

Supplementary Information for:

Naphthoquinone Derivatives as Potential Immunomodulators: Prospective for COVID-19 Treatment

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1. Experimental spectra

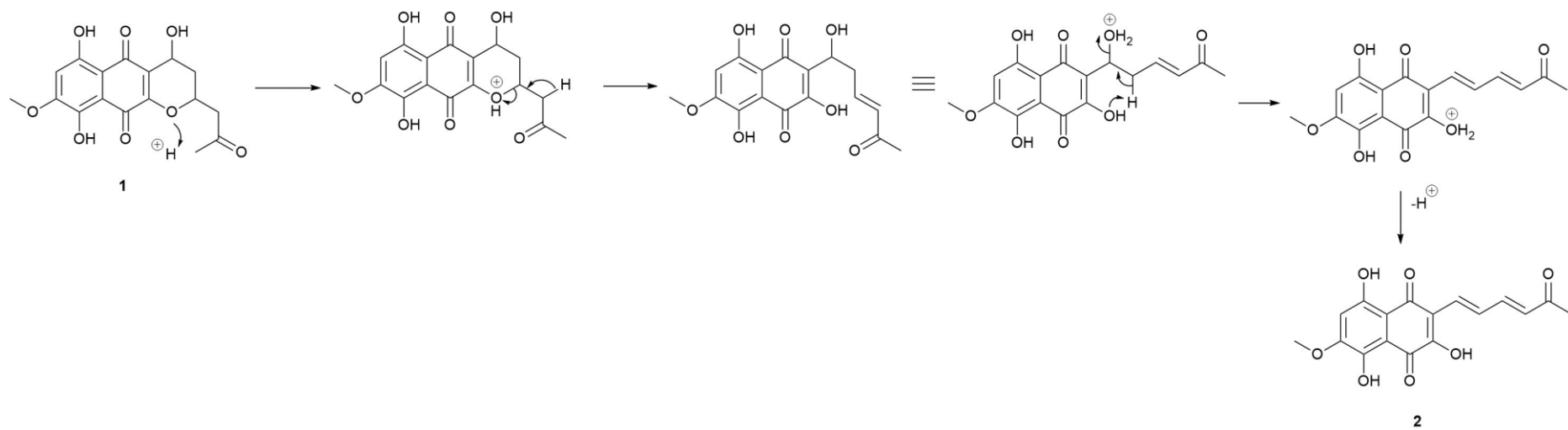


Figure S1. Plausible mechanism for the conversion of Erythrostominone (1) into 3,5,8-TMON (2).

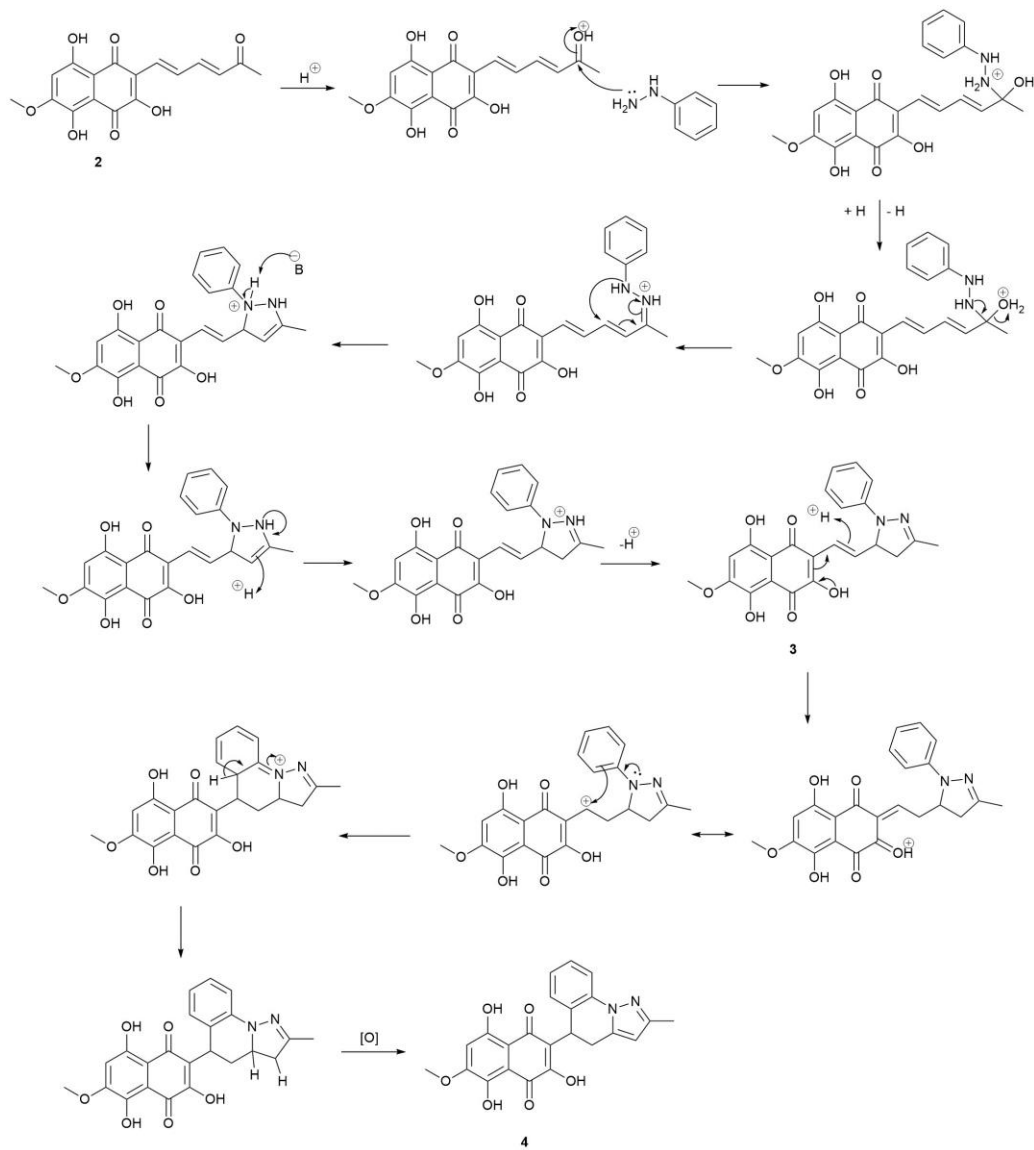


Figure S1. Plausible mechanism for the synthesis of 3 and 4.

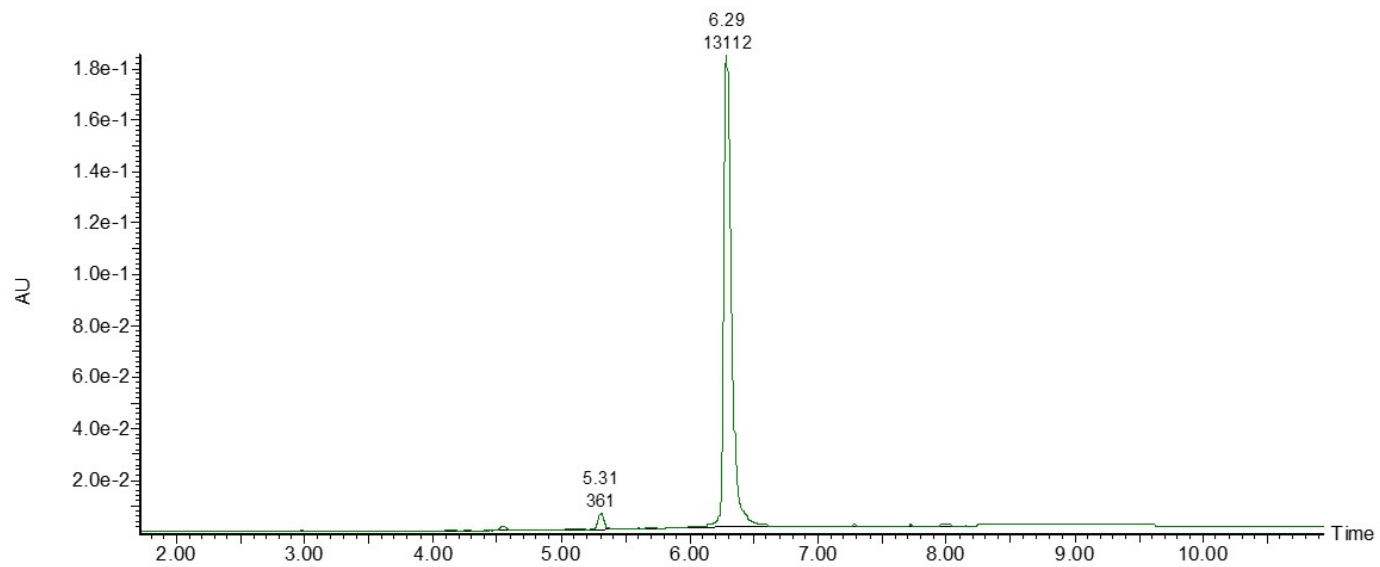


Figure S2. 3,5,8-TMON (2) UPLC-DAD chromatogram. Relative peak purity (97.3%).

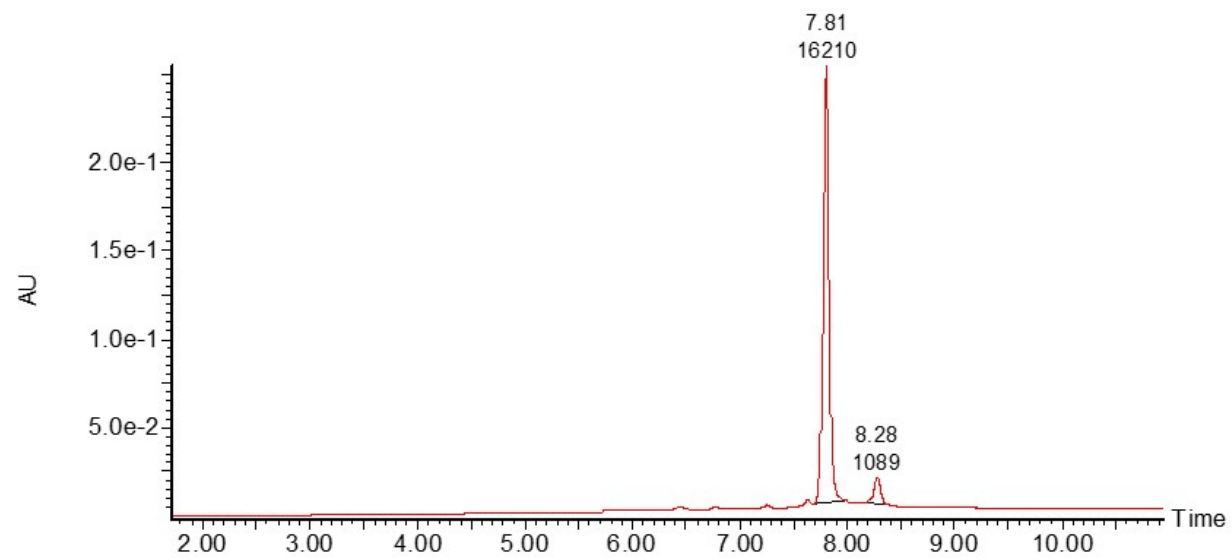


Figure S3. Compound 3 UPLC-DAD chromatogram. Relative peak purity (93.7%)

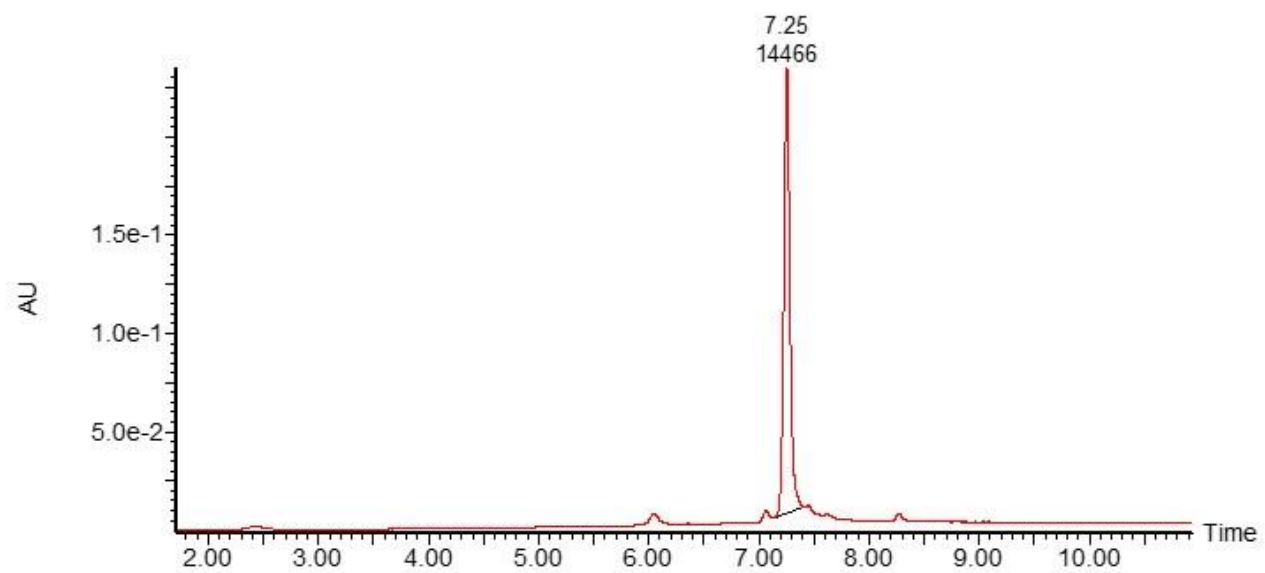


Figure S4. Compound 4 UPLC-DAD. Relative peak purity (~100%)

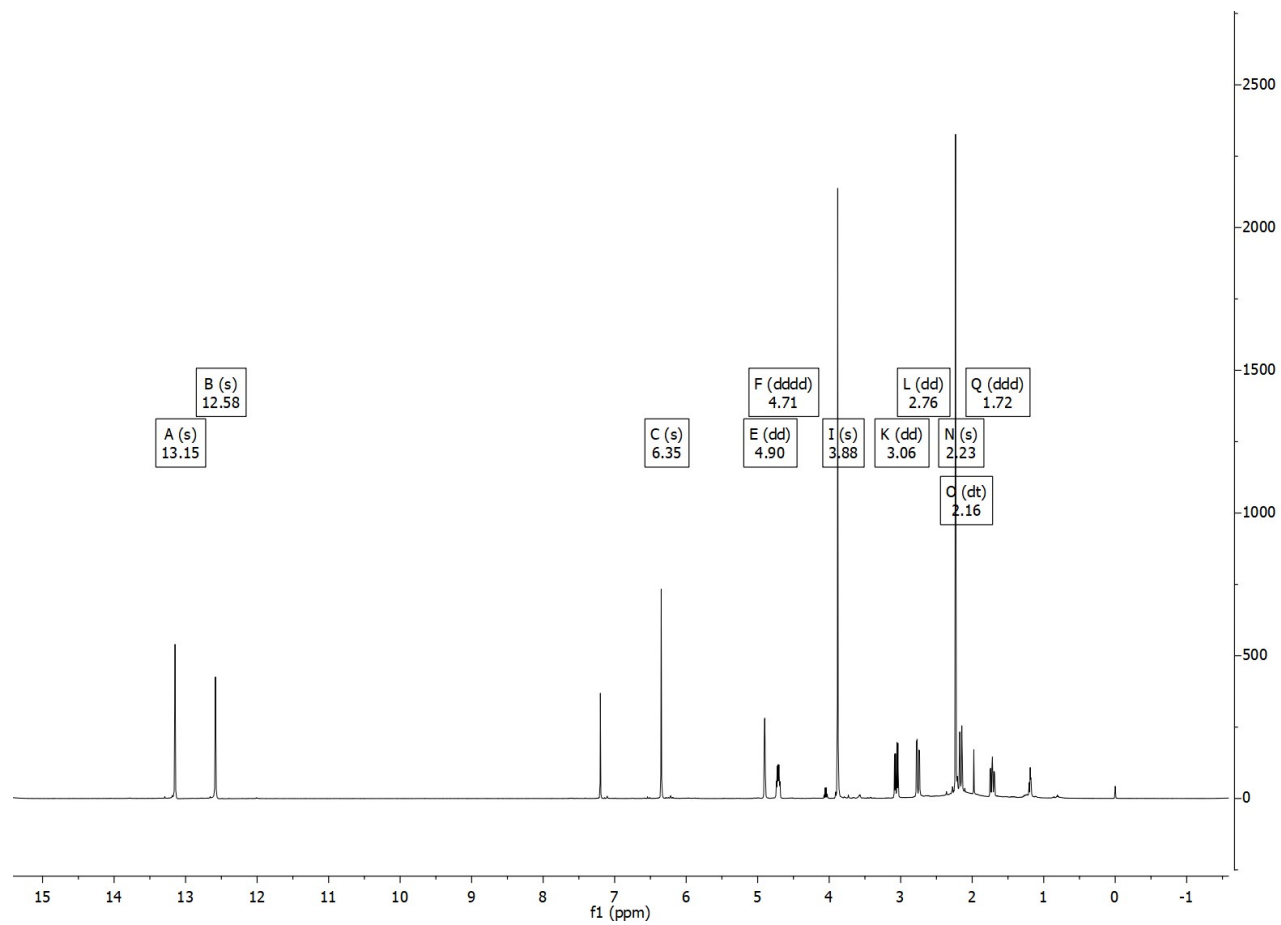


Figure S5. ¹H NMR spectra of Erythrostominone in CdCl₃, 500 MHz.

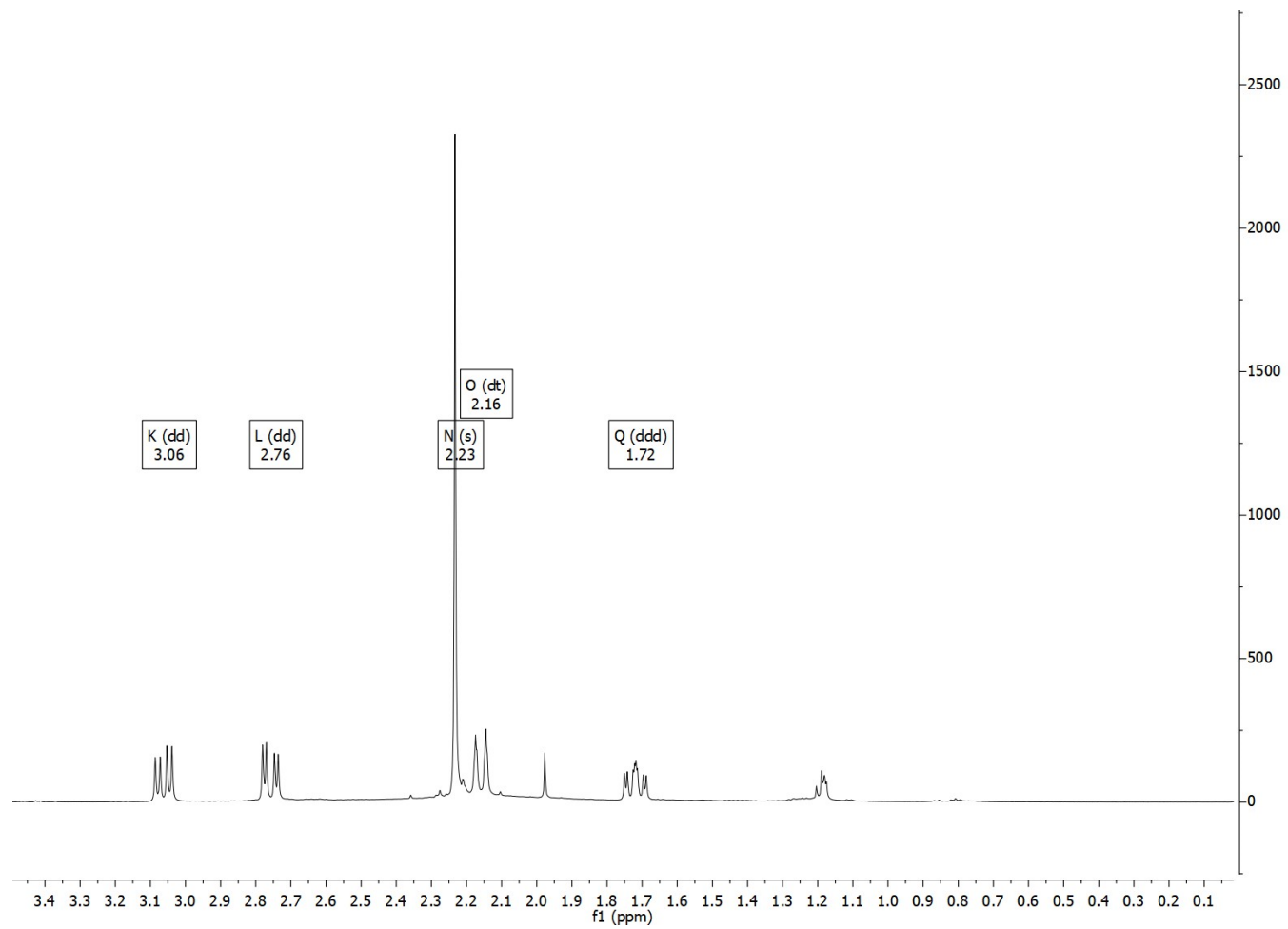


Figure S6. ¹H NMR spectra of Erythrostominone from 0 to 3.5 ppm in CDCl₃, 500 MHz.

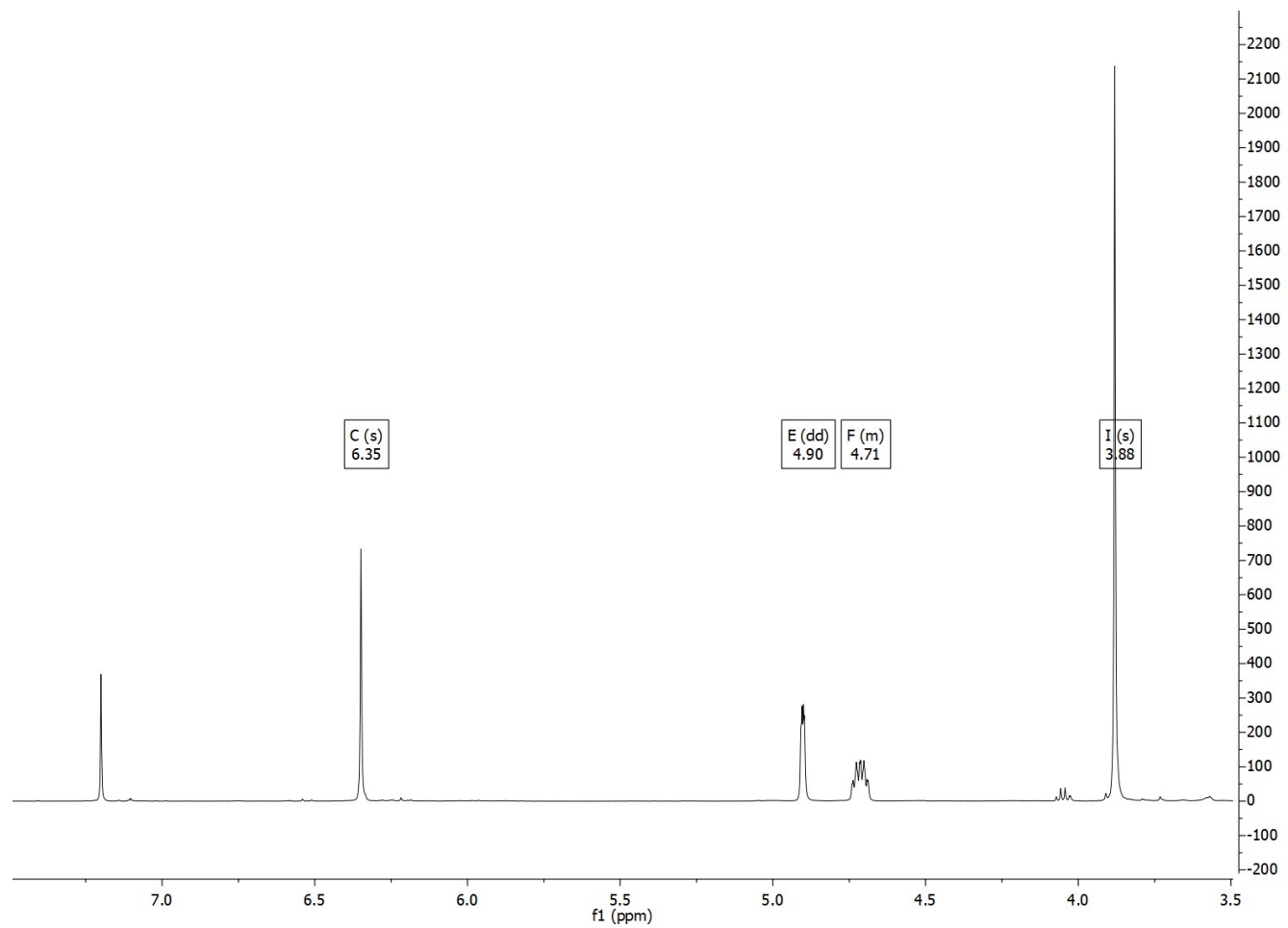


Figure S7. ^1H NMR spectra of Erythrostominone from 3.5 to 7.5 ppm in CDCl_3 , 500 MHz.

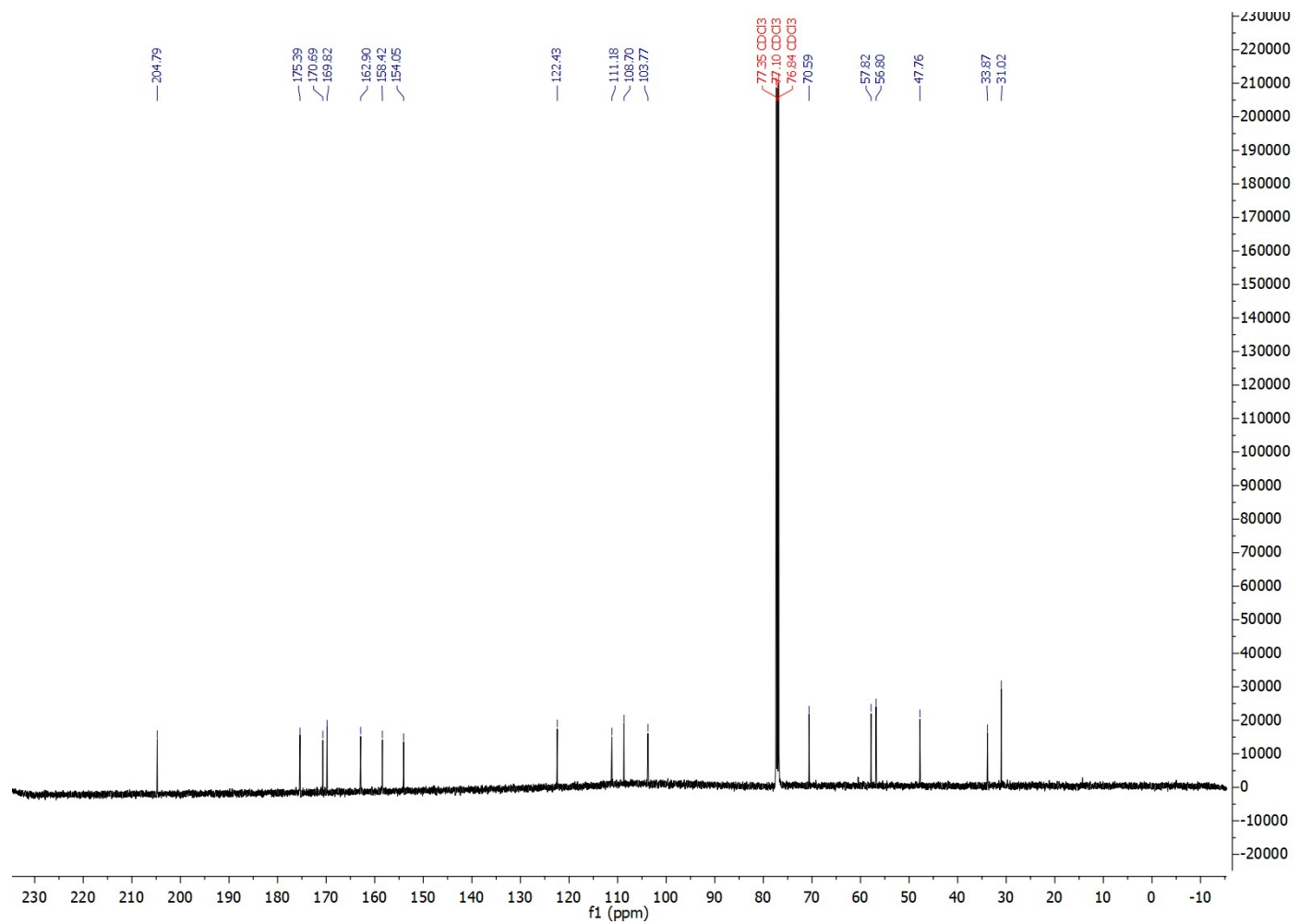


Figure S8. ^{13}C NMR spectra of Erythrostominone in CDCl_3 , 125 MHz.

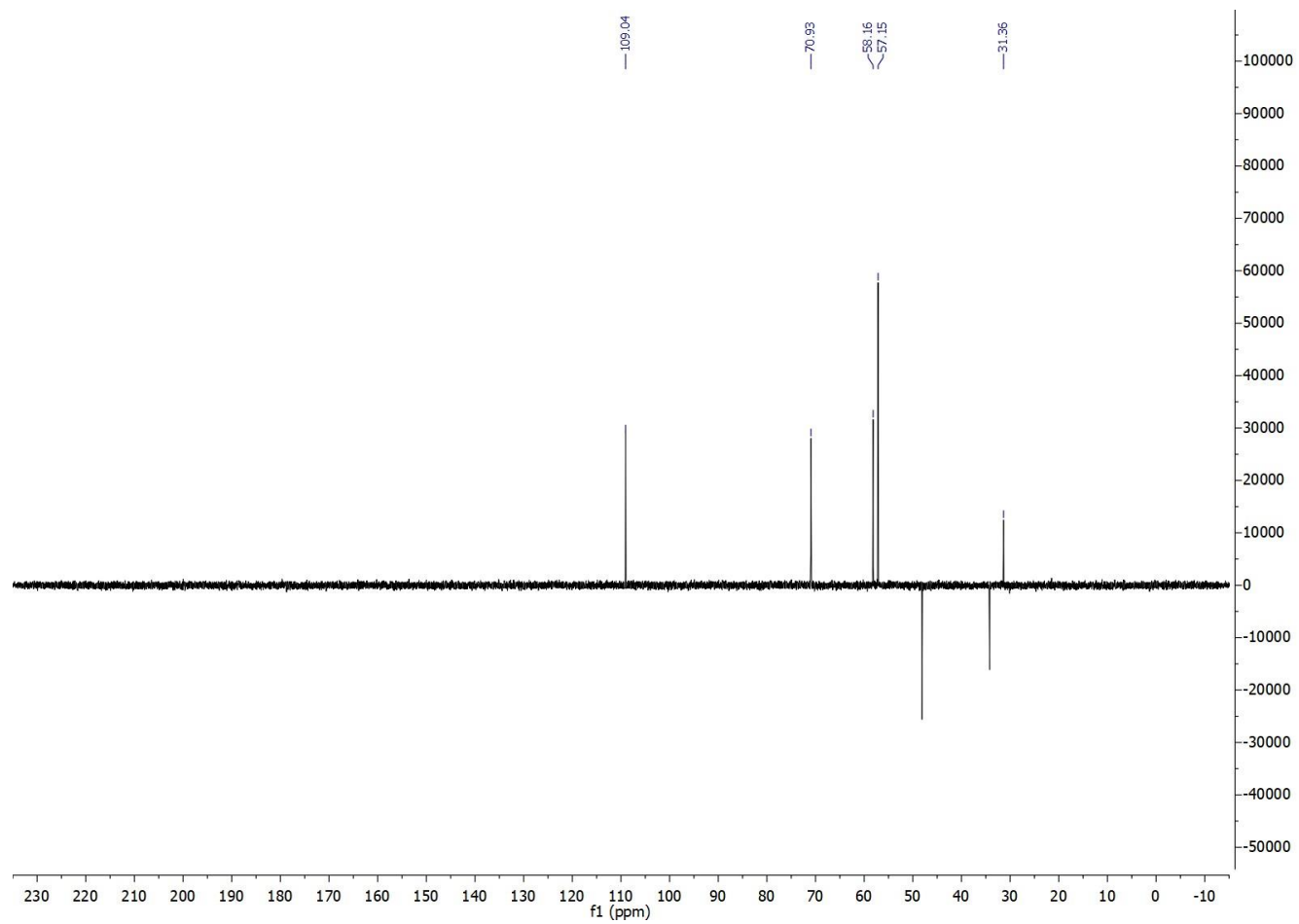


Figure S9. DEPT-136 NMR spectra of Erythrostominone in CDCl₃.

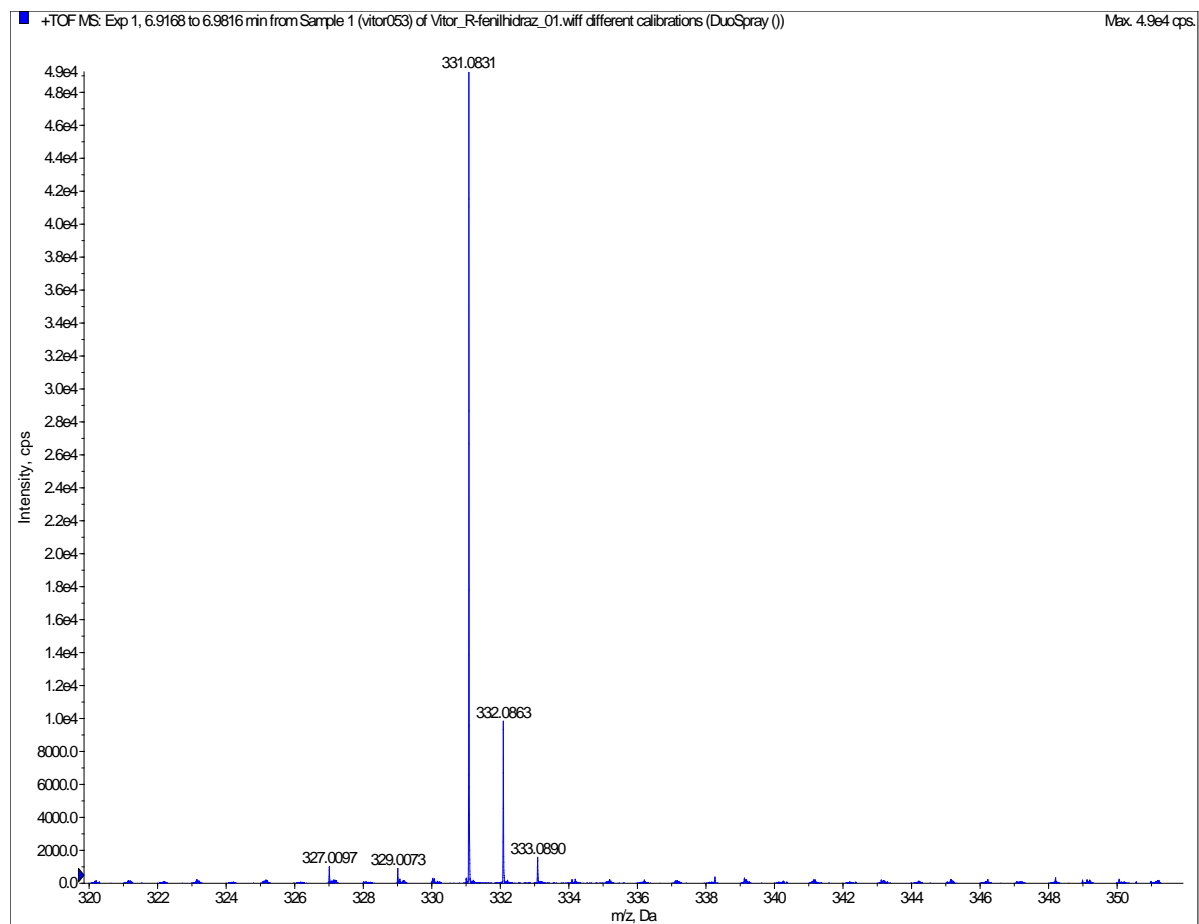


Figure S11. HRMS ESI+ spectra obtained in positive mode for 3,5,8-TMON (2). The molecular formula $C_{17}H_{14}O_7$ corresponds to the exact calculated mass of 330.0740 u for the deprotonated molecule, with a 3.9385 ppm error compared to the spectra.

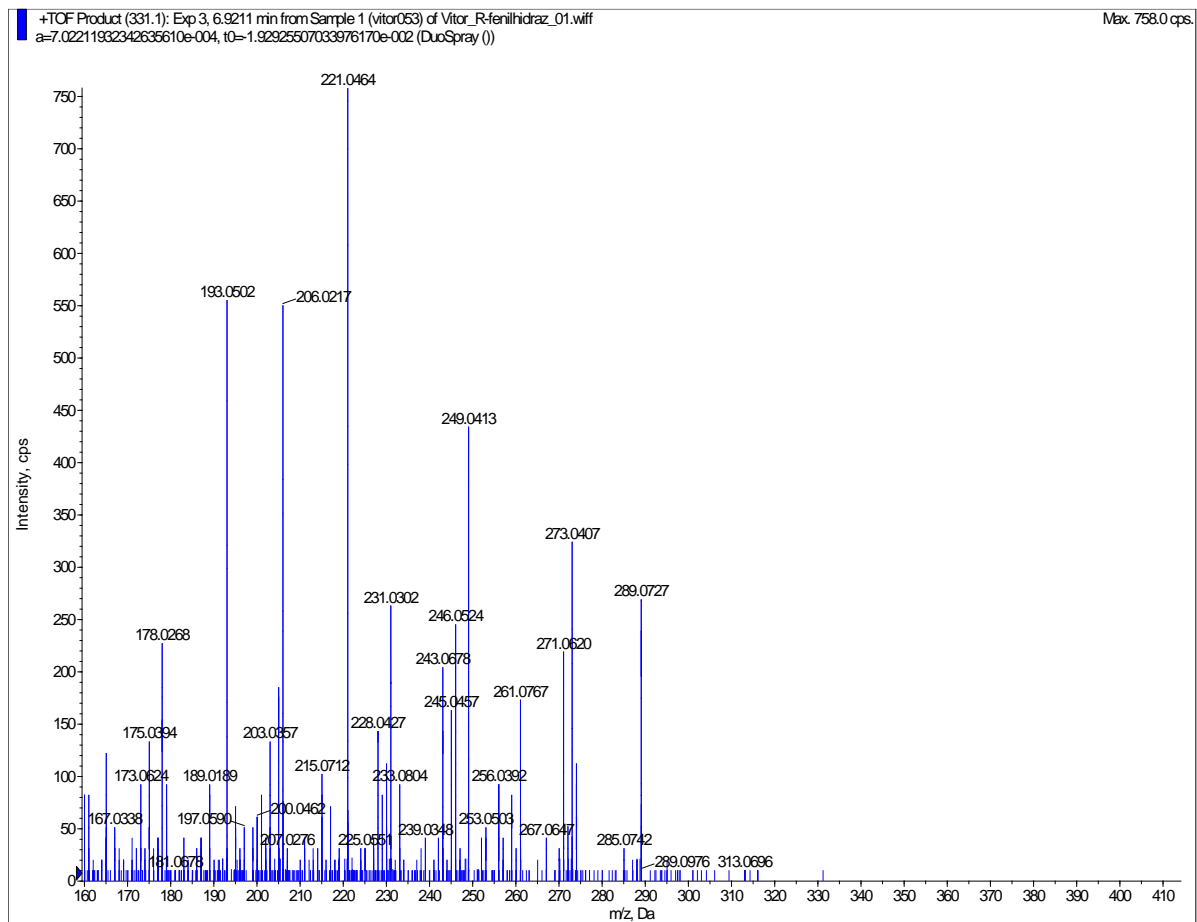


Figure S12. ESI+ CID spectra (30eV, N₂) of 3,5,8-TMON (2).

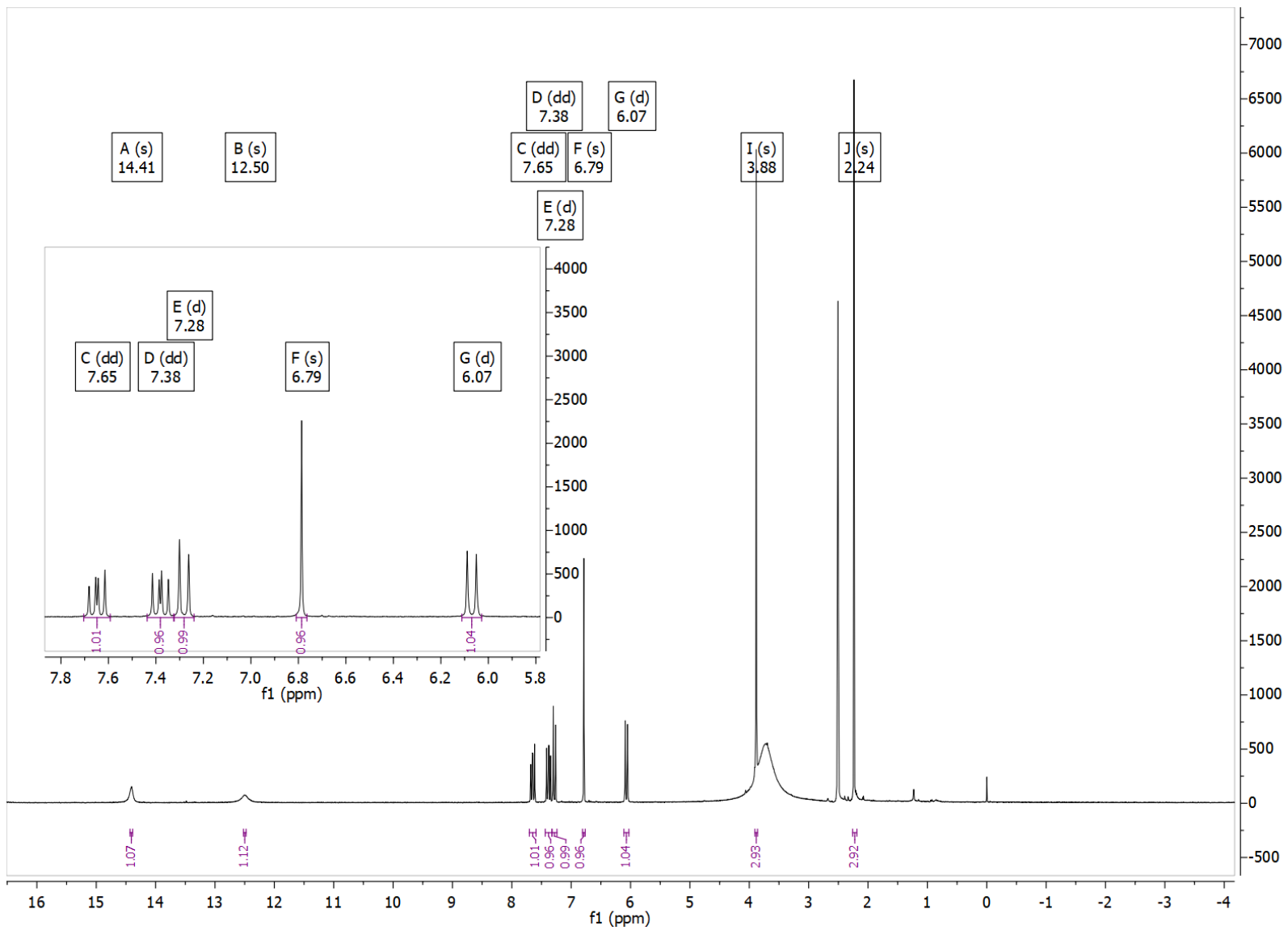


Figure S12. ¹H NMR spectra of 3,5,8-TMON in DMSO-d₆, 400 MHz.

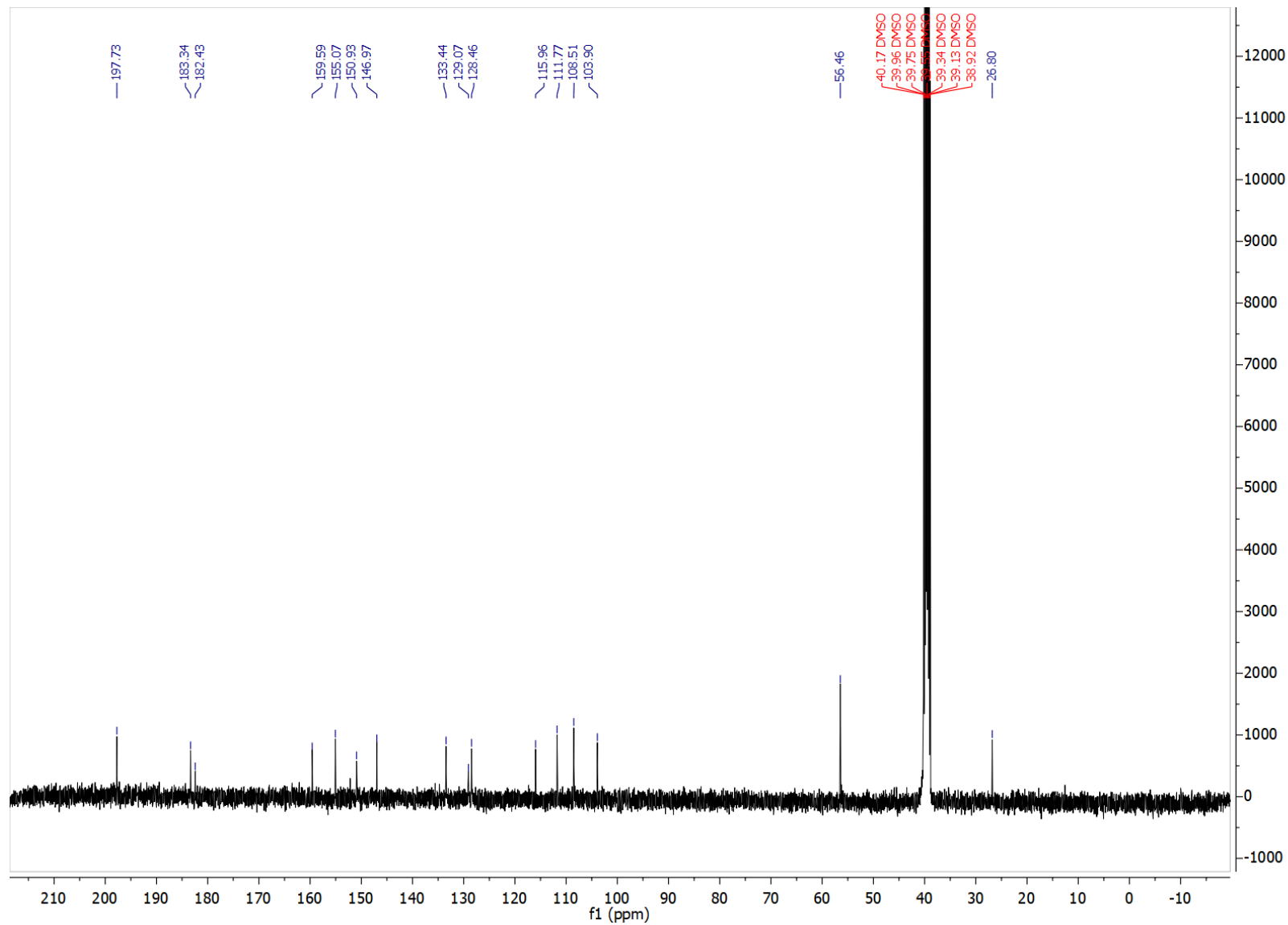


Figure S13. ^{13}C NMR spectra of 3,5,8-TMON in DMSO- d_6 , 100 MHz

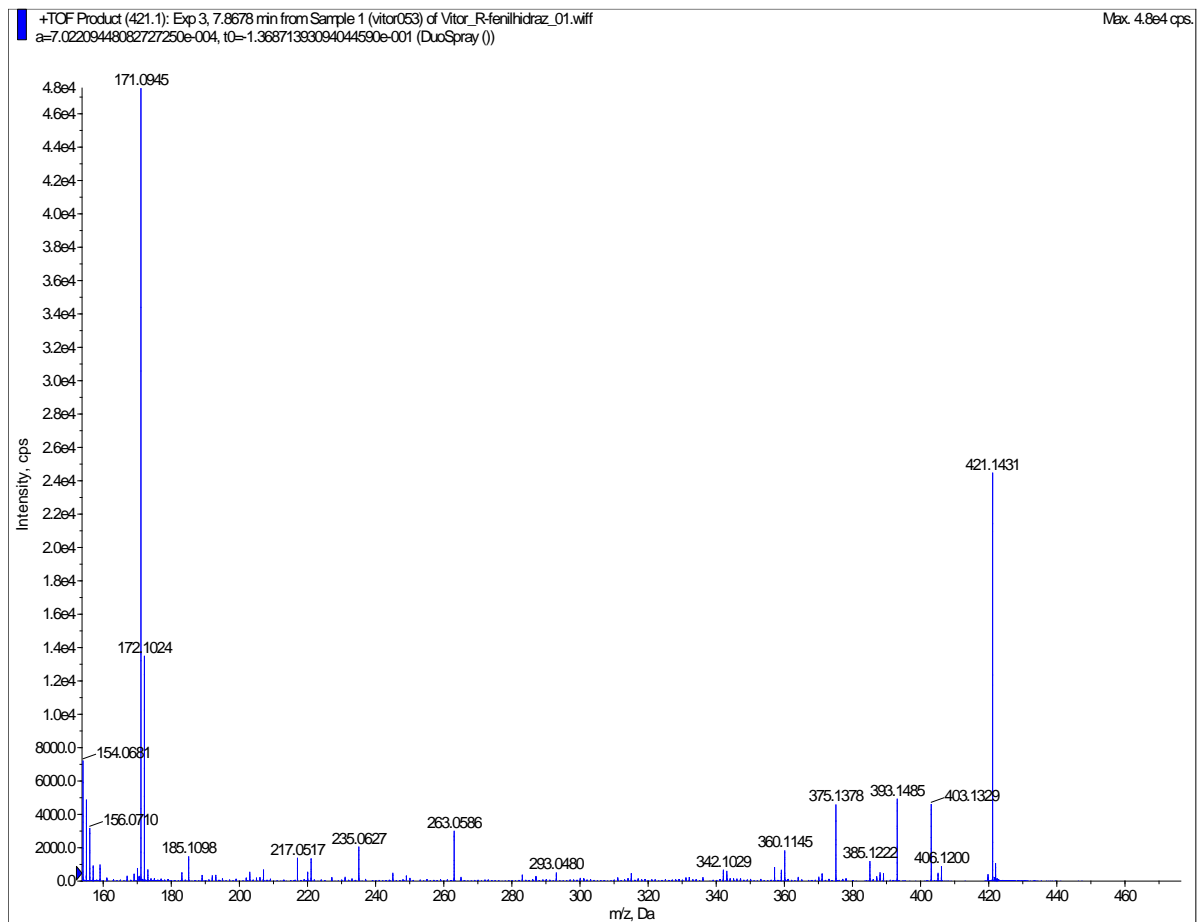


Figure S14. ESI+ CID spectra (30eV, N₂) of 3.

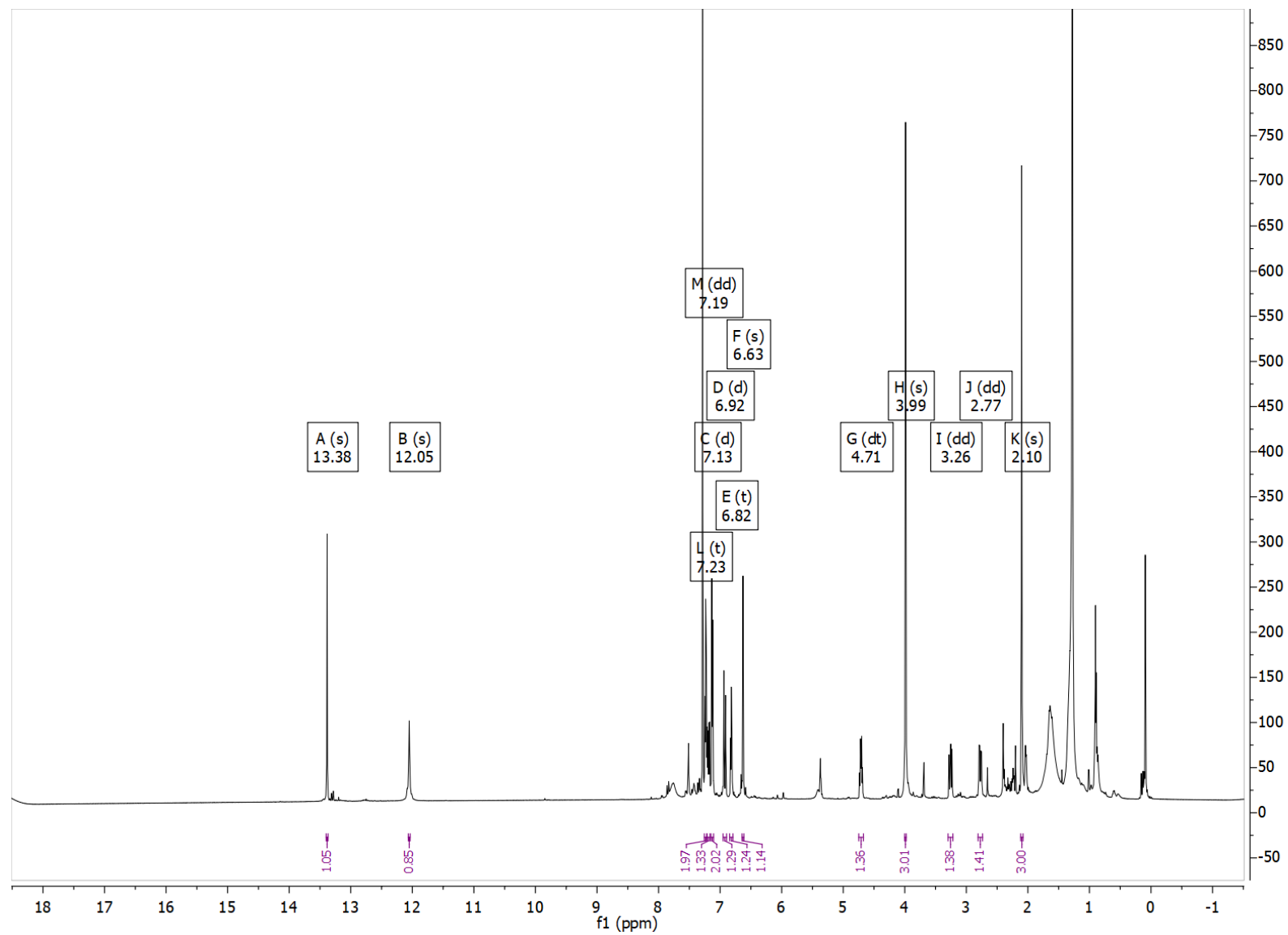


Figure S15. ^1H NMR spectra of **3** in CDCl_3 , 600 MHz.

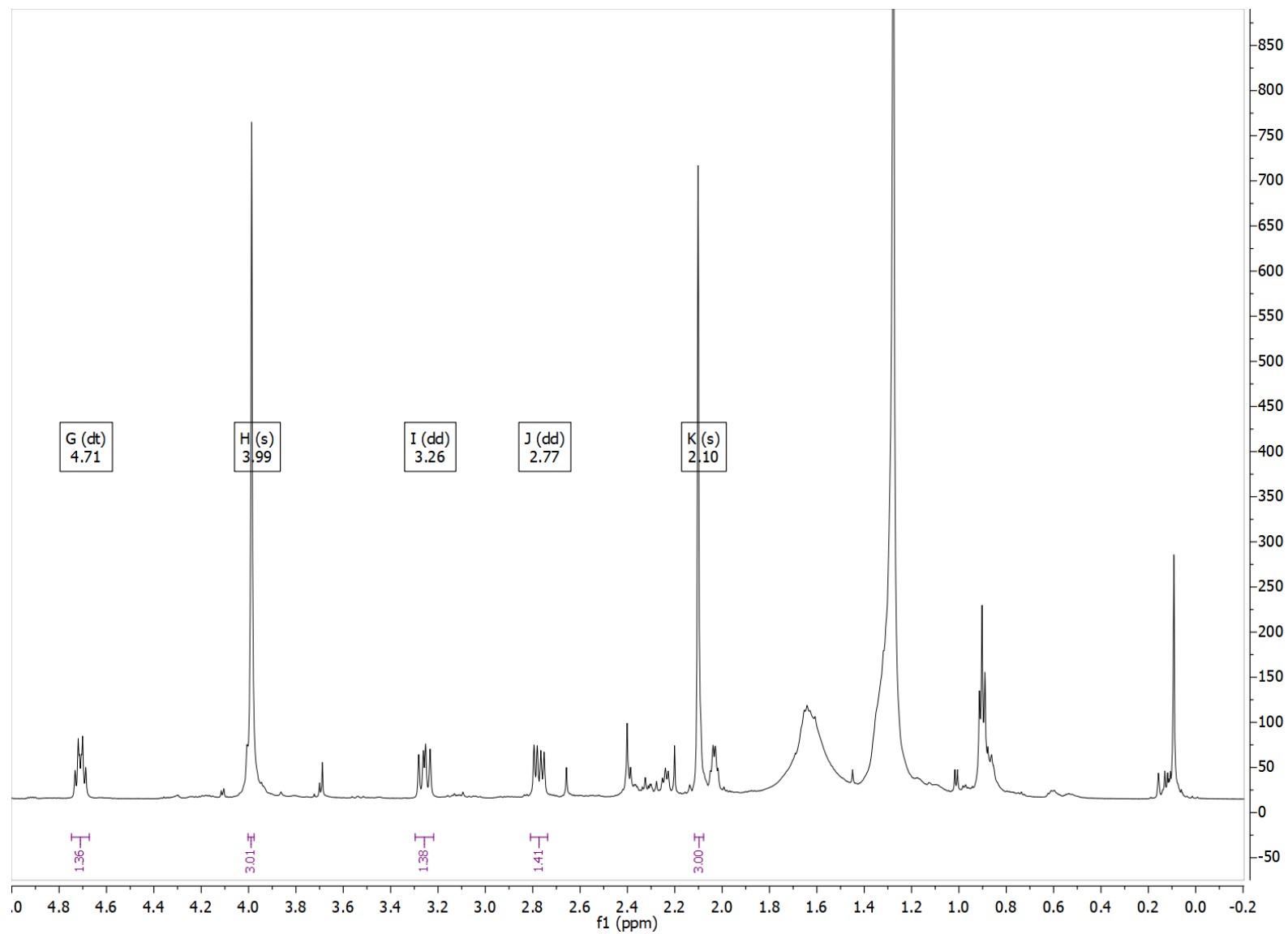


Figure S16. ¹H NMR spectra of 3 from 0 to 5 ppm in CDCl₃, 600 MHz.

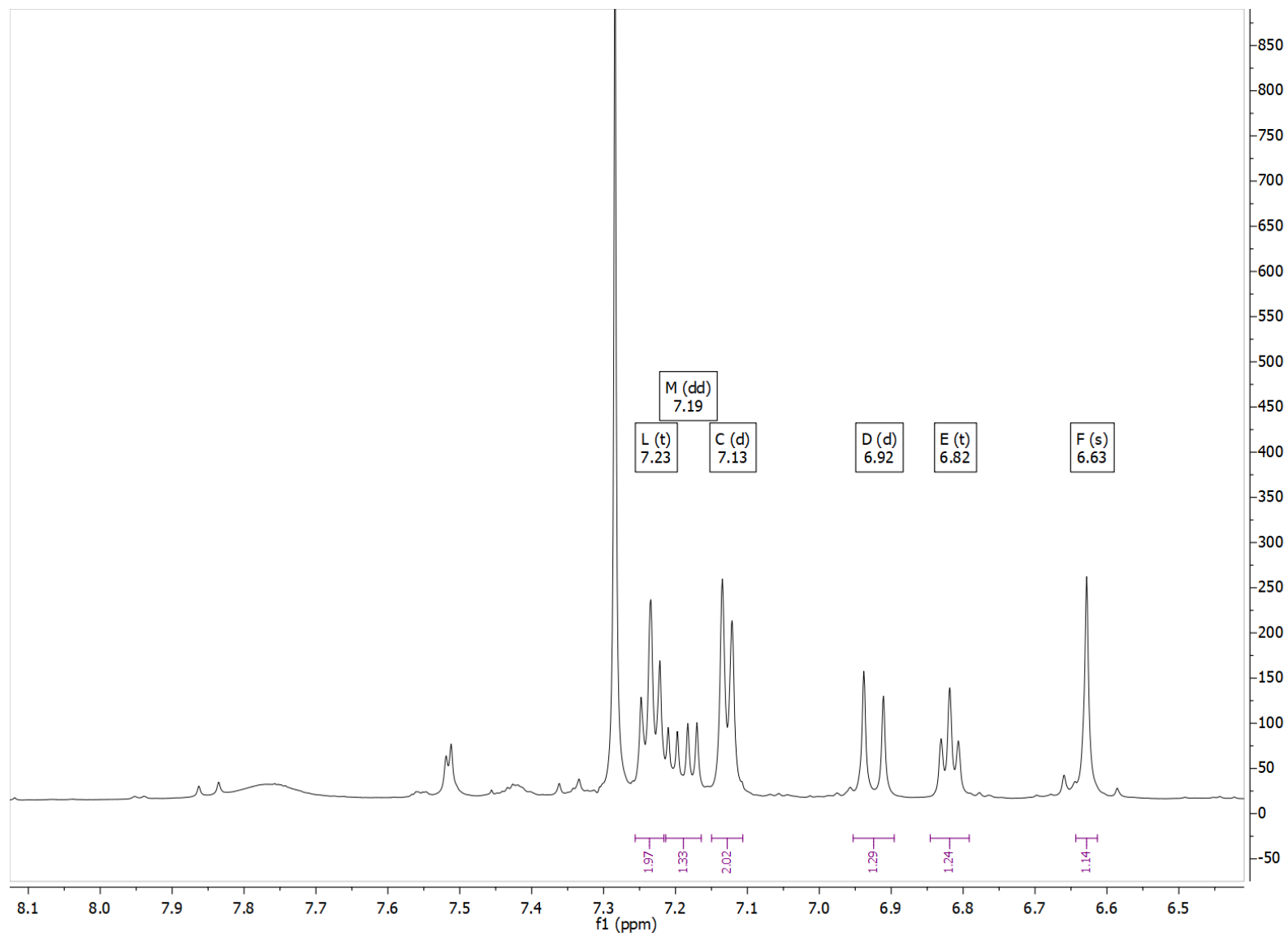


Figure S17. ¹H NMR spectra of 3 from 6.5 to 8.0 ppm in CDCl₃, 600 MHz.

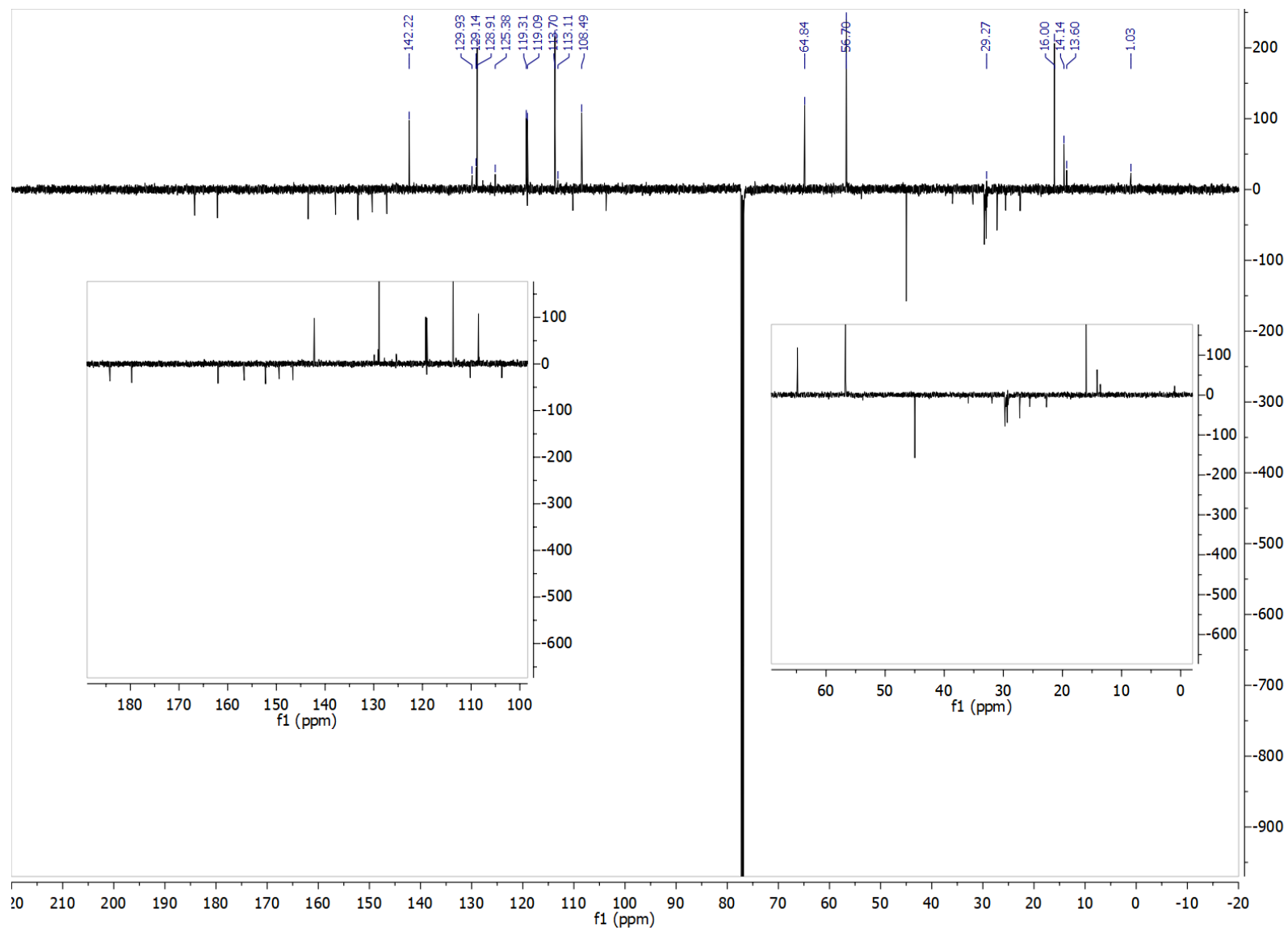


Figure S18. ^{13}C APT NMR spectra of 3 in CDCl_3 , 150 MHz.

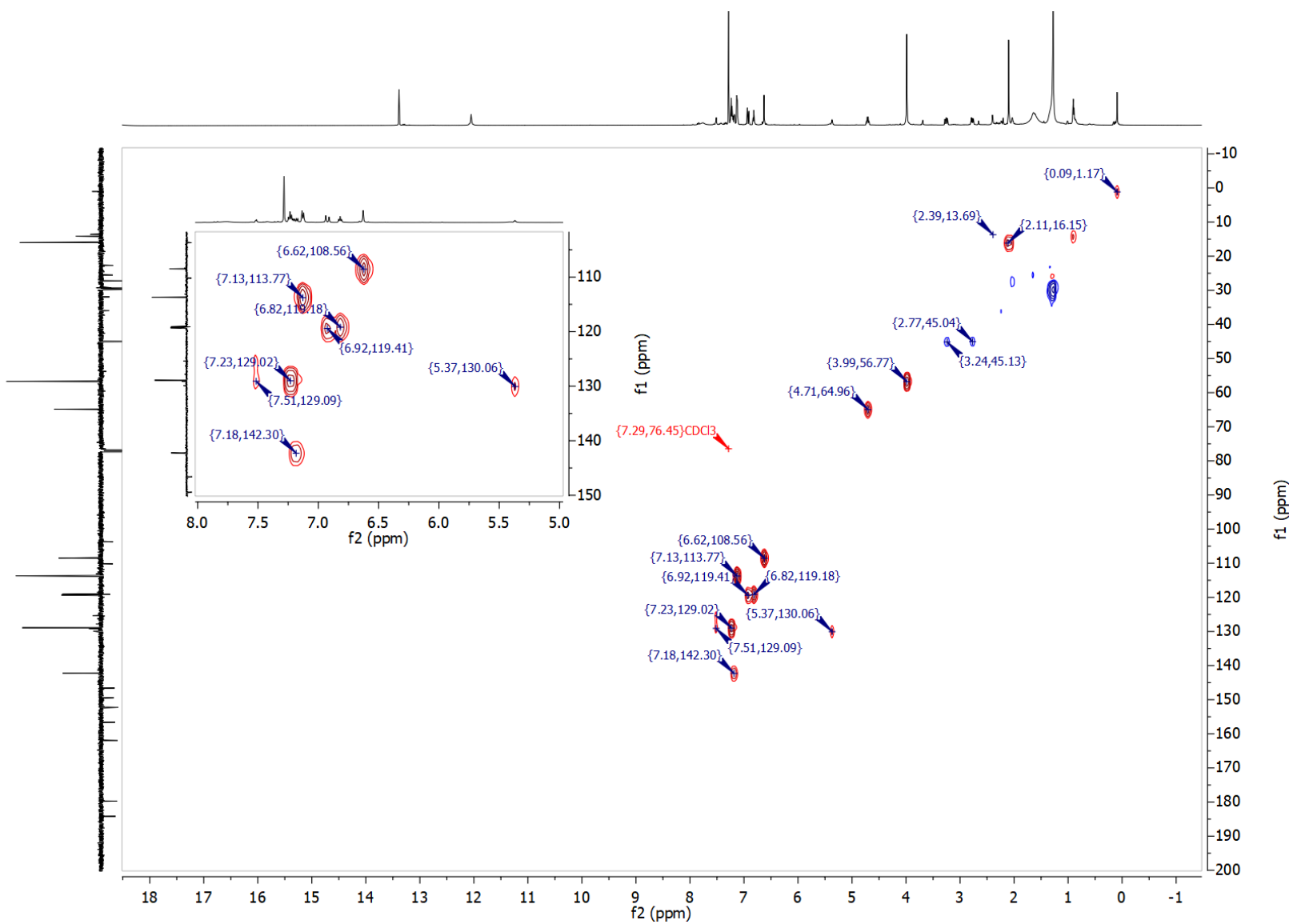


Figure S20. HMQC map for 3 in CDCl₃.

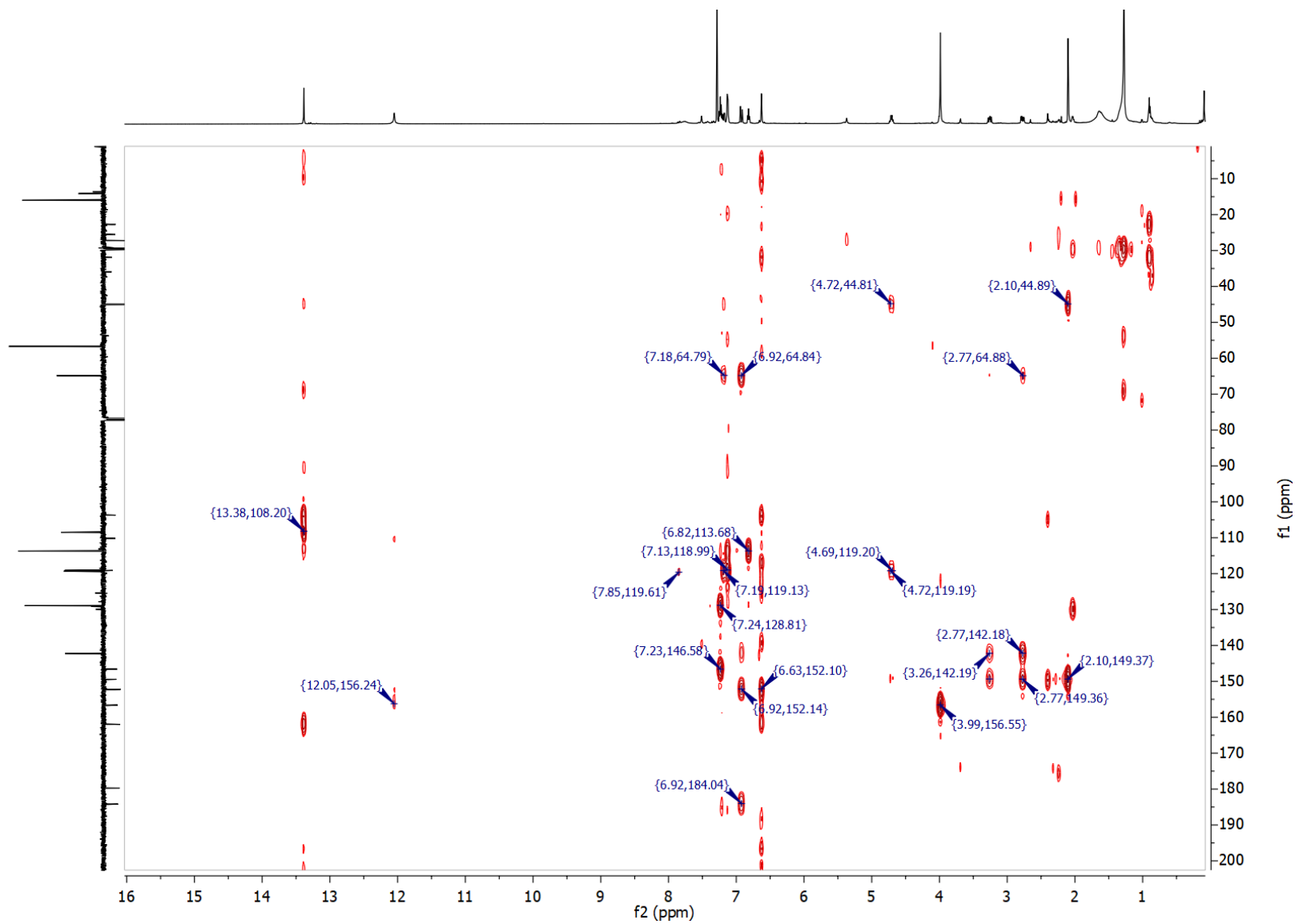


Figure S29. HMBC map for 3 in CDCl_3 .

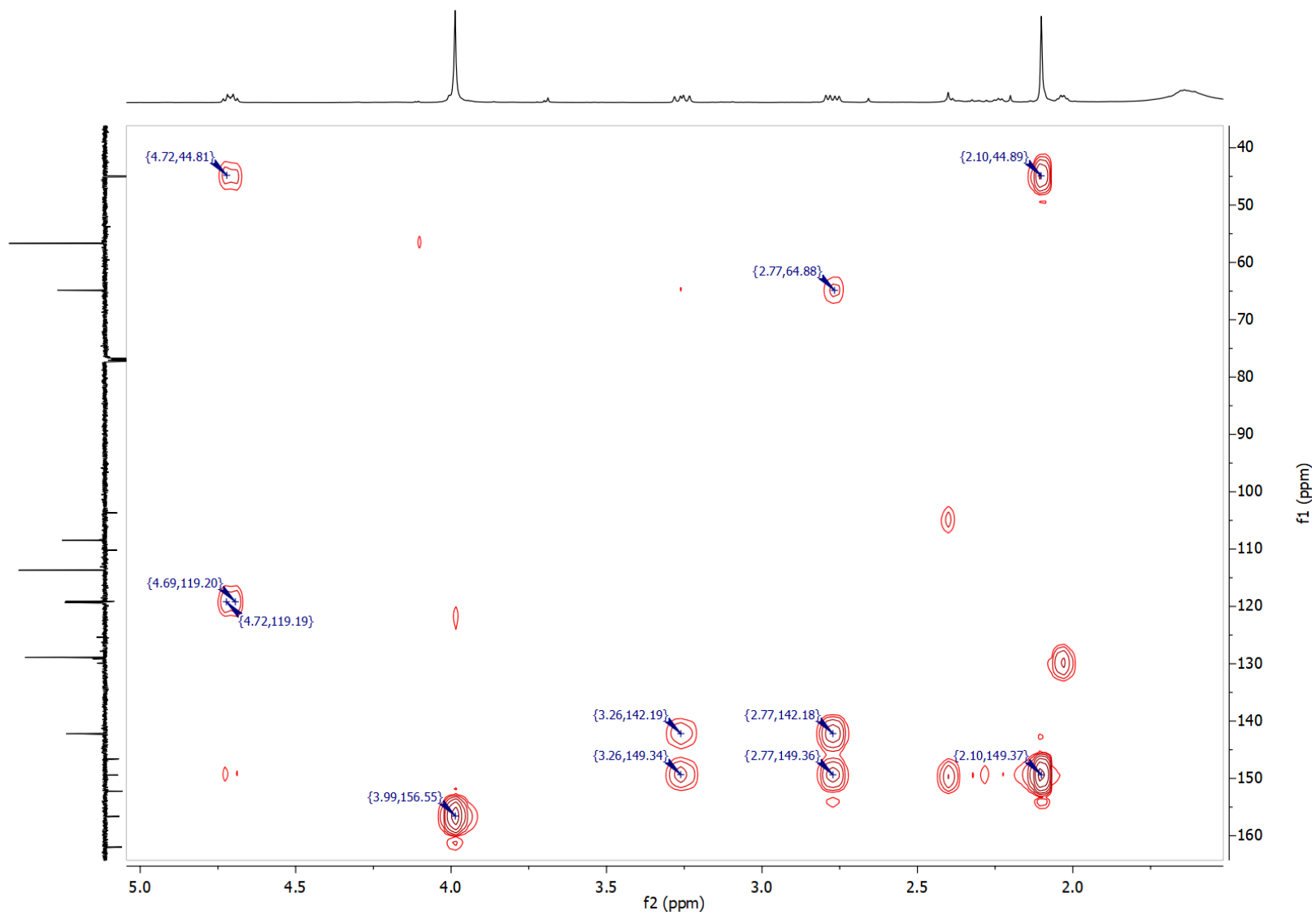


Figure S210. HMBC map for 3 from 1.0 to 5.0 ppm in CDCl₃.

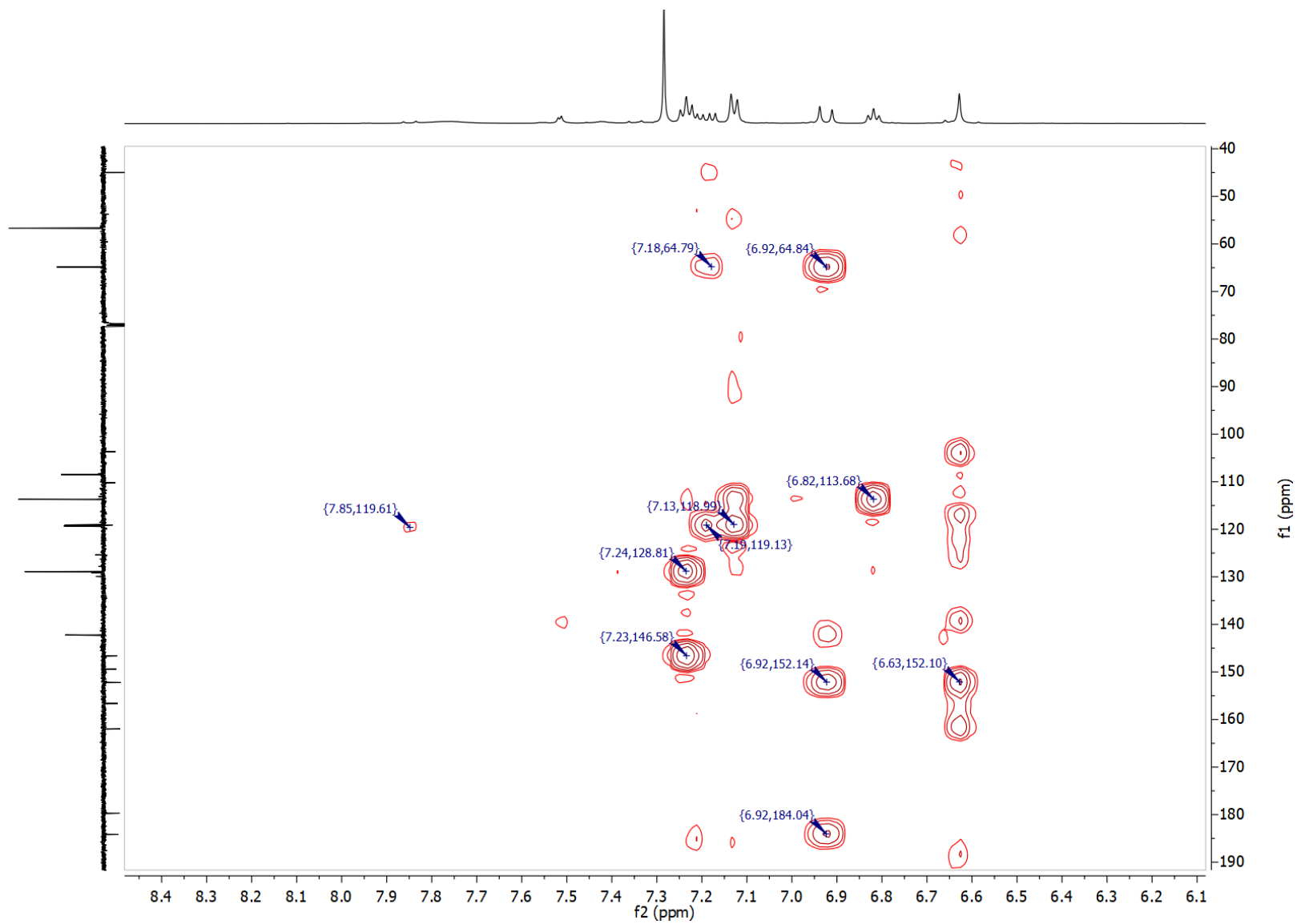


Figure S11. HMBC map for 3 from 6.0 to 8.5 ppm in CDCl₃.

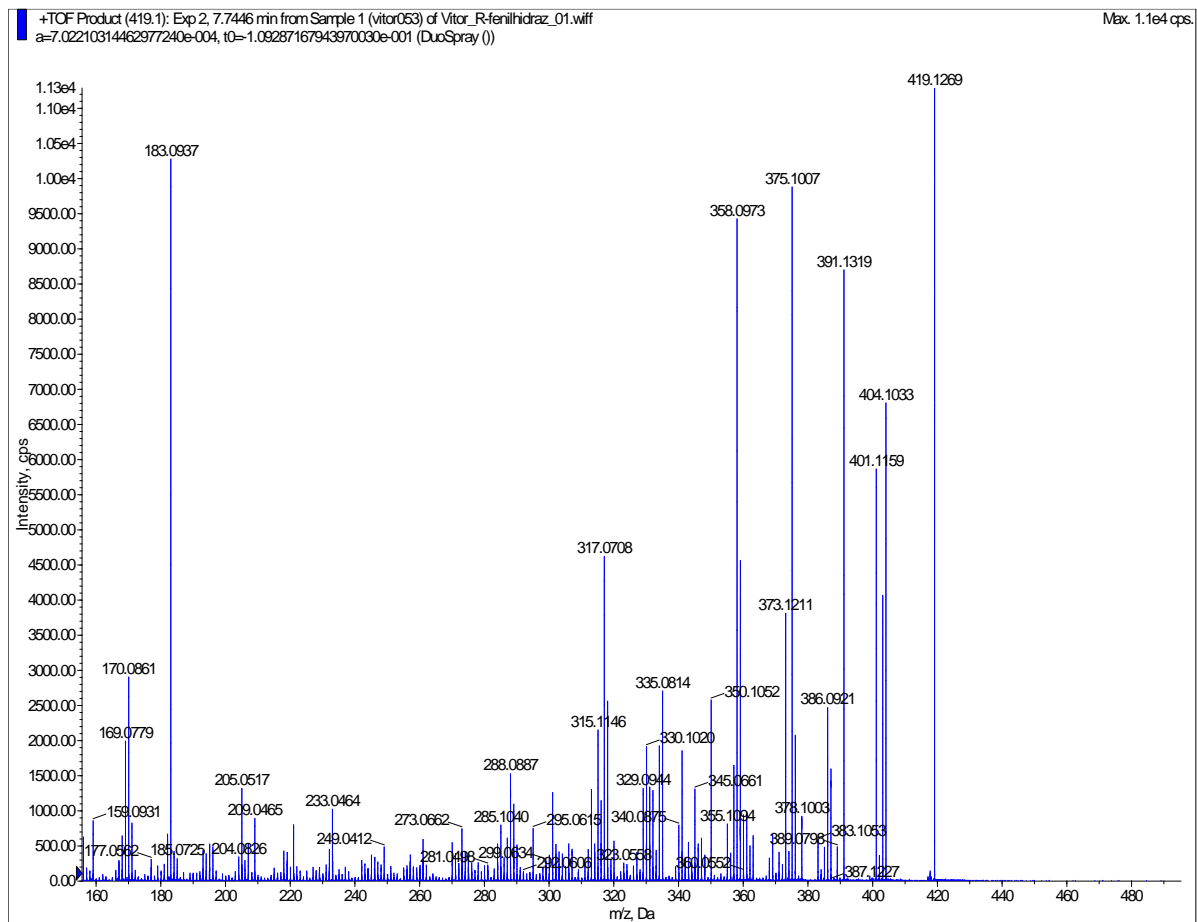


Figure S12. ESI+ CID spectra (30eV, N₂) of 4.

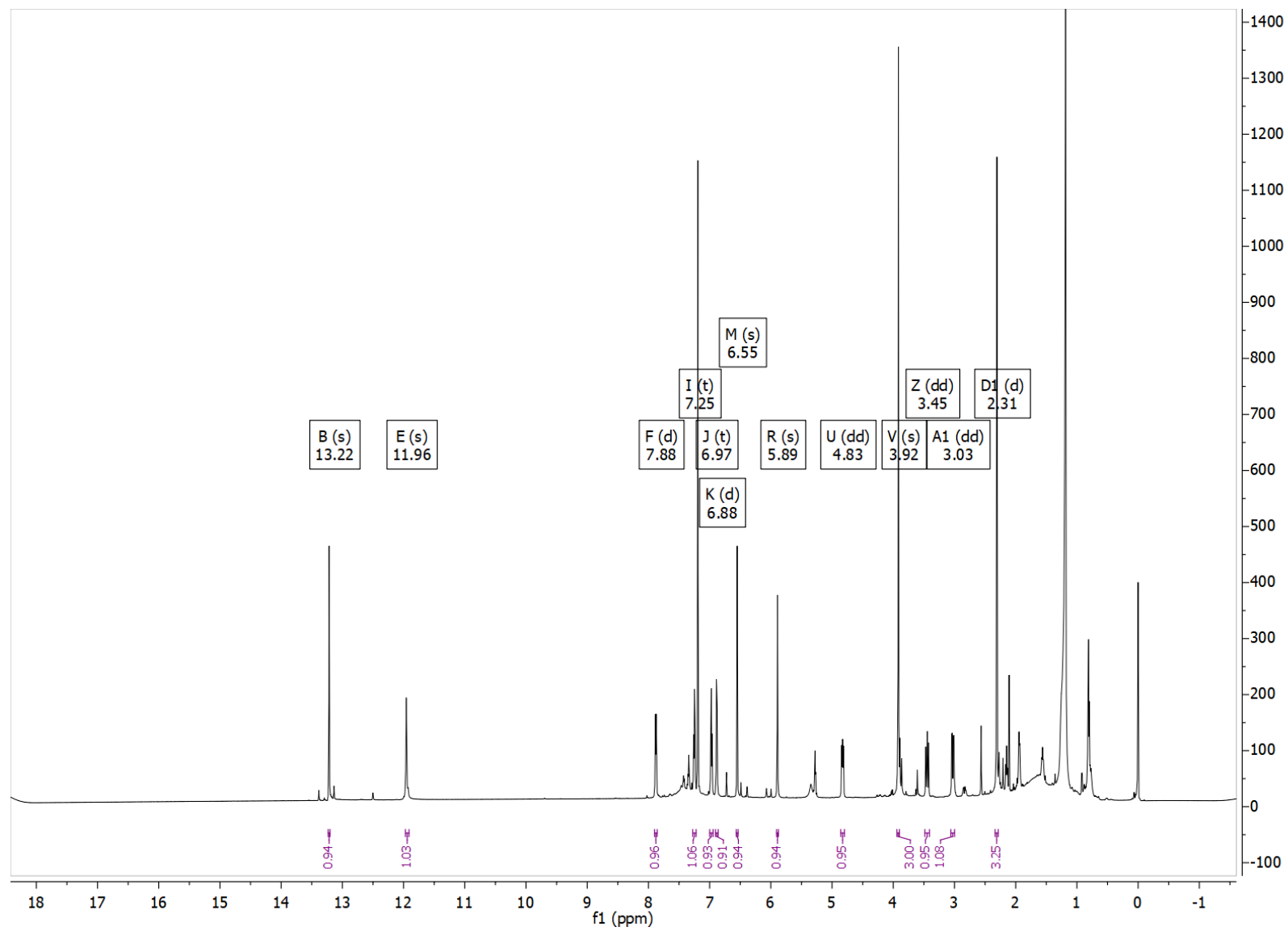


Figure S13. ¹H NMR spectra of 4 in CDCl₃, 600 MHz.

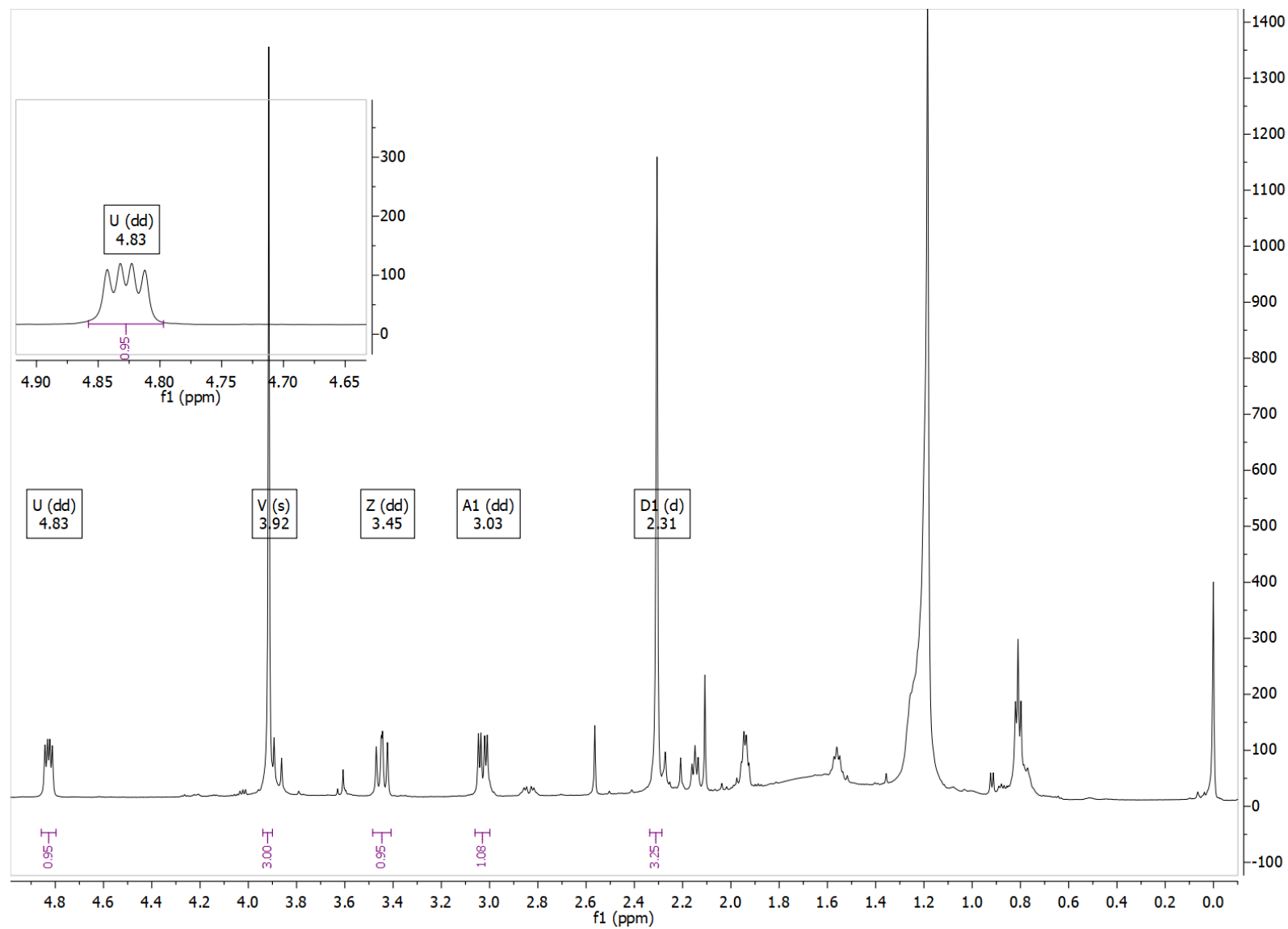


Figure S14. ¹H NMR spectra of 4 from 0 to 5 ppm in CDCl₃, 600 MHz.

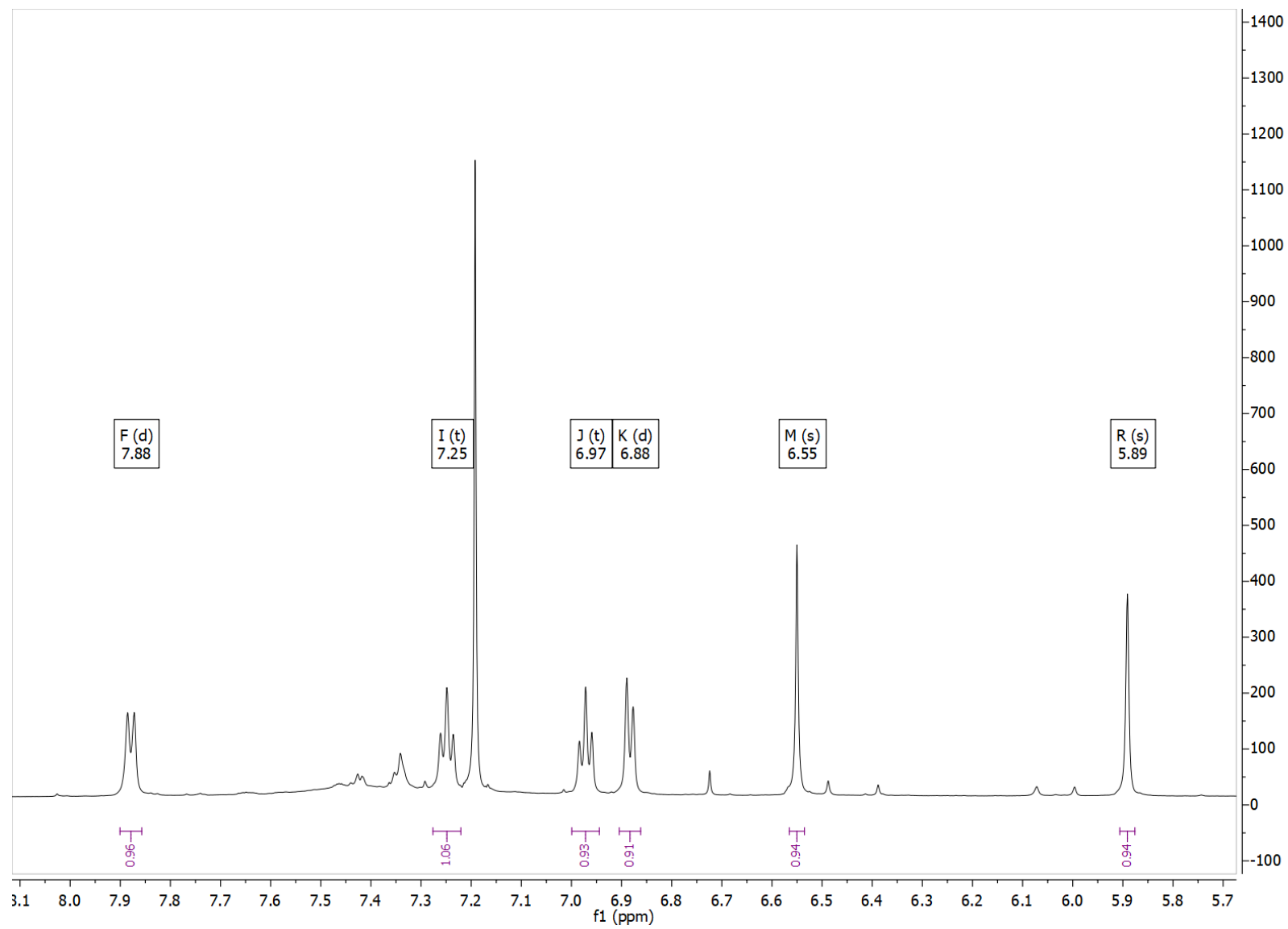


Figure S15. ¹H NMR spectra of 4 from 5.5 to 8.0 ppm in CDCl₃, 600 MHz.

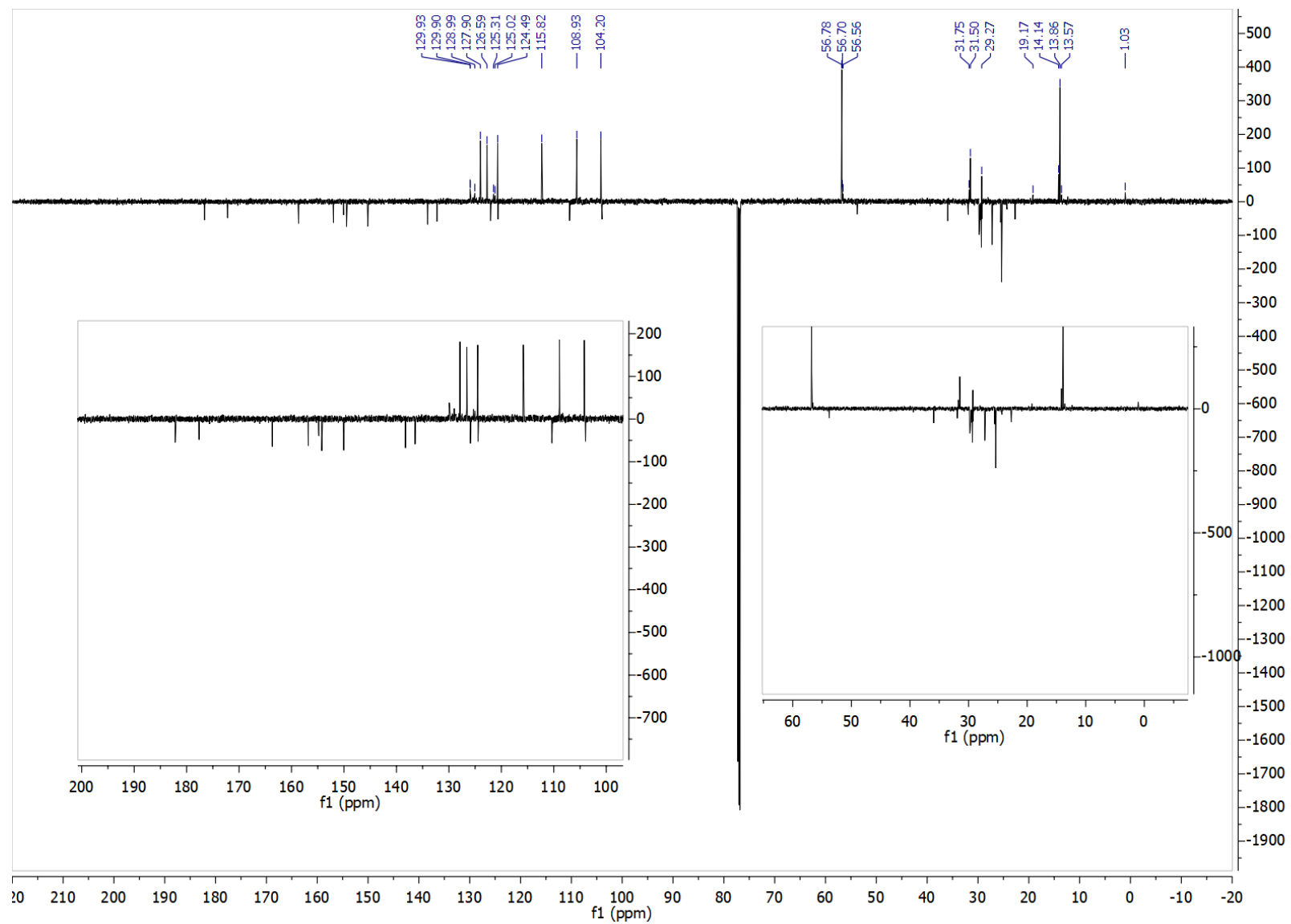


Figure S16. ^{13}C APT NMR spectra for 4 in CDCl_3 , 150 MHz.

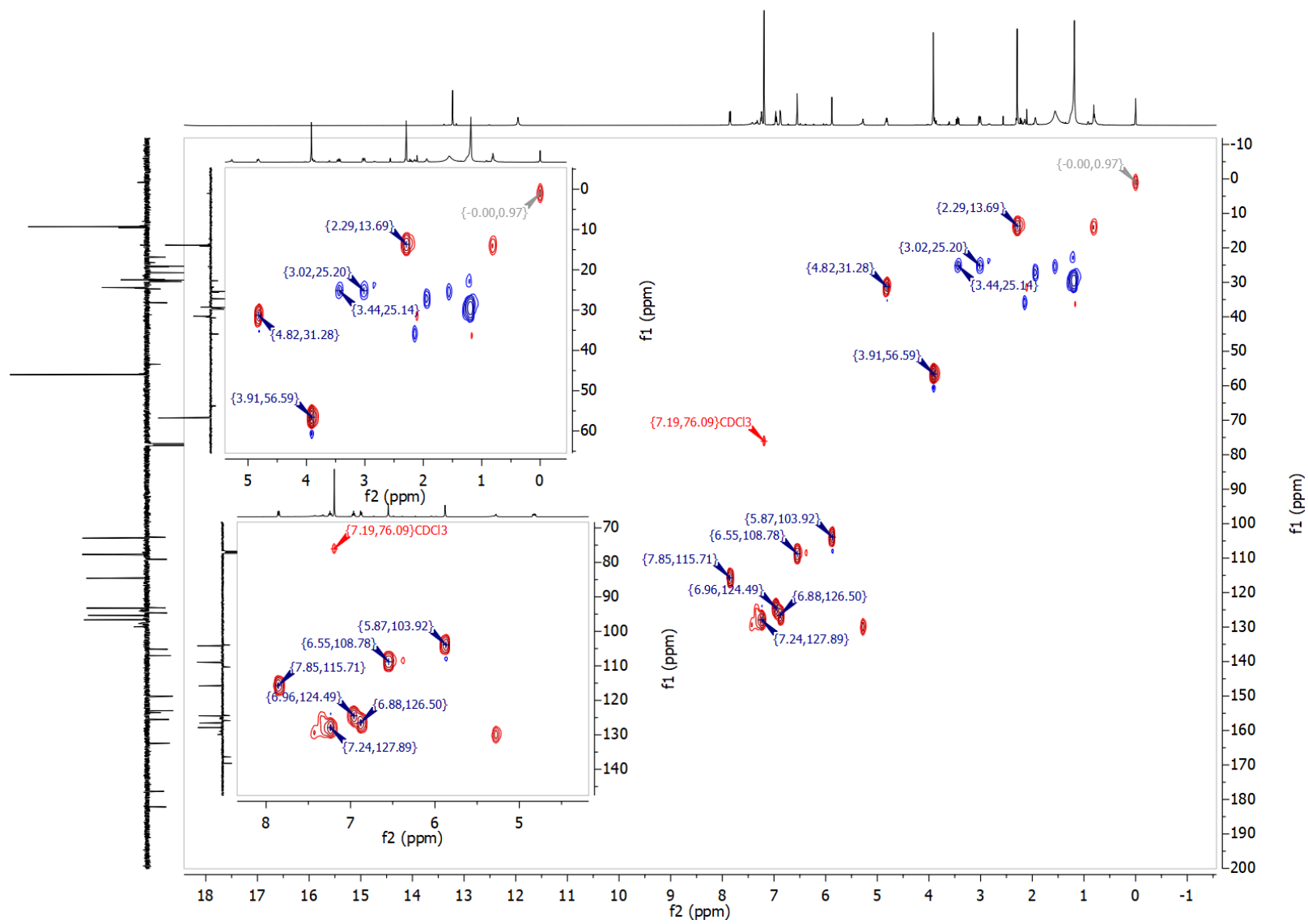


Figure S17. HMQC map for 4 in CDCl₃.

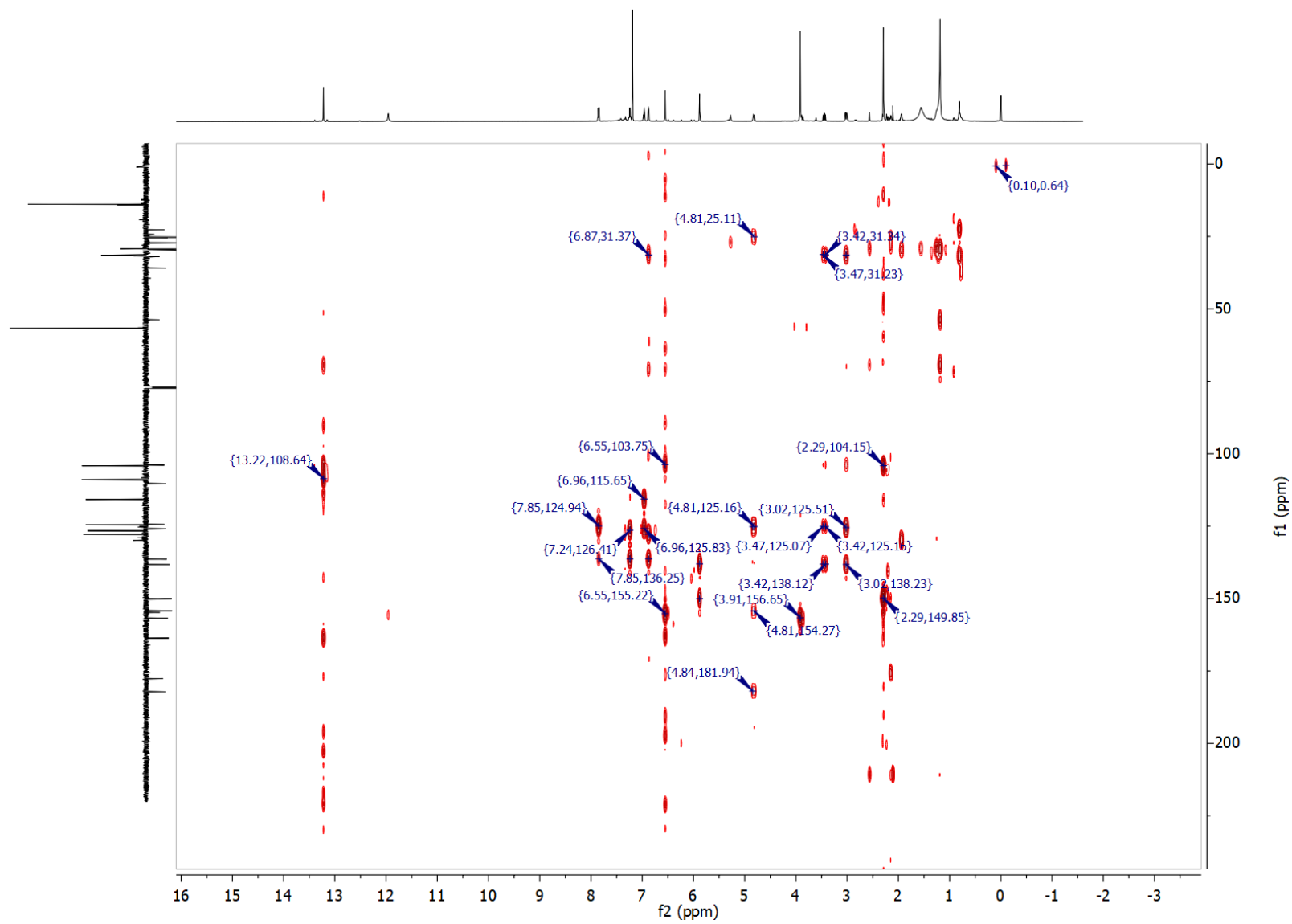


Figure S18. HMBC map for 4 in CDCl₃.

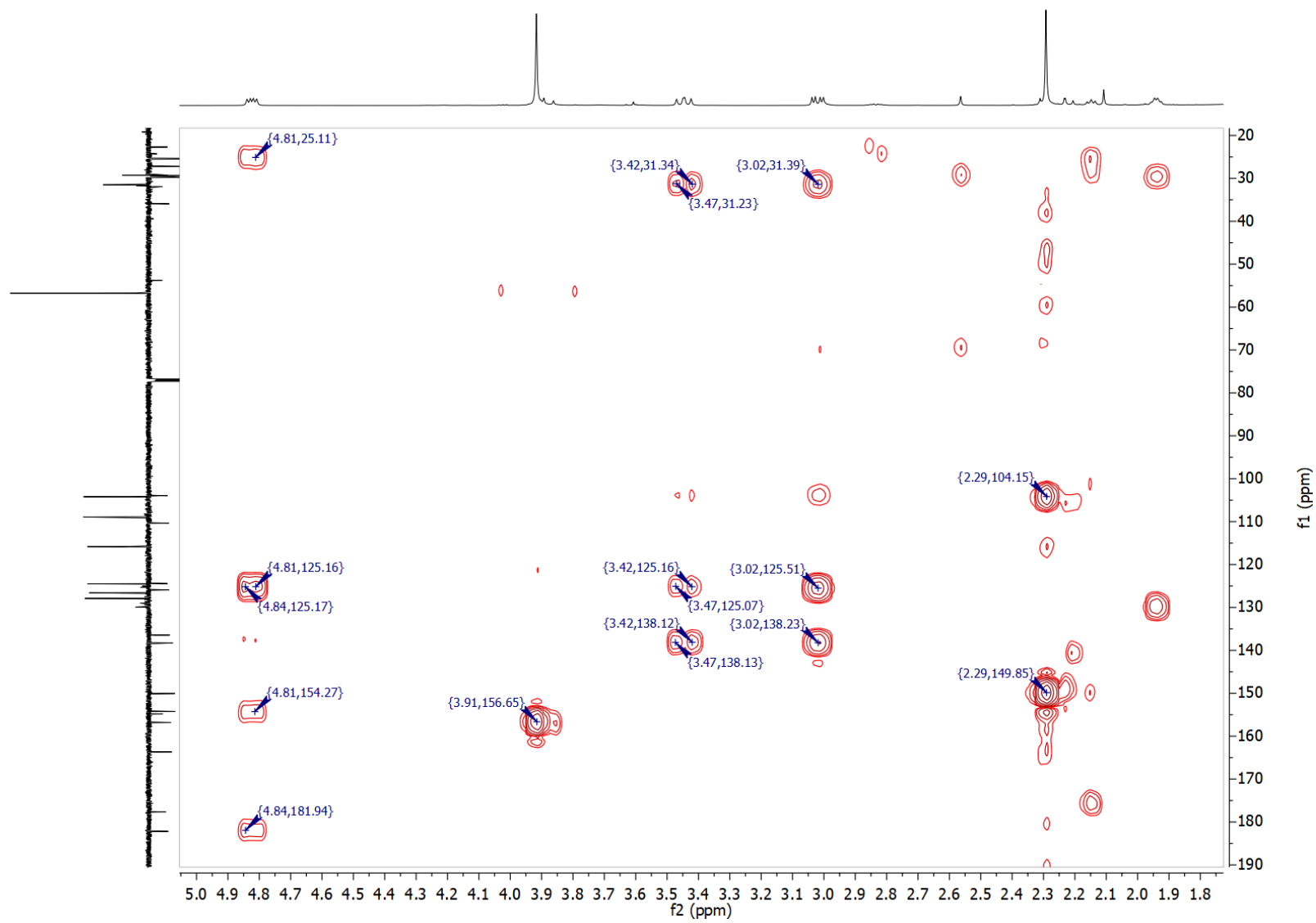


Figure S19. HMBC map from 1.5 to 5.0 ppm for 4 in CDCl₃.

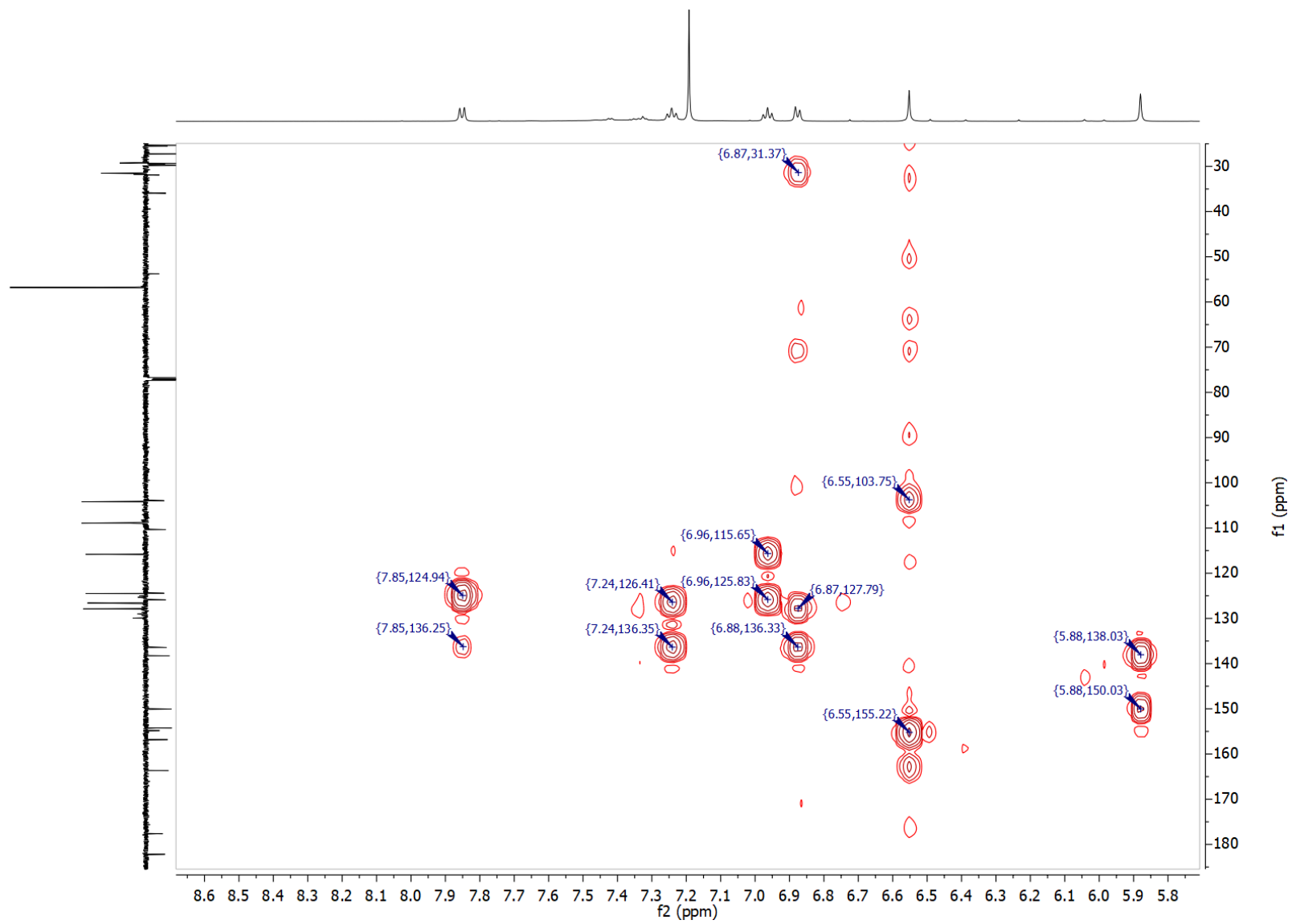


Figure S20. HMBC map from 5.5 to 8.5 ppm for 4 in CDCl₃.

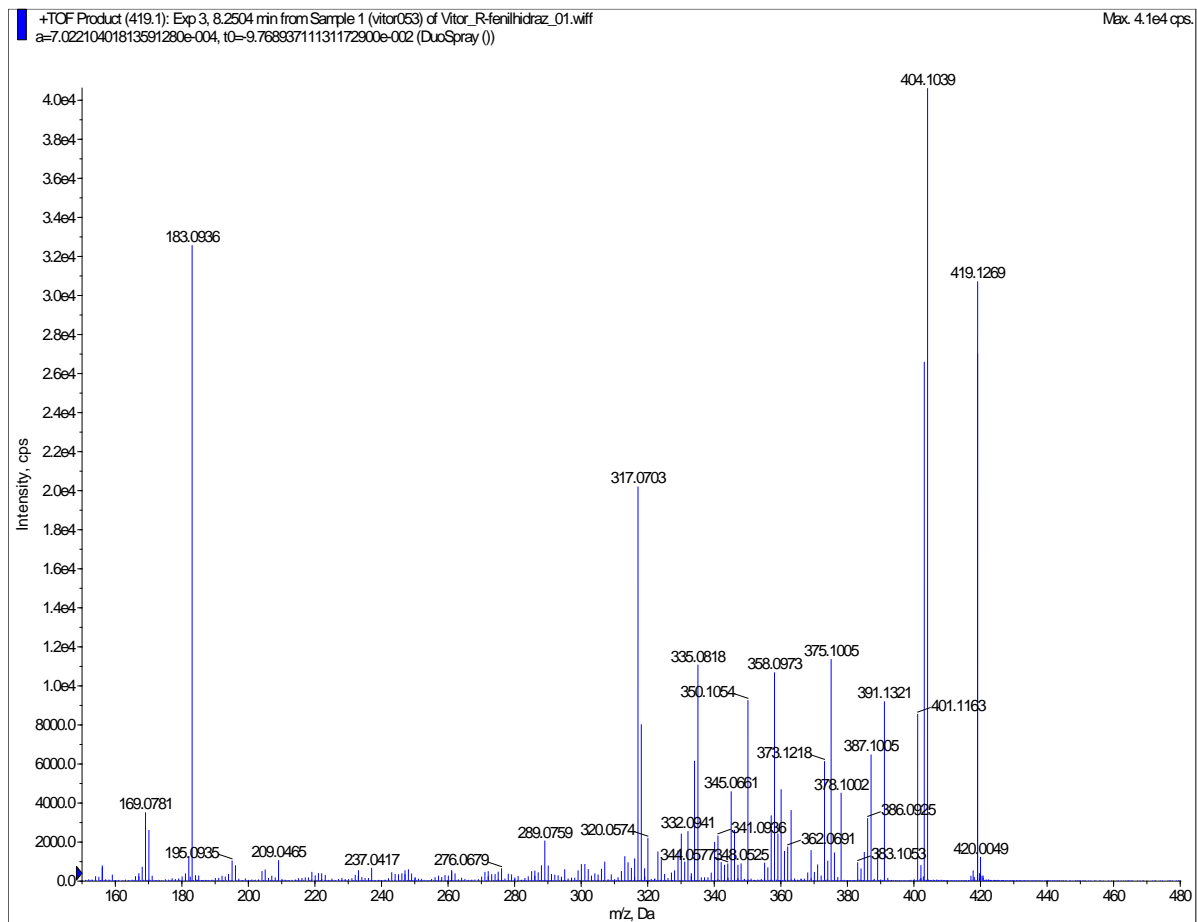


Figure S21. ESI+ CID spectra (30eV, N₂) of 5.