SUPPLEMENTARY MATERIAL

Structure elucidation and NMR assignments of a new sesquiterpene of volatile oil from *Artemisia frigida* Willd

Saranchimeg Borchuluun, Qinghu Wang *, Yanhua Xu, Xiang He, Wenqiang Bao, Biligetu Pa

College of Traditional Mongolian Medicine, Inner Mongolia University for Nationalities, Tongliao 028000, Inner Mongolia, China

A new sesquiterpene, artefrigin (**5**), together with four known sesquiterpenes were isolated from the volatile oil of *Artemisia frigida* Willd. The structure of **5** was elucidated by spectroscopic methods, including UV, IR, HR-ESI-MS and extensive 1D and 2D NMR techniques.

Keywords: *Artemisia frigida* Willd.; Compositae; Sesquiterpene; Artefrigin

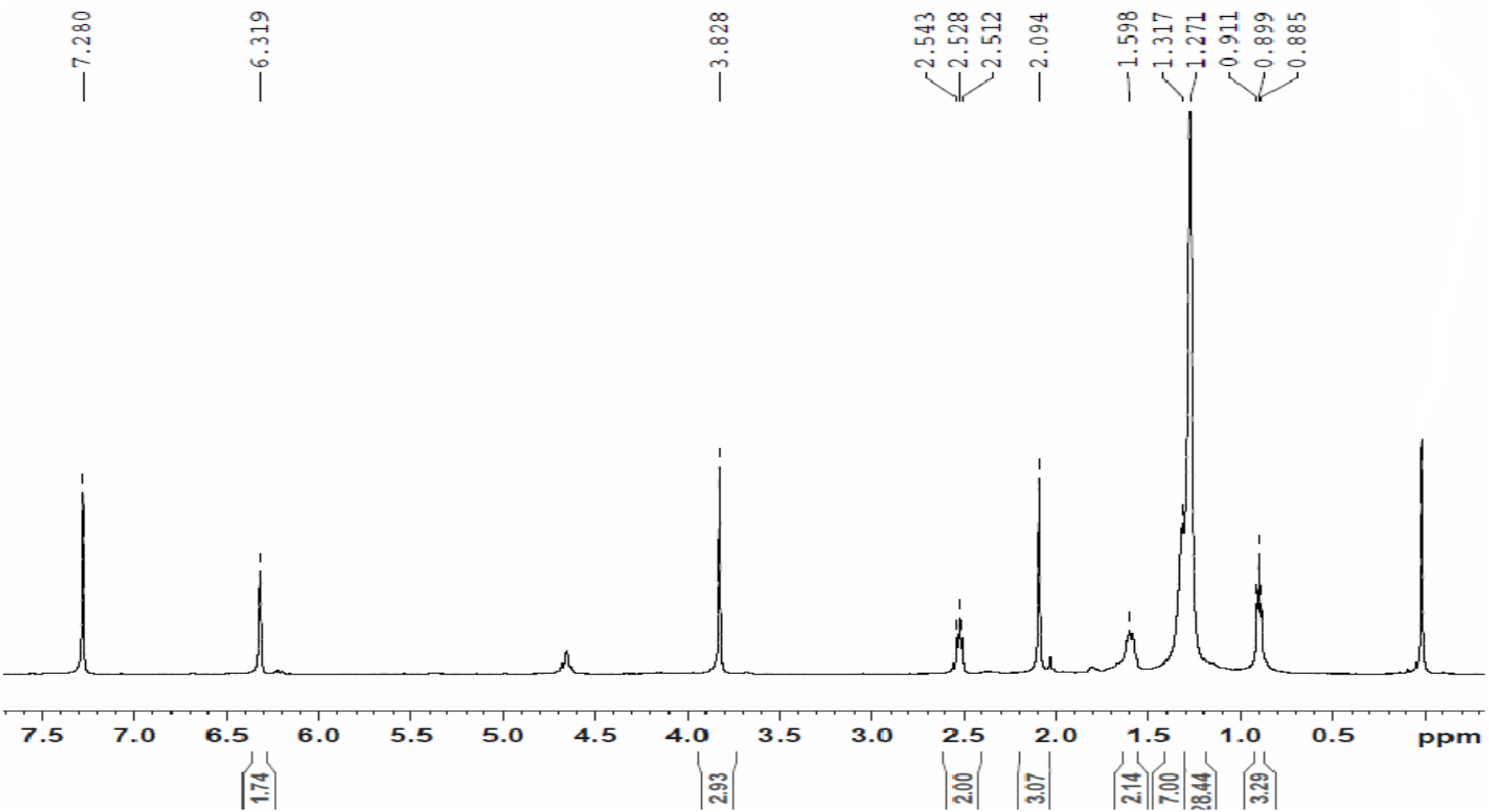

Figure S1. ^{1}H-NMR spectrum of compound **5**

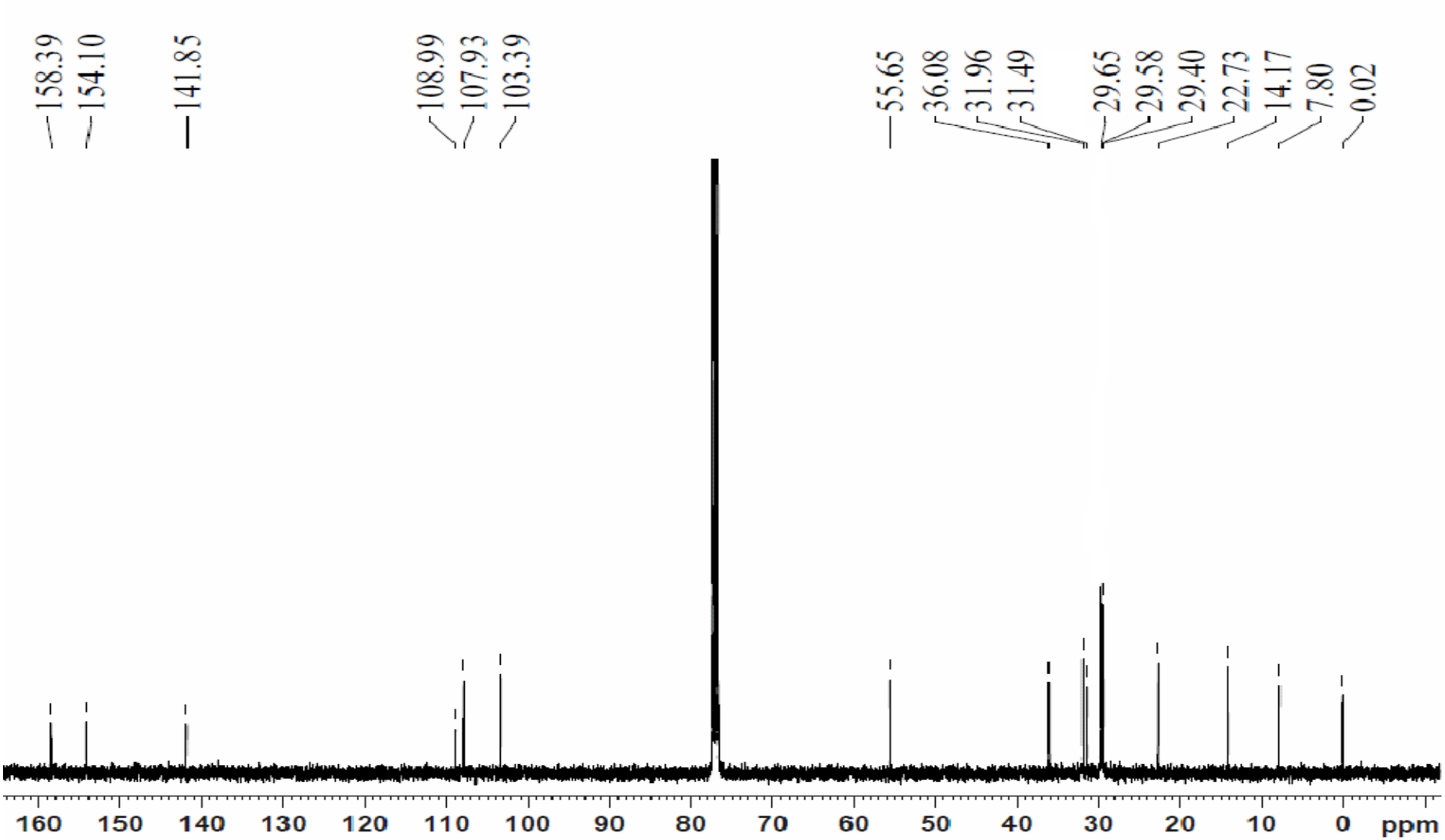

Figure S2. ^{13}C-NMR spectrum of compound **5**

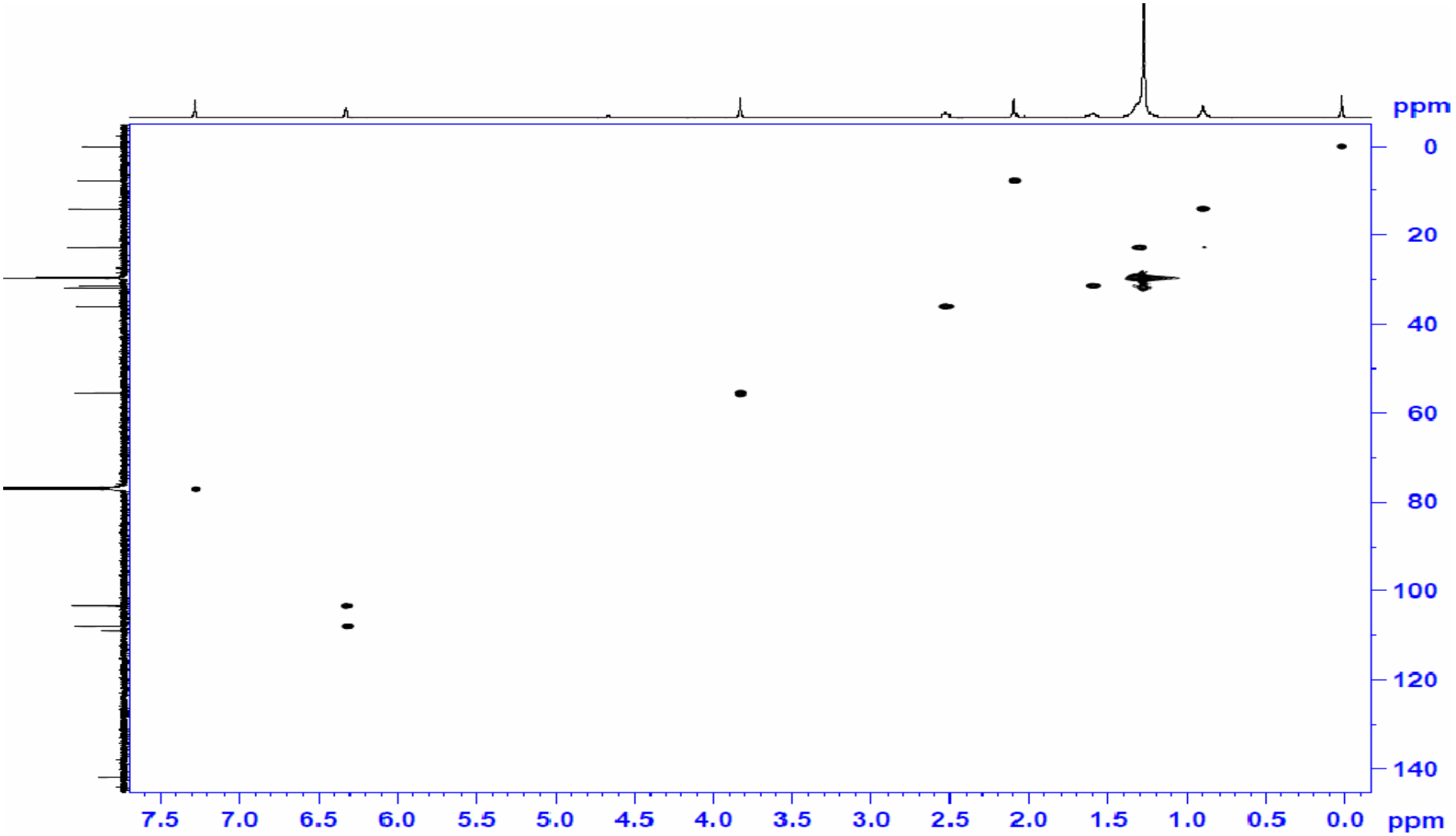

Figure S3. HSQC spectrum of compound **5**

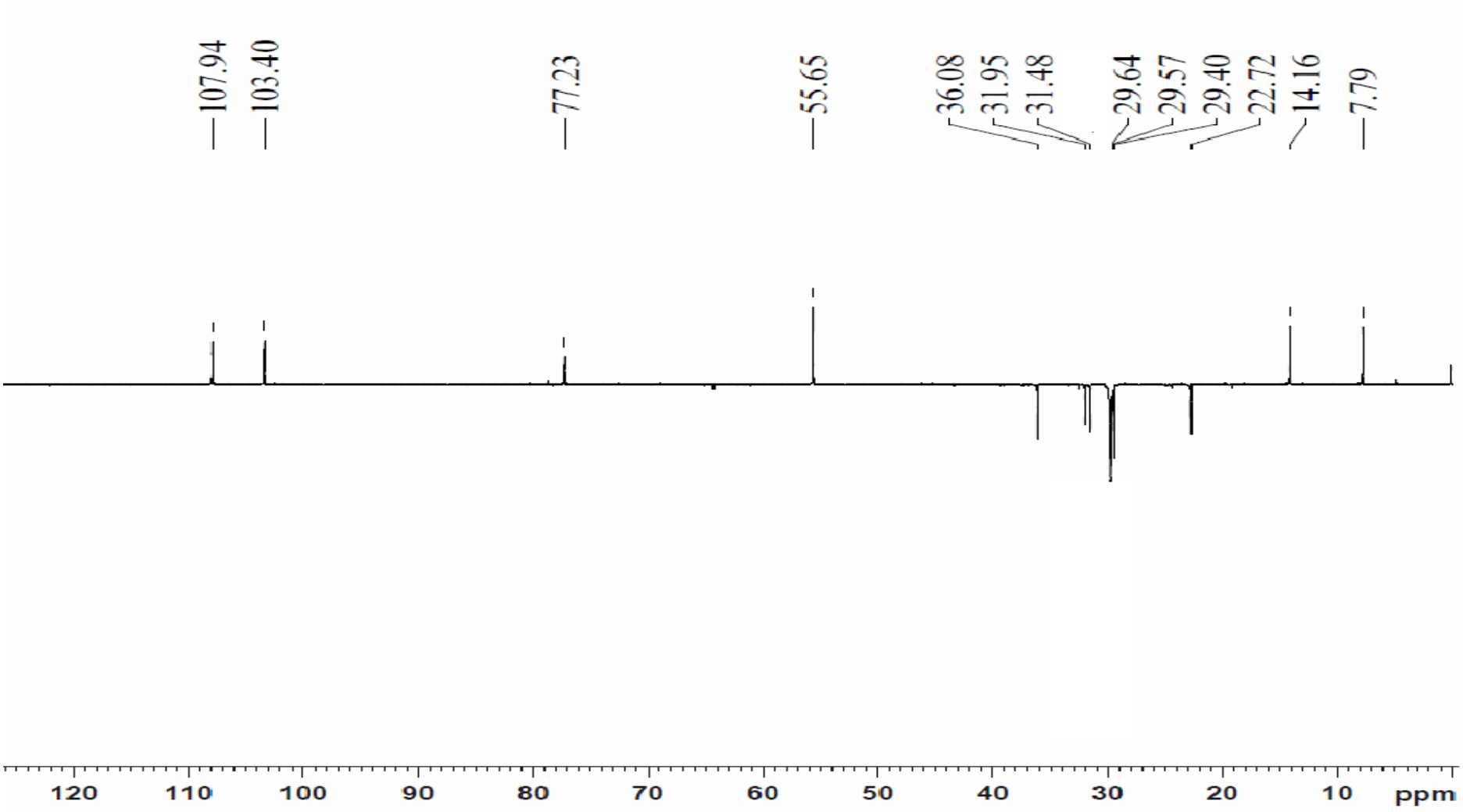

Figure S4. DEPT spectrum of compound **5**

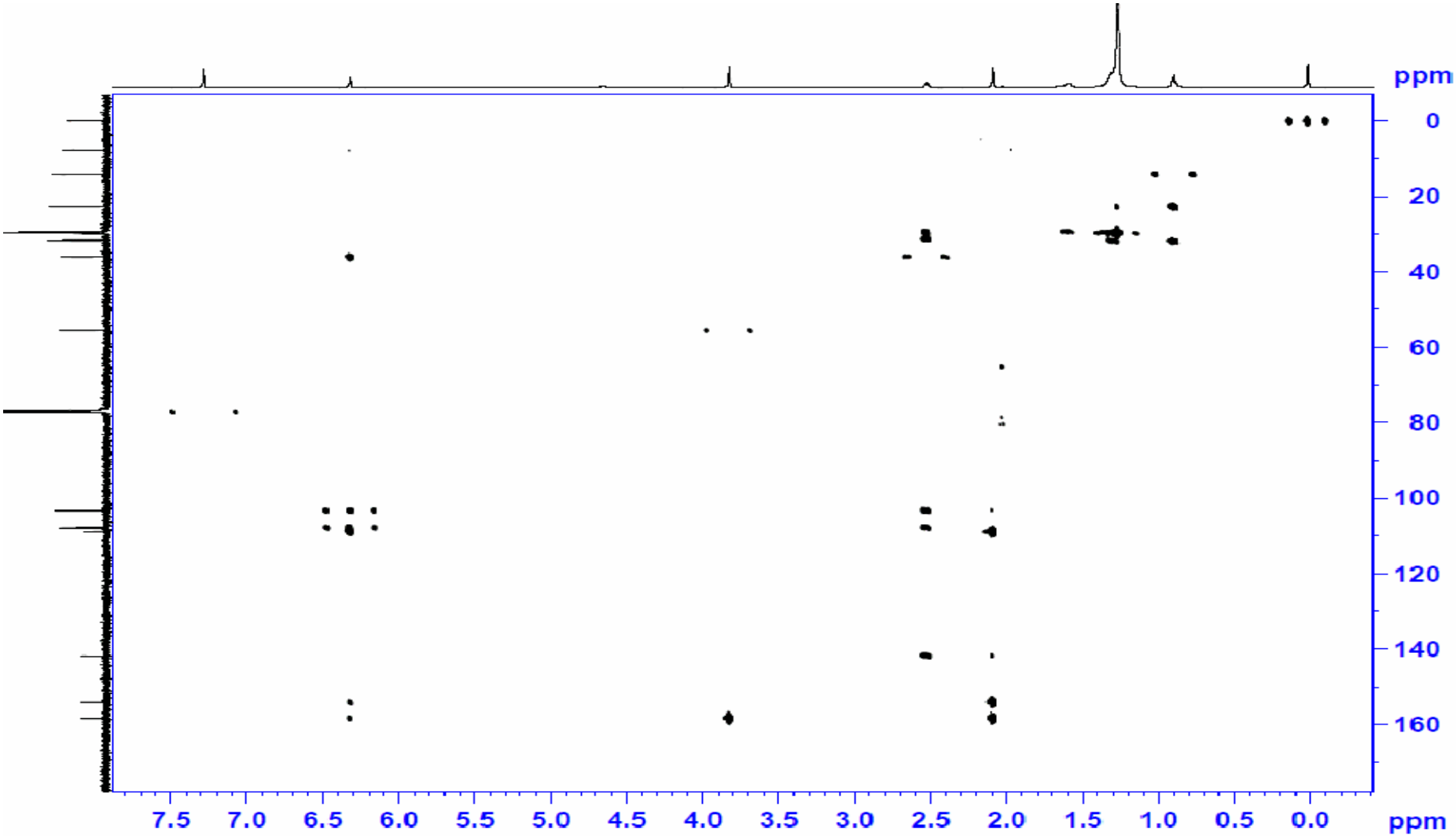

Figure S5 HMBC spectrum of compound **5**

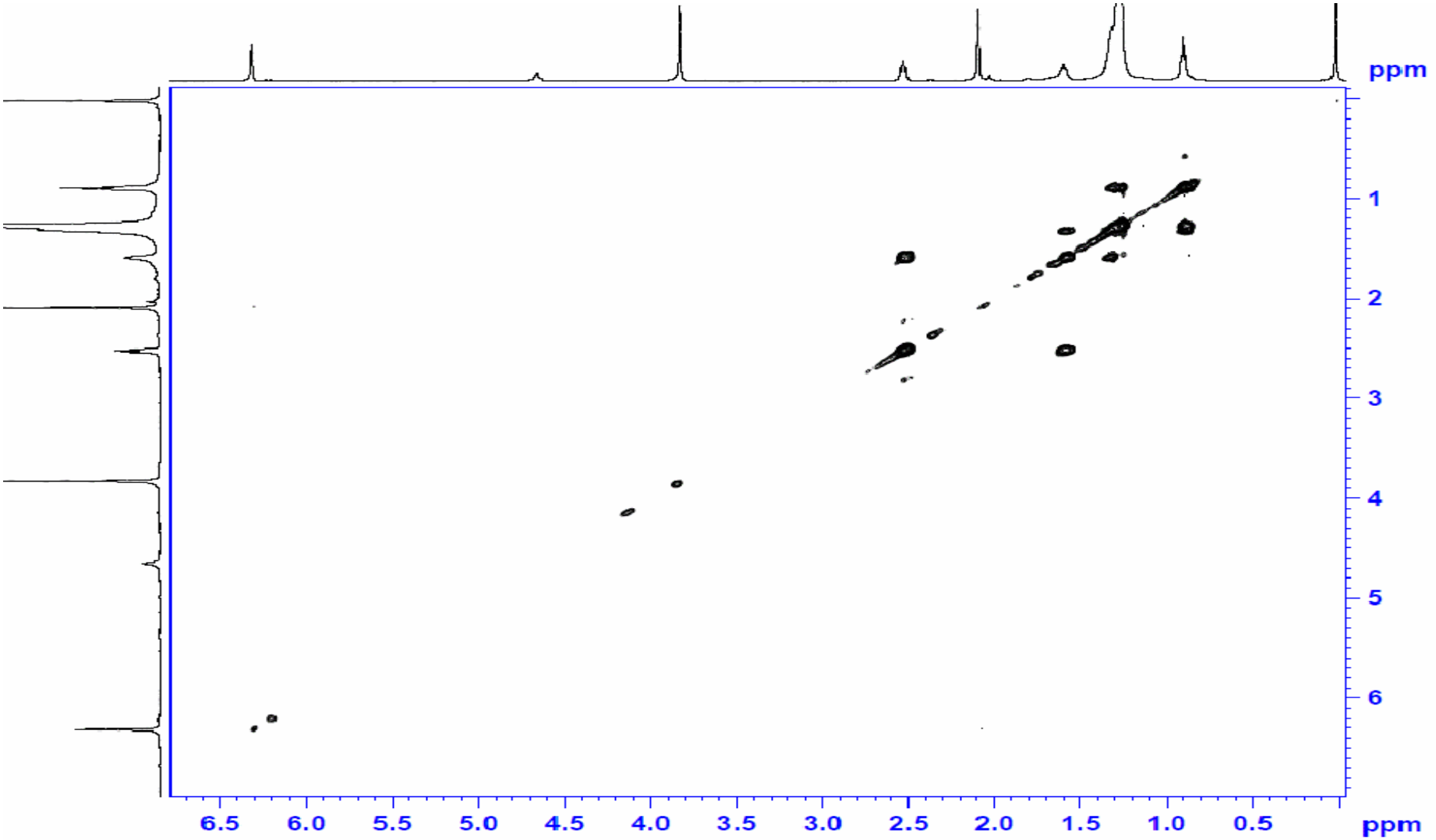

Figure S6. COSY spectrum of compound **5**

Single Mass Analysis
Tolerance = 500.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 16-16 H: 25-25 O: 0-2 23Na: 0-1

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	O	23Na
249.1845	249.1855	-12.0	-11.5	4.5	C16 H25 O2	16	25	2	

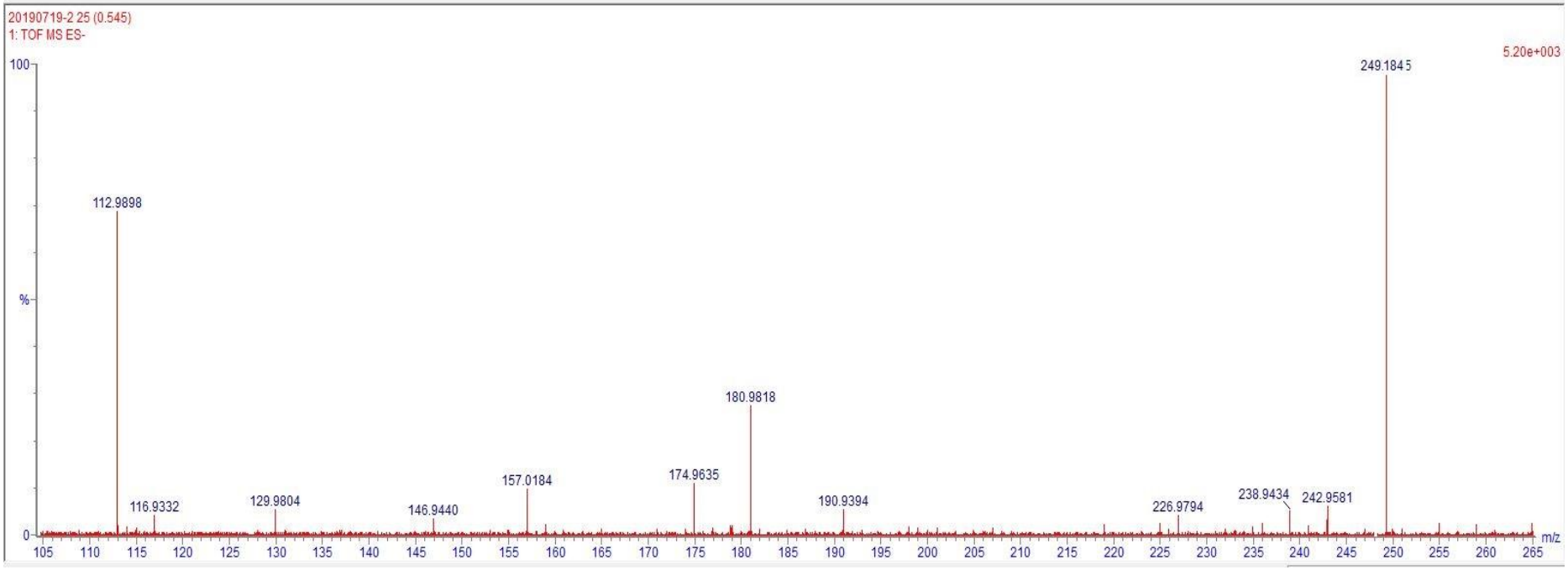

Figure S7. MS spectrum of compound **5**

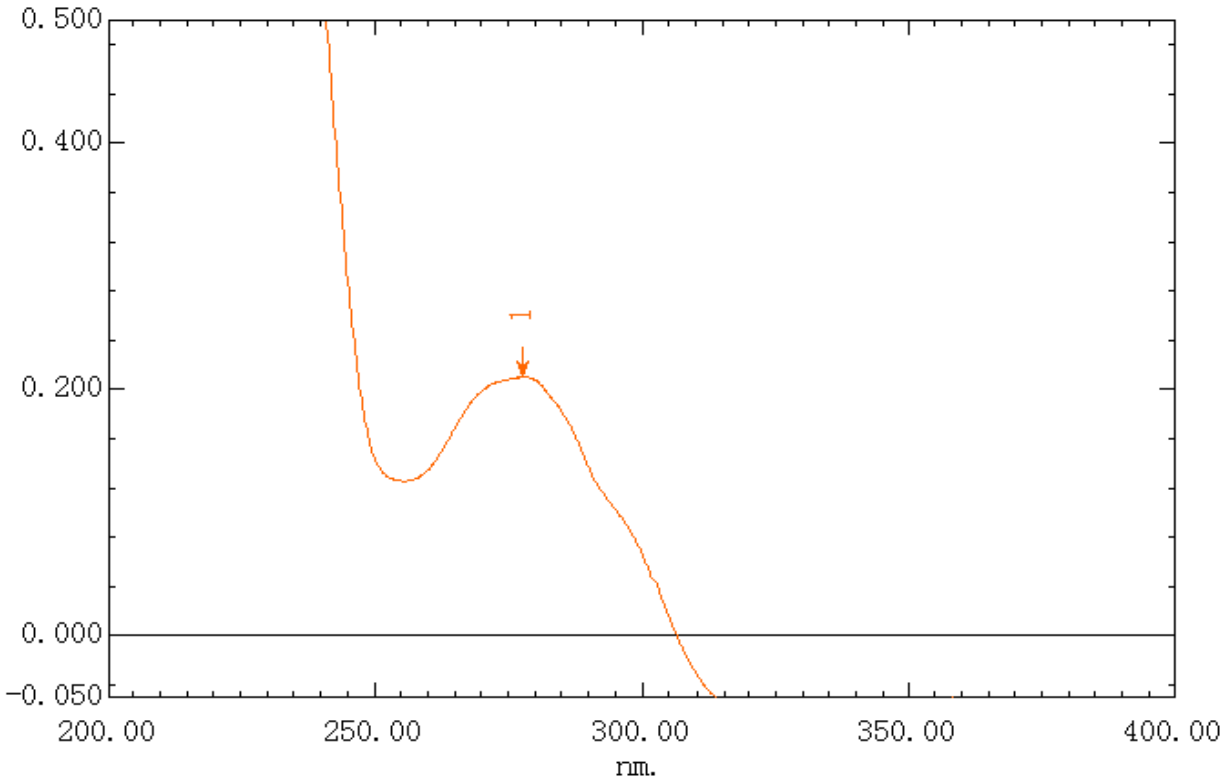

Figure S8. UV spectrum of compound **5**

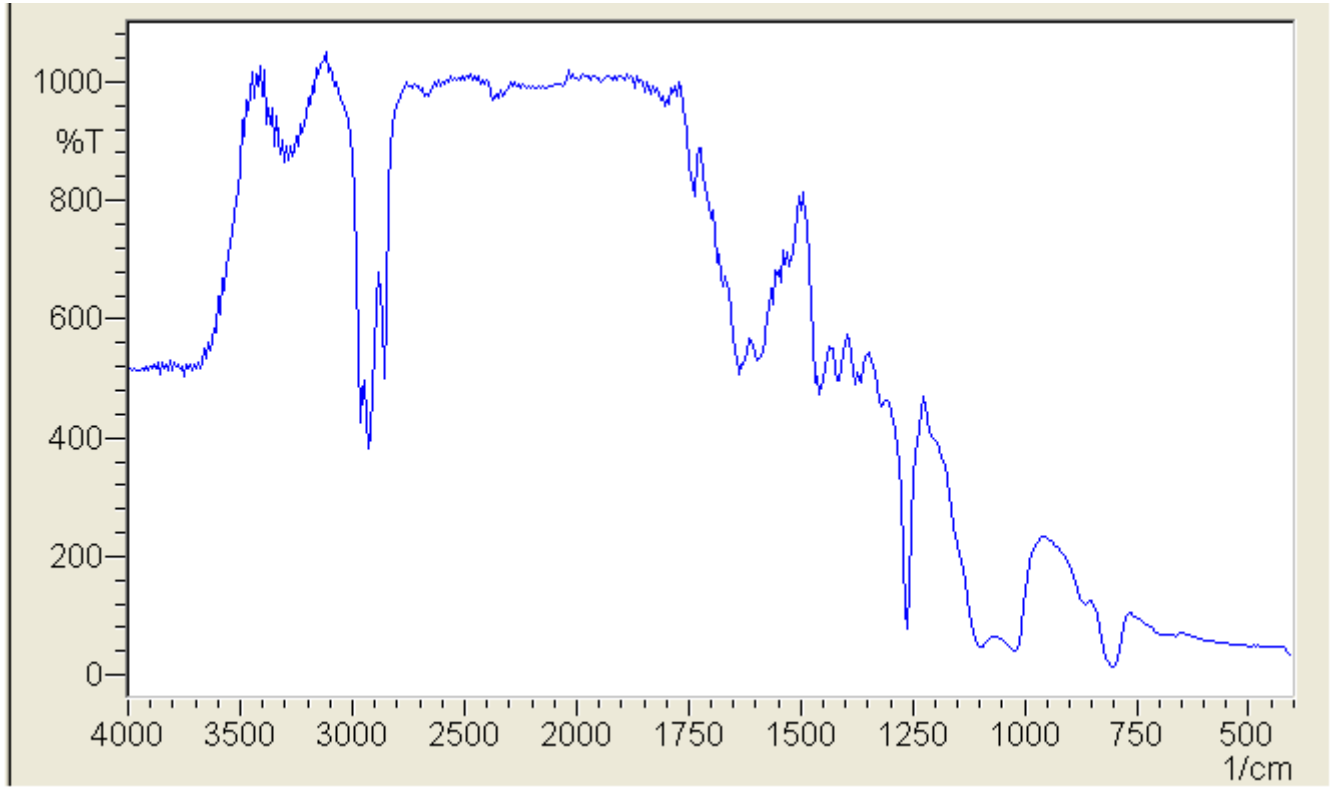

Figure S9. IR spectrum of compound **5**

Table S1. ^{1}H and ^{13}C-NMR data (500 and 125 MHz, resp.; $CDCl_3$) of compound **5**.

Position	δ_H (ppm), *J* (Hz)	δ_c (ppm)	HMBC
1	—	141.9	
2	6.32 (1H, brs)	103.4	C-3, C-4, C-6, C-7
3	—	158.4	
4	—	109.0	
5	—	154.1	
6	6.32 (1H, brs)	108.0	C-2, C-4, C-5, C-7
7	2.52 (2H, t, *J* = 7.05Hz)	36.1	C-1, C-2, C-6, C-8, C-9
8	1.60 (2H, m)	31.5	
9	1.31-1.33 (2H, m)	29.7	
10	1.31-1.33 (2H, m)	29.4	
11	1.31-1.33 (2H, m)	29.6	
12	1.18 (2H, m)	32.0	
13	1.31-1.33 (2H, m)	22.7	
14	0.90 (3H, t, *J* = 6.5 Hz)	14.2	C-12, C-13
15	2.09 (3H, s)	7.80	C-3, C-4, C-5
3-OCH_3	3.82 (3H, s)	55.7	C-3