

## Supporting Information

*Rec. Nat. Prod.* X:X (2025) XX-XX

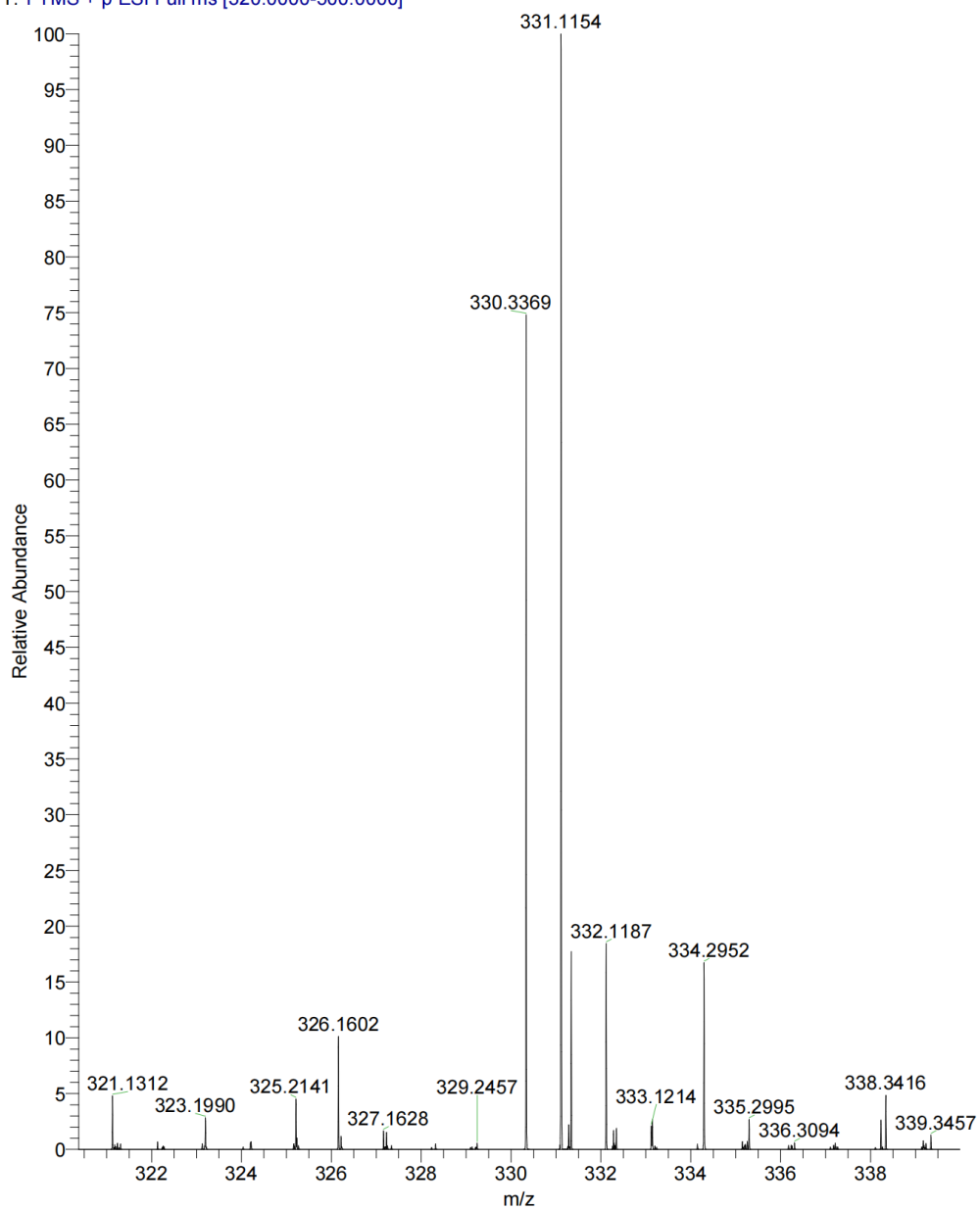
### Chemical Constituents of *Siegesbeckia orientalis* and Their Anti-proliferative Activity

Rongxian Li<sup>#</sup>, Di Ge<sup>#</sup>, Wenyong Yin, Yongqi Zhang, Mengjia Liu,  
Han Xue, Xianshou Zhao and Na Liu\*

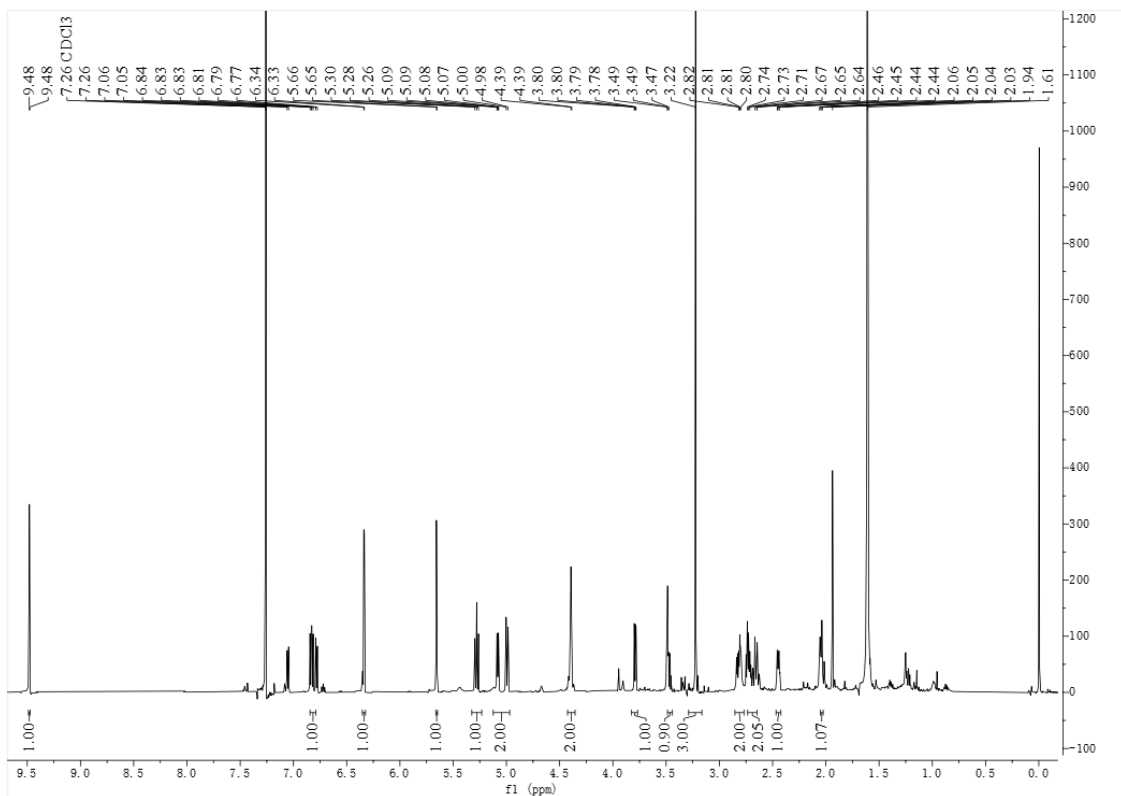
*School of Biological Science and Technology, University of Jinan, Jinan 250022, China Jinan,  
Shandong 250000, P. R. China*

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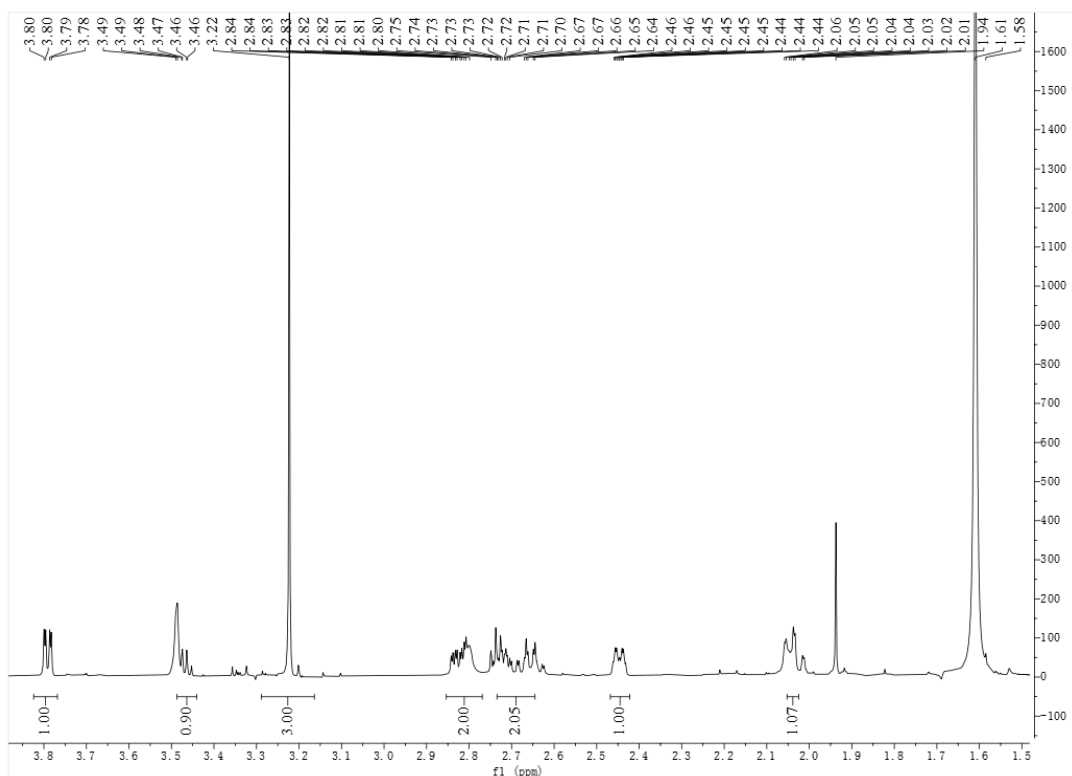
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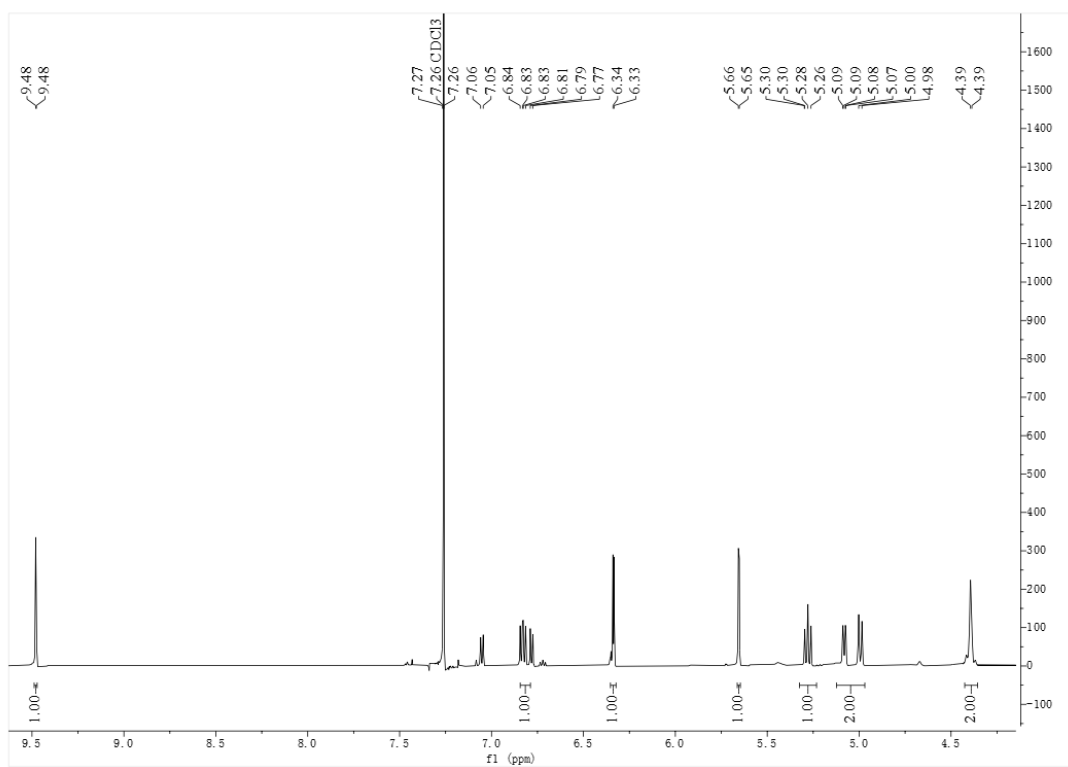
**Figure S1: HR-ESI-MS Spectrum of 1.**



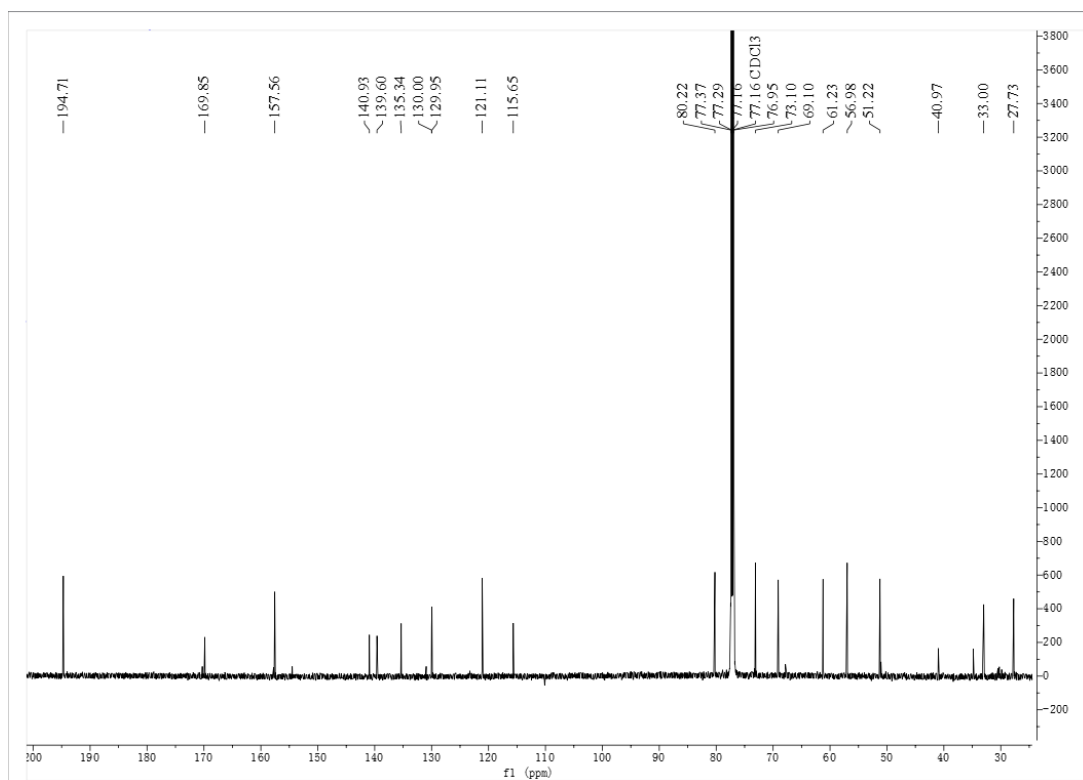
**Figure S2:** <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>) Spectrum of **1**.



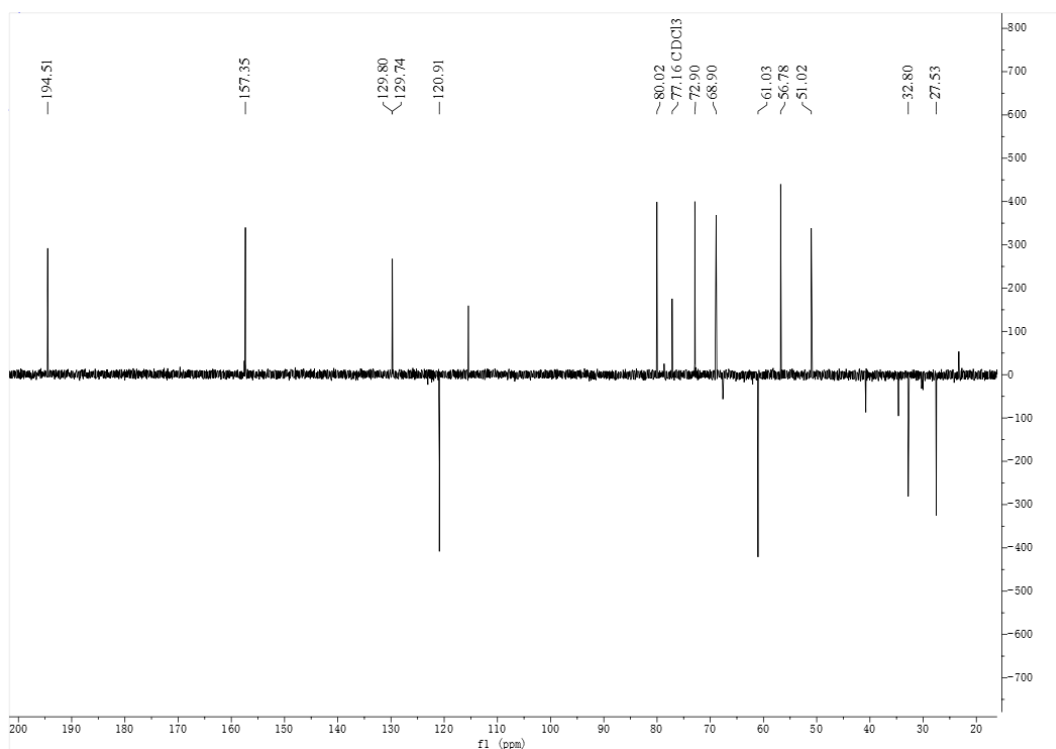
**Figure S3:** <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>) Spectrum of **1** (From  $\delta_H$  1.6 ppm to  $\delta_H$  3.8 ppm).



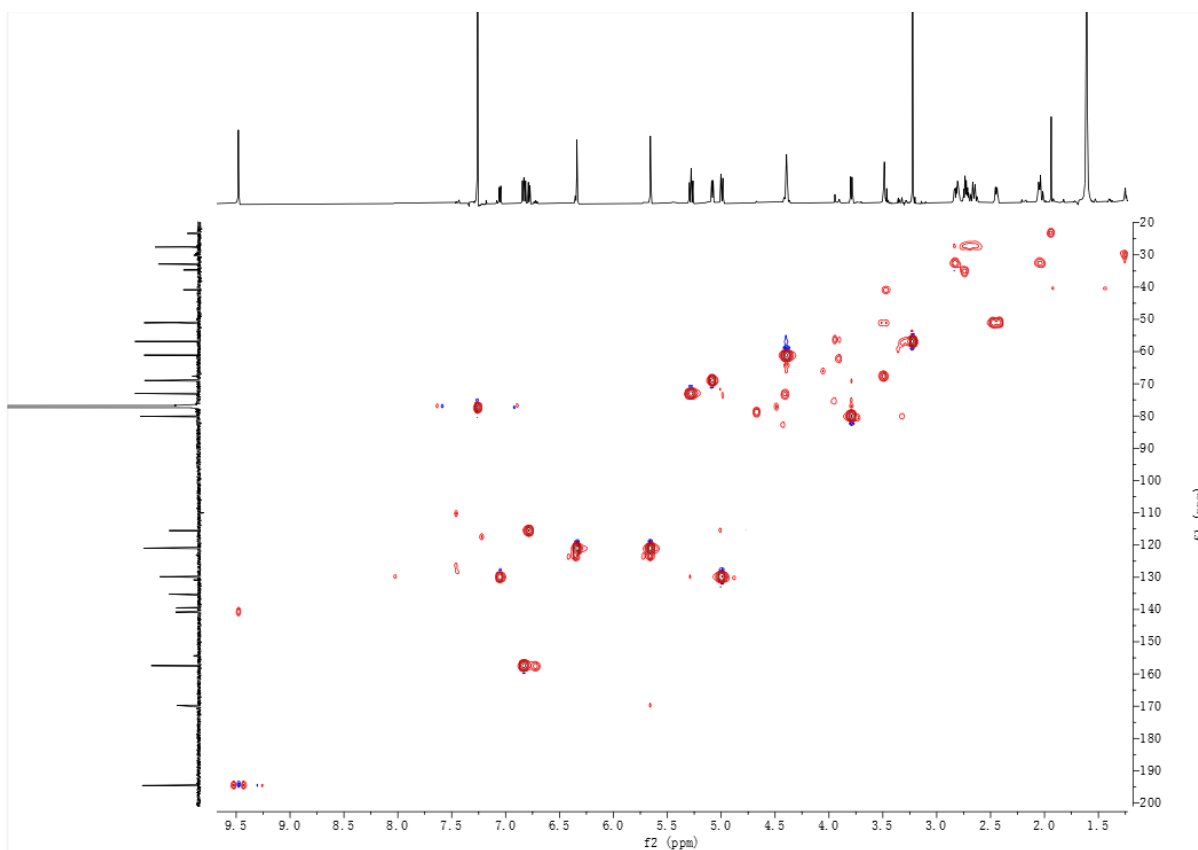
**Figure S4:**  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ ) Spectrum of **1** (From  $\delta_{\text{H}}$  4.4 ppm to  $\delta_{\text{H}}$  9.5 ppm).



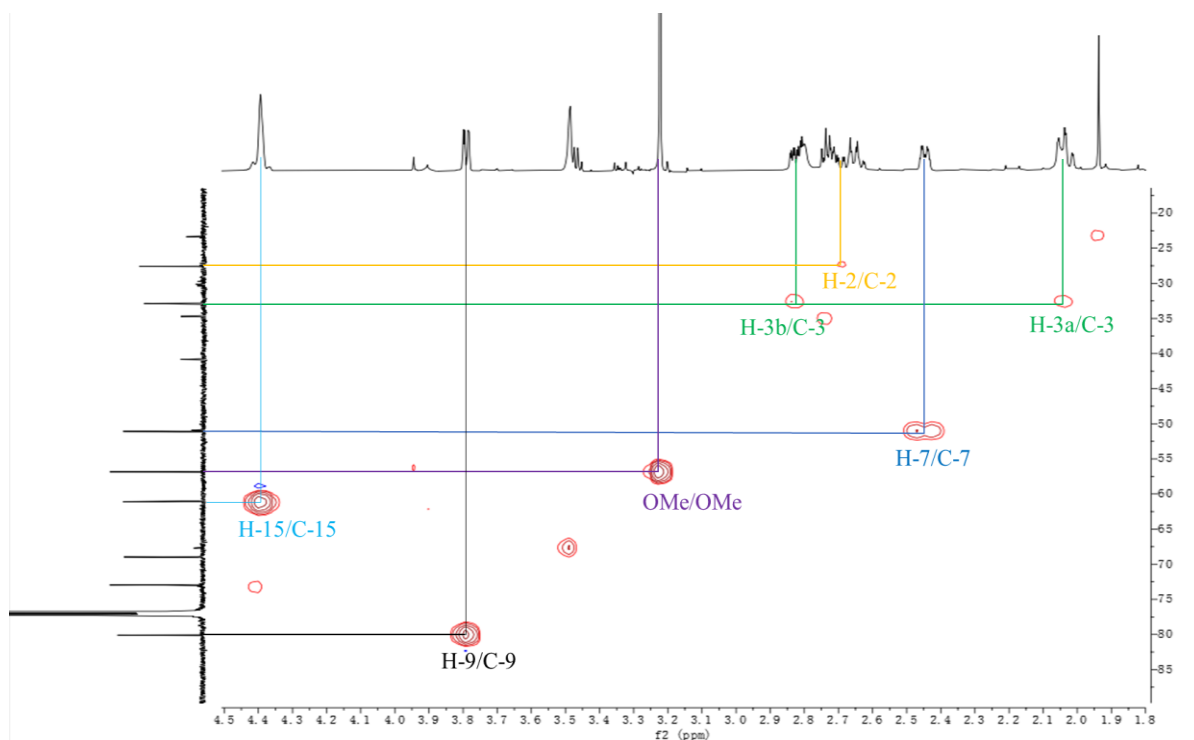
**Figure S5:**  $^{13}\text{C-NMR}$  (600 MHz,  $\text{CDCl}_3$ ) Spectrum of **1**.



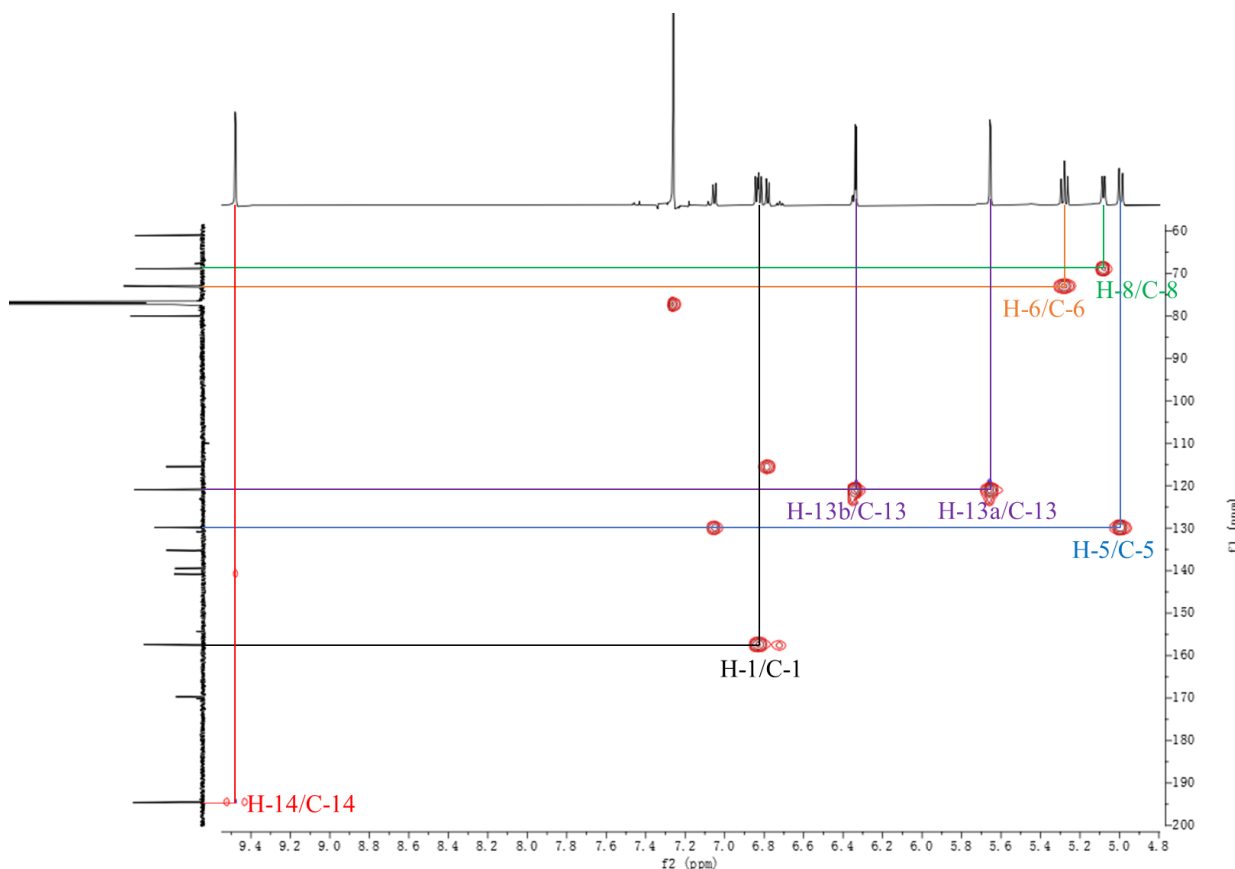
**Figure S6:** DEPT135 (600 MHz, CDCl<sub>3</sub>) Spectrum of **1**.



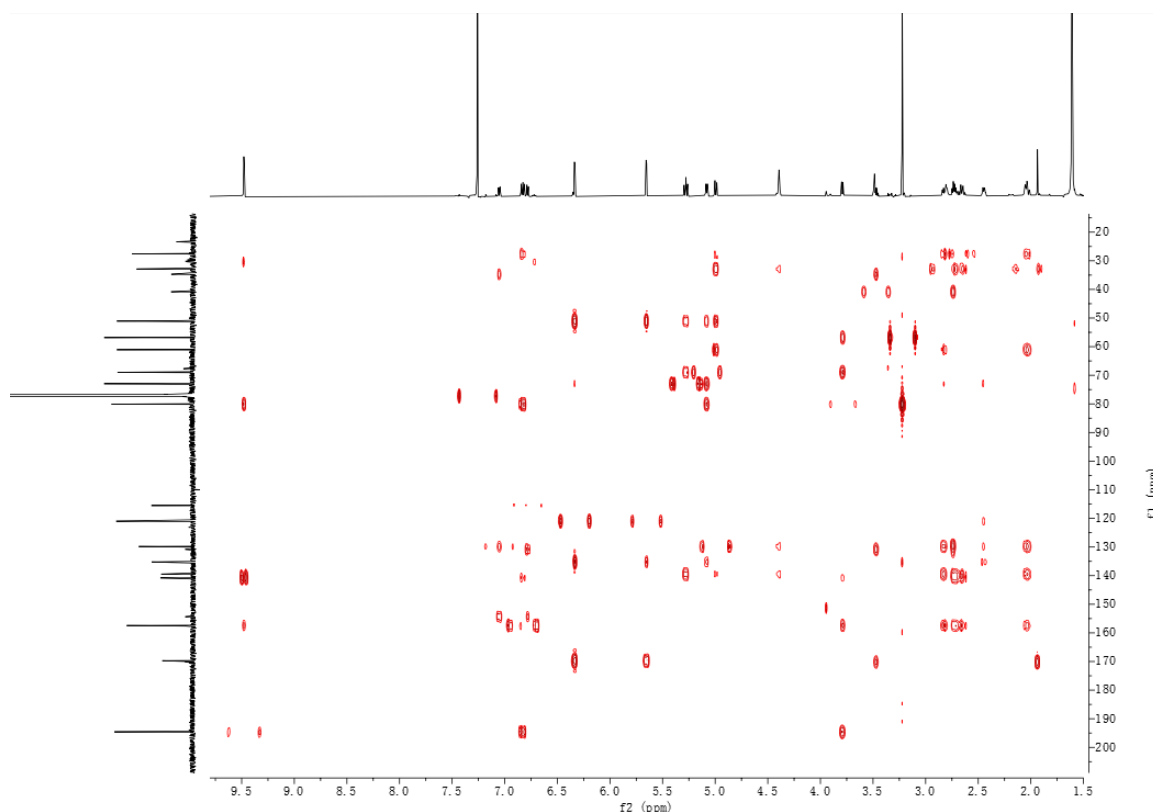
**Figure S7:** HSQC Spectrum of **1**.



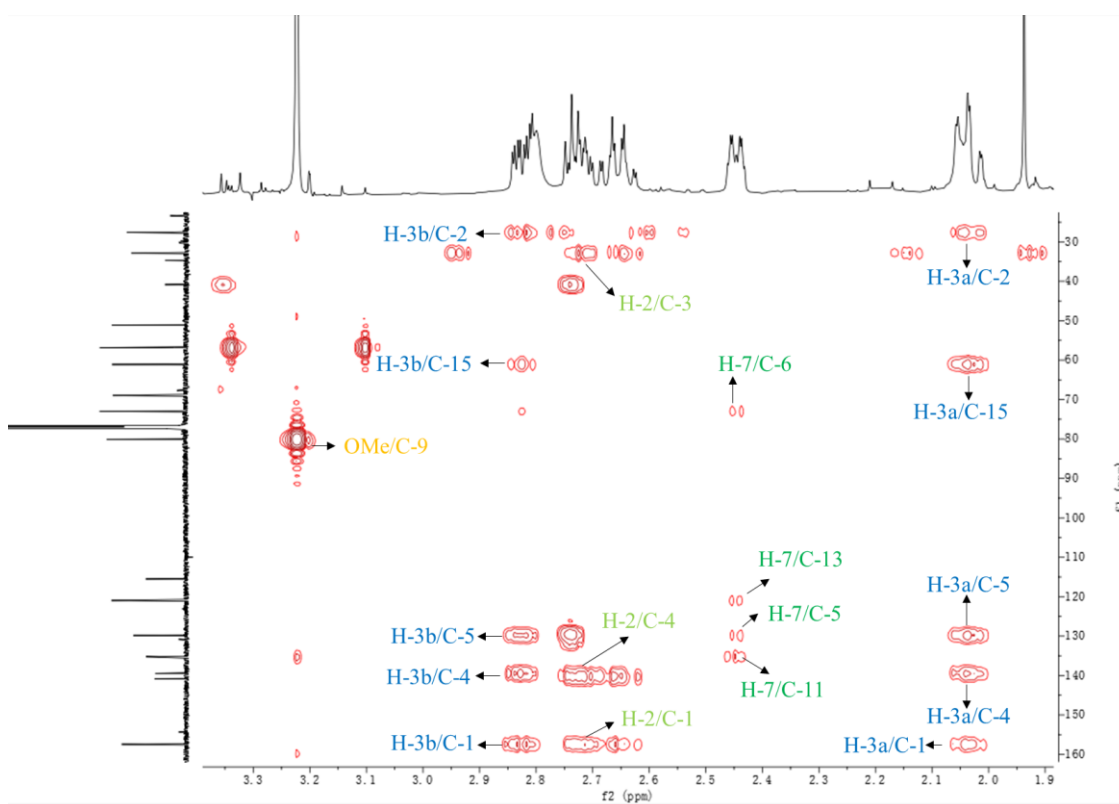
**Figure S8:** HSQC Spectrum of **1** (From  $\delta_{\text{H}}$  1.9 ppm to  $\delta_{\text{H}}$  4.4 ppm).



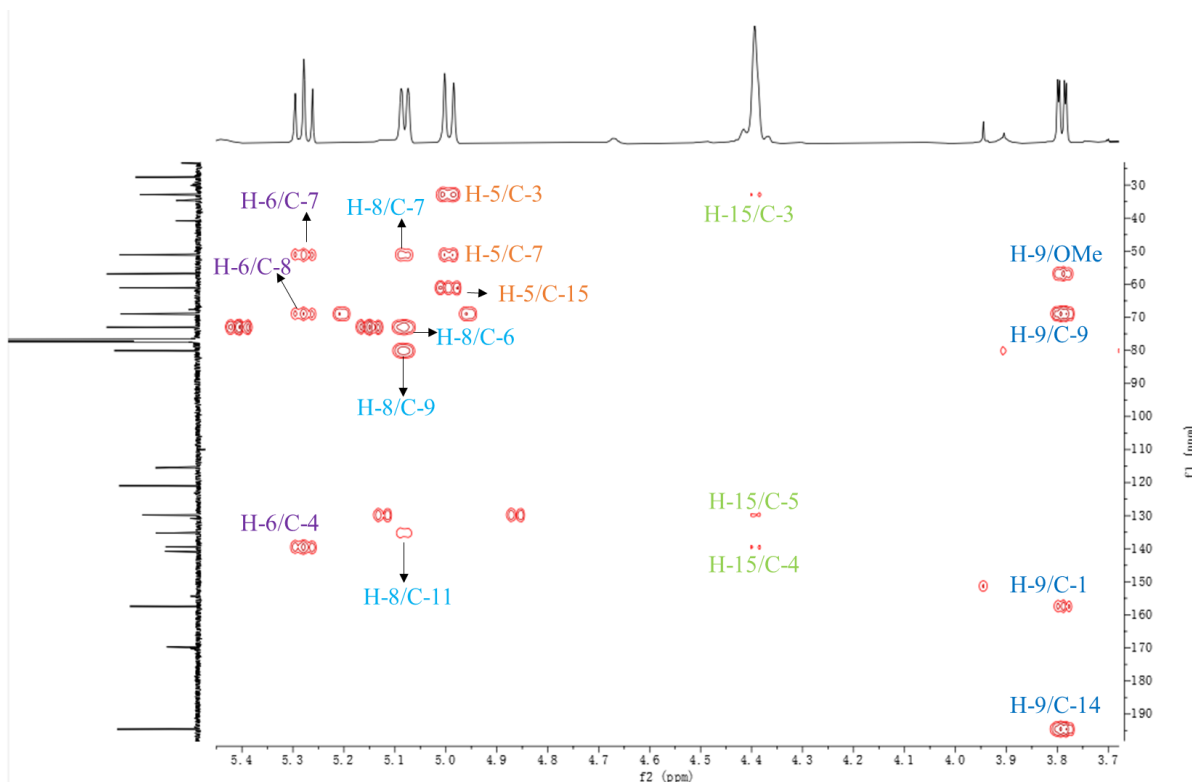
**Figure S9:** HSQC Spectrum of **1** (From  $\delta_{\text{H}}$  5.0 ppm to  $\delta_{\text{H}}$  9.5 ppm).



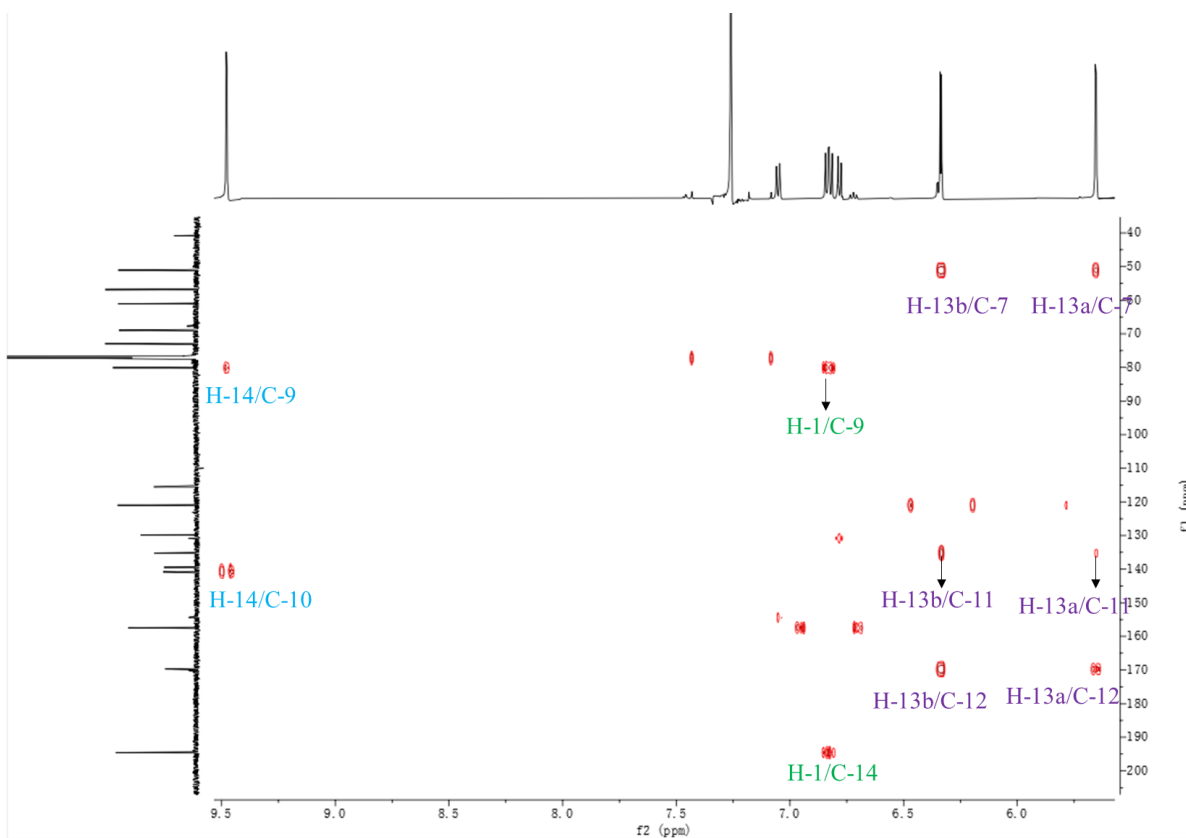
**Figure S10:** HMBC Spectrum of **1**.



**Figure S11:** HMBC Spectrum of **1** (From  $\delta_{\text{H}}$  1.9 ppm to  $\delta_{\text{H}}$  3.2 ppm ).

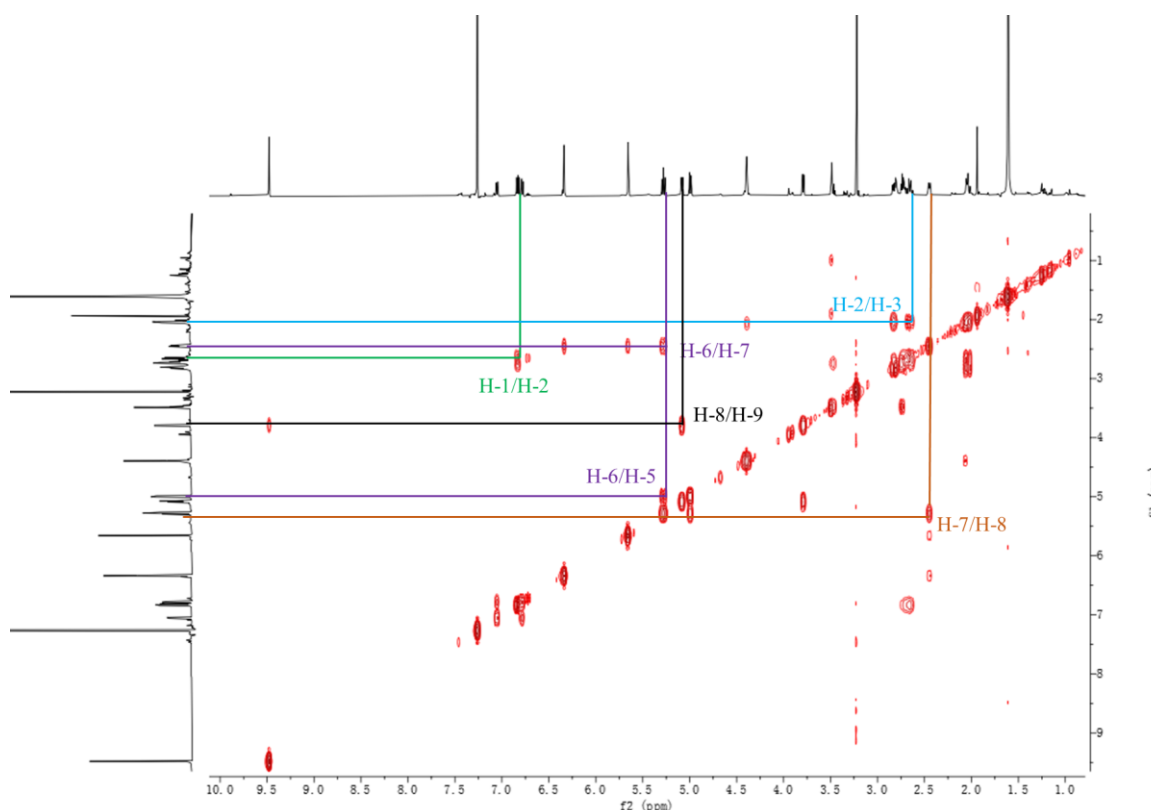


**Figure S12:** HMBC Spectrum of **1** (From  $\delta_H$  3.8 ppm to  $\delta_H$  5.3 ppm ).

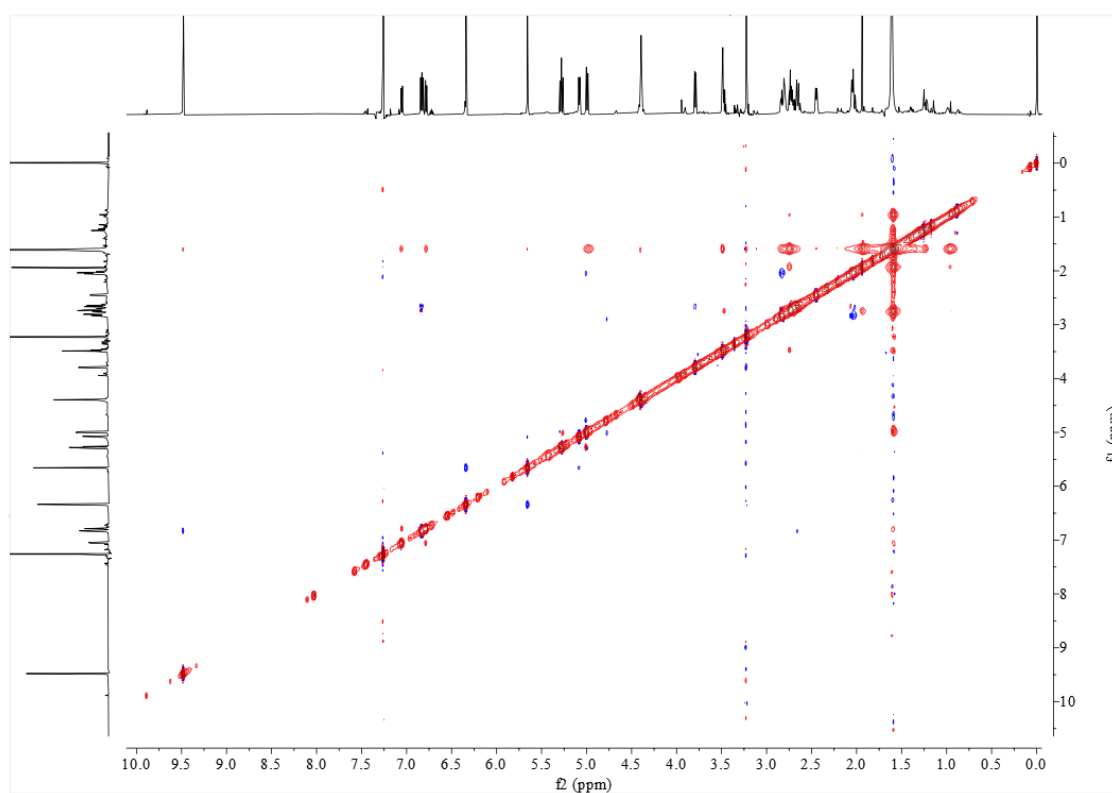


**Figure S13:** HMBC Spectrum of **1** (From  $\delta_H$  5.6 ppm to  $\delta_H$  9.5 ppm ).

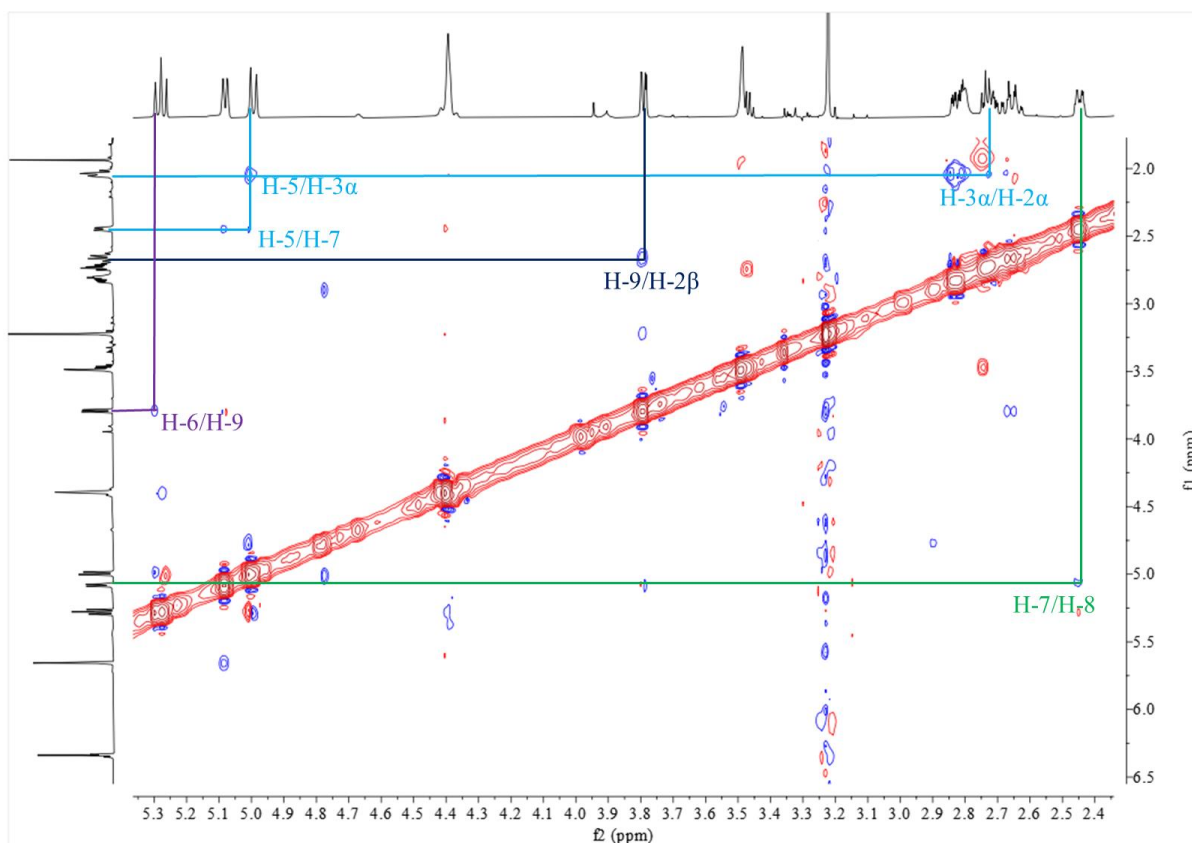




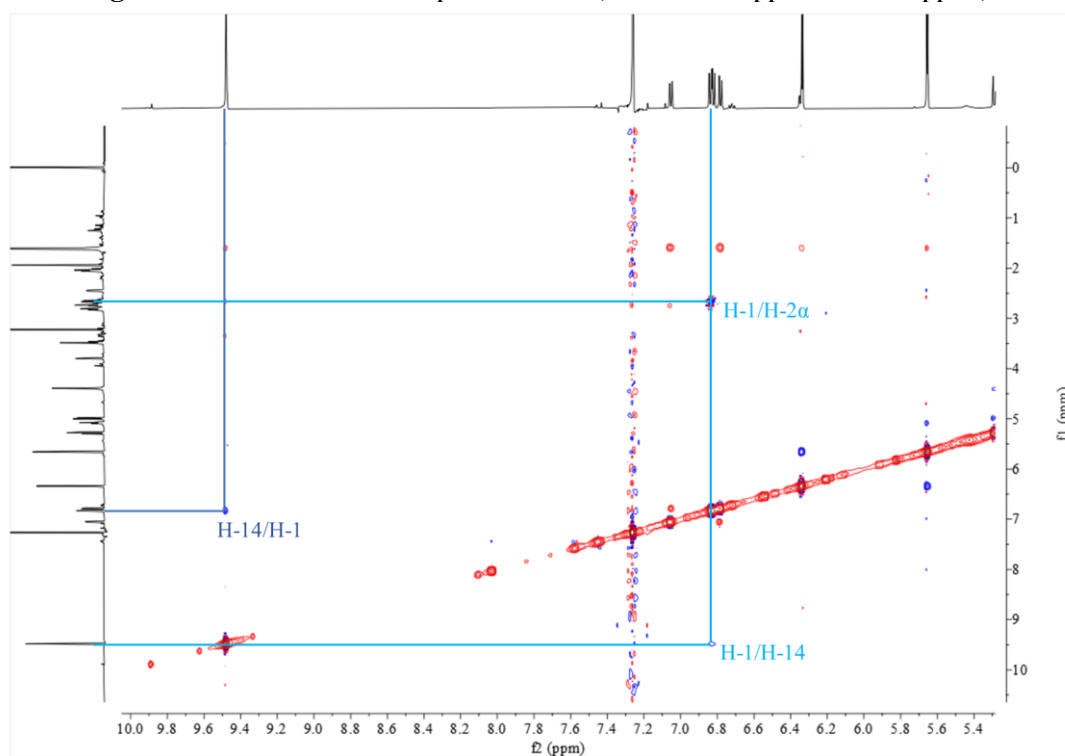
**Figure S14:**  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of **1**.



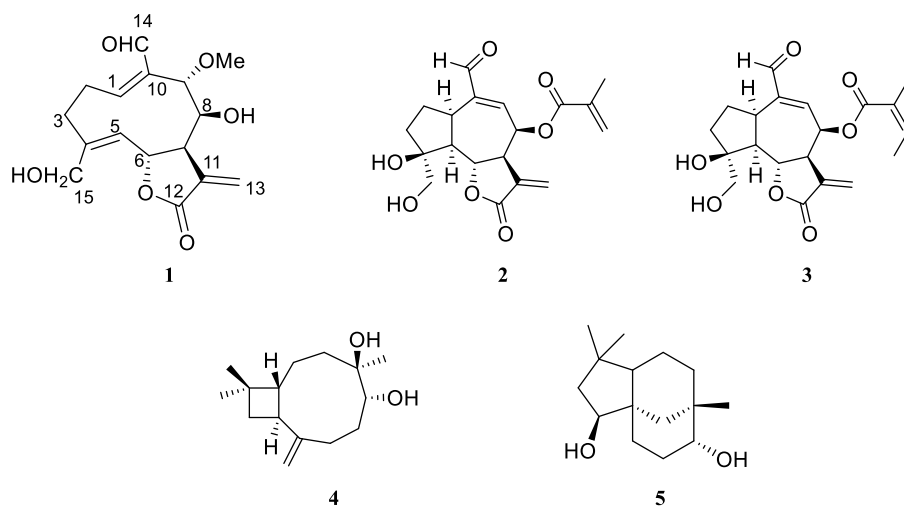
**Figure S15:**  $^1\text{H}$ - $^1\text{H}$  NOESY Spectrum of **1**.



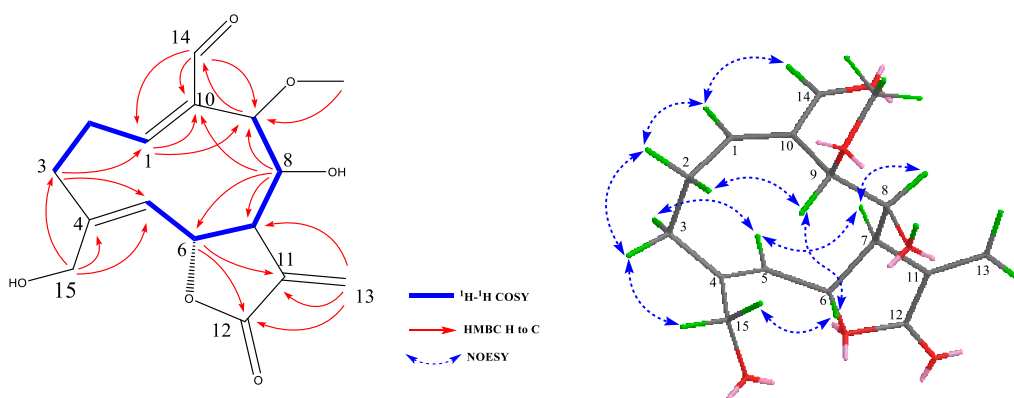
**Figure S16:** <sup>1</sup>H-<sup>1</sup>H NOESY Spectrum of **1** (From  $\delta_H$  2.4 ppm to  $\delta_H$  5.3 ppm ).



**Figure S17:** <sup>1</sup>H-<sup>1</sup>H NOESY Spectrum of **1** (From  $\delta_H$  5.6 ppm to  $\delta_H$  9.6 ppm ).



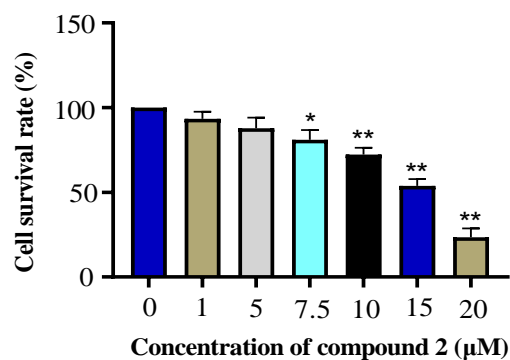
**Figure S18:** The structures of compounds 1-5.



**Figure S19:** COSY, HMBC and NOESY correlations of compound 1.

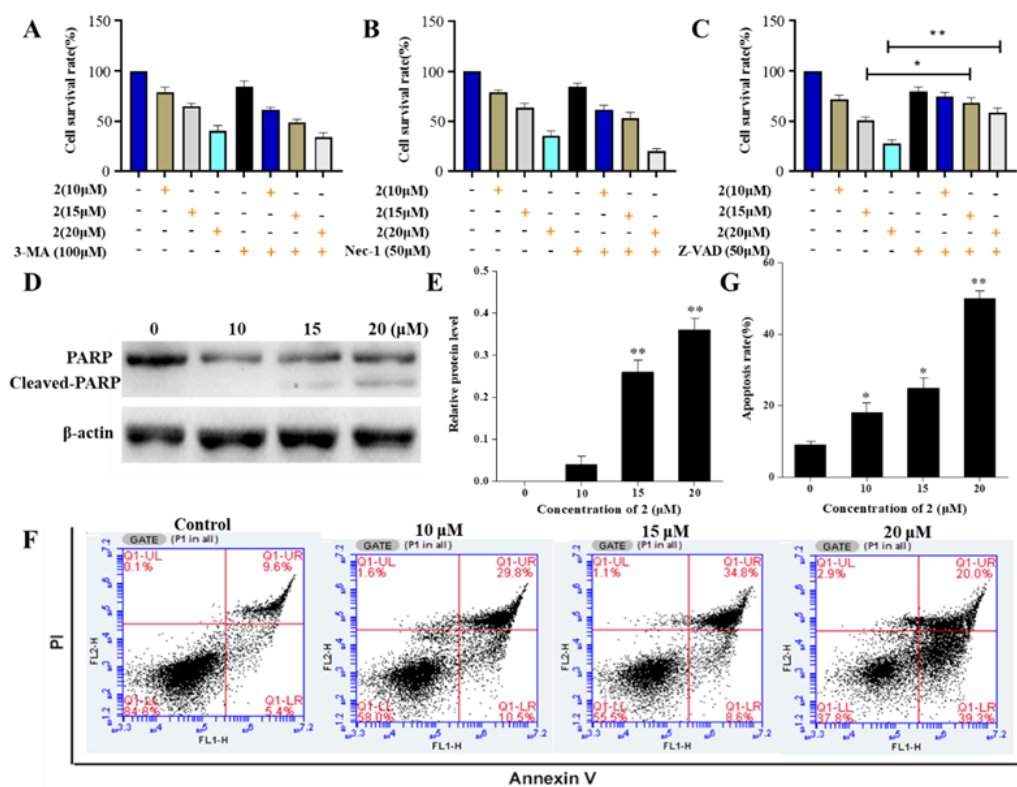
**Table S1:** NMR spectral data for compound **1** in CDCl<sub>3</sub> (600/150 MHz).

No.	<b>1</b>				
	$\delta_{\text{H}}$ (J, Hz)	$\delta_{\text{C}}$	<sup>1</sup> H- <sup>13</sup> C HMBC	<sup>1</sup> H- <sup>1</sup> H COSY	<sup>1</sup> H- <sup>1</sup> H NOESY
1	6.81 dd (10.0, 7.6)	157.6	C-3, C-9, C-10, C-14	H-2	H-2 $\alpha$ , H-14
2 $\alpha$	2.66 m	27.7	C-1, C-3, C-4	H-1	H-1, H-3 $\alpha$
2 $\beta$	2.73 m				H-9
3 $\alpha$	2.04 m	33.0	C-1, C-2, C-5, C-15		H-2 $\alpha$ , H-5, H-15 $\alpha$
3 $\beta$	2.82 m				
4		139.6			
5	4.99 d (10.6)	130.0	C-3, C-4, C-7, C-15	H-6	H-3 $\alpha$ , H-7
6	5.28 t (10.2)	73.1	C-4, C-7, C-8	H-5, H-7	H-15 $\beta$ , H-9
7	2.45 m	51.2	C-5, C-6, C-8, C-13	H-6, H-8	H-5, H-8
8	5.08 d (8.0)	69.1	C-6, C-7, C-10, C-9	H-7, H-9	H-7
9	3.79 dd (8.0, 2.2)	80.2	C-1, C-8, C-10, C-14		H-2 $\beta$ , H-6
10		140.9			
11		135.3			
12		169.9			
13a	5.65 d (3.1)	121.1	C-7, C-11, C-12		
13b	6.34 d (3.5)				
14	9.48 d	194.7	C-1, C-9, C-10		H-1
15	4.39 s (2H)	61.2	C-3, C-4, C-5		H-3 $\alpha$
-OMe	3.22 s	57.0	C-9		H-6

**Figure S20:** Compound **2** had cytotoxic effect on MDA-MB-231 cells.

**Table S2:** Anti-breast cancer activity of isolated compounds (IC<sub>50</sub> in μM).

	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	Adriamycin
MDA-MB-231	>20	13.73 ± 1.24	>20	>20	>20	4.35 ± 1.08



**Figure S21.** Apoptosis induced by Compound 2 in MDA-MB-231 cells.

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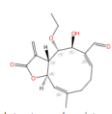
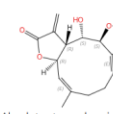
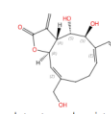
References Reactions Suppliers

Structure Match: As Drawn (0), Substructure (0), Similarity (36K)

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17 Results Sort: Relevance View: Partial

<p>1 96</p> <p>246516-30-3</p>  <p>Absolute stereochemistry shown E/Z labels describe double bond geometry</p> <p>C<sub>17</sub>H<sub>22</sub>O<sub>5</sub> (3aS,4S,5S,6E,10E,11aR)-4-Ethoxy-2,3,3a,4,</p>	<p>2 96</p> <p>146564-54-7</p>  <p>Absolute stereochemistry shown E/Z labels describe double bond geometry</p> <p>C<sub>16</sub>H<sub>20</sub>O<sub>5</sub> Cyclodeca[b]furan-6-carboxaldehyde, 2,3,</p>	<p>3 96</p> <p>145042-18-8</p>  <p>Absolute stereochemistry shown E/Z labels describe double bond geometry</p> <p>C<sub>15</sub>H<sub>18</sub>O<sub>6</sub> Cyclodeca[b]furan-6-carboxaldehyde, 2,3,</p>
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CAS SciFinder Substances Enter a query... Edit

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Similarity:
 

- 95-98 (3)
- 90-94 (14)
- 85-89 (83)
- 80-84 (287)
- 75-79 (881)

 View All

Reaction Role:
 

- Product (41)
- Reactant (4)

Reference Role:
 

- Preparation (59)

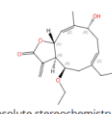
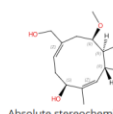
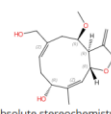
<p>1 Reference 0 Reactions 0 Suppliers</p> <p>4 93</p> <p>3061330-54-6</p>  <p>Absolute stereochemistry shown E/Z labels describe double bond geometry</p> <p>C<sub>17</sub>H<sub>24</sub>O<sub>5</sub> Cyclodeca[b]furan-2(3H)-one, 4-ethoxy-3a,4,5,8,9,11a-hexahydro-9-hydroxy-6-(hydr...</p> <p>2 References 1 Reaction 0 Suppliers</p>	<p>1 Reference 0 Reactions 0 Suppliers</p> <p>5 93</p> <p>3061330-73-9</p>  <p>Absolute stereochemistry shown E/Z labels describe double bond geometry</p> <p>C<sub>16</sub>H<sub>22</sub>O<sub>5</sub></p> <p>2 References 1 Reaction 0 Suppliers</p>	<p>1 Reference 0 Reactions 0 Suppliers</p> <p>6 93</p> <p>3061330-53-5</p>  <p>Absolute stereochemistry shown E/Z labels describe double bond geometry</p> <p>C<sub>16</sub>H<sub>22</sub>O<sub>5</sub> Cyclodeca[b]furan-2(3H)-one, 3a,4,5,8,9,11a-hexahydro-9-hydroxy-6-(hydroxy methyl...</p> <p>2 References 1 Reaction 0 Suppliers</p>
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Figure S22: The Scifinder similarity report for new compound 1.

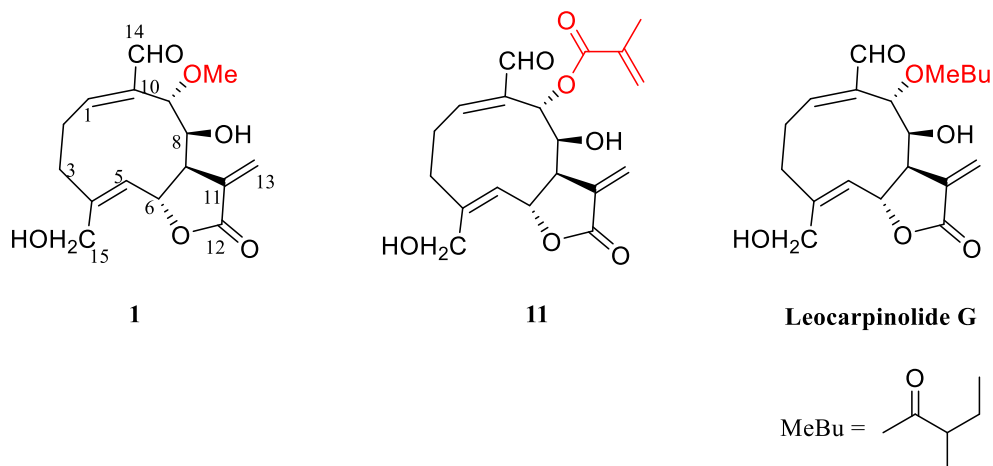


Figure S23: The structure is most similar to compound 1.

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**Table S3:** The <sup>1</sup>H NMR data for compound **1** and the similar compounds.

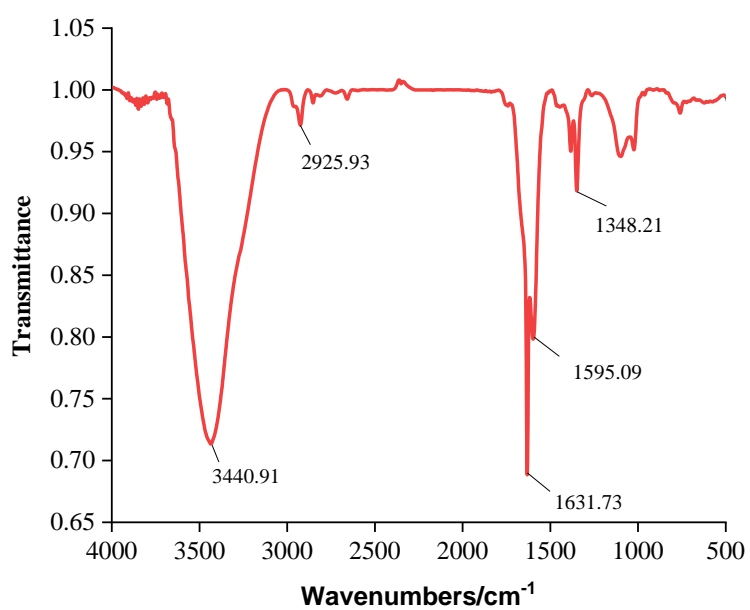
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1	6.81 dd (10.0, 7.6)	6.77 dd (10.0, 7.6)	6.61 dd
2	2.66 m 2.73 m	2.69 m 3.01 m	2.50 dddd 2.79 dddd
3	2.04 m 2.82 m	2.03 t (12.1) 2.82 m	2.04 ddd 2.72 ddd
5	4.99 d (10.6)	5.03 d (10.6)	5.17 d
6	5.28 t (10.2)	5.43 t (10.2)	5.31 dd
7	2.45 m	2.48 d (9.5)	2.49 dddd
8	5.08 d (7.9)	5.31 d (8.2)	5.46 dd
9	3.79 dd (8.0, 2.2)	5.37 dd (8.3, 1.6)	5.56 br d
13	5.65 d (3.1) 6.34 d (3.5)	5.67 d (3.1) 6.36 d (3.1)	5.68 d 6.42 d
14	9.48 d	9.46 s	9.40 d
15	4.39 s	4.49 m	4.06 br s
2'			2.41 tq
3'		6.13 s	1.60 ddq
		5.62 s	1.42 ddq
4'		1.92 s	0.85 t
5'			1.07 d

**Table S4:** The <sup>13</sup>C NMR data for compound **1** and the similar compounds.

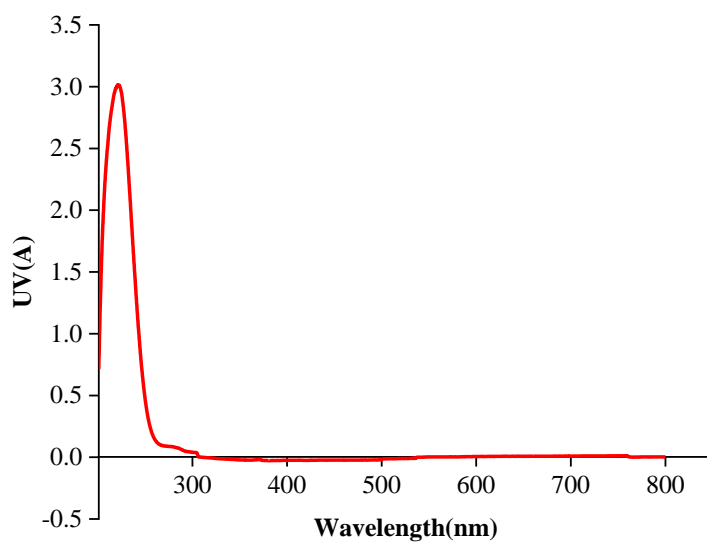
Position	<b>1</b> (600MHz, CDCl <sub>3</sub> )	<b>11</b> <sup>[1]</sup> (600MHz, CDCl <sub>3</sub> )	<b>LeocarpinolideG</b> <sup>[2]</sup> (400MHz, CDCl <sub>3</sub> )
1	157.6	158.9	155.04
2	27.6	28.0	27.39
3	33.0	33.0	32.49
4	139.6	140.6	140.30
5	130.0	129.5	128.99
6	73.1	73.0	73.75
7	51.2	52.0	51.51
8	69.1	68.5	70.38
9	80.2	73.2	71.24
10	140.9	141.4	139.51
11	135.3	135.9	133.99
12	169.9	169.6	168.95
13	121.1	120.8	123.10
14	194.7	194.4	195.37
15	61.2	61.3	60.72
1'		167.2	176.03
2'		135.6	41.24
3'		127.2	26.79
4'		18.4	11.48
5'			16.78
-OMe	56.8		

[1] N. Liu, C. Wu, J. H. Yu, K. K. Zhu, M. N. Song, F. Y. Yang, R. L. Feng, Y. Y. Zhang, W. Q. Chang and H. Zhang (2019). Germacrane-type sesquiterpenoids with cytotoxic activity from *Sigesbeckia orientalis*, *Bioorg Chem.* **92**, 103196.

[2] F. A. Macías and N. H. Fischer (1992). Melampolides from *Lecocarpus pinnatifidus*, *Phytochemistry.* **31(8)**, 2747-2754.

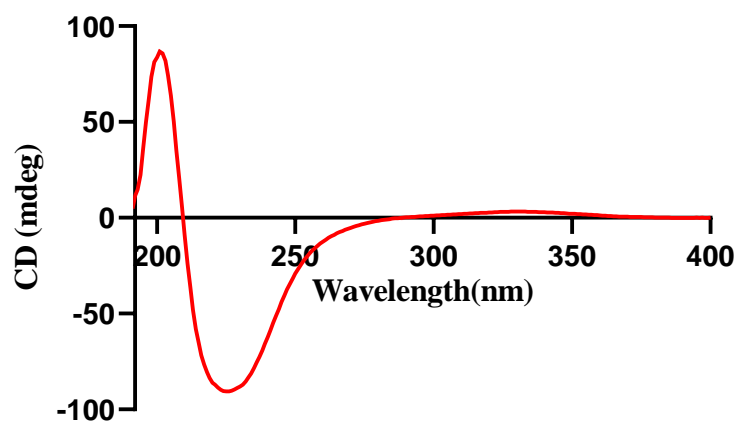


**Figure S24:** IR spectrum of compound 1.



**Figure S25:** UV spectrum of compound 1.





**Figure S26:** CD spectrum of compound **1**.



Compound1.zip

**Figure S27:** FID (NMR) files of compound **1**.