

# Supporting Information

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## Lactones from *Glomerella cingulata* Cultivated in Rice: Structural Studies and Antimicrobial Evaluation

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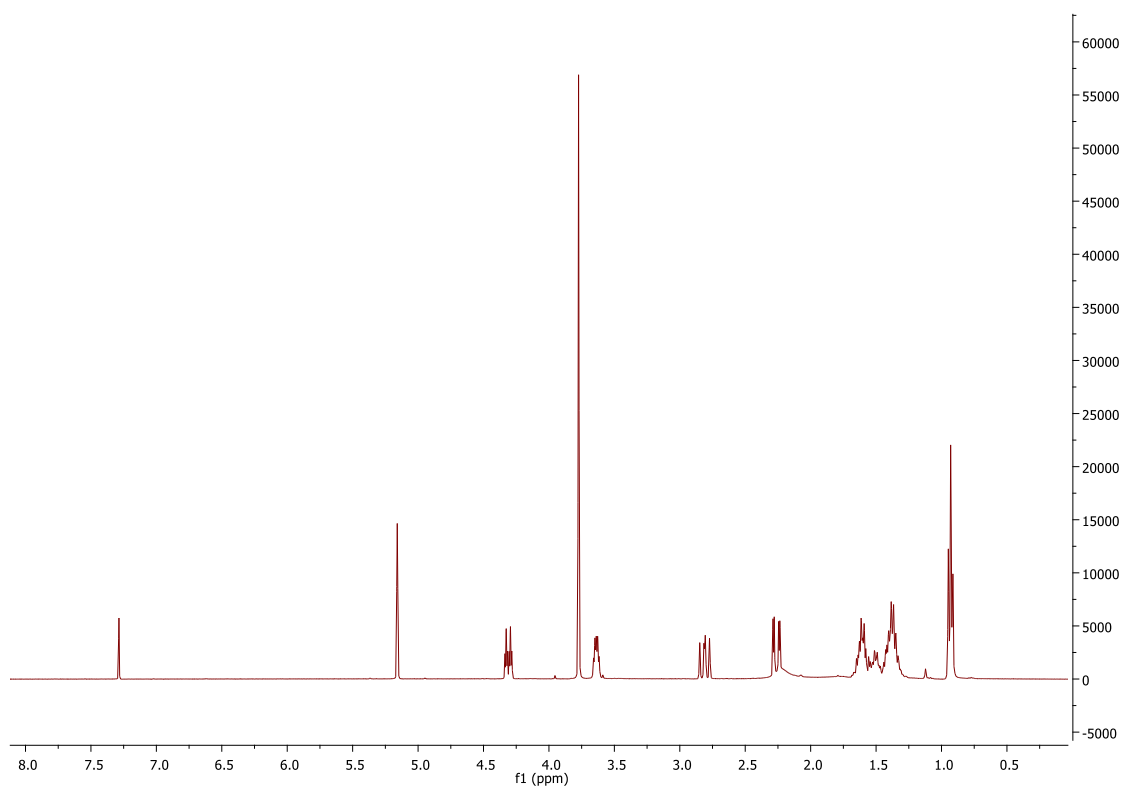
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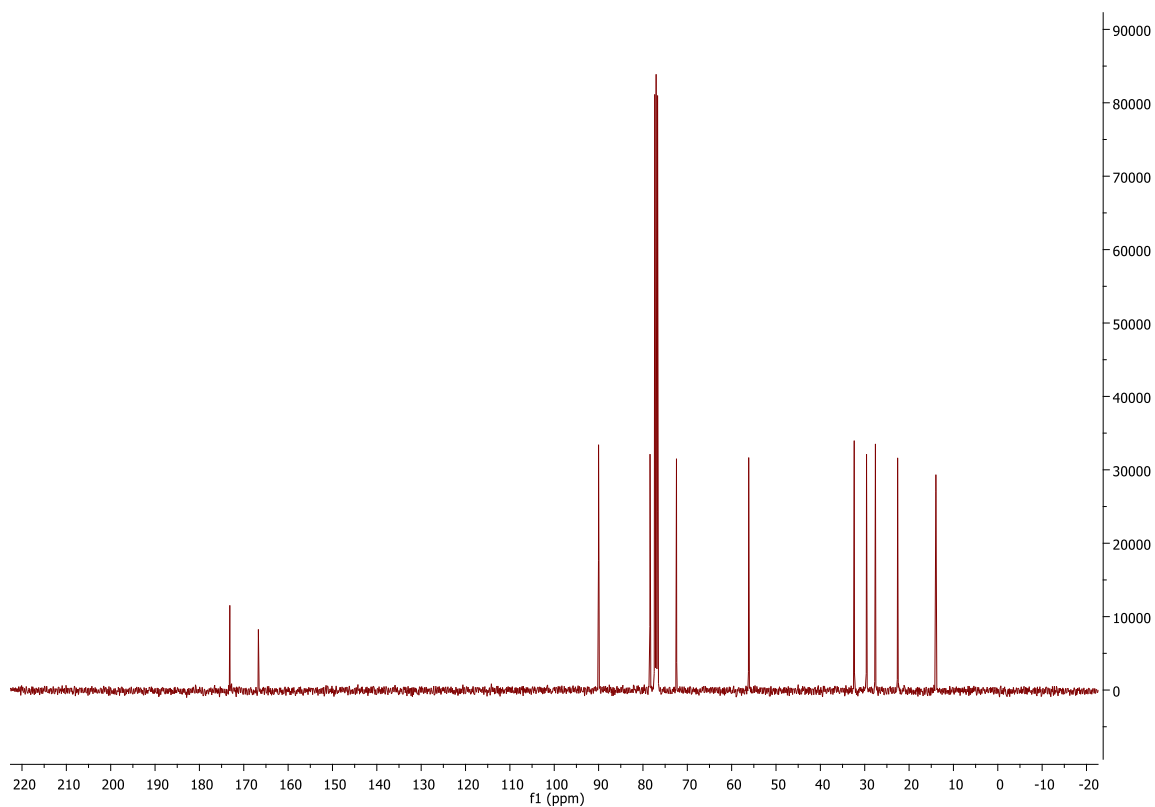
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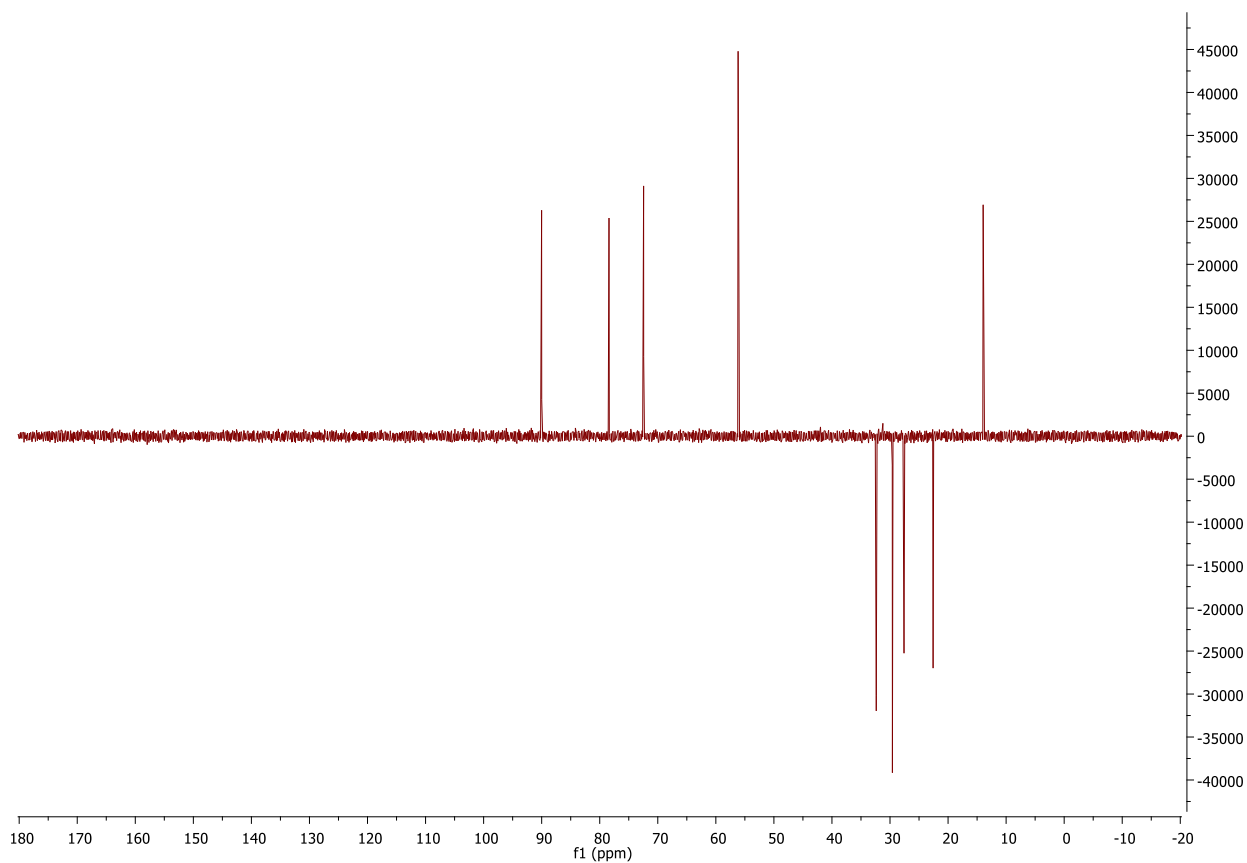
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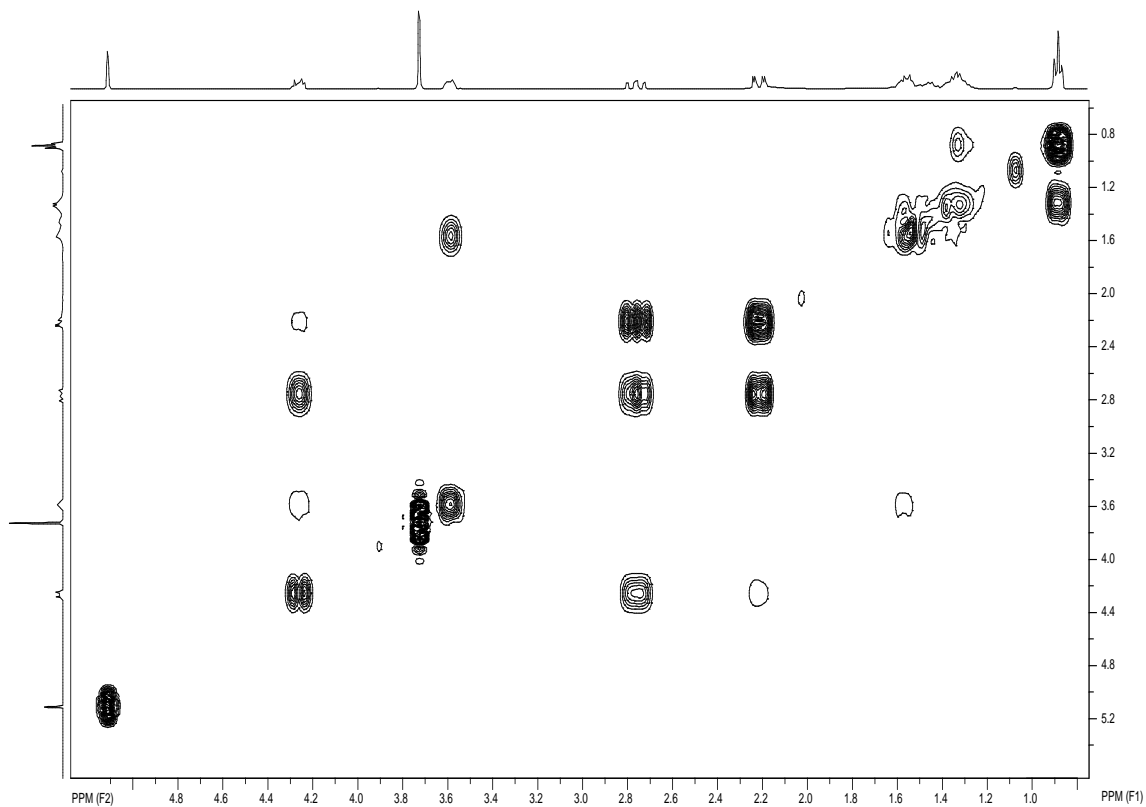
**Figure S1:**  $^1\text{H}$  NMR spectrum of pestalotin (1) at 400 MHz



**Figure S2:**  $^{13}\text{C}$  NMR spectrum of pestalotin (1) at 100 MHz

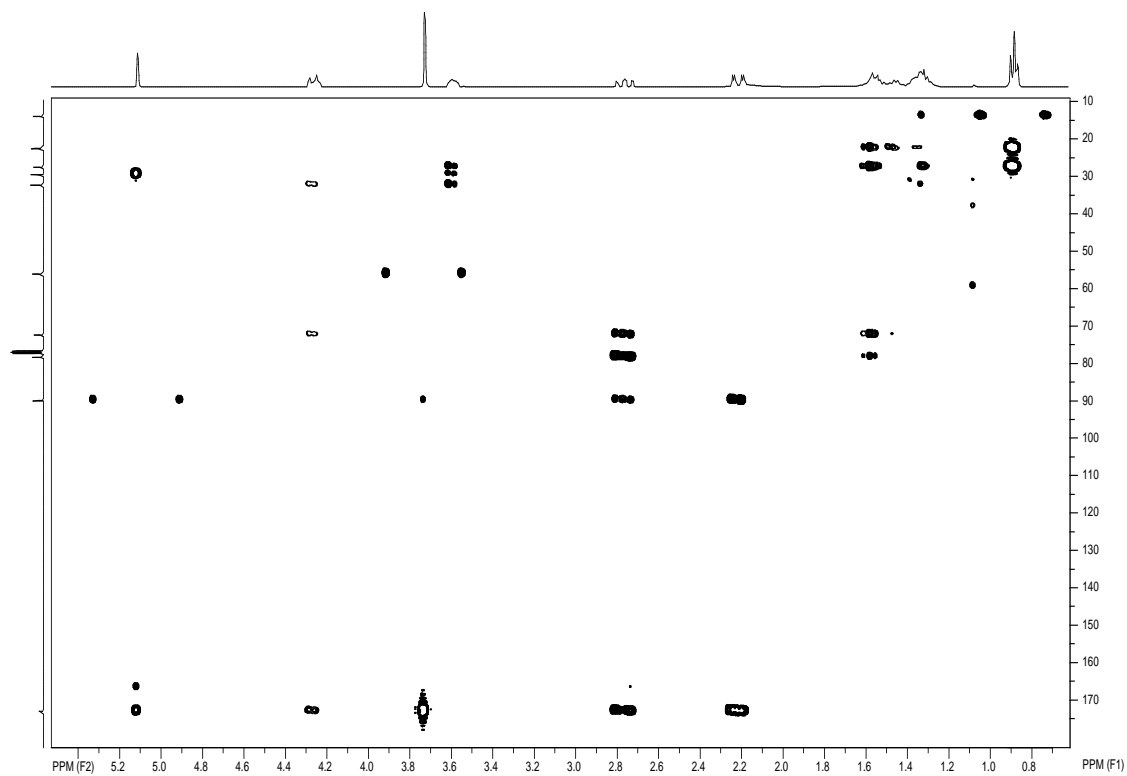


**Figure S3:** DEPT 135 NMR spectrum of pestalotin (**1**) at 100 MHz.

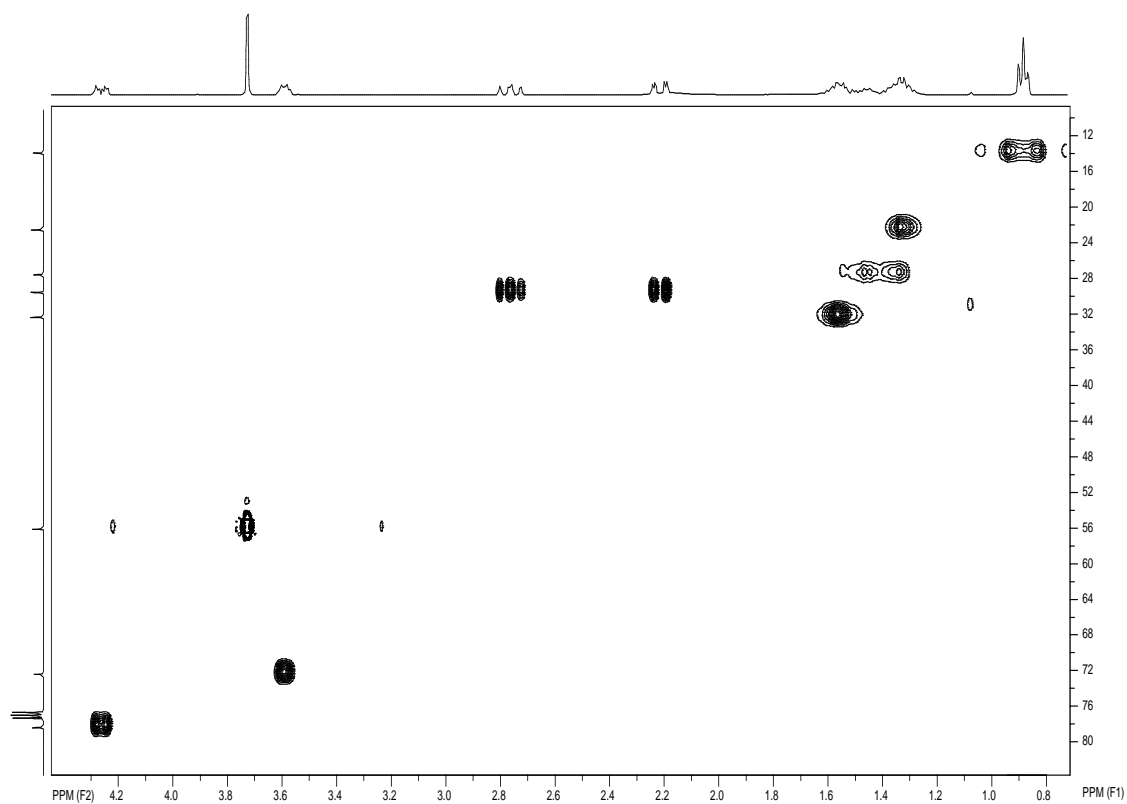


**Figure S4:**  $^1\text{H}$ - $^1\text{H}$  correlation map from COSY NMR of pestalotin (**1**)

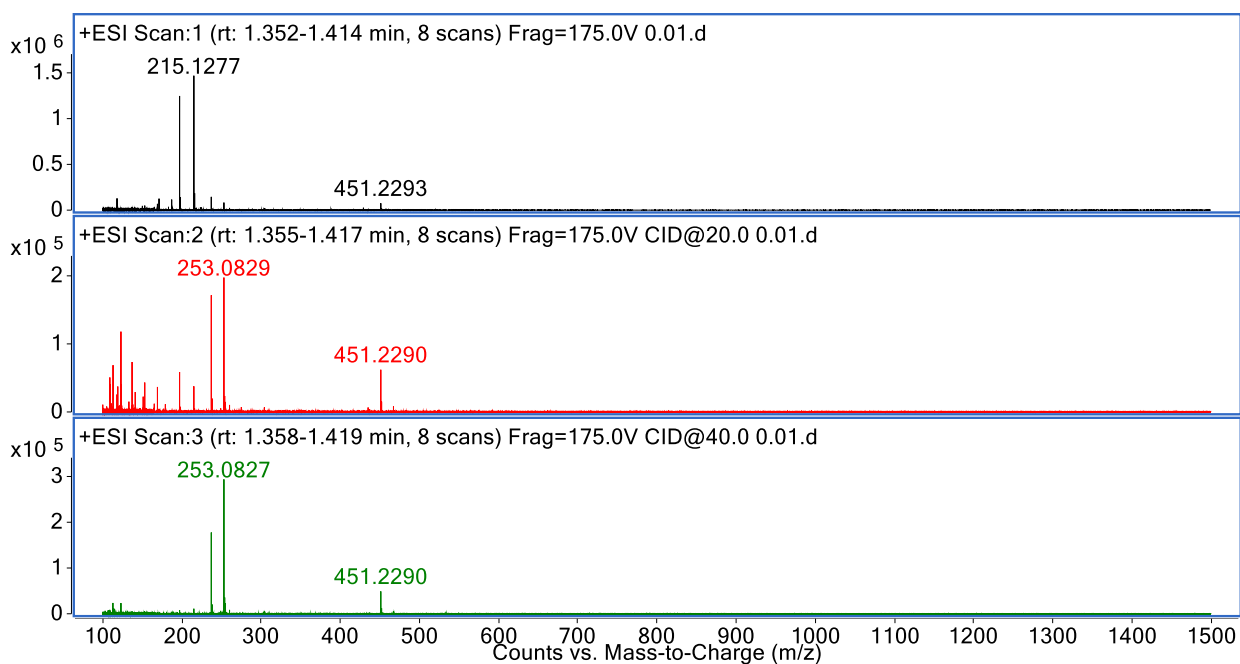
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**Figura S5:**  $^1\text{H}$ - $^{13}\text{C}$  correlation map from HMBC NMR of pestalotin (**1**)



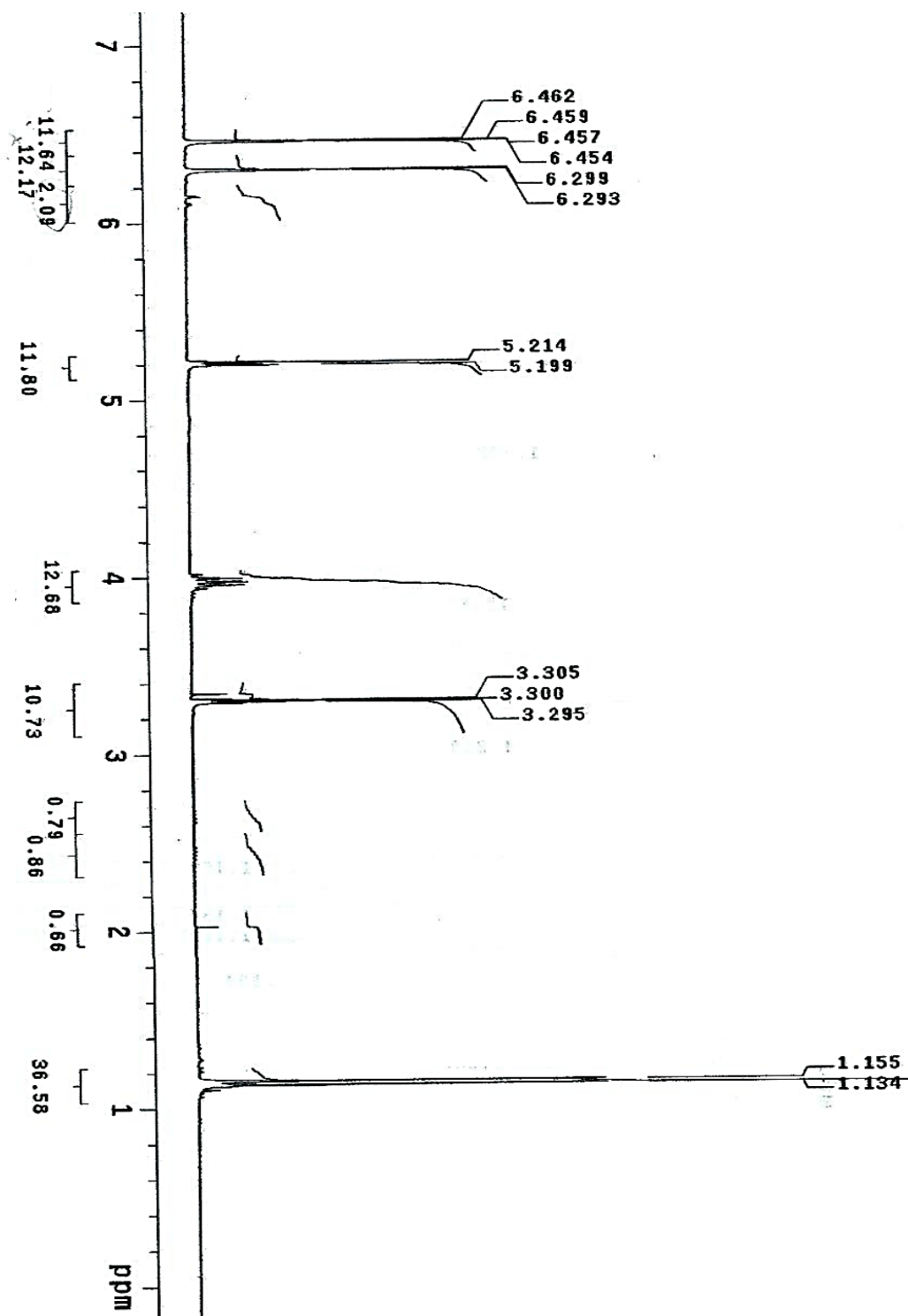
**Figura S6:**  $^1\text{H}$ - $^{13}\text{C}$  correlation map from HSQC NMR of pestalotin (**1**)



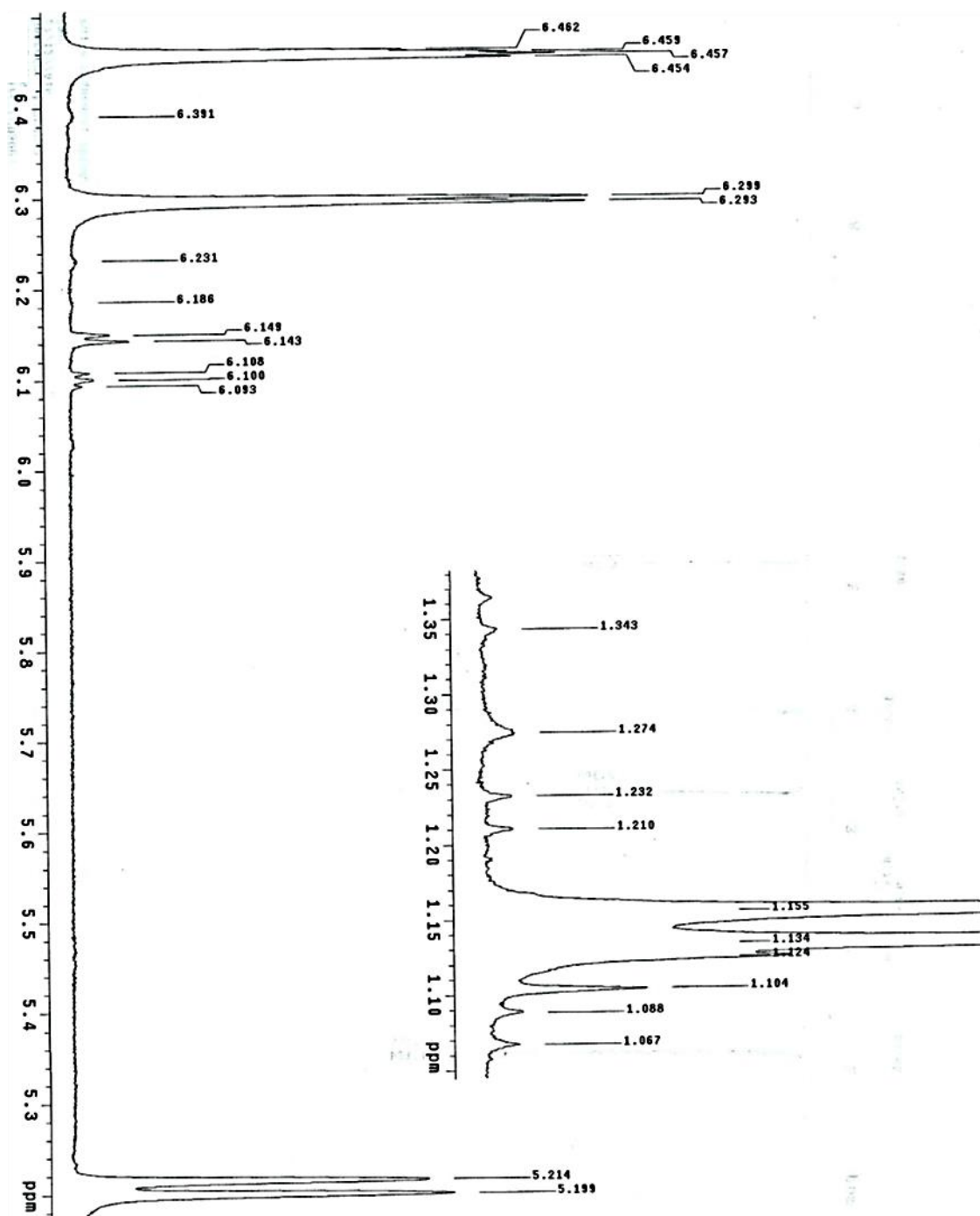
**Figure S7:** General Mass Spectra (100-150 m/z) of pestalotin (**1**)

**Table S1:**  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR data for compound **1** (at 400 and 100 MHz in  $\text{CD}_3\text{OD}$   $\delta$  in ppm).

Position (H)	<b>1</b>	Position (C)	<b>1</b>
<b>1'</b>	3.63 (m)	<b>1'</b>	72.4
<b>2'</b>	1.57-1.64 (m)	<b>2'</b>	32.5
<b>3</b>	5.15 (1H, s)	<b>3'</b>	27.6
<b>3'</b>	1.40 (m)	<b>4'</b>	22.5
<b>4'</b>	1.34 (m)	<b>5'</b>	166.7; 13.9
<b>5'</b>	0.93 (3H, d; J = 6.9)	<b>3</b>	90.0
<b>5<sup>a</sup></b>	2.25 (dd, J = 3.9, 17.1)	<b>4</b>	173.1
<b>5<sup>b</sup></b>	2.81 (dd, J = 3.9, 17.1)	<b>5</b>	29.6
<b>6</b>	4.31 (dt, J = 4.0, 12.8)	<b>6</b>	78.4
<b>OCH<sub>3</sub></b>	3.77 (3H, s)	<b>OCH<sub>3</sub></b>	56.1

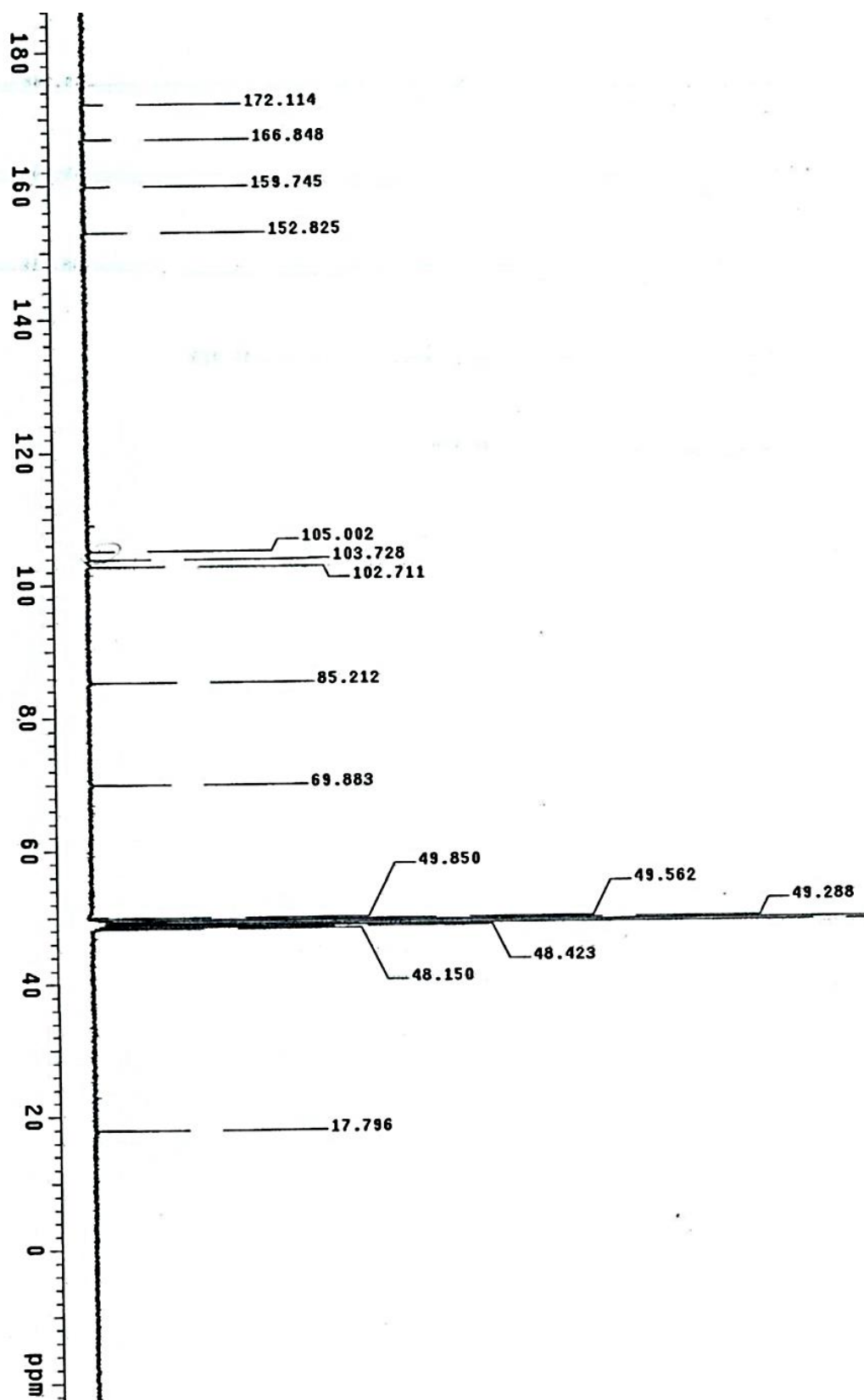


**Figure S8:** <sup>1</sup>H NMR spectrum of (3R,8S) - 5,7-dihydroxy-3-(1-hydroxyethyl) - phthalide (2) at 300 MHz.

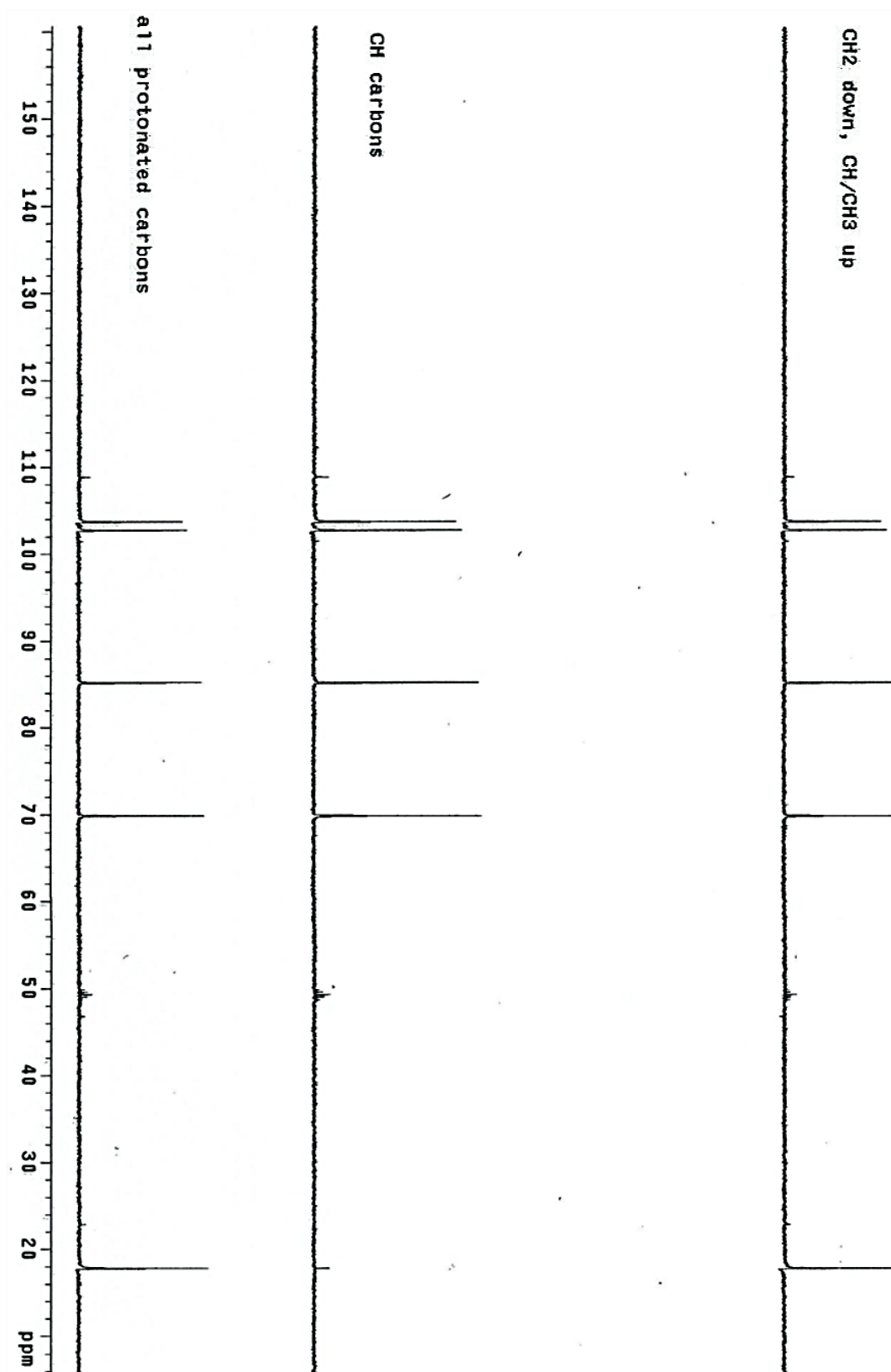


**Figure S9:** <sup>1</sup>H NMR (expansion) spectrum of (3R,8S) - 5,7-dihydroxy-3-(1-hydroxyethyl)-phthalide (2) at 300 MHz





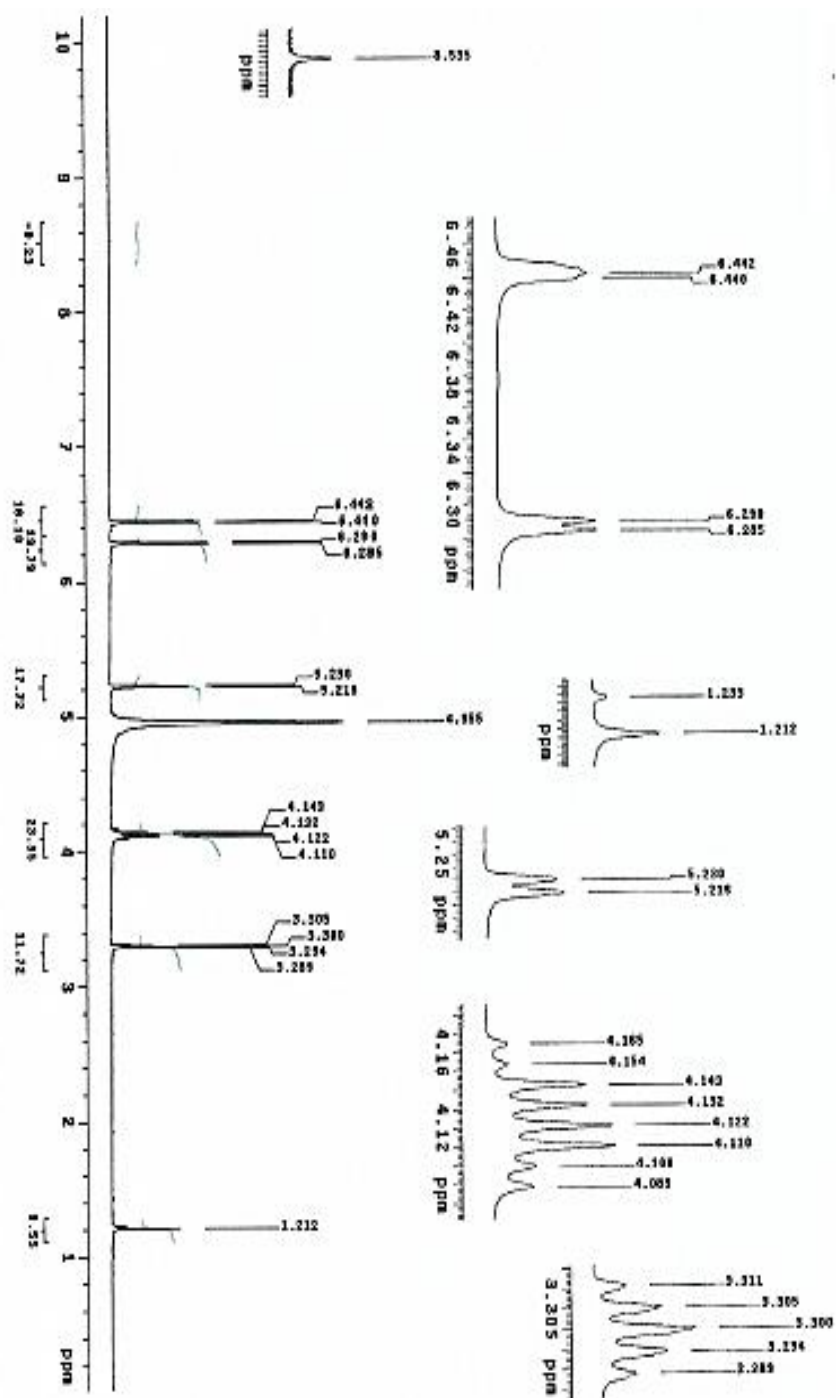
**Figure S10:**  $^{13}\text{C}$  NMR spectrum of (3R,8S)-5,7-dihydroxy-3-(1-hydroxyethyl)-phthalide (**2**) at 75 MHz



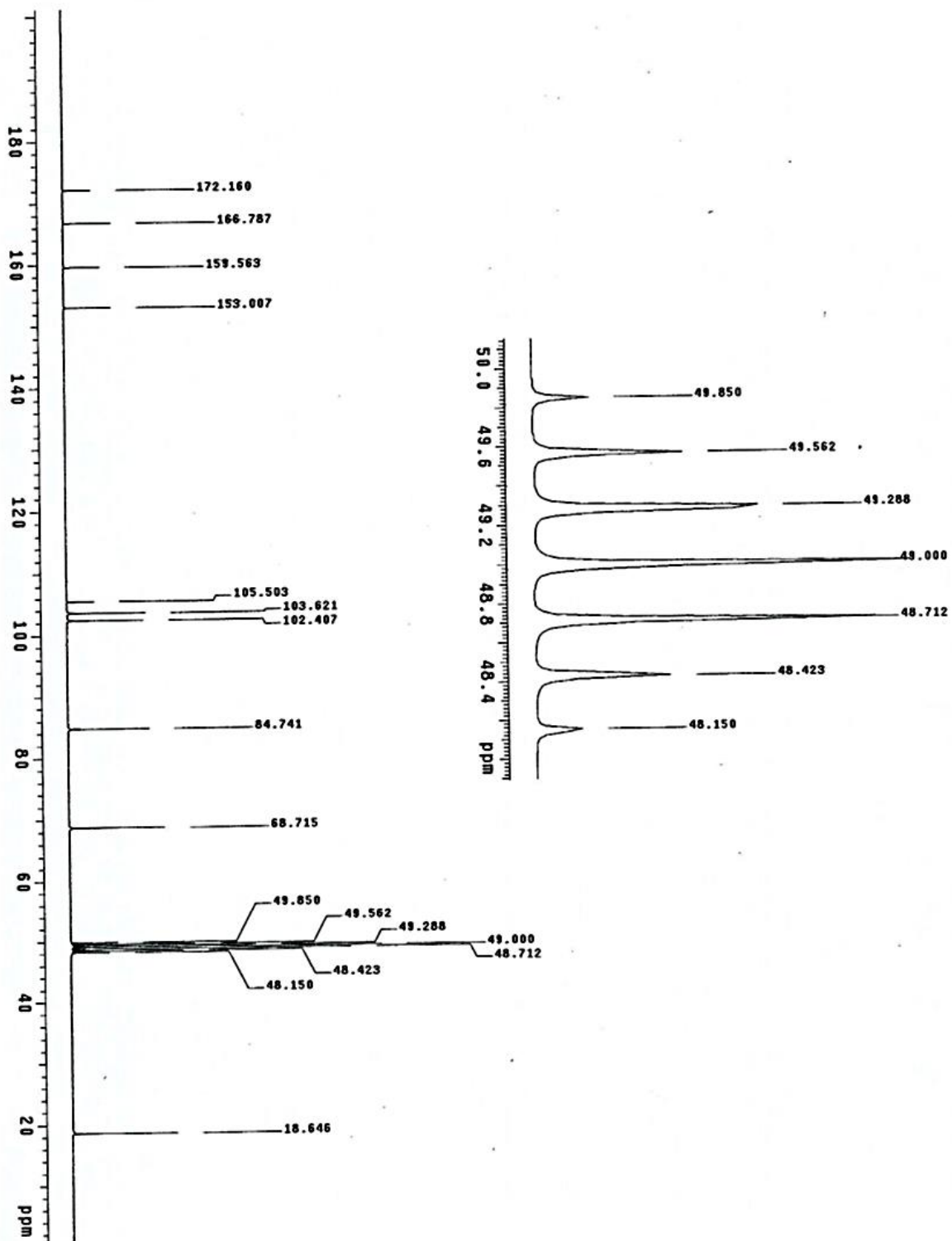
**Figure S11:** DEPT 135 NMR spectrum of (3R,8S)-5,7-dihydroxy-3-(1-hydroxyethyl)-phthalide (2) at 75 MHz



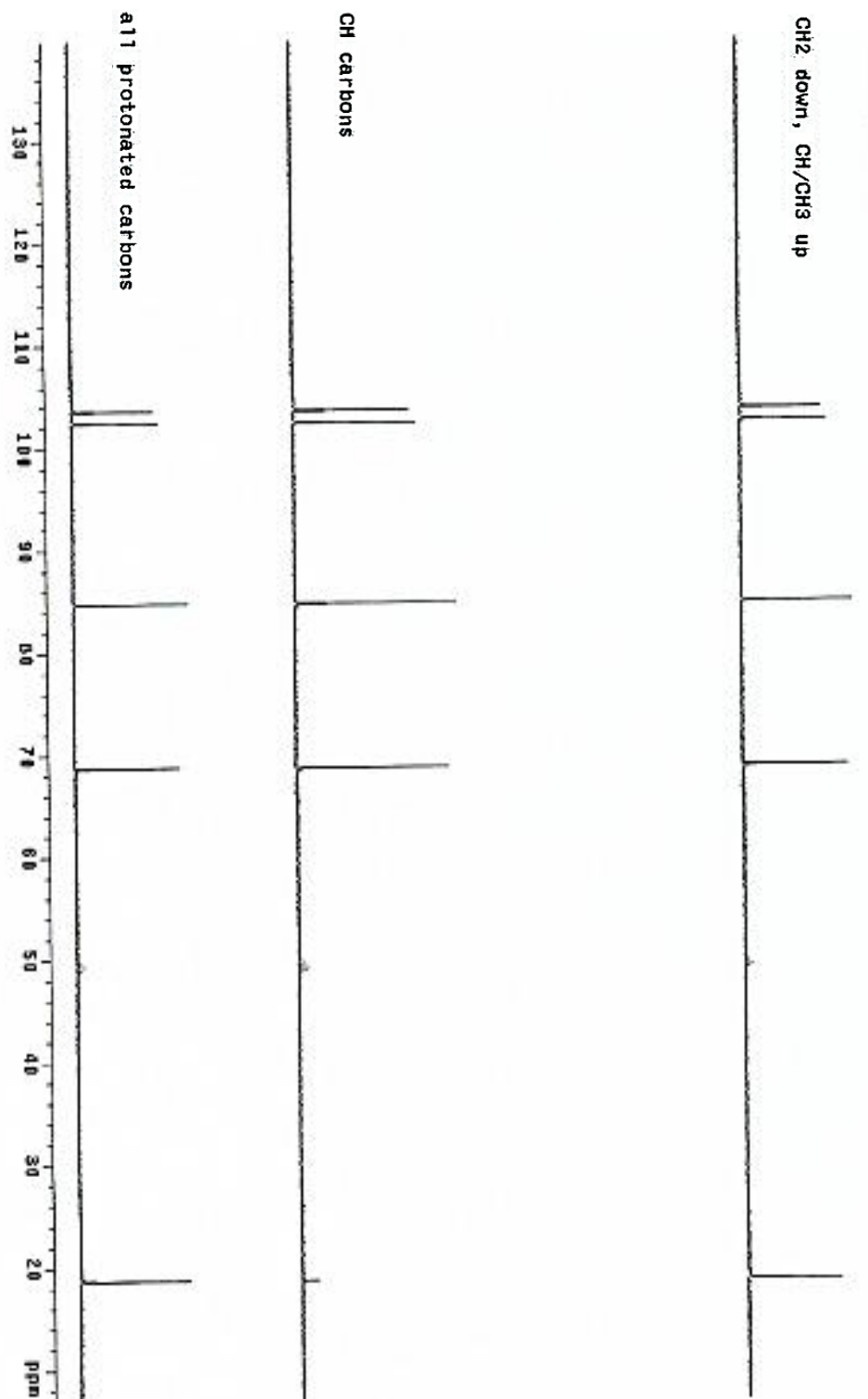




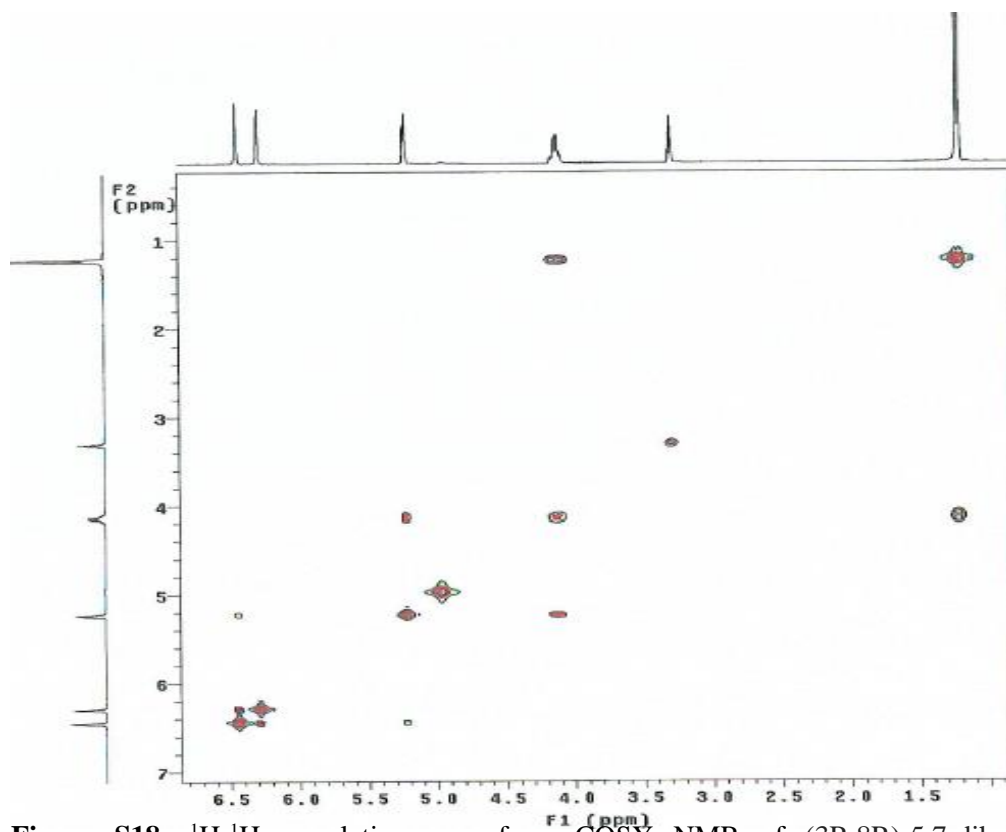
**Figure S15:** <sup>1</sup>H NMR spectrum of (3R,8R)-5,7-dihydroxy-3-(1-hydroxyethyl)-phthalide (**3**) at 300 MHz



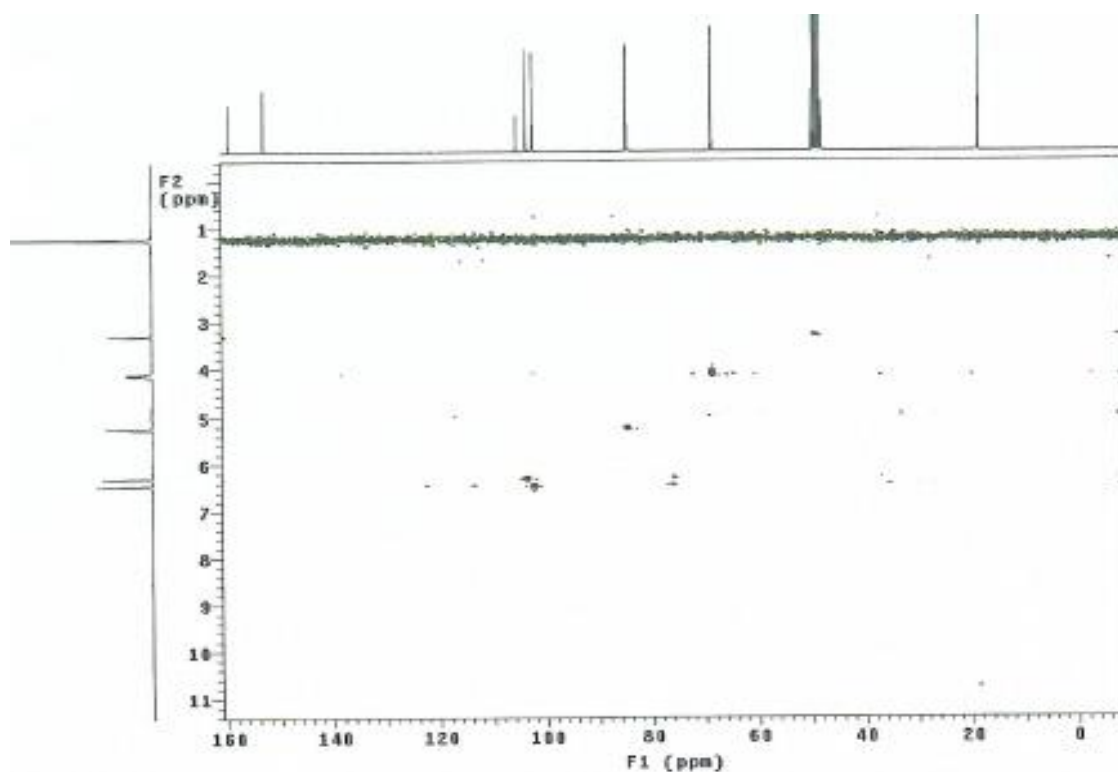
**Figure S16:** <sup>13</sup>C NMR spectrum of (3R,8R)-5,7-dihydroxy-3-(1-hydroxyethyl)-phthalide (**3**) at 75 MHz.



**Figure S17:** DEPT 135 NMR spectrum of (3R,8R)-5,7-dihydroxy-3-(1-hydroxyethyl)-phthalide (3) at 75 MHz

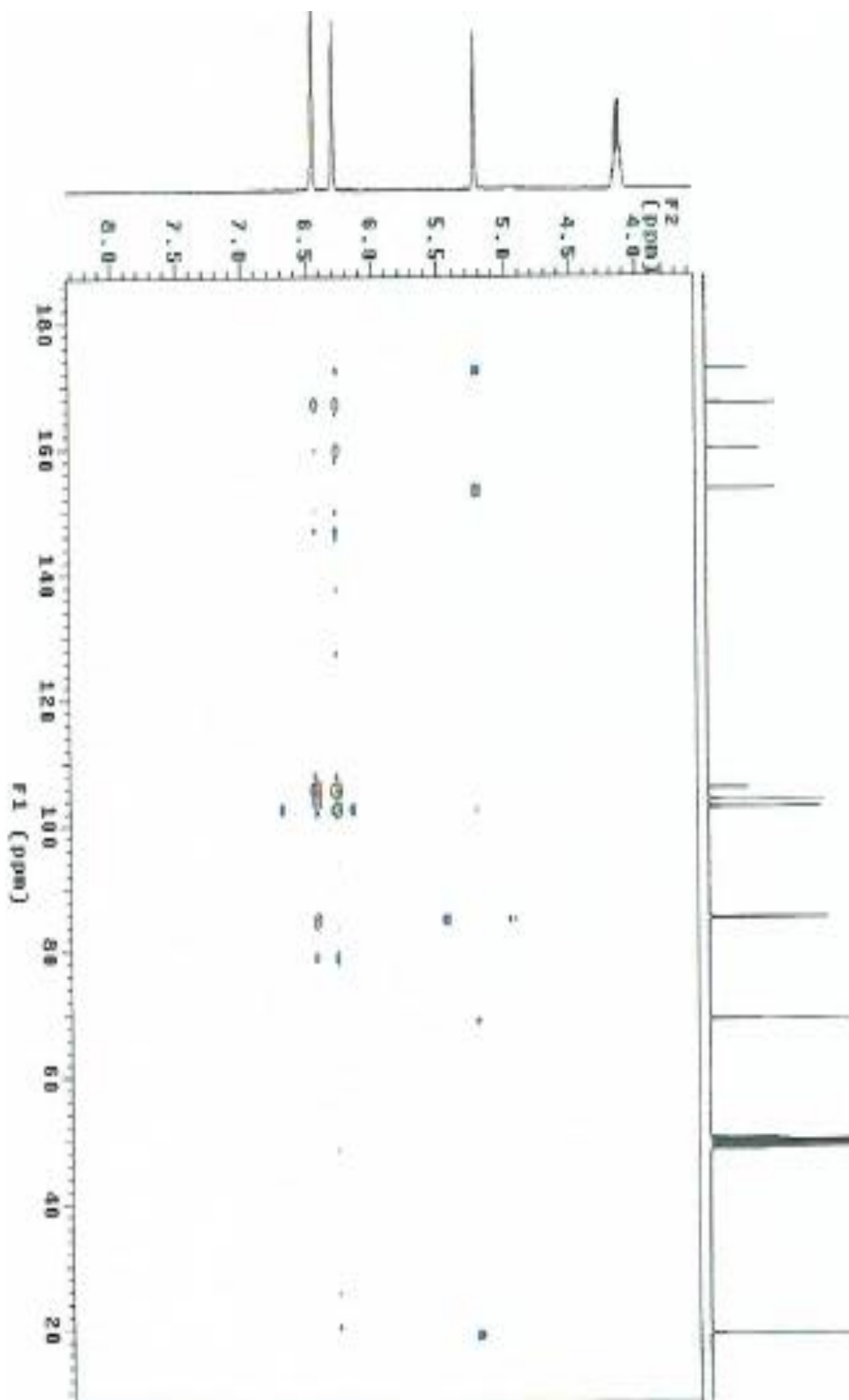


**Figure S18:** <sup>1</sup>H-<sup>1</sup>H correlation map from COSY NMR of (3R,8R)-5,7-dihydroxy-3-(1-hydroxyethyl)-phthalide (**3**) at 75 MHz

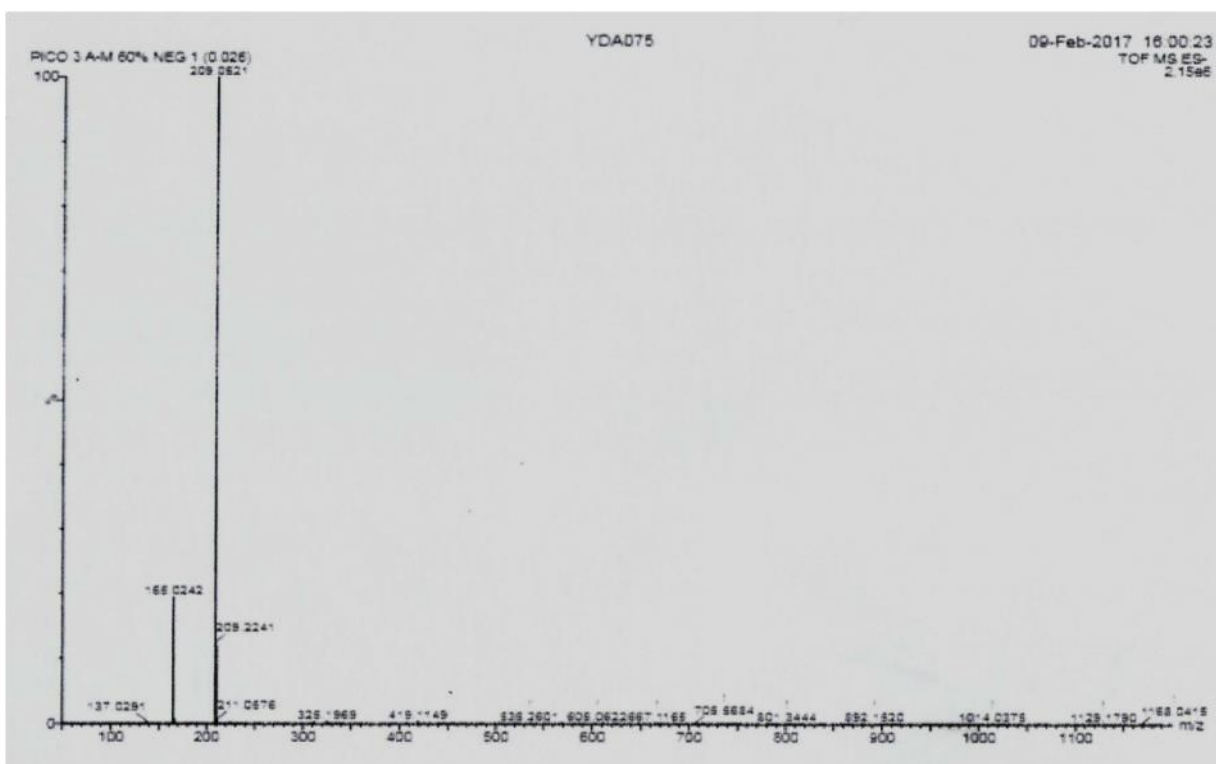


**Figure S19:** One bond <sup>1</sup>H-<sup>13</sup>C correlation map from HSQC NMR of (3R,8R)-5,7-dihydroxy-3-(1-hydroxyethyl)-phthalide (**3**) at 300 MHz (<sup>1</sup>H) and 75 MHz (<sup>13</sup>C)





**Figure S20:** Long range  $^1\text{H}$ - $^{13}\text{C}$  correlation map from HMBC NMR of (3R,8R)-5,7-dihydroxy-3-(1-hydroxyethyl)phthalide (**3**) at 300 MHz ( $^1\text{H}$ ) and 75 MHz ( $^{13}\text{C}$ ).



**Figure S21:** General Mass Spectra (100-150 m/z) of phthalides

**Table S2:** <sup>1</sup>H NMR and <sup>13</sup>C NMR data for compound **2** and **3** (at 300 and 75 MHz in CD<sub>3</sub>OD δ in ppm).

Position (H)	<b>2</b>	<b>3</b>	Position (C)	<b>2</b>	<b>3</b>
<b>3</b>	5.20 (1H, d, J = 3.3 Hz)	5.22 (1H, d, J = 3.3)	<b>1</b>	172.1	172.1
<b>4</b>	6.45 (1H, dd, J = 0.6, 1.5)	6.44 (1H, dd, J = 0.6, 1.5)	<b>3</b>	84.7	84.7
<b>4'</b>	-	-	<b>4</b>	102.4	102.4
<b>5'</b>	-	-	<b>5</b>	166.7	166.7
<b>5b</b>	-	-	<b>6</b>	103.6	103.6
<b>6</b>	6.29 (1H, d, J = 1.5)	6.28 (1H, d, J = 1.5)	<b>7</b>	159.5	159.5
<b>8</b>	3.98 (1H, m)	4.12 (1H, m)	<b>7<sup>a</sup></b>	105.0	105.0
<b>9</b>	1.14 (3H, d, J = 6.3)	1.22 (3H, d, J = 6.3)	<b>9</b>	18.6	18.6

**Table S3:** Antimicrobial tests of the F-H/AC fraction and of substances **2** and **3**.

Bacteria	Minimum Inhibitory Concentration (µg/mL)		
	AcOEt extract	<b>2</b>	<b>3</b>
<i>Escherichia coli</i>	X	250 <sup>(+)</sup> ; 62.5 <sup>(-)</sup>	X
<i>Staphylococcus aureus</i>	X	500 <sup>(+)</sup>	X
<i>Klebsiella pneumoniae</i>	X	X	X
<i>Enterococcus faecalis</i>	500 <sup>(-)</sup>	31.2 <sup>(-)</sup>	X