

## Supporting Information

### Further Verticillene Diterpenoids, Eudesmane Sesquiterpenoids, and Hydroperoxysteroids from a Taiwanese Soft Coral *Cespitularia* sp.

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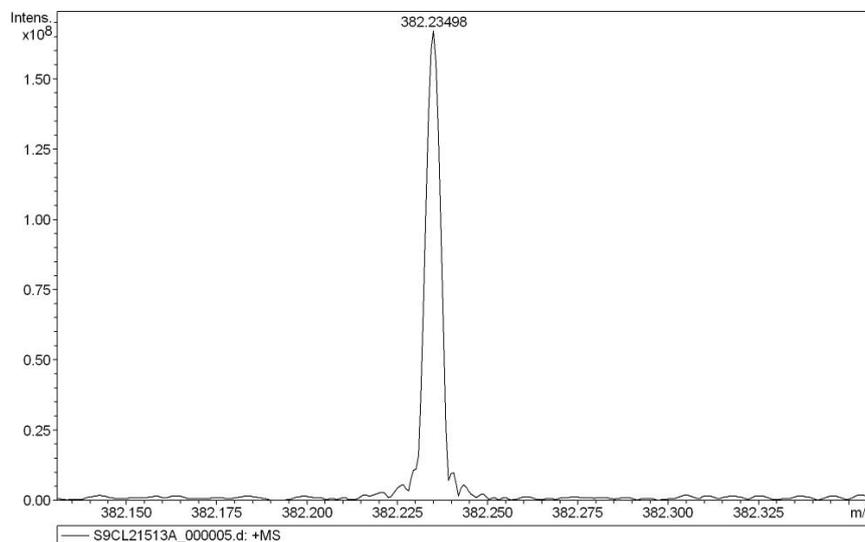
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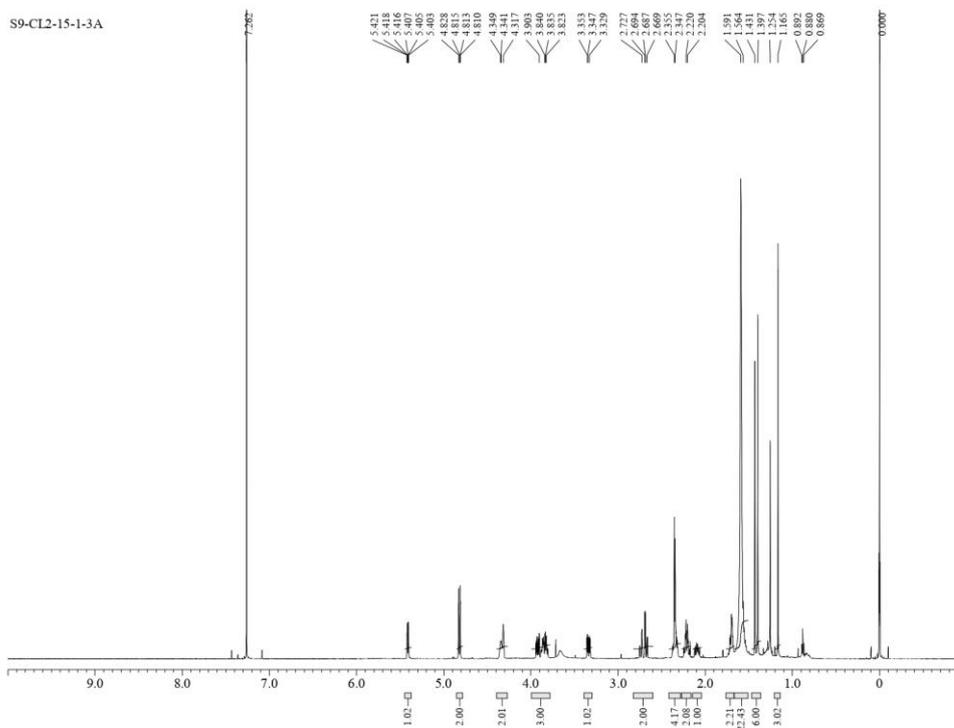
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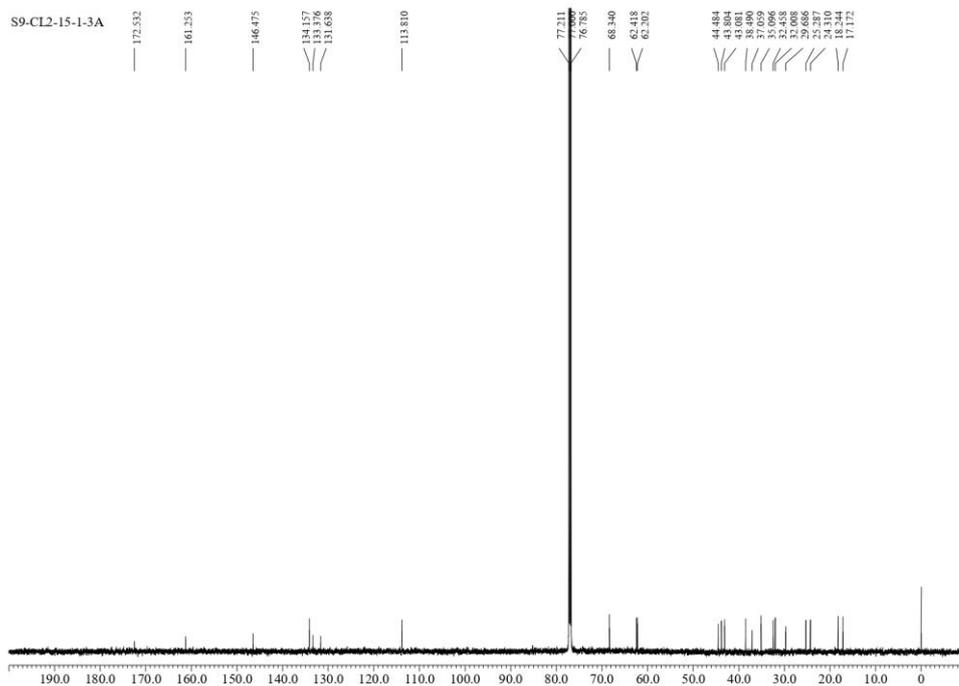


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**Figure S1.** HRESIMS of compound **1**

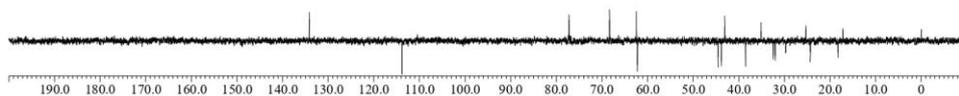


**Figure S2.** <sup>1</sup>H NMR spectrum (600MHz) of compound **1** in CDCl<sub>3</sub>

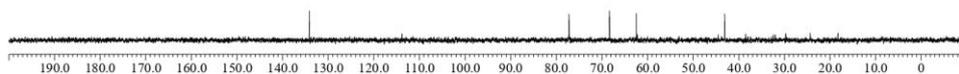


**Figure S3.**  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **1** in  $\text{CDCl}_3$

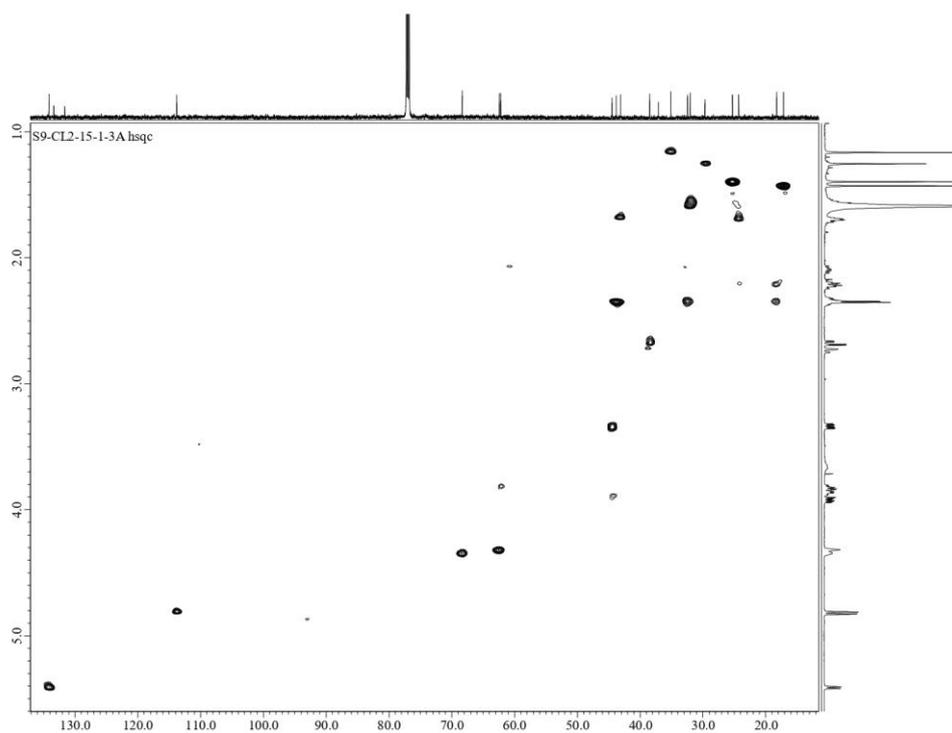
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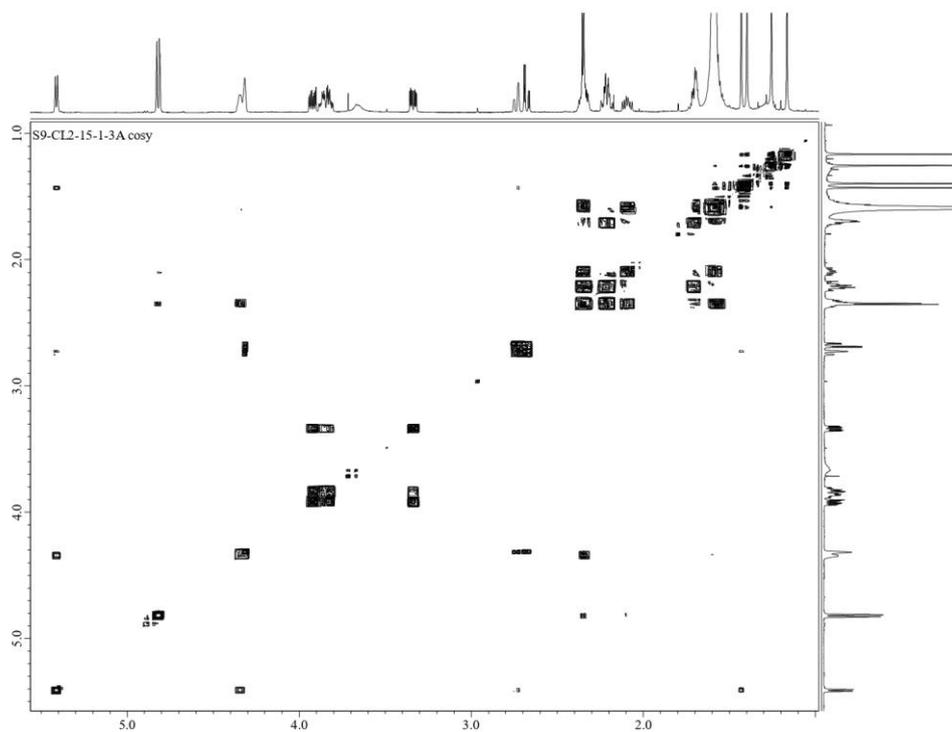
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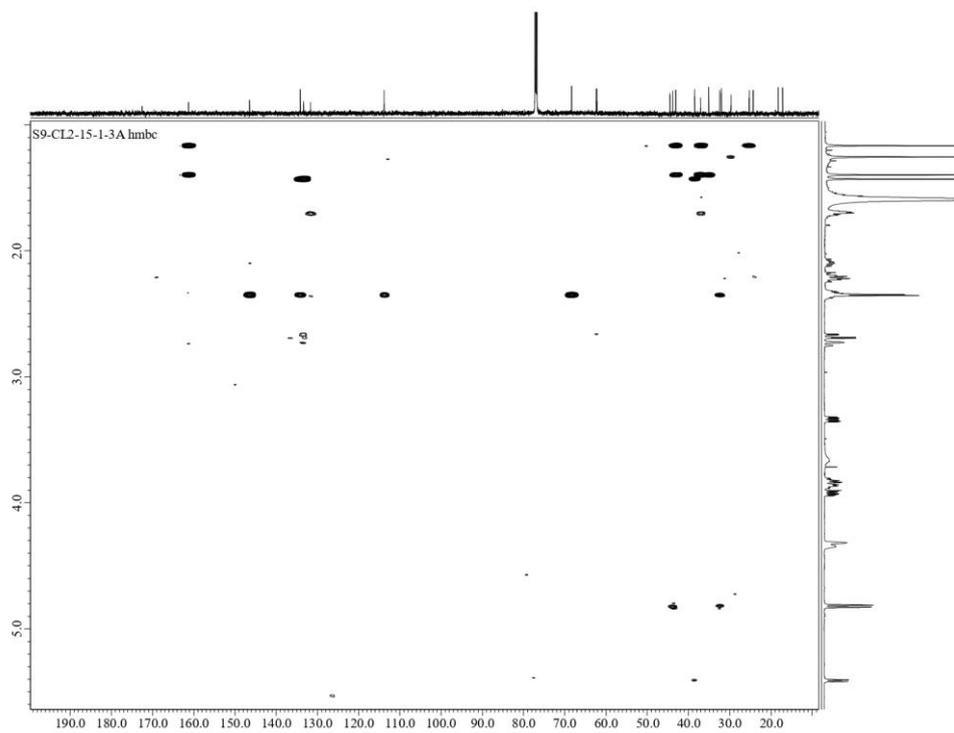
**Figure S4.** DEPT spectrum (150 MHz) of compound **1** in  $\text{CDCl}_3$



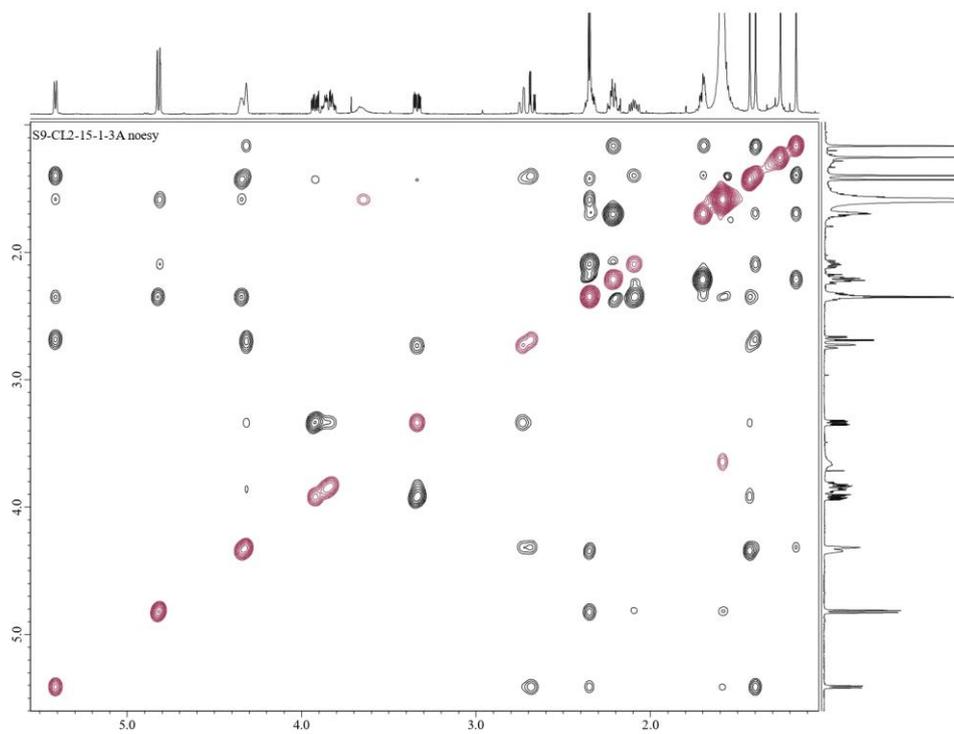
**Figure S5.** HSQC spectrum of compound **1** in CDCl<sub>3</sub>



**Figure S6.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **1** in CDCl<sub>3</sub>



**Figure S7.** HMBC spectrum of compound **1** in  $\text{CDCl}_3$



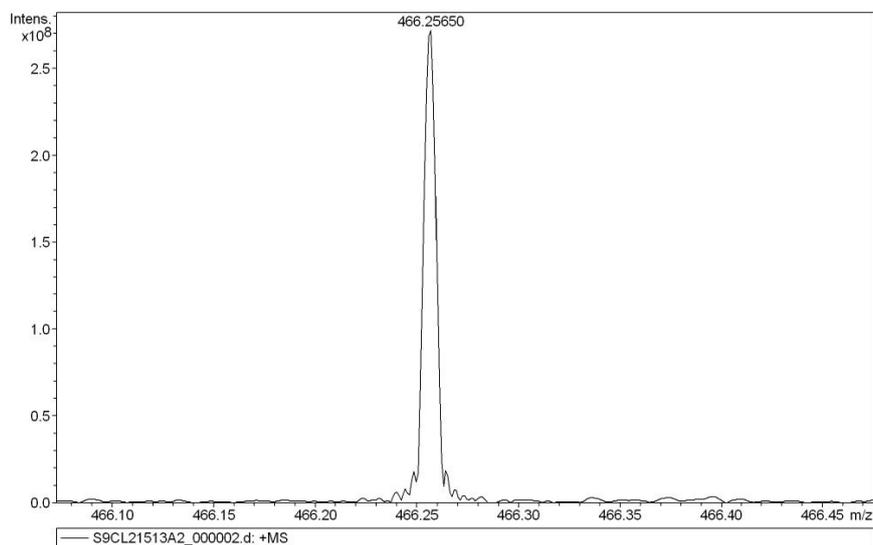
**Figure S8.** NOESY spectrum of compound **1** in  $\text{CDCl}_3$

## Mass Spectrum SmartFormula Report

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Instrument: BRUKER FT-MS solariX



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466.25650	1	C <sub>26</sub> H <sub>37</sub> NNaO <sub>5</sub>	100.00	466.25639	-0.11	-0.23	13.6	8.5	even	ok

Figure S9. HRESIMS of compound 1a

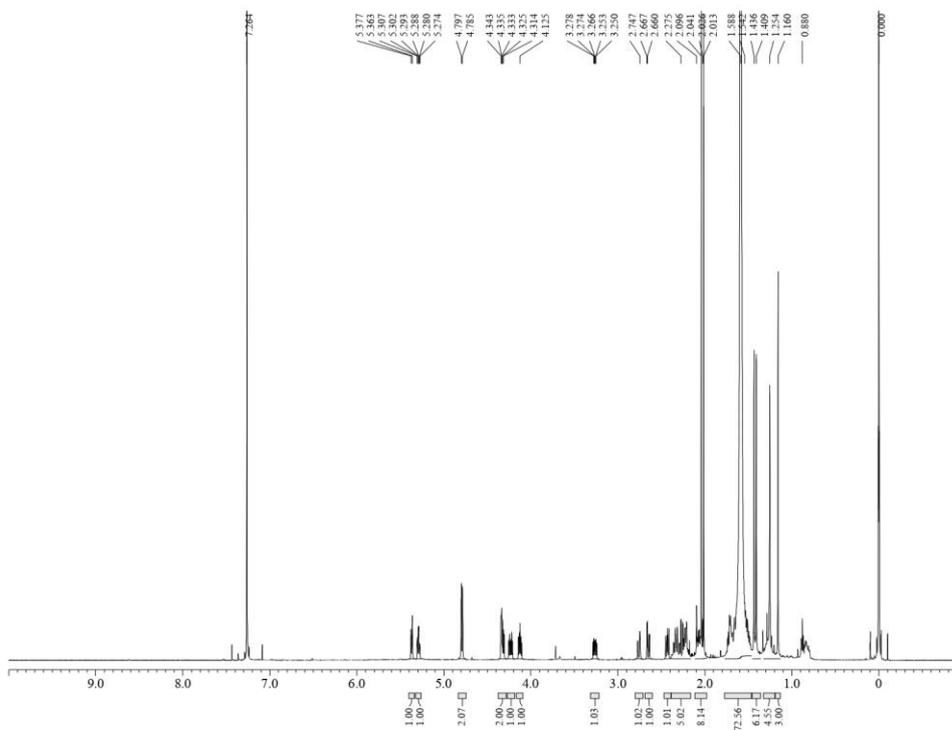
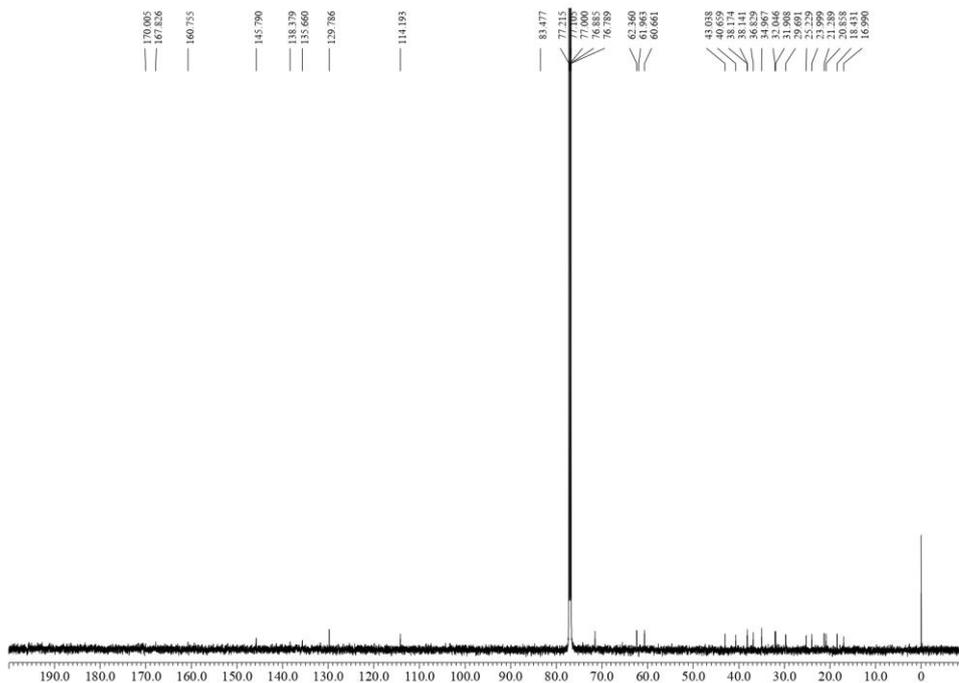


Figure S10. <sup>1</sup>H NMR spectrum (600MHz) of compound 1a in CDCl<sub>3</sub>

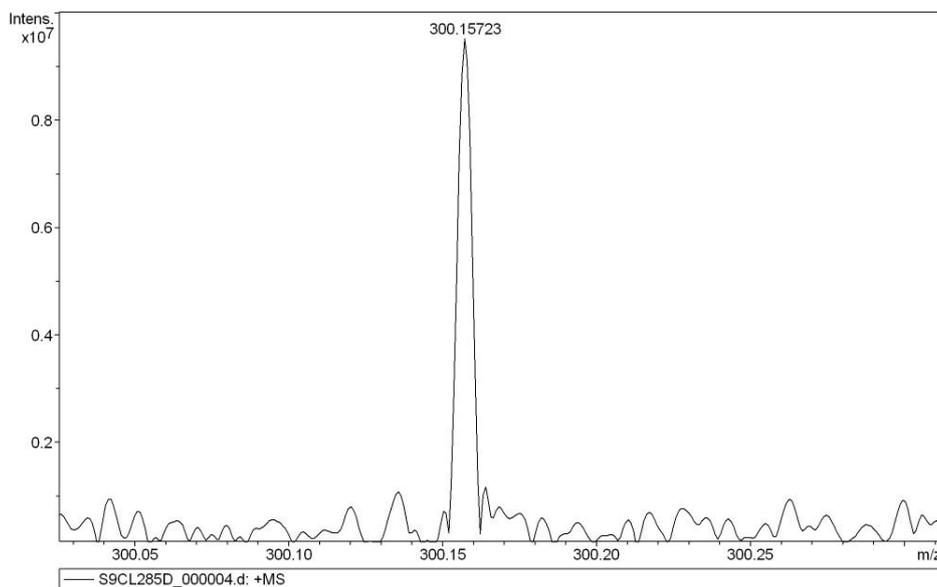


**Figure S11.**  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **1a** in  $\text{CDCl}_3$

**Analysis Info**

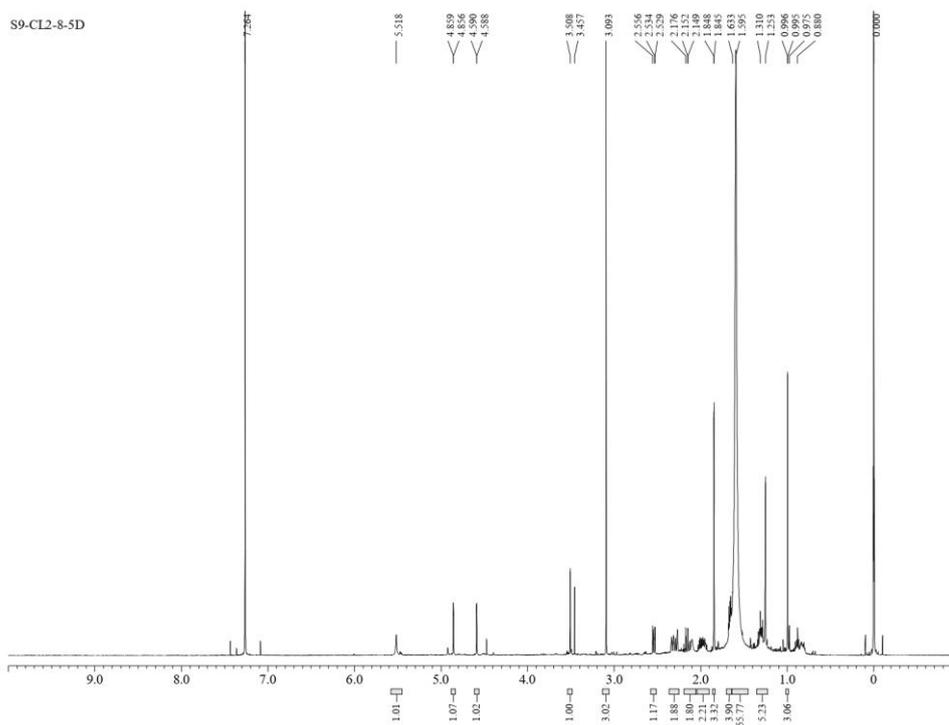
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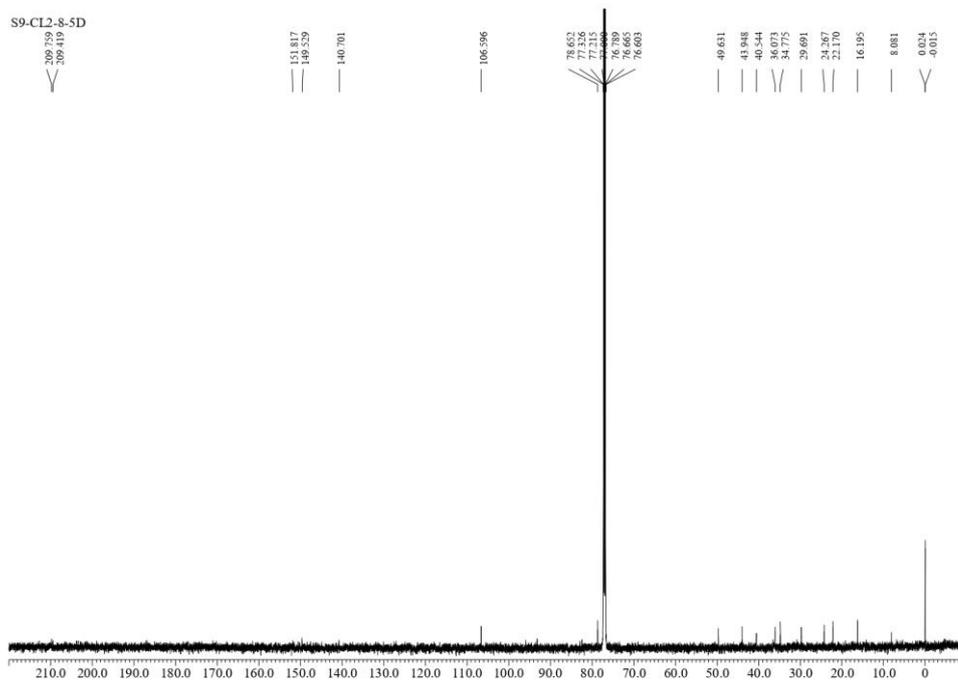


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300.15723	1	C <sub>16</sub> H <sub>23</sub> NNaO <sub>3</sub>	100.00	300.15701	-0.22	-0.72	16.8	5.5	even	ok

**Figure S12.** HRESIMS of compound **2**

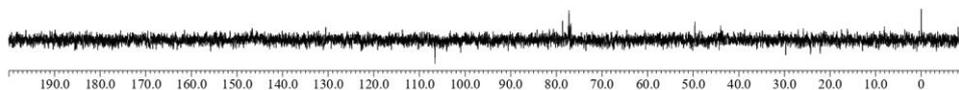


**Figure S13.**  $^1\text{H}$  NMR spectrum (600MHz) of compound **2** in  $\text{CDCl}_3$

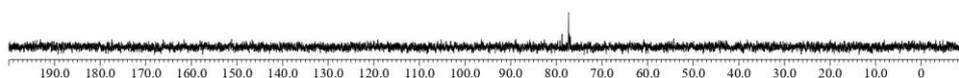


**Figure S14.**  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **2** in  $\text{CDCl}_3$

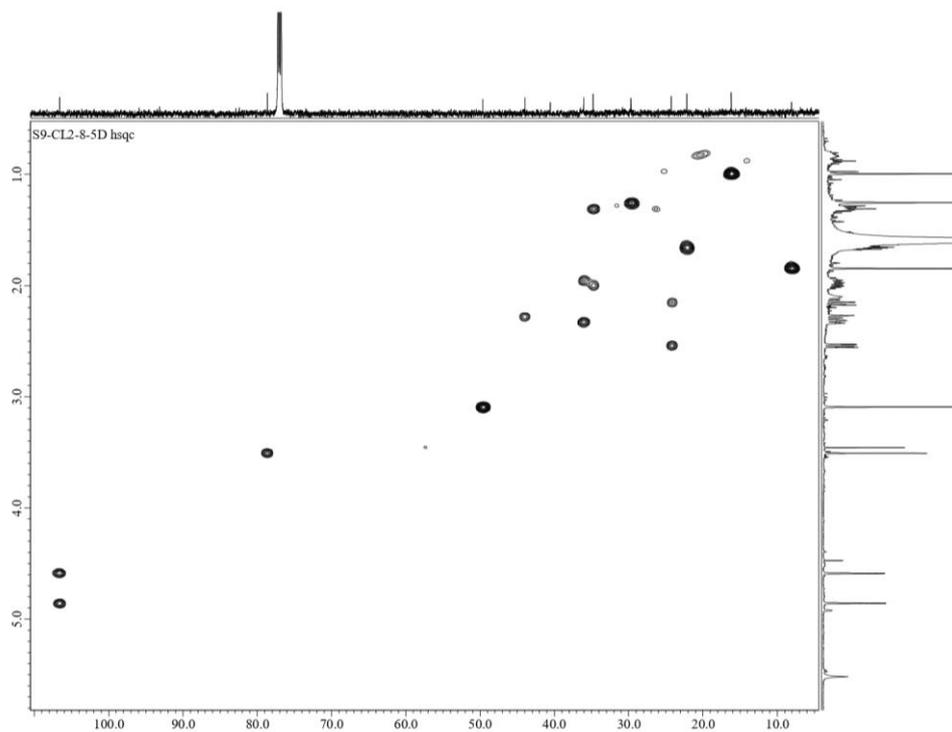
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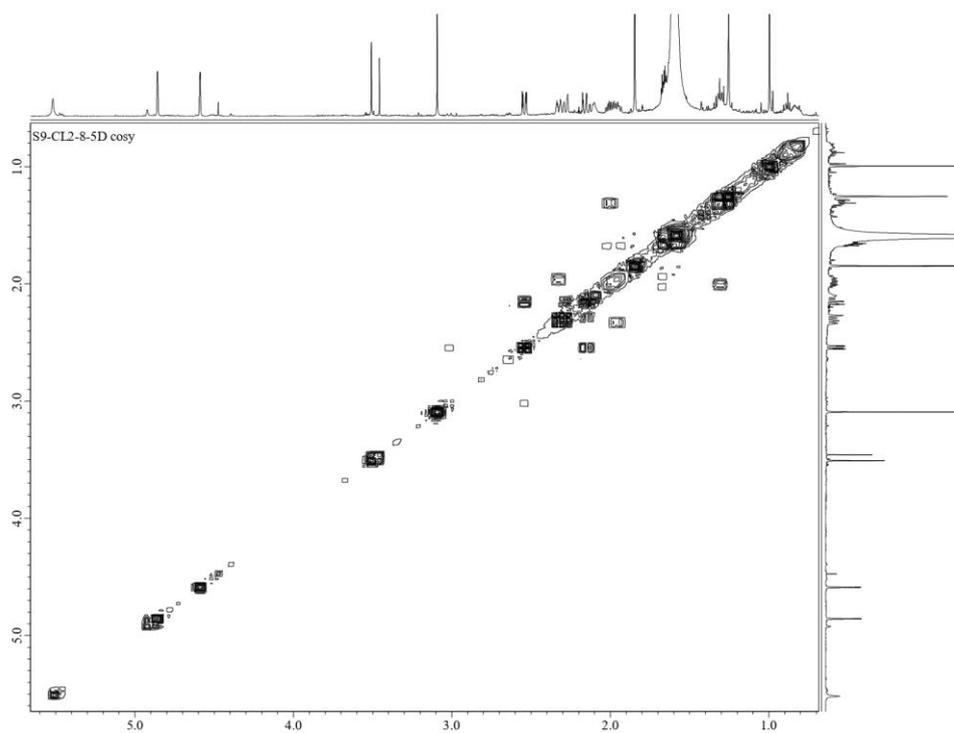
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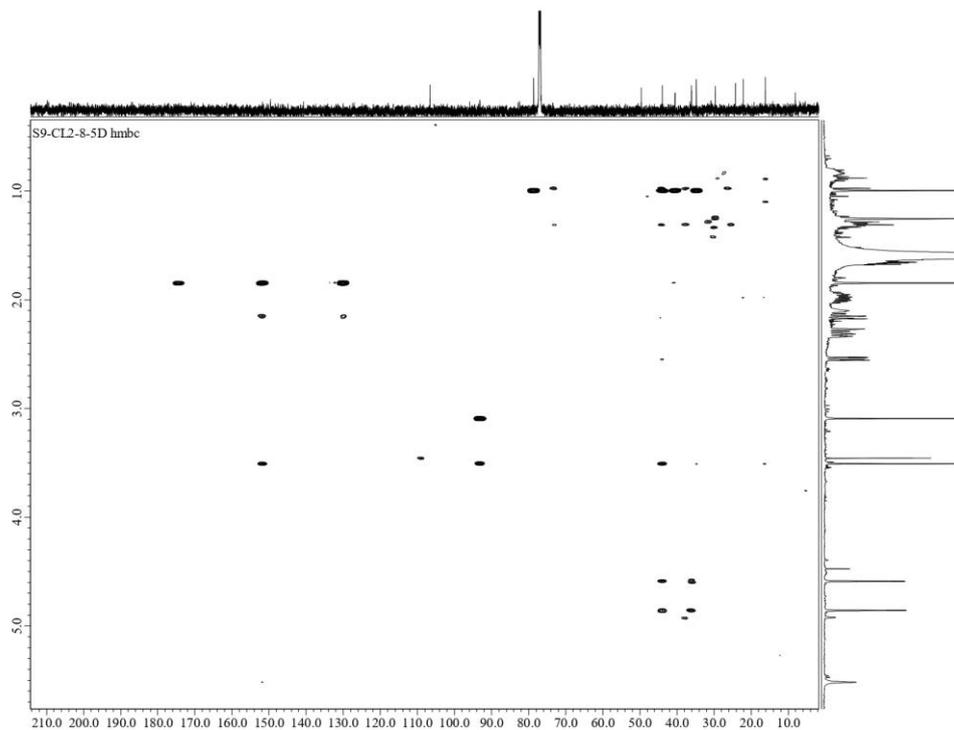
**Figure S15.** DEPT spectrum (150 MHz) of compound **2** in CDCl<sub>3</sub>



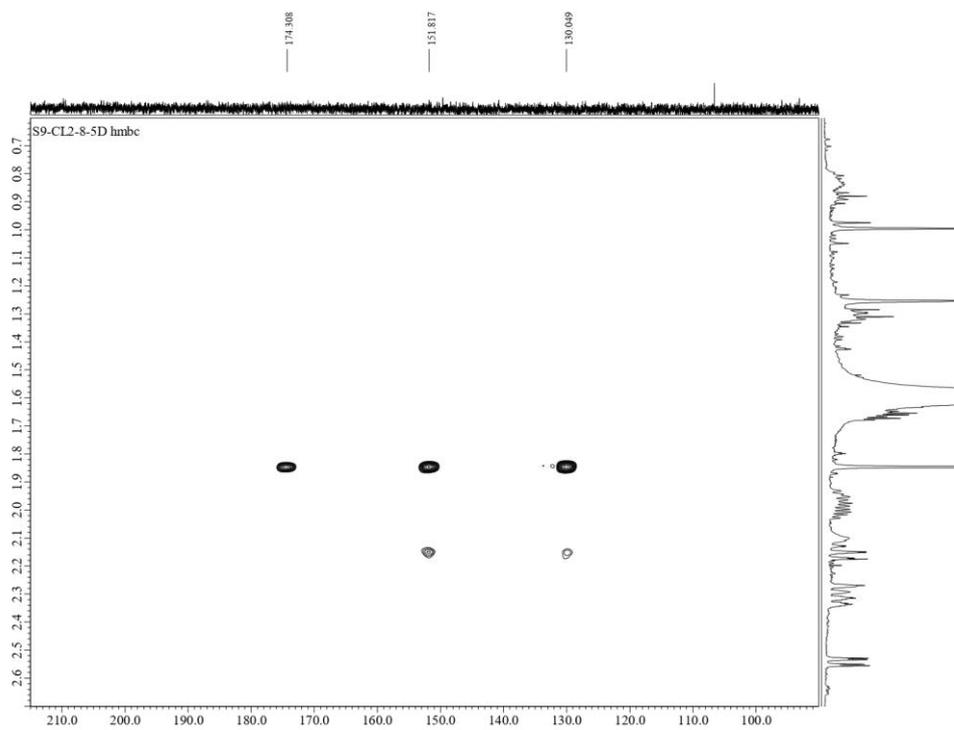
**Figure S16.** HSQC spectrum of compound **2** in CDCl<sub>3</sub>



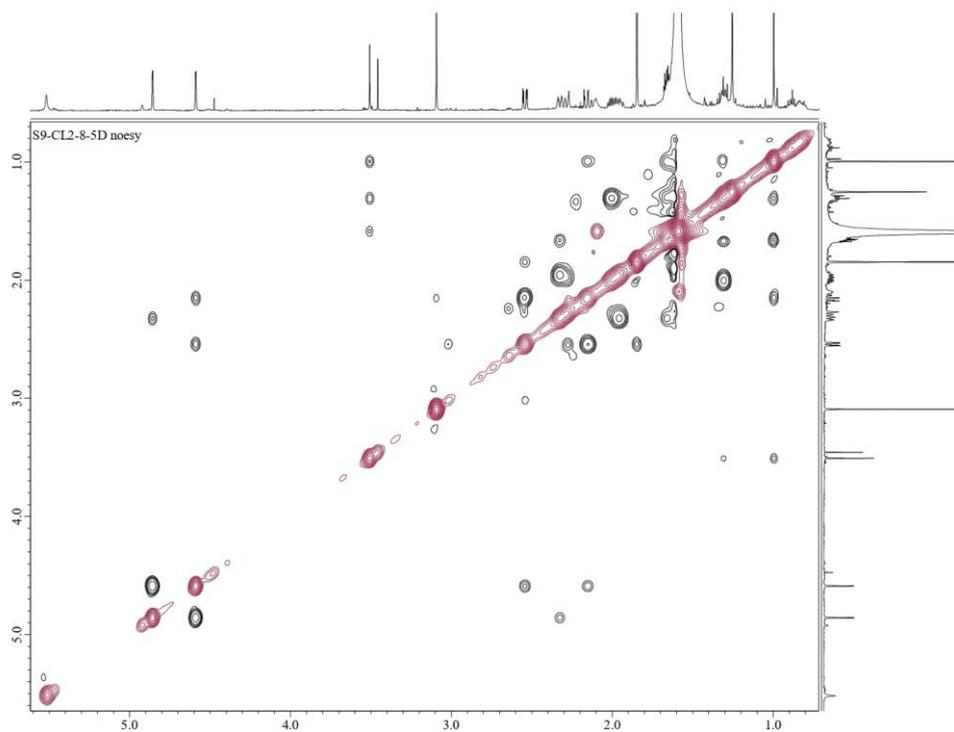
**Figure S17.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **2** in CDCl<sub>3</sub>



**Figure S18.** HMBC spectrum of compound **2** in CDCl<sub>3</sub>



**Figure S19.** The amplificatory HMBC spectrum of compound **2** in CDCl<sub>3</sub>

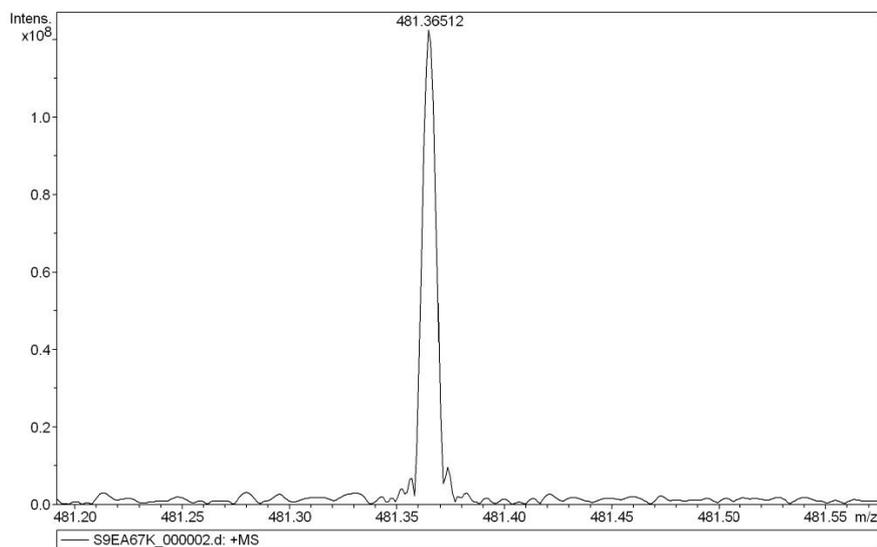


**Figure S20.** NOESY spectrum of compound **2** in CDCl<sub>3</sub>

**Analysis Info**

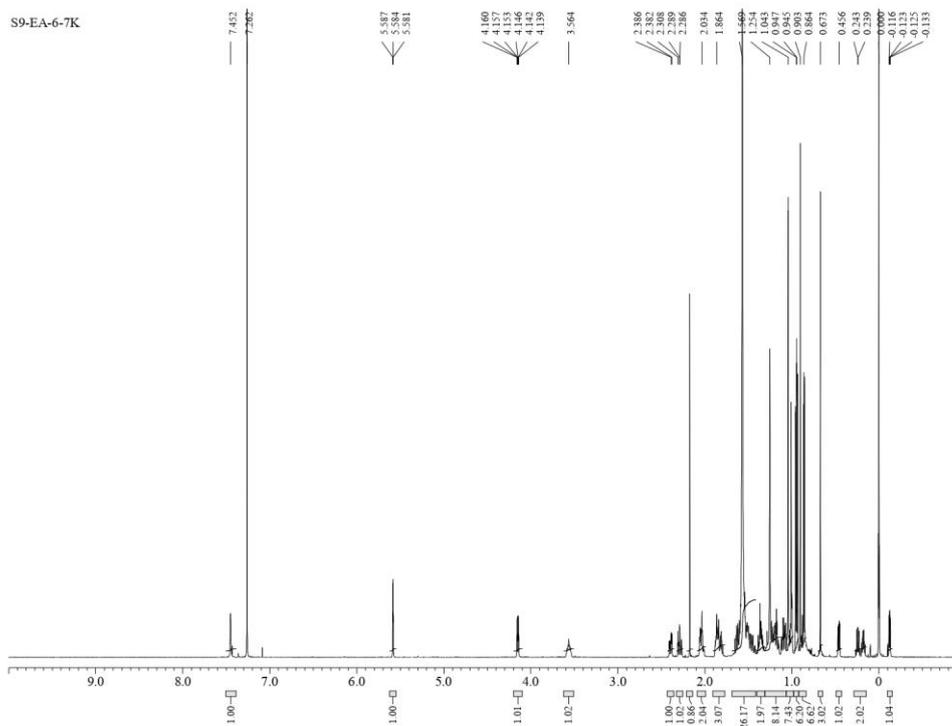
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Comment ESI Positive

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Instrument: BRUKER FT-MS solariX

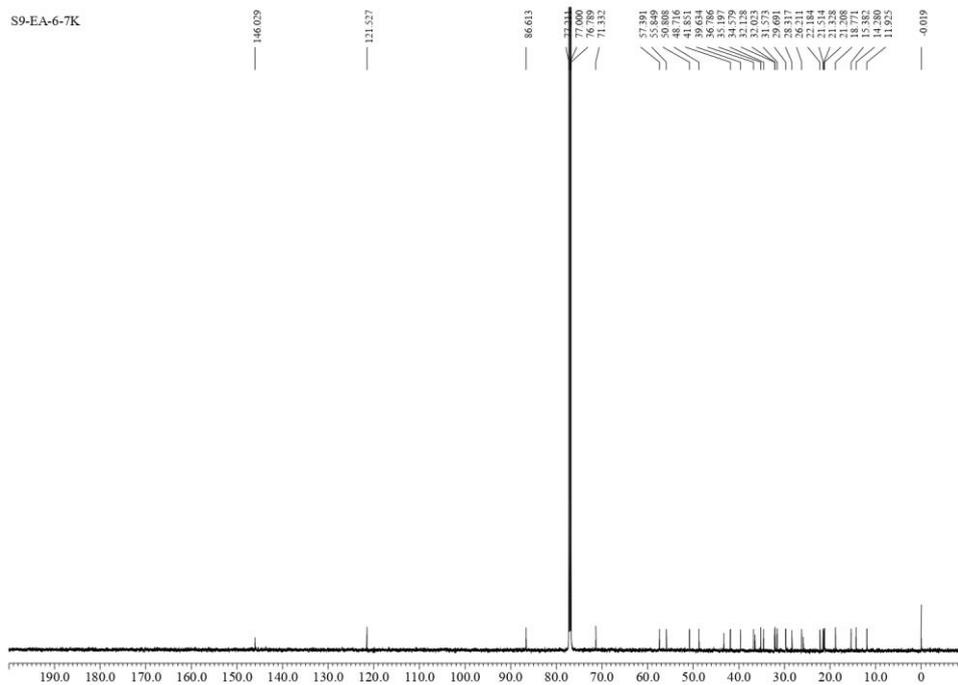


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**Figure S21.** HRESIMS of compound **3**

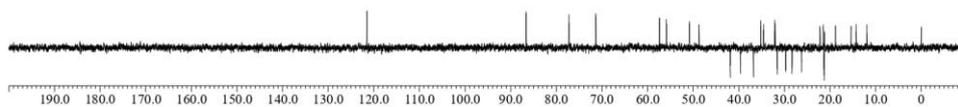


**Figure S22.** <sup>1</sup>H NMR spectrum (600MHz) of compound **3** in CDCl<sub>3</sub>

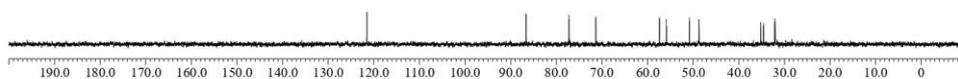


**Figure S23.**  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **3** in  $\text{CDCl}_3$

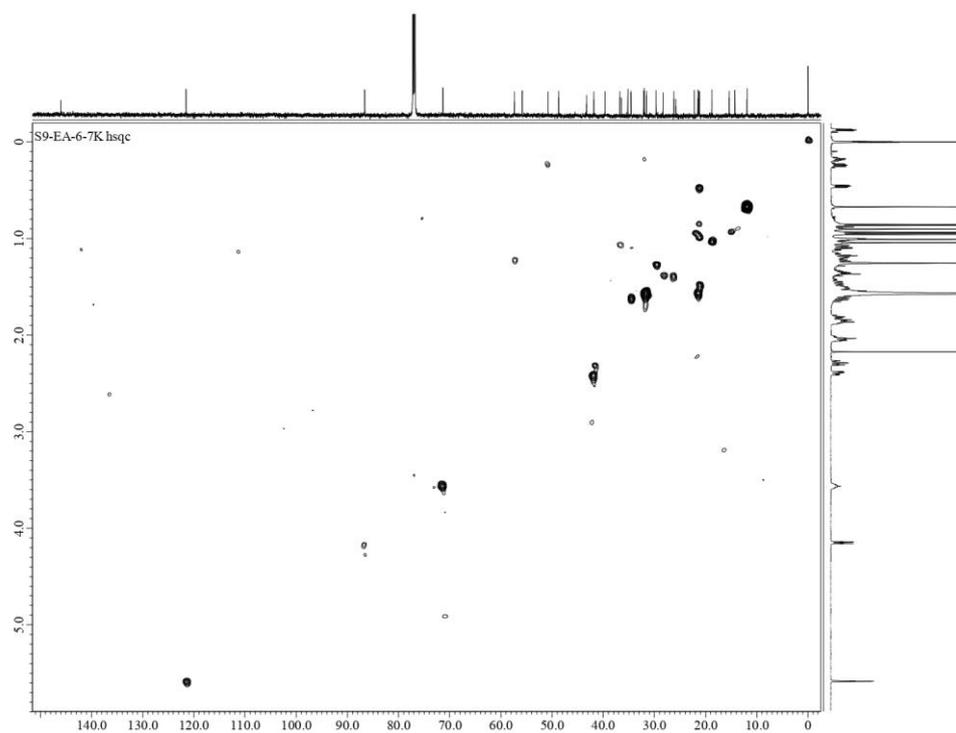
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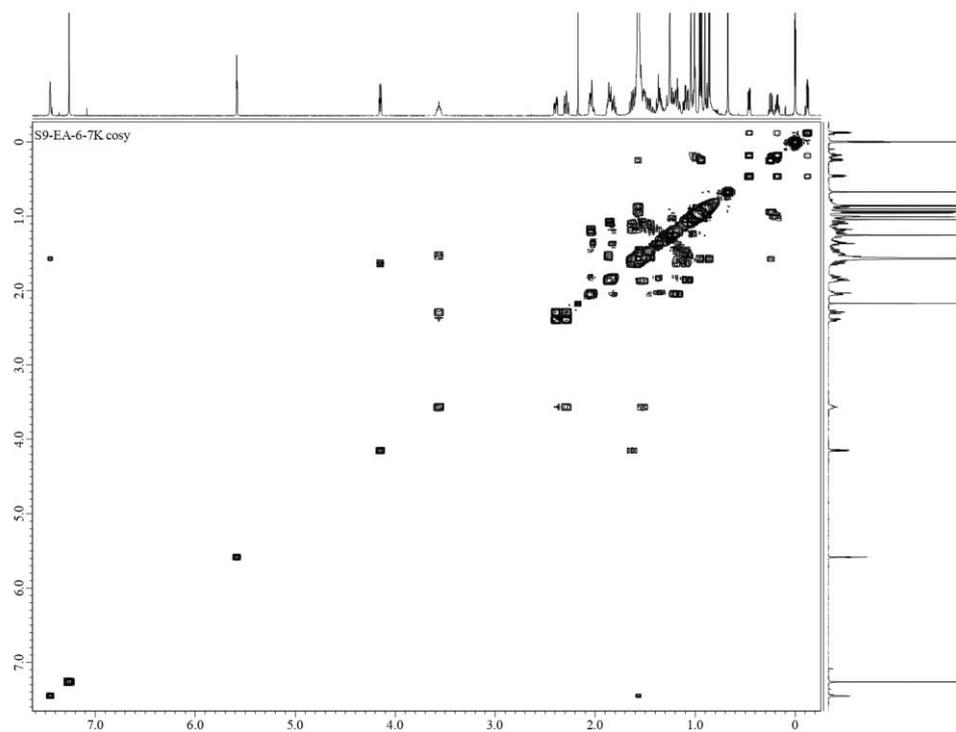
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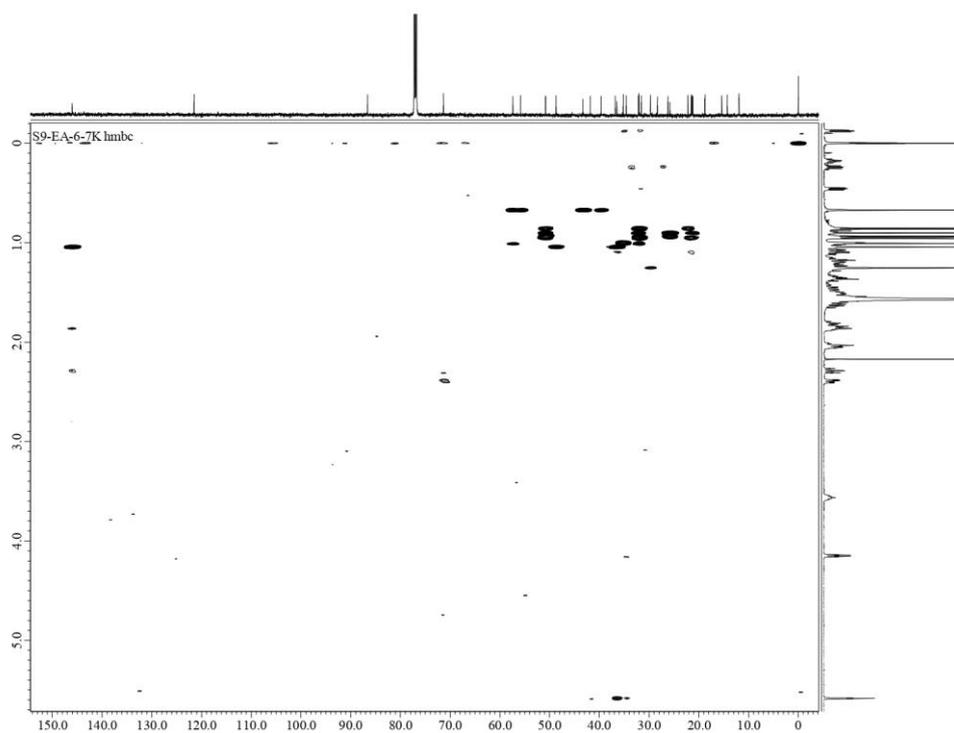
**Figure S24.** DEPT spectrum (150 MHz) of compound **3** in  $\text{CDCl}_3$



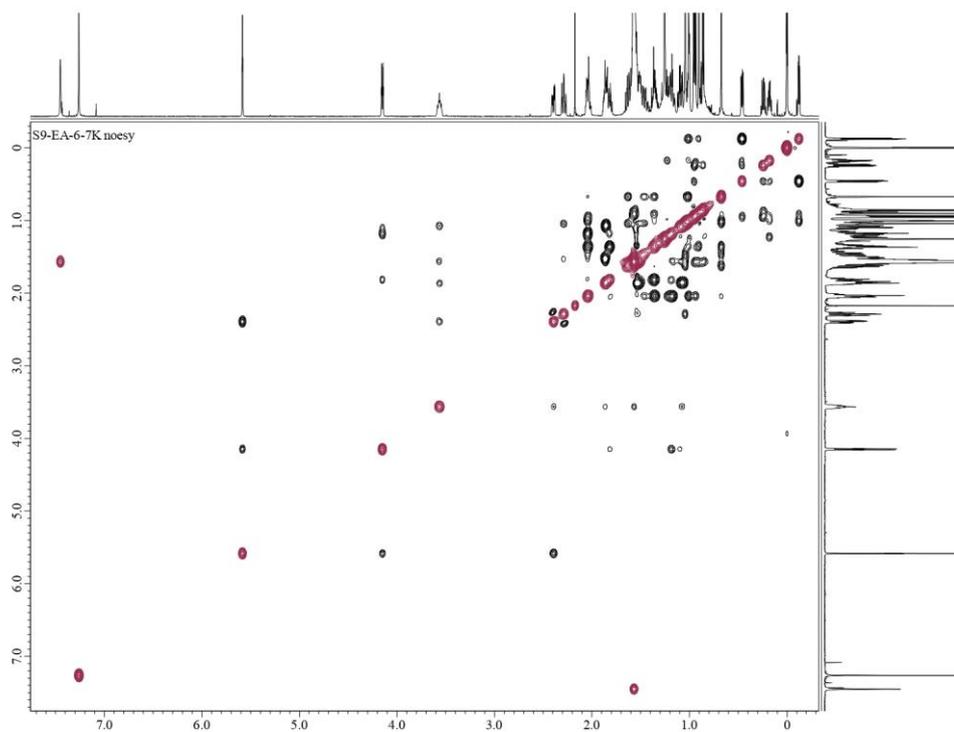
**Figure S25.** HSQC spectrum of compound **3** in CDCl<sub>3</sub>



**Figure S26.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **3** in CDCl<sub>3</sub>



**Figure S27.** HMBC spectrum of compound **3** in CDCl<sub>3</sub>

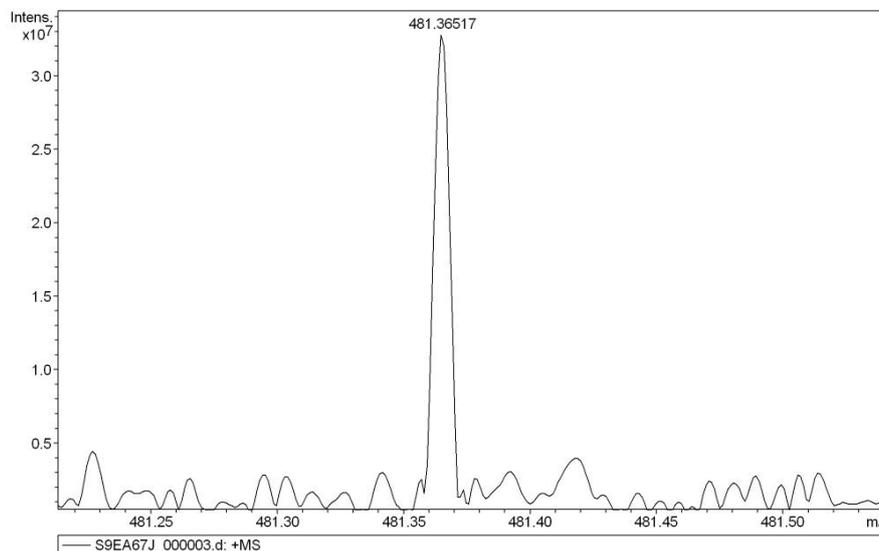


**Figure S28.** NOESY spectrum of compound **3** in CDCl<sub>3</sub>

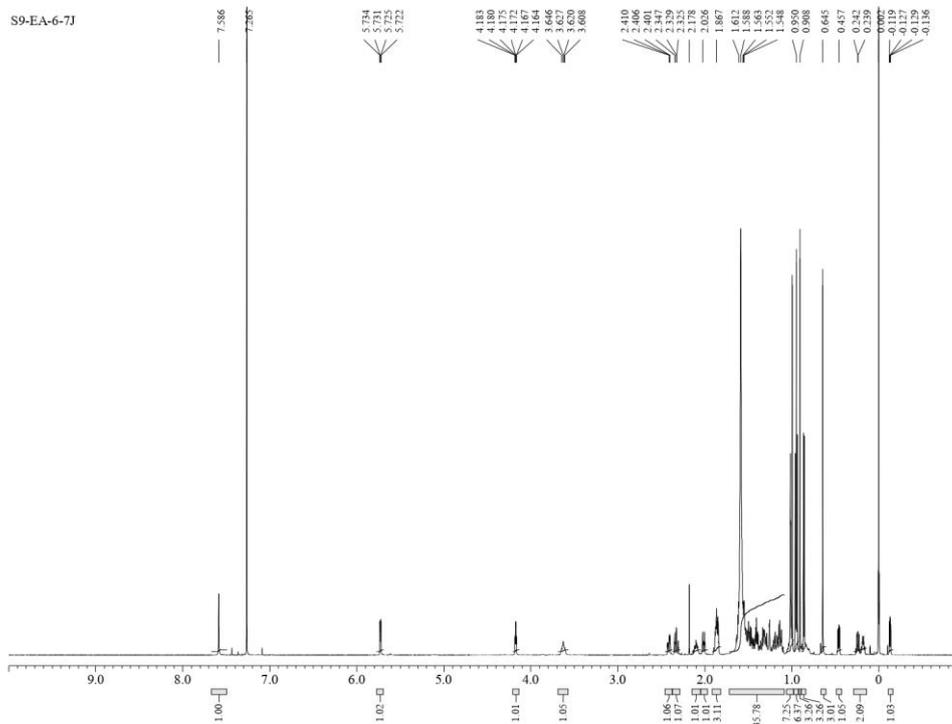
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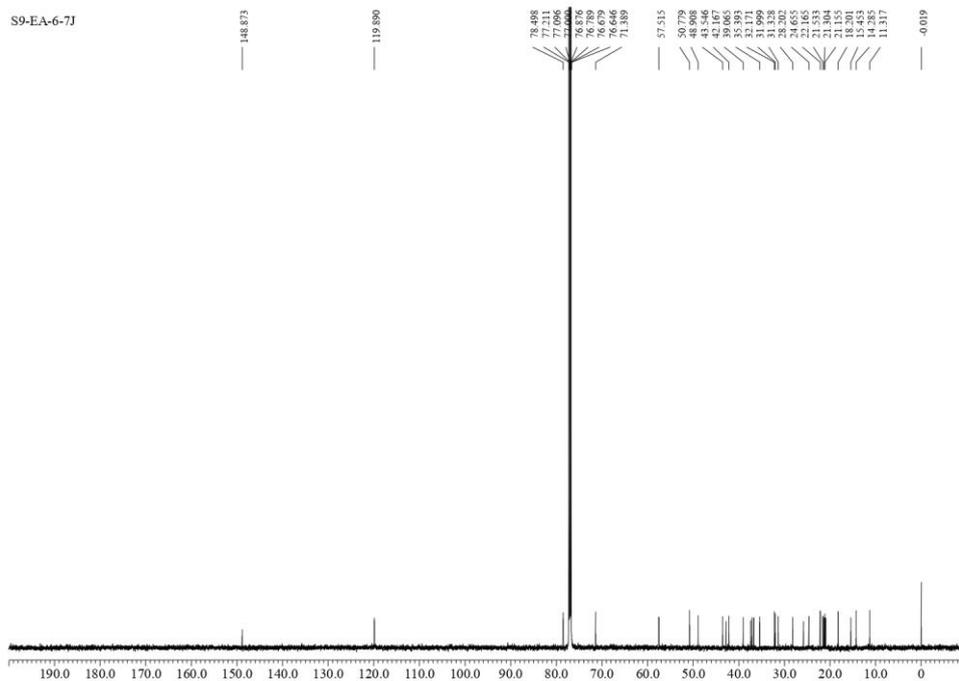
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Sample Name S9-EA-6-7-J  
Comment ESI Positive

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Operator: YU HSIAO-CHING  
Instrument: BRUKER FT-MS solariX



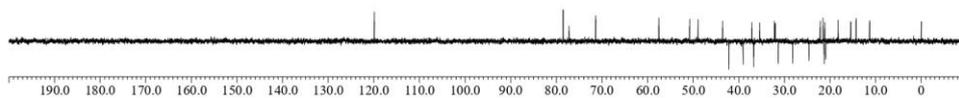
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
481.36517	1	C 30 H 50 Na O 3	100.00	481.36522	0.05	0.10	37.5	5.5	even	ok

**Figure S29. HRESIMS of compound 4****Figure S30. <sup>1</sup>H NMR spectrum (600MHz) of compound 4 in CDCl<sub>3</sub>**

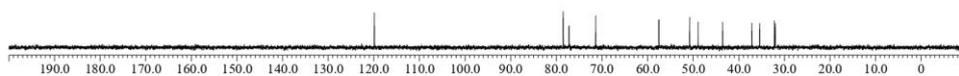


**Figure S31.**  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **4** in  $\text{CDCl}_3$

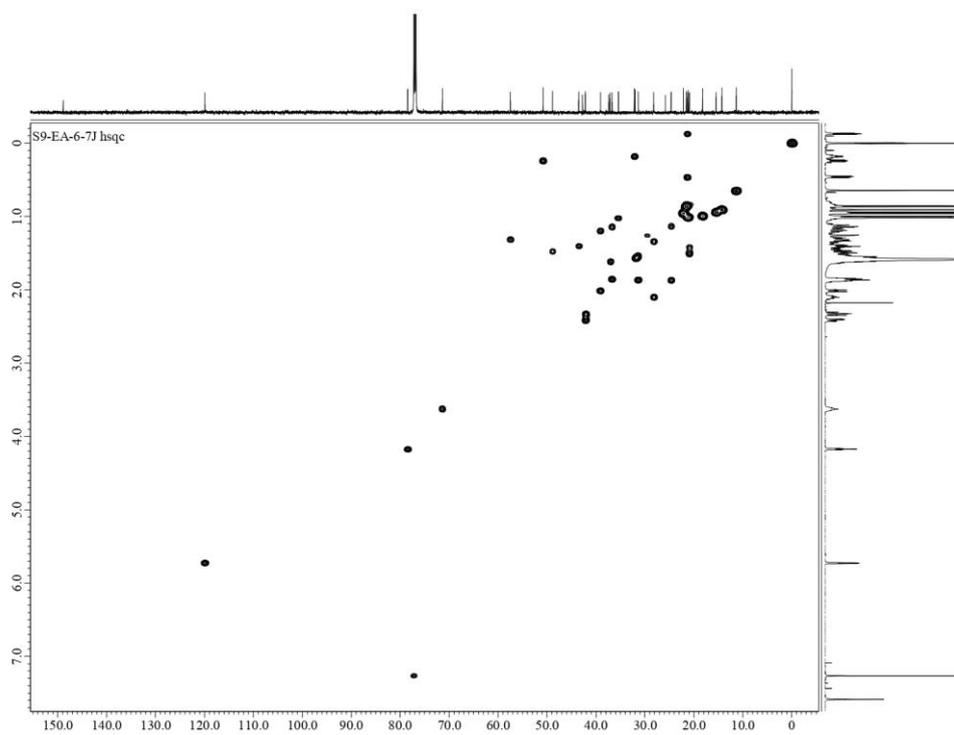
Y = 135[deg]  
S9-EA-6-7J



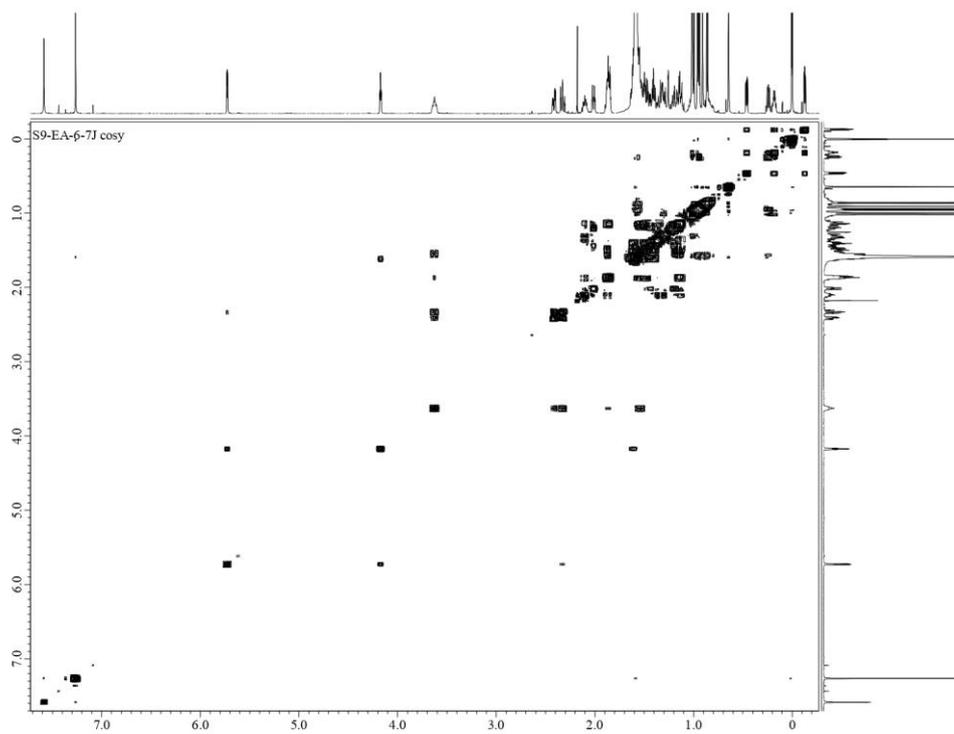
Y = 90[deg]  
S9-EA-6-7J



**Figure S32.** DEPT spectrum (150 MHz) of compound **4** in  $\text{CDCl}_3$



**Figure S33.** HSQC spectrum of compound **4** in  $\text{CDCl}_3$



**Figure S34.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **4** in  $\text{CDCl}_3$

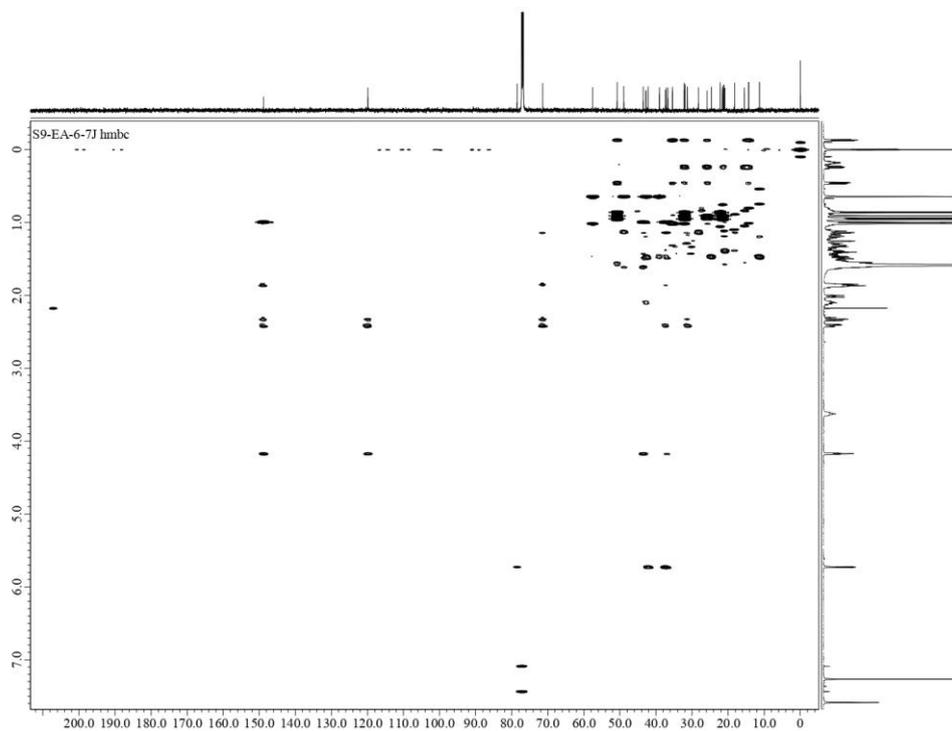


Figure S35. HMBC spectrum of compound **4** in CDCl<sub>3</sub>

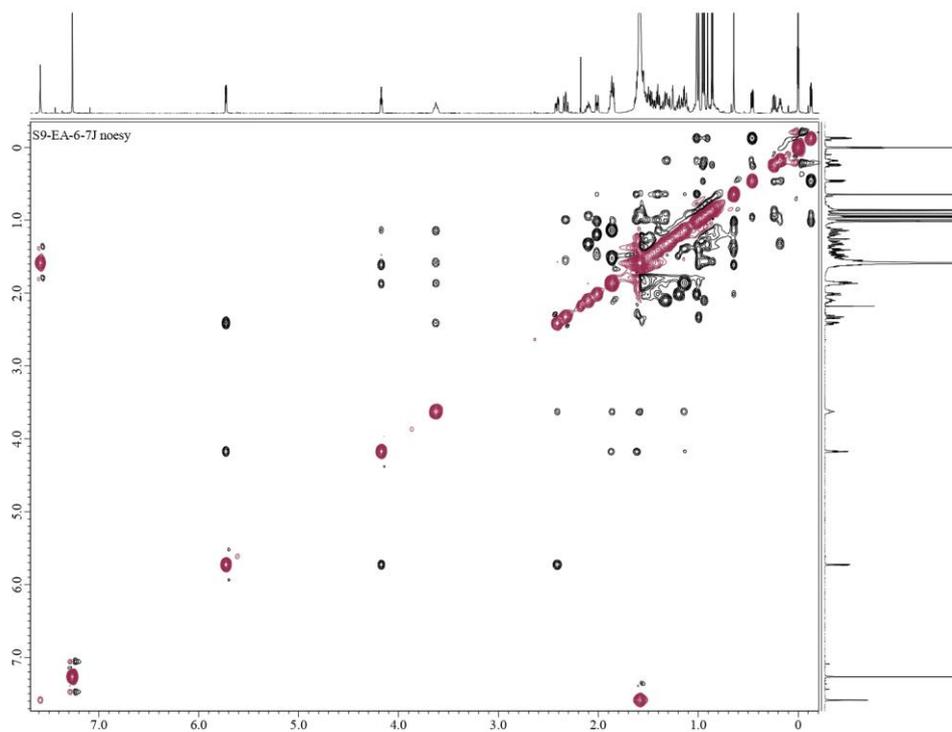
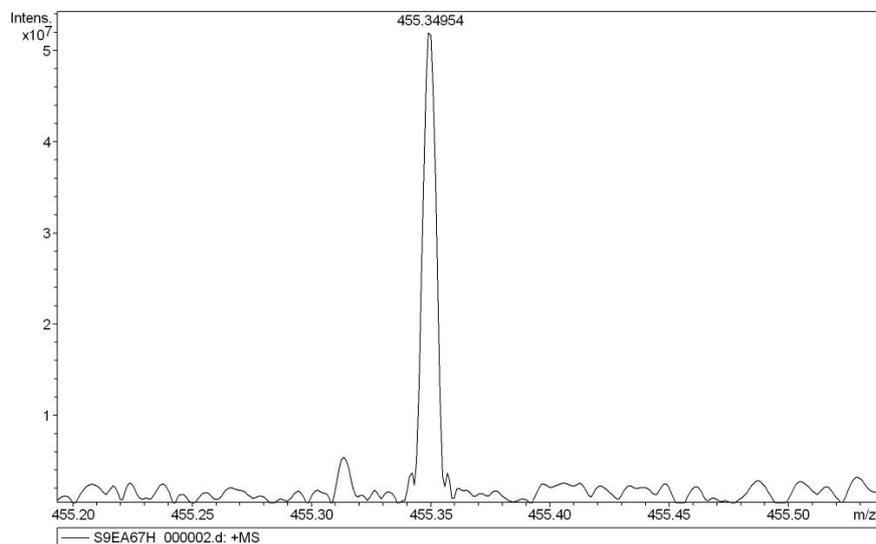


Figure S36. NOESY spectrum of compound **4** in CDCl<sub>3</sub>

**Analysis Info**

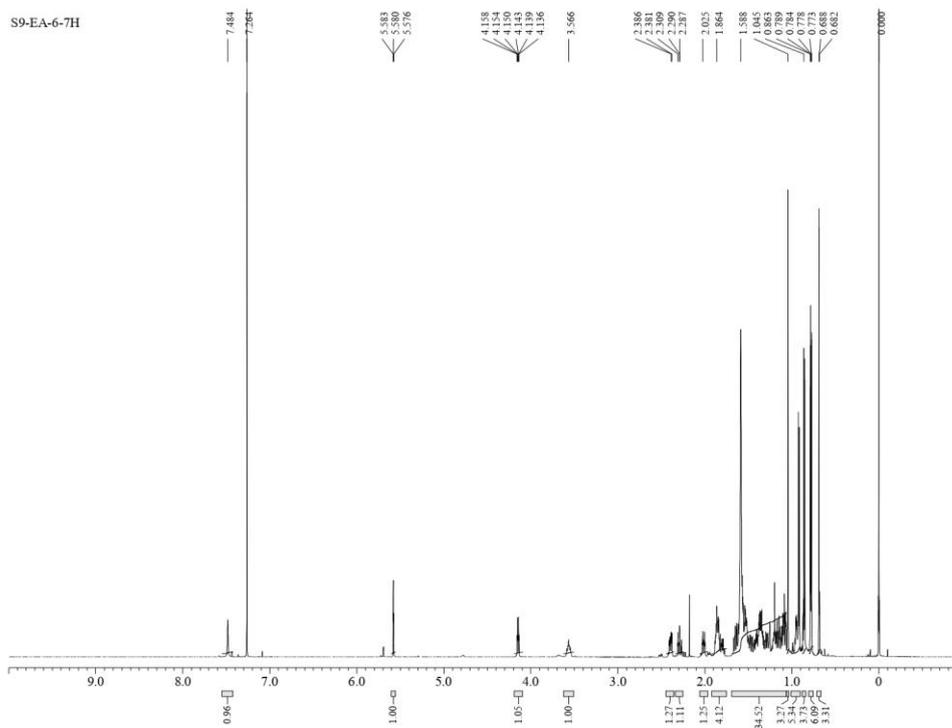
Analysis Name D:\Data\1\S9EA67H\_000002.d  
Method broadband first signal  
Sample Name S9-EA-6-7-H  
Comment ESI Positive

3/26/2021 11:35:26 AM  
Operator: YU HSIAO-CHING  
Instrument: BRUKER FT-MS solariX

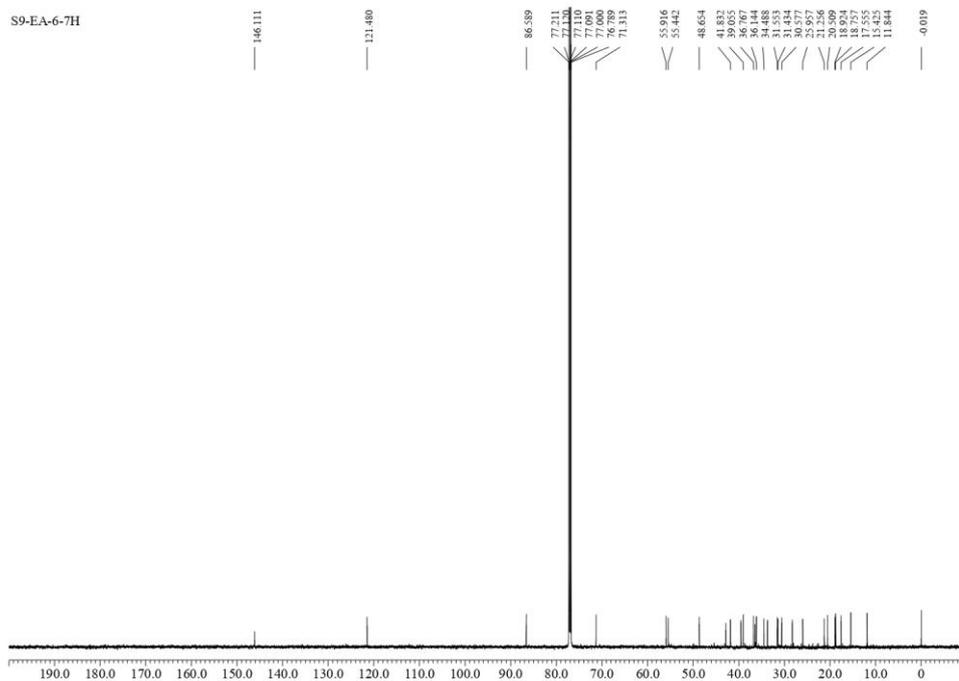


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
455.34954	1	C 28 H 48 Na O 3	100.00	455.34957	0.02	0.05	36.2	4.5	even	ok

**Figure S37.** HRESIMS of compound **5**

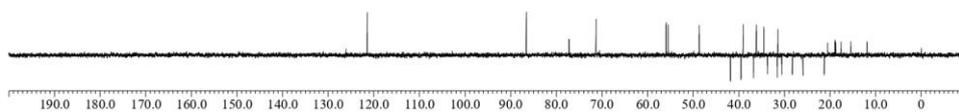


**Figure S38.** <sup>1</sup>H NMR spectrum (600MHz) of compound **5** in CDCl<sub>3</sub>

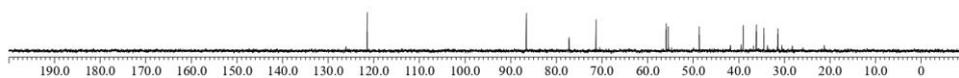


**Figure S39.**  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **5** in  $\text{CDCl}_3$

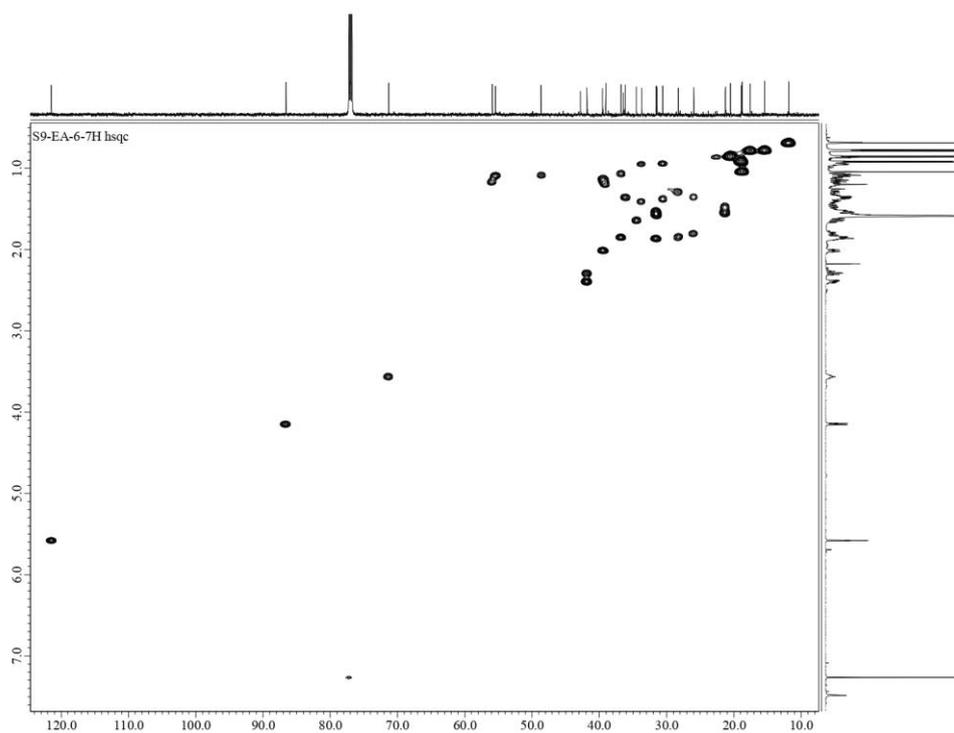
Y = 135[deg]  
S9-EA-6-7H



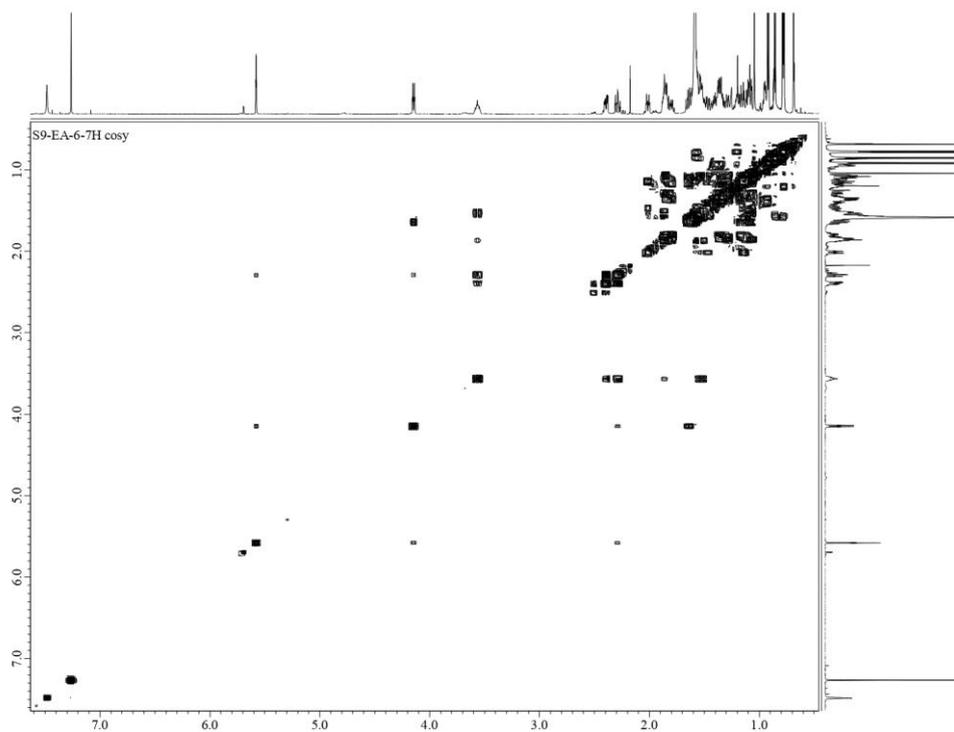
Y = 90[deg]  
S9-EA-6-7H



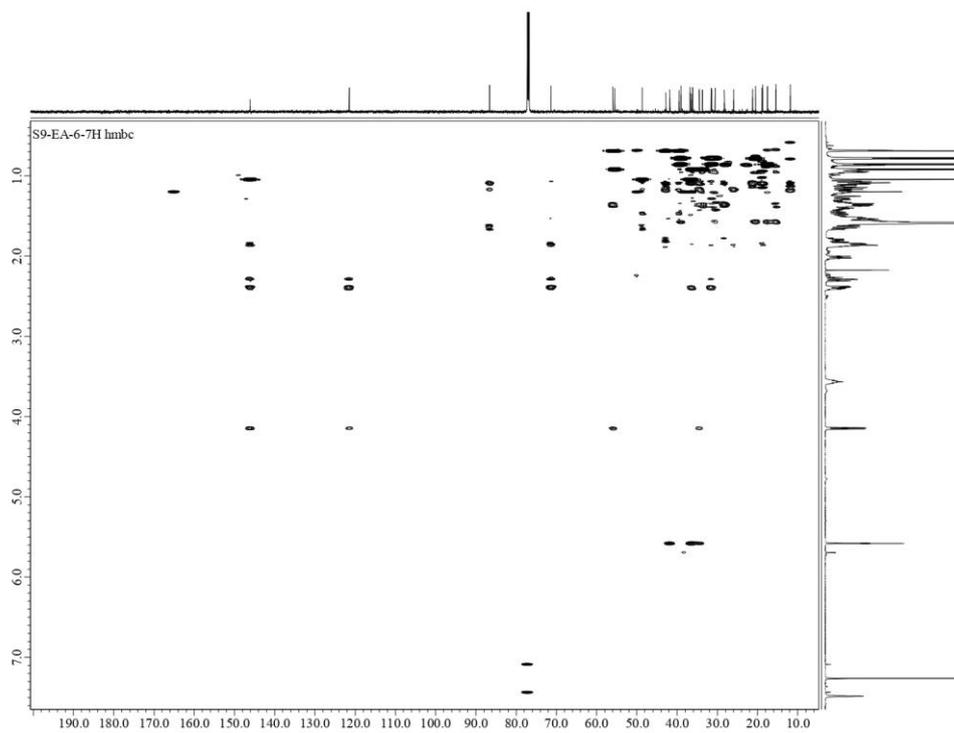
**Figure S40.** DEPT spectrum (150 MHz) of compound **5** in  $\text{CDCl}_3$



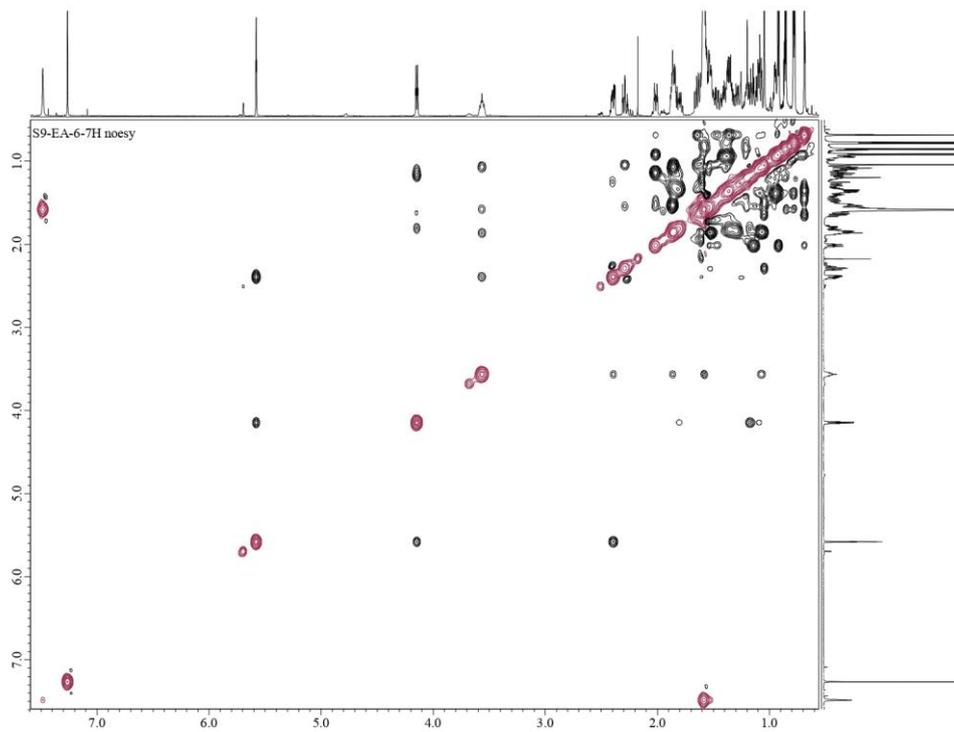
**Figure S41.** HSQC spectrum of compound **5** in  $\text{CDCl}_3$



**Figure S42.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **5** in  $\text{CDCl}_3$



**Figure S43.** HMBC spectrum of compound **5** in  $\text{CDCl}_3$



**Figure S44.** NOESY spectrum of compound **5** in  $\text{CDCl}_3$

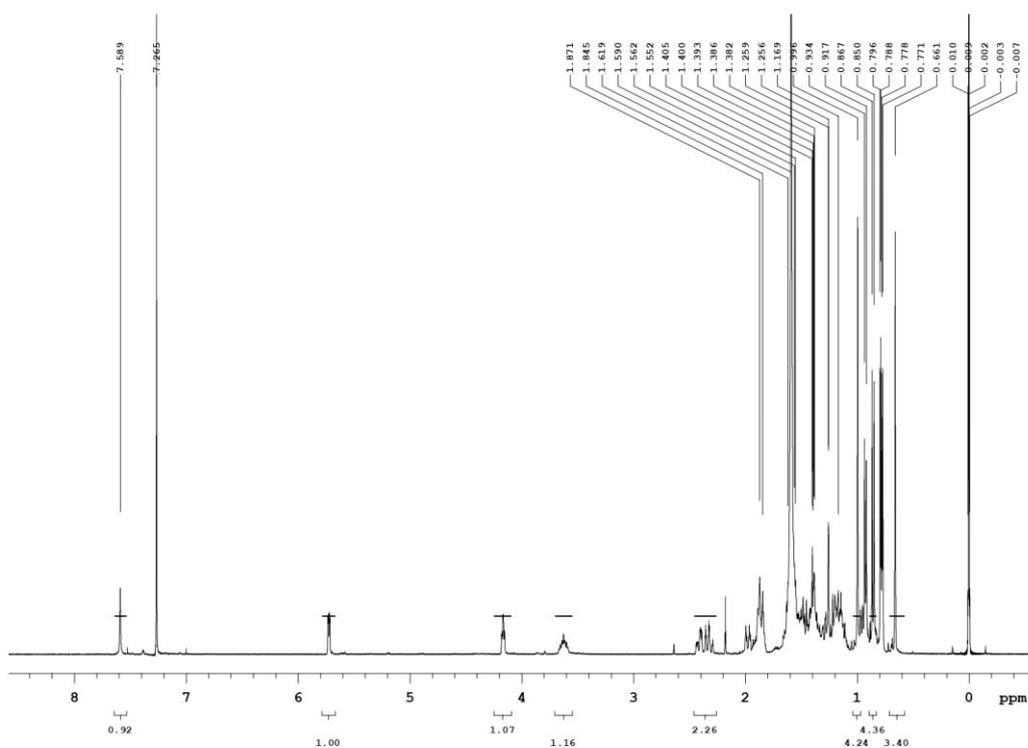


Figure S45.  $^1\text{H}$  NMR spectrum (400MHz) of compound **6** in  $\text{CDCl}_3$

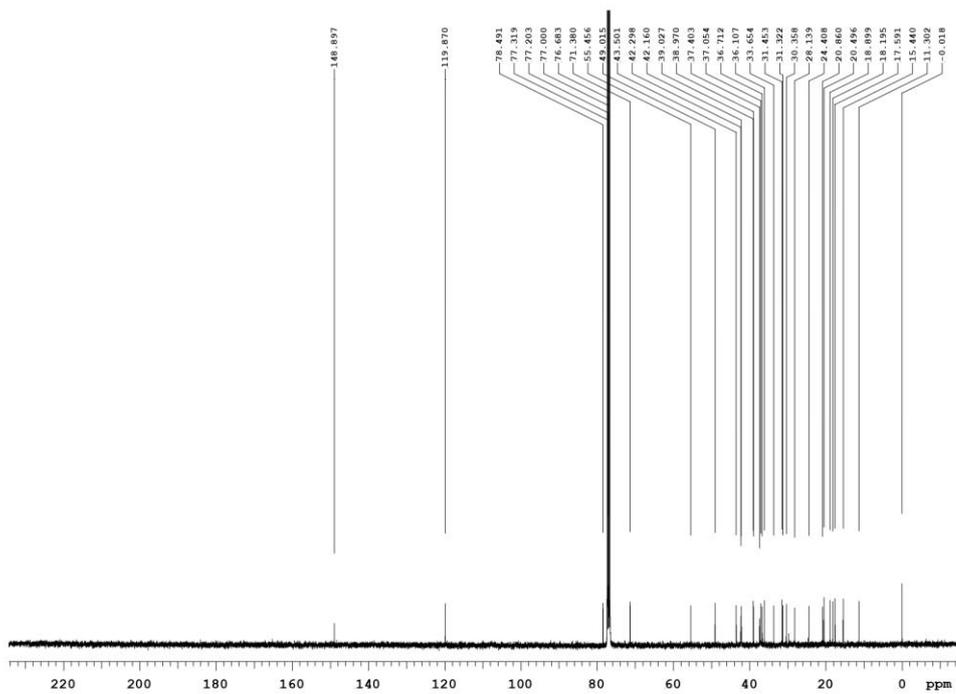


Figure S46.  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **6** in  $\text{CDCl}_3$

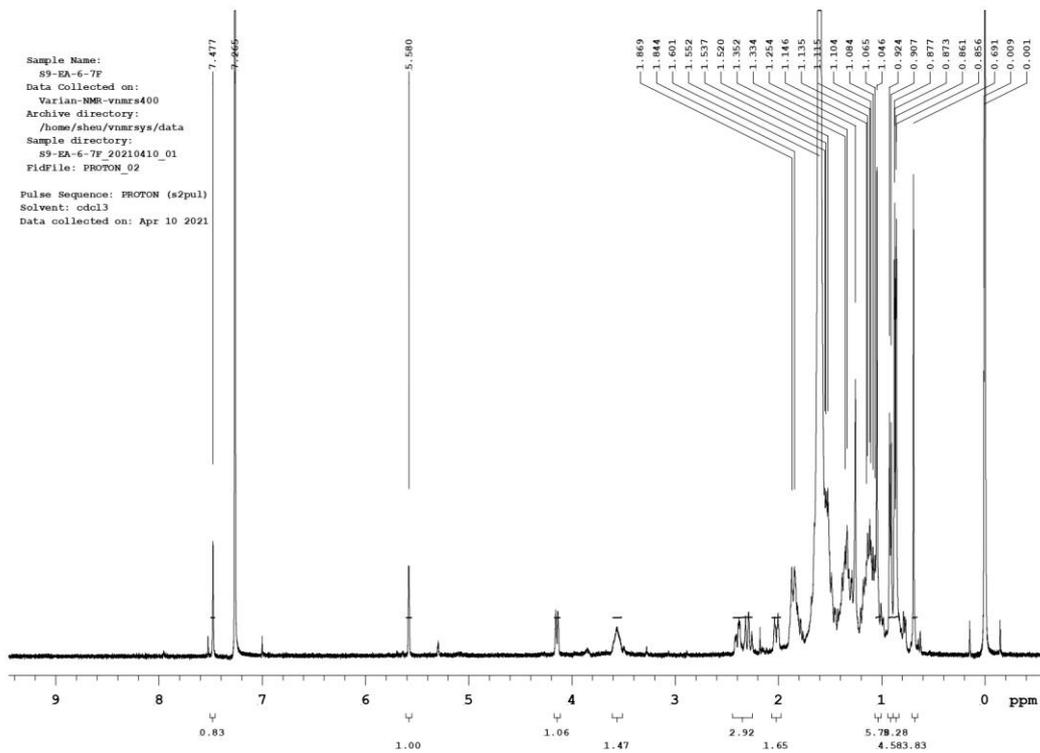


Figure S47.  $^1\text{H}$  NMR spectrum (400MHz) of compound 7 in  $\text{CDCl}_3$

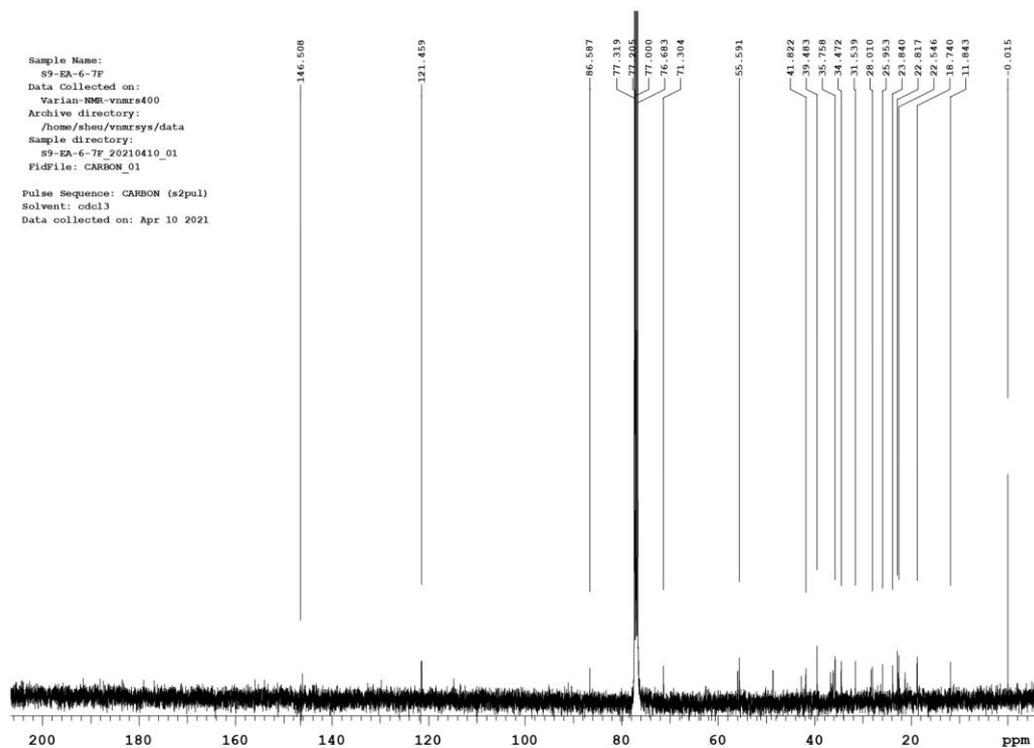


Figure S48.  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound 7 in  $\text{CDCl}_3$



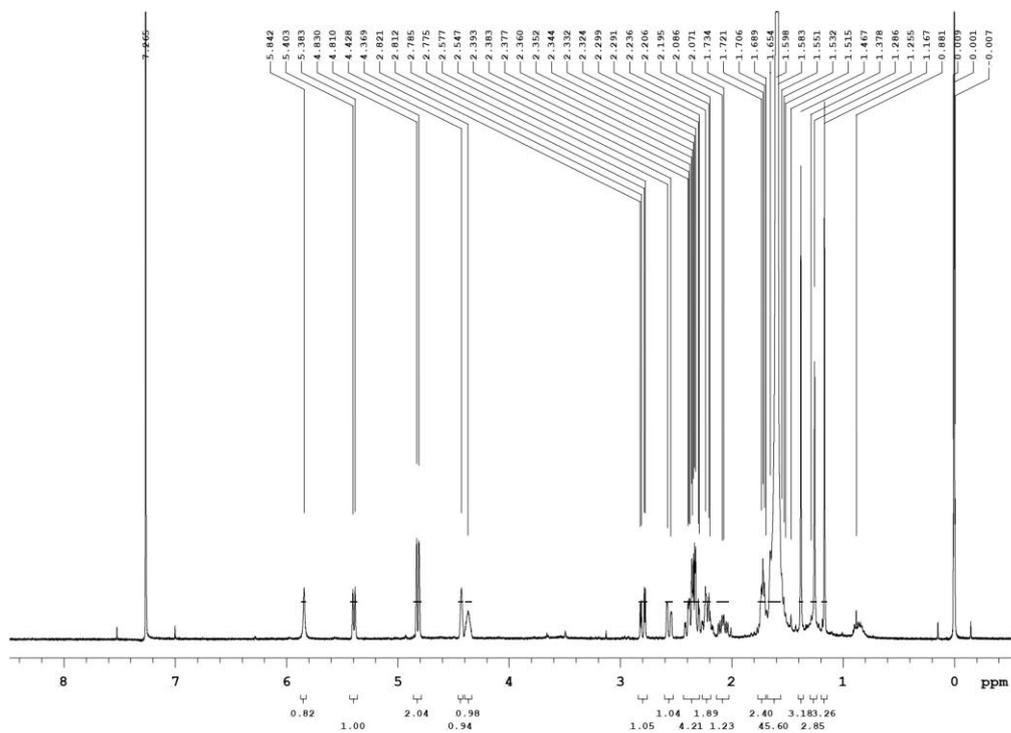


Figure S51.  $^1\text{H}$  NMR spectrum (400MHz) of compound **9** in  $\text{CDCl}_3$

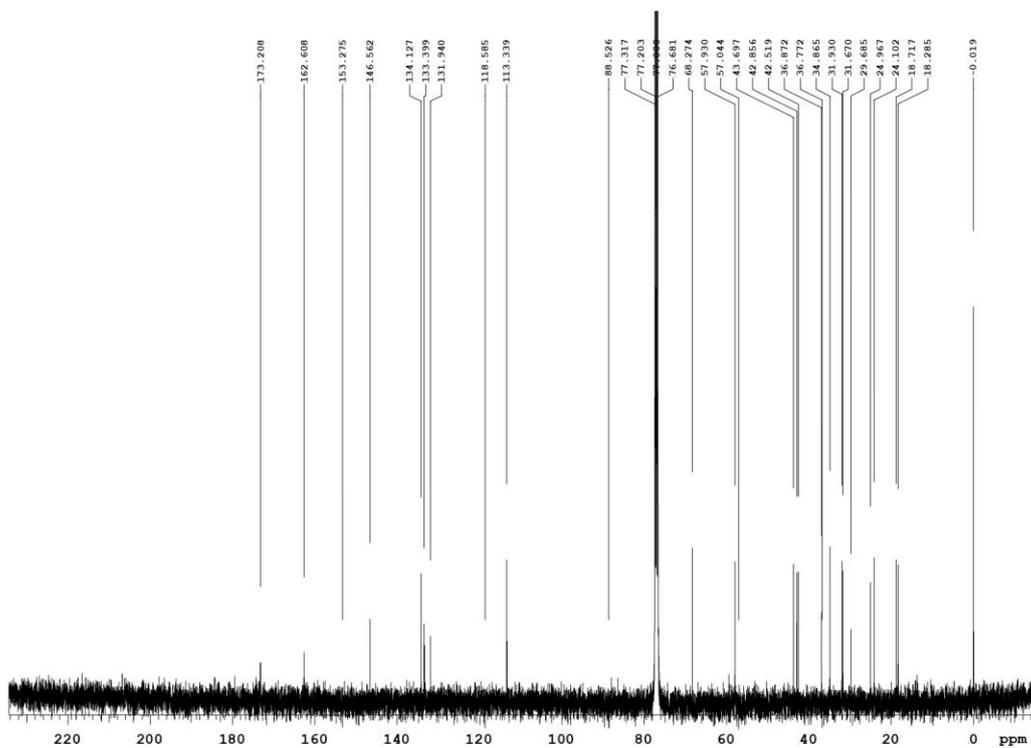


Figure S52.  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **9** in  $\text{CDCl}_3$

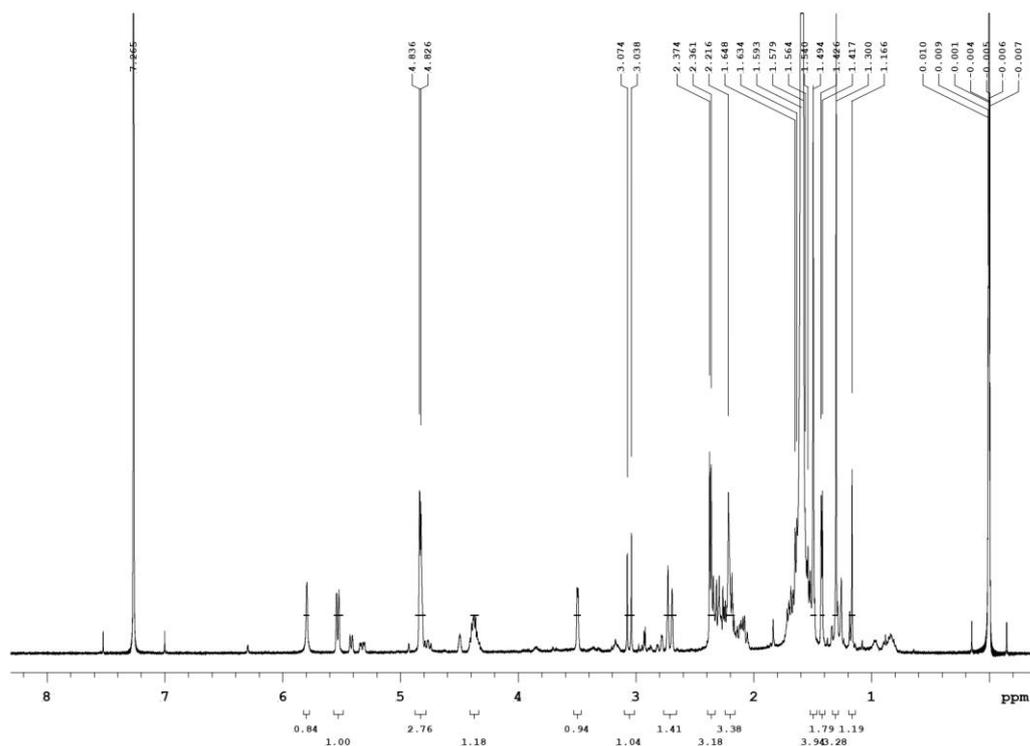


Figure S53.  $^1\text{H}$  NMR spectrum (400MHz) of compound **10** in  $\text{CDCl}_3$

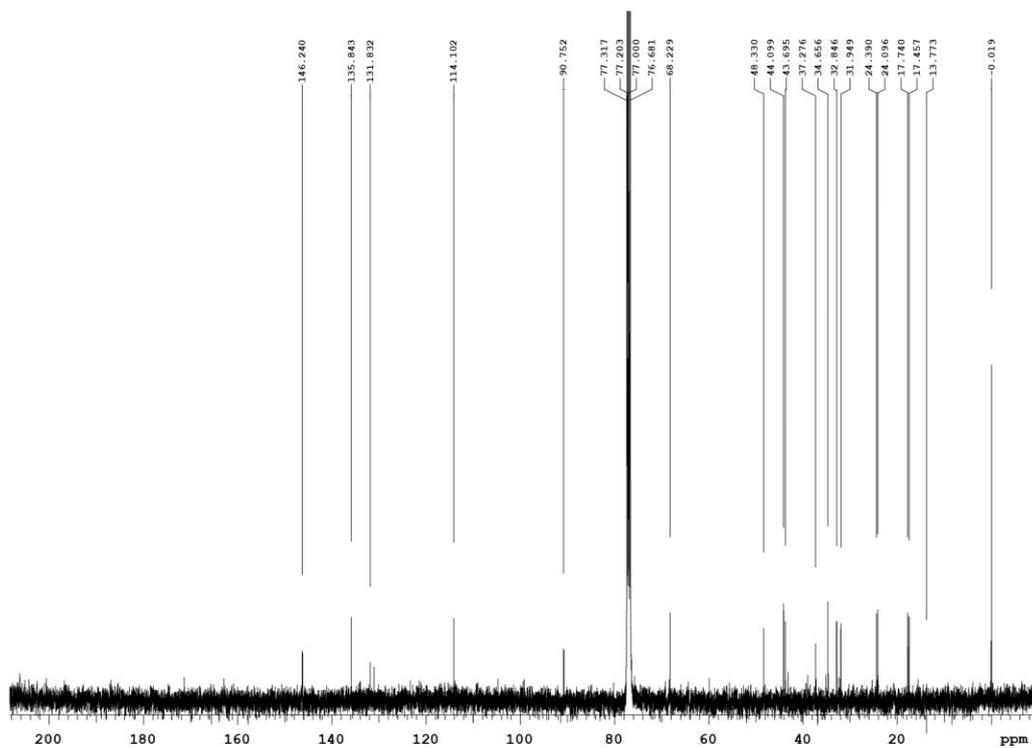
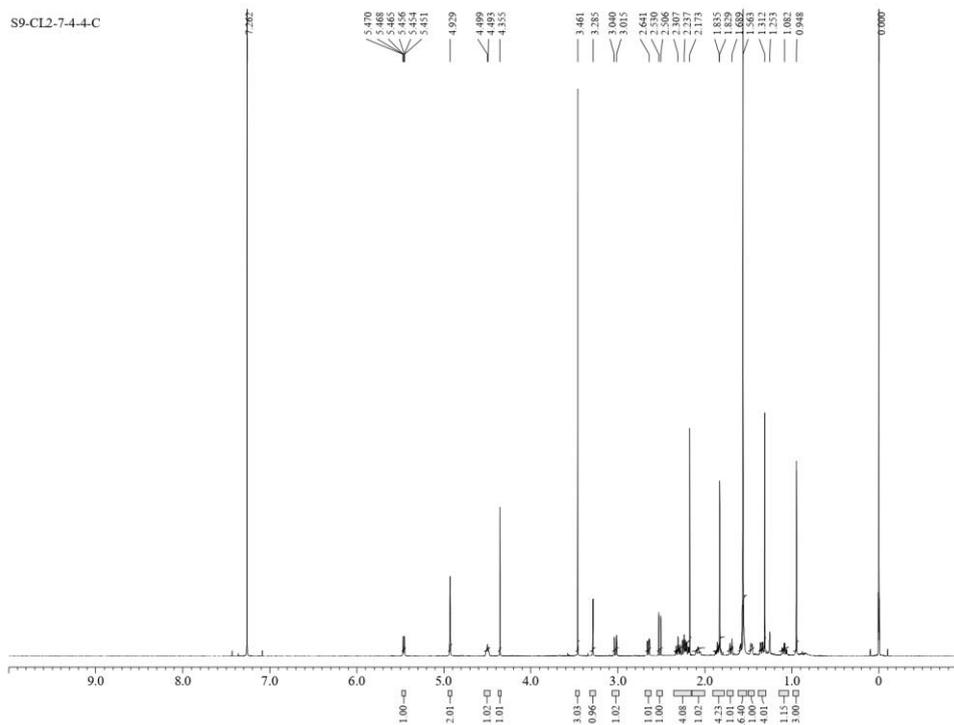
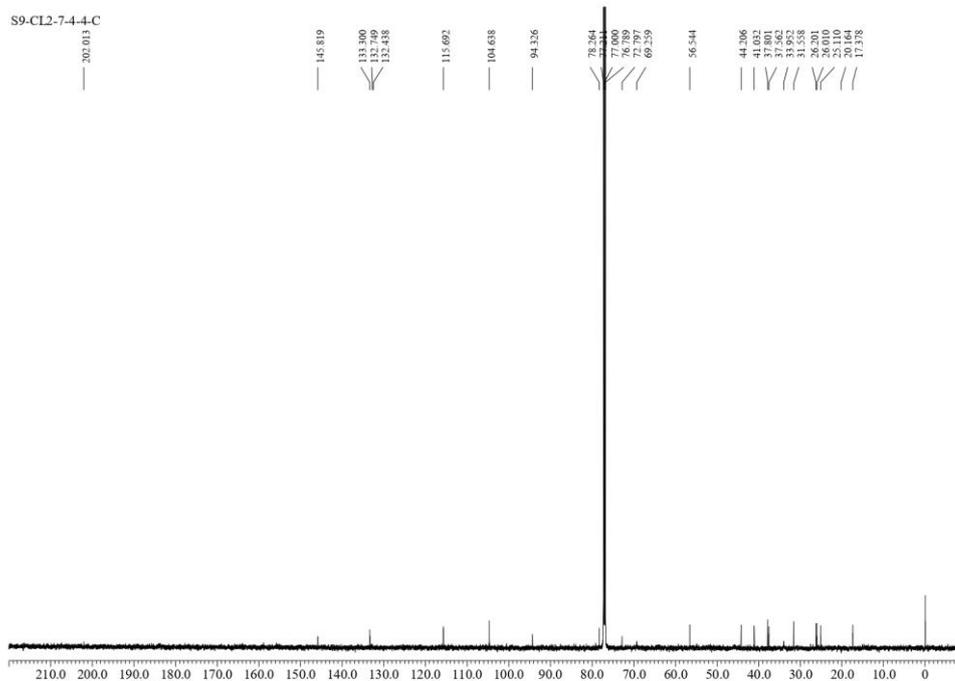


Figure S54.  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **10** in  $\text{CDCl}_3$



**Figure S55.**  $^1\text{H}$  NMR spectrum (600MHz) of compound **11** in  $\text{CDCl}_3$



**Figure S56.**  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **11** in  $\text{CDCl}_3$

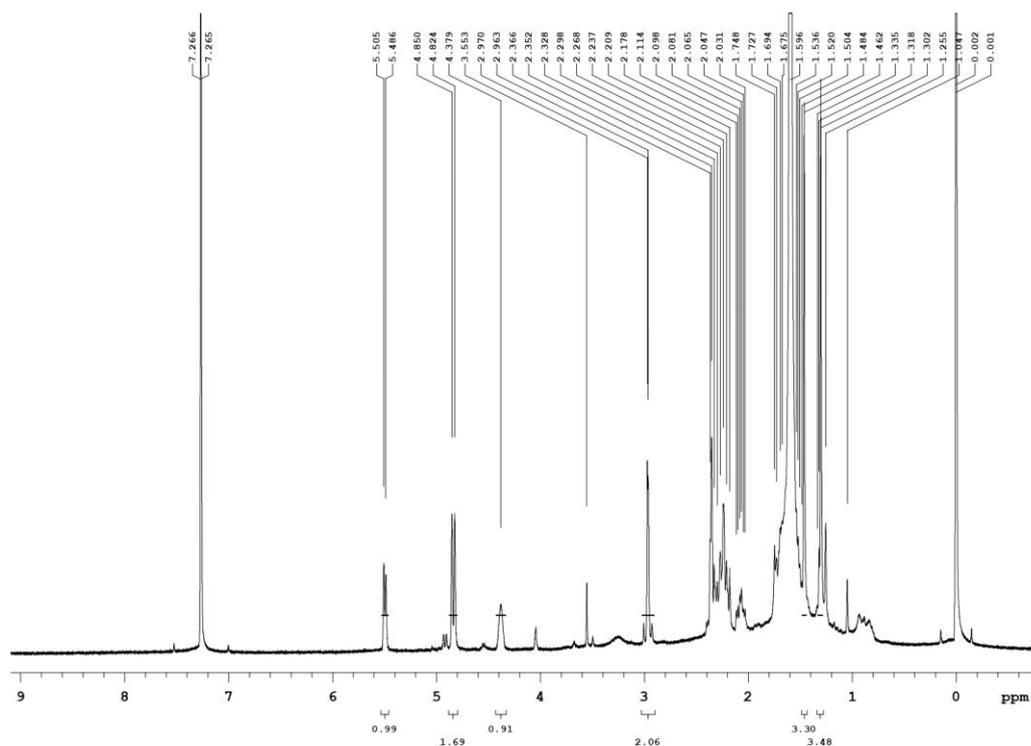


Figure S57.  $^1\text{H}$  NMR spectrum (400MHz) of compound **12** in  $\text{CDCl}_3$

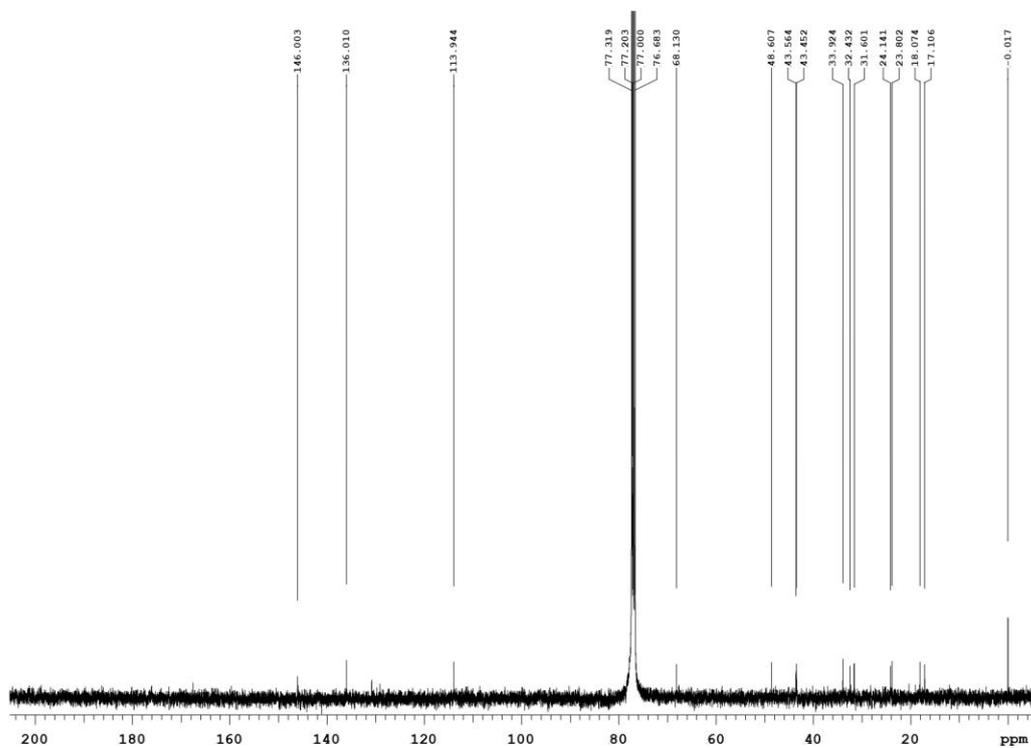


Figure S58.  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **12** in  $\text{CDCl}_3$

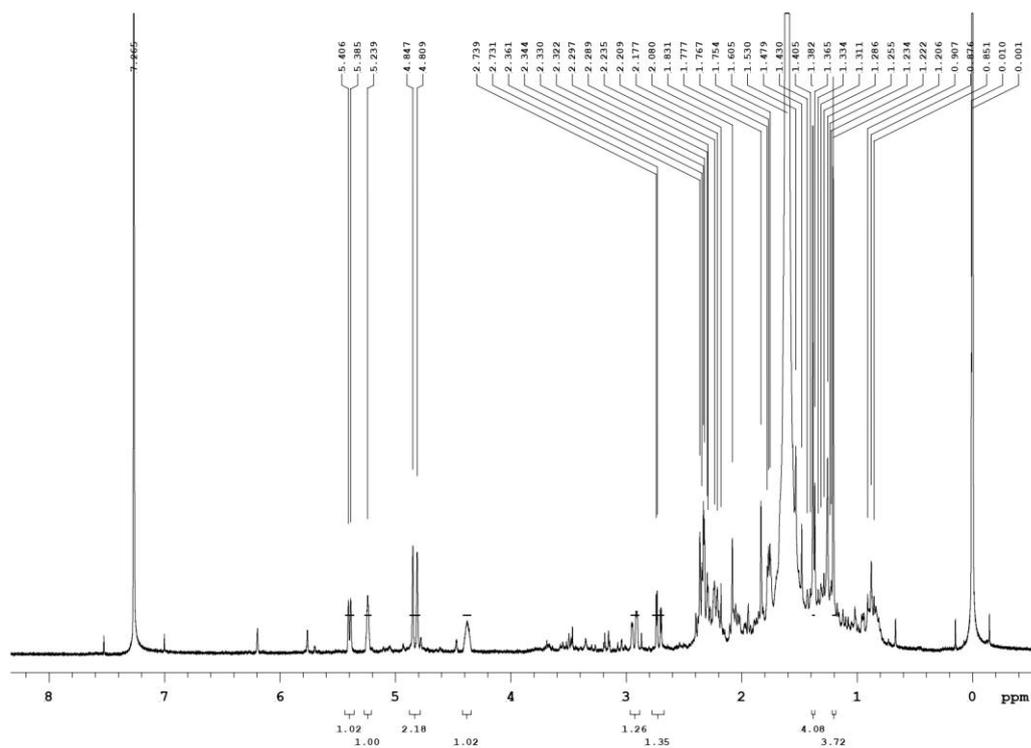


Figure S59.  $^1\text{H}$  NMR spectrum (400MHz) of compound **13** in  $\text{CDCl}_3$

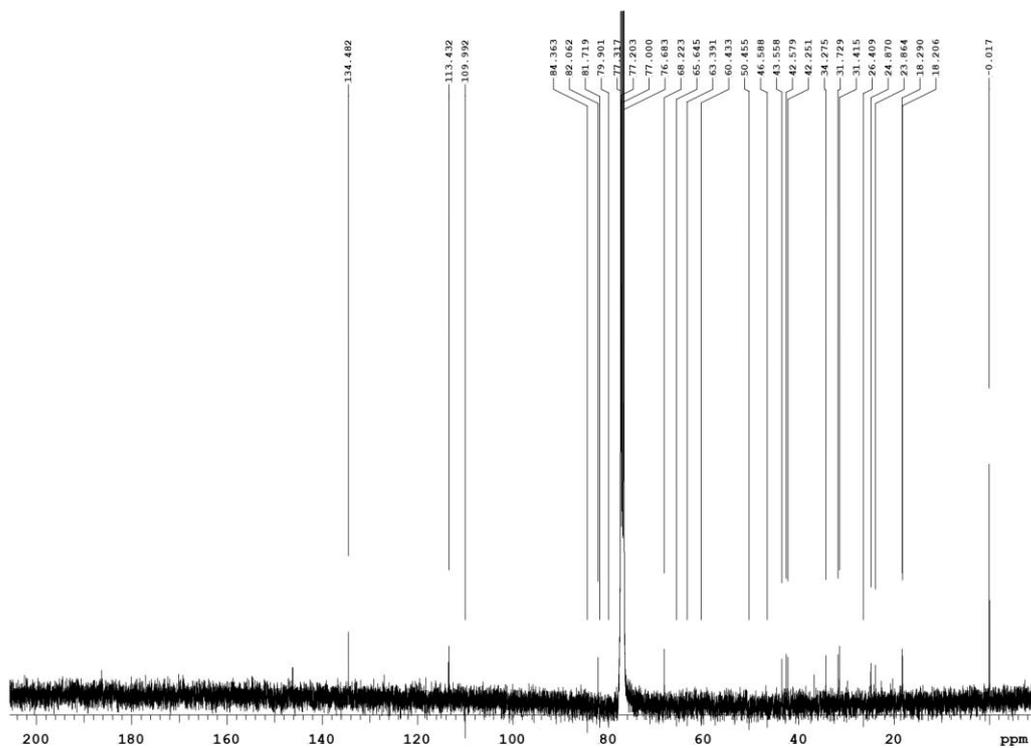


Figure S60.  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **13** in  $\text{CDCl}_3$

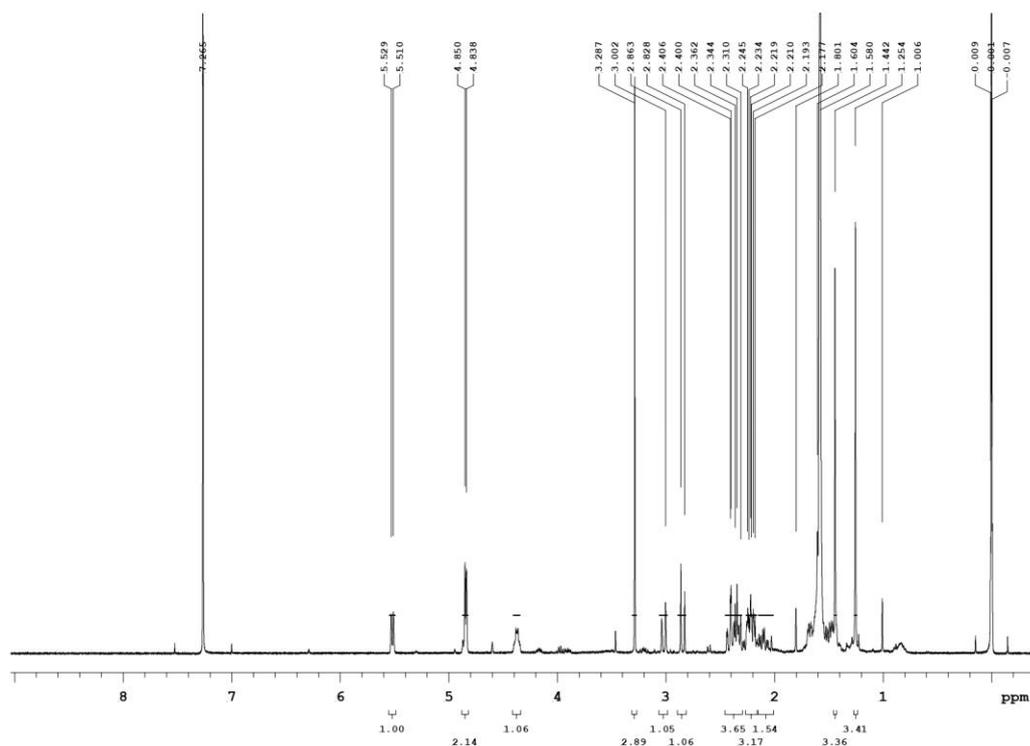


Figure S61.  $^1\text{H}$  NMR spectrum (400MHz) of compound **14** in  $\text{CDCl}_3$

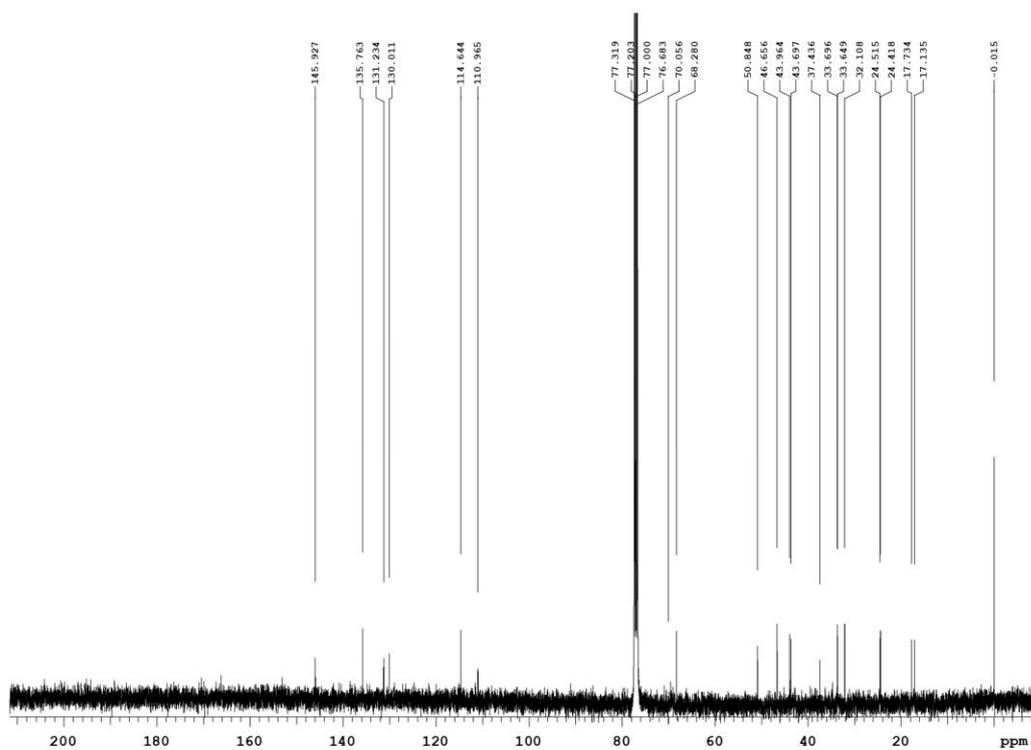


Figure S62.  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **14** in  $\text{CDCl}_3$

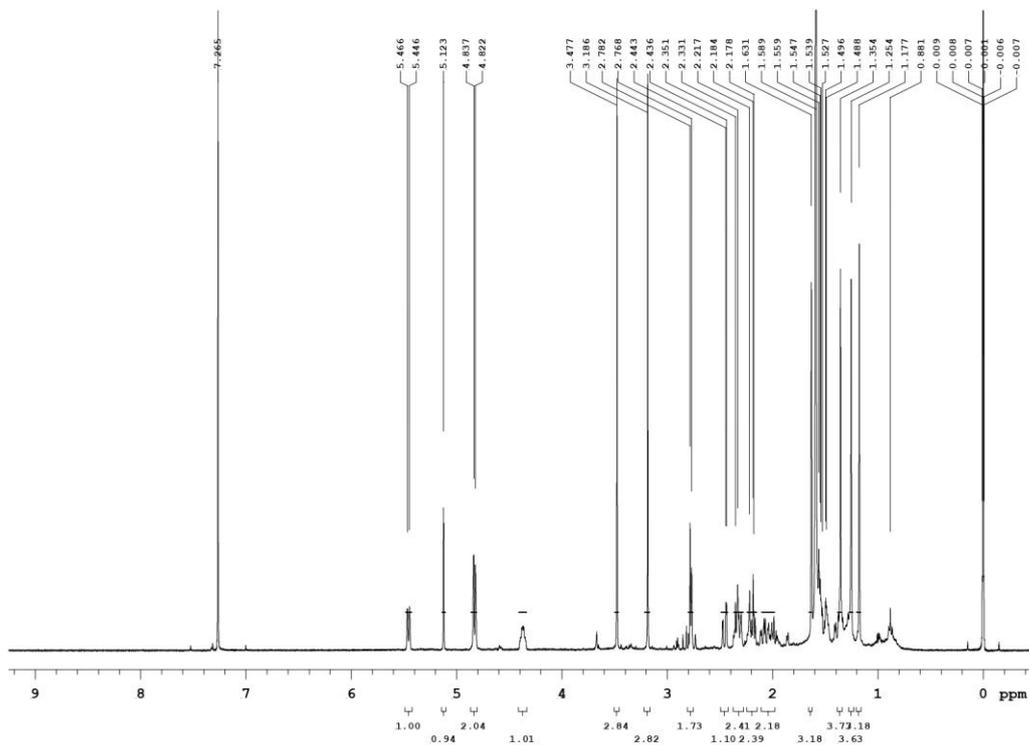


Figure S63.  $^1\text{H}$  NMR spectrum (400MHz) of compound 15 in  $\text{CDCl}_3$

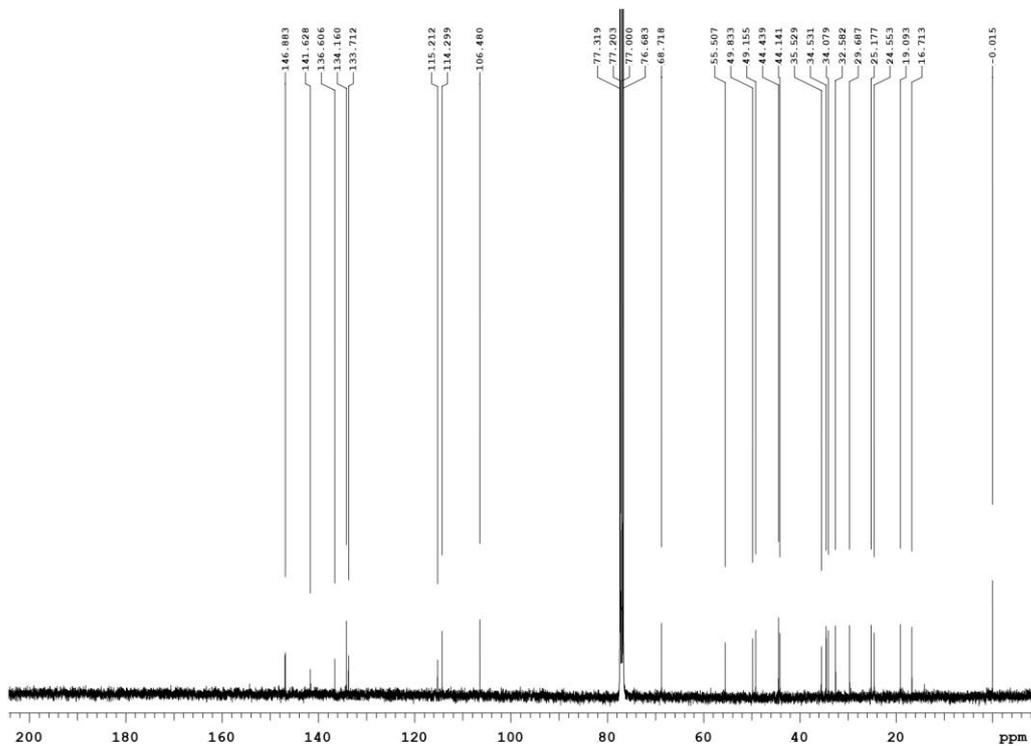


Figure S64.  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound 15 in  $\text{CDCl}_3$

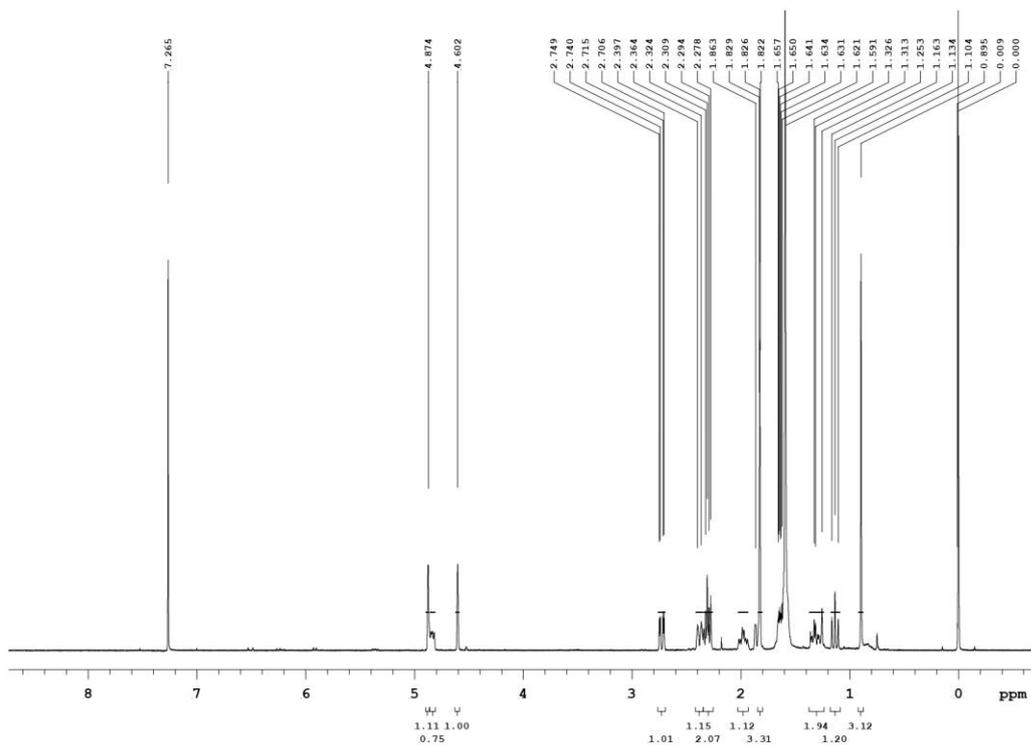


Figure S65.  $^1\text{H}$  NMR spectrum (400MHz) of compound 16 in  $\text{CDCl}_3$

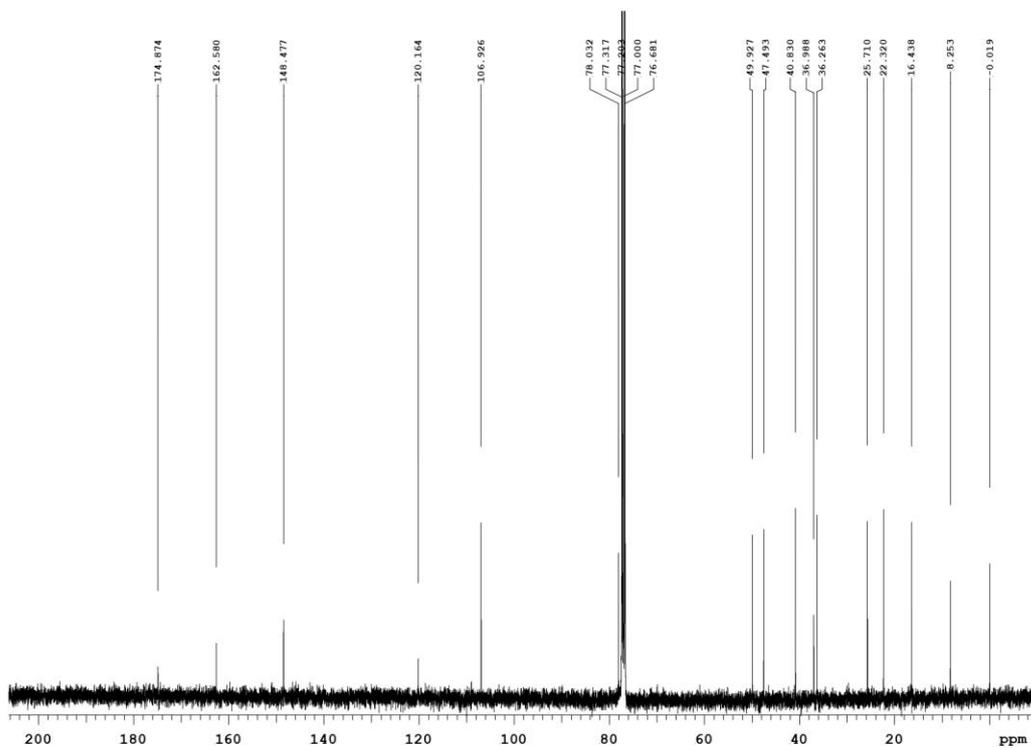
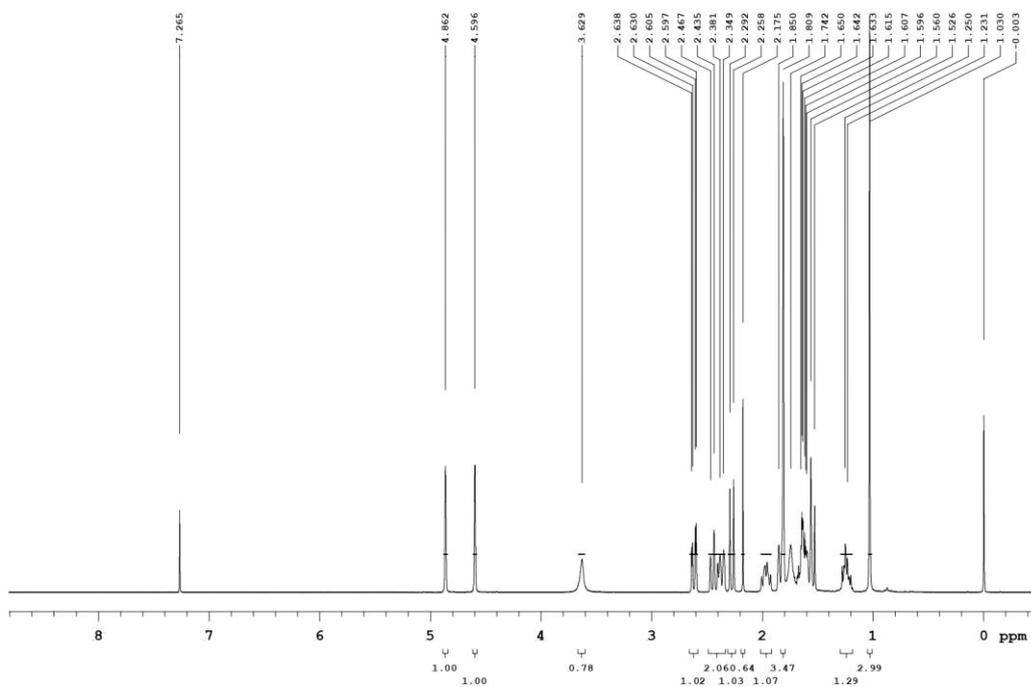
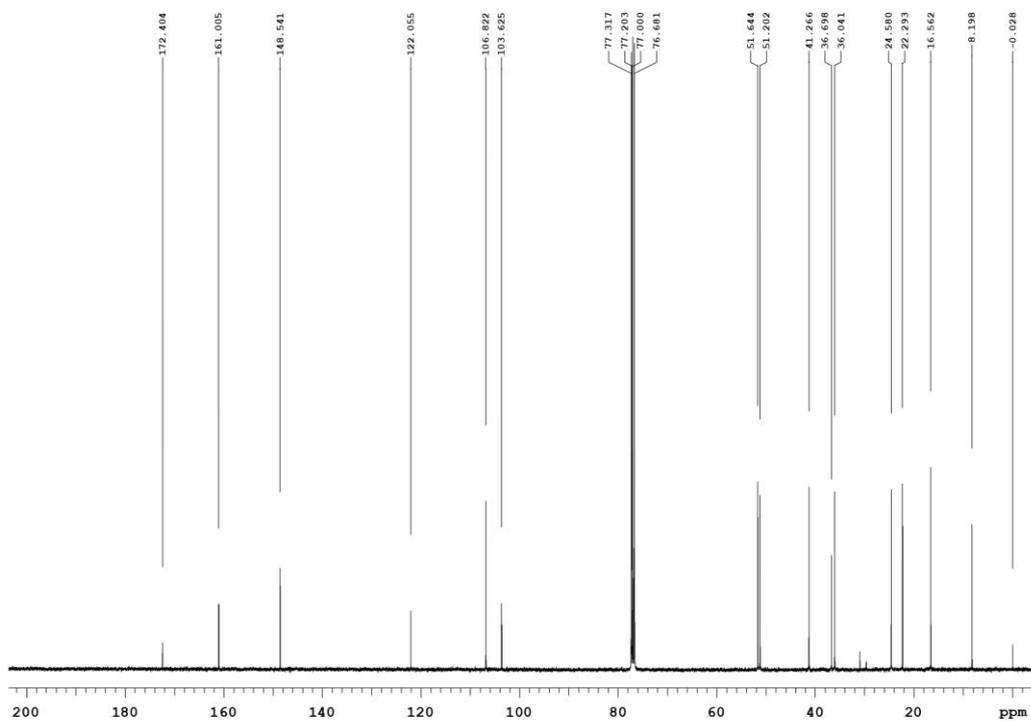


Figure S66.  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound 16 in  $\text{CDCl}_3$



**Figure S67.**  $^1\text{H}$  NMR spectrum (400MHz) of compound **17** in  $\text{CDCl}_3$



**Figure S68.**  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **17** in  $\text{CDCl}_3$

Table S1. The cytotoxicity data of compounds **1–16** and **1a**.

Compounds	Cell lines IC <sub>50</sub> (μg/mL)		
	HepG2	MDA-MB231	A549
<b>1</b>	> 20	> 20	> 20
<b>1a</b>	> 20	> 20	> 20
<b>2</b>	> 20	> 20	> 20
<b>3</b>	> 20	> 20	> 20
<b>4</b>	> 20	> 20	> 20
<b>5</b>	> 20	15.40	18.74
<b>6</b>	> 20	> 20	> 20
<b>7</b>	> 20	> 20	> 20
<b>8</b>	> 20	> 20	> 20
<b>9</b>	> 20	> 20	> 20
<b>10</b>	> 20	> 20	> 20
<b>11</b>	> 20	> 20	> 20
<b>12</b>	> 20	> 20	> 20
<b>13</b>	> 20	> 20	> 20
<b>14</b>	> 20	> 20	> 20
<b>15</b>	> 20	> 20	> 20
<b>16</b>	> 20	> 20	> 20
Doxorubicin	0.37	0.30	0.15

Table S2. Antibacterial activity (zone of inhibition in mm).

Compounds (25 µg/disk)	Inhibition zone (mm)									
	<i>B. s.</i>	<i>S. a.</i>	<i>S. e.</i>	<i>E. a.</i>	<i>E. c.</i>	<i>K. p.</i>	<i>S. m.</i>	<i>S. s.</i>	<i>S. t.</i>	<i>Y. e.</i>
<b>3</b>	–	–	–	–	–	–	–	–	–	–
<b>4</b>	–	–	–	–	–	–	–	–	–	–
<b>5</b>	–	–	6	–	–	5	–	–	–	–
<b>6</b>	–	–	–	–	–	–	–	–	–	–
<b>7</b>	–	–	–	–	–	–	–	–	–	–
<b>9</b>	–	–	–	–	–	9	–	–	–	–
<b>12</b>	–	–	–	–	–	–	–	–	–	–
Ampicillin	9	12	10	5	5	5	8	9	8	18

–: Inactive

Ampicillin: Positive control

*B. s.*: *Bacillus subtilis* (ATCC6051)

*S. a.*: *Staphylococcus aureus* (ATCC9144)

*S. e.*: *Salmonella enterica* (ATCC13076)

*E. a.*: *Enterobacter aerogenes* (ATCC13048)

*E. c.*: *Escherichia coli* (ATCC25922)

*K. p.*: *Klebsiella pneumoniae* (ATCC10031)

*S. m.*: *Serratia marcescens* (ATCC25419)

*S. s.*: *Shigella sonnei* (ATCC11060)

*S. t.*: *Salmonella typhimurium* (ATCC14028)

*Y. e.*: *Yersinia enterocolitica* (ATCC23715)

Table S3. Inhibitory effects of compounds **1–10**, **1a**, **14**, and **15** on TNF- $\alpha$  expression, PGE<sub>2</sub>, and NO production in LPS induced dendritic cells.

Compounds	Inh % <sup>1</sup>		
	TNF- $\alpha$	PGE <sub>2</sub>	NO
<b>1</b>	2.3 ± 2.0	2.9 ± 1.5	11.0 ± 2.4
<b>1a</b>	-0.1 ± 1.6	-0.8 ± 5.9	14.0 ± 1.5 *
<b>2</b>	7.3 ± 3.2	12.8 ± 3.5	19.6 ± 4.0 ***
<b>3</b>	8.0 ± 3.0	11.4 ± 2.1	33.8 ± 1.5 ***
<b>4</b>	3.8 ± 2.7	2.4 ± 2.1	34.9 ± 3.9 ***
<b>5</b>	0.8 ± 1.8	3.5 ± 4.2	16.0 ± 3.7 **
<b>6</b>	5.0 ± 2.9	-4.4 ± 0.4	14.6 ± 3.9 *
<b>7</b>	1.9 ± 5.1	-7.6 ± 2.8	3.7 ± 5.7
<b>8</b>	0.2 ± 0.5	-4.9 ± 3.2	10.2 ± 3.2
<b>9</b>	3.3 ± 1.7	1.2 ± 5.9	16.8 ± 4.7 **
<b>10</b>	-3.9 ± 1.1	-11.5 ± 4.6	11.9 ± 2.7
<b>14</b>	5.2 ± 1.8	-8.8 ± 6.3	24.8 ± 1.4***
<b>15</b>	23.6 ± 2.5 ***	21.2 ± 0.9 *	35.0 ± 3.7 ***
DEX <sup>2</sup>	85.6 ± 3.4 ****	–	73.4 ± 1.3 ****

1. Percentage of inhibition (Inh %) at the concentration 100  $\mu$ M for **1–3**, **5**, **7**, **9**, **11**, **14** and **15** and 25  $\mu$ M for **4**, **6**, and **8** compared with the control group (100 % for stimulated LPS alone). Results are presented as mean  $\pm$  SEM. (n = 3). \* p < 0.05, \*\* p < 0.01, \*\*\* p < 0.001, \*\*\*\* p < 0.0001.

2. Positive control: dexamethasone (DEX) at 100  $\mu$ M.