Supporting Information

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Peniciloxatone A, a New Polyoxygenated Ergostane Steroid Isolated from the Marine Alga-Sourced Fungus *Penicillium oxalicum* 2021CDF-3

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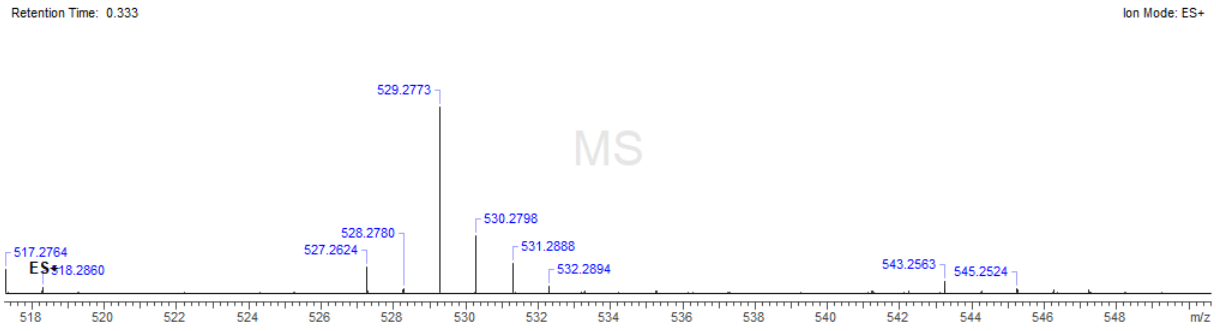


Figure S1: HRESIMS spectrum of **1**

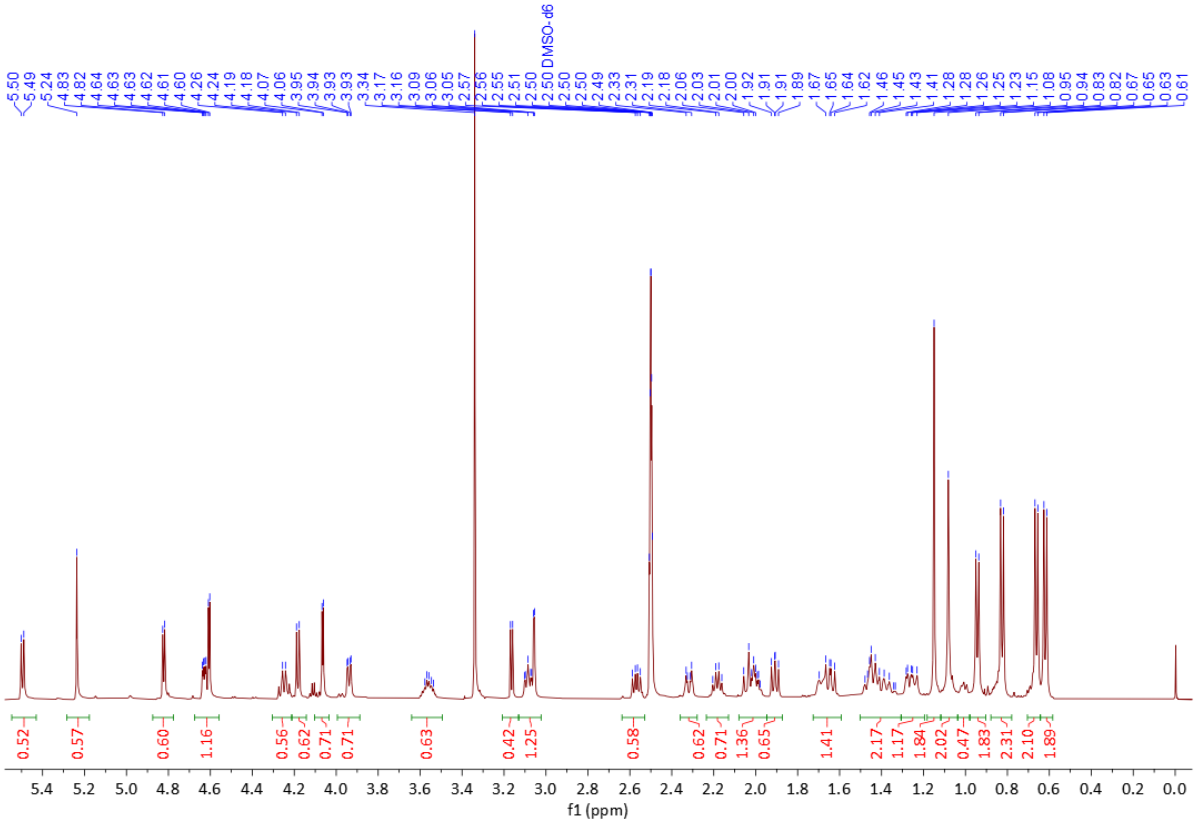


Figure S2: ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **1**

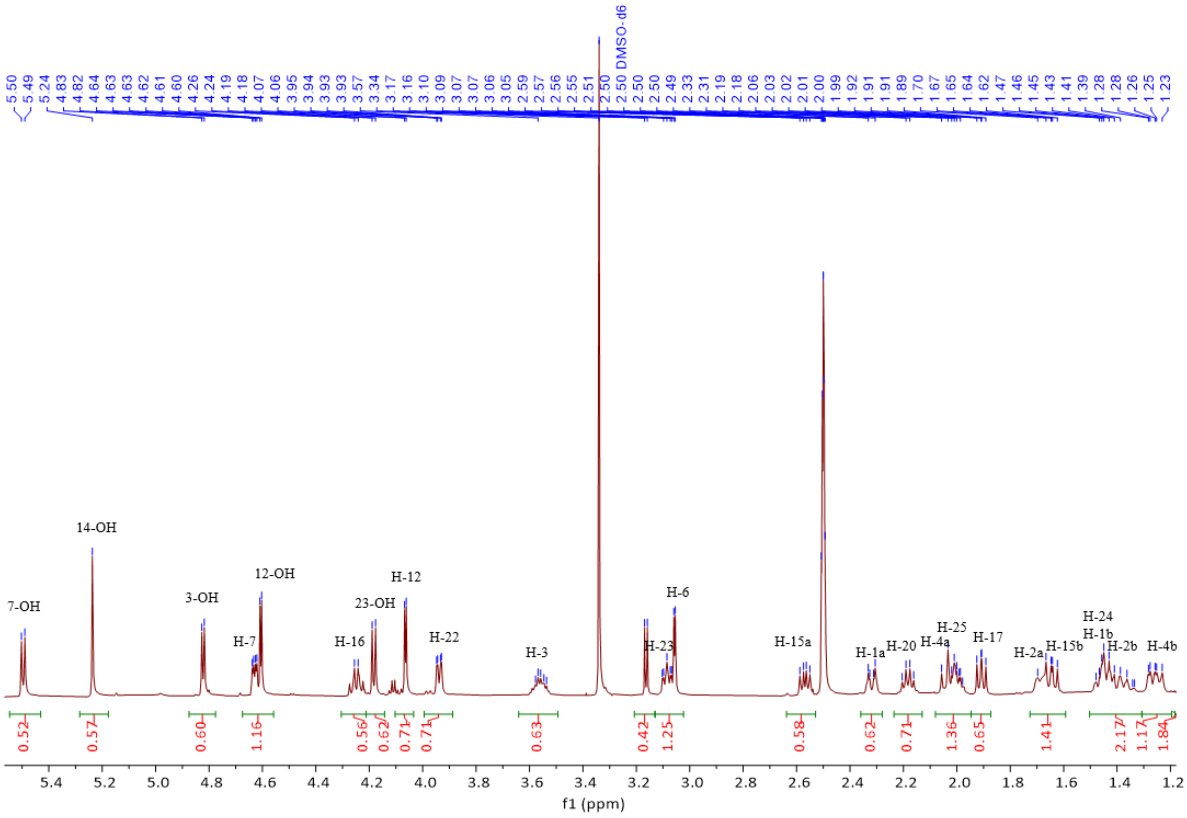


Figure S3: Enlarged ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **1**

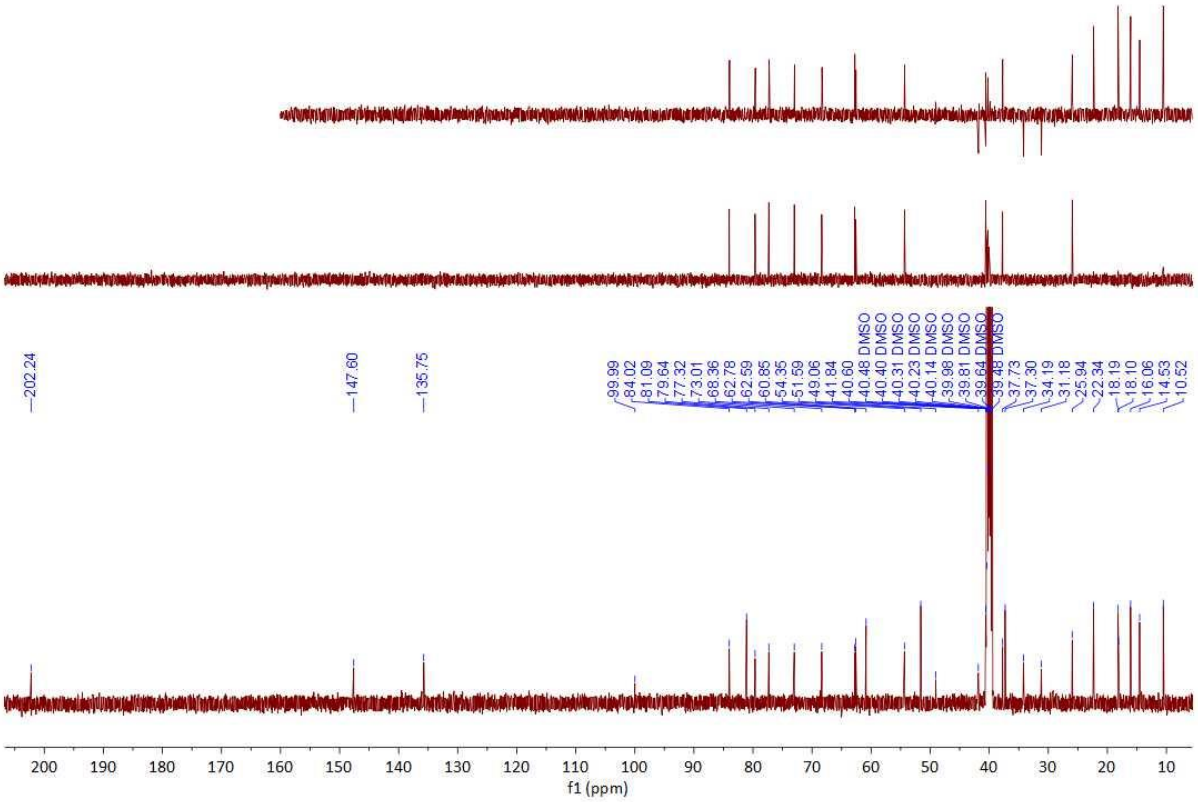


Figure S4: ^{13}C NMR and DEPT (125 MHz, DMSO-d_6) spectra of **1**

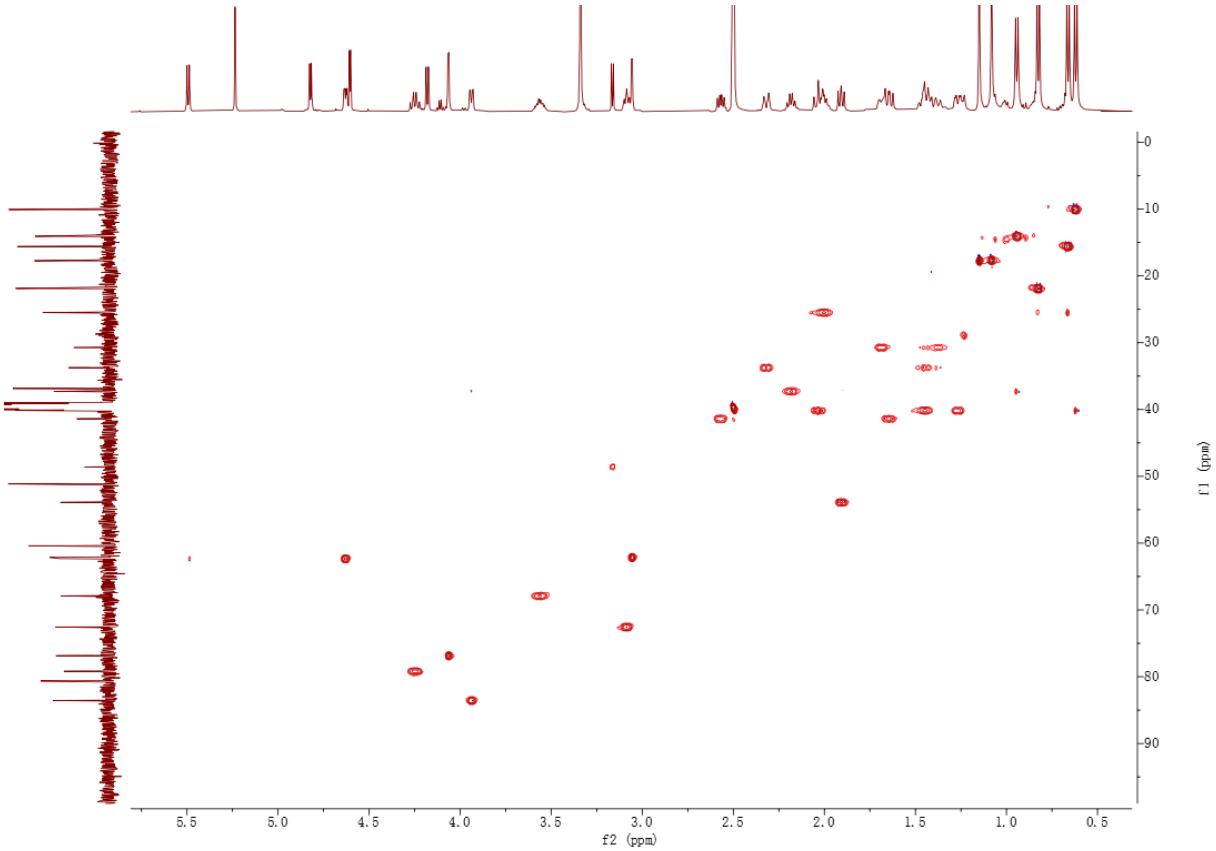


Figure S5: HSQC spectrum of **1**

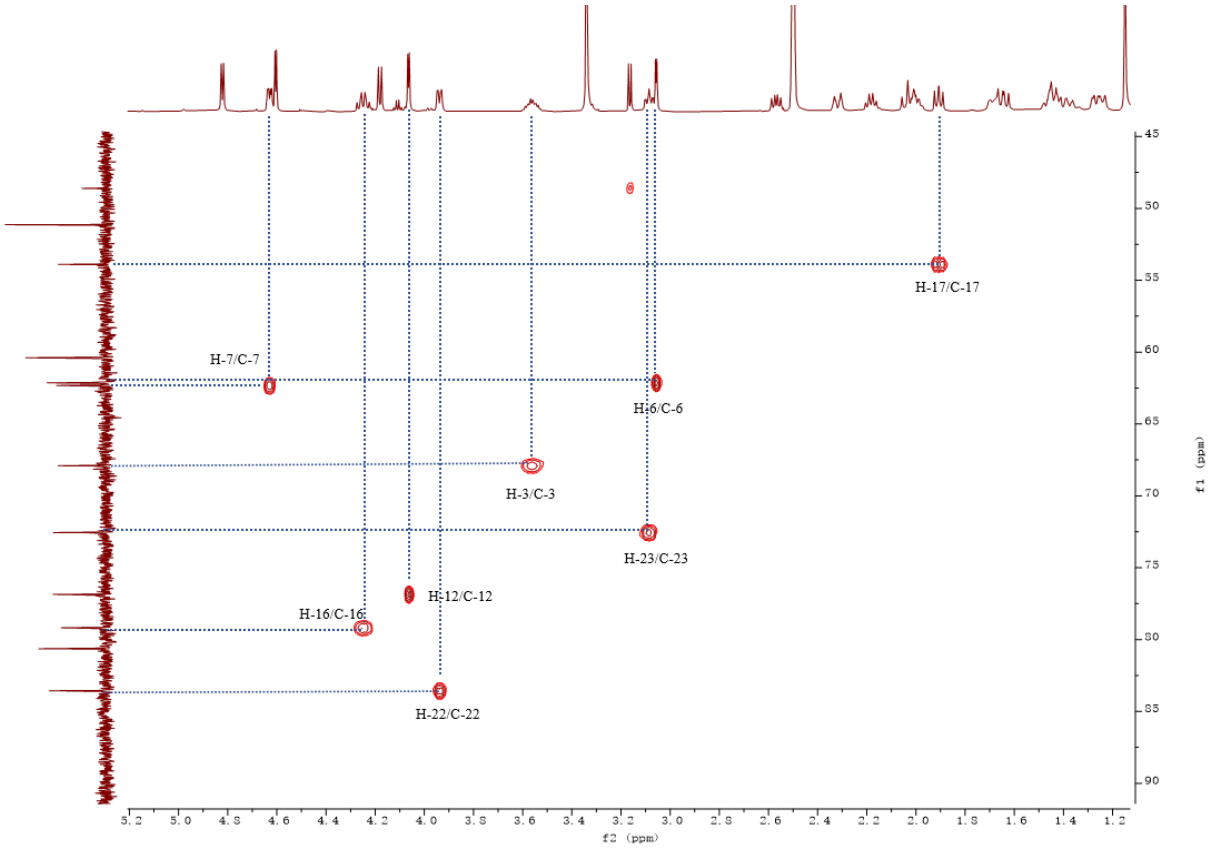


Figure S6: Enlarged HSQC spectrum of **1**

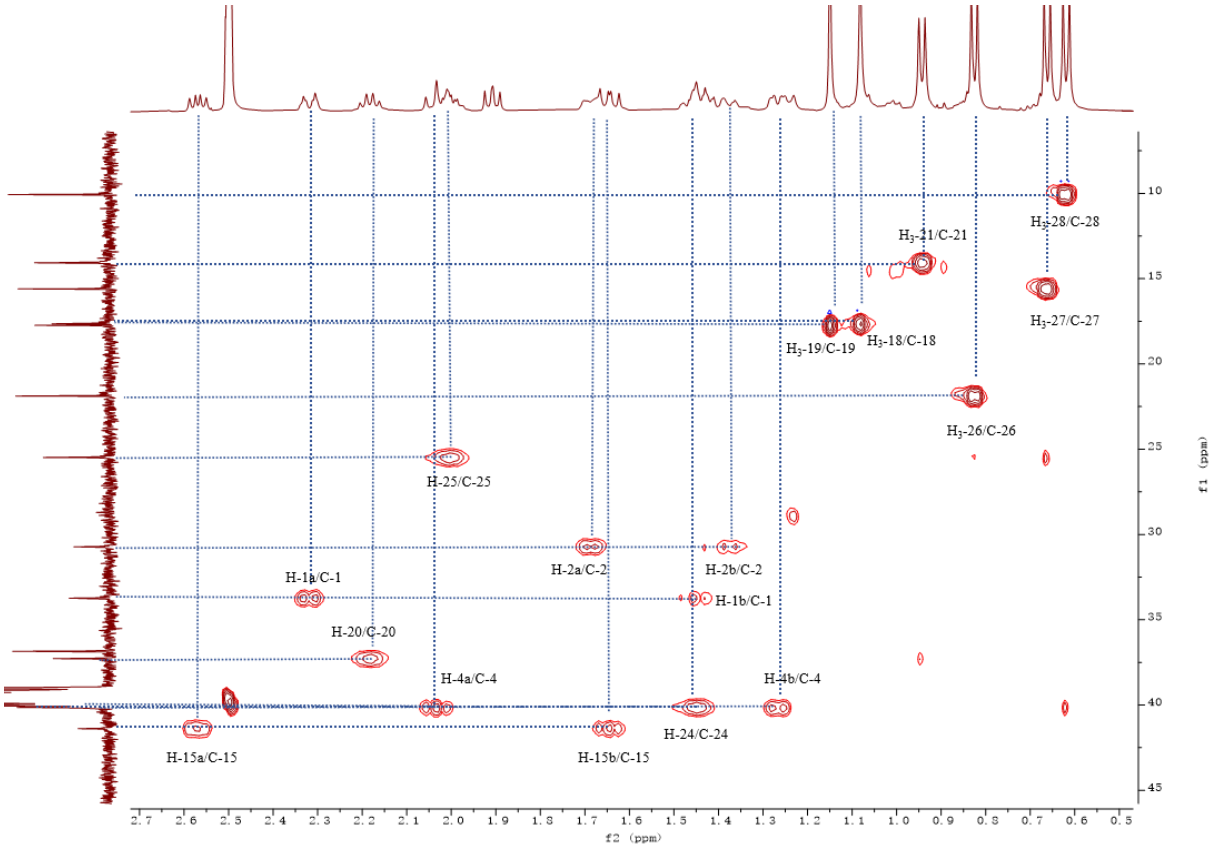


Figure S7: Enlarged HSQC spectrum of **1**

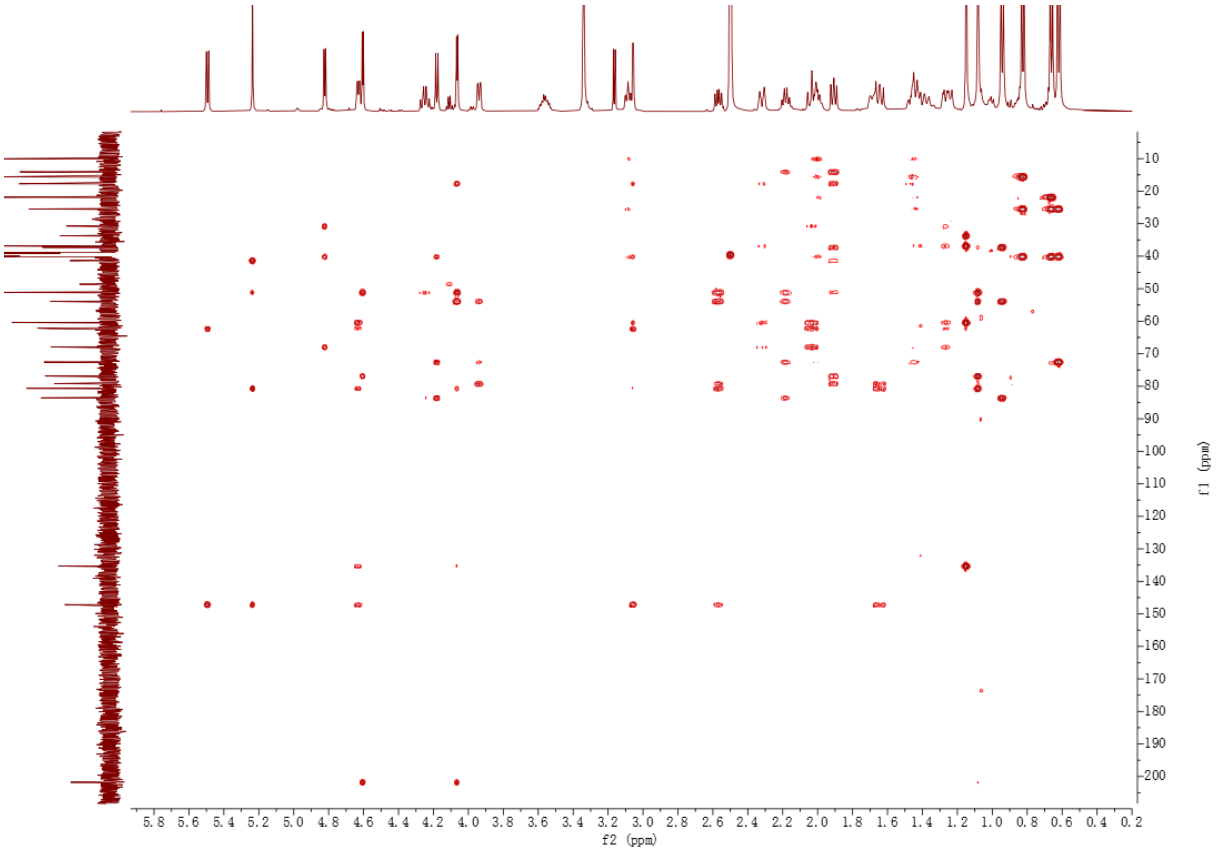


Figure S8: HMBC spectrum of **1**

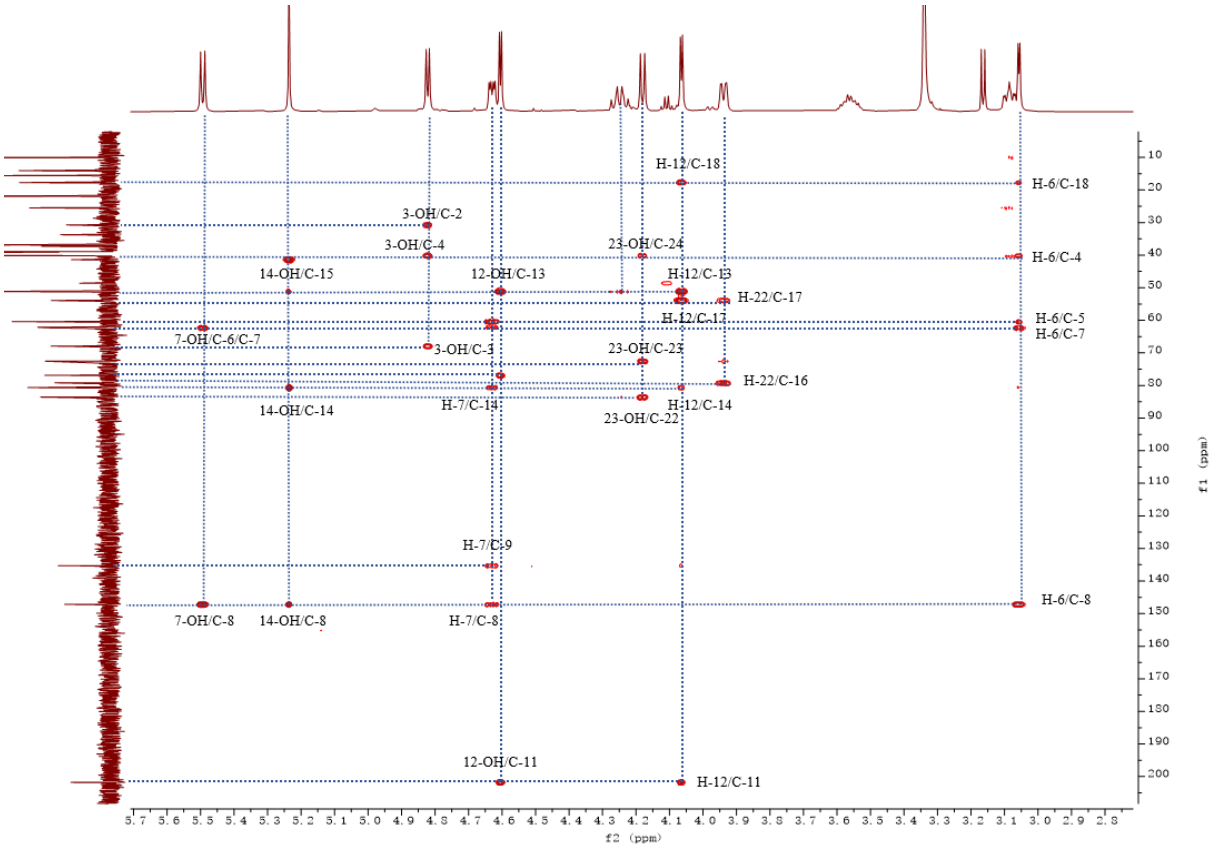


Figure S9: Enlarged HMBC spectrum of **1**

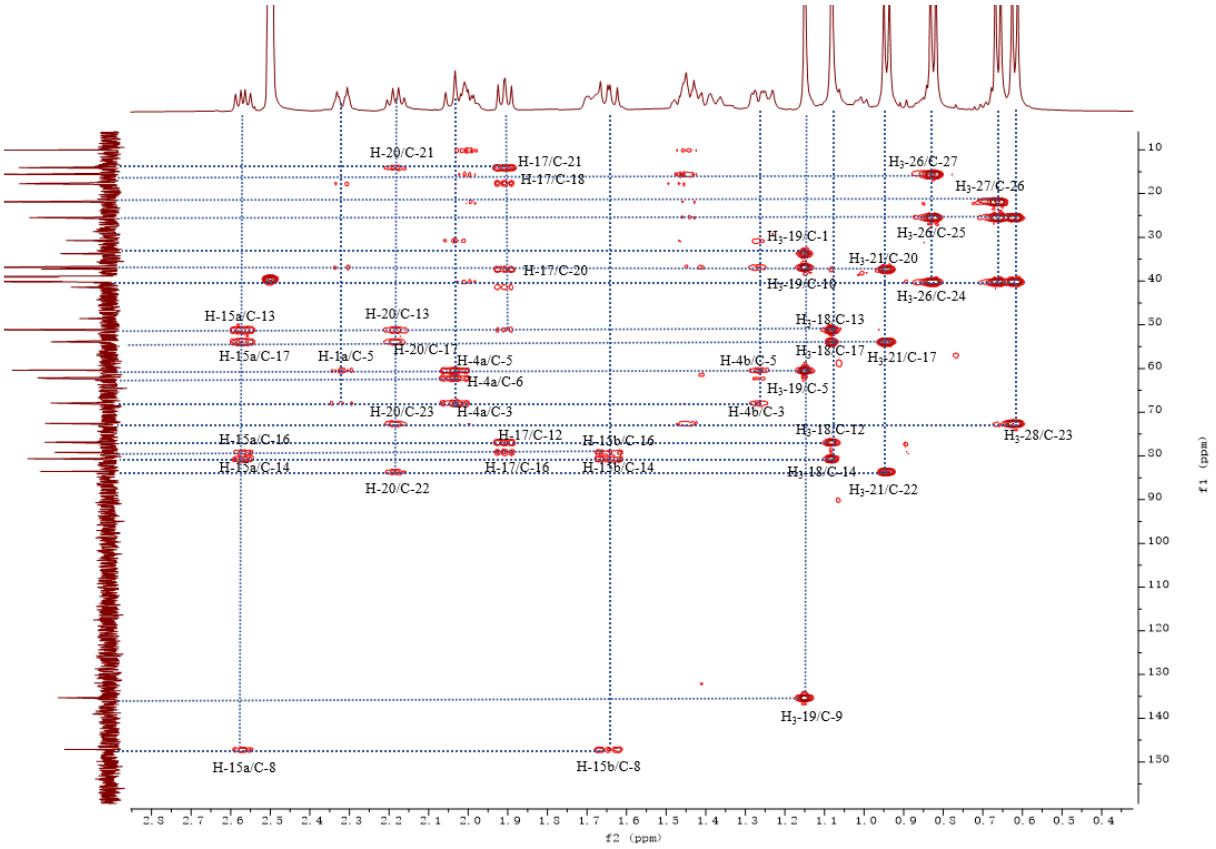


Figure S10: Enlarged HMBC spectrum of **1**

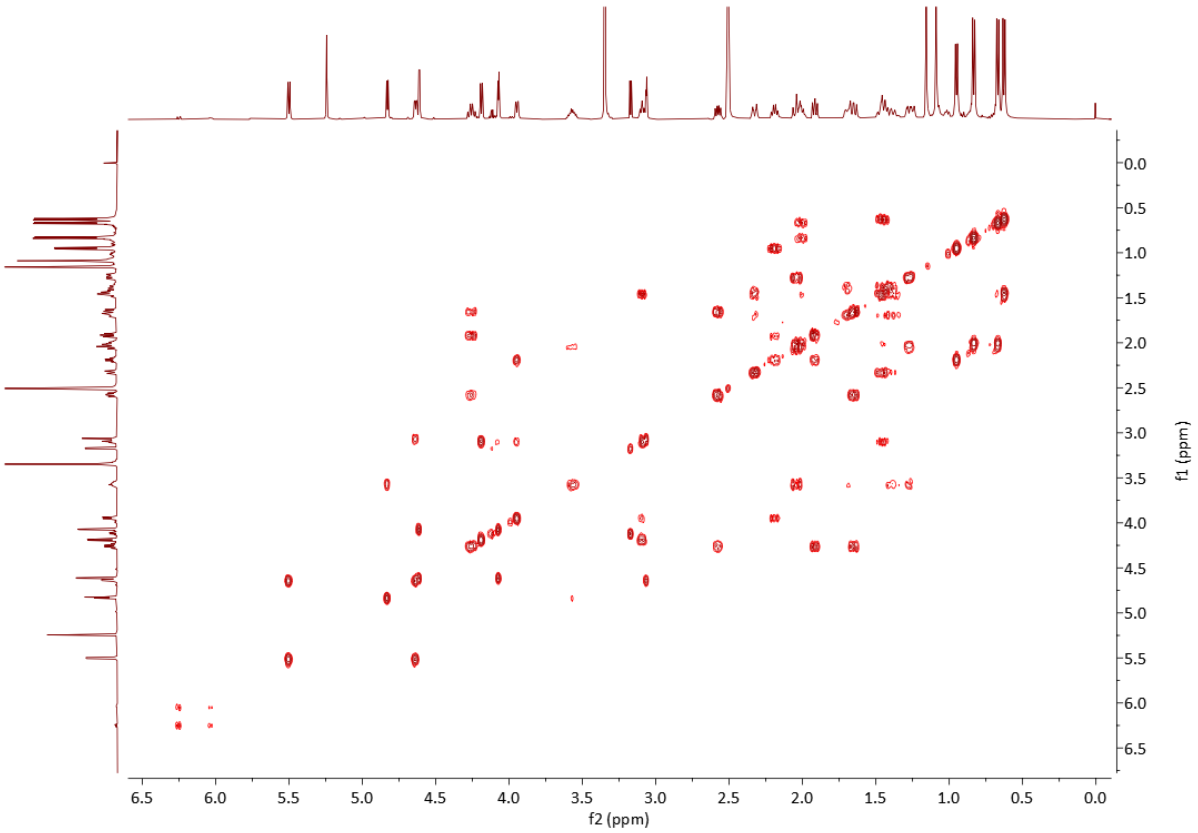


Figure S11: ^{1}H-^{1}H COSY spectrum of **1**

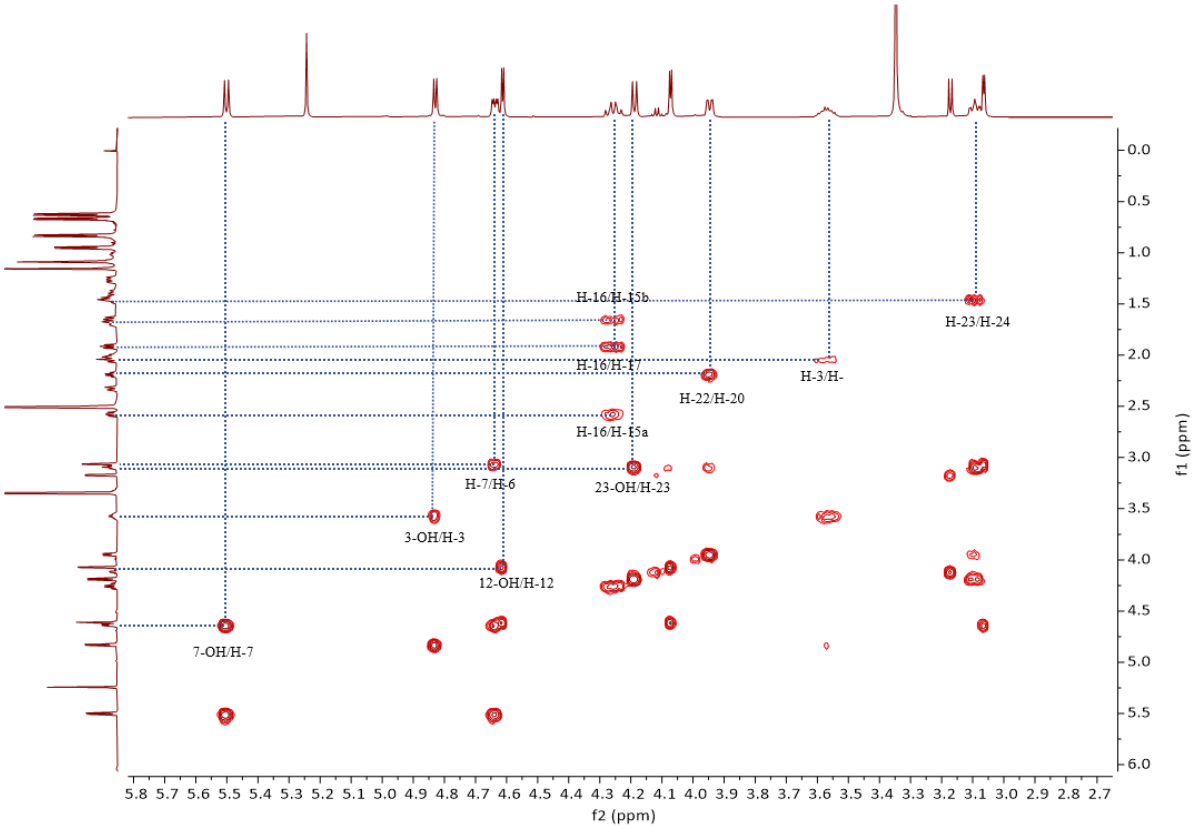


Figure S12: Enlarged ^{1}H-^{1}H COSY spectrum of **1**

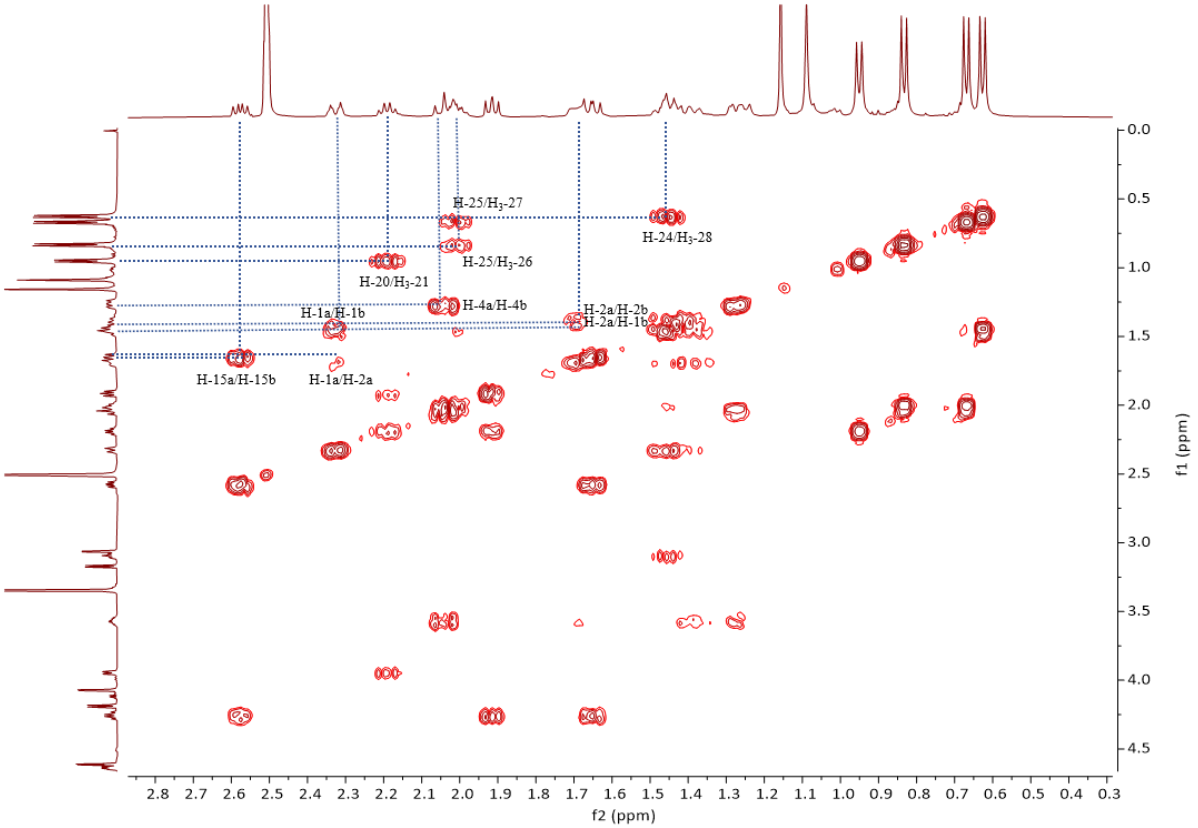


Figure S13: Enlarged ^{1}H-^{1}H COSY spectrum of **1**

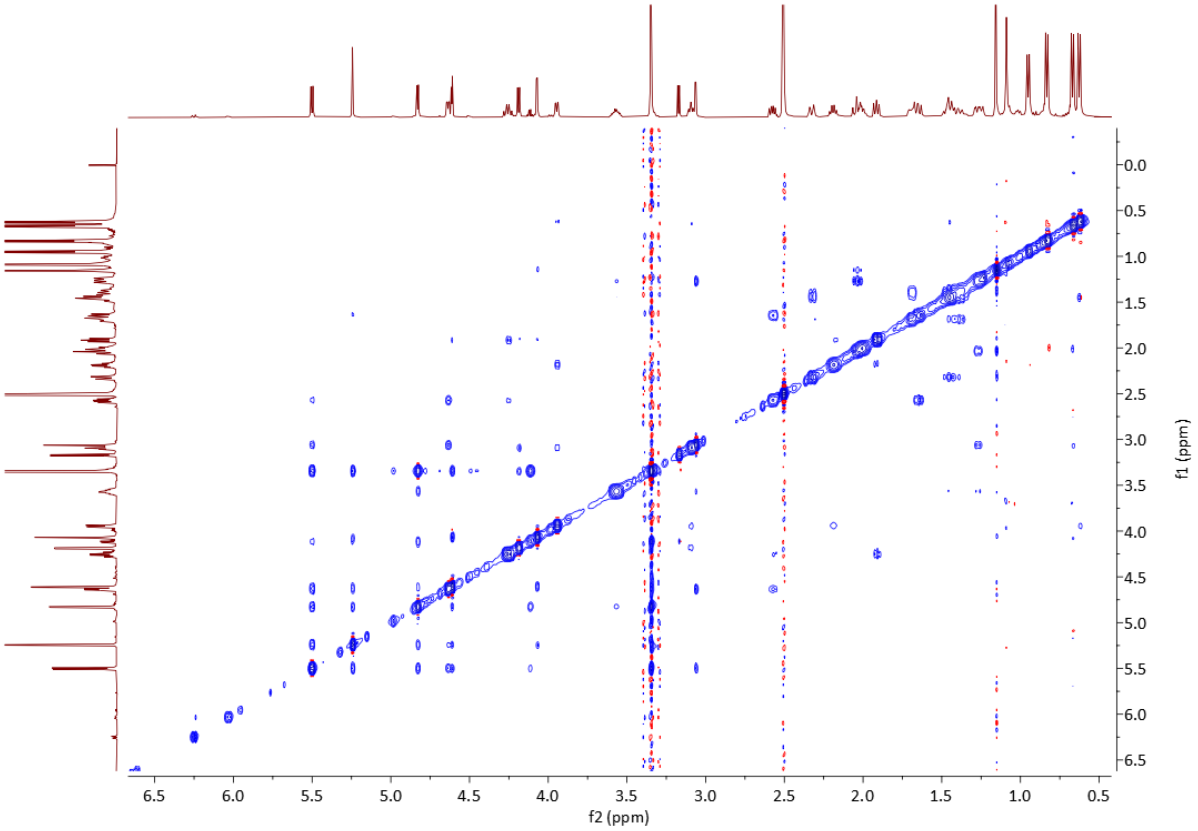


Figure S14: NOESY spectrum of **1**

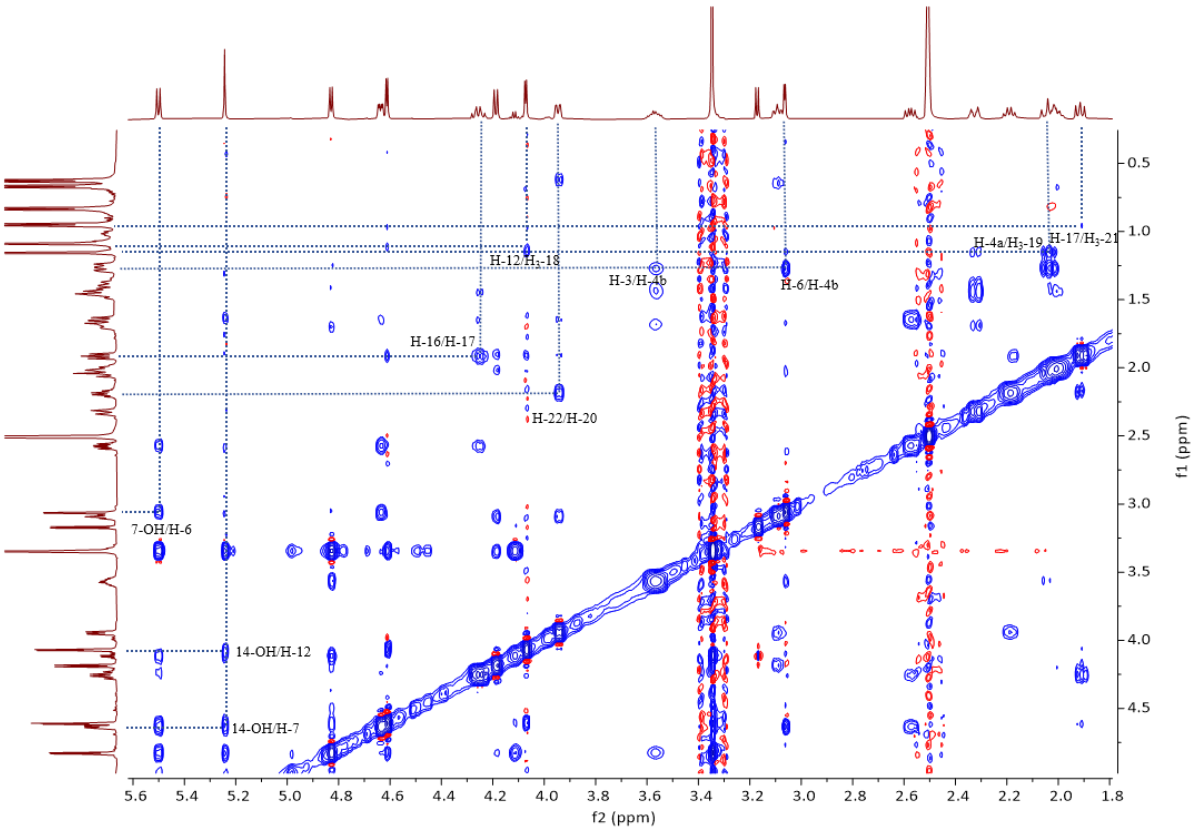


Figure S15: Enlarged NOESY spectrum of **1**

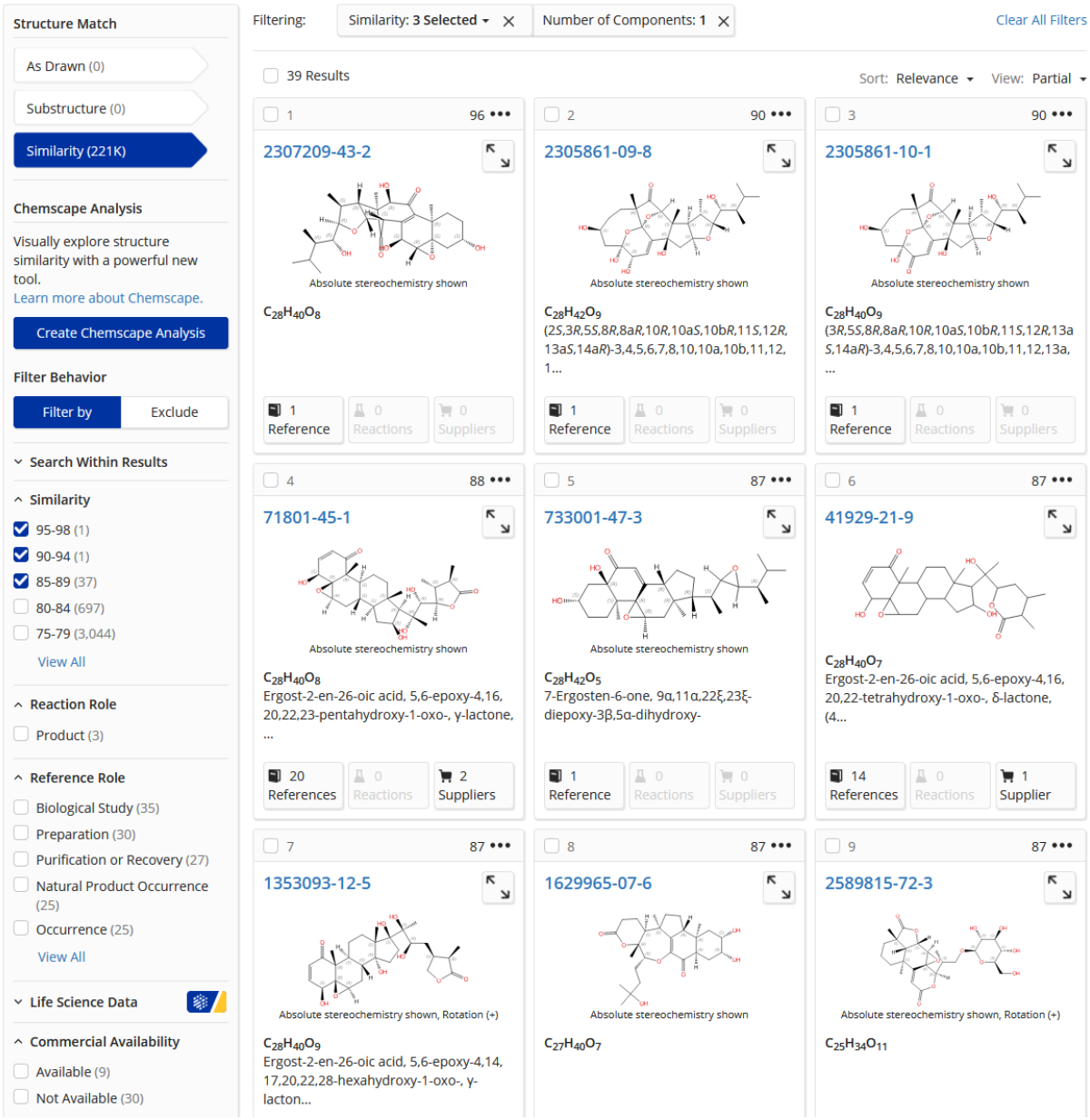
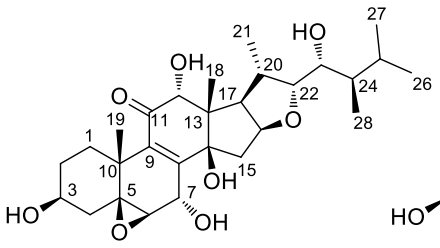
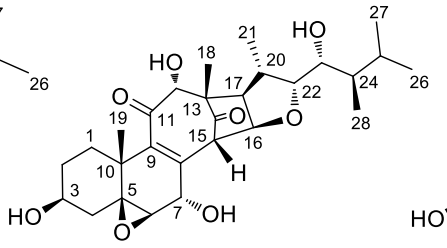


Figure S16: Scifinder search results of **1**

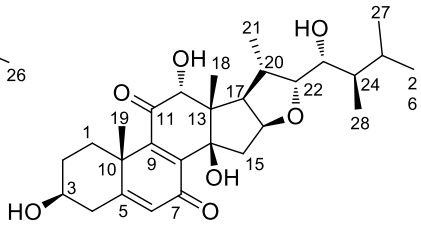
Table S1: The comparison of NMR data of compound **1**, asperflotone, and asperfloroid



1



asperflotone



asperfloroid

No	Compound 1		Asperflotone		asperfloroid	
	δ_H (*J* in Hz)	δ_C, type	δ_H (*J* in Hz)	δ_C, type	δ_H (*J* in Hz)	δ_C, type
1	2.33 dt (12.7, 3.2) 1.44 m	33.7 CH_2	2.36 br d (13.8) 1.41 br t (13.8)	35.1 CH_2	2.43 dt (13.9, 3.4) 1.06 td (13.9, 4.0)	31.9 CH_2
2	1.68 m 1.37 m	30.7 CH_2	1.69 m 1.34 m	30.5 CH_2	1.76 m 1.60 tdd (13.9, 11.0, 3.4)	29.8 CH_2
3	3.56 m	67.9 CH	3.50 m	67.7 CH	3.46 tt (11.0, 4.7)	70.3 CH
4	2.03 m 1.26 m	40.1 CH_2	1.95 t (12.0) 1.26 br d (12.0)	39.9 CH_2	2.60 m 2.47 ddd (13.1, 11.0, 1.4)	41.5 CH_2
5		60.4 C		61.3 C		168.4 C
6	3.06 d (2.7)	62.1 CH	3.01 br s	61.0 CH	6.24 d (1.4)	125.4 CH
7	4.63 dd (6.4, 2.7)	62.3 CH	4.07 br d (7.6)	67.9 CH		187.8 C
8		147.2 C		133.7 C		144.1 C
9		135.3 C		139.9 C		147.2 C
10		36.9 C		38.1 C		40.6 C
11		201.8 C		207.2 C		200.7 C
12	4.06 d (3.2)	76.9 CH	3.77 d (4.3)	82.0 CH	3.60 d (3.6)	80.2 CH
13		51.1 C		64.6, C		52.2 C
14		80.6 C		209.4 C		81.0 C

15	2.58 dd (12.0, 6.8) 1.65 m	41.4 CH_2	2.81 s	59.4 CH	2.34 dd (14.3, 7.9) 2.07 dd (14.3, 3.2)	47.9 CH_2
16	4.25 td (9.1, 6.8)	79.2 CH	4.23 d (8.1)	84.3 CH	4.60 td (8.2, 3.2)	83.9 CH
17	1.91 dd (9.1, 7.6)	53.9 CH	2.76 t (9.3)	50.2 CH	2.30 t (8.5)	57.7 CH
18	1.08 s	17.6 CH_3	1.15 s	14.9 CH_3	1.00 s	15.2 CH_3
19	1.15 s	17.7 CH_3	0.90 s	16.8 CH_3	1.46 s	22.3 CH_3
20	2.18 q (7.2)	37.3 CH	1.79 m	38.8 CH	2.60 m	38.4 CH
21	0.94 d (7.2)	14.1 CH_3	1.02 d (6.8)	13.6 CH_3	1.04 d (7.0)	14.7 CH_3
22	3.94 dd (7.3, 2.2)	83.6 CH	3.90 br d (7.9)	82.2 CH	4.01 dd (7.7, 1.6)	82.4 CH
23	3.09 ddd (8.8, 6.4, 2.2)	72.6 CH	3.08 br t (8.5)	71.9 CH	3.12 ddd (9.0, 7.2, 1.6)	72.7 CH
24	1.44 m	40.0 CH	1.51 m	39.8 CH	1.54 m	40.2 CH
25	2.00 m	25.5 CH	2.06 m	25.2 CH	2.07 m	25.4 CH
26	0.83 d (6.8)	21.9 CH_3	0.83 d (6.8)	21.6 CH_3	0.85 d (7.0)	21.7 CH_3
27	0.66 d (6.8)	15.6 CH_3	0.66 d (6.8)	15.2 CH_3	0.69 d (6.8)	15.5 CH_3
28	0.62 d (7.0)	10.1 CH_3	0.59 d (6.9)	9.7 CH_3	0.65 d (6.9)	10.0 CH_3
3-OH	4.82 d (4.7)		4.85 br s		5.09 br s	
7-OH	5.49 d (6.4)		5.90 d (7.6)		-	
12-OH	4.60 d (3.2)		5.54 d (4.3)		4.71 s	
14-OH	5.24 s		-		5.99 s	
23-OH	4.18 d (6.4)		4.43 d (7.1)		4.04 d (7.2)	