SUPPLEMENTARY MATERIAL

New cadinane sesquiterpenoids from *Mikania micrantha*

Yao Zhang,[a] You-Mei Zeng,[a] You-Kai Xu,[b] Shu-Qi Wu,[a] Shen Li,[a] Hai-Yan Tian[c*] and Sheng Yin[a*]

[a]*School of Pharmaceutical Sciences, Sun Yat-sen University, Guangzhou 510006, China*

[b]*Key Laboratory of Tropical Plant Resource and Sustainable Use, Xishuangbanna Tropical Botanica Garden, Chinese Academy of Science, Menglun, Yunnan 666303, China*

[c]*Institute of Traditional Medicine and Natural Products,, College of Pharmacy, Jinan University, Guangzhou 510006, China*

[*]Corresponding author. E-mail:yinsh2@mail.sysu.edu.cn (S. Yin); thytian@jnu.edu.cn (H. Y. Tian).

ABSTRACT

Chemical investigation of the aerial parts of *Mikania micrantha* led to the isolation of eight sesquiterpenoids and ten diterpenoids, including five cadinane sesquiterpenoids (**1**–**5**), three bisabolene sesquiterpenoids (**6–8**), nine *ent*-kaurane diterpenoids (**9**–**17**), and an abietane diterpenoid (**18**). Among them, **1–3** are new and feature a rare lactone or furan ring derived from C-6 isopropyl group side chain. Compound **18** was isolated from genus *Mikania* for the first time, and was also the first example of abietane-type diterpenoids from this plant. Their structures were elucidated on the basis of an extensive spectroscopic analysis (1D and 2D NMR, HRESIMS, and ECD). All compounds were examined for their inhibitory effects on lipopolysaccharide (LPS)-induced nitric oxide

(NO) production in RAW 264.7 macrophage cells, and compound **18** exhibited pronounced inhibition on NO production (IC_{50} = 11.04 μM), being comparable to the positive control, quercetin (IC_{50} = 11.15 μM).

Keywords: *Mikania micrantha*; Cadinane sesquiterpenoids; Anti-inflammatory activities

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Table S1. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data for **1**–**3** (δ in ppm) in $CDCl_3$.

No.	**1**		**2**		**3**	
	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C
1	2.19, m	26.4	2.01, m	24.0	1,98, m	25.4
	1.31 m		1.66,m		1.77, m	
2	2.04, m	31.2	1.95,m	25.2	1.98, m	26.3
	1.82, m		1.86,m		1.98, m	
3		81.8		136.4		135.5
4	5.84, s	132.3	5.02, s	119.6	5.34, s	119.2
5		134.4	3.57, s	38.1	3.54, dd (4.7,2.3)	33.7
6		158.6		165.9		140.5
7	4.69, m	79.8	4.64, m	78.5		146.2
8	2.38, m	39.7	2.33, m	41.5		188.7
	1.20 m		1.00, m			
9	1.44, m	34.9	1.75, m	26.1	2.59, m	41.3
10	1.77, m	44.2	1.42, m	40.9	2.23, m	40.2
11		121.0		119.5		120.6
12		174.6		175.0	7.35, s	144.8
13	1.92, s	9.1	1.82, s	8.2	2.07, s	8.2
14	1.07, d (6.5)	19.1	0.99, d (6.7)	19.2	1.24, d (7.0)	12.1
15	1.33,s	23.9	1.66, s	23.5	1.69, s	23.4

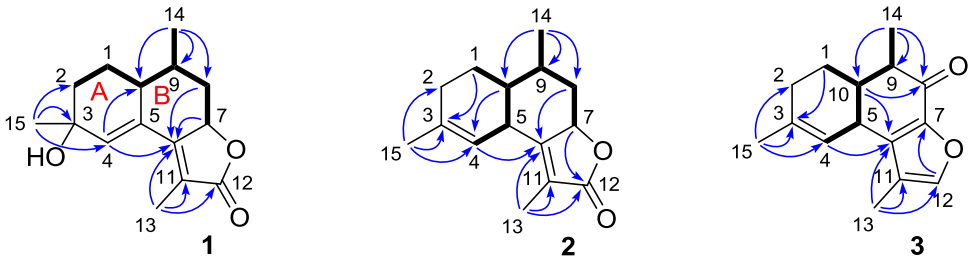


Figure S1. Key ^{1}H–^{1}H COSY and HMBC correlations of compounds **1**–**3**

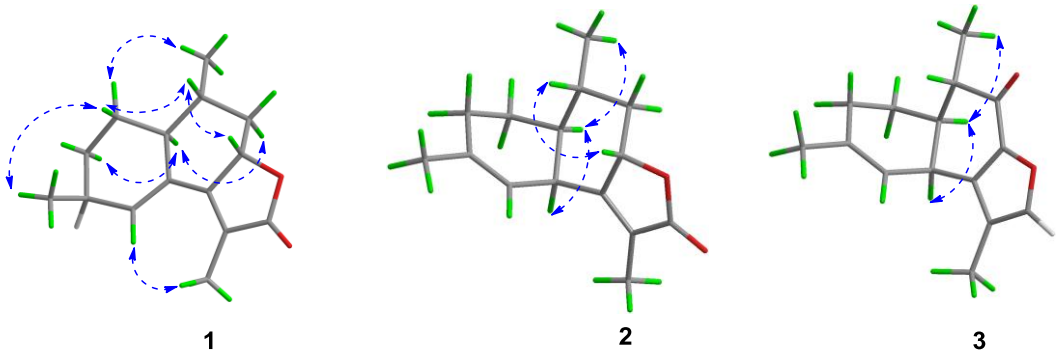


Figure S2. Key NOESY correlations of compounds **1–3**

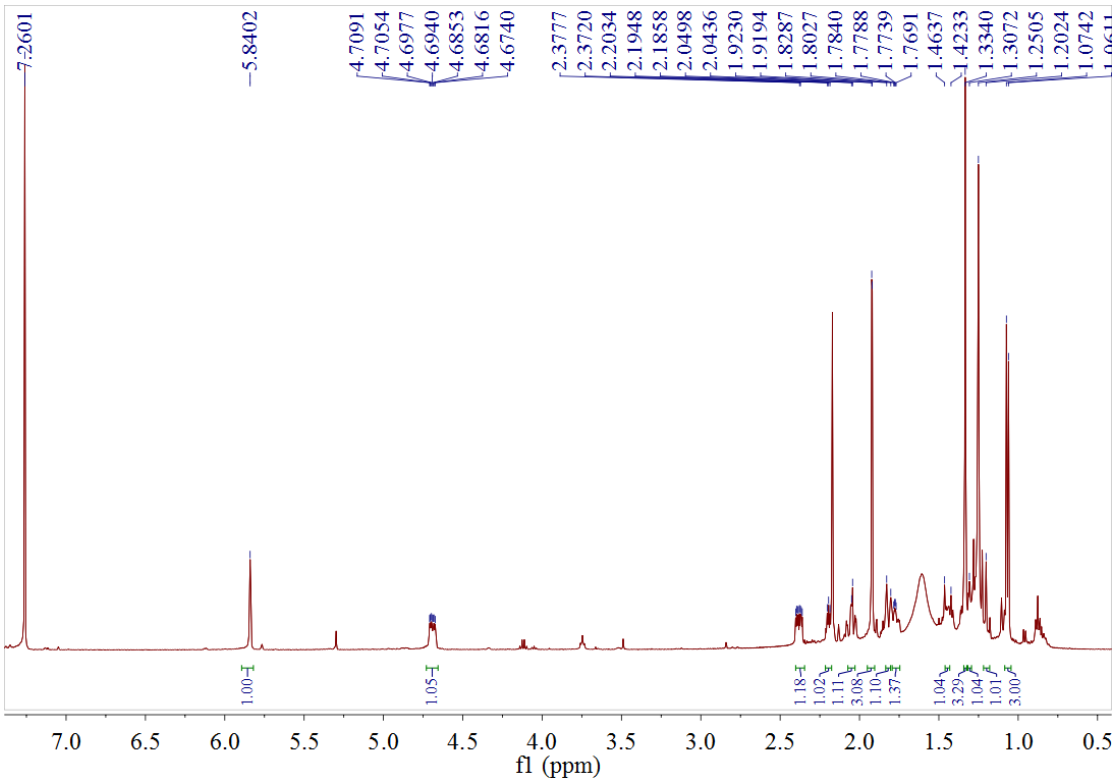


Figure S3. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **1**

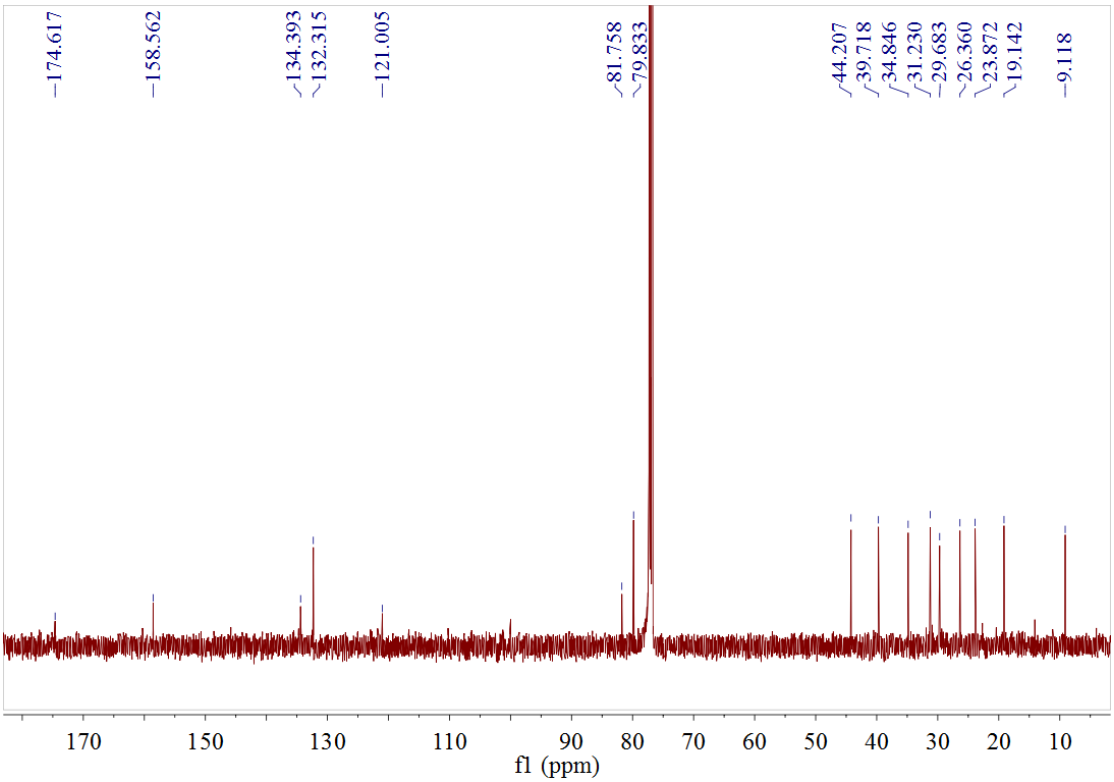


Figure S4. ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **1**

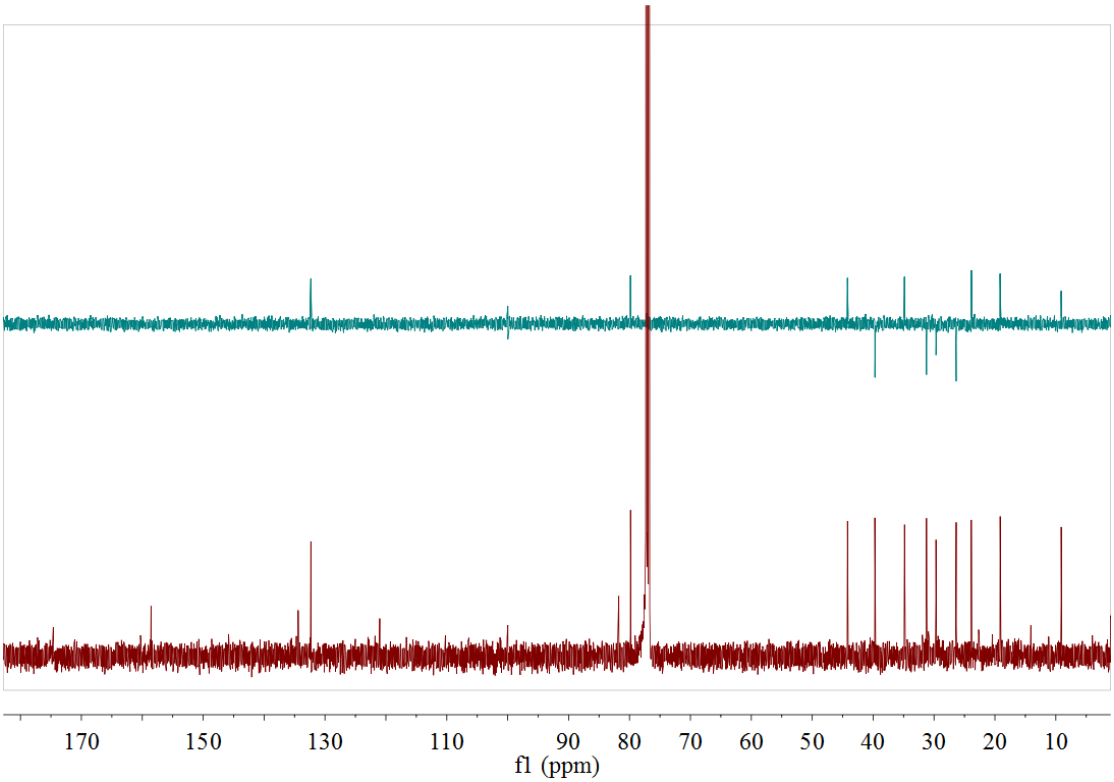


Figure S5. DEPT135 spectrum of compound **1** in$CDCl_3$

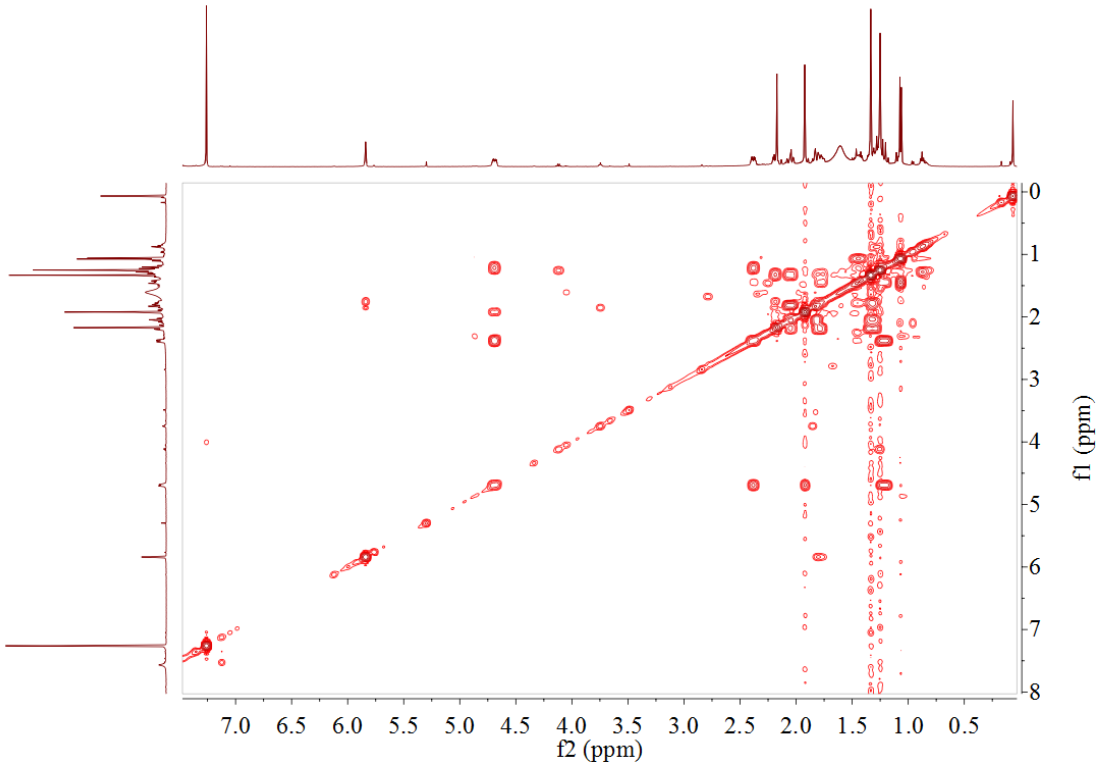


Figure S6. ^{1}H- ^{1}H COSY spectrum of compound **1** in $CDCl_3$

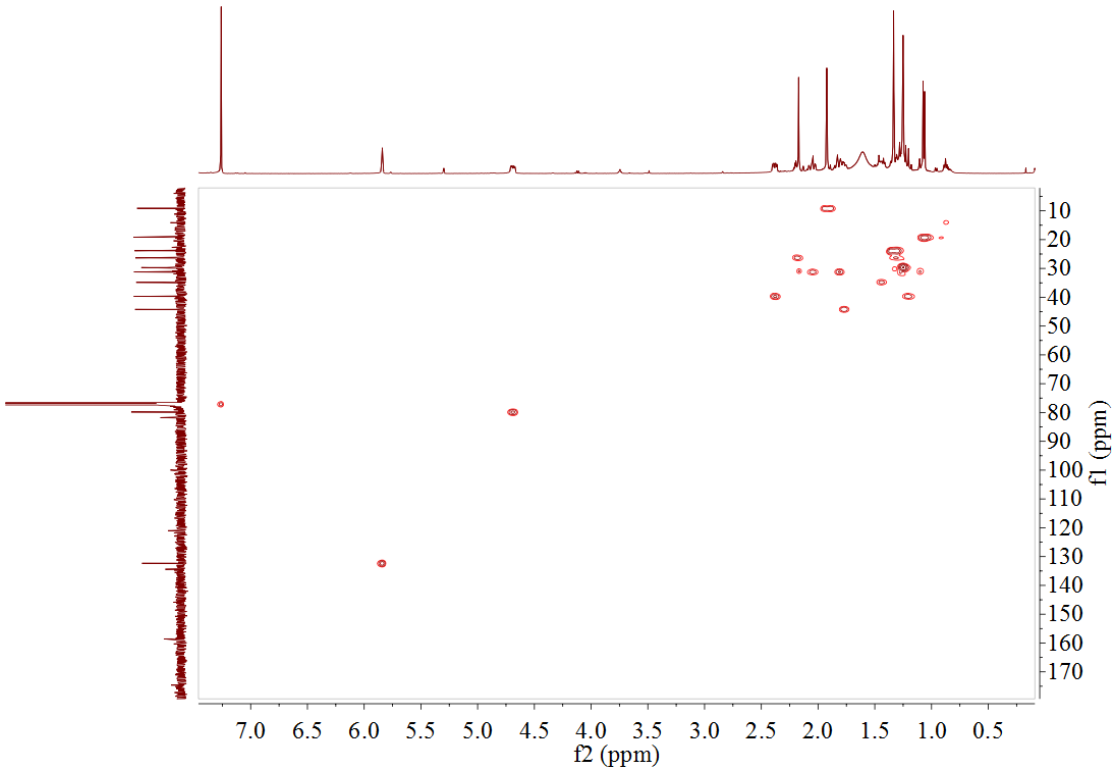


Figure S7. HSQC spectrum of compound **1** in $CDCl_3$

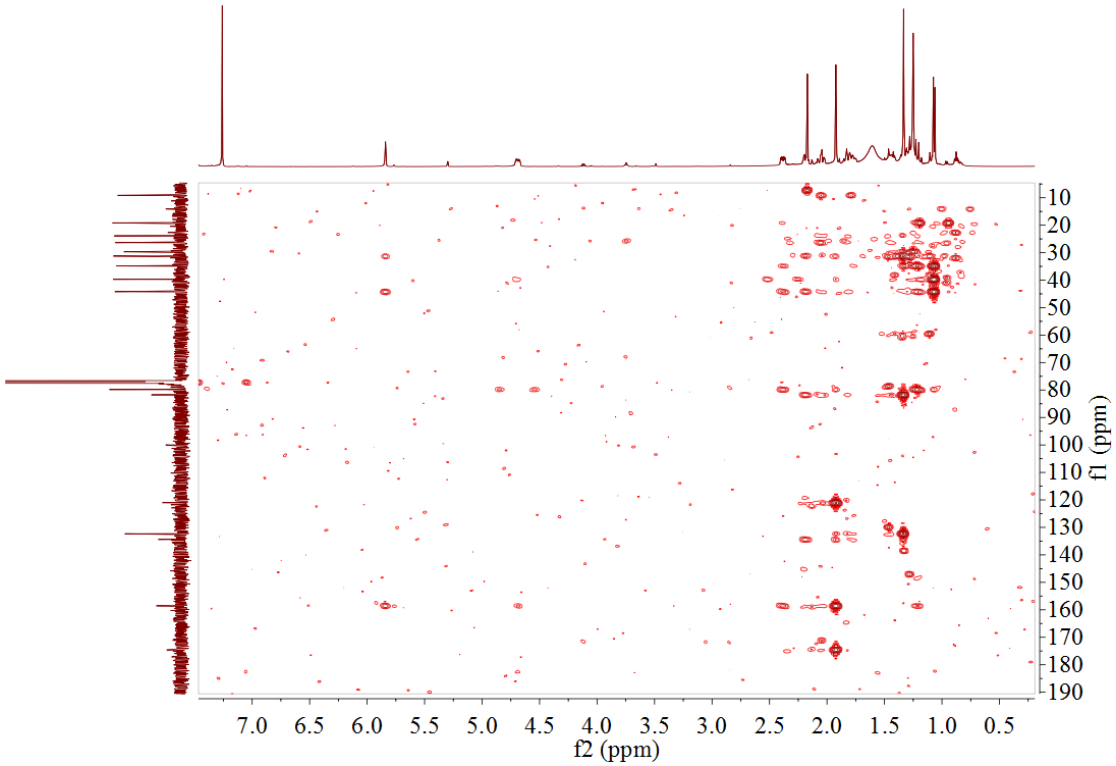


Figure S8. HMBC spectrum of compound **1** in $CDCl_3$

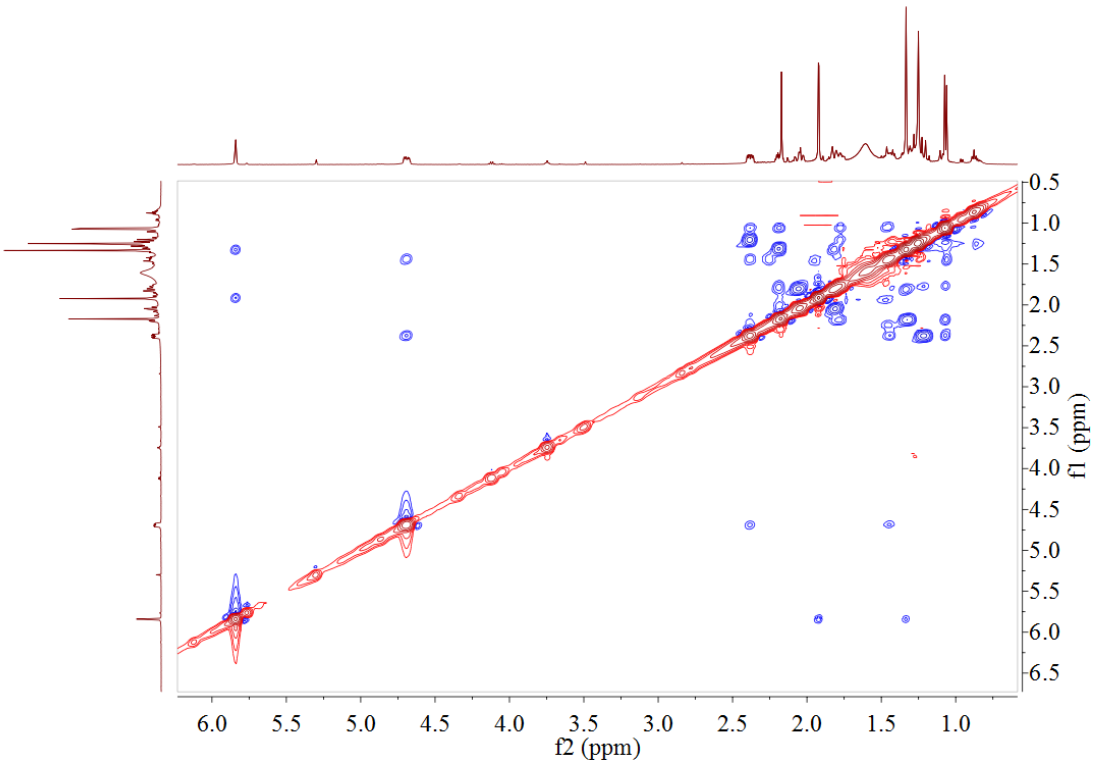


Figure S9. NOESY spectrum of compound **1** in $CDCl_3$

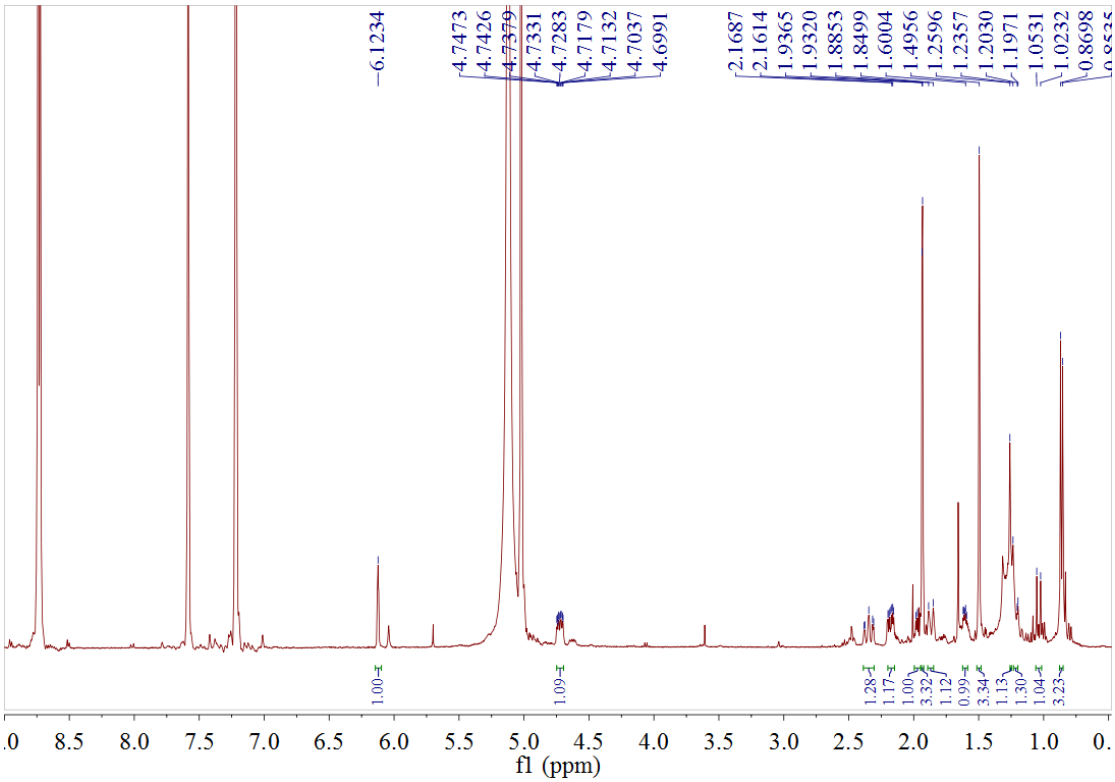


Figure S10. ^{1}H NMR (pyridine-d_5, 400 MHz) spectrum of compound **1**

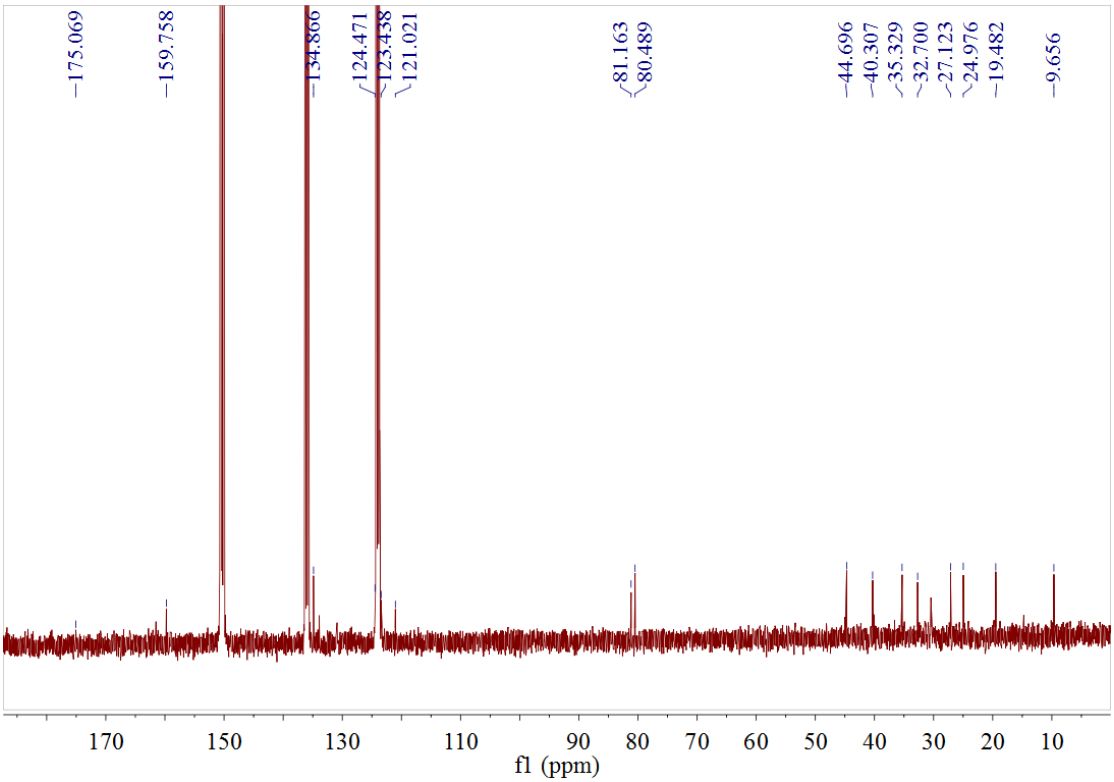


Figure S11. ^{13}C NMR (pyridine-d_5, 100 MHz) spectrum of compound **1**

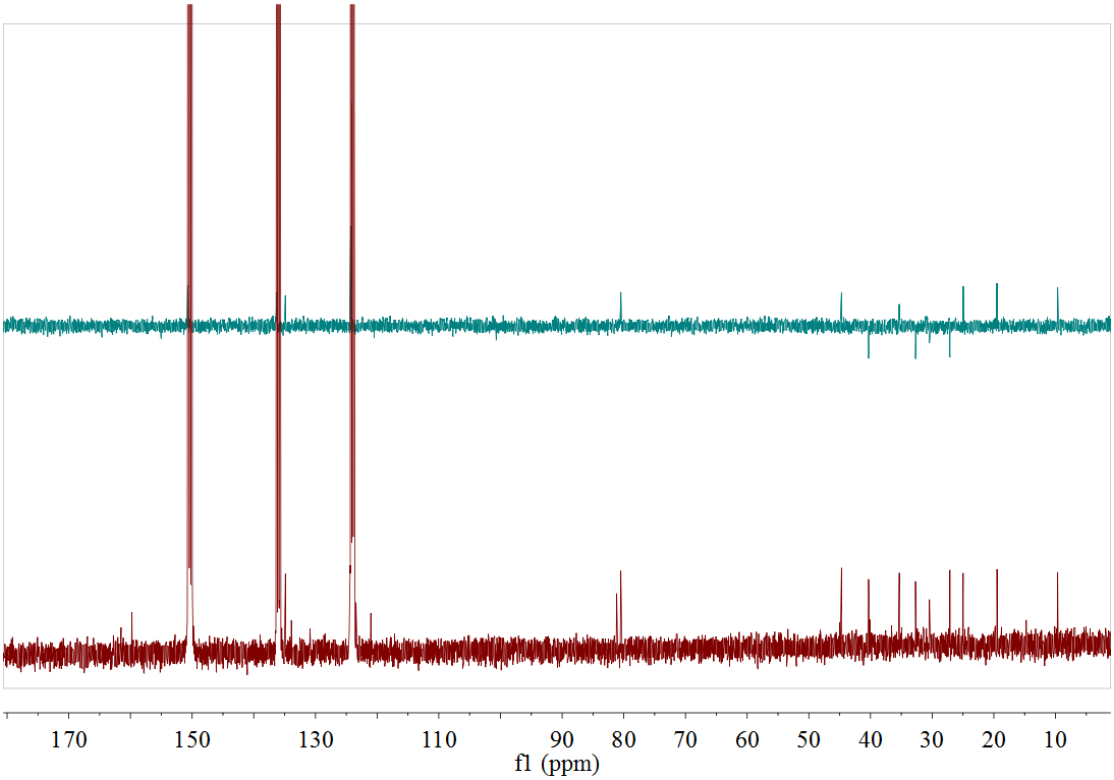


Figure S12. DEPT135 spectrum of compound **1** in pyridine-d_5

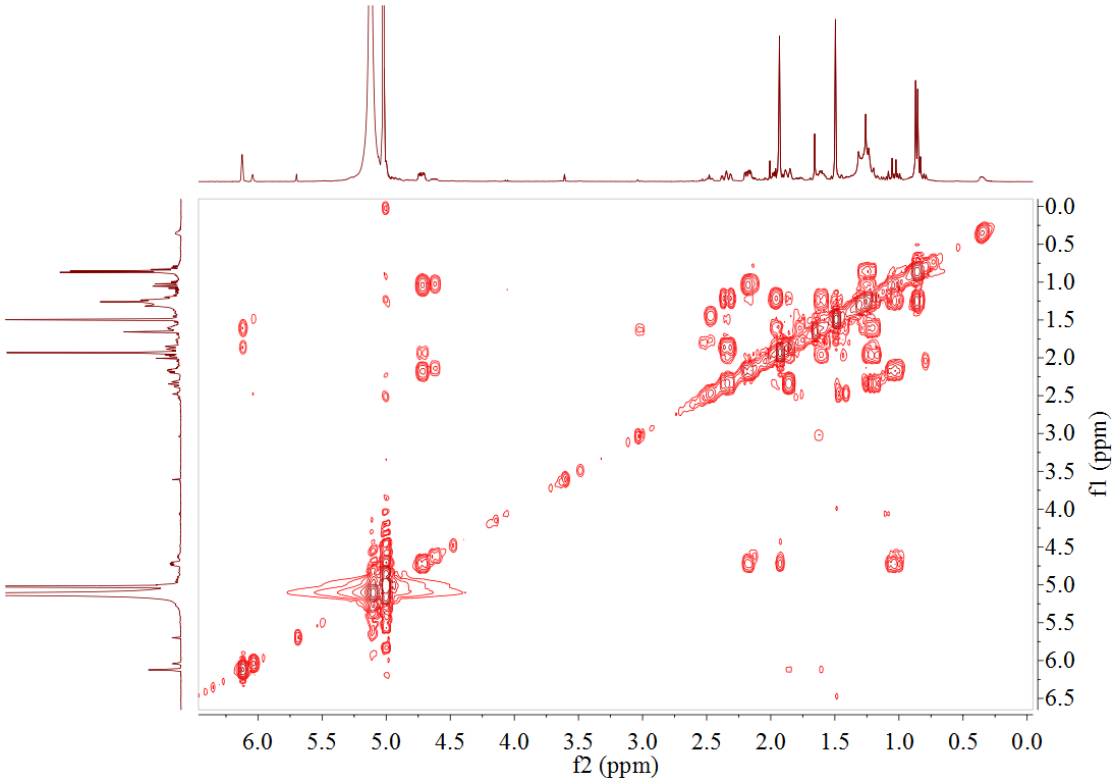


Figure S13. ^{1}H- ^{1}H COSY spectrum of compound **1** in pyridine-d_5

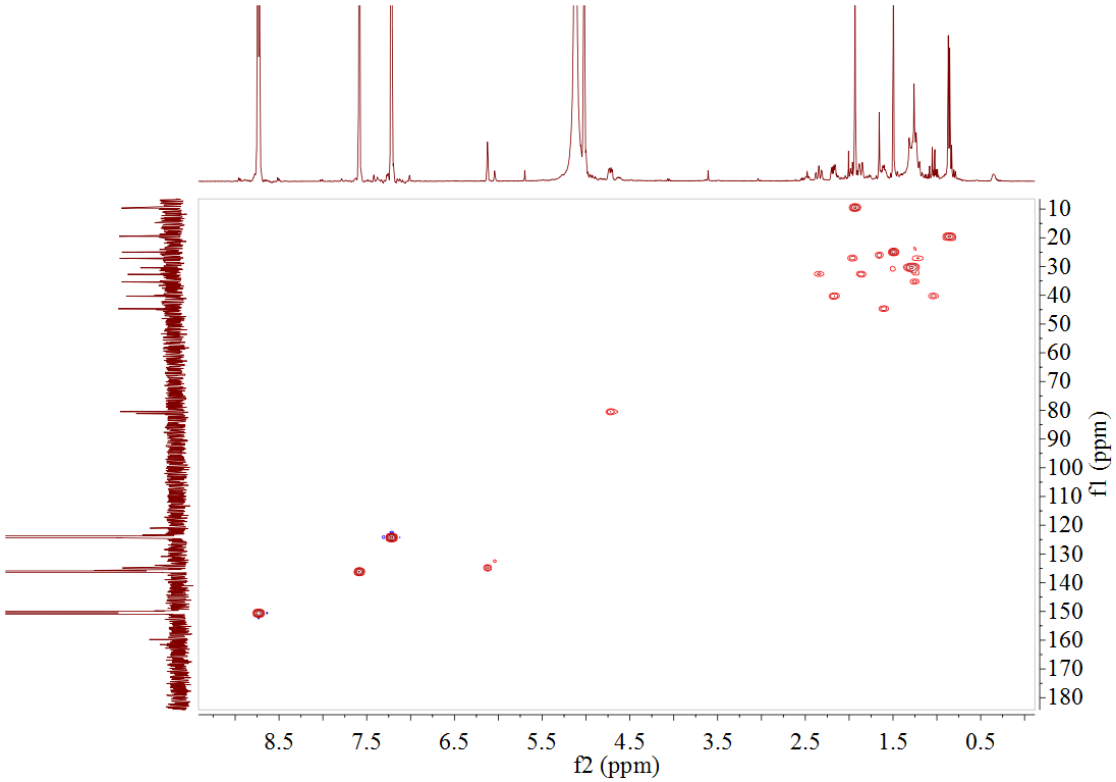


Figure S14. HSQC spectrum of compound **1** in pyridine-d_5

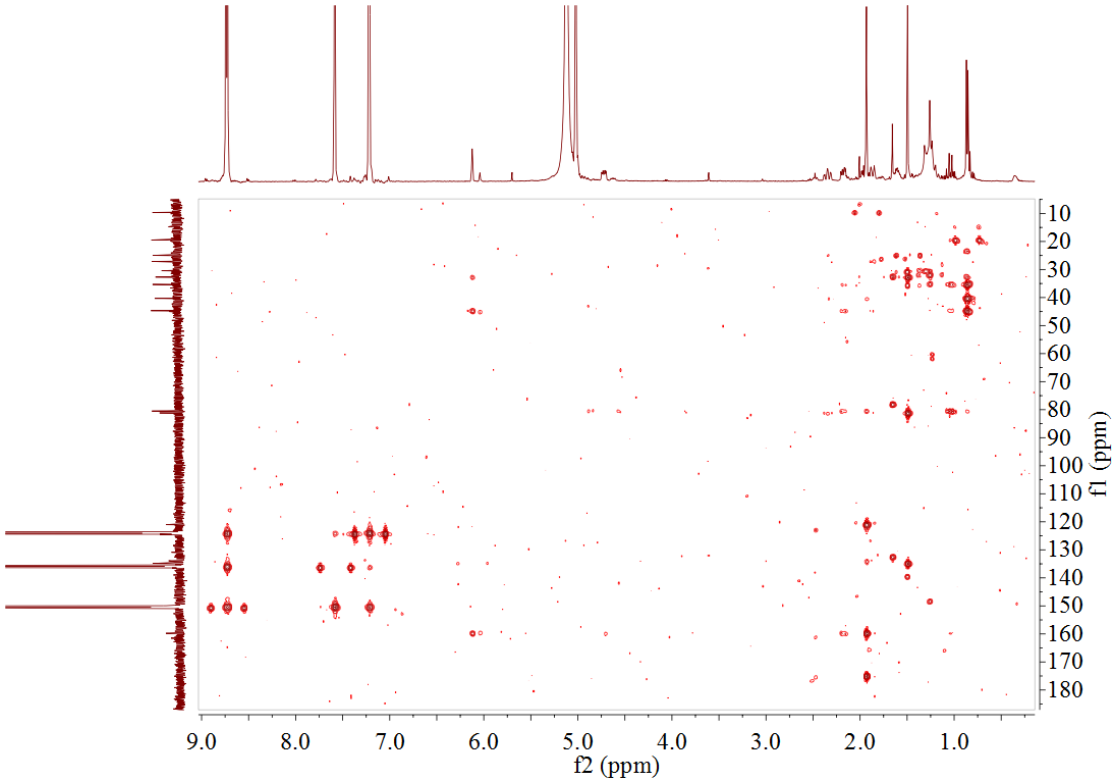


Figure S15. HMBC spectrum of compound **1** in pyridine-d_5

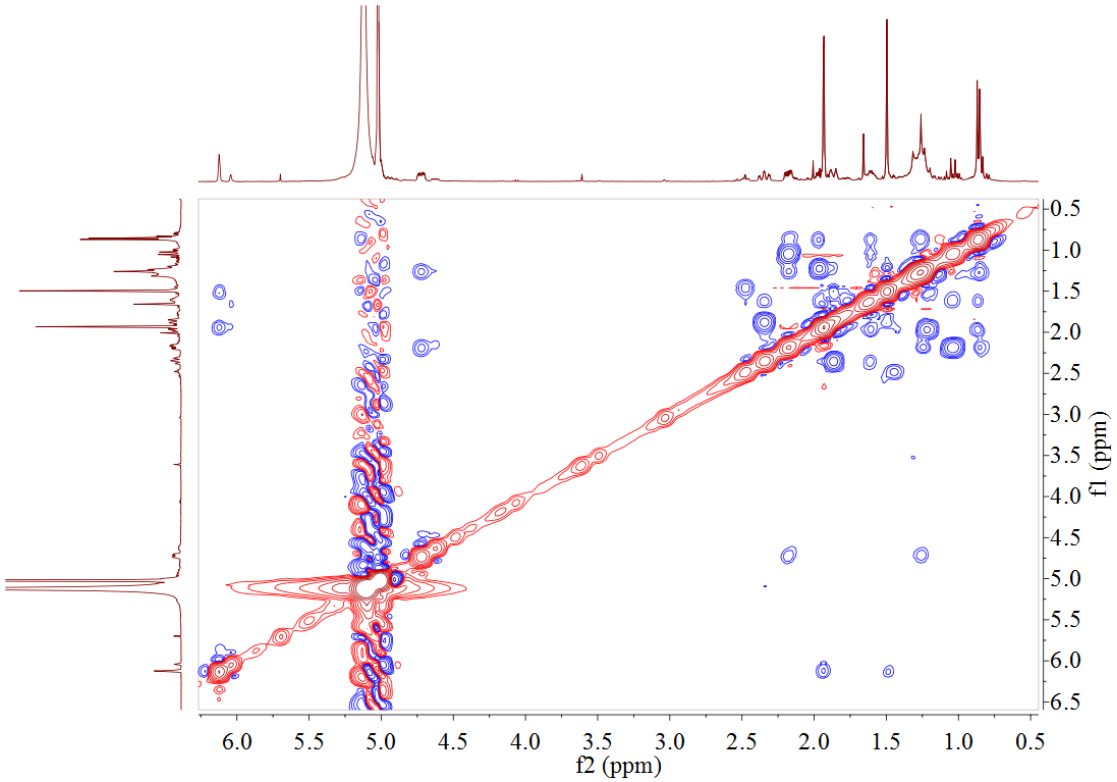
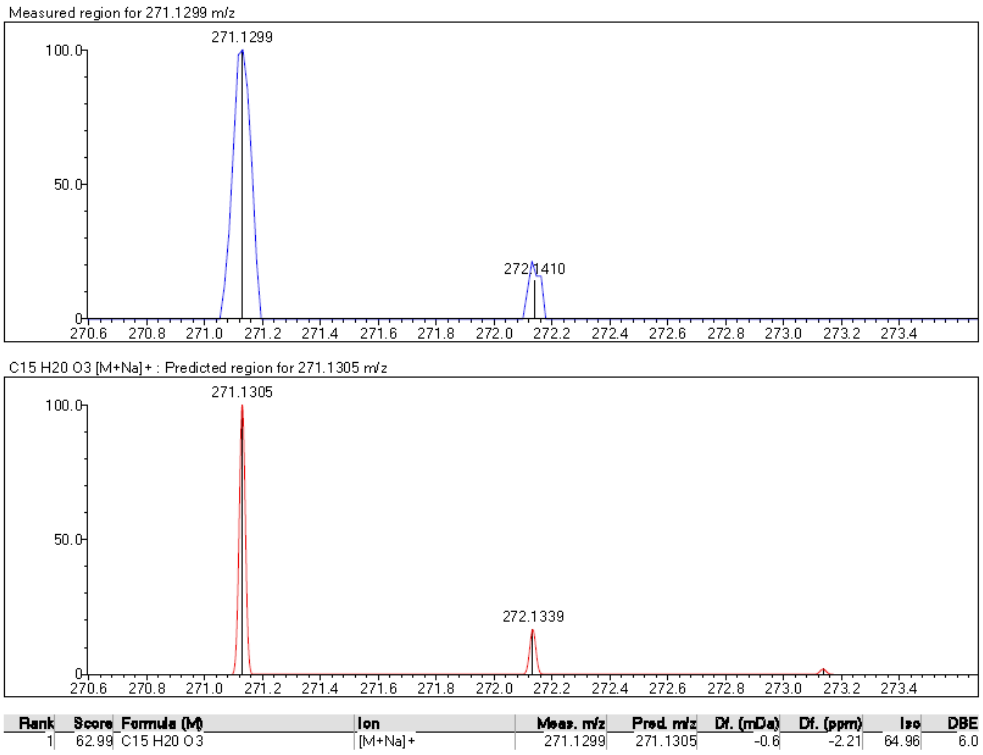


Figure S16. NOESY spectrum of compound **1** in pyridine-d_5



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	62.99	C15 H20 O3	[M+Na]+	271.1299	271.1305	-0.6	-2.21	64.96	6.0

Figure S17. HRESIMS spectrum of **1**

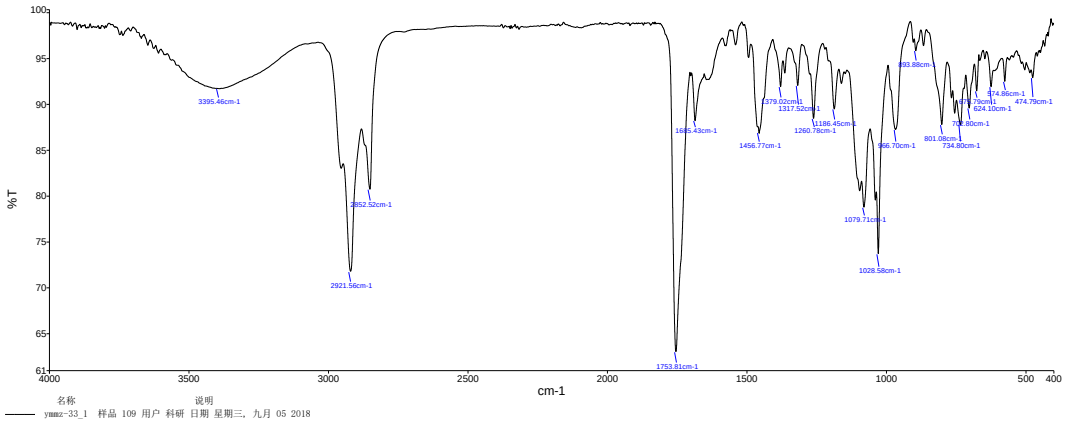


Figure S18. IR (KBr disc) spectrum of **1**

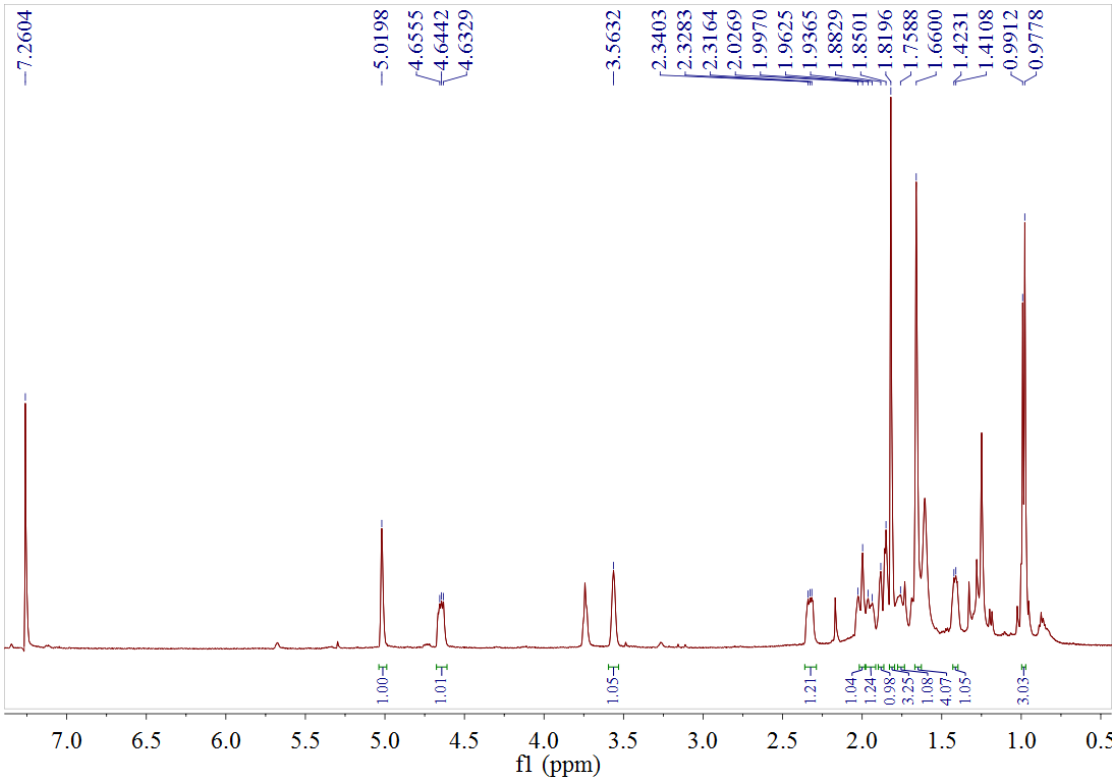


Figure S19. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **2**

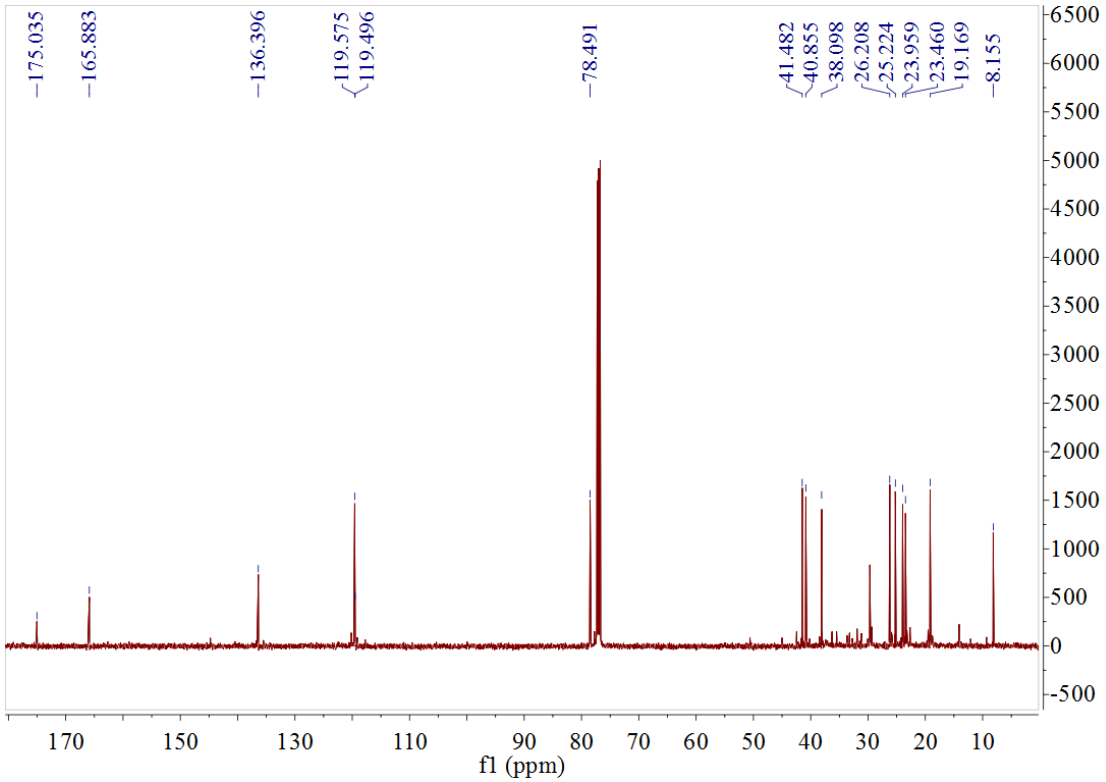


Figure S20. ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **2**

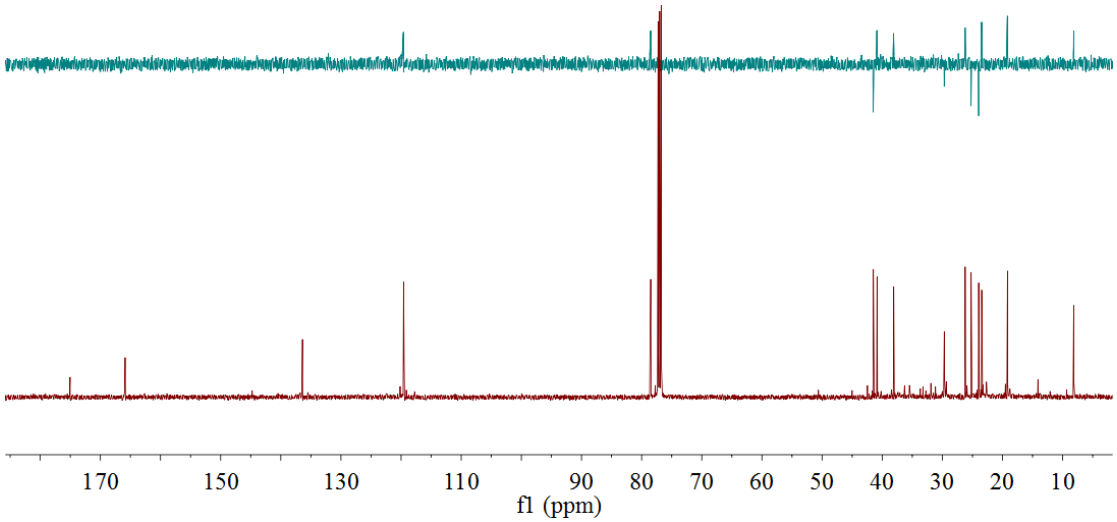


Figure S21. DEPT135 spectrum of compound **2** in$CDCl_3$

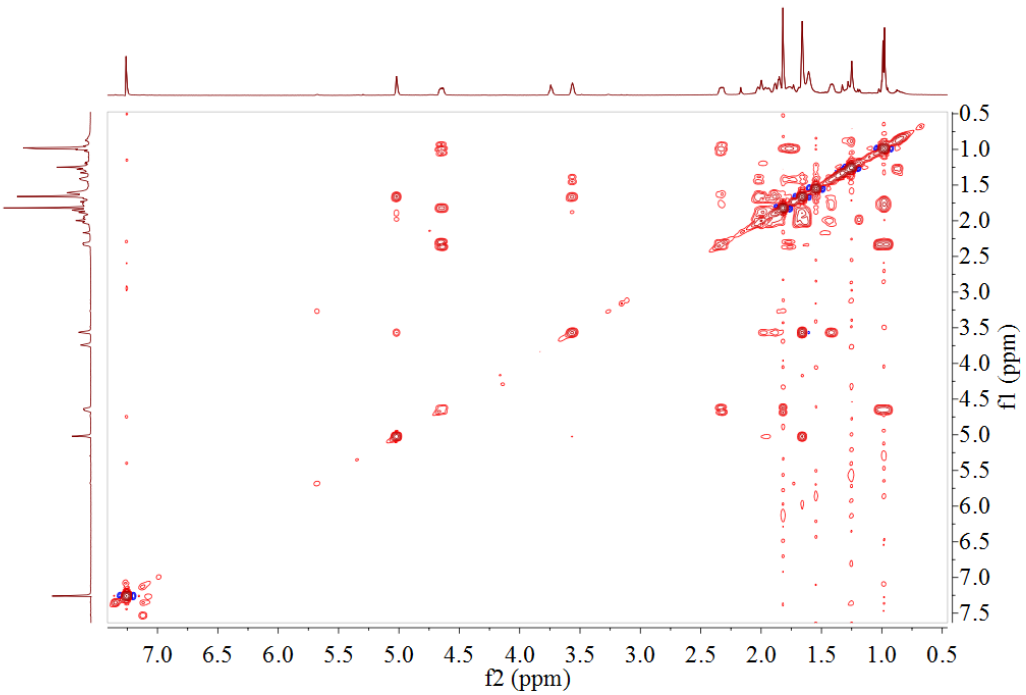


Figure S22. ^{1}H- ^{1}H COSY spectrum of compound **2** in $CDCl_3$

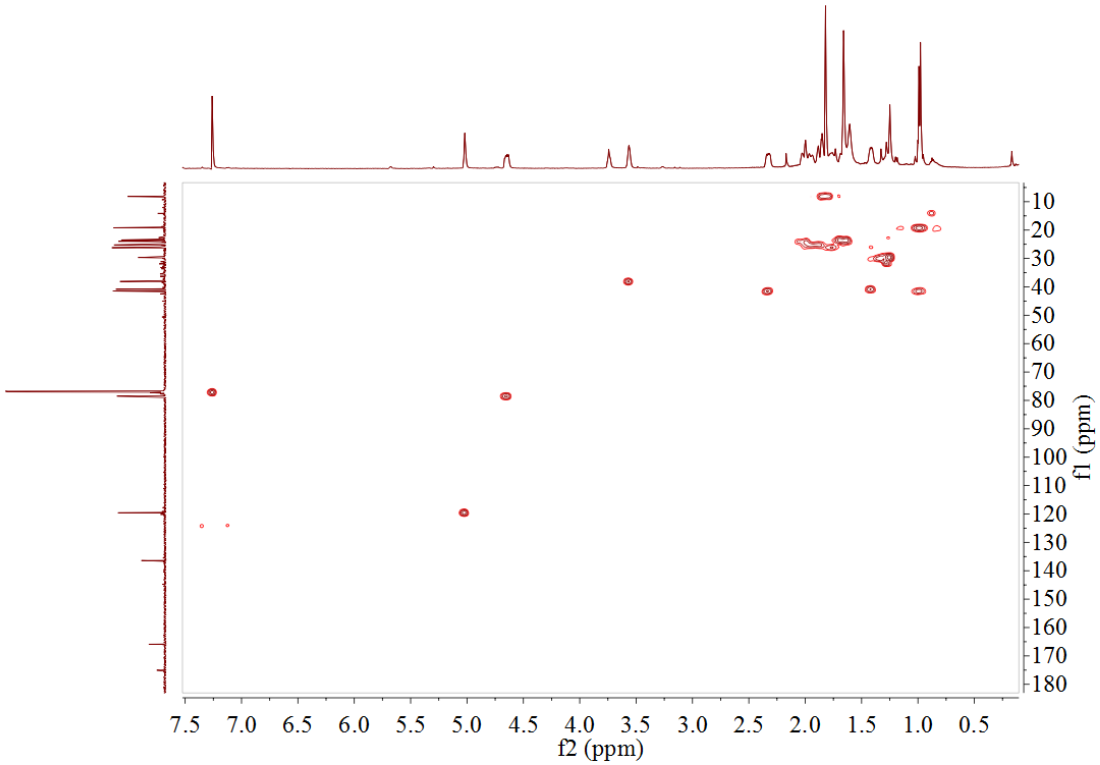


Figure S23. HSQC spectrum of compound **2** in $CDCl_3$

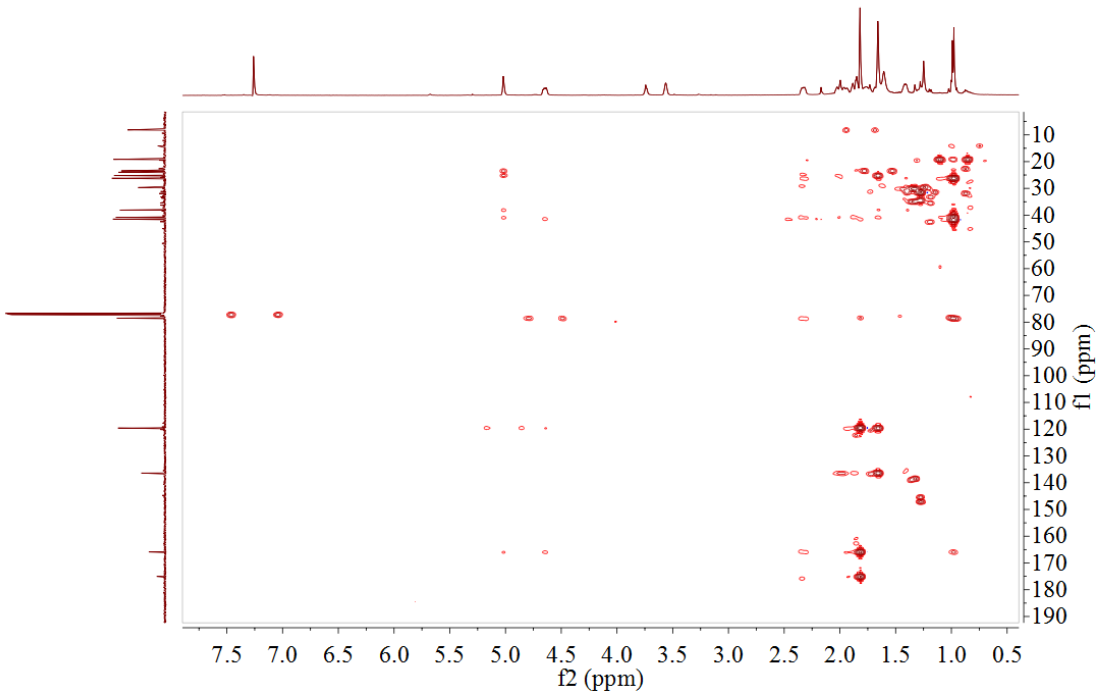


Figure S24. HMBC spectrum of compound **2** in $CDCl_3$

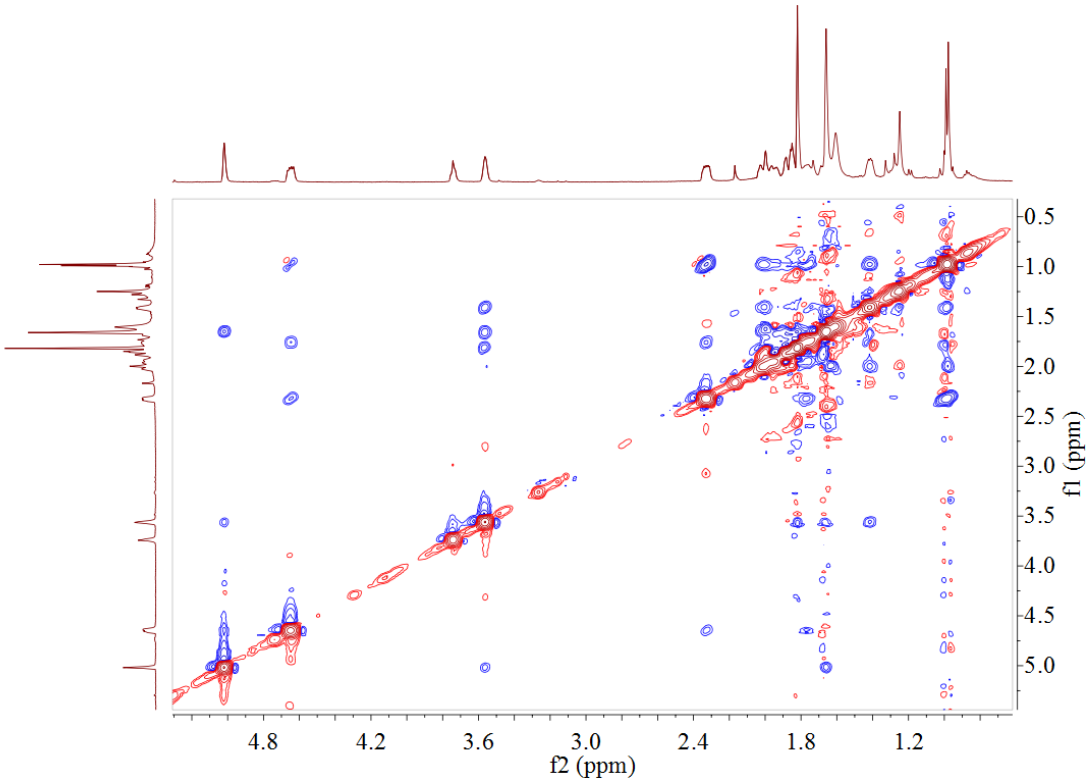


Figure S25. NOESY spectrum of compound **2** in $CDCl_3$

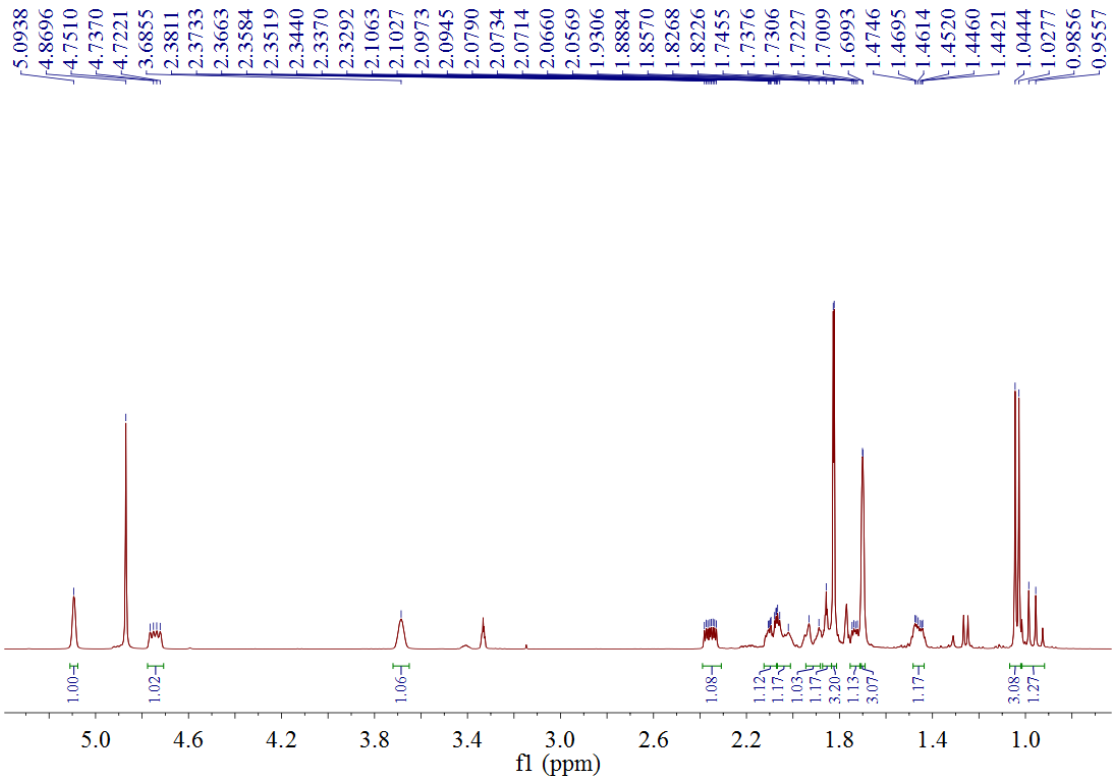


Figure S26. ^{1}H NMR (CD_3OD, 400 MHz) spectrum of compound **2**

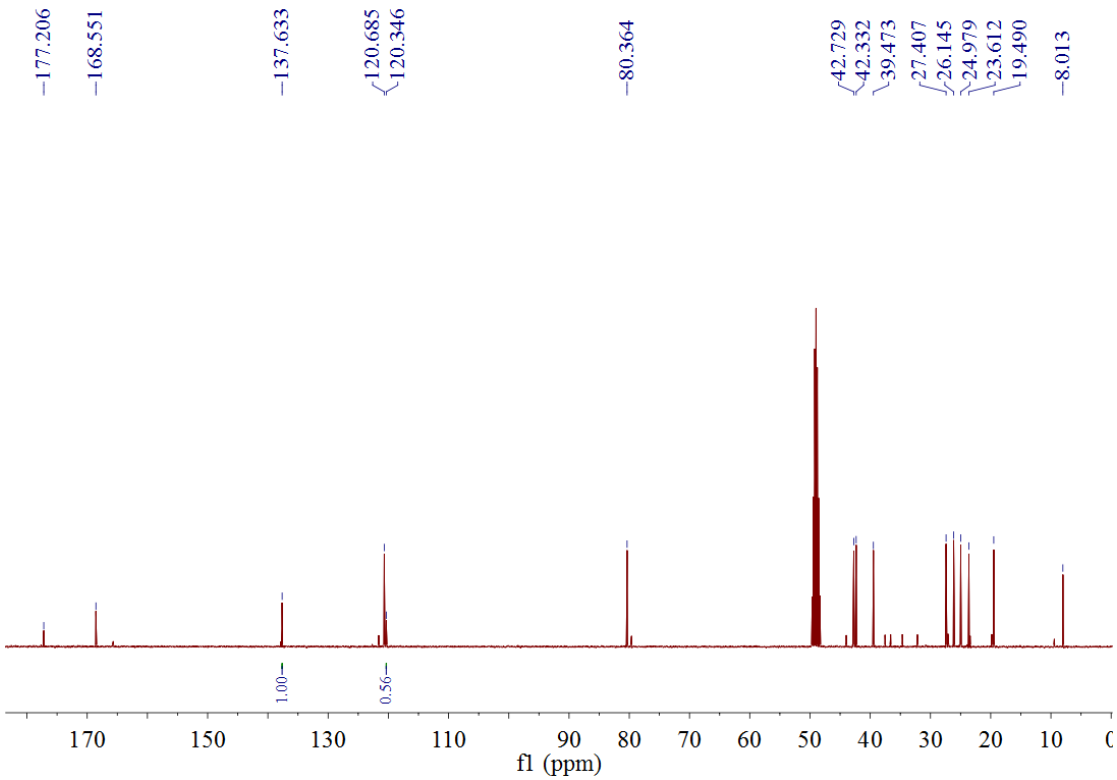


Figure S27. ^{13}C NMR (CD_3OD, 100 MHz) spectrum of compound **2**

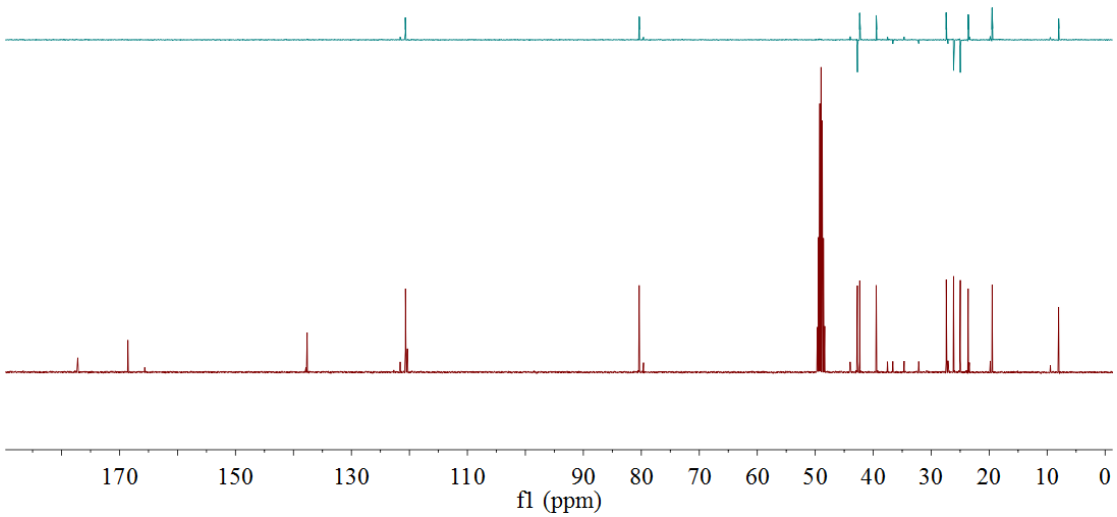


Figure S28. DEPT135 spectrum of compound **2** in CD_3OD

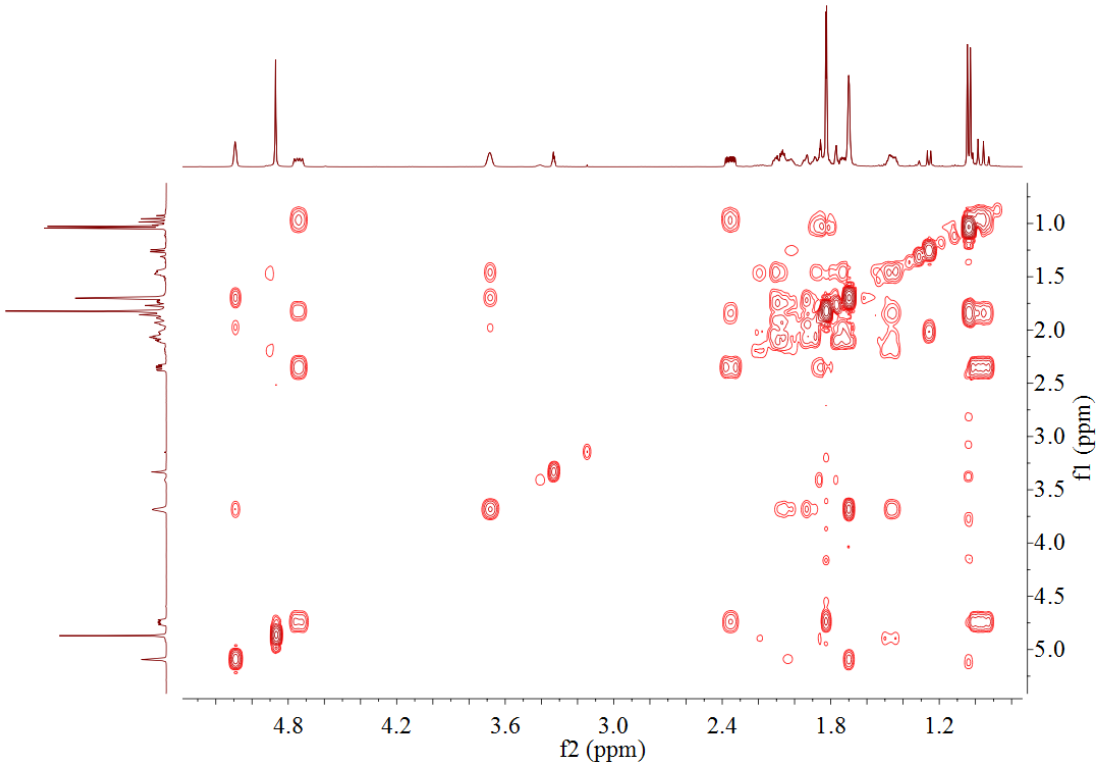


Figure S29. ^{1}H- ^{1}H COSY spectrum of compound **2** in CD_3OD

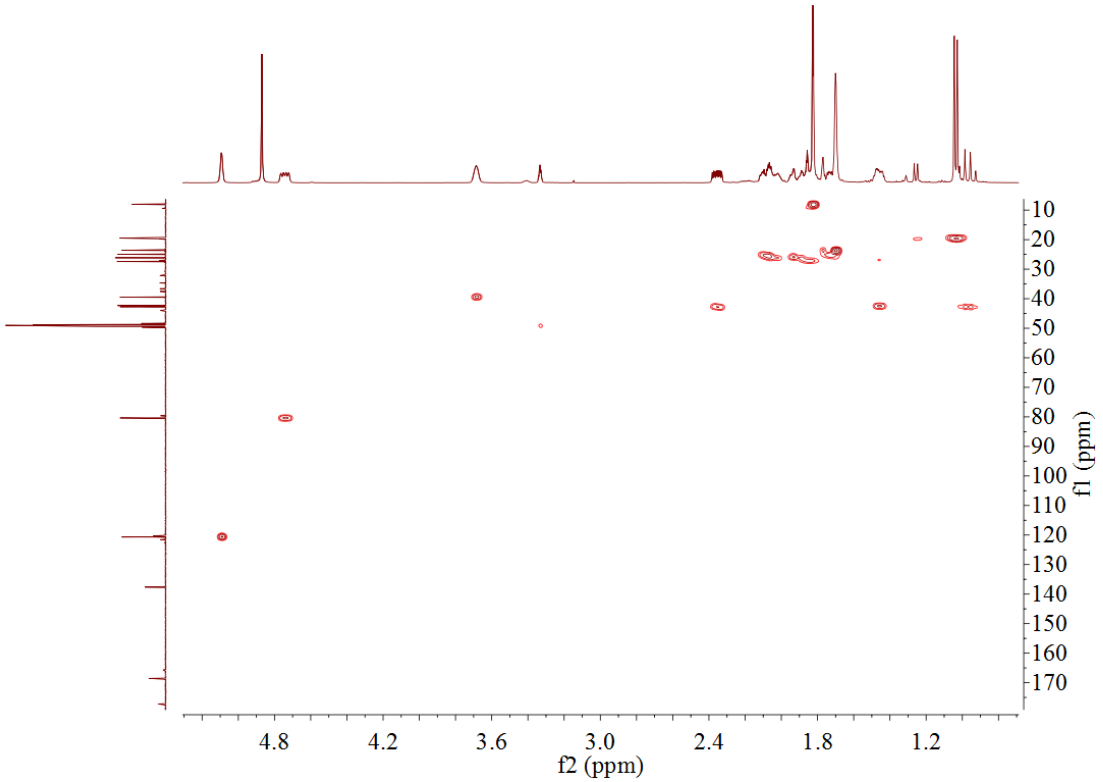


Figure S30. HSQC spectrum of compound **2** in CD_3OD

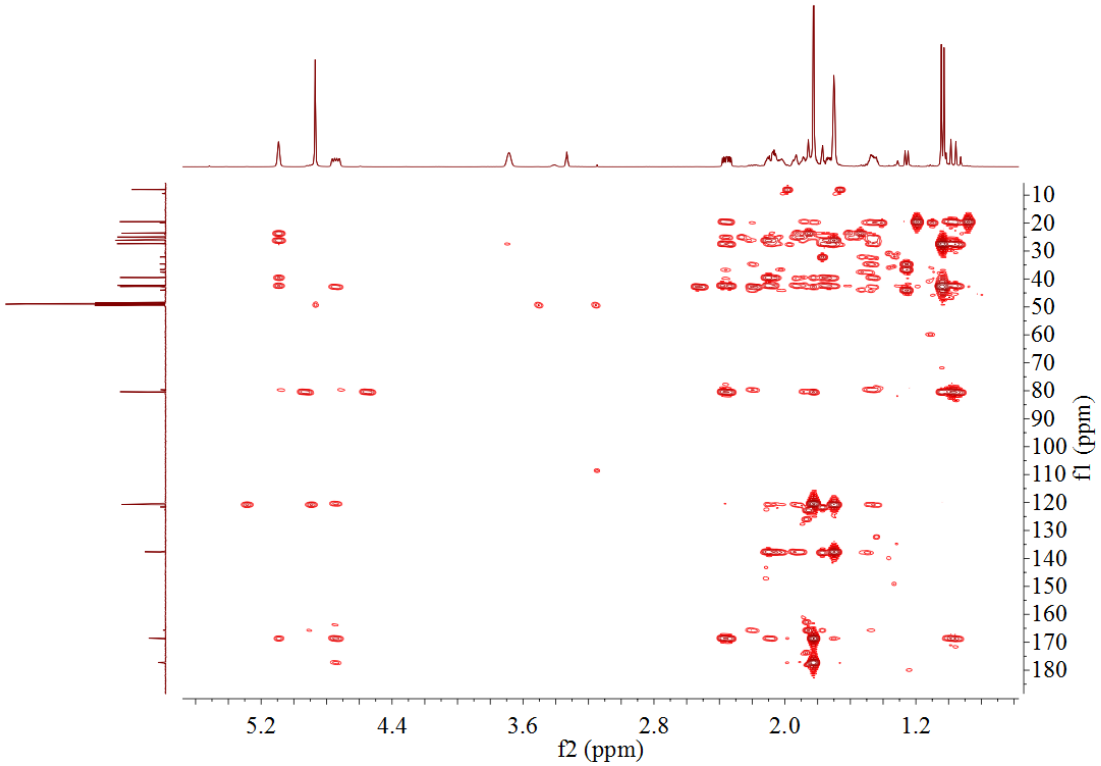


Figure S31. HMBC spectrum of compound **2** in CD_3OD

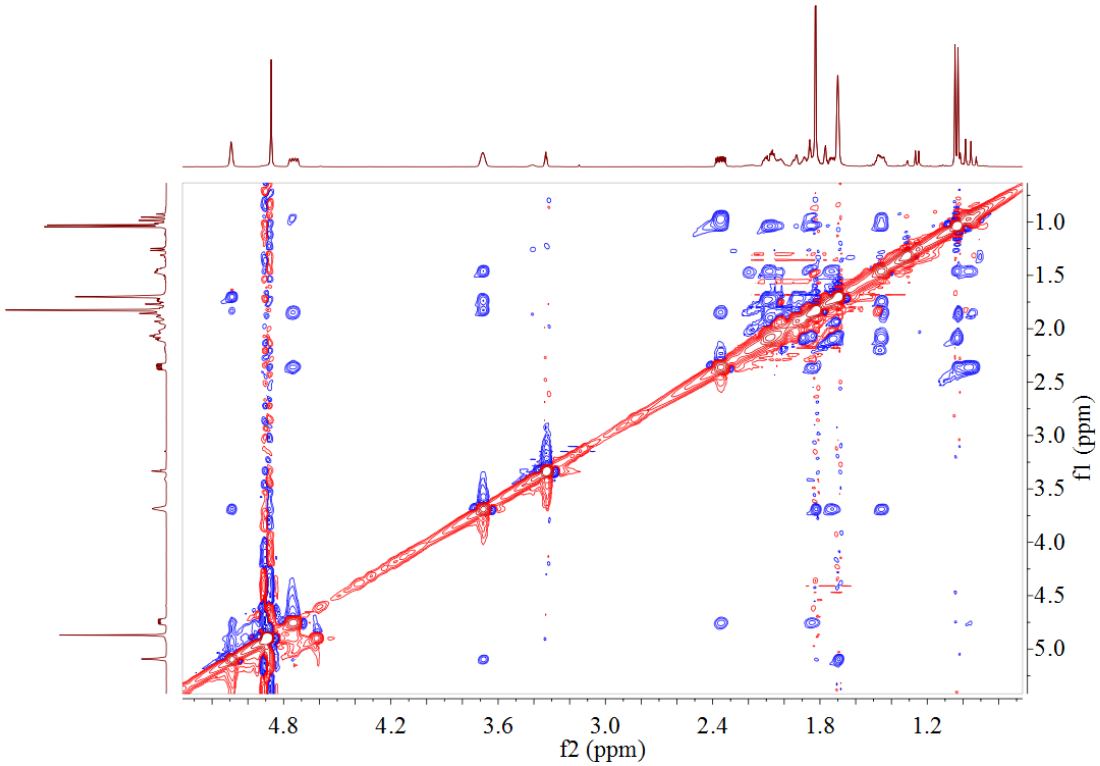
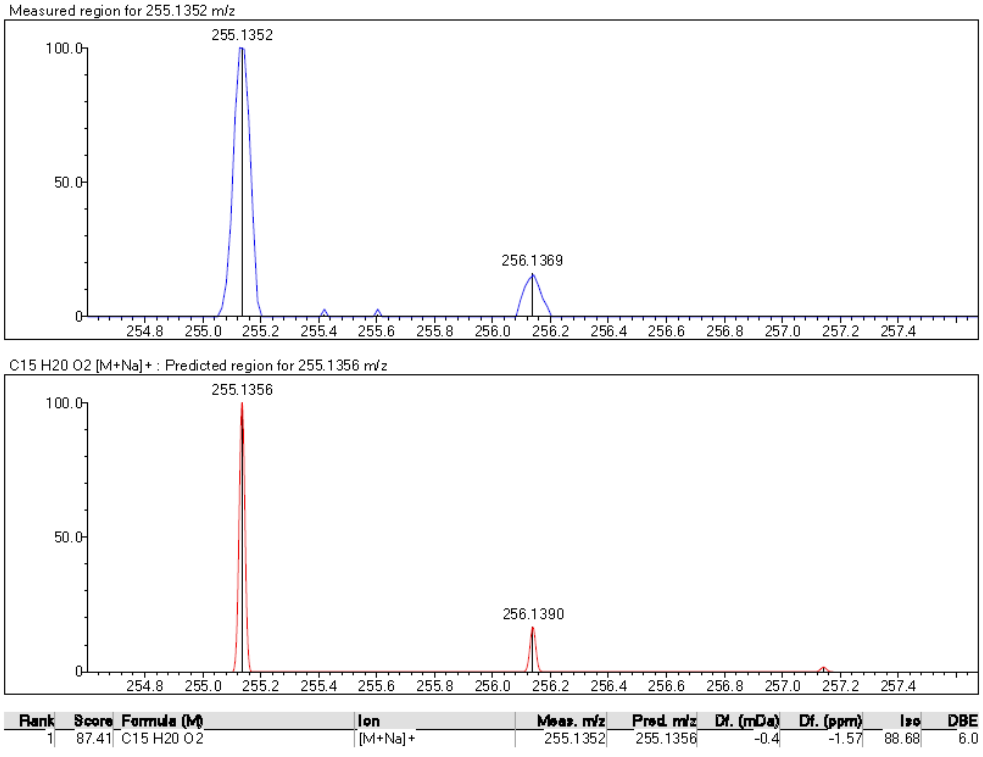


Figure S32. NOESY spectrum of compound **2** in $CD_{3L}OD$



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Dt. (mDa)	Dt. (ppm)	Iso	DBE
1	87.41	C15 H20 O2	[M+Na]+	255.1352	255.1356	-0.4	-1.57	88.68	6.0

Figure S33. HRESIMS spectrum of **2**

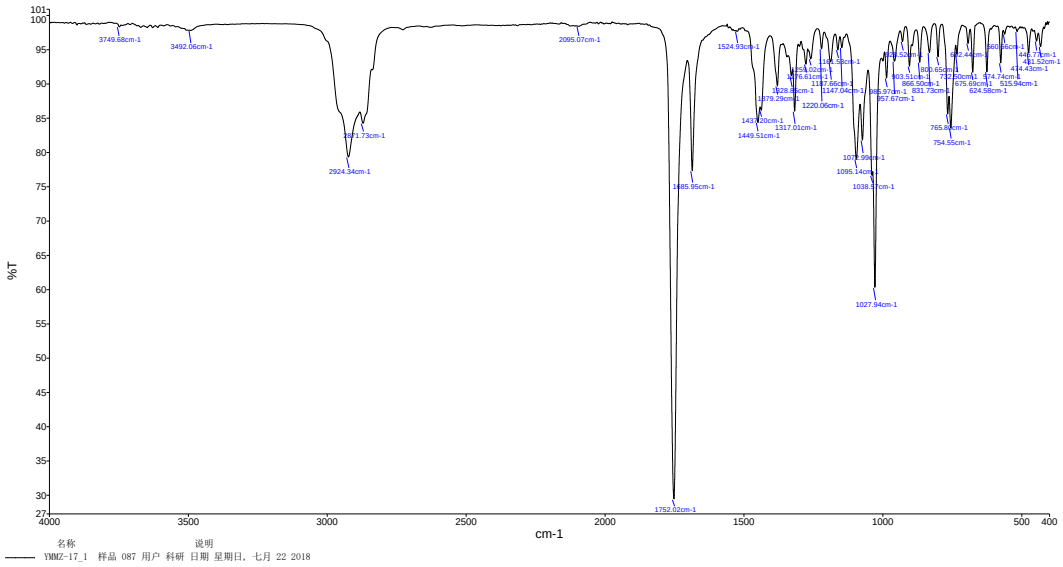


Figure S34. IR (KBr disc) spectrum of **2**

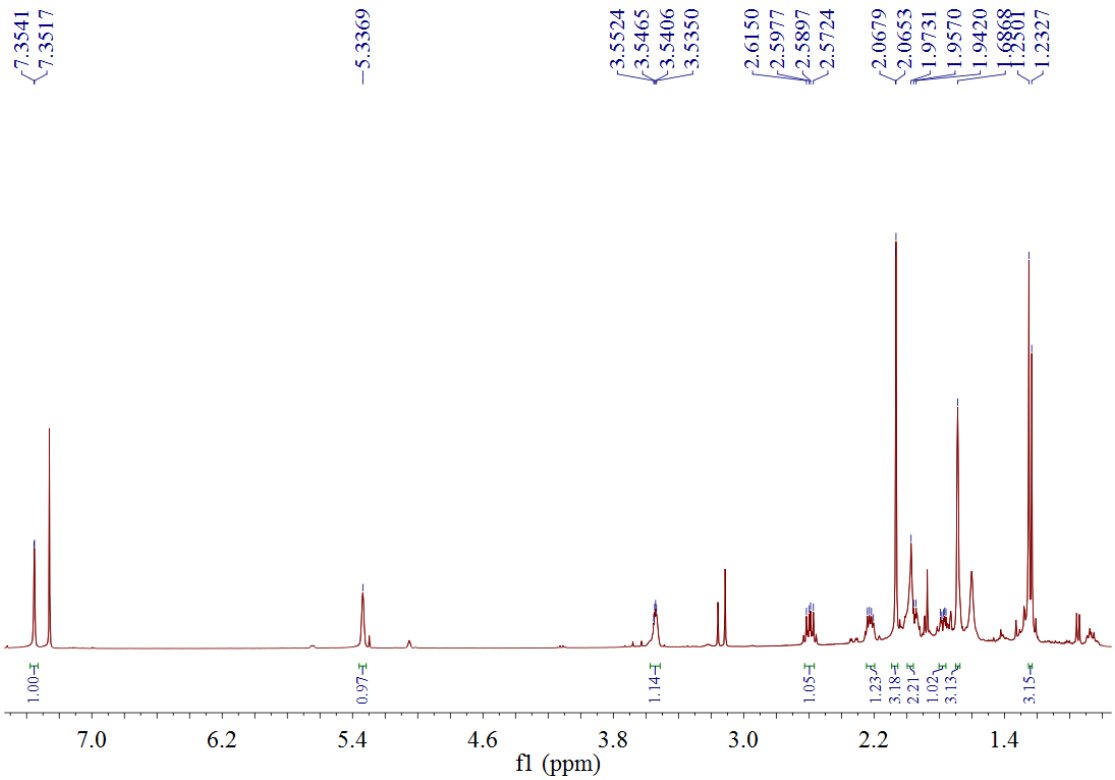


Figure S35. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **3**

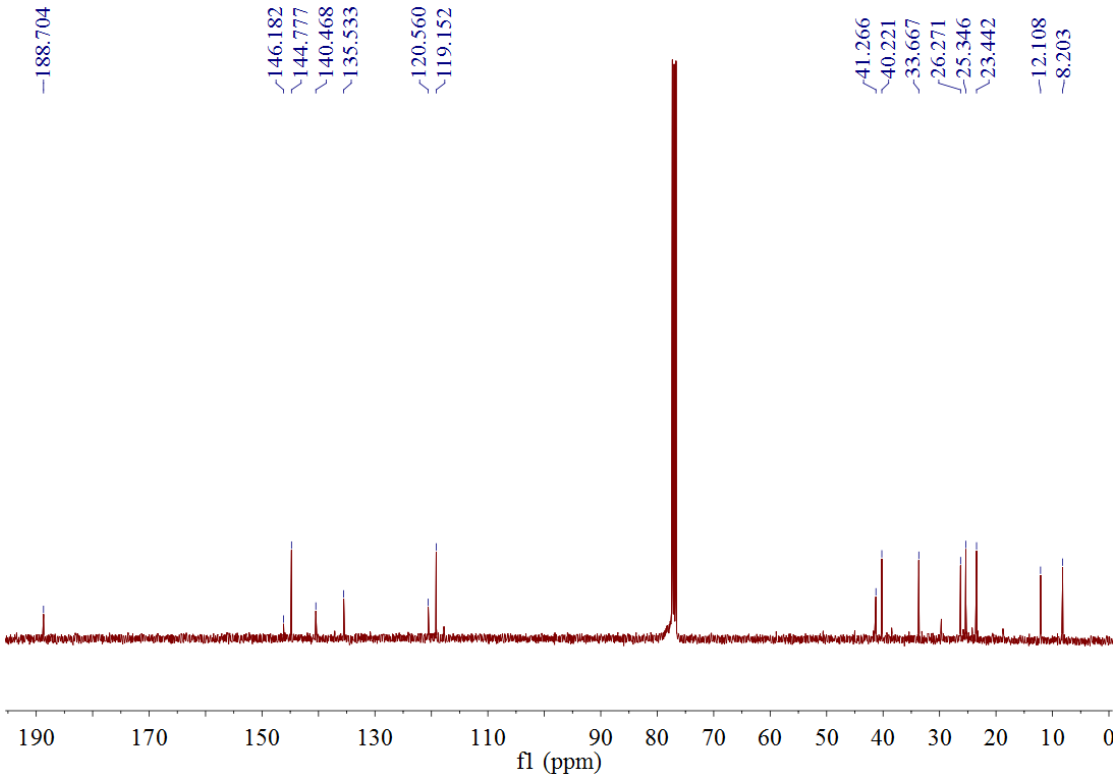


Figure S36. ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **3**

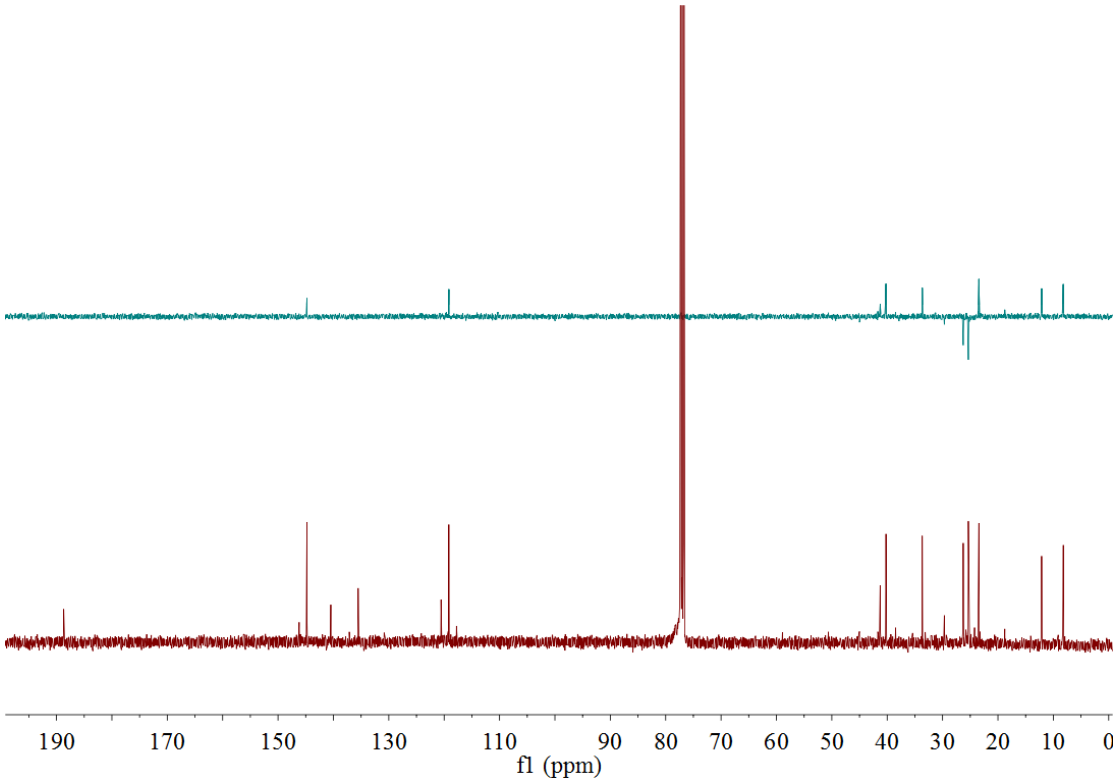


Figure S37. DEPT135 spectrum of compound **3** in$CDCl_3$

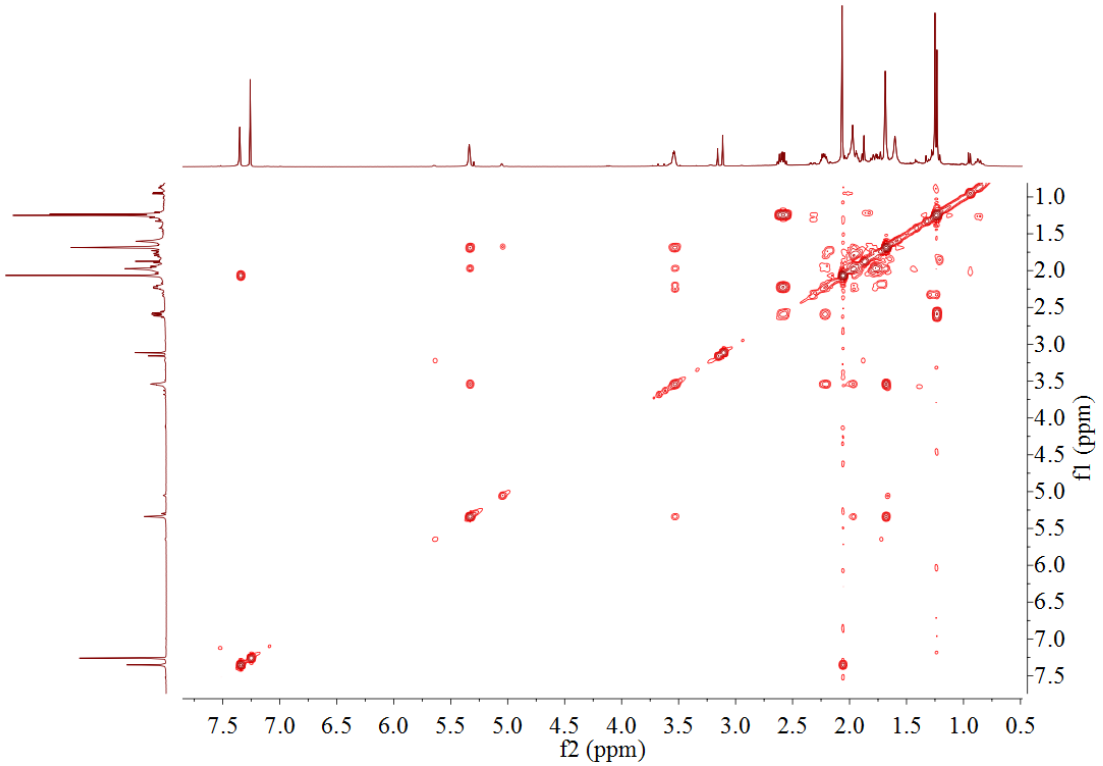


Figure S38. ^{1}H- ^{1}H COSY spectrum of compound **3** in $CDCl_3$

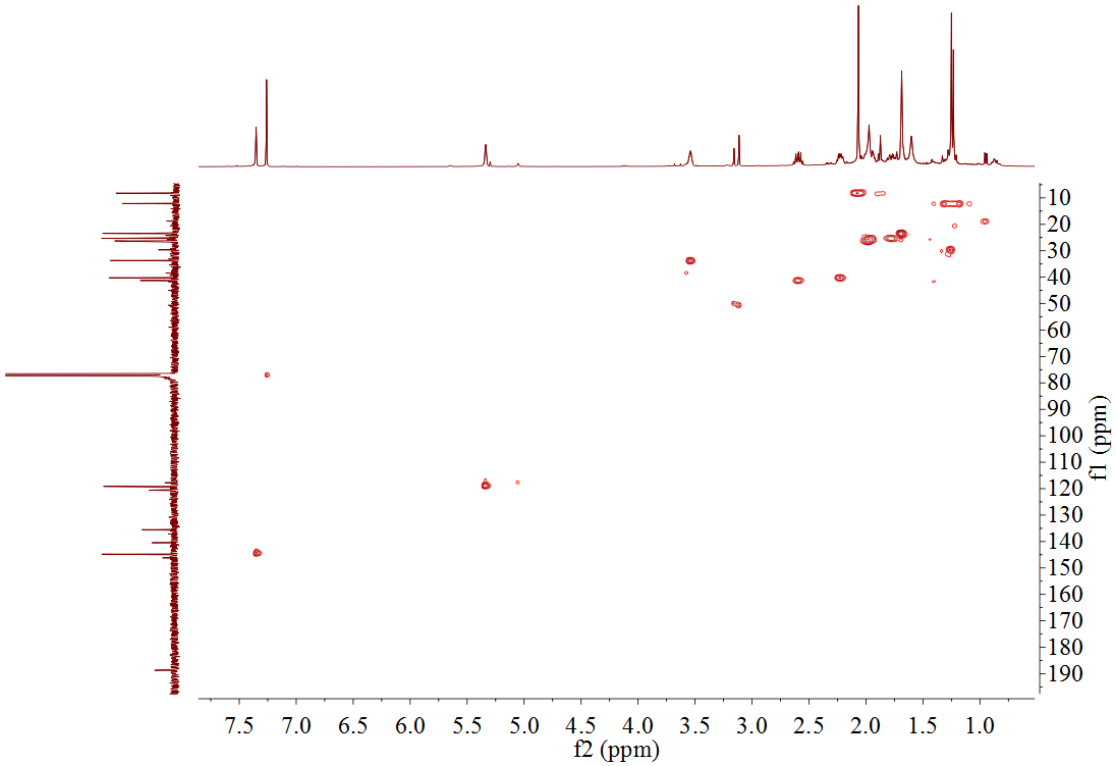


Figure S39. HSQC spectrum of compound **3** in $CDCl_3$

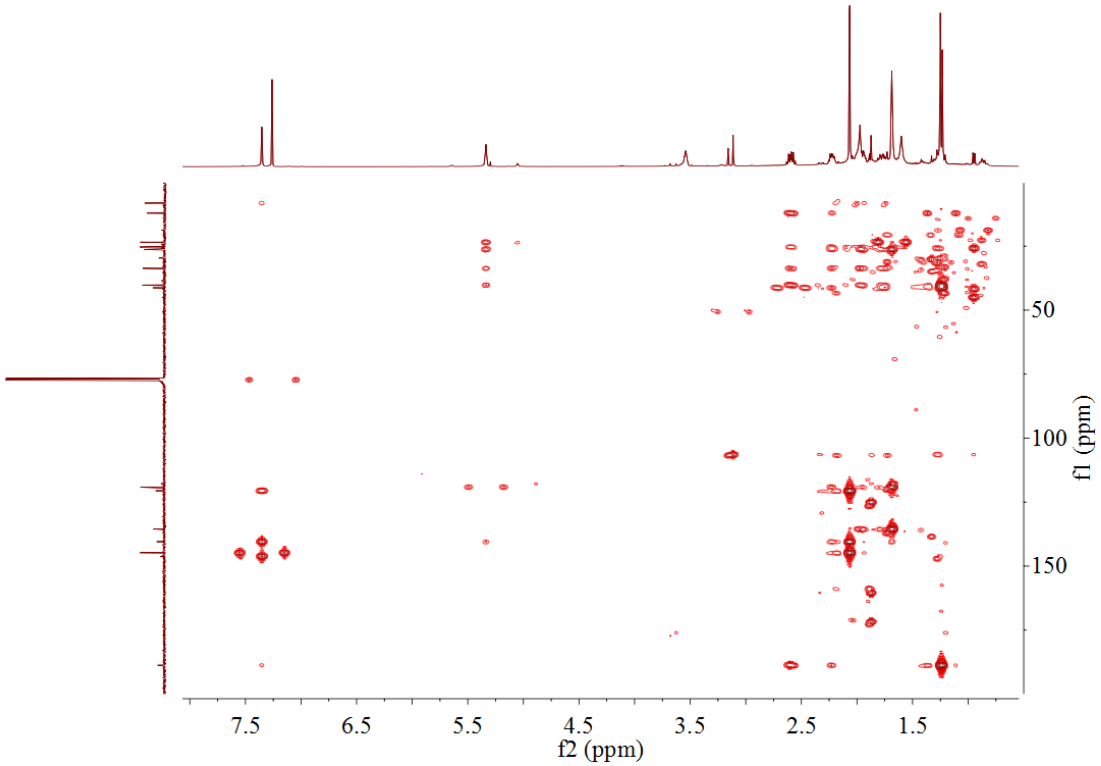


Figure S40. HMBC spectrum of compound **3** in $CDCl_3$

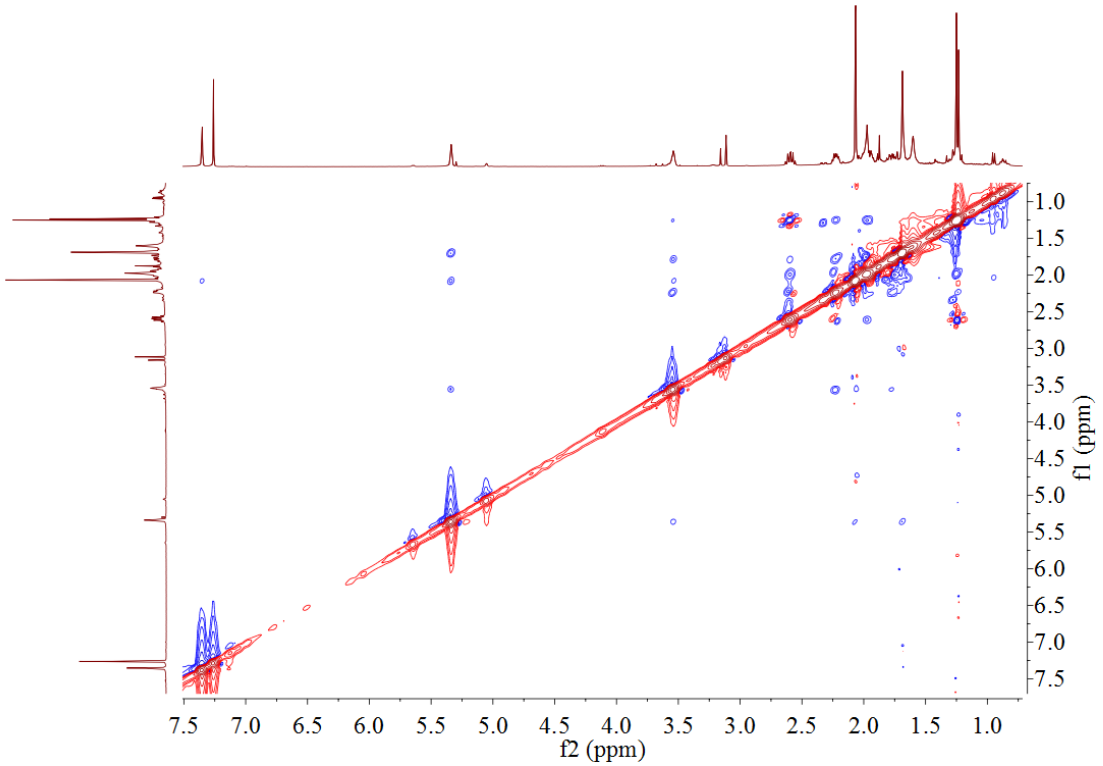
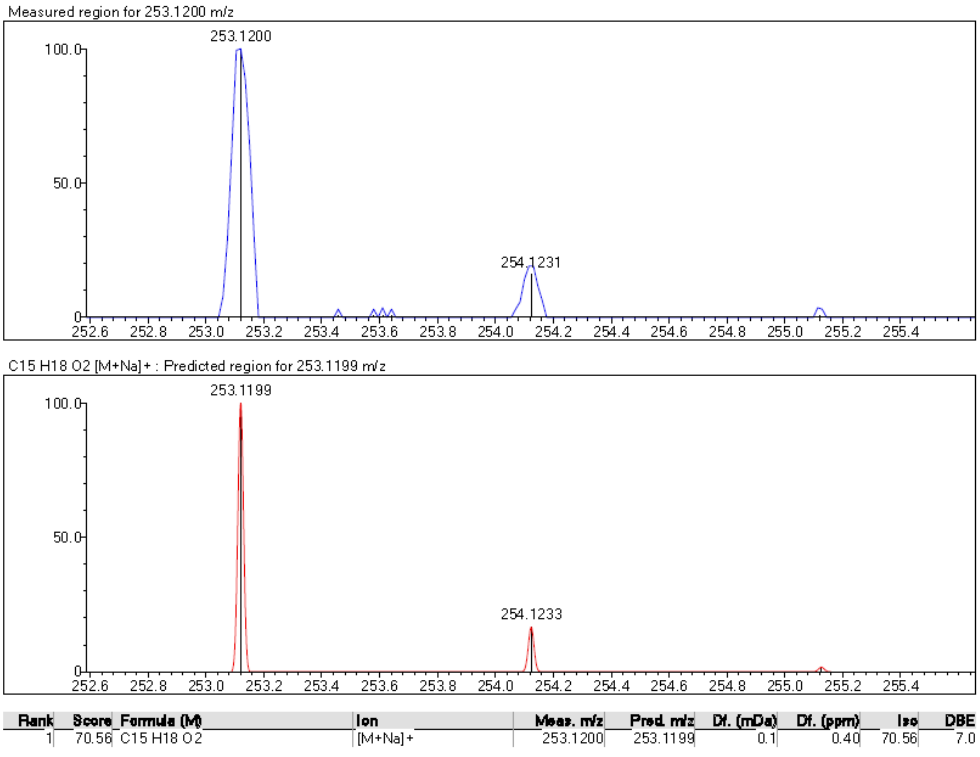


Figure S41. NOESY spectrum of compound **3** in $CDCl_3$



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Dif. (mDa)	Dif. (ppm)	Iso	DBE
1	70.56	C15 H18 O2	[M+Na]+	253.1200	253.1199	0.1	0.40	70.56	7.0

Figure S42. HRESIMS spectrum of **3**

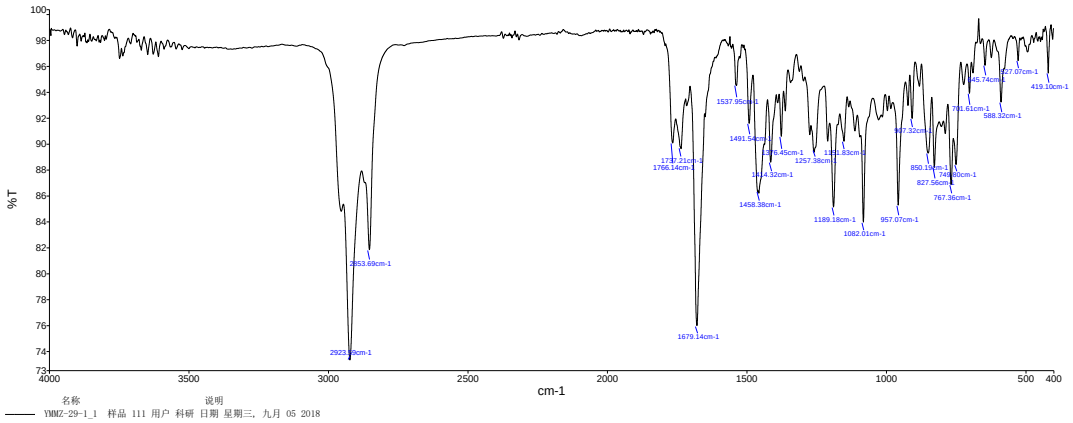


Figure S43. IR (KBr disc) spectrum of **3**

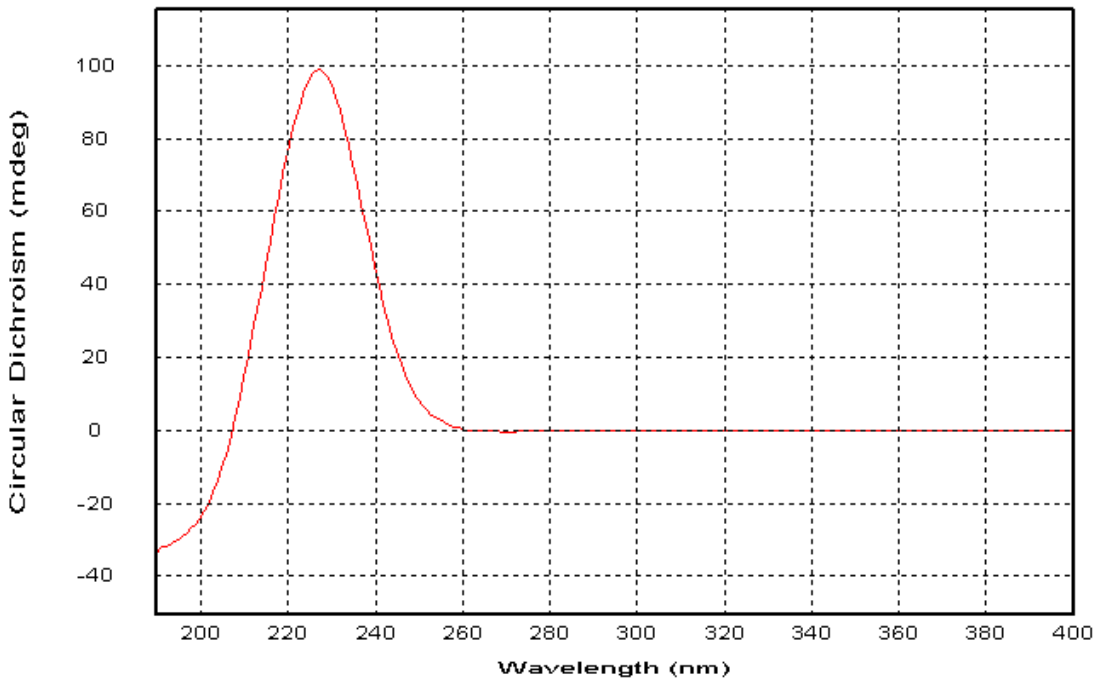


Figure S44. CD spectrum of **2**