SUPPLEMENTARY MATERIAL

A New Antiviral Pregnane from A Gorgonian-Derived *Cladosporium* sp. Fungus

Mei-Lin Yu[a,b], Fei-Fei Guan[a,b], Fei Cao[a,c], Yan-Lai Jia[a,b], and Chang-Yun Wang[a,b,*]

[a]*Key Laboratory of Marine Drugs, the Ministry of Education of China, School of Medicine and Pharmacy, Ocean University of China, Qingdao 266003, People's Republic of China.*

[b]*Laboratory for Marine Drugs and Bioproducts, Qingdao National Laboratory for Marine Science and Technology, Qingdao 266200, People's Republic of China.*

[c] *Key Laboratory of Pharmaceutical Quality Control of Hebei Province, College of Pharmaceutical Sciences, Hebei University, Baoding 071002, China.*

Correspondence

Prof. Dr. Chang-Yun Wang

School of Medicine and Pharmacy, Ocean University of China; Key Laboratory of Marine Drugs, the Ministry of Education, 5 Yushan Road, Qingdao, 266003, Shandong, P. R. China.

Tel: +86/532/82031536

Fax: +86/532/82031536

E-mail:changyun@ouc.edu.cn

E-mails: changyun@ouc.edu.cn

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*Corresponding author. Email: changyun@ouc.edu.cn

Abstract

A new pregnane, 3*α*-hydroxy-7-ene-6,20-dione (**1**), and five known steroids (**2**–**6**), along with one known steroidal glycoside (**7**) were obtained from the fungus *Cladosporium* sp. WZ-2008-0042 cultured from a gorgonian *Dichotella gemmacea* collected from the South China Sea. The structure and absolute configuration of the new compound (**1)** were elucidated by comprehensive spectroscopic data and X-ray diffraction data. The compound has a rare configuration of 3*α*-OH that is different from most of pregnanes. All of the isolated compounds were evaluated for their antiviral activities against respiratory syncytial virus (RSV). Among them, **1** exhibited potential antiviral activity with the IC_{50} value of 0.12 mM.

Keywords: *Cladosporium* sp.; gorgonian *Dichotella gemmacea*; 3*α*-OH pregnane; structure elucidation; antiviral activity.

List of supporting information

Table S1. ^{1}H and ^{13}C NMR data ($CDCl_3$) of compound **1**

position	δ_C, type	δ_H, (J in Hz)	HMBC
1	31.8, CH_2	1.62 (m), 1.54 (m)	C-5
2	28.0, CH_2	1.76 (m), 1.67 (m)	C-10
3	65.3, CH	2.01 (m)	C-1
4	27.8, CH_2	1.79 (m), 1.51 (m)	C-3, 5, 10
5	48.6, CH	2.71 (m)	C-6
6	201.4, C	-	_
7	123.9, CH	5.71 (s)	C-5, 9, 14
8	161.8, C	_	_
9	49.8, CH	2.31 (t, 2.3)	C-8, 11
10	38.9, C	_	_
11	21.5, CH_2	1.91 (m), 1.58 (m)	C-8, 9, 13
12	37.9, CH_2	1.81 (m), 1.62 (m)	C-11, 18
13	45.4, C	_	_
14	55.5, CH	2.20 (m)	C-8
15	22.7, CH_2	1.73 (m), 1.64 (m)	C-13
16	22.9, CH_2	2.17 (m), 1.64 (m)	C-13, 14
17	63.2, CH	2.68 (m)	C-18, 20, 21
18	13.8, CH_3	0.55 (3H, s)	C-12, 14, 17
19	12.5, CH_3	0.82 (3H, s)	C-1, 5, 10
20	208.7, C	_	_
21	31.5, CH_3	2.14 (3H, s)	C-17, 20
3-OH		4.19 (s)	

Spectra were recorded at 500 MHz for ^{1}H NMR and at 125MHz for ^{13}C NMR using $CDCl_3$ as solvent.

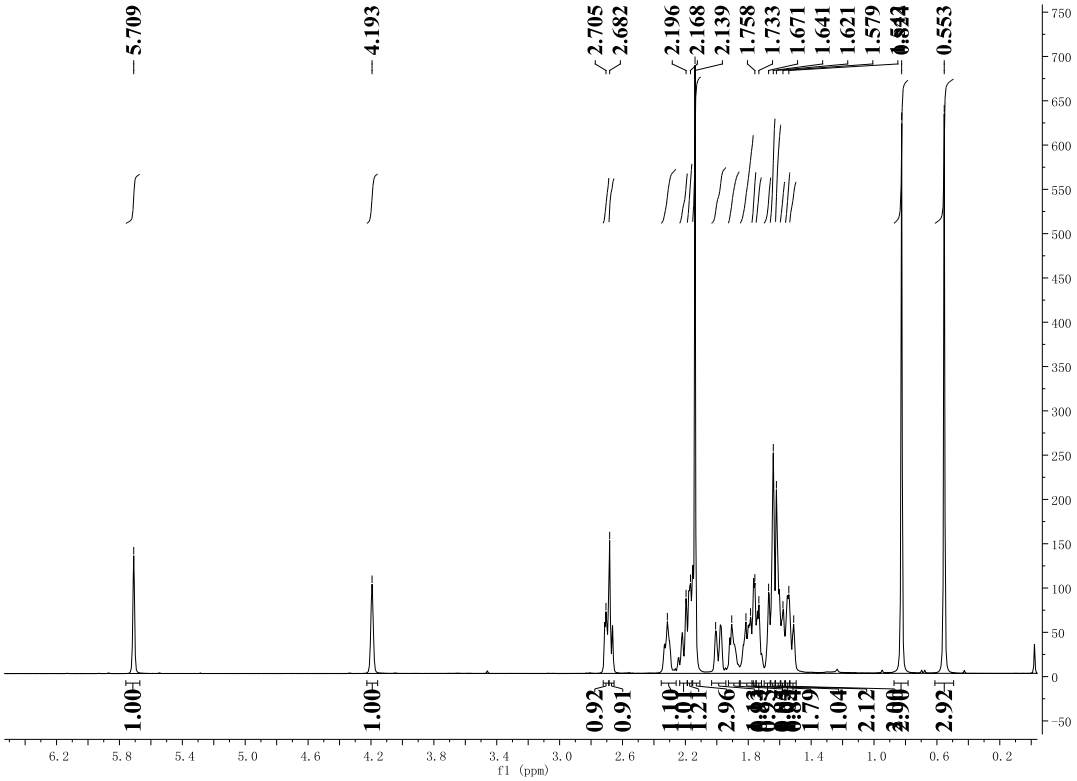

Figure S1. ^{1}H NMR (500MHz, $CDCl_3$) spectrum of compound **1**

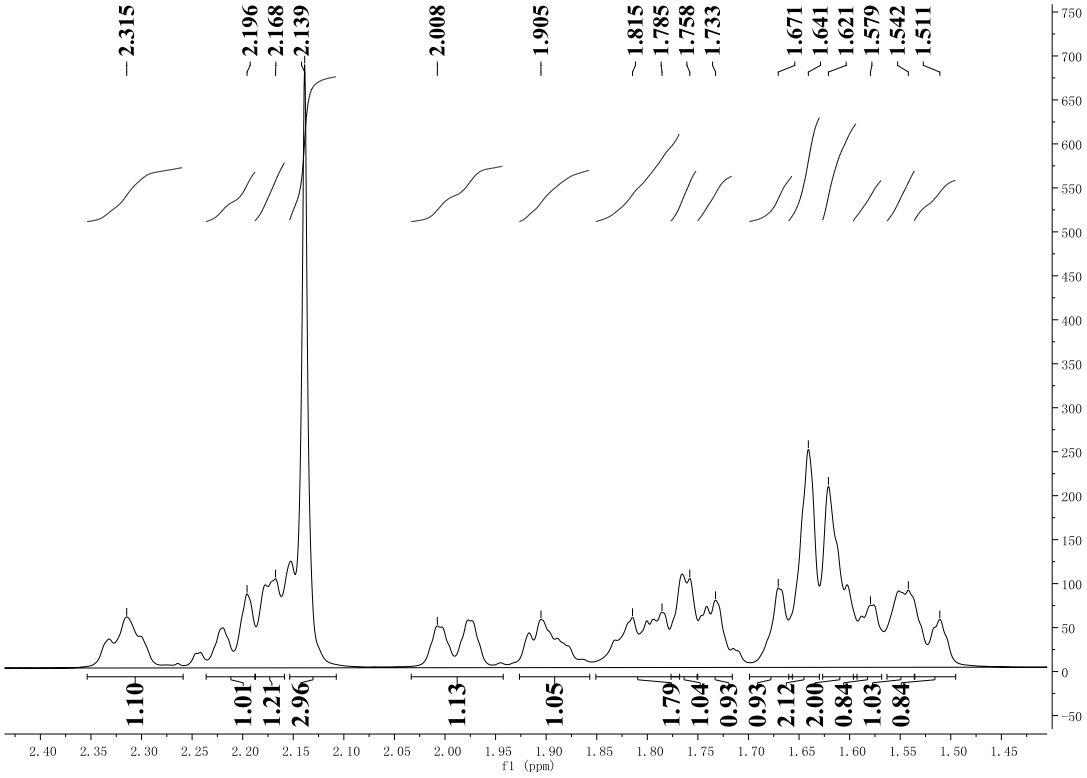

Figure S2. Partial ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **1**

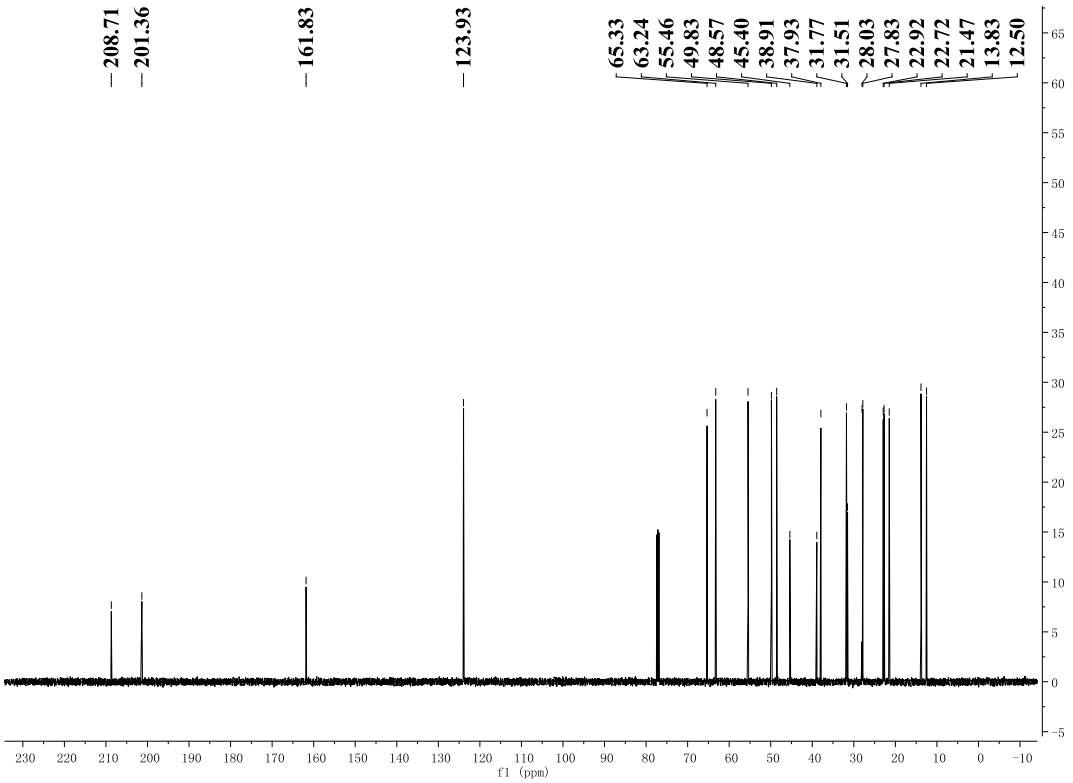

Figure S3. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **1**

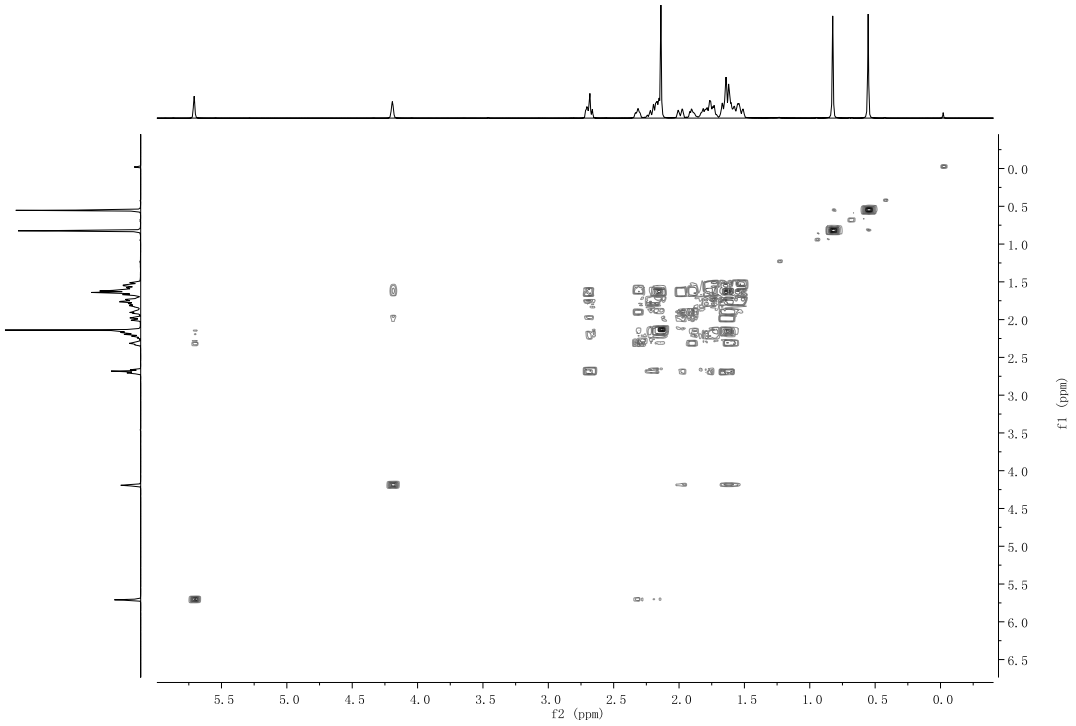

Figure S4. $^{1}H–^{1}H$ COSY ($CDCl_3$) spectrum of compound **1**

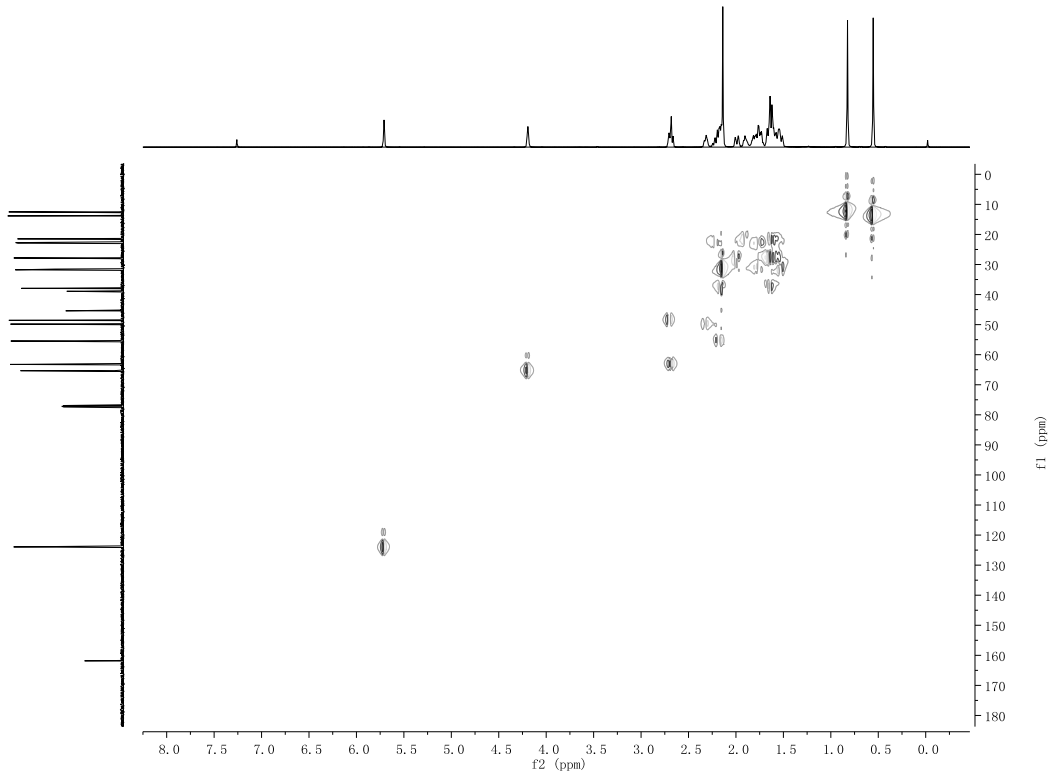

Figure S5. HMQC ($CDCl_3$) spectrum of compound **1**

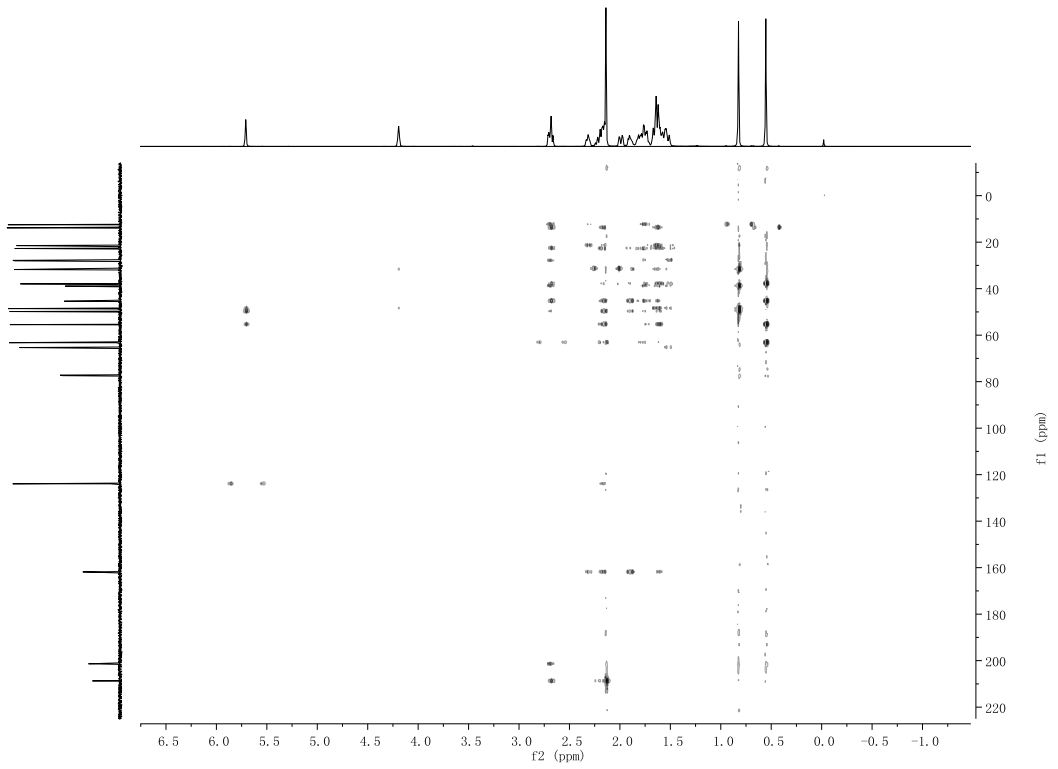

Figure S6. HMBC ($CDCl_3$) spectrum of compound **1**

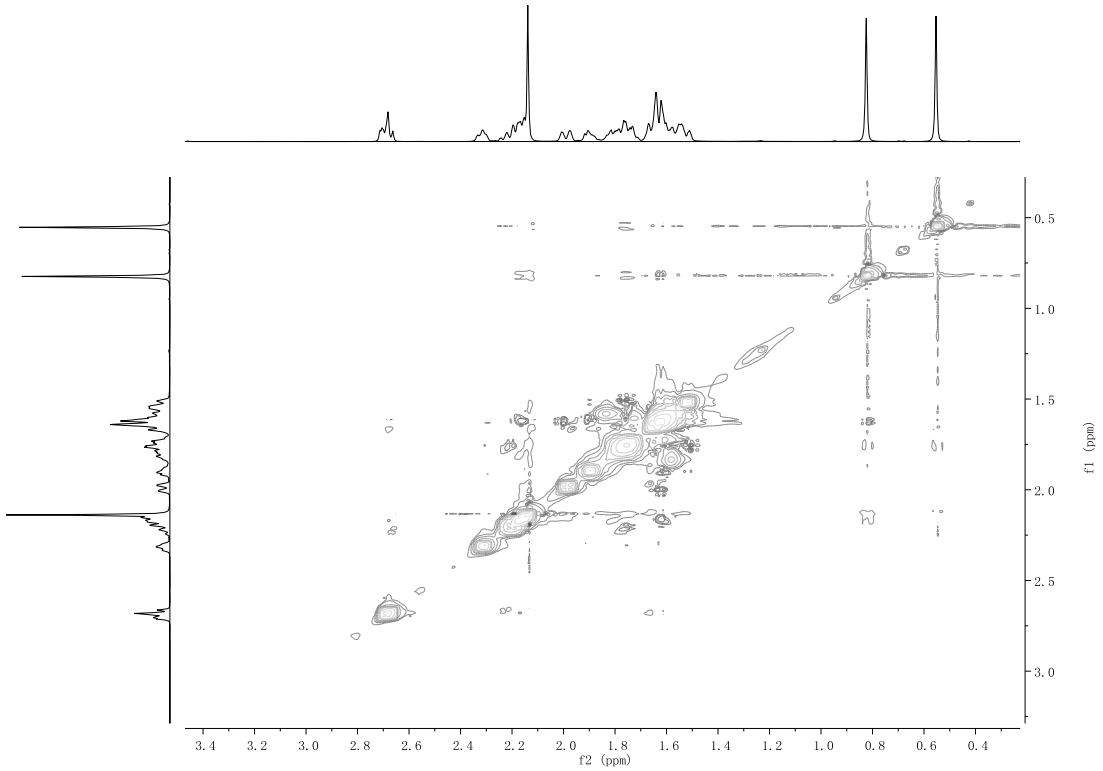

Figure S7. NOESY ($CDCl_3$) spectrum of compound **1**

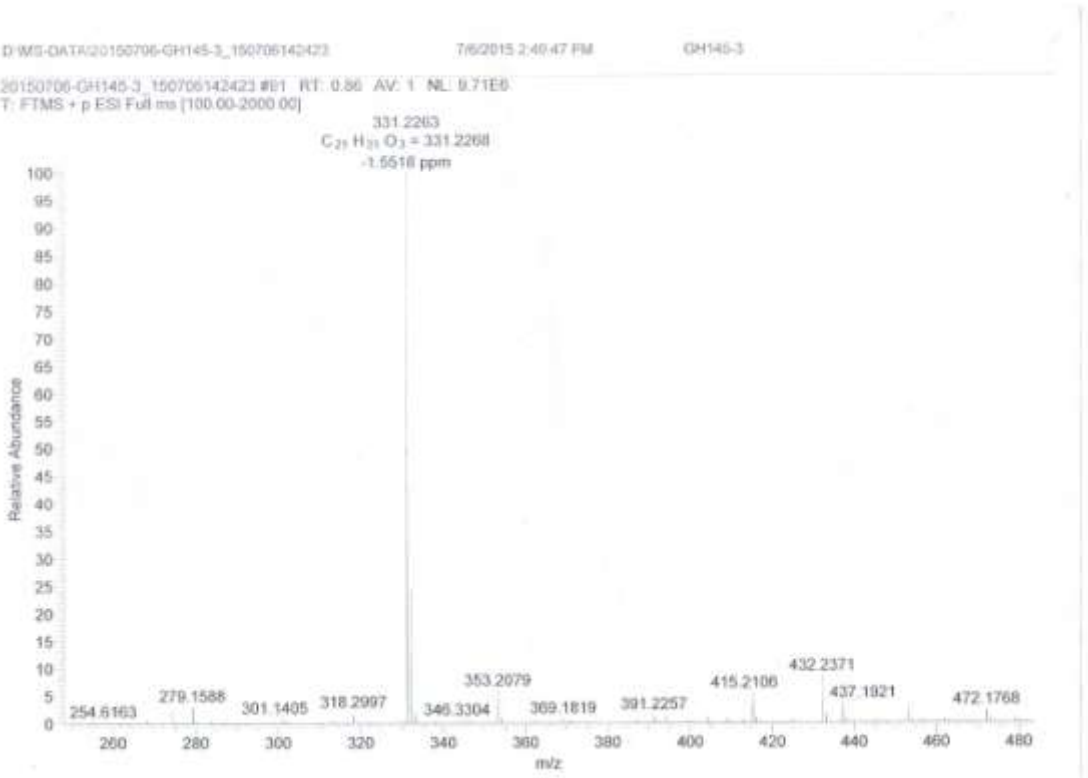

Figure S8. HRESIMS spectrum of compound **1**

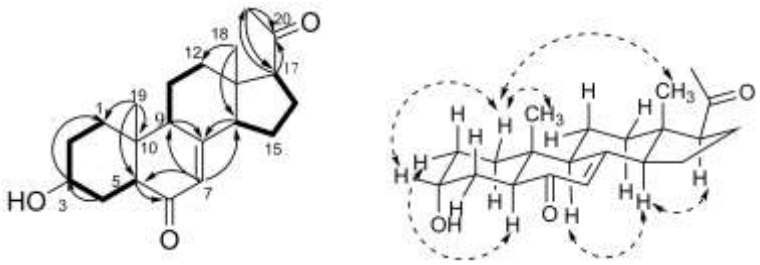

Figure S9. ^{1}H–^{1}H COSY (—), key HMBC ( ) and NOESY ( ) correlations of compound **1**