

Sequential Biotransformation of Antcin K by *Bacillus subtilis* ATCC 6633

Te-Sheng Chang ¹, Chien-Min Chiang ², Yi-Yun Siao ¹ and Jiumn-Yih Wu ^{3,*}

¹ Department of Biological Sciences and Technology, National University of Tainan, No. 33, Sec. 2, Shu-Lin St., Tainan 70005, Taiwan; mozyme2001@gmail.com (T-S.C.); nightcat0@gmail.com (Y-Y.S.)

² Department of Biotechnology, Chia Nan University of Pharmacy and Science, No. 60, Sec. 1, Erh-Jen Rd., Jen-Te District, Tainan 71710, Taiwan; cmchiang@mail.cnu.edu.tw

³ Department of Food Science, National Quemoy University, No. 1, University Rd., Jin-Ning Township, Kinmen County 892, Taiwan

* Correspondence: wujy@nqu.edu.tw; Tel.: +886-82-313310; Fax: +886-82-313797

Received: 6 August 2018; Accepted: 22 August; Published: date

Supplementary Materials

Table S1. NMR spectroscopic data for compound (1)/(2) (in pyridine-*d*₅; 700MHz).

Position	type	Compound (1)		Compound (2)		HMBC
		δ _C	δ _H (<i>J</i> in Hz)	δ _C	δ _H (<i>J</i> in Hz)	
Antcin K moiety						
1	CH ₂	29.7	3.12, dt (12.8, 3.6) 2.08, m	29.5	3.11, dt (12.9, 3.5); 2.07, m	H-3, H-19
2	CH ₂	26.8	2.75, m 1.95, m	26.5	2.74, m 1.94, m	
3	CH	74.7	4.08, m	74.5	4.08, m	H-1, H-29
4	C	74.0	-	73.8	-	H-2, H-3, H-29,
5	CH	43.5	2.17, dd (13.7, 2.0)	43.3	2.16, dd (13.7, 2.0)	H-3, H-6, H-19, H-29
6	CH ₂	30.2	2.72, m 2.45, m	30.0	2.73, m; 2.45, m;	H-5, H-7
7	CH	70.8	4.63, t (8.5)	70.6	4.63, t (8.5)	H-5, H-6
8	C	154.4	-	154.1	-	H-6, H-7, H-14
9	C	144.0	-	143.7	-	H-5, H-7, H-12, H-14, H-19
10	C	38.8	-	38.5	-	H-2, H-5, H-6, H-19
11	C	201.6	-	201.3	--	H-12
12	CH ₂	58.8	2.95, d (13.4) 2.44, d (13.4)	58.6	2.97, d (13.4) 2.46, d (13.4)	H-14, H-17, H-18
13	C	48.0	-	47.7	-	H-12, H-14, H-15, H-16, H-17, H-18,
14	CH	53.8	2.66, dd (12.7, 7.0)	53.6	2.67, dd (12.8, 7.2)	H-7, H-12, H-16, H-18
15	CH ₂	25.5	2.51, m 2.12, m	25.3	2.51, m 2.12, m	H-14
16	CH ₂	28.3	1.93, m 1.25, m	28.0	1.93, m 1.27, m	H-17
17	CH	54.8	1.41, m	54.6	1.41, m	H-14, H-18, H-21, H-22
18	CH ₃	12.5	0.88, s	12.3	0.90, s	H-12, H-14, H-17
19	CH ₃	21.0	2.08, s	20.7	2.07, s	H-5
20	CH	36.3	1.30, m	36.0	1.33, m	H-21
21	CH ₃	18.6	0.86, d (6.3)	18.4	0.89, d (6.4)	H-22
22	CH ₂	34.2	1.60, m 1.23, m	33.9	1.62, m 1.23, m	H-21, H-23
23	CH ₂	31.4	2.36, m - 2.07, m	31.3	2.36, m - 2.08, m	H-25, H-28,
24	C	149.0	-	148.6	-	H-23, H-25 , H-27, H-28
25	CH	46.4	3.42, q (7.0)	45.8	3.37, q (7.0)	H-27, H-28,
26	C	173.7	-	173.4	-	H-25, H-27, Glc H-1'
27	CH ₃	16.7	1.38, d (7.0)	16.3	1.36, d (7.0)	H-25
28	CH ₂	111.4	5.15, s 4.98, s	111.1	5.14, s 5.01, s	H23, H-25
29	CH ₃	28.1	1.74, s	27.8	1.74, s	H-3
Glucose moiety						
1'	CH	96.3	6.40, d (8.2)	95.8	6.32, d (8.2)	H-2',
2'	CH	74.2	4.19, t (8.5)	73.7	4.20, t (8.6)	H-1', H-4',
3'	CH	78.7	4.29, m	78.5	4.25, m	H-1', H-2',
4'	CH	71.1	4.33, m	70.7	4.11, m	H-3', H-6',
5'	CH	79.5	4.04, m	76.0	4.12, m	H-4', H-6'
6'	CH ₂	62.3	4.45, dd (11.9, 2.5) 4.38, dd (11.9, 4.5)	64.2	4.88, dd (11.8, 1.9) 4.80, dd (11.8, 5.3)	H-4',
Succinyl moiety						
1''	C	-	-	172.8	-	Glc H6' , H2'', H3''
2'' and 3''	CH ₂	-	-	29.5	2.84,	H3'', H2''
	CH ₂			29.5	2.74,	
4''	C	-	-	174.5	-	H2'', H3''

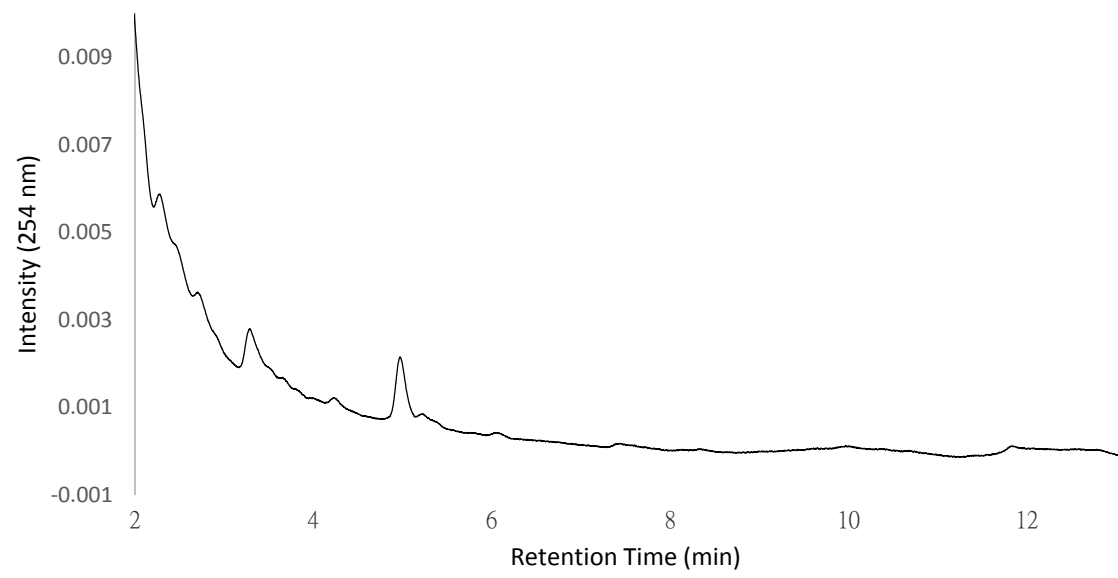


Figure S1. UPLC analysis of the fermentation broth by *B. subtilis* ATCC 6633 without adding of antcin K.

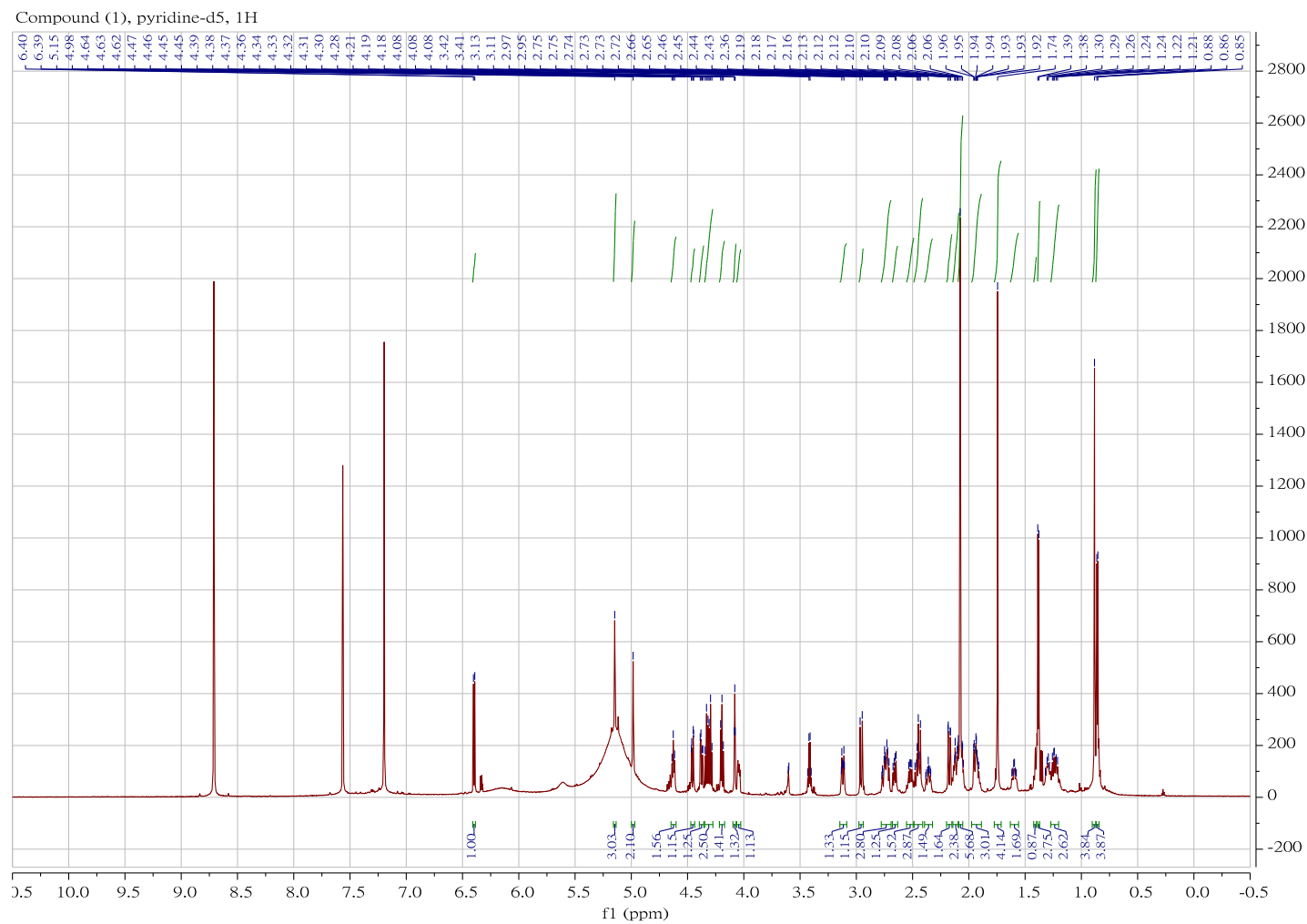


Figure S2. The ¹H-NMR (700 MHz, Pyridine-d₅) spectrum of compound (1).

Compound (1), pyridine-d₅, ¹³C

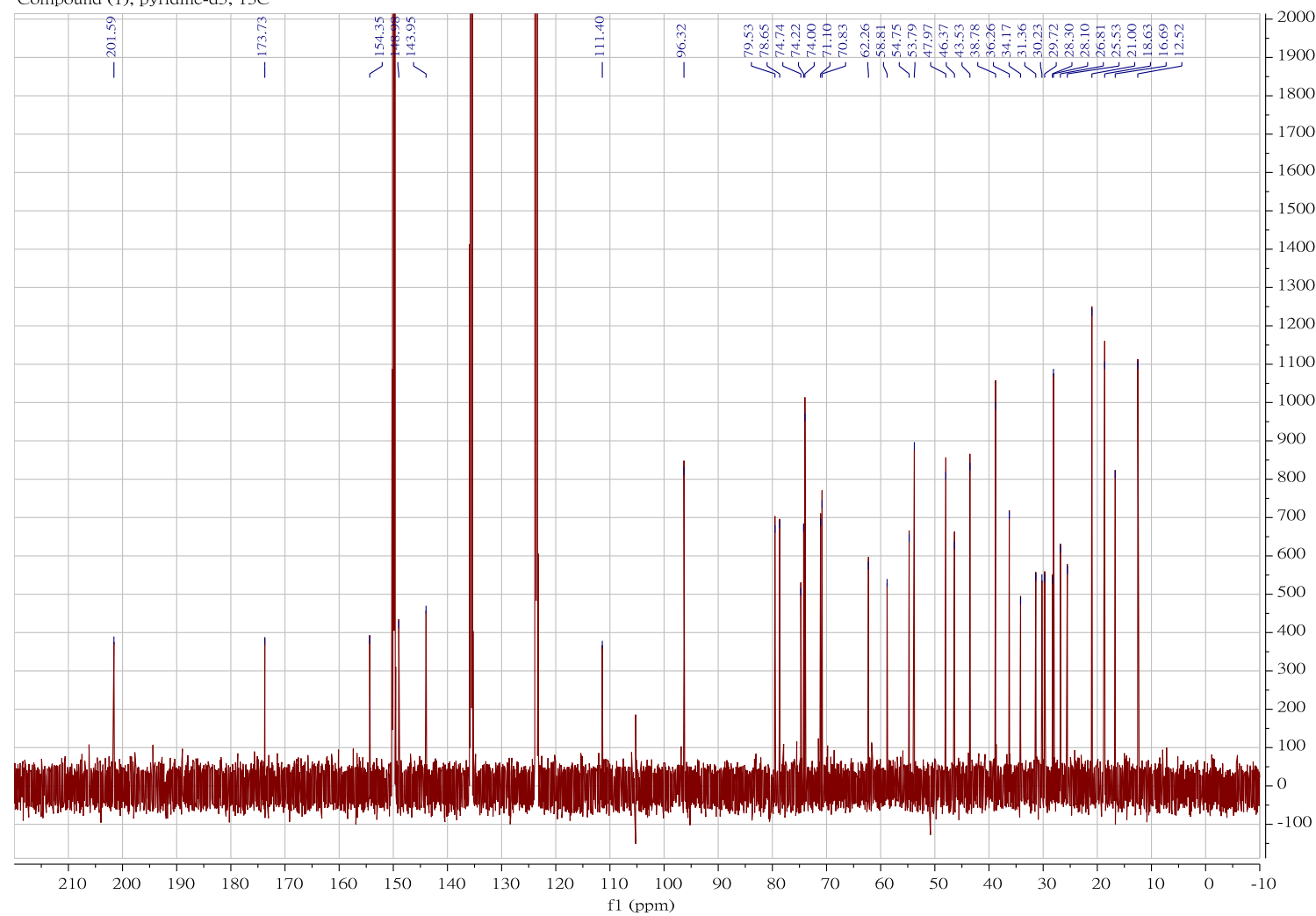


Figure S3. The ¹³C-NMR (176 MHz, Pyridine-d₅) spectrum of compound (1).

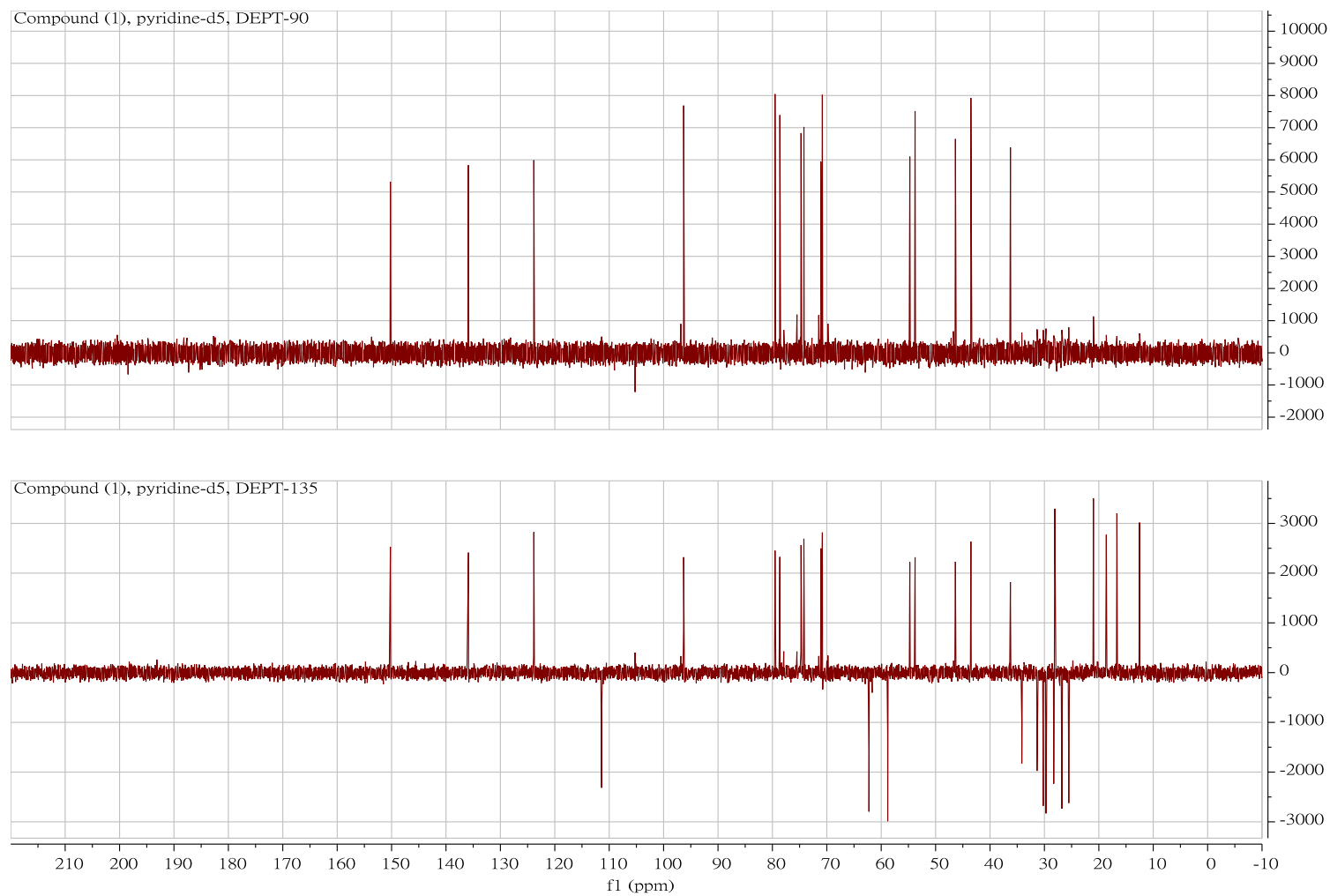


Figure S4. The DEPT-90 and DEPT-135 (176 MHz, Pyridine-d₅) spectra of compound (1).

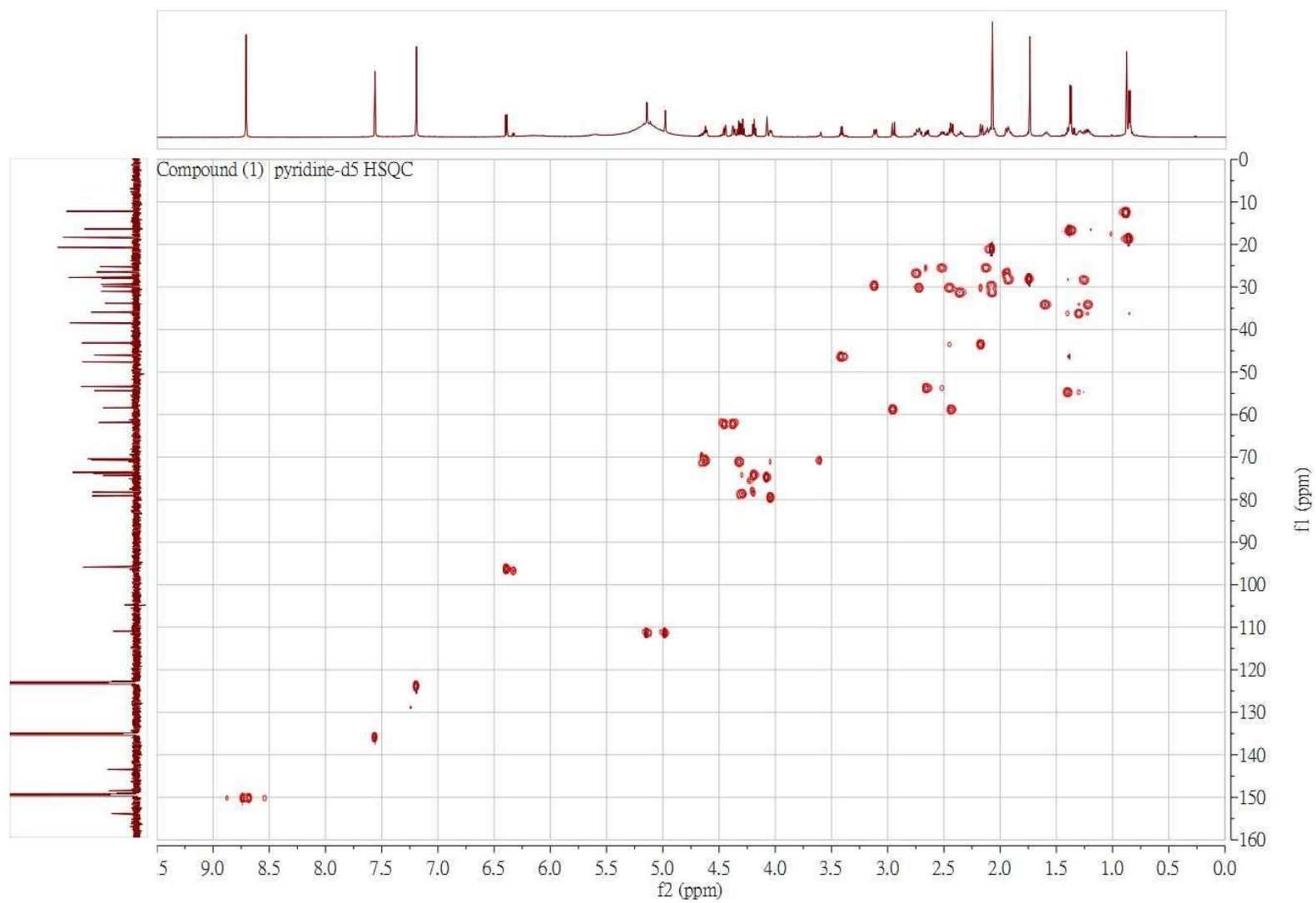


Figure S5. The HSQC (700 MHz, Pyridine-d5) spectrum of compound (1).

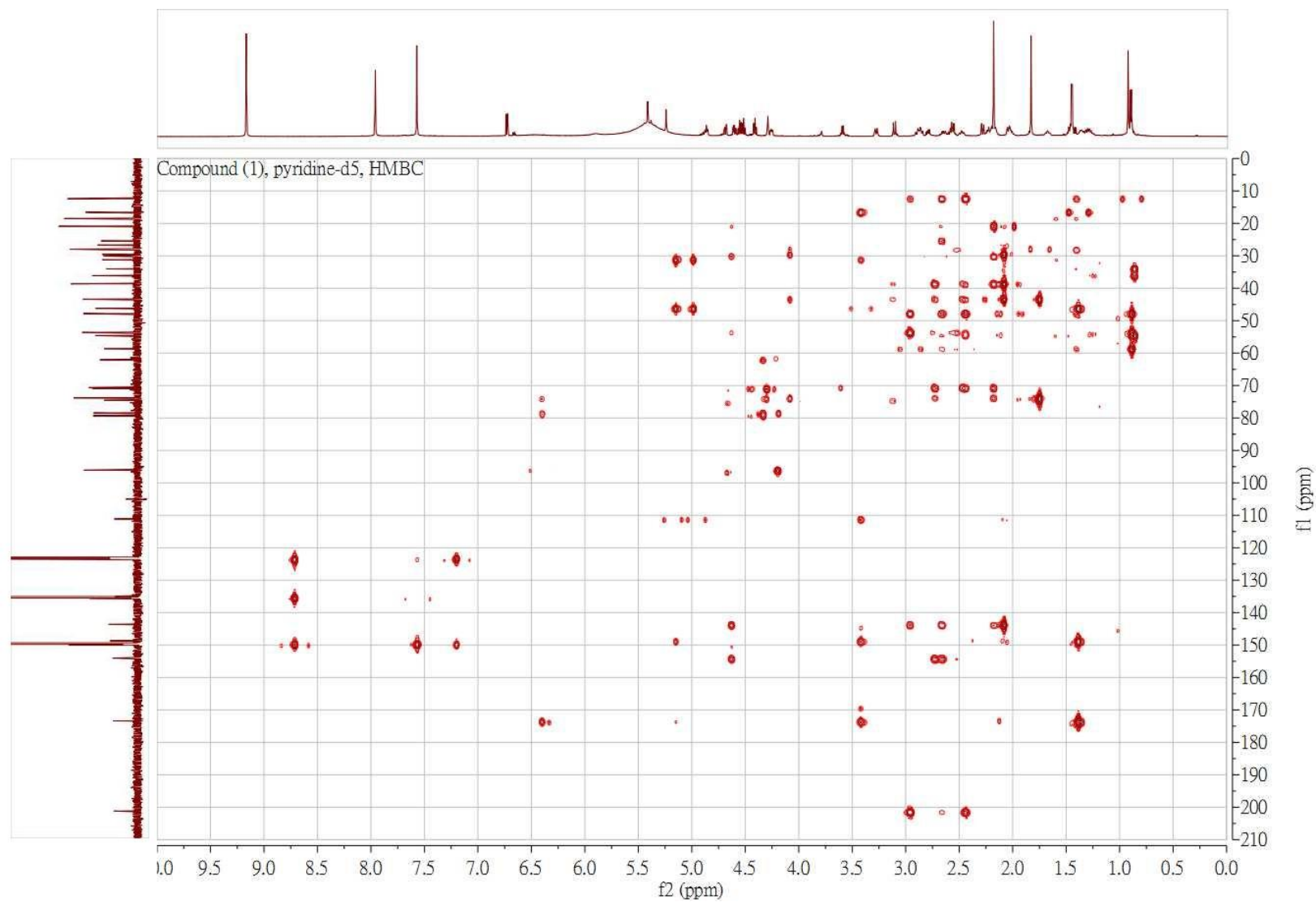


Figure S6. The HMBC (700 MHz, Pyridine-d₅) spectrum of compound (1).

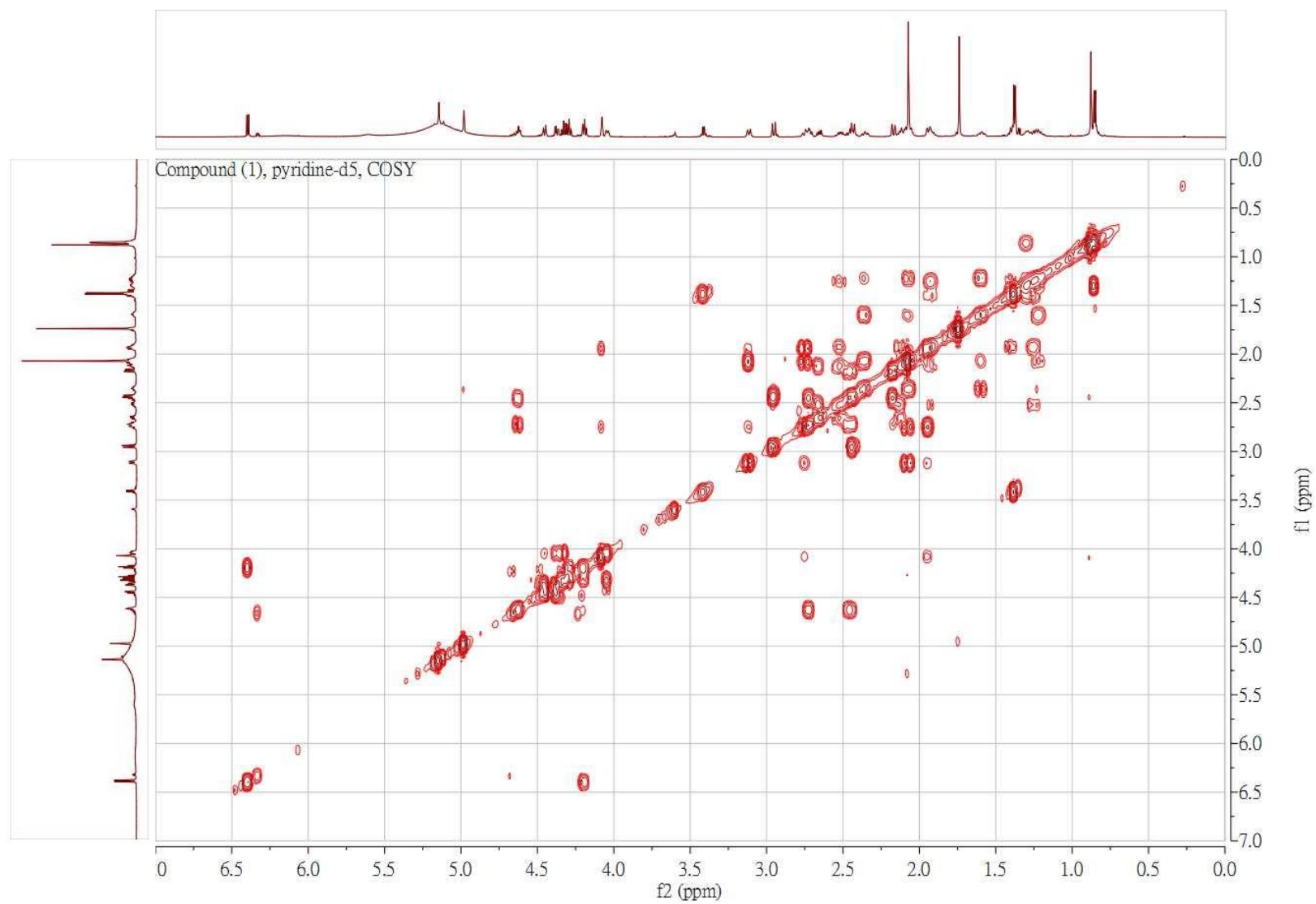


Figure S7. The H-H COSY (700 MHz, Pyridine-d₅) spectrum of compound (**1**).

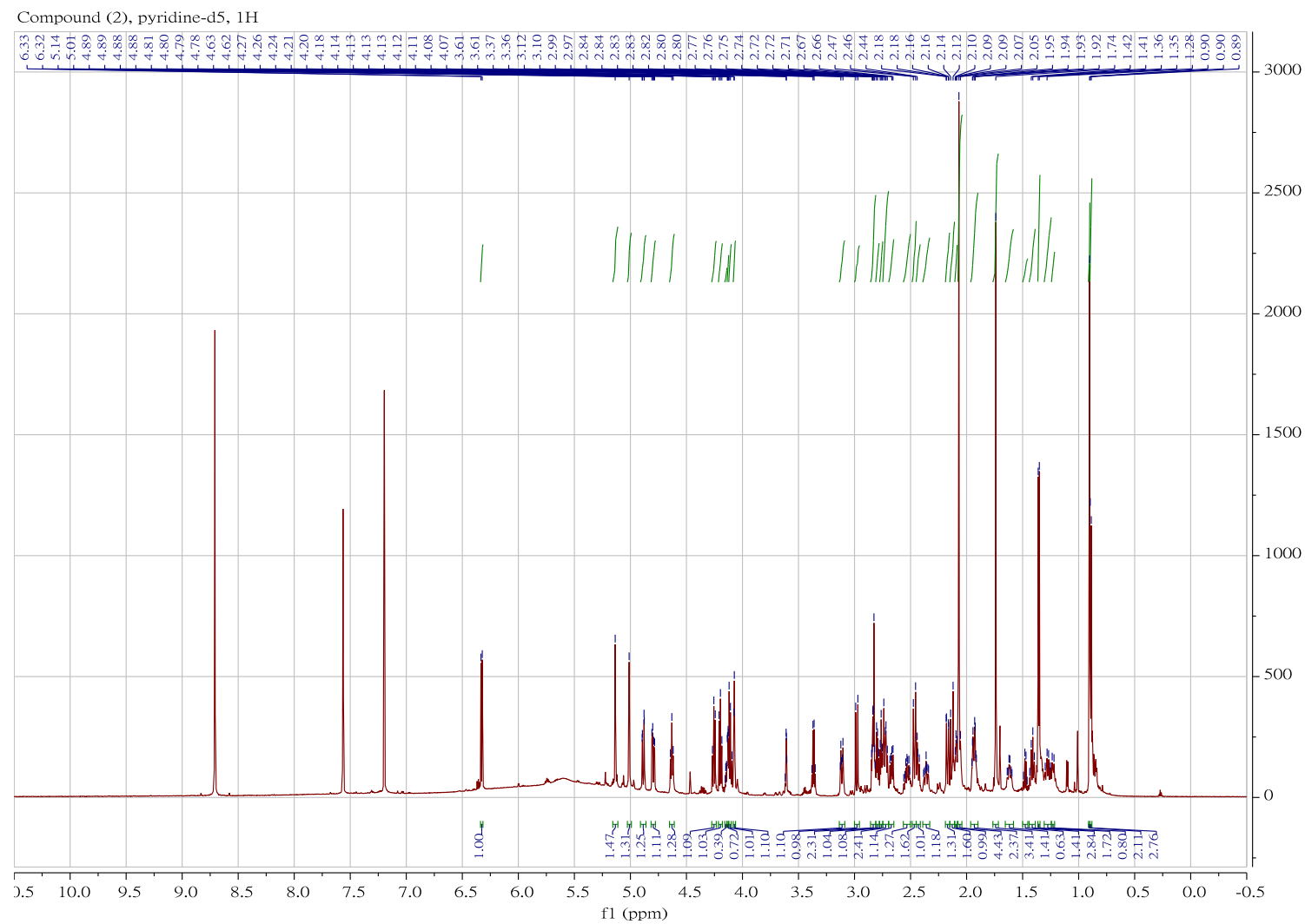


Figure S8. The ¹H-NMR (700 MHz, Pyridine-d₅) spectrum of compound (2).

Compound (2), pyridine-d₅, ¹³C

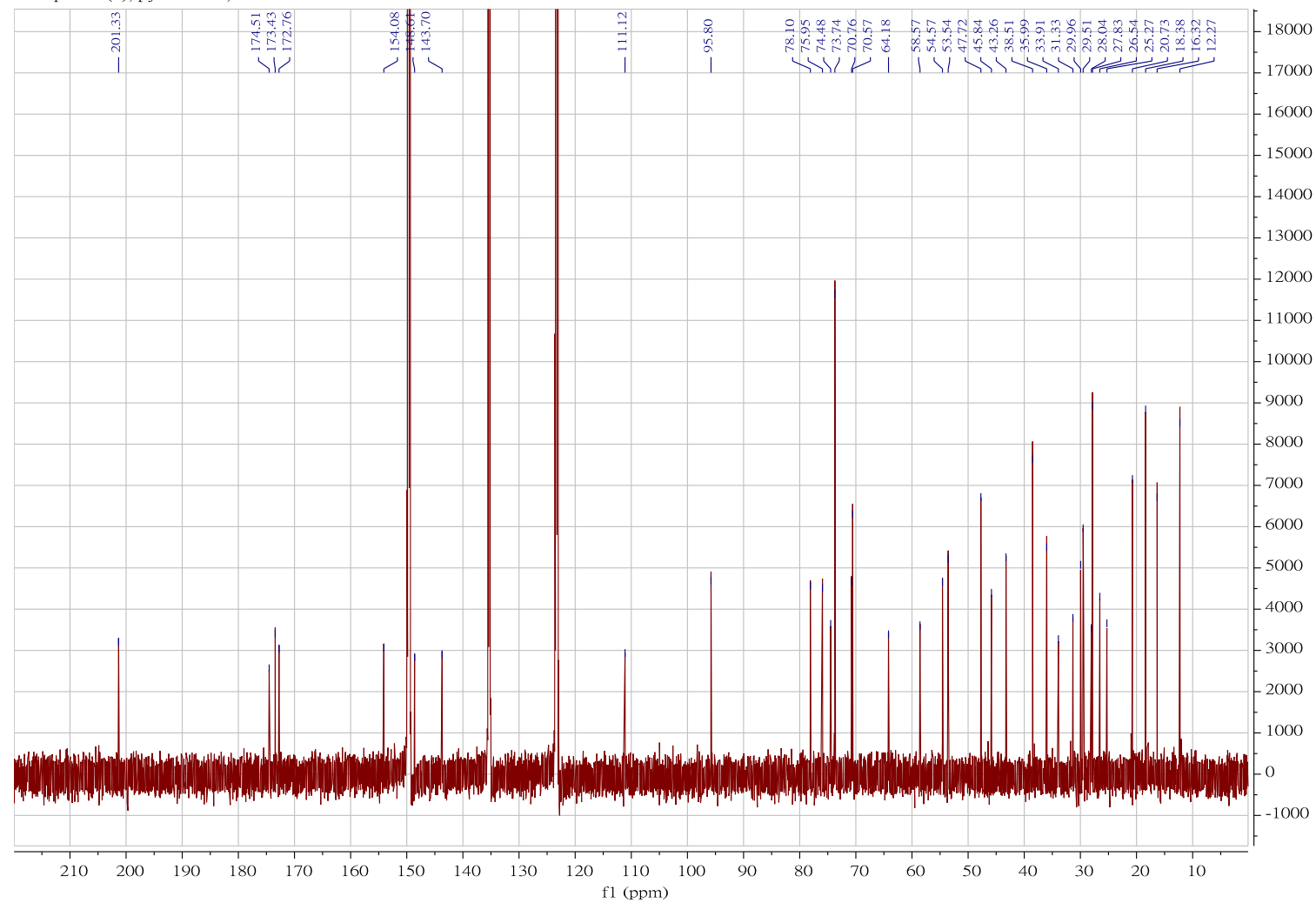


Figure S9. The ¹³C-NMR (176 MHz, Pyridine-d₅) spectrum of compound (2).

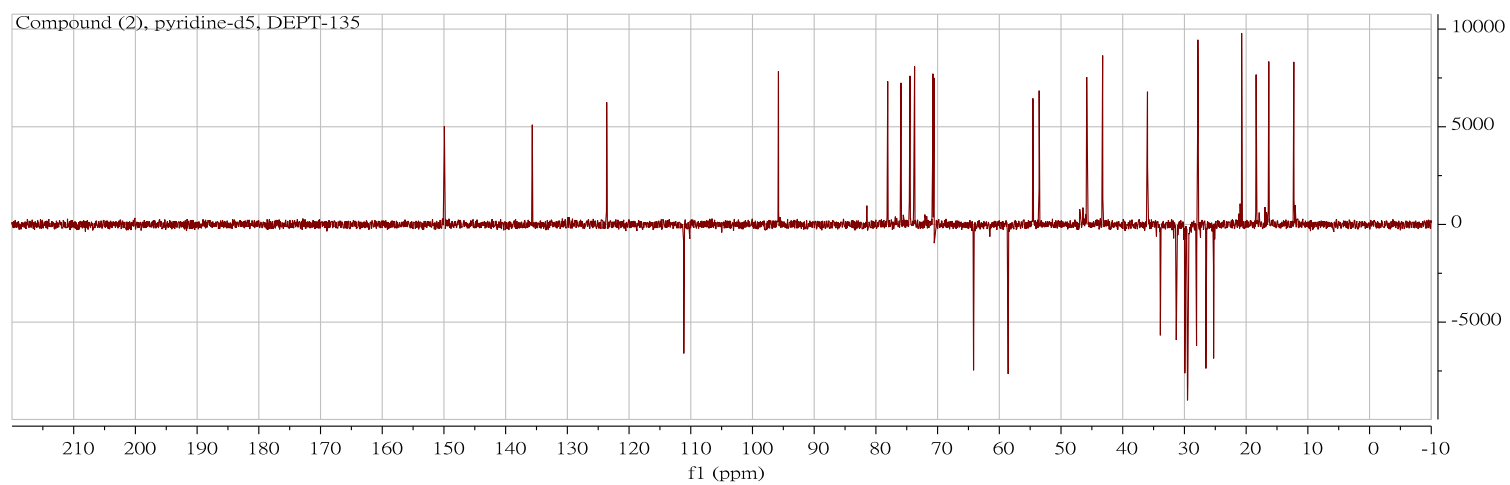
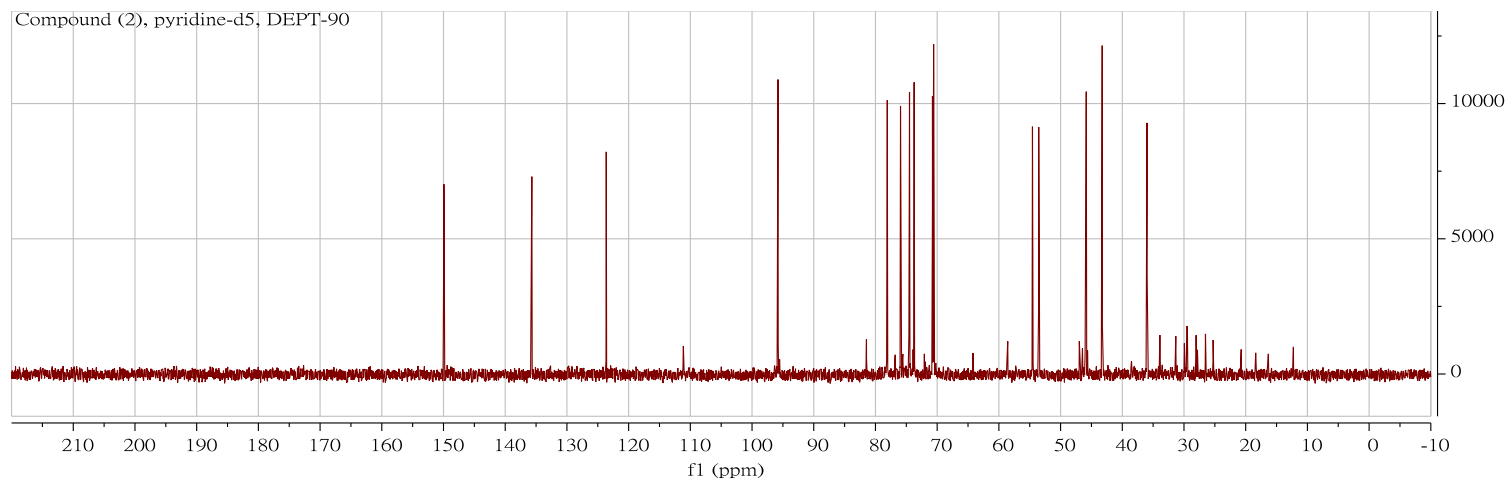


Figure S10. The DEPT-90 and DEPT-135 (176 MHz, Pyridine-d₅) spectra of compound (2).

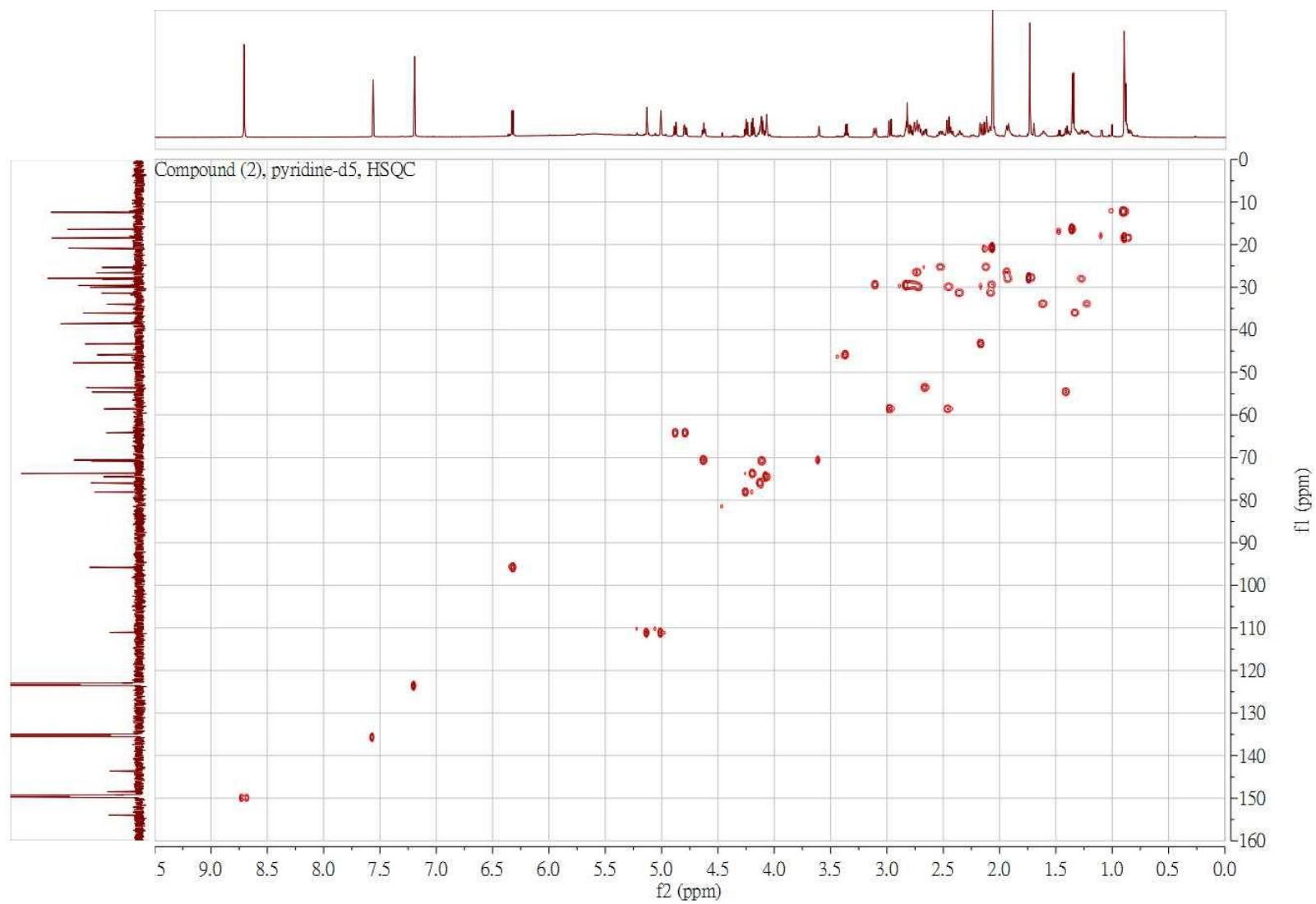


Figure S11. The HSQC (700 MHz, Pyridine-d₅) spectrum of compound (2).

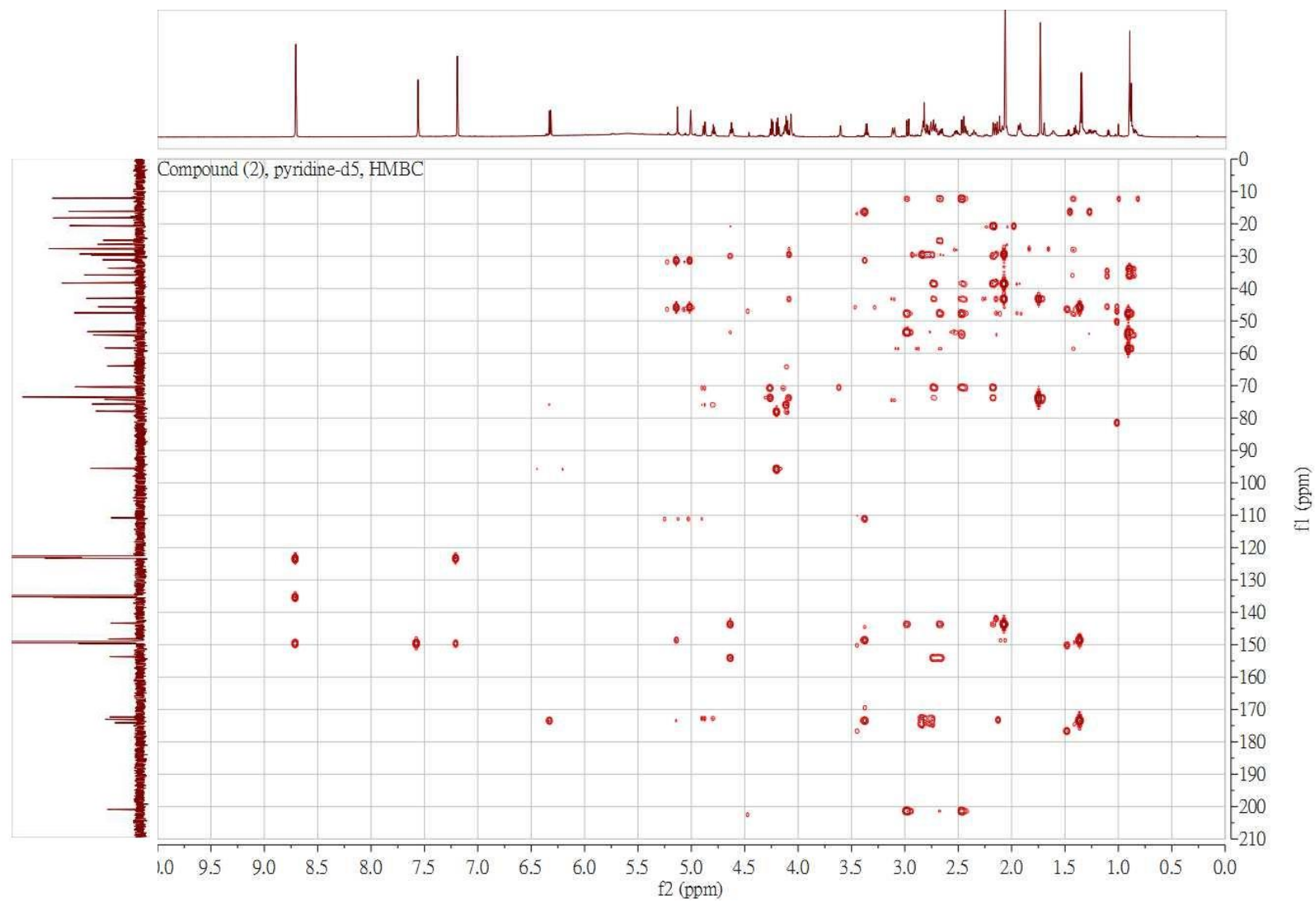


Figure S12. The HMBC (700 MHz, Pyridine-d₅) spectrum of compound (2).

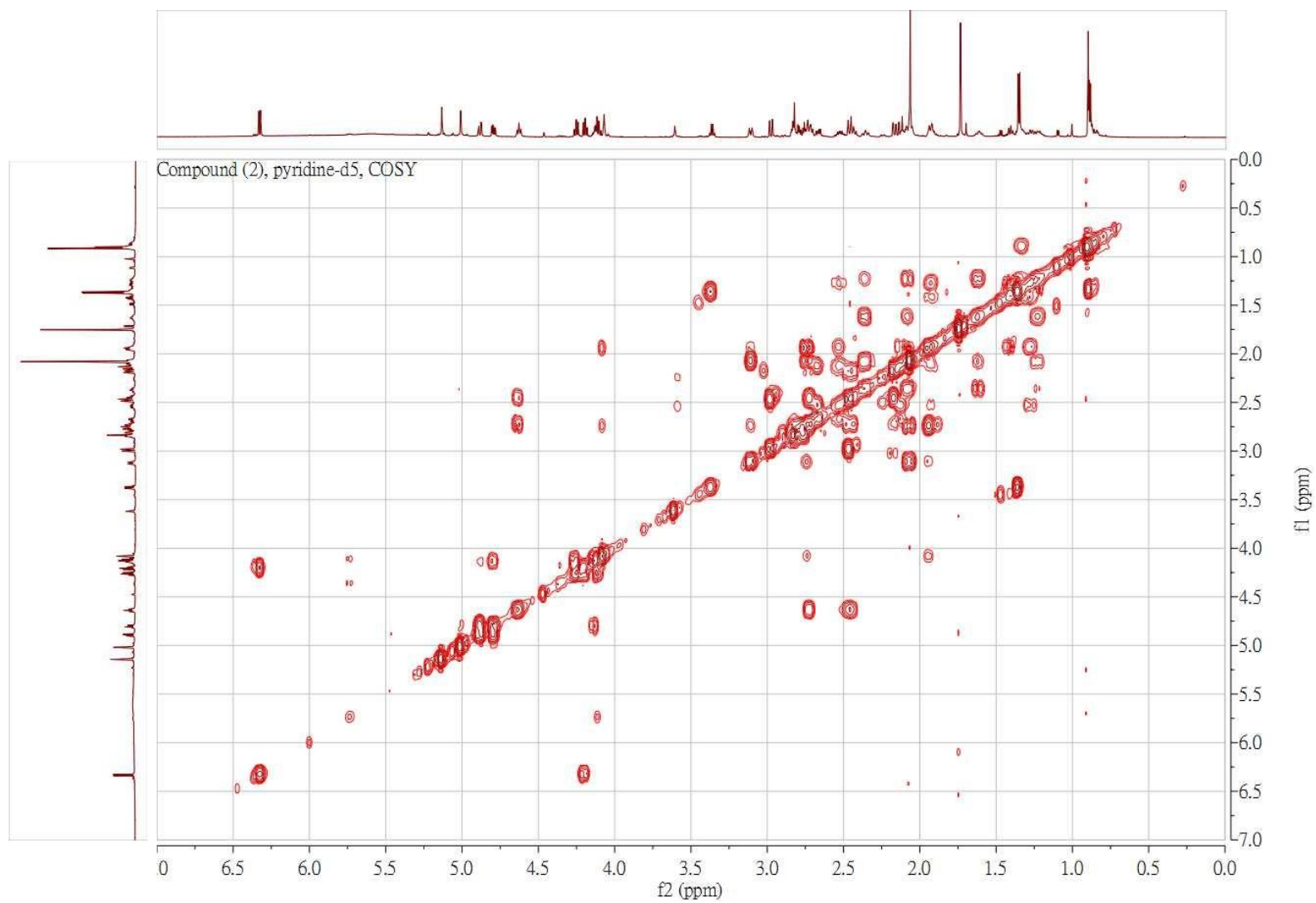


Figure S13. The HMBC (700 MHz, Pyridine-d₅) spectrum of compound (2).