

补充数据

乌药中3个新的倍半萜

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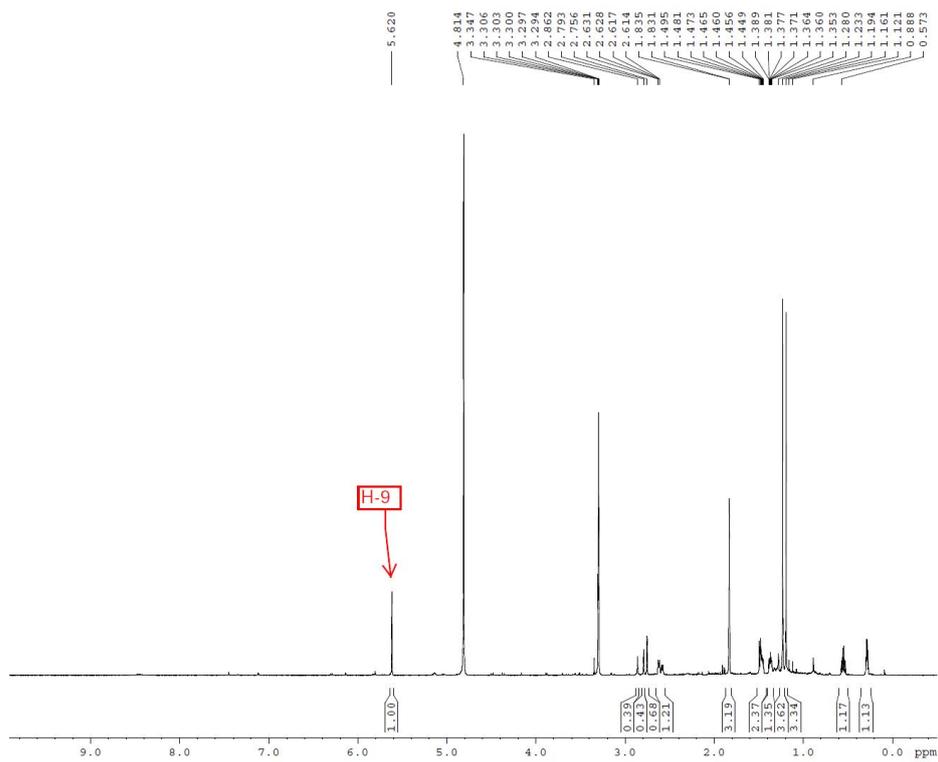


图1 化合物1的¹H NMR图（全谱）(500 MHz, CD₃OD)

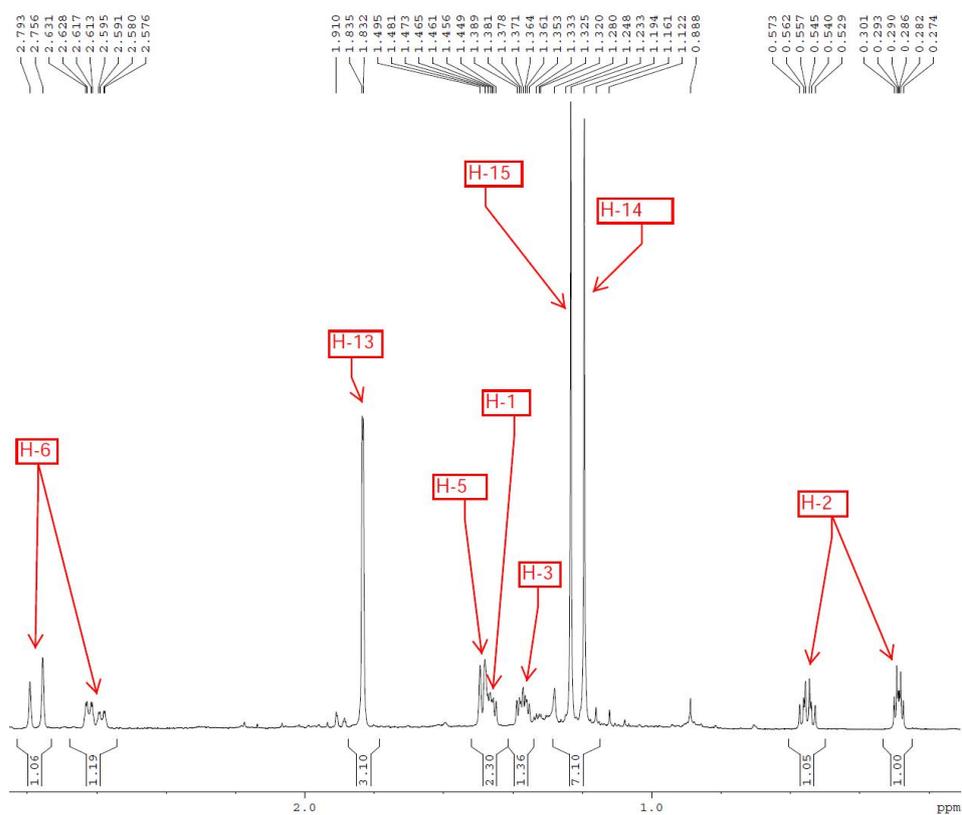


图1-1 化合物1的¹H NMR图（放大谱）

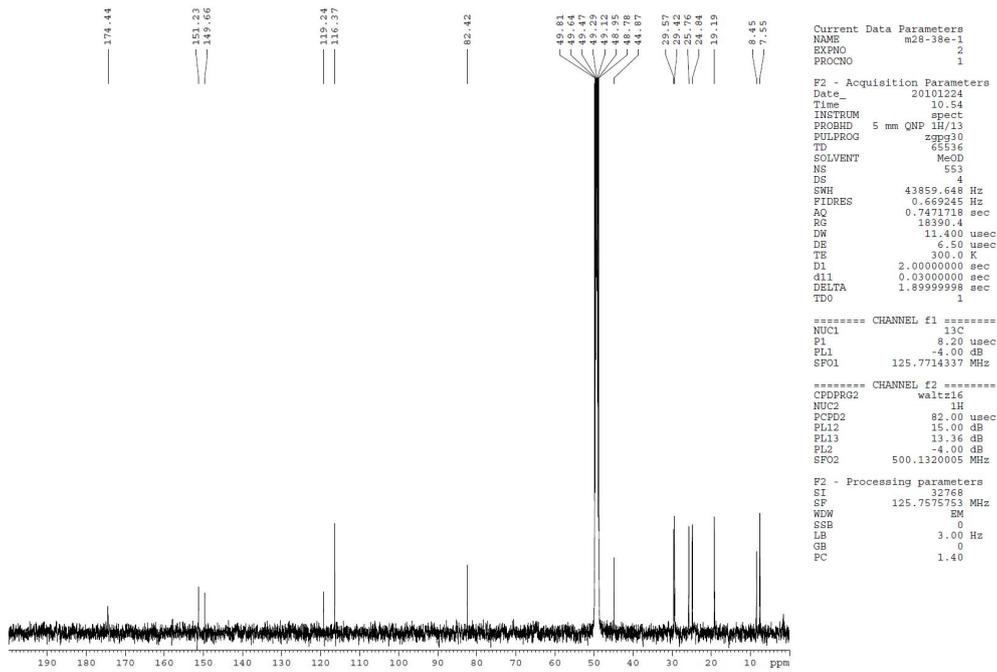


图2 化合物1的¹³C NMR图(125 MHz, CD₃OD)

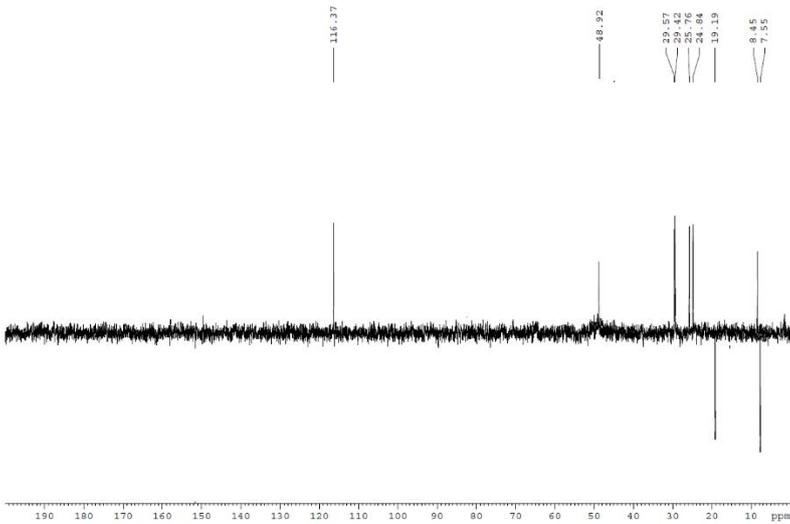


图3 化合物1的DEPT图

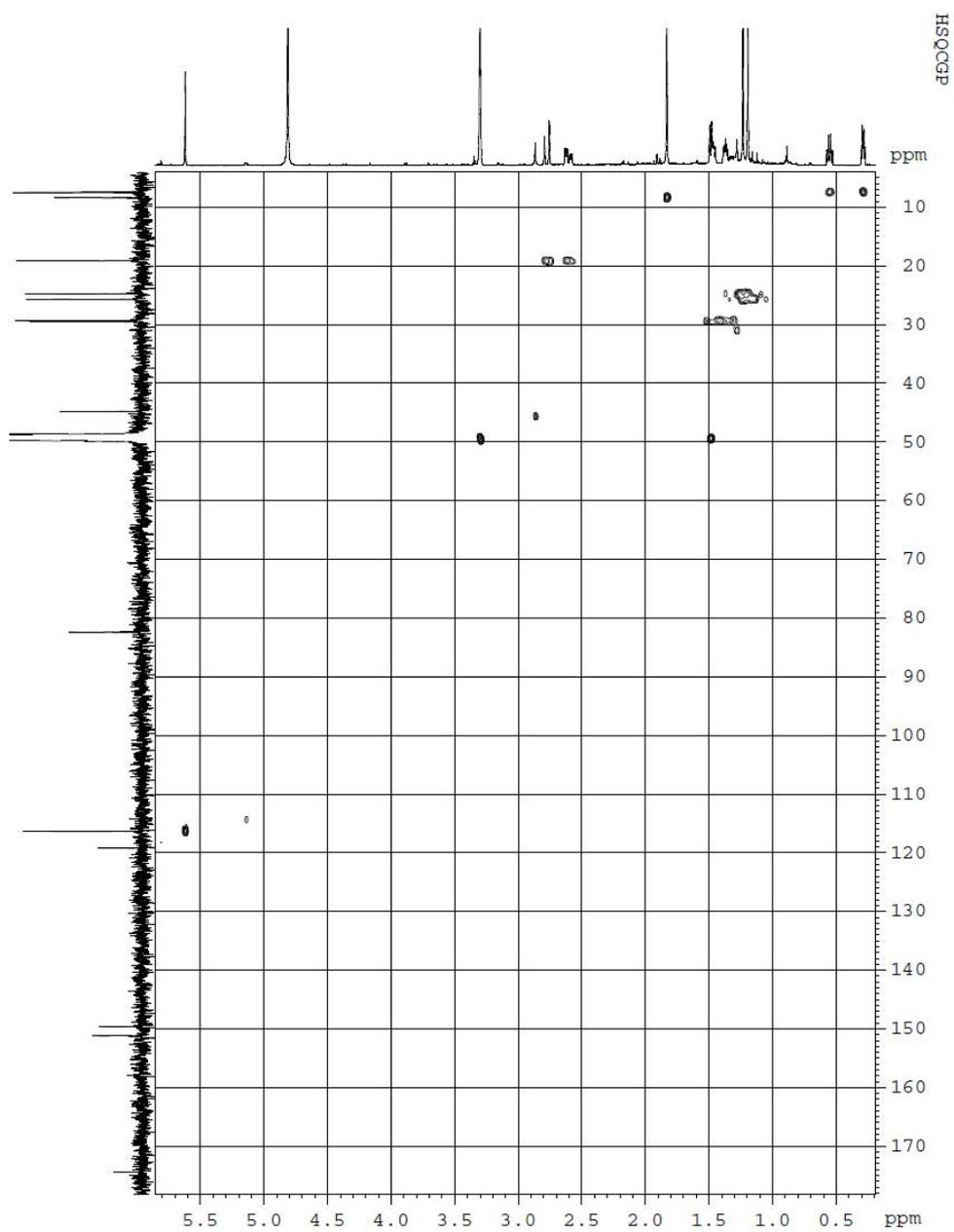


图4 化合物1的HSQC图

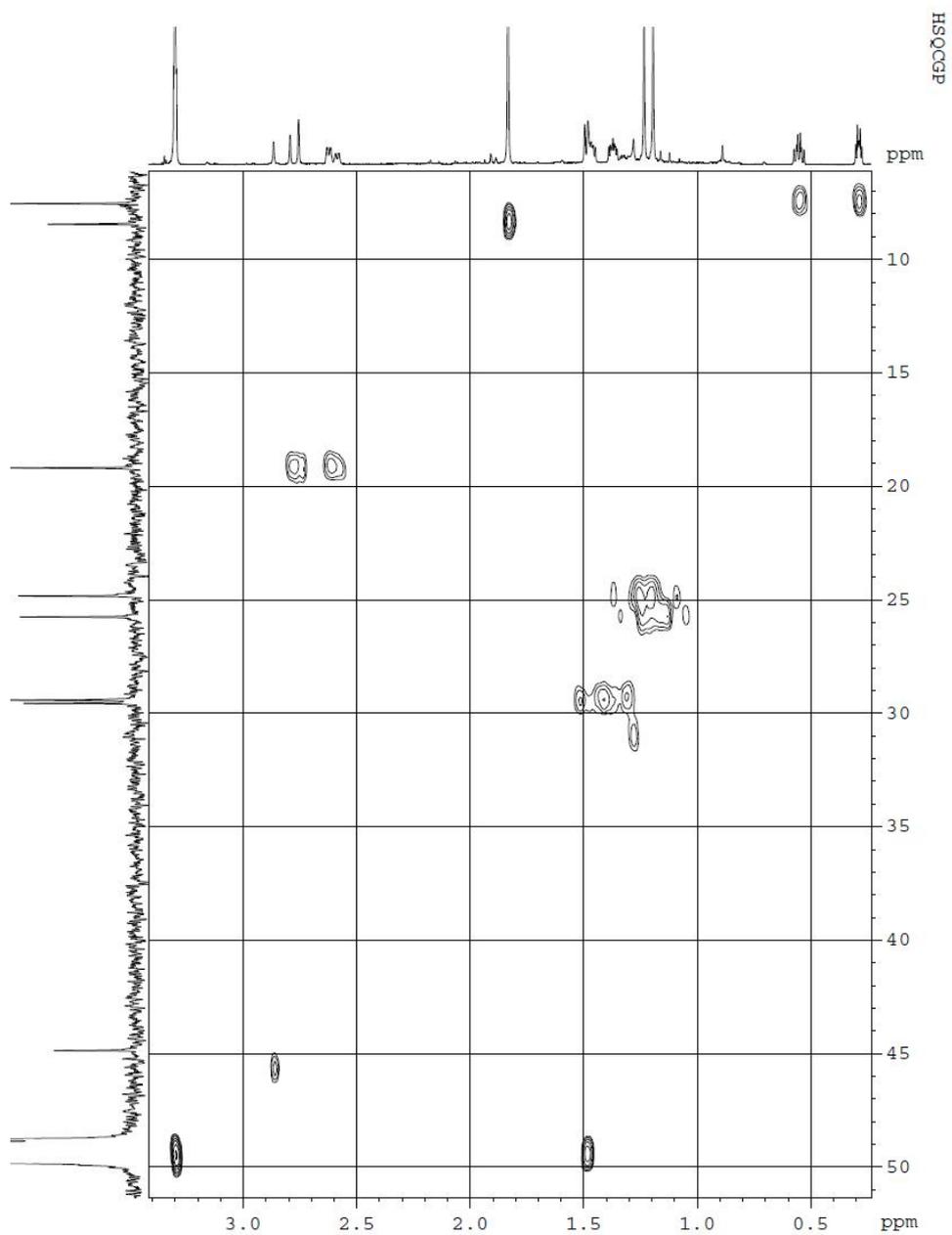


图4-1 化合物1的HSQC图（放大谱）

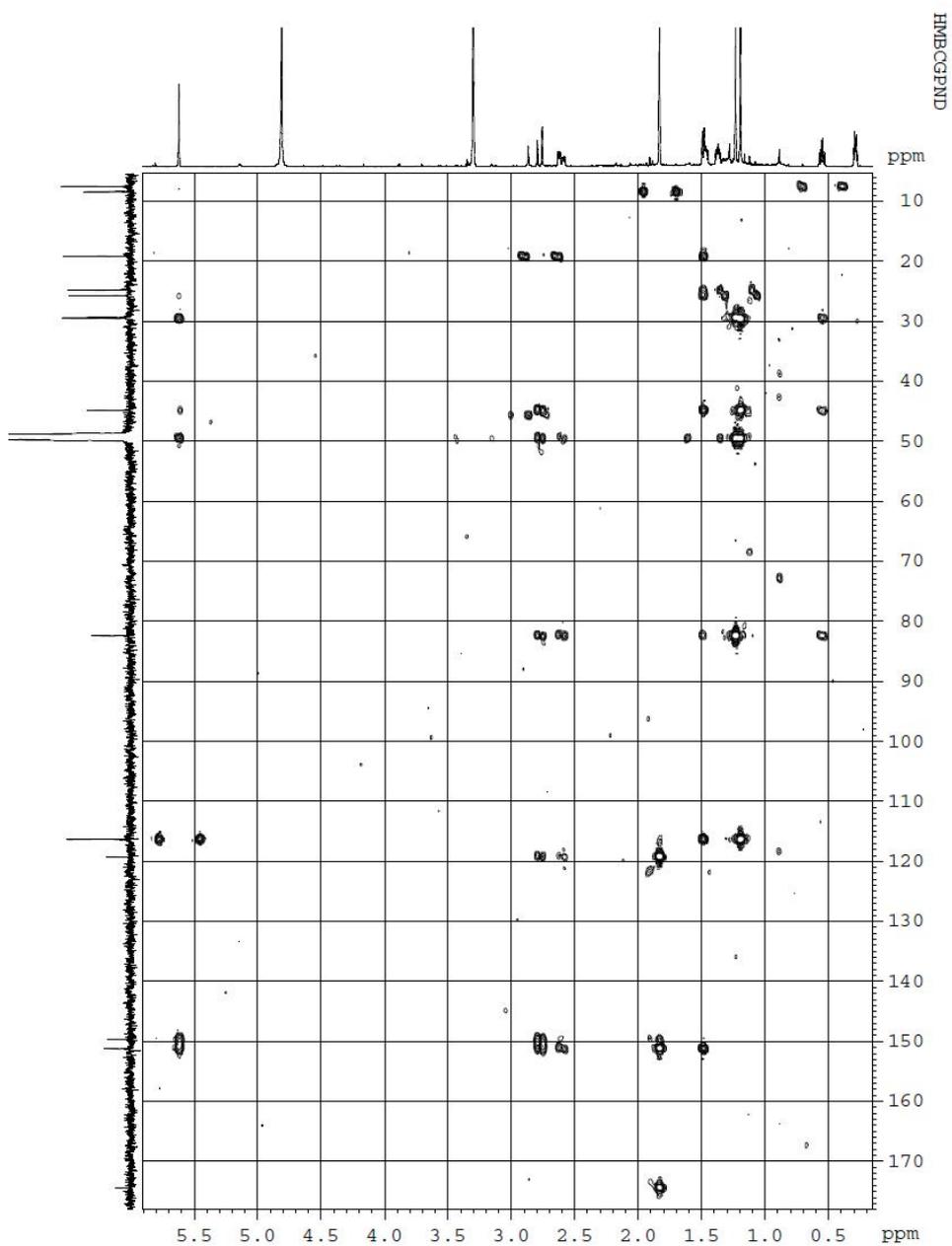


图5 化合物1的HMBC图

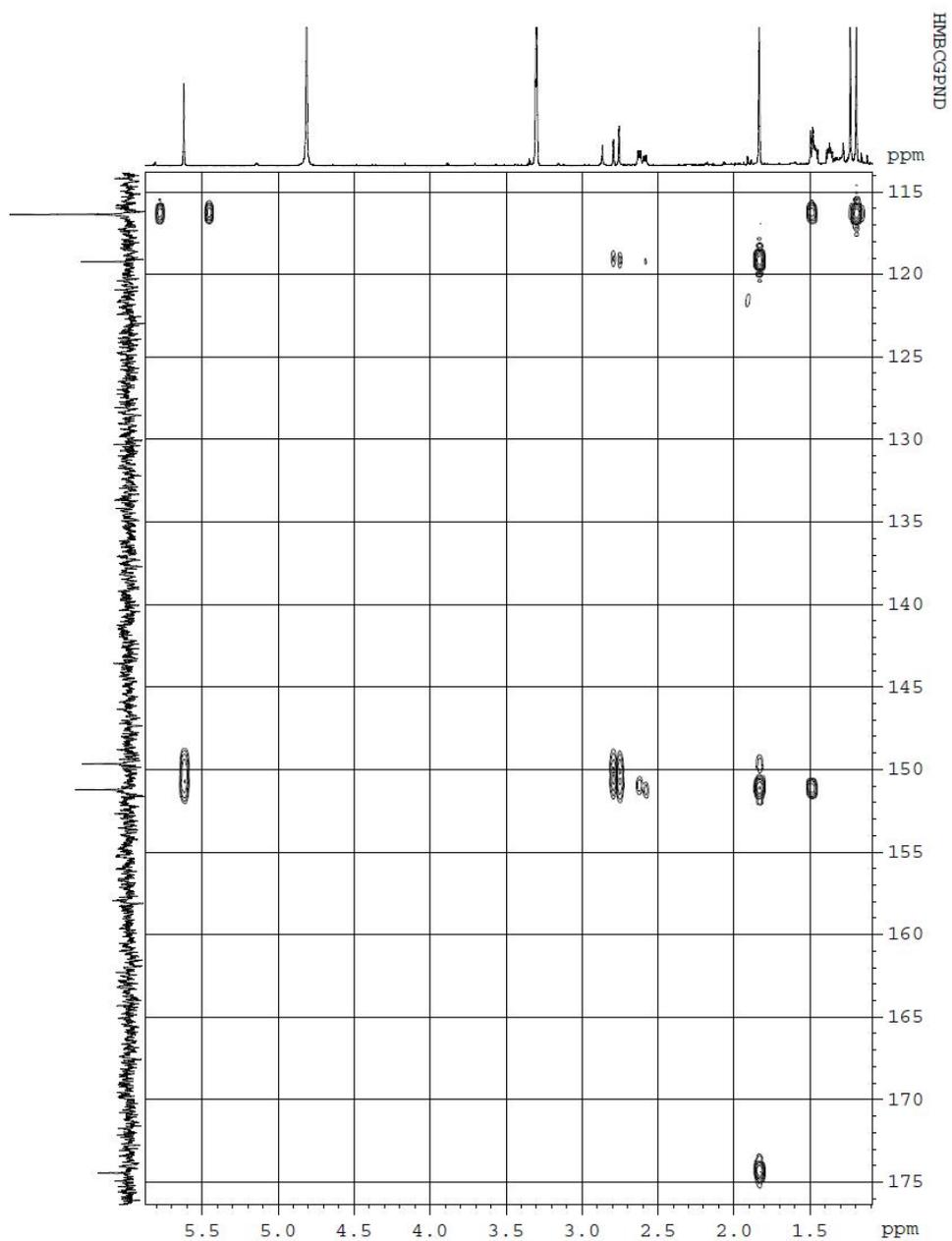


图5-1 化合物1的HMBC图（放大谱1）

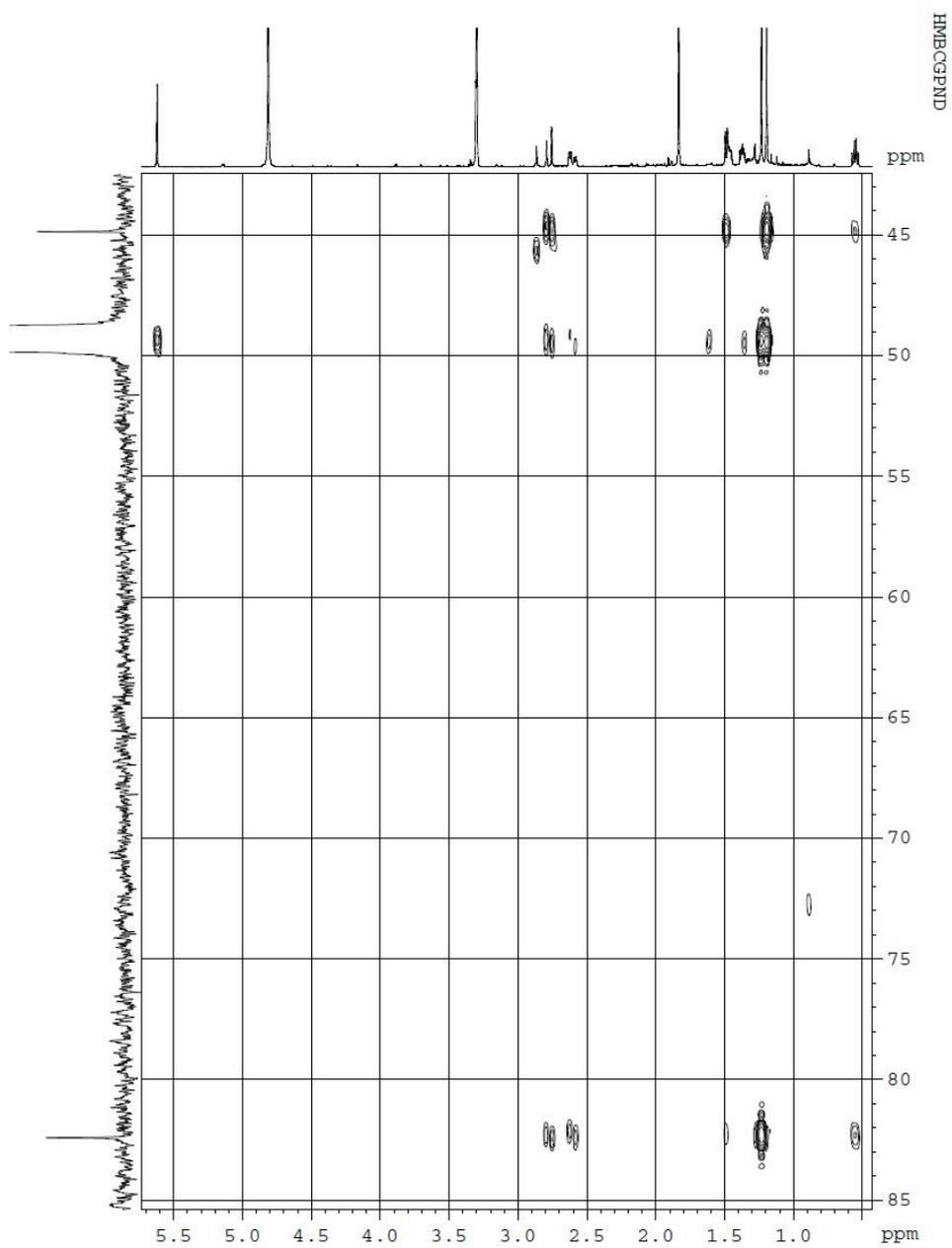


图5-2 化合物1的HMBC图（放大谱2）

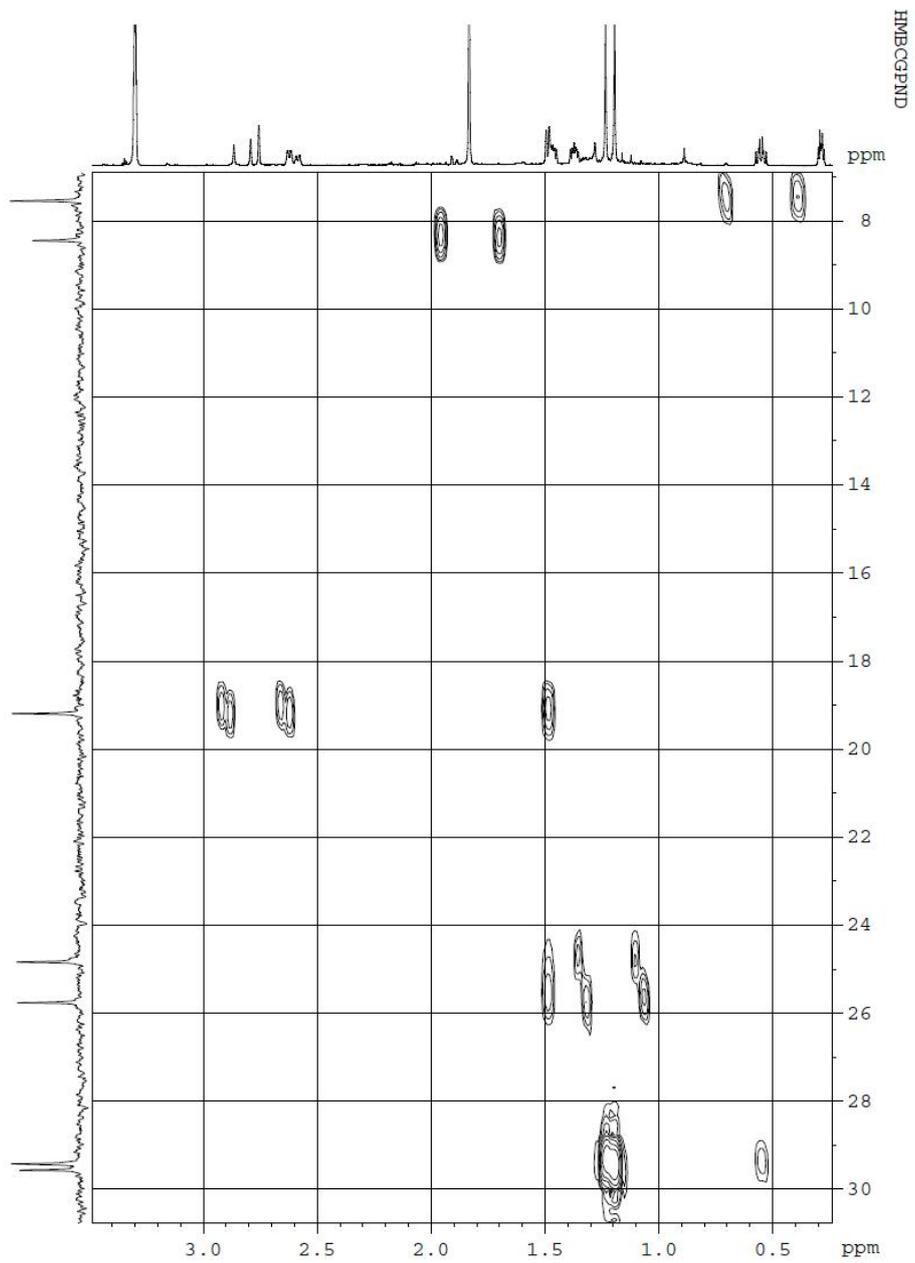


图5-3 化合物1的HMBC图（放大谱3）

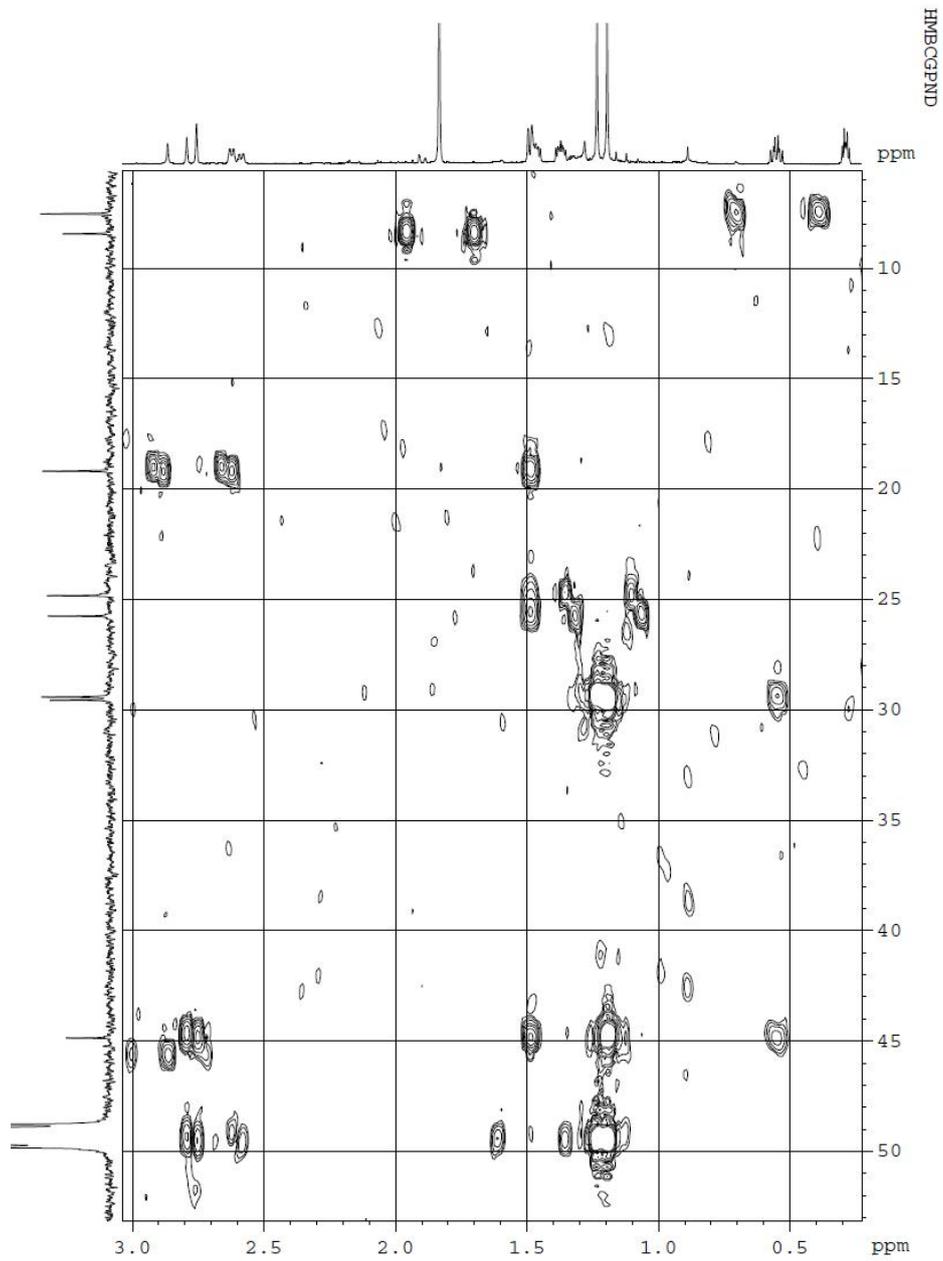


图5-4 化合物1的HMBC图（放大谱4）

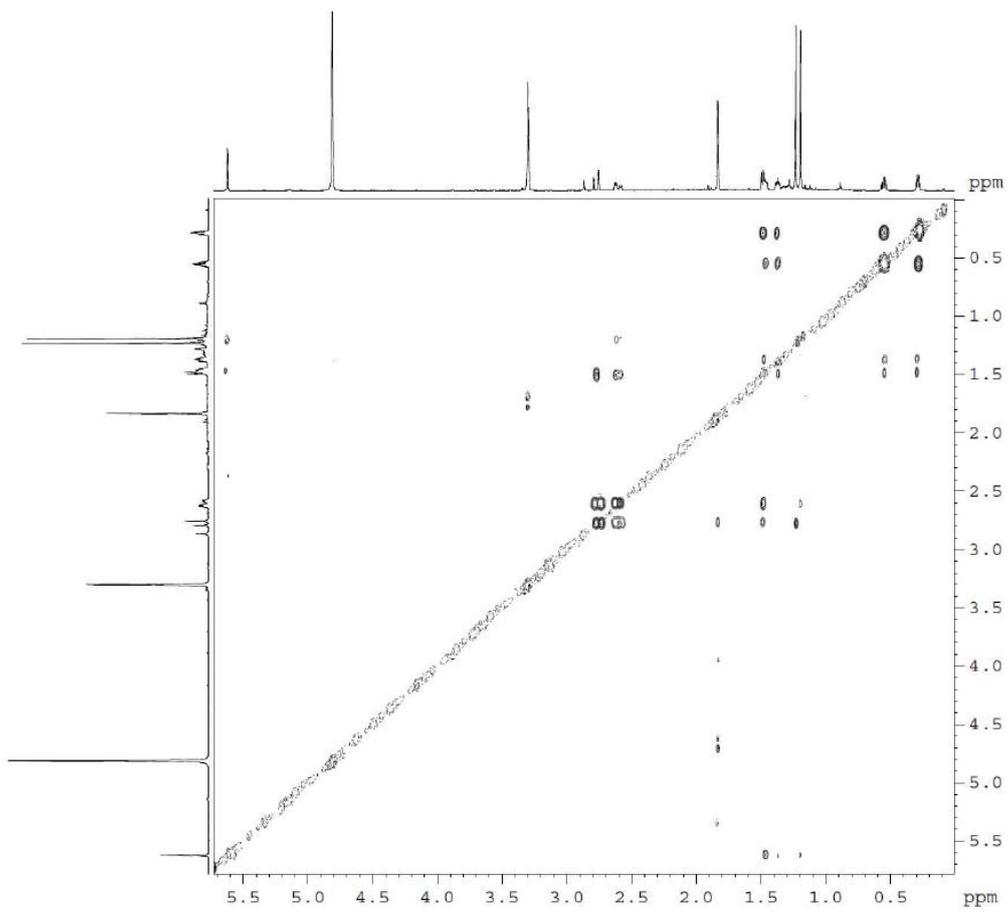


图6 化合物1的 ^1H - ^1H COSY图

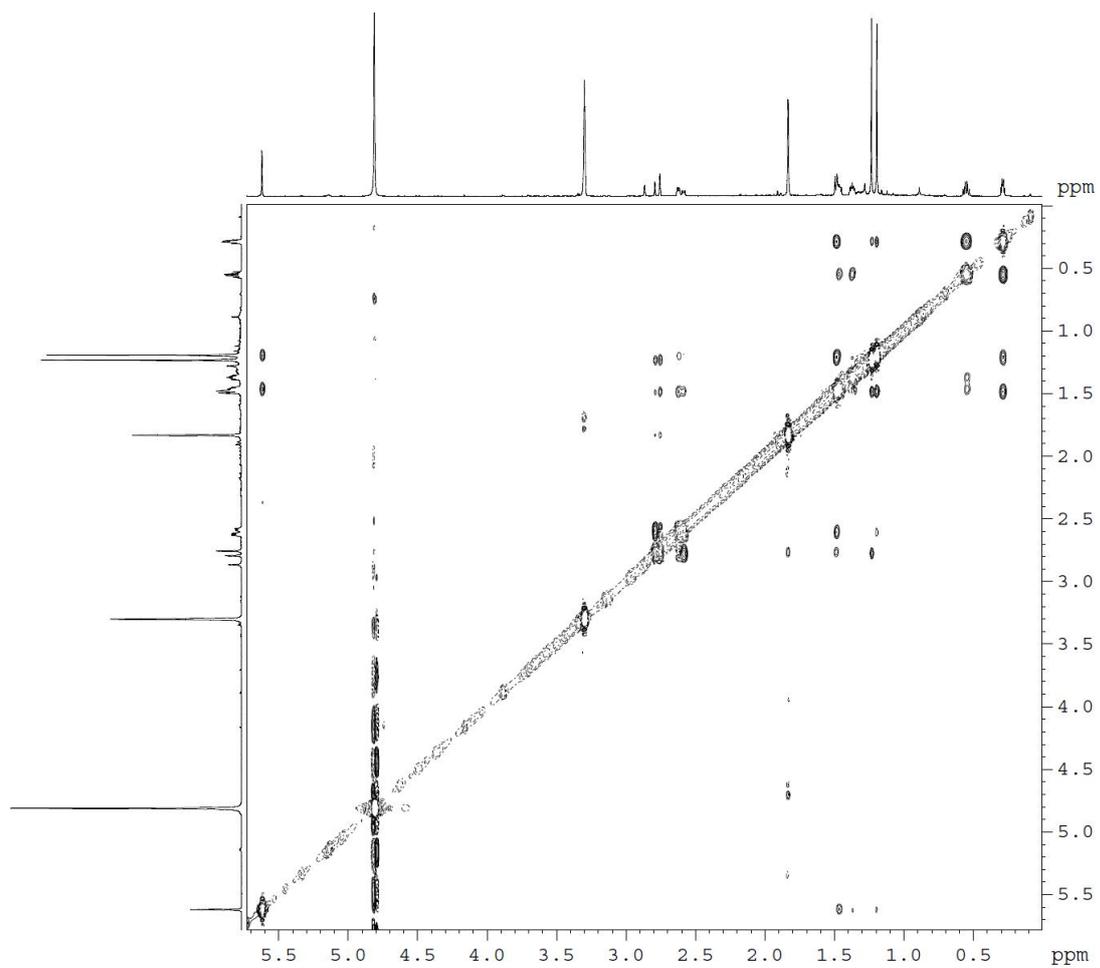


图7 化合物1的NOESY图

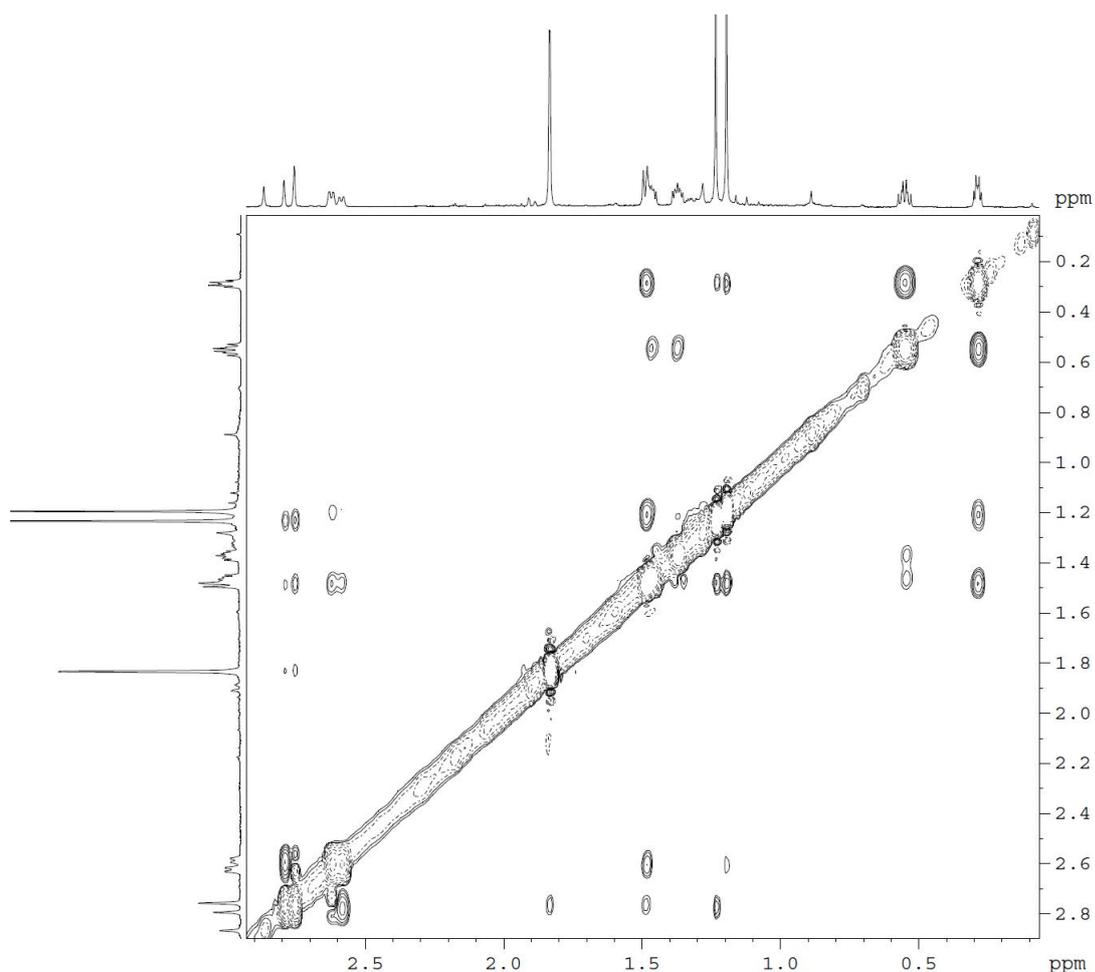


图7-1 化合物1的NOESY图（放大谱）

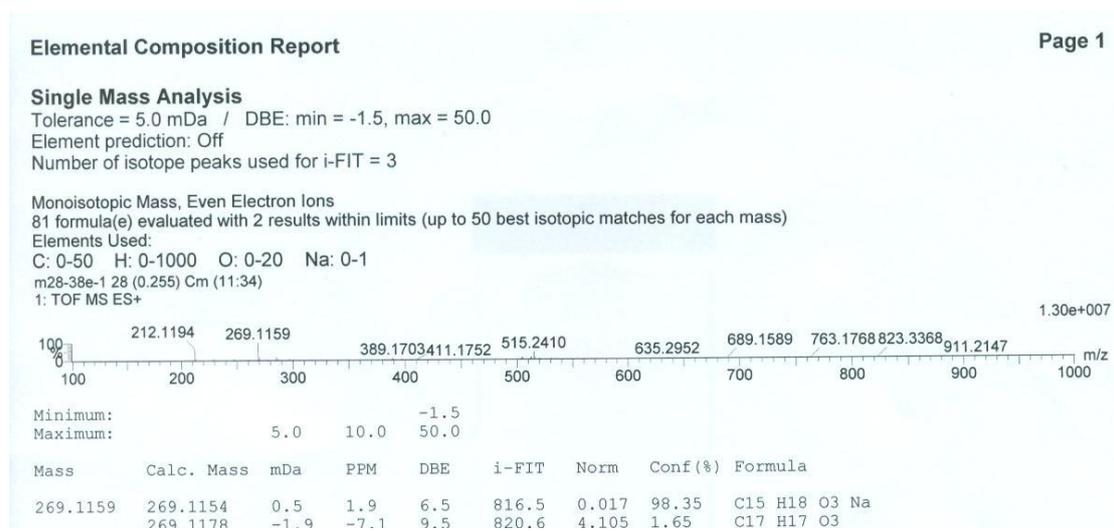


图8 化合物1的HR-ESI-MS图

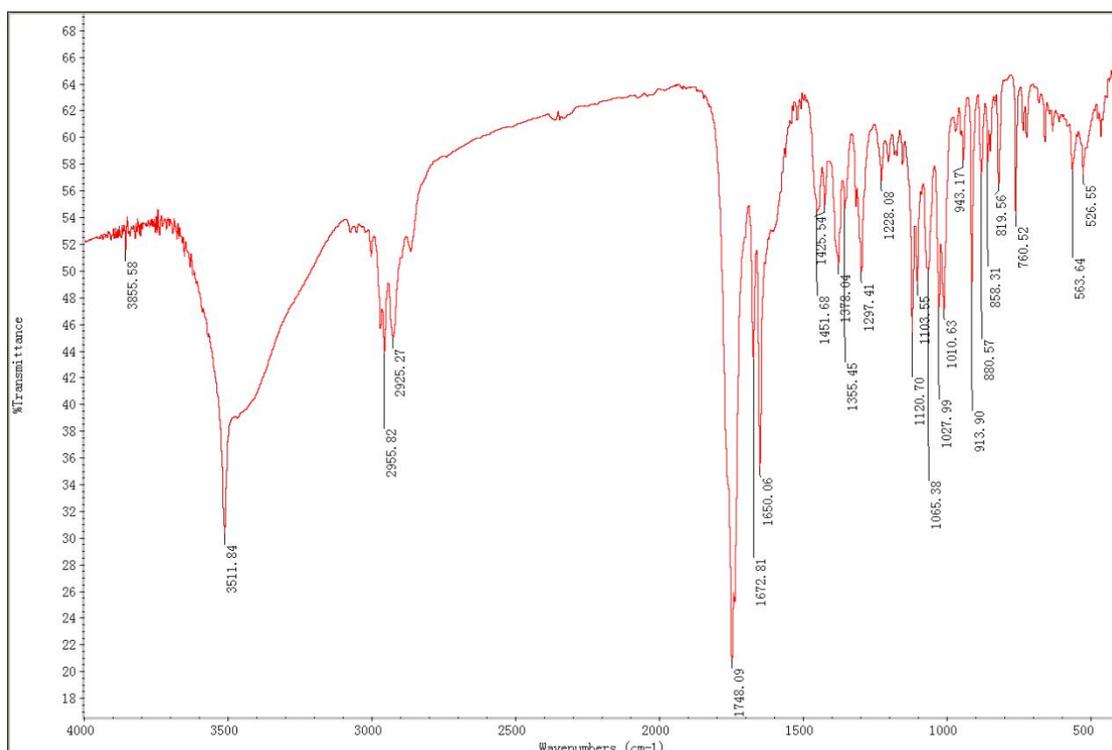
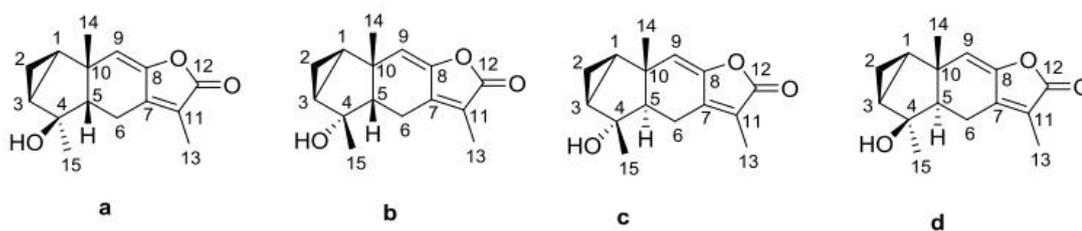


图9 化合物1的IR图



	A	B	C	D	E	F	G
1	Functional		Solvent?		Basis Set		Type of
2	mPW1PW91		PCM		6-31G(d)		Shielding
3							
12			DP4+	0.00%	100.00%	0.00%	0.00%
14	Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4
15	C		7.5	187.6	185.4	180.0	180.3
16	C		29.4	166.7	165.7	162.5	163.2
17	C		82.4	117.0	115.8	119.4	119.4
18	C		48.9	147.9	148.2	128.9	130.9
19	C		44.8	150.9	150.1	152.1	149.9
20	C		29.5	165.9	165.7	166.8	165.1
21	C		19.1	172.8	173.4	171.8	171.7
22	C	x	151.2	50.8	50.2	49.2	49.1
23	C	x	149.6	51.6	50.7	49.9	50.0
24	C	x	116.3	80.0	81.2	73.2	73.1
25	C	x	119.2	76.9	77.7	74.3	74.7
26	C	x	174.4	31.91	31.80	32.36	32.33
27	C		8.4	183.19	183.42	183.29	183.17
28	C		25.7	169.03	169.19	170.86	169.54
29	C		24.8	166.90	171.48	171.98	166.61

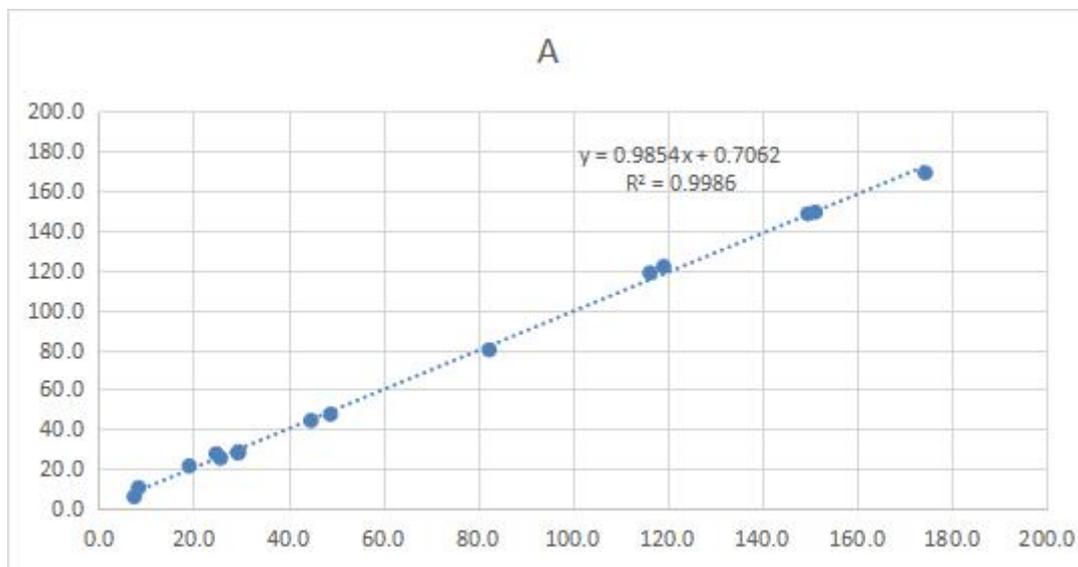
	A	B	C	D	E	F
1	Functional		Solvent?		Basis Set	
2	mPW1PW91		PCM		6-31G(d)	
3						
4			Isomer 1	Isomer 2	Isomer 3	Isomer 4
5	sDP4+ (H data)		0.73%	99.27%	0.00%	0.00%
6	sDP4+ (C data)		0.19%	99.81%	0.00%	0.00%
7	sDP4+ (all data)		0.00%	100.00%	0.00%	0.00%
8	uDP4+ (H data)		4.10%	95.90%	0.00%	0.00%
9	uDP4+ (C data)		0.80%	99.20%	0.00%	0.00%
10	uDP4+ (all data)		0.03%	99.97%	0.00%	0.00%
11	DP4+ (H data)		0.03%	99.97%	0.00%	0.00%
12	DP4+ (C data)		0.00%	100.00%	0.00%	0.00%
13	DP4+ (all data)		0.00%	100.00%	0.00%	0.00%

A-DP4+		构象		1	2					
		权重 (%)		91.29	8.71					
实验编号	实验值	计算编号		权重后	计算值	计算-实验	取平方	平均值	RMSE	
2	7.5	1	187.5797	187.7356	187.5933	5.9	-1.6	2.567417	5.155832	2.27
3	29.4	2	166.5748	167.5348	166.6584	27.8	-1.6	2.40595		
4	82.4	3	116.9484	117.2828	116.9775	79.9	-2.5	6.043371		
5	48.9	4	148.1616	145.6741	147.9449	47.5	-1.4	2.042435		
10	44.8	5	150.9616	150.5217	150.9233	44.3	-0.5	0.204373		
1	29.5	6	165.7997	167.1026	165.9132	28.6	-0.9	0.756378		
6	19.1	7	172.7854	173.2285	172.824	21.4	2.3	5.216585		
7	151.2	8	50.7394	51.3107	50.78916	149.3	-1.9	3.4472		
8	149.6	9	51.5209	51.883	51.55244	148.5	-1.1	1.117245		
9	116.3	10	80.0227	79.6445	79.98976	118.7	2.4	5.881178		
11	119.2	11	76.911	76.9229	76.91204	122.0	2.8	7.574896		
12	174.4	12	31.8989	32.0346	31.91072	169.1	-5.3	27.68567		
13	8.4	15	183.1869	183.2375	183.1913	10.5	2.1	4.466296		
14	25.7	18	169.0178	169.1161	169.0264	25.4	-0.3	0.111567		
15	24.8	19	166.8676	167.2363	166.8997	27.6	2.8	7.816918		

B-DP4+		构象		1	2					
		权重 (%)		99.17	0.83					
实验编号	实验值	计算编号		权重后	计算值	计算-实验	取平方	平均值	RMSE	
2	7.5	1	185.3535	185.7009	185.3564	8.2	0.7	0.55231	3.340468	1.83
3	29.4	2	165.6874	164.9754	165.6815	28.9	-0.5	0.277475		
4	82.4	3	115.8238	115.6746	115.8226	81.2	-1.2	1.555735		
5	48.9	4	148.2329	147.8319	148.2296	47.2	-1.7	2.984564		
10	44.8	5	150.1527	149.1988	150.1448	45.2	0.4	0.132657		
1	29.5	6	165.666	165.552	165.6651	28.9	-0.6	0.37152		
6	19.1	7	173.367	173.5012	173.3681	20.8	1.7	2.935907		
7	151.2	8	50.2525	49.2526	50.2442	149.9	-1.3	1.651862		
8	149.6	9	50.7054	51.1838	50.70937	149.4	-0.2	0.029929		
9	116.3	10	81.1595	81.2633	81.16036	117.5	1.2	1.43444		
11	119.2	11	77.6374	79.8787	77.656	121.2	2.0	3.889449		
12	174.4	12	31.8036	31.4691	31.80082	169.3	-5.1	26.48632		
13	8.4	15	183.4211	183.5762	183.4224	10.3	1.9	3.500876		
14	25.7	18	169.1922	169.1491	169.1918	25.2	-0.5	0.257588		
15	24.8	19	171.5059	168.9358	171.4846	22.8	-2.0	4.046388		

C-DP4+		构象			1	2	3				
		权重 (%)			44.09	45.64	10.27				
计算编号					权重后	计算值	计算-实验	取平方	平均值	RMSE	
1	180.0855	179.8967	180.2028	180.0114	13.8	6.3	40.2929	40.0939	6.33		
2	162.2092	162.6207	163.4725	162.5267	32.2	2.8	7.734724				
3	119.471	119.2253	119.4602	119.3578	77.4	-5.0	24.54319				
4	131.5189	126.5796	128.3654	128.9407	67.4	18.5	342.1639				
5	152.0254	152.3862	151.3173	152.1173	43.1	-1.7	2.903982				
6	166.7393	166.7945	167.0637	166.7978	27.7	-1.8	3.23019				
7	171.6366	171.8353	172.0491	171.7697	22.5	3.4	11.48881				
8	49.1431	49.1908	49.6786	49.21987	151.0	-0.2	0.044599				
9	49.8797	49.8567	50.1833	49.90038	150.3	0.7	0.455979				
10	73.3047	73.2173	73.0317	73.23677	125.8	9.5	90.36292				
11	74.3984	74.229	74.4869	74.33017	124.7	5.5	29.80568				
12	32.3002	32.4087	32.4169	32.3617	168.7	-5.7	32.88559				
15	183.2691	183.3111	183.3217	183.2937	10.4	2.0	4.024149				
18	170.8333	170.8622	170.9527	170.8588	23.4	-2.3	5.086675				
19	170.8167	173.429	170.4962	171.976	22.3	-2.5	6.385191				

D-DP4+		构象			1	2	3				
		权重 (%)			48.71	47.8	3.49				
实验编号	实验值	计算编号			权重后	计算值	计算-实验	取平方	平均值	RMSE	
2	7.5	1	180.2724	180.284	180.3146	180.2794	13.6	6.1	36.80384	34.31307	5.86
3	29.4	2	163.2075	163.2105	164.0306	163.2377	31.4	2.0	4.144129		
4	82.4	3	119.3895	119.3744	119.9471	119.4017	77.4	-5.0	25.00233		
5	48.9	4	130.8818	130.8545	131.0581	130.8749	65.4	16.5	271.248		
10	44.8	5	149.8282	149.8482	150.3028	149.8543	45.5	0.7	0.447268		
1	29.5	6	165.0989	165.0945	164.9611	165.092	29.5	0.0	7.46E-05		
6	19.1	7	171.7321	171.7093	172.345	171.7426	22.5	3.4	11.68195		
7	151.2	8	49.0538	49.0492	49.7617	49.07631	151.1	-0.1	0.003679		
8	149.6	9	50.0243	50.0422	50.2754	50.04162	150.1	0.5	0.277906		
9	116.3	10	73.1436	73.1433	73.2299	73.14647	125.9	9.6	92.17211		
11	119.2	11	74.7216	74.7297	74.6884	74.72431	124.2	5.0	25.46399		
12	174.4	12	32.3298	32.3228	32.4922	32.33212	168.7	-5.7	32.5308		
13	8.4	15	183.1468	183.1919	183.16	183.1688	10.5	2.1	4.566521		
14	25.7	18	169.5078	169.5433	169.9169	169.539	24.8	-0.9	0.759671		
15	24.8	19	166.5975	166.6036	166.9342	166.6122	27.9	3.1	9.593776		



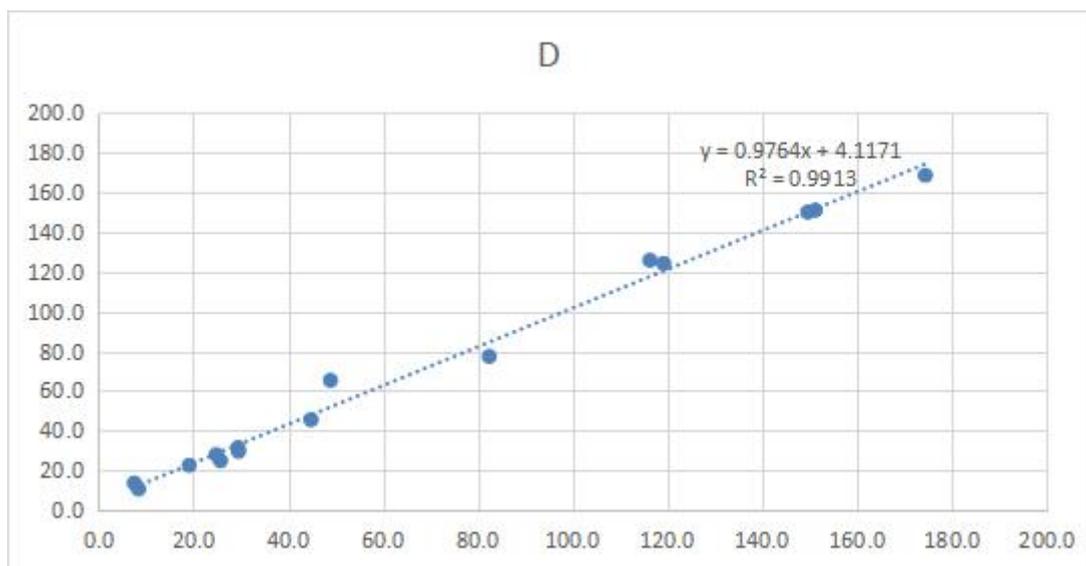
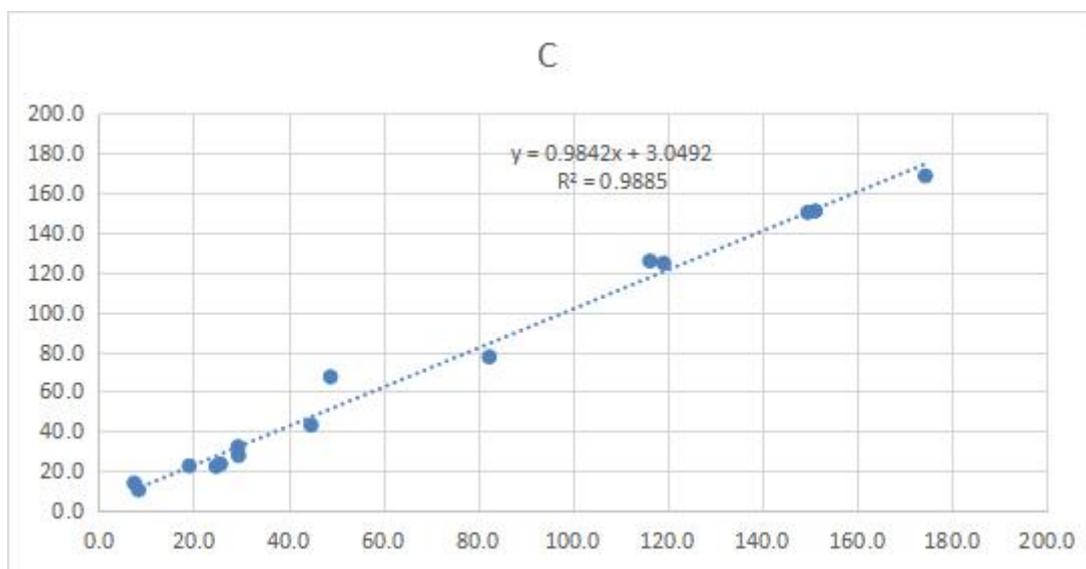
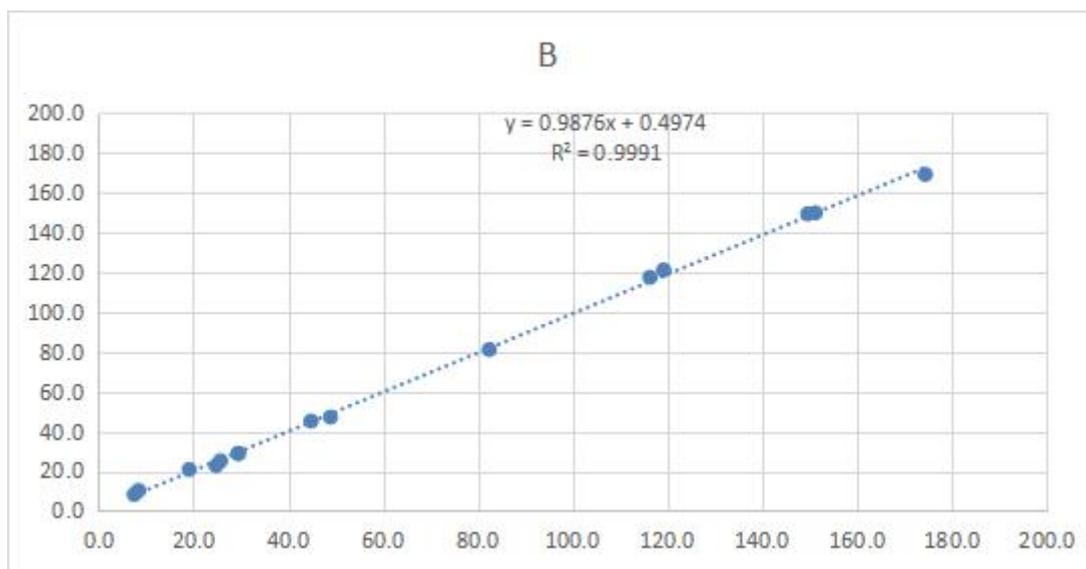


图 10 化合物 1 的 DP4+分析结果

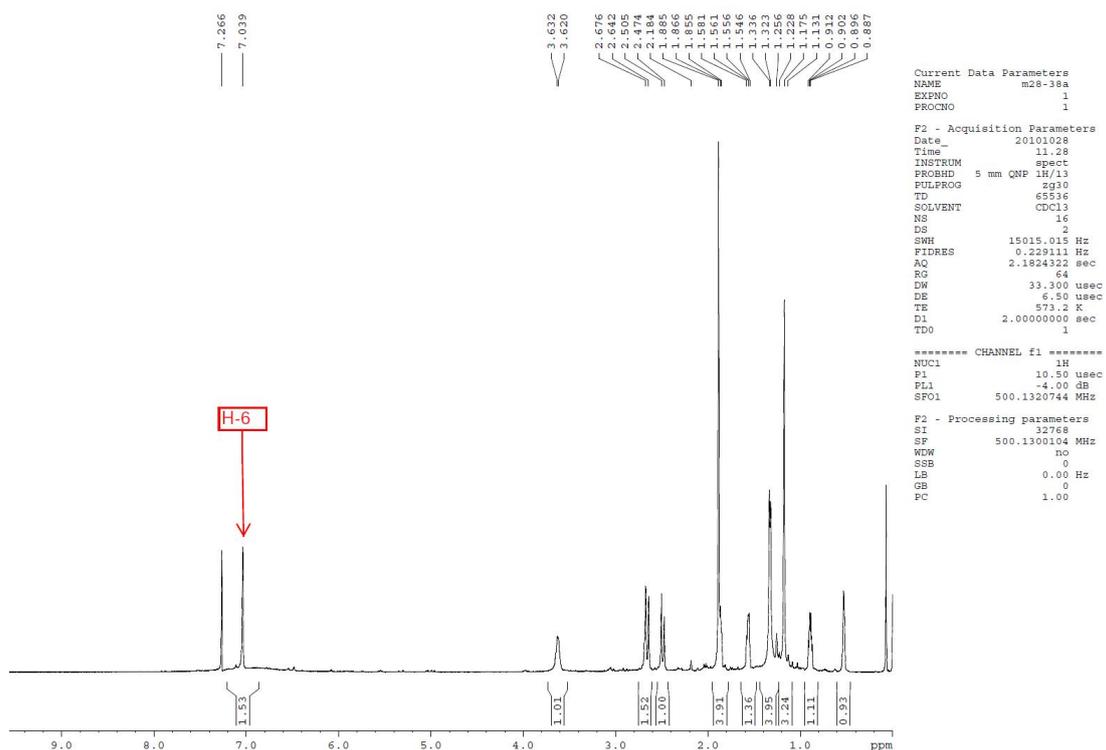


图11 化合物2的¹H NMR图(500 MHz, CDCl₃)

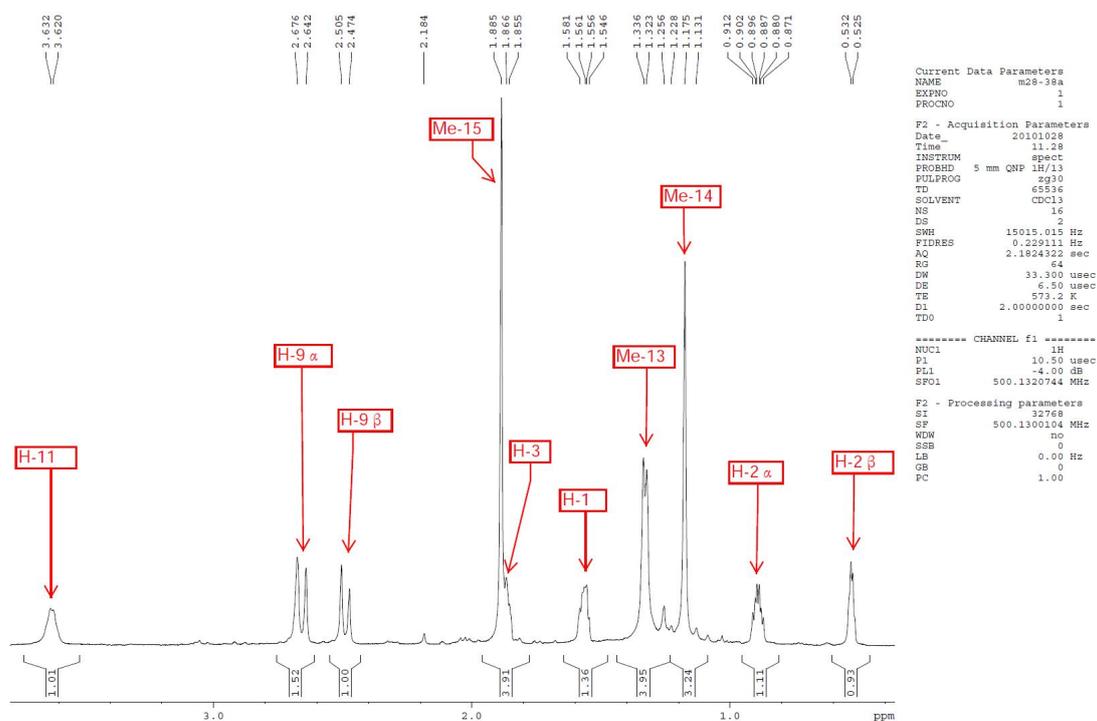


图11-1 化合物2的¹H NMR图(放大谱)

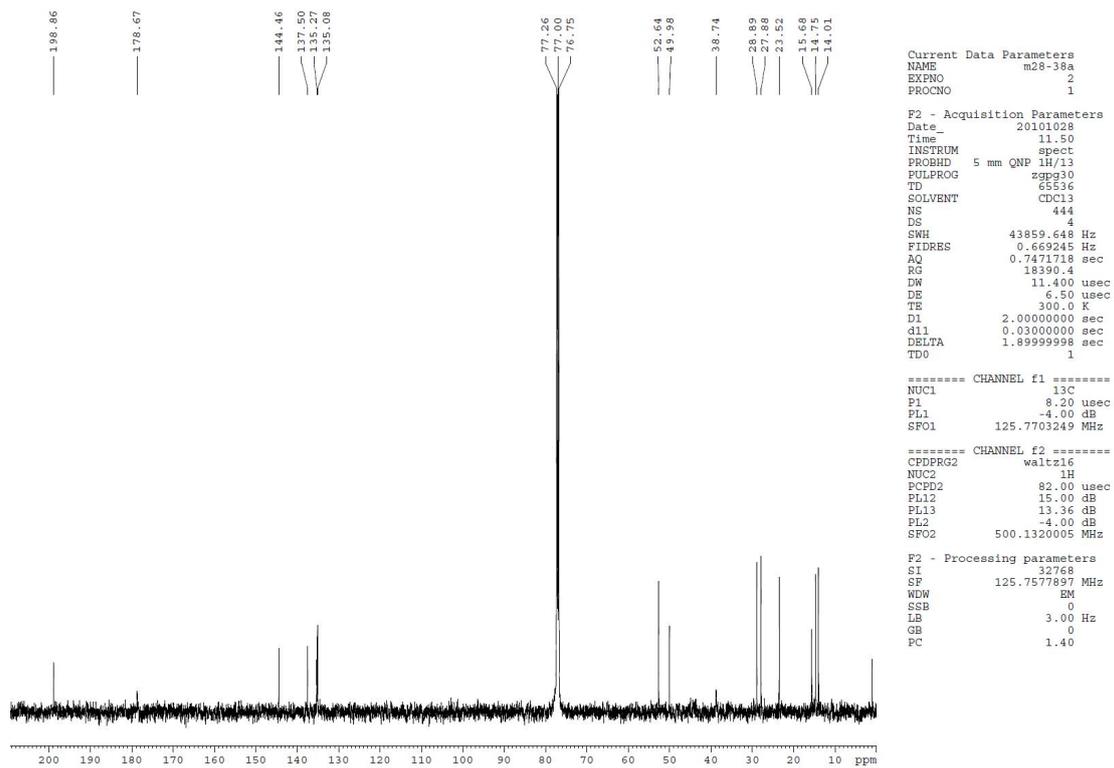


图12 化合物2的¹³C NMR图(125 MHz, CDCl₃)

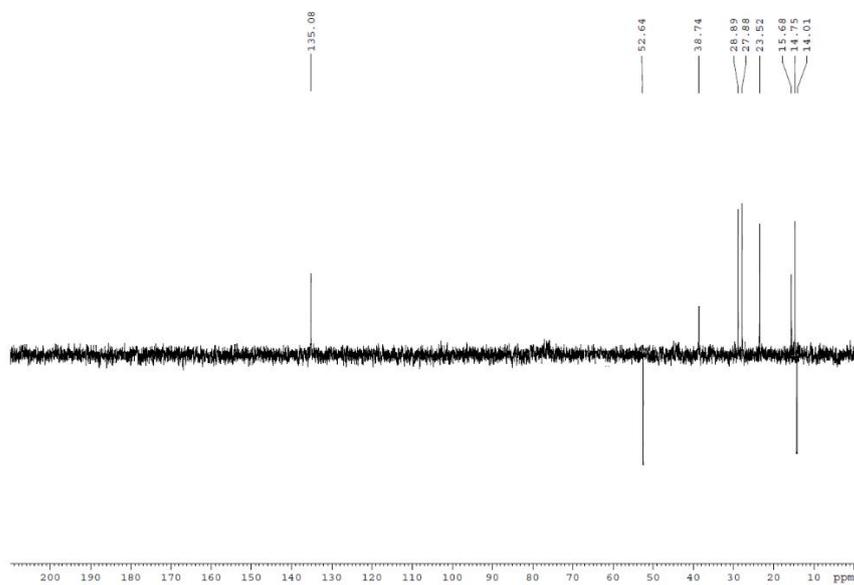


图13 化合物2的DEPT图

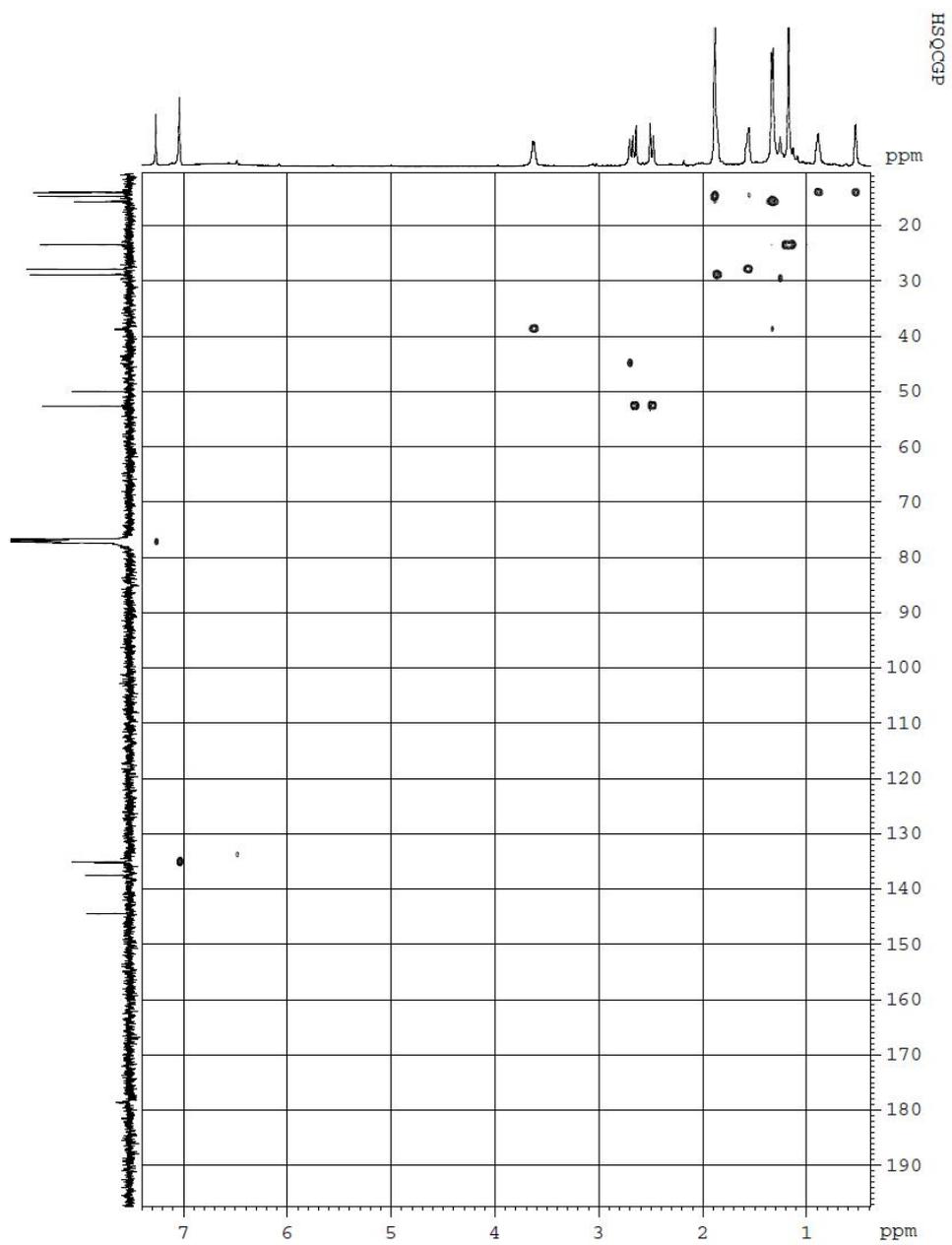


图14 化合物2的HSQC图

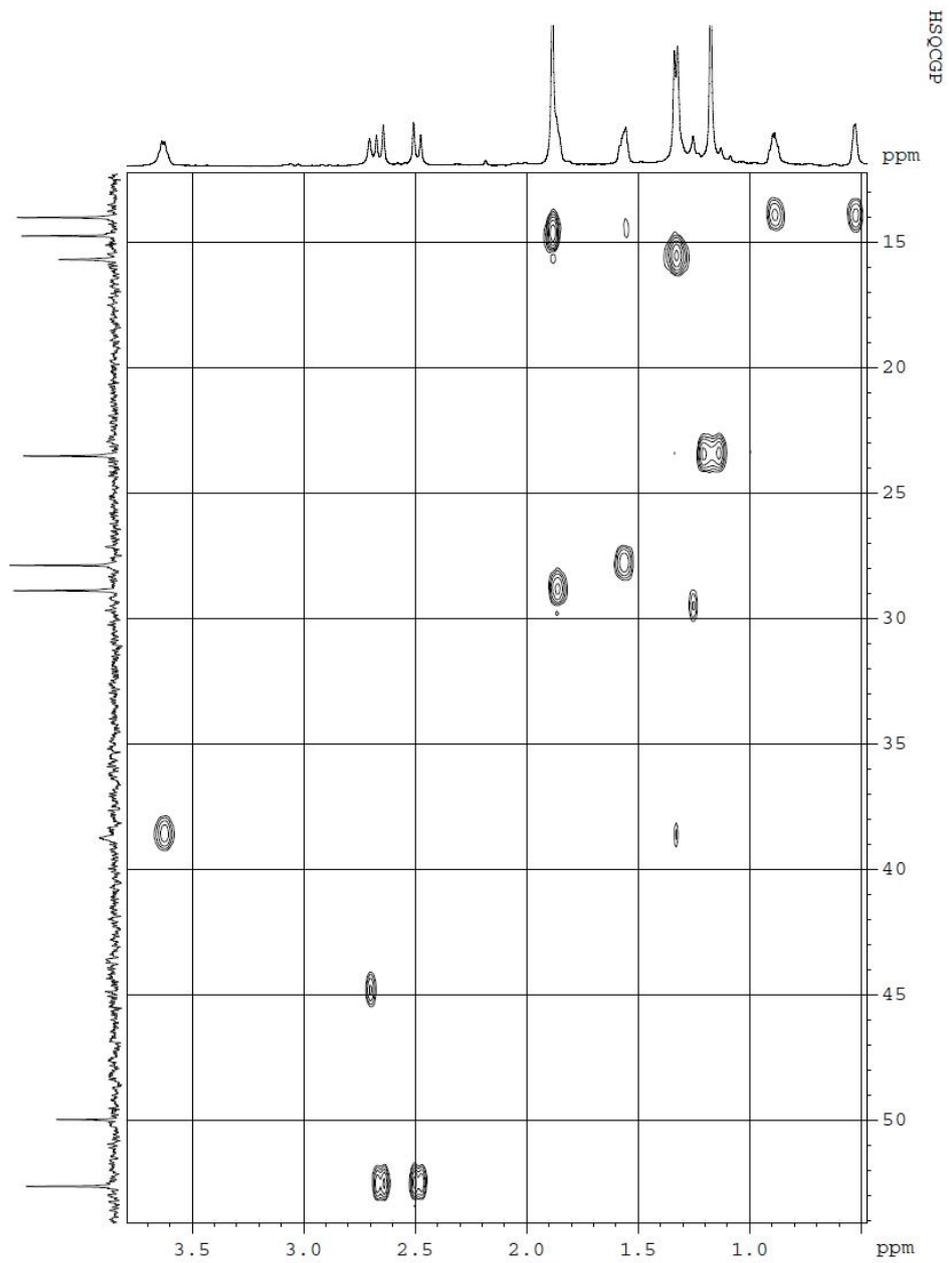


图14-1 化合物2的HSQC图（放大图）

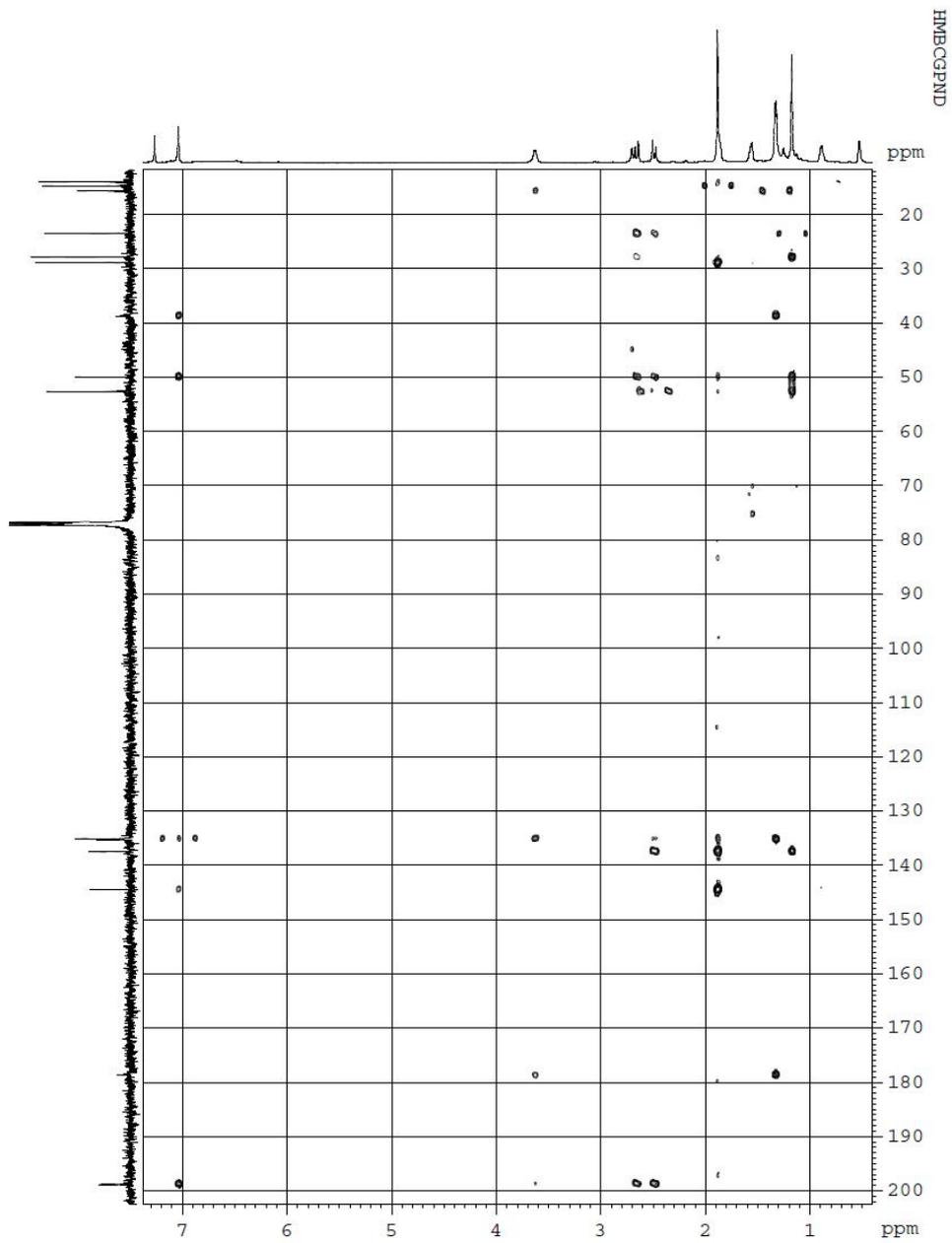


图15 化合物2的HMBC图

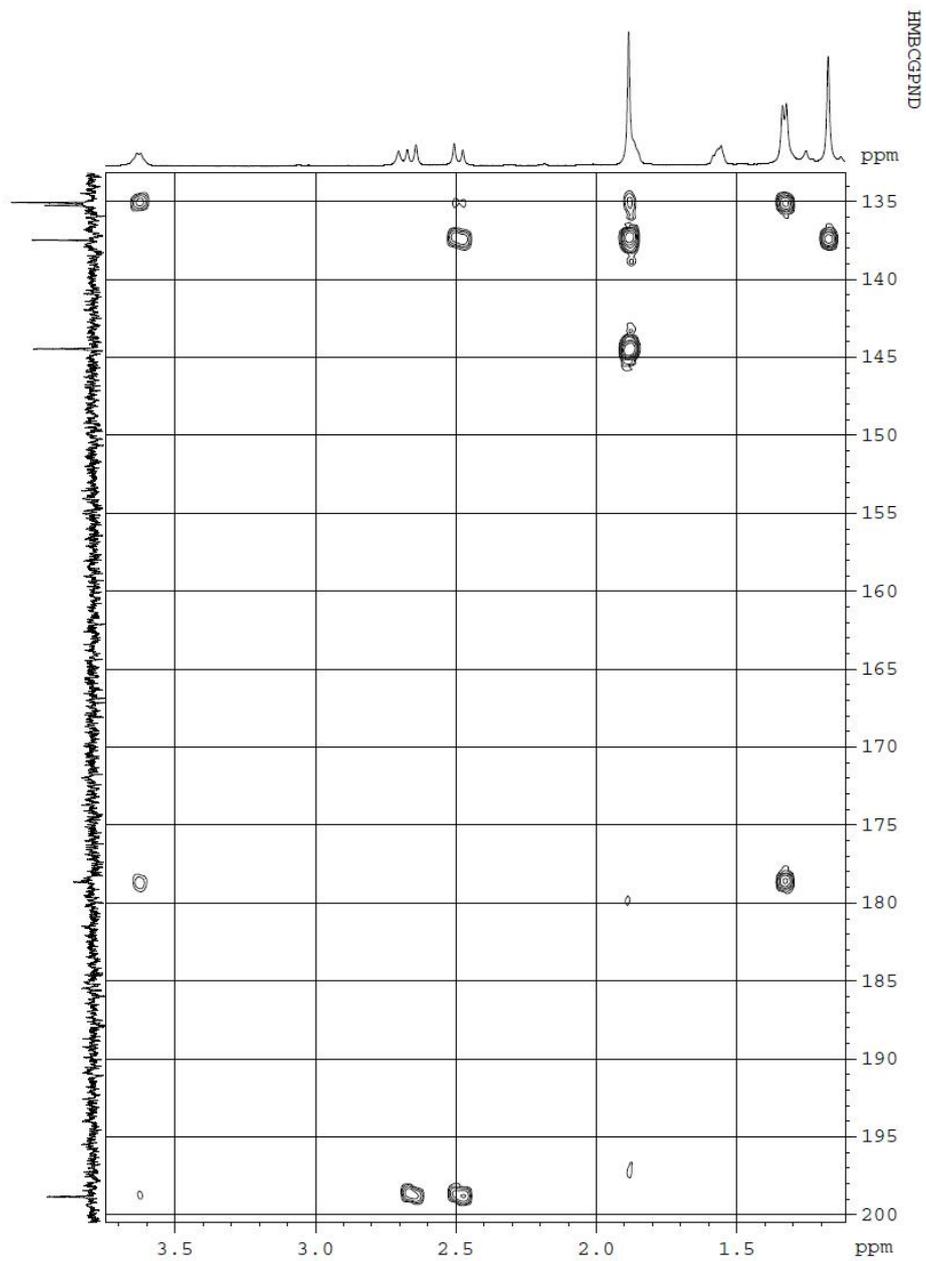


图15-1 化合物2的HMBC图（放大图1）

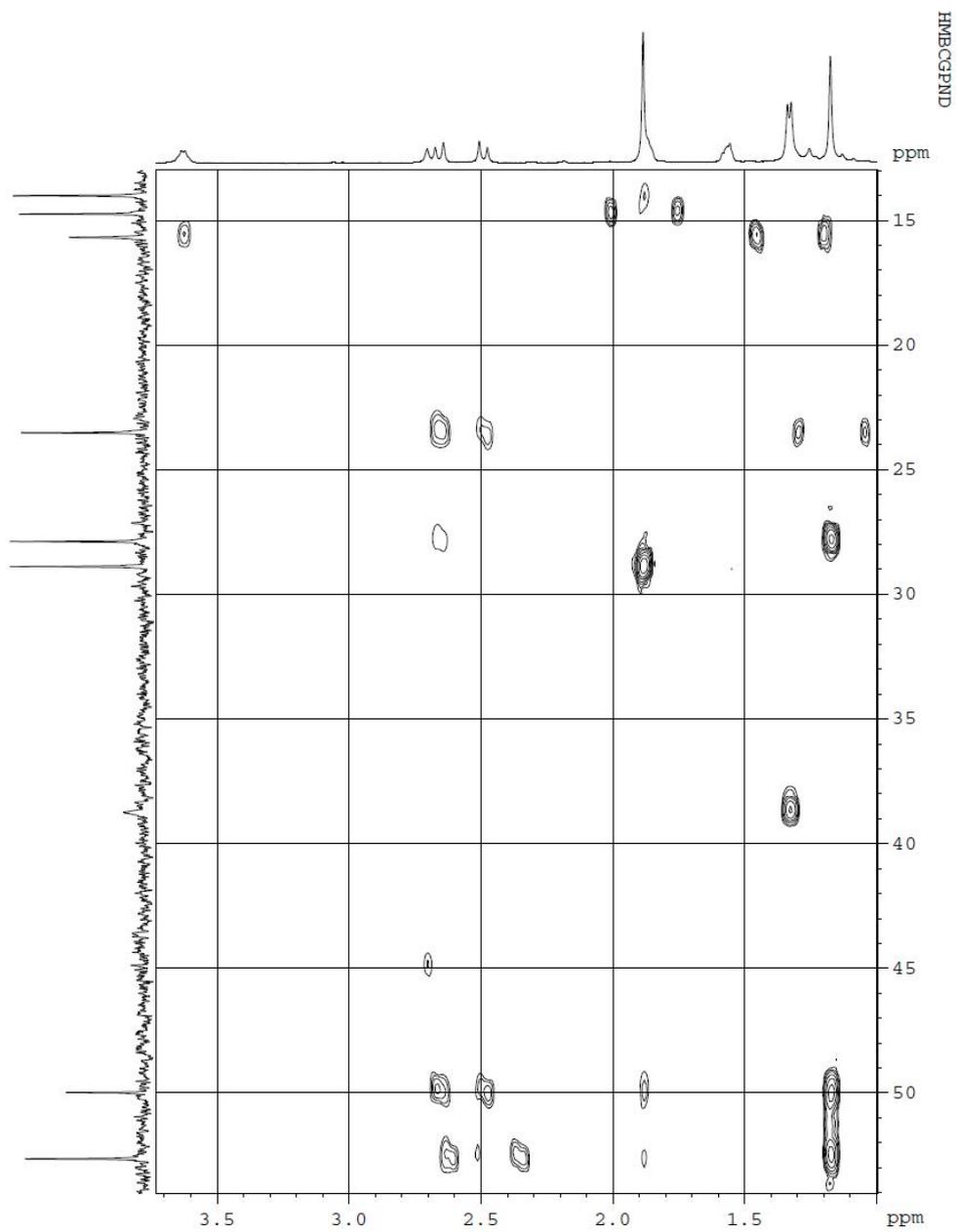


图15-2 化合物2的HMBC图（放大图2）

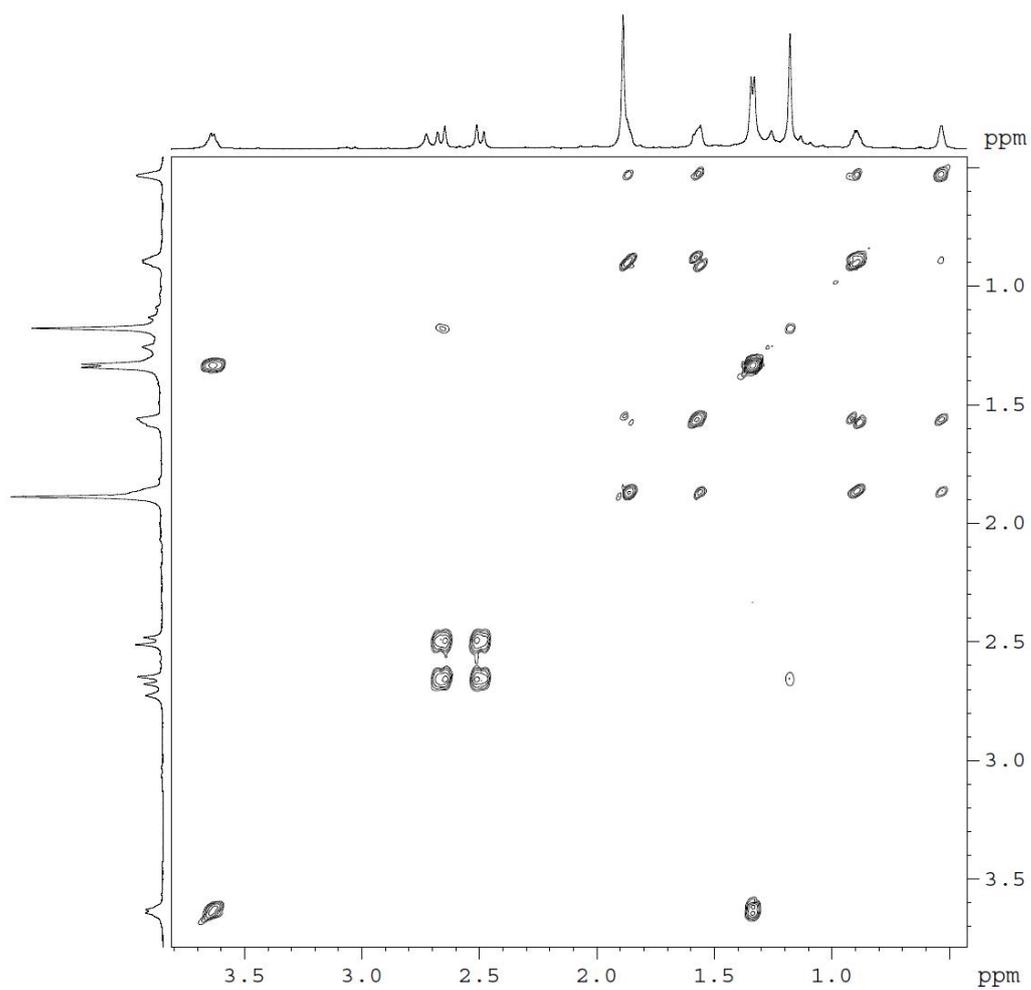


图16 化合物2的 ^1H - ^1H COSY图

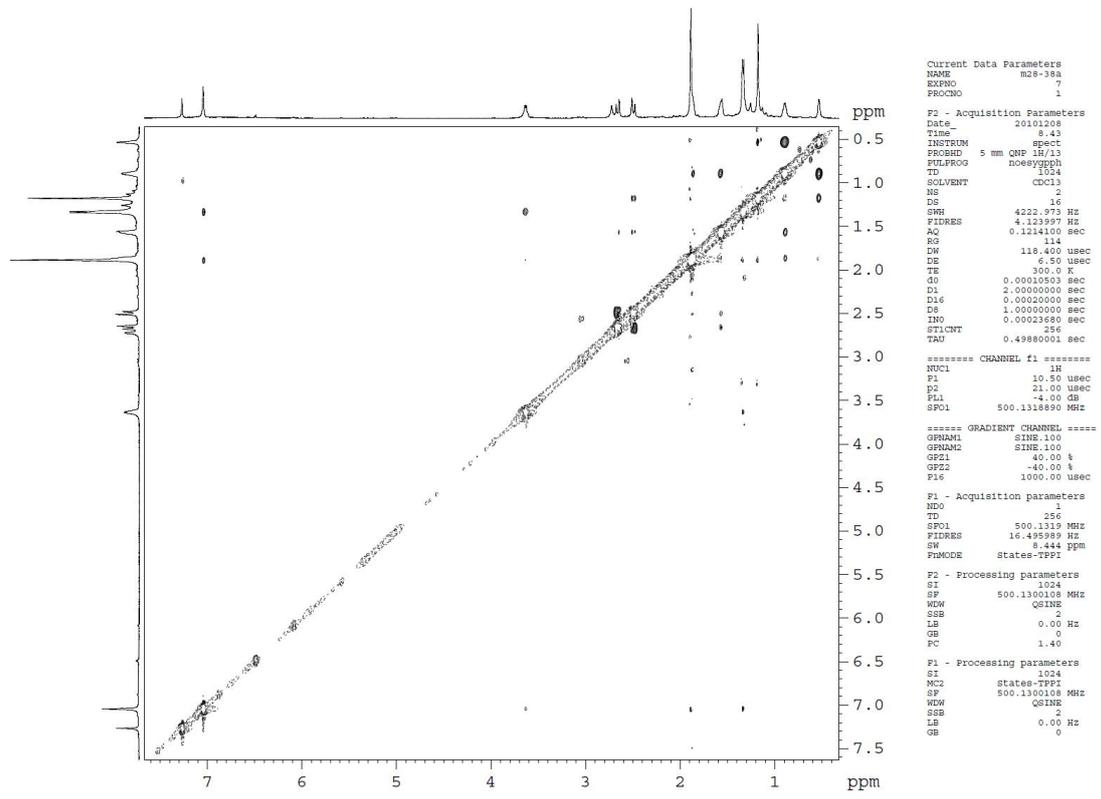


图17 化合物2的NOESY图

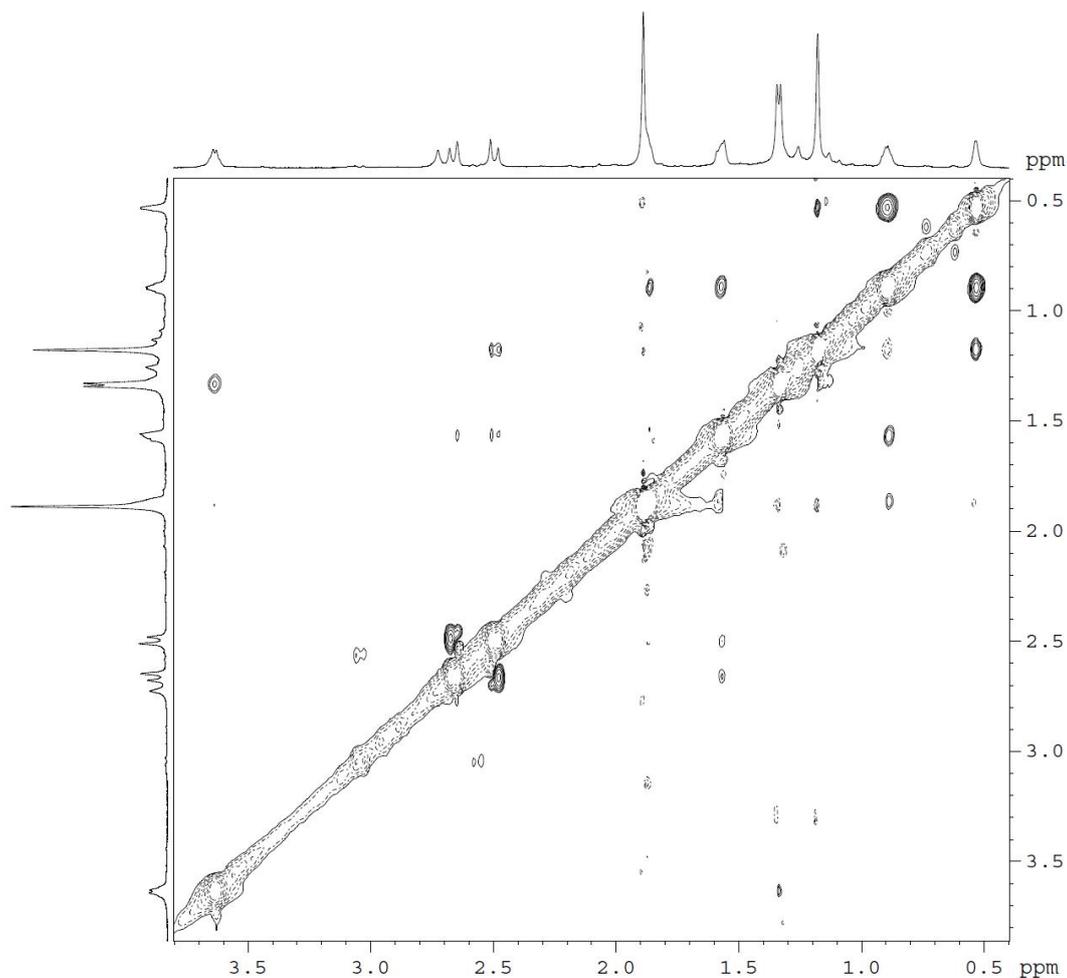


图17-1 化合物2的NOESY图（放大谱）

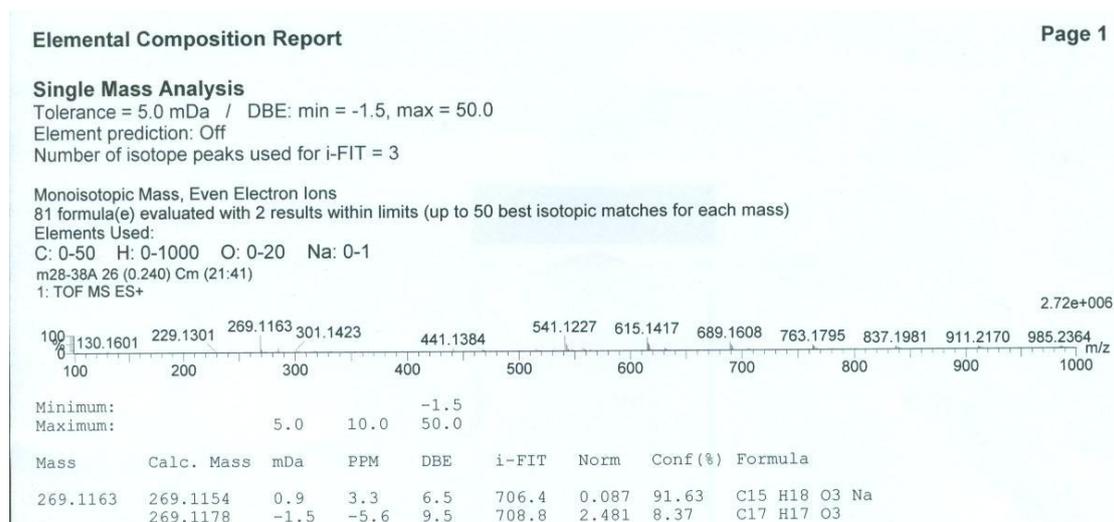


图18 化合物2的HR-ESI-MS图

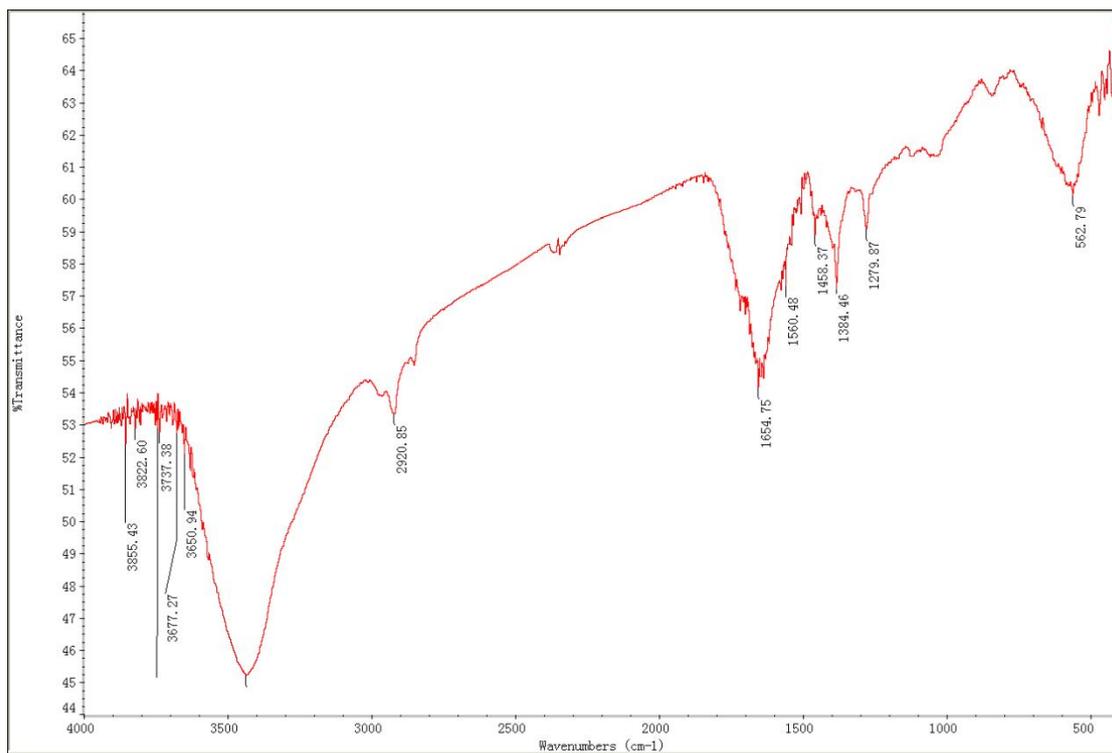
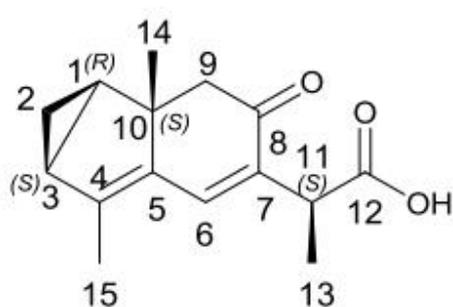
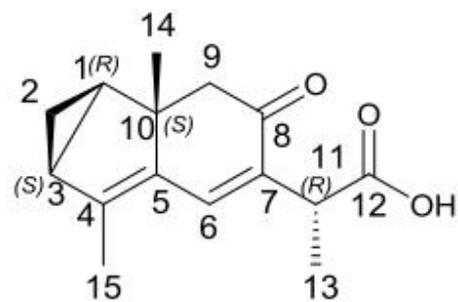


图19 化合物2的IR图



A



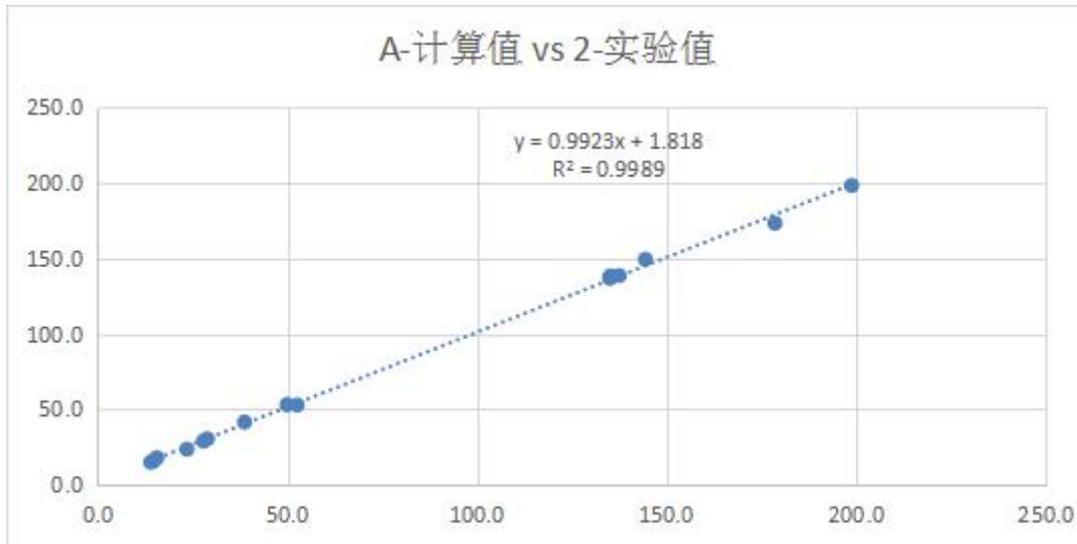
B

Nuclei	sp2?	DP4+	100.00%	0.00%
		xperimenta	Isomer 1	Isomer 2
C		14	179.1	179.2
C		28.9	164.3	164.6
C	x	144.4	50.7	51.4
C	x	137.5	61.0	61.0
C		49.9	142.7	142.0
C		27.9	165.7	166.0
C		135	62.7	61.6
C	x	135.2	61.2	60.8
C	x	198.8	4.0	3.3
C		52.6	142.9	142.8
C		38.7	153.7	152.5
C	x	178.6	27.86	28.44
C		15.6	176.19	176.77
C		14.7	178.18	178.25
C		23.5	170.85	170.86

	Isomer 1	Isomer 2
sDP4+ (H data)	100.00%	0.00%
sDP4+ (C data)	93.82%	6.18%
sDP4+ (all data)	100.00%	0.00%
uDP4+ (H data)	50.36%	49.64%
uDP4+ (C data)	48.18%	51.82%
uDP4+ (all data)	48.54%	51.46%
DP4+ (H data)	100.00%	0.00%
DP4+ (C data)	93.38%	6.62%
DP4+ (all data)	100.00%	0.00%

	构象 权重 (%)	1	2	3	4	5	6							
		17	16.52	36.8	1.78	19.17	8.73							
实验编号	2-实验值	计算编号	权重后						计算值	计算-实验	取平方	平均值	RMSE	
2	14.0	1	179.1269	179.1803	179.0081	179.3501	179.205	179.159	179.1138	14.8	0.8	0.622323	6.321266	2.51
3	28.9	2	164.3352	164.3233	164.2319	164.4473	164.5399	164.2542	164.3294	30.3	1.4	1.934847		
4	144.4	3	50.2935	50.3503	50.6498	50.764	51.334	50.7707	50.6835	149.5	5.1	25.54419		
5	137.5	4	61.1827	61.1619	61.0699	61.0048	60.7547	61.1076	61.04598	138.6	1.1	1.18498		
10	49.9	5	142.9982	142.9802	142.6393	142.964	142.1898	142.5668	142.6699	53.0	3.1	9.622285		
1	27.9	6	165.4685	165.4768	165.5131	165.4932	166.2717	165.62	165.6539	28.9	1.0	1.004297		
6	135.0	7	63.3433	63.3543	61.5751	63.5464	64.331	61.4744	62.72422	136.8	1.8	3.344707		
7	135.2	8	61.8967	61.859	60.3143	62.2763	62.0138	59.9164	61.16447	138.5	3.3	10.65582		
8	198.8	9	5.5805	5.5795	3.4707	5.0577	2.3222	3.3445	3.974804	198.4	-0.4	0.136586		
9	52.6	10	142.7705	142.7629	143.0262	142.5398	143.1652	142.8163	142.9389	52.7	0.1	0.014384		
11	38.7	11	156.8088	156.8572	151.5188	153.7349	154.1892	150.147	153.7316	41.4	2.7	7.307632		
12	178.6	12	26.2368	26.2384	29.0226	28.9273	27.9742	28.7687	27.86422	173.4	-5.2	27.23559		
13	15.6	13	175.3966	175.3845	175.6187	175.5857	178.8593	175.9529	176.1921	17.9	2.3	5.073314		
15	14.7	17	178.2202	178.2161	178.1427	178.2275	178.1903	178.1828	178.1821	15.8	1.1	1.135753		
14	23.5	18	170.7977	170.8189	170.852	170.895	170.9242	170.8481	170.8516	23.5	0.0	0.002288		

实验编号	2-实验值	计算编号	B-计算值	计算-实验	取平方	平均值	RMSE
2	14.0	1	14.6	0.6	0.420265	7.52226	2.74
3	28.9	2	30.1	1.2	1.338799		
4	144.4	3	148.7	4.3	18.45877		
5	137.5	4	138.7	1.2	1.363381		
10	49.9	5	53.7	3.8	14.80543		
1	27.9	6	28.5	0.6	0.369195		
6	135.0	7	138.0	3.0	9.014554		
7	135.2	8	138.9	3.7	13.46209		
8	198.8	9	199.2	0.4	0.139821		
9	52.6	10	52.9	0.3	0.064522		
11	38.7	11	42.7	4.0	15.75446		
12	178.6	12	172.8	-5.8	33.91816		
13	15.6	13	17.3	1.7	2.726524		
15	14.7	17	15.7	1.0	0.994335		
14	23.5	18	23.4	-0.1	0.003592		



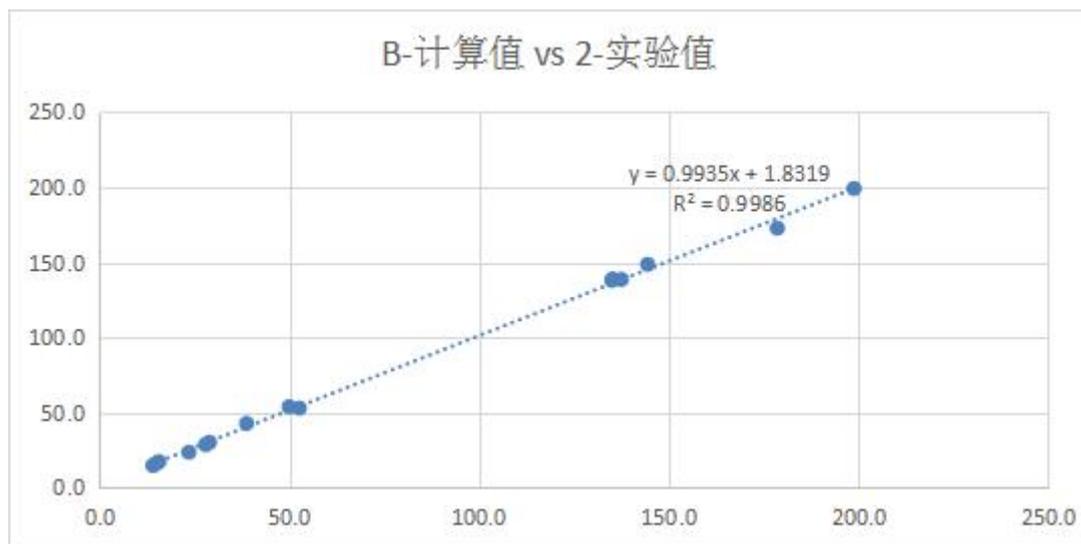


图20 化合物2的DP4+分析结果

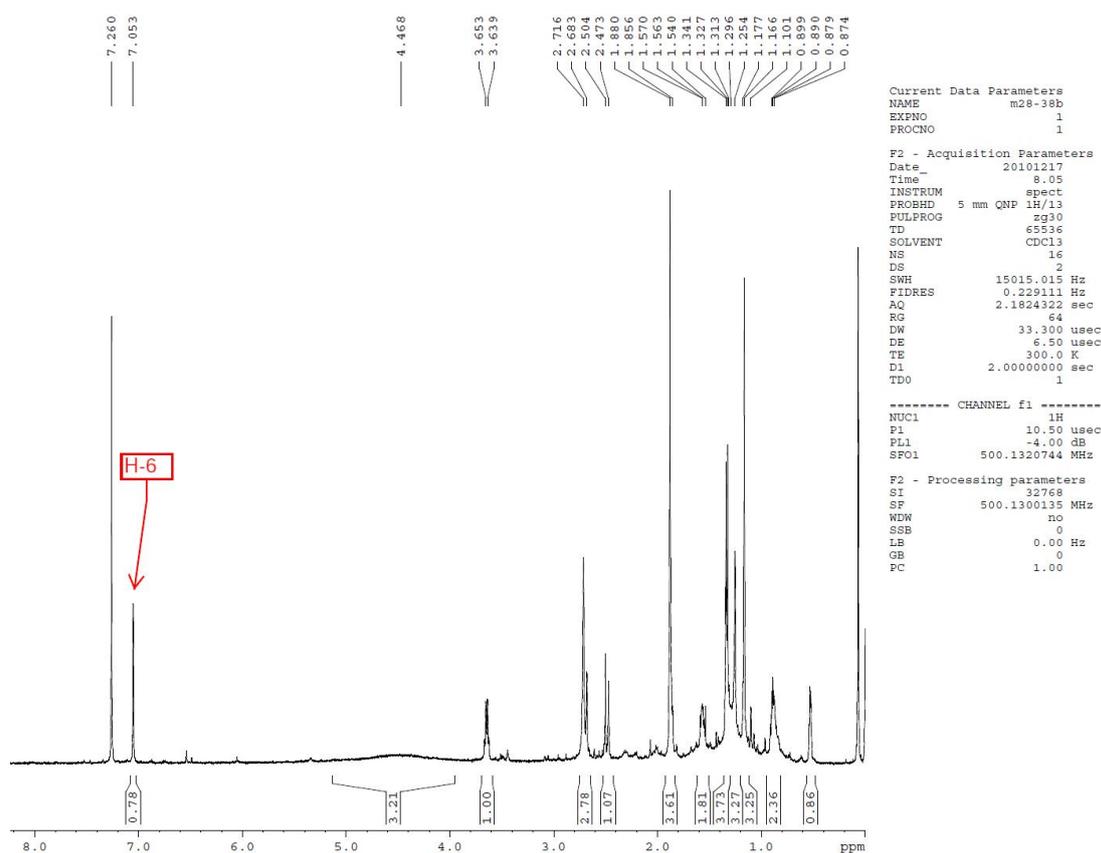


图21 化合物3的¹H NMR图(500 MHz, CDCl₃)

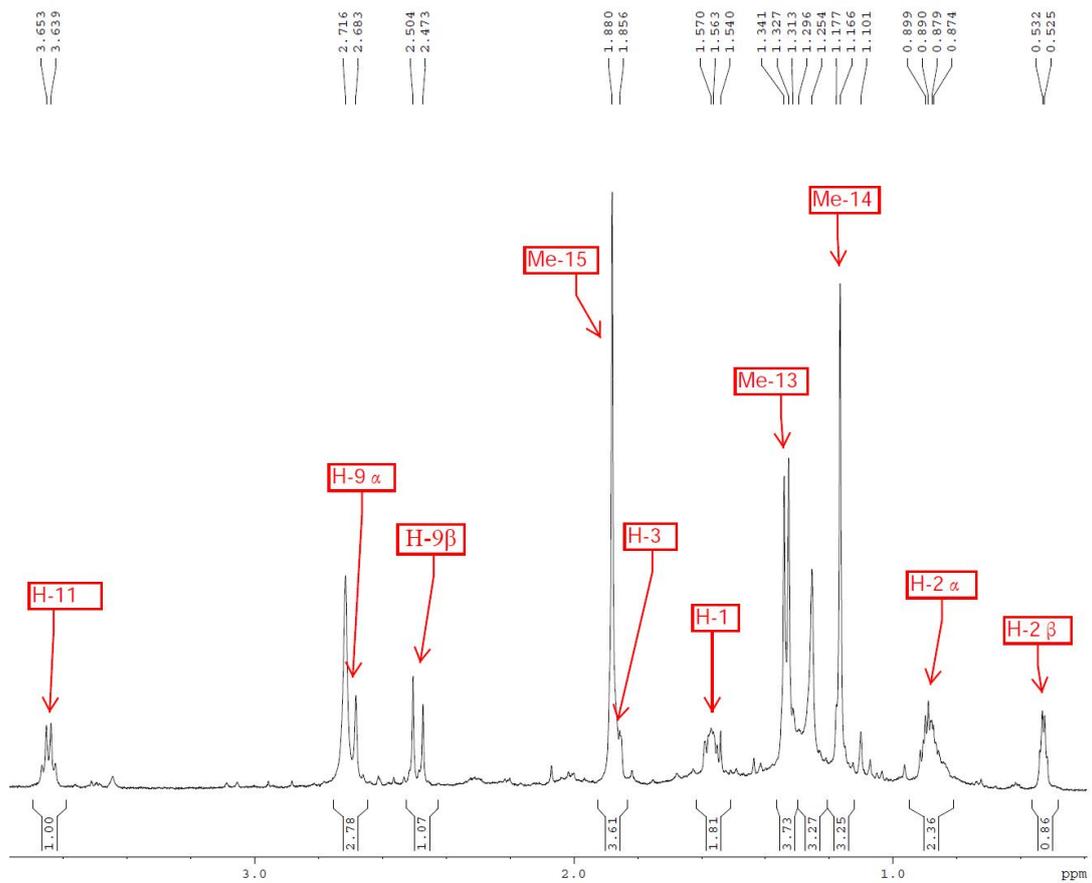


图21-1 化合物3的¹H NMR图（放大谱）

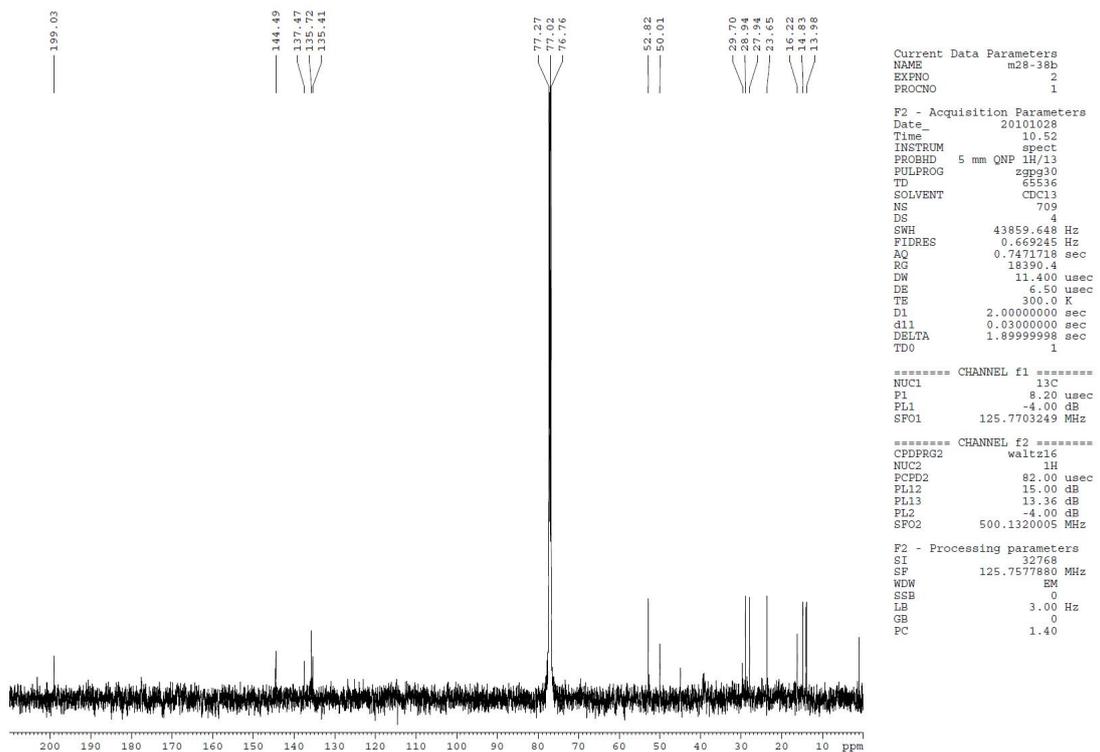


图22 化合物3的¹³C NMR图(125 MHz, CDCl₃)

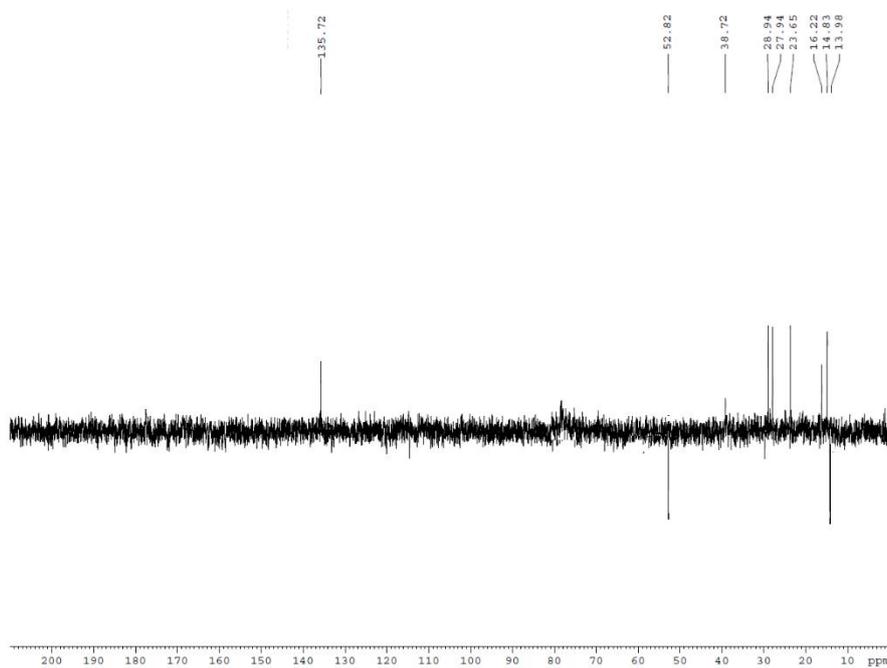


图23 化合物3的DEPT图

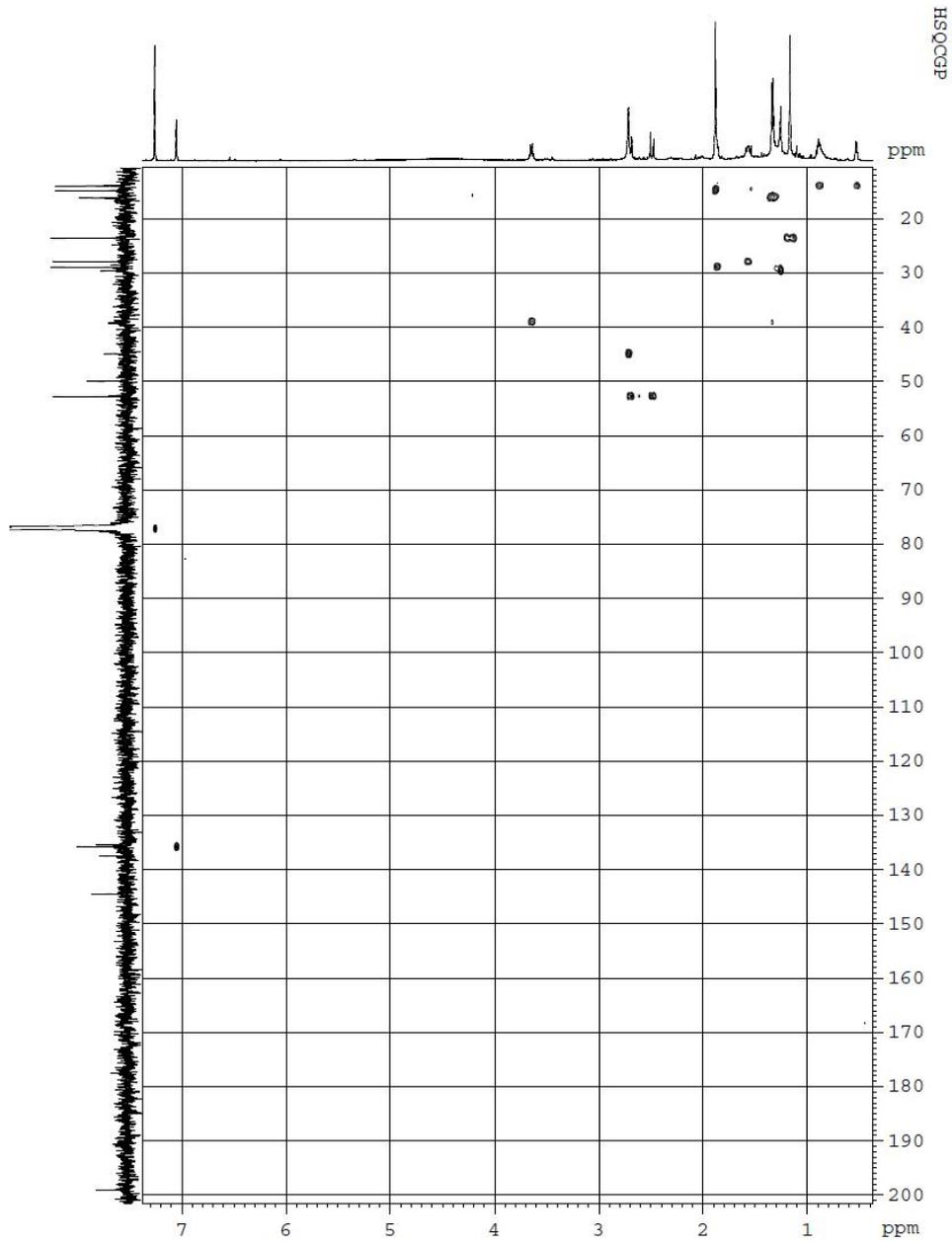


图24 化合物3的HSQC图

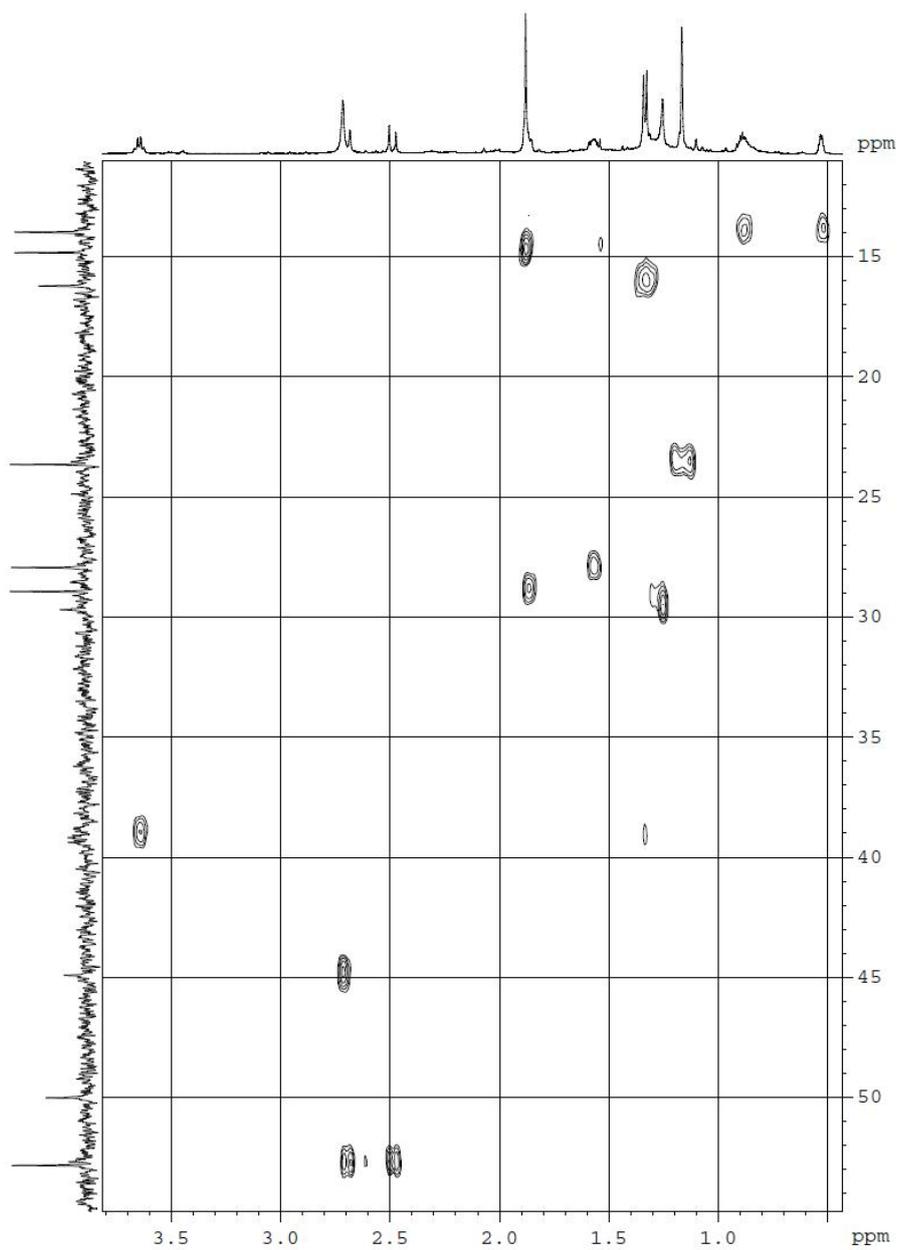


图24-1 化合物3的HSQC图（放大谱）

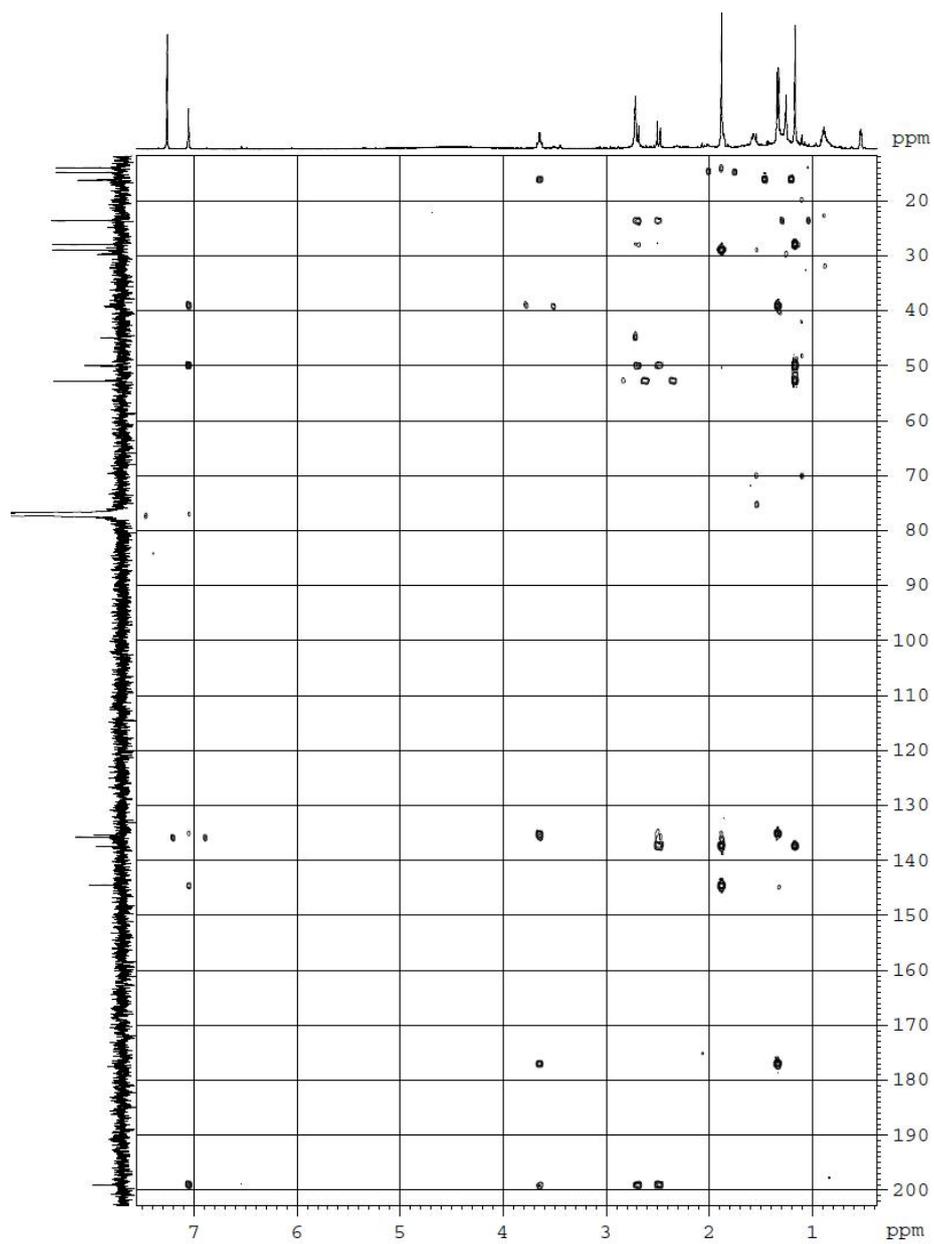


图25 化合物3的HMBC图

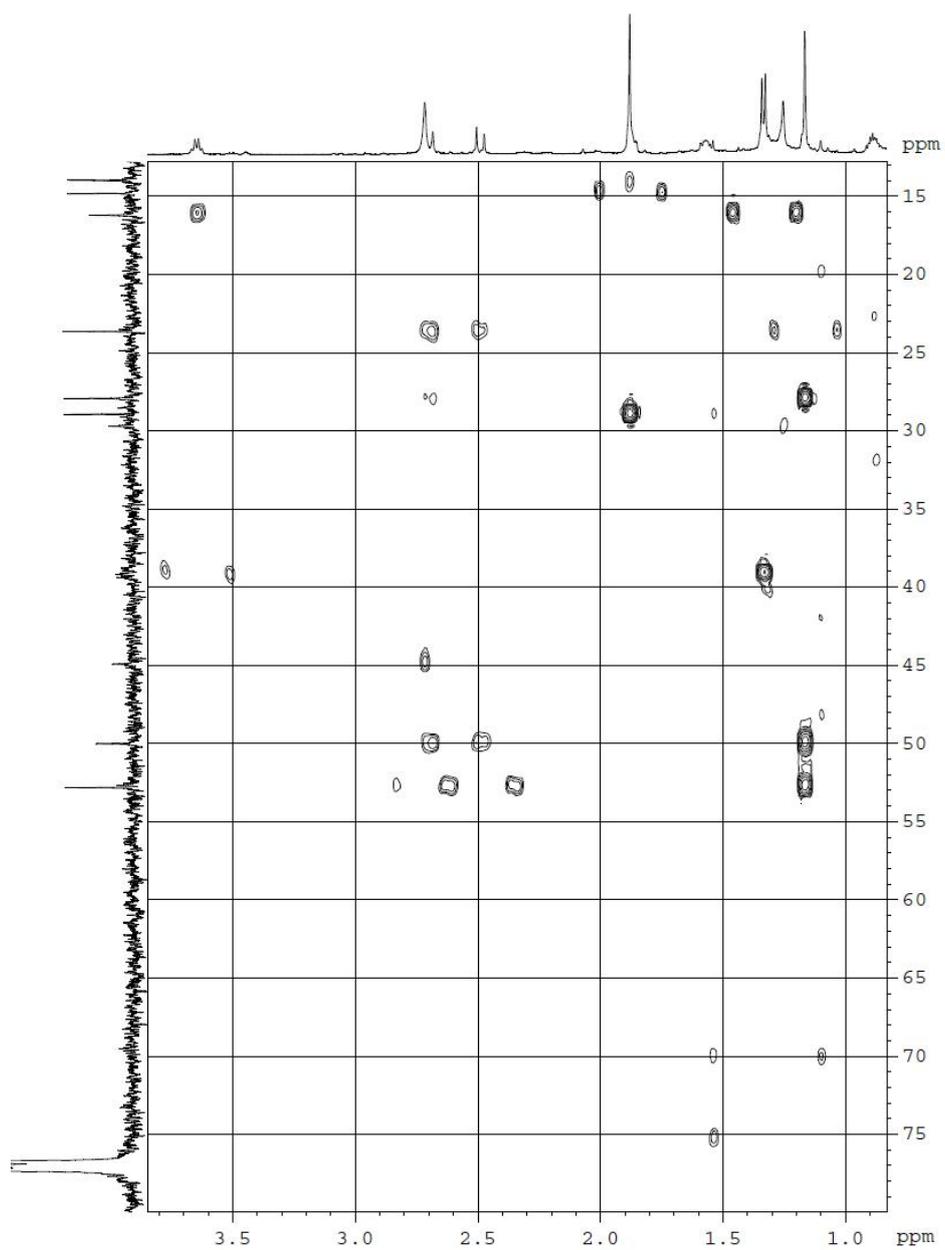


图25-1 化合物3的HMBC图（放大谱1）

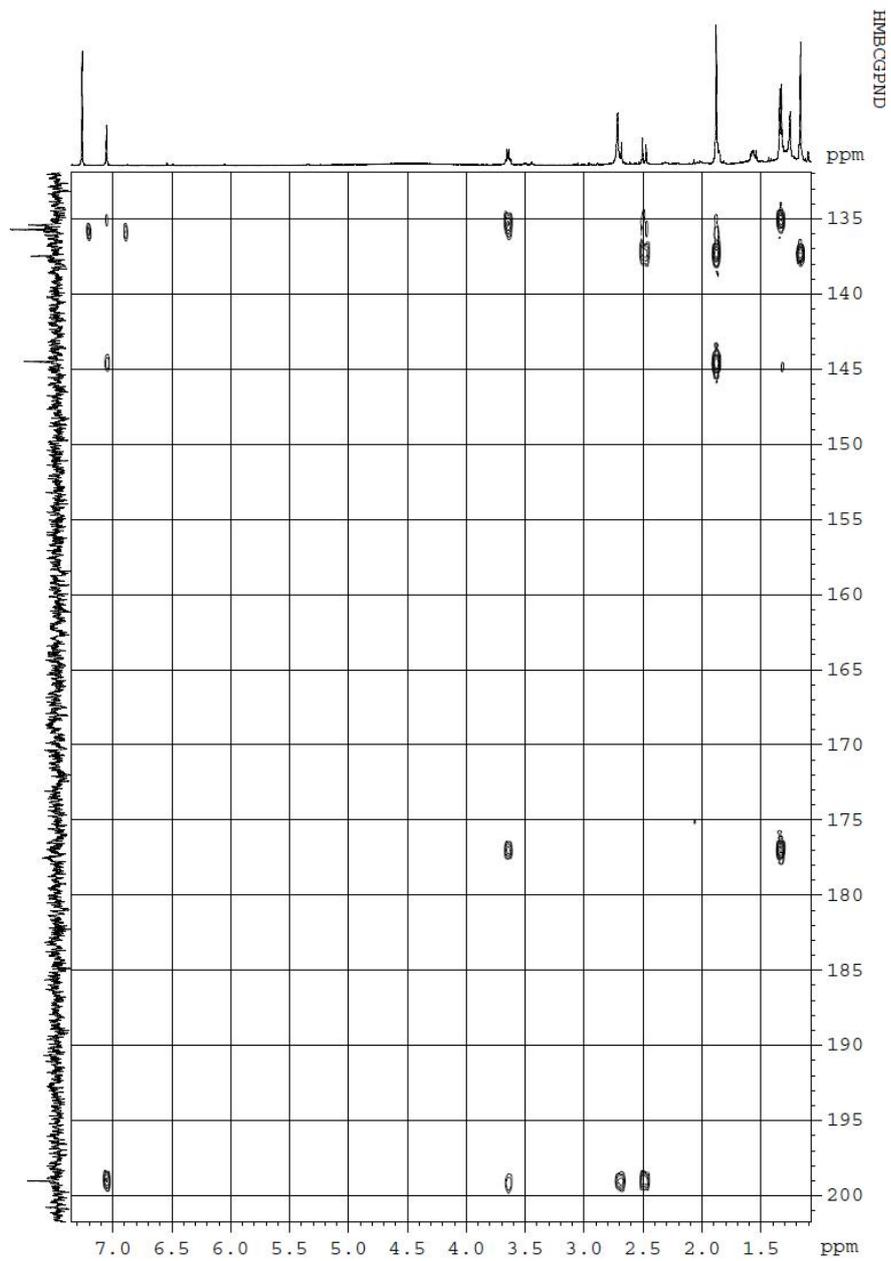


图25-2 化合物3的HMBC图（放大谱2）

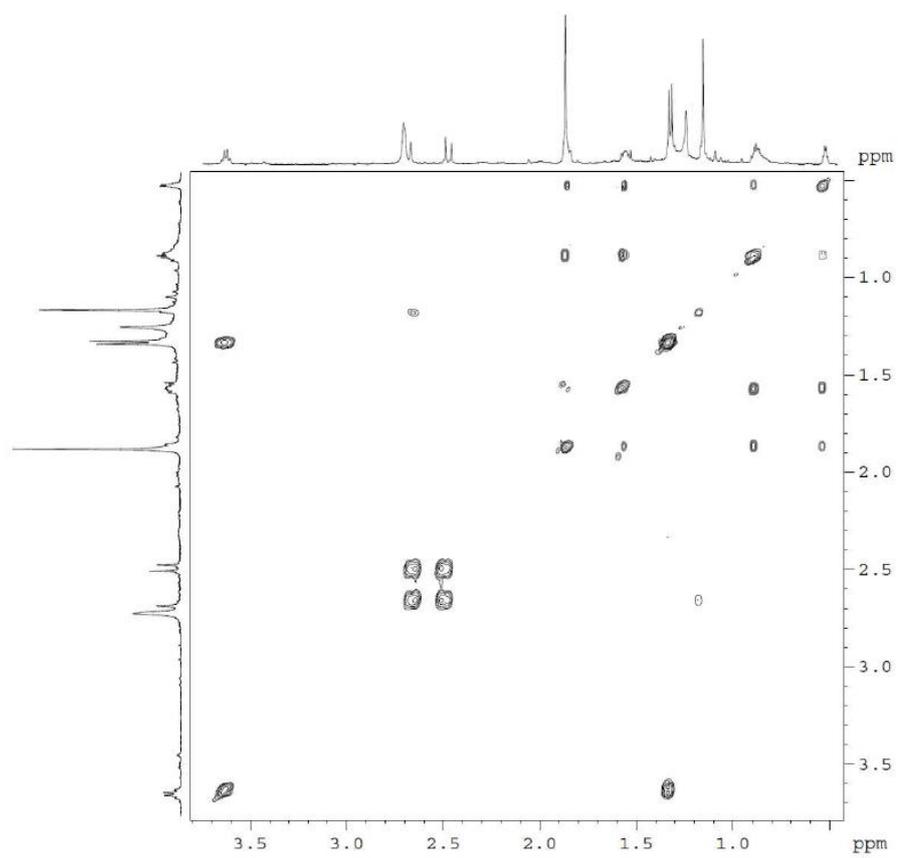


图26 化合物3的 ^1H - ^1H COSY图

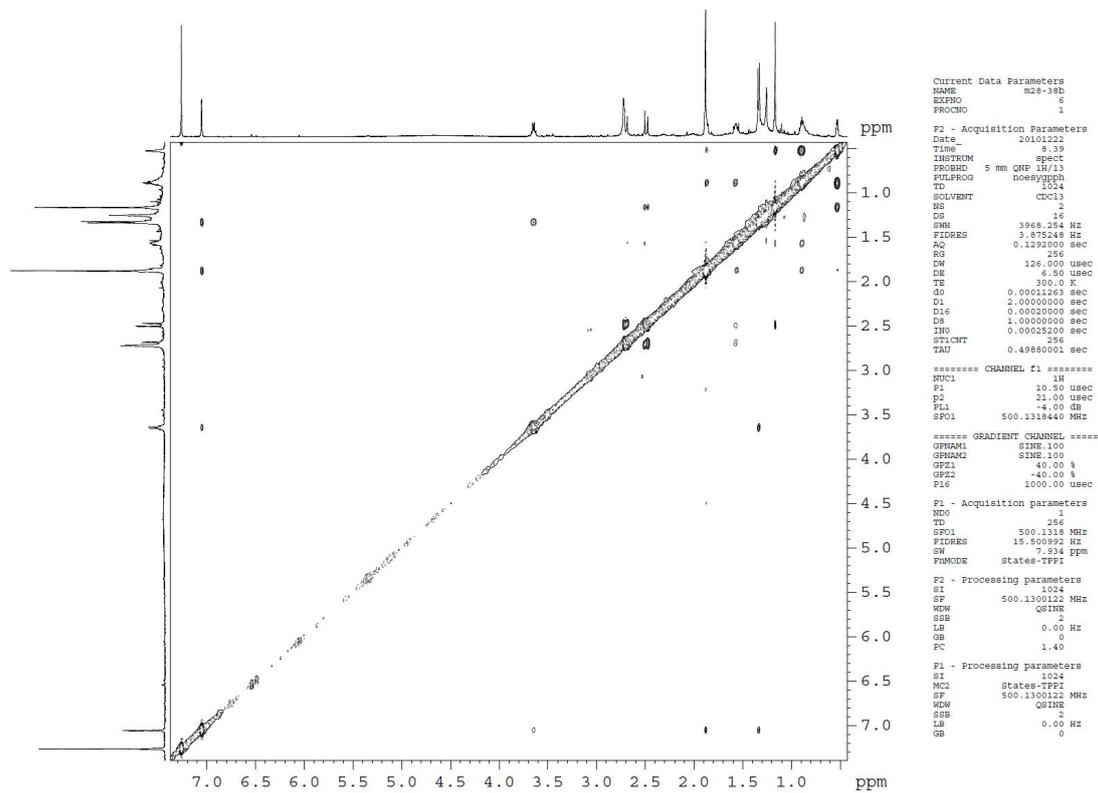


图27 化合物3的NOESY图

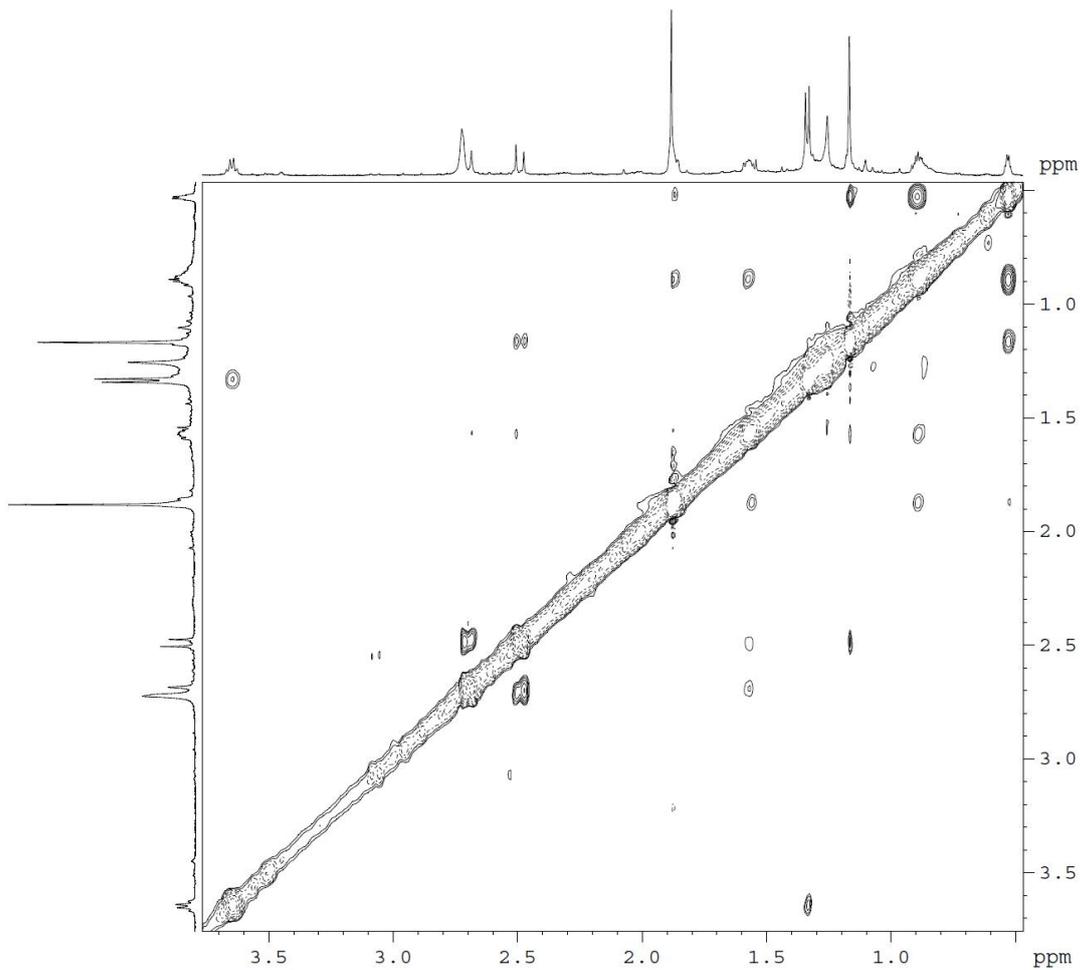


图27-1 化合物3的NOESY图（放大谱）

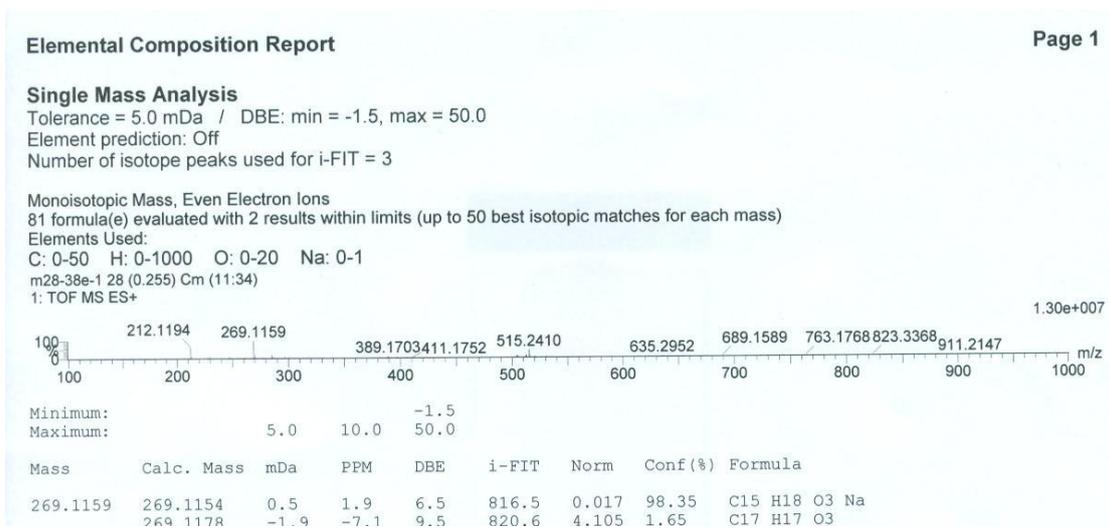


图28 化合物3的HR-ESI-MS图

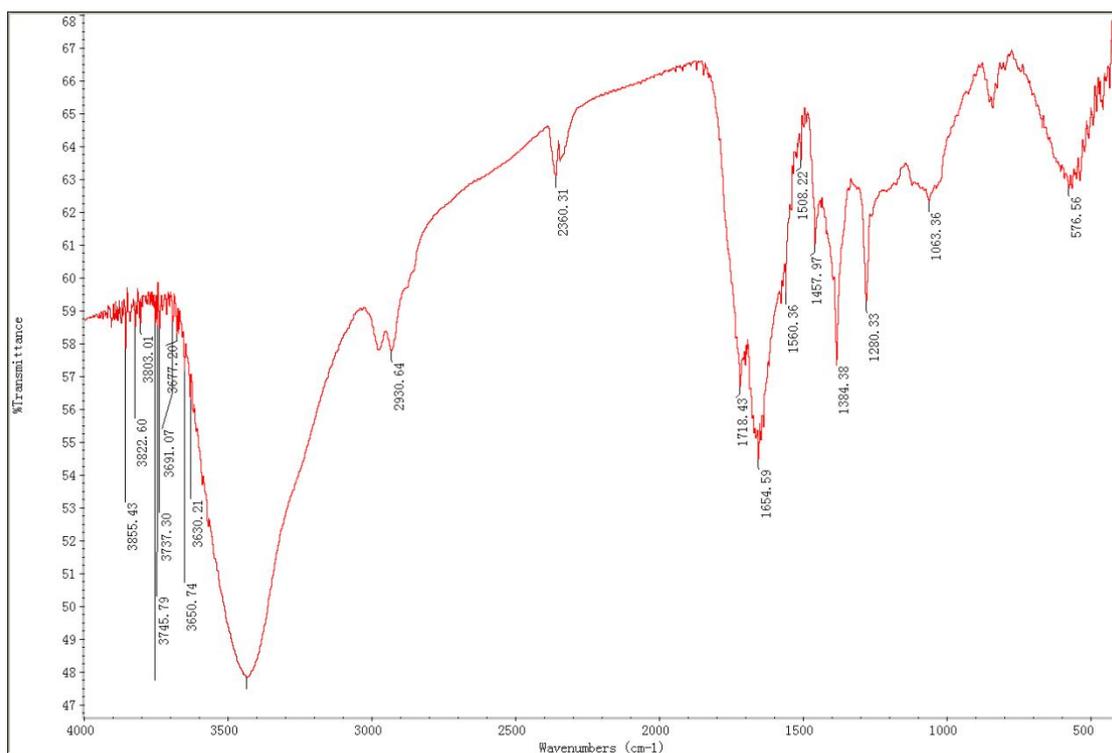
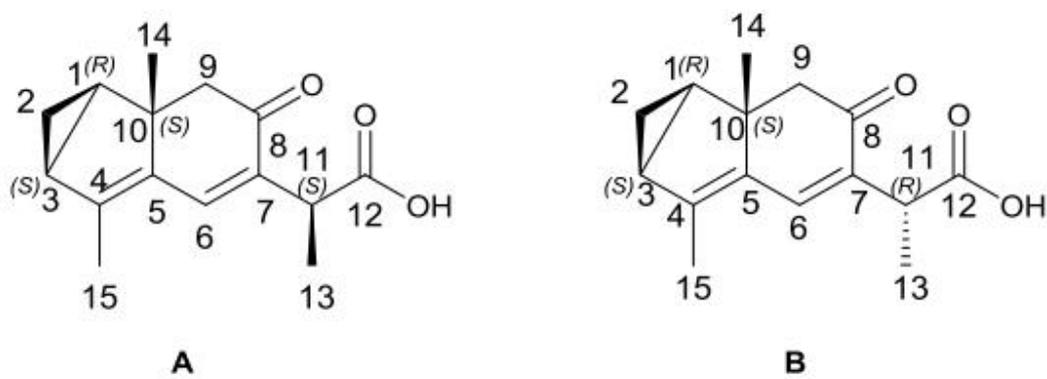


图29 化合物3的IR图



Nuclei	sp2?	DP4+	100.00%	0.00%
		xperimenta	Isomer 1	Isomer 2
C		13.9	179.1	179.2
C		28.9	164.3	164.6
C	x	144.4	50.7	51.4
C	x	137.4	61.0	61.0
C		50	142.7	142.0
C		27.9	165.7	166.0
C	x	135.7	62.7	61.6
C	x	135.4	61.2	60.8
C		199	4.0	3.3
C		52.8	142.9	142.8
C		38.7	153.7	152.5
C	x	178.6	27.86	28.44
C		16.2	176.19	176.77
C		14.8	178.18	178.25
C		23.6	170.85	170.86

	Isomer 1	Isomer 2
sDP4+ (H data)	100.00%	0.00%
sDP4+ (C data)	96.56%	3.44%
sDP4+ (all data)	100.00%	0.00%
uDP4+ (H data)	50.36%	49.64%
uDP4+ (C data)	75.62%	24.38%
uDP4+ (all data)	75.89%	24.11%
DP4+ (H data)	100.00%	0.00%
DP4+ (C data)	98.87%	1.13%
DP4+ (all data)	100.00%	0.00%

实验编号	3-实验值	计算编号	构象权重 (%)						计算值	计算-实验	取平方	平均值	RMSE	
			1	2	3	4	5	6						
2	13.9	1	179.0691	179.0484	179.2967	179.1505	179.2449	179.231	179.2478	14.6	0.7	0.559921	7.023762	2.65
3	28.9	2	164.3594	164.5894	164.5593	164.4272	164.8454	164.4089	164.5525	30.1	1.2	1.338799		
4	144.4	3	50.2936	50.4602	51.5705	50.4331	51.7558	51.2334	51.40617	148.7	4.3	18.45877		
5	137.4	4	61.2584	60.7597	61.0116	61.303	60.7383	60.9477	60.97057	138.7	1.3	1.606908		
10	50.0	5	142.7261	143.0181	141.7695	142.9417	141.7119	143.0443	141.9586	53.7	3.7	14.04588		
1	27.9	6	165.7256	165.6882	166.1442	165.555	165.9993	165.6674	166.0302	28.5	0.6	0.369195		
6	135.7	7	63.6823	59.8408	61.3307	63.8828	61.288	63.9652	61.60499	138.0	2.3	5.30116		
7	135.4	8	62.3643	63.6708	60.5196	62.2613	59.9069	62.0645	60.77847	138.9	3.5	12.03446		
8	199.0	9	4.7149	3.8102	3.0366	4.5075	3.0905	2.6909	3.265726	199.2	0.2	0.03025		
9	52.8	10	142.8313	142.7509	142.818	142.6992	142.7905	142.8932	142.811	52.9	0.1	0.002917		
11	38.7	11	156.2881	159.139	151.9552	153.1079	150.7665	153.9265	152.5243	42.7	4.0	15.75446		
12	178.6	12	26.7672	27.3544	28.9972	28.9651	27.9332	27.9213	28.44136	172.8	-5.8	33.91816		
13	16.2	13	174.1641	171.609	177.1937	174.5408	177.7485	178.7759	176.7654	17.3	1.1	1.105061		
15	14.8	17	178.2328	178.0326	178.271	178.147	178.2354	178.2662	178.2475	15.7	0.9	0.804902		
14	23.6	18	170.9051	170.9421	170.8423	170.9683	170.9054	170.6481	170.8631	23.4	-0.2	0.02558		

实验编号	3-实验值	计算编号	A-计算值	计算-实验	取平方	平均值	RMSE
2	13.9	1	14.8	0.9	0.790098	5.928091	2.43
3	28.9	2	30.3	1.4	1.934847		
4	144.4	3	149.5	5.1	25.54419		
5	137.4	4	138.6	1.2	1.412693		
10	50.0	5	53.0	3.0	9.011889		
1	27.9	6	28.9	1.0	1.004297		
6	135.7	7	136.8	1.1	1.274311		
7	135.4	8	138.5	3.1	9.390086		
8	199.0	9	198.4	-0.6	0.324416		
9	52.8	10	52.7	-0.1	0.00641		
11	38.7	11	41.4	2.7	7.307632		
12	178.6	12	173.4	-5.2	27.23559		
13	16.2	13	17.9	1.7	2.730432		
15	14.8	17	15.8	1.0	0.932609		
14	23.6	18	23.5	-0.1	0.021854		

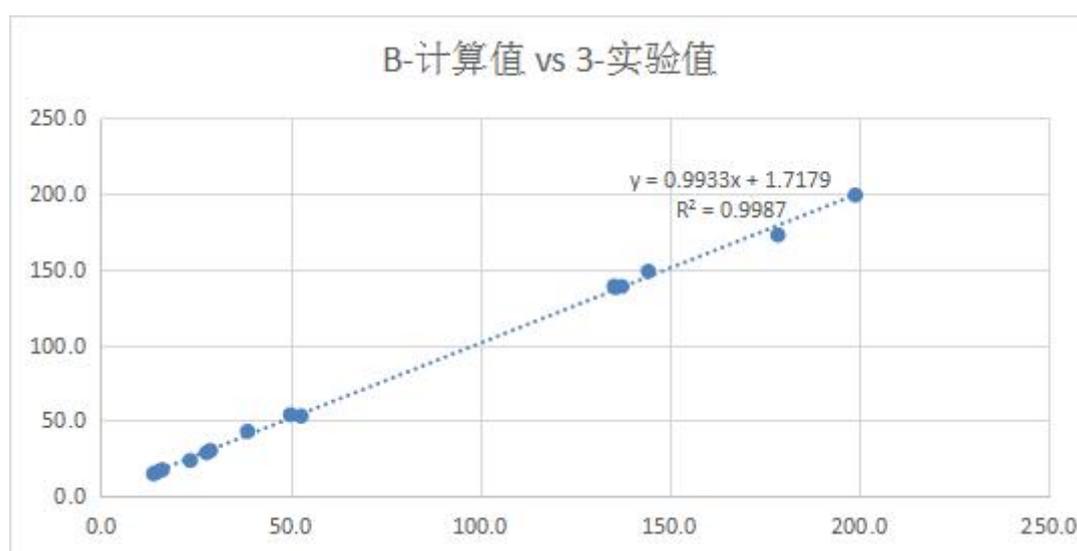
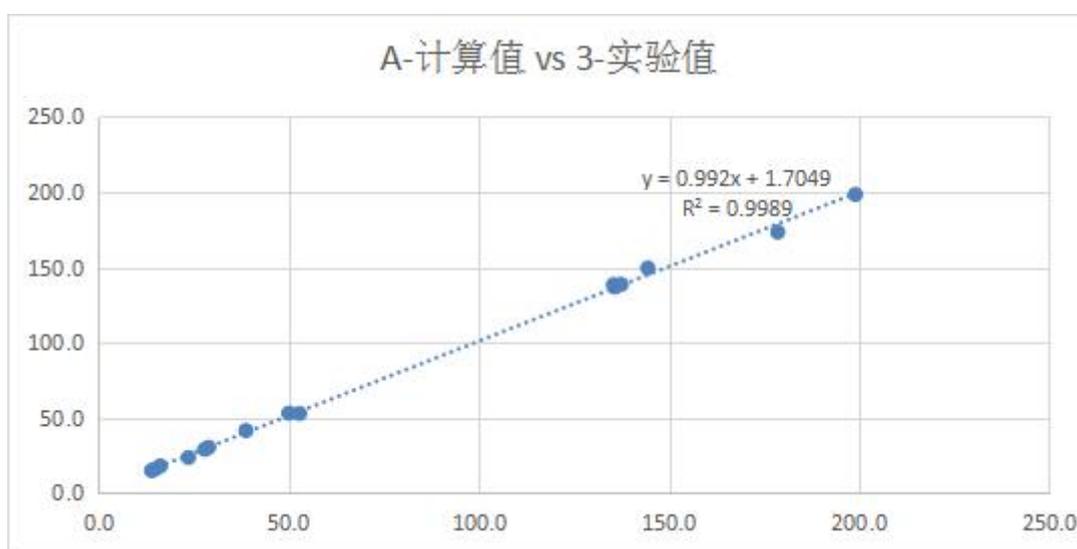


图30 化合物3的DP4+分析结果

jonathan
goodman

contact us

data

people

programs

publications

highlights:

#sketchBINOL
c2k
CP3: NMR data
DP4: NMR data
force field
evaluation
InChIKey collision
RinChi project
solubility
challenge

wiki (intranet)

Assignment of stereochemistry and structure using NMR and CP3

Please select version of database to use:

CP3-original
CP3-database2
CP3-database3

Enter two ¹H and ¹³C experimental spectra then two calculated spectra:

¹³ C Expt A	14.0, 28.9, 144.4, 137.5, 49.9, 27.9, 135.0, 135.2, 198.8, 52.6, 38.7, 178.6, 15.6, 14.7, 23.5
¹³ C Expt B	13.9, 28.9, 144.4, 137.4, 50.0, 27.9, 135.7, 135.4, 199.0, 52.8, 38.7, 178.6, 16.2, 14.8, 23.6
¹³ C Calc A	14.8, 30.3, 149.5, 138.6, 53.0, 28.9, 136.8, 138.5, 198.4, 52.7, 41.4, 173.4, 17.9, 15.8, 23.5
¹³ C Calc B	14.6, 30.1, 148.7, 138.7, 53.7, 28.5, 138.0, 138.9, 199.2, 52.9, 42.7, 172.8, 17.3, 15.7, 23.4
¹ H Expt A	0.52, 0.89, 1.85, 1.56, 7.03, 2.65, 2.49, 3.62, 1.33, 1.30, 1.30, 1.87, 1.90, 1.90, 1.10, 1.13, 1.10
¹ H Expt B	0.52, 0.89, 1.87, 1.56, 7.04, 2.66, 2.49, 3.64, 1.33, 1.30, 1.30, 1.87, 1.90, 1.90, 1.10, 1.13, 1.10
¹ H Calc A	1.05, 0.69, 2.03, 1.63, 7.03, 2.37, 2.82, 3.30, 1.43, 1.14, 1.38, 1.86, 1.97, 1.94, 1.24, 1.18, 1.48
¹ H Calc B	1.04, 0.70, 2.01, 1.61, 7.06, 2.34, 2.81, 3.12, 0.91, 1.52, 1.55, 1.89, 1.85, 2.01, 1.04, 1.68, 1.35

CP3 thinks ExpA goes with CalcB and ExpB with CalcA:

ExpA with CalcA and ExpB with CalcB: 0.0%
ExpA with CalcB and ExpB with CalcA: 100.0%

CP3 values:

	C data	H data	All data
ExpA-CalcA & ExpB-CalcB	-0.25	-3.87	-2.06
ExpA-CalcB & ExpB-CalcA	-0.60	0.04	-0.28

Probabilities:

	C data	H data	All data
ExpA-CalcA & ExpB-CalcB	98.9%	0.0%	0.0%
ExpA-CalcB & ExpB-CalcA	1.1%	100.0%	100.0%

Assign resonances

Calculate

Re-read input

Clear text

图31 CP3分析结果：小程序中的A和B分别表示化合物3和2。

图 32 化合物 2 和 3 的 HPLC 图谱