

Supporting Information

Briarenols C–E, New Polyoxygenated Briaranes from the Octocoral *Briareum excavatum*

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Yang-Chang Wu and Ping-Jyun Sung

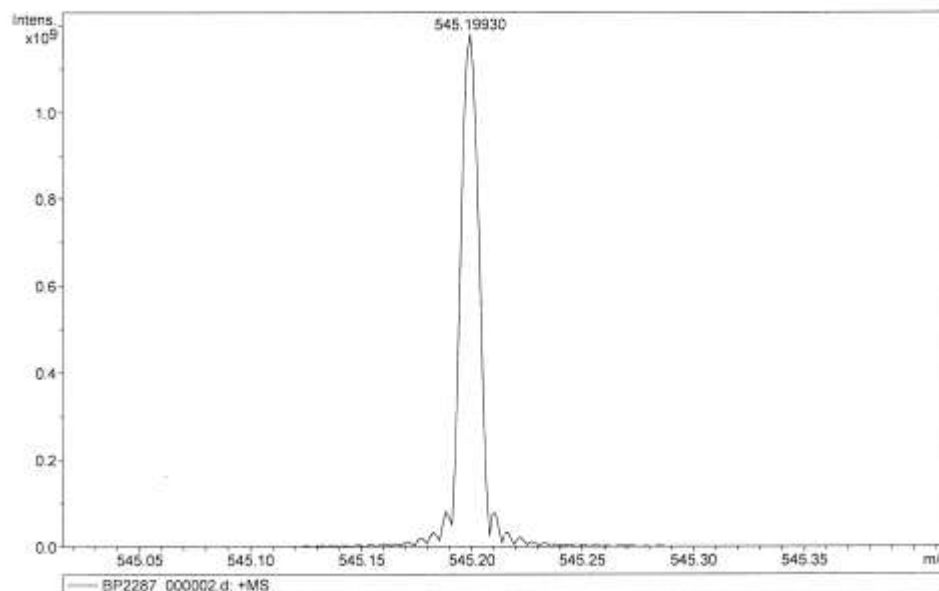
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Mass Spectrum SmartFormula Report

Analysis Info

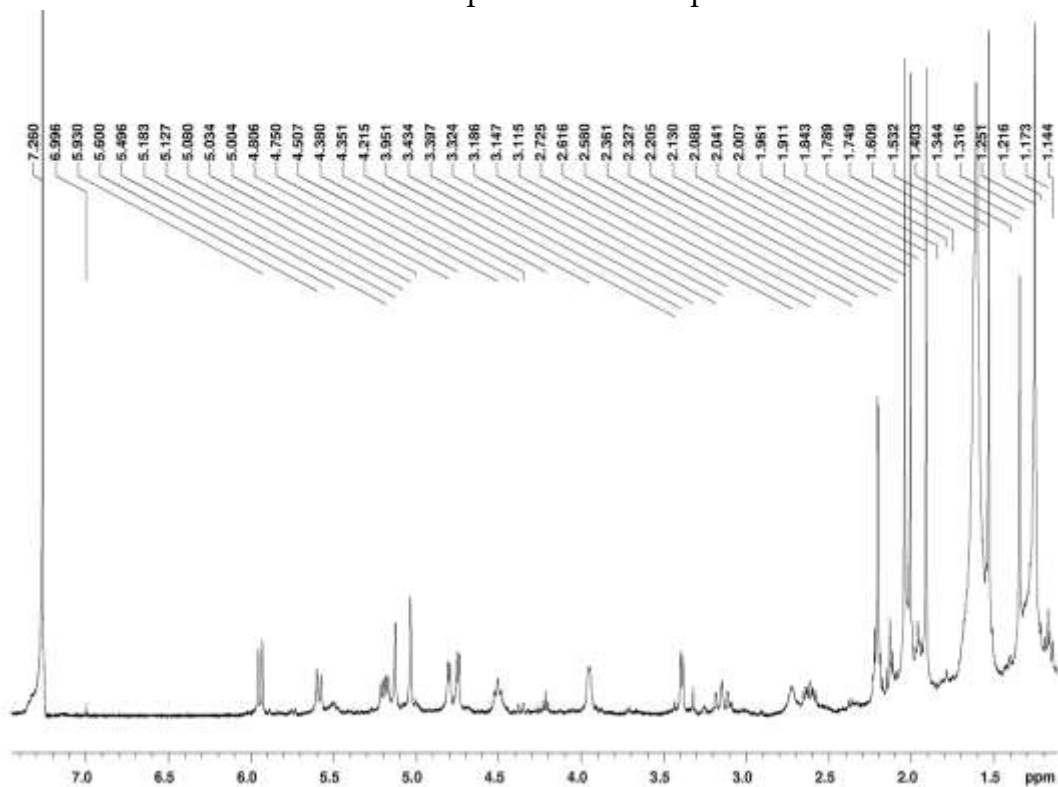
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Method broadband first signal
Sample Name BP-22-8-7
Comment ESI Positive

8/22/2016 3:16:59 PM
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Instrument: BRUKER FT-MS solarix

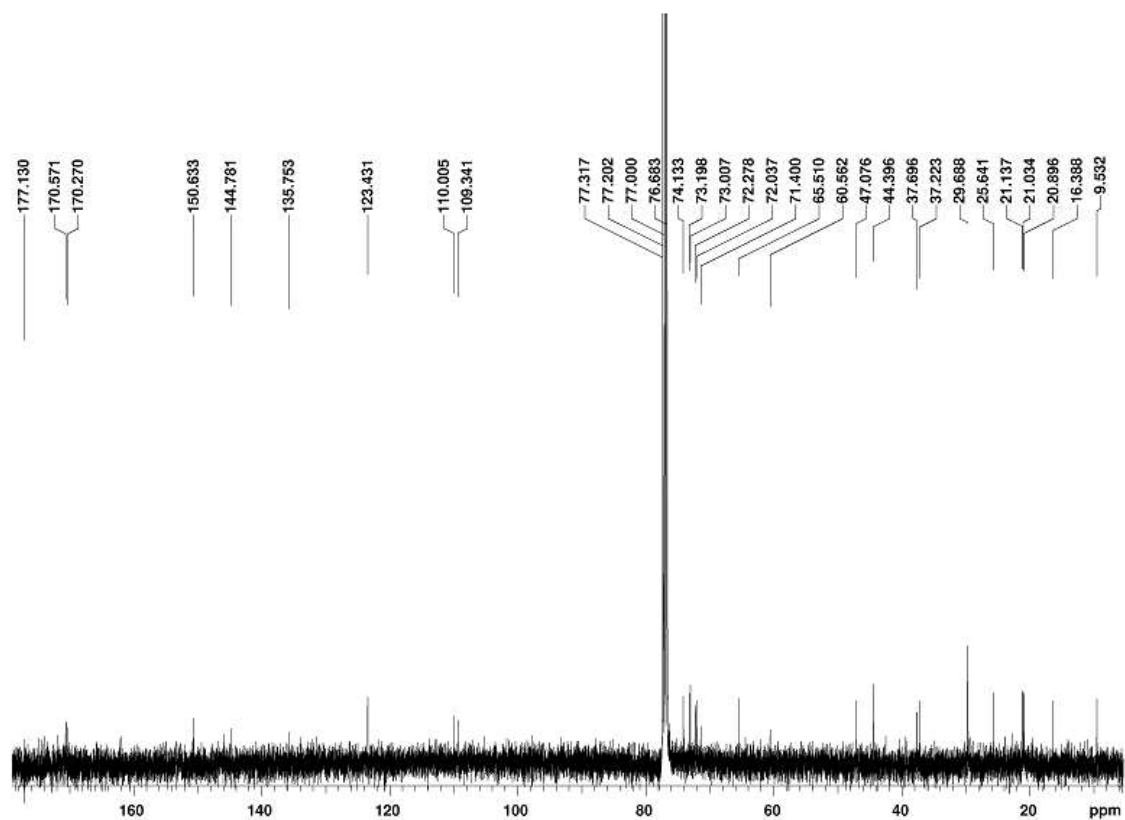


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
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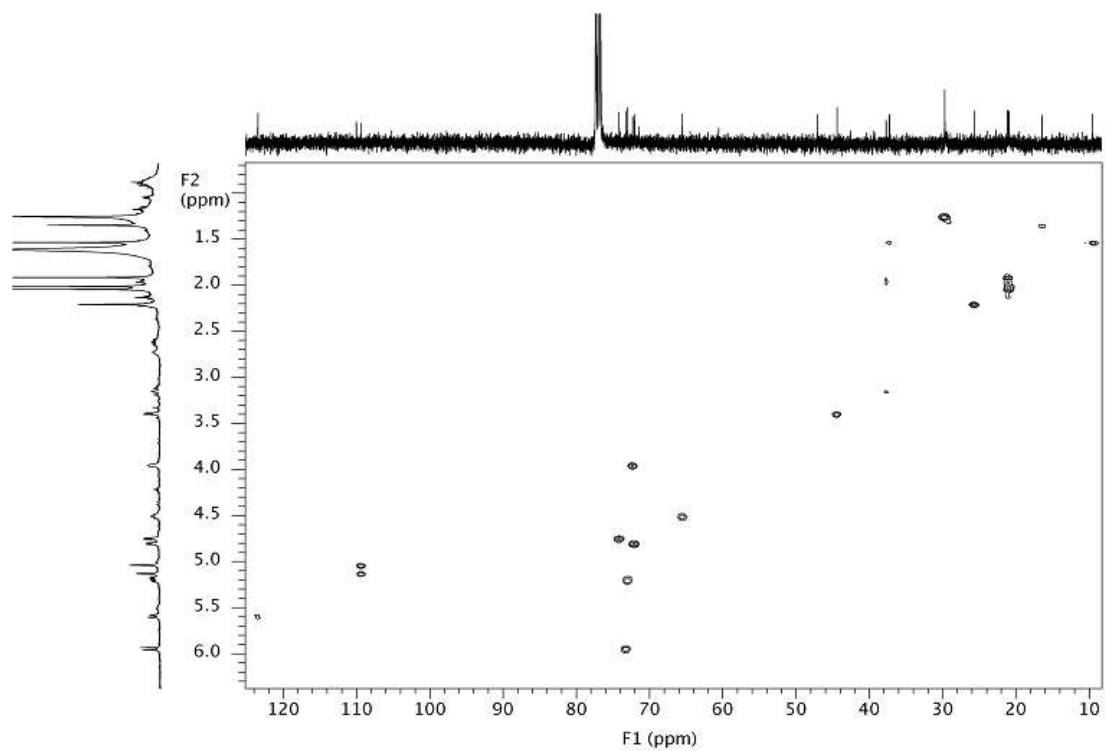
S1. HRESIMS spectrum of compound 1.



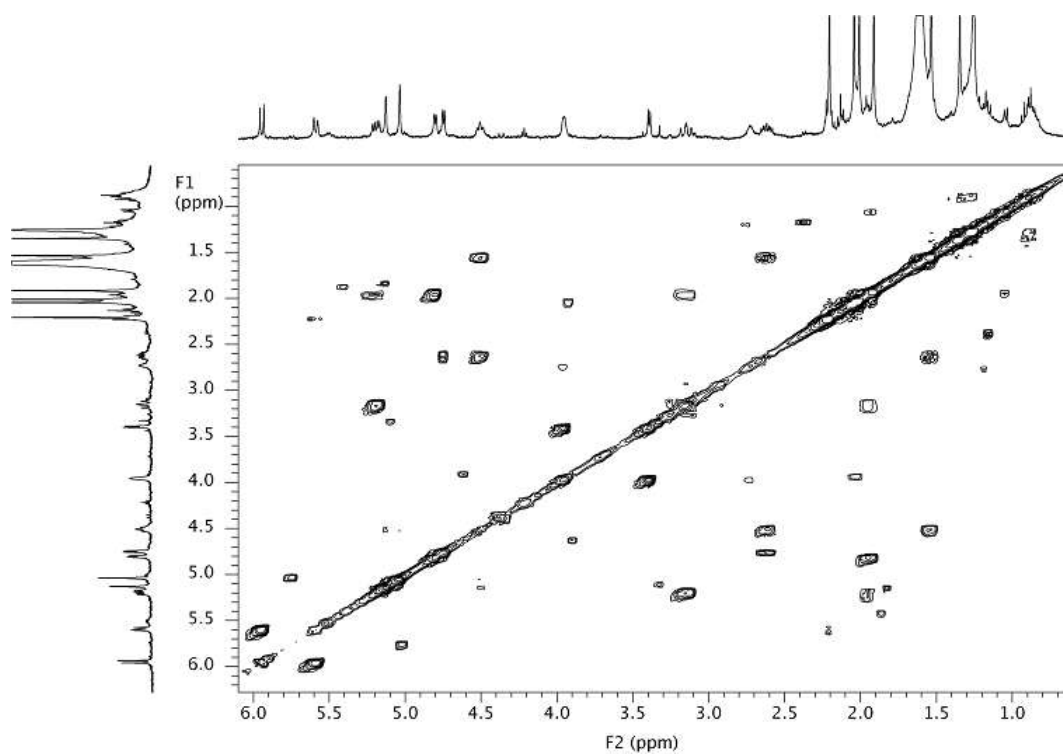
S2. ¹H NMR spectrum (400 MHz) of compound 1 in CDCl₃.



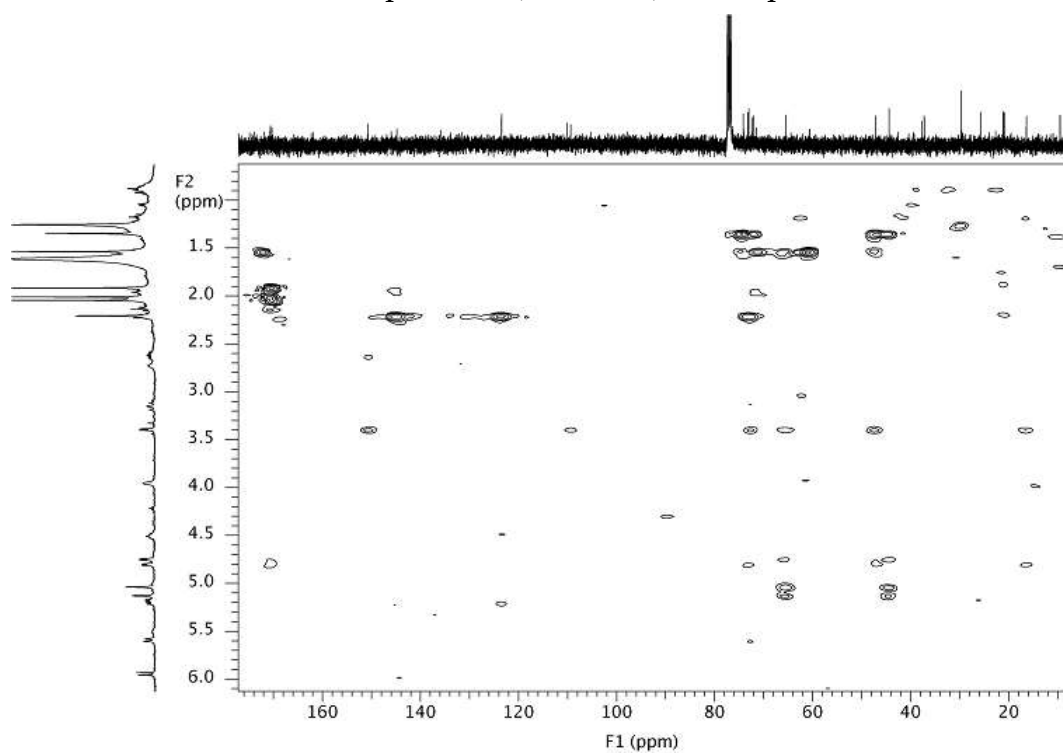
S3. ¹³C NMR spectrum (100 MHz) of compound 1 in CDCl₃.



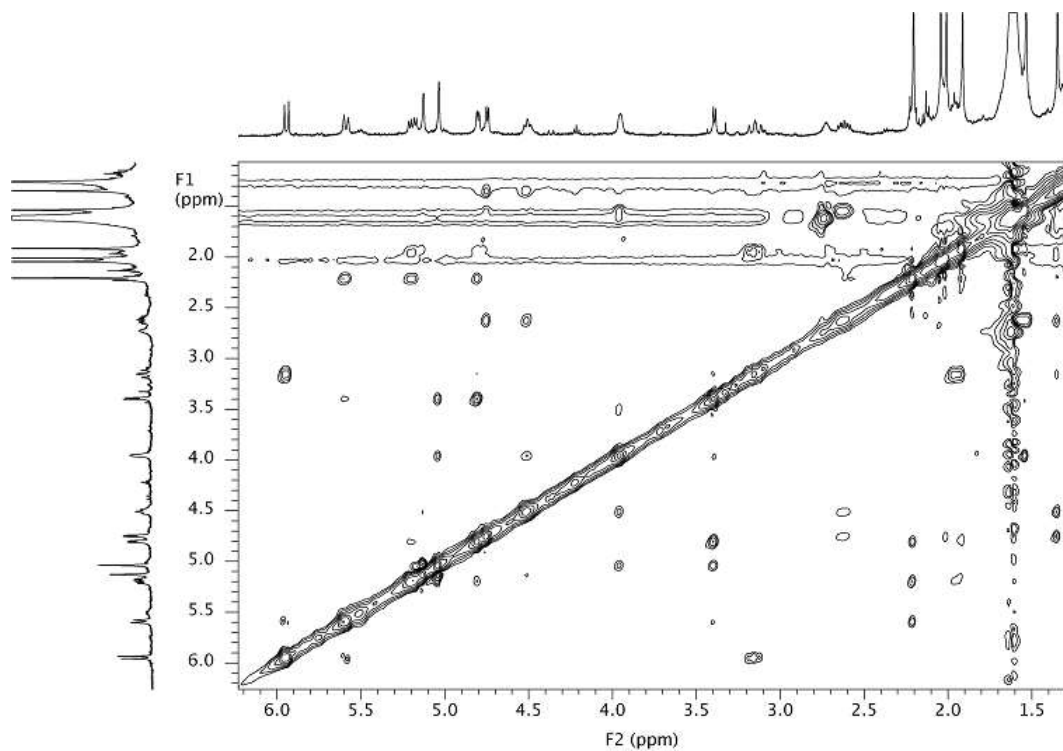
S4. gHSQC spectrum (400 MHz) of compound **1** in CDCl₃.



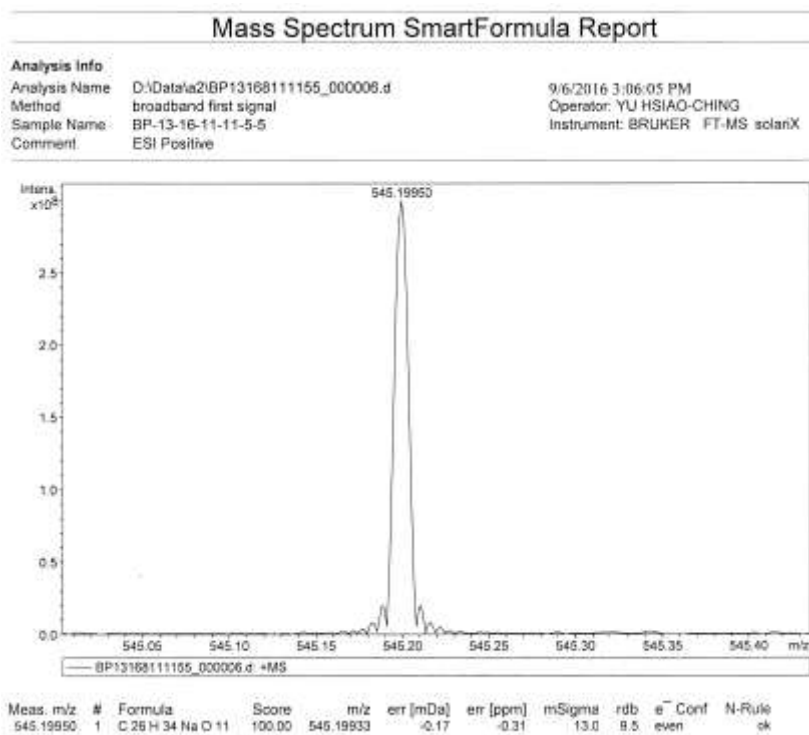
S5. ¹H-¹³C COSY spectrum (400 MHz) of compound **1** in CDCl₃.



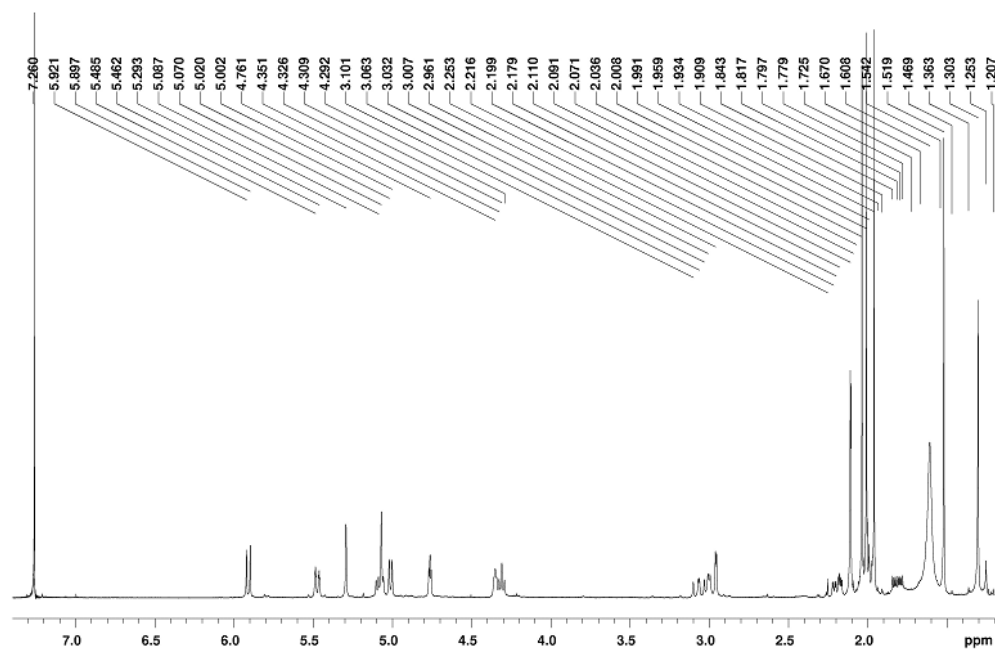
S6. gHMBC spectrum (400 MHz) of compound **1** in CDCl₃.



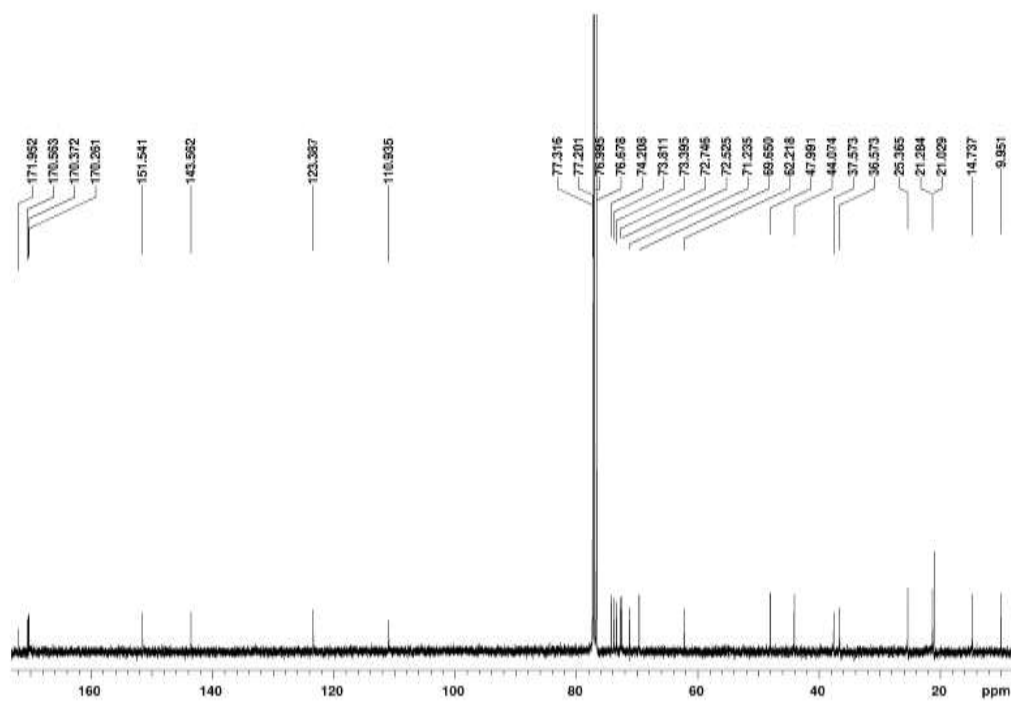
S7. NOESY spectrum (400 MHz) of compound **1** in CDCl₃.



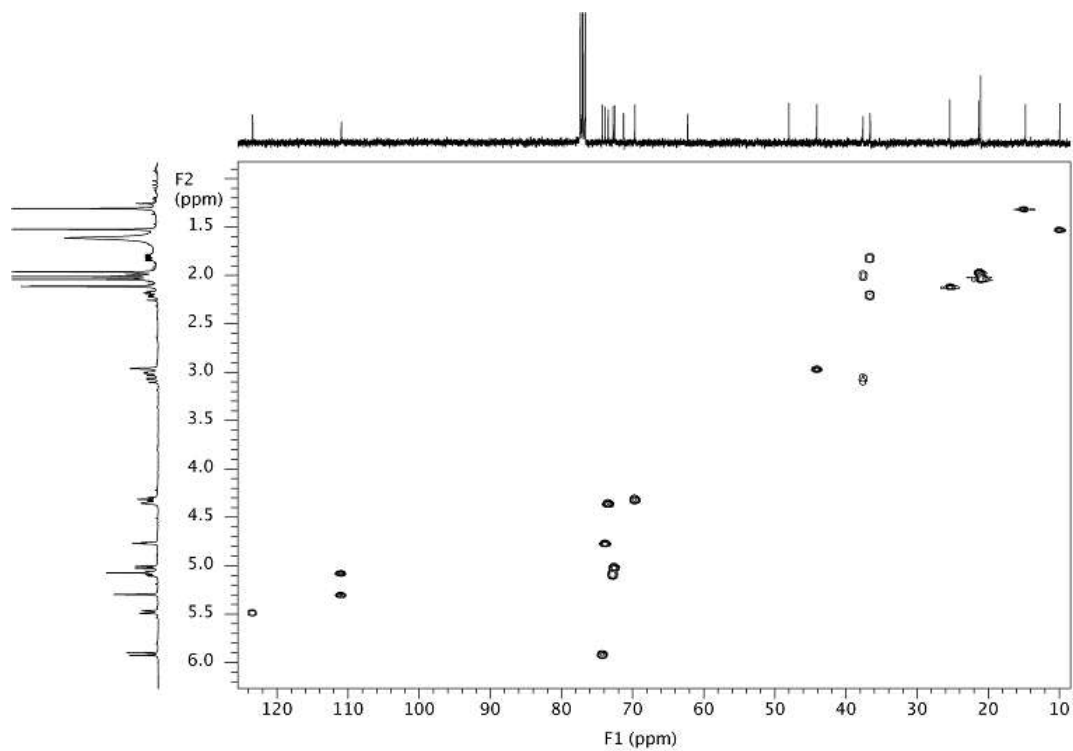
S8. HRESIMS spectrum of compound 2.



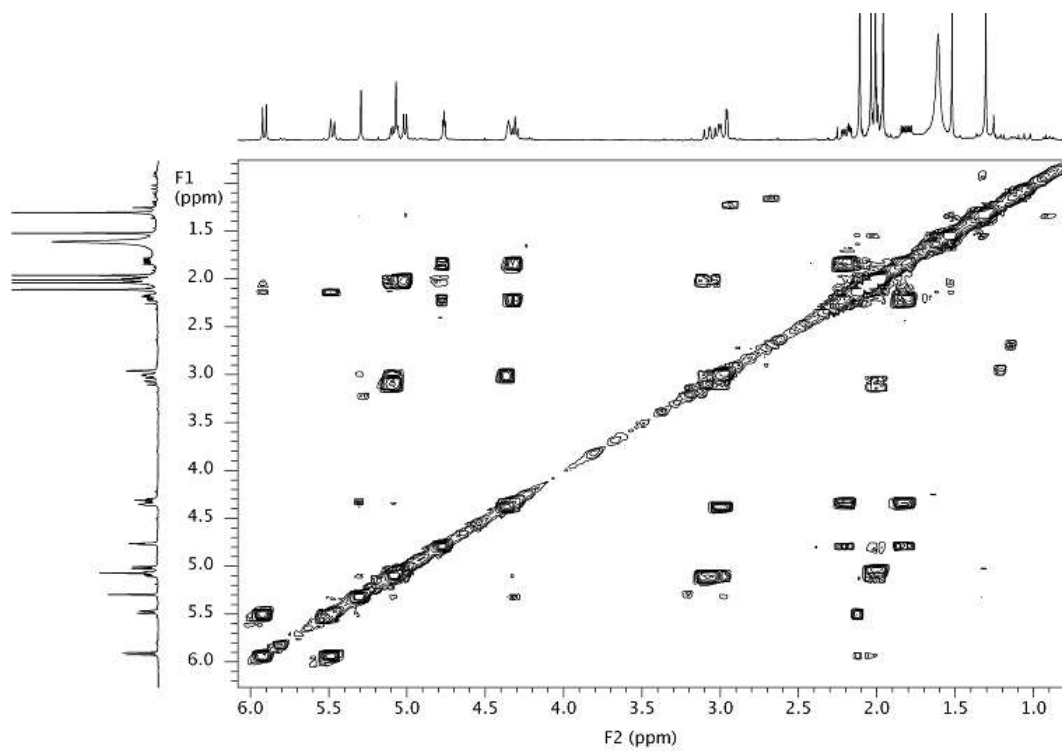
S9. ^1H NMR spectrum (400 MHz) of compound 2 in CDCl_3 .



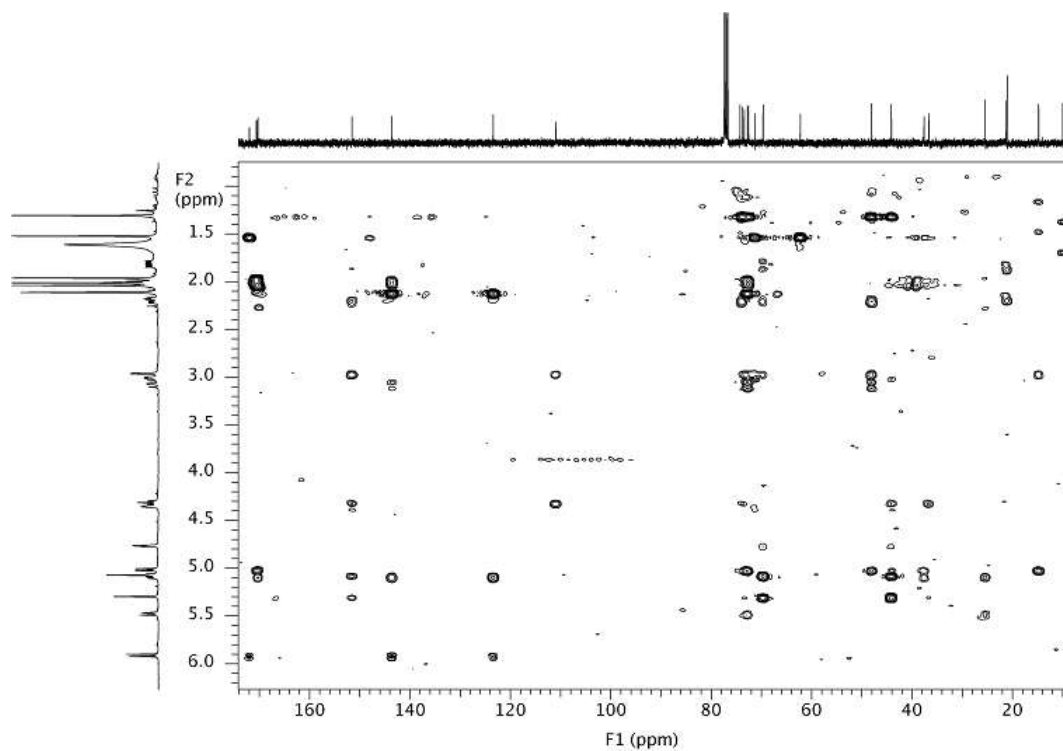
S10. ^{13}C NMR spectrum (100 MHz) of compound **2** in CDCl_3 .



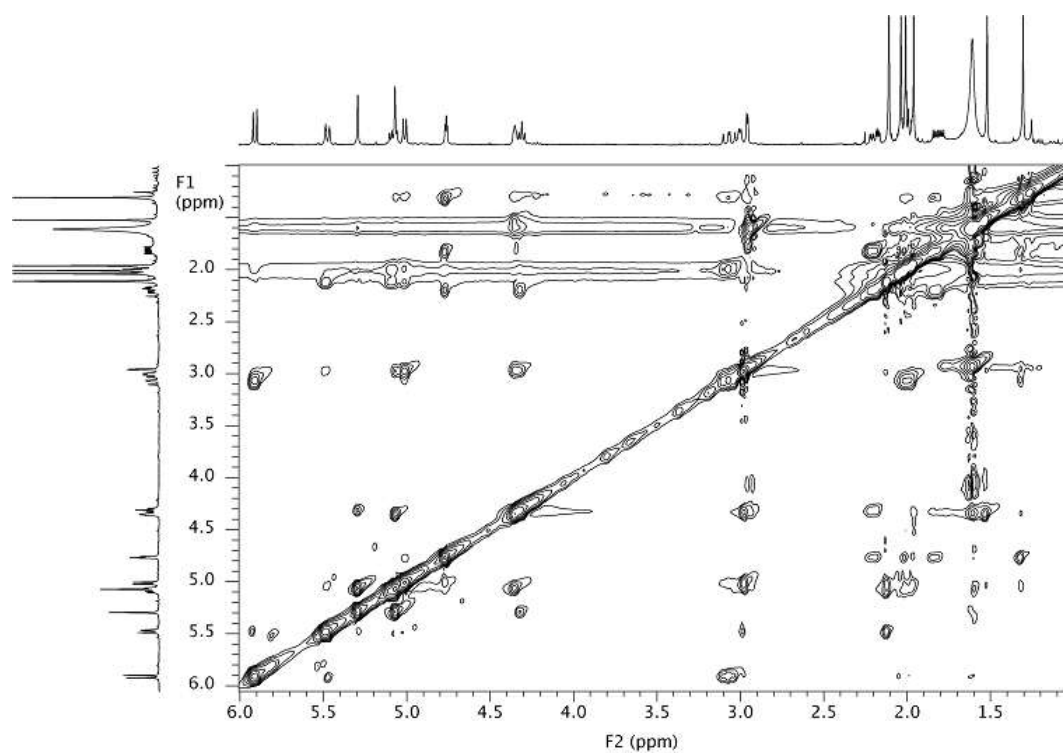
S11. gHSQC spectrum (400 MHz) of compound **2** in CDCl_3 .



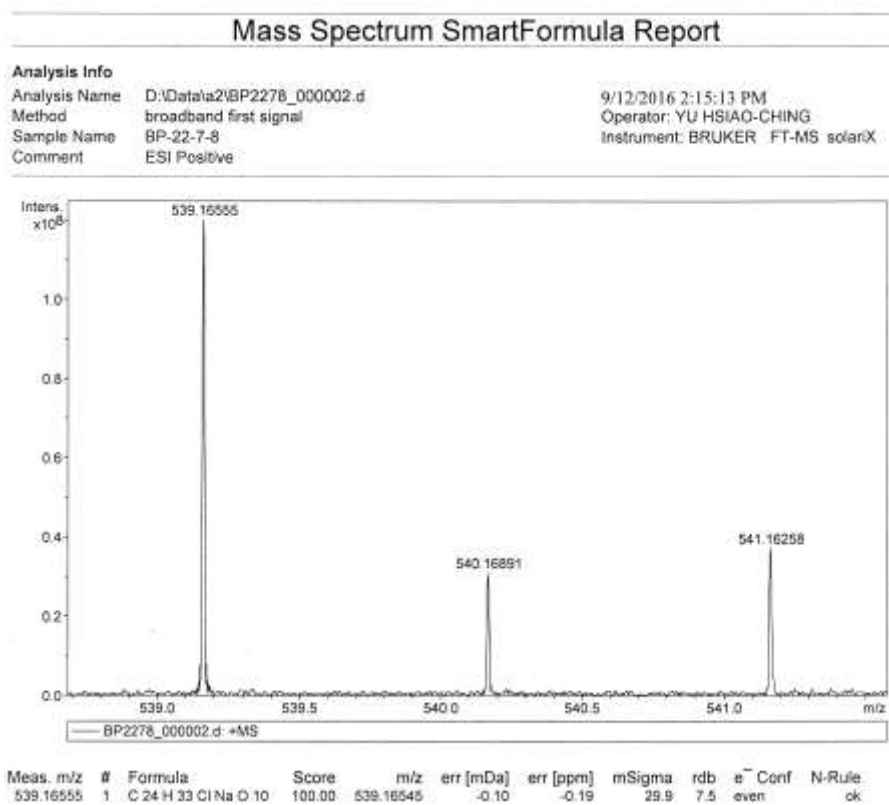
S12. ^1H - ^1H COSY spectrum (400 MHz) of compound **2** in CDCl_3 .



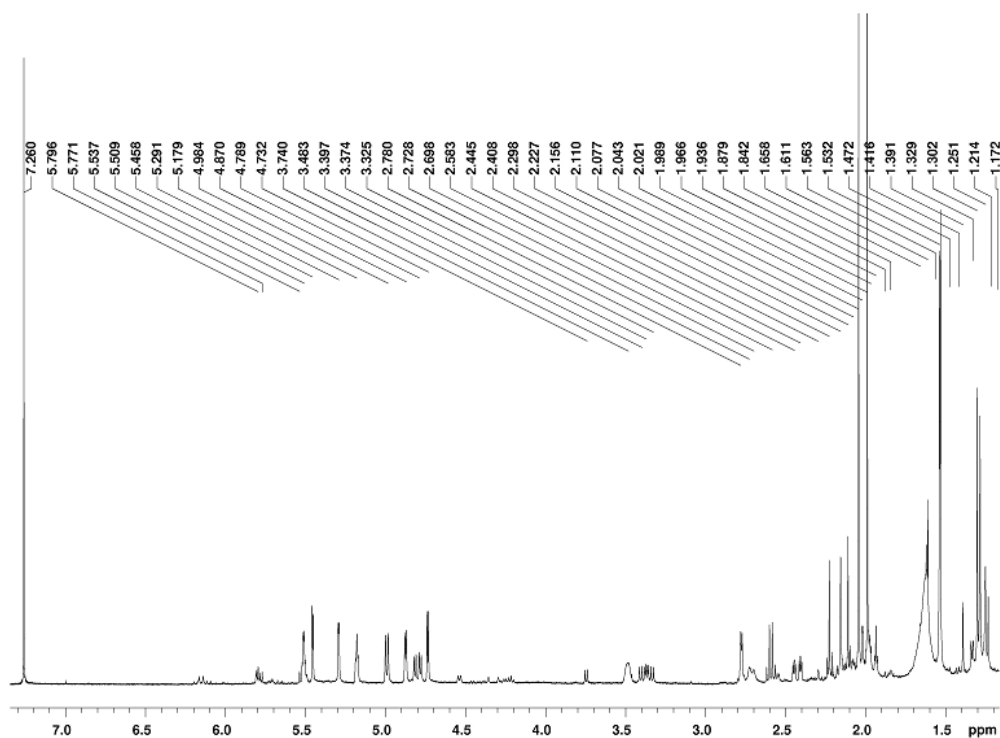
S13. gHMBC spectrum (400 MHz) of compound **2** in CDCl_3 .



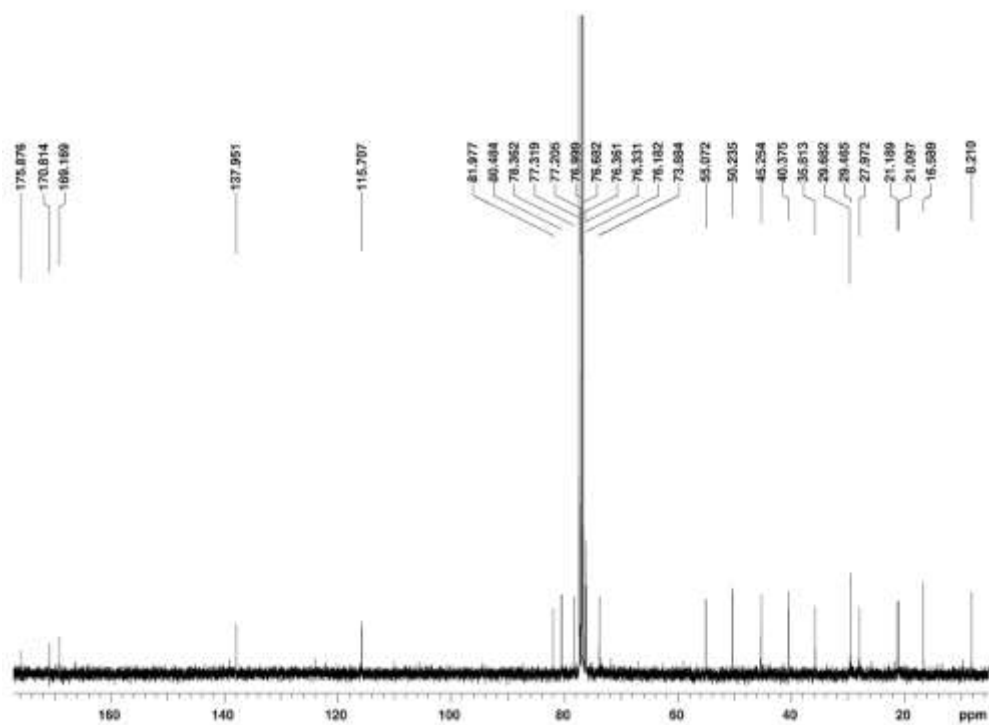
S14. NOESY spectrum (400 MHz) of compound **2** in CDCl₃.



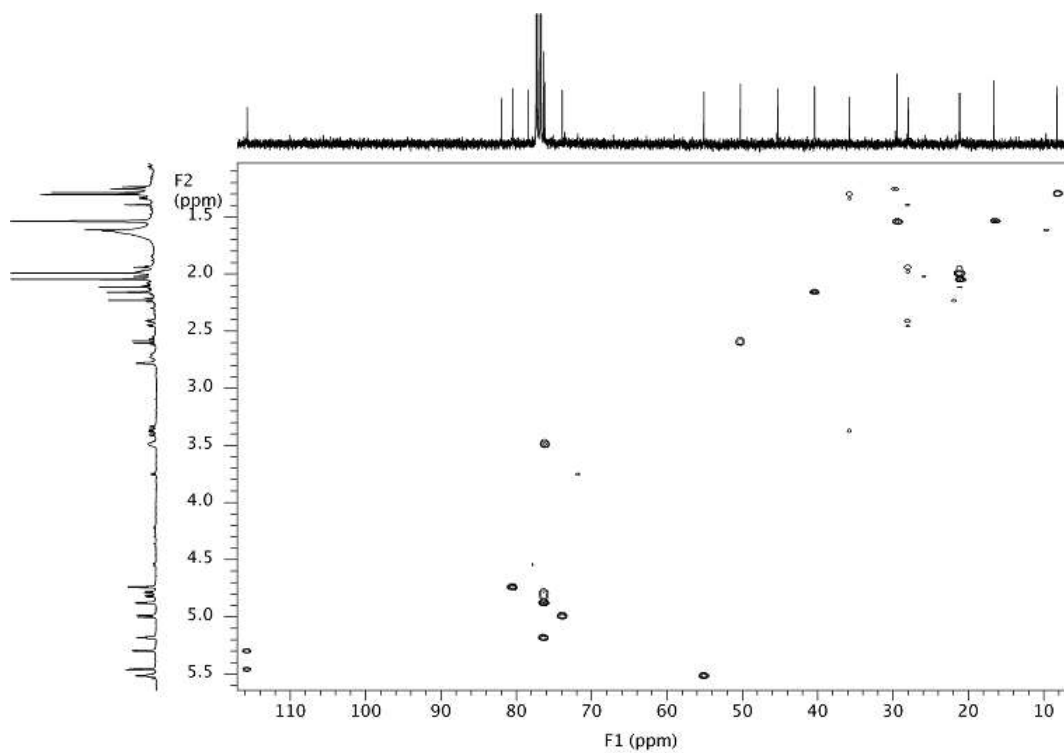
S15. HRESIMS spectrum of compound **3**.



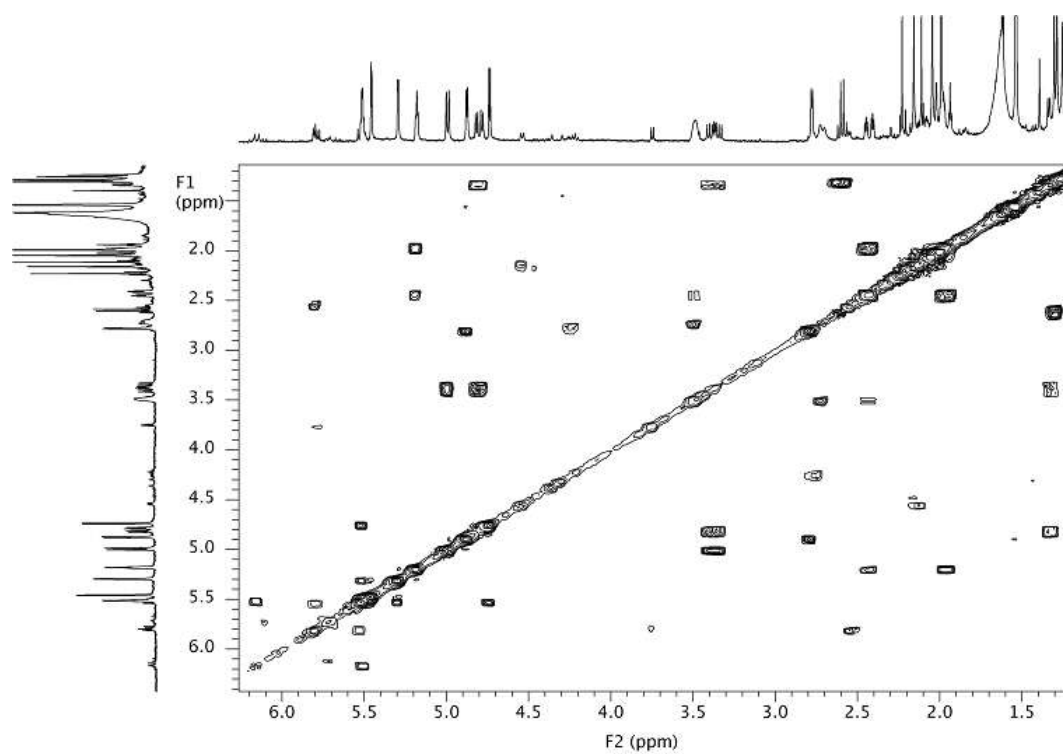
S16. ^1H NMR spectrum (400 MHz) of compound **3** in CDCl_3 .



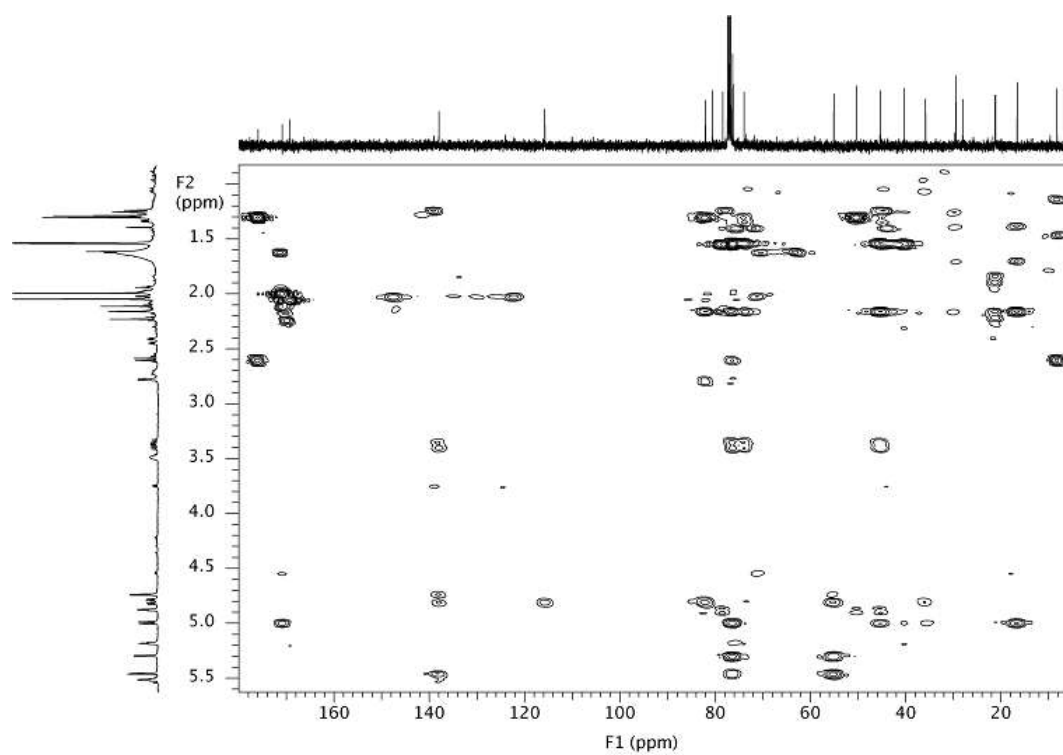
S17. ^{13}C NMR spectrum (100 MHz) of compound **3** in CDCl_3 .



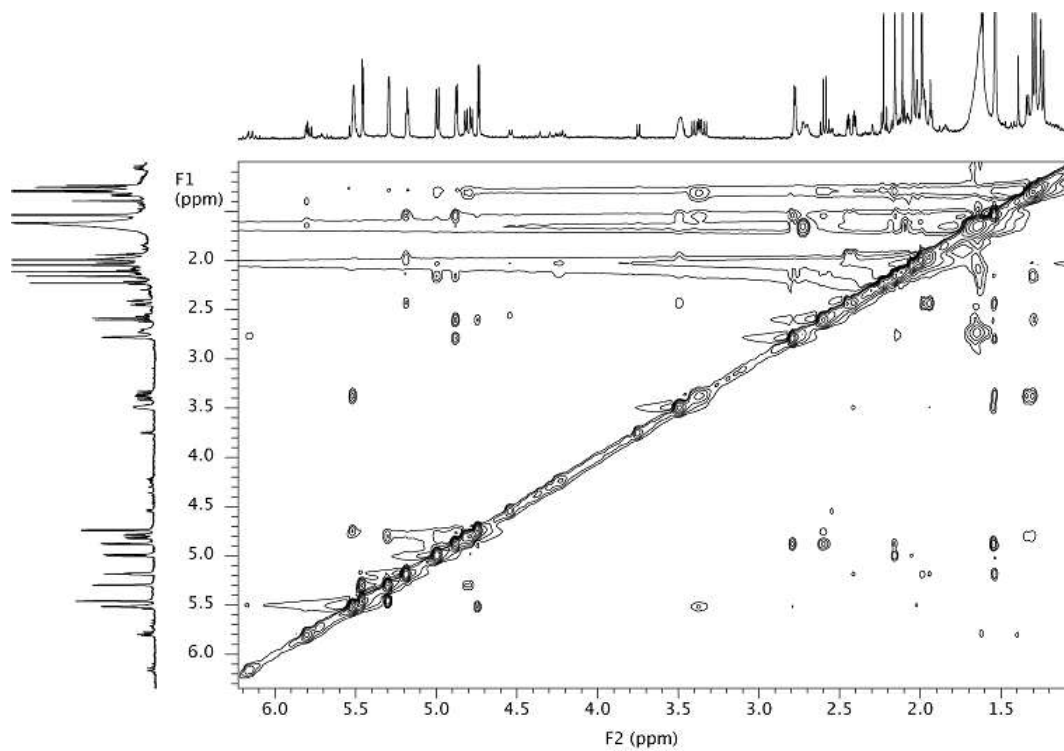
S18. gHSQC spectrum (400 MHz) of compound **3** in CDCl₃.



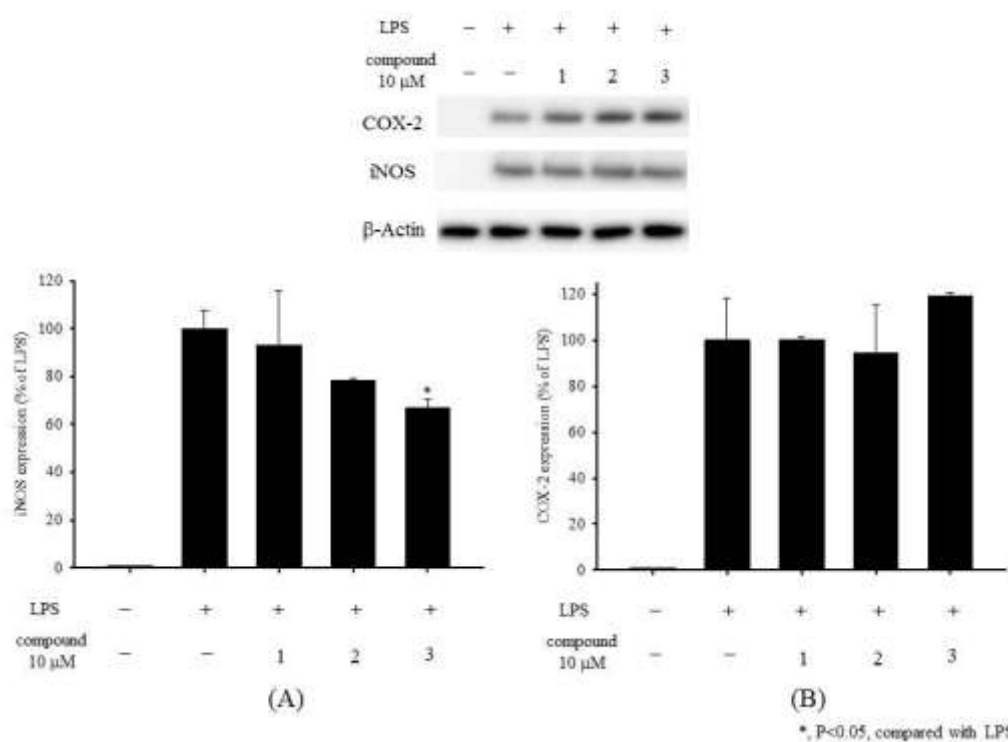
S19. ¹H-¹³C COSY spectrum (400 MHz) of compound **3** in CDCl₃.



S20. gHMBC spectrum (400 MHz) of compound **3** in CDCl₃.



S21. NOESY spectrum (400 MHz) of compound **3** in CDCl₃.



S22. Effects of compounds briarenols C-E (1-3) on pro-inflammatory iNOS and COX-2 protein expression in the LPS-stimulated murine macrophage cell line RAW264.7. (A) The relative density of iNOS immunoblot; (B) the relative density of COX-2 immunoblot. The relative intensity of the LPS-stimulated group was taken to be 100%. Band intensities were quantified by densitometry and are indicated as the percent change relative to that of the LPS-stimulated group. briarenols C-E (1-3) significantly inhibited LPS-induced iNOS and COX-2 protein expression in macrophages. The experiments were repeated three times (* $p < 0.05$, significantly different from the LPS-stimulated group).