SUPPLEMENTARY MATERIAL

12-*Epi*-9-deacetoxyxenicin, New Cytotoxic Diterpenoid from a Bornean Soft Coral, *Xenia* sp.

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One new compound, 12-*epi*-9-deacetoxyxenicin (**1**) along with a hydoperoxide product, 12-*epi*-9-deacetoxy-8-hydroperoxyxenicin (**2**) and two known sesquiterpenoids (**3**-**4**) were isolated from a population of Bornean soft coral *Xenia* sp. The structures of these metabolites were elucidated based on their spectroscopic data. Compounds **1** and **2** showed cytotoxic activity against ATL cell line, S1T. In addition, compound **3** exhibited hyphal inhibition of *Lagenidium thermophilum*.

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

Supplementary Information

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Figure S16. NOESY spectrum of **2** in $CDCl_3$.
Figure S17. HR-ESI-MS spectrum of **2**.

Table S1. ^{13}C and ^{1}H NMR (150 and 600 MHz) data of **1-2** ($CDCl_3$, δ in ppm, J in Hz).

	1		**2**	
No	δ_C	δ_H	δ_C	δ_H
1	91.5	5.85 d (1.8)	92.9	6.00 d (4.8)
3	137.4	6.39 br s	138.5	6.34 br s
4	113.4		111.8	
4α	37.7	2.00 m	33.8	2.29 m
5	29.6	1.95 m; 1.53 m	28.9	2.24 m; 1.83 m
6	40.1	2.26 m; 2.06 m	26.3	2.42 m; 2.26 m
7	135.9		145.9	
8	124.2	5.34 t (8.3)	89.6	4.42 dd (10.0, 5.1)
9	25.1	2.48 m; 2.09 m	27.1	2.05 m; 1.74 m
10	35.6	2.26 m	31.4	2.34 m; 2.17 m
11	151.1		146.6	
11a	49.2	1.95 m	40.8	2.68 t (4.8)
12	71.7	5.67 d (3.4)	71.3	5.60 d (3.4)
13	70.7	5.63 dd (9.6, 3.4)	70.6	5.57 dd (8.9, 3.4)
14	117.7	5.27 d (9.6)	117.4	5.20 d (9.2)
15	141.1		140.8	
16	25.8	1.75 s	25.8	1.74 s
17	18.8	1.72 s	18.7	1.67 s
18	16.8	1.66 s	118.7	5.42 s; 5.35 s
19	113.1	4.86 s; 4.77 s	112.7	4.93 s; 4.81 s
1-OAc	169.8		169.5	
	21.1	2.04 s	21.0	2.06 s
12-OAc	170.3		170.3	
	21.1	2.02 s	21.1	2.02 s
13-OAc	169.8		169.8	
	21.0	2.12 s	21.0	2.10 s

Table S2. MICs of compounds **1-4** against seven strains of marine fungi.

Strains	MIC (μg/mL)			
	1	**2**	**3**	**4**
F. moniliforme	100	100	100	100
F. oxysporum	100	100	100	100
F. solani	100	100	100	100
Exophiala sp.	50	50	50	50
O. humicola	100	100	100	100
L. thermophilum	50	50	25	50
H. sabahensis	50	50	50	50

Positive control: itraconazole with MIC 3.2 μg/mL.

Figure S2. The ^{1}H-^{1}H COSY and selective HMBC correlations of **1**.

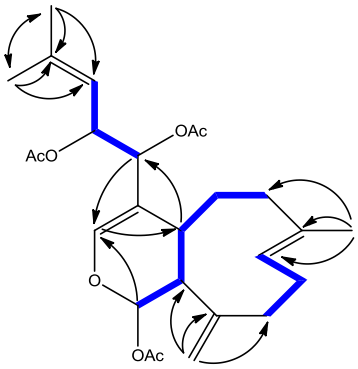


Figure S3. The summary of diastereomeric xenicins with relative configurations β-OAc/α-OAc, α-OAc/β-OAc and α-OAc/α-OAc at C-12/C-13.

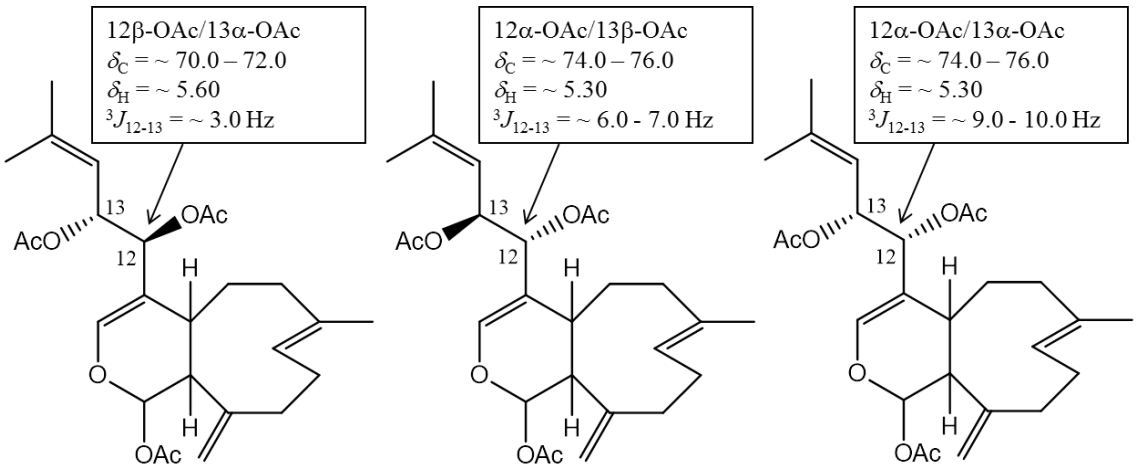


Figure S4. ^{1}H NMR spectrum of **1** in $CDCl_3$ (600 MHz).

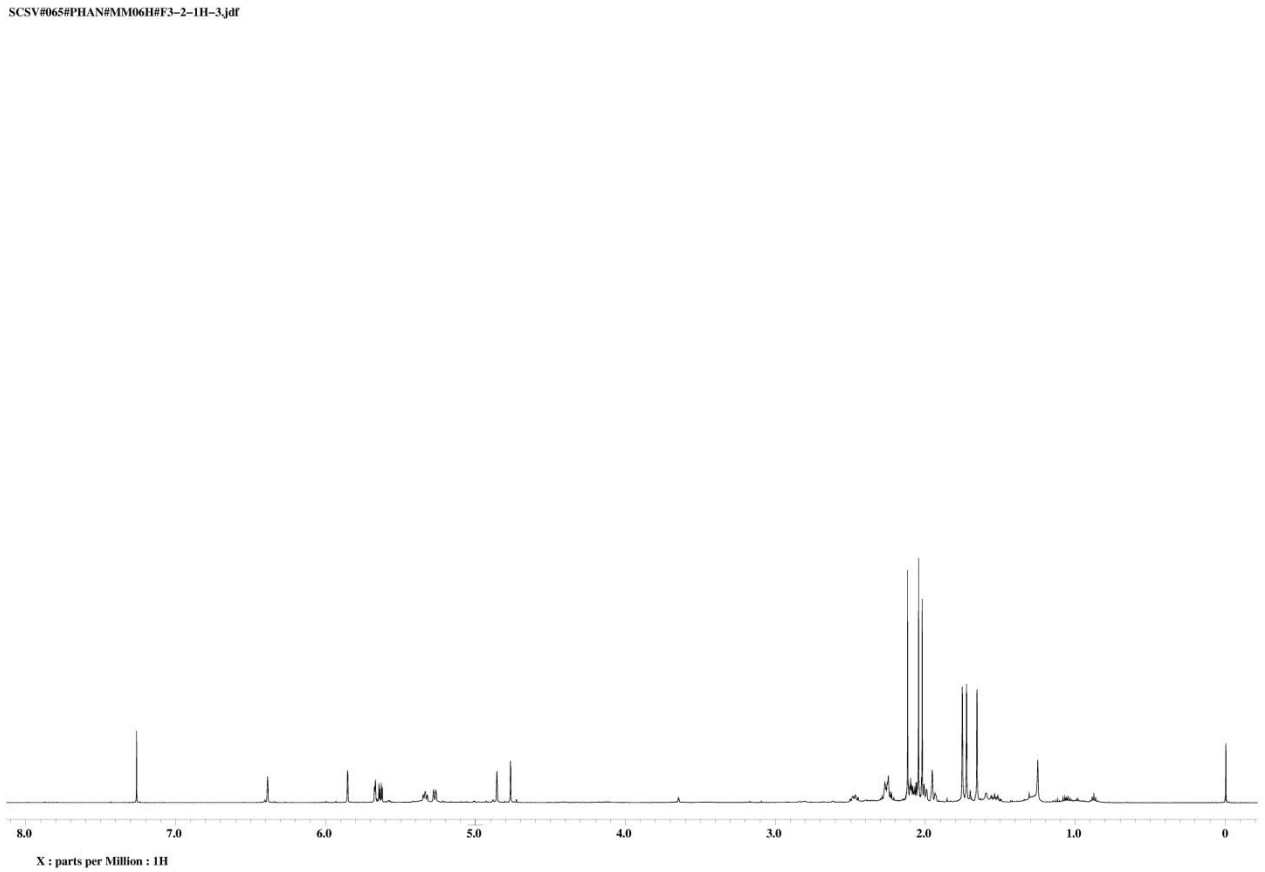


Figure S5. ^{13}C NMR spectrum of **1** in $CDCl_3$ (150 MHz).

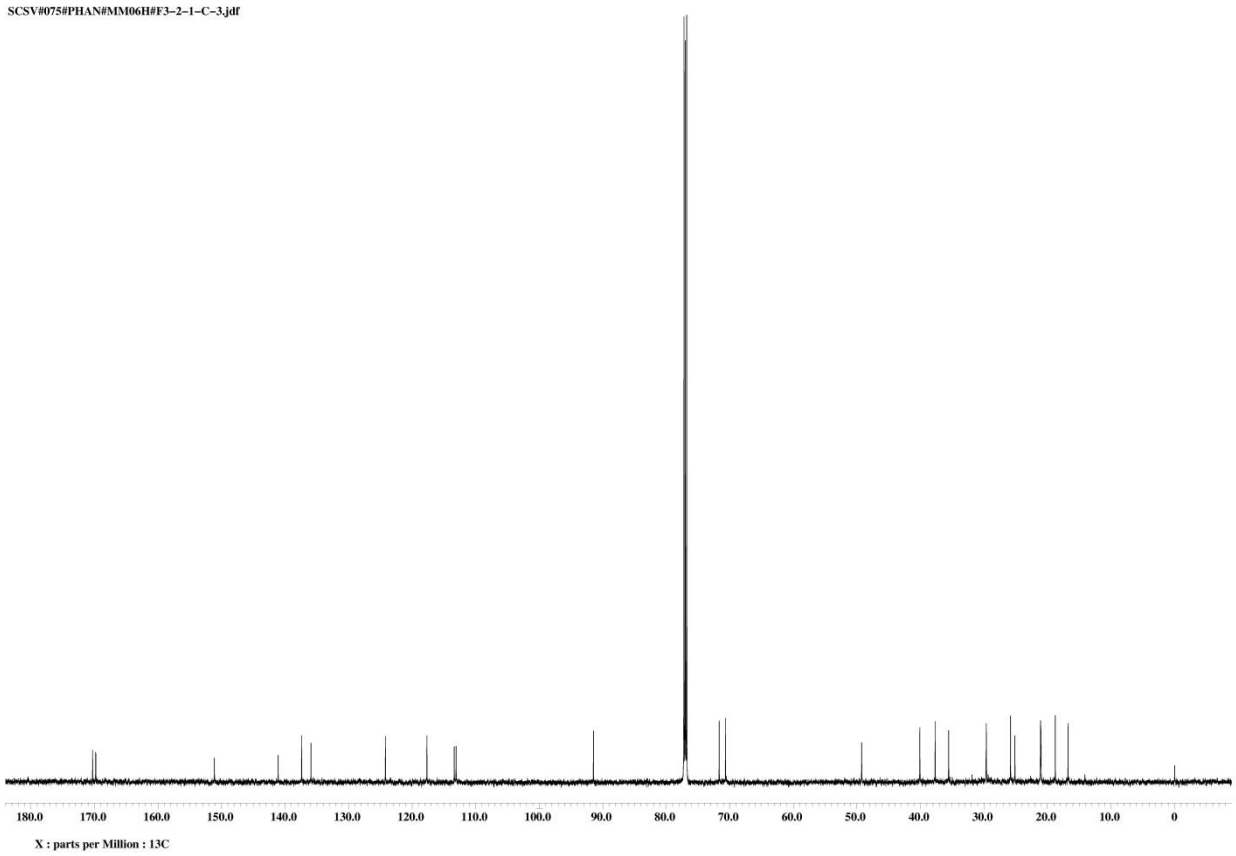


Figure S6. HSQC spectrum of **1** in $CDCl_3$.

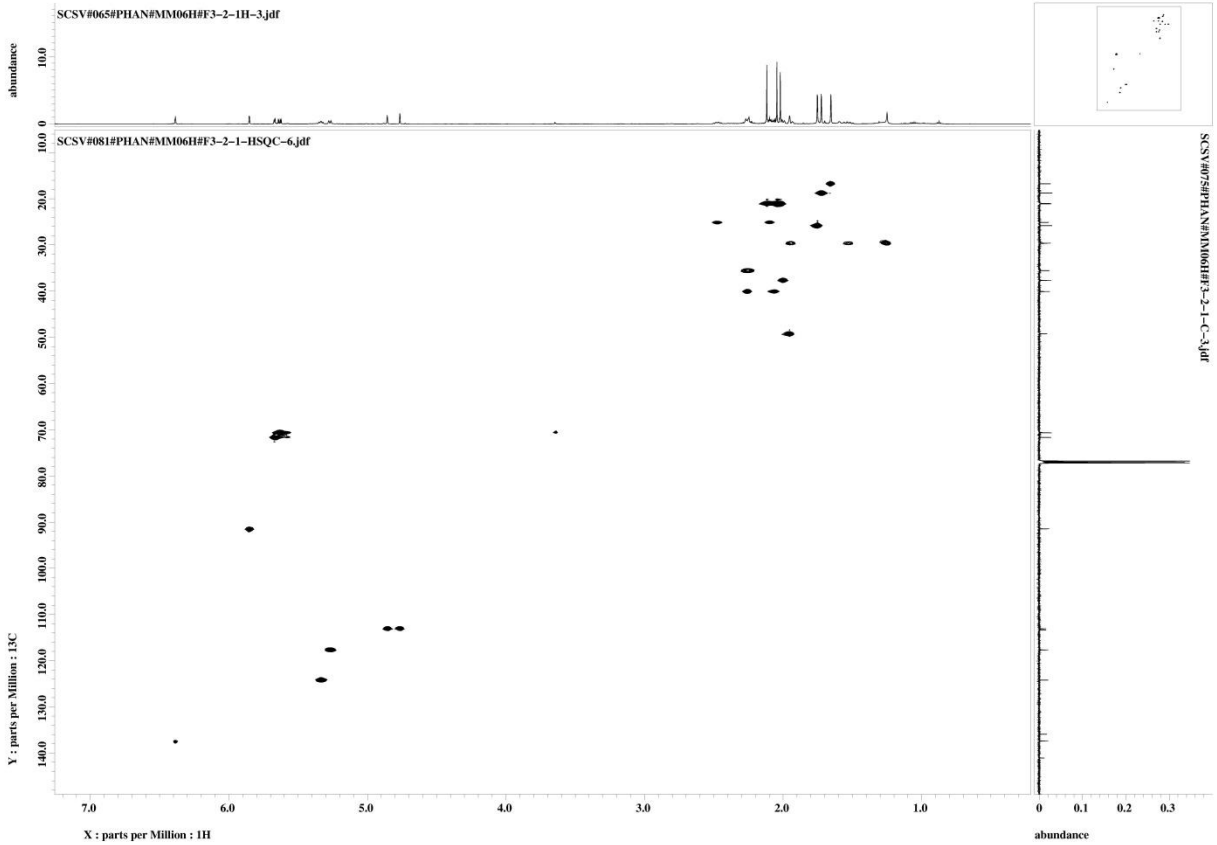


Figure S7. ^{1}H-^{1}H COSY spectrum of **1** in $CDCl_3$.

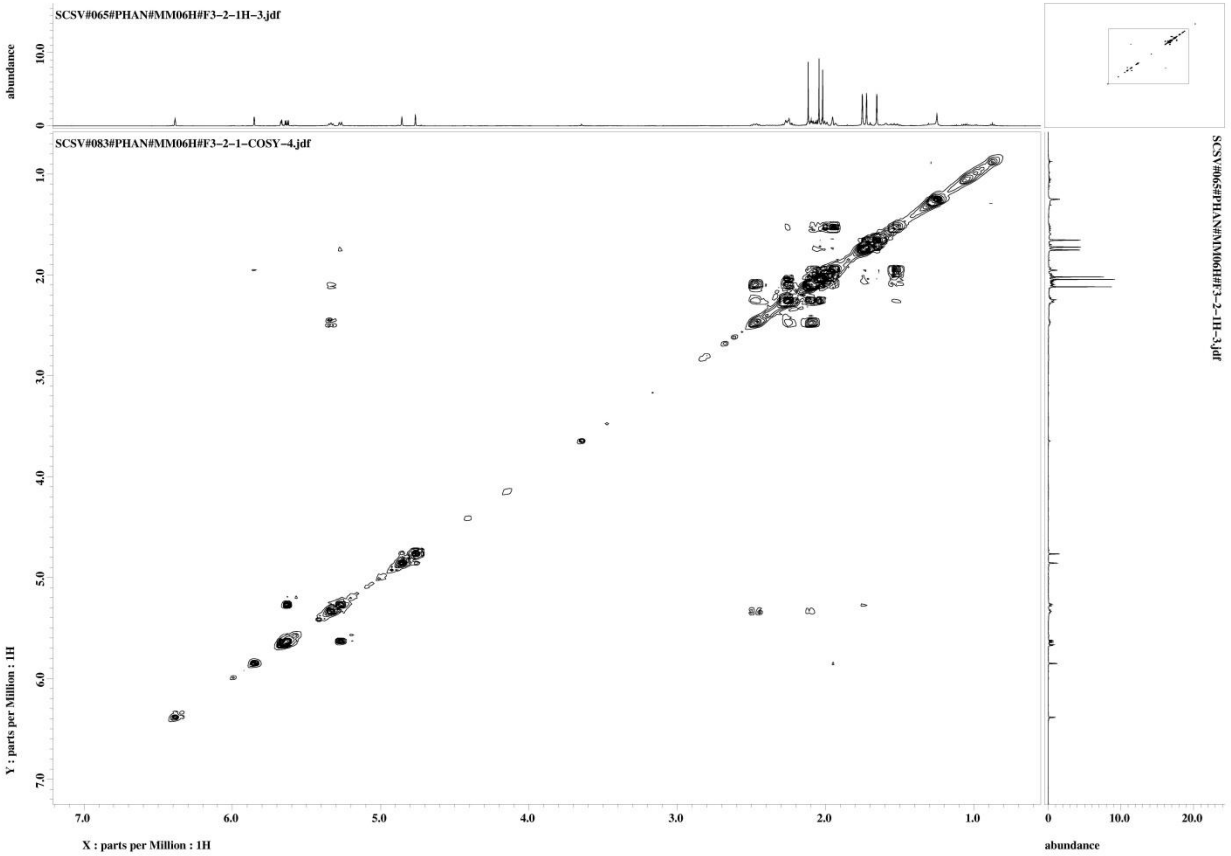


Figure S8. HMBC spectrum of **1** in $CDCl_3$.

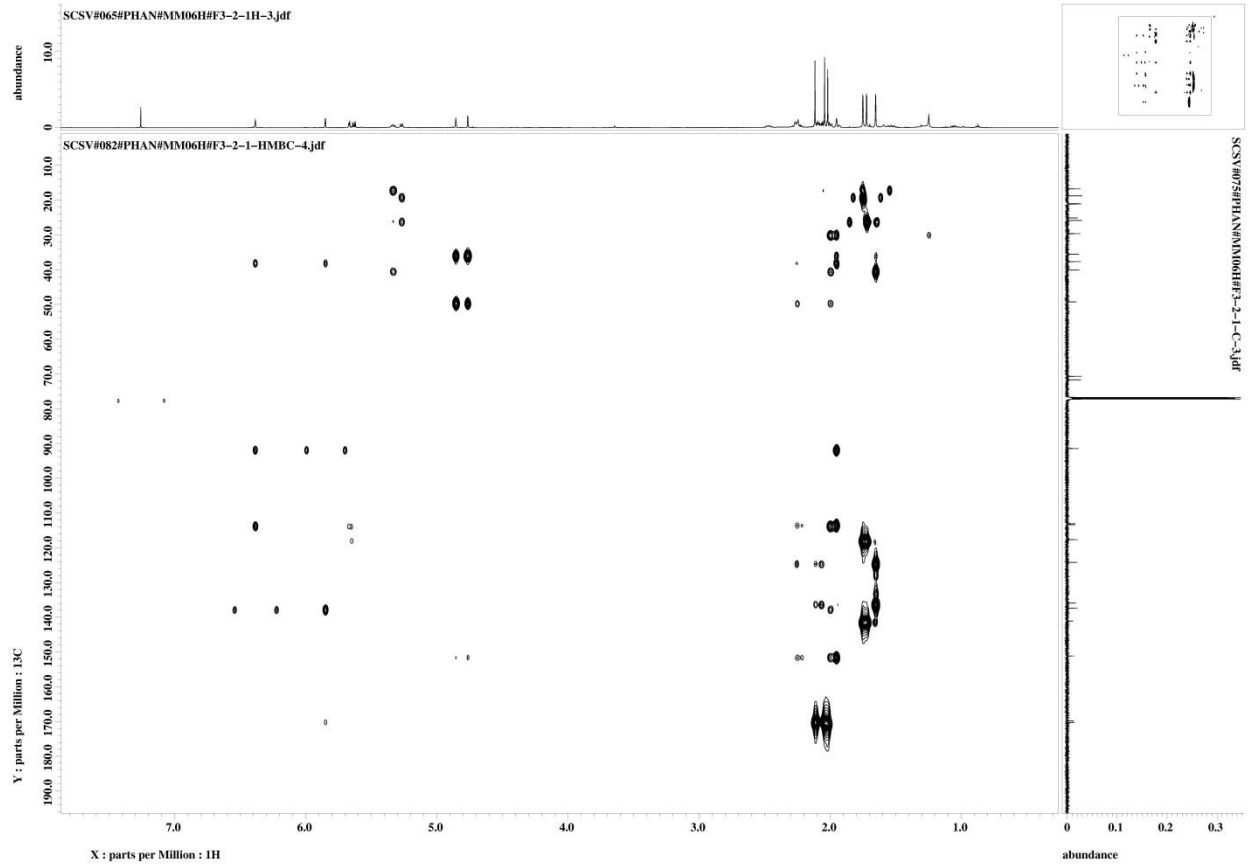


Figure S9. NOESY spectrum of **1** in $CDCl_3$.

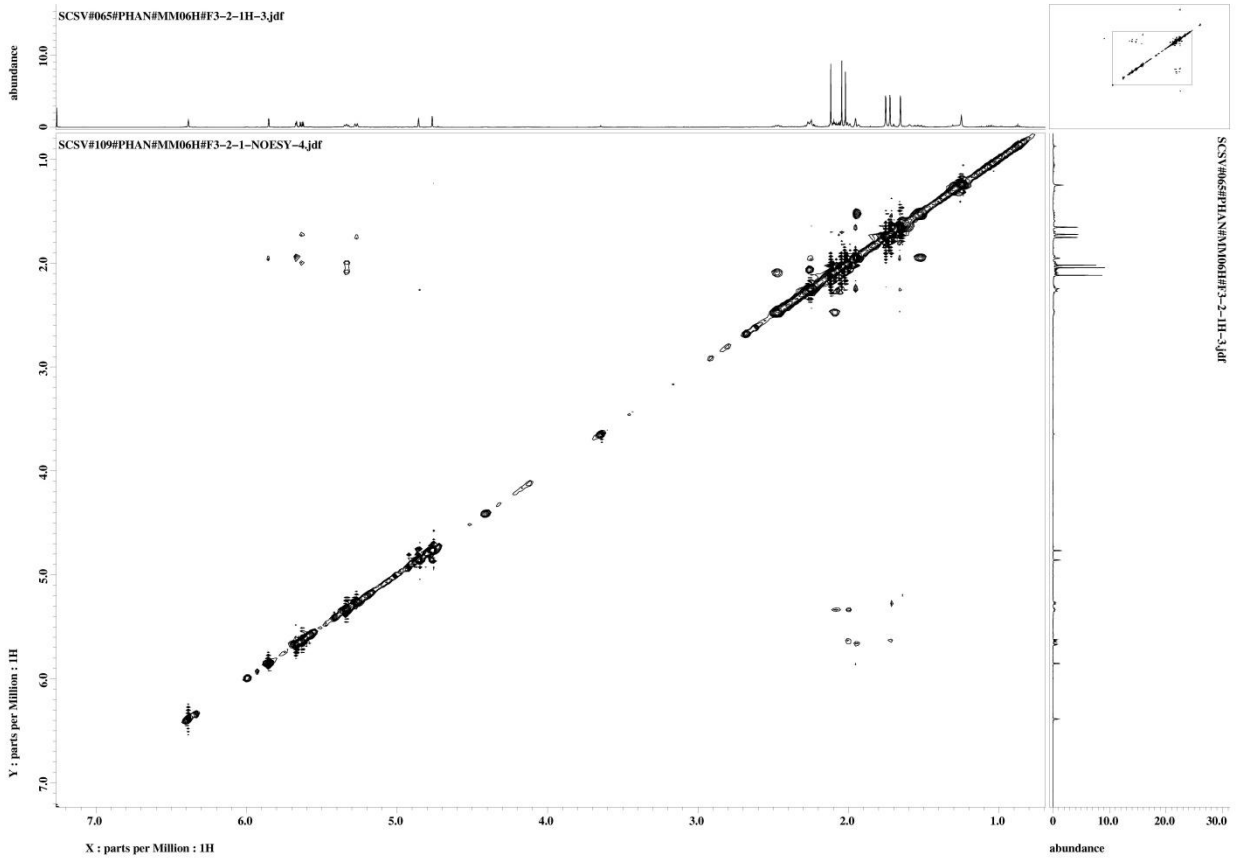
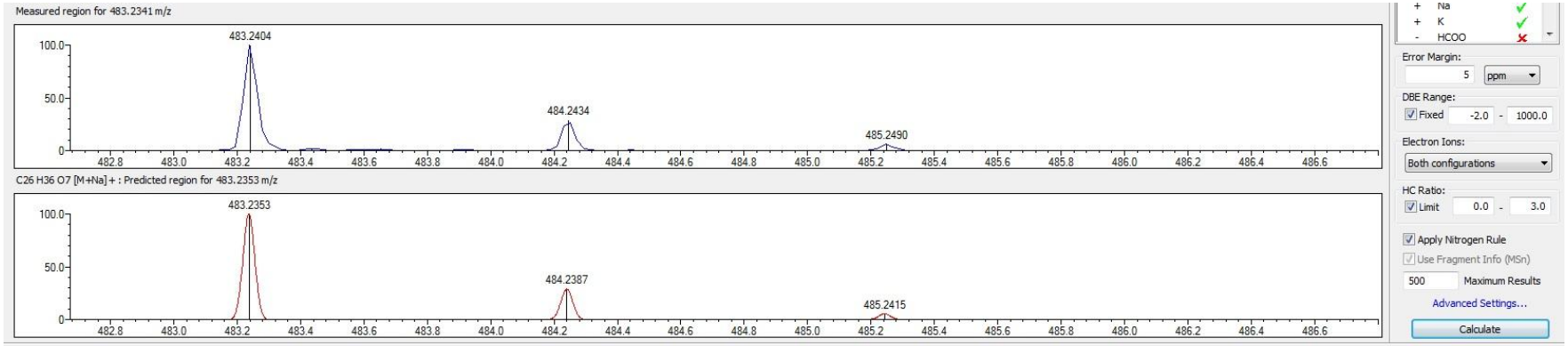


Figure S10. HRESIMS spectrum of **1**.



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	83.19	C26 H36 O7	[M+Na]+	483.2341	483.2353	-1.2	-2.48	86.39	9.0
2	73.22	C23 H34 N2 O9	[M+H]+	483.2341	483.2337	0.4	0.83	73.22	8.0
3	73.22	C23 H31 N O9	[M+NH4]+	483.2341	483.2337	0.4	0.83	73.22	9.0
4	56.84	C23 H40 O8	[M+K]+	483.2341	483.2355	-1.4	-2.90	59.68	4.0
5	40.03	C35 H30 O2	[M+H]+	483.2341	483.2319	2.2	4.55	43.92	21.0

Figure S11. ^{1}H NMR spectrum of **2** in $CDCl_3$ (600 MHz).

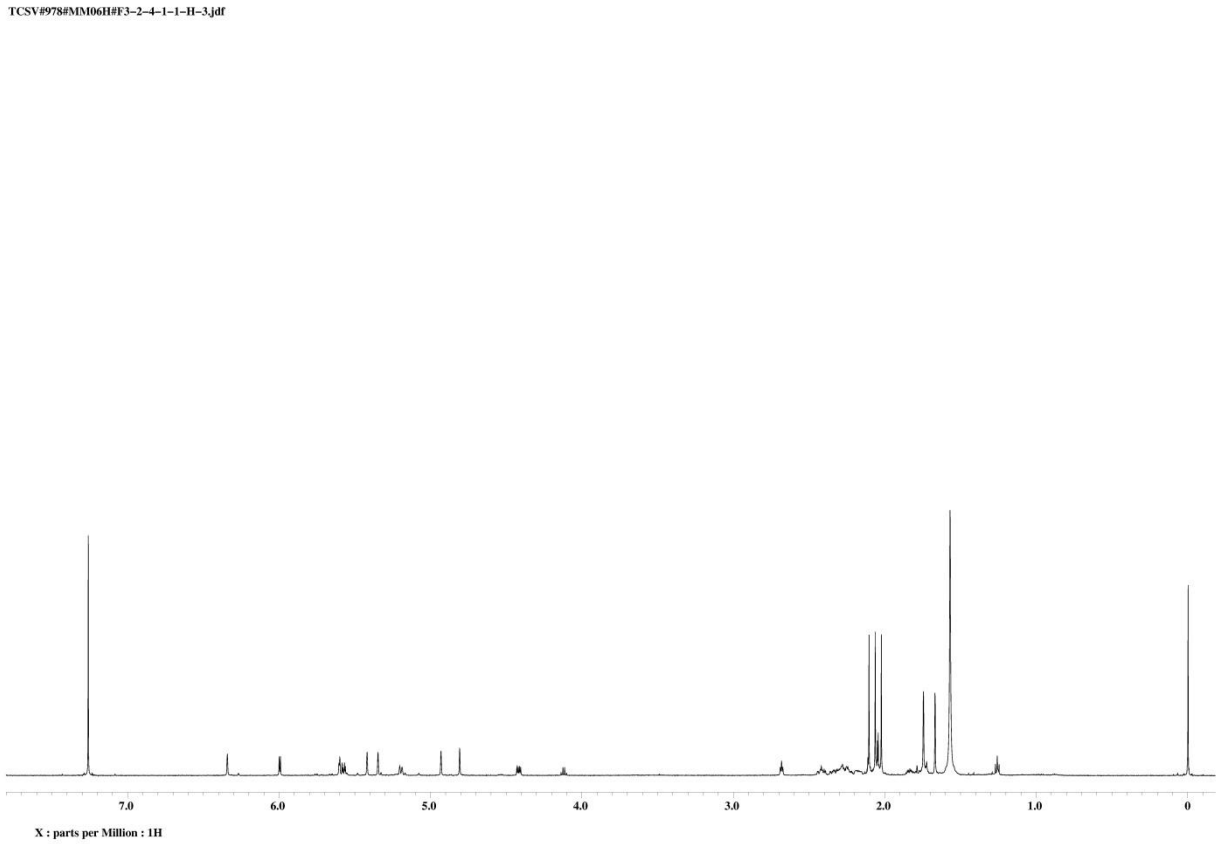


Figure S12. ^{13}C NMR spectrum of **2** in $CDCl_3$ (150 MHz).

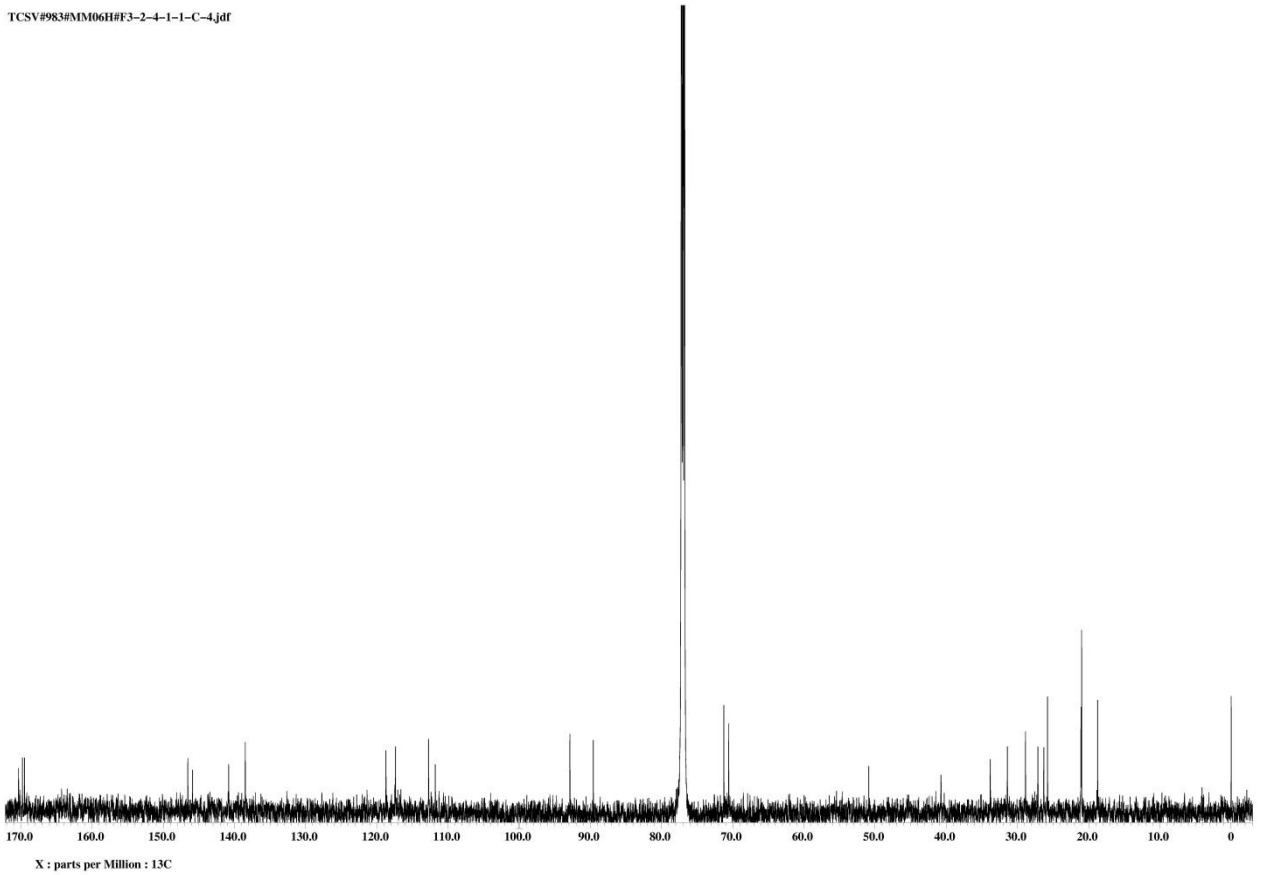


Figure S13. HSQC spectrum of **2** in $CDCl_3$.

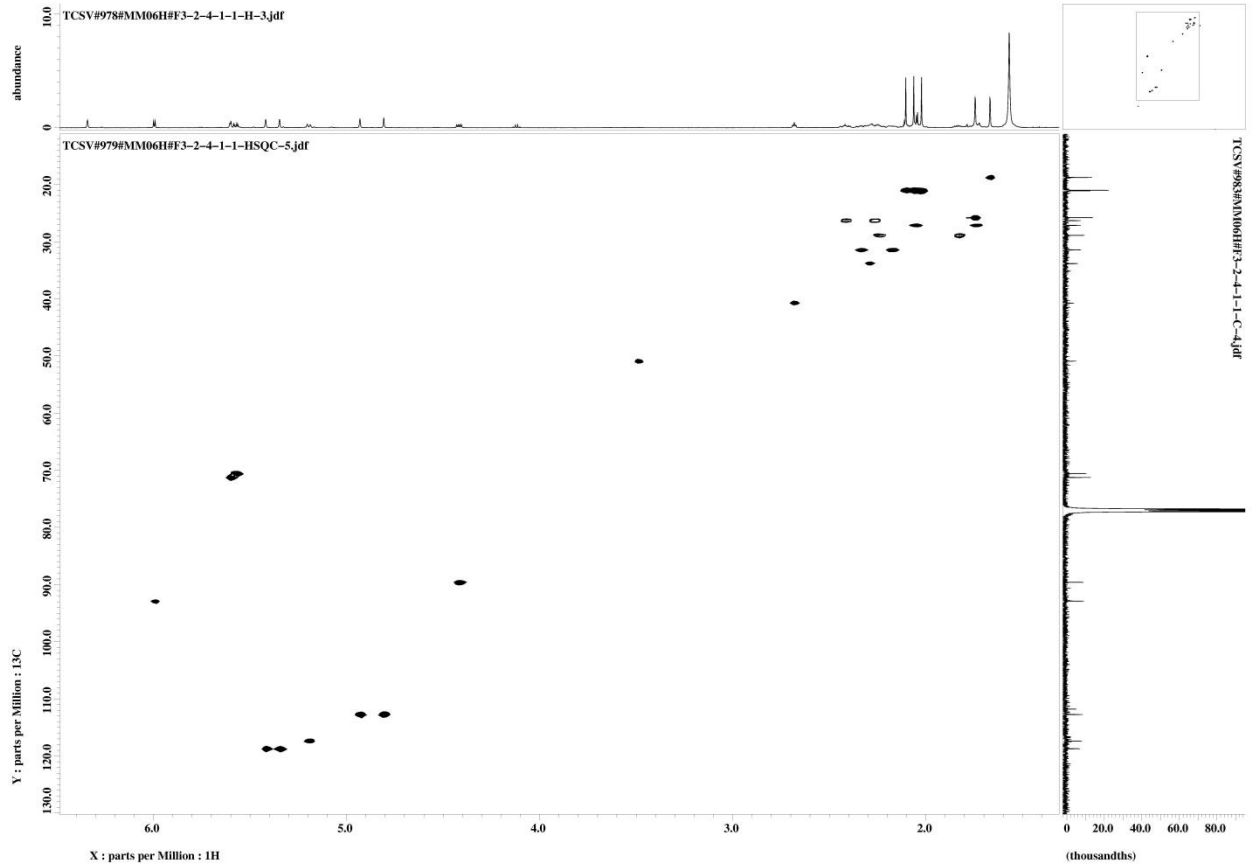


Figure S14. ^{1}H-^{1}H COSY spectrum of **2** in $CDCl_3$.

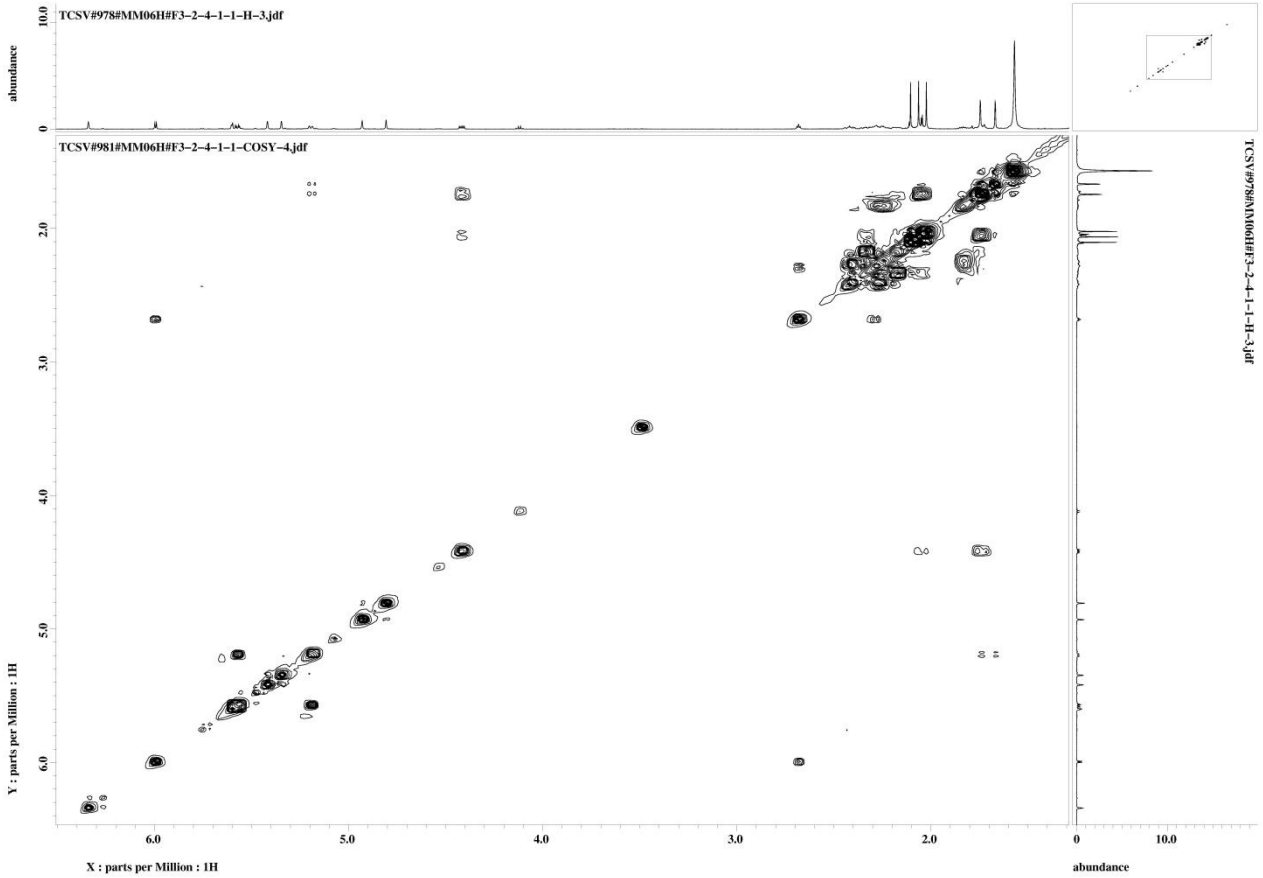


Figure S15. HMBC spectrum of **2** in $CDCl_3$.

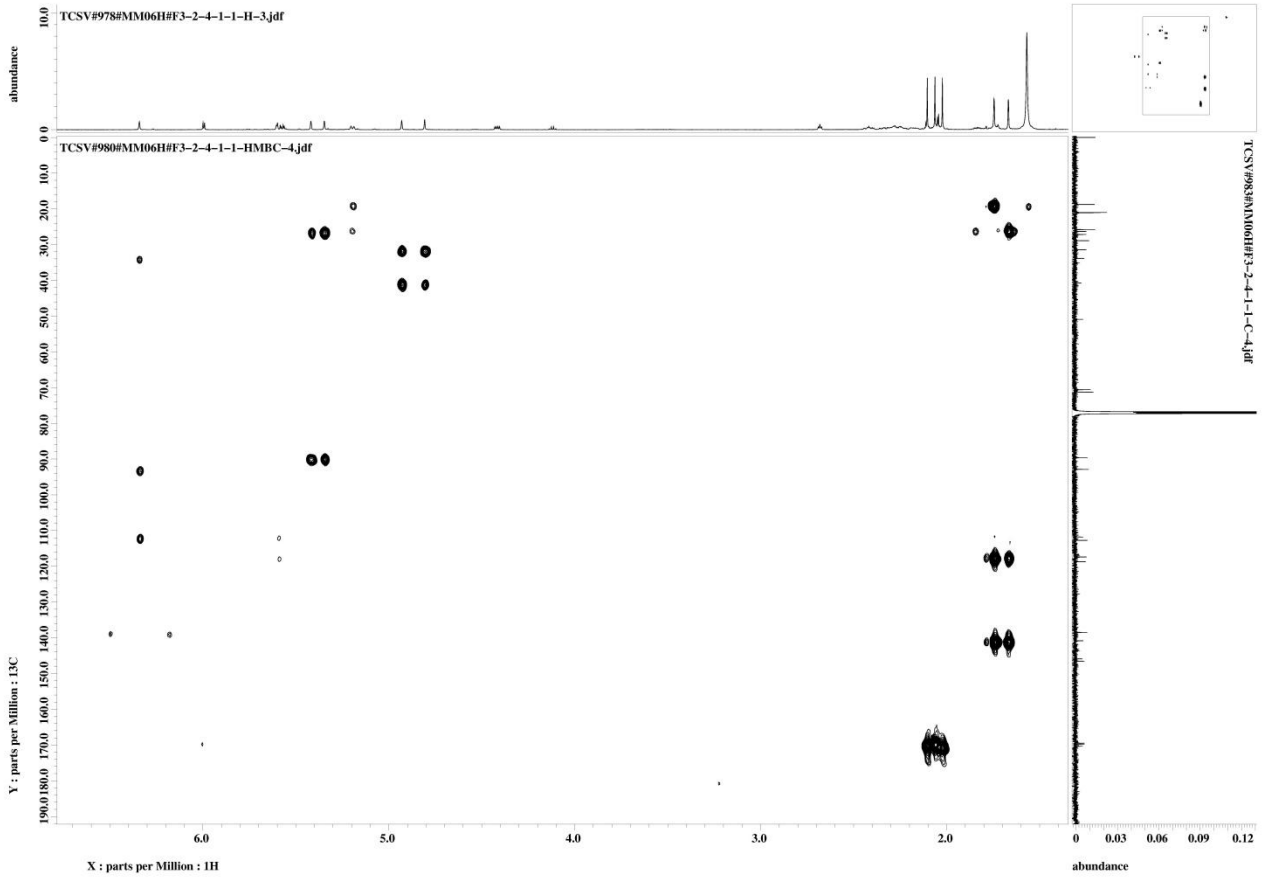


Figure S16. NOESY spectrum of **2** in $CDCl_3$.

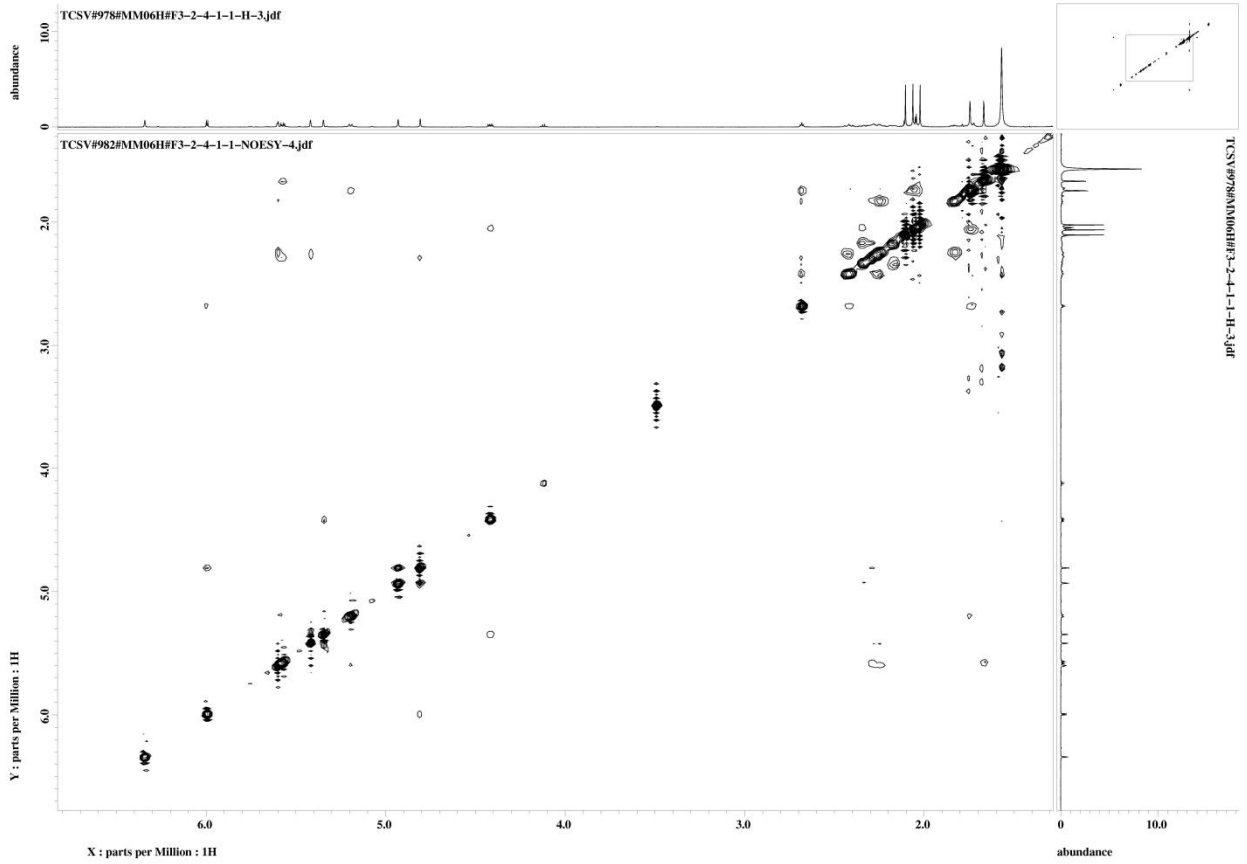
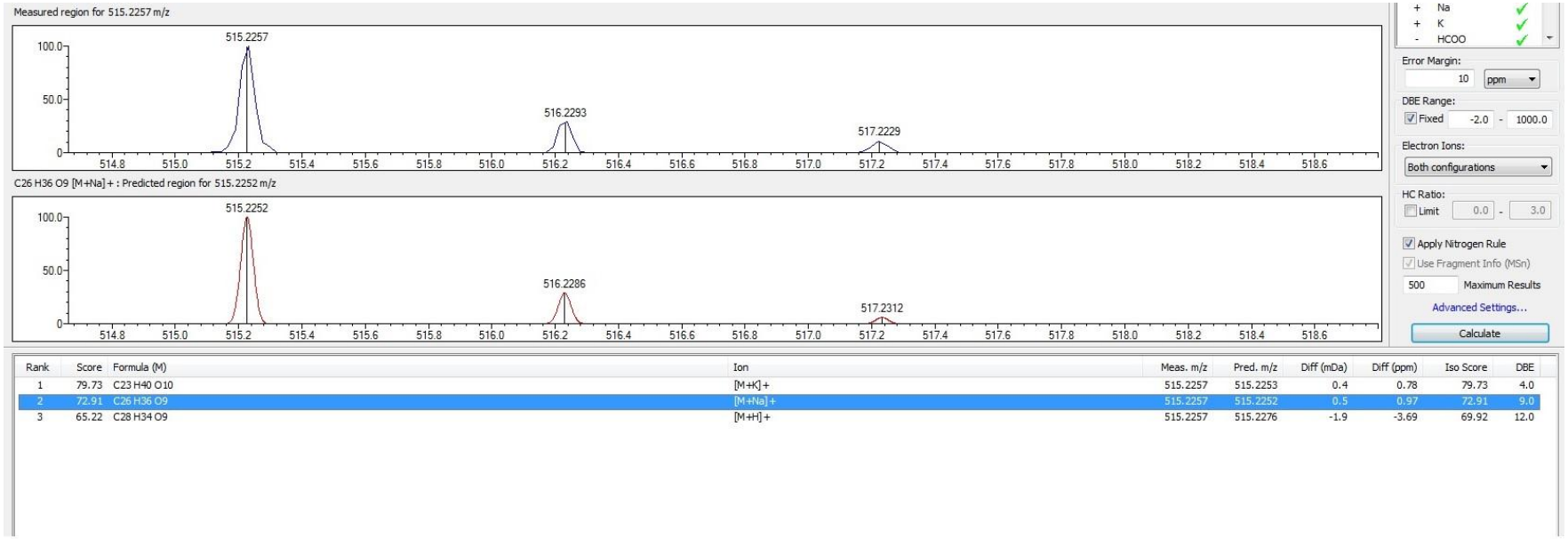


Figure S17. HRESIMS spectrum of **2**.



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff (mDa)	Diff (ppm)	Iso Score	DBE
1	79.73	C23 H40 O10	[M+K]+	515.2257	515.2253	0.4	0.78	79.73	4.0
2	72.91	C26 H36 O9	[M+Na]+	515.2257	515.2252	0.5	0.97	72.91	9.0
3	65.22	C28 H34 O9	[M+H]+	515.2257	515.2276	-1.9	-3.69	69.92	12.0