

SUPPLEMENTARY MATERIAL

15-Deoxy-Isoxeniolide-A, New Diterpenoid from a Bornean Soft Coral, *Xenia* sp.

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Abstract: A new xenicane diterpenoid, 15-deoxy-isoxeniolide-A (**1**) along with four known compounds 9-deoxy-isoxeniolide-A (**2**), isoxeniolide-A (**3**), xeniolide-A (**4**) and coraxeniolide-B (**5**) were isolated from the Bornean soft coral *Xenia* sp. The structure of this metabolite was elucidated on the basis of spectral analysis NMR and HRESIMS. Compound **5** showed potent cytotoxic activity against ATL cell line, S1T.

Keywords: soft coral; *Xenia* sp.; xenicane; diterpene; adult T-cell leukemia; S1T

Supplementary Information

Table S1. ^{13}C and ^1H NMR (600 and 150 MHz) data of **1** (CDCl_3 , δ in ppm, J in Hz).

Table S2. Cytotoxicity of compounds **1-5**.

Figure S2. COSY, selective HMBC and NOE correlations of compound **1**.

Figure S3. ^1H NMR spectrum of 15-deoxy-isoxeniolide-A (**1**) in CDCl_3 (600 MHz).

Figure S4. ^{13}C NMR spectrum of 15-deoxy-isoxeniolide-A (**1**) in CDCl_3 (150 MHz).

Figure S5. HSQC spectrum of 15-deoxy-isoxeniolide-A (**1**) in CDCl_3 .

Figure S6. ^1H - ^1H COSY spectrum of 15-deoxy-isoxeniolide-A (**1**) in CDCl_3 .

Figure S7. HMBC spectrum of 15-deoxy-isoxeniolide-A (**1**) in CDCl_3 .

Figure S8. NOESY spectrum of 15-deoxy-isoxeniolide-A (**1**) in CDCl_3 .

Figure S9. HRESIMS spectrum of 15-deoxy-isoxeniolide-A (**1**).

Table S1. ¹³C and ¹H NMR (600 and 150 MHz) data of 1 (CDCl₃, δ in ppm, *J* in Hz).

No	1	
	δ _C	δ _H
1	71.0 (t)	4.06 dd (11.7, 5.8, β-H) 3.63 t (11.7, α-H)
3	169.2 (s)	
4	130.4 (s)	
4a	50.9 (d)	2.57 dt (8.9, 3.4)
5	37.9 (t)	1.61-1.63 m
6	39.8 (t)	2.16-2.18 m
7	132.9 (s)	
8	130.4 (d)	5.20 d (6.9)
9	67.1 (d)	4.77 t (6.9)
10	45.6 (t)	2.44 dd (13.8, 6.9, β-H) 2.39 d (13.8, α-H)
11	147.9 (s)	
11a	50.0 (d)	1.99 ddd (11.7, 5.8, 3.4)
12	137.4 (d)	6.33 d (11.0)
13	123.4 (d)	6.67 dd (15.8, 11.0)
14	149.2 (d)	5.92 dd (15.8, 6.9)
15	31.5 (d)	2.41 m
16	22.0 (q)	1.04 d (6.9)
17	22.0 (q)	1.03 d (6.9)
18	17.3 (q)	1.69 s
19	114.7 (t)	5.06 s 4.96 s

Table S2. Cytotoxicity of compounds 1-5.

Compound	Cell line IC ₅₀ (μg/mL)
	S1T
1	49.75
2	40.25
3	46.07
4	34.75
5	4.12

Figure S2. COSY, selective HMBC and NOE correlations of 1.

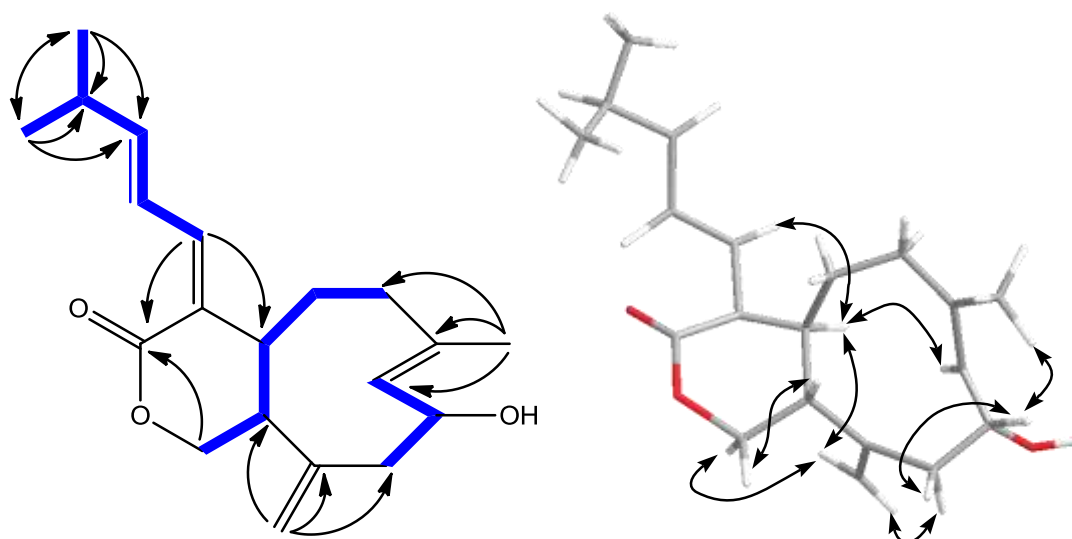


Figure S3. ^1H NMR spectrum of 15-deoxy-isoxeniolide-A (**1**) in CDCl_3 (600 MHz).

WCSY929923M04-1-1-01-2,00

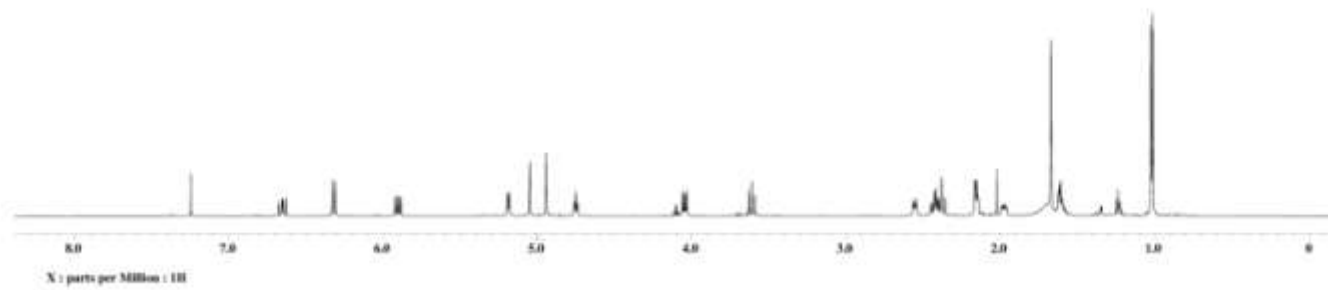


Figure S4. ^{13}C NMR spectrum of 15-deoxy-isoxeniolide-A (**1**) in CDCl_3 (150 MHz).

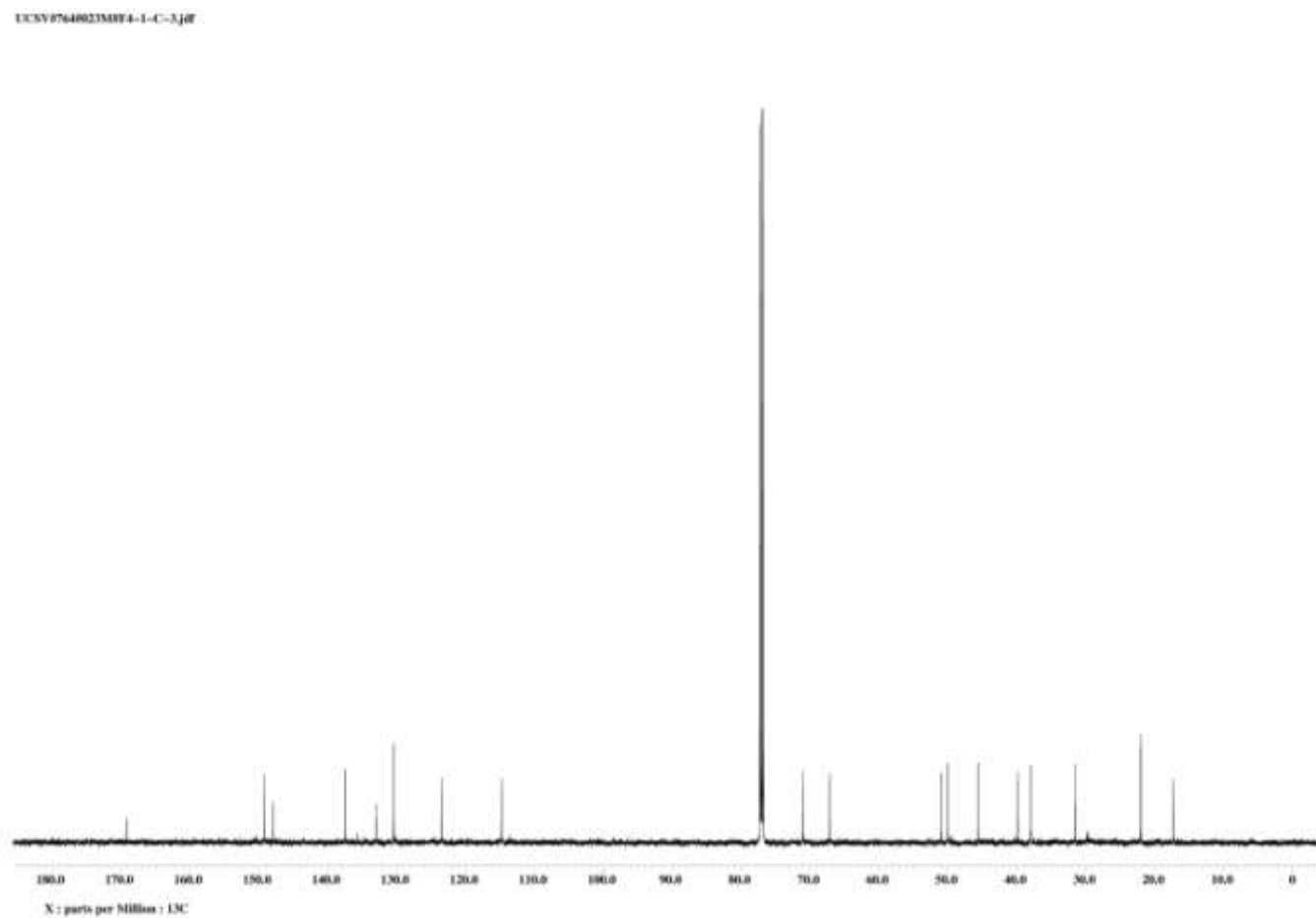


Figure S5. HSQC spectrum of 15-deoxy-isoxeniolide-A (**1**) in CDCl₃.

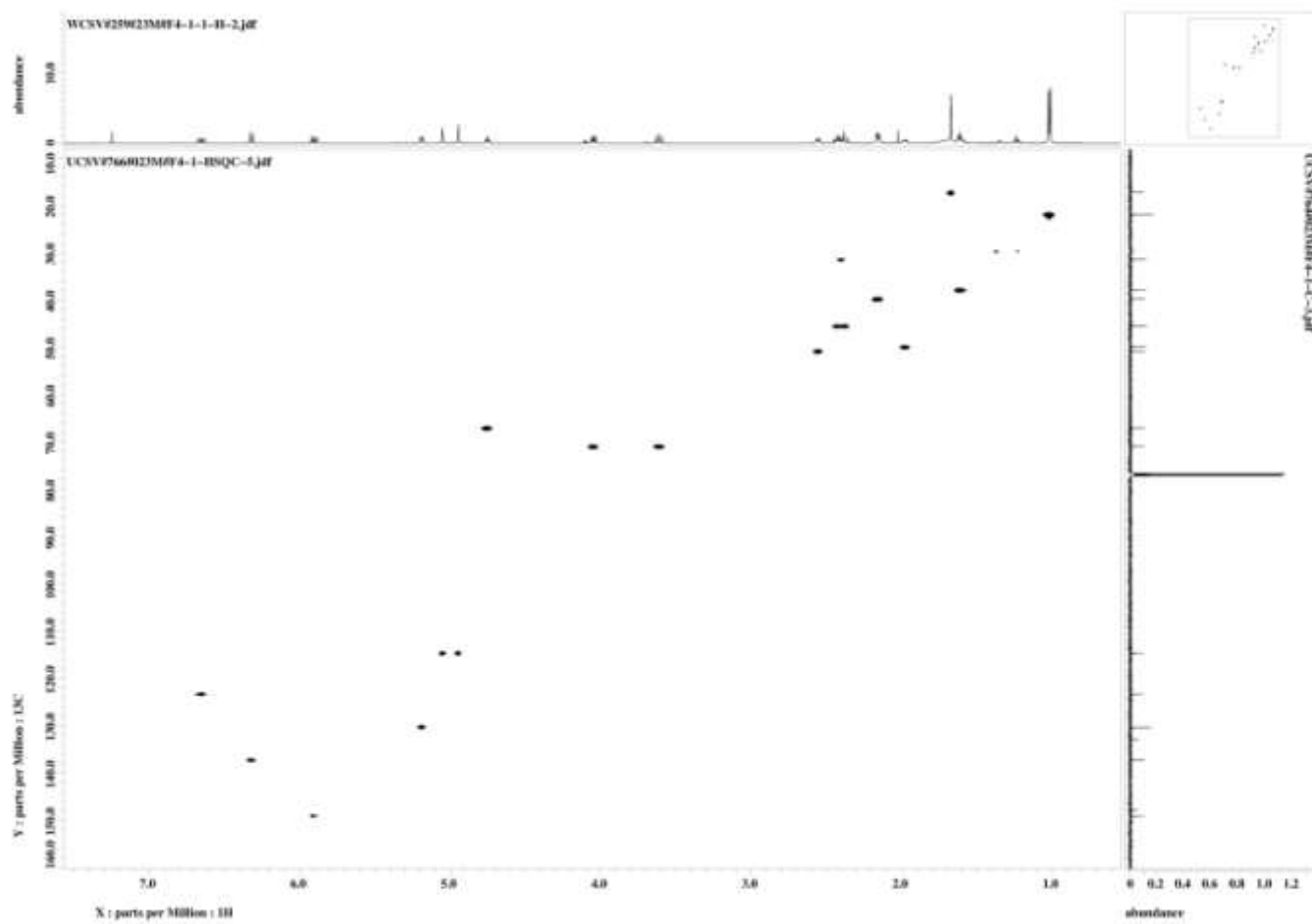


Figure S6. ^1H - ^1H COSY spectrum of 15-deoxy-isoxeniolide-A (**1**) in CDCl_3 .

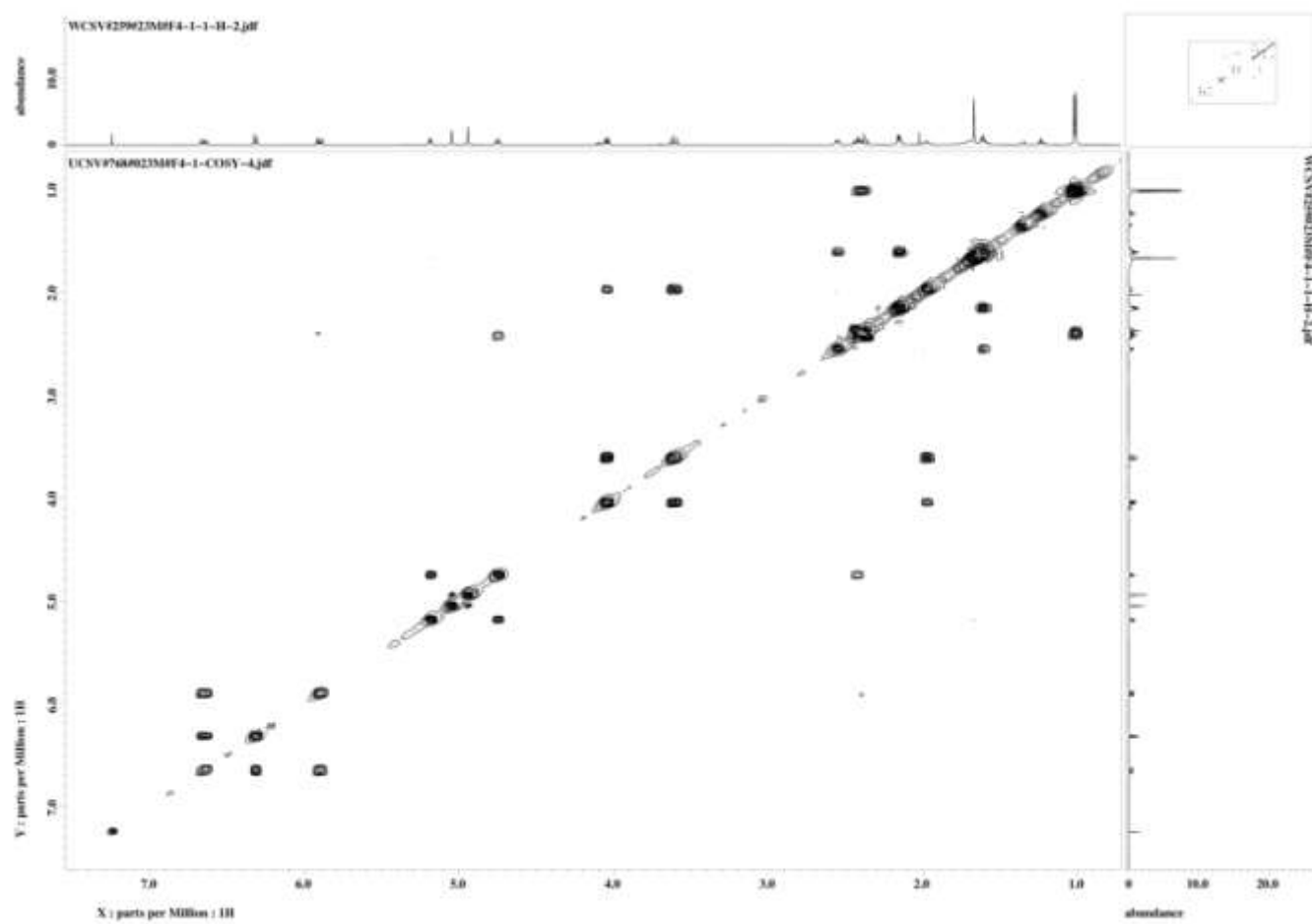


Figure S7. HMBC spectrum of 15-deoxy-isoxeniolide-A (1) in CDCl₃.

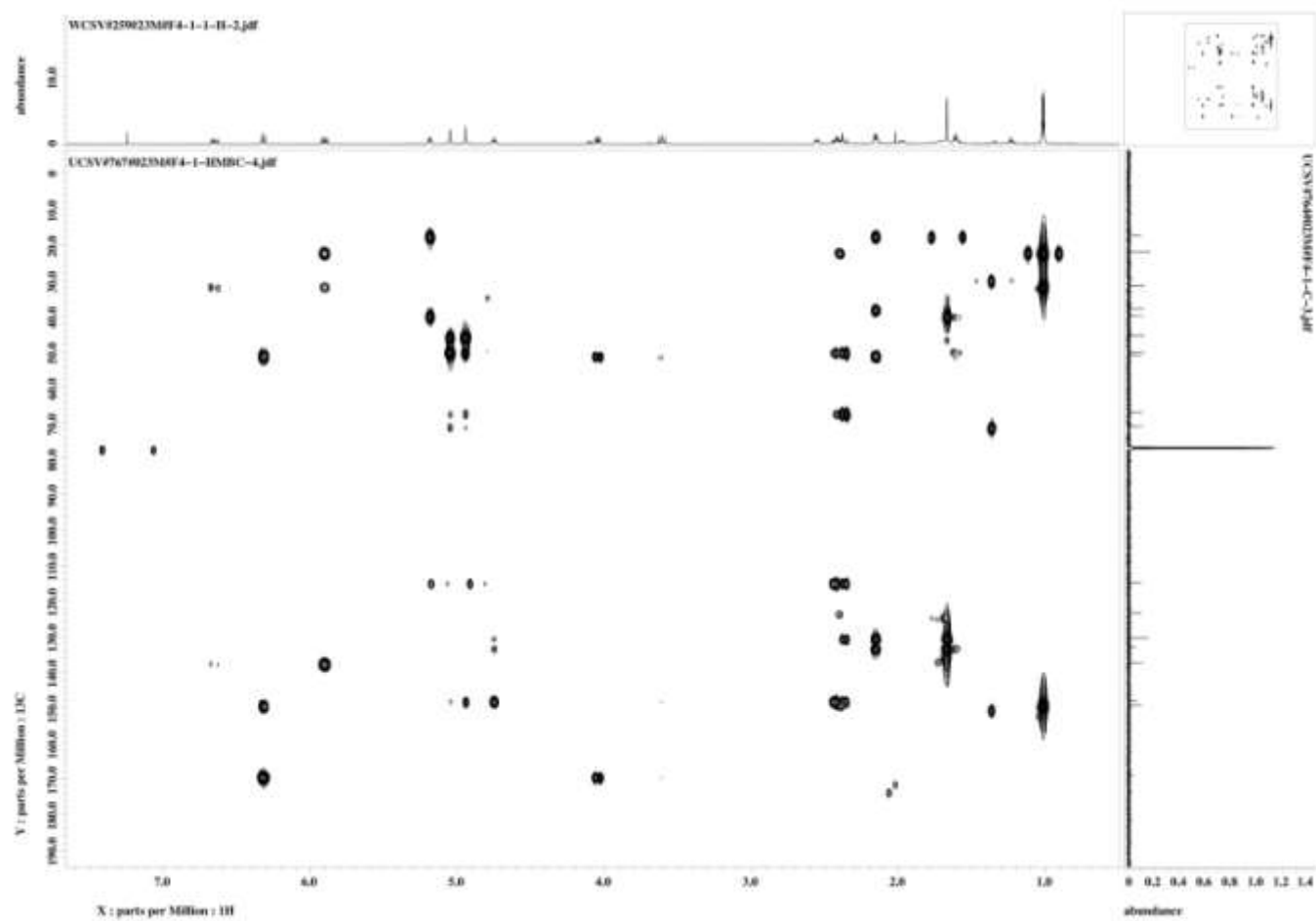


Figure S8. NOESY spectrum of 15-deoxy-isoxeniolide-A (1) in CDCl_3 .

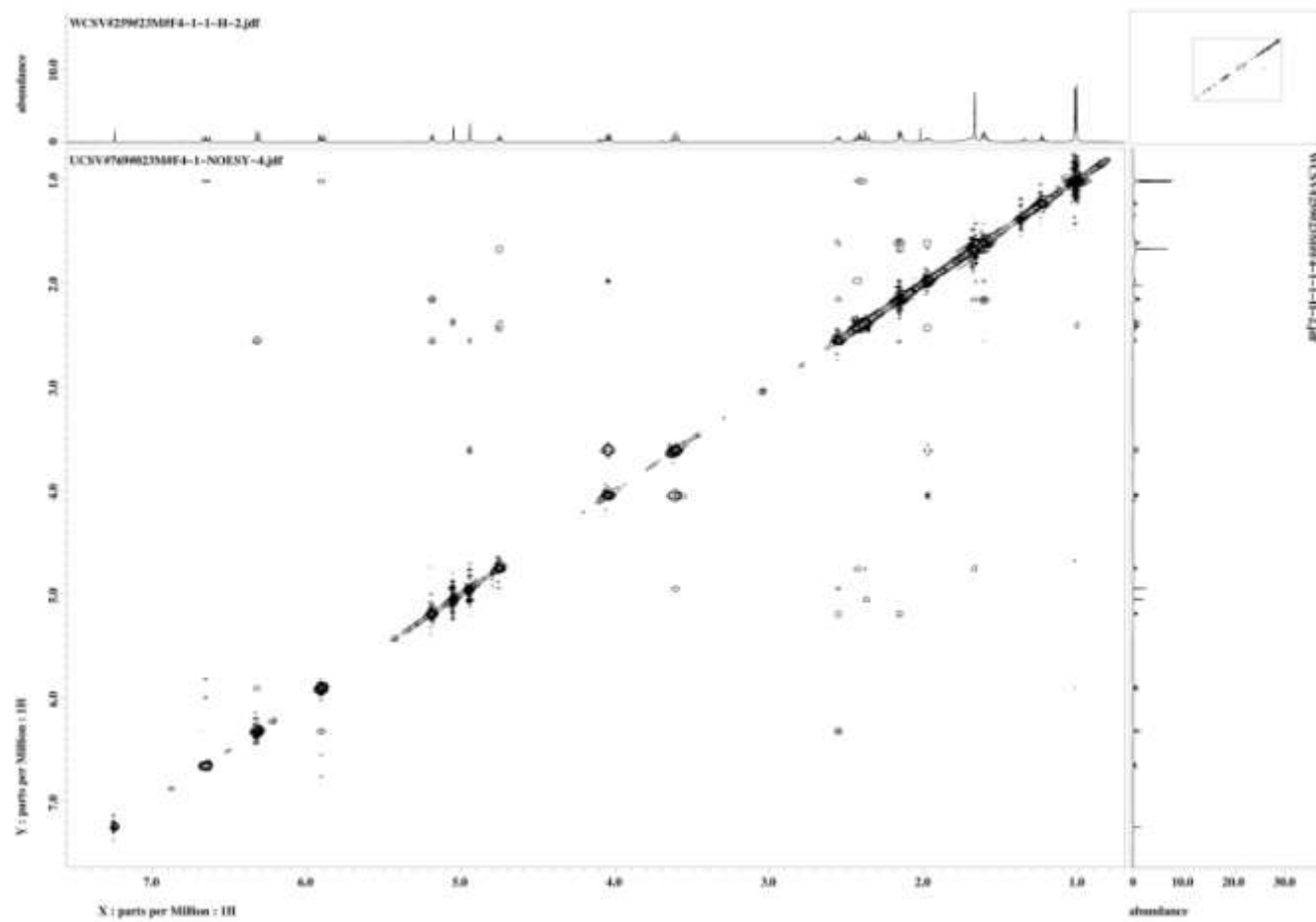


Figure S9. HRESIMS spectrum of 15-deoxy-isoxeniolide-A (1).

