

Lactoquinomycin C and D , two new medermycin derivatives from the marine-derived *Streptomyces* sp. SS17A

Biao Zhou, Yong-Jun Jiang, Yuan-Yuan Ji, Hao-Jian Zhang, Li Shen *

Institute of Marine Biology, Ocean College, Zhejiang University, No. 1 Zheda Rd., Zhoushan
316021, People's Republic of China

*Tel: +86-0580-2092601. Fax: +86-0580-2092601. E-mail: shenli@zju.edu.cn

ABSTRACT

Lactoquinomycin C (**1**) and Lactoquinomycin D (**2**), two new medermycin derivatives together with six known compounds (**3-8**) were isolated from the rice solid fermentation of the marine-derived *Streptomyces* sp. SS17A. The intriguing structural features of the Lactoquinomycin D (**2**) which contains 5,14-epoxidation is relatively rare in medermycin derivatives. Compounds **1** and **2** exhibited no cytotoxicity against PC-3 and HCT-116 cancer cell lines, whereas compound **3** showed stronger cytotoxicity with IC₅₀ values of 0.02 and 0.04 μ M, respectively. A structure-activity relationship was observed for the cytotoxicity of the medermycin derivatives with a γ -lactone unit is required for significant cytotoxicity based on compounds **1-3**.

KEYWORDS: Lactoquinomycin C; Lactoquinomycin D; 5,14-epoxidation.

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Table S1. Cytotoxic activity assay for Compounds **1-3**.

Compounds	1	2	3 ^a
PC3 (IC ₅₀ , μM)	>20	>20	0.02
HCT-116 (IC ₅₀ , μM)	>20	>20	0.04
^a medermycin (3) was considered as a positive control.			

Table S2. ¹H and ¹³C NMR Data of Compound **1** ¹H and ¹³C NMR (600 and 150 MHz in DMSO-*d*₆).

no.	δ_H^a	δ_C^b
1	7.49, d (2.5)	112.2
2		162.7
3	7.09, d (2.5)	124.7
4		145.7
5		122.4
6		182.2
7		131.7
8	7.72, d (8.0)	118.4
9	7.86, d (8.0)	132.6
10		137.1
11		157.6
12		116.4
13		189.8
14		128.7
1'	4.96, dd (11.0, 1.5)	70.3
2'	1.68, q (11.0)	29.2
	2.37, m	
3'	3.60, m	65.8
4'	3.41, m	69.5
5'	3.55, m	76.5
6'	1.32, d (6.0)	18.0
2-OH	11.21, br s	
4-Me	2.74, s	23.8
11-OH	13.63, s	
3'-N(Me) ₂	2.72, s	37.4
	2.76, s	41.3
4'-OH	6.06, br s	

Table S3. ^1H and ^{13}C NMR Data of Compound **2** ^1H and ^{13}C NMR (600 and 150 MHz in methanol- d_4).

no.	δ_{H}^a	δ_{C}^b
1	4.25, q (6.0)	66.0
3	4.45, t (5.0)	66.8
4	2.23, dd (14.0, 1.5)	24.7
	2.55, m	
5		84.9
6		189.6
7		132.9
8	7.65, d (8.0)	119.9
9	7.97, d (8.0)	134.8
10		137.9
11		158.6
12		116.6
13		202.3
14		77.1
15	2.88, dt (18.0, 2.0)	36.1
	2.98, dd (18.0, 5.0)	
16		169.4
1'	5.02, dd (11.0, 1.5)	72.4
2'	1.67, q (11.0)	30.5
	2.57, m	
3'	3.62, m	68.5
4'	3.47, dd (10.0, 9.0)	71.2
5'	3.57, m	78.5
6'	1.42, d (6.0)	18.2
3'-N(Me) ₂	2.80, s	37.5
	2.92, s	42.1

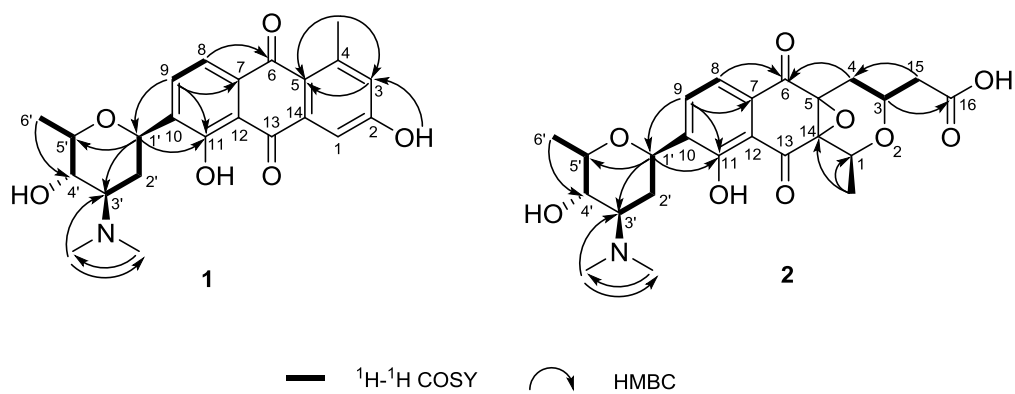


Figure S1. ^1H - ^1H COSY and selected HMBC correlations for compounds **1** and **2**.

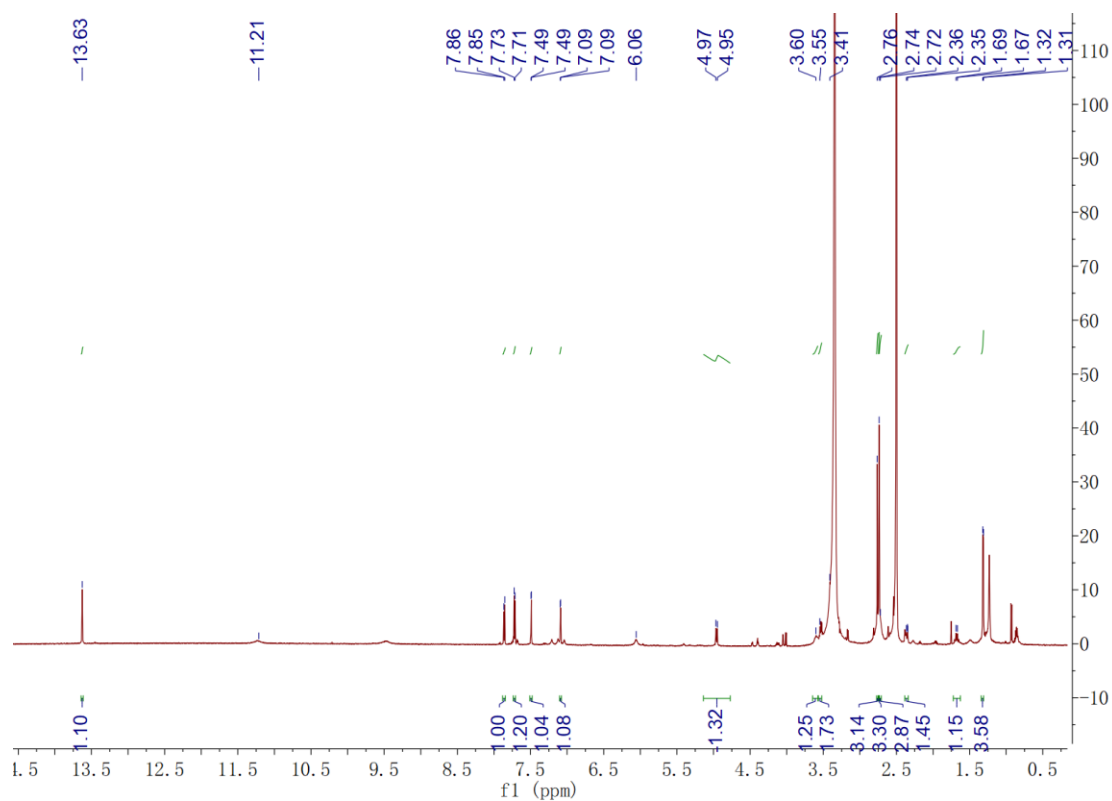


Figure S2. ^1H NMR spectrum of **1** in $\text{DMSO}-d_6$.

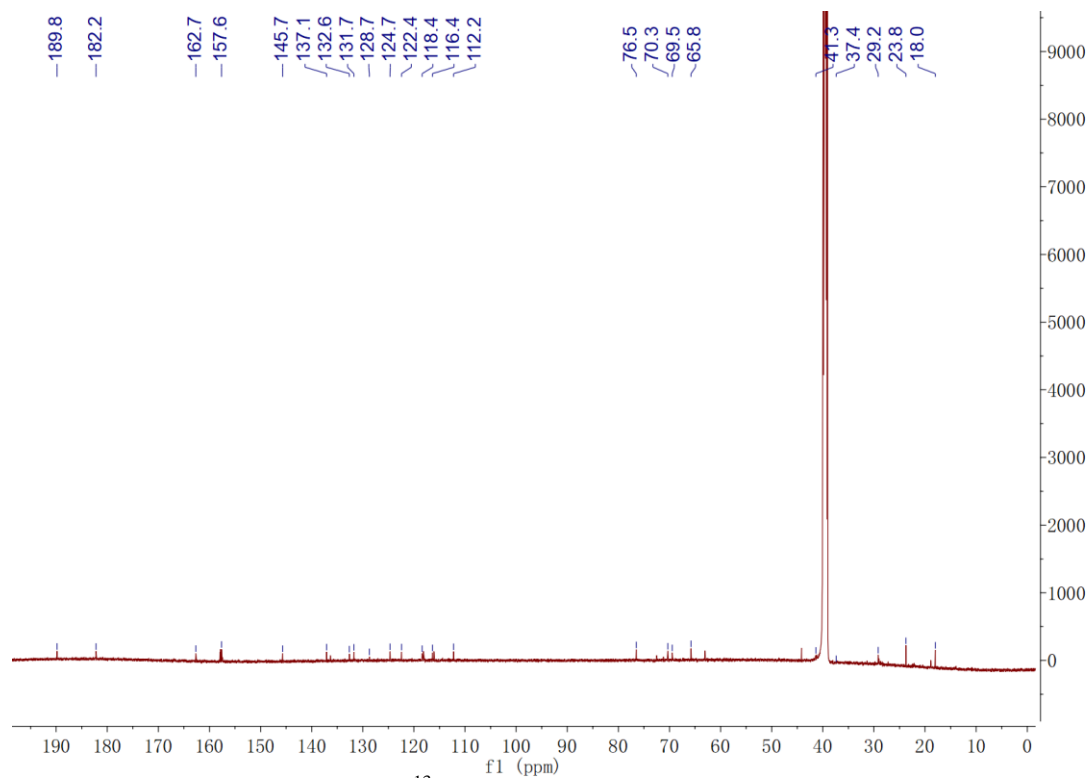


Figure S3. ^{13}C NMR spectrum of **1** in $\text{DMSO-}d_6$.

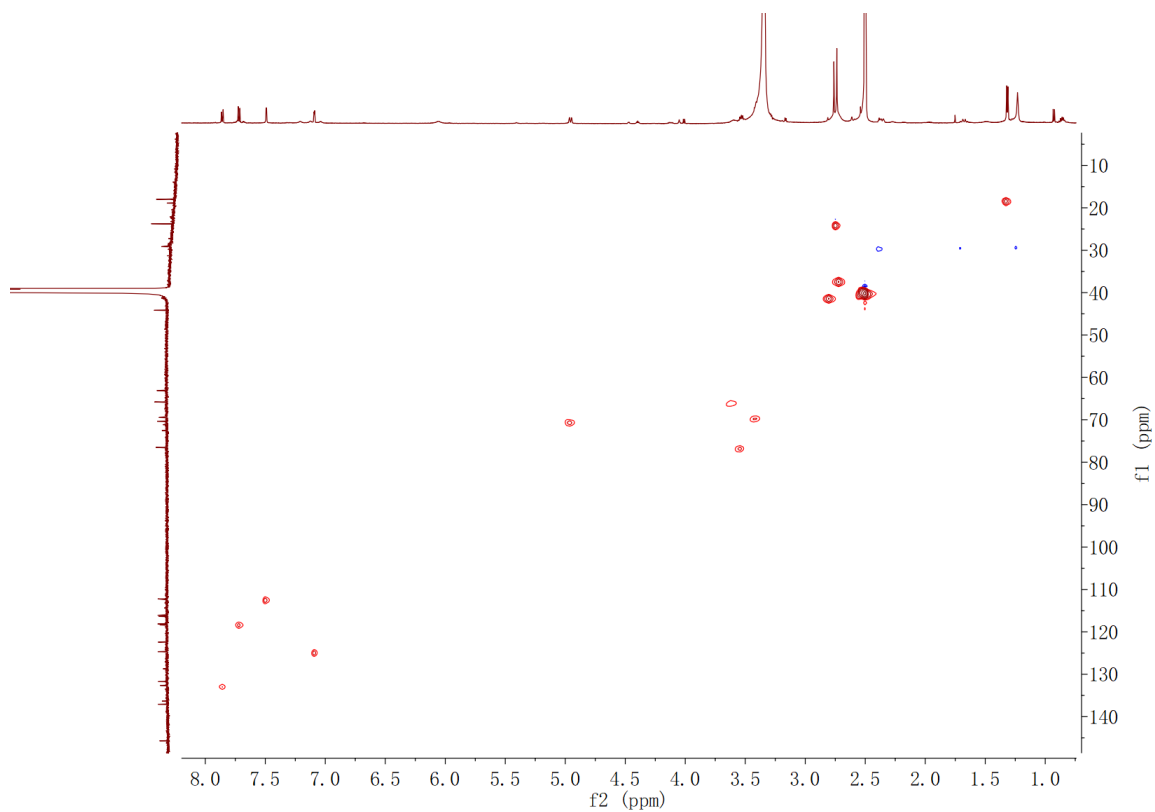


Figure S4. HSQC spectrum of **1** in $\text{DMSO-}d_6$.

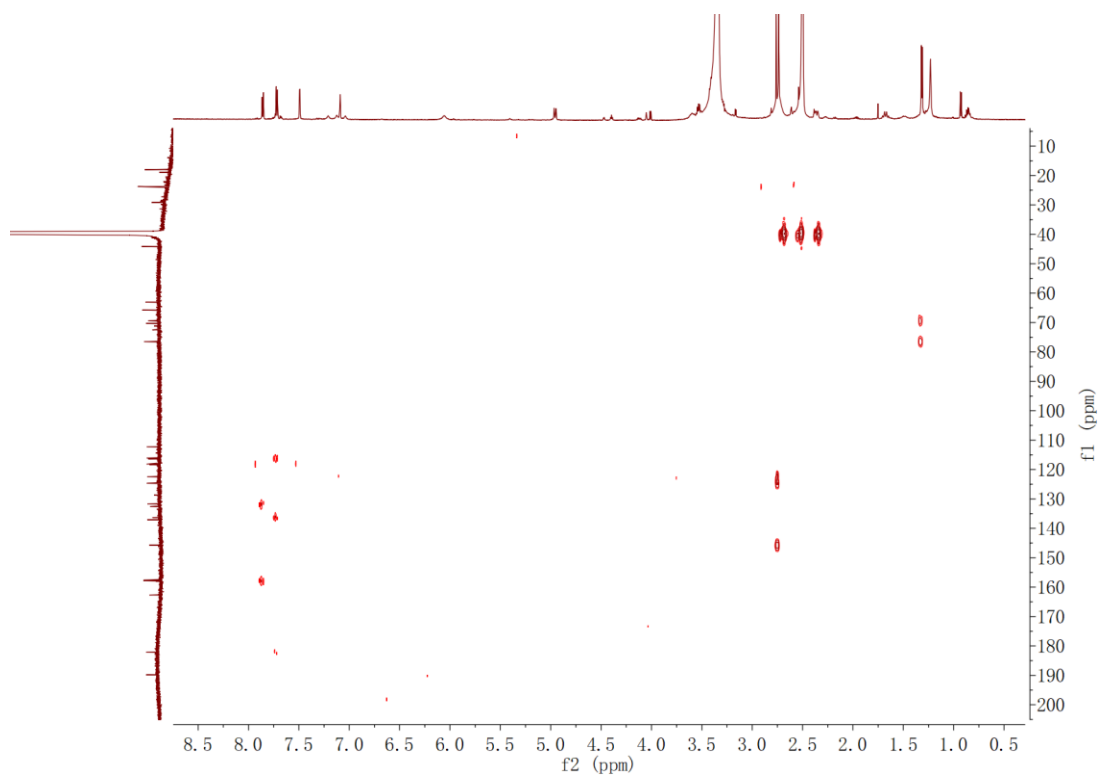


Figure S5. HMBC spectrum of **1** in DMSO- d_6 .

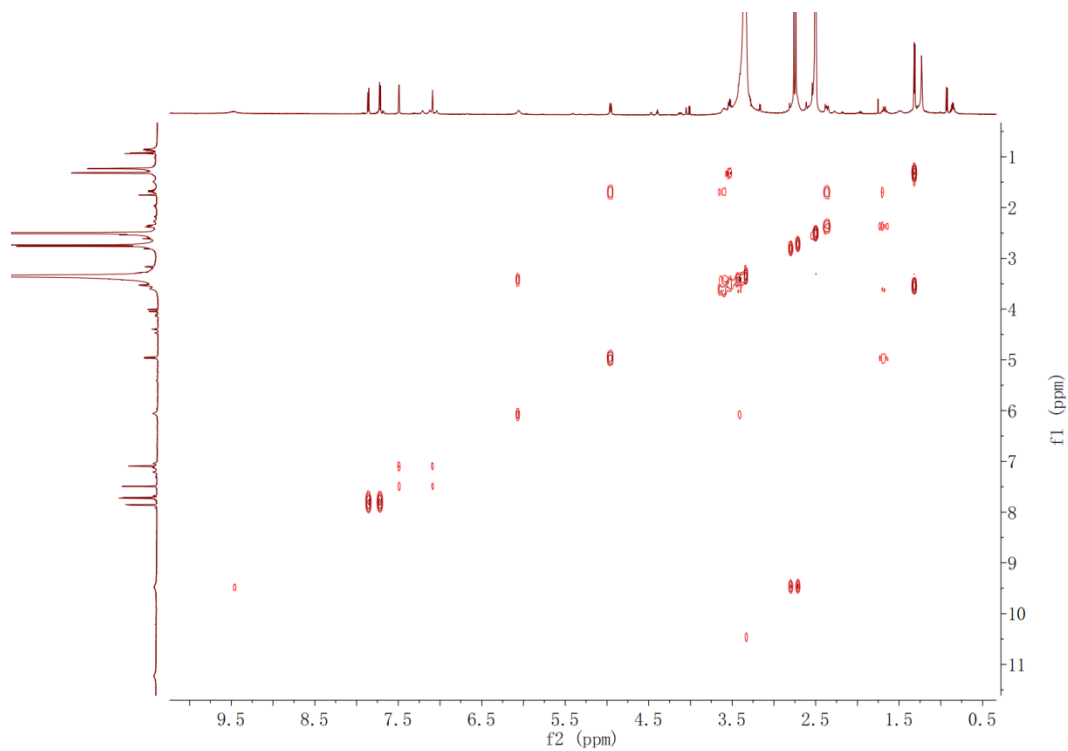


Figure S6. ^1H - ^1H COSY spectrum of **1** in DMSO- d_6 .

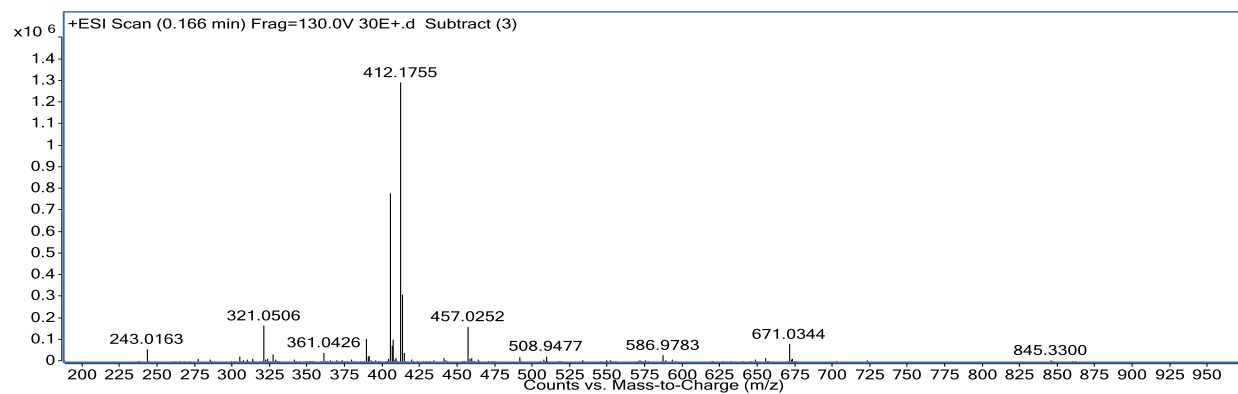


Figure S7. HRESIMS spectrum of **1**.

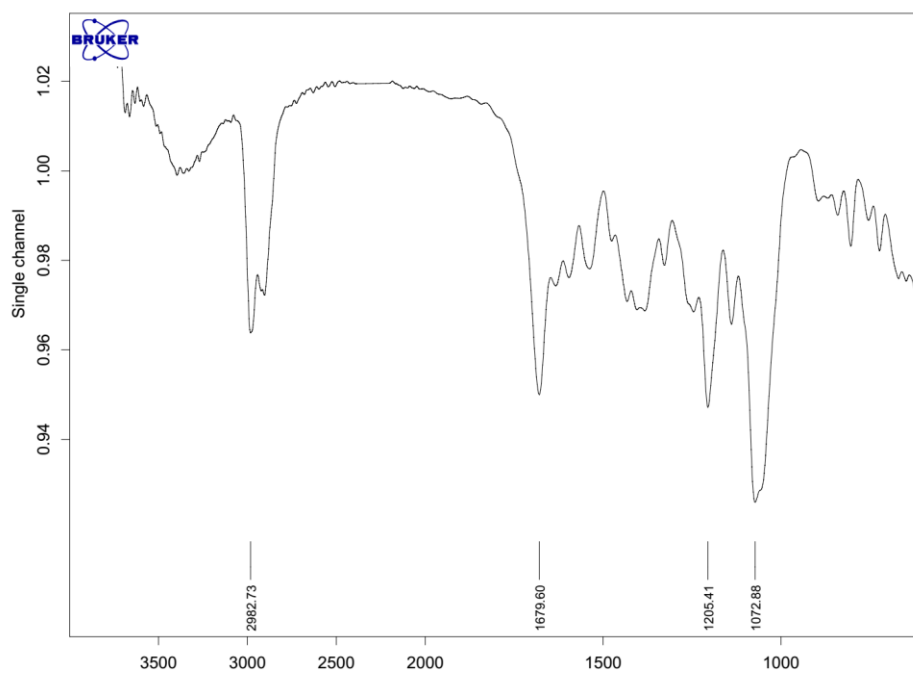


Figure S8. IR spectrum of **1**.

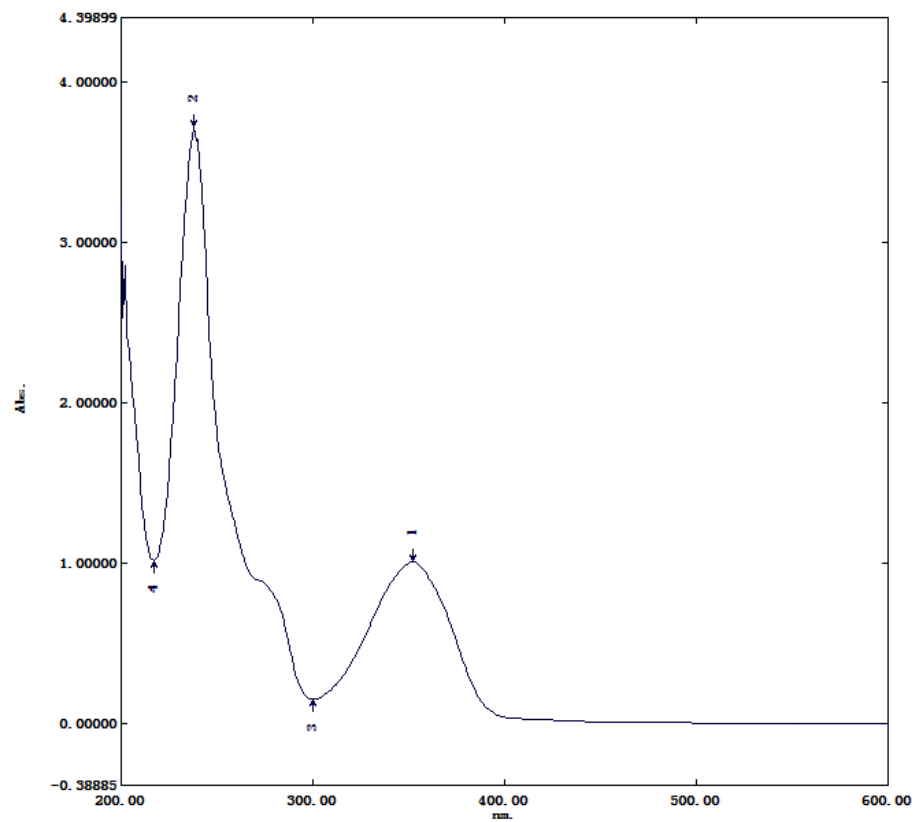


Figure S9. DAD UV-Vis spectrum of **1**.

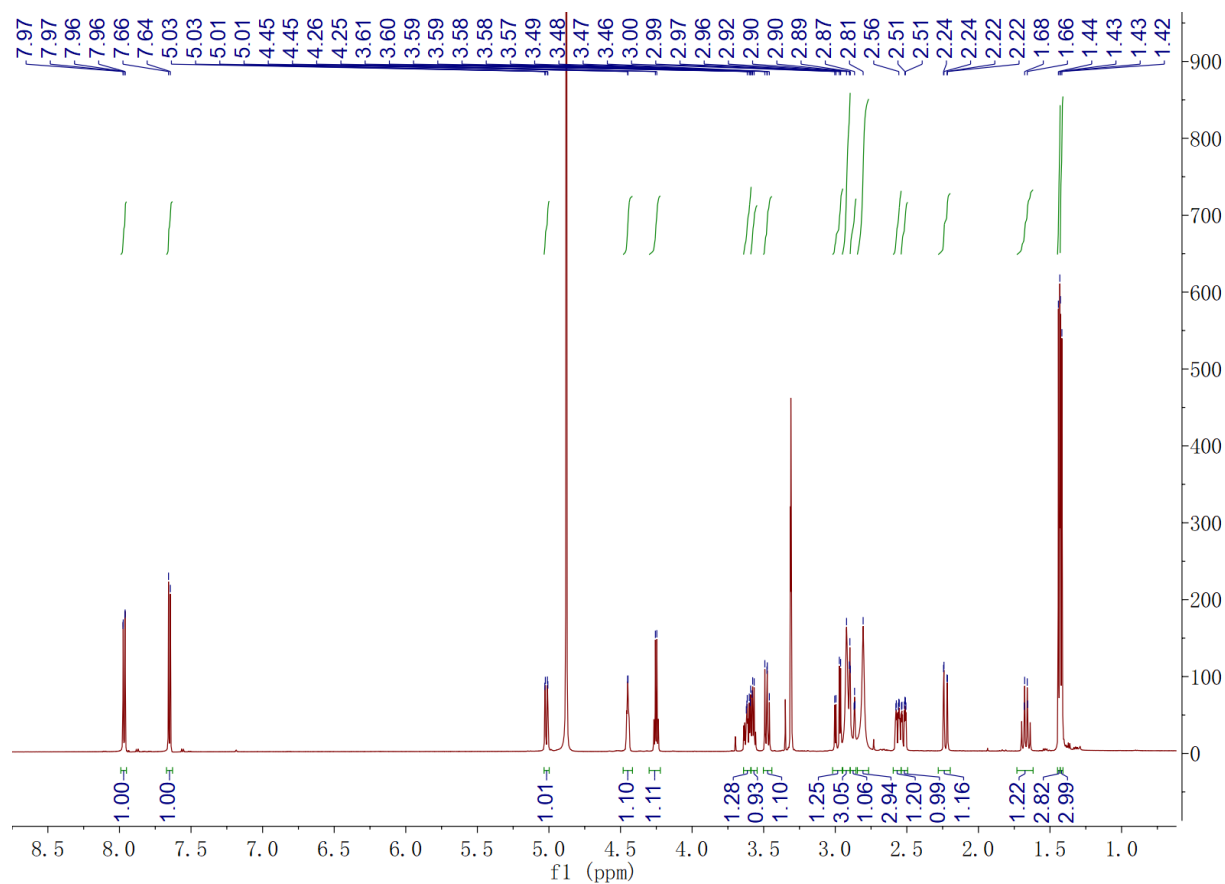


Figure S10. ¹H NMR spectrum of **2** methanol-*d*₄.

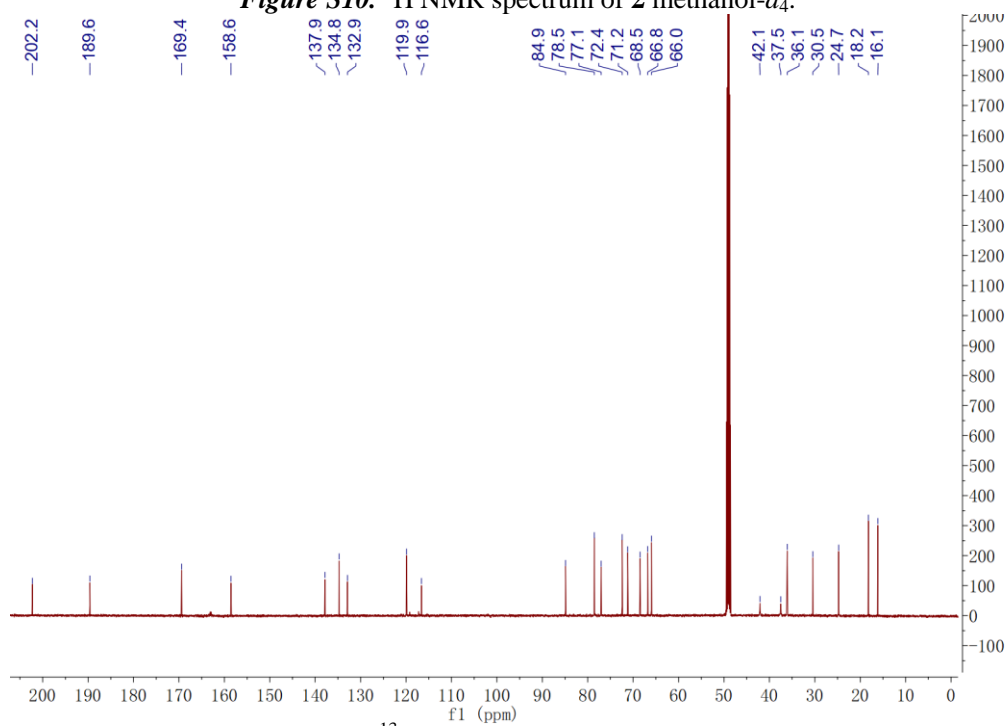


Figure S11. ¹³C NMR spectrum of **2** methanol-*d*₄.

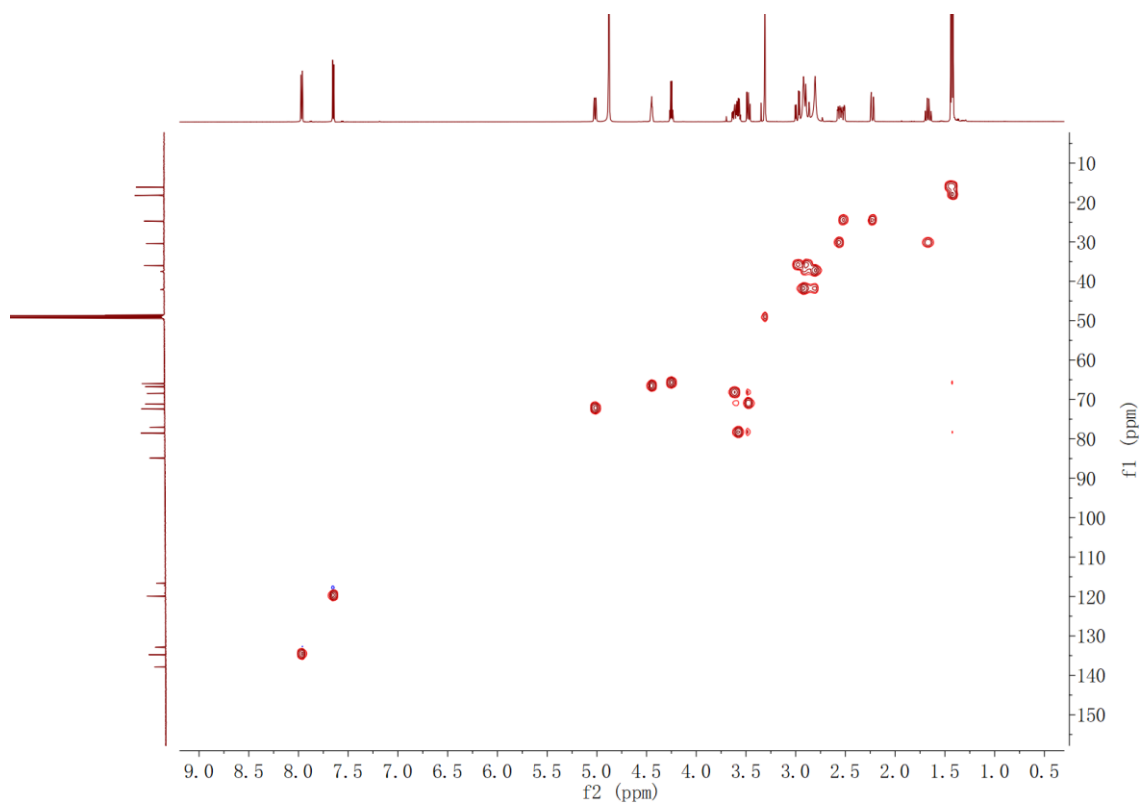


Figure S12. HSQC spectrum of **2** methanol- d_4 .

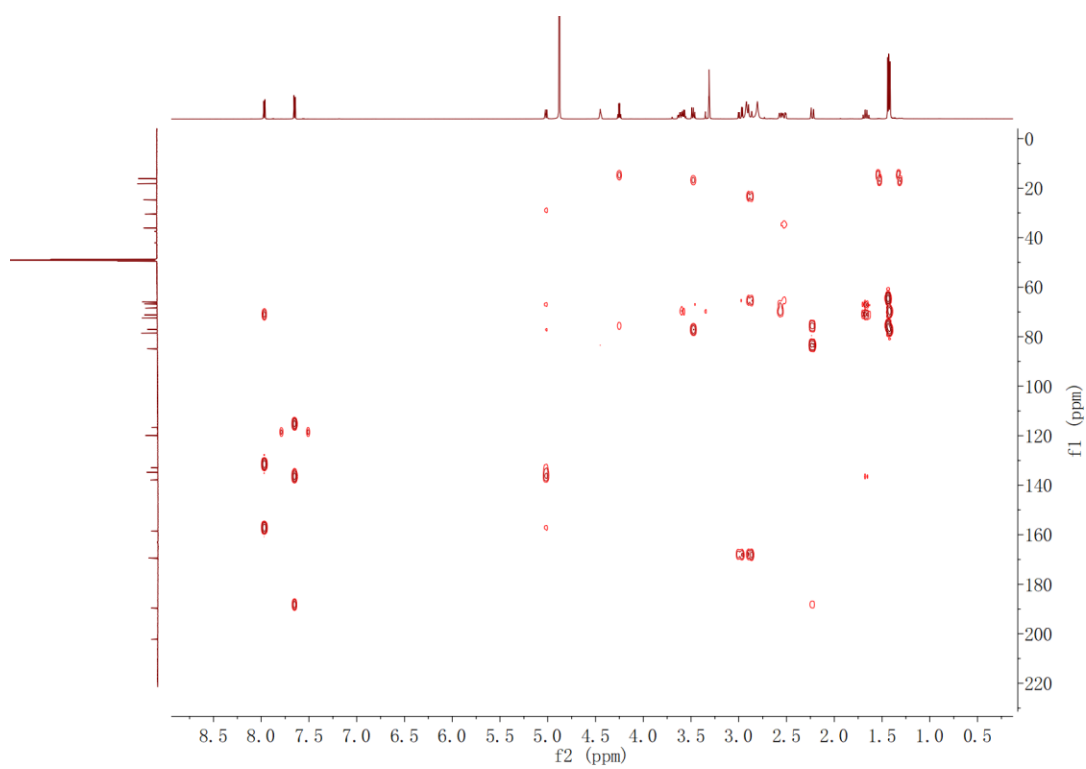


Figure S13. HMBC spectrum of **2** methanol- d_4 .

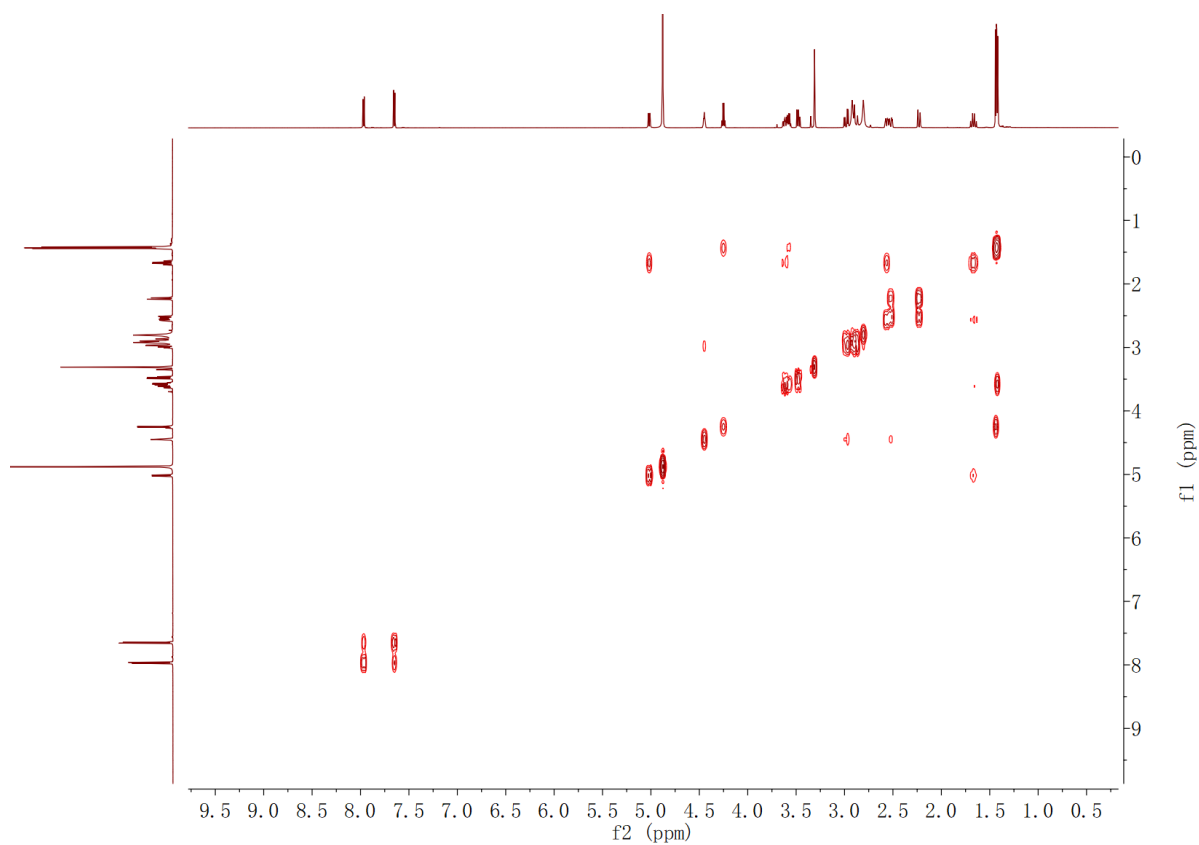


Figure S14. ^1H - ^1H COSY spectrum of **2** methanol- d_4 .

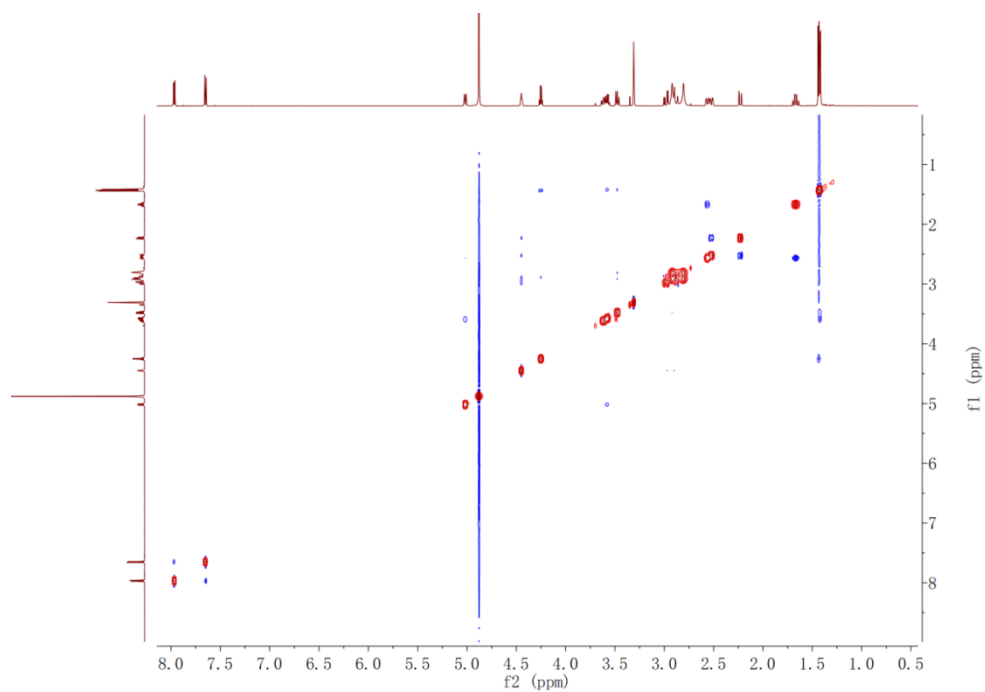


Figure S15. NOESY spectrum of **2** methanol- d_4 .

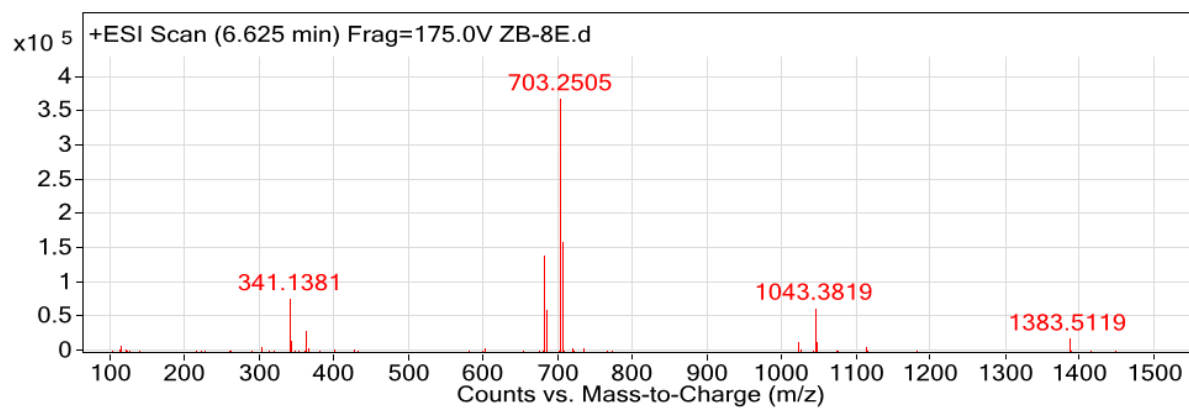


Figure S16. HRESIMS spectrum of **2**.

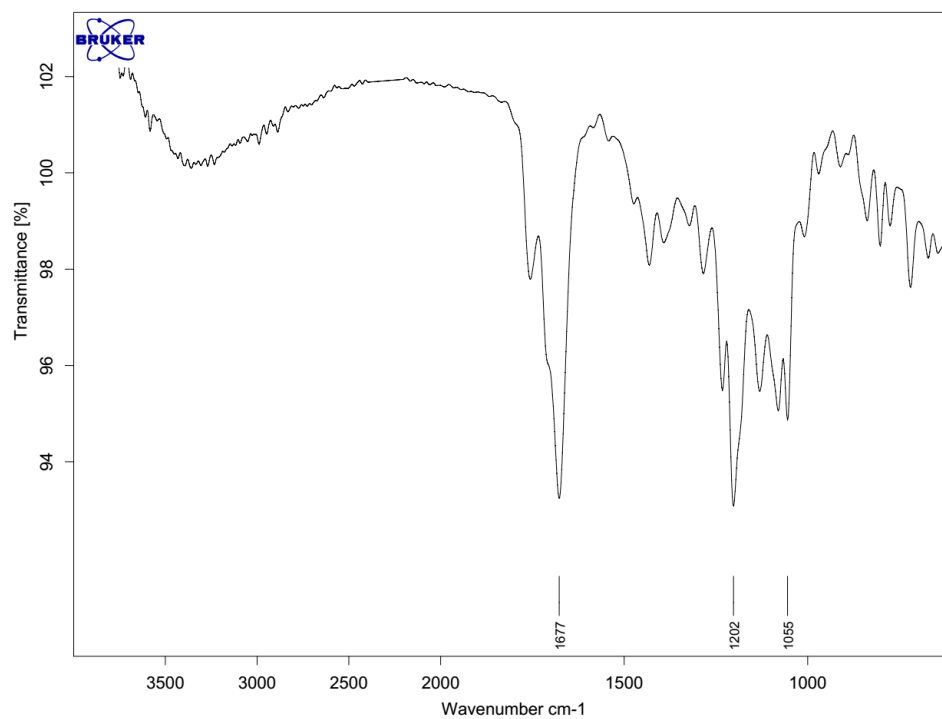


Figure S17. IR spectrum of **2**.

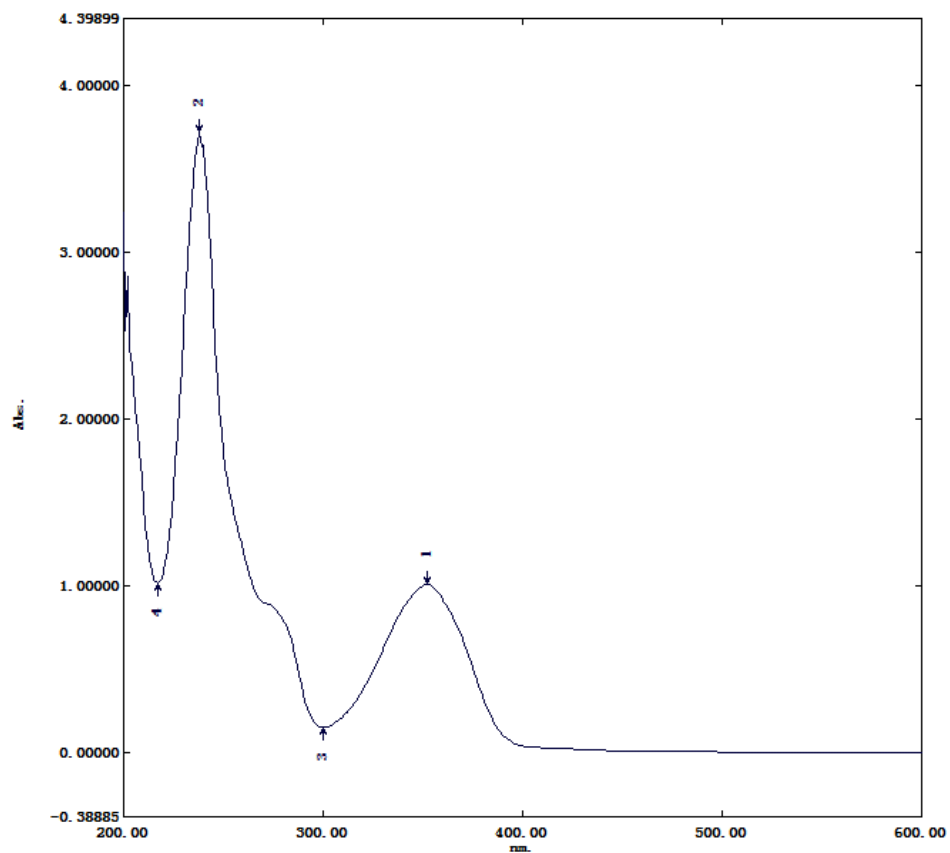


Figure S18. DAD UV-Vis spectrum of **2**.