

## Supporting Information

*Rec. Nat. Prod.* 18:2 (2024) 245-250

### A New Diphenyl Ether Derivative from an Endolichenic Fungus

#### *Preussia africana*

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## S1. <sup>1</sup>H and <sup>13</sup>C NMR data for compounds 2–6

Barceloneic lactone B (**2**), <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) of compound **2**: δ<sub>H</sub> 7.09 (1H, d, *J* = 2.4 Hz, H-4), 7.57 (1H, t, *J* = 8.3 Hz, H-5), 6.79 (1H, d, *J* = 8.3 Hz, H-6), 6.92 (1H, s, H-10), 5.05 (1H, s, H-14), 4.35 (1H, d, *J* = 8.3 Hz, H-15), 3.86 (3H, s, H-3a), 9.71 (1H, br s, OH-9), 5.15 (1H, t, *J* = 5.7 Hz, OH-15); <sup>13</sup>C NMR (600 MHz, DMSO-*d*<sub>6</sub>): 166.8 (C-1), 115.6 (C-2), 157.2 (C-3), 110.0 (C-4), 134.3 (C-5), 114.7 (C-6), 152.8 (C-7), 142.8 (C-8), 149.1 (C-9), 116.2 (C-10), 139.7 (C-11), 117.8 (C-12), 68.9 (C-14), 62.6 (C-15), 56.7 (C-3a).

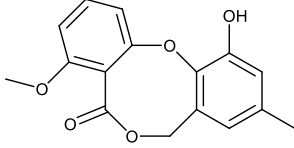
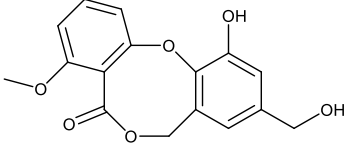
Quercilolin (**3**), <sup>1</sup>H NMR (600 MHz, Aceton-*d*<sub>6</sub>) of compound **3**: δ<sub>H</sub> 6.34 (1H, d, *J* = 1.8 Hz, H-2), 6.21 (1H, d, *J* = 2.0 Hz, H-6), 6.28 (1H, s, H-2'), 6.12 (1H, s, H-4'), 6.02 (1H, s, H-6'), 3.74 (1H, s, 4-OMe), 2.17 (1H, s, 5'-Me), 2.02 (1H, s, 5-Me); <sup>13</sup>C NMR (150 MHz, Aceton-*d*<sub>6</sub>) δ: 134.0 (C-1), 100.1 (C-2), 150.6 (C-3), 157.3 (C-4), 133.4 (C-5), 106.7 (C-6), 139.9 (C-1'), 99.1 (C-2'), 159.5 (C-3'), 106.8 (C-4'), 158.4 (C-5'), 109.3 (C-6'), 54.7 (4-OMe), 20.7 (5'-Me), 15.6 (5-Me).

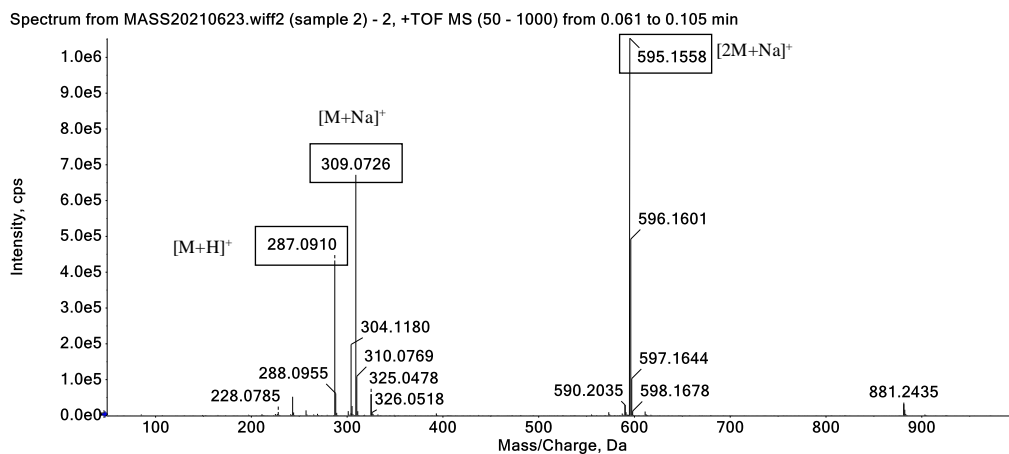
3-hydroxy-5-methylphenyl ether (**4**), <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) of compound **4**: δ<sub>H</sub> 6.39 (1H, d, *J* = 2.5 Hz, H-3'), 6.31 (1H, s, H-4), 6.29 (1H, d, *J* = 2.5 Hz, H-5'), 6.26 (1H, s, H-6), 6.10 (1H, s, H-2), 2.21 (3H, s, 4'-Me), 2.01 (3H, s, 3-Me); <sup>13</sup>C NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: 159.6 (C-5), 158.2 (C-1'), 157.6 (C-6'), 150.4 (C-2'), 139.7 (C-3), 134.1 (C-1), 130.2 (C-4'), 109.4 (C-4), 107.0 (C-6), 107.0 (C-2), 100.2 (C-3'), 99.0 (C-5'), 21.7 (3-Me), 16.5 (4'-Me).

2,2',3,4'-tetrahydroxy-5,6'-dimethyldiphenyl ether (**5**), <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) of compound **5**: δ<sub>H</sub> 6.35 (1H, d, *J* = 3.0 Hz, H-3'), 6.29 (1H, d, *J* = 3.0 Hz, H-5'), 6.21 (1H, d, *J* = 1.2 Hz, H-6), 5.62 (1H, d, *J* = 1.2 Hz, H-4), 3.69 (3H, s, 4'-OMe), 2.00 (3H, s, 6'-Me), 1.97 (3H, s, 5-Me); <sup>13</sup>C NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: 156.2 (C-4'), 150.6 (C-2'), 146.8 (C-3), 146.1 (C-1), 134.4 (C-1'), 132.3 (C-6'), 131.6 (C-2), 126.8 (C-5), 109.8 (C-6), 106.0 (C-5'), 104.9 (C-4), 100.4 (C-3'), 55.0 (4'-OMe), 20.8 (5-Me), 16.1 (6'-Me).

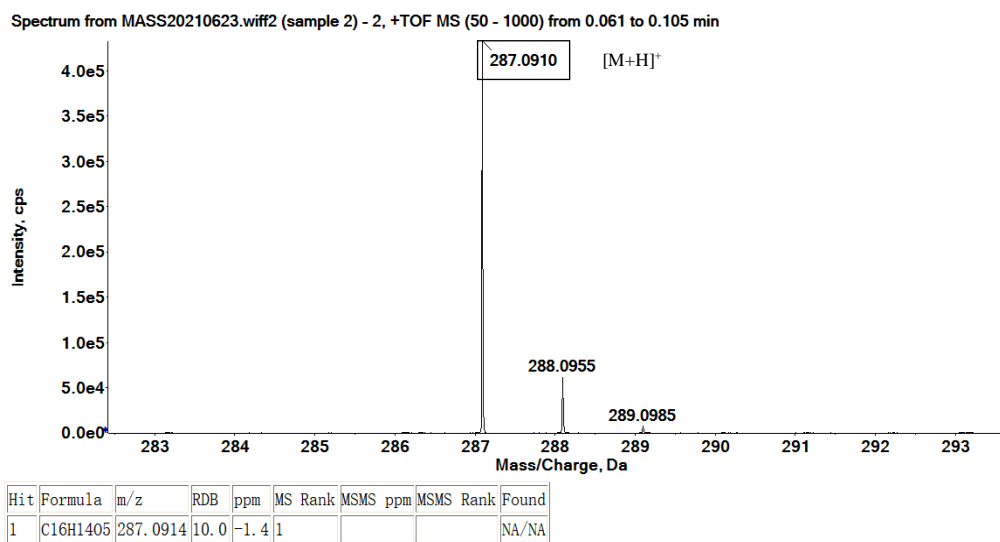
1,3,6-trihydroxy-8-methyl-9H-xanthen-9-one (**6**), <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) of compound **6**: δ<sub>H</sub> 6.64 (1H, d, *J* = 2.3 Hz, H-5), 6.62 (1H, dd, *J* = 1.1, 2.4 Hz, H-7), 6.26 (1H, d, *J* = 2.2 Hz, H-4), 6.11 (1H, d, *J* = 2.2 Hz, H-2), 2.72 (3H, s, 8-Me); <sup>13</sup>C NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: 181.8 (C-9), 165.5 (C-3), 163.7 (C-1), 163.5 (C-6), 159.3 (C-10a), 157.0 (C-4a), 143.2 (C-8), 116.8 (C-7), 111.1 (C-8a), 102.5 (C-9a), 100.1 (C-5), 98.3 (C-2), 93.7 (C-4), 23.5 (8-Me).

**Table S1:** Comparison of NMR data between compound **1** and barceloneic lactone B in DMSO-*d*<sub>6</sub>

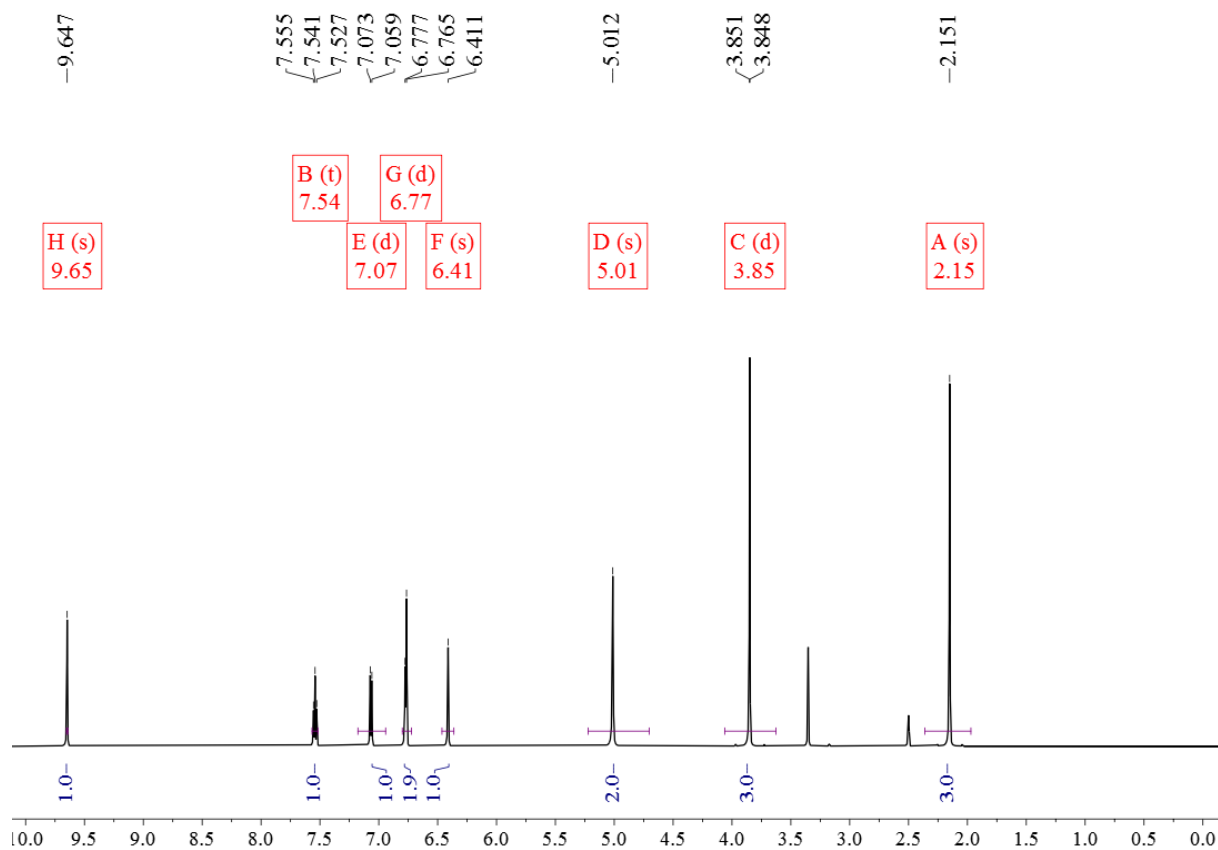
No.				
	$\delta_{\text{H}}$ (integral, mult., <i>J</i> in Hz)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ (integral, mult., <i>J</i> in Hz)	$\delta_{\text{C}}$
1	-	166.3	-	166.8
2	-	115.1	-	115.6
3	-	156.7	-	157.2
4	7.07 (1H, d, <i>J</i> = 8.4 Hz)	109.5	7.09 (1H, d, <i>J</i> = 8.3 Hz)	110.0
5	7.54 (1H, t, <i>J</i> = 8.4 Hz)	133.8	7.57 (1H, t, <i>J</i> = 8.3 Hz)	134.3
6	6.77 (1H, d, <i>J</i> = 8.4 Hz, overlapped)	114.3	6.79 (1H, d, <i>J</i> = 8.3 Hz)	114.7
7	-	152.3	-	152.8
8	-	141.6	-	142.8
9	-	148.5	-	149.1
10	6.77 (1H, br s)	118.2	6.92 (1H, s)	116.2
11	-	134.0	-	139.7
12	6.41 (1H, br s)	119.9	6.56 (1H, s)	117.8
13	-	127.3	-	127.7
14	5.01 (2H, s)	68.4	5.05 (2H, s)	68.9
15	2.15 (3H, s)	20.4	4.35 (2H, d, <i>J</i> = 5.7 Hz)	62.6
3- OMe	3.85 (3H, s)	56.2	3.86 (3H, s)	56.7
9-OH	9.65 (s)	-	9.71 (br s)	-
15-OH	-	-	5.15 (t, <i>J</i> = 5.7 Hz)	-



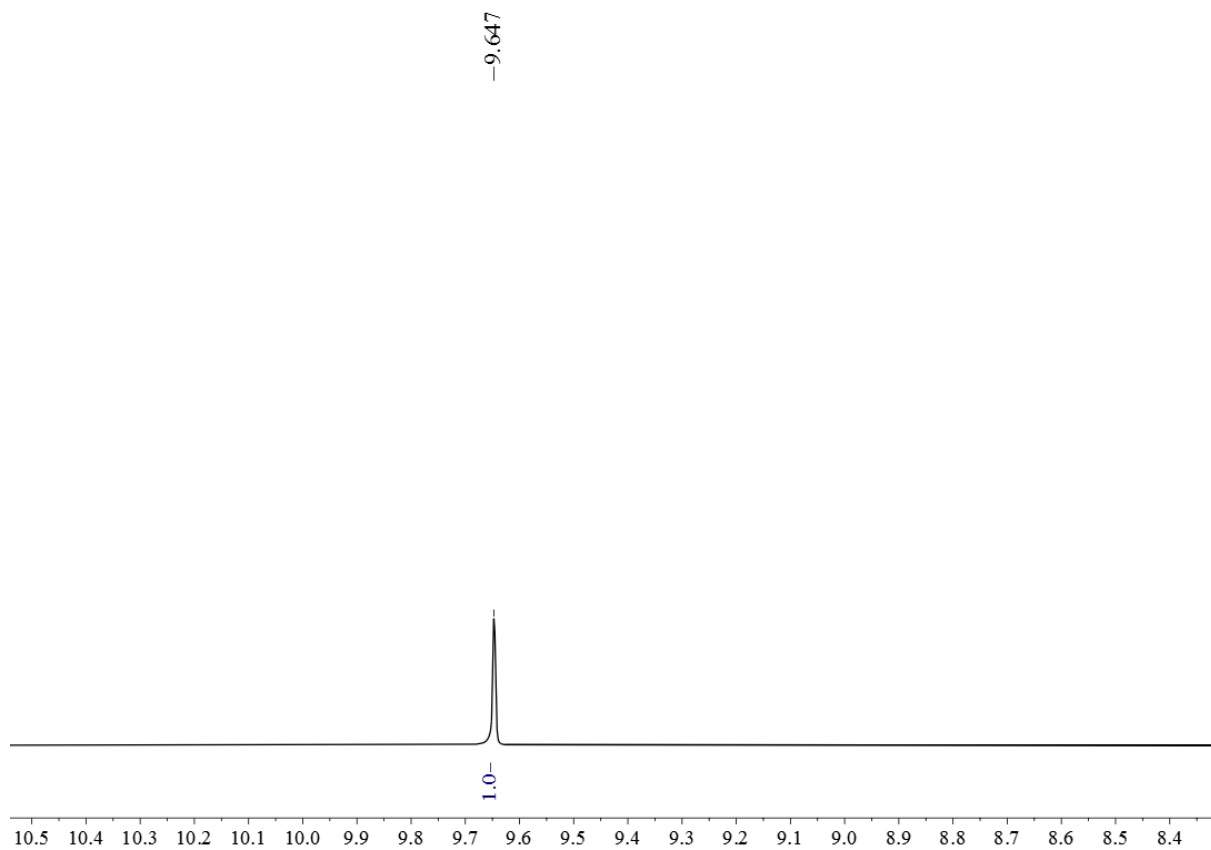
**Figure S1:** HR-ESI-MS spectrum of **1** (barceloneic lactone D) (From 100 Da to 900 Da)



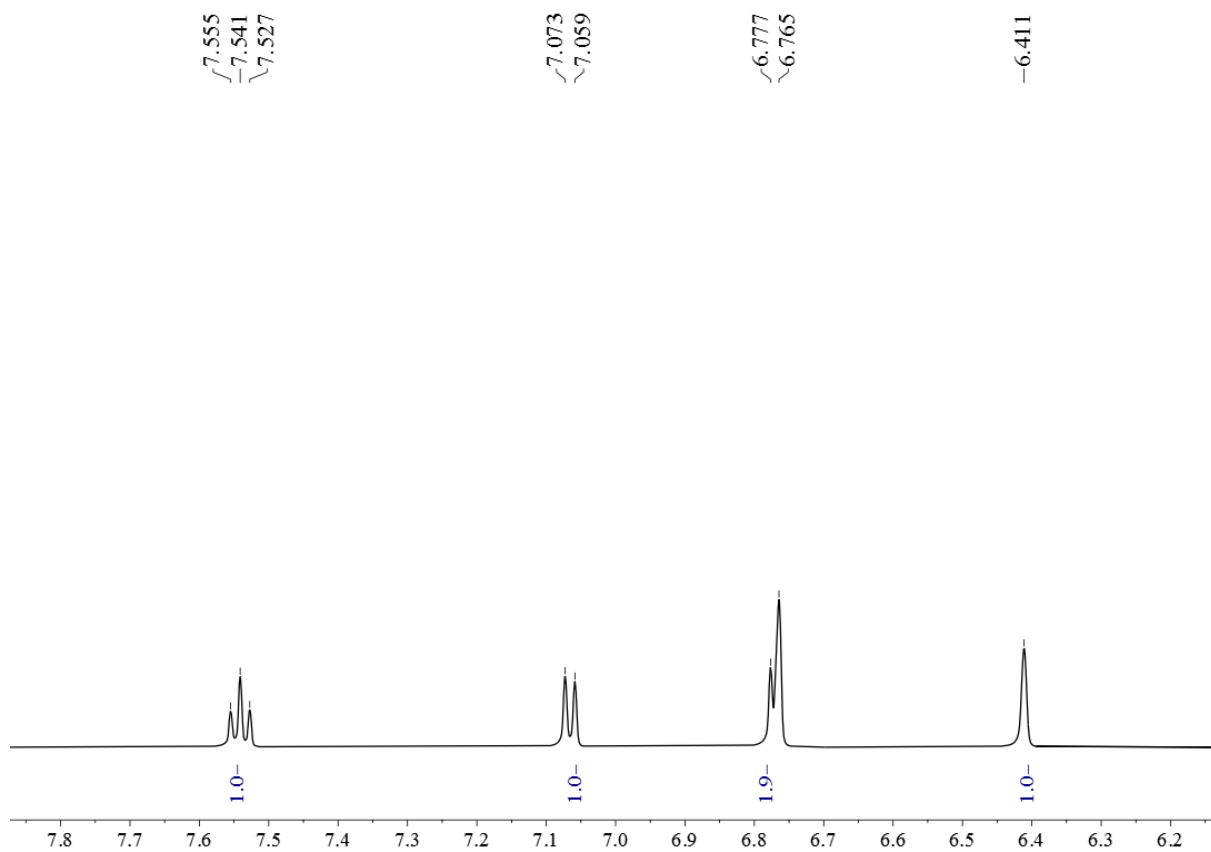
**Figure S2:** HR-ESI-MS spectrum of **1** (barceloneic lactone D) (From 283 Da to 293 Da)



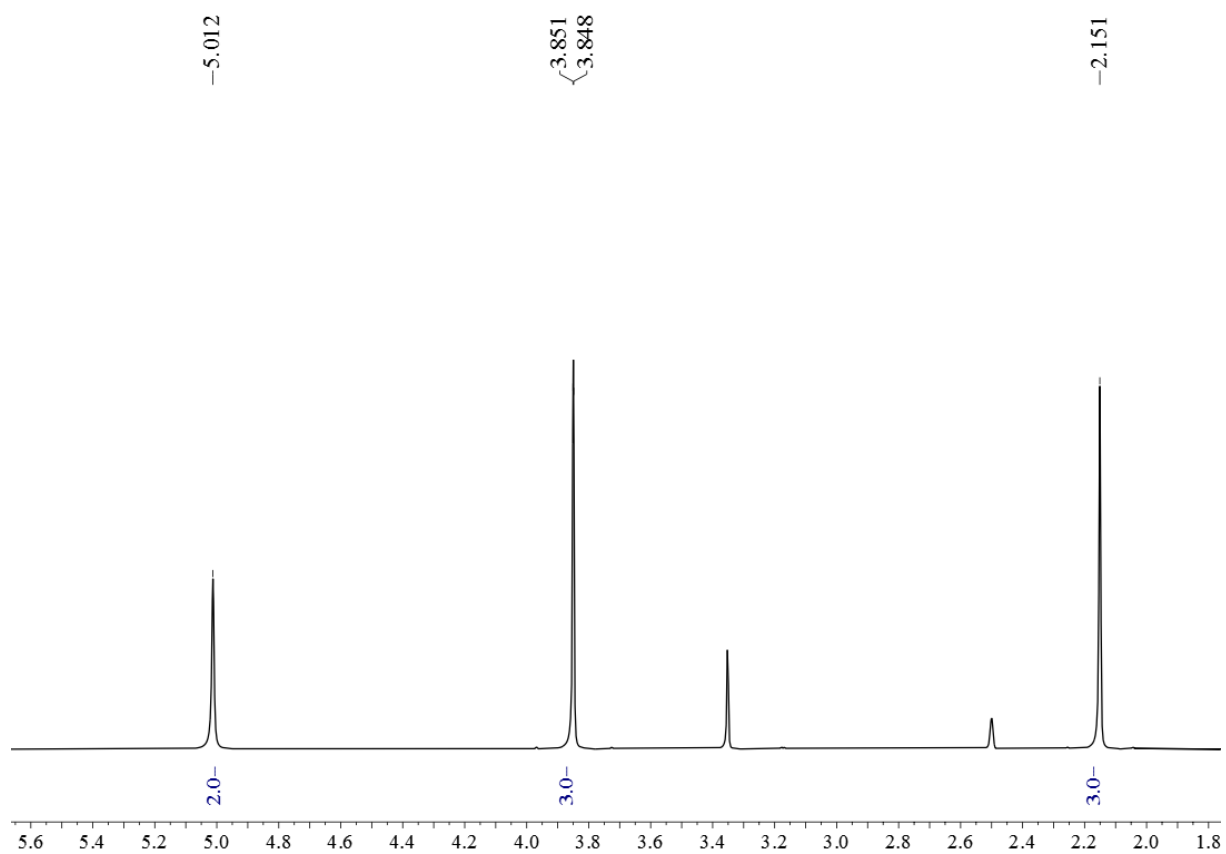
**Figure S3:**  $^1\text{H-NMR}$  (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **1** (barceloneic lactone D)



**Figure S4:** <sup>1</sup>H-NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of **1** (barceloneic lactone D) (From  $\delta_{\text{H}}$  8.4 ppm to 10.5 ppm)

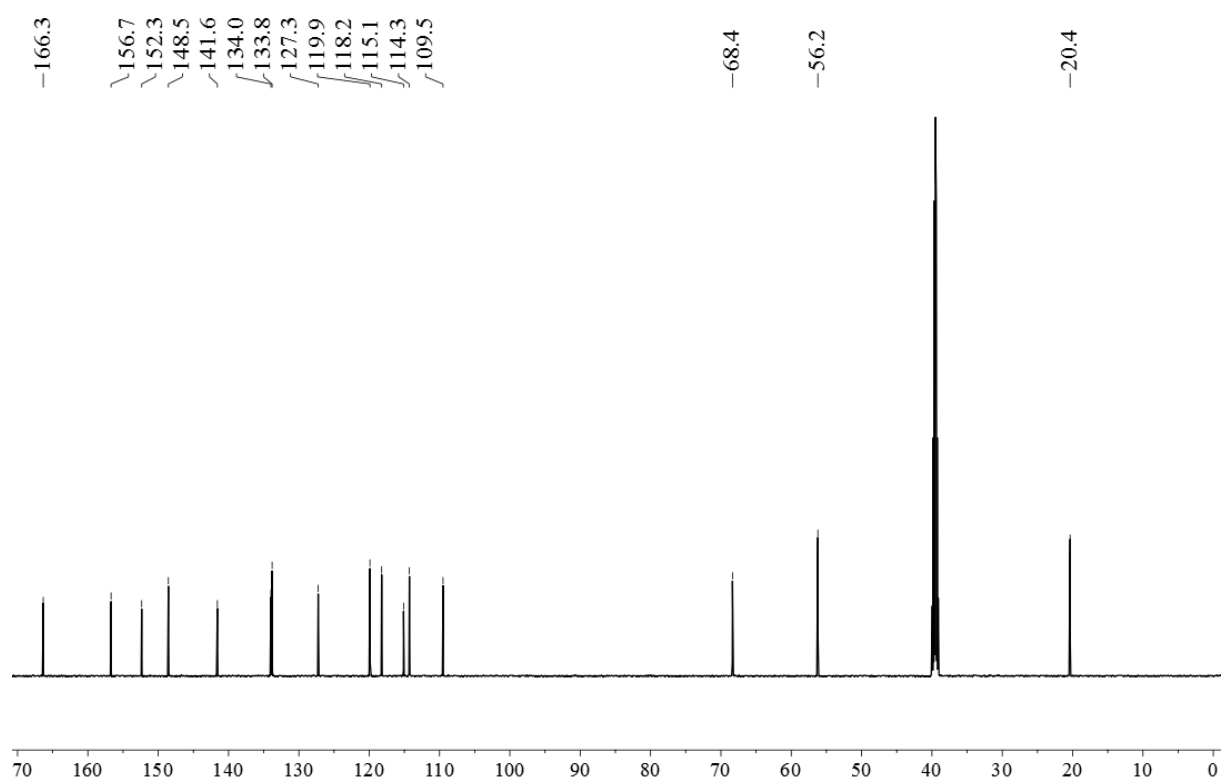


**Figure S5:** <sup>1</sup>H-NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of **1** (barceloneic lactone D) (From  $\delta_{\text{H}}$  6.2 ppm to 7.8 ppm)

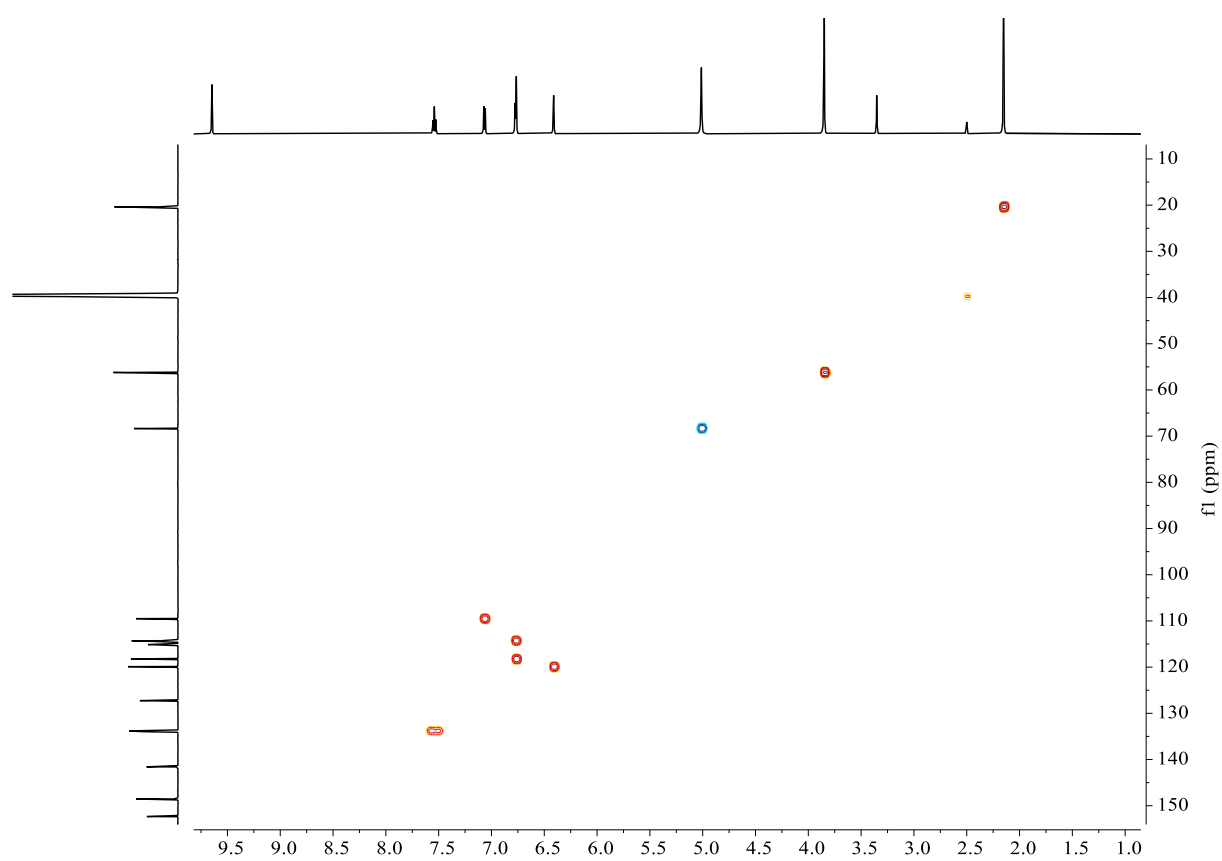


**Figure S6:** <sup>1</sup>H-NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of **1** (barceloneic lactone D) (From  $\delta_{\text{H}}$  1.8 ppm to 5.6 ppm)

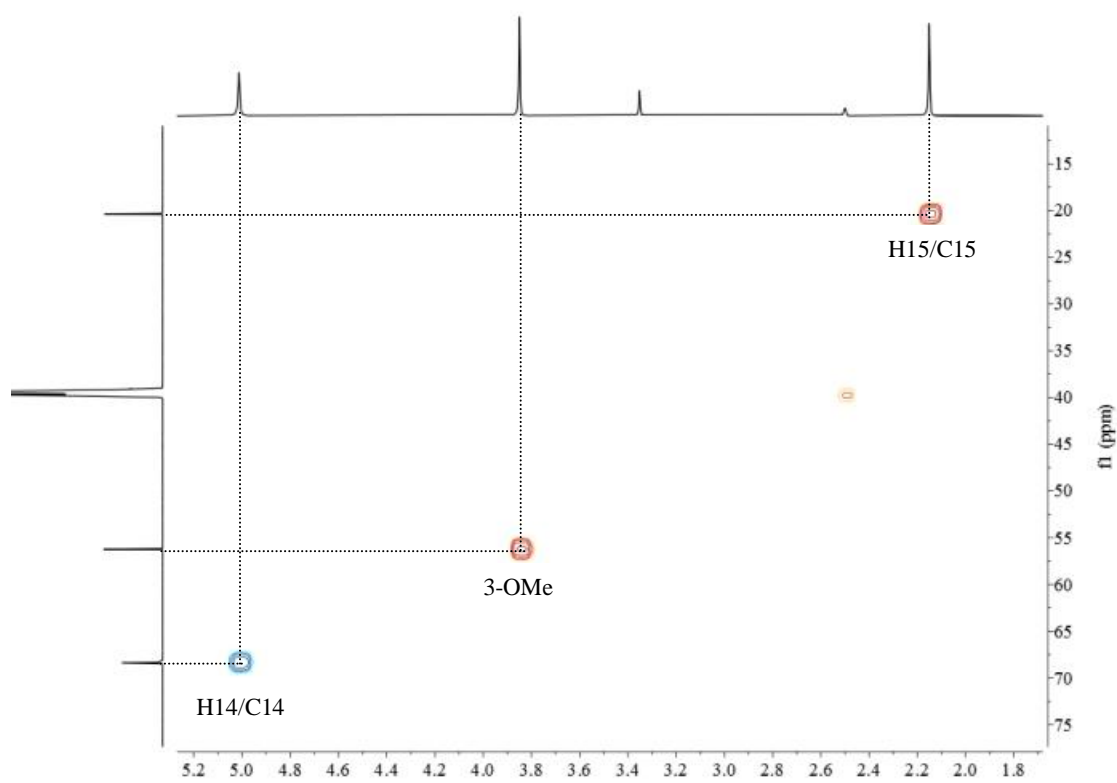




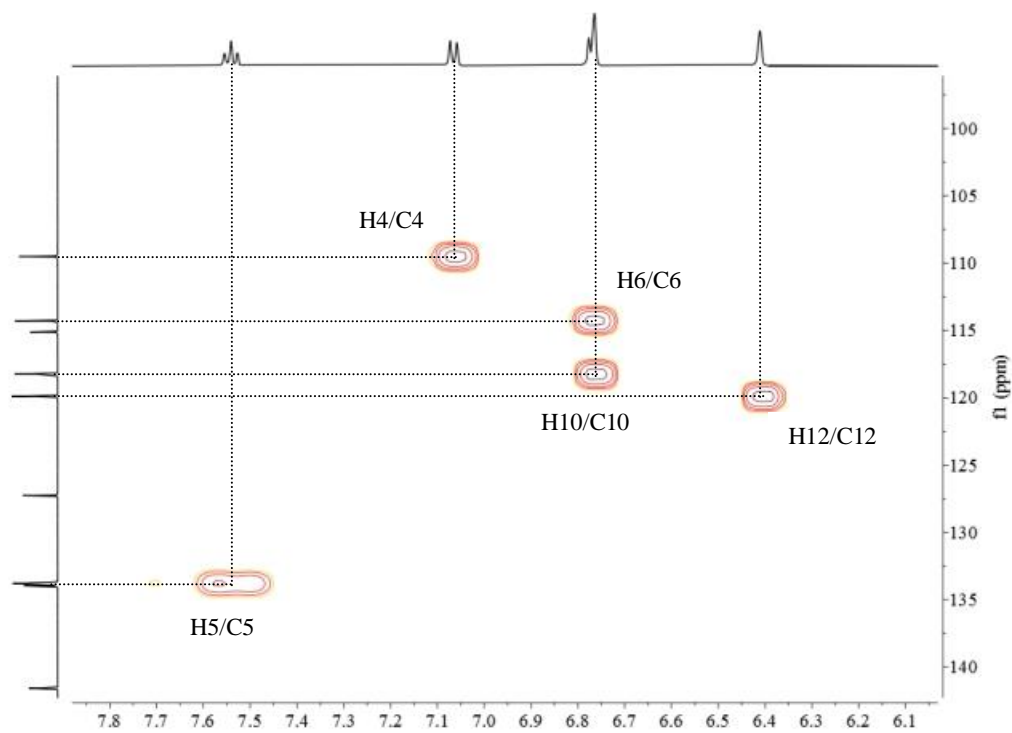
**Figure S7:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **1** (barceloneic lactone D)



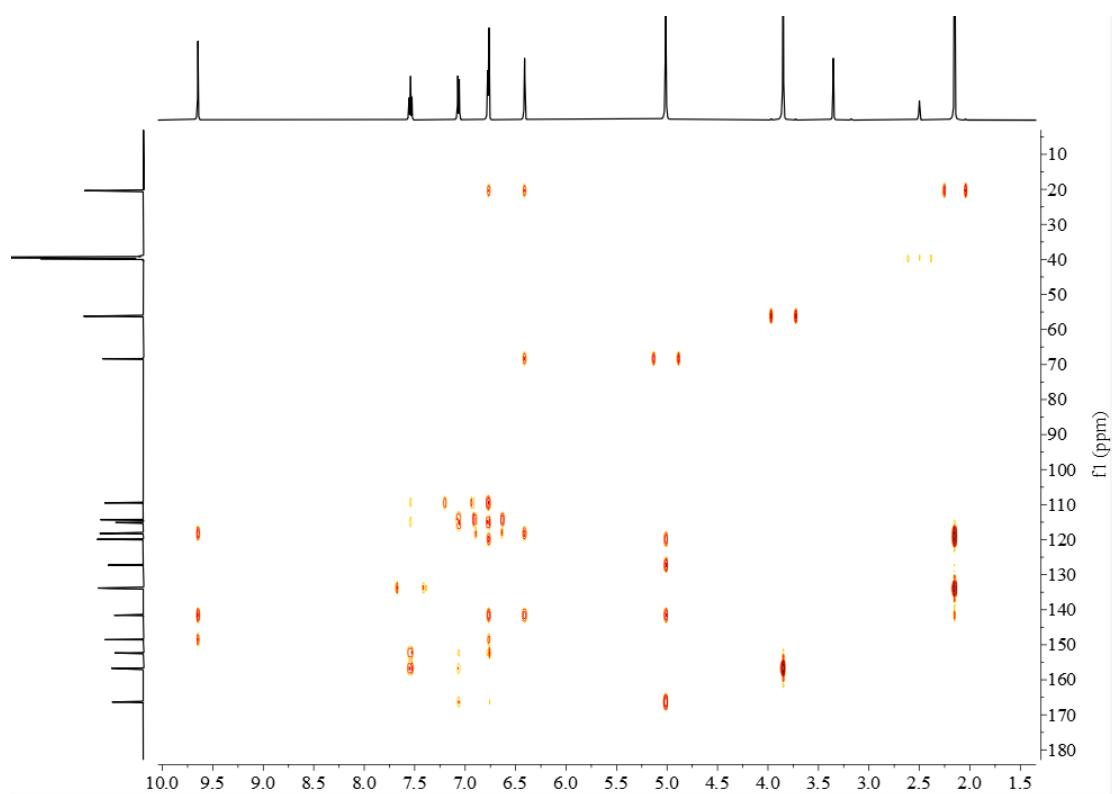
**Figure S8:** HSQC spectrum of **1** (barceloneic lactone D)



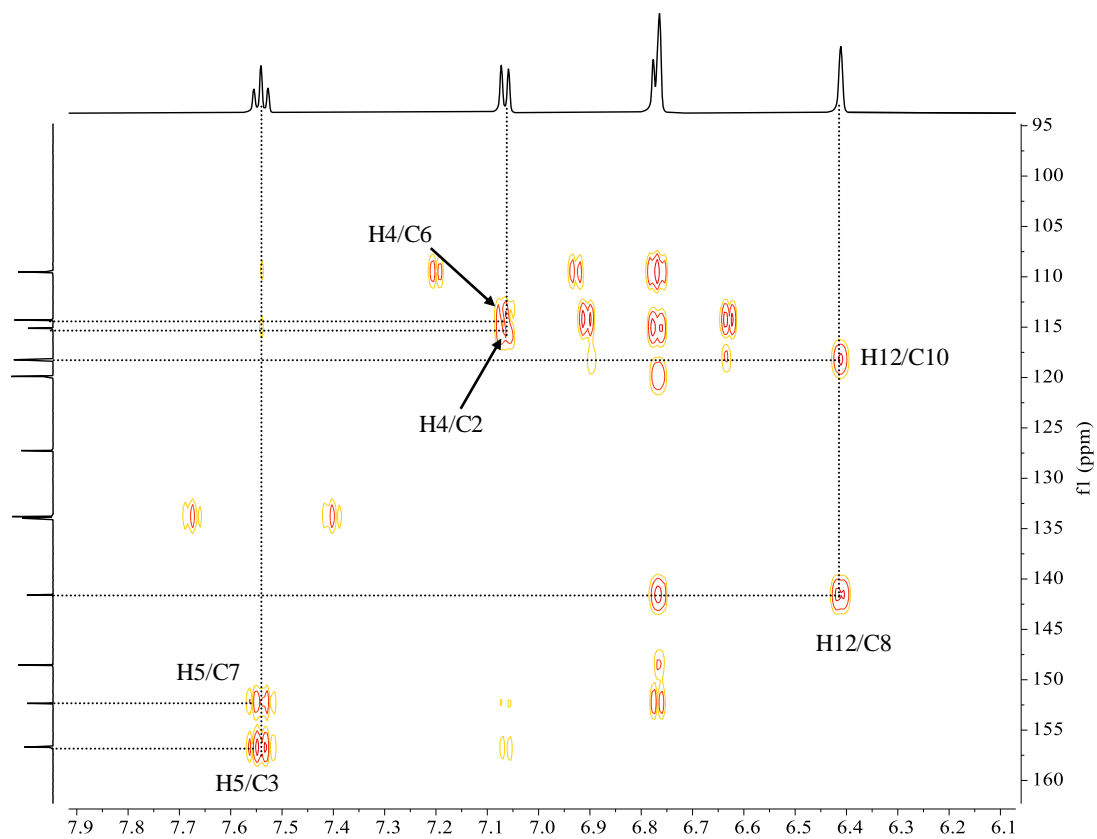
**Figure S9:** HSQC spectrum of **1** (barceloneic lactone D) (From  $\delta_{\text{C}}$  15 ppm to 75 ppm)



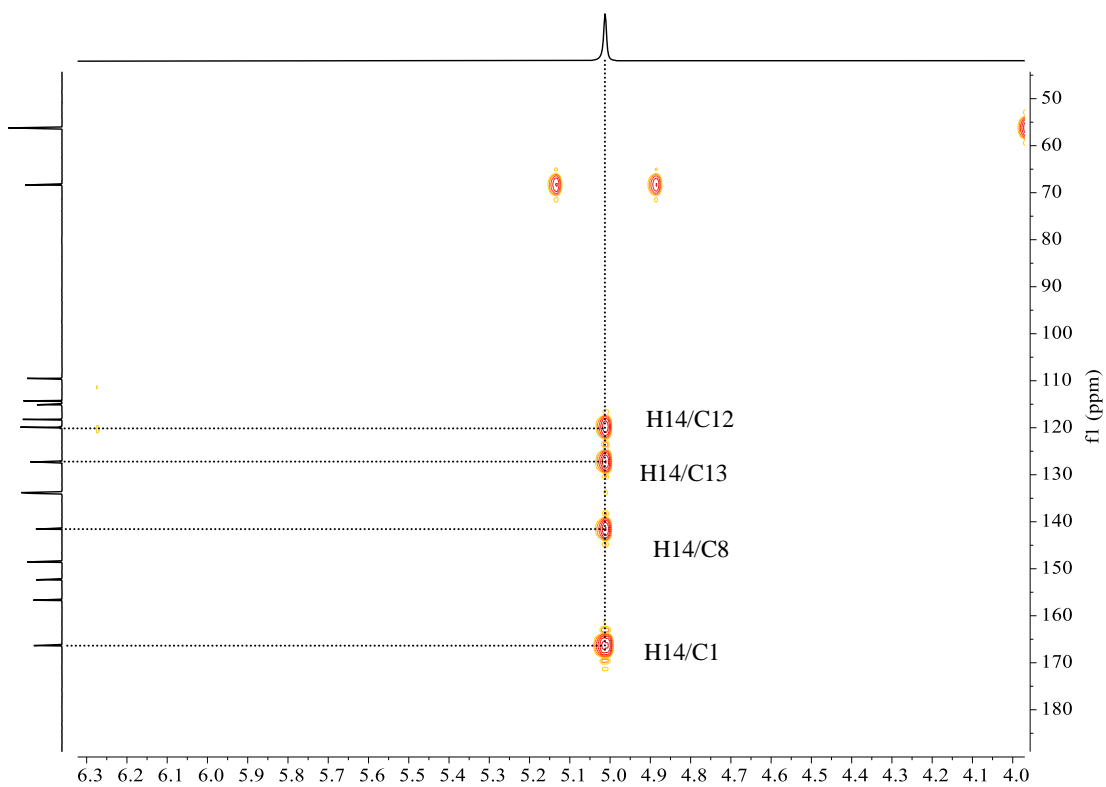
**Figure S10:** HSQC spectrum of **1** (barceloneic lactone D) (From  $\delta_{\text{C}}$  100 ppm to 140 ppm)



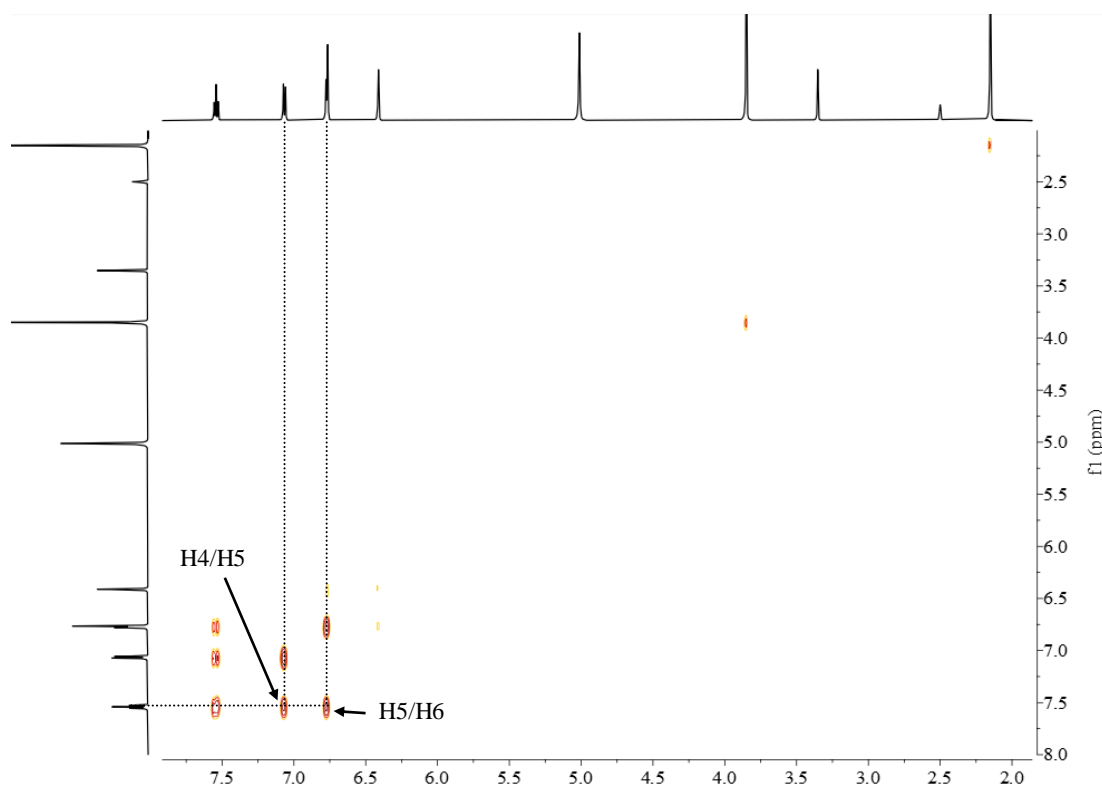
**Figure S11:** HMBC spectrum of **1** (barceloneic lactone D)



**Figure S12:** HMBC spectrum of **1** (barceloneic lactone D) (From  $\delta_C$  95 ppm to 160 ppm)



**Figure S13:** HMBC spectrum of **1** (barceloneic lactone D) (From  $\delta_{\text{C}}$  50 ppm to 180 ppm)

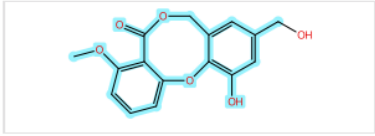
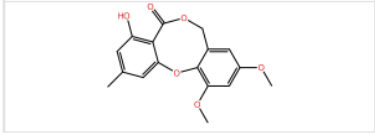


**Figure S14:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** (barceloneic lactone D)



## Substances (7)

[View in SciFinder®](#)

1		Similarity Score: 96																
<p><b>1443221-26-8</b></p>  <p><b>C<sub>16</sub>H<sub>14</sub>O<sub>6</sub></b> 11-Hydroxy-9-(hydroxymethyl)-4-methoxy-5H,7H-dibenzo[<i>b,g</i>][1,5]dioxocin-5-one</p> <p>1 Reference    0 Reactions    0 Suppliers</p>		<table border="1"> <thead> <tr> <th>Key Physical Properties</th> <th>Value</th> <th>Condition</th> </tr> </thead> <tbody> <tr> <td>Molecular Weight</td> <td>302.28</td> <td>-</td> </tr> <tr> <td>Boiling Point (Predicted)</td> <td>604.2±55.0 °C</td> <td>Press: 760 Torr</td> </tr> <tr> <td>Density (Predicted)</td> <td>1.396±0.06 g/cm<sup>3</sup></td> <td>Temp: 20 °C; Press: 760 Torr</td> </tr> <tr> <td>pKa (Predicted)</td> <td>8.21±0.20</td> <td>Most Acidic Temp: 25 °C</td> </tr> </tbody> </table> <p>Spectra</p>		Key Physical Properties	Value	Condition	Molecular Weight	302.28	-	Boiling Point (Predicted)	604.2±55.0 °C	Press: 760 Torr	Density (Predicted)	1.396±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr	pKa (Predicted)	8.21±0.20	Most Acidic Temp: 25 °C
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<p><b>2824125-39-3</b></p>  <p><b>C<sub>17</sub>H<sub>16</sub>O<sub>6</sub></b> 5H,7H-Dibenzo[<i>b,g</i>][1,5]dioxocin-5-one, 4-hydroxy-9,11-dimethoxy-2-methyl-</p> <p>1 Reference    0 Reactions    0 Suppliers</p>		<table border="1"> <thead> <tr> <th>Key Physical Properties</th> <th>Value</th> <th>Condition</th> </tr> </thead> <tbody> <tr> <td>Molecular Weight</td> <td>316.31</td> <td>-</td> </tr> <tr> <td>Boiling Point (Predicted)</td> <td>568.3±50.0 °C</td> <td>Press: 760 Torr</td> </tr> <tr> <td>Density (Predicted)</td> <td>1.302±0.06 g/cm<sup>3</sup></td> <td>Temp: 20 °C; Press: 760 Torr</td> </tr> <tr> <td>pKa (Predicted)</td> <td>7.34±0.20</td> <td>Most Acidic Temp: 25 °C</td> </tr> </tbody> </table>		Key Physical Properties	Value	Condition	Molecular Weight	316.31	-	Boiling Point (Predicted)	568.3±50.0 °C	Press: 760 Torr	Density (Predicted)	1.302±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr	pKa (Predicted)	7.34±0.20	Most Acidic Temp: 25 °C
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**Figure S15:** SciFinder search report for the non dimer version of compound **1** with 90-98 % similarity.