

## Supporting Information

New Cytotoxic Cytochalasans from A Plant-Associated Fungus *Chaetomium globosum* kz-19

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Figure S1:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}D_6$ ) spectrum of **1**

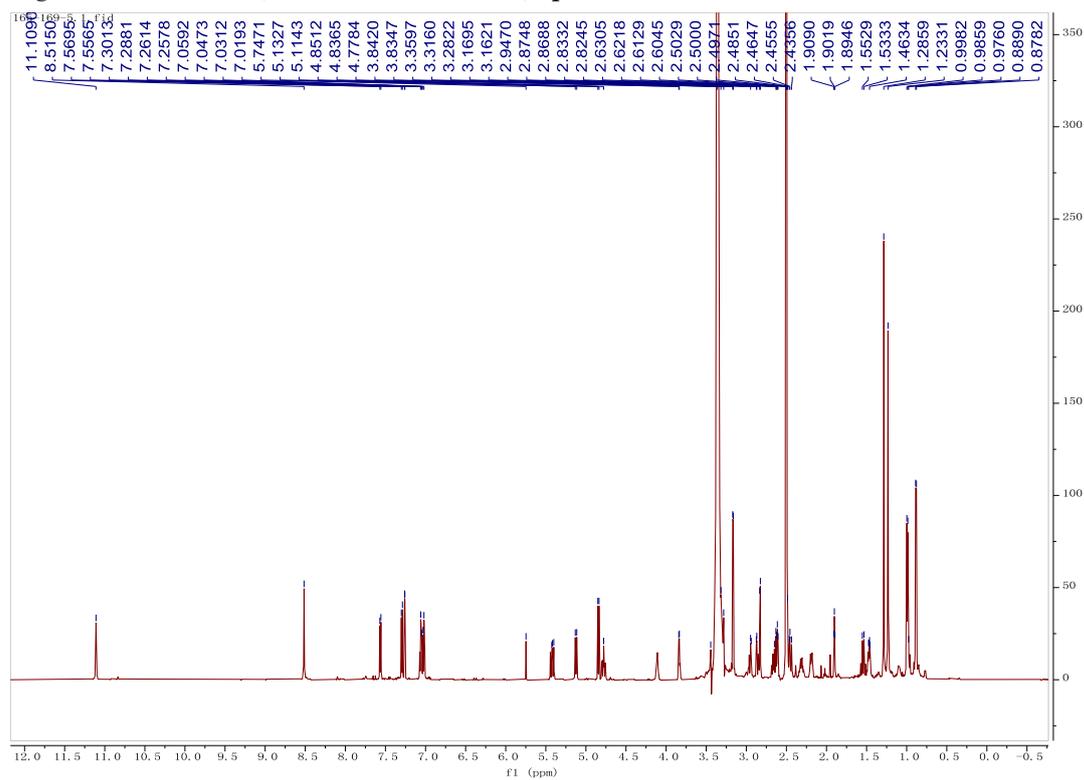


Figure S2:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}D_6$ ) spectrum of **1**

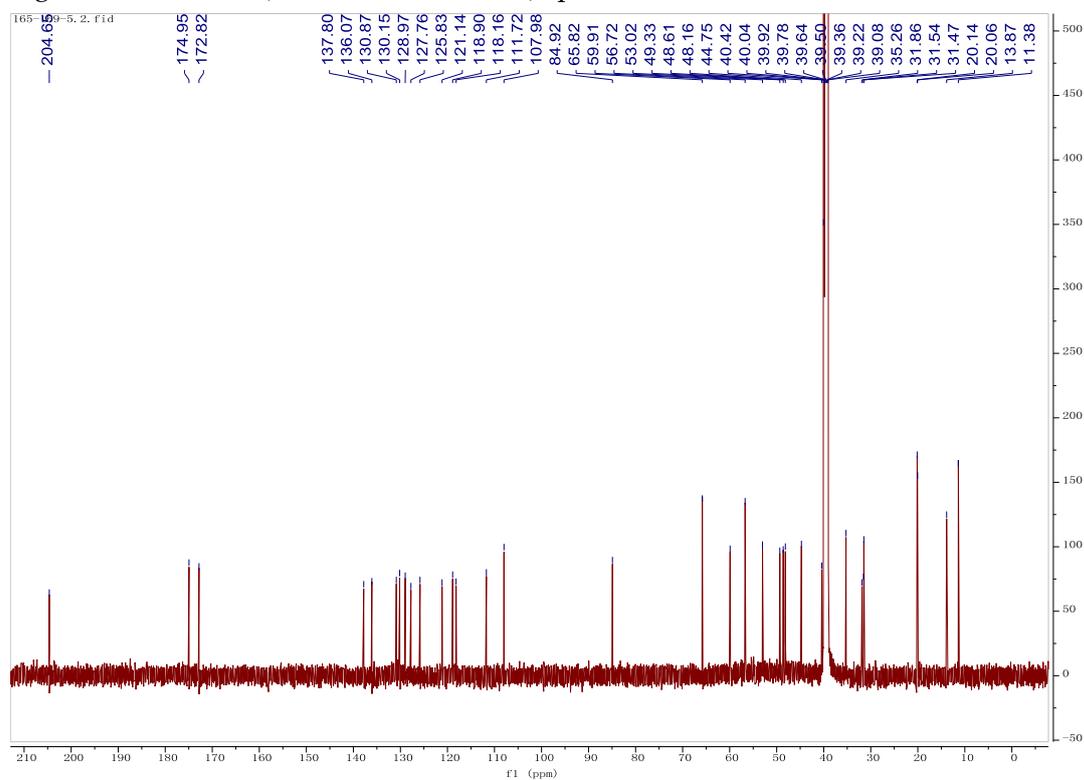


Figure S3: HSQC spectrum of 1

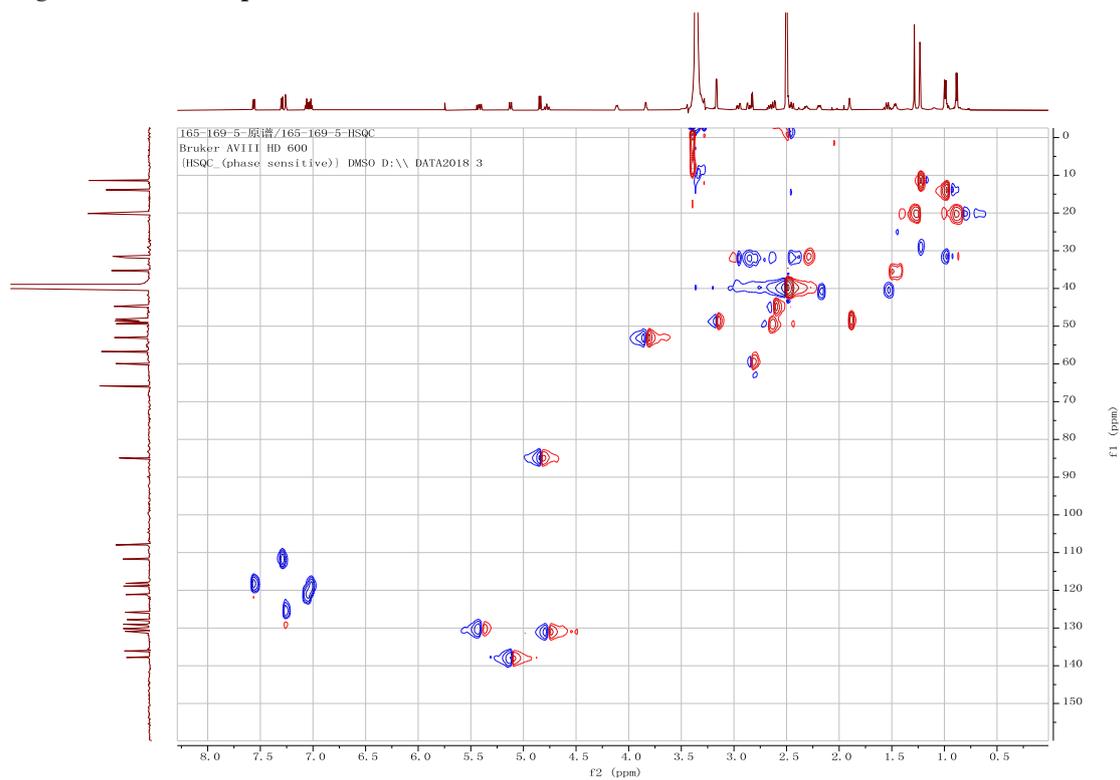


Figure S4: HMBC spectrum of 1

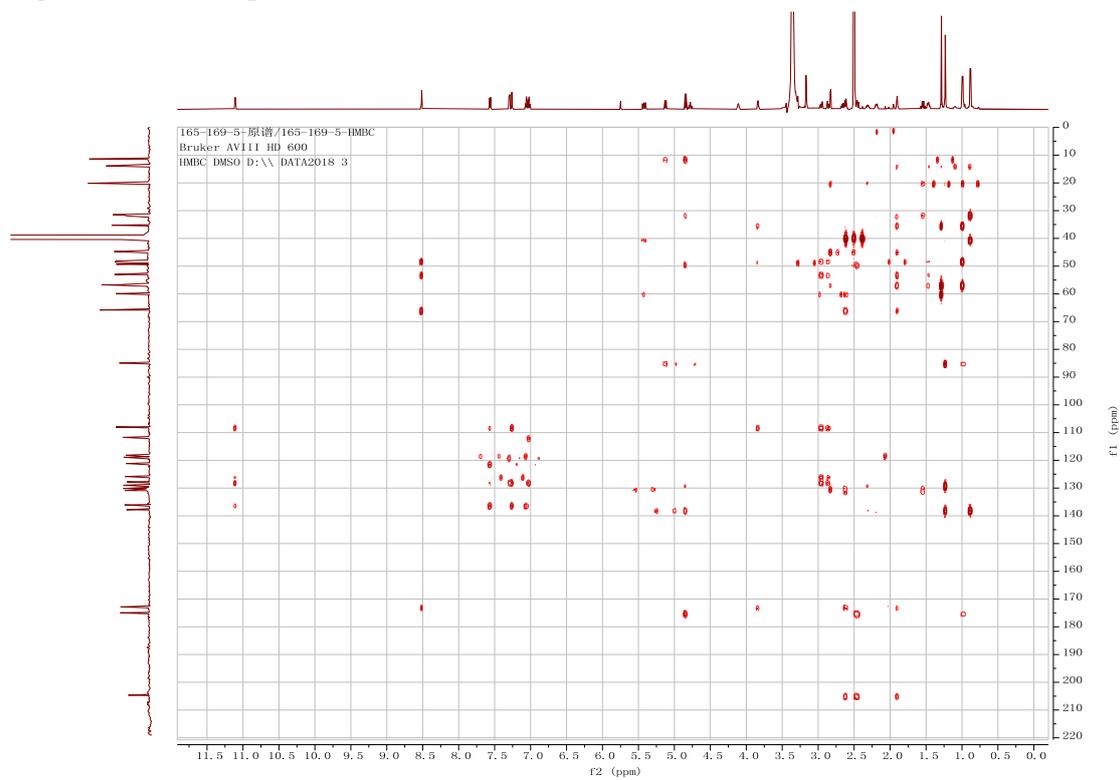


Figure S5:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**

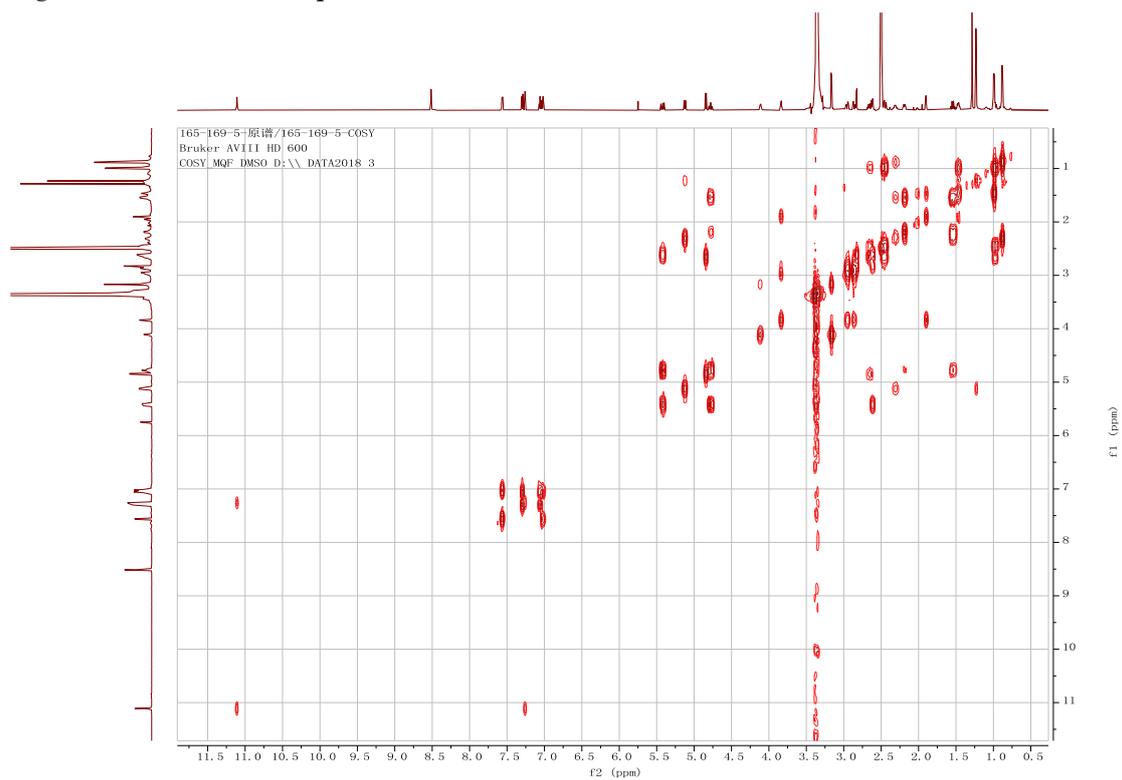


Figure S6: TOCSY spectrum of **1**

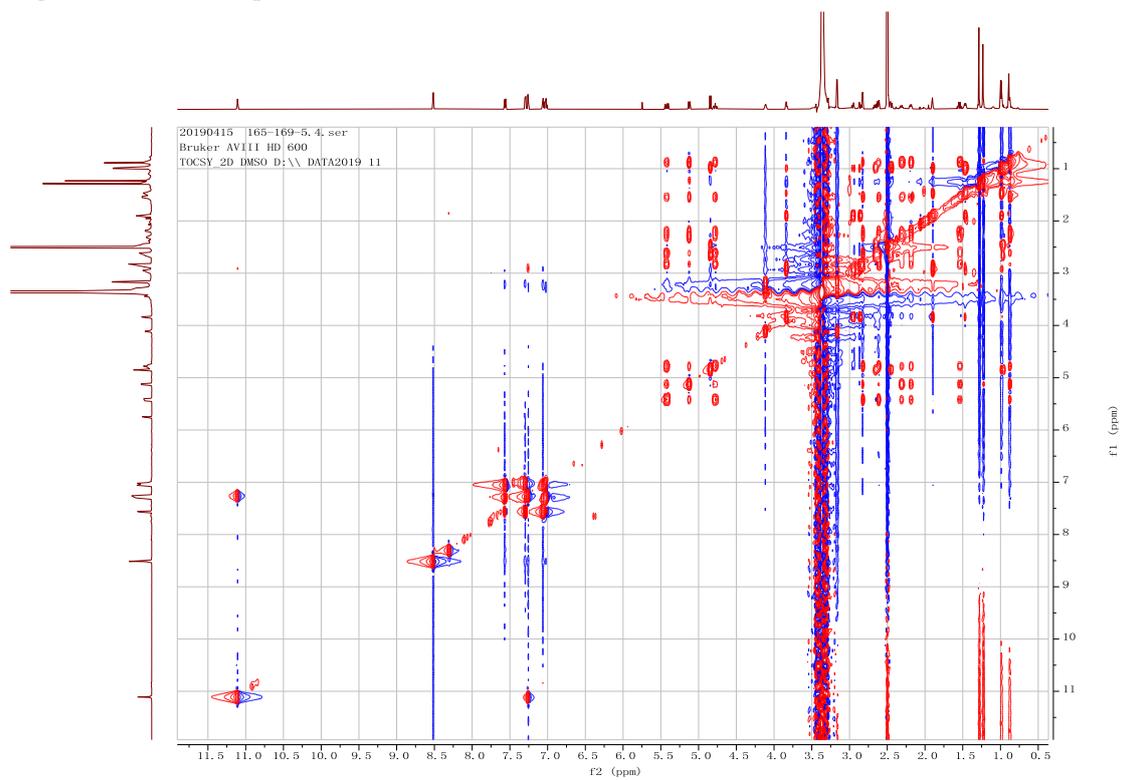


Figure S7: NOESY spectrum of **1**

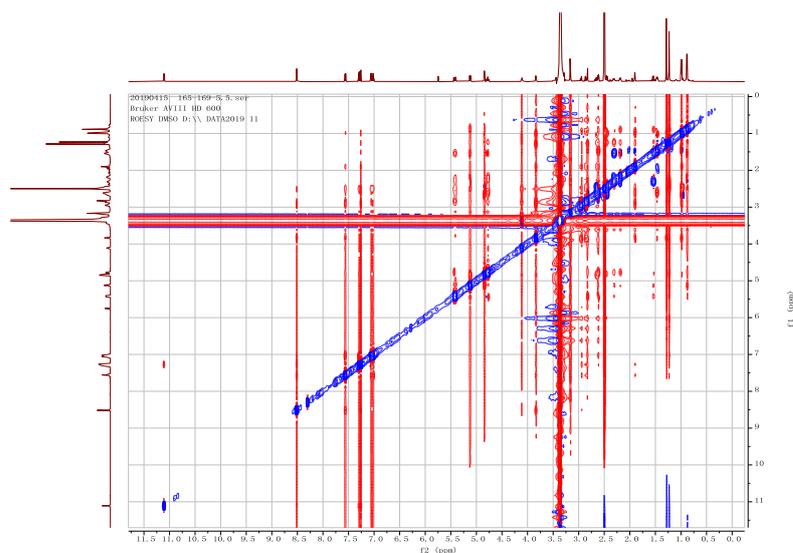


Figure S8: HR ESIMS spectrum of **1**

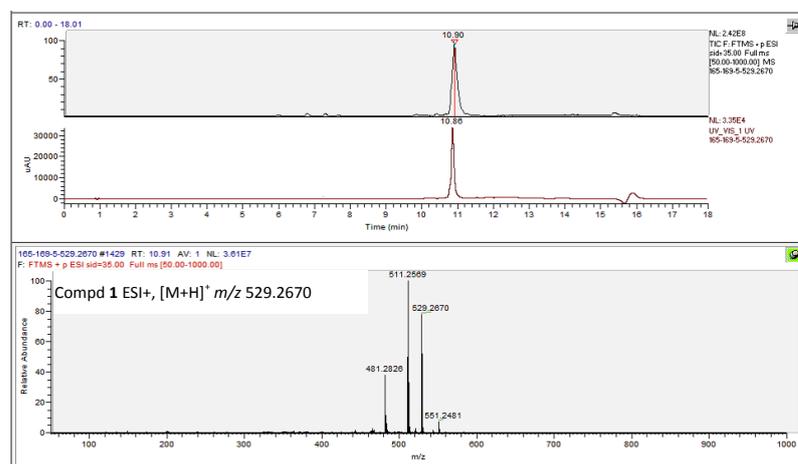


Figure S9: ECD and UV spectrum of **1**

TDDFT theory,  $\omega$ B3LYP functional and 6-311G(d,p) level of theory, methanol as solvent for structural optimization, compound **1** have 9 conformations, of which 2 conformations have Boltzmann content >1%, listed in the table. The calculated result of **1** is consistent with the experimental result, and the absolute configuration of **1** is confirmed as shown in the figure below ( $\sigma=0.30\text{eV}$ ).

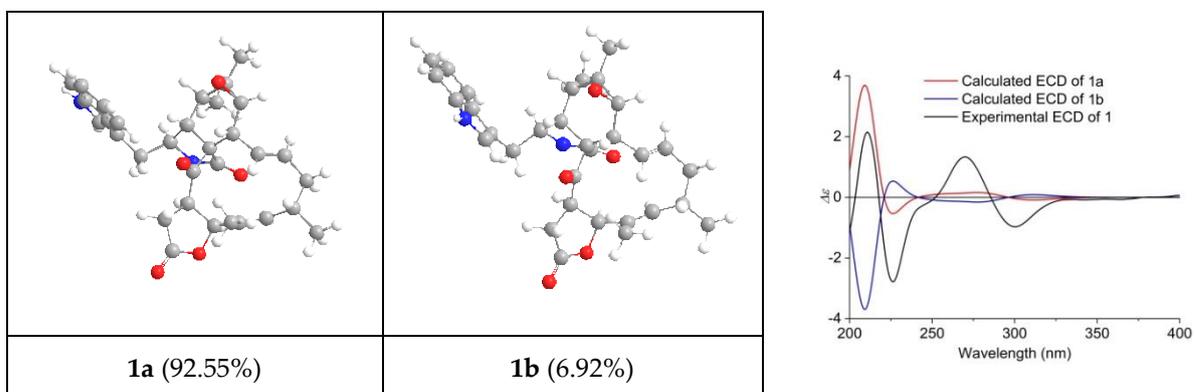


Figure S10:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}D_6$ ) spectrum of **2**

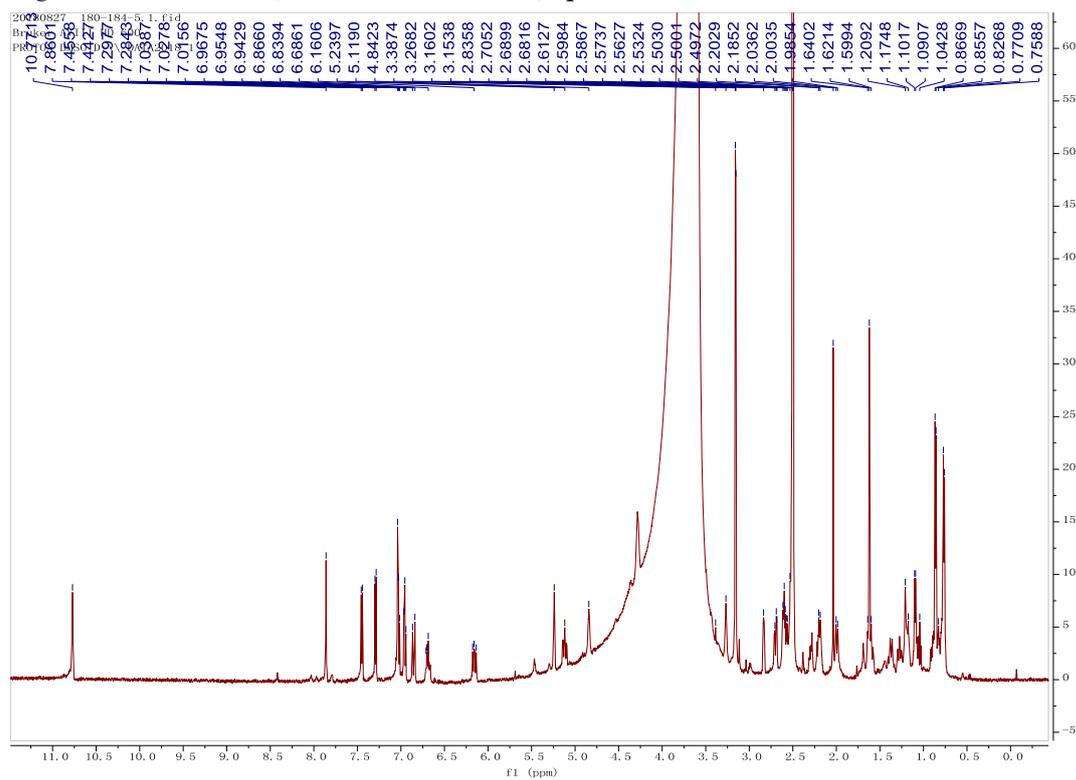


Figure S11:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}D_6$ ) spectrum of **2**

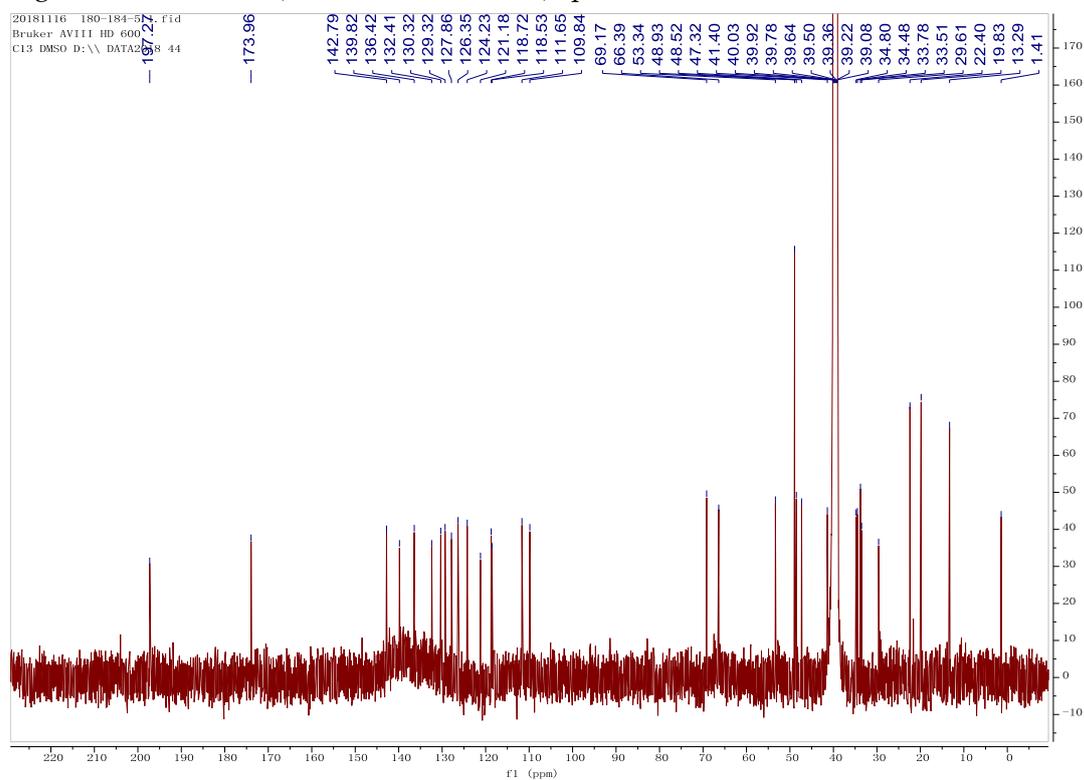


Figure S12: HSQC spectrum of 2

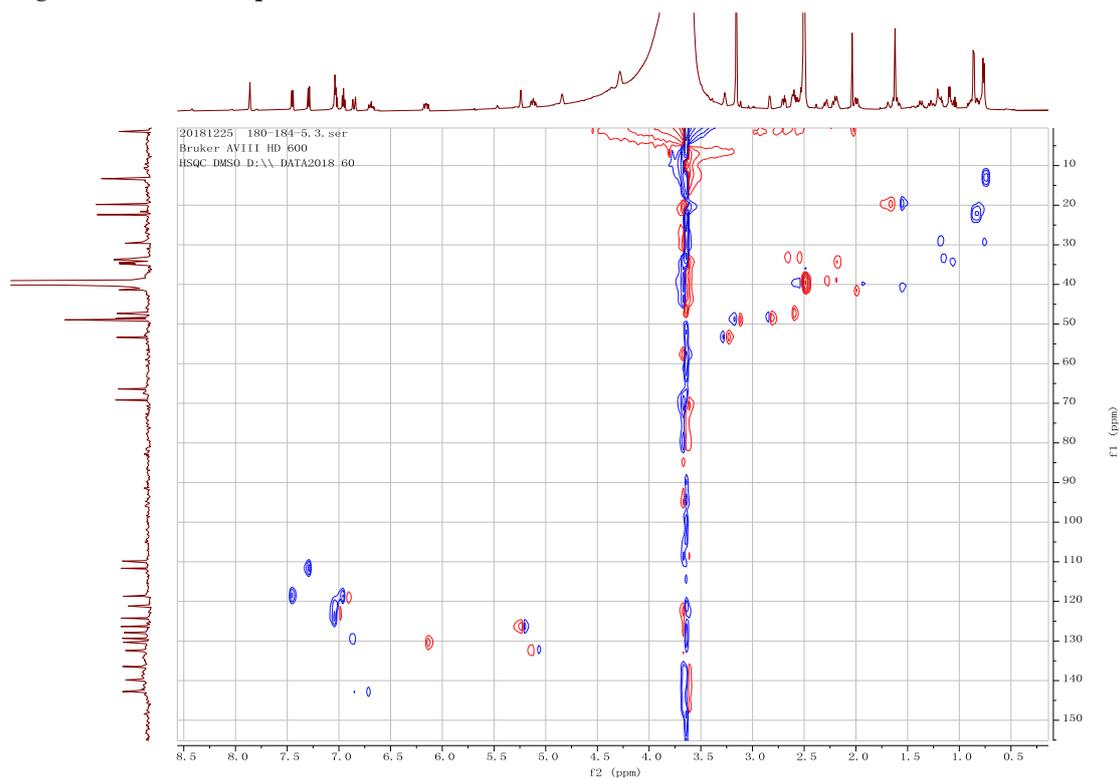


Figure S13: HMBC spectrum of 2

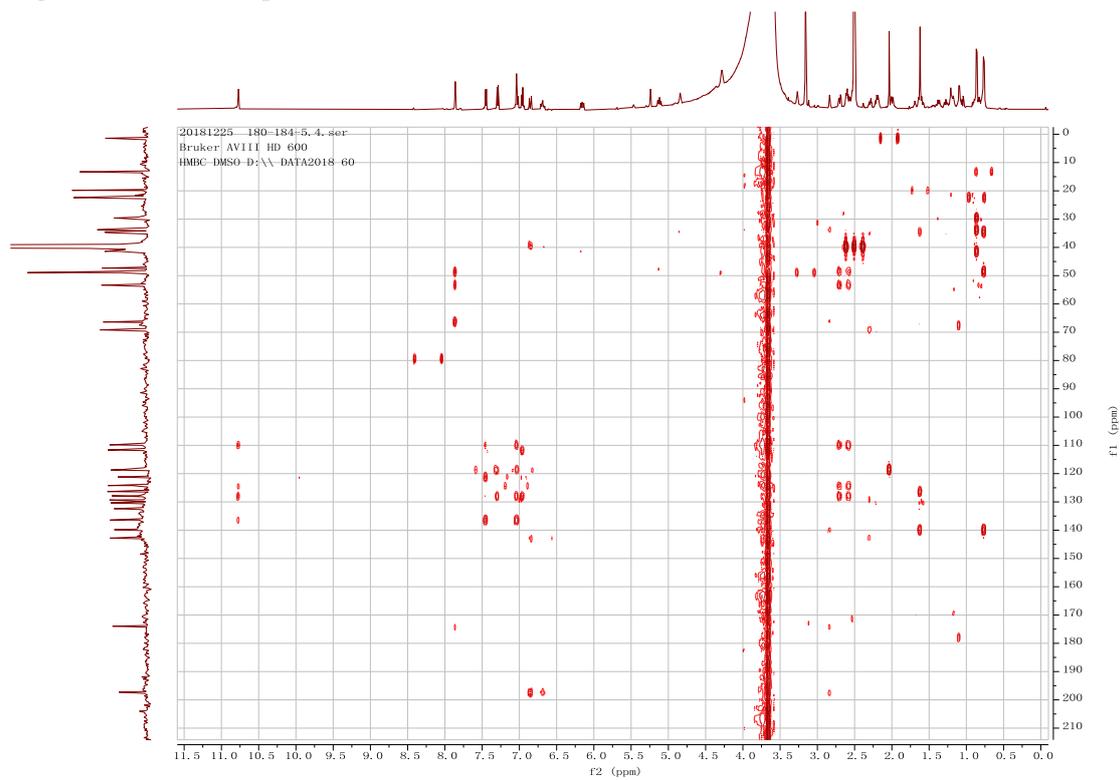


Figure S14:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 2

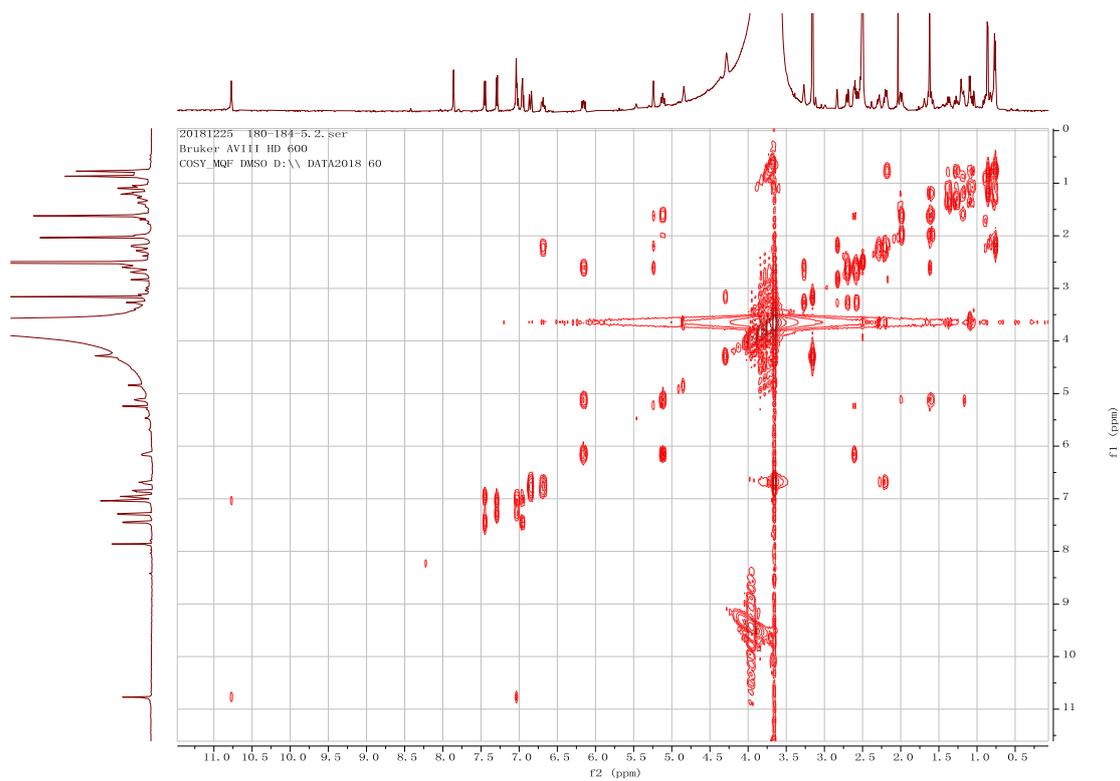


Figure S15: TOCSY spectrum of 2

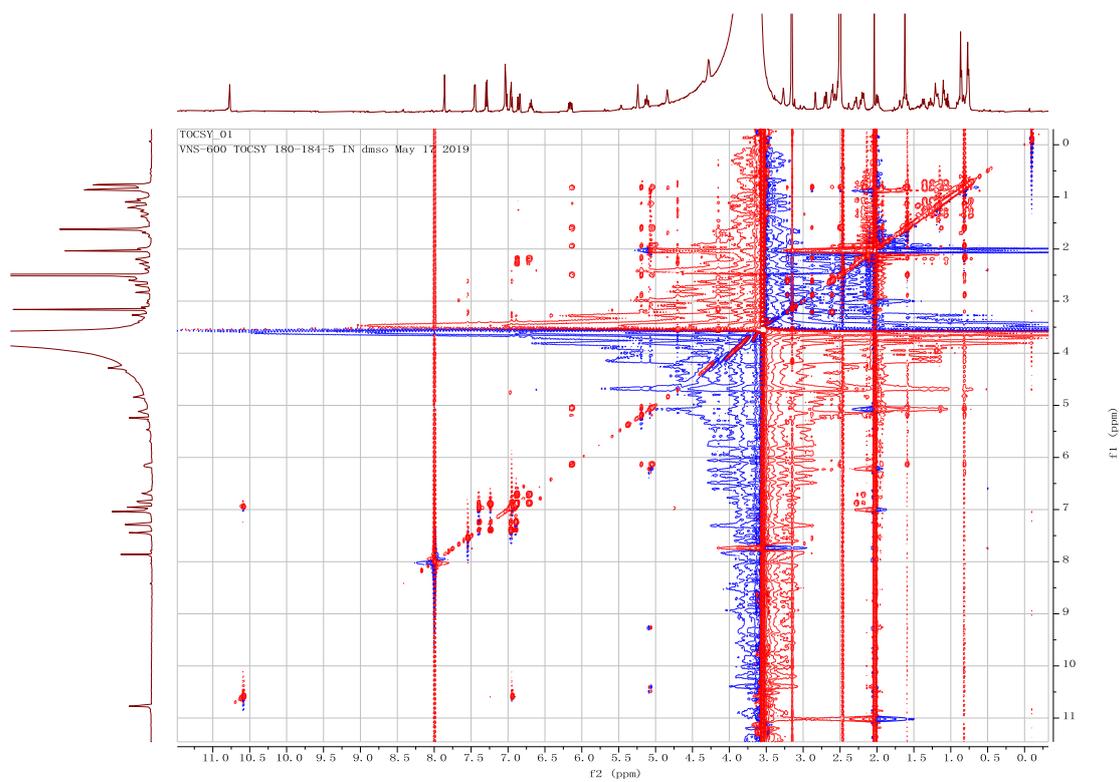


Figure S16: NOESY spectrum of **2**

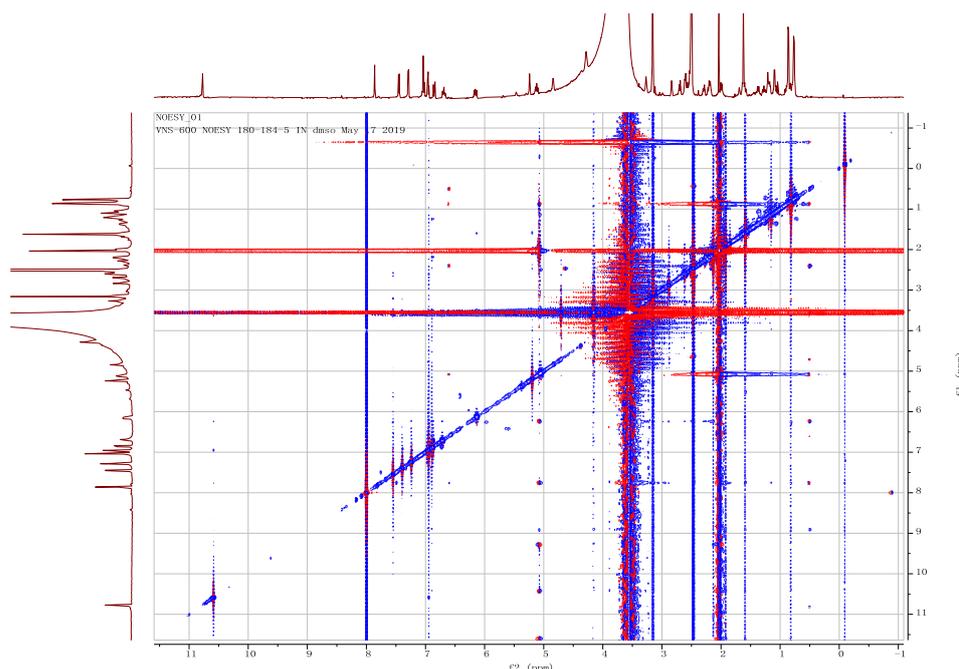


Figure S17: HR ESIMS spectrum of **2**

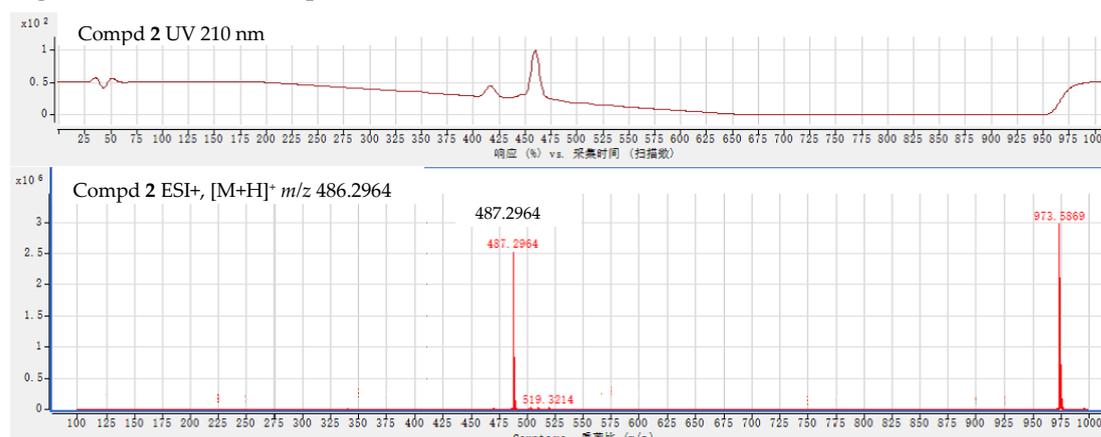
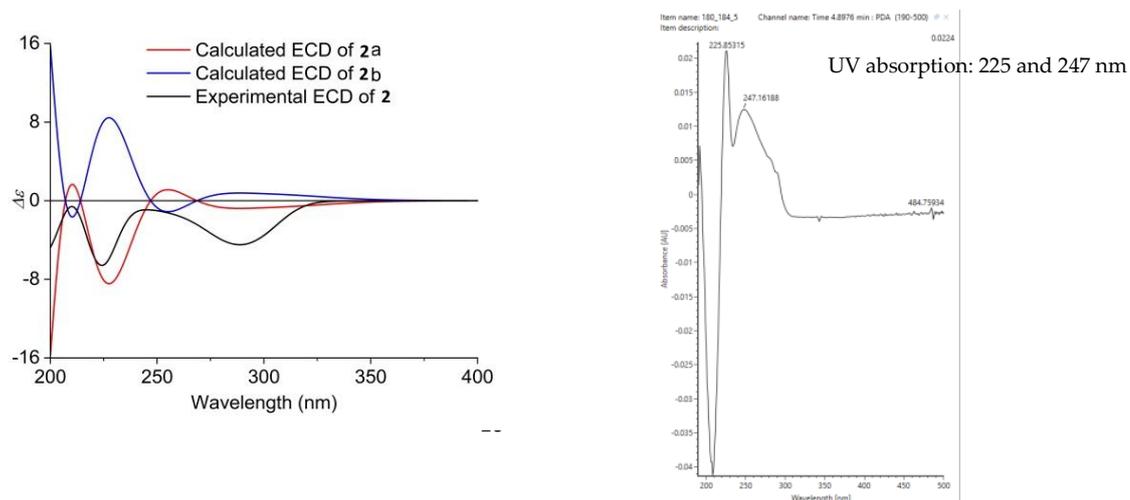


Figure S18: ECD and UV spectrum of **2**

TDDFT theory,  $\omega$ B97XD functional and TZVP level of theory, **2** has 58 conformations, of which 14 conformations have Boltzmann content  $>1\%$ , listed in the table below. Cam-B3LYP functional and TZVP level calculate 70 excited states, the solvent is methanol,  $\sigma=0.40\text{eV}$ , the result is shown in the figure.



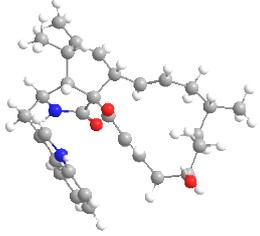
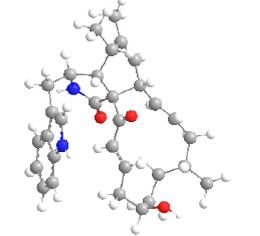
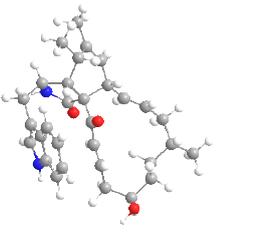
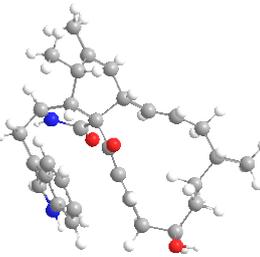
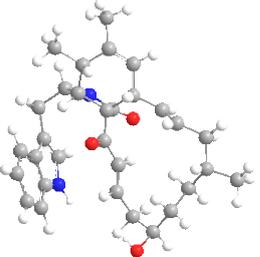
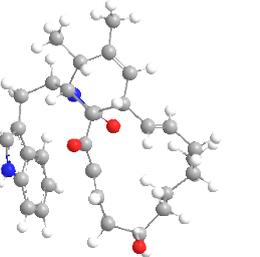
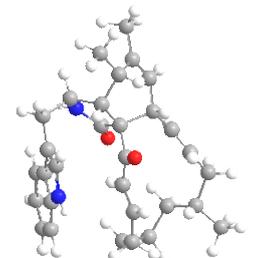
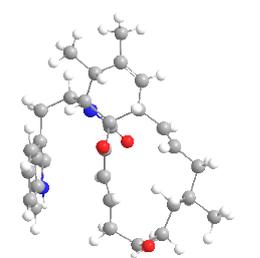
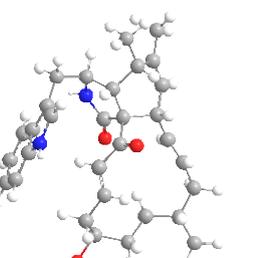
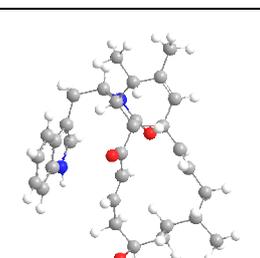
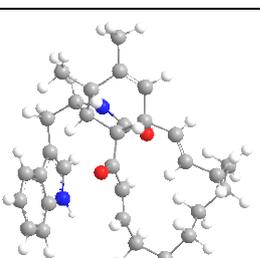
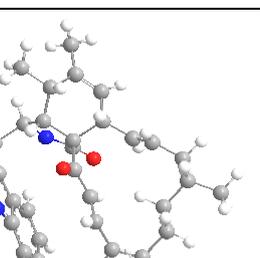
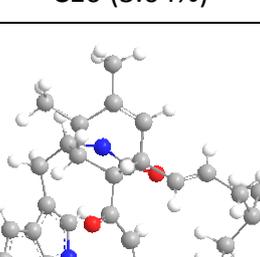
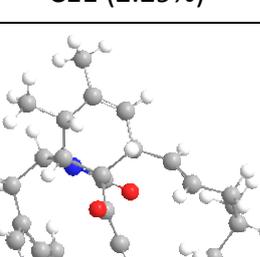
		
C1 (16.70%)	C2 (16.18%)	C3 (11.95%)
		
C4 (9.76%)	C5 (9.21%)	C6 (8.23%)
		
C7 (7.77%)	C8 (4.31%)	C9 (3.55%)
		
C10 (3.04%)	C11 (2.29%)	C12 (2.20%)
		
C13 (2.01%)	C14 (1.20%)	

Figure S19:  $^1\text{H}$  NMR spectrum of **2c**

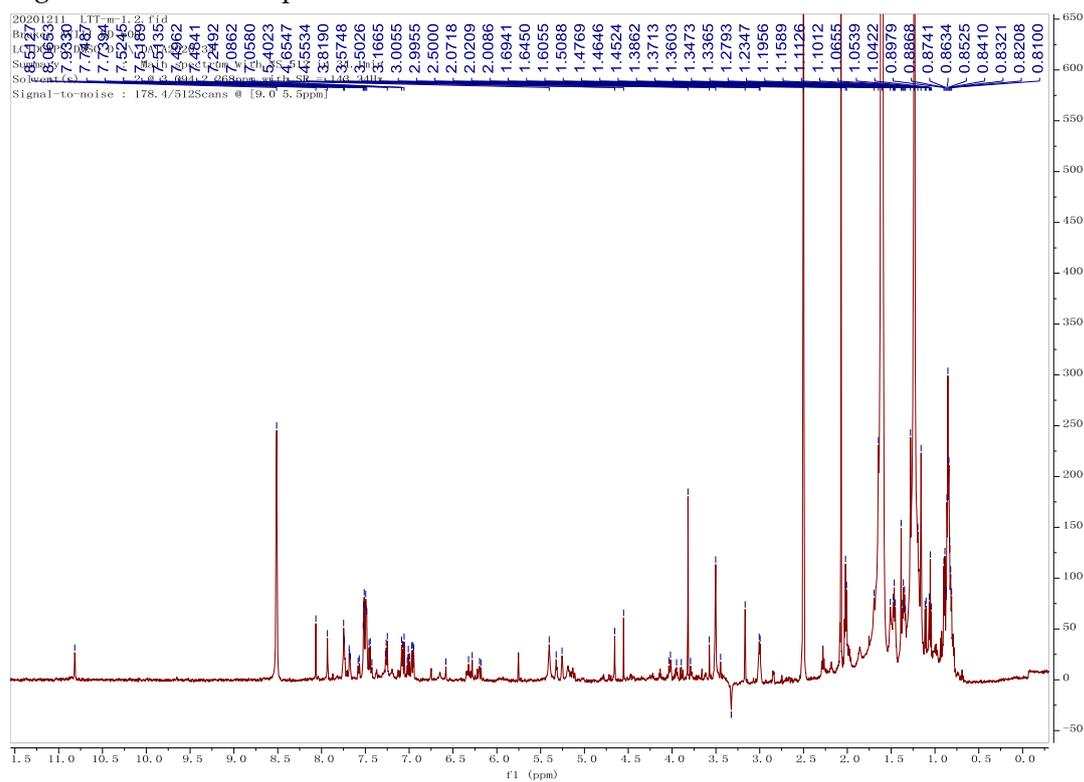


Figure S20:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2c**

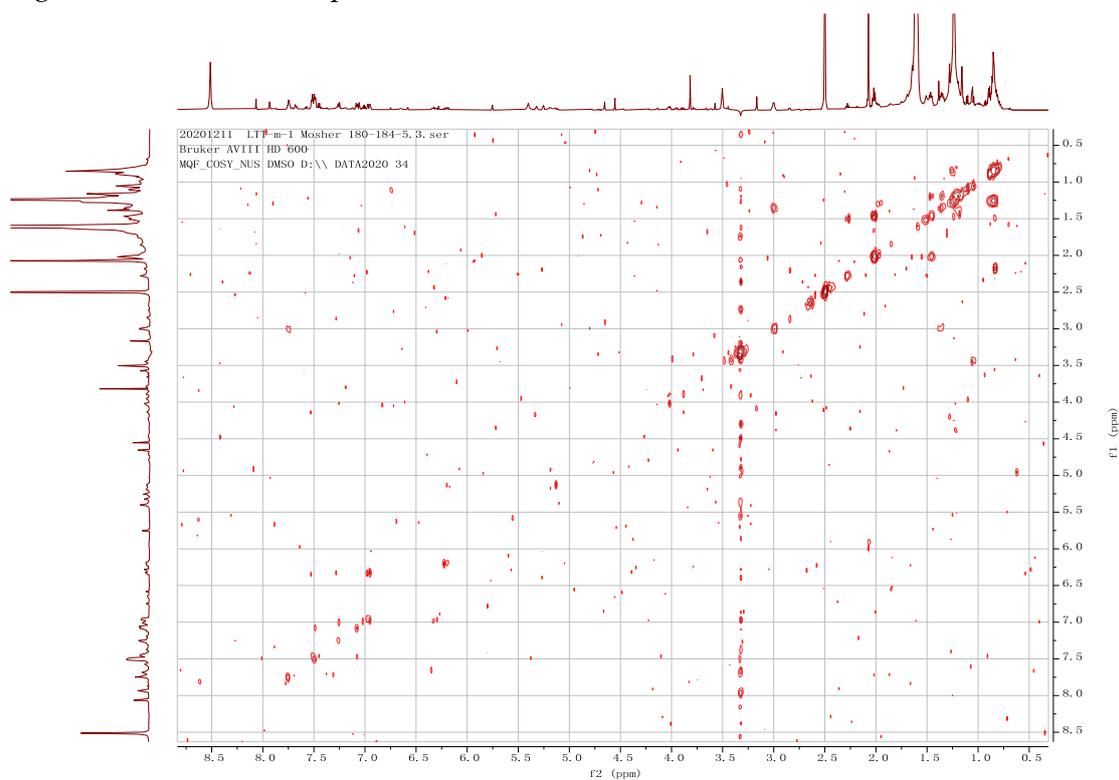




Figure S23: <sup>1</sup>H NMR (600 MHz, DMSO-*D*<sub>6</sub>) spectrum of **3**

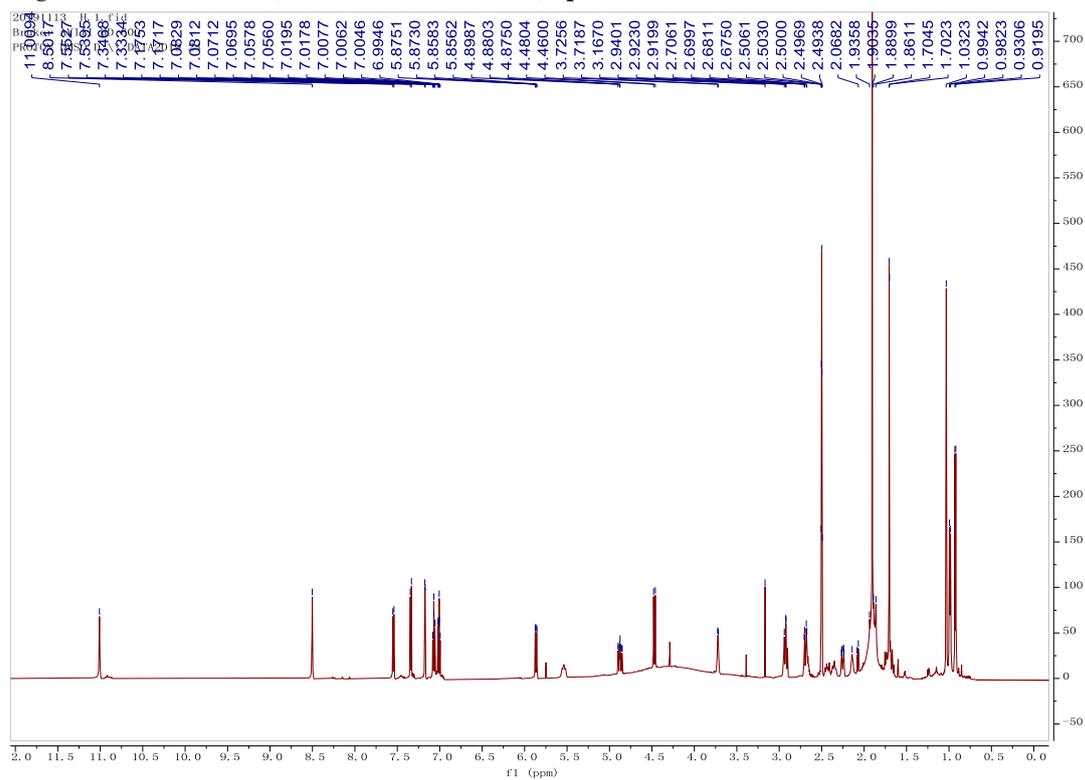


Figure S24: <sup>13</sup>C NMR (150 MHz, DMSO-*D*<sub>6</sub>) spectrum of **3**

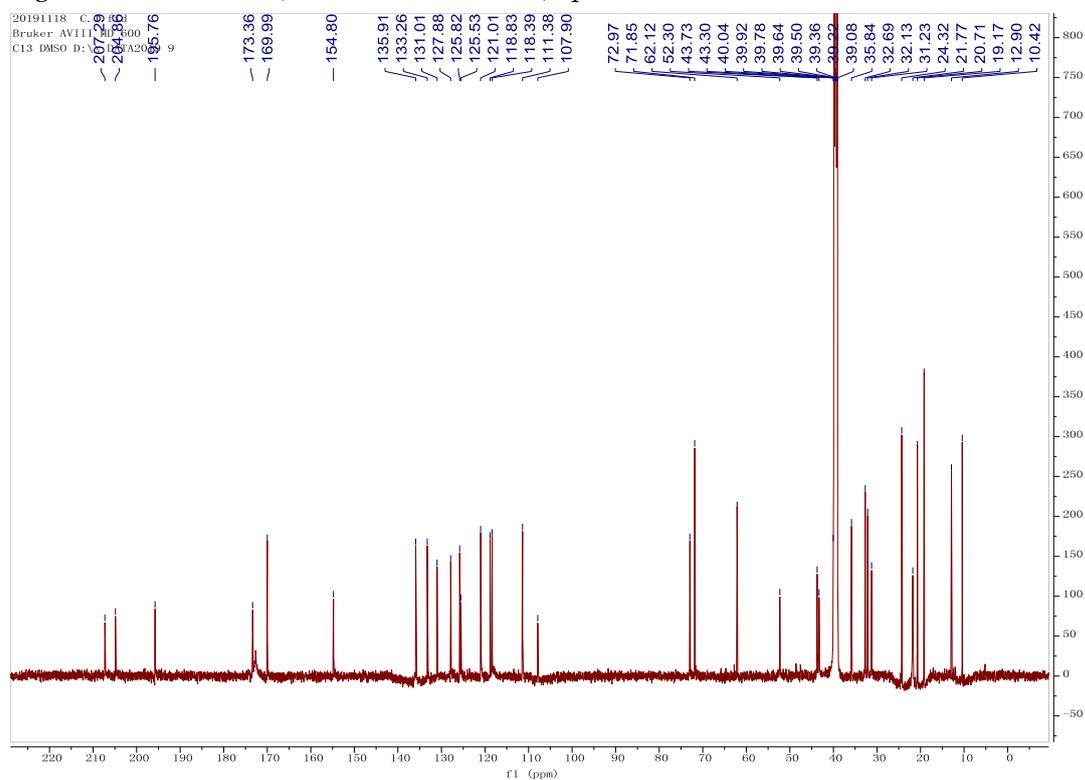


Figure S25: HSQC spectrum of 3

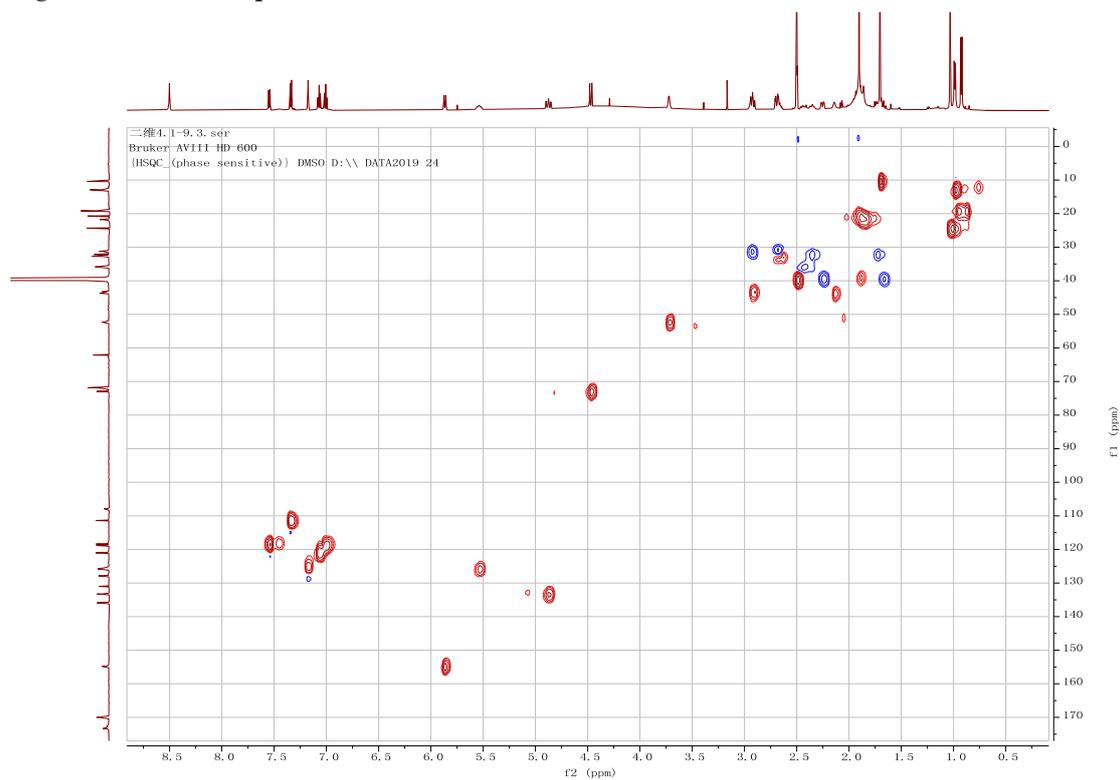


Figure S26: HMBC spectrum of 3

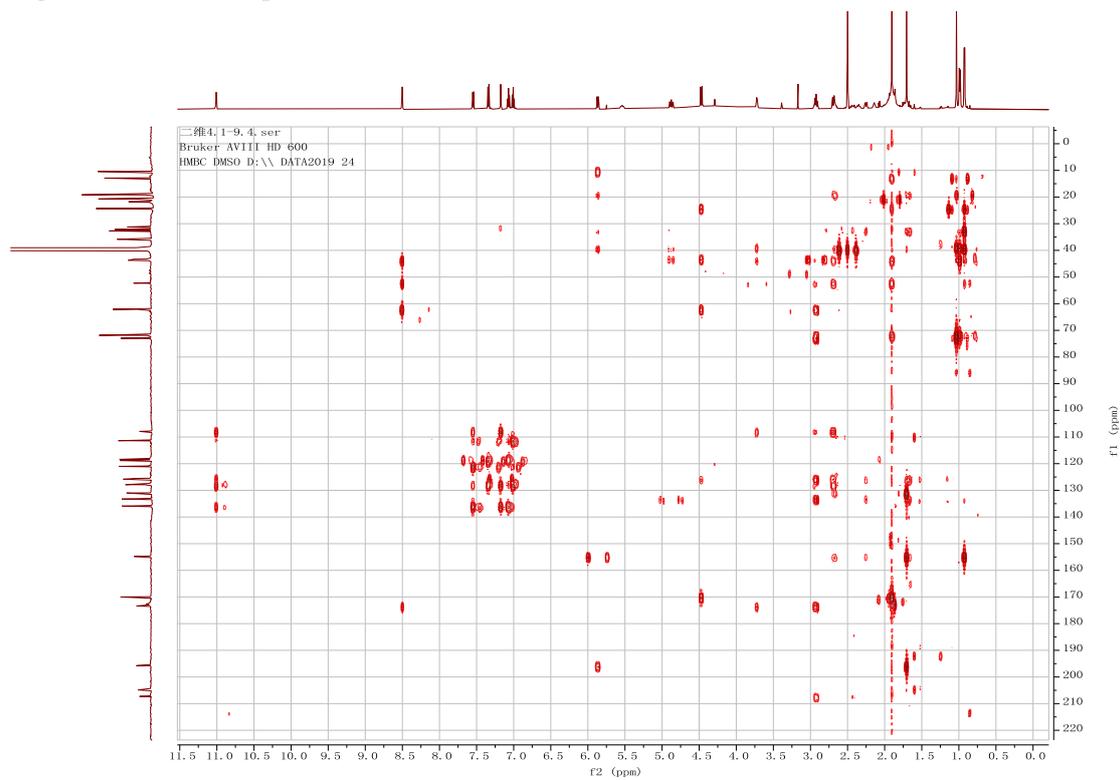


Figure S27:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3**

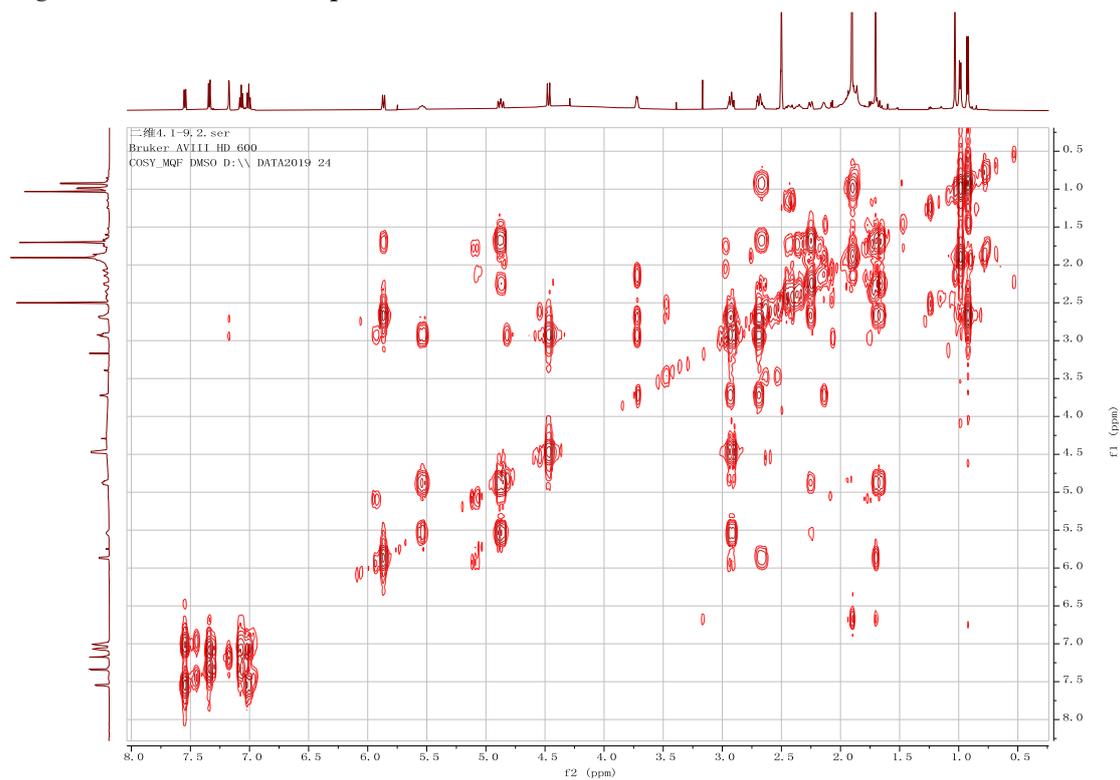


Figure S28: ROESY spectrum of **3**

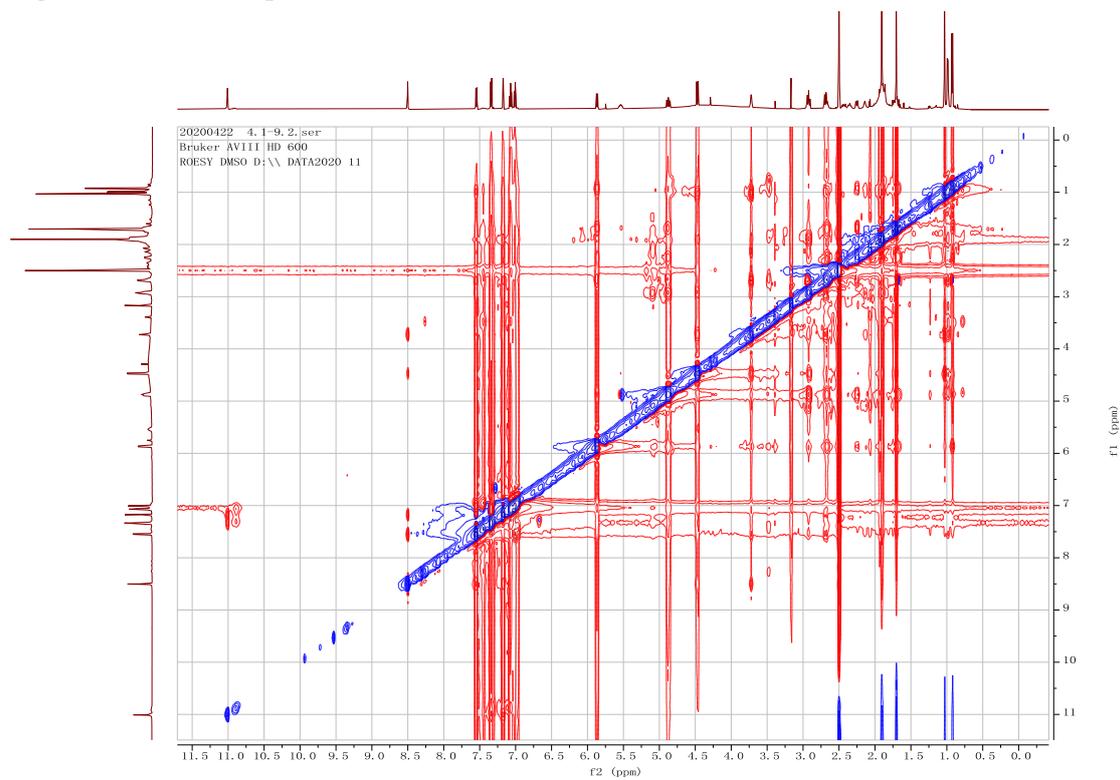


Figure S29: HR-ESIMS spectrum of **3**

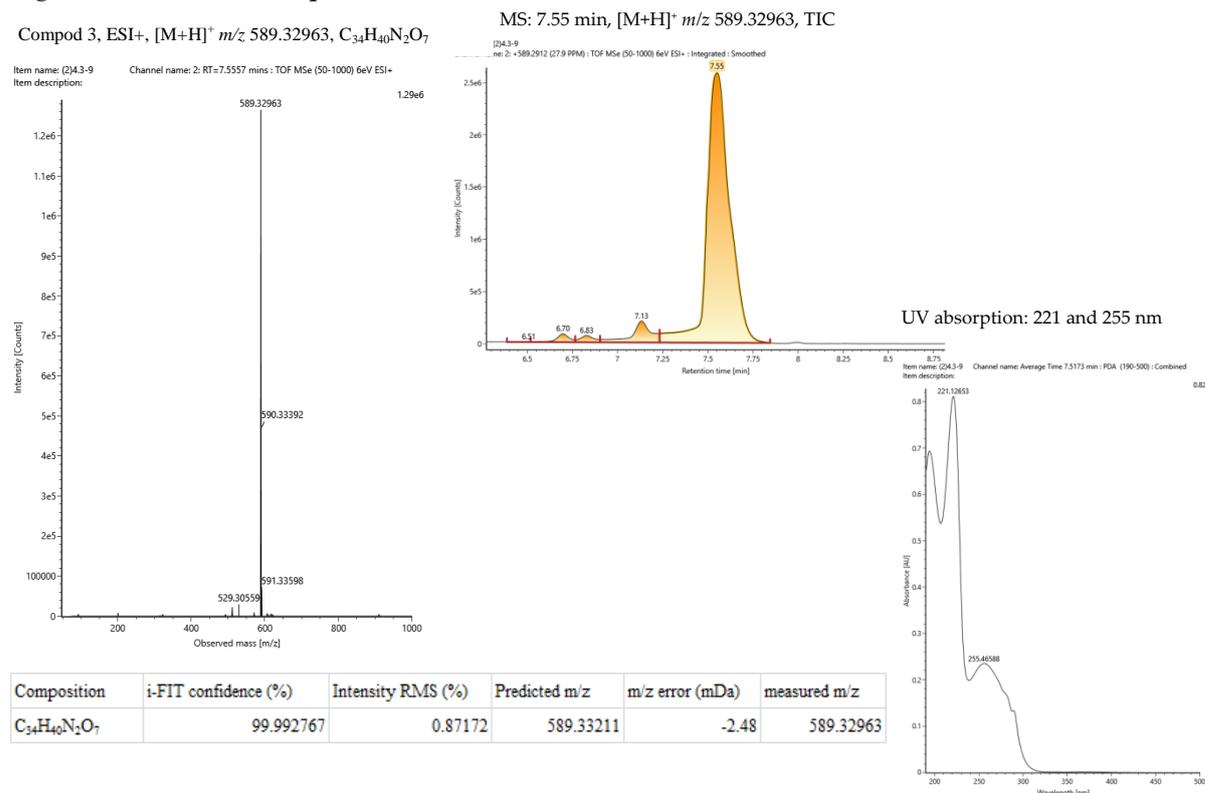


Figure S30: ECD and UV spectrum of **3** (in MeOH)

TDDFT theory, ωB3LYP functional and 6-311G(d,p) level of theory, methanol as solvent for structural optimization, compound **3** has 13 conformations, of which 5 conformations have Boltzmann content >1%, listed in the table below. The calculated result of **3** is consistent with the experimental result, and the absolute configuration of **3** is determined as shown in the right figure.

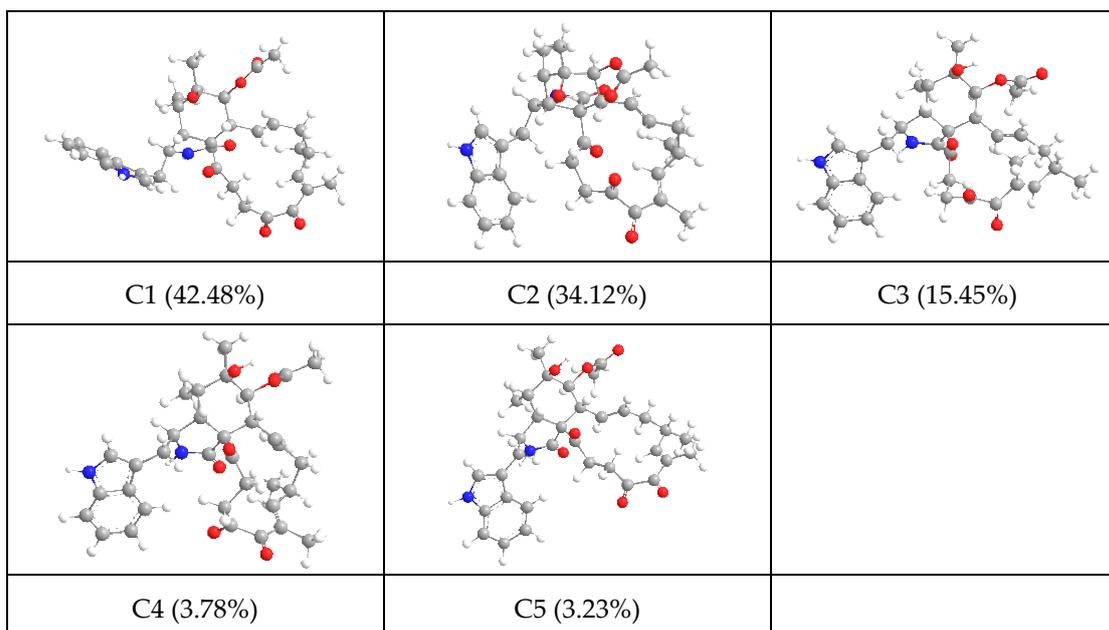
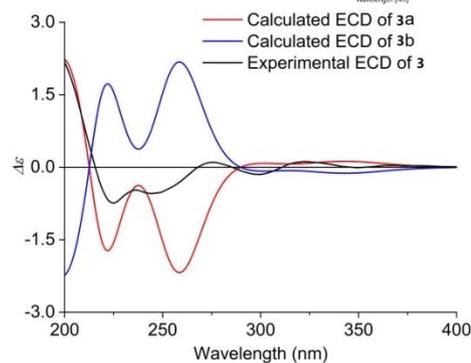


Figure S31  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}D_6$ ) spectrum of 4

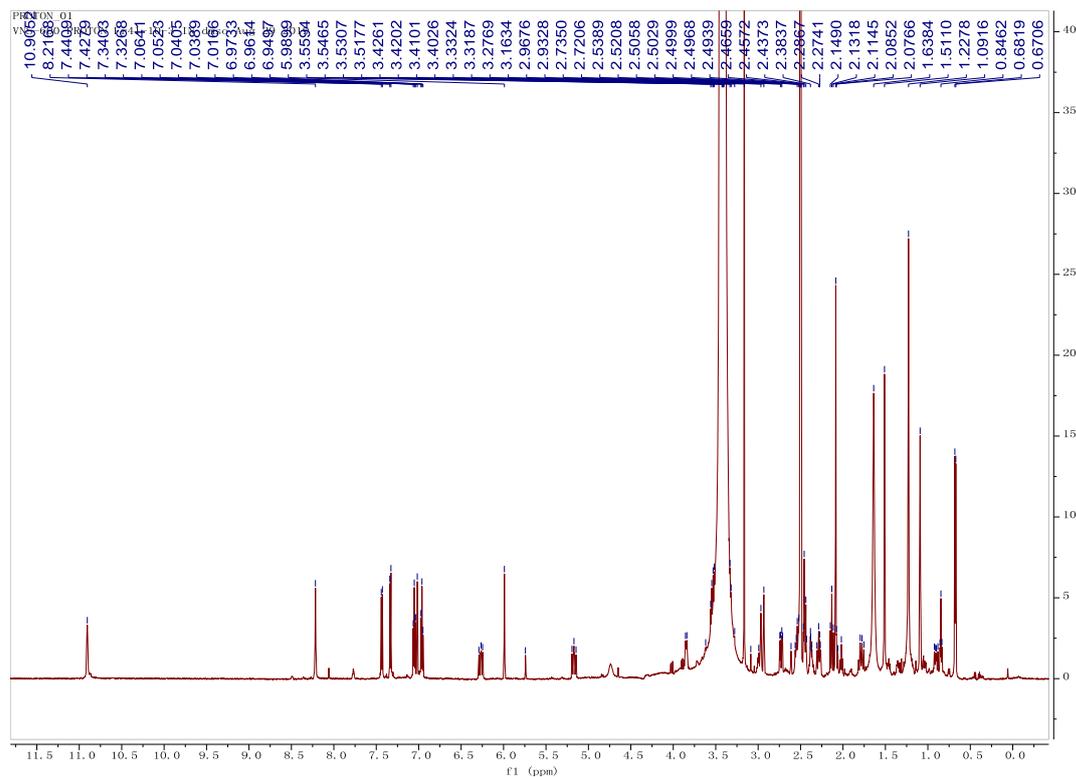


Figure S32:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}D_6$ ) spectrum of 4

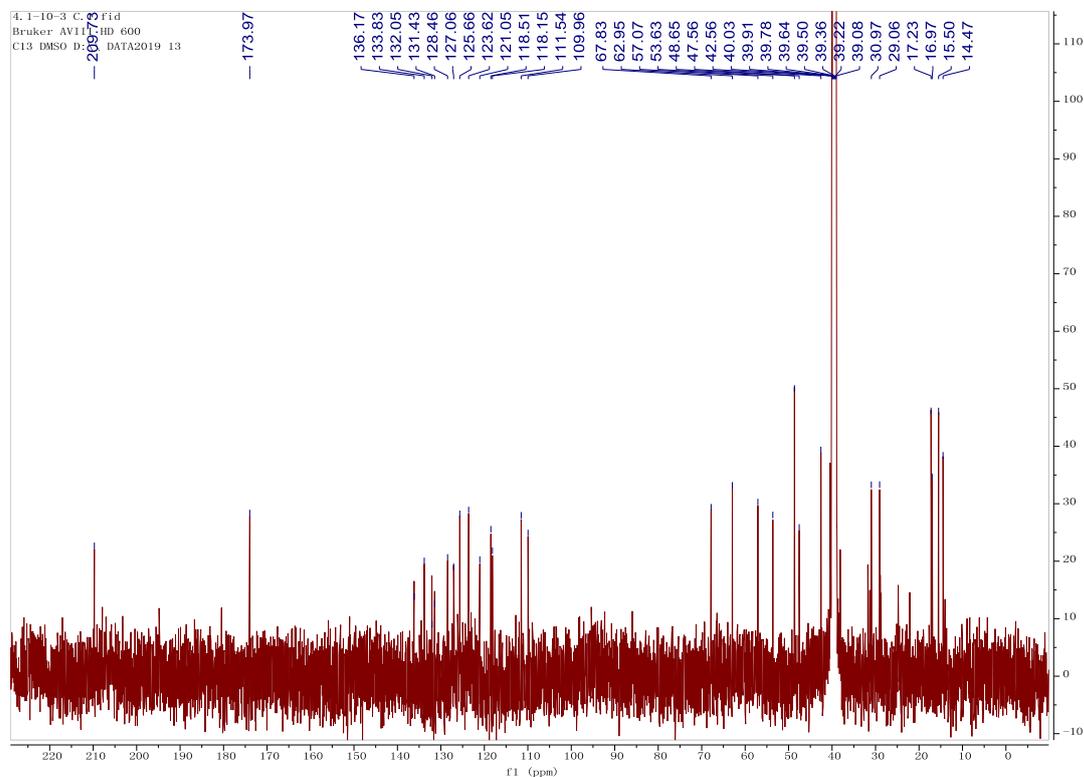


Figure S33: HSQC spectrum of 4

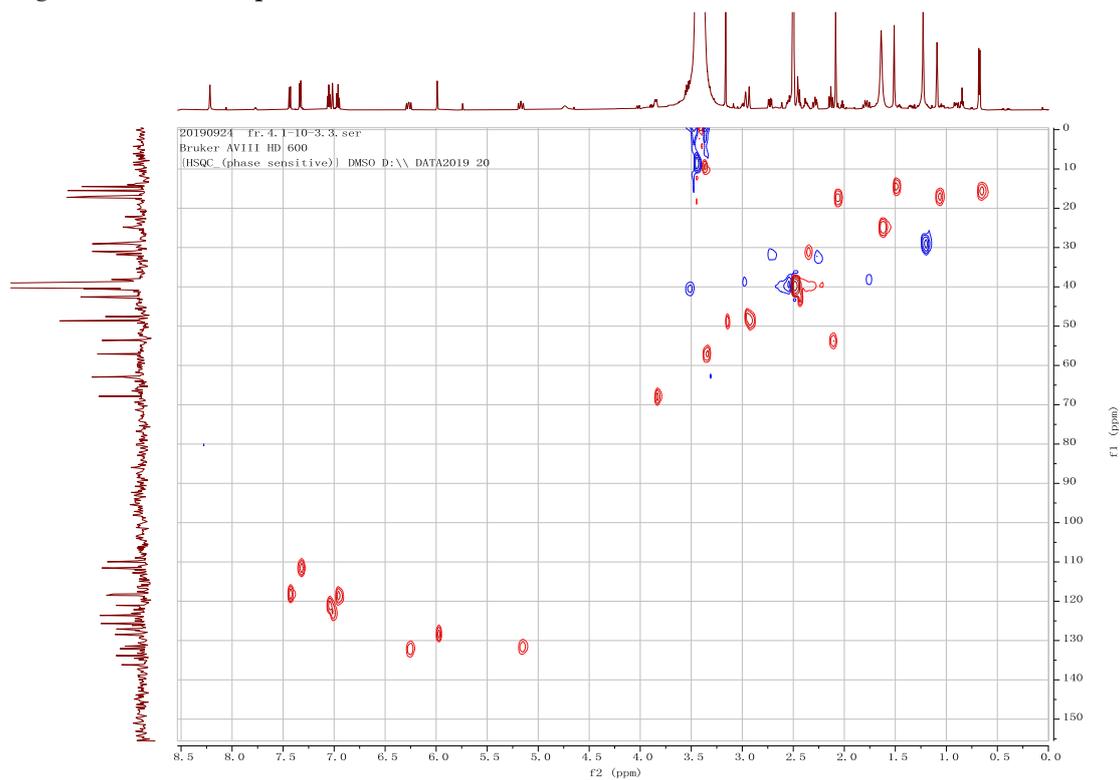


Figure S34: HMBC spectrum of 4

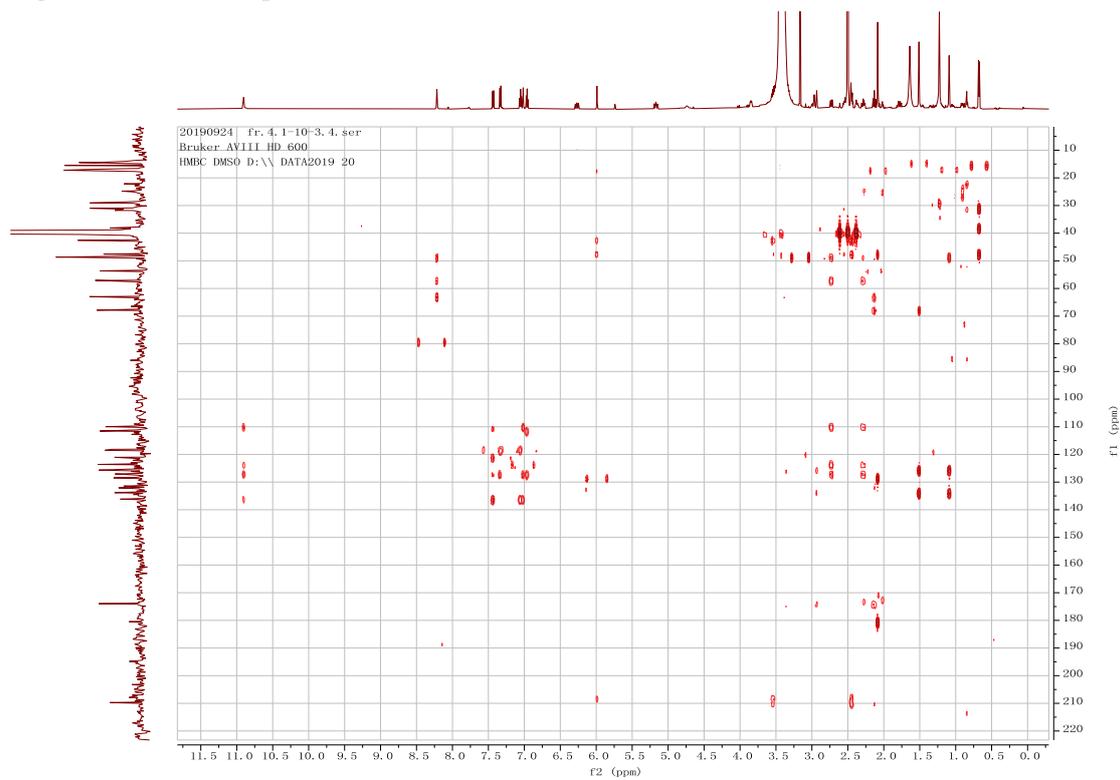


Figure S35:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 4

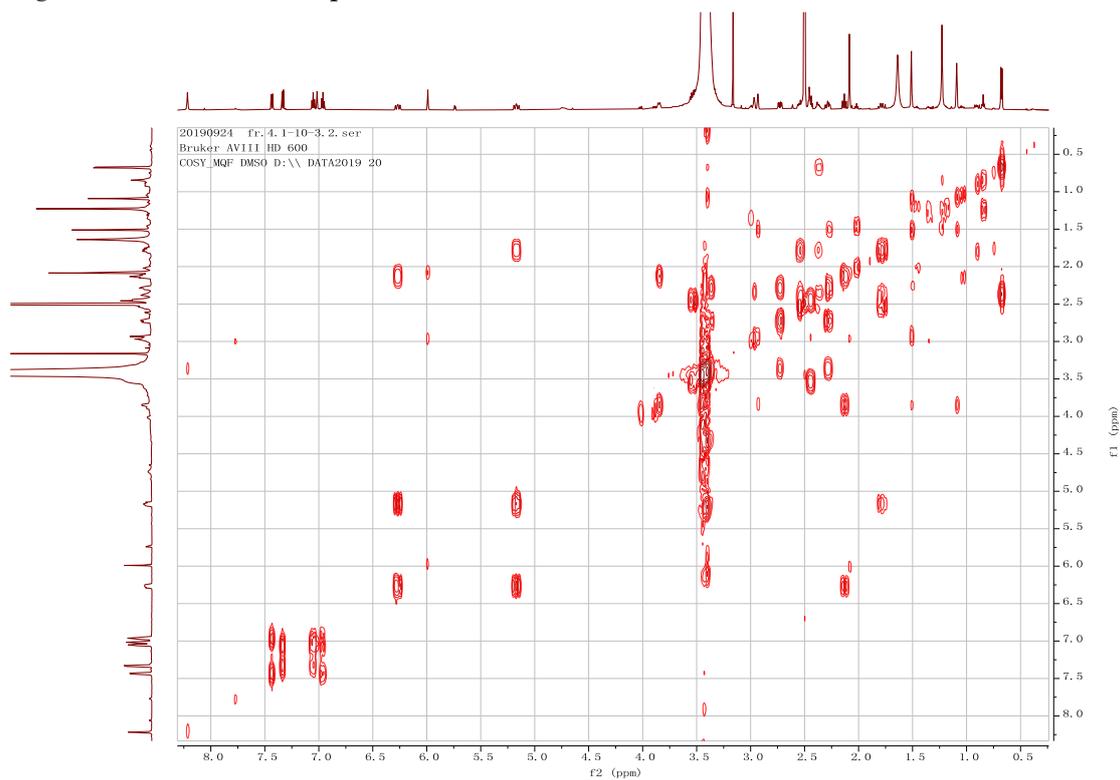


Figure S36: TOCSY spectrum of 4

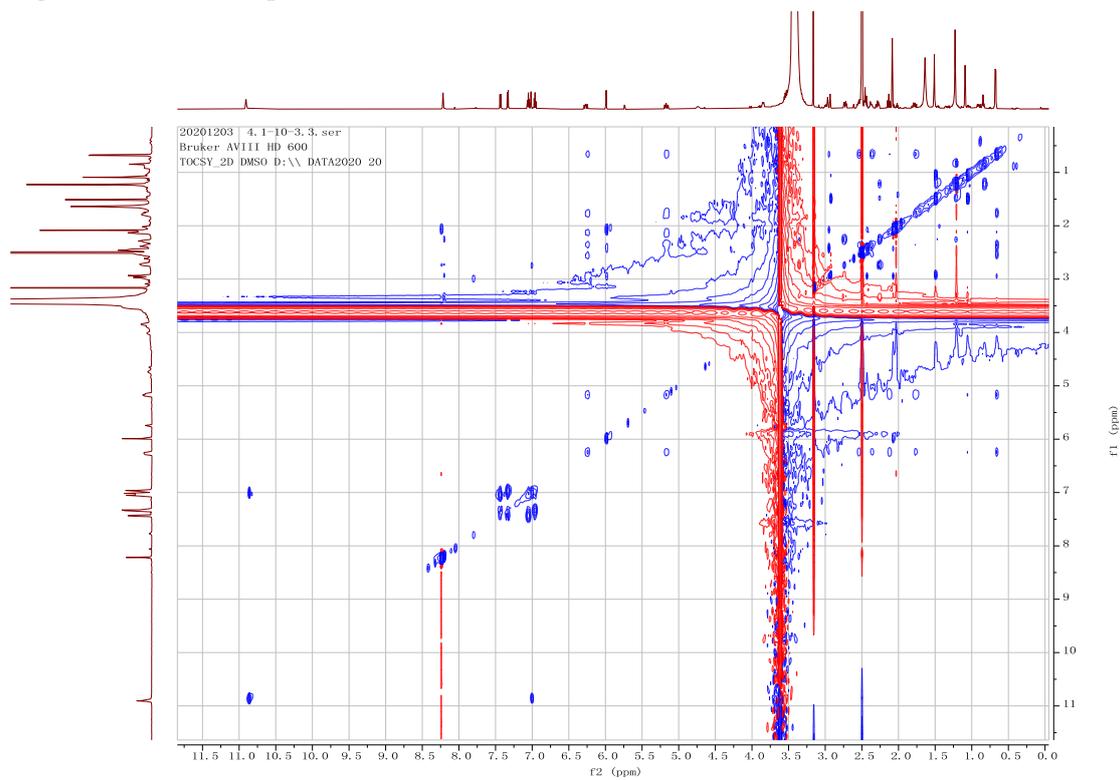


Figure S37: NOESY spectrum of 4

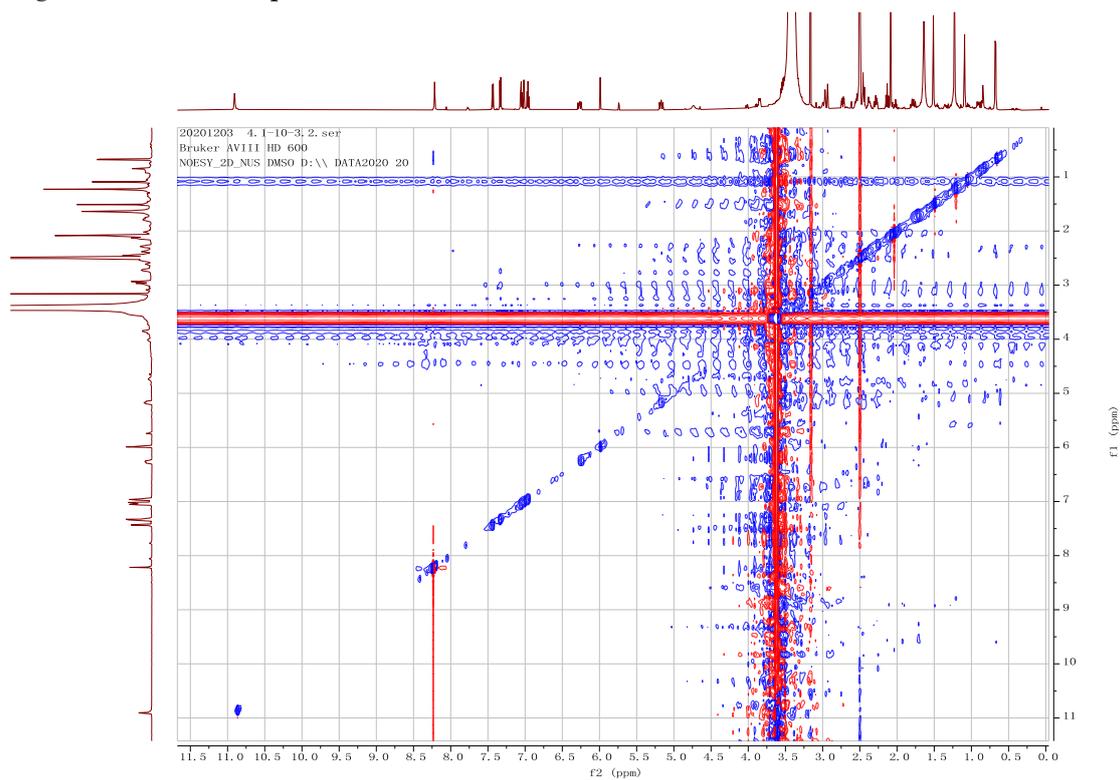
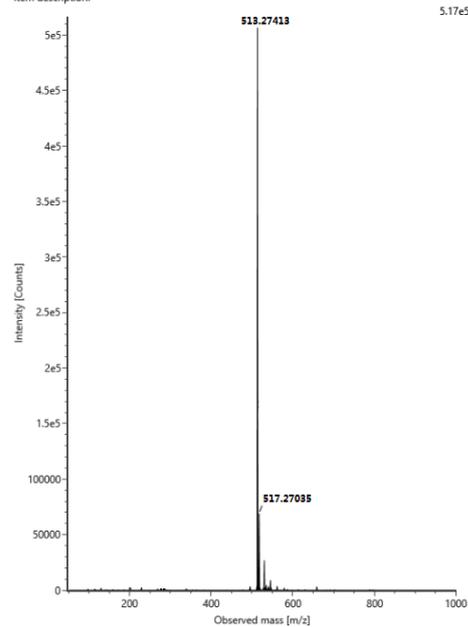


Figure S38: HR-ESI-MS spectrum of 4

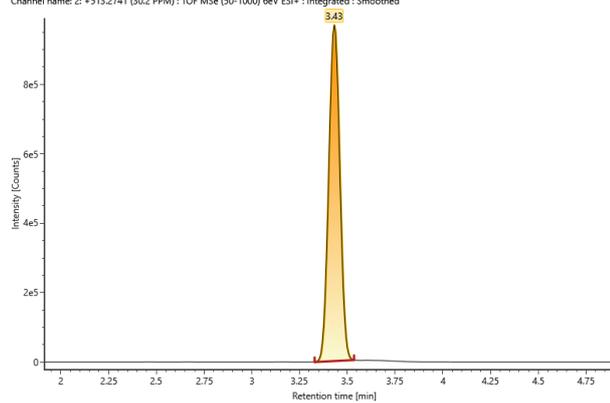
Compd 4 ESI+, [M+H]<sup>+</sup> m/z 513.27413, t<sub>R</sub>=3.42 min

Item name: fr:4.1-10-3 Channel name: 2: RT=3.4 2 mins : TOF MSe (50-1000) 6eV ESI+  
 Item description:



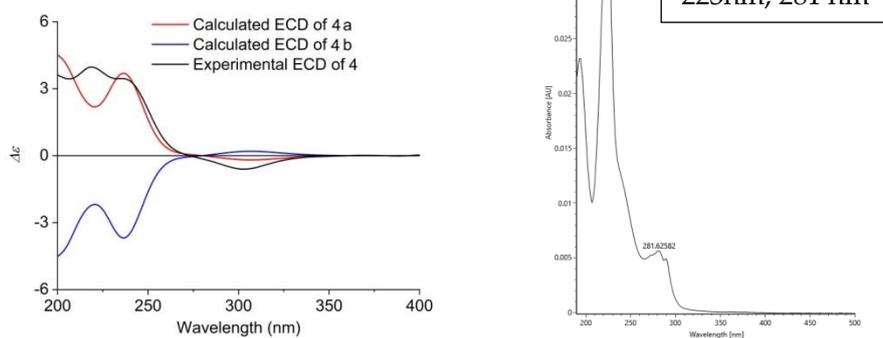
Compd 4. 513.2741, t<sub>R</sub> = 3.43 min

Item name: fr:4.1-10-3  
 Channel name: 2: +513.2741 (30.2 PPM) : TOF MSe (50-1000) 6eV ESI+ : Integrated : Smoothed



Results (1 found)								
	Composition	i-FIT Confidence (%)	m/z RMS (PPM)	Intensity RMS (%)	Predicted m/z	m/z error (PPM)	m/z error (mDa)	DBE
1	C32H36N2O4	99.992657	1.325362	0.683619	513.274784	-1.276882	-0.654104	16.000000

Figure S39: ECD and UV spectrum of **4**



TDDFT theory,  $\omega$ B3LYP functional and 6-311G(d,p) level of theory, methanol as solvent for structural optimization, compound **4** have 14 conformations, of which 8 conformations have Boltzmann content >1%, listed in the table below. The calculated result of **4** is consistent with the experimental result, and the absolute configuration of **4** is confirmed as shown in the figure above.

C1 (35.33%)	C2 (23.15%)	C3 (17.16%)
C4 (9.64%)	C5 (6.10%)	C6 (4.61%)
C7 (2.01%)	C8 (1.87%)	

Figure S40: <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of 5

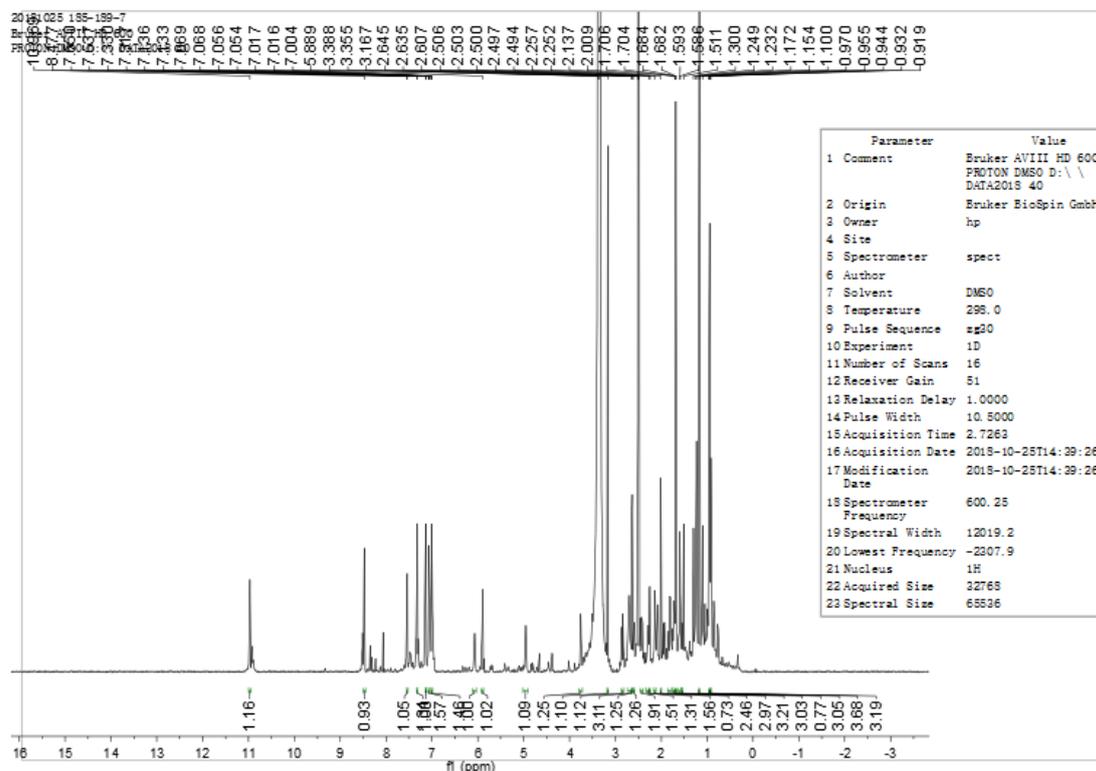


Figure S41: <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of 5

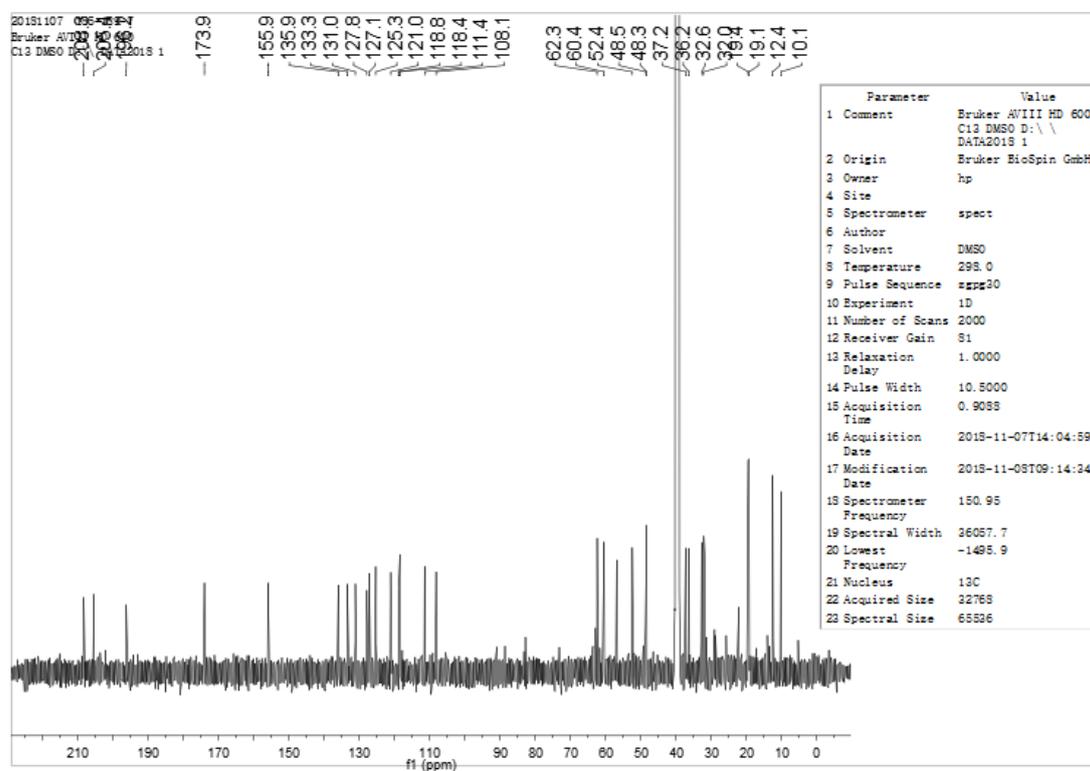


Figure S42:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **6**

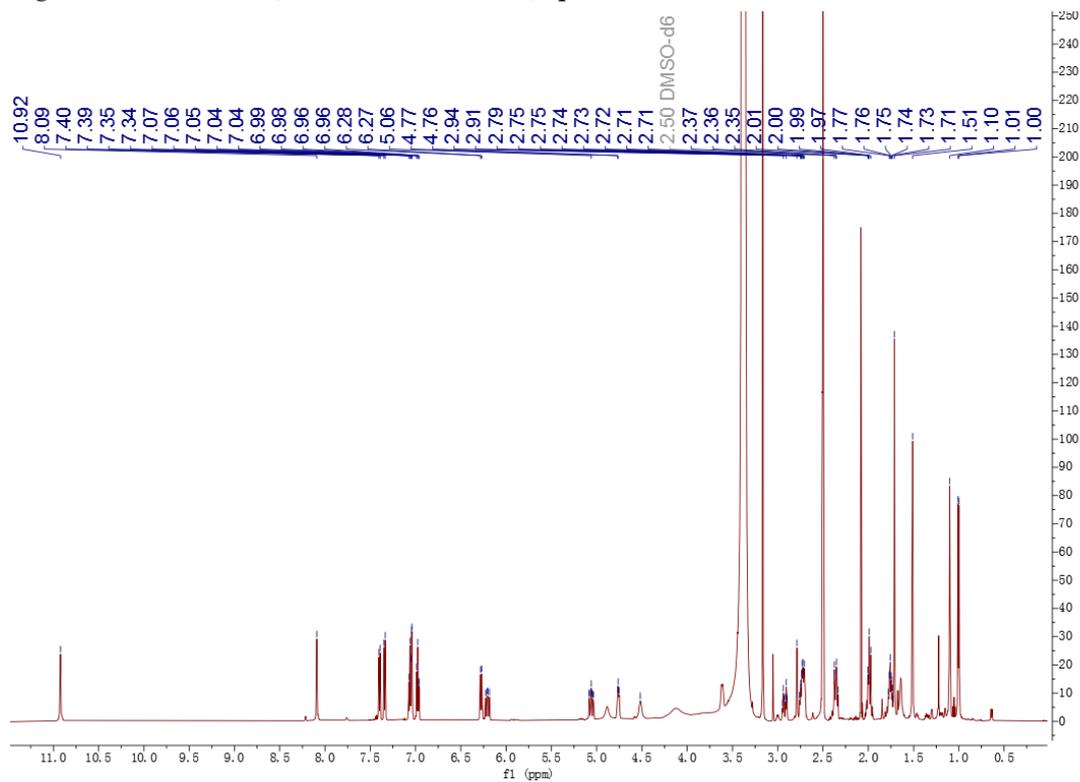


Figure S43:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **6**

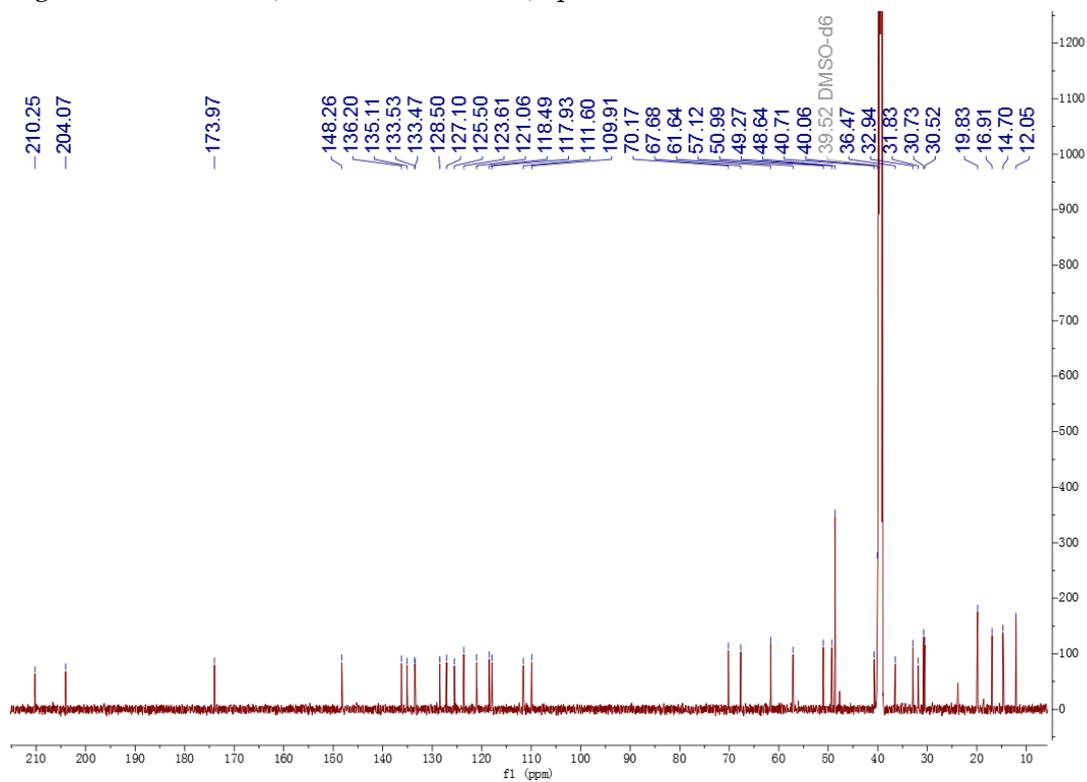


Figure S44:  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ ) spectrum of **7**

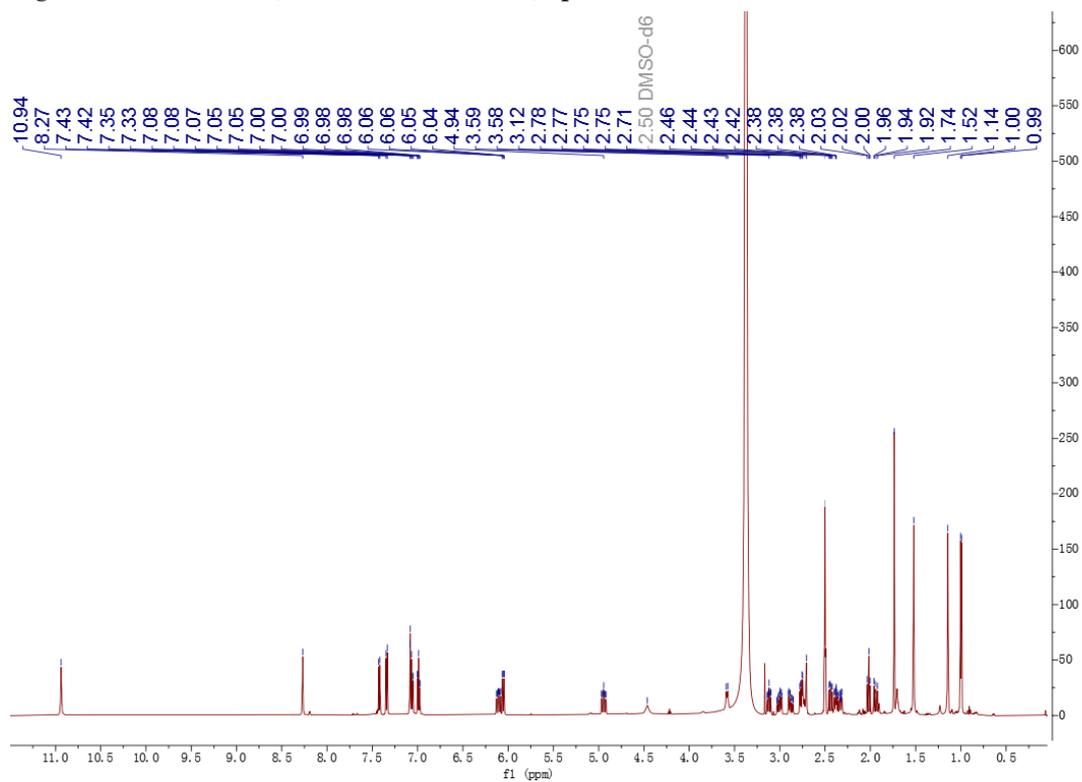


Figure S45:  $^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ ) spectrum of **7**

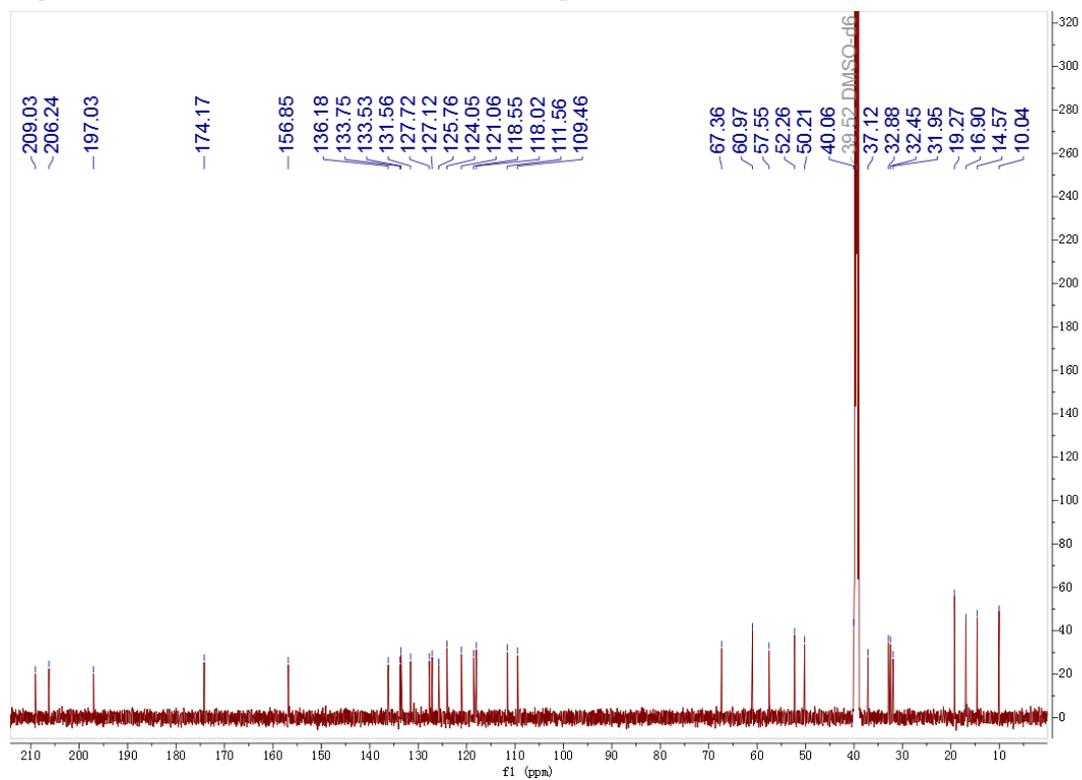


Figure S46:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **8**

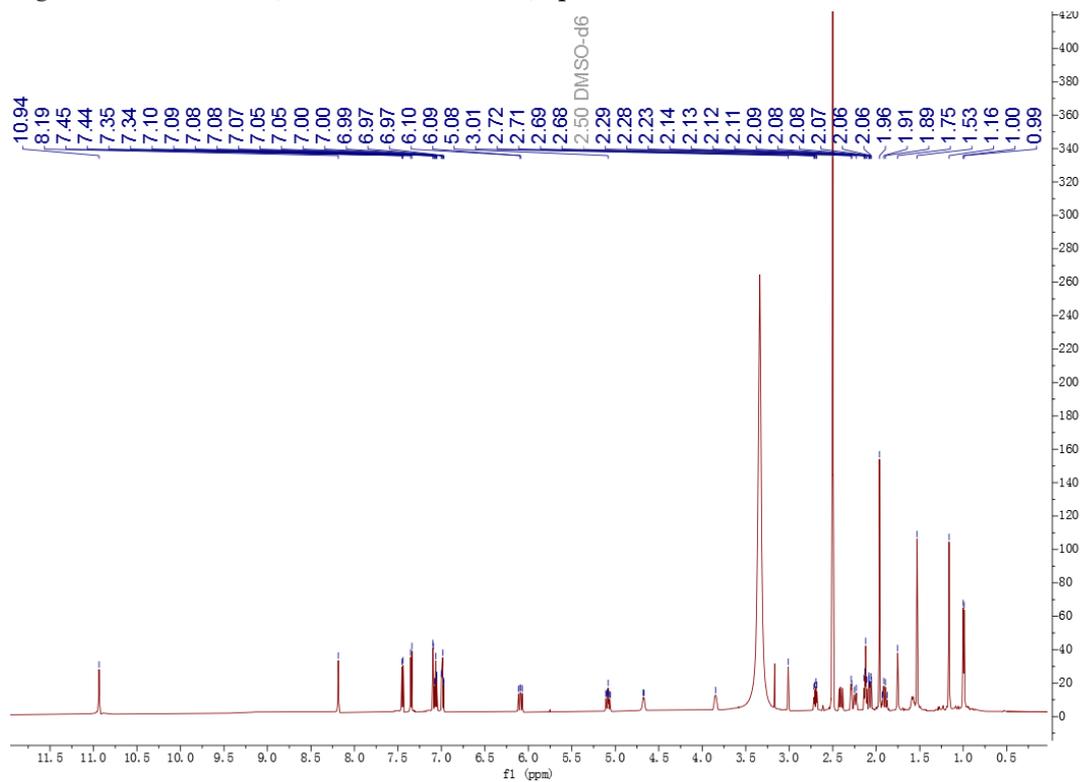


Figure S47:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **8**

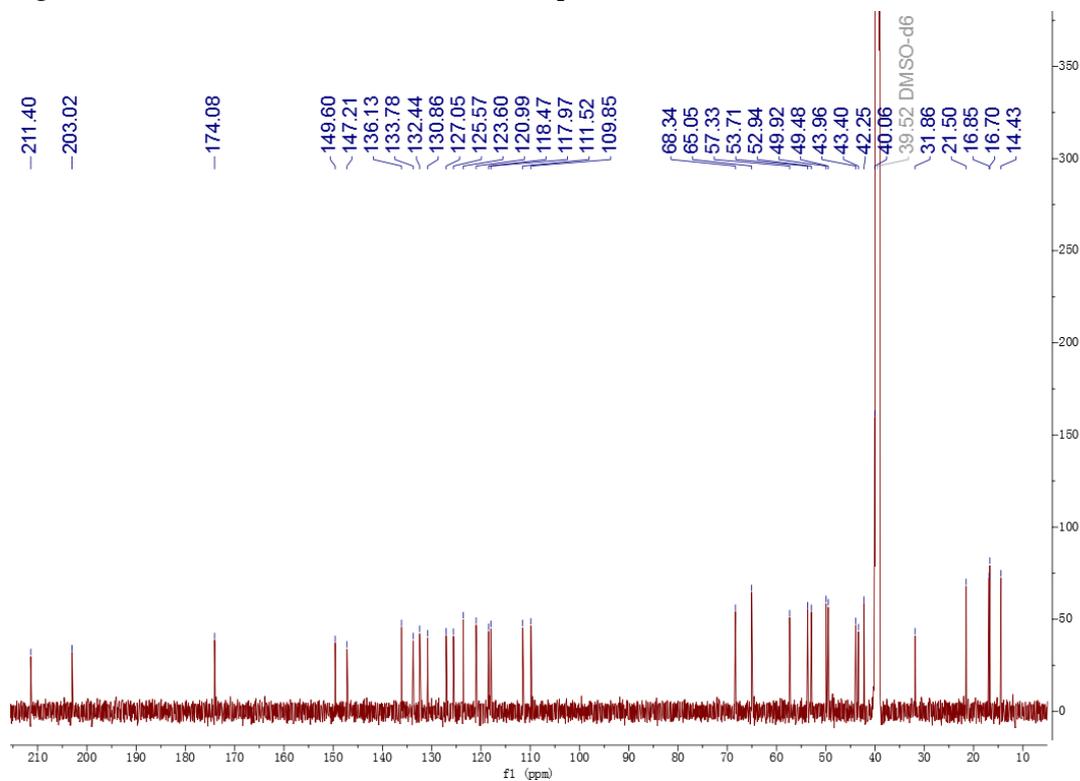


Figure S48:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **9**

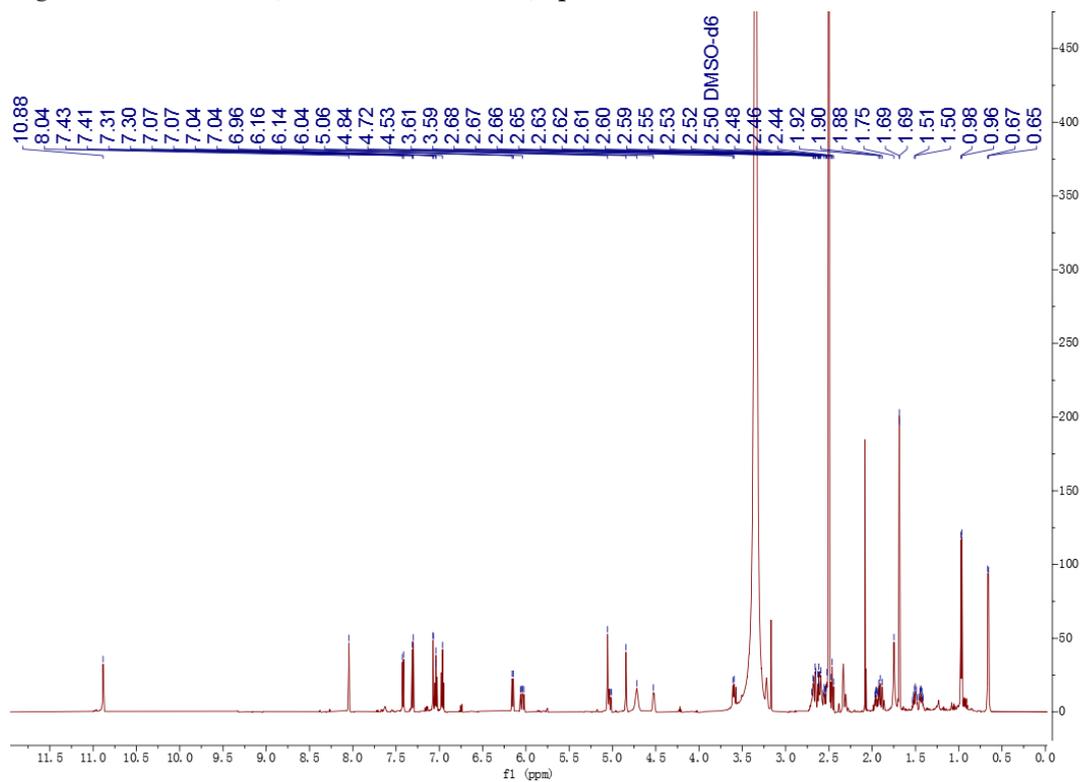


Figure S49:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **9**

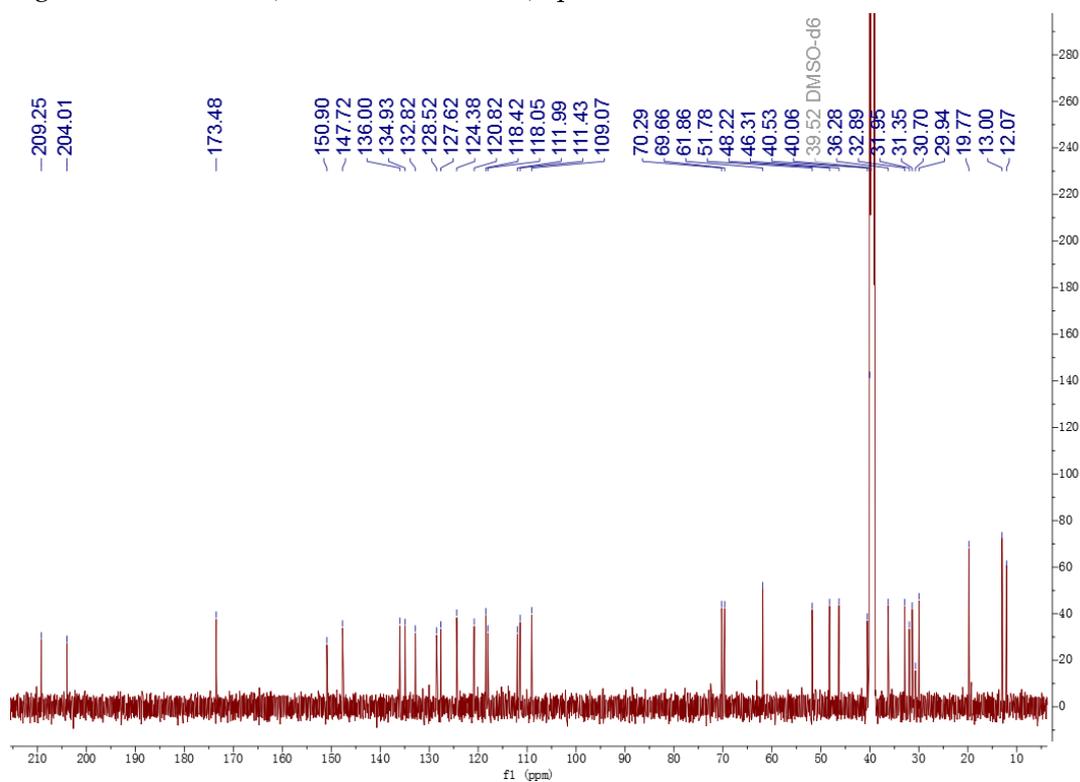


Figure S50:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **10**

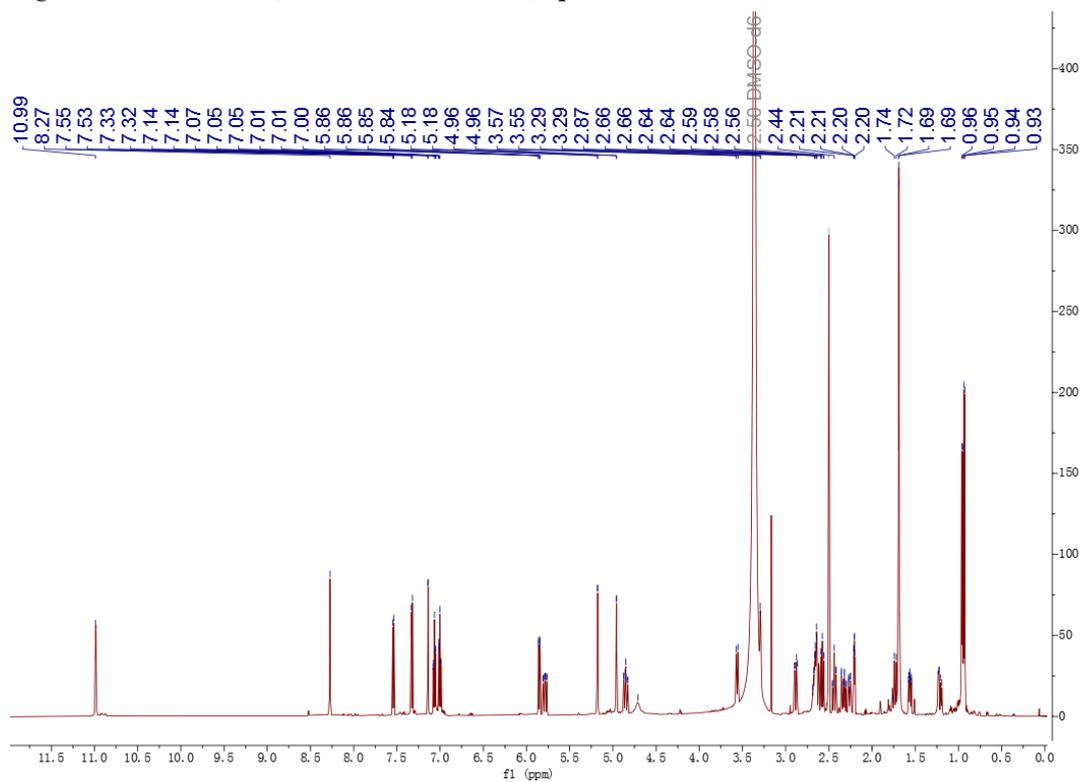


Figure S51:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **10**

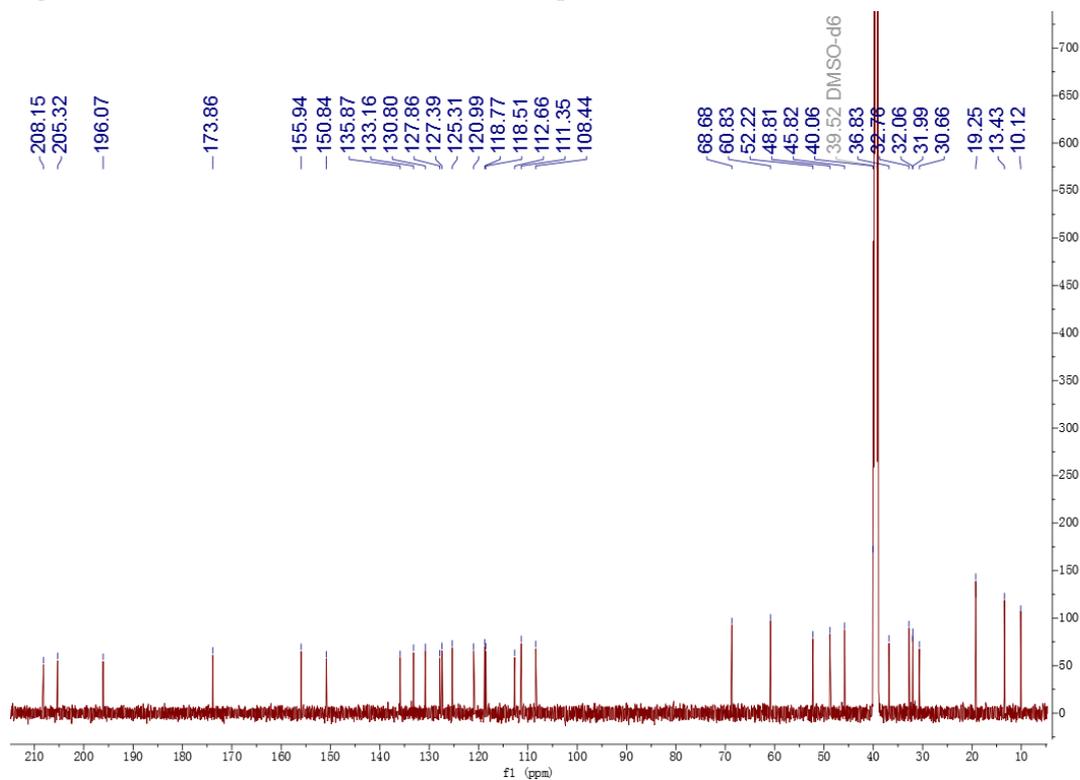


Figure S52: <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of **11**

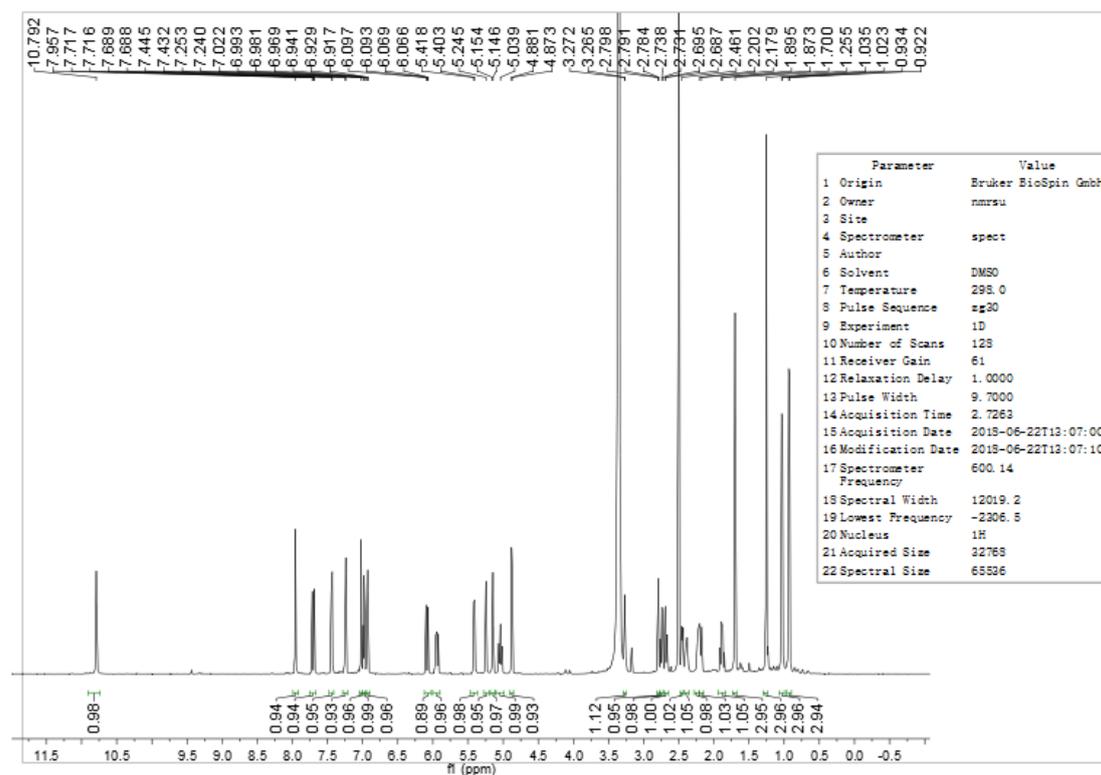


Figure S53: <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of **11**

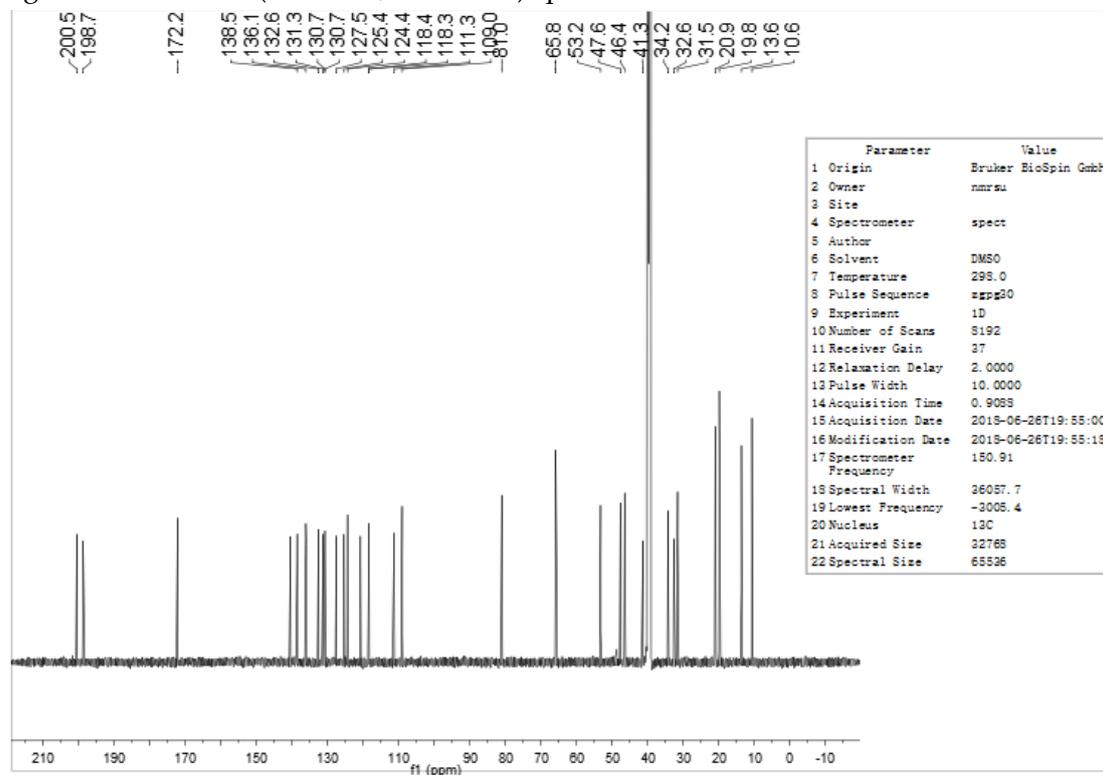


Figure S54: <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of **12**

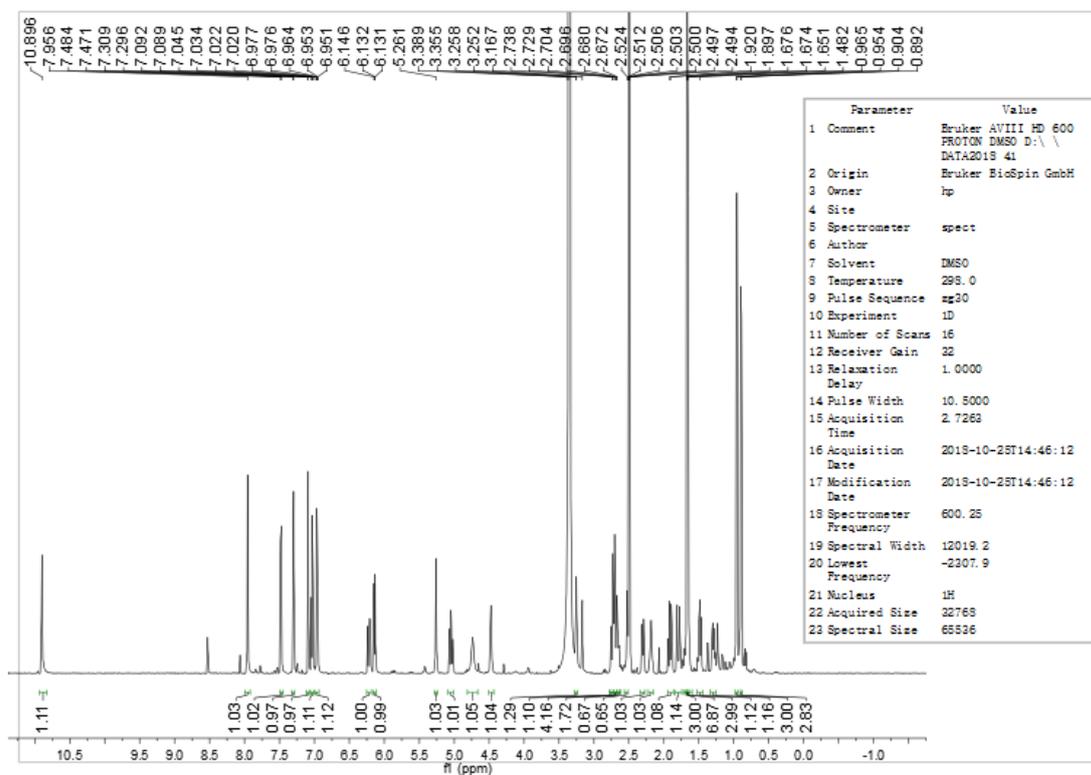


Figure S55: <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of **12**

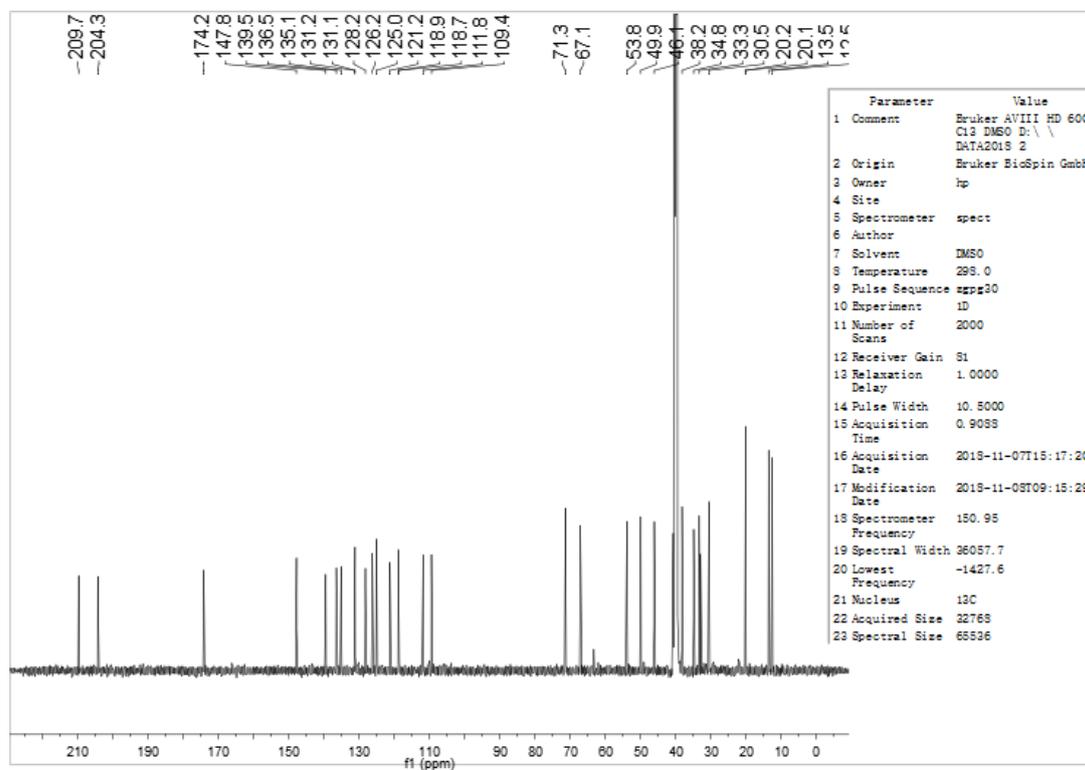


Figure S56: <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of **13**

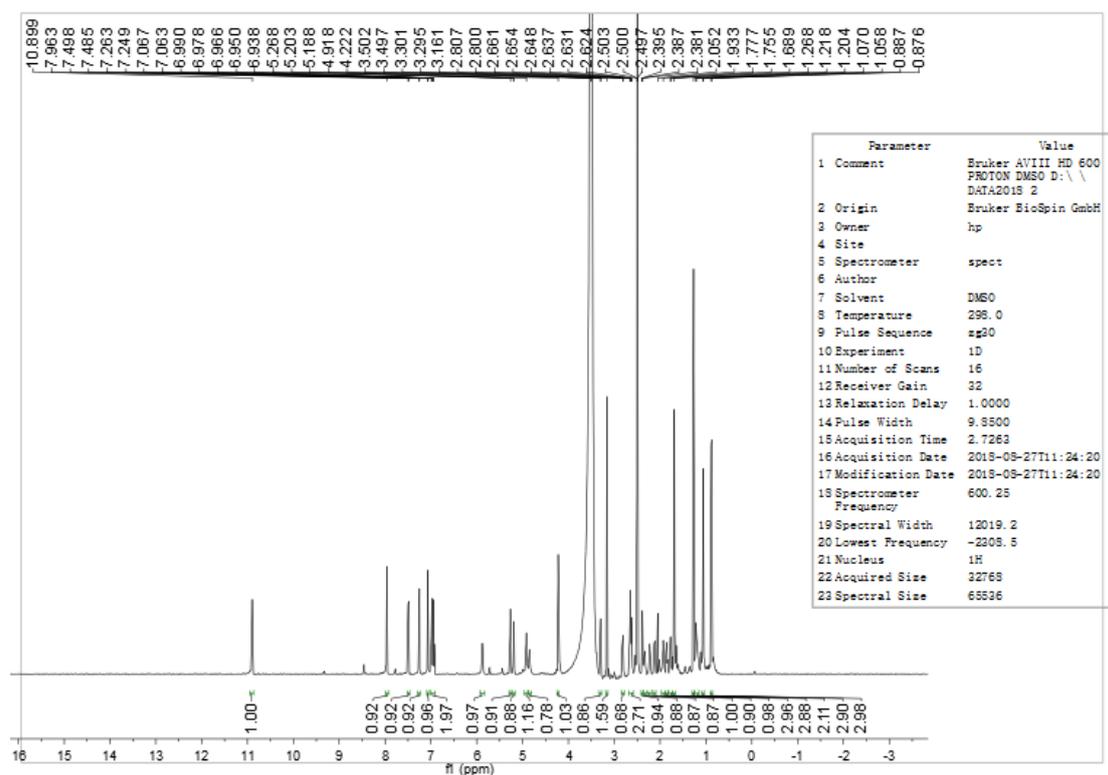


Figure S57: <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of **13**

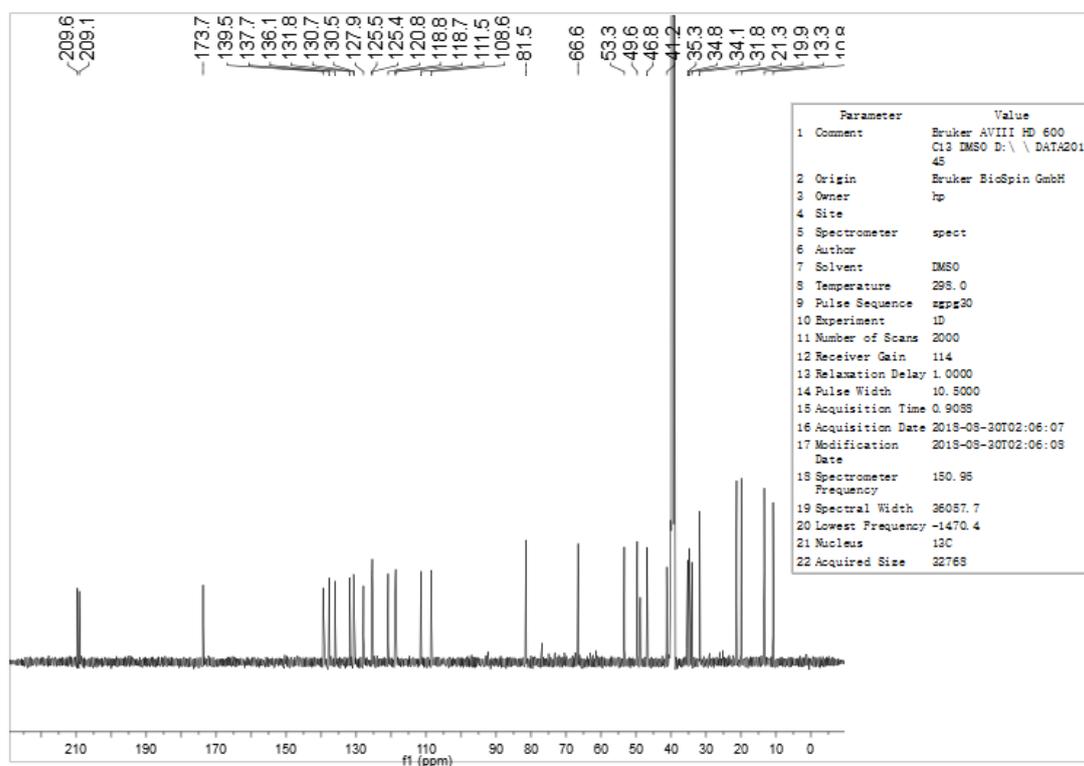


Figure S58: <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of **14**

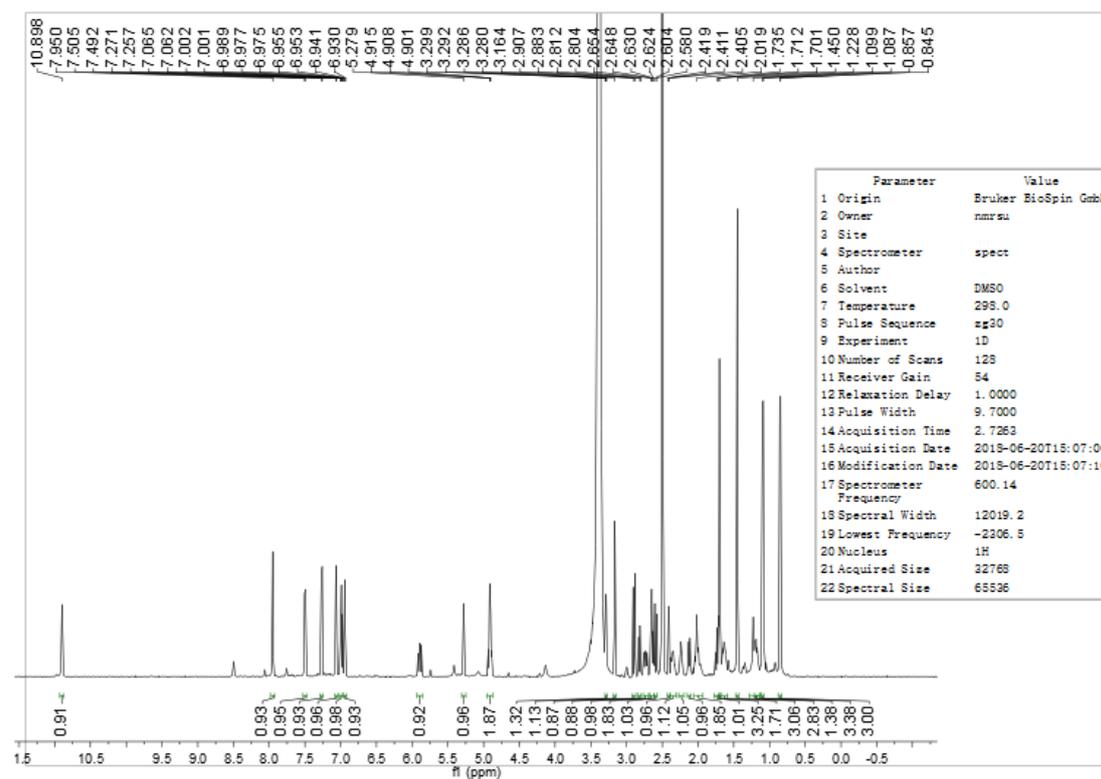


Figure S59: <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of **14**

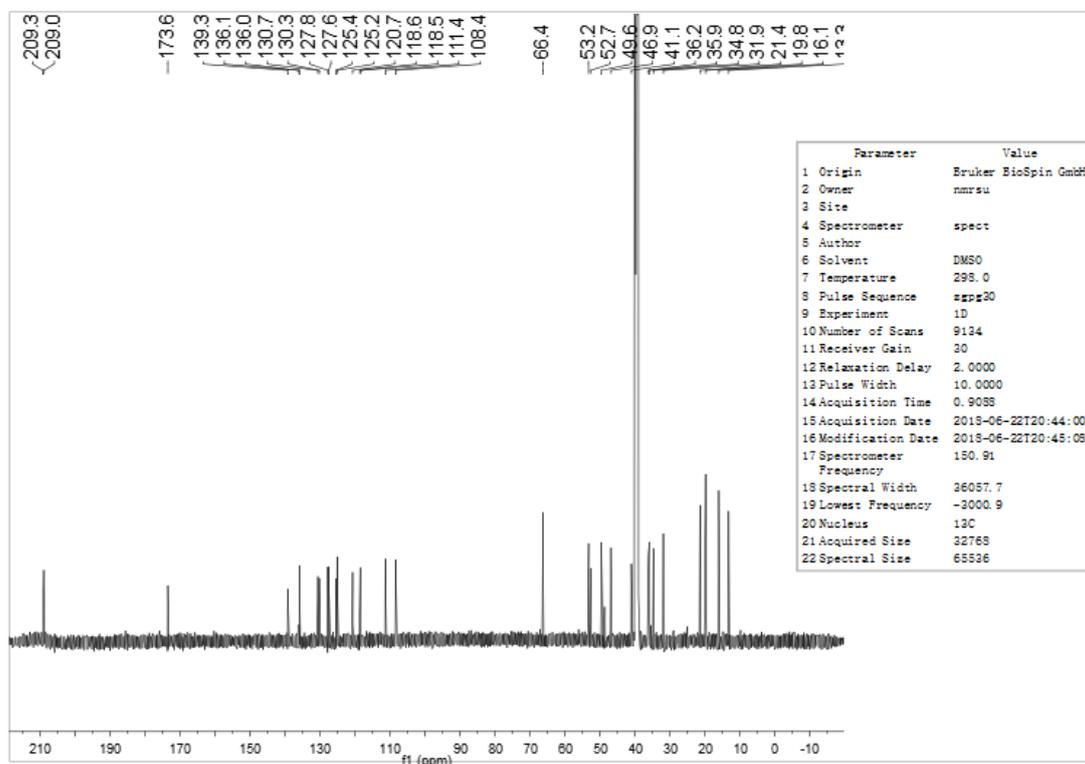


Figure S60: <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of **15**

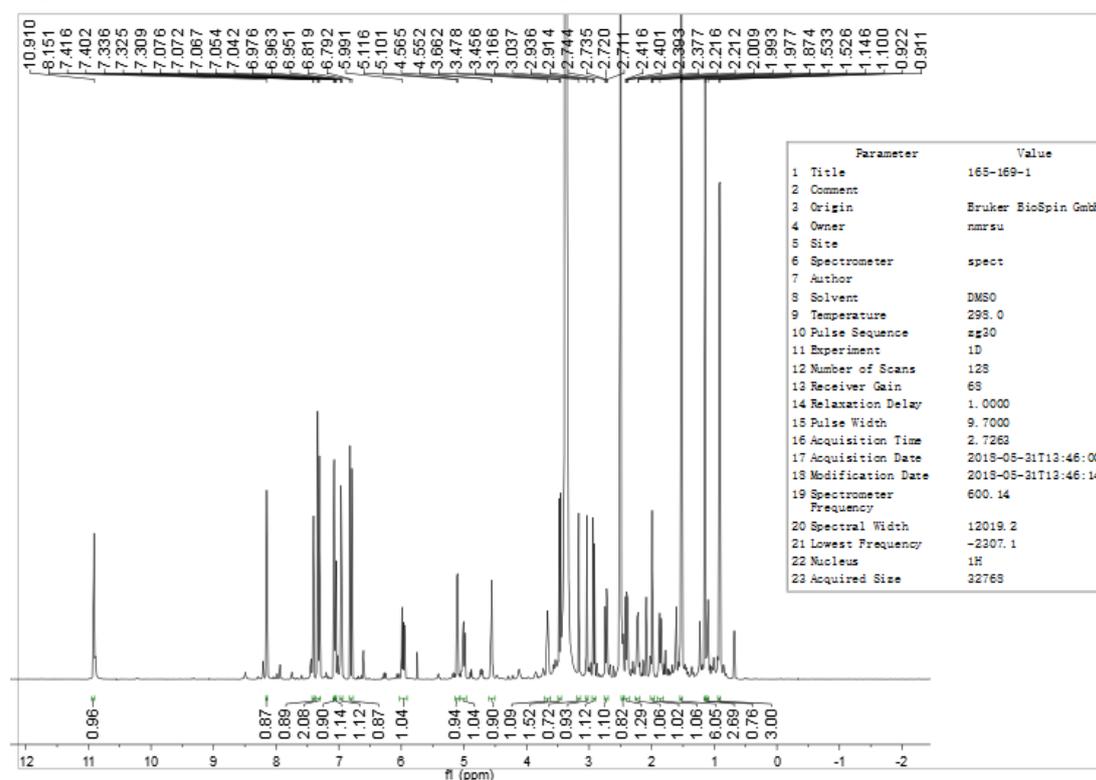


Figure S61: <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of **15**

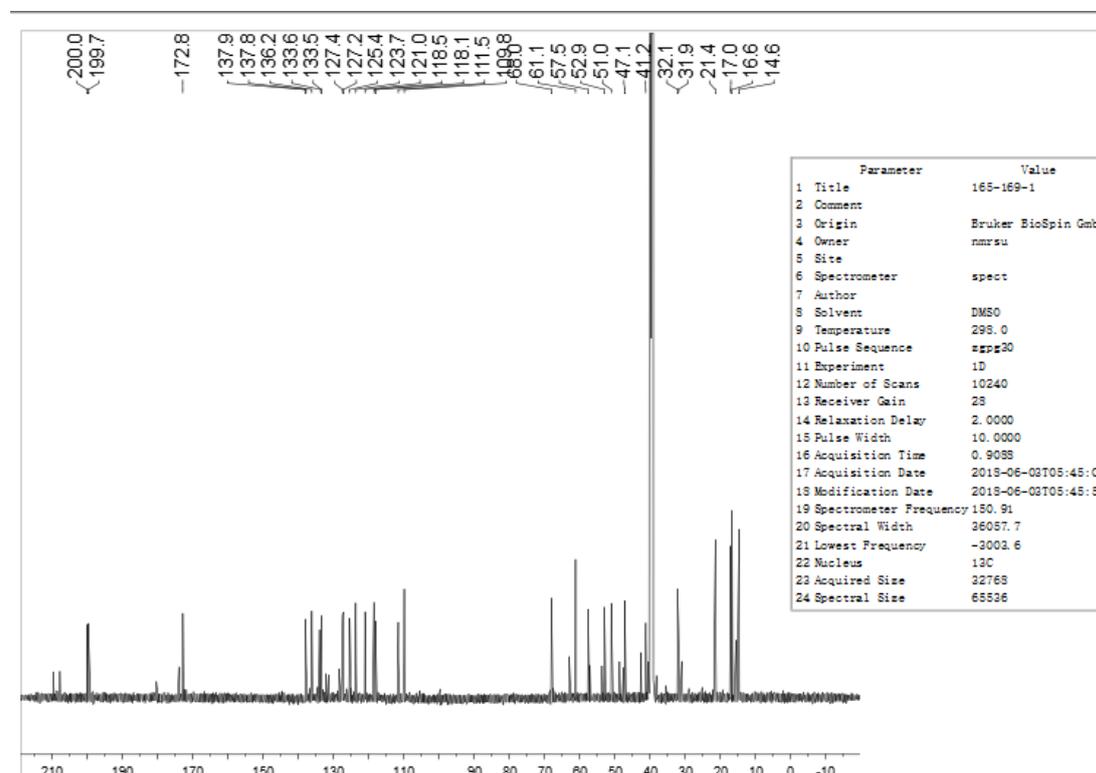


Figure S62: <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of **16**

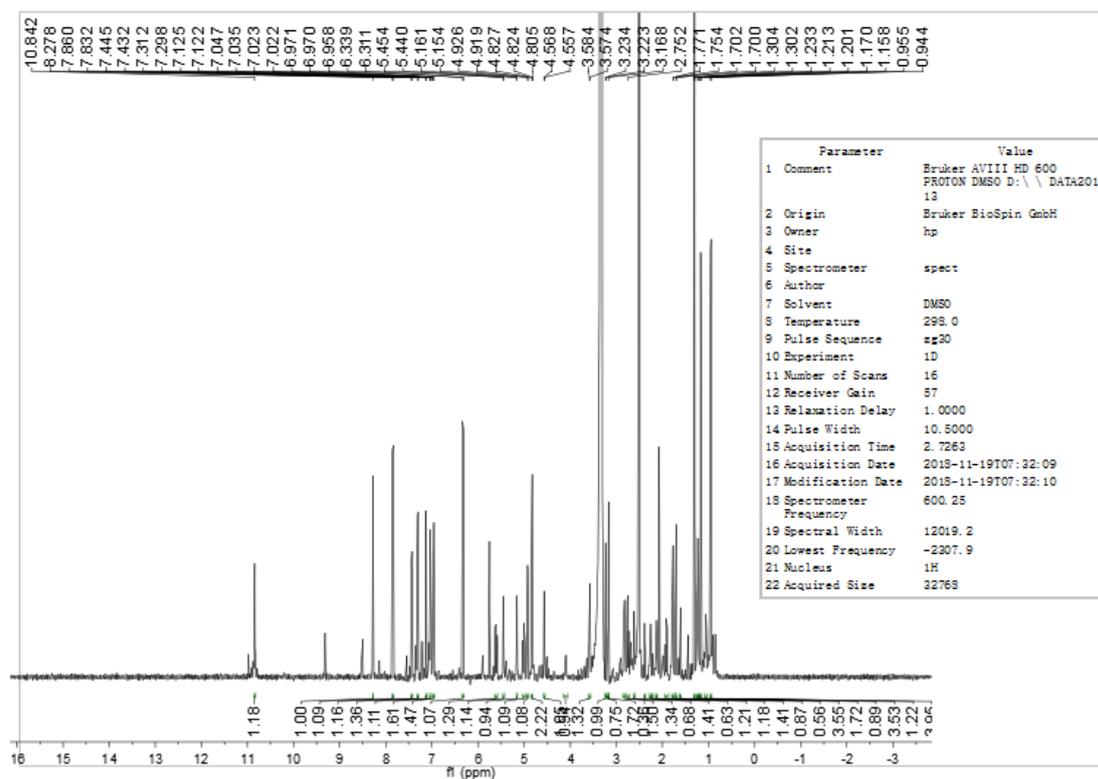


Figure S63: <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of **16**

