Supporting Information

Hirundigenin type C_{21} steroidal glycosides from *Cynanchum stauntonii* and their anti-inflammatory activity

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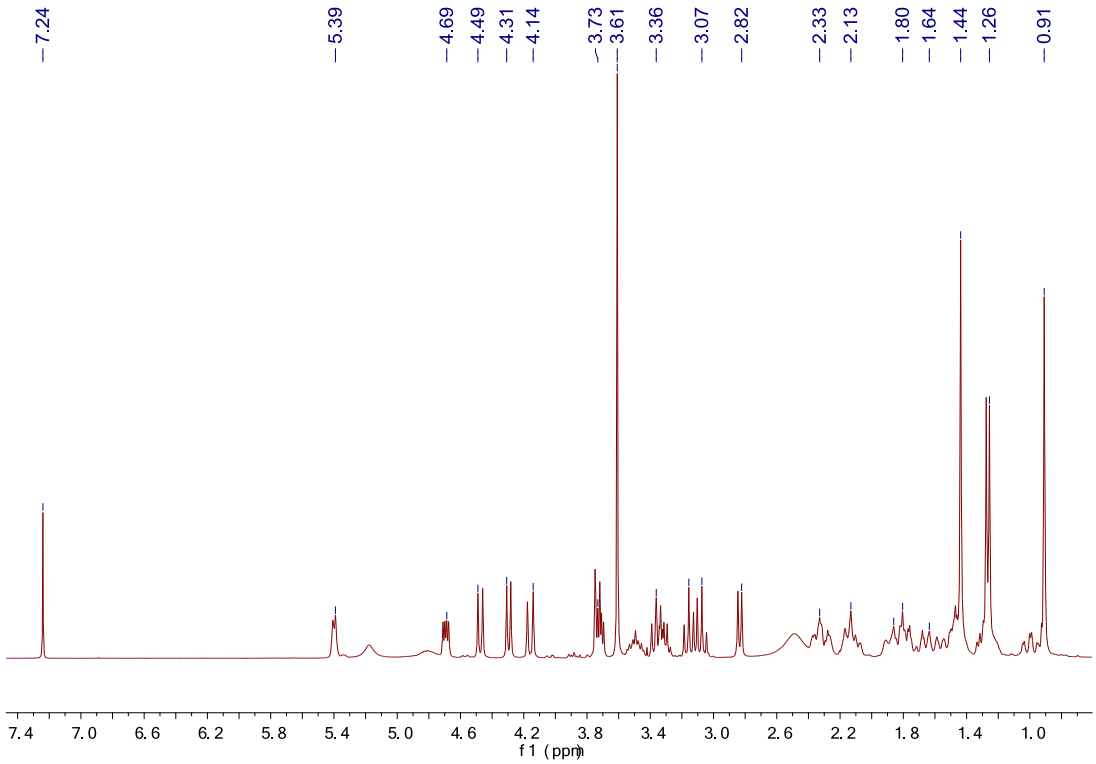

Figure S1 ^{1}H NMR spectrum of compound **1**

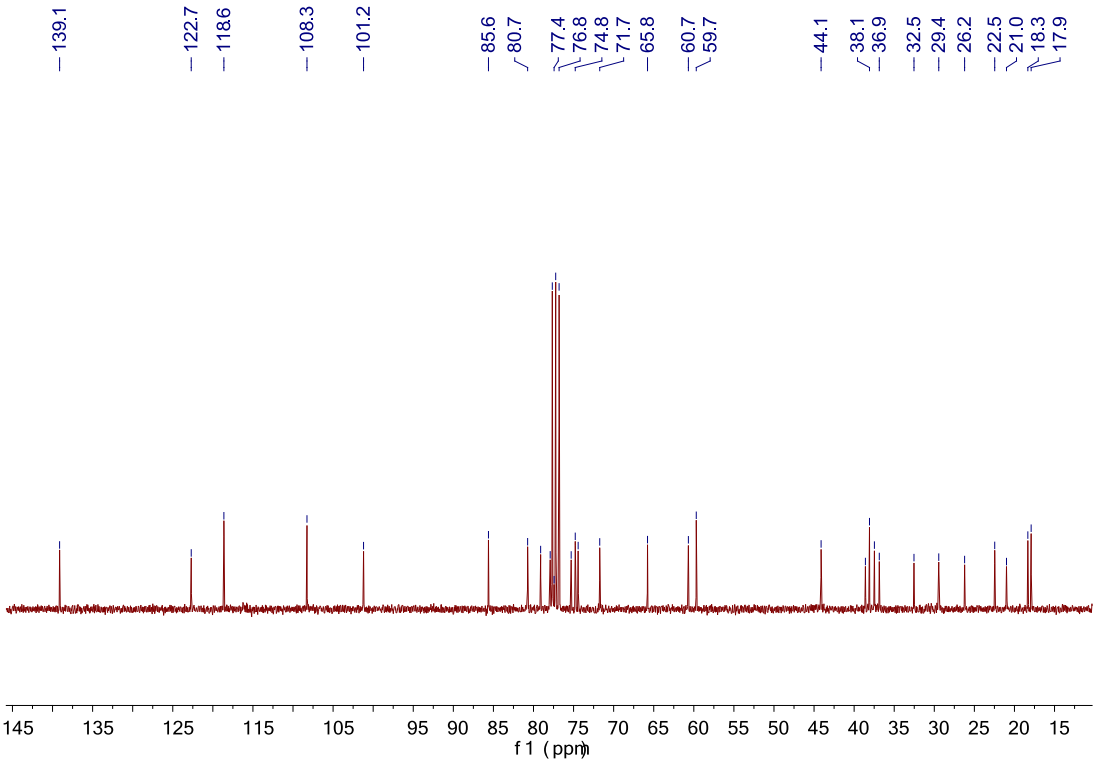

Figure S2 ^{13}C NMR spectrum of compound **1**

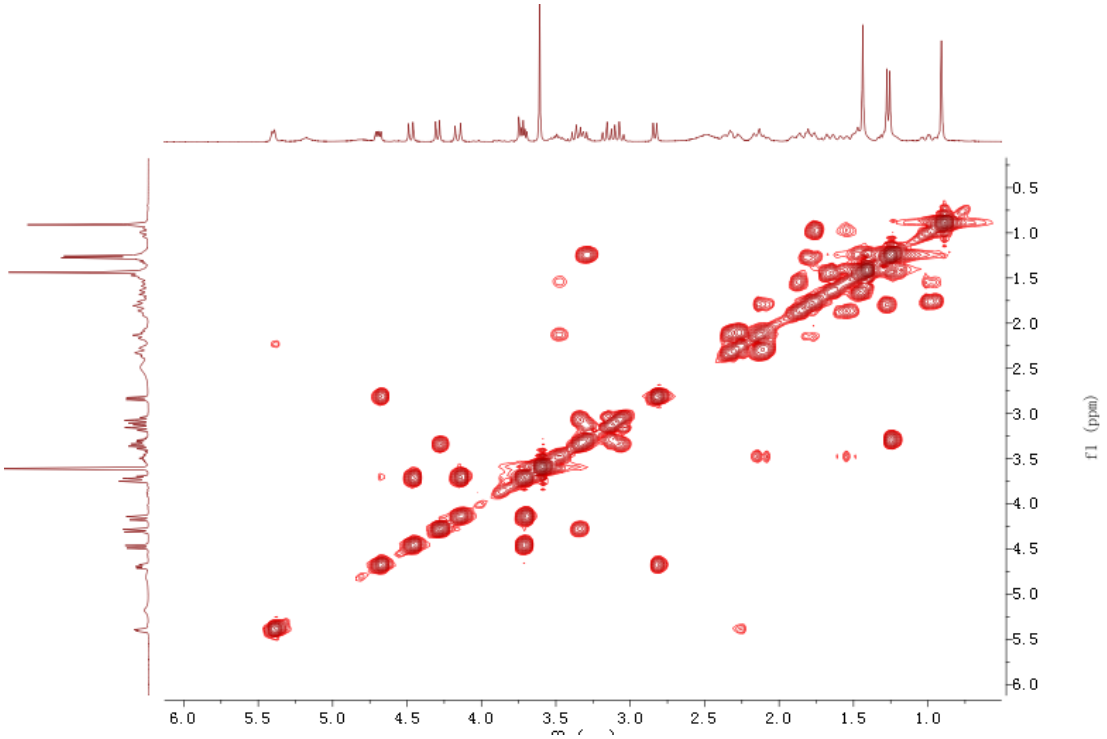

Figure S3 ^{1}H-^{1}H COSY spectrum of compound **1**

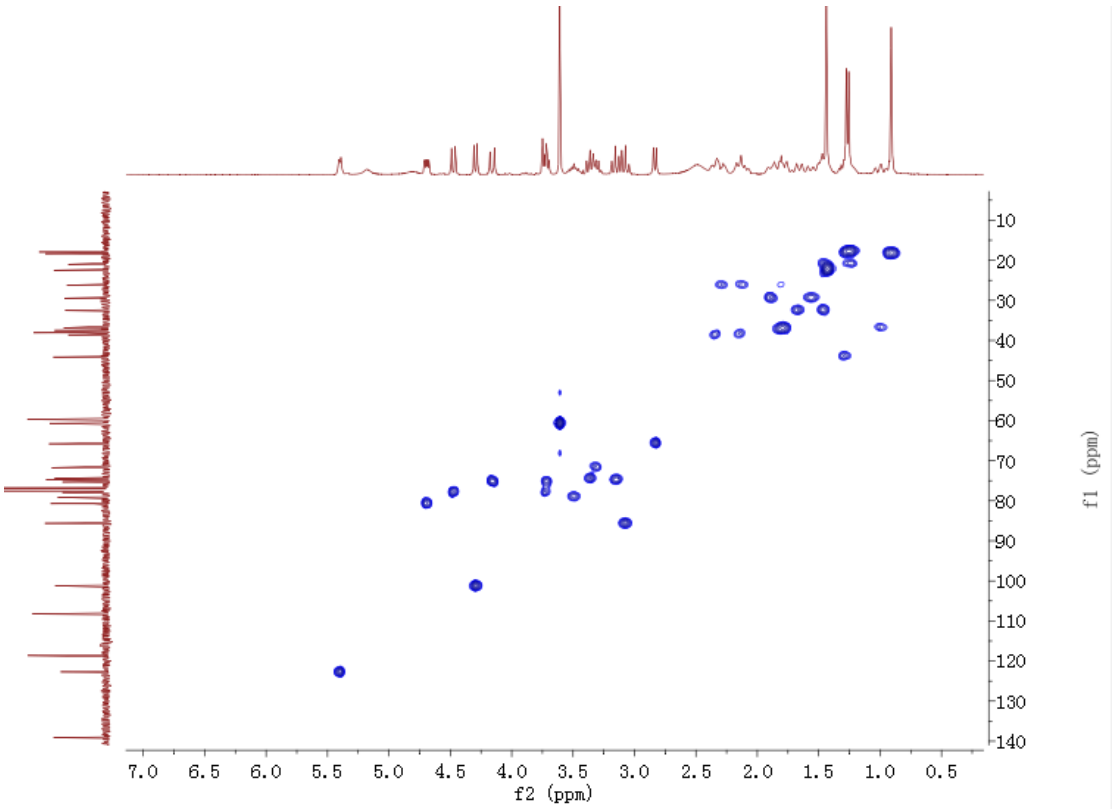

Figure S4 HSQC spectrum of compound **1**

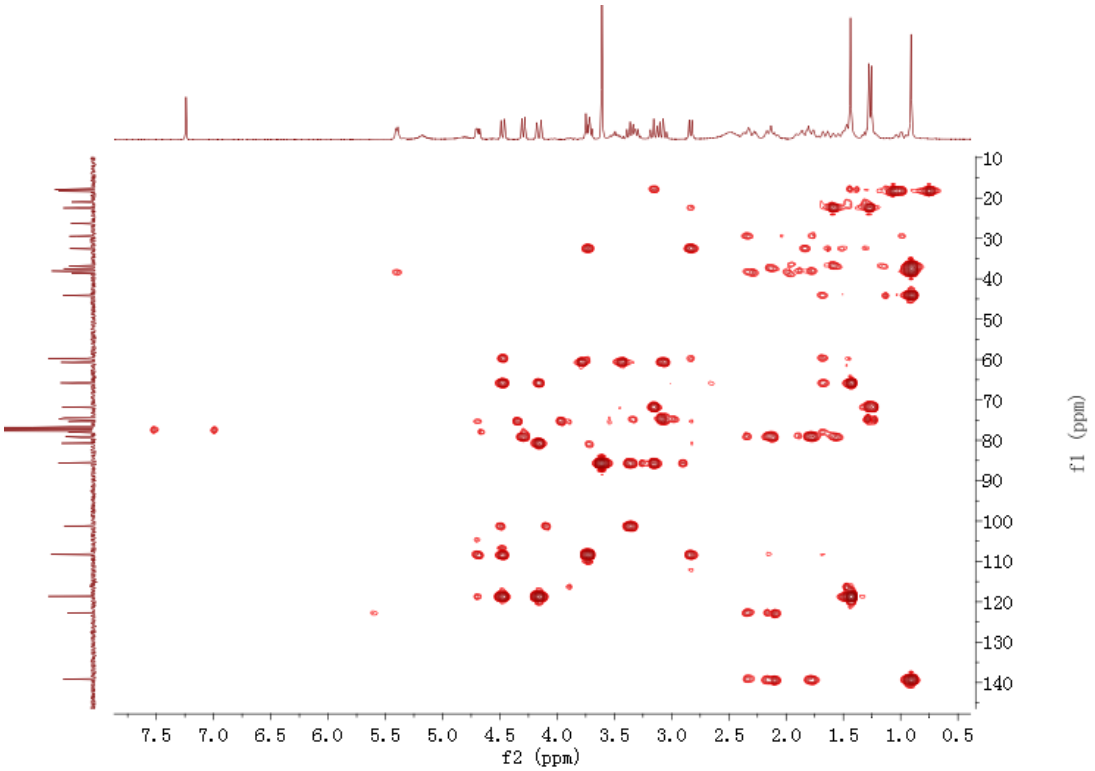

Figure S5 HMBC spectrum of compound **1**

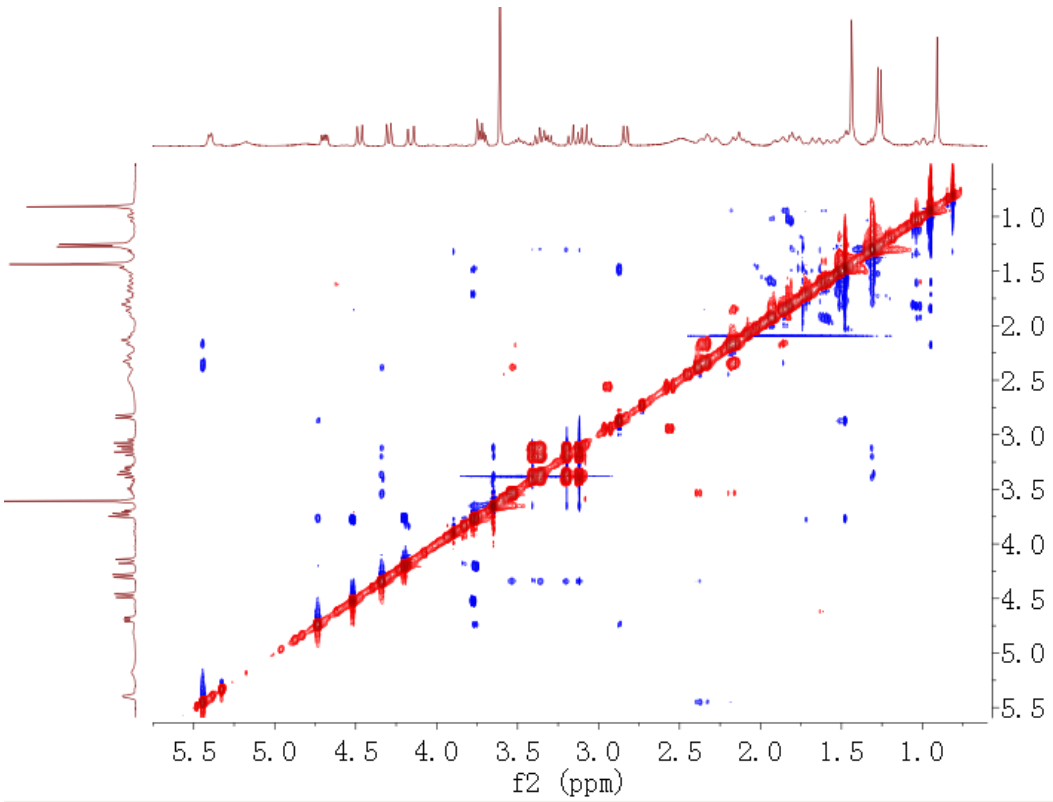

Figure S6 ROESY spectrum of compound **1**

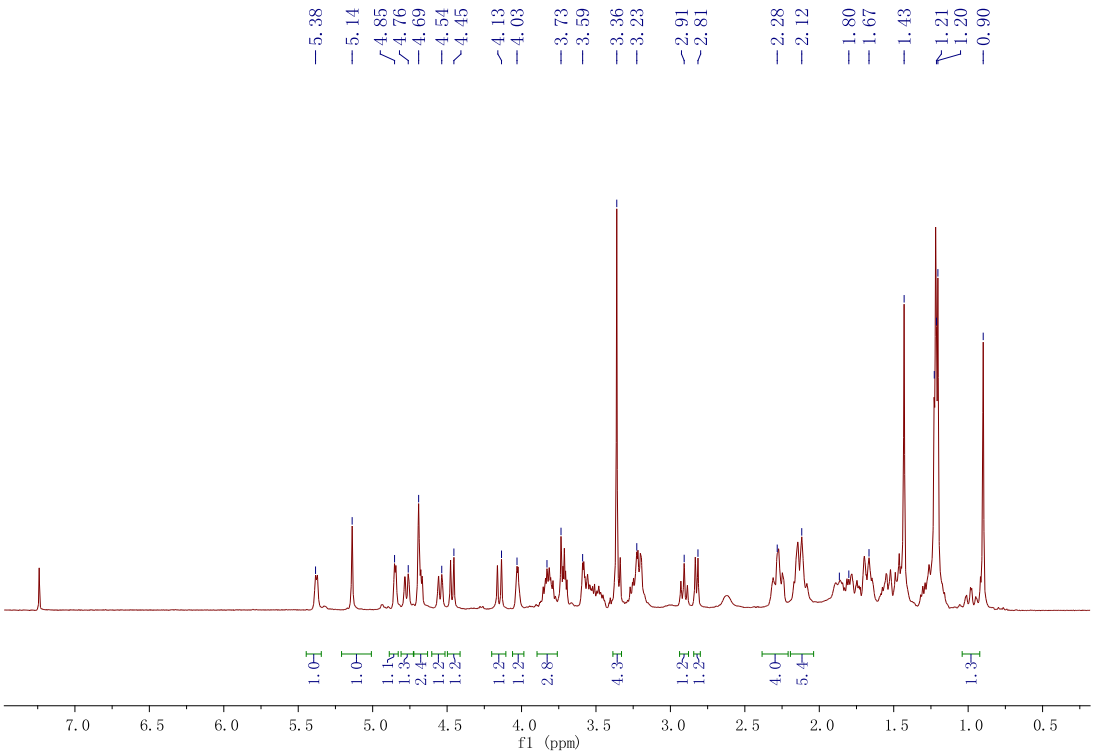

Figure S7 ^{1}H NMR spectrum of compound **2**

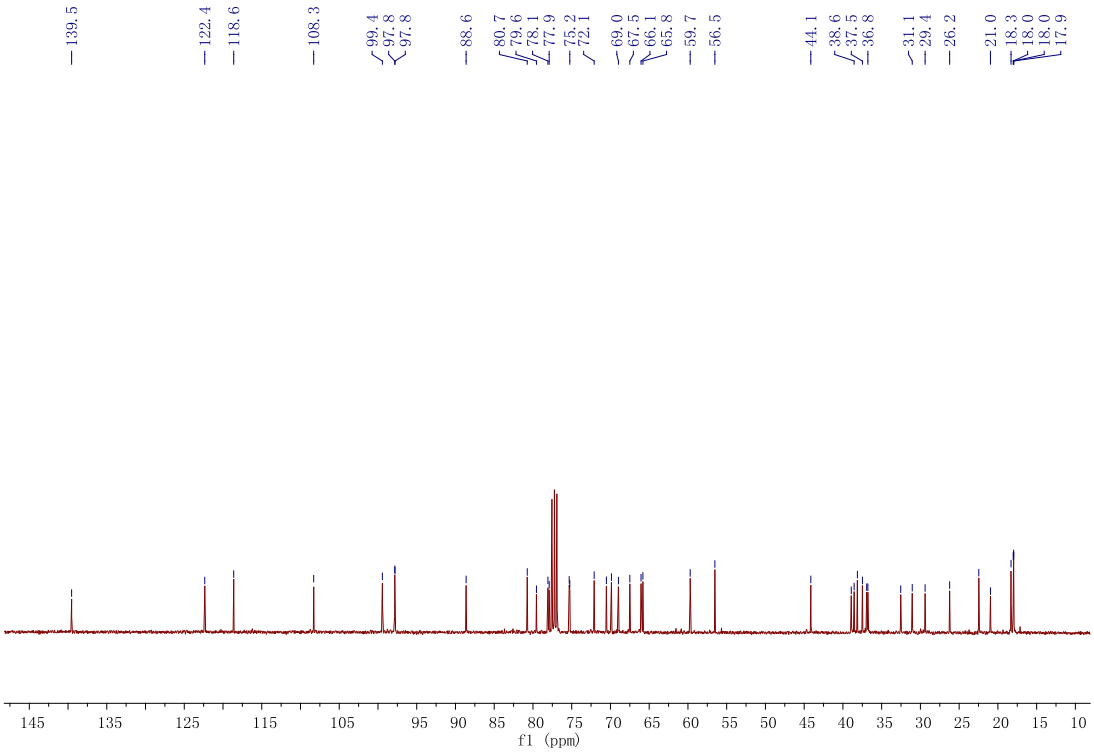

Figure S8 ^{13}C NMR spectrum of compound **2**

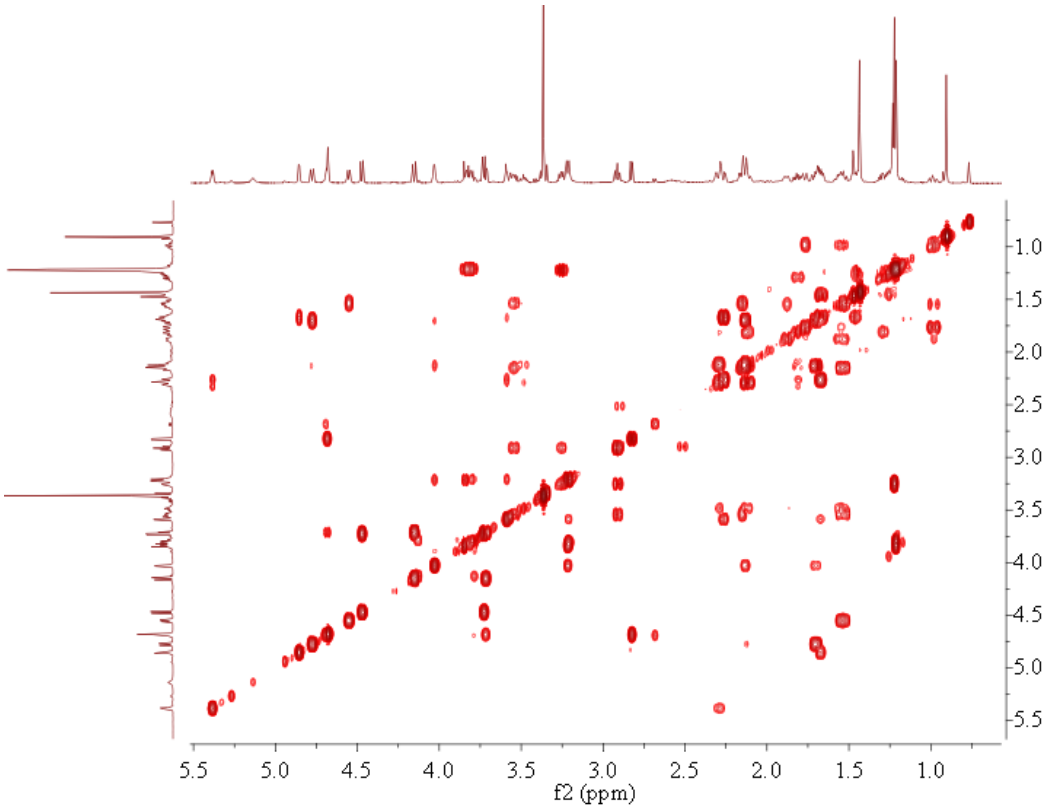

Figure S9 ^{1}H-^{1}H COSY spectrum of compound **2**

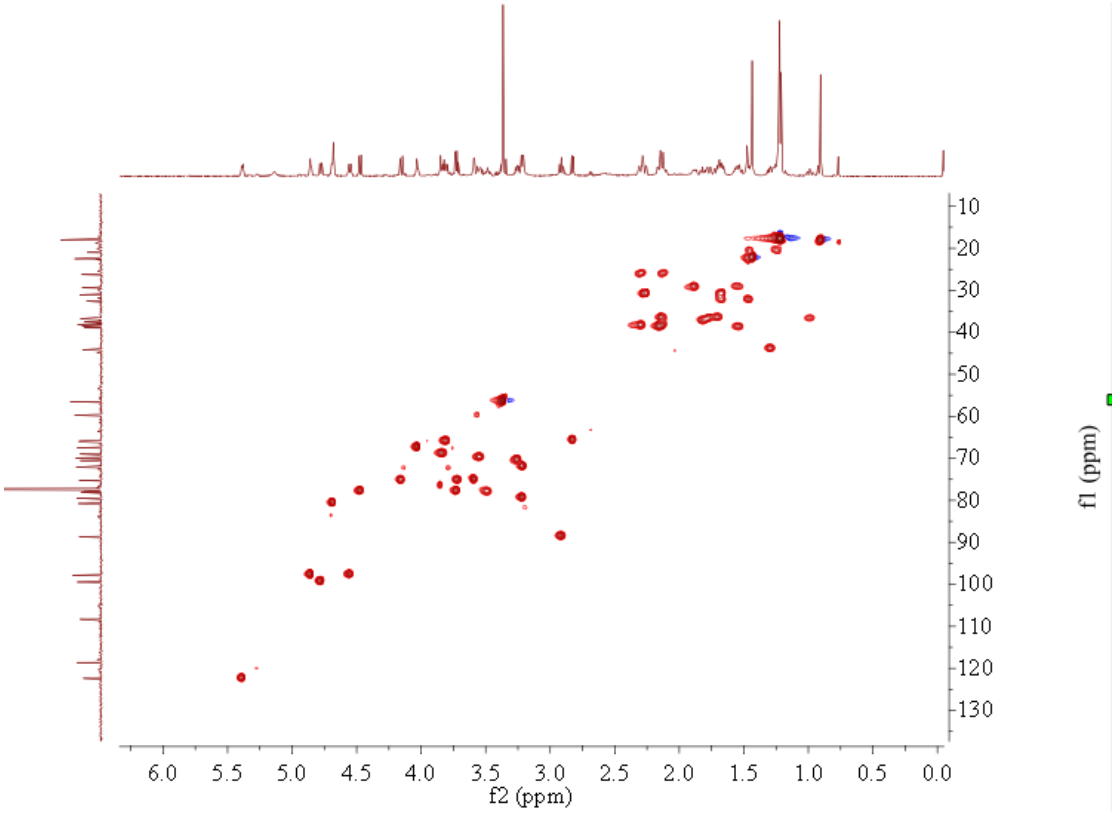

Figure S10 HSQC spectrum of compound **2**

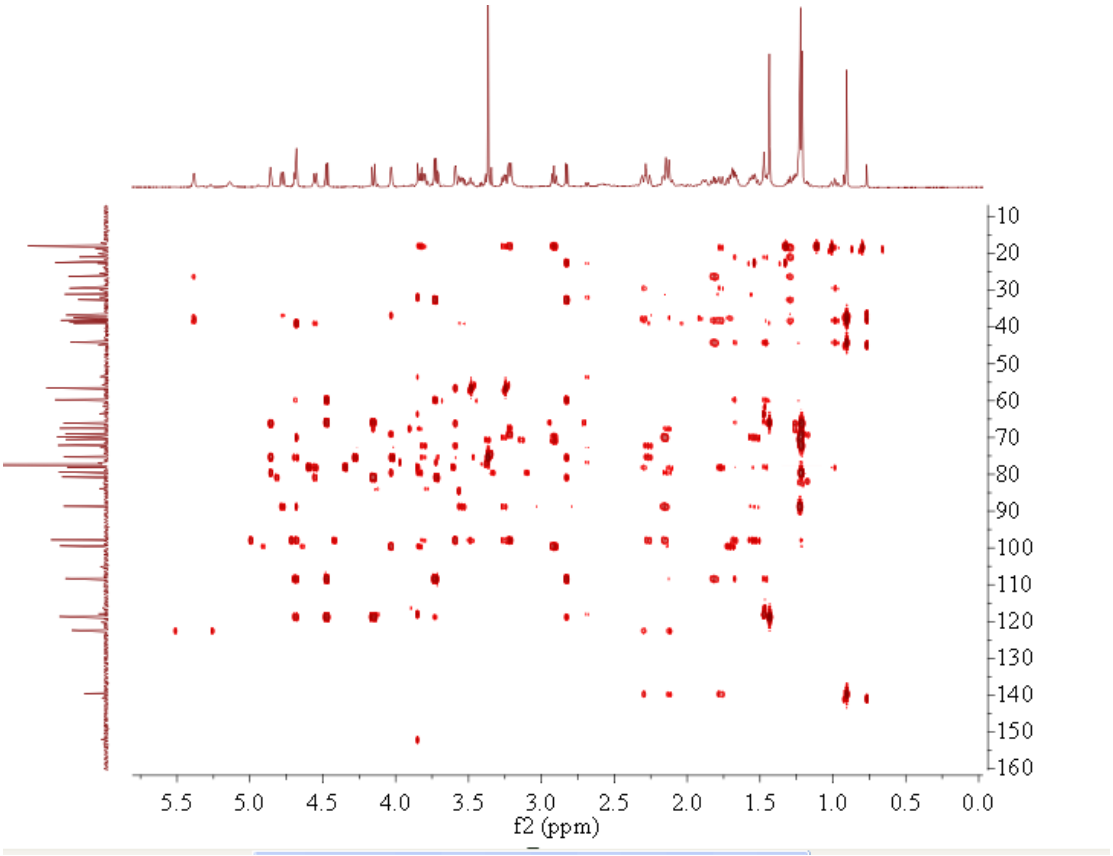

Figure S11 HMBC spectrum of compound **2**

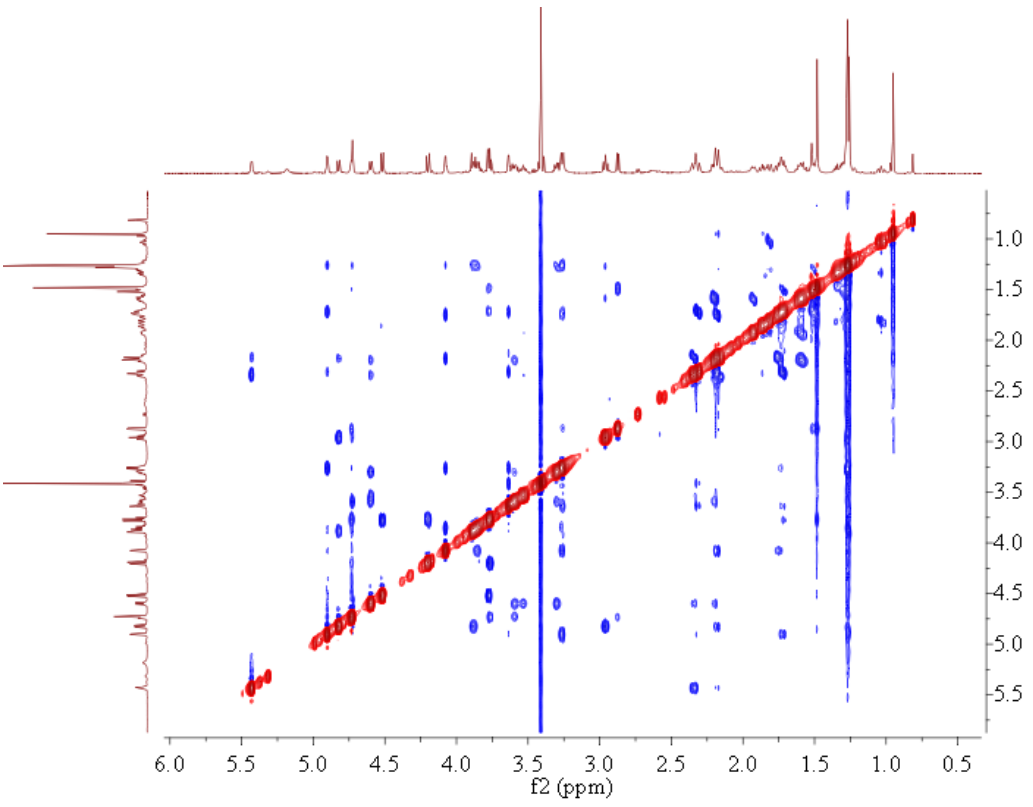

Figure S12 ROESY spectrum of compound **2**

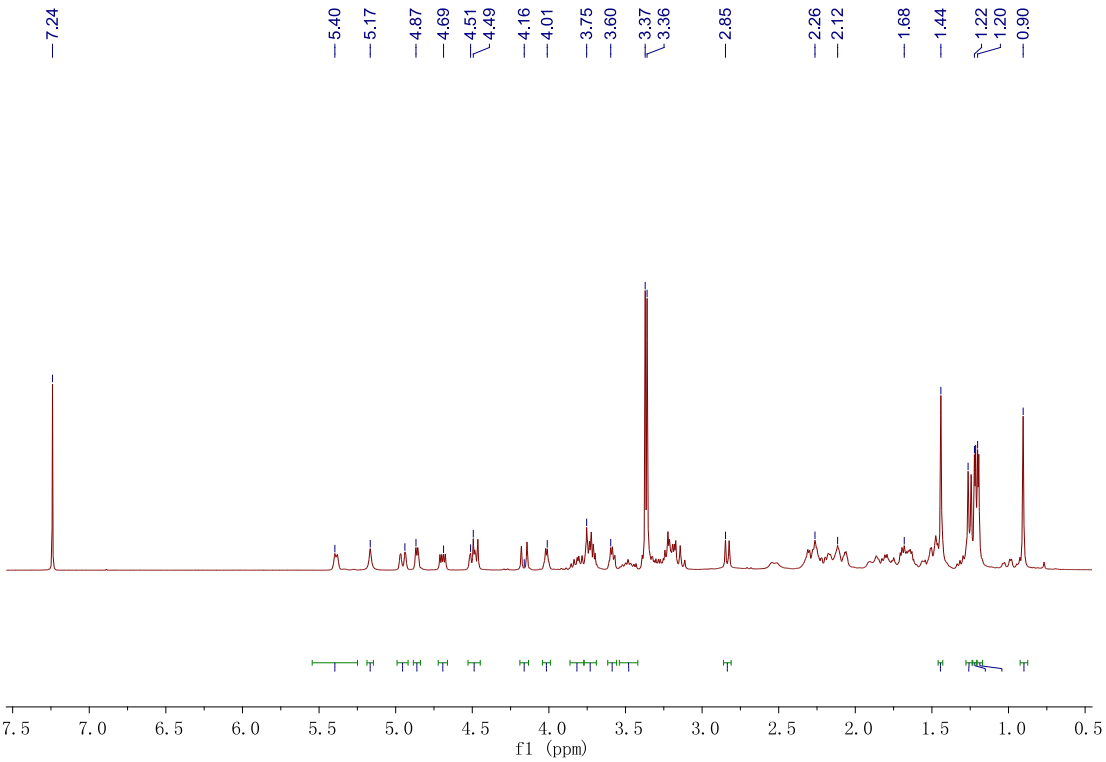

Figure S13 ^{1}H NMR spectrum of compound **3**

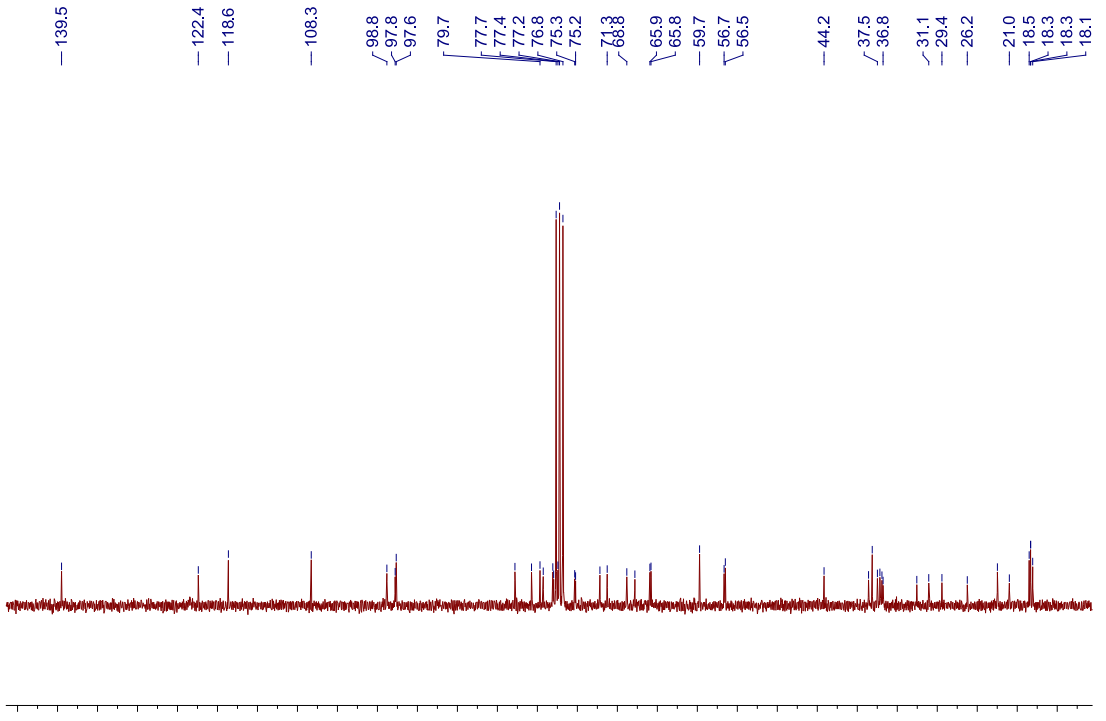

Figure S14 ^{13}C NMR spectrum of compound **3**

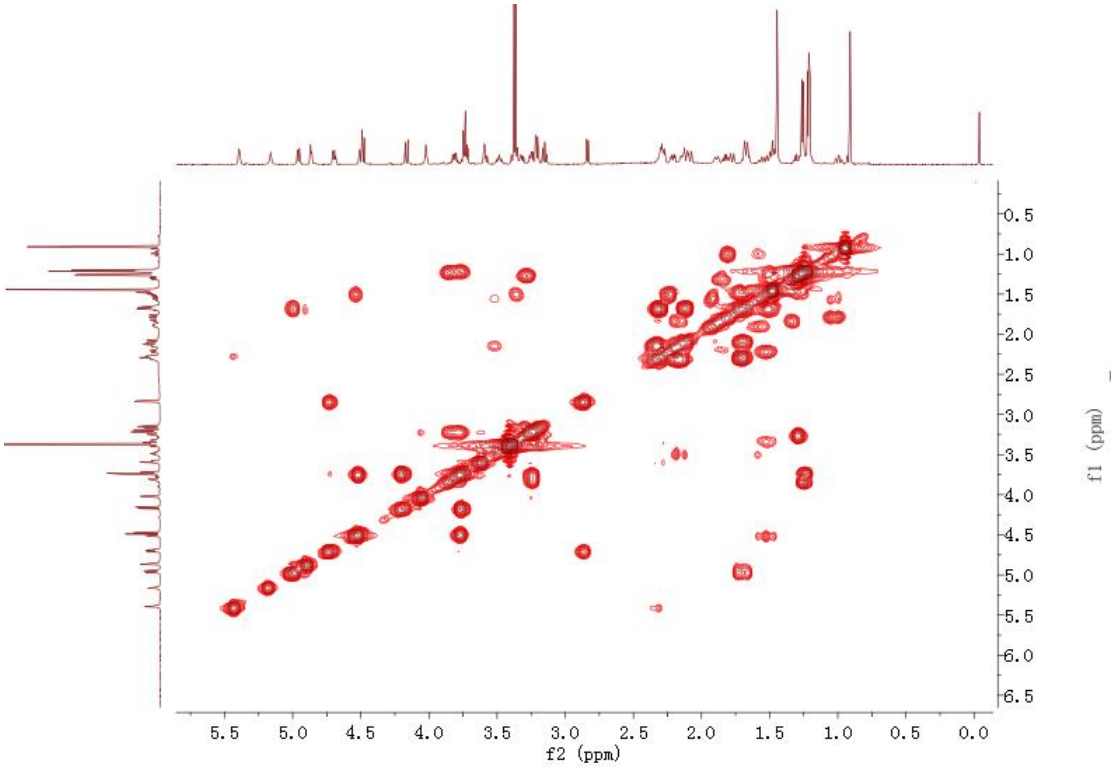

Figure S15 ^{1}H-^{1}H COSY spectrum of compound **3**

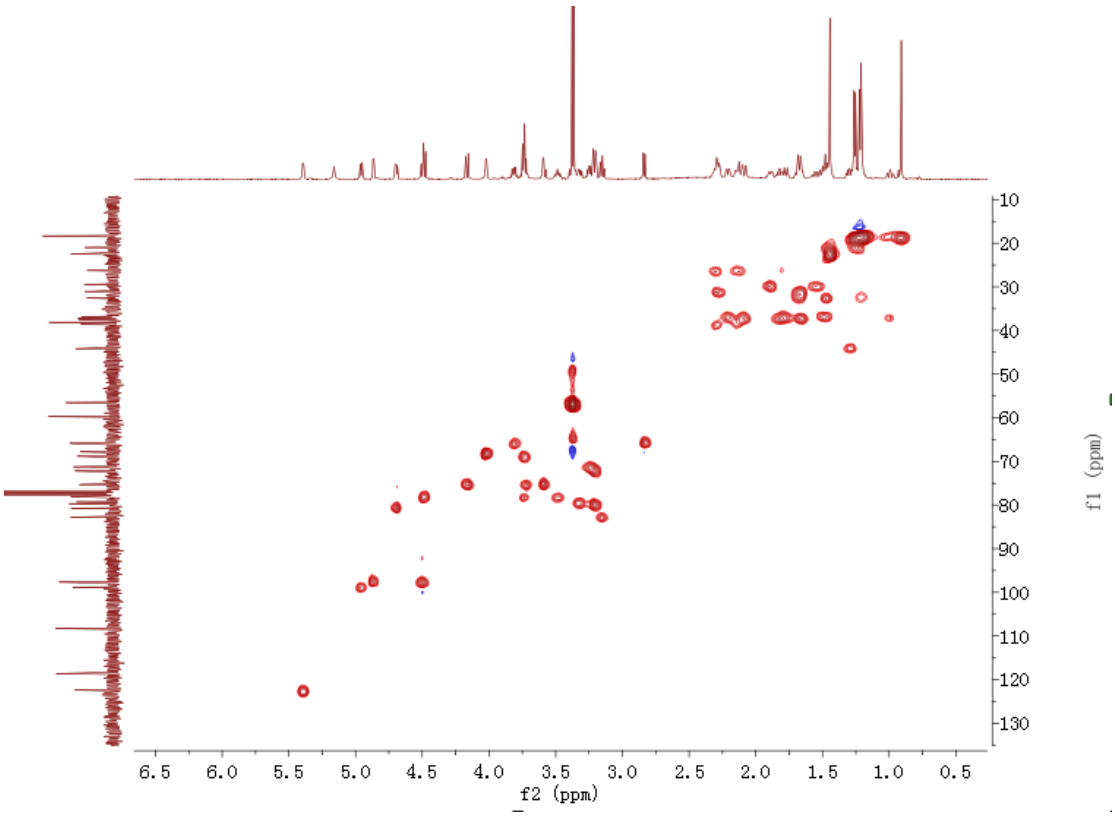

Figure S16 HSQC spectrum of compound **3**

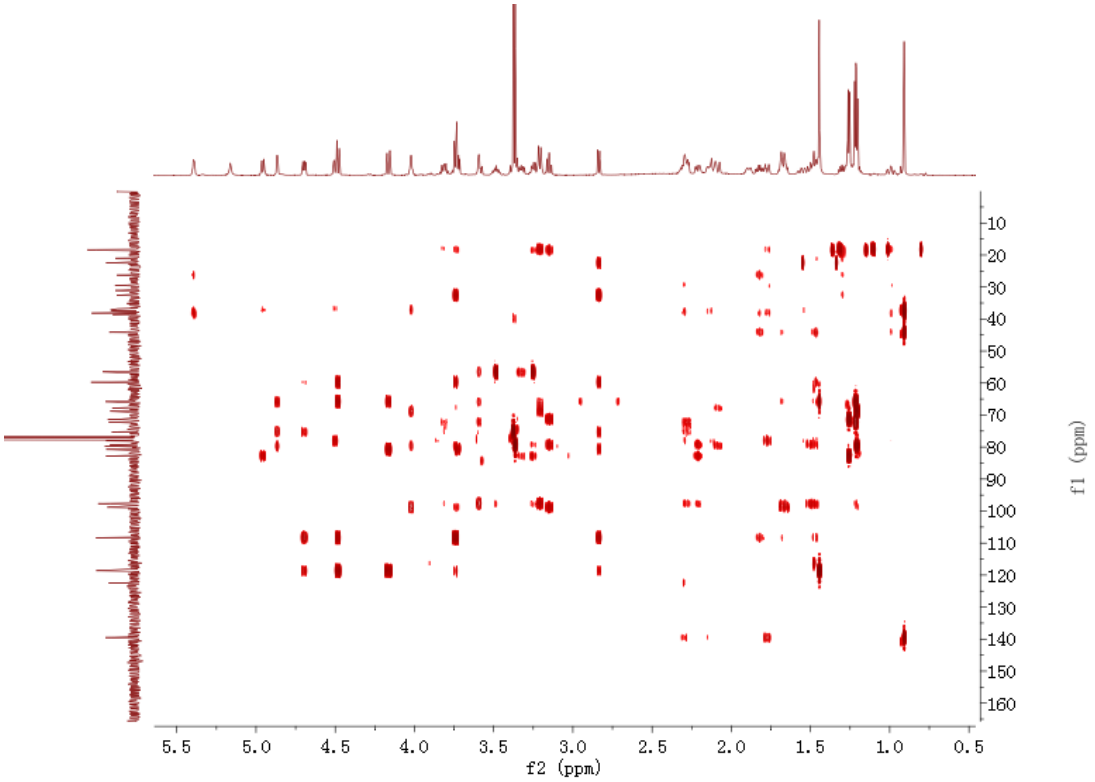

Figure S17 HMBC spectrum of compound **3**

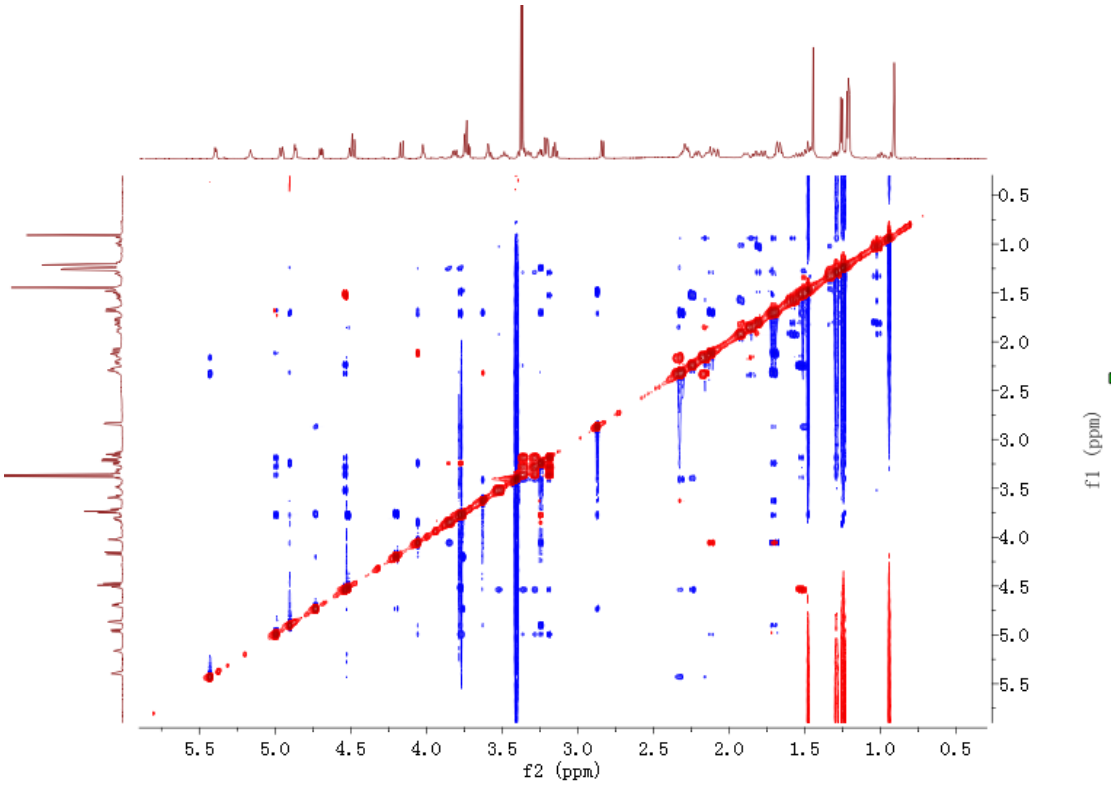

Figure S18 ROESY spectrum of compound **3**

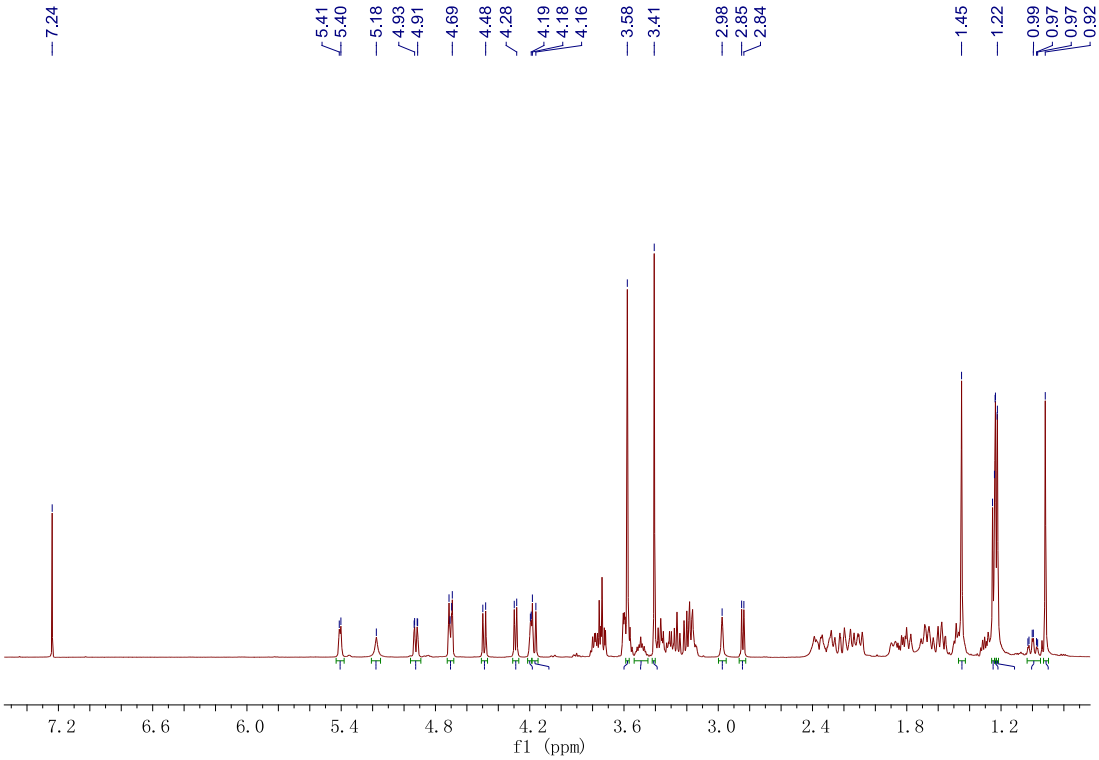

Figure S19 ^{1}H NMR spectrum of compound **4**

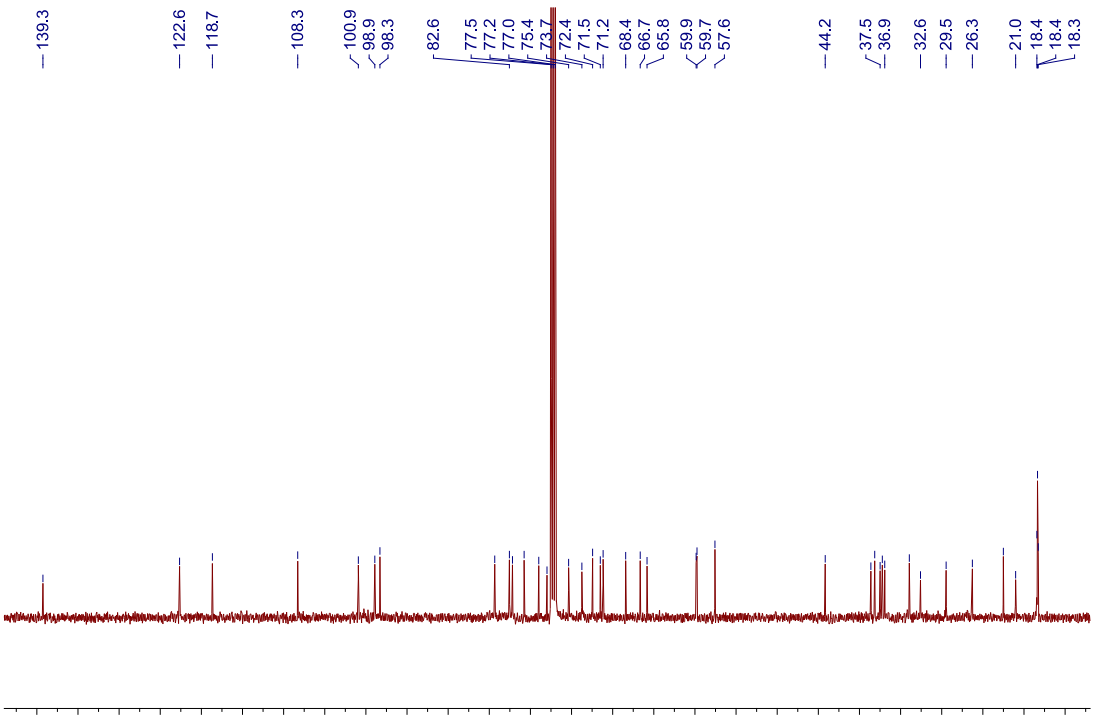

Figure S20 ^{13}C NMR spectrum of compound **4**

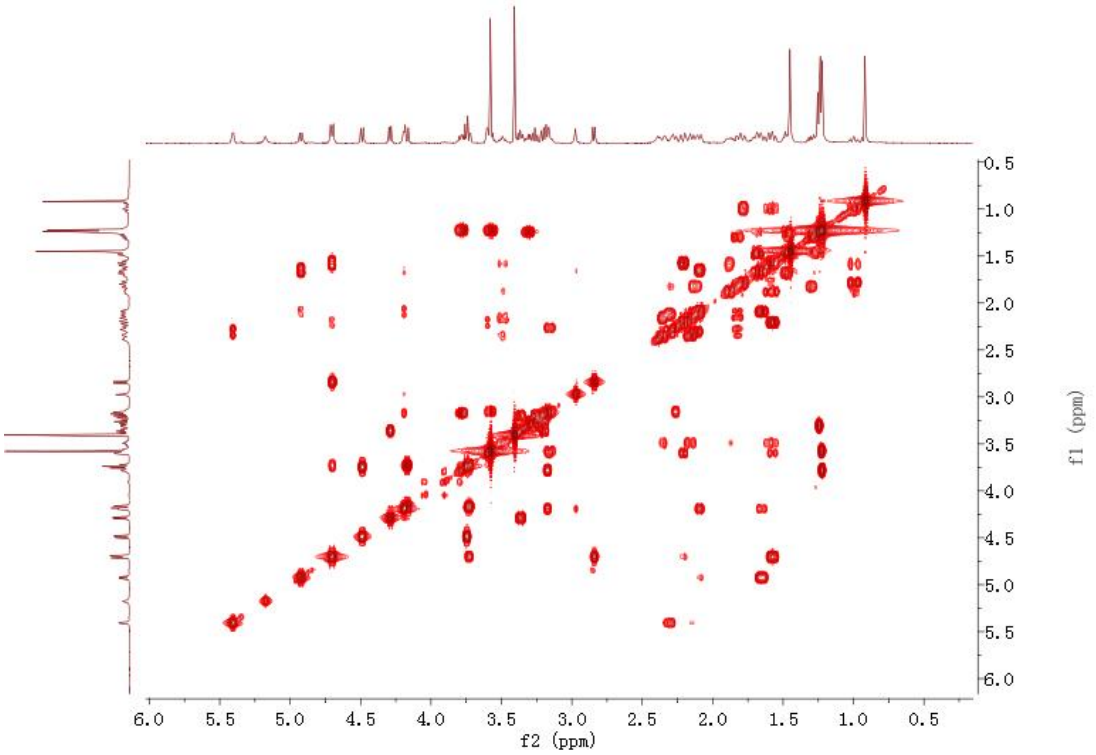

Figure S21 ^{1}H-^{1}H COSY spectrum of compound **4**

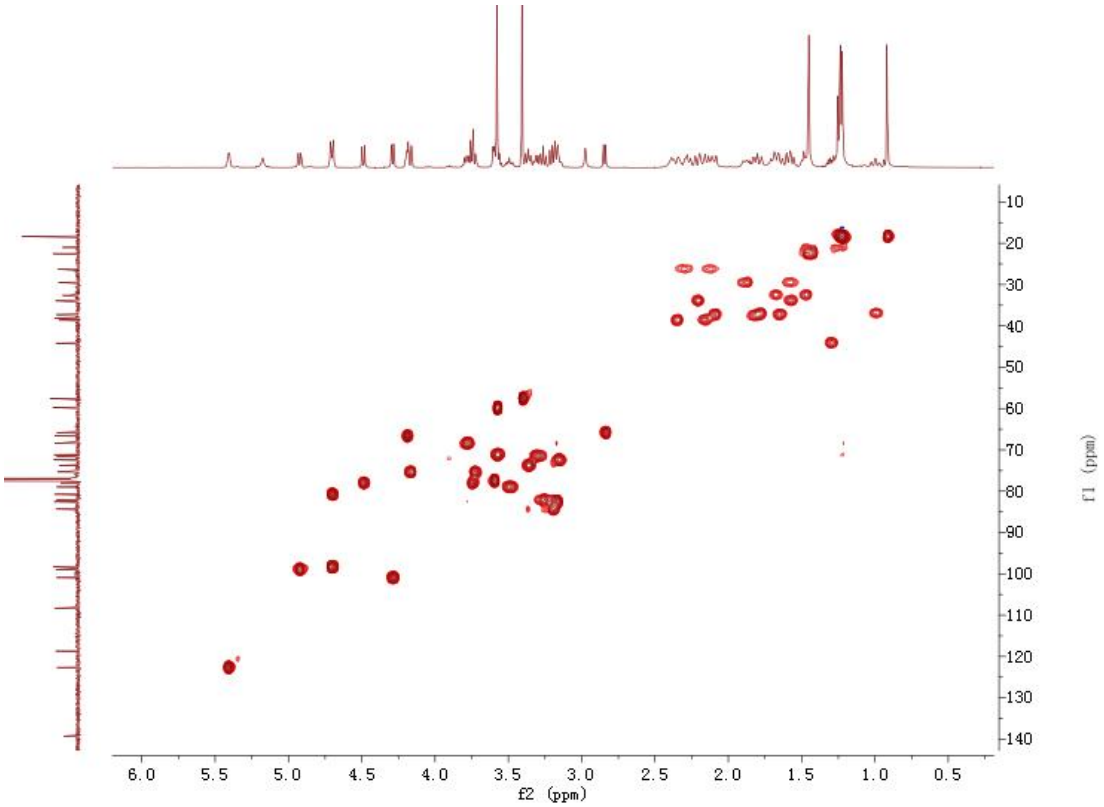

Figure S22 HSQC spectrum of compound **4**

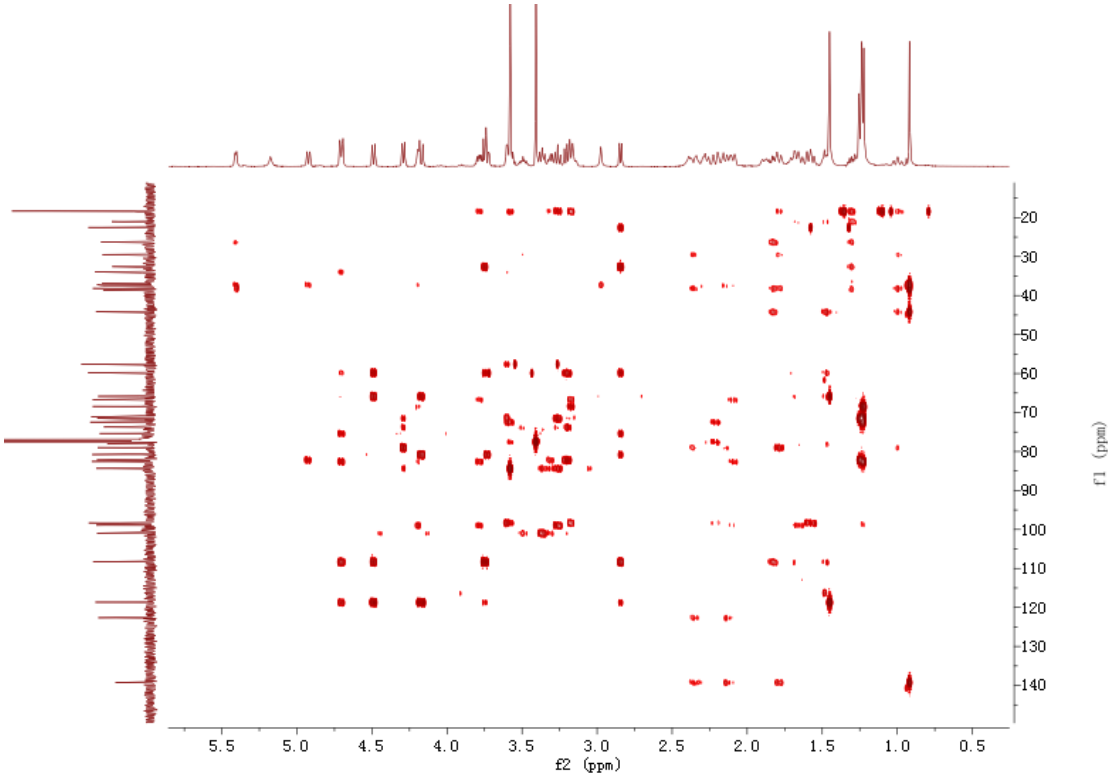

Figure S23 HMBC spectrum of compound **4**

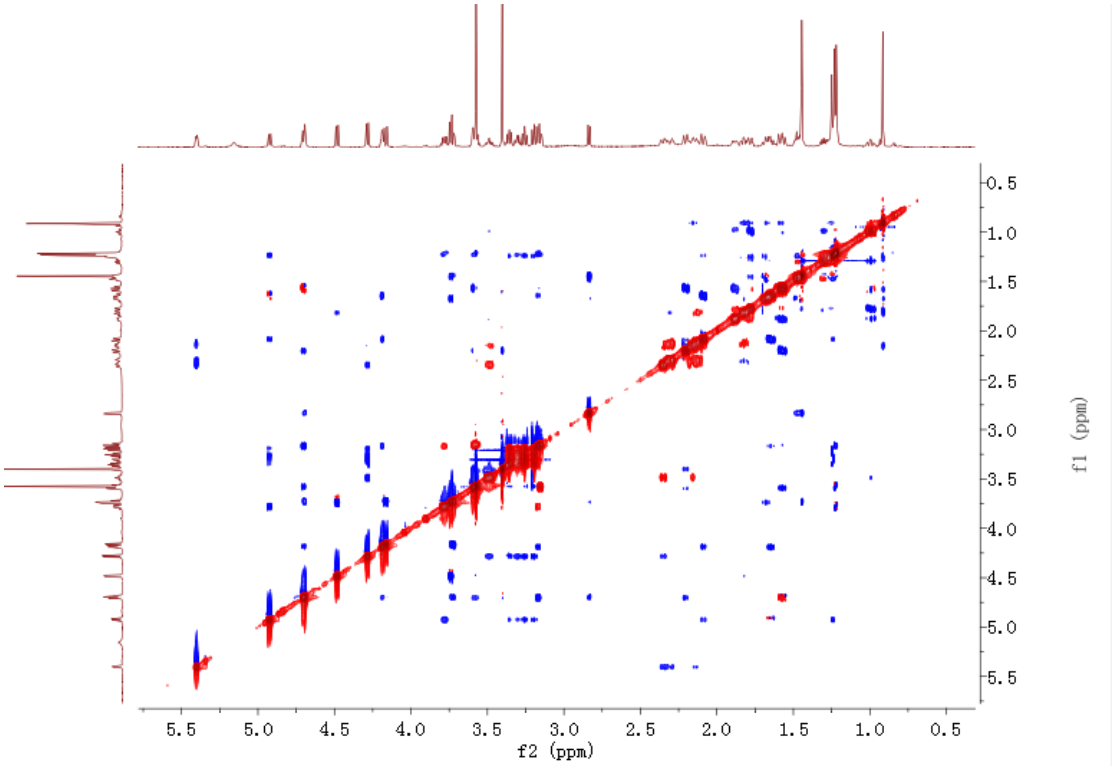

Figure S24 ROESY spectrum of compound **4**

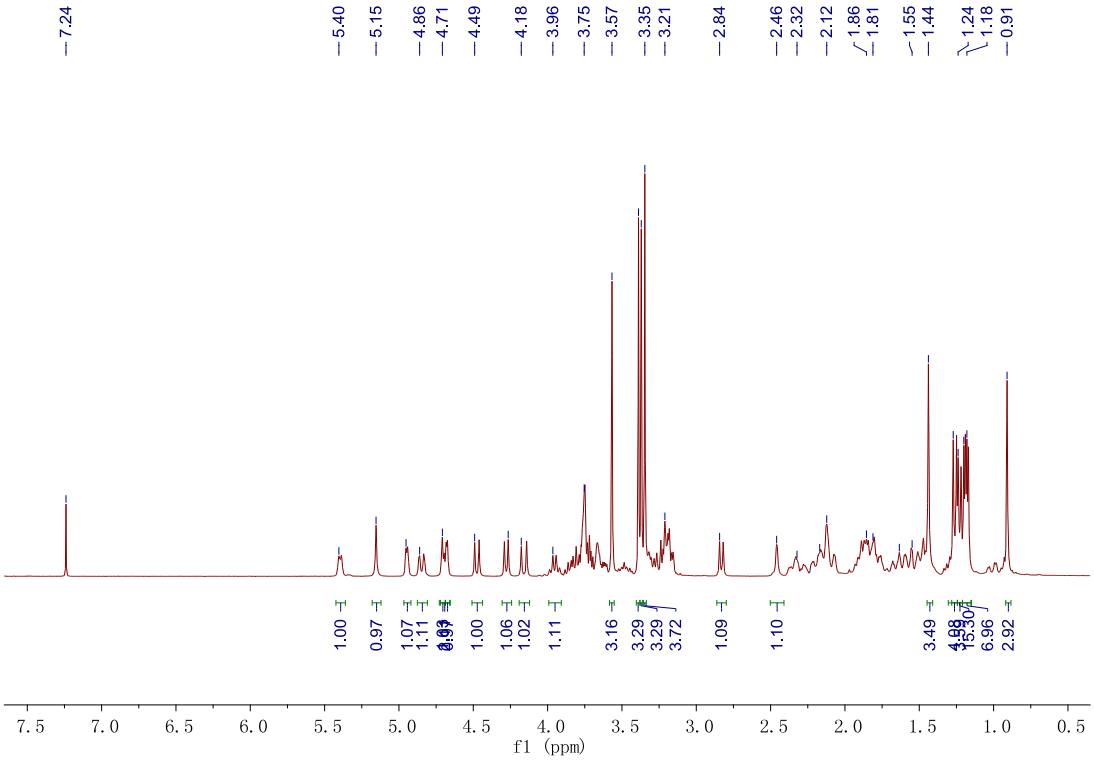

Figure S25 ^{1}H NMR spectrum of compound **5**

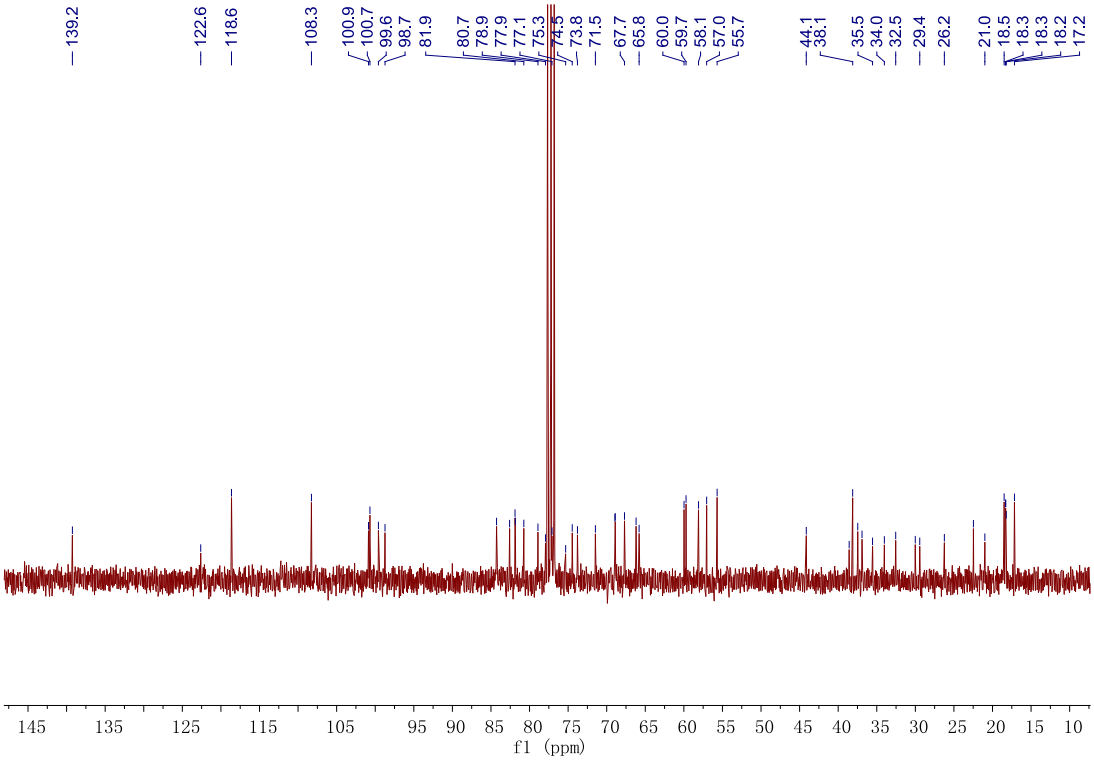

Figure S26 ^{13}C NMR spectrum of compound **5**

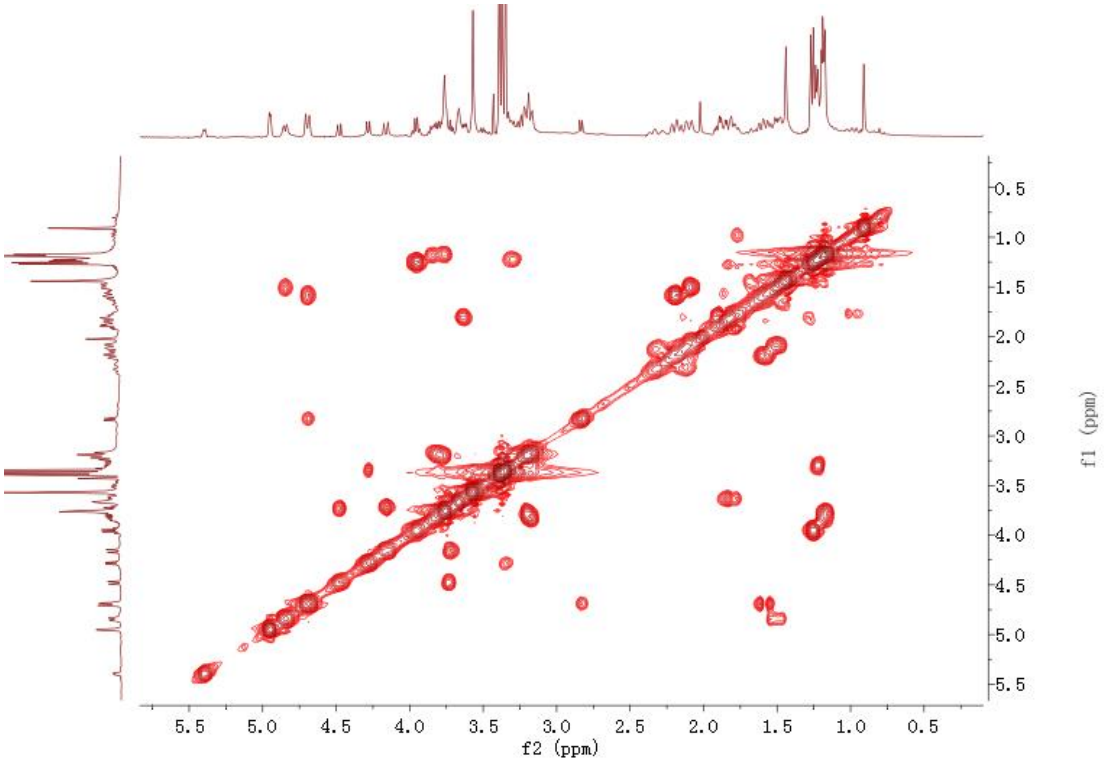

Figure S27 ^{1}H-^{1}H COSY spectrum of compound **5**

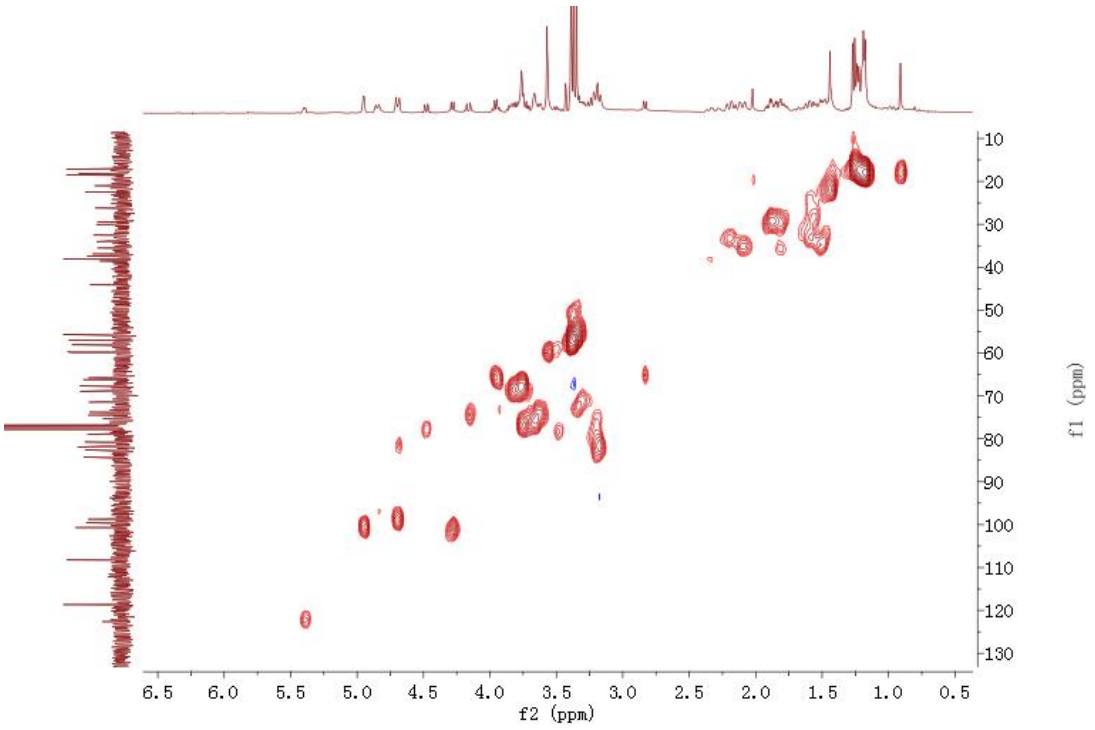

Figure S28 HSQC spectrum of compound **5**

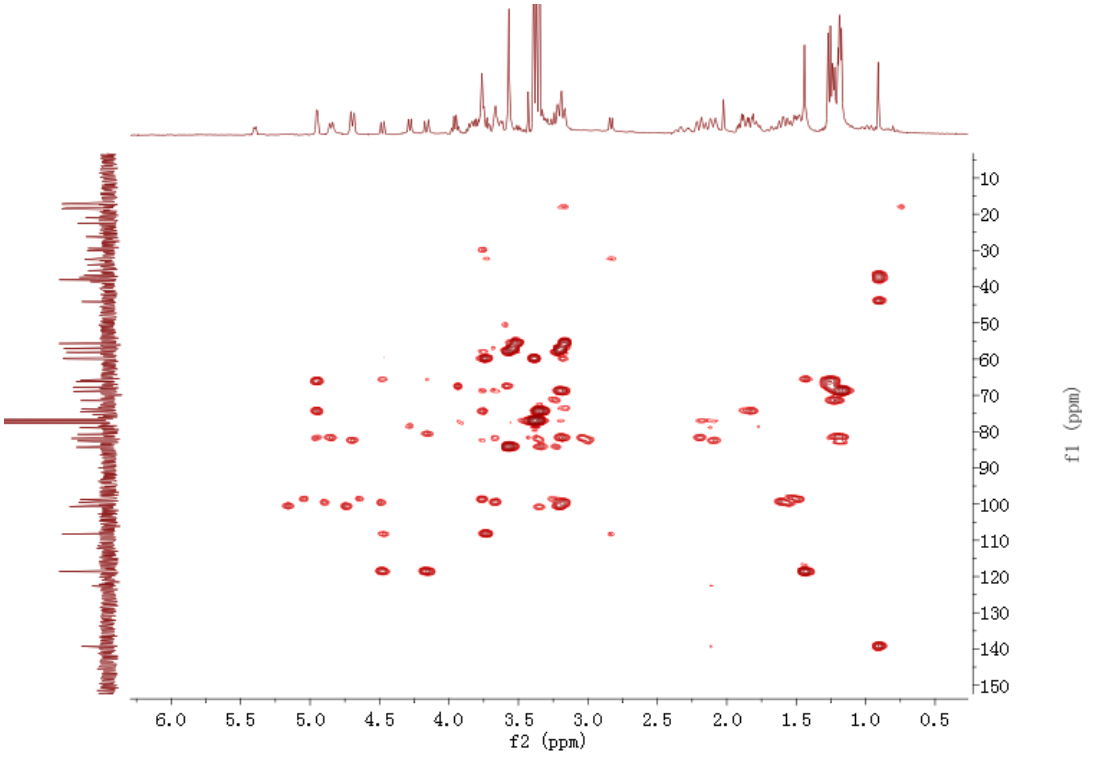

Figure S29 HMBC spectrum of compound **5**

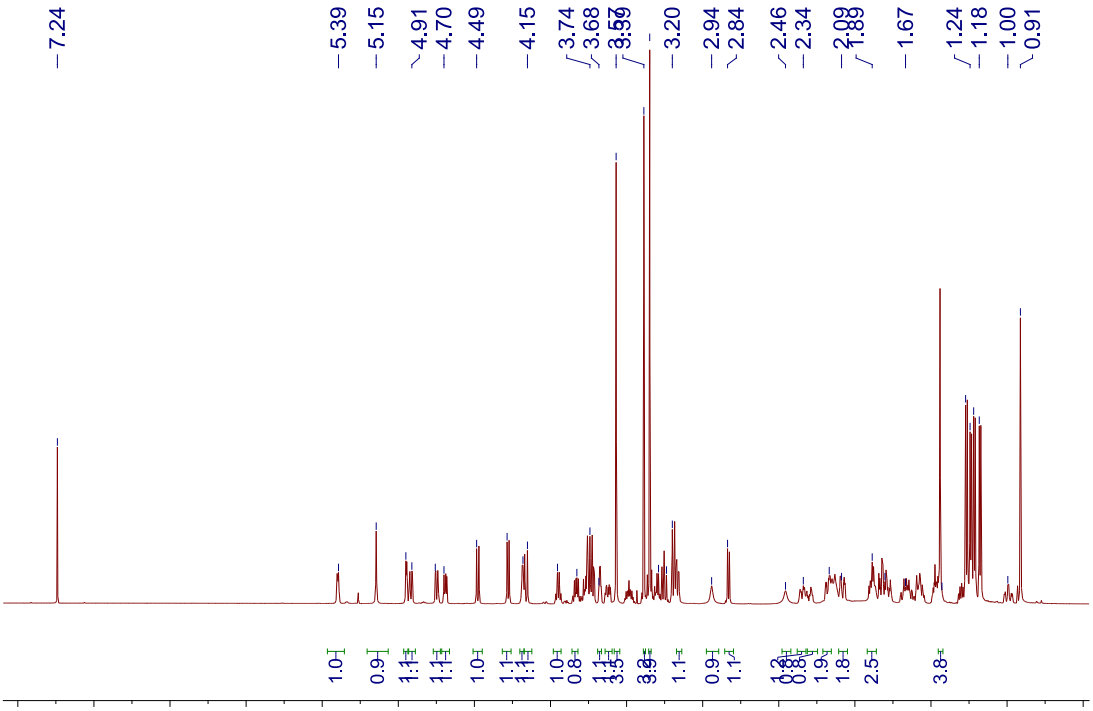

Figure S30 ^{1}H NMR spectrum of compound **6**

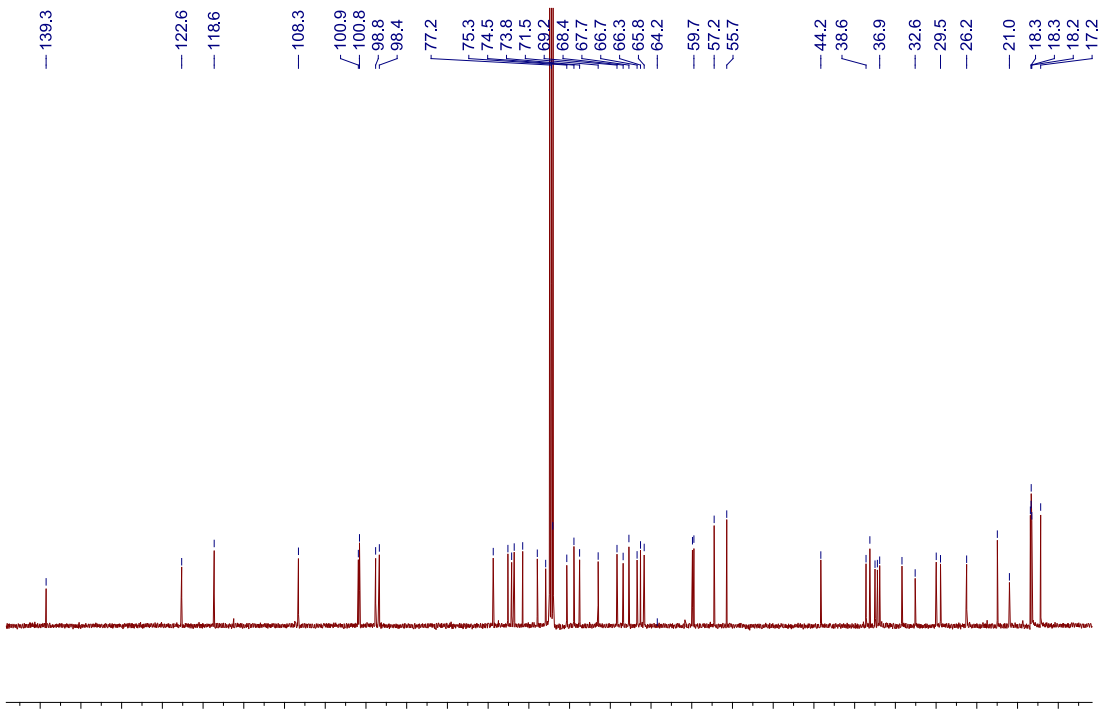

Figure S31 ^{13}C NMR spectrum of compound **6**

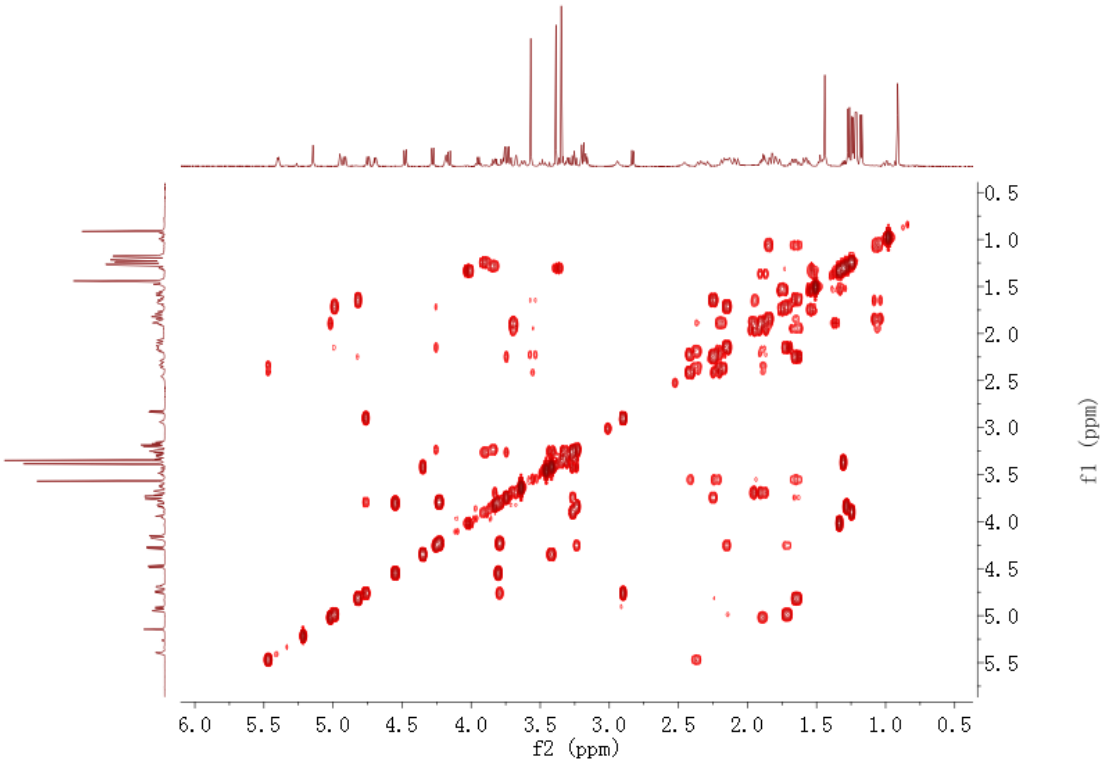

Figure S32 ^{1}H-^{1}H COSY spectrum of compound **6**

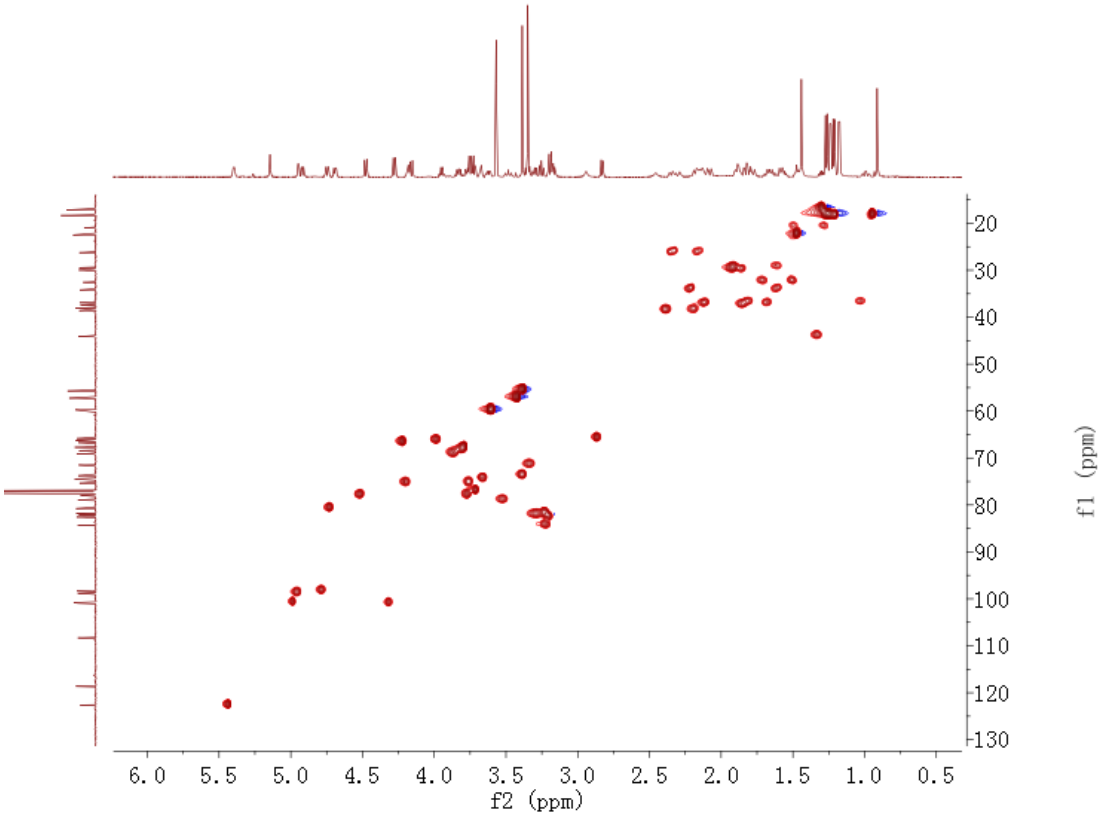

Figure S33 HSQC spectrum of compound **6**

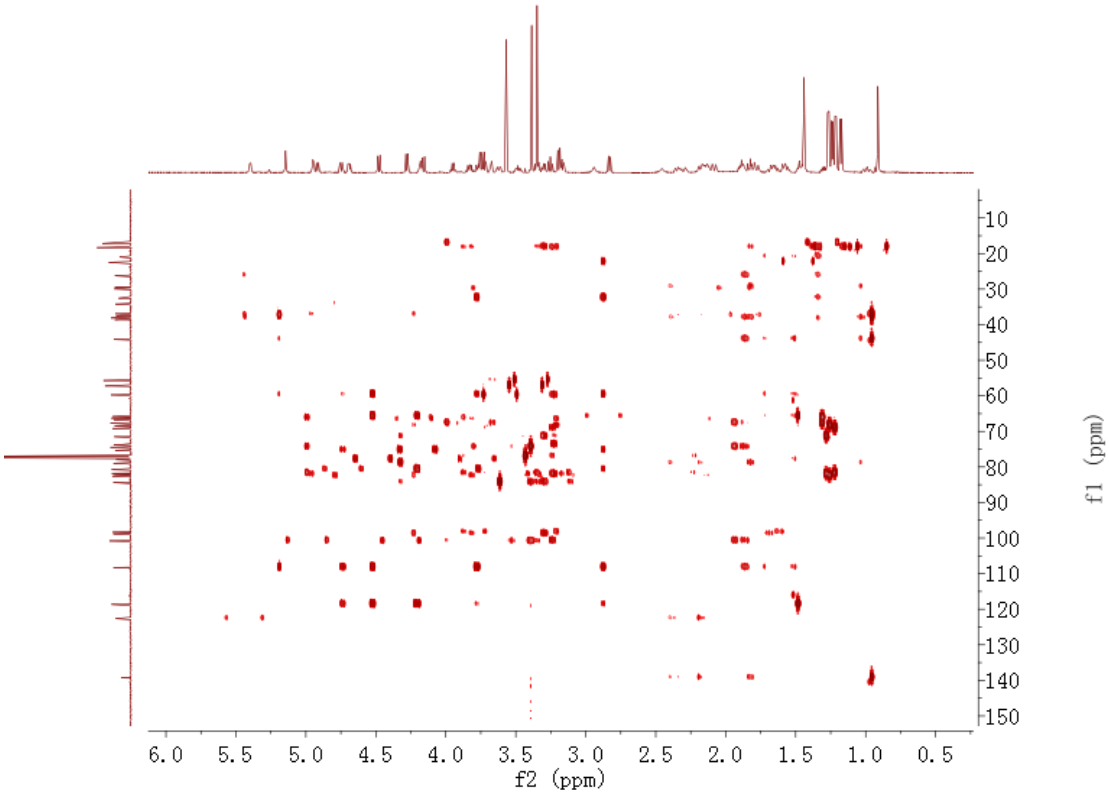

Figure S34 HMBC spectrum of compound **6**

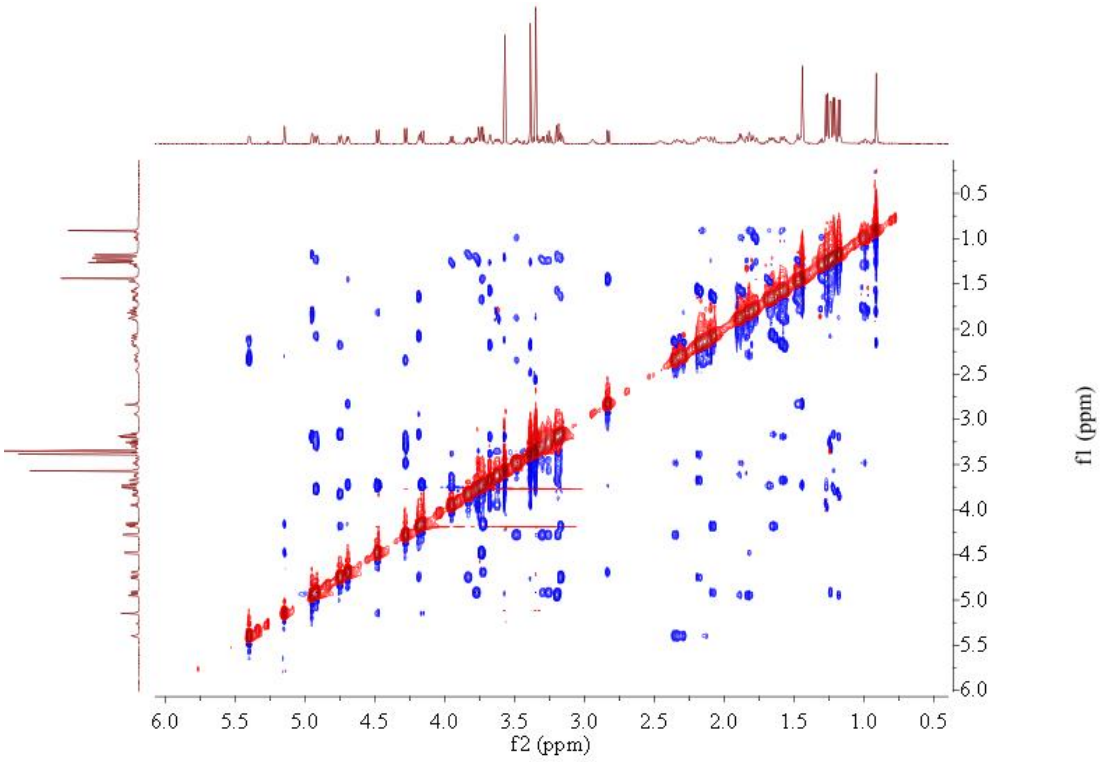

Figure S35 ROESY spectrum of compound **6**

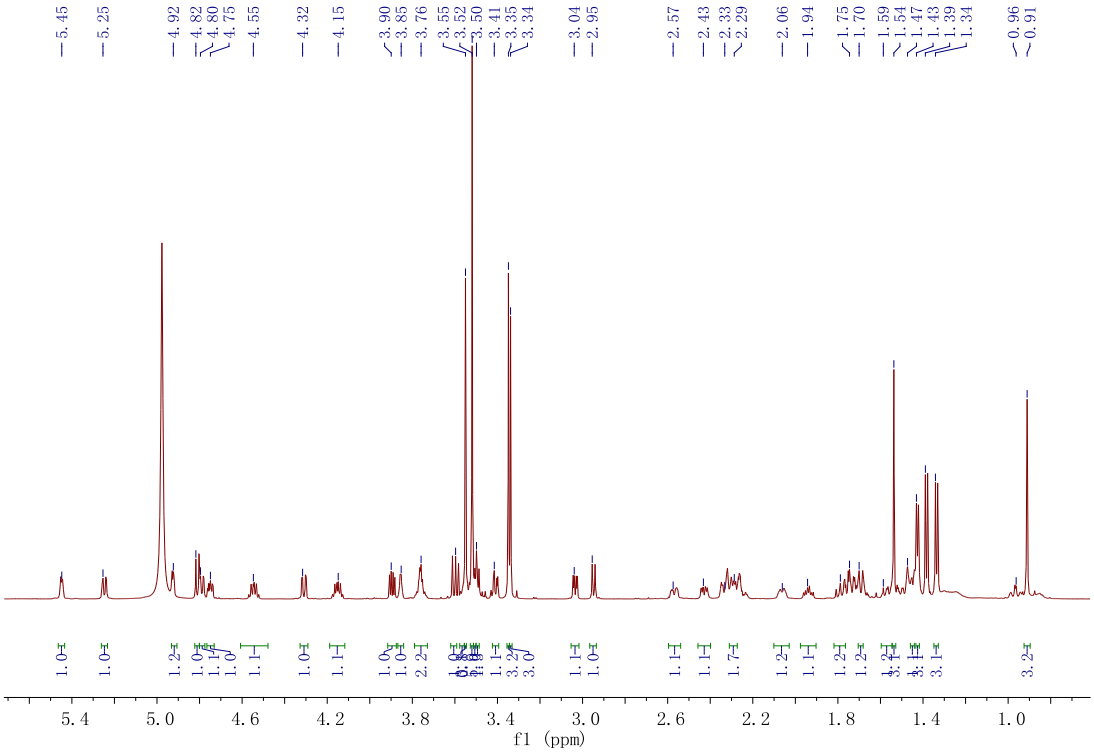

Figure S36 ^{1}H NMR spectrum of compound **2a**

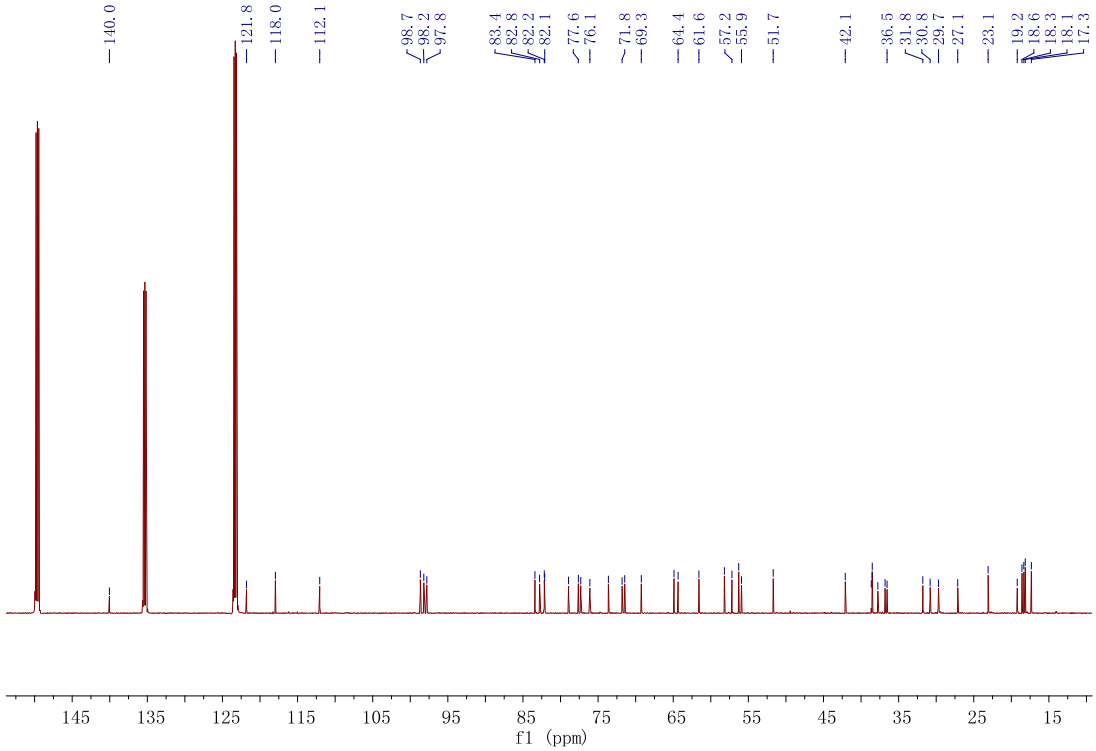

Figure S37 ^{13}C NMR spectrum of compound **2a**

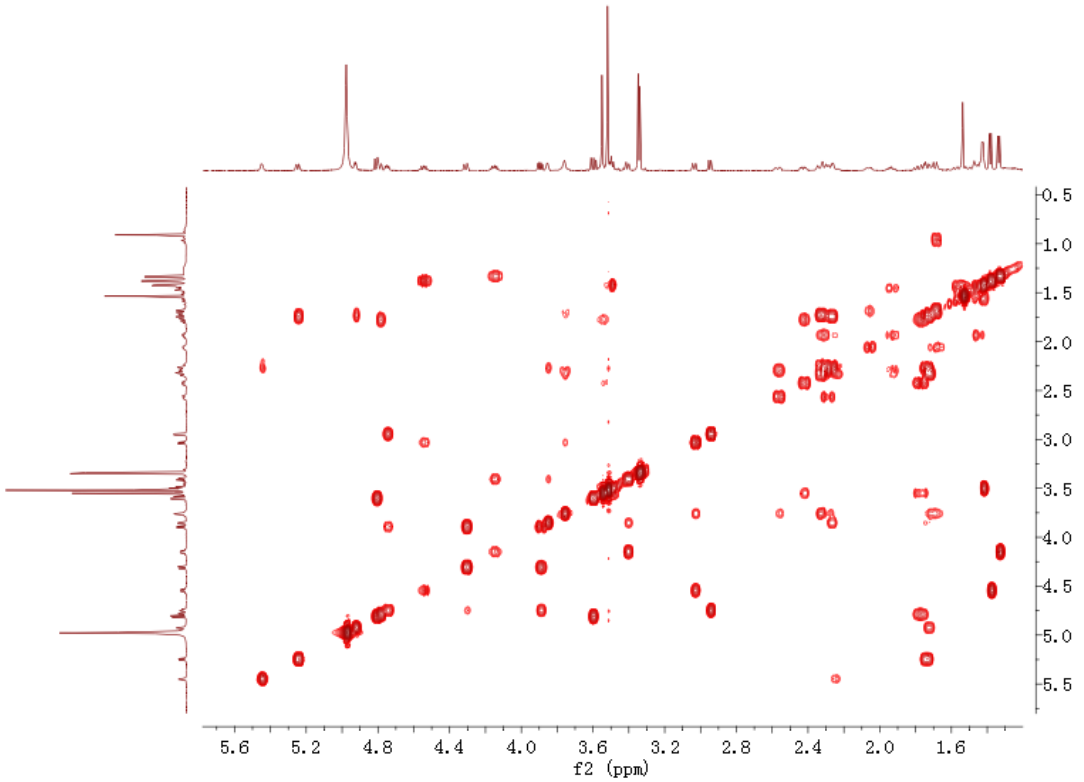

Figure S38 ^{1}H-^{1}H COSY spectrum of compound **2a**

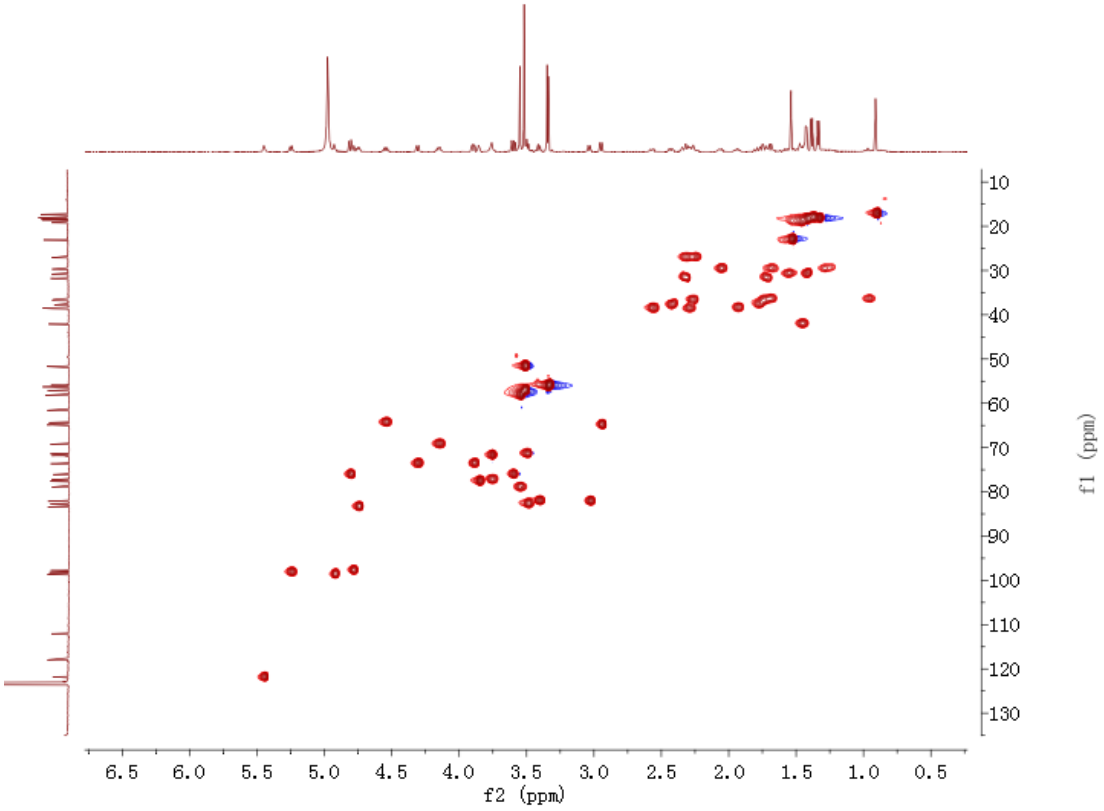

Figure S39 HSQC spectrum of compound **2a**

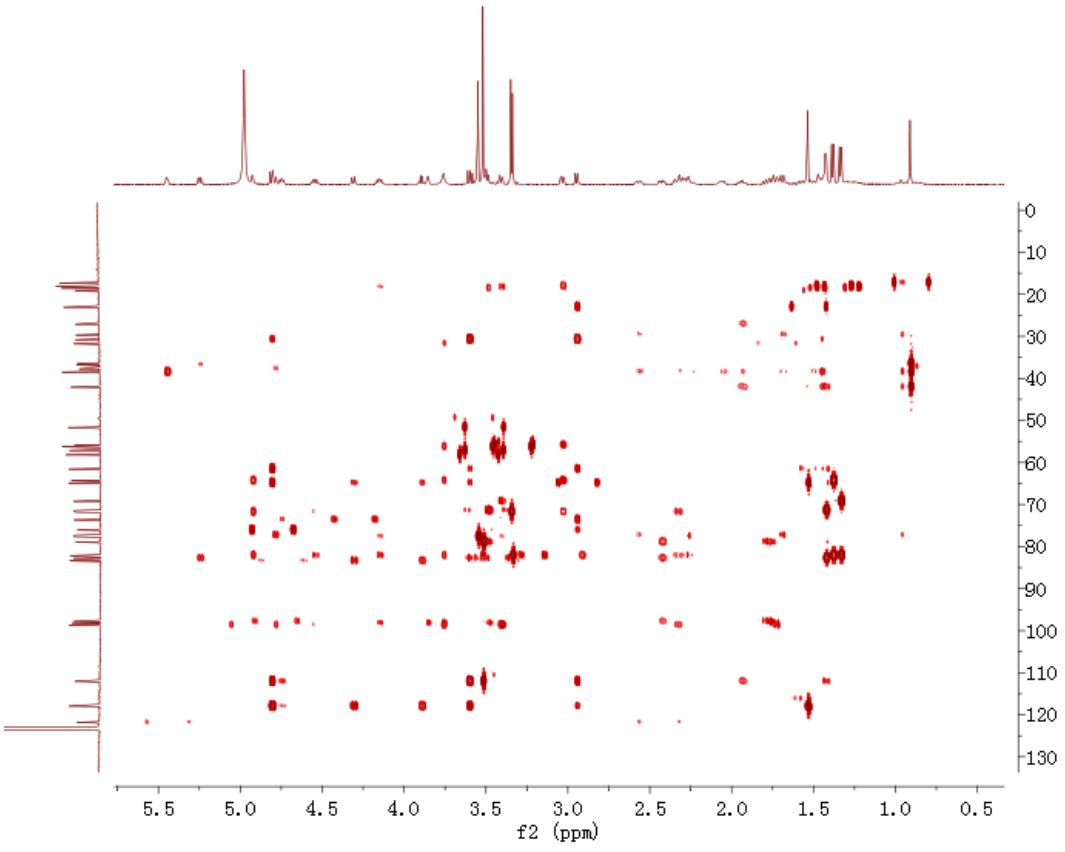

Figure S40 HMBC spectrum of compound **2a**

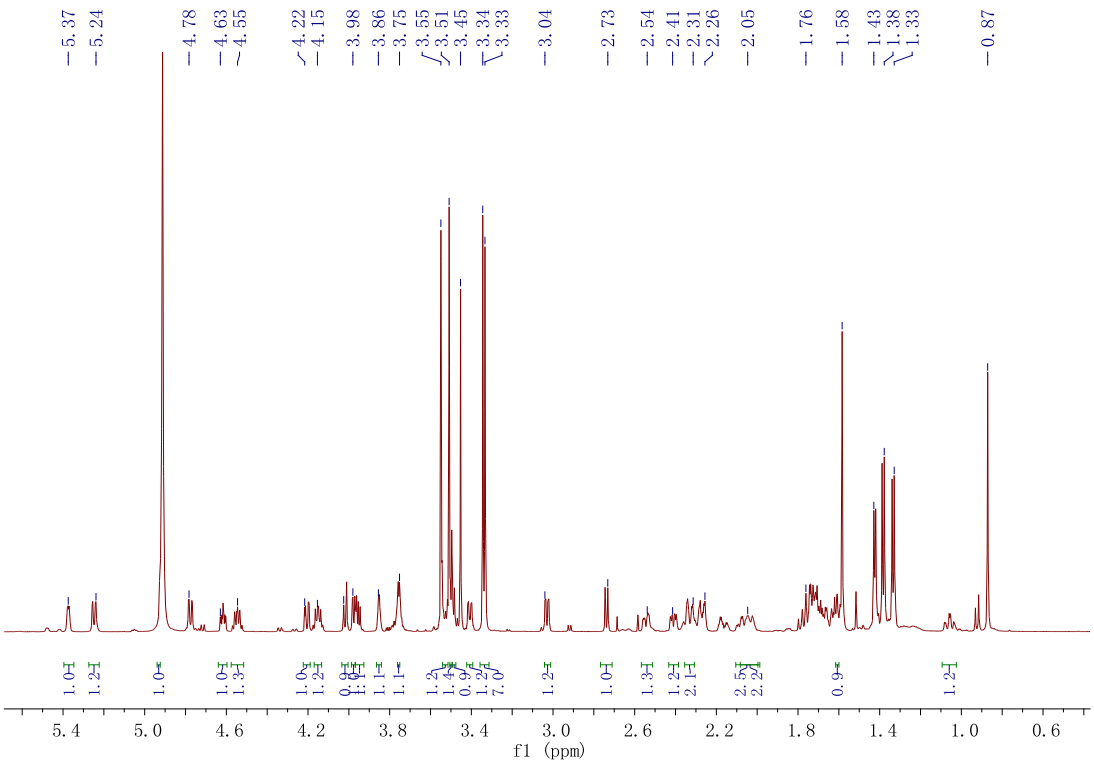

Figure S41 ^{1}H NMR spectrum of compound **2b**

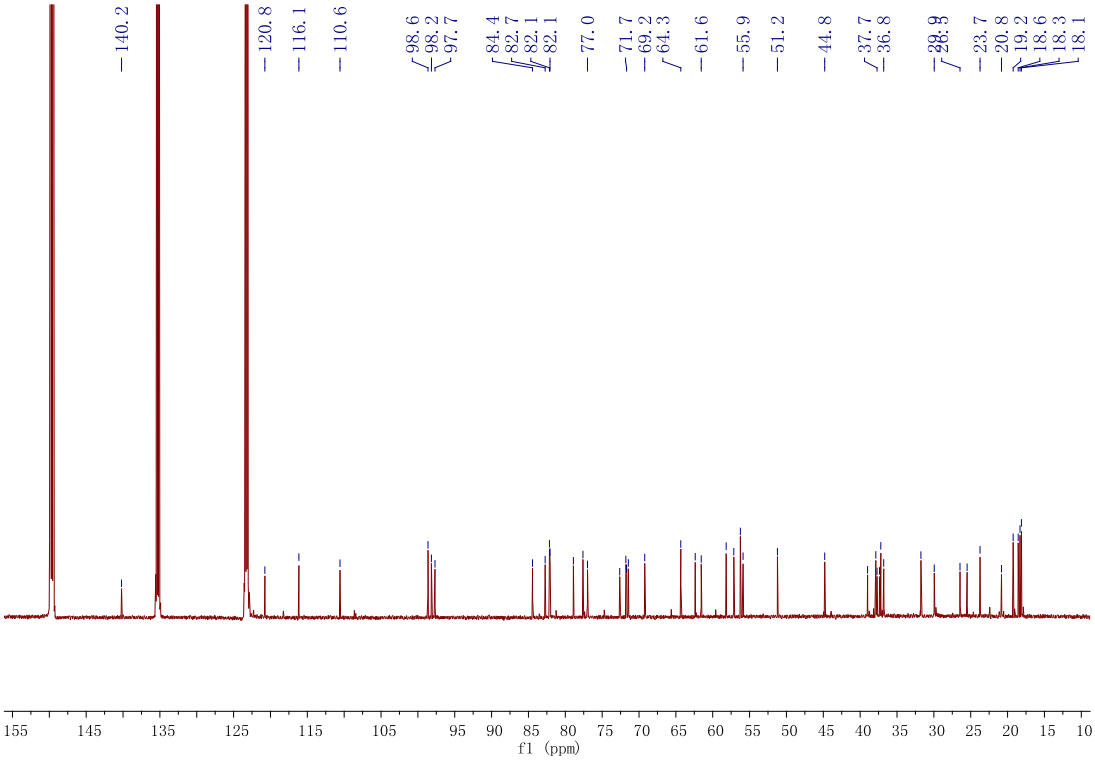

Figure S42 ^{13}C NMR spectrum of compound **2b**

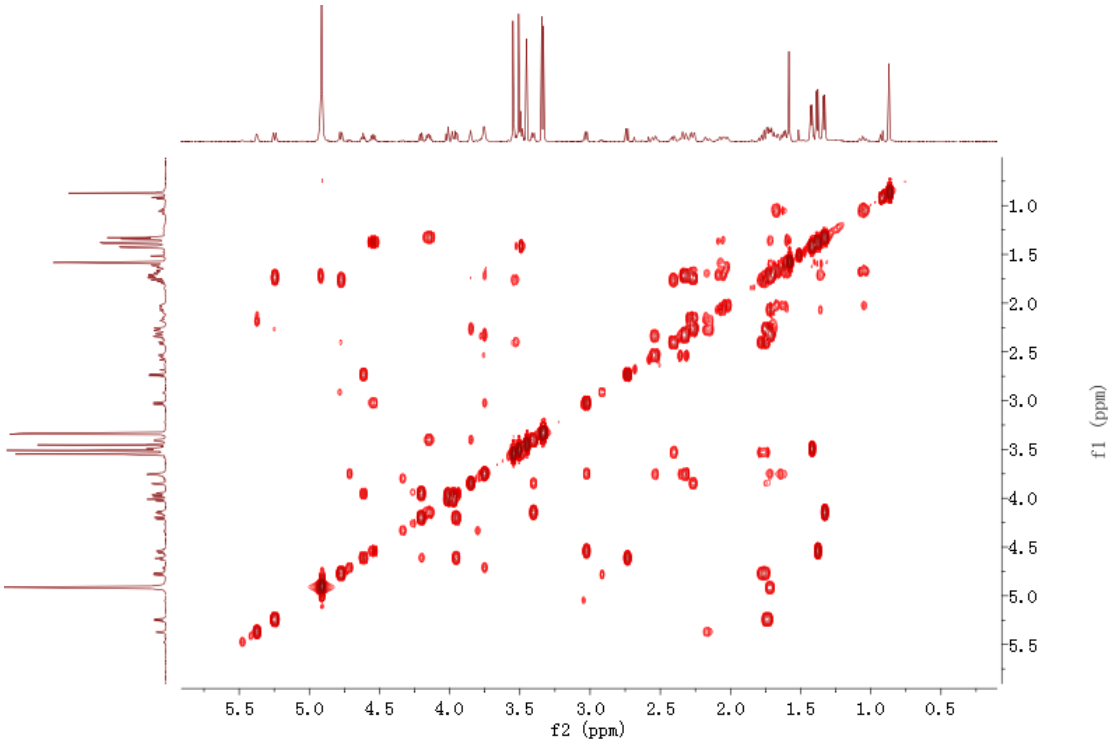

Figure S43 ^{1}H-^{1}H COSY spectrum of compound **2b**

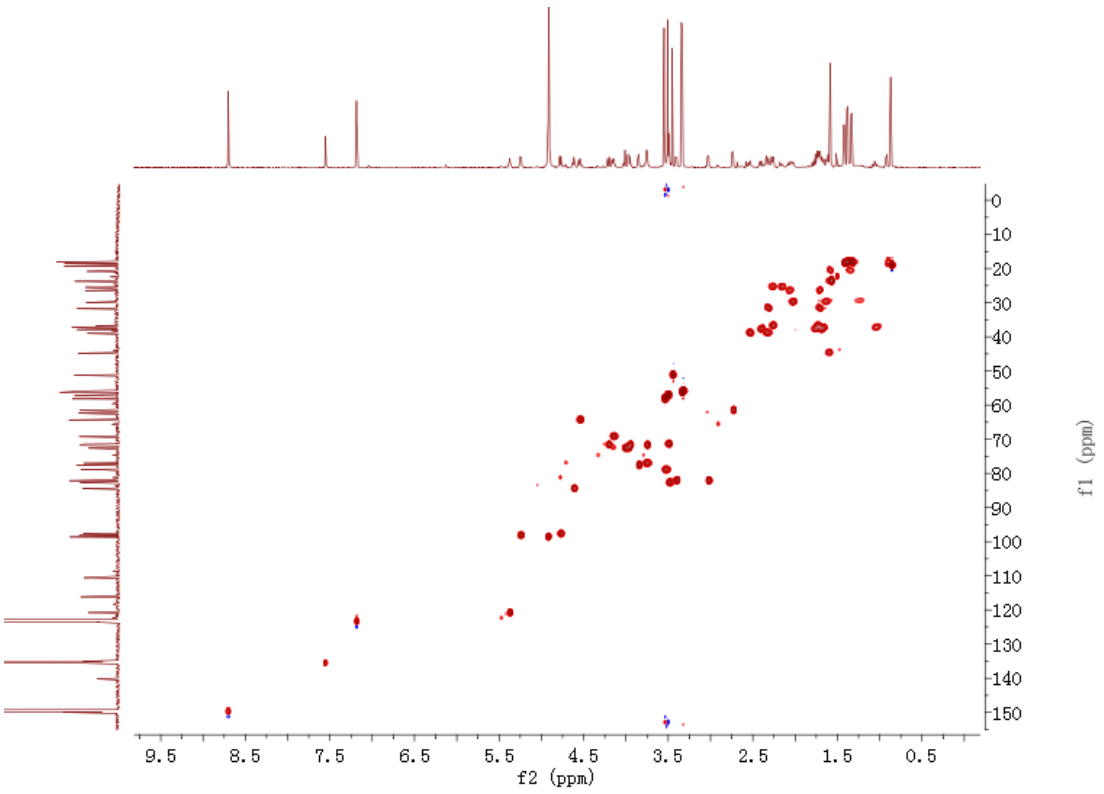

Figure S44 HSQC spectrum of compound **2b**

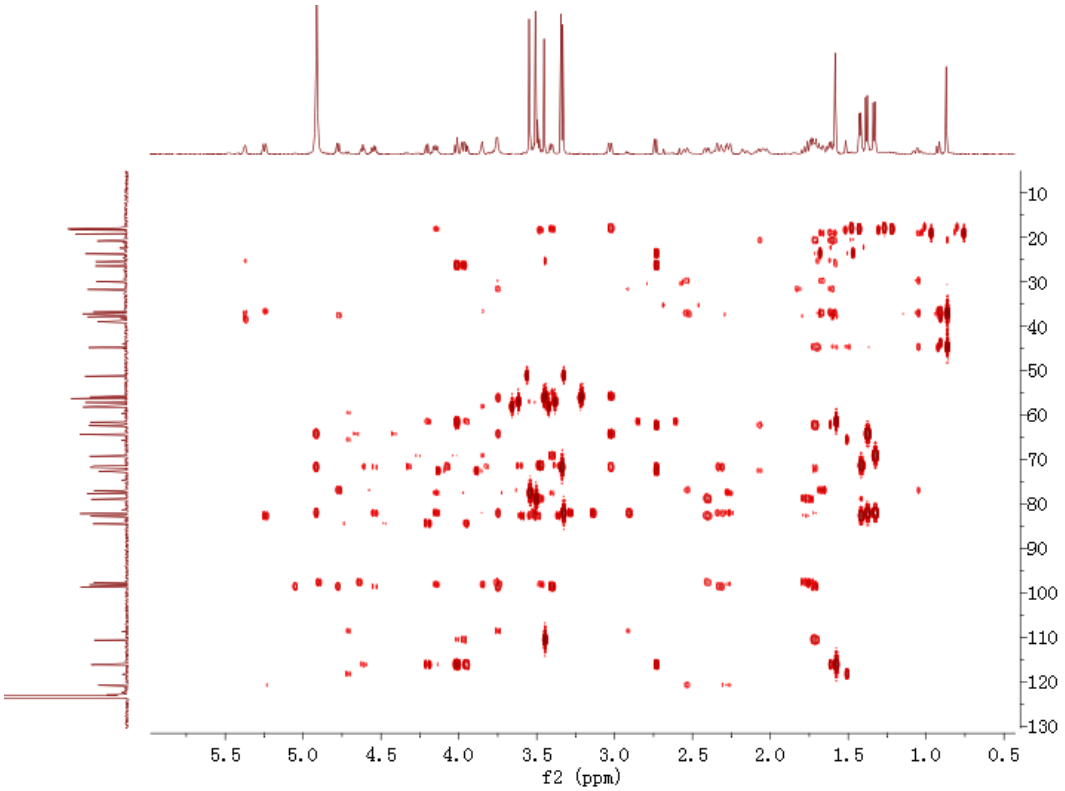

Figure S45 HMBC spectrum of compound **2b**

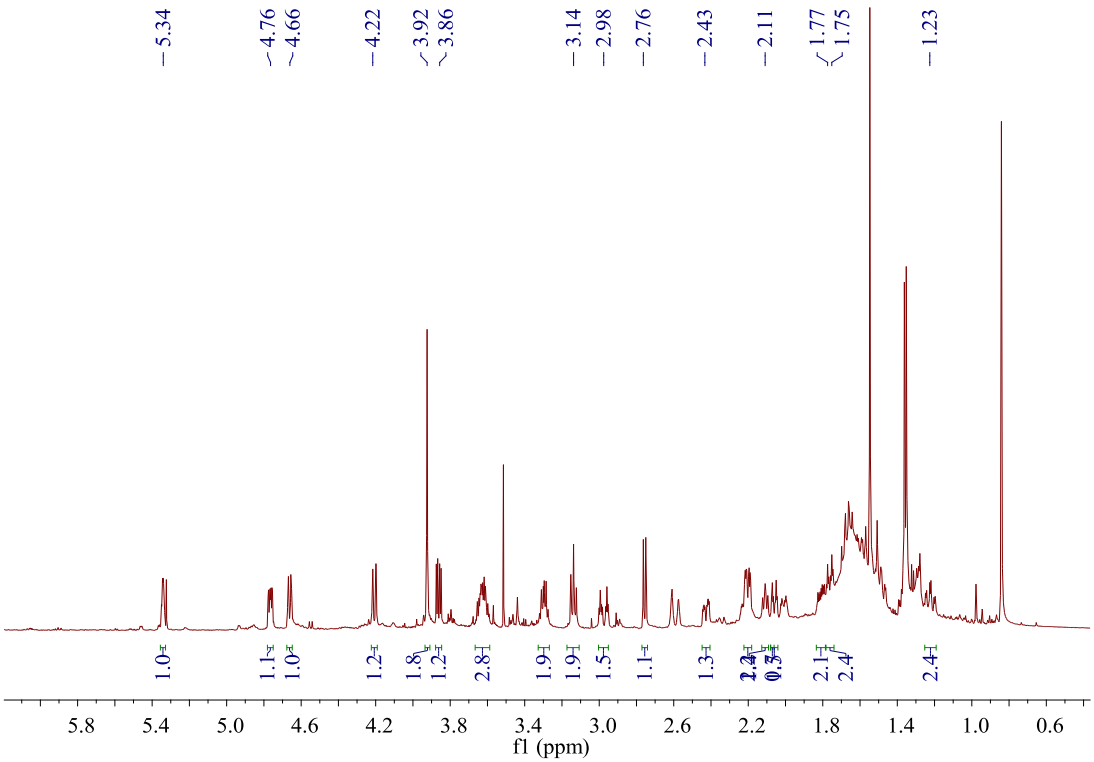

Figure S46 ^{1}H NMR spectrum of compound **2d**

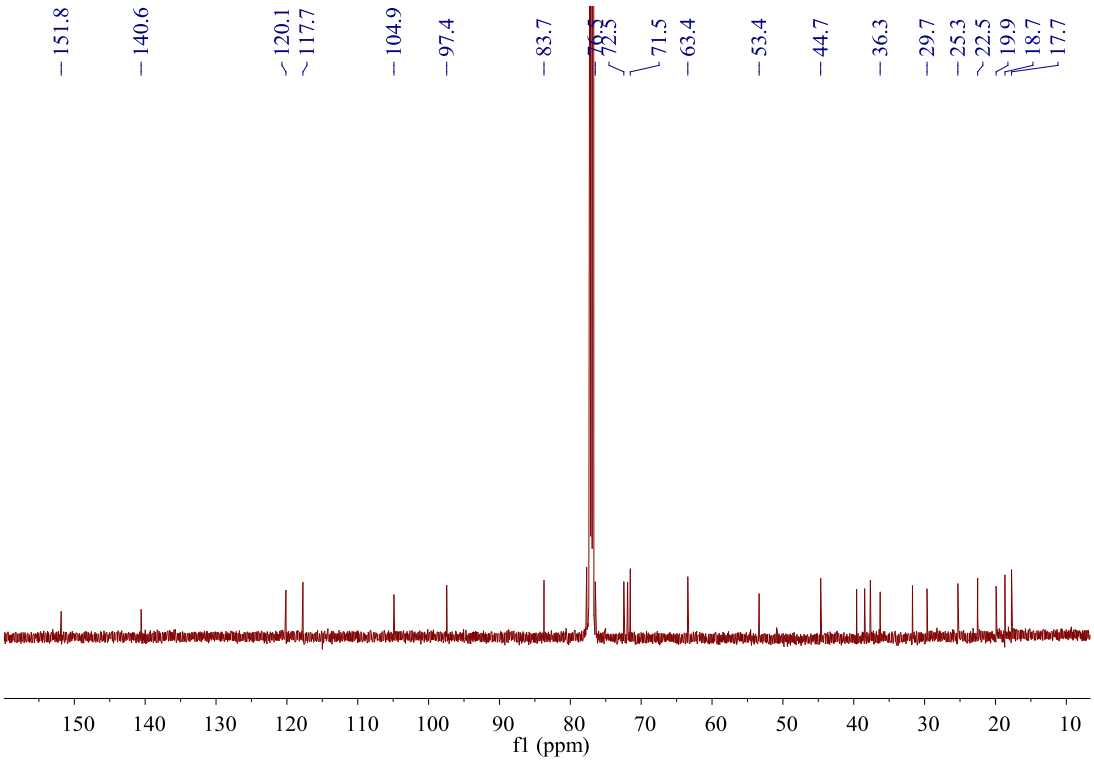

Figure S47 ^{13}C NMR spectrum of compound **2d**

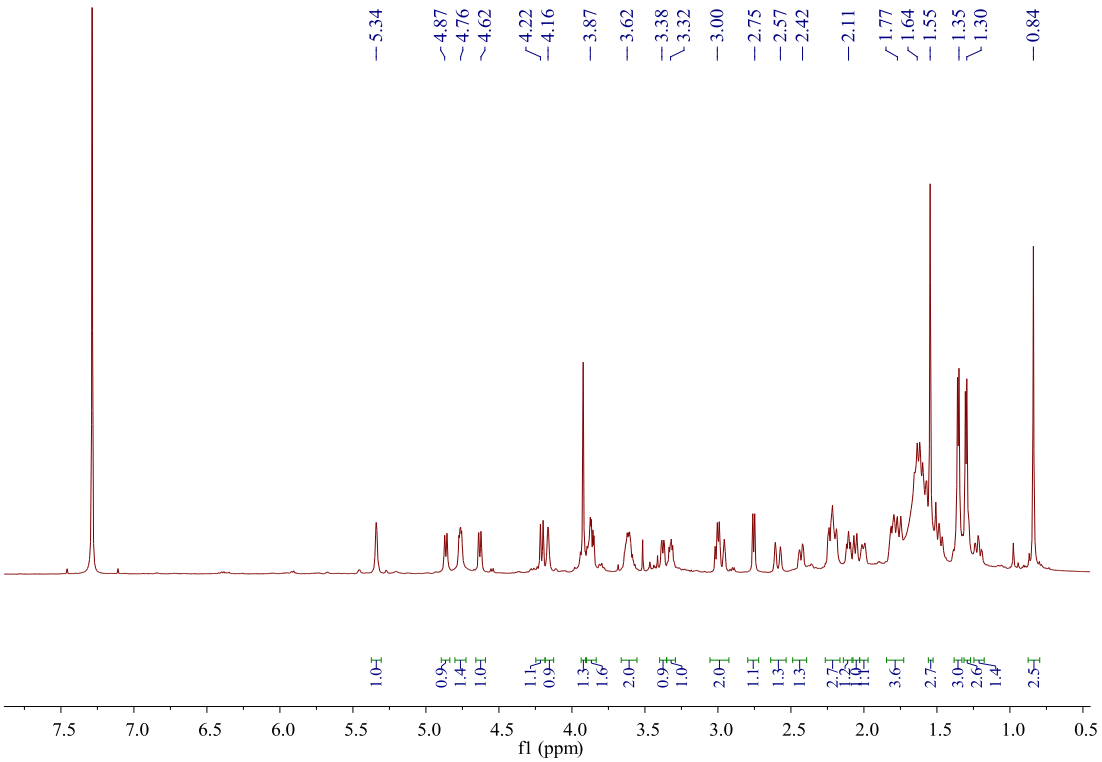

Figure S48 ^{1}H NMR spectrum of compound **2e**

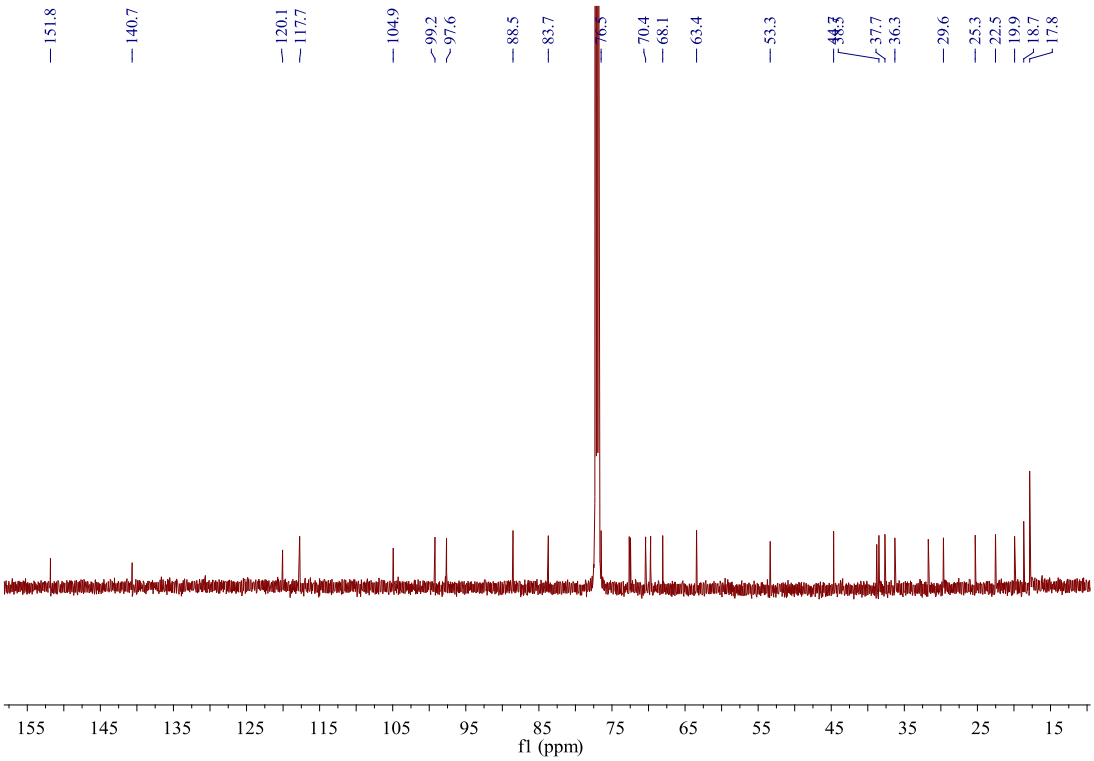

Figure S49 ^{13}C NMR spectrum of compound **2e**

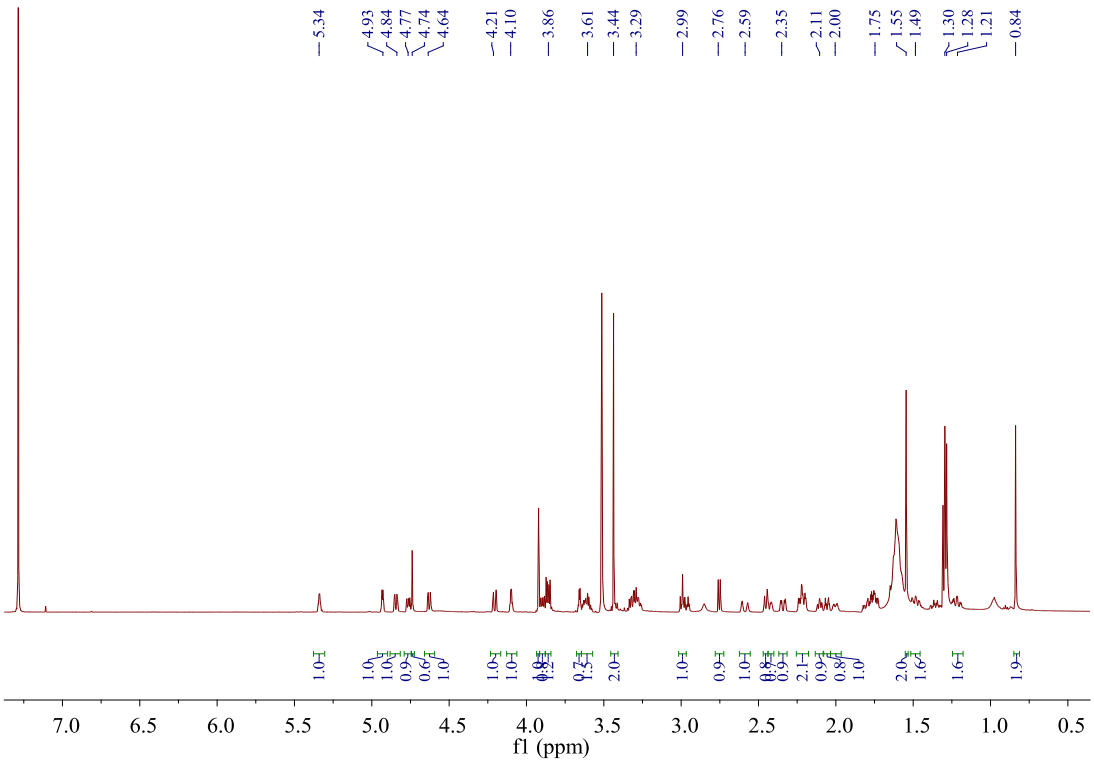

Figure S50 ^{1}H NMR spectrum of compound **2f**

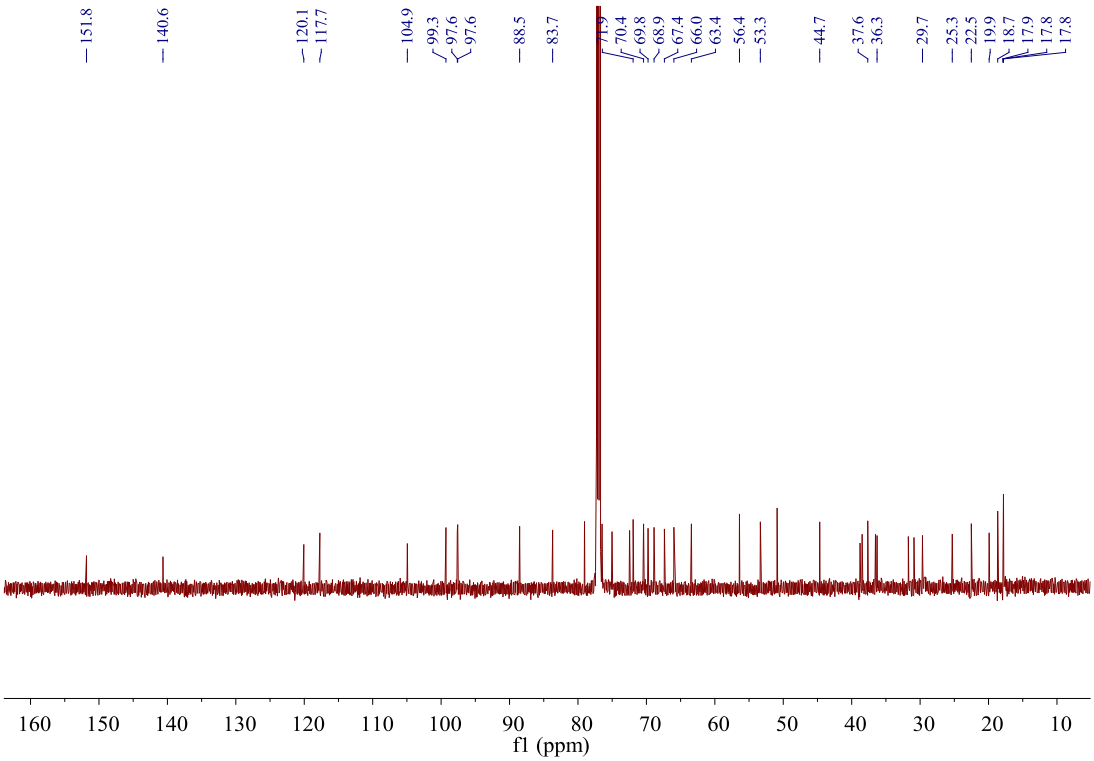

Figure S51 ^{13}C NMR spectrum of compound **2f**

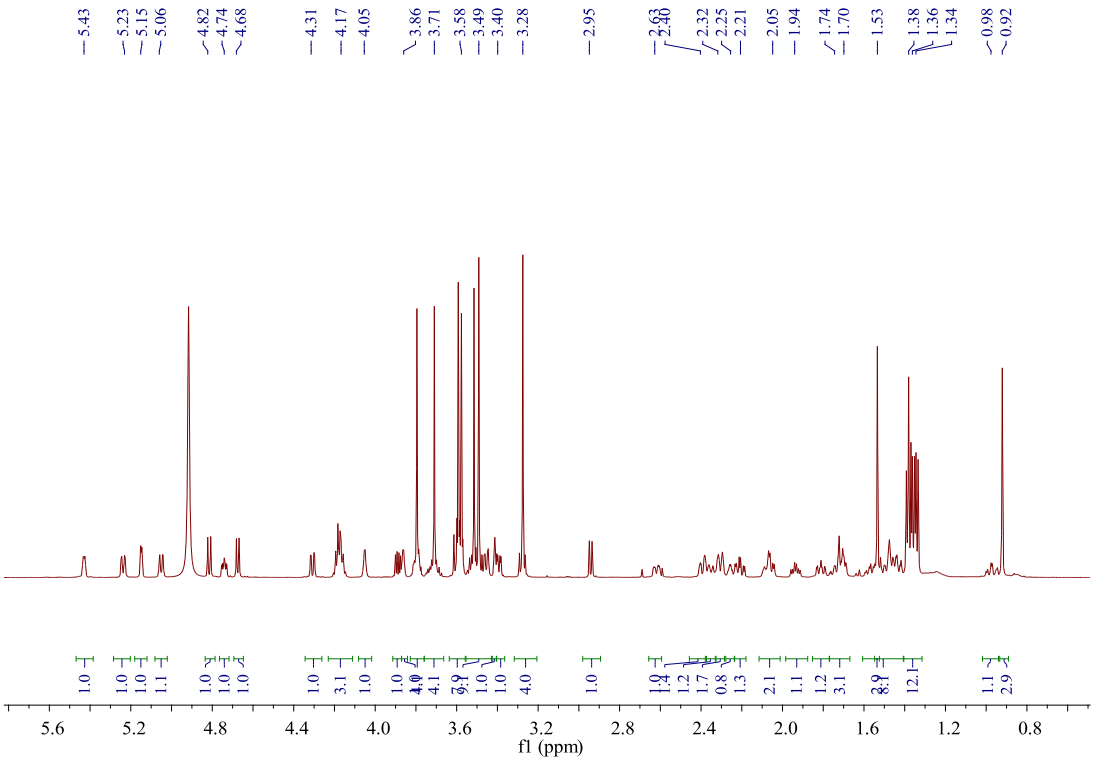

Figure S52 ^{1}H NMR spectrum of compound **6a**

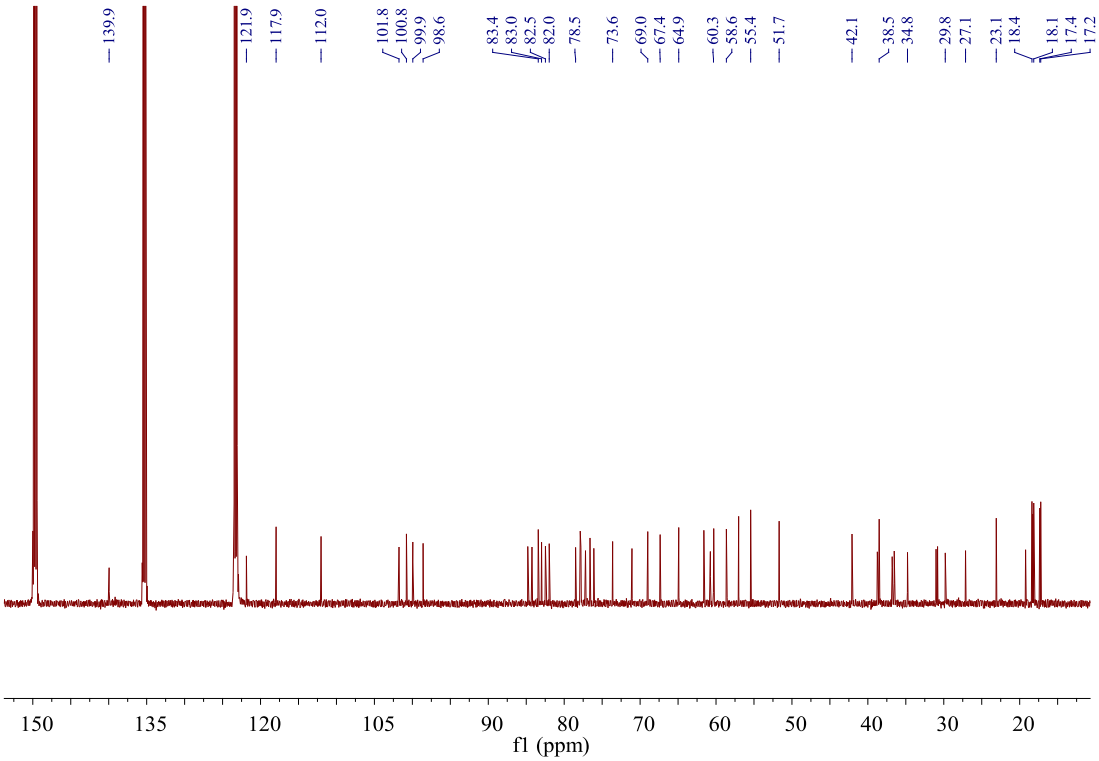

Figure S53 ^{13}C NMR spectrum of compound **6a**

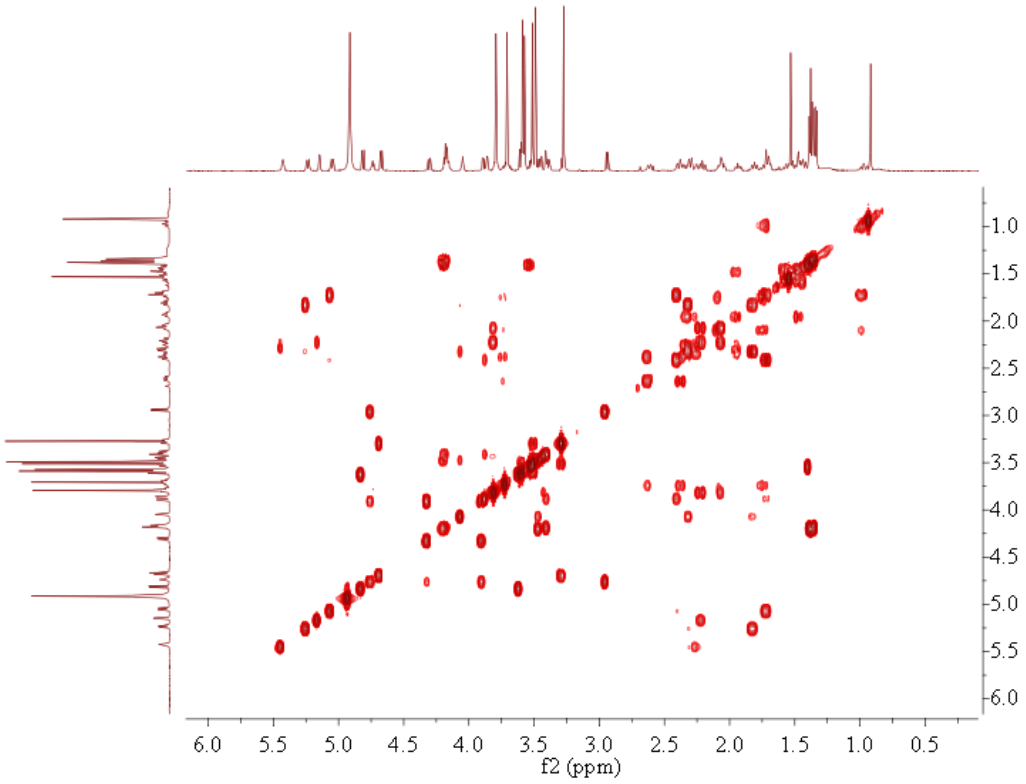

Figure S54 ^{1}H-^{1}H COSY spectrum of compound **6a**

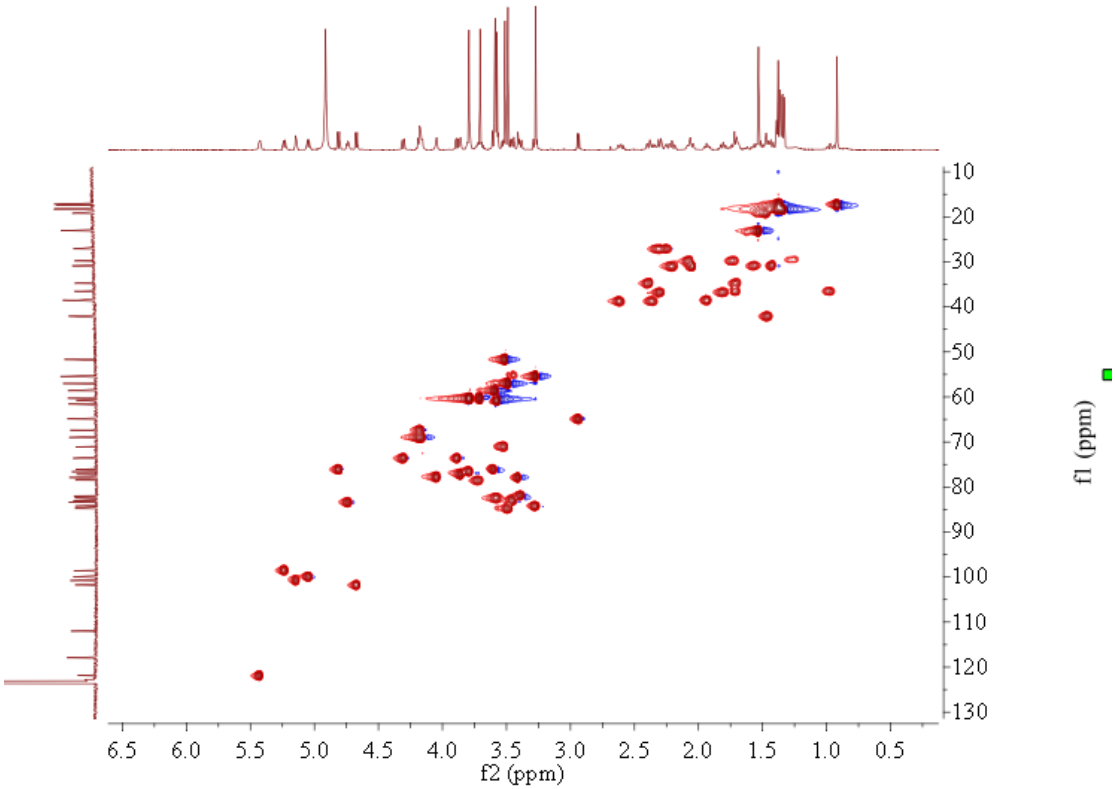

Figure S55 HSQC spectrum of compound **6a**

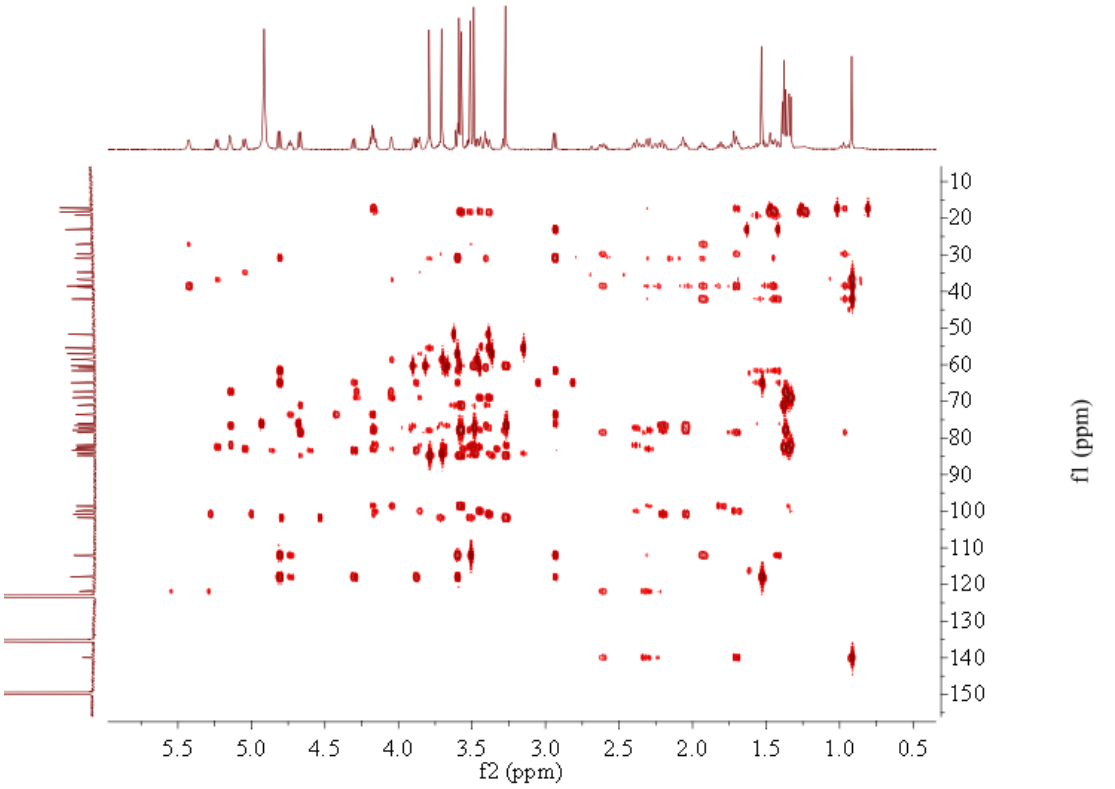

Figure S56 HMBC spectrum of compound **6a**

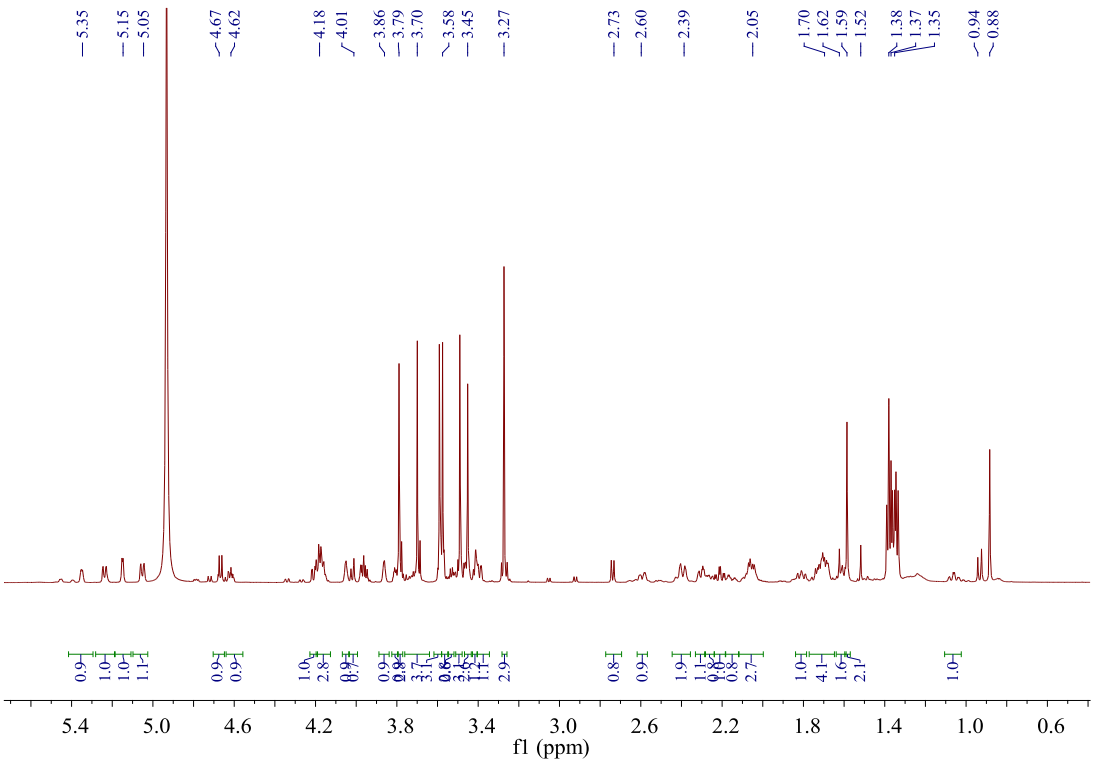

Figure S57 ^{1}H NMR spectrum of compound **6b**

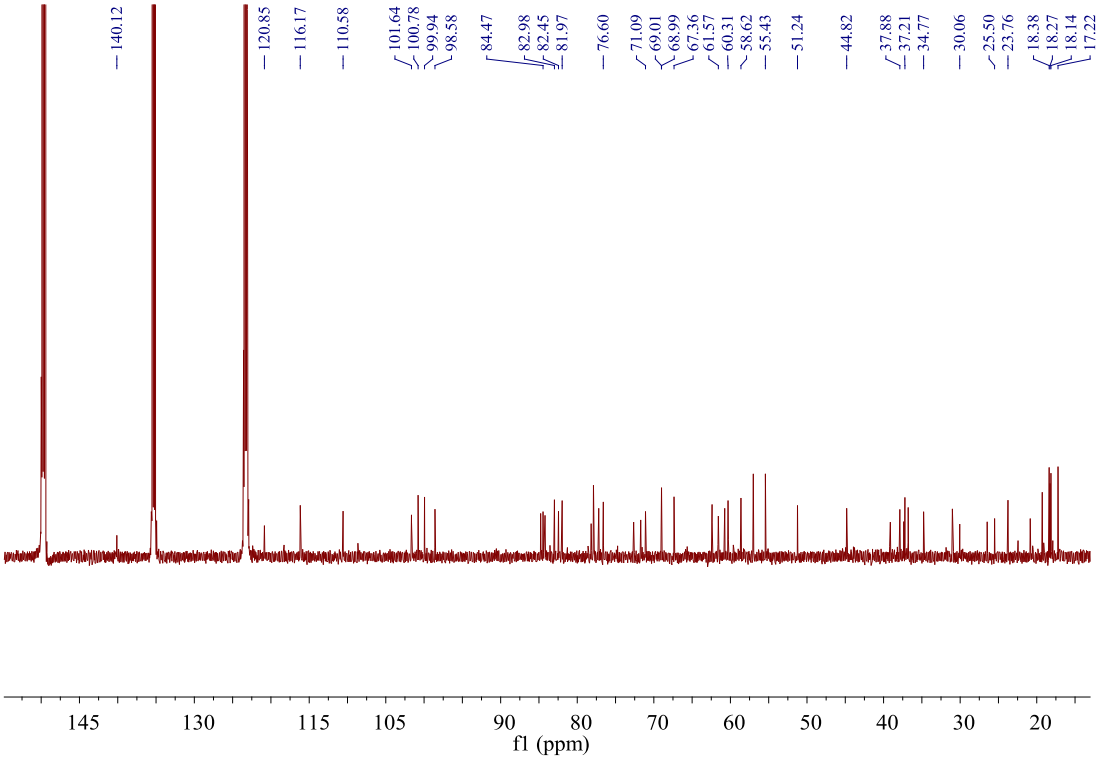

Figure S58 ^{13}C NMR spectrum of compound **6b**

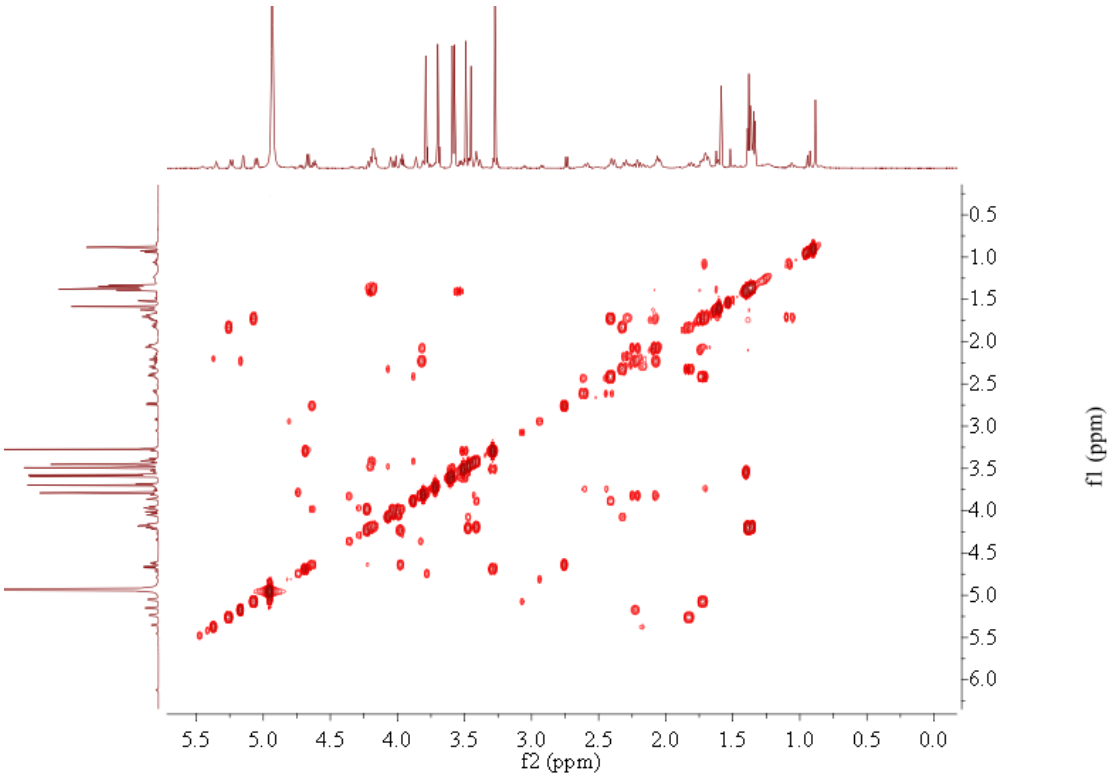

Figure S59 ^{1}H-^{1}H COSY spectrum of compound **6b**

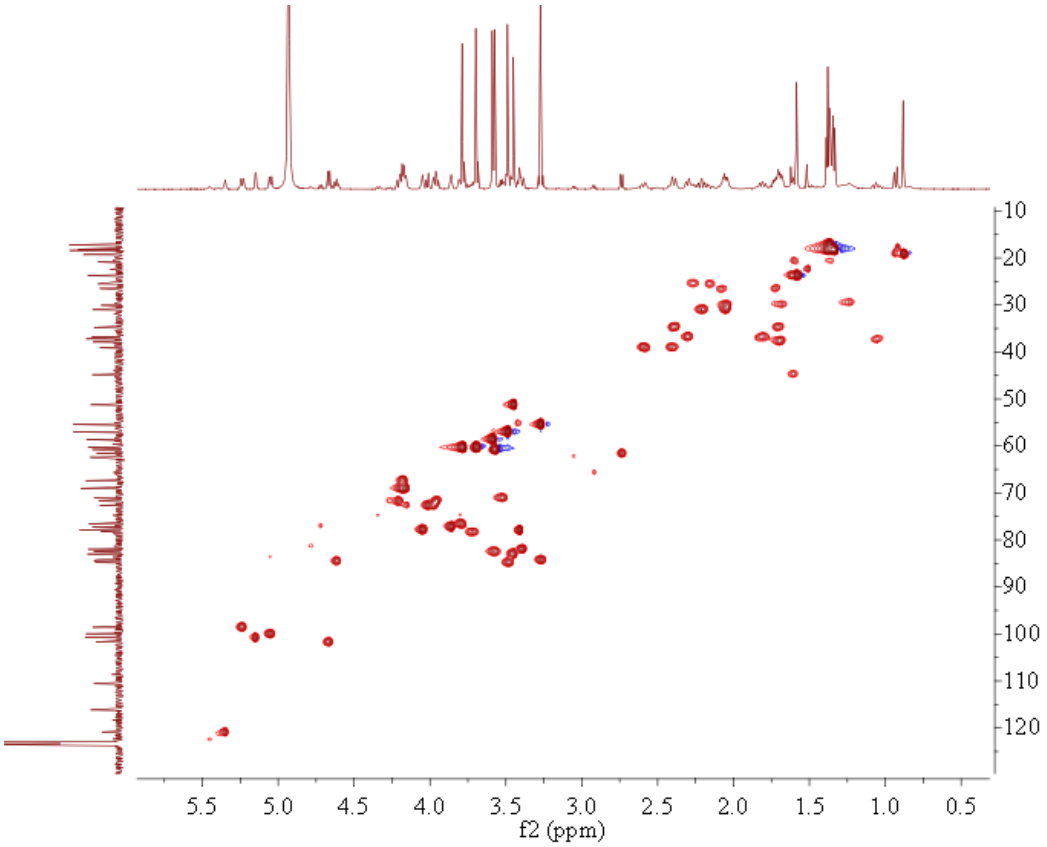

Figure S60 HSQC spectrum of compound **6b**

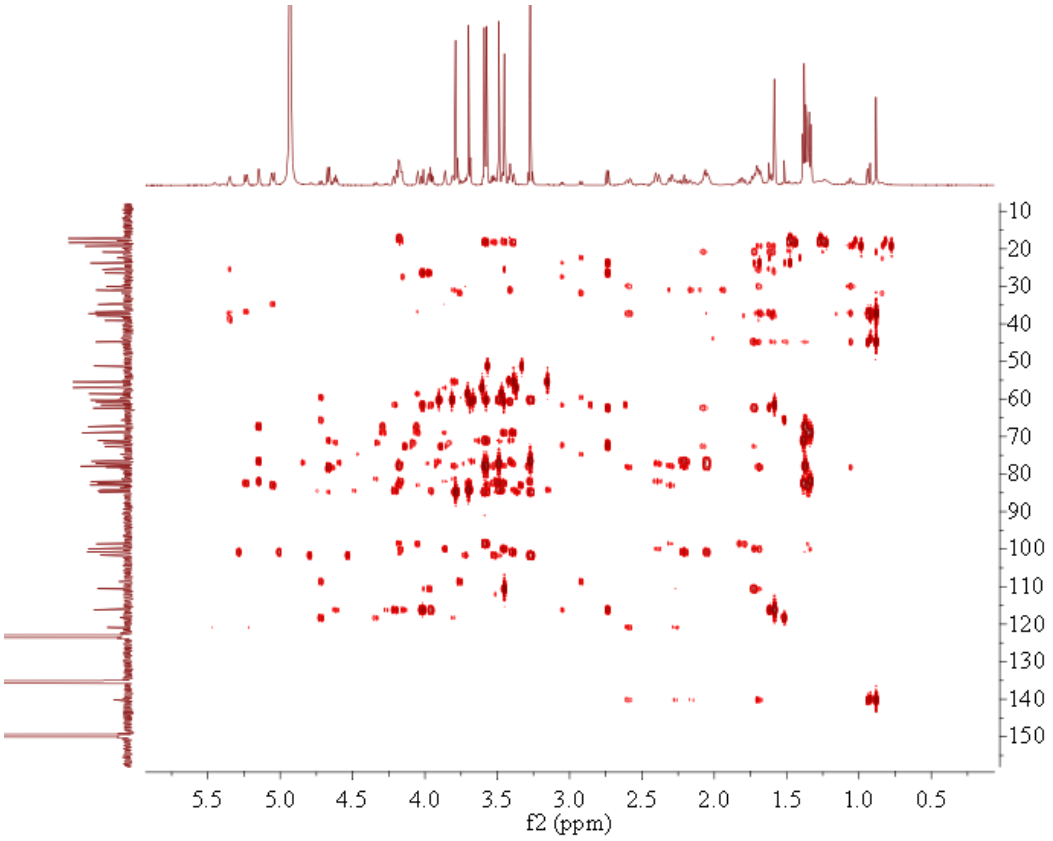

Figure S61 HMBC spectrum of compound **6b**

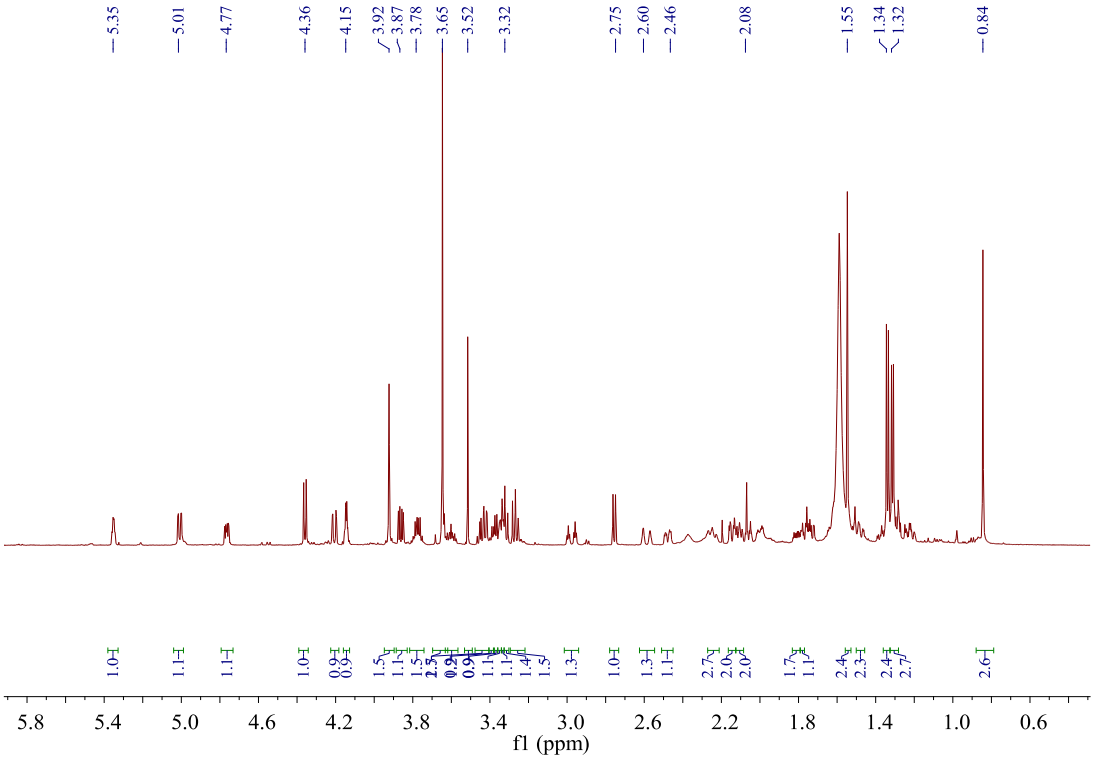

Figure S62 ^{1}H NMR spectrum of compound **6d**

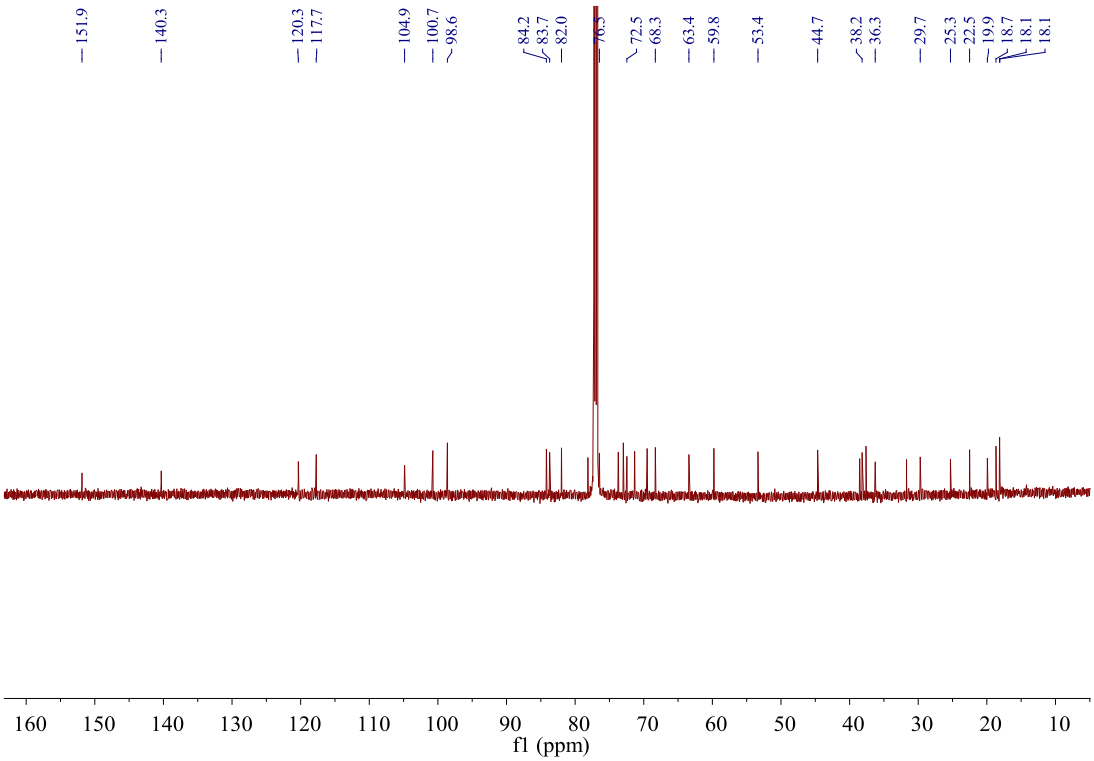

Figure S63 ^{13}C NMR spectrum of compound **6d**

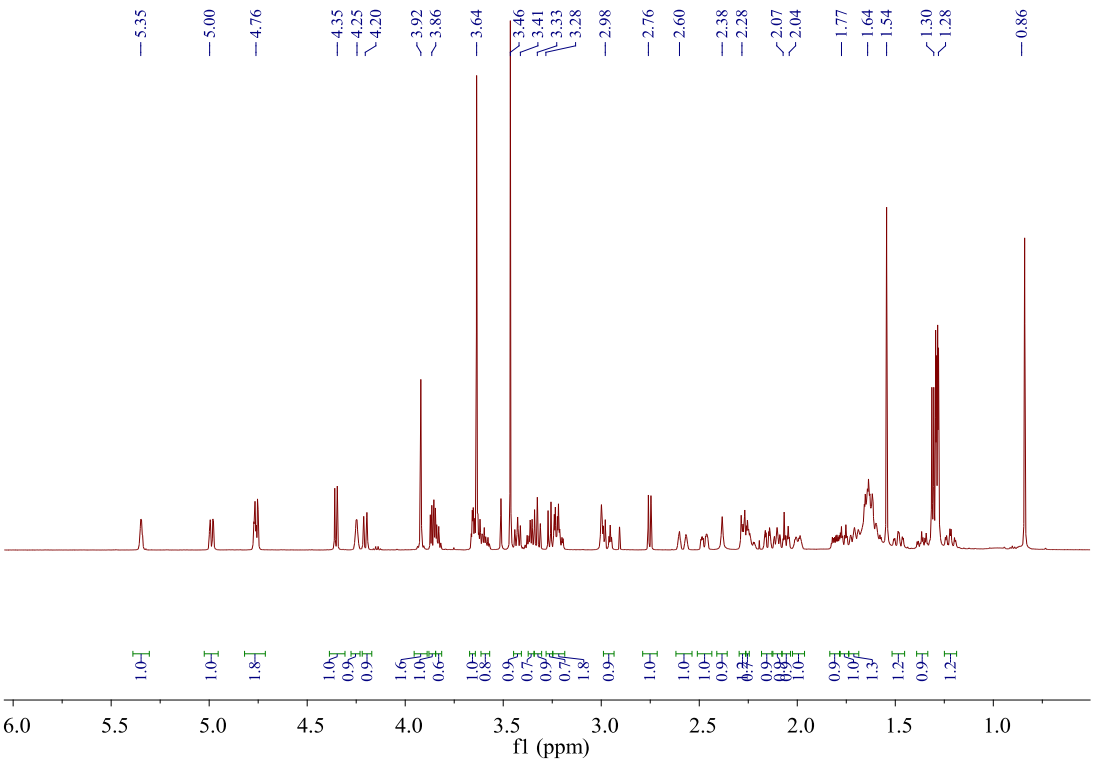

Figure S64 ^{1}H NMR spectrum of compound **6e**

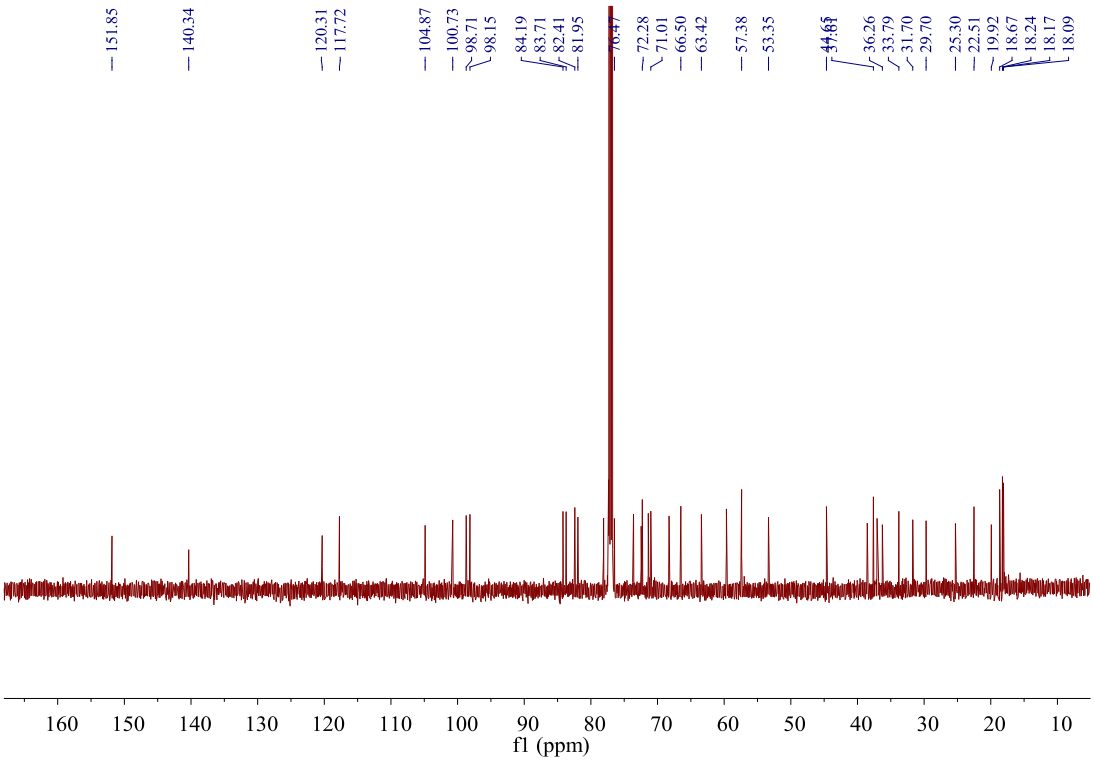

Figure S65 ^{13}C NMR spectrum of compound **6e**

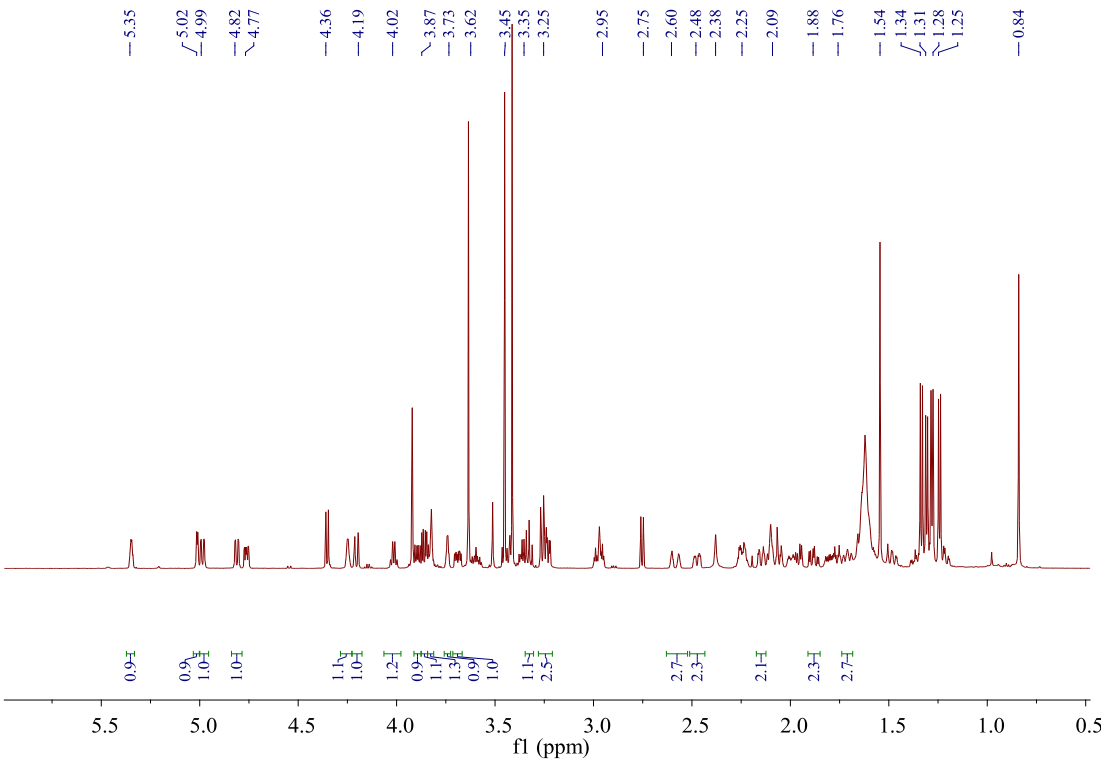

Figure S66 ^{1}H NMR spectrum of compound **6f**

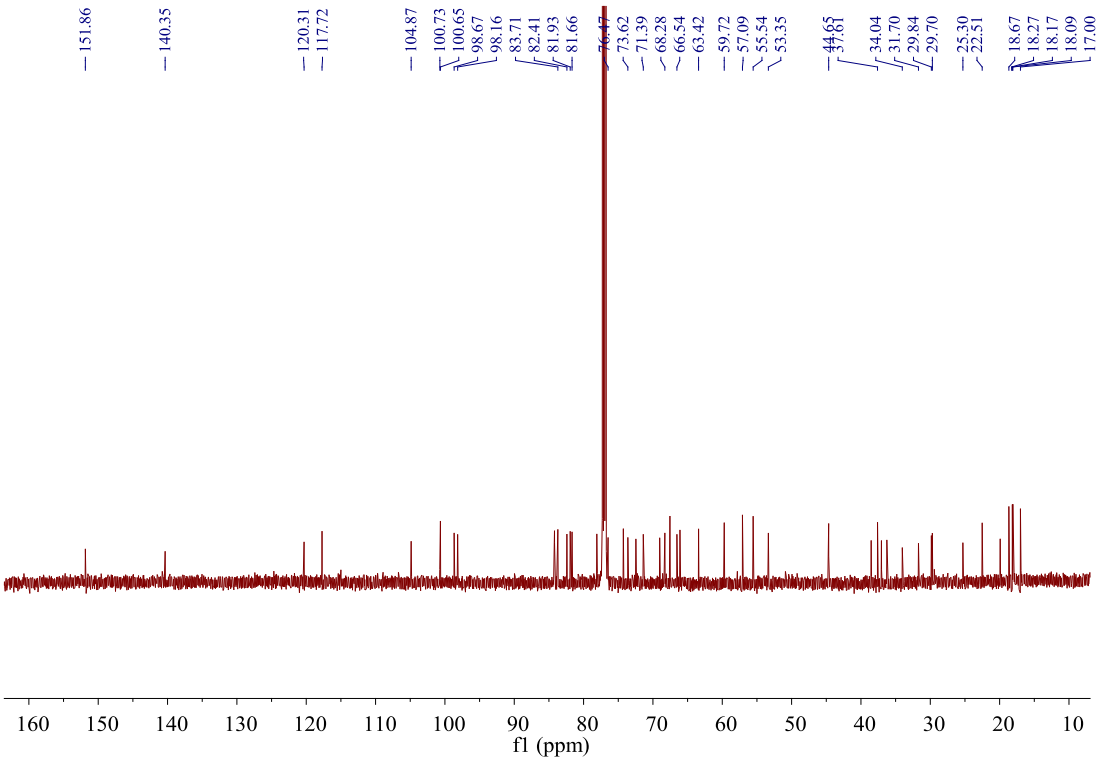

Figure S67 ^{13}C NMR spectrum of compound **6f**

Table S1 Assignment of ^{1}H NMR data for the aglycone part of compounds **2a-2f,6a-6f** in 600MHz (δ in ppm, *J* values in Hz)

positon	[a]2a	[a]2b	[b]2d	[b]2e	[b]2f	[a]6a	[a]6b	[b]6c	[b]6d	[b]6e	[b]6f
1	2.26,m/1.71,m	1.67,m/1.06,m	1.77,m/1.22,m	1.76,m/1.21,td(14.0,3.3)	1.77,m/1.21,td(14.1,3.5)	1.72,m/0.97,m	1.71,m/1.05,td(14.5,3.7)	1.71,m/1.19,td(13.8,3.6)	1.78,m/1.22,m	1.76,dt(13.6,3.6)/1.22,td(13.9,4.0)	1.76,m/1.22,m
2	2.06,d(10.1)/1.69,d(10.1)	2.04,m/1.66,m	2.01,m/1.58,m	2.00,bd(12.3)/1.58,m	2.00,m/1.29,m	2.07,m/1.73,m	2.05,m/1.71,m	1.95,m/1.58,m	2.00,m/1.62,m	2.00,m/1.61,m	2.00,m/1.61,m
3	3.76,m	3.76,m	3.63,m	3.61,m	3.61,m	3.72,m	3.72,m	3.58,m	3.60,m	3.60,m	3.60,m
4	2.57,m/2.28.m	2.54,m/2.33,m	2.43,m/2.20,m	2.43,bd(14.0)/2.21,m	2.43,bd(14.4)/2.23,m	2.62,m/2.36,m	2.59,bd(13.8)/2.39,bd(13.3)	2.44,m/1.76,m	2.48,m/2.25,m	2.47,dq(13.7,2.1)/2.25,m	2.47,d like(14.1)/2.25,m
5											
6	5.45,m	5.37.m	5.34,m	5.34,br s	5.34,q(3.1)	5.43,t(2.6)	5.43,t(2.5)	5.32,q(2.3)	5.35,q(2.3)	5.35,q(2.4)	5.35,q(2.4)
7	2.32,m/2.26,m	2.27,m/2.17,m	2.98,m/2.59,m	2.97,m/bd（21.0）	2.99,m/2.59,bd(21.1)	2.30,bd(13.1)/2.26,m	2.27,m/2.15,m	2.93,m/2.58,m	2.98,dt(21.0,3.7)/2.59,m	3.01,m/2.58,d like(21.3)	2.99,m/2.58,d like(21.3)
8	1.94,m	2.03,m				1.94,m	1.69,m				
9	1.47,m	1.61,d(1.7)	2.11,m	2.10，t(8.2)	2.11.t(8.3)	1.47,m	1.61,m	2.07,m	2.11,m	2.10,bt(8.8）	2.10,m
10											
11	1.49,m/1.47,m	1.60,m/1.37,m	1.81,m/1.36,m	1.80,m/1.35,m	1.81,m/1.35,m	1.49,m/1.48,m	1.61,m/1.37,m	1.79,m/1.33,m	1.81,m/1.37,m	1.81,m/1.36,m	1.81,m/1.36,m
12	1.57,m/1.43,m	2.07,m/1.72,m	2.06,m/1.49,m	2.06,bd(12.3)/1.49,m	2.06,m/1.48,td(14.1,3	1.57,m/1.43,m	2.06,m/1.71,m	2.02,m/1.47,m	2.06,m/1.49,m	2.06,dt like(12.5,3.	2.06,m/1.48,m

					.5)					3)/1.48,td(13.1,3.4)	
13											
14											
15	4.31,dd(10.3,2.3)/3.90,q(4.3)	4.21,dd(10.5,2.5)/3.95,m	4.21,dd(10.9,1.2)/3.86,m	4.21,d(11.1)/3.86,dd(11.1,4.3)	4.21,dd(11.1,1.2)/3.86,dd(10.8,4.6)	4.31,dd(10.3,2.2)/3.88,q(5.4)	4.21,dd(10.3,2.4)/3.95,m	4.17,dd(10.9,1.0)/3.82,dd(10.8,4.4)	4.21,dd(11.1,1.2)/3.86,dd(11.0,4.6)	4.20,dd(10.9,1.2)/3.86,dd(10.9,4.4)	4.20,dd(10.9,1.2)
16	4.75,m	4.62,m	4.76,m	4.76,m	4.76,m	4.74,m	4.62,m	4.73,m	4.77,m	4.76,m	4.76,m
17	2.95,d(8.5)	2.74,d(7.8)	2.76,d(7.9）	2.76,d(7.8）	2.75,d(8.0)	2.94,d(8.0)	2.74,d(8.0)	2.72,d(7.9)	2.75,d(8.0)	2.75,d(7.9)	2.75,d(7.9)
18	4.81,d(9.0)/3.60,d(9.0)	4.02,d(8.6)/3.98,dd(7.0,1.6)	3.92,br s	3.92,br s	3.92,br s	4.81,d(8.8)/3.61,d(8.8)	4.01,d(8.5)/3.97,m	3.88,br s	3.92,br s	3.92,br s	3.92,br s
19	0.91,s	0.87,s	0.84,s	0.84,s	0.84,s	0.92,s	0.88,s	0.80,s	0.84,s	0.84,s	0.84,s
20											
21	1.54,s	1.58,s	1.55,s	1.54,s	1.54,s	1.53,s	1.59,s	1.51,s	1.59,s	1.54,s	1.54,s
22	3.52,s	3.45,s				3.51,s	3.45,s				

[a]Spectra in pyding-d5. [b]Spectra in $CDCl_3$.

Table S2 Assignment of ^{1}H NMR data for the sugar chains of compounds **2a-2f,6a-6f** in 600MHz (δ in ppm, *J* values in Hz)

position	[a]**2a**	[a]**2b**	[b]**2d**	[b]**2e**	[b]**2f**	[a]**6a**	[a]**6b**	[b]**6c**	[b]**6d**	[b]**6e**	[b]**6f**
	M-can	M-can	can	can	can	M-the	M-the	the	the	the	the
1'	4.79,dd(9.6	4.78,dd(9.7	4.66,dd(9.7	4.63,d(9.5)	4.63,dd(9.9	4.67,d(7.8)	4.67,d(7.8)	4.34,d(7.8)	4.36,d(7.8)	4.35 ,	4.35,d(7.8)

	,1.8)	,1.7)	,2.0)		,1.7)					d(7.8)	
2'	2,43,m/1.78,m	2.41,m/1.69,m	2.20,m/1.68,m	2.21,m/1.63,m	2.22,m/1.62,m	3.49,m	3.49,m	3.41,m	3.43,m	3.43,t(8.7)	3.43,m
3'	3.56,m	3.53,m	3.64,m	3.62,m	3.63,m	3.28,m	3.28,m	3.12,q(8.9)	3.27,t(8.7)	3.26,d(8.9)	3.26,d(8.9)
4'	3.50,m	3.49,m	3.14,m	3.01,m	3.0,d(8.7)	3.58,overlap	3.58,overlap	3.20,t(8.9)	3.33,m	3.33,m	3.33,t(9.3）
5'	3.51,m	3.5,d(4.3)	3.31,m	3.32,m	3.33,m	3.53,m	3.53,m	3.34,m	3.38.m	3.36,m	3.36，m
6'	1.43,d(5.3)	1.42,d(5.4)	1.36.d(6.1）	1.30,d(6.0)	1.28,bs	1.36,d(6.3)	1.36,d(6.3)	1.30,d(6.1)	1.31,d(5.9)	1.31,d(6.0)	1.31,d(5.9)
2'-OCH3						3.80,s	3.79,s				
3'-OCH3	3.53,s	3.51,s				3.71,s	3.70,s	3.64,s	3.65,s	3.64,s	3.64,s
	M-digt	M-digt	digt	digt	digt	M-digt	M-digt	digt	digt	digt	digt
1"	5.25,dd(9.8,1.8)	5.25,dd(9.6,1.7)		4.86,d(9.6)	4.84,dd(9.8,2.1)	5.24,dd(9.8,1.7)	5.23,dd(9.8,1.7)		5.01,dd(9.7,1.2)	4.99,dd(9.7,2.0)	4.99,dd(9.7,2.0)
2"	2.28,m/1.75,m	2.27,m/1.73,m		2.21,m/1.79,m	2.23,m/1.77,m	2.31,bd(13.1)/1.81,m	2.31,bd(13.1)/1.81,m		2.14,m/1.74,m	2.15,bd like(13.9)/1.71,m	2.15,m/1.71,m
3"	3.86,m	3.85,m		4.16,br s	4.10,d like(3.2)	4.05,qd(2.8)	4.05,qd(2.8)		4.14,m	2.84,m	3.86,dd(9.9,4.5)
4"	3.41,dd(9.7,2.4)	3.41,dd(9.5,2.6)		3.38,d(9.0)	3.30,dd(9.5,3.1)	3.45,dd(9.5,2.6)	3.45,dd(9.5,2.6)		3.35,m	3,23,m	3.23,dd(9.0,3.1)
5"	4.15,m	4.15,m		3.88,m	3.90,m	4.18,m	4.18,m		3.78,m	3.64,m	3.89,m
6"	1.34,d(6.2)	1.34,d(6.0)		1.55,d(5.8)	1.29,bs	1.37,d(4.3)	1.37,d(4.3)		1.34,d(6.3)	1.28,d（2.4）	1.28,d(6.4)
3"-OCH3	3.55,s	3.55,s				3.59,s	3.59,s				
	M-cym	M-cym				M-cym	M-cym			cym	cym
1'"	4.92,dd(4.8	4.92,overla			4.93,d(3.9)	5.05,dd(9.8	5.05,dd(9.8			4.76 ，	4.81,dd(9.8

	,1.6)	p				,1.6)	,1.6)			dd(9.6,1.2)	,2.0)
2‴	2.34,m/1.34,m	2.33,m/1.71,m			2.34,bd(14.8)/1.75,m	2.39,bd(12.8)/1.72,m	2.39,bd(12.8)/1.72,m			2.27,m/1.63,m	2.25,m/1.65,m
3‴	3.76,m	3.75,d(4.1)			3.66,m	3.86,qd(2.8)	3.86,qd(2.8)			3.65,m	3.74,q(2.7)
4‴	3.04,dd(8.6,2.8)	3.03,dd(8.7,2.9)			3.28,m	3.39,dd(9.5,2.7)	3.39,dd(9.5,2.7)			3.22.m	3.26,dd(9.7,3.1)
5‴	4.55,m	4.55,m			3.87,m	4.18,m	4.18,m			4.25,q(2.8)	3.83,m
6‴	1.38,d(6.4)	1.38,d(6.4)			1.31,bs	1.34,d(6.2)	1.34,d(6.2)			1.29,d(2.5)	1.24,d(6.3)
2‴-OCH3	3.35,s	3.34,s									
3‴-OCH3	3.34,s	3.33,s			3.44,s	3.49,s	3.49,s			3.46,s	3.45,s
						M-dign	M-dign			dign	dign
1⁗						5.14,d(3.5)	5.15,d(3.5)				5.01,bd(3.7)
2⁗						2.21,m/2.06,m	2.21,m/2.06,m				1.88,m/1.29,m
3⁗						3.80,m	3.80,m				3.69,m
4⁗						3.41,br s	3.41,br s				4.25,m
5⁗						4.18,m	4.18,m				4.01,bd(7.0)
6⁗						1.39,s	1.39,s				1.33,d(7.0)
3⁗-OCH3						3.28,s	3.28,s				3,41,s
4⁗-OCH3						3.58,s	3.58,s				

[a]Spectra in pyding-d5. [b]Spectra in $CDCl_3$

Table S3 Assignment of ^{13}C NMR data for compounds **2a-2f**,**6a-6f** in 150MHz (δ in ppm)

position	[a]**2a**	[a]**2b**	[b]**2c**	[b]**2d**	[b]**2e**	[b]**2f**	[a]**6a**	[a]**6b**	[b]**6c**	[b]**6d**	[b]**6e**	[b]**6f**
1	36.5	37.4	36.4	36.3	36.3	36.3	36.5	37.4	36.3	36.3	36.3	36.3
2	29.7	30.0	31.9	29.7	29.7	29.7	29.8	30.1	29.8	29.7	29.7	29.7
3	77.3	77.0	71.3	77.2	77.2	77.2	78.5	78.2	78.3	78.1	78.1	78.1
4	38.6	39.0	42.1	38.5	38.5	38.5	38.8	39.1	38.6	38.5	38.5	38.5
5	140.0	140.2	140.8	140.6	140.7	140.7	140.0	140.1	140.3	140.3	140.3	140.4
6	121.8	120.8	120.2	120.1	120.1	120.1	121.9	120.9	120.5	120.3	120.3	120.3
7	27.1	25.5	25.4	25.3	25.3	25.3	27.1	25.5	25.4	25.3	25.3	25.3
8	38.5	37.8	105.1	104.9	104.9	104.9	38.5	37.9	105.0	104.6	104.9	104.9
9	42.1	44.8	44.8	44.7	44.7	44.7	42.1	44.8	44.7	44.7	44.7	44.7
10	38.5	37.2	37.5	37.7	37.7	37.7	38.5	37.2	37.7	37.6	37.6	37.6
11	19.2	20.8	20.1	19.9	19.9	19.9	19.2	20.9	20.0	19.9	19.9	19.9
12	30.8	26.5	31.9	31.7	31.7	31.7	30.8	26.5	31.8	31.7	31.7	31.7
13	61.6	62.4	53.5	53.4	53.4	53.4	61.6	62.4	53.5	53.4	53.4	53.4
14	112.1	110.6	151.9	151.9	151.8	151.8	112.1	110.6	151.9	151.9	151.9	151.9
15	73.6	71.7	72.6	72.5	72.5	72.5	73.6	71.7	72.5	72.5	72.5	72.5
16	83.4	84.5	83.9	83.7	83.7	83.7	83.4	84.5	83.8	83.7	83.7	83.7
17	64.9	61.6	63.6	63.4	63.4	63.4	65.0	61.6	63.5	63.4	63.4	63.4
18	76.1	72.6	76.6	76.5	76.5	76.5	76.1	72.6	76.5	76.5	76.5	76.5
19	17.3	19.2	18.9	18.7	18.7	18.7	17.3	19.3	18.8	18.7	18.7	18.7
20	118.0	116.1	117.7	117.7	117.7	117.7	118.0	116.2	117.9	117.7	117.7	117.7
21	23.1	23.7	22.6	22.5	22.5	22.5	23.1	23.8	22.6	22.5	22.5	22.5
22	51.7	51.2					51.7	51.2				

	M-can	M-can		can	can	can	M-the	M-the	the	the	the	the
1'	97.8	97.7		97.5	97.6	97.6	101.8	101.6	101.1	100.7	100.7	100.7
2'	37.8	37.7		39.6	38.8	38.8	84.8	84.8	74.4	73.7	73.6	73.6
3'	78.9	78.9		71.9	69.8	69.8	84.2	84.2	85.5	84.2	84.2	84.2
4'	82.8	82.7		77.7	88.5	88.5	82.5	82.5	74.7	82.0	82.0	81.9
5'	71.5	71.5		71.5	70.4	70.4	71.1	71.1	71.7	71.3	71.4	71.4
6'	18.6	18.6		17.7	17.9	17.9	18.3	18.3	17.9	18.1	18.2	18.1
2'-OCH3							60.3	60.3				
3'-OCH3	57.2	57.1					60.3	60.3	60.6	59.8	59.7	59.7
	M-digt	M-digt			digt	digt	M-digt	M-digt		digt	digt	digt
1"	98.2	98.2			99.2	99.3	98.6	98.6		98.6	98.7	98.7
2"	36.8	36.8			37.7	36.5	36.8	36.8		38.2	37.1	37.0
3"	77.6	77.6			68.1	67.4	77.8	77.8		68.3	68.3	68.3
4"	82.1	82.1			72.6	79.0	83.0	83.0		72.9	82.4	82.4
5"	69.3	69.2			69.7	68.9	69.0	69.0		69.5	71.0	69.0
6"	18.3	18.3			17.9	17.9	18.2	18.2		18.1	18.2	18.2
3"-OCH3	58.2	58.2					58.6	58.6				
	M-cym	M-cym				cym	M-cym	M-cym			cym	cym
1'"	98.7	98.6				97.6	100.0	99.9			98.2	98.2
2'"	31.8	31.8				30.9	34.8	34.8			33.8	34.0
3'"	71.8	71.8				75.0	77.2	77.2			77.3	76.9
4'"	82.2	82.2				71.9	82.0	82.0			72.3	81.7
5'"	64.4	64.3				66.0	69.0	69.0			66.5	67.6
6'"	18.1	18.1				17.8	18.4	18.4			18.1	18.3
2'"-OCH3	56.3	56.3										

3'''-OCH3	55.9	55.9				56.4	57.0	57.0			57.4	57.1
							M-dign	M-dign				dign
1''''							100.8	100.8				100.7
2''''							31.0	31.0				29.8
3''''							76.6	76.6				74.3
4''''							77.9	77.9				66.5
5''''							67.4	67.4				66.1
6''''							17.2	17.2				17.0
3''''-OCH3							55.4	55.4				55.5
4''''-OCH3							60.8	60.8				

[a]Spectra in pyding-d5. [b]Spectra in $CDCl_3$.