

## Supporting Information

### **Isolation, structural characterization and antidiabetic activity of new diketopiperazine alkaloids from mangrove endophytic fungus *Aspergillus* sp. 16-5c**

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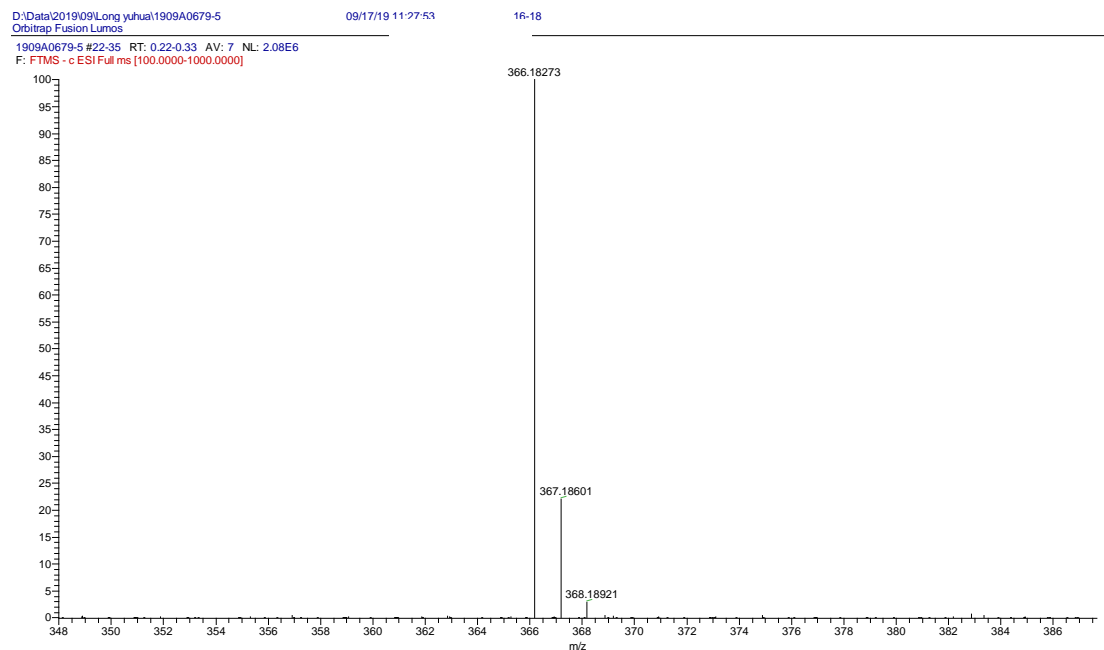
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SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
366.18273	366.18231	1.13	11.5	C <sub>21</sub> H <sub>24</sub> O <sub>3</sub> N <sub>3</sub>

Figure S1 HRESIMS of compound **1**

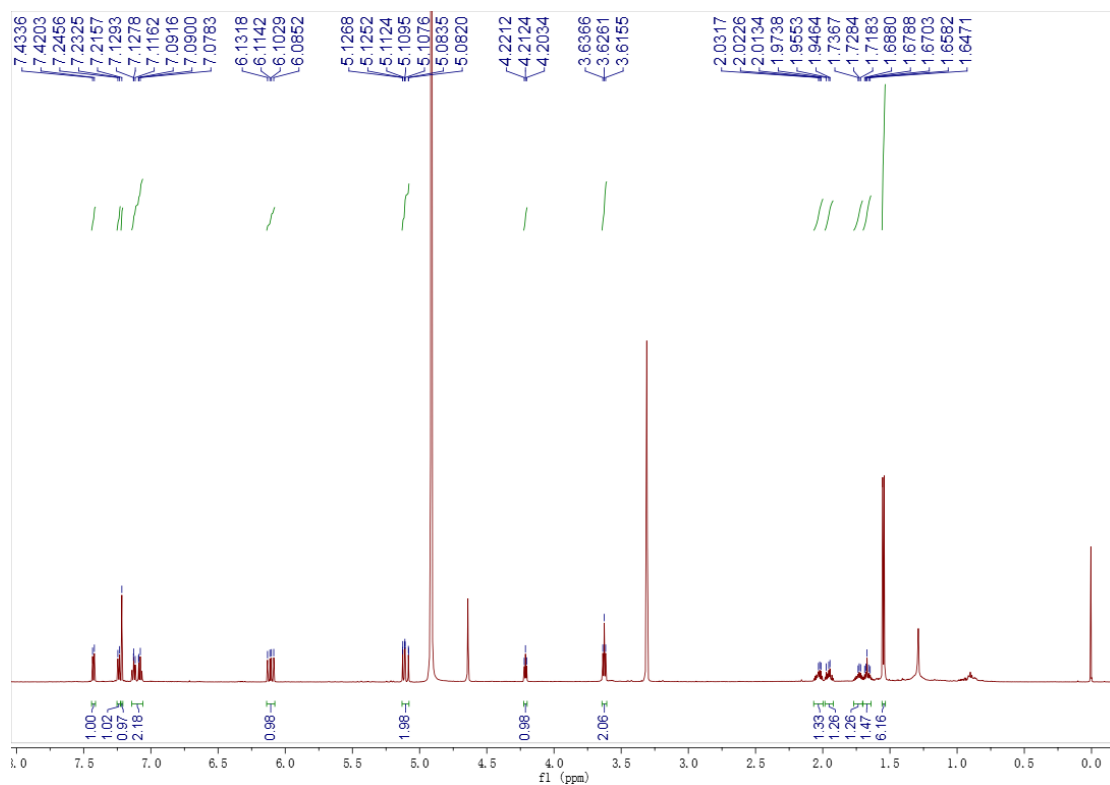


Figure S2 <sup>1</sup>H NMR spectrum (600 MHz, methanol-*d*<sub>4</sub>) of compound **1**

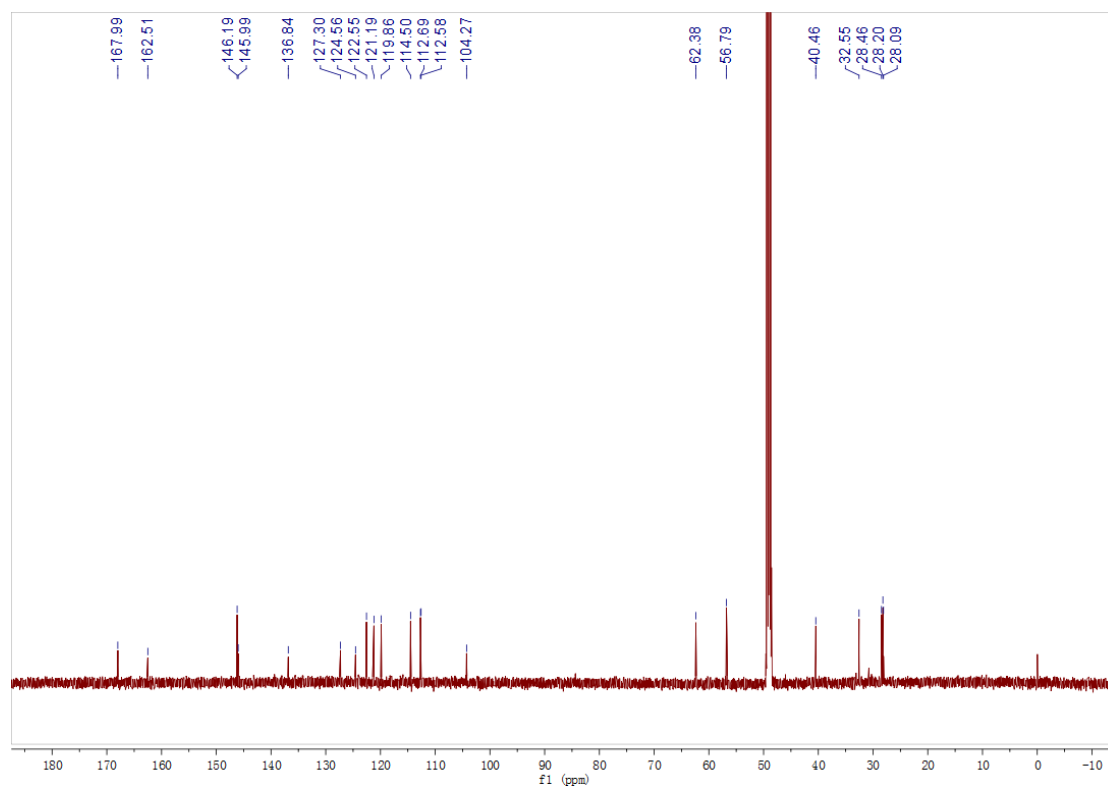


Figure S3  $^{13}\text{C}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **1**

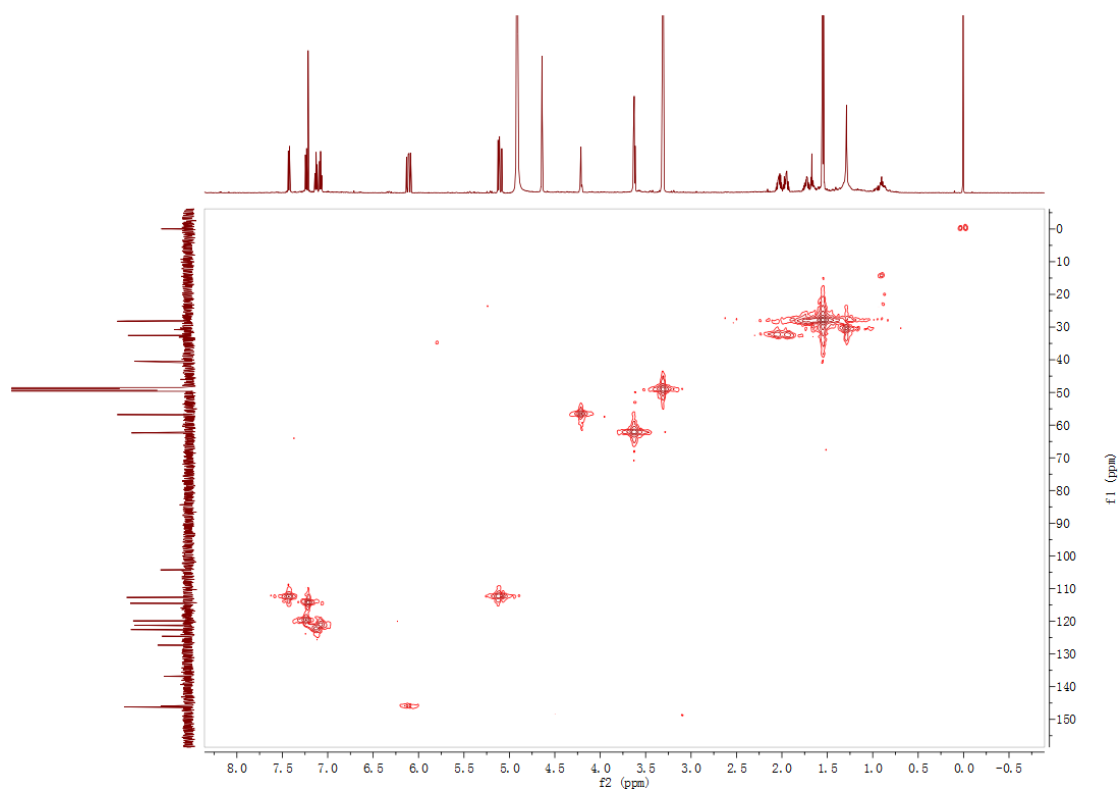


Fig.S4 HMQC spectrum (600 MHz, methanol- $d_4$ ) of compound **1**

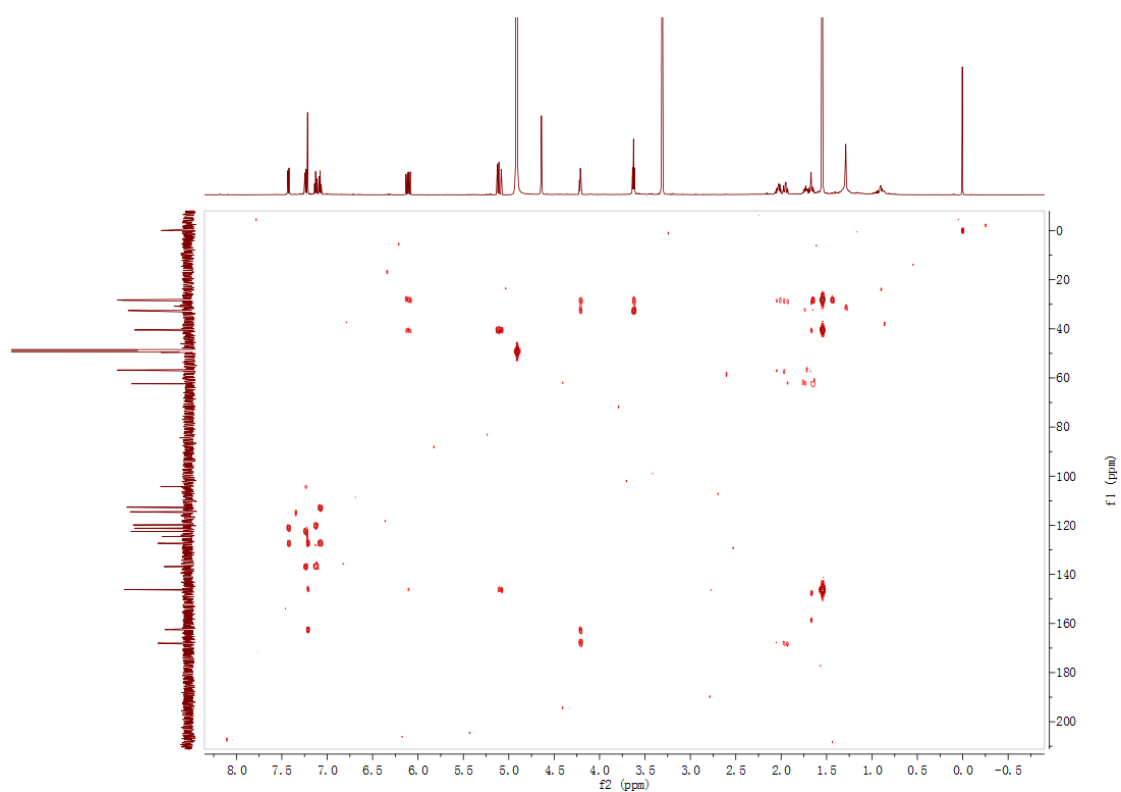


Figure S5 HMBC spectrum (600 MHz, methanol- $d_4$ ) of compound **1**

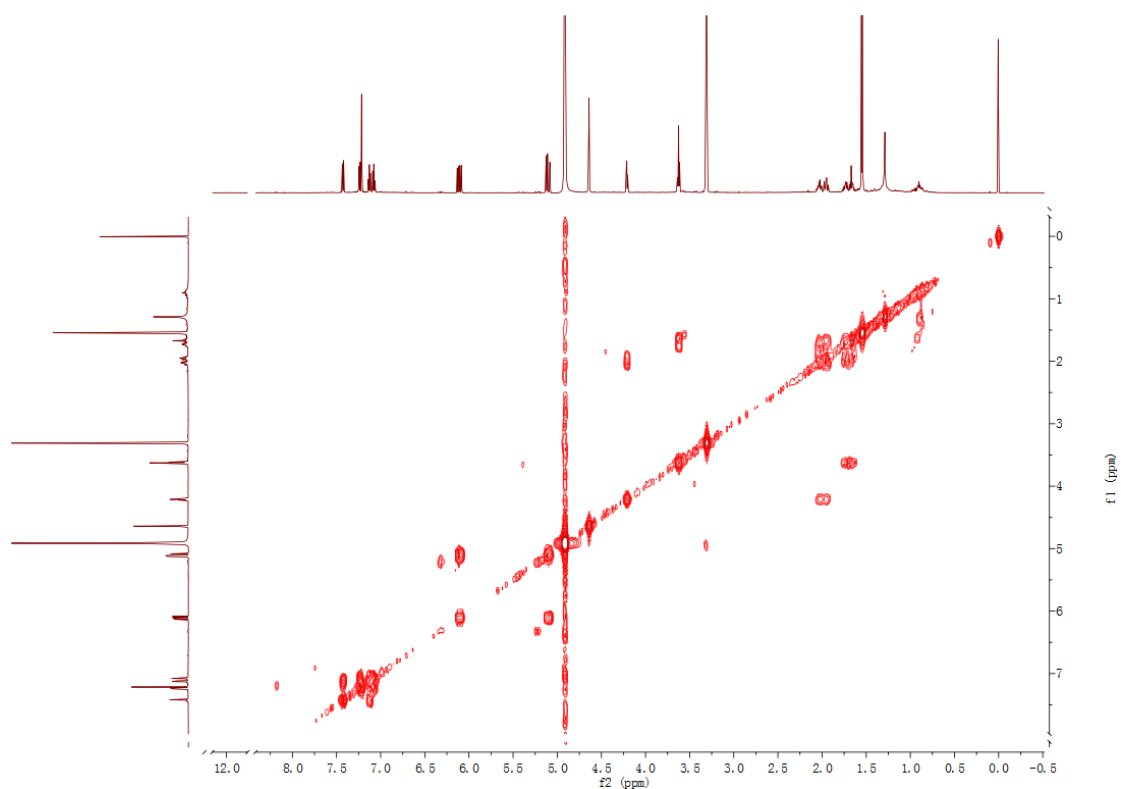


Figure S6  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz, methanol- $d_4$ ) of compound **1**

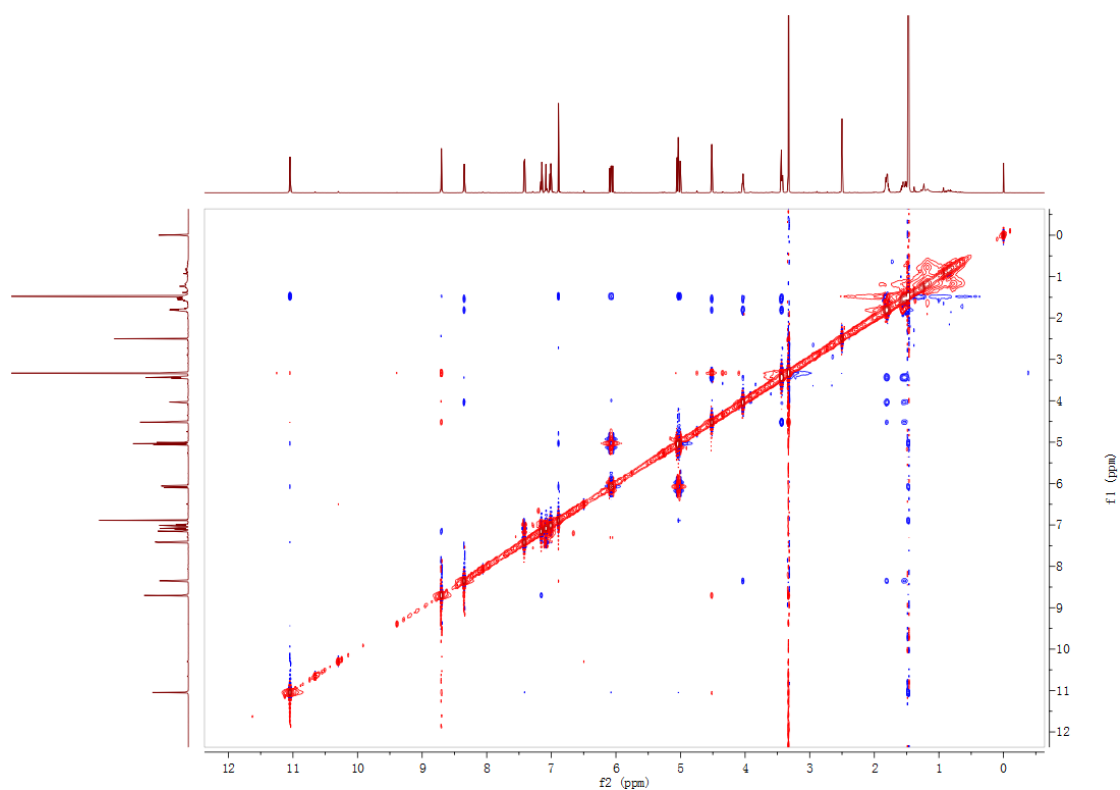


Figure S7 NOESY spectrum (600 MHz, DMSO- $d_6$ ) of compound **1**

#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

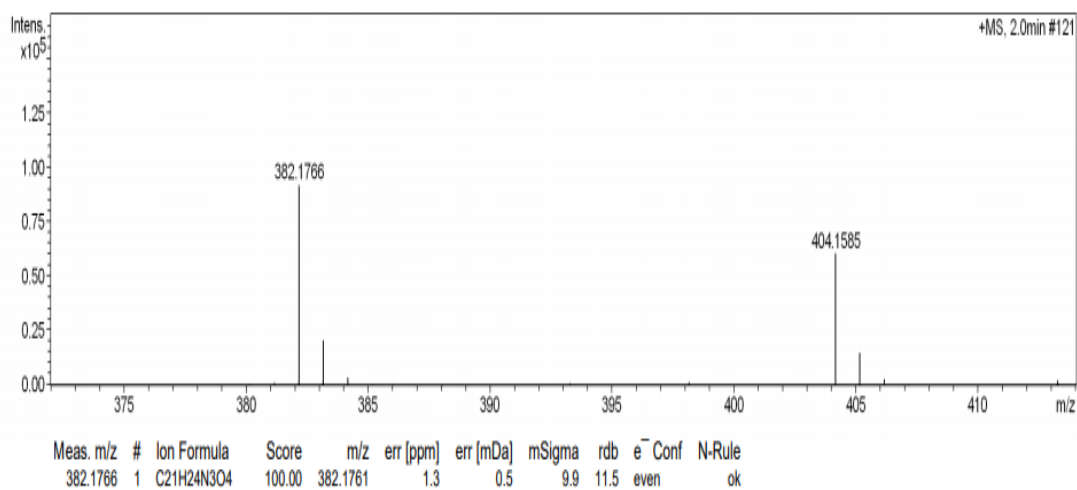


Figure S8 HRESIMS of compound **2**

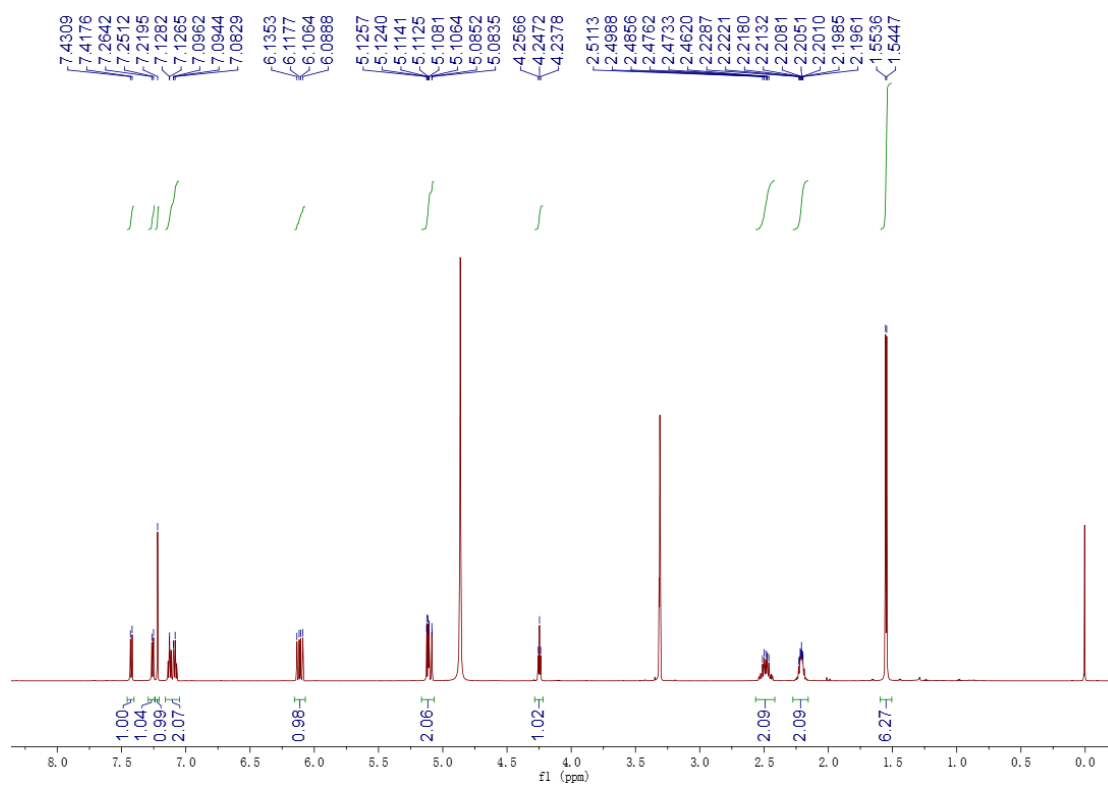


Figure S9 <sup>1</sup>H NMR spectrum (600 MHz, methanol-*d*<sub>4</sub>) of compound **2**

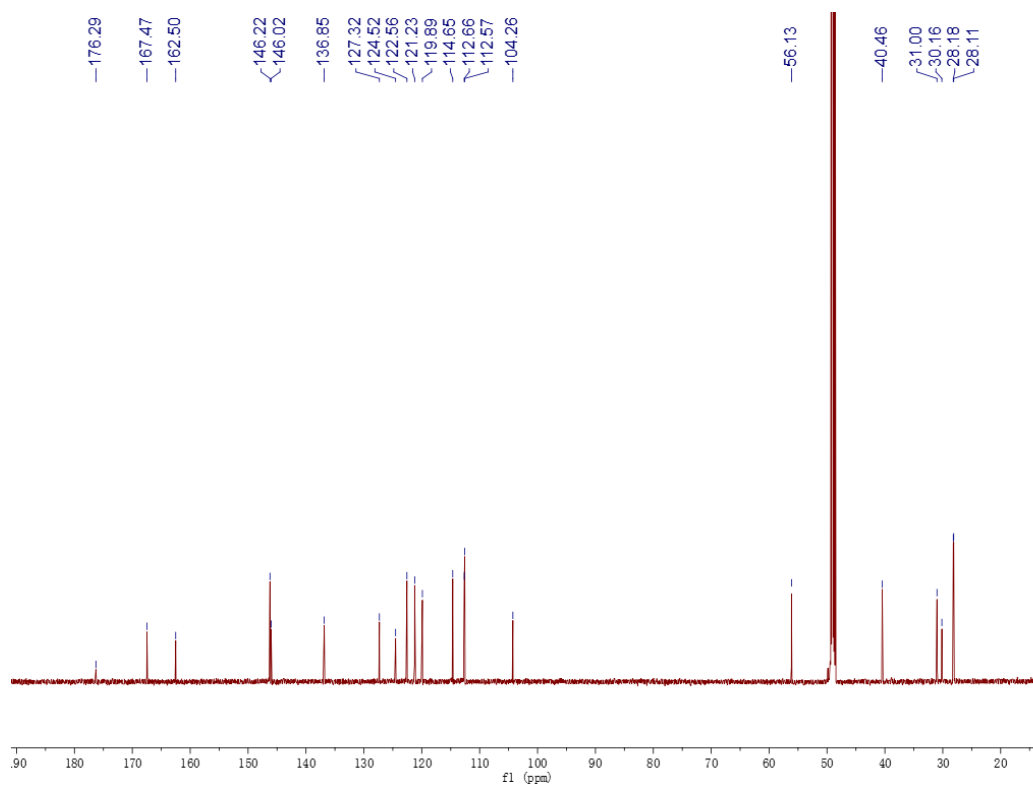


Figure S10 <sup>13</sup>C NMR spectrum (600 MHz, methanol-*d*<sub>4</sub>) of compound **2**



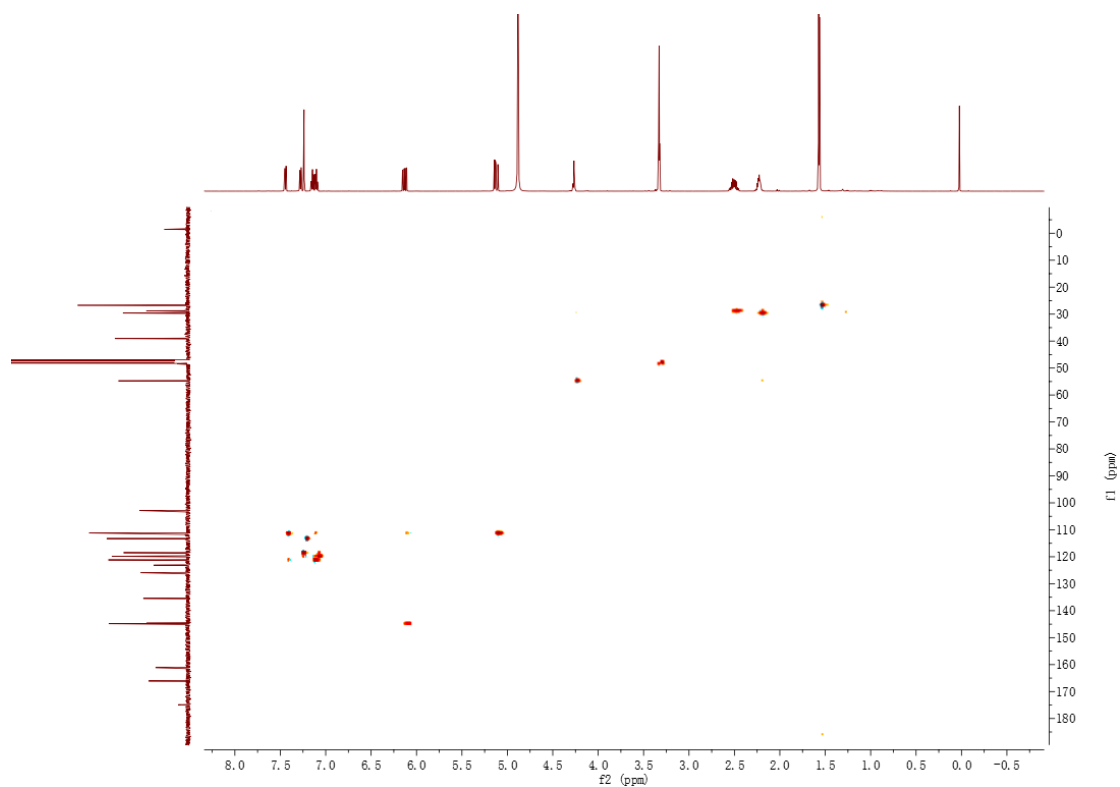


Figure S11 HMQC spectrum (600 MHz, methanol- $d_4$ ) of compound **2**

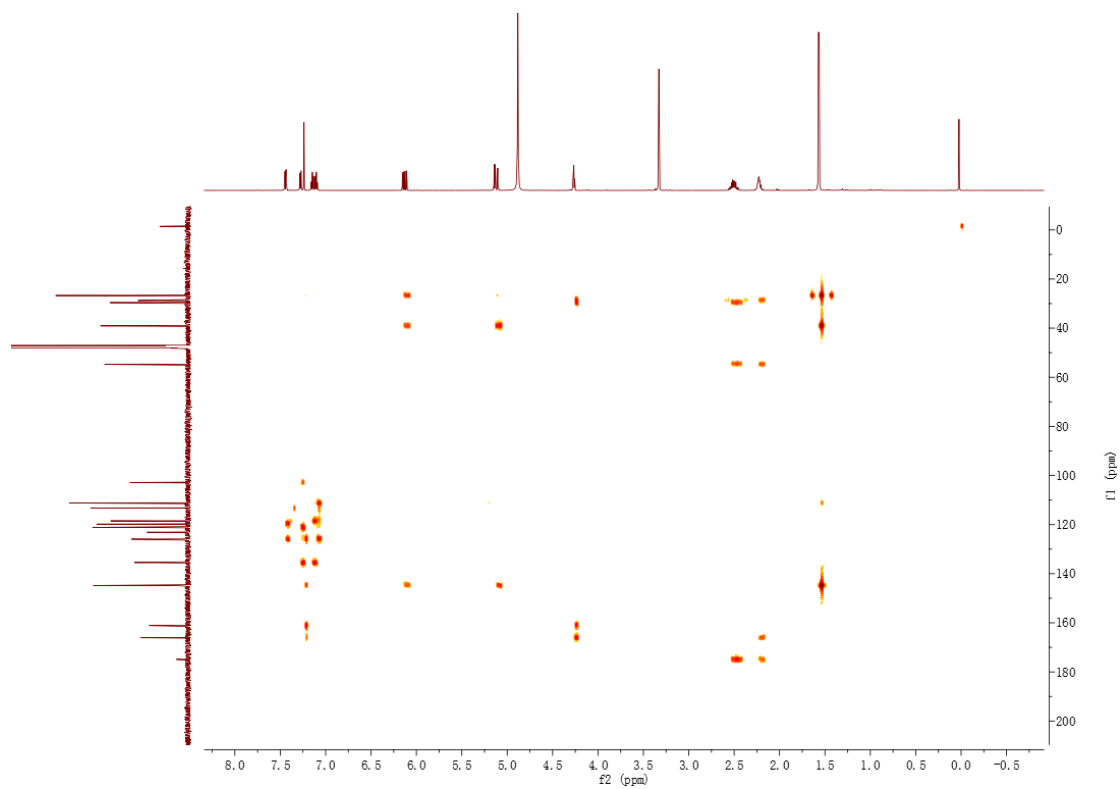


Figure S12 HMBC spectrum (600 MHz, methanol- $d_4$ ) of compound **2**

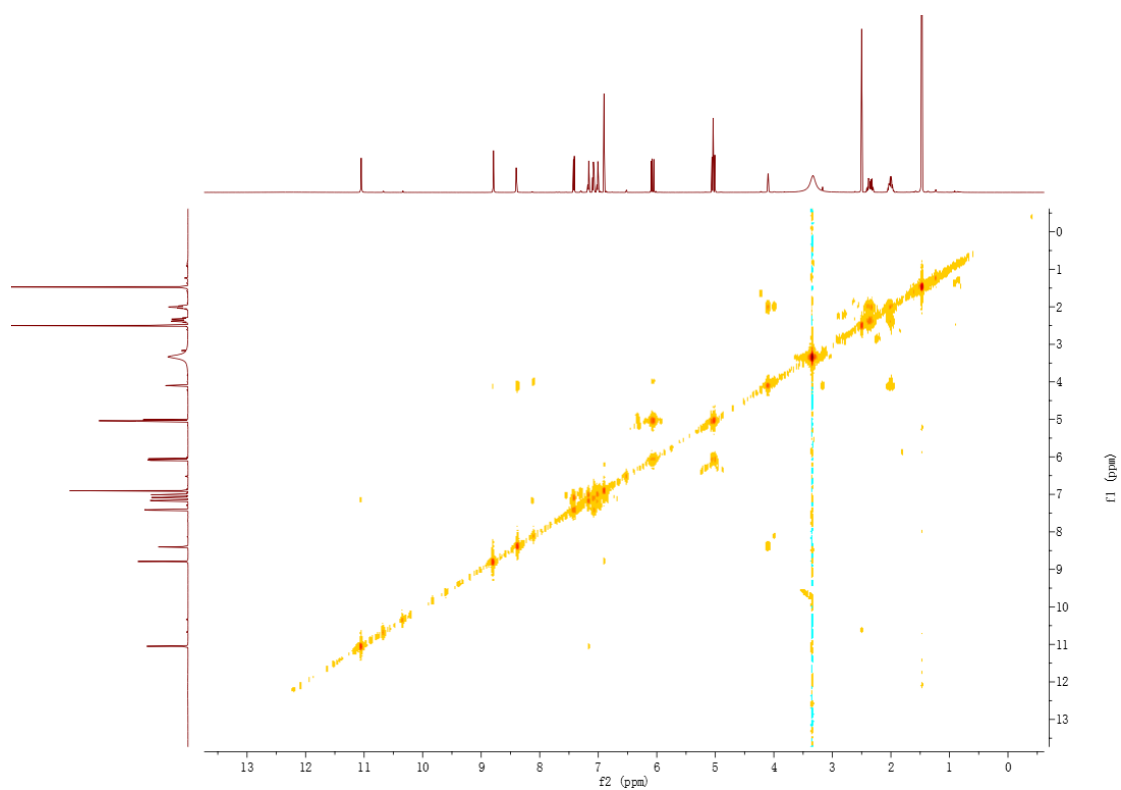


Figure S13  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz,  $\text{DMSO-}d_4$ ) of compound **2**

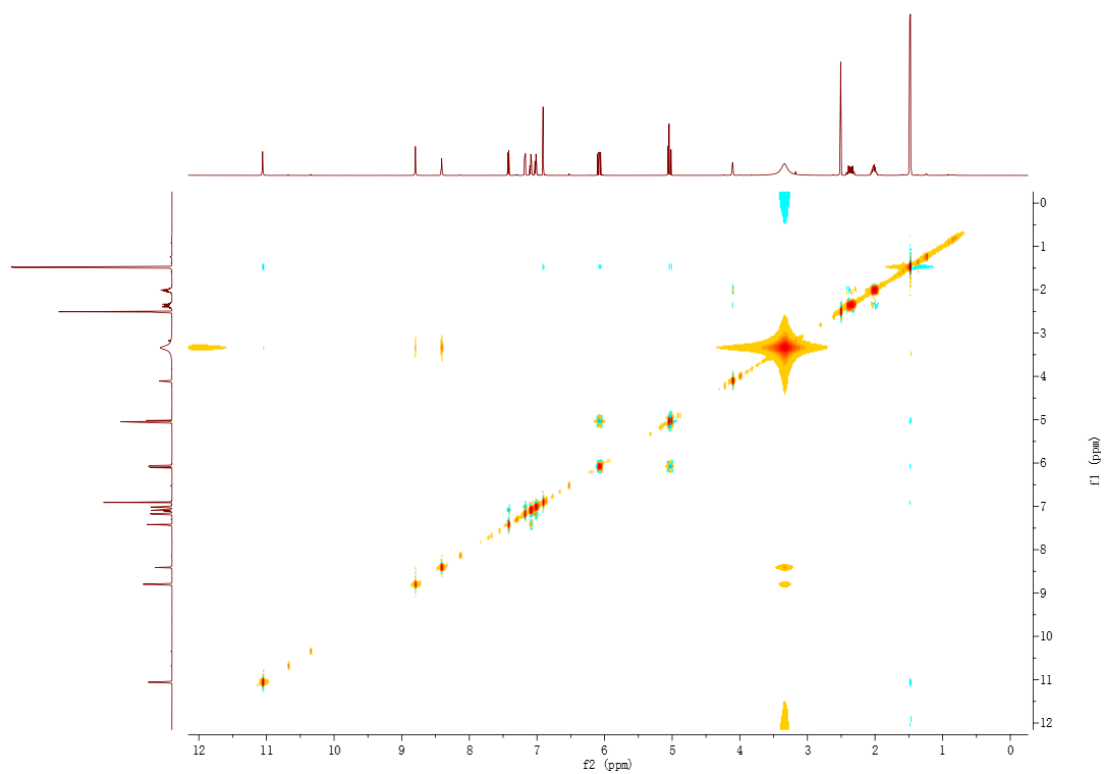
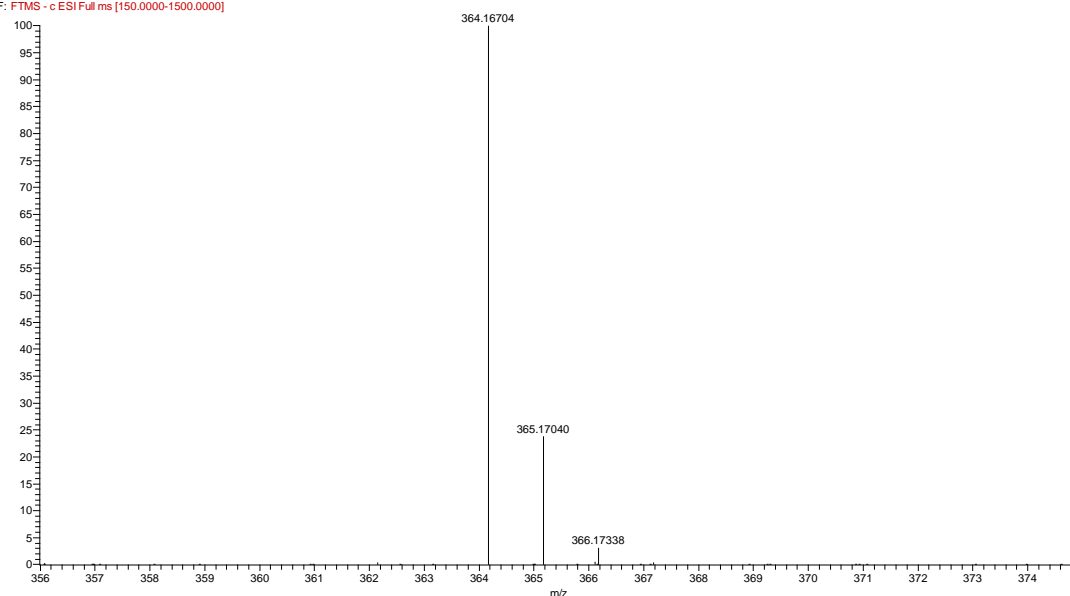


Figure S14 NOESY spectrum (600 MHz,  $\text{DMSO-}d_6$ ) of compound **2**



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
364.16704	364.16666	1.03	12.5	C <sub>21</sub> H <sub>22</sub> O <sub>3</sub> N <sub>3</sub>

Figure S15 HRESIMS of compound **3**

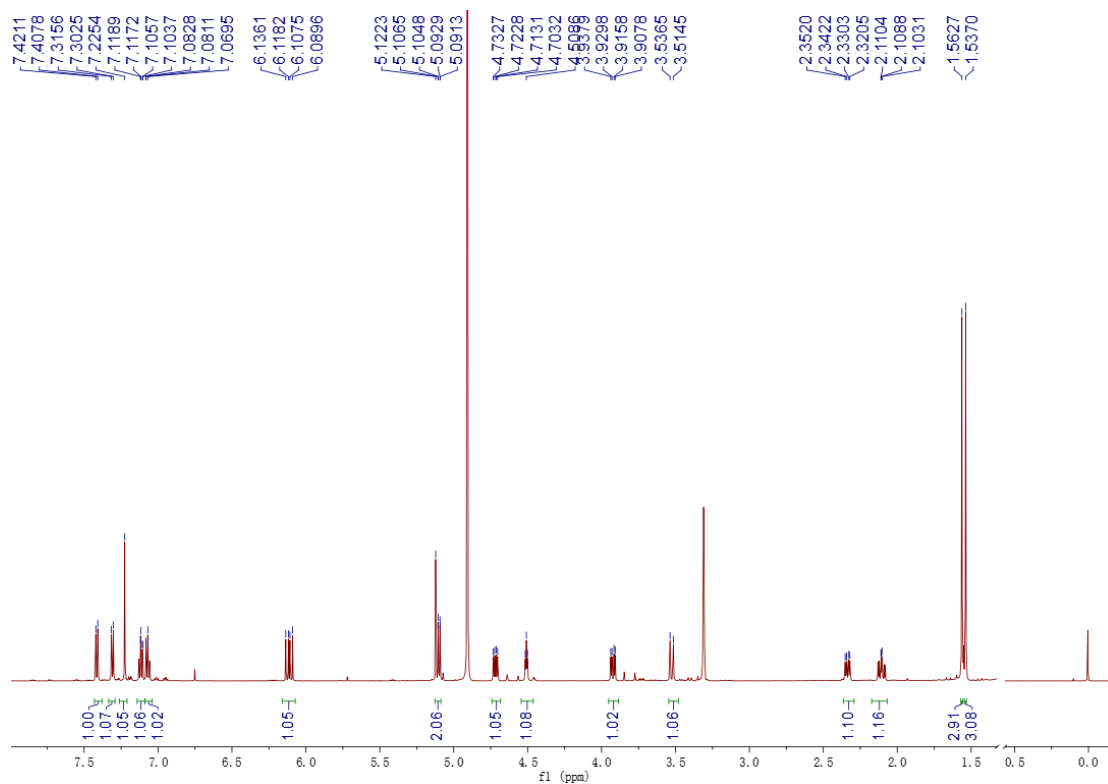


Figure S16 <sup>1</sup>H NMR spectrum (600 MHz, methanol-*d*<sub>4</sub>) of compound **3**

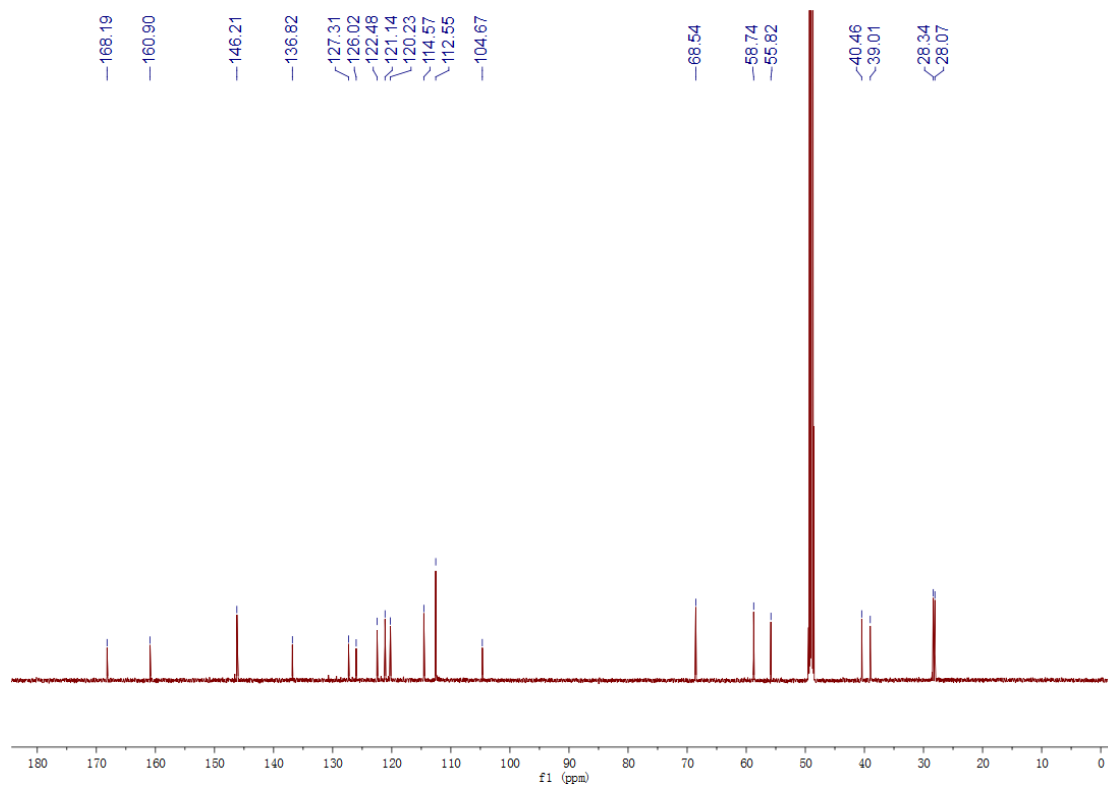


Figure S17  $^{13}\text{C}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **3**

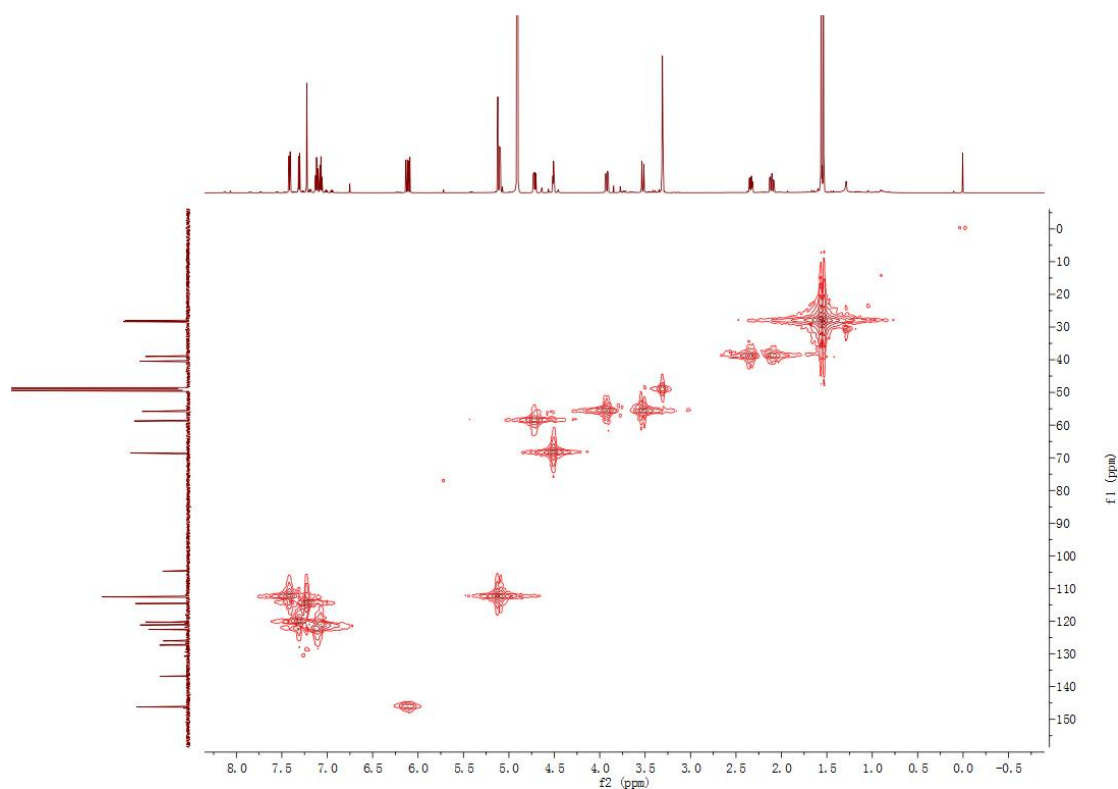


Figure.S18 HMQC spectrum (600 MHz, methanol- $d_4$ ) of compound **3**

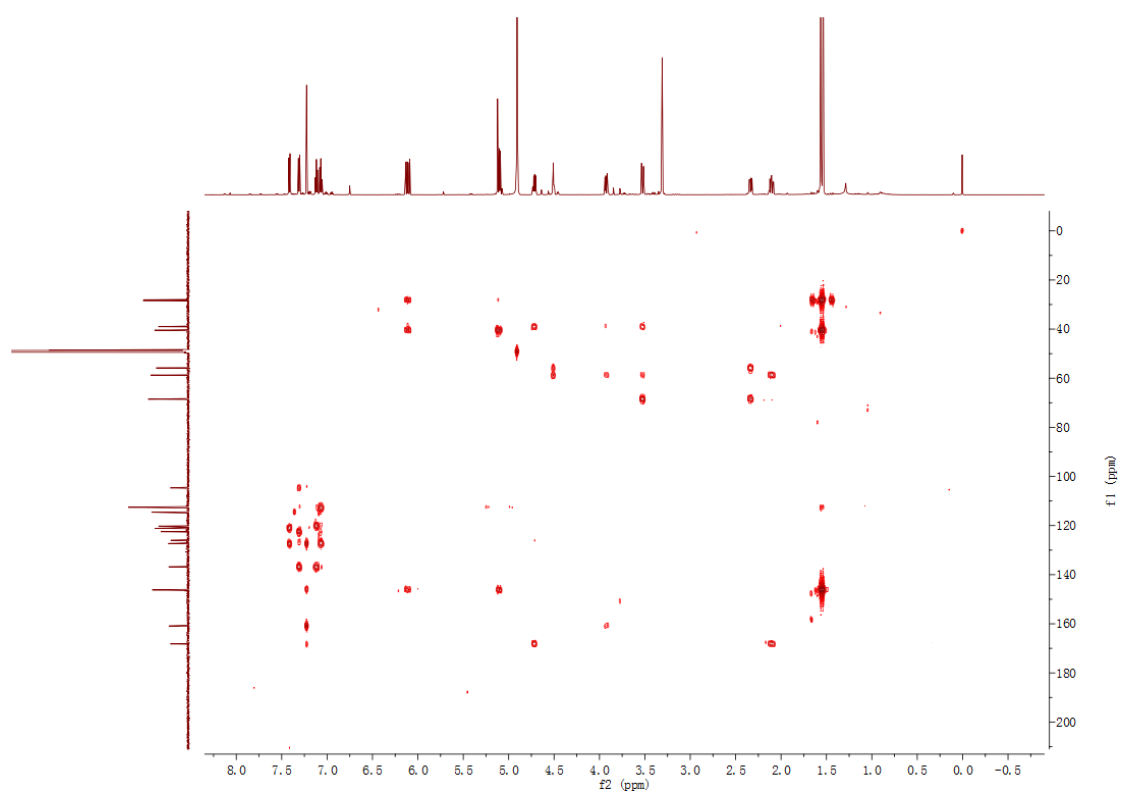


Figure S19 HMBC spectrum (600 MHz, methanol- $d_4$ ) of compound **3**

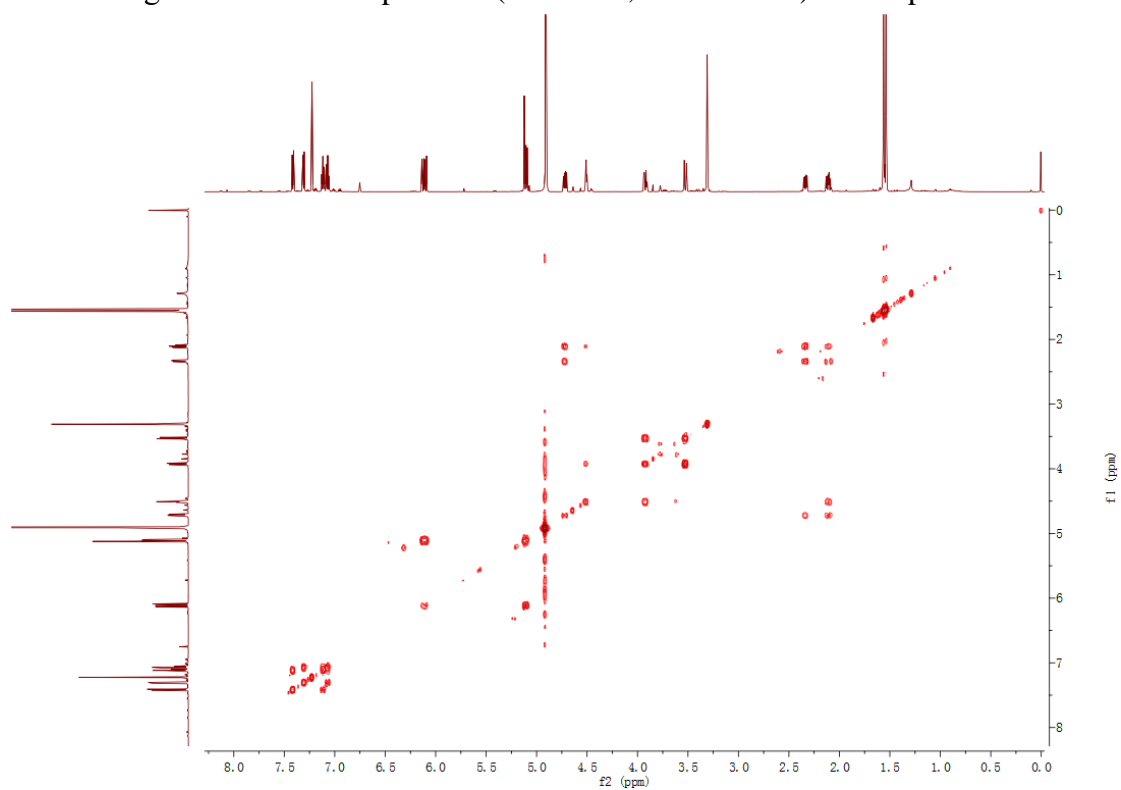


Figure S20  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz, methanol- $d_4$ ) of compound **3**

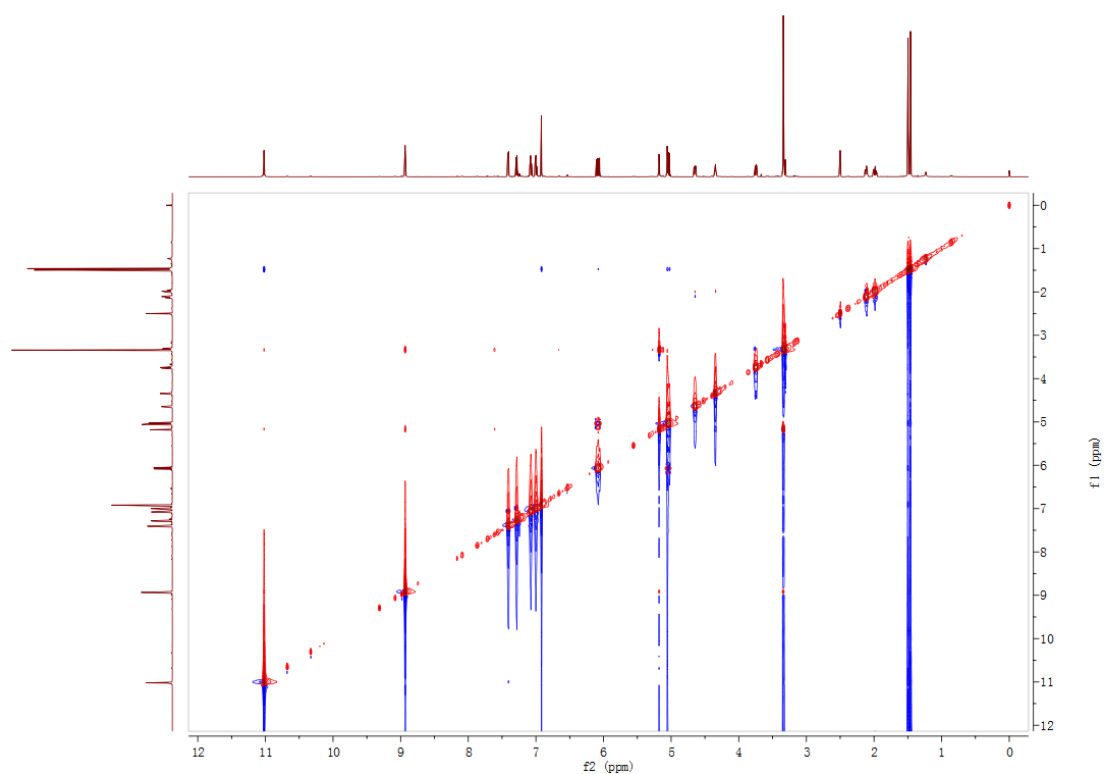
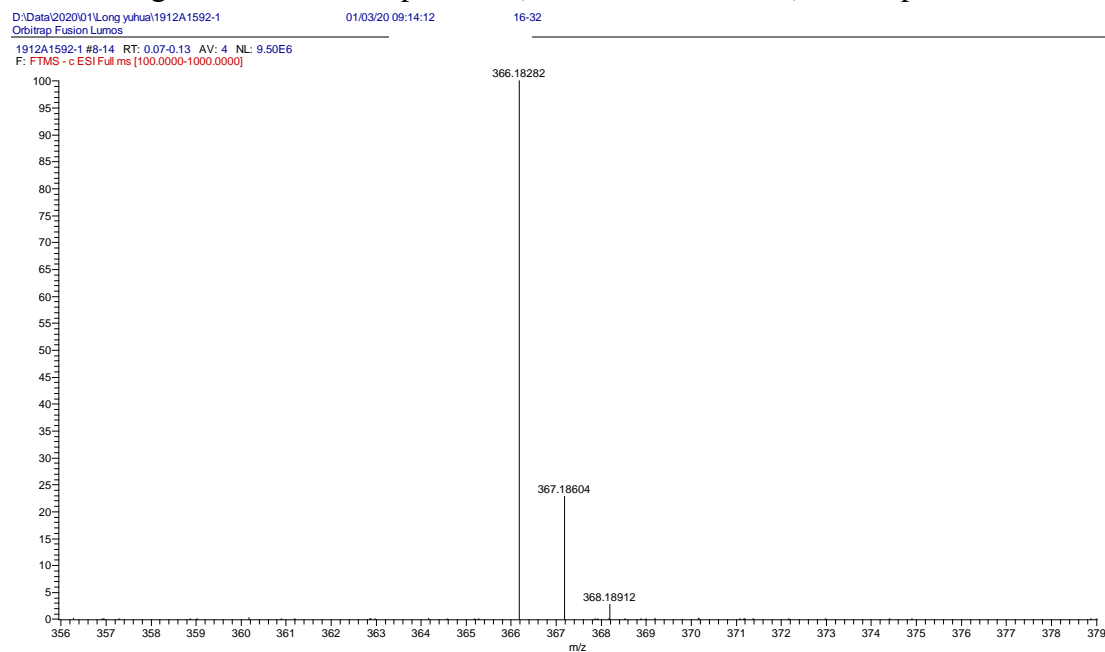


Figure S21 NOESY spectrum (600 MHz, DMSO- $d_6$ ) of compound **3**



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
366.18282	366.18231	1.38	11.5	C <sub>21</sub> H <sub>24</sub> O <sub>3</sub> N <sub>3</sub>

Figure S22 HRESIMS of compound **4**

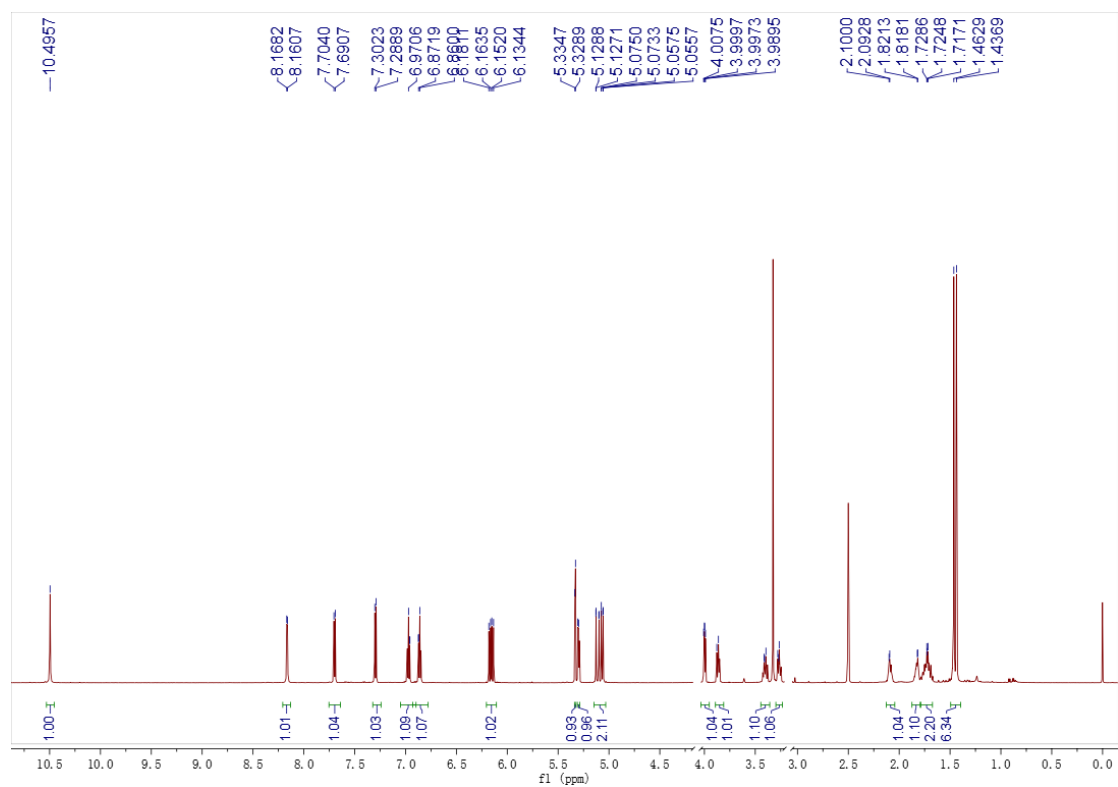


Figure S23 <sup>1</sup>H NMR spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound **4**

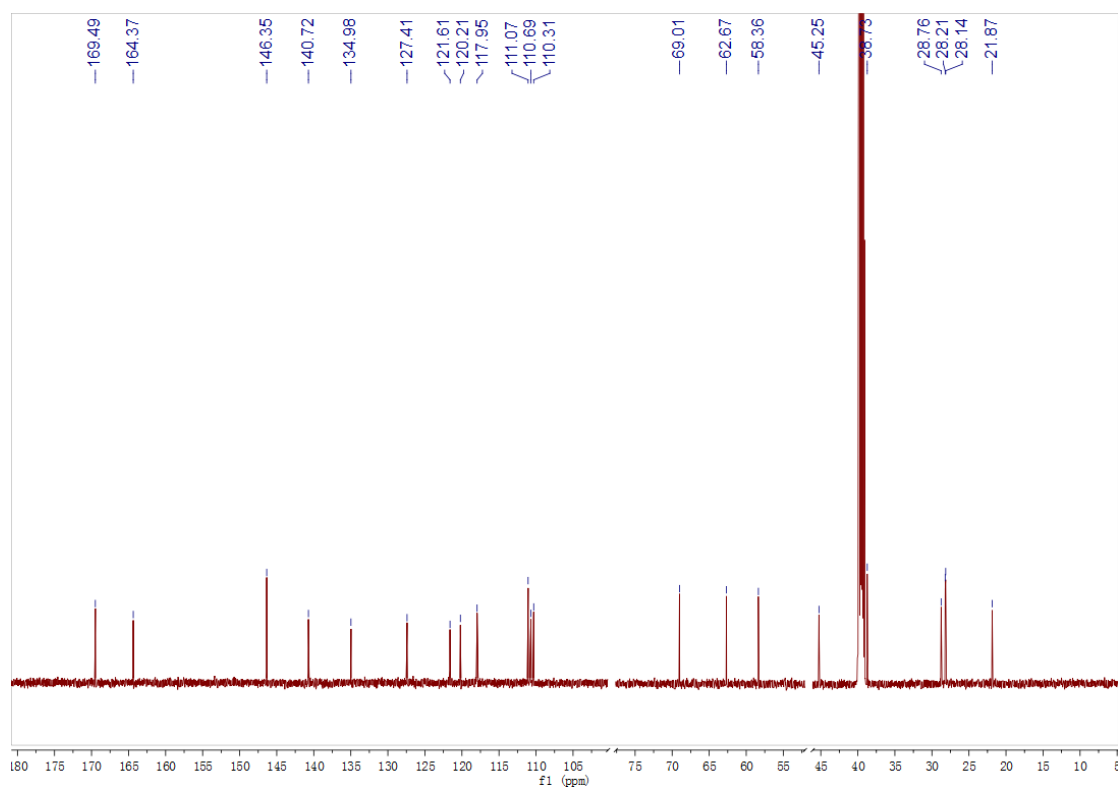


Figure S24 <sup>13</sup>C NMR spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound **4**

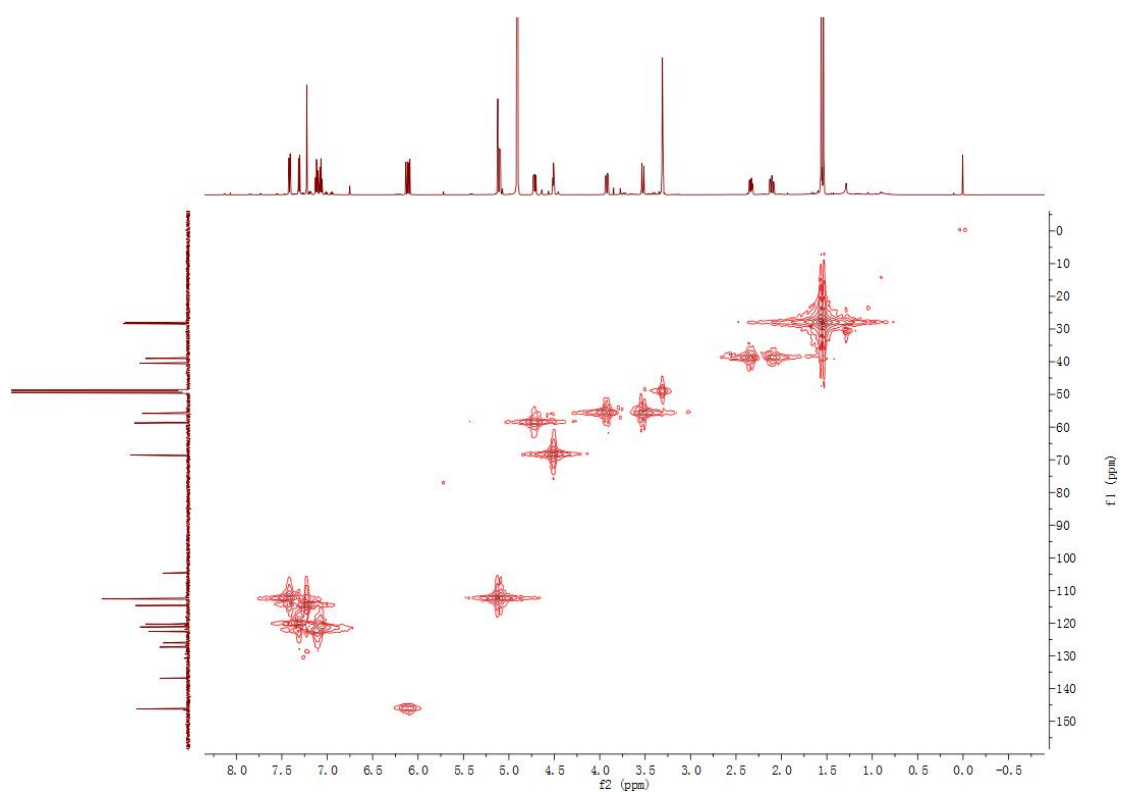


Figure S25 HMQC spectrum (600 MHz, DMSO- $d_6$ ) of compound **4**

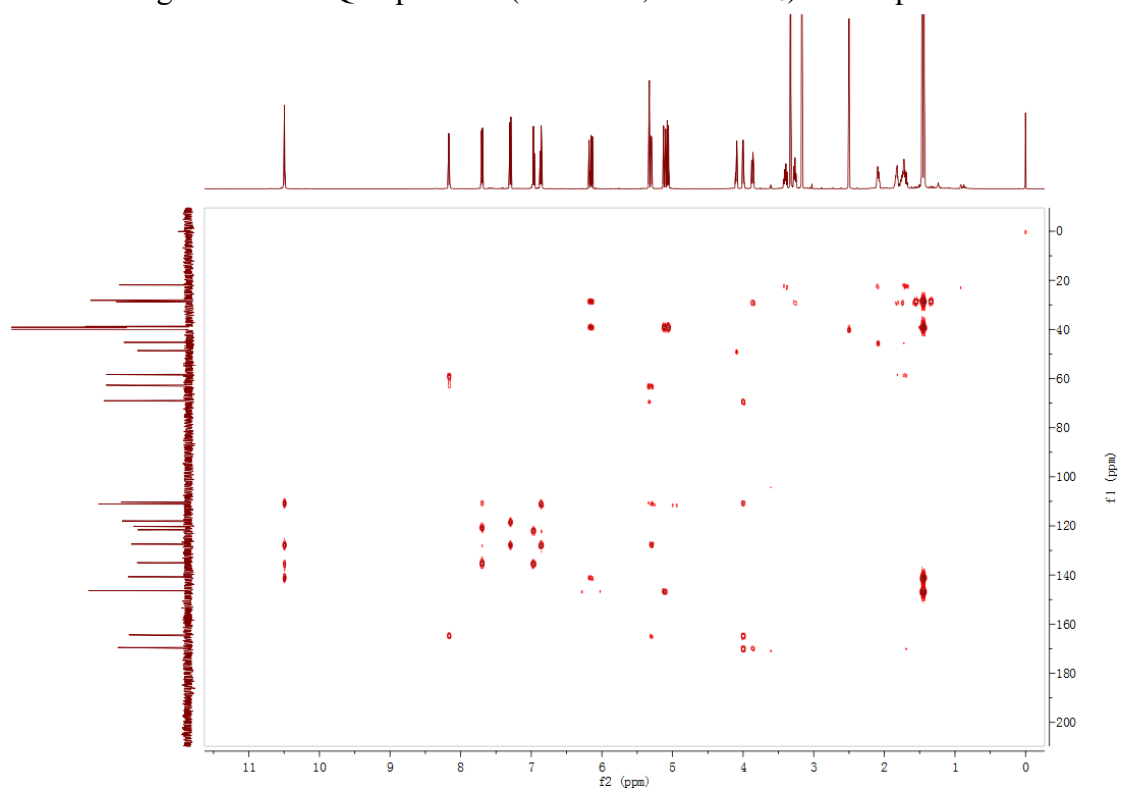


Figure S26 HMBC spectrum (600 MHz, DMSO- $d_6$ ) of compound **4**



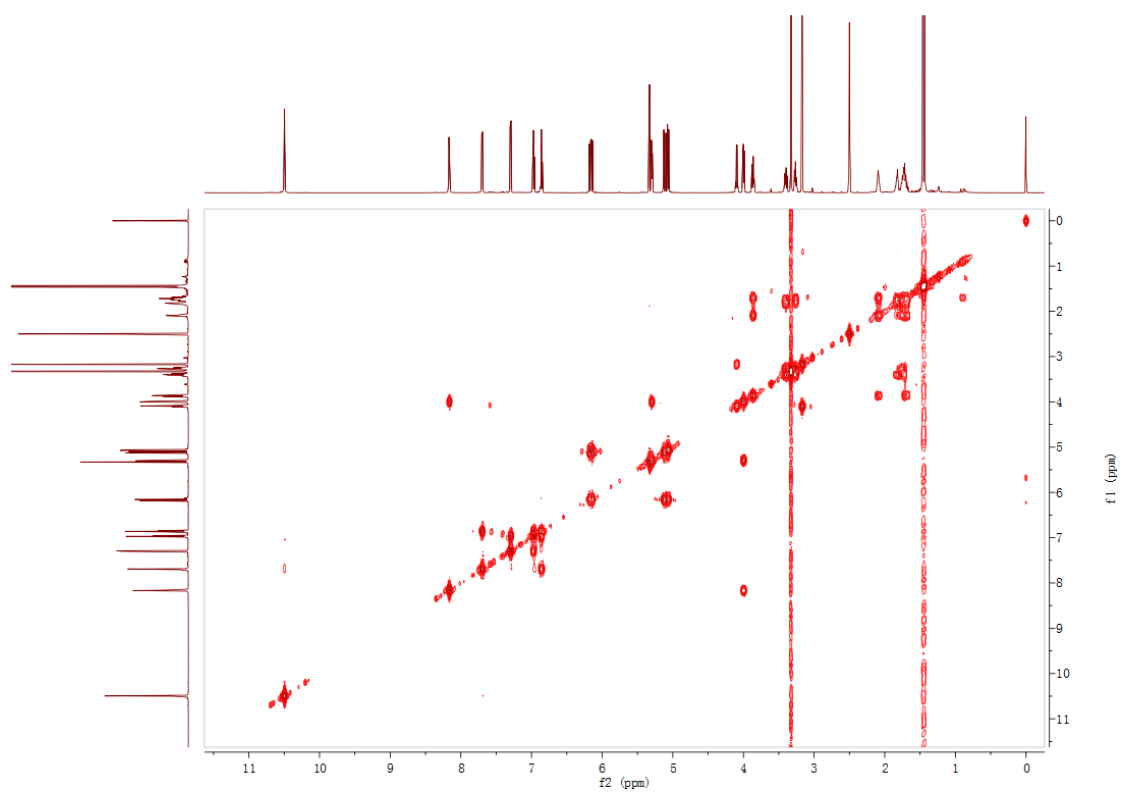


Figure S27  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz,  $\text{DMSO}-d_6$ ) of compound **4**

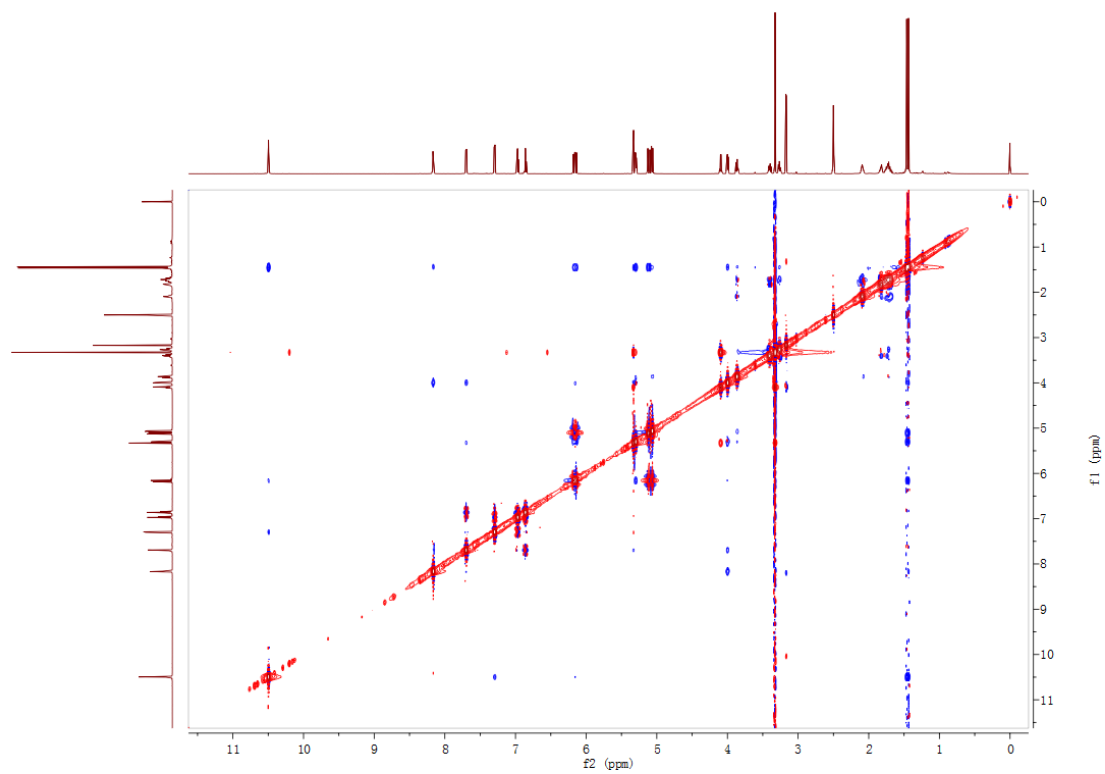
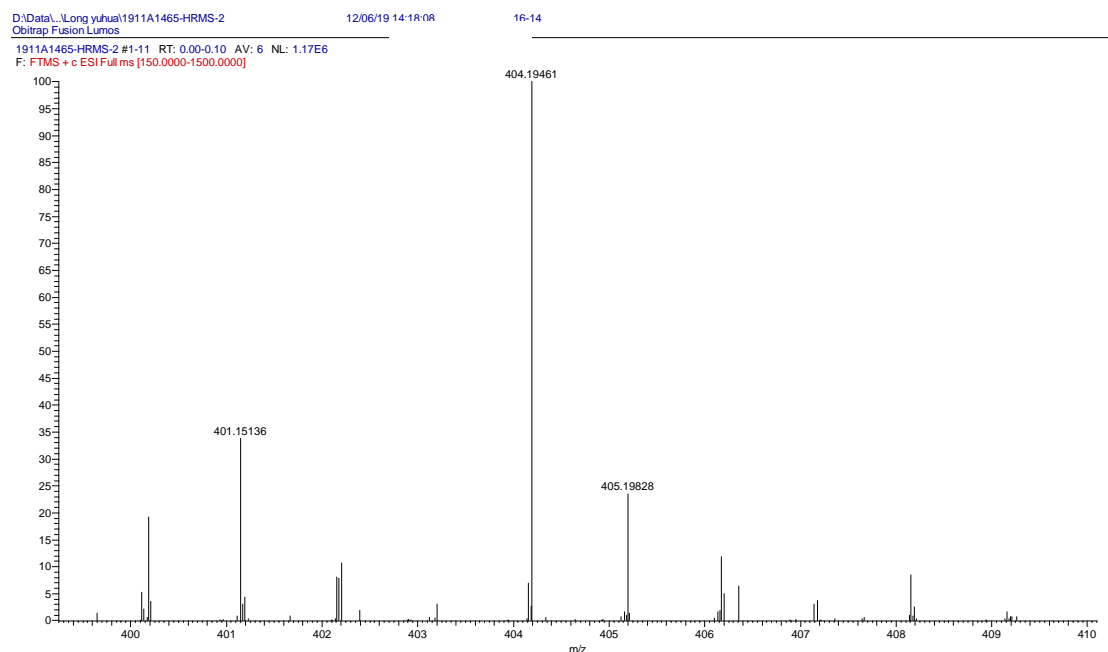


Figure S28 NOESY spectrum (600 MHz,  $\text{DMSO}-d_6$ ) of compound **4**



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
404.19461	404.19446	0.36	10.5	C <sub>22</sub> H <sub>27</sub> O <sub>3</sub> N <sub>3</sub> Na

Figure S29 HRESIMS of compound **5**

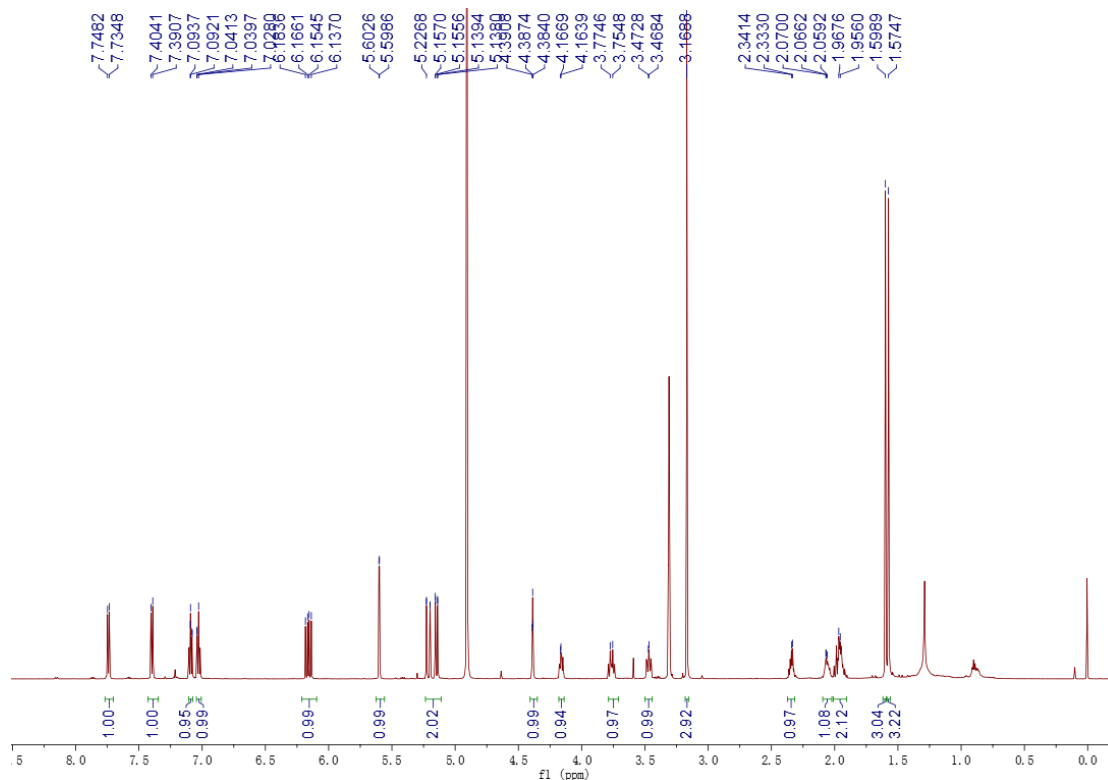


Figure S30 <sup>1</sup>H NMR spectrum (600 MHz, methanol-*d*<sub>4</sub>) of compound **5**

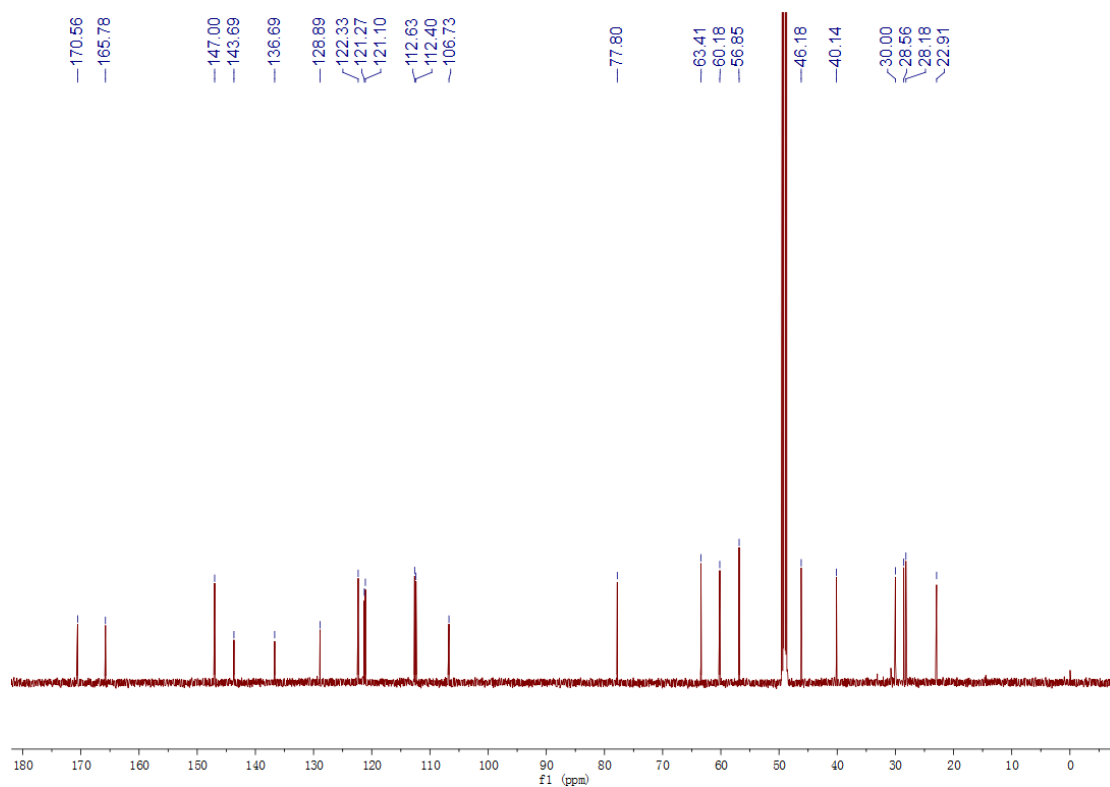


Figure S31  $^{13}\text{C}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **5**

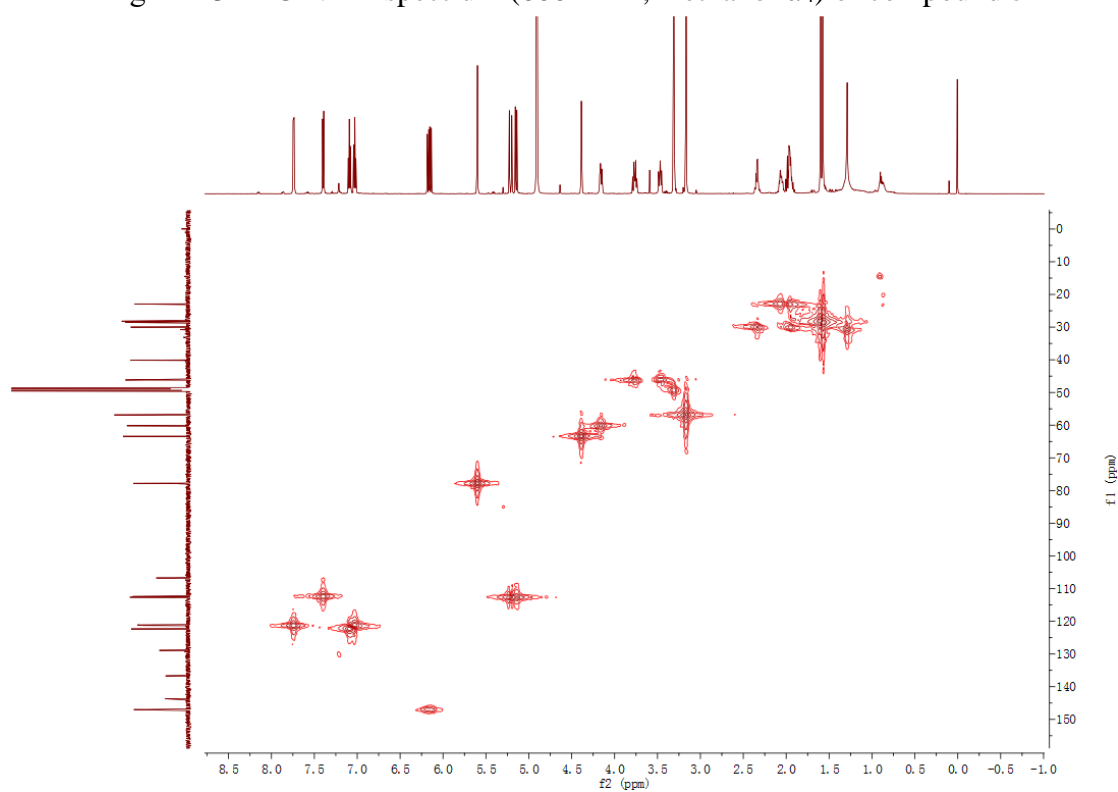


Figure S32 HMQC spectrum (600 MHz, methanol- $d_4$ ) of compound **5**

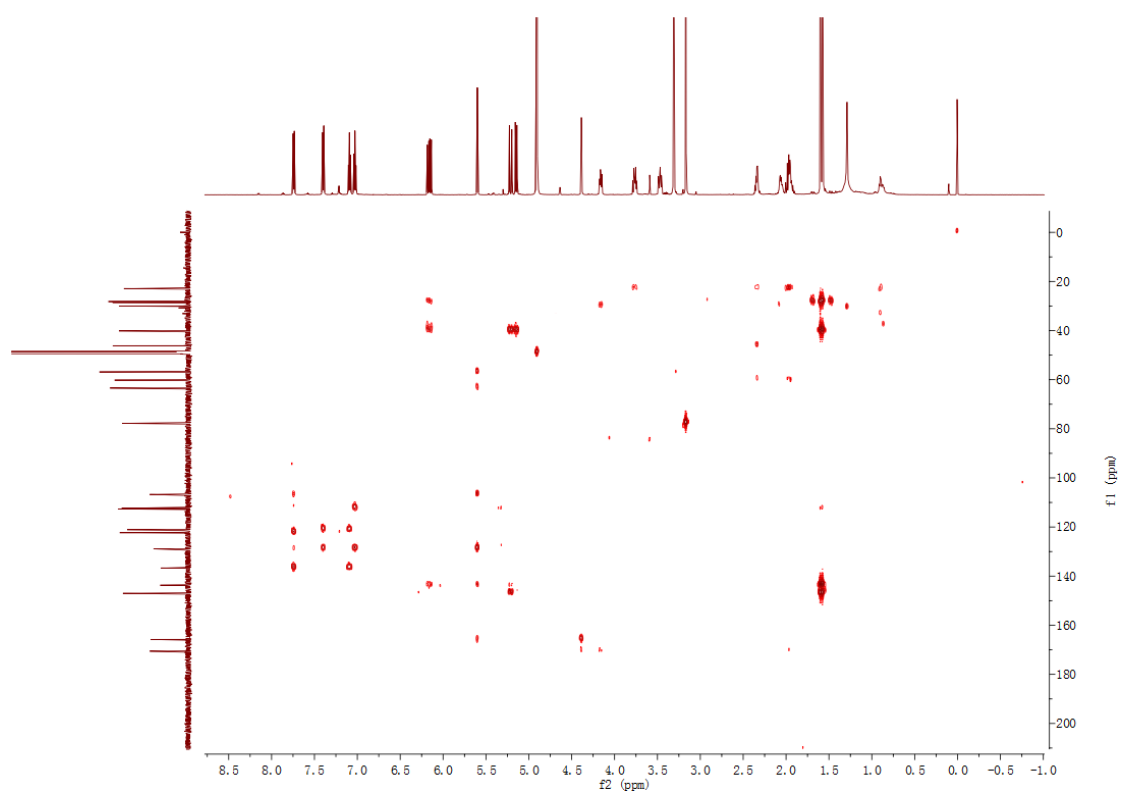


Figure S33 HMBC spectrum (600 MHz, methanol- $d_4$ ) of compound **5**

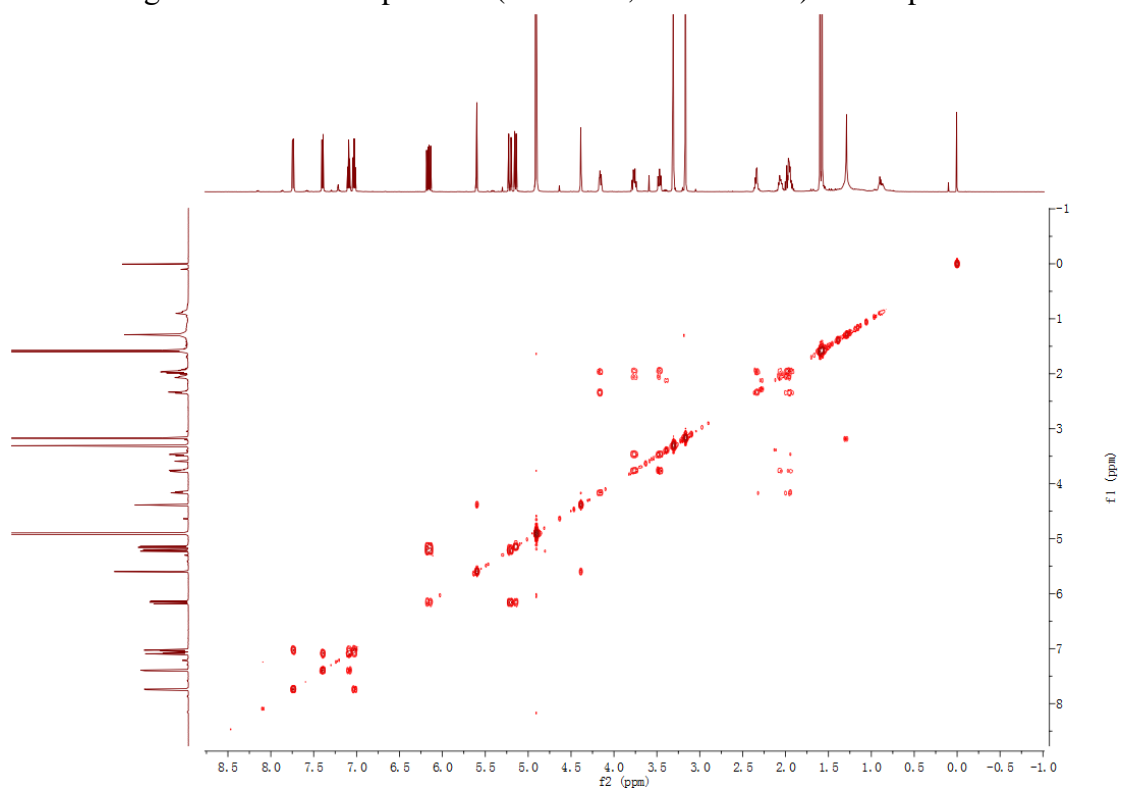
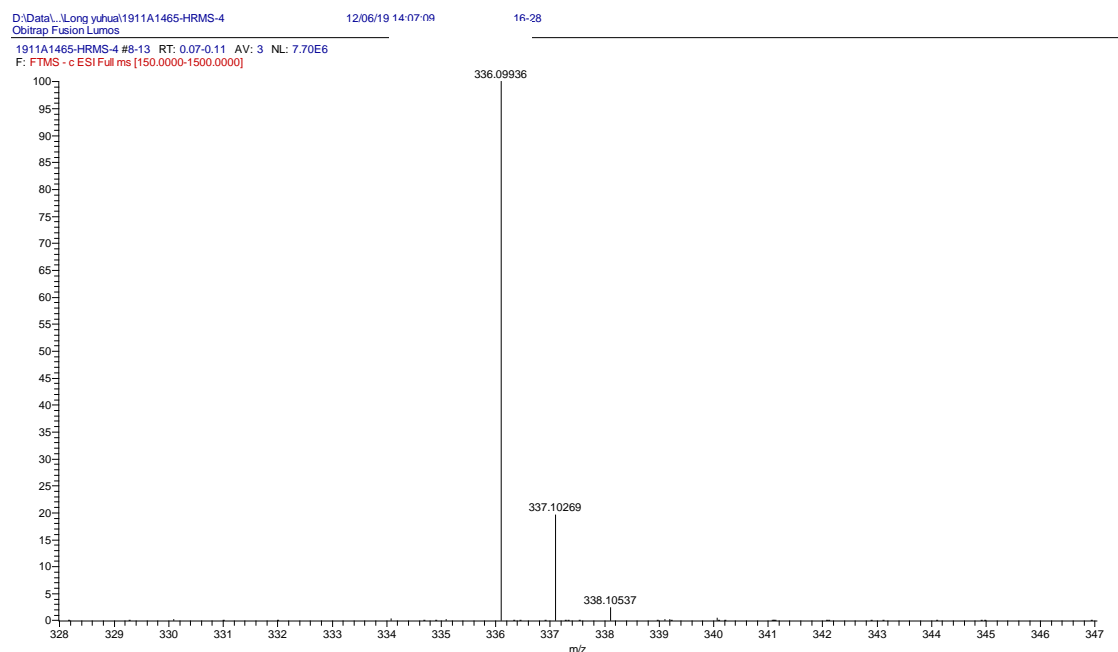


Figure S34  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz, methanol- $d_4$ ) of compound **5**



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
336.09936	336.09898	1.13	13.5	C <sub>18</sub> H <sub>14</sub> O <sub>4</sub> N <sub>3</sub>

Figure S35 HRESIMS of compound **6**

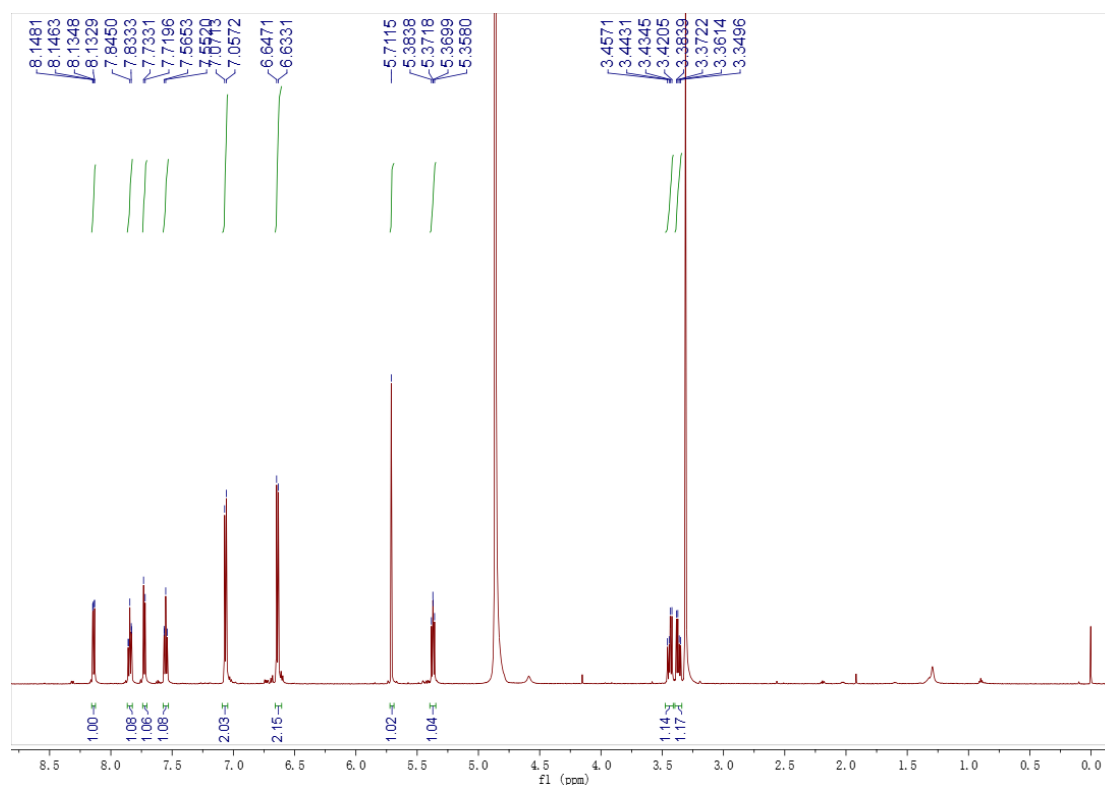


Figure S36 <sup>1</sup>H NMR spectrum (600 MHz, methanol-*d*<sub>4</sub>) of compound **6**

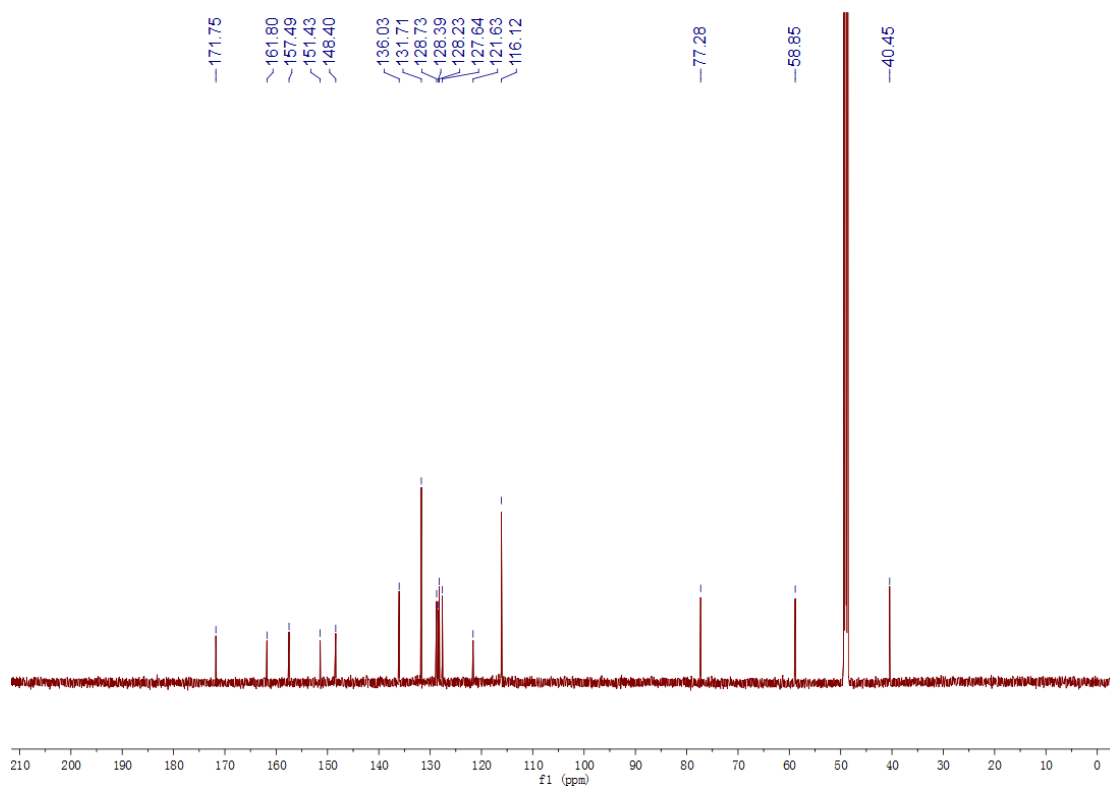


Figure S37  $^{13}\text{C}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **6**

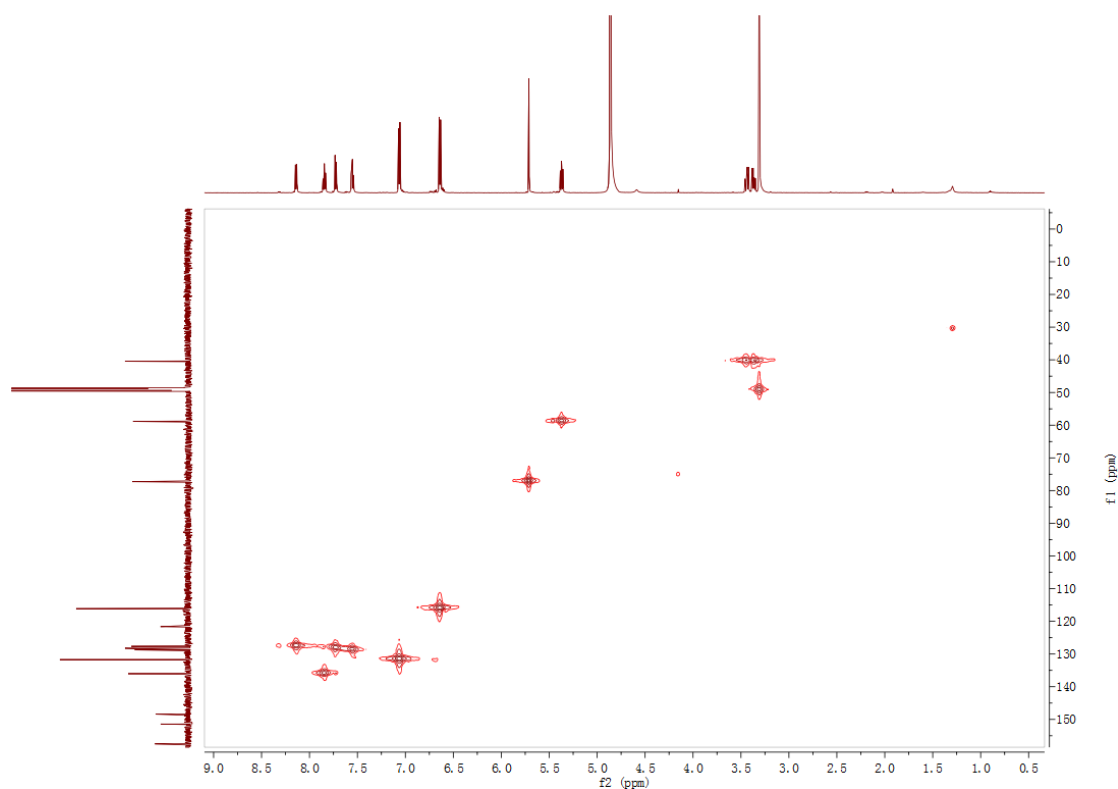


Figure S38 HMQC spectrum (600 MHz, methanol- $d_4$ ) of compound **6**

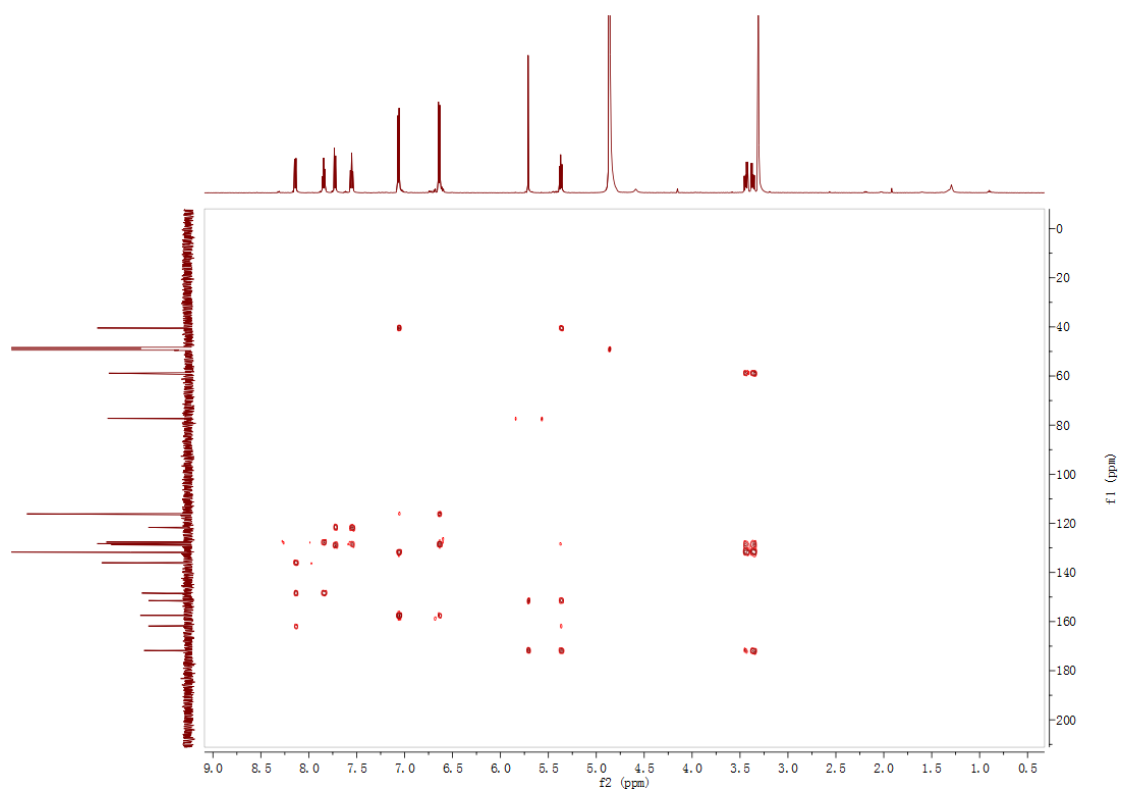


Figure S39 HMBC spectrum (600 MHz, methanol- $d_4$ ) of compound **6**

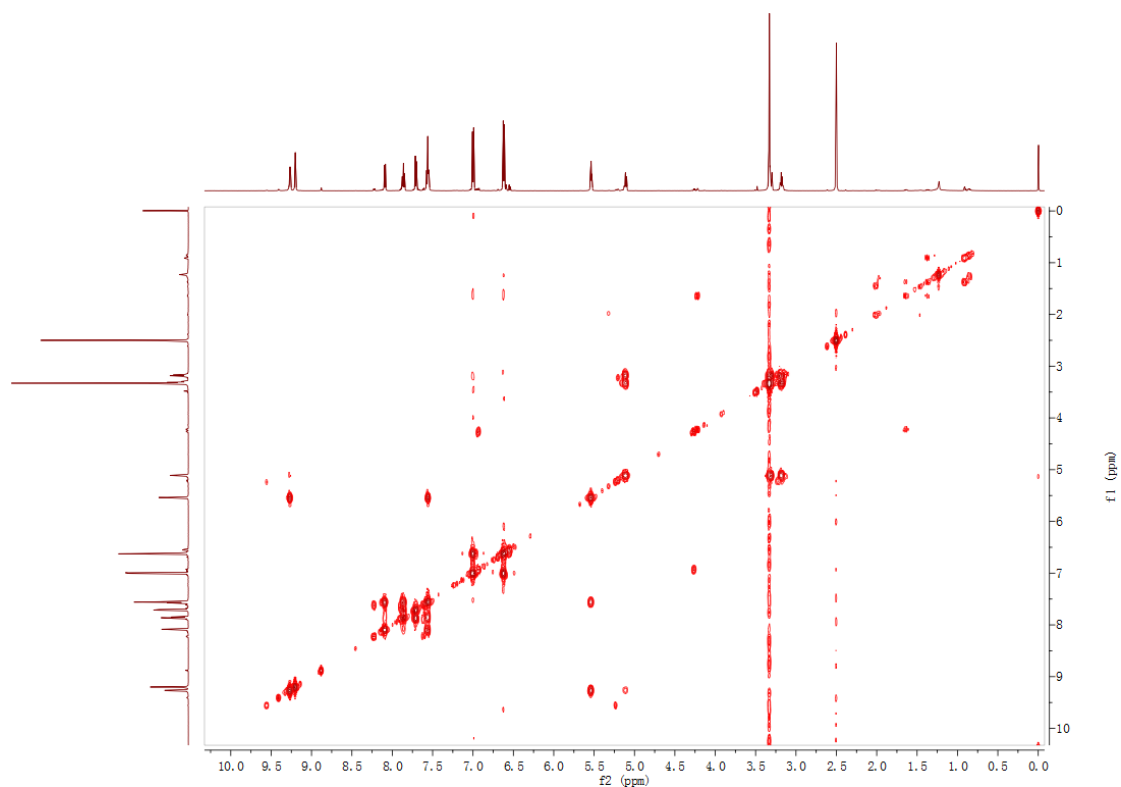


Figure S40  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz, methanol- $d_4$ ) of compound **6**

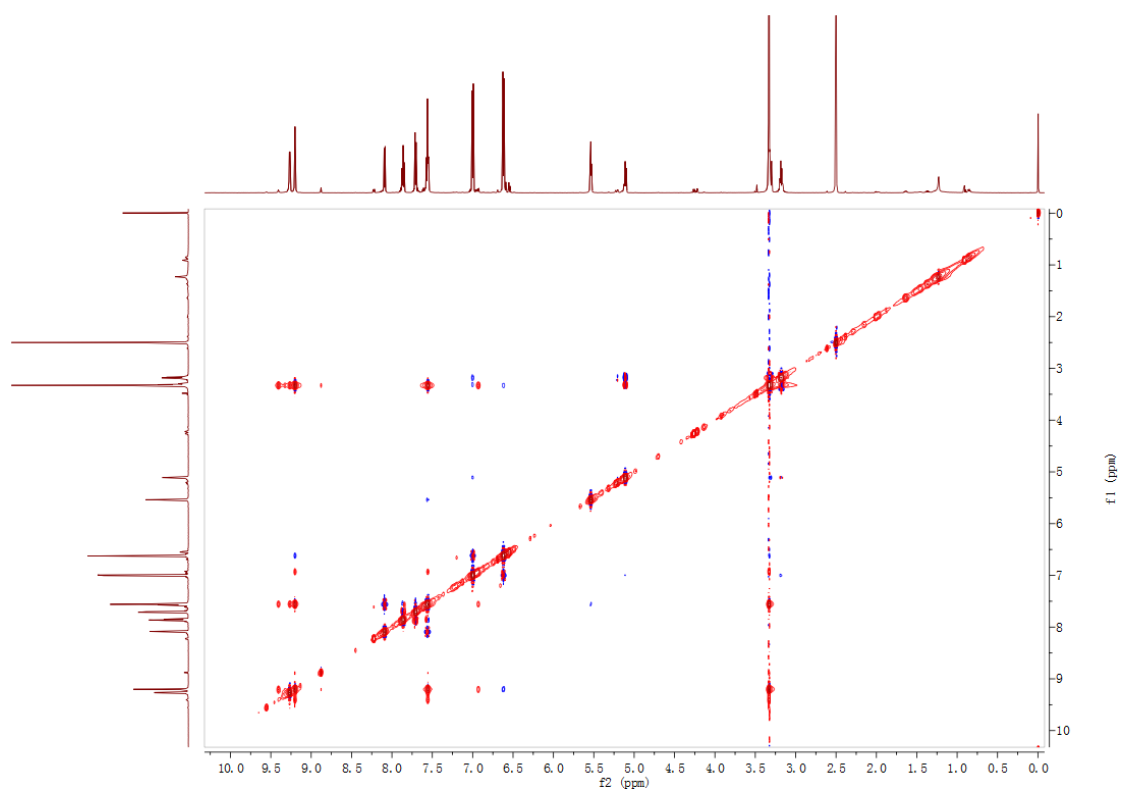


Figure S41 NOESY spectrum (600 MHz, DMSO- $d_6$ ) of compound **6**

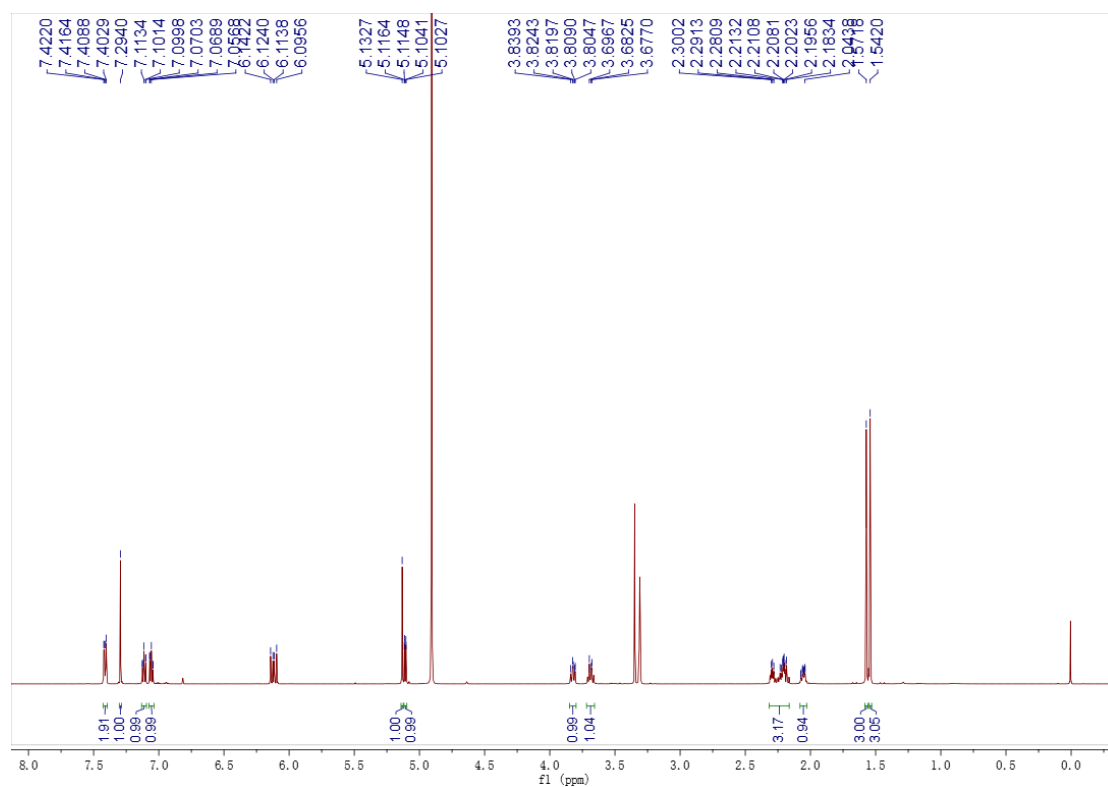


Figure S42  $^1\text{H}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **7**



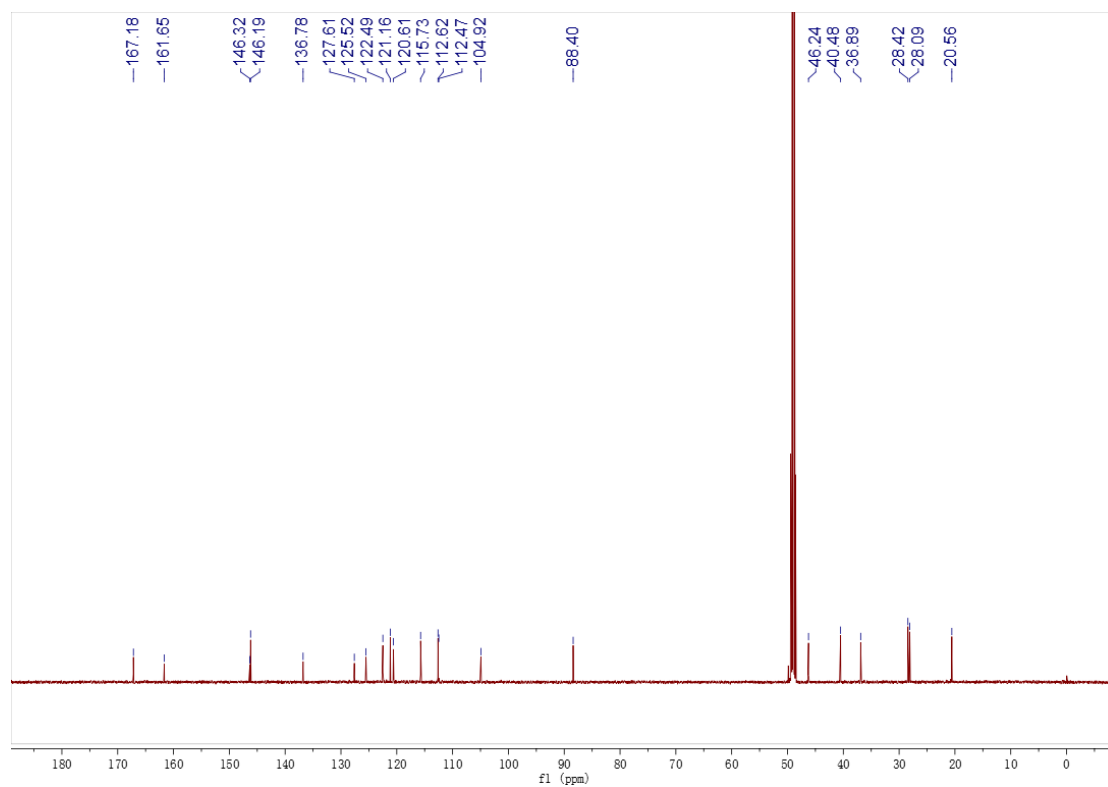


Figure S43  $^{13}\text{C}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **7**

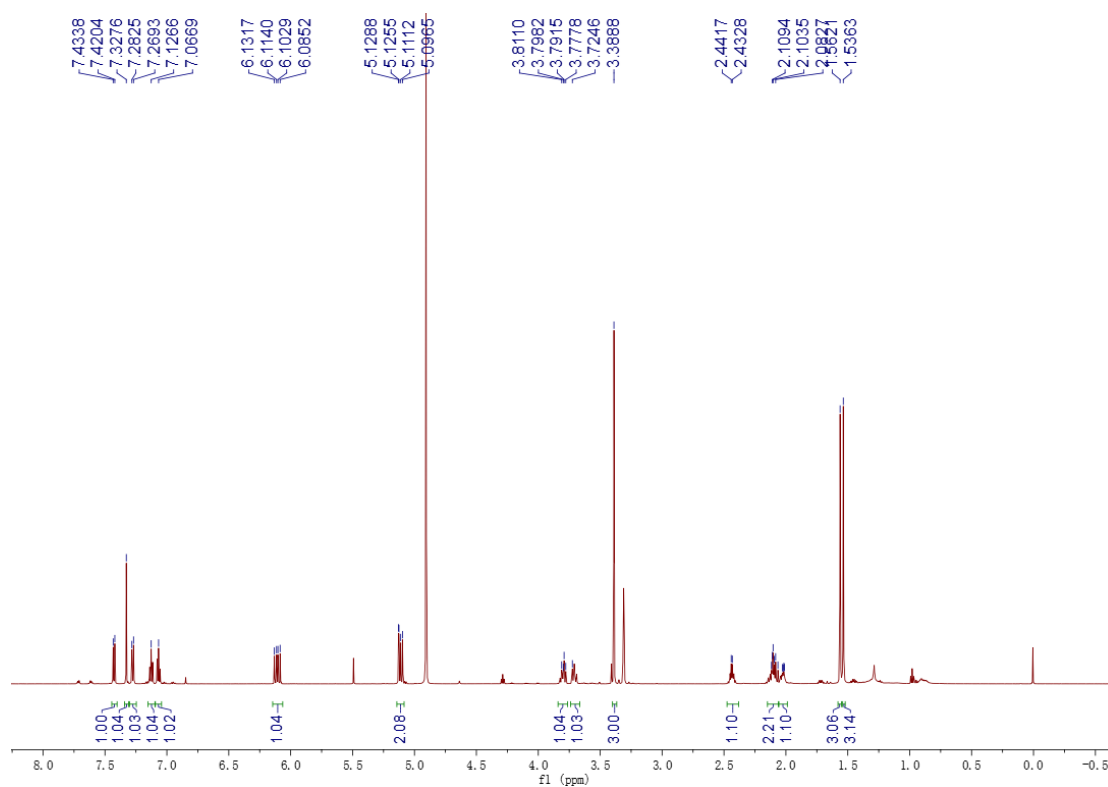


Figure S44  $^1\text{H}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **8**

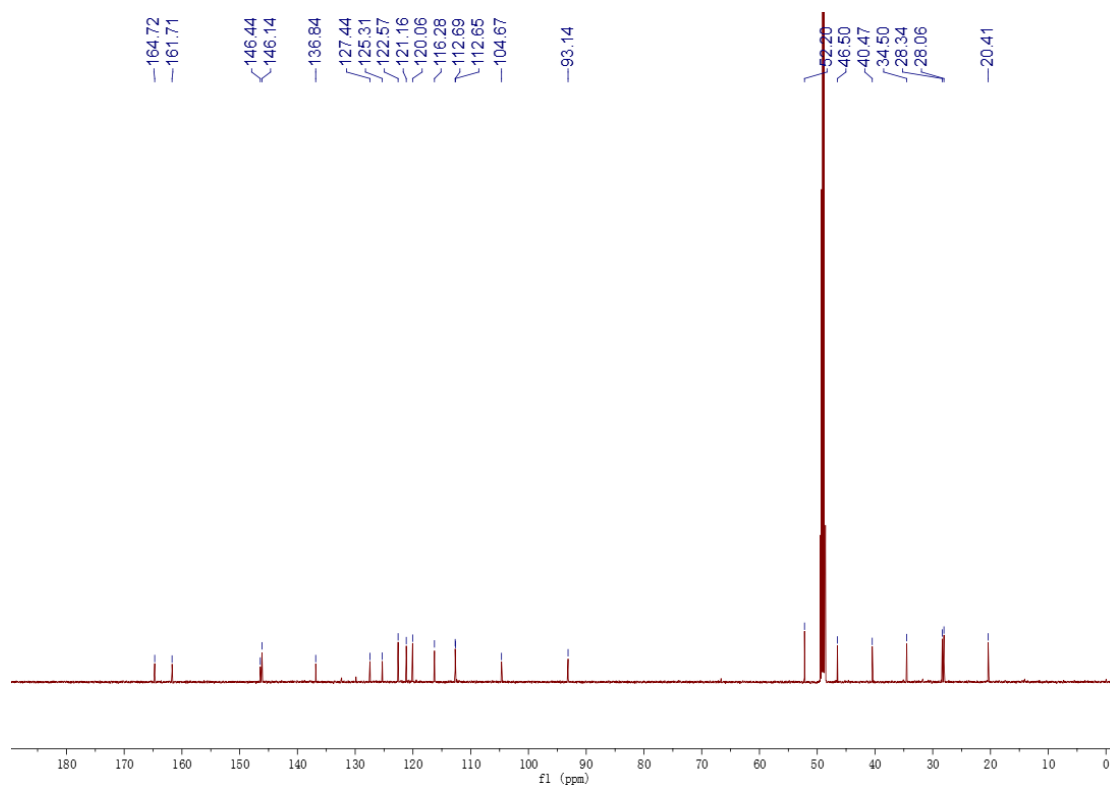


Figure S45  $^{13}\text{C}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **8**

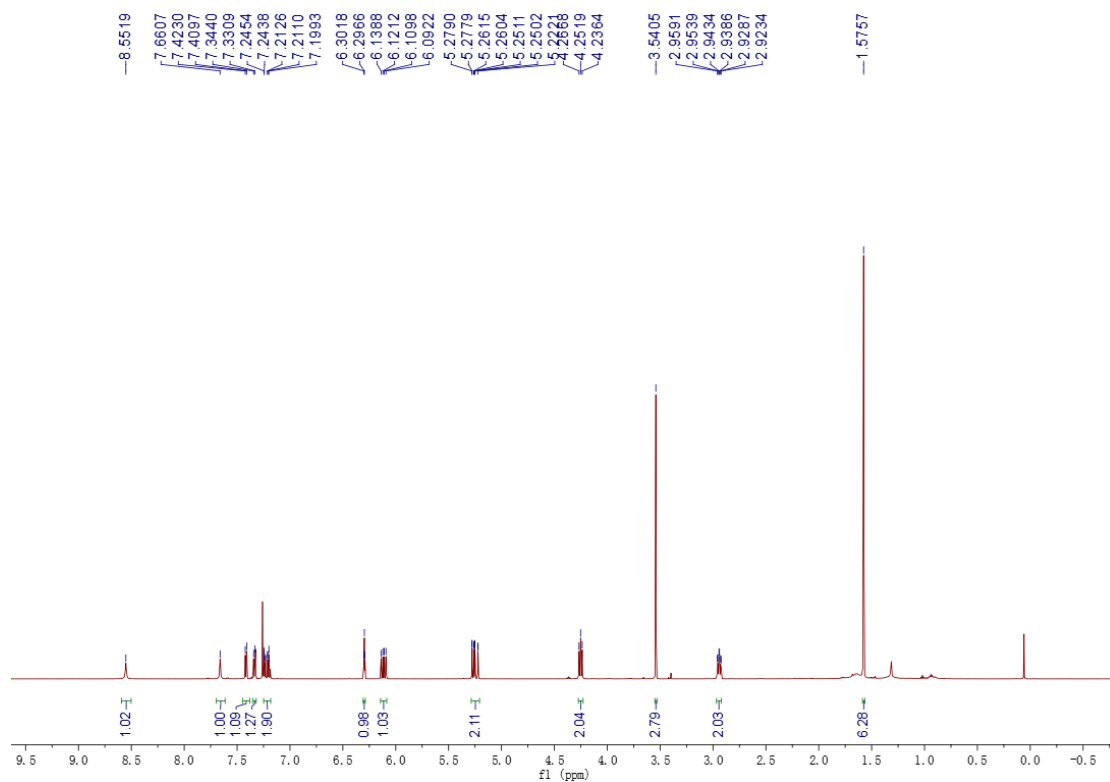


Figure S46  $^1\text{H}$  NMR spectrum (600 MHz, chloroform- $d$ ) of compound **9**

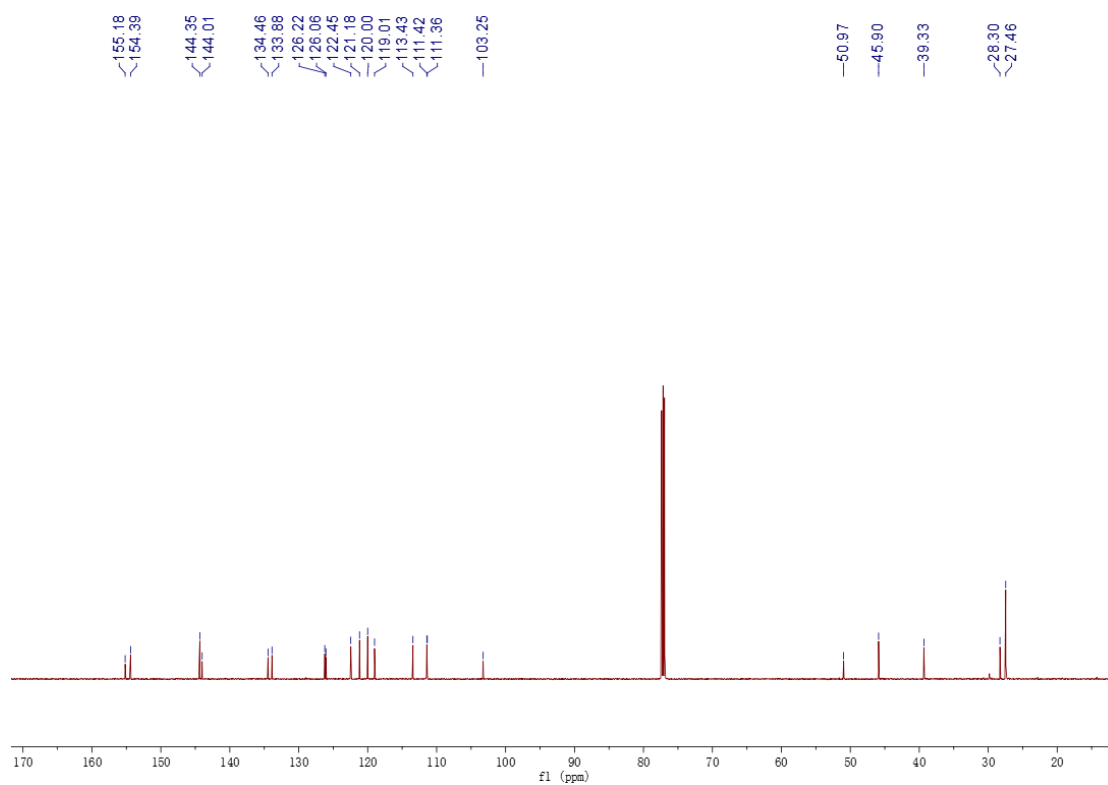


Figure S47  $^{13}\text{C}$  NMR spectrum (600 MHz, chloroform- $d$ ) of compound **9**

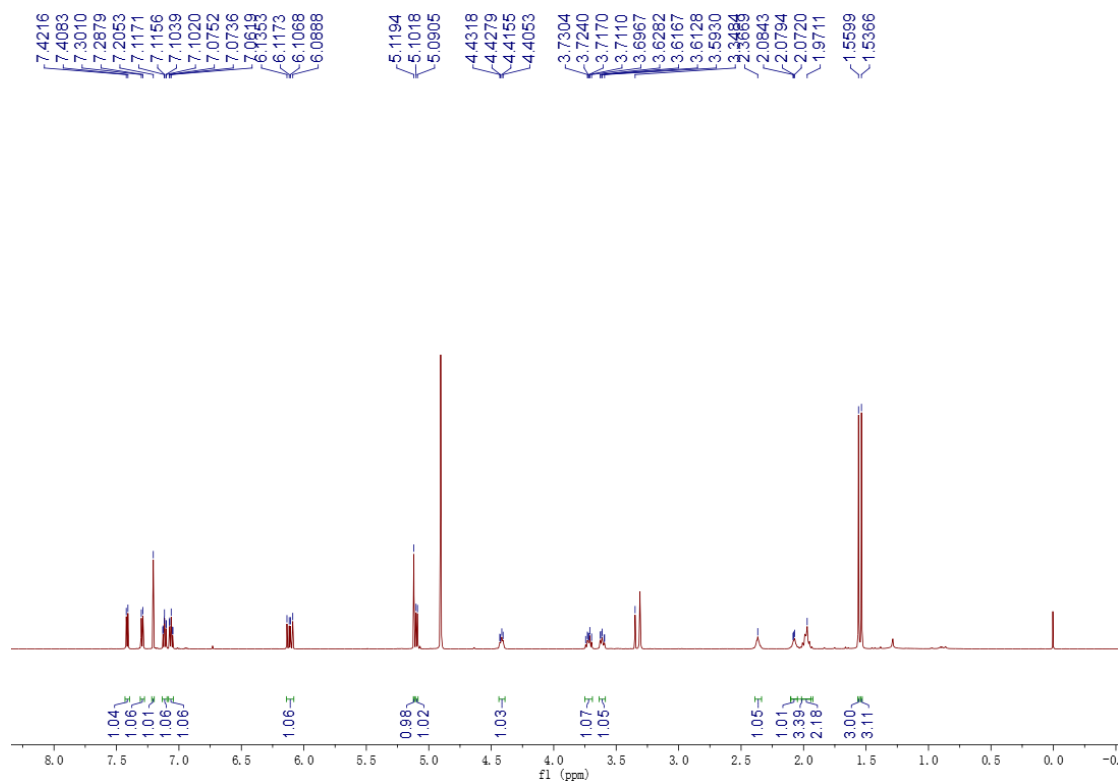


Figure S48  $^1\text{H}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **10**

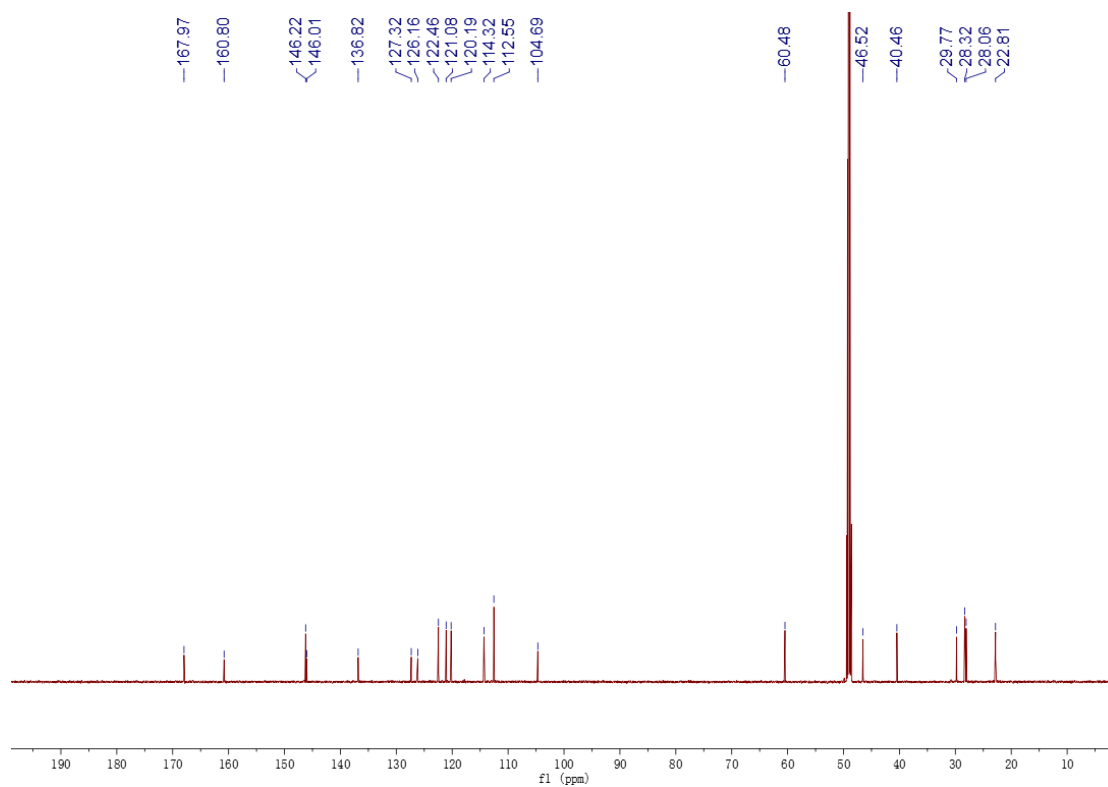


Figure S49  $^{13}\text{C}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **10**

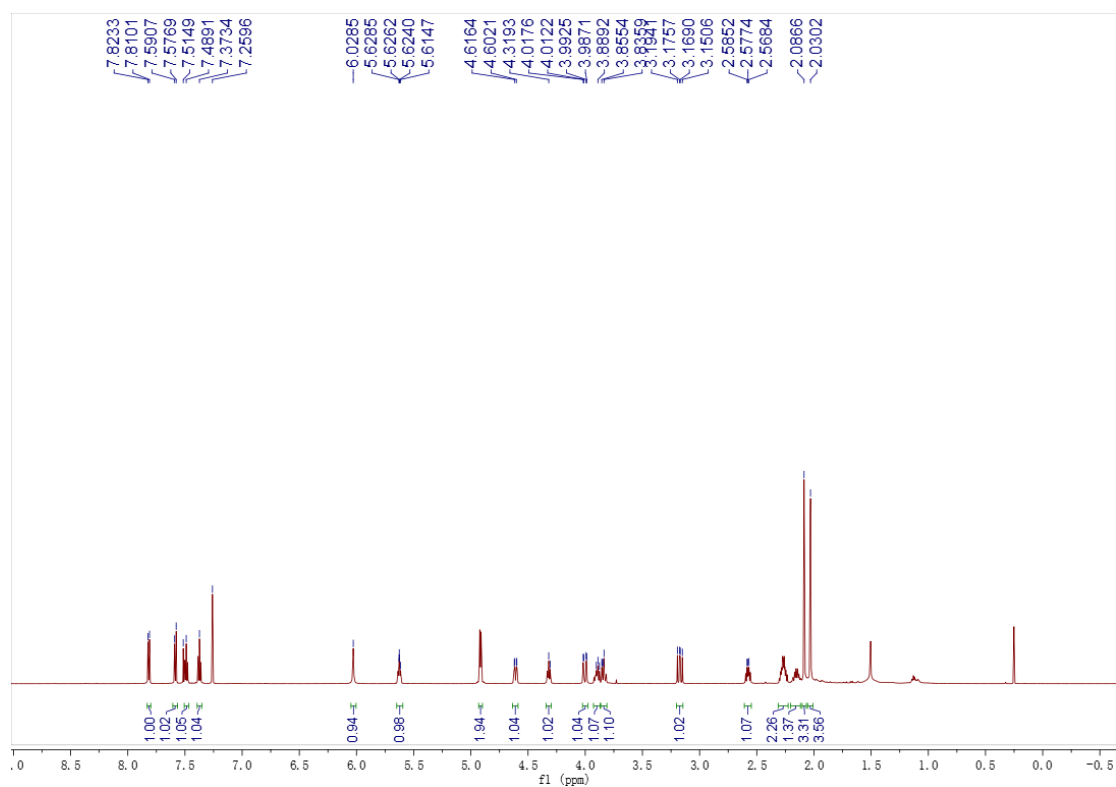


Figure S50  $^1\text{H}$  NMR spectrum (600 MHz, chloroform- $d$ ) of compound **11**

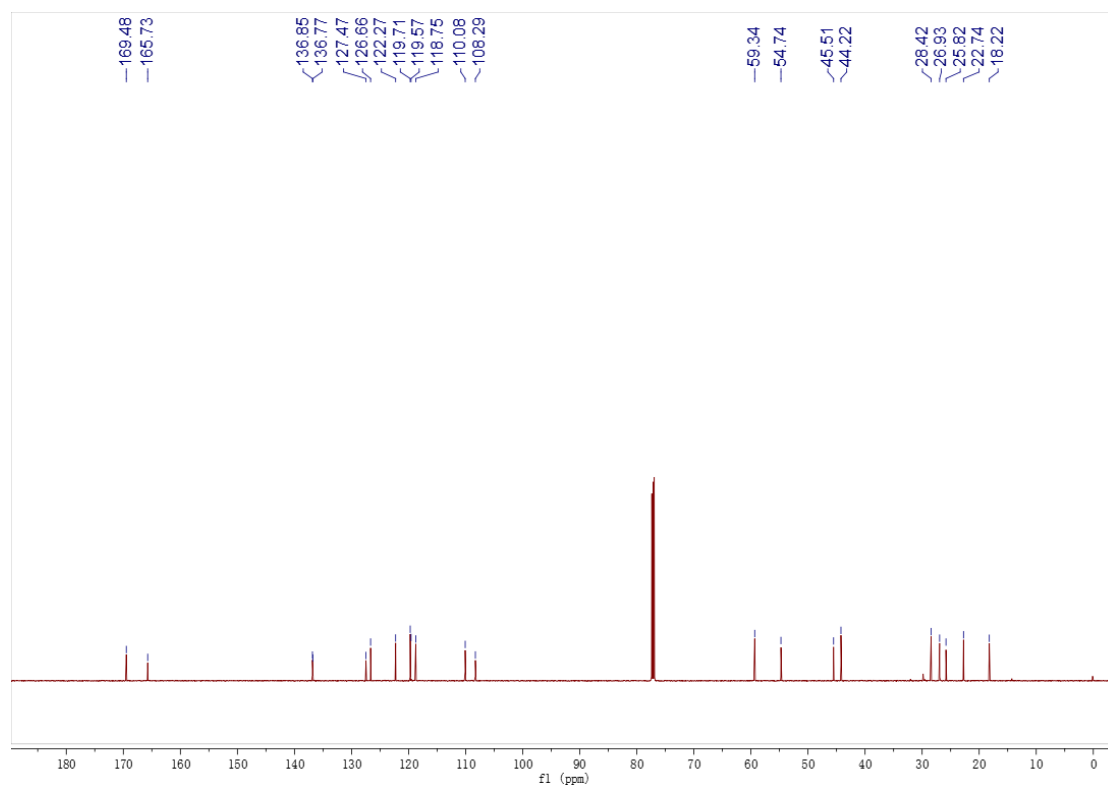


Figure S51  $^{13}\text{C}$  NMR spectrum (600 MHz, chloroform-*d*) of compound **11**

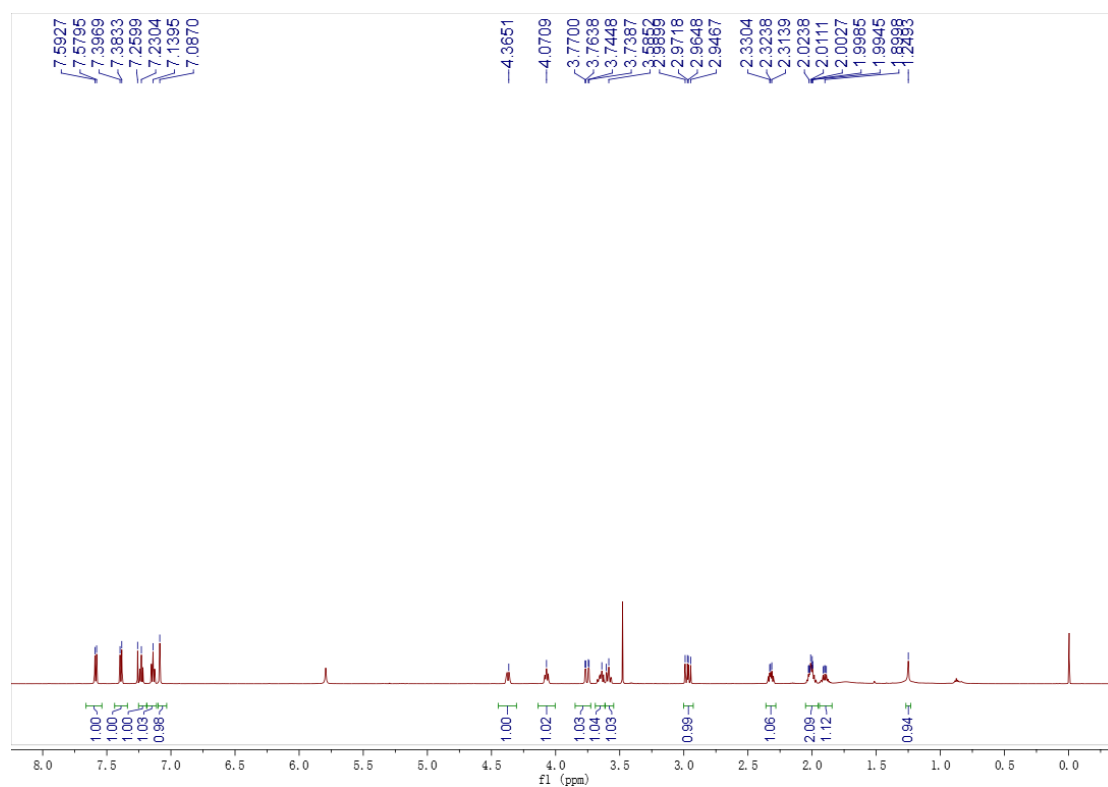


Figure S52  $^1\text{H}$  NMR spectrum (600 MHz, chloroform-*d*) of compound **12**

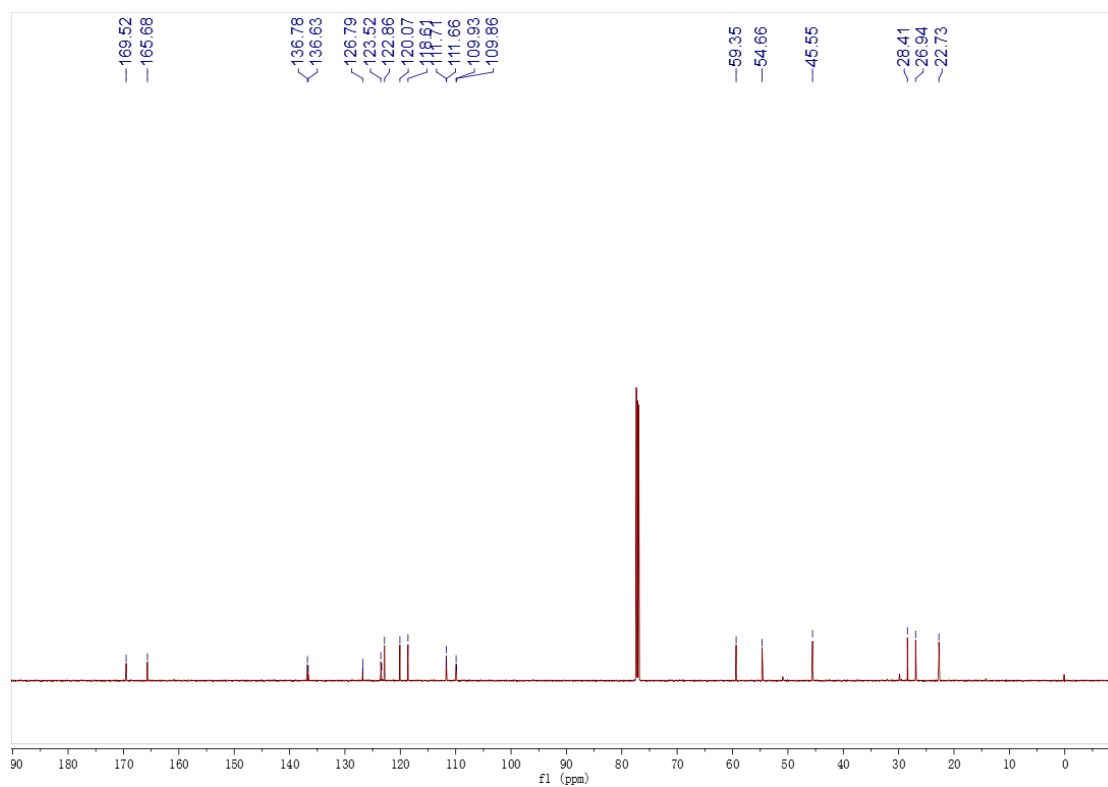


Figure S53  $^{13}\text{C}$  NMR spectrum (600 MHz, chloroform- $d$ ) of compound **12**

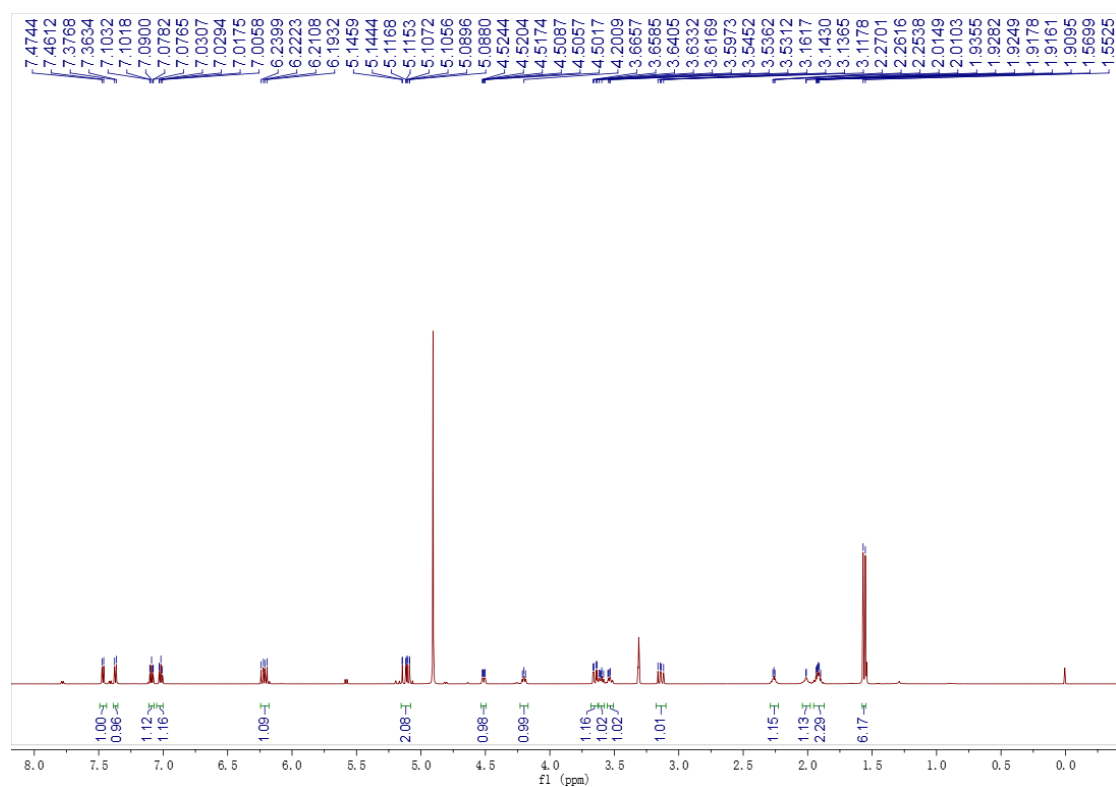


Figure S54  $^1\text{H}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **13**

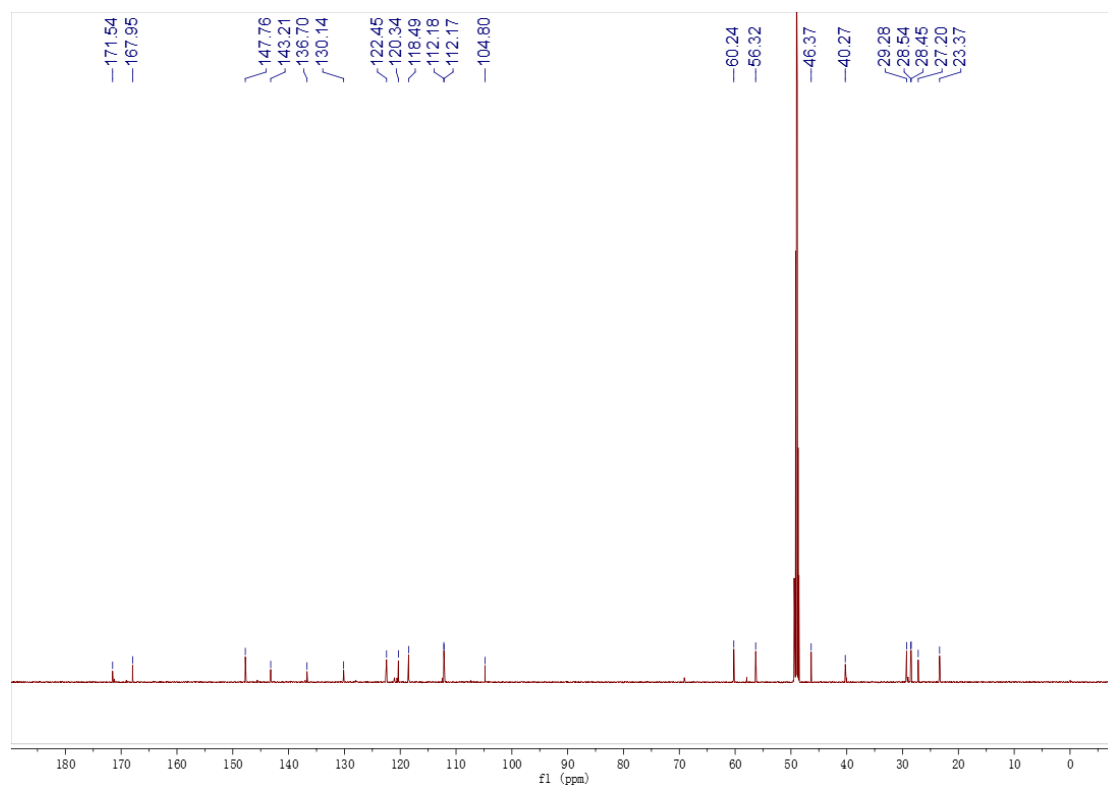


Figure S55  $^{13}\text{C}$  NMR spectrum (600 MHz, methanol- $d_4$ ) of compound **13**

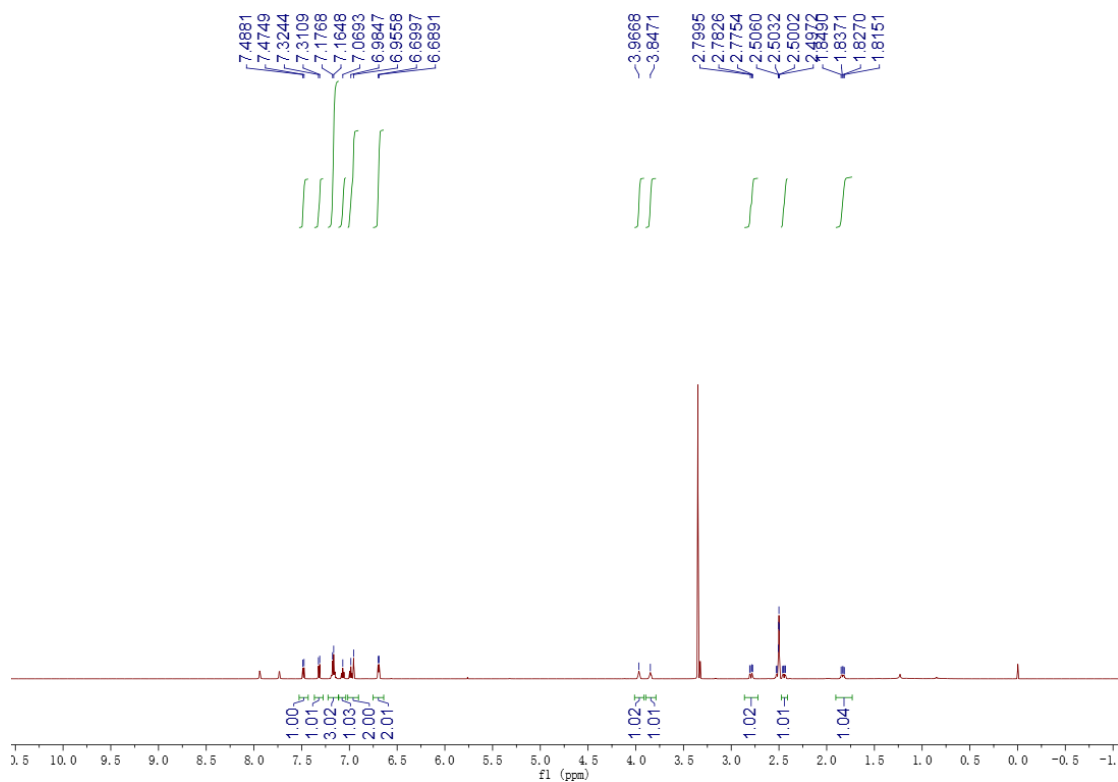


Figure S56  $^1\text{H}$  NMR spectrum (600 MHz, DMSO- $d_6$ ) of compound **14**

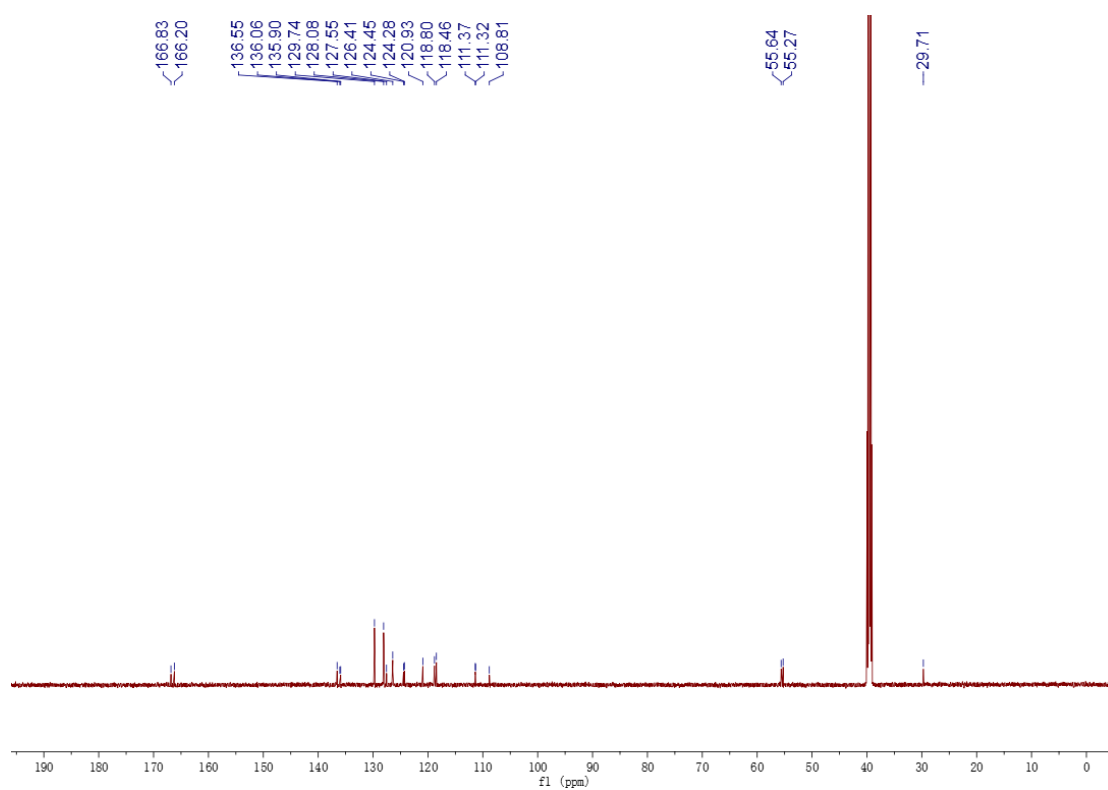


Figure S57  $^{13}\text{C}$  NMR spectrum (600 MHz,  $\text{DMSO-}d_4$ ) of compound **14**

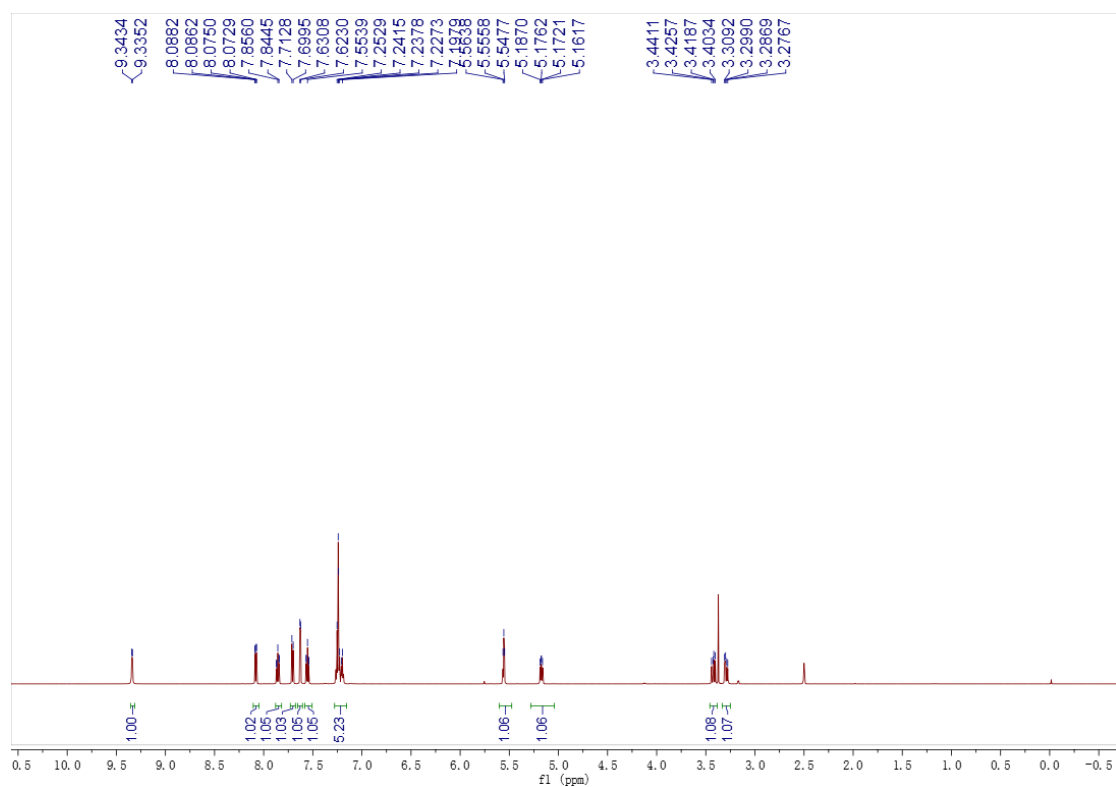


Figure S58  $^1\text{H}$  NMR spectrum (600 MHz,  $\text{DMSO-}d_6$ ) of compound **15**



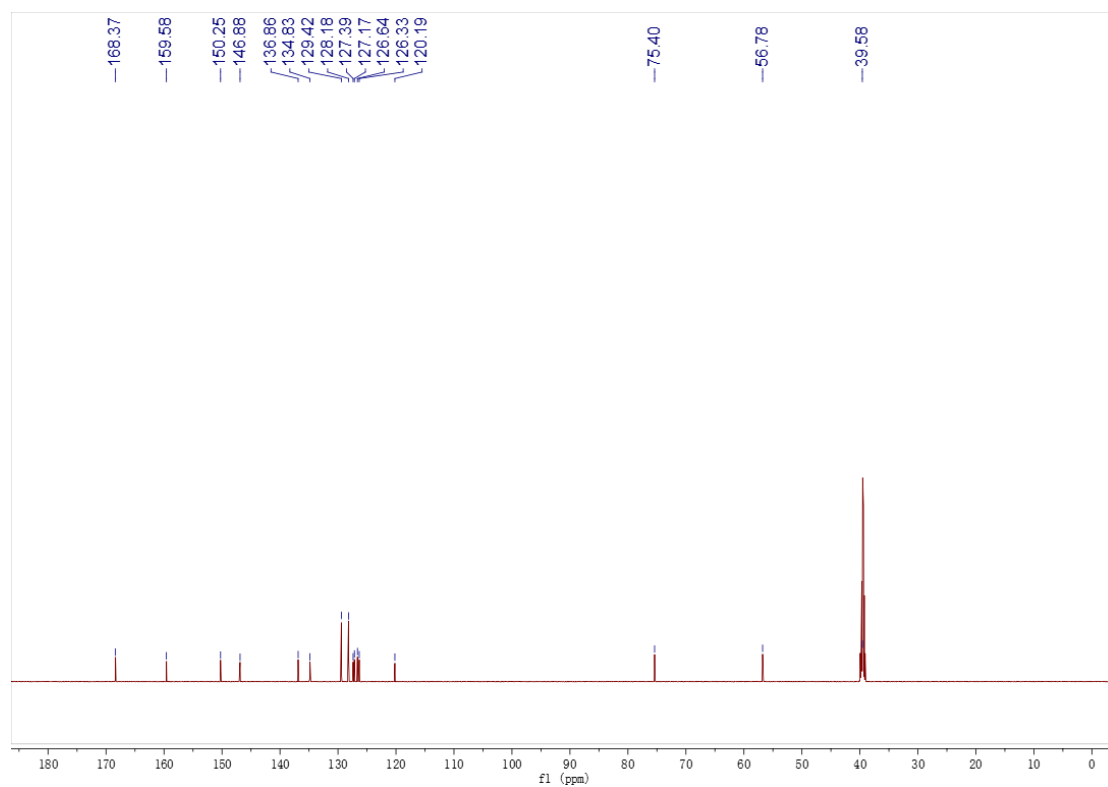


Figure S59 <sup>13</sup>C NMR spectrum (600 MHz, DMSO-*d*<sub>4</sub>) of compound **15**

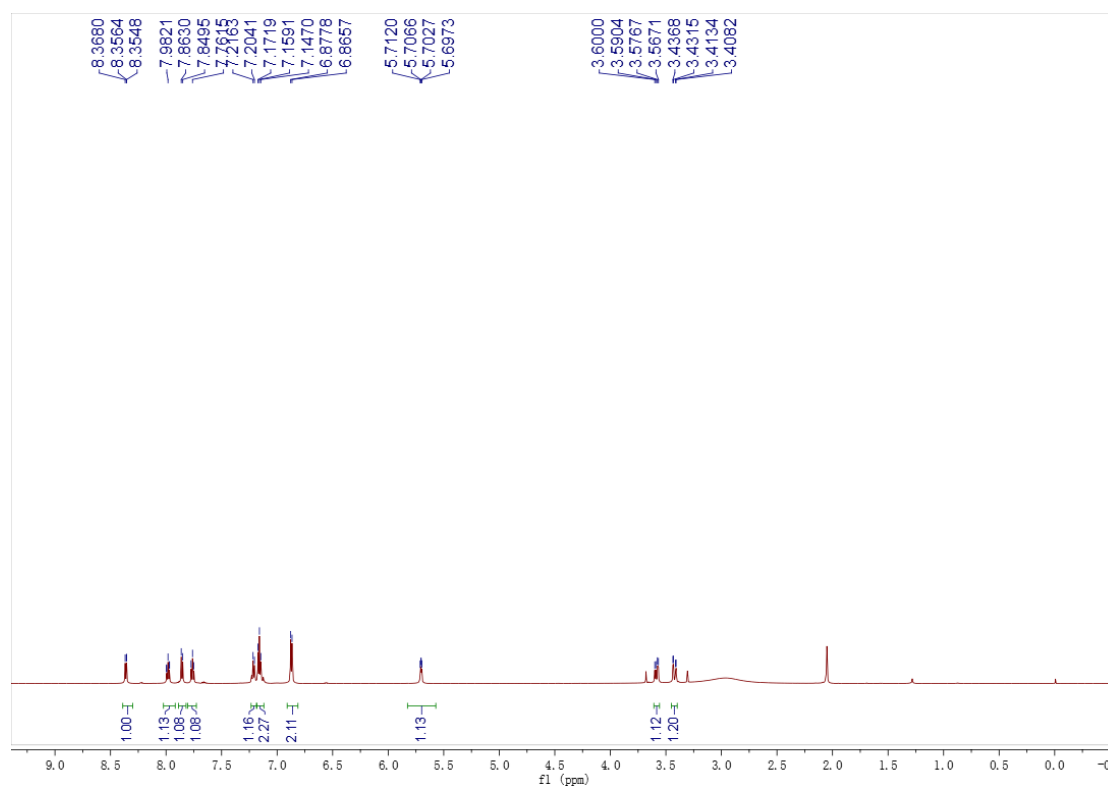


Figure S60 <sup>1</sup>H NMR spectrum (600 MHz, acetone-*d*<sub>6</sub>) of compound **16**

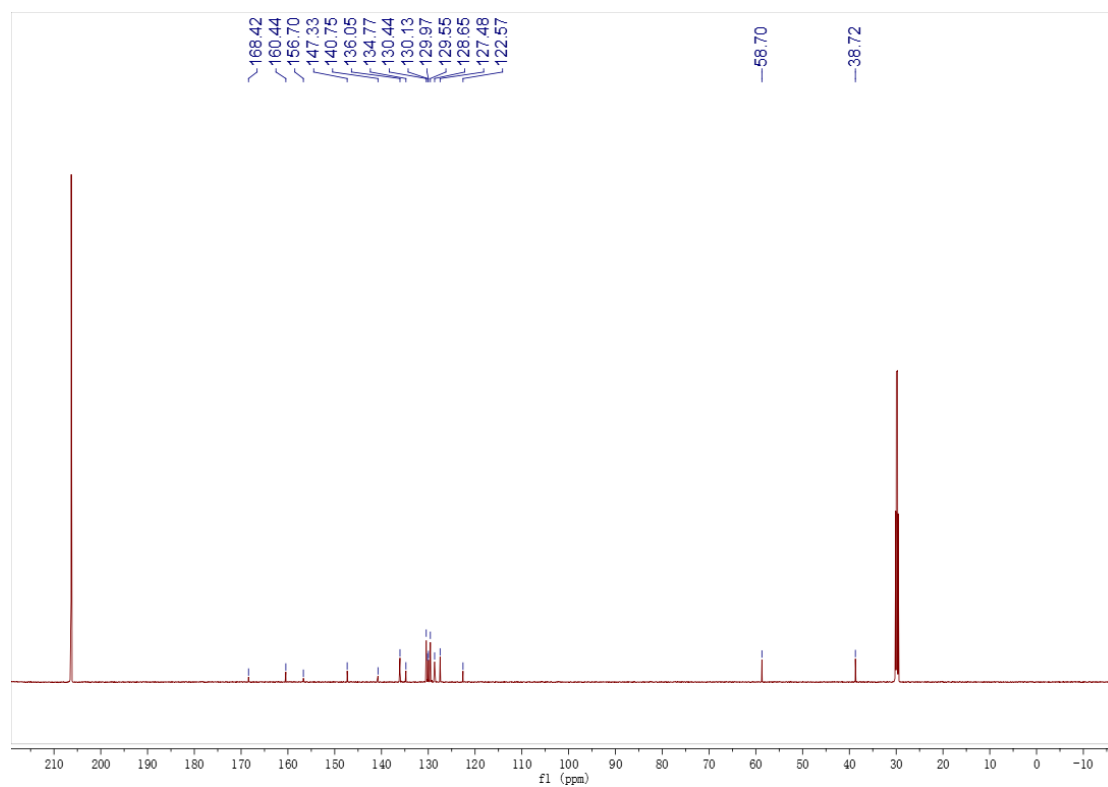


Figure S61  $^{13}\text{C}$  NMR spectrum (600 MHz, acetone- $d_4$ ) of compound **16**