

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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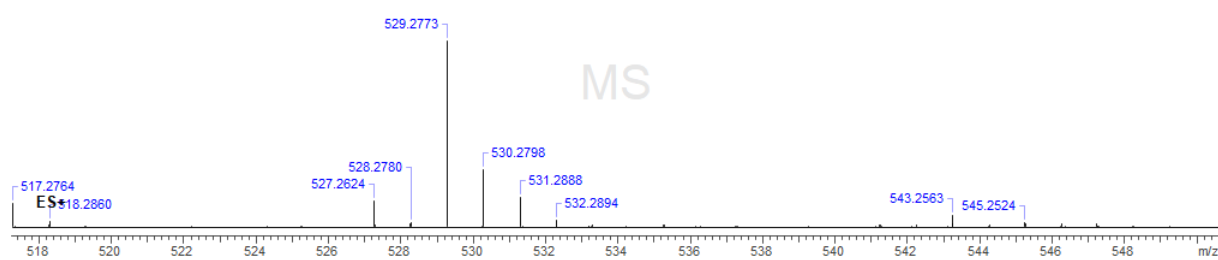


Figure S1: HRESIMS spectrum of 1

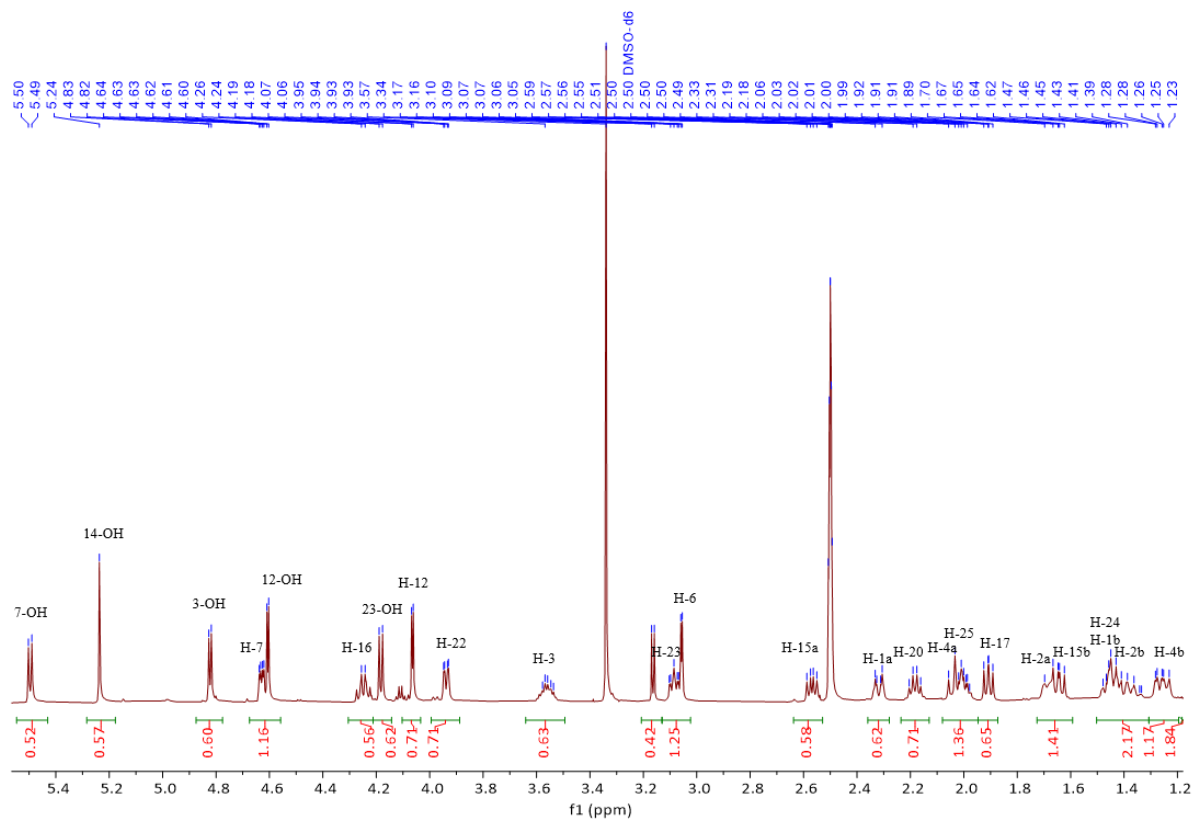


Figure S3: Enlarged ^1H NMR (500 MHz, $\text{DMSO-}d_6$) spectrum of **1**

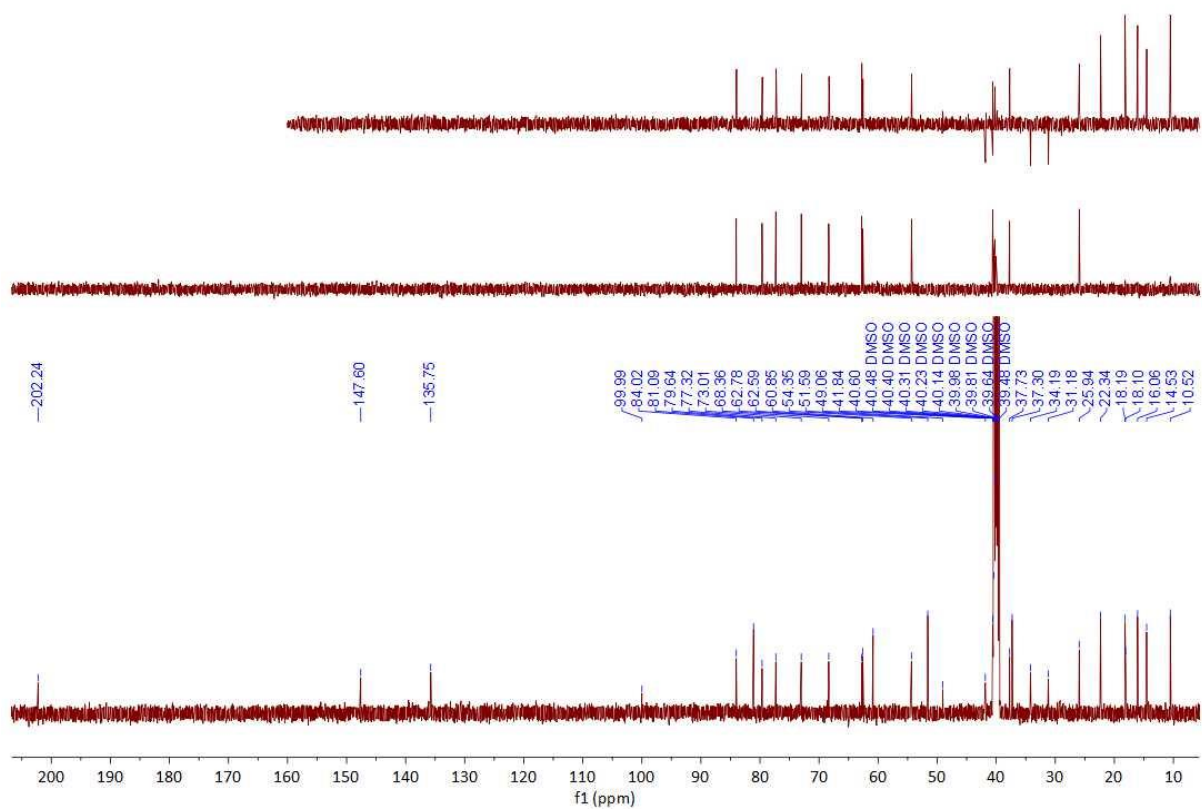


Figure S4: ^{13}C NMR and DEPT (125 MHz, $\text{DMSO-}d_6$) spectra of **1**

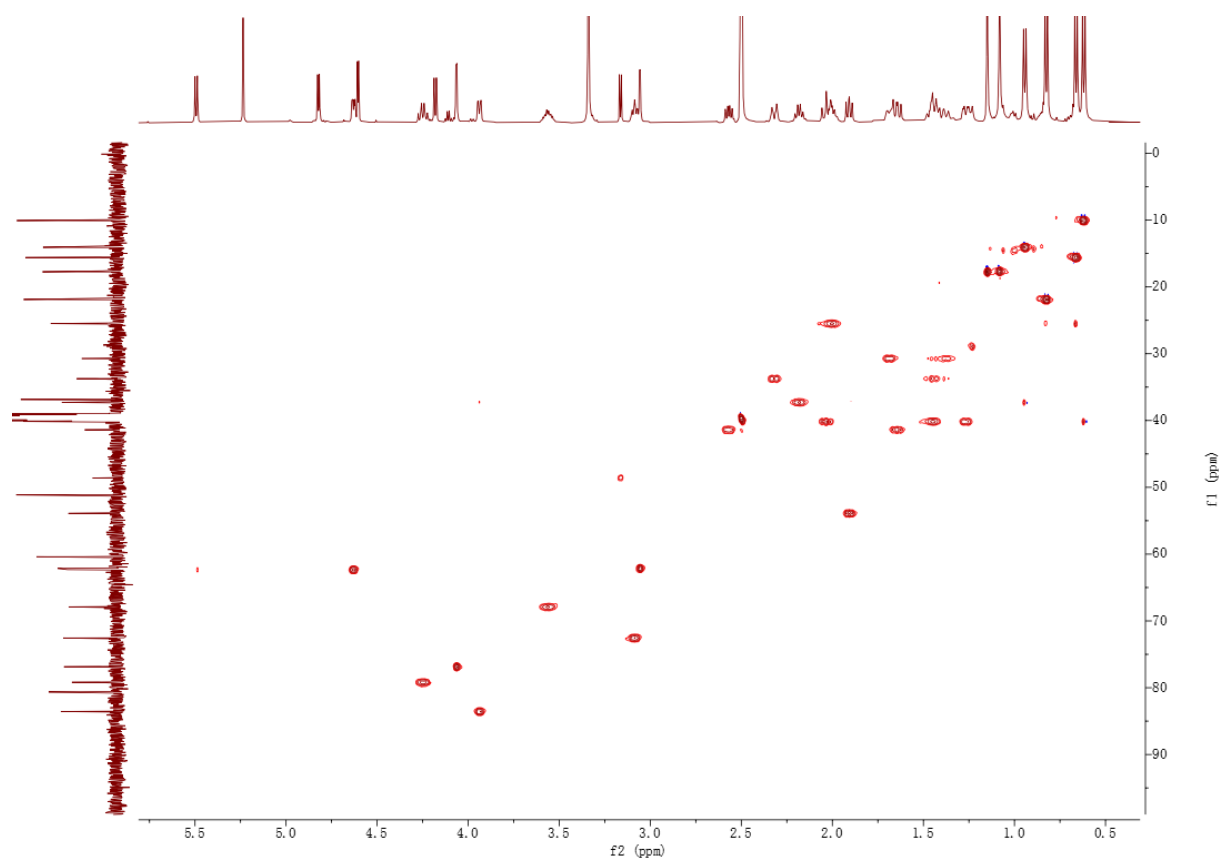


Figure S5: HSQC spectrum of **1**

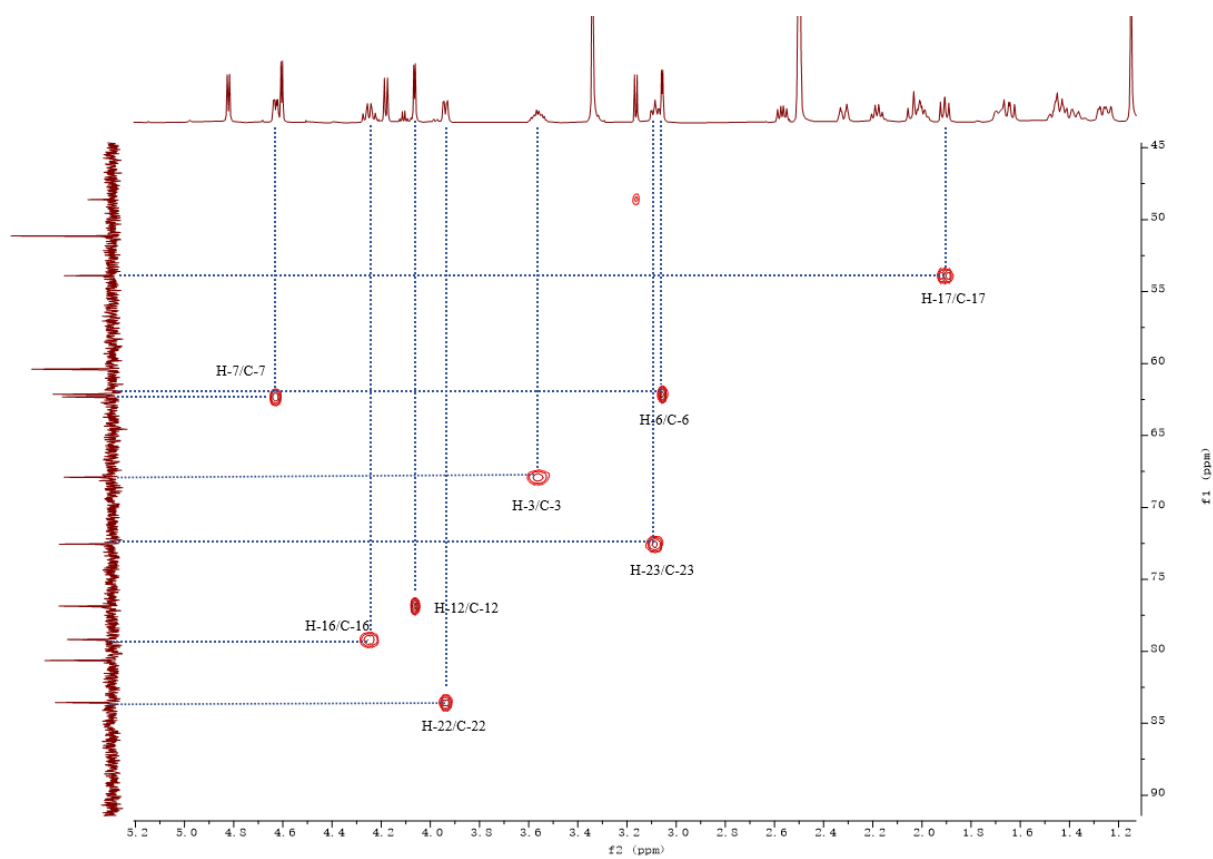


Figure S6: Enlarged HSQC spectrum of **1**

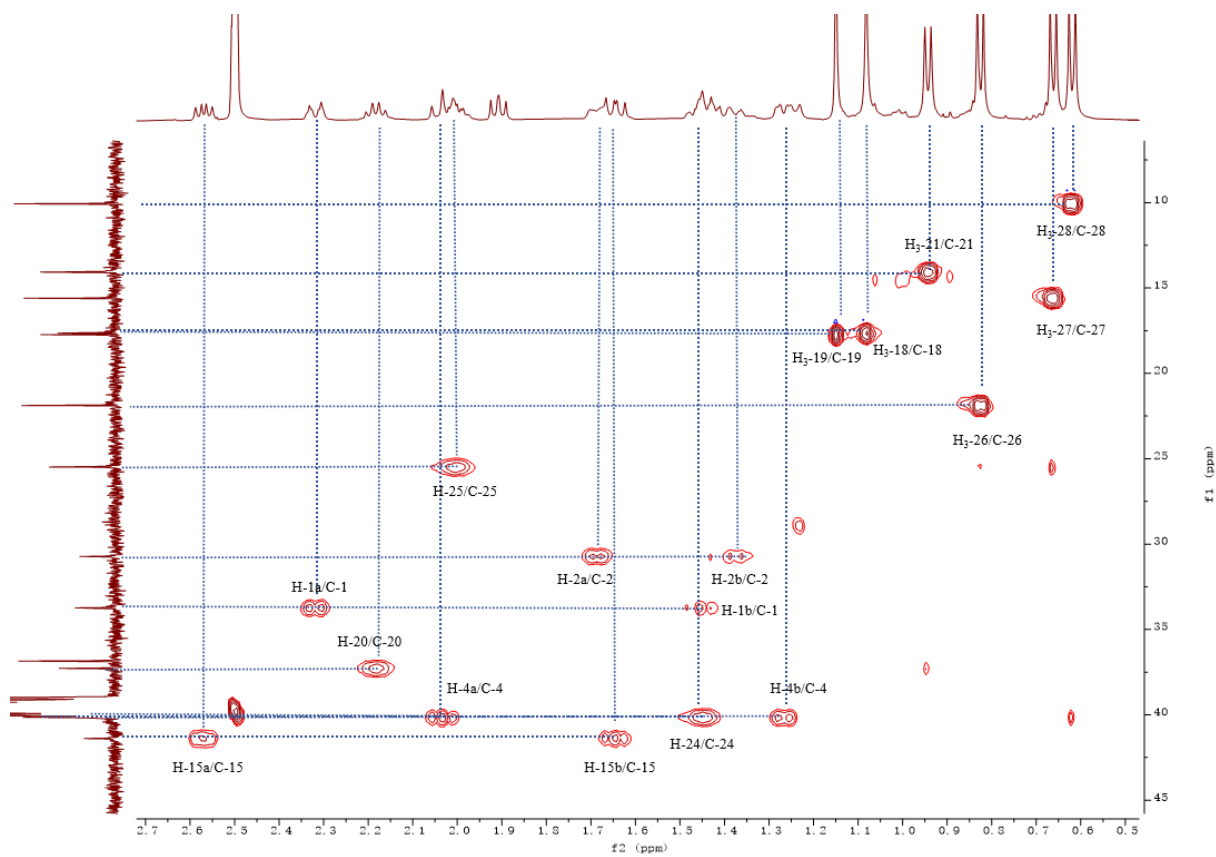


Figure S7: Enlarged HSQC spectrum of **1**

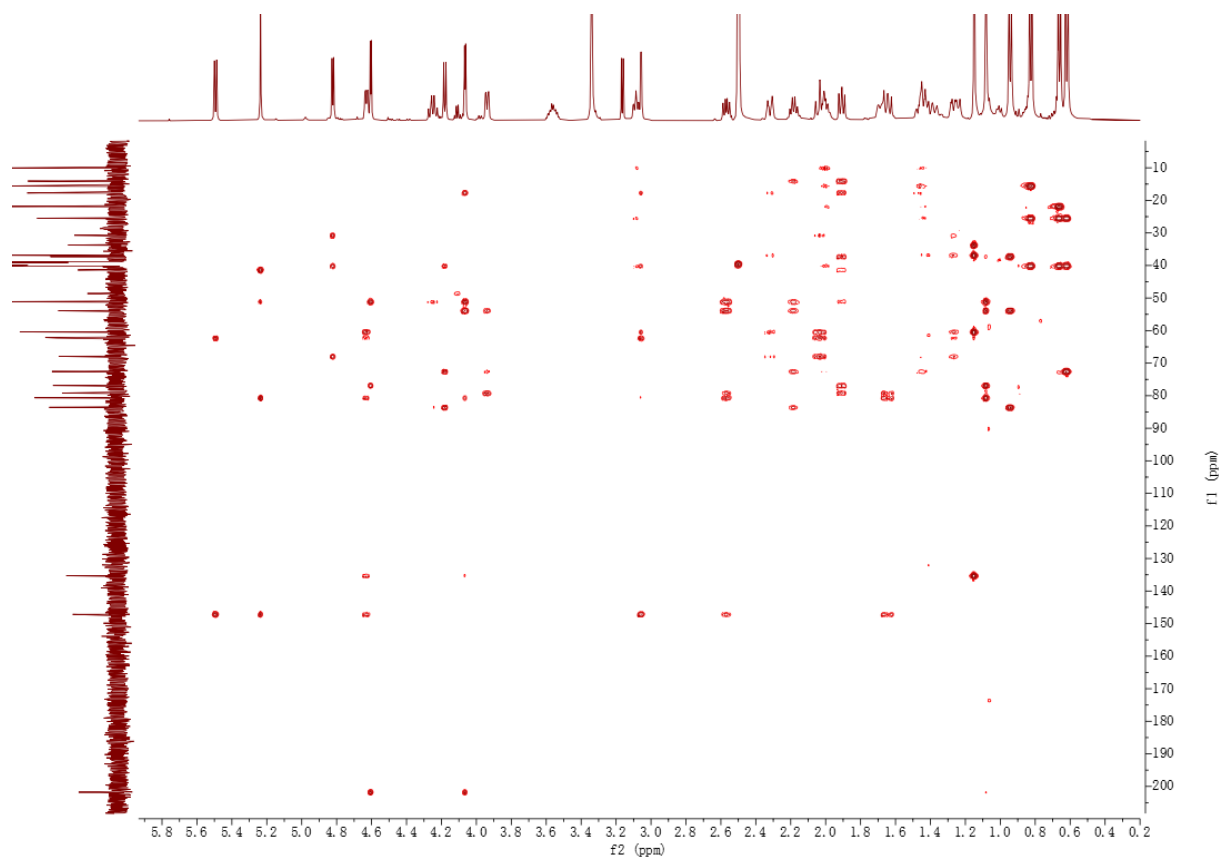


Figure S8: HMBC spectrum of **1**

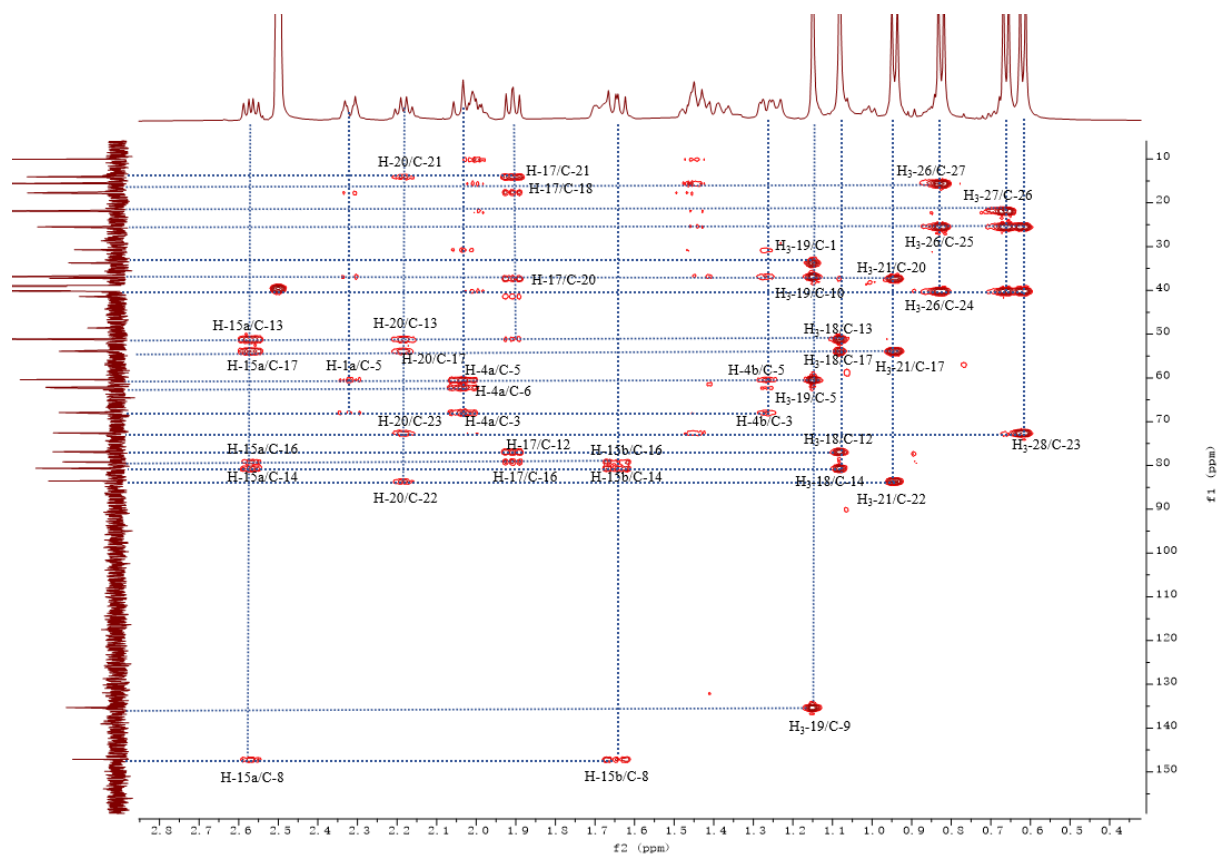


Figure S10: Enlarged HMBC spectrum of **1**

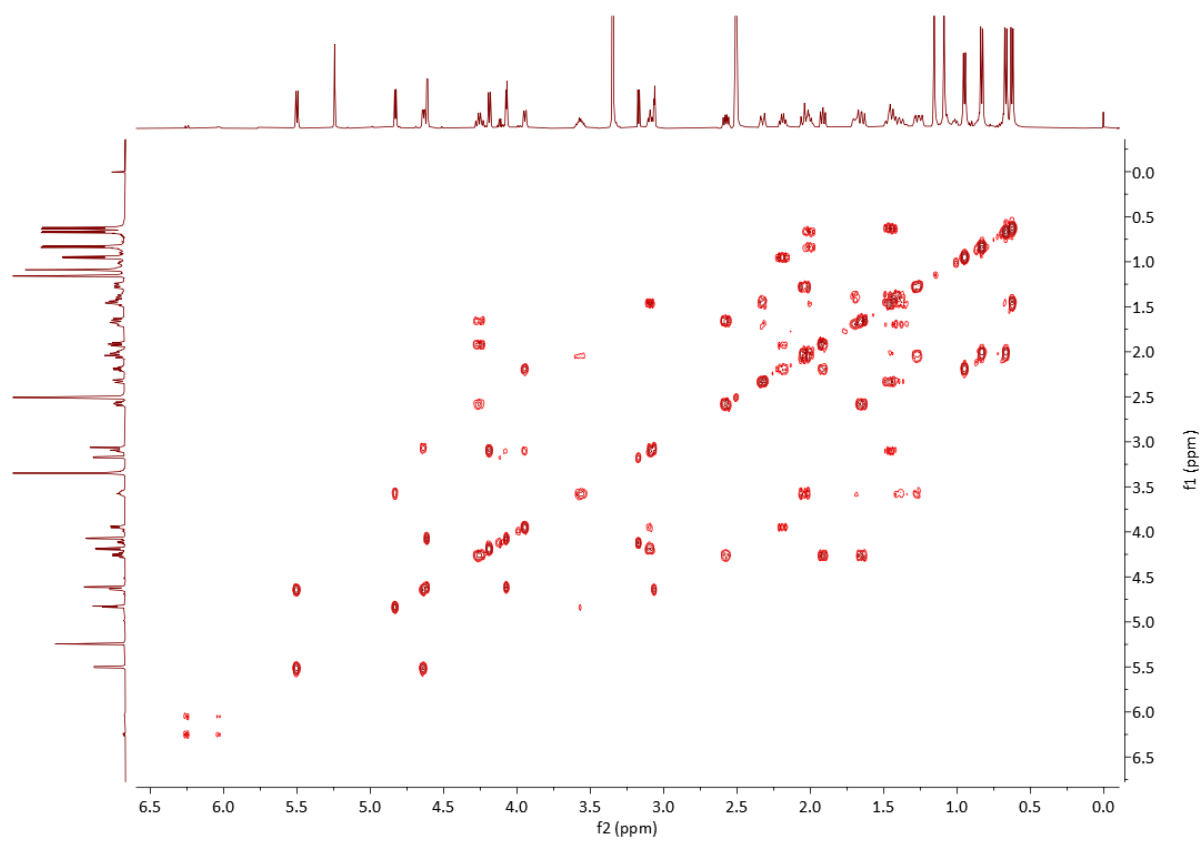


Figure S11: ^1H - ^1H COSY spectrum of **1**

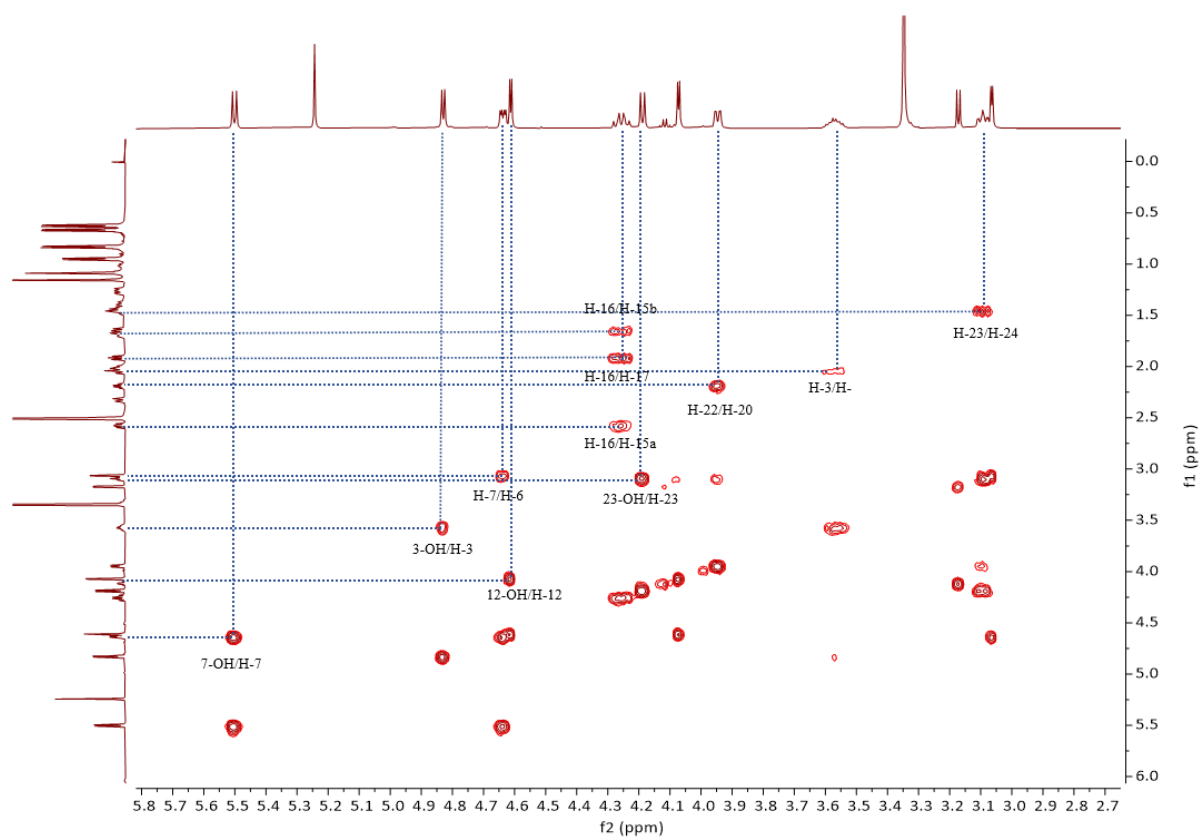


Figure S12: Enlarged ^1H - ^1H COSY spectrum of **1**

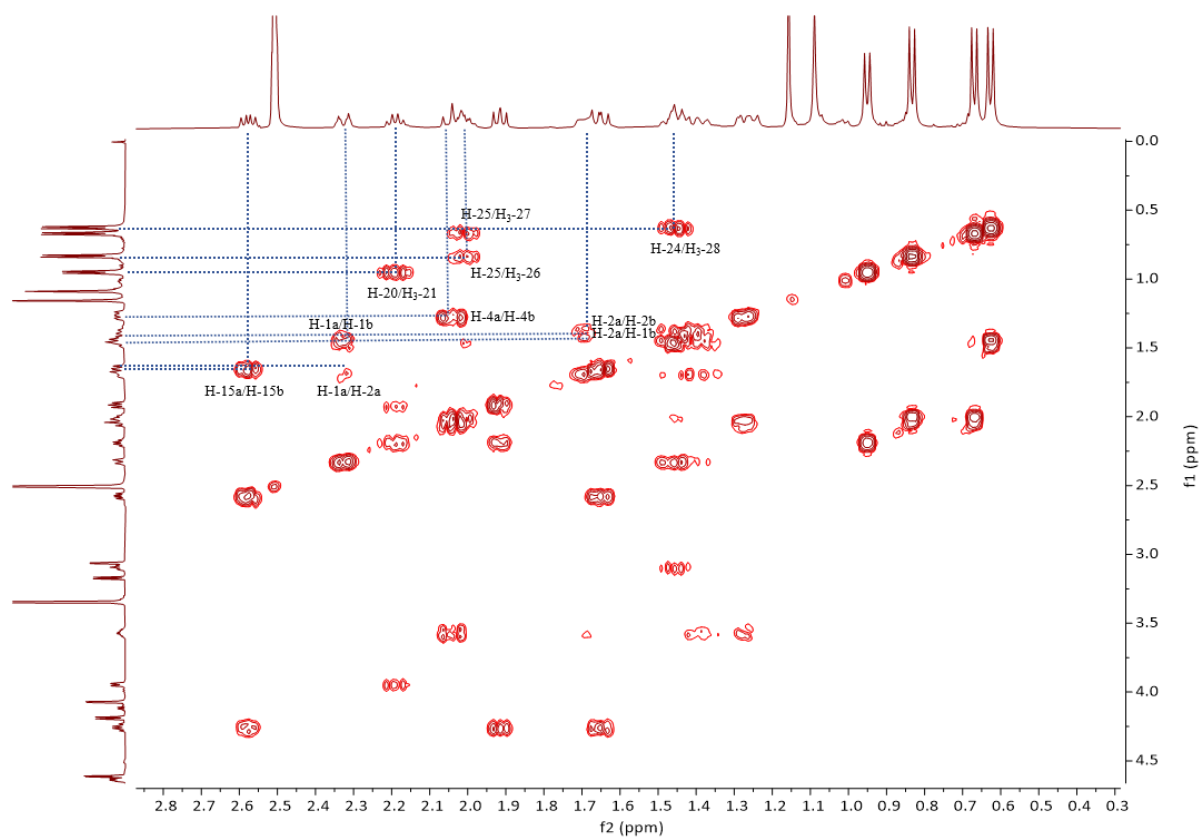


Figure S13: Enlarged ^1H - ^1H COSY spectrum of **1**

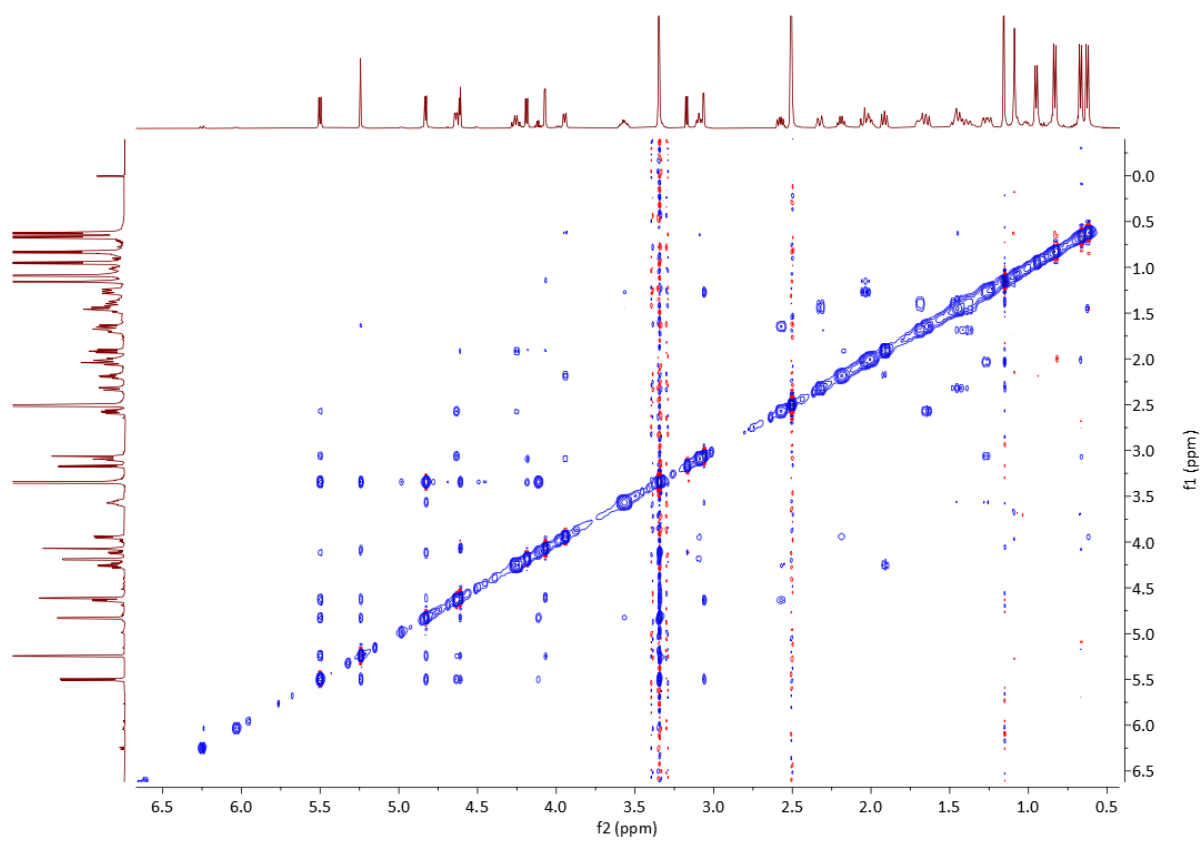


Figure S14: NOESY spectrum of **1**

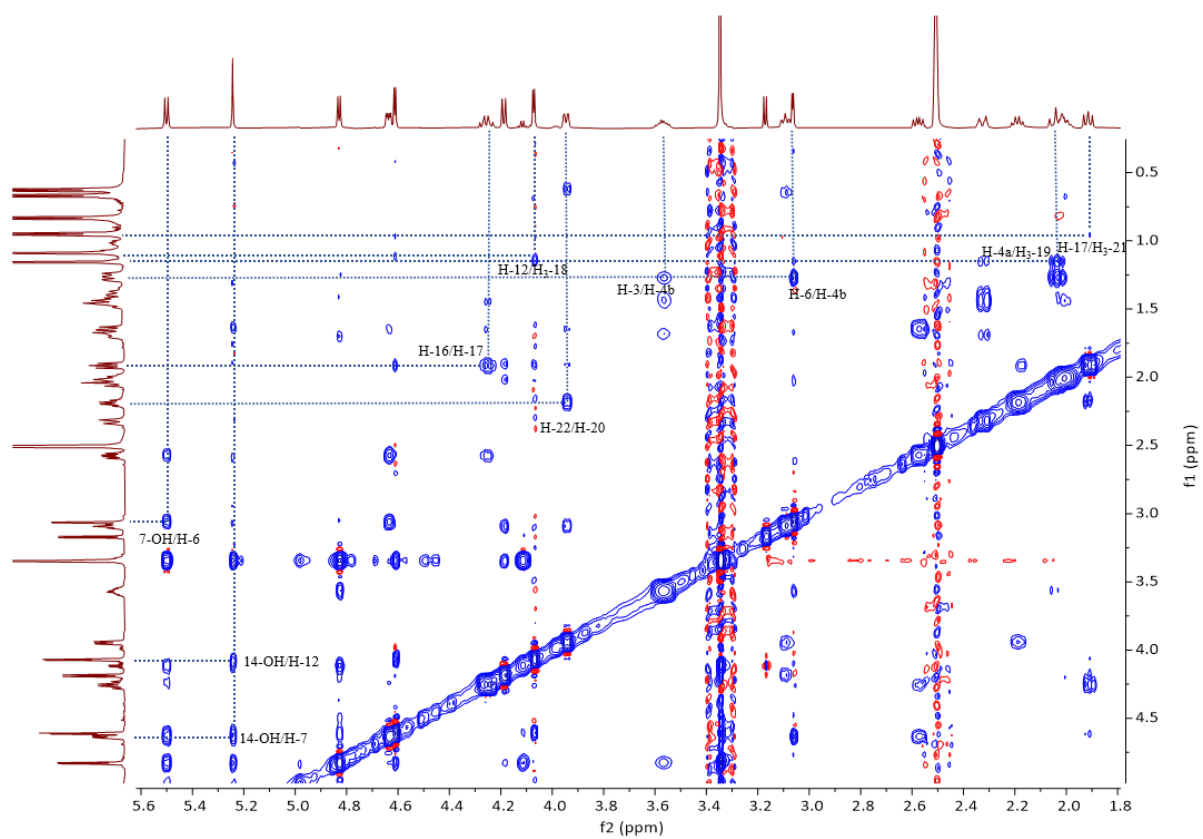


Figure S15: Enlarged NOESY spectrum of **1**

Structure Match

As Drawn (0)

Substructure (0)

Similarity (221K)

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Filter by Exclude

Search Within Results

Similarity

95-98 (1)

90-94 (1)

85-89 (37)

80-84 (697)

75-79 (3,044)

[View All](#)

Reaction Role

Product (3)

Reference Role

Biological Study (35)

Preparation (30)

Purification or Recovery (27)

Natural Product Occurrence (25)

Occurrence (25)

[View All](#)

Life Science Data

Commercial Availability

Available (9)

Not Available (30)

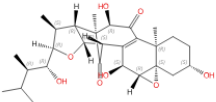
Filtering: Similarity: 3 Selected X Number of Components: 1 X [Clear All Filters](#)

39 Results

Sort: Relevance View: Partial

1 96 ...

2307209-43-2



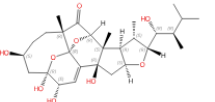
Absolute stereochemistry shown

$C_{28}H_{40}O_8$

1 Reference 0 Reactions 0 Suppliers

2 90 ...

2305861-09-8



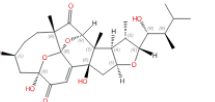
Absolute stereochemistry shown

$C_{28}H_{42}O_9$
(2*S*,3*R*,5*S*,8*R*,8*aR*,10*R*,10*aS*,10*bR*,11*S*,12*R*,13*aS*,14*aR*)-3,4,5,6,7,8,10,10*a*,10*b*,11,12,1...

1 Reference 0 Reactions 0 Suppliers

3 90 ...

2305861-10-1



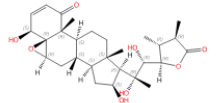
Absolute stereochemistry shown

$C_{28}H_{40}O_9$
(3*R*,5*S*,8*R*,8*aR*,10*R*,10*aS*,10*bR*,11*S*,12*R*,13*aS*,14*aR*)-3,4,5,6,7,8,10,10*a*,10*b*,11,12,13*a*,14...

1 Reference 0 Reactions 0 Suppliers

4 88 ...

71801-45-1



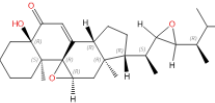
Absolute stereochemistry shown

$C_{28}H_{40}O_8$
Ergost-2-en-26-oic acid, 5,6-epoxy-4,16,20,22,23-pentahydroxy-1-oxo-, γ -lactone, ...

20 References 0 Reactions 2 Suppliers

5 87 ...

733001-47-3



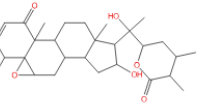
Absolute stereochemistry shown

$C_{28}H_{42}O_5$
7-Ergosten-6-one, 9*a*,11*a*,22*E*,23*E*-diepoxy-3*B*,5*a*-dihydroxy-

1 Reference 0 Reactions 0 Suppliers

6 87 ...

41929-21-9



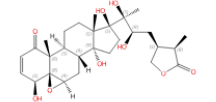
Absolute stereochemistry shown

$C_{28}H_{40}O_7$
Ergost-2-en-26-oic acid, 5,6-epoxy-4,16,20,22-tetrahydroxy-1-oxo-, δ -lactone, (4...

14 References 0 Reactions 1 Supplier

7 87 ...

1353093-12-5

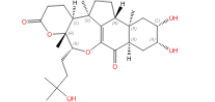


Absolute stereochemistry shown, Rotation (+)

$C_{28}H_{40}O_9$
Ergost-2-en-26-oic acid, 5,6-epoxy-4,14,17,20,22,28-hexahydroxy-1-oxo-, γ -lactone...

8 87 ...

1629965-07-6

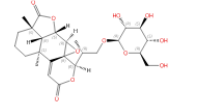


Absolute stereochemistry shown

$C_{27}H_{40}O_7$

9 87 ...

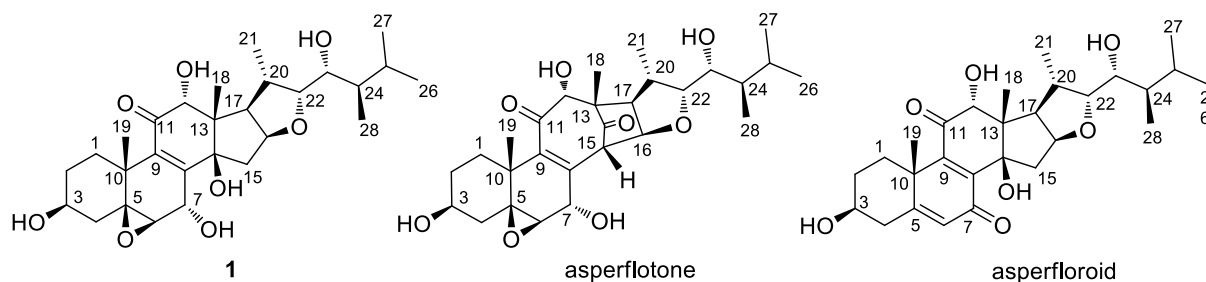
2589815-72-3



Absolute stereochemistry shown, Rotation (+)

$C_{25}H_{34}O_{11}$

Figure S16: Scifinder search results of 1

Table S1: The comparison of NMR data of compound **1**, asperflotone, and 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)	33.7 CH ₂	2.36 br d (13.8)	35.1 CH ₂	2.43 dt (13.9, 3.4)	31.9 CH ₂
	1.44 m		1.41 br t (13.8)		1.06 td (13.9, 4.0)	
2	1.68 m	30.7 CH ₂	1.69 m	30.5 CH ₂	1.76 m	29.8 CH ₂
	1.37 m		1.34 m		1.60 tdd (13.9, 11.0, 3.4)	
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	40.1 CH ₂	1.95 t (12.0)	39.9 CH ₂	2.60 m	41.5 CH ₂
	1.26 m		1.26 br d (12.0)		2.47 ddd (13.1, 11.0, 1.4)	
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)	