

## SUPPLEMENTARY MATERIAL

### New Isocoumarin Analogues from the Marine-derived Fungus *Paraphoma* sp. CUGBMF180003

**Xiuli Xu<sup>1</sup>, Jiangpeng Li<sup>1</sup>, Kai Zhang<sup>2</sup>, Shangzhu Wei<sup>1</sup>, Rui Lin<sup>1</sup>, Steven W. Polyak<sup>3</sup>, Na Yang<sup>4,5,\*</sup> and Fuhang Song<sup>2,\*</sup>**

<sup>1</sup> School of Ocean Sciences, China University of Geosciences, Beijing, 100083, P. R. China; xuxl@cugb.edu.cn (X.X); lijiangpeng@cugb.edu.cn (J.L.); weishangzhu@cugb.edu.cn (S.W.); linrui@cugb.edu.cn (R.L.)

<sup>2</sup> School of Light Industry, Beijing Technology and Business University, Beijing, 100048, P. R. China; zhangkai2030302071@st.btbu.edu.cn (K.Z.)

<sup>3</sup> School of Biological Sciences, University of South Australia, Adelaide, 5005, Australia; Steven.Polyak@unisa.edu.au (S.W.P.)

<sup>4</sup> CAS Key Laboratory of Experimental Marine Biology, Institute of Oceanology, Chinese Academy of Sciences, Qingdao, 266071, P. R. China

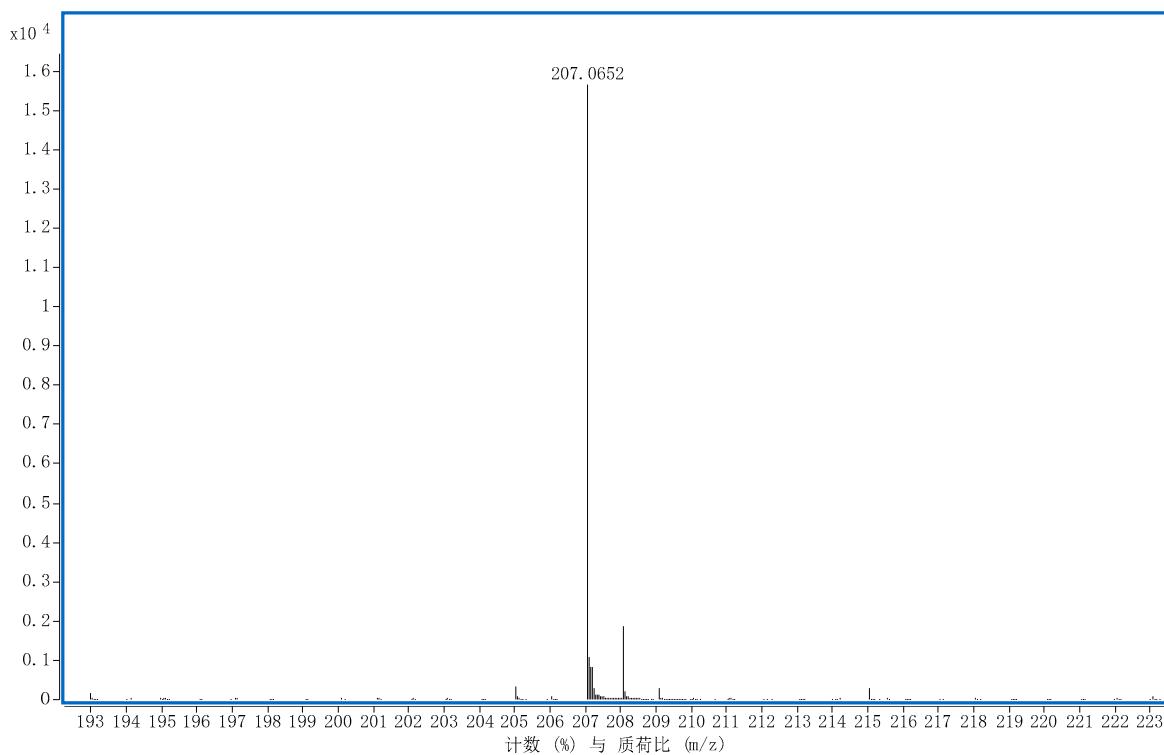
<sup>5</sup> Laboratory for Marine Biology and Biotechnology, Qingdao National Laboratory for Marine Science and Technology, Qingdao, 266071, P. R. China

\* Correspondence: songfuhang@btbu.edu.cn (F.S.); yangna@qdio.ac.cn (N.Y.)

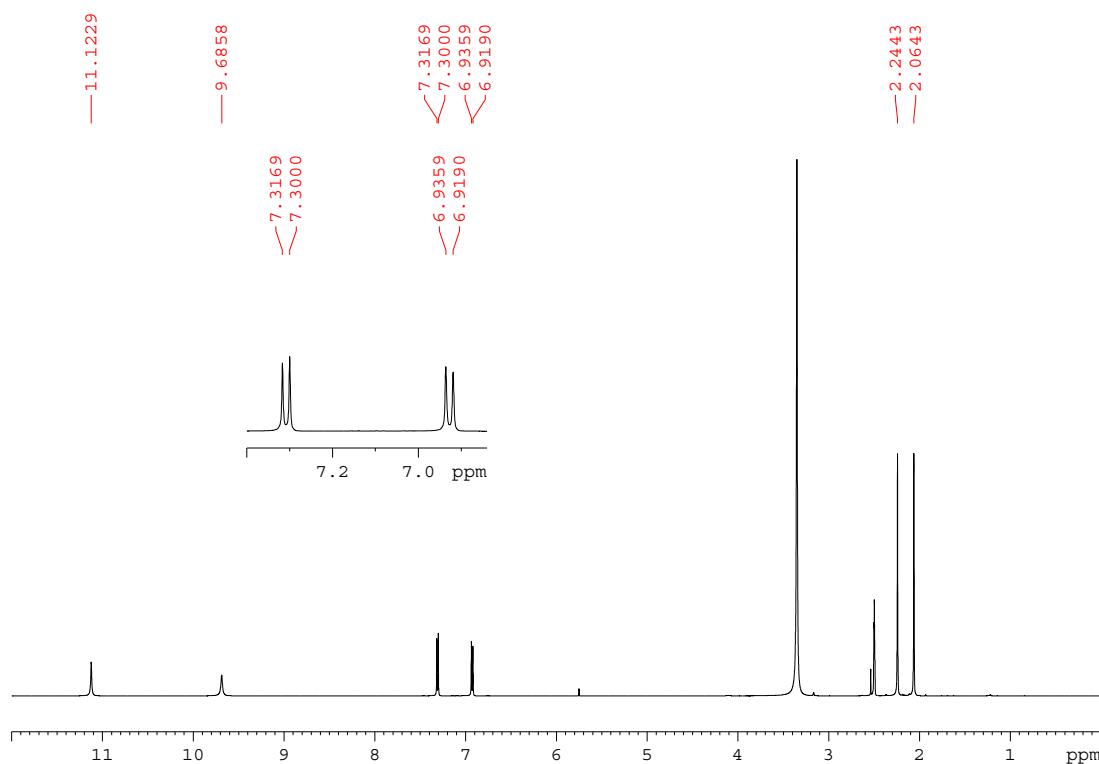
**Table of Contents**

<b>Figure S1.</b> HRESIMS spectrum for <b>1</b> .....	4
<b>Figure S2.</b> $^1\text{H}$ NMR spectrum (500 MHz, DMSO- $d_6$ ) of <b>1</b> .....	4
<b>Figure S3.</b> $^{13}\text{C}$ NMR spectrum (125 MHz, DMSO- $d_6$ ) of <b>1</b> .....	5
<b>Figure S4.</b> HSQC spectrum (500 MHz, Acetone- $d_6$ ) of <b>1</b> .....	5
<b>Figure S5.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum (500 MHz, Acetone- $d_6$ ) of <b>1</b> .....	6
<b>Figure S6.</b> HMBC spectrum (500 MHz, DMSO- $d_6$ ) of <b>1</b> .....	6
<b>Figure S7.</b> HRESIMS spectrum for <b>2</b> .....	7
<b>Figure S8.</b> $^1\text{H}$ NMR spectrum (500 MHz, DMSO- $d_6$ ) of <b>2</b> .....	7
<b>Figure S9.</b> $^{13}\text{C}$ NMR spectrum (125 MHz, DMSO- $d_6$ ) of <b>2</b> .....	8
<b>Figure S10.</b> HSQC spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>2</b> .....	8
<b>Figure S11.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum (500MHz, CDCl <sub>3</sub> ) of <b>2</b> .....	9
<b>Figure S12.</b> HMBC spectrum (500MHz, DMSO) <b>2</b> .....	9
<b>Figure S13.</b> HRESIMS spectrum for <b>3</b> .....	10
<b>Figure S14.</b> $^1\text{H}$ NMR spectrum (500 MHz, DMSO- $d_6$ ) of <b>3</b> .....	10
<b>Figure S15.</b> $^{13}\text{C}$ NMR spectrum (125 MHz, DMSO- $d_6$ ) of <b>3</b> .....	11
<b>Figure S16.</b> HSQC spectrum (500 MHz, DMSO- $d_6$ ) of <b>3</b> .....	11
<b>Figure S17.</b> HMBC spectrum (500 MHz, DMSO- $d_6$ ) of <b>3</b> .....	12
<b>Figure S18.</b> HRESIMS spectrum for <b>4</b> .....	12
<b>Figure S19.</b> $^1\text{H}$ NMR spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>4</b> .....	13
<b>Figure S20.</b> $^{13}\text{C}$ NMR spectrum (125 MHz, CDCl <sub>3</sub> ) of <b>4</b> .....	13
<b>Figure S21.</b> HSQC spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>4</b> .....	14
<b>Figure S22.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>4</b> .....	14
<b>Figure S23.</b> HMBC spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>4</b> .....	15
<b>Figure S24.</b> HRESIMS spectrum for <b>5</b> .....	15
<b>Figure S25.</b> $^1\text{H}$ NMR spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>5</b> .....	16
<b>Figure S26.</b> $^{13}\text{C}$ NMR spectrum (125 MHz, CDCl <sub>3</sub> ) of <b>5</b> .....	16
<b>Figure S27.</b> HSQC spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>5</b> .....	17
<b>Figure S28.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>5</b> .....	17
<b>Figure S29.</b> HMBC spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>5</b> .....	18

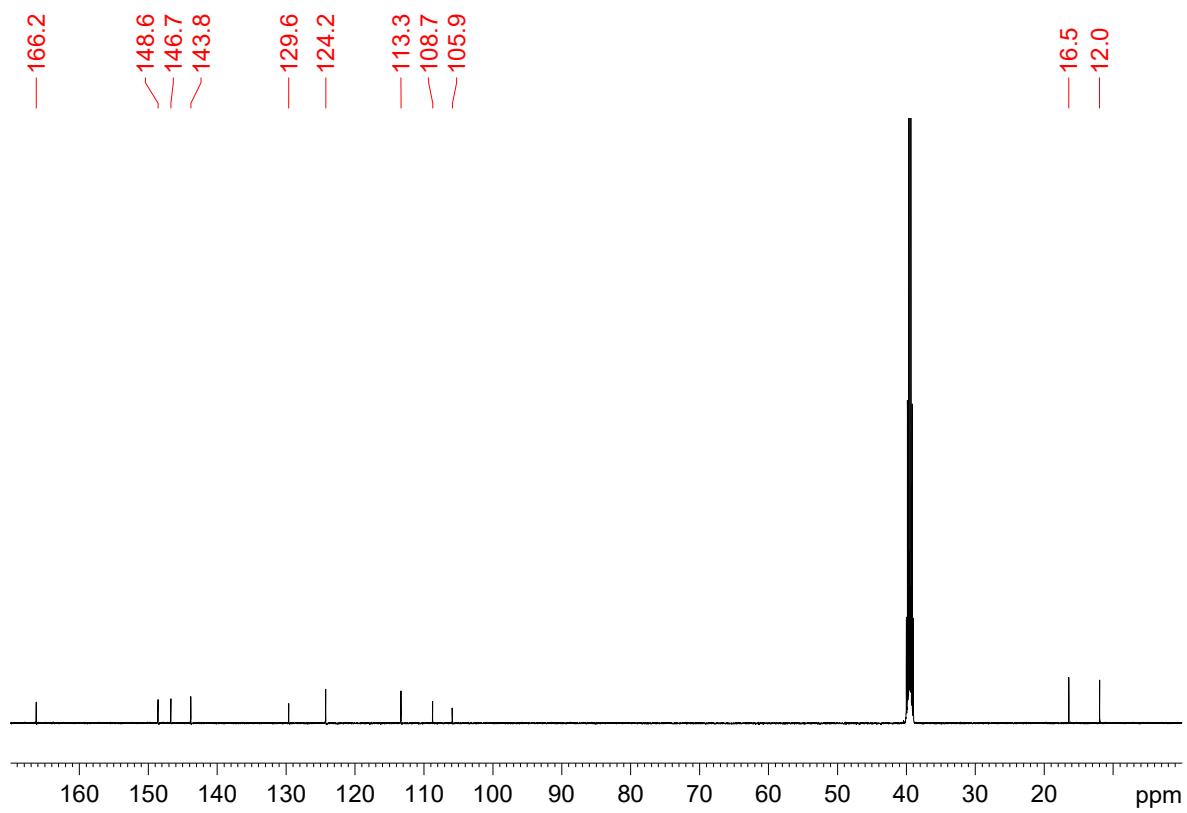
<b>Figure S30.</b> HRESIMS spectrum for <b>6</b> .....	18
<b>Figure S31.</b> $^1\text{H}$ NMR spectrum (500 MHz, Acetone- $d_6$ ) of <b>6</b> .....	19
<b>Figure S32.</b> $^{13}\text{C}$ NMR spectrum (125 MHz, Acetone- $d_6$ ) of <b>6</b> .....	19
<b>Figure S33.</b> HSQC spectrum (500 MHz, Acetone- $d_6$ ) of <b>6</b> .....	20
<b>Figure S34.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum (500 MHz, Acetone- $d_6$ ) of <b>6</b> .....	20
<b>Figure S35.</b> HMBC spectrum (500 MHz, Acetone- $d_6$ ) of <b>6</b> .....	21
<b>Figure S36.</b> HRESIMS spectrum for <b>12</b> .....	21
<b>Figure S37.</b> $^1\text{H}$ NMR spectrum (500 MHz, DMSO- $d_6$ ) of <b>12</b> .....	22
<b>Figure S38.</b> $^{13}\text{C}$ NMR spectrum (125 MHz, DMSO- $d_6$ ) of <b>12</b> .....	22
<b>Figure S39.</b> HSQC spectrum (500 MHz, DMSO- $d_6$ ) of <b>12</b> .....	23
<b>Figure S40.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum (500 MHz, DMSO- $d_6$ ) of <b>12</b> .....	23
<b>Figure S41.</b> HMBC spectrum (500 MHz, DMSO- $d_6$ ) of <b>12</b> .....	24
<b>Figure S42.</b> HRESIMS spectrum for <b>13</b> .....	24
<b>Figure S43.</b> $^1\text{H}$ NMR spectrum (500 MHz, DMSO- $d_6$ ) of <b>13</b> .....	25
<b>Figure S44.</b> $^{13}\text{C}$ NMR spectrum (125 MHz, DMSO- $d_6$ ) of <b>13</b> .....	25
<b>Figure S45.</b> HSQC spectrum (500 MHz, DMSO- $d_6$ ) of <b>13</b> .....	26
<b>Figure S46.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum (500 MHz, DMSO- $d_6$ ) of <b>13</b> .....	26
<b>Figure S47.</b> HMBC spectrum (500 MHz, DMSO- $d_6$ ) of <b>13</b> .....	27
<b>Figure S48.</b> HRESIMS spectrum for <b>14</b> .....	27
<b>Figure S49.</b> $^1\text{H}$ NMR spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>14</b> .....	28
<b>Figure S50.</b> $^{13}\text{C}$ NMR spectrum (125 MHz, CDCl <sub>3</sub> ) of <b>14</b> .....	28
<b>Figure S51.</b> HSQC spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>14</b> .....	29
<b>Figure S52.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>14</b> .....	29
<b>Figure S53.</b> HMBC spectrum (500 MHz, CDCl <sub>3</sub> ) of <b>14</b> .....	30
<b>Figure S54.</b> Neighbor-joining phylogenetic tree of strain CUGBMF180003 .....	31



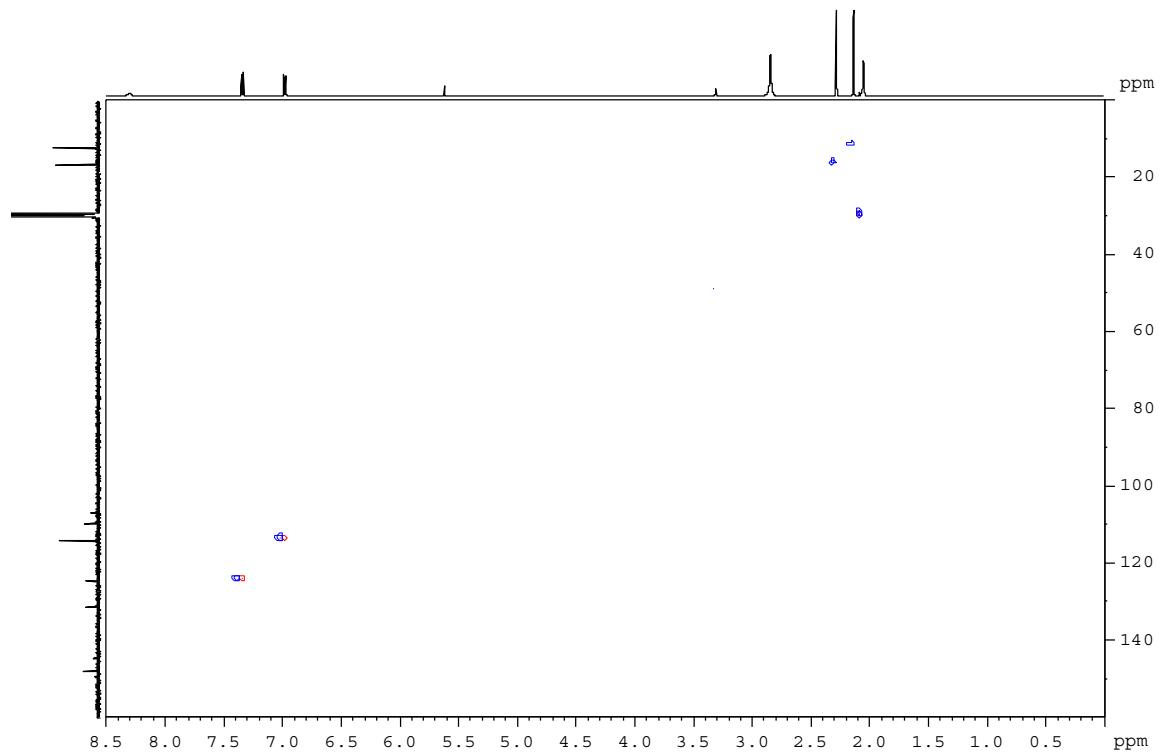
**Figure S1.** HRESIMS spectrum for compound **1**



**Figure S2.**  $^1\text{H}$  NMR spectrum (500 MHz, DMSO- $d_6$ ) of **1**

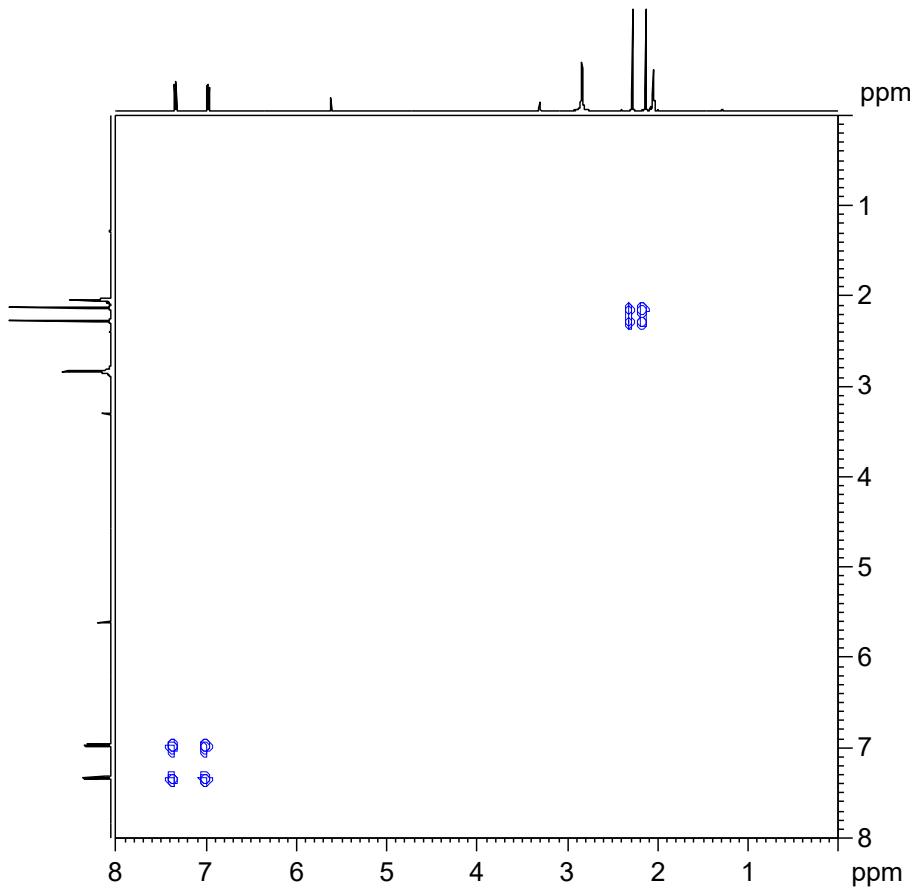


**Figure S3.**  $^{13}\text{C}$  NMR spectrum (125 MHz, DMSO- $d_6$ ) of **1**

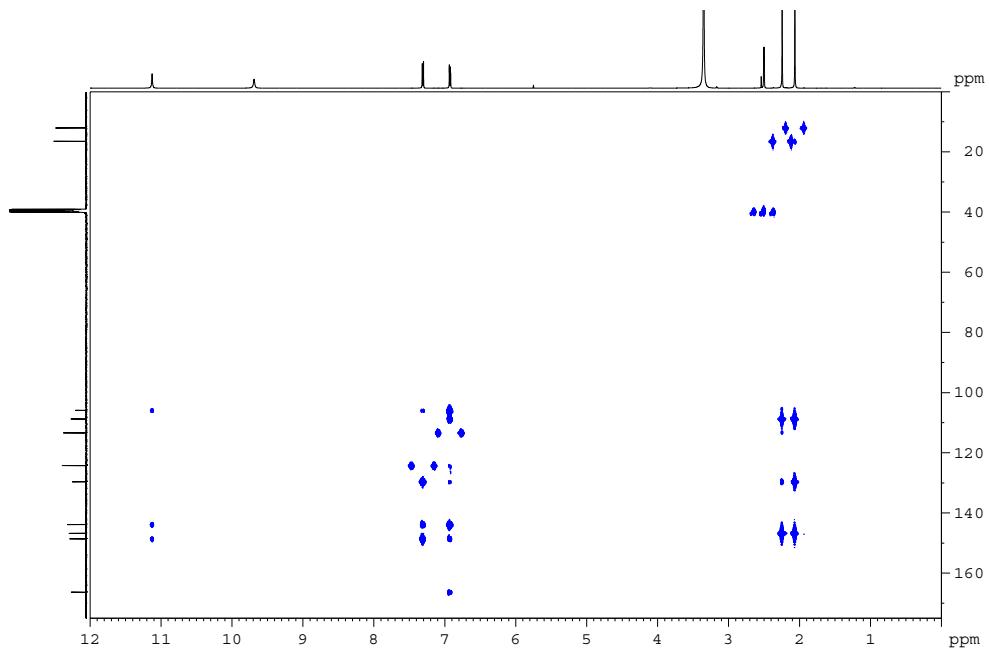


**Figure S4.** HSQC spectrum (500 MHz, Acetone- $d_6$ ) of **1**

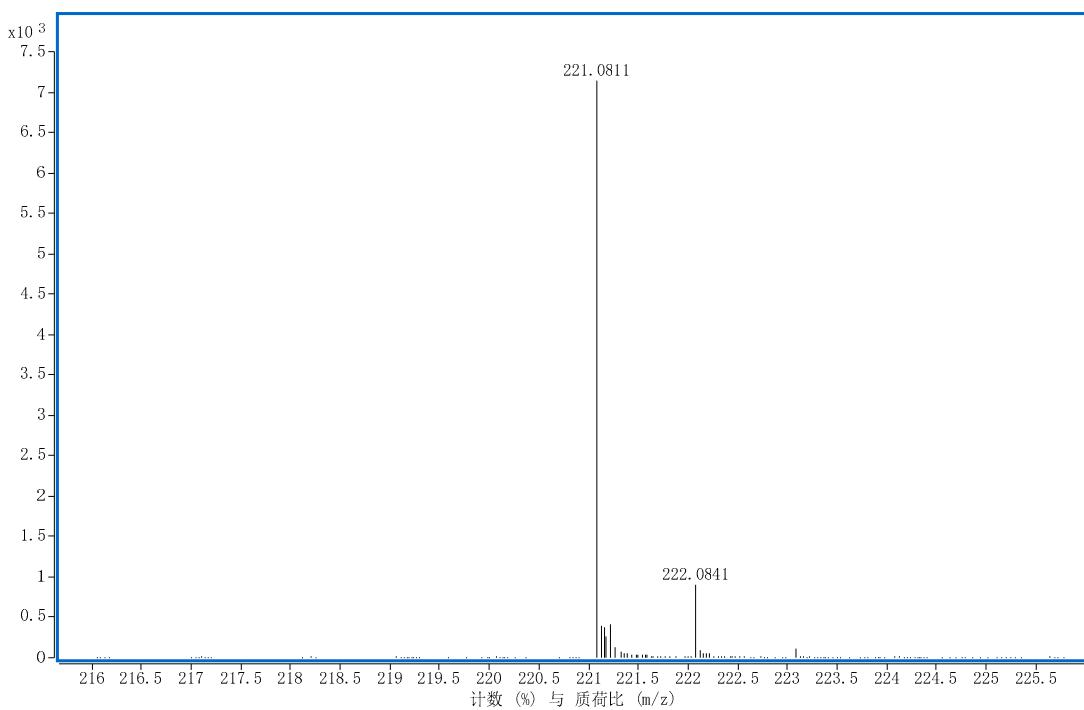
Supplementary Material



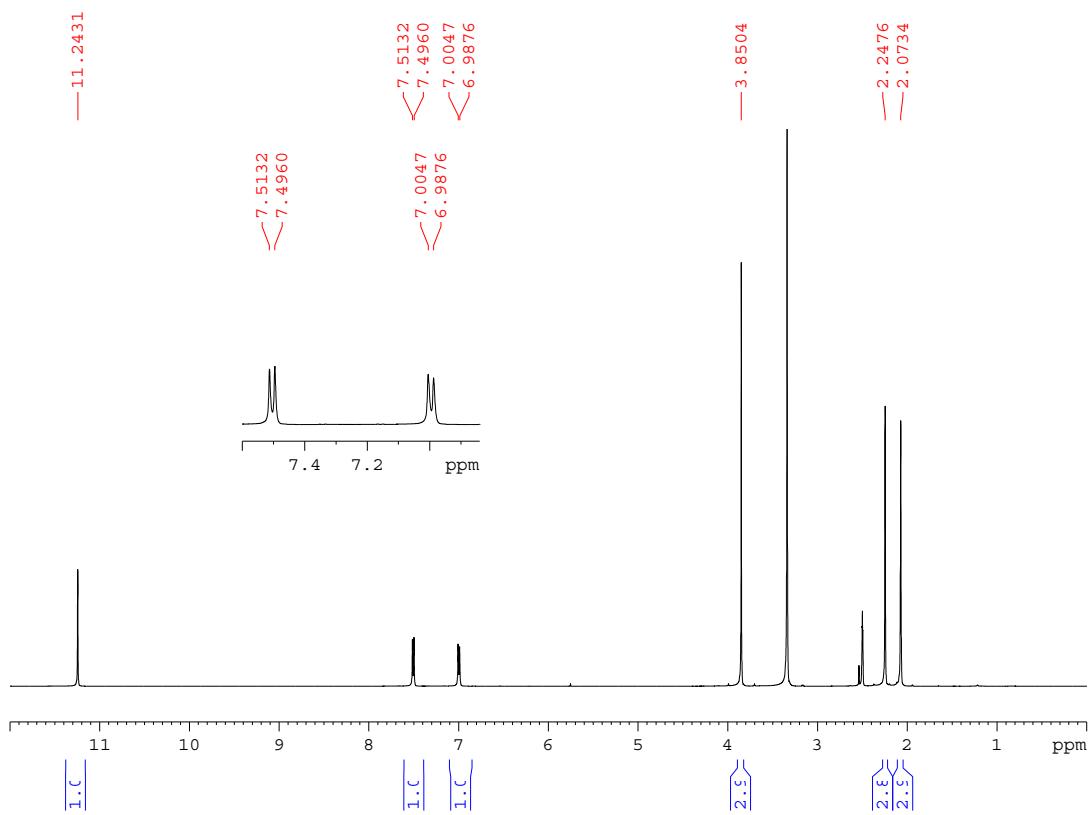
**Figure S5.** <sup>1</sup>H -<sup>1</sup>H COSY spectrum (500 MHz, Acetone-*d*<sub>6</sub>) of **1**



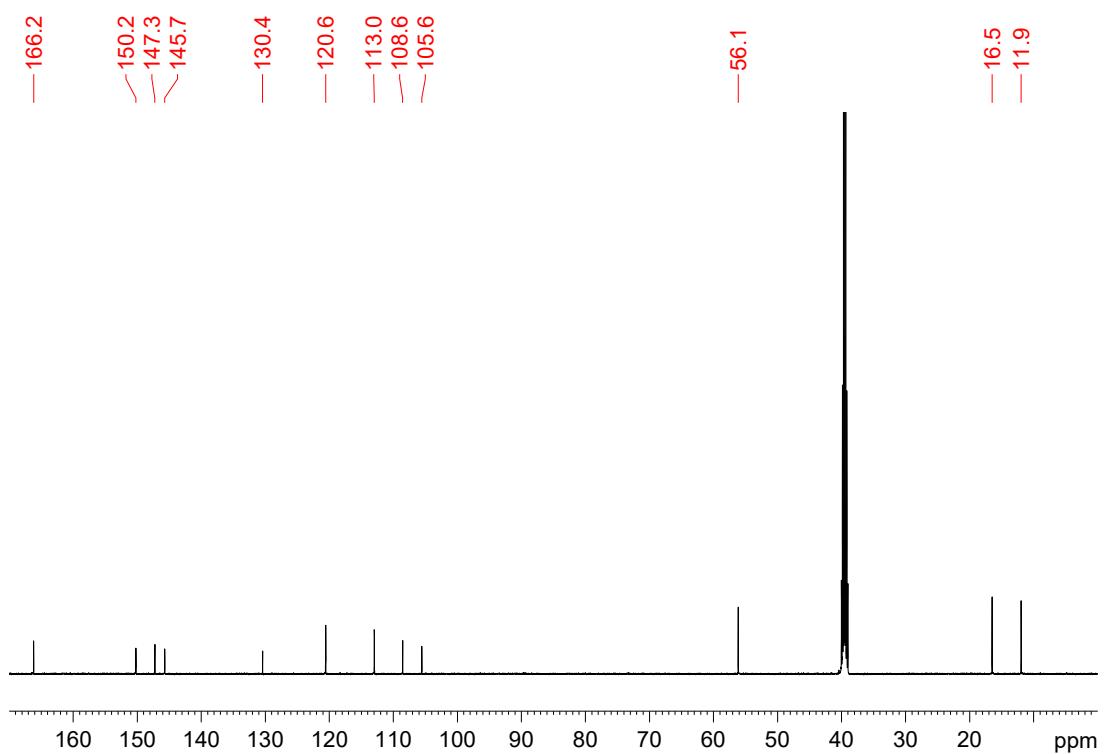
**Figure S6.** HMBC spectrum (500 MHz, DMSO-*d*<sub>6</sub>) of **1**



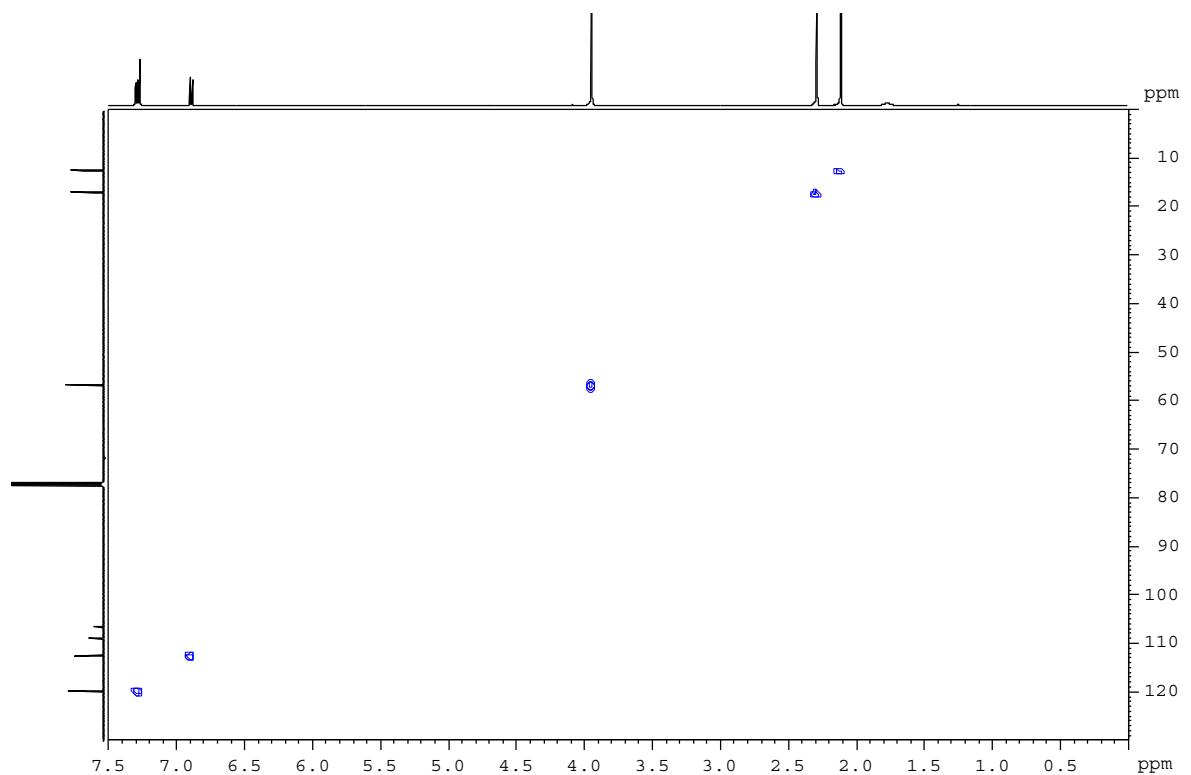
**Figure S7.** HRESIMS spectrum for **2**



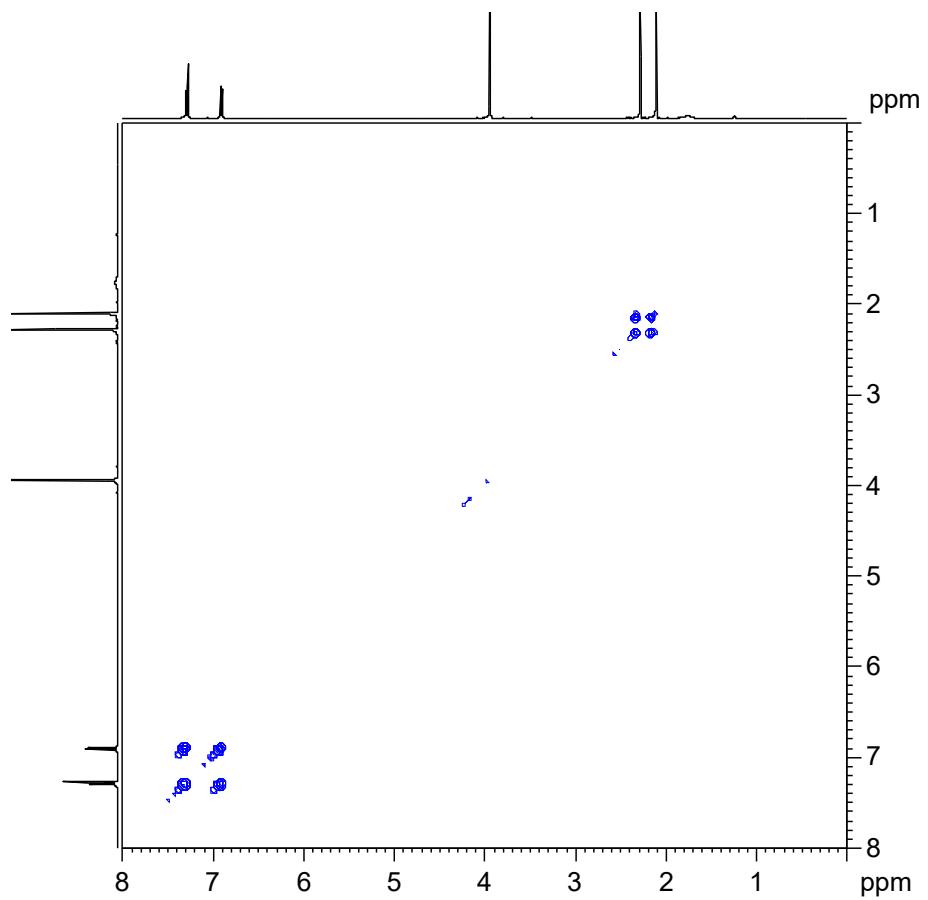
**Figure S8.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{DMSO}-d_6$ ) of **2**



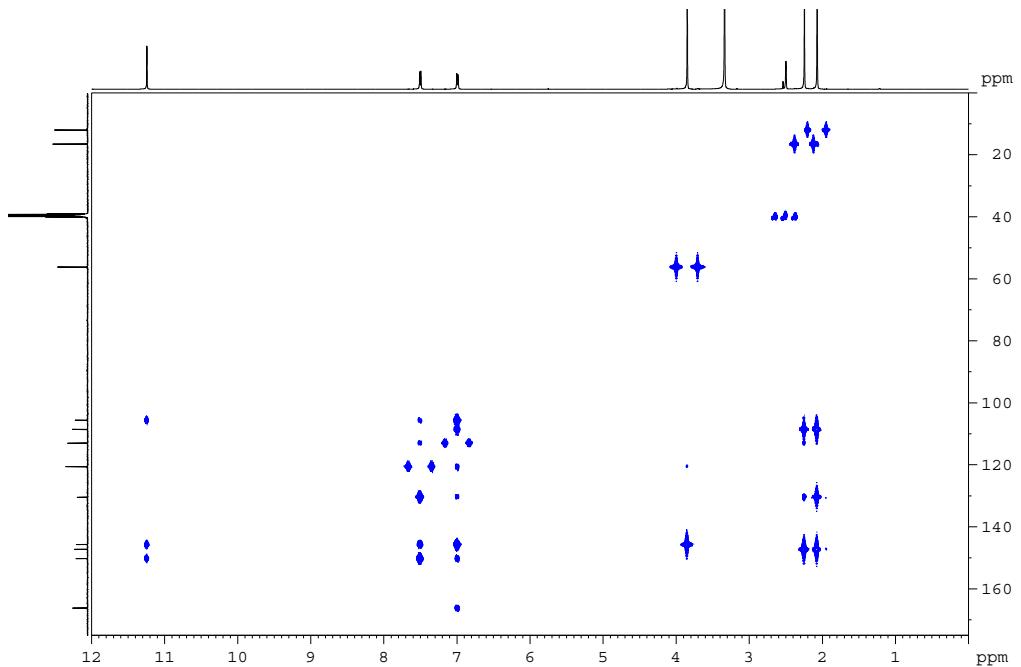
**Figure S9.** <sup>13</sup>C NMR spectrum (125 MHz, DMSO-*d*<sub>6</sub>) of **2**



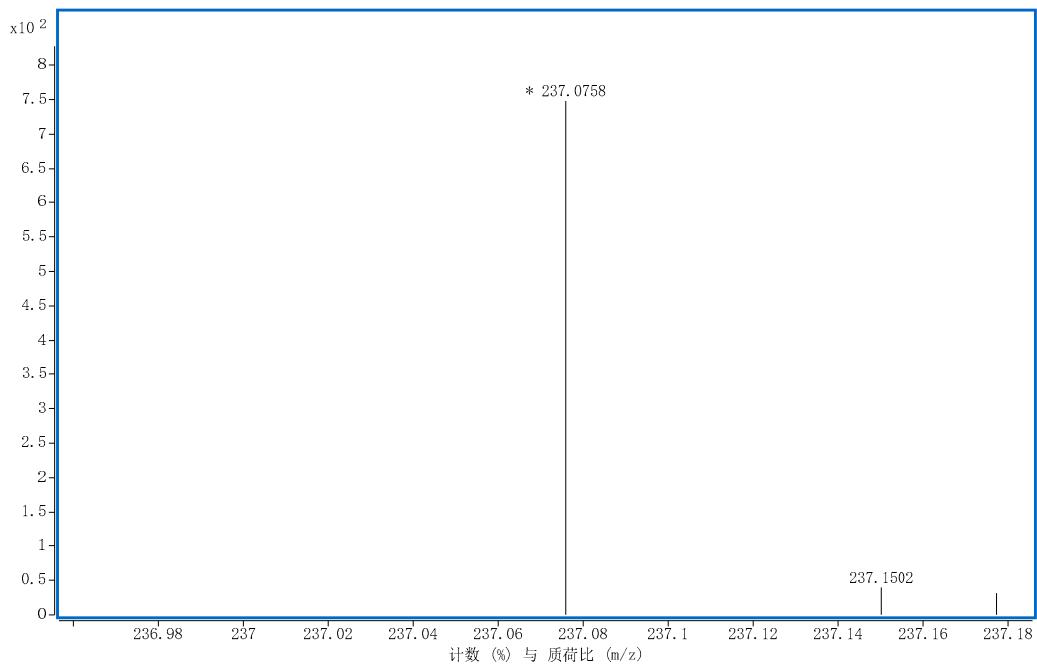
**Figure S10.** HSQC spectrum (500 MHz, CDCl<sub>3</sub>) of **2**



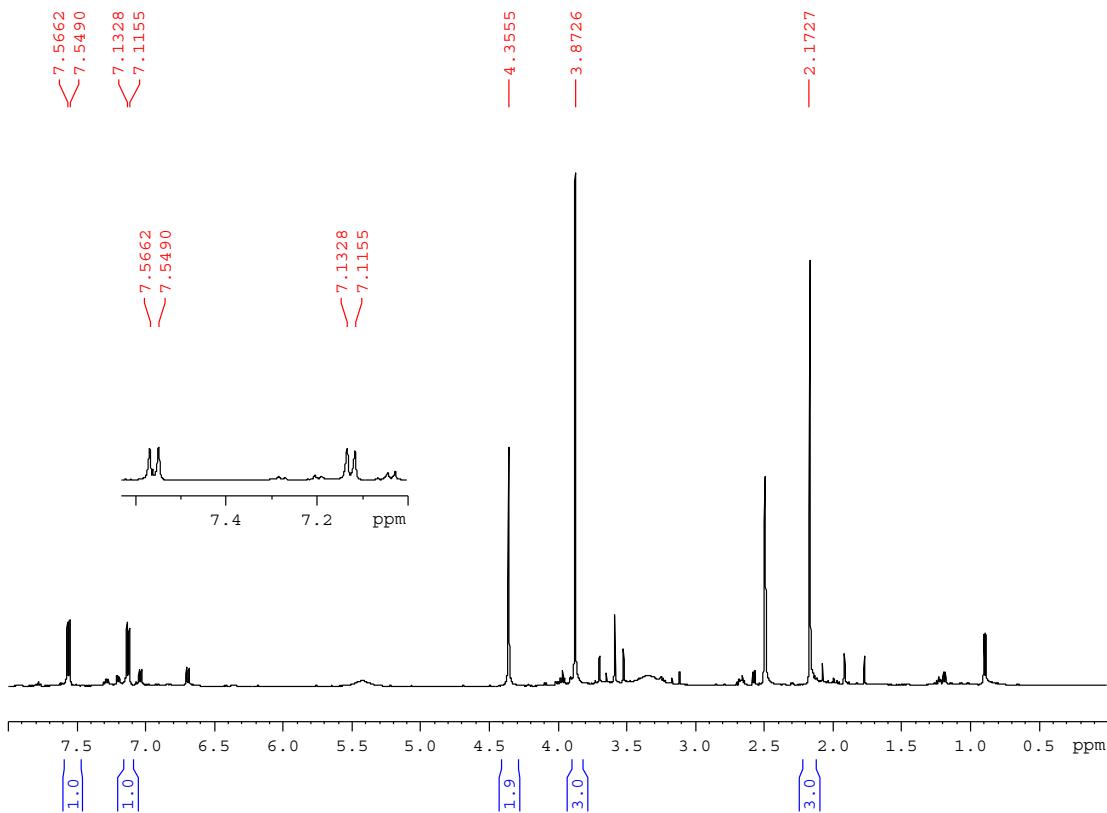
**Figure S11.**  $^1\text{H}$  -  $^1\text{H}$  COSY spectrum (500MHz,  $\text{CDCl}_3$ ) of **2**



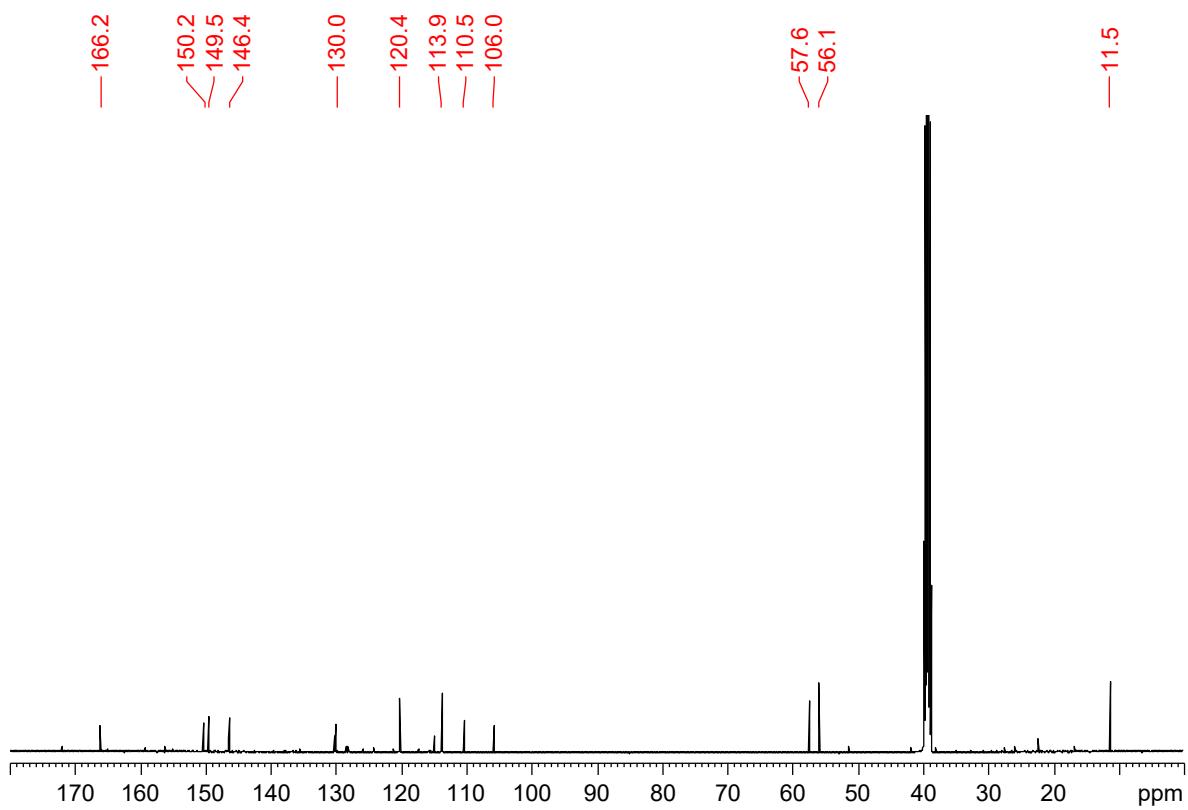
**Figure S12.** HMBC spectrum (500 MHz,  $\text{DMSO}-d_6$ ) of **2**



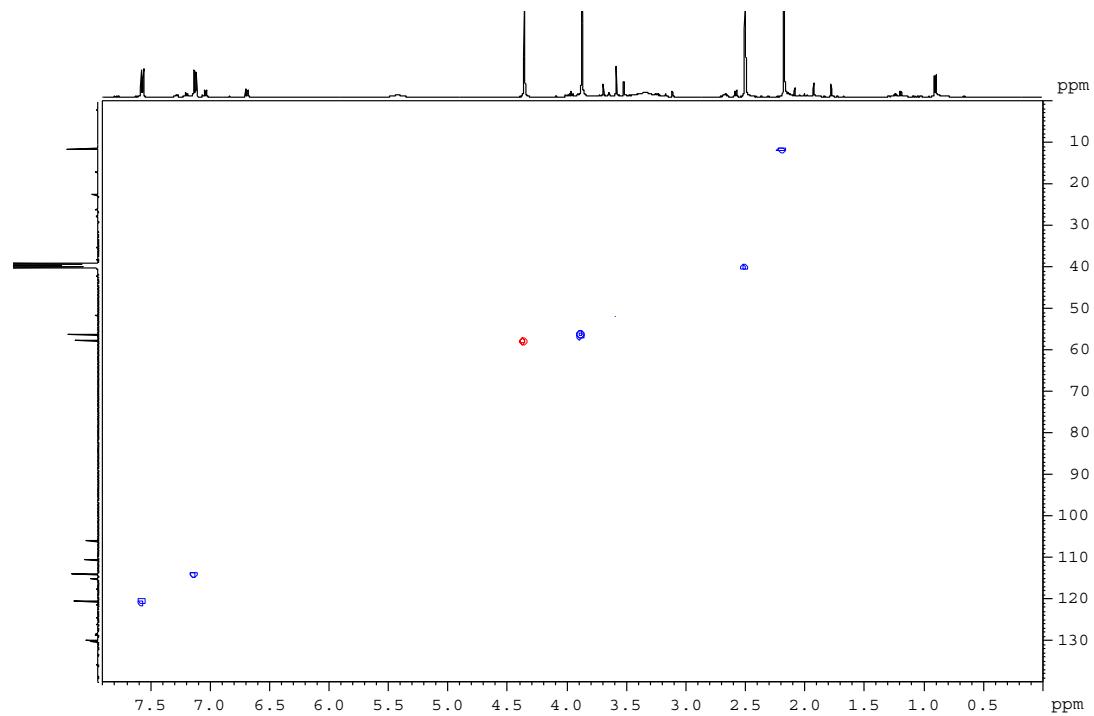
**Figure S13.** HRESIMS spectrum for **3**



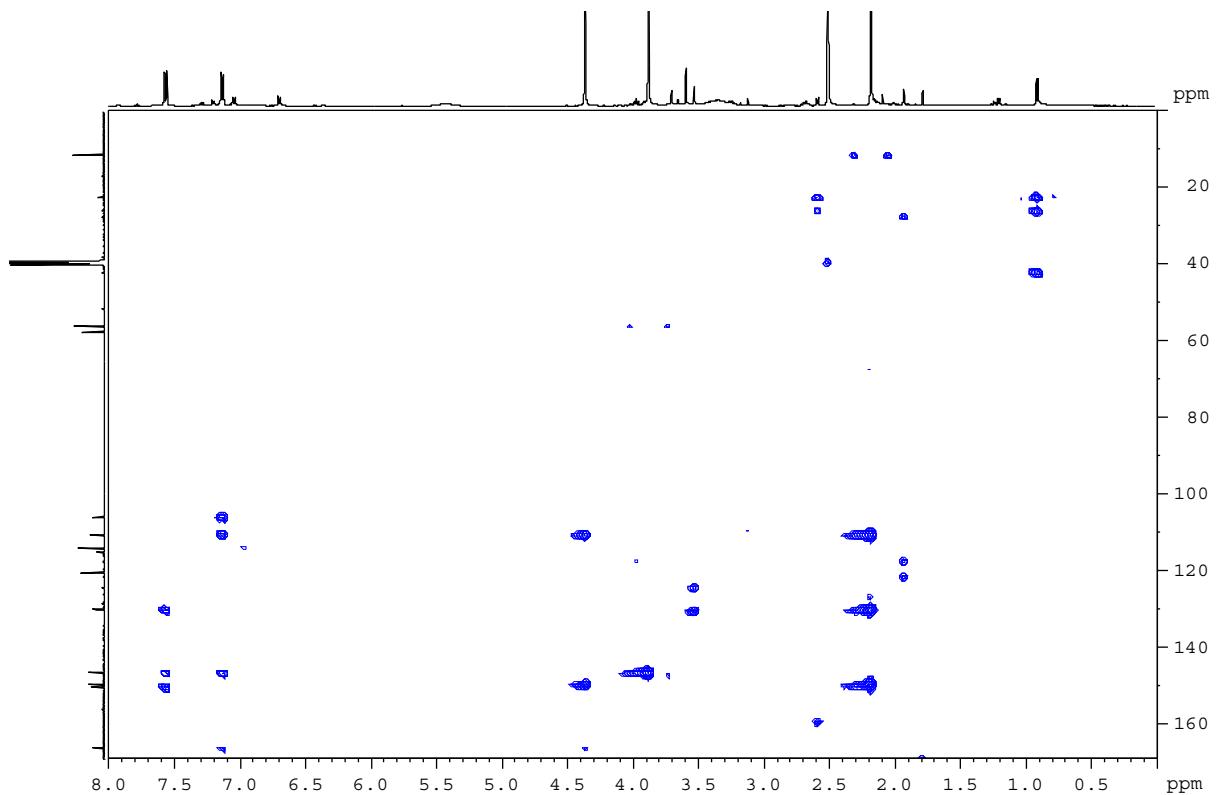
**Figure S14.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{DMSO}-d_6$ ) of **3**



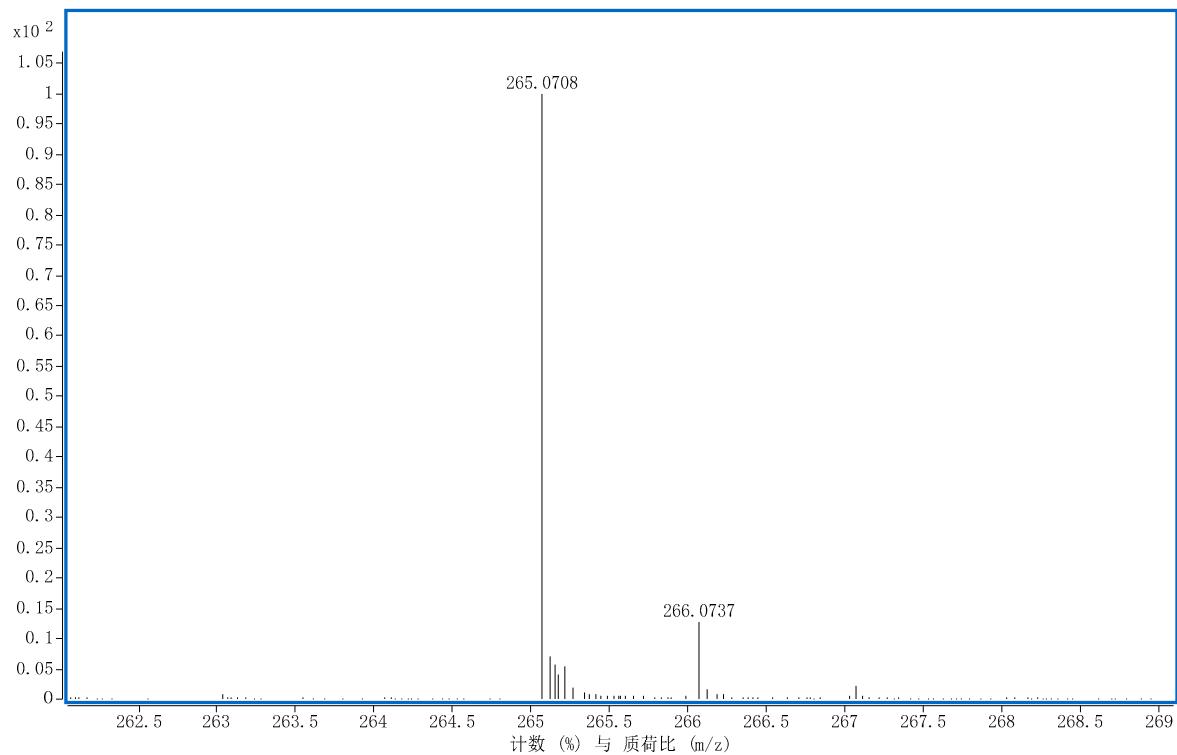
**Figure S15.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{DMSO}-d_6$ ) of **3**



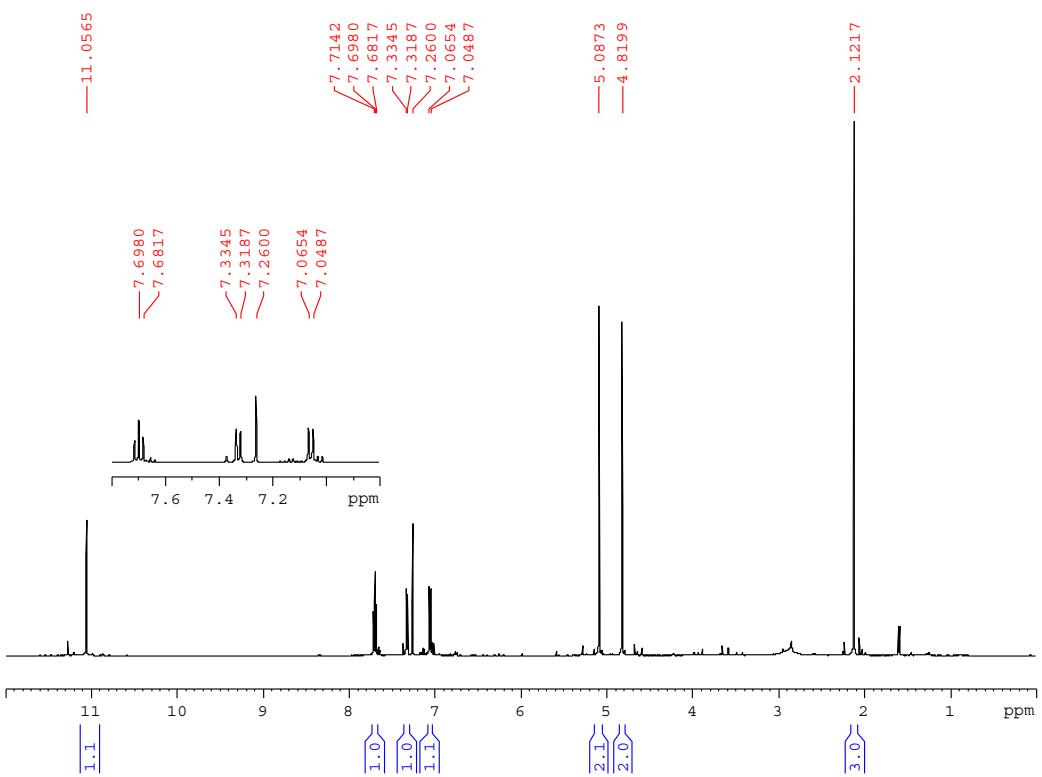
**Figure S16.** HSQC spectrum (500 MHz,  $\text{DMSO}-d_6$ ) of **3**



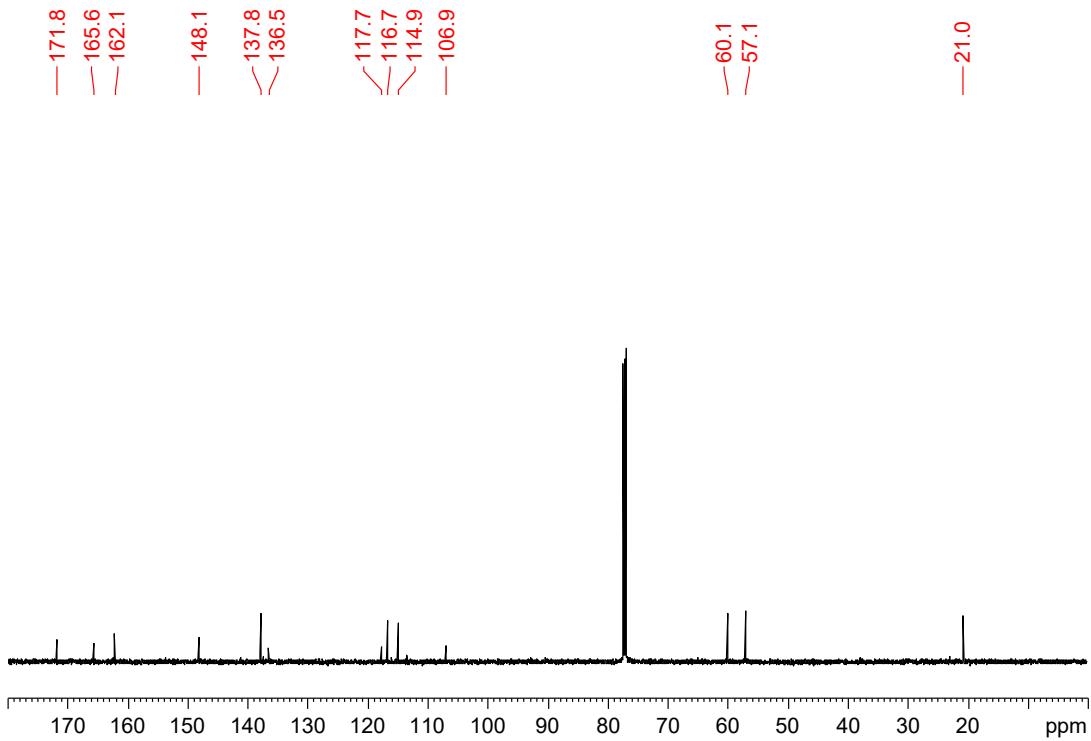
**Figure S17.** HMBC spectrum (500 MHz, DMSO-*d*<sub>6</sub>) of **3**



**Figure S18.** HRESIMS spectrum for **4**

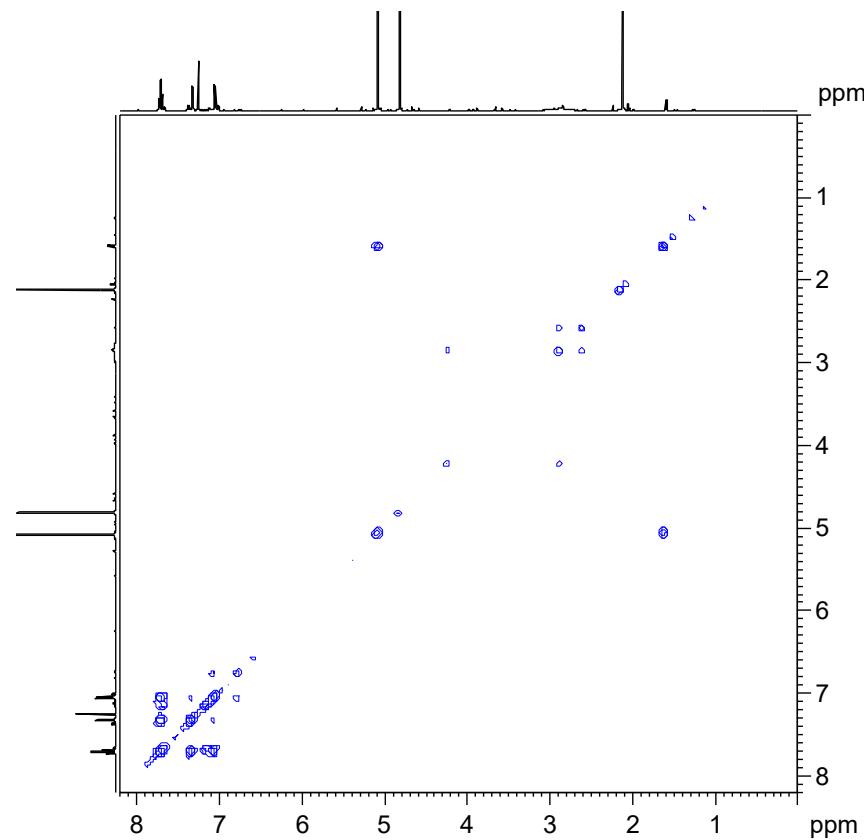
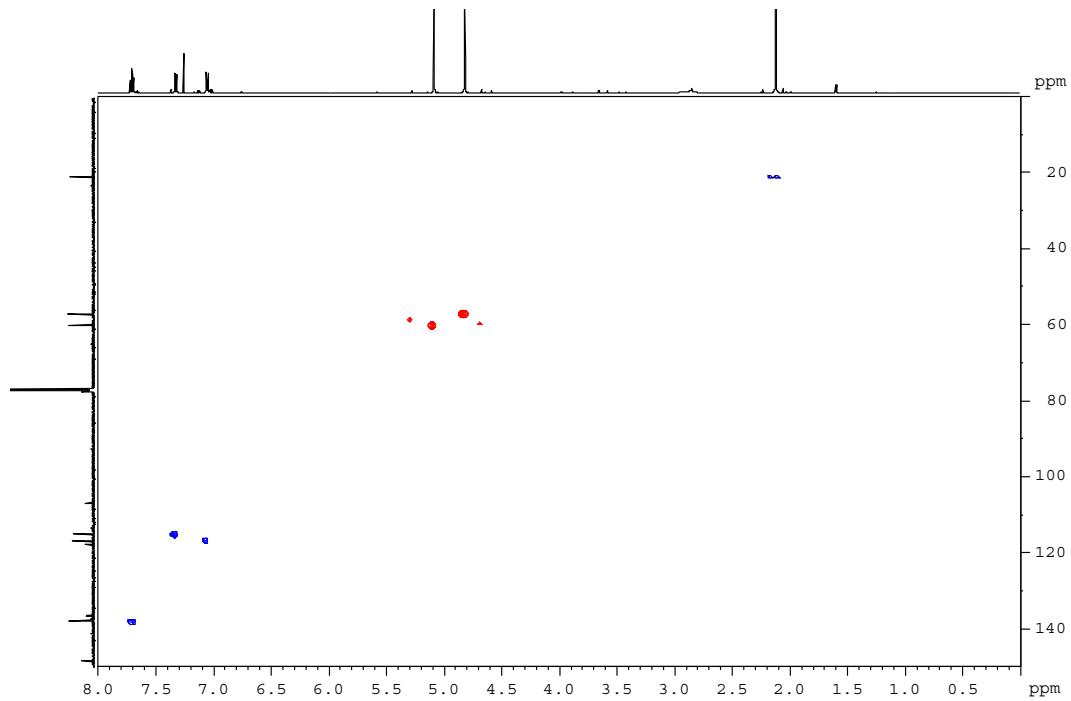


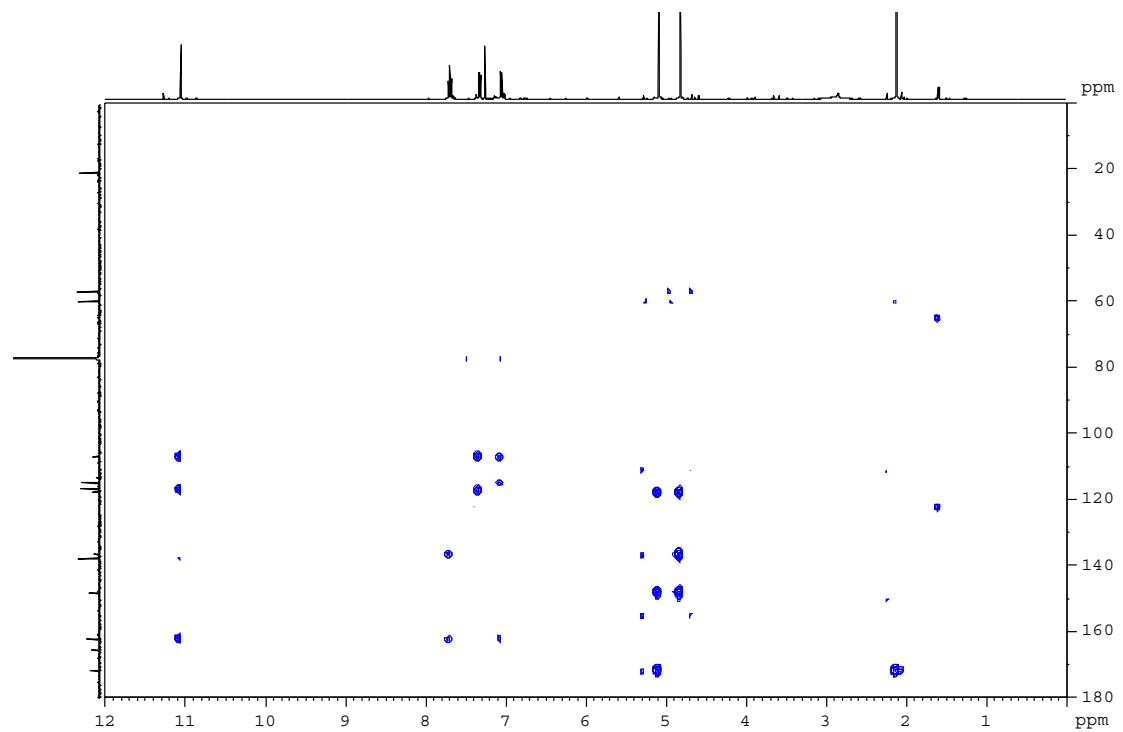
**Figure S19.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of **4**



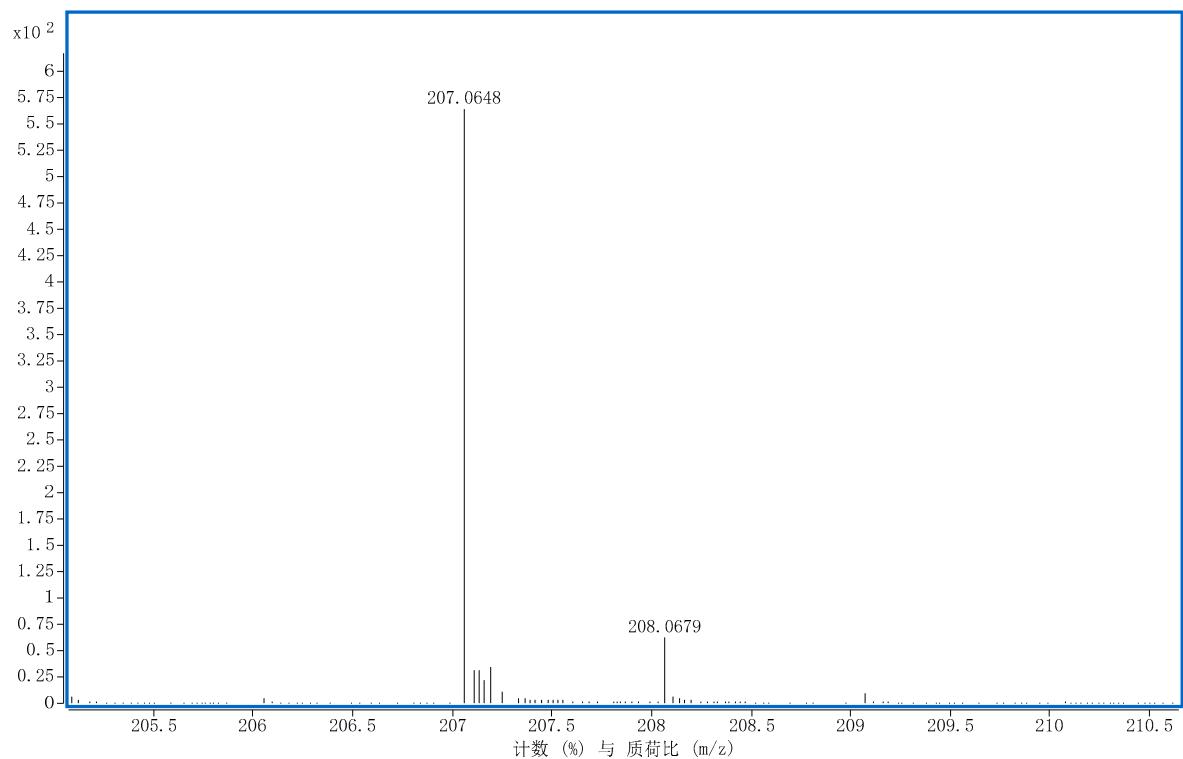
**Figure S20.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of **4**

Supplementary Material



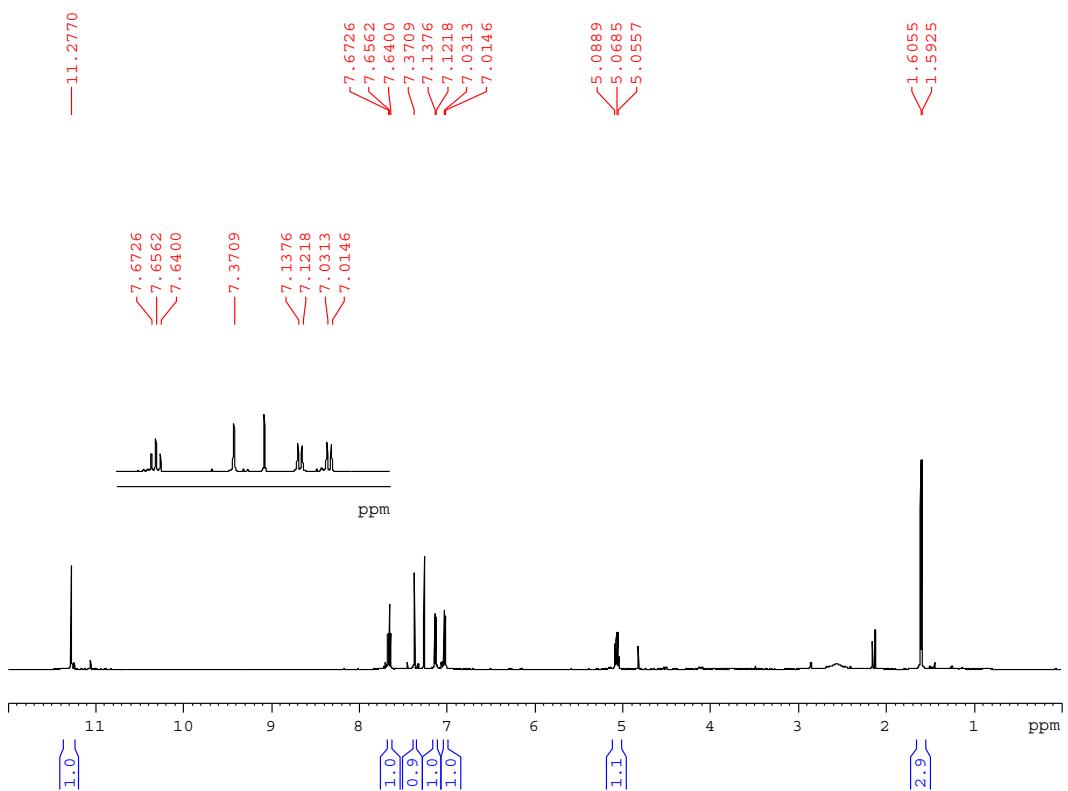


**Figure S23.** HMBC spectrum (500 MHz,  $\text{CDCl}_3$ ) of **4**

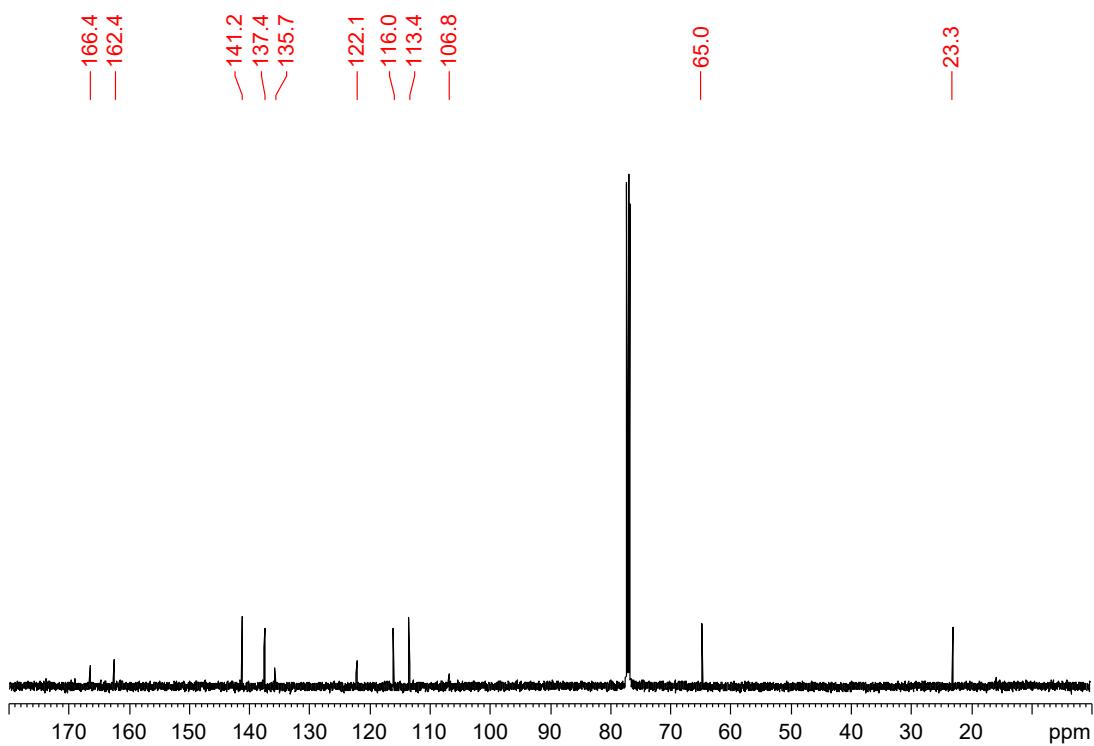


**Figure S24.** HRESIMS spectrum for **5**

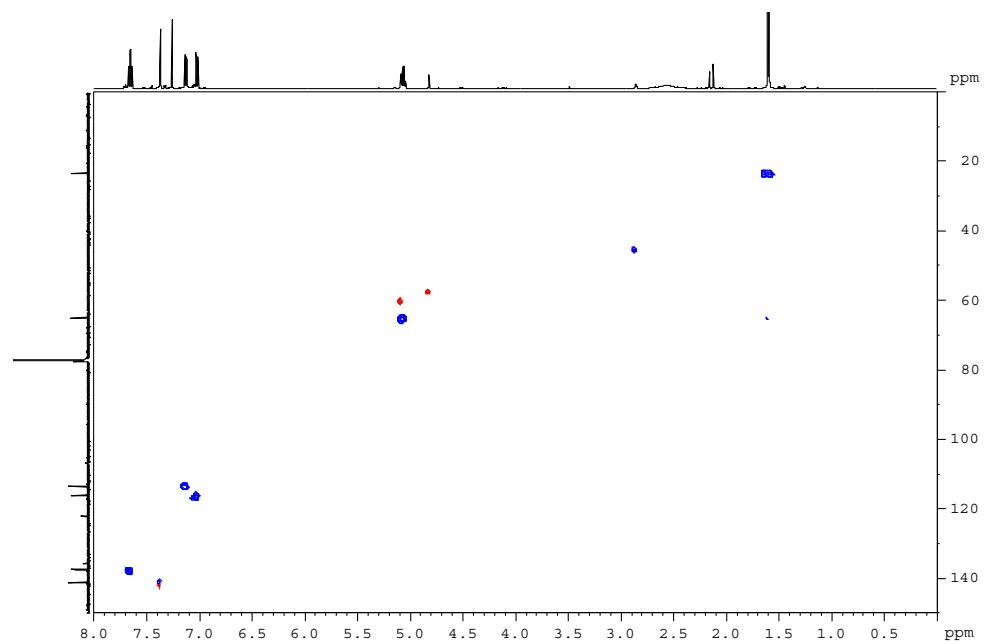
Supplementary Material



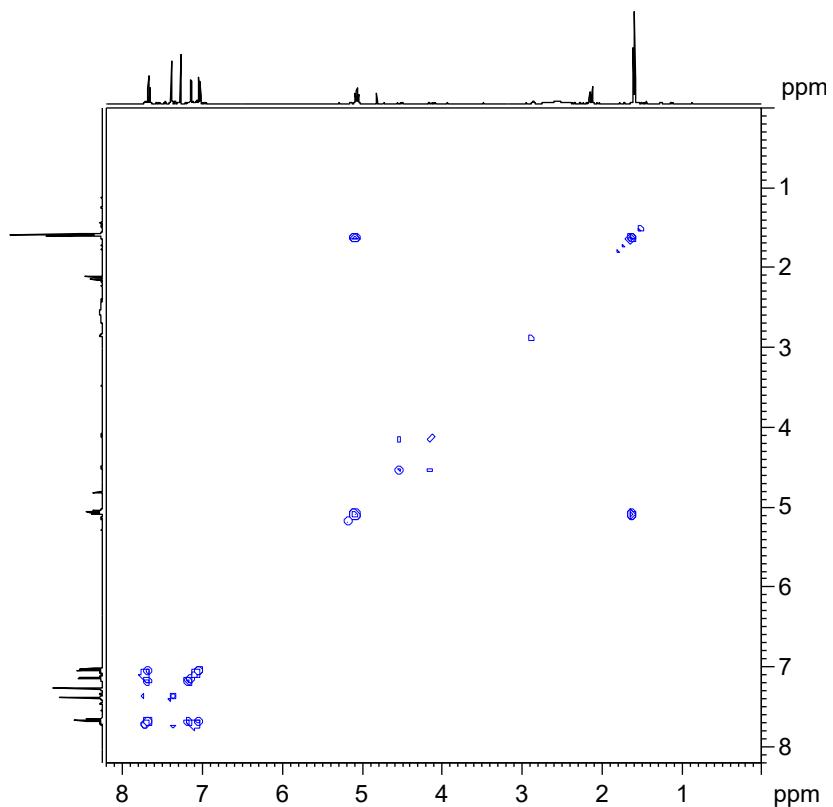
**Figure S25.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of **5**



**Figure S26.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of **5**

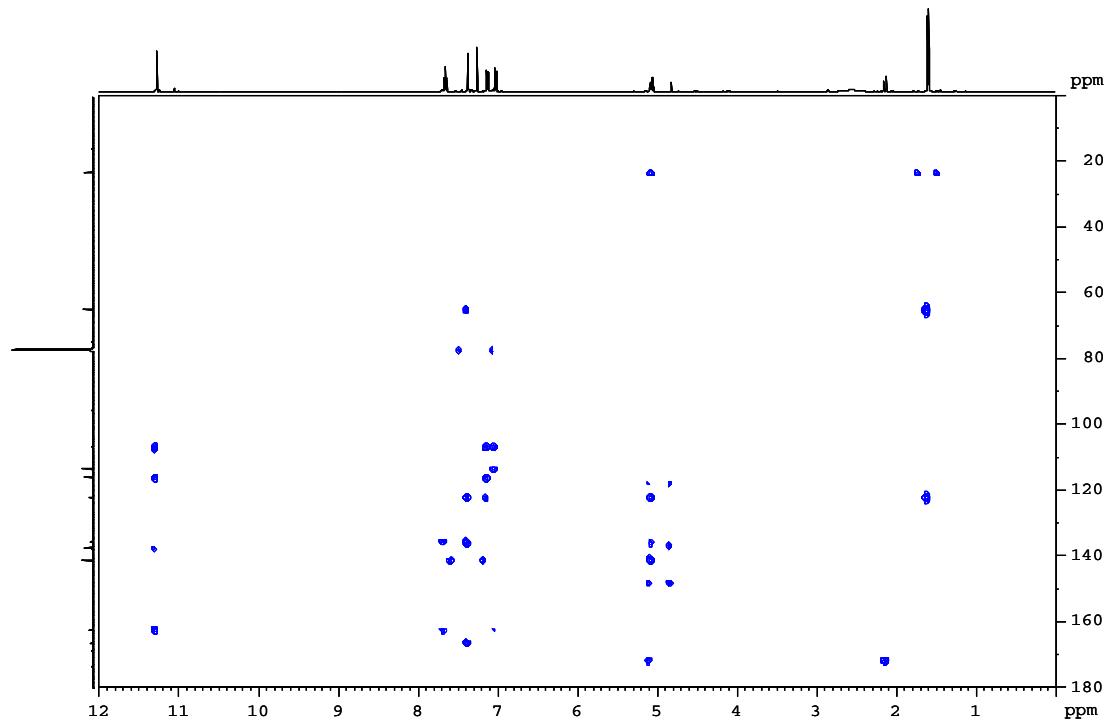


**Figure S27.** HSQC spectrum (500 MHz,  $\text{CDCl}_3$ ) of **5**

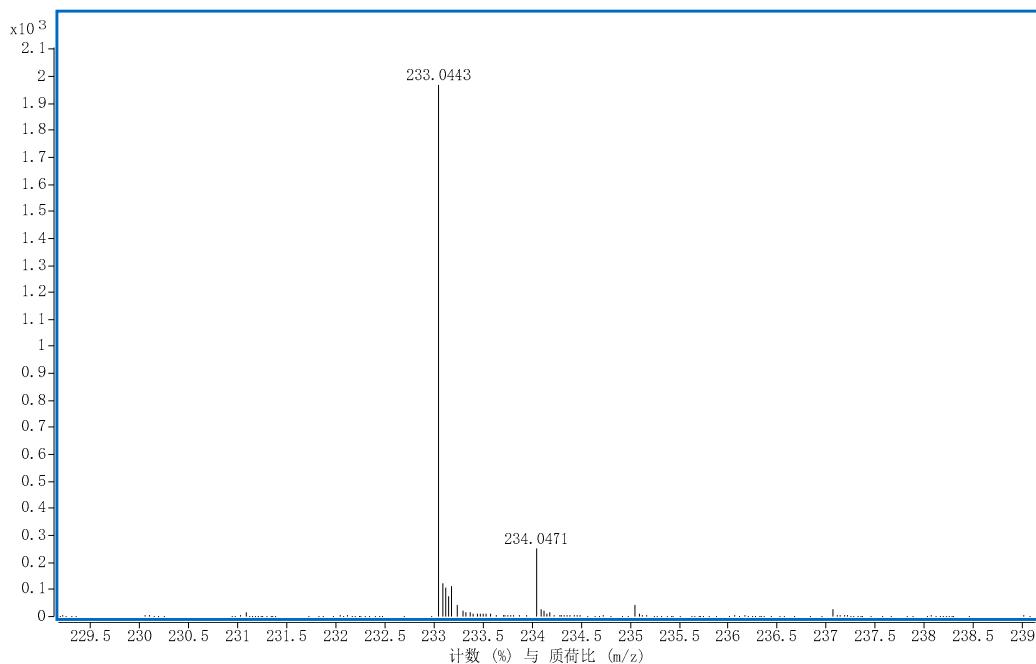


**Figure S28.**  $^1\text{H}$  - $^1\text{H}$  COSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of **5**

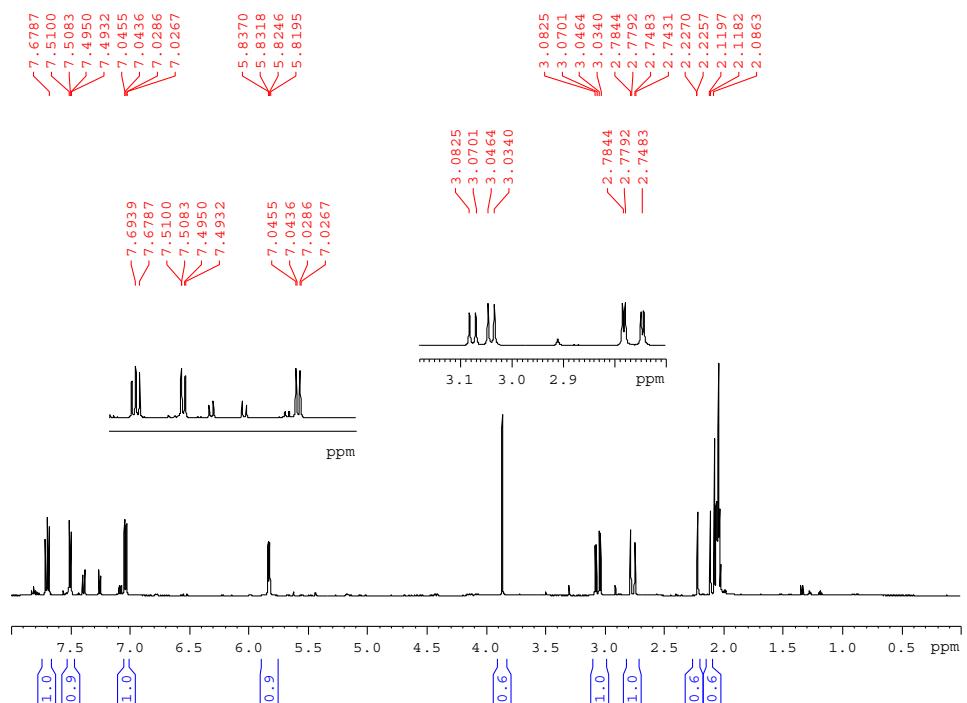
Supplementary Material



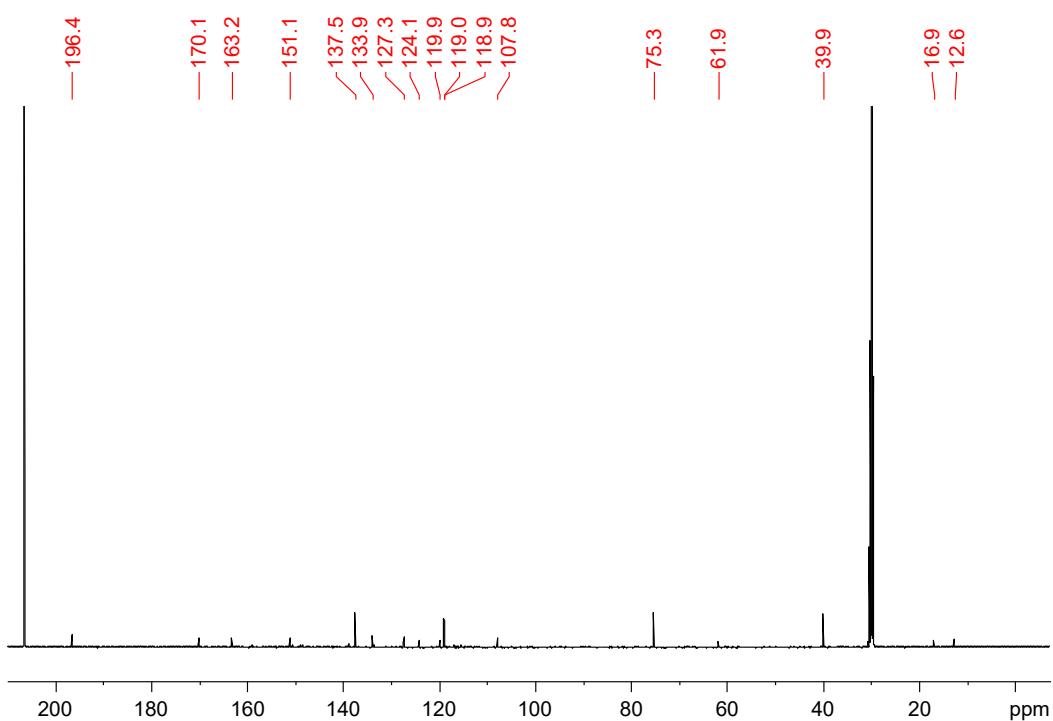
**Figure S29.** HMBC spectrum (500 MHz,  $\text{CDCl}_3$ ) of **5**



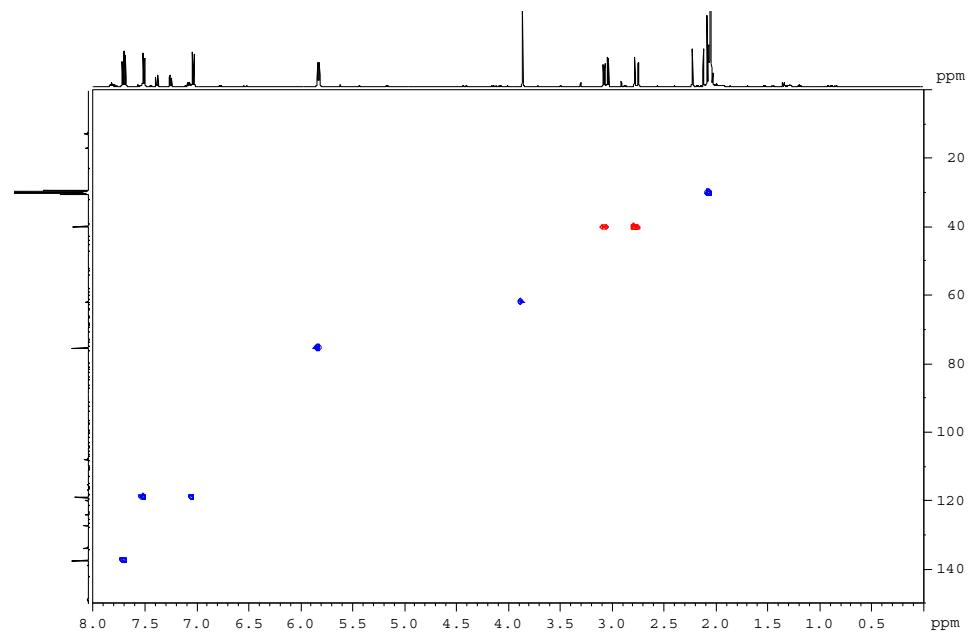
**Figure S30.** HRESIMS spectrum for **6**



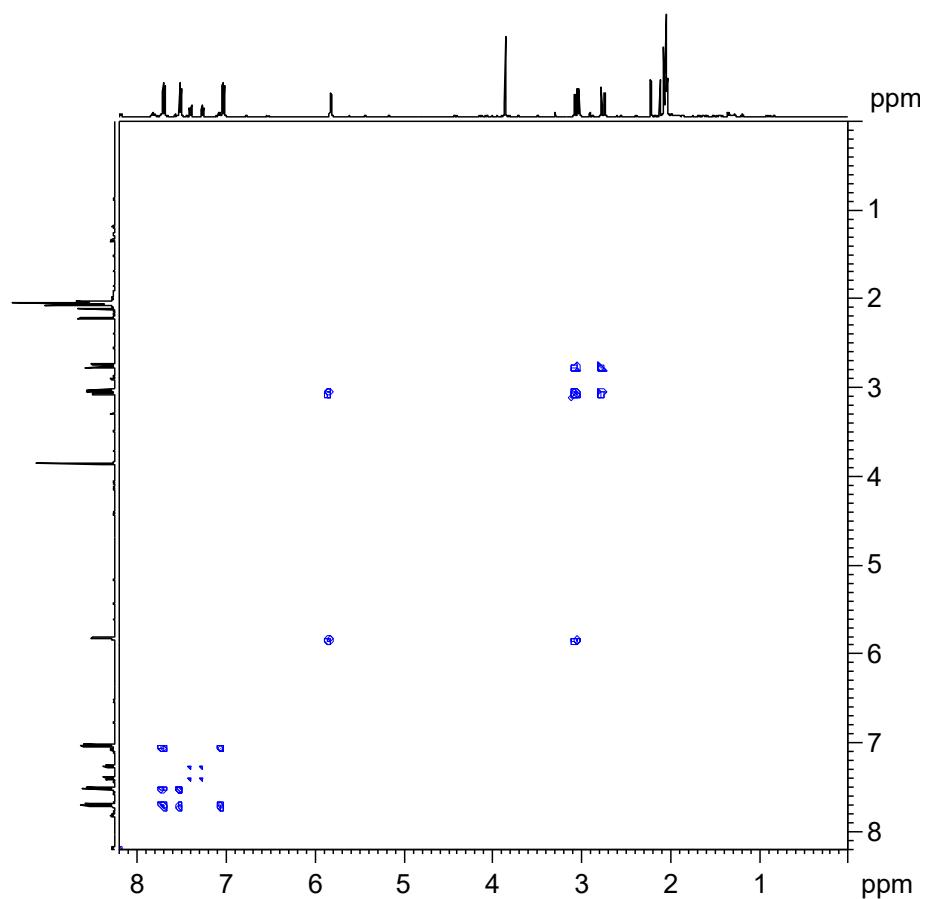
**Figure S31.**  $^1\text{H}$  NMR spectrum (500 MHz, Acetone- $d_6$ ) of **6**



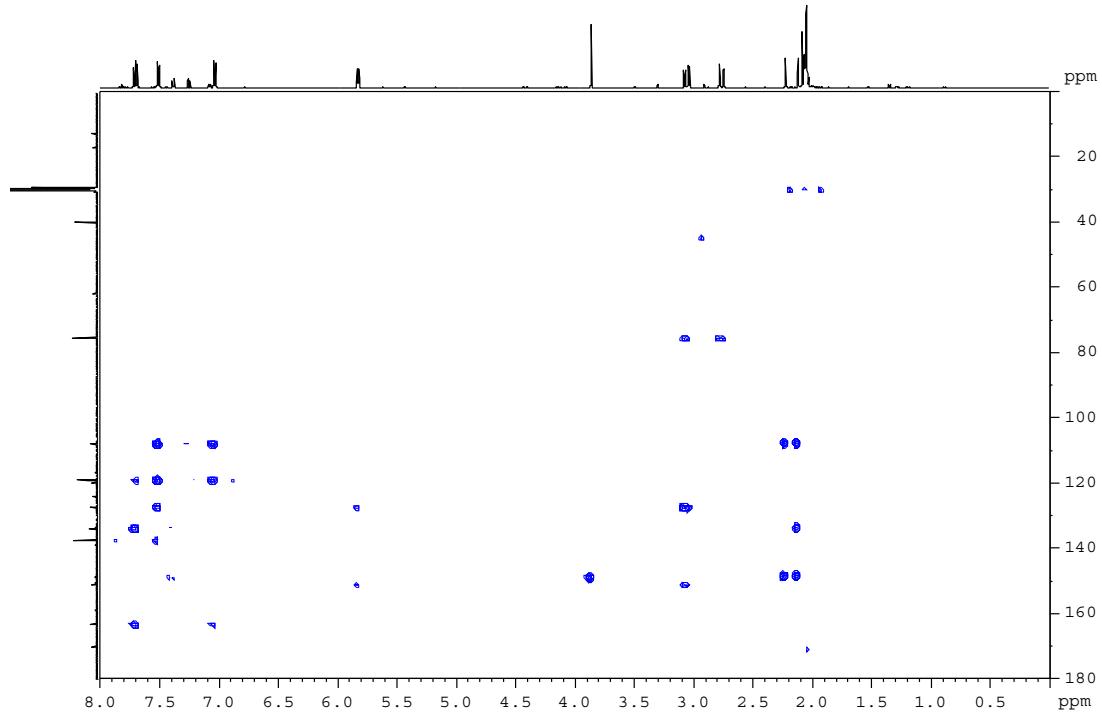
**Figure S32.**  $^{13}\text{C}$  NMR spectrum (125 MHz, Acetone- $d_6$ ) of **6**



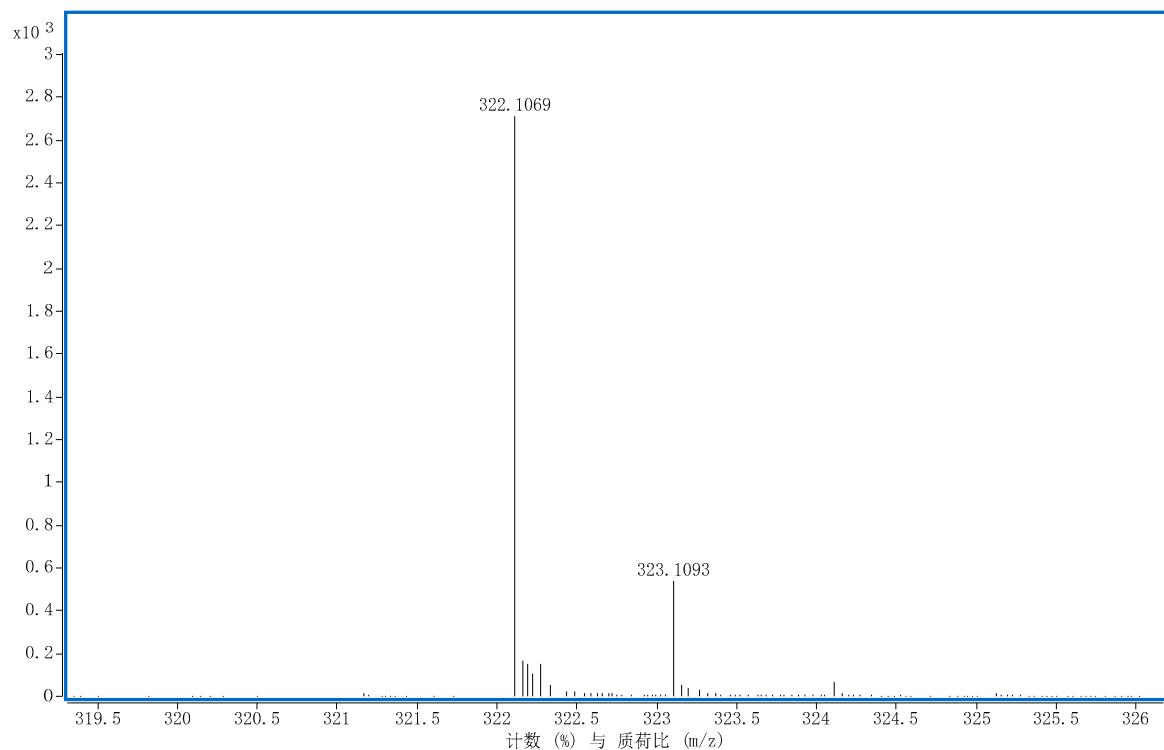
**Figure S33.** HSQC spectrum (500 MHz, Acetone- $d_6$ ) of **6**



**Figure S34.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz, Acetone- $d_6$ ) of **6**

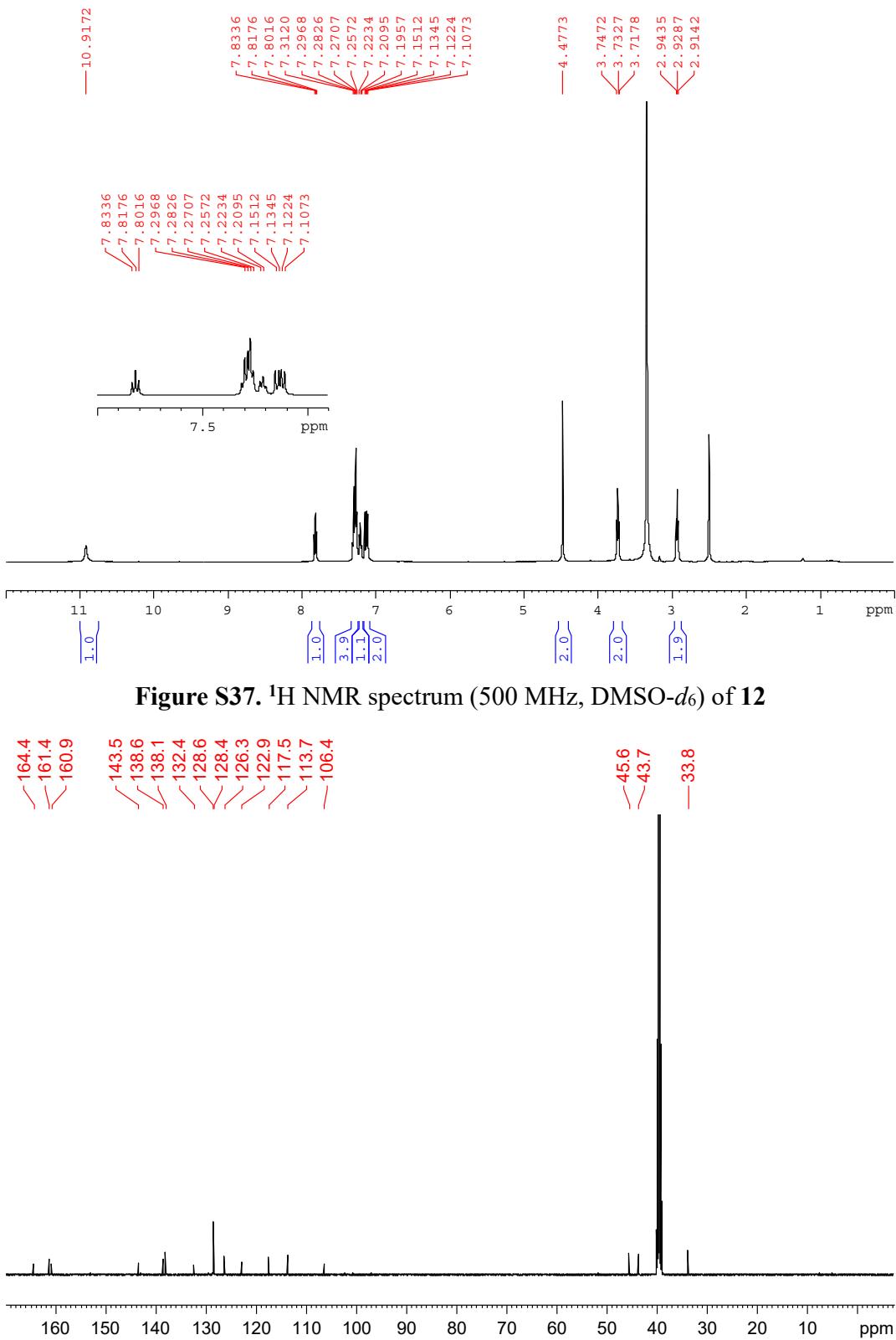


**Figure S35.** HMBC spectrum (500 MHz, Acetone-*d*<sub>6</sub>) of **6**

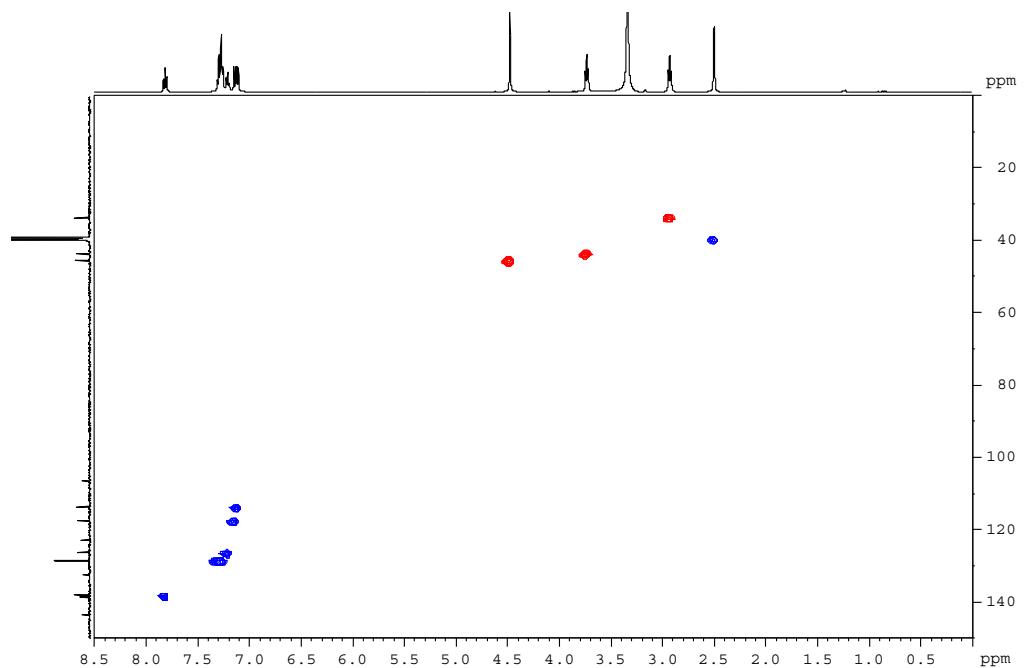


**Figure S36.** HRESIMS spectrum for **12**

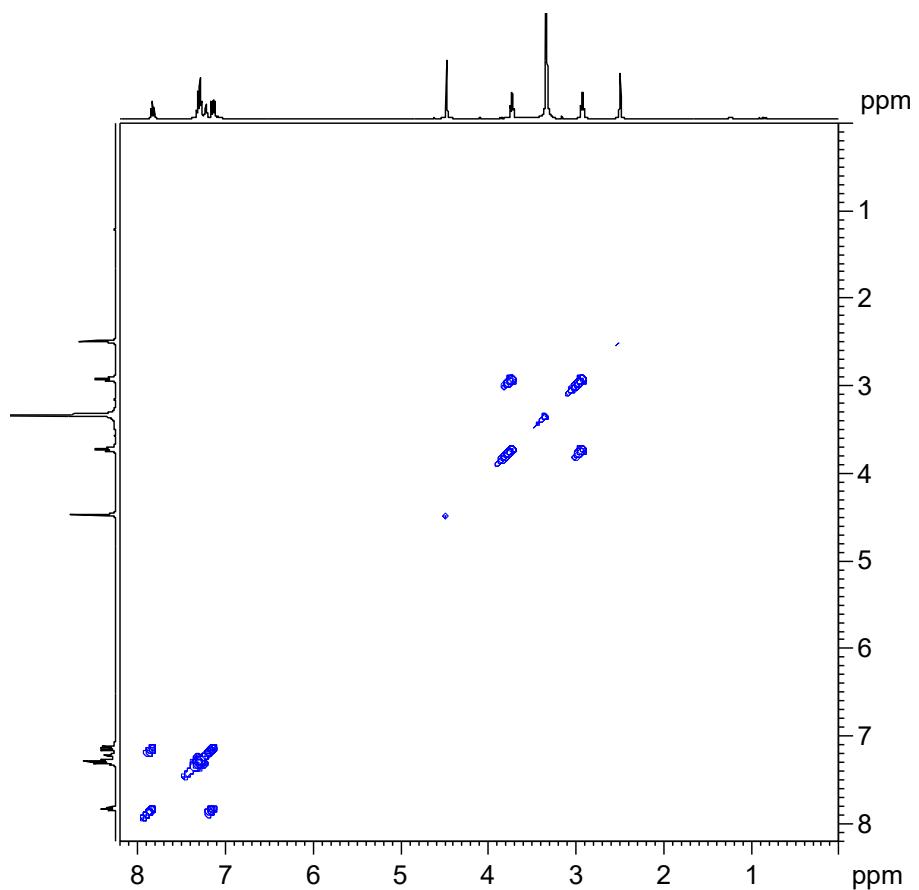
Supplementary Material



**Figure S38.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{DMSO}-d_6$ ) of **12**

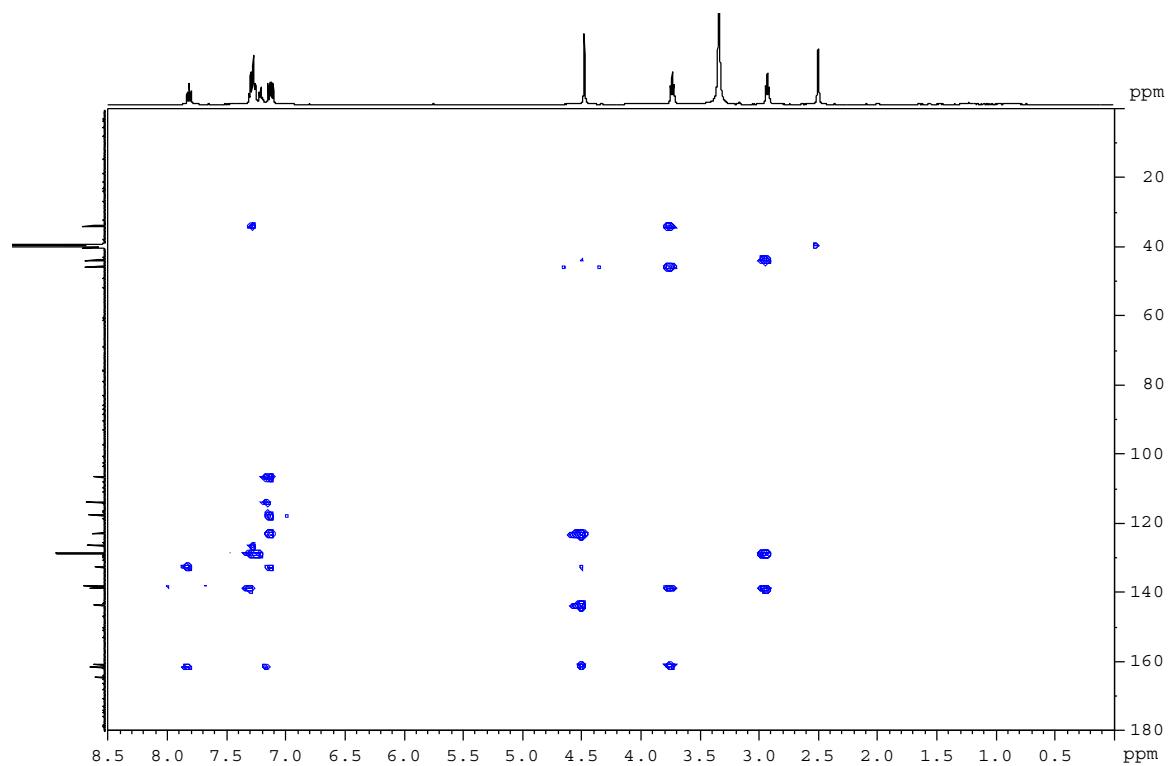


**Figure S39.** HSQC spectrum (500 MHz,  $\text{DMSO}-d_6$ ) of **12**

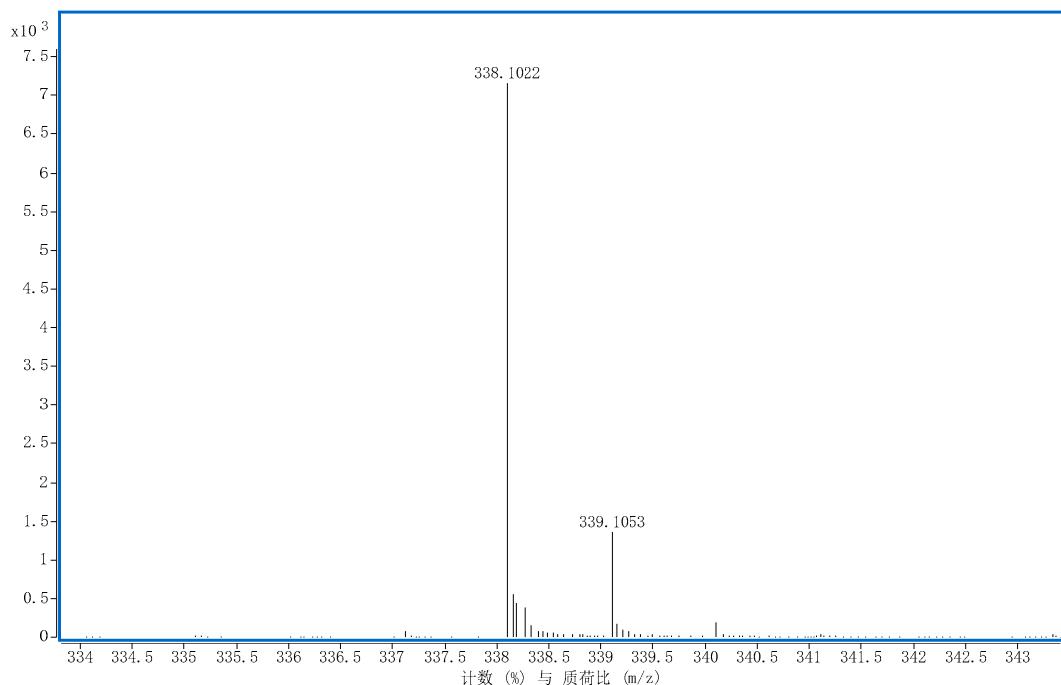


Supplementary Material

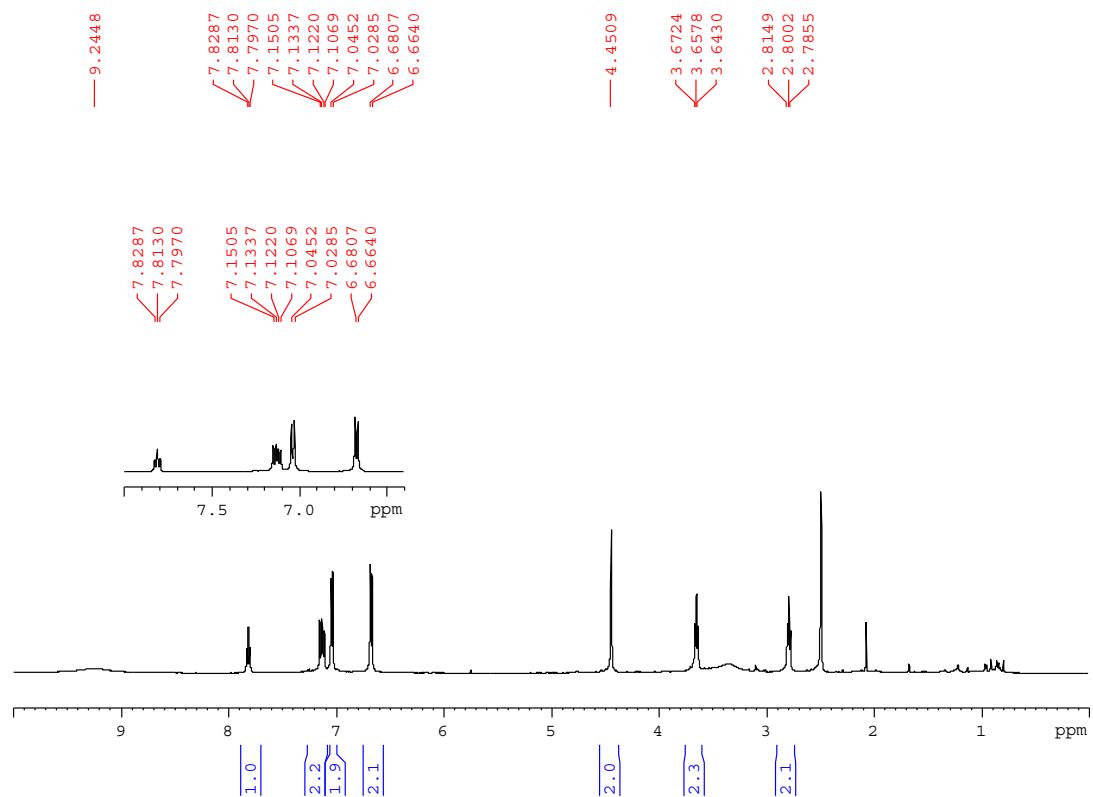
**Figure S40.**  $^1\text{H}$  - $^1\text{H}$  COSY spectrum (500 MHz, DMSO- $d_6$ ) of **12**



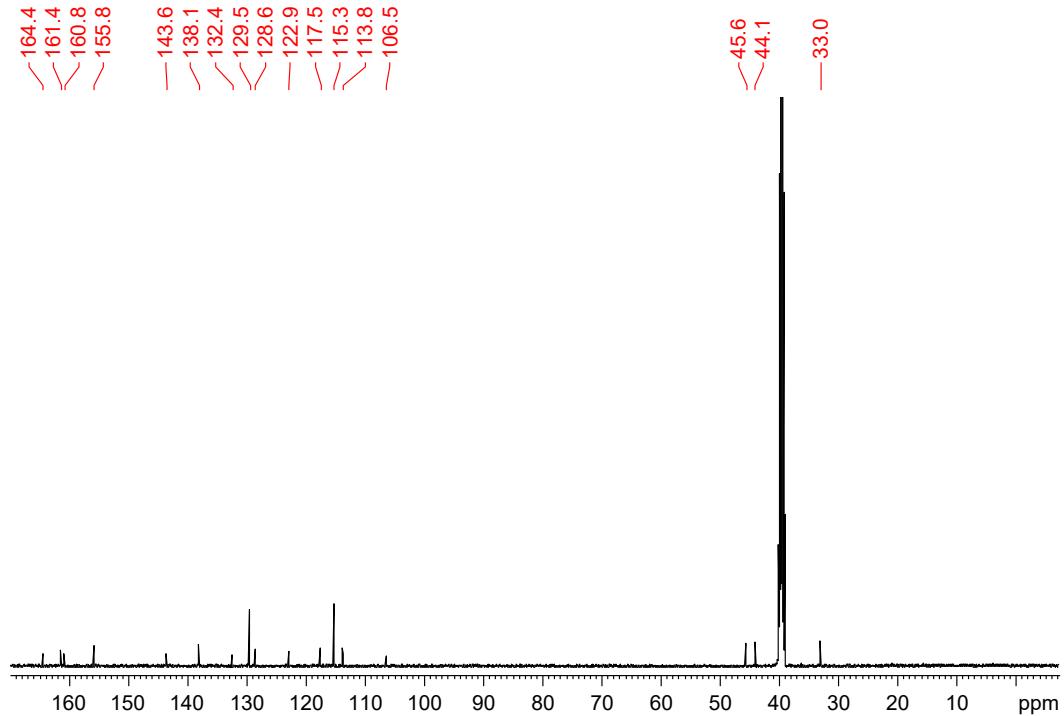
**Figure S41.** HMBC spectrum (500 MHz, DMSO- $d_6$ ) of **12**



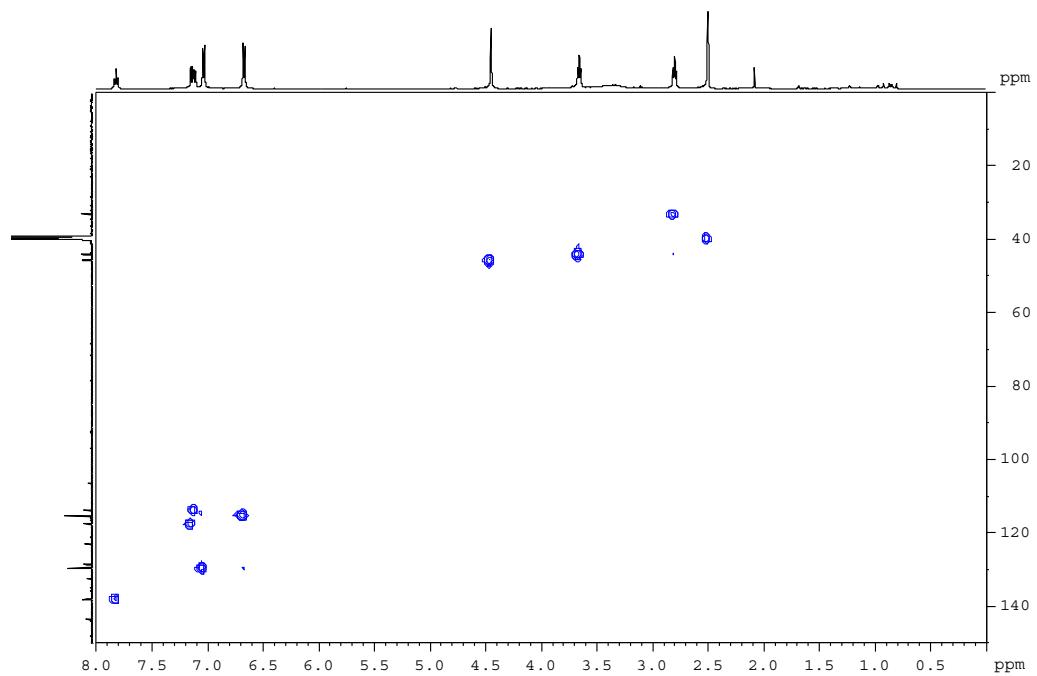
**Figure S42.** HRESIMS spectrum for **13**



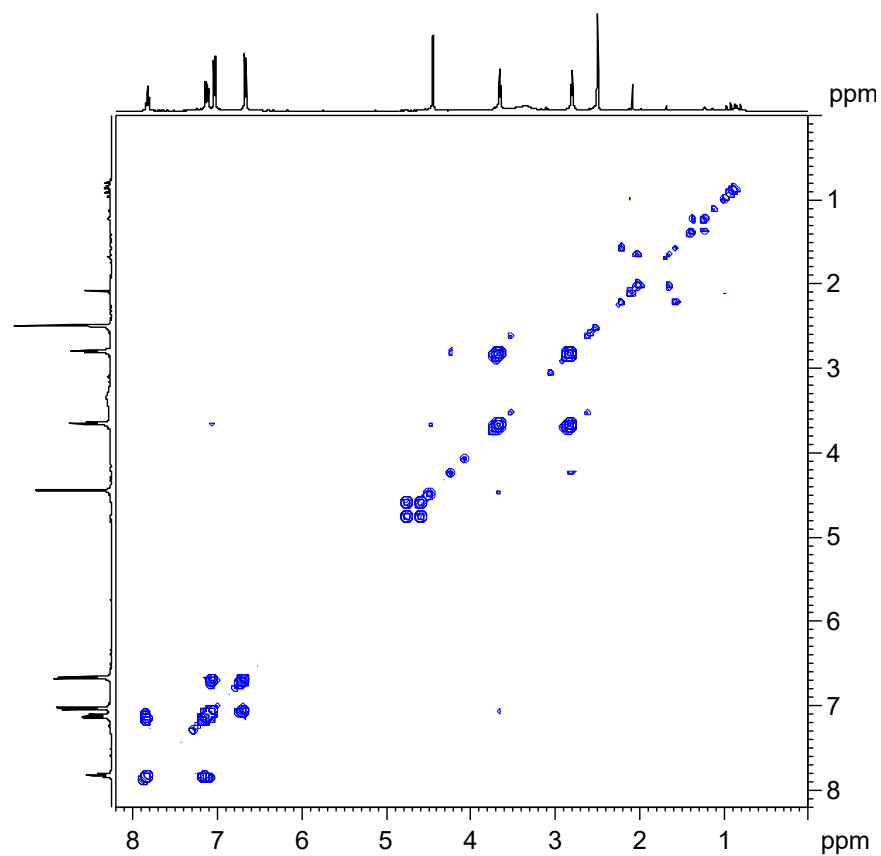
**Figure S43.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{DMSO}-d_6$ ) of **13**



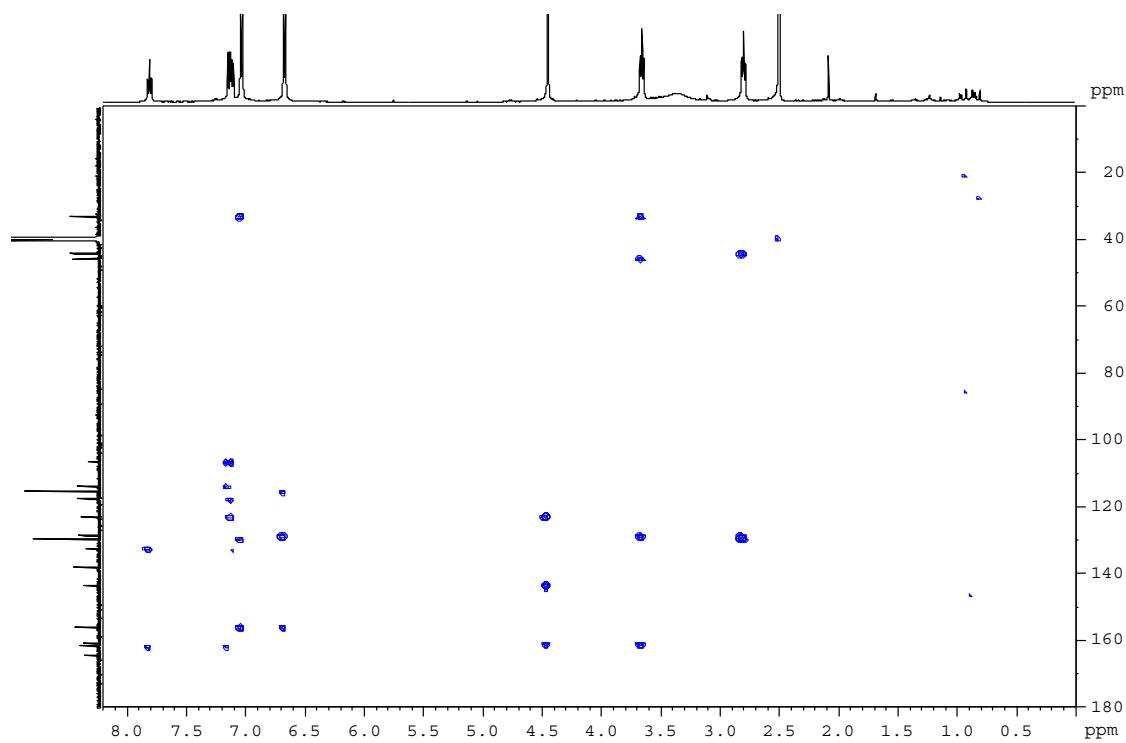
**Figure S44.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{DMSO}-d_6$ ) of **13**



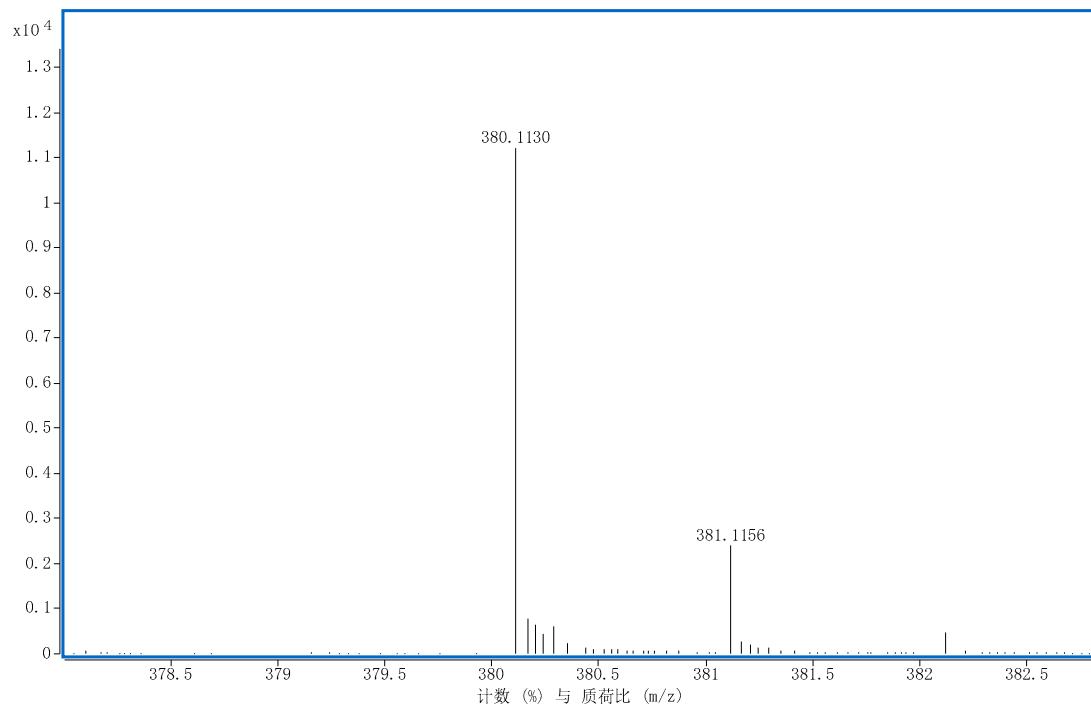
**Figure S45.** HSQC spectrum (500 MHz,  $\text{DMSO}-d_6$ ) of **13**



**Figure S46.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz,  $\text{DMSO}-d_6$ ) of **13**

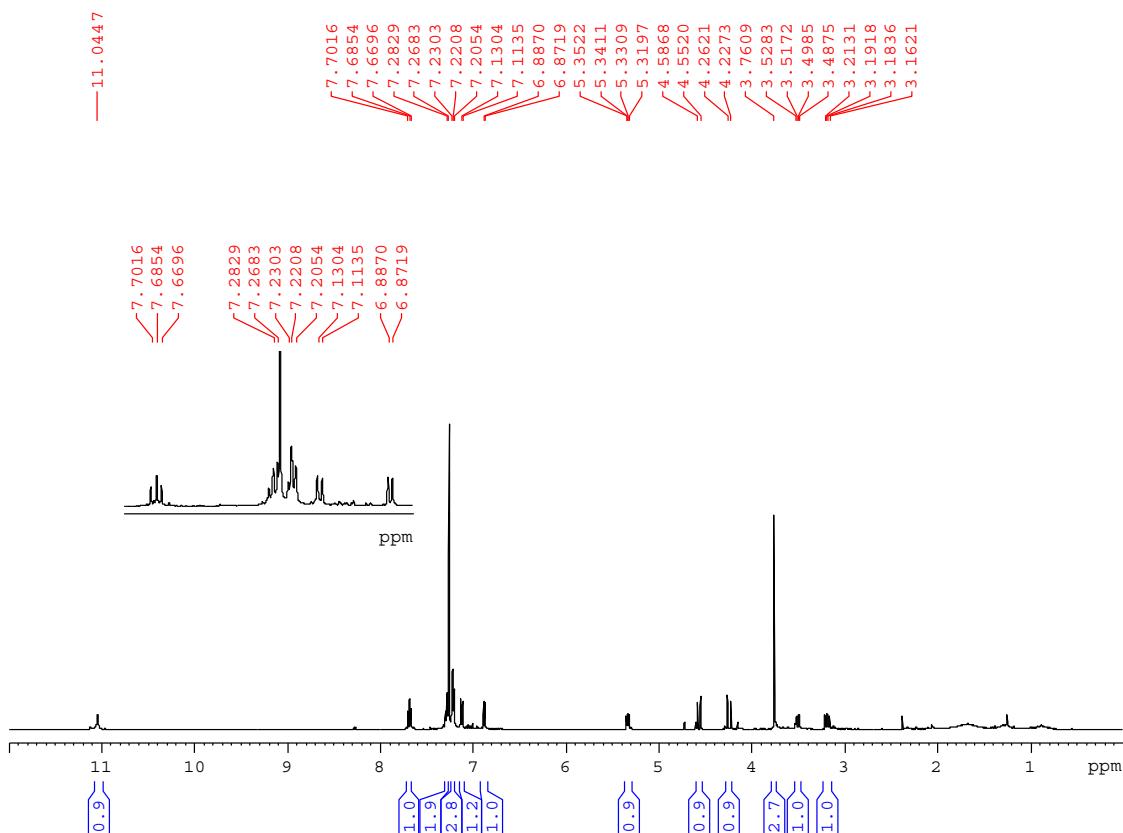


**Figure S47.** HMBC spectrum (500 MHz,  $\text{DMSO}-d_6$ ) of **13**

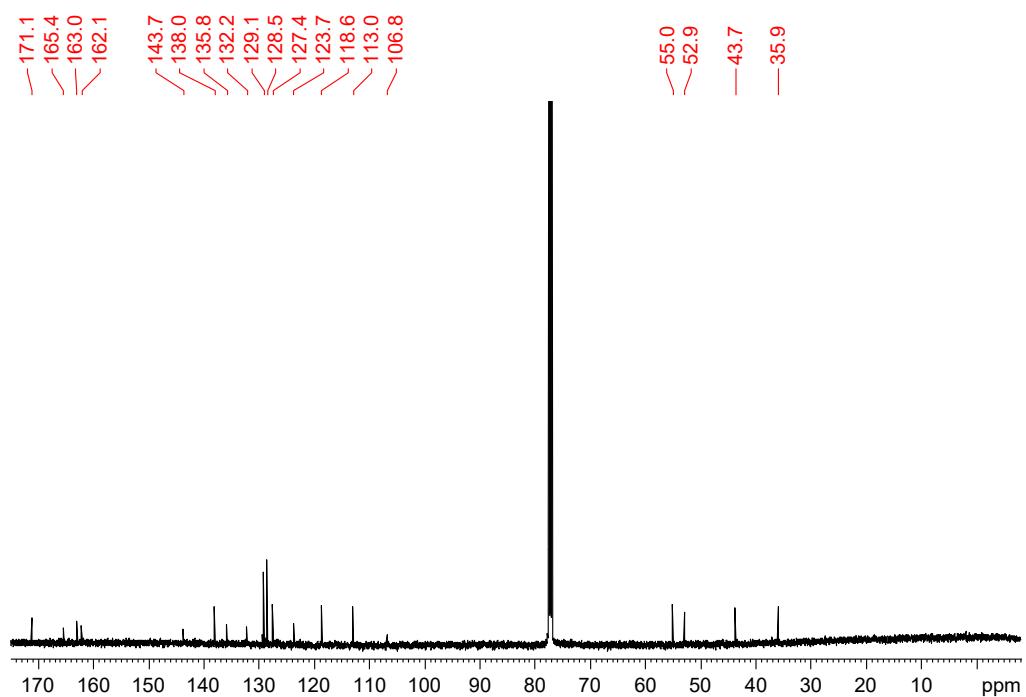


**Figure S48.** HRESIMS spectrum for **14**

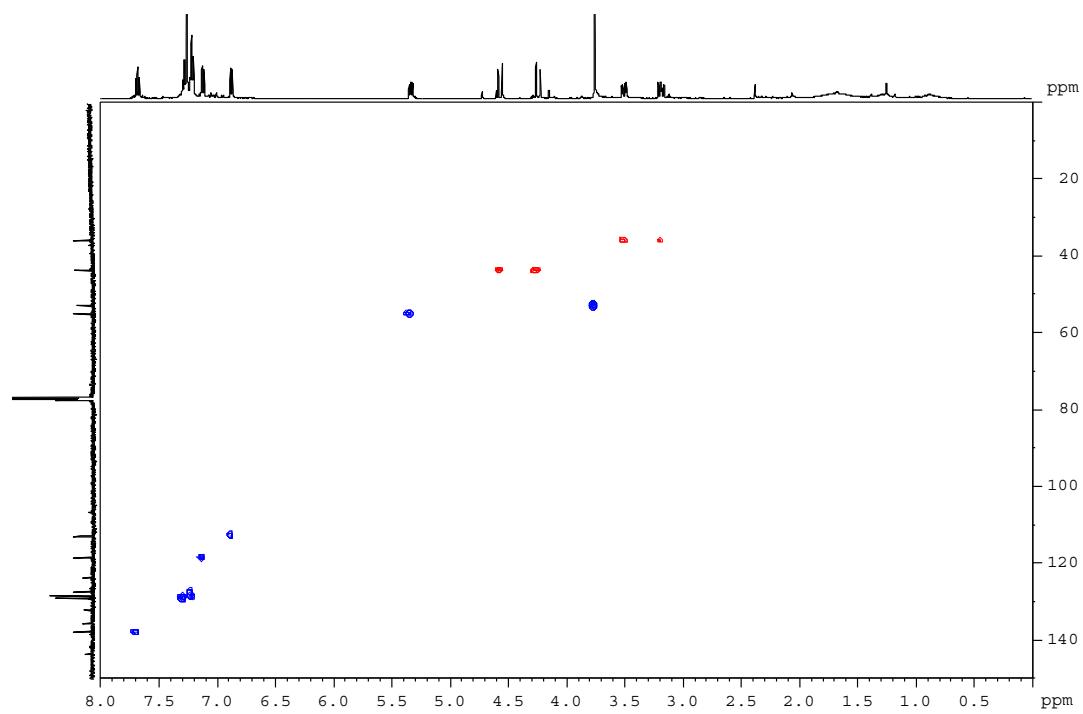
Supplementary Material



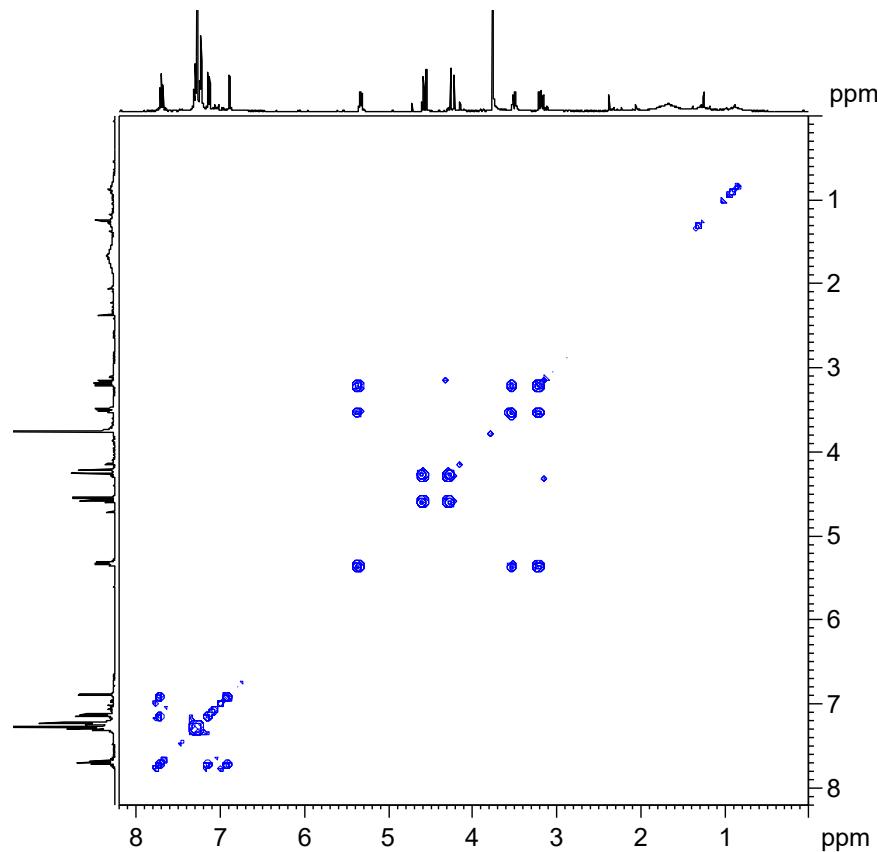
**Figure S49.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of **14**



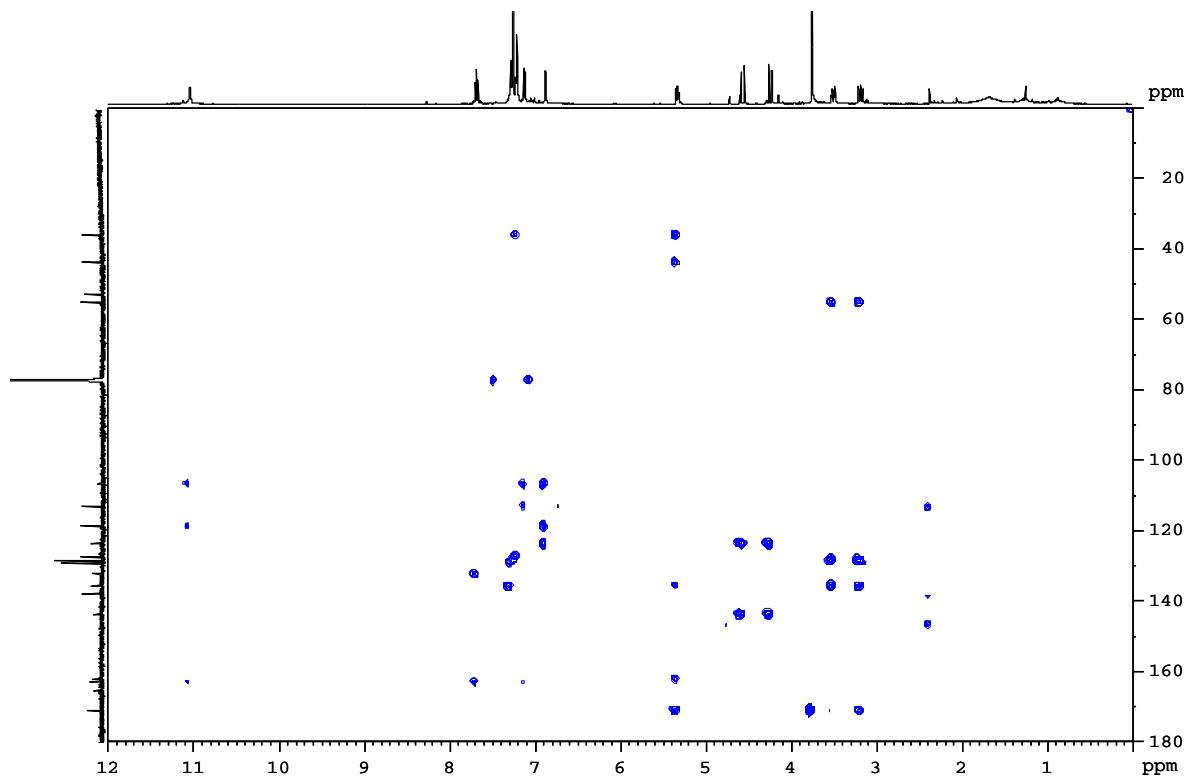
**Figure S51.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of **14**



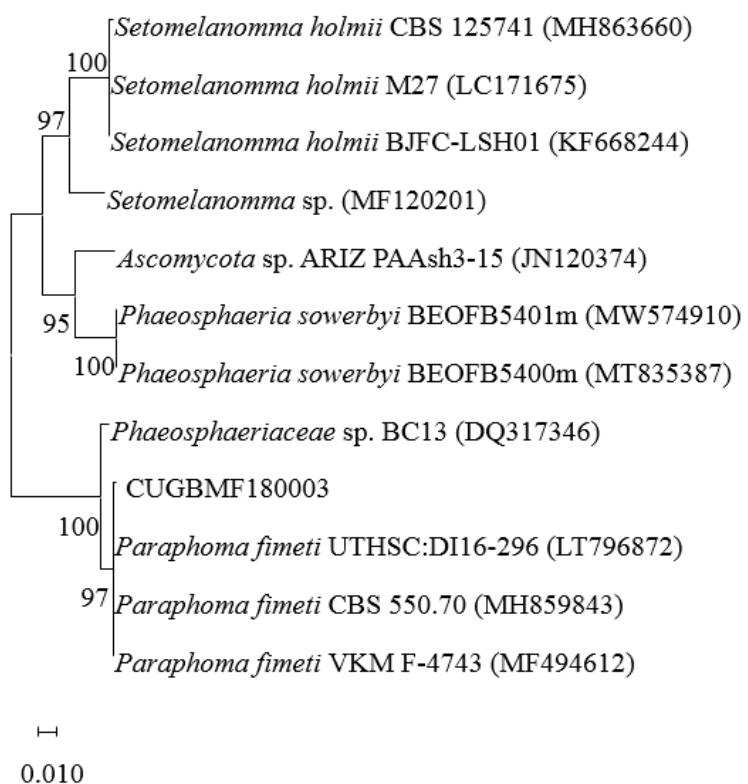
**Figure S52.** HSQC spectrum (500 MHz,  $\text{CDCl}_3$ ) of **14**



**Figure S53.**  $^1\text{H}$  - $^1\text{H}$  COSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of **14**



**Figure S54.** HMBC spectrum (500 MHz,  $\text{CDCl}_3$ ) of **14**



**Figure S55.** Neighbor-joining phylogenetic tree of CUGBMF180003 and its most related type strains based on internal transcribed spacer region (ITS) from NCBI ITS database. Numbers at nodes indicate levels of bootstrap support (%) based on a neighbor joining analysis of 1,000 resampled datasets; only values >50 % are given. NCBI accession numbers are given in parentheses. Bar 0.010 nucleotide substitutions per site.