

## Supporting Information

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### Cytotoxic Drimane-type Sesquiterpenoids from the Fungus *Aspergillus flavipes* 297

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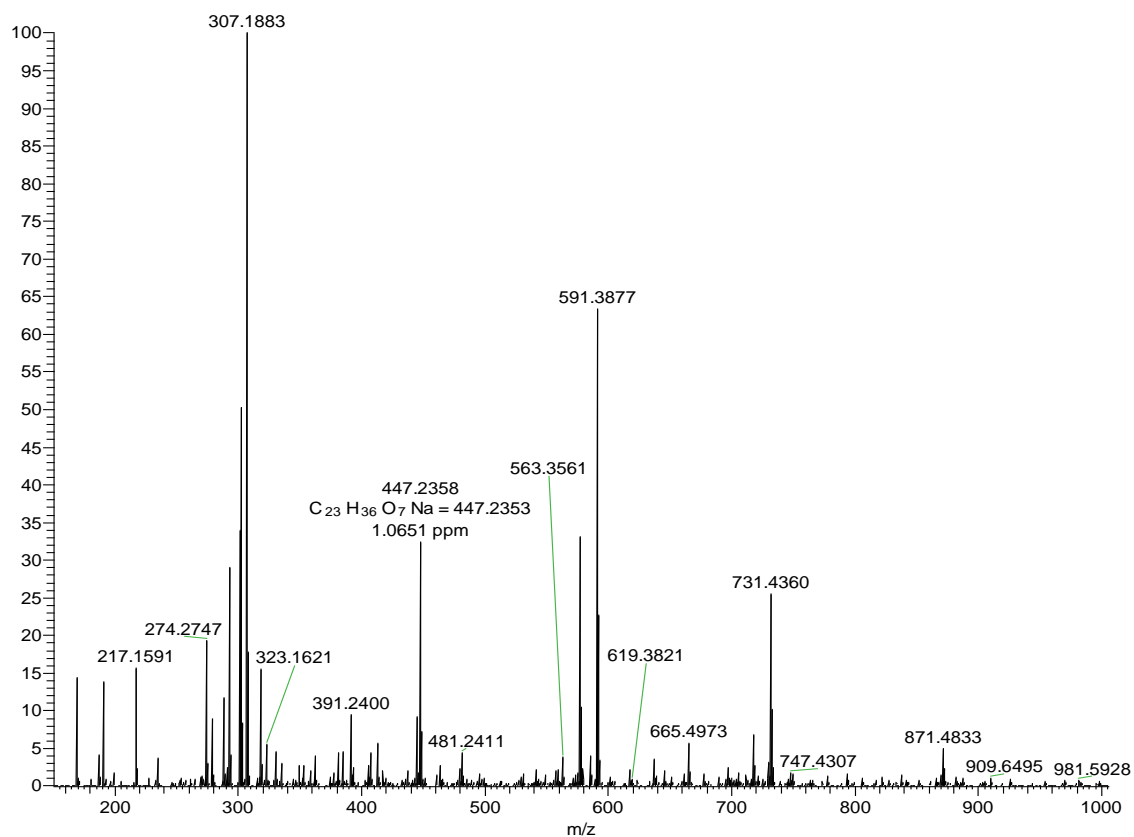
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20211020-17A\_211020105751 #114-115 RT: 0.91-0.92 AV: 2 SB: 28 0.04-0.26 NL: 2.93E7  
T: FTMS + p ESI Full ms [150.00-1000.00]



**Figure S1:** HRESIMS spectrum of **1a**

20211020-17B\_211020102914 #113-115 RT: 0.94-0.96 AV: 3 SB: 26 0.16-0.38 NL: 1.16E7  
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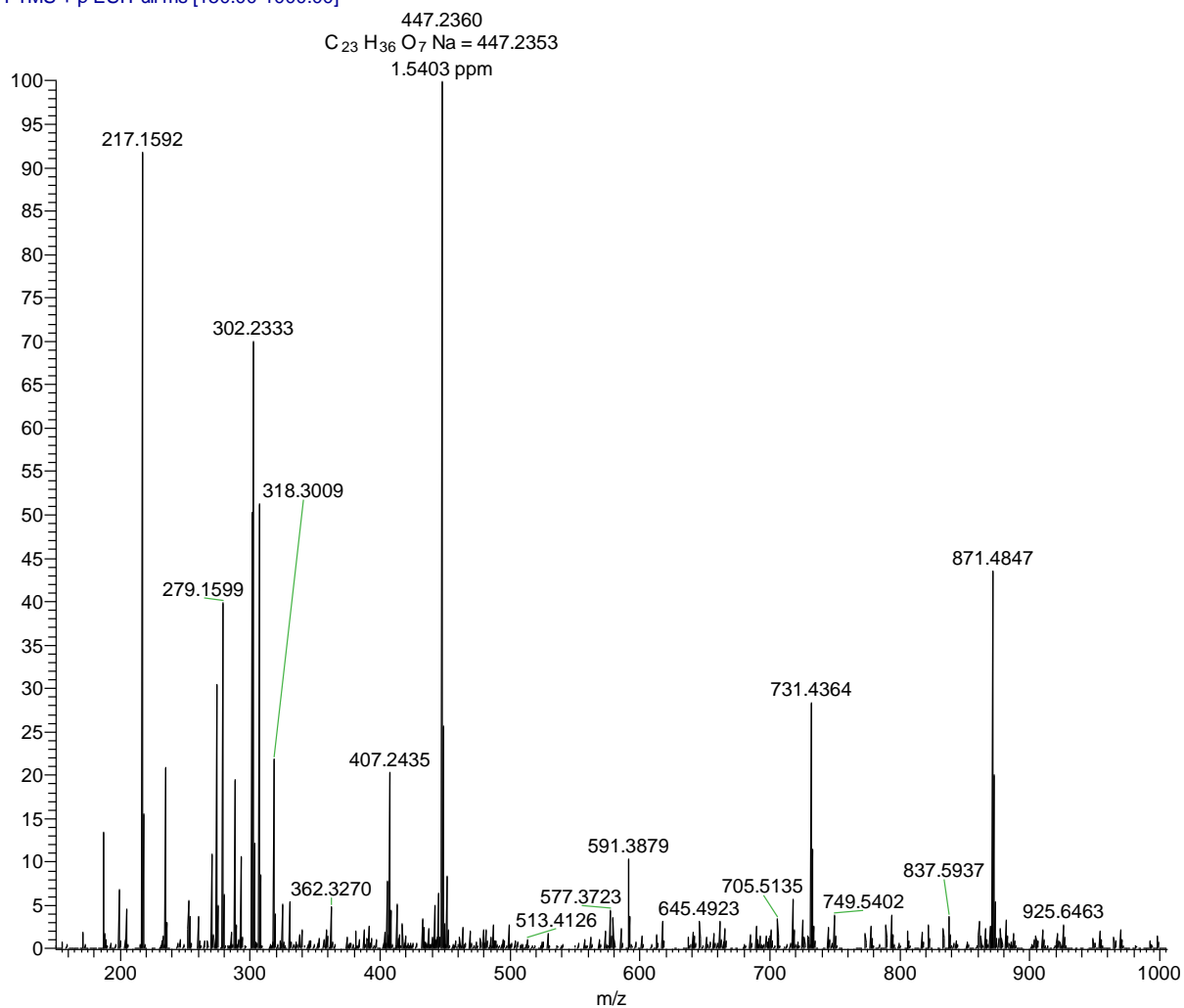


Figure S2: HRESIMS spectrum of **1b**

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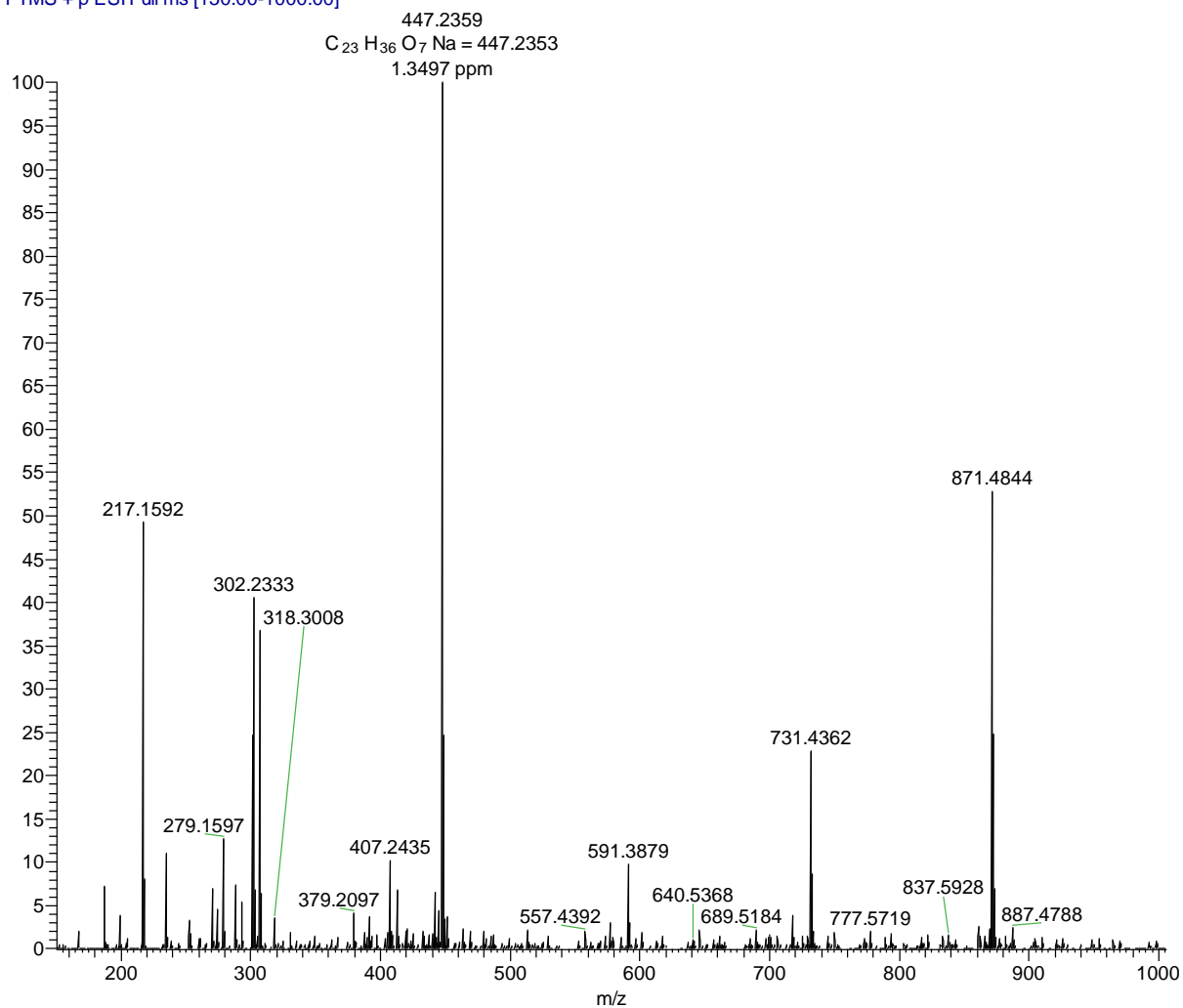
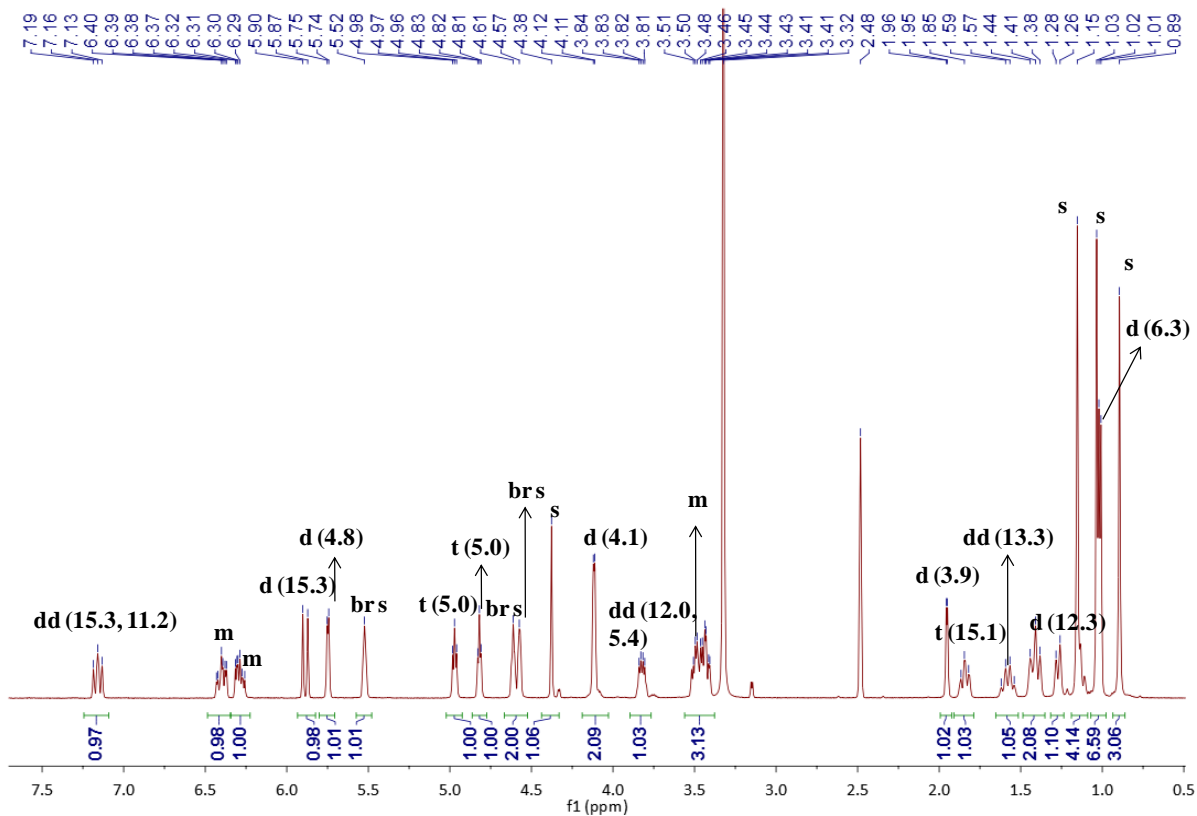
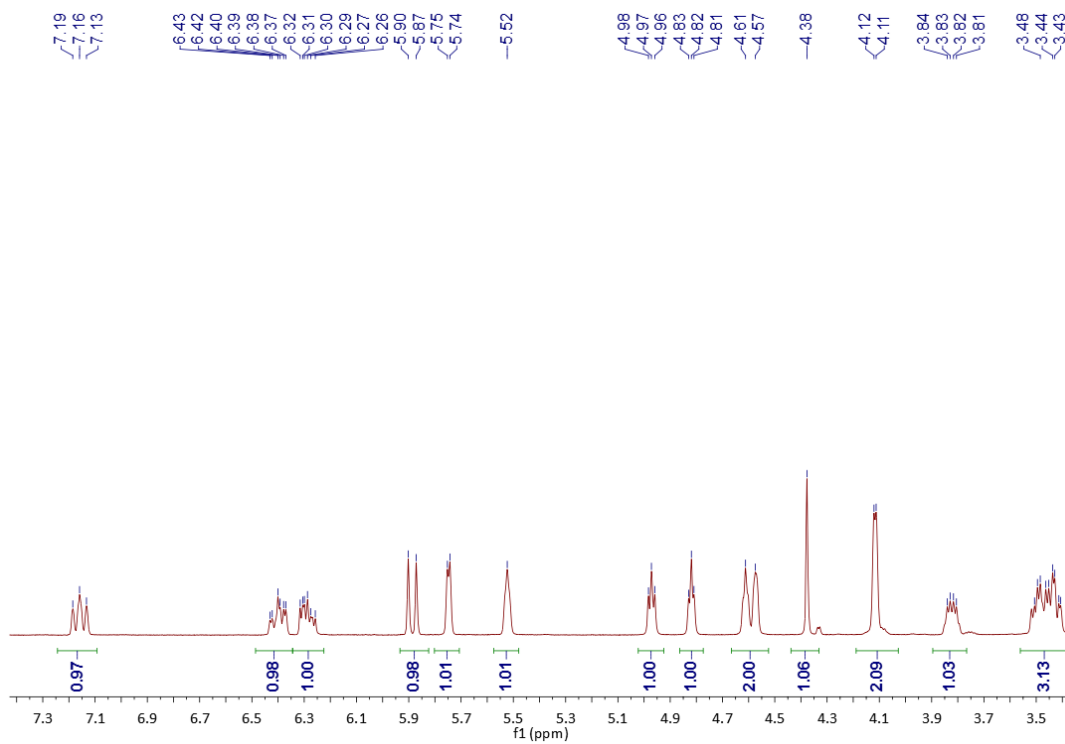


Figure S3: HRESIMS spectrum of **1c**



**Figure S4:**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of **1**



**Figure S5:** Enlarged  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of **1**

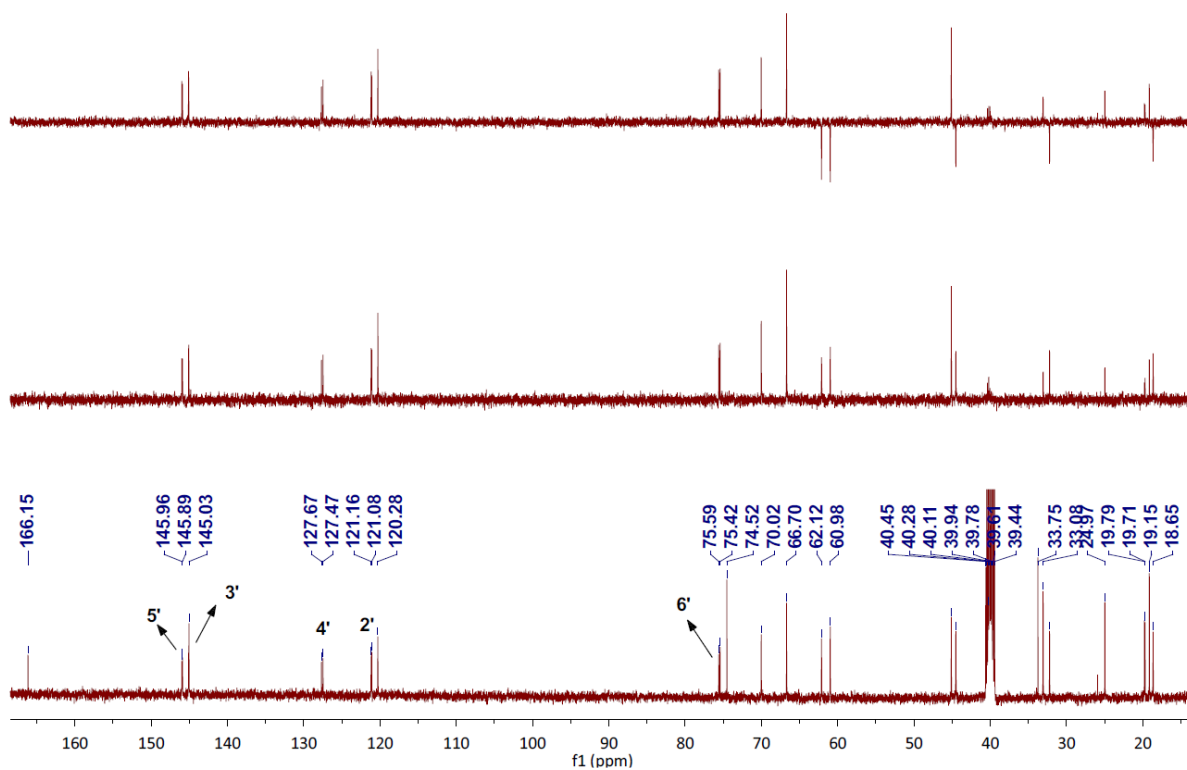


Figure S6:  $^{13}\text{C}$  NMR and DEPT (125 MHz,  $\text{DMSO-}d_6$ ) spectra of **1**

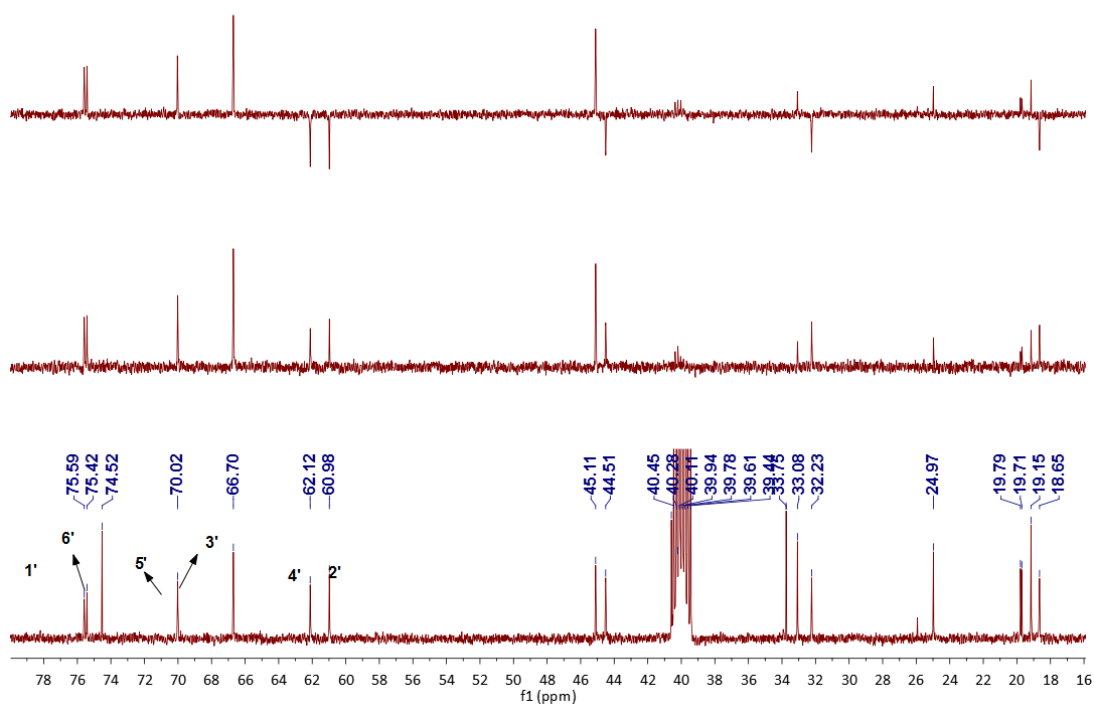


Figure S7: Enlarged  $^{13}\text{C}$  NMR and DEPT (125 MHz,  $\text{DMSO-}d_6$ ) spectra of **1**

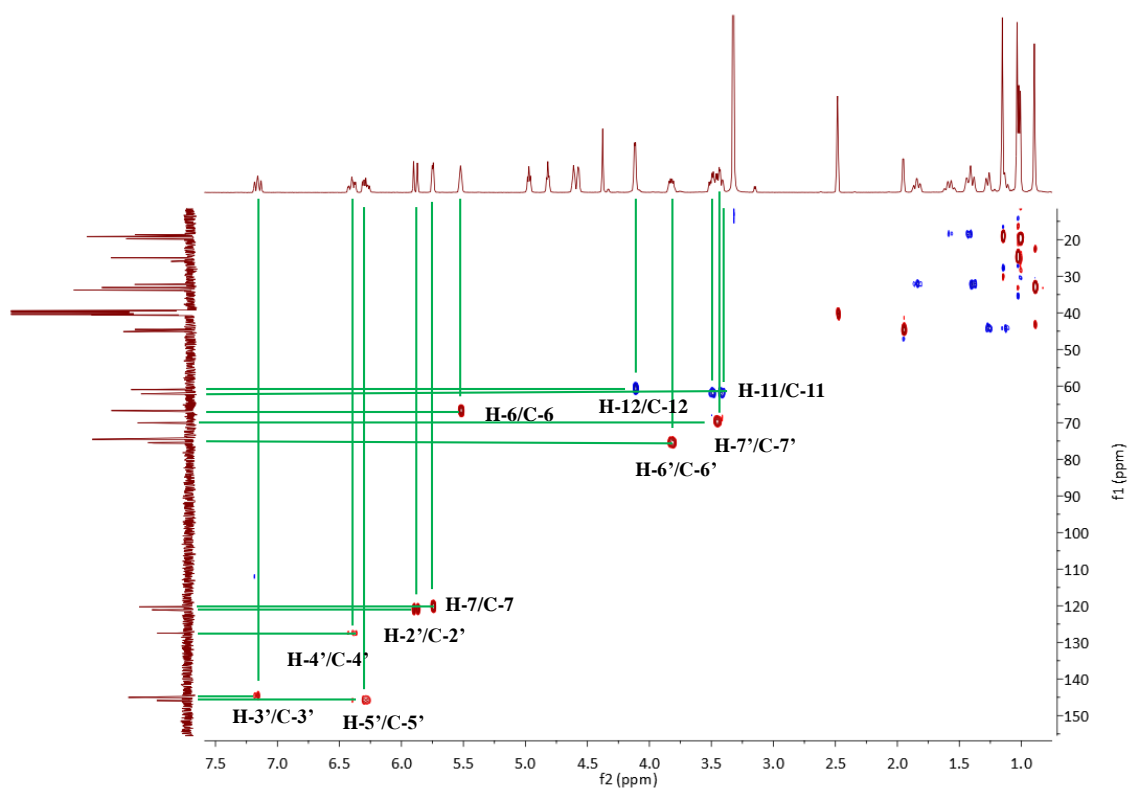


Figure S8: HSQC spectrum of 1

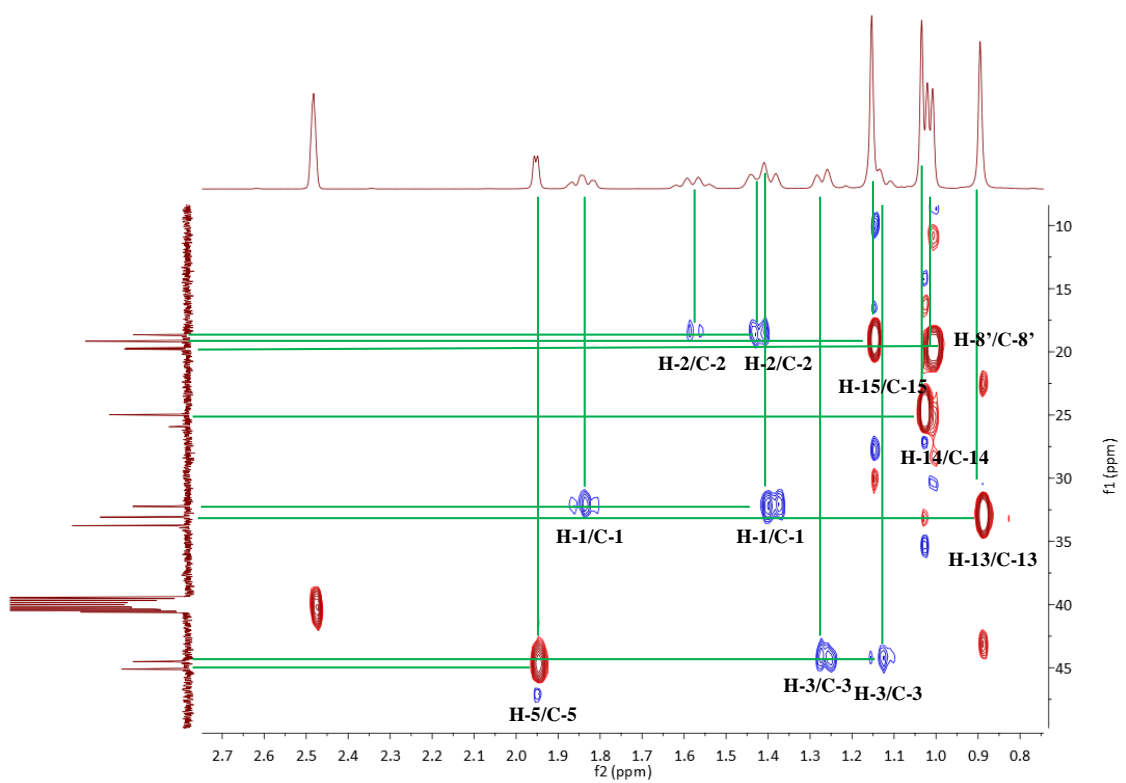
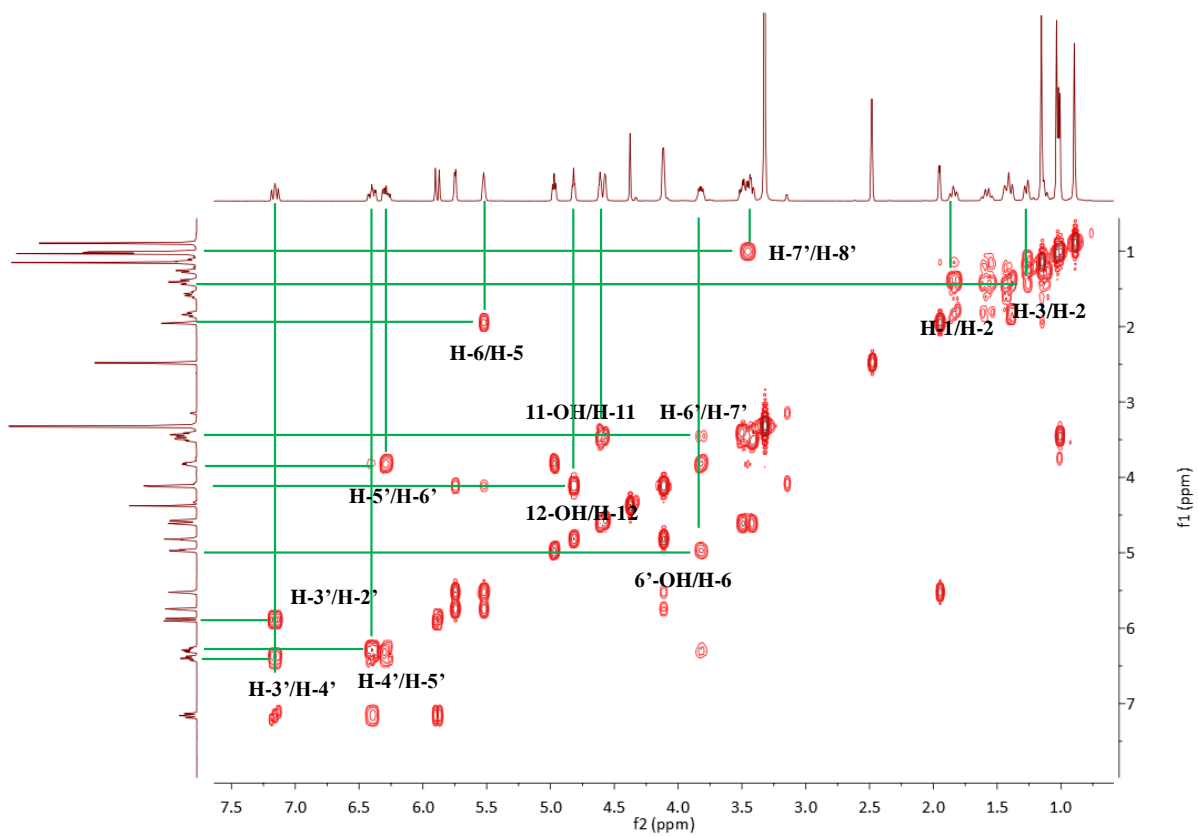


Figure S9: Enlarged HSQC spectrum of 1



**Figure S10:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**



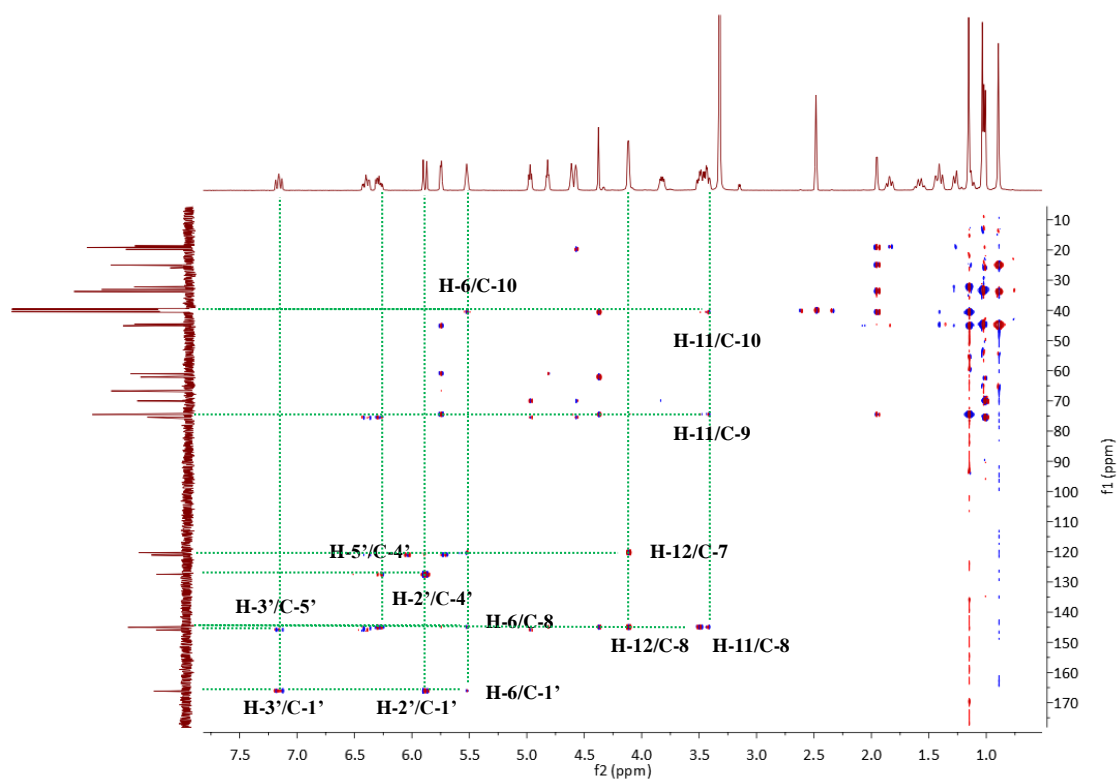


Figure S11: HMBC spectrum of **1**

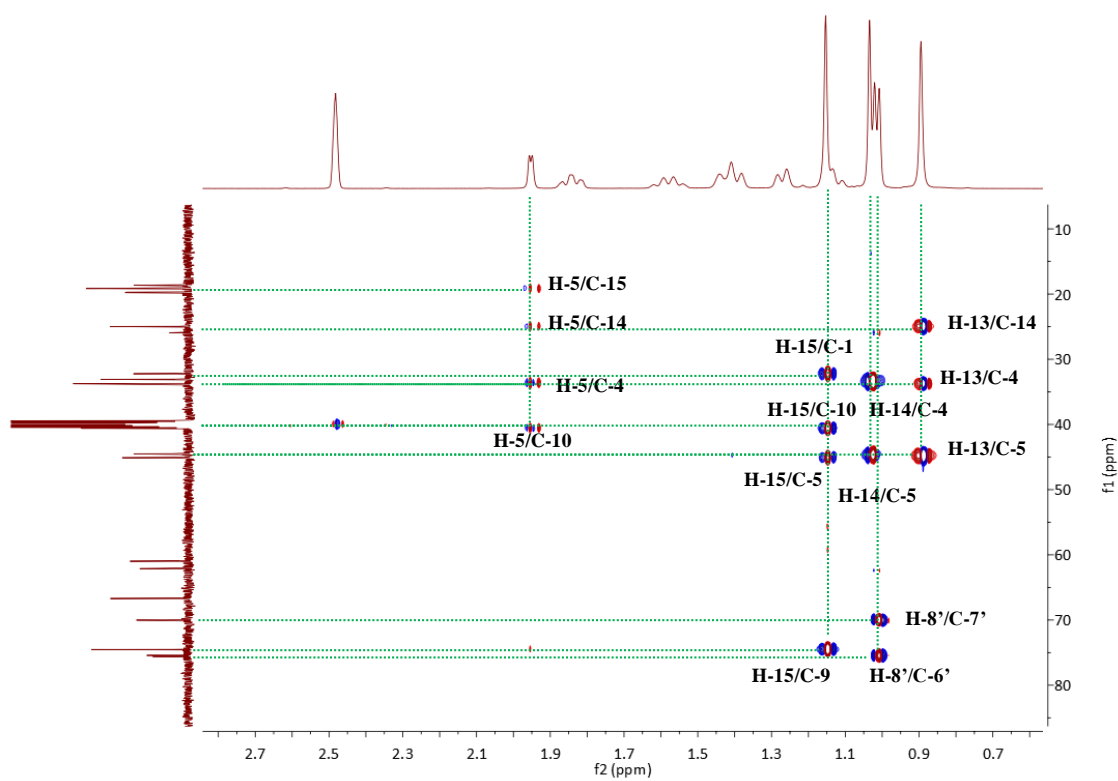
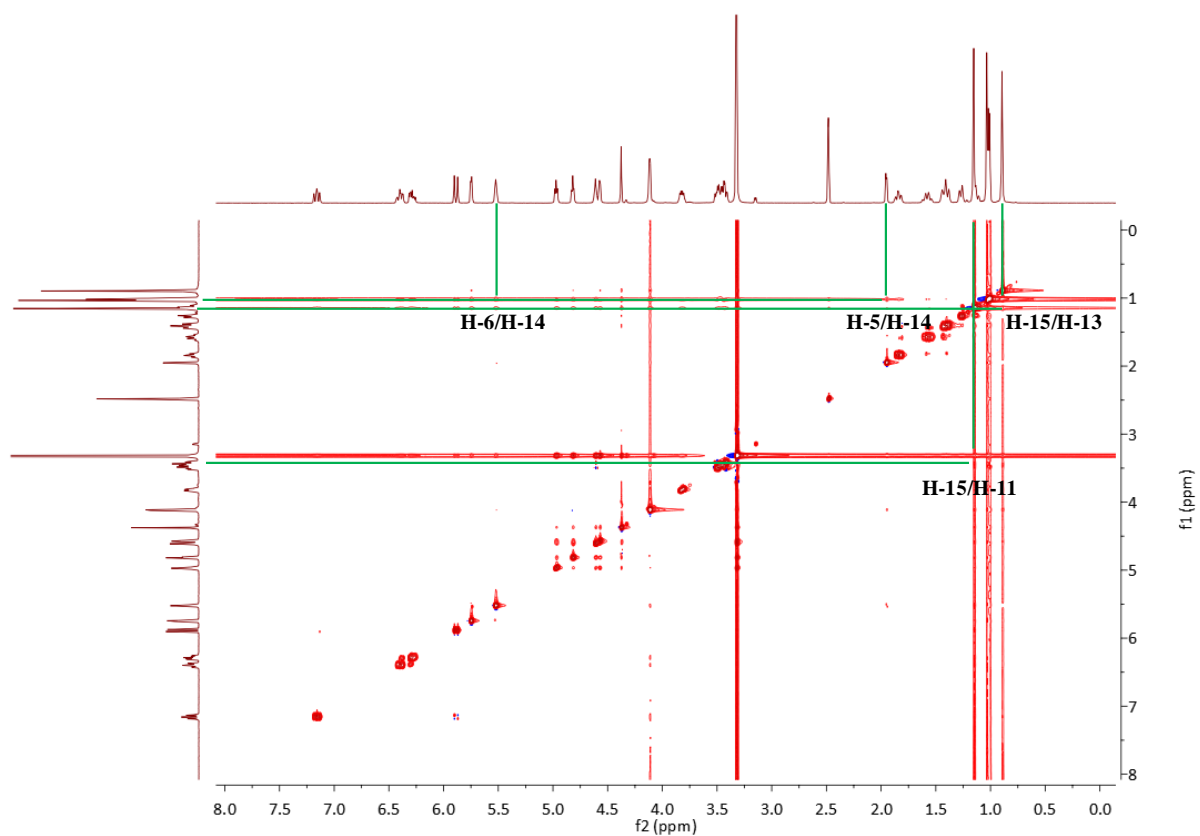


Figure S12: Enlarged HMBC spectrum of **1**



**Figure S13:** NOESY spectrum of **1**

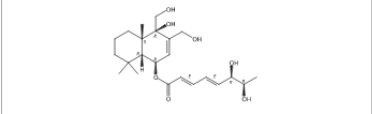
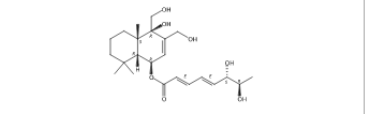
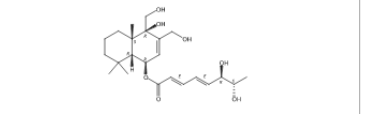
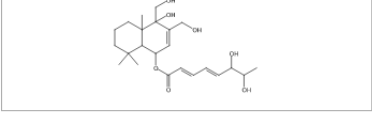
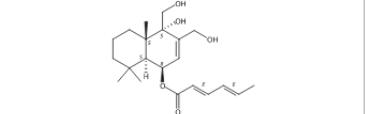
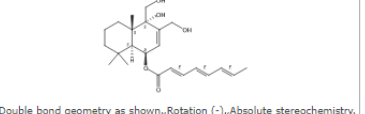
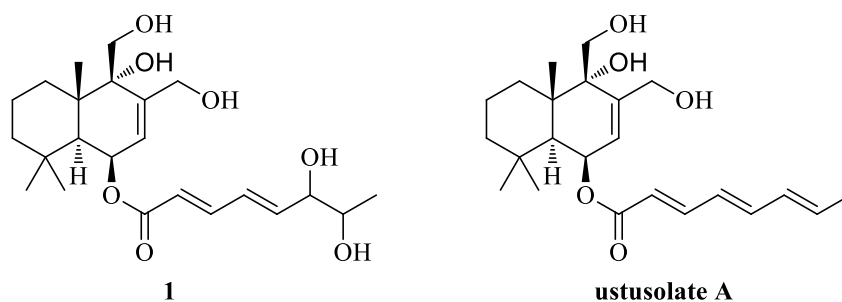
<p>Score: ≥ 99 1. 1175635-93-4</p>  <p>Double bond geometry as shown, Absolute stereochemistry.</p> <p><b>C23 H36 O7</b> 2,4-Octadienoic acid, 6,7-dihydroxy-, (1R,4R,4a,5,8aR)-1,4,4a,5,6,7,8,8a-octahydro-4-hydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-1-naphthalenyl ester, (2E,4E,6R,7R)-</p> <p>▶ Key Physical Properties</p>	<p>Score: ≥ 99 2. 1175883-16-5</p>  <p>Double bond geometry as shown, Absolute stereochemistry.</p> <p><b>C23 H36 O7</b> 2,4-Octadienoic acid, 6,7-dihydroxy-, (1R,4R,4a,5,8aR)-1,4,4a,5,6,7,8,8a-octahydro-4-hydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-1-naphthalenyl ester, (2E,4E,6S,7R)-</p> <p>▶ Key Physical Properties</p>	<p>Score: ≥ 99 3. 1176542-42-9</p>  <p>Double bond geometry as shown, Absolute stereochemistry.</p> <p><b>C23 H36 O7</b> 2,4-Octadienoic acid, 6,7-dihydroxy-, (1R,4R,4a,5,8aR)-1,4,4a,5,6,7,8,8a-octahydro-4-hydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-1-naphthalenyl ester, (2E,4E,6R,7S)-</p> <p>▶ Key Physical Properties</p>
<p>Score: ≥ 99 4. 1217875-41-6</p>  <p><b>C23 H36 O7</b> 2,4-Octadienoic acid, 6,7-dihydroxy-, 1,4,4a,5,6,7,8,8a-octahydro-4-hydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-1-naphthalenyl ester</p> <p>▶ Key Physical Properties</p>	<p>Score: 95 5. 1136245-81-2</p>  <p>Double bond geometry as shown, Absolute stereochemistry.</p> <p><b>C21 H32 O5</b> 2,4-Hexadienoic acid, (1R,4S,4a,5,8a,5)-1,4,4a,5,6,7,8,8a-octahydro-4-hydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-1-naphthalenyl ester, (2E,4E)-</p> <p>▶ Key Physical Properties</p>	<p>Score: 95 6. 1136611-58-9</p>  <p>Double bond geometry as shown, Rotation (-), Absolute stereochemistry.</p> <p><b>C23 H34 O5</b> 2,4,6-Octatrienoic acid, (1R,4S,4a,5,8a,5)-1,4,4a,5,6,7,8,8a-octahydro-4-hydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-1-naphthalenyl ester, (2E,4E,6E)-</p> <p>▶ Key Physical Properties Spectra</p>

Figure S14: Scifinder search results of 1

**Table S1:** Comparison of the NMR data with ustusolate A [1]

Compound 1 (DMSO- <i>d</i> <sub>6</sub> )			Ustusolate A (DMSO- <i>d</i> <sub>6</sub> )		
No.	$\delta_{\text{H}}$ (mult., <i>J</i> in Hz)	$\delta_{\text{C}}$ , type	No.	$\delta_{\text{H}}$ (mult., <i>J</i> in Hz)	$\delta_{\text{C}}$ , type
1	1.84, t (15.1); 1.41, m	32.2, CH <sub>2</sub>	1	1.86, dt (13.3, 3.7); 1.43, m	31.8, CH <sub>2</sub>
2	1.58, dd (13.3); 1.41, m	18.6, CH <sub>2</sub>	2	1.60, m; 1.44, m	18.2, CH <sub>2</sub>
3	1.27, d (12.3); 1.11, m	44.5, CH <sub>2</sub>	3	1.28, m; 1.17, m	44.1, CH <sub>2</sub>
4		33.7, C	4		33.3, C
5	1.95, d (3.9)	45.4, CH	5	1.97, d (4.6)	44.7, CH
6	5.52, br s	66.7, CH	6	5.54, d (4.4)	66.2, CH
7	5.75, d (4.8)	120.3, CH	7	5.77, d (5.0)	120.0, CH
8		145.1, C	8		144.5, C
9		74.5, C	9		74.1, C
10		40.6, C	10		40.1, C
11	3.49, m; 3.43, m	62.1, CH <sub>2</sub>	11	3.52, m; 3.45, m	61.7, CH <sub>2</sub>
12	4.12, d (4.1)	61.0, CH <sub>2</sub>	12	4.14, d (5.0)	60.6, CH <sub>2</sub>
13	0.89, s	33.1, CH <sub>3</sub>	13	0.91, s	32.6, CH <sub>3</sub>
14	1.03, s	25.0, CH <sub>3</sub>	14	1.06, s	24.5, CH <sub>3</sub>
15	1.15, s	19.2, CH <sub>3</sub>	15	1.17, s	18.3, CH <sub>3</sub>
1'		166.1, C	1'		165.7, C
2'	5.89, d (15.3)	121.1, CH	2'	5.89, br d (15.1)	120.4, CH
3'	7.16, dd (15.3, 11.2)	145.0, CH	3'	7.19, dd (15.1, 11.5)	144.8, CH
4'	6.40, m	127.7, CH	4'	6.34, dd (14.7, 11.5)	127.6, CH
5'	6.29, m	146.0, CH	5'	6.68, dd (14.7, 11.0)	141.4, CH
6'	3.82, dd (12.0, 5.4)	75.4, CH	6'	6.20, dd (15.1, 11.0)	131.3, CH
7'	3.47, m	70.0, CH	7'	6.01, dq (15.1, 6.9)	135.3, CH
8'	1.01, d (6.3)	19.7, CH <sub>3</sub>	8'	1.79, d (6.9)	18.7, CH <sub>3</sub>
9-OH	4.38, s		9-OH	4.40, s	
11-OH	4.61, br s		11-OH	4.63, t (5.0)	
12-OH	4.82, t (5.0)		12-OH	4.85, t (5.0)	
6'-OH	4.97, d (5.0)		-		
7'-OH	4.57, br s		-		

**References**

[1] Z. Lu, Y. Wang, C. Miao, P. Liu, K. Hong and W. Zhu (2009). Sesquiterpenoids and benzofuranoids from the marine-derived fungus *Aspergillus ustus* 094102, *J. Nat. Prod.* 72, 1761–1767.