

Supporting Information

**Metabolites with Anti-inflammatory Activities Isolated from the
Mangrove Endophytic Fungus *Dothiorella* sp. ZJQQYZ-1**

Zhaokun Li, Junhao Zhu, Ruxue Mu, Chenxi Wang, Yuru Sun, Bingbing Qian, Ning
Li* and Yan Chen*

School of Pharmacy, Anhui Medical University, Hefei, 230032, China

*Corresponding authors

E-mail addresses: cychemistry@163.com (Y. Chen); 1993500019@ahmu.edu.cn (N. Li)

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Figure S31. The IC₅₀ value of compounds **5** and **7** against LPS-induced NO production in RAW264.7 cells were calculated and presented.

Table S1. The DP4+ evaluation of **3**.

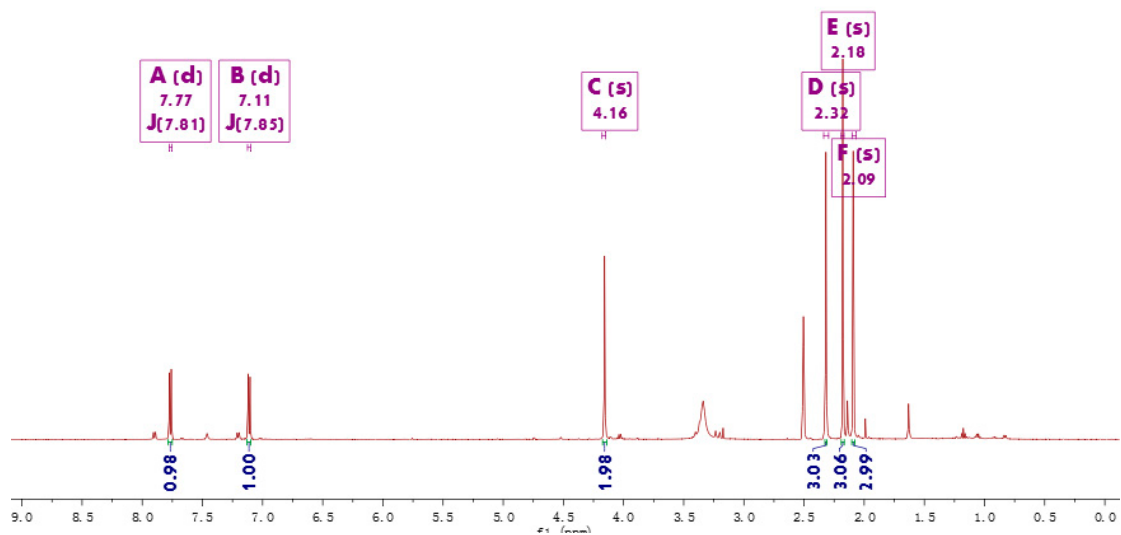


Figure. S1 ^1H -NMR spectrum of compound **1** in $\text{DMSO-}d_6$

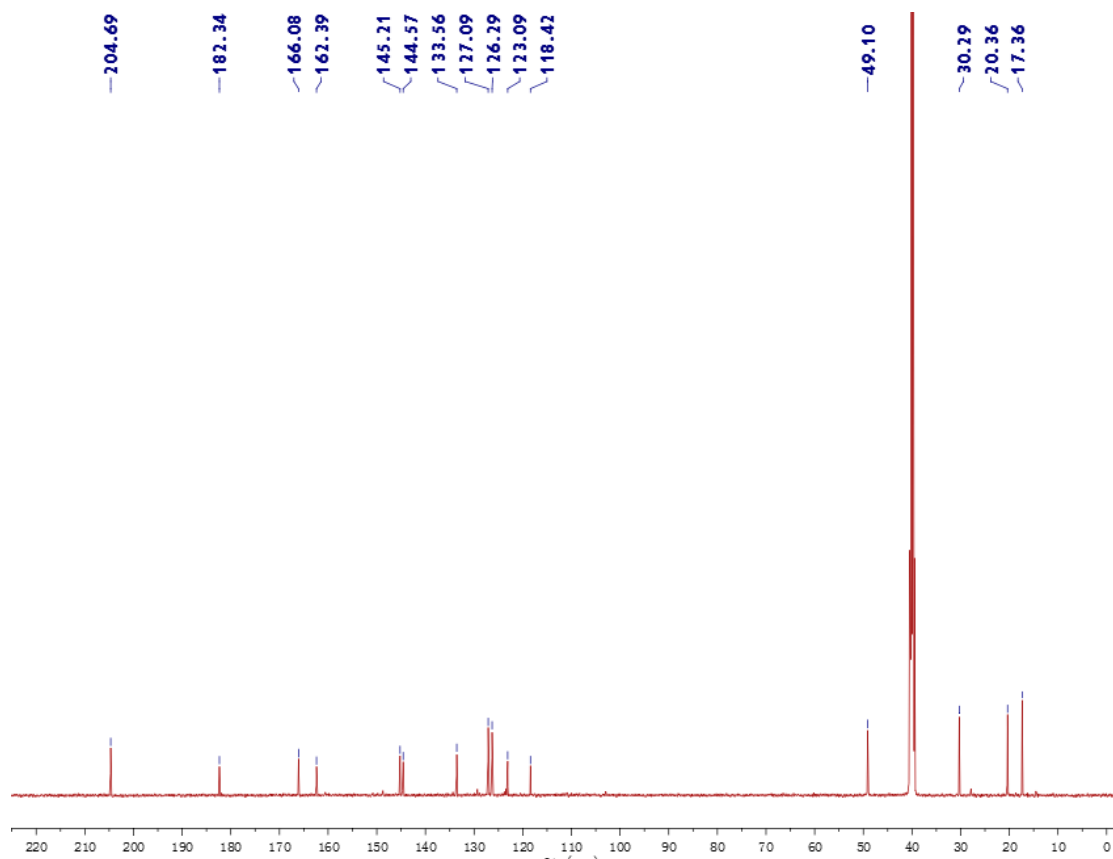


Figure. S2 ^{13}C -NMR spectrum of compound **1** in $\text{DMSO-}d_6$

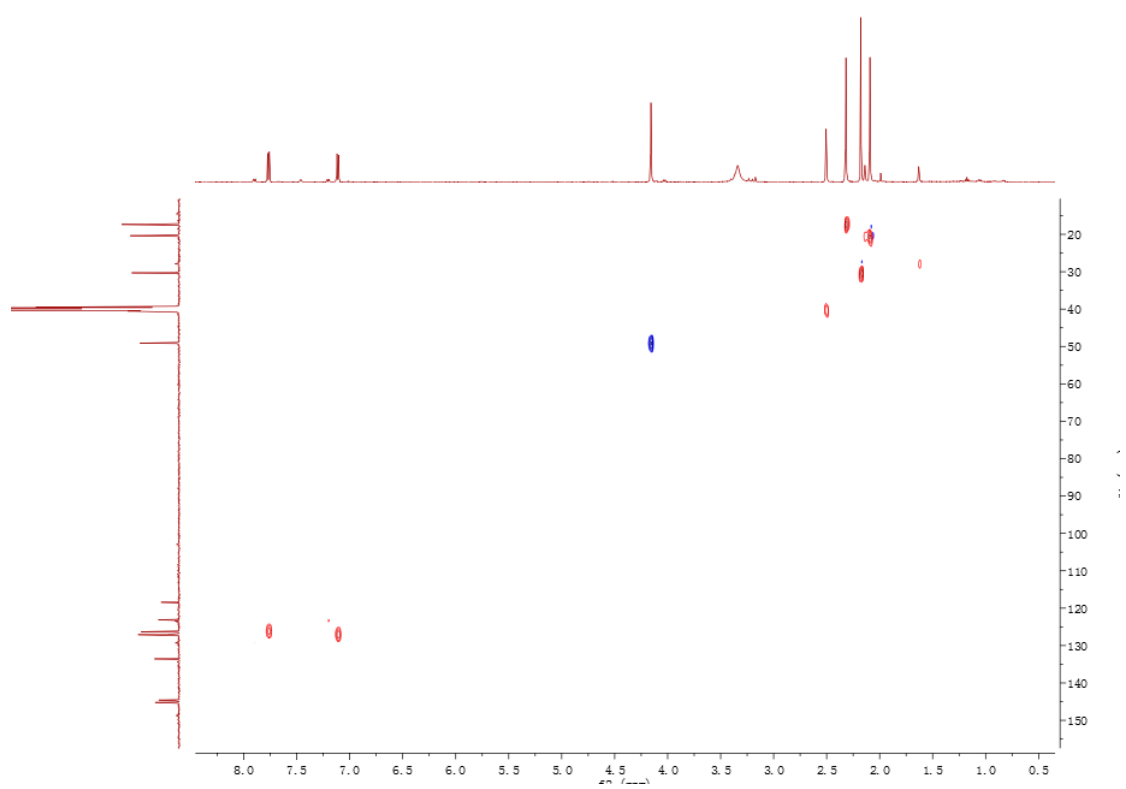


Figure. S3 HSQC spectrum of compound **1**

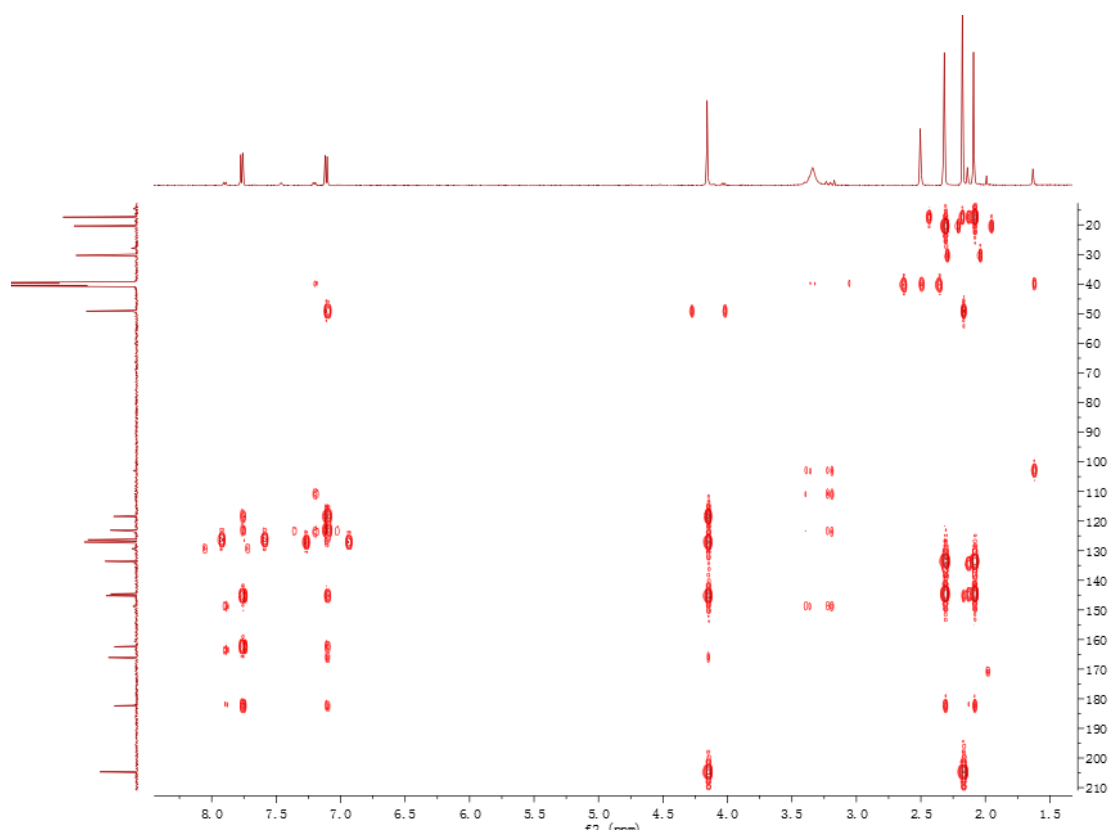


Figure. S4 HMBC spectrum of compound **1**

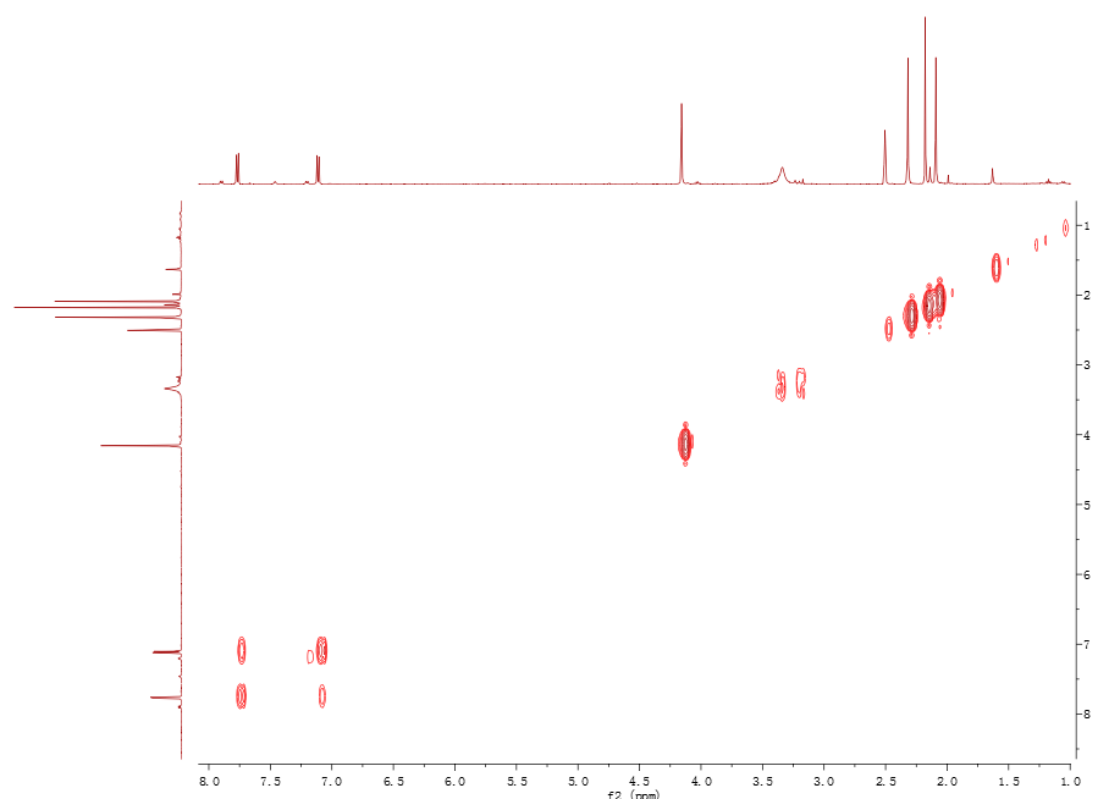


Figure S5 ^1H - ^1H COSY spectrum of compound **1**

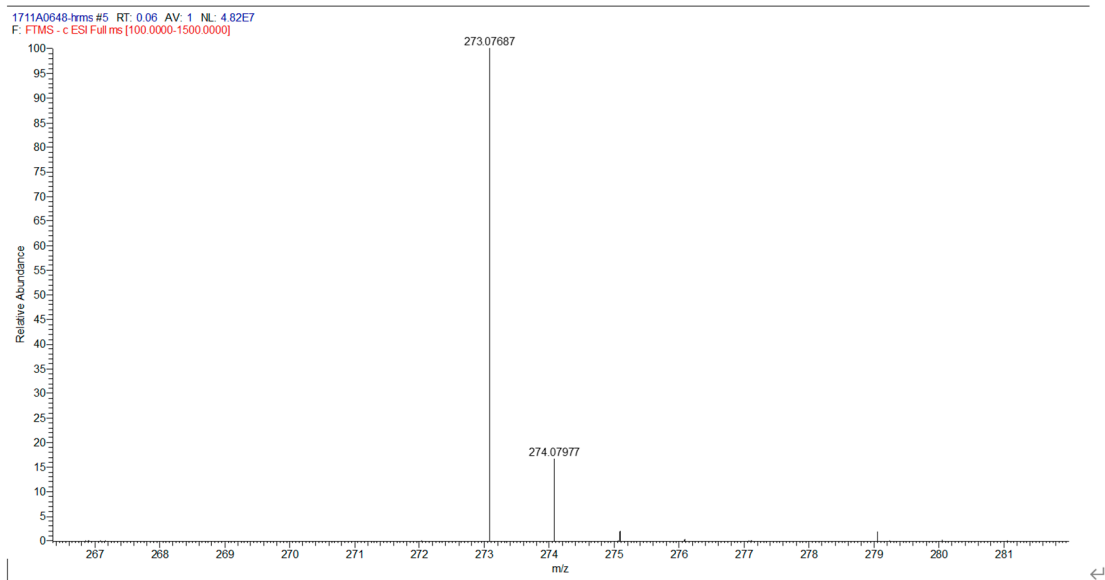


Figure S6. HRESIMS spectrum of compound **1**

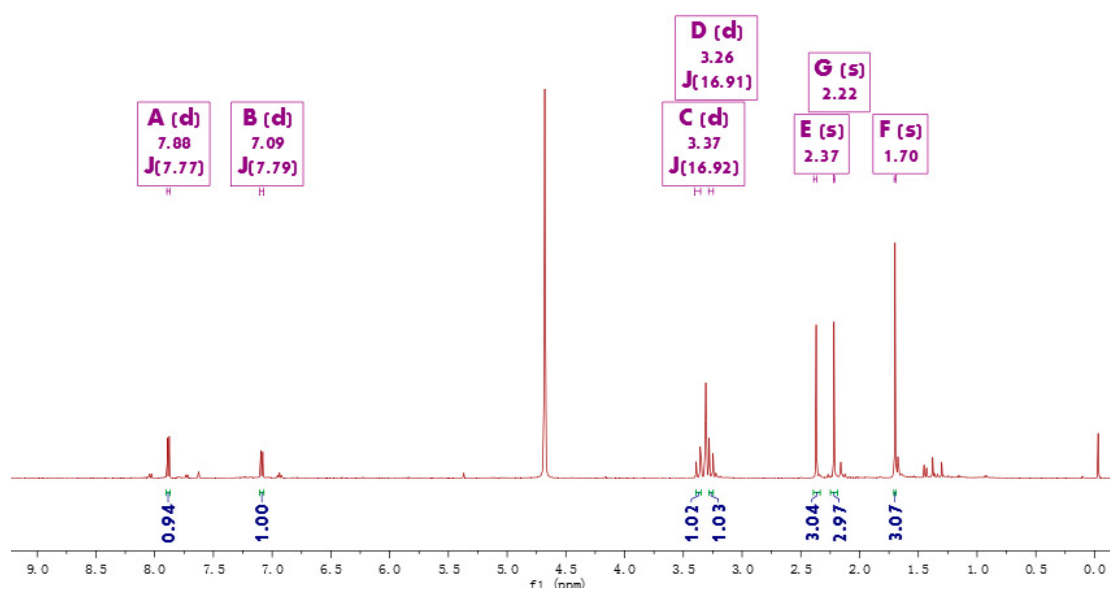


Figure S7. ^1H NMR spectrum of compound **2** (500 MHz, CD_3OD and CDCl_3).

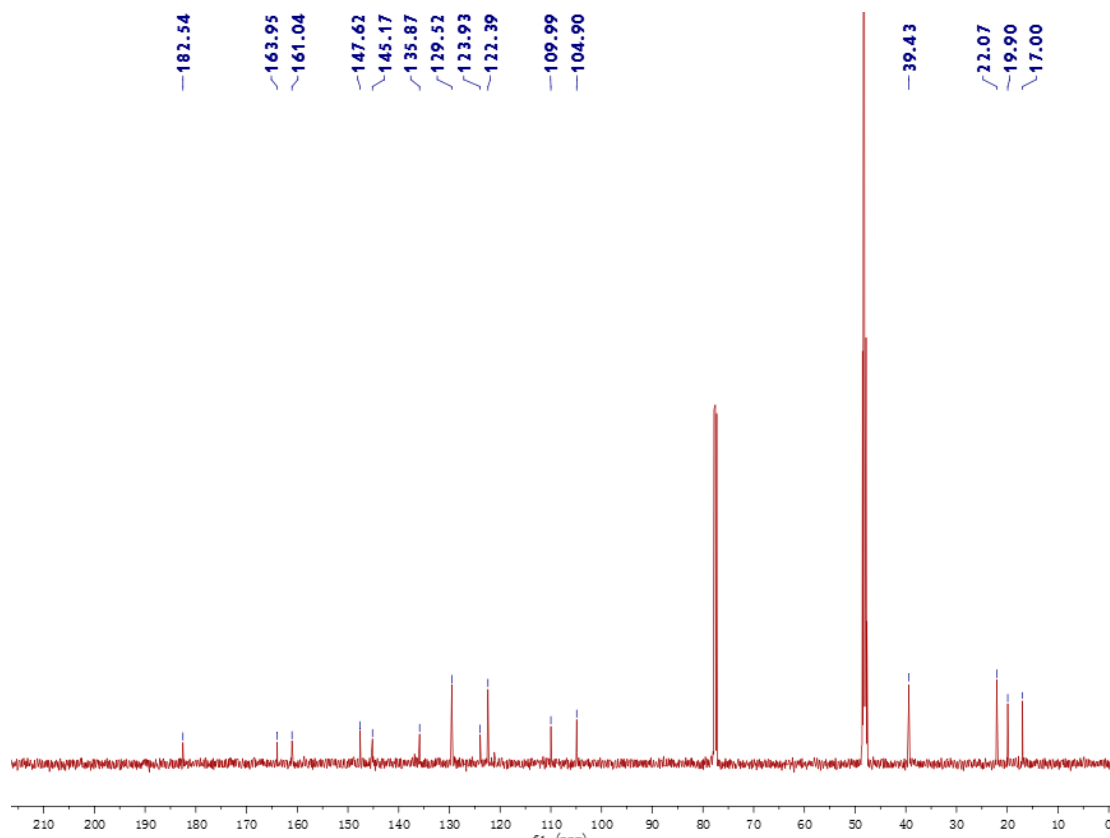


Figure S8. ^{13}C NMR spectrum of compound **2** (125 MHz, CD_3OD and CDCl_3).

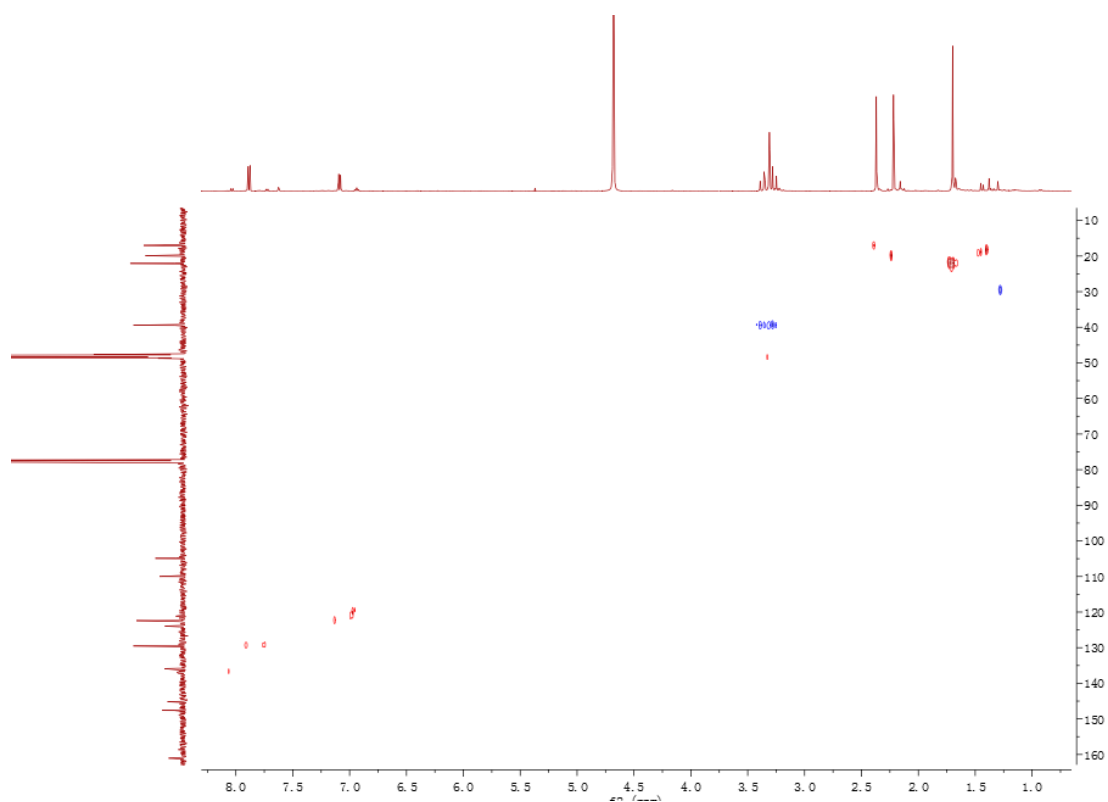


Figure S9. HSQC spectrum of compound 2

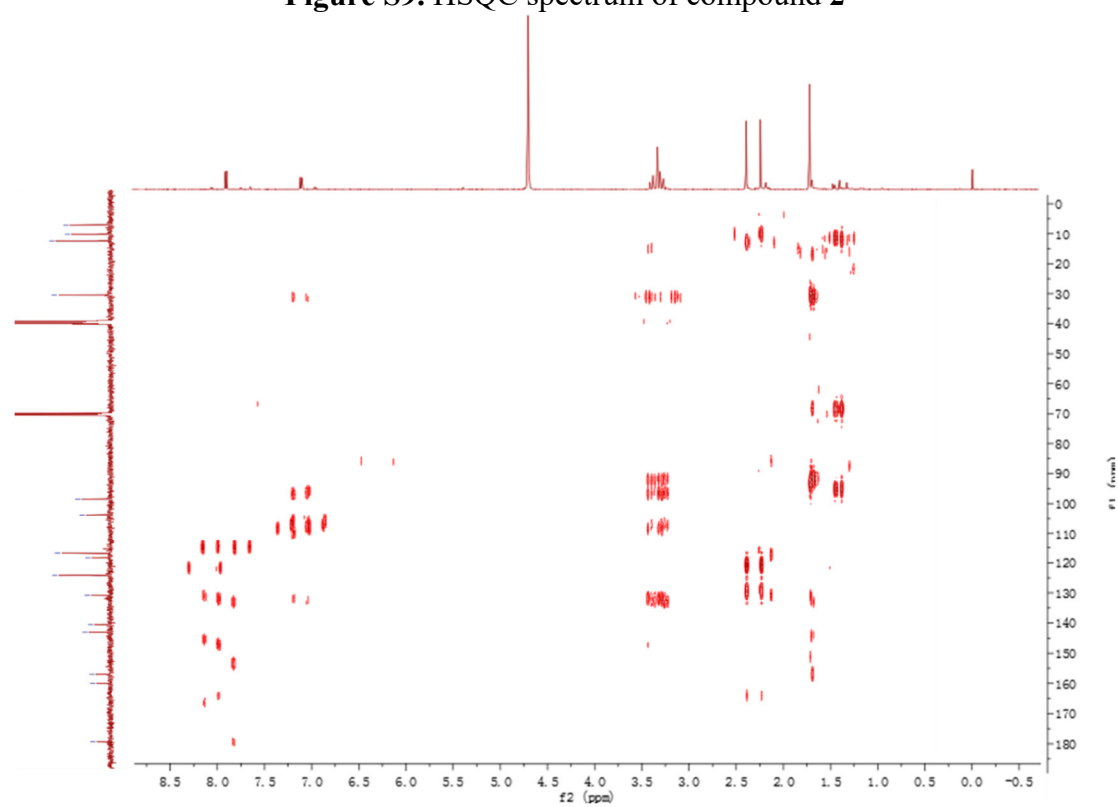


Figure S10. HMBC spectrum of compound 2

1712A0839 #5-11 RT: 0.06-0.10 AV: 3 NL: 6.47E6
F: FTMS - c ESI Full ms [100.0000-600.0000]

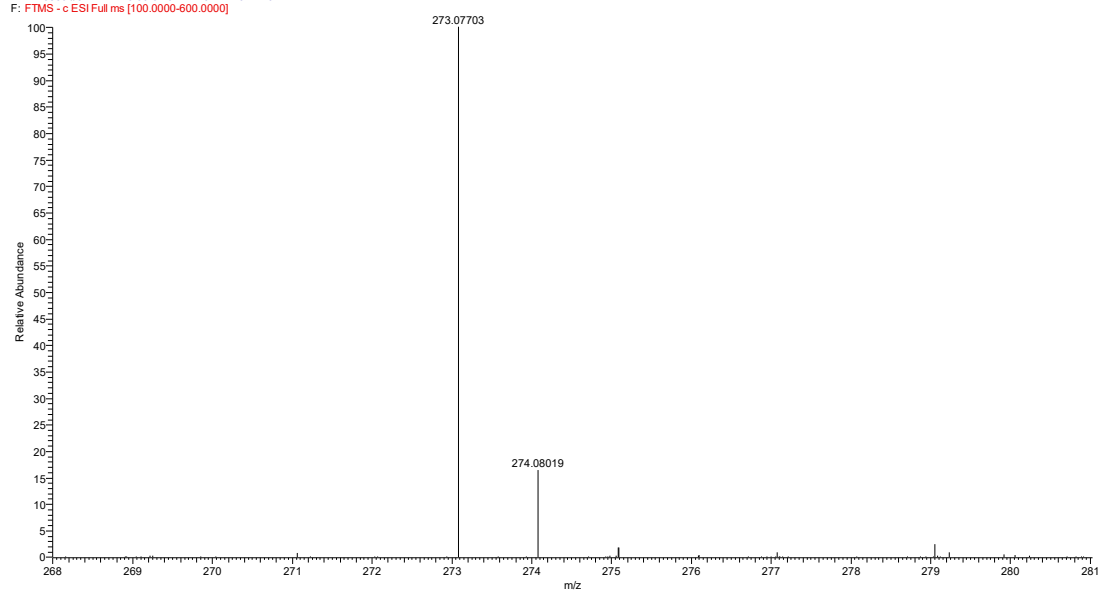


Figure S11. HRESIMS spectrum of compound 2.

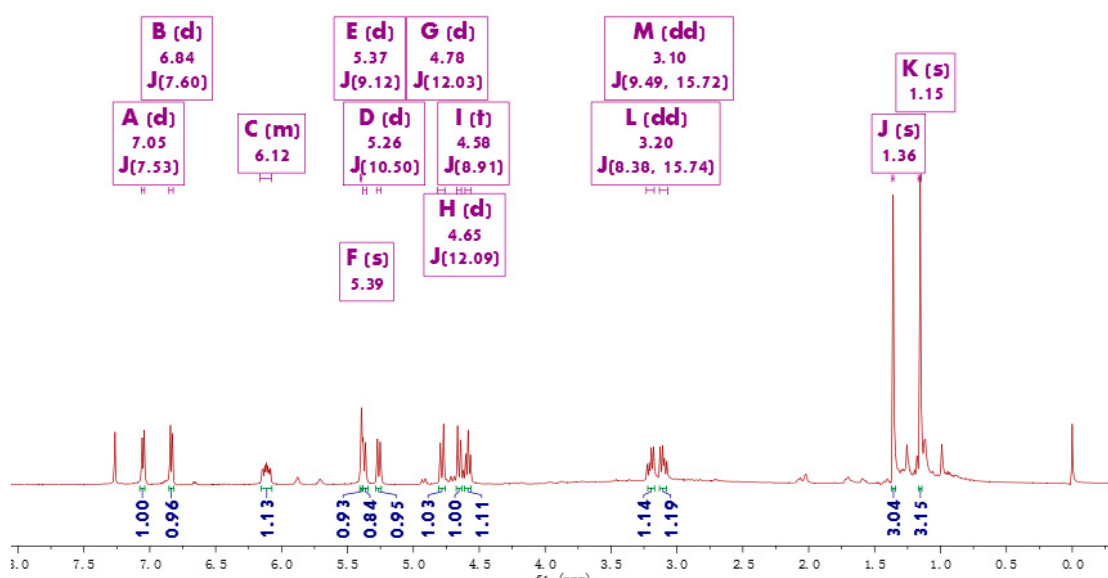


Figure S12. ¹H-NMR spectrum of compound 3 in CDCl₃

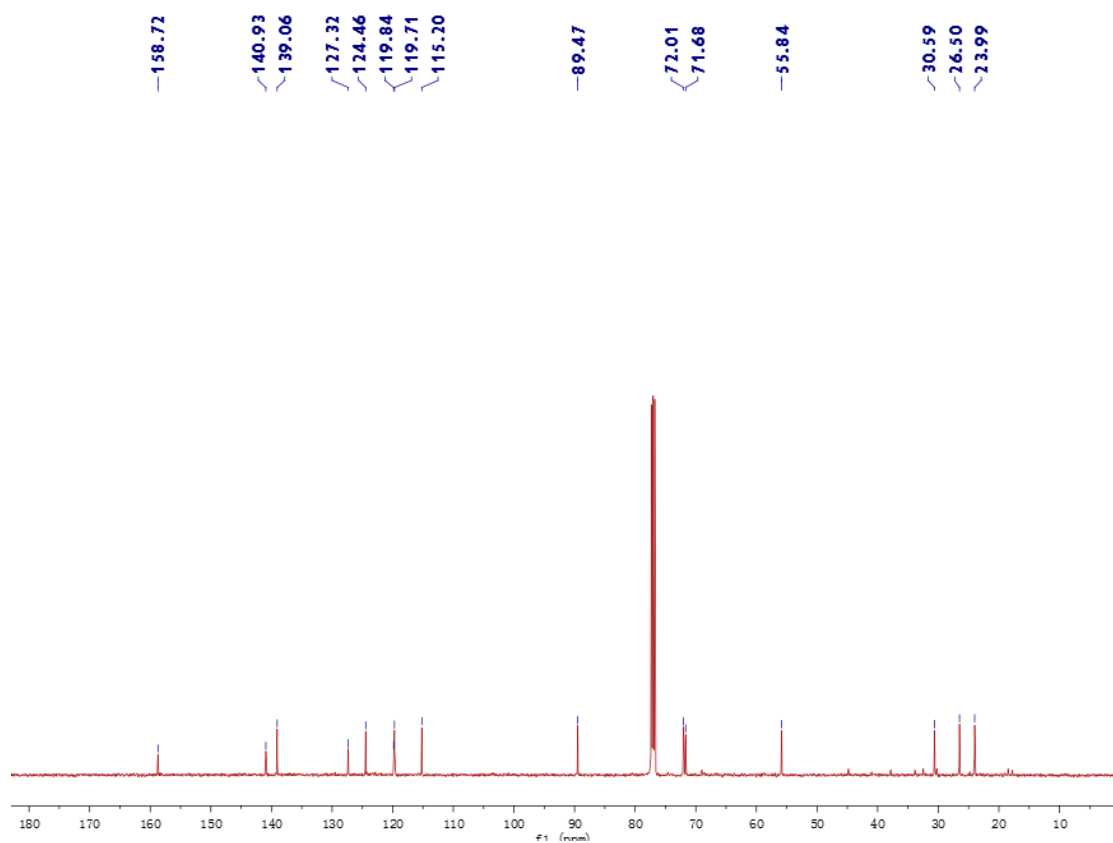


Figure S13. ^{13}C -NMR spectrum of compound **3** in CDCl_3

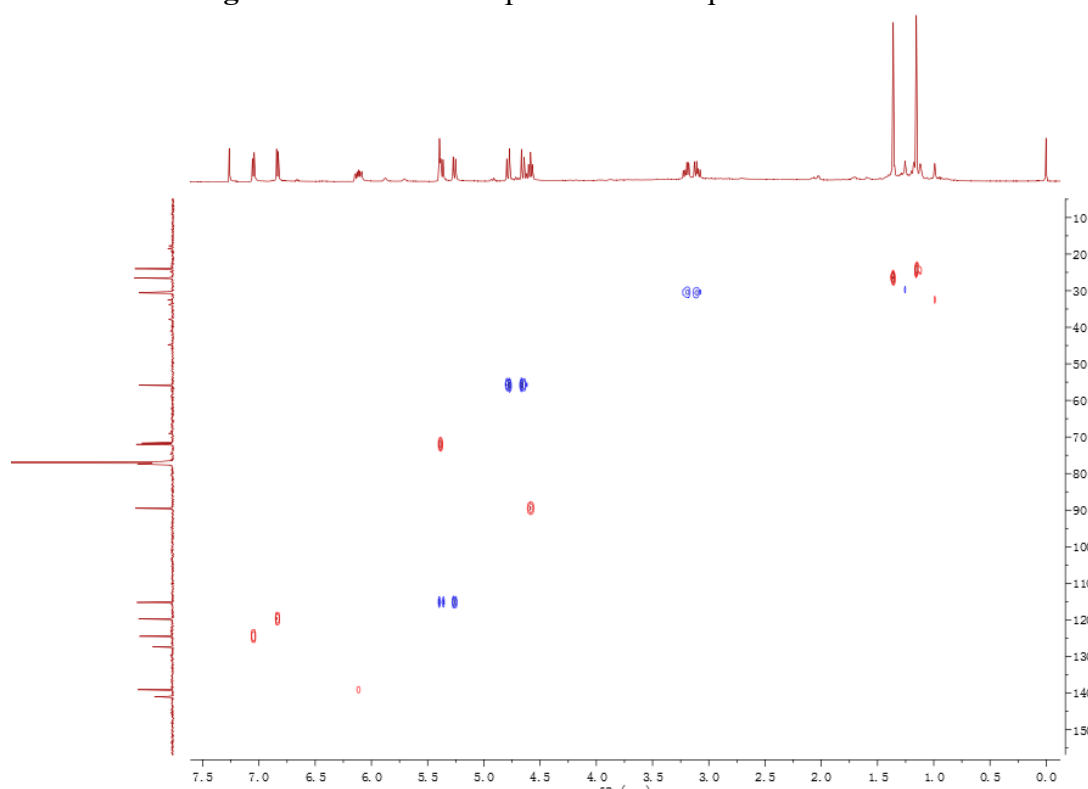


Figure S14 HSQC spectrum of compound **3**

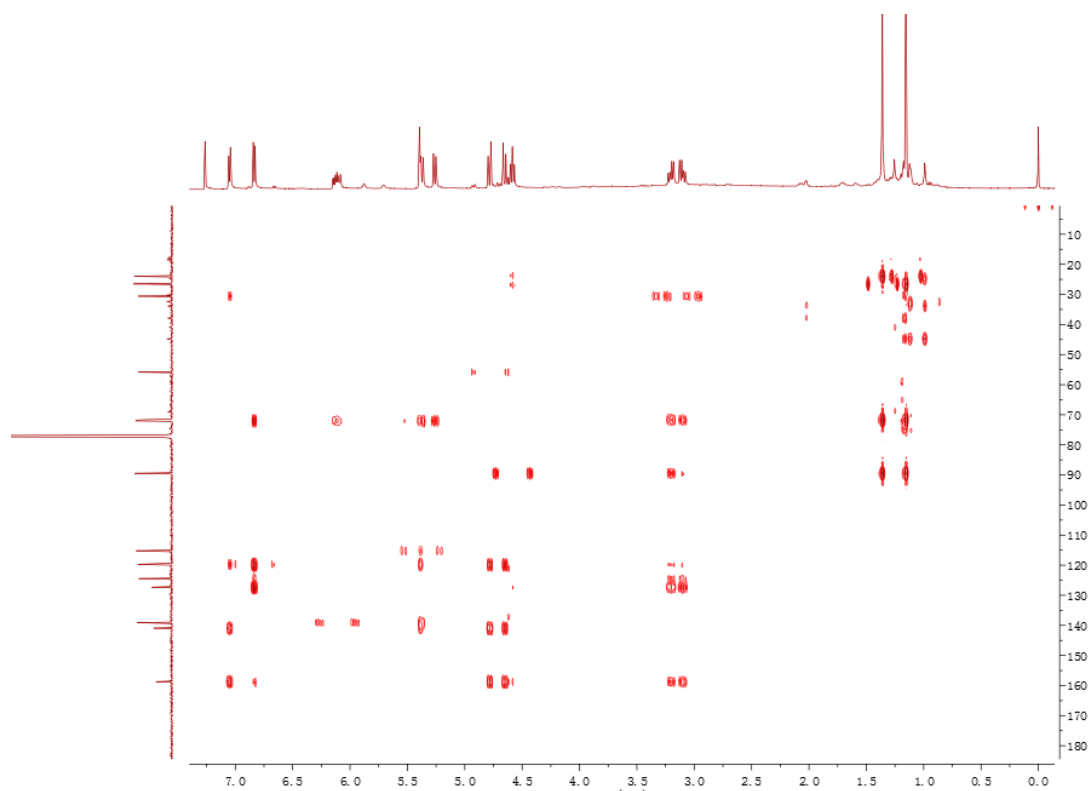


Figure S15. HMBC spectrum of compound **3**

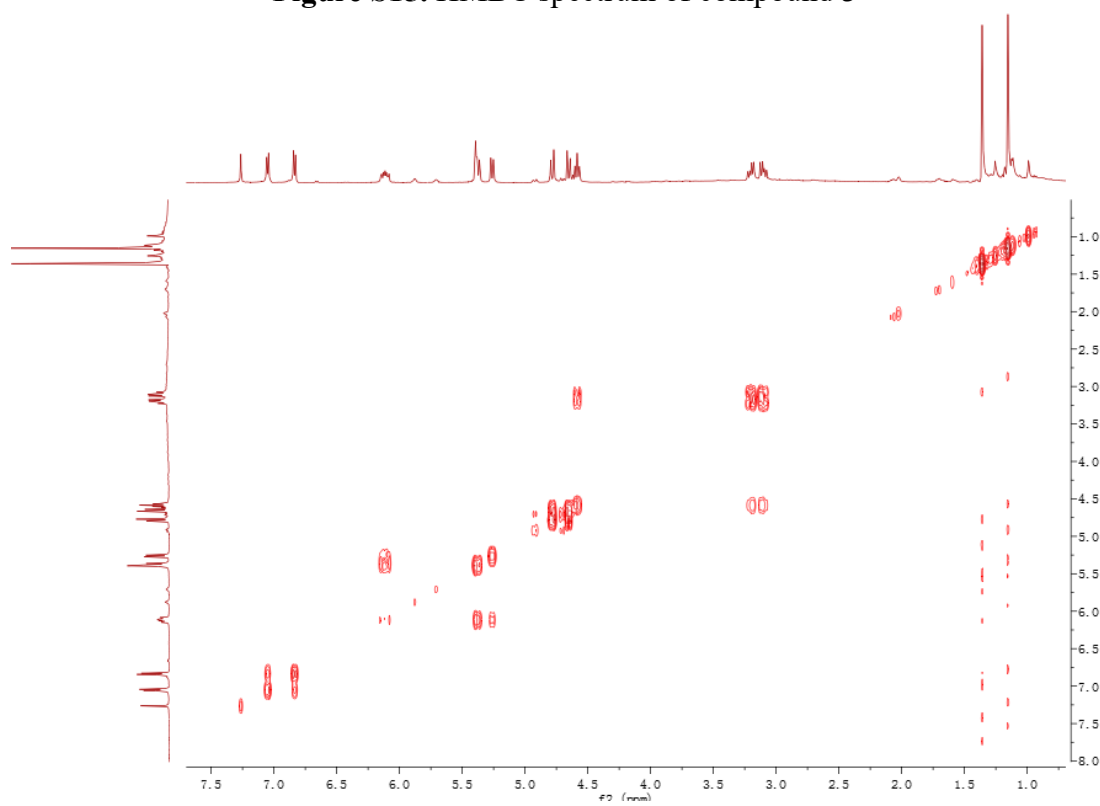


Figure S16. ^1H - ^1H COSY spectrum of compound **3**

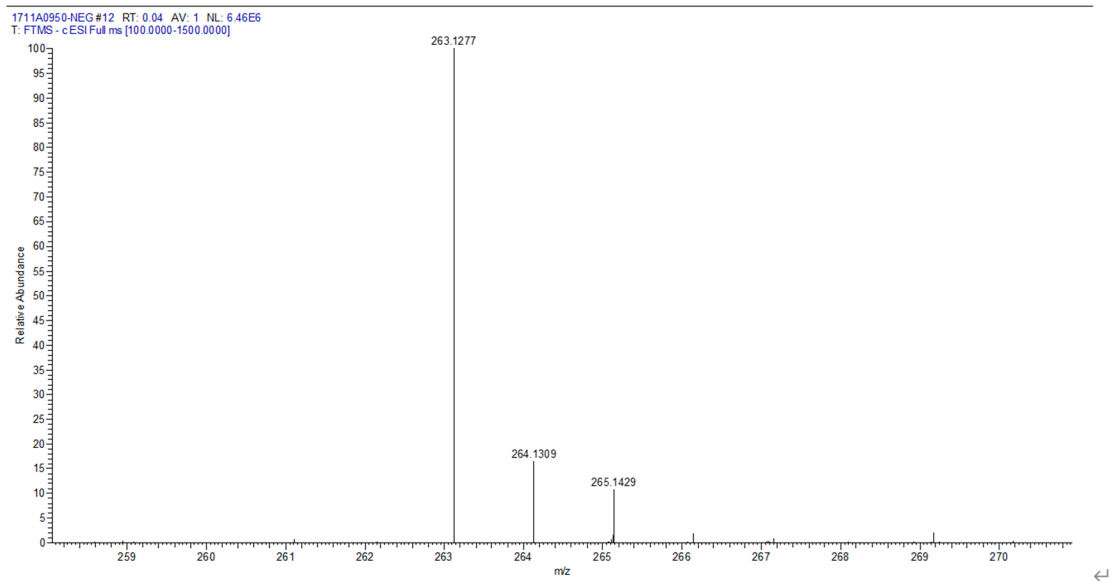


Figure S17. HRESIMS spectrum of compound **3**

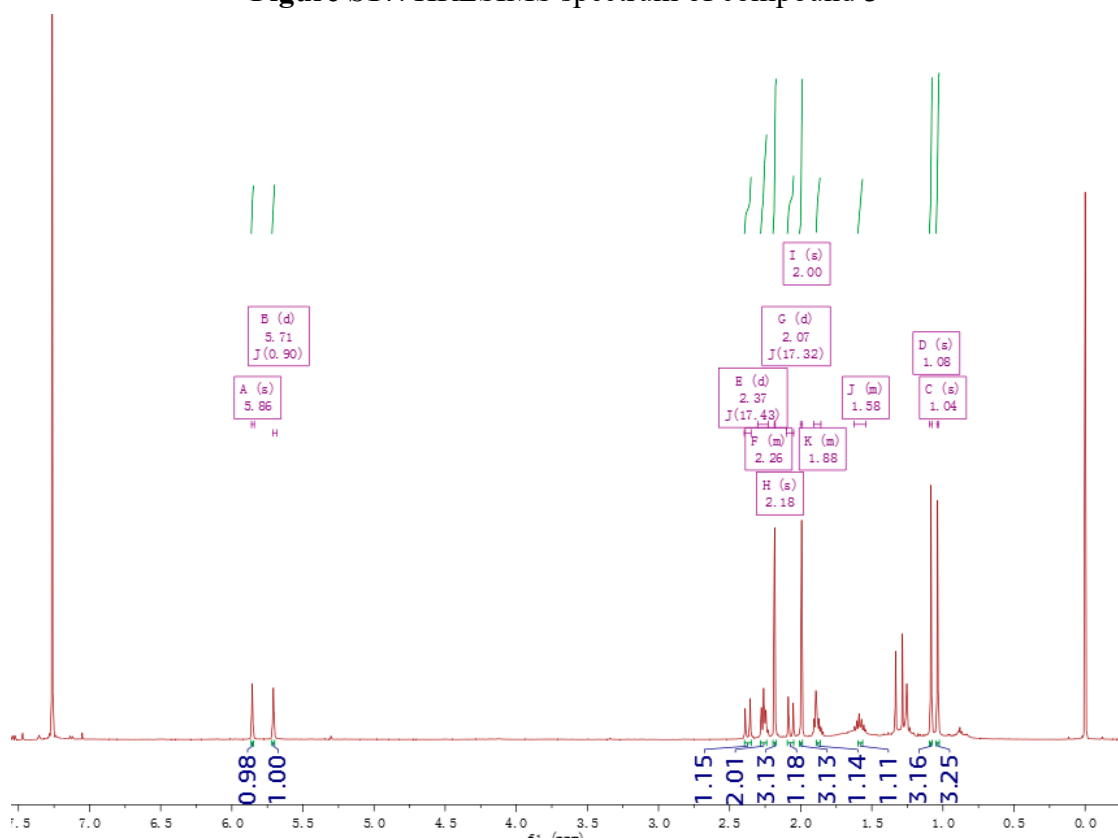


Figure S18 ^1H NMR spectrum of compound **4** in CDCl_3

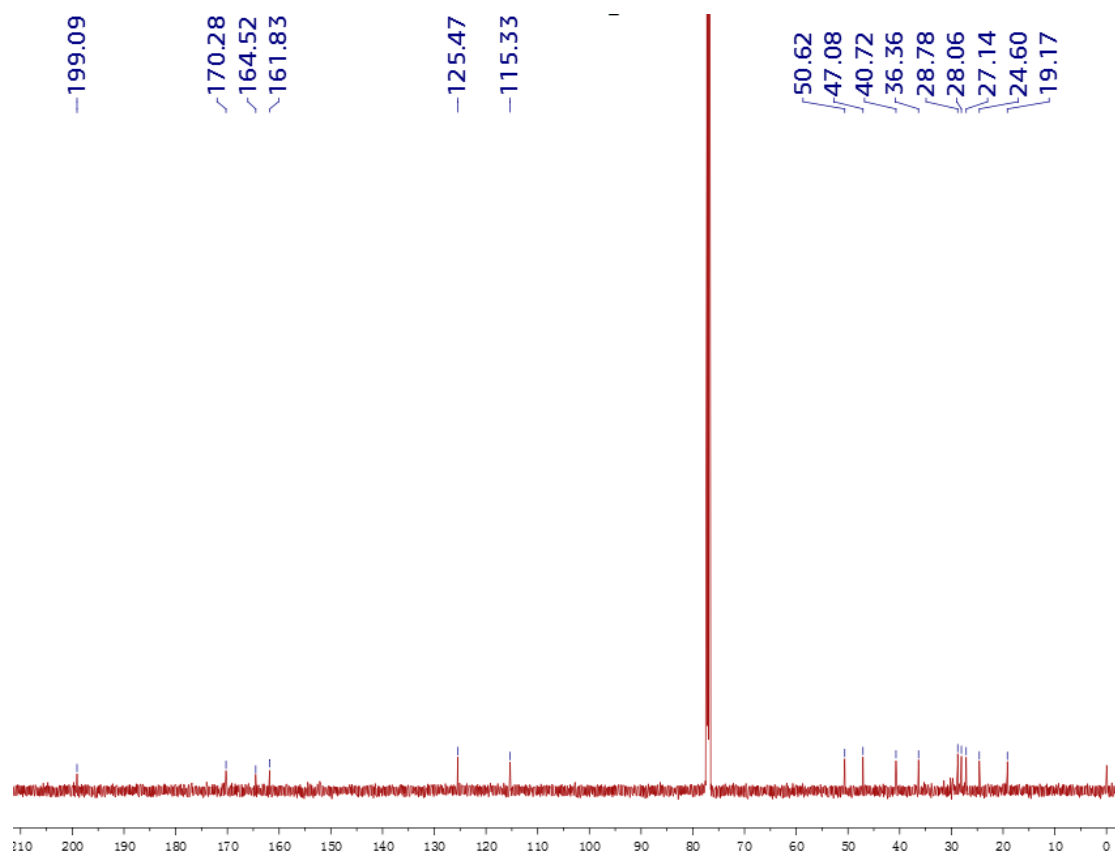


Figure S19. ¹³C NMR spectrum of compound **4** in CDCl₃

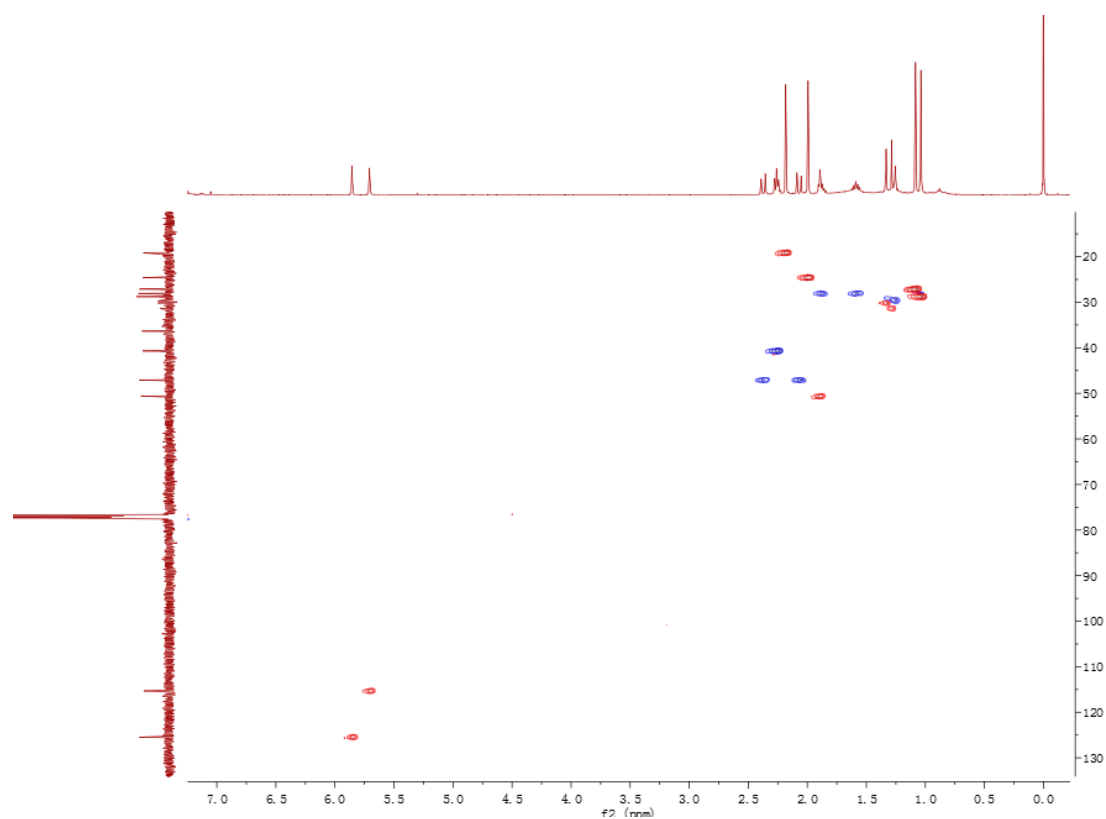


Figure S20. HSQC spectrum of compound **4**

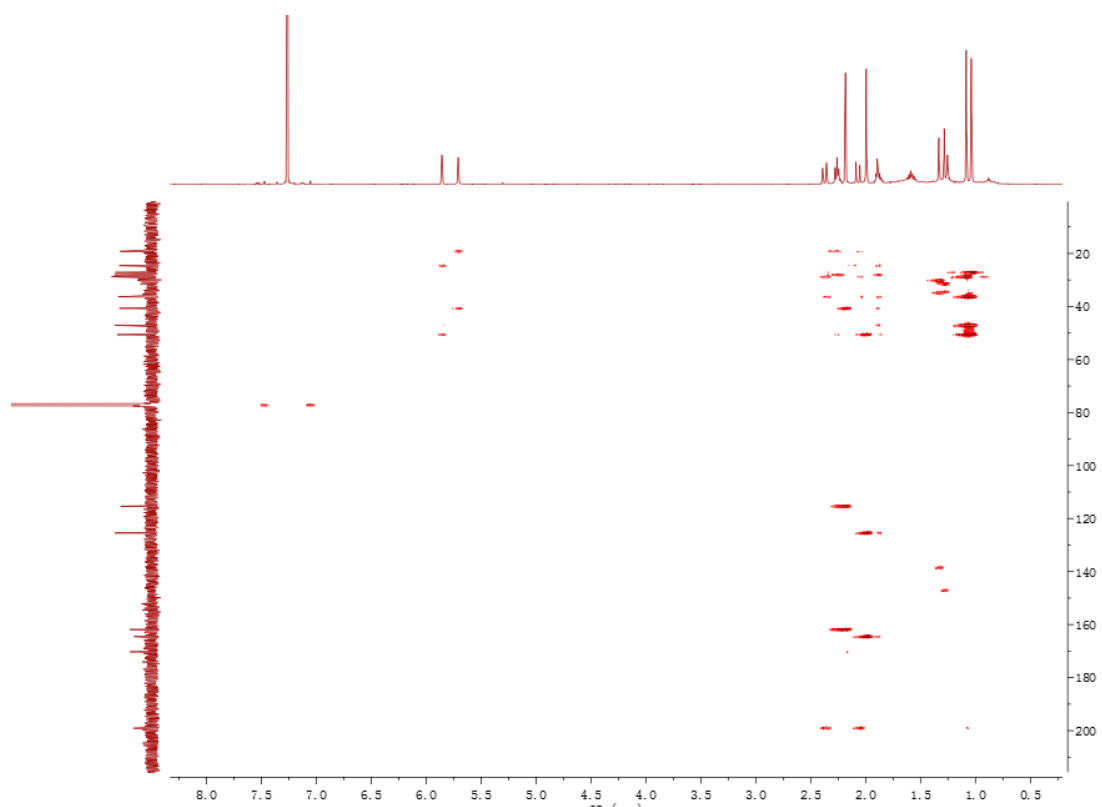


Figure S21. HMBC spectrum of compound **4**

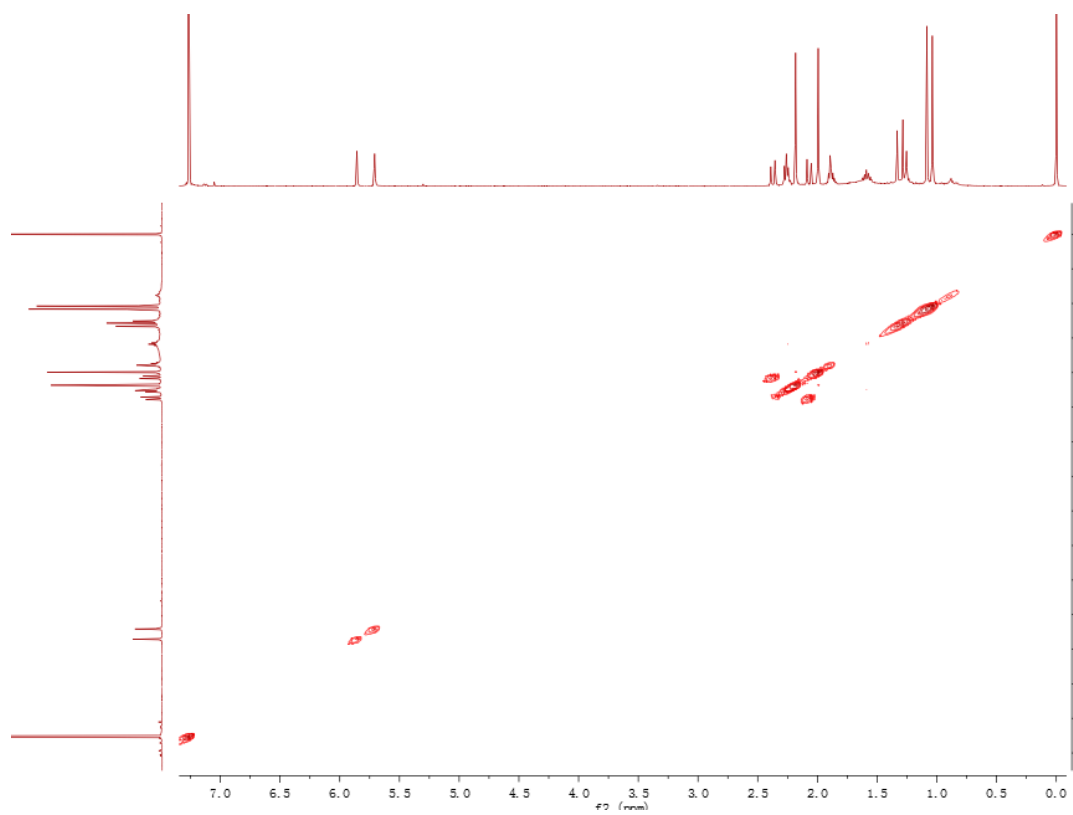
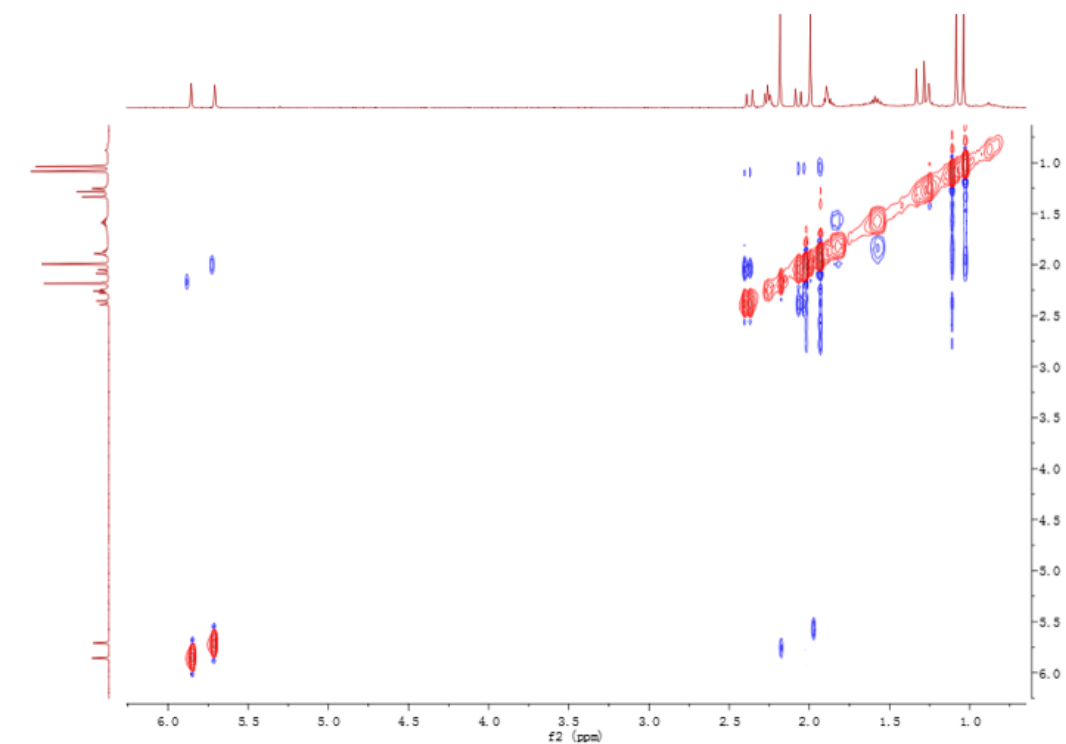


Figure S22. ^1H - ^1H COSY spectrum of compound **4**



27 #50-62 RT: 0.89-1.11 AV: 13 NL: 2.33E8
T: FTMS + pESI Full ms [200.0000-1000.0000]

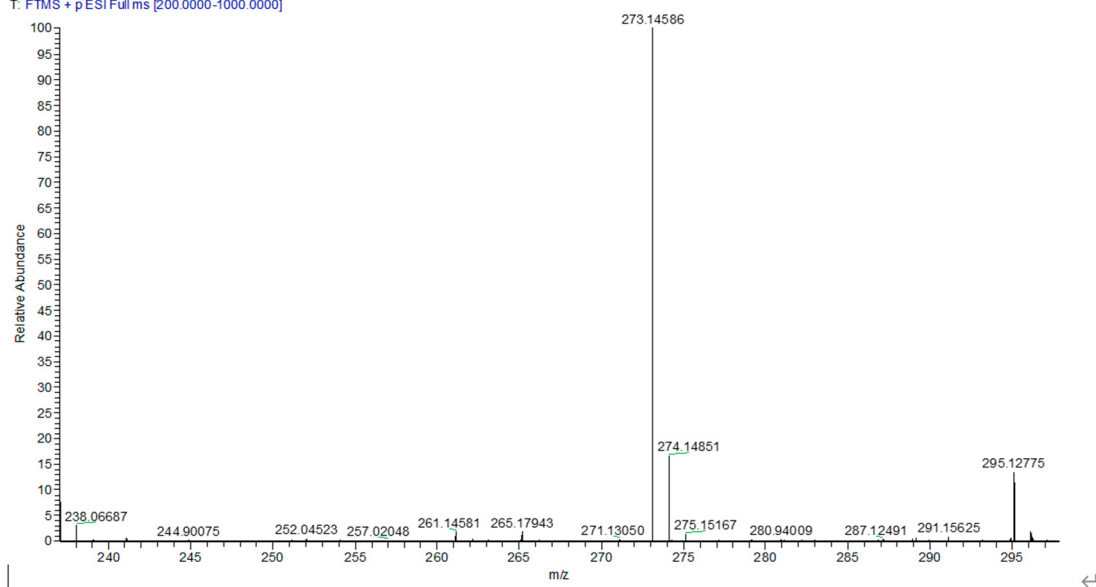


Figure S23. HRESIMS spectrum of compound **4**

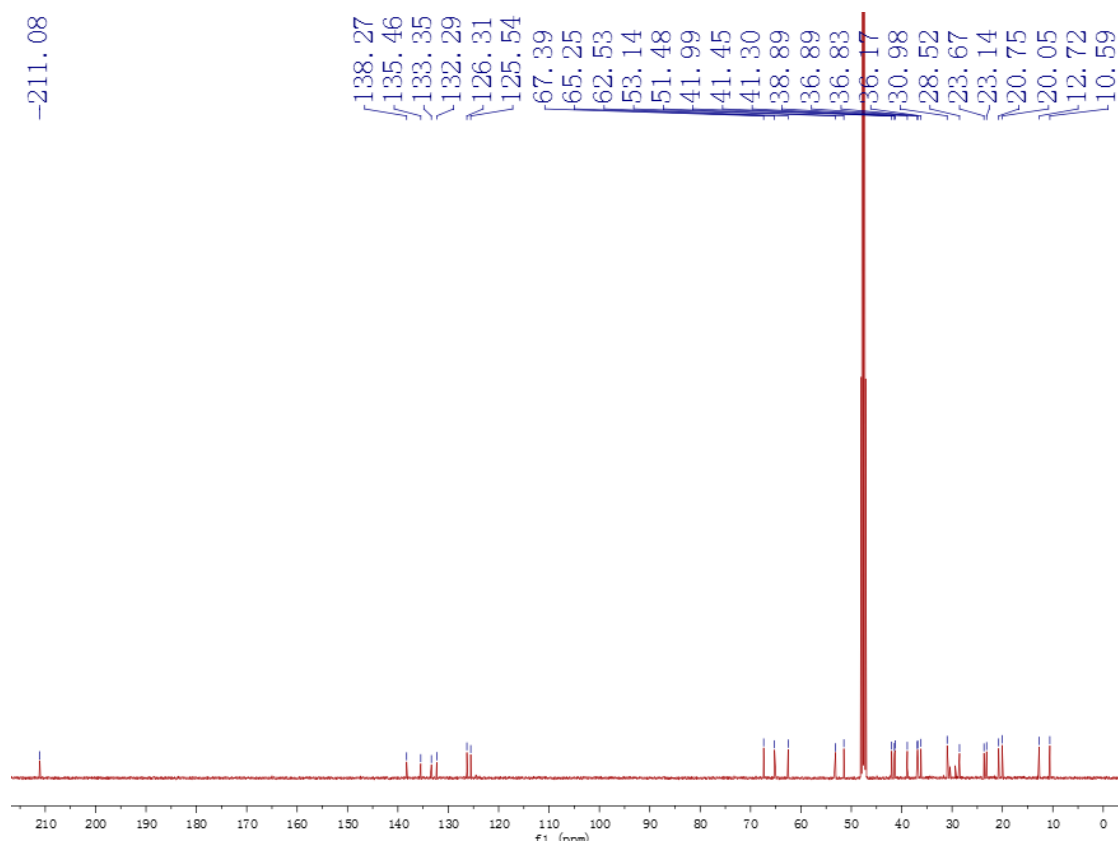
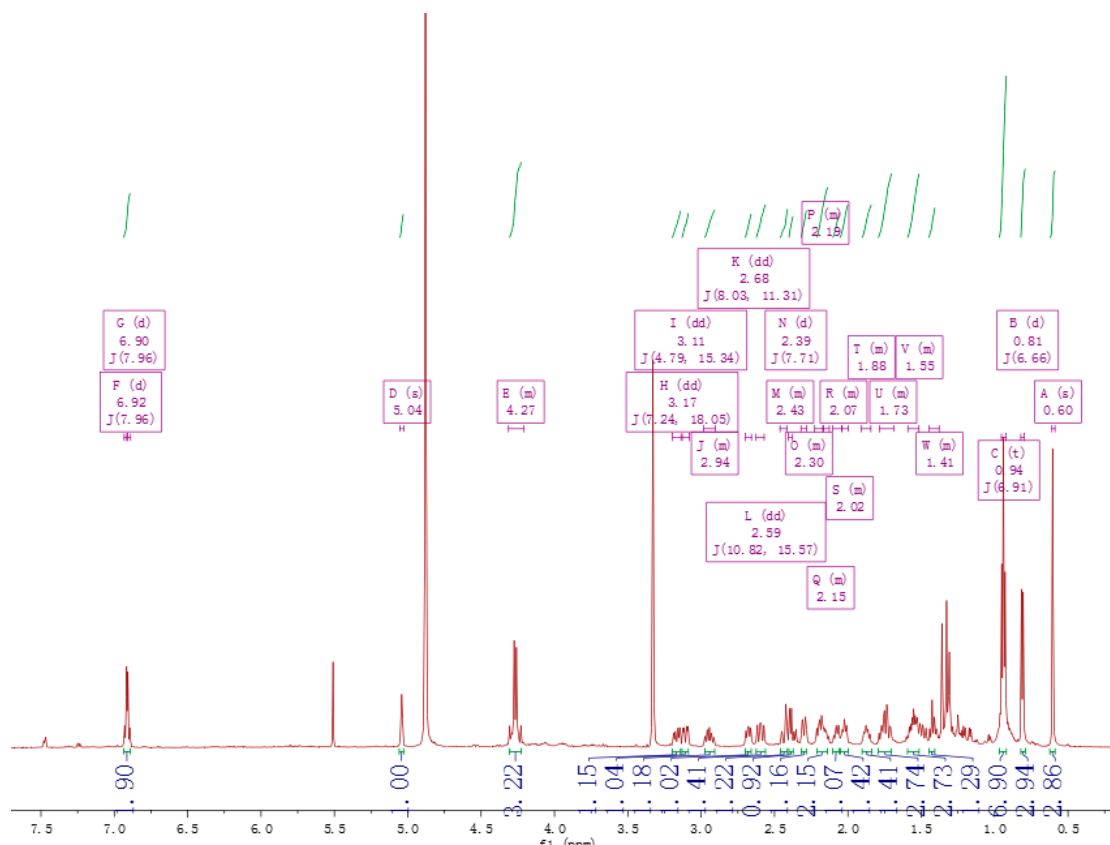


Figure S25. ^{13}C NMR spectrum of compound **5** (500 MHz, CD_3OD).

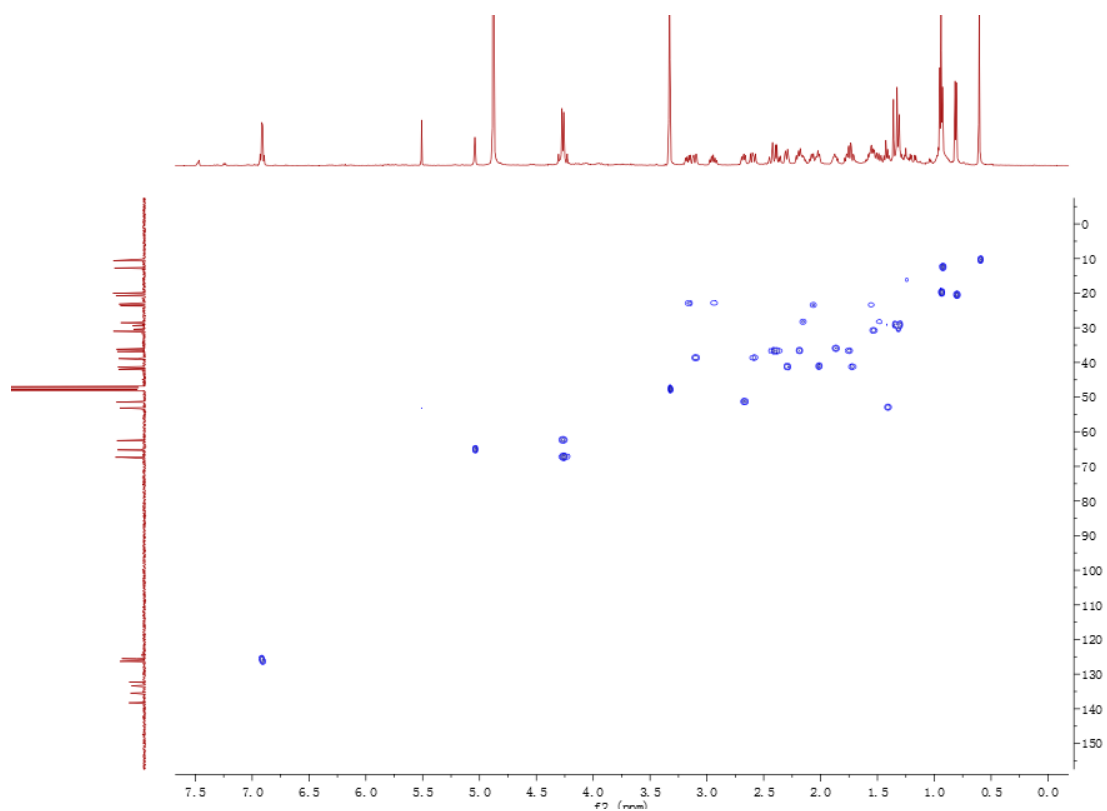


Figure S26. HSQC spectrum of compound **5**

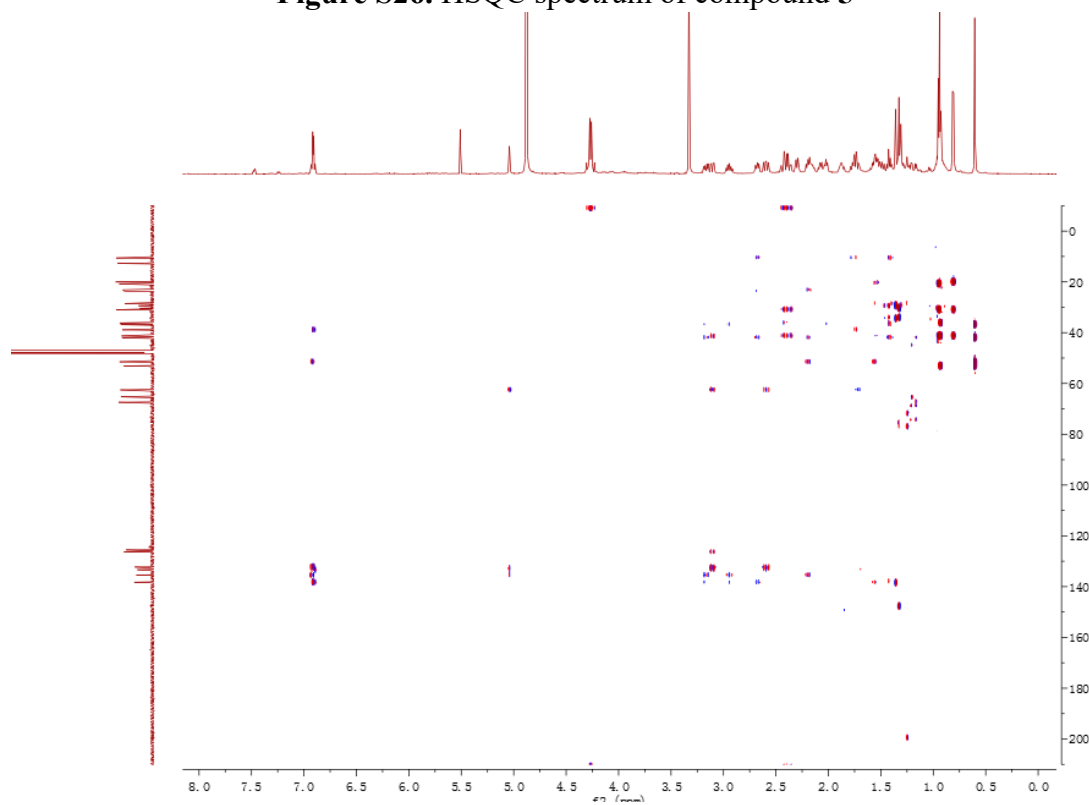


Figure S27. HMBC spectrum of compound **5**.

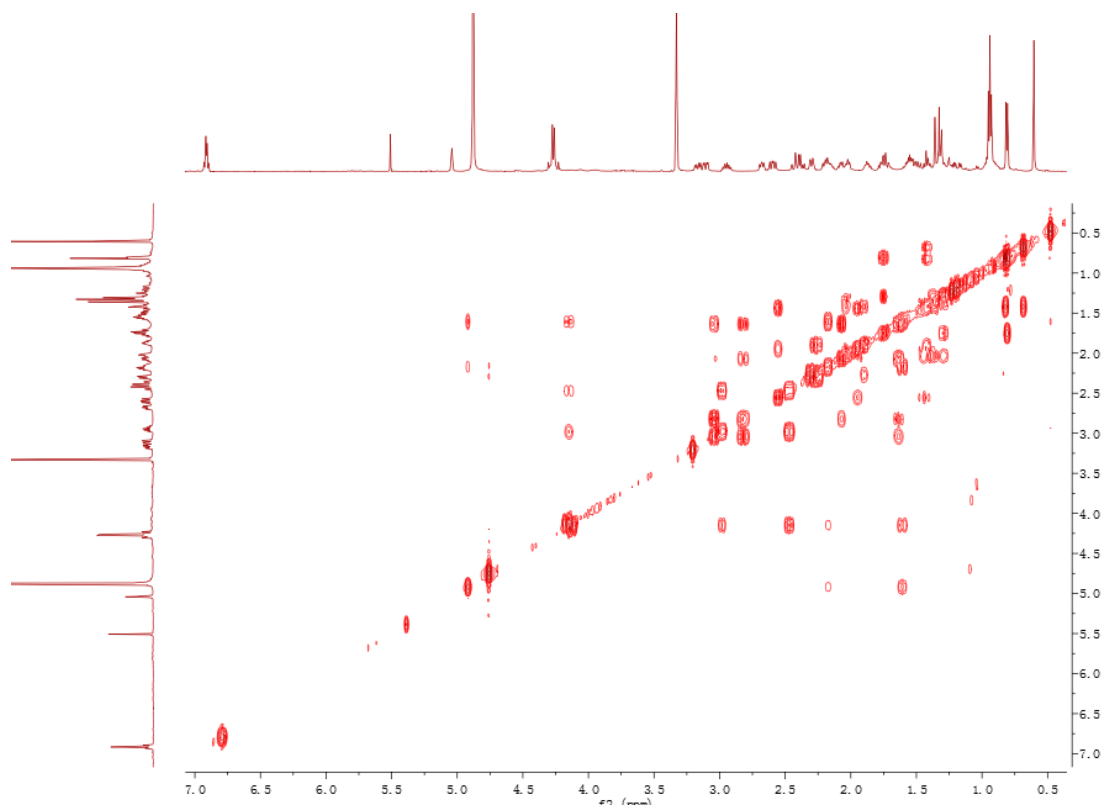


Figure S28. ^1H - ^1H COSY spectrum of compound **5**

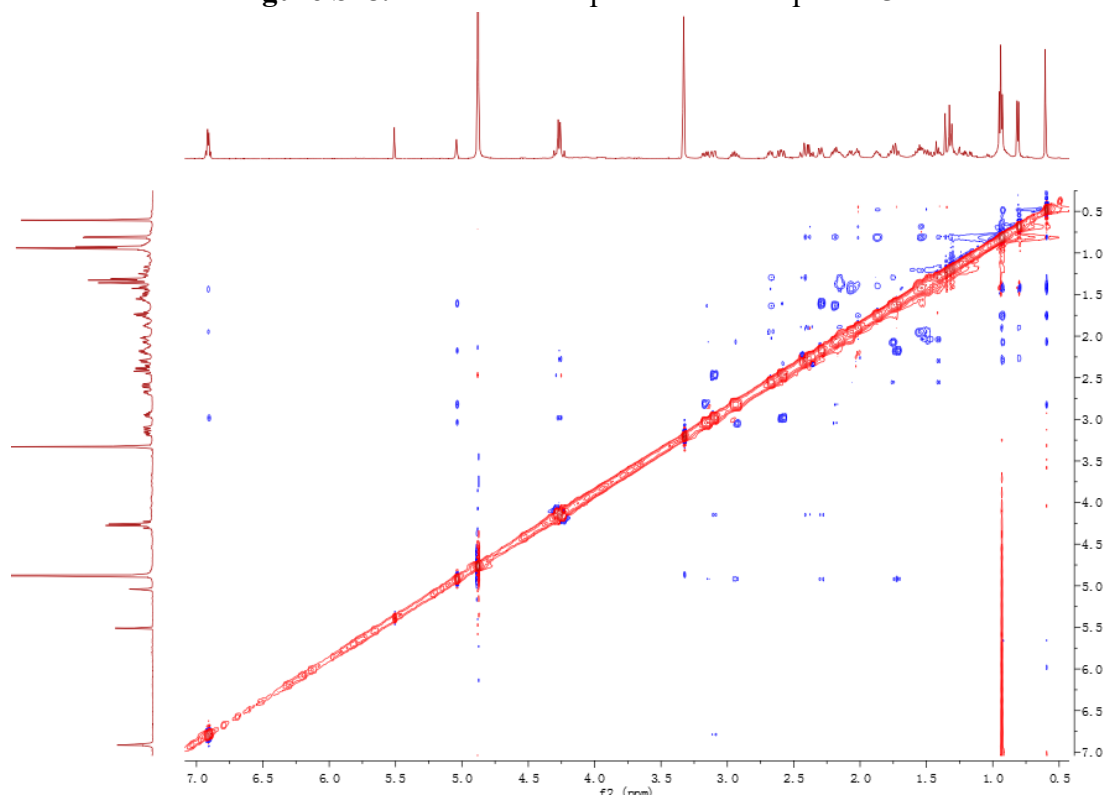


Figure S29. NOESY spectrum of compound **5**

2YZ-12 #50-61 RT: 0.89-1.09 AV: 12 NL: 6.76E7
T: FTMS + p ESI Full ms [200.0000-1000.0000]

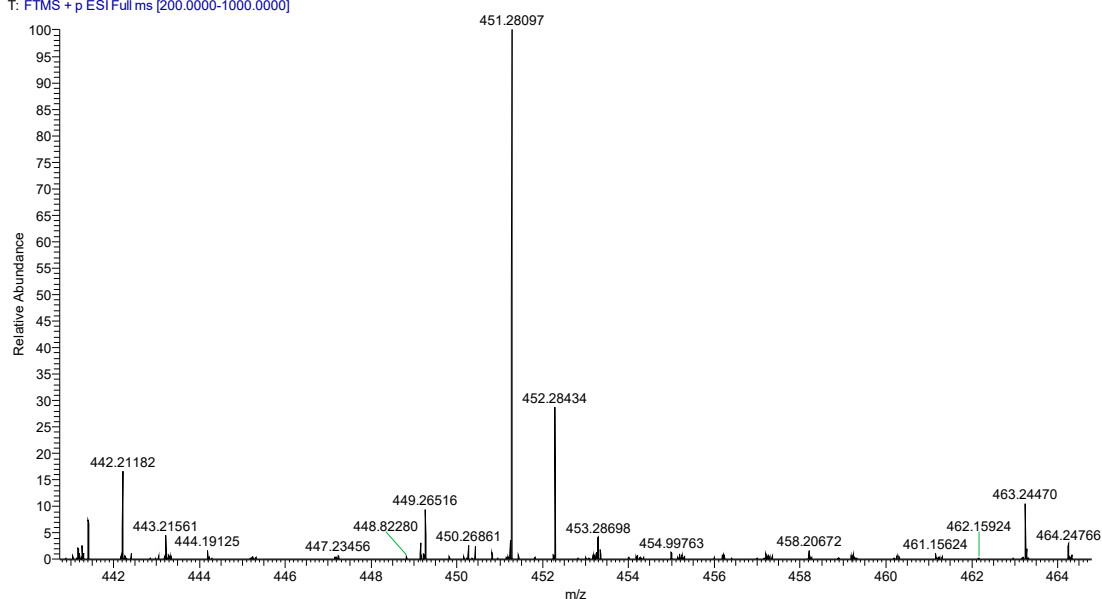


Figure S30. HRESIMS spectrum of compound **5**

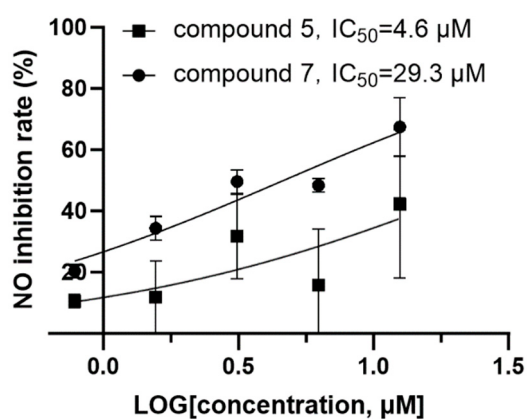


Figure S31. The IC₅₀ value of compounds **5** and **7** against LPS-induced NO production in RAW264.7 cells were calculated and presented. Data were expressed as mean values $\pm$ SD, $n = 3$.

Table S1. The DP4+ evaluation of **3**.

Functional		Solvent?	Basis Set		Type of Data		
mPW1PW91		PCII	6-31G(d,p)		Unscaled Shifts		
		DP4+	0.00%	100.00%	–	–	–
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	127.2	129.3	128.8			
C	x	124.4	124.4	124.4			
C	x	119.6	121.0	120.8			
C	x	140.9	143.7	142.2			
C	x	119.8	120.2	120.5			
C	x	158.7	159.0	158.7			
C		89.4	90.6	90.5			
C		30.5	32.2	31.3			
C		71.6	72.4	72.5			
C		23.9	22.4	22.2			
C		26.4	26.6	26.5			
C		55.8	56.70	56.00			
C		72	76.00	73.30			
C	x	139	143.30	140.00			
C	x	115.2	113.00	113.70			
H	x	7.05	7.11	7.11			
H	x	6.83	6.77	6.76			
H		4.59	4.58	4.58			
H		3.1	3.01	3.02			
H		3.19	3.37	3.27			
H		1.15	1.19	1.20			
H		1.36	1.43	1.40			
H		4.65	4.82	4.68			
H		4.78	4.84	4.80			
H		5.39	5.28	5.42			
H		6.11	6.18	6.18			
H	x	5.25	5.41	5.3			
H	x	5.37	5.76	5.54			

Functional		Solvent?	Basis Set		Type of Data		
mPW1PW91		PCII	6-31G(d,p)		Unscaled Shifts		
		Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)		0.11%	99.89%	–	–	–	–
sDP4+ (C data)		0.09%	99.91%	–	–	–	–
sDP4+ (all data)		0.00%	100.00%	–	–	–	–
uDP4+ (H data)		5.68%	94.32%	–	–	–	–
uDP4+ (C data)		4.65%	95.35%	–	–	–	–
uDP4+ (all data)		0.29%	99.71%	–	–	–	–
DP4+ (H data)		0.01%	99.99%	–	–	–	–
DP4+ (C data)		0.00%	100.00%	–	–	–	–
DP4+ (all data)		0.00%	100.00%	–	–	–	–