

## 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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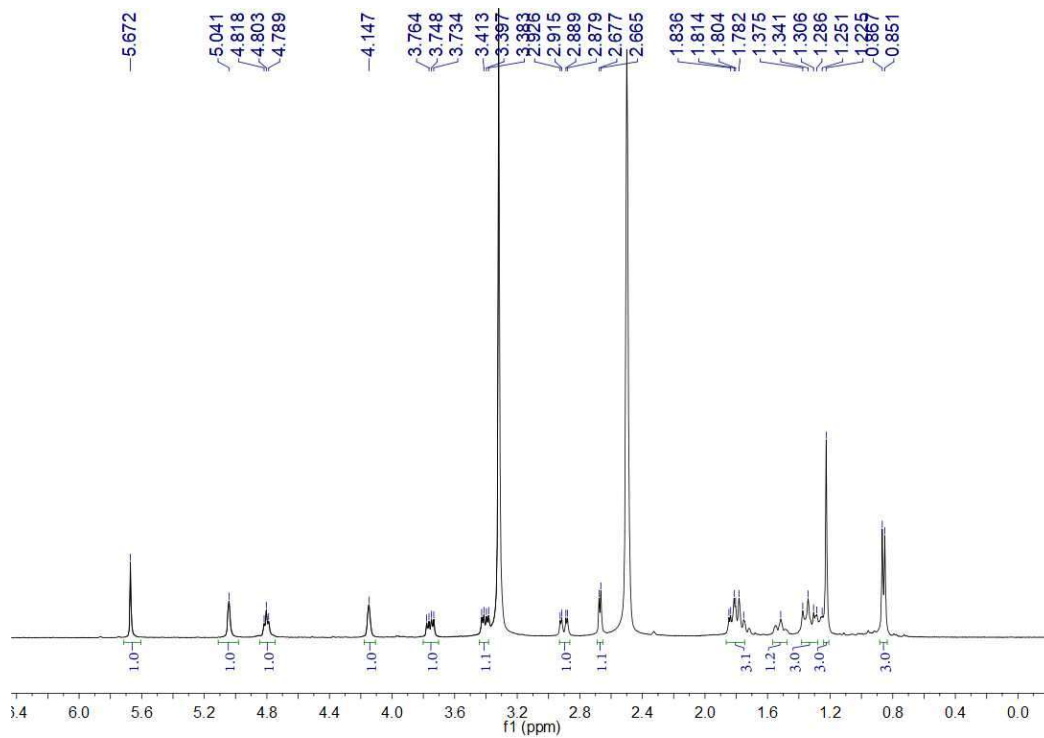


Figure S1:  $^1\text{H}$  NMR Spectrum of **1** in  $\text{DMSO-}d_6$  (400 MHz)

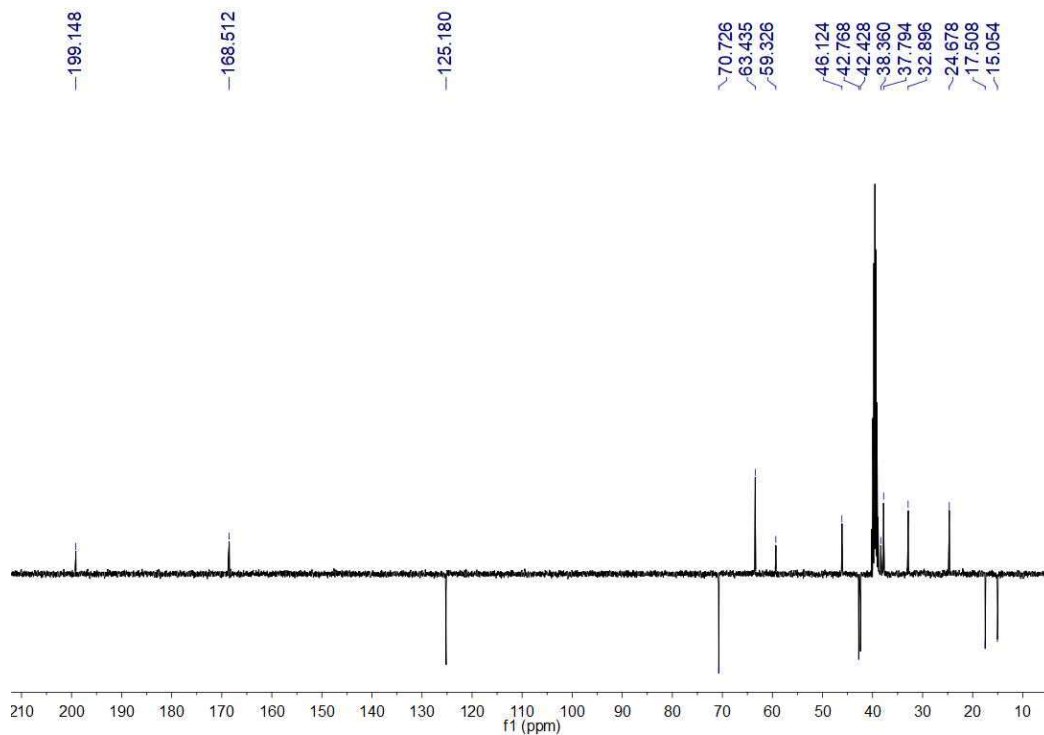
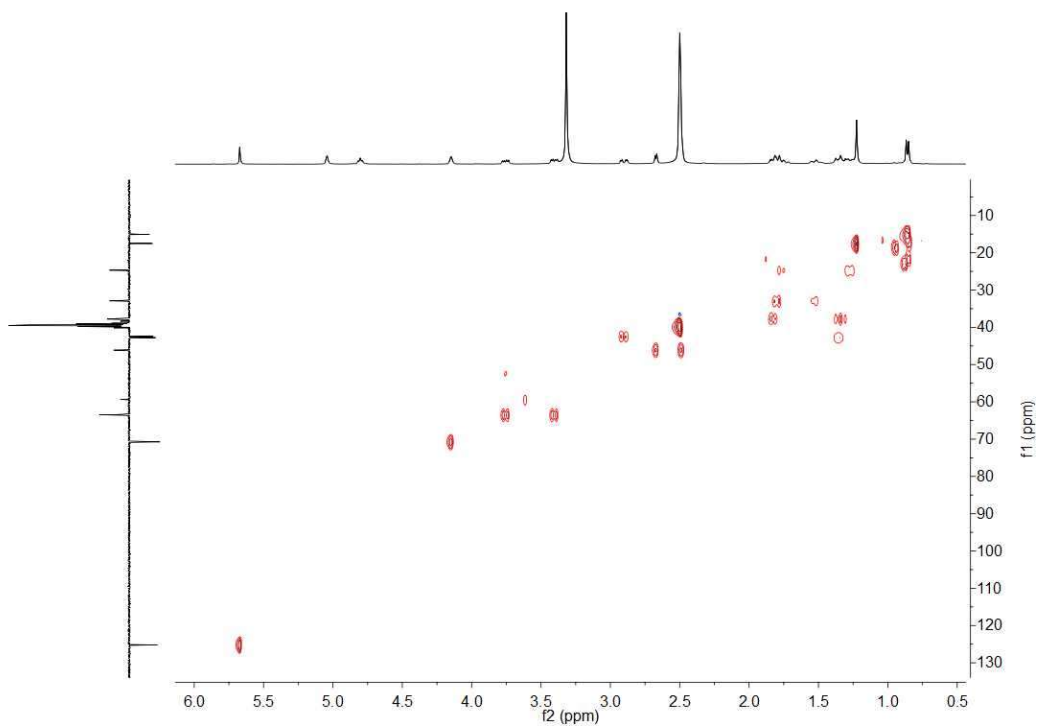
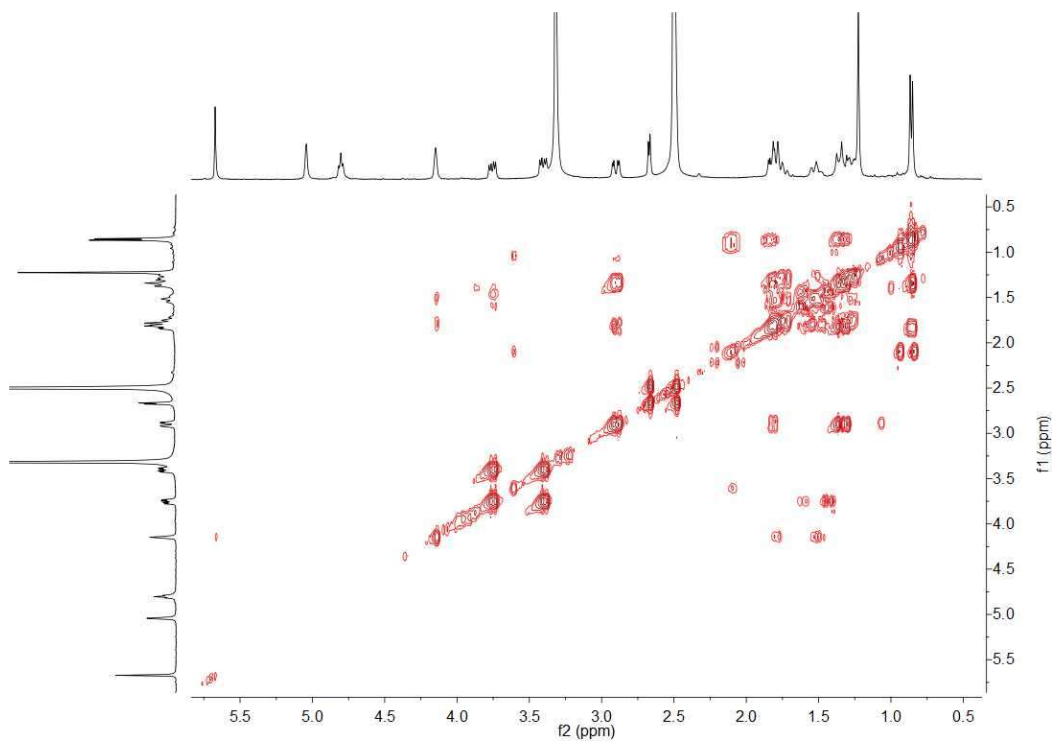


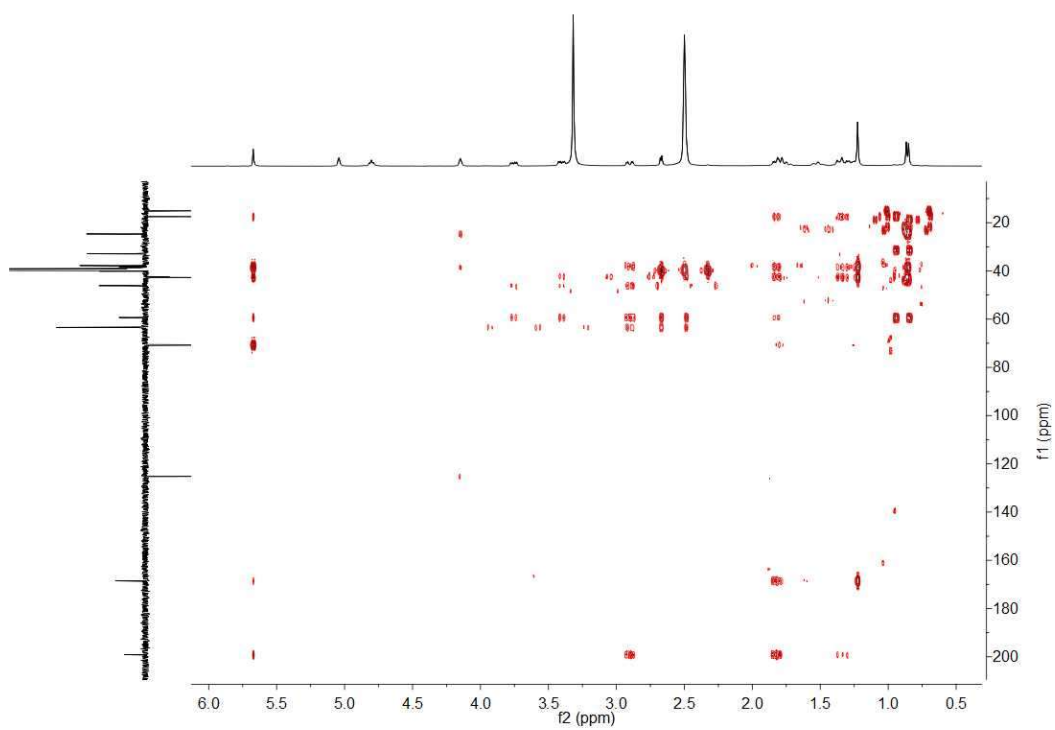
Figure S2:  $^{13}\text{C}$  NMR Spectrum of **1** in  $\text{DMSO-}d_6$  (100 MHz)



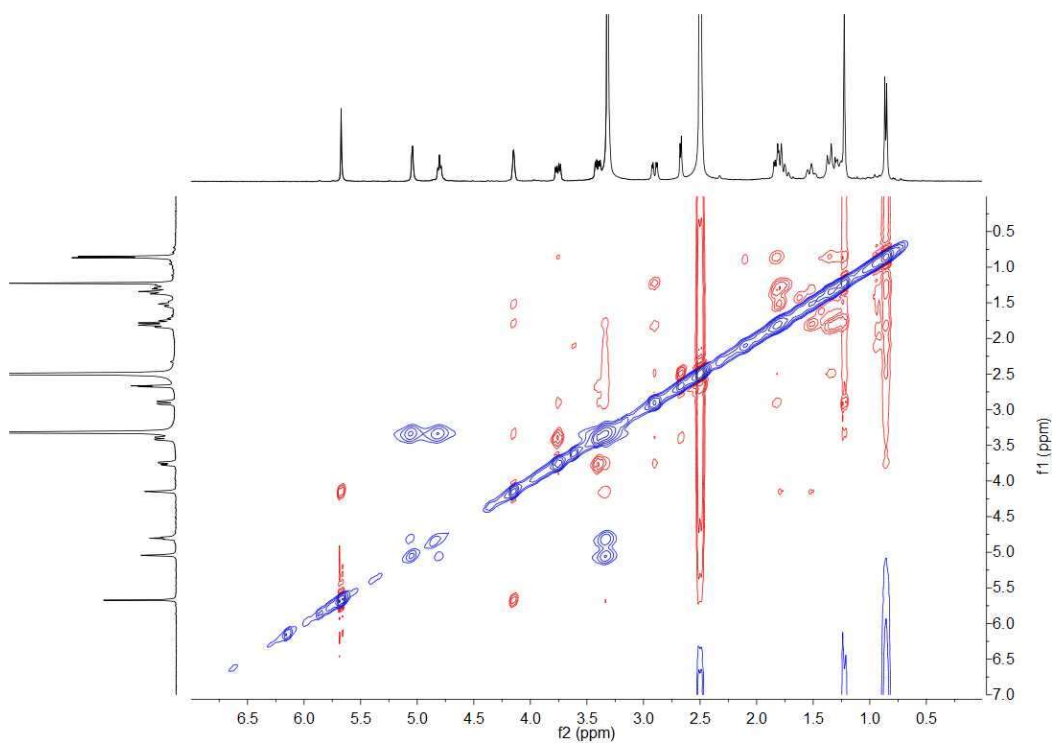
**Figure S3:** HSQC Spectrum of **1** in DMSO-*d*<sub>6</sub>



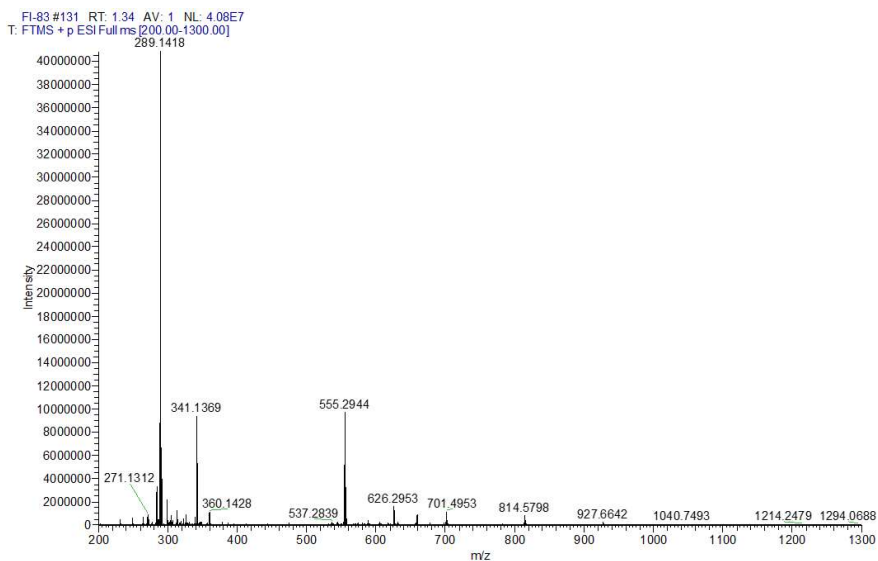
**Figure S4:** <sup>1</sup>H-<sup>1</sup>H COSY Spectrum of **1** in DMSO-*d*<sub>6</sub>



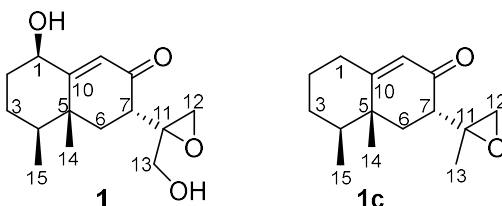
**Figure S5:** HMBC Spectrum of **1** in DMSO- $d_6$



**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.	<b>1</b> <sup>a</sup>		<b>1c</b> <sup>b</sup>	
	$\delta_{\text{H}}$	$\delta_{\text{C}}$	$\delta_{\text{H}}$	$\delta_{\text{C}}$
1	4.15, br s	70.7, CH	2.08–2.10, m 2.44, overlapped	33.0, CH <sub>2</sub>
2	1.29–1.38, m 1.79–1.86, m	37.8, CH <sub>2</sub>	1.24–1.26, m; 1.96–1.99, m	29.5, CH <sub>2</sub>
3	1.23–1.31, m 1.74–1.81, m	24.7, CH <sub>2</sub>	1.51–1.54, m 1.59–1.64, m	30.4, CH <sub>2</sub>
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 <sub>2</sub>	2.08, dd (4.7, 14.0) 1.51, dd (13.7, 14.0)	34.3, CH <sub>2</sub>
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 <sub>2</sub>	2.55, d (4.3) 2.60, d (4.3)	51.2, CH <sub>2</sub>
13	3.41, d (12.3, 5.7) 3.76, d (12.3, 5.9)	63.9, CH <sub>2</sub>	1.44, s	21.2, CH <sub>3</sub>
14	1.22, s	17.5, CH <sub>3</sub>	1.08, s	20.8, CH <sub>3</sub>
15	0.86, d (6.7)	15.1, CH <sub>3</sub>	0.93, d (6.7)	16.2, CH <sub>3</sub>
1-OH	5.05, br s			
13-OH	4.80, dd (5.9, 5.7)			

<sup>a</sup> <sup>1</sup>H NMR recorded at 400 MHz in DMSO-*d*<sub>6</sub>, <sup>13</sup>C NMR recorded at 100 MHz in DMSO-*d*<sub>6</sub>.

<sup>b</sup> <sup>1</sup>H NMR recorded at 500 MHz in CDCl<sub>3</sub>, <sup>13</sup>C NMR recorded at 125 MHz CDCl<sub>3</sub>

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Chemical Structure similarity

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

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0 of 5 Substances Selected

Score: 91

1. 129602-10-4

-5

Absolute stereochemistry.

**C<sub>15</sub> H<sub>20</sub> O<sub>3</sub>**  
2-(3*R*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-6-hydroxy-4a,5-dimethyl-3-(2-methyloxiranyl), [3*S*][3a(*R*),4aβ,5β,6a]]- (9CI)

▶ Key Physical Properties

Score: 85

2. 85431-61-4

-20

Absolute stereochemistry.

**C<sub>15</sub> H<sub>20</sub> O<sub>3</sub>**  
Naphth[1,2-*b*]oxiren-2(1a*H*)-one, 4,5,6,7,7a,7b-hexahydro-6-hydroxy-1a-[(2*R*)-2-(hydroxymethyl)oxiranyl]-7,7a-dimethyl-, (1a,5,6*R*,7*R*,7a*R*,7b*R*)

▶ Key Physical Properties

Score: 85

3. 1304771-32-1

-2

Rotation (+), Absolute stereochemistry.

**C<sub>15</sub> H<sub>22</sub> O<sub>3</sub>**  
2-(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-8-hydroxy-4,4a-dimethyl-6-[(2*R*)-2-methyl-2-oxiranyl], (4*R*,4a,5,6,5,8*R*)

▶ Key Physical Properties

Score: 85

4. 1638621-55-2

-1

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

**C<sub>15</sub> H<sub>20</sub> O<sub>3</sub>**  
2-(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4a,5-dimethyl-3-(2-methyl-2-oxiranyl)-, (3*S*,4a*R*,5*S*)

▶ Key Physical Properties

Score: 85

5. 1638621-56-3

-3

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

**C<sub>15</sub> H<sub>20</sub> O<sub>3</sub>**  
2-(3*H*)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4a,5-dimethyl-3-(2-methyl-2-oxiranyl)-, (3*R*,4a*R*,5*S*)

▶ Key Physical Properties

Figure S8: Scifinder report for 1