

## 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**

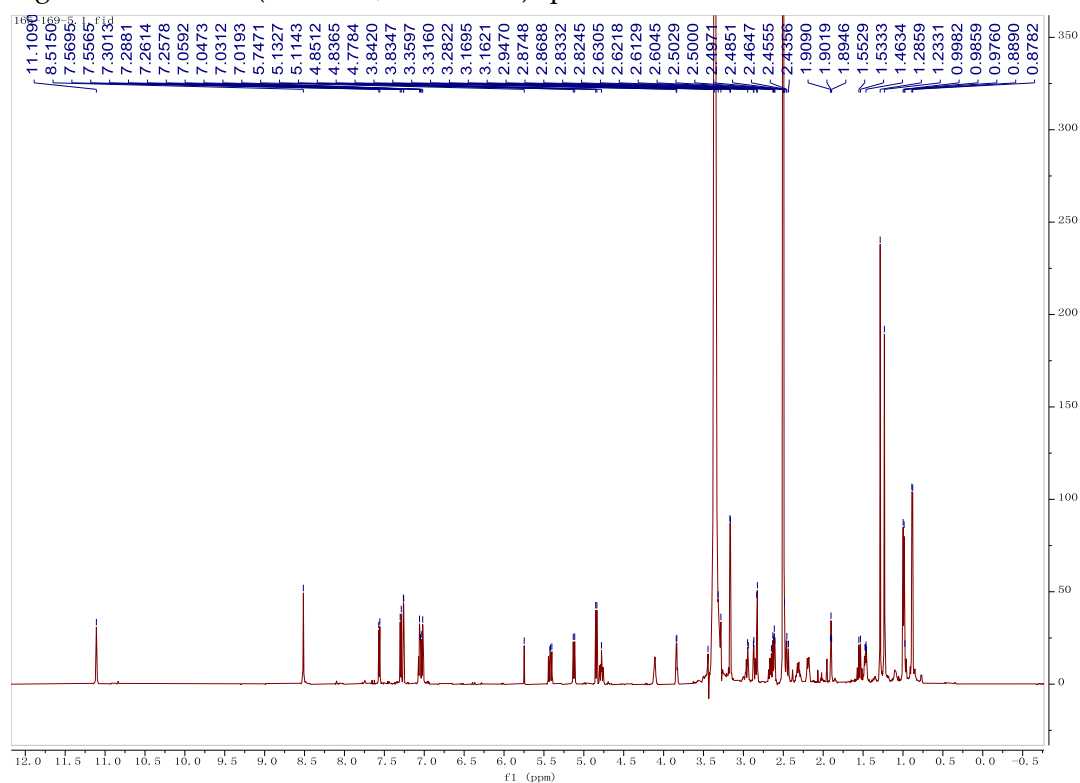


Figure S2:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}D_6$ ) spectrum of **1**

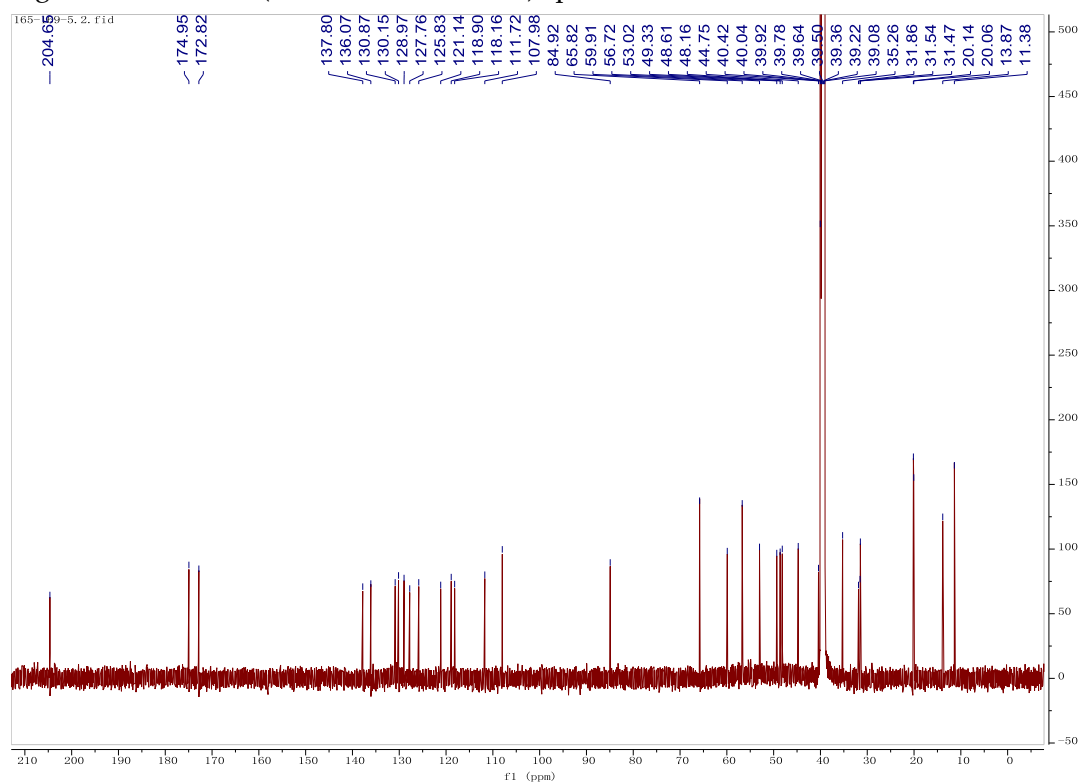




Figure S3: HSQC spectrum of **1**

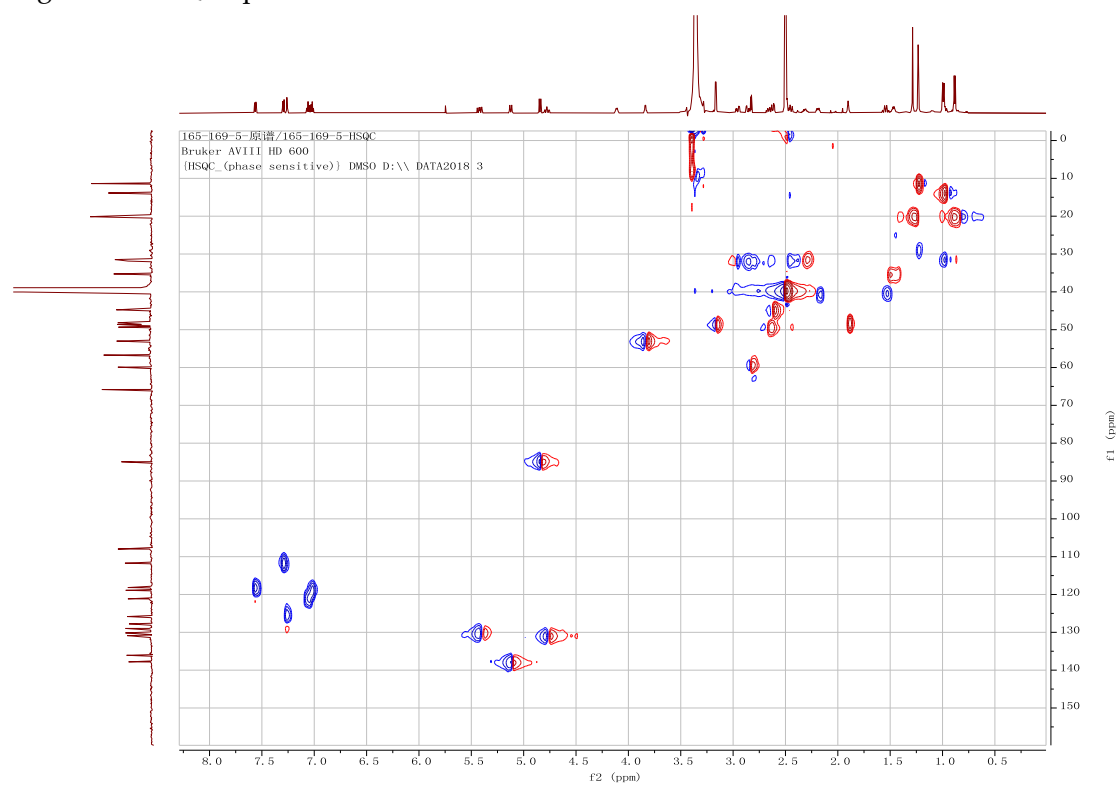


Figure S4: HMBC spectrum of **1**

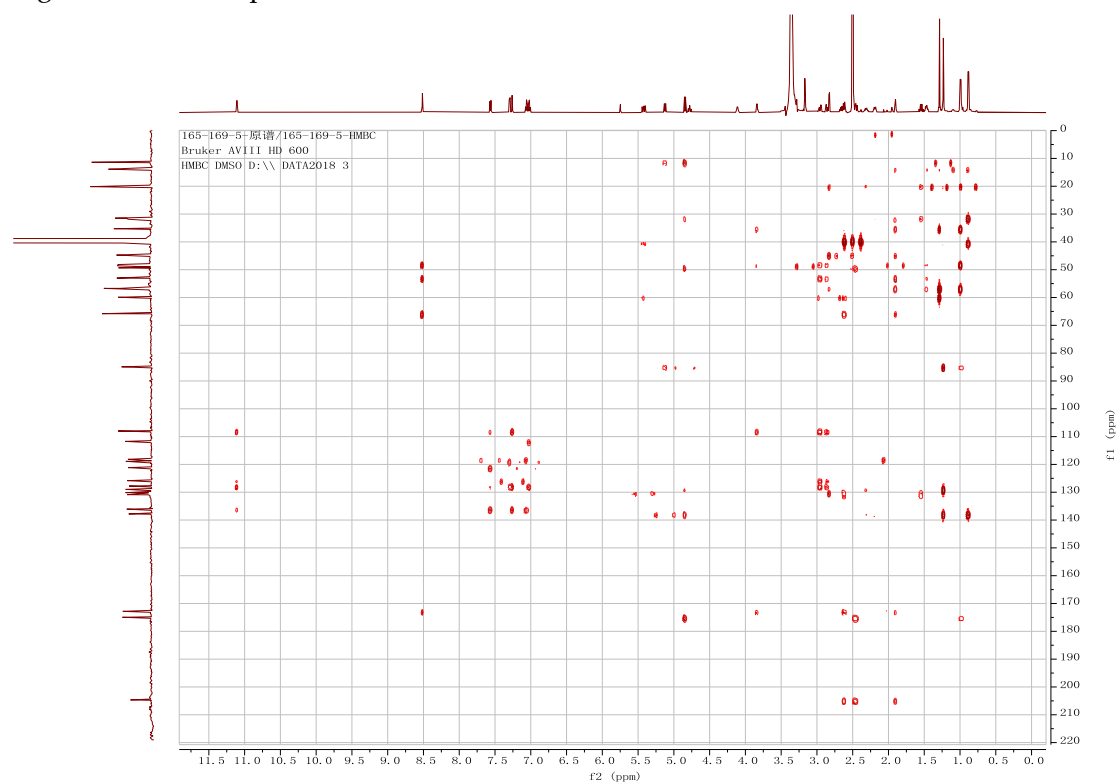


Figure S5:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**

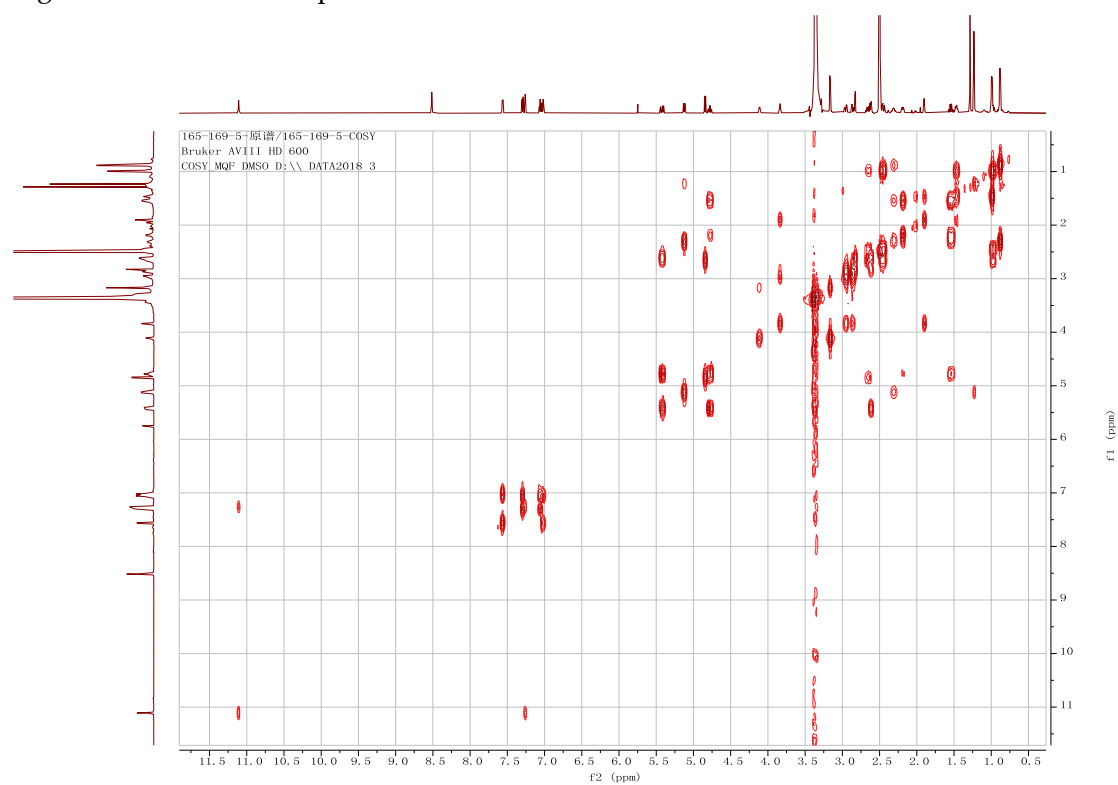


Figure S6: TOCSY spectrum of **1**



Figure S7: NOESY spectrum of **1**

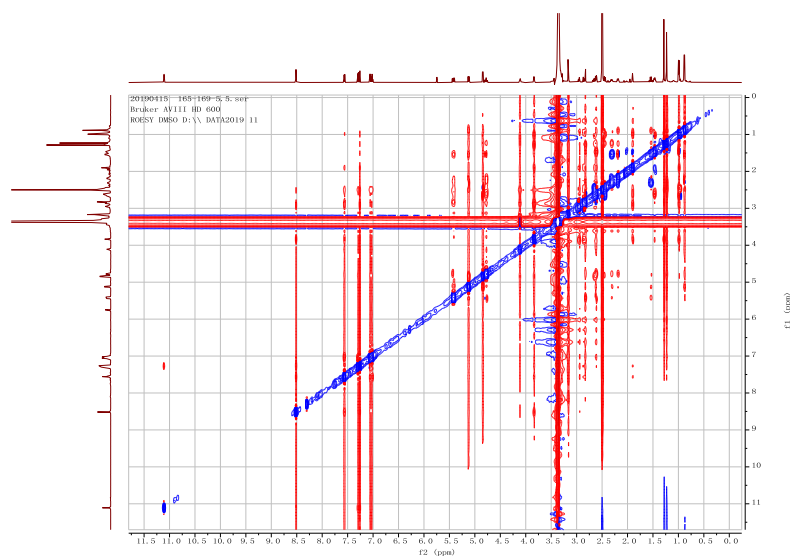


Figure S8: HR ESIMS spectrum of **1**

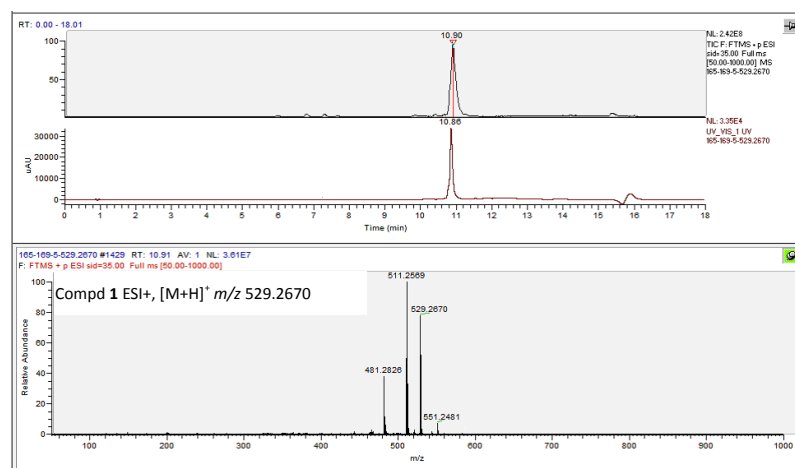


Figure S9: ECD and UV spectrum of **1**

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 ( $\sigma=0.30\text{eV}$ ).

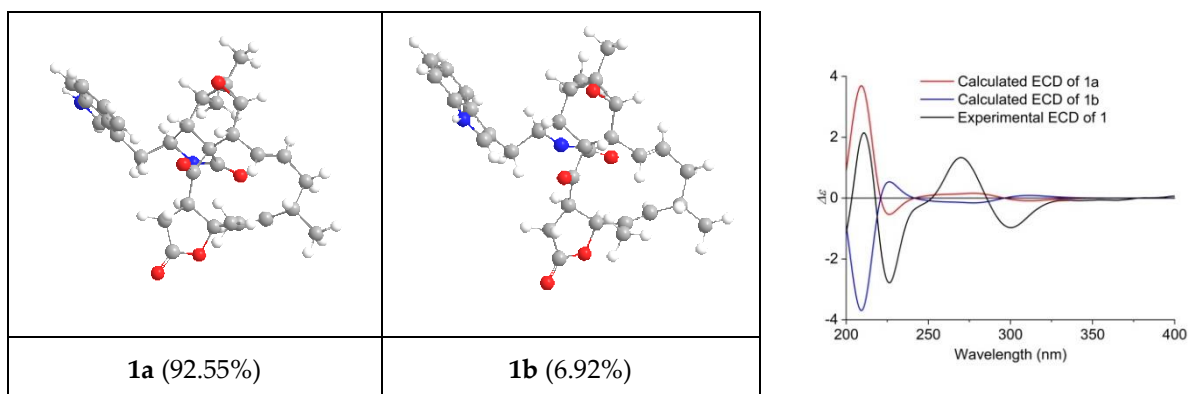


Figure S10:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}D_6$ ) spectrum of **2**

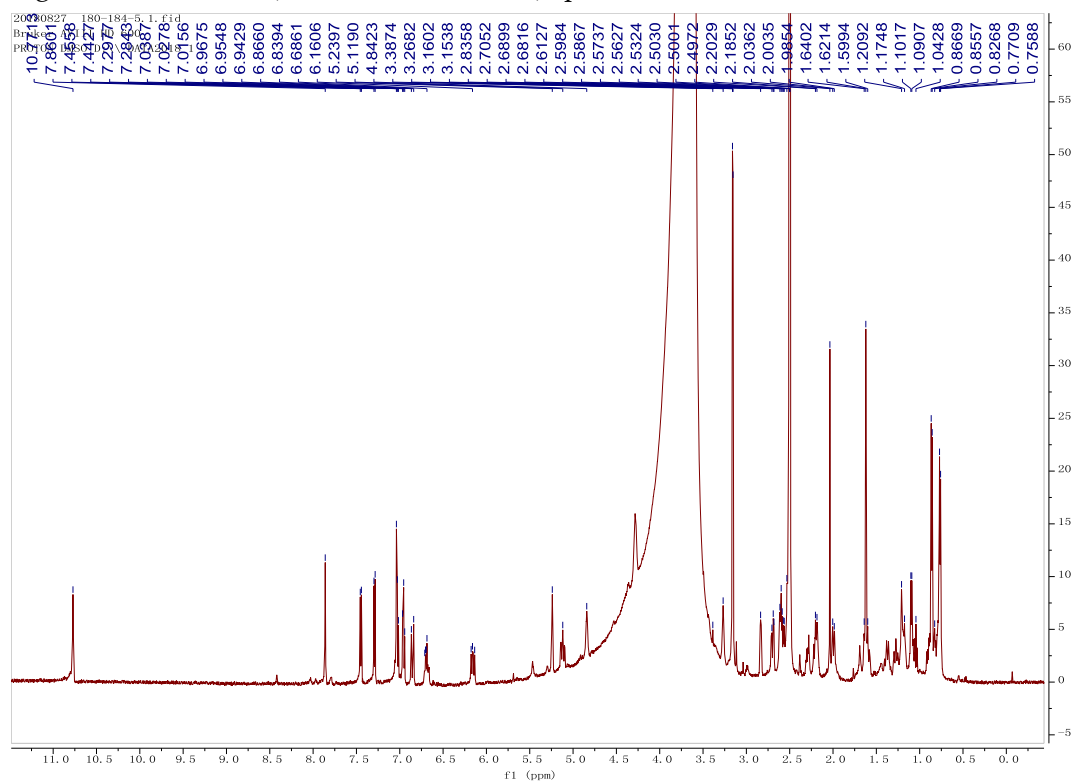


Figure S11:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}D_6$ ) spectrum of **2**

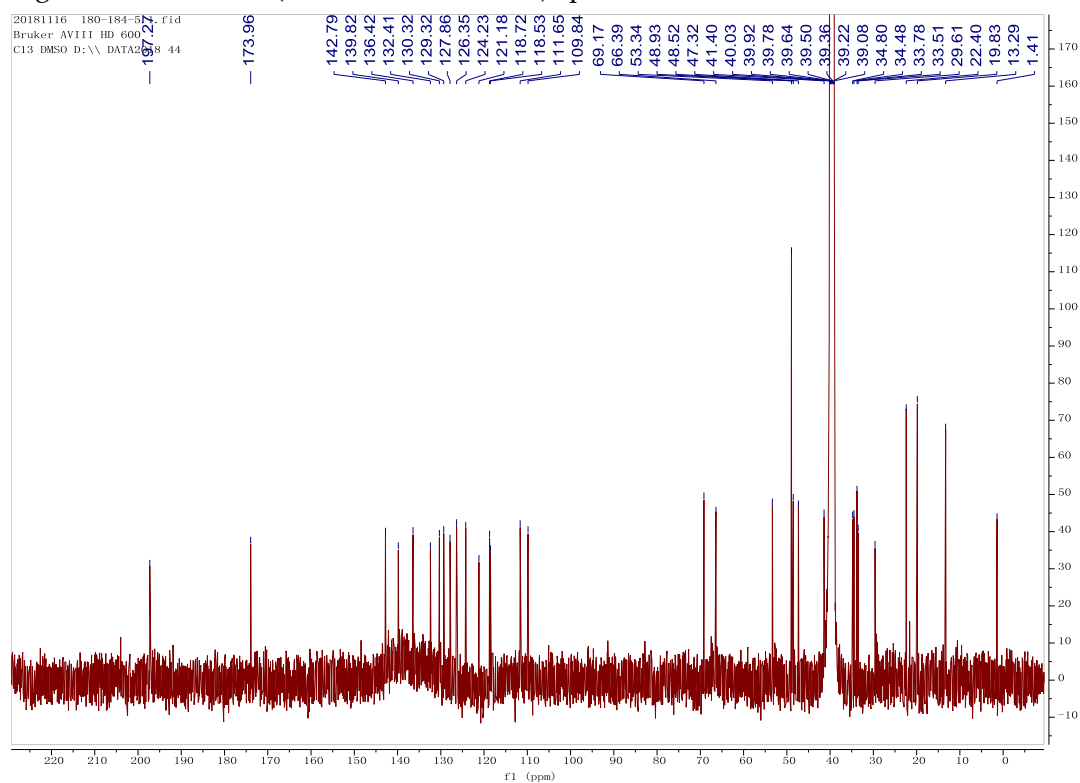


Figure S12: HSQC spectrum of 2

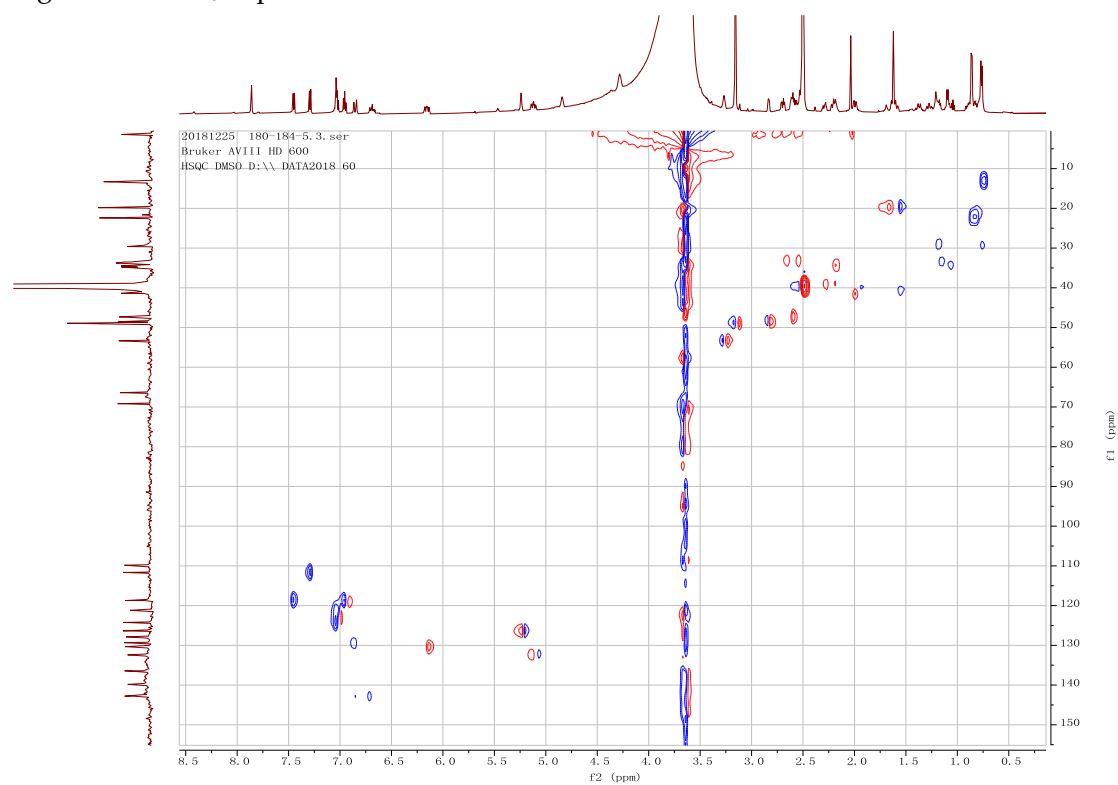


Figure S13: HMBC spectrum of 2

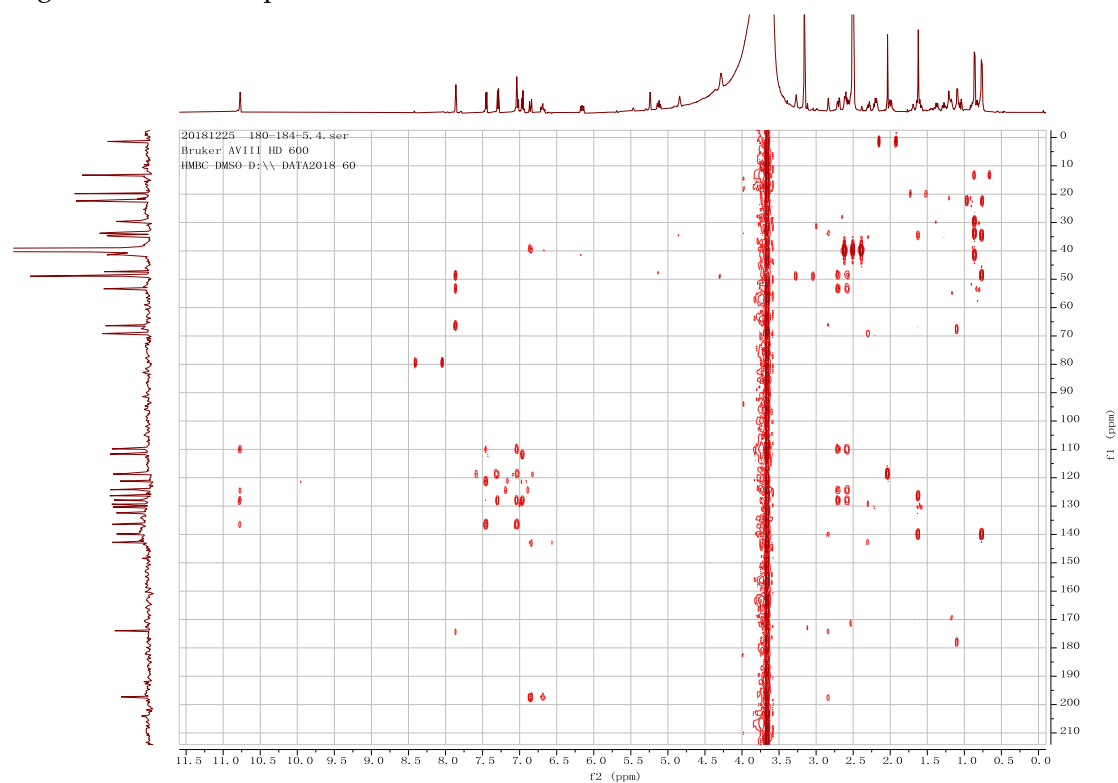


Figure S14:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2**

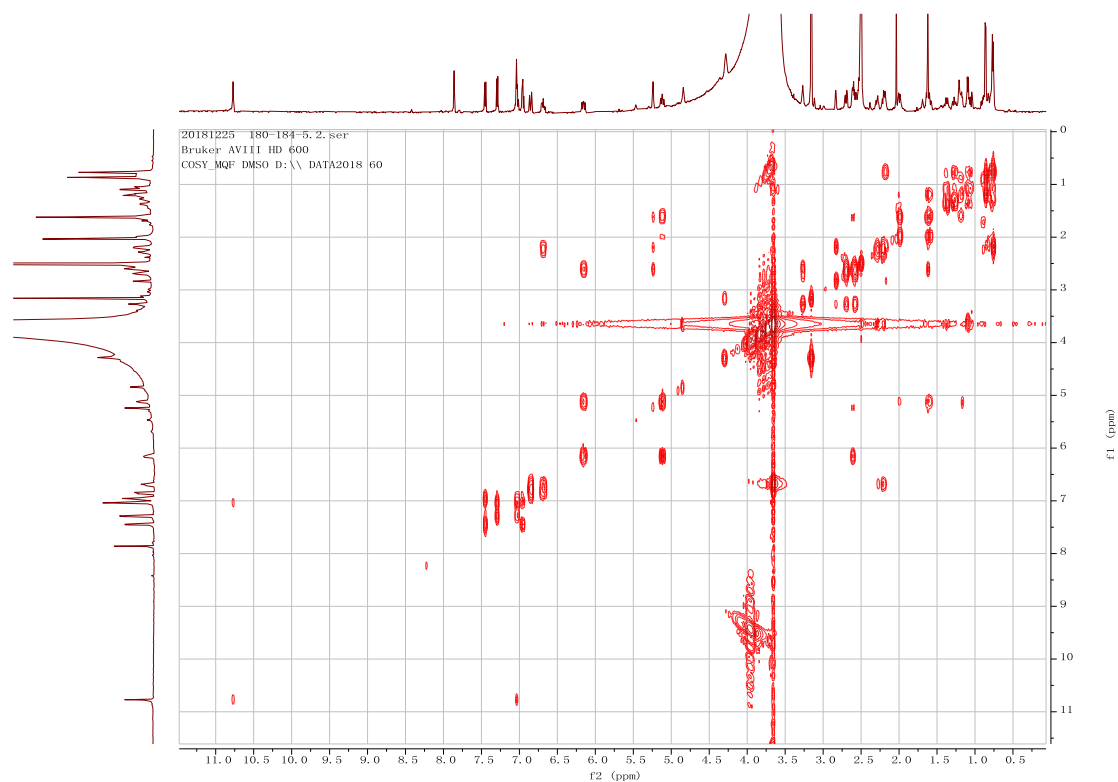


Figure S15: TOCSY spectrum of **2**

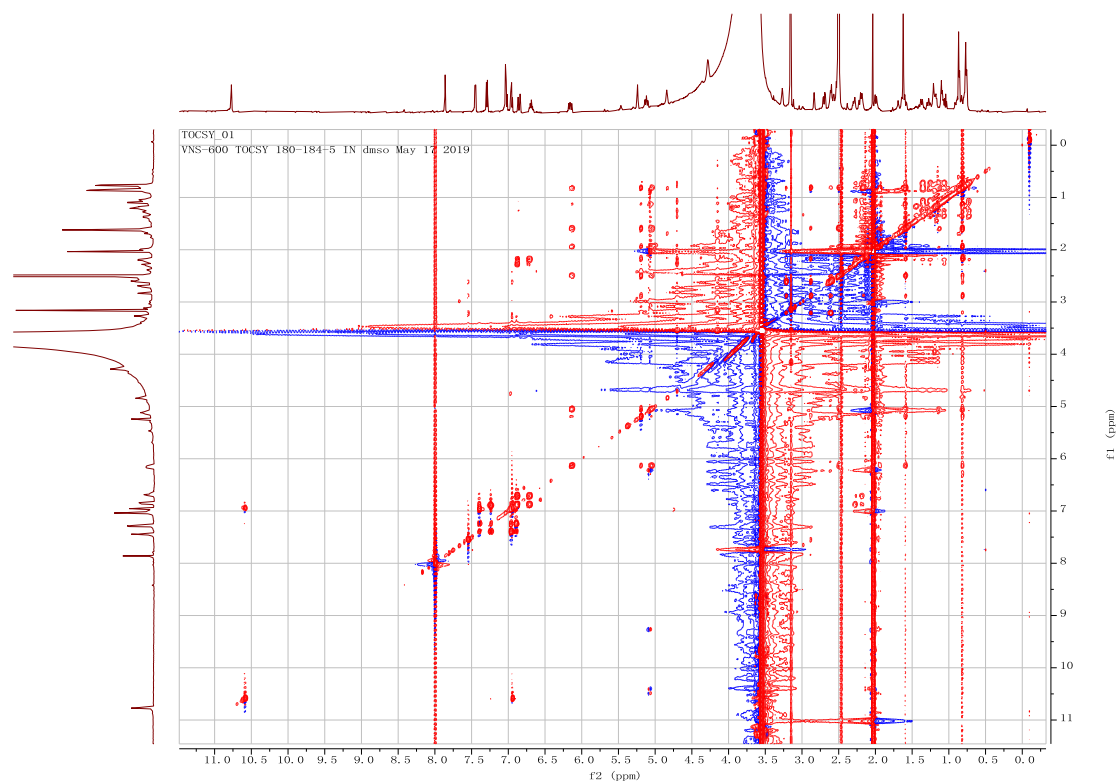


Figure S16: NOESY spectrum of **2**

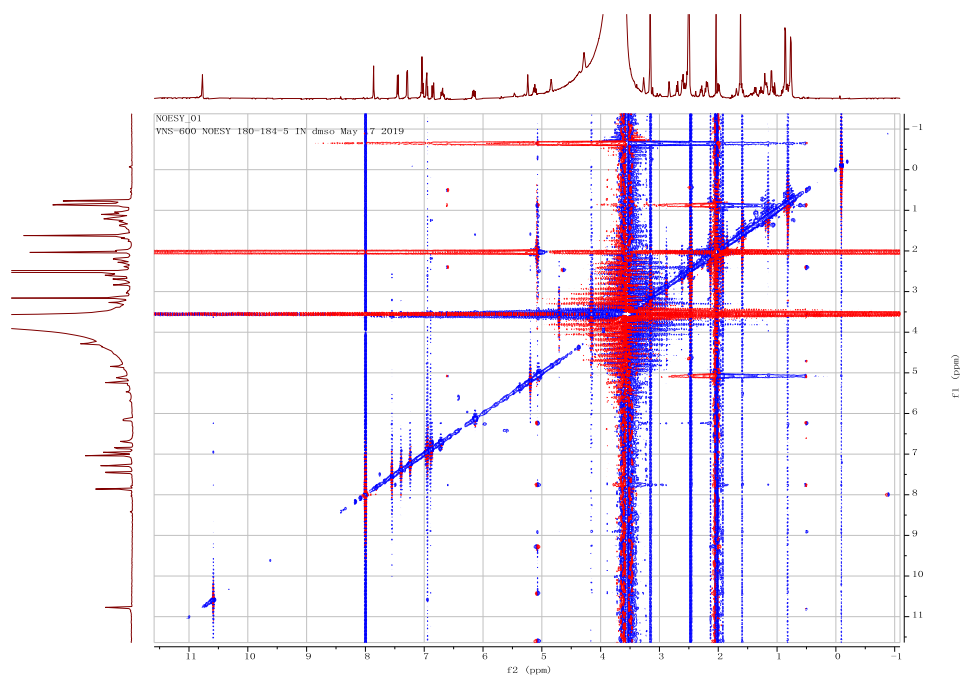


Figure S17: HR ESIMS spectrum of **2**

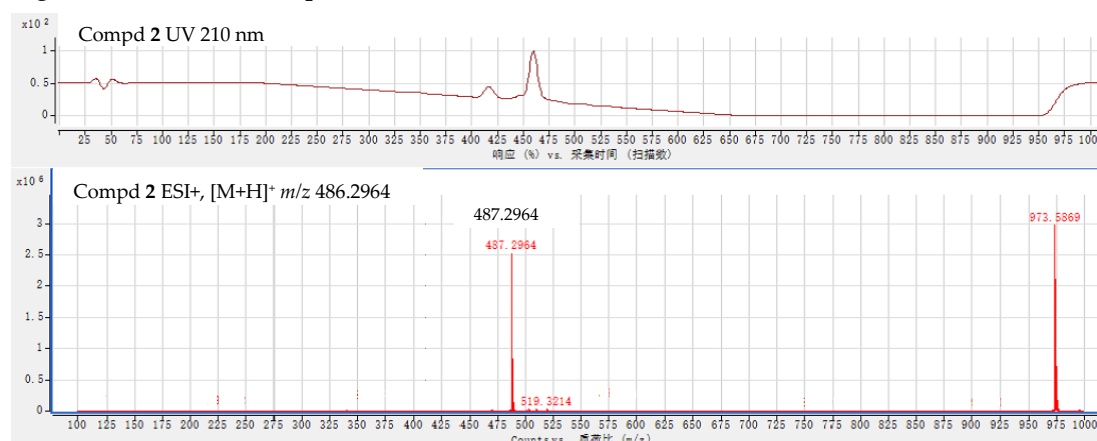
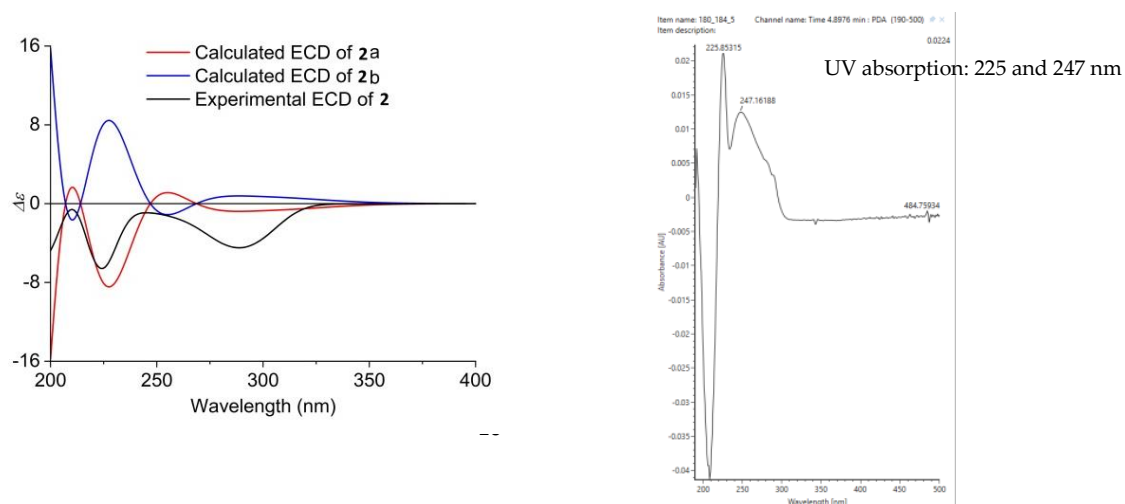


Figure S18: ECD and UV spectrum of **2**

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.



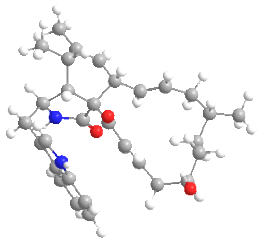
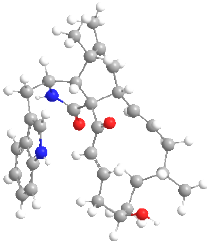
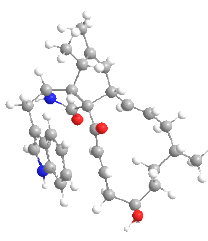
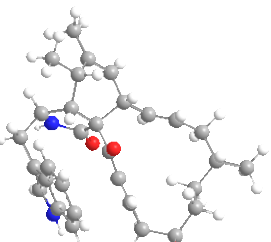
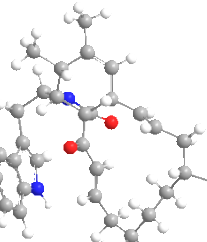
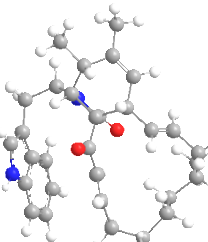
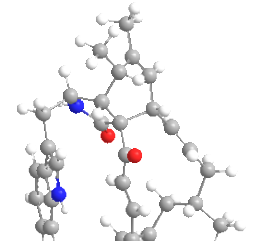
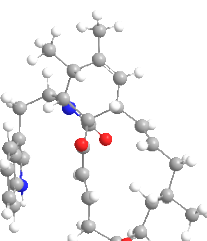
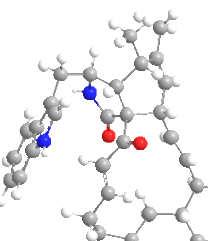
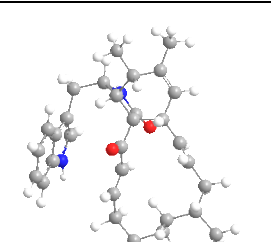
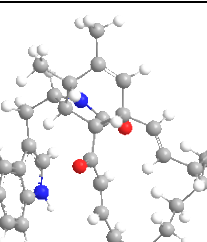
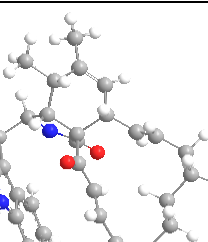
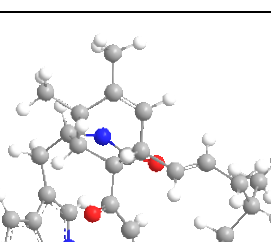
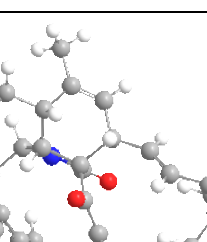
		
C1 (16.70%)	C2 (16.18%)	C3 (11.95%)
		
C4 (9.76%)	C5 (9.21%)	C6 (8.23%)
		
C7 (7.77%)	C8 (4.31%)	C9 (3.55%)
		
C10 (3.04%)	C11 (2.29%)	C12 (2.20%)
		
C13 (2.01%)	C14 (1.20%)	



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

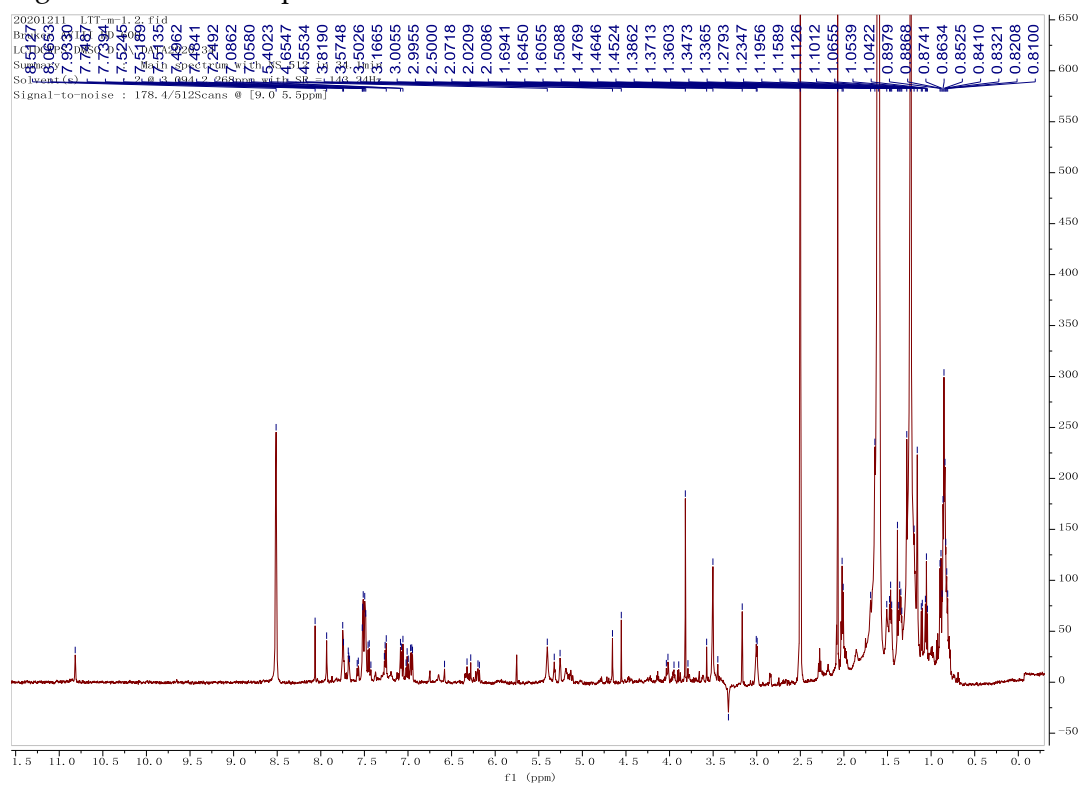
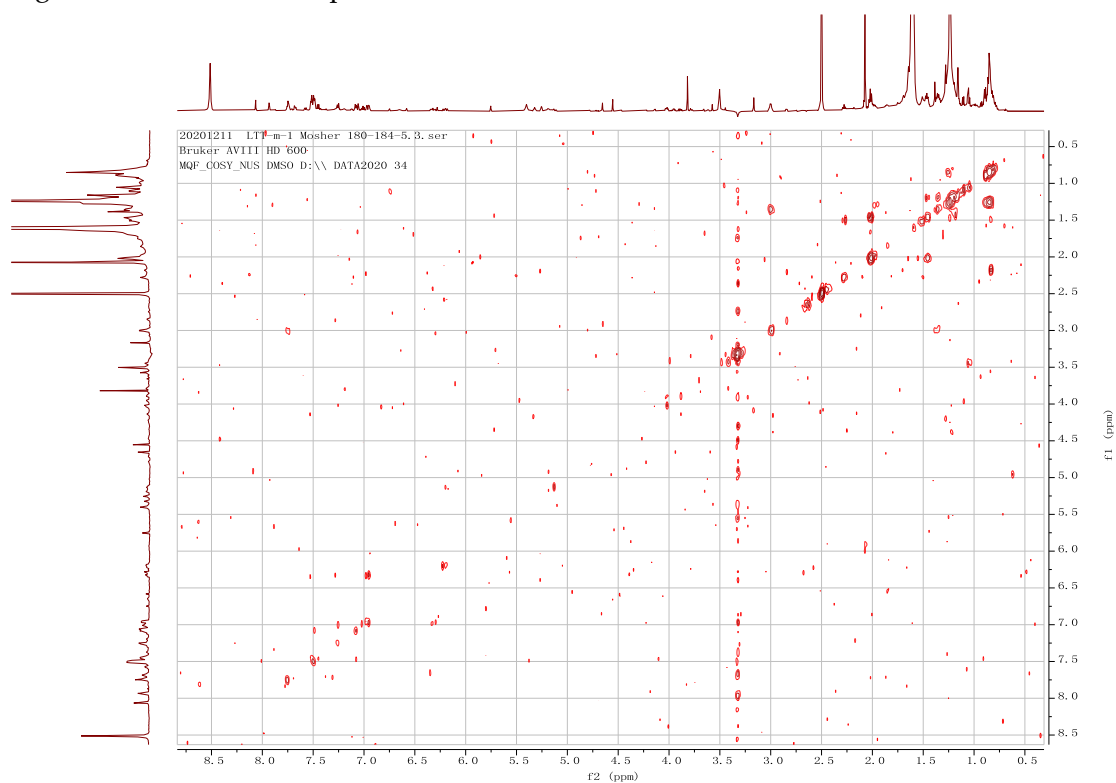


Figure S20:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2c**



[illegible]

20210112\_LIT-m-1.2.ser  
Bruker AVIII HD 600  
MQF-COSY\_NUS-DMSO-D6-\\DATA2021-13

Chemical shifts (ppm) listed on the right side of the spectrum:

- 11.0695
- 8.5017
- 7.5027
- 7.5395
- 7.3468
- 7.3334
- 7.1753
- 7.1317
- 7.0829
- 7.0812
- 7.0712
- 7.0695
- 7.0578
- 7.0560
- 7.0195
- 7.0178
- 7.0077
- 7.0062
- 7.0046
- 6.9946
- 5.8751
- 5.8730
- 5.8583
- 5.8562
- 4.8987
- 4.8803
- 4.8750
- 4.4804
- 4.4600
- 3.7256
- 3.7187
- 3.1670
- 2.9401
- 2.9230
- 2.9199
- 2.7061
- 2.6997
- 2.6811
- 2.6750
- 2.5061
- 2.5030
- 2.5000
- 2.4969
- 2.4938
- 2.0682
- 1.9358
- 1.9095
- 1.8899
- 1.8611
- 1.7045
- 1.7023
- 1.0323
- 0.9942
- 0.9823
- 0.9306
- 0.9195

20191118 C. C.  
Bruker AVIII 500  
C13 DMSO D<sub>6</sub> 9

Chemical shift labels (ppm):

- 207.29
- 204.36
- 185.76
- 173.36
- 169.99
- 154.80
- 135.91
- 133.26
- 131.01
- 127.88
- 125.82
- 125.53
- 121.01
- 118.83
- 118.39
- 111.38
- 107.90
- 72.97
- 71.85
- 62.12
- 52.30
- 43.73
- 43.30
- 40.04
- 39.92
- 39.78
- 39.64
- 39.50
- 39.36
- 39.22
- 39.08
- 35.84
- 32.69
- 32.13
- 31.23
- 24.32
- 21.77
- 20.71
- 19.17
- 12.90
- 10.42

Figure S25: HSQC spectrum of **3**

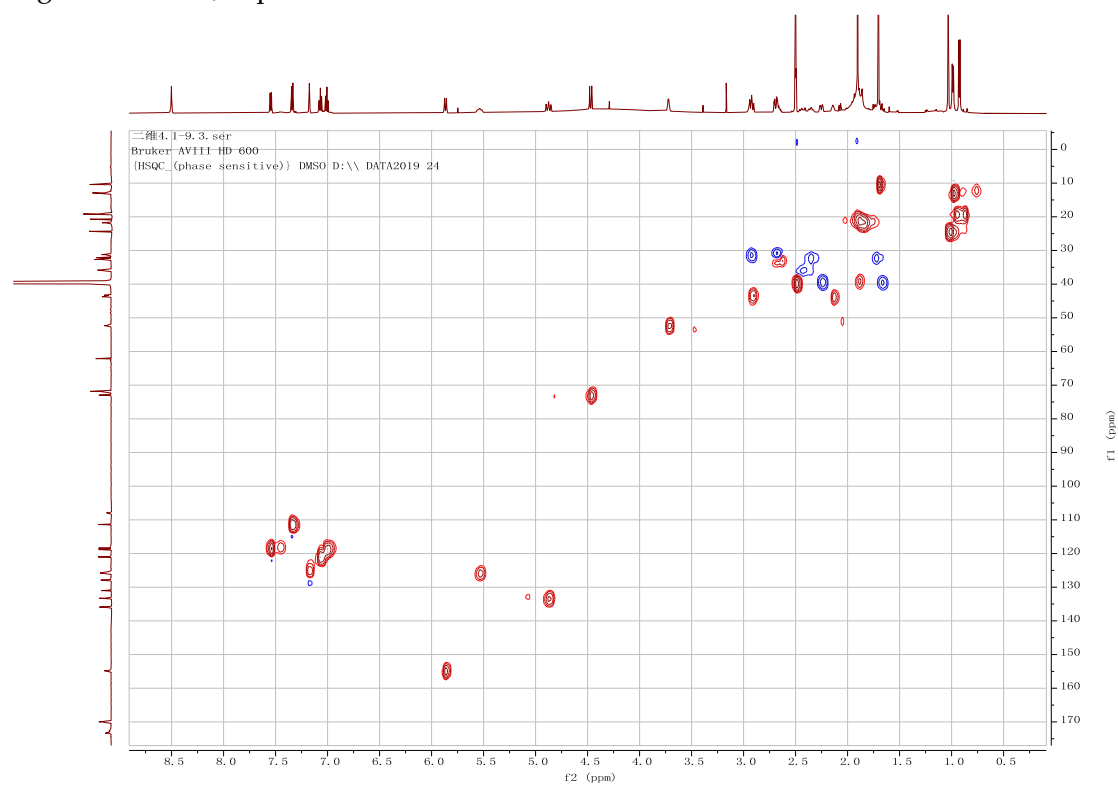


Figure S26: HMBC spectrum of **3**

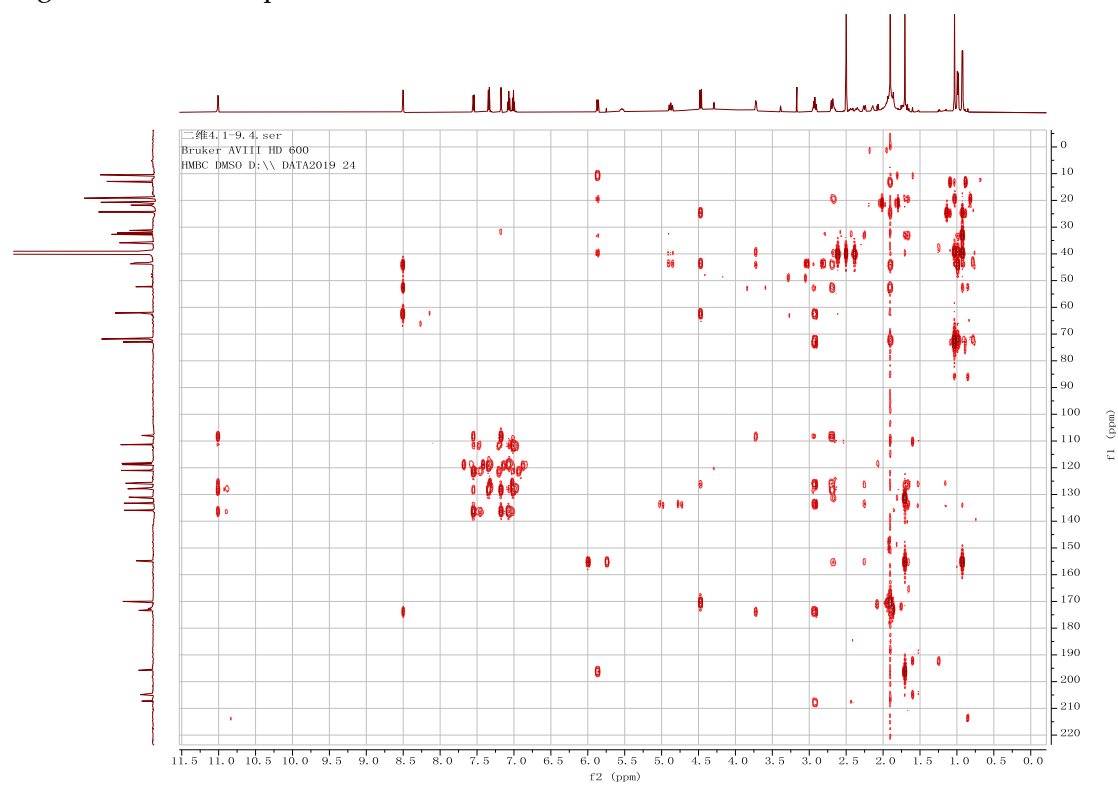


Figure S27:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3**

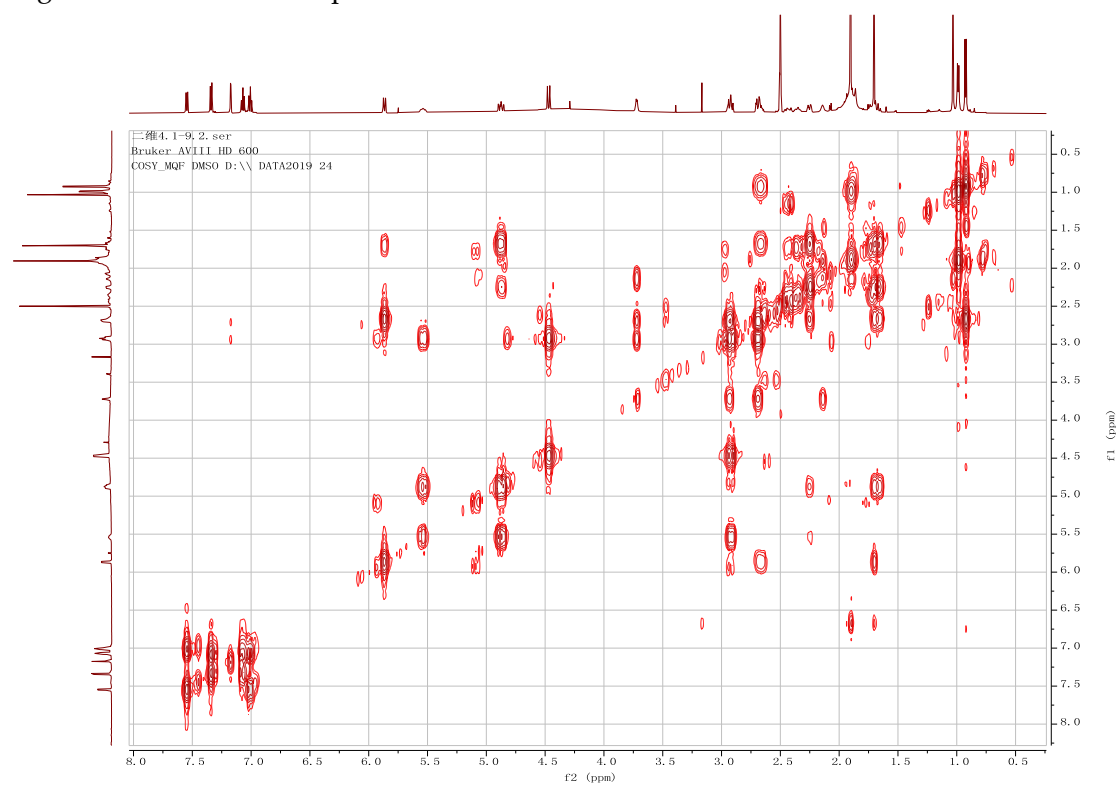


Figure S28: ROESY spectrum of **3**

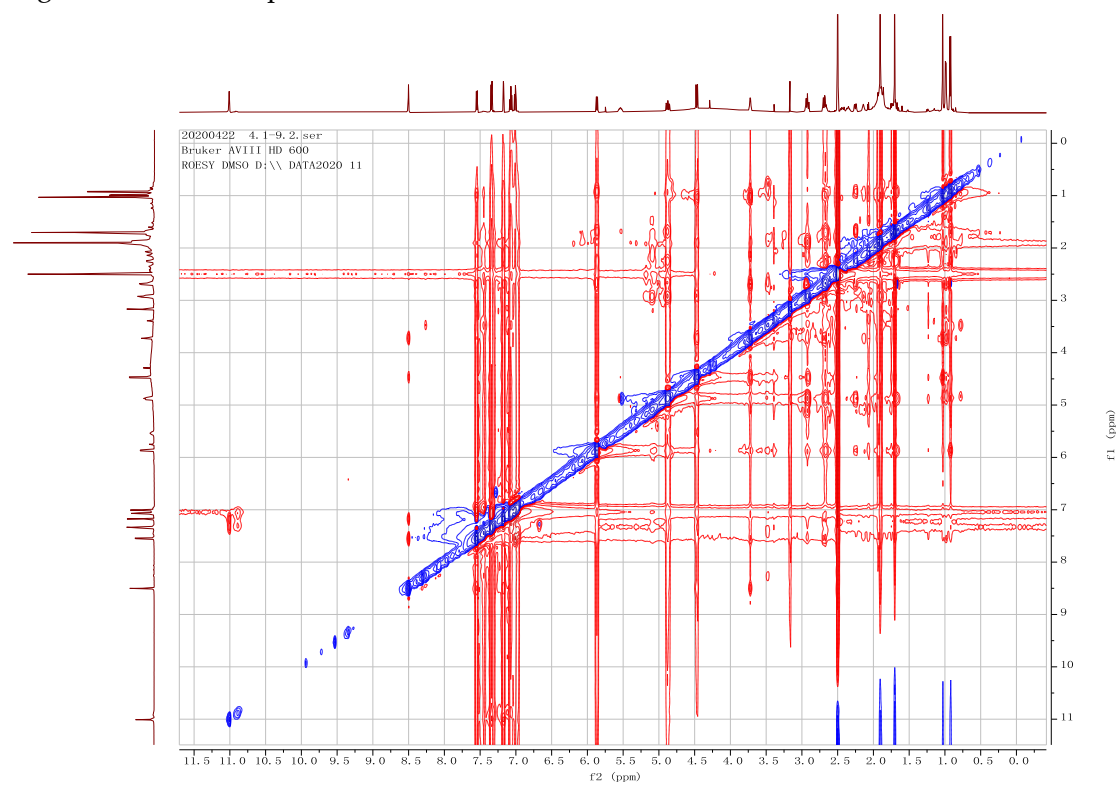


Figure S29: HR-ESIMS spectrum of **3**

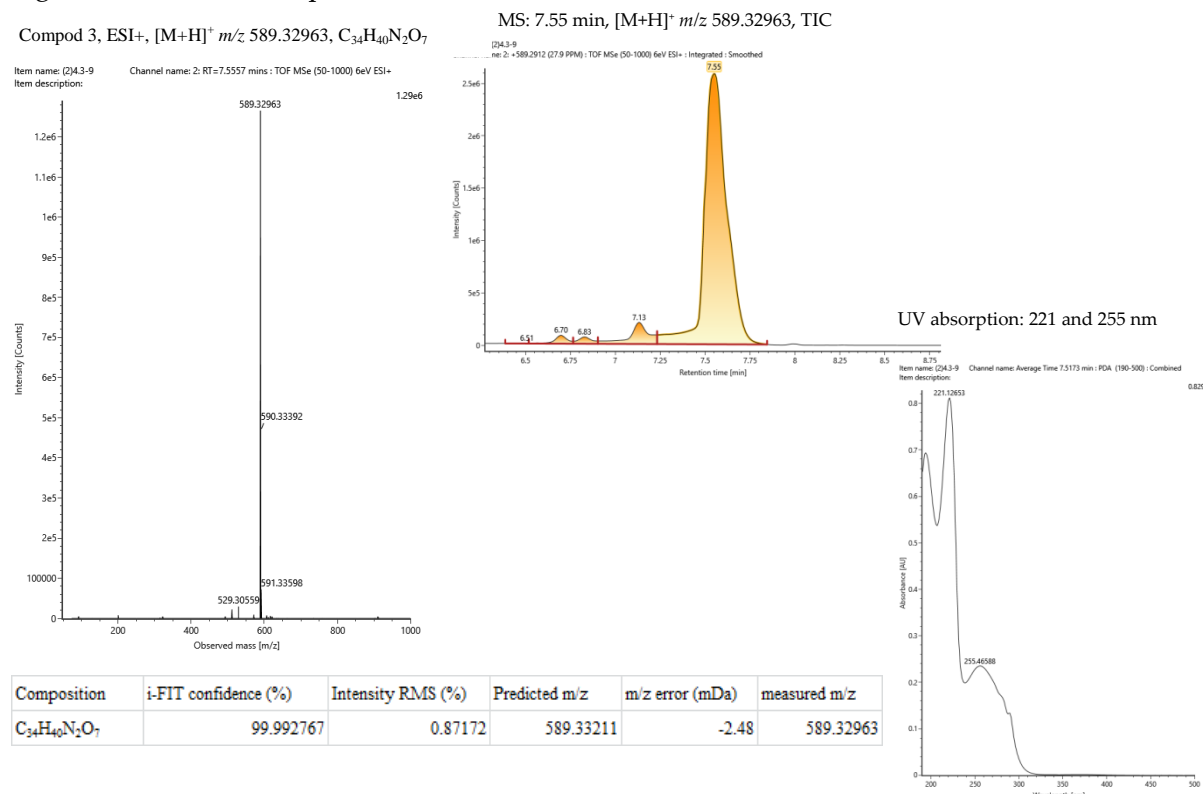
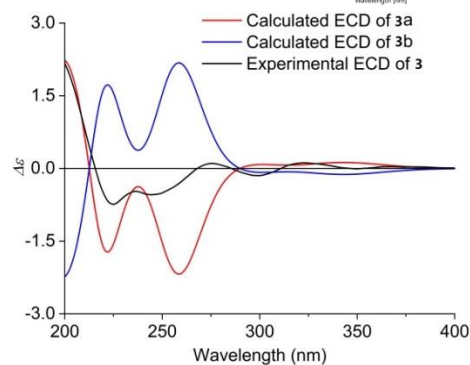


Figure S30: ECD and UV spectrum of **3** (in MeOH)

TDDFT theory,  $\omega$ B3LYP 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.



C1 (42.48%)	C2 (34.12%)	C3 (15.45%)
C4 (3.78%)	C5 (3.23%)	

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

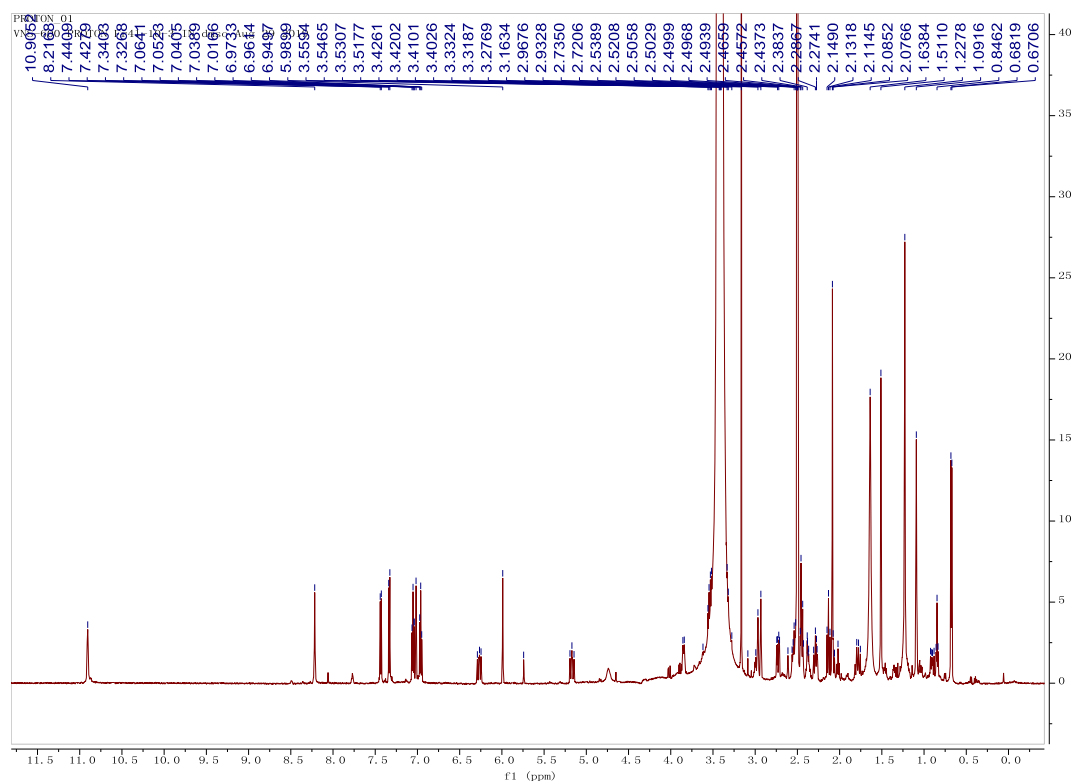


Figure S32:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}D_6$ ) spectrum of **4**

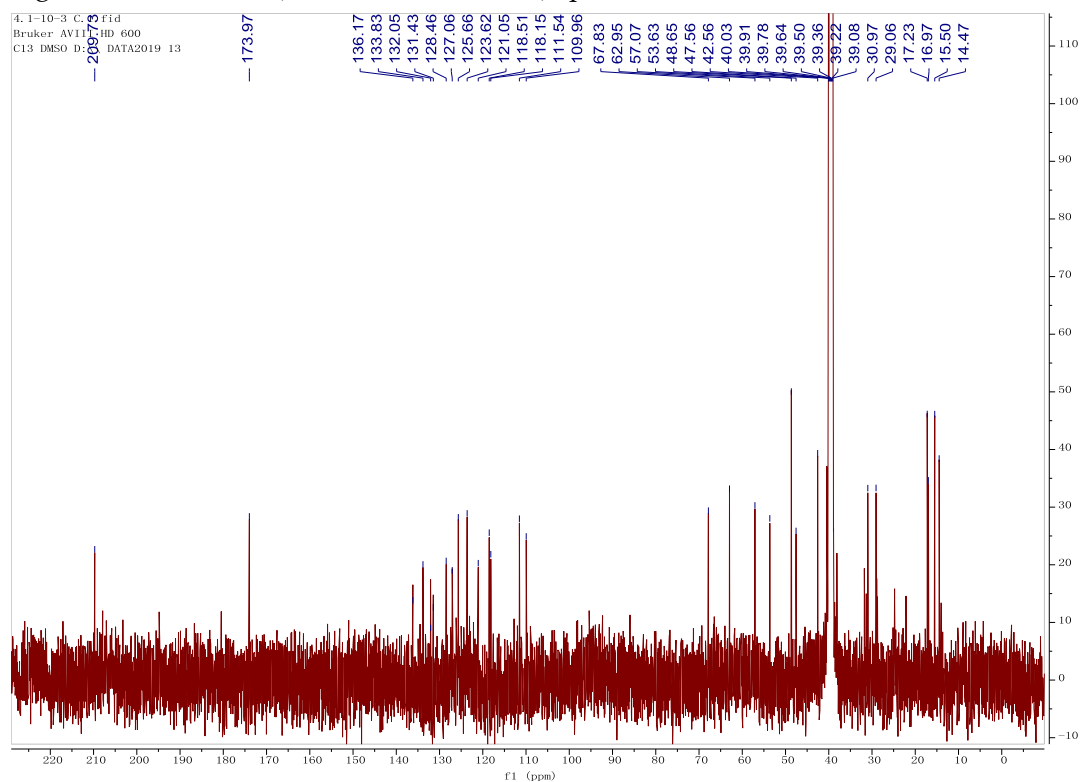


Figure S33: HSQC spectrum of **4**

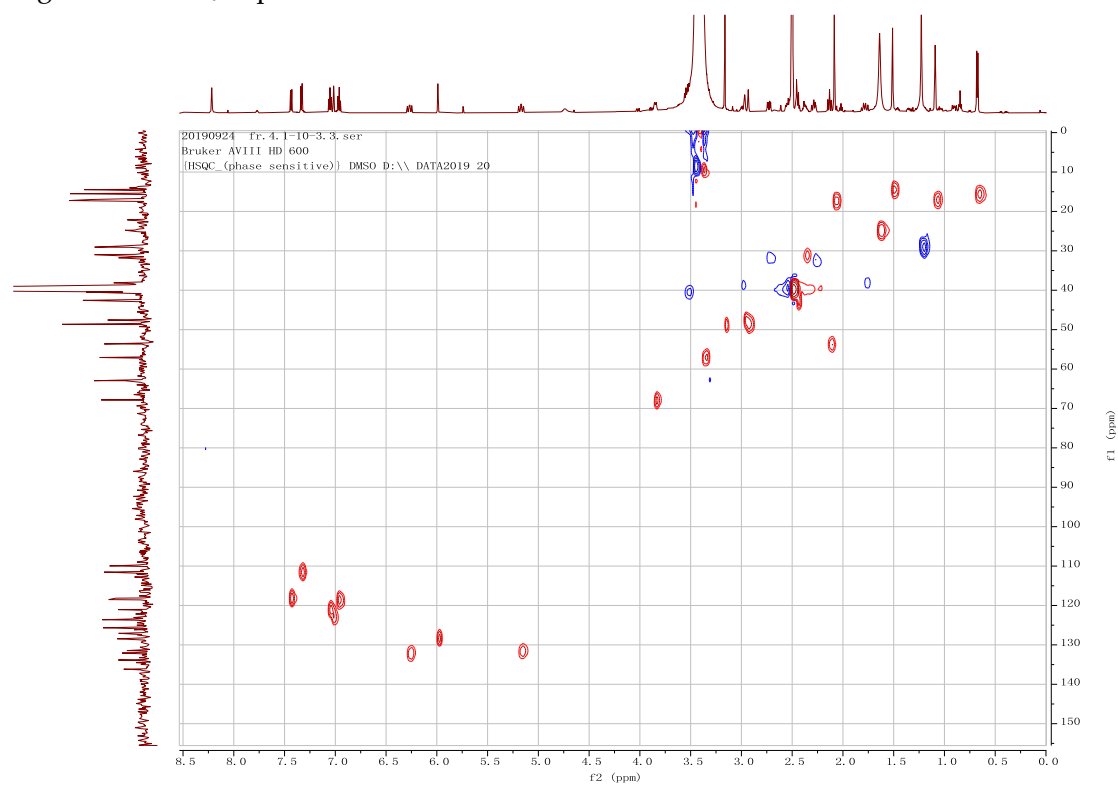


Figure S34: HMBC spectrum of **4**

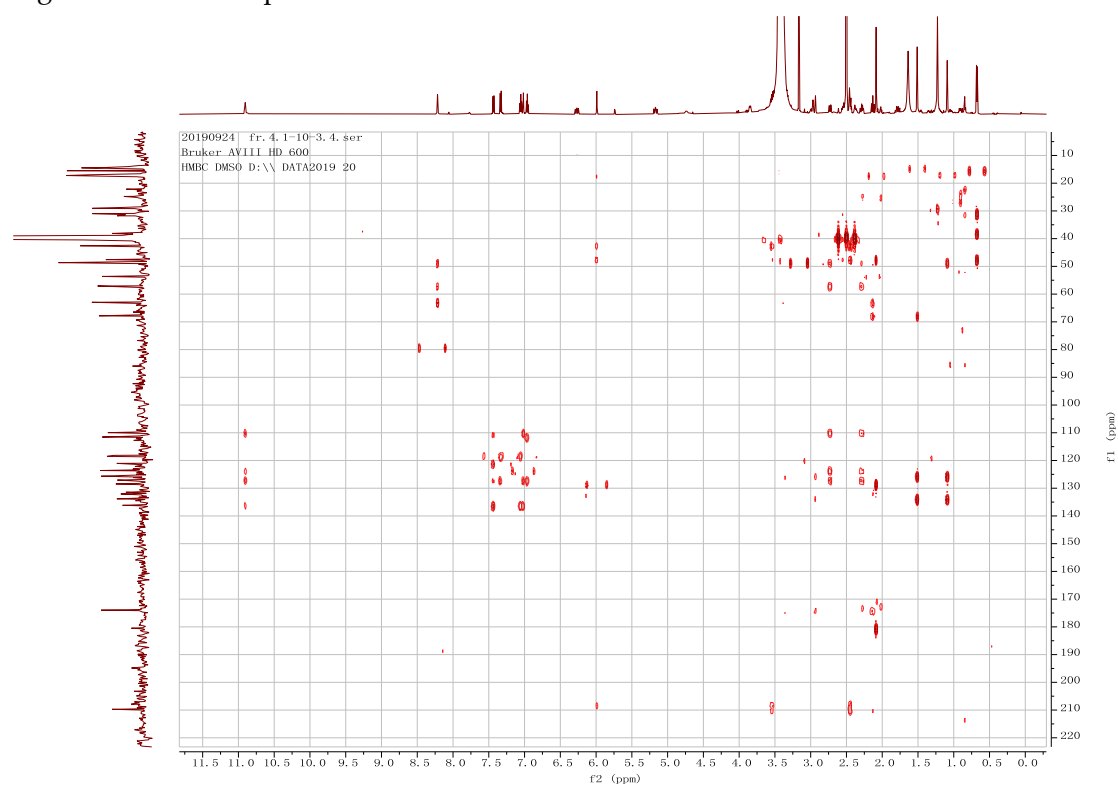




Figure S35:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4**

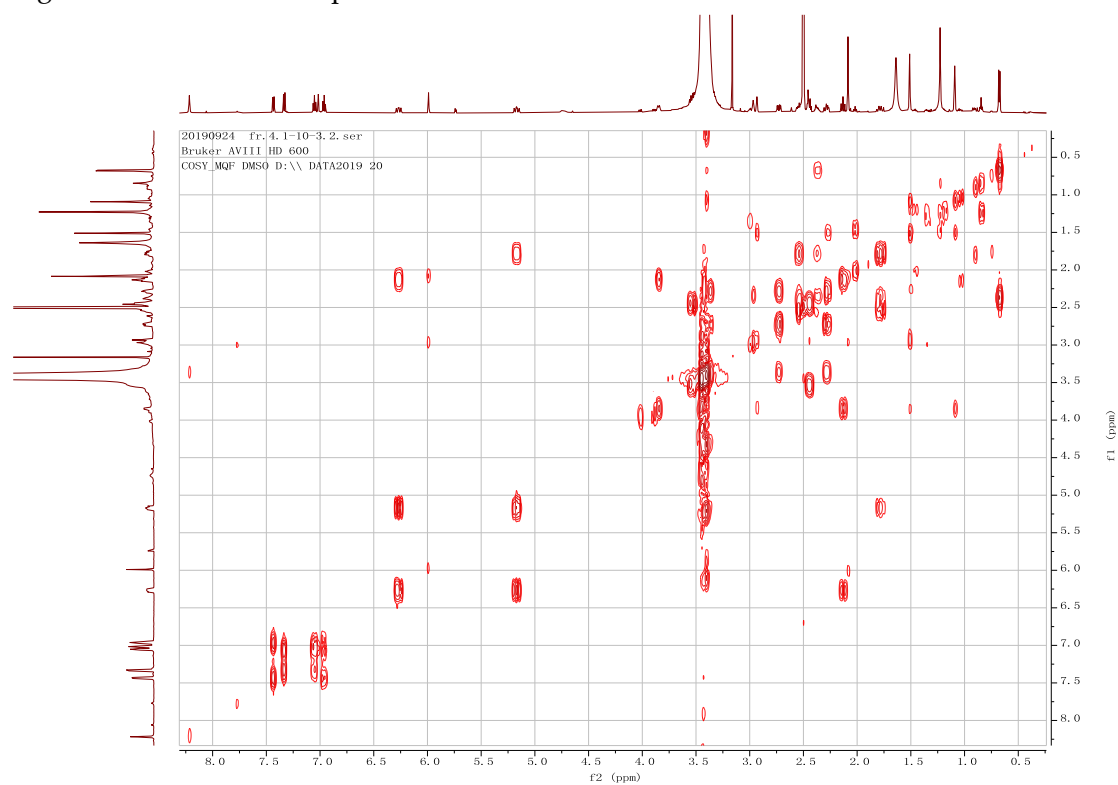


Figure S36: TOCSY spectrum of **4**

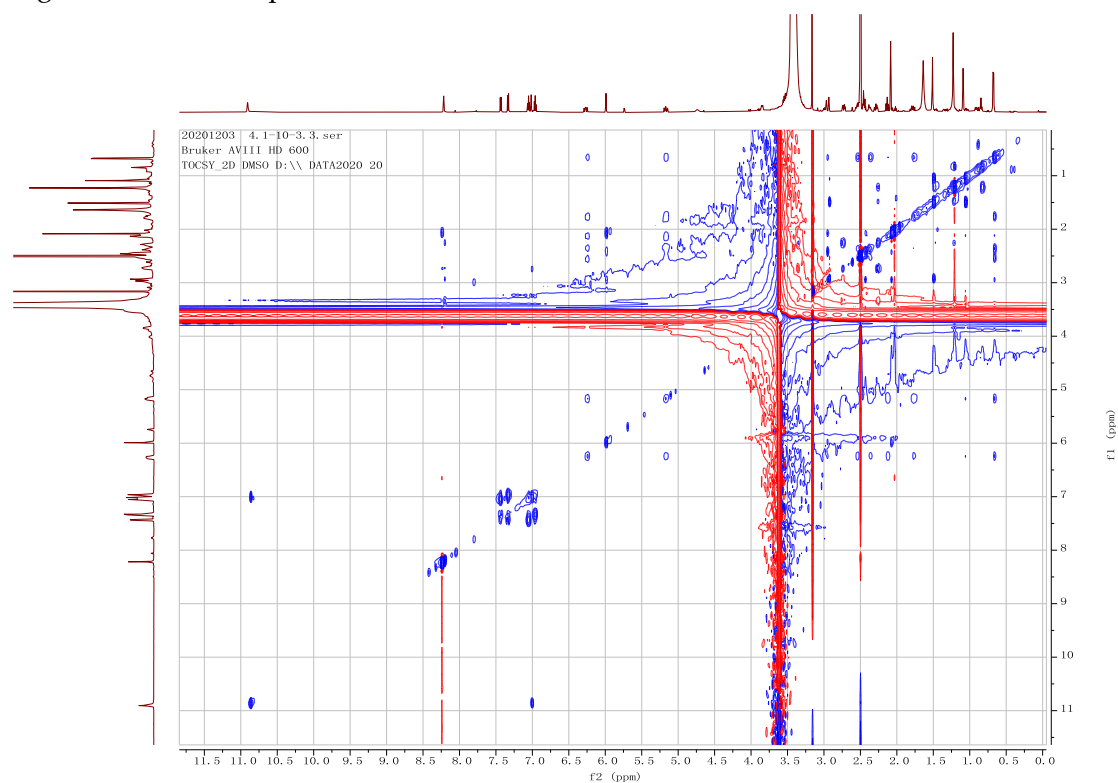


Figure S37: NOESY spectrum of 4

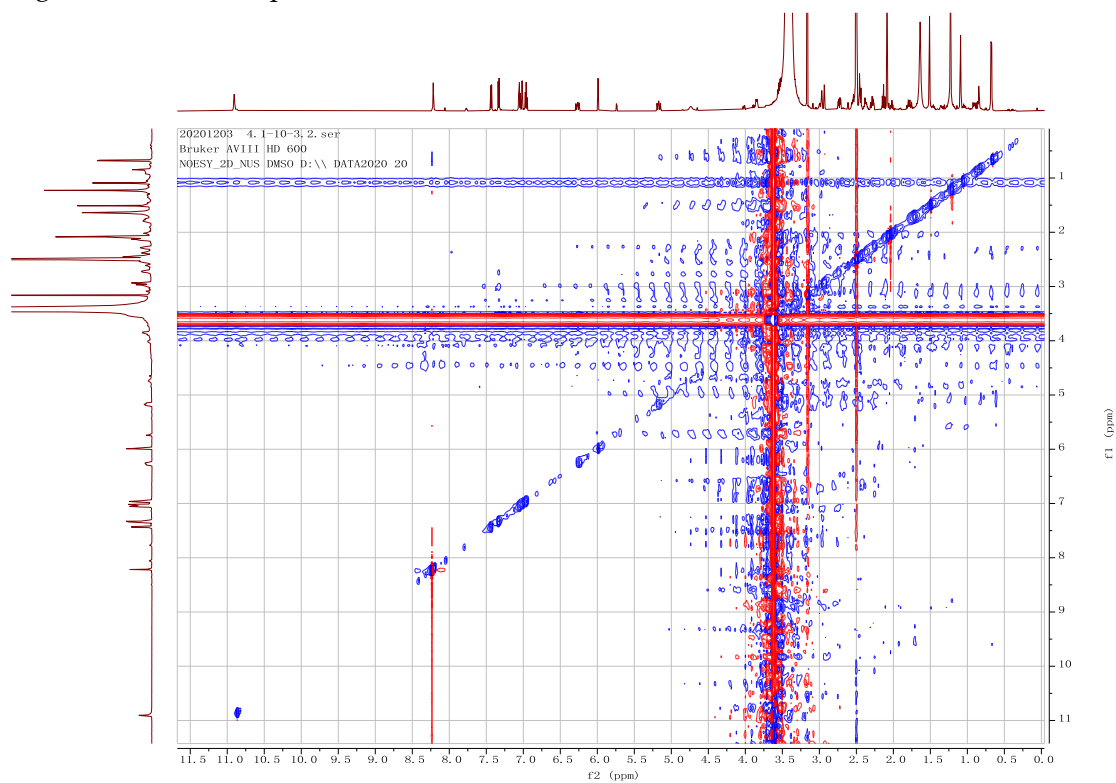
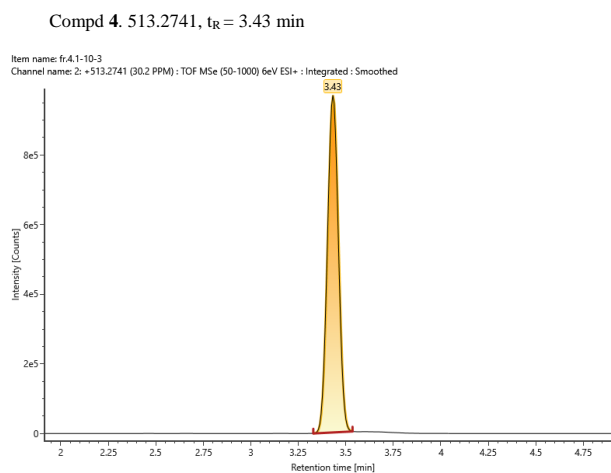
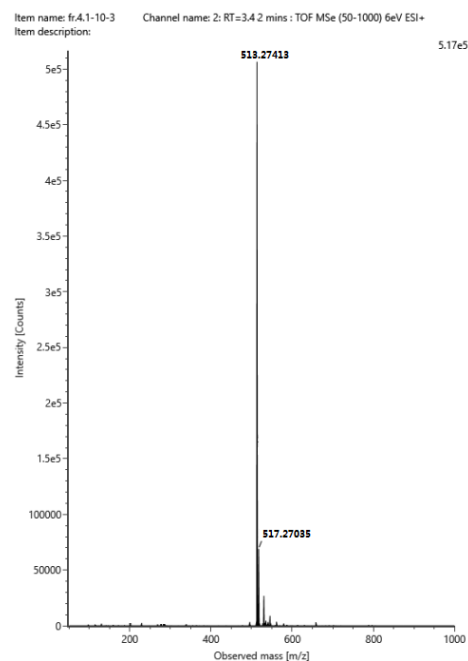


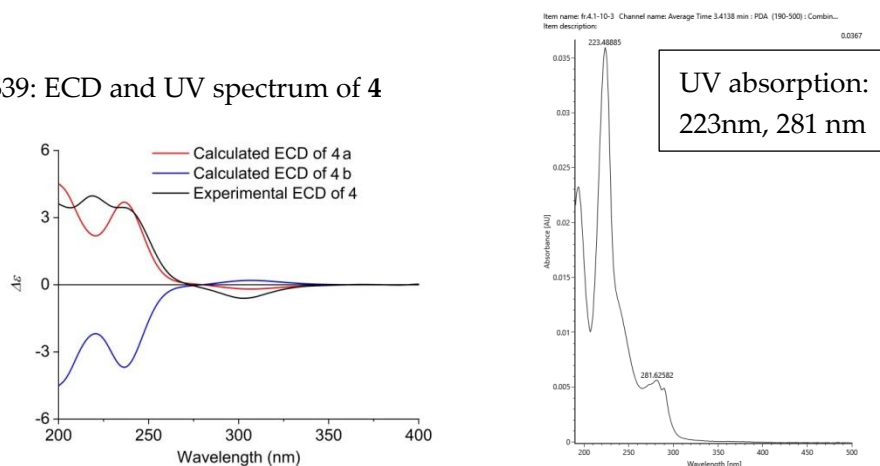
Figure S38: HR-ESI-MS spectrum of 4

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



Results (1 found)							
	Composition	i-FIT Confidence (%)	m/z RMS (PPM)	Intensity RMS (%)	Predicted m/z	m/z error (PPM)	m/z error (mDa)
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:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **5**

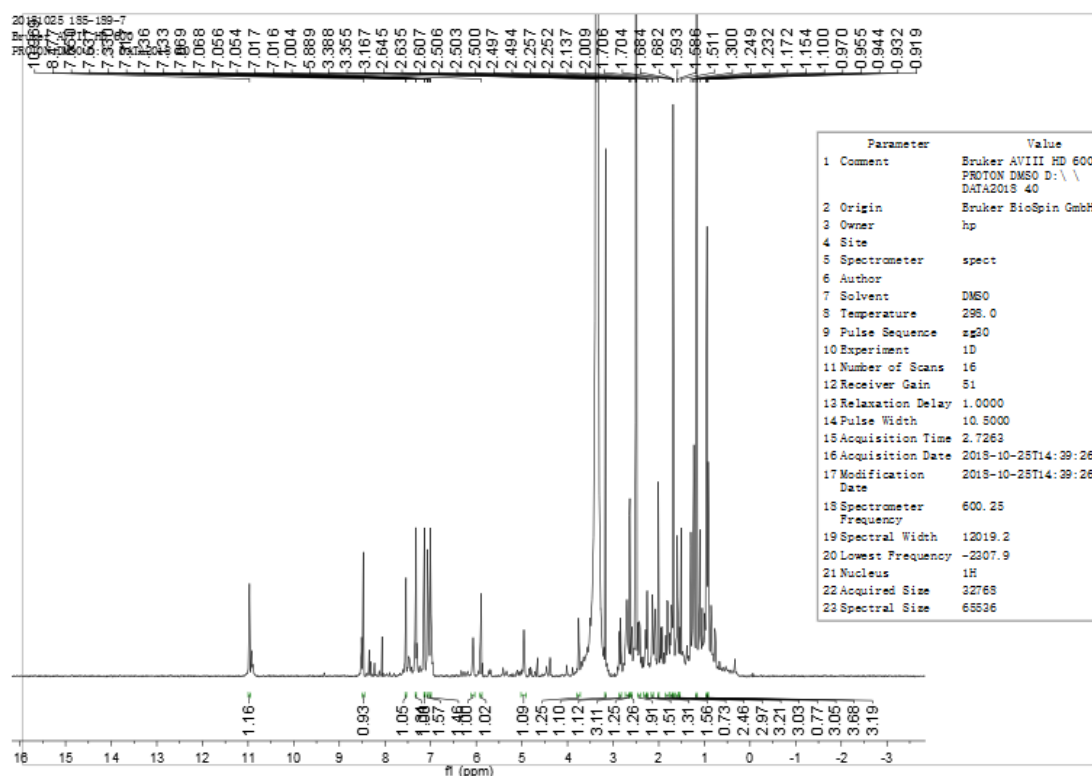


Figure S41:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **5**

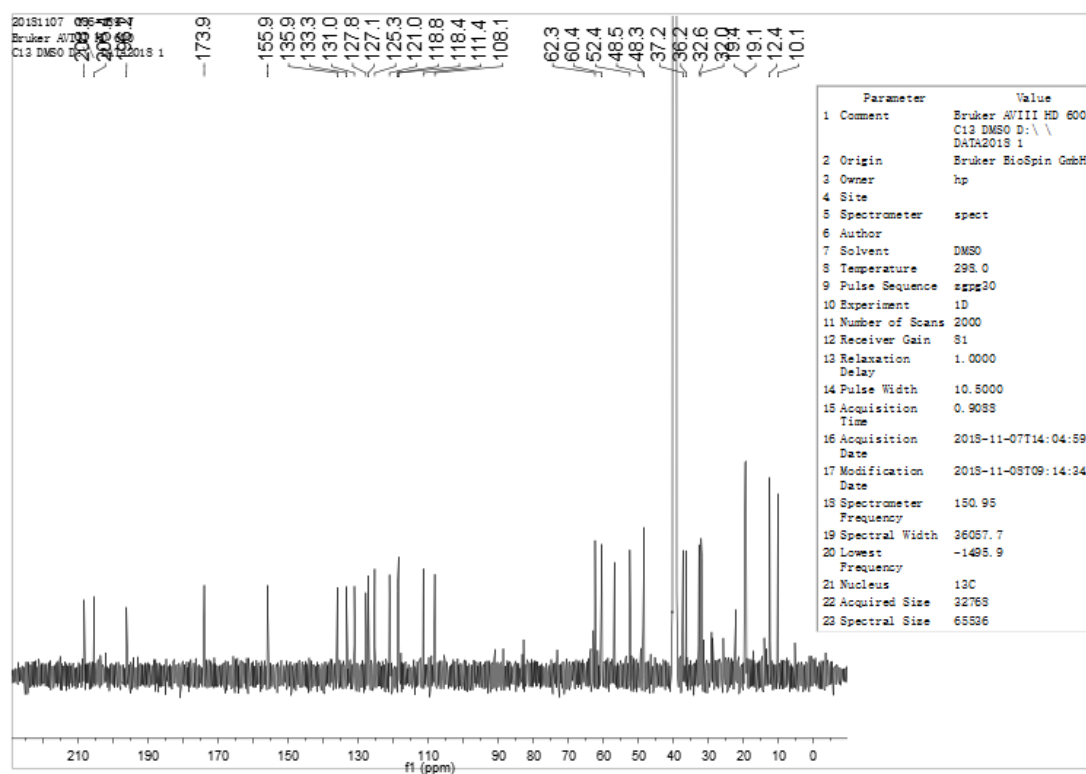


Figure S42:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **6**

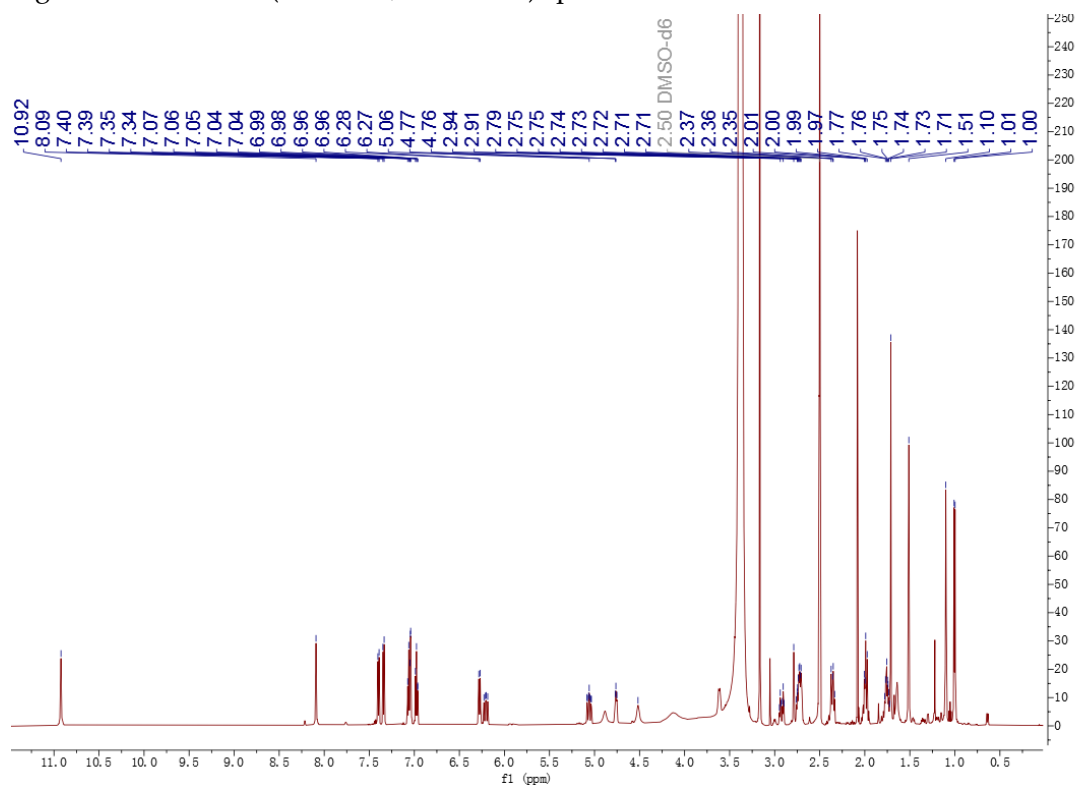


Figure S43:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **6**

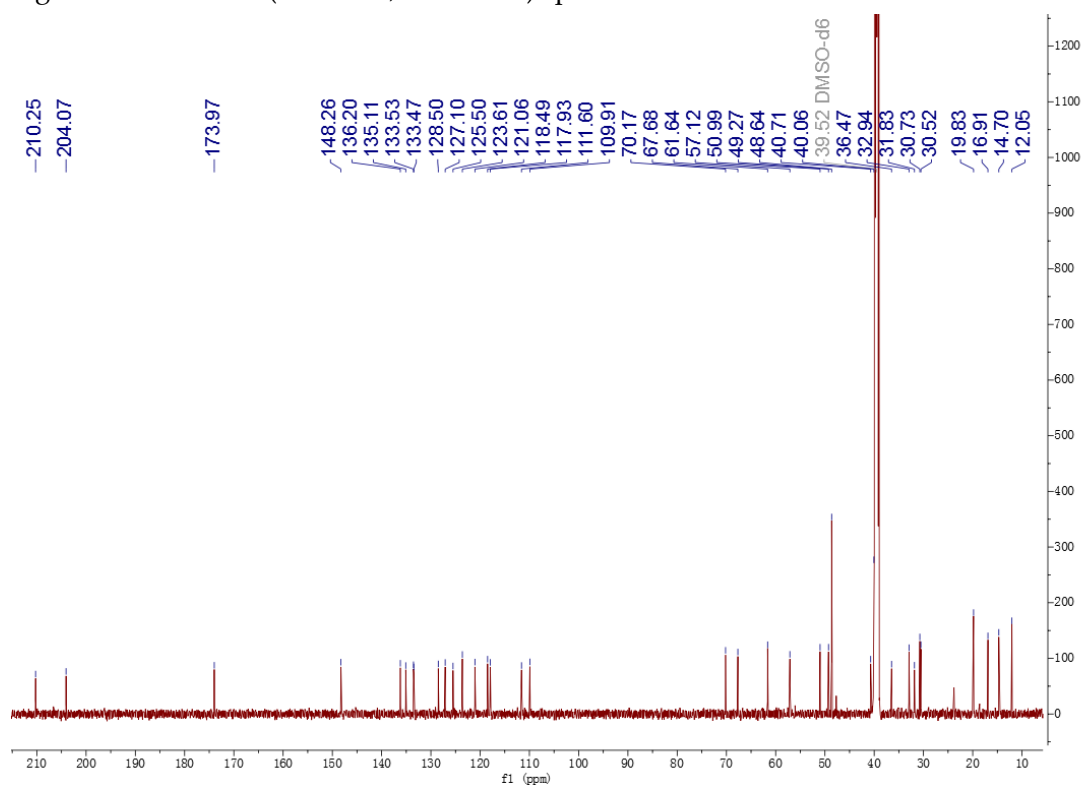


Figure S44:  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ ) spectrum of **7**

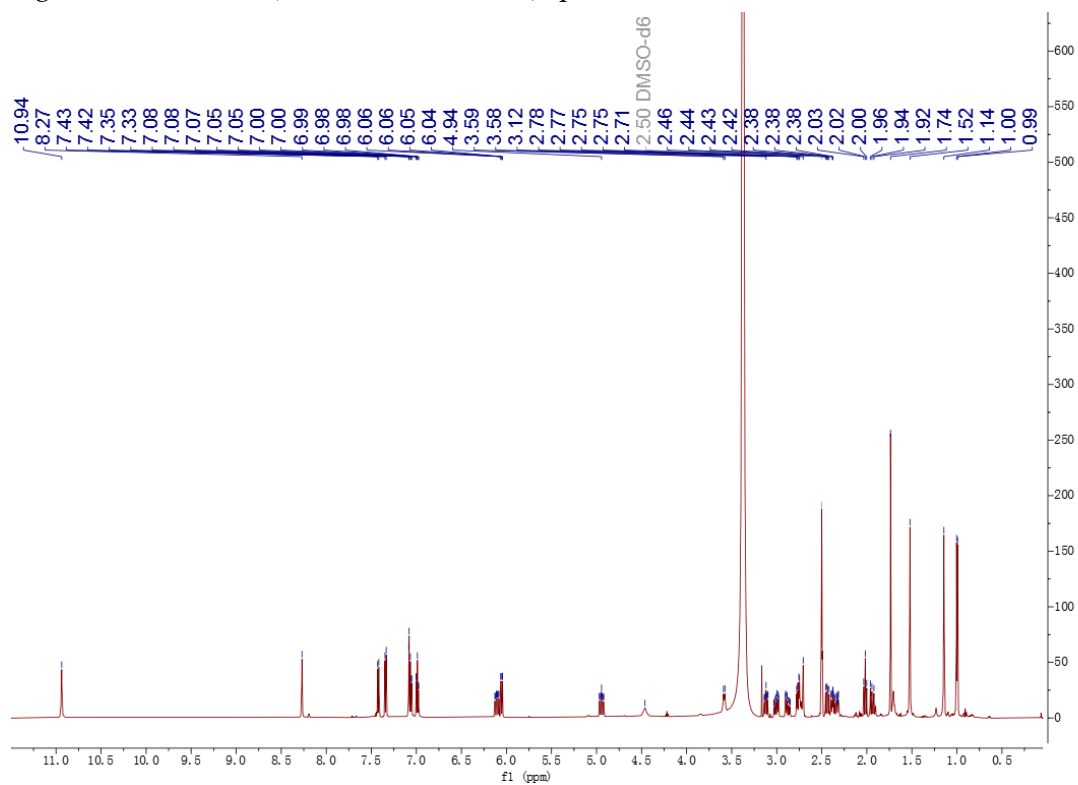


Figure S45:  $^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ ) spectrum of **7**

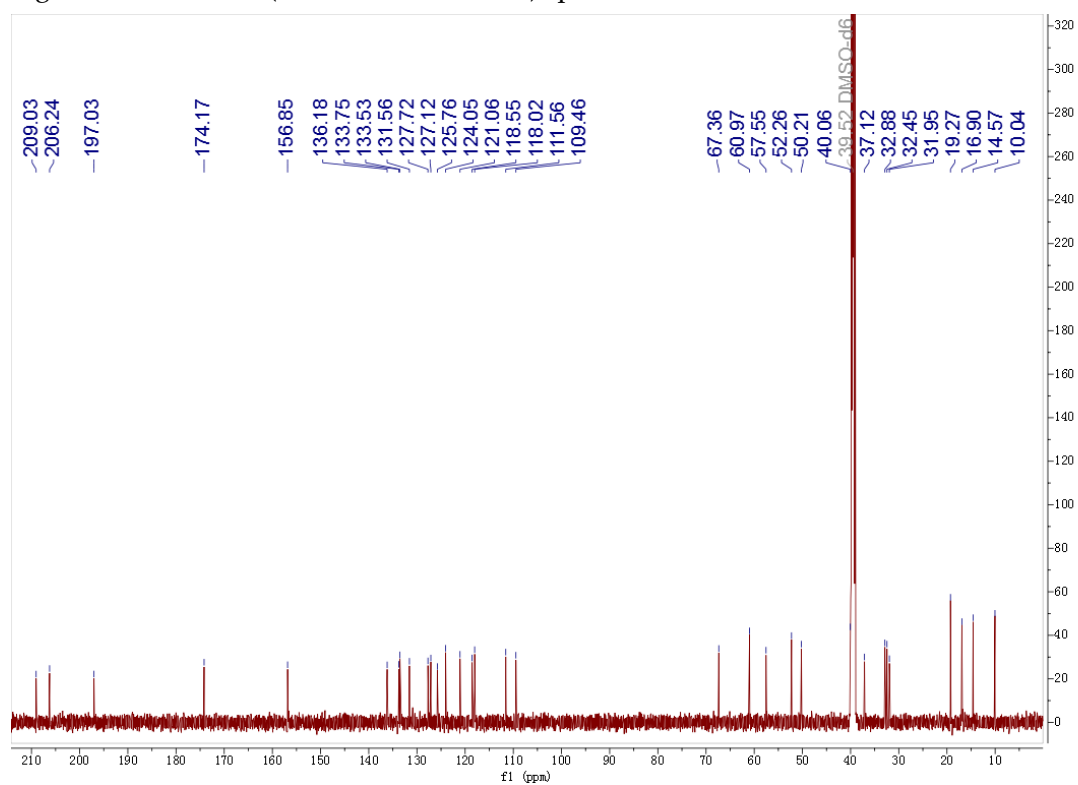


Figure S46:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **8**

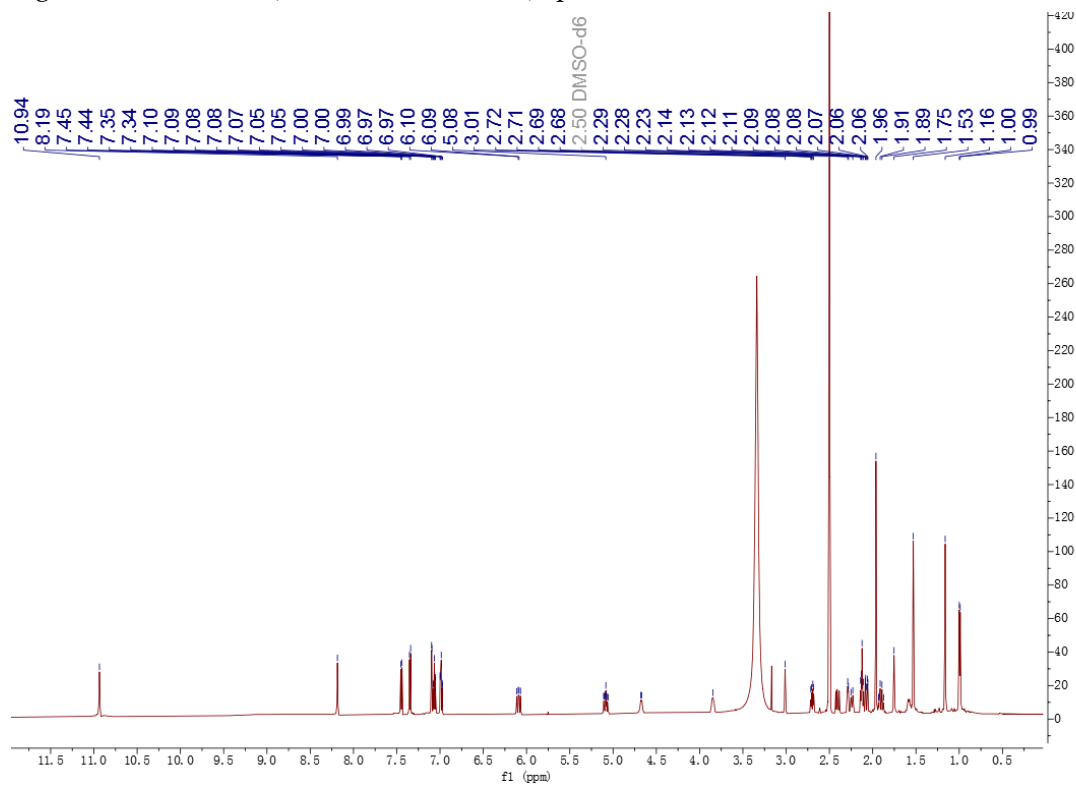


Figure S47:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **8**

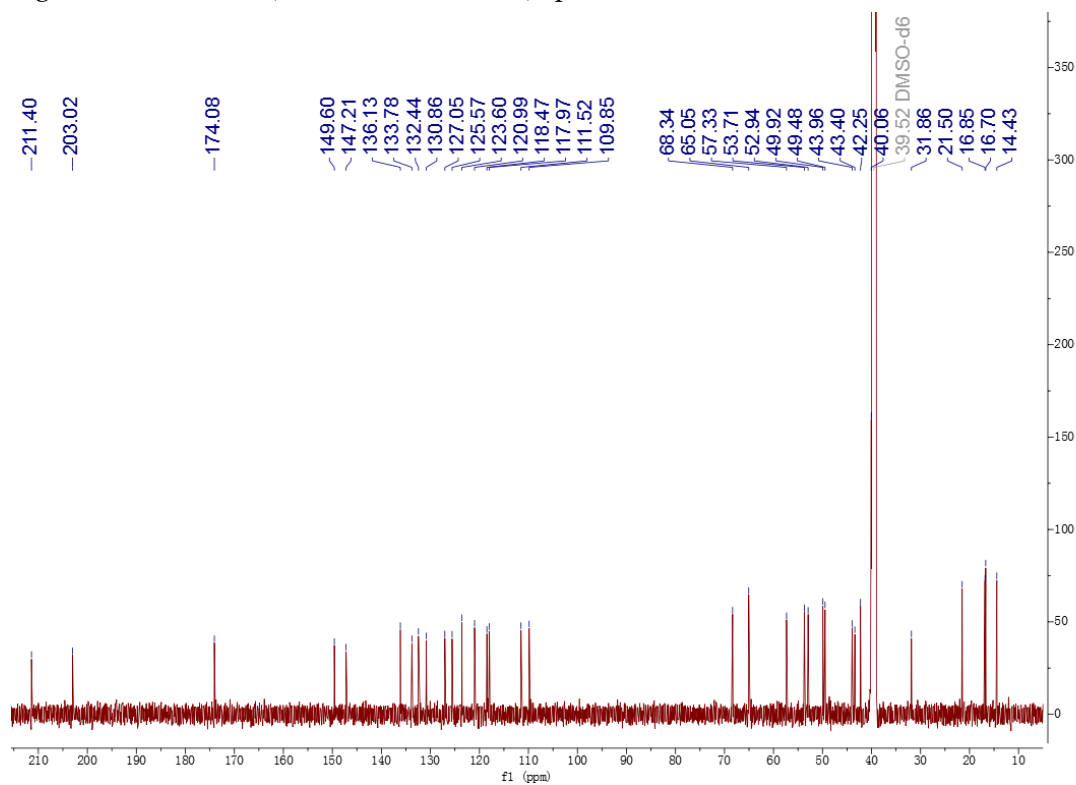


Figure S48:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **9**

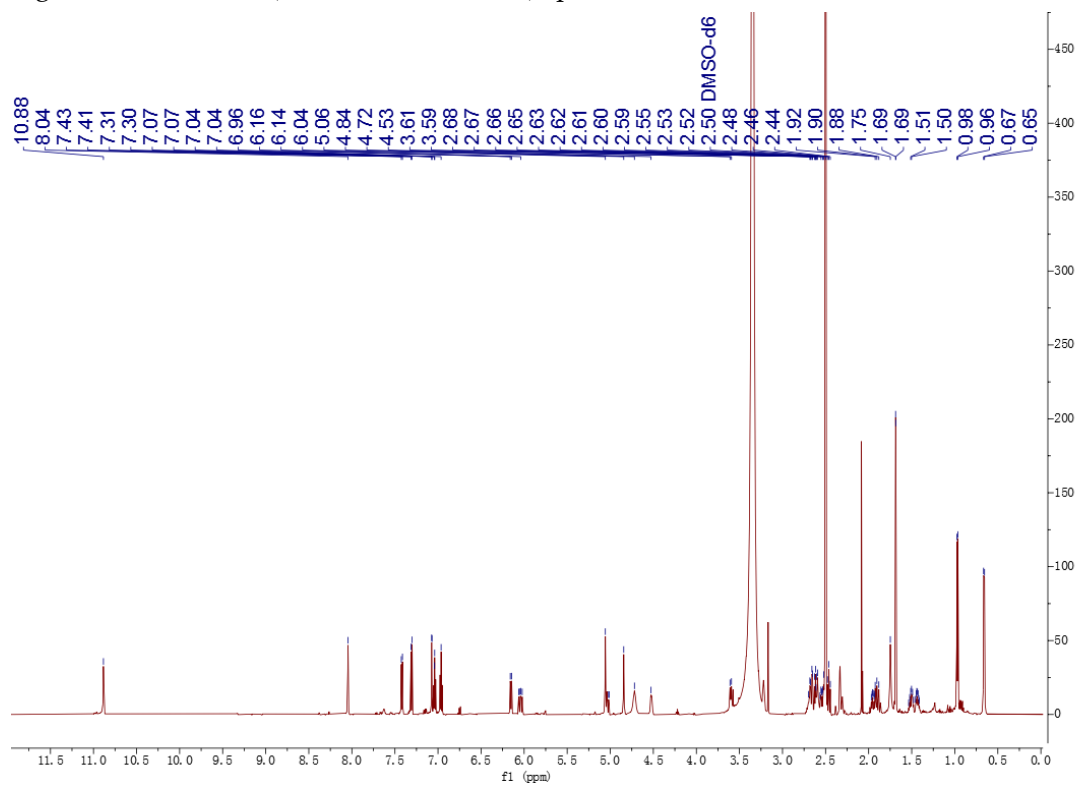


Figure S49:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **9**

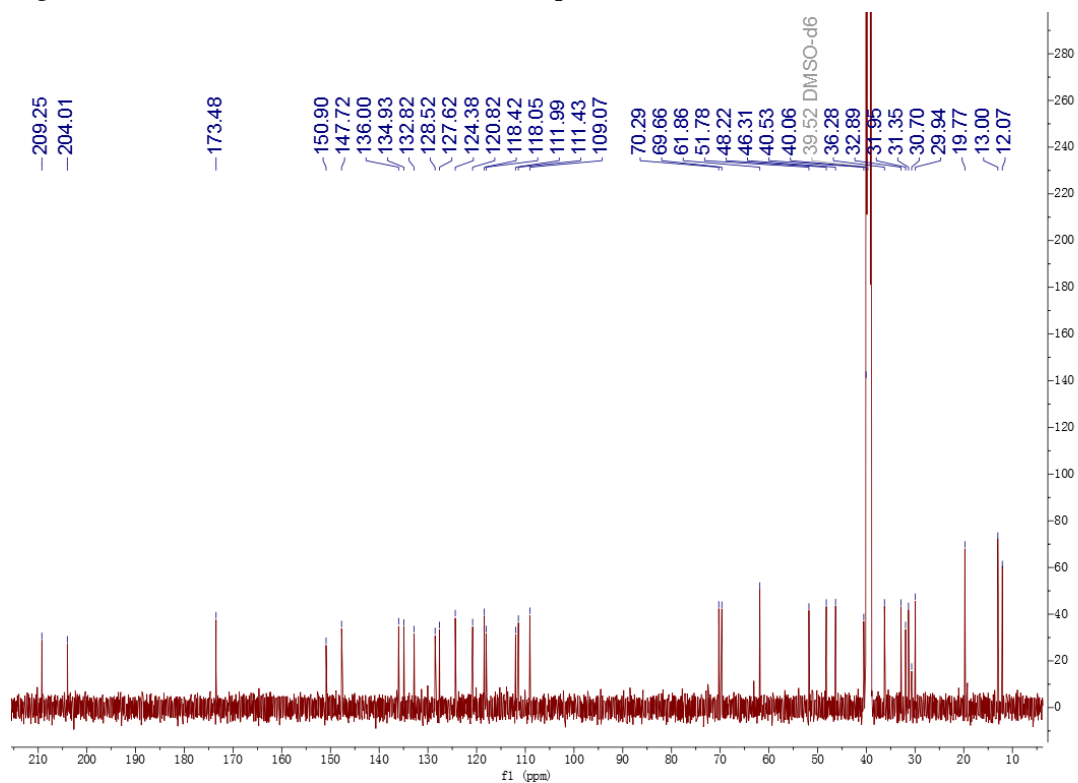




Figure S50:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **10**

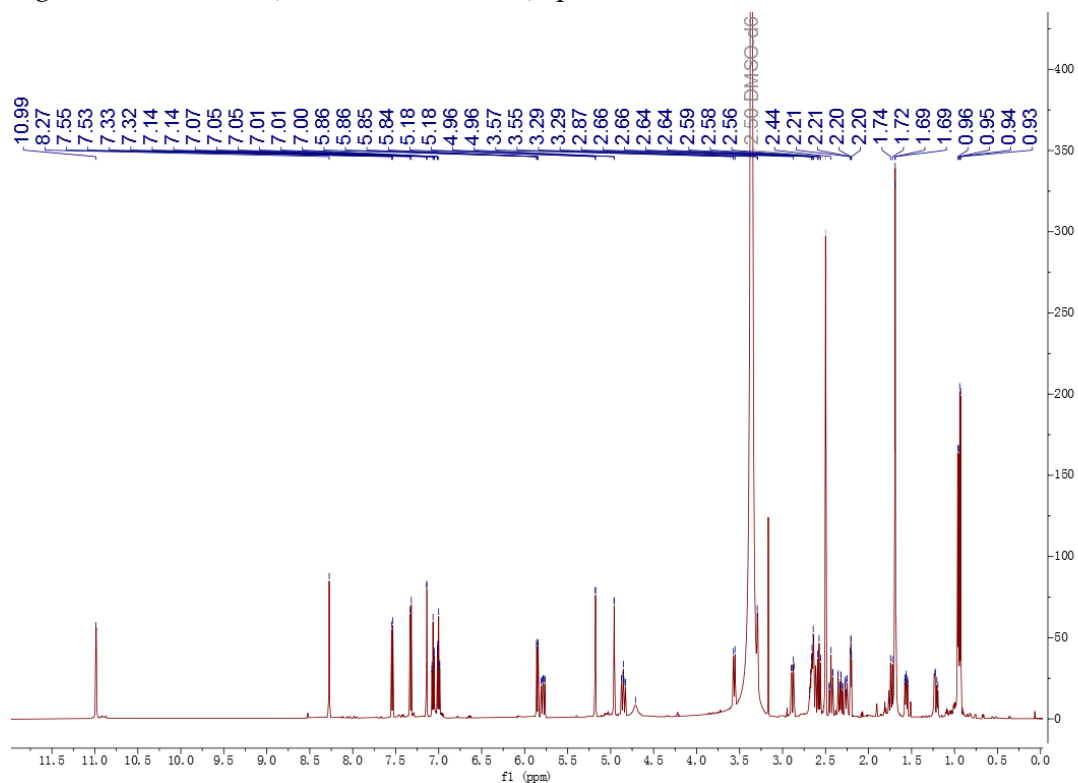


Figure S51:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **10**

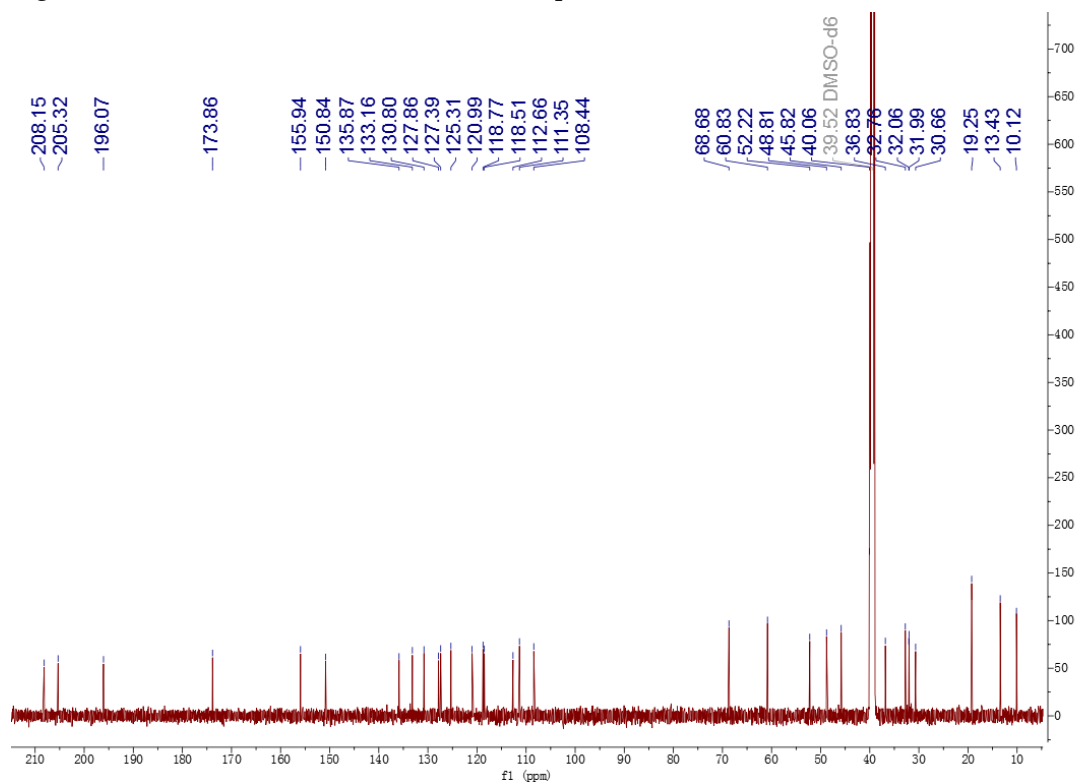


Figure S52:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **11**

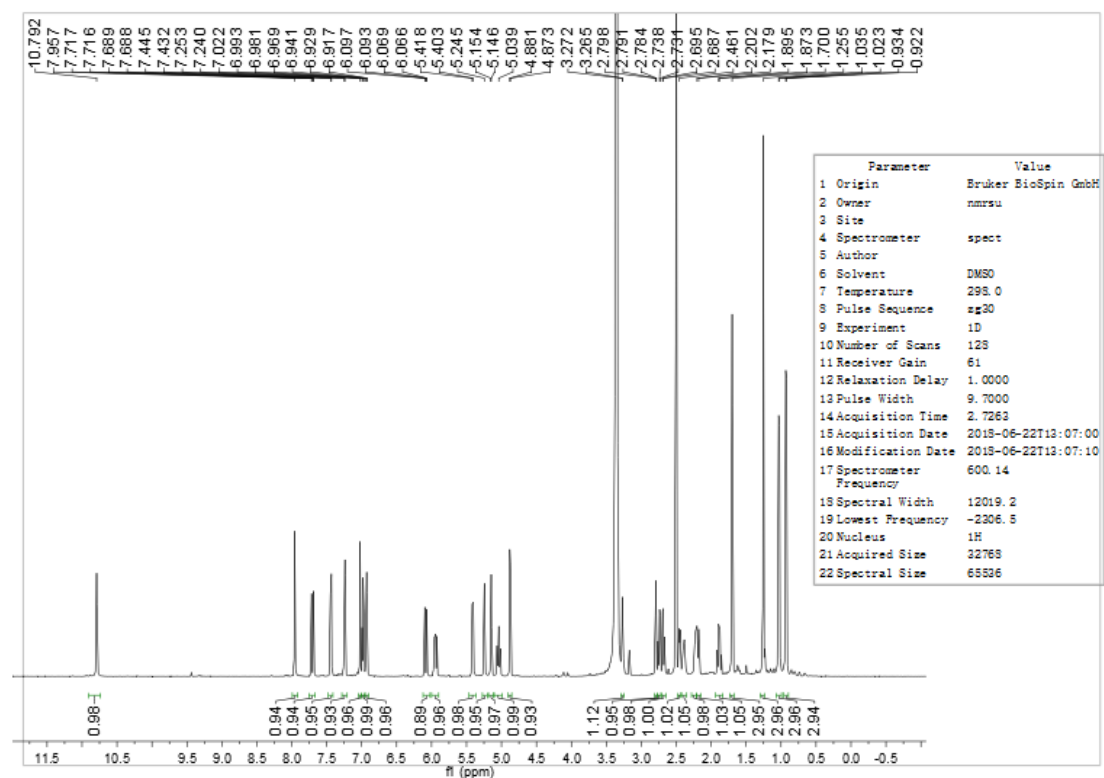


Figure S53:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **11**

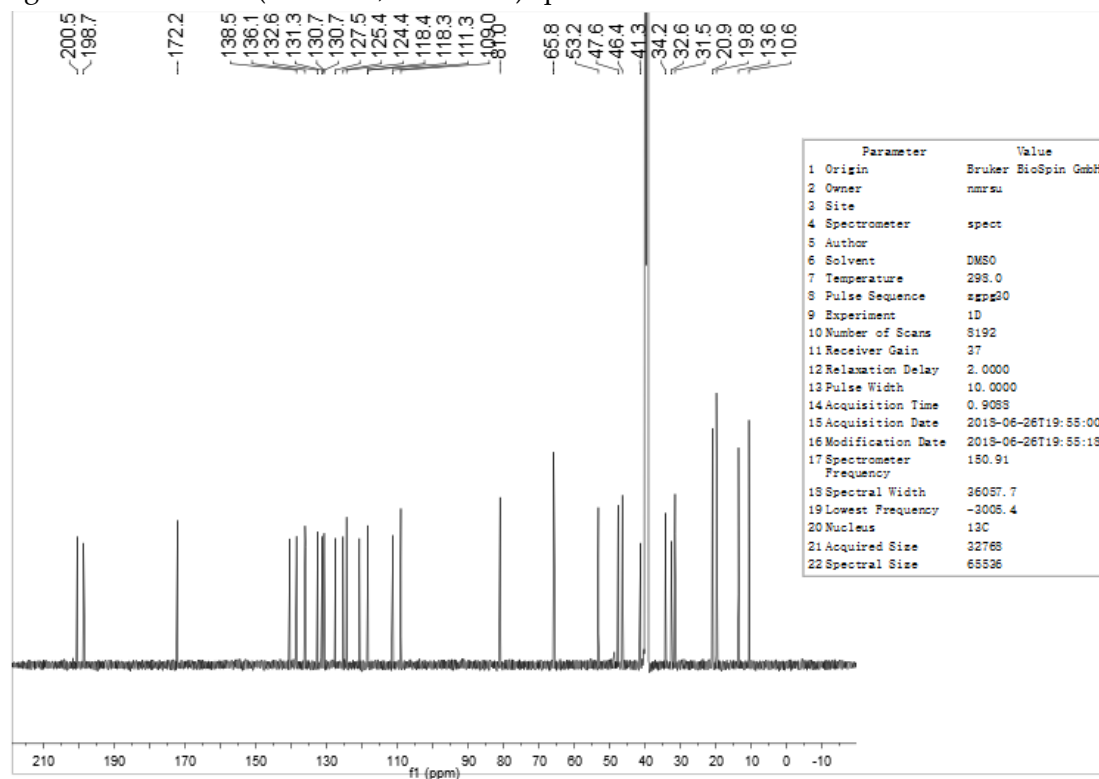


Figure S54:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of **12**

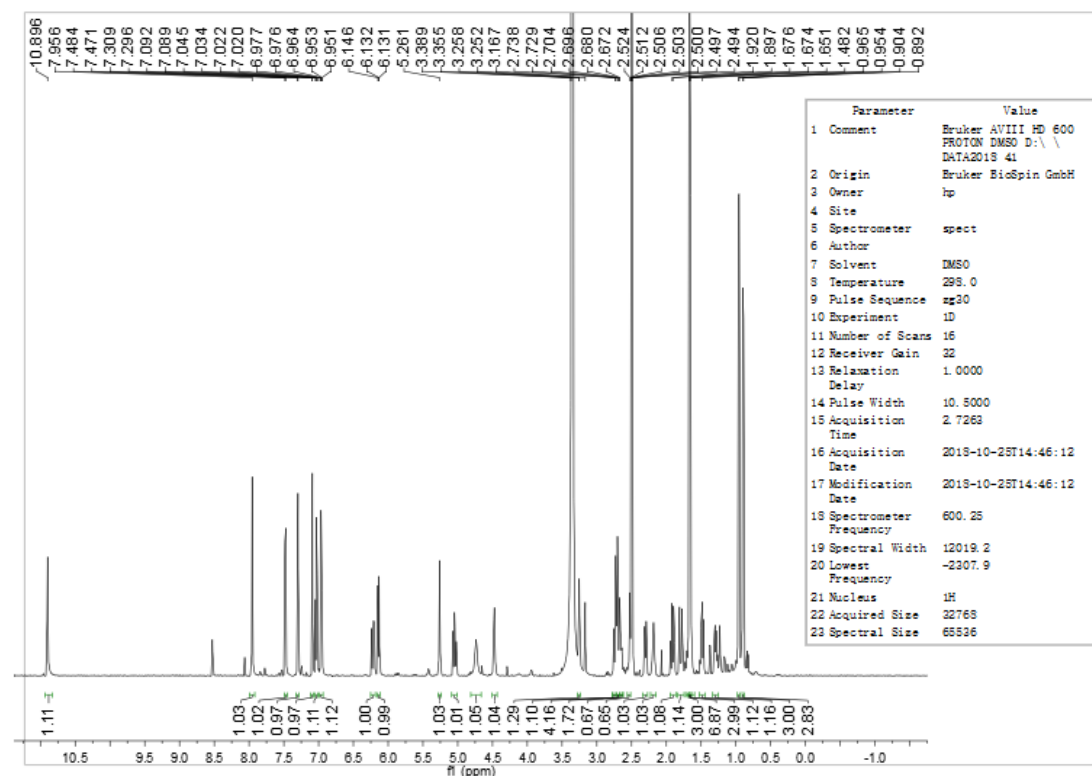


Figure S55:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of **12**

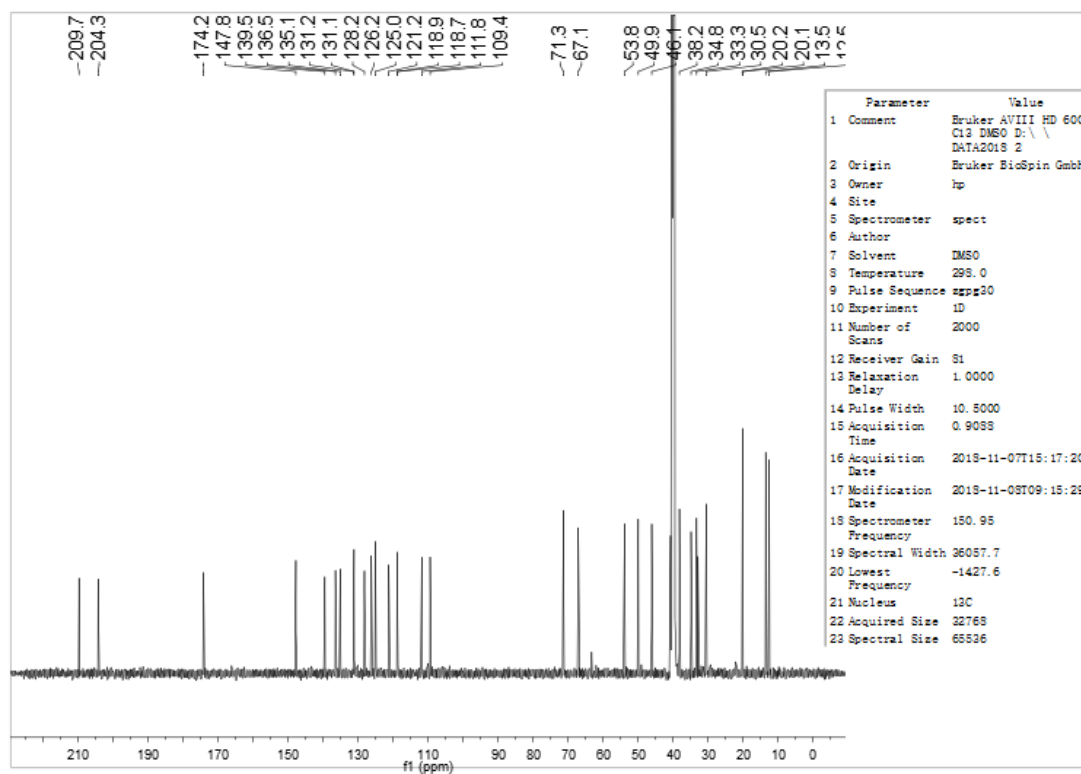


Figure S56:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of **13**

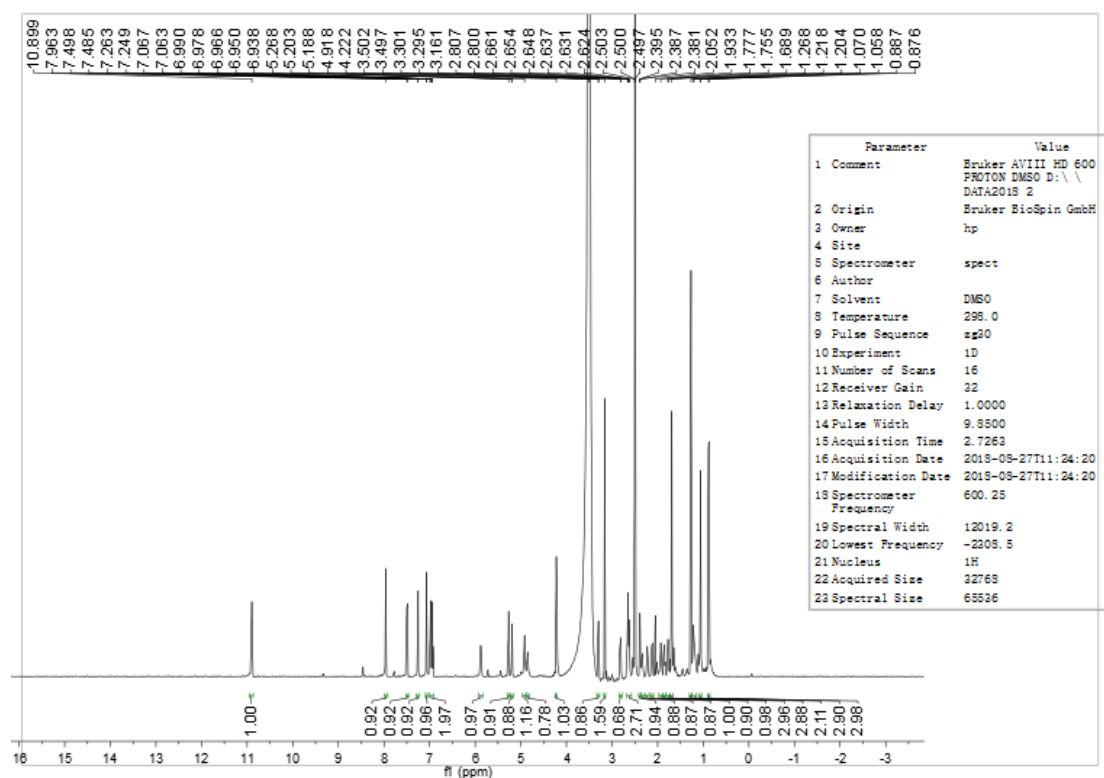


Figure S57:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of **13**

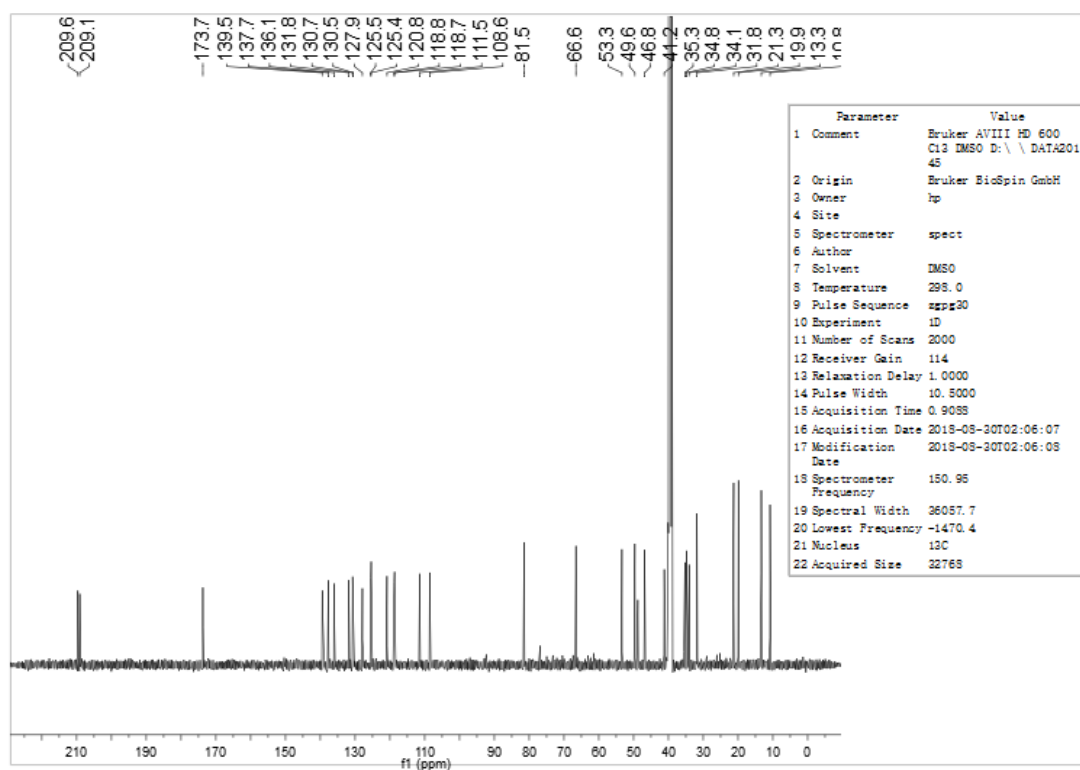


Figure S58:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **14**

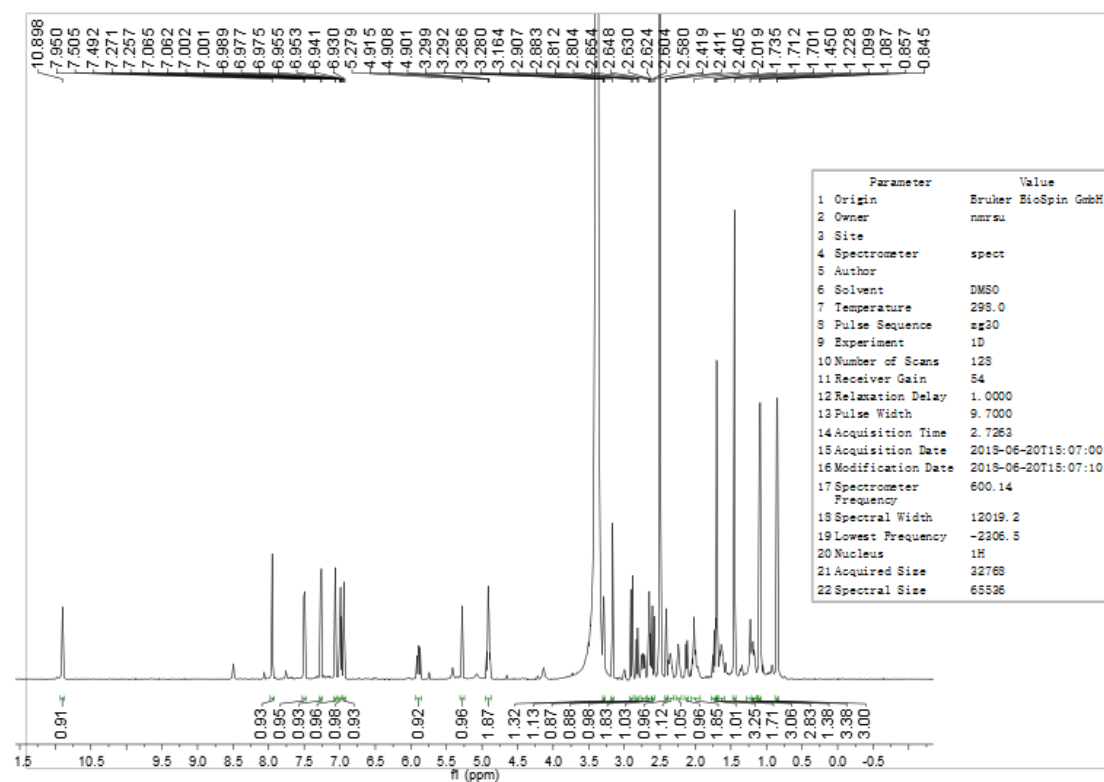


Figure S59:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **14**

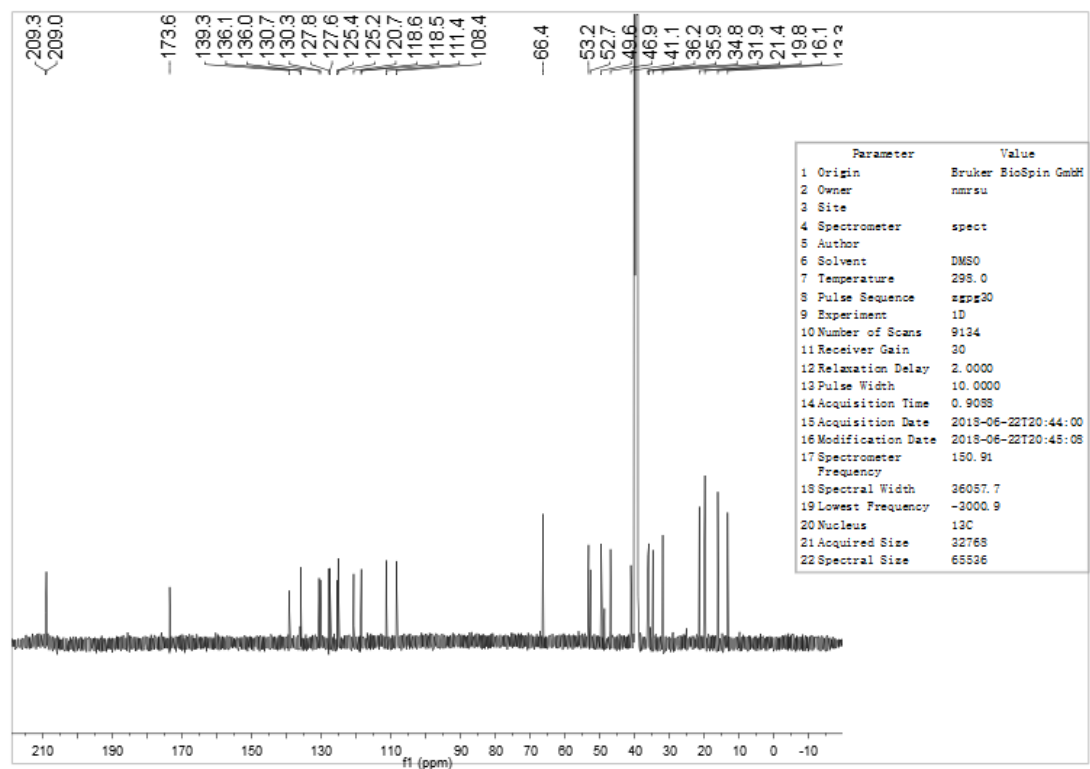


Figure S60:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of **15**

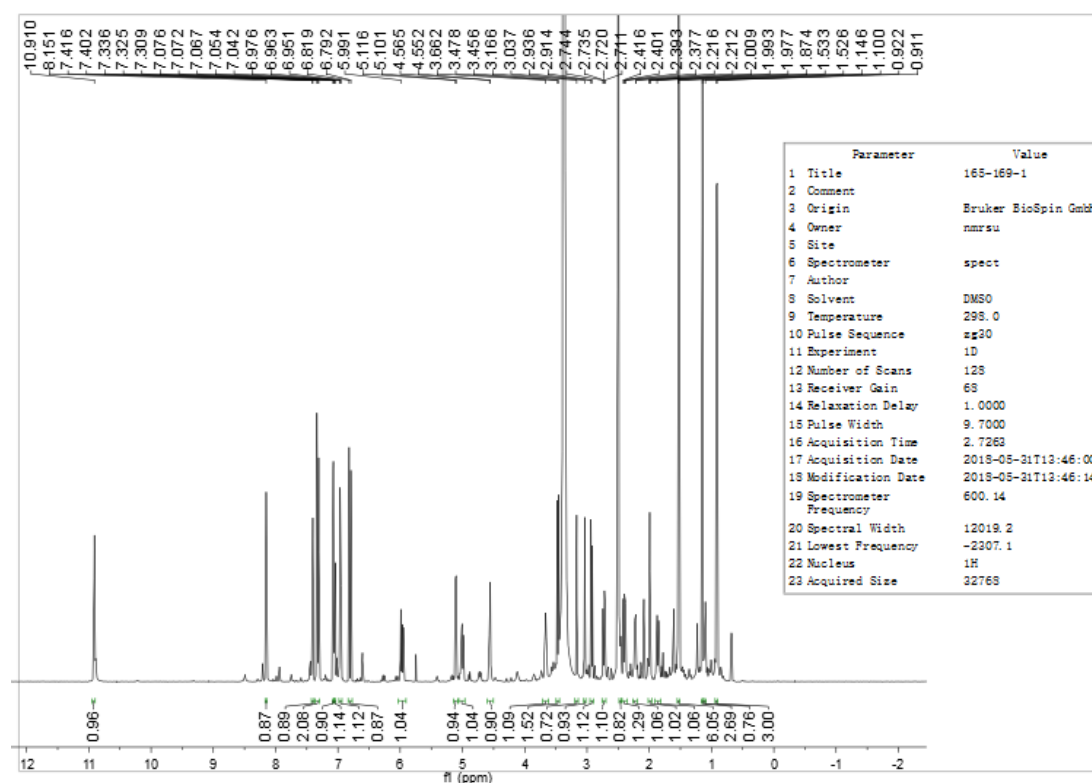


Figure S61:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ ) spectrum of **15**

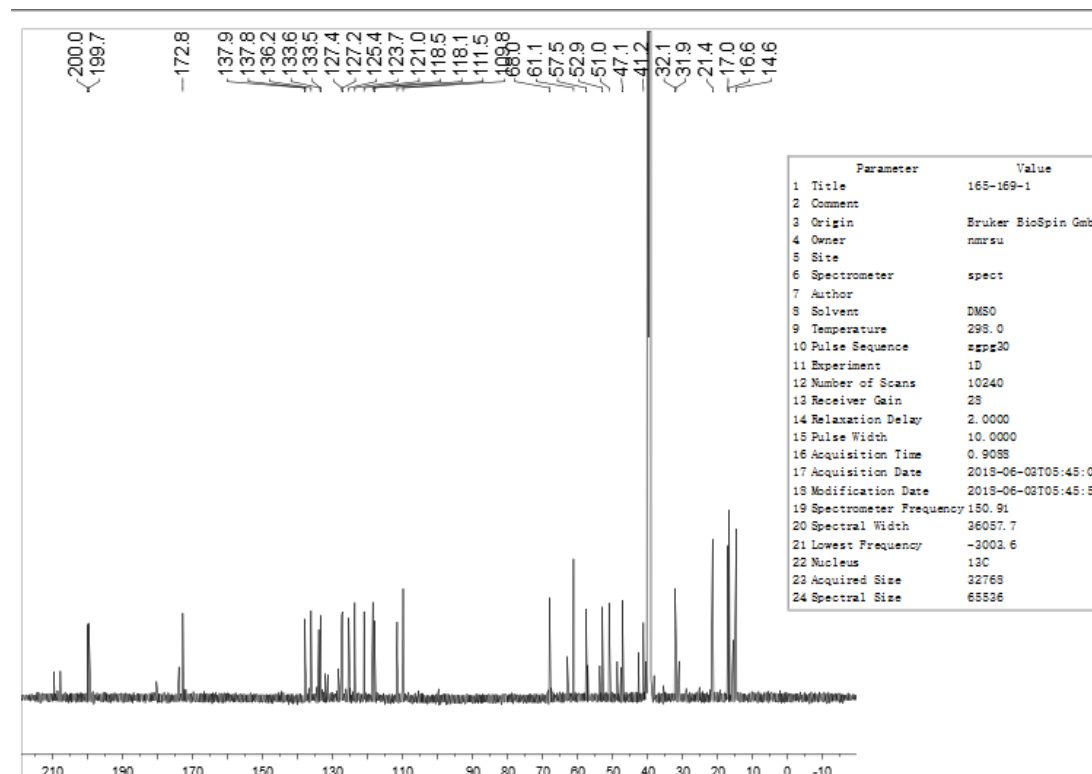


Figure S62:  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of **16**

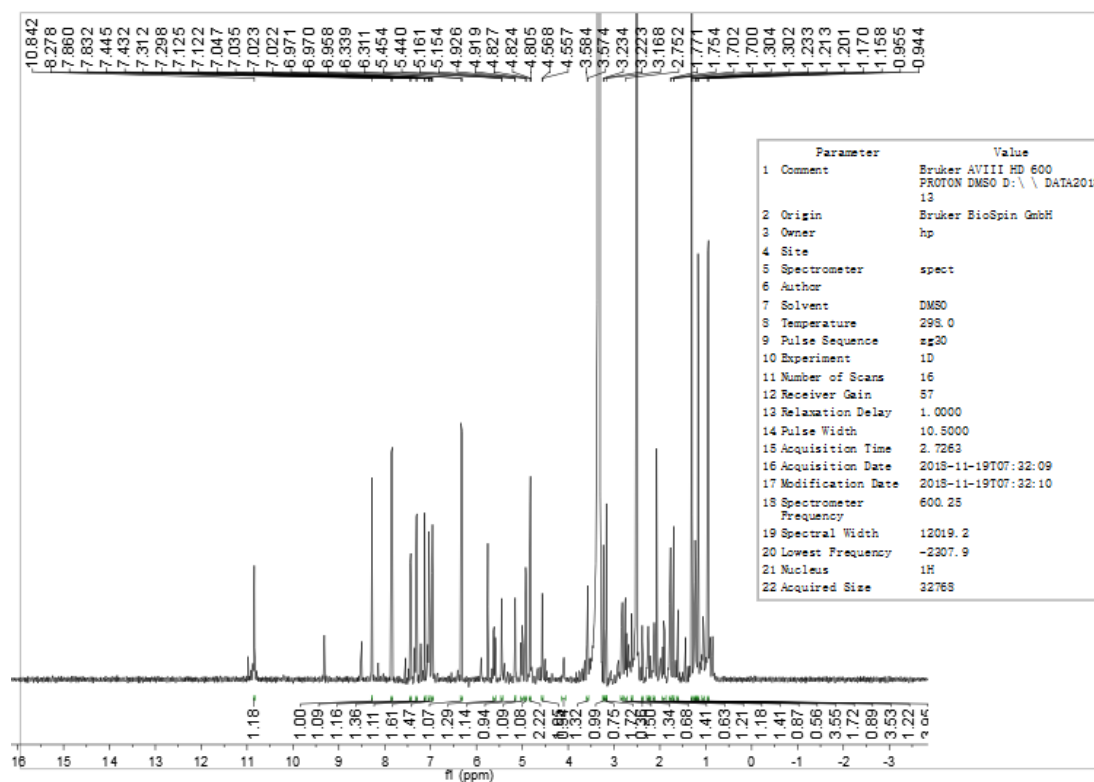


Figure S63:  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of **16**

