

Supporting Information

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A New Ssquiterpene and Known Alkaloids from *Toddalia asiatica* and Their Inhibitions Against Phosphodiesterase-4

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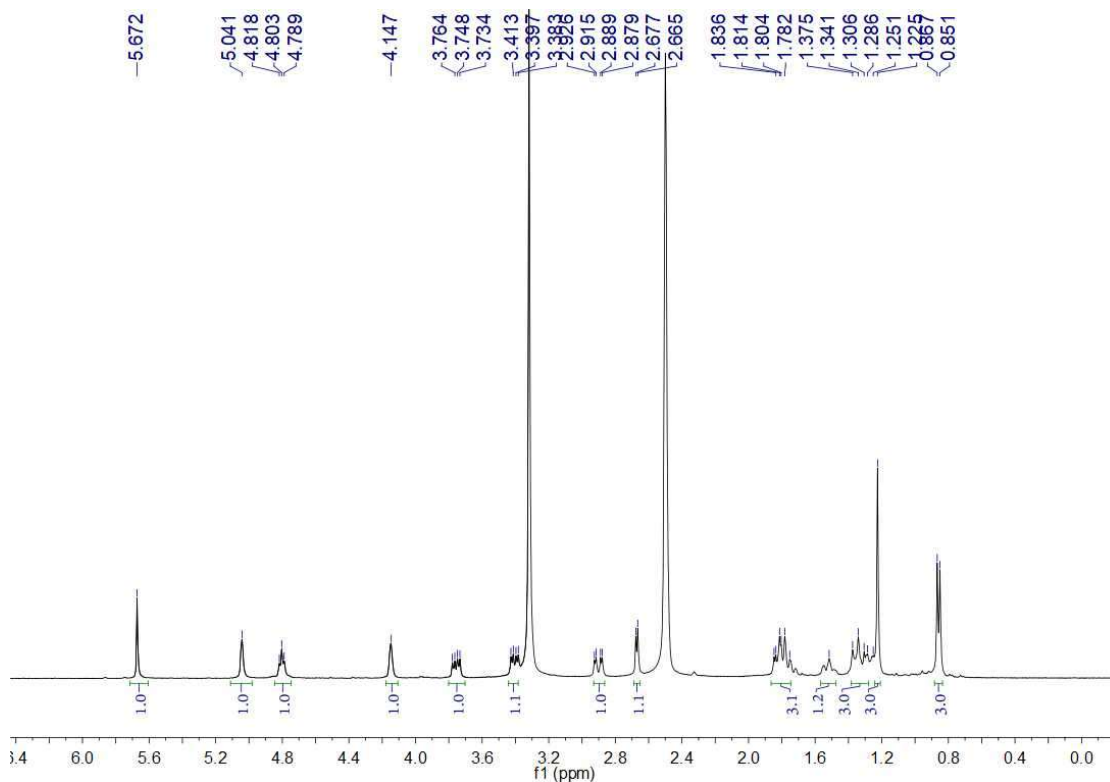


Figure S1: ^1H NMR Spectrum of **1** in $\text{DMSO-}d_6$ (400 MHz)

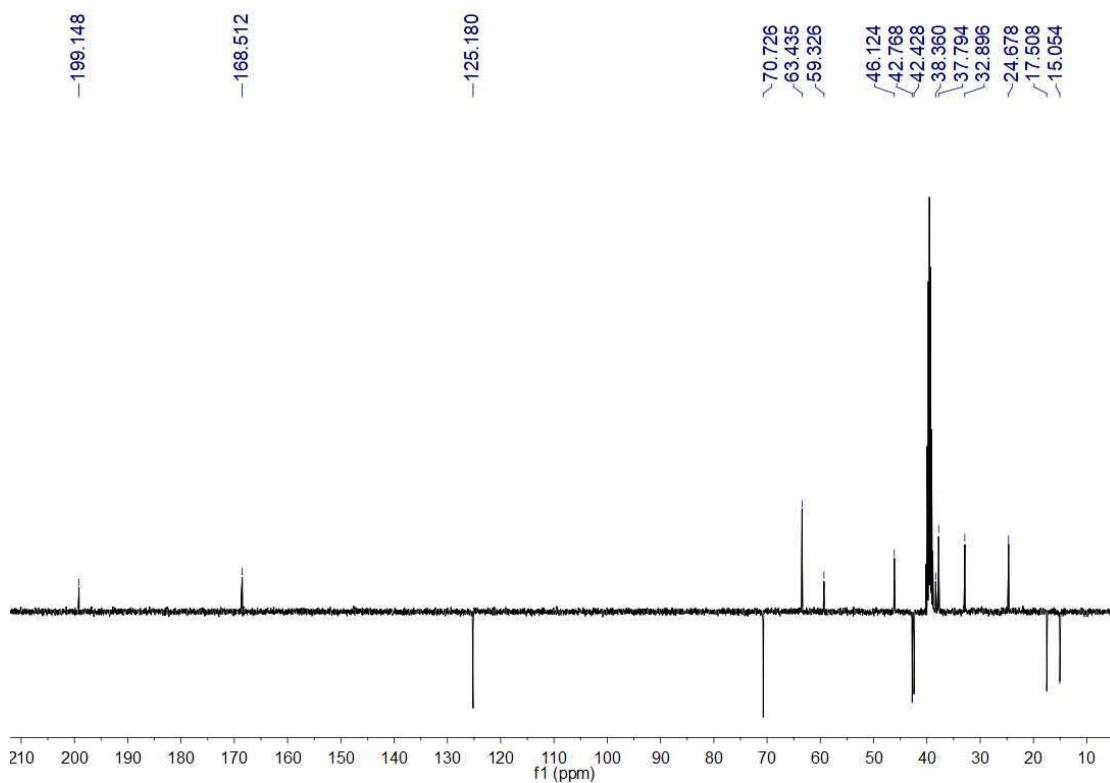


Figure S2: ^{13}C NMR Spectrum of **1** in $\text{DMSO-}d_6$ (100 MHz)

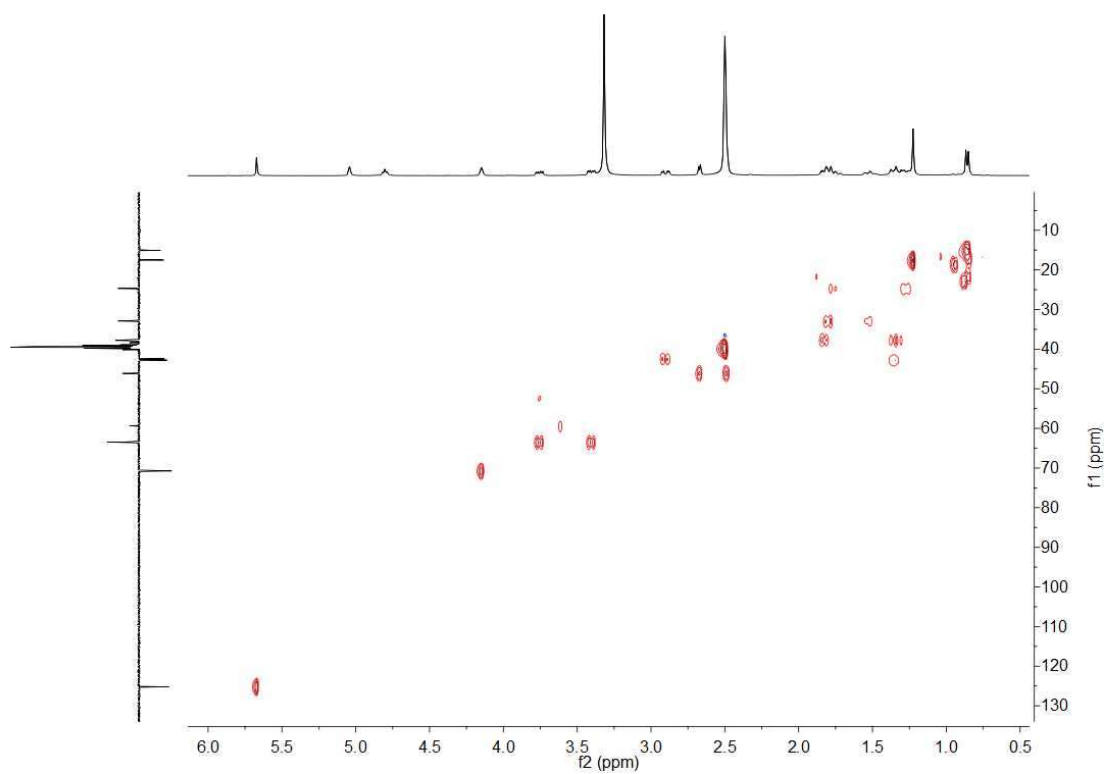


Figure S3: HSQC Spectrum of **1** in DMSO- d_6

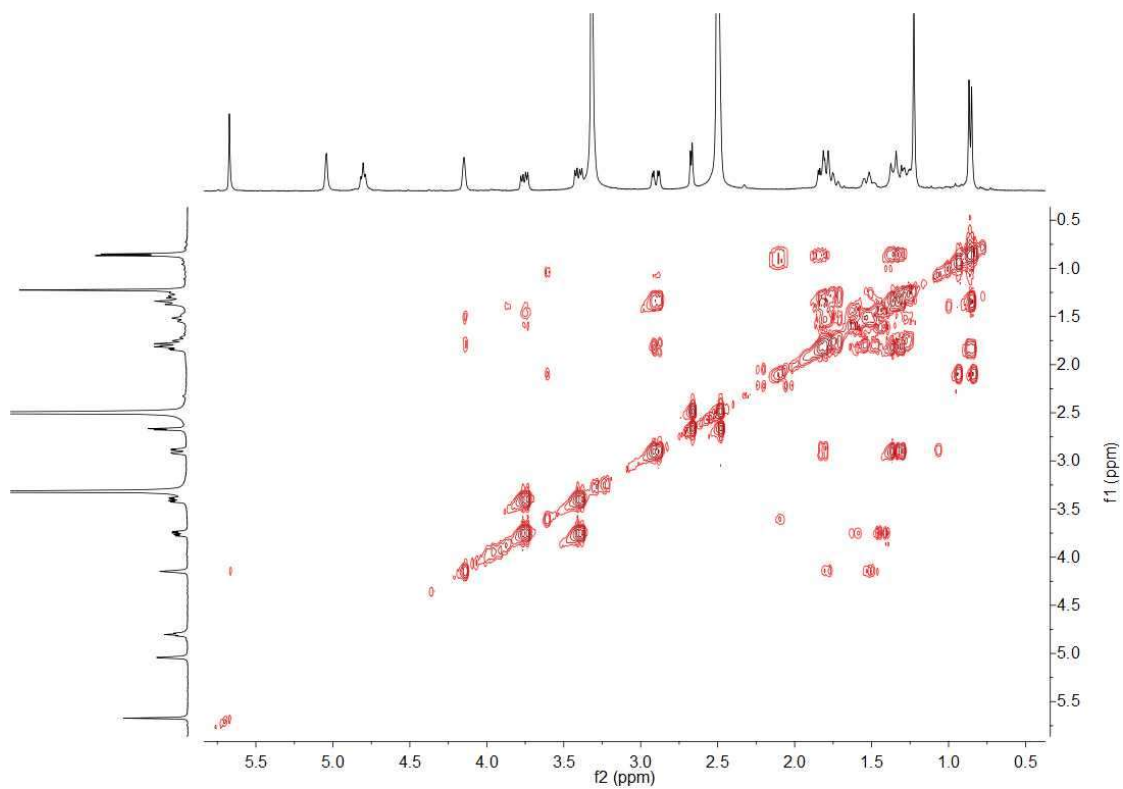


Figure S4: ^1H - ^1H COSY Spectrum of **1** in DMSO- d_6

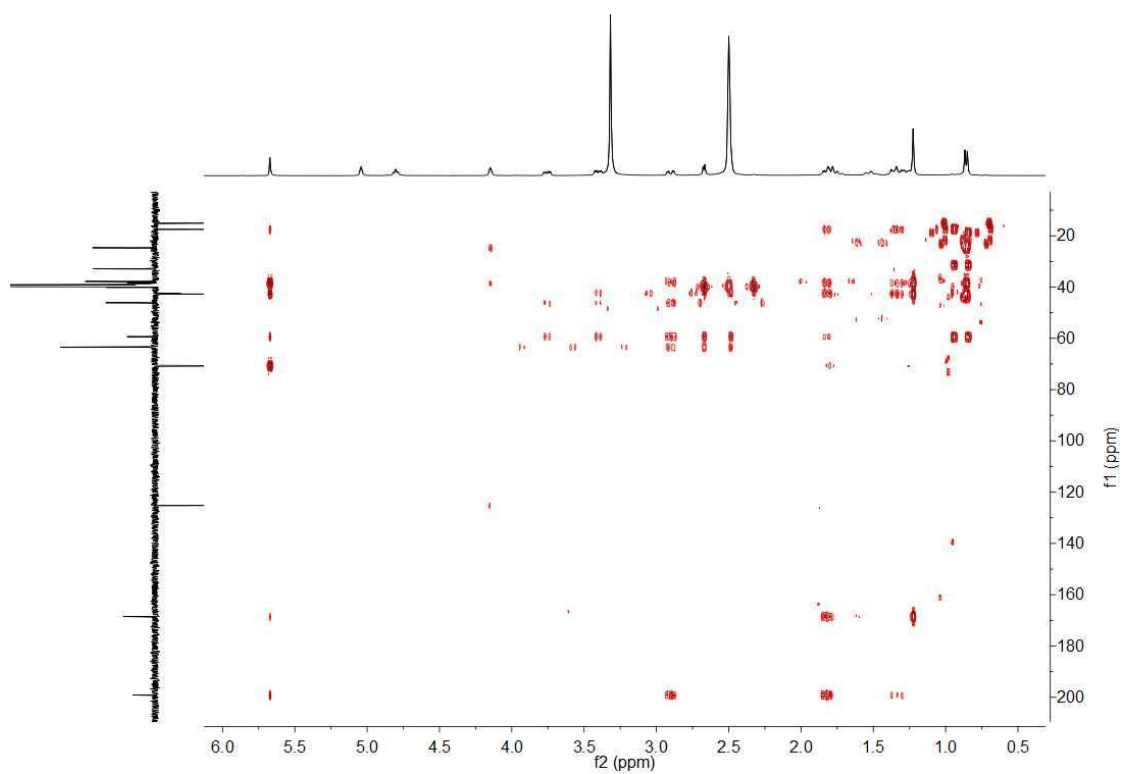


Figure S5: HMBC Spectrum of **1** in DMSO- d_6

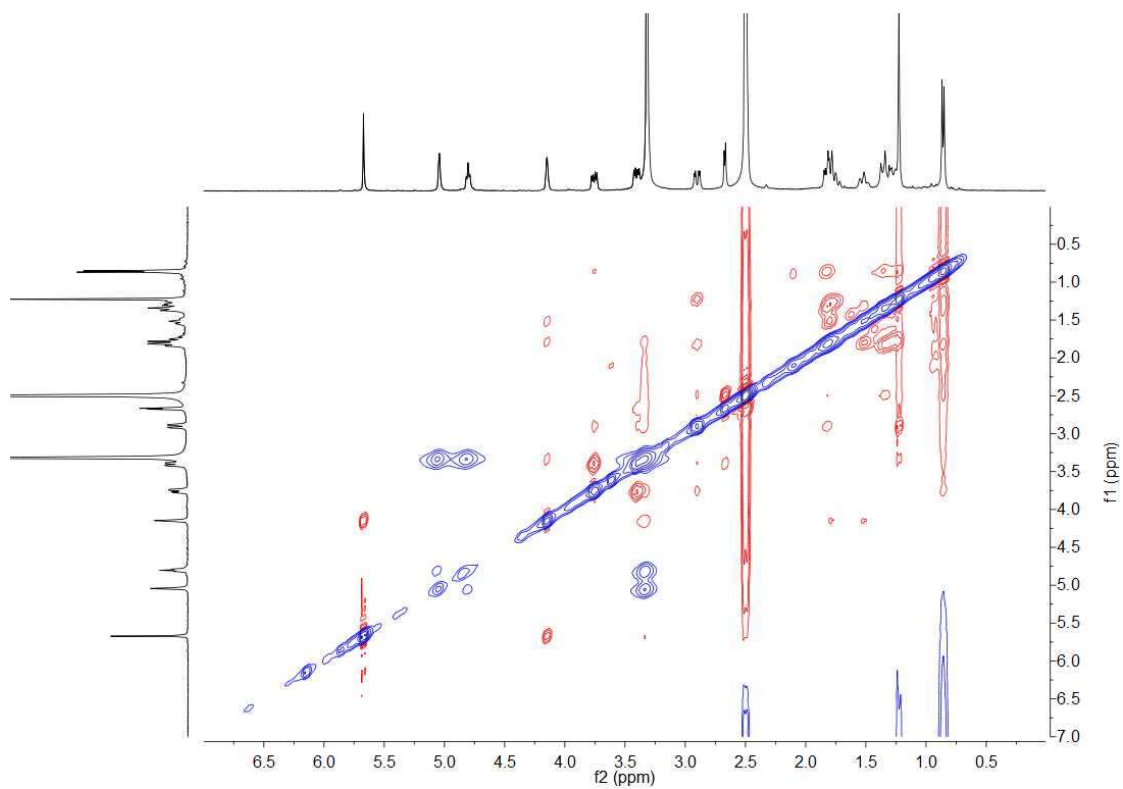


Figure S6: NOESY Spectrum of **1** in DMSO- d_6

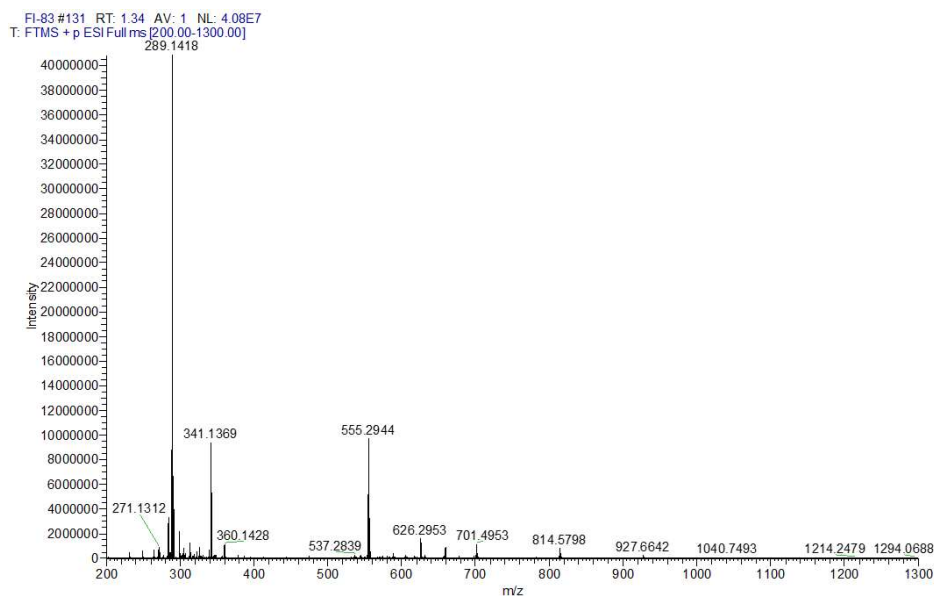


Figure S7: HRESIMS spectrum of **1**.

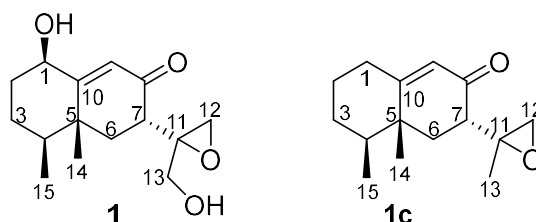


Table S1. NMR data of **1** and its analogue (**1c**: 7β-H-9(10)-ene-11,12-epoxy-8-oxoeremophilane)

No.	1 ^a		1c ^b	
	δ _H	δ _C	δ _H	δ _C
1	4.15, br s	70.7, CH	2.08–2.10, m 2.44, overlapped	33.0, CH ₂
2	1.29–1.38, m 1.79–1.86, m	37.8, CH ₂	1.24–1.26, m; 1.96–1.99, m 1.51–1.54, m	29.5, CH ₂
3	1.23–1.31, m 1.74–1.81, m	24.7, CH ₂	1.59–1.64, m	30.4, CH ₂
4	1.31–1.39, m	42.8, CH	1.83–1.85, m	38.6, CH
5		38.3, C		40.3, C
6	1.50–1.56, m 1.77–1.82, m	32.9, CH ₂	2.08, dd (4.7, 14.0) 1.51, dd (13.7, 14.0)	34.3, CH ₂
7	2.90, dd (14.6, 3.8)	42.4, CH	2.45, dd (4.7, 13.7)	47.5, CH
8		199.2, C		198.5, C
9	5.69, s	125.2, CH	5.74, s	122.9, CH
10		168.5, C		172.2, C
11		59.3, C		56.2, C
12	2.49, d (4.4); 2.67, d (4.4)	46.1, CH ₂	2.55, d (4.3) 2.60, d (4.3)	51.2, CH ₂
13	3.41, d (12.3, 5.7) 3.76, d (12.3, 5.9)	63.9, CH ₂	1.44, s	21.2, CH ₃
14	1.22, s	17.5, CH ₃	1.08, s	20.8, CH ₃
15	0.86, d (6.7)	15.1, CH ₃	0.93, d (6.7)	16.2, CH ₃
1-OH	5.05, br s			
13-OH	4.80, dd (5.9, 5.7)			

^a ¹H NMR recorded at 400 MHz in DMSO-*d*₆, ¹³C NMR recorded at 100 MHz in DMSO-*d*₆.

^b ¹H NMR recorded at 500 MHz in CDCl₃, ¹³C NMR recorded at 125 MHz CDCl₃

Figure S8: Scifinder report for 1

Explore ▾ Saved Searches ▾ SciPlanner

Chemical Structure similarity

SUBSTANCES

Select All Deselect All

0 of 7 Similarity Candidates Selected

Similarity Range	Substances
≥ 99 (most similar)	0
95-98	0
90-94	1
85-89	4
80-84	11
75-79	28
70-74	127
65-69	727
0-64 (least similar)	6939

Get Substances

0 of 5 Substances Selected

Score: 91

1. **129602-10-4**

~5

Absolute stereochemistry.

C₁₅H₂₂O₃
2-(3H)-Naphthalene, 4,4a,5,6,7,8-hexahydro-6-hydroxy-4a,5-dimethyl-3-(2-methyloxiranyl)-, [3S-[3a(R*),4aβ,5β,6α]]-, (9CI)

Key Physical Properties

Score: 85

2. **85431-61-4**

~20

Absolute stereochemistry.

C₁₅H₂₂O₄
Naphthyl 1,2-b)oxiren-2(1aH)-one, 4,5,6,7,7a,7b-hexahydro-6-hydroxy-1a-[[2R)-2-(hydroxymethyl)oxiranyl]-7,7a-dimethyl-, (1a,5,6R,7R,7aR,7bR)-

Key Physical Properties

Score: 85

3. **1304771-32-1**

~2

Rotation (+), Absolute stereochemistry.

C₁₈H₂₂O₃
2-(3H)-Naphthalene, 4,4a,5,6,7,8-hexahydro-8-hydroxy-4,4a-dimethyl-6-[[2R)-2-methyl-2-oxiranyl]-, (4R,4a,5,6,5,8R)-

Key Physical Properties

Score: 85

4. **1638621-55-2**

~1

Currently available stereo shown., Rotation (-), Absolute stereochemistry.

C₁₅H₂₂O₃
2-(3H)-Naphthalene, 4,4a,5,6,7,8-hexahydro-4a,5-dimethyl-3-(2-methyl-2-oxiranyl)-, (3S,4aR,5S)-

Key Physical Properties

Score: 85

5. **1638621-56-3**

~3

Currently available stereo shown., Rotation (-), Absolute stereochemistry.

C₁₅H₂₂O₃
2-(3H)-Naphthalene, 4,4a,5,6,7,8-hexahydro-4a,5-dimethyl-3-(2-methyl-2-oxiranyl)-, (3R,4aR,5S)-

Key Physical Properties