

## Supporting Information

*Rec. Nat. Prod.* 17:4 (2023) 622-627

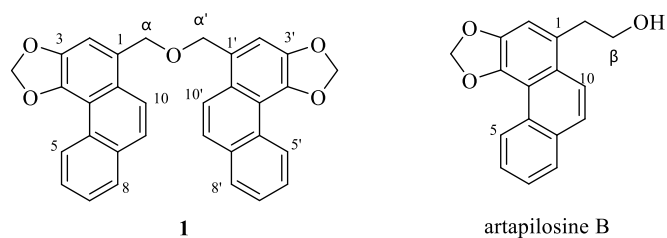
### A Novel Phenanthrene and An Undescribed Alkaloid from the Roots of *Stephania tetrandra*

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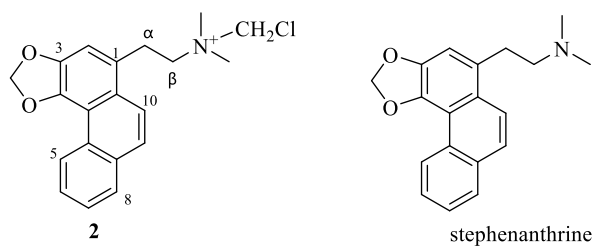
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**Table 1.** The most similar compound data to compound **1**

Position	<b>1</b>		artapilosine B	
	$\delta_{\text{H}}$ ( $J$ in Hz)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ ( $J$ in Hz)	$\delta_{\text{C}}$
1 (1')		131.1		128.7
2 (2')	7.32 s	109.8	7.18 s	111.0
3 (3')		145.0		144.9
4 (4')		143.5		142.5
4a (4a')		117.3		117.1
4b (4b')		128.7		129.0
5 (5')	9.09 dd (7.8, 1.0)	127.0	9.10 dd (8.0, 2.0)	127.3
6 (6')	7.62 overlapped	126.5	7.58 overlapped	126.3
7 (7')	7.62 overlapped	127.4	7.62 overlapped	126.8
8 (8')	7.85 dd (7.8, 1.0)	127.9	7.84 dd (8.0, 2.0)	127.6
8a (8a')		132.1		131.9
9 (9')	7.62 overlapped	125.8	7.60 d (10.0)	125.2
10 (10')	7.93 d (9.0)	122.6	7.86 d (10.0)	122.6
10a (10a')		126.2		126.2
$\alpha$ ( $\alpha'$ )	5.11 s	63.9	3.33 t (6.8)	36.7
$\beta$ ( $\beta'$ )			3.37 t (6.8)	63.2
OCH <sub>2</sub> O (OCH <sub>2</sub> O')	6.26 s	101.4	6.24 s	101.1

Recorded in CDCl<sub>3</sub>

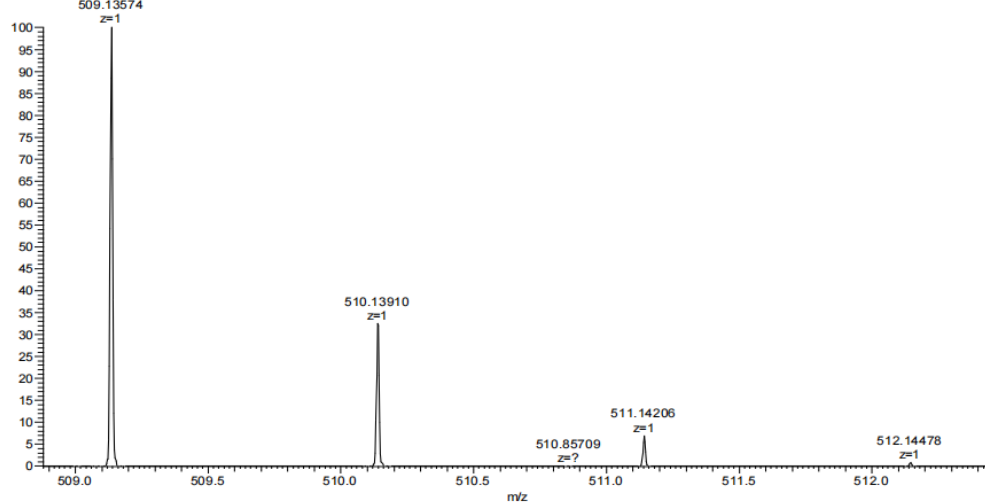


**Table 2.** The most similar compound data to compound **2**

Position	<b>2</b> <sup>a</sup>		stephenanthrine <sup>b</sup>	
	$\delta_{\text{H}}$ ( <i>J</i> in Hz)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ ( <i>J</i> in Hz)	$\delta_{\text{C}}$
1		126.5		131.9
2	7.37 s	112.3	7.16 s	110.1
3		146.8		145.0
4		144.7		142.3
4a		118.4		117.1
4b		129.8		128.6
5	9.12 dd (7.8, 1.8)	128.3	9.08 br d (9.6)	127.3
6	7.63 overlapped	128.3	7.83 br d (9.6)	127.3
7	7.63 overlapped	127.7	7.58-7.61 m	126.8
8	7.90 overlapped	128.9	7.58-7.61 m	126.3
8a		133.4		131.3
9	7.73 d (9.6)	127.3	7.62 br d (9.6)	125.5
10	7.90 overlapped	122.7	7.87 d (9.6)	122.4
10a		127.4		125.9
$\alpha$	3.63 m	27.2	3.38 ddd (16.8, 11.2, 5.6)	30.9
$\beta$	3.76 m	64.3	2.85 ddd (16.8, 11.2, 5.6)	60.2
OCH <sub>2</sub> O	6.30 s	102.9	6.21 s	101.1
<i>N</i> -CH <sub>3</sub>	3.41 s	50.3	2.56 s	44.5
<i>N</i> -CH <sub>2</sub> Cl	5.48 s	69.6		

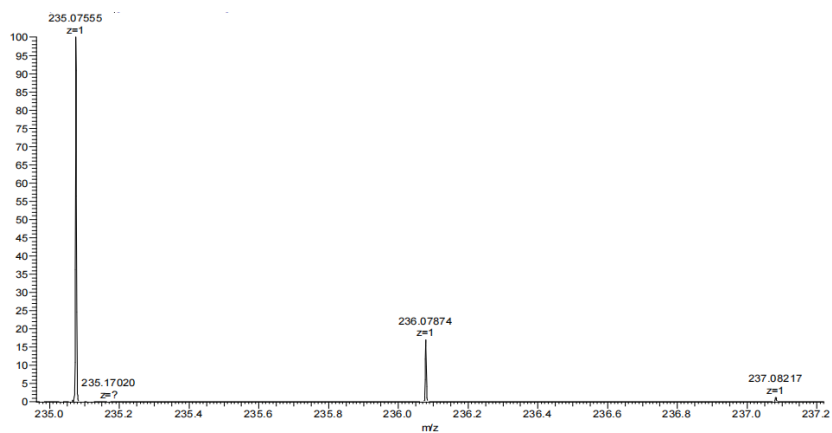
<sup>a</sup>Recorded in CD<sub>3</sub>OD, <sup>b</sup>Recorded in CDCl<sub>3</sub>.

FJ-12 #935 RT: 9.29 AV: 1 NL: 1.24E8  
 T: FTMS + p ESI Full ms [100.0000-1500.0000]  
 509.13574



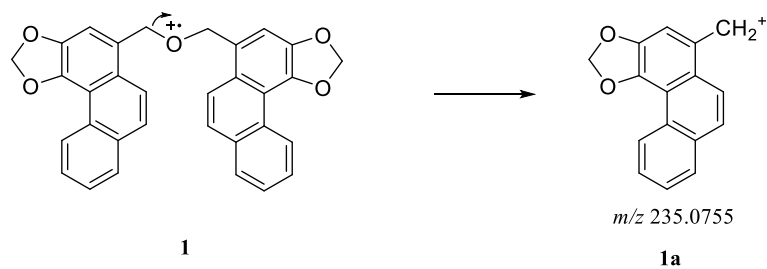
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
509.13574	509.13594	-0.4	21.5	C32 H22 O5 Na	M+Na

**Figure S1:**The HR-ESIMS spectrum of compound **1**

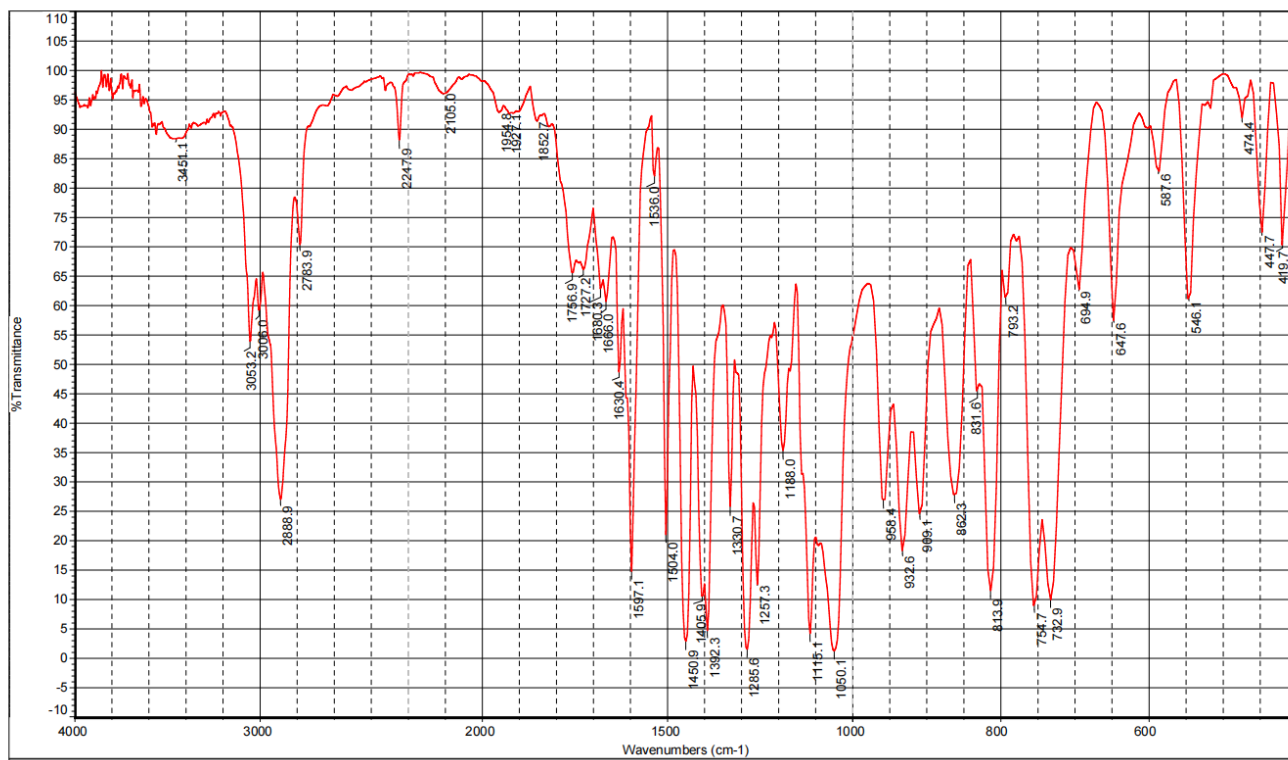


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
235.07555	235.07536	0.82	11.5	C16 H11 O2

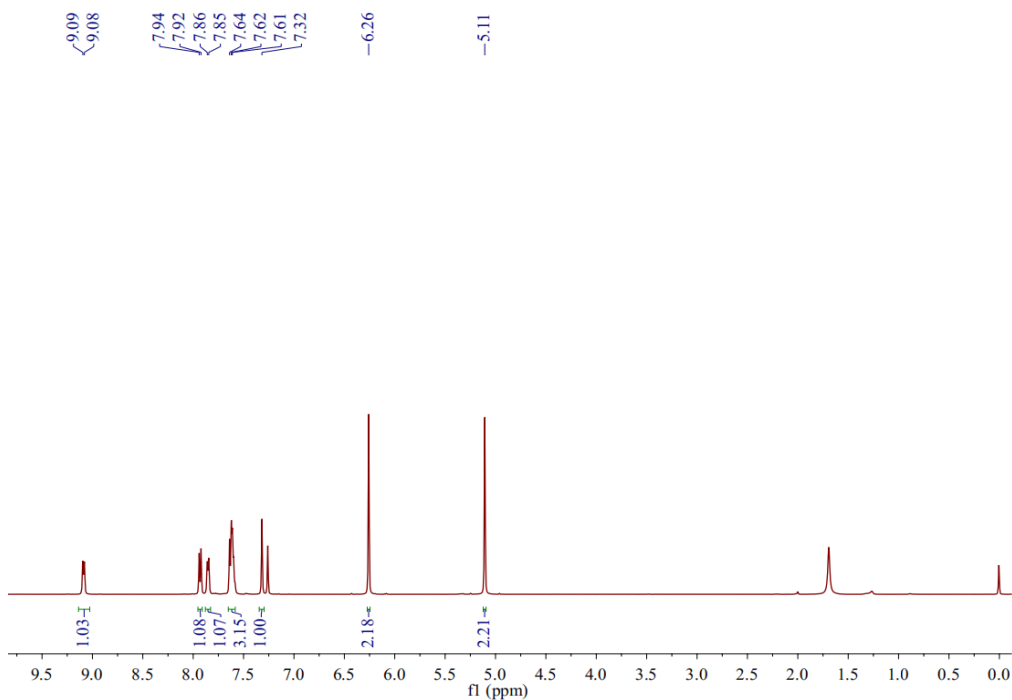
**Figure S2:**The HR-ESIMS data between  $m/z$  50 to 350 in compound **1**



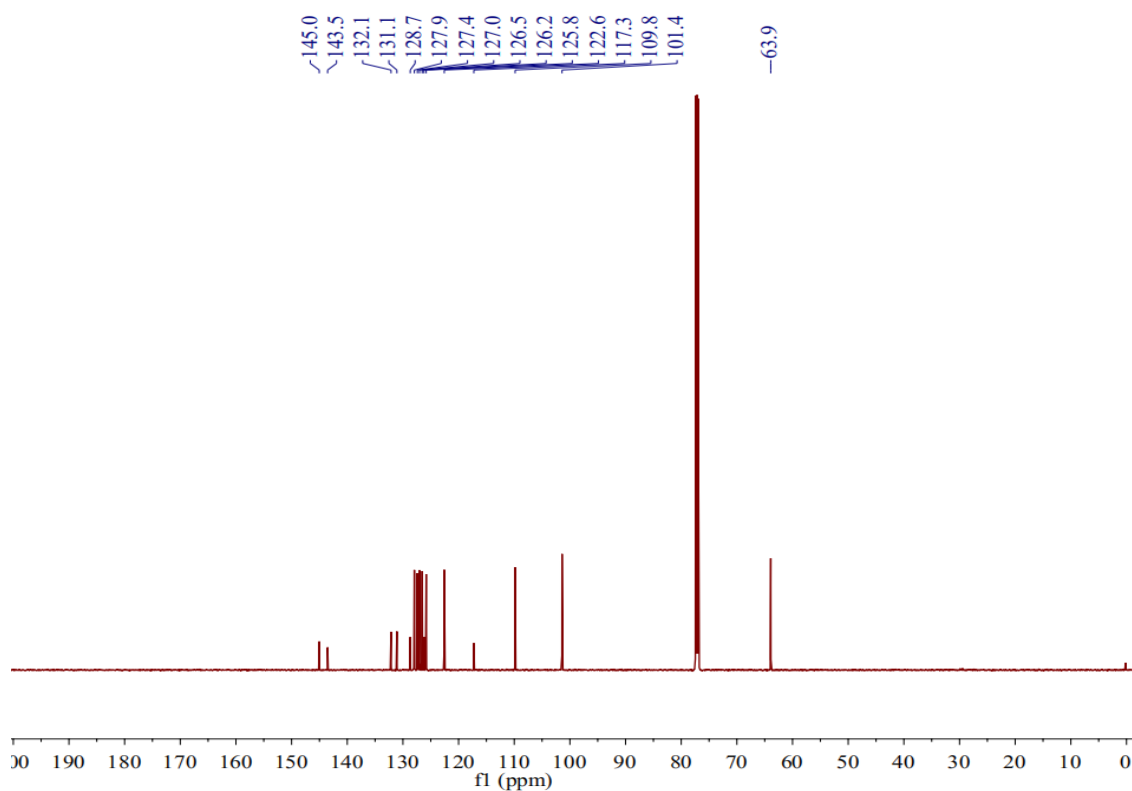
**Figure S3:** Fragment ion of compound **1**



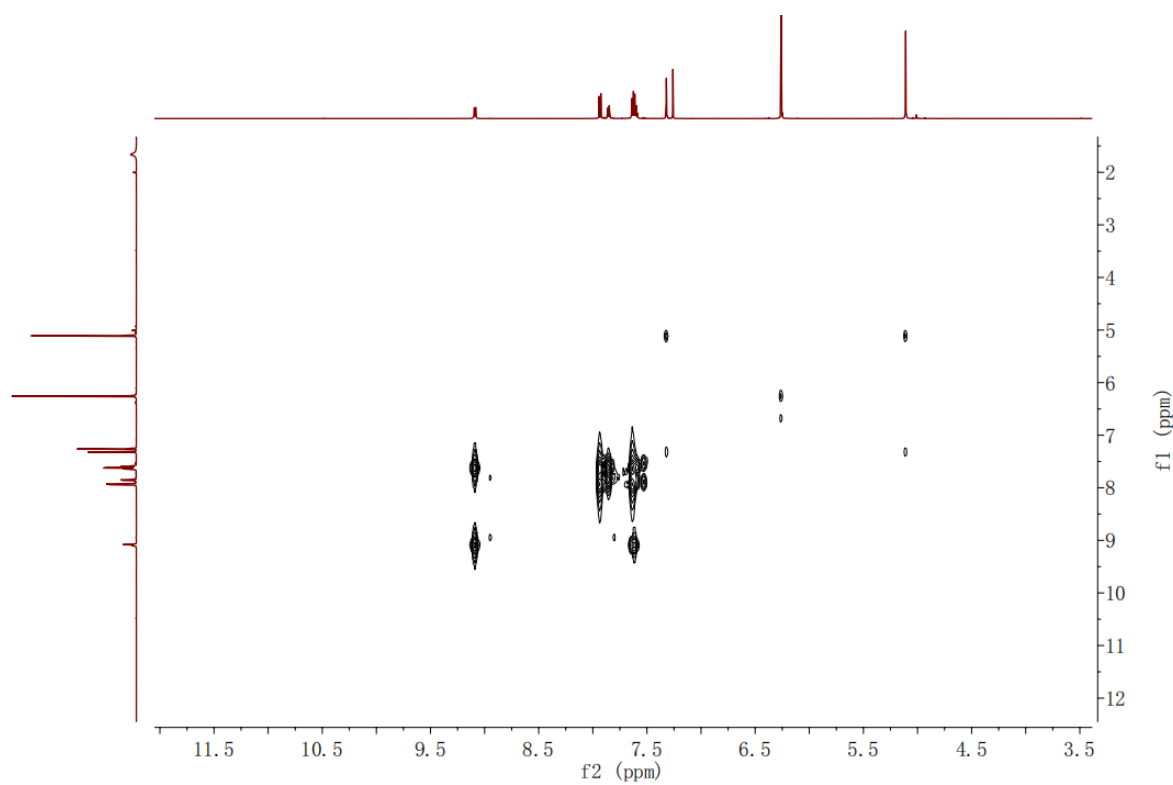
**Figure S4:** The IR spectrum of compound **1**



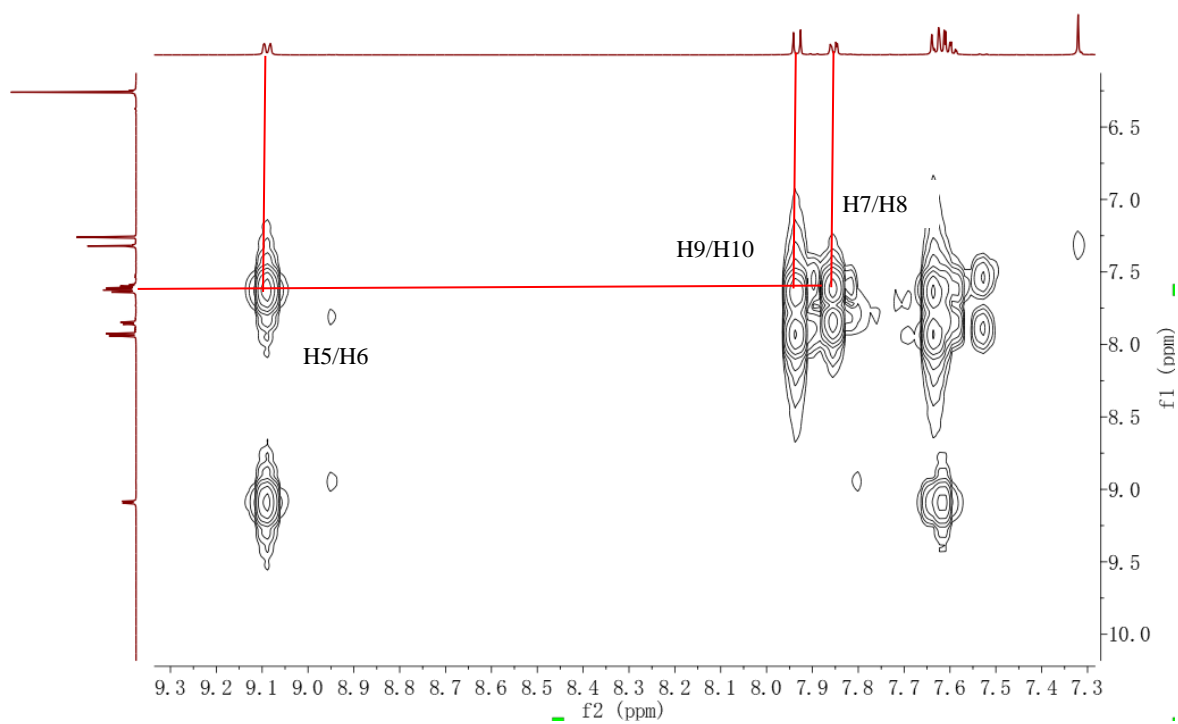
**Figure S5:** The  $^1\text{H}$ -NMR spectrum of compound **1** in  $\text{CDCl}_3$  (600 MHz)



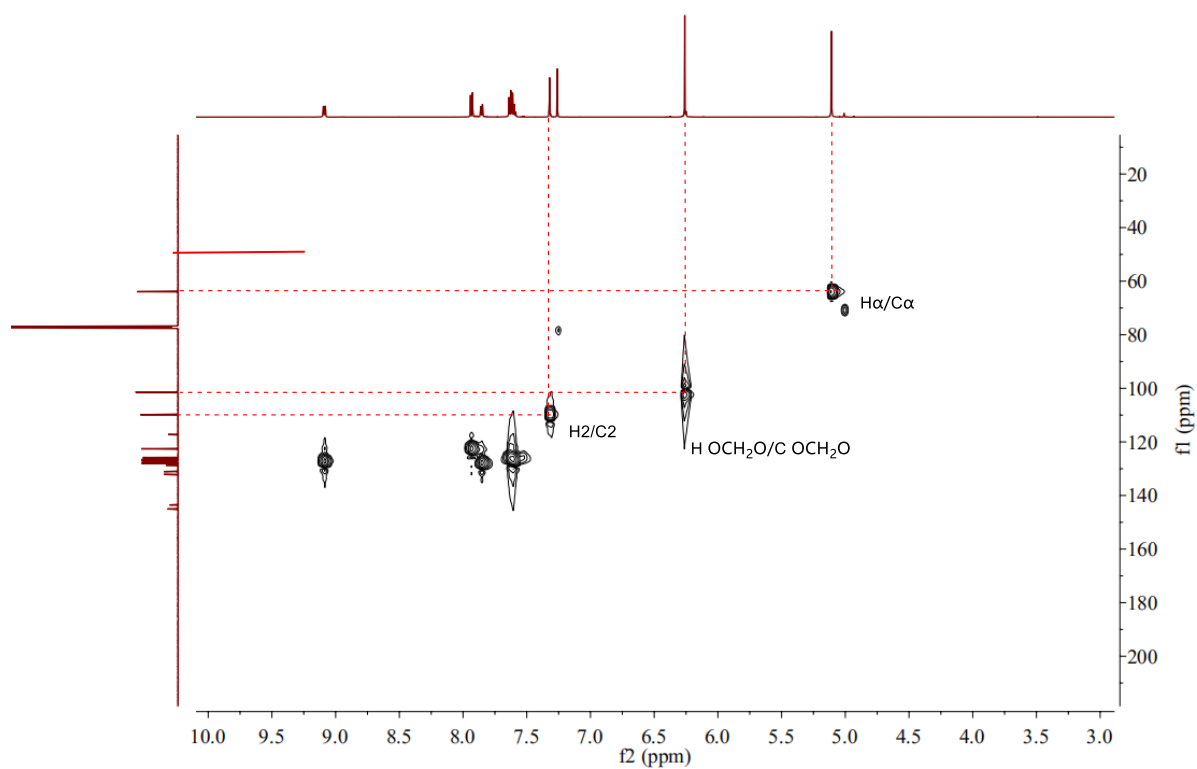
**Figure S6:** The  $^{13}\text{C}$ -NMR spectrum of compound **1** in  $\text{CDCl}_3$  (150 MHz)



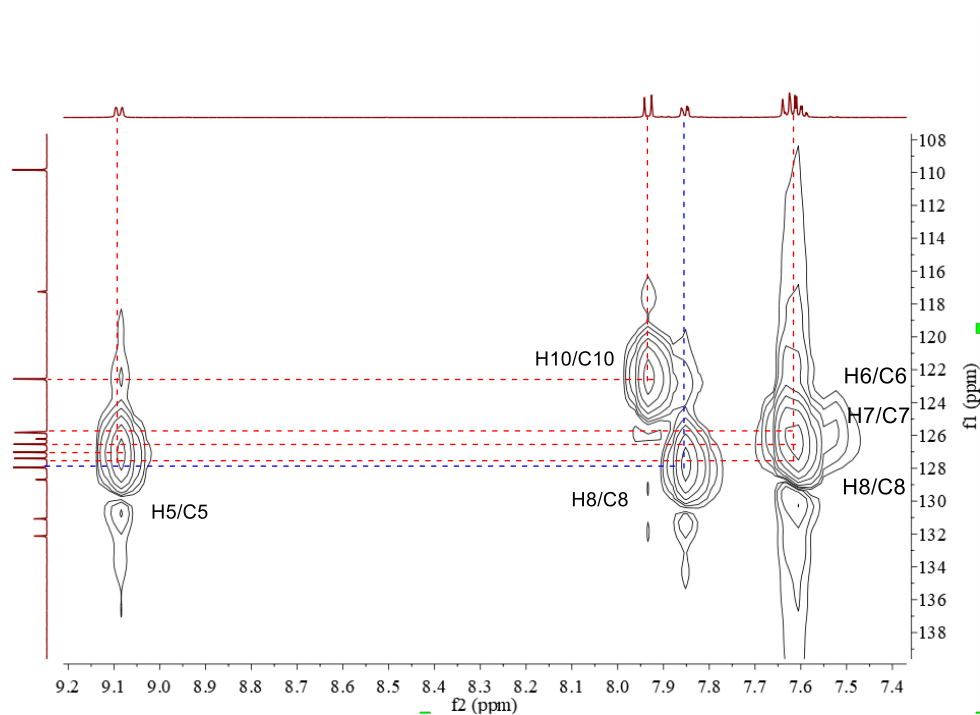
**Figure S7:** The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** in  $\text{CDCl}_3$



**Figure S8:** The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** in  $\text{CDCl}_3$  (From  $\delta_{\text{H}}$  7.3 to 9.3)

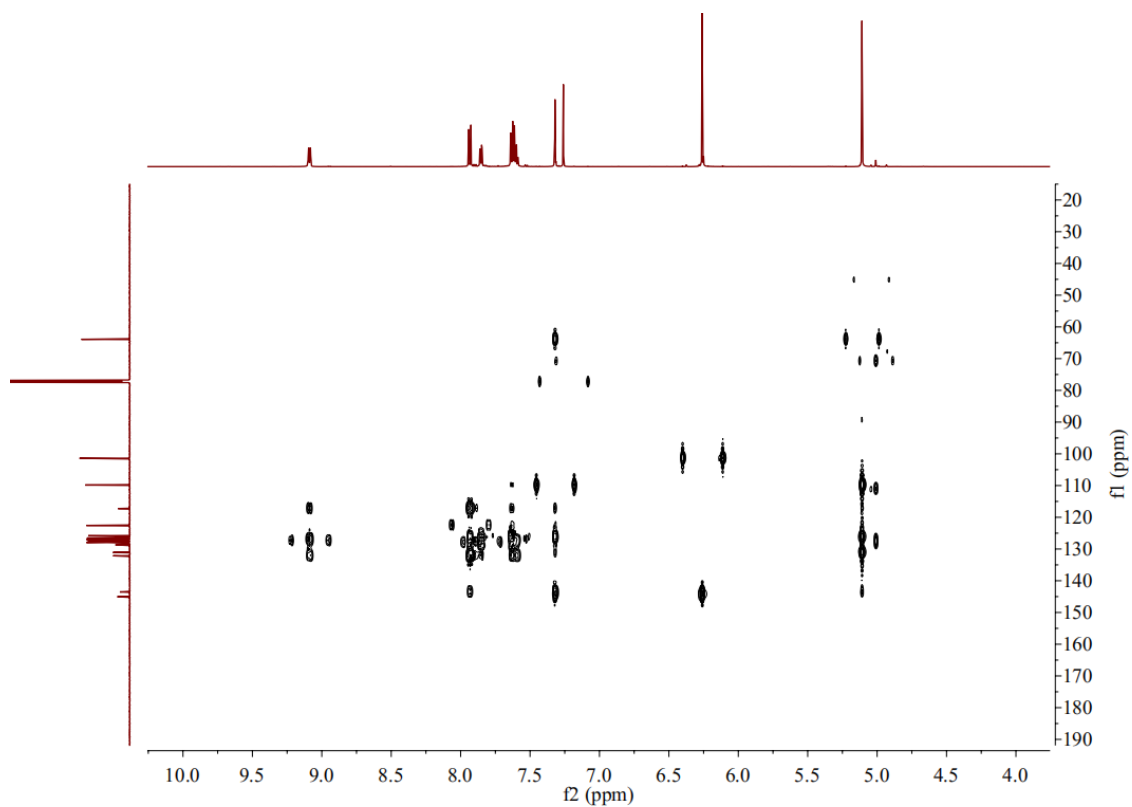


**Figure S9:** The HSQC spectrum of compound **1** in  $\text{CDCl}_3$

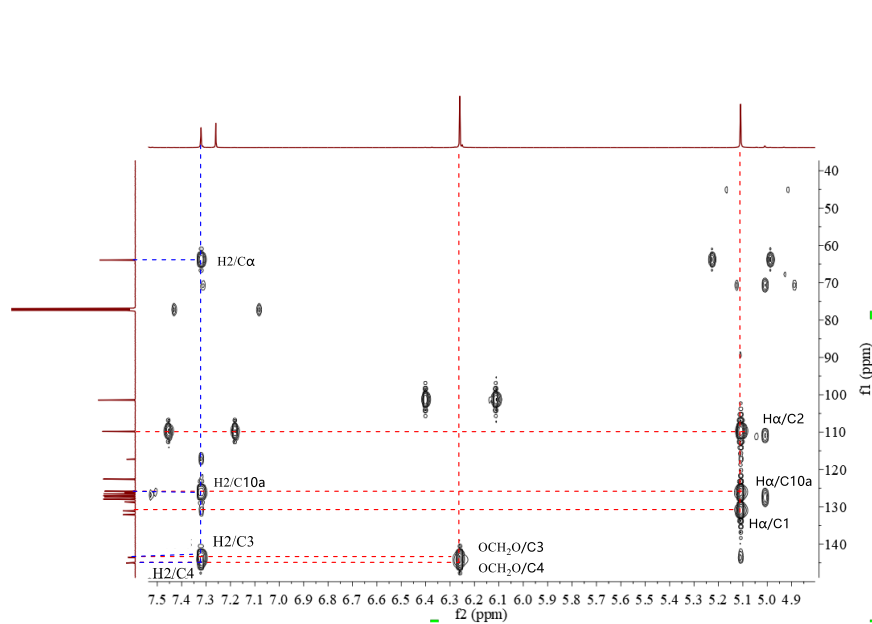




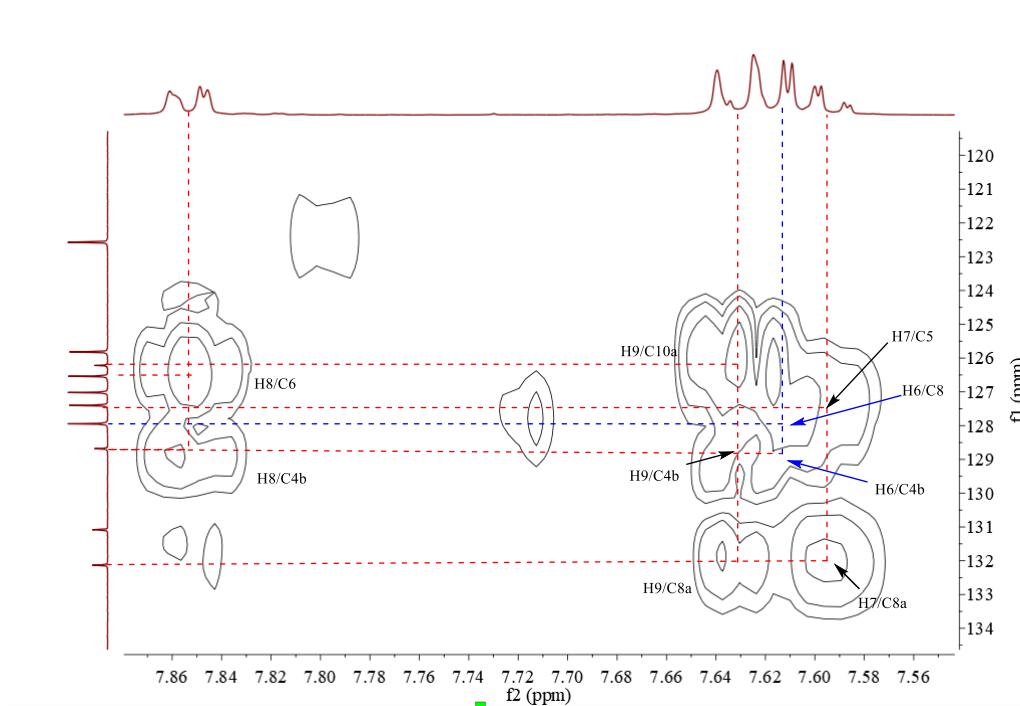
**Figure S10:** The HSQC spectrum of compound **1** in CDCl<sub>3</sub> (From  $\delta_C$  108 to 138)



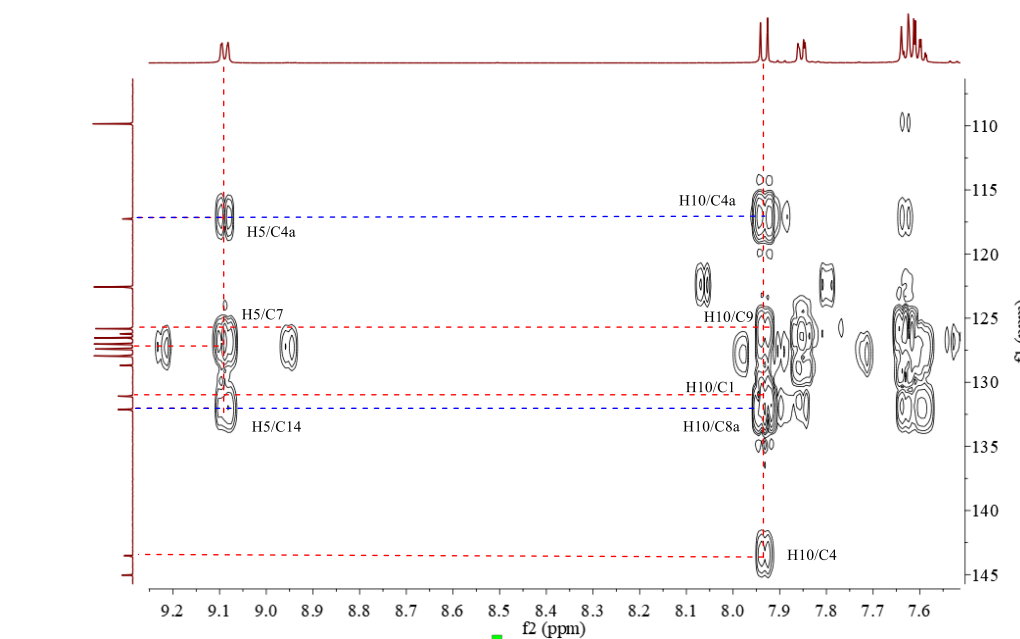
**Figure S11:** The HMBC spectrum of compound **1** in CDCl<sub>3</sub>



**Figure S12:** The HMBC spectrum of compound **1** in CDCl<sub>3</sub> (From  $\delta_H$  4.9 to 7.5)

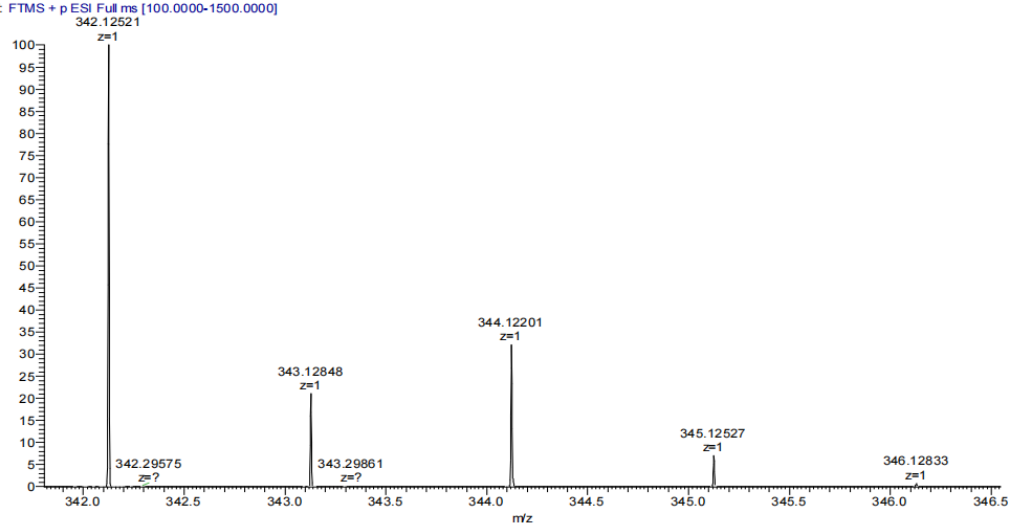


**Figure S13:** The HMBC spectrum of compound **1** in CDCl<sub>3</sub> (From δ<sub>H</sub> 7.5 to 7.9)



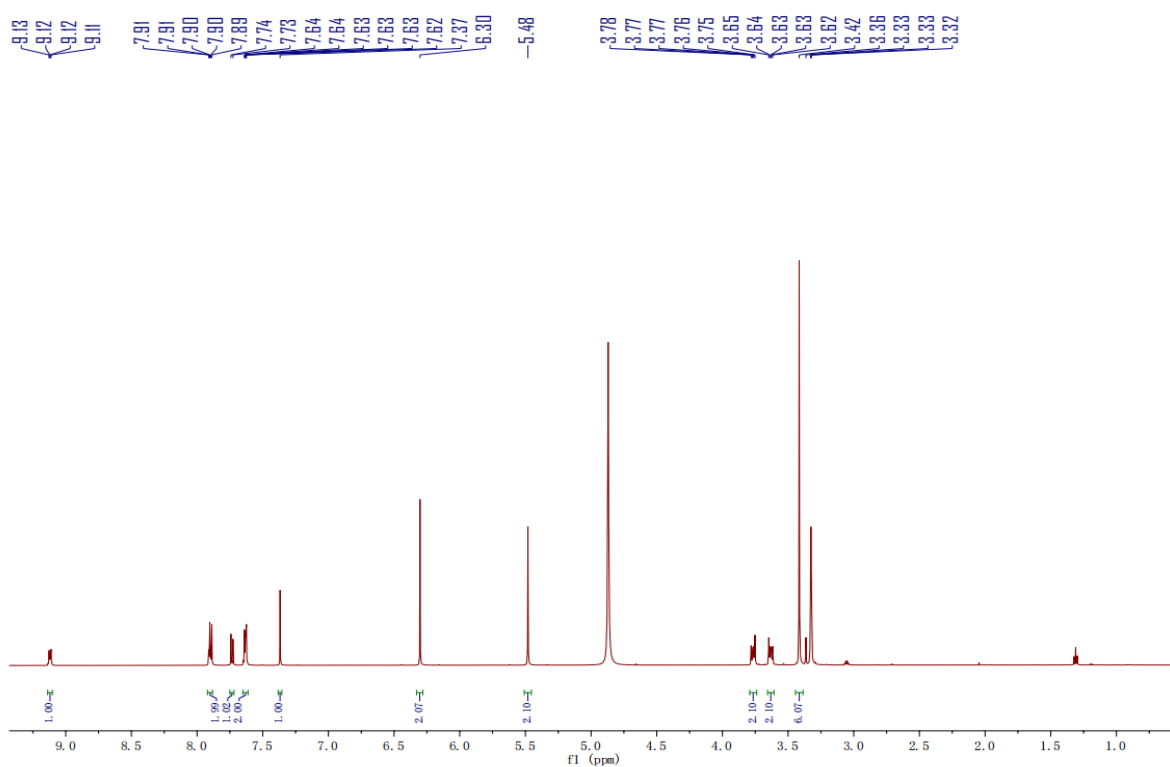
**Figure S14:** The HMBC spectrum of compound **1** in CDCl<sub>3</sub> (From δ<sub>H</sub> 7.9 to 9.2)

FJ-48 #581 RT: 5.80 AV: 1 NL: 8.30E9  
 T: FTMS + pESI Full ms [100.0000-1500.0000]

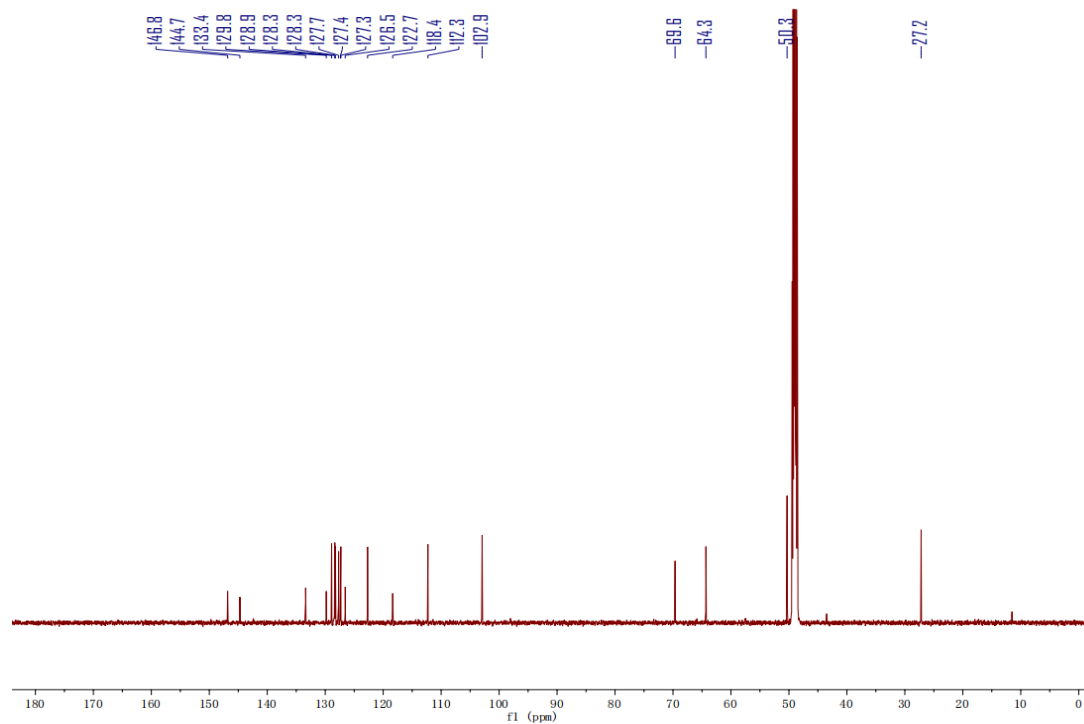


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
342.12521	342.12553	-0.94	10.5	C20 H21 O2 N Cl	M+H

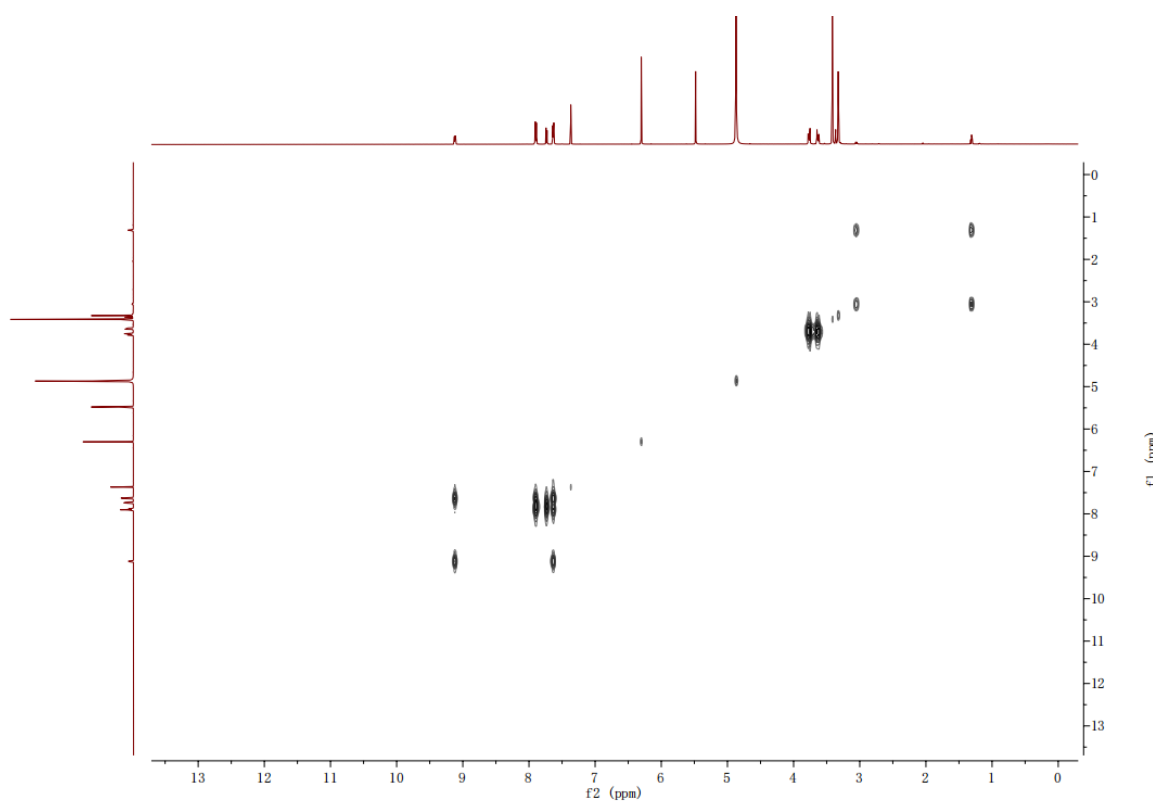
**Figure S15:** The HR-ESIMS spectrum of compound **2**



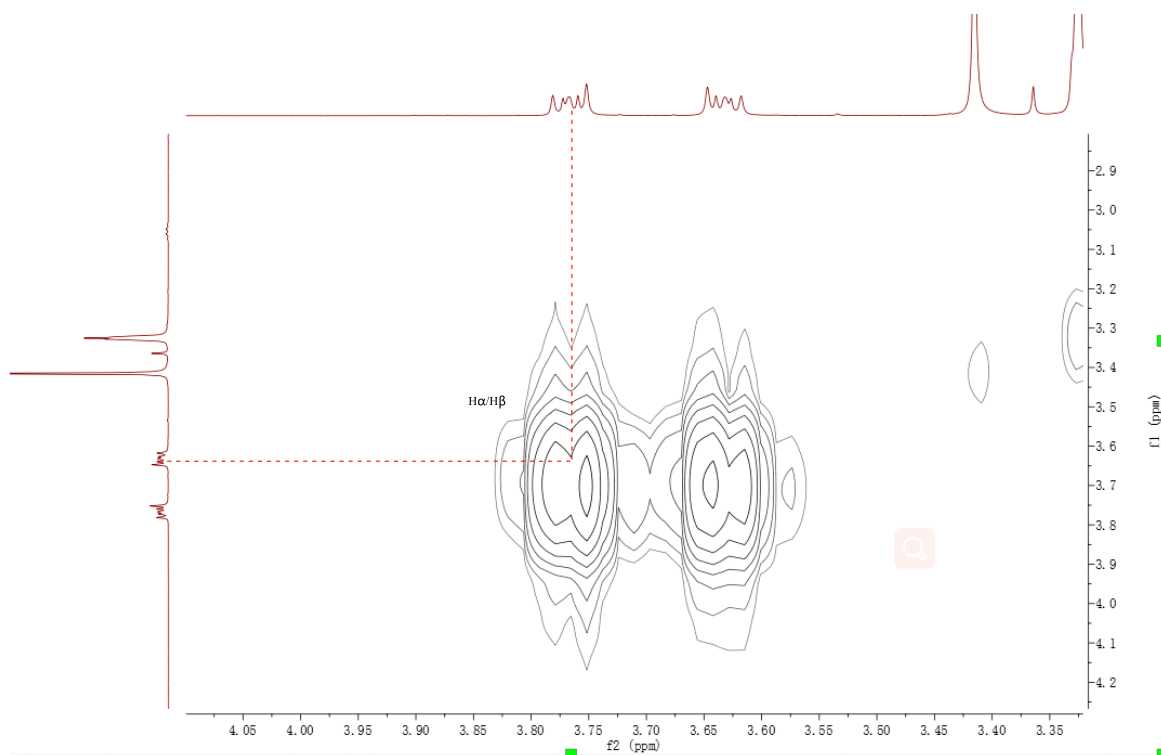
**Figure S16:** The <sup>1</sup>H-NMR spectrum of compound **2** in CD<sub>3</sub>OD (600 MHz)



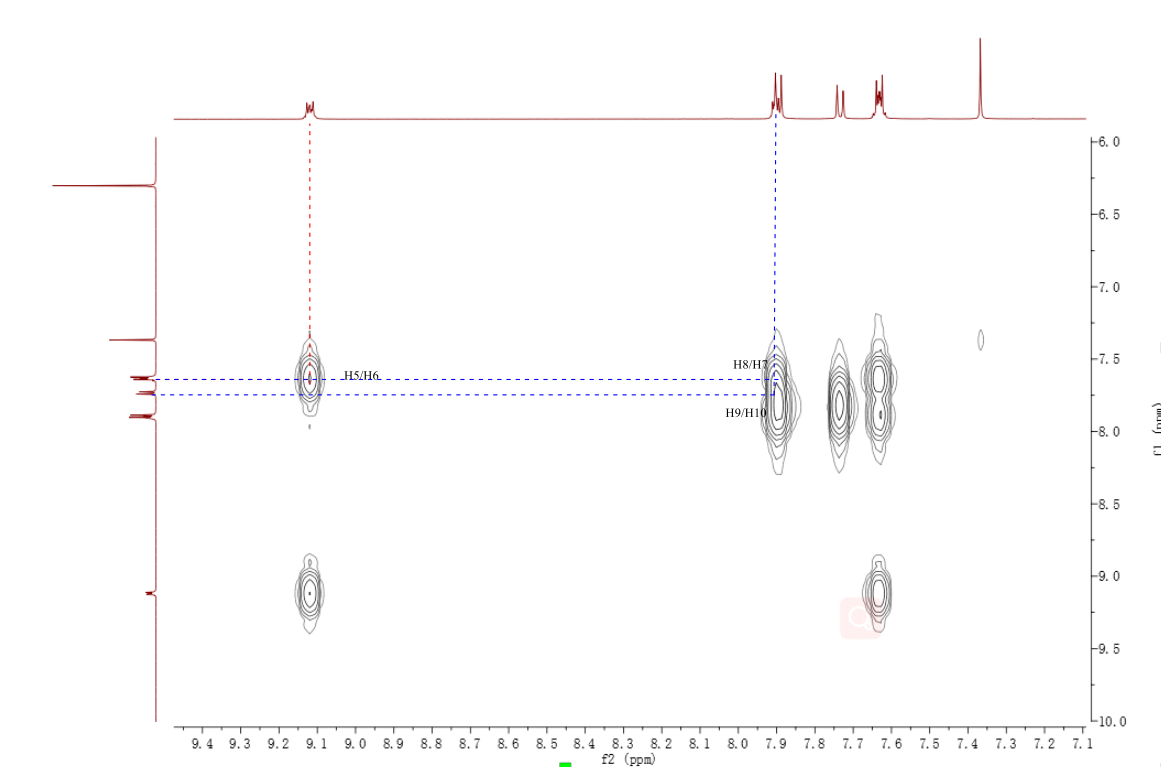
**Figure S17:** The  $^{13}\text{C}$ -NMR spectrum of compound **2** in  $\text{CD}_3\text{OD}$  (150 MHz)



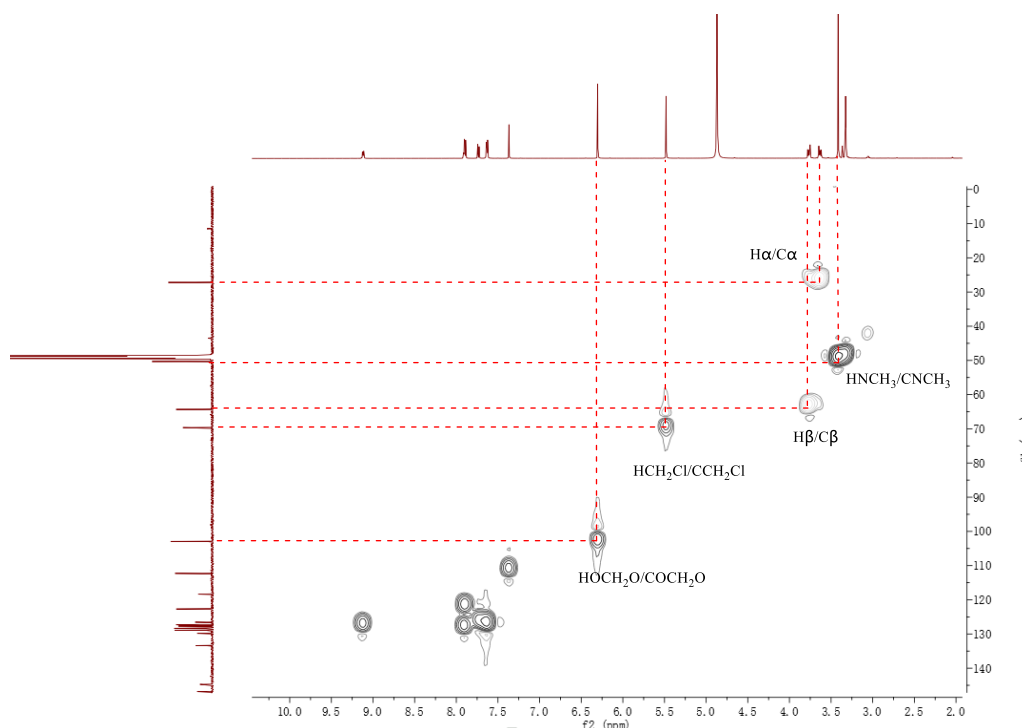
**Figure S18:** The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2** in  $\text{CD}_3\text{OD}$



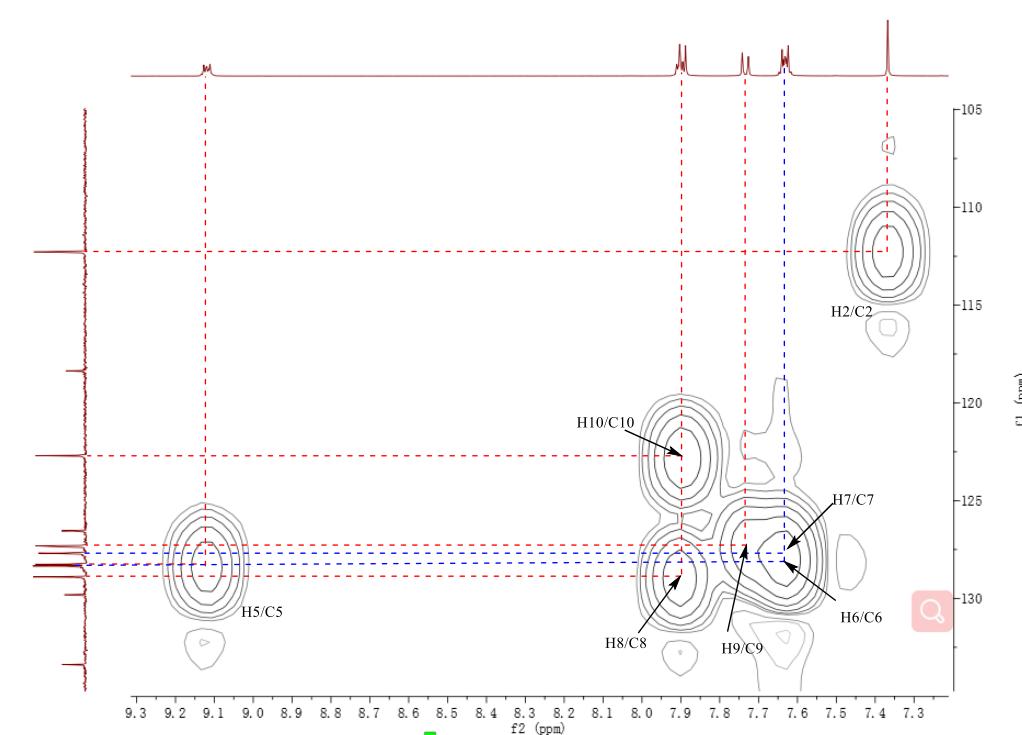
**Figure S19:** The <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **2** in CD<sub>3</sub>OD (From  $\delta_{\text{H}}$  2.9 to 4.2)



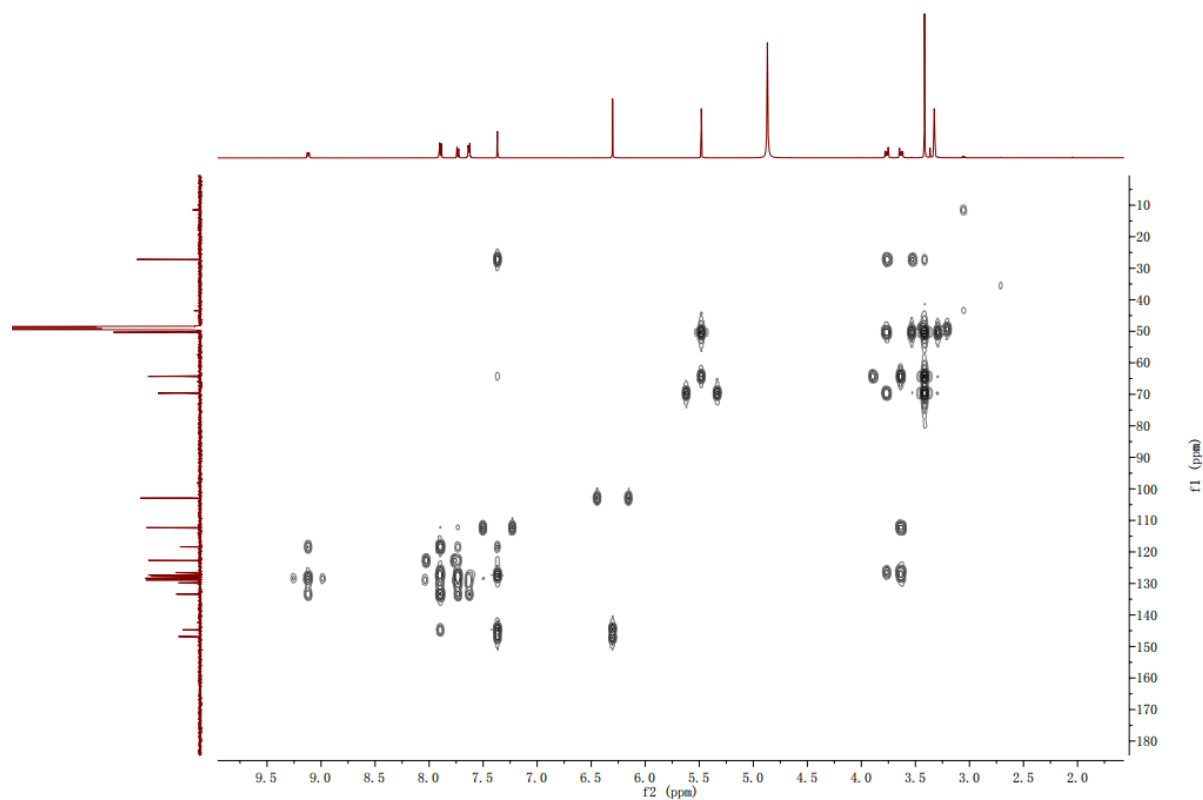
**Figure S20:** The <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **2** in CD<sub>3</sub>OD (From  $\delta_{\text{H}}$  6.0 to 10)



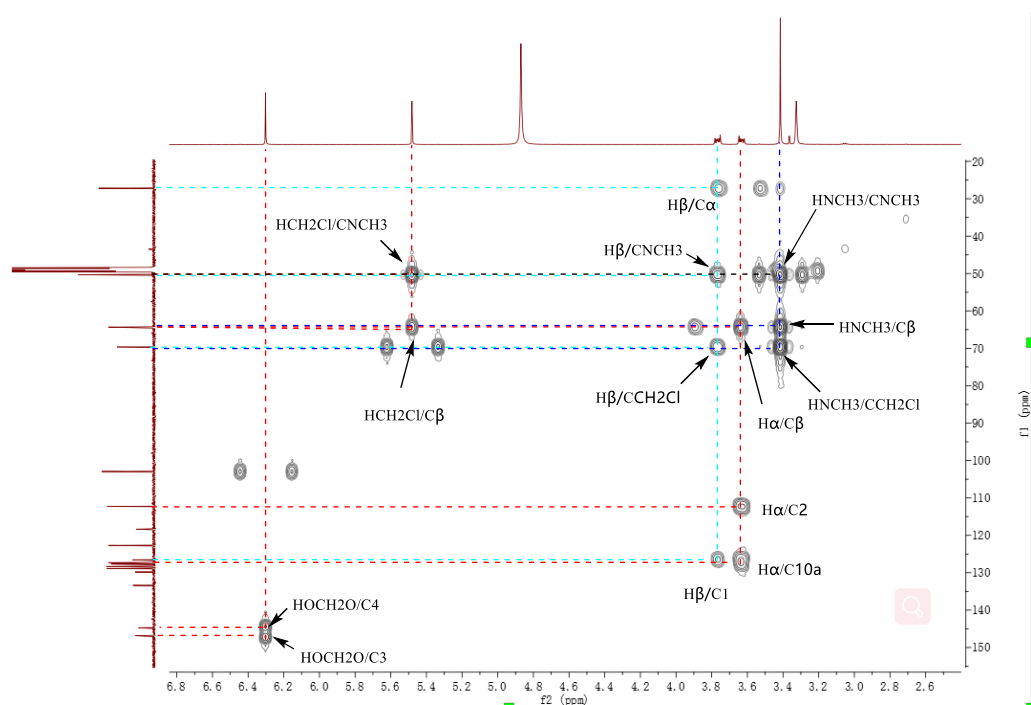
**Figure S21:** The HSQC spectrum of compound **2** in CD<sub>3</sub>OD



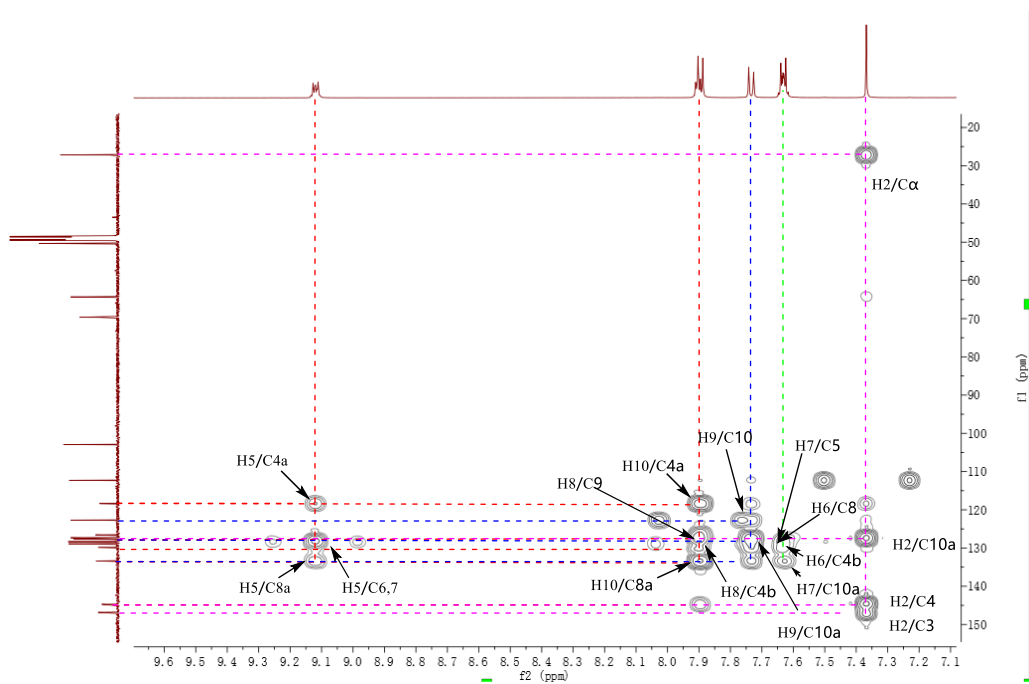
**Figure S22:** The HSQC spectrum of compound **2** in CD<sub>3</sub>OD (From  $\delta_C$  110 to 140)



**Figure S23:** The HMBC spectrum of compound **2** in CD<sub>3</sub>OD



**Figure S24:** The HMBC spectrum of compound **2** in CD<sub>3</sub>OD (From  $\delta_H$  2.6 to 6.8)

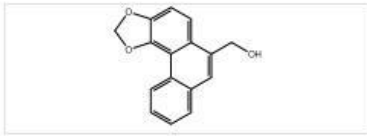
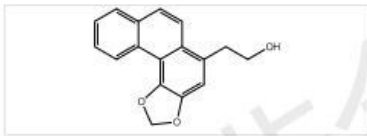


**Figure S25:** The HMBC spectrum of compound **2** in CD<sub>3</sub>OD (From  $\delta_{\text{H}}$  7.1 to 9.6)



## Substances (2)

[View in SciFinder®](#)

1		Similarity Score: 99																
<b>500554-75-6</b>  <b>C<sub>16</sub>H<sub>12</sub>O<sub>3</sub></b> Phenanthro[3,4- <i>d</i> ]-1,3-dioxole-6-methanol 1 Reference    0 Reactions    0 Suppliers		<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>252.27</td> <td>-</td> </tr> <tr> <td>Boiling Point (Predicted)</td> <td>489.2±14.0 °C</td> <td>Press: 760 Torr</td> </tr> <tr> <td>Density (Predicted)</td> <td>1.381±0.06 g/cm<sup>3</sup></td> <td>Temp: 20 °C; Press: 760 Torr</td> </tr> <tr> <td>pKa (Predicted)</td> <td>14.03±0.10</td> <td>Most Acidic Temp: 25 °C</td> </tr> </tbody> </table>		Key Physical Properties	Value	Condition	Molecular Weight	252.27	-	Boiling Point (Predicted)	489.2±14.0 °C	Press: 760 Torr	Density (Predicted)	1.381±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr	pKa (Predicted)	14.03±0.10	Most Acidic Temp: 25 °C
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<b>2881056-41-1</b>  <b>C<sub>17</sub>H<sub>14</sub>O<sub>3</sub></b> Phenanthro[4,3- <i>d</i> ]-1,3-dioxole-5-ethanol 1 Reference    0 Reactions    0 Suppliers		<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>266.29</td> <td>-</td> </tr> <tr> <td>Boiling Point (Predicted)</td> <td>488.4±14.0 °C</td> <td>Press: 760 Torr</td> </tr> <tr> <td>Density (Predicted)</td> <td>1.337±0.06 g/cm<sup>3</sup></td> <td>Temp: 20 °C; Press: 760 Torr</td> </tr> <tr> <td>pKa (Predicted)</td> <td>14.66±0.10</td> <td>Most Acidic Temp: 25 °C</td> </tr> </tbody> </table>		Key Physical Properties	Value	Condition	Molecular Weight	266.29	-	Boiling Point (Predicted)	488.4±14.0 °C	Press: 760 Torr	Density (Predicted)	1.337±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr	pKa (Predicted)	14.66±0.10	Most Acidic Temp: 25 °C
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pKa (Predicted)	14.66±0.10	Most Acidic Temp: 25 °C																

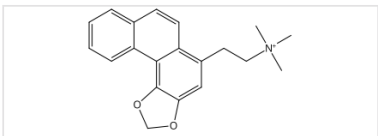
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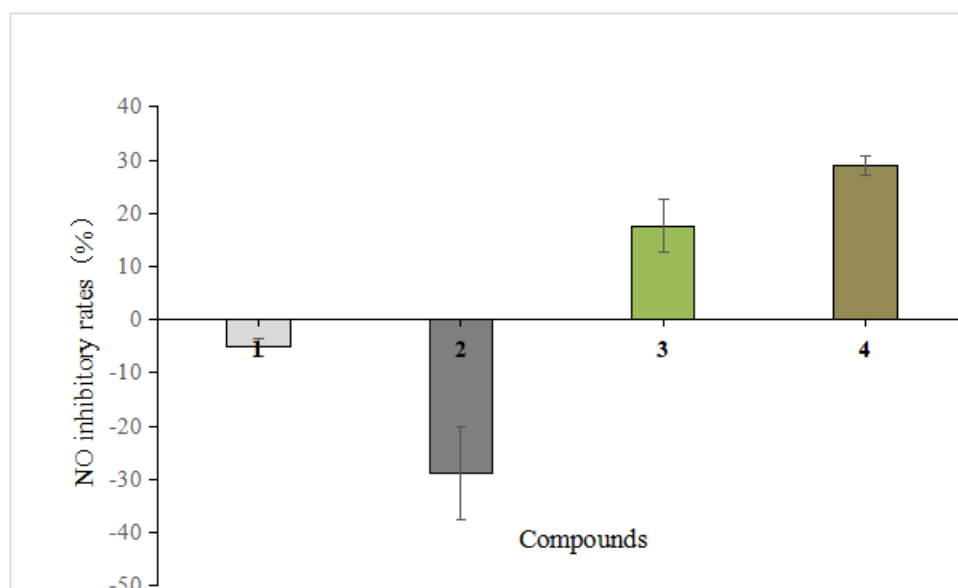
**Figure S26:** SciFinder search report for the non dimer version of compound 1 with 90-99 % similarity.

## Substances (1)

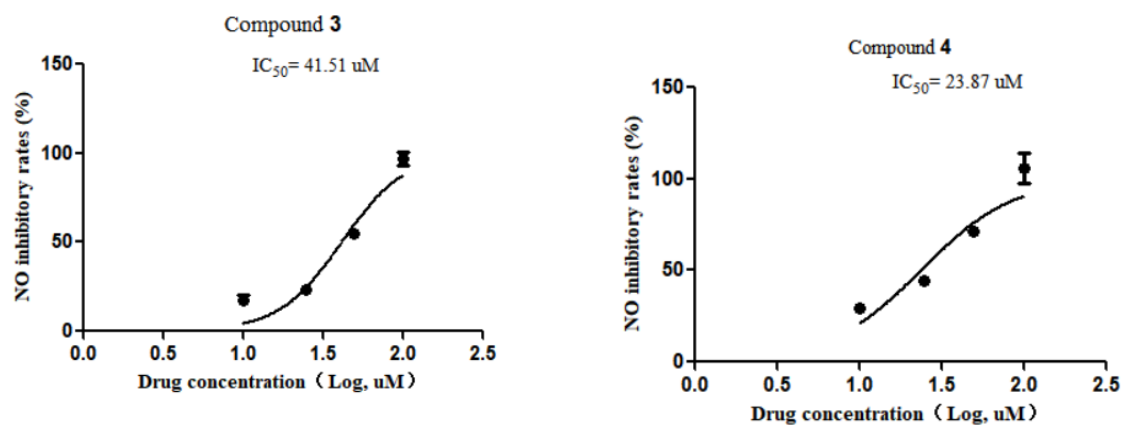
[View in SciFinder®](#)

1	Similarity Score: 91						
<b>785744-42-5</b>  <b>C<sub>20</sub>H<sub>22</sub>NO<sub>2</sub></b> <i>N,N,N</i> -Trimethylphenanthro[3,4- <i>d</i> ]-1,3-dioxole-5-ethanaminium 3 References    11 Reactions    1 Supplier	<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>308.39</td><td>-</td></tr></tbody></table>	Key Physical Properties	Value	Condition	Molecular Weight	308.39	-
Key Physical Properties	Value	Condition					
Molecular Weight	308.39	-					

**Figure S27:** SciFinder search report of compound **2** with 90-99 % similarity.



**Figure S28:** The NO inhibitory rates of compounds **1-4** at the concentration of 10  $\mu$ M



**Figure S29:** NO inhibition curve of compounds 3 and 4