Electronic Supplementary Material (ESI) for RSC Advances.

Adamantyl derivatives and rearranged benzophenones from *Garcinia xanthochymus* fruits

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‡ These authors contributed equally to this work.

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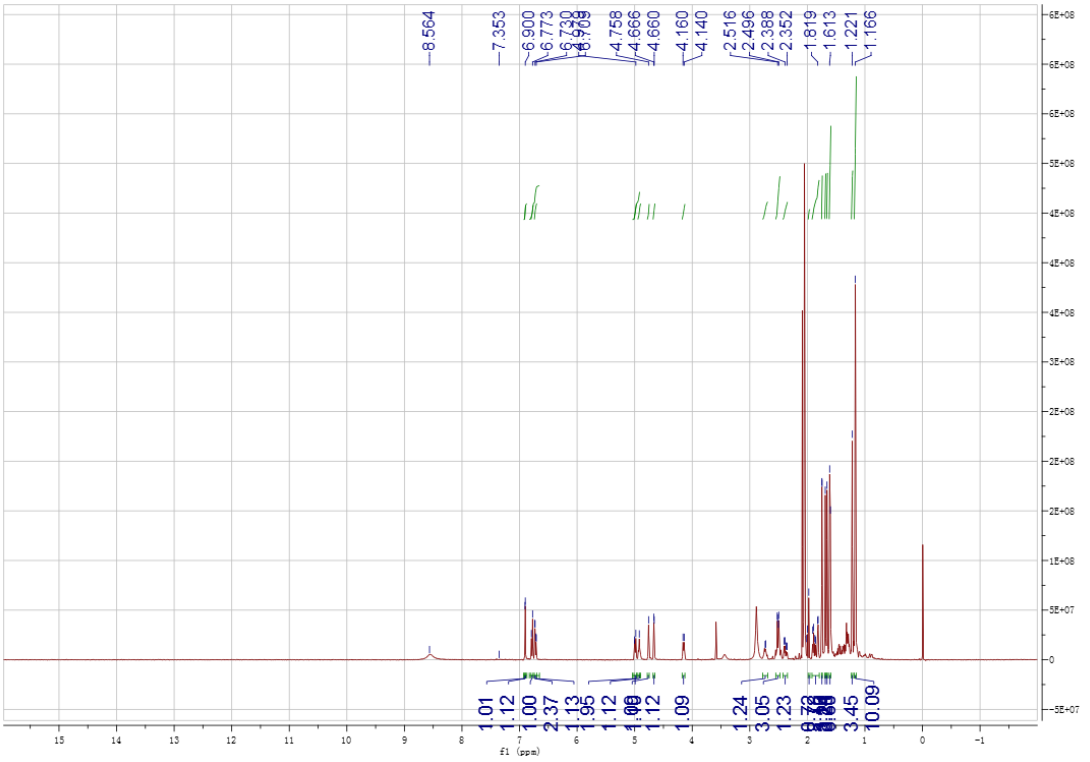
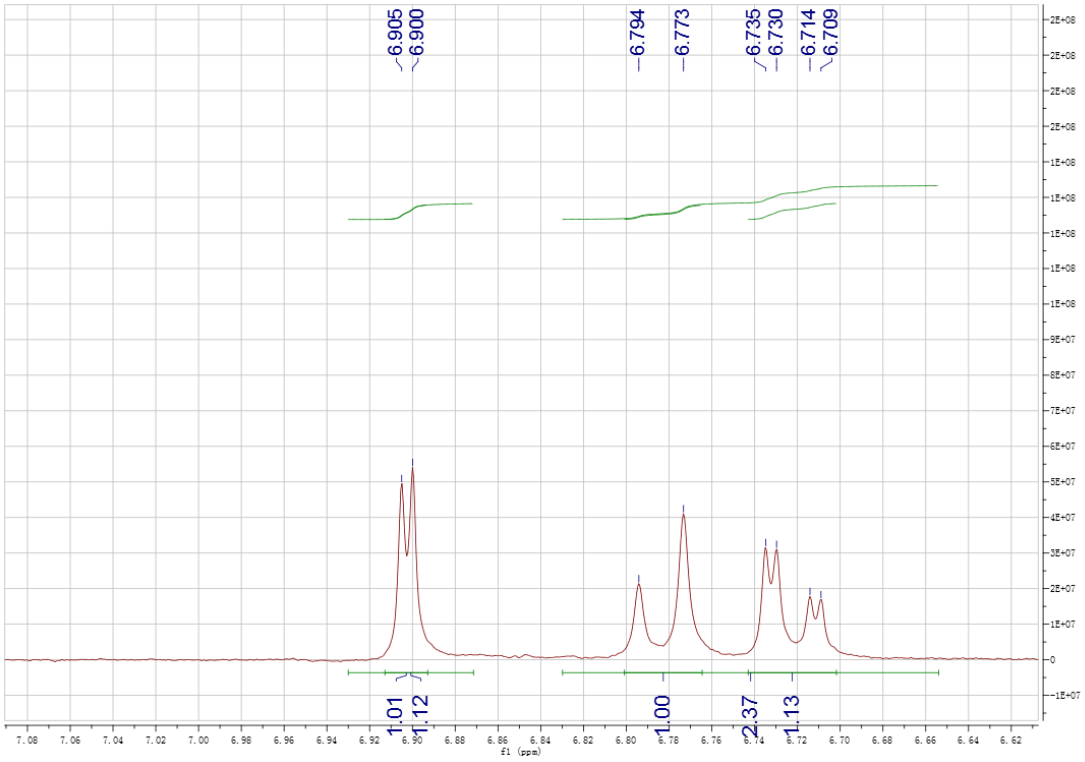
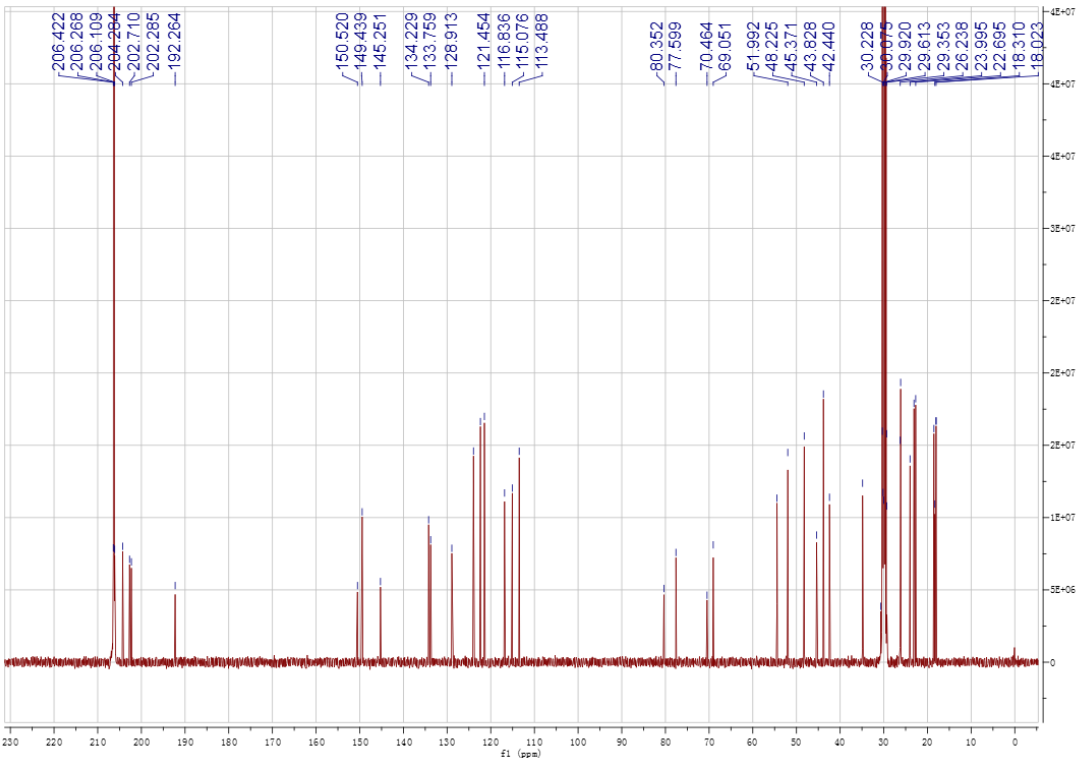
Electronic Supplementary Information



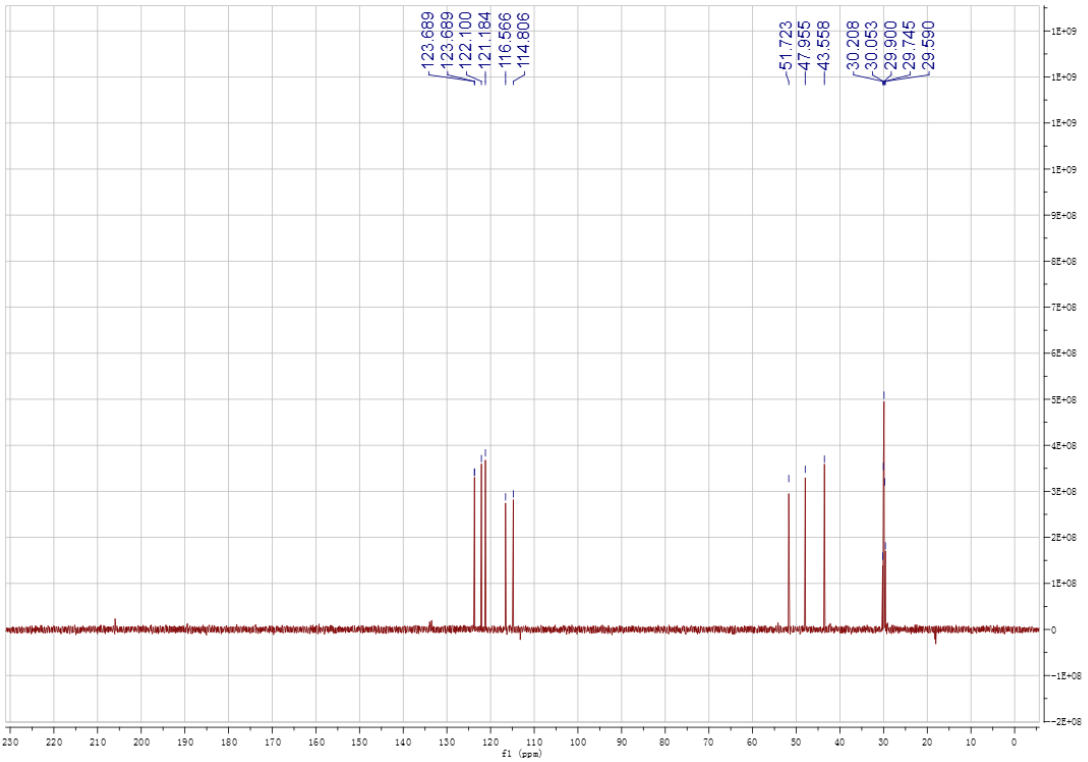
^{1}H-NMR spectrum of compound **1**



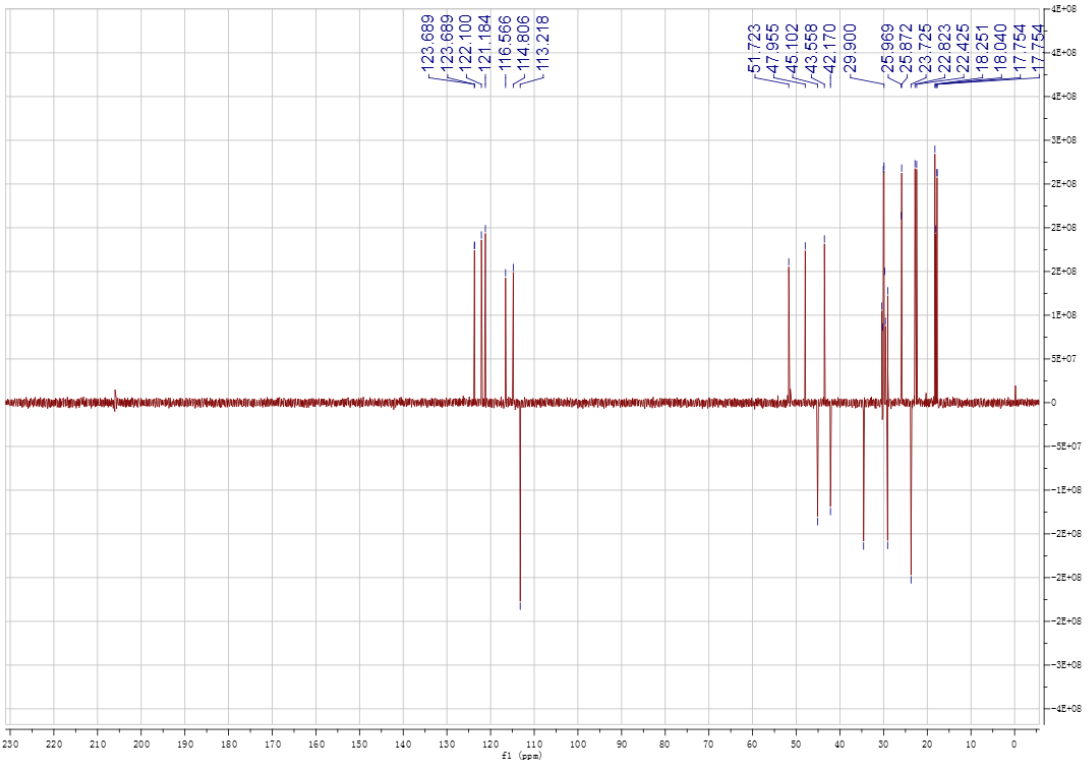
^{1}H-NMR spectrum of compound **1**(expanded region to confirm the 1,3,4-trisubstituted benzene system.)



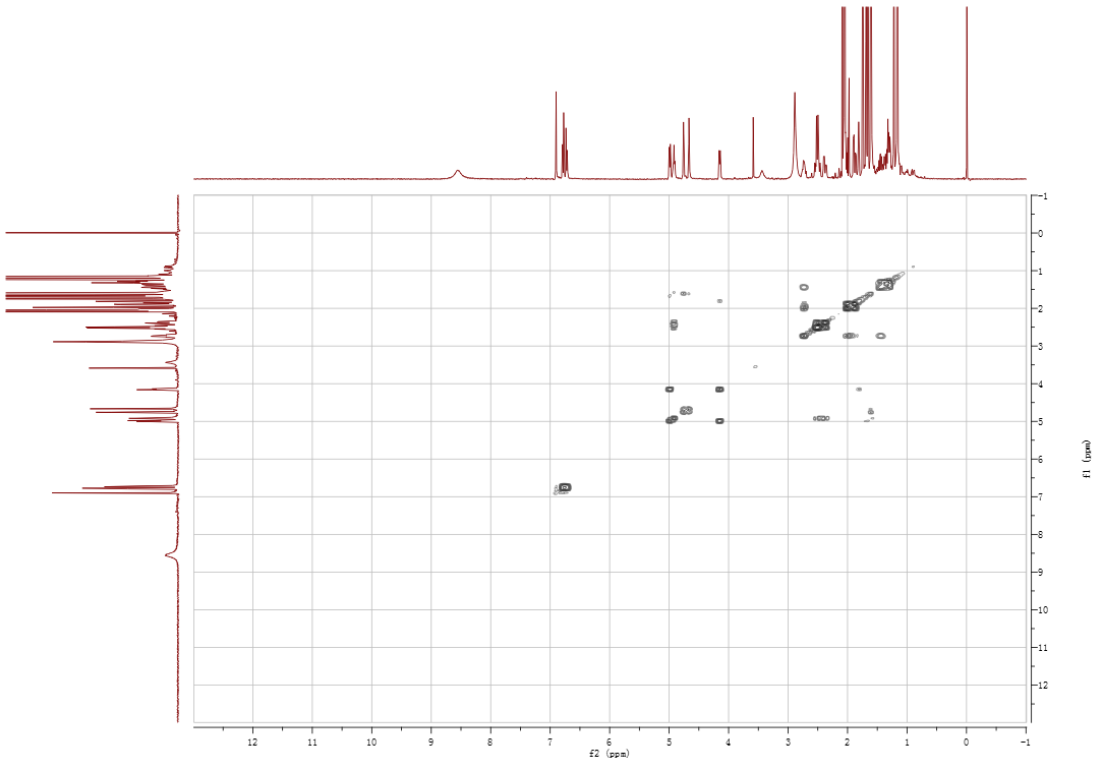
^{13}C-NMR spectrum of compound **1**



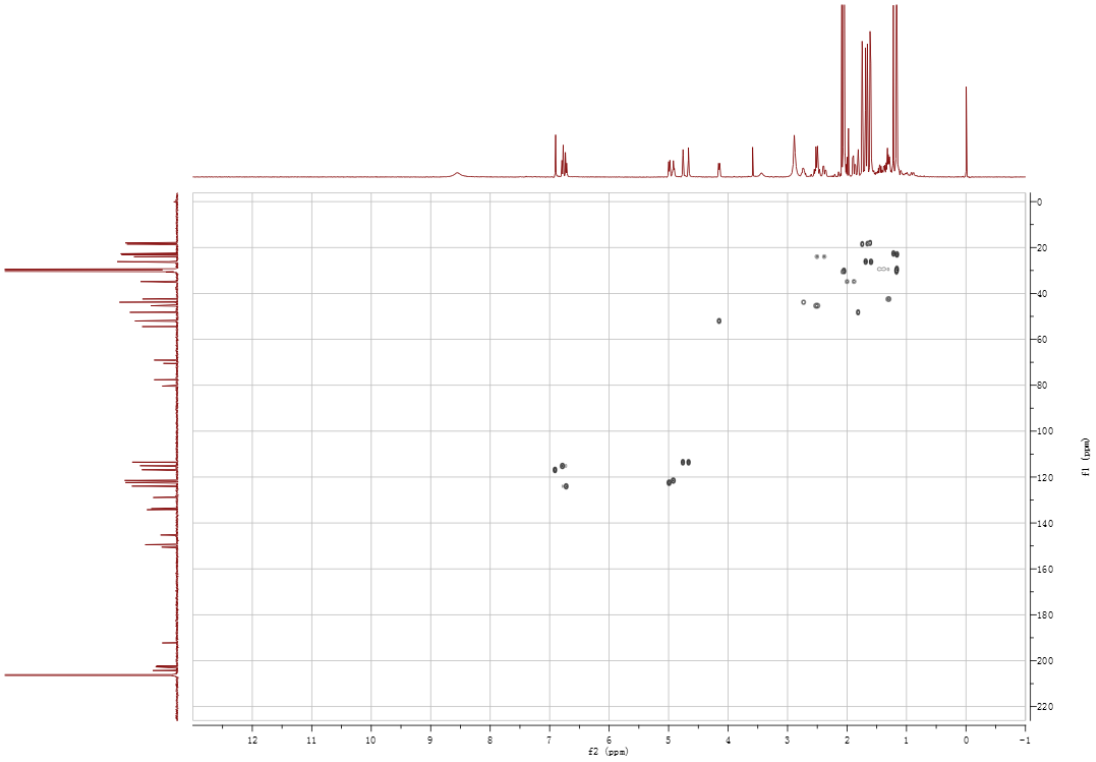
DEPT spectrum of compound **1**



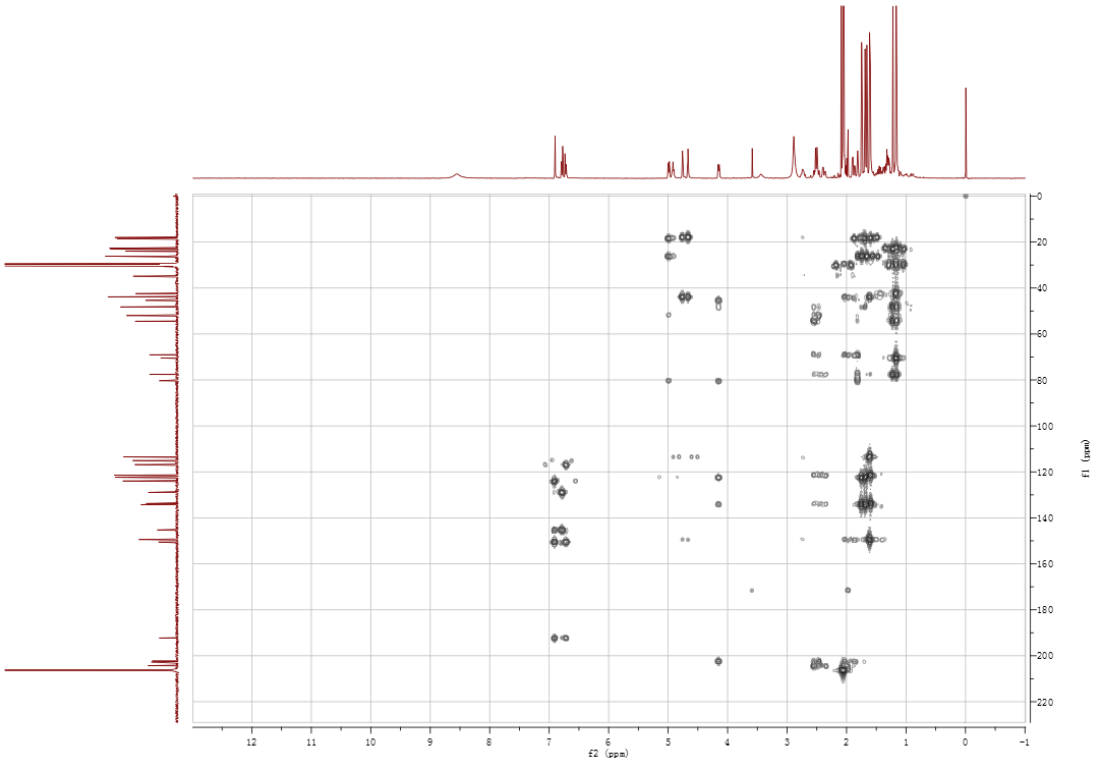
DEPT spectrum of compound **1**



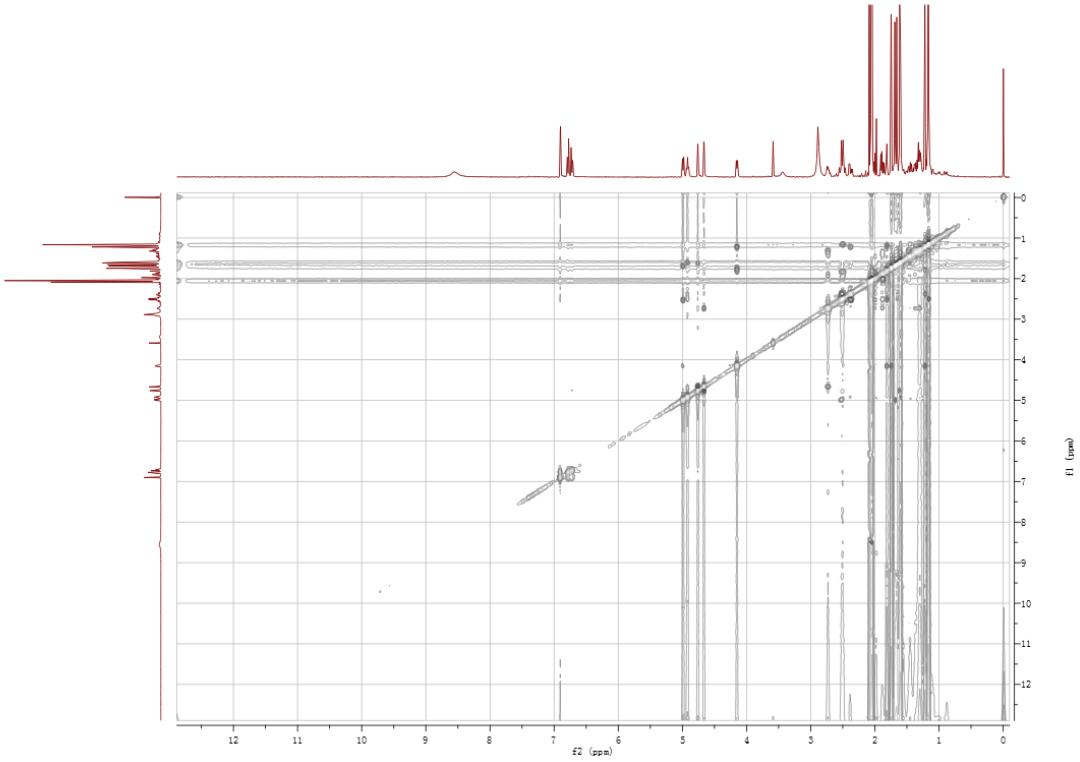
^{1}H-^{1}HCOSY spectrum of compound **1**



HSQC spectrum of compound **1**



HMBC spectrum of compound **1**



ROESY spectrum of compound **1**

Elemental Composition Report **Page 1**

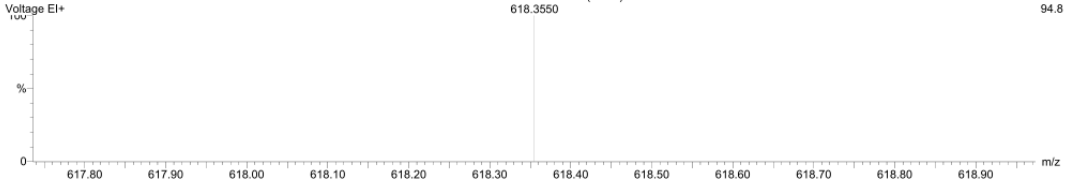
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
74 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 O: 6-15

gf-41
12:26:17 02-Dec-2015
Voltage EI+

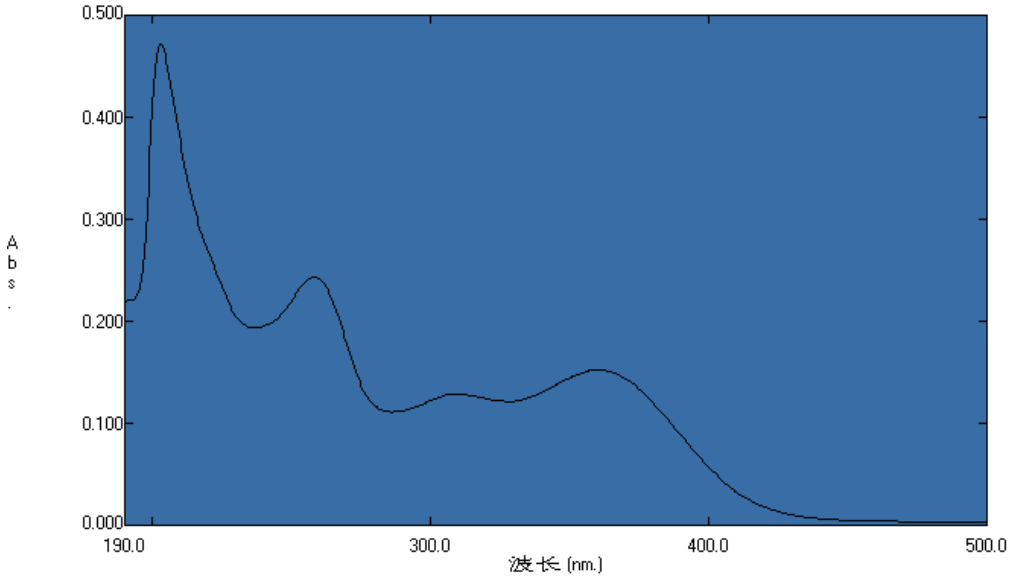
KIB
M151202EA-01AFAMM 19 (1.744)
618.3550

Autospec Premier
P776
94.8

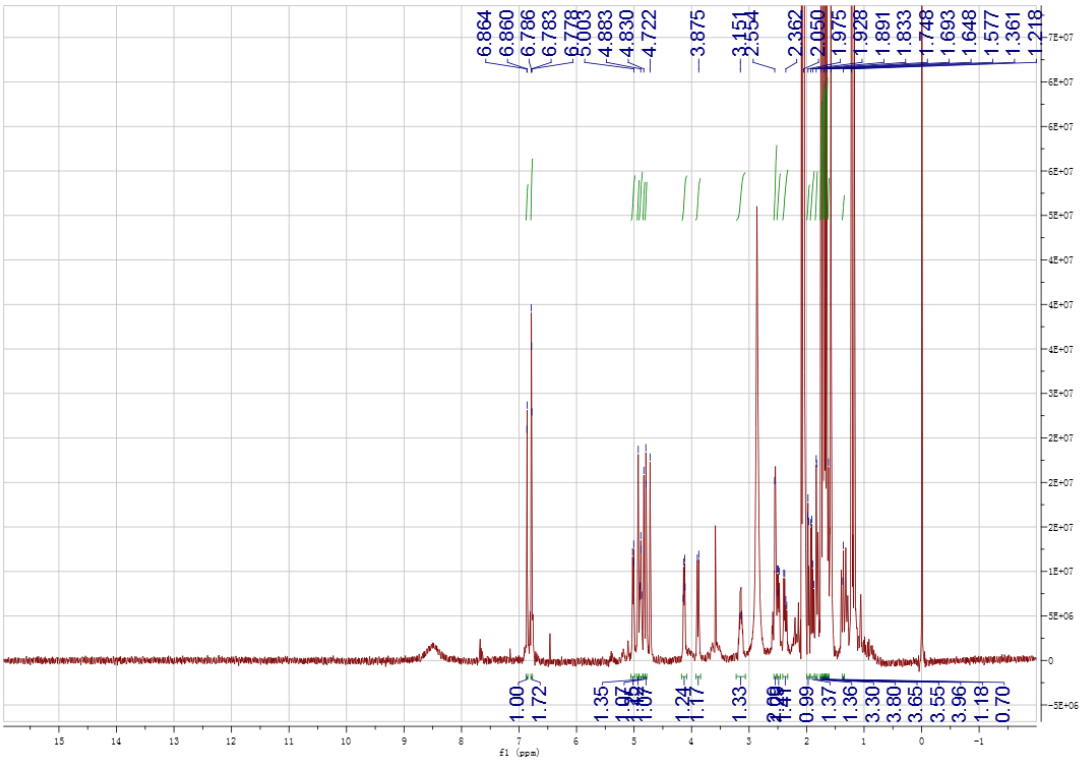


Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
618.3550	618.3557	-0.7	-1.1	14.0	5546067.5	C38 H50 O7

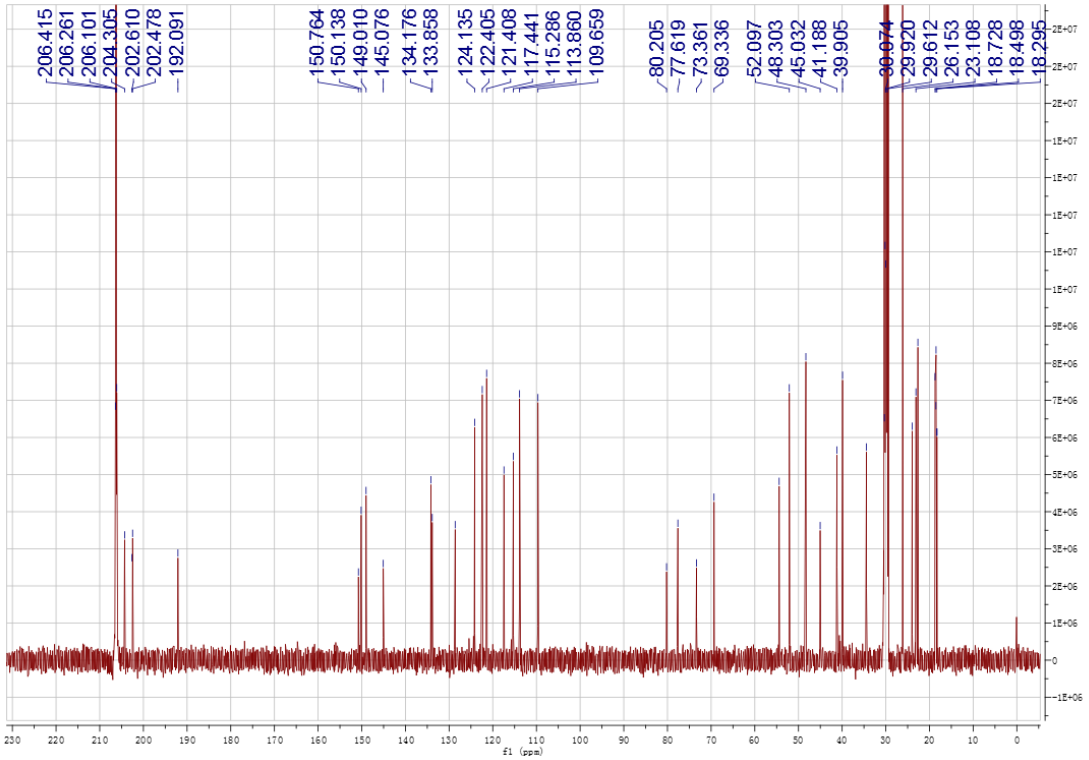
HR-EI-MS spectrum of compound **1**



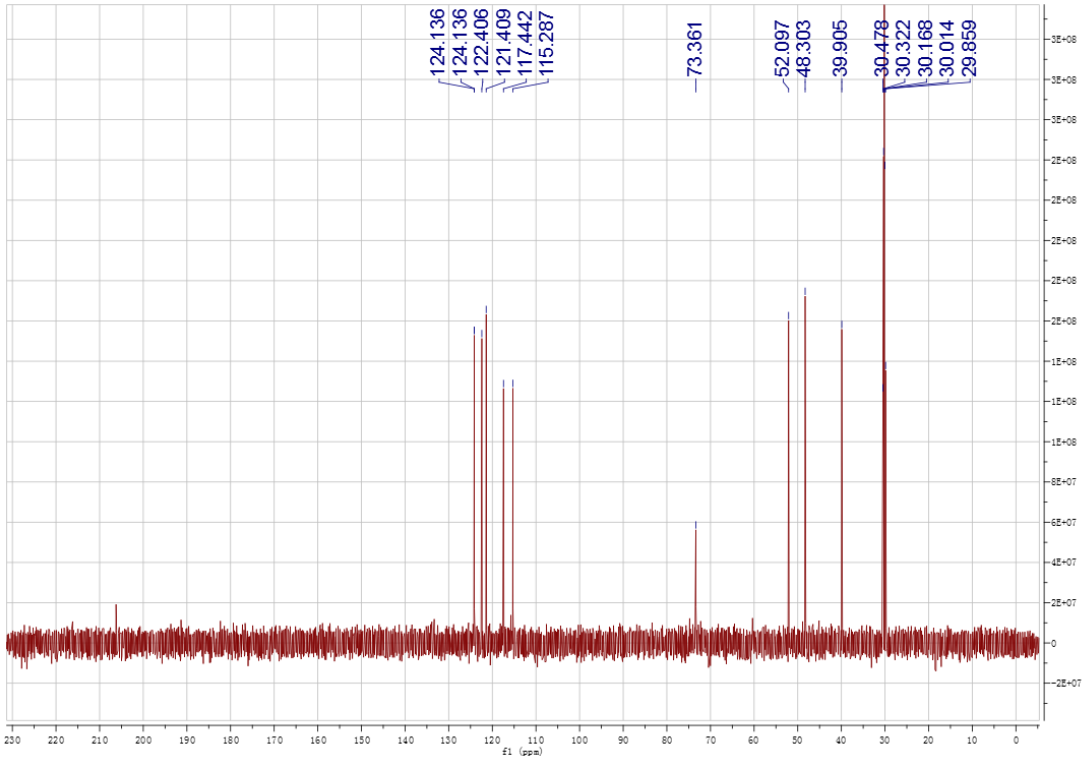
UV spectrum of compound **1**



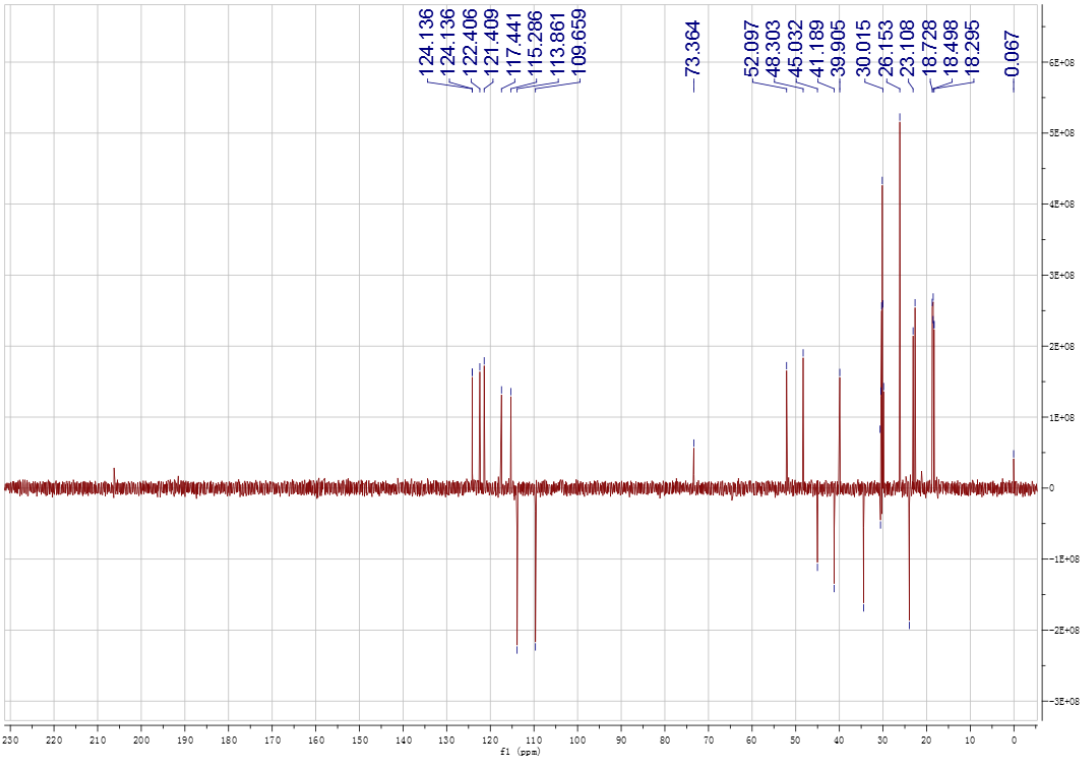
^{1}H-NMR spectrum of compound **2**



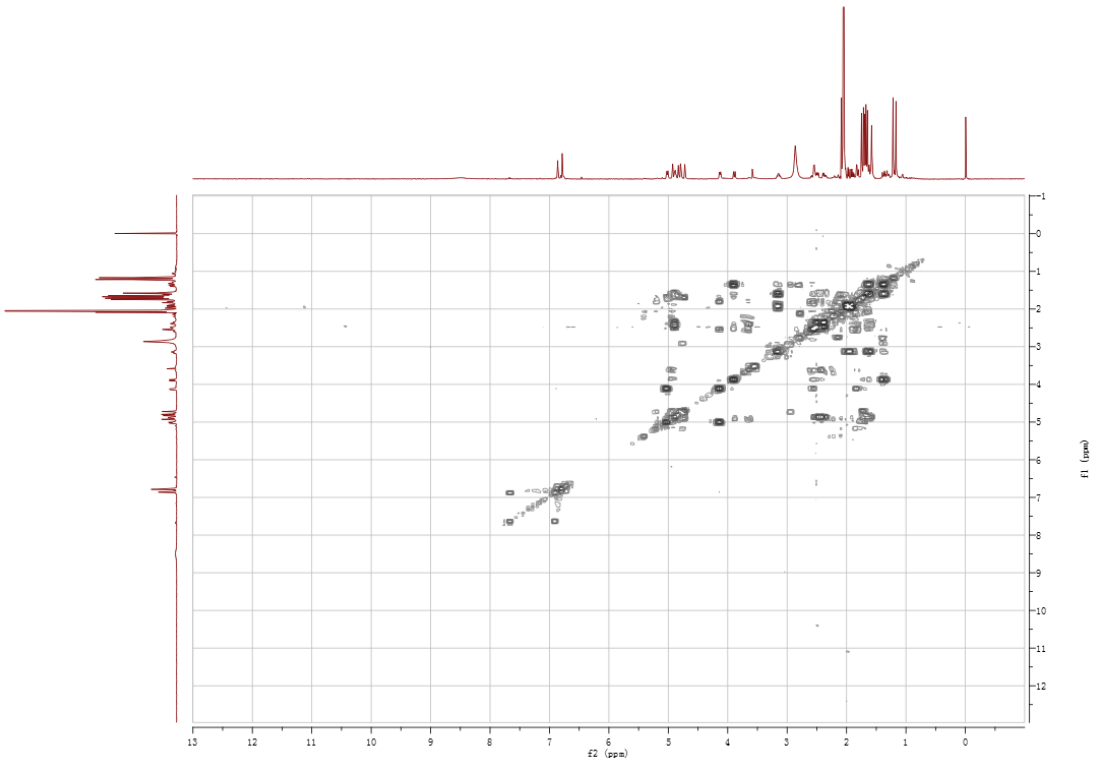
^{13}C-NMR spectrum of compound **2**



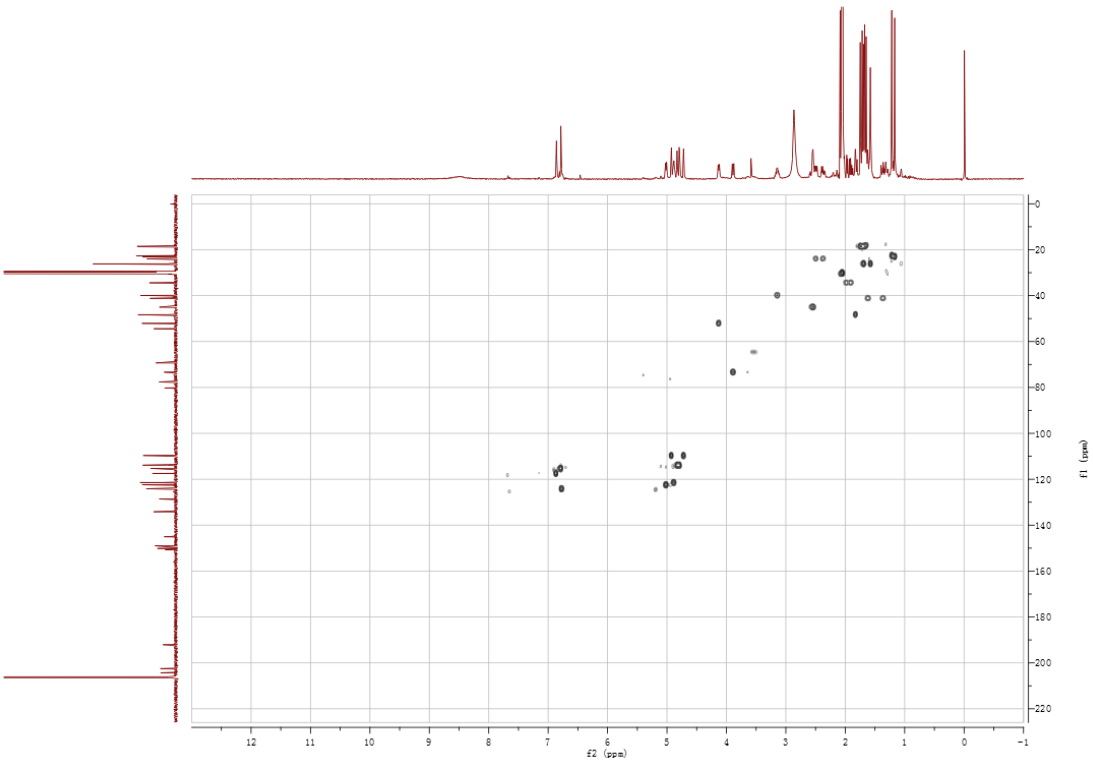
DEPT spectrum of compound **2**



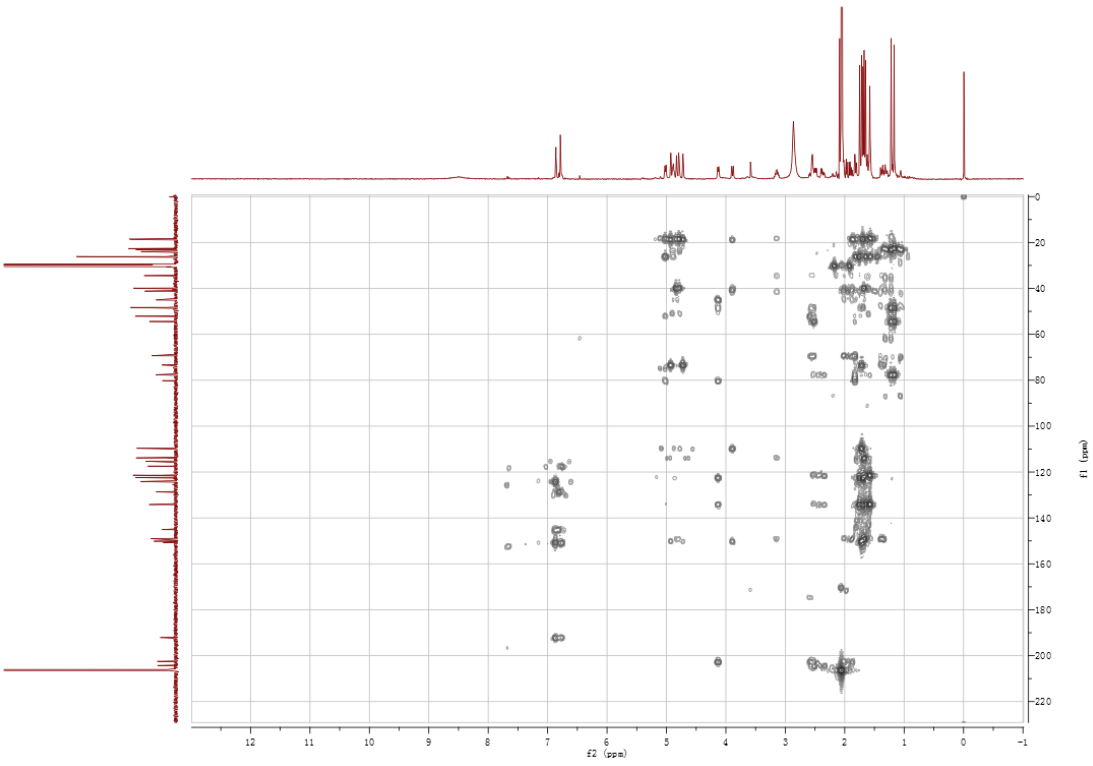
DEPT spectrum of compound **2**



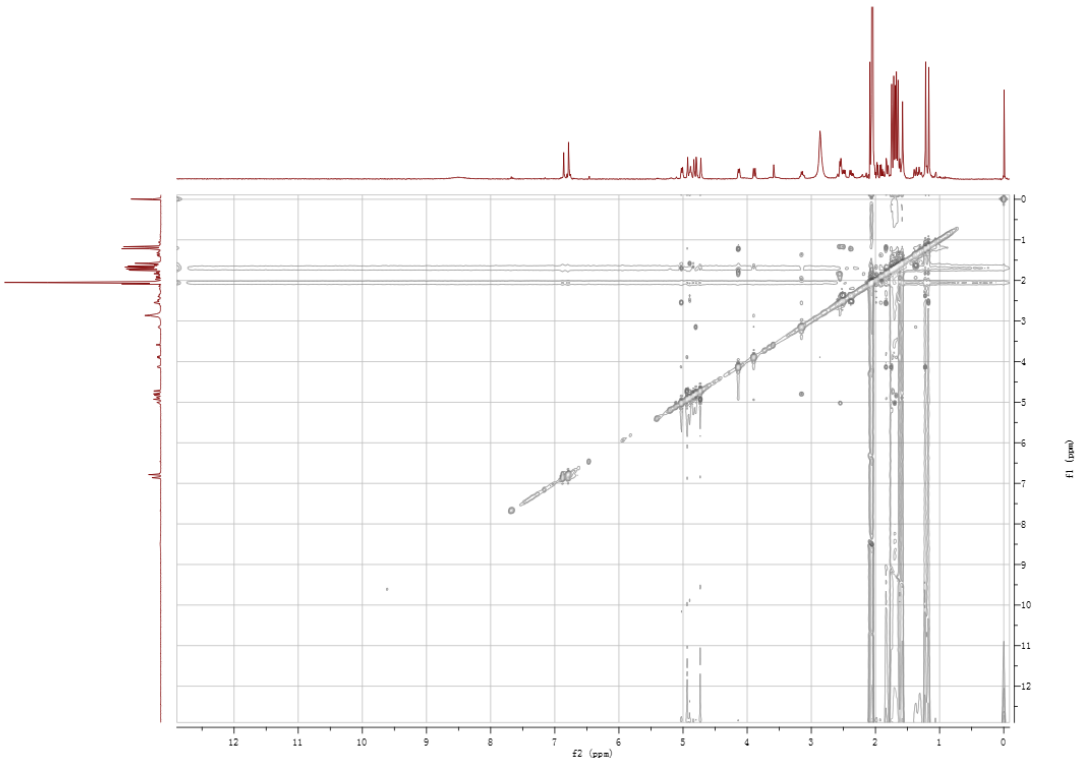
^{1}H-^{1}HCOSY spectrum of compound **2**



HSQC spectrum of compound **2**



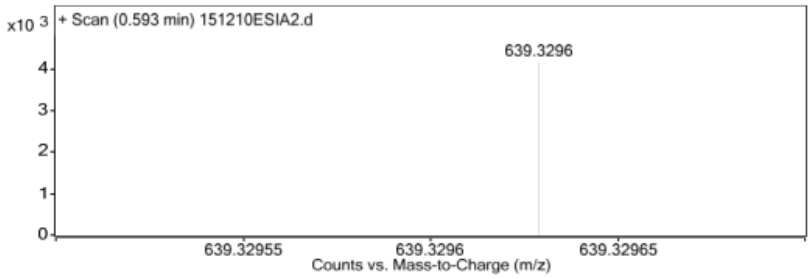
HMBC spectrum of compound **2**



ROESY spectrum of compound **2**

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
274.274	1	2135.6		
639.3296	1	4180.78	C38 H48 Na O7	M+
640.3328	1	1630.64	C38 H48 Na O7	M+
655.3097	1	1284.74		
922.0098	1	1322.09		
1255.6703		5355.09		
1256.6753	1	4333.14		
1257.6784	1	2740.9		
1271.6492		2339.48		
1272.6541	1	1705.43		

Formula Calculator Element Limits

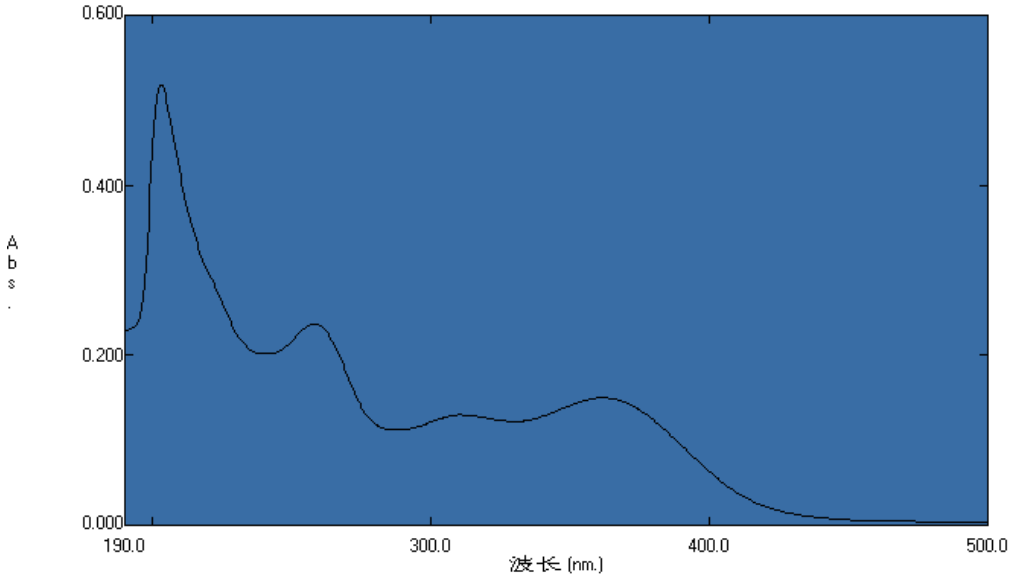
Element	Min	Max
C	0	200
H	0	400
O	0	10
Na	1	1

Formula Calculator Results

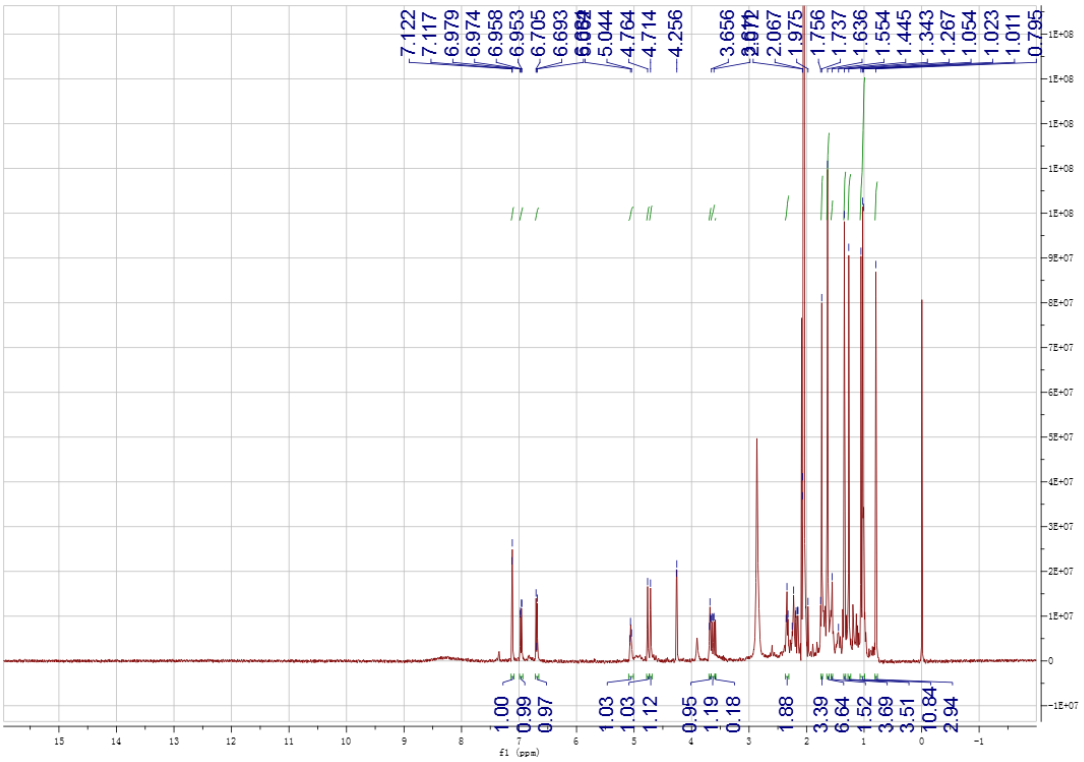
Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C38 H48 Na O7	639.3298	639.3292	639.3296	-0.8	-1.2	14.5000

--- End Of Report ---

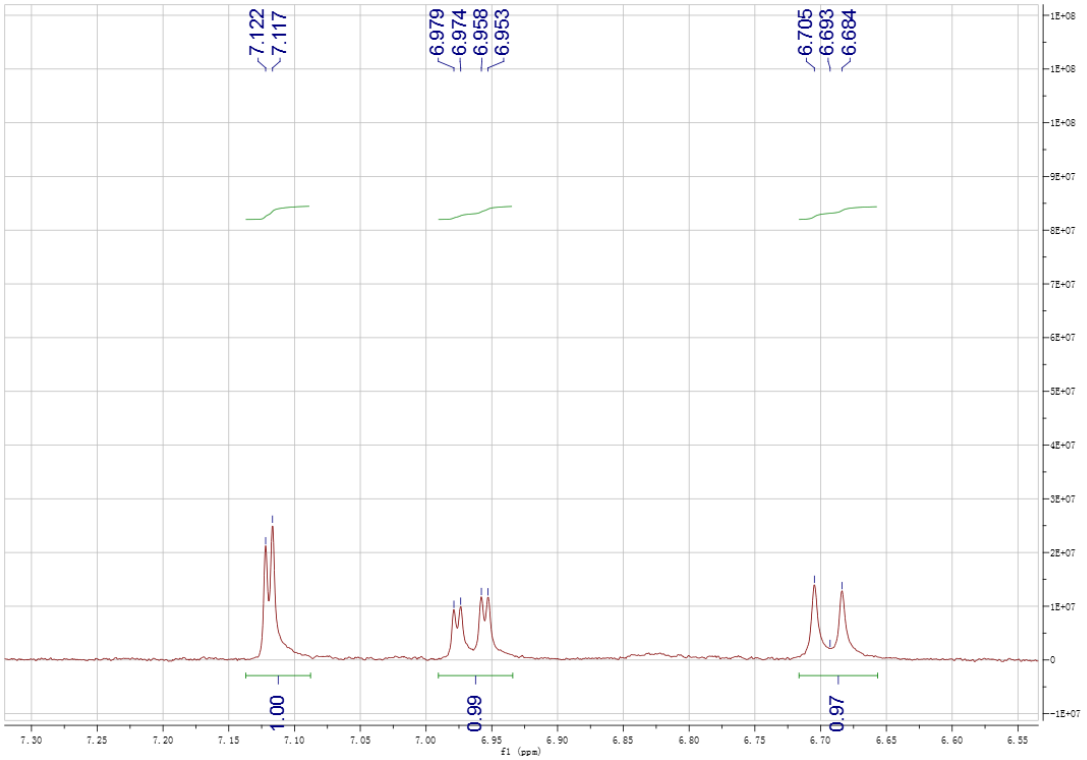
HR-ESI-MS spectrum of compound **2**



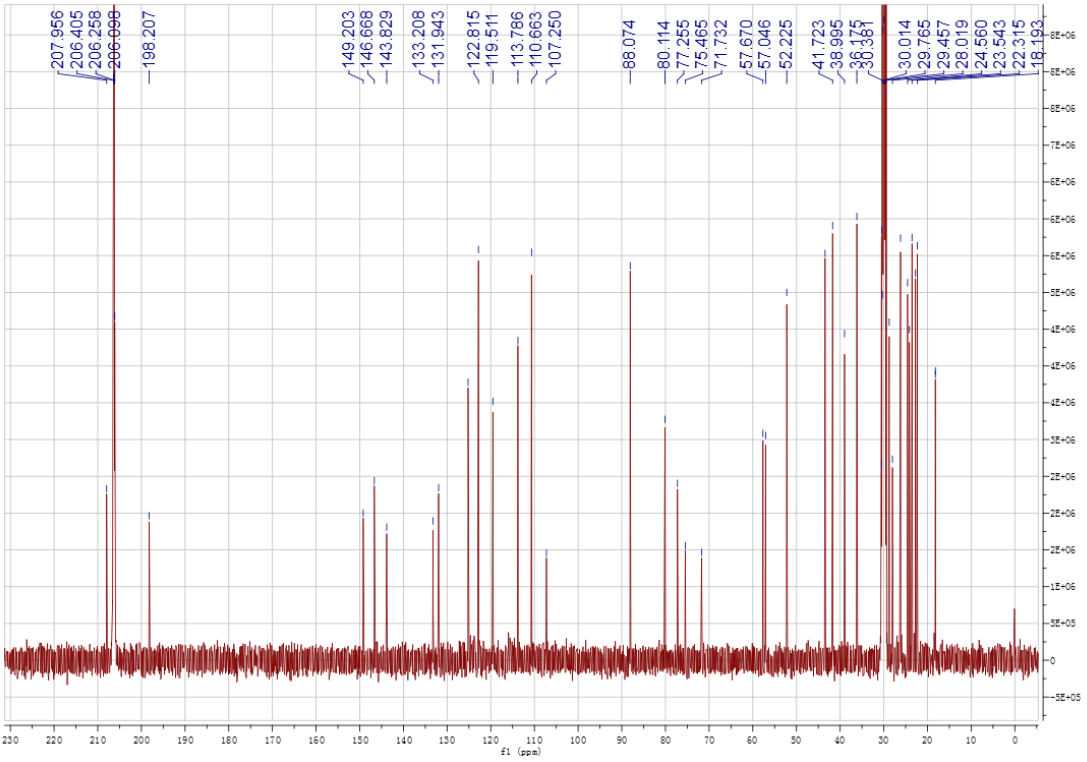
UV spectrum of compound **2**



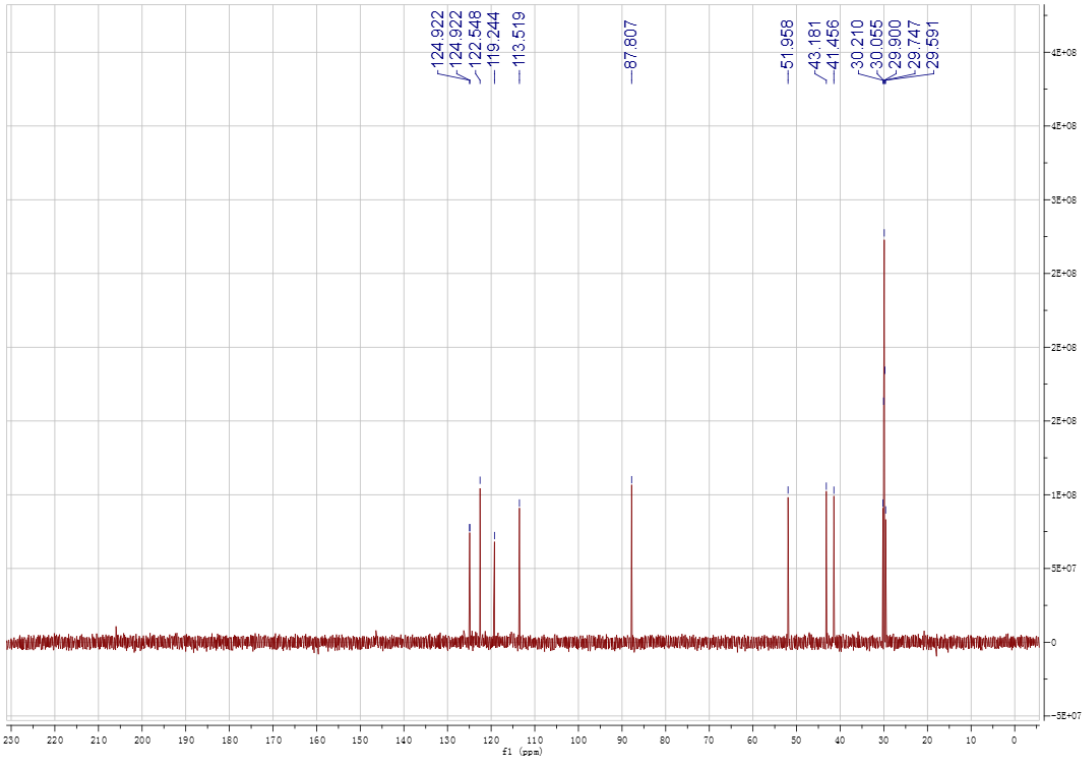
[1]H-NMR spectrum of compound **3**



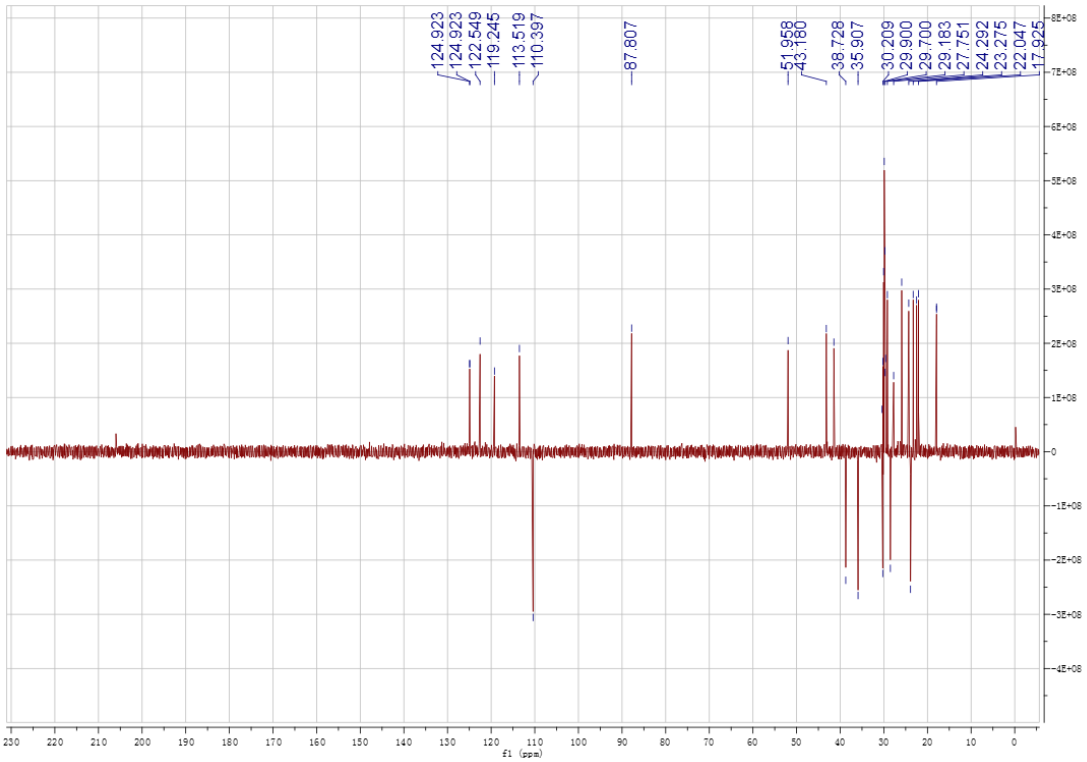
^{1}H-NMR spectrum of compound **3**(expanded region to confirm the 1,3,4-trisubstituted benzene system.)



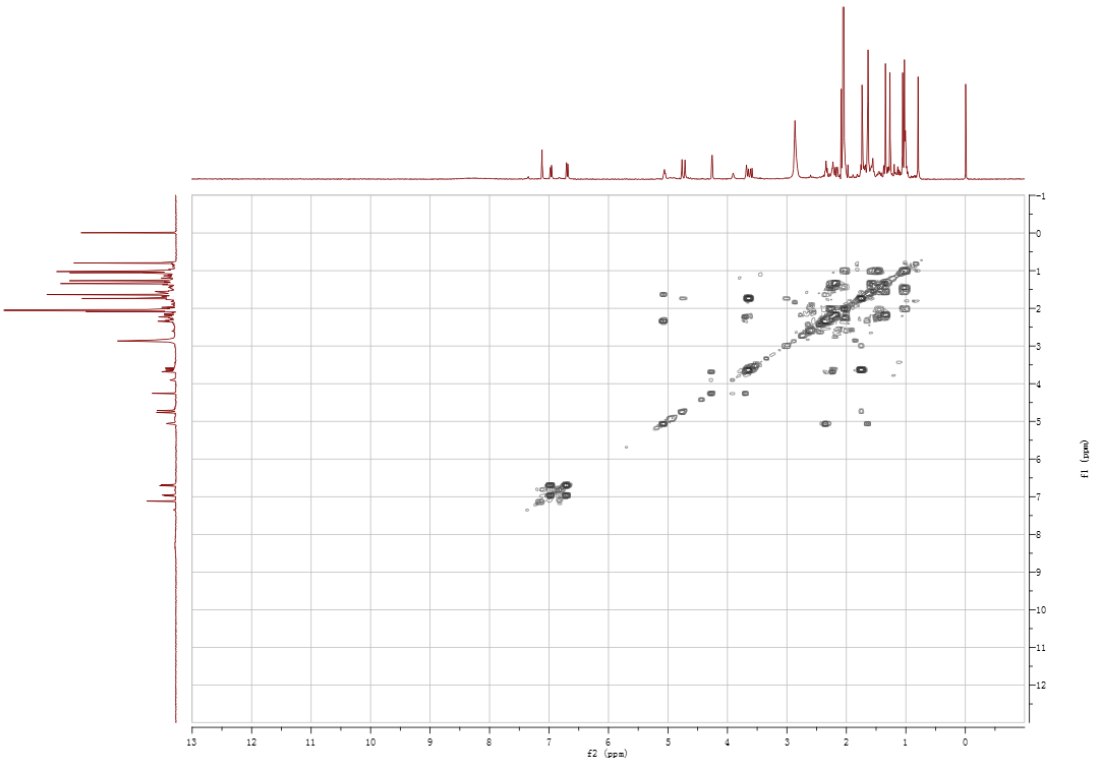
^{13}C-NMR spectrum of compound **3**



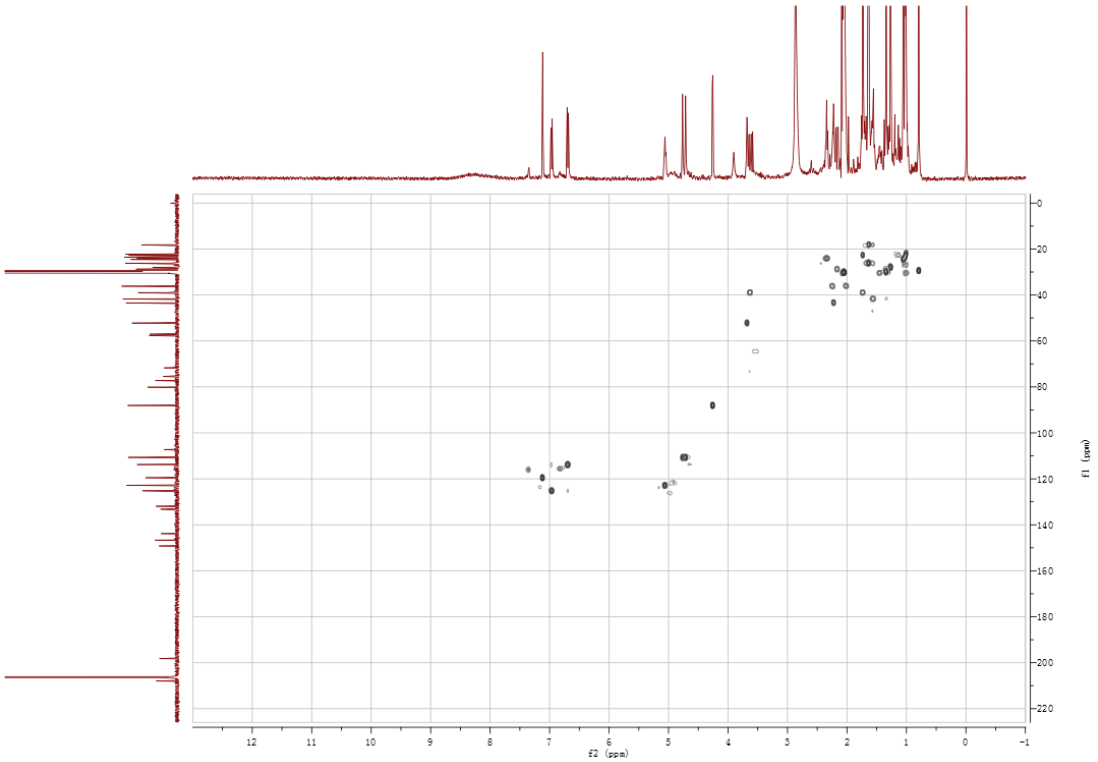
DEPT spectrum of compound **3**



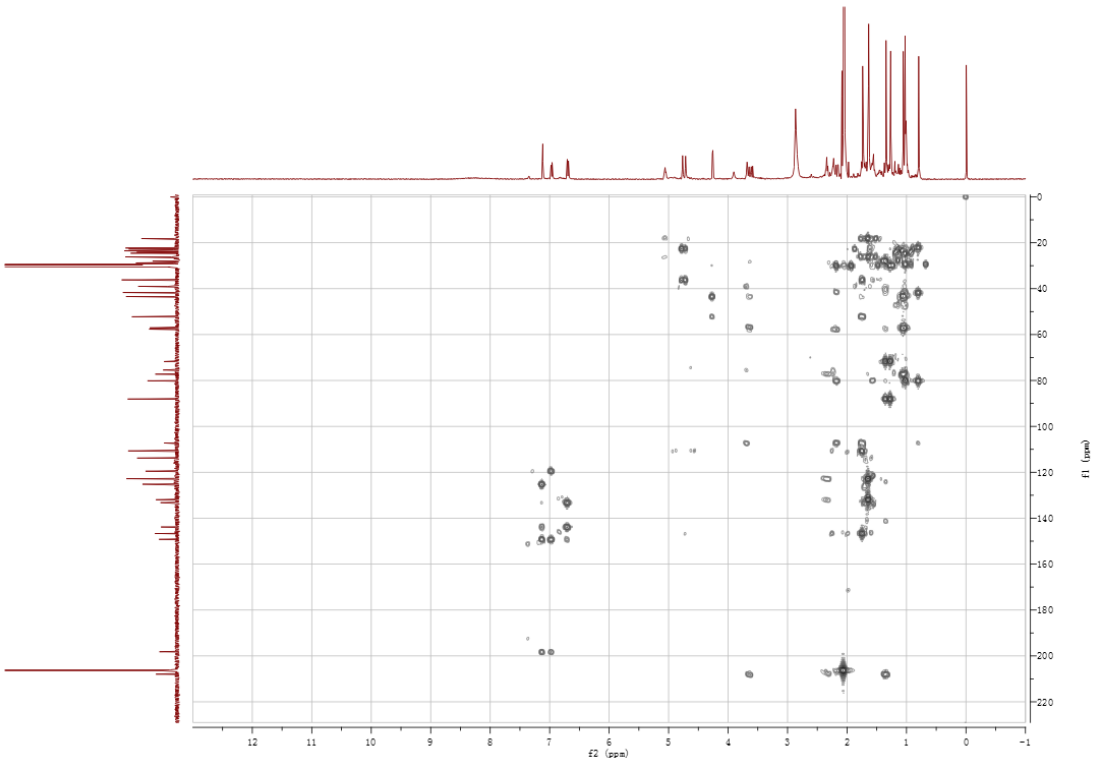
DEPT spectrum of compound **3**



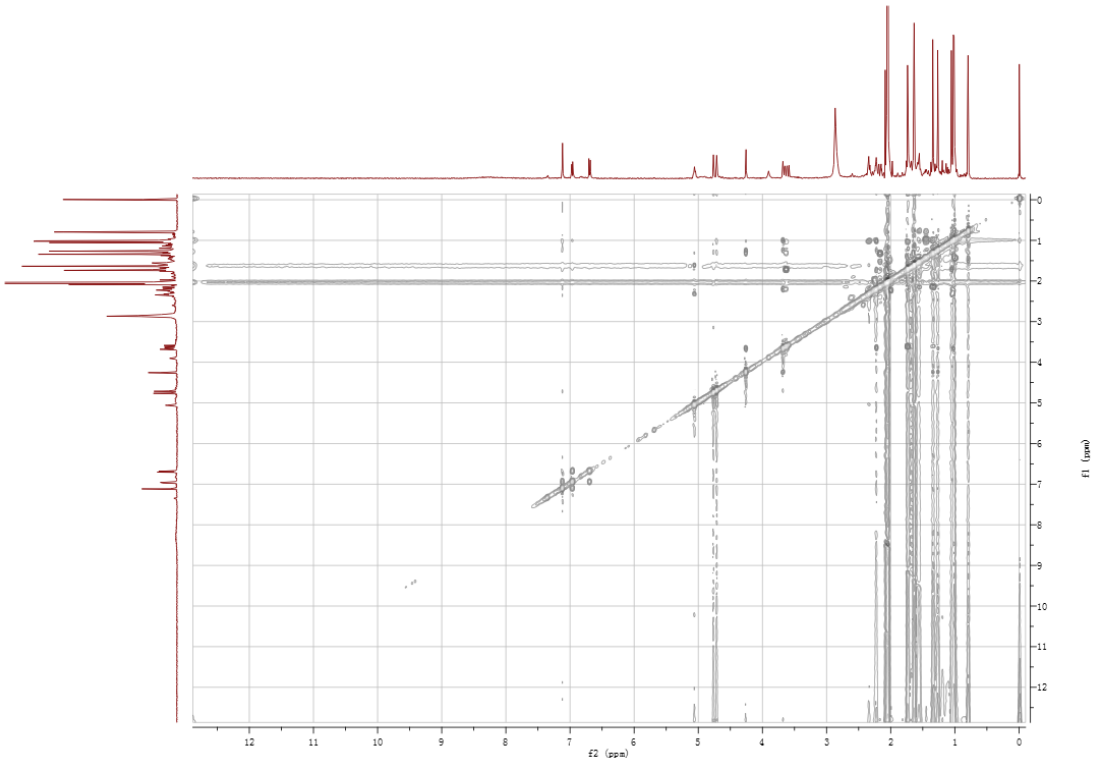
^{1}H-^{1}HCOSY spectrum of compound **3**



HSQC spectrum of compound **3**



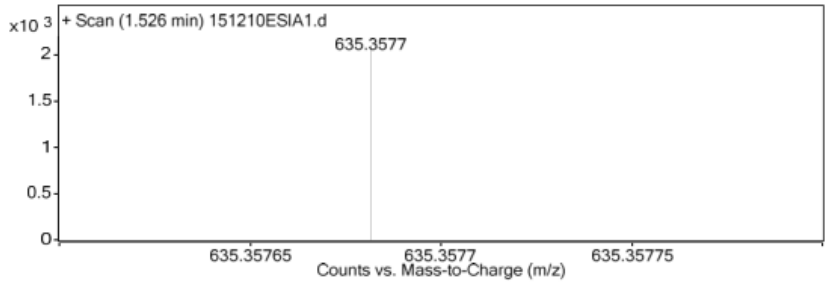
HMBC spectrum of compound **3**



ROESY spectrum of compound **3**

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
121.0509	1	5899.1		
218.0718		854.92		
232.1116	1	2360.25		
587.336	1	804.4		
635.3577	1	2097.88	C38 H51 O8	M+
636.3615	1	965.81	C38 H51 O8	M+
657.3394	1	725.14		
665.4035	1	685.57		
922.0098	1	4328.78		
923.01	1	759.95		

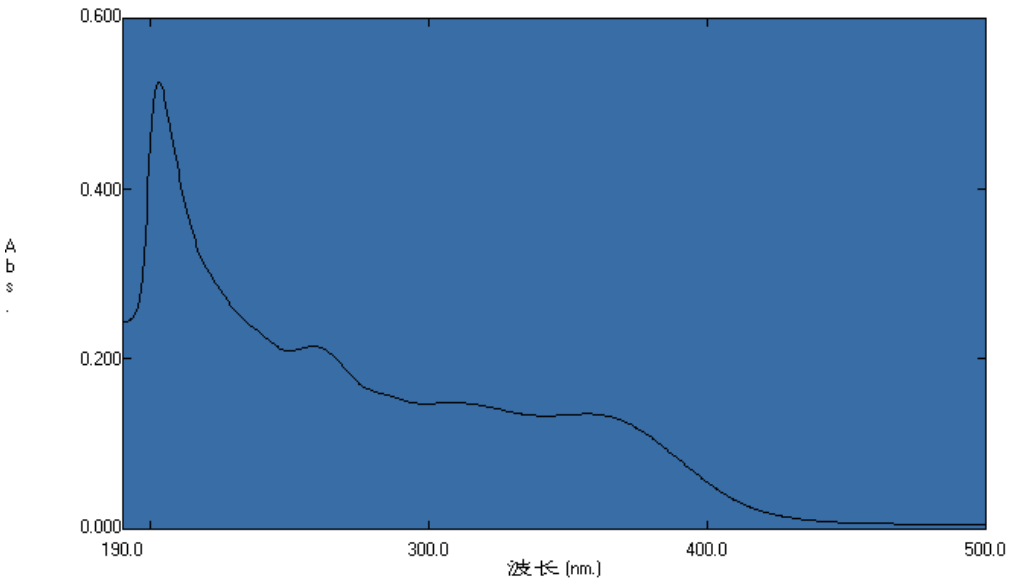
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	10

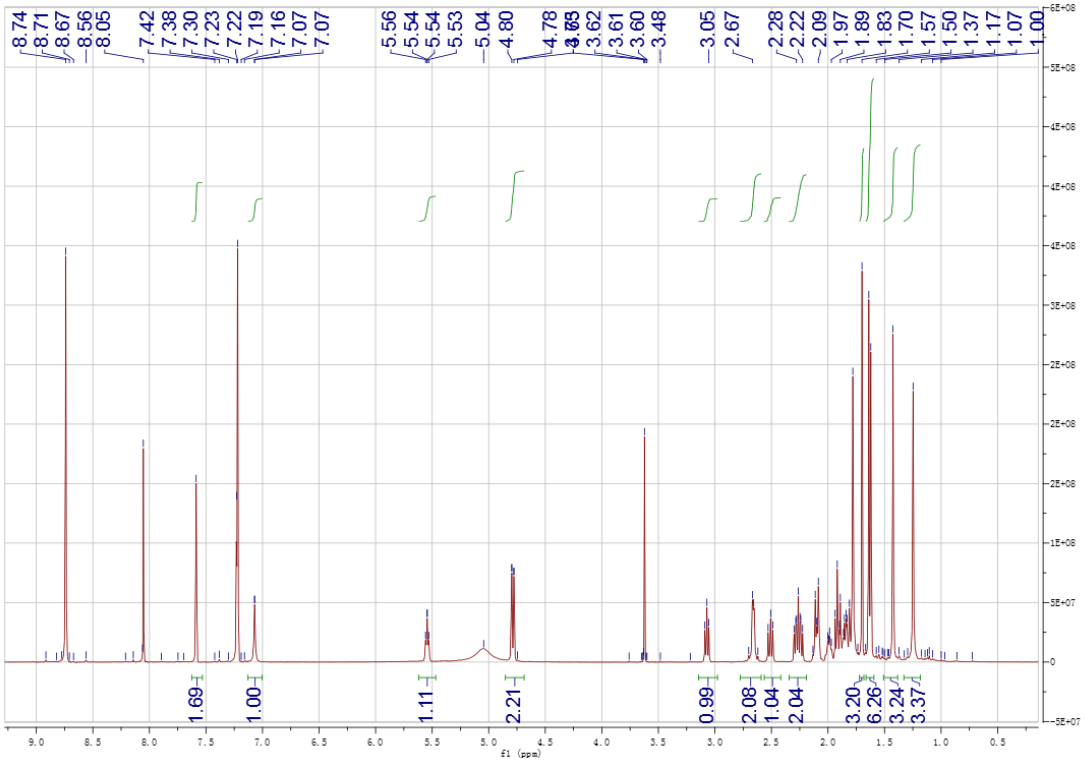
Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C38 H51 O8	635.3584	635.3578	635.3577	-0.2	-0.2	13.5000

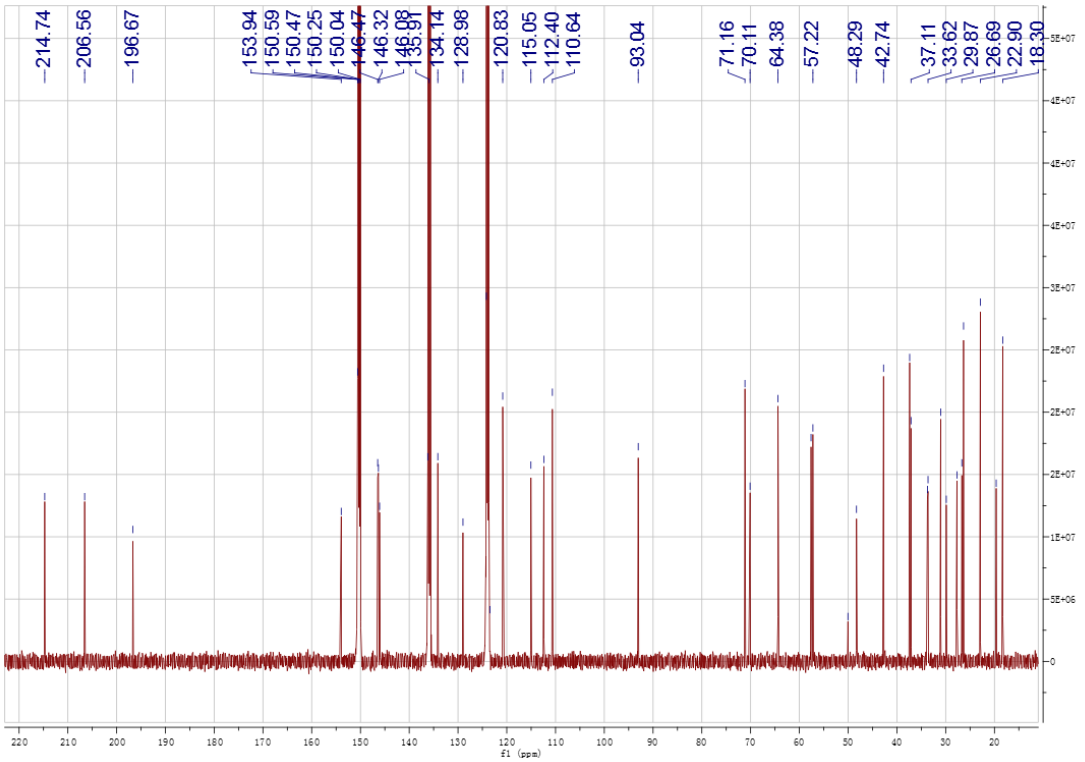
HR-ESI-MS spectrum of compound **3**



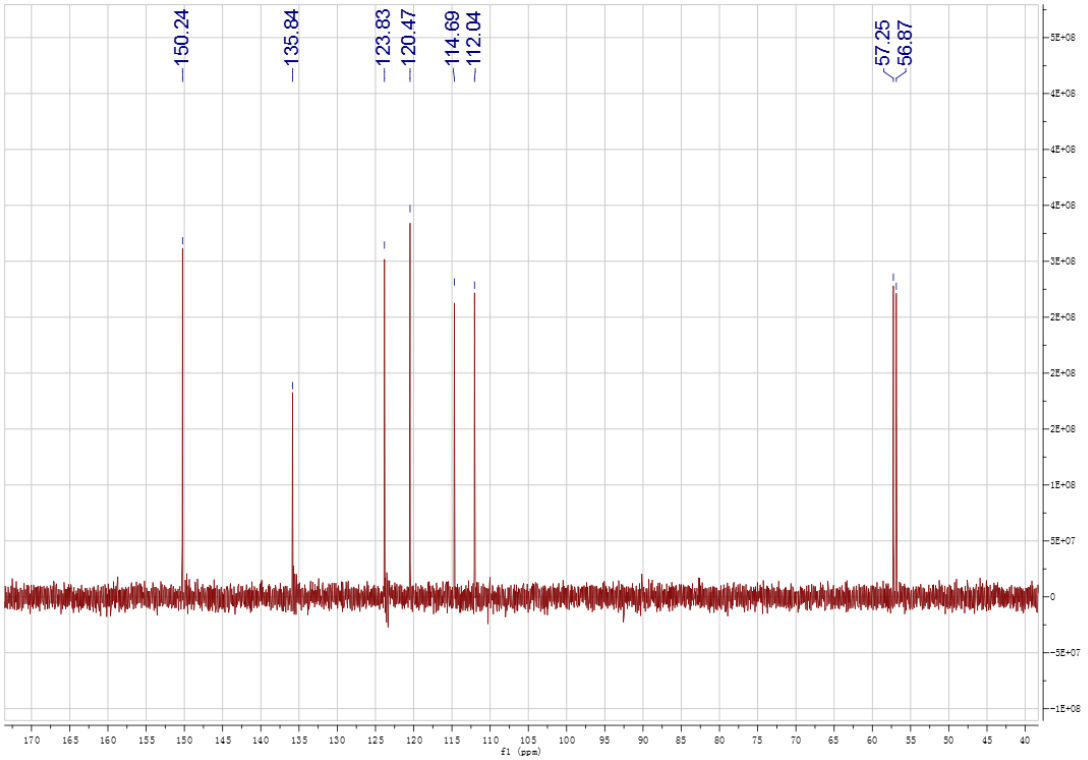
UV spectrum of compound **3**



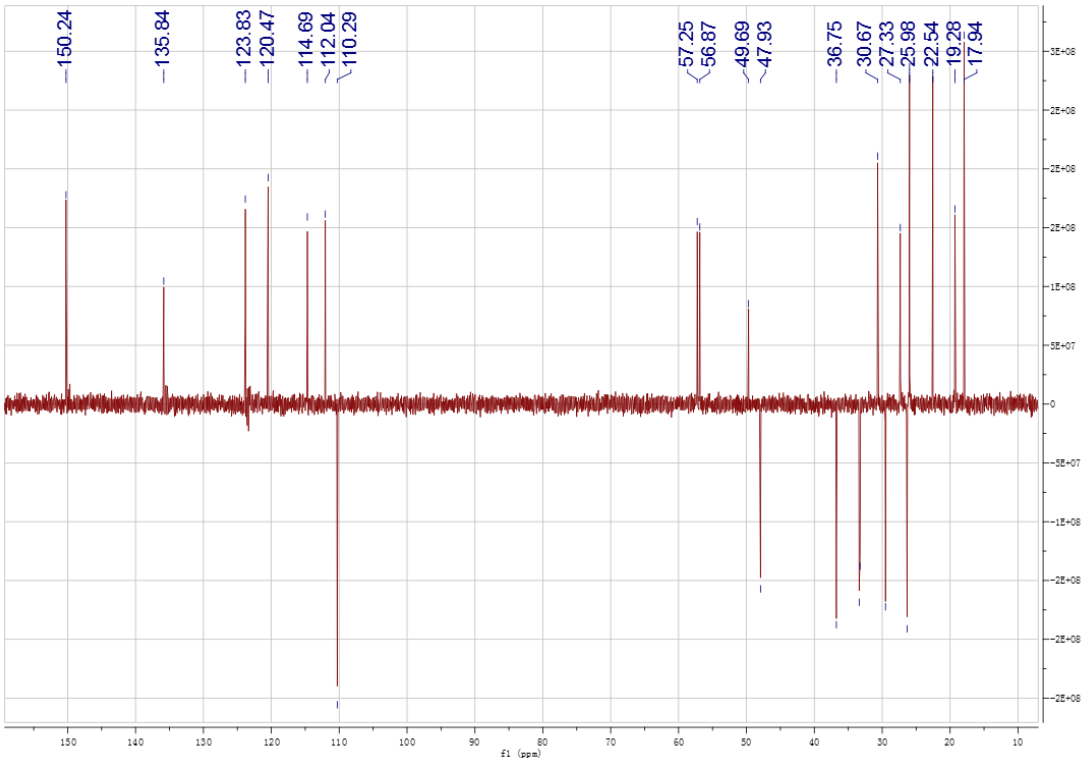
^{1}H-NMR spectrum of compound **4** in CD_5N_5



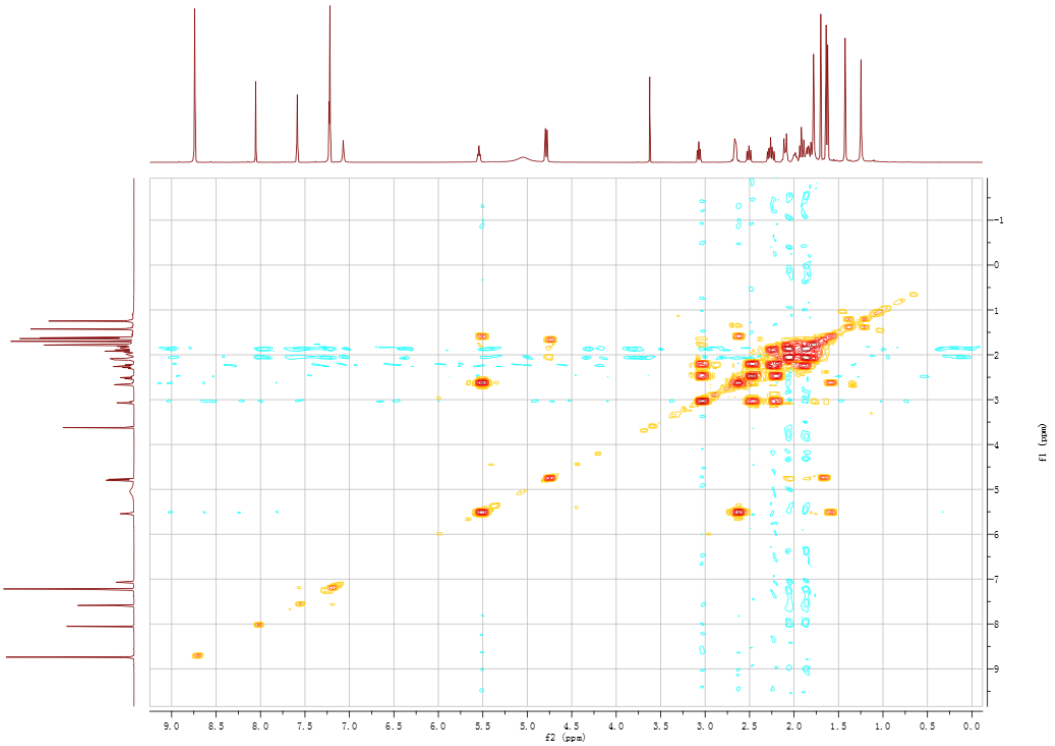
^{13}C-NMR spectrum of compound **4** in CD_5N_5



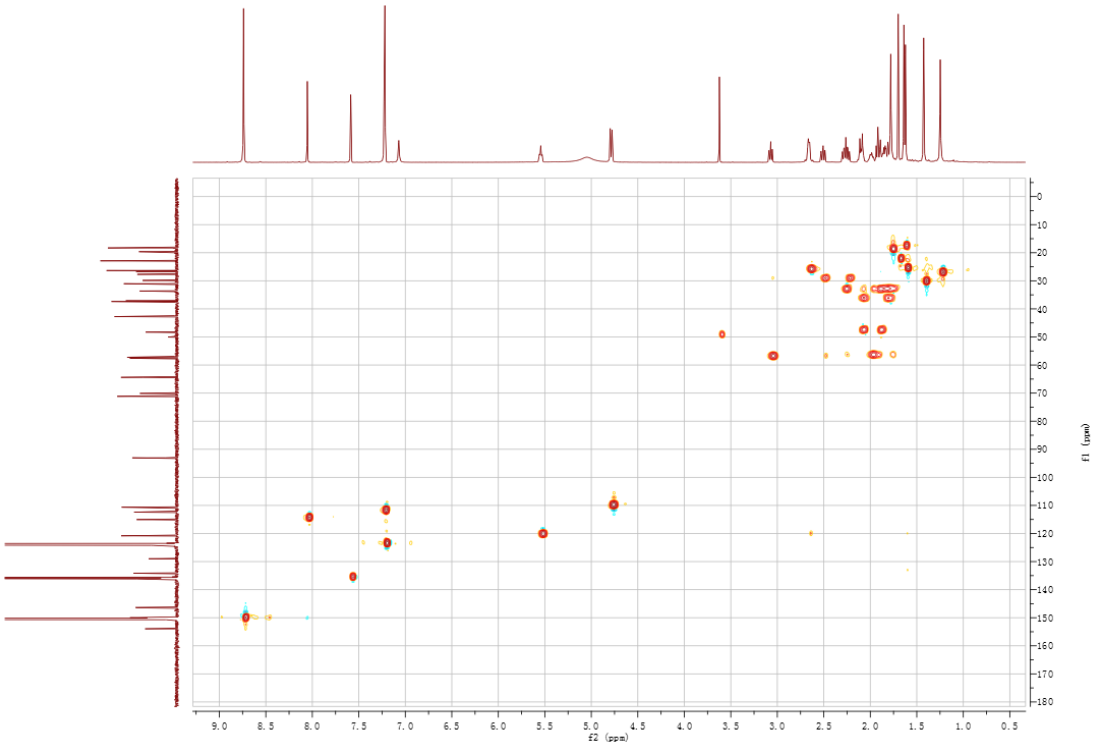
DEPT spectrum of compound **4** in CD_5N_5



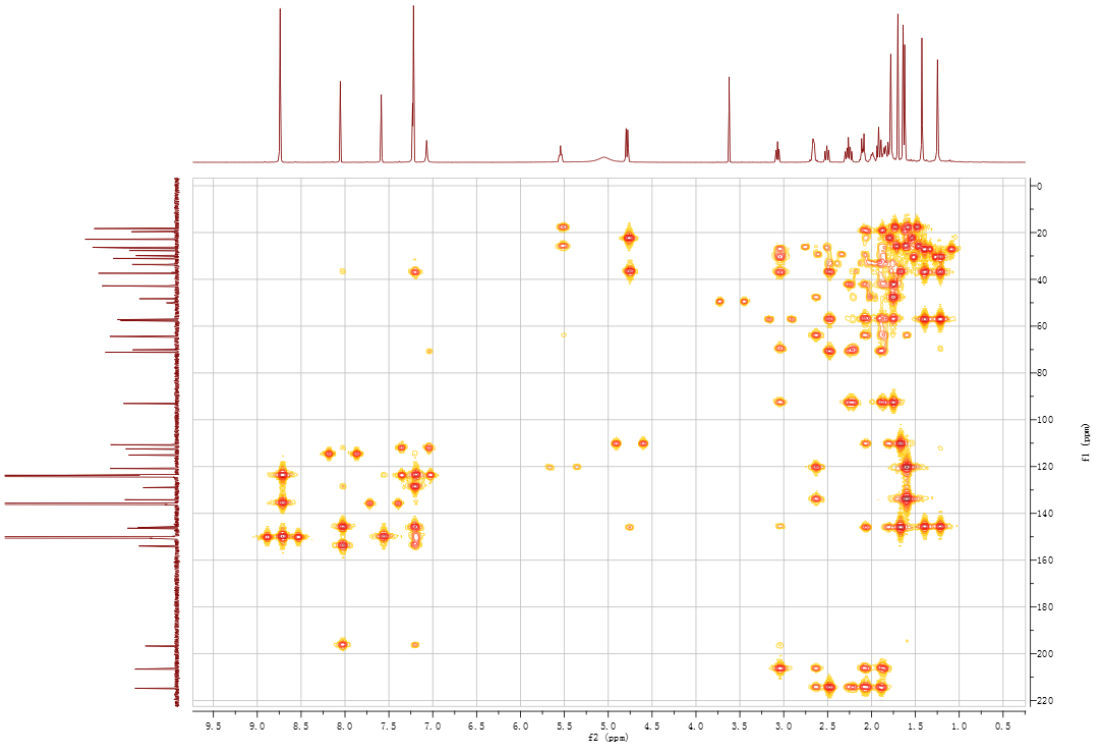
DEPT spectrum of compound **4** in CD_5N_5



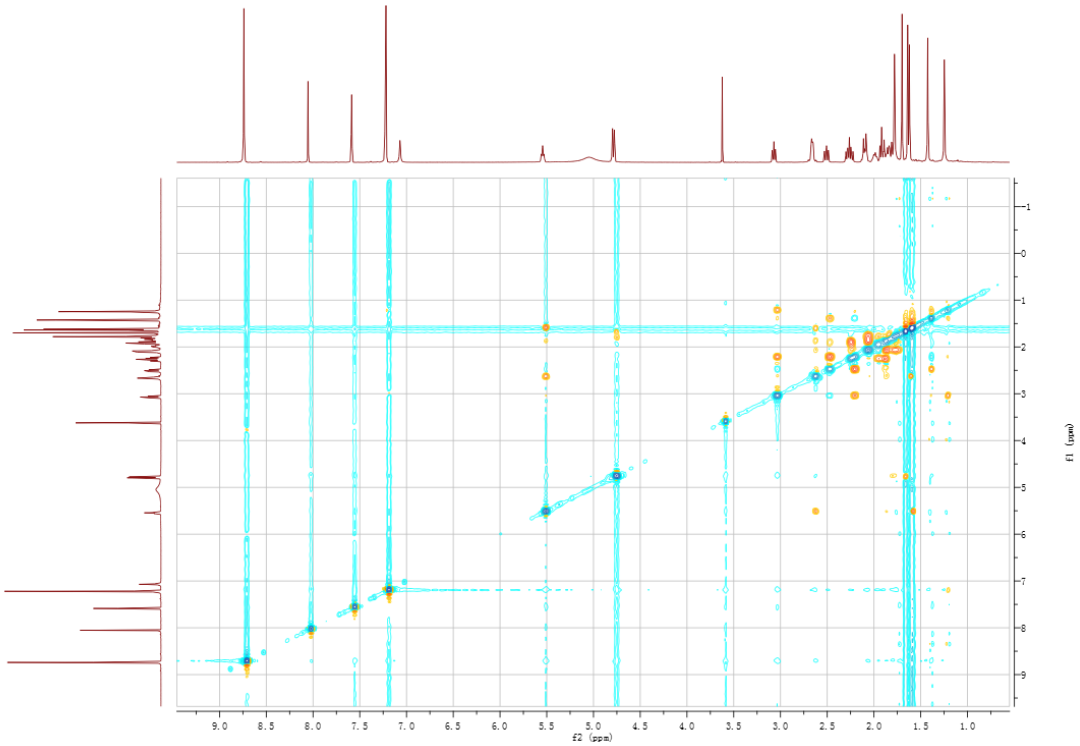
^{1}H-^{1}HCOSY spectrum of compound **4** in CD_5N_5



HSQC spectrum of compound **4** in CD_5N_5



HMBC spectrum of compound **4** in CD_5N_5



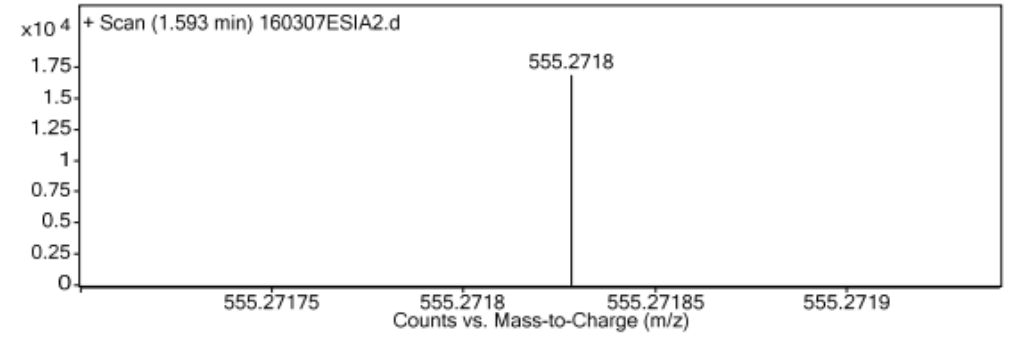
ROESY spectrum of compound **4** in CD_5N_5

Data Filename	160307ESIA2.d	**Sample Name**	GF-63
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	3/8/2016 9:21:10 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

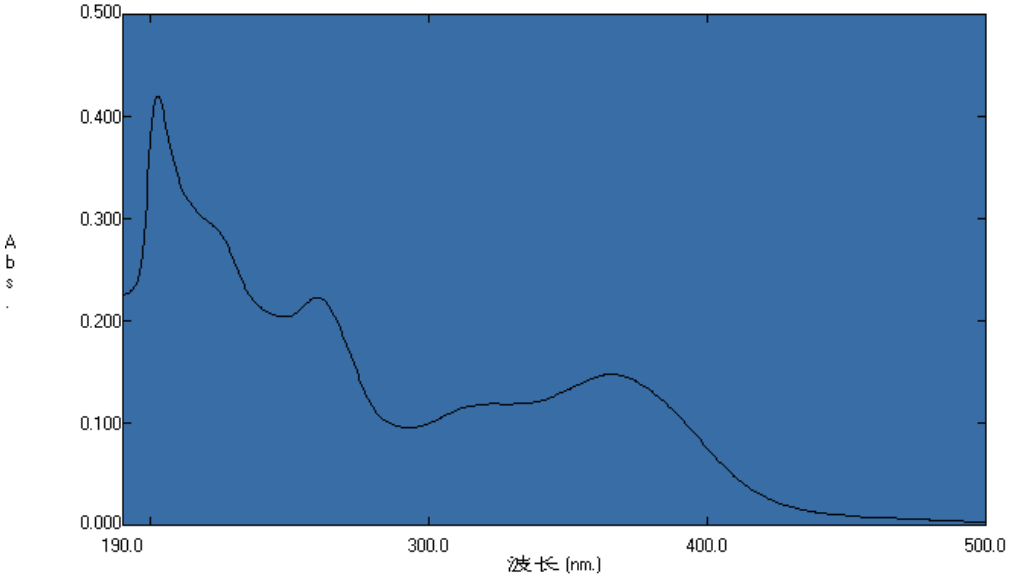
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

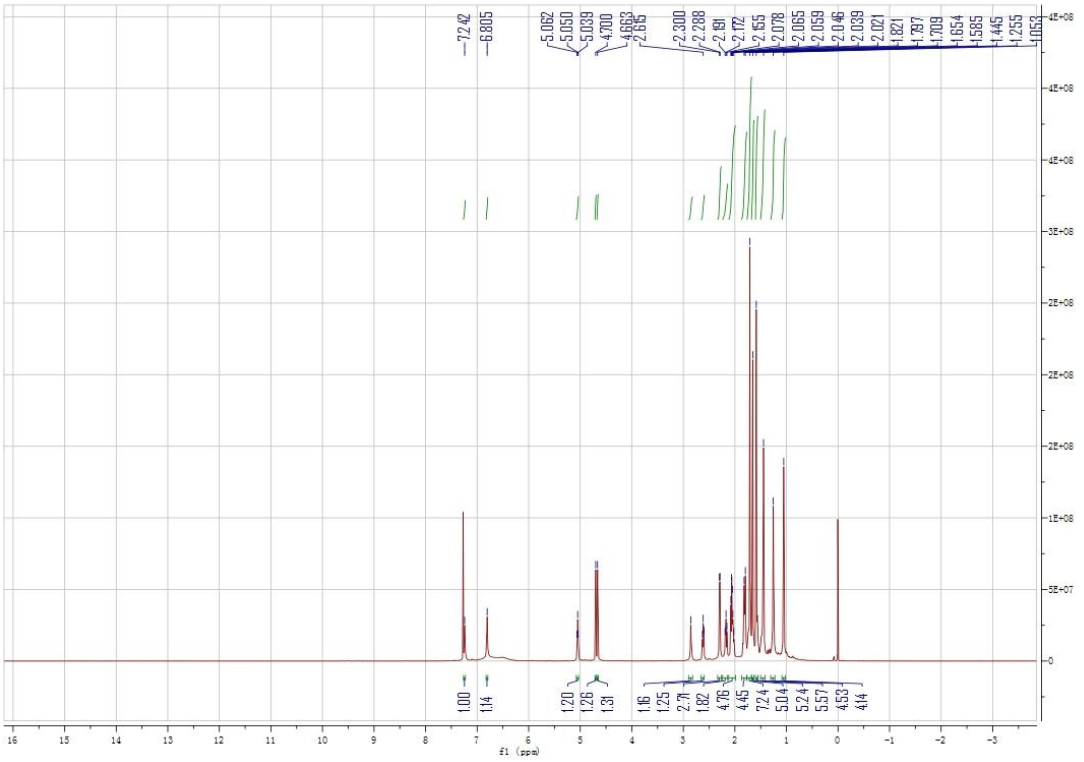
Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



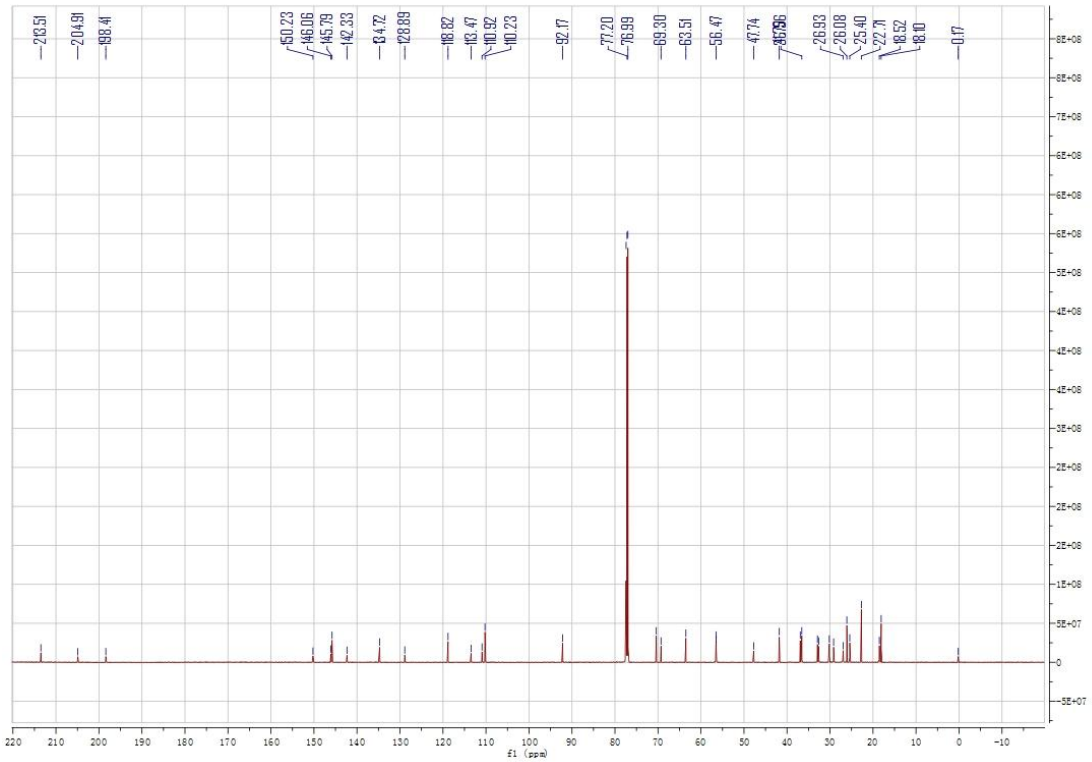
HR-ESI-MS spectrum of compound **4**



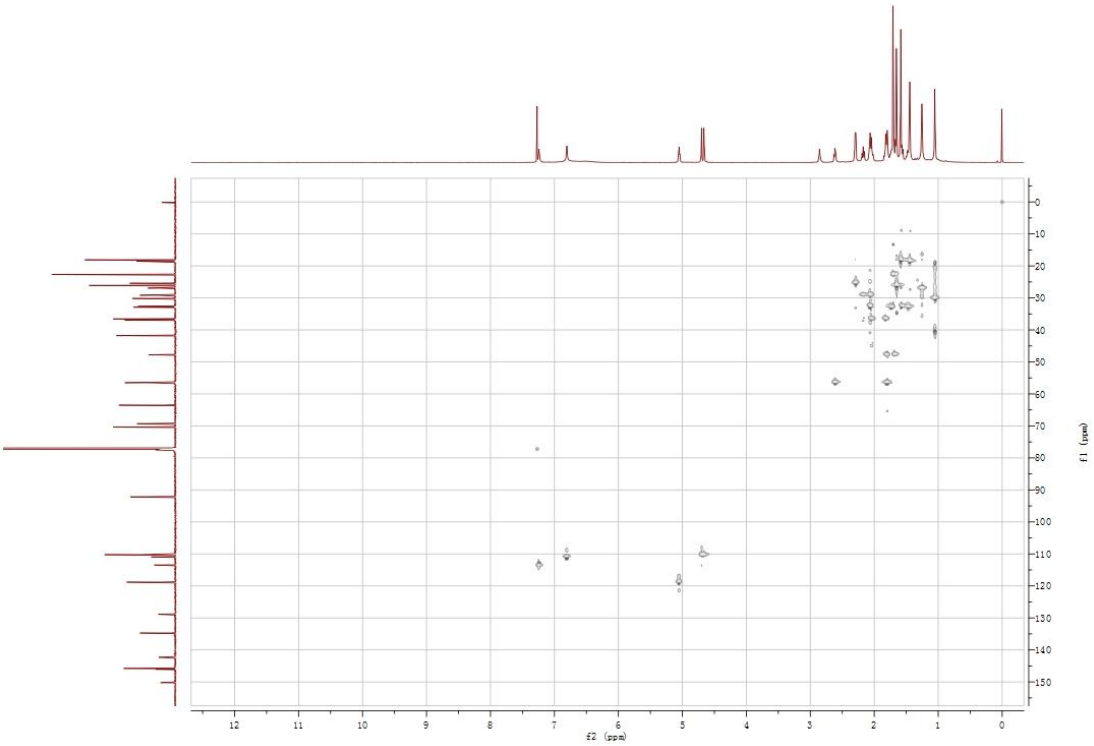
UV spectrum of compound **4**



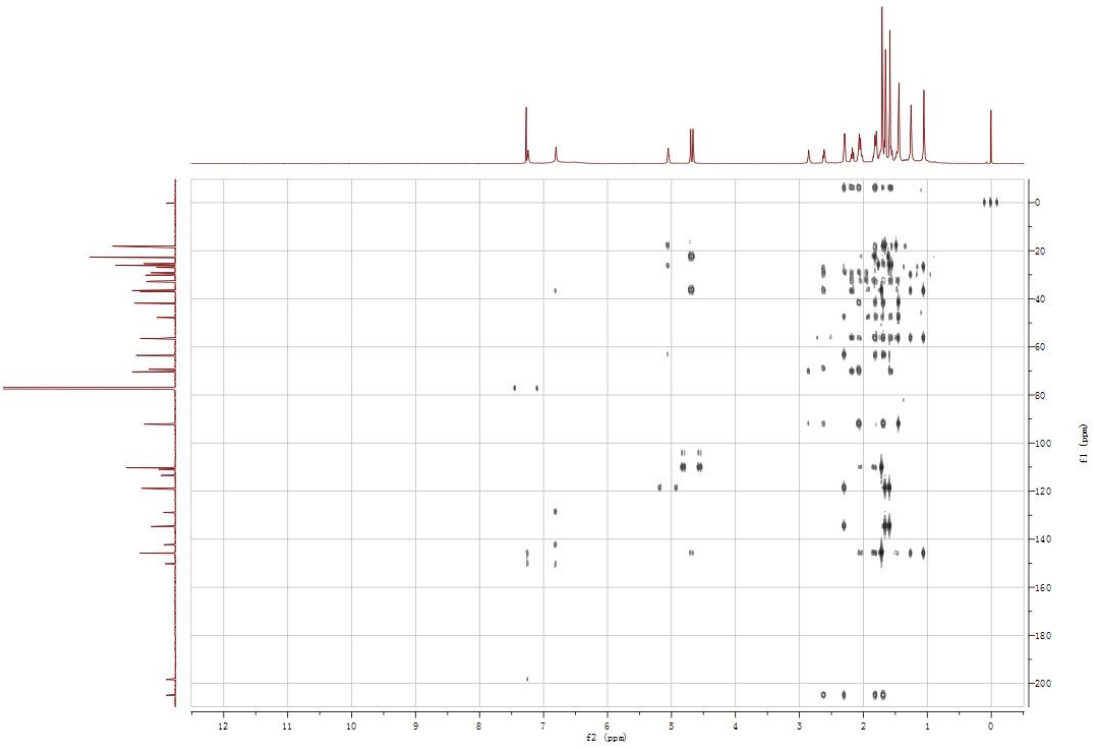
^{1}H-NMR spectrum of compound **4** in $CDCl_3$



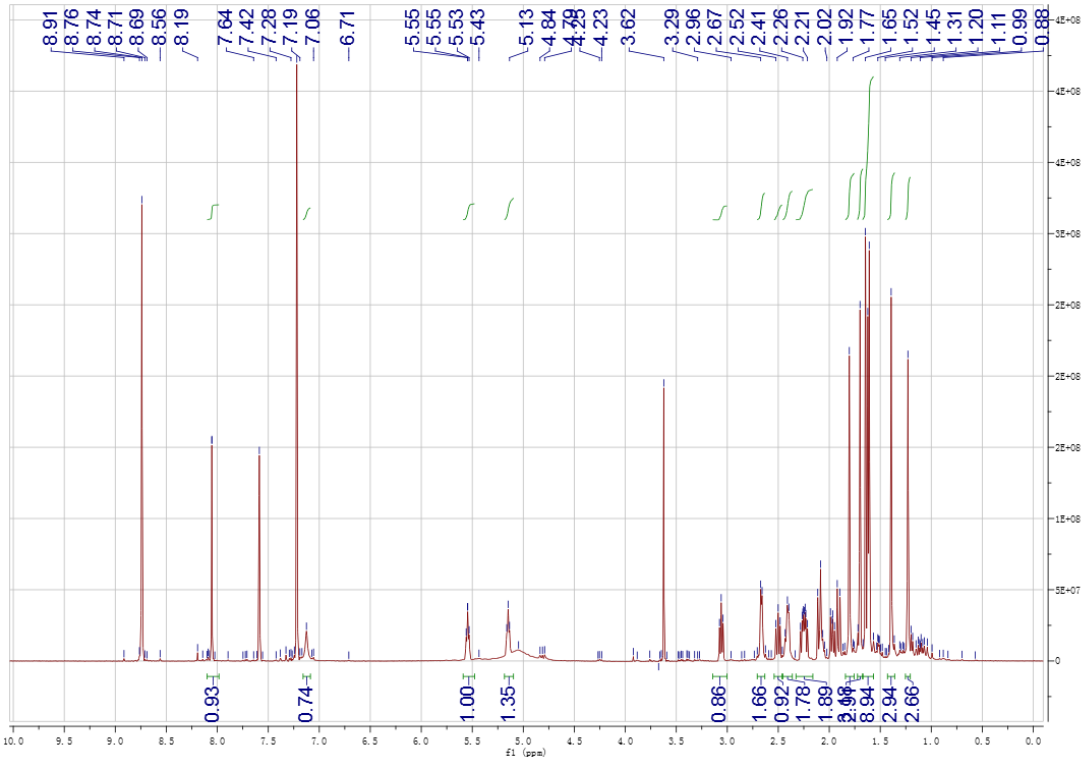
^{13}C-NMR spectrum of compound **4** in $CDCl_3$



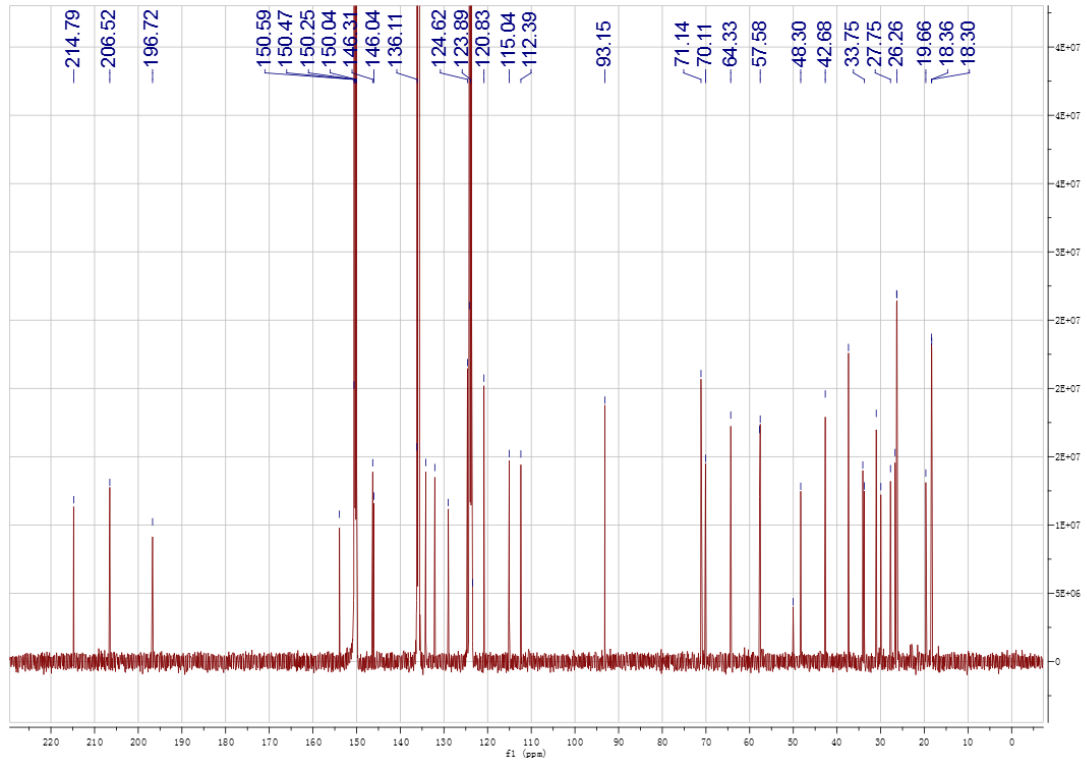
HSQC of compound **4** in $CDCl_3$



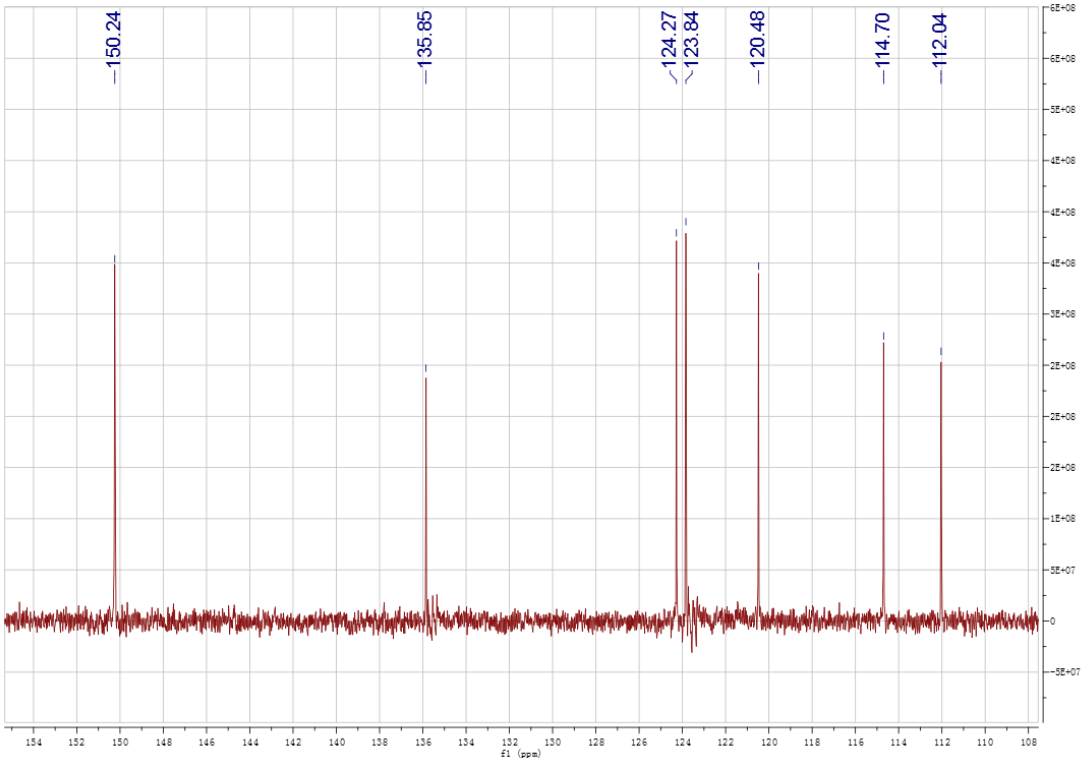
HMBC of compound **4** in $CDCl_3$



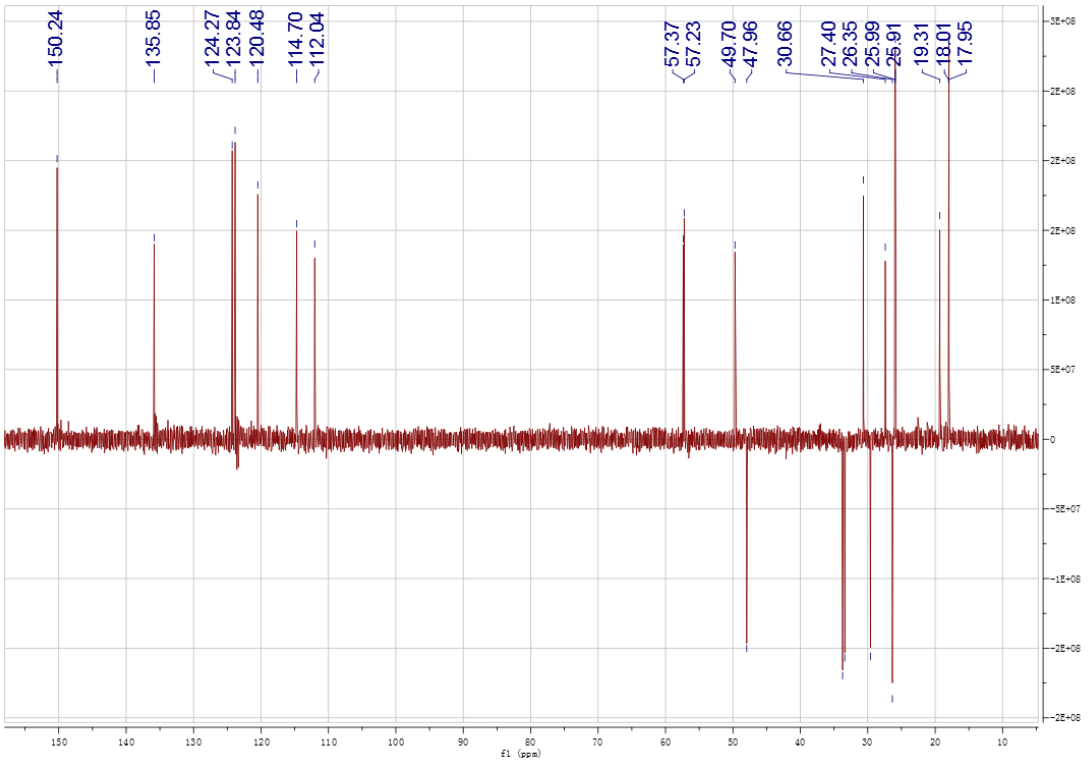
^{1}H-NMR spectrum of compound **5** in CD_5N_5



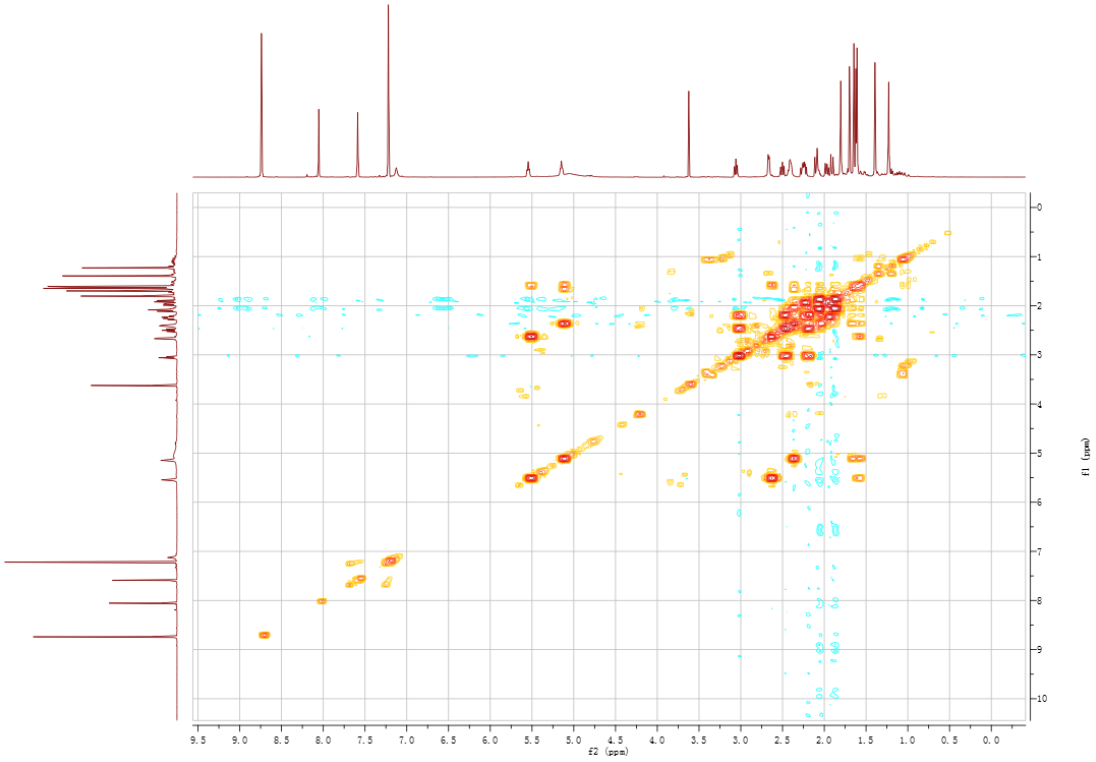
^{13}C-NMR spectrum of compound **5** in CD_5N_5



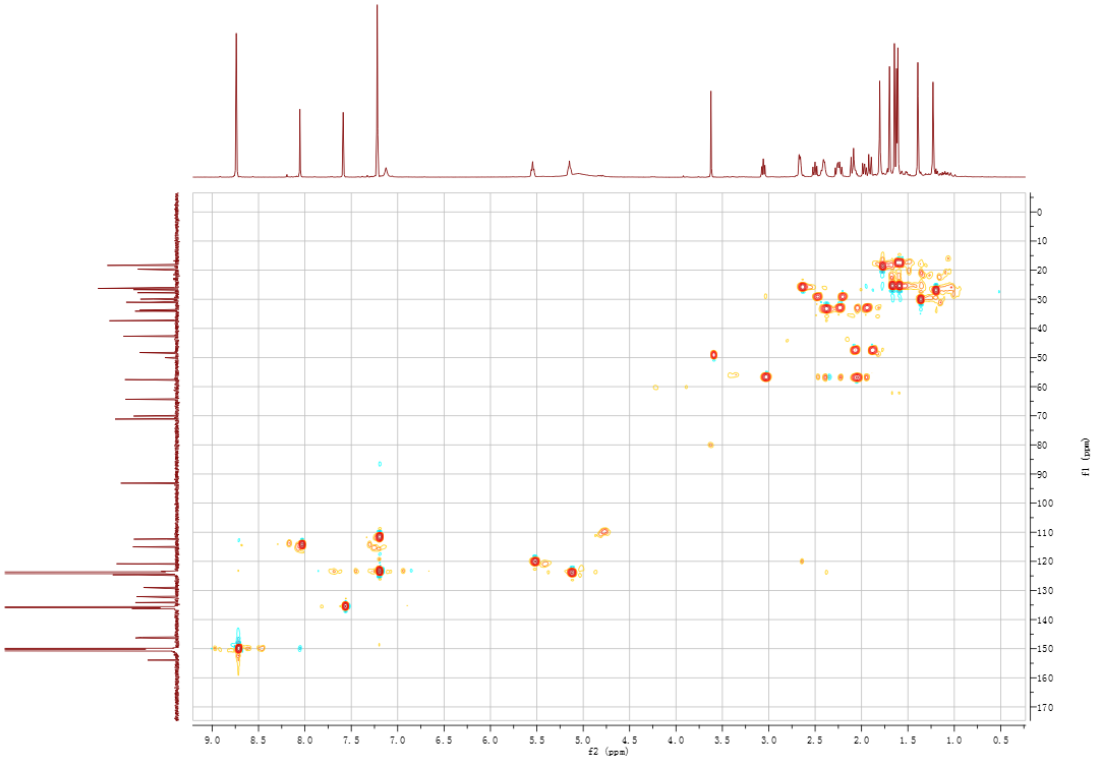
DEPT spectrum of compound **5** in CD_5N_5



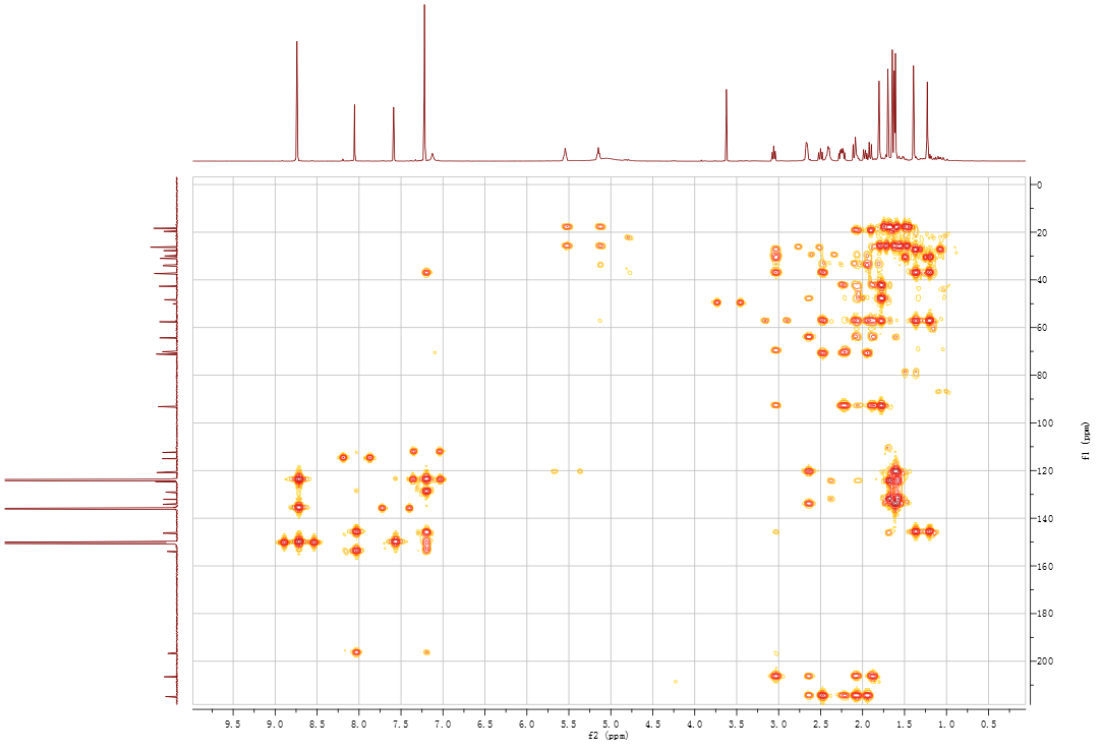
DEPT spectrum of compound **5** in CD_5N_5



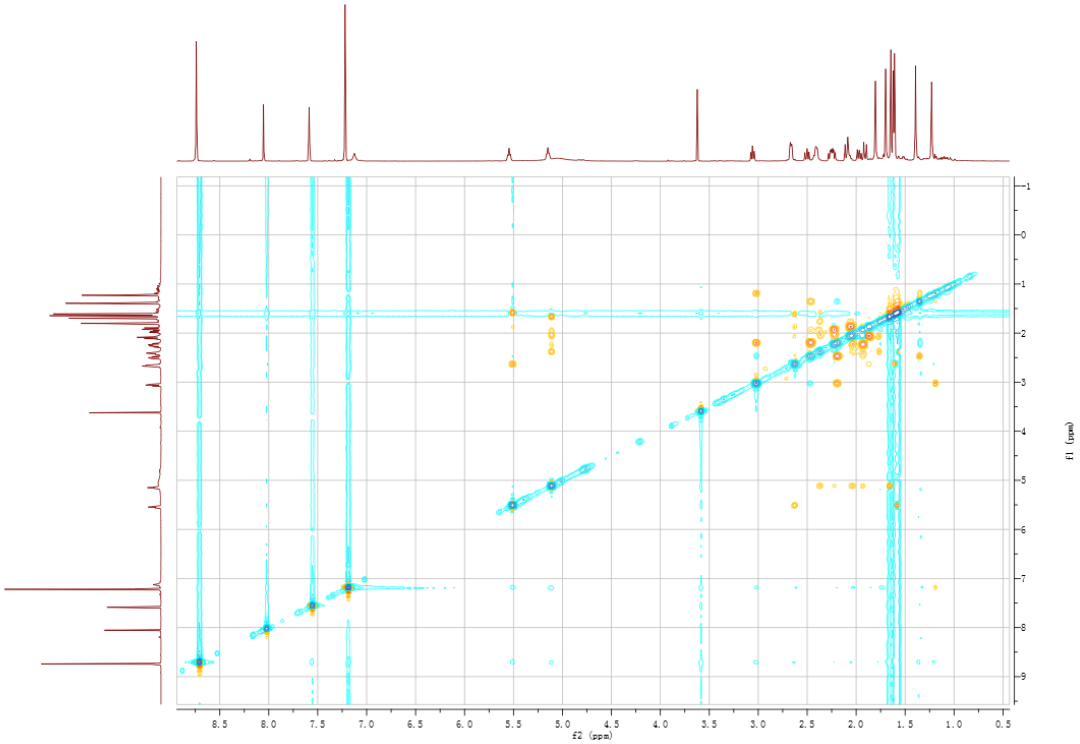
^{1}H-^{1}HCOSY spectrum of compound **5** in CD_5N_5



HSQC spectrum of compound **5** in CD_5N_5



HMBC spectrum of compound **5** in CD_5N_5



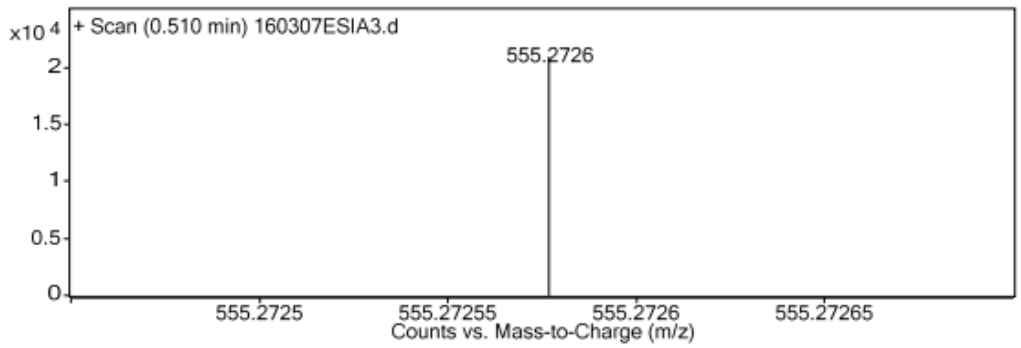
ROESY spectrum of compound **5** in CD_5N_5

Data Filename	160307ESIA3.d	**Sample Name**	GF-66
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	3/8/2016 9:23:35 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

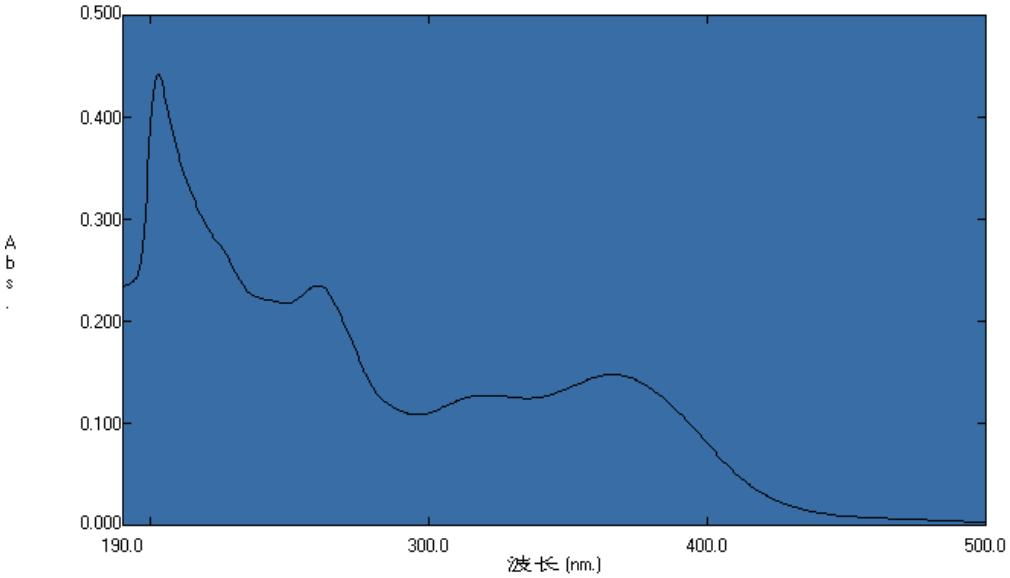
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

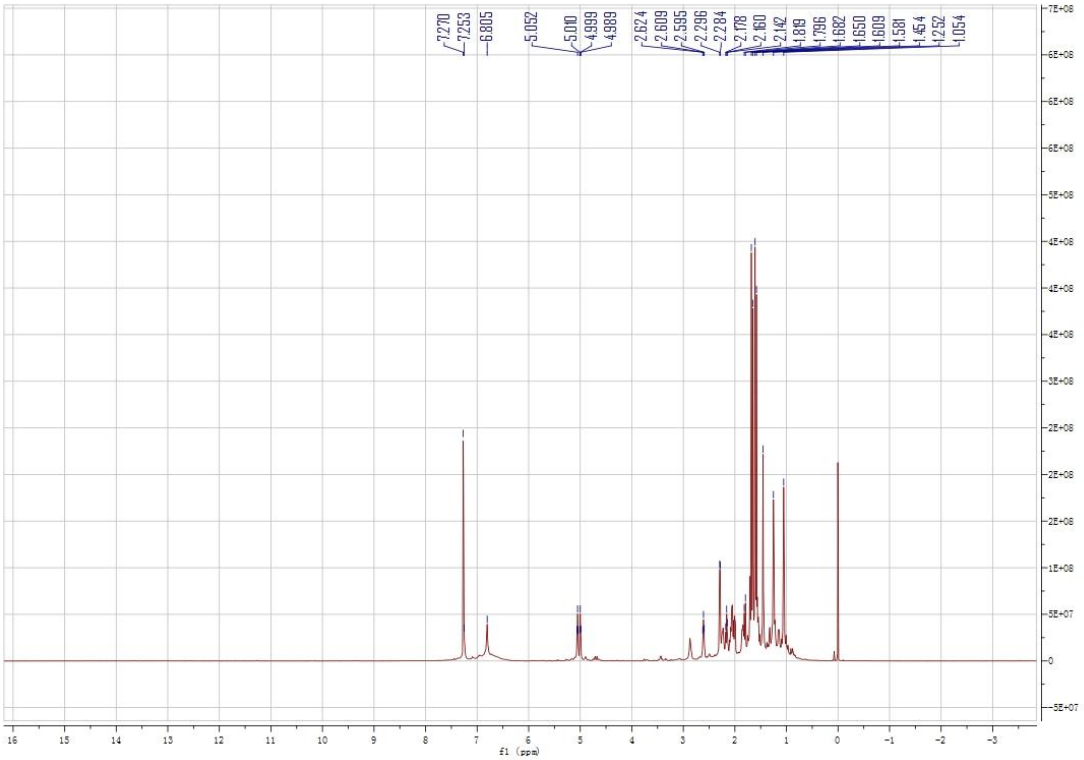
Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



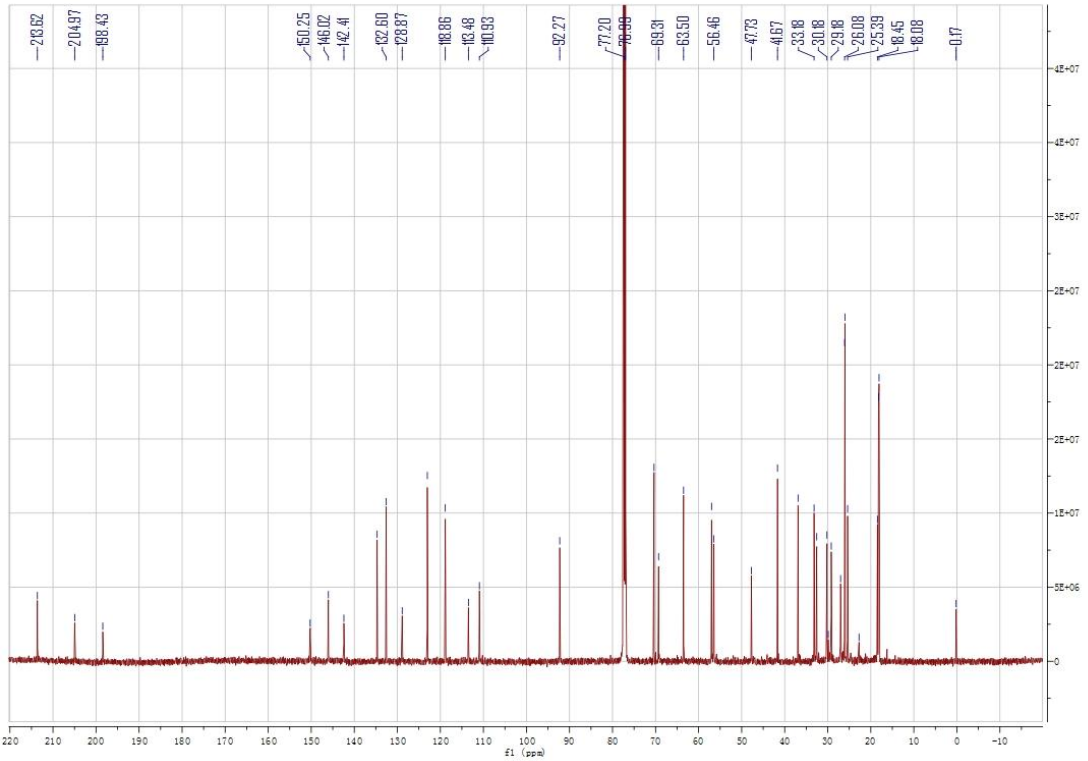
HR-ESI-MS spectrum of compound **5**



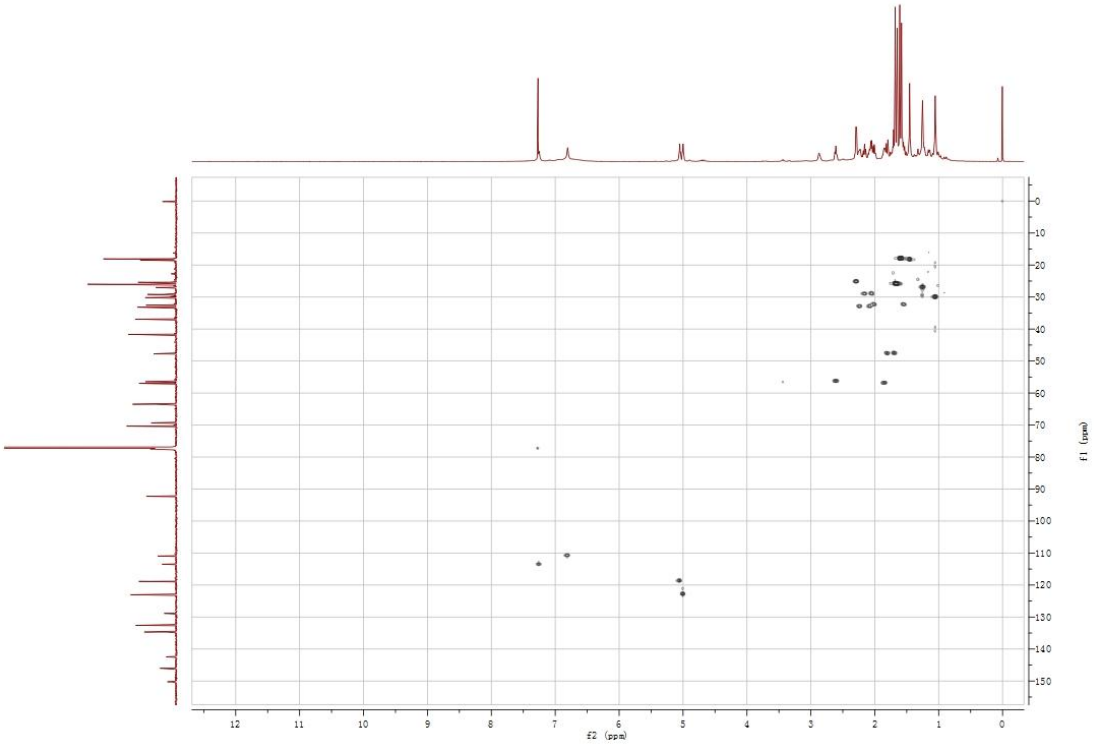
UV spectrum of compound **5**



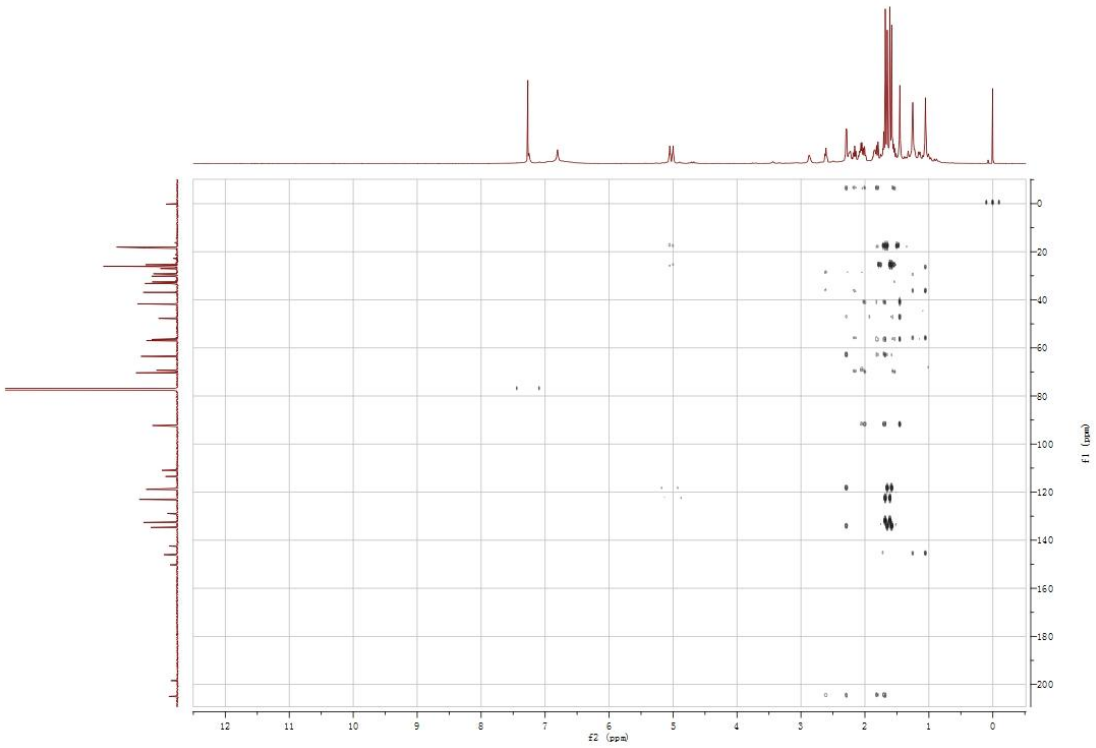
^{1}H-NMR spectrum of compound **5** in $CDCl_3$



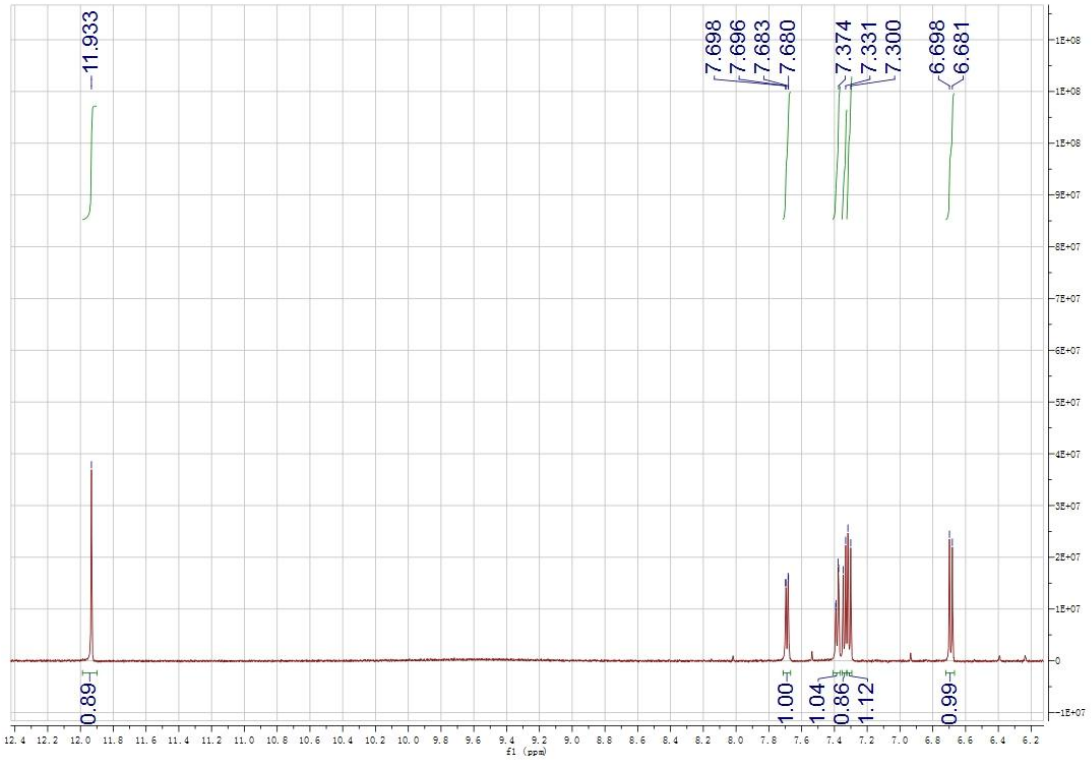
^{13}C-NMR spectrum of compound **5** in $CDCl_3$



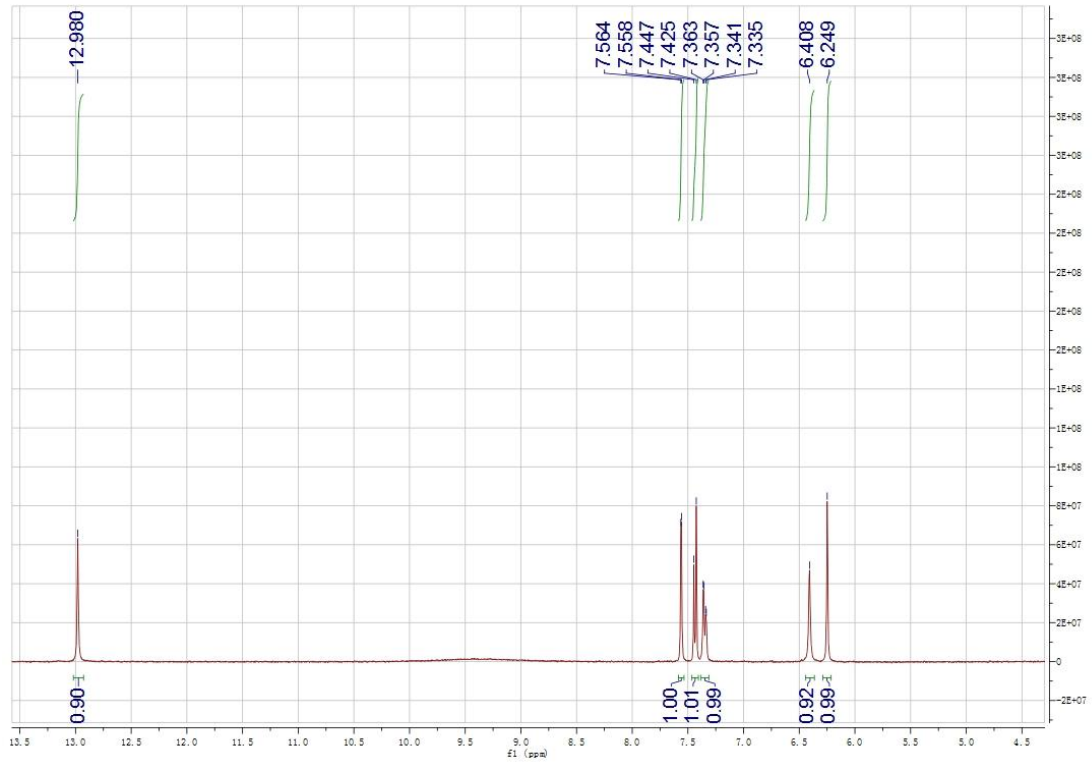
HSQC spectrum of compound **5** in $CDCl_3$



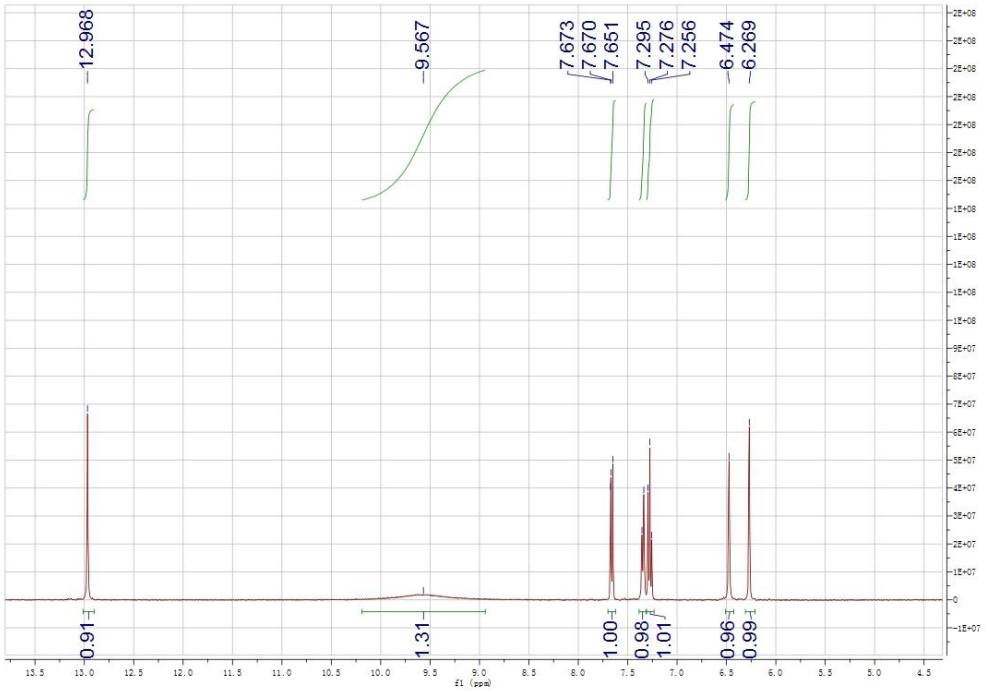
HMBC spectrum of compound **5** in $CDCl_3$



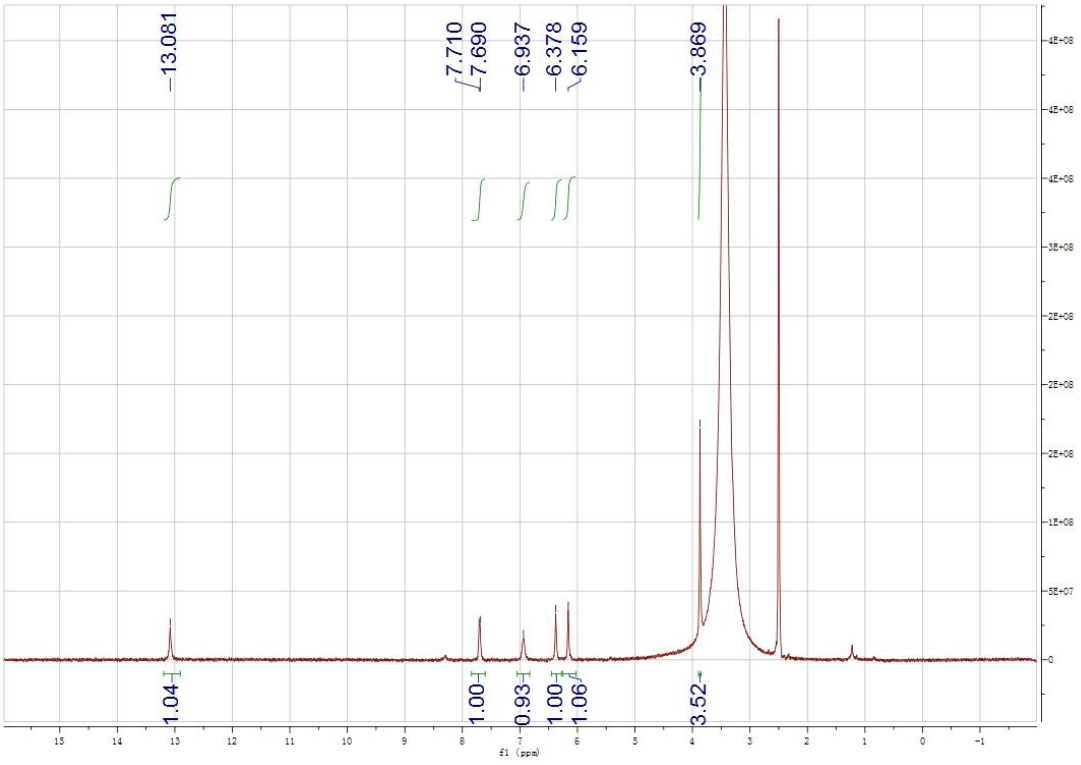
^{1}H-NMR of compound 6



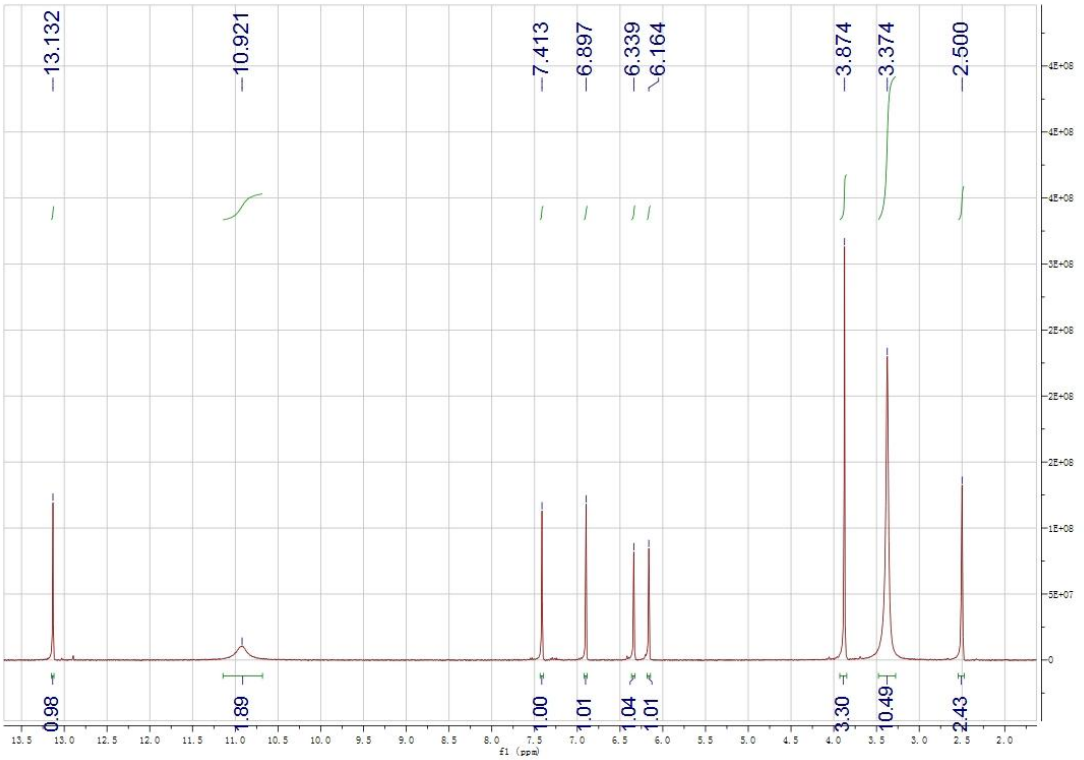
^{1}H-NMR of compound 7



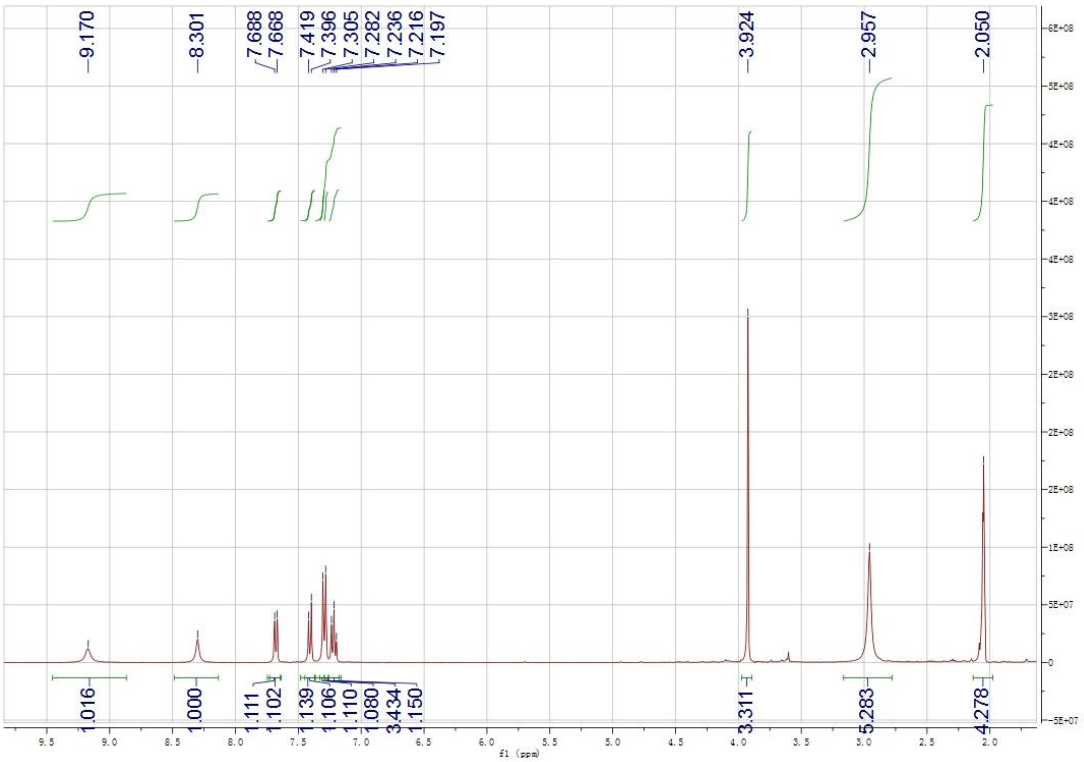
^{1}H-NMR of compound 8



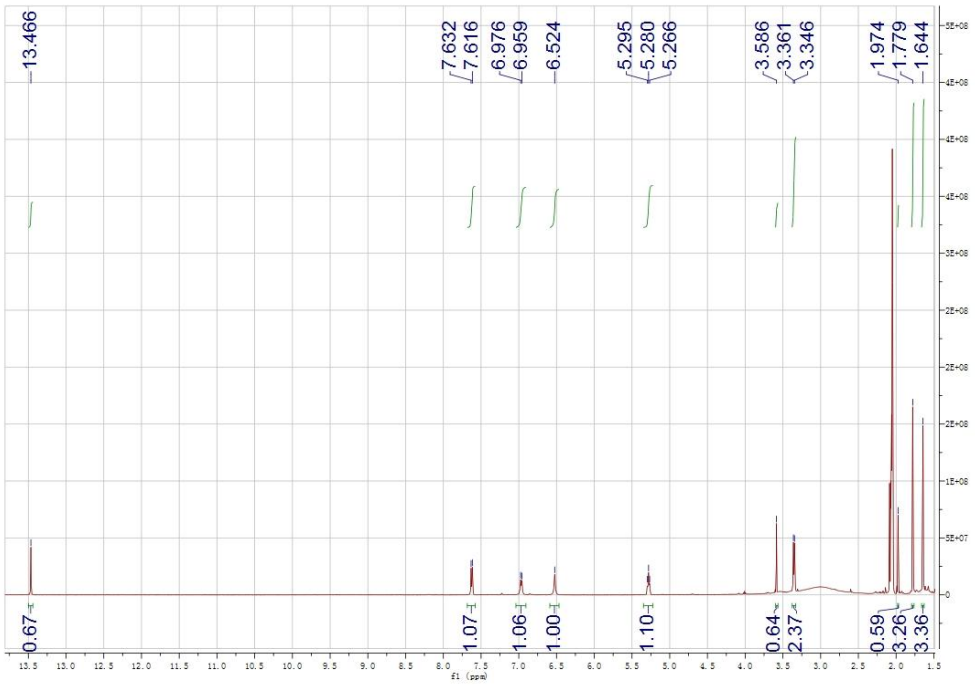
^{1}H-NMR of compound 9



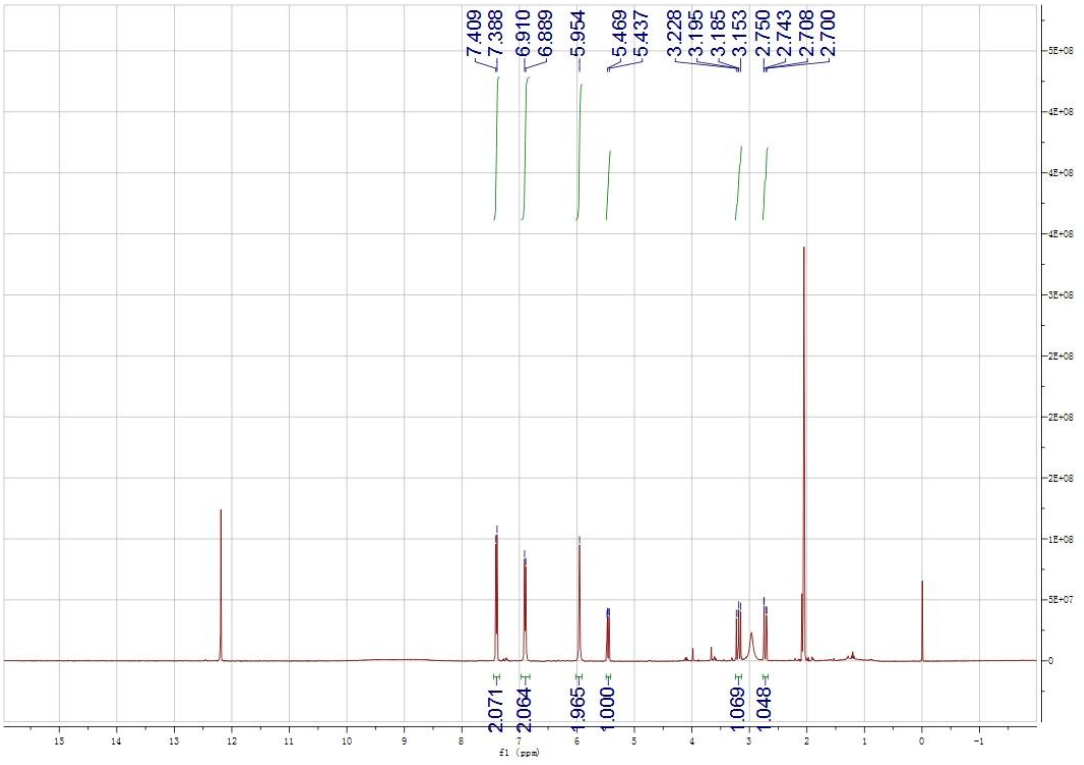
^{1}H-NMR of compound 10



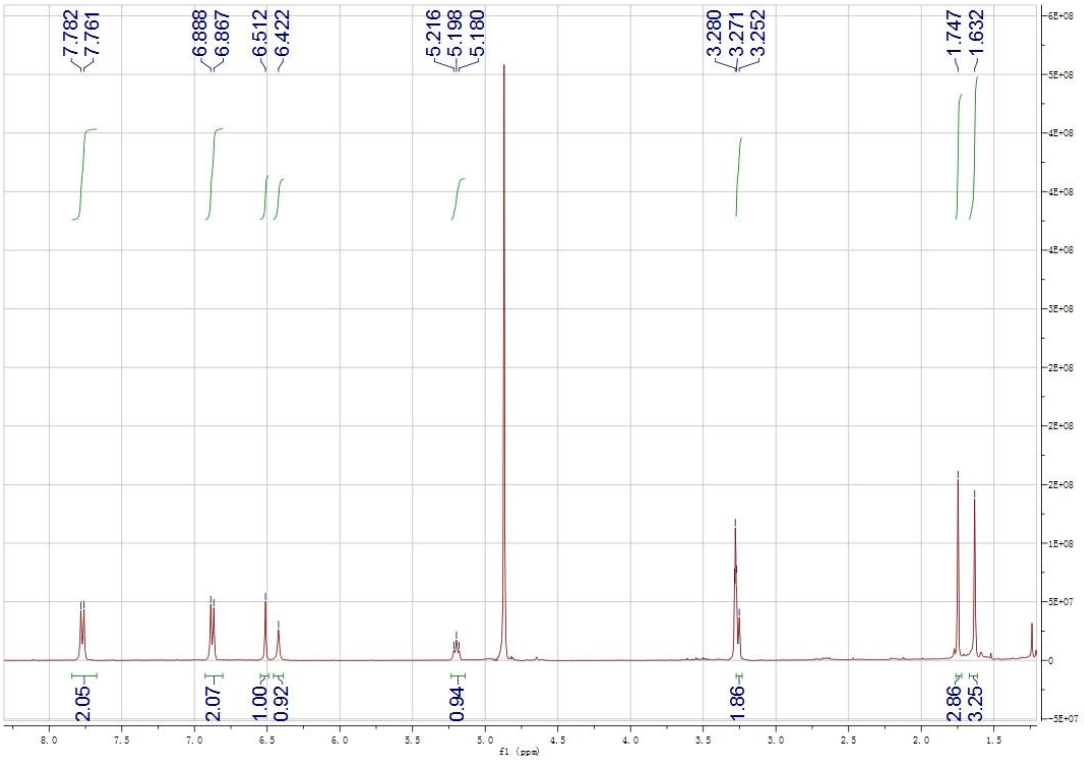
^{1}H-NMR of compound 11



^{1}H-NMR of compound 12



^{1}H-NMR of compound 13



^{1}H-NMR of compound 14

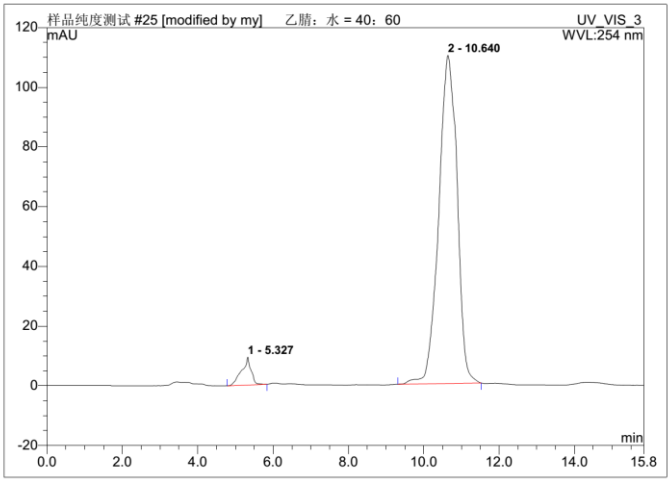
Table 1: Full HMBCs of compounds **1**-**3**

No	**1**	**2**	**3**
1			
2			
3			
4			
5			
6	C-7, 34, 5, 4, 8	C-7, 5, 4	C-17, 7, 8, 9, 34, 4
7			
8			
9			
10			
11			
12	C-16, 13, 14, 10	C-16, 13, 14, 10	C-16, 13, 14, 10
13			
14			
15	C-11, 13		C-11, 13, 14
16	C-12, 14, 10	C-10, 14, 12	C-12, 14, 10
17		C-5, 18, 19, 4	C-18, 5, 19, 4, 22
18	C-20, 17, 19, 21	C-21, 17, 22, 20, 19	
19			
20	C-21, 18, 19	C-18, 21, 19	C-21, 19, 18
21	C-19, 20		C-20, 19, 18
22			
23		C-26, 22, 25, 24	
24			
25	C-23, 24	C-23, 24, 26	C-26, 23, 24
26	C-23, 24		C-24, 25, 23
27	C-1, 28, 29, 9	C-1, 28, 29, 9	C-1, 28, 29
28	C-30, 31		
29			
30	C-28, 29		C-28, 29
31	C-28, 29		C-28, 29
32	C-1, 8, 7, 33	C-33, 8, 1, 7	C-33, 7, 8, 1
33	C-1, 8, 7, 32	C-32, 8, 1, 7	C-32, 7, 8, 1
34	C-36, 35, 4, 3, 6, 7	C-6, 7, 3, 35, 2, 4	C-6, 3, 4
35	C-37, 38, 34, 3	C-37, 38, 34, 3	C-7, 34
36			
37	C-35, 36		C-38, 36, 35
38	C-35, 36		C-37, 36, 35

Table **2** ^{1}H, ^{13}C NMR data of compounds **4** and **5** (in $CDCl_3$)

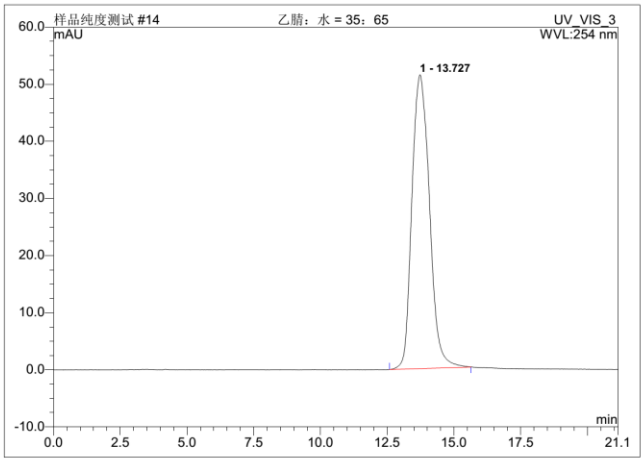
No	4		5	
	^{13}C-NMR	^{1}H-NMR	^{13}C-NMR	^{1}H-NMR
1	63.5		63.5	
2	213.5		213.6	
3	70.4		70.4	
4	32.7	2.06, 1.57 m, 2H	32.6	2.01, 1.55 m, 2H
5	56.4	1.80 m	57.0	1.86 m
6	41.8		41.7	
7	92.2		92.3	
8	69.3		69.3	
9	204.9		205.0	
10	47.7	1.80, 1.68 m 2H	47.7	1.80 d (13.8), 1.71 m 2H
11	25.4	2.29 d (7.2)	25.4	2.29 d (6.9)
12	118.8	5.05 t (7.2)	118.9	5.06 t (6.9)
13	134.7		134.7	
14	26.1	1.65 s 3H	26.1	1.65 s 3H
15	18.1	1.58 s 3H	18.1	1.58 s 3H
16	29.2	2.18 dd (11.4, 9.6), 2.06 m 2H	29.2	2.18 dd (10.8, 9.4), 2.05 m 2H
17	56.5	2.61 dd (9.6, 8.4)	56.5	2.61 dd (9.4, 8.4)
18	36.9		36.9	
19	26.9	1.25 s 3H	27.0	1.25 s 3H
20	30.2	1.05 s 3H	33.2	1.05 s 3H
21	32.9	1.73, 1.47 m, 2H	32.9	2.24, 2.08 m, 2H
22	36.6	2.04, 1.82 m, 2H	123.0	5.00 t (6.6)
23	146.1		132.6	
24	110.2	4.70 s, 4.66 s	18.2	1.61 s 3H
25	22.7	1.70 s 3H	26.0	1.68 s 3H
26	18.5	1.44 s 3H	18.5	1.45 s 3H
27	198.4		198.4	
28	128.9		128.9	
29	145.8		146.0	
30	110.9	6.81 s	110.9	6.81 s
31	142.3		142.4	
32	150.2		150.3	
33	113.5	7.24 s	113.5	7.26 s

HPLC condition: UV λmax 254 nm, column: YMC-Pack ODS-A column (250 × 10 mm, 5 μm); flow rate: 3 mL/min



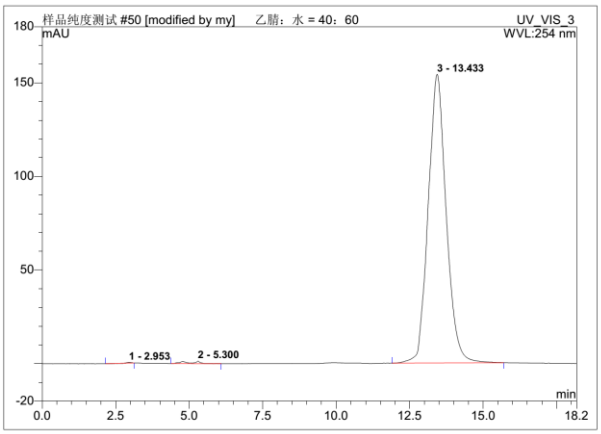
No.	Ret.Time min	Plates(EP)	Height mAU	Area mAU*min	Rel.Area %	Resolution(EP)	S/N
1	5.33	2049	9.375	2.713	4.17	7.80	12.5
2	10.64	2258	109.916	62.290	95.83	n.a.	222.6
Total:			119.291	65.003	100.00	7.798	

HPLC Chromatographic profiles of compound 15 (CH_3CN : H_2O = 40 : 60)



No.	Ret.Time min	Plates(EP)	Height mAU	Area mAU*min	Rel.Area %	Resolution(EP)	S/N
1	13.73	1991	51.452	39.288	100.00	n.a.	480.4
Total:			51.452	39.288	100.00	0.000	

HPLC Chromatographic profiles of compound 16 (CH_3CN : H_2O = 35 : 65)



No.	Ret.Time min	Plates(EP)	Height mAU	Area mAU*min	Rel.Area %	Resolution(EP)	S/N
1	2.95	1336	0.411	0.028	0.03	3.26	4.6
2	5.30	358	1.309	0.595	0.54	7.35	5.9
3	13.43	2391	154.186	109.509	99.43	n.a.	693.8
Total:			155.906	110.131	100.00	10.607	

HPLC Chromatographic profiles of compound 17
(CH_3CN : H_2O = 40 : 60)