

SUPPLEMENTARY MATERIAL

A new sesquiterpene from the gorgonian coral *Menella* sp.

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A new sesquiterpene from the gorgonian coral *Menella* sp.

A new sesquiterpene named menecubebane B (**1**) and a known analogue (**2**) were isolated from the gorgonian coral *Menella* sp.. Their structures were elucidated by the extensive analyses of spectroscopic data, and by the comparison with related literature. Cytotoxic effect against both Eca9706 and HeLa cell lines was evaluated, revealing **1** exhibited moderate cytotoxicity against the two cell lines involved with IC₅₀ values being 20.8 and 30.6 μ M, respectively.

Keywords: Gorgonian coral; *Menella* sp.; sesquiterpene; cytotoxicity

Table S1: ^1H (500 MHz), ^{13}C (125 MHz) data of compound **1** in CD_3OD

No.	1	
	δ_{C} (mult.)	δ_{H} (mult., J in Hz)
1	160.5 (C)	
2	63.8 (CH)	4.94 (ddd, $J = 5.0, 4.5, 2.0$ Hz)
3	46.2 (CH_2)	2.19 (dd, $J = 14.0, 4.5$ Hz)
		2.11 (dd, $J = 14.0, 5.0$ Hz)
4	73.2 (C)	
5	204.1 (C)	
6	136.0 (C)	
7	39.0 (CH)	2.75 (m)
8	19.5 (CH_2)	1.74 (m), 1.56 (m)
9	38.4 (CH_2)	1.82 (m), 1.58 (m)
10	72.2 (C)	
11	29.9 (CH)	2.06 (m)
12	17.8 (CH_3)	0.75 (d, $J = 6.5$ Hz)
13	21.0 (CH_3)	0.89 (d, $J = 6.5$ Hz)
14	28.5 (CH_3)	1.50 (s)
15	27.5 (CH_3)	1.46 (s)

Figure legends

Figure S1. Key ^1H - ^1H COSY and HMBC correlations of **1**

Figure S2. Key NOESY correlations of **1**

Figure S3. ^1H NMR (500 MHz, CD_3OD) of **1**

Figure S4. ^{13}C NMR (125 MHz, CD_3OD) of **1**

Figure S5. COSY (500 MHz, CD_3OD) of **1**

Figure S6. HSQC (500 MHz, CD_3OD) of **1**

Figure S7. HMBC (500 MHz, CD_3OD) of **1**

Figure S8. NOESY (500 MHz, CD_3OD) of **1**

Figure S9. HRMS of **1**

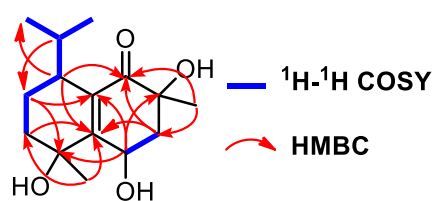


Figure S1. Key ^1H - ^1H COSY and HMBC correlations of **1**

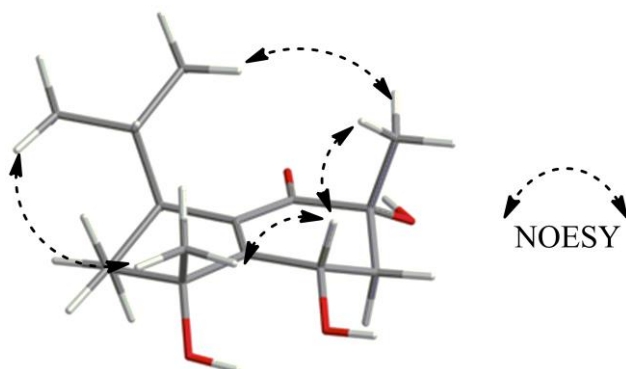


Figure S2. Key NOESY correlations of **1**

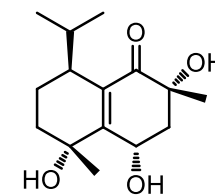
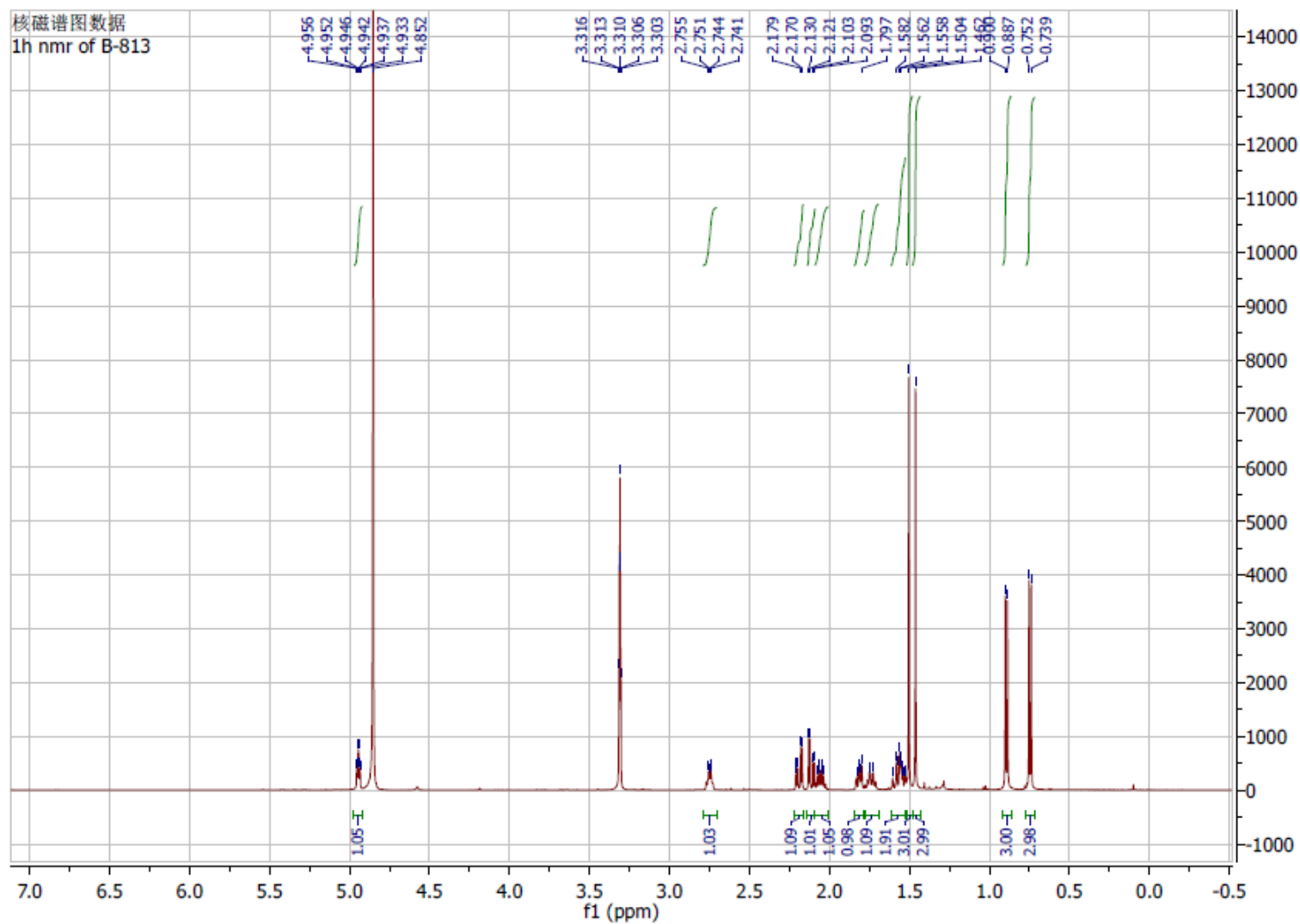


Figure S3. ^1H NMR (500 MHz, CD_3OD) of compound **1**.

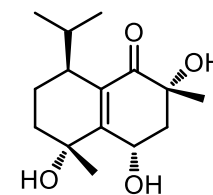
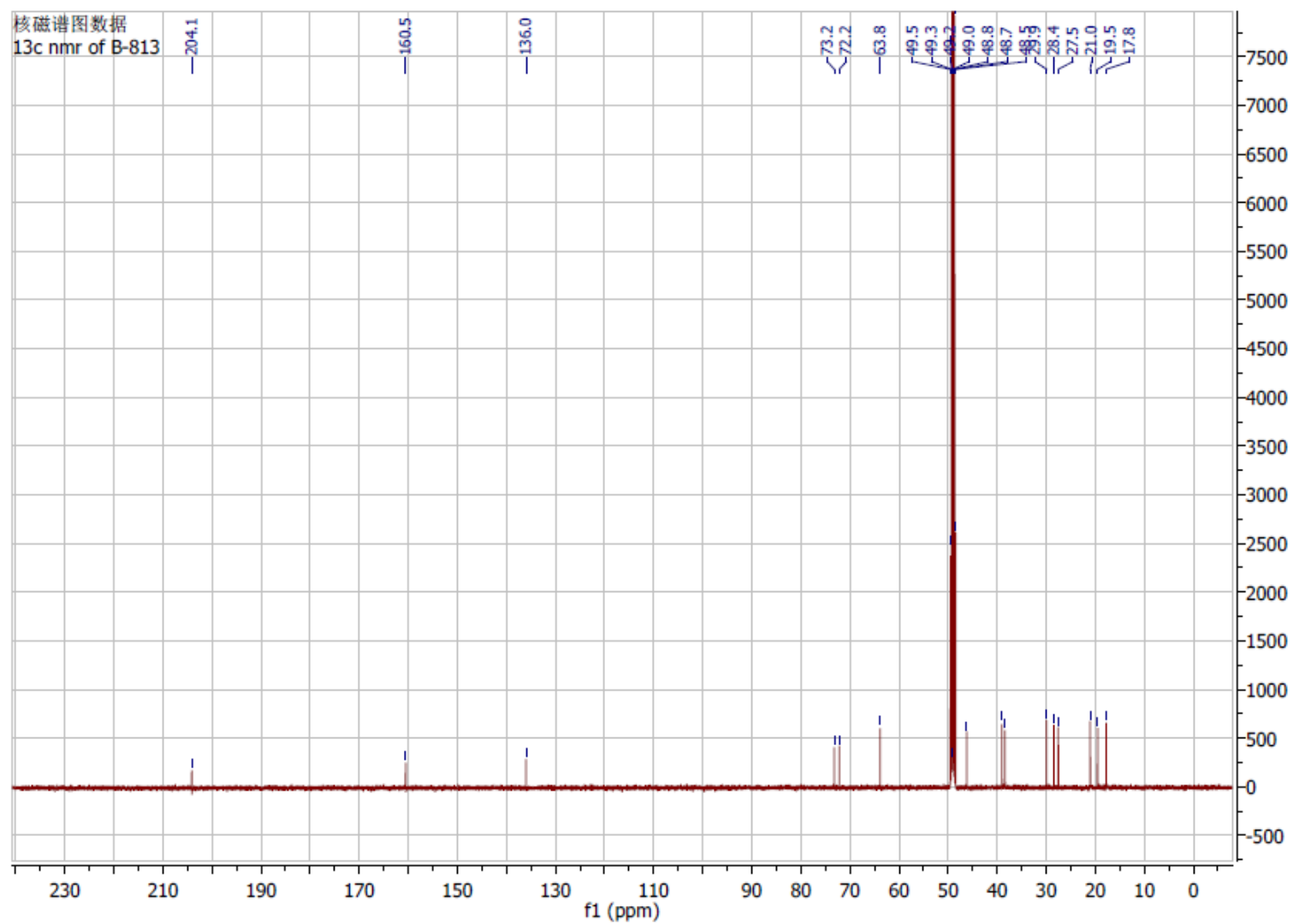


Figure S4. ^{13}C NMR (125 MHz, CD_3OD) of compound **1**.

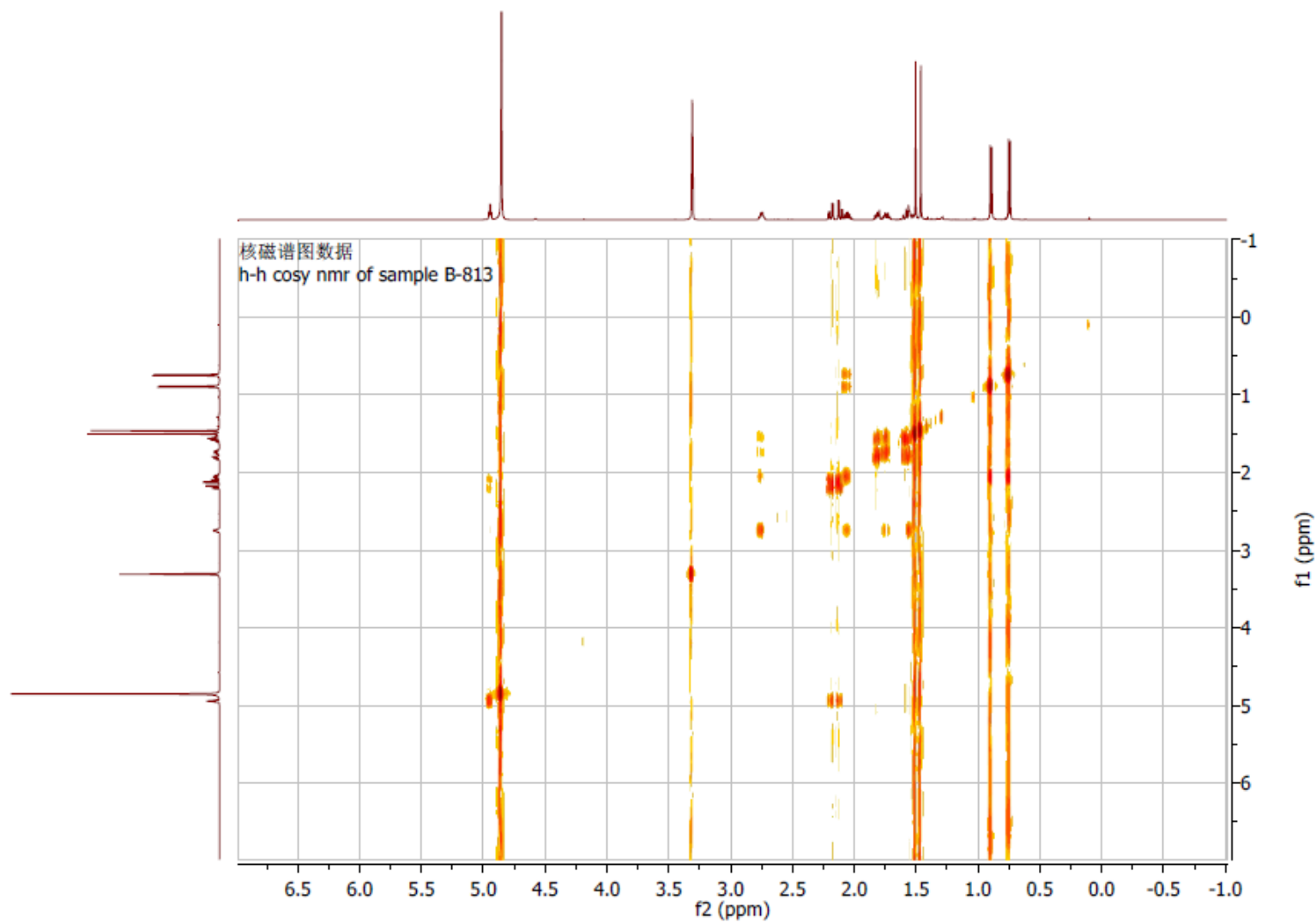
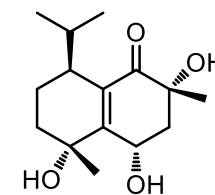


Figure S5. ^1H - ^1H COSY (500 MHz, CD_3OD) of compound **1**.

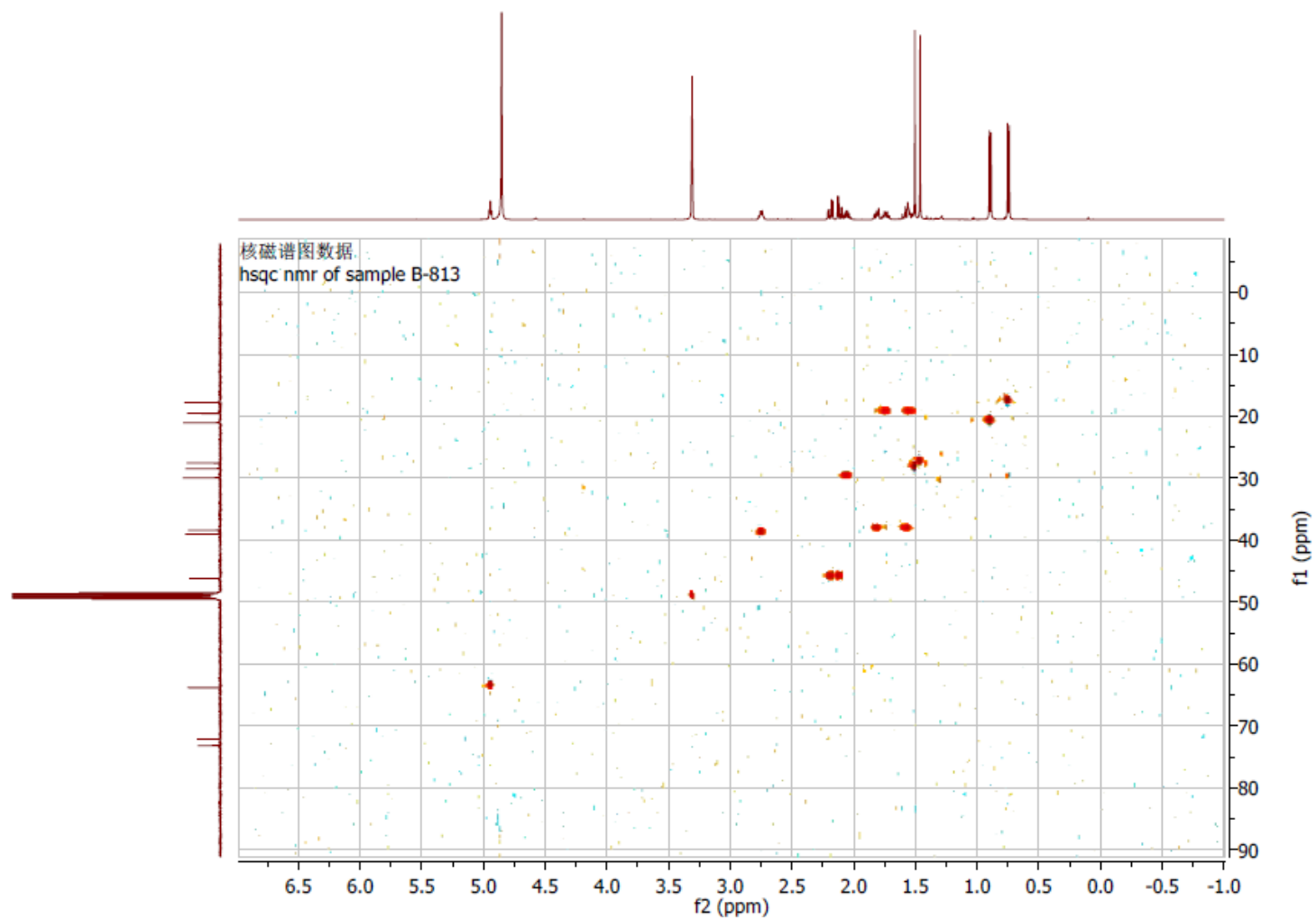
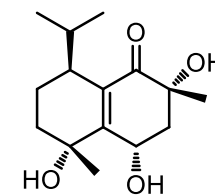


Figure S6. HSQC (500 MHz, CD₃OD) of compound **1**.

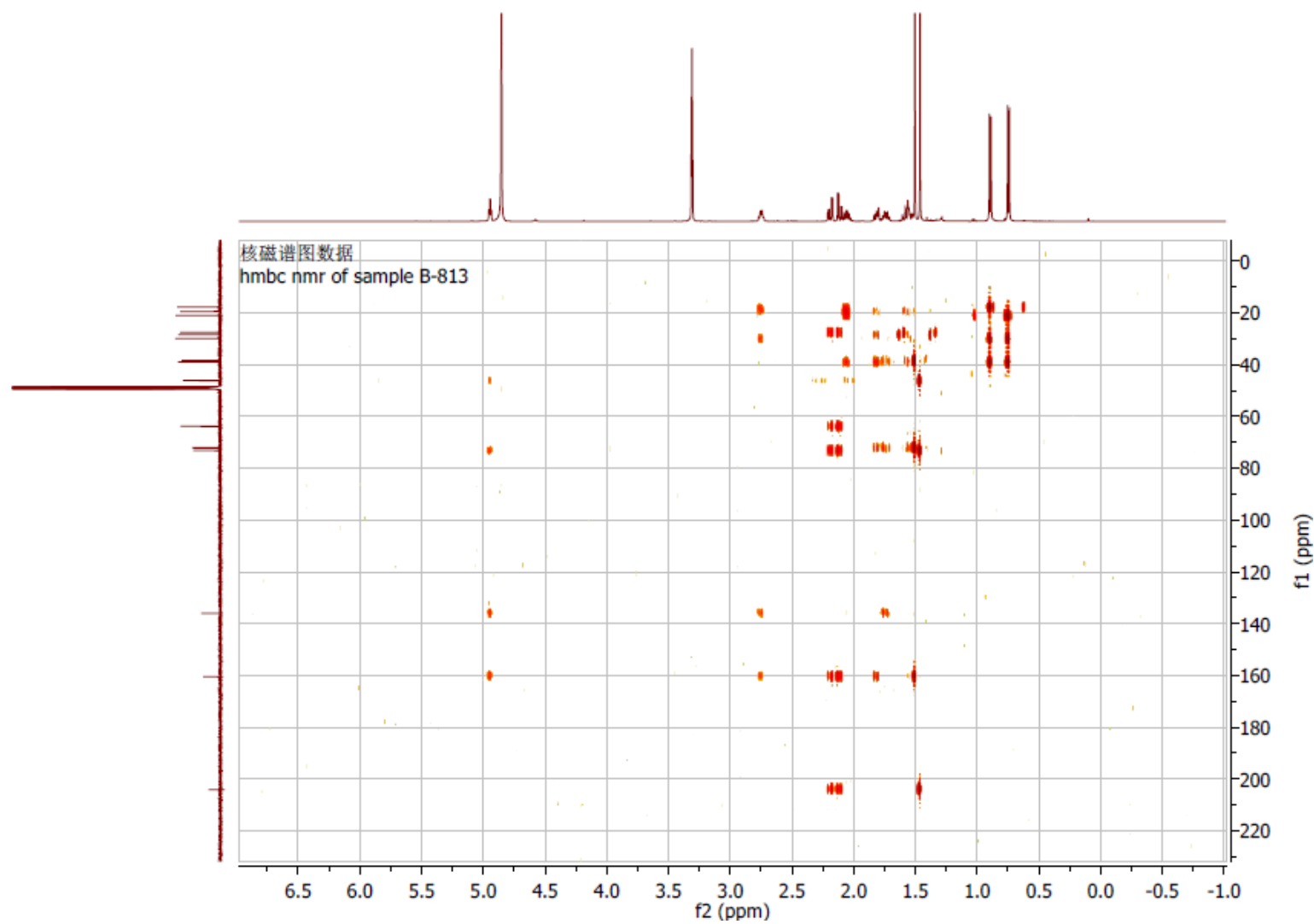
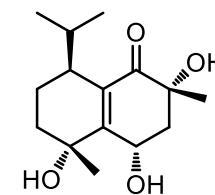


Figure S7. HMBC (500 MHz, CD₃OD) of compound **1**

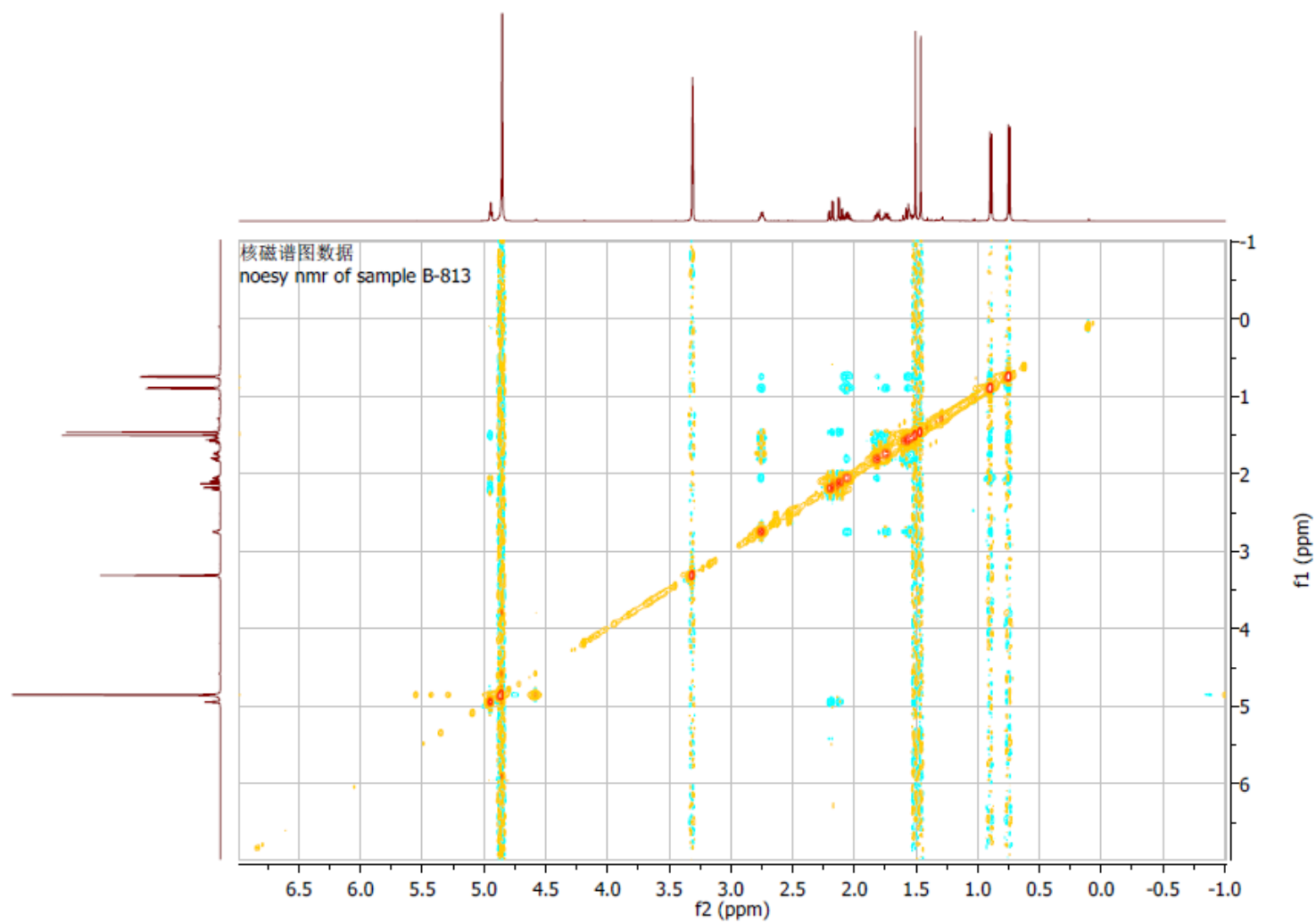
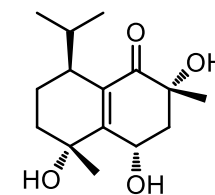
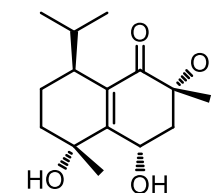


Figure S8. NOESY (500 MHz, CD₃OD) of compound **1**

Summary

✓✓✓✓✓	Compound Name (Library Hit)	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Purity (%)
✓ ● ● ● ●	268.16745952 (No Match)	C ₁₅ H ₂₄ O ₄	609825	50	267.1602	267.1598	-1.3	0.00	5.08	5.08	1.4%	0.0%



● Spectrum from Sample813.wiff (sample 1) - Sample813, Experiment 1, -TOF MS (100 - 1000) from 5.133 to 5.155 min
 ● C₁₅H₂₄O₄ -H

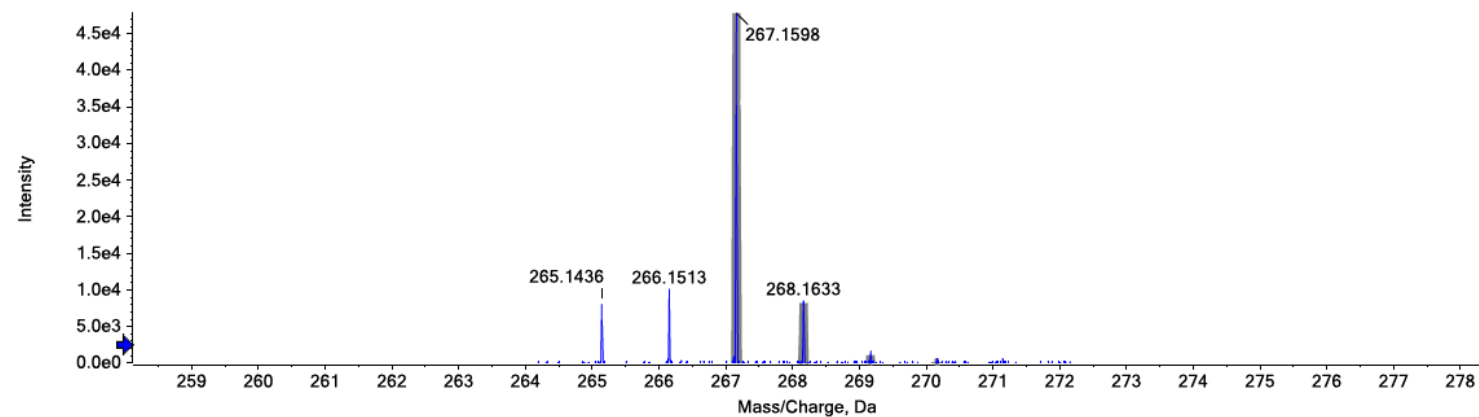


Figure S9. HRMS of compound **1**.