

SUPPLEMENTARY MATERIAL

A new polyoxygenated cyclohexene derivative from *Artabotrys hainanensis*

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ABSTRACT

A new polyoxygenated cyclohexene derivative, artahainanol A (**1**), together with three known analogues (**2–4**), was isolated from the stems and leaves of *Artabotrys hainanensis*. Among them, **1** is an unusual polyoxygenated cyclohexene containing 14 carbon atoms on the carbon skeleton. All known compounds (**2–4**) were isolated from the genus *Artabotrys* for the first time. The structure of **1** was elucidated by extensive spectroscopic methods and the known compounds were identified by comparisons with data reported in the literature. All isolated compounds were evaluated for their cytotoxicities against five human cancer cell lines: HL-60, SMMC-7721, A-549, MCF-7 and SW480 *in vitro*. Compounds **1–4** showed significant inhibitory effects against various human cancer cell lines with IC₅₀ values ranging from 2.68 to 18.32 μM.

Keywords: *Artabotrys hainanensis*; polyoxygenated cyclohexene; artahainanol A; cytotoxicities.

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List of Supplementary Material

Table S1. ^1H and ^{13}C NMR data of artahainanol A (**1**) in CDCl_3 .

Figure S1. Selected 2D NMR correlations for artahainanol A (**1**).

Figure S2. ^1H -NMR spectrum of artahainanol A (**1**) in CDCl_3 .

Figure S3. ^{13}C -NMR spectrum of artahainanol A (**1**) in CDCl_3 .

Figure S4. HSQC spectrum of artahainanol A (**1**) in CDCl_3 .

Figure S5. HMBC spectrum of artahainanol A (**1**) in CDCl_3 .

Figure S6. ^1H - ^1H COSY spectrum of artahainanol A (**1**) in CDCl_3 .

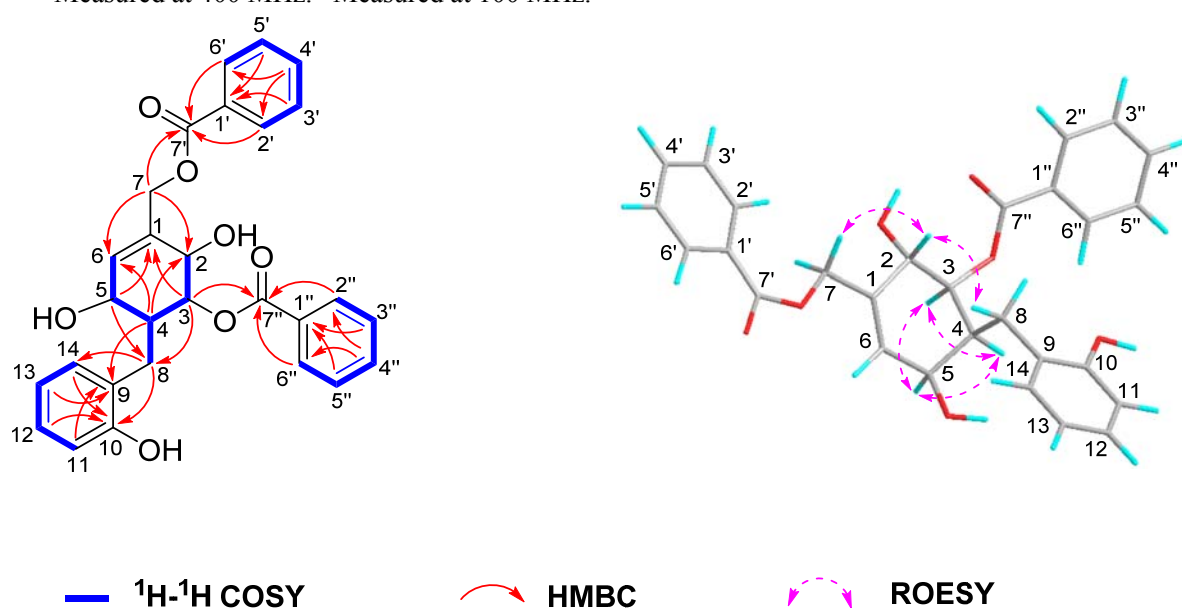
Figure S7. ROESY spectrum of artahainanol A (**1**) in CDCl_3 .

Figure S8. Enlarged ROESY spectrum 1 of artahainanol A (**1**) in CDCl_3 .

Figure S9. Enlarged ROESY spectrum 2 of artahainanol A (**1**) in CDCl_3 .

Table S1 ^1H and ^{13}C NMR data of artahainanol A (**1**) in CDCl_3 .

Position	$\delta_{\text{H}}^{\text{a}}$	$\delta_{\text{C}}^{\text{b}}$
1		135.2 s
2	4.59 (1H, d, $J = 5.8$ Hz)	67.4 d
3	5.44 (1H, dd, $J = 5.8, 3.5$ Hz)	77.1 d
4	2.90 (1H, m)	33.1 d
5	5.01 (1H, br s)	70.1 d
6	6.17 (1H, br s)	128.6 d
7a	5.13 (1H, d, $J = 13.4$ Hz)	64.7 t
7b	4.86 (1H, d, $J = 13.4$ Hz)	
8a	3.04 (1H, dd, $J = 15.8, 6.2$ Hz)	23.4 t
8b	2.80 (1H, dd, $J = 15.8, 8.6$ Hz)	
9		120.2 s
10		153.4 s
11	6.86 (1H, d, $J = 7.6$ Hz)	116.6 d
12	7.08 (1H, dd, $J = 7.8, 7.6$ Hz)	127.4 d
13	6.81 (1H, dd, $J = 7.8, 7.6$ Hz)	120.5 d
14	7.02 (1H, d, $J = 7.6$ Hz)	129.2 d
1'		129.4 s
2', 6'	7.88 (2H, d, $J = 7.6$ Hz')	129.7 d
3', 5'	7.37 (2H, dd, $J = 7.8, 7.6$ Hz)	128.3 d
4'	7.53 (1H, m)	133.2 d
7'		166.6 s
1''		129.6 s
2'', 6''	8.03 (2H, d, $J = 8.0$ Hz)	129.7 d
3'', 5''	7.42 (2H, dd, $J = 8.0, 7.8$ Hz')	128.4 d
4''	7.58 (1H, m)	133.2 d
7''		166.7 s

^a Measured at 400 MHz. ^b Measured at 100 MHz.**Figure S1.** Selected 2D NMR correlations for artahainanol A (**1**).

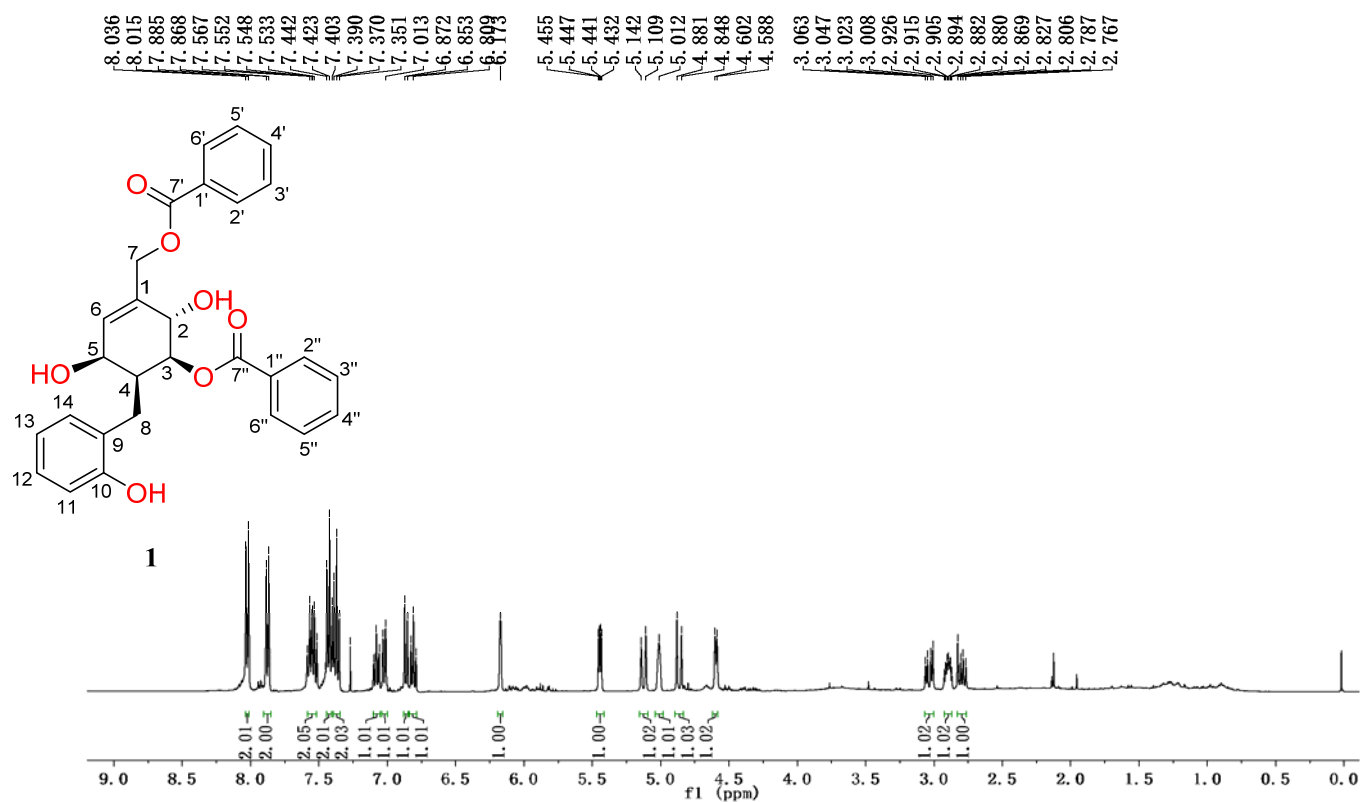


Figure S2. ¹H-NMR spectrum of artahainanol A (**1**) in CDCl₃.

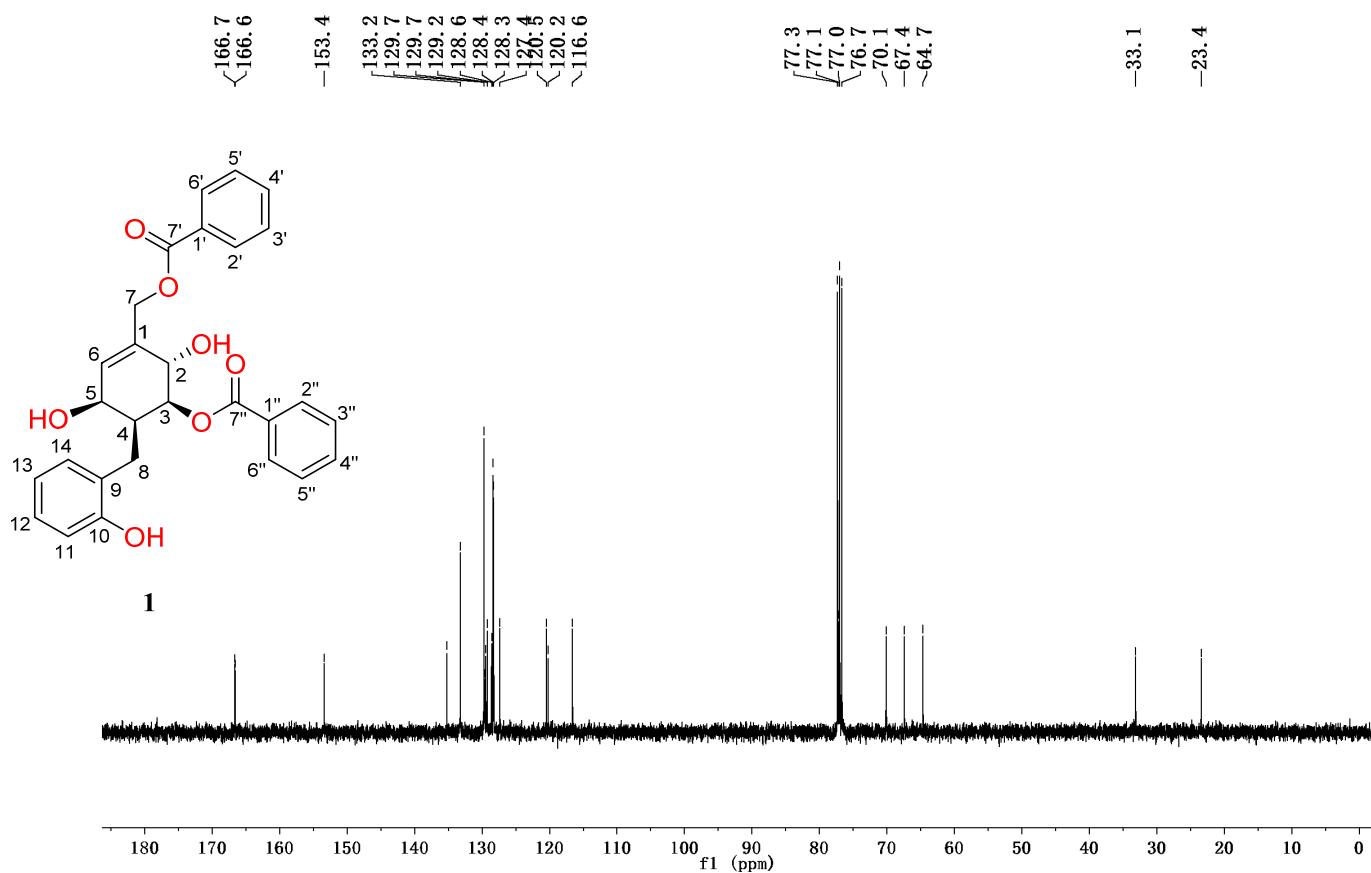


Figure S3. ¹³C-NMR spectrum of artahainanol A (**1**) in CDCl₃.

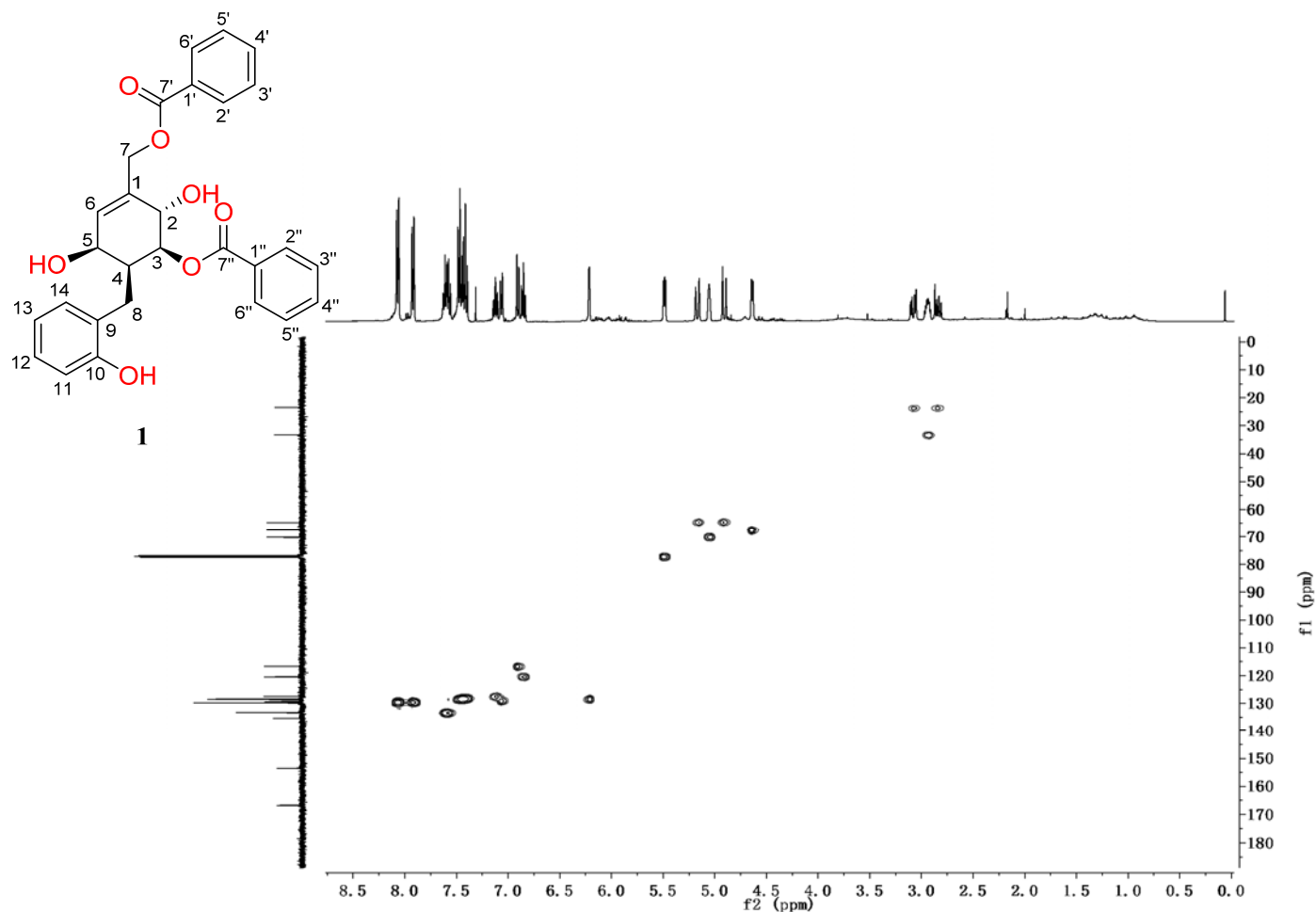


Figure S4. HSQC spectrum of artahainanol A (1) in CDCl_3 .

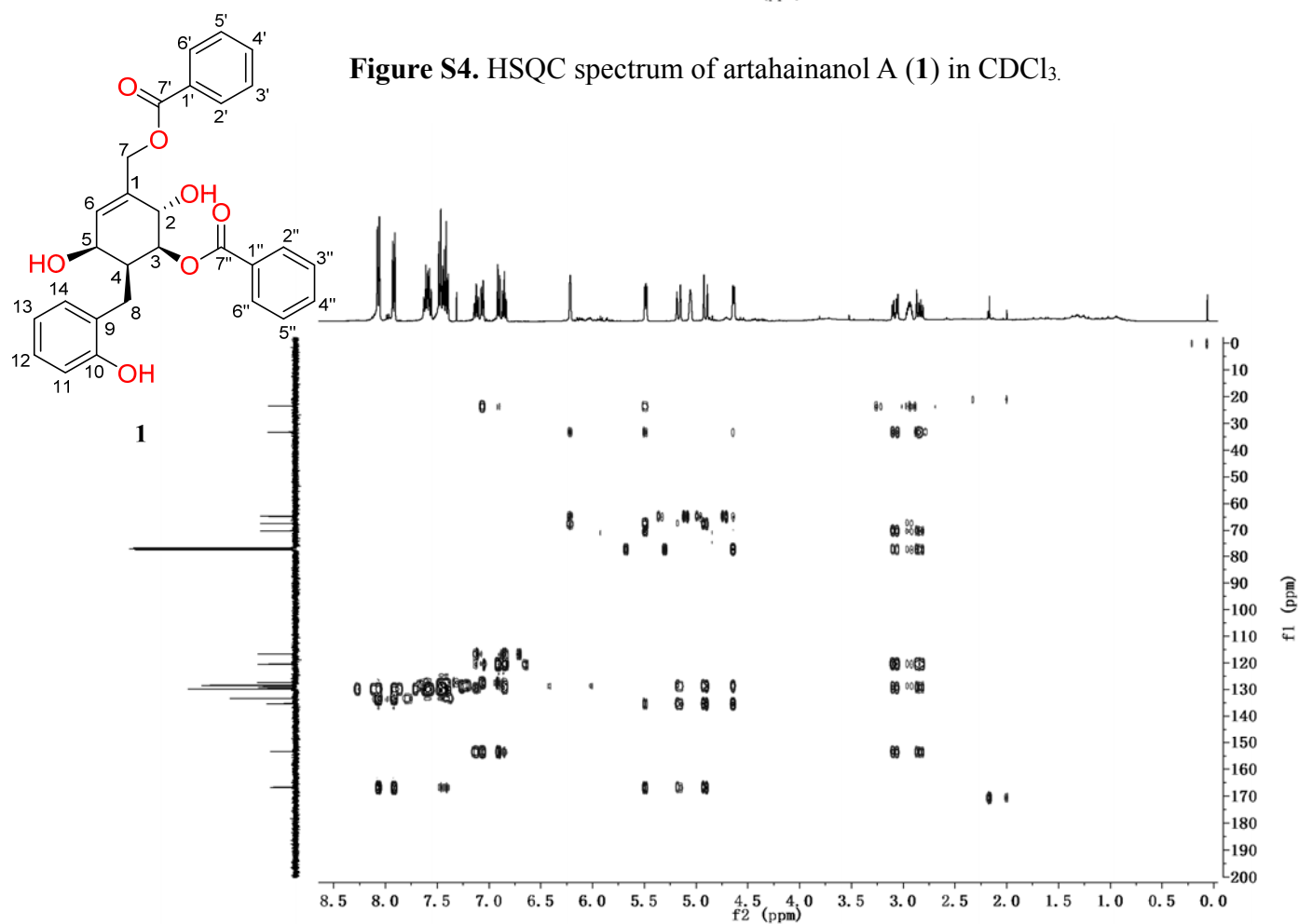


Figure S5. HMBC spectrum of artahainanol A (1) in CDCl_3 .

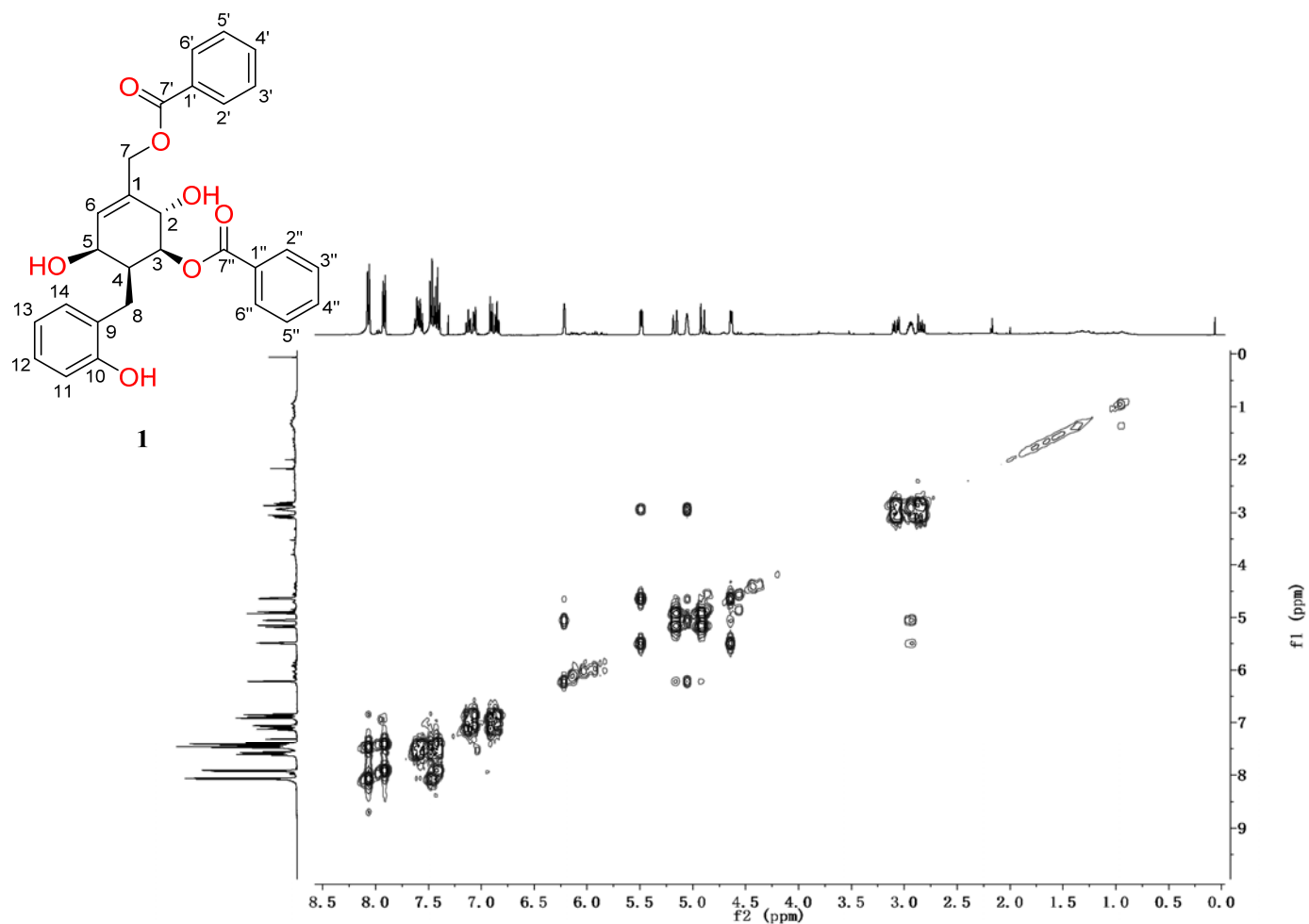


Figure S6. ^1H - ^1H COSY spectrum of artahainanol A (**1**) in CDCl_3 .

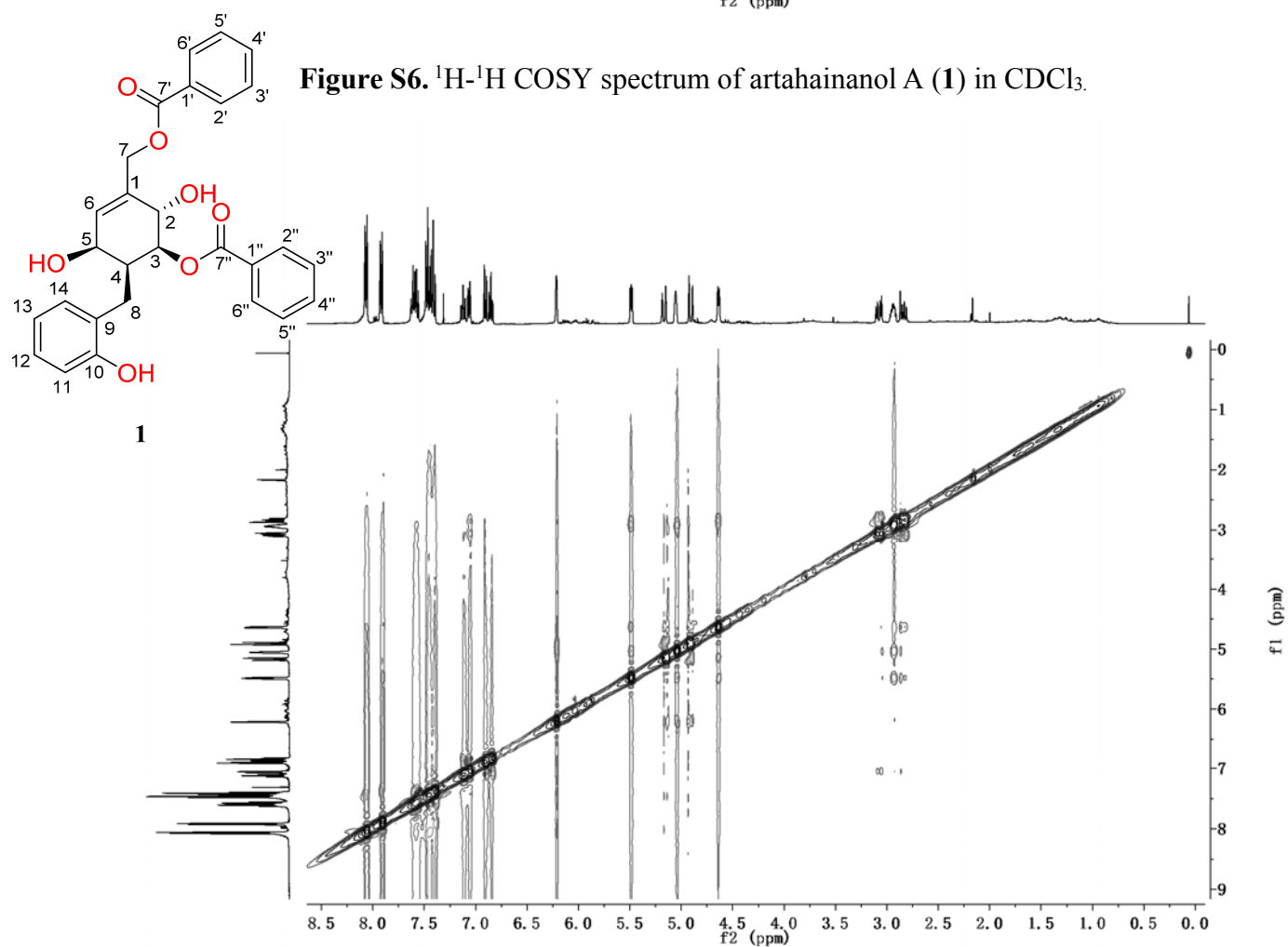


Figure S7. ROESY spectrum of artahainanol A (**1**) in CDCl_3 .

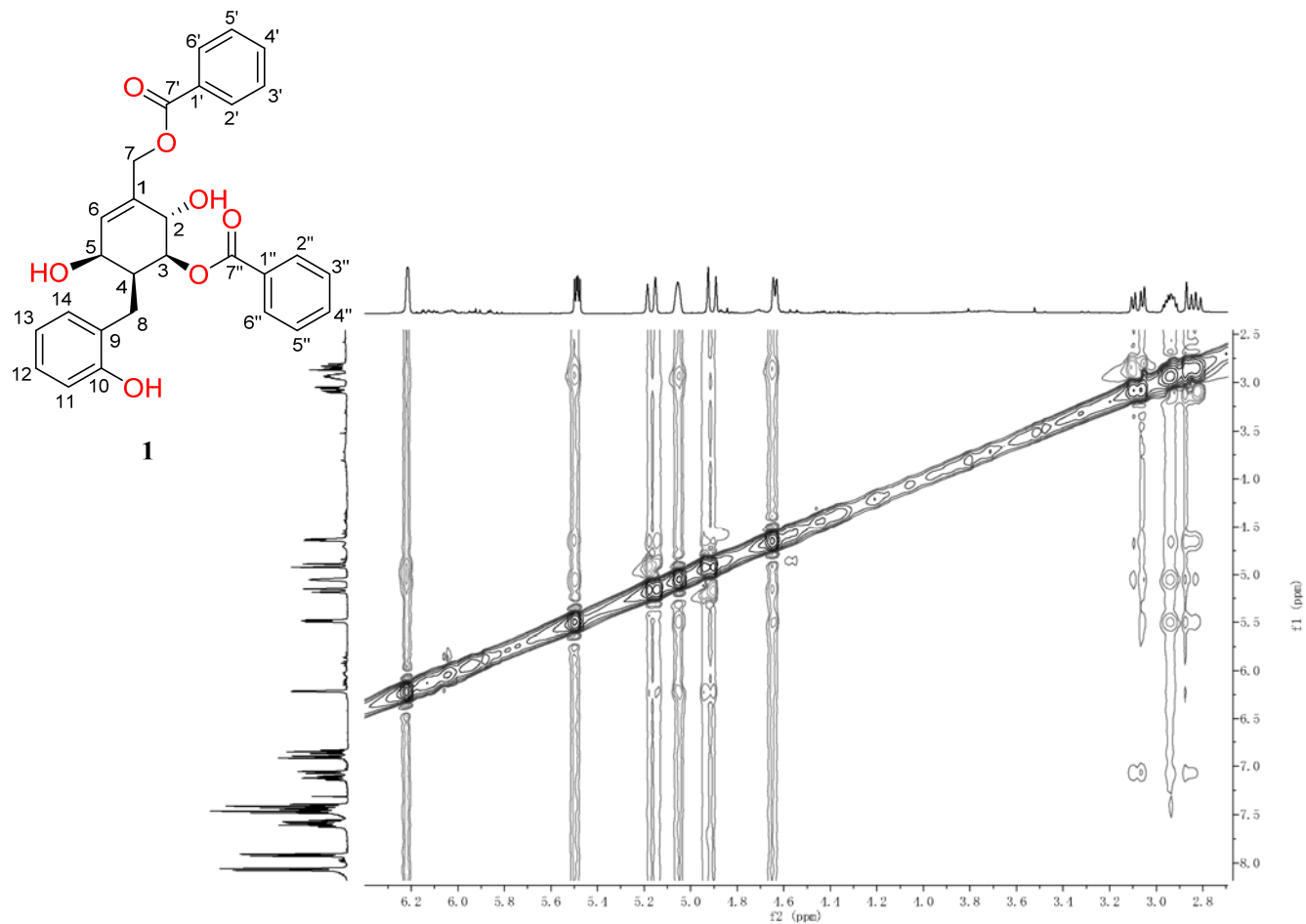


Figure S8. Enlarged ROESY spectrum 1 of artahainanol A (**1**) in CDCl₃.

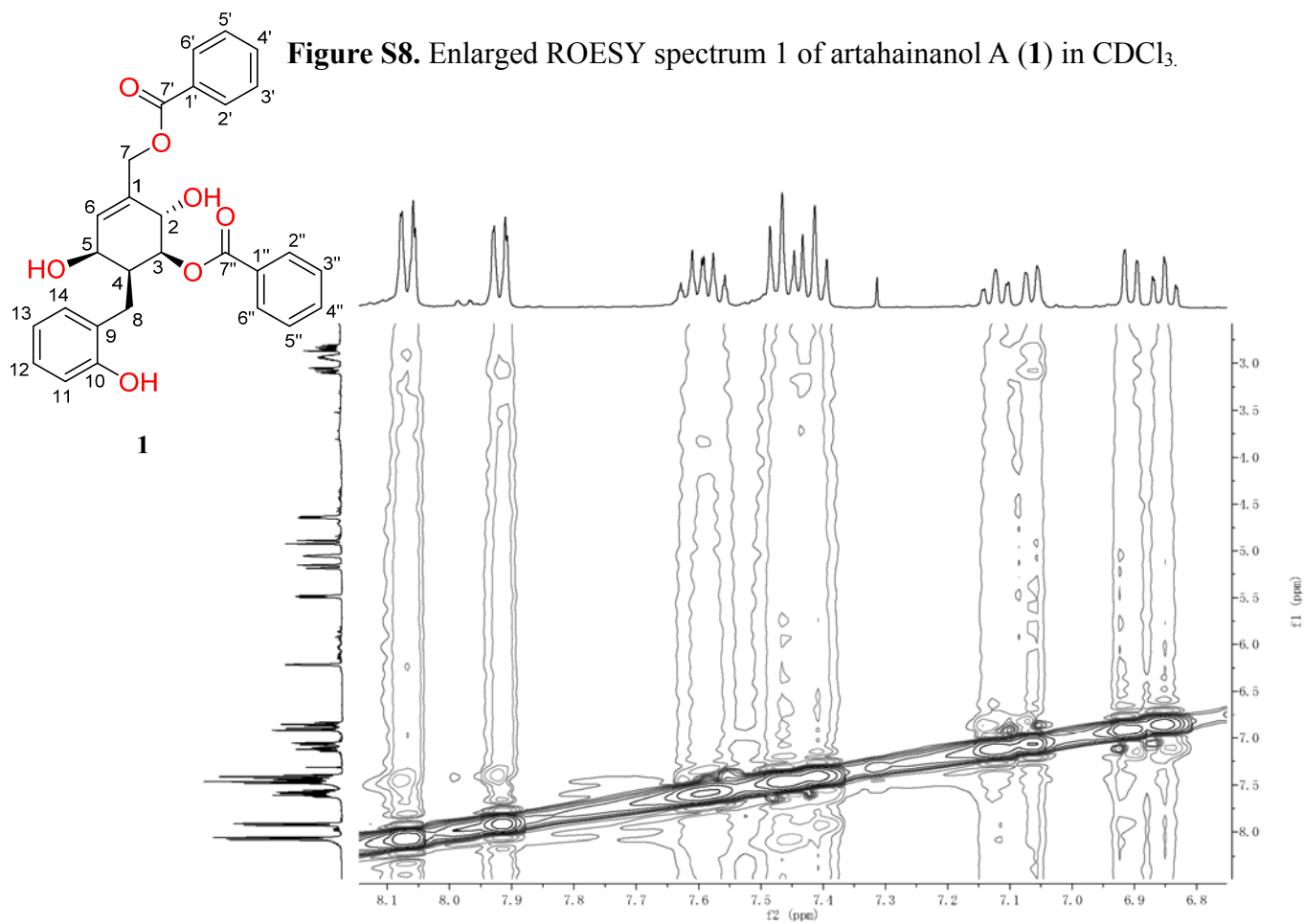


Figure S9. Enlarged ROESY spectrum 2 of artahainanol A (**1**) in CDCl₃.