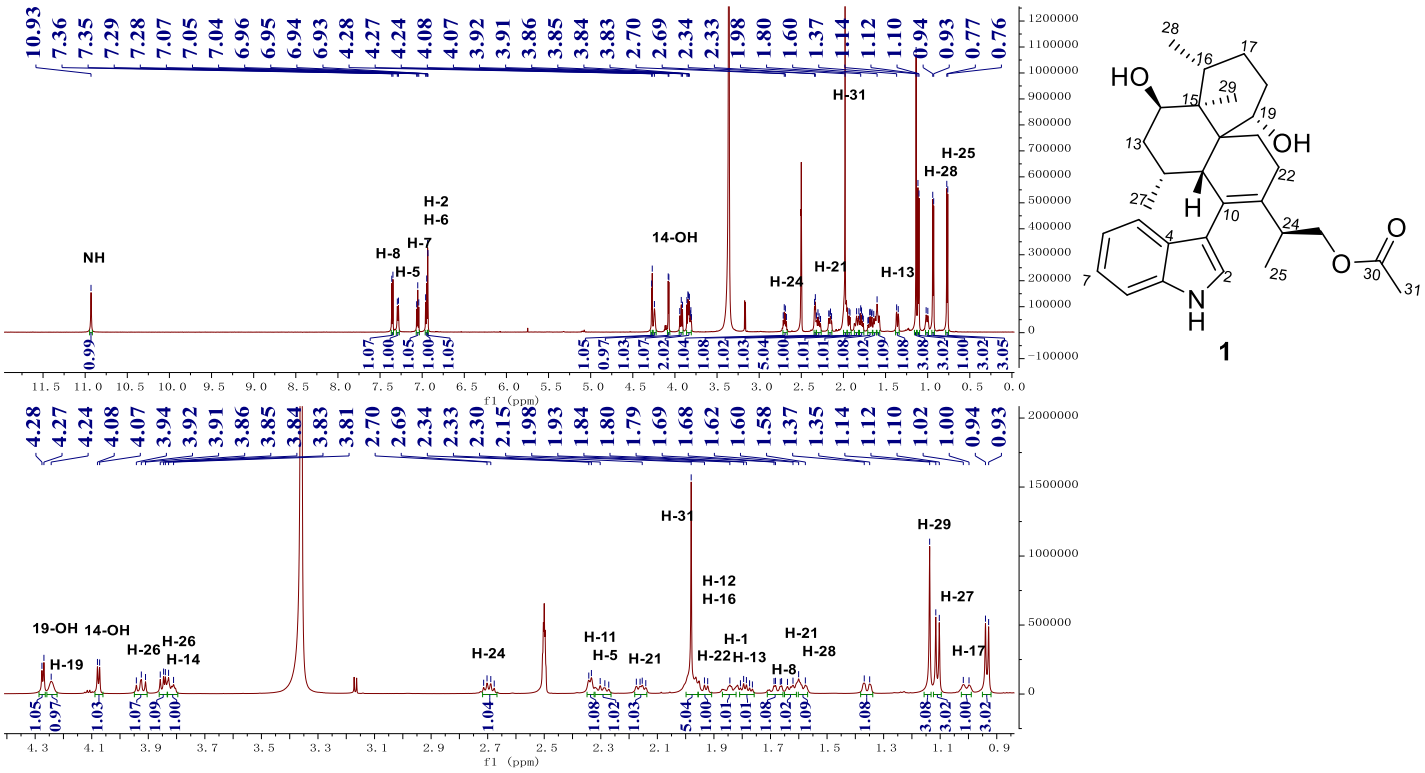
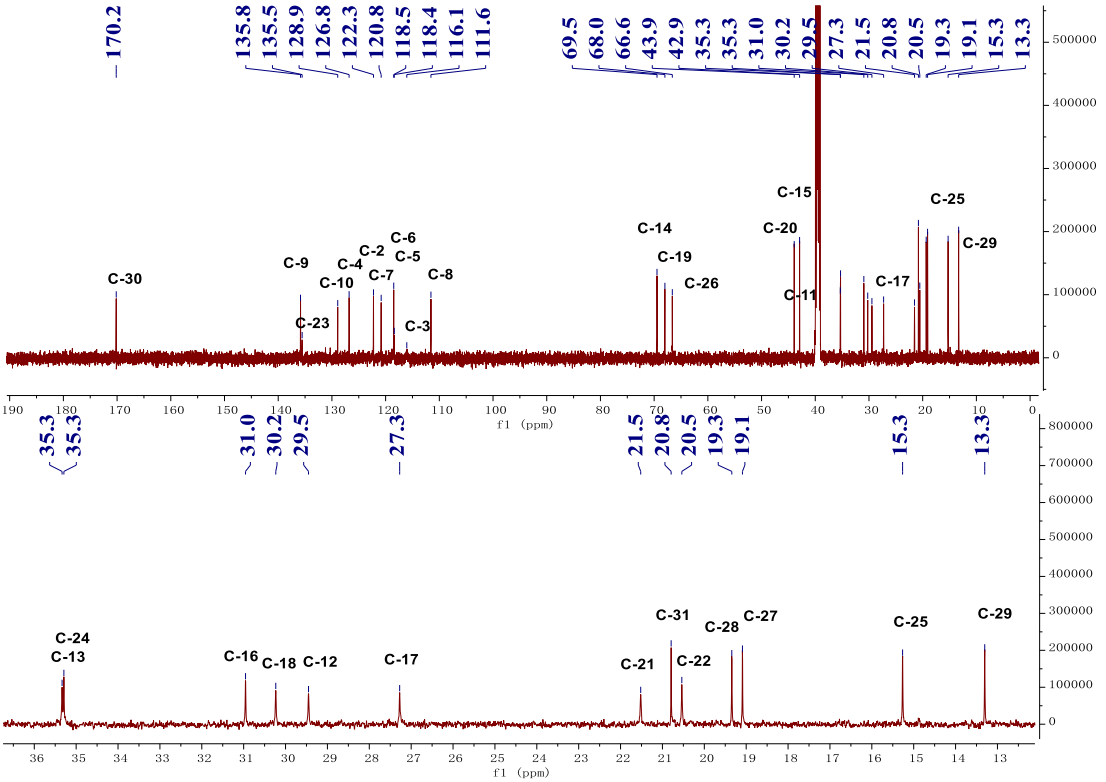


Figure S3. ^{13}C-NMR spectrum of compound **1** in DMSO-d_6 (150 MHz).



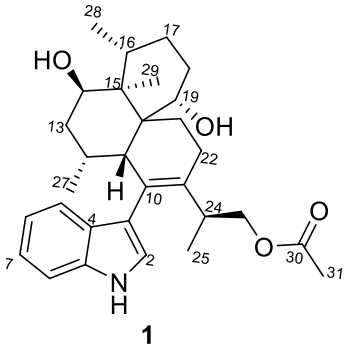
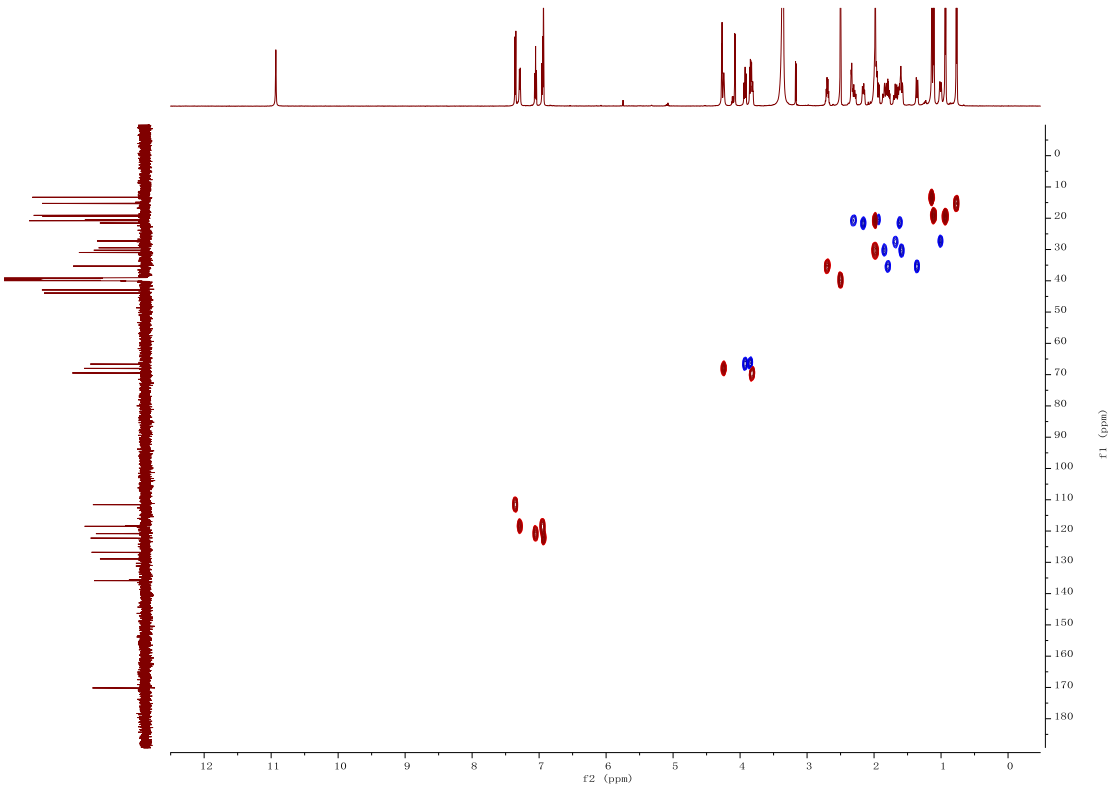


Figure S4. HSQC spectrum of compound **1** in DMSO-d_6 (600*150 MHz).



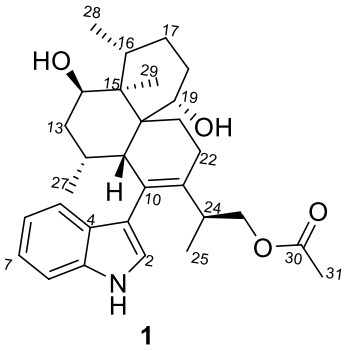


Figure S5. HMBC spectrum of compound **1** in DMSO-d_6 (600*150 MHz).

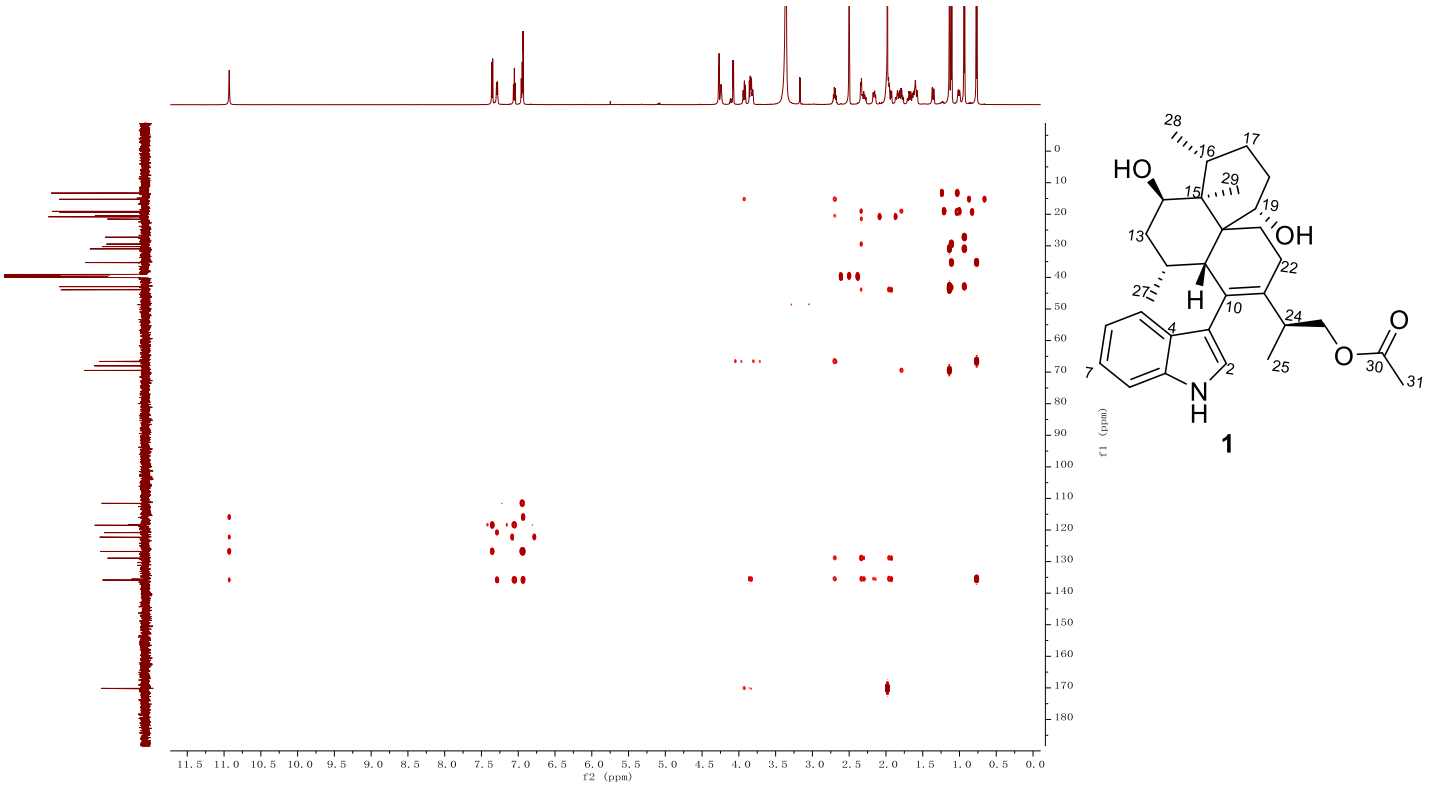


Figure S6. ^{1}H-^{1}H COSY spectrum of compound **1** in DMSO-d_6 (600 MHz).

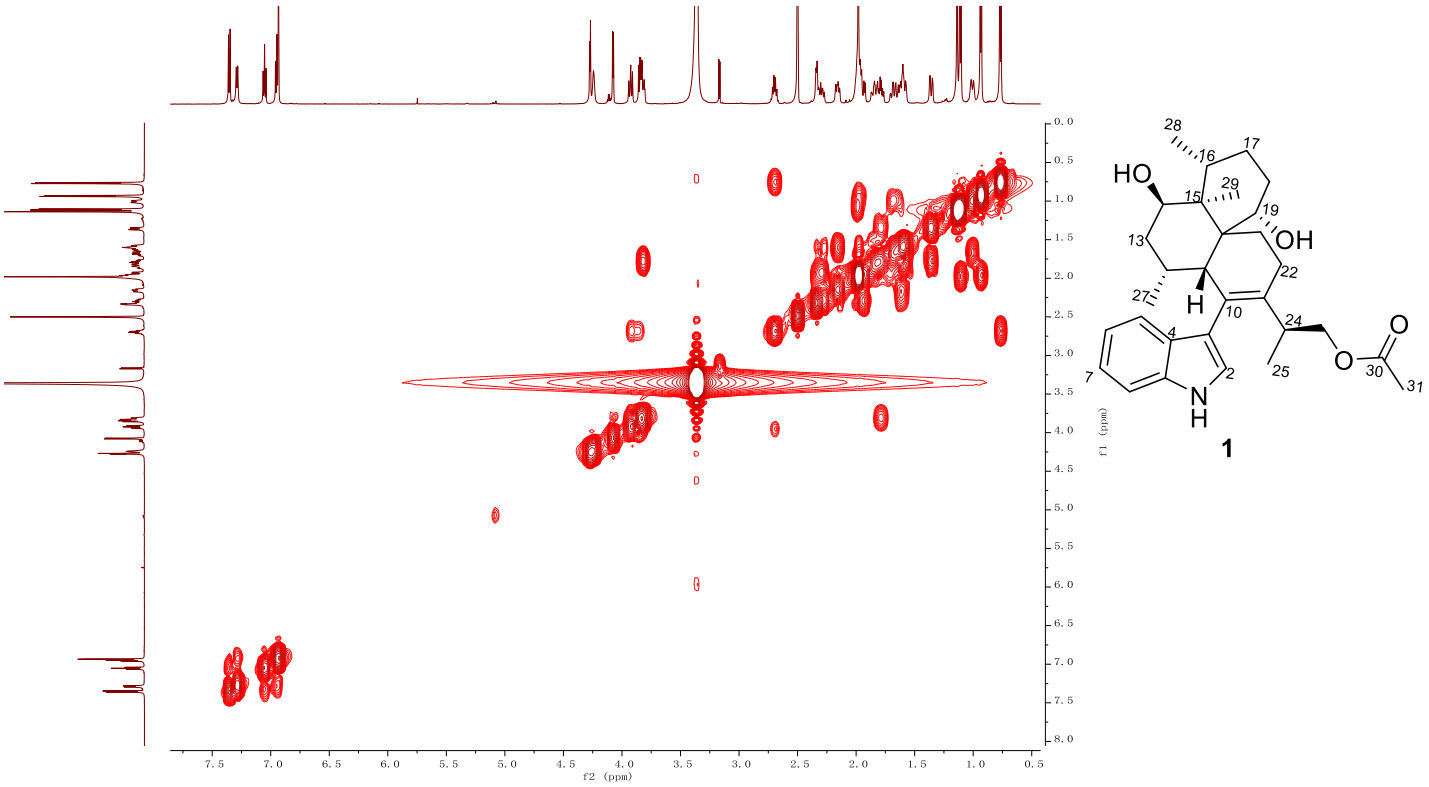


Figure S7. NOESY spectrum of compound **1** in DMSO-d_6 (600 MHz).

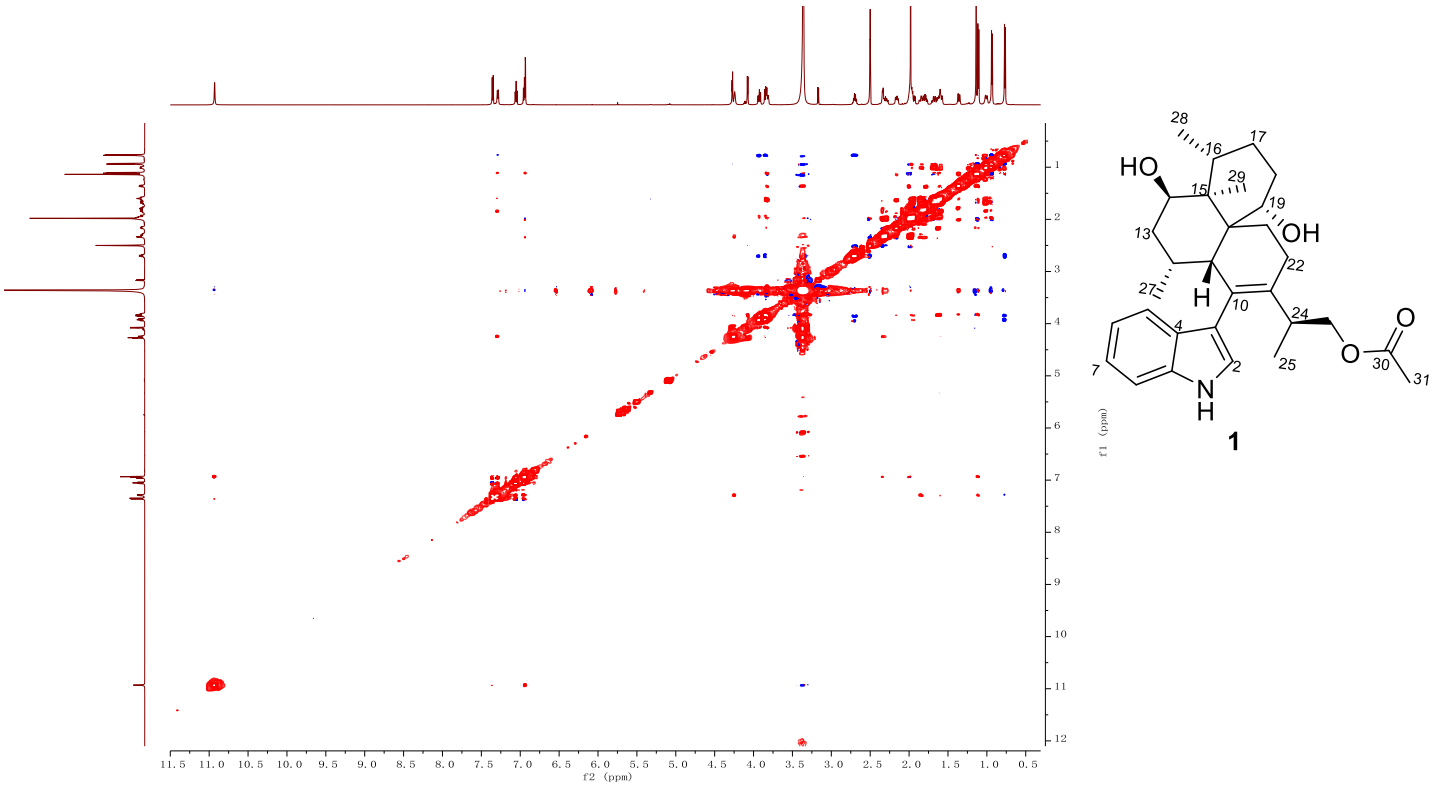


Figure S8. ^{1}H-NMR spectrum of compound **2** in DMSO-d_6 (600 MHz).

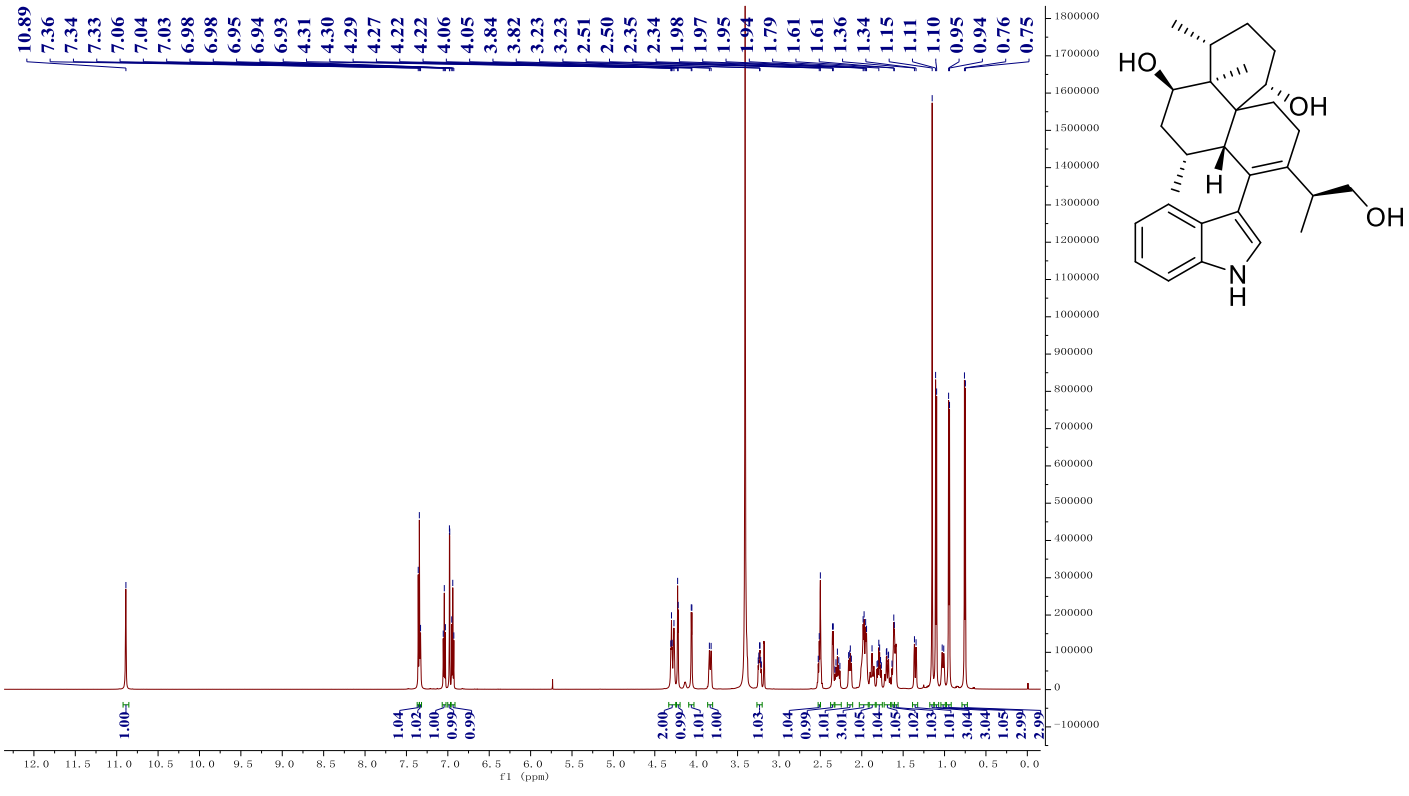


Figure S9. ^{13}C-NMR spectrum of compound **2** in DMSO-d_6 (150 MHz).

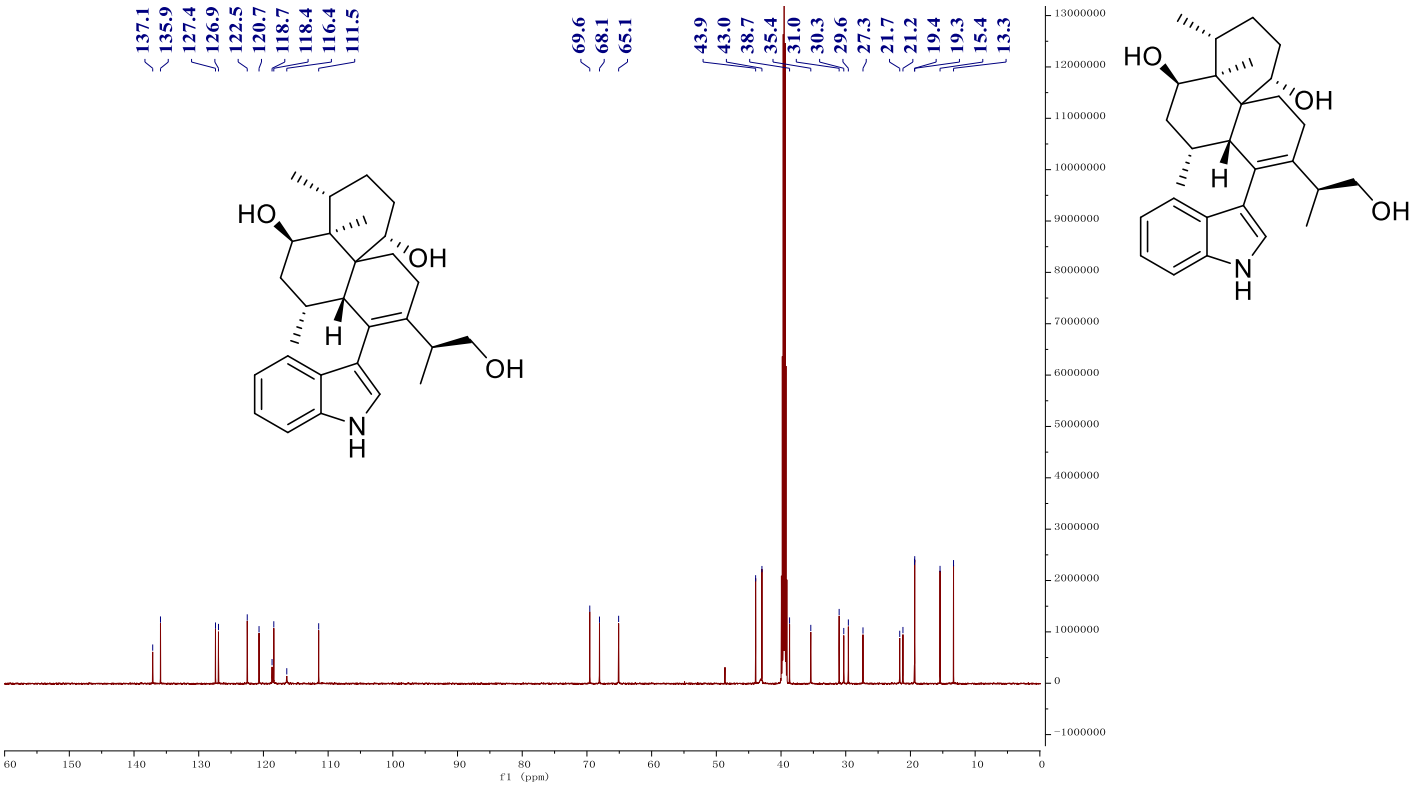


Figure S10. ^{1}H-NMR spectrum of compound **3** in Chloroform-d_3 (600 MHz).

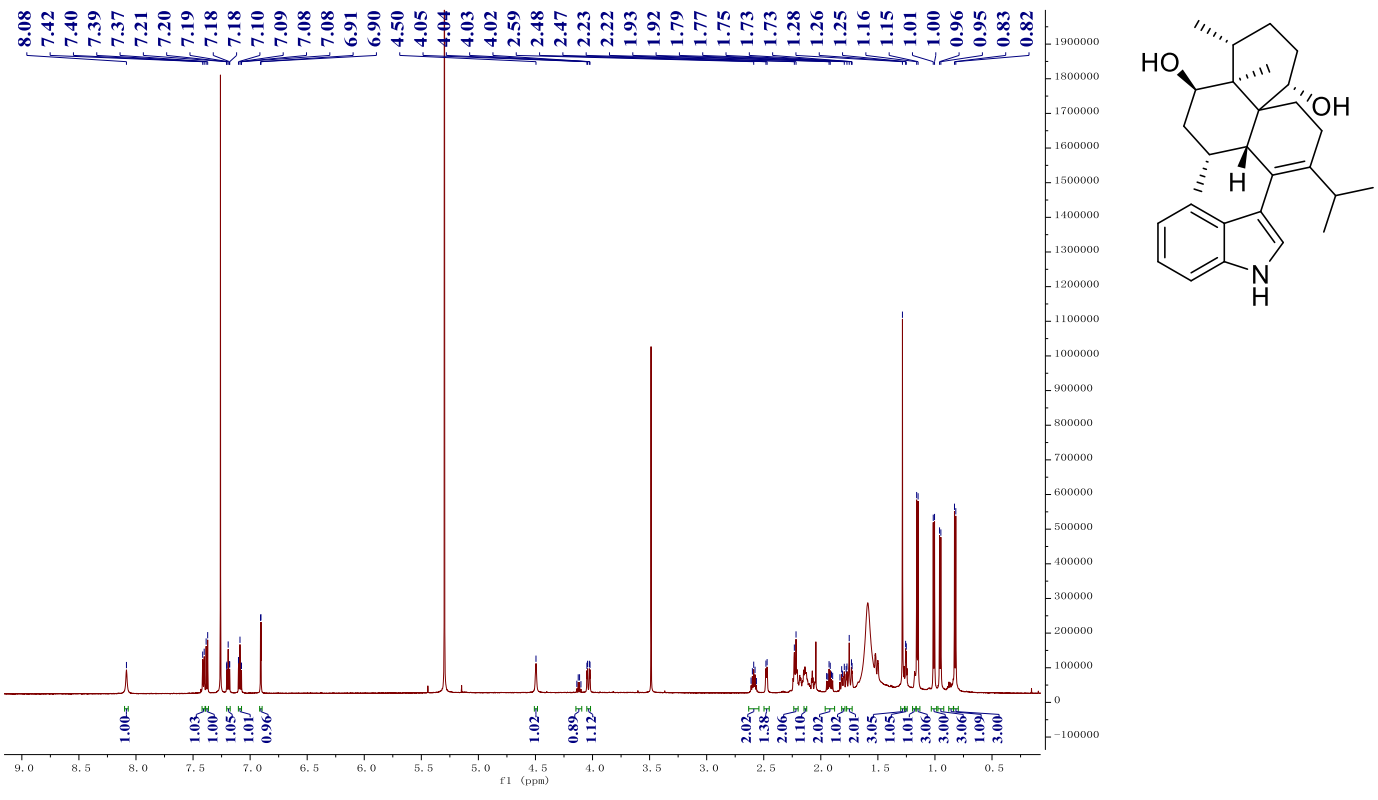


Figure S11. ^{13}C-NMR spectrum of compound **3** in DMSO-d_6 (150 MHz).

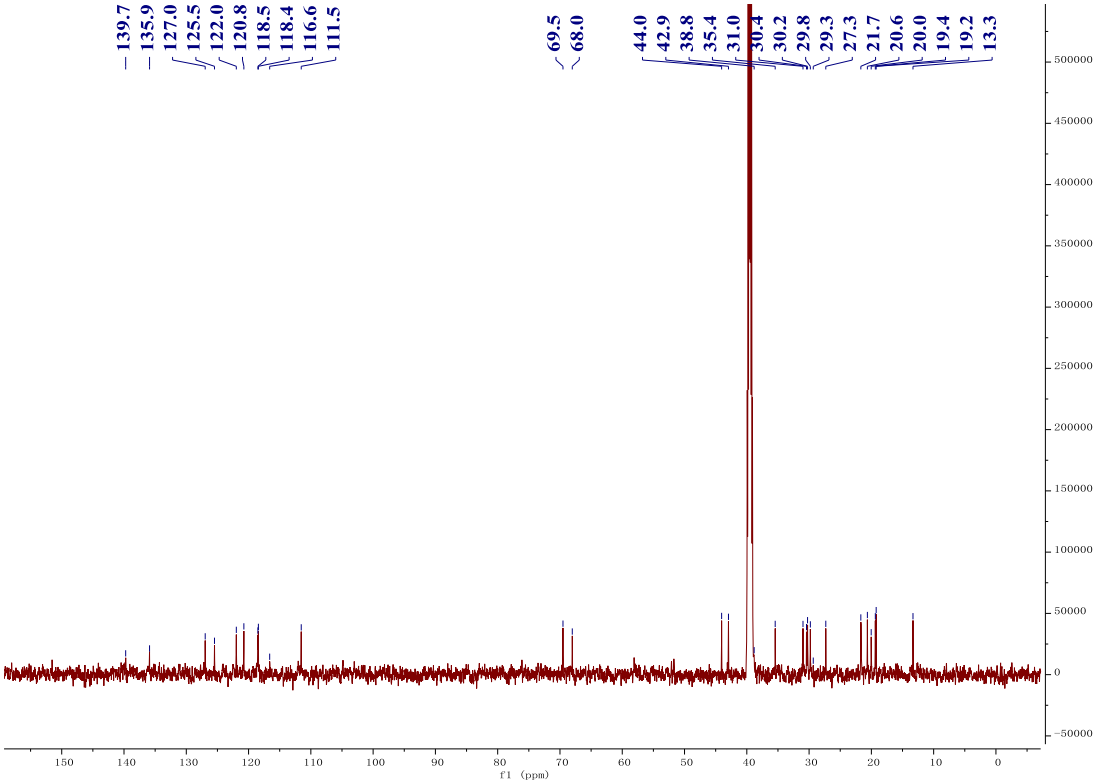
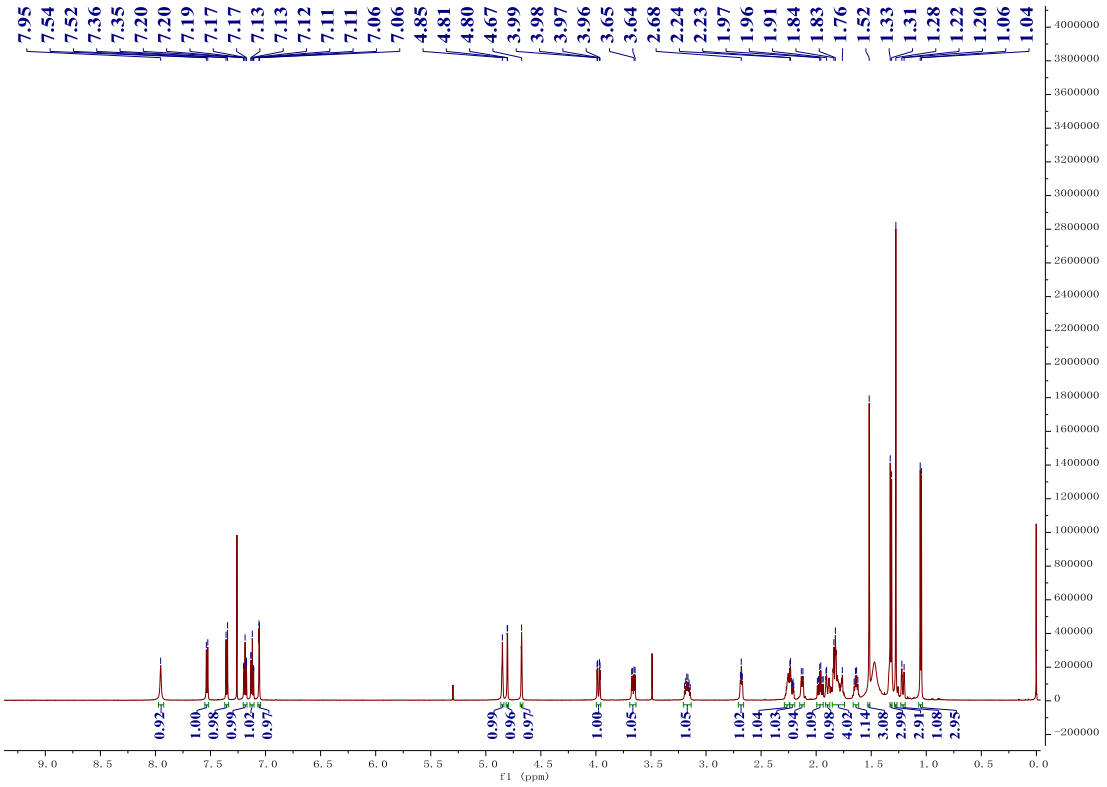


Figure S12. ^{1}H-NMR spectrum of compound **4** in Chloroform-d_3 (600 MHz).



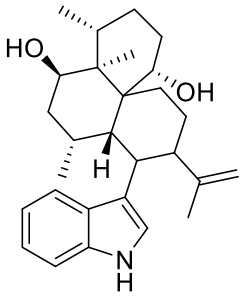


Figure S13. ^{13}C-NMR spectrum of compound **4** in DMSO-d_6 (150 MHz).

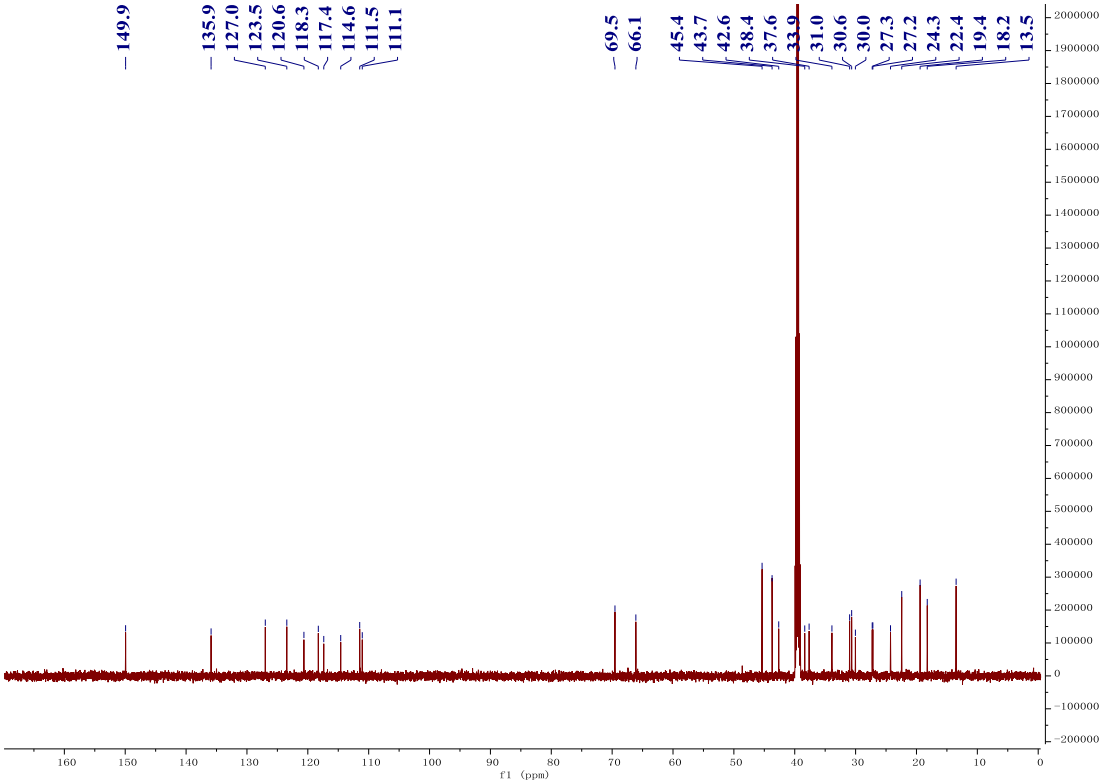


Figure S14. ^{1}H-NMR spectrum of compound **5** in Chloroform-d_3 (600 MHz).

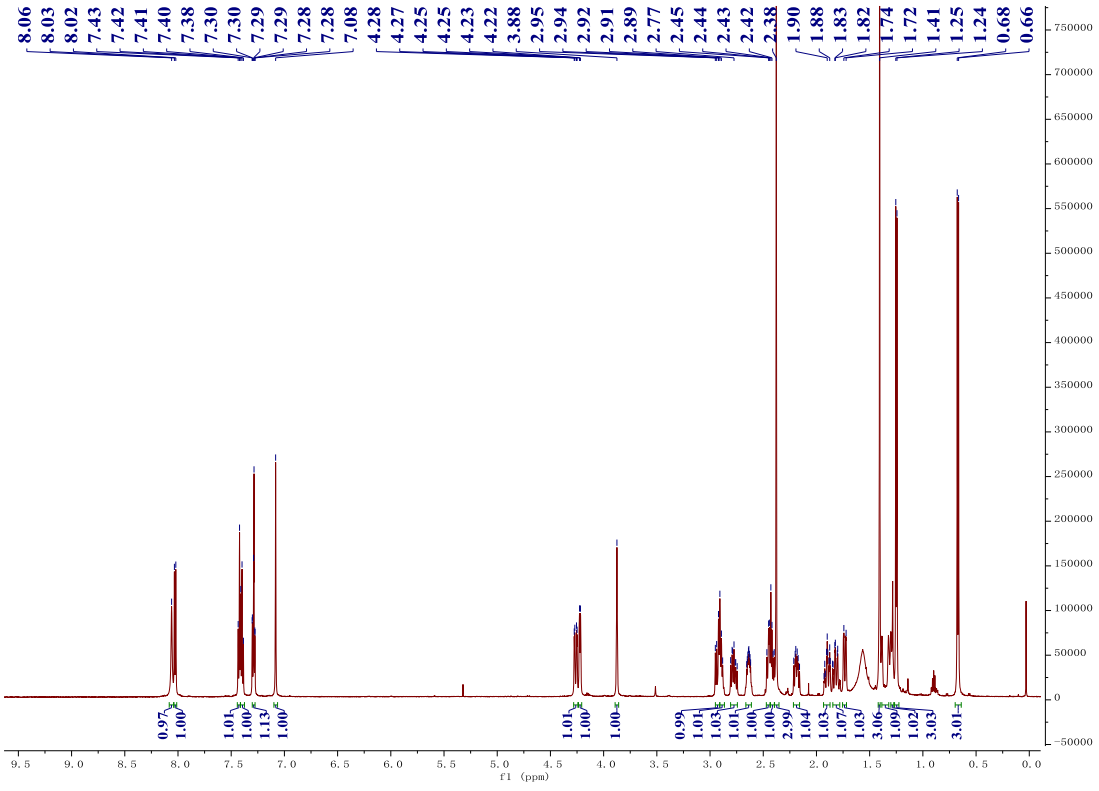


Figure S15. ^{13}C-NMR spectrum of compound **5** in Chloroform-d_3 (150 MHz).

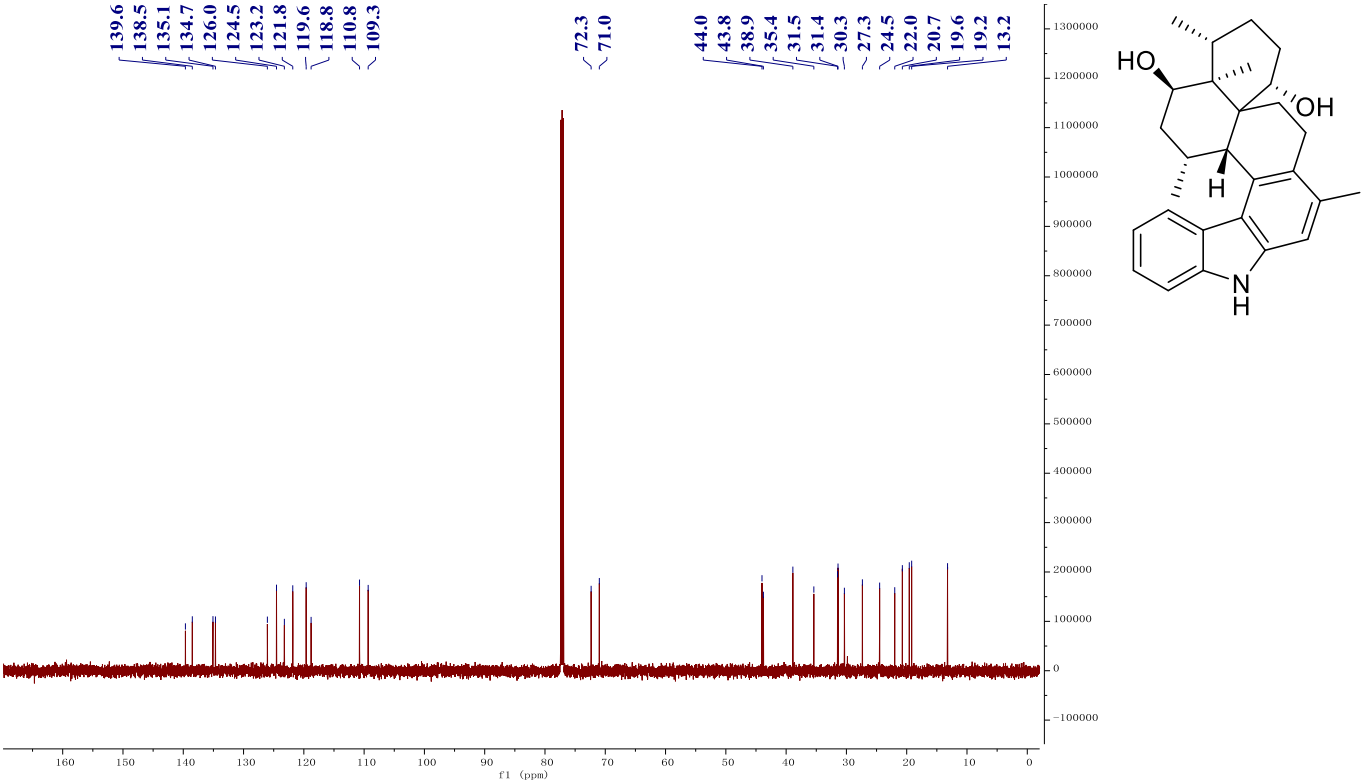


Figure S16. ^{1}H-NMR spectrum of compound **6** in Chloroform-d_3 (600 MHz).

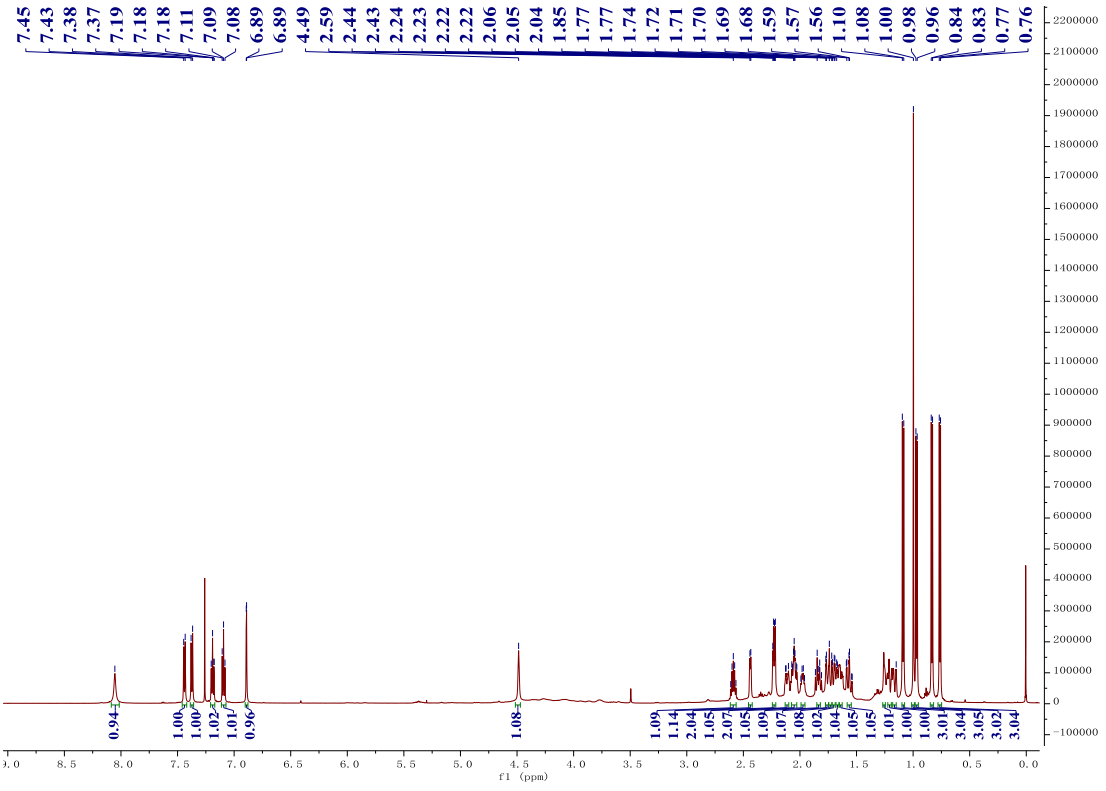


Figure S17. ^{13}C-NMR spectrum of compound **6** in Chloroform-d_3 (150 MHz).

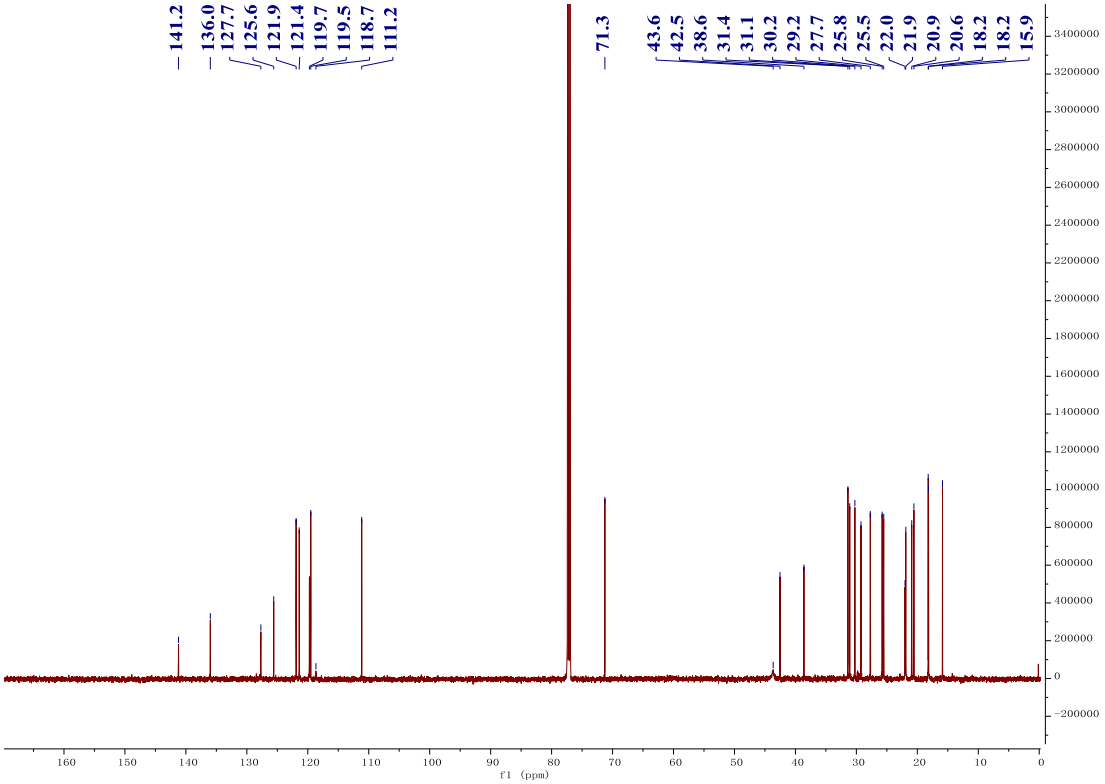


Figure S18. ^{1}H-NMR spectrum of hydrolysate of compound **1** in DMSO-d_6 (600 MHz).