SUPPLEMENTARY MATERIAL

New butenolides with anti-inflammatory activity from *Balanophora simaoensis*

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Abstract: Two new butenolides, balanolides A (**1**) and B (**1**), were isolated from the aerial parts of the parasitic plant *Balanophora simaoensis*. Their structures were established by comprehensive spectroscopic analysis and quantum chemical ECD calculation. The new butenolides were evaluated for their inhibitory effects against nitric oxide (NO) production in LPS-induced RAW 264.7 macrophage cells. Compounds **1** and **2** displayed moderate anti-inflammatory activity with IC_{50}values of 11.8 and 12.9 μM, respectively.

Key words: *Balanophora simaoensis*; butenolides; anti-inflammatory activity

List of supporting information

Table S1. ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR data for compounds **1** and **2** in $CDCl_3$

Position	**1**		**2**	
	δ_H(J in Hz)	δ_C	δ_H(J in Hz)	δ_C
1		129.5		120.7
2	6.67 d (2.9)	116.5		158.2
3		151.6	6.44 d (2.4)	98.5
4		153.5		159.8
5	6.77 d (8.8)	111.0	6.40 dd (8.2, 2.4)	104.0
6	6.73 dd (8.8, 2.9)	111.6	6.95 d (8.2)	130.1
7	2.76 m	28.9	2.73 m	28.2
8	2.71 m	26.8	2.68 m	26.9
	2.54 m		2.50 m	
9		163.7		164.0
10		123.3		123.2
11		174.6		174.7
12	4.87 q (6.8)	78.6	4.84 q (6.8)	78.7
13	1.68 s	8.4	1.66 s	8.4
14	1.40 d (6.8)	18.2	1.38 d (6.8)	18.2
2-OCH_3			3.80 s	55.4
3-OCH_3	3.78 s	55.6		
4-OCH_3	3.76 s	55.7	3.79 s	55.2

Figure S1. Selected COSY (—) and HMBC (⤳) correlations of **1**

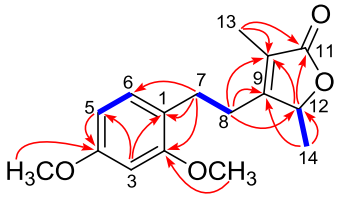


Figure S2. Experimental/calculated ECD spectra of **1** and experimental ECD spectra **2** (in MeOH)

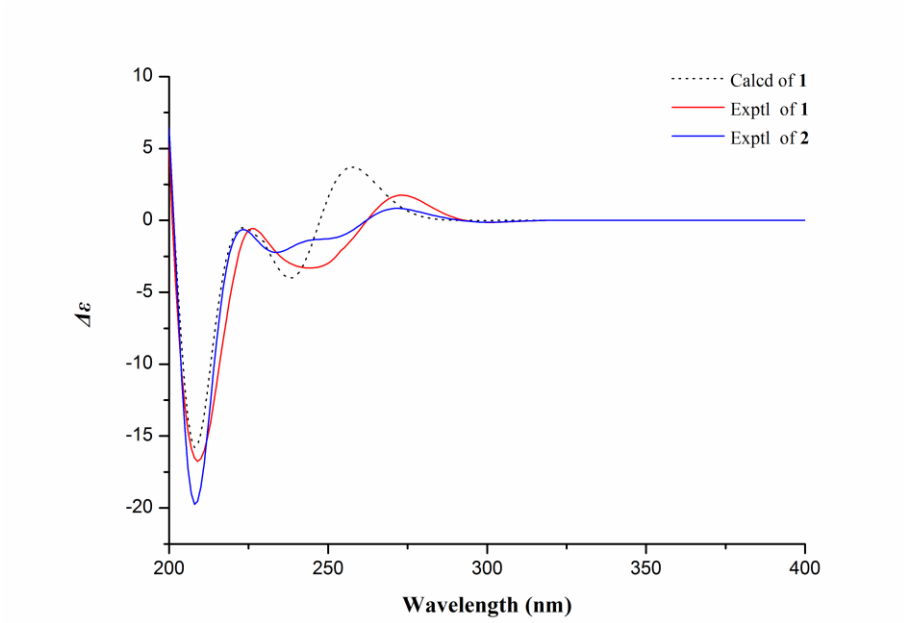
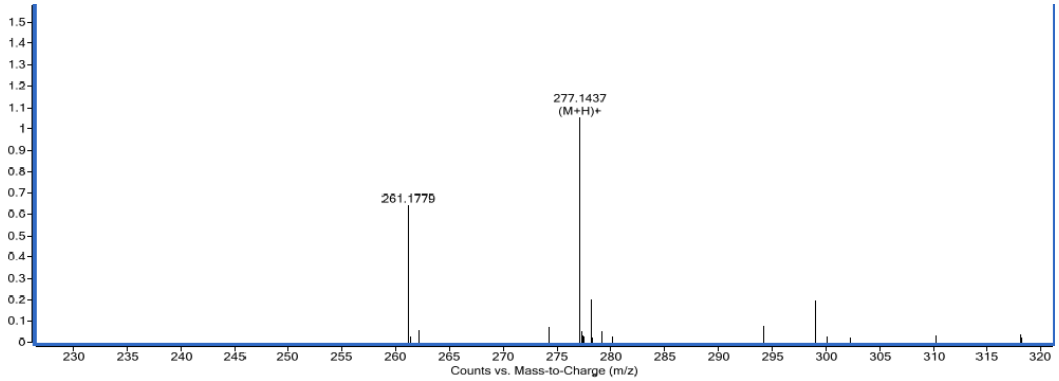


Figure S3. HR-ESI-MS spectrum of compound **1**



Name	Formula	Score	Mass	Mass (MFG)	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)
	C16 H20 O4	91.55	276.1364	276.1362	-1.05	1.05	-0.29

Species	Ion Formula	m/z	Height	Score (MFG)	Score (MFG, MS)	Score (MFG, mass)	Score (MFG, abund)	Score (MFG, iso. spacing)
(M+H)+	C16 H21 O4	277.1434	10507	91.55	91.55	99.33	93.59	73.53

m/z	m/z (Calc)	Diff (ppm)	Diff (mDa)	Height	Height (Calc)	Height %	Height % (Calc)	Height Sum %	Height Sum% (Calc)
277.1437	277.1434	-1.1	-0.3	10507	10807.7	100	100	81	83.3
278.145	278.1468	6.71	1.9	1973.1	1912.9	18.8	17.7	15.2	14.7
279.1526	279.1493	-11.73	-3.3	488.4	248	4.6	2.3	3.8	1.9

Figure S4. ^{1}H NMR (600 MHz) spectrum of compound **1**

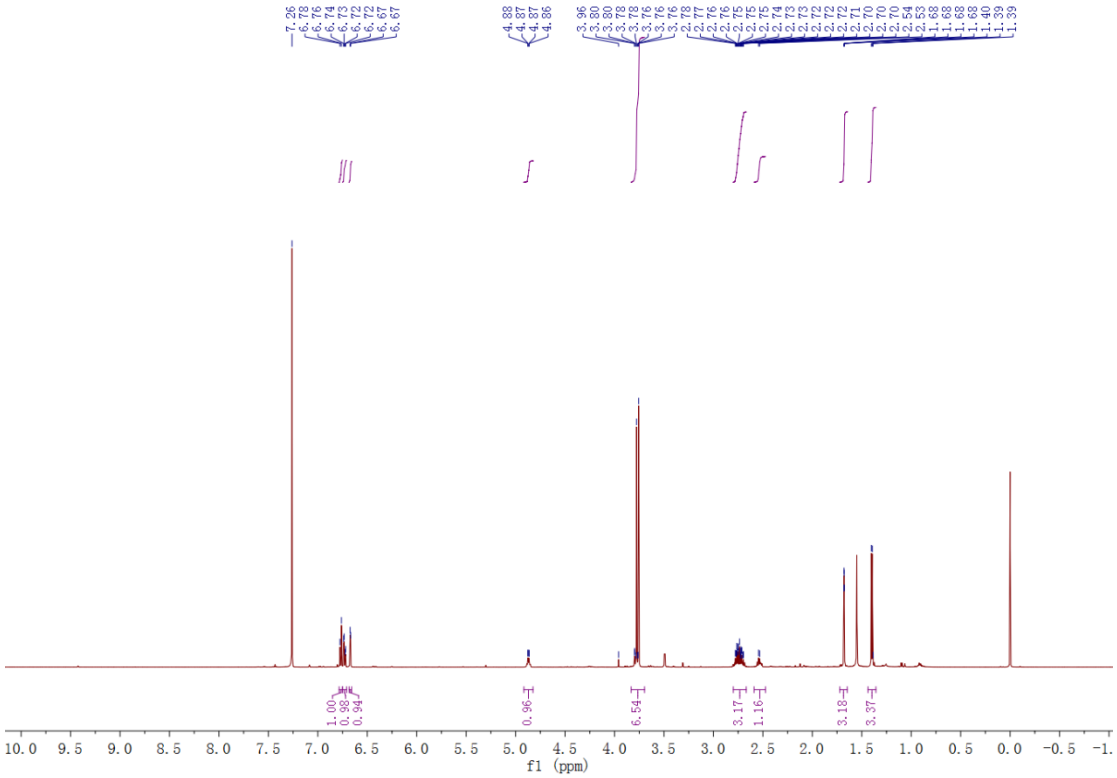


Figure S5. 13C NMR (150 MHz) spectrum of compound **1**

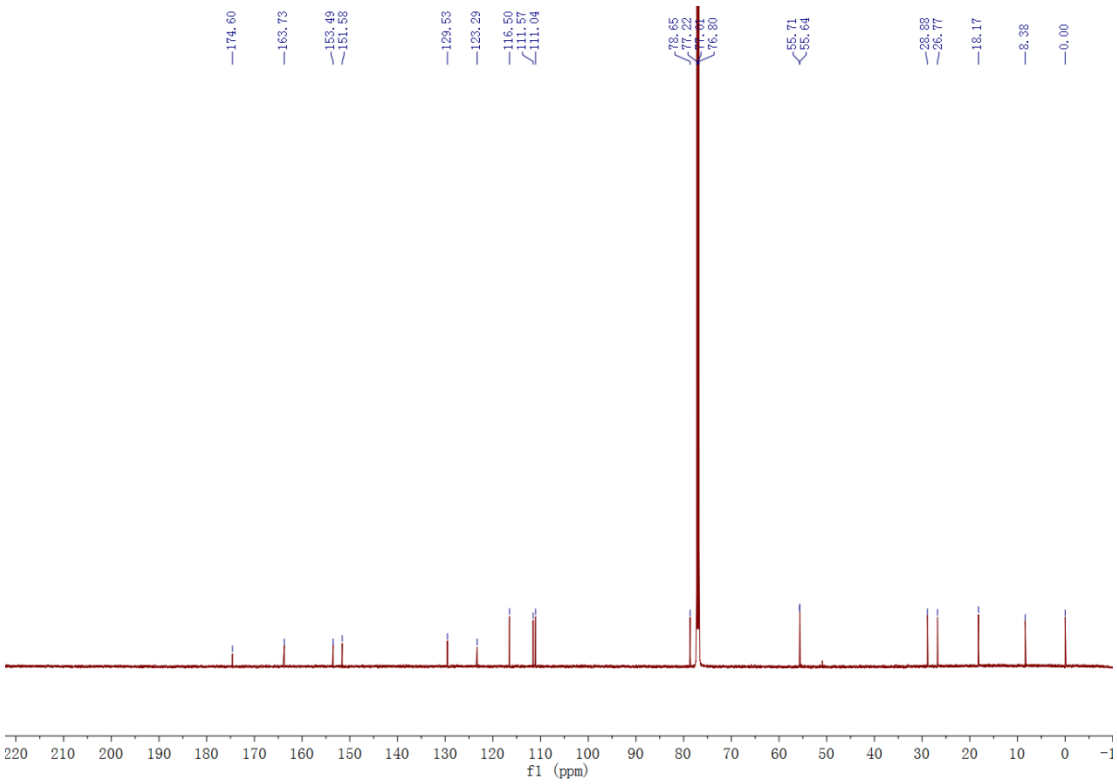


Figure S6. 1H-1H COSY spectrum of compound **1**

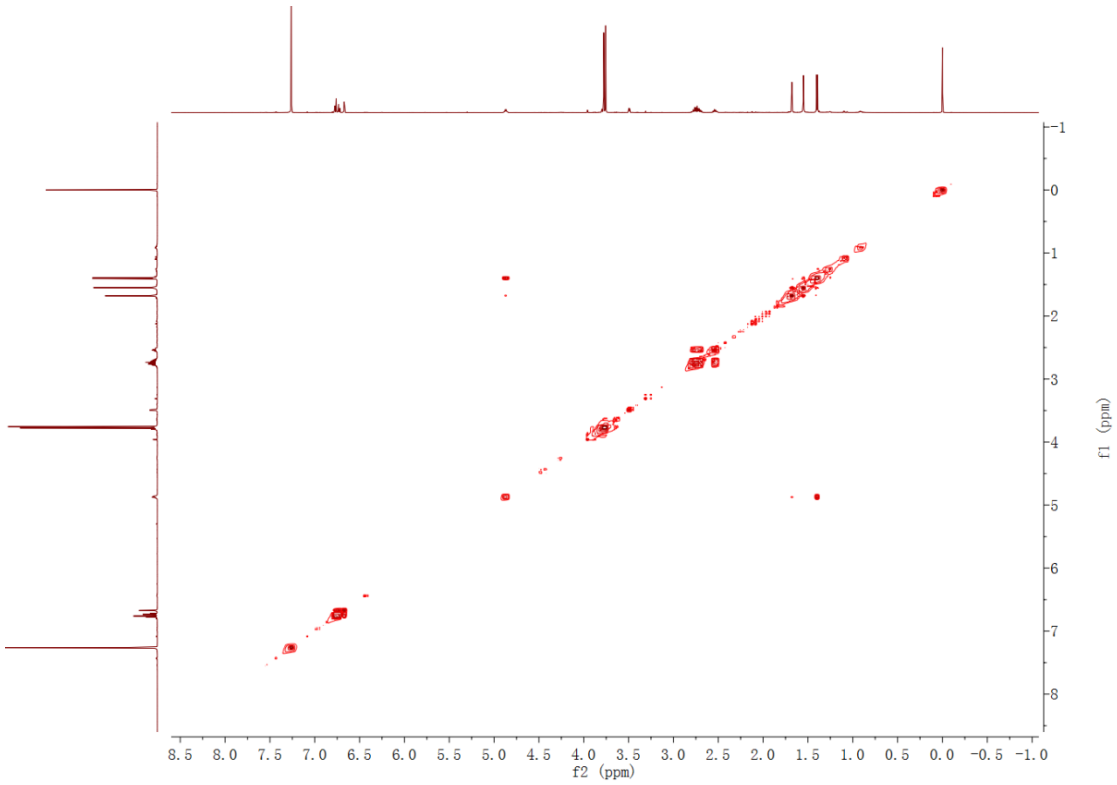


Figure S7. HSQC spectrum of compound **1**

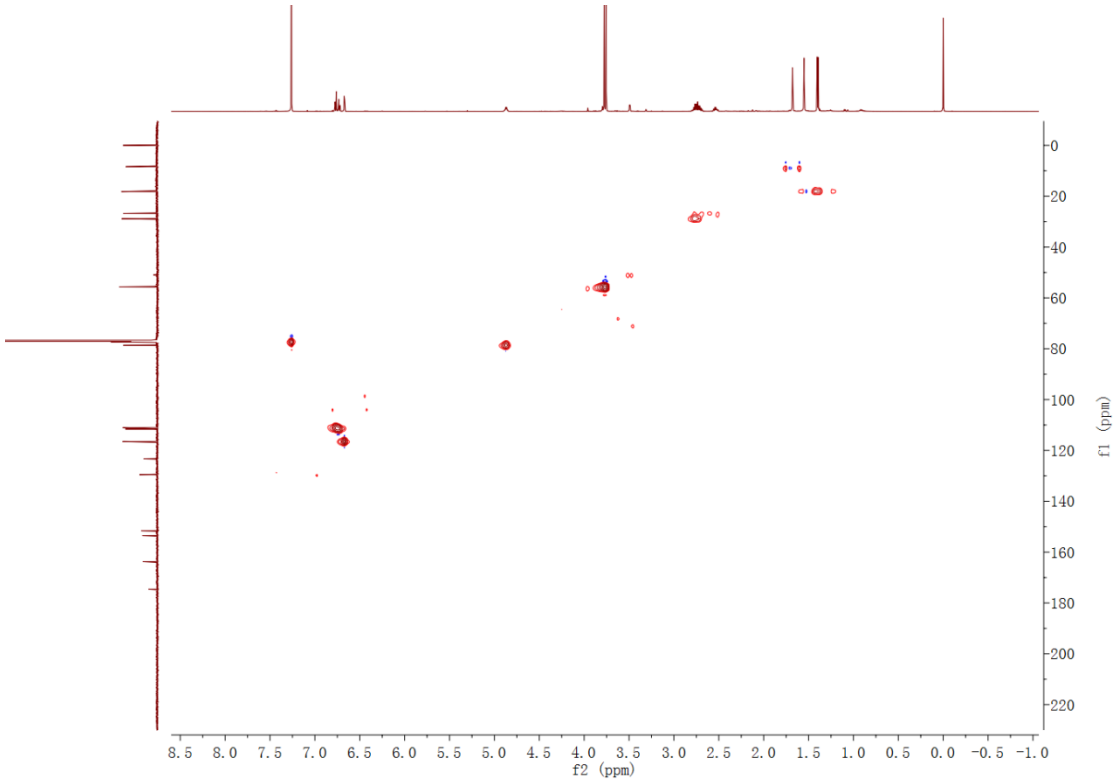


Figure S8. HMBC spectrum of compound **1**

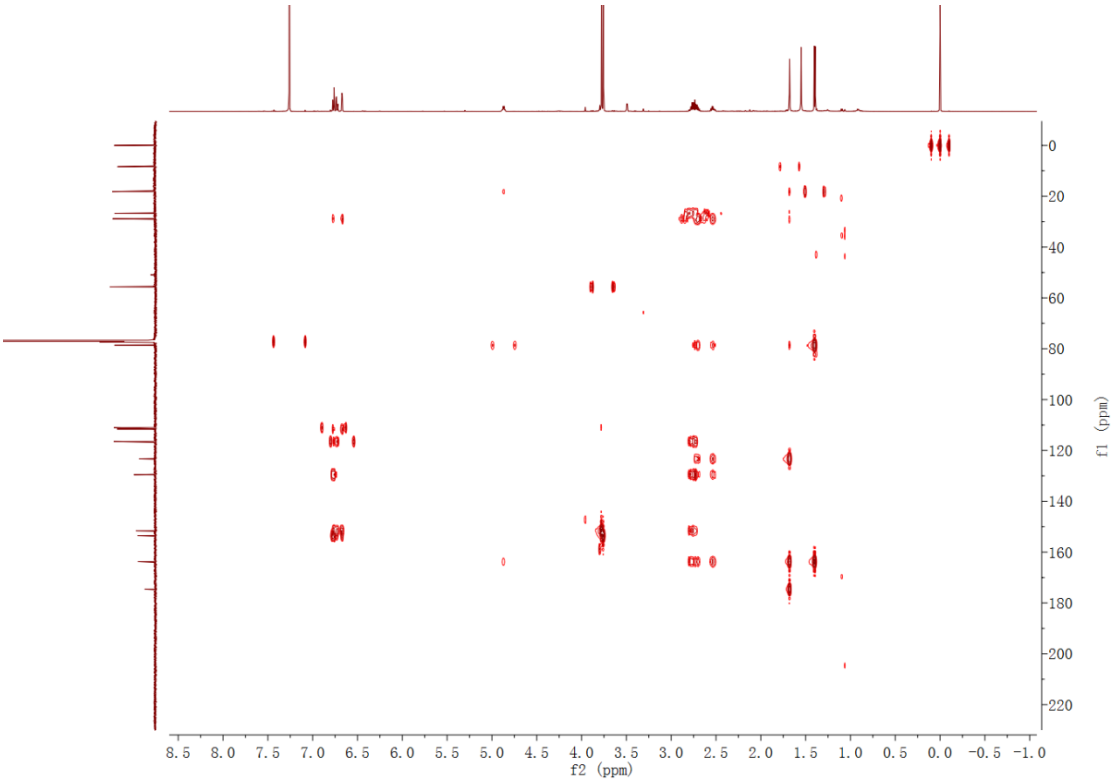


Figure S9. IR spectrum of compound **1**

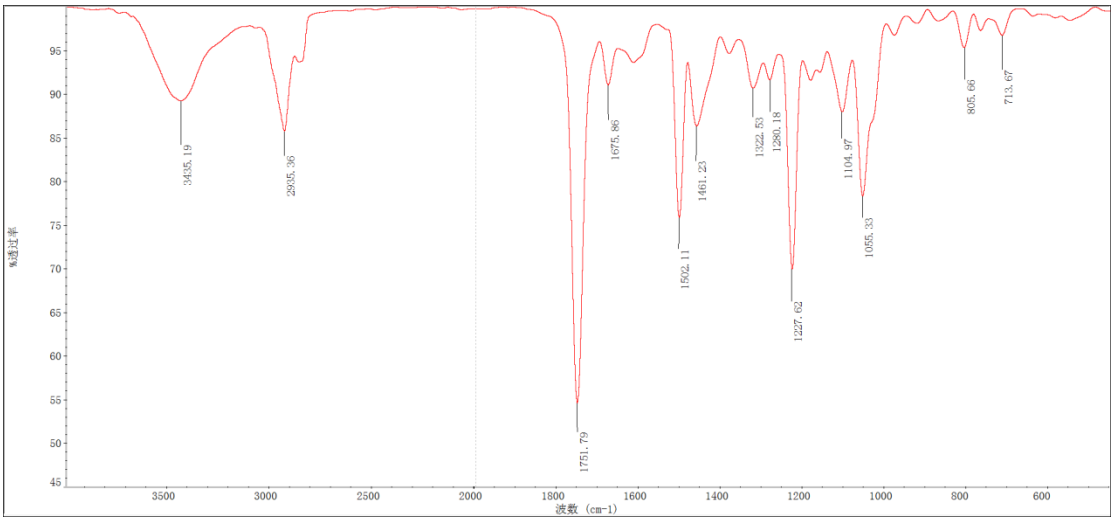
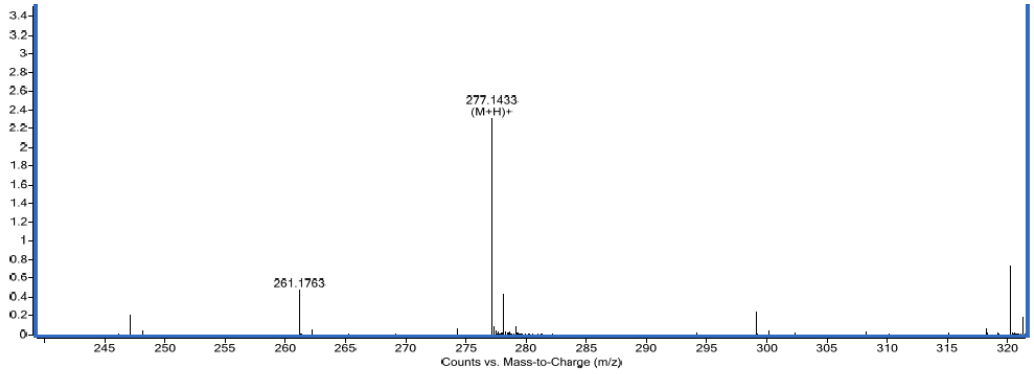


Figure S10. HR-ESI-MS spectrum of compound **2**



Name	Formula	Score	Mass	Mass (MFG)	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)
	C16 H20 O4	98.61	276.136	276.1362	0.65	0.65	0.18

Species	Ion Formula	m/z	Height	Score (MFG)	Score (MFG, MS)	Score (MFG, mass)	Score (MFG, abund)	Score (MFG, iso. spacing)
(M+H)+	C16 H21 O4	277.1434	23050	98.61	98.61	99.75	98.27	96.75

m/z	m/z (Calc)	Diff (ppm)	Diff (mDa)	Height	Height (Calc)	Height %	Height % (Calc)	Height Sum %	Height Sum% (Calc)
277.1433	277.1434	0.63	0.2	23050	23409.9	100	100	82.1	83.3
278.1459	278.1468	3.21	0.9	4261	4143.3	18.5	17.7	15.2	14.7
279.1494	279.1493	-0.41	-0.1	779.4	537.2	3.4	2.3	2.8	1.9

Figure S11. ^{1}H NMR (600 MHz) spectrum of compound **2**

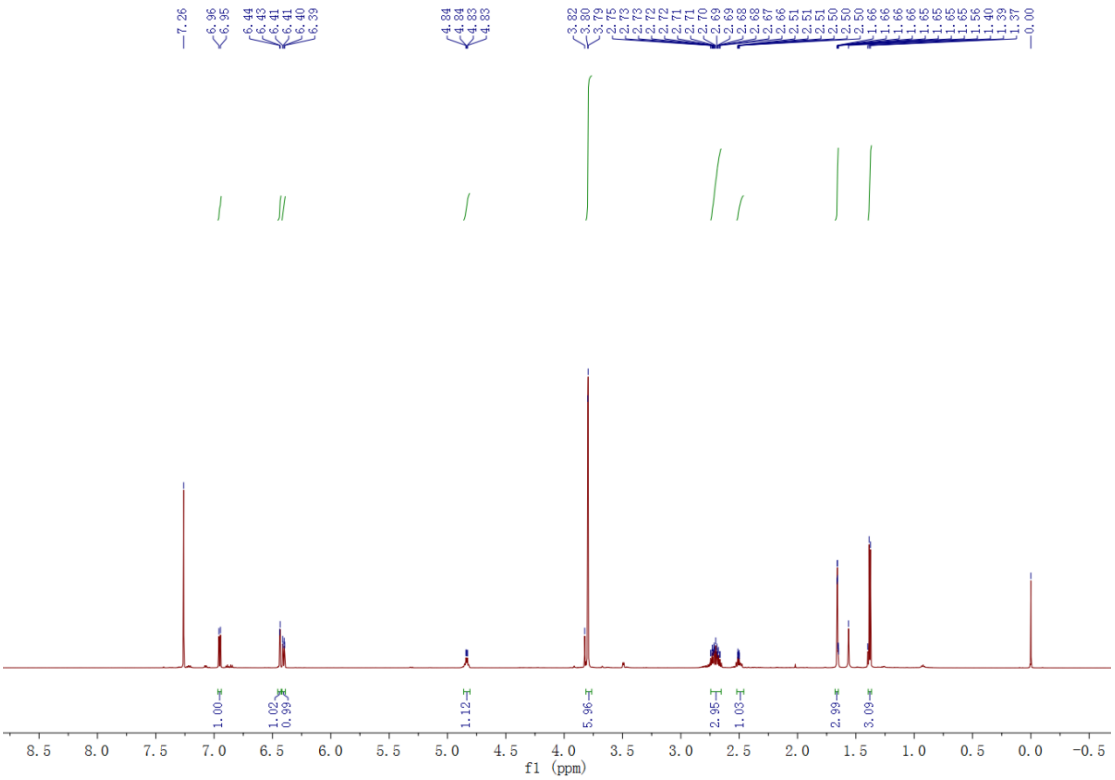


Figure S12. 13C NMR (150 MHz) spectrum of compound **2**

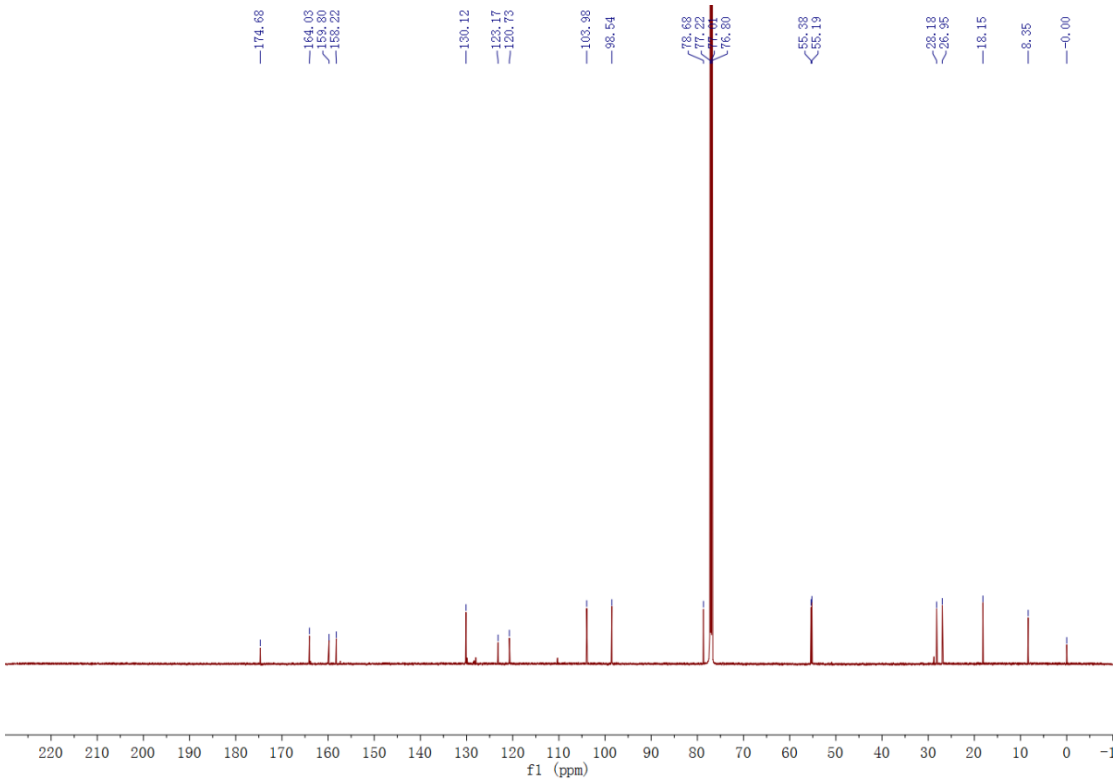


Figure S13. 1H-1H COSY spectrum of compound **2**

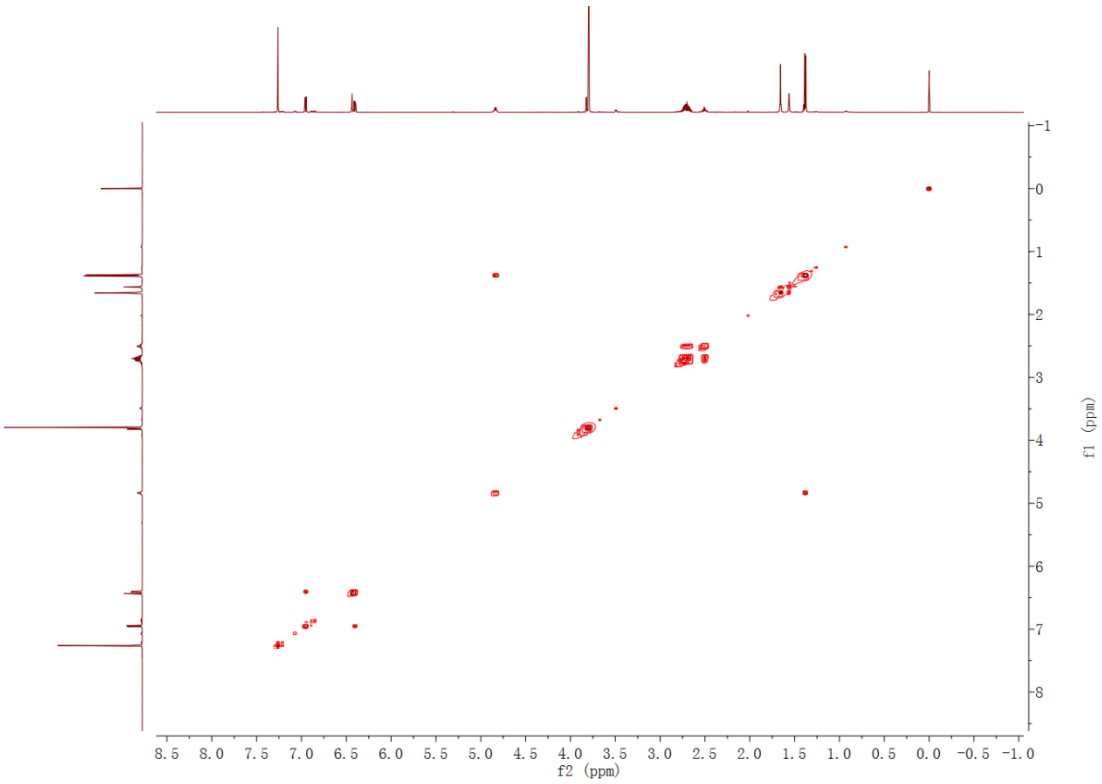


Figure S14. HSQC spectrum of compound **2**

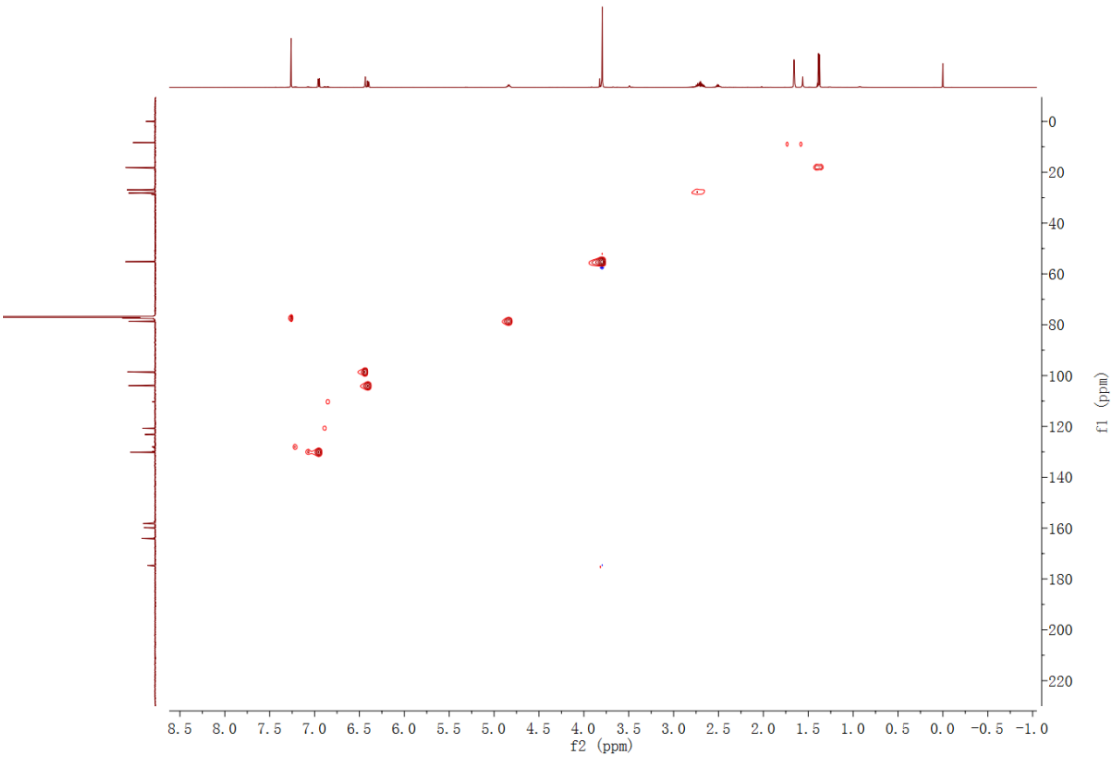


Figure S15. HMBC spectrum of compound **2**

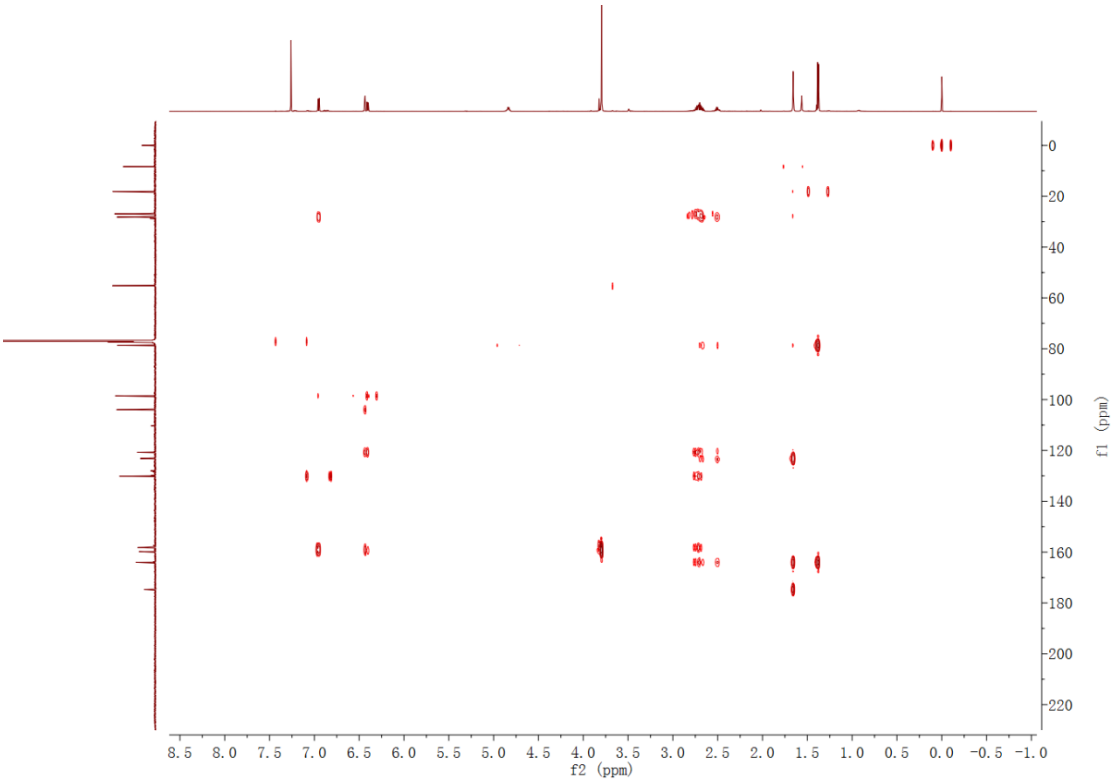


Figure S16. IR spectrum of compound **2**