

# Supporting Information

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## A New Clerodane-type Diterpene from *Conyza blinii*

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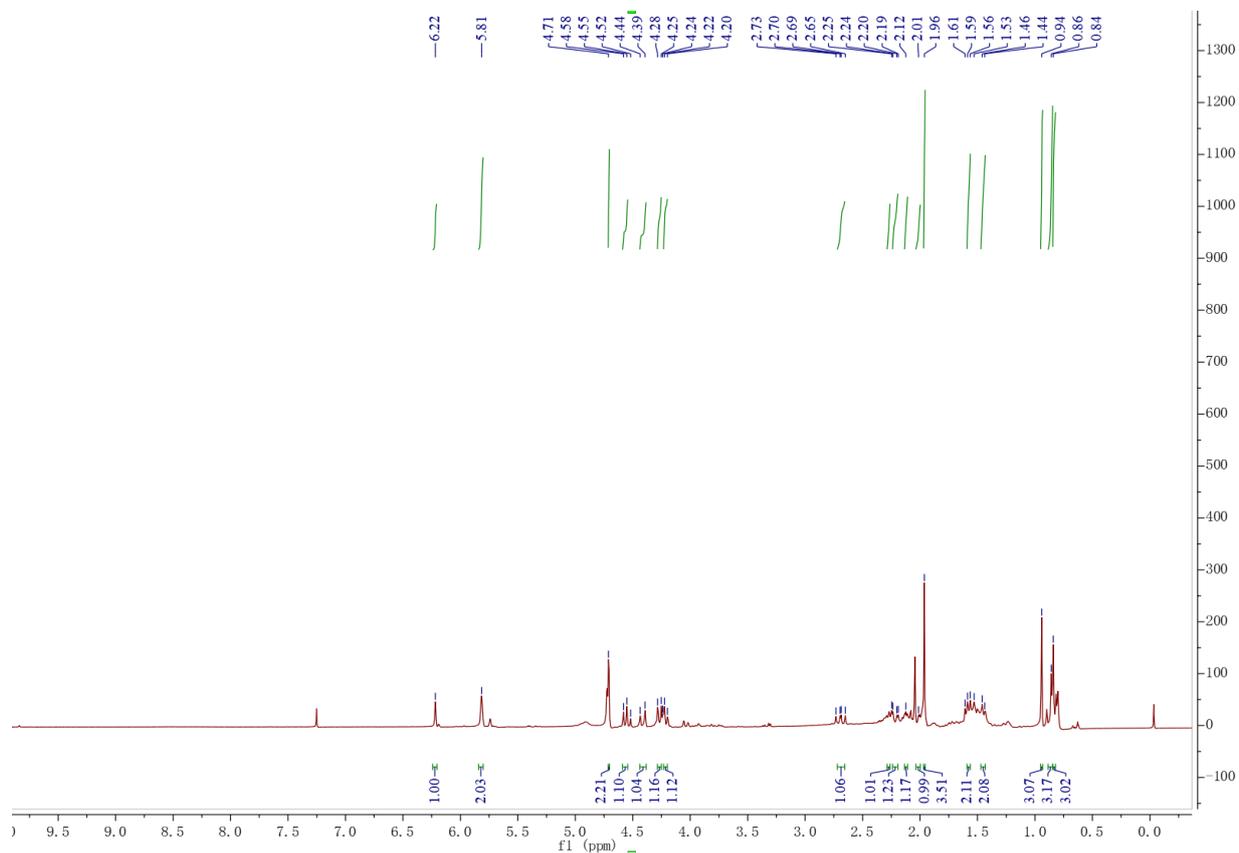
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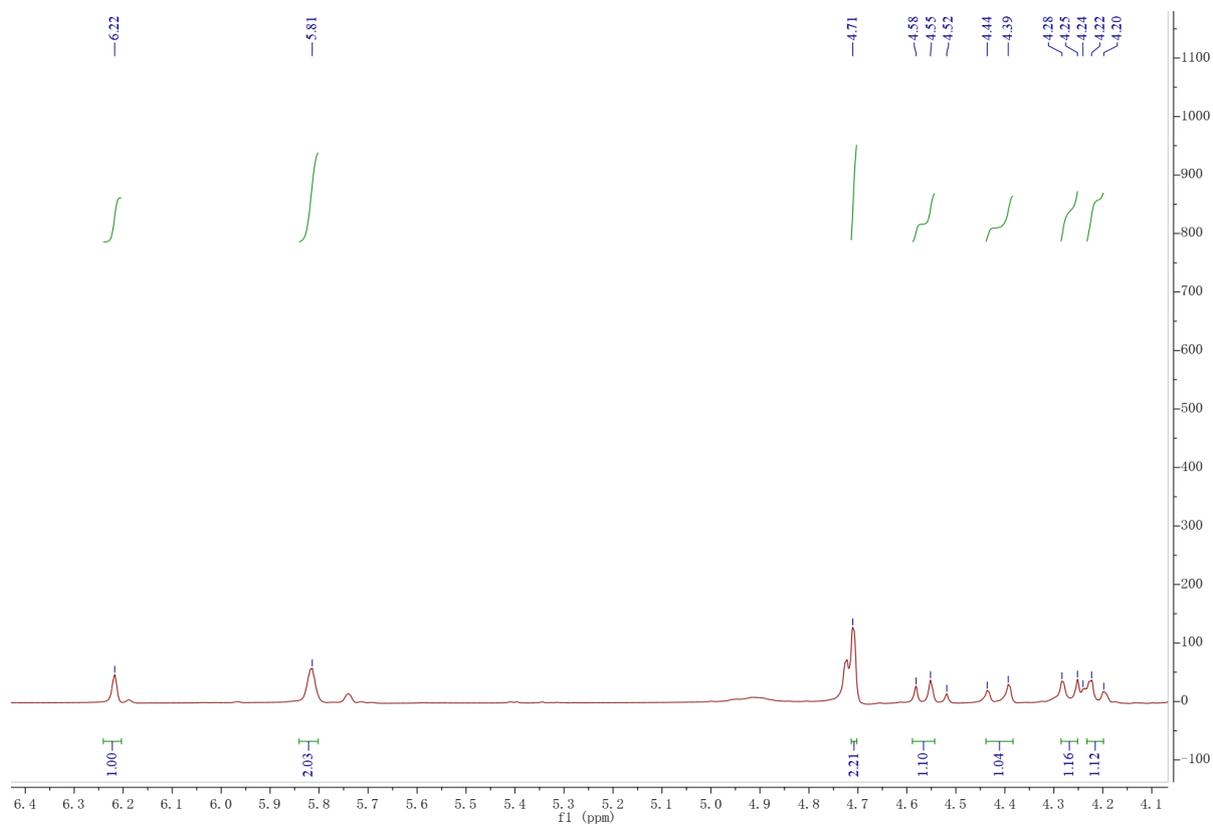
# These authors contributed equally to this work.

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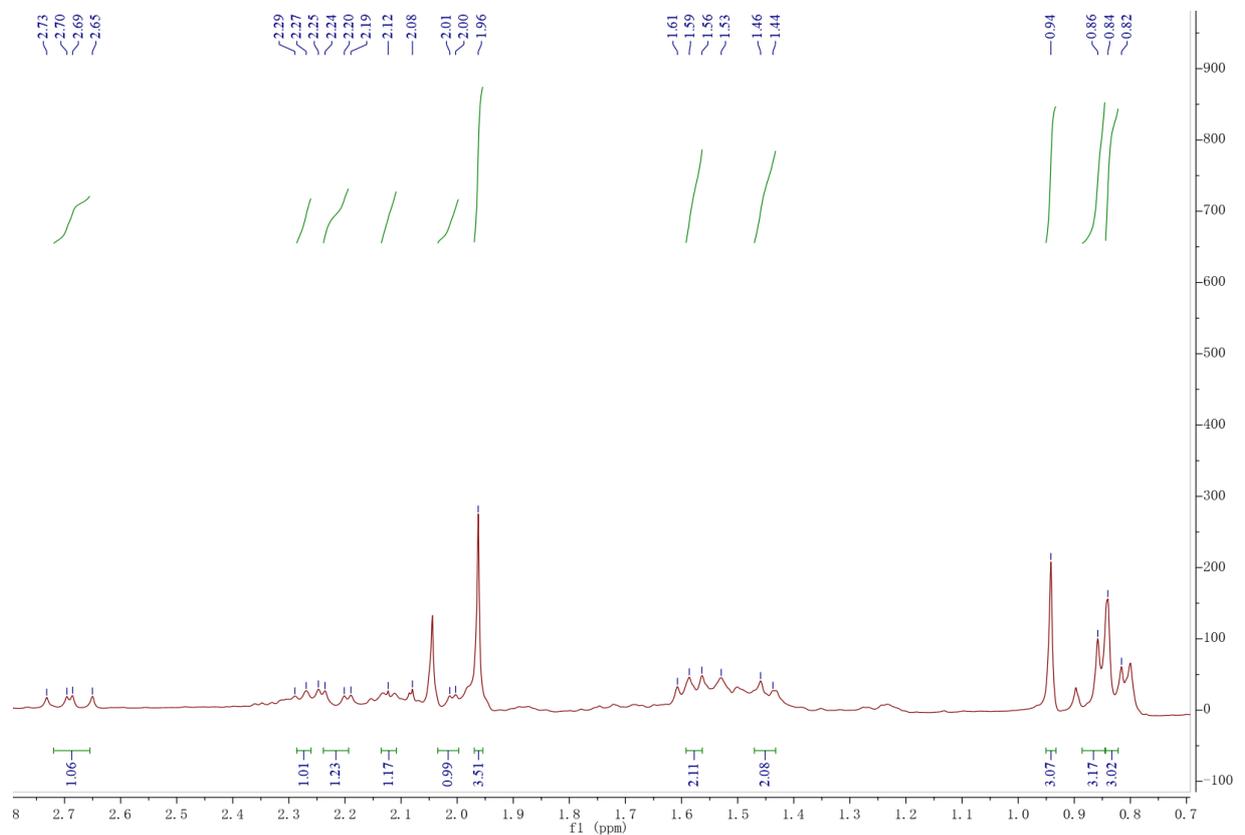
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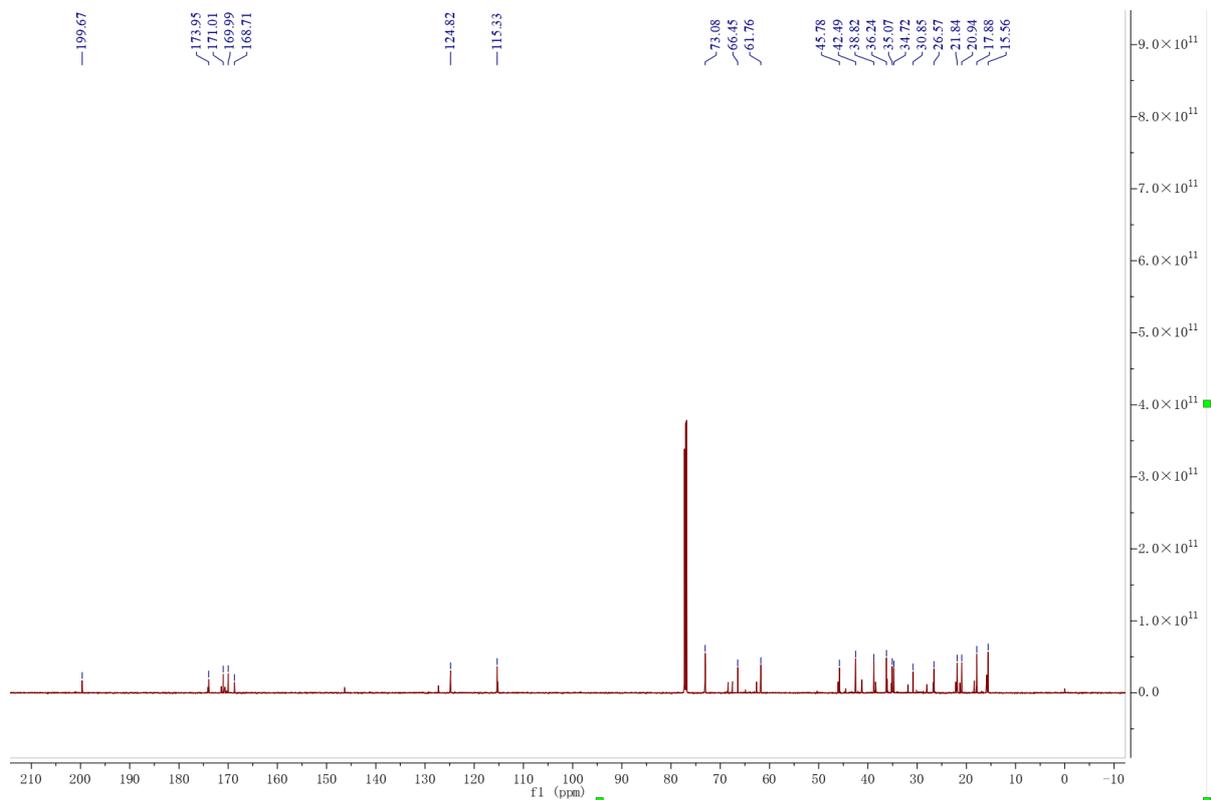
**Figure S1:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of **1**



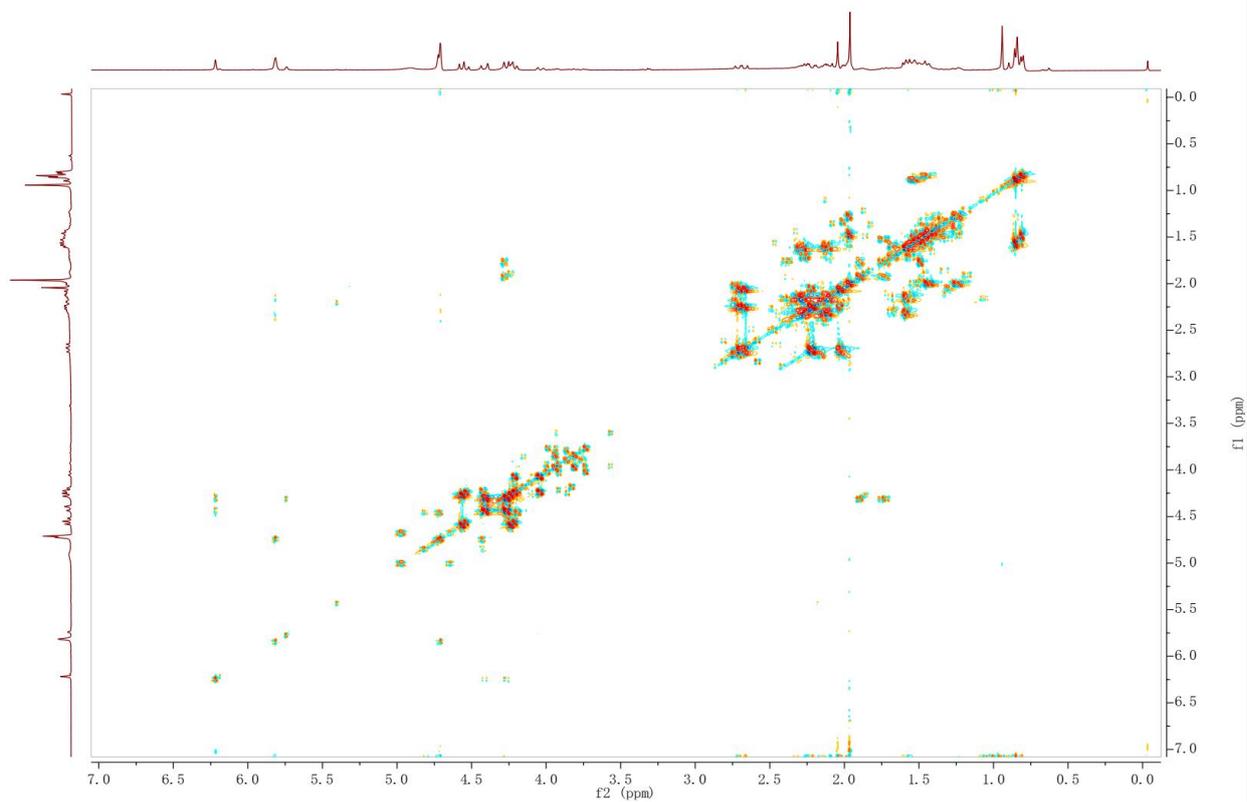
**Figure S2:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of **1** (From  $\delta_{\text{H}}$  4.00 ppm to  $\delta_{\text{H}}$  6.30 ppm)



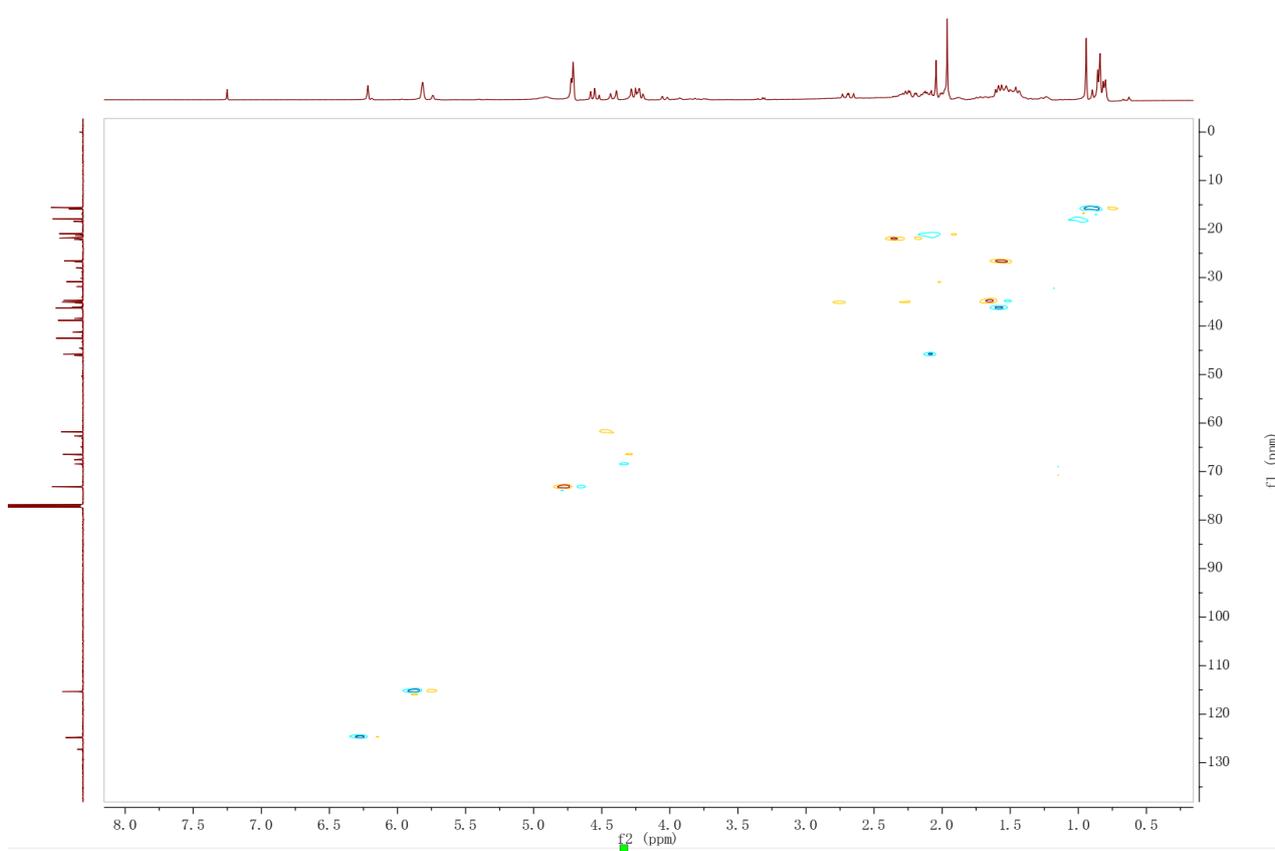
**Figure S3:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of **1** (From  $\delta_{\text{H}}$  0.70 ppm to  $\delta_{\text{H}}$  2.80 ppm)



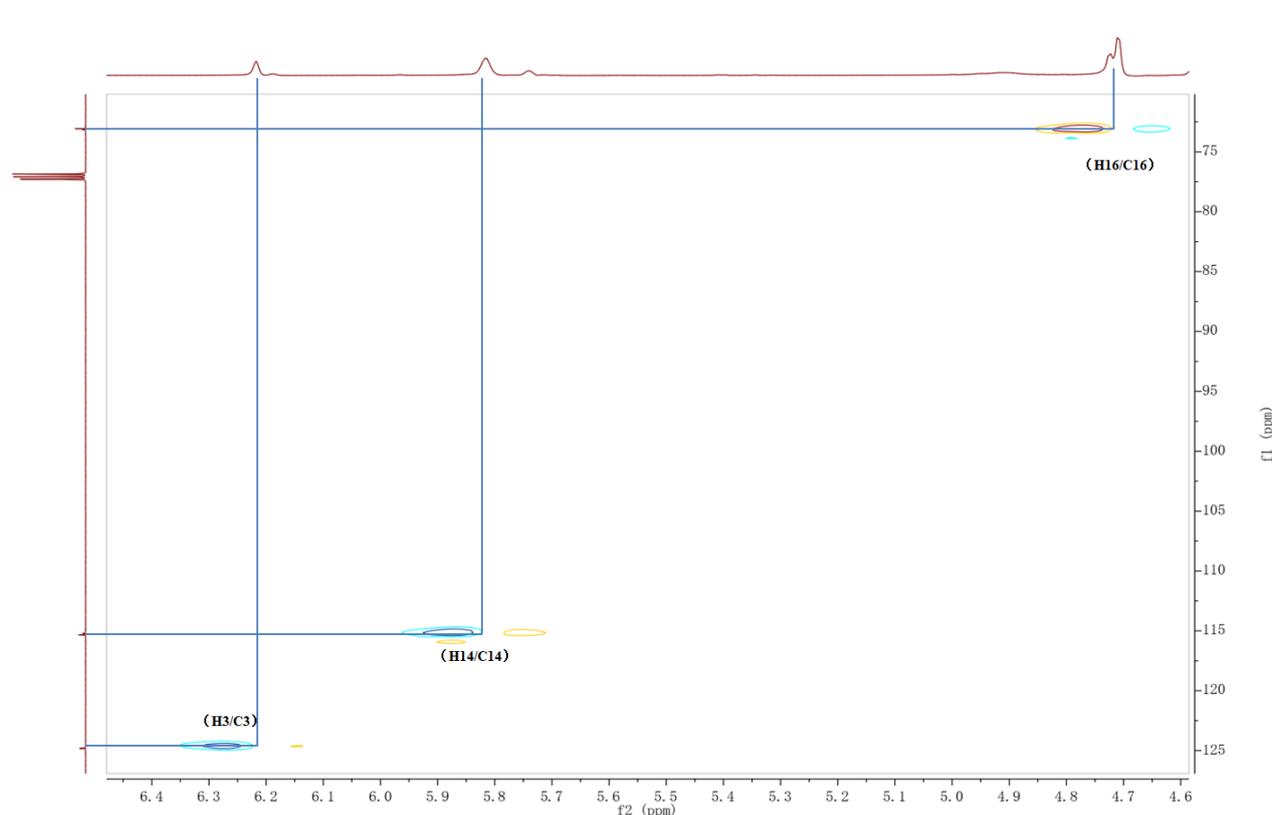
**Figure S4:**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of **1**



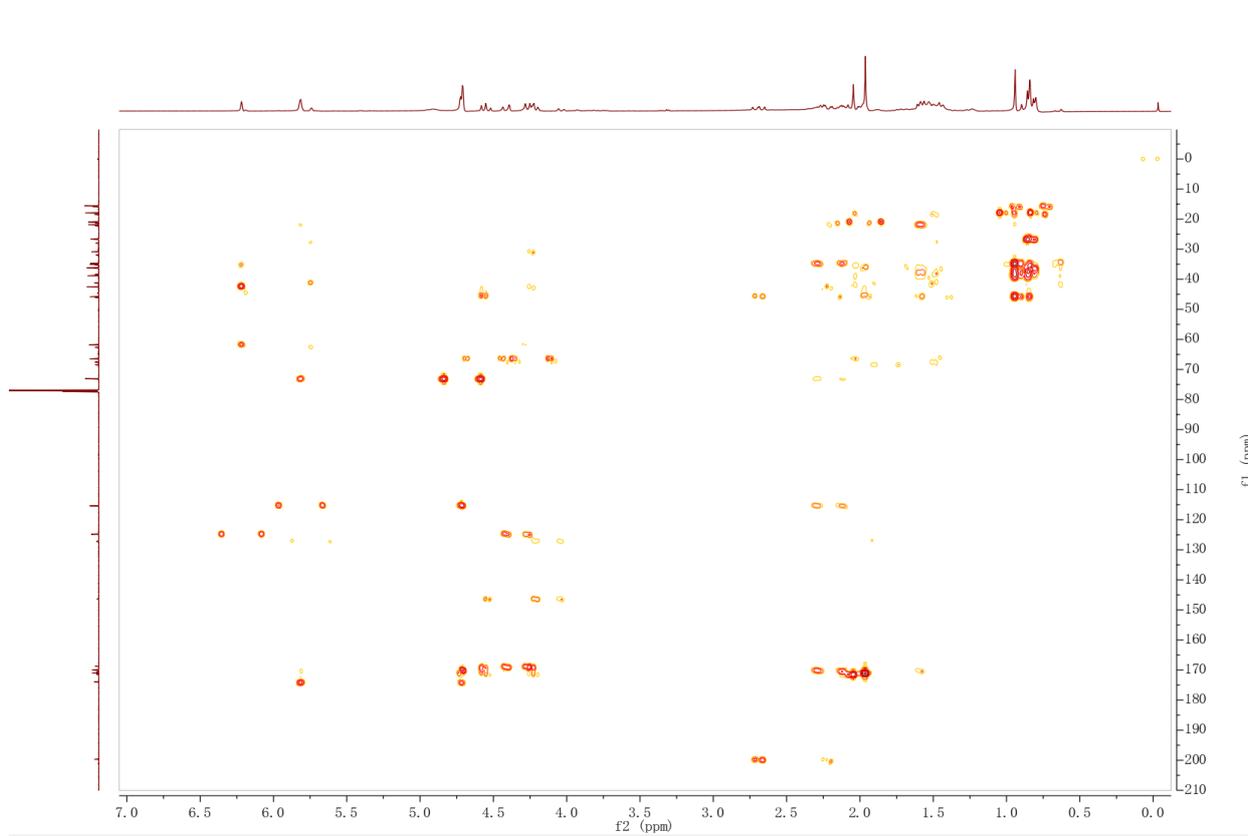
**Figure S5: COSY spectrum of 1**



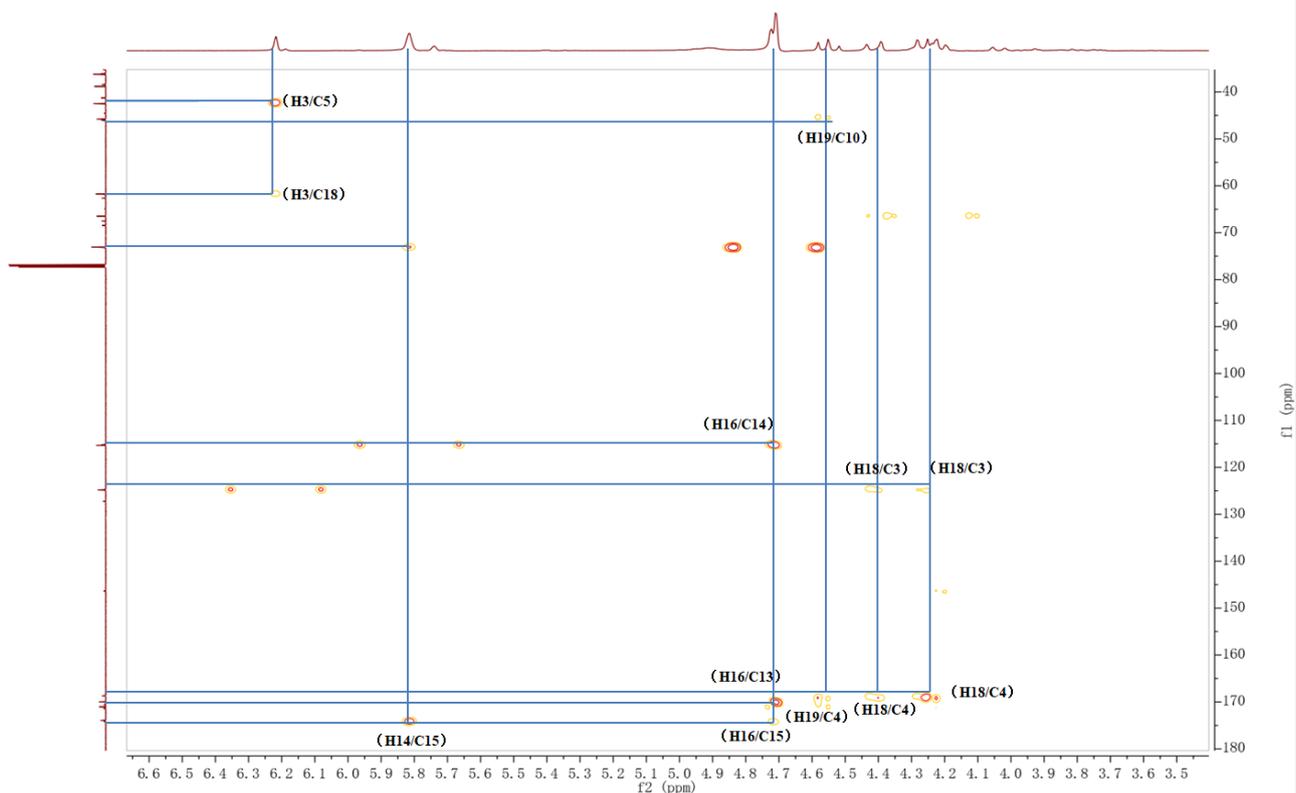
**Figure S6: HSQC spectrum of 1**



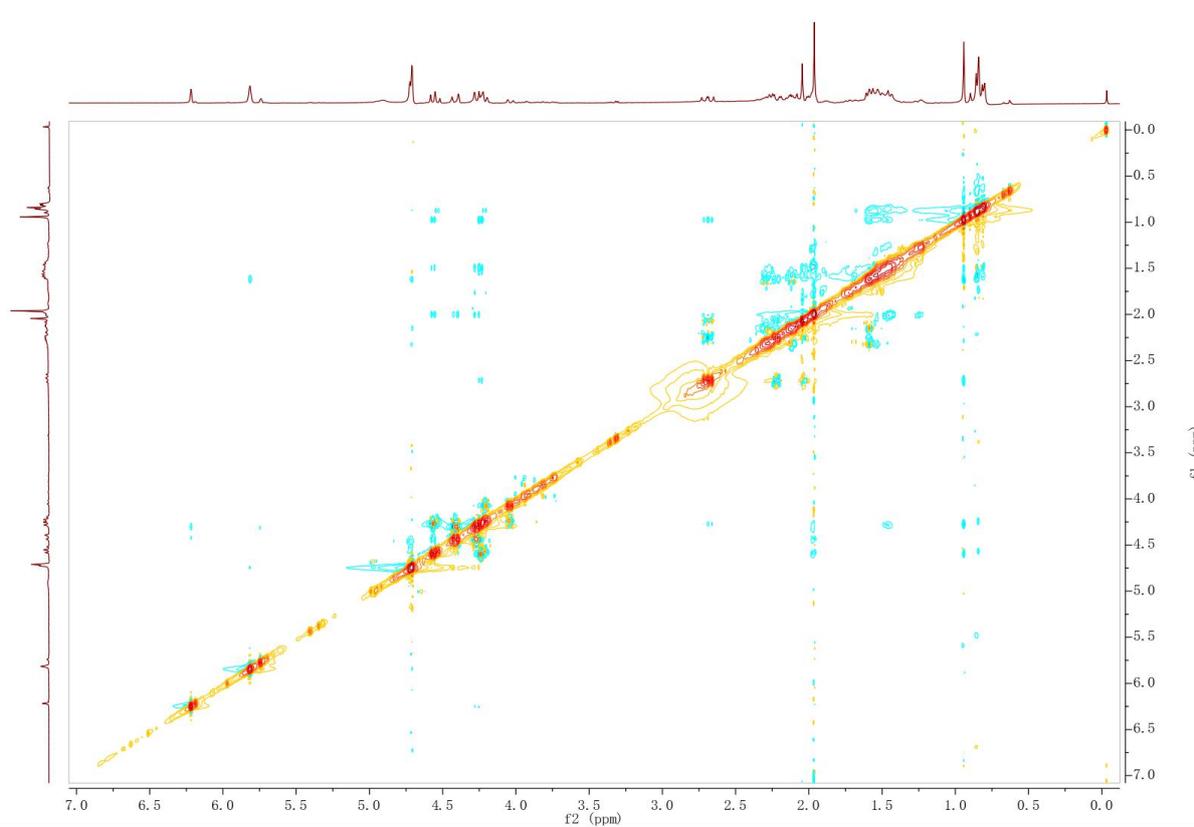
**Figure S7:** HSQC spectrum of **1** (From  $\delta_C$  70.0 ppm to  $\delta_C$  127.0 ppm)



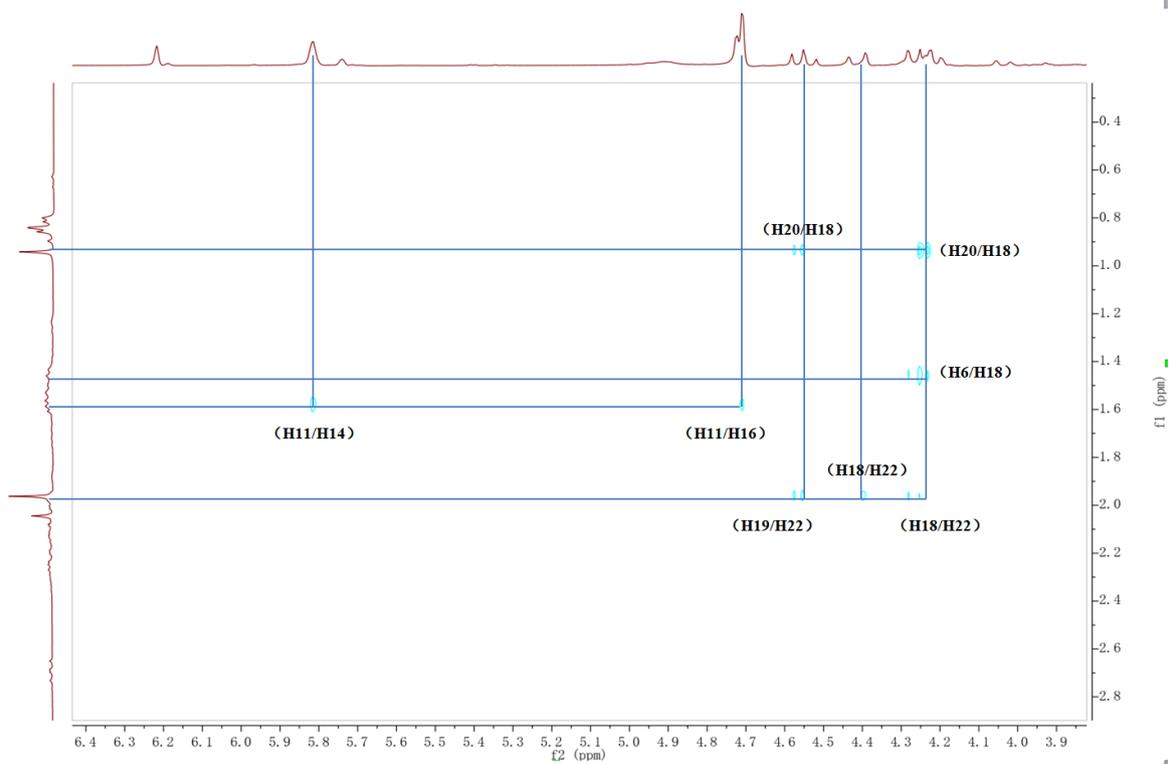
**Figure S8:** HMBC spectrum of **1**



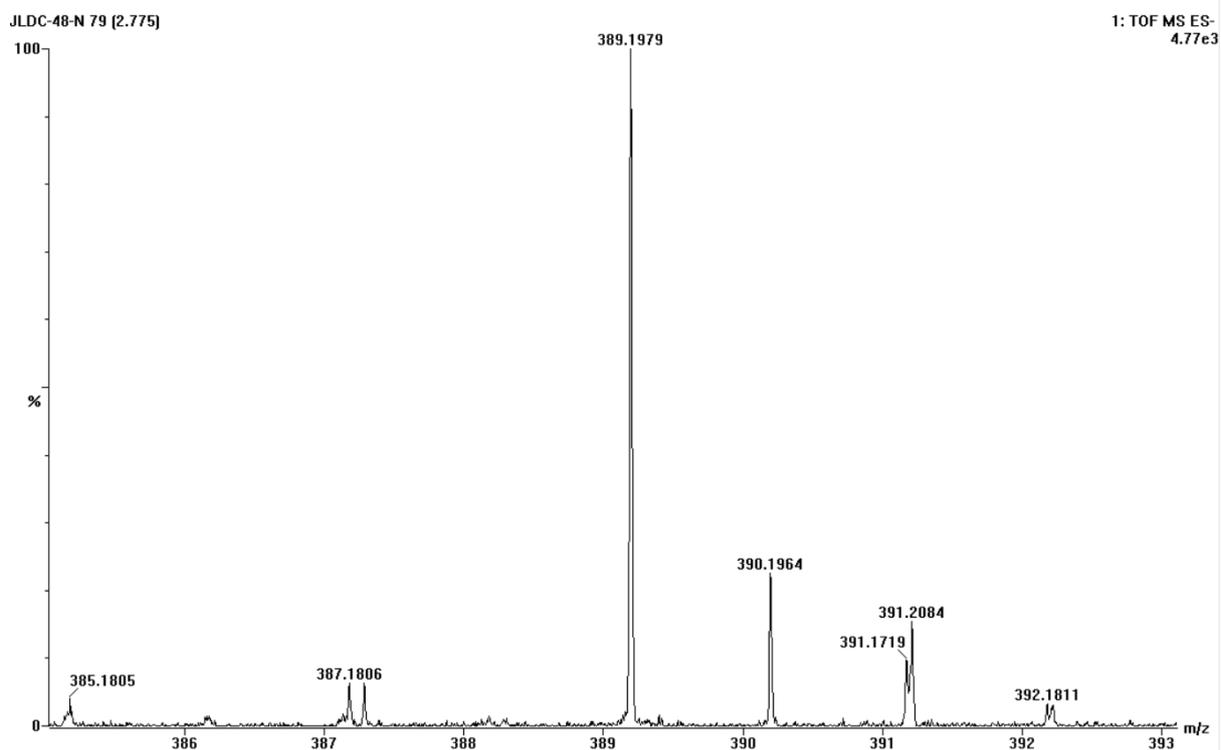
**Figure S9:** HMBC spectrum of **1** (From  $\delta_C$  40.0 ppm to  $\delta_C$  180.0 ppm)



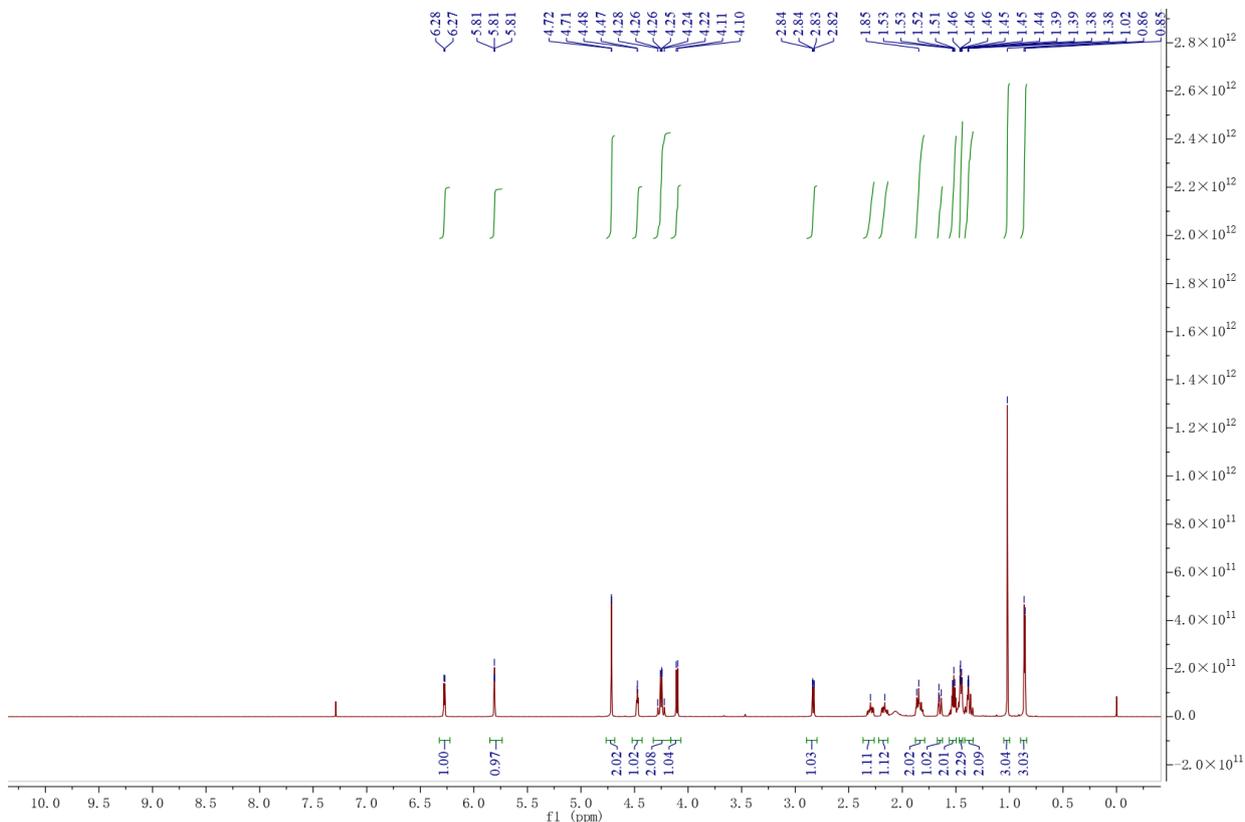
**Figure S10:** NOESY spectrum of **1**



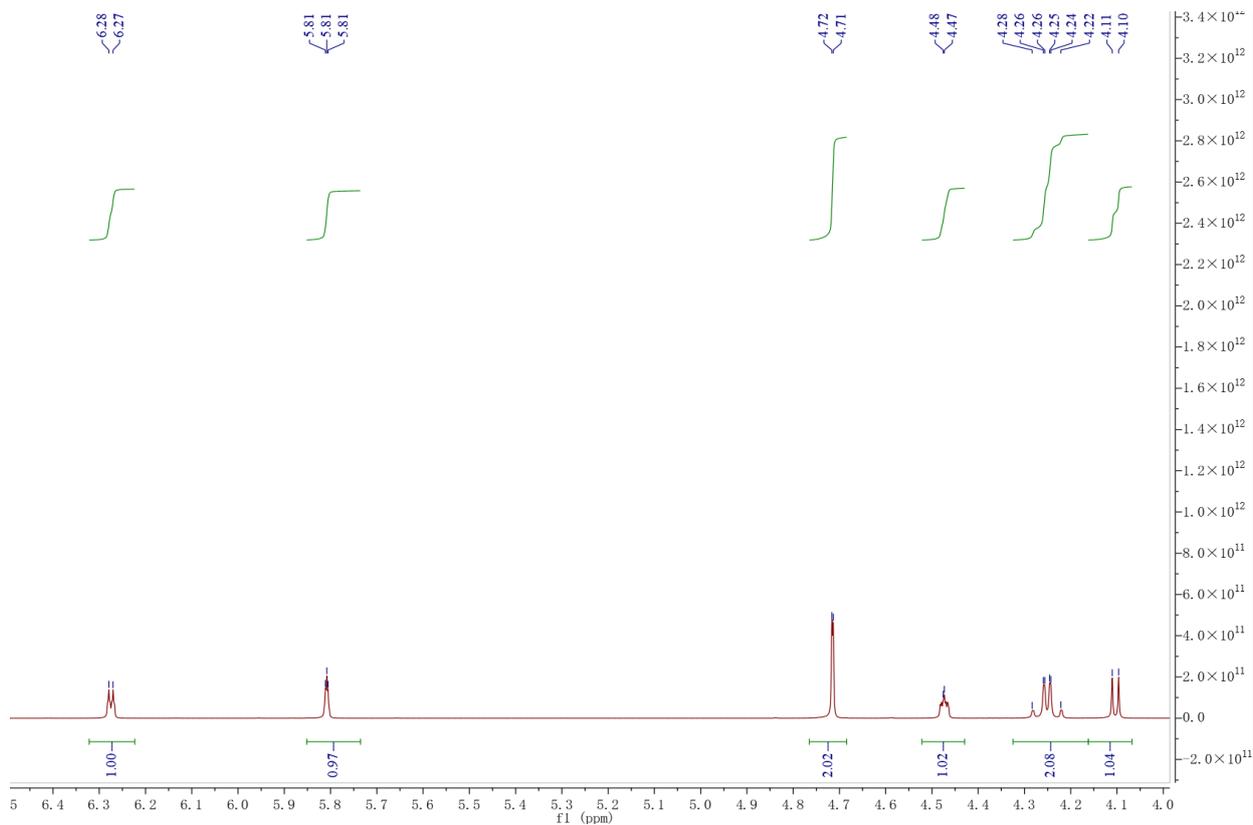
**Figure S11:** NOESY spectrum of **1** (expand)



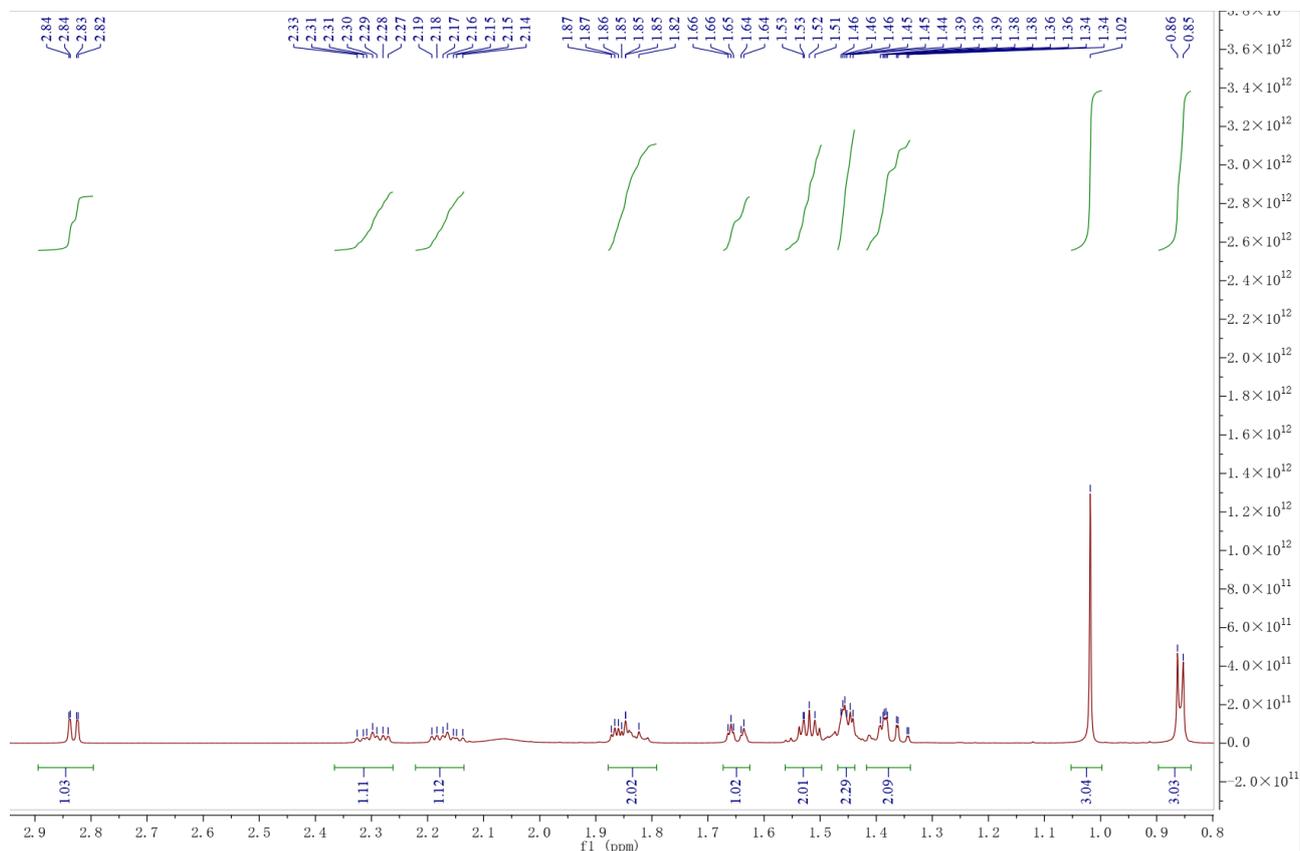
**Figure S12:** HR-ESI-MS spectrum of **1**



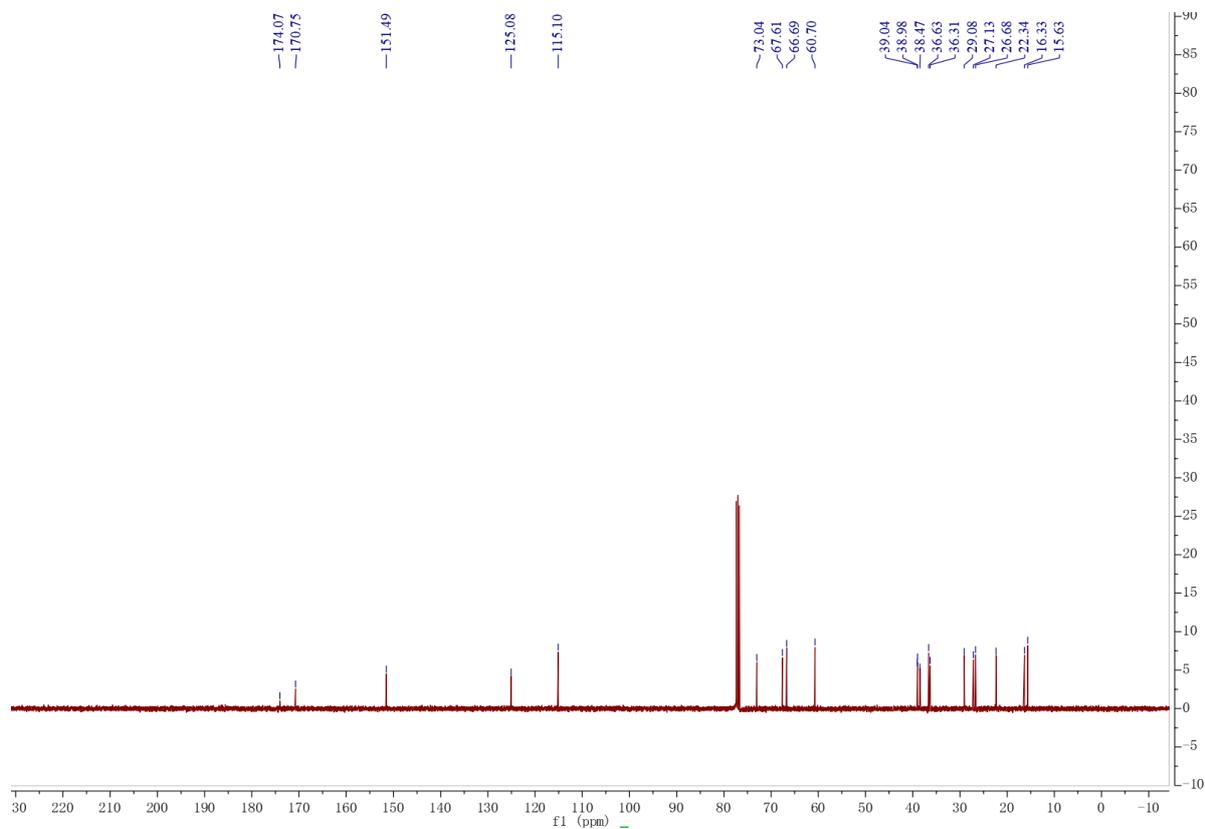
**Figure S13:**  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ ) of **2**



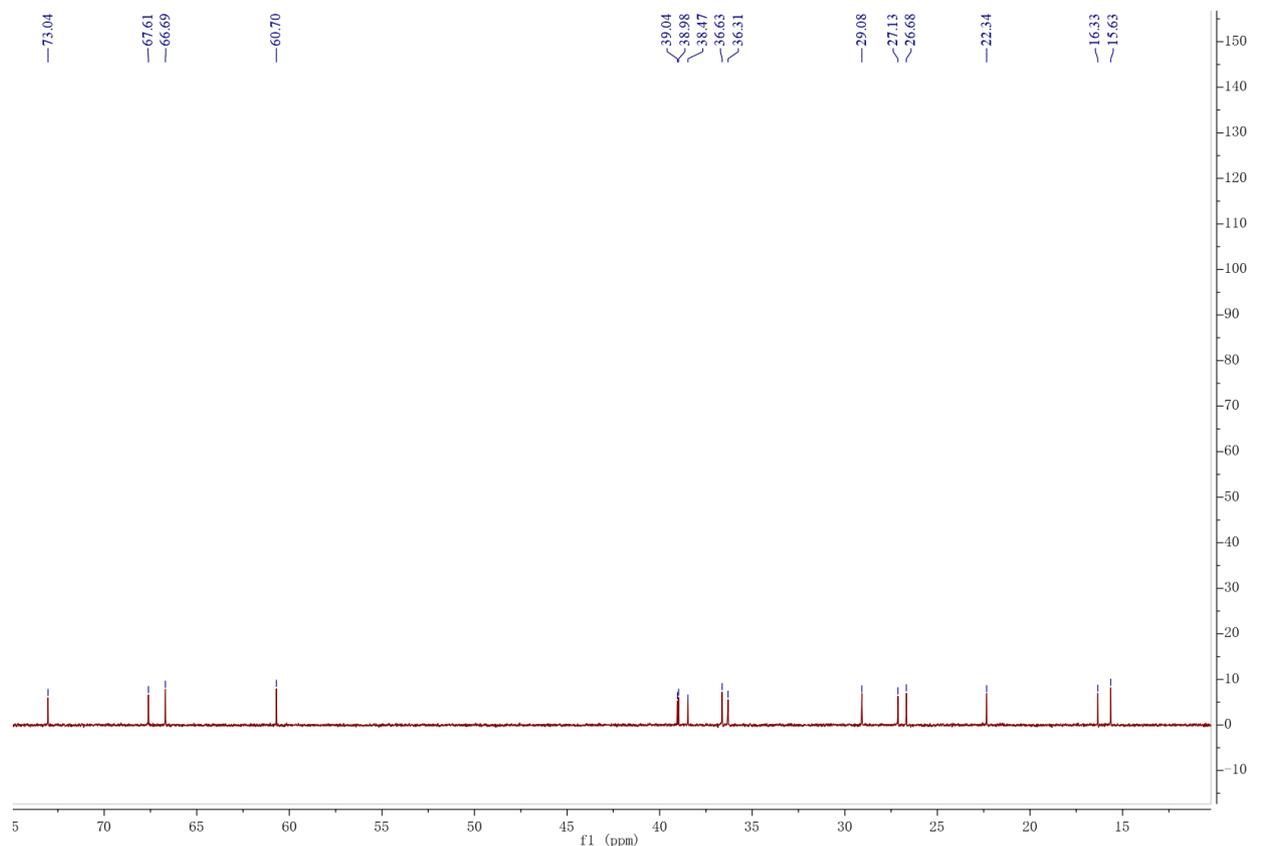
**Figure S14:**  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ ) of **2** (From  $\delta_{\text{H}}$  4.00 ppm to  $\delta_{\text{H}}$  6.50 ppm)



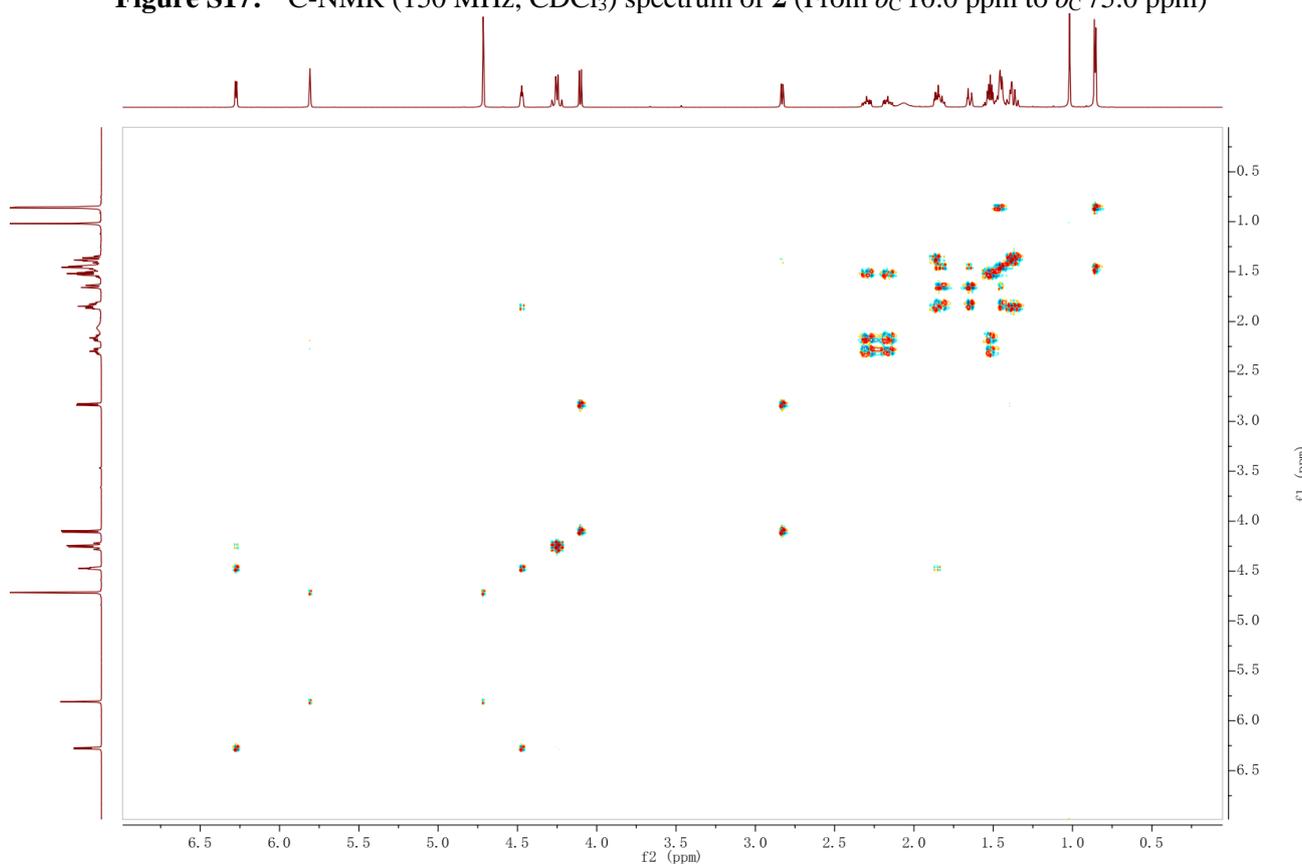
**Figure S15:**  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ ) of **2** (From  $\delta_{\text{H}}$  0.80 ppm to  $\delta_{\text{H}}$  3.00 ppm)



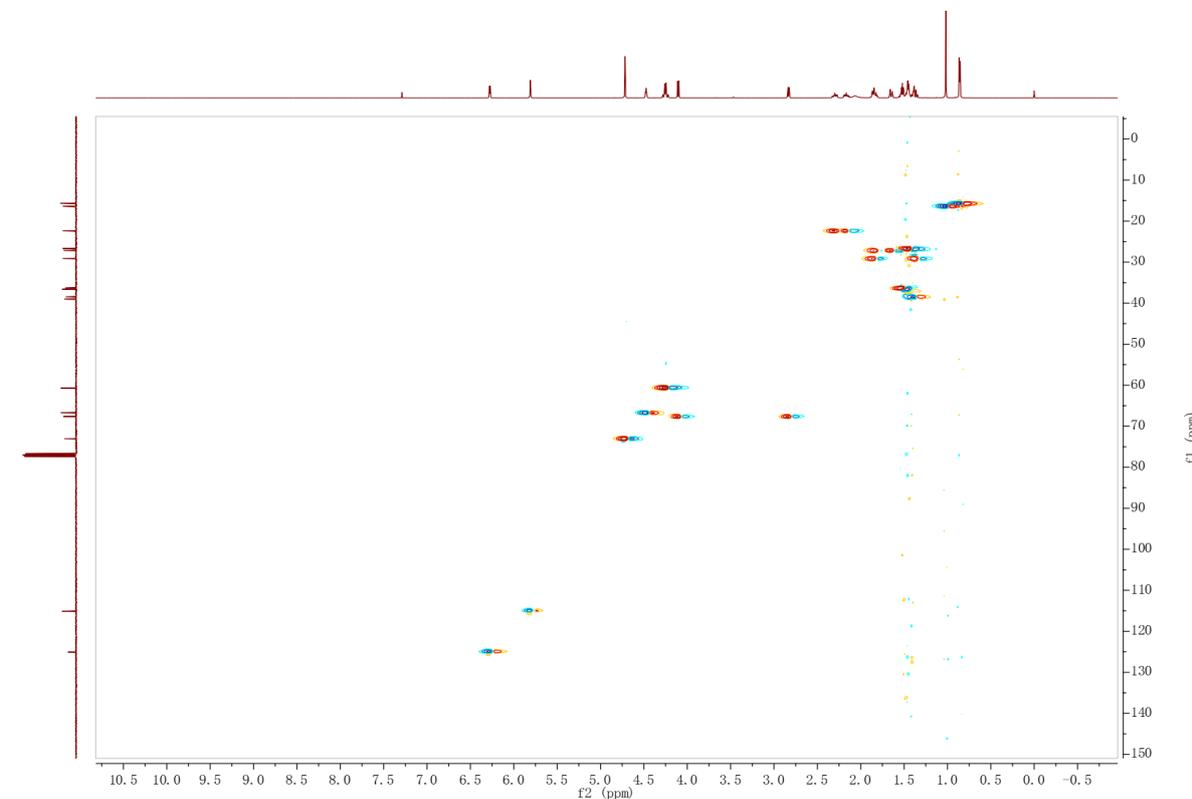
**Figure S16:**  $^{13}\text{C-NMR}$  (150 MHz,  $\text{CDCl}_3$ ) spectrum of **2**



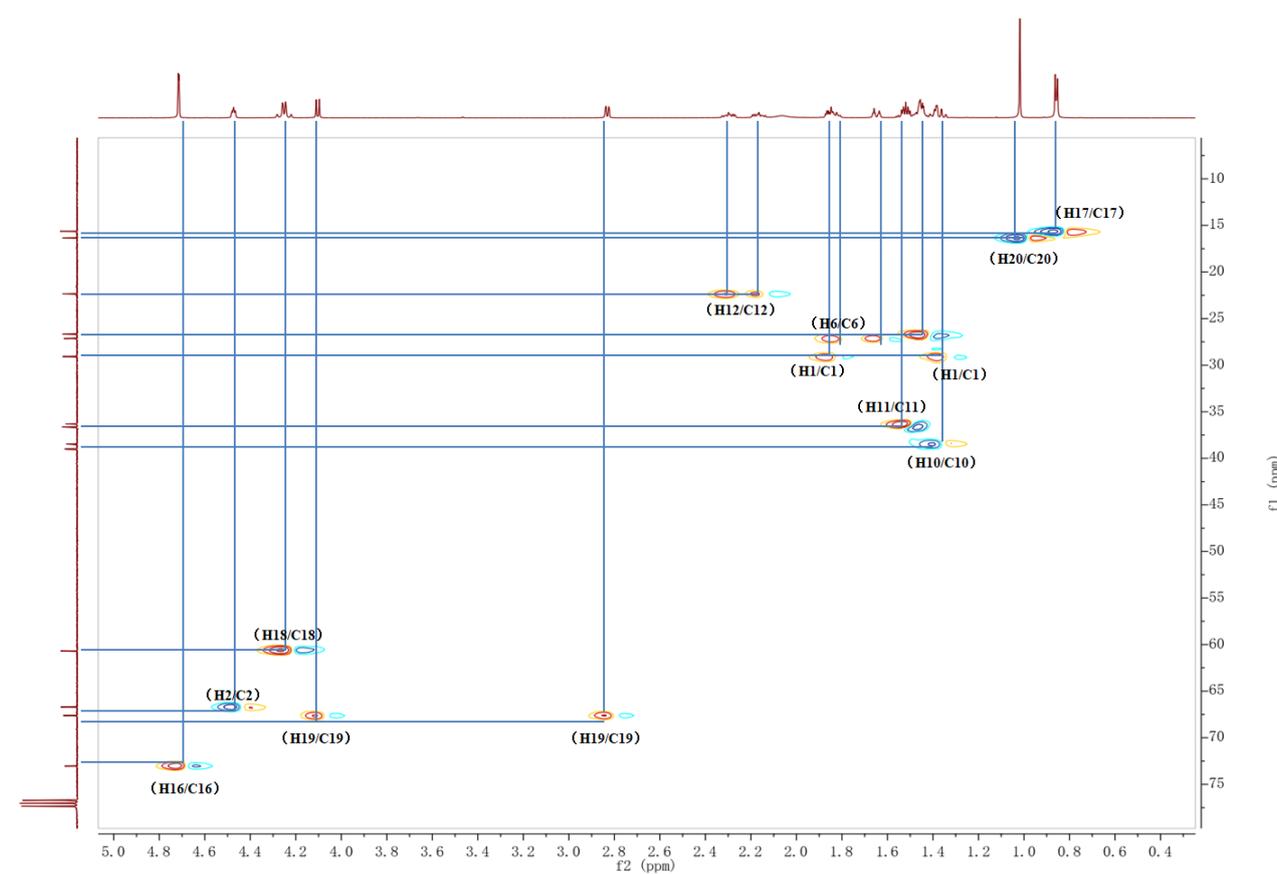
**Figure S17:**  $^{13}\text{C}$ -NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of **2** (From  $\delta_{\text{C}}$  10.0 ppm to  $\delta_{\text{C}}$  75.0 ppm)



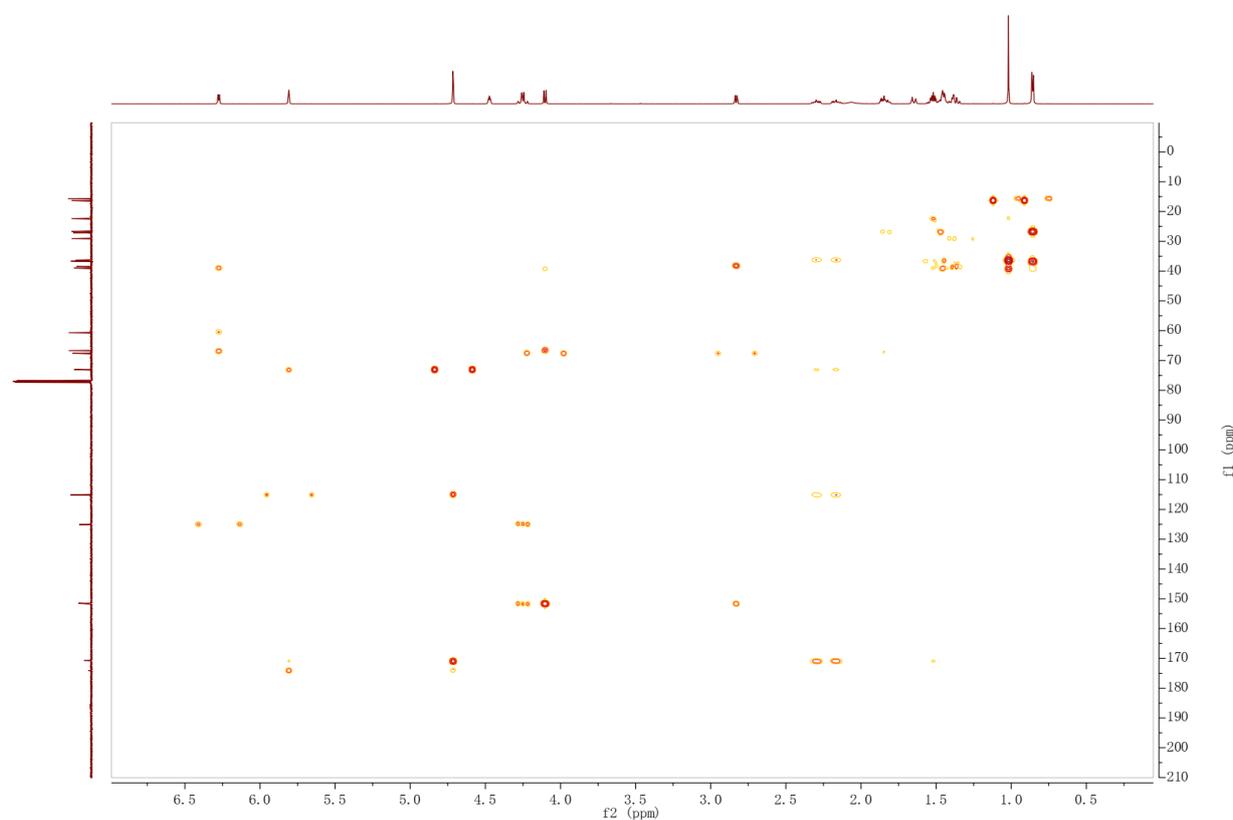
**Figure S18:** COSY spectrum of **2**



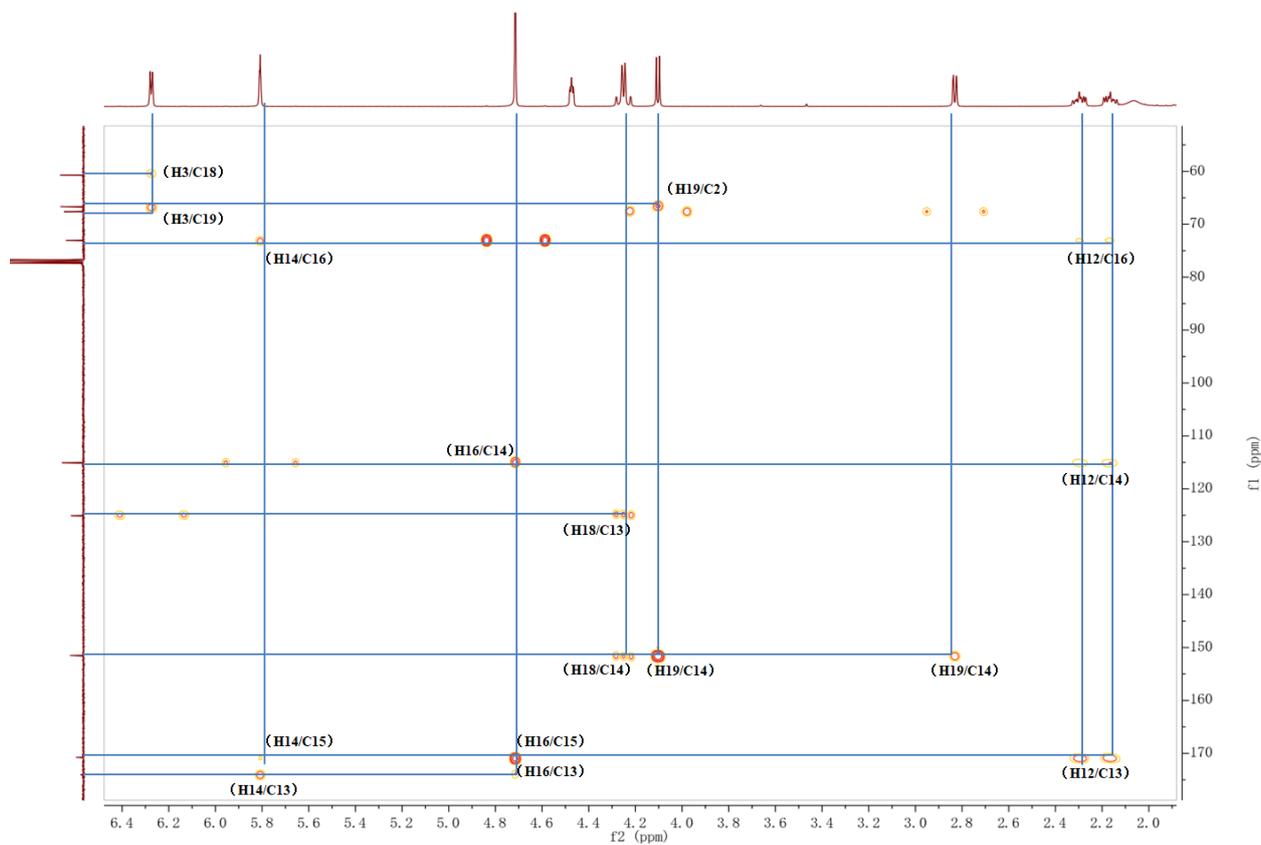
**Figure S19:** HSQC spectrum of **2**



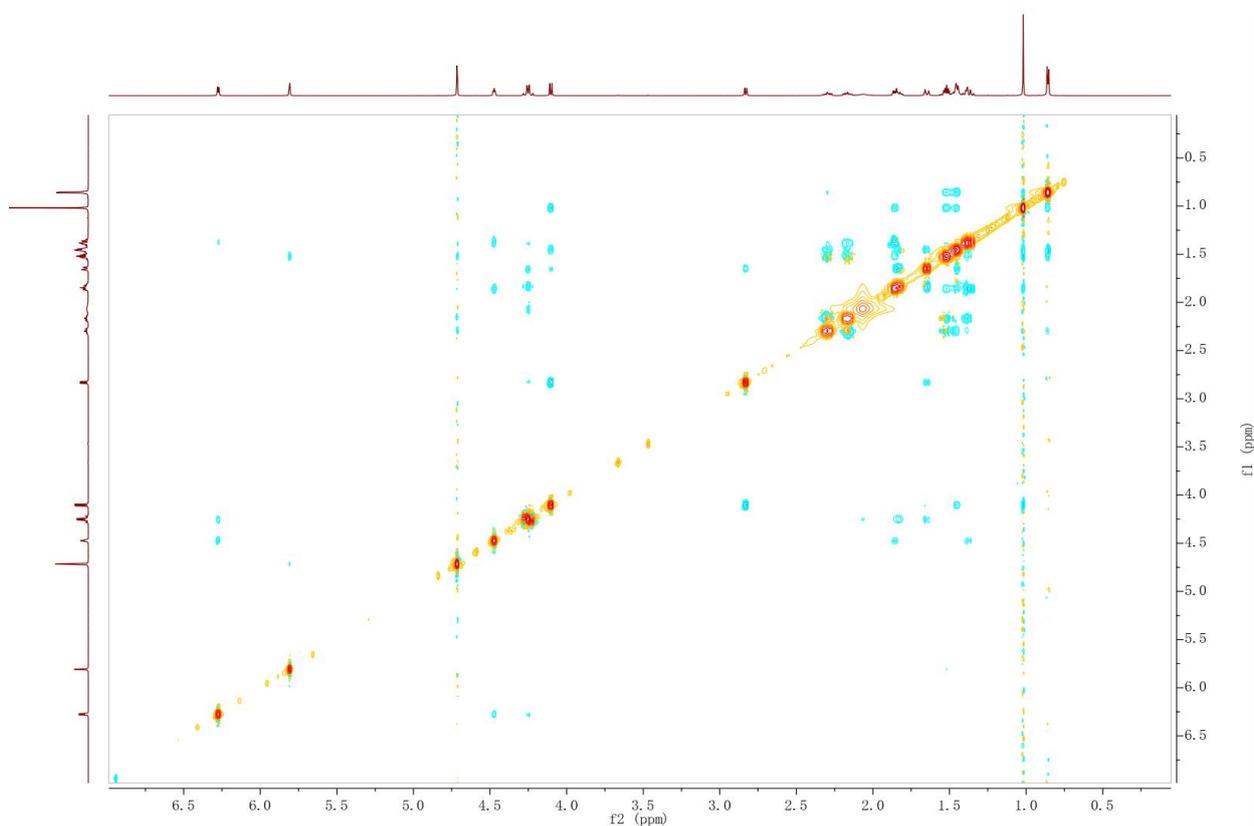
**Figure S20:** HSQC spectrum of **2** (From  $\delta_c$  10.0 ppm to  $\delta_c$  75.0 ppm)



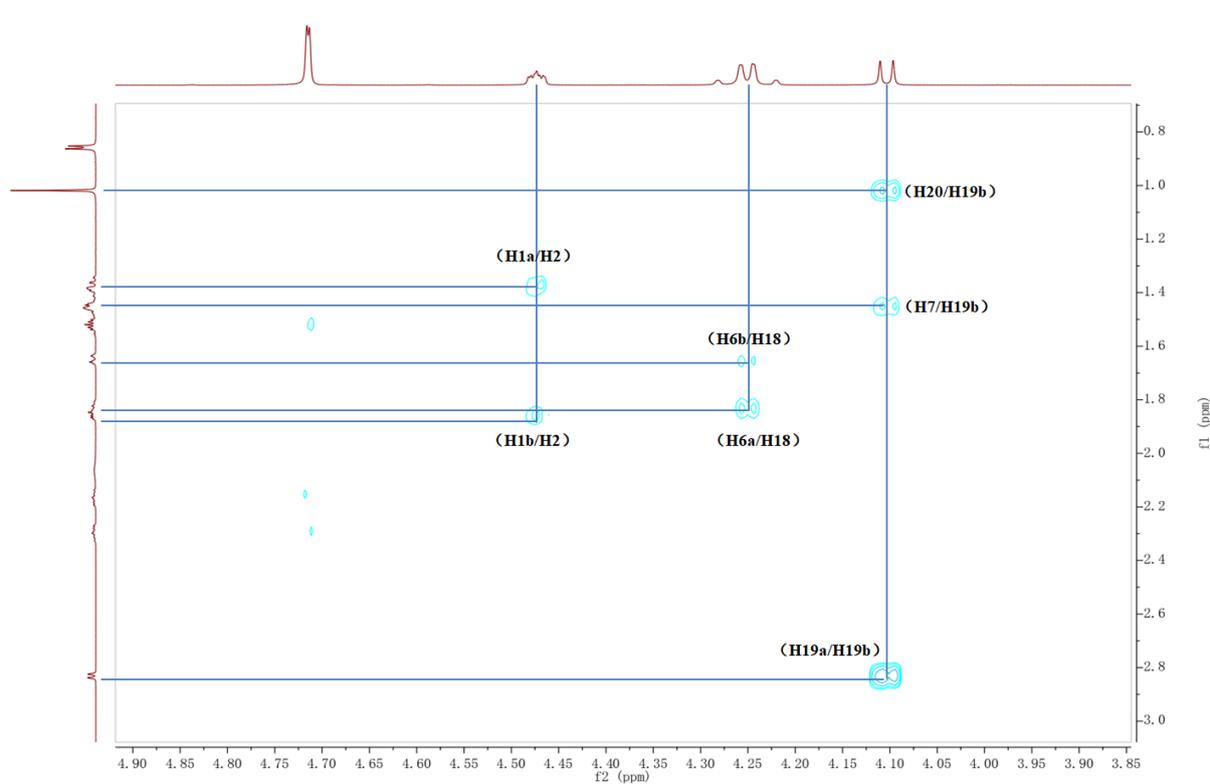
**Figure S21: HMBC spectrum of 2**



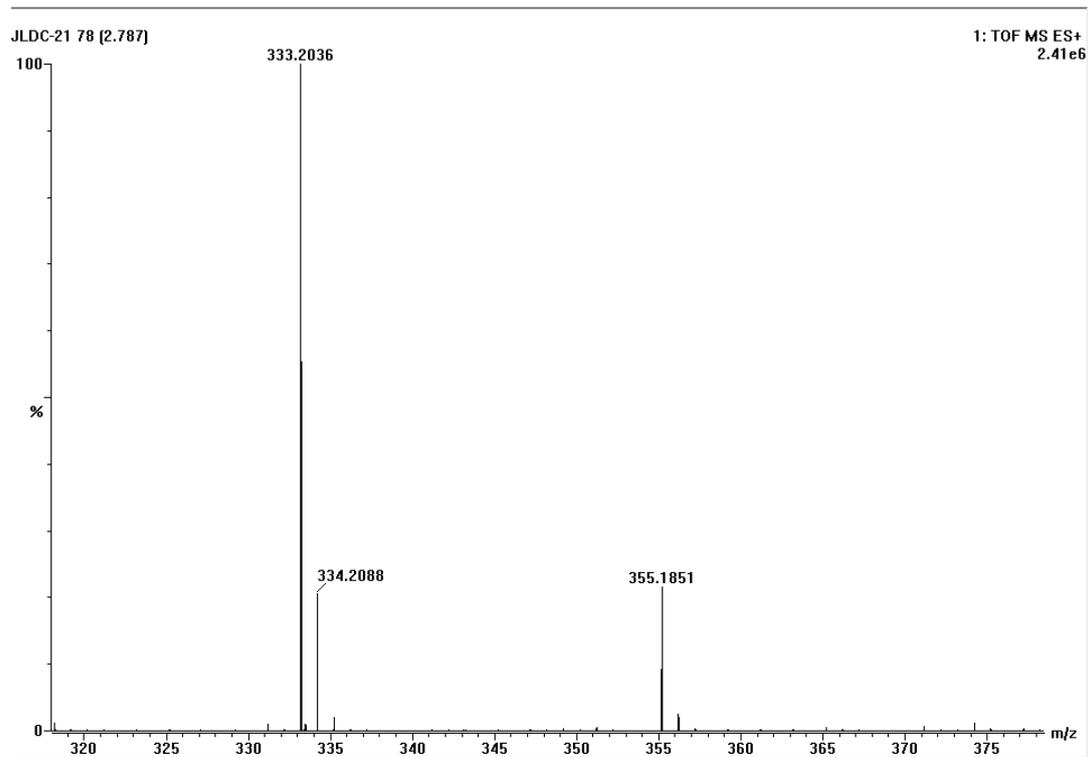
**Figure S22: HMBC spectrum of 2 (From  $\delta_C$  60.0 ppm to  $\delta_C$  175.0 ppm)**



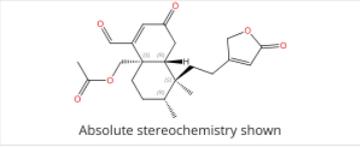
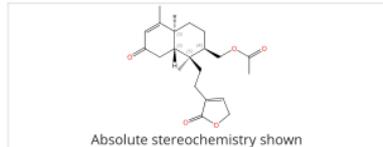
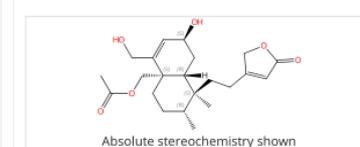
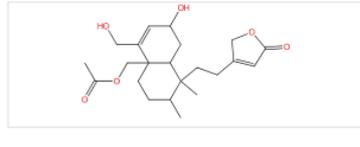
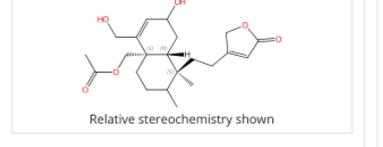
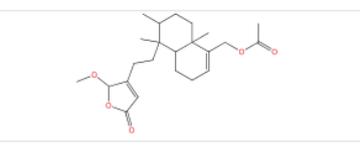
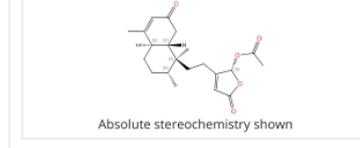
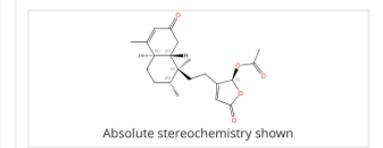
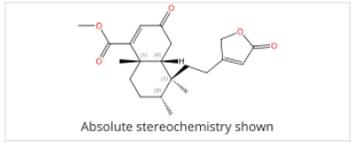
**Figure S23: NOESY spectrum of 2**



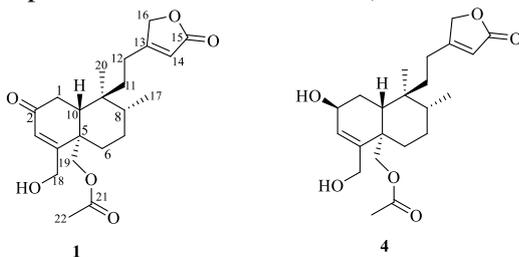
**Figure S24: NOESY spectrum of 2 (expand)**



**Figure S25:** HR-ESI-MS spectrum of **2**

<p>1</p> <p><b>125675-12-9</b></p>  <p>Absolute stereochemistry shown</p> <p><b>C<sub>22</sub>H<sub>28</sub>O<sub>6</sub></b>  1-Naphthalenecarboxaldehyde, 8a-[[acetyloxy)methyl]-5-[2-(2,5-dihydro-5-oxo-3-furanyl)ethyl]-3,4,4a,5,6,7,8,8a-octahydro-5,6-dimethyl-3-oxo-, [4a<i>R</i>-(4aα,5α,6β,8aβ)]-</p> <p>1 Reference    0 Reactions    0 Suppliers</p>	<p>2</p> <p><b>1210501-97-5</b></p>  <p>Absolute stereochemistry shown</p> <p><b>C<sub>22</sub>H<sub>30</sub>O<sub>5</sub></b>  3-[2-[[1<i>S</i>,2<i>R</i>,4a<i>S</i>,5,8a<i>S</i>)-2-[[Acetyloxy)methyl]-1,2,3,4,4a,7,8,8a-octahydro-1,4a,5-trimethyl-7-oxo-1-naphthalenyl]ethyl]-2(5<i>H</i>)-furanone</p> <p>3 References    1 Reaction    1 Supplier</p>	<p>3</p> <p><b>125675-09-4</b></p>  <p>Absolute stereochemistry shown</p> <p><b>C<sub>22</sub>H<sub>32</sub>O<sub>6</sub></b>  4-[2-[[1<i>S</i>,2<i>R</i>,4a<i>S</i>,5,7,8a<i>R</i>)-4a-[[Acetyloxy)methyl]-1,2,3,4,4a,7,8,8a-octahydro-7-hydroxy-5-(hydroxymethyl)-1,2-dimethyl-1-naphthalenyl]ethyl]-2(5<i>H</i>)-furanone</p> <p>20 References    0 Reactions    48 Suppliers</p>
<p>4</p> <p><b>2931740-67-7</b></p>  <p>Absolute stereochemistry shown</p> <p><b>C<sub>22</sub>H<sub>32</sub>O<sub>6</sub></b>  2(5<i>H</i>)-Furanone, 4-[2-[4a-[[acetyloxy)methyl]-1,2,3,4,4a,7,8,8a-octahydro-7-hydroxy-5-(hydroxymethyl)-1,2-dimethyl-1-naphthalenyl]ethyl]-</p> <p>0 References    0 Reactions    1 Supplier</p>	<p>5</p> <p><b>2508139-59-9</b></p>  <p>Relative stereochemistry shown</p> <p><b>C<sub>22</sub>H<sub>32</sub>O<sub>6</sub></b>  <i>rel</i>-4-[2-[[1<i>R</i>,4a<i>R</i>,8a<i>S</i>)-4a-[[Acetyloxy)methyl]-1,2,3,4,4a,7,8,8a-octahydro-7-hydroxy-5-(hydroxymethyl)-1,2-dimethyl-1-naphthalenyl]ethyl]-2(5<i>H</i>)-furanone</p> <p>0 References    0 Reactions    1 Supplier</p>	<p>6</p> <p><b>107424-16-8</b></p>  <p>Absolute stereochemistry shown</p> <p><b>C<sub>23</sub>H<sub>34</sub>O<sub>5</sub></b>  4-[2-[5-[[Acetyloxy)methyl]-1,2,3,4,4a,7,8,8a-octahydro-1,2,4a-trimethyl-1-naphthalenyl]ethyl]-5-methoxy-2(5<i>H</i>)-furanone</p> <p>1 Reference    0 Reactions    0 Suppliers</p>
<p>7</p> <p><b>126616-72-6</b></p>  <p>Absolute stereochemistry shown</p> <p><b>C<sub>22</sub>H<sub>30</sub>O<sub>5</sub></b>  2(5<i>H</i>)-Furanone, 5-(acetyloxy)-4-[2-(1,2,3,4,4a,7,8,8a-octahydro-1,2,4a,5-tetramethyl-7-oxo-1-naphthalenyl)ethyl]-, [1<i>S</i>-[1α(<i>S</i>*),2β,4aβ,8aα]]-</p> <p>1 Reference    0 Reactions    0 Suppliers</p>	<p>8</p> <p><b>126582-63-6</b></p>  <p>Absolute stereochemistry shown</p> <p><b>C<sub>22</sub>H<sub>30</sub>O<sub>5</sub></b>  2(5<i>H</i>)-Furanone, 5-(acetyloxy)-4-[2-(1,2,3,4,4a,7,8,8a-octahydro-1,2,4a,5-tetramethyl-7-oxo-1-naphthalenyl)ethyl]-, [1<i>S</i>-[1α(<i>R</i>*),2β,4aβ,8aα]]-</p> <p>1 Reference    0 Reactions    0 Suppliers</p>	<p>9</p> <p><b>51117-32-9</b></p>  <p>Absolute stereochemistry shown</p> <p><b>C<sub>21</sub>H<sub>28</sub>O<sub>5</sub></b>  1-Naphthalenecarboxylic acid, 5-[2-(2,5-dihydro-5-oxo-3-furanyl)ethyl]-3,4,4a,5,6,7,8,8a-octahydro-5,6,8a-trimethyl-3-oxo-, methyl ester, [4a<i>R</i>-(4aα,5α,6β,8aα)]-</p> <p>1 Reference    1 Reaction    0 Suppliers</p>

**Figure S26:** Compound similarity assessment of 1

**Table S1:** NMR data comparison of **1** and **4** in CDCl<sub>3</sub> (600/150MHz,  $\delta$  in ppm,  $J$  in Hz)

No.	<b>1</b>		<b>4</b>	
	$\delta_H$ ( $J$ in Hz)	$\delta_C$	$\delta_H$ ( $J$ in Hz)	$\delta_C$
1	2.22, dd (18.3, 4.8); 2.69, dd (18.3, 4.2)	35.1		27.7
2		199.7	4.21, m	63.8
3	6.22, s	124.8	5.79, d (4.2)	124.4
4		168.7		147.4
5		42.5		41.0
6	2.02, m; 1.44, m	30.8		31.2
7	1.49, m	26.6		26.8
8	1.50, m	36.2		38.1
9		38.8		36.0
10	2.04, m	45.8		40.8
11	1.57, m	34.7		34.8
12	2.23, m; 2.10, m	21.8		21.6
13		170.0		172.6
14	5.81, s	115.3	5.75, s	114.2
15		174.0		174.9
16	4.71, s	73.1	4.69, s	73.5
17	0.85, d (6.0)	15.6	0.76, d (6.0)	15.6
18	4.41, d (17.2); 4.26, d (17.2)	61.8	4.13, d (14.2); 4.04, d (14.2)	62.2
19	4.55, m; 4.23, m	66.4	4.45, d (11.3); 4.01, d (11.3)	66.9
20	0.94, s	17.9	0.75, s	18.2
21		171.0		171.0
22	1.96, s	20.9	1.94, s	21.0