Electronic Supplementary Information

Identification of new bisabosqual-type meroterpenoids reveals non-enzymatic conversion of bisabosquals to *seco*-bisabosquals

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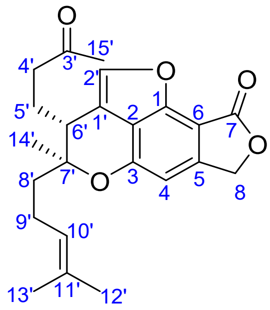
Supplementary Tables

Table S1 NMR data of 1 (^{1}H for 600 MHz and ^{13}C for 150 MHz in $CDCl_3$)

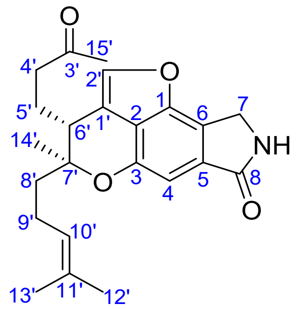


No.	δ_C, type	δ_H (J in Hz)[a]	^{1}H-^{1}H COSY	HMBC	ROESY
1	148.9, C				
2	117.8, C				
3	155.7, C				
4	101.2, CH	6.63, br s	8	2, 3, 5, 6, 8	8
5	149.0, C				
6	103.9, C				
7	168.3, C				
8	70.3, CH_2	5.35, br s	4	4, 5, 6, 7	4
1′	116.0, C				
2′	139.2, CH	7.44, br s	6′	1, 1′, 2, 6′	4′a, 4′b
3′	207.7, C				
4′	41.0, CH_2	a: 2.59, ddd (18.0, 8.4, 5.4)	4′b, 5′a, 5′b	3′, 5′, 6′	2′
		b: 2.44, dt (18.0, 7.8)	4′a, 5′a, 5′b	3′, 5′, 6′	2′, 6′
5′	23.3, CH_2	a: 2.19	4′a, 4′b, 5′b, 6′	1′, 3′, 4′, 6′, 7′	14′
		b: 1.54	4′a, 4′b, 5′a, 6′	1′, 3′, 4′, 6′, 7′	
6′	39.4, CH	3.03, br dd (11.4, 3.6)	2′, 5′a, 5′b	1′, 2, 2′, 4′, 5′, 7′, 8′, 14′	4′b, 8′a, 9′a, 9′b, 14′[b]
7′	86.4, C				
8′	38.6, CH_2	a: 1.67, ddd (14.4, 11.4, 4.8)	8′b, 9′a, 9′b	6′, 7′, 9′, 10′, 14′	6′
		b: 1.54	8′a, 9′a, 9′b	6′, 7′, 9′, 10′, 14′	
9′	22.2, CH_2	a: 2.10	8′a, 8′b, 9′b, 10′	7′, 8′, 10′, 11′	6′, 13′
		b: 2.03	8′a, 8′b, 9′a, 10′	7′, 8′, 10′, 11′	6′, 13′
10′	123.2, CH	4.94, br t (7.2)	9′a, 9′b ,12′, 13′	8′, 9′, 12′, 13′	12′
11′	132.3, C				
12′	25.6, CH_3	1.60, br s	10′	10′, 11′, 13′	10′
13′	17.5, CH_3	1.50, br s	10′	10′, 11′, 12′	9′a, 9′b
14′	21.8, CH_3	1.49, s		6′, 7′, 8′	5′a, 6′[b]
15′	30.2, CH_3	2.15, s		3′, 4′	

[a] The indiscernible signals from overlap or the complex multiplicity are reported without designating multiplicity.

[b] The NOE correlation was observed through the 1D-selective NOE experiment.

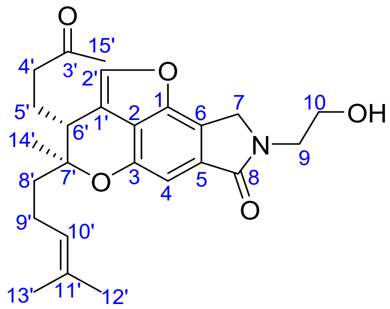
Table S2 NMR data of 2 (^{1}H for 400 MHz and ^{13}C for 100 MHz in $CDCl_3$)



No.	δ_C, type	δ_H (*J* in Hz)[a]	^{1}H-^{1}H COSY	HMBC	ROESY
1	147.7, C				
2	120.4, C				
3	149.7, C				
4	102.8, CH	7.12, s		2, 3, 6, 8	
5	131.7, C				
6	119.8, C				
7	42.8, CH_2	4.59, br s	N<u>H</u>	1, 5, 6, 8	
8	172.2, C				
1′	117.0, C				
2′	139.7, CH	7.42, s		1, 1′, 2	4′a, 4′b, 6′
3′	208.0, C				
4′	41.0, CH_2	a: 2.58, ddd (17.2, 8.4, 5.2)	4′b, 5′a, 5′b	3′, 5′	2′
		b: 2.40, dt (17.6, 7.6)	4′a, 5′a, 5′b	3′, 5′, 6′	2′
5′	23.6, CH_2	a: 2.19	4′a, 4′b, 5′b, 6′	1′, 4′	
		b: 1.62	4′a, 4′b, 5′a, 6′		
6′	39.6, CH	2.97, dd (10.4, 3.6)	5′a, 5′b	1′, 2, 2′, 4′, 5′	2′, 9′
7′	84.2, C				
8′	38.4, CH_2	a: 1.62	8′b, 9′		
		b: 1.46	8′a, 9′		
9′	22.2, CH_2	2.05	8′a, 8′b, 10′	8′, 10′, 11′	6′
10′	123.5, CH	4.90, br t (7.2)	9′, 12′, 13′	9′, 12′, 13′	12′
11′	132.0, C				
12′	25.5, CH_3	1.58, br s	10′	10′, 11′, 13′	10′
13′	17.5, CH_3	1.48, br s	10′	10′, 11′, 12′	
14′	21.9, CH_3	1.48, s		6′, 7′, 8′	
15′	30.1, CH_3	2.12, s		3′, 4′	
NH		7.41, br s	7	5, 6, 7, 8	

[a] The indiscernible signals from overlap or the complex multiplicity are reported without designating multiplicity.

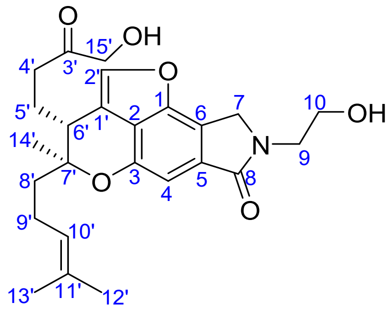
Table S3 NMR data of 3 (^{1}H for 600 MHz and ^{13}C for 150 MHz in $CDCl_3$)



No.	δ_C, type	δ_H (*J* in Hz)[a]	^{1}H-^{1}H COSY	HMBC	ROESY
1	147.4, C				
2	120.2, C				
3	149.7, C				
4	102.9, CH	7.10, s		2, 3, 6, 8	
5	132.1, C				
6	117.6, C				
7	48.8, CH_2	4.64, s		1, 5, 6, 8, 9	
8	170.2, C				
9	46.6, CH_2	3.79, t (4.8)	10	7, 8	
10	62.0, CH_2	3.92, t (4.8)	9		
1′	116.9, C				
2′	139.7, CH	7.41, d (0.6)	6′	1, 1′, 2	4′a, 4′b
3′	208.0, C				
4′	41.0, CH_2	a: 2.57, ddd (18.0, 7.8, 4.8)	4′b, 5′a, 5′b	3′, 5′, 6′	2′
		b: 2.39, dt (18.0, 7.8)	4′a, 5′a, 5′b	3′, 5′, 6′	2′
5′	23.6, CH_2	a: 2.18	4′a, 4′b, 5′b, 6′	1′, 3′, 4′, 6′, 7′	
		b: 1.61	4′a, 4′b, 5′a, 6′	1′, 3′, 4′, 6′, 7′	
6′	39.6, CH	2.97, br dd (10.8, 4.2)	2′, 5′a, 5′b	1′, 2, 2′, 4′, 5′, 7′	
7′	84.2, C				
8′	38.4, CH_2	a: 1.61	8′b, 9′a, 9′b	6′, 7′, 9′	
		b: 1.46	8′a, 9′a, 9′b	9′	
9′	22.2, CH_2	a: 2.08	8′a, 8′b, 9′b, 10′	10′, 11′	
		b: 2.01	8′a, 8′b, 9′a, 10′	10′, 11′	
10′	123.5, CH	4.90, br t (6.6)	9′a, 9′b ,12′, 13′	12′, 13′	12′
11′	132.1, C				
12′	25.6, CH_3	1.58, br s	10′	10′, 11′, 13′	10′
13′	17.5, CH_3	1.49, br s	10′	10′, 11′, 12′	
14′	21.8, CH_3	1.47, s		6′, 7′, 8′	
15′	30.1, CH_3	2.12, s		3′, 4′, 5′	

[a] The indiscernible signals from overlap or the complex multiplicity are reported without designating multiplicity.

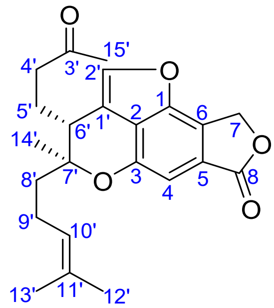
Table S4 NMR data of 4 (^{1}H for 600 MHz and ^{13}C for 150 MHz in $CDCl_3$)



No.	δ_C, type	δ_H (J in Hz)[a]	^{1}H-^{1}H COSY	HMBC	ROESY
1	147.5, C				
2	120.1, C				
3	149.6, C				
4	103.1 CH	7.12, s		2, 3, 6, 8	
5	132.3, C				
6	117.7, C				
7	48.9, CH_2	4.64, s		1, 5, 6, 8, 9	9, 10
8	170.2, C				
9	46.6, CH_2	3.80, t (4.8)	10	7, 8, 10	7
10	62.0, CH_2	3.93, t (4.8)	9		7
1′	116.6, C				
2′	139.8, CH	7.42, s		1, 1′, 2, 6′	4′a, 4′b
3′	208.9, C				
4′	35.7, CH_2	a: 2.54, ddd (18.0, 9.0, 4.8)	4′b, 5′a, 5′b	3′, 5′, 6′	2′, 15′a, 15′b
		b: 2.36, dt (17.4, 8.4)	4′a, 5′a, 5′b	3′, 5′, 6′	2′, 15′a, 15′b
5′	23.6, CH_2	a: 2.24	4′a, 4′b, 5′b, 6′	1′, 6′, 7′	14′
		b: 1.71	4′a, 4′b, 5′a, 6′	1′, 3′, 4′, 6′, 7′	
6′	39.6, CH	2.99, dd (10.2, 3.6)	5′a, 5′b	1′, 2, 2′, 4′, 5′, 7′, 8′	8′a, 8′b, 9′a, 9′b, 14′
7′	84.0, C				
8′	38.4, CH_2	a: 1.61	8′b, 9′a, 9′b	6′, 7′, 9′, 14′	6′
		b: 1.44	8′a, 9′a, 9′b	6′, 7′, 9′, 14′	6′
9′	22.2, CH_2	a: 2.07	8′a, 8′b, 9′b, 10′	8′, 10′, 11′	6′, 14′
		b: 2.00	8′a, 8′b, 9′a, 10′	8′, 10′, 11′	6′, 14′
10′	123.4, CH	4.89, br t (7.2)	9′a, 9′b ,12′, 13′	9′, 12′, 13′	12′
11′	132.2, C				
12′	25.6, CH_3	1.58, br s	10′	10′, 11′, 13′	10′
13′	17.6, CH_3	1.48, br s	10′	10′, 11′, 12′	
14′	22.0, CH_3	1.50, s		6′, 7′, 8′	5′a, 6′, 9′a, 9′b
15′	68.2, CH_2	a: 4.23, d (18.6)	15′b	3′	4′a, 4′b
		b: 4.16, d (18.6)	15′a	3′	4′a, 4′b

[a] The indiscernible signals due to overlap or the complex multiplicity are reported without designating multiplicity.

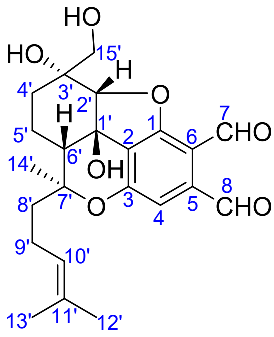
Table S5 NMR data of 5 (^{1}H for 600 MHz and ^{13}C for 150 MHz in $CDCl_3$)



No.	δ_C, type	δ_H (J in Hz)[a]	^{1}H-^{1}H COSY	HMBC	ROESY
1	146.4, C				
2	122.3, C				
3	150.4, C				
4	104.1, CH	7.13, s		2, 3, 6, 8	
5	125.0, C				
6	123.1, C				
7	66.9, CH_2	5.44, s		1, 5, 6, 8	
8	171.3, C				
1′	117.2, C				
2′	141.0, CH	7.50, d (0.6)	6′	1, 1′, 2	4′a, 4′b
3′	207.8, C				
4′	40.9, CH_2	a: 2.58, ddd (18.0, 7.8, 5.4)	4′b, 5′a, 5′b	3′, 5′, 6′	2′, 6′
		b: 2.40, dt (18.0, 7.8)	4′a, 5′a, 5′b	3′, 5′, 6′	2′, 6′
5′	23.5, CH_2	a: 2.18	4′a, 4′b, 5′b, 6′	1′, 6′, 7′	
		b: 1.57	4′a, 4′b, 5′a, 6′	1′, 3′, 4′, 6′, 7′	
6′	39.5, CH	3.00, br dd (10.8, 3.6)	2′, 5′a, 5′b	1′, 2, 2′, 4′, 5′	4′a, 4′b, 9′a, 9′b
7′	84.7, C				
8′	38.4, CH_2	a: 1.61	8′b, 9′a, 9′b	6′, 7′, 14′	
		b: 1.48	8′a, 9′a, 9′b	9′, 14′	
9′	22.2, CH_2	a: 2.08	8′a, 8′b, 9′b, 10′	8′, 10′, 11′	6′
		b: 2.02	8′a, 8′b, 9′a, 10′	8′, 10′, 11′	6′
10′	123.3, CH	4.91, br t (7.2)	9′a, 9′b ,12′, 13′	9′, 12′, 13′	12′
11′	132.2, C				
12′	25.6, CH_3	1.59, br s	10′	10′, 11′, 13′	10′
13′	17.5, CH_3	1.48, br s	10′	10′, 11′, 12′	
14′	21.8, CH_3	1.48, s		6′, 7′, 8′	
15′	30.1, CH_3	2.14, s		3′, 4′	

[a] The indiscernible signals from overlap or the complex multiplicity are reported without designating multiplicity.

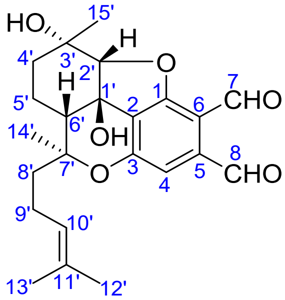
Table S6 NMR data of 6 (^{1}H for 400 MHz and ^{13}C for 100 MHz in DMSO-d_6)



No.	δ_C, type	δ_H (J in Hz)[a]	^{1}H-^{1}H COSY	HMBC	ROESY
1	167.7, C				
2	118.9, C				
3	155.6, C				
4	108.8, CH	6.67, s		2, 3, 6, 8	8
5	140.4, C				
6	112.1, C				
7	187.2, CH	10.16, s		1, 5, 6	
8	192.8, CH	10.40, s		4, 5	4
1′	71.8, C				
2′	96.8, CH	4.99, s		1, 1′, 2, 15′	6′, 15′a, 15′b, 1′-OH
3′	71.8, C				
4′	29.9, CH_2	a: 1.48	4′b, 5′a, 5′b	5′, 6′	
		b: 1.35	4′a, 5′a, 5′b	2′, 3′, 5′, 6′	
5′	17.1 CH_2	a: 1.50	4′a, 4′b, 5′b, 6′	4′	
		b: 1.04	4′a, 4′b, 5′a, 6′	3′, 6′	
6′	41.7, CH	2.22	5′a, 5′b	1′, 5′	2′, 1′-OH
7′	84.9, C				
8′	39.9, CH_2	a: 2.17	8′b, 9′a, 9′b	7′, 9′, 14′	
		b: 1.77	8′a, 9′a, 9′b	6′, 7′	
9′	23.3, CH_2	a: 2.19	8′a, 8′b, 9′b, 10′	8′, 10′	
		b: 1.89	8′a, 8′b, 9′a, 10′	8′, 10′, 11′	
10′	124.3, CH	5.03	9′a, 9′b, 12′, 13′	9′, 12′, 13′	12′
11′	130.7, C				
12′	25.4, CH_3	1.61, br s	10′	10′, 11′, 13′	10′
13′	17.5, CH_3	1.56, br s	10′	10′, 11′, 12′	
14′	23.6, CH_3	1.41, s		6′, 7′, 8′	
15′	66.1, CH_2	a: 3.43, d (10.9)	15′b	2′, 3′, 4′	2′
		b: 3.04, d (10.9)	15′a	2′, 3′, 4′	2′
1′-OH		5.92, s		2	2′, 6′

[a] The indiscernible signals from overlap or the complex multiplicity are reported without designating multiplicity.

Table S7 NMR data of 7 (^{1}H for 400 MHz and ^{13}C for 100 MHz in DMSO-d_6)



No.	δ_C[a], type	δ_H (J in Hz)[a, b]	δ_C, type	δ_H (J in Hz)[b]	^{1}H-^{1}H COSY	HMBC	ROESY
1	166.3, C		167.7, C				
2	118.0, C		118.8, C				
3	156.7, C		155.6, C				
4	113.2, CH	6.90, s	108.7, CH	6.66, s		2, 3, 6, 8	8
5	141.2, C		140.4, C				
6	112.5, C		112.1, C				
7	187.7, CH	10.38, s	187.2, CH	10.18, s		5, 6	
8	192.3, CH	10.37, s	192.8, CH	10.41, s		4, 5	4
1′	70.9, C		69.3, C				
2′	101.6, CH	4.76, s	101.8, CH	4.66, s		1, 1′, 2, 15′	4′b, 6′, 15′, 1′-OH
3′	70.1, C		68.6, C				
4′	34.2, CH_2	a: 1.75	34.4, CH_2	a: 1.47	4′b, 5′a, 5′b	2′, 3′, 6′	
		b: 1.35		b: 1.31	4′a, 5′a, 5′b		2′, 6′
5′	18.0, CH_2	a: 1.59	17.6 CH_2	a: 1.46	4′a, 4′b, 5′b, 6′	3′, 6′	
		b: 1.18		b: 1.05	4′a, 4′b, 5′a, 6′	4′, 6′, 7′	3′-OH
6′	41.2, CH	2.29, dd (12.9, 6.0)	41.5, CH	2.23, dd (13.2, 5.2)	5′a, 5′b	1′, 5′, 8′	2′, 4′b, 1′-OH
7′	85.3, C		84.9, C				
8′	40.5, CH_2	a: 2.14	39.9, CH_2	a: 2.15	8′b, 9′a, 9′b	7′, 9′, 10′, 14′	1′-OH
		b: 1.86		b: 1.78	8′a, 9′a, 9′b	6′, 7′, 9′, 14′	
9′	23.8, CH_2	a: 2.22	23.3, CH_2	a: 2.17	8′a, 8′b, 9′b, 10′	7′, 10′	
		b: 1.97		b: 1.91	8′a, 8′b, 9′a, 10′	8′	
10′	123.6, CH	5.06, br t (6.0)	124.2, CH	5.03, br t (6.4)	9′a, 9′b, 12′, 13′	9′, 12′, 13′	12′
11′	132.0, C		130.7, C				
12′	25.6, CH_3	1.64, br s	25.4, CH_3	1.61, br s	10′	10′, 11′, 13′	10′
13′	17.7, CH_3	1.59, br s	17.5, CH_3	1.56, br s	10′	10′, 11′, 12′	
14′	23.8, CH_3	1.47, s	23.4, CH_3	1.40, s		6′, 7′, 8′	
15′	29.3, CH_3	1.35, s	28.6, CH_3	1.22, s		2′, 3′, 4′	2′
1′-OH				5.85, s		1′, 2, 6′	2′, 6′, 8′a
3′-OH				4.15, s		2′, 3′, 4′	5′b

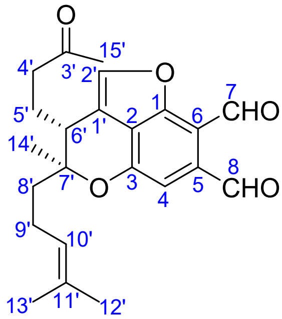
[a] The data were recorded at 400 MHz (^{1}H NMR) and 100 MHz (^{13}C NMR) in $CDCl_3$.

[b] The indiscernible signals from overlap or the complex multiplicity are reported without designating multiplicity.

Table S8 Comparison of experimental and calculated ^{13}C NMR data of 6

No.	6	6a	AE	6b	AE
C-1	167.7	165.8	1.9	166.8	0.9
C-2	118.9	118.0	0.9	119.5	0.6
C-3	155.6	154.1	1.5	154.3	1.3
C-4	108.8	109.3	0.5	109.1	0.3
C-5	140.4	137.8	2.6	137.8	2.6
C-6	112.1	110.5	1.6	110.7	1.4
C-7	187.2	184.8	2.4	184.8	2.4
C-8	192.8	191.7	1.1	191.7	1.1
C-1′	71.8	74.2	2.4	74.1	2.3
C-2′	96.8	100.6	3.8	102.0	5.2
C-3′	71.8	74.8	3.0	74.0	2.2
C-4′	29.9	32.6	2.7	32.6	2.7
C-5′	17.1	23.5	6.4	23.5	6.4
C-6′	41.7	43.0	1.3	44.1	2.4
C-7′	84.9	87.2	2.3	86.9	2.0
C-8′	39.9	42.5	2.6	41.6	1.7
C-9′	23.3	28.9	5.6	28.3	5.0
C-14′	23.6	29.1	5.5	30.7	7.1
C-15′	66.1	71.9	5.8	73.7	7.6
MAE		2.83		2.92	
R^2		0.9991		0.9986	
DP4+		98.30%		1.70%	

Table S9 NMR data of 8 (^{1}H for 400 MHz and ^{13}C for 100 MHz in $CDCl_3$)



No.	δ_C, type	δ_H (J in Hz)[a]	^{1}H-^{1}H COSY	HMBC	ROESY
1	153.8, C				
2	121.8, C				
3	154.1, C				
4	110.7, CH	7.23, s		2, 3, 6, 8	8
5	137.2, C				
6	115.7[b], C				
7	187.7, CH	10.77, s		1, 5, 6	
8	192.1, CH	10.58, s		4, 5, 6	4
1′	115.8[b], C				
2′	142.2, CH	7.58, br s	6′	1, 1′, 2	4′a, 4′b
3′	207.5, C				
4′	40.9, CH_2	a: 2.56	4′b, 5′a, 5′b	3′, 5′	2′
		b: 2.43	4′a, 5′a, 5′b	3′, 5′, 6′	2′
5′	23.4, CH_2	a: 2.20	4′a, 4′b, 5′b, 6′	4′	
		b: 1.54	4′a, 4′b, 5′a, 6′		
6′	39.5, CH	3.06, br dd (10.9, 3.4)	2′, 5′a, 5′b	1′, 2, 2′, 4′, 5′	9′
7′	86.7, C				
8′	38.5, CH_2	a: 1.65	8′b, 9′		
		b: 1.55	8′a, 9′		
9′	22.2, CH_2	2.06	8′a, 8′b, 10′	8′, 10′, 11′	6′
10′	123.0, CH	4.92, br t (7.0)	9′, 12′, 13′	9′, 12′, 13′	12′
11′	132.4, C				
12′	25.5, CH_3	1.59, br s	10′	10′, 11′, 13′	10′
13′	17.5, CH_3	1.49, br s	10′	10′, 11′, 12′	
14′	21.7, CH_3	1.49, s		6′, 7′, 8′	
15′	30.1, CH_3	2.14, s		3′, 4′	

[a] The indiscernible signals from overlap or the complex multiplicity are reported without designating multiplicity.

[b] The data are interchangeable.

Table S10 Primers used in the study

Primer	Sequence (5' to 3')	Usage
Inf-Bar-F-EcoRV	CCAAGCATCGAAGATATGAGCCCAGAACGACGCC	Cloning the *bar* gene from pPTRI
Inf-Bar-R-EcoRV	TCGGCATCTACTGATTCAGATCTCGGTGACGGGCAG	
TtrPC-Bar-ANN1-F	TATTCTTTTGATTTAGCAATTAACCCTCACTAAAG	Cloning the *bar* gene expression cassette from pBSKII-PtrPC-BAR-TtrPC
TtrPC-Bar-ANN1-R	CGGCAAAATCCCTTATATCGATAAGCTTCAGGGCT	
gRNA-gstbA-F	TAATACGACTCACTATAGGAGTCGCAGAACTCGCGGCGTTTTAGAGCTAGAAATAGC	Cloning gRNA scaffold from pUCm-gRNAscaffold-*eGFP*
eGFP-R	TTACACCTTCCTCTTCTTC	
PtrpC-XbaI-F	GCTCTAGAGCGCAATTAACCCTCACTAA	Cloning the *neo* marker gene cassette from pBSKII-PtrPC-*neo*-TtrPC
TtrpC-HindIII-R	CCCAAGCTTCAGGGCTGGTGACGGAATTTTCATAG	
pUCm-F	TCGCGCGTTTCGGTGATGAC	Cloning the gRNA cassette from pUCm-gRNA-*stbA*
gRNA-R	AAAAGCACCGACTCGGTGCC	

Table S11 Plasmids used in the study

Plasmid	**Characteristic**	**Source**
pUCm-T	A commercial vector for cloning and *in vitro* transcription	Sangon Biotech Co., Ltd. (China)
pBARI	Plasmid containing *bar* marker gene cassette (Amp^R)	Matsuda, Y. *et al.*[1]
pBSKII-PtrPC-EcoRV-TtrPC	Plasmid containing the *trpC* promoter and terminator (Amp^R)	Zheng, Y.-M. *et al.*[2]
pBSKII-PtrPC-Flag-*toCas9*-TtrPC	Plasmid containing *Cas9* whose expression is regulated by the *trpC* promoter (Amp^R)	Zheng, Y.-M. *et al.*[2]
pUCm-gRNAscaffold-*eGFP*	Plasmid containing gRNA scaffold	Zheng, Y.-M. *et al.*[2]
pBSKII-PtrPC-*neo*-TtrPC	Plasmid containing *neo* whose expression is regulated by the *trpC* promoter (Amp^R)	Zheng, Y.-M. *et al.*[2]
pBSKII-PtrPC-BAR-TtrPC	Plasmid containing *bar* whose expression is regulated by the *trpC* promoter (Amp^R)	This work
pBSKII-*toCas9*-*bar*	Plasmid containing *Cas9* and *bar* whose expressions are independently regulated by the *trpC* promoter (Amp^R)	This work
pUCm-gRNA-*stbA*	Recombinant pUCm used for *in vitro* transcription to generate gRNA targeting *stbA* (Amp^R)	This work

Supplementary Figures

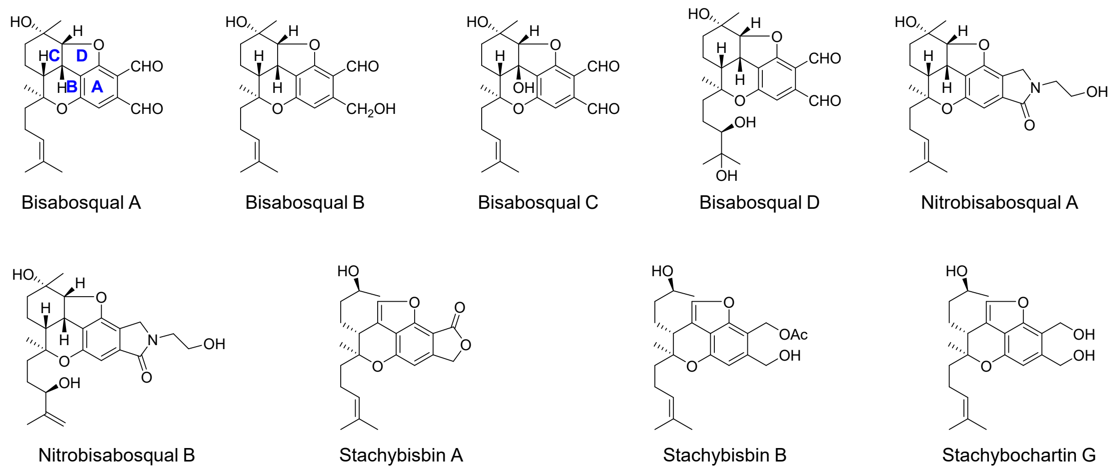


Fig. S1 Structures of known bisabosqual-type meroterpenoids

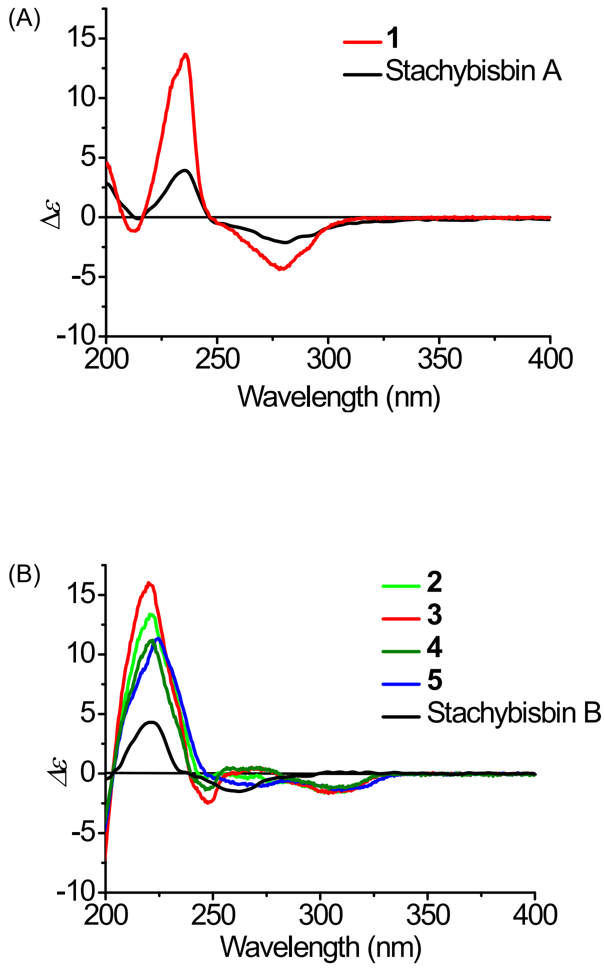


Fig. S2 Comparison of ECD spectra of 1-5 with those of stachybisbins A and B

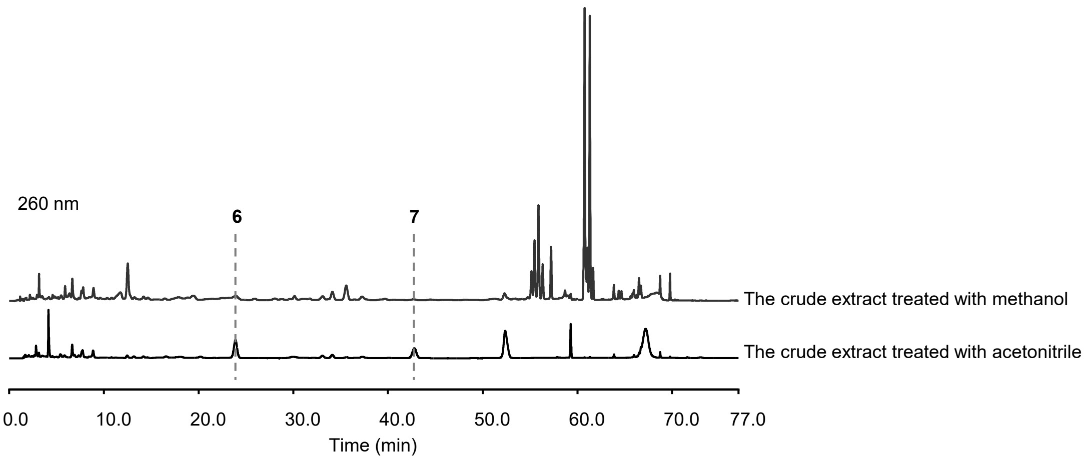


Fig. S3 HPLC analysis of the *S. bisbyi* PYH05-7 extract treated with methanol or acetonitrile

The culture broth of *S. bisbyi* PYH05-7 grown in liquid maltose medium was extracted with ethyl acetate. Subsequently, the resulted crude extract was stored in methanol or acetonitrile for one day, and then used for HPLC analysis.

(1′*R**,2′*R**,3′*R**,6′*R**,7′*S**)-**6a**

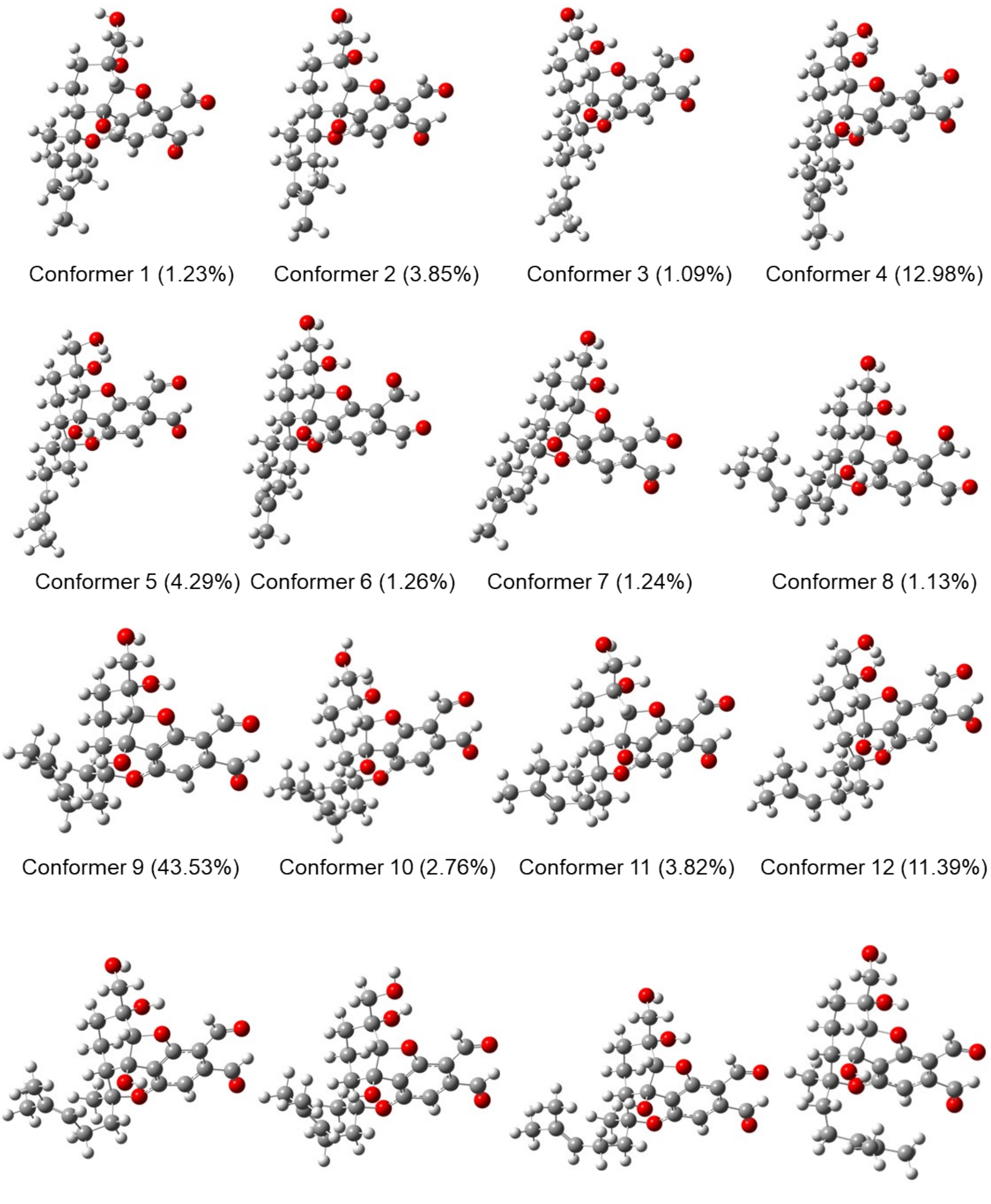


Fig. S4 Most stable conformers of (1′*R,2′*R**,3′*R**,6′*R**,7′*S**)-6a**

(1′*R**,2′*R**,3′*R**,6′*R**,7′*R**)-**6b**

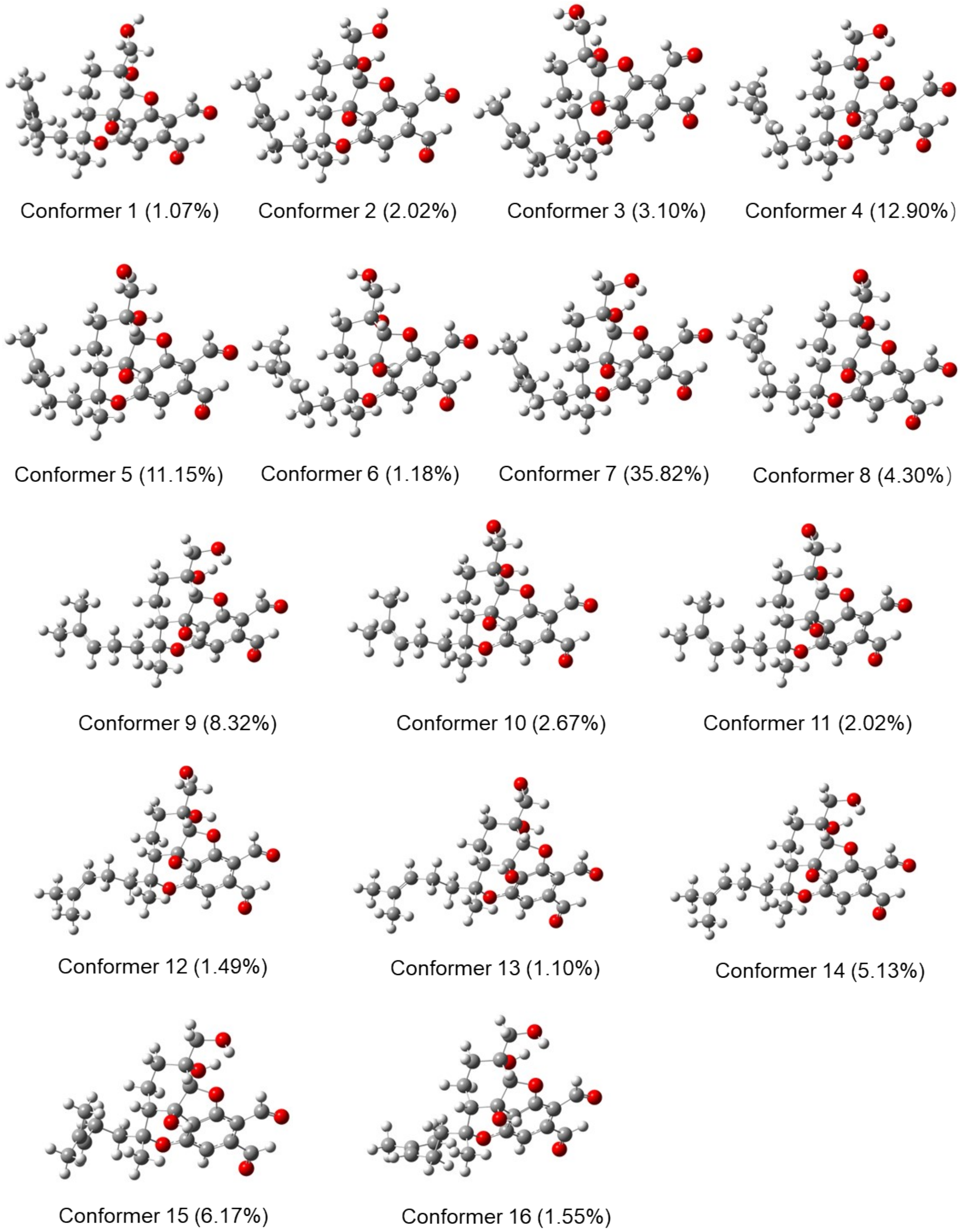
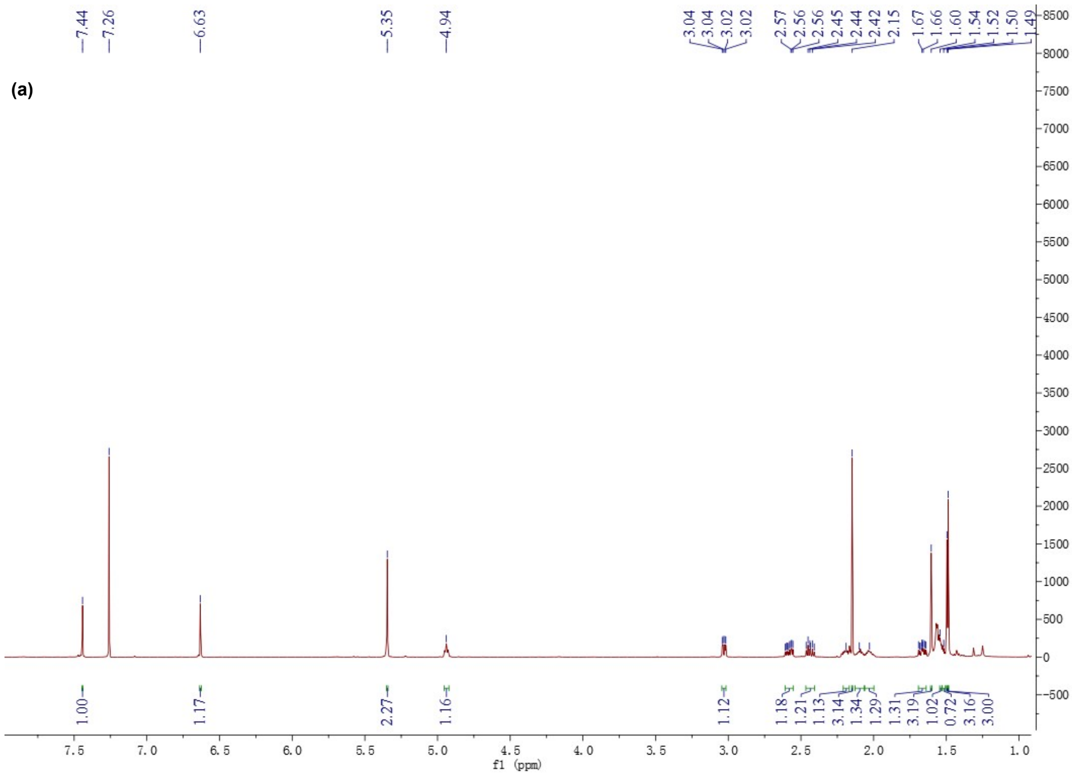
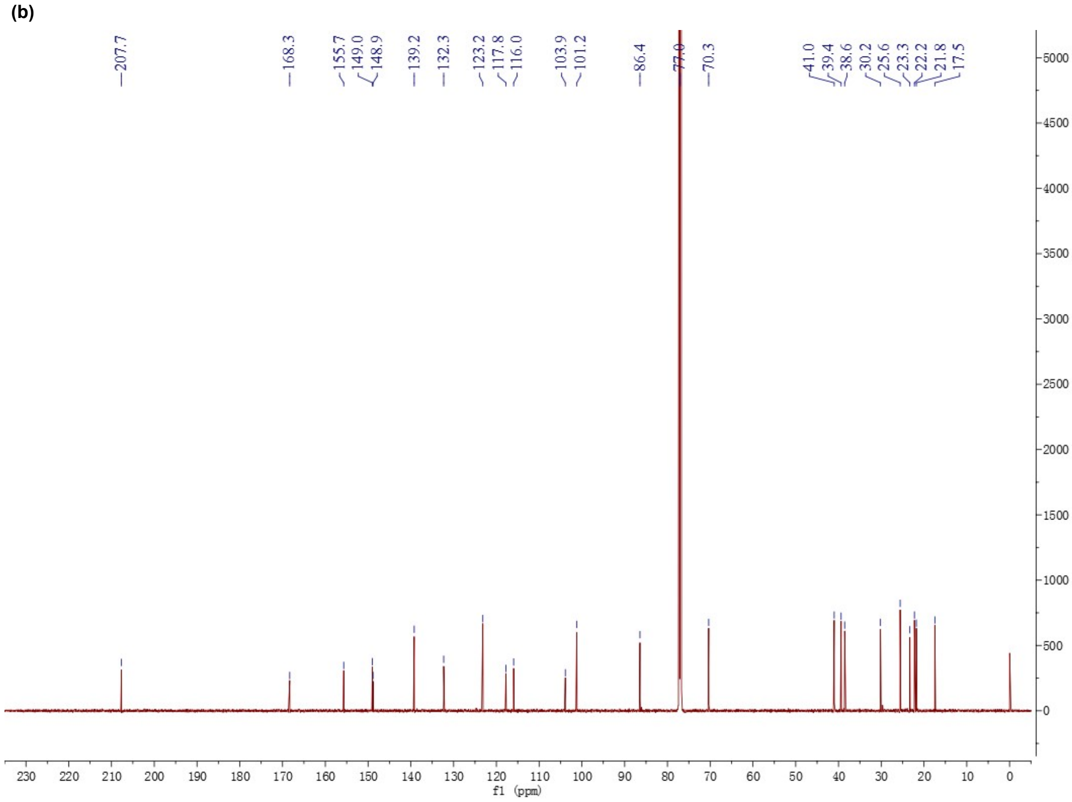


Fig. S5 Most stable conformers of (1′*R,2′*R**,3′*R**,6′*R**,7′*R**)-6b**

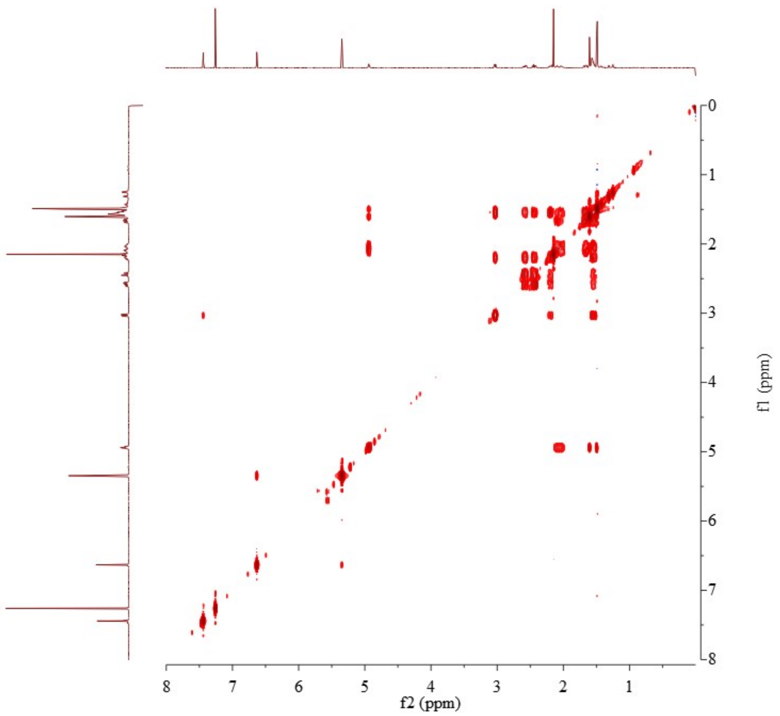
(a)


7.44
7.26
6.63
5.35
4.94
3.04
3.04
3.02
3.02
2.57
2.56
2.56
2.45
2.44
2.42
2.15
1.67
1.66
1.60
1.54
1.52
1.50
1.49
1.00
1.17
2.27
1.16
1.12
1.18
1.21
1.13
3.14
1.34
1.29
1.31
3.19
1.02
0.72
3.16
3.00
f1 (ppm)

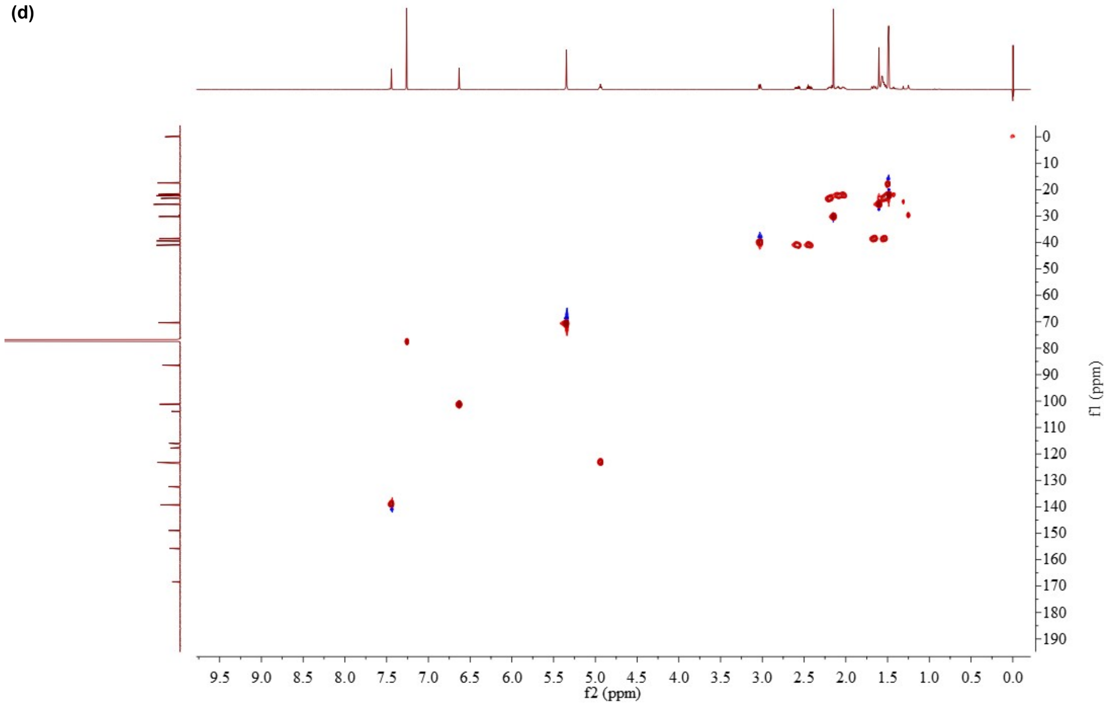
(b)


207.7
168.3
155.7
149.0
148.9
139.2
132.3
123.2
117.8
116.0
103.9
101.2
86.4
77.0
70.3
41.0
39.4
38.6
30.2
25.6
23.3
22.2
21.8
17.5
f1 (ppm)

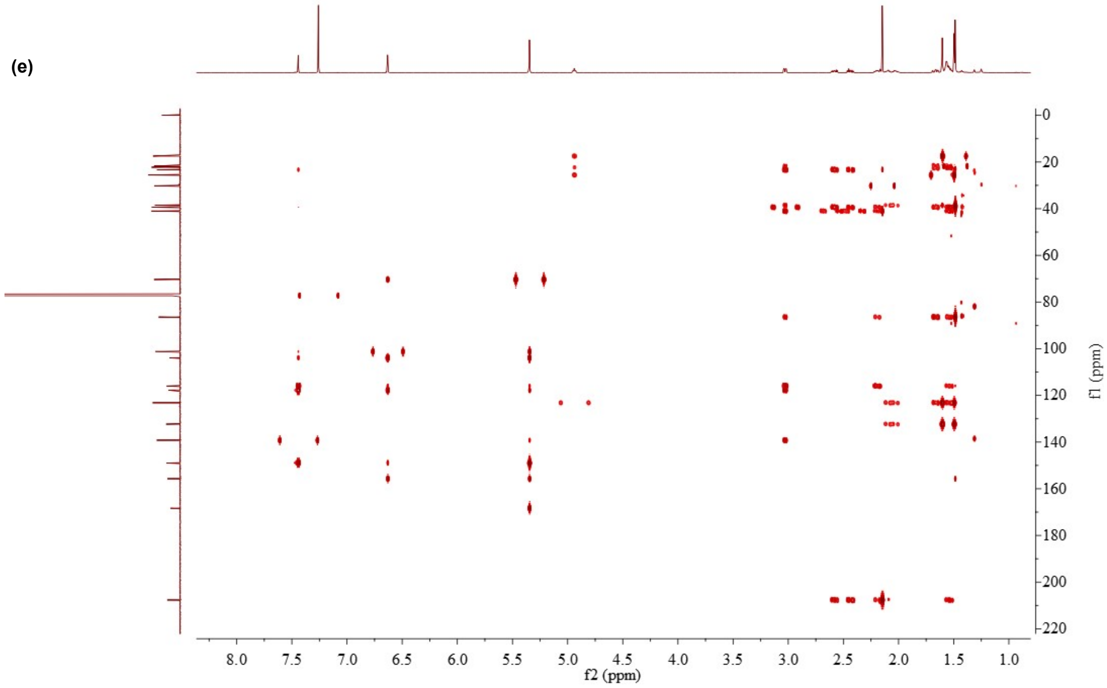
(c)



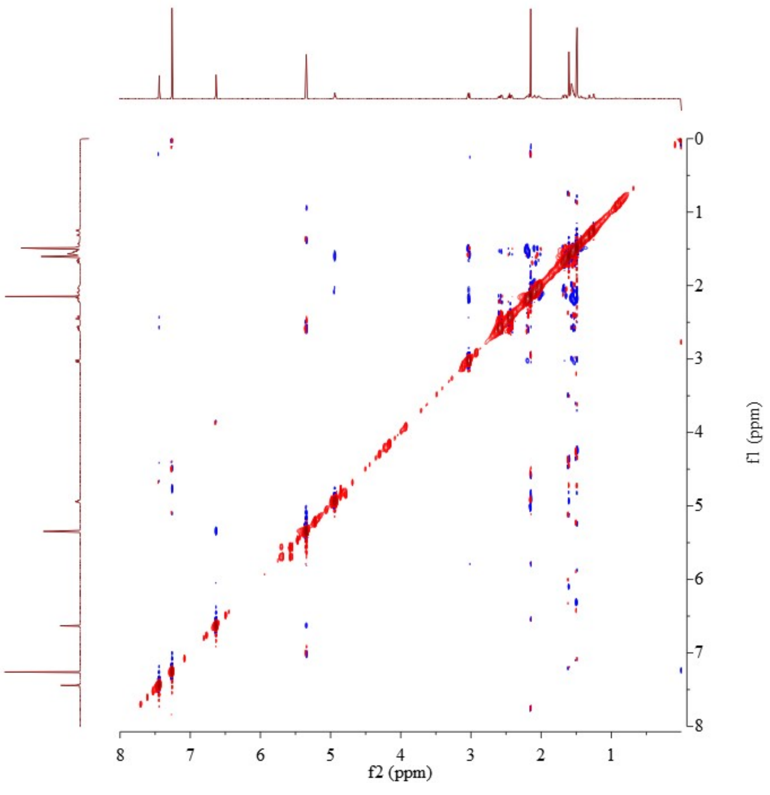
(d)



(e)



(f)



(g)

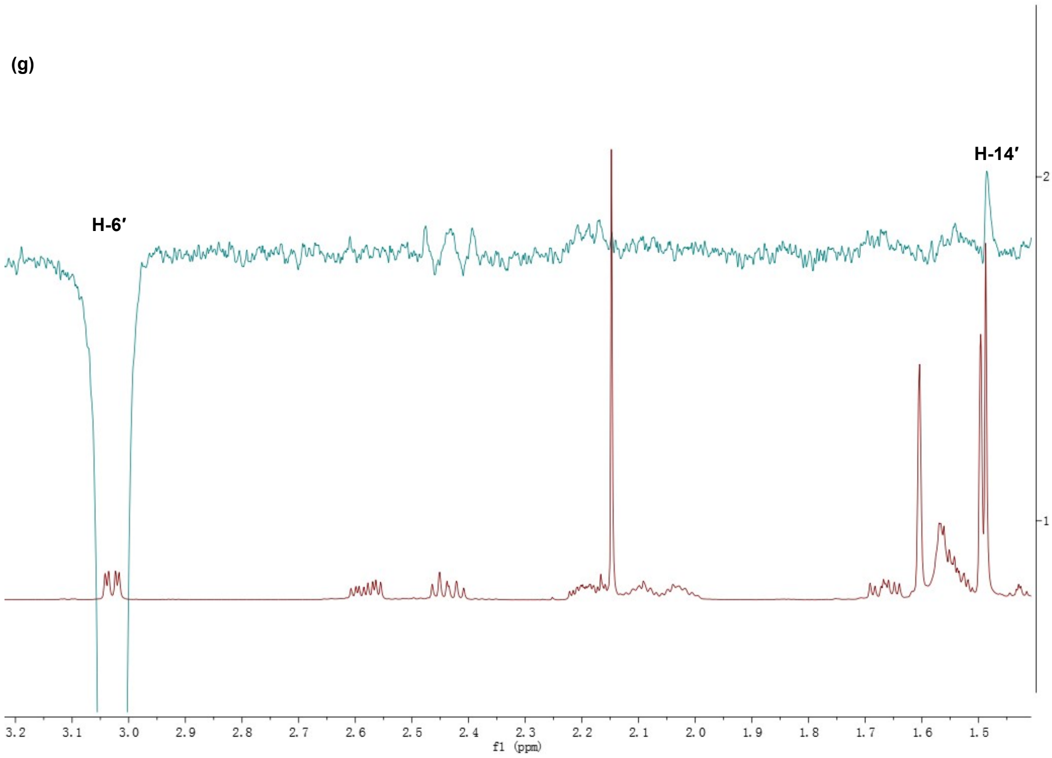
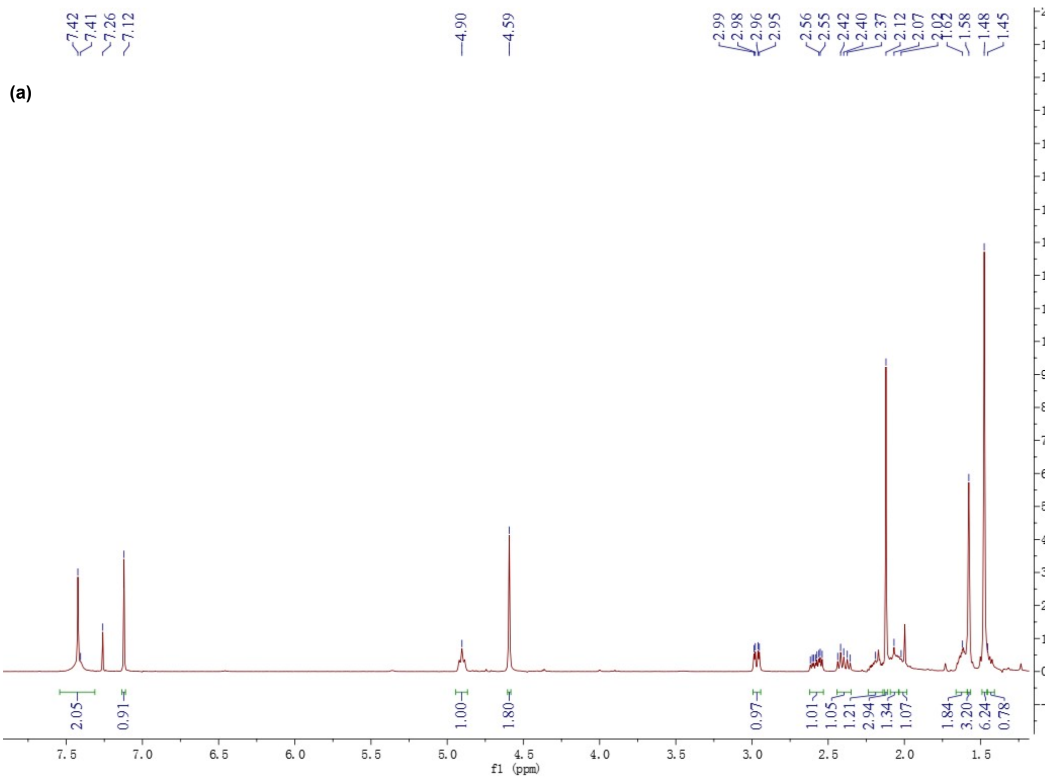


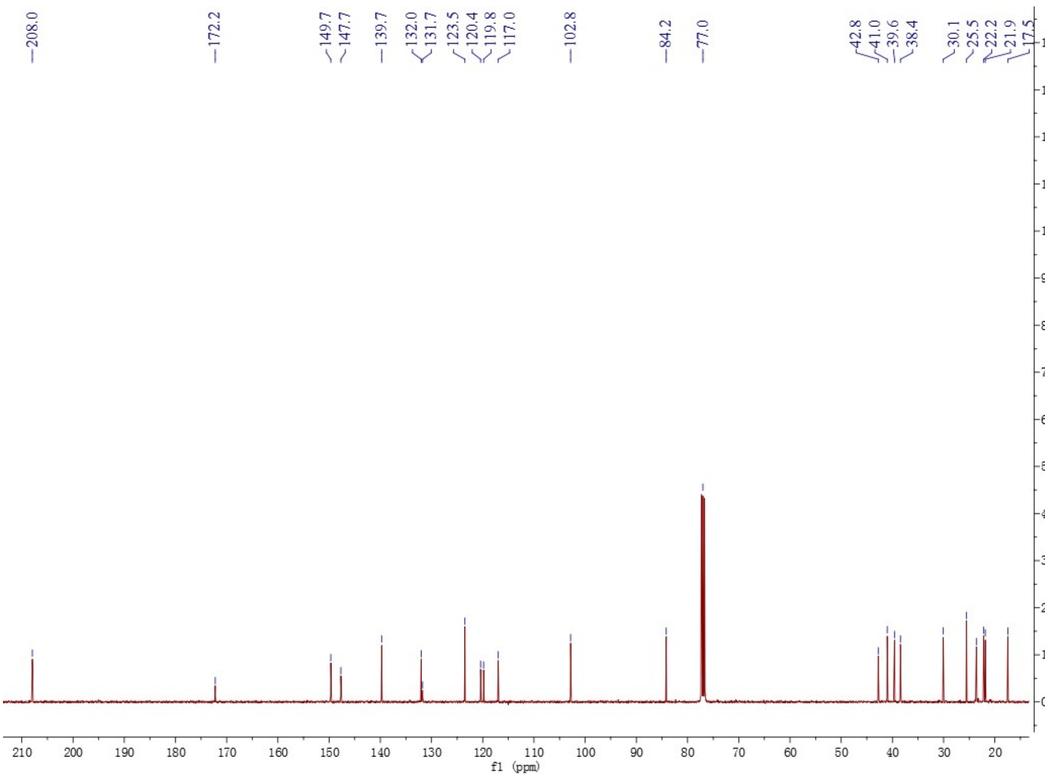
Fig. S6 NMR spectra of 1

(a) ^{1}H NMR spectrum in $CDCl_3$ at 600 MHz; (b) ^{13}C NMR spectrum in $CDCl_3$ at 150 MHz; (c) ^{1}H-^{1}H COSY spectrum in $CDCl_3$ at 600 MHz; (d) HSQC spectrum in $CDCl_3$ at 600 MHz; (e) HMBC spectrum in $CDCl_3$ at 600 MHz; (f) ROESY spectrum in $CDCl_3$ at 600 MHz; (g) 1D-selective NOE experiment in $CDCl_3$ at 400 MHz.

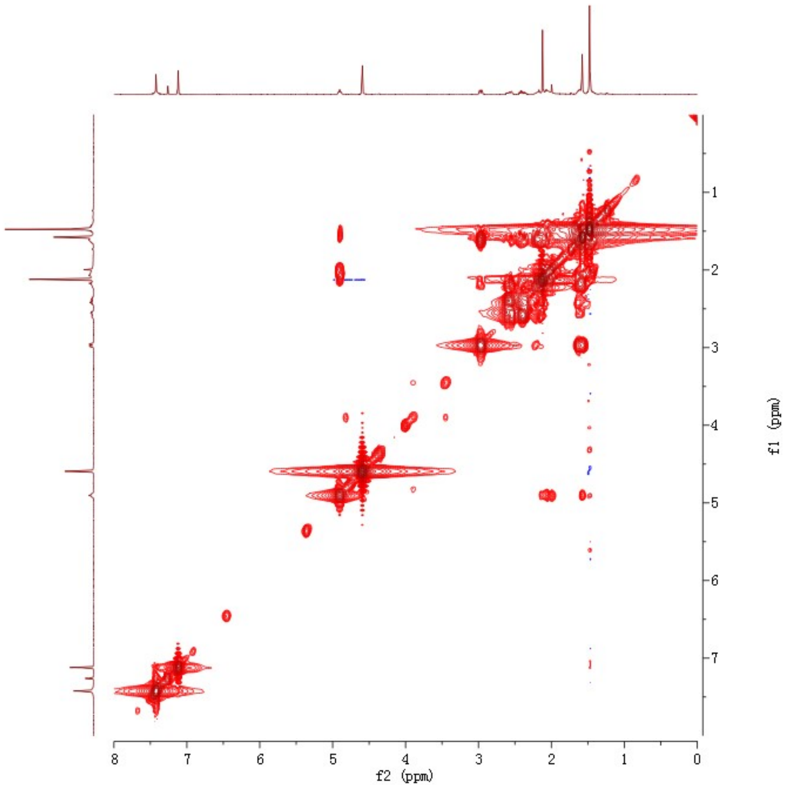
(a)


7.42
7.41
7.26
7.12
4.90
4.59
2.99
2.98
2.96
2.95
2.56
2.55
2.42
2.40
2.37
2.12
2.07
2.02
1.62
1.58
1.48
1.45
2.05
0.91
1.00
1.80
0.97
1.01
1.05
1.21
2.94
1.34
1.07
1.84
3.20
6.24
0.78
f1 (ppm)

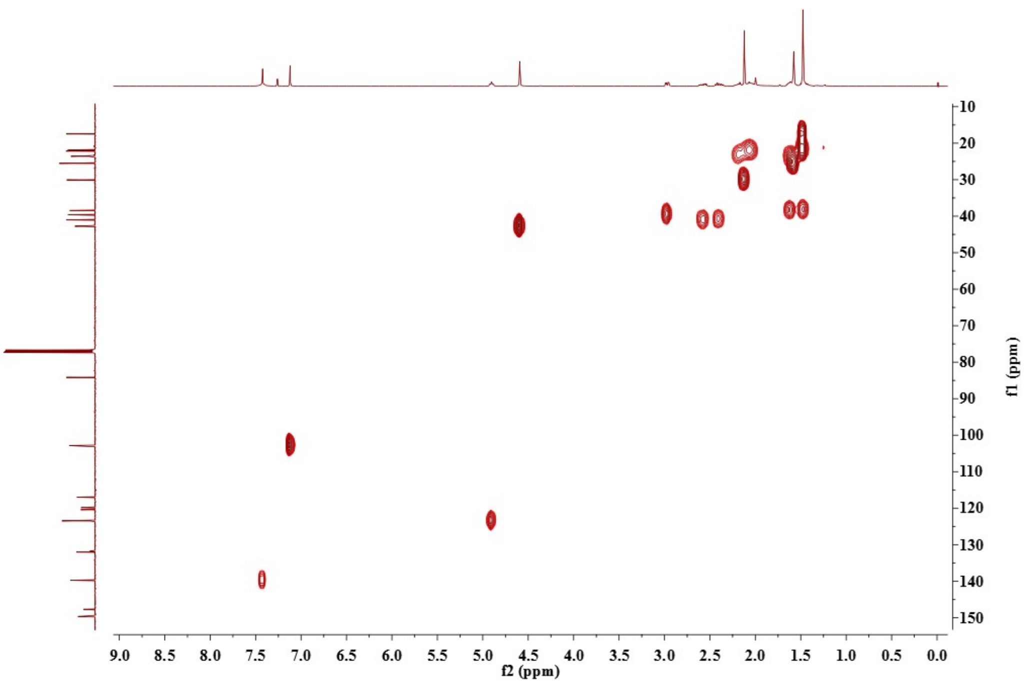
(b)


208.0
172.2
149.7
147.7
139.7
132.0
131.7
123.5
120.4
119.8
117.0
102.8
84.2
77.0
42.8
41.0
39.6
38.4
30.1
25.5
22.2
21.9
17.5
f1 (ppm)

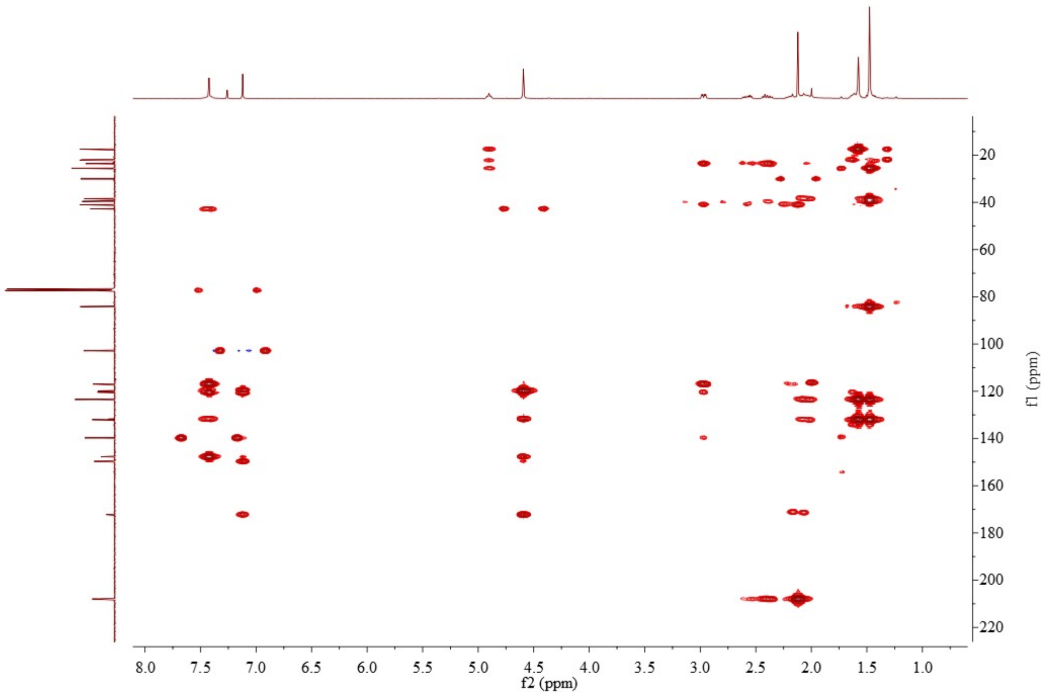
(c)



(d)



(e)



(f)

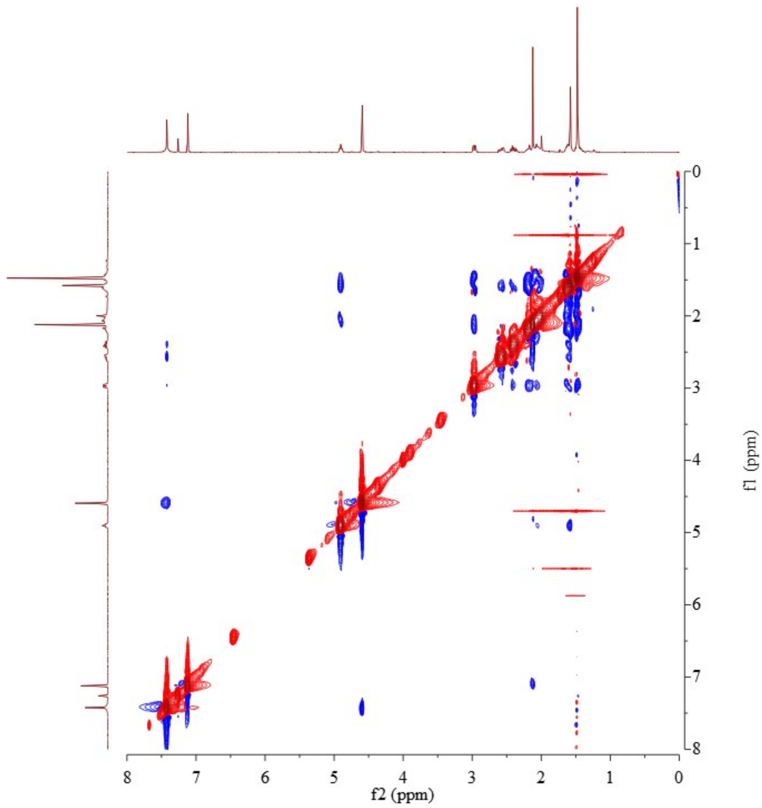
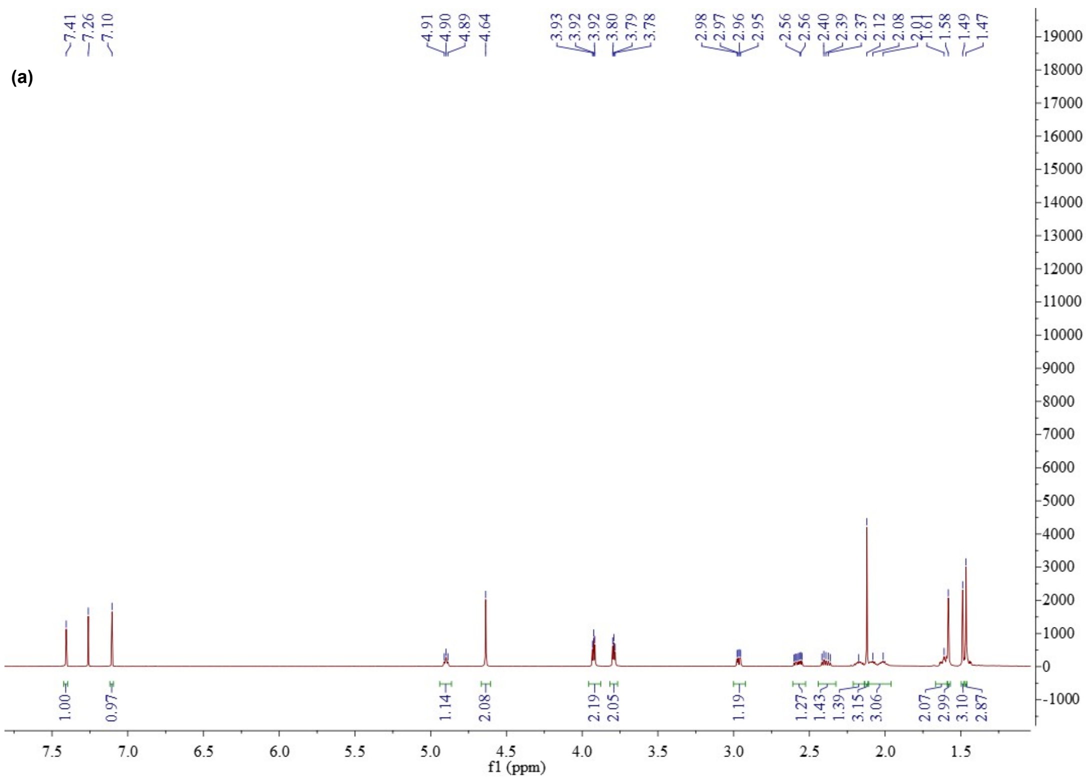
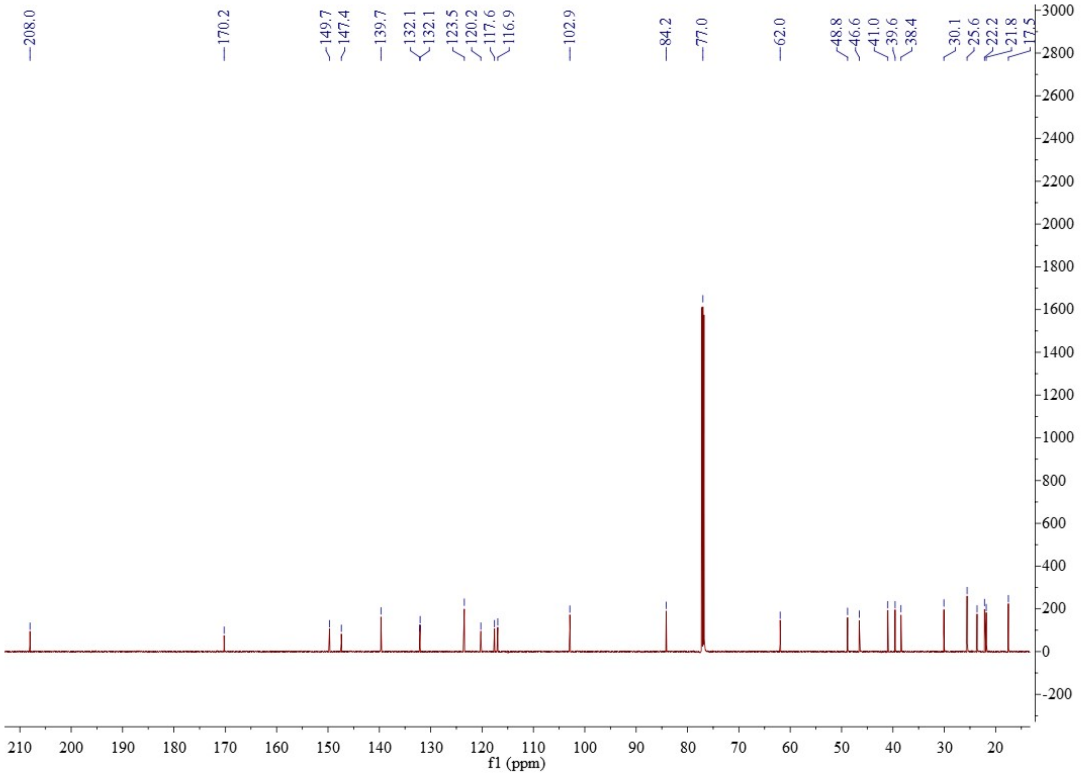


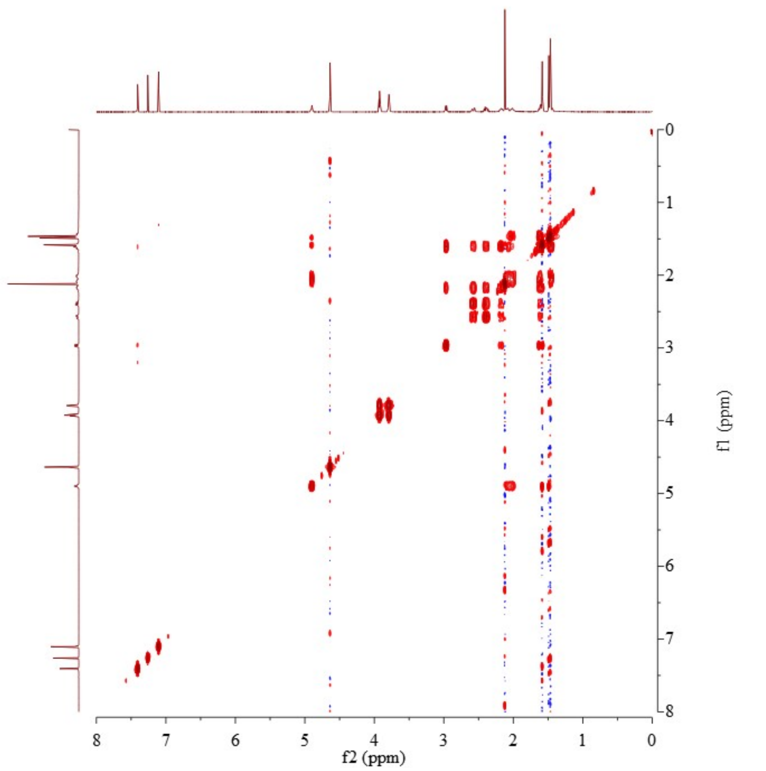
Fig. S7 NMR spectra of 2

(a) ^{1}H NMR spectrum in $CDCl_3$ at 400 MHz; (b) ^{13}C NMR spectrum in $CDCl_3$ at 100 MHz; (c) ^{1}H-^{1}H COSY spectrum in $CDCl_3$ at 400 MHz; (d) HSQC spectrum in $CDCl_3$ at 400 MHz; (e) HMBC spectrum in $CDCl_3$ at 400 MHz; (f) ROESY spectrum in $CDCl_3$ at 400 MHz.

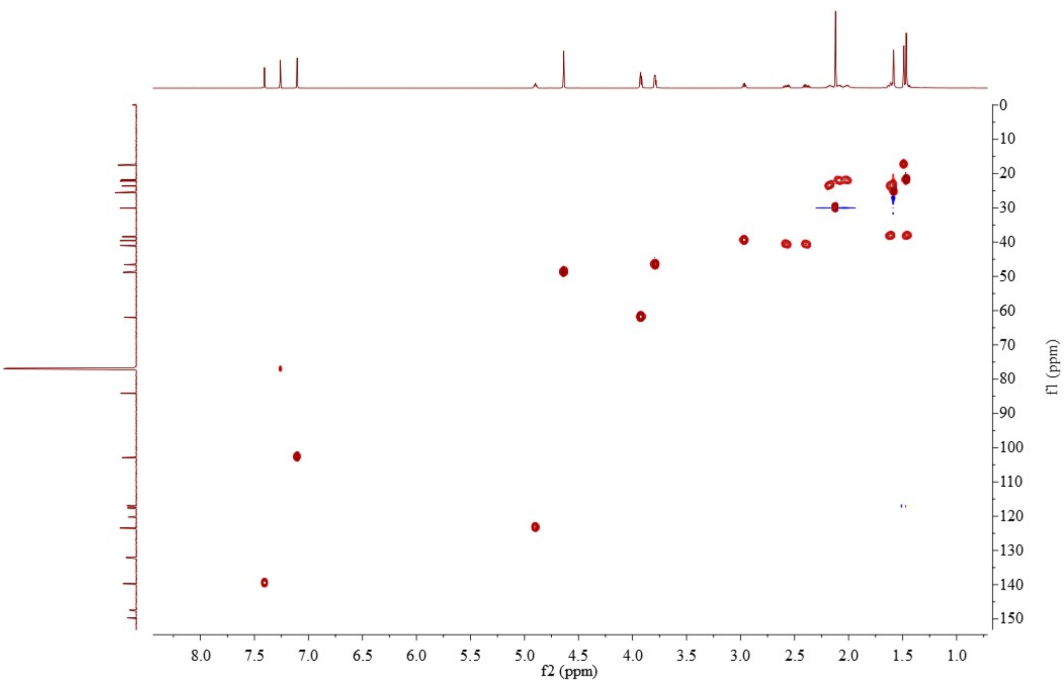

(a)
7.41
7.26
7.10
4.91
4.90
4.89
4.64
3.93
3.92
3.92
3.80
3.79
3.78
2.98
2.97
2.96
2.95
2.56
2.56
2.40
2.39
2.37
2.12
2.08
2.01
1.61
1.58
1.49
1.47
1.00
0.97
1.14
2.08
2.19
2.05
1.19
1.27
1.43
1.39
3.15
3.06
2.07
2.99
3.10
2.87
f1 (ppm)


(b)
208.0
170.2
149.7
147.4
139.7
132.1
132.1
123.5
120.2
117.6
116.9
102.9
84.2
77.0
62.0
48.8
46.6
41.0
39.6
38.4
30.1
25.6
22.2
21.8
17.5
f1 (ppm)

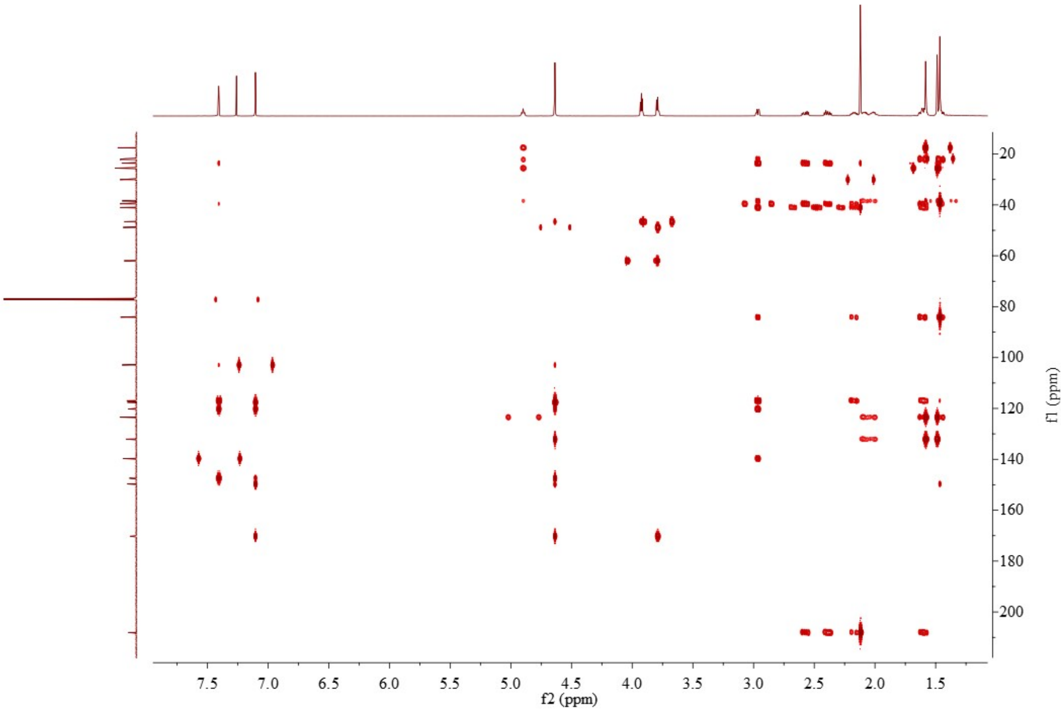
(c)



(d)



(e)



(f)

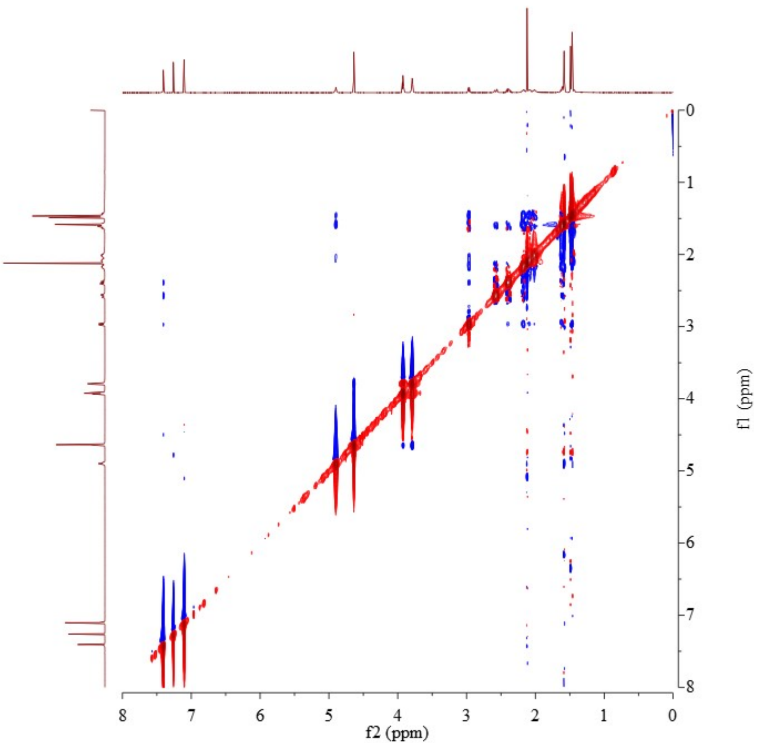
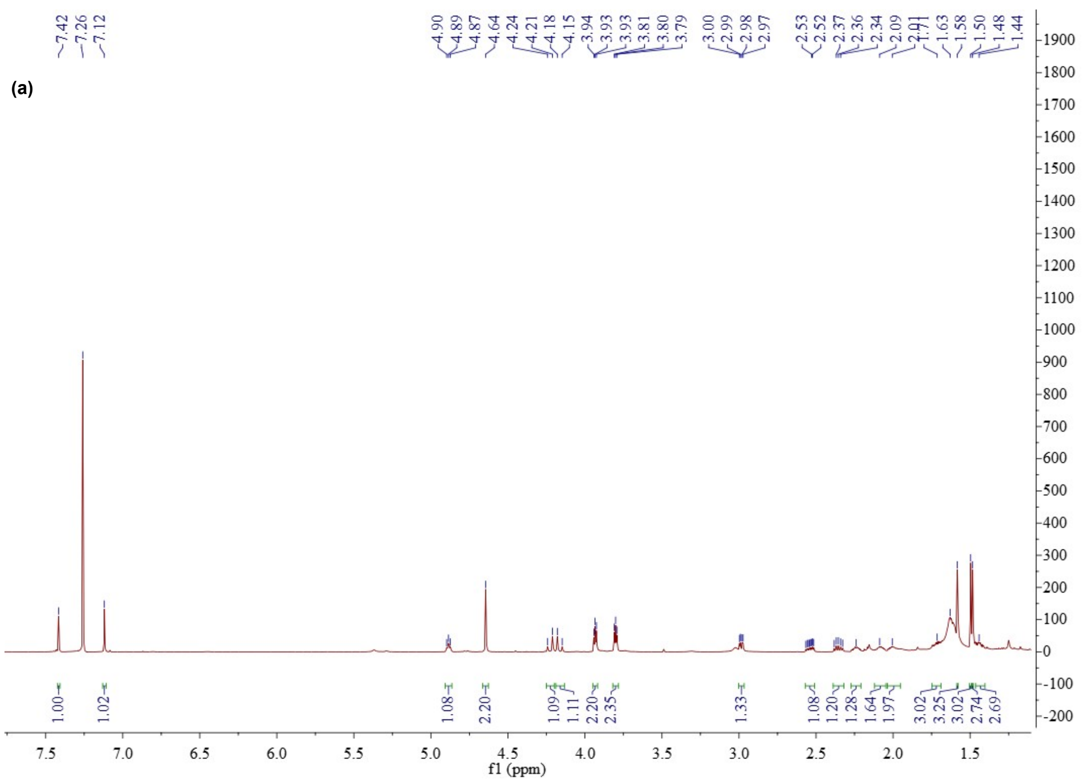


Fig. S8 NMR spectra of 3

(a) ^{1}H NMR spectrum in $CDCl_3$ at 600 MHz; (b) ^{13}C NMR spectrum in $CDCl_3$ at 150 MHz; (c) ^{1}H-^{1}H COSY spectrum in $CDCl_3$ at 600 MHz; (d) HSQC spectrum in $CDCl_3$ at 600 MHz; (e) HMBC spectrum in $CDCl_3$ at 600 MHz; (f) ROESY spectrum in $CDCl_3$ at 600 MHz.

(a)


7.42
7.26
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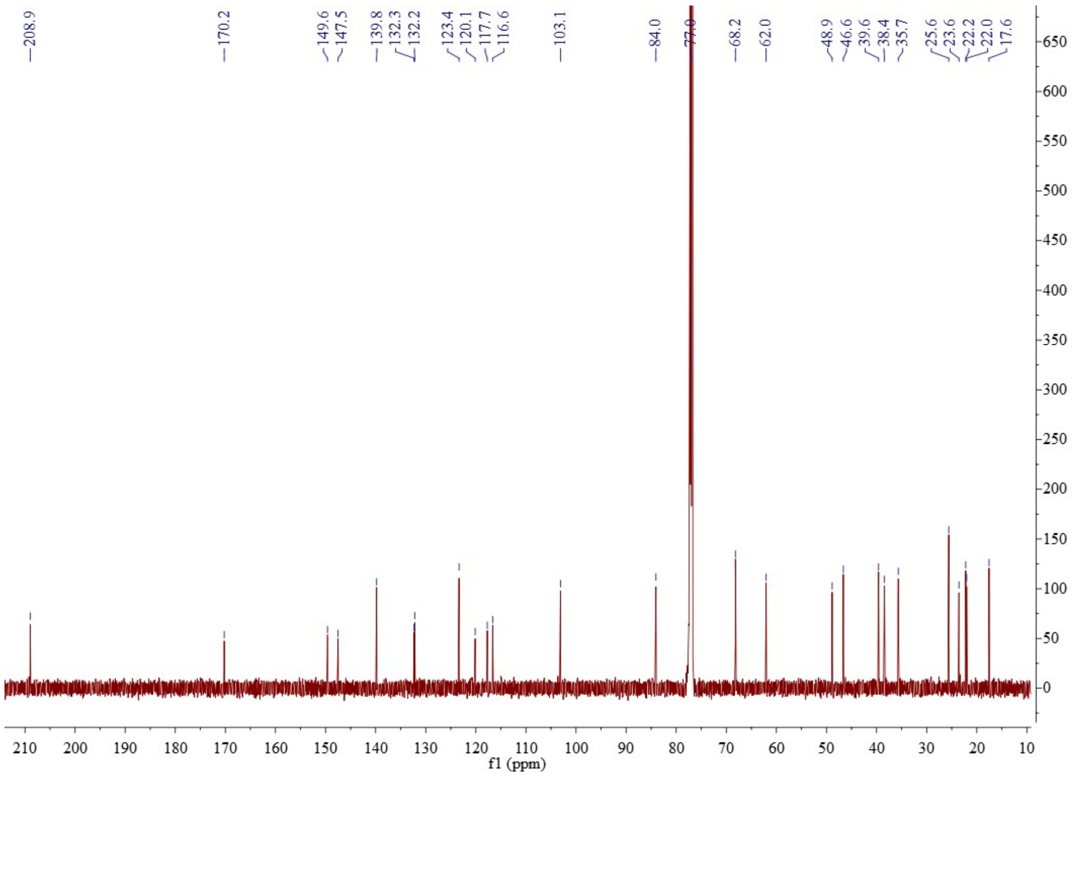
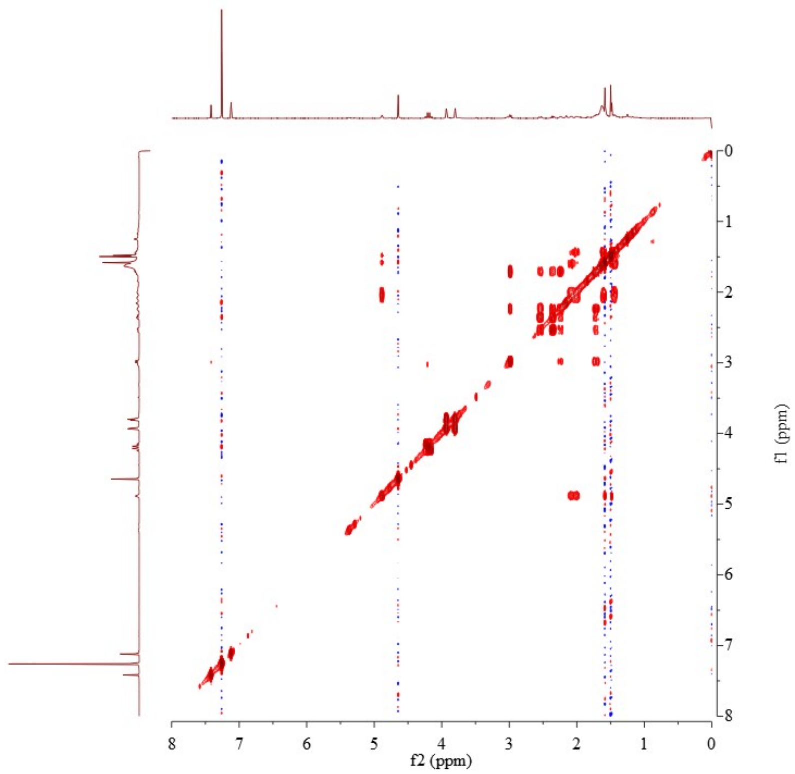
4.90
4.89
4.87
4.64
4.24
4.21
4.18
4.15
3.94
3.93
3.93
3.81
3.80
3.79
3.00
2.99
2.98
2.97
2.53
2.52
2.37
2.36
2.34
2.09
2.01
1.71
1.63
1.58
1.50
1.48
1.44
1.00
1.02
1.08
2.20
1.09
1.11
2.20
2.35
1.33
1.08
1.20
1.28
1.64
1.97
3.02
3.25
3.02
2.74
2.69
f1 (ppm)

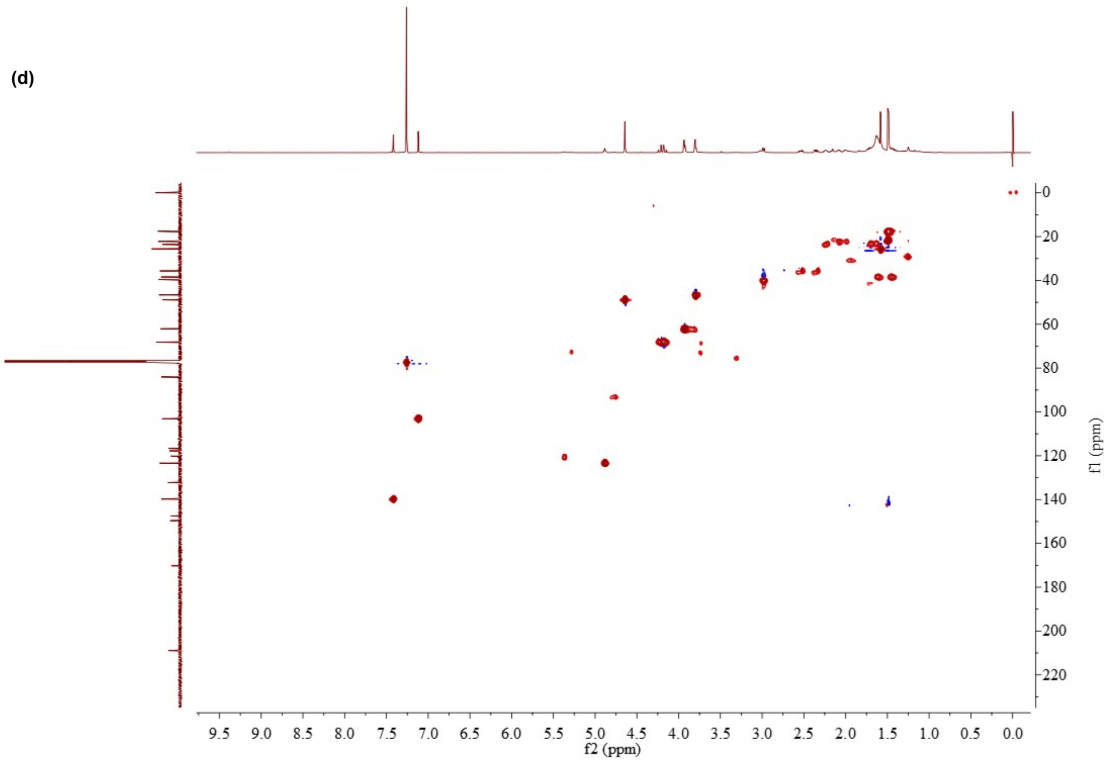
(b)


208.9
170.2
149.6
147.5
139.8
132.3
132.2
123.4
120.1
117.7
116.6
103.1
84.0
77.0
68.2
62.0
48.9
46.6
39.6
38.4
35.7
25.6
23.6
22.2
22.0
17.6
f1 (ppm)

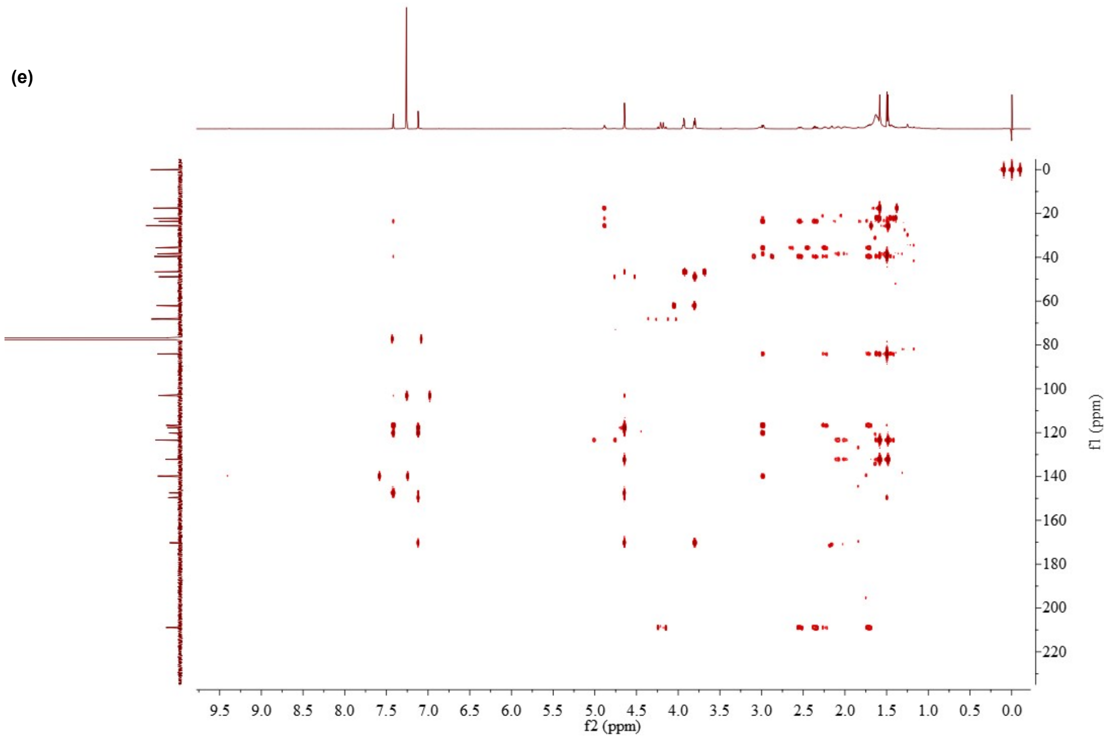
(c)



(d)



(e)



(f)

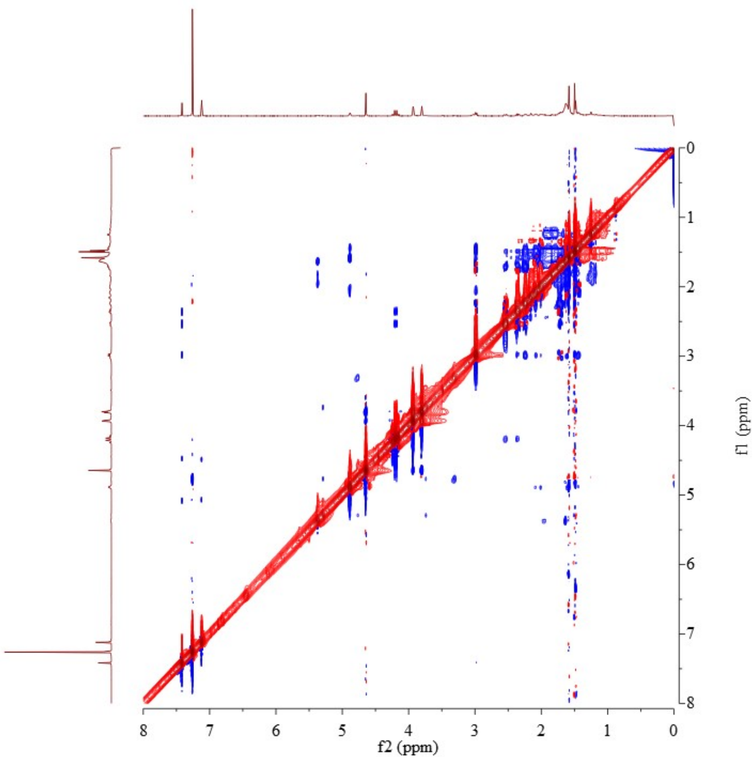
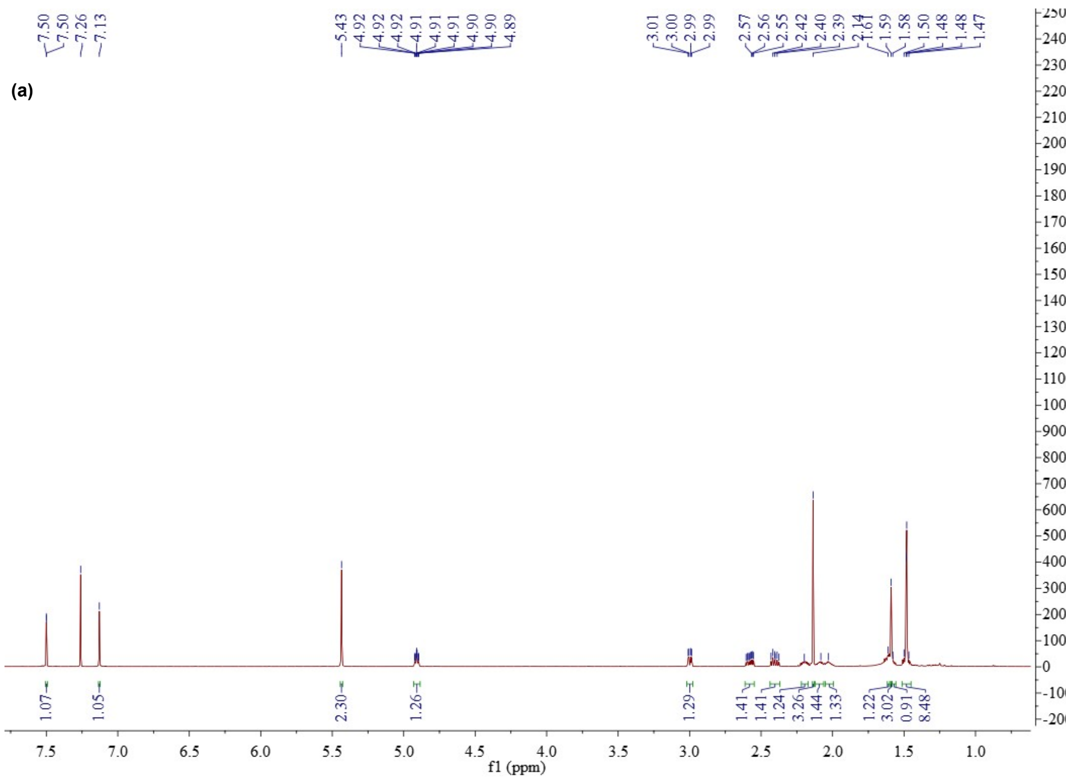


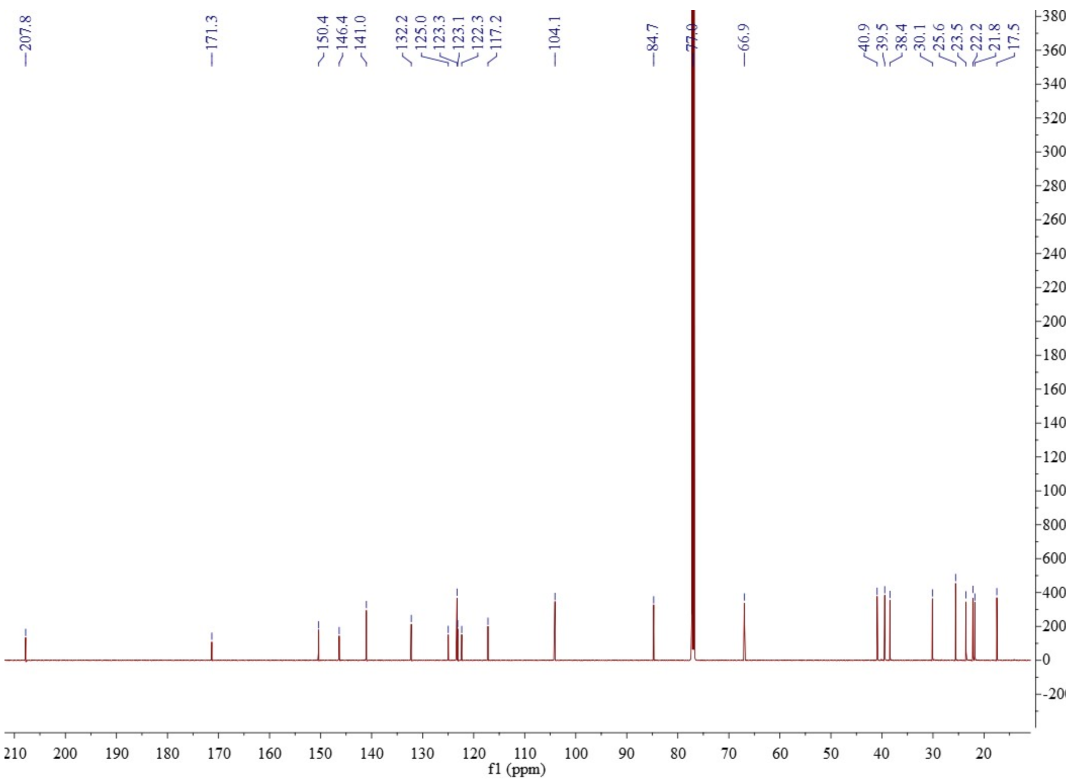
Fig. S9 NMR spectra of 4

(a) [1]H NMR spectrum in $CDCl_3$ at 600 MHz; (b) [13]C NMR spectrum in $CDCl_3$ at 150 MHz; (c) [1]H-[1]H COSY spectrum in $CDCl_3$ at 600 MHz; (d) HSQC spectrum in $CDCl_3$ at 600 MHz; (e) HMBC spectrum in $CDCl_3$ at 600 MHz; (f) ROESY spectrum in $CDCl_3$ at 600 MHz.

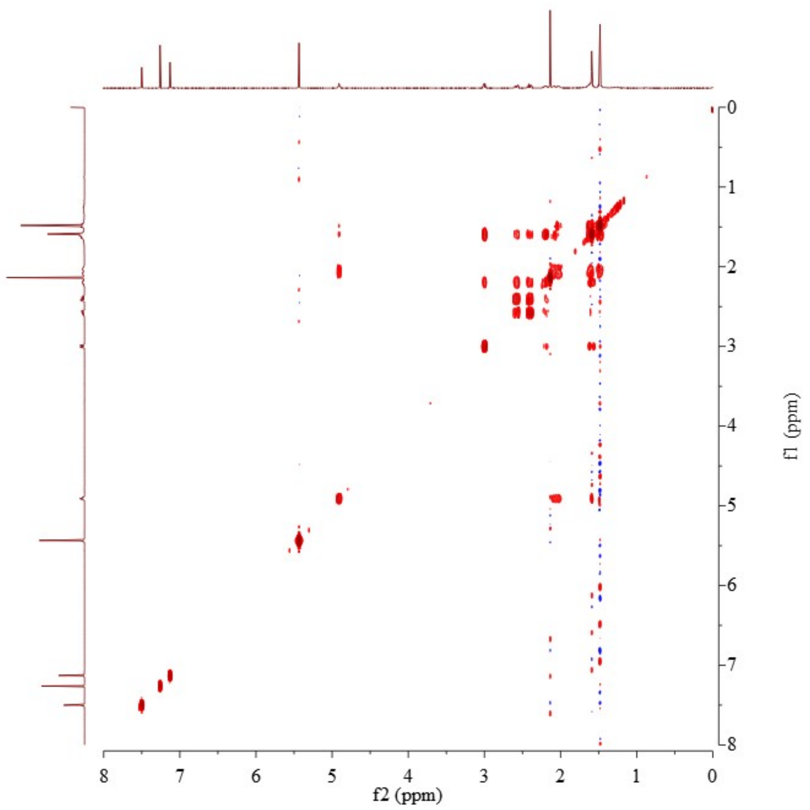
(a)



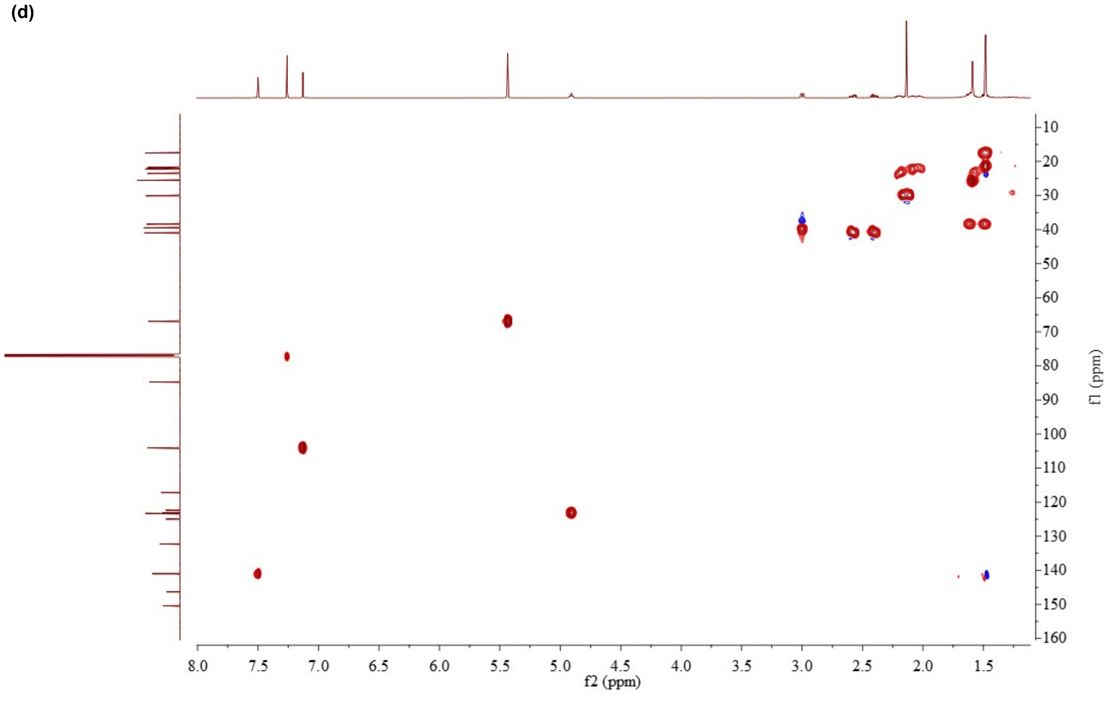
(b)



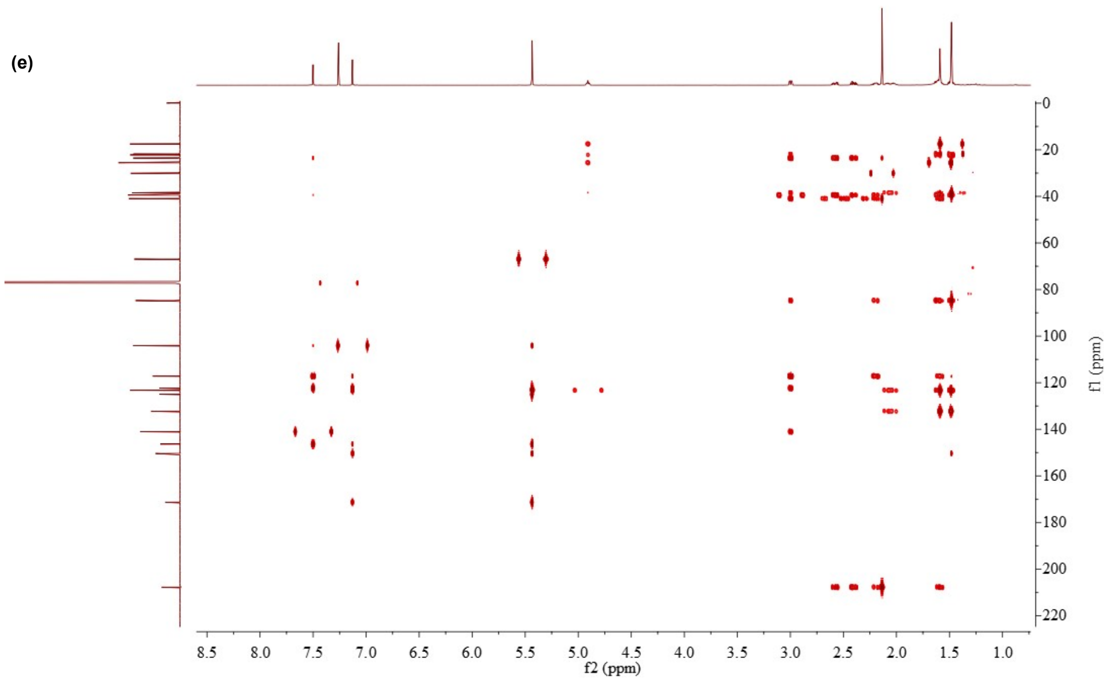
(c)



(d)



(e)



(f)

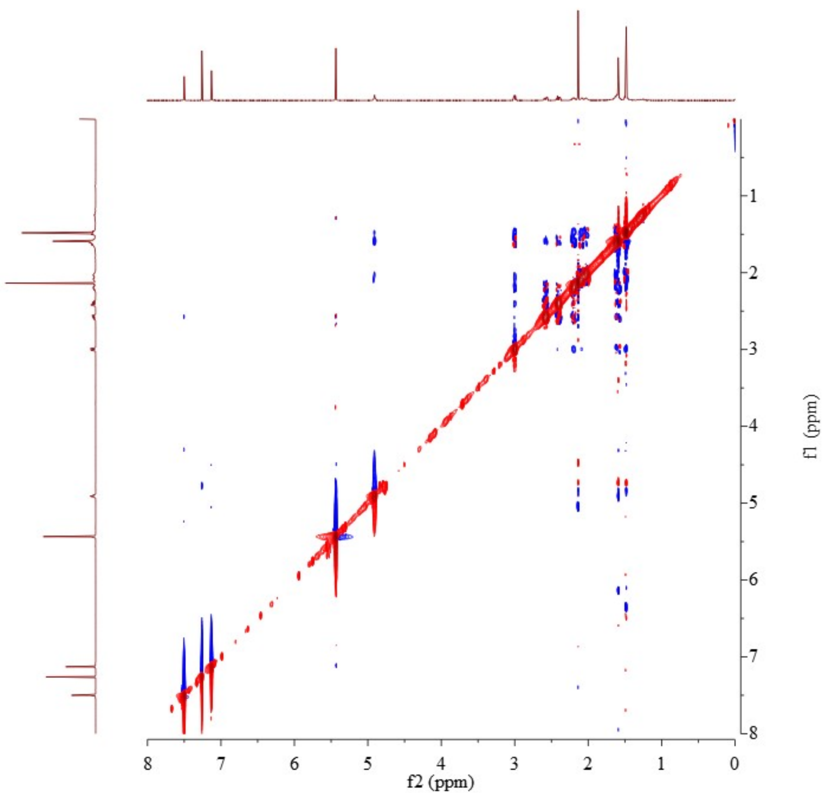
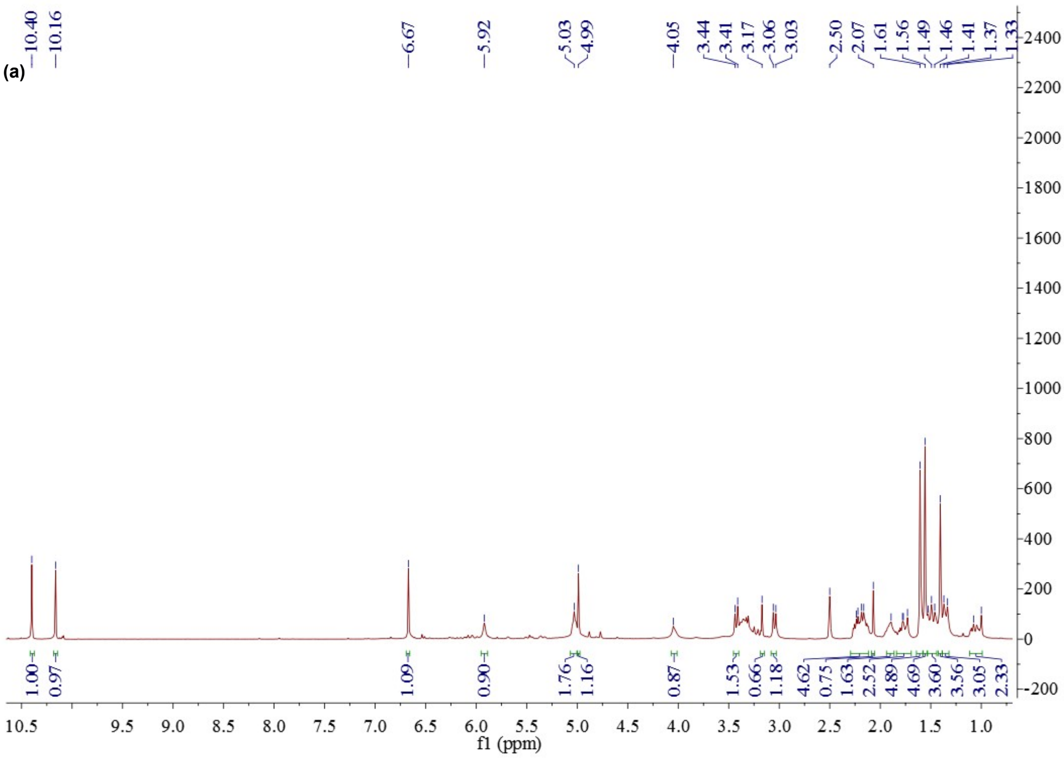


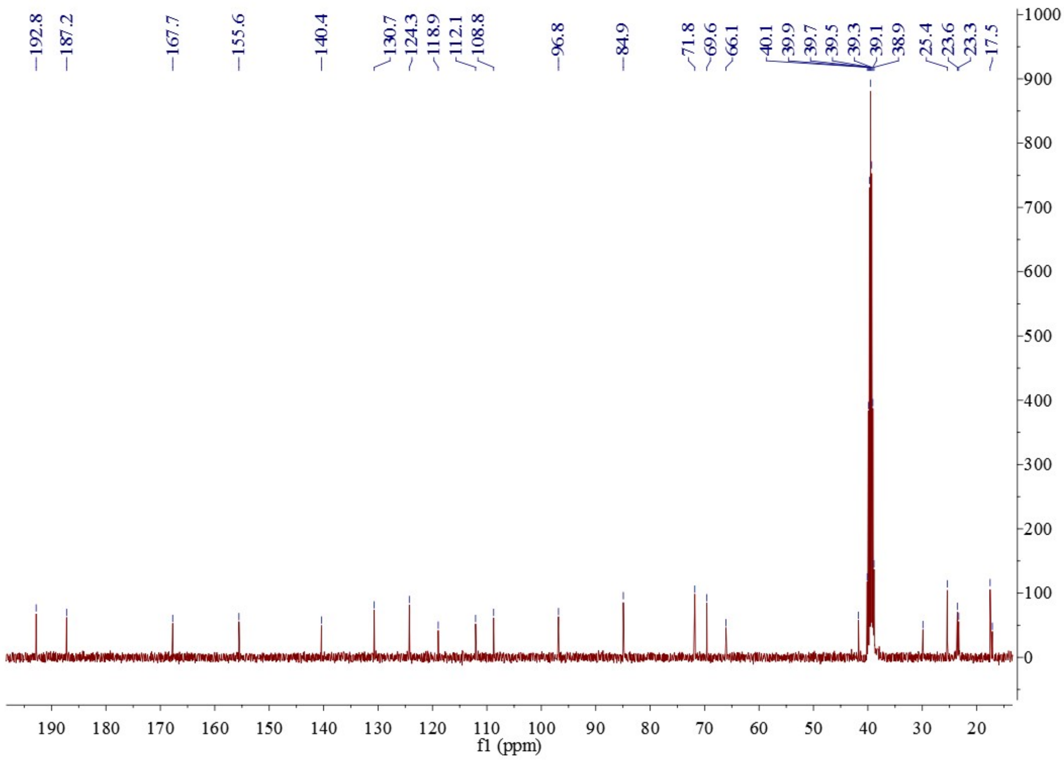
Fig. S10 NMR spectra of 5

(a) ^{1}H NMR spectrum in $CDCl_3$ at 600 MHz; (b) ^{13}C NMR spectrum in $CDCl_3$ at 150 MHz; (c) ^{1}H-^{1}H COSY spectrum in $CDCl_3$ at 600 MHz; (d) HSQC spectrum in $CDCl_3$ at 600 MHz; (e) HMBC spectrum in $CDCl_3$ at 600 MHz; (f) ROESY spectrum in $CDCl_3$ at 600 MHz.

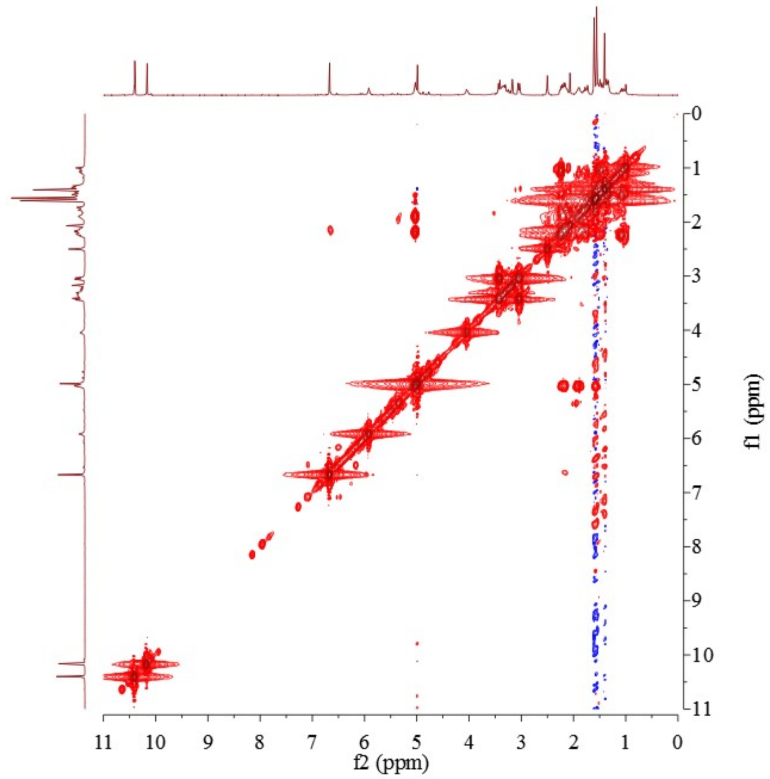
(a)


10.40
10.16
6.67
5.92
5.03
4.99
4.05
3.44
3.41
3.17
3.06
3.03
2.50
2.07
1.61
1.56
1.49
1.46
1.41
1.37
1.33
f1 (ppm)

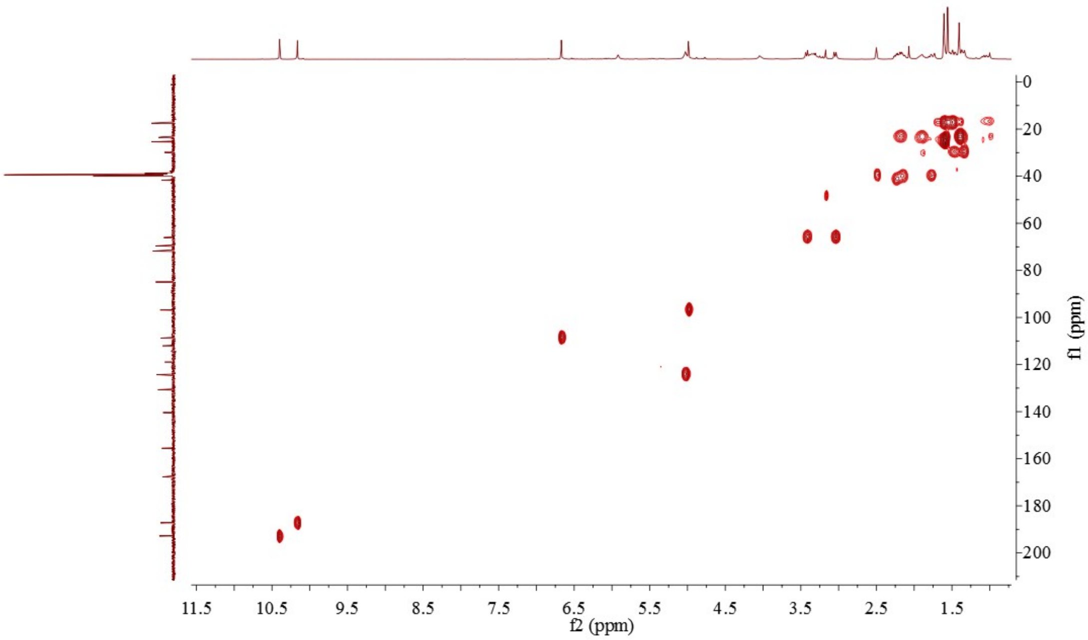
(b)


192.8
187.2
167.7
155.6
140.4
130.7
124.3
118.9
112.1
108.8
96.8
84.9
71.8
69.6
66.1
40.1
39.9
39.7
39.5
39.3
39.1
38.9
25.4
23.6
23.3
17.5
f1 (ppm)

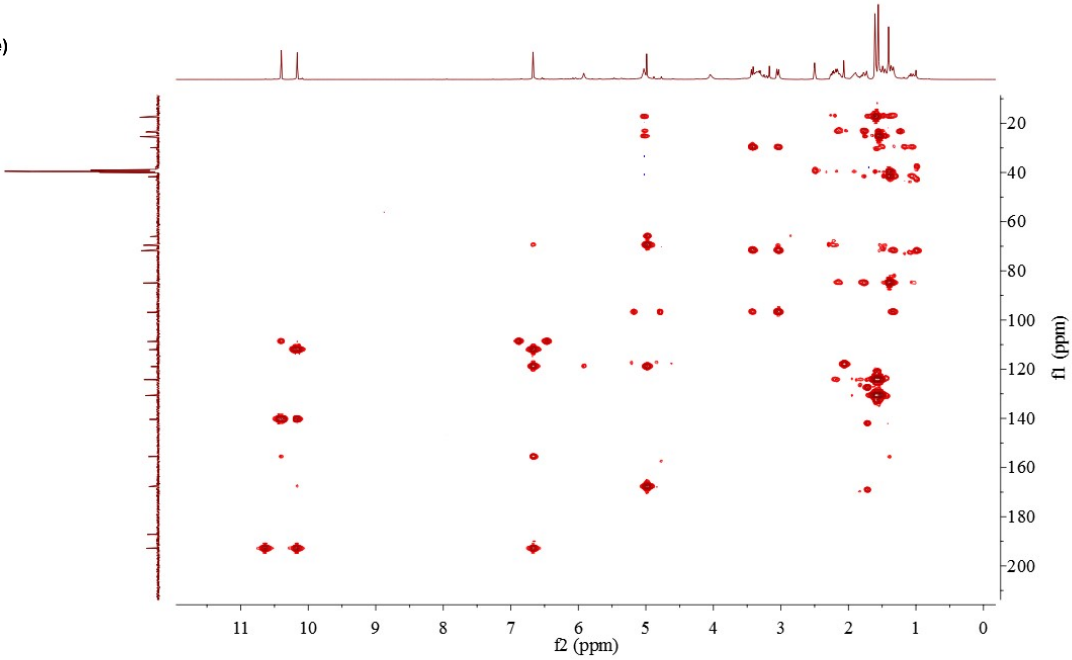
(c)



(d)



(e)



(f)

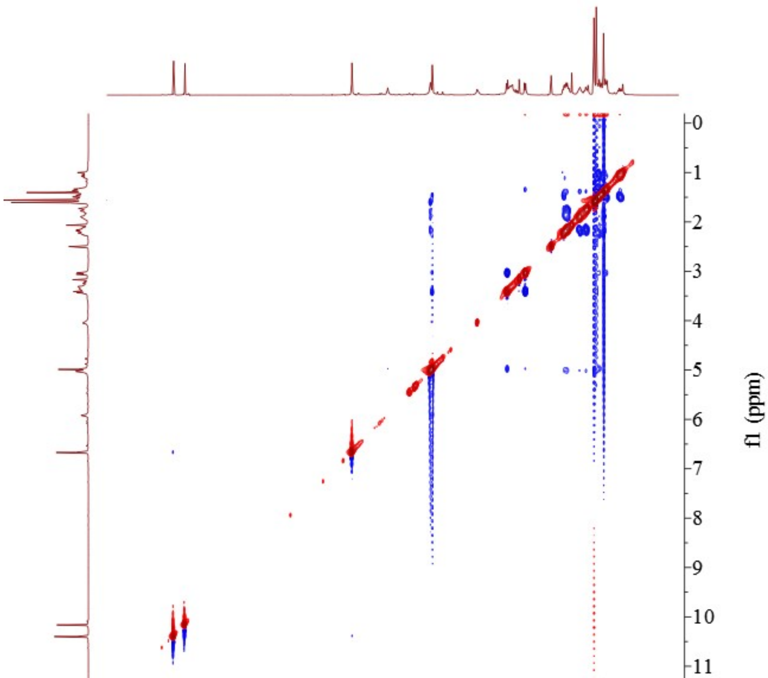
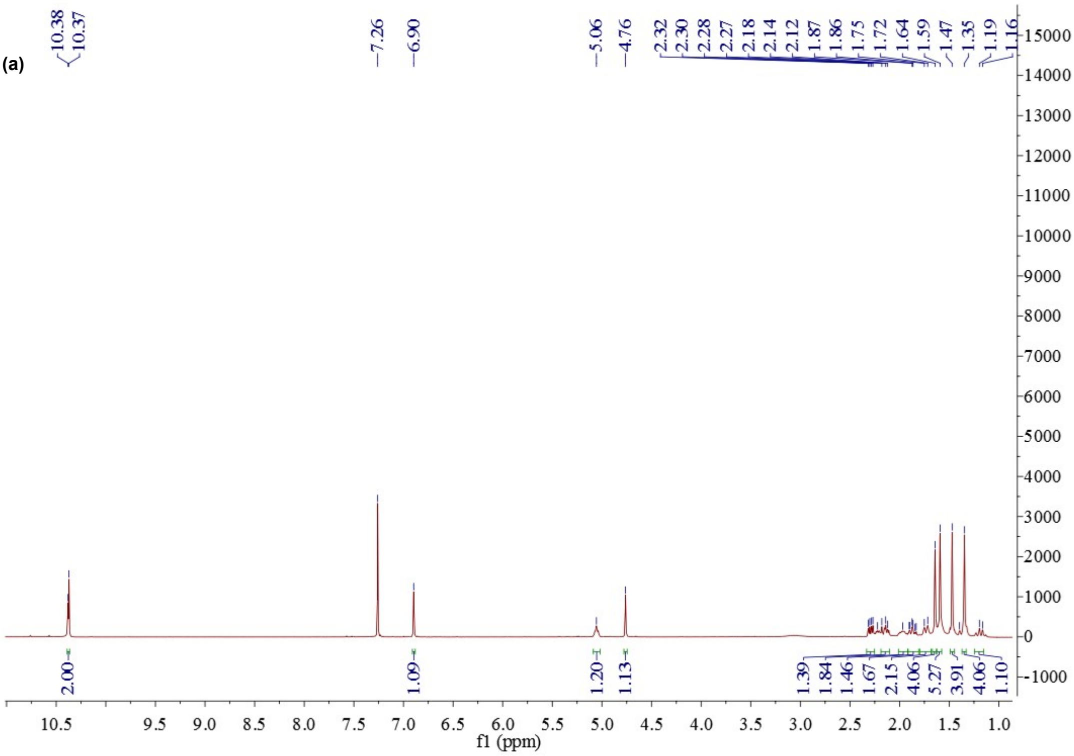


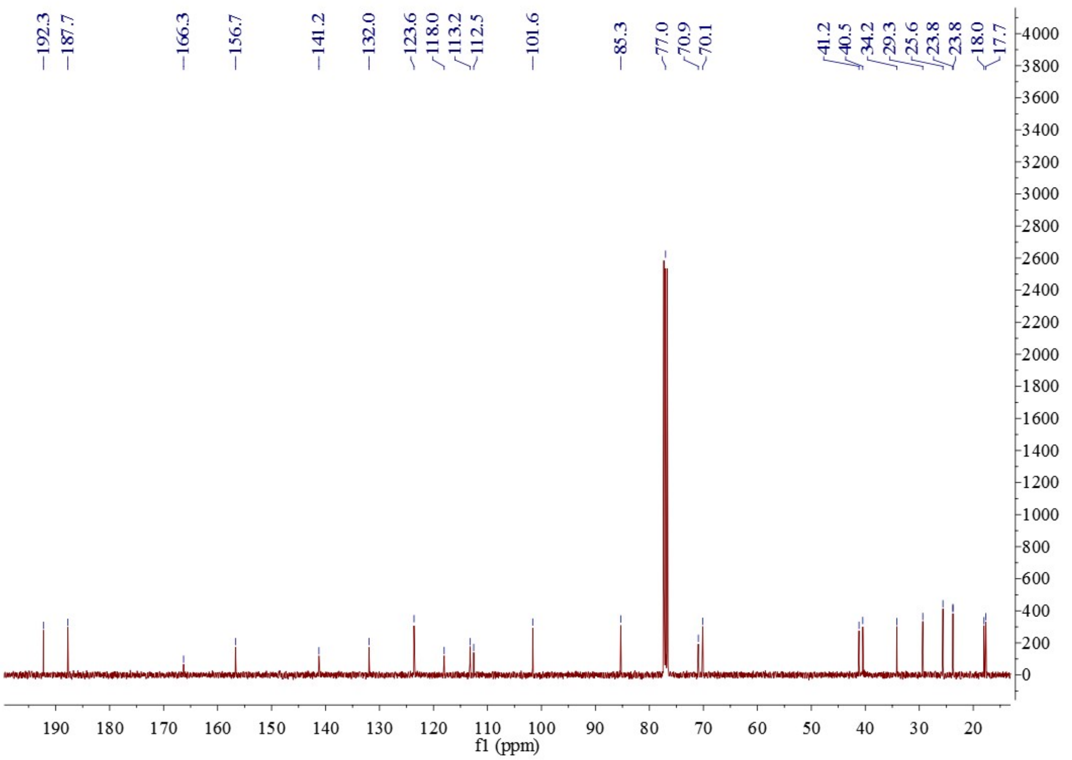
Fig. S11 NMR spectra of 6

(a) ^{1}H NMR spectrum in DMSO-d_6 at 400 MHz; (b) ^{13}C NMR spectrum in DMSO-d_6 at 100 MHz; (c) ^{1}H-^{1}H COSY spectrum in DMSO-d_6 at 400 MHz; (d) HSQC spectrum in DMSO-d_6 at 400 MHz; (e) HMBC spectrum in DMSO-d_6 at 400 MHz; (f) ROESY spectrum in DMSO-d_6 at 400 MHz.

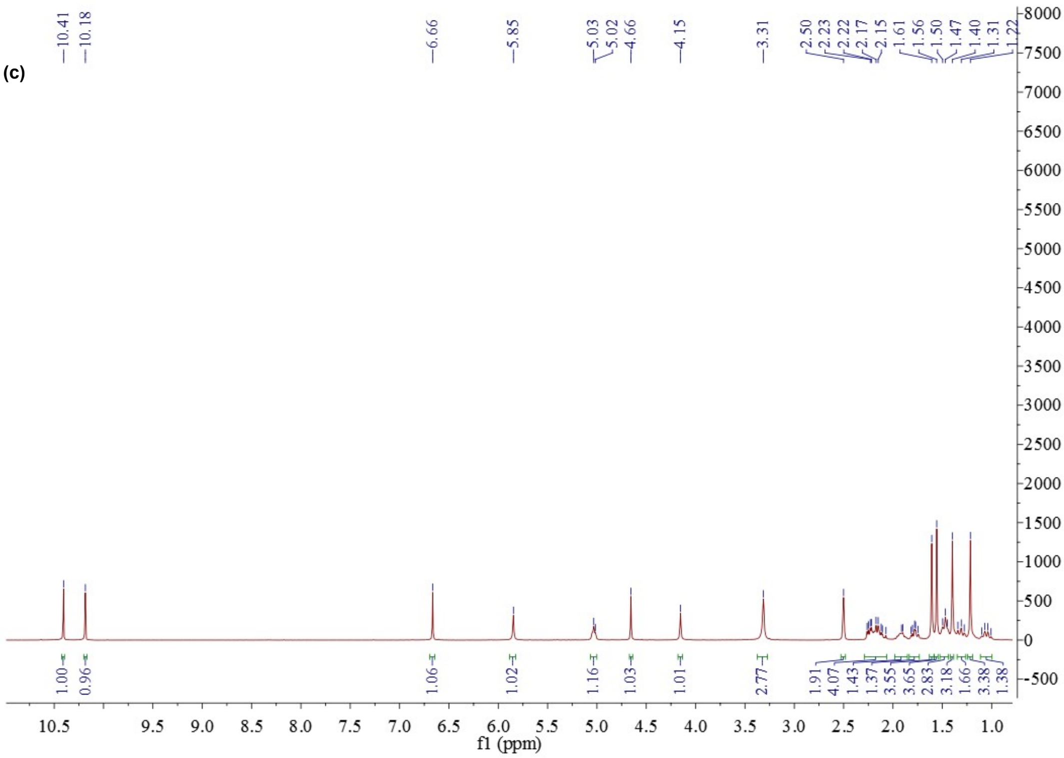
(a)


10.38
10.37
7.26
6.90
5.06
4.76
2.32
2.30
2.28
2.27
2.18
2.14
2.12
1.87
1.86
1.75
1.72
1.64
1.59
1.47
1.35
1.19
1.16
2.00
1.09
1.20
1.13
1.39
1.84
1.46
1.67
2.15
4.06
5.27
3.91
4.06
1.10
f1 (ppm)

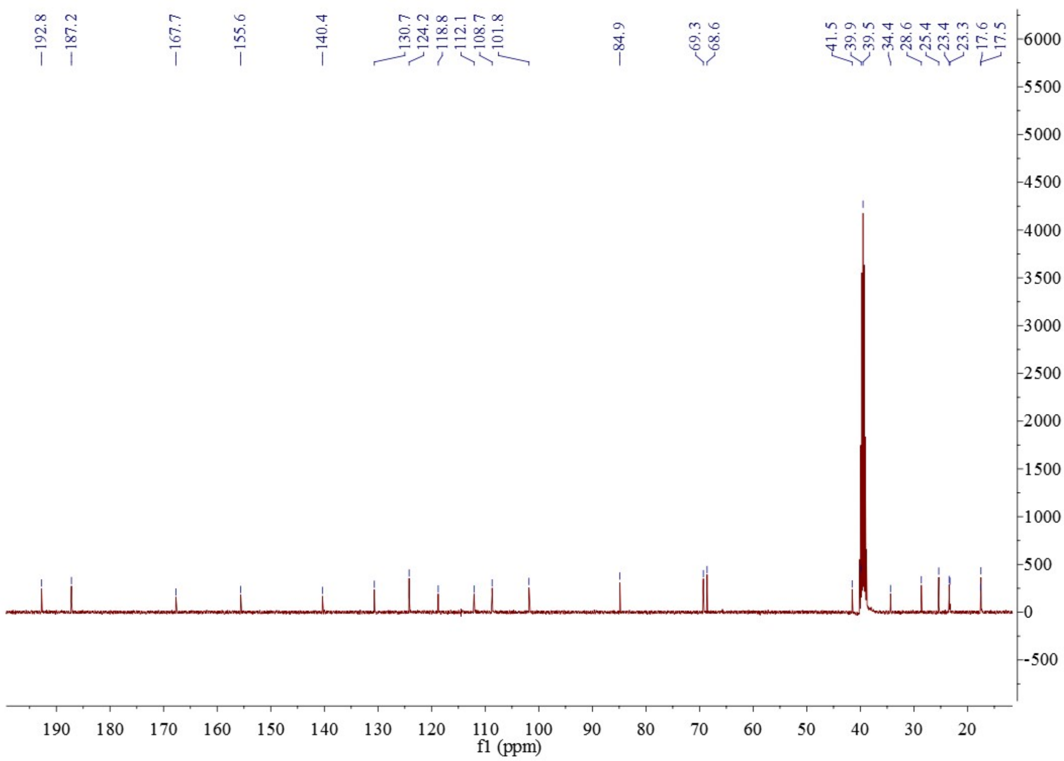
(b)


192.3
187.7
166.3
156.7
141.2
132.0
123.6
118.0
113.2
112.5
101.6
85.3
77.0
70.9
70.1
41.2
40.5
34.2
29.3
25.6
23.8
23.8
18.0
17.7
f1 (ppm)

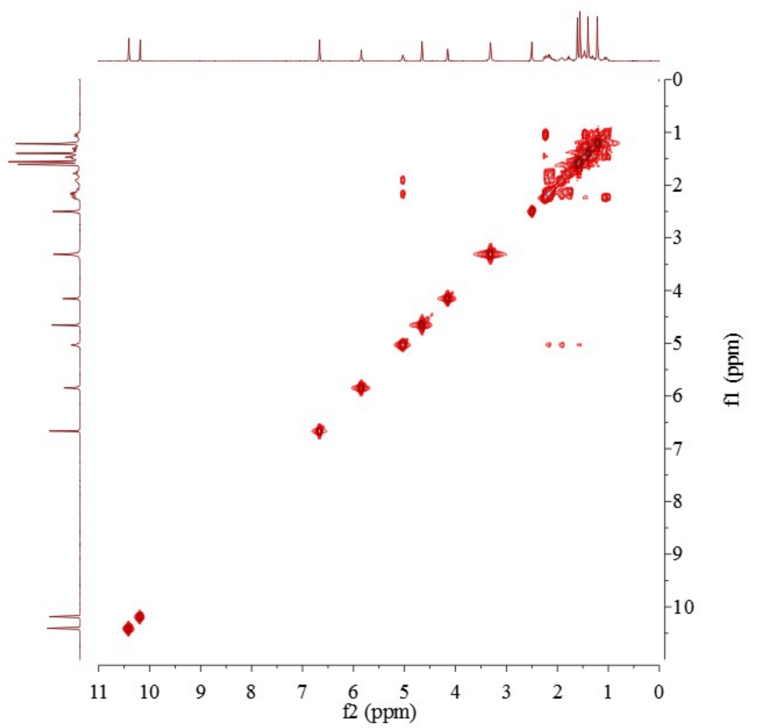
(c)


10.41
10.18
6.66
5.85
5.03
5.02
4.66
4.15
3.31
2.50
2.23
2.22
2.17
2.15
1.61
1.56
1.50
1.47
1.40
1.31
1.22
1.00
0.96
1.06
1.02
1.16
1.03
1.01
2.77
1.91
4.07
1.43
1.37
3.55
3.65
2.83
3.18
1.66
3.38
1.38
f1 (ppm)

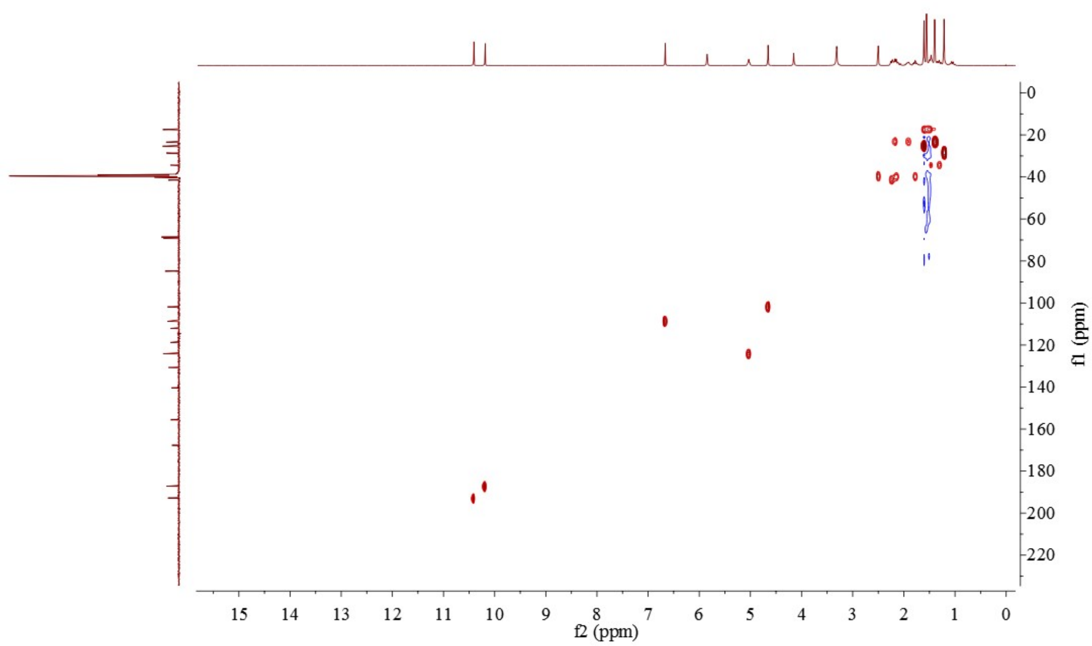
(d)


192.8
187.2
167.7
155.6
140.4
130.7
124.2
118.8
112.1
108.7
101.8
84.9
69.3
68.6
41.5
39.9
39.5
34.4
28.6
25.4
23.4
23.3
17.6
17.5
f1 (ppm)

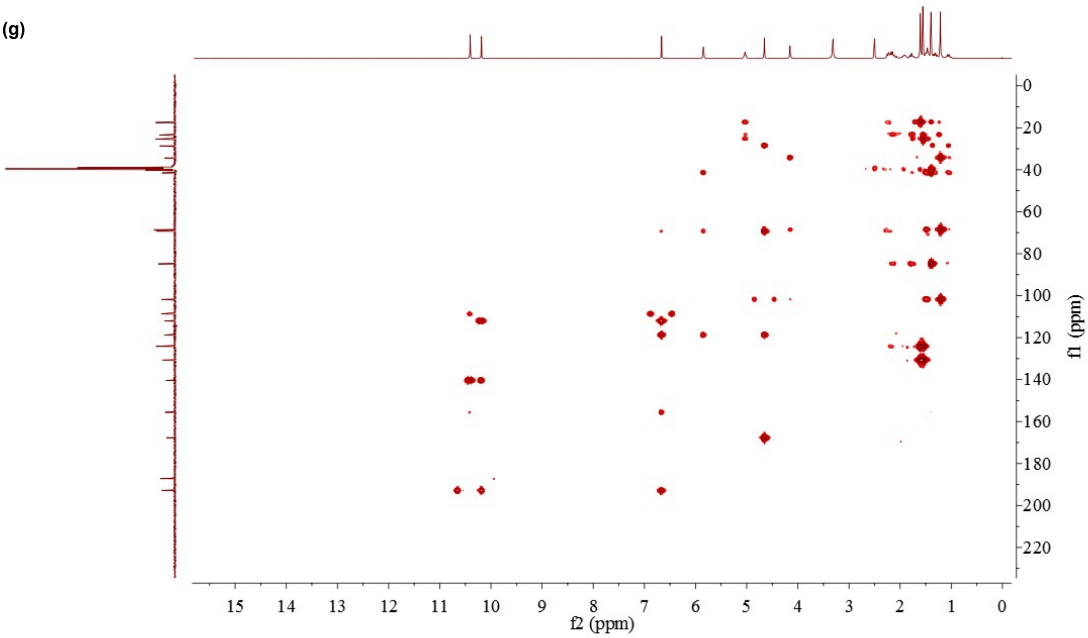
(e)



(f)



(g)



(h)

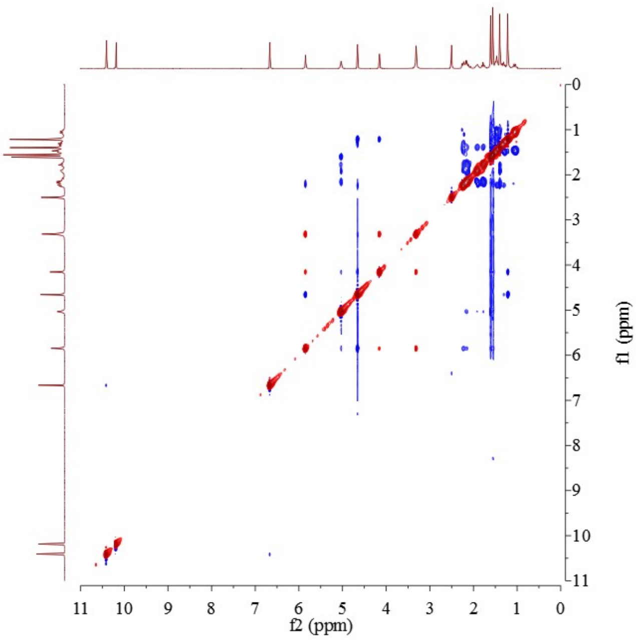
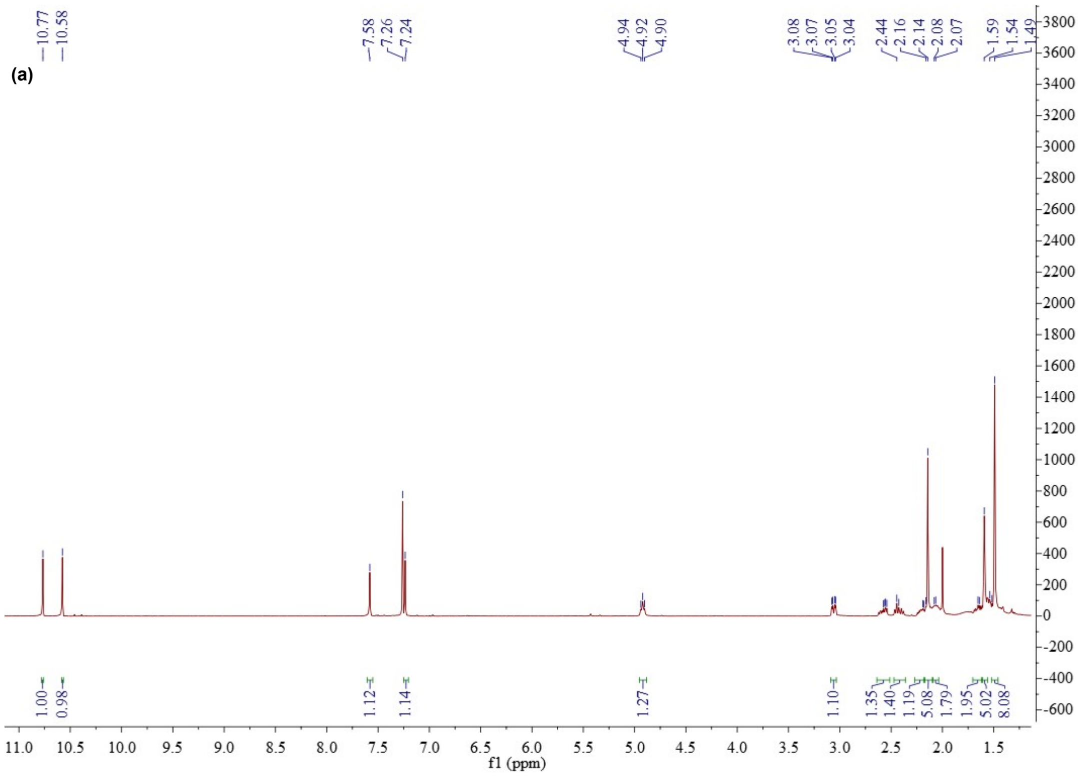


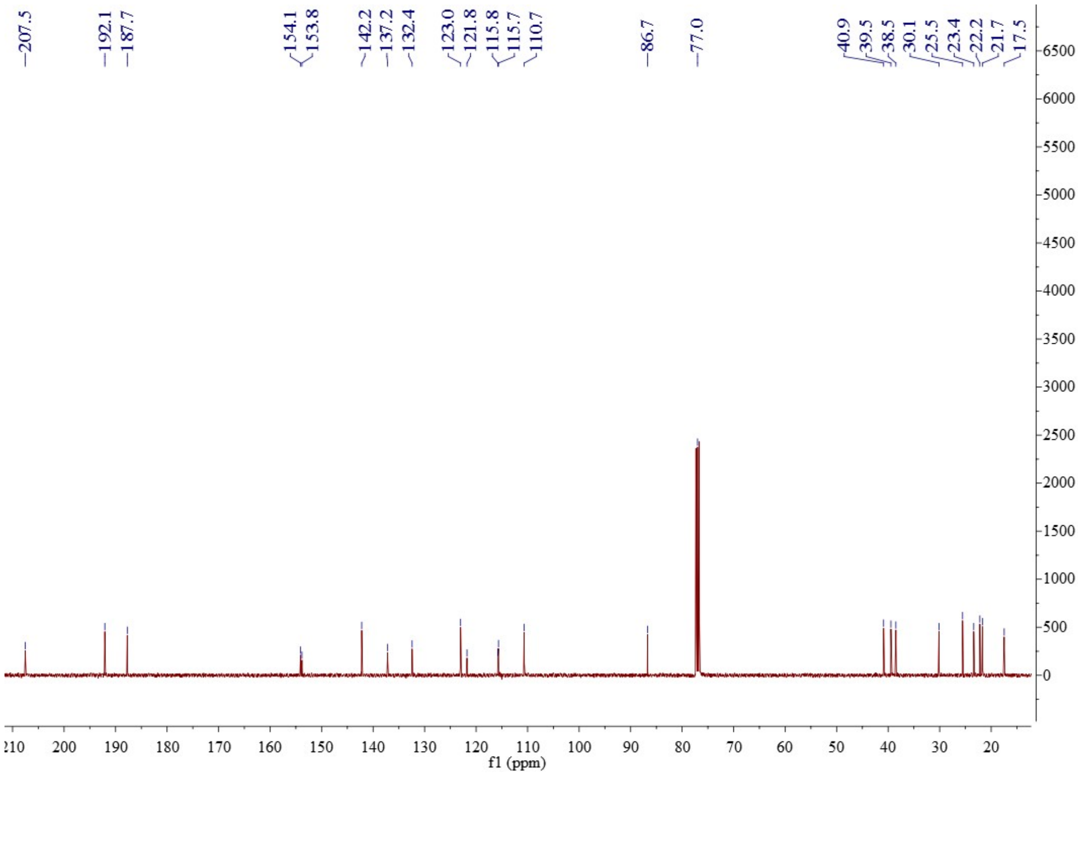
Fig. S12 NMR spectra of 7

(a) ^{1}H NMR spectrum in $CDCl_3$ at 400 MHz; (b) ^{13}C NMR spectrum in $CDCl_3$ at 100 MHz; (c) ^{1}H NMR spectrum in DMSO-d_6 at 400 MHz; (d) ^{13}C NMR spectrum in DMSO-d_6 at 100 MHz; (e) ^{1}H-^{1}H COSY spectrum in DMSO-d_6 at 400 MHz; (f) HSQC spectrum in DMSO-d_6 at 400 MHz; (g) HMBC spectrum in DMSO-d_6 at 400 MHz; (h) ROESY spectrum in DMSO-d_6 at 400 MHz.

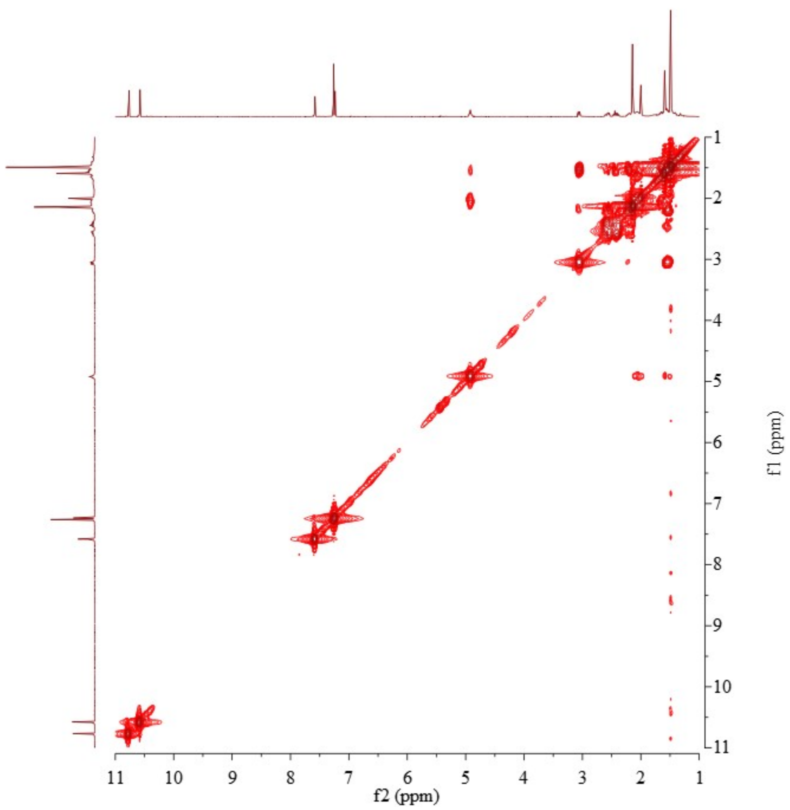
(a)


10.77
10.58
7.58
7.26
7.24
4.94
4.92
4.90
3.08
3.07
3.05
3.04
2.44
2.16
2.14
2.08
2.07
1.59
1.54
1.49
1.00
0.98
1.12
1.14
1.27
1.10
1.35
1.40
1.19
5.08
1.79
1.95
5.02
8.08
f1 (ppm)

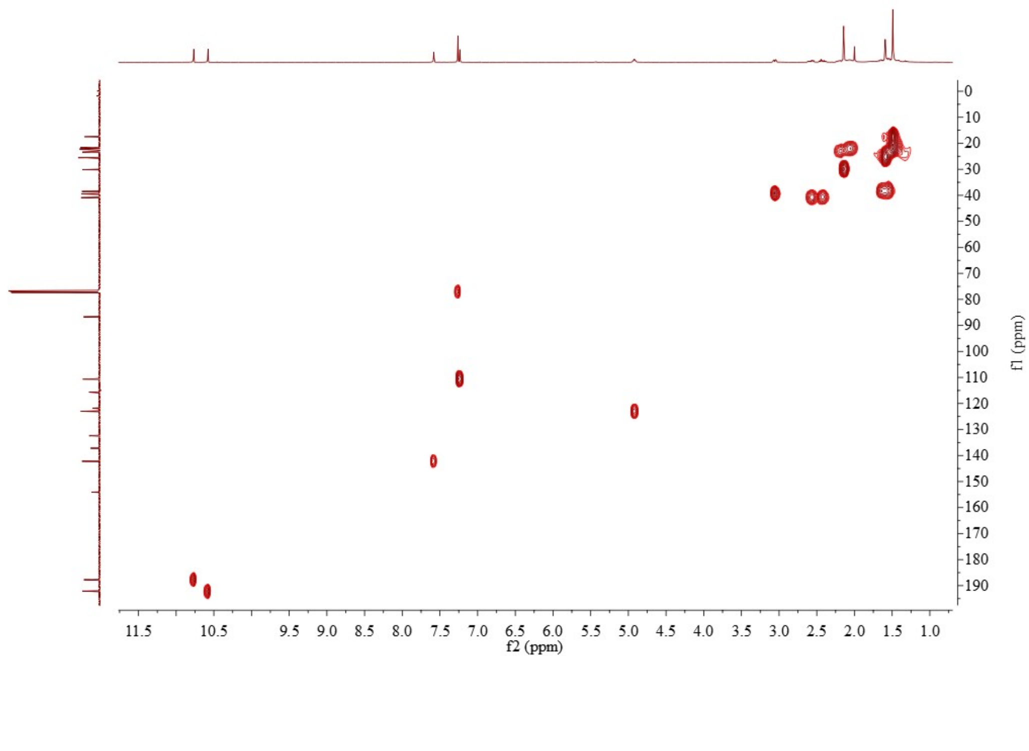
(b)


207.5
192.1
187.7
154.1
153.8
142.2
137.2
132.4
123.0
121.8
115.8
115.7
110.7
86.7
77.0
40.9
39.5
38.5
30.1
25.5
23.4
22.2
21.7
17.5
f1 (ppm)

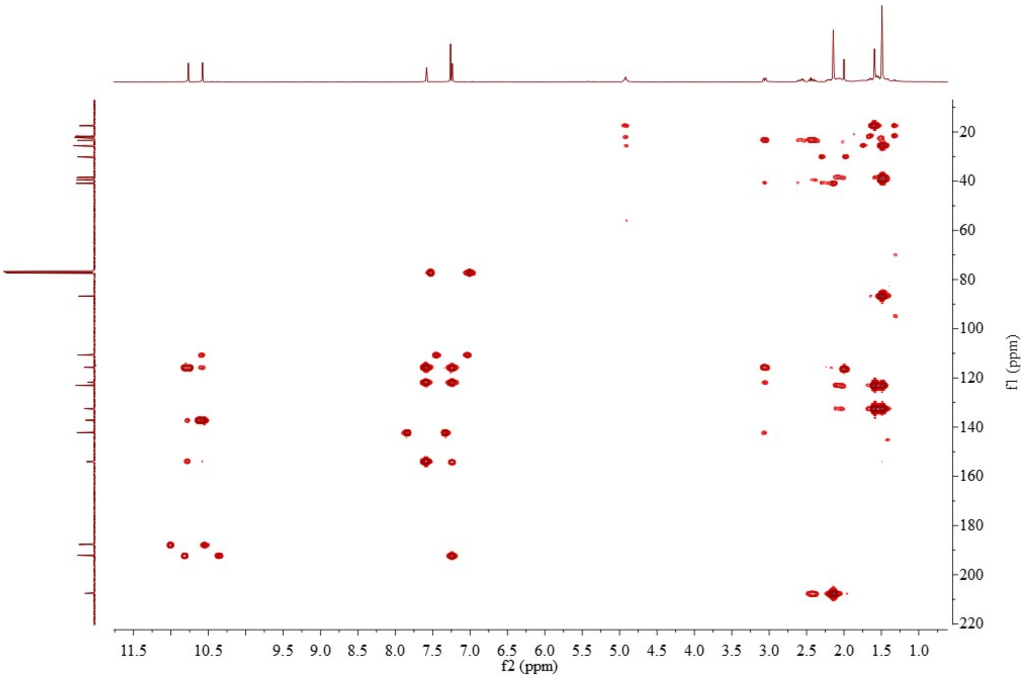
(c)



(d)



(e)



(f)

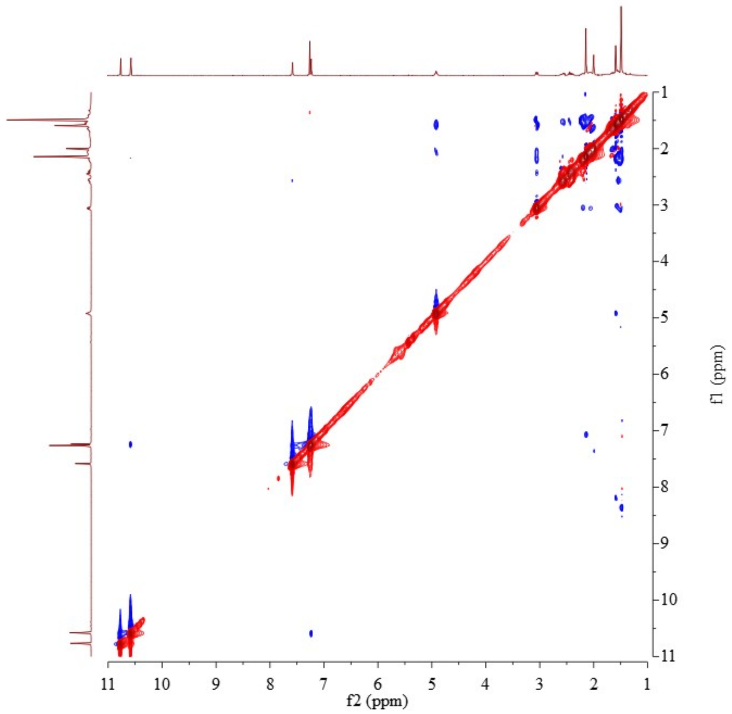


Fig. S13 NMR spectra of 8

(a) ^{1}H NMR spectrum in $CDCl_3$ at 400 MHz; (b) ^{13}C NMR spectrum in $CDCl_3$ at 100 MHz; (c) ^{1}H-^{1}H COSY spectrum in $CDCl_3$ at 400 MHz; (d) HSQC spectrum in $CDCl_3$ at 400 MHz; (e) HMBC spectrum in $CDCl_3$ at 400 MHz; (f) ROESY spectrum in $CDCl_3$ at 400 MHz.

Supplementary References

[1] Y. Matsuda, T. Wakimoto, T. Mori, T. Awakawa, I. Abe, *J Am Chem Soc* **2014**, *136*, 15326-15336.

[2] Y. M. Zheng, F. L. Lin, H. Gao, G. Zou, J. W. Zhang, G. Q. Wang, G. D. Chen, Z. H. Zhou, X. S. Yao, D. Hu, *Sci Rep* **2017**, *7*, 9250.