

Supporting Information

New Marine Sterols from a Gorgonian *Pinnigorgia* sp.

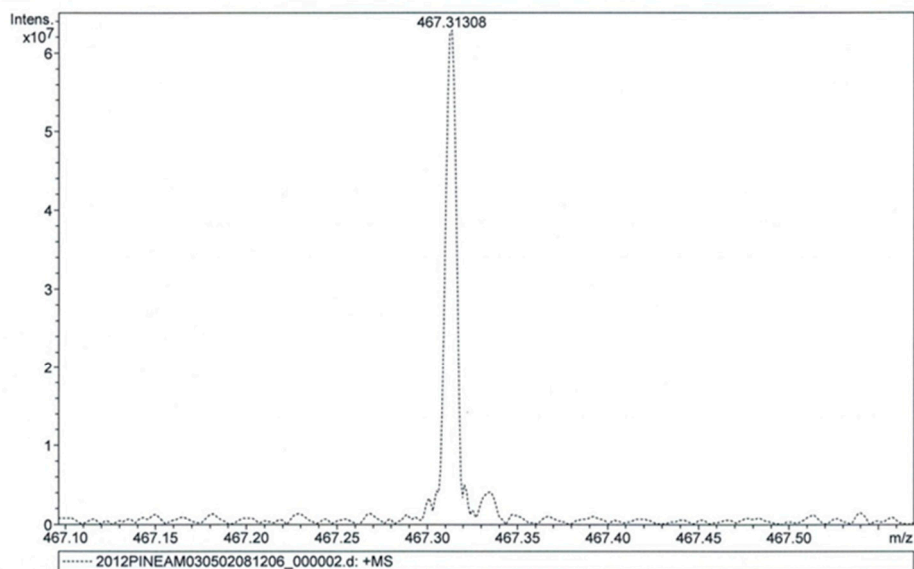
Yu-Chia Chang , Tsong-Long Hwang , Chih-Hua Chao , Ping-Jyun Sung *

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Mass Spectrum SmartFormula Report

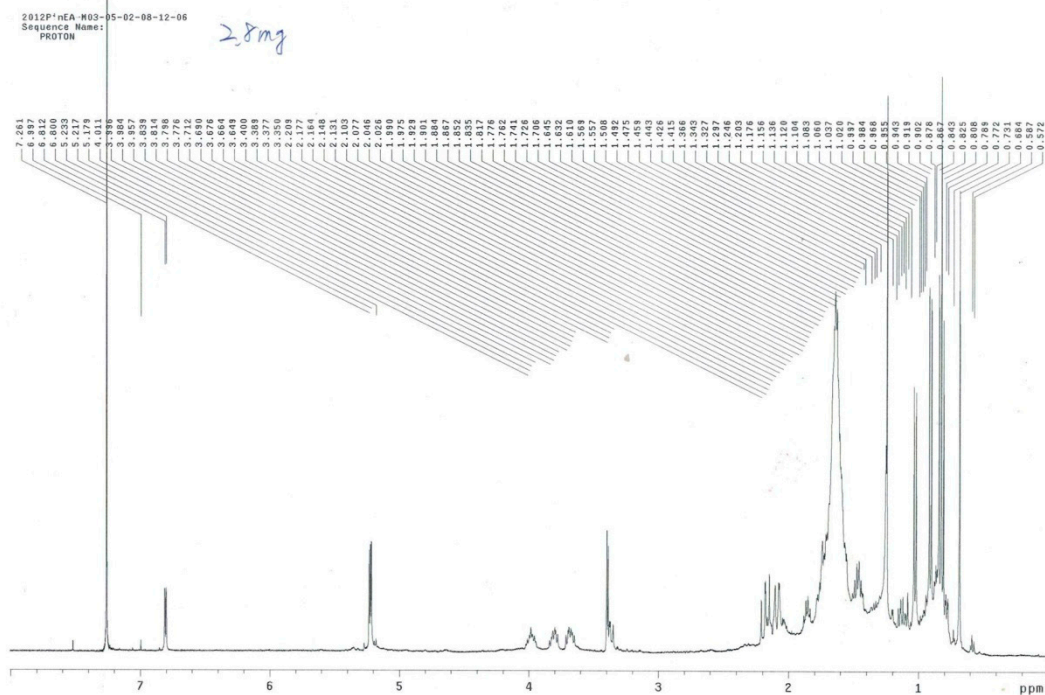
Analysis Info

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Method broadband first signal
Sample Name 2012PinEA-M03-05-02-08-12-06 Instrument: FT-MS solarix
Comment ESI Positive

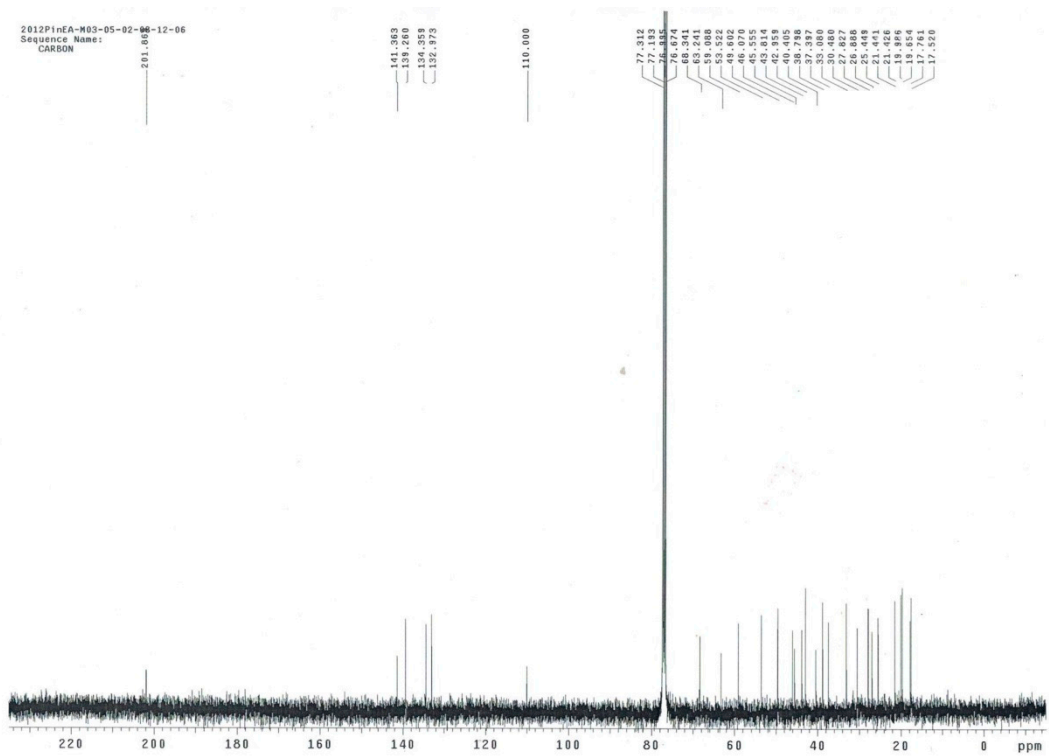


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
467.31308	1	C ₂₈ H ₄₄ NaO ₄	100.00	467.31318	0.11	0.23	31.0	6.5	even	ok

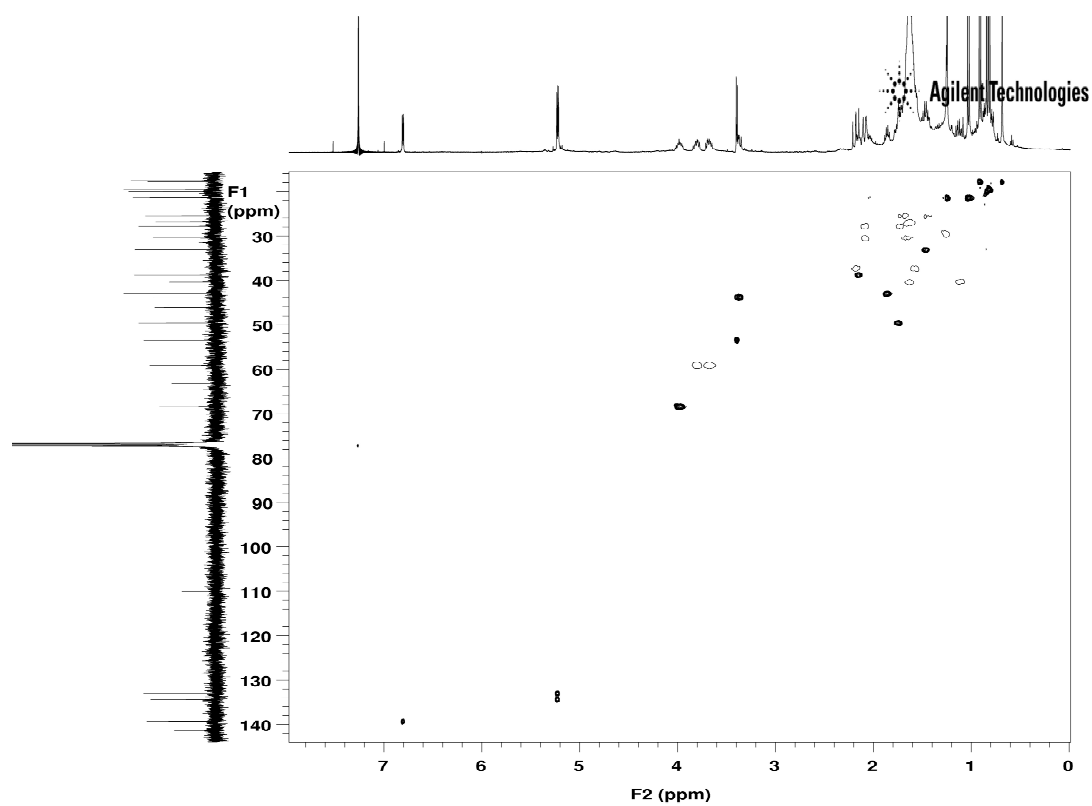
S1. HRESIMS spectrum of compound 1.



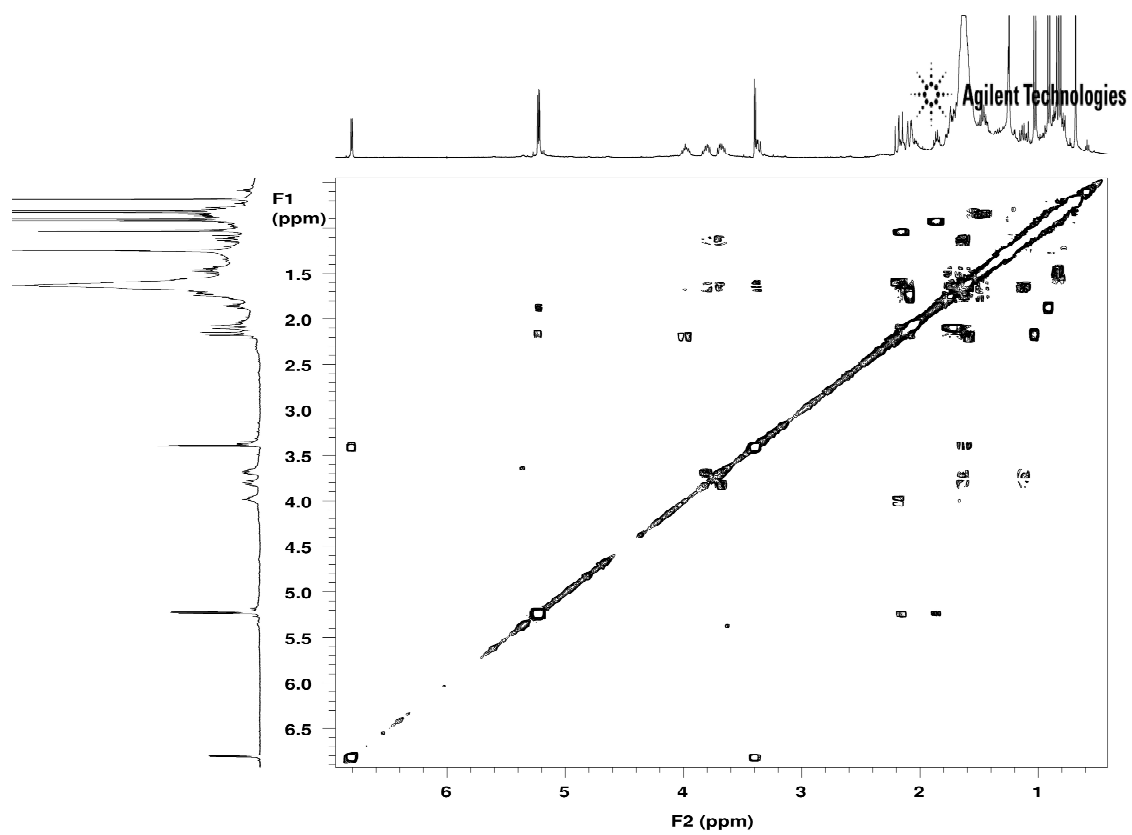
S2. ¹H NMR spectrum (400 MHz) of compound 1 in CDCl₃.



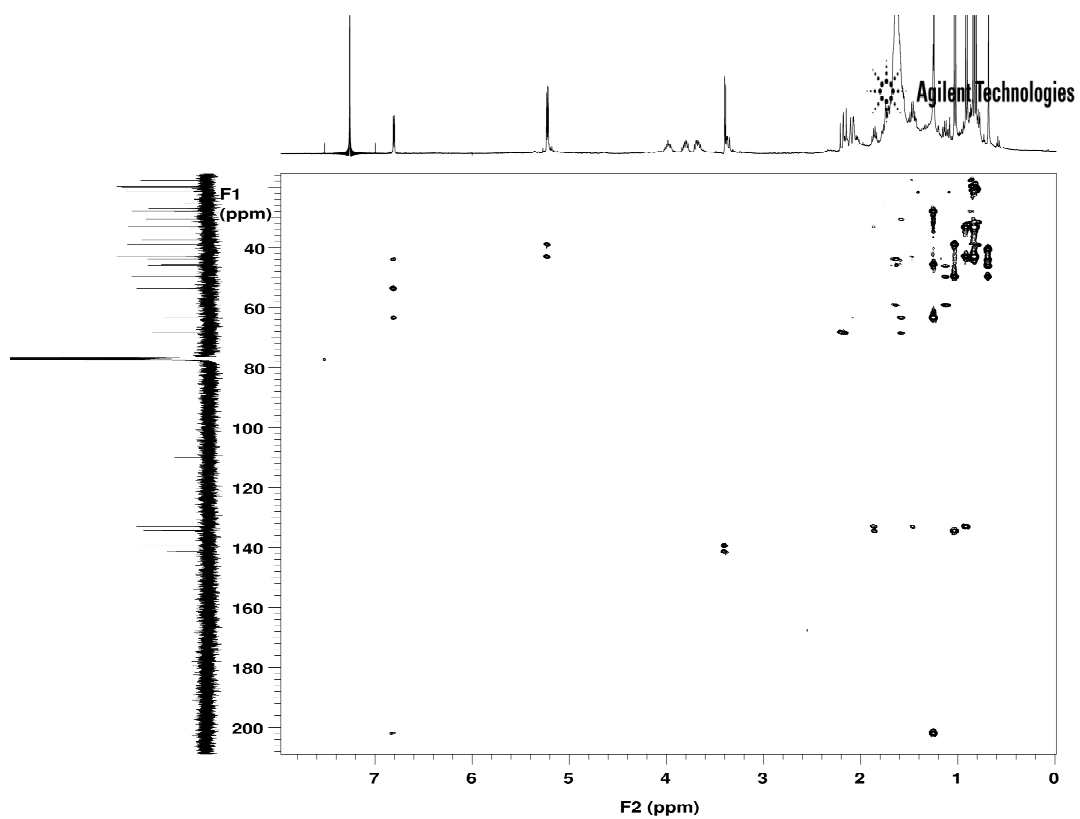
S3. ^{13}C NMR spectrum (100 MHz) of compound **1** in CDCl_3 .



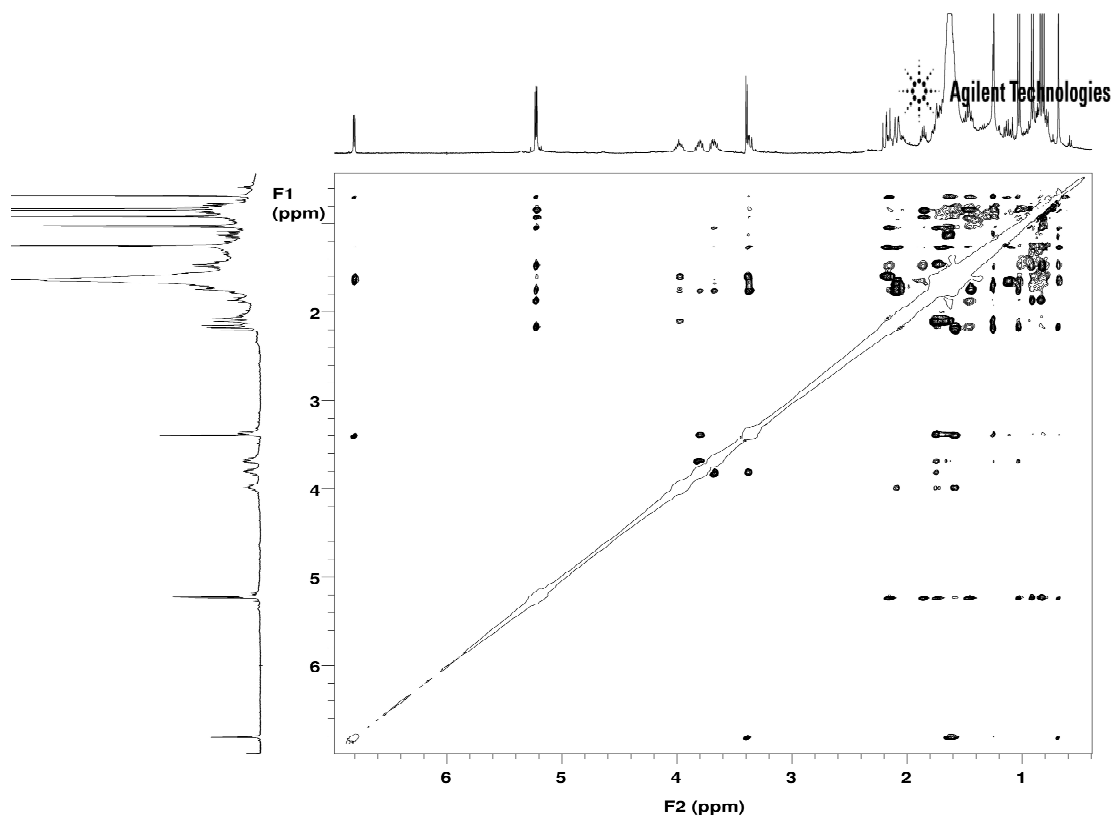
S4. gHSQC spectrum (400 MHz) of compound **1** in CDCl₃.



S5. ^1H - ^1H COSY spectrum (400 MHz) of compound **1** in CDCl_3 .



S6. gHMBC spectrum (400 MHz) of compound **1** in CDCl_3 .



S7. NOESY spectrum (400 MHz) of compound **1** in CDCl₃.

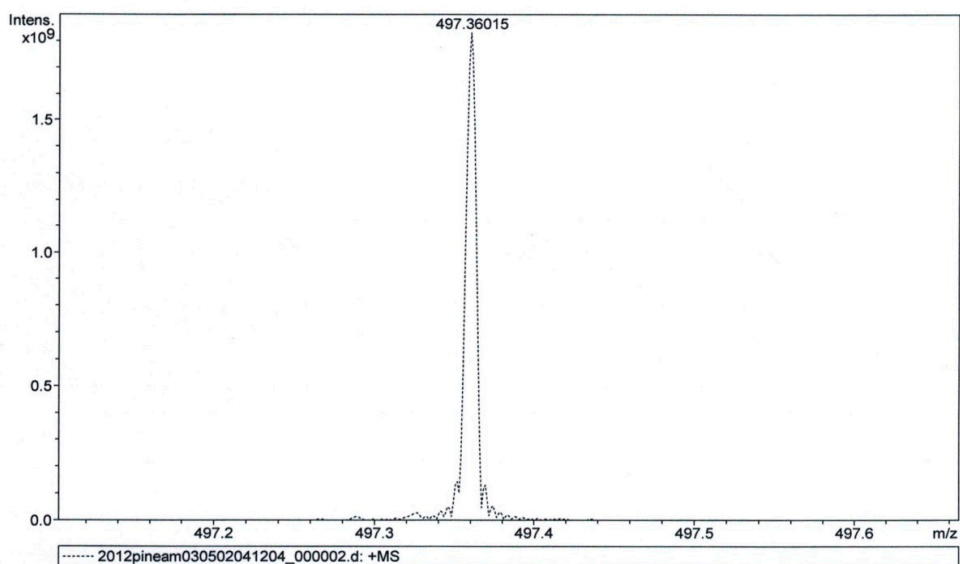
Mass Spectrum SmartFormula Report

Analysis Info

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Comment ESI Positive

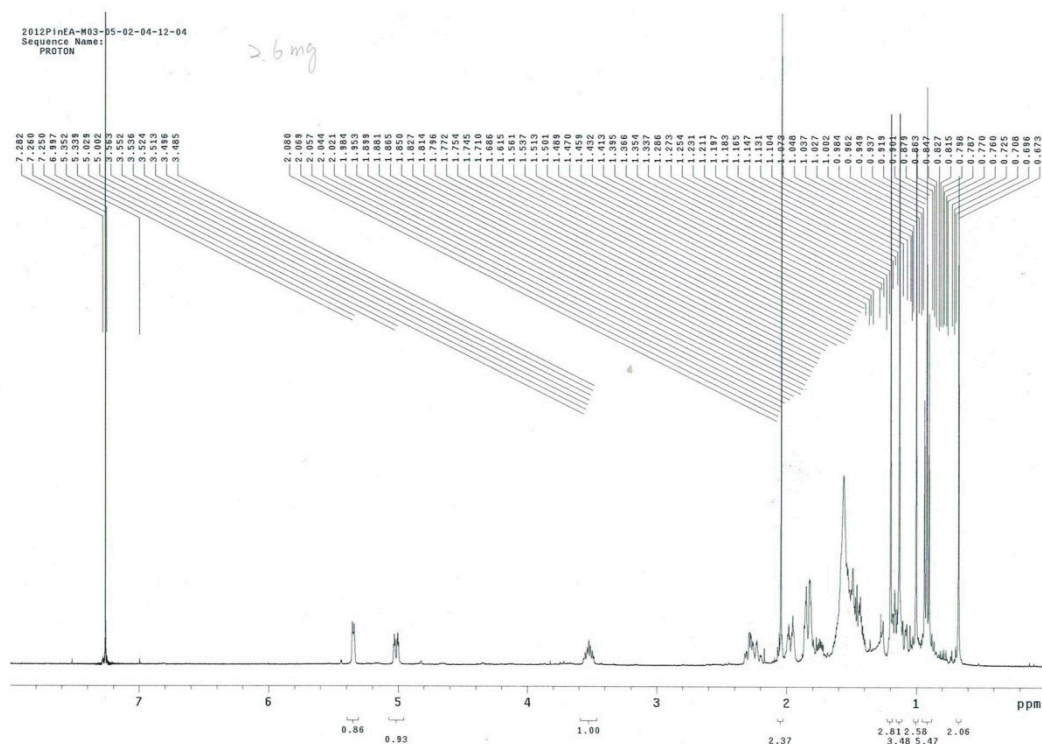
6/5/2014 3:22:02 PM

Instrument: FT-MS solarix

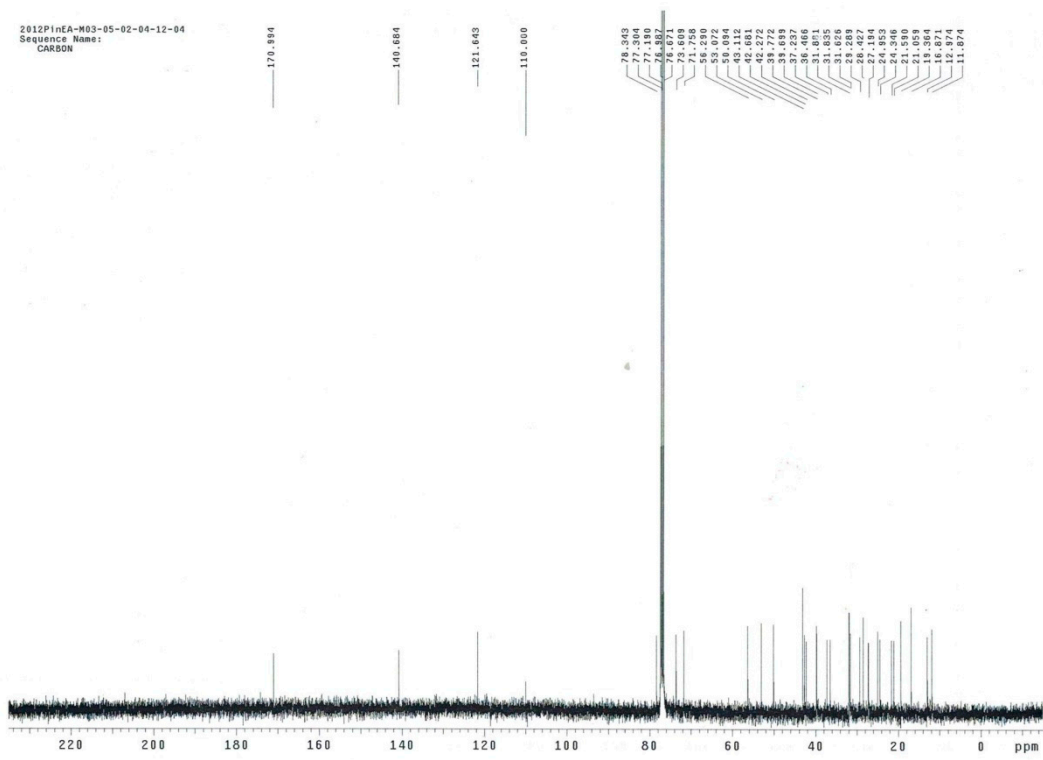


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
497.36015	1	C ₃₀ H ₅₀ NaO ₄	100.00	497.36013	-0.02	-0.03	13.5	5.5	even	ok

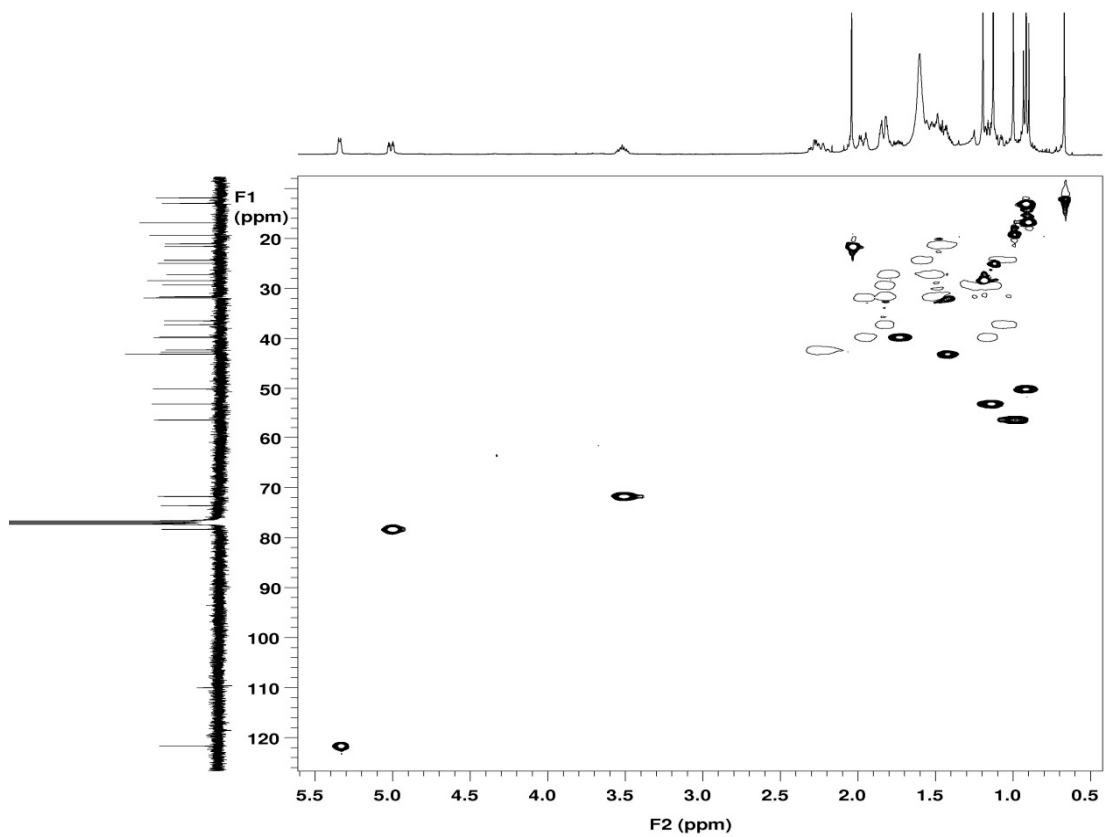
S8. HRESIMS spectrum of compound 2.



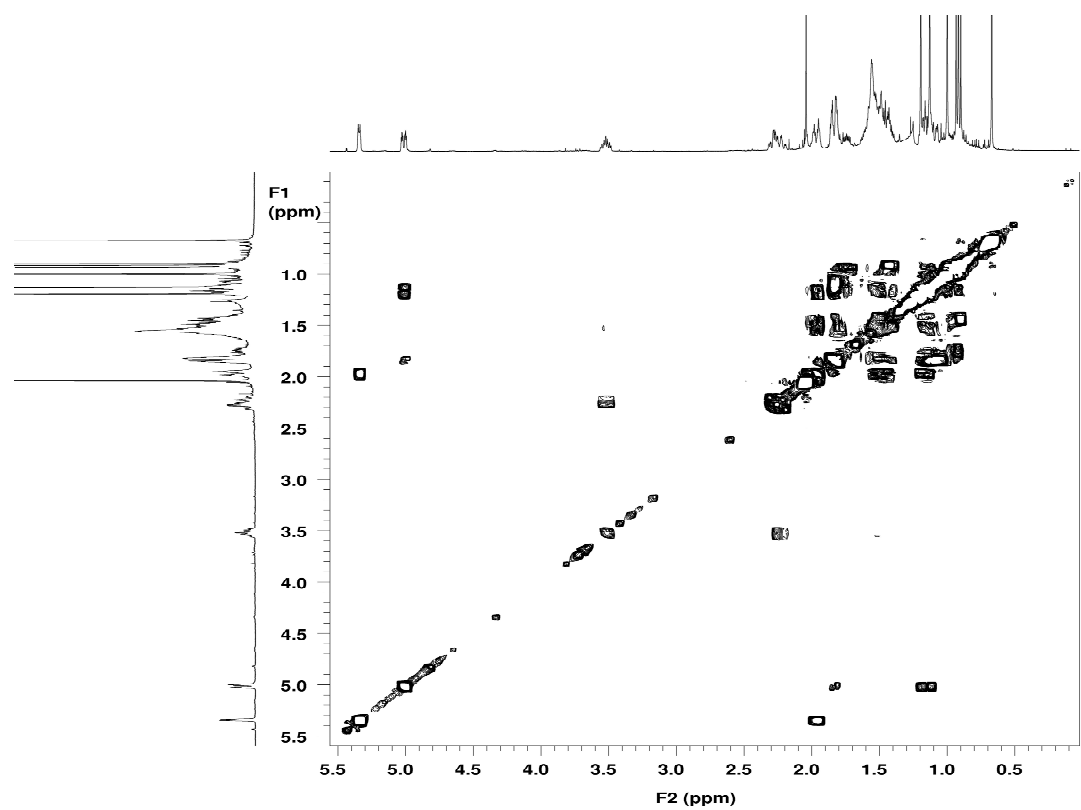
S9. ¹H NMR spectrum (400 MHz) of compound 2 in CDCl₃.



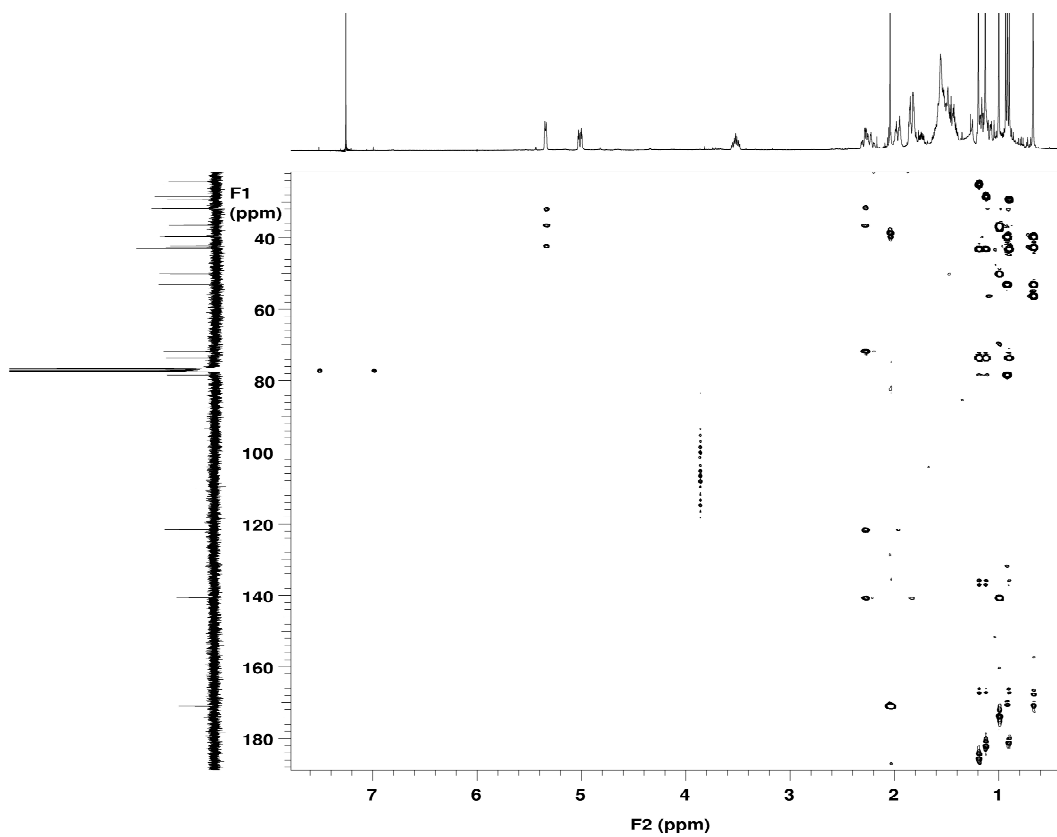
S10. ^{13}C NMR spectrum (100 MHz) of compound **2** in CDCl_3 .



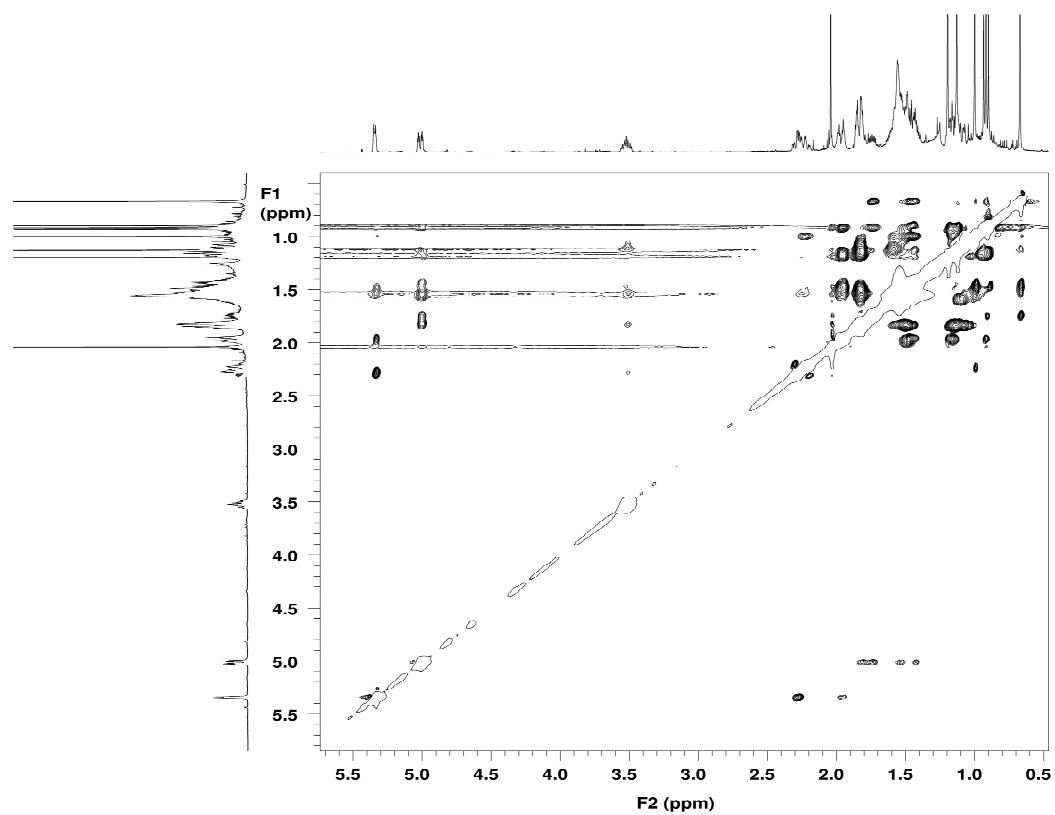
S11. gHSQC spectrum (400 MHz) of compound **2** in CDCl_3 .



S12. ^1H - ^1H COSY spectrum (400 MHz) of compound **2** in CDCl_3 .



S13. gHMBC spectrum (400 MHz) of compound **2** in CDCl₃.



S14. NOESY spectrum (400 MHz) of compound **2** in CDCl₃.