

SUPPLEMENTARY MATERIAL

Two new anthraquinone derivatives and one new triarylbenzophenone analog from *Selaginella tamariscina*

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Abstract

Two new anthraquinone derivatives, selaginones A (**1**) and B (**2**), and one new triarylbenzophenone analog, selagibenzophenone B (**3**), were isolated from *Selaginella tamariscina* (Beauv.) Spring. Their structures were established by 1D-, 2D-NMR and HR-ESI-MS data. Compounds **1** and **2** represent the uncommon examples of aryl substituted anthraquinone derivatives. Especially, compound **2** is a unique anthranone with exceptional structural feature, in which a *p*-hydroxyphenyl moiety is attached to the C-10 position. Compound **3** is the second naturally occurring triarylbenzophenone and showed moderate activity against SMCC-7721 and MHCC97-H cell line with IC₅₀ values of 39.8, 51.5 μ M respectively.

Keywords

Selaginella tamariscina; anthraquinone; aryl anthraquinone; selaginone A;
selaginone B; selagibenzophenone B; hepatocellular carcinoma

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Table S1. ^1H (500 MHz) and ^{13}C (125 MHz) NMR data of compound **1** in CD_3OD and compound **2** in $\text{DMSO}-d_6$

Position	Compound 1		Compound 2	
	δ_{H} (J in Hz)	δ_{C}	δ_{H} (J in Hz)	δ_{C}
1		145.2		141.7

2		140.2		137.3
3	7.90 d (8.0)	131.4	7.62 d (7.8)	125.2
4	7.60 d (8.0)	138.6	7.38 d (7.8)	134.6
5	7.85 d (8.5)	130.4	7.26 d (8.5)	129.7
6	7.07 d (8.5)	123.5	6.94 d (8.5)	121.4
7		167.8		156.4
8	7.45 s	113.9	7.35 s	111.2
9		187.4		187.3
10		184.8	5.50 s	45.2
1a		134.7		130.4
4a		133.5		143.8
5a		126.1		135.8
8a		137.2		132.5
1'		135.1		129.6
2'/6'	7.10 d (7.5)	130.4	6.78 m	130.0
3'/5'	6.83 d (7.5)	115.8	6.75 m	115.1
4'		157.6		156.8
1''	5.96 s	66.4	5.96 d (16.0)	64.8
			5.87 d (16.0)	
2''		167.9		165.5
3''		121.8		119.4
4''/8''	8.02 d (8.0)	132.9	7.91 d (8.0)	131.5
5''/7''	6.89 d (8.0)	116.4	6.89 d (8.0)	115.6
6''		164.2		163.2

1'''	134.4
2'''(6''')	128.0
3'''(5''')	115.0
4'''	155.4

Table S2. ^1H (400 MHz) and ^{13}C (100 MHz) NMR data of compound **3** in CD_3OD

Position	Compound 3	
	δ_{H} (J in Hz)	δ_{C}
1		162.2
2/6	6.61 d (8.6)	114.5
3/5	7.42 d (8.6)	132.0
4		130.2
7		199.2

8/12	7.51 s	126.2
9/11		141.0
10		141.6
13		136.2
14/18/20/24	7.11 d (8.4)	130.0
15/17/21/23	6.65 d (8.4)	114.4
16/22		156.4
19/25		131.8
26/30	7.58 d (8.4)	127.8
27/29	6.91 d (8.4)	115.4
28		157.3
31		131.4

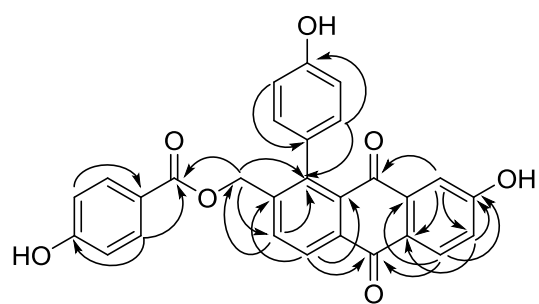


Figure S1. The Key HMBC correlations of compound **1**.

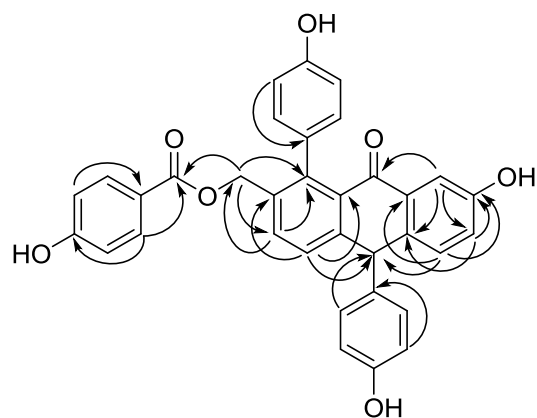


Figure S2. The Key HMBC correlations of compound **2**.

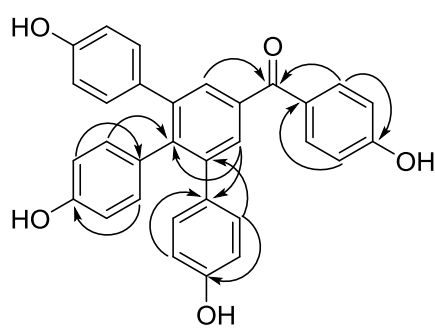


Figure S3. The Key HMBC correlations of compound **3**.

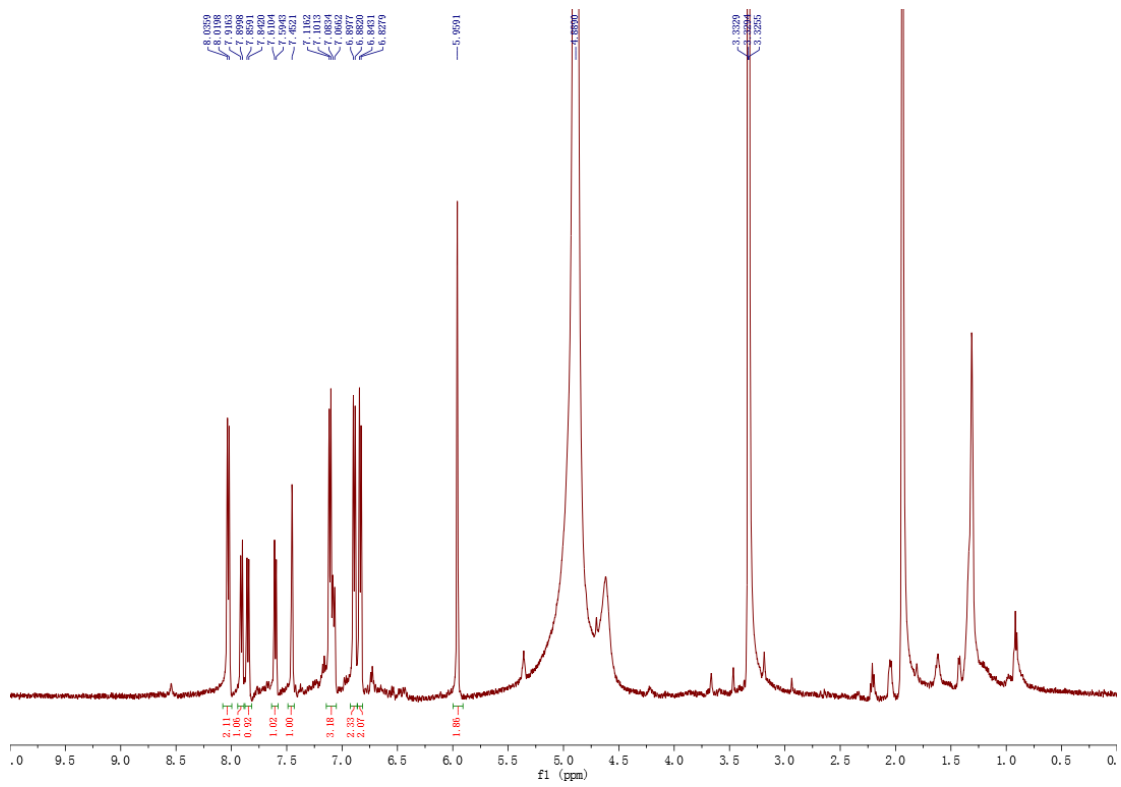


Figure S4. The ^1H NMR (500MHz, CD_3OD) spectrum of compound **1**.

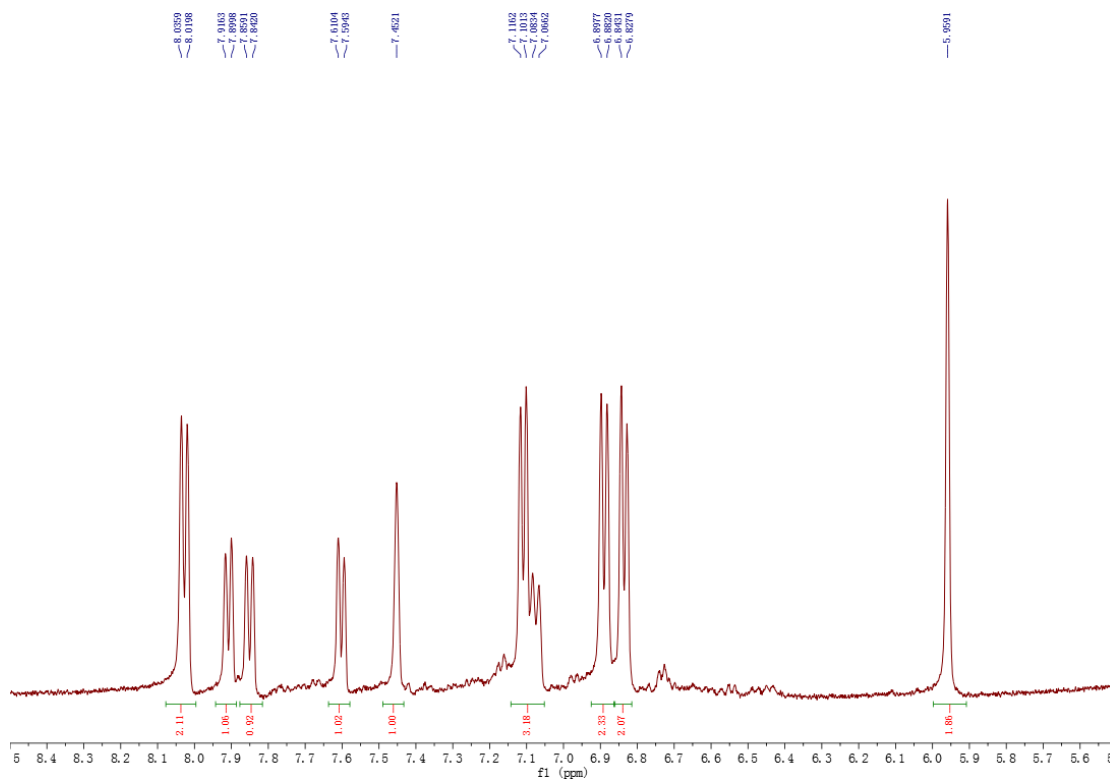


Figure S5. The ^1H NMR (500MHz, CD_3OD) spectrum of compound **1**.

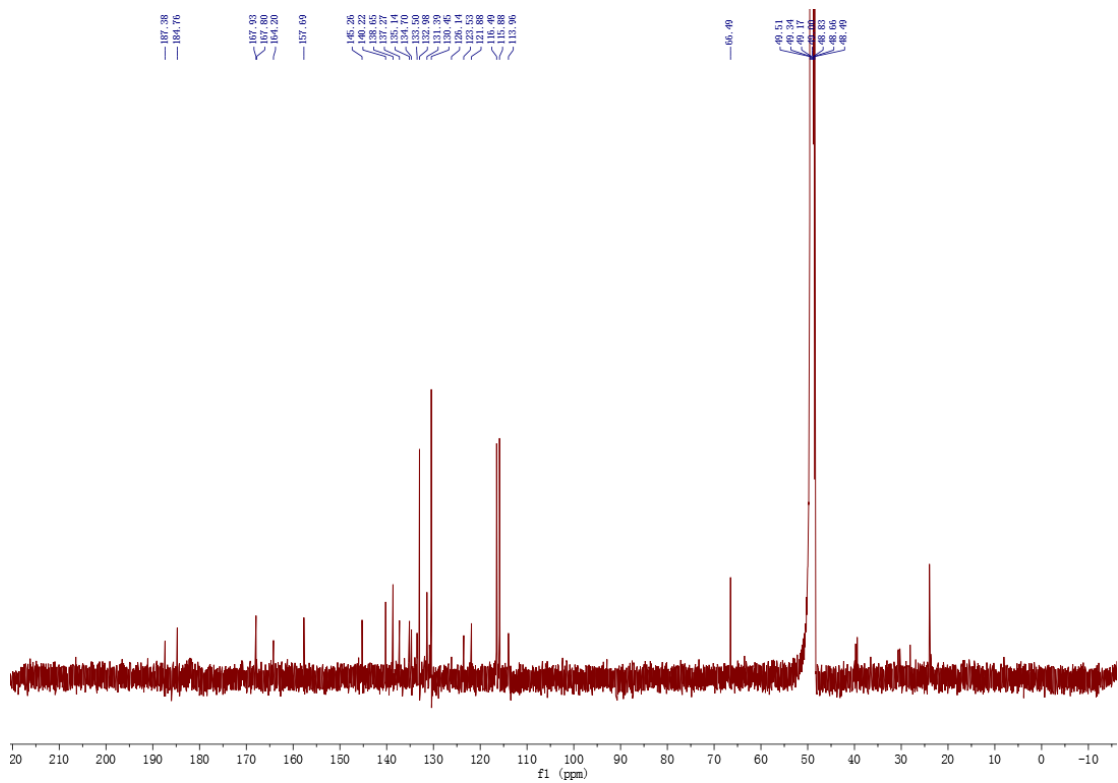


Figure S6. The ¹³C NMR (125MHz, CD₃OD) spectrum of compound **1**.

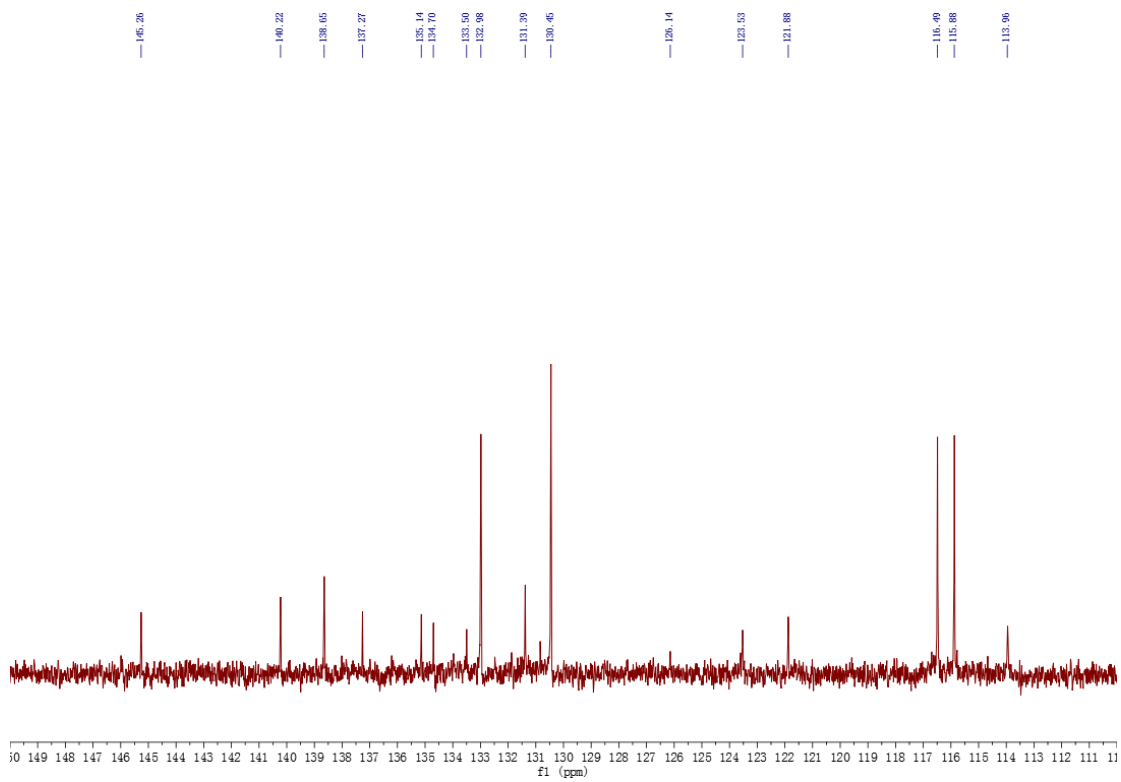


Figure S7. The ¹³C NMR (125MHz, CD₃OD) spectrum of compound **1**.

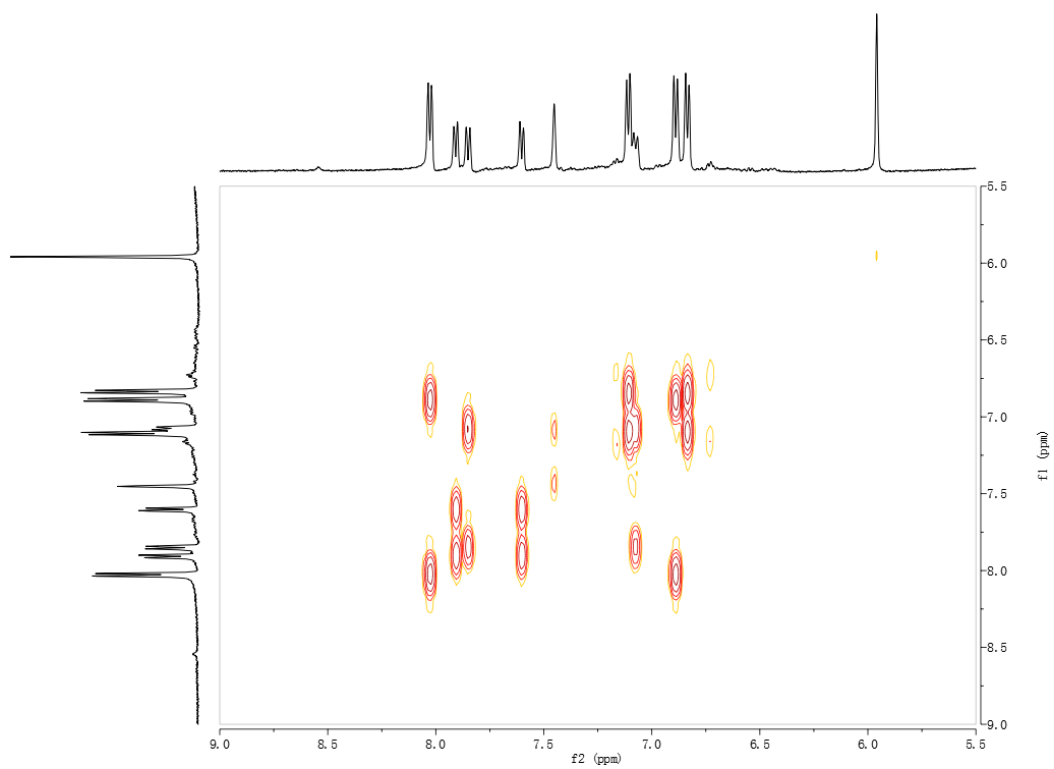


Figure S8. The COSY spectrum of compound **1**.

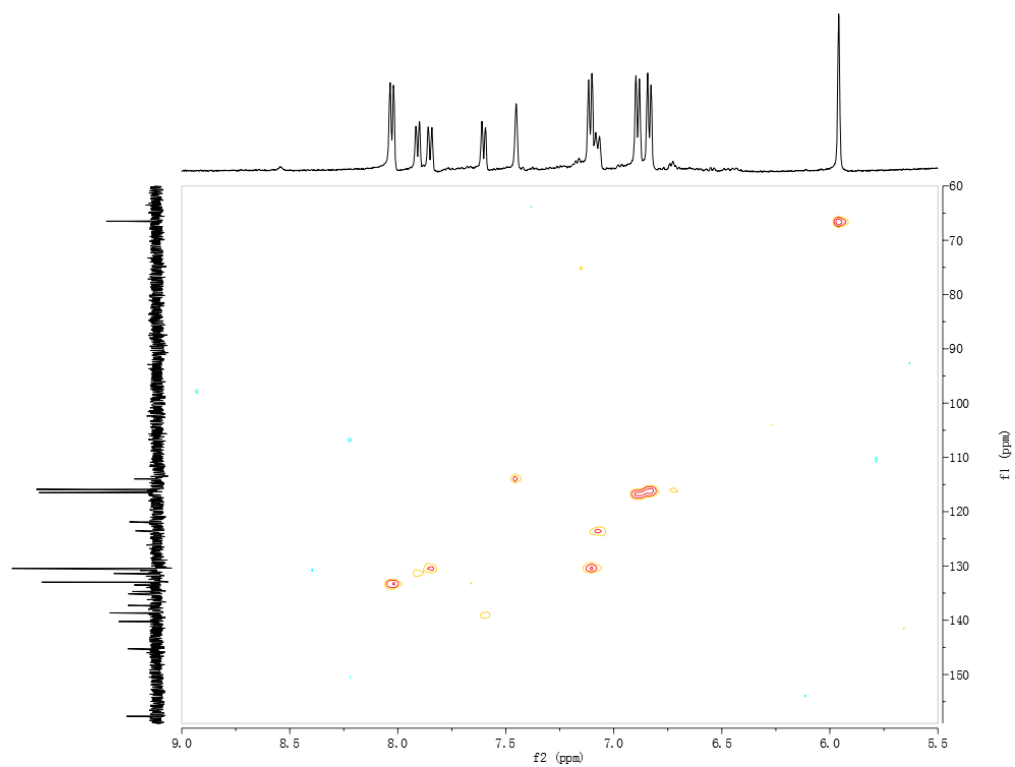


Figure S9. The HSQC spectrum of compound **1**.

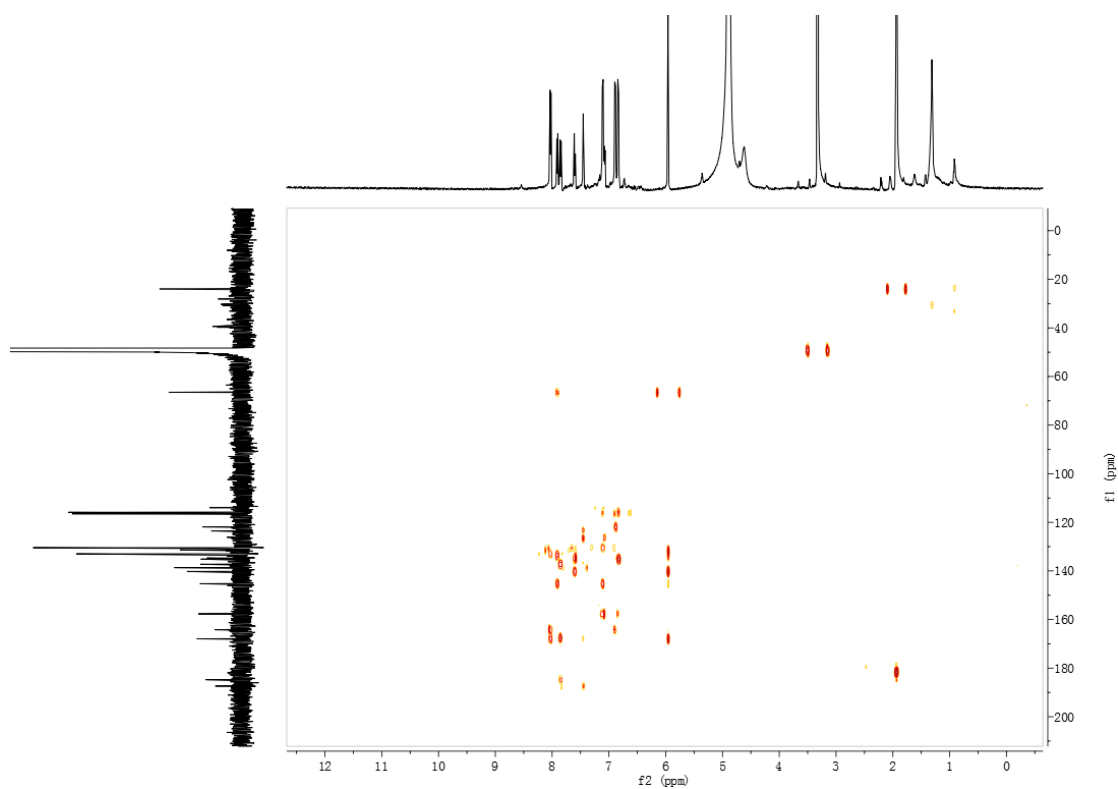


Figure S10. The HMBC spectrum of compound **1**.

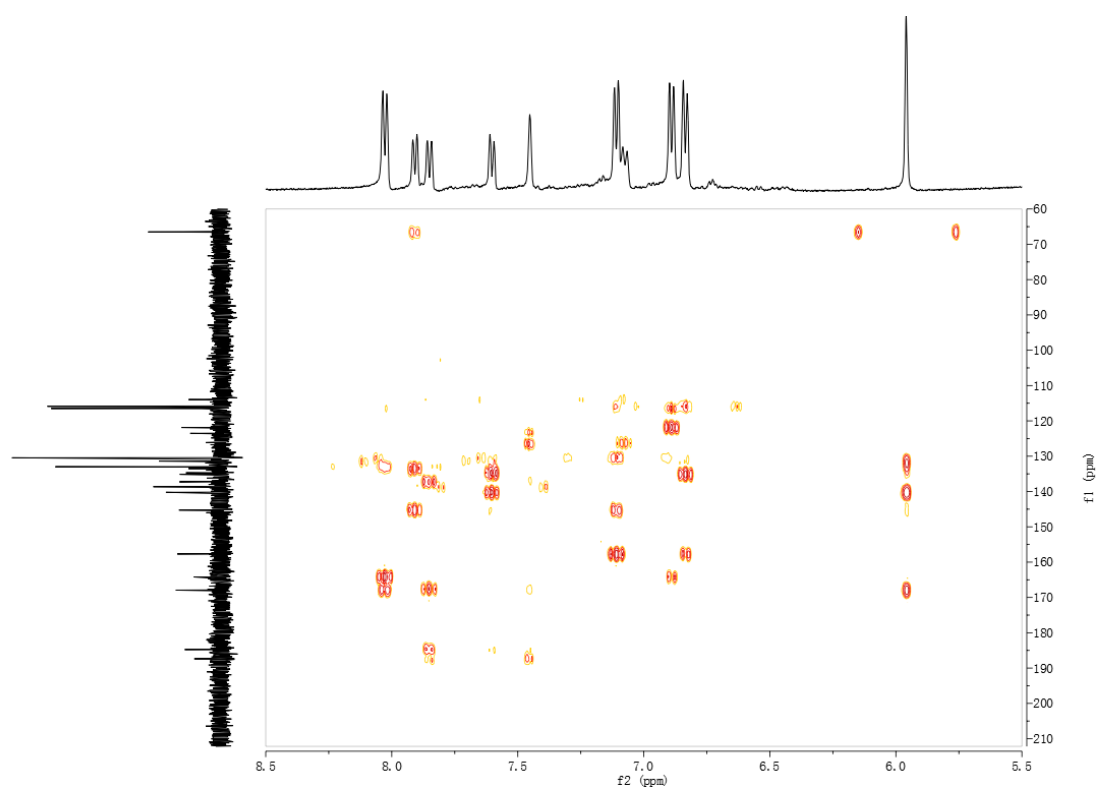


Figure S11. The HMBC spectrum of compound **1**.

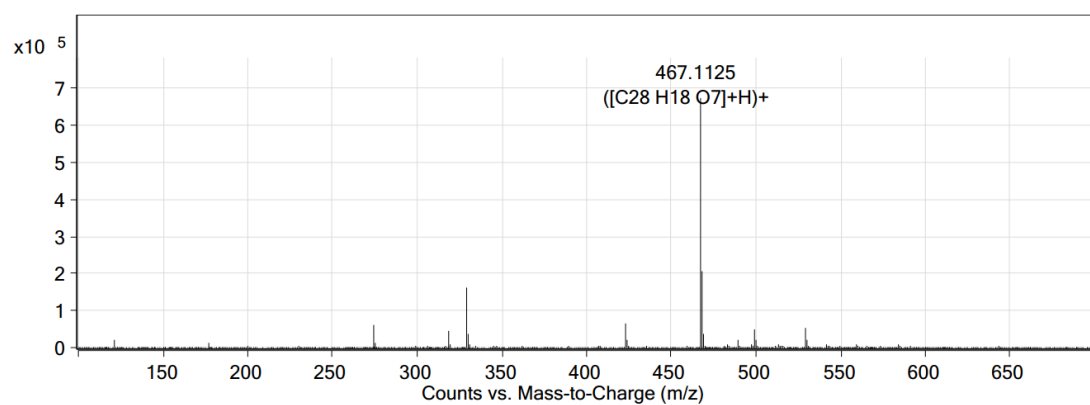


Figure S12. The HR-ESIMS sepctrum of compound **1**.

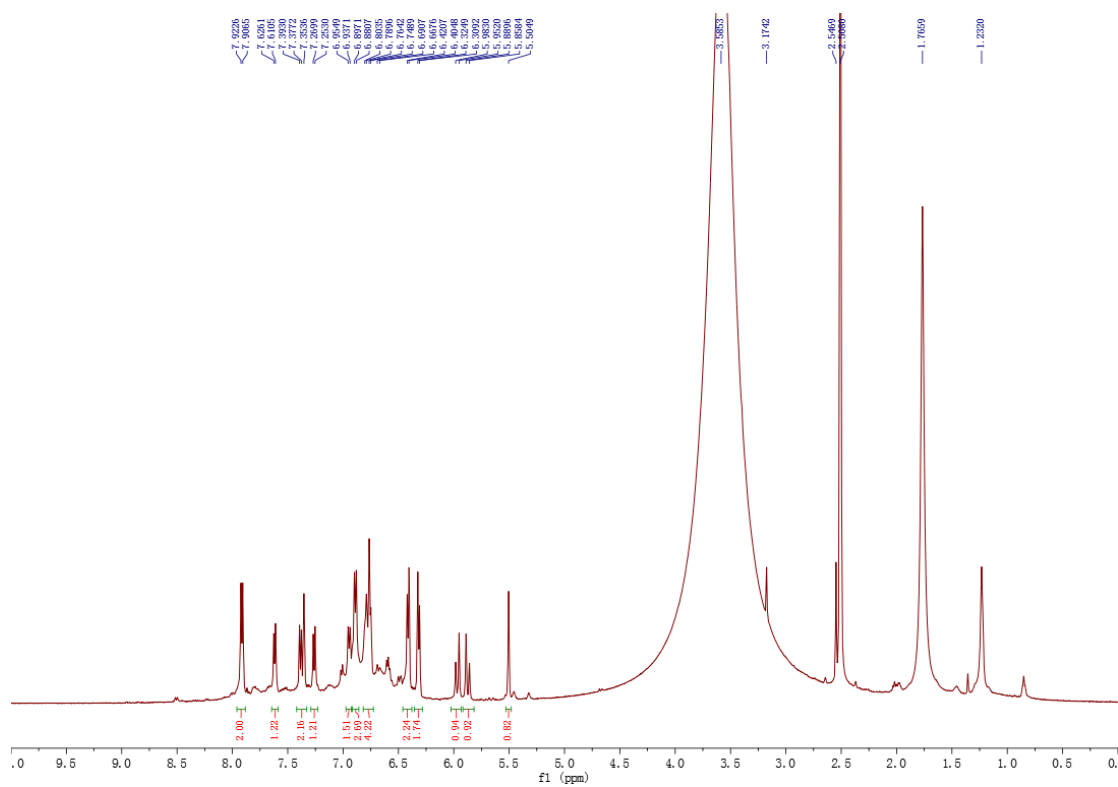


Figure S13. The ^1H NMR (500MHz, $\text{DMSO}-d_6$) spectrum of compound **2**.

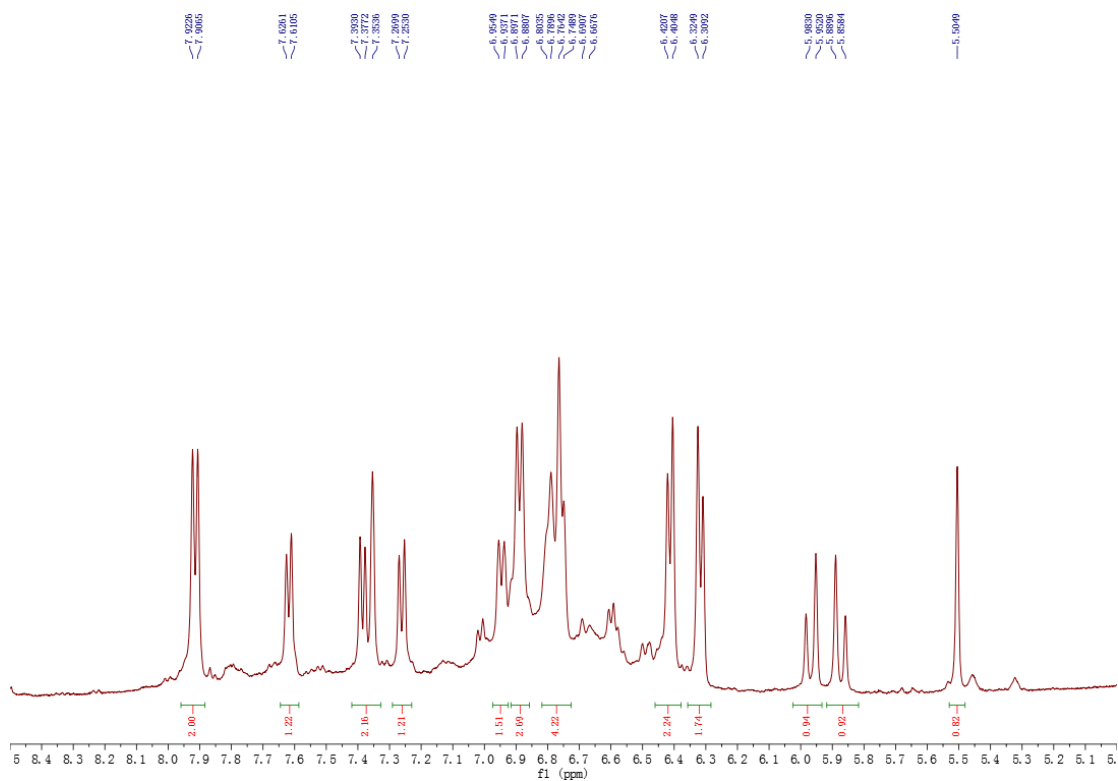


Figure S14. The ^1H NMR (500MHz, $\text{DMSO}-d_6$) spectrum of compound **2**.

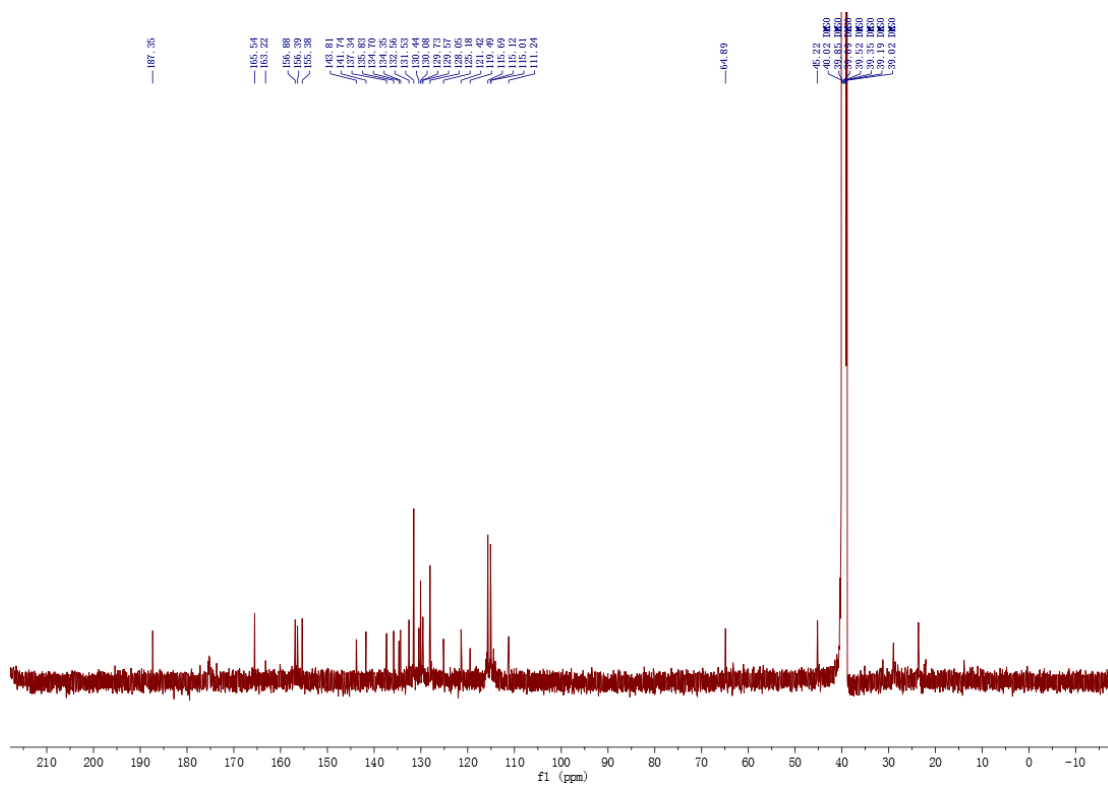


Figure S15. The ^{13}C NMR (125MHz, $\text{DMSO-}d_6$) spectrum of compound **2**.

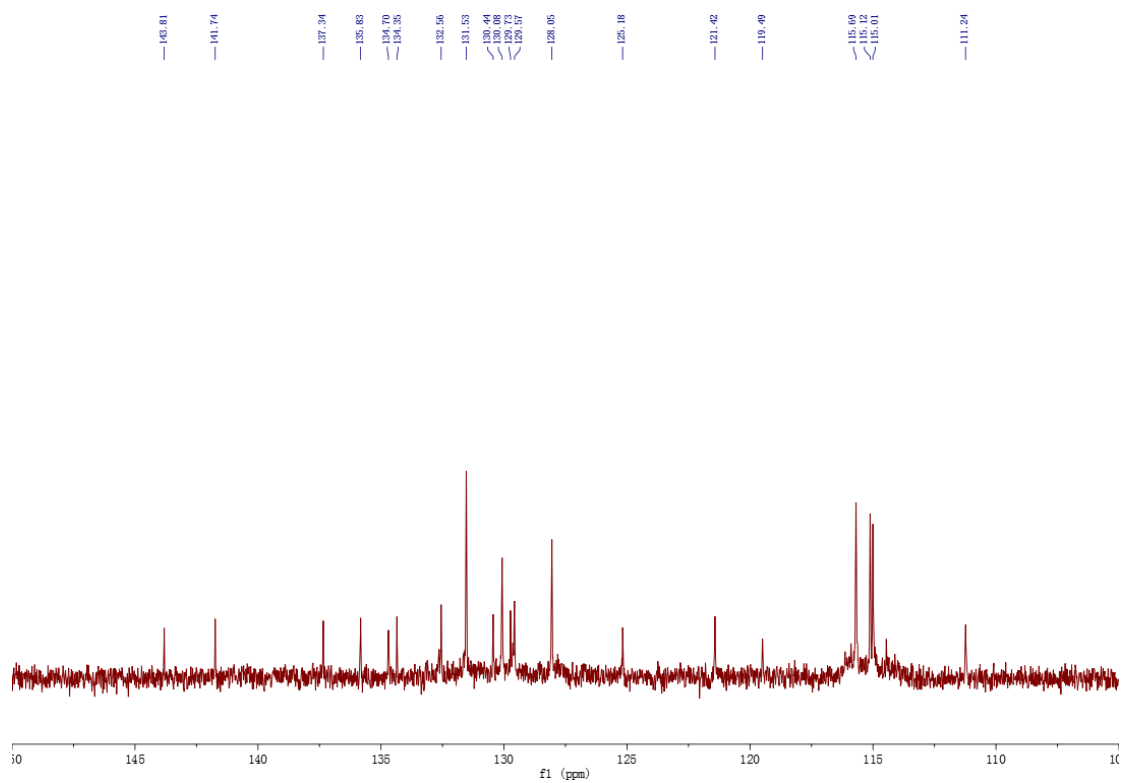


Figure S16. The ^{13}C NMR (125MHz, $\text{DMSO}-d_6$) spectrum of compound **2**.

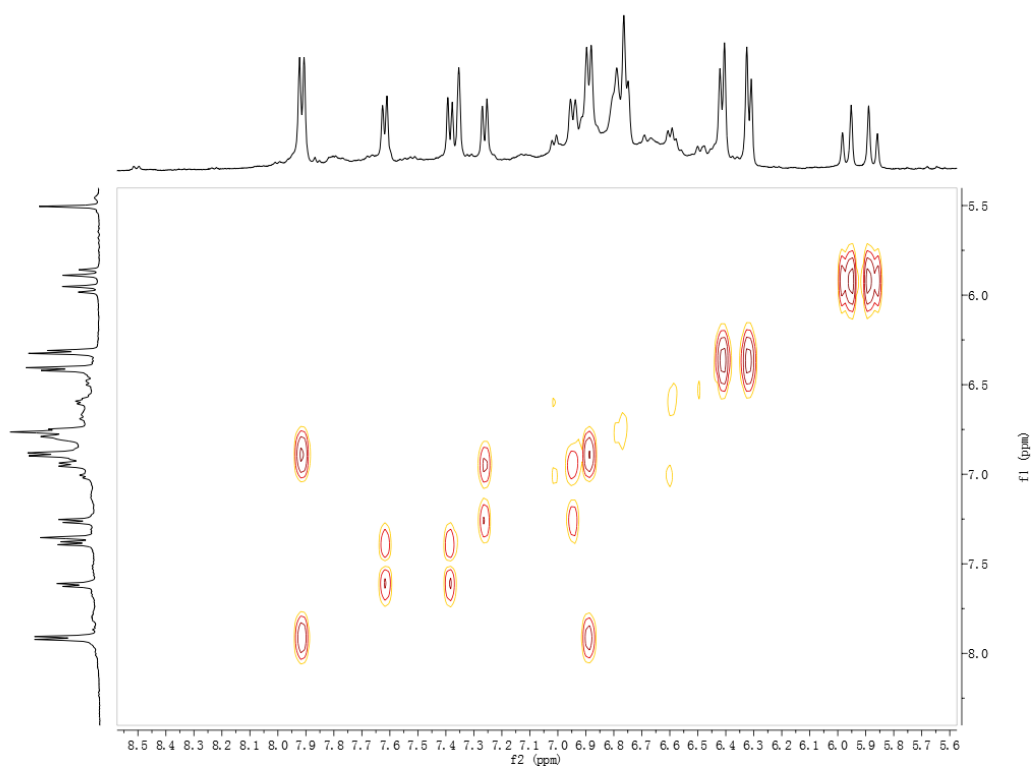


Figure S17. The COSY spectrum of compound **2**.

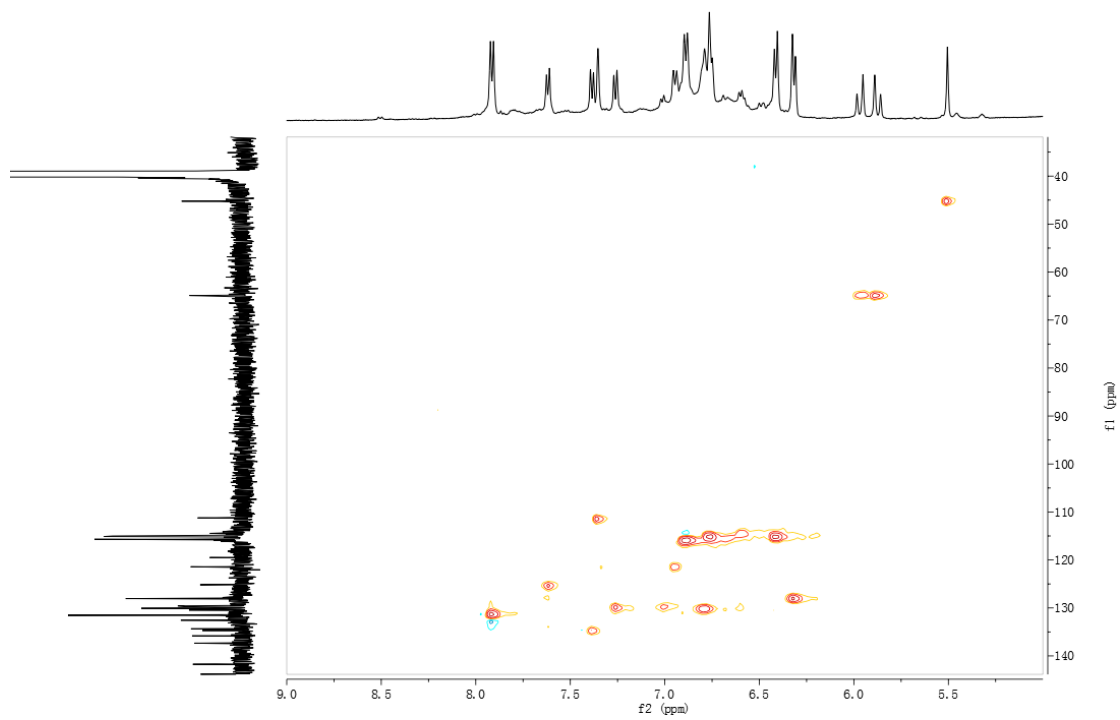


Figure S18. The HSQC spectrum of compound **2**.

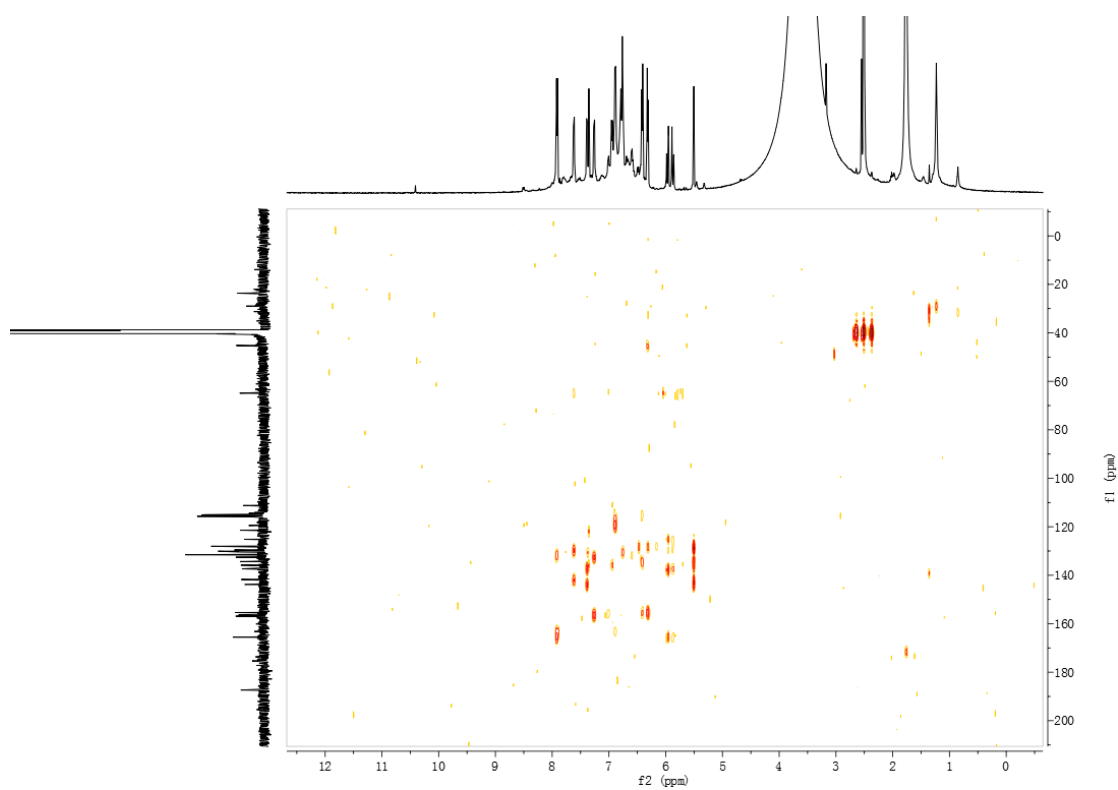


Figure S19. The HMBC spectrum of compound **2**.

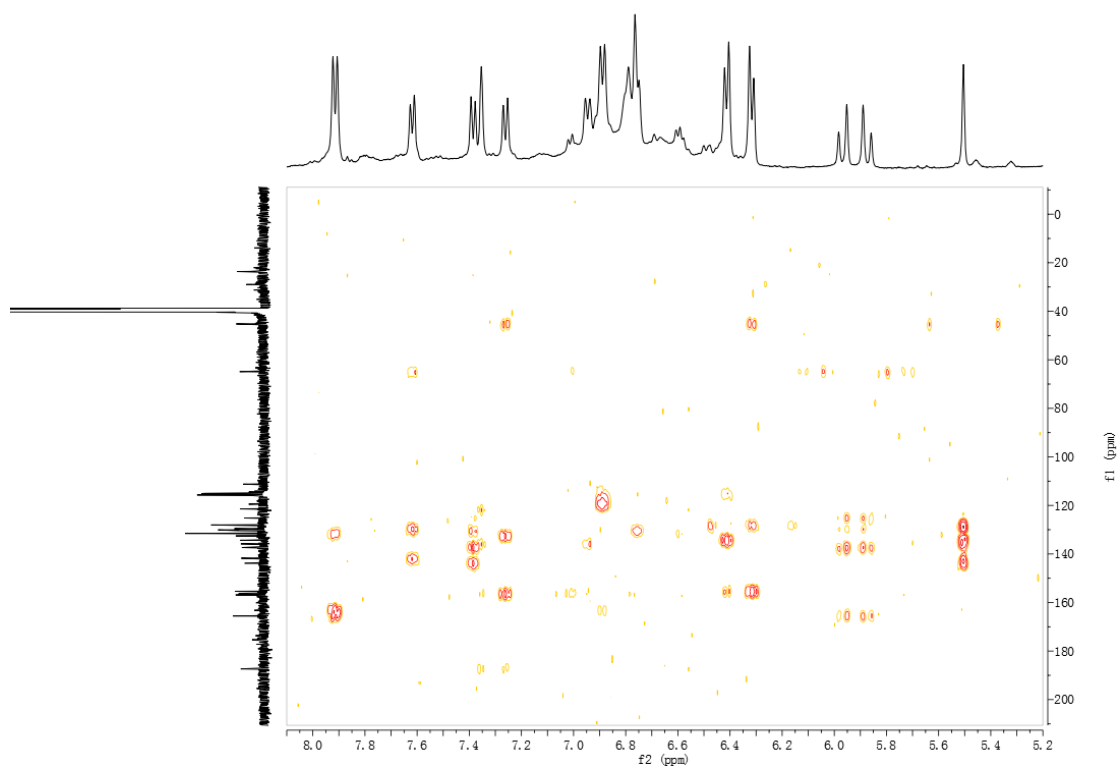


Figure S20. The HMBC spectrum of compound **2**.

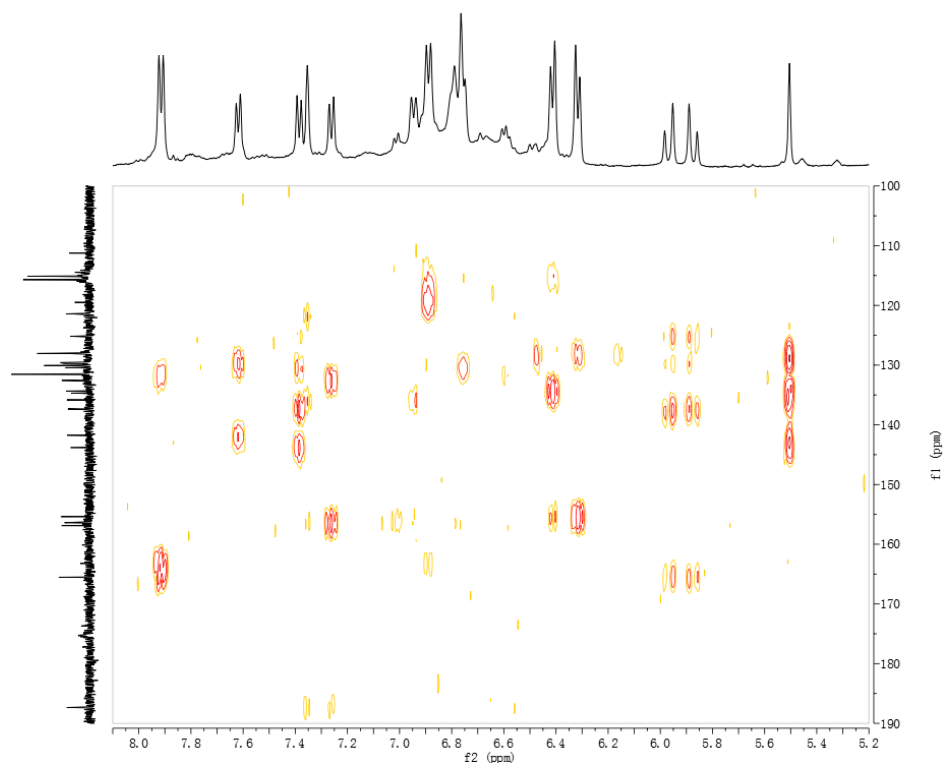


Figure S21. The HMBC spectrum of compound **2**.

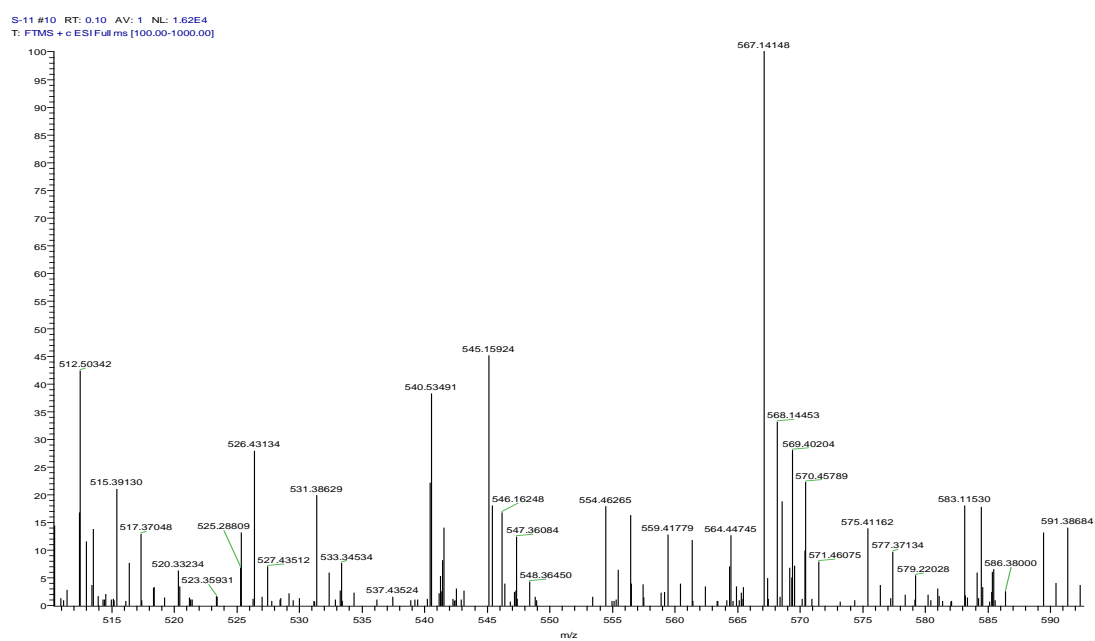


Figure S22. The HR-ESI-MS sepctrum of compound **2**.

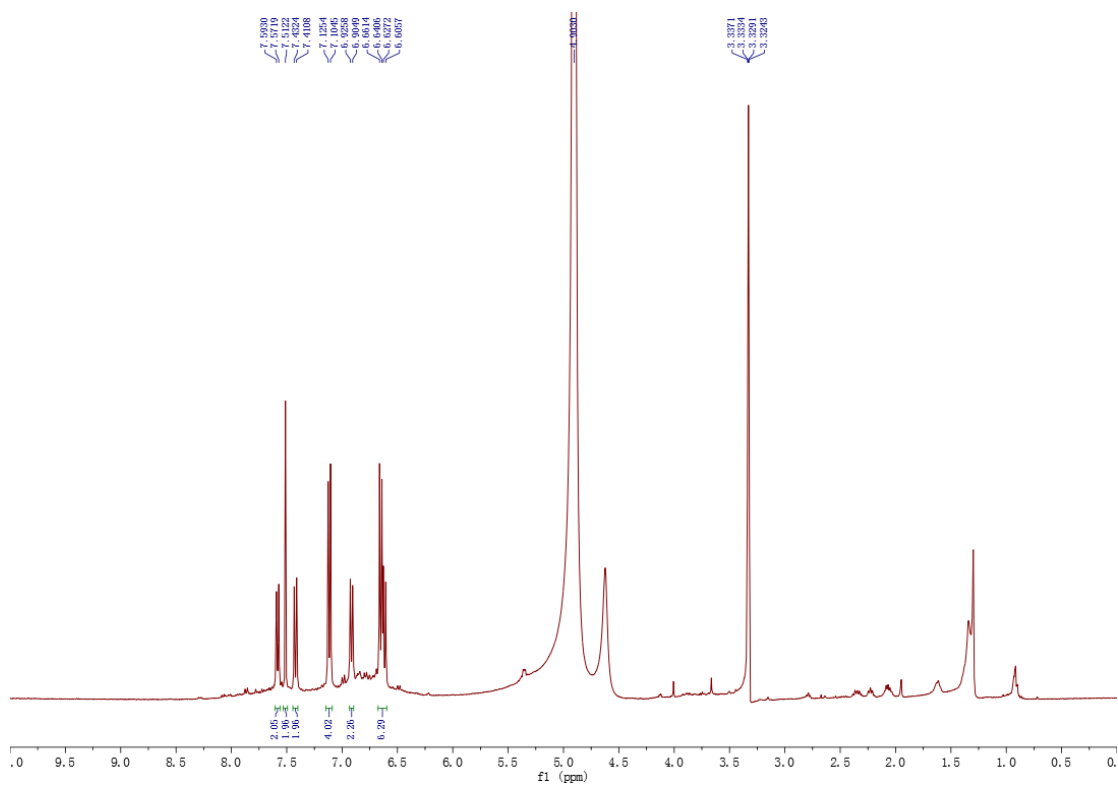


Figure S23. The ¹H NMR (500MHz, CD₃OD) spectrum of compound **3**.

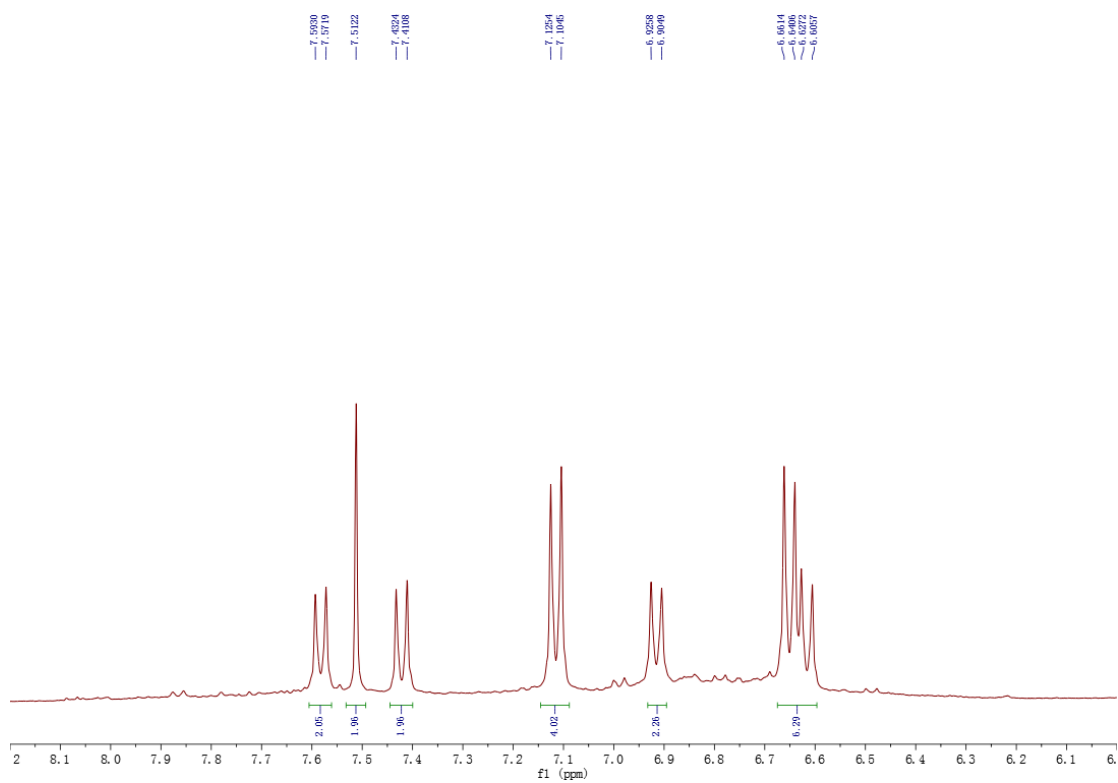


Figure S24. The ^1H NMR (500MHz, CD_3OD) spectrum of compound **3**.

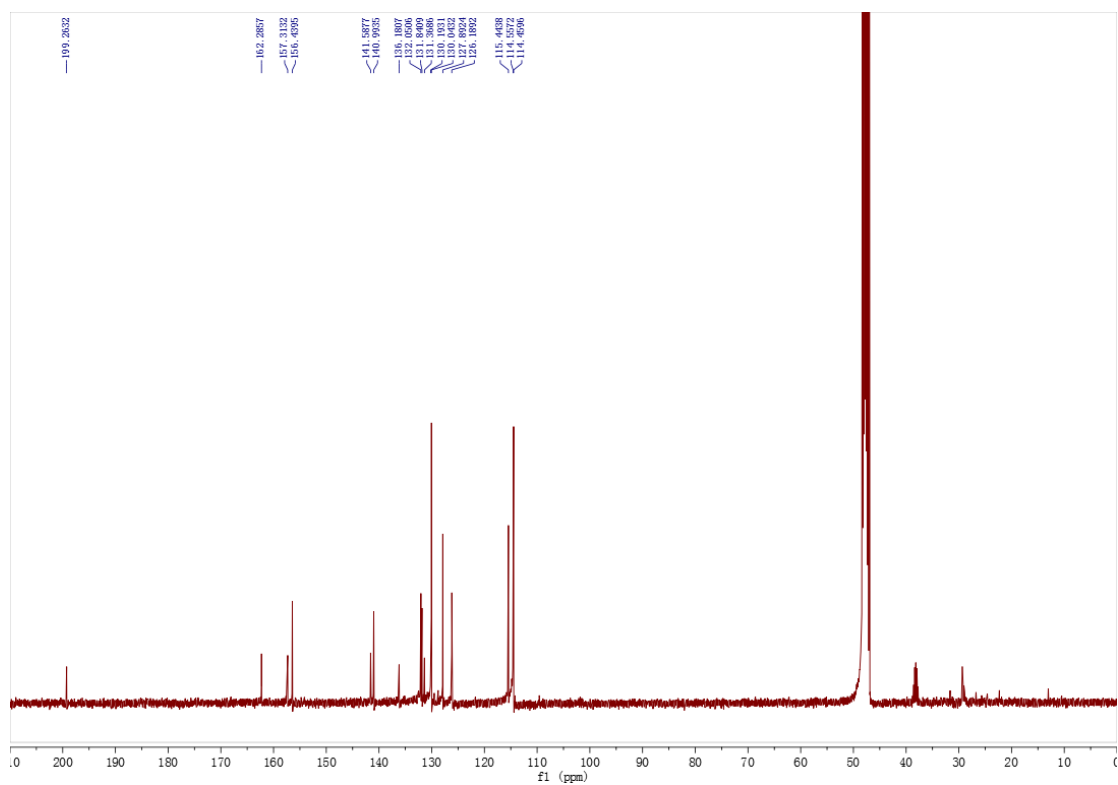


Figure S25. The ^{13}C NMR (125MHz, CD_3OD) spectrum of compound **3**.

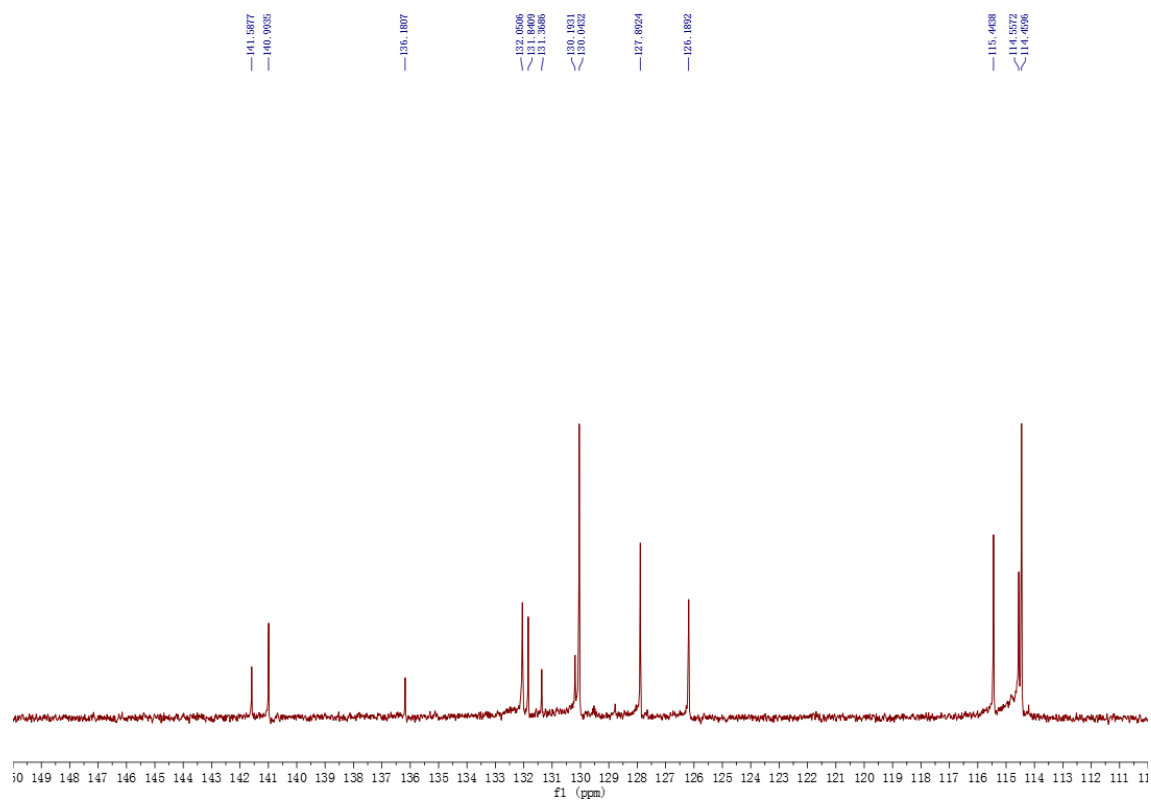


Figure S26. The ^{13}C NMR (125MHz, CD_3OD) spectrum of compound **3**.

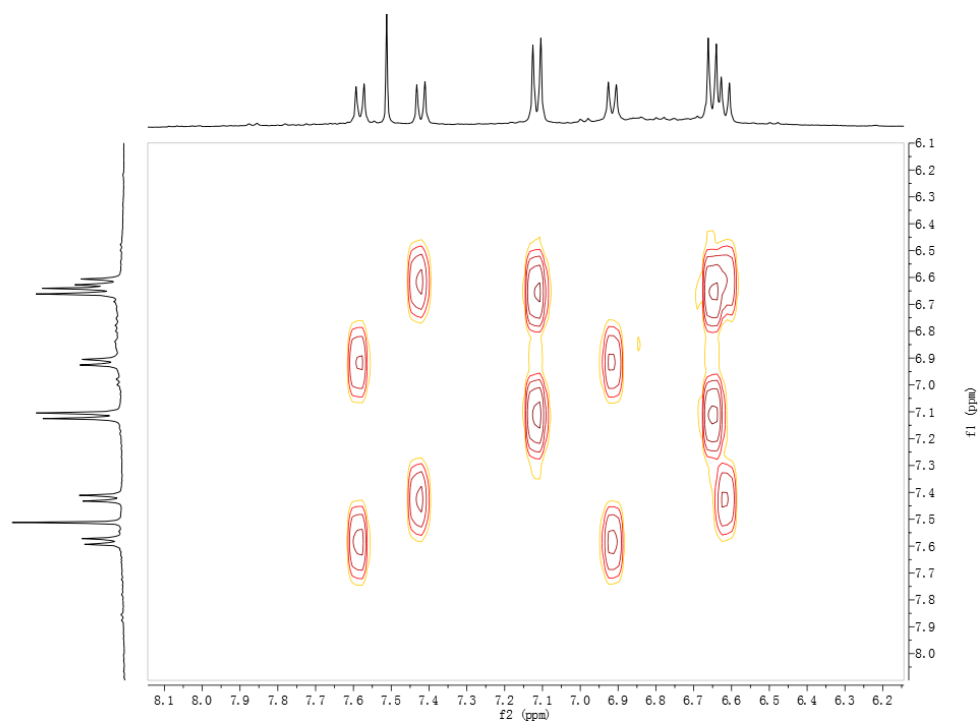


Figure S27. The COSY spectrum of compound **3**.

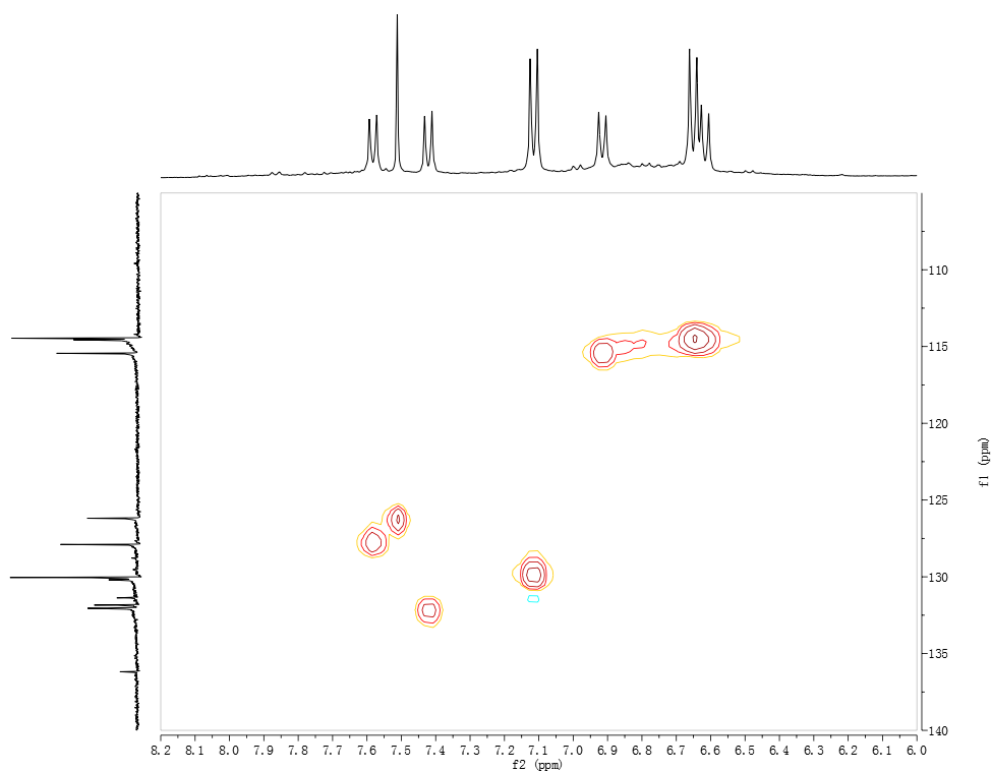


Figure S28. The HSQC spectrum of compound **3**.

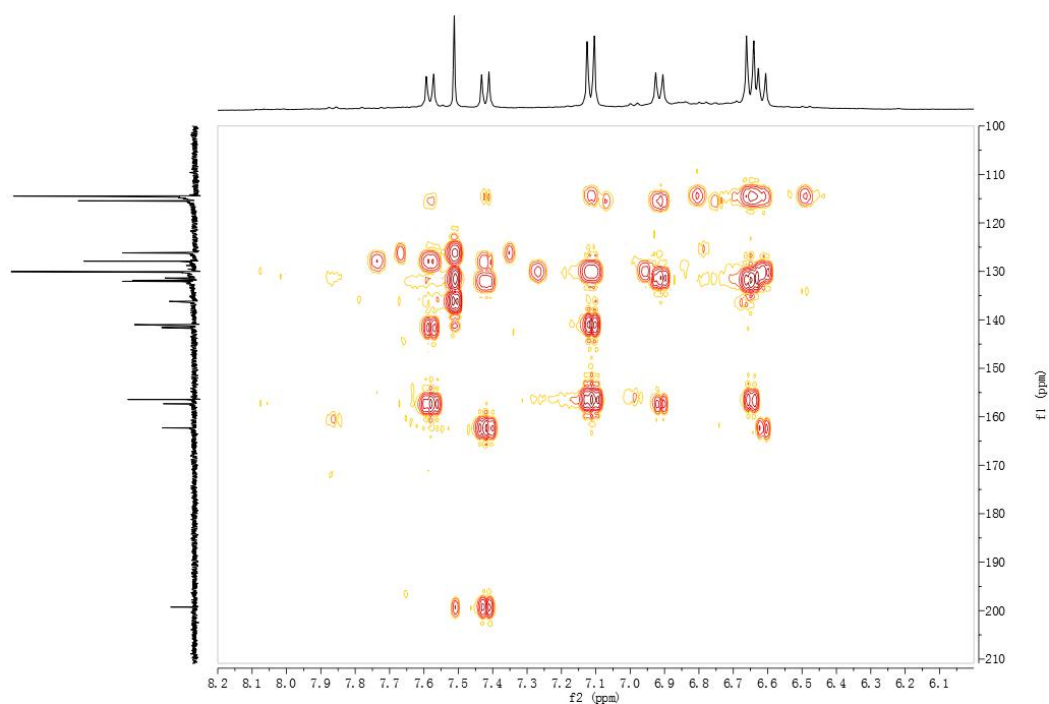


Figure S29. The HMBC spectrum of compound **3**.

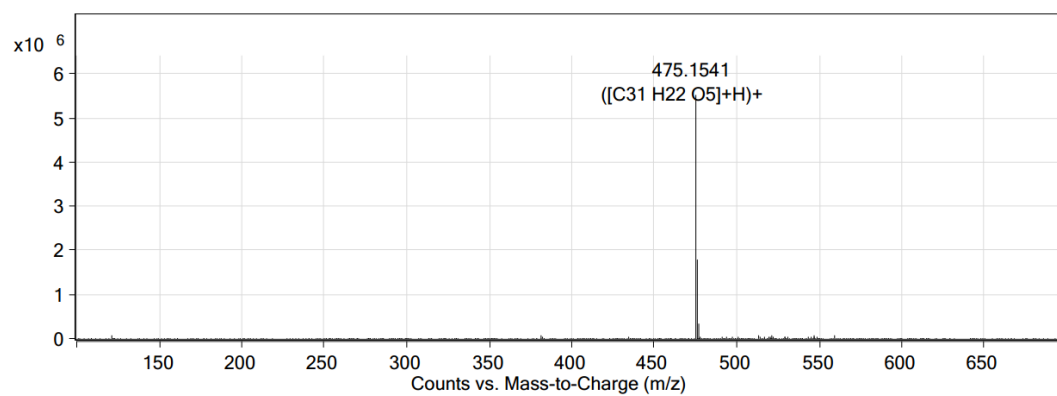


Figure S30. The HR-ESI-MS spectrum of compound **3**.