Supporting Information

Rec. Nat. Prod. 17:4 (2023) 689-704

Three New Chemical Constituents of *Dryopteris Crassirhizoma* Nakai in Lianhua Qingwen Capsule and Investigation on Their Antiviral Potential Based On 3CL Hydrolase of SARS-CoV-2

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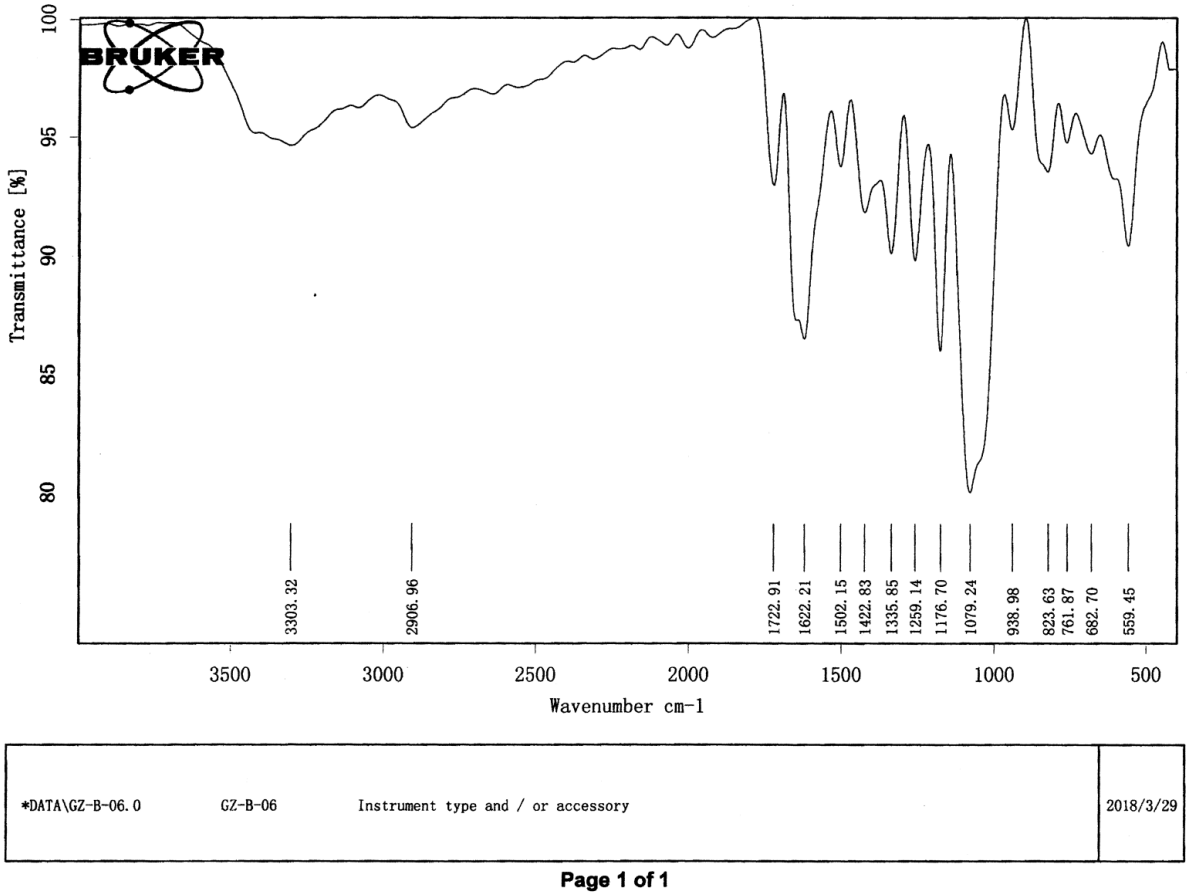

Figure S1: IR spectrum of Spectrum of **1**

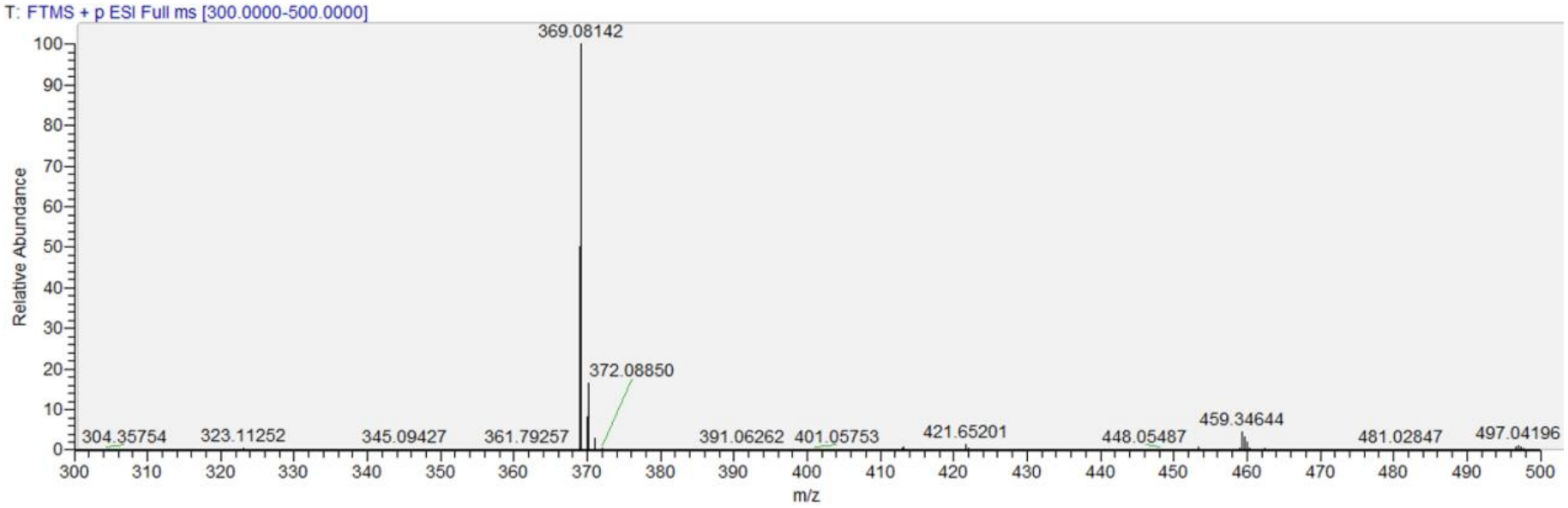

Figure S2: HR-ESI-MS Spectrum of **1**

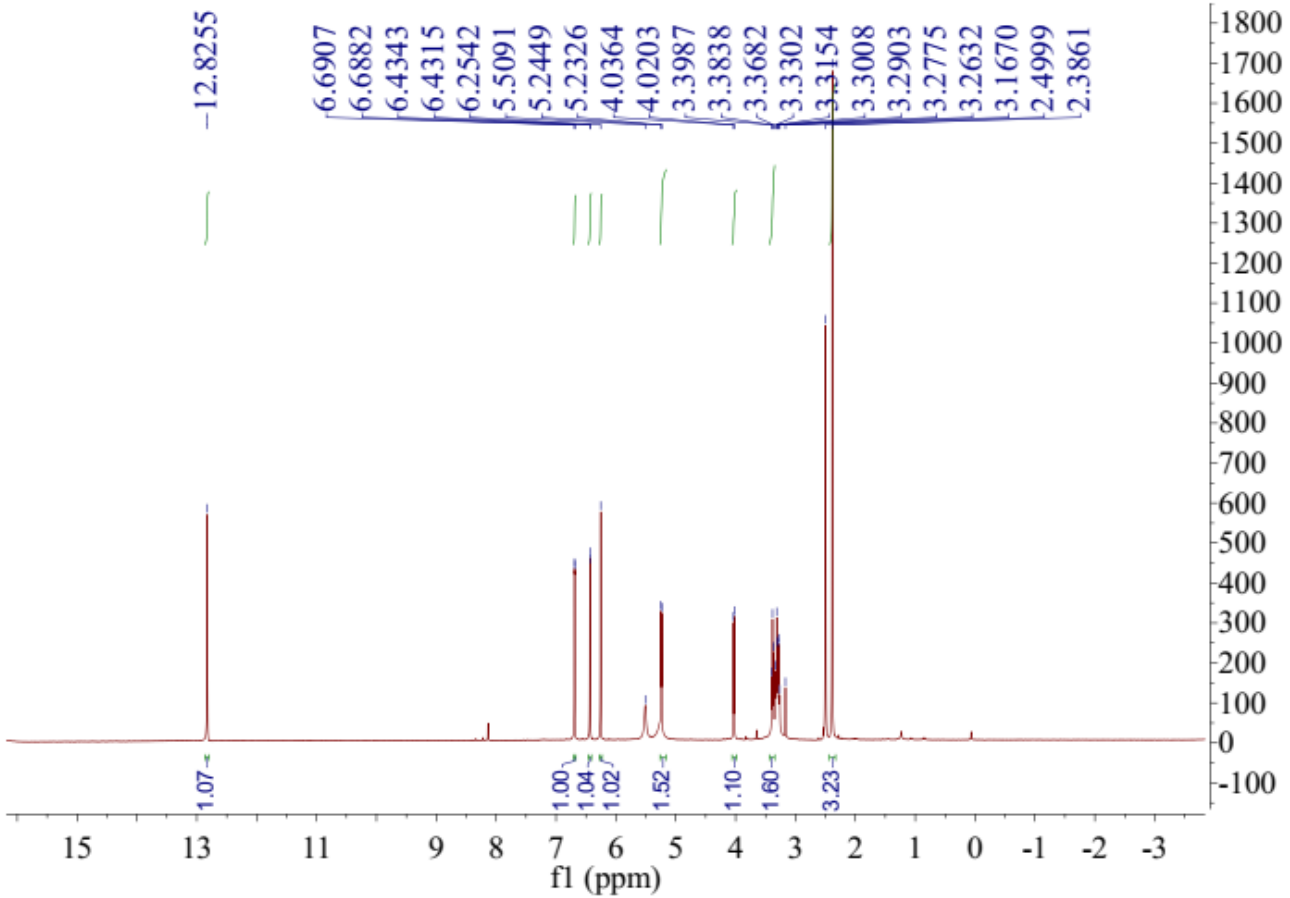

Figure S3: ^{1}H-NMR (600 MHz, DMSO-d_6) Spectrum of **1**

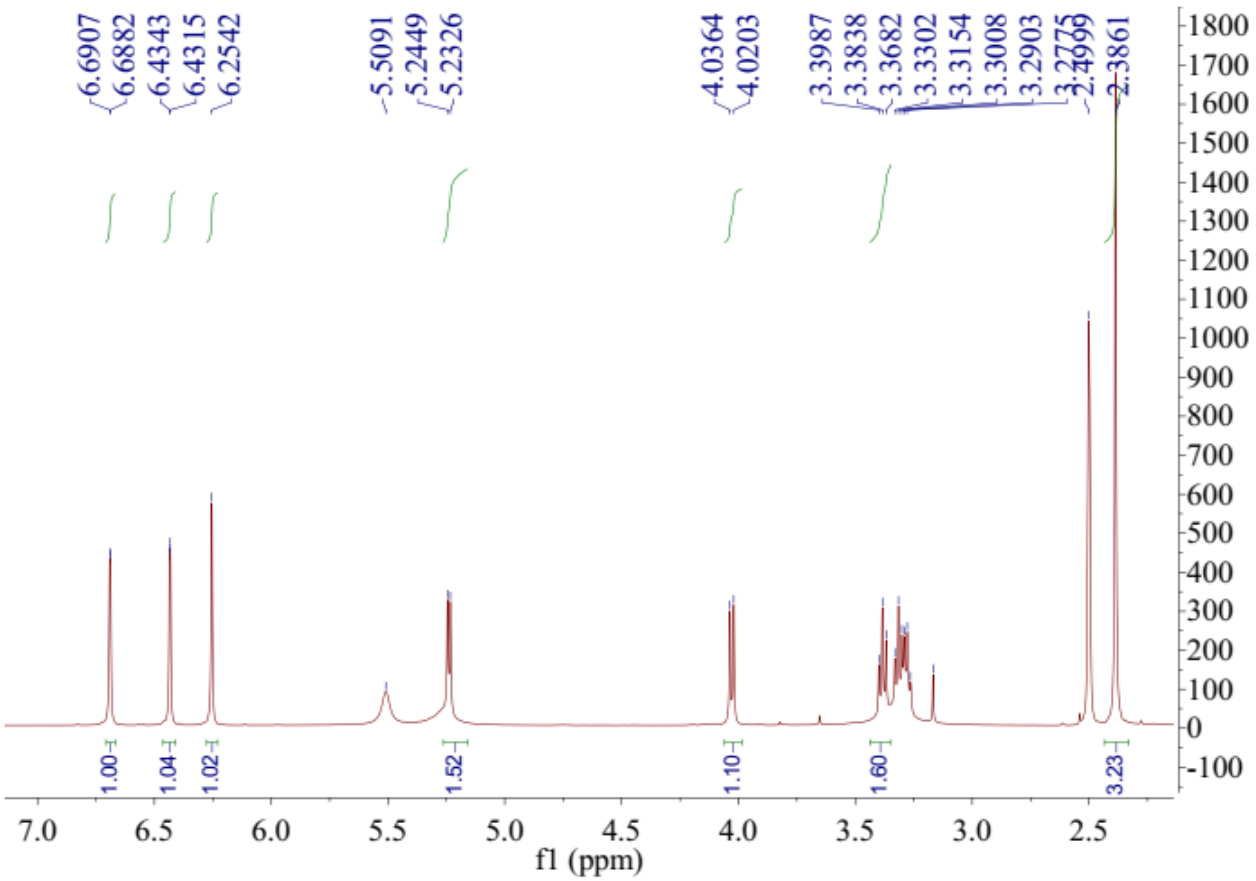

Figure S4: ^{1}H-NMR (600 MHz, DMSO-d_6) Spectrum of **1**

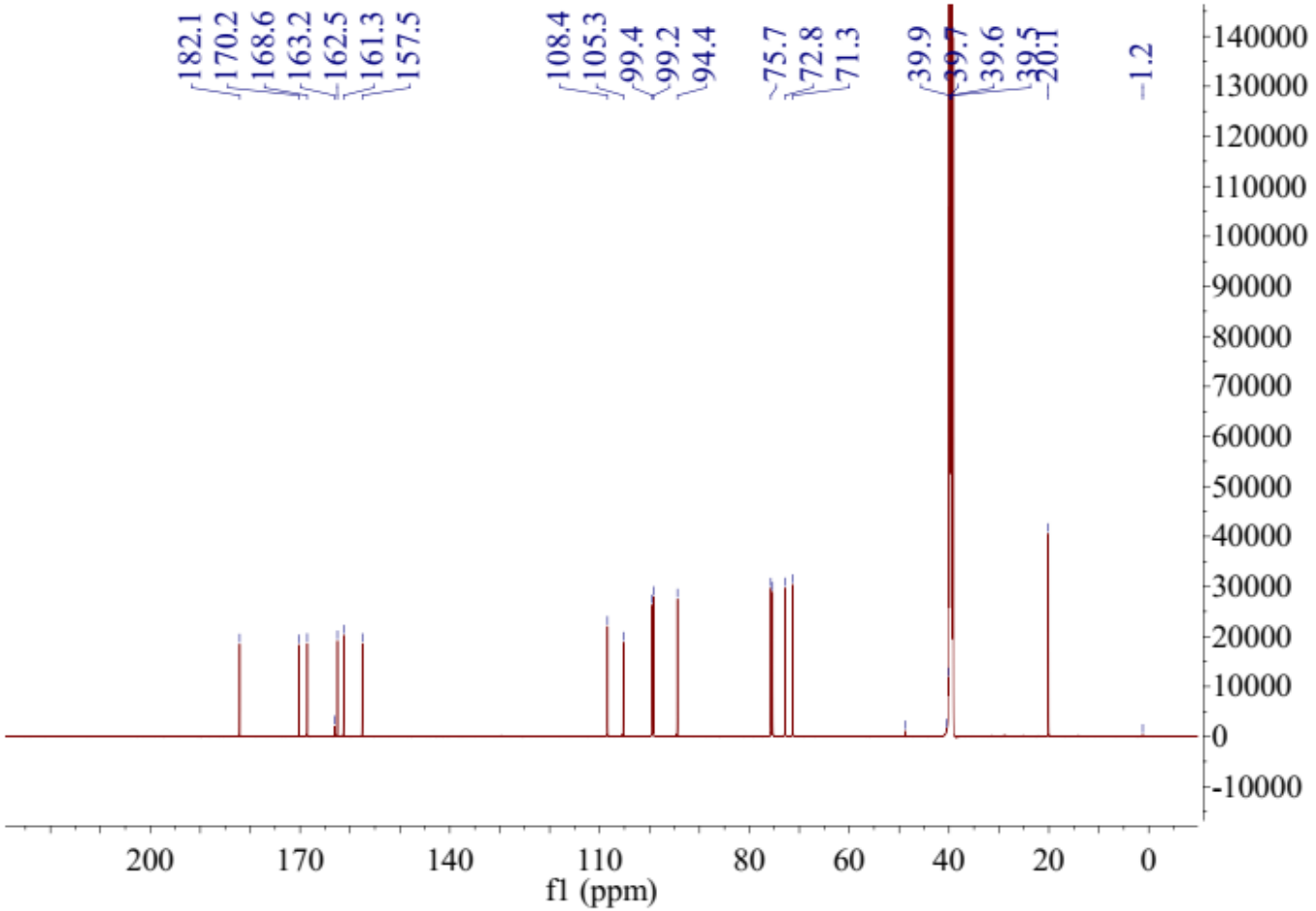

Figure S5: ^{13}C-NMR (150 MHz, DMSO -d_6) Spectrum of **1**

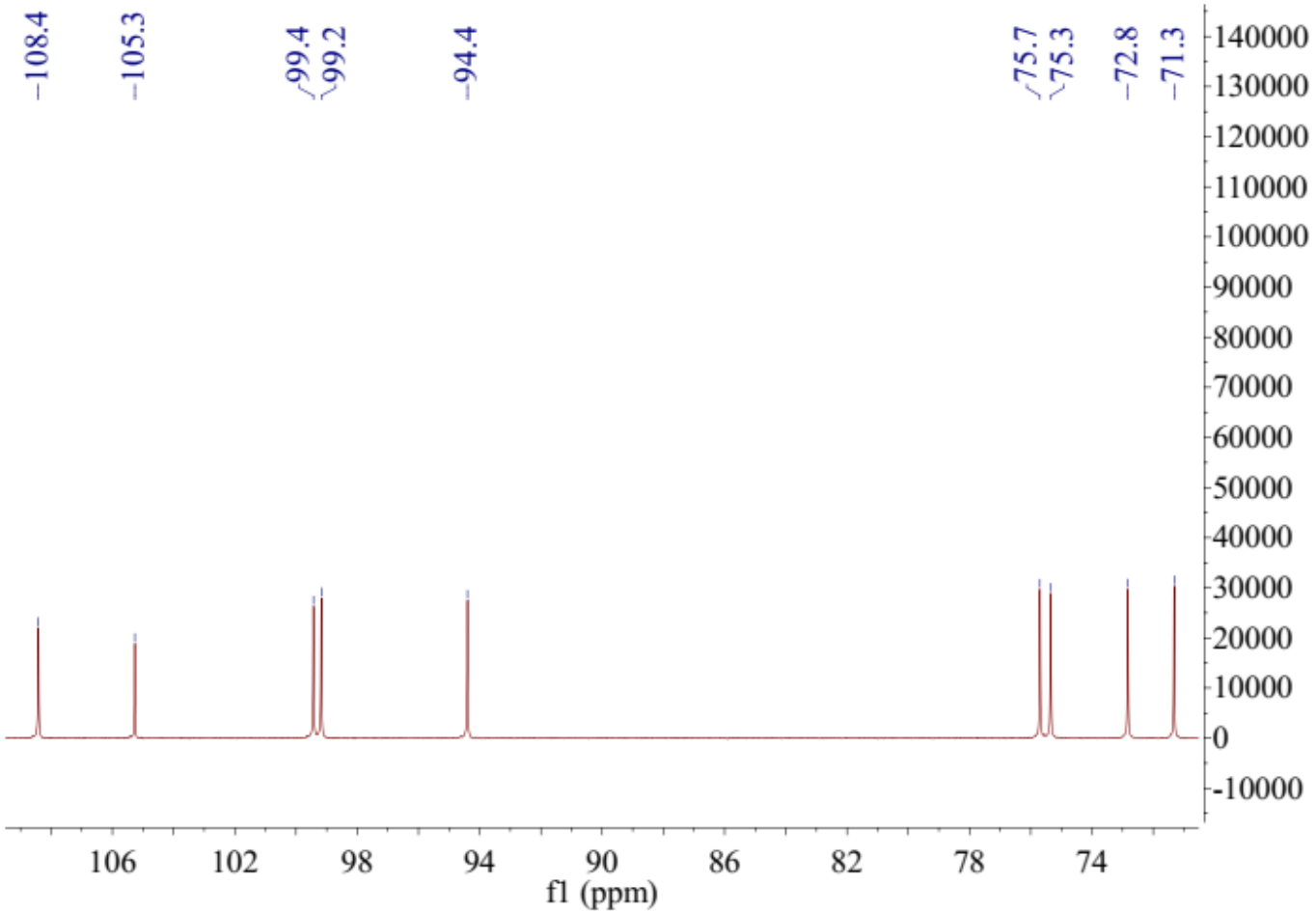

Figure S6: ^{13}C-NMR (150 MHz, DMSO -d_6) Spectrum of **1**

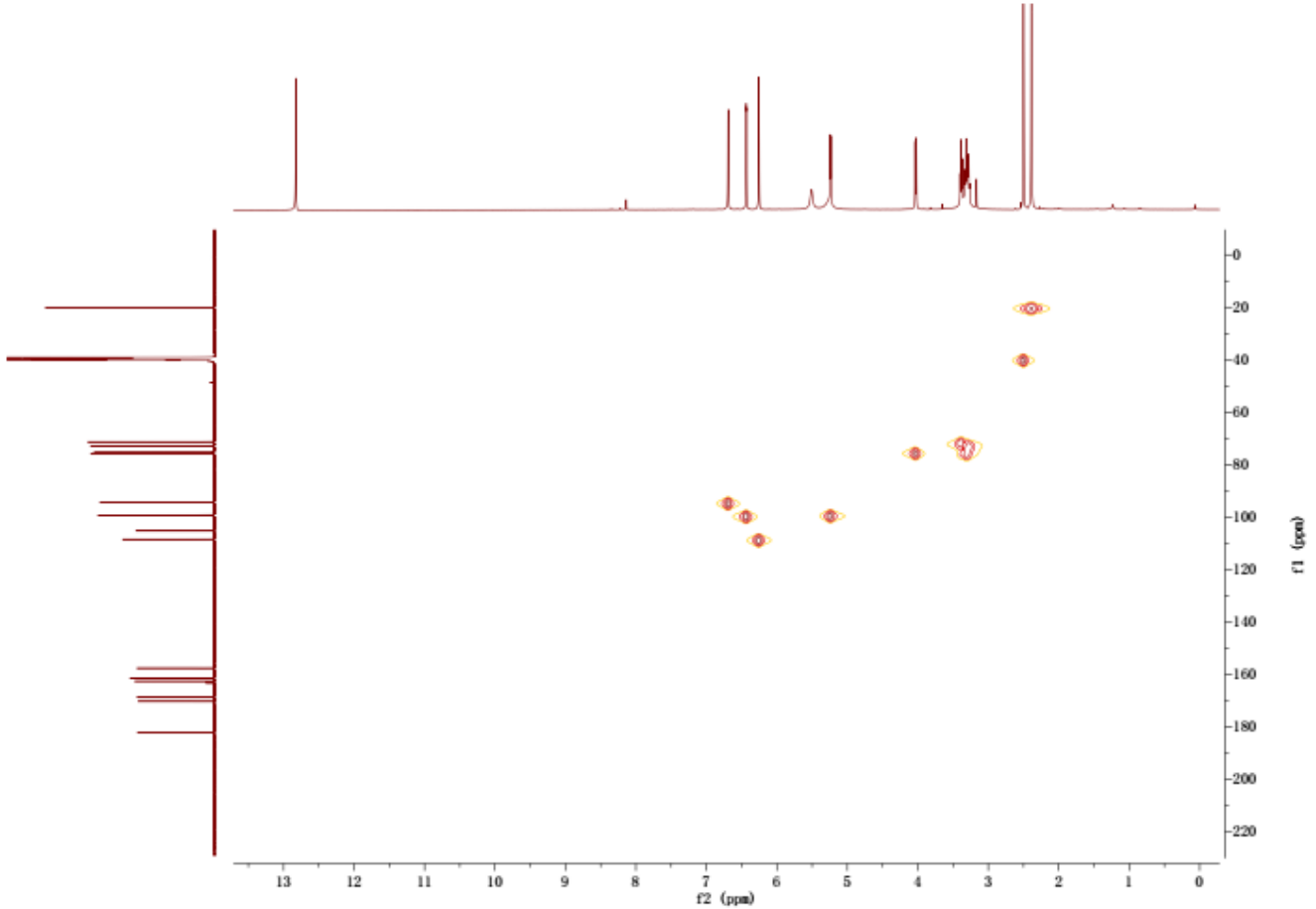

Figure S7: HSQC Spectrum of **1**

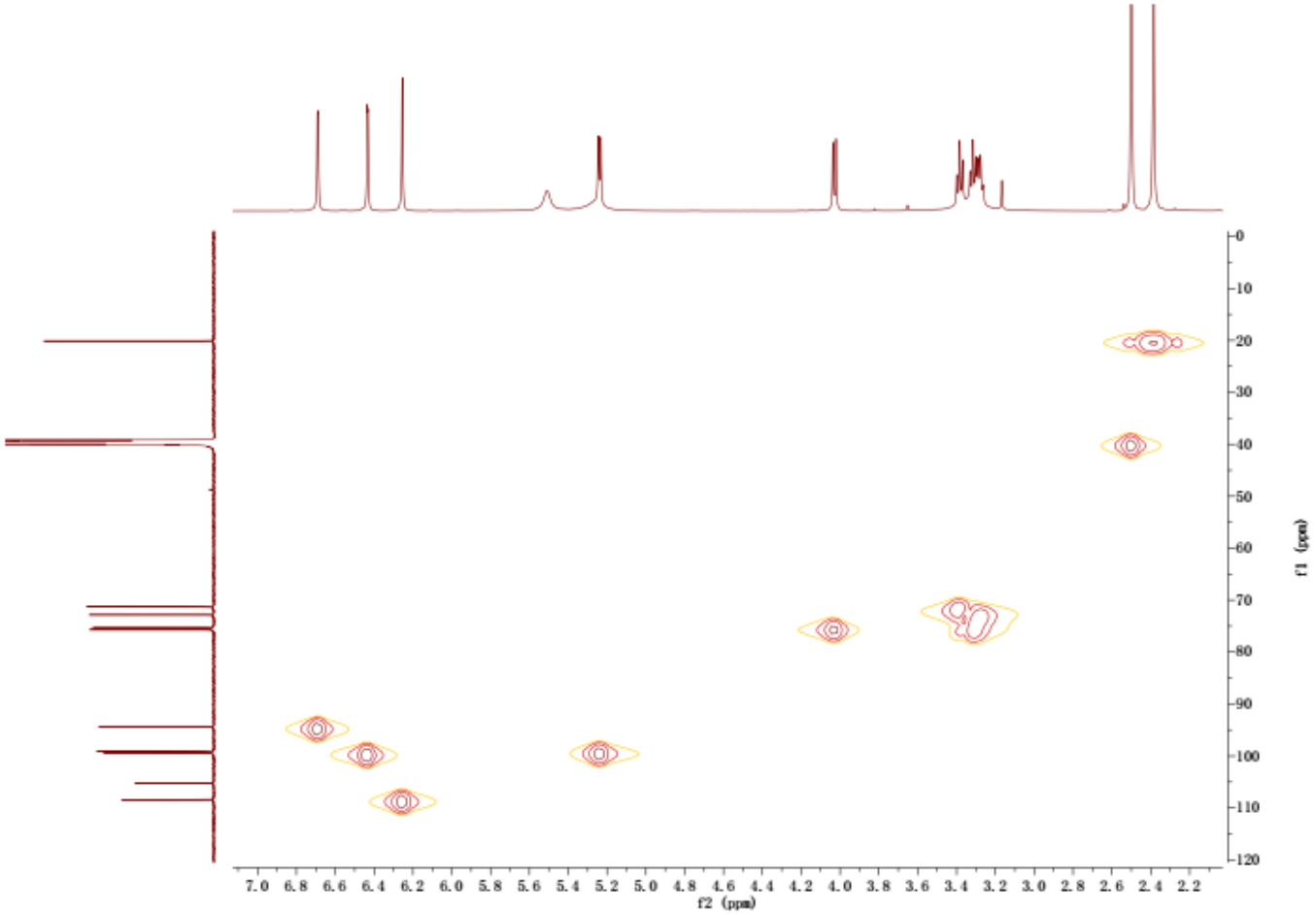

Figure S8: HSQC Spectrum of **1**

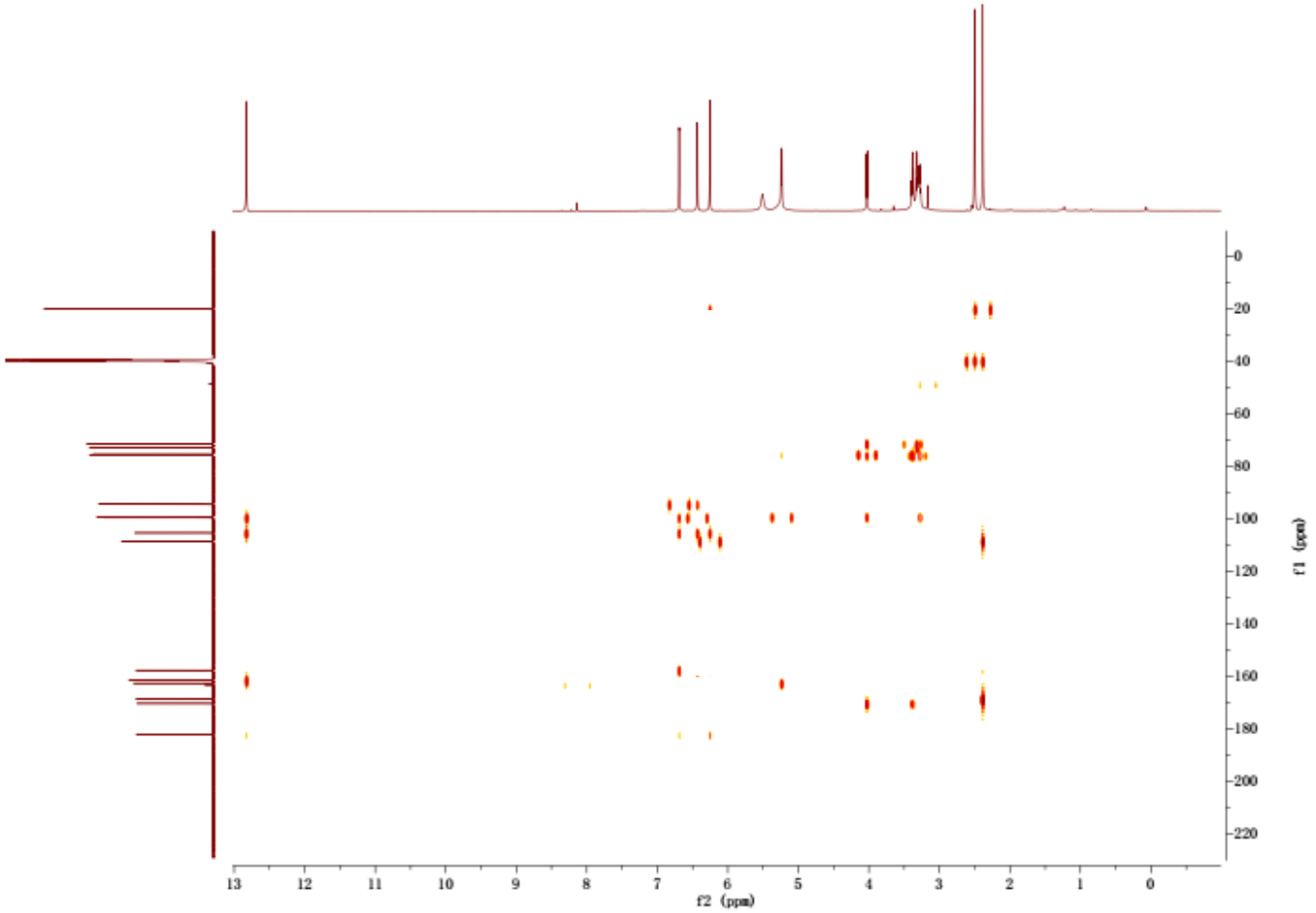

Figure S9: HMBC Spectrum of **1**

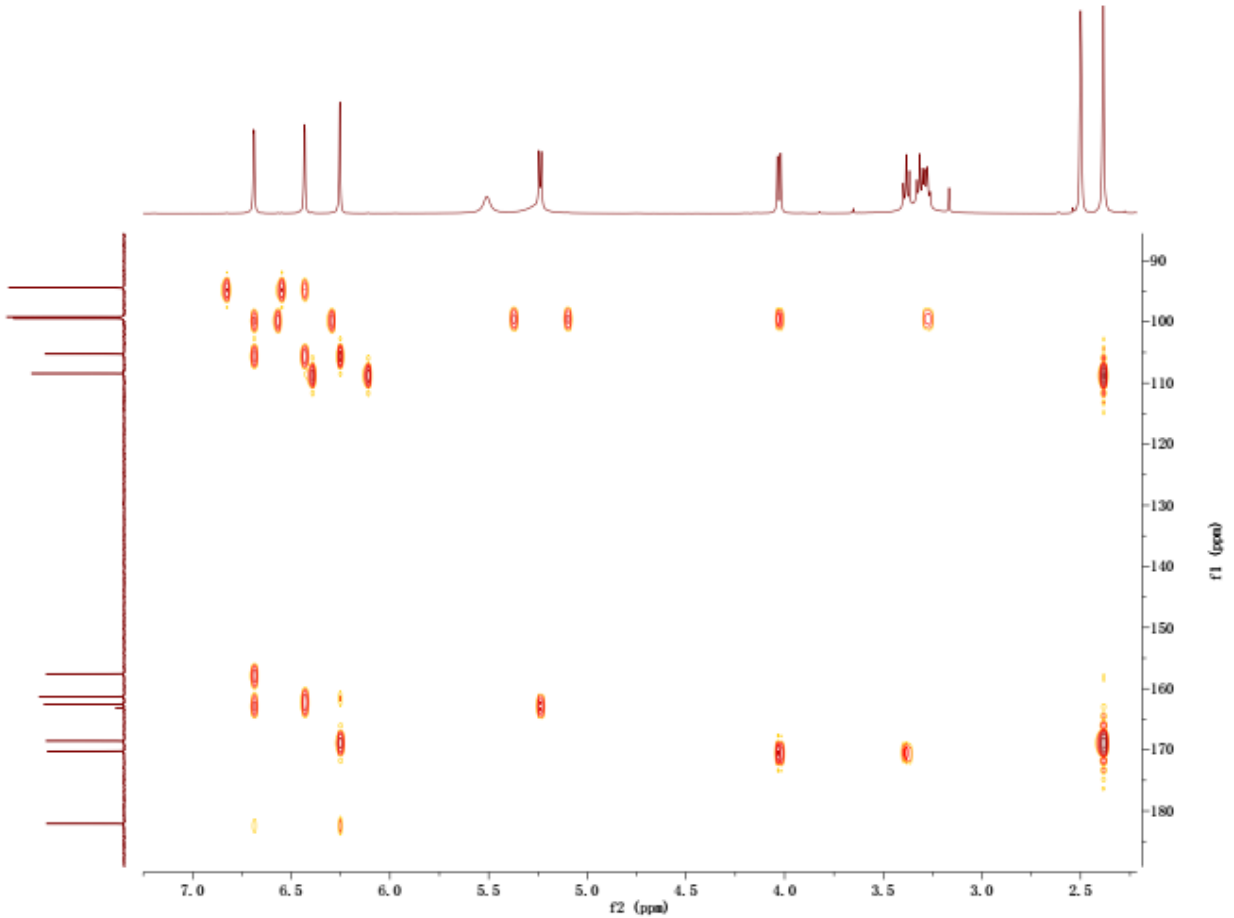

Figure S10: HMBC Spectrum of **1**

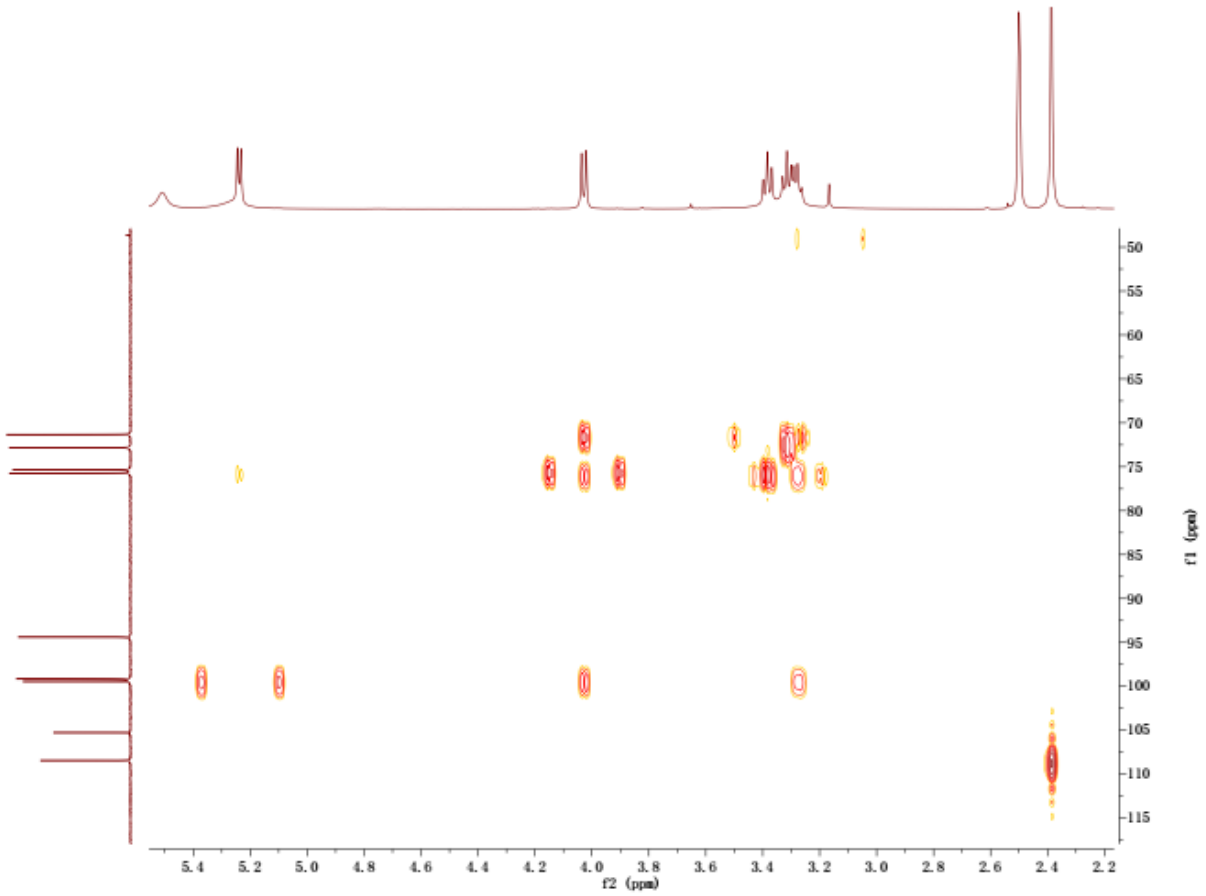

Figure S11: HMBC Spectrum of **1**

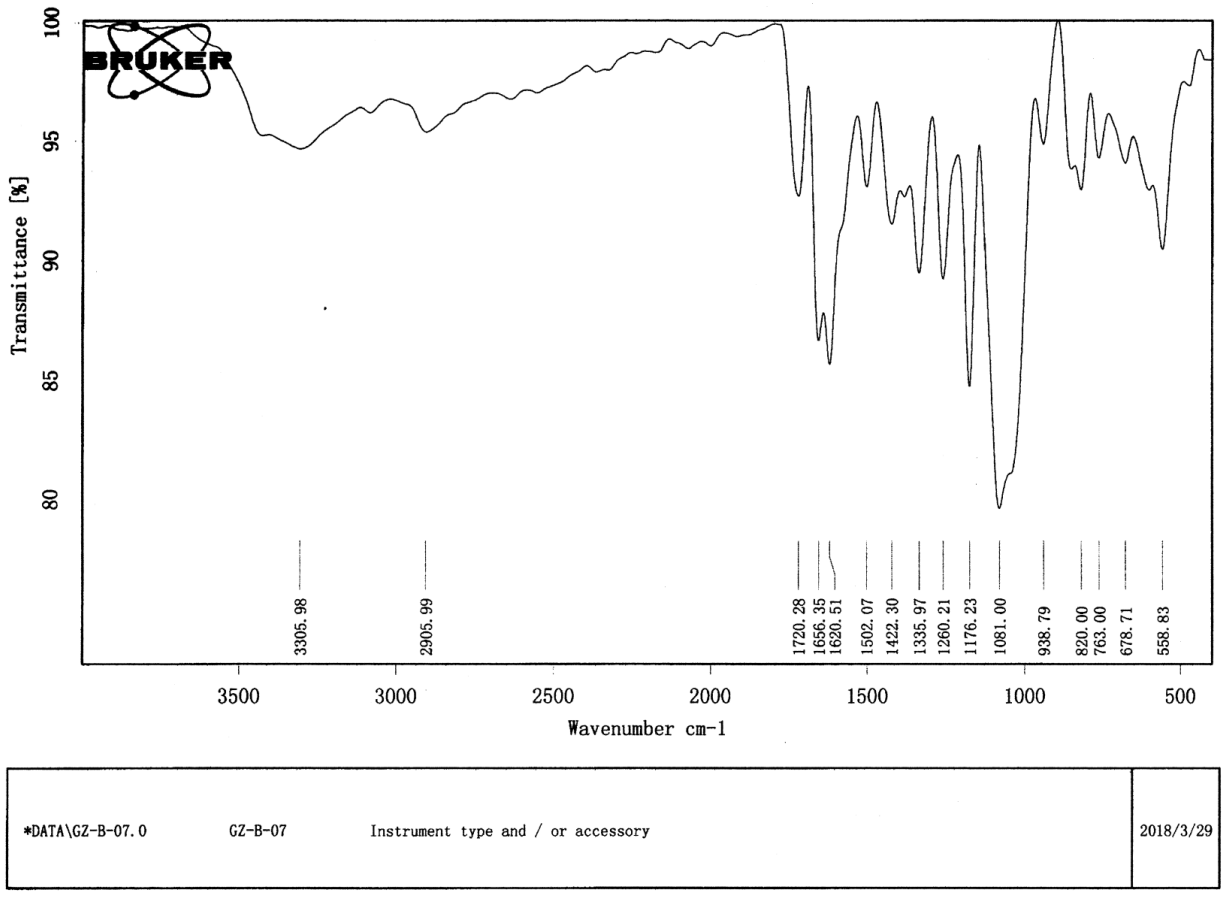

Figure S12: IR spectrum of Spectrum of **2**

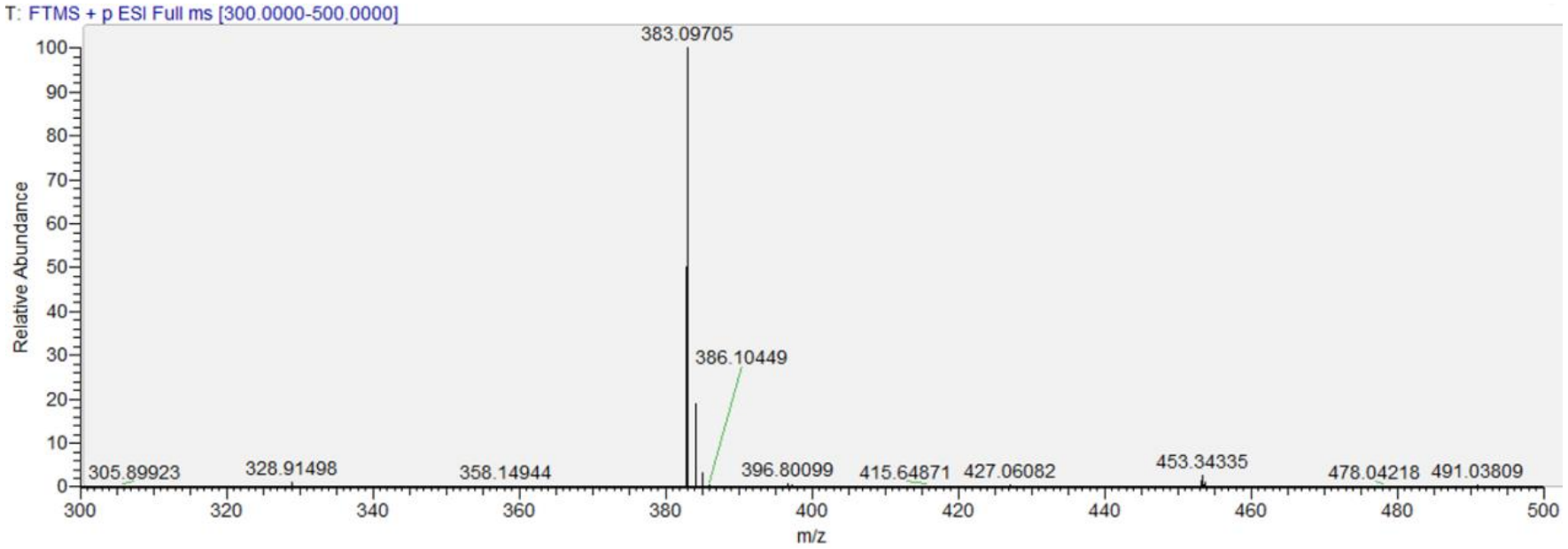

Figure S13: HR-ESI-MS Spectrum of **2**

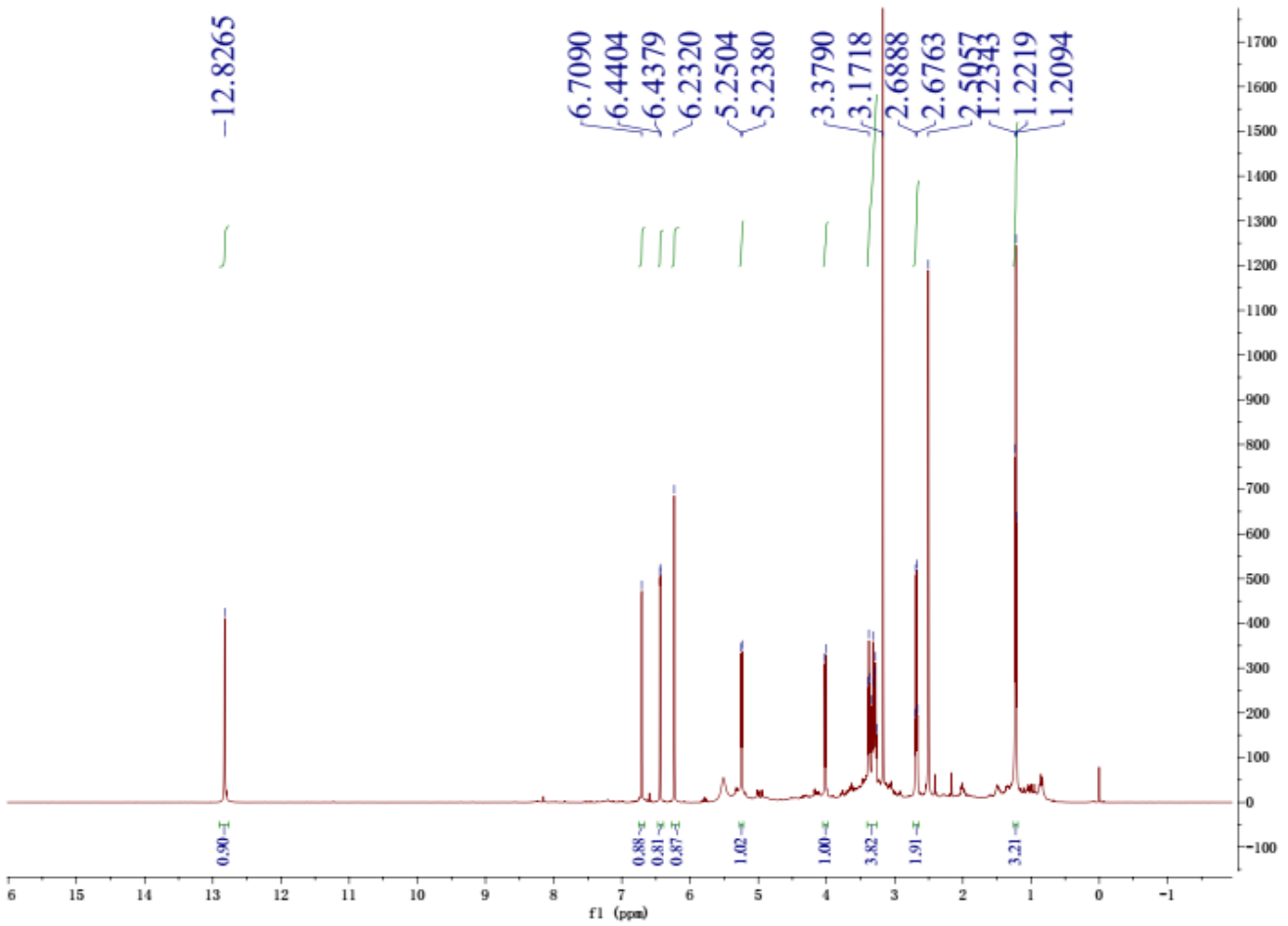

Figure S14: ^{1}H-NMR (600 MHz, DMSO-d_6) Spectrum of **2**

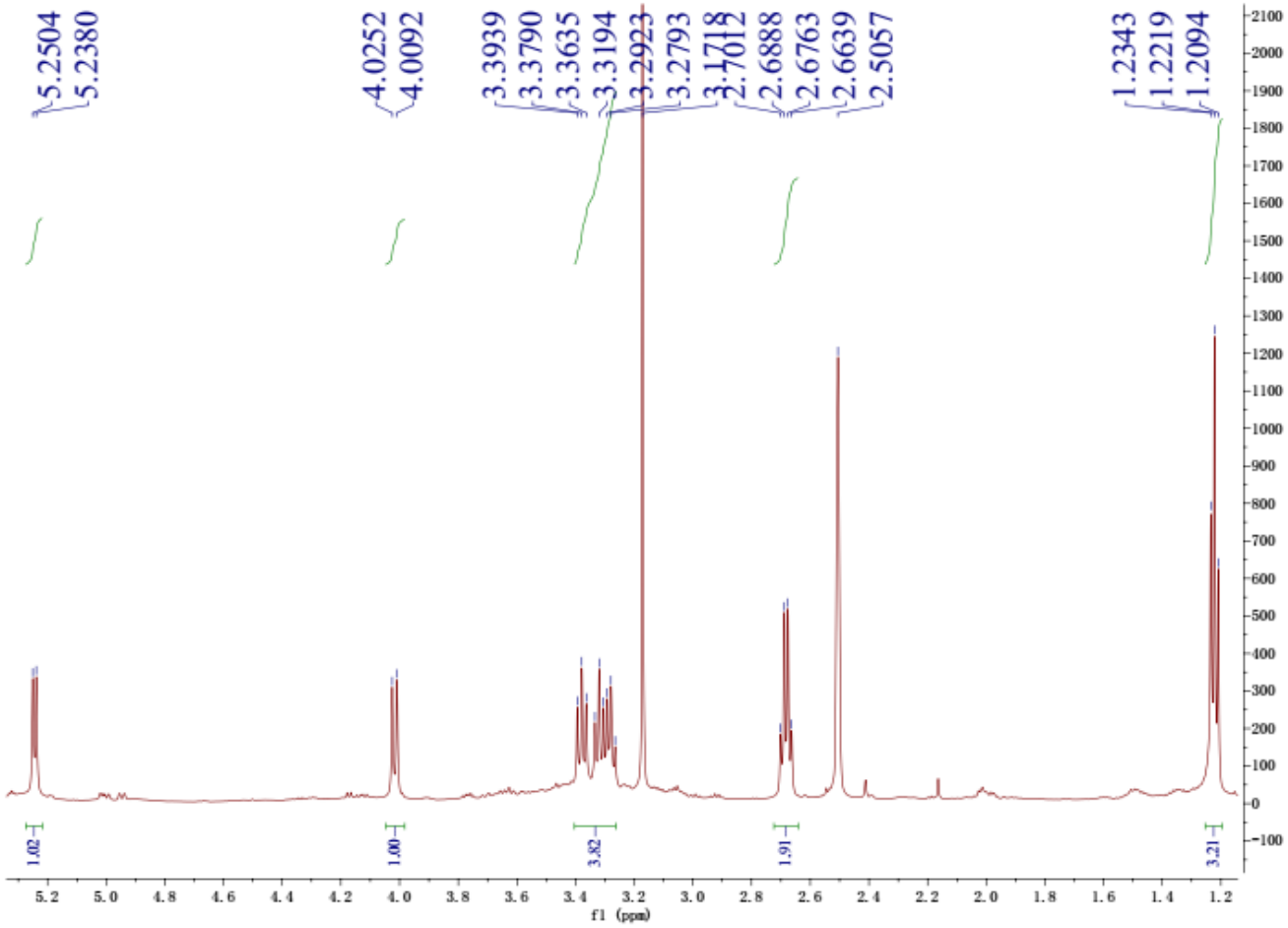

Figure S15: ^{1}H-NMR (600 MHz, DMSO-d_6) Spectrum of **2**

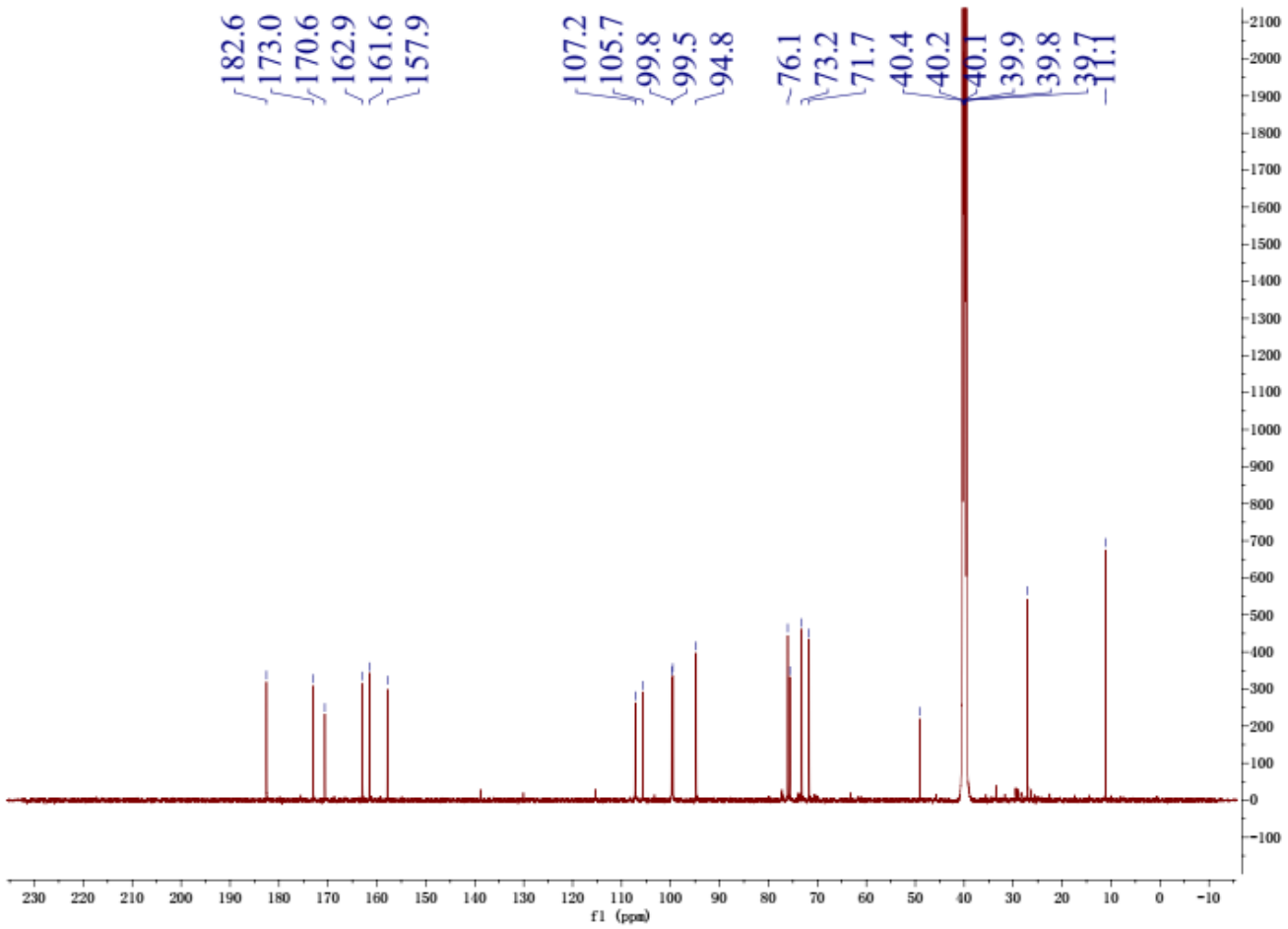

Figure S16: ^{13}C-NMR (150 MHz, DMSO-d_6) Spectrum of **2**

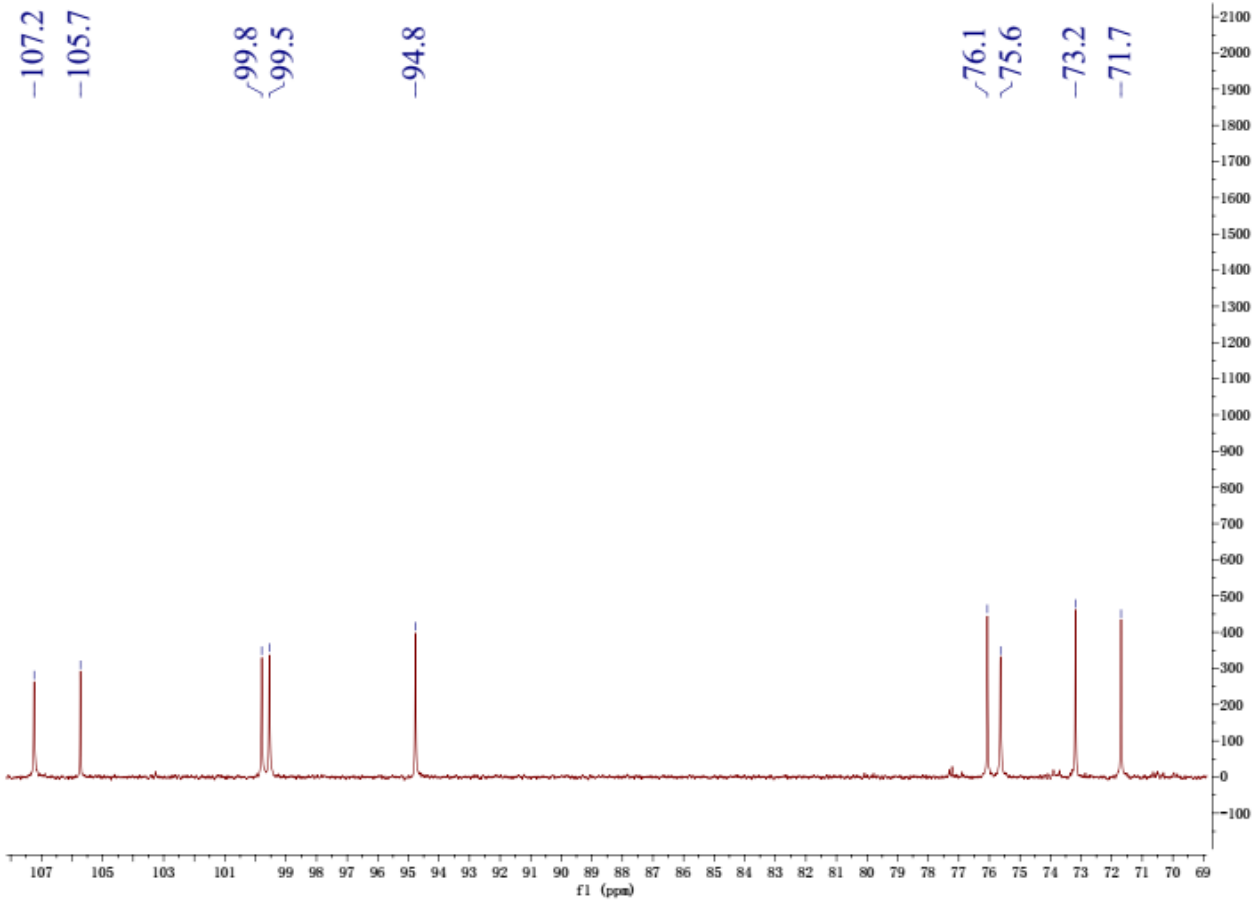

Figure S17: ^{13}C-NMR (150 MHz, DMSO-d_6) Spectrum of **2**

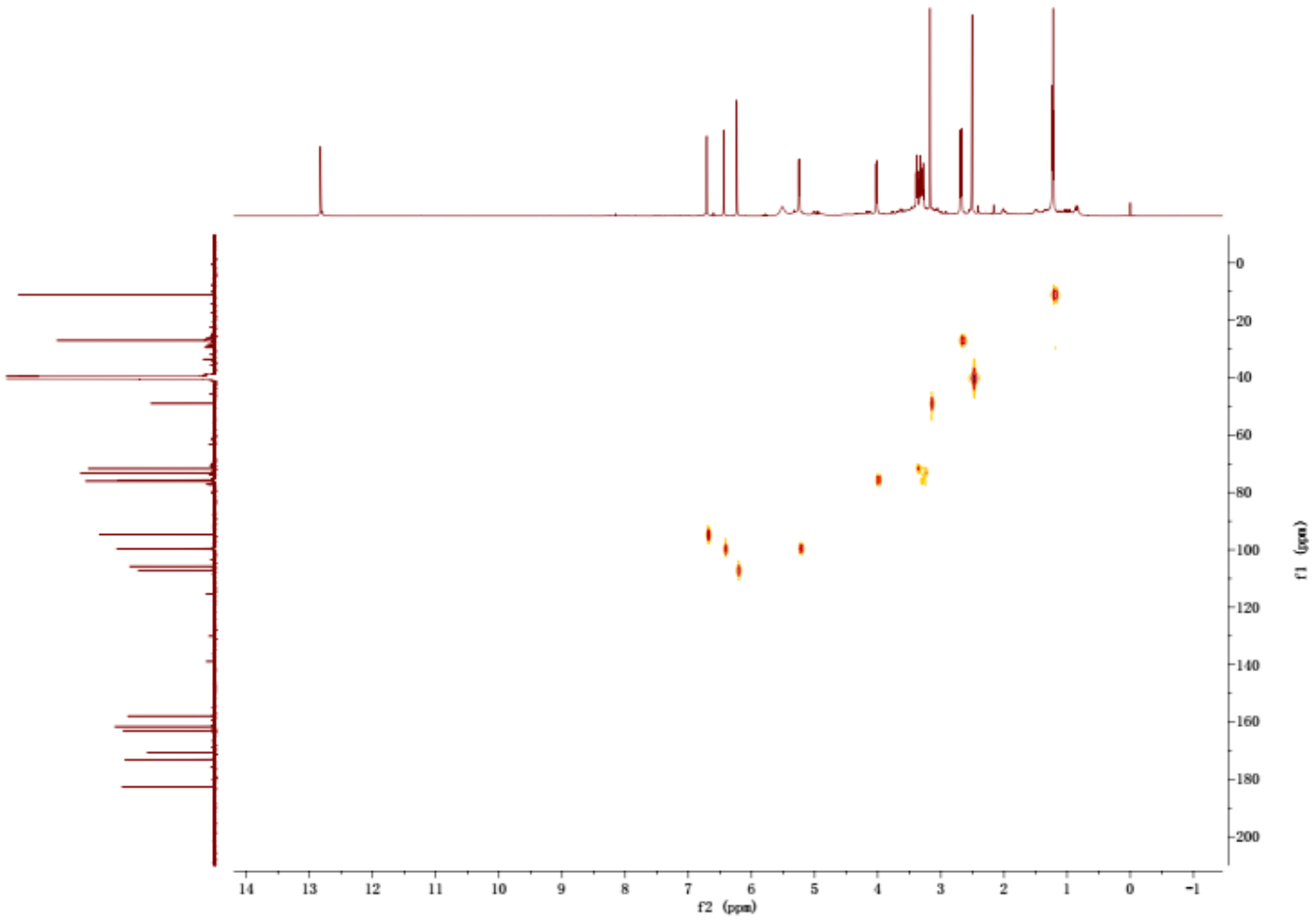

Figure S18: HSQC Spectrum of **2**

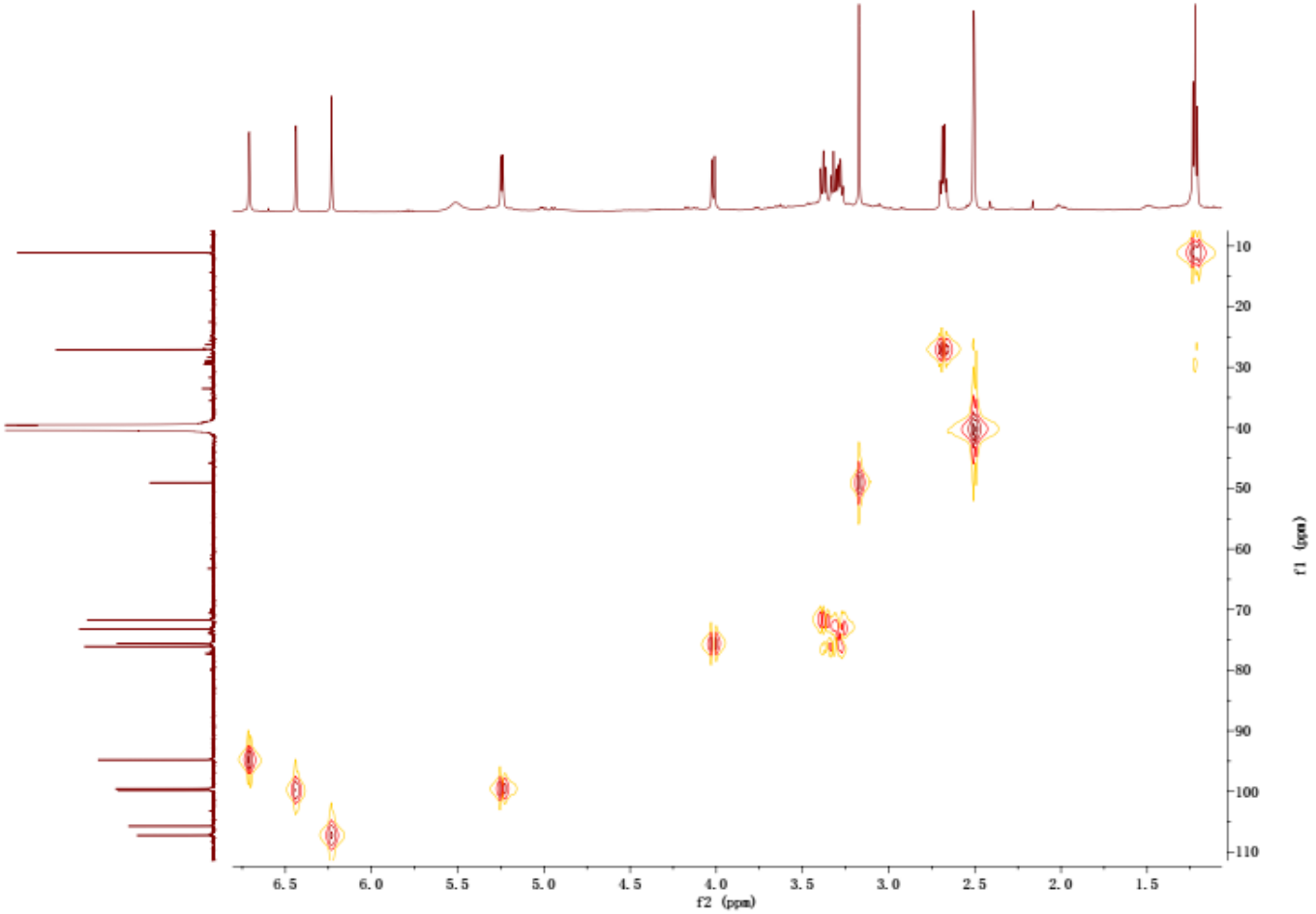

Figure S19: HSQC Spectrum of **2**

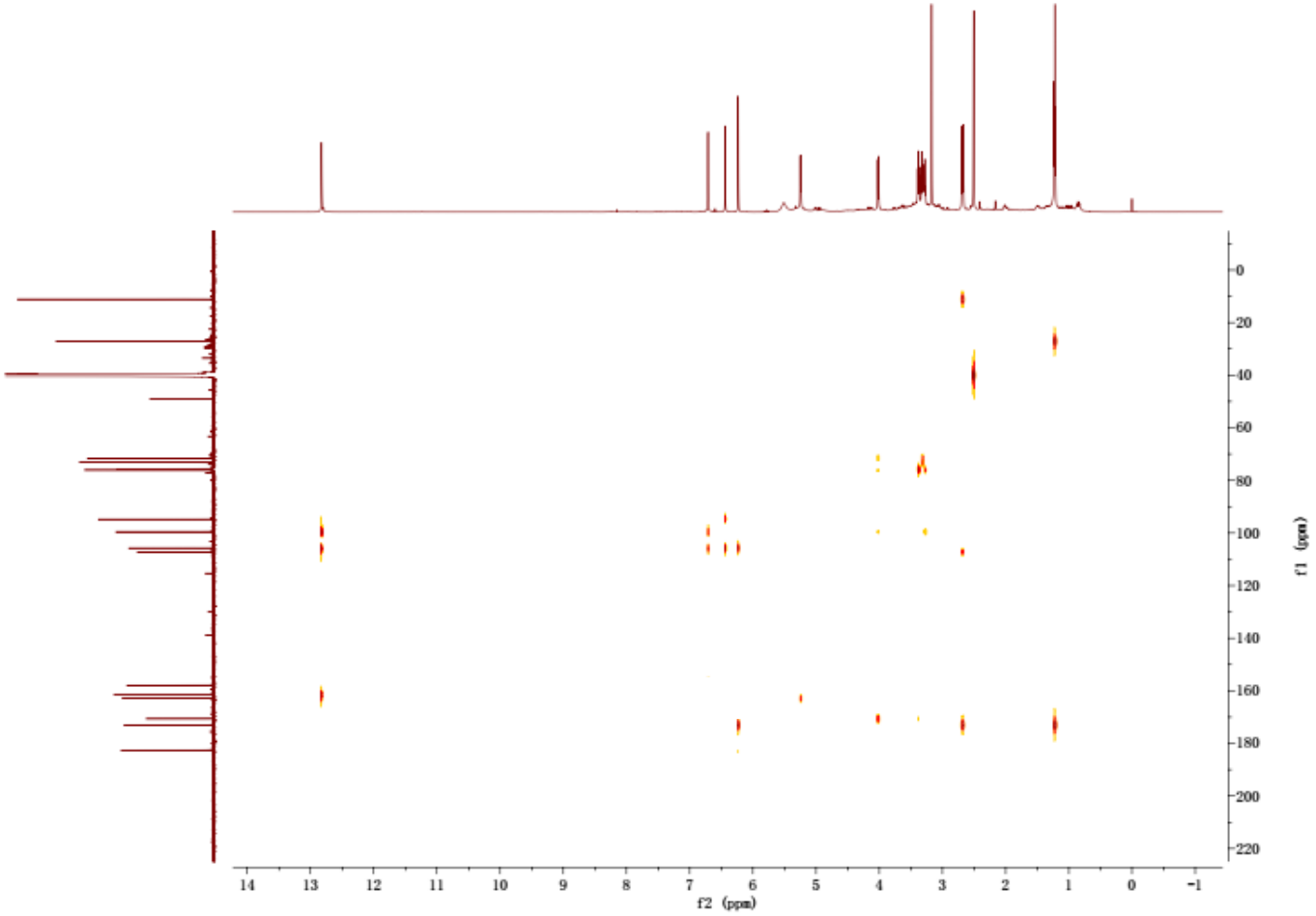

Figure S20: HMBC Spectrum of **2**

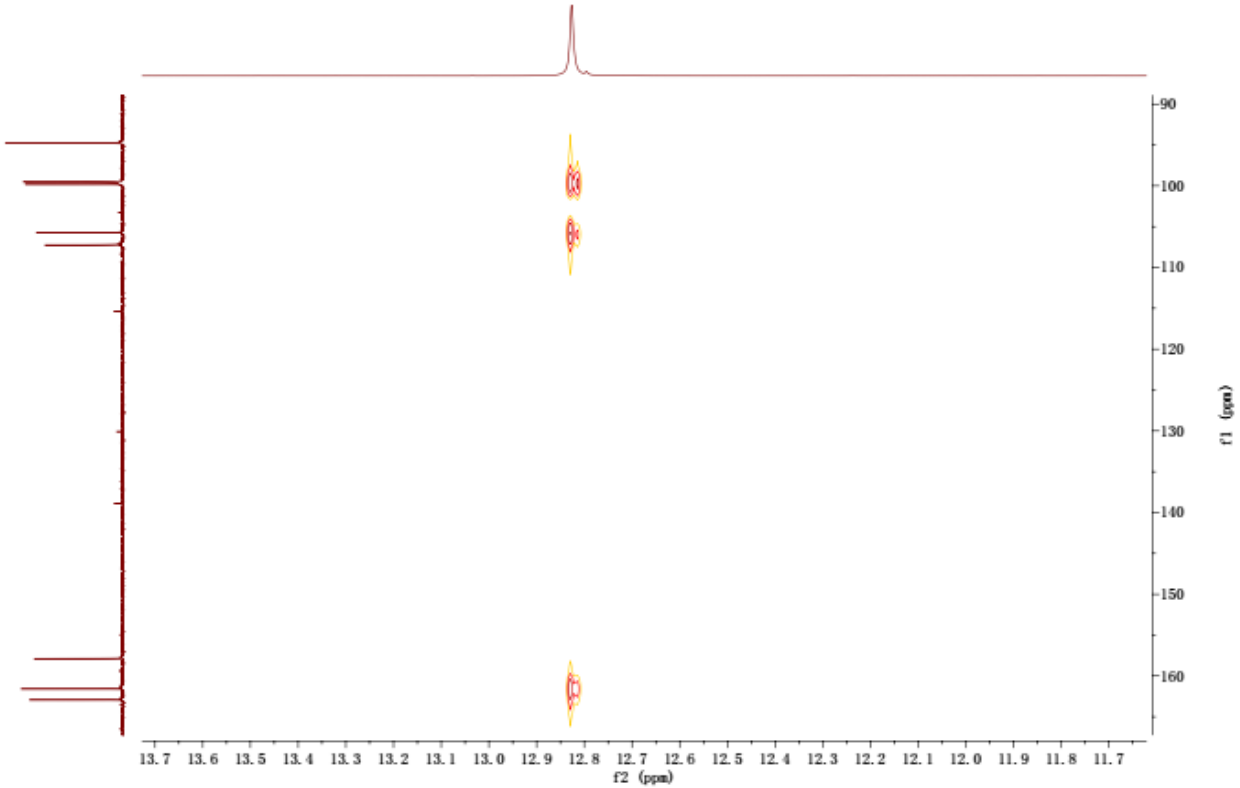

Figure S21: HMBC Spectrum of **2**

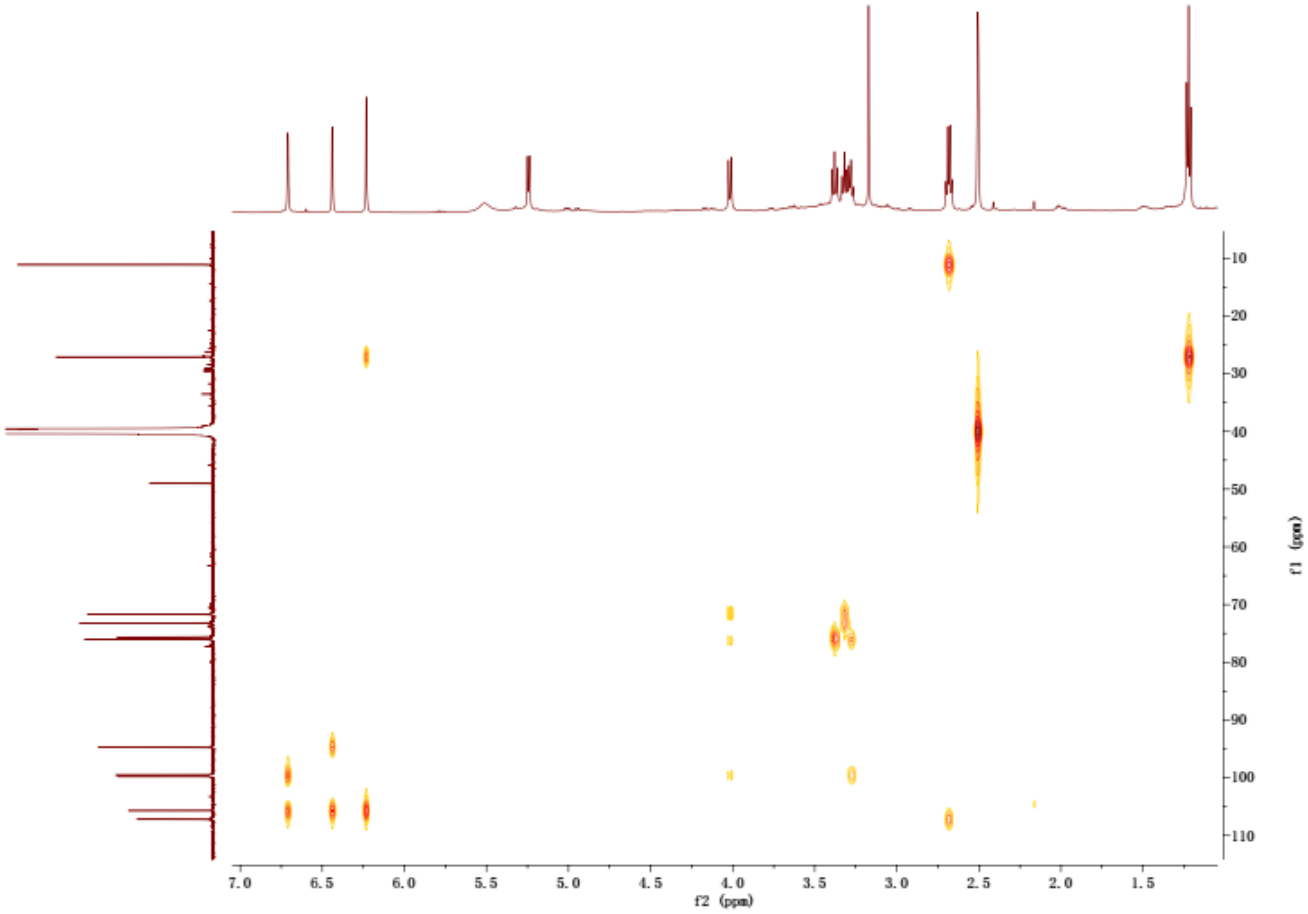

Figure S22: HMBC Spectrum of **2**

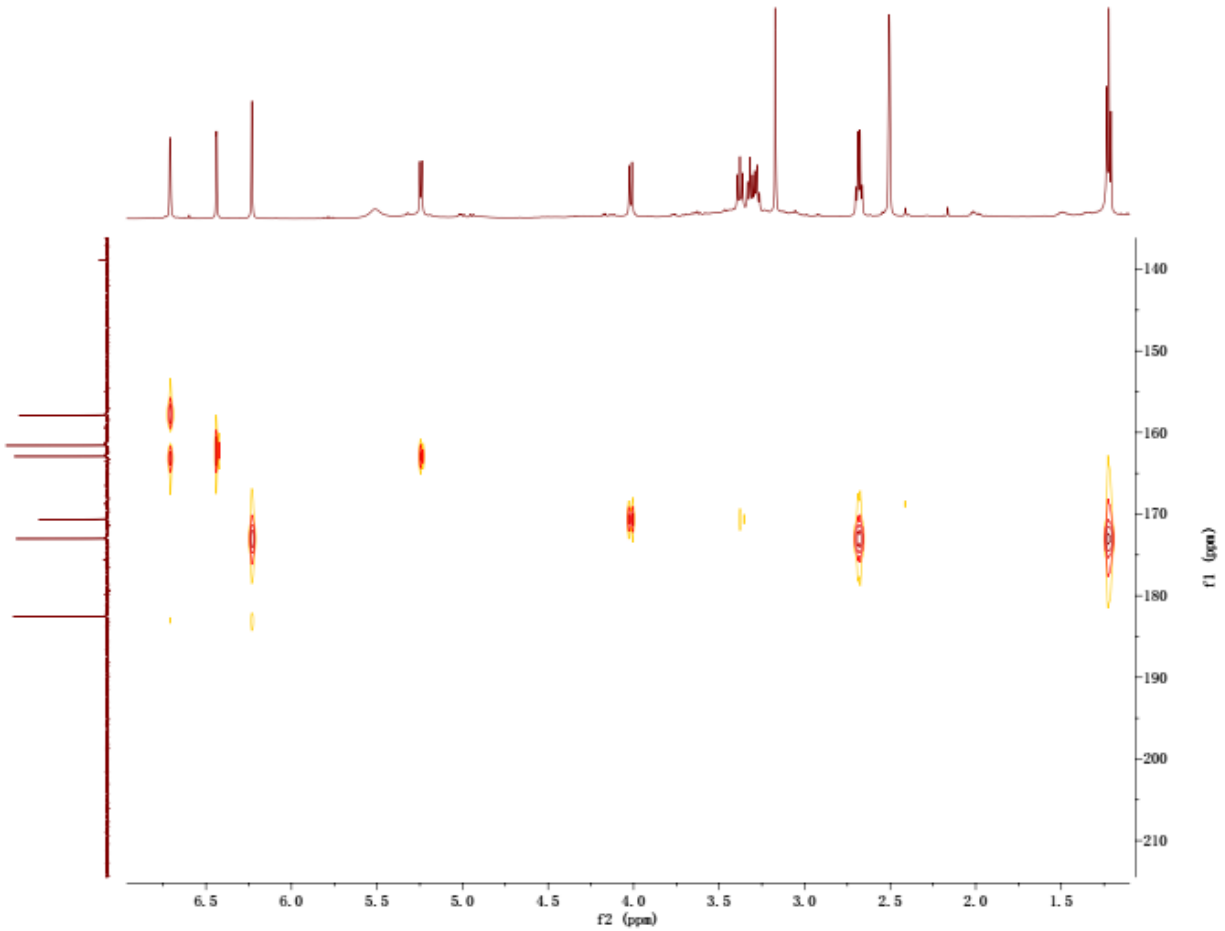

Figure S23: HMBC Spectrum of **2**

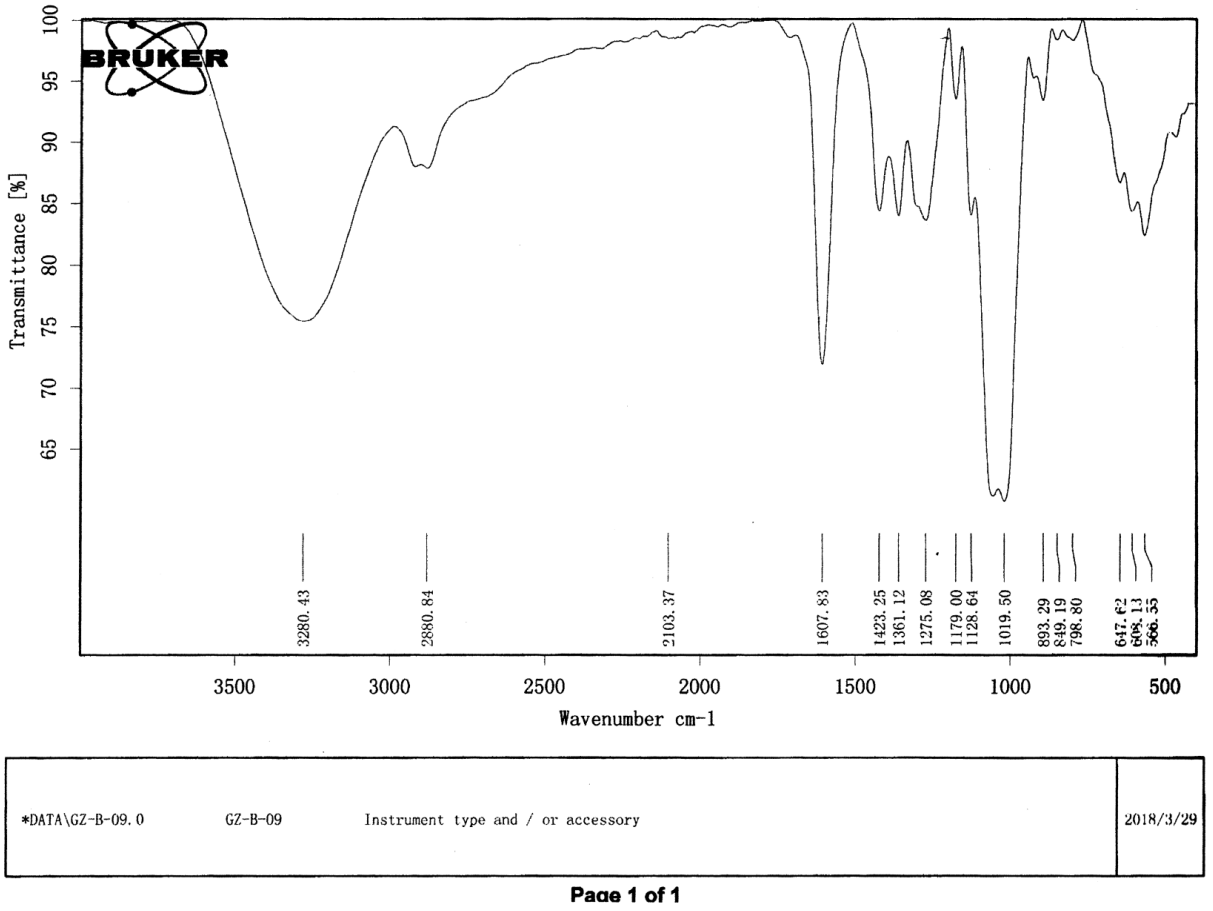

Figure S24: IR spectrum of Spectrum of **6**

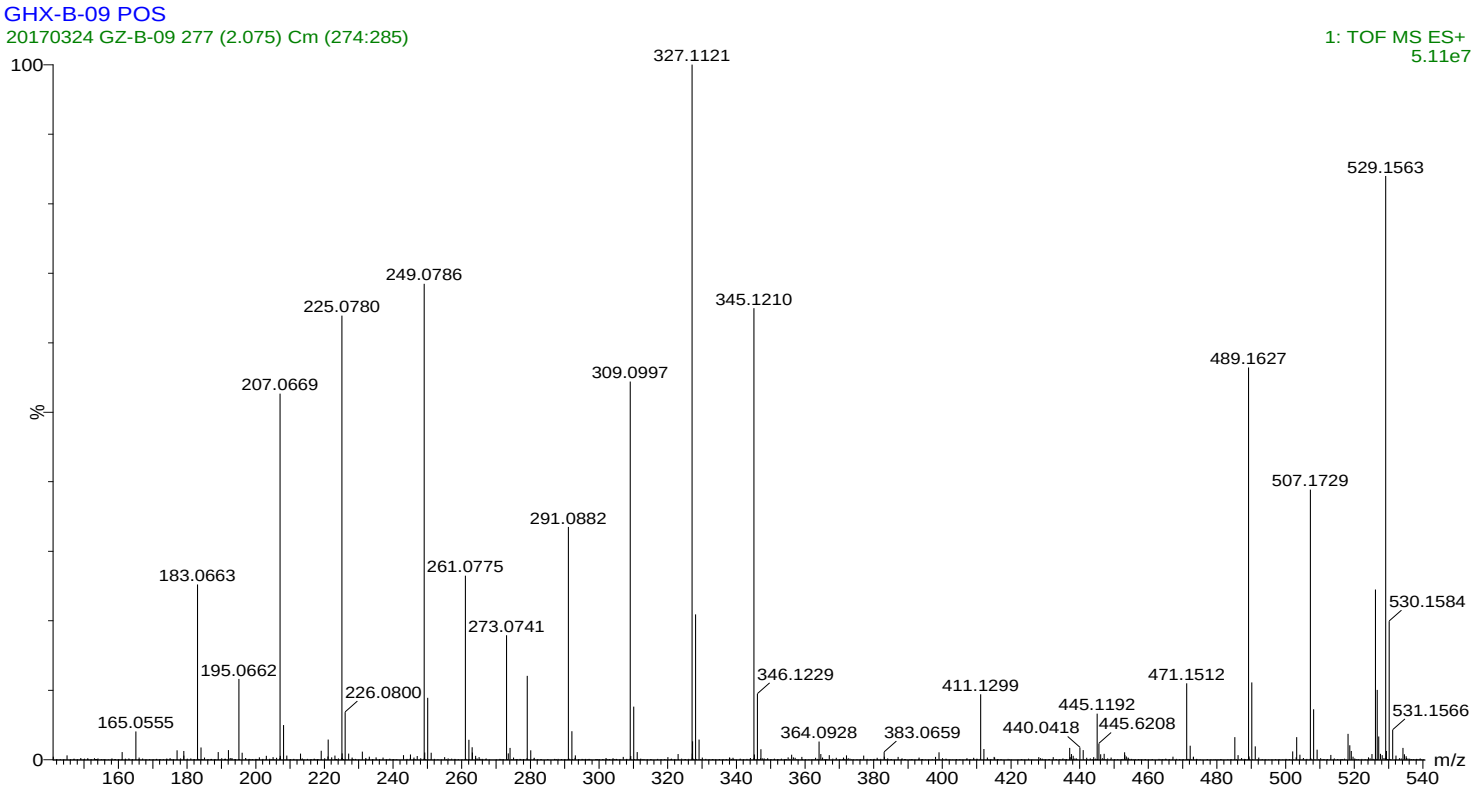

Figure S25: HR-ESI-MS Spectrum of **6**

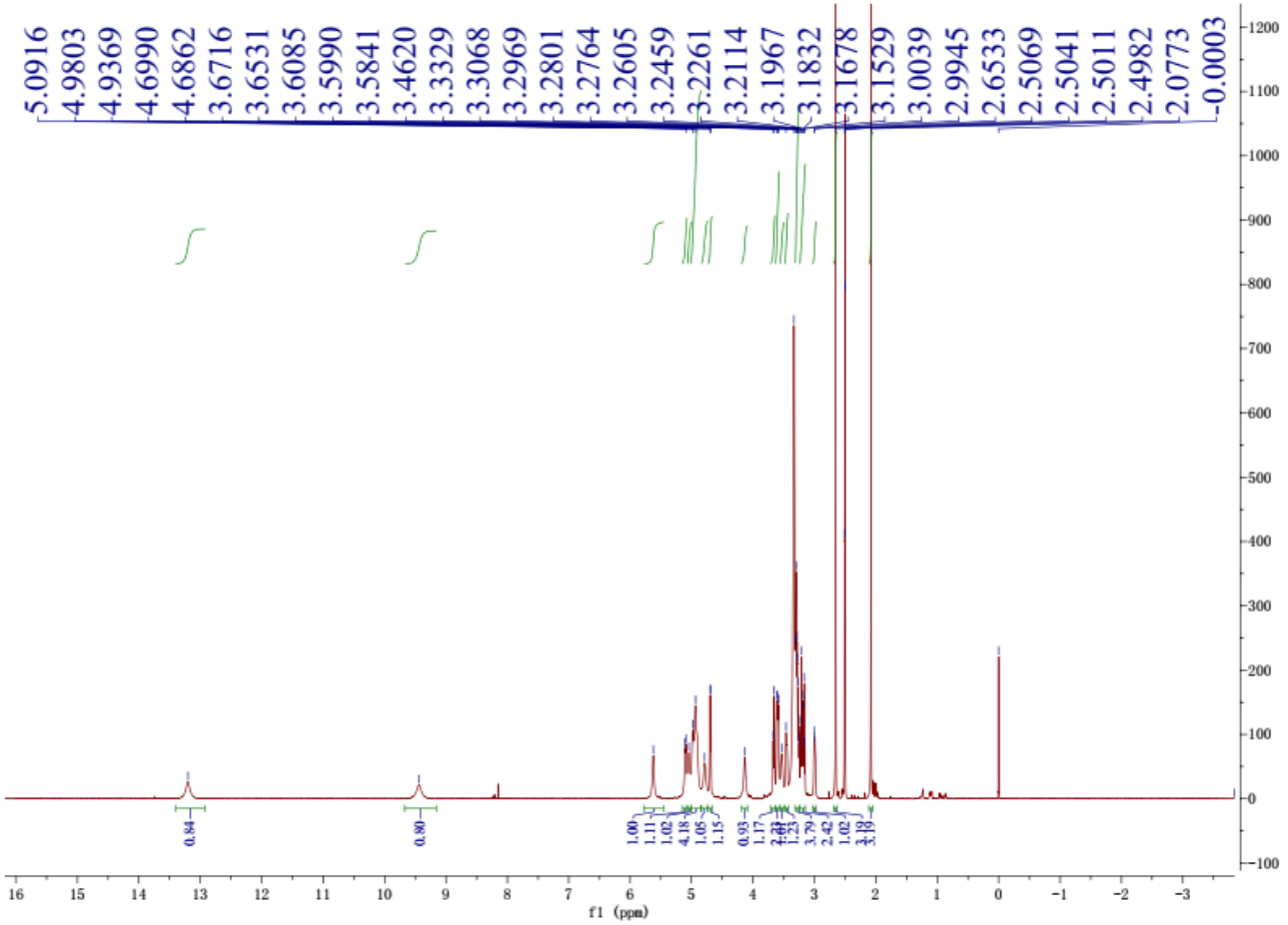

Figure S26: ^{1}H-NMR (600 MHz, DMSO-d_6) Spectrum of **6**

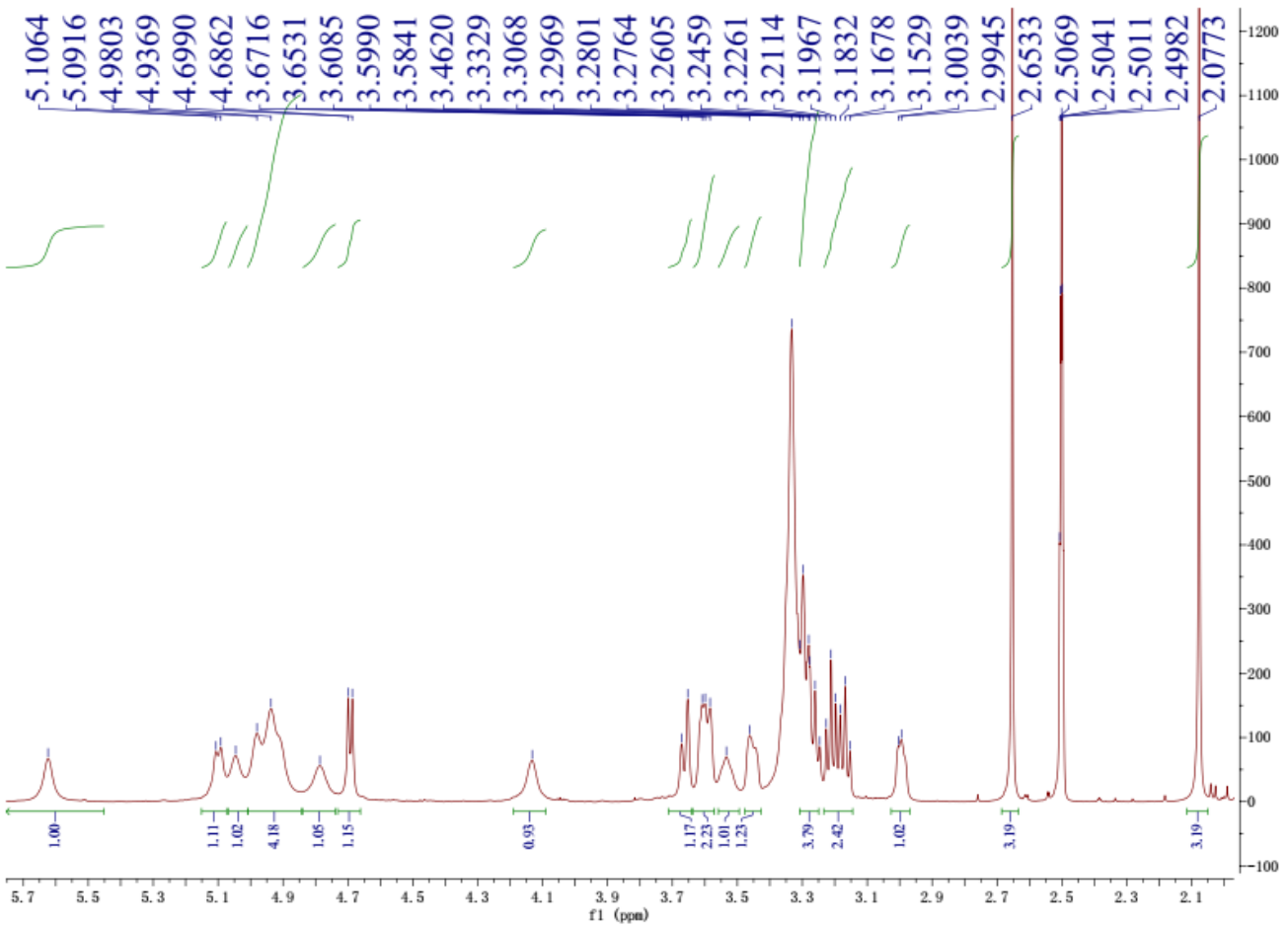

Figure S27: ^{1}H-NMR (600 MHz, DMSO-d_6) Spectrum of **6**

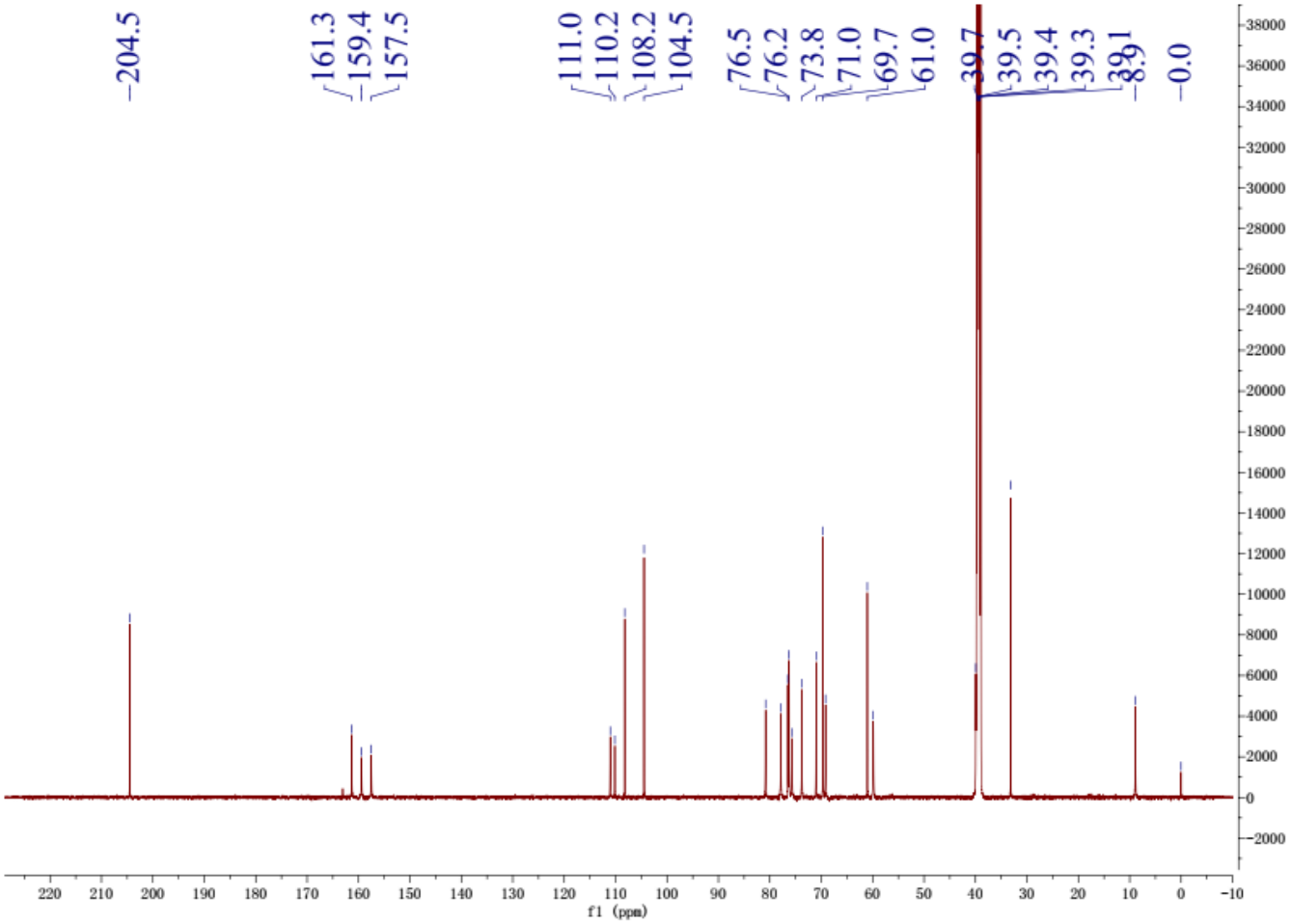

Figure S28: ^{13}C-NMR (150 MHz, DMSO-d_6) Spectrum of **6**

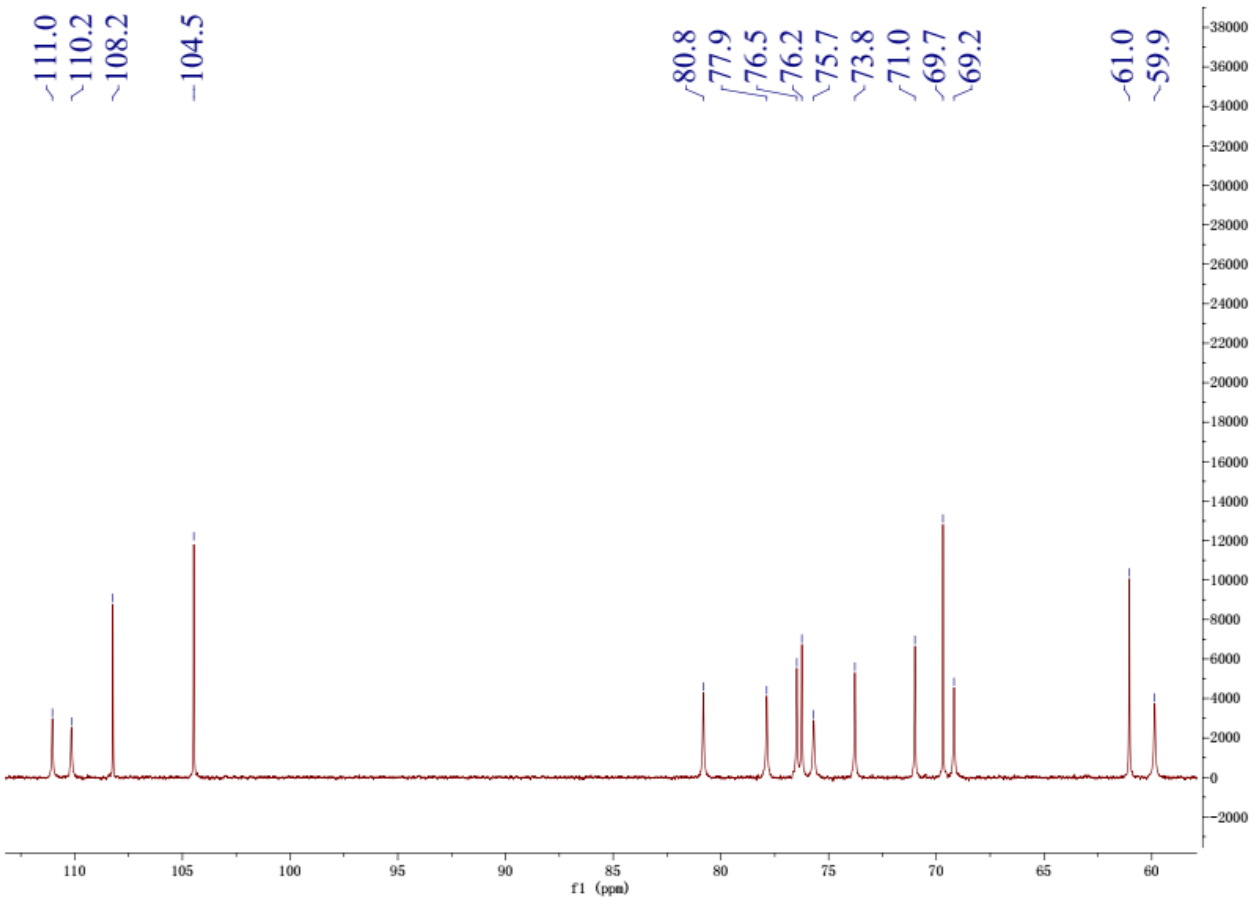

Figure S29: ^{13}C-NMR (150 MHz, DMSO-d_6) Spectrum of **6**

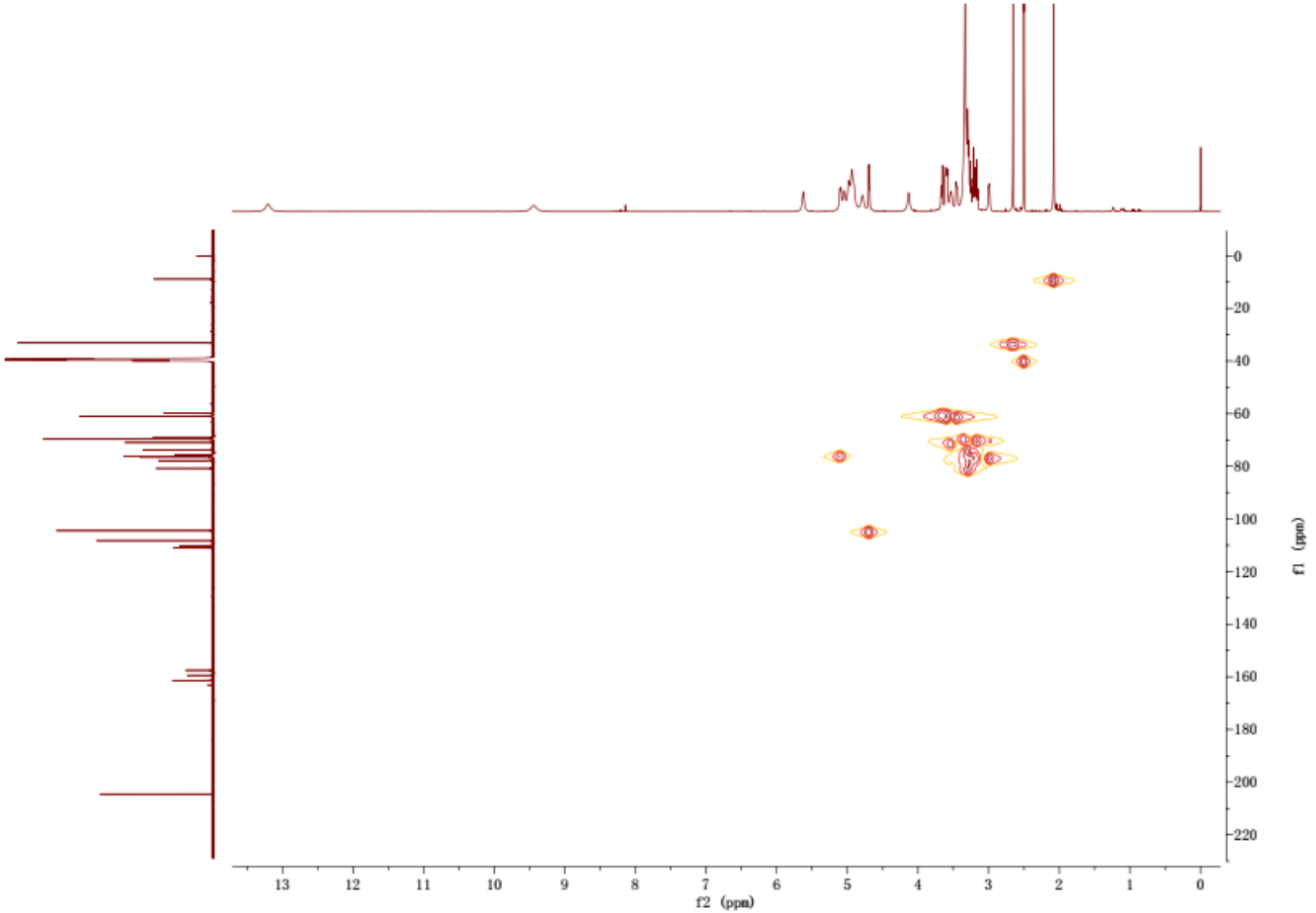

Figure S30: HSQC Spectrum of **6**

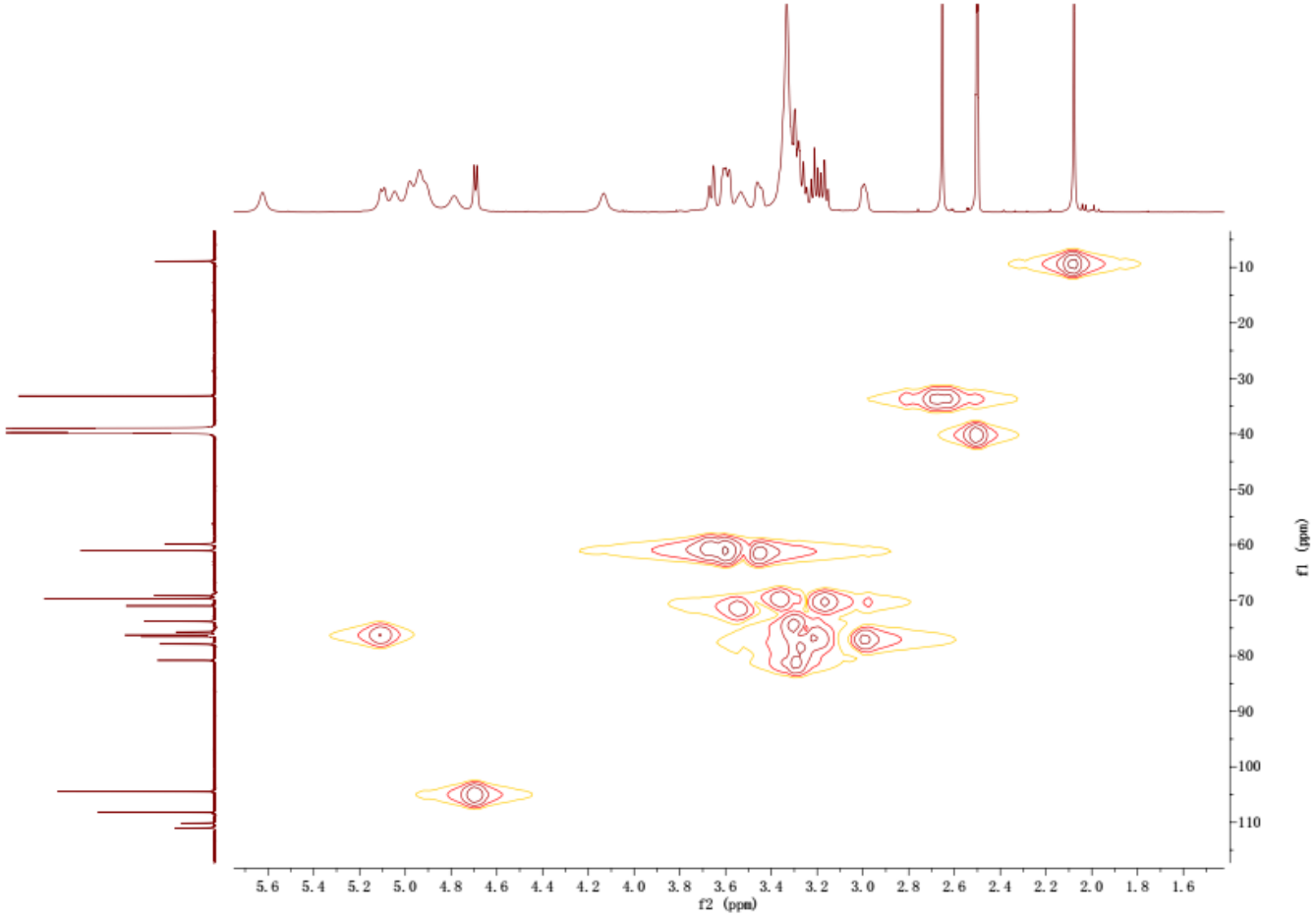

Figure S31: HSQC Spectrum of **6**

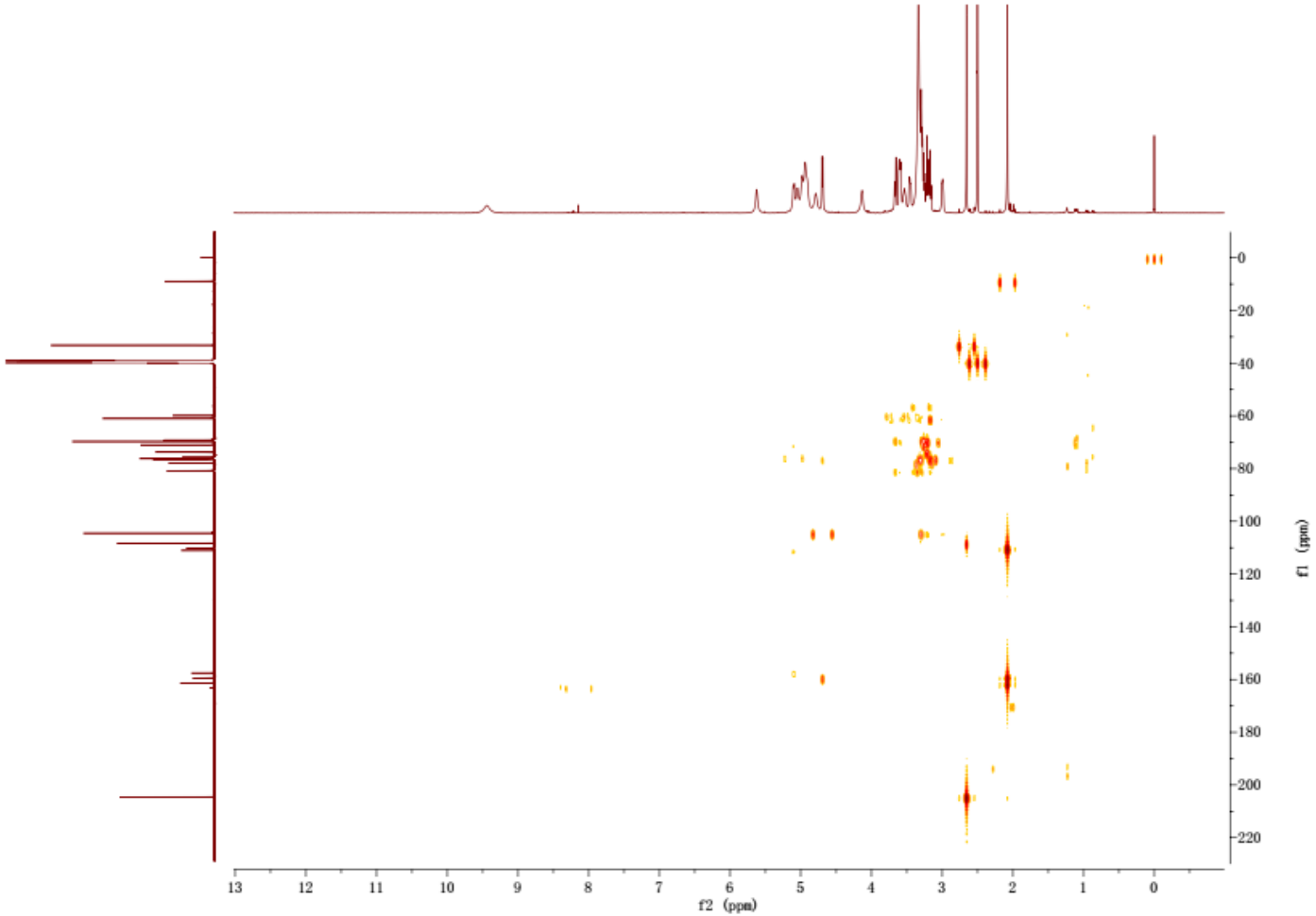

Figure S32: HMBC Spectrum of **6**

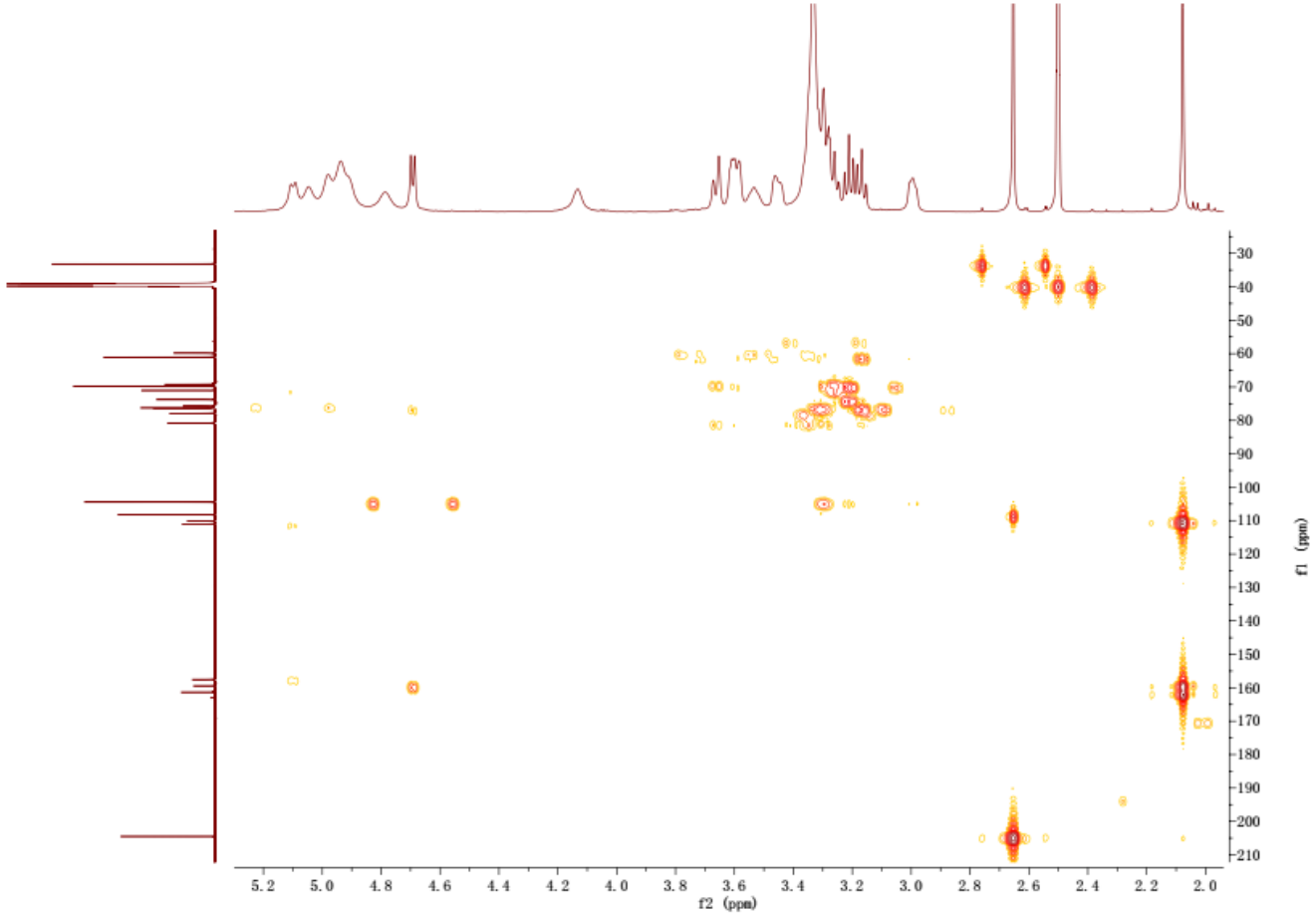

Figure S33: HMBC Spectrum of **6**

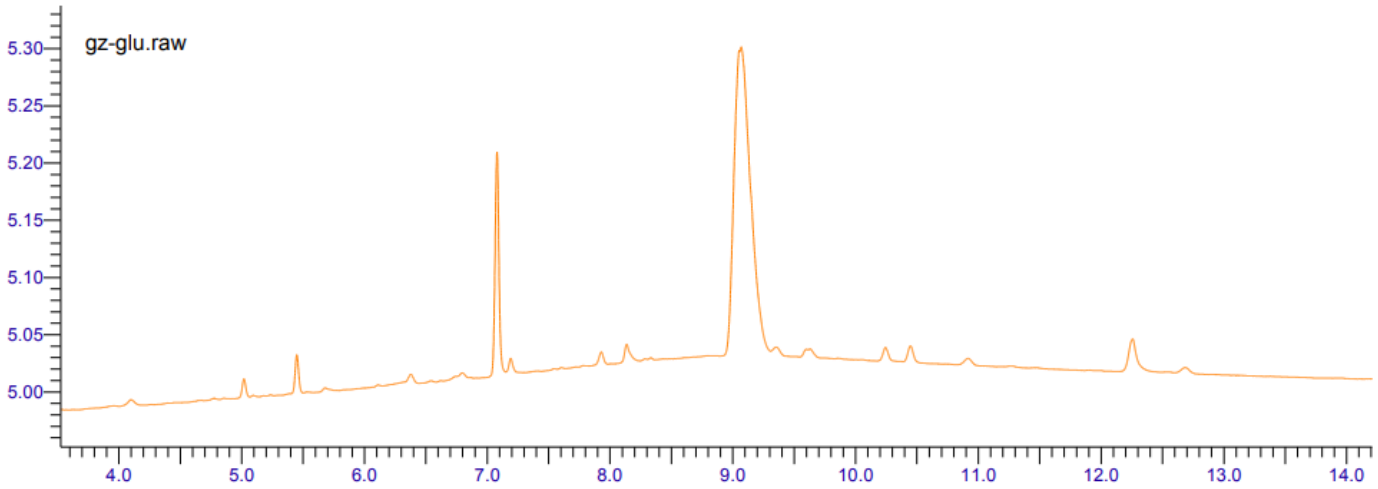

Figure S34: GC sugar moieties of **6** after hydrolysis

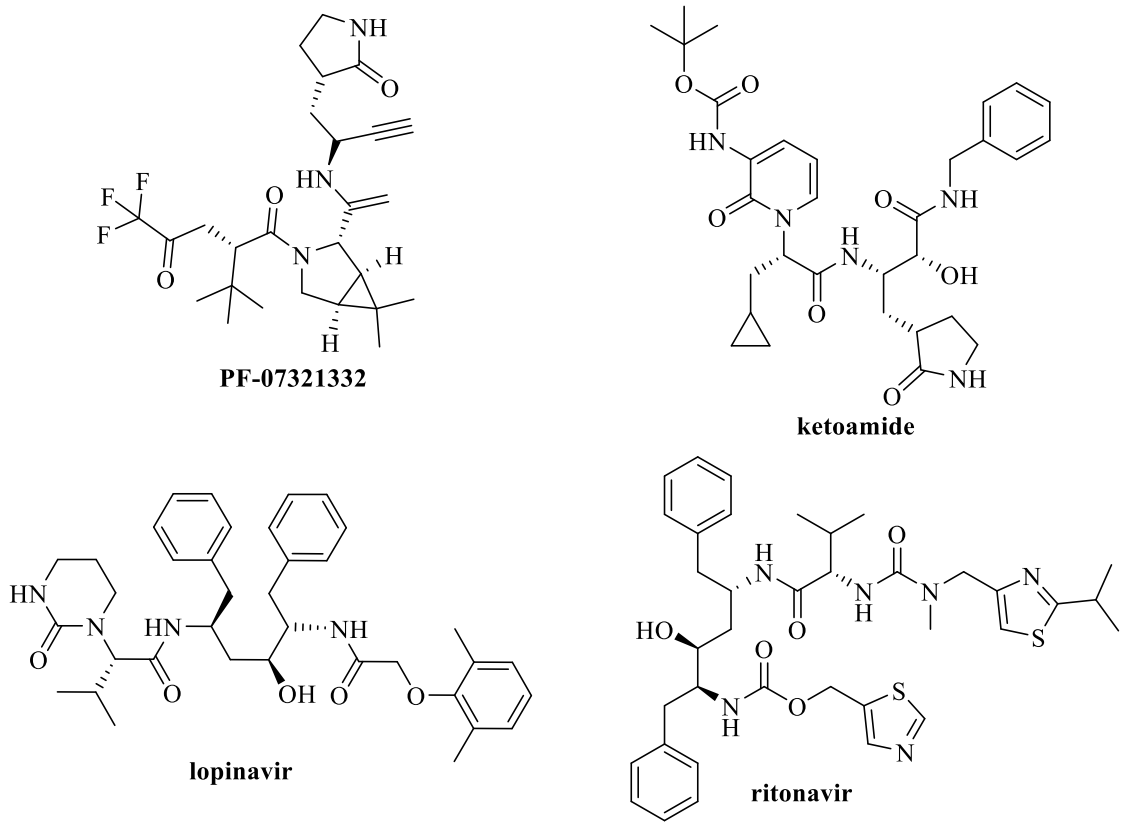

Figure S35: Structure of positive control compounds

Table S1 : The NMR data comparison between the new compounds (1 and 2) and the Known compounds (CAS No. 2627272-31-3)

Position	1		2		2627272-31-3	
	δ_H, (*J* in Hz)	δ_C	δ_H, (*J* in Hz)	δ_C	δ_H, (*J* in Hz)	δ_C
1						
2		168.5		173.0	6.33 (s)	172.2
3	6.25 (s)	108.4	6.23 (s)	107.2		107.0
4		182.1		182.5		184.2
5		161.3		161.6		107.3
6	6.43 (d,1.7)	99.2	6.44 (d,1.5)	99.5	6.48 (s)	163.1
7		162.5		162.9		101.2
8	6.69 (brs)	94.4	6.71 (brs)	94.8	6.66 (s)	164.9
9		157.5		157.9	4.47 (s, 2H)	61.4
10		105.3		105.7		
11	2.39 (s)	20.1	2.68 (q, 7.5)	27.0		
12			1.22 (t, 7.5)	11.1		
2-OH					13.20 (brs)	
4-OH					9.44 (brs)	
5-OH	12.83 (brs)		12.83 (brs)			
1′	5.24 (d,7.4)	99.4	5.25 (d,7.4)	99.8	5.02 (d, 6.8)	101.5
2′	3.28 (m)	72.8	3.28 (m)	73.2	3.47 (m)	74.6
3′	3.30 (m)	75.7	3.30 (m)	76.0	3.41 (m)	78.3
4′	3.38 (t, 9.2)	71.3	3.38 (t, 9.1)	71.7	3.40 (m)	71.1
5′	4.03 (d, 9.7)	75.3	4.02 (d, 9.6)	75.6	3.47 (m)	77.8
6′		170.2		170.6	3.99 (dd, 12.0, 1.8), 3.70 (dd, 12.0, 5.4)	62.3

Table S2 : The NMR data comparison between the new compound (**3**) and the known compounds (CAS No. 906081-66-1)

Position	**6**		**906081-66-1**	
	δ_H, (J in Hz)	δ_C	δ_H, (J in Hz)	δ_C
1		111.0		112.9
2		159.4		159.6
3		108.2		109.8
4		161.3		161.6
5		110.2		111.4
6		157.5		156.6
7		204.5		208.9
8	2.65 (s)	33.2	3.24 (ddd, 17.0, 8.7, 6.1) 3.61 (17.0, 8.7, 6.1)	46.4
9	2.08 (s)	8.9	1.66 (m) 1.73 (m)	14.1
10			0.81 (t, 7.5)	18.5
11			2.54 (s)	9.6
12				
2-OH	13.20 (brs)		13.20 (brs)	
4-OH	9.44 (brs)		9.44 (brs)	
5-OH				
1′	5.10 (d, 8.9)	75.7	5.79 (d, 9.8)	76.8
2′	3.53 (m)	71.0	4.51 (t, 9.8)	74.3
3′	3.26 (m)	77.9	4.36 (t, 9.2)	79.7
4′	3.33 (m)	69.2	4.49 (t, 9.4)	70.8
5′	3.30 (m)	80.8	4.06 (dt, 9.7, 2.9)	82.7
6′	3.61 (m), 3.64 (brd, 11.1)	59.9	4.45 (dd, 11.8, 2.2), 4.48 (dd, 11.8, 3.2)	61.5
1″	4.69 (d, 7.7)	104.5	5.22 (d, 7.4)	105.9
2″	3.31 (m)	73.8	4.31 (dd, 8.0, 7.4)	75.8
3″	3.21 (t, 8.8)	76.2	4.30 (t, 8.0)	78.3
4″	3.17 (t, 9.1)	69.7	4.25 (t, 8.3)	71.8
5″	2.99 (m)	76.5	3.88 (ddd, 9.3, 5.7, 2.8)	78.5
6″	3.46 (m), 3.60 (m)	61.0	4.26 (dd, 11.4, 5.3), 4.37 (dd, 11.4, 2.8)	62.7