Supporting Information

***Rec. Nat. Prod*. 14:5 (2020) 312-318**

New Spectinabilin and Hexadienamide Derivatives from *Streptomyces* sp. S012

Zhiqiang Zhang[1], Xiaochun Zhang[1], Qianjin Kang[2] and Chunhua Lu[1,*]

[1]Key Laboratory of Chemical Biology (Ministry of Education), School of Pharmaceutical Sciences, Shandong University, Jinan 250012, China

[2]State key Laboratory of Microbial Metabolism, Shanghai Jiaotong University, Shanghai, 200240, China

Table of Contents page

Table S1. The NMR data of **1** (600 MHz, δ in ppm, J in Hz, In CD_3OD)

Pos.	δ_H (mult., J Hz)	δ_C	^1H-^1H COSY	HMBC
1	/	164.5s		
1a	3.94 (s)	56.5q		C-1
2	/	100.6s		
2a	1.75 (s)	7.0q		C-1, C-2, C-3
3	/	182.8s		
4	/	121.0s		
4a	1.81 (s)	9.3q		C-3, C-4, C-5
5	/	157.0s		
6	4.41 (t, 7.3)	74.4d	H-7	C-5, C-7, C-8a, C-8
7a	2.49 (dd, 15.0, 6.6)	38.2t	H-6	C-9, C-8, C-5, C-6, C-8a
7b	2.71 (dd, 15.0, 7.9)			
8	/	138.1s		
8a	3.54 (d, 13.1) 4.36 (d, 13.1)	69.5t		C-6, C-8, C-9
9	5.31 (s)	129.8d		C-10a, C-7, C-10, C-8a, C-11
10	/	45.2s		
10a	1.24 (s)	29.0q		C-10, C-15, C-9
11	5.25 (s)	126.8d	H-12a	C-12a, C-10, C-15, C-13, C-9
12	/	131.9s		
12a	1.82 (s)	21.6q		C-13, C-11, C-12
13	5.87 (s)	124.7d	H-14a	C-14a, C-15, C-11, C-12,
14	/	137.1s		
14a	1.66 (s)	22.8q		C-13, C-14, C-15
15	3.19 (s)	57.4d		C-14a, C-10a, C-10, C-11, C-13, C-16, C-17, C-21
16	/	149.5s		
17	7.39 (d, 8.5)	131.9d	H-18	C-15, C-18, C-21, C-16
18	8.07 (d, 8.5)	123.5d	H-17	C-19, C-20
19		148.4s		
20	8.07 (d, 8.5)	123.5d	H-21	
21	7.39 (d, 8.5)	131.9d	H-20	

Table S2. The NMR data of **2** (600 MHz, δ in ppm, J in Hz, in C_5D_5N)

Pos.	δ_H (mult., J Hz)	δ_C	^1H-^1H COSY	HMBC
1	/	162.1s		
1a	3.85 (s)	55.3q		C-1
2	/	99.3s		
2a	2.01(s)	7.3q		C-1, C-2, C-3
3	/	180.0s		
4	/	120.3s		
4a	2.18 (s)	9.5q		C-3, C-4, C-5
5	/	155.8s		
6	5.28 (dd, 6.1, 7.3)	73.5d	H-7	C-5, C-7, C-8, C-8a, C-9
7a	3.01(dd, 5.1, 15.8)	38.2t		C-5, C-6, C-8, C-8a, C-9
7b	3.08 (dd, 7.4, 14.7)			
8	/	139.7s		
8a	5.04 (m) 4.87 (d, 14.0)	70.8t		C-6, C-8, C-9
9	6.22 (s)	126.9d		C-7, C-8a, C-10a, C-10
10	/	134.9s		
10a	2.10 (s)	18.4q		
11	6.06 (s)	136.0d		C-9, C-10a, C-13
12	/	135.5s		
12a	2.08(s)	17.8q		
13	6.19 (s)	135.5d	H-14a	C-11, C-12a, C-14a, C-15
14	/	139.9s		
14a	2.10(s)	19.7q		
15	6.62 (s)	128.6d		C-13, C-14a, C-17, C-21
16	/	145.0s		
17	7.51 (d, 8.8)	129.9d	H-18	C-18, C-21
18	8.27 (d, 8.8)	123.7d	H-17	C-16, C-20
19	/	146.7s		
20	8.27 (d, 8.8)	123.7d	H-21	C-16, C-18
21	7.51 (d, 8.8)	129.9d	H-20	C-19, C-21

Table S3. The NMR data of **3** (400 MHz, δ in ppm, J in Hz, in C_5D_5N.)

Pos.	**3**			
	δ_H	δ_C	HMBC	COSY
1	/	166.6s	/	/
2	5.96 (d, 11.2)	120.1d	C-1, C-4	H-3
3	6.49 (t, 11.2)	141.7d	C-1, C-5	H-4
4	8.18 (dd, 15.0, 12.8)	130.2d	/	H-3, H-5
5	5.91 (dd, 15.0, 6.7)	137.8d	C-6, C-3	H-6
6	1.68 (d, 6.7)	18.8q	C-4, C-5	H-5
1′	1.31 (d, 6.8)	20.7q	C-2′, C-3′	H-2′
2′	5.22 (m)	44.1d	C-3′, C-4′	H-1′, H-3′
3′	6.91 (d, 9.1)	144.4d	C-5′, C-6′	H-2′
4′	/	128.5s		
5′	/	169.1s		
5′a	3.65 (s)	52.1q	C-5′	
6′	2.10 (s)	13.3q	C-4′, C-3′, C-5′	

Table S4. The NMR data of **4** (400 MHz δ in ppm, J in Hz, in CD_3OD)

Pos.	δ_H (δ in ppm, J in Hz)	δ_C	COSY	HMBC
1	/	168.3s		
2	5.58 (d, 11.4)	119.3d		C-1, C-4
3	6.43 (t, 11.4)	142.7d	H-2	C-1, C-5
4	7.43 (dt, 14.8, 11.4)	129.9d	H-3	
5	6.05 (dd, 14.8, 6.8)	139.1d	H-4	C-3, C-6
6	1.84 (dd, 6.8,1.0)	18.8q	H-5	C-4, C-5
1′	1.26 (d, 6.8)	20.7q	H-2′	C-3′
2′	4.81 (dq, 8.6, 6.8)	44.4d		C-4′, C-3′, C-1′
3′	6.25 (dd, 8.8,1.3)	139.2d	H-2′	C-5′, C-6′, C-1′
4′	/	132.4s		
5′	/	174.3s		
6′	1.93 (d, 1.2)	13.3q		C-4′, C-3′, C-5′

Table S5. The NMR and optical rotation data of **2** (C_5D_5N) and spectinabilin ($CDCl_3$)

.	**2**		spectinabilin※	
NO.	δ_H (mult., *J* Hz)[a]	δ_C	δ_H (mult., *J* Hz)[b]	δ_C
1	/	162.1 (C)		162.1 (C)
1a	3.85 (s)	55.3 (CH_3)	3.99 (s)	55.3
2	/	99.3(C)		99.1(C)
2a	2.01 (s)	7.3 (CH_3)	1.86(s)	6.9 (CH_3)
3	/	180.0 (C)		180.6 (C)
4	/	120.3 (C)		119.9 (C)
4a	2.18 (s)	9.5 (CH_3)	2.04(s)	9.4 (CH_3)
5	/	155.8 (C)		155.2(C)
6	5.28 (dd, *J* = 6.1, 7.3 Hz)	73.5 (CH)	5.20 (t, *J* = 7.0 Hz)	73.3 (CH)
7a	3.01(dd, *J* = 5.1, 15.8 Hz)	38.2 (CH_2)	3.04 (qd, *J* = 7.0, 15.0 Hz)	38.3 (CH_2)
7b	3.09 (dd, *J* = 7.4, 14.7 Hz)			
8	/	139.7 (C)		139.4 (C)
8a	5.04 (m) 4.87 (d, *J* =14.0 Hz)	70.8 (CH)	4.86 (qb *J* = 13 Hz)	70.1 (CH)
9	6.22 (s)	126.9 (CH)	6.54(s)	128.1 (CH
10	/	134.9 (C)		134.0(C)
10a	2.10 (s)	18.4 (CH_3)	2.06 (s)	19.5 (CH_3)
11	6.06 (s)	136.0 (CH)	6.13(s)	135.3 (CH)
12	/	135.5(C)		135.6(C)
12a	2.08 (s)	17.8 (CH_3)	2.09(s)	19.6 (CH_3)
13	6.19, s	135.5 (CH)	6.08(s)	134.4 (CH)
14	/	139.9 (C)		
14a	2.10 (s)	19.7 (CH_3)	2.13(s)	17.9 (CH_3)
15	6.62 (s)	128.6 (CH)	5.92(s)	126.8 (CH)
16	/	145.0 (C)		144.7 (C)
17	7.51 (d, *J* = 8.8 Hz)	129.9 (CH)	7.51 (d, *J* = 9.0 Hz)	129.5 (CH)
18	8.27 (d, *J* = 8.8 Hz)	123.7 (CH)	8.02 (d, *J* = 9.0 Hz)	123.5 (CH)
19	/	146.7(C)		145.9(C)
20	8.27 (d, *J* = 8.8 Hz)	123.7 (CH)	7.51 (d, *J* = 9.0 Hz)	123.5 (CH)
21	7.51 (d, *J* = 8.8 Hz)	129.9 (CH)	8.02 (d, *J* = 9.0 Hz)	145.9(C)
$[\alpha]_D$	- 40 (c 0.1, $CHCl_3$)		+60 (c 5.0, $CHCl_3$) ※	

※The NMR and $[\alpha]_D$ data of spectinabilin was reported by Kakinuma et al., Spectinabilin, a new nitro-containing metabolite isolated from *Streptomyces spectabilis*. *Tetrahedron*, 1976, **32**(2): 217-222

[a]. the NMR data of **2** was recorded on a Bruker DRX-600 MHz NMR spectrometer

[b]. The NMR data were recorded at a Varian XL 100 MHz spectrometer.

Table S6. The NMR data of **4** (CD_3OD) and sarmentosamide (CD_3OD)

No	**4**		sarmentosamide※	
	δ_H[a]	δ_C[b]	δ_H[a]	δ_C[b]
1	/	168.3 (C)	/	168.2 (C)
2	5.58 (d, *J* = 11.4 Hz)	119.3 (CH)	5.55 (dd, *J* = 11.8, 0.7 Hz)	119.1 (CH)
3	6.43 (t, *J* = 11.4 Hz)	142.7 (CH)	6.39 (dd, *J* = 11.8, 11.4 Hz)	142.6 (CH)
4	7.43 (dt, *J* = 14.8, 11.4 Hz)	129.9 (CH)	7.39 (dt, *J* = 15.1, 11.4 Hz)	129.8 (CH)
5	6.05 (dd, *J* =14.8, 6.8 Hz)	139.1 (CH)	5.99 (dq, *J* =15.1, 6.8 Hz)	138.9 (CH)
6	1.84 (dd, *J* = 6.8, 1.0 Hz)	18.8 (CH_3)	1.82 (dd, *J* = 6.8, 1.7 Hz)	18.6 (CH_3)
1′	1.26 (d, *J* = 6.8 Hz)	20.7 (CH_3)	1.24 (d, *J* = 7.0 Hz)	20.5 (CH_3)
2′	4.81 (dq, J = 8.6, 7.0 Hz)	44.4 (CH)	4.77 (dq, J = 8.8, 7.0 Hz)	44.3 (CH)
3′	6.25 (dd, *J* = 8.8,1.3 Hz)	139.2 (CH)	6.22 (dd, *J* = 8.8,1.5 Hz)	139.0 (CH)
4′	/	132.4 (C)	/	132.3 (C)
5′	/	174.3 (C)	/	174.2 (C)
5′a				
6′	1.93 (d, *J* =1.2 Hz)	13.3 (CH_3)	1.92 (d, *J* =1.5 Hz)	13.2 (CH_3)

※The NMR data of sarmentosamide was reported by Kitani et al., *Natural Product Research*, 2013, 27(3): 226-231.

[a]. the ^1H NMR data were recorded at 400 MHz.

[b]. The ^{13}C NMR data were recorded at 100 MHz.

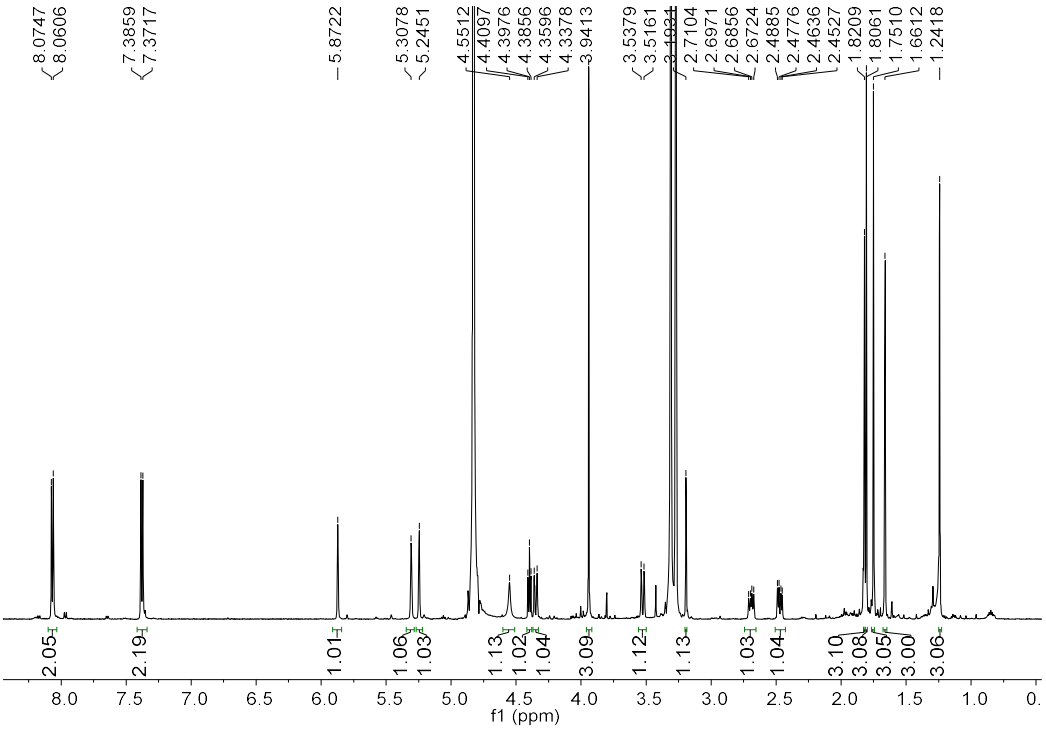

Figure S1: The ^{1}H NMR spectrum of compound **1 i**n CD_3OD at 600MHz

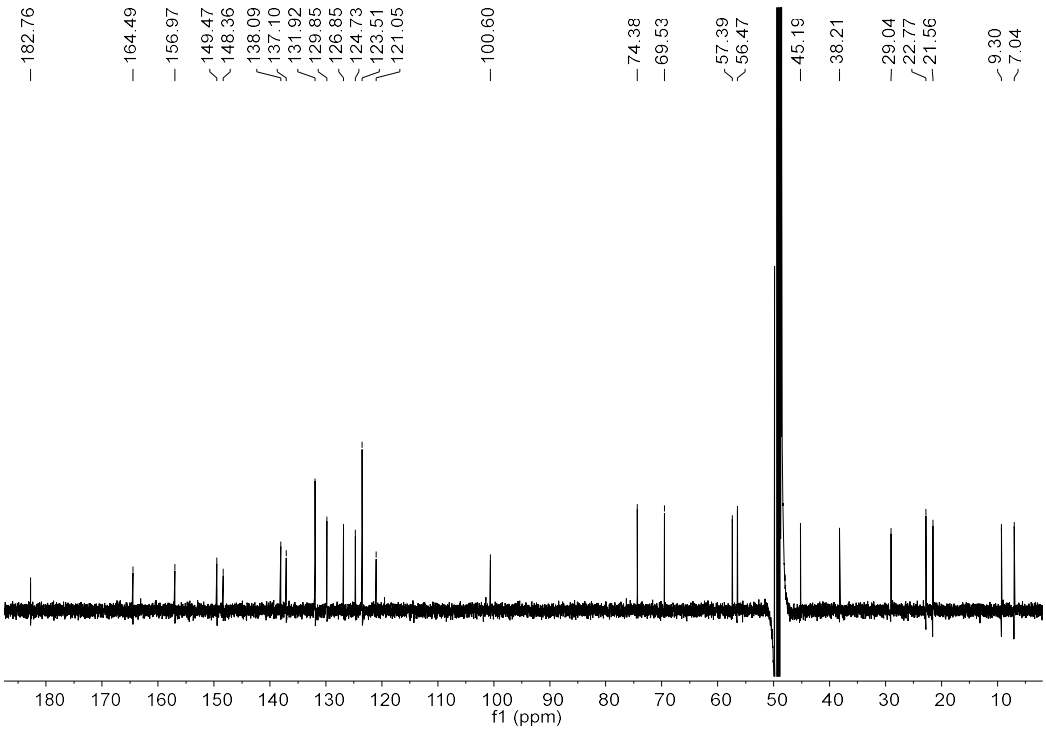

Figure S2: The ^{13}C NMR spectrum of compound **1** n CD_3OD at 150 MHz

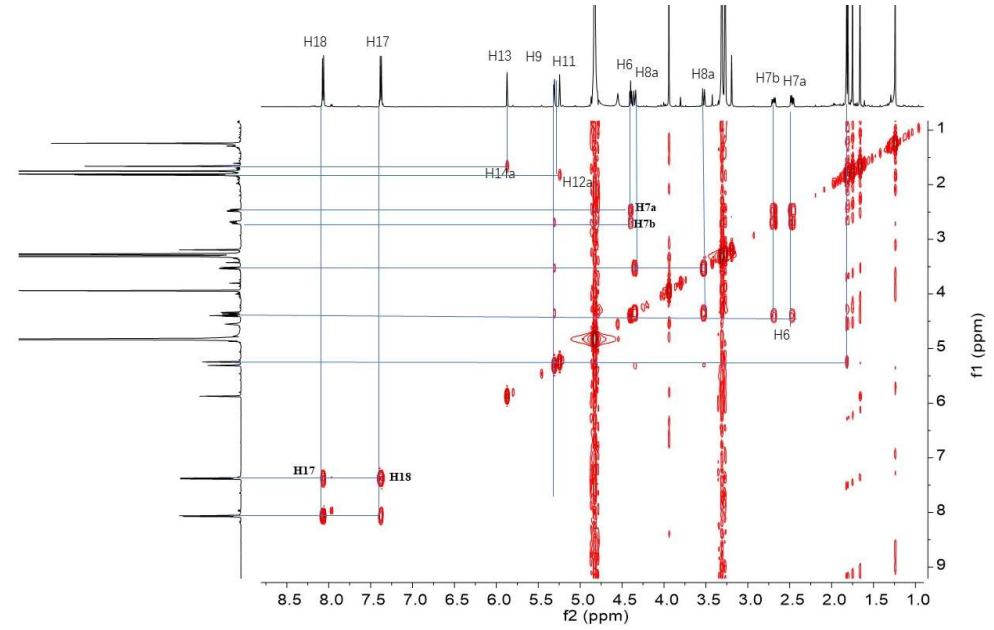

Figure S3: The ^{1}H-^{1}H COSY spectrum of compound **1**

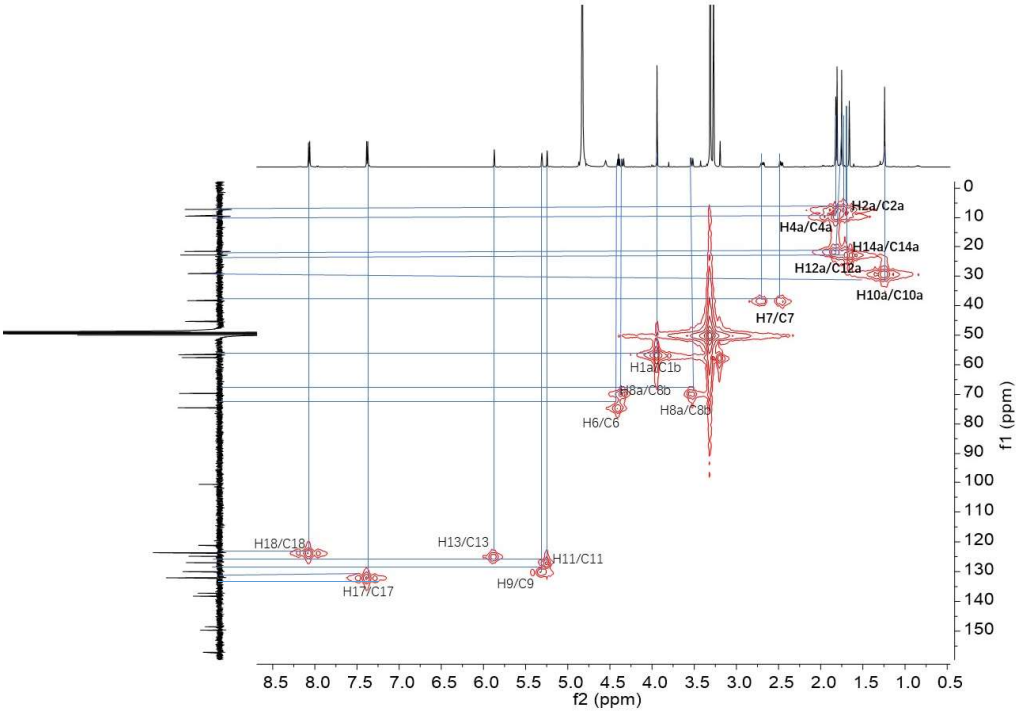

Figure S4: The HMQC spectrum of compound **1**

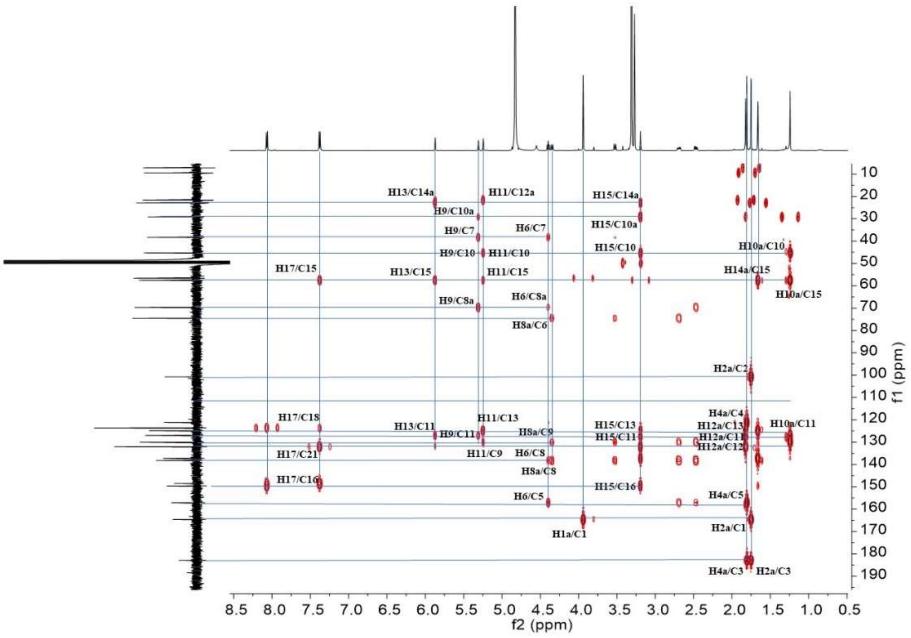

Figure S5: The HMBC spectrum of compound **1**

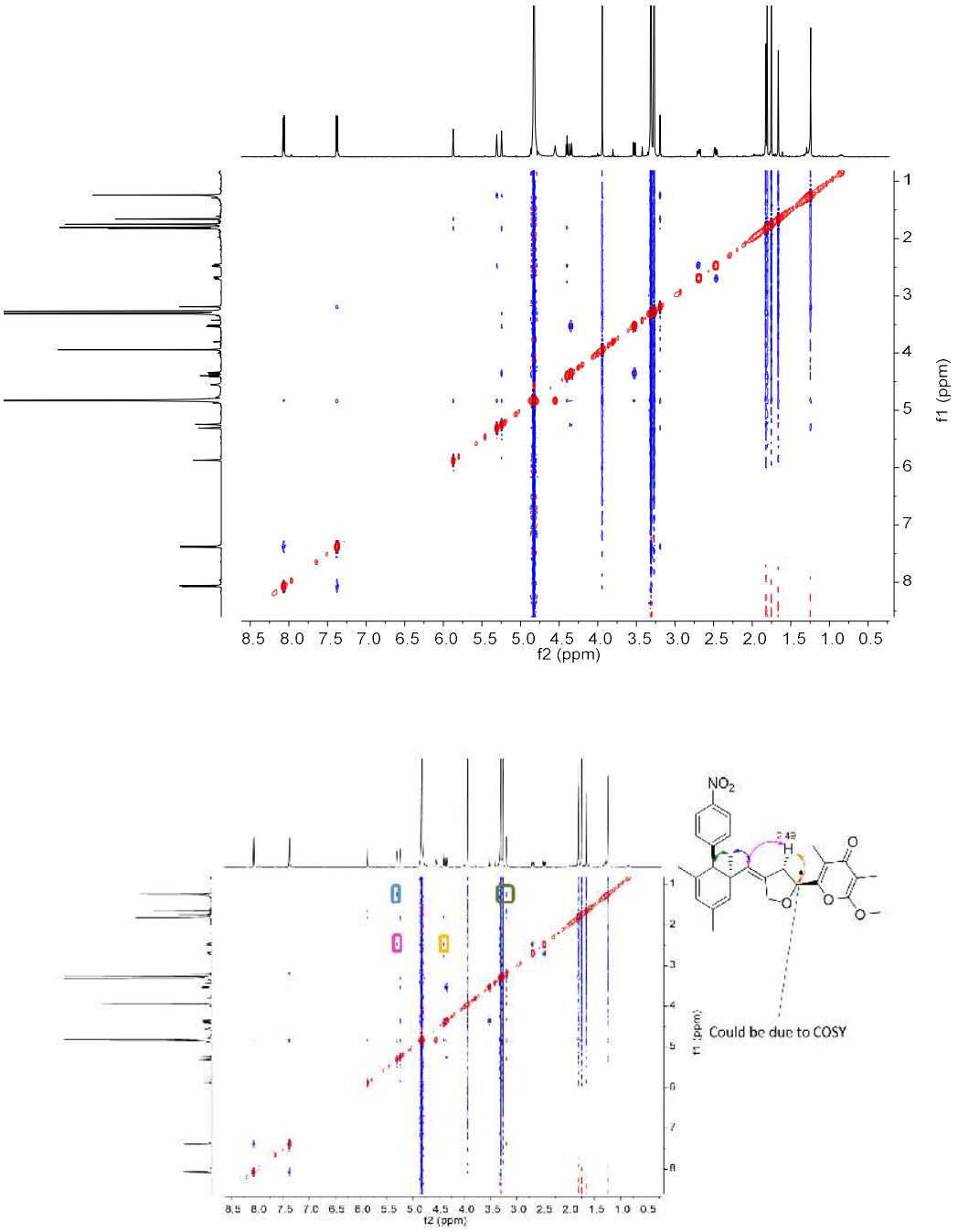

Figure S6: The ROESY spectrum of compound **1**

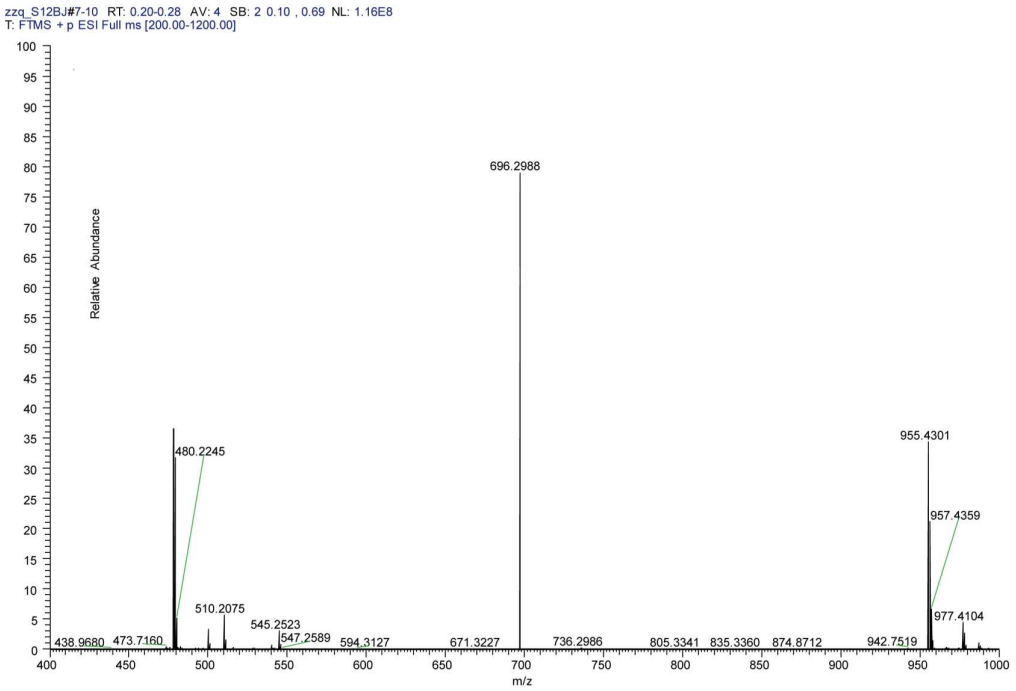

Figure S7: The HRESIMS spectrum of compound **1**

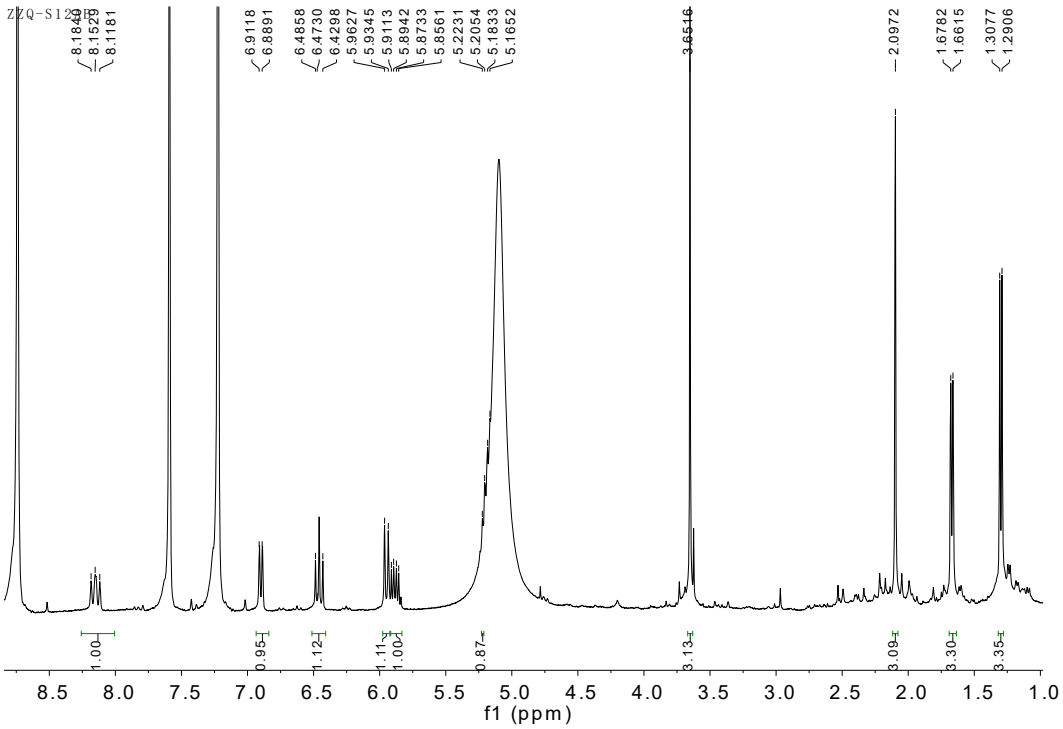

Figure S8: The ^{1}H NMR spectrum of compound **3** 1n C_5D_5N at 400 MHz

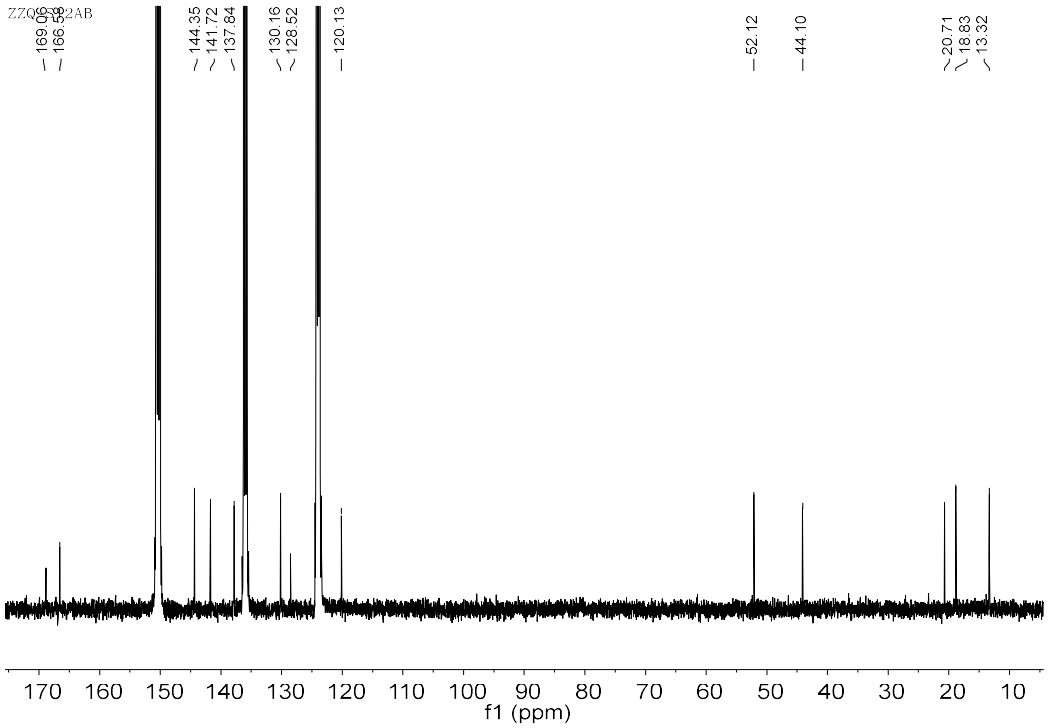

Figure S9: The ^{13}C NMR spectrum of compound **3 i**n C_5D_5N at 100 MHz

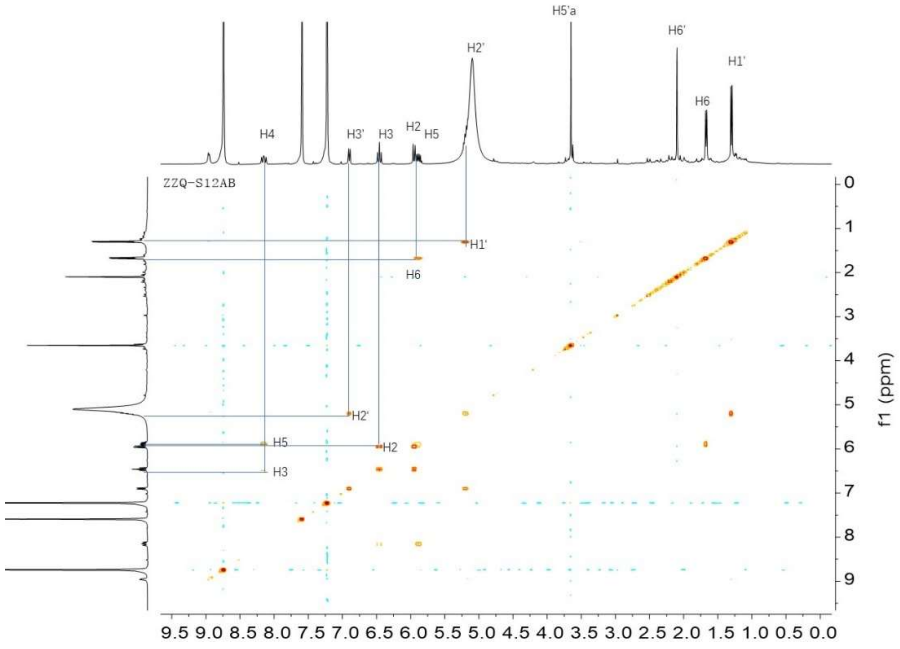

Figure S10: The ^{1}H-^{1}H COSY spectrum of compound **3**

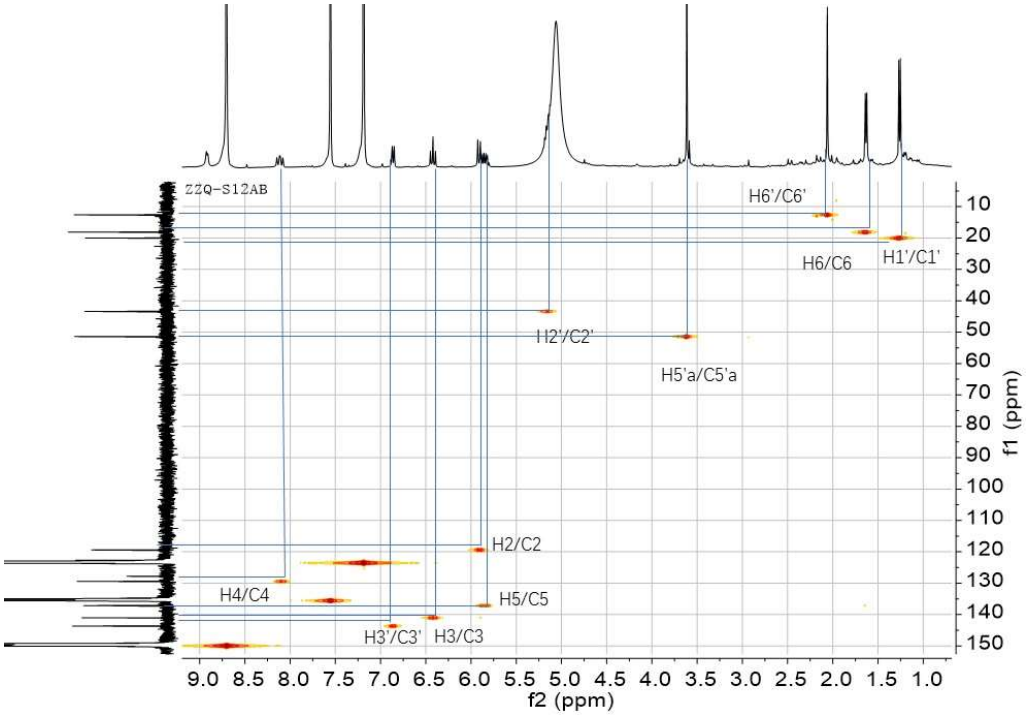

Figure S11: The HMQC spectrum of compound **3**

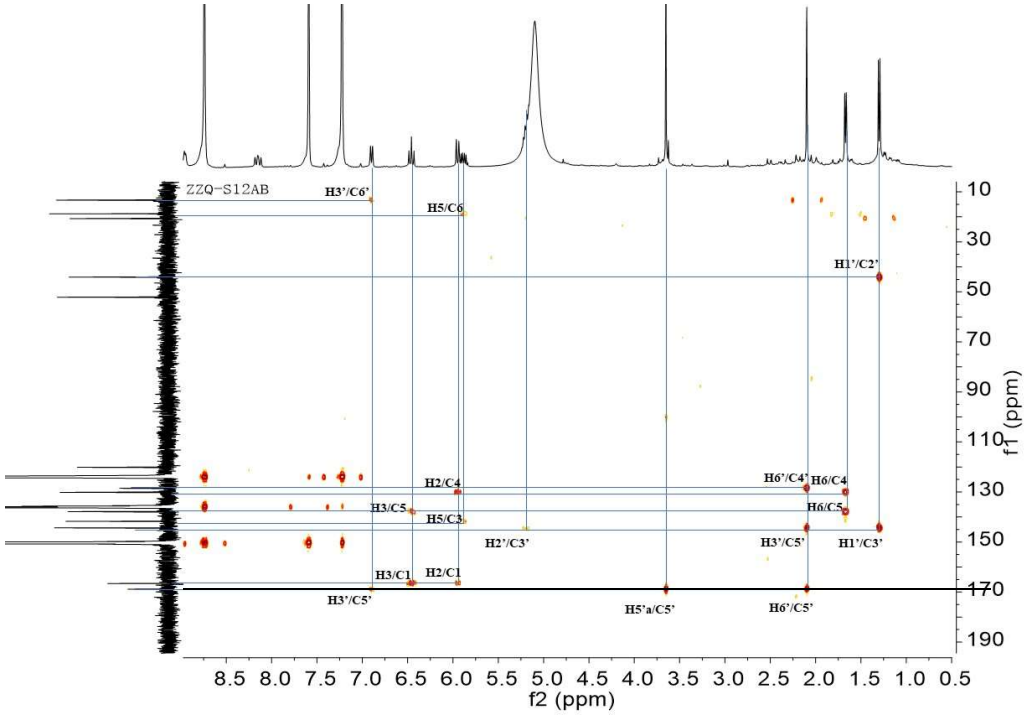

Figure S12: The HMBC spectrum of compound **3**

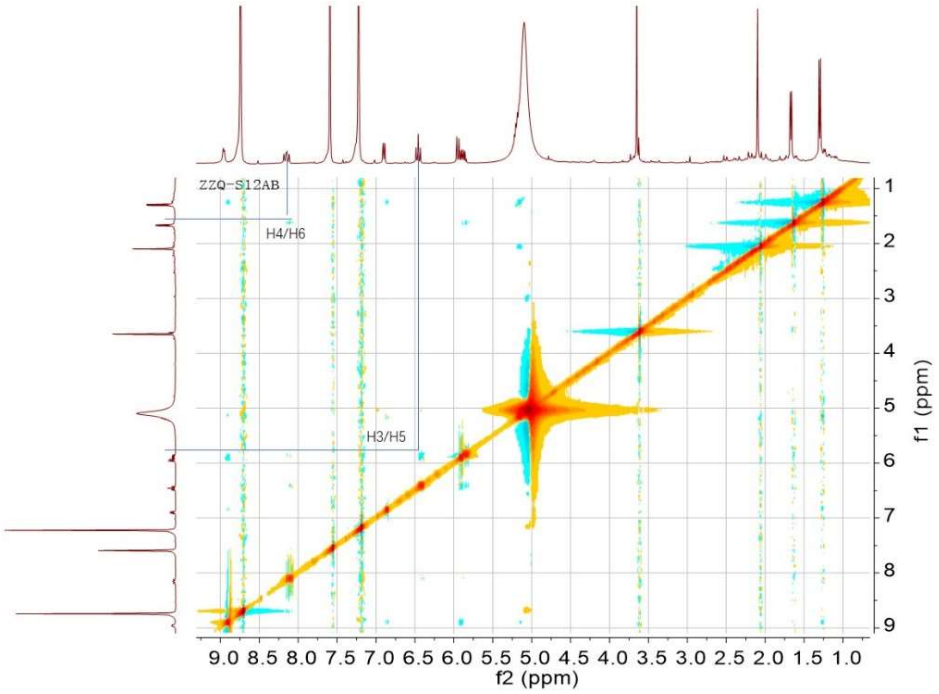

Figure S13: The ROESY spectrum of compound **3**

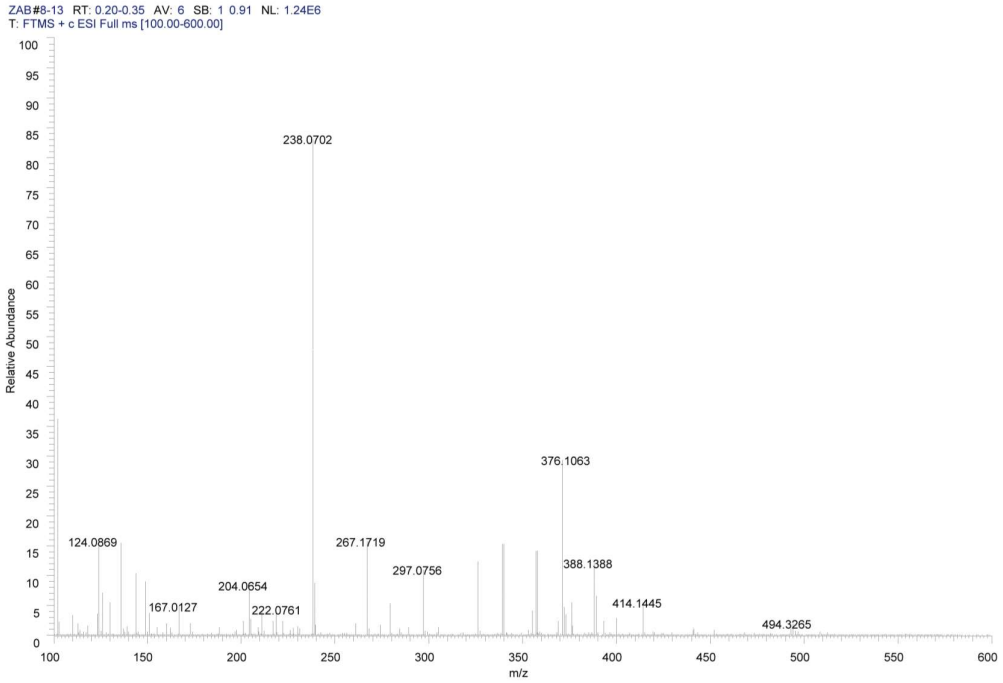

Figure S14: The HRESIMS spectrum of compound **3**

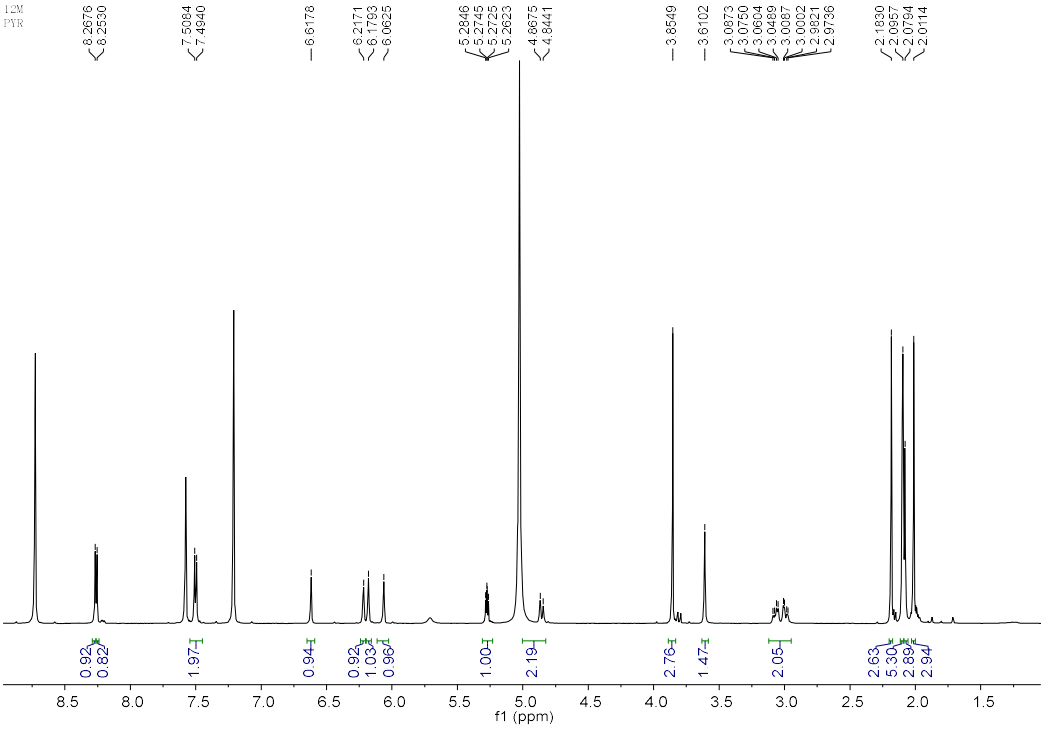

Figure S15: The ^{1}H NMR spectrum of compound **2 i**n C_5D_5N at 600 MHz

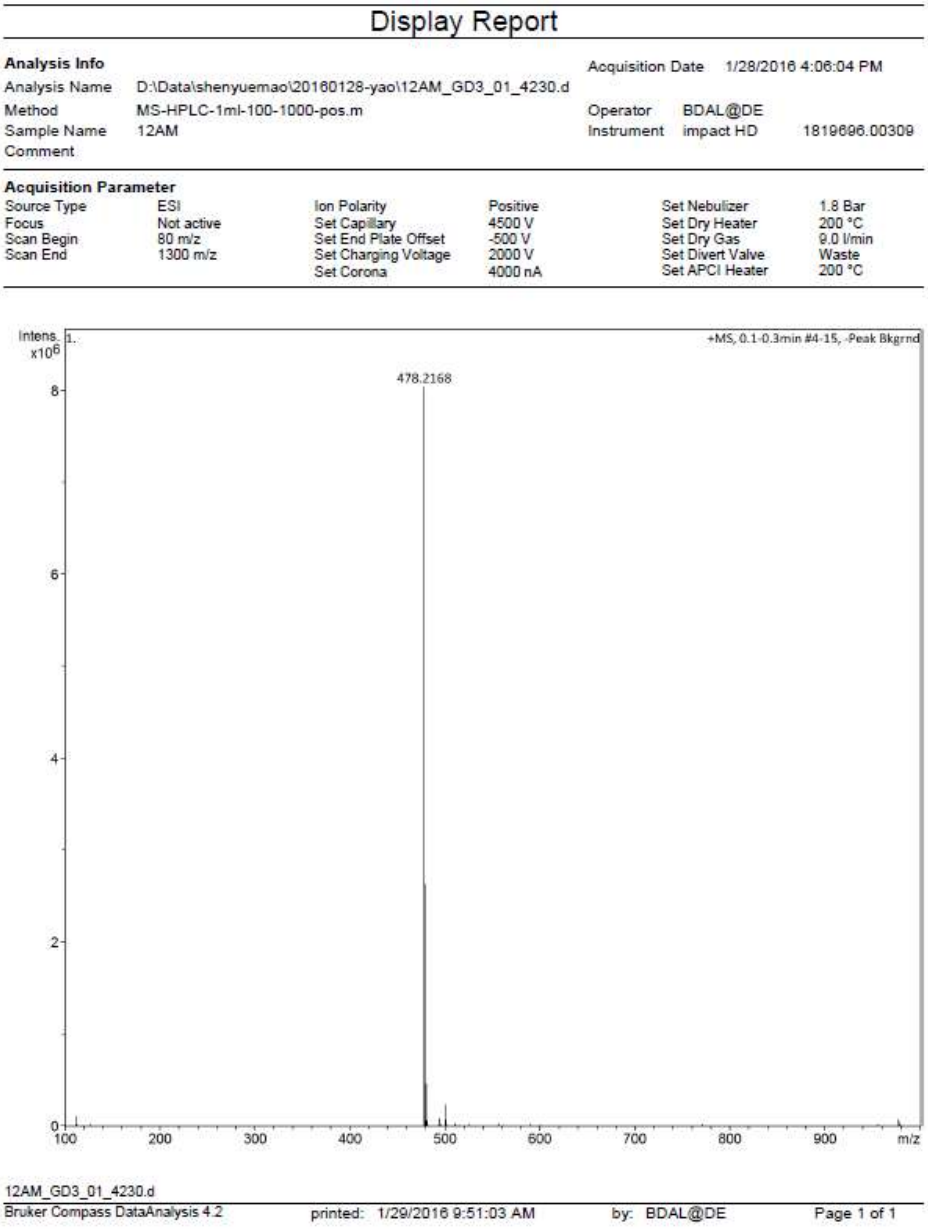

Figure S16: The HRESIMS spectrum of compound **2**

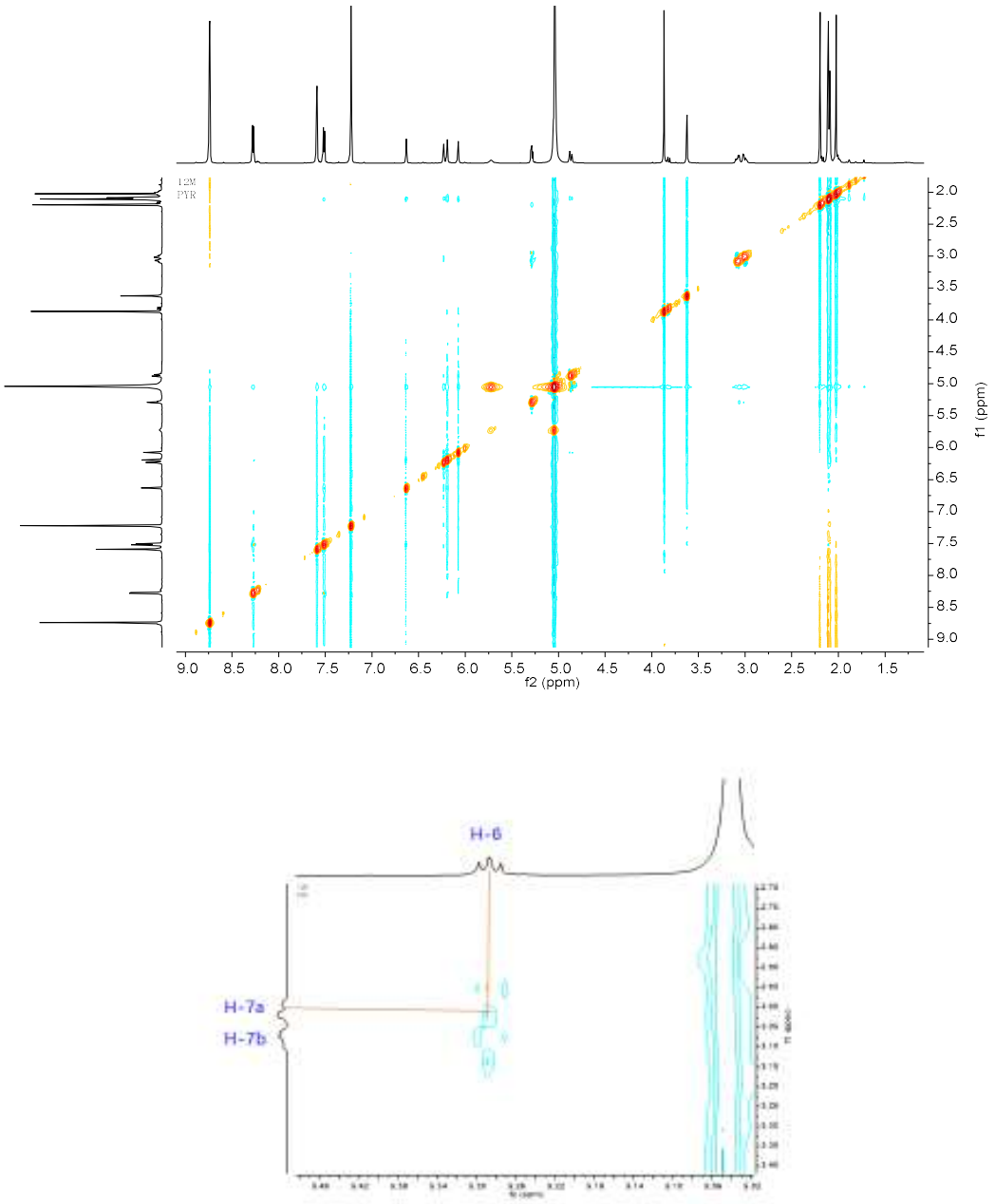

Figure S17: The ROESY spectrum of compound **2**

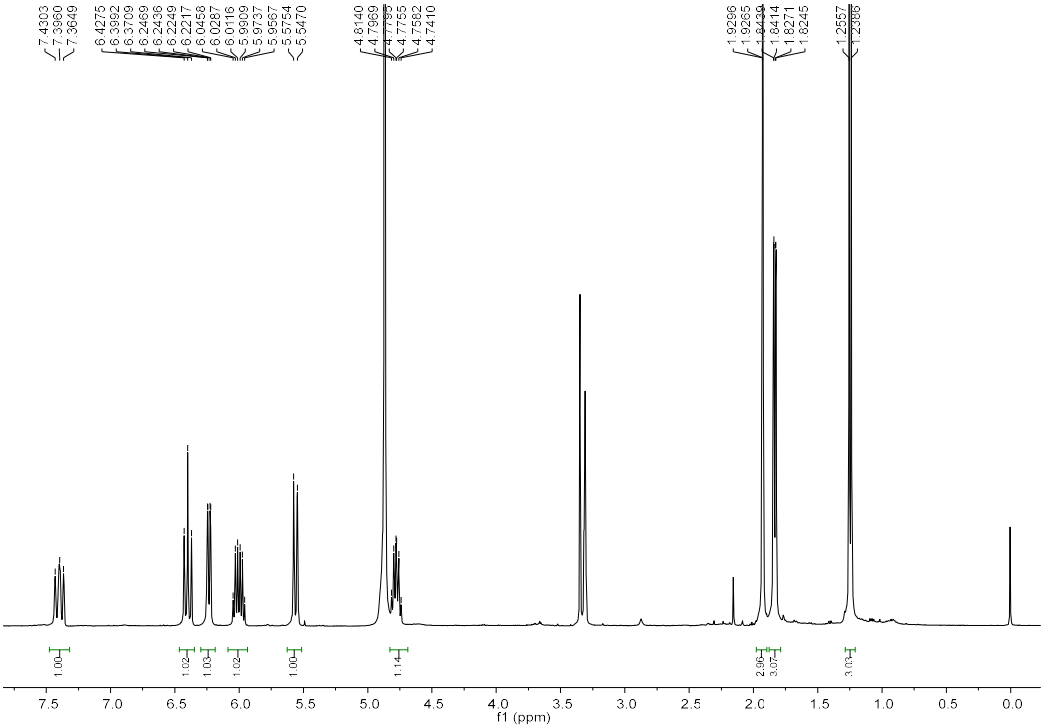

Figure S18: The ^{1}H NMR spectrum of compound **4 i**n CD_3OD at 400 MHz

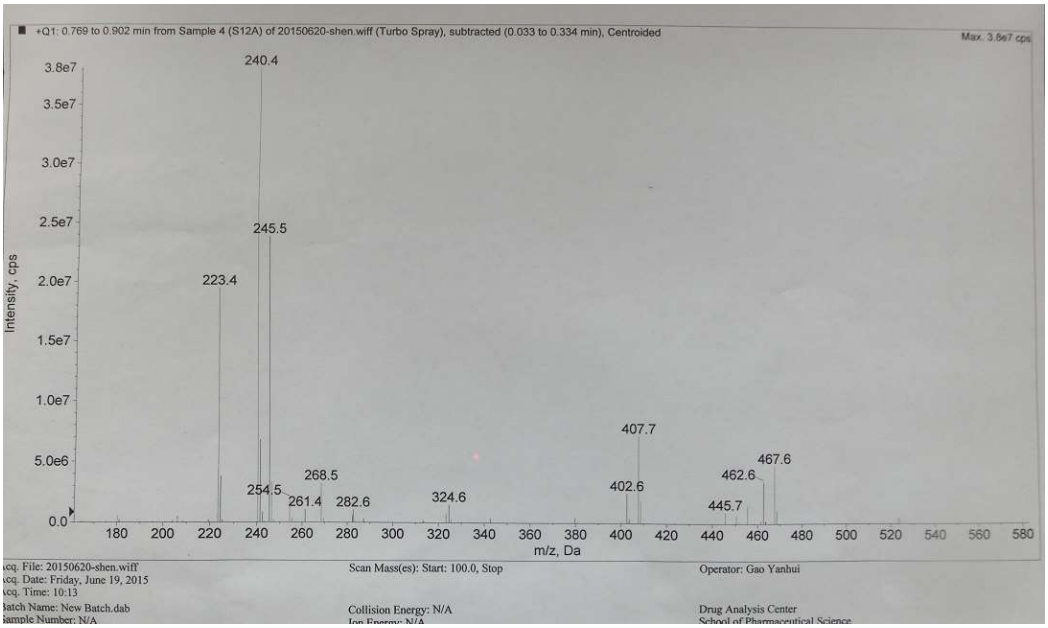

Figure S19: The ESIMS spectrum of compound **4**