

SUPPLEMENTARY MATERIAL

Chemical constituents from *Curcuma longa* L. and their inhibitory effects of nitric oxide production

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A new bisabolane-type sesquiterpenoid, turmerone Q (**1**), along with six known compounds (**2-7**), were isolated from the rhizomes of *Curcuma longa* L. The structural elucidation of the new compound was conducted using ¹H NMR, ¹³C NMR, HSQC, HMBC, and NOESY spectroscopic analyses. The absolute configuration of **1** was elucidated by comparison of the experimental and calculated ECD spectra. The anti-inflammatory effects of **1-7** were evaluated through lipopolysaccharide-induced nitric oxide (NO) production in RAW 264.7 macrophages assays, and compounds **6** and **7** showed potent inhibitory activity against NO production.

Keywords: *Curcuma longa* L.; sesquiterpenoids; nitric oxide.

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Table S1 The ^1H and ^{13}C NMR spectroscopic data of **1** in CDCl_3

No.	1	
	$\delta_{\text{C}}^{\text{a}}$, type	$\delta_{\text{H}}^{\text{b}}$ (<i>J</i> in Hz)
1'	35.8, CH	2.49 brd (11.7)
2'	133.3, CH	5.74 d (10.0)
3'	127.6, CH	6.17 dd (10.0, 2.0)
4'	145.0, C	--
5'	69.4, CH	4.44 dd (3.0, 3.5)
6'	31.9, CH ₂	1.49 ddd (11.8, 2.6, 3.0)
		1.88 m
7'	114.1, CH ₂	4.99 br s,
		5.08 br s
1	29.5, CH ₃	1.25 s
2	69.9, C	--
3	53.8, CH ₂	2.61 d (17.1)
		2.59 d (17.1)
4	212.9, C	--
5	49.0, CH ₂	2.26 overlapped
		2.47 overlapped
6	32.3, CH	2.26 overlapped
7	16.9, CH ₃	0.92 d (6.4)
8	29.5, CH ₃	1.25 s

Table S2. Inhibitory effects of compounds 1-7 on NO production induced by LPS in RAW 264.7 macrophages ($\text{IC}_{50}^{\text{a}}$: μM)

Compound	IC_{50}	Compound	IC_{50}
1	97.57	5	53.96
2	80.19	6	12.93
3	83.82	7	14.42
4	38.85	-	-
hydrocortisone ^b	37.64	-	-

a : Inhibitory effects of compounds **1-7** on NO production induced by LPS in RAW 264.7 macrophages.

b : Positive control.

Figure S1 HR-ESI-MS spectrum of compound 1

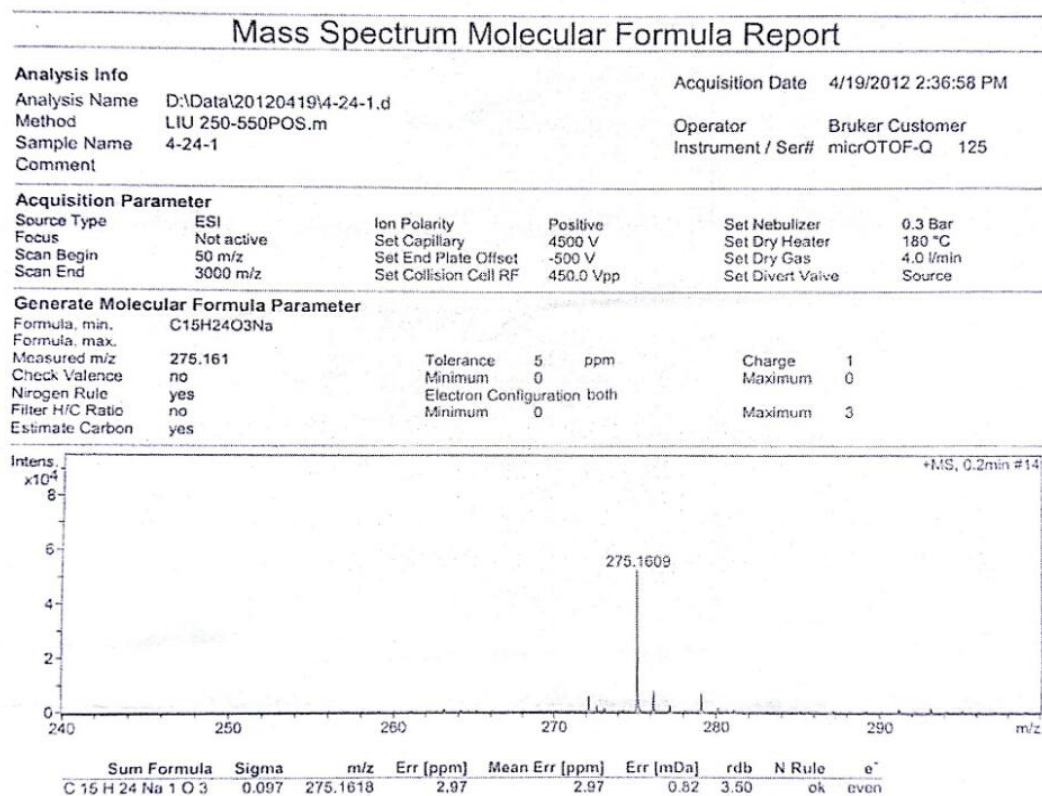


Figure S2 IR spectrum of compound 1

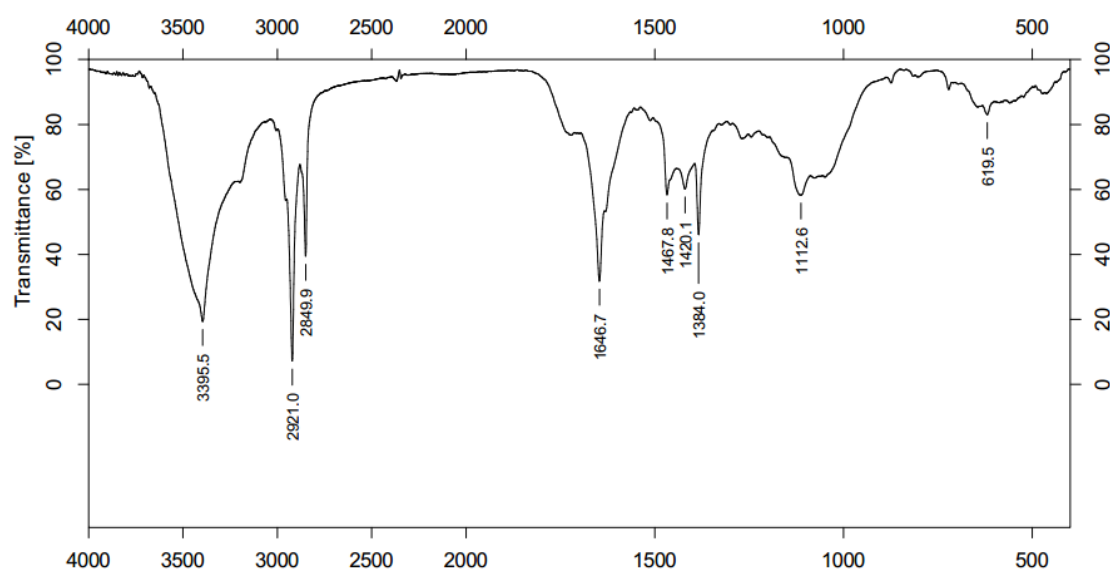


Figure S3. Key HMBC and NOESY correlations of compound 1.

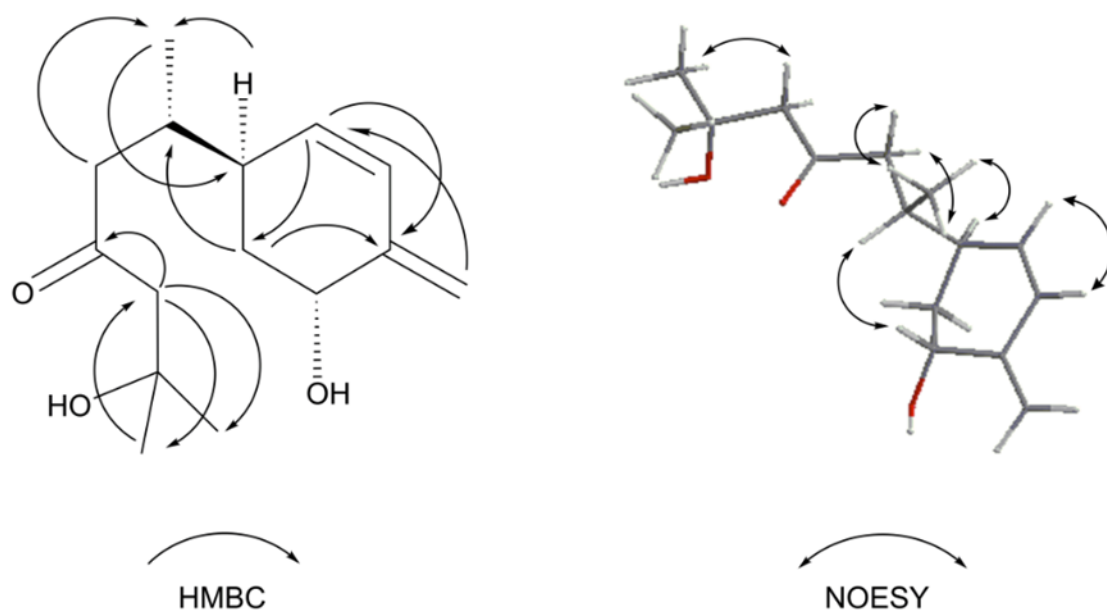


Figure S4. Experimental ECD of compound 1 in methanol.

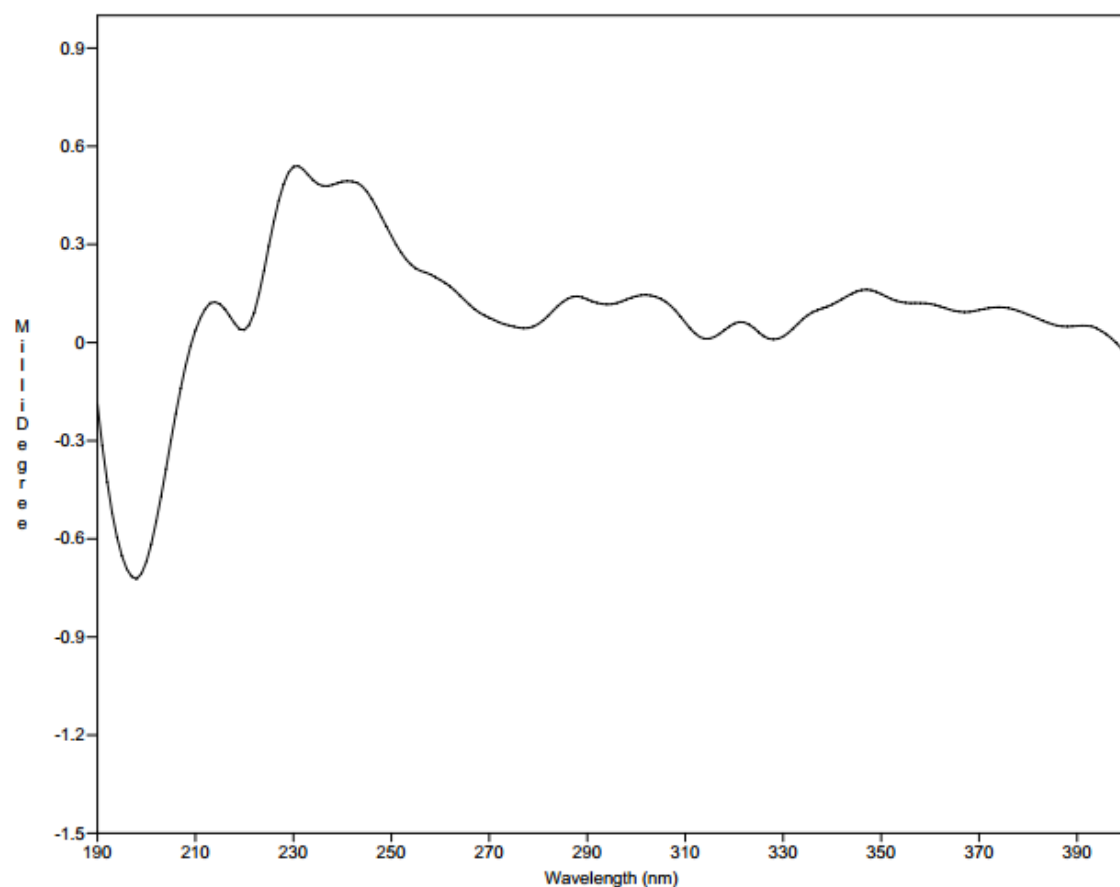


Figure S5. Calculated ECD spectra of 1a (1'S, 5'R, 6S)-isomer and 1b (1'R, 5'S, 6R)-isomer and the experimental ECD spectrum of 1 in methanol.

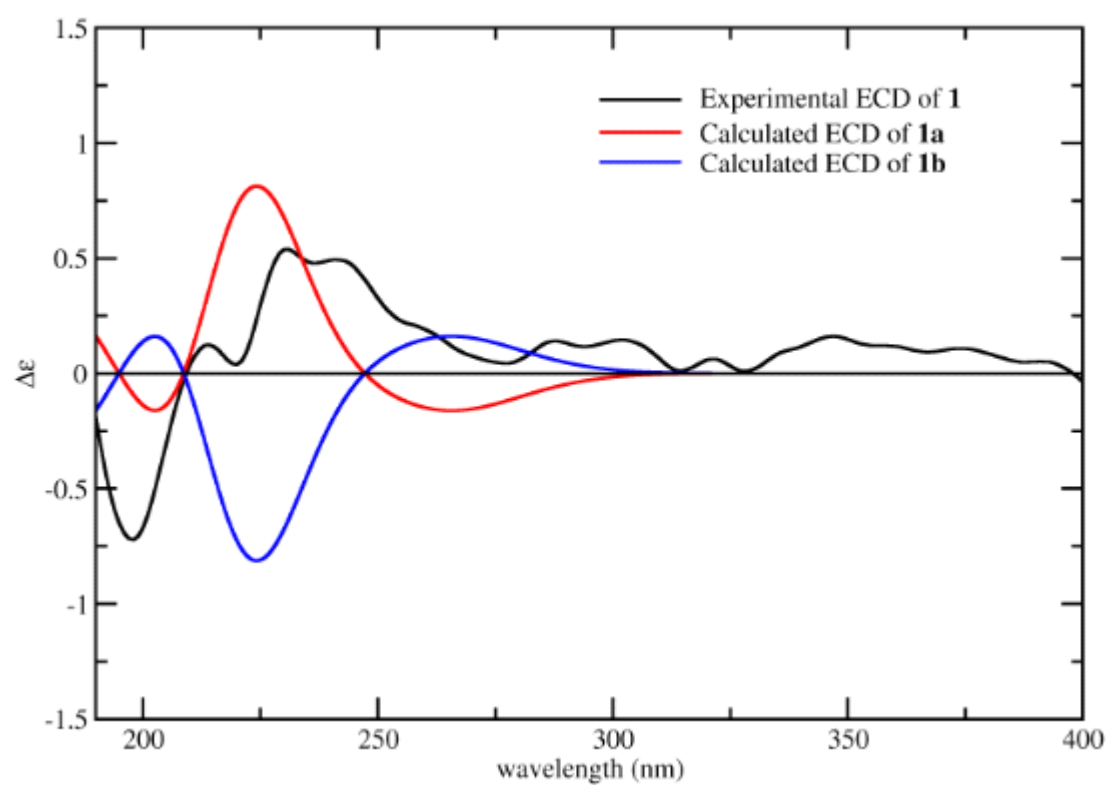
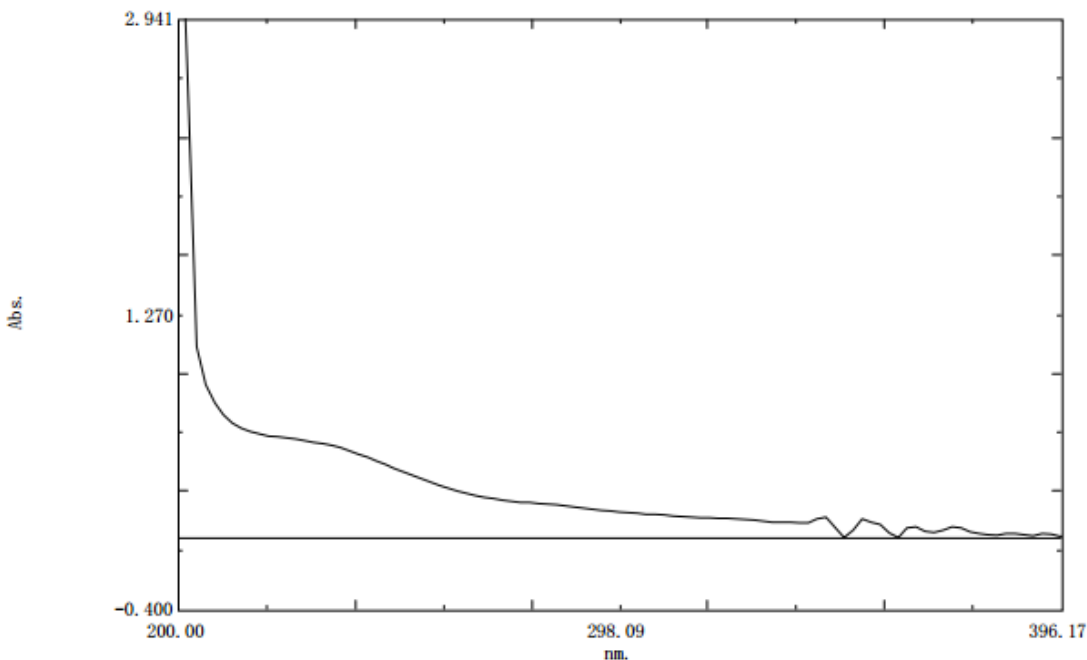


Figure S6. UV spectrum of compound 1.



No.	Wavelength	吸收值	描述
1	206.00	.872	
2	228.00	.555	
3	352.00	.110	
4	344.00	.121	
5	364.00	.065	
6	232.00	.538	
7	266.00	.242	
8			

Figure S7 The ¹H NMR spectrum of compound 1 in CDCl₃

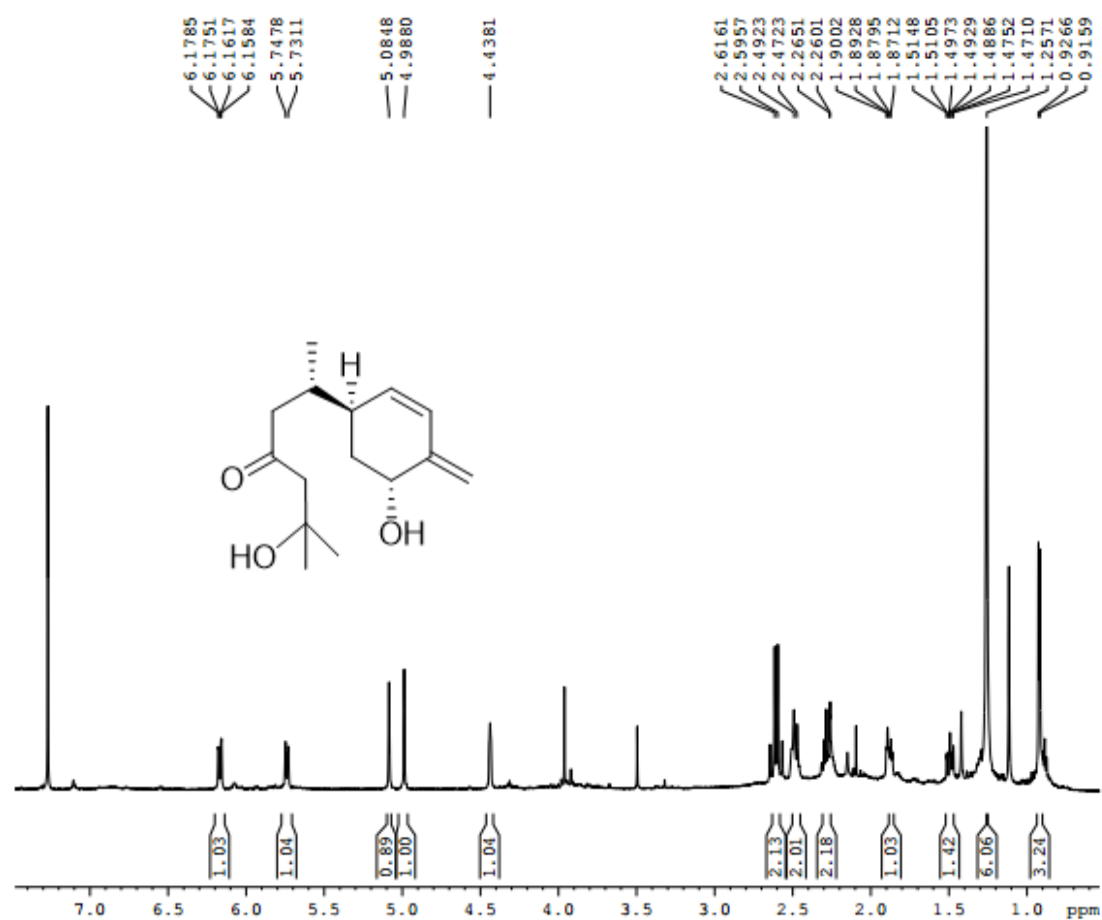


Figure S8 The ¹³C NMR spectrum of compound 1 in CDCl₃

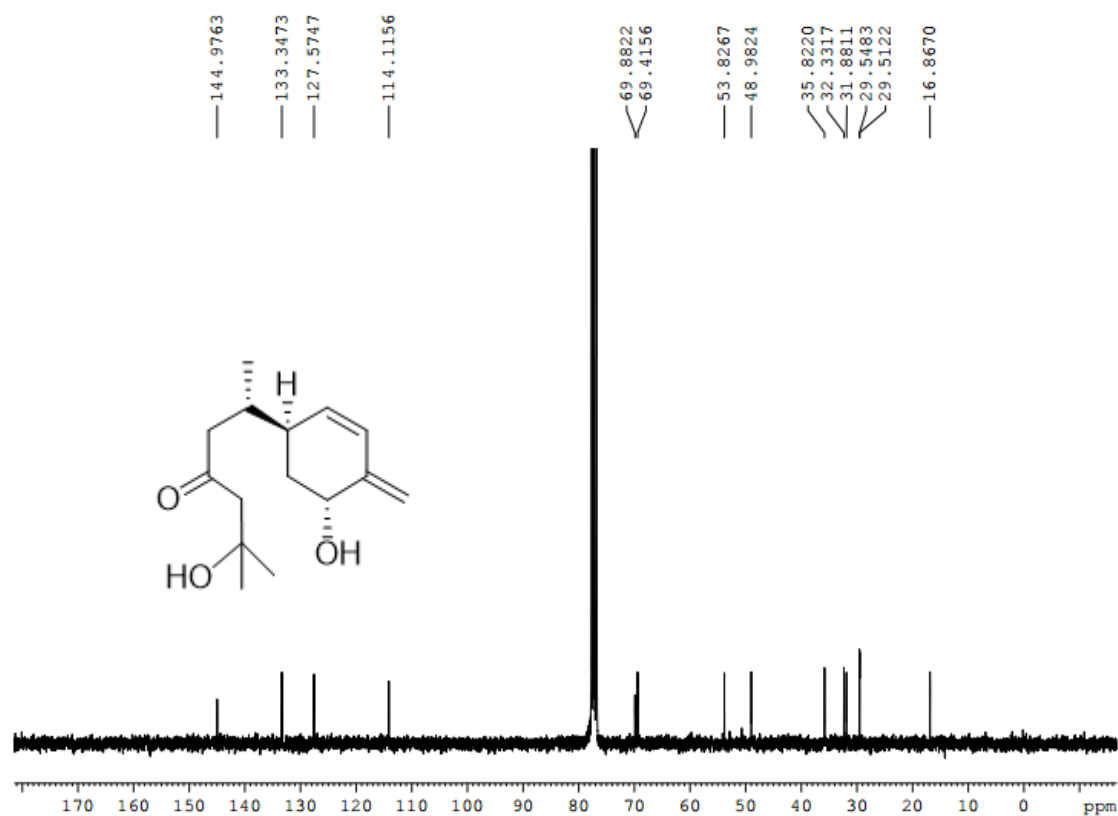


Figure S9 The HSQC spectrum of compound **1** in CDCl₃

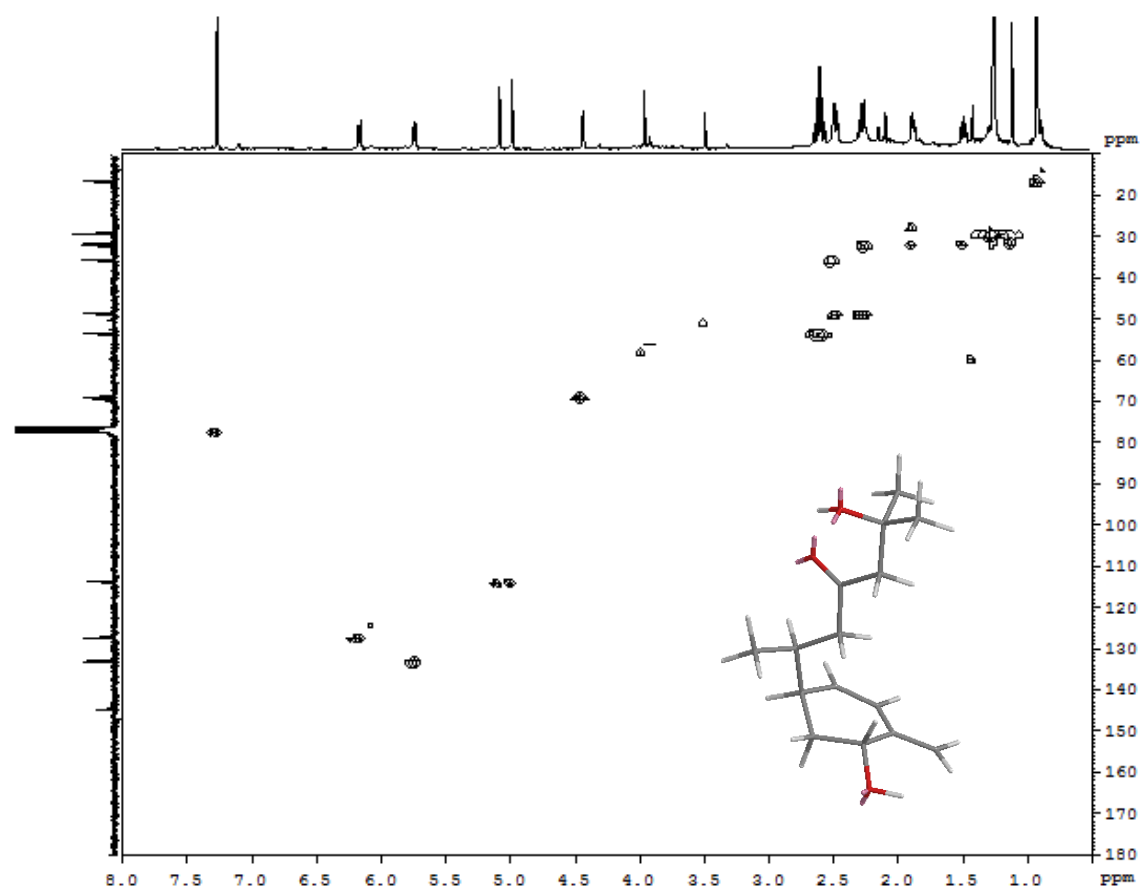


Figure S10 The HMBC spectrum of compound **1** in CDCl₃

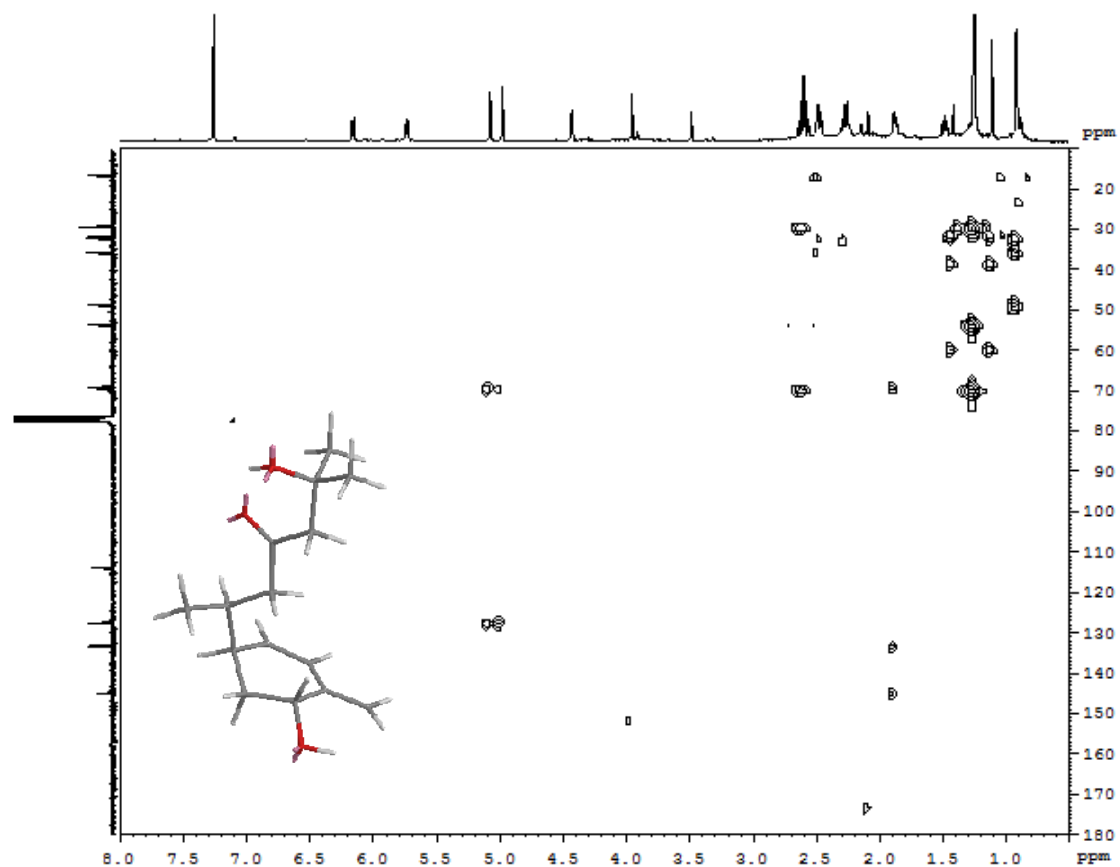


Figure S11 The NOESY spectrum of compound 1 in CDCl₃

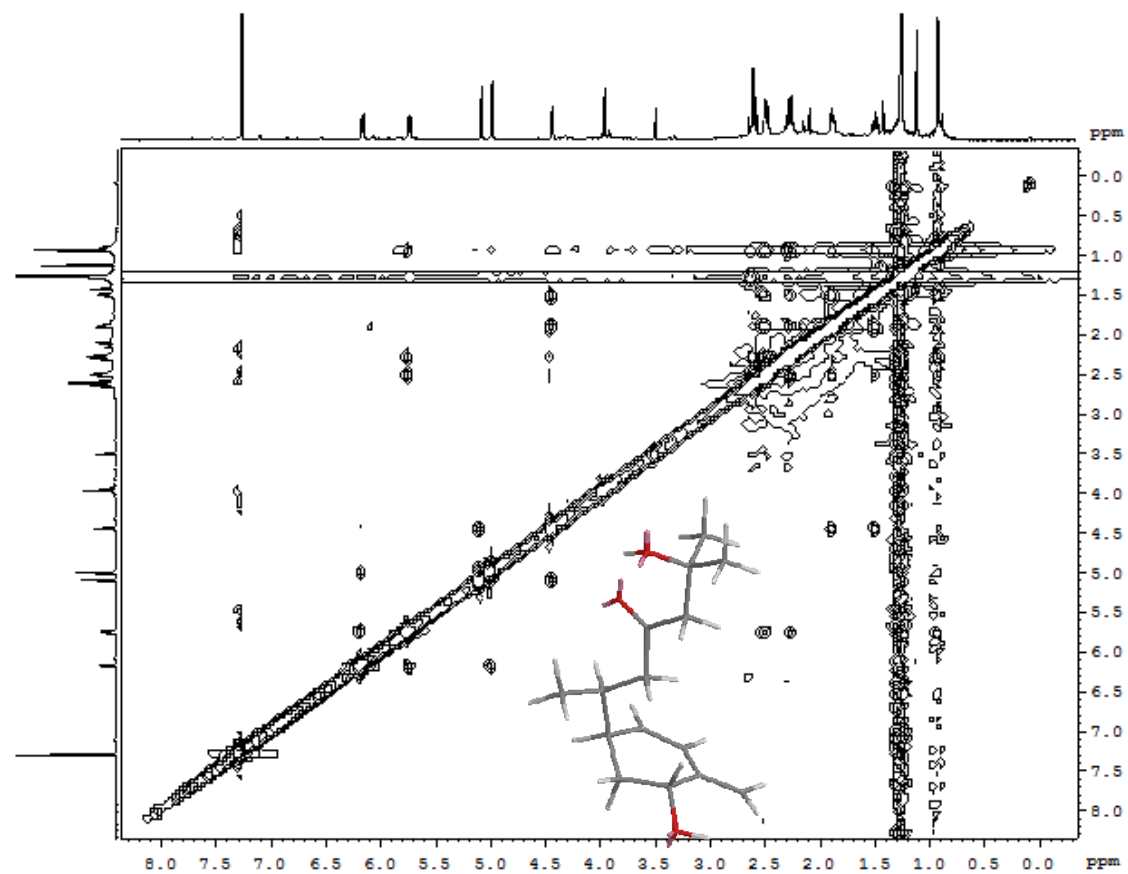


Figure S12. The ^1H - ^1H COSY spectrum of compound 1.

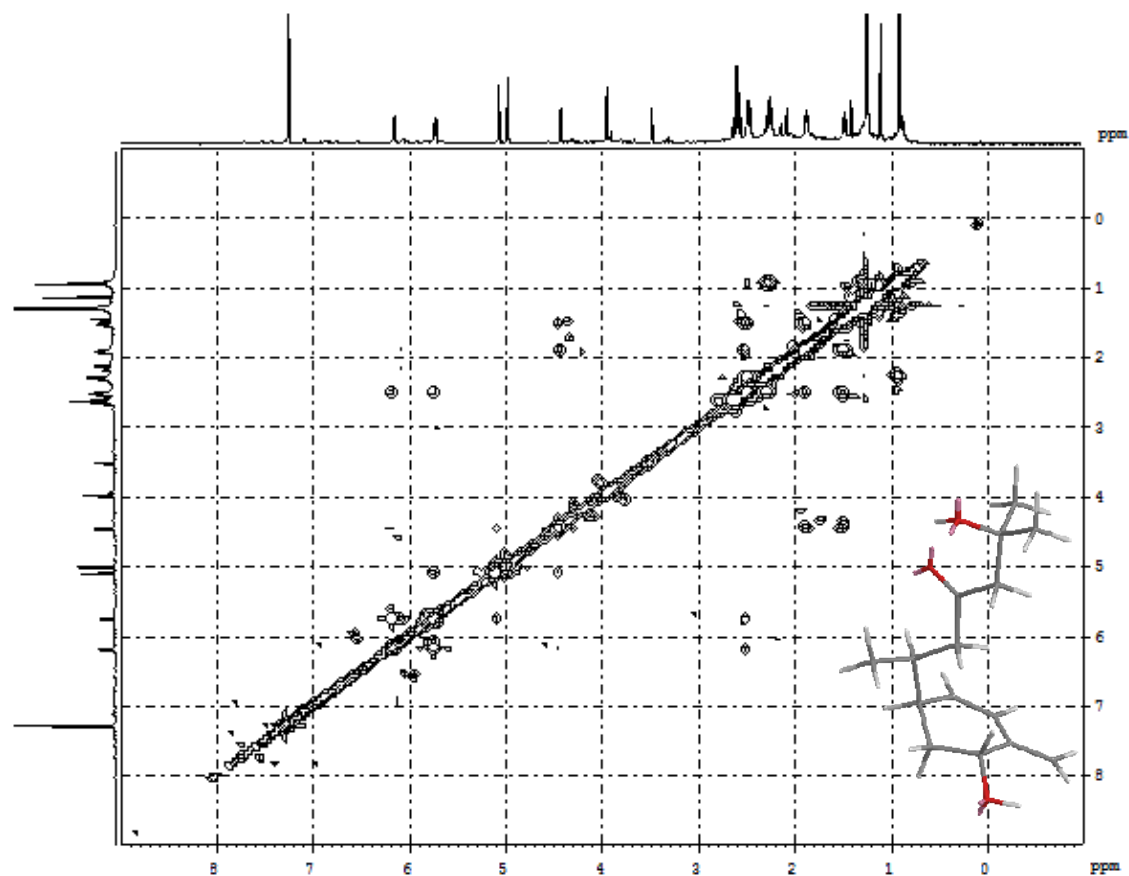


Figure S13 The ^1H NMR spectrum of compound 2 in CDCl_3

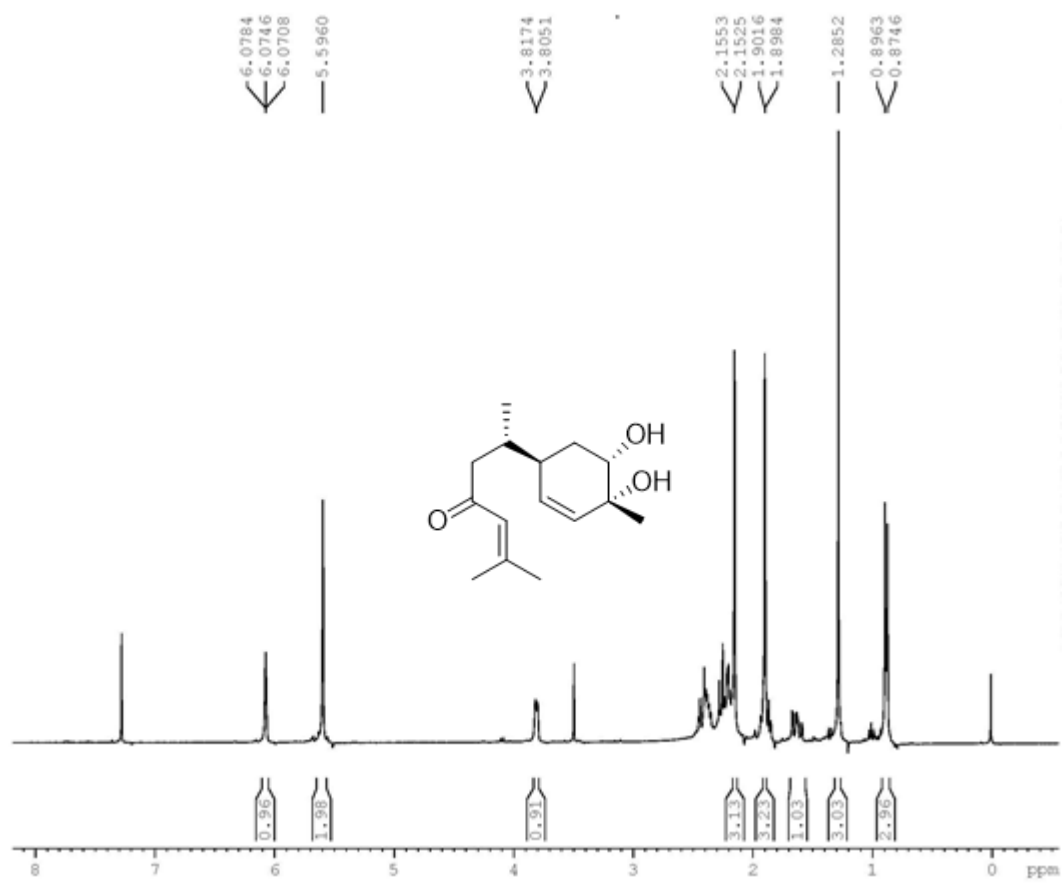


Figure S14 The ¹³C NMR spectrum of compound 2 in CDCl₃

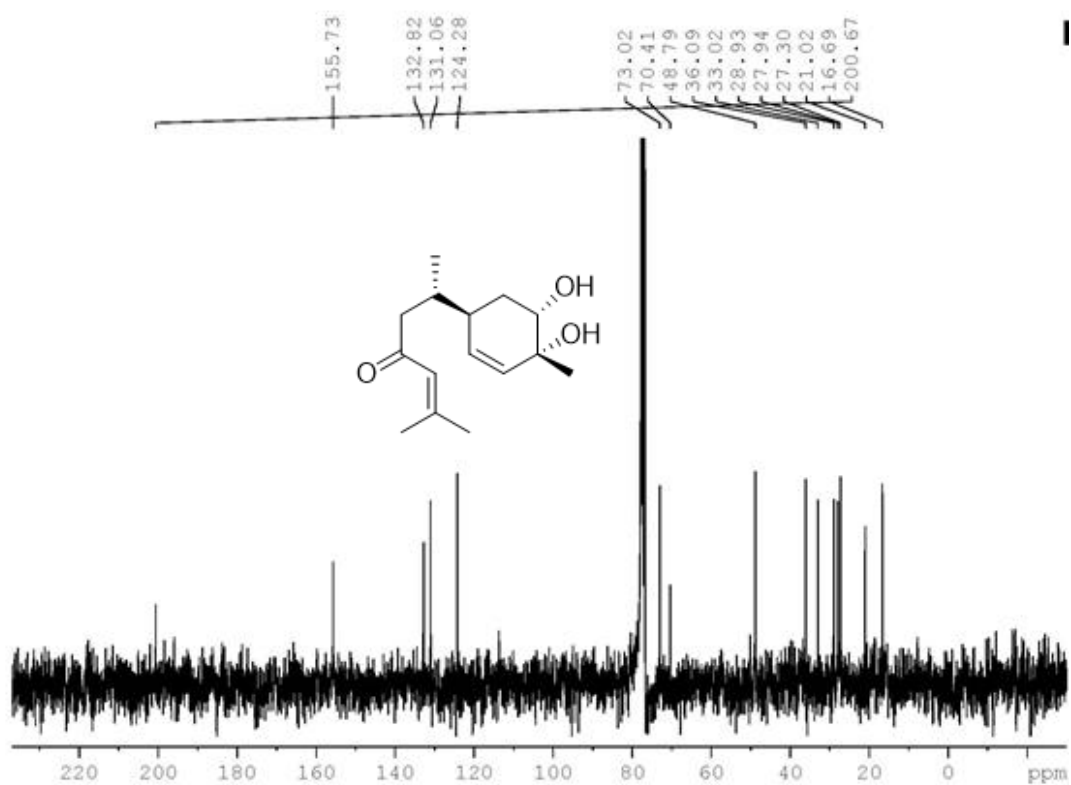


Figure S15 The ^1H NMR spectrum of compound 3 in CDCl_3

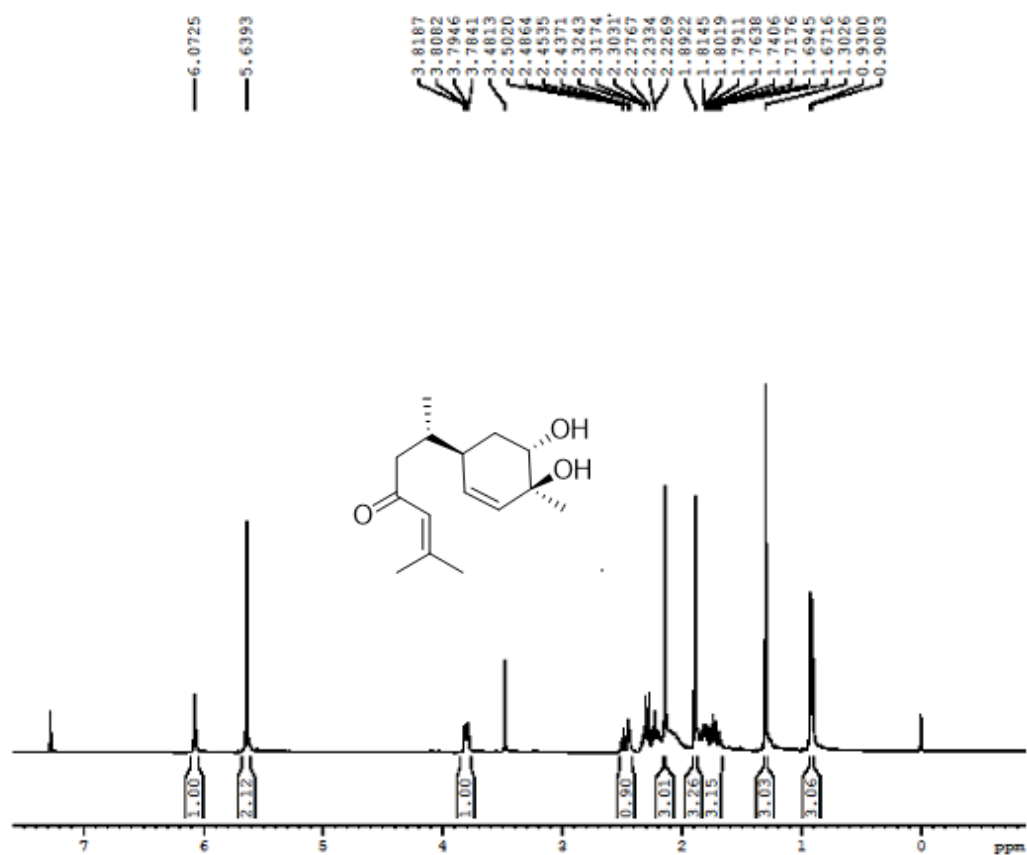


Figure S16 The ^{13}C NMR spectrum of compound 3 in MeOH

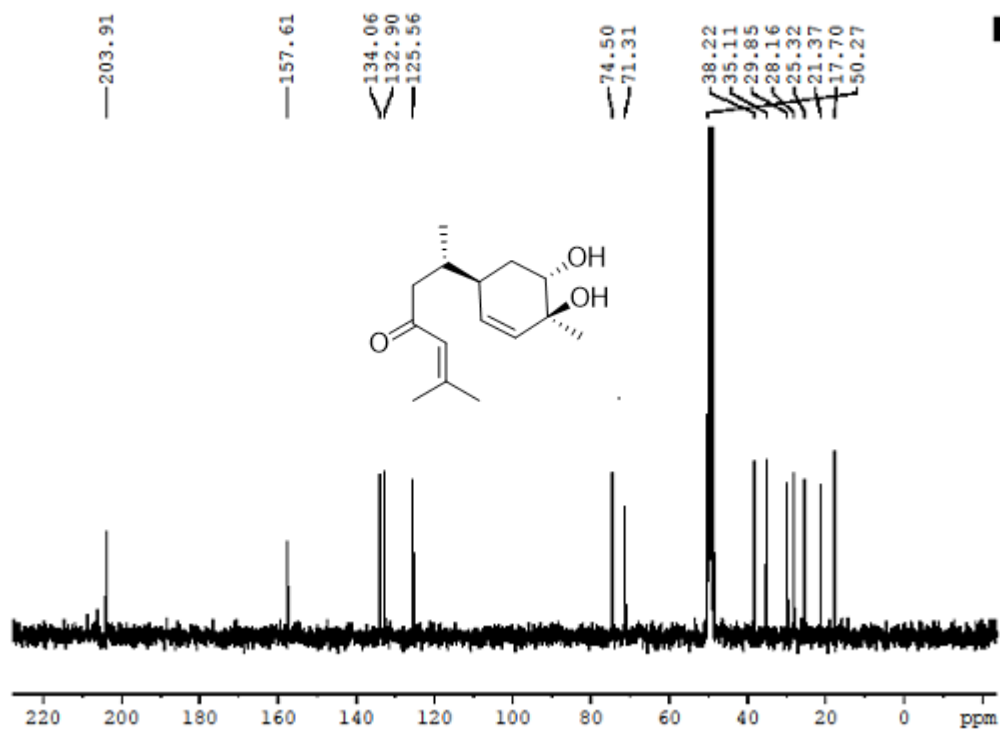


Figure S17 The ¹H NMR spectrum of compound 4 in CDCl₃

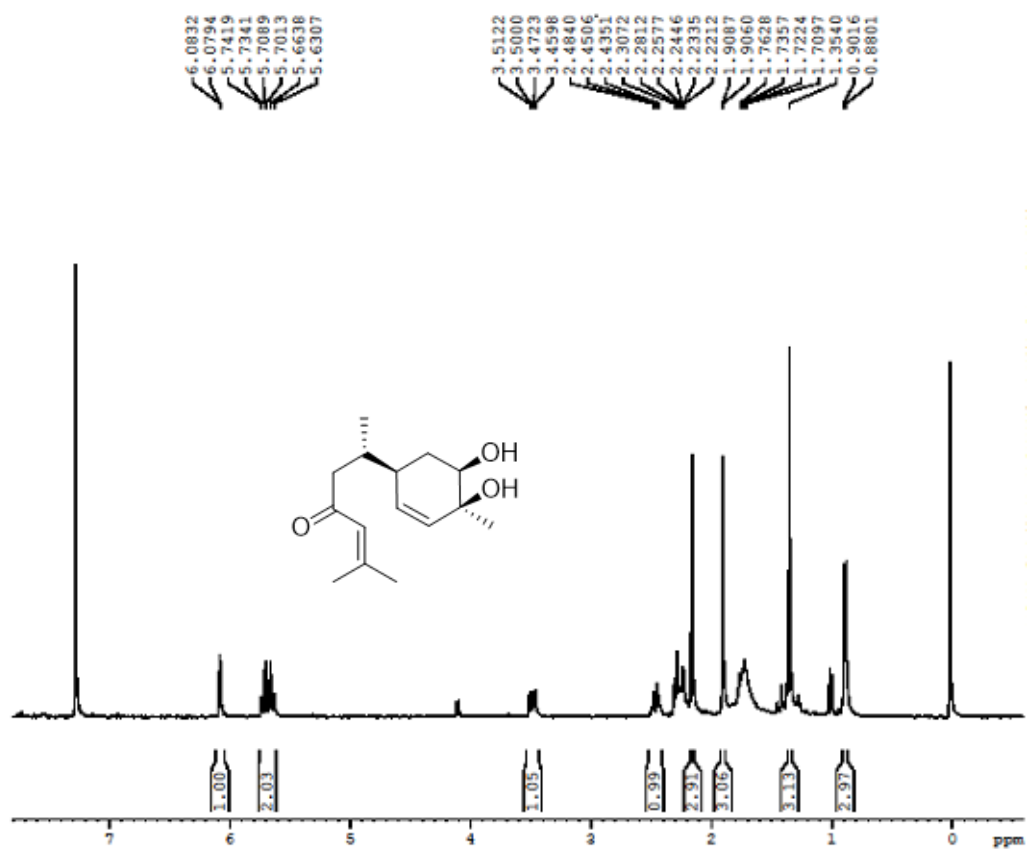


Figure S18 The ^{13}C NMR spectrum of compound 4 in CDCl_3

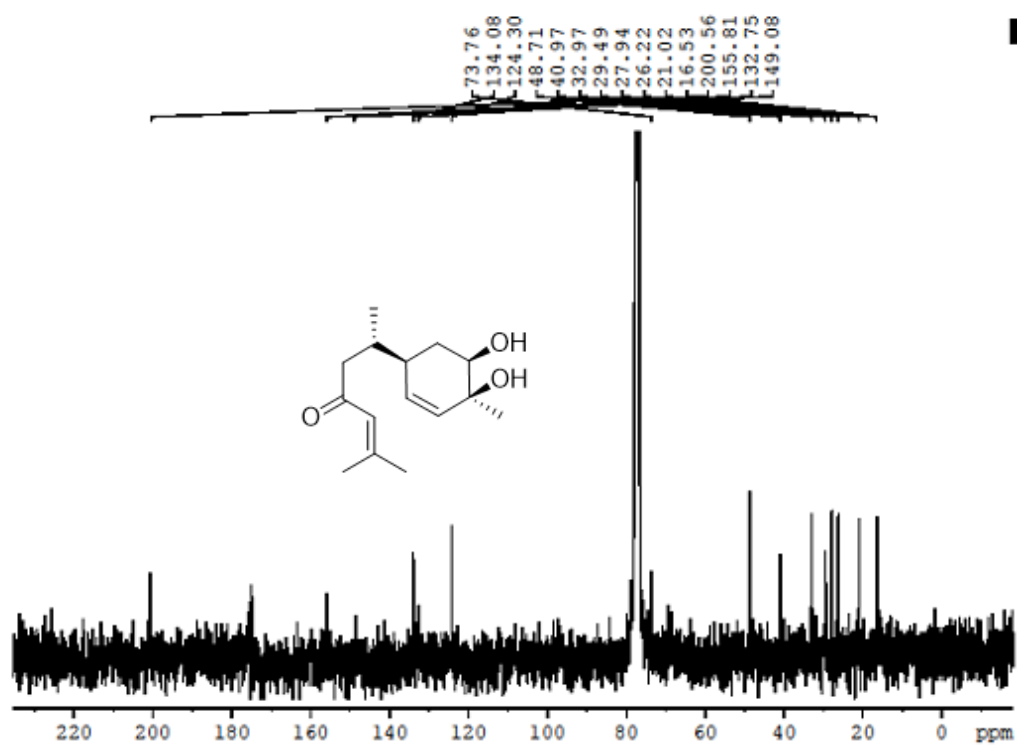


Figure S19 The ^1H NMR spectrum of compound 5 in $\text{DMSO}-d_6$

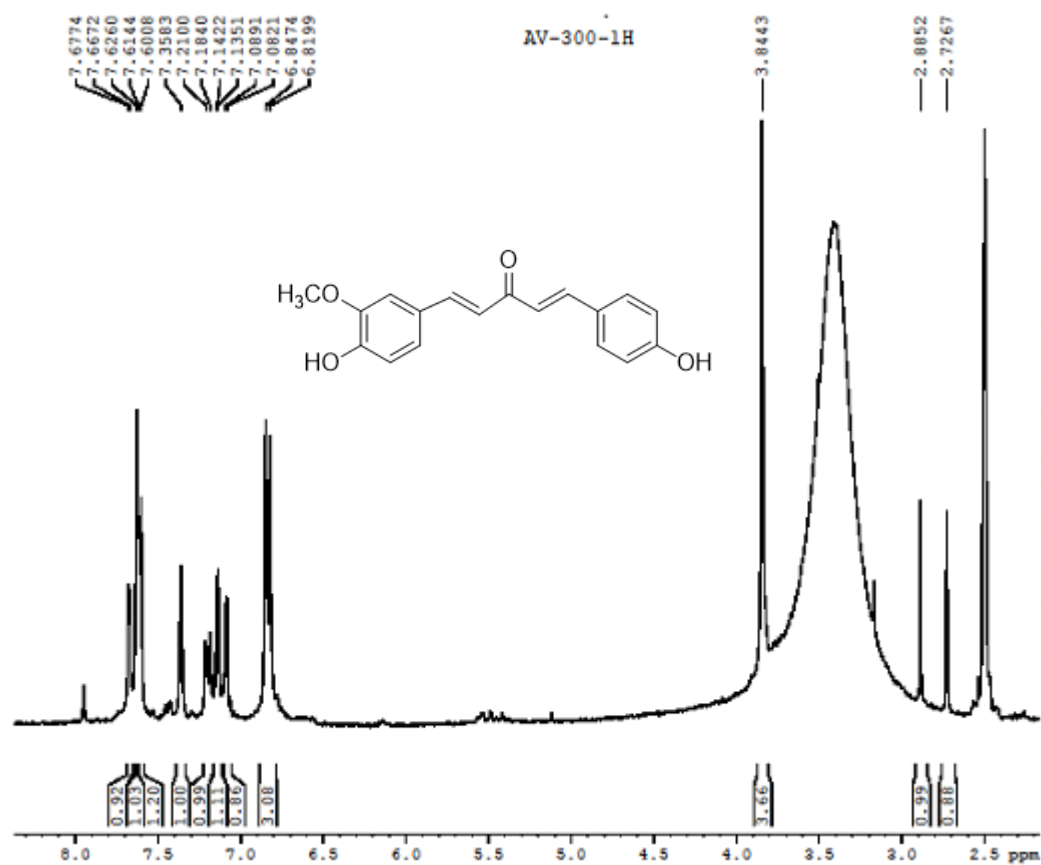


Figure S20 The ¹³C NMR spectrum of compound 5 in DMSO-*d*₆

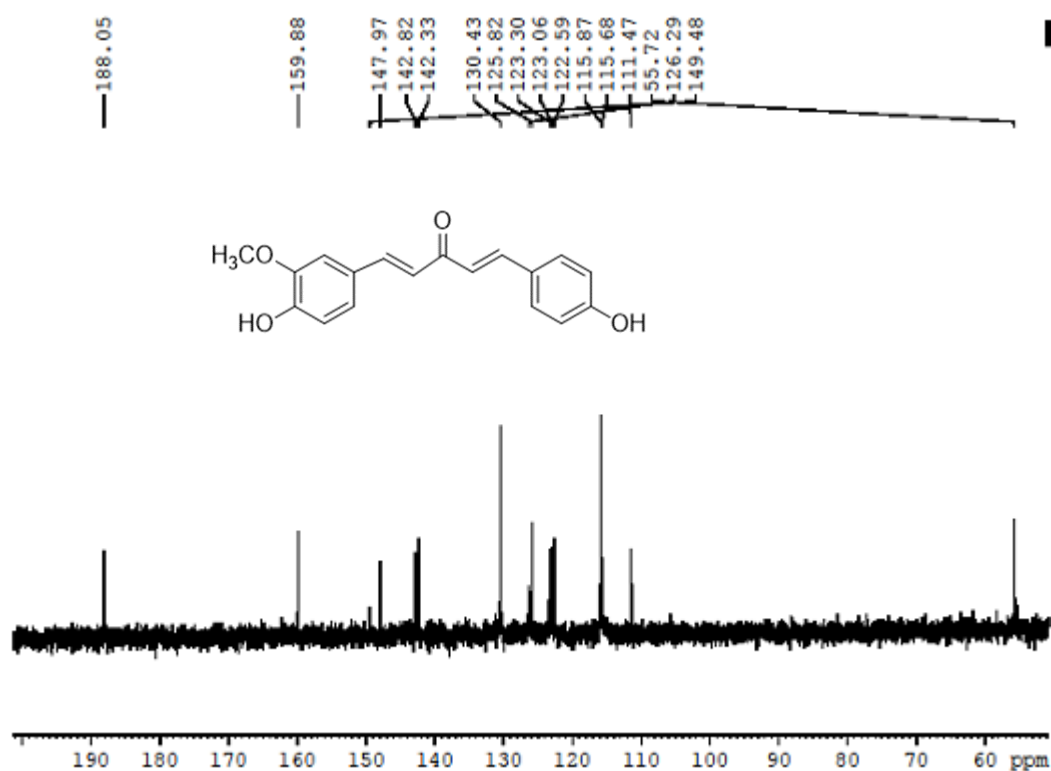


Figure S21 The ^1H NMR spectrum of compound 6 in $\text{DMSO}-d_6$

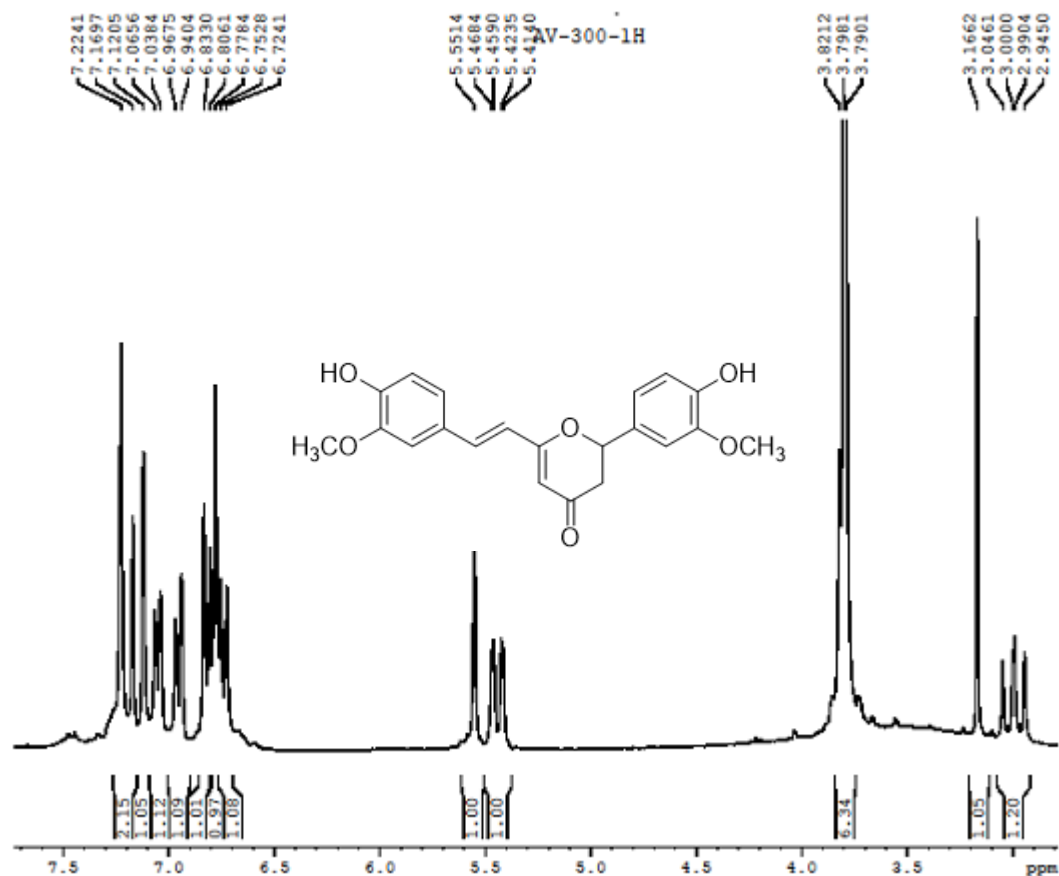


Figure S22 The ^{13}C NMR spectrum of compound 6 in $\text{DMSO}-d_6$

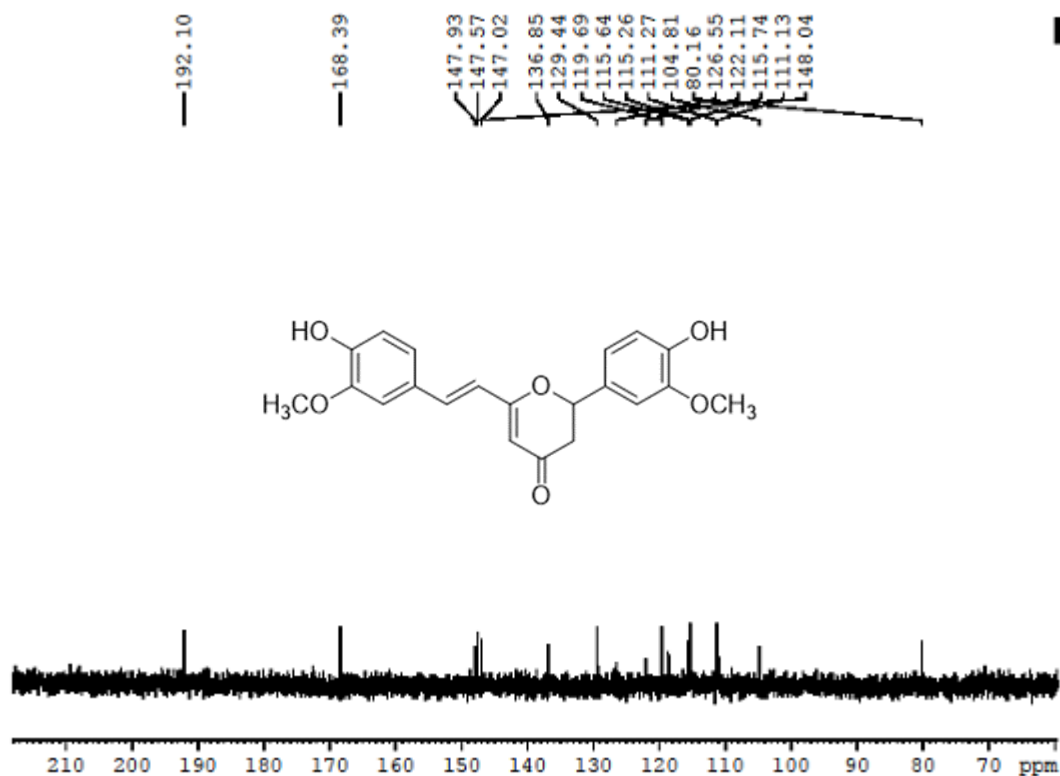


Figure S23 The ¹H NMR spectrum of compound 7 in DMSO-*d*₆

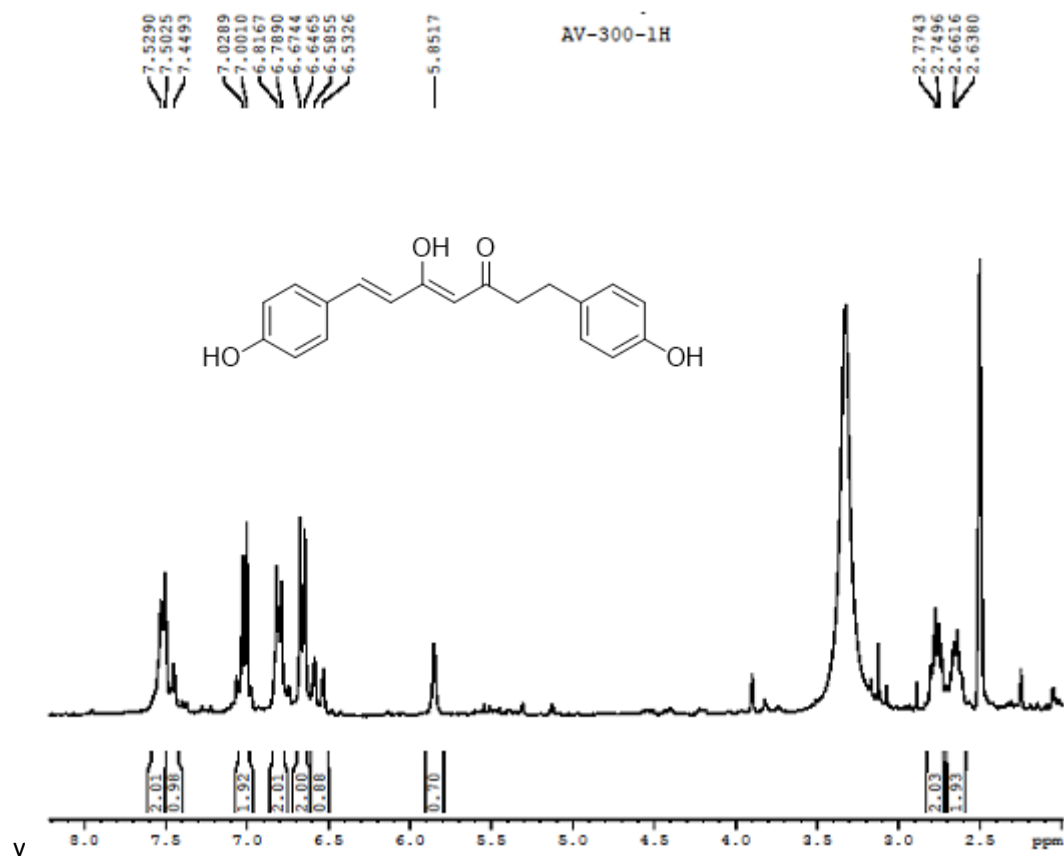


Figure S24 The ^{13}C NMR spectrum of compound 7 in $\text{DMSO}-d_6$

