

Supporting Material:

¹H NMR-based isolation of anti-inflammatory 9,11-secosteroids from the octocoral *Sinularia leptoclados*

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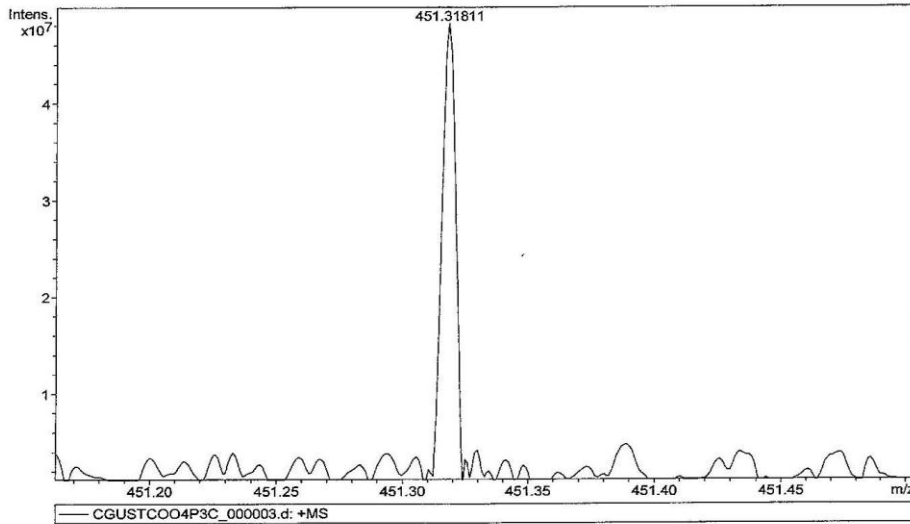
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Mass Spectrum SmartFormula Report

Analysis Info

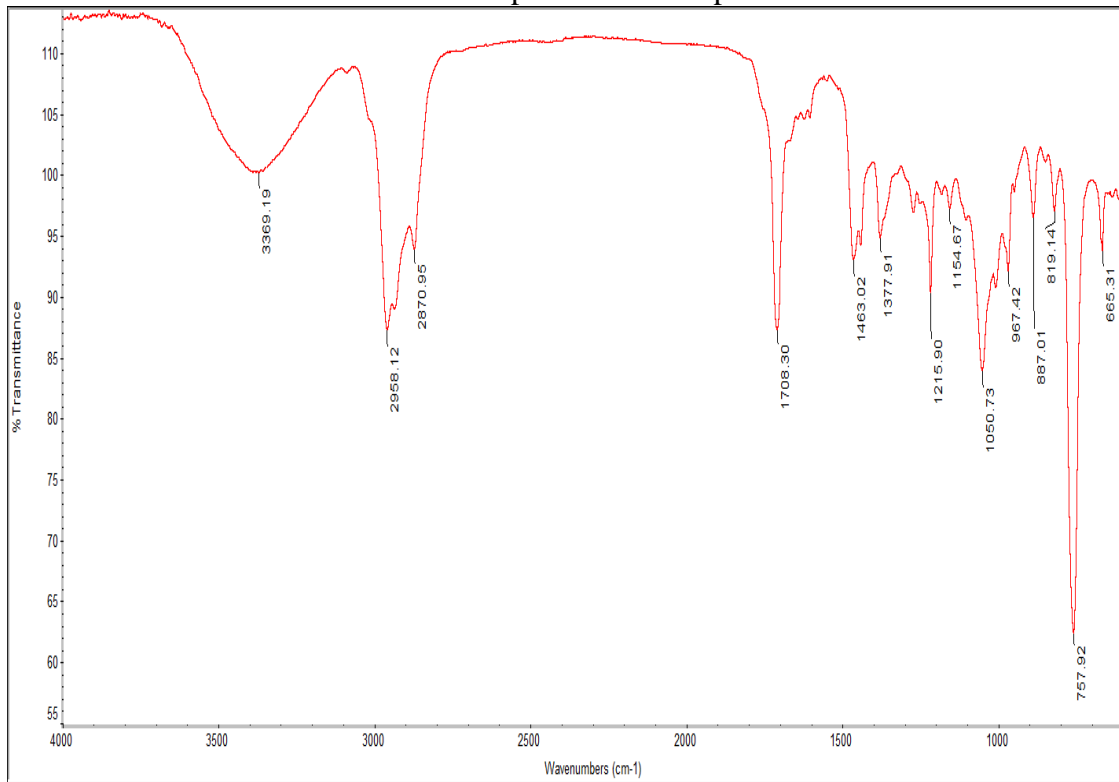
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Method broadband first signal
Sample Name Cgust-c004p3c
Comment ESI Positive

5/28/2019 4:52:36 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solarix

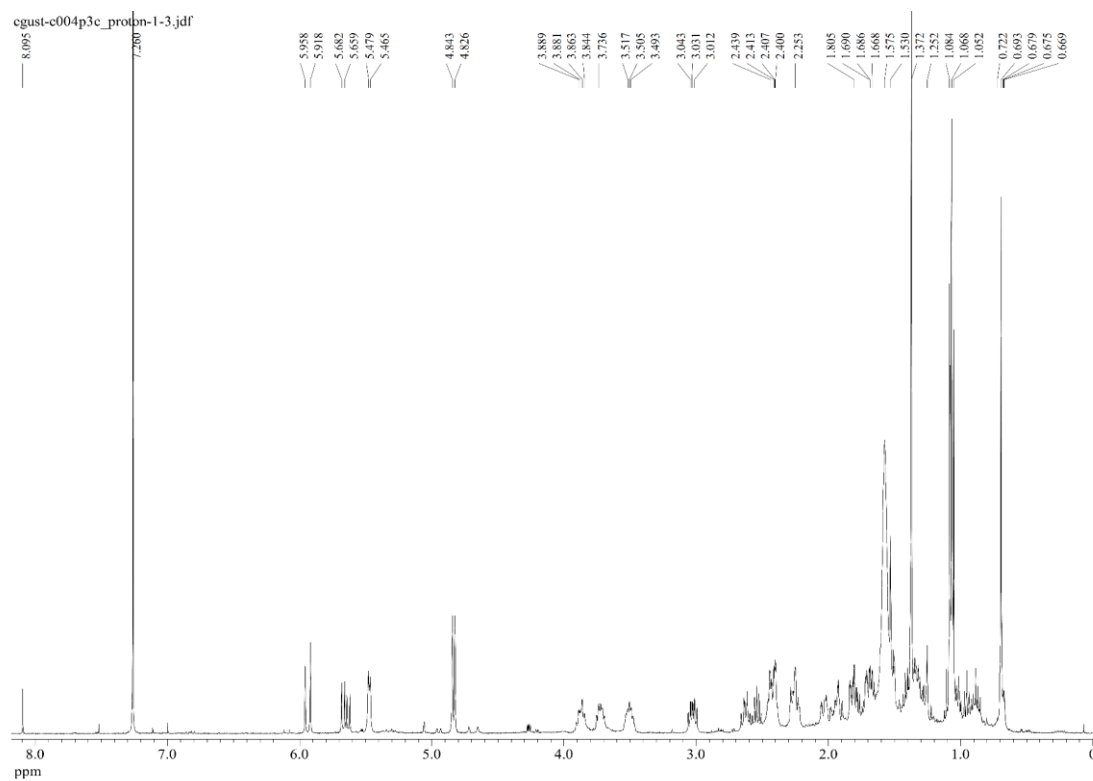


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
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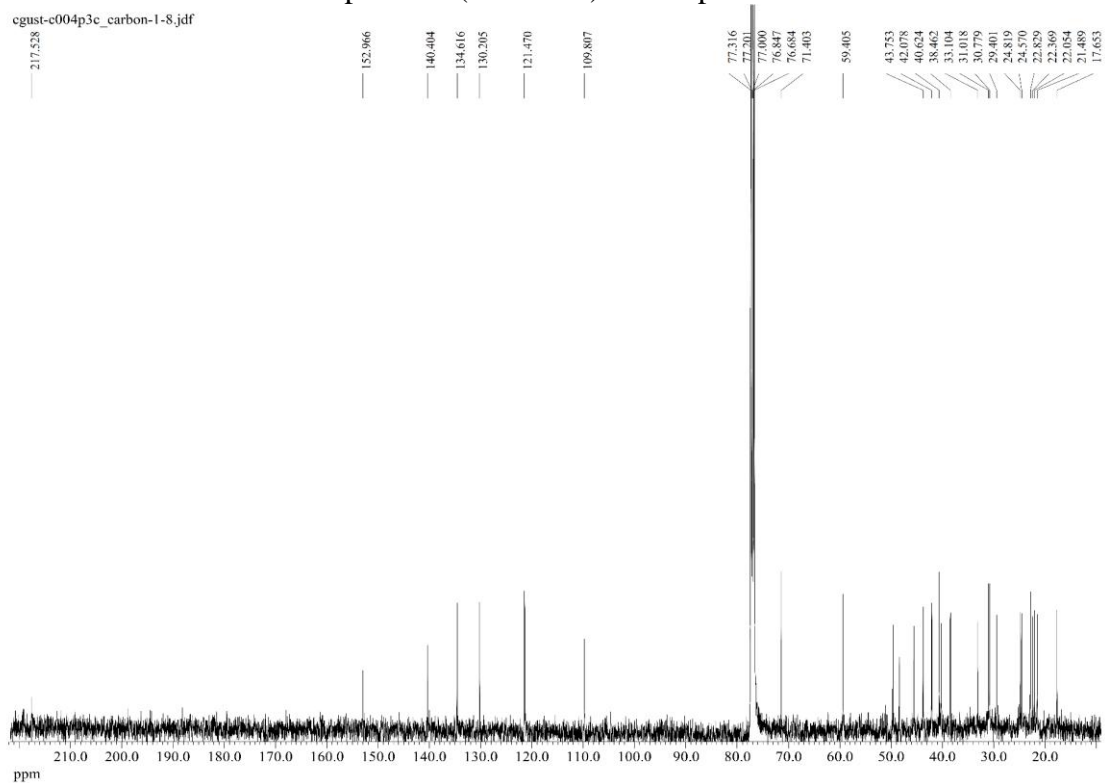
S1. HRESIMS spectrum of compound 1



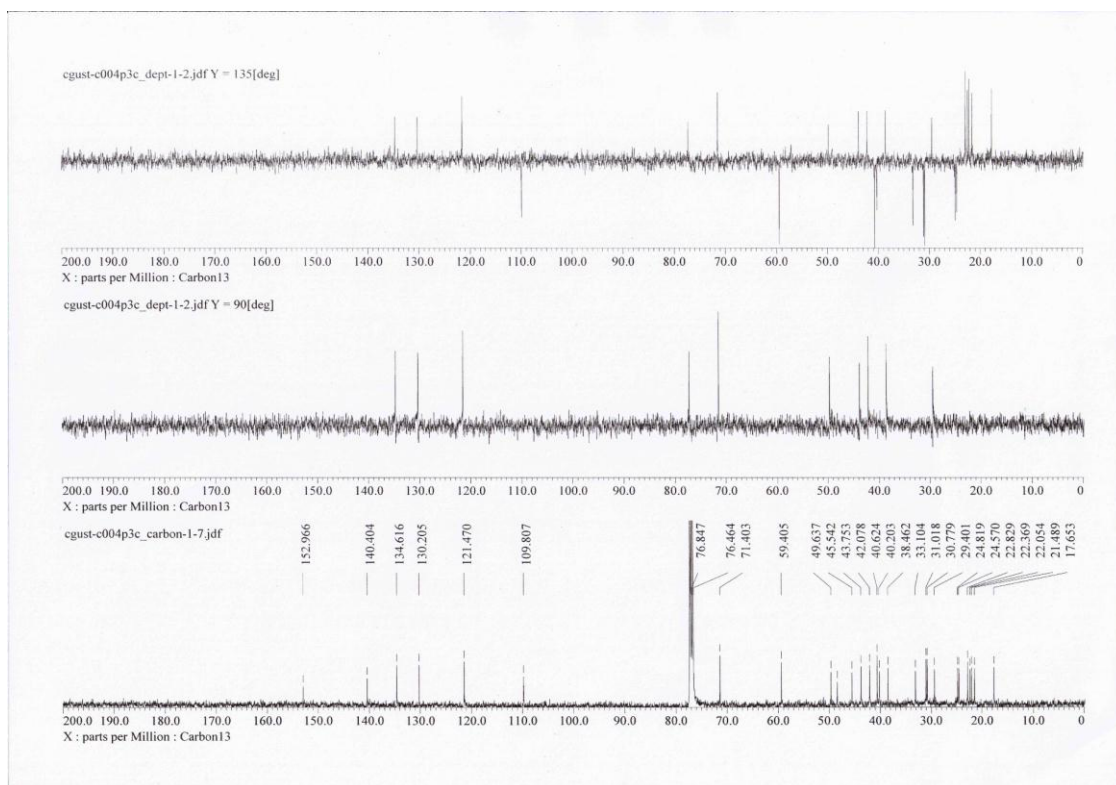
S2. IR spectrum of compound 1



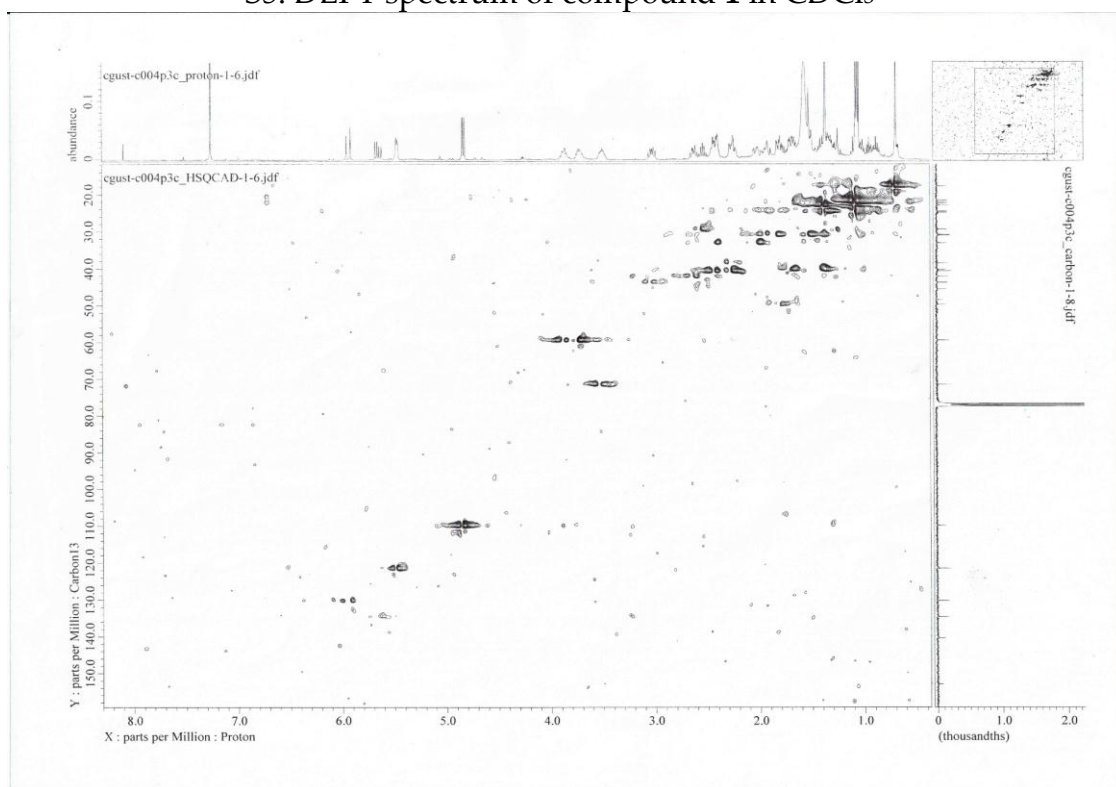
S3. ^1H NMR spectrum (400 MHz) of compound **1** in CDCl_3



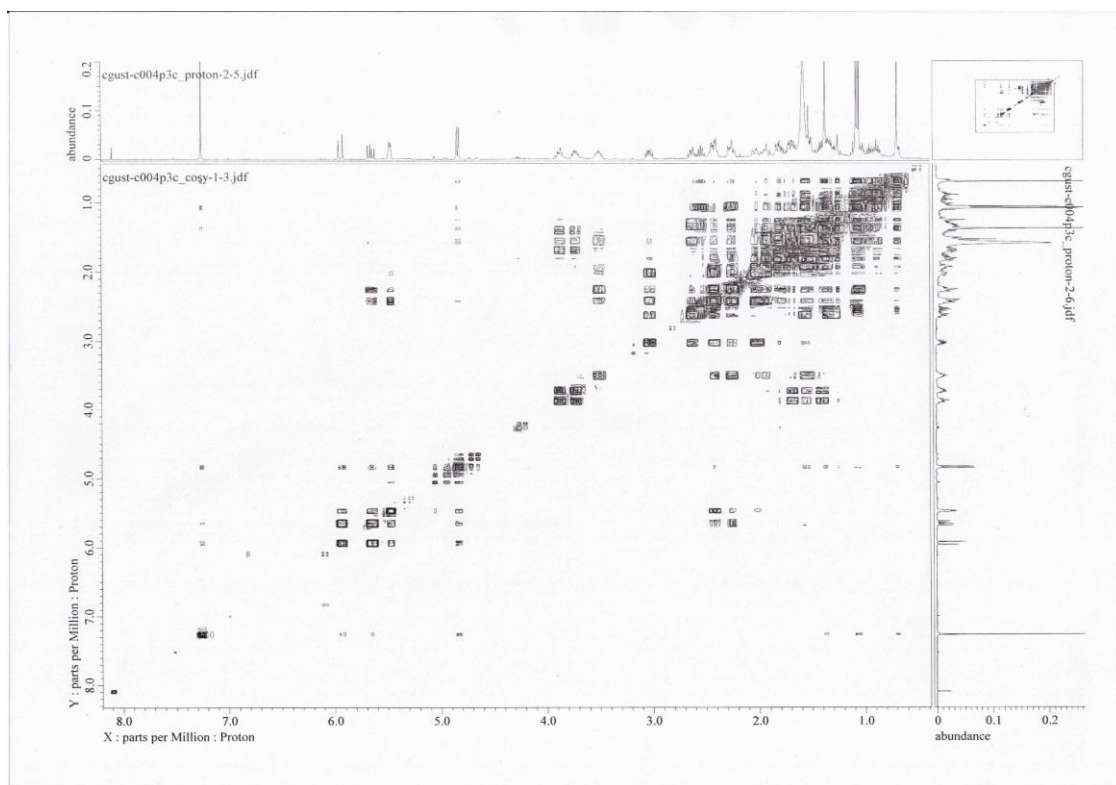
S4. ^{13}C NMR spectrum (100 MHz) of compound **1** in CDCl_3



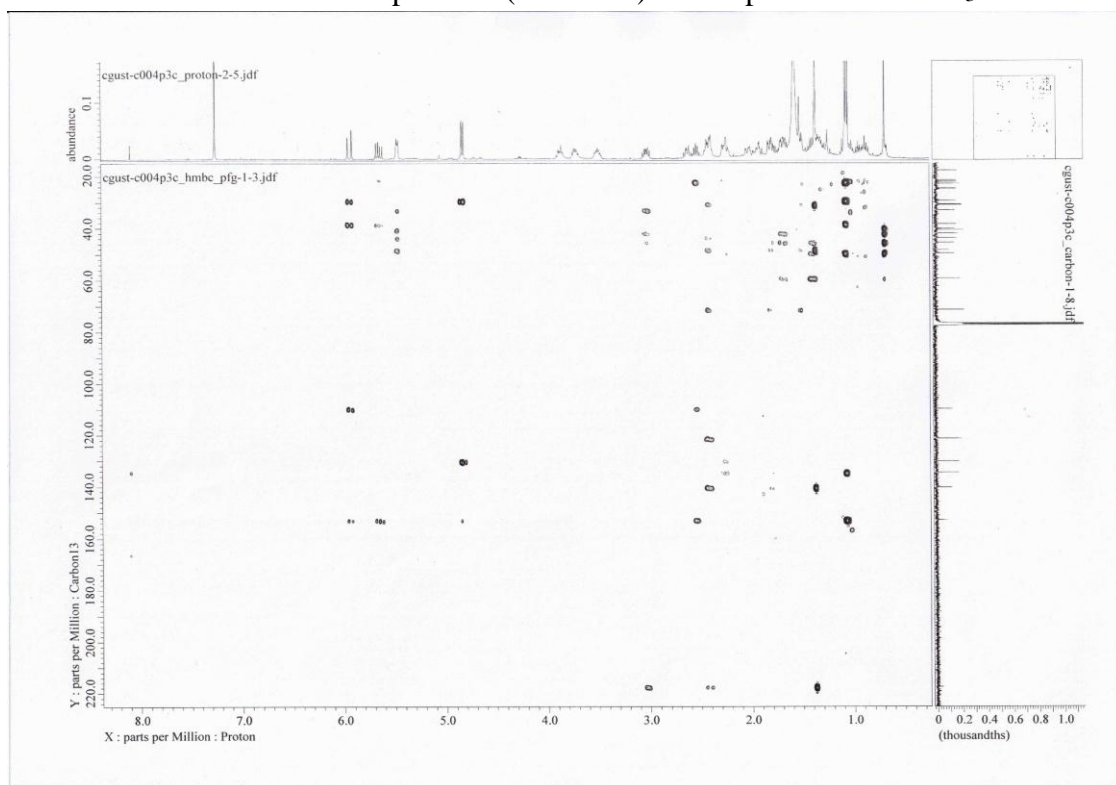
S5. DEPT spectrum of compound **1** in CDCl₃



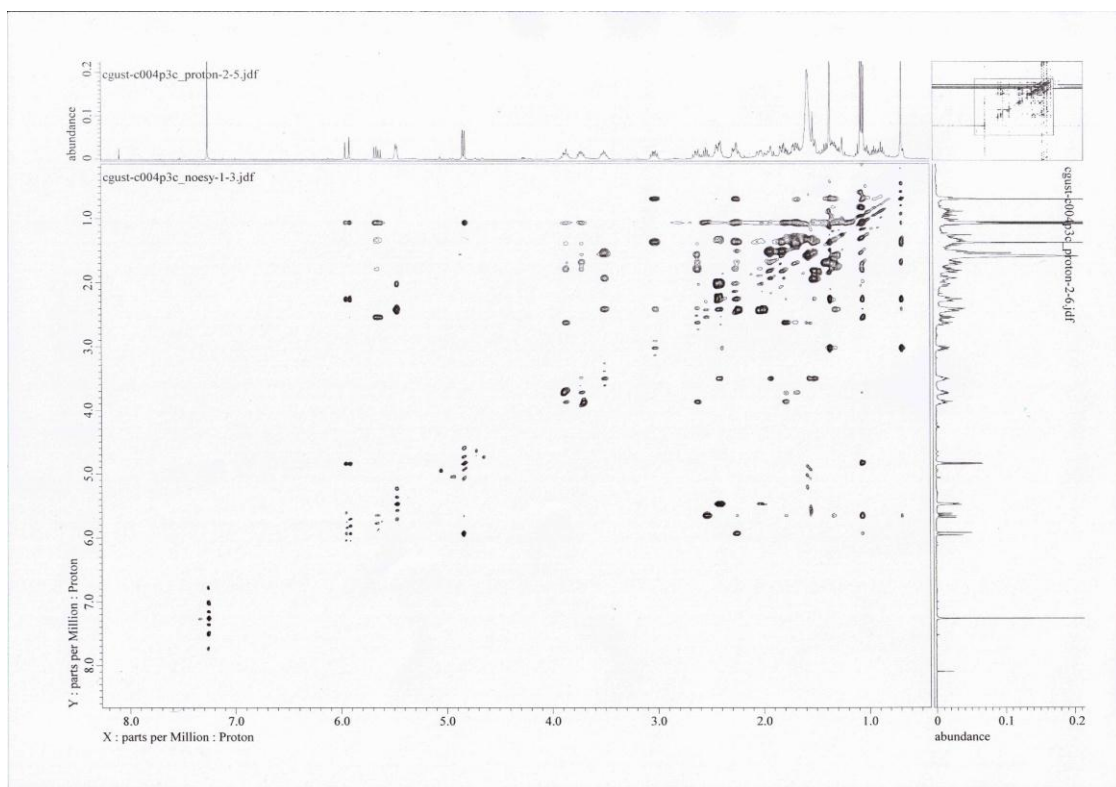
S6. gHSQC spectrum (400 MHz) of compound **1** in CDCl₃



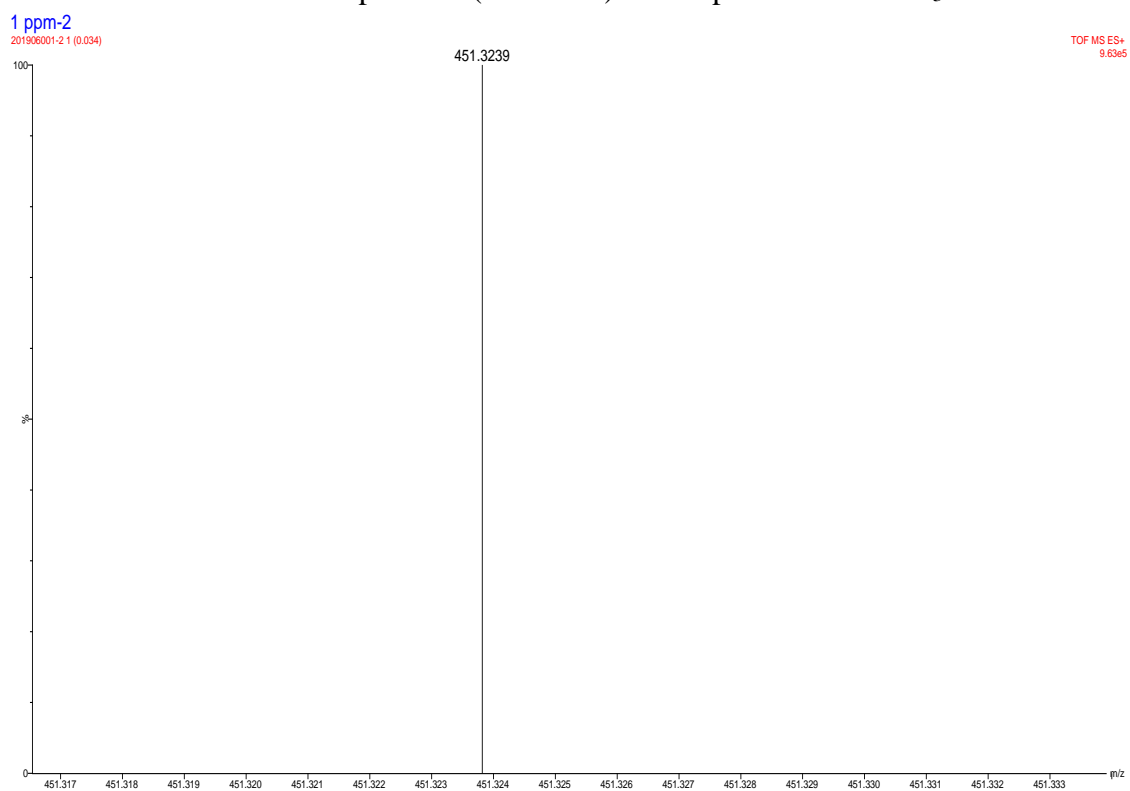
S7. ^1H - ^1H COSY spectrum (400 MHz) of compound **1** in CDCl_3



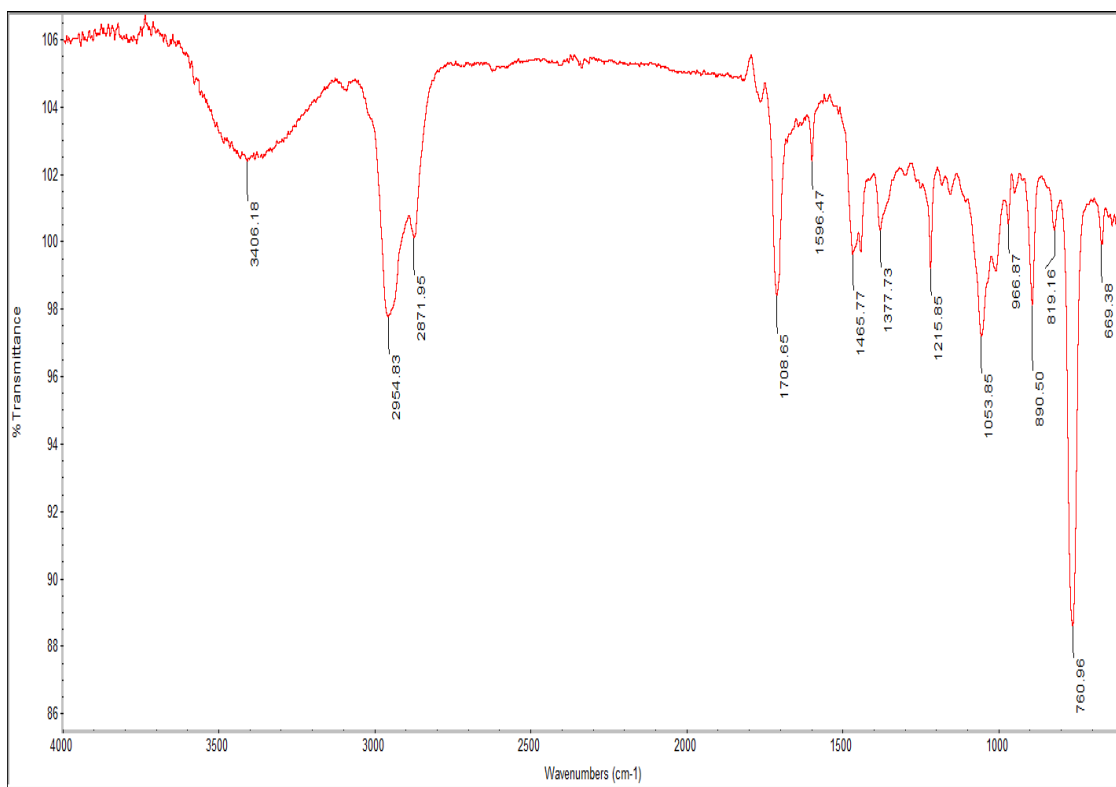
S8. gHMBC spectrum (400 MHz) of compound **1** in CDCl_3



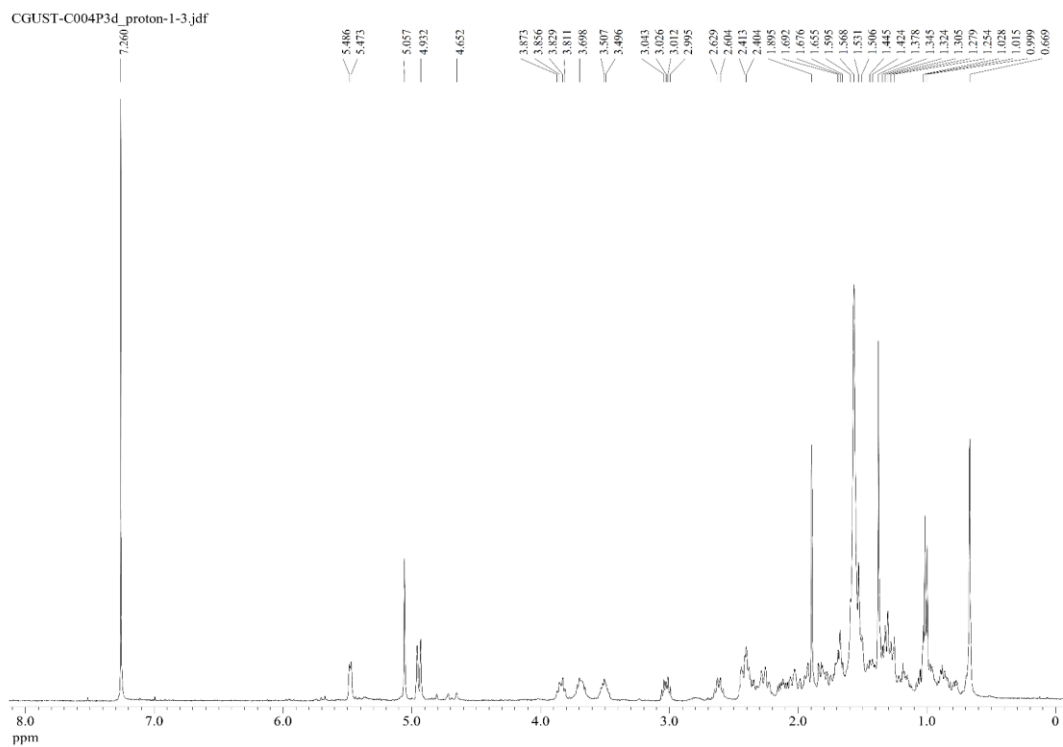
S9. NOESY spectrum (400 MHz) of compound **1** in CDCl_3



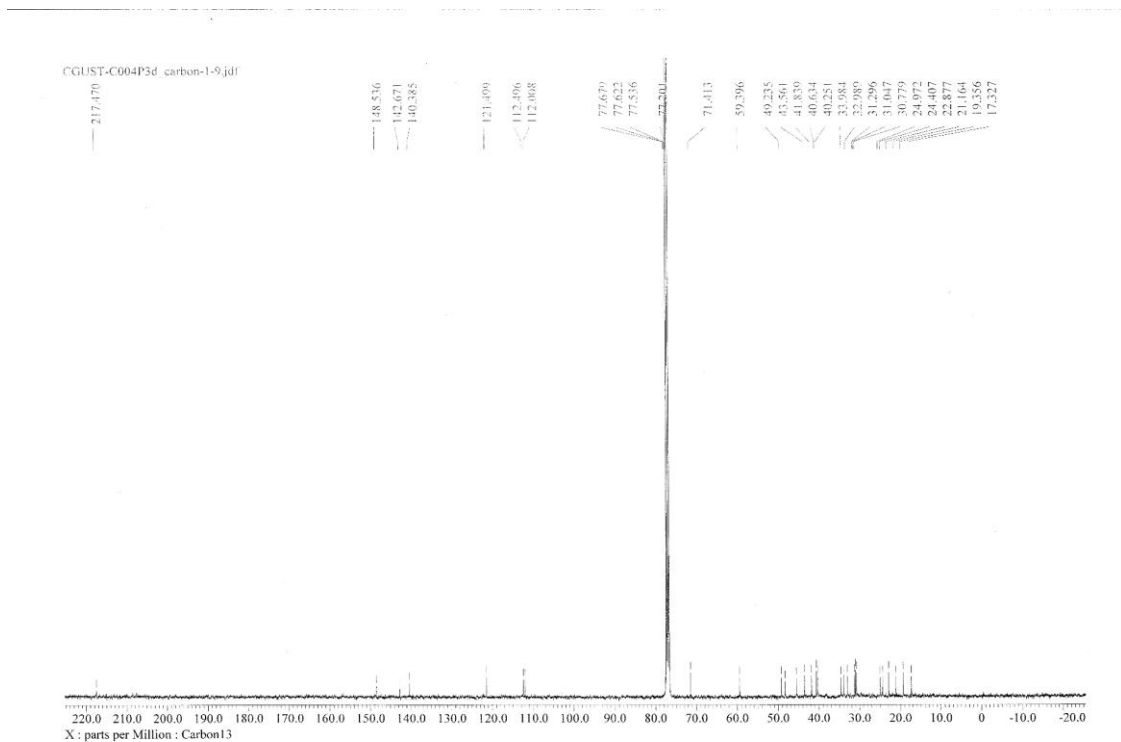
S10. HRMS spectrum of compound **2**



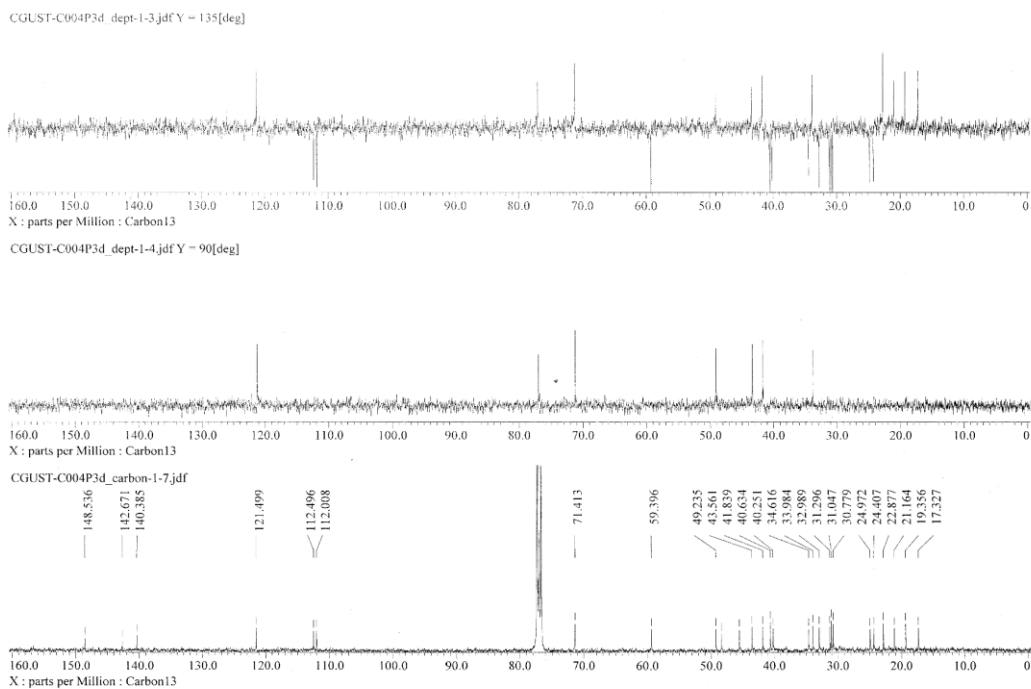
S11. IR spectrum of compound 2



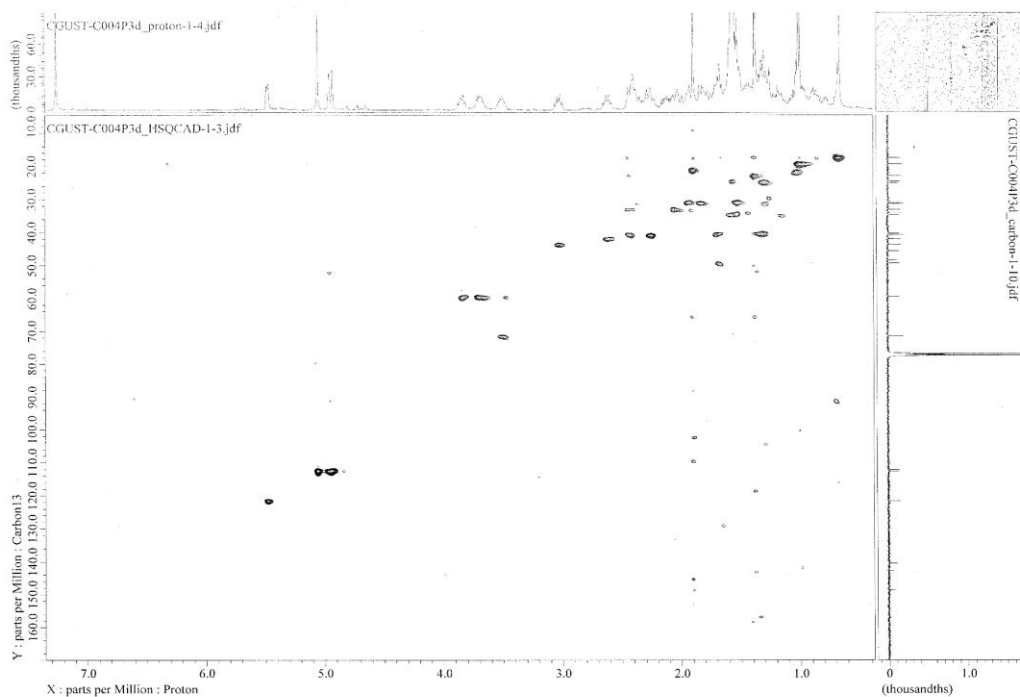
S12. ¹H NMR spectrum (400 MHz) of compound 2 in CDCl₃



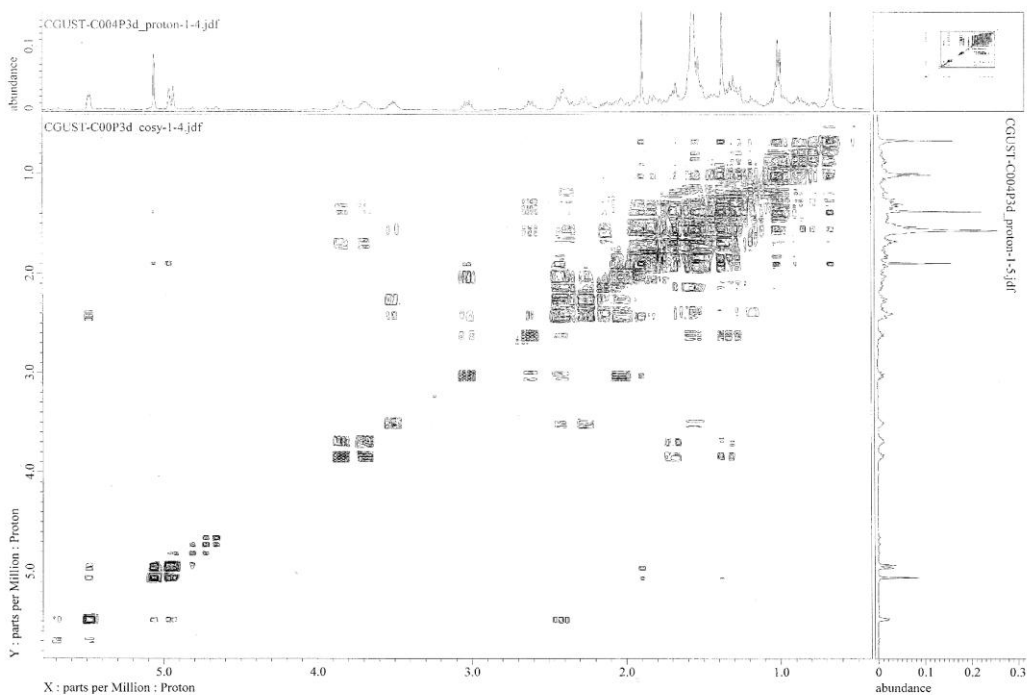
S13. ^{13}C NMR spectrum (100 MHz) of compound **2** in CDCl_3



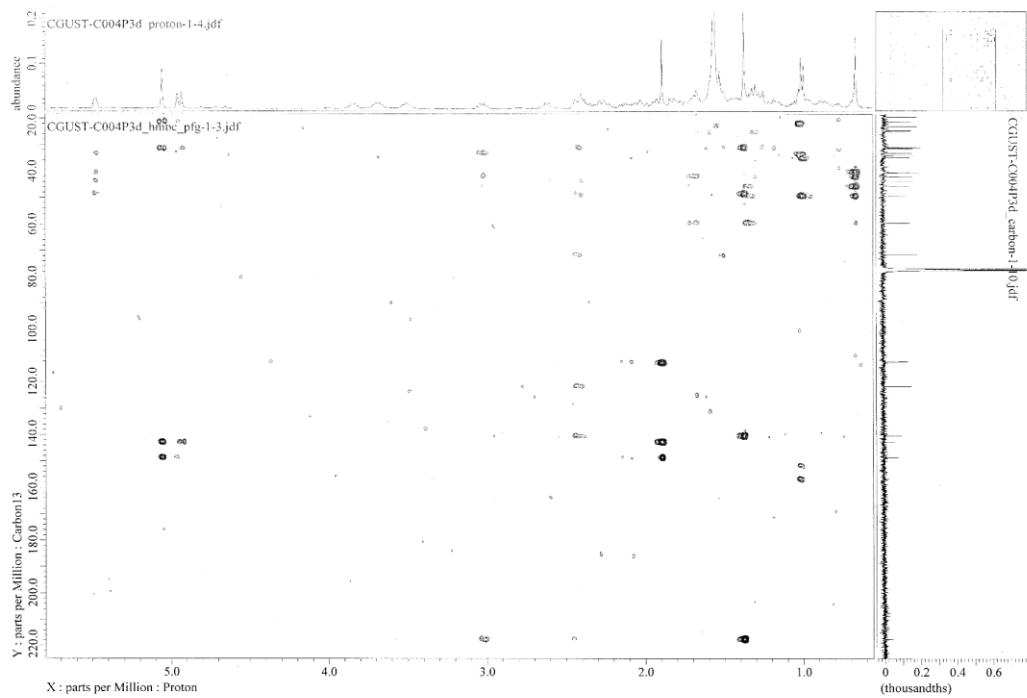
S14. DEPT spectrum of compound **2** in CDCl_3 .



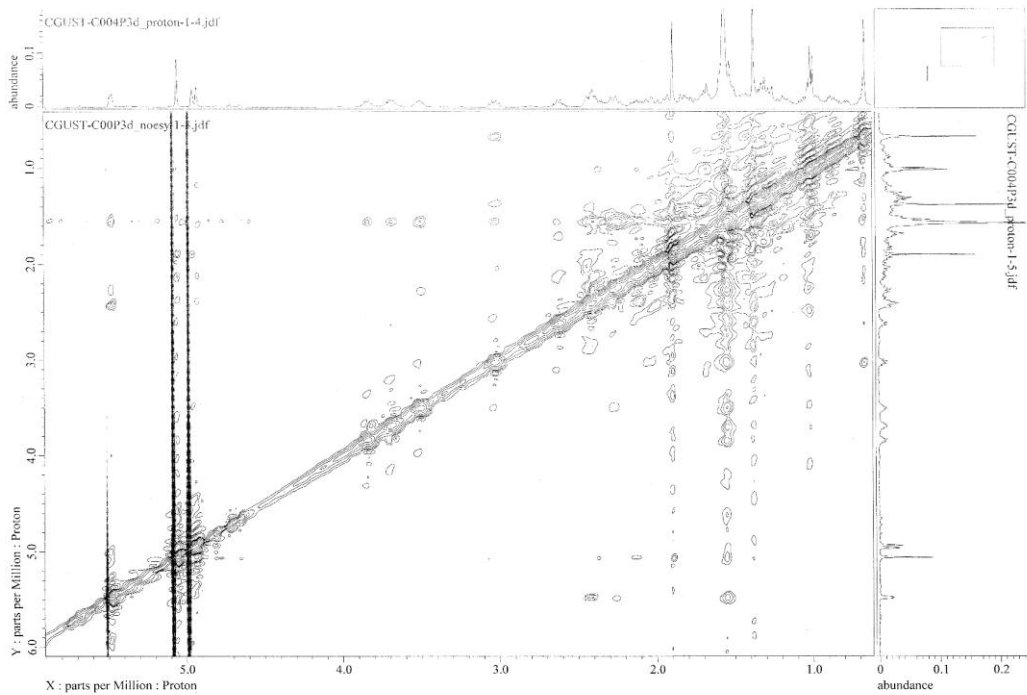
S15. gHSQC spectrum (400 MHz) of compound **2** in CDCl₃



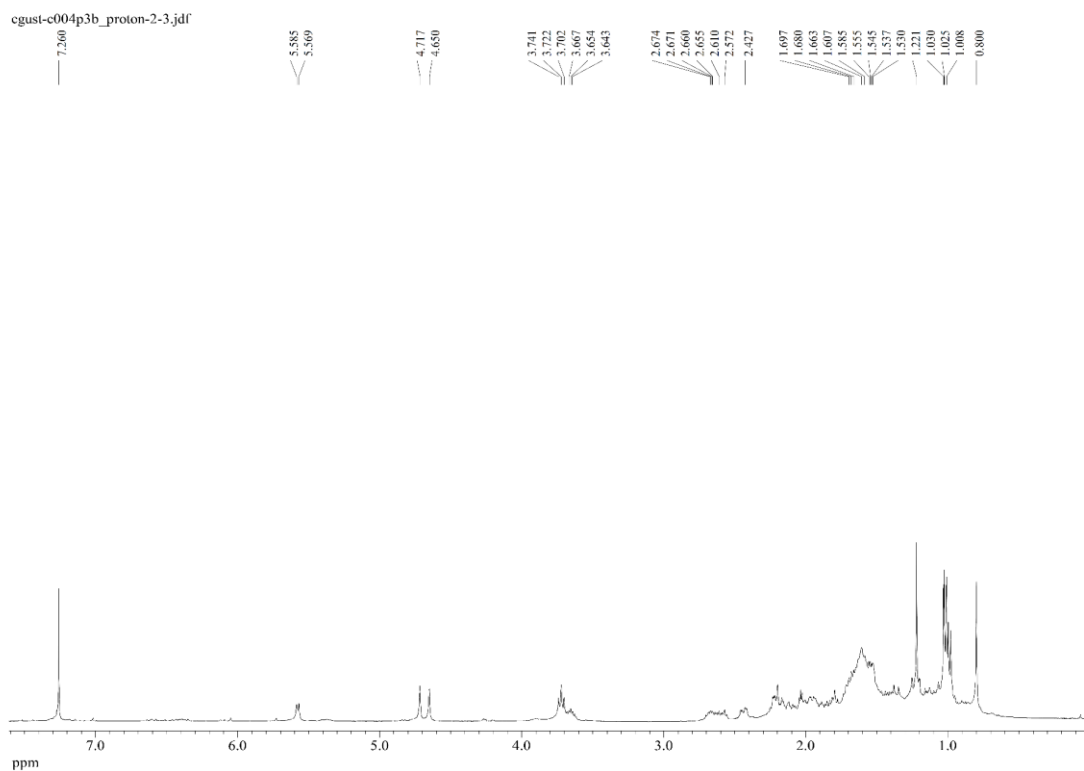
S16. ¹H-¹H COSY spectrum (400 MHz) of compound **2** in CDCl₃



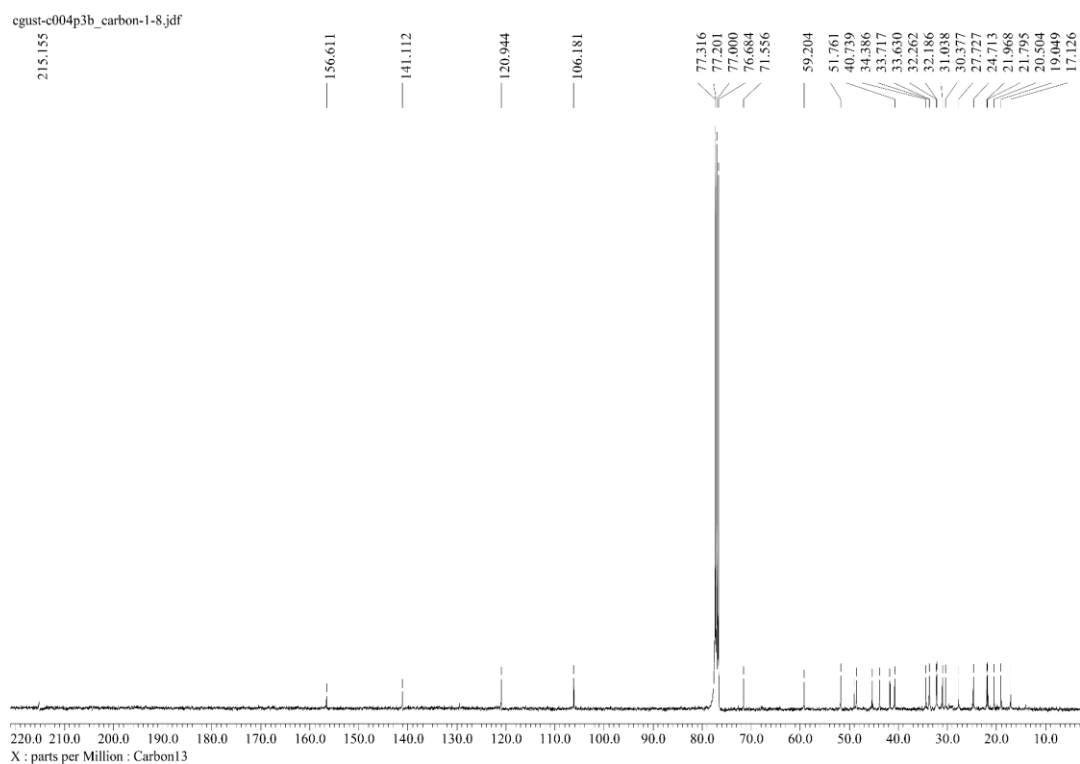
S17. gHMBC spectrum (400 MHz) of compound **2** in CDCl_3



S18. NOESY spectrum (400 MHz) of compound **2** in CDCl_3

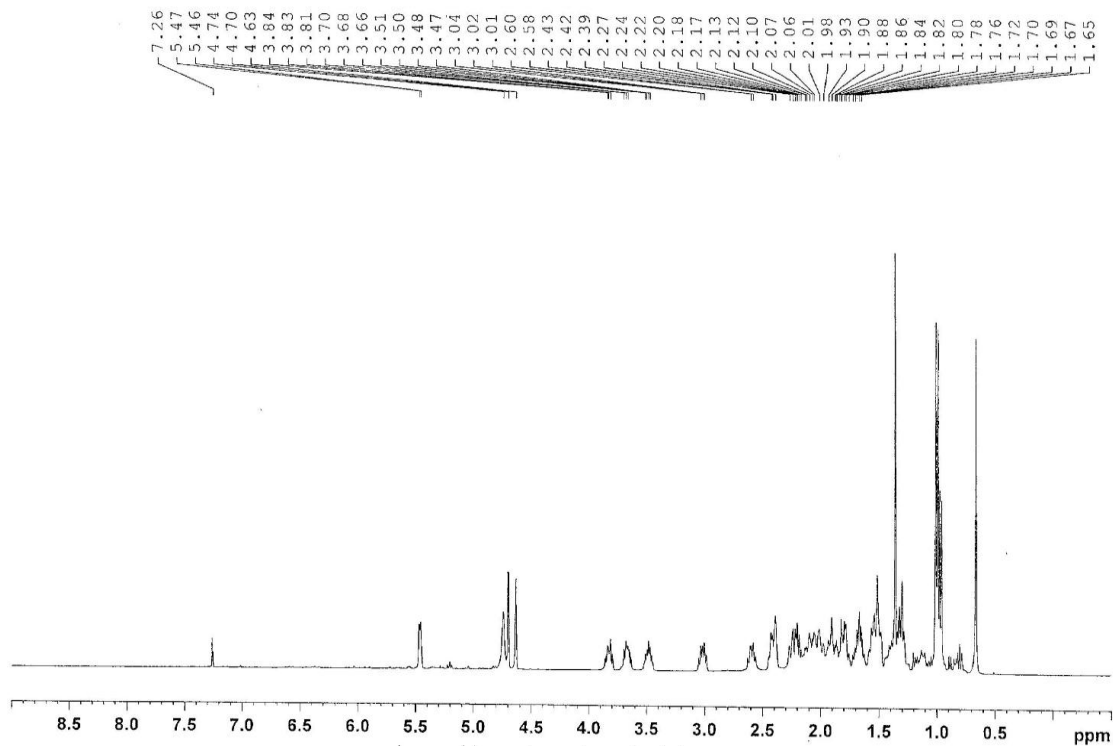


S19. ^1H NMR spectrum (400 MHz) of compound **3** in CDCl_3



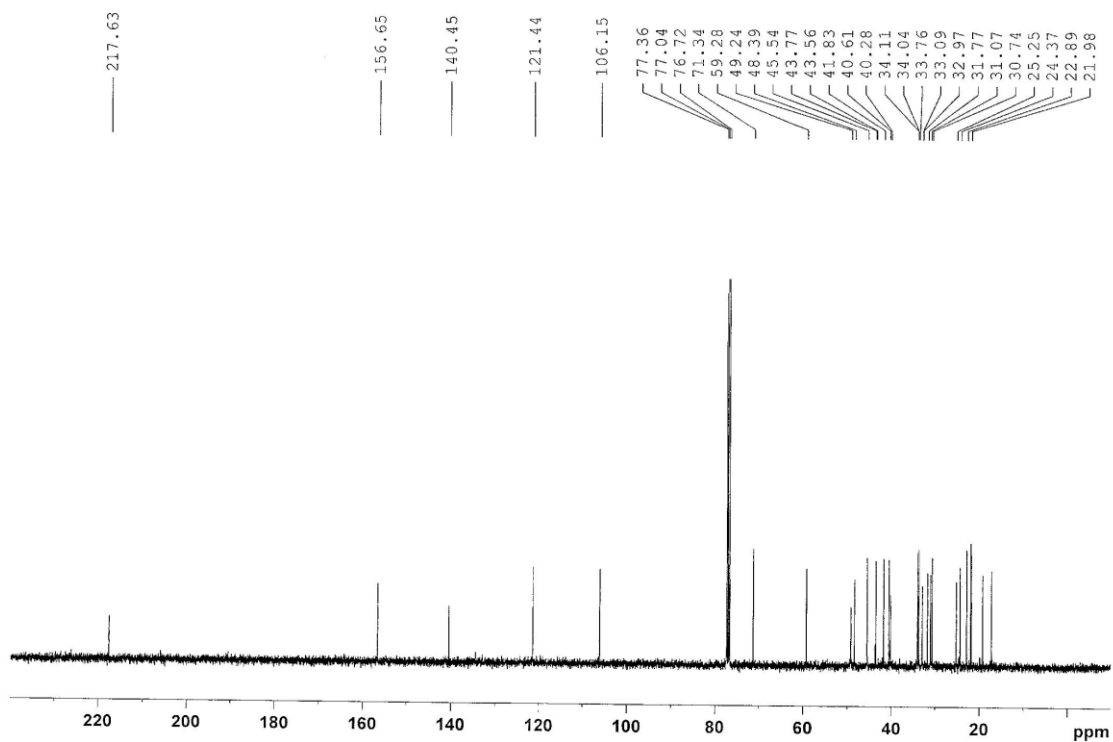
S20. ^{13}C NMR spectrum (100 MHz) of compound **3** in CDCl_3

CGUST-C004P3



S21. ¹H NMR spectrum (400 MHz) of compound **4** in CDCl₃

CGUST-C004P3-C13



S22. ¹³C NMR spectrum (100 MHz) of compound **4** in CDCl₃