

## **Supporting Information**

# **Polyhydroxy *p*-Terphenyls from a Mangrove Endophytic Fungus *Aspergillus candidus* LDJ-5**

Guoliang Zhou,<sup>1</sup> Xiaomin Zhang,<sup>1</sup> Mudassir Shah,<sup>1</sup> Qian Che,<sup>1</sup> Guojian Zhang,<sup>1,2</sup>

Qianqun Gu,<sup>1</sup> Tianjiao Zhu,<sup>\*,1</sup> and Dehai Li<sup>\*,1,2,3</sup>

<sup>1</sup> Key Laboratory of Marine Drugs, Chinese Ministry of Education, School of

Medicine and Pharmacy, Ocean University of China, Qingdao 266003, People's  
Republic of China

<sup>2</sup> Laboratory for Marine Drugs and Bioproducts, Pilot National Laboratory for Marine  
Science and Technology, Qingdao, 266237, P. R. China

<sup>3</sup> Open Studio for Druggability Research of Marine Natural Products, Pilot National  
Laboratory for Marine Science and Technology, Qingdao, 266237, People's  
Republic of China

\* Corresponding authors: Tel: 0086-532-82031619. E-mail: dehaili@ouc.edu.cn (D. Li);  
zhutj@ouc.edu.cn (T. Zhu).

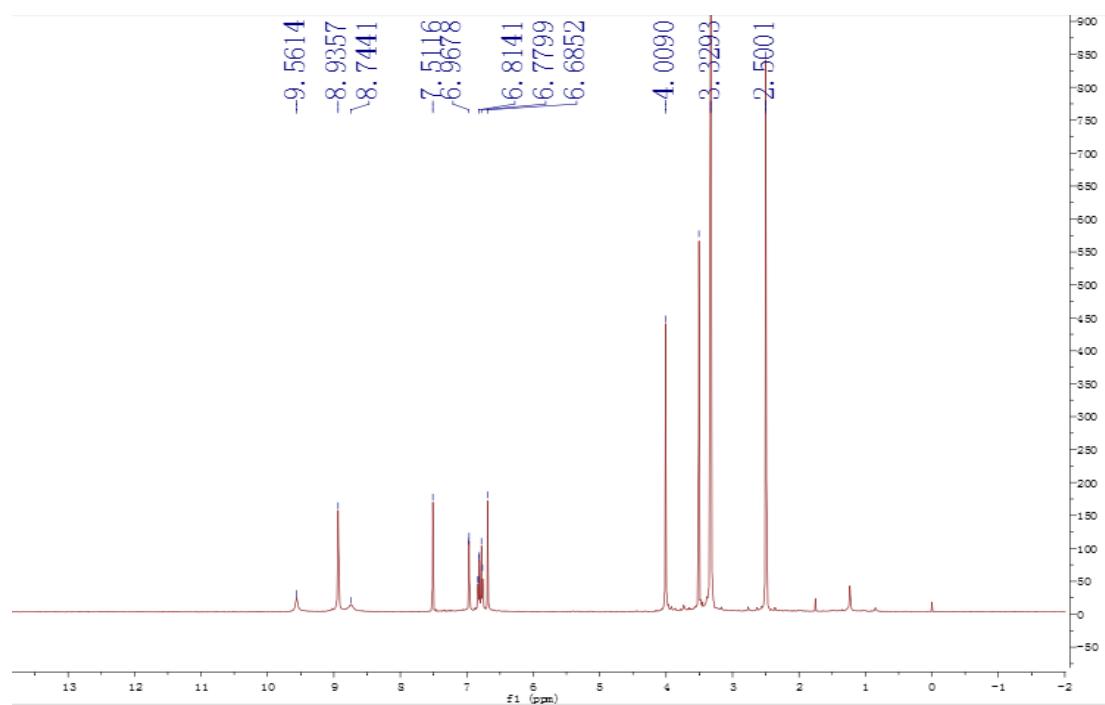
## List of supporting information

<b>Figure S1.</b> $^1\text{H}$ NMR (500 MHz, DMSO- $d_6$ ) spectrum of <b>1</b> .....	S5
<b>Figure S2.</b> $^{13}\text{C}$ NMR (125 MHz, DMSO- $d_6$ ) spectrum of <b>1</b> . .....	S5
<b>Figure S3.</b> DEPT (125 MHz, DMSO- $d_6$ ) spectrum of <b>1</b> . .....	S6
<b>Figure S4.</b> HSQC spectrum of <b>1</b> in DMSO- $d_6$ .....	S6
<b>Figure S5.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>1</b> in DMSO- $d_6$ . .....	S7
<b>Figure S6.</b> HMBC spectrum of <b>1</b> in DMSO- $d_6$ .....	S7
<b>Figure S7.</b> NOESY spectrum of <b>1</b> in DMSO- $d_6$ . .....	S8
<b>Figure S8.</b> HRESIMS spectrum of <b>1</b> .....	S8
<b>Figure S9.</b> $^1\text{H}$ NMR (500 MHz, DMSO- $d_6$ ) spectrum of <b>2</b> .....	S9
<b>Figure S10.</b> $^{13}\text{C}$ NMR (125 MHz, DMSO- $d_6$ ) spectrum of <b>2</b> .....	S9
<b>Figure S11.</b> DEPT (125 MHz, DMSO- $d_6$ ) spectrum of <b>2</b> . .....	S10
<b>Figure S12.</b> HSQC spectrum of <b>2</b> in DMSO- $d_6$ .....	S10
<b>Figure S13.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>2</b> in DMSO- $d_6$ . .....	S11
<b>Figure S14.</b> HMBC spectrum of <b>2</b> in DMSO- $d_6$ .....	S11
<b>Figure S15.</b> HRESIMS spectrum of <b>2</b> .....	S12
<b>Figure S16.</b> $^1\text{H}$ NMR (500 MHz, DMSO- $d_6$ ) spectrum of <b>3</b> .....	S12
<b>Figure S17.</b> $^{13}\text{C}$ NMR (125 MHz, DMSO- $d_6$ ) spectrum of <b>3</b> .....	S13
<b>Figure S18.</b> DEPT (125 MHz, DMSO- $d_6$ ) spectrum of <b>3</b> .....	S13
<b>Figure S19.</b> HSQC spectrum of <b>3</b> in DMSO- $d_6$ .....	S14
<b>Figure S20.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>3</b> in DMSO- $d_6$ . .....	S14
<b>Figure S21.</b> HMBC spectrum of <b>3</b> in DMSO- $d_6$ .....	S15
<b>Figure S22.</b> HRESIMS spectrum of <b>3</b> .....	S15
<b>Figure S23.</b> $^1\text{H}$ NMR (500 MHz, DMSO- $d_6$ ) spectrum of <b>4</b> .....	S16
<b>Figure S24.</b> $^{13}\text{C}$ NMR (125 MHz, DMSO- $d_6$ ) spectrum of <b>4</b> .....	S16
<b>Figure S25.</b> DEPT (125 MHz, DMSO- $d_6$ ) spectrum of <b>4</b> .....	S17
<b>Figure S26.</b> HSQC spectrum of <b>4</b> in DMSO- $d_6$ .....	S17
<b>Figure S27.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>4</b> in DMSO- $d_6$ . .....	S18

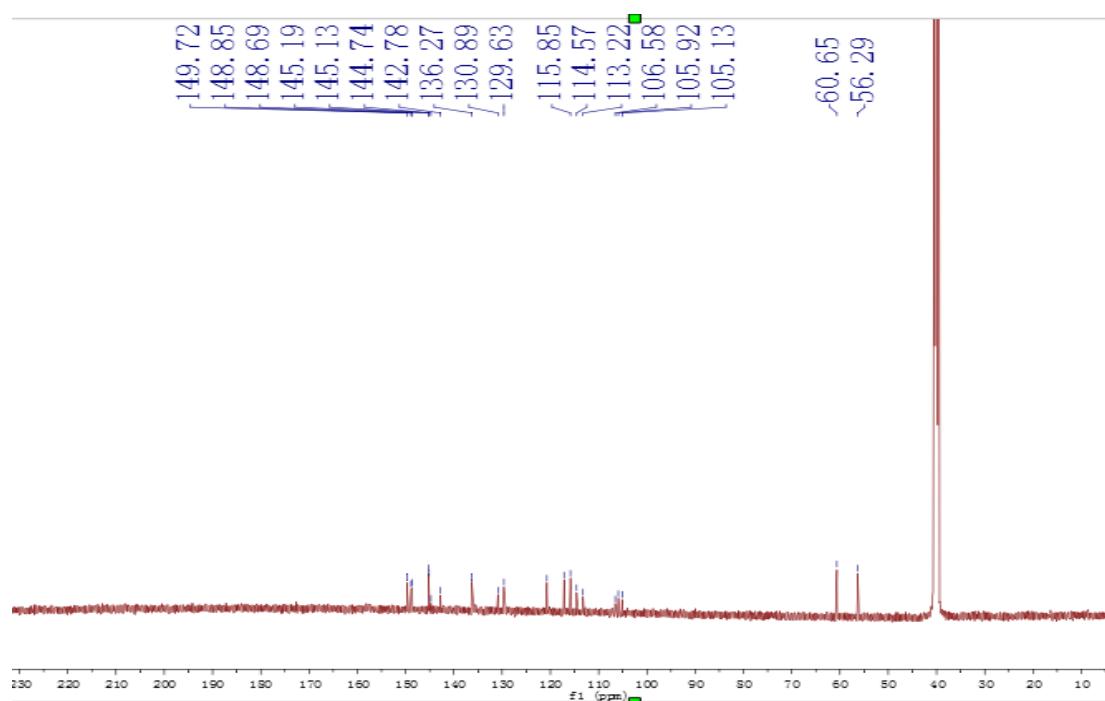
<b>Figure S28.</b> HMBC spectrum of <b>4</b> in DMSO- <i>d</i> <sub>6</sub> .....	S18
<b>Figure S29.</b> HRESIMS spectrum of <b>4</b> .....	S19
<b>Figure S30.</b> <sup>1</sup> H NMR (500 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of <b>5</b> .....	S19
<b>Figure S31.</b> <sup>13</sup> C NMR (125 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of <b>5</b> .....	S20
<b>Figure S32.</b> DEPT (125 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of <b>5</b> .....	S20
<b>Figure S33.</b> HSQC spectrum of <b>5</b> in DMSO- <i>d</i> <sub>6</sub> .....	S21
<b>Figure S34.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>5</b> in DMSO- <i>d</i> <sub>6</sub> . .....	S21
<b>Figure S35.</b> HMBC spectrum of <b>5</b> in DMSO- <i>d</i> <sub>6</sub> .....	S22
<b>Figure S36.</b> HRESIMS spectrum of <b>5</b> .....	S22
<b>Figure S37.</b> <sup>1</sup> H NMR (500 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of <b>6</b> .....	S23
<b>Figure S38.</b> <sup>13</sup> C NMR (125 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of <b>6</b> .....	S23
<b>Figure S39.</b> DEPT (125 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of <b>6</b> .....	S24
<b>Figure S40.</b> HSQC spectrum of <b>6</b> in DMSO- <i>d</i> <sub>6</sub> .....	S24
<b>Figure S41.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>6</b> in DMSO- <i>d</i> <sub>6</sub> . .....	S25
<b>Figure S42.</b> HMBC spectrum of <b>6</b> in DMSO- <i>d</i> <sub>6</sub> .....	S25
<b>Figure S43.</b> HRESIMS spectrum of <b>6</b> .....	S26
<b>Figure S44.</b> <sup>1</sup> H NMR (500 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of <b>7</b> .....	S26
<b>Figure S45.</b> <sup>13</sup> C NMR (125 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of <b>7</b> .....	S27
<b>Figure S46.</b> DEPT (125 MHz, DMSO- <i>d</i> <sub>6</sub> ) spectrum of <b>7</b> .....	S27
<b>Figure S47.</b> HSQC spectrum of <b>7</b> in DMSO- <i>d</i> <sub>6</sub> .....	S28
<b>Figure S48.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>7</b> in DMSO- <i>d</i> <sub>6</sub> . .....	S28
<b>Figure S49.</b> HMBC spectrum of <b>7</b> in DMSO- <i>d</i> <sub>6</sub> .....	S29
<b>Figure S50.</b> NOESY spectrum of <b>7</b> in DMSO- <i>d</i> <sub>6</sub> . .....	S29
<b>Figure S51.</b> HRESIMS spectrum of <b>7</b> .....	S30
<b>Figure S52.</b> HPLC of LDJ-5 crude extract.....	S30
<b>Figure S53.</b> Chiral HPLC analysis of <b>1</b> .....	S31
<b>Figure S54.</b> IR spectrum of <b>1</b> .....	S31
<b>Figure S55.</b> IR spectrum of <b>2</b> .....	S31
<b>Figure S56.</b> IR spectrum of <b>3</b> .....	S32
<b>Figure S57.</b> IR spectrum of <b>4</b> .....	S32

<b>Figure S58.</b> IR spectrum of <b>5</b> .....	S32
<b>Figure S59.</b> IR spectrum of <b>6</b> .....	S33
<b>Figure S60.</b> IR spectrum of <b>7</b> .....	S33
<b>Table S1.</b> Antimicrobial activity of <b>1-7</b> .....	S33

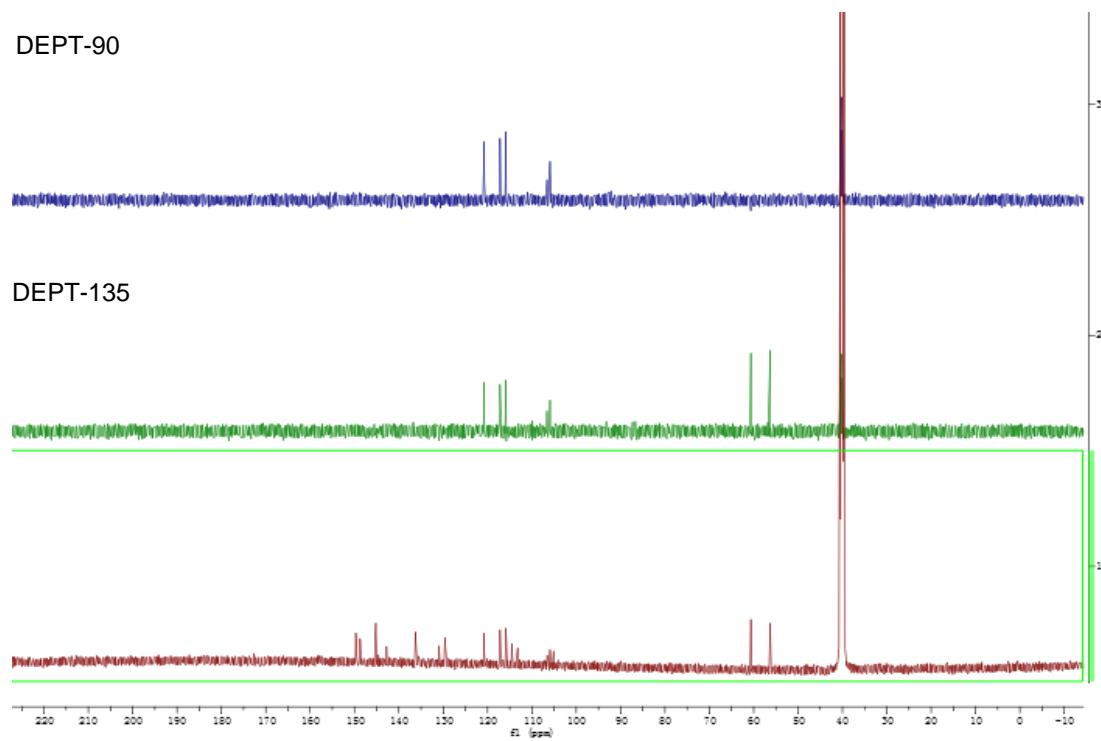
**Figure S1.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of **1**.



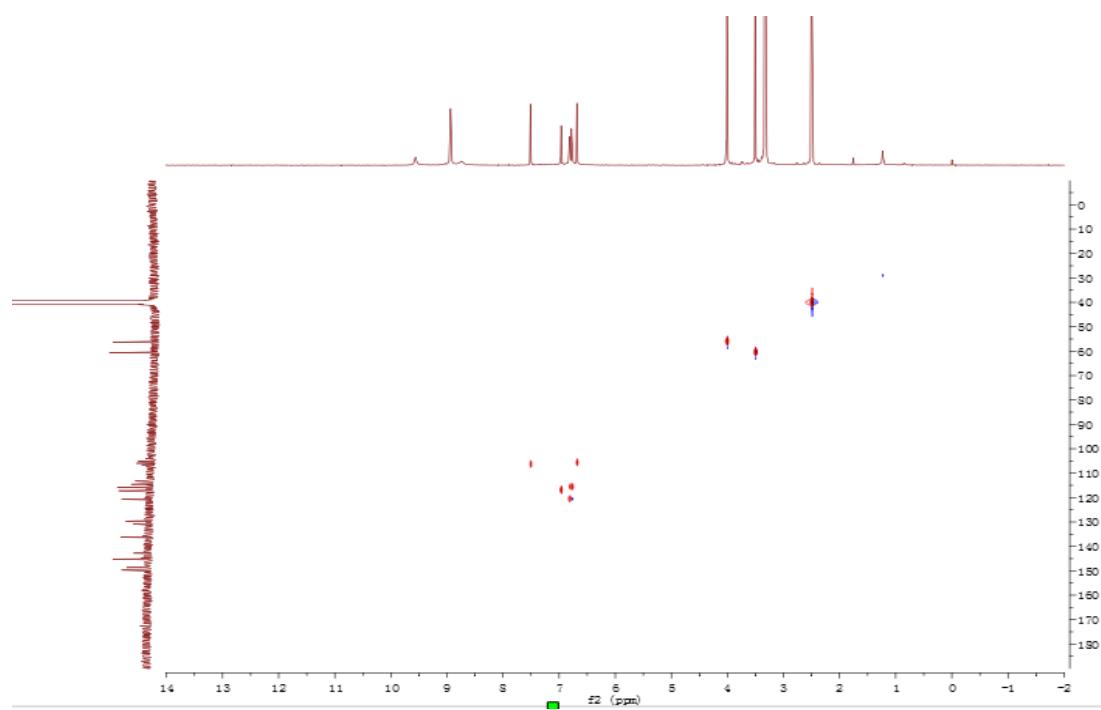
**Figure S2.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) spectrum of **1**.



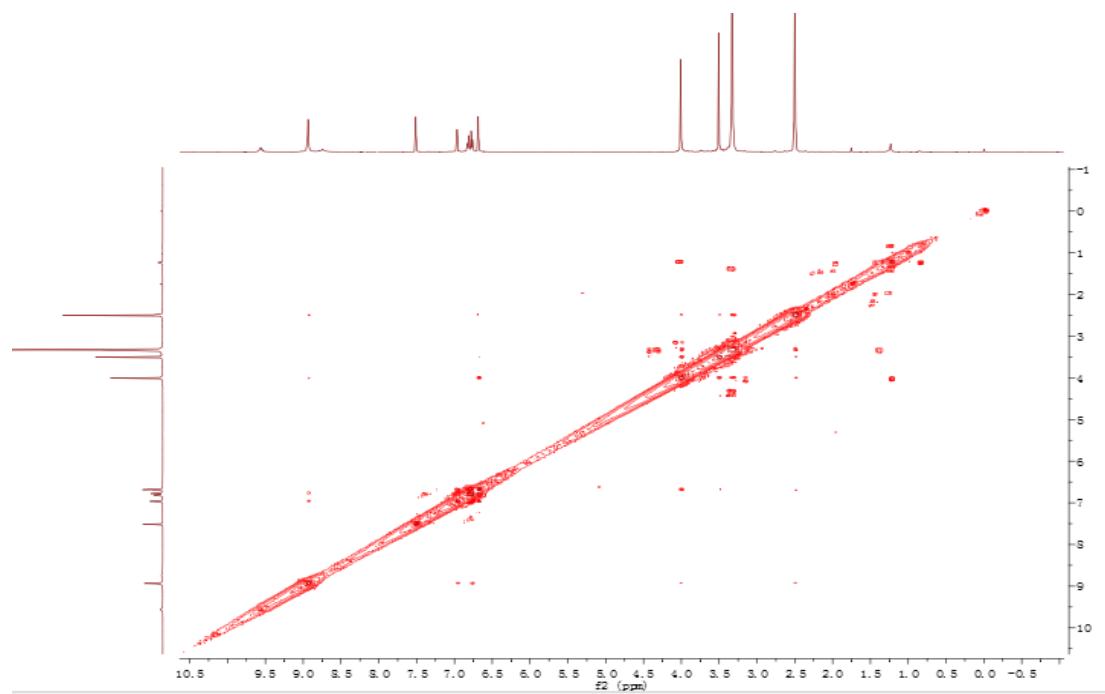
**Figure S3.** DEPT (125 MHz, DMSO-*d*<sub>6</sub>) spectrum of **1**.



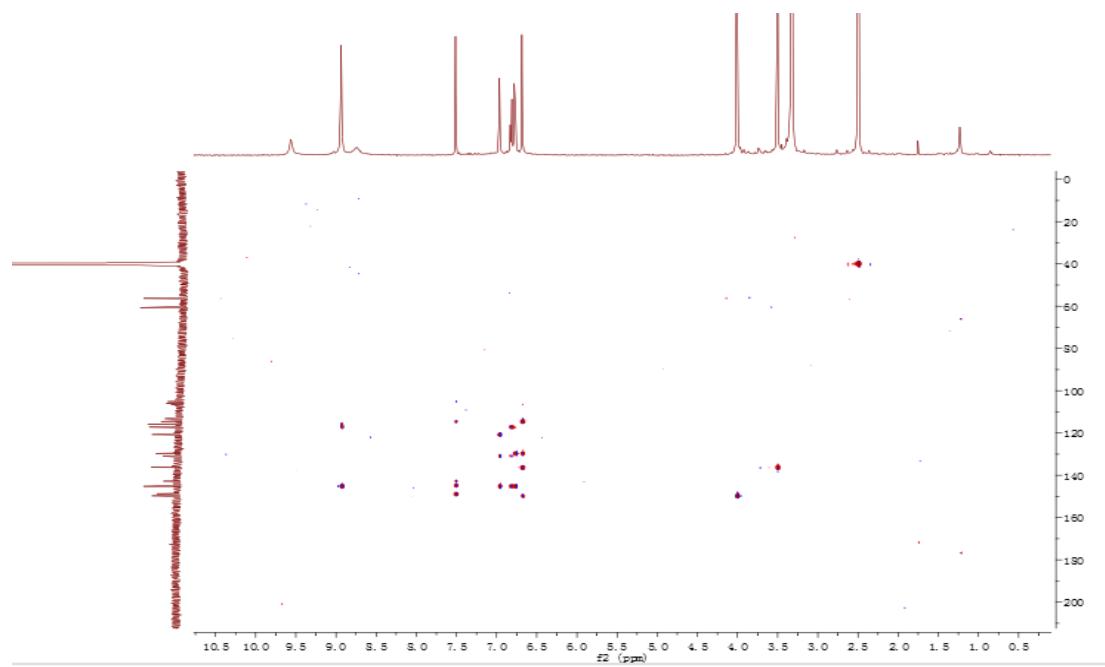
**Figure S4.** HSQC spectrum of **1** in DMSO-*d*<sub>6</sub>.



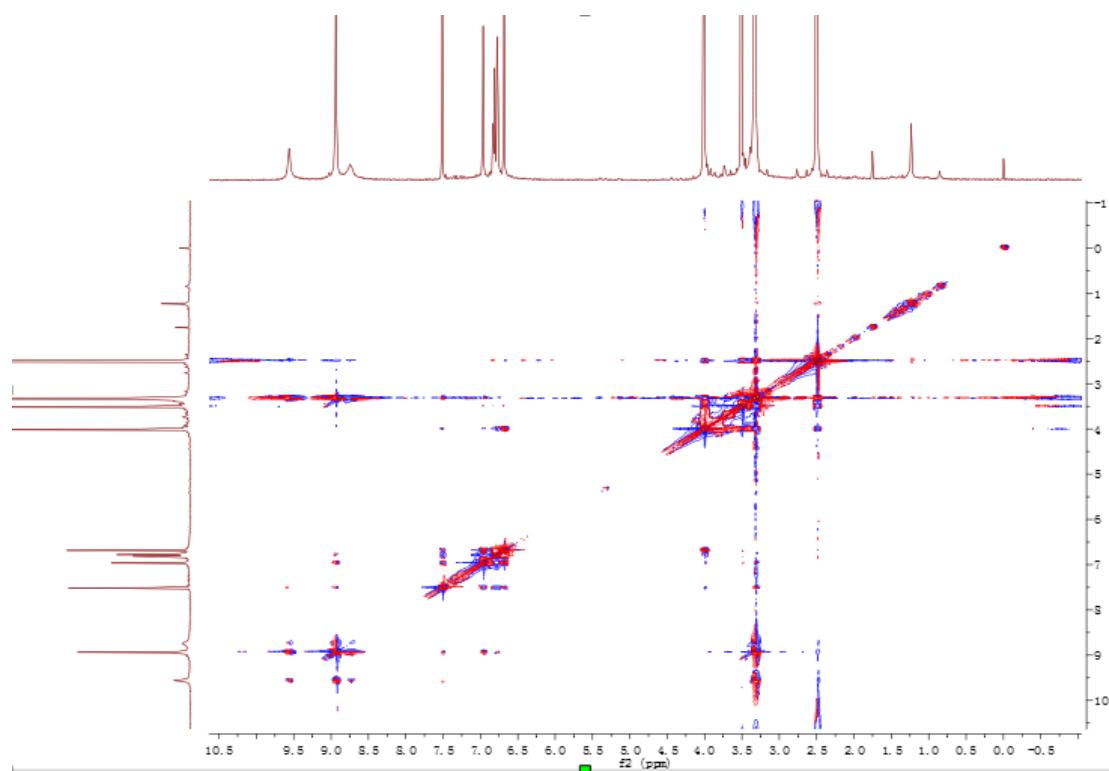
**Figure S5.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in  $\text{DMSO}-d_6$ .



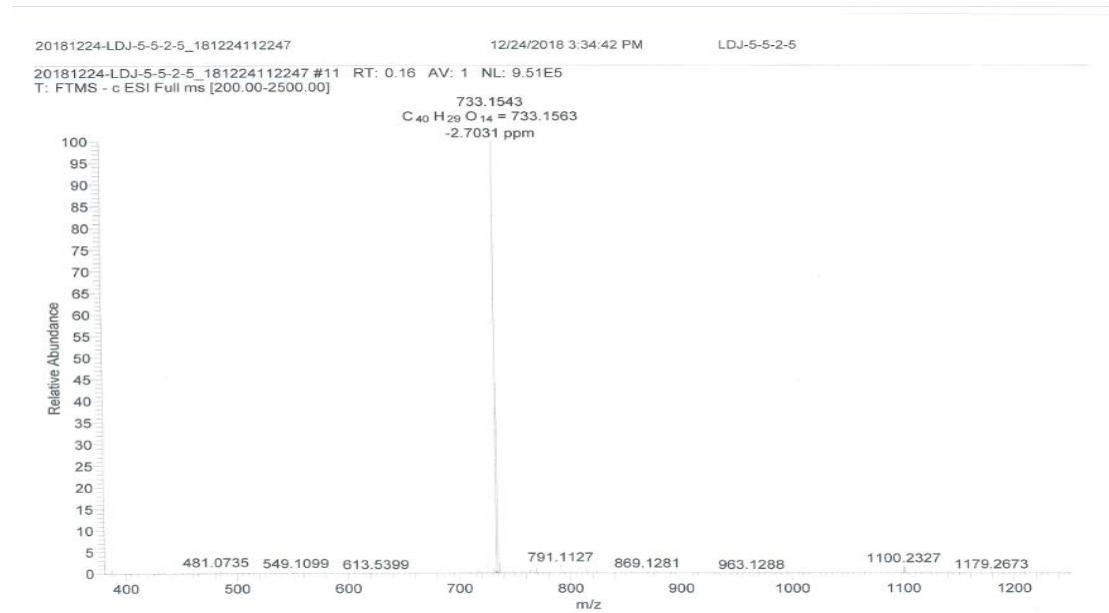
**Figure S6.** HMBC spectrum of **1** in  $\text{DMSO}-d_6$ .



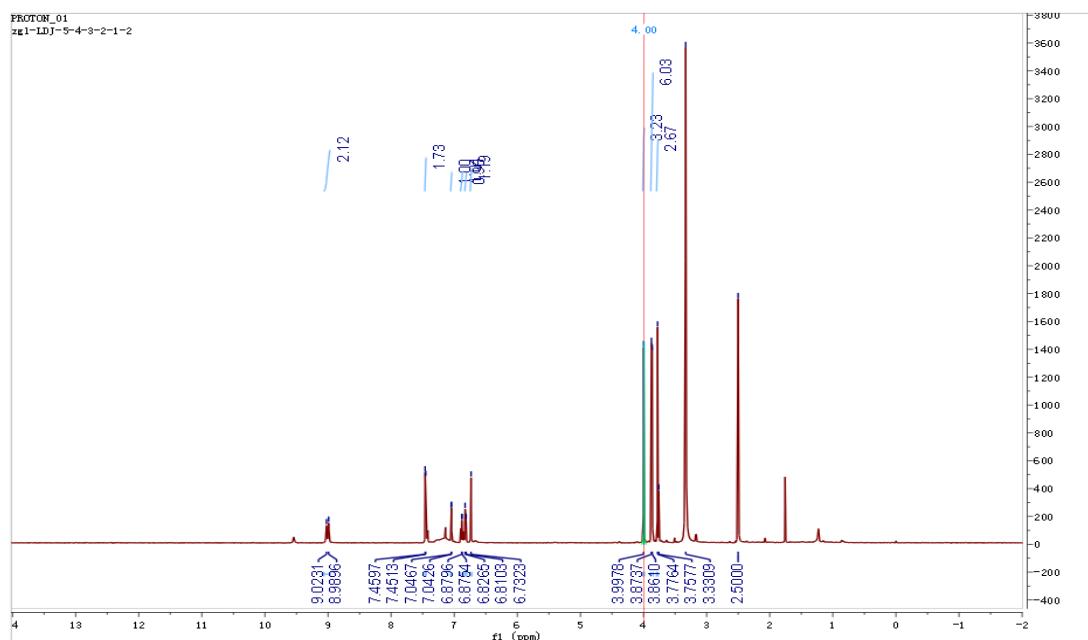
**Figure S7.** NOESY spectrum of **1** in DMSO-*d*<sub>6</sub>.



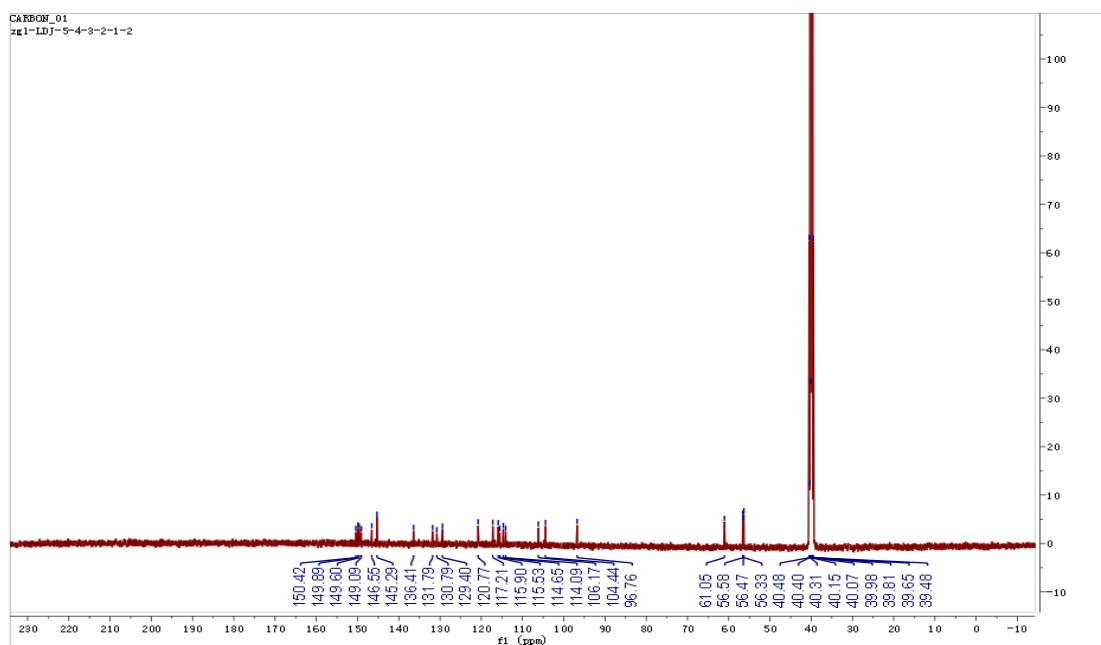
**Figure S8.** HRESIMS spectrum of **1**.



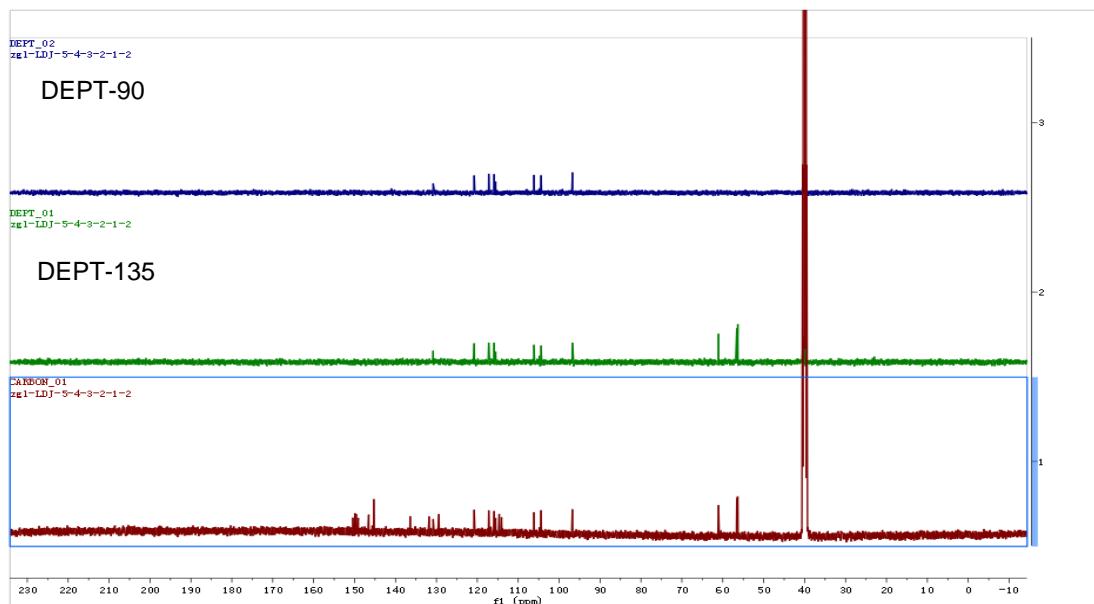
**Figure S9.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of **2**.



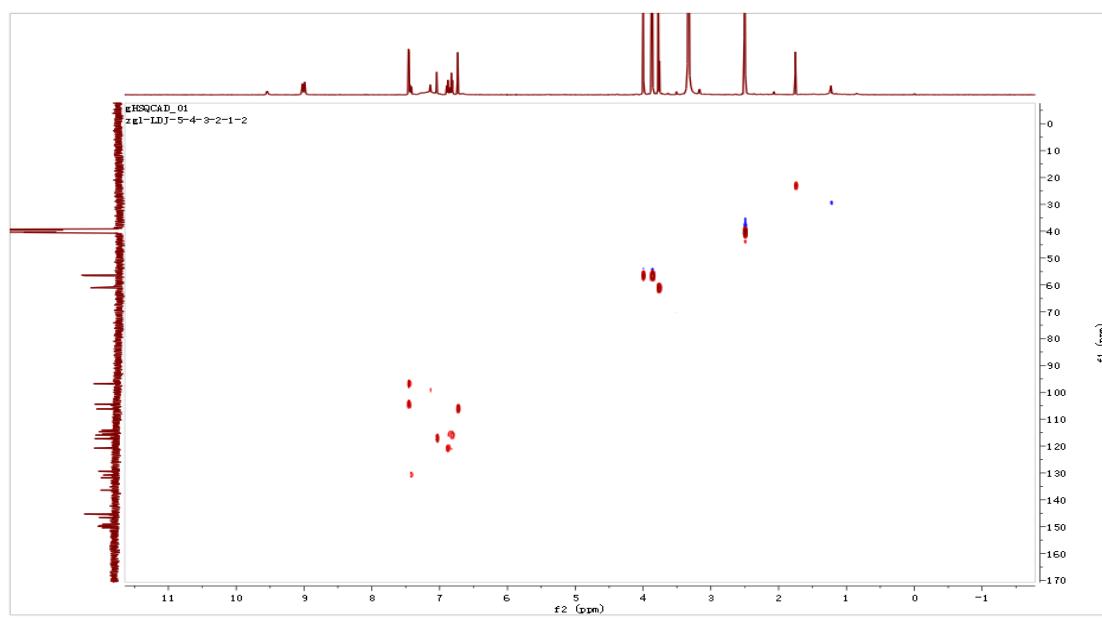
**Figure S10.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) spectrum of **2**.



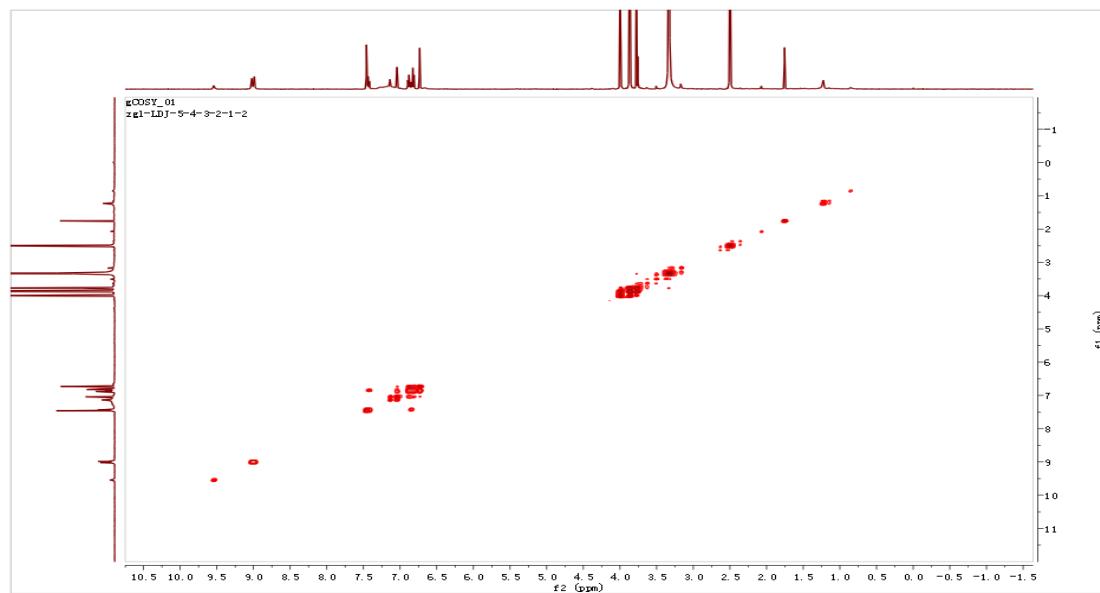
**Figure S11.** DEPT (125 MHz, DMSO-*d*<sub>6</sub>) spectrum of **2**.



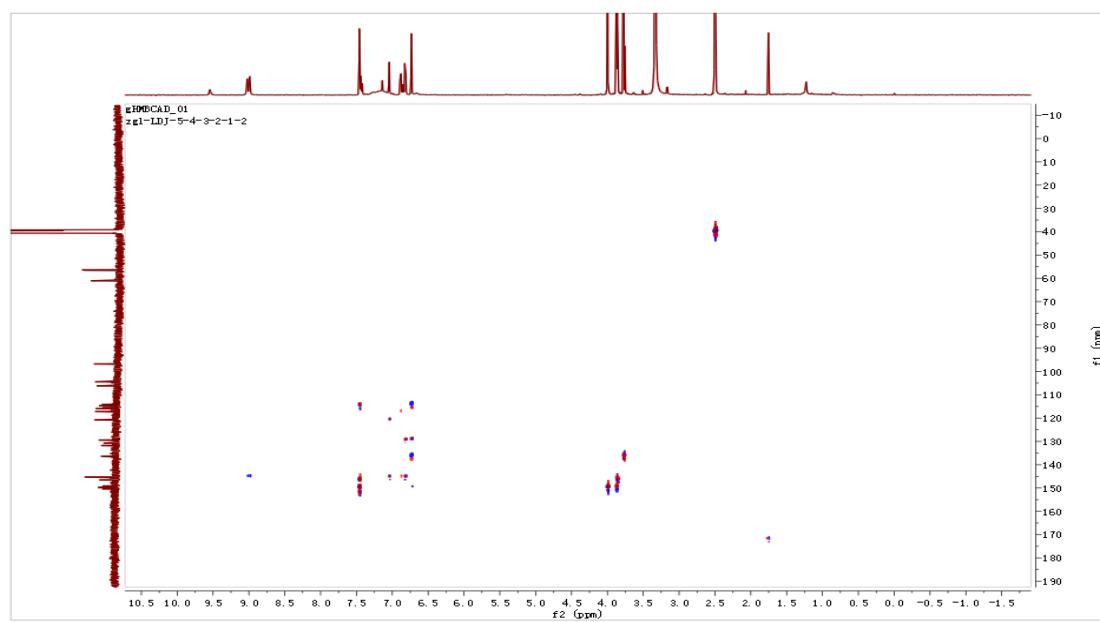
**Figure S12.** HSQC spectrum of **2** in DMSO-*d*<sub>6</sub>.



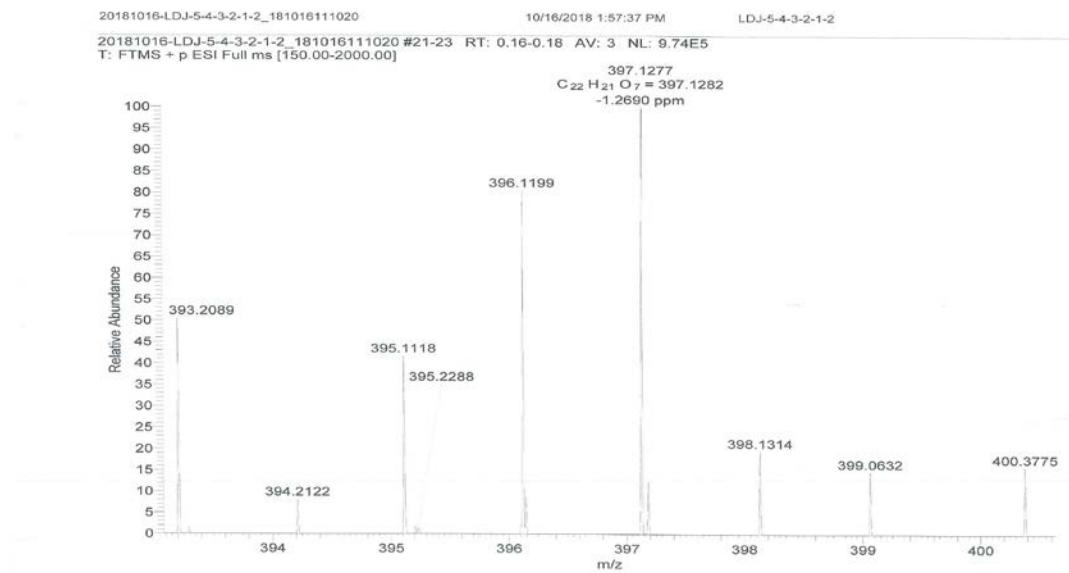
**Figure S13.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in  $\text{DMSO}-d_6$ .



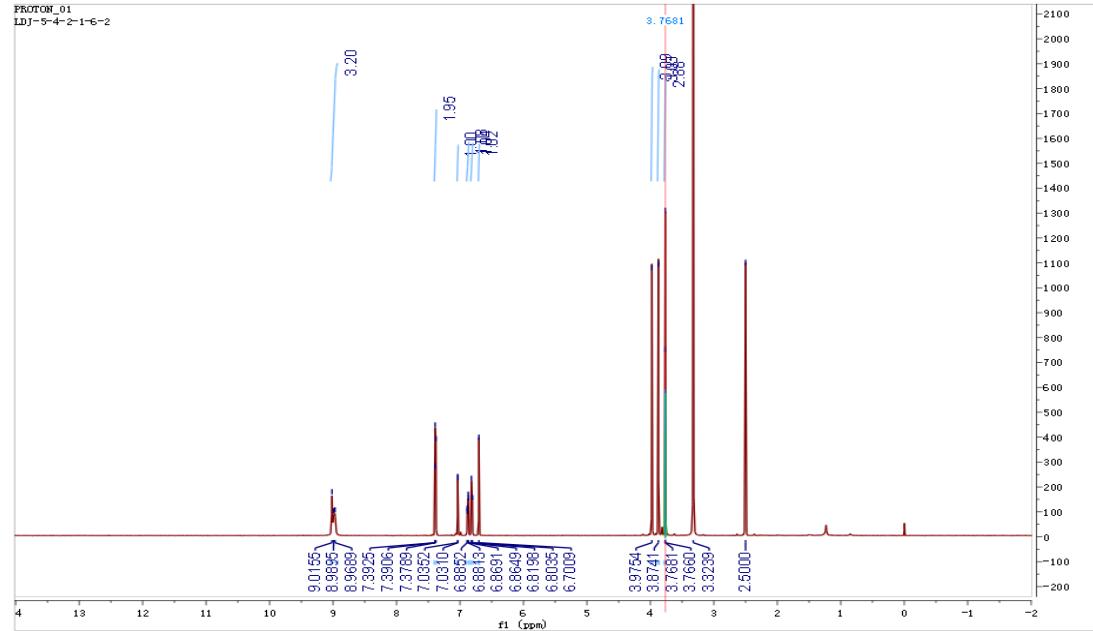
**Figure S14.** HMBC spectrum of **2** in  $\text{DMSO}-d_6$ .



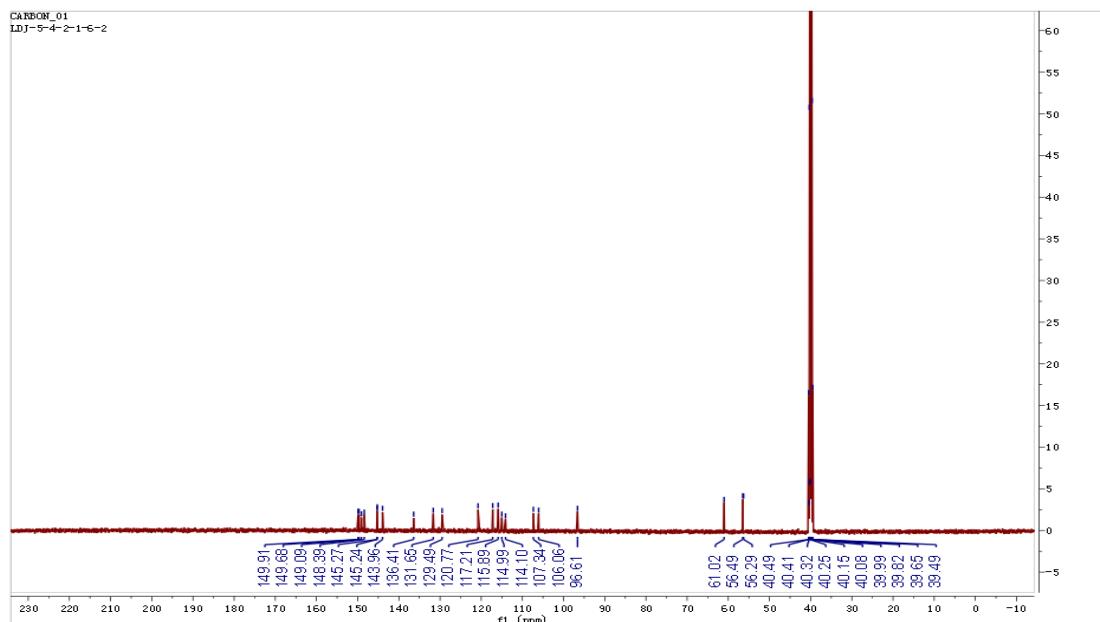
**Figure S15.** HRESIMS spectrum of **2**.



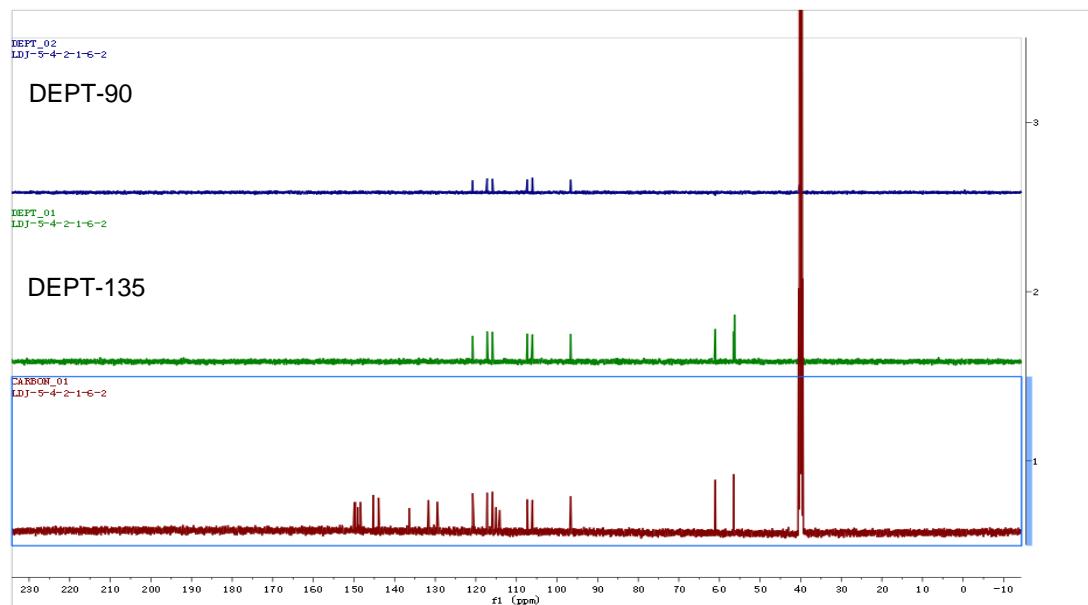
**Figure S16.**  $^1H$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of **3**.



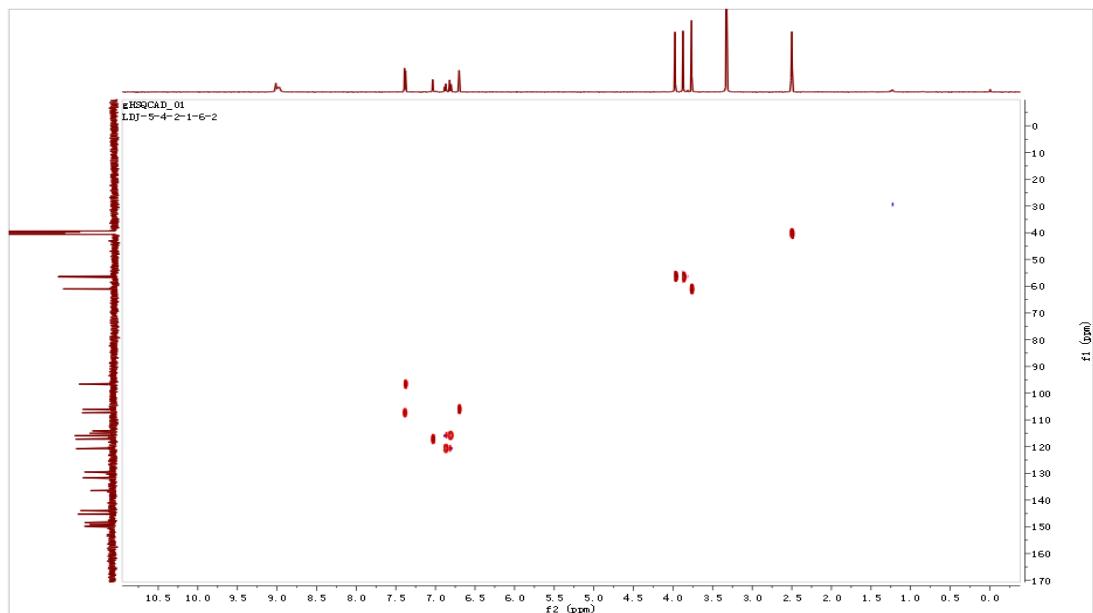
**Figure S17.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) spectrum of **3**.



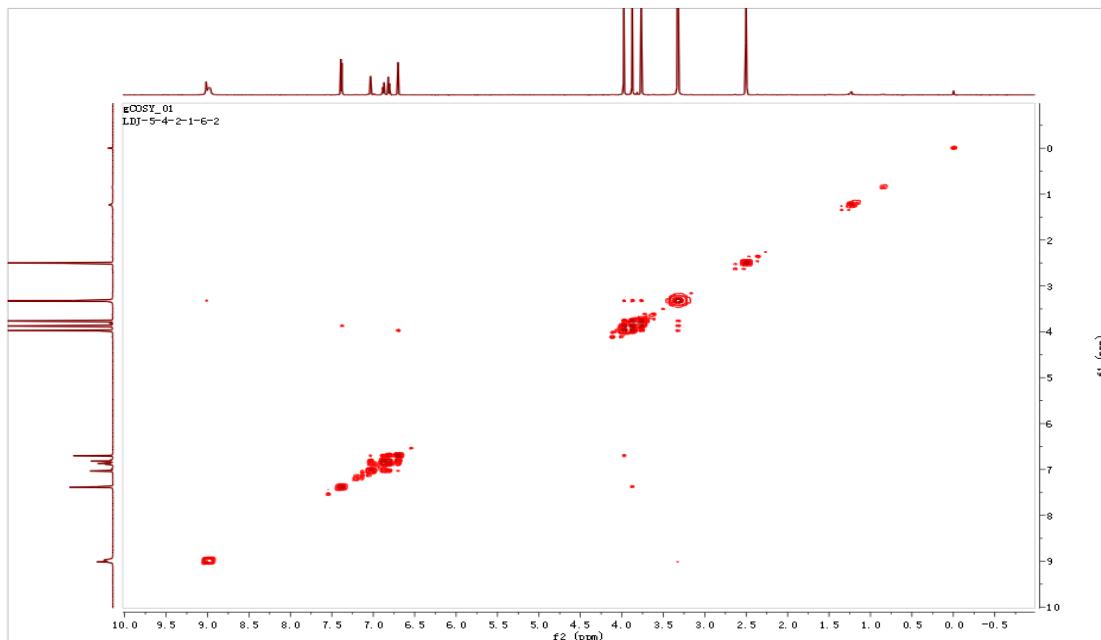
**Figure S18.** DEPT (125 MHz, DMSO- $d_6$ ) spectrum of **3**.



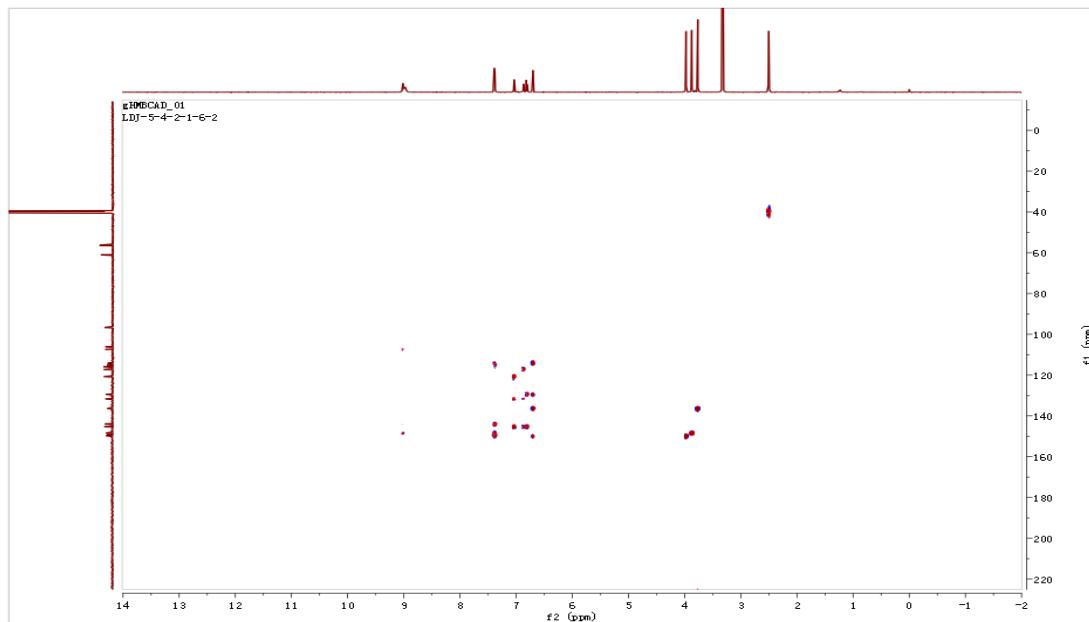
**Figure S19.** HSQC spectrum of **3** in DMSO-*d*<sub>6</sub>.



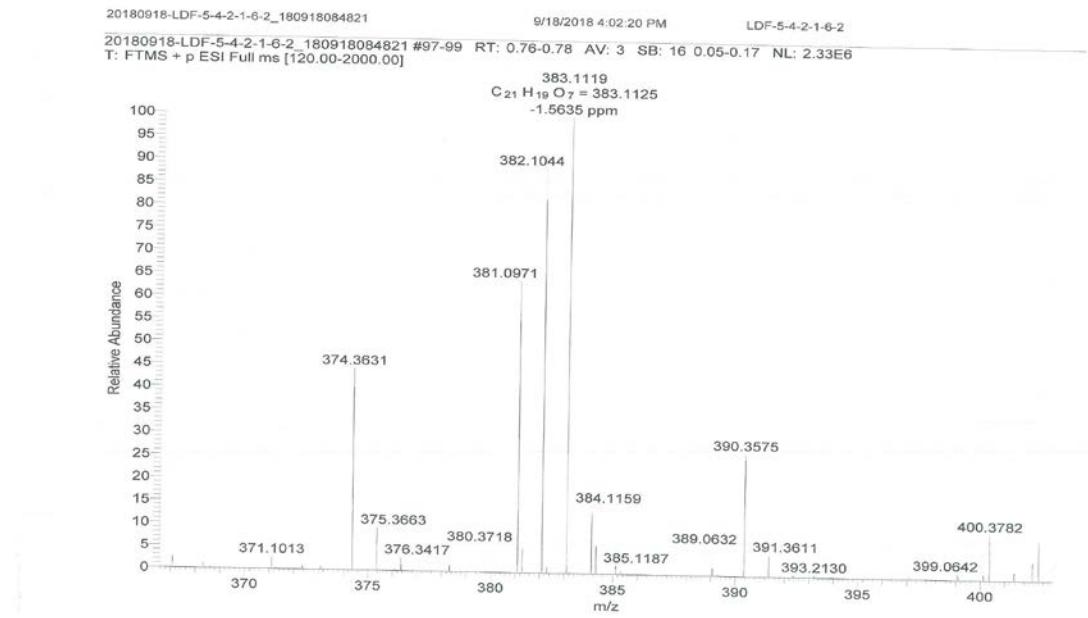
**Figure S20.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **3** in DMSO-*d*<sub>6</sub>.



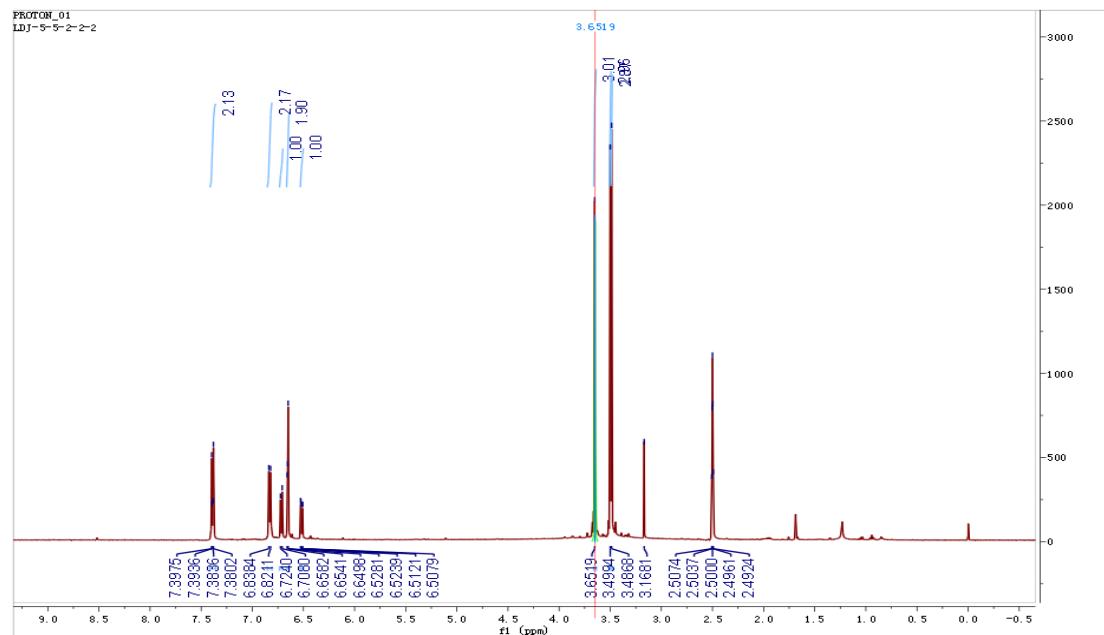
**Figure S21.** HMBC spectrum of **3** in DMSO-*d*<sub>6</sub>.



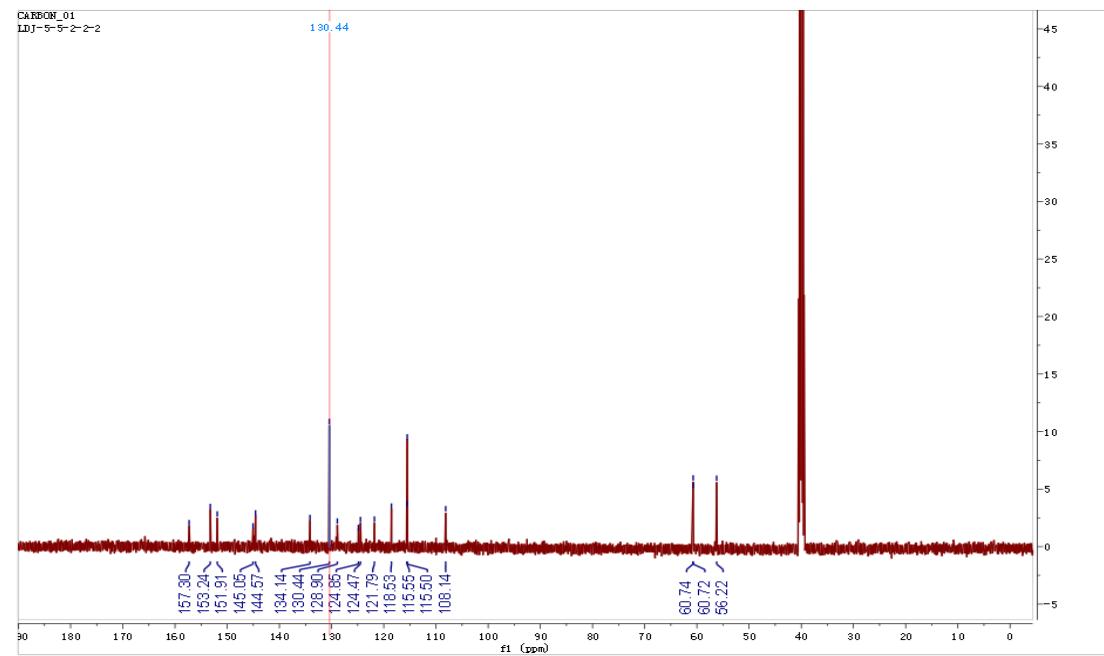
**Figure S22.** HRESIMS spectrum of **3**.



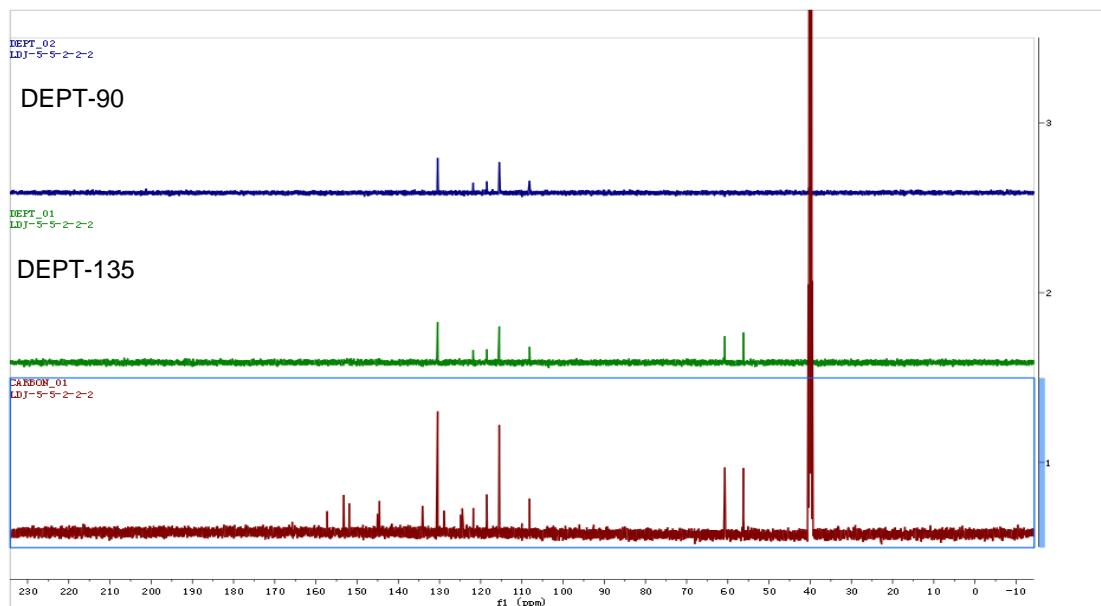
**Figure S23.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of **4**.



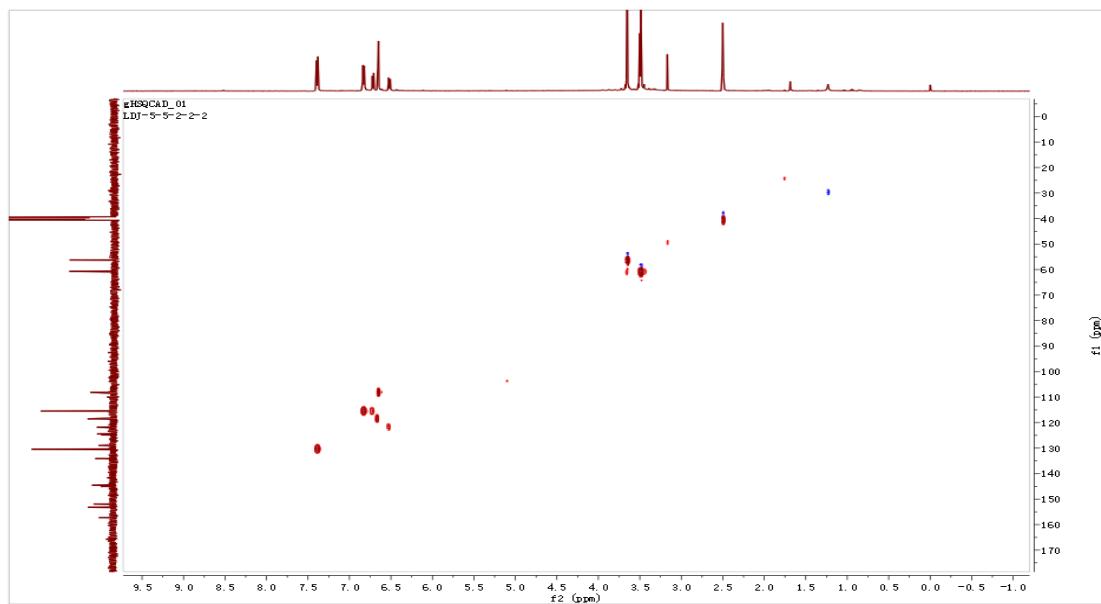
**Figure S24.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO}-d_6$ ) spectrum of **4**.



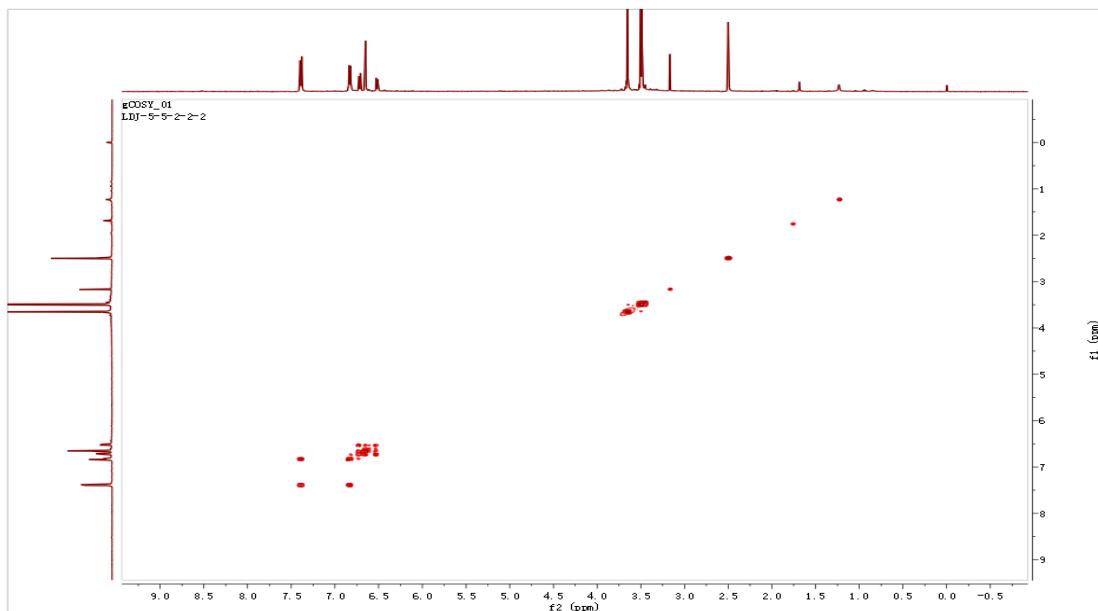
**Figure S25.** DEPT (125 MHz, DMSO-*d*<sub>6</sub>) spectrum of **4**.



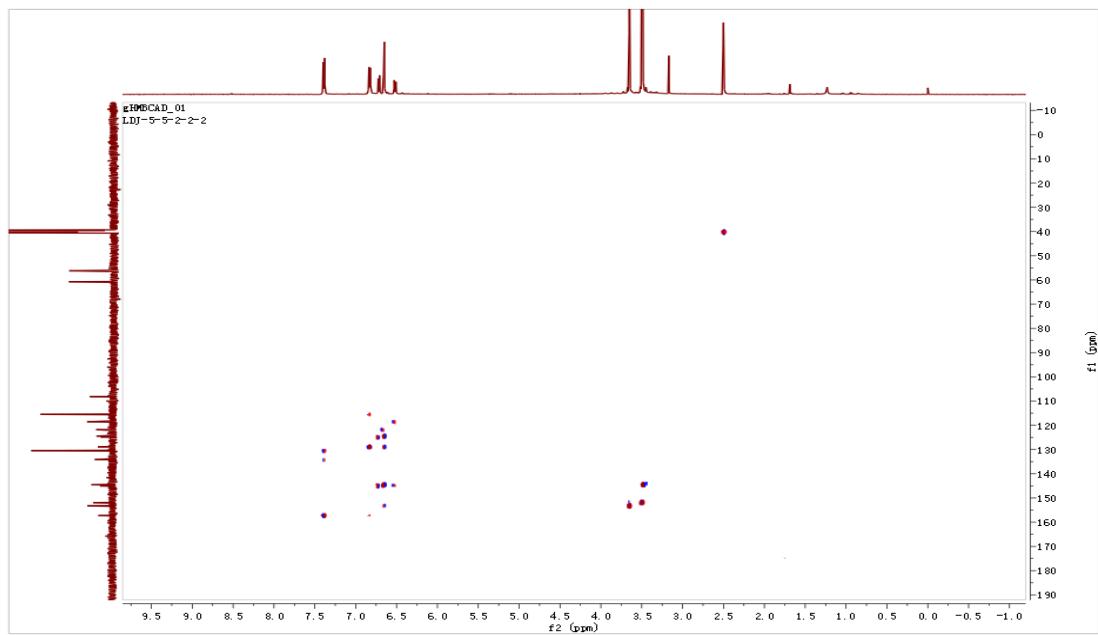
**Figure S26.** HSQC spectrum of **4** in DMSO-*d*<sub>6</sub>.



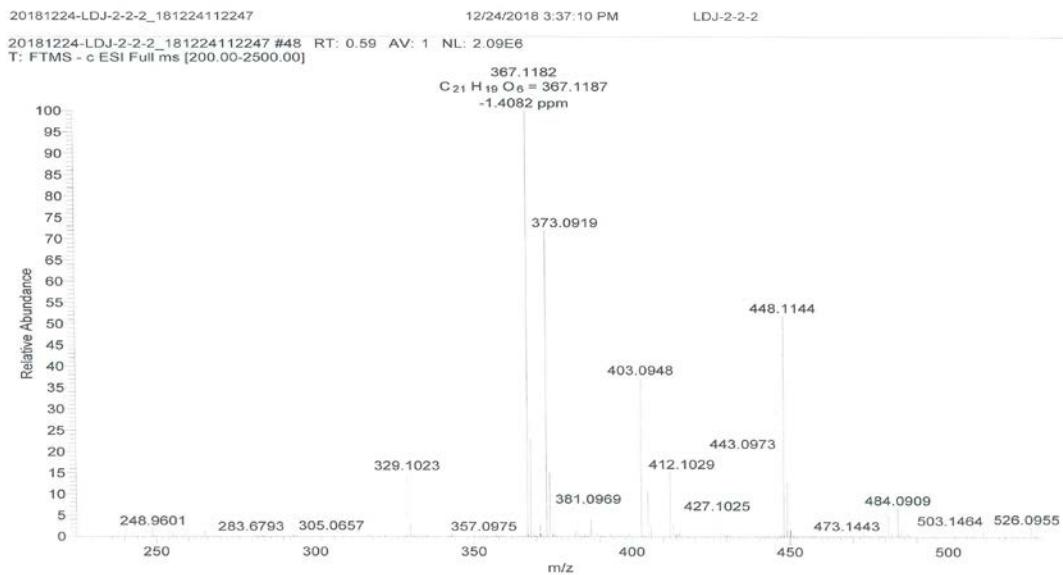
**Figure S27.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4** in  $\text{DMSO}-d_6$ .



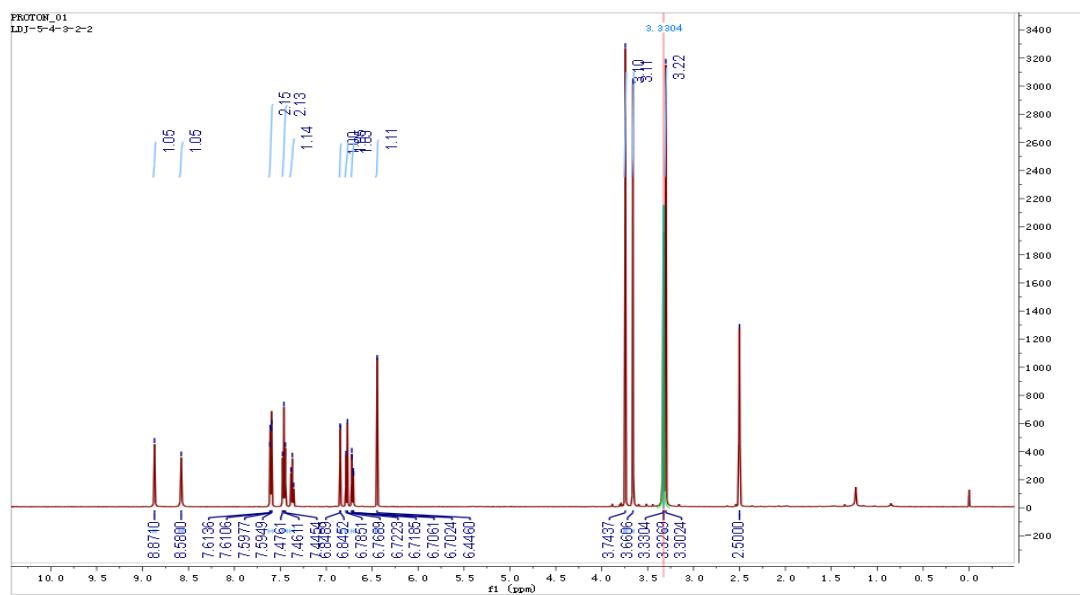
**Figure S28.** HMBC spectrum of **4** in  $\text{DMSO}-d_6$ .



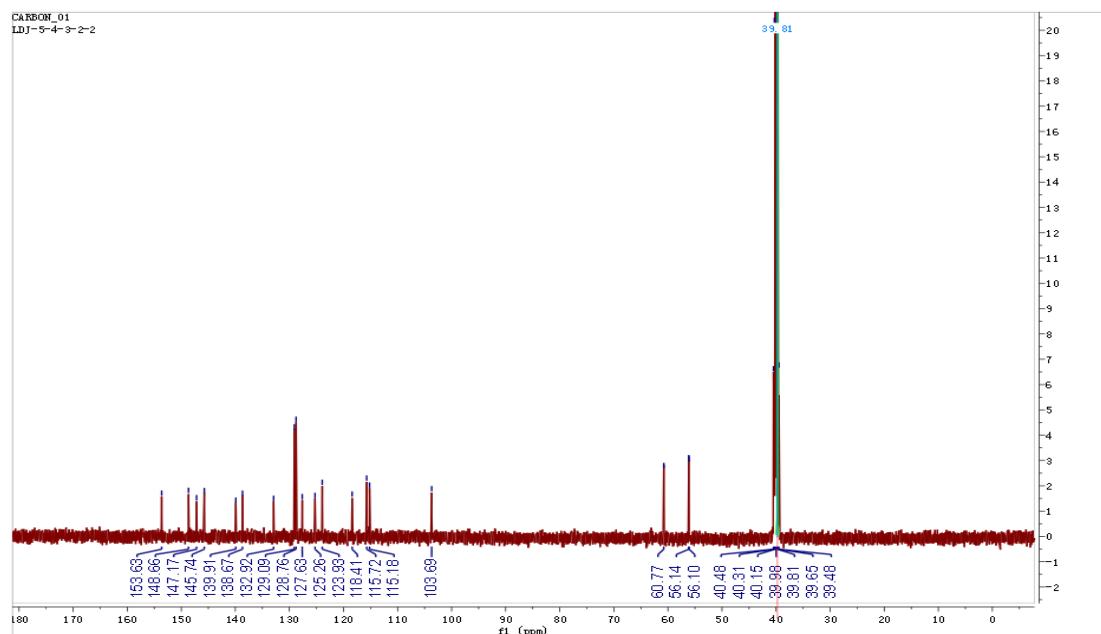
**Figure S29.** HRESIMS spectrum of **4**.



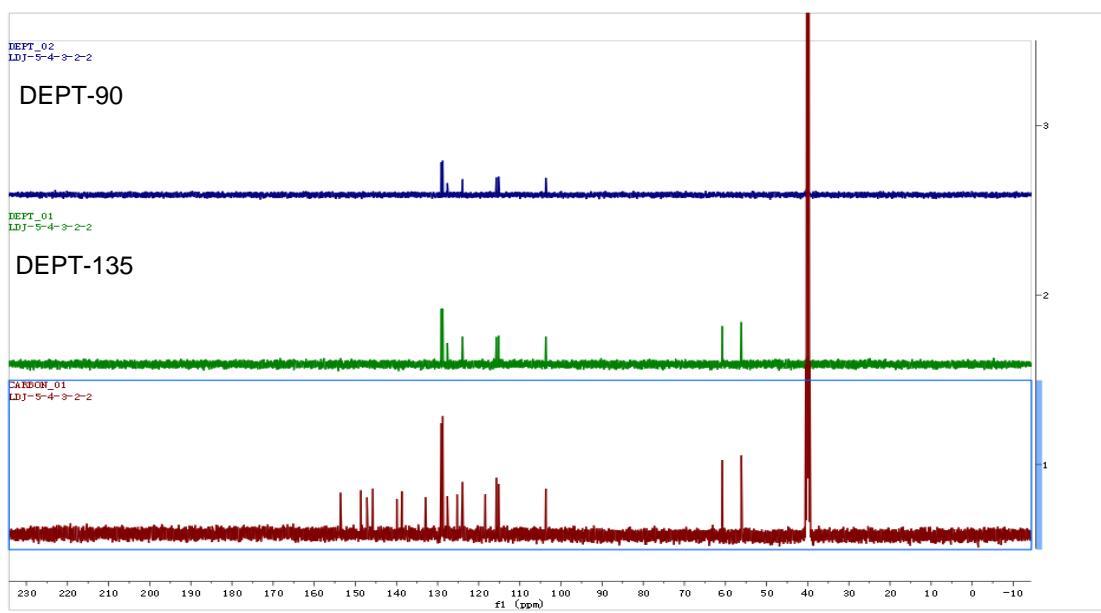
**Figure S30.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of 5.



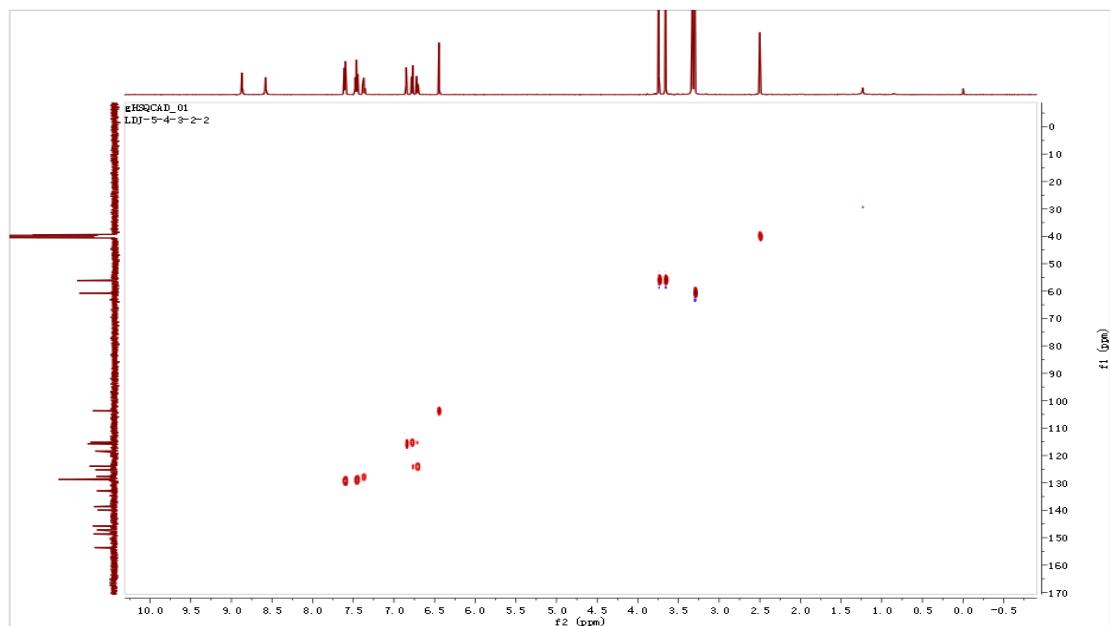
**Figure S31.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) spectrum of **5**.



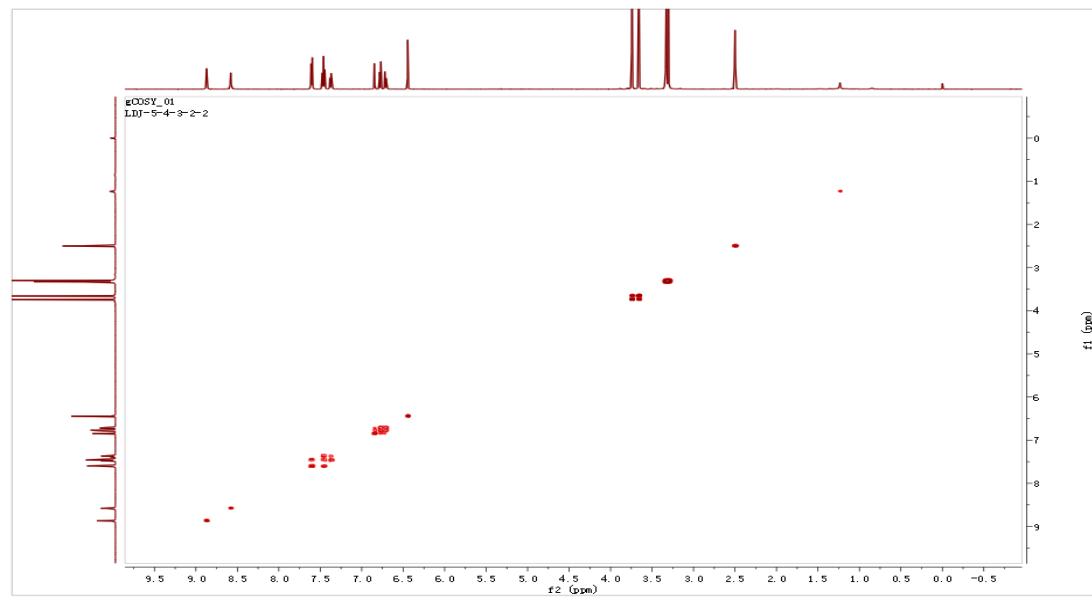
**Figure S32.** DEPT (125 MHz, DMSO- $d_6$ ) spectrum of **5**.



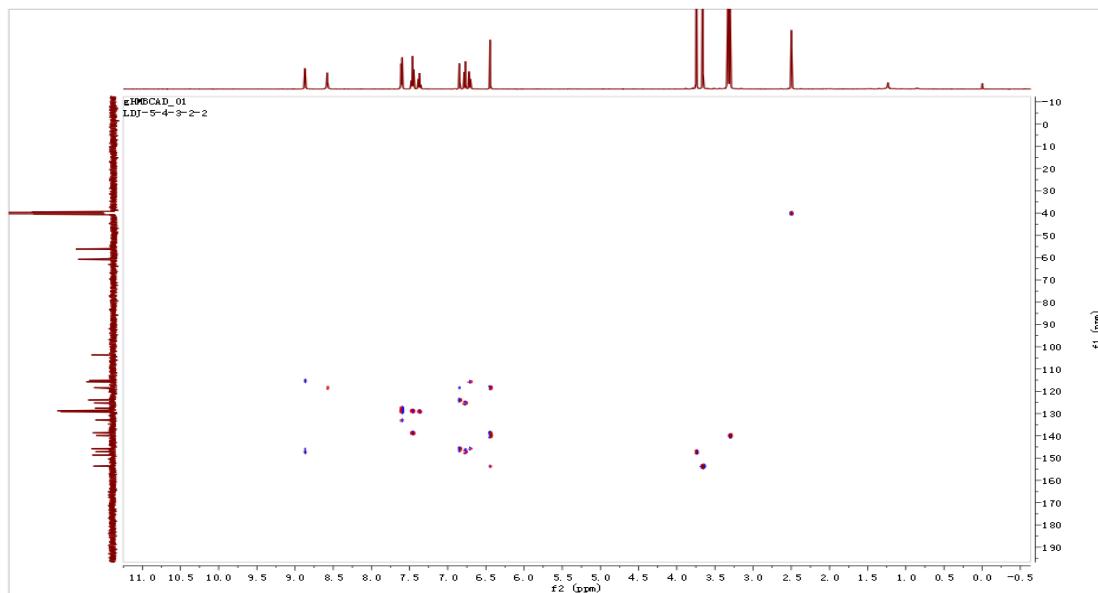
**Figure S33.** HSQC spectrum of **5** in DMSO-*d*<sub>6</sub>.



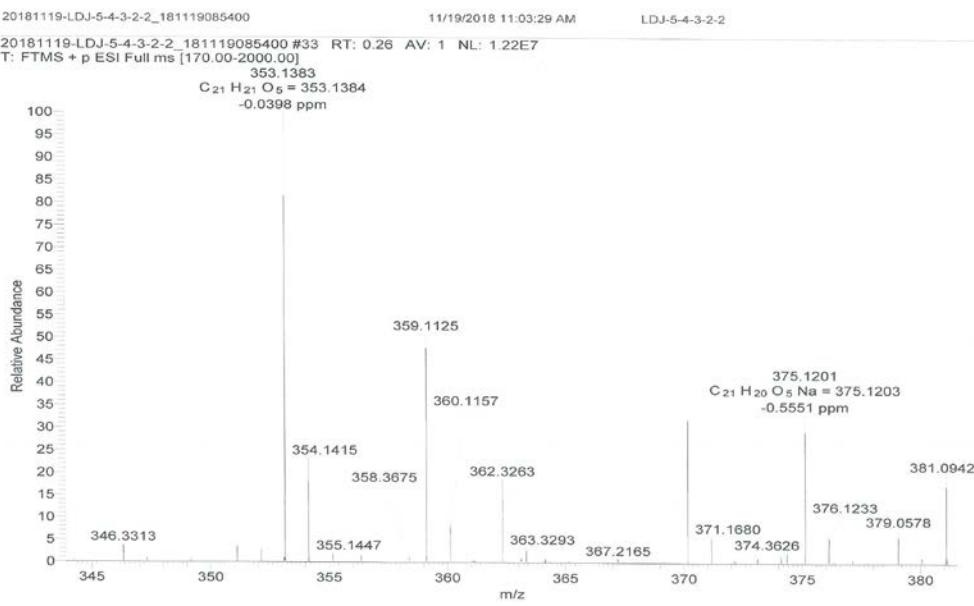
**Figure S34.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **5** in DMSO-*d*<sub>6</sub>.



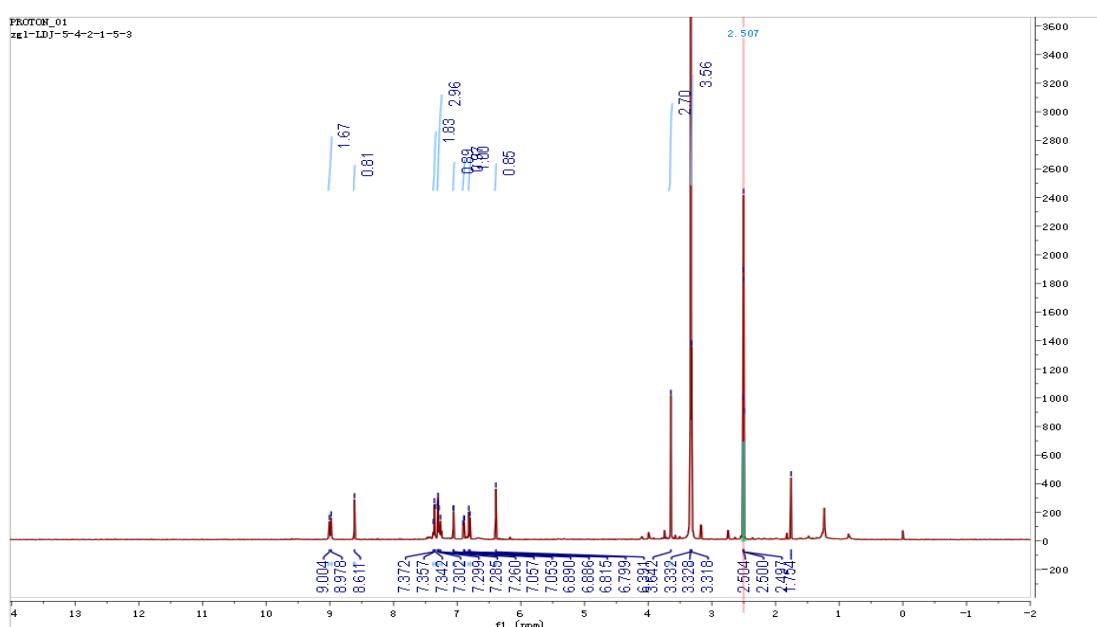
**Figure S35.** HMBC spectrum of **5** in DMSO-*d*<sub>6</sub>.



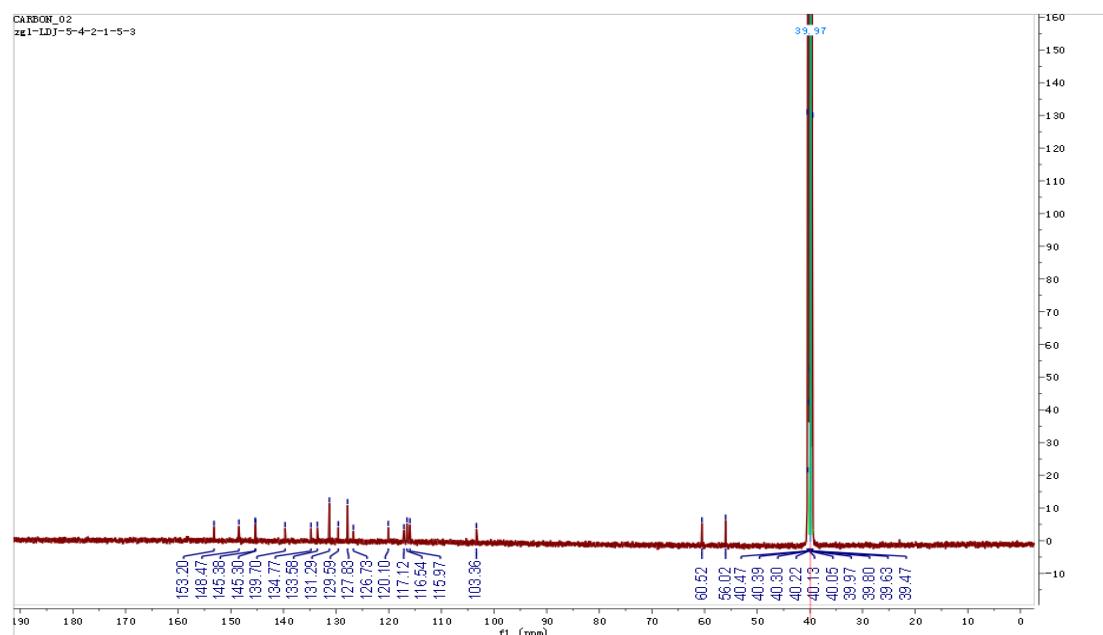
**Figure S36.** HRESIMS spectrum of **5**.



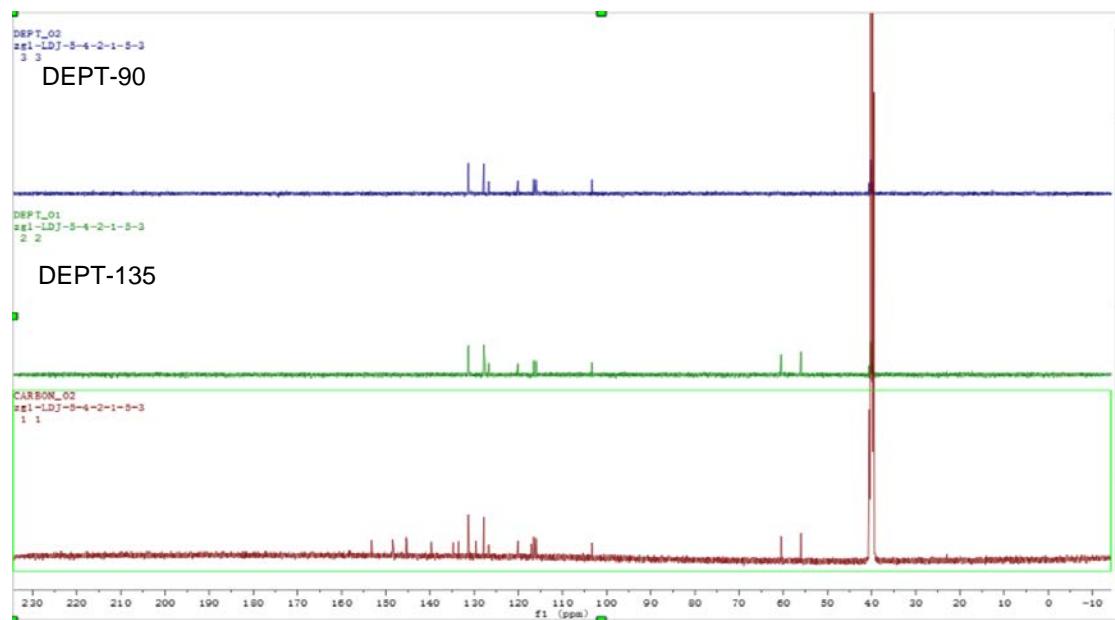
**Figure S37.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of **6**.



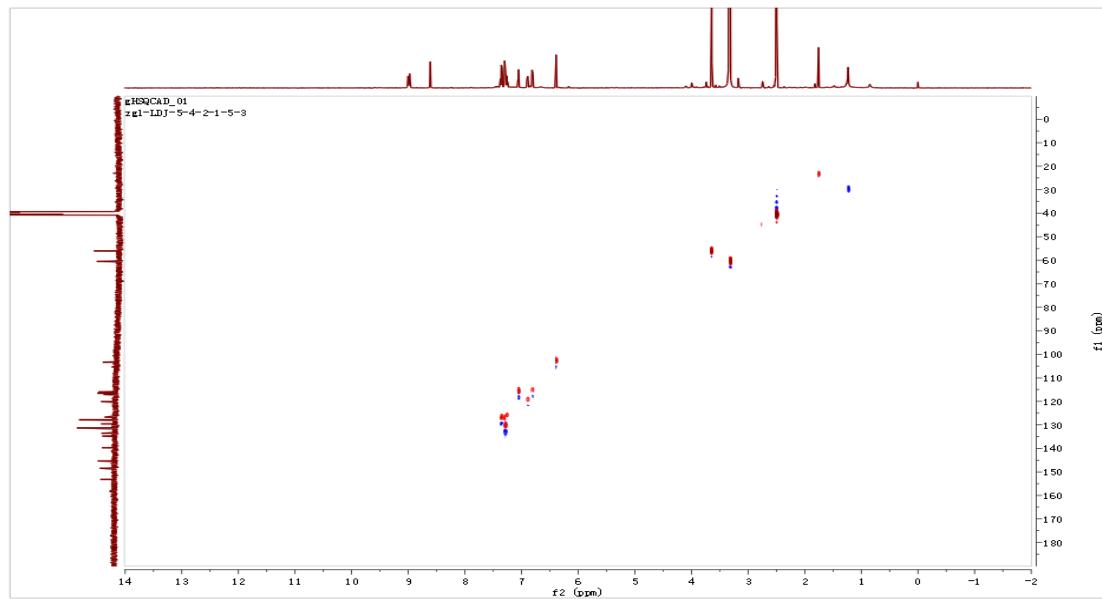
**Figure S38.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) spectrum of **6**.



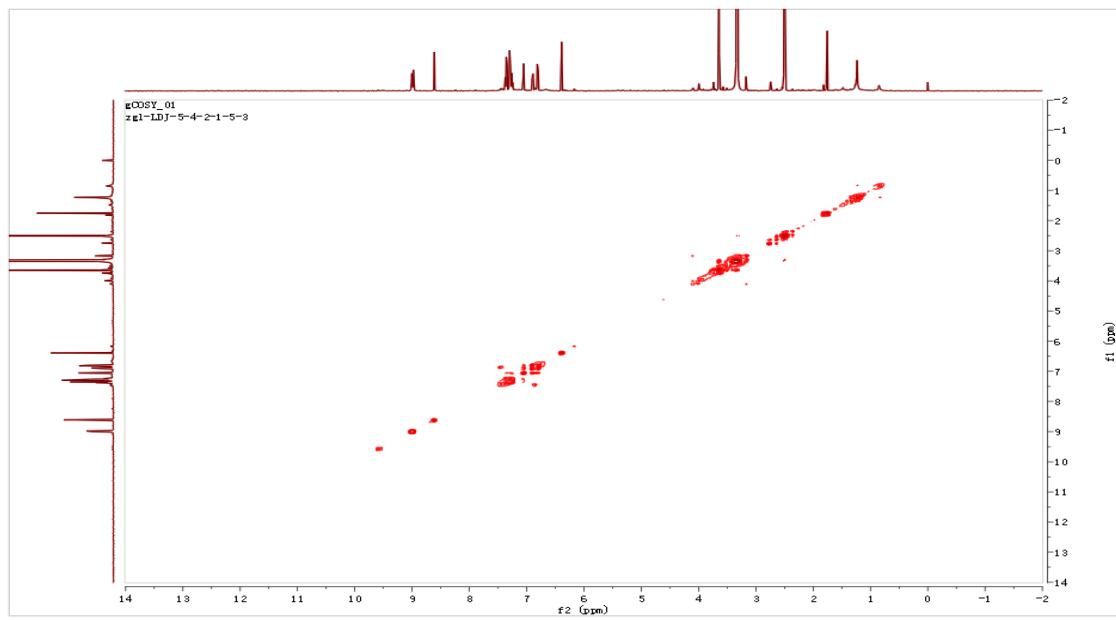
**Figure S39.** DEPT (125 MHz, DMSO-*d*<sub>6</sub>) spectrum of **6**.



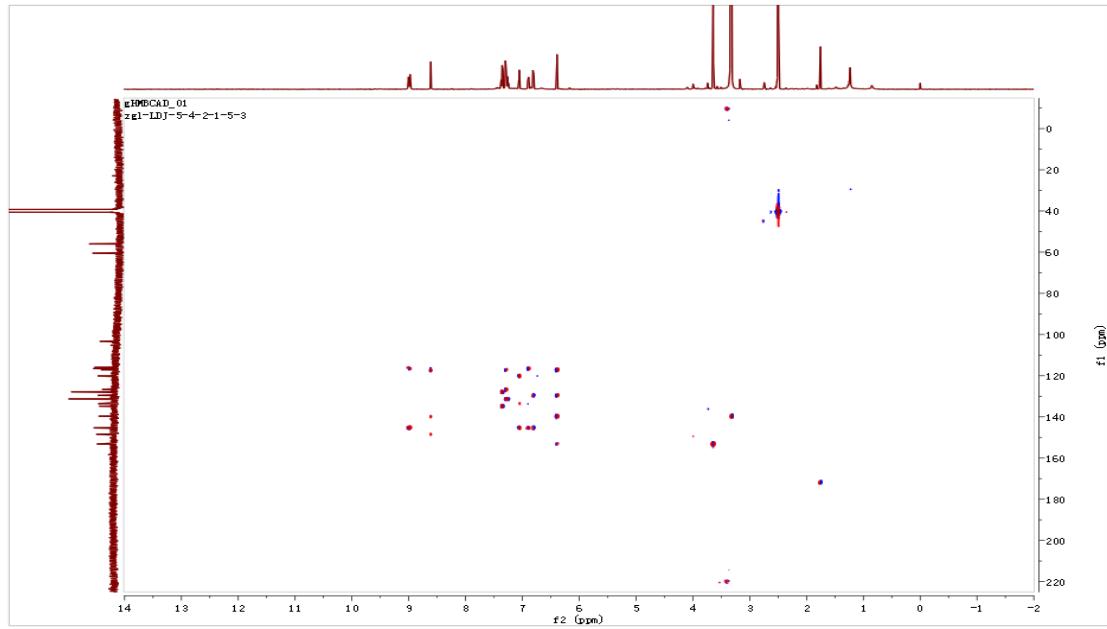
**Figure S40.** HSQC spectrum of **6** in DMSO-*d*<sub>6</sub>.



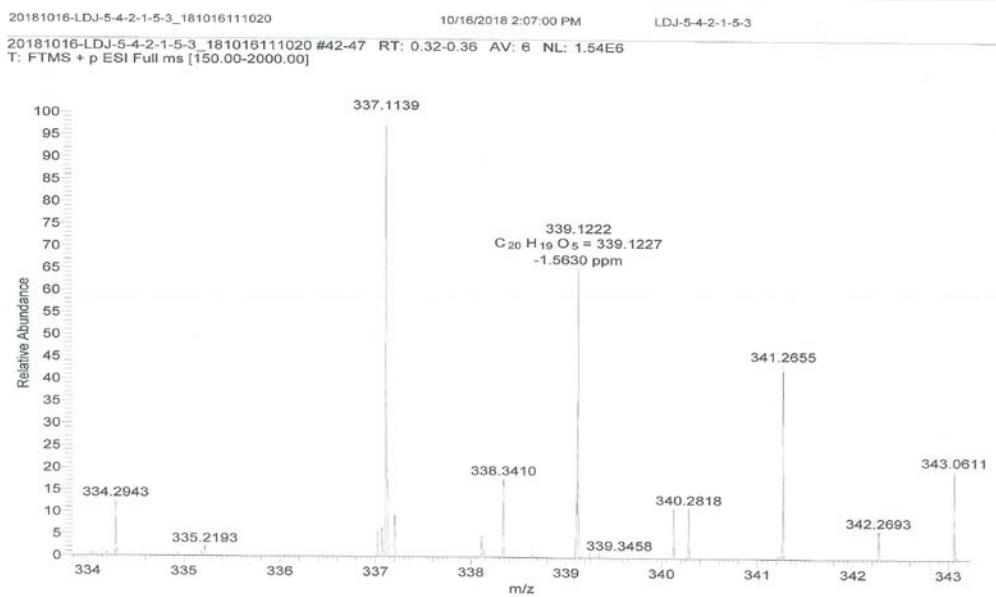
**Figure S41.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **6** in  $\text{DMSO}-d_6$ .



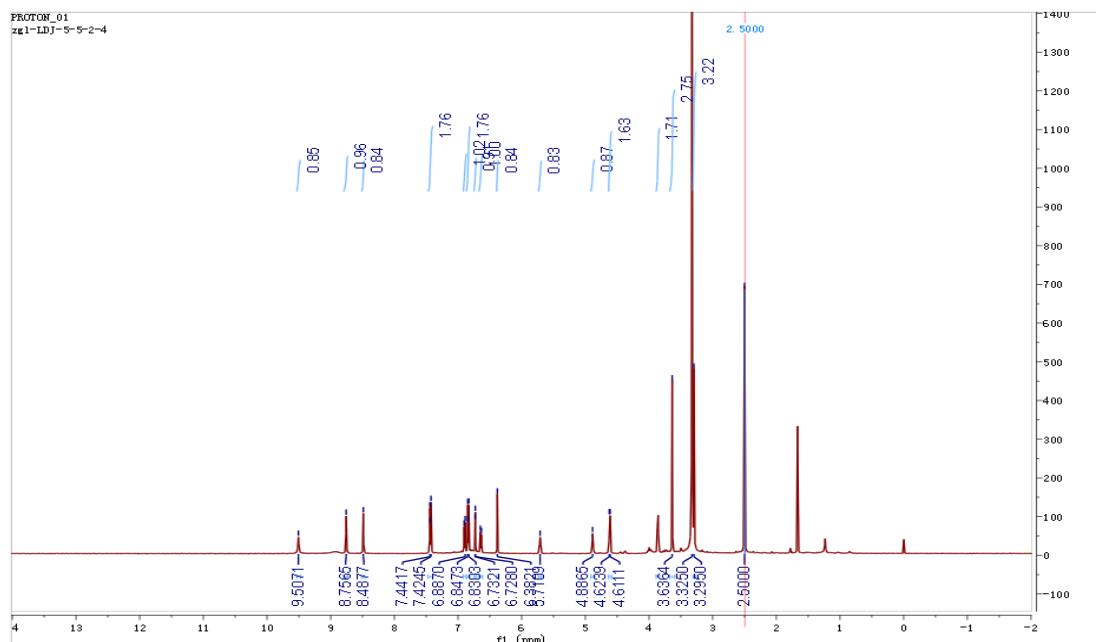
**Figure S42.** HMBC spectrum of **6** in  $\text{DMSO}-d_6$ .



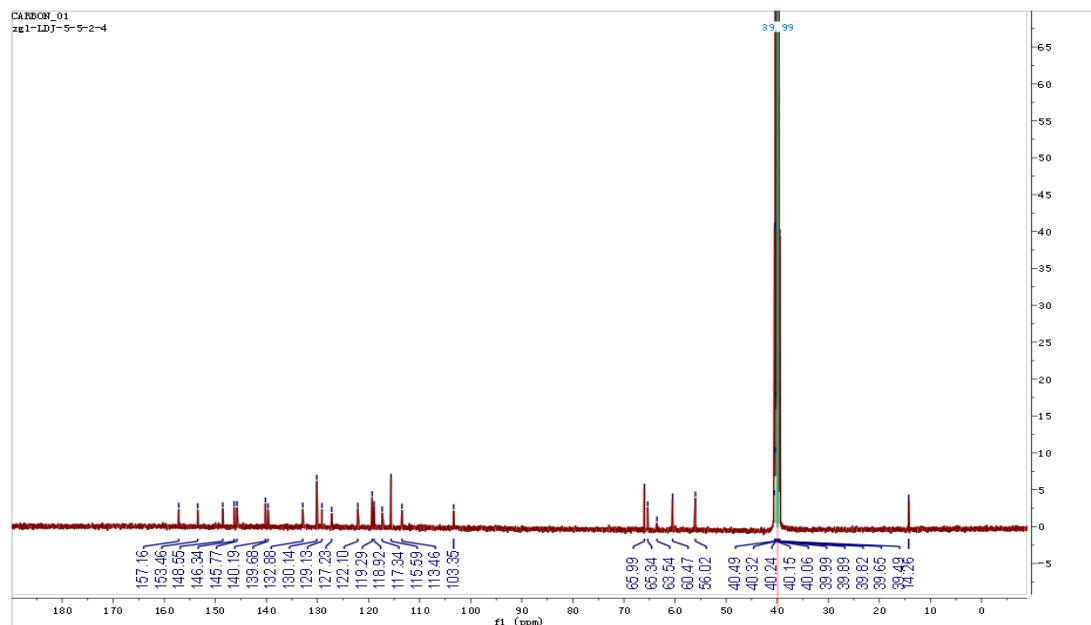
**Figure S43.** HRESIMS spectrum of **6**.



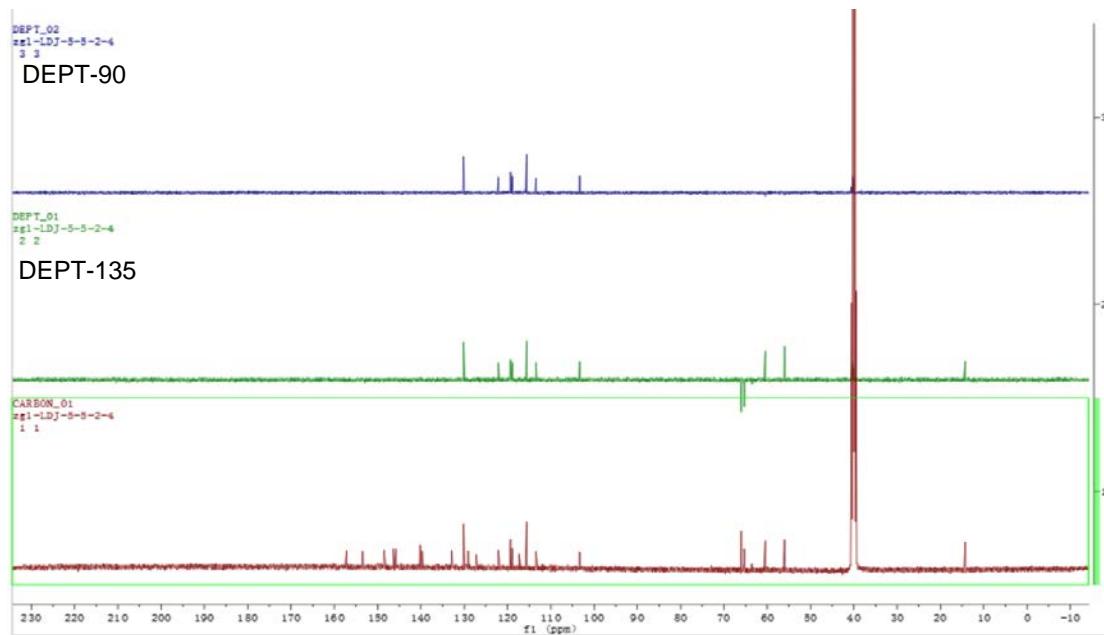
**Figure S44.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of **7**.



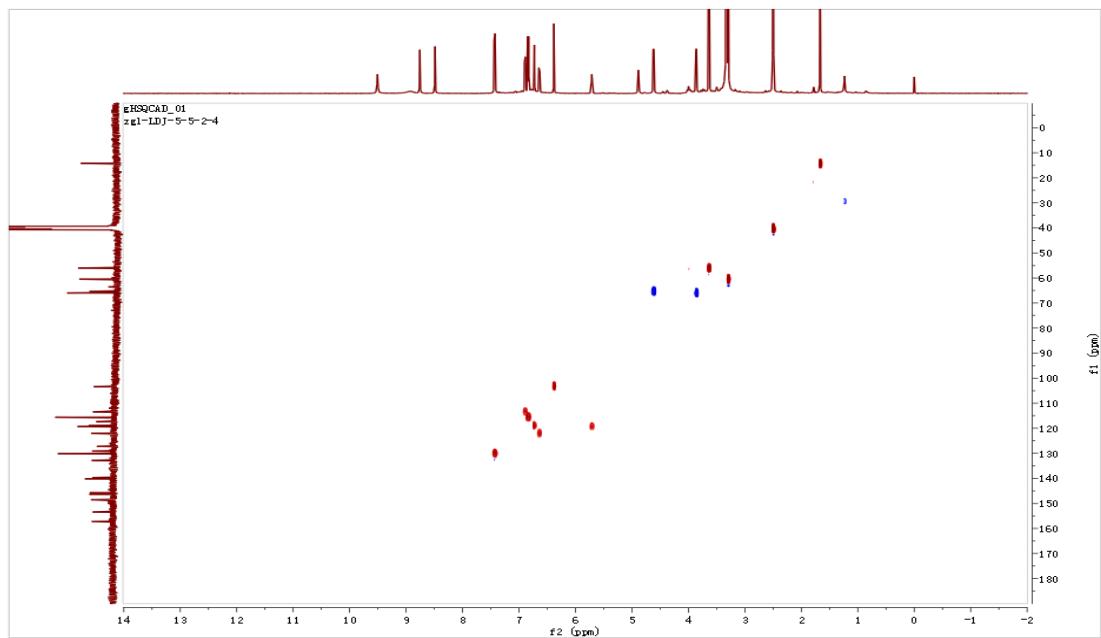
**Figure S45.**  $^{13}\text{C}$  NMR (125 MHz, DMSO-d<sub>6</sub>) spectrum of **7**.



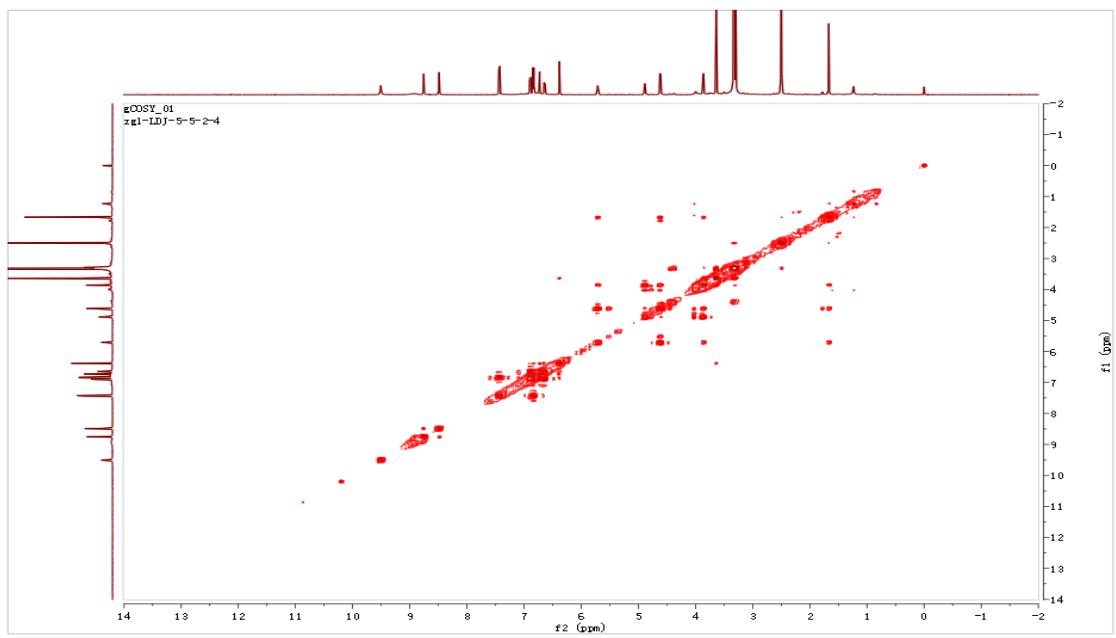
**Figure S46.** DEPT (125 MHz, DMSO-d<sub>6</sub>) spectrum of **7**.



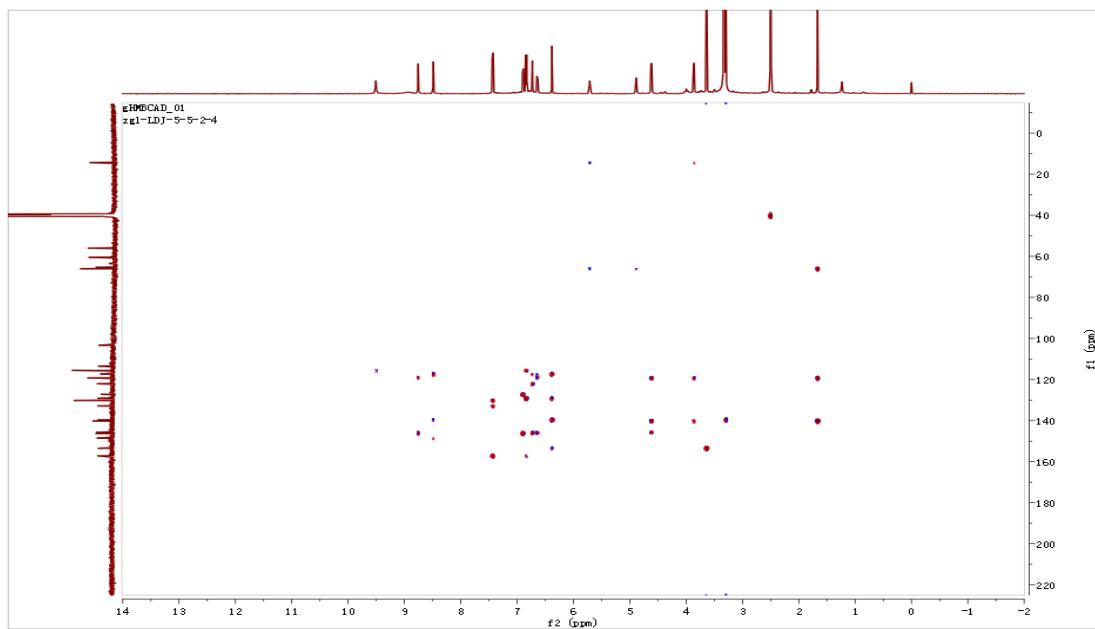
**Figure S47.** HSQC spectrum of **7** in DMSO-*d*<sub>6</sub>.



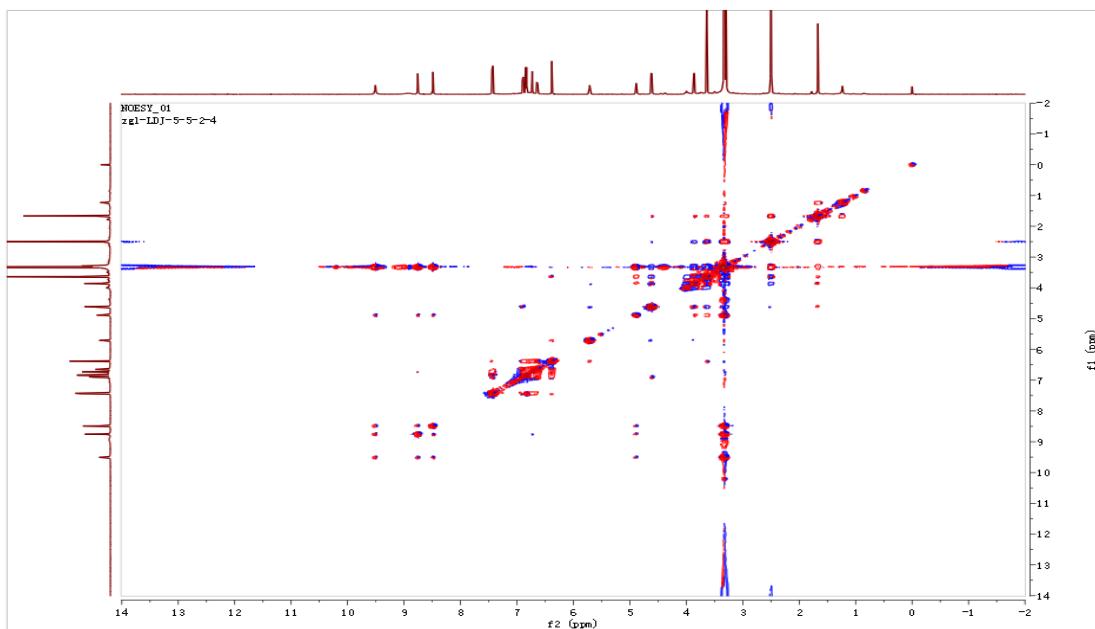
**Figure S48.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **7** in DMSO-*d*<sub>6</sub>.



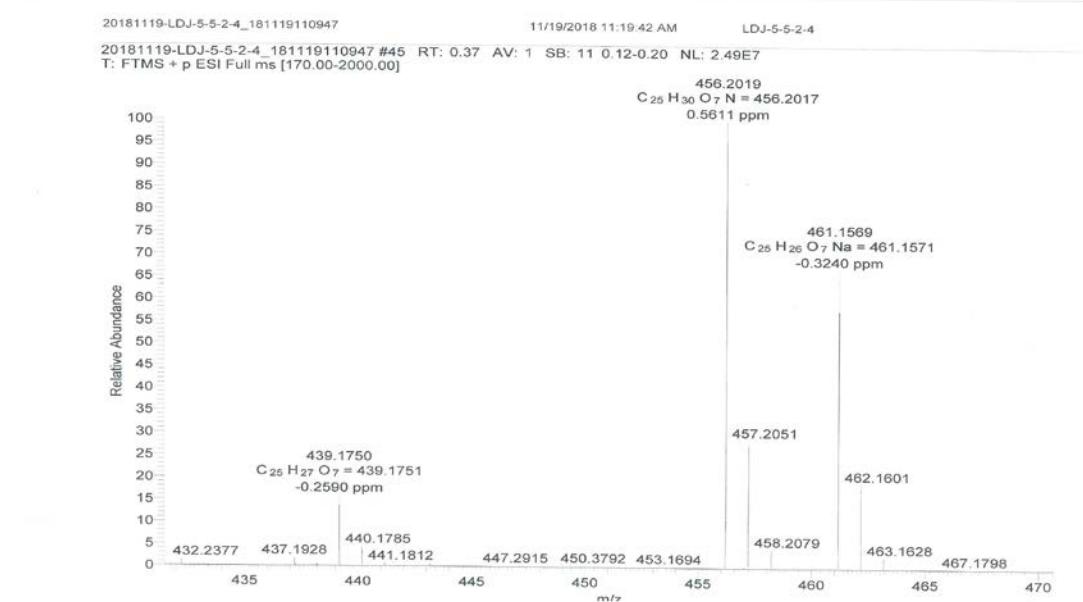
**Figure S49.** HMBC spectrum of **7** in DMSO-*d*<sub>6</sub>.



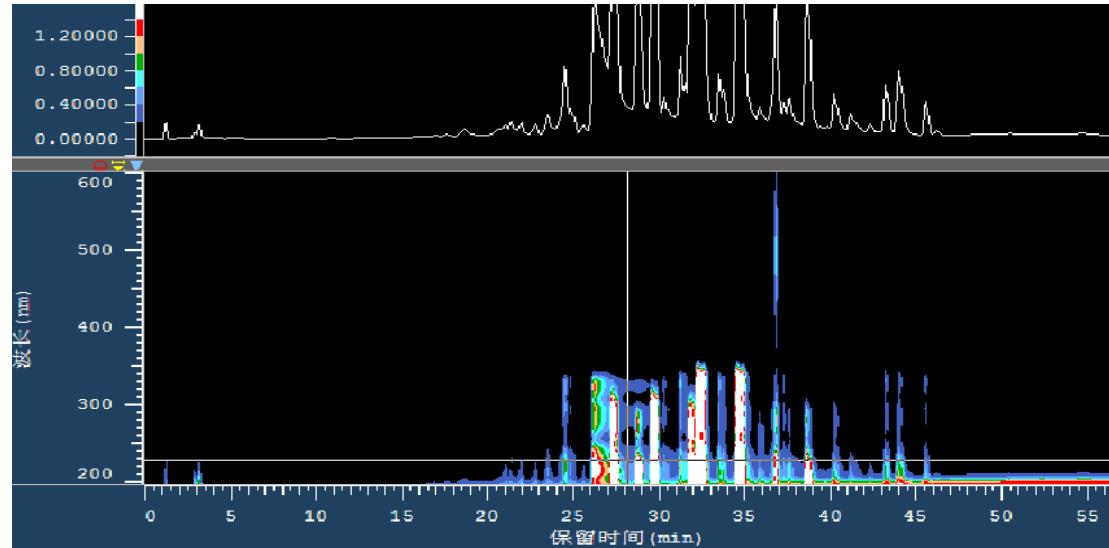
**Figure S50.** NOESY spectrum of **7** in DMSO-*d*<sub>6</sub>.



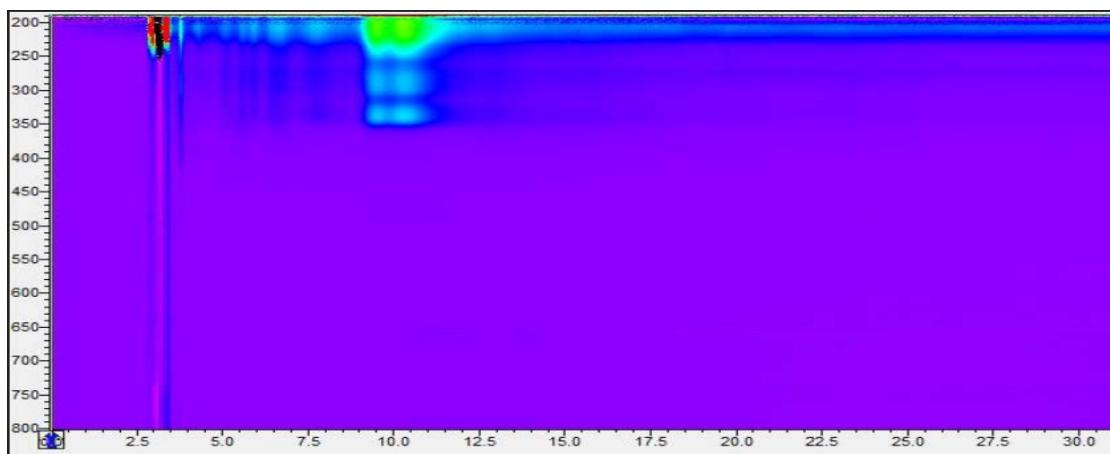
**Figure S51.** HRESIMS spectrum of **7**.



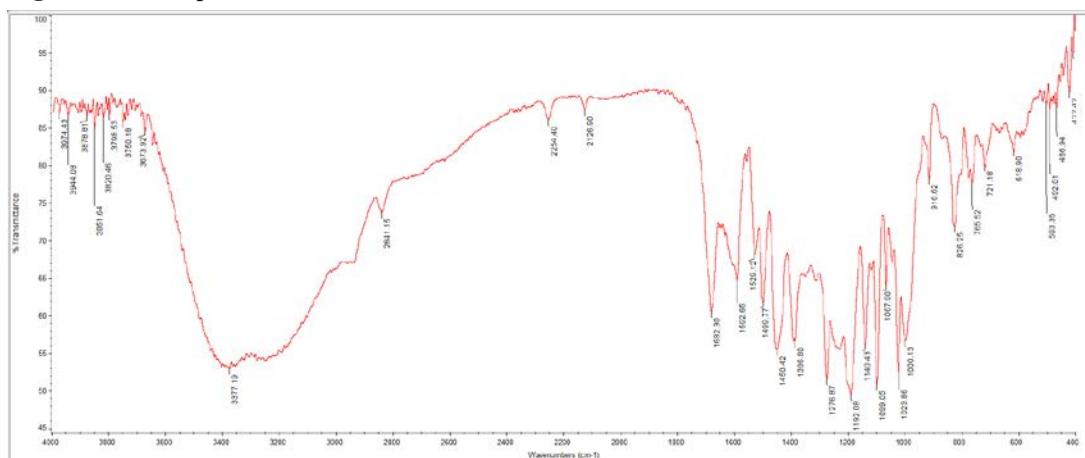
**Figure S52.** HPLC of LDJ-5 crude extract.



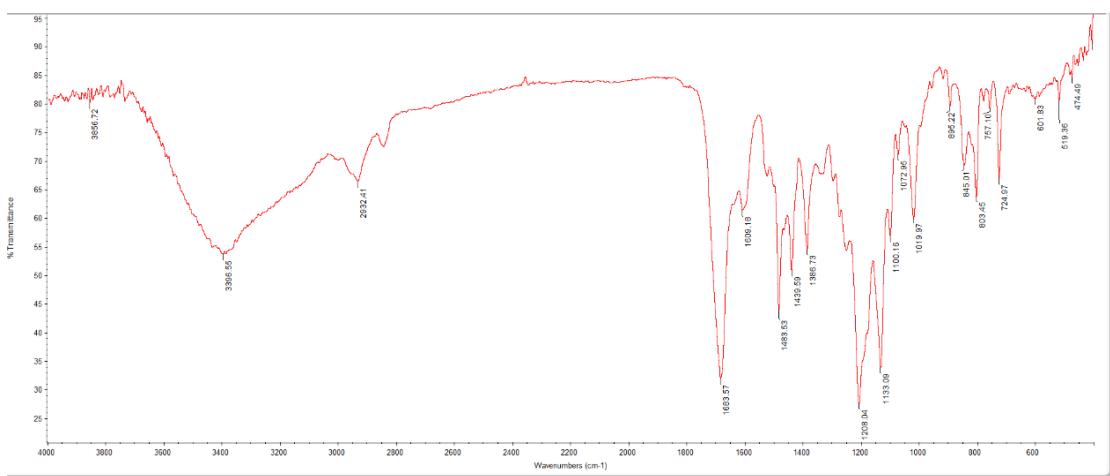
**Figure S53.** Chiral HPLC analysis of **1**.



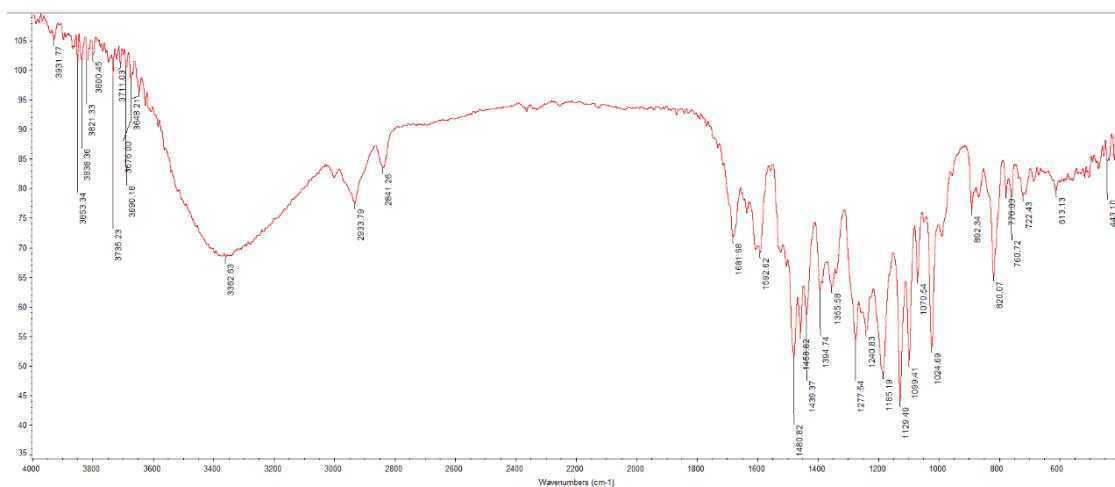
**Figure S54.** IR spectrum of **1**.



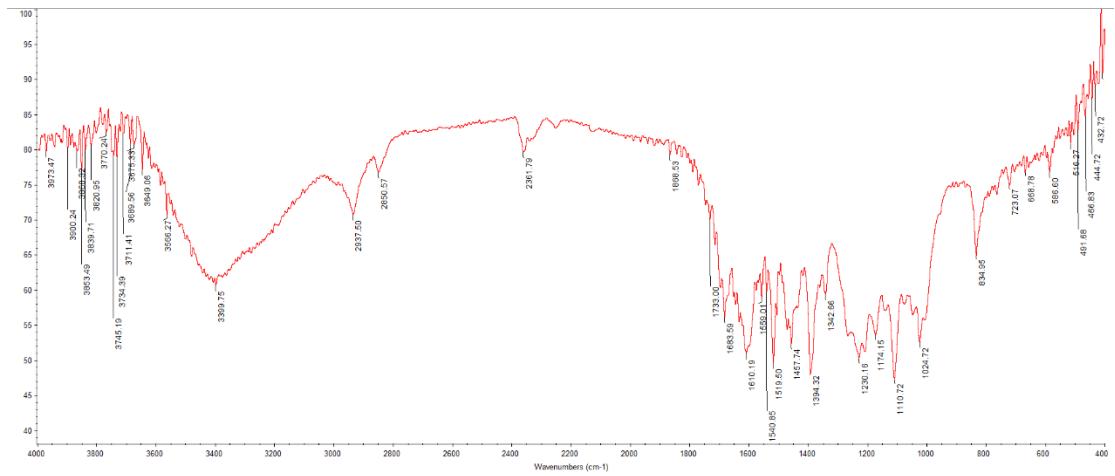
**Figure S55.** IR spectrum of **2**.



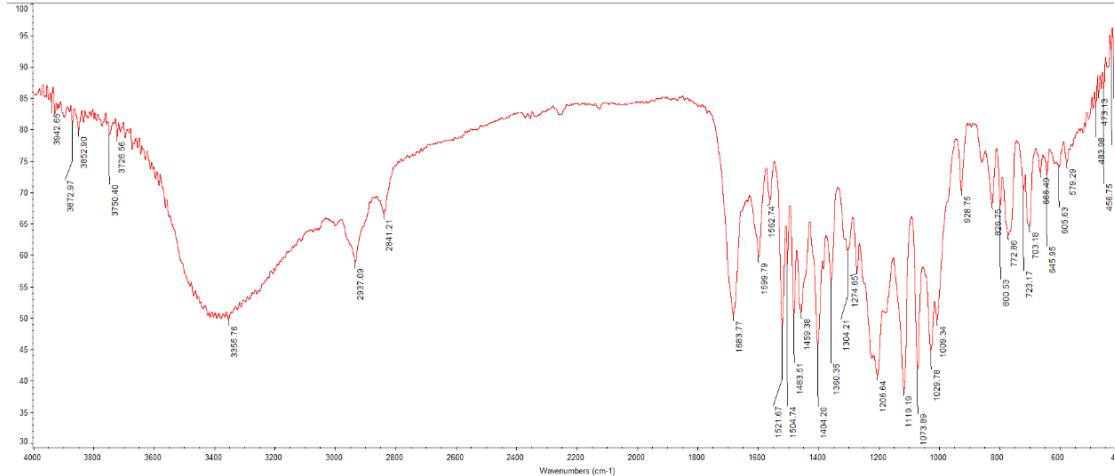
**Figure S56.** IR spectrum of **3**.



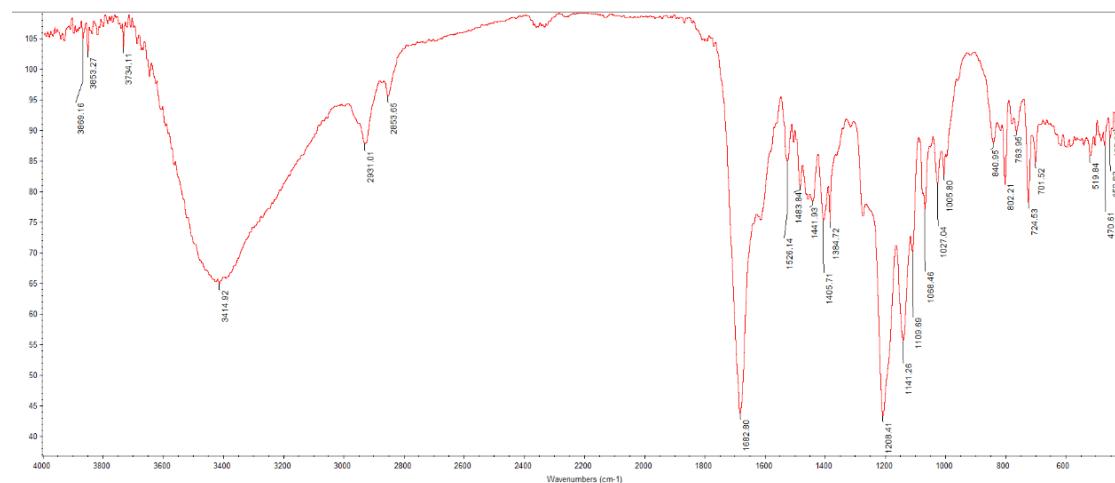
**Figure S57.** IR spectrum of 4.



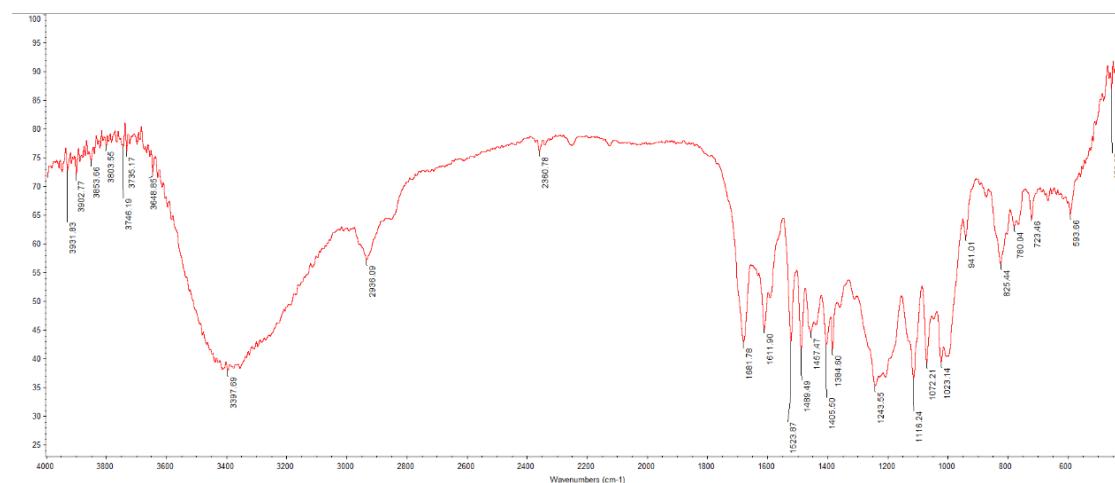
**Figure S58.** IR spectrum of 5.



**Figure S59.** IR spectrum of **6**.



**Figure S60.** IR spectrum of **7**.



**Table S1.** Antimicrobial activity of **1-7**.

Compound	MIC ( $\mu\text{g/mL}$ )				
	<i>Proteus</i> species	<i>Pseudomonas</i> <i>aeruginosa</i>	<i>Bacillus</i> <i>subtilis</i>	<i>Bacillus</i> <i>cereus</i>	<i>Mycobacterium</i> <i>phlei</i>
<b>1</b>	>200	>200	>200	>200	>200
<b>2</b>	>200	40	>200	>200	79
<b>3</b>	19	>200	38	>200	38
<b>4</b>	>200	>200	>200	70	>200
<b>5</b>	35	70	70	70	70
<b>6</b>	>200	>200	>200	>200	>200
<b>7</b>	>200	>200	>200	87	>200
Positive drug <sup>a</sup>	0.26	0.52	4.14	2.07	0.52

<sup>a</sup>: Ciprofloxacin = positive control for *P. species*, *P. aeruginosa*, *B. subtilis*, *Bacillus cereus* and *Mycobacterium phlei*.