

Supplementary material

Synthesis, Analysis, Cholinesterase-Inhibiting Activity and Molecular Modelling Studies of 3-(Dialkylamino)-2-hydroxypropyl 4-[(Alkoxy-carbonyl)amino]benzoates and Their Quaternary Ammonium Salts

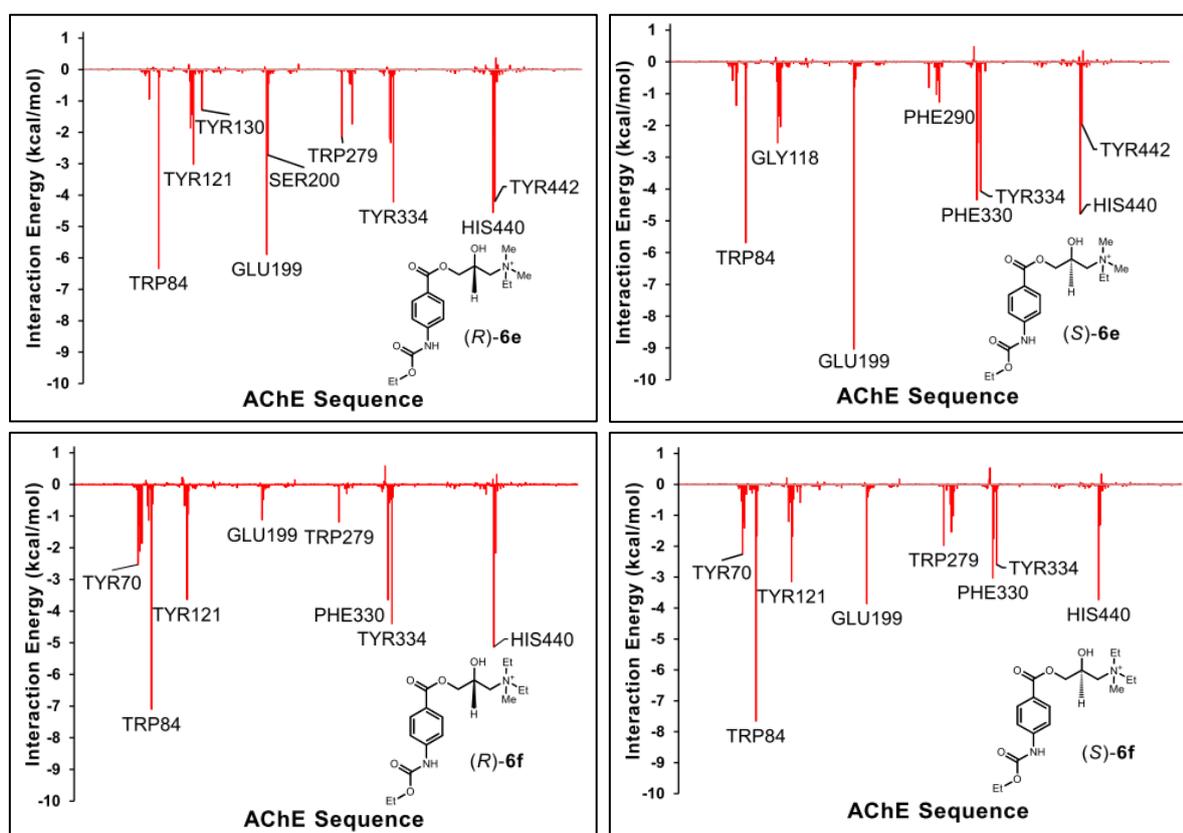


Figure S1. Histograms of interaction energies partitioned with respect to the AChE, amino acids in complex with (R)-6e, (S)-6e, (R)-6f and (S)-6f.

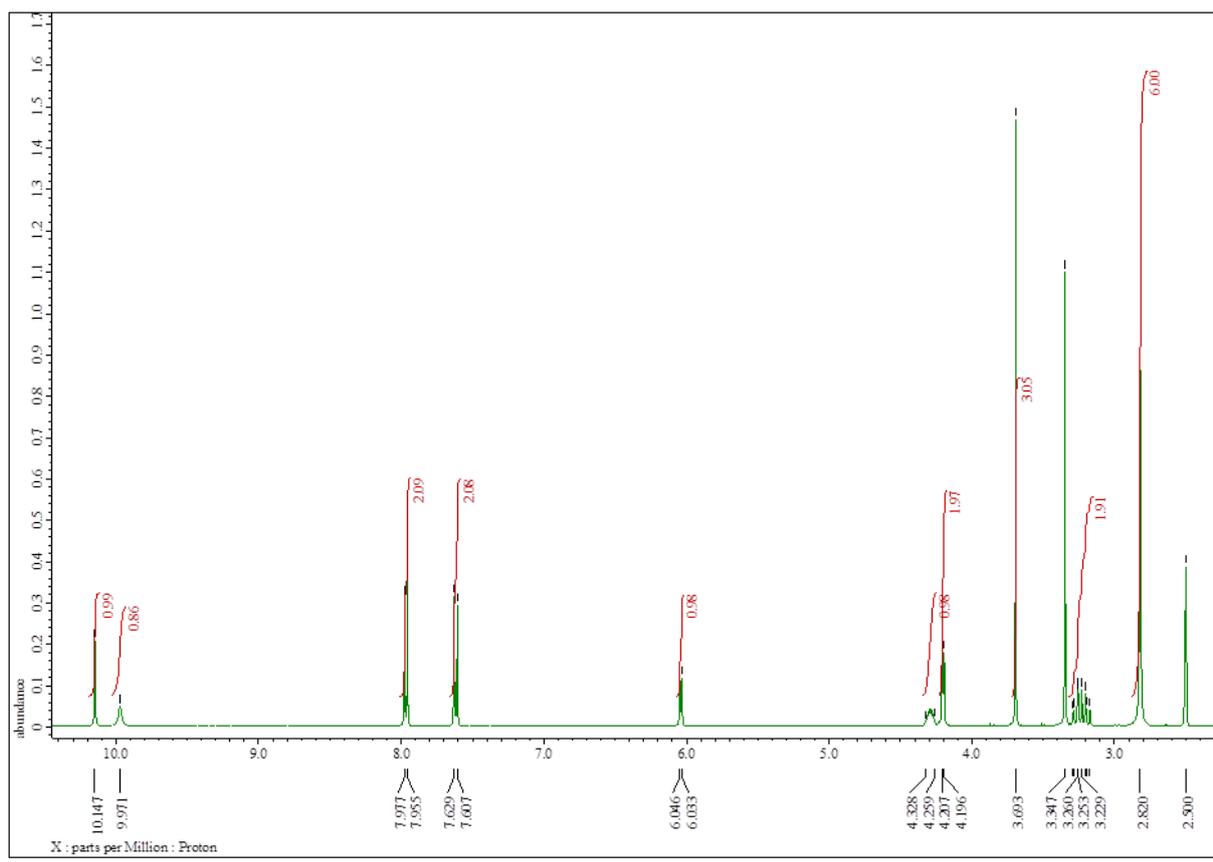


Figure S2. ¹H-NMR spectrum of 5a

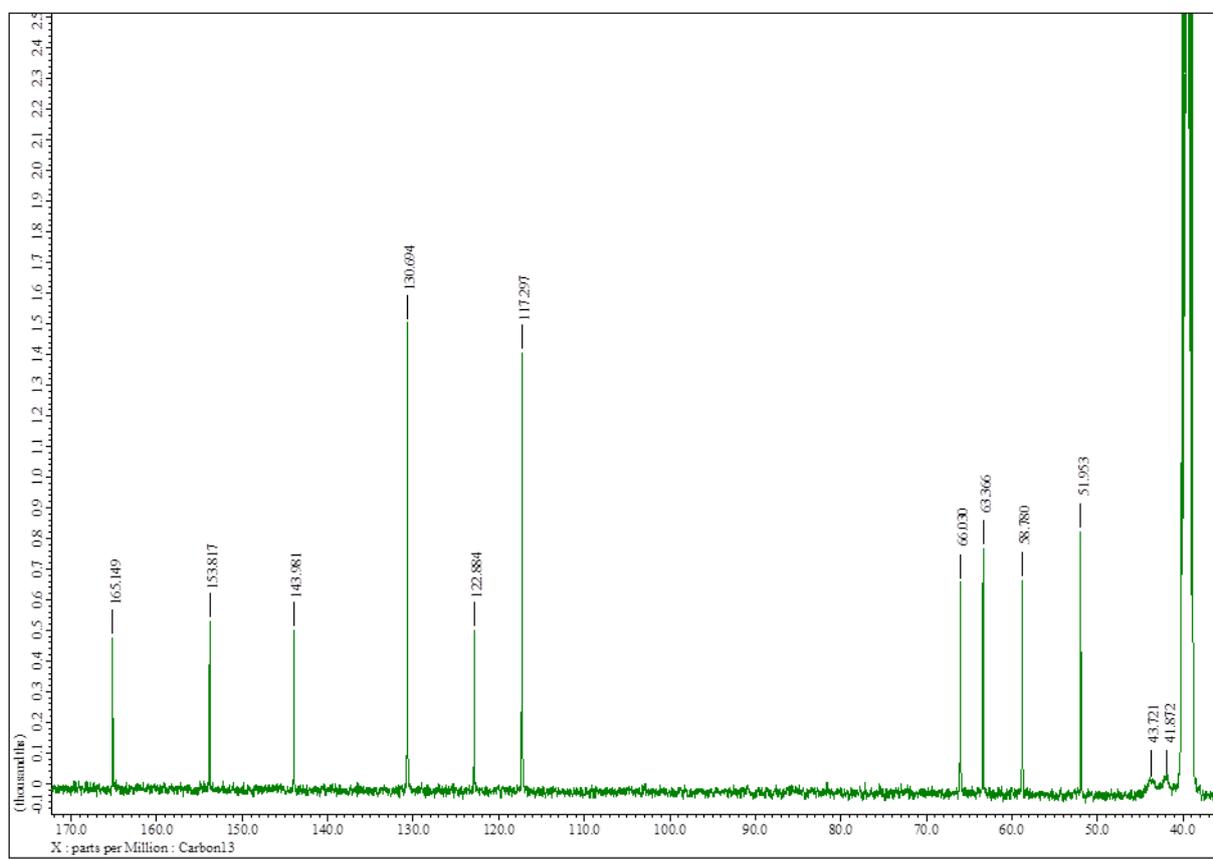


Figure S3. ¹³C-NMR spectrum of 5a

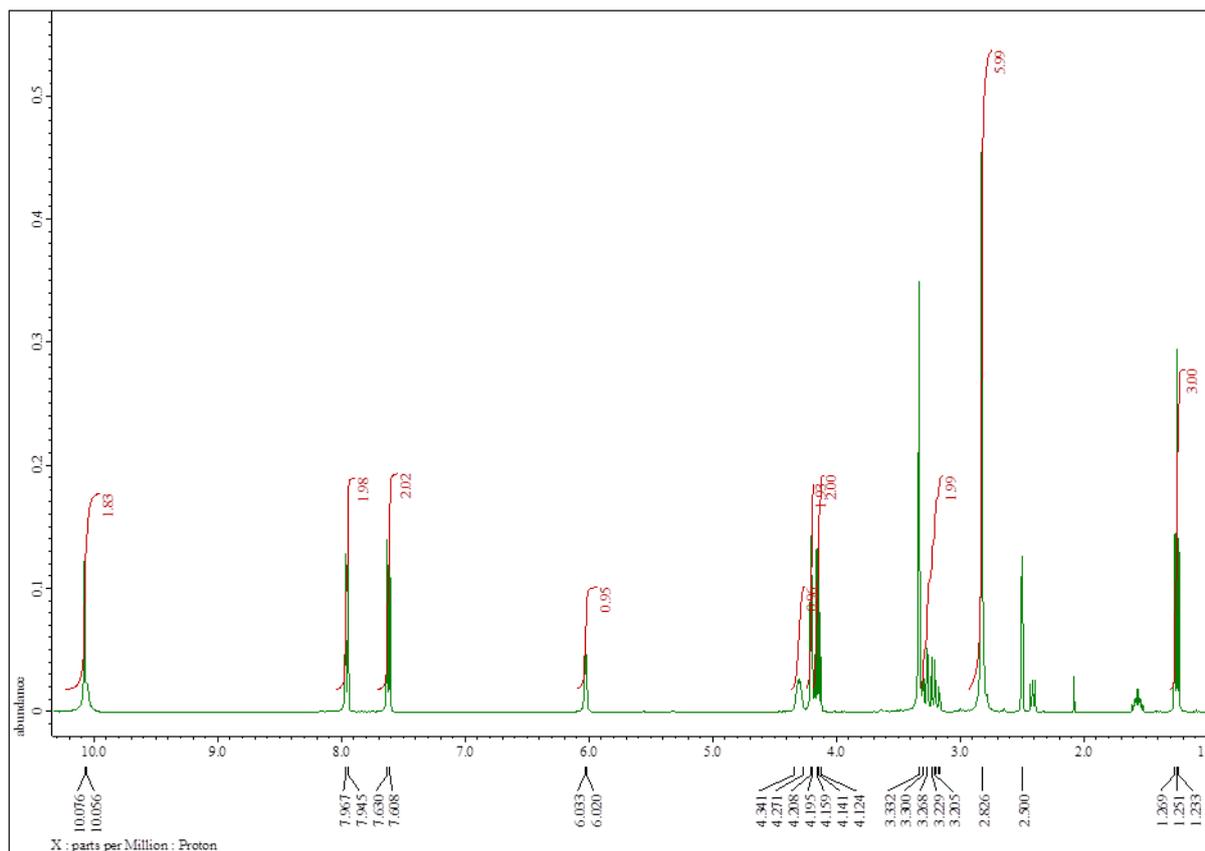


Figure S4. ¹H-NMR spectrum of 5b

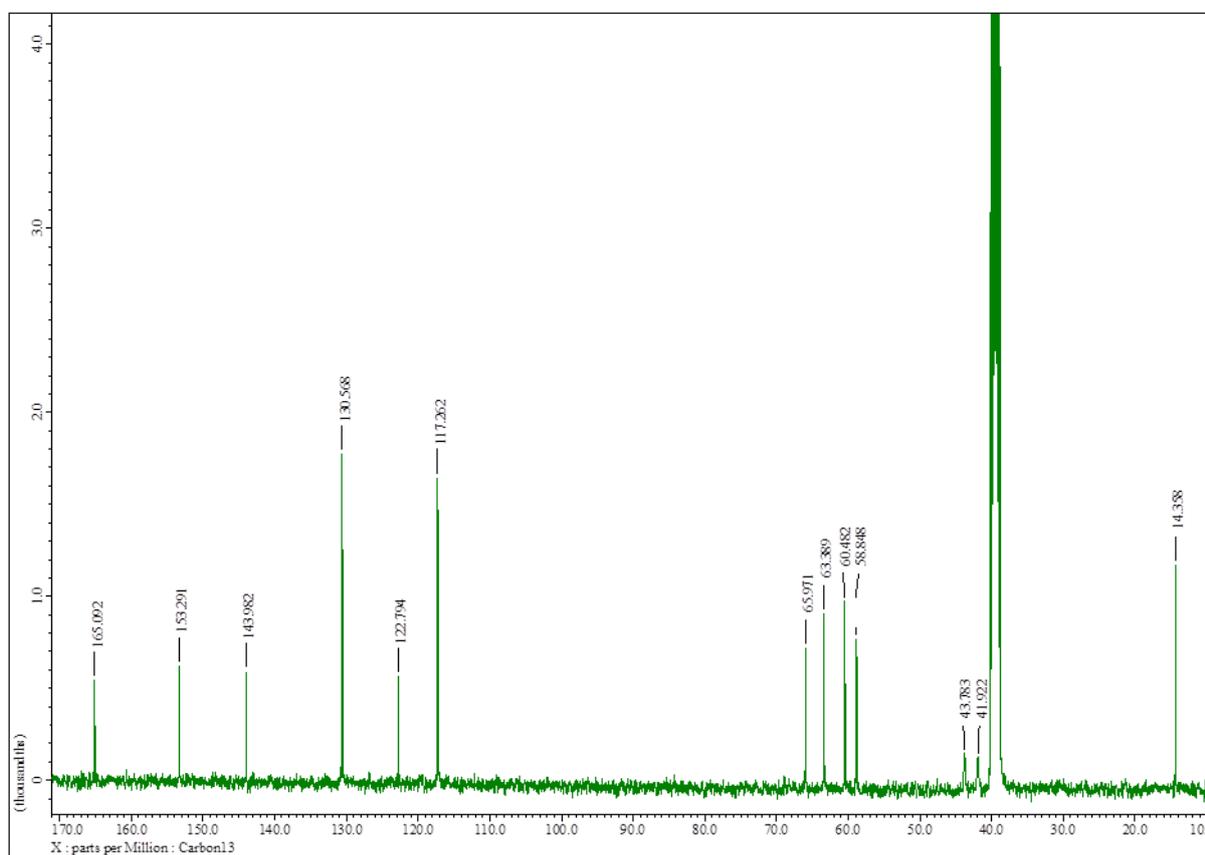


Figure S5. ¹³C-NMR spectrum of 5b

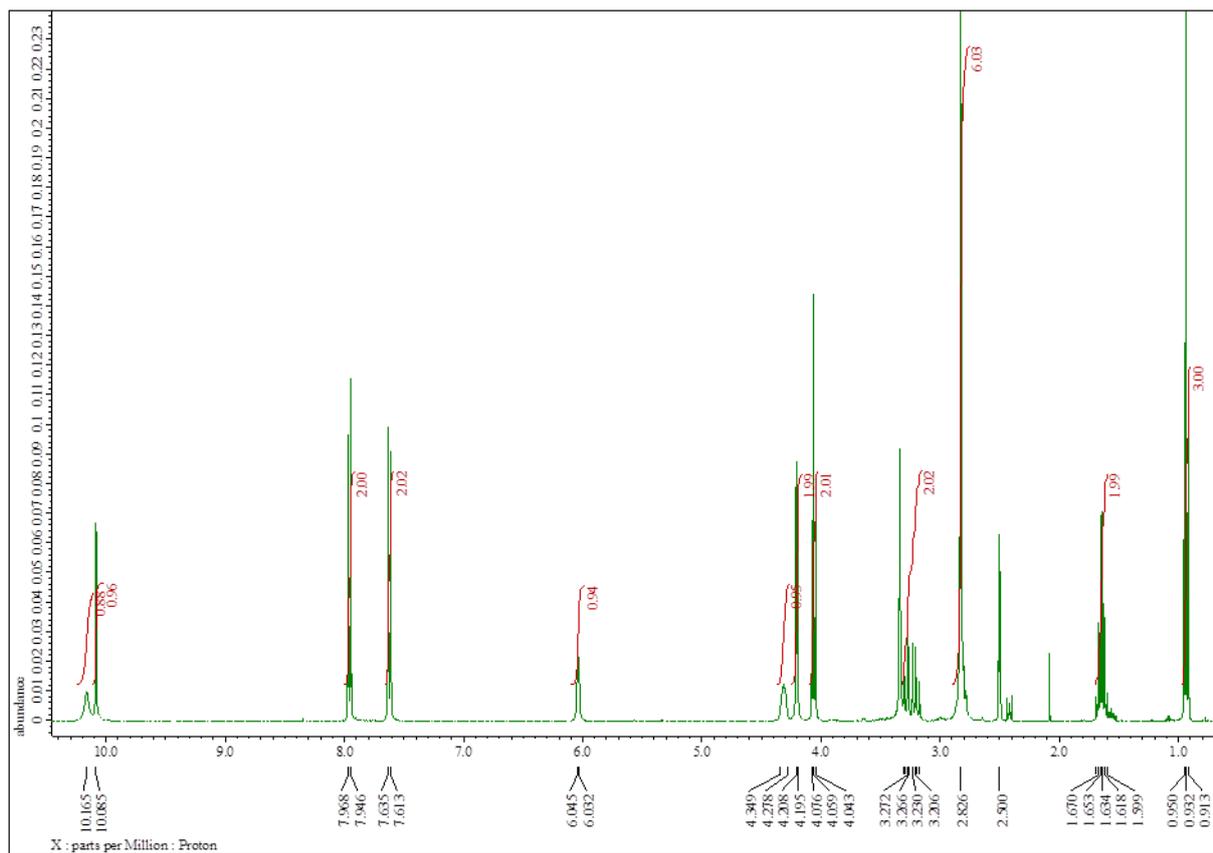


Figure S6. ¹H-NMR spectrum of 5c

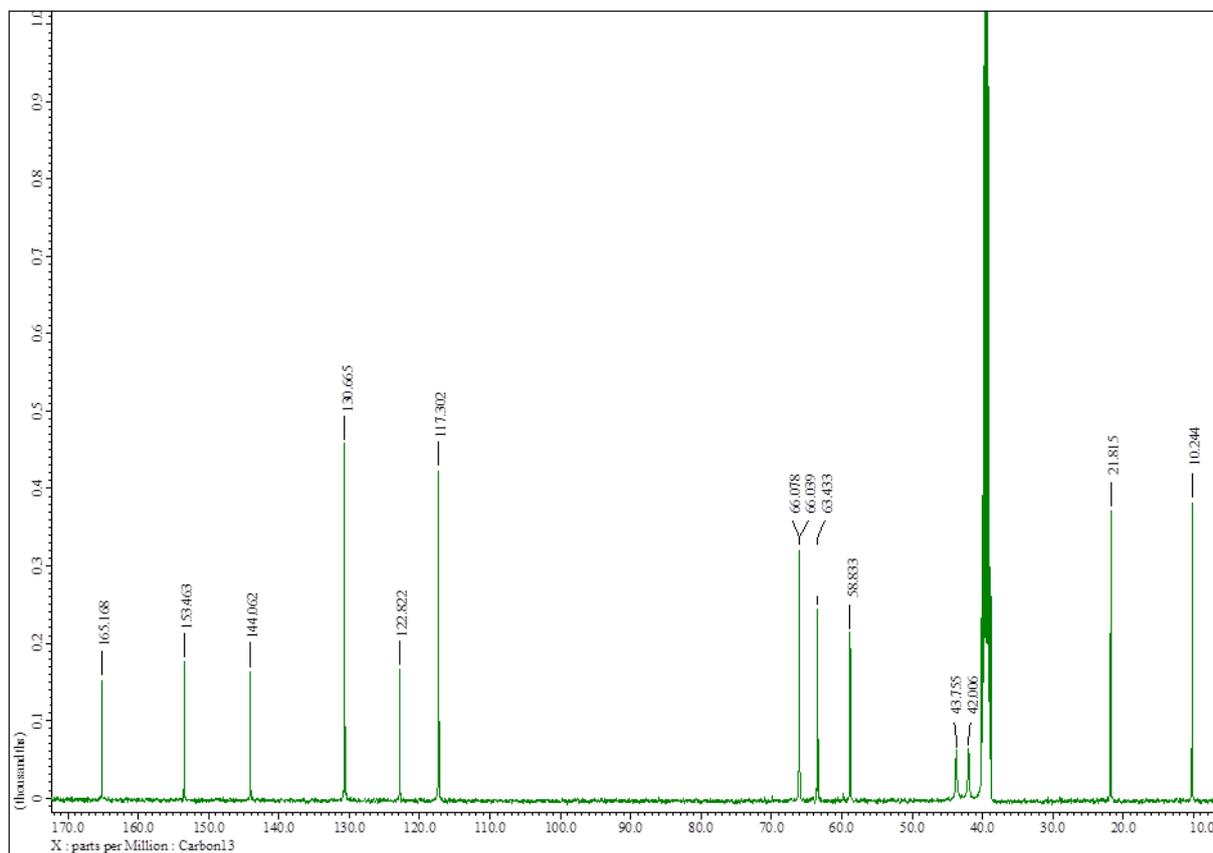


Figure S7. ¹³C-NMR spectrum of 5c

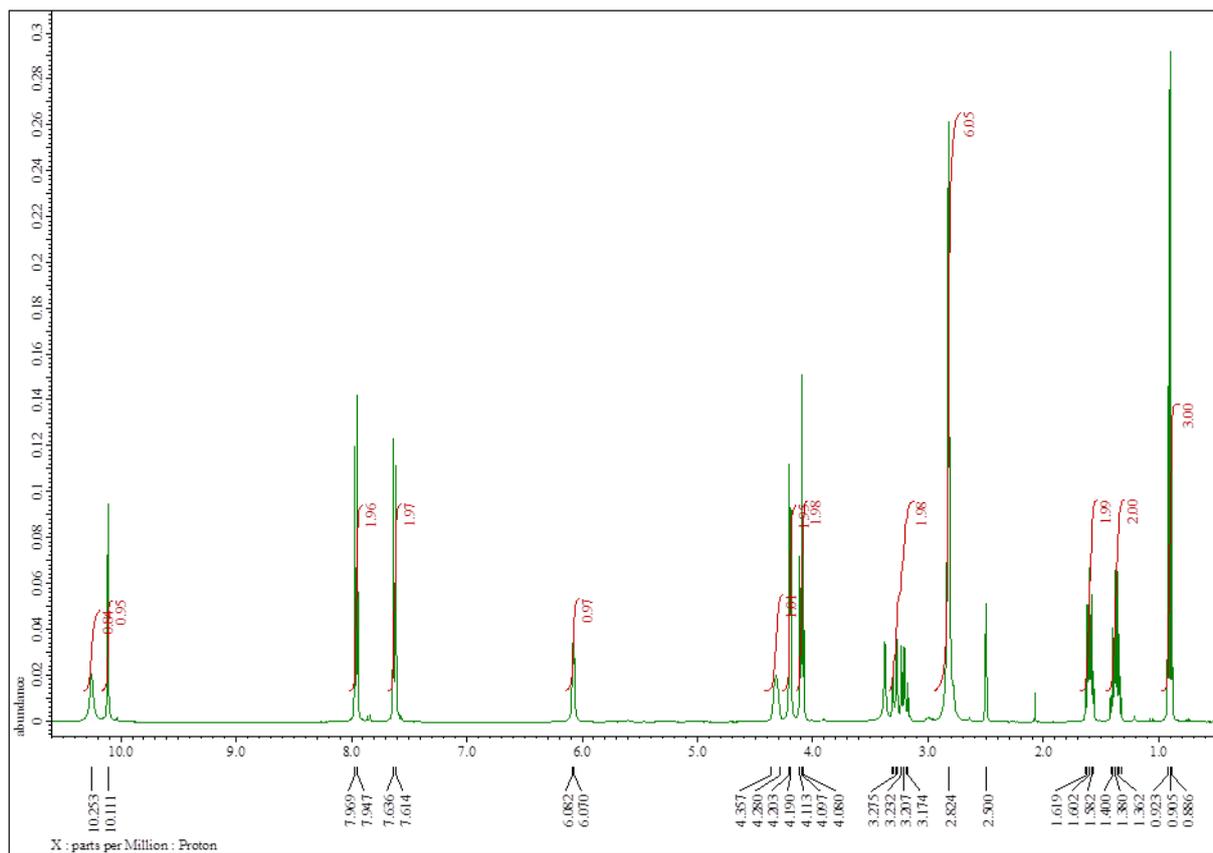


Figure S8. ¹H-NMR spectrum of 5d

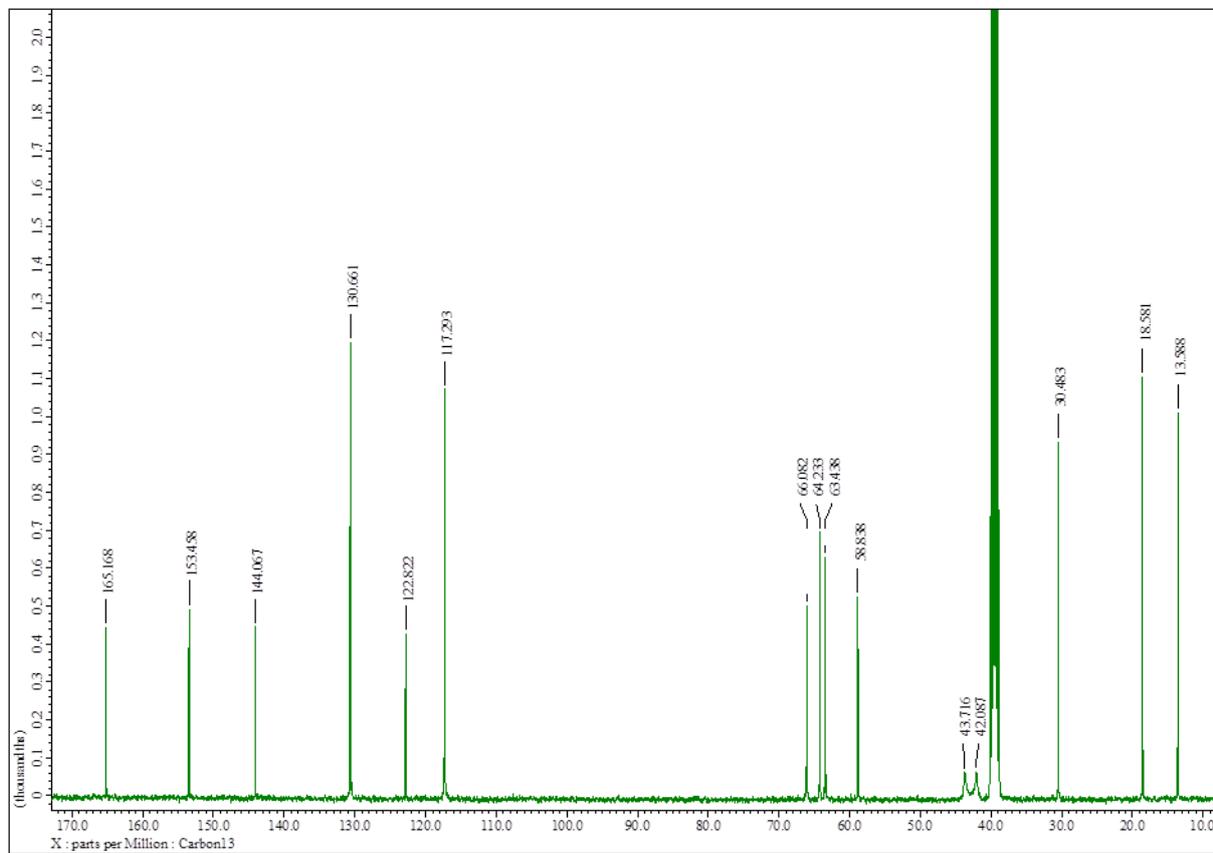


Figure S9. ¹³C-NMR spectrum of 5d

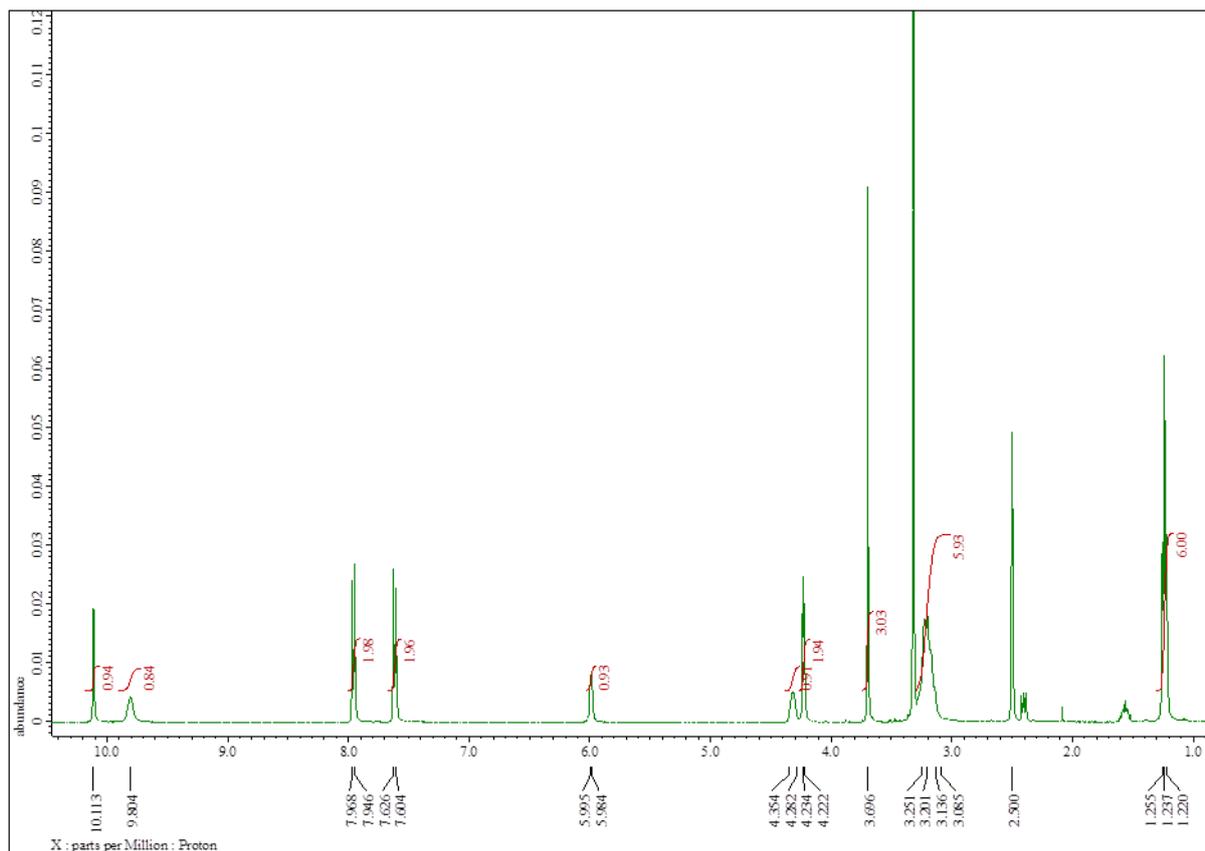


Figure S10. ¹H-NMR spectrum of 5e

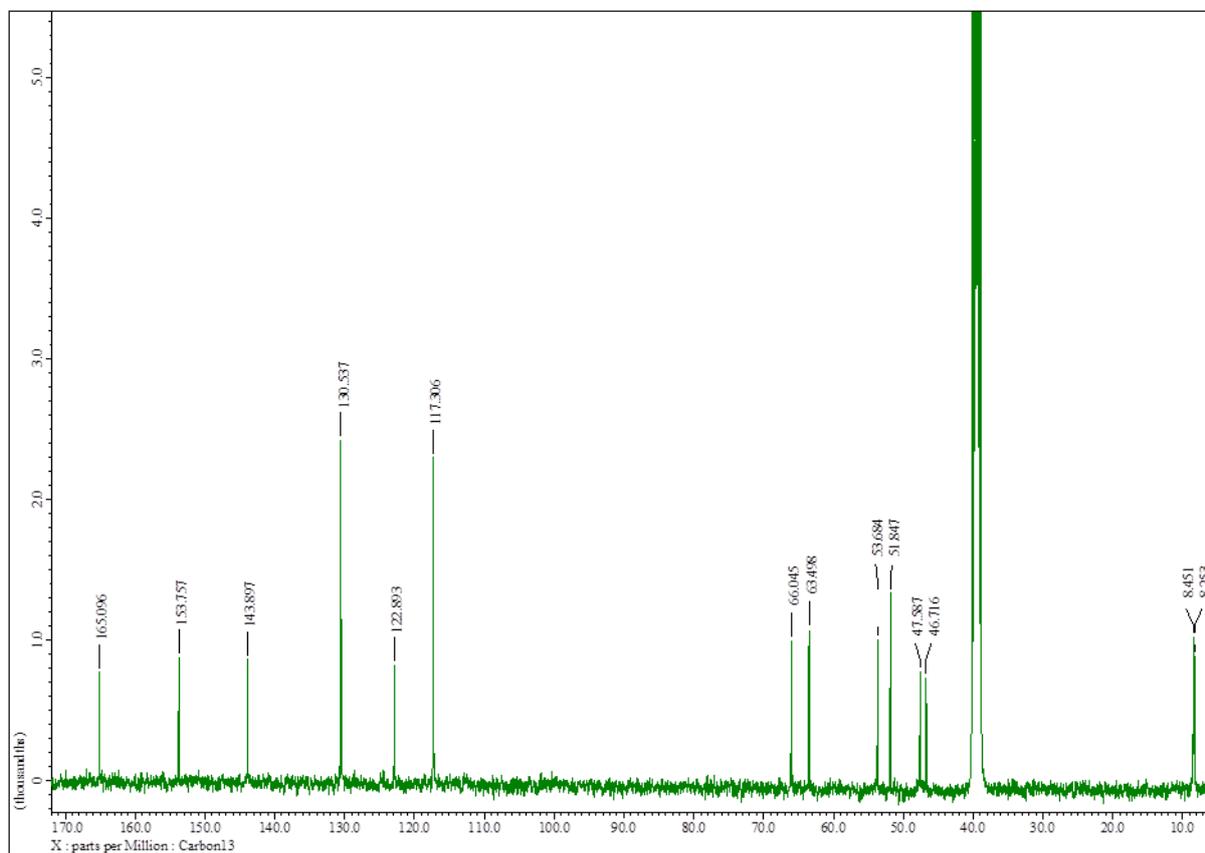


Figure S11. ¹³C-NMR spectrum of 5e

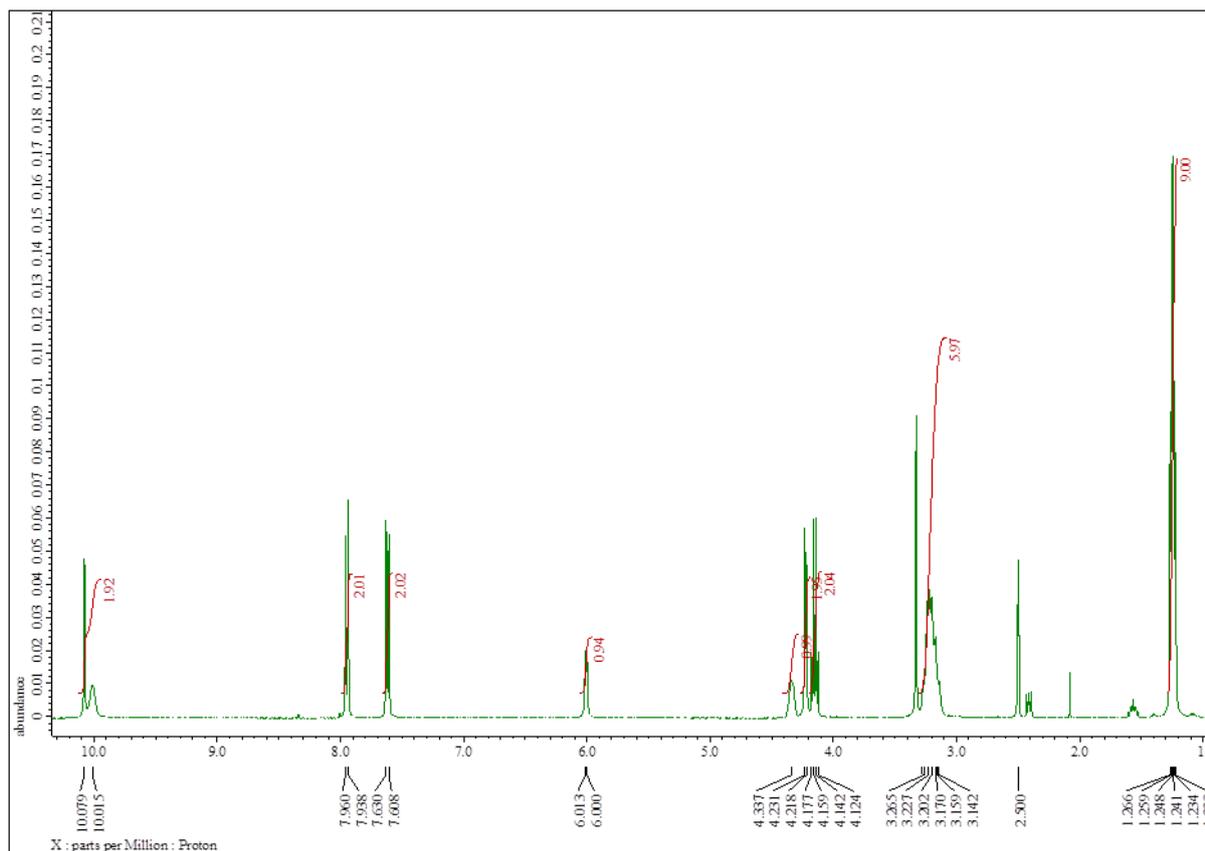


Figure S12. ¹H-NMR spectrum of 5f

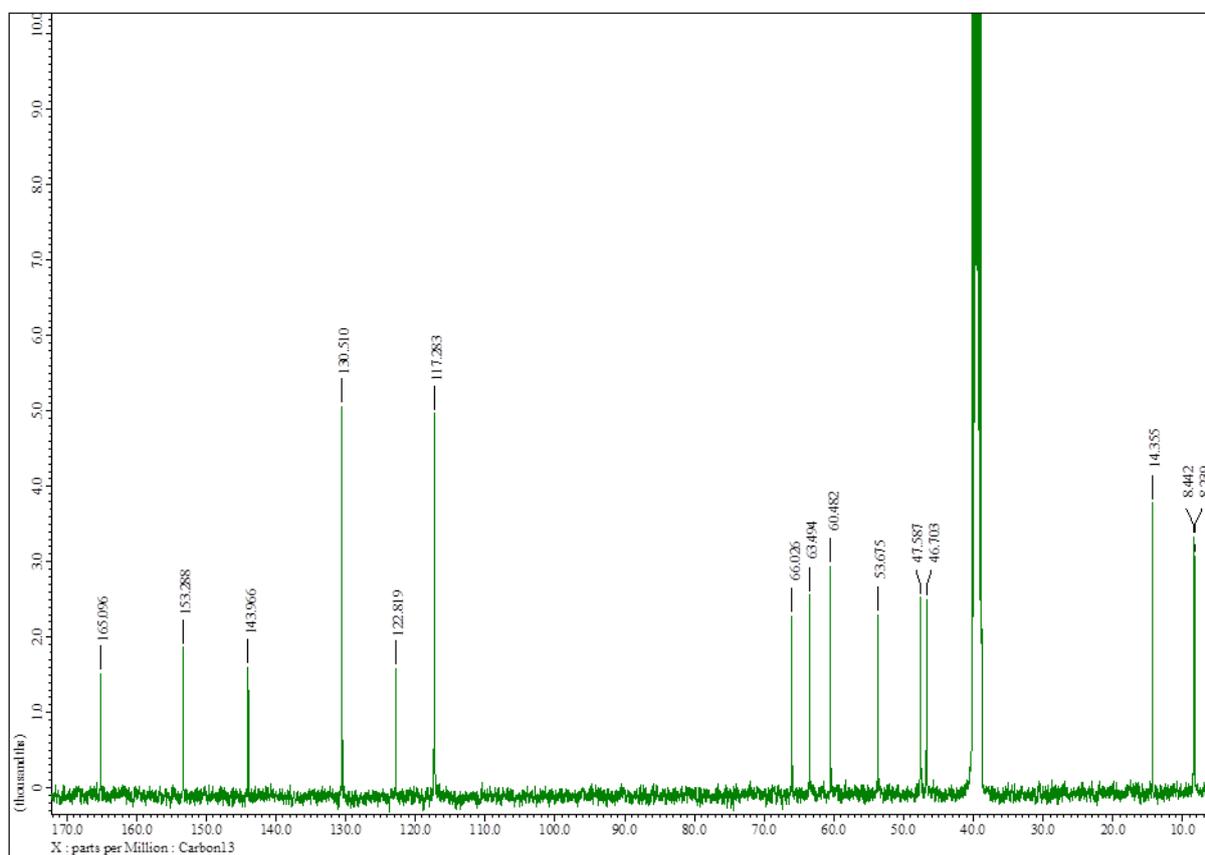


Figure S13. ¹³C-NMR spectrum of 5f

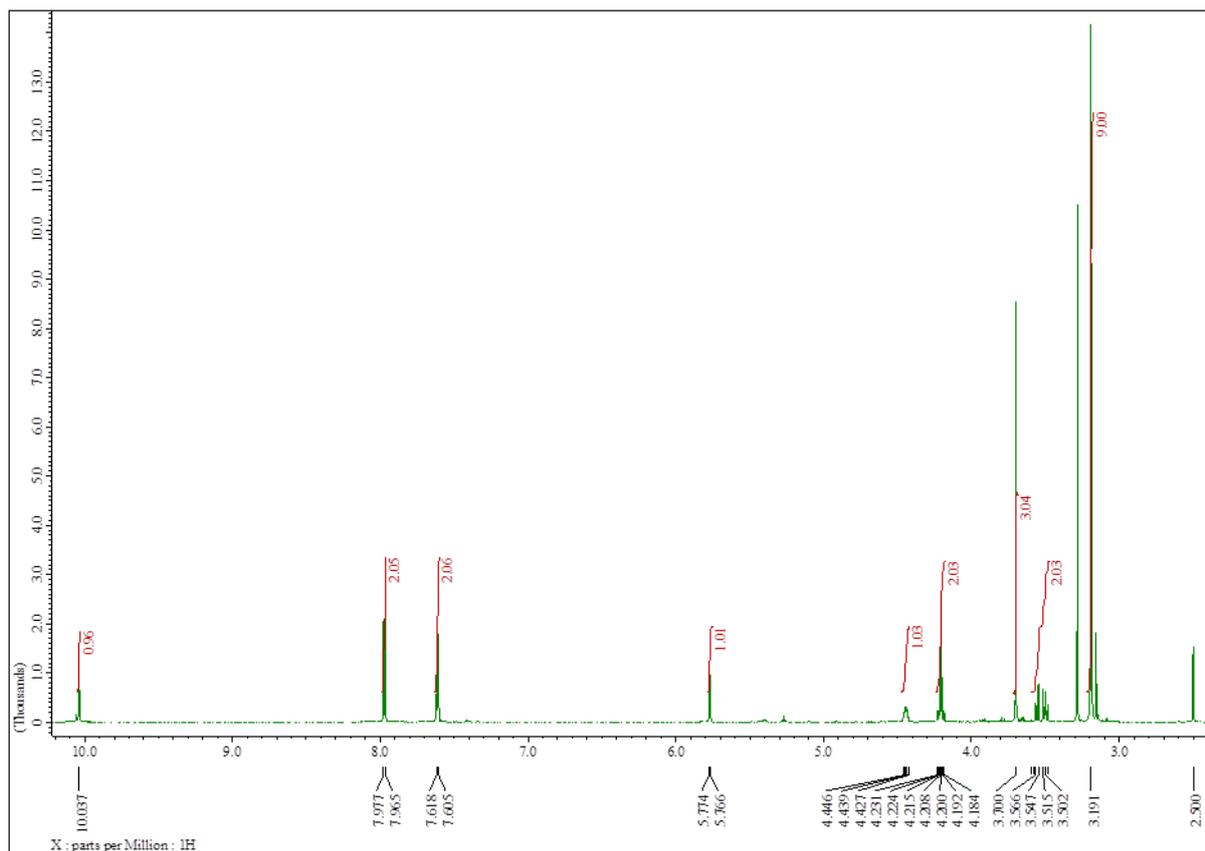


Figure S14. ^1H -NMR spectrum of **6a**

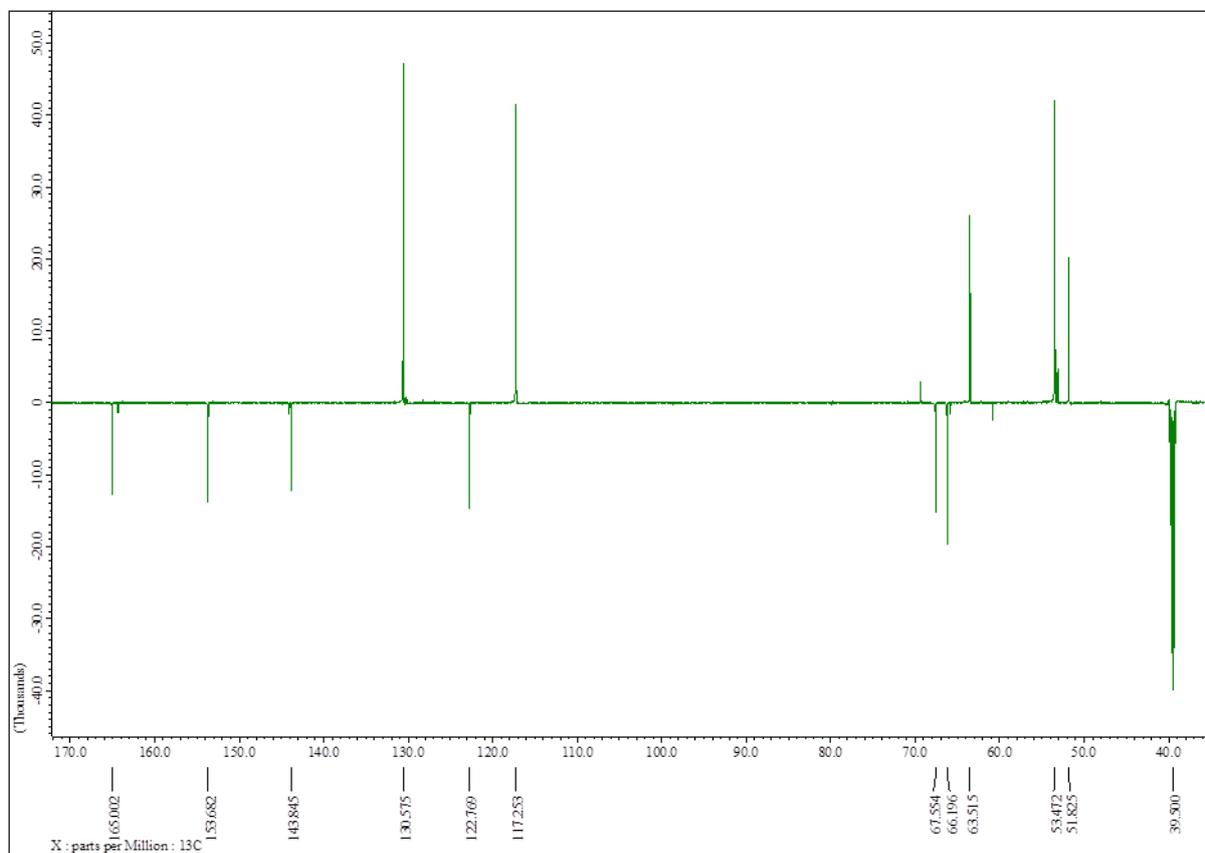


Figure S15. ^{13}C -NMR (APT) spectrum of **6a**

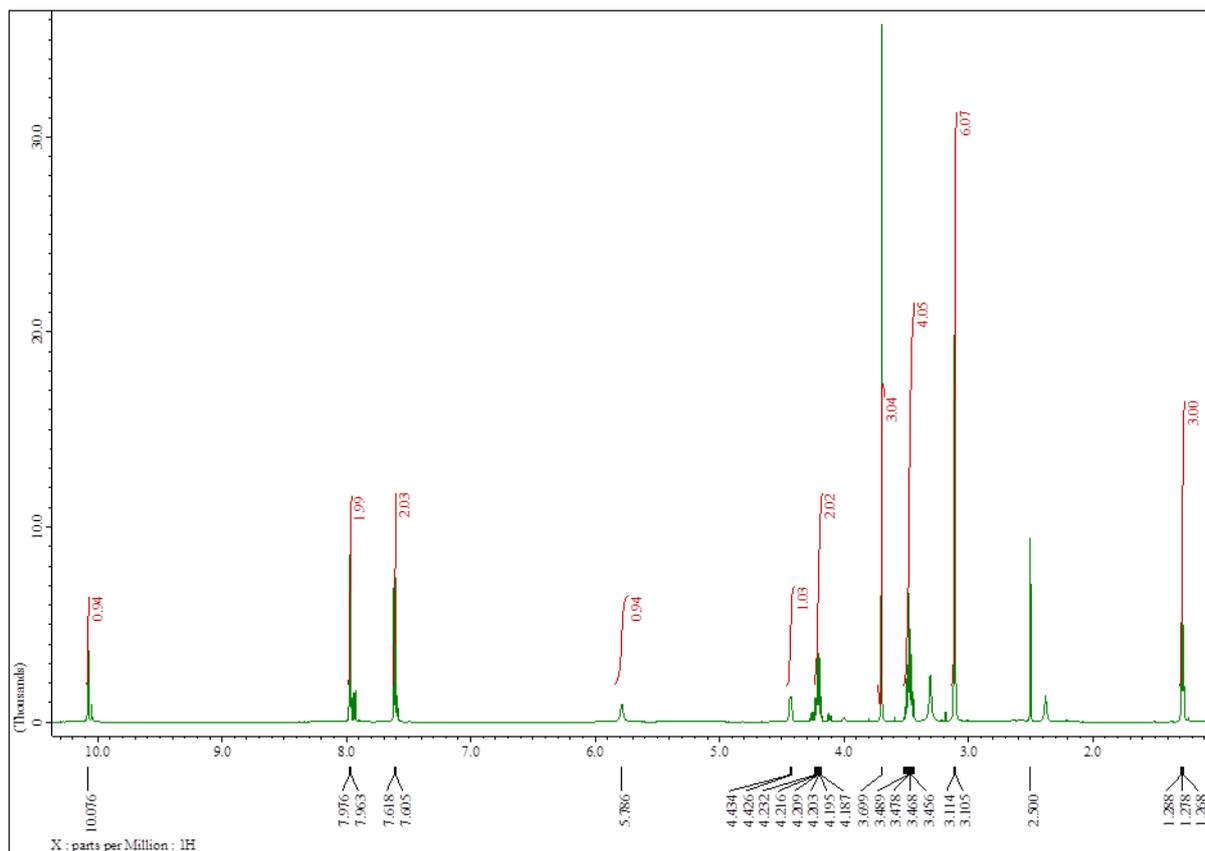


Figure S16. ¹H-NMR spectrum of 6b

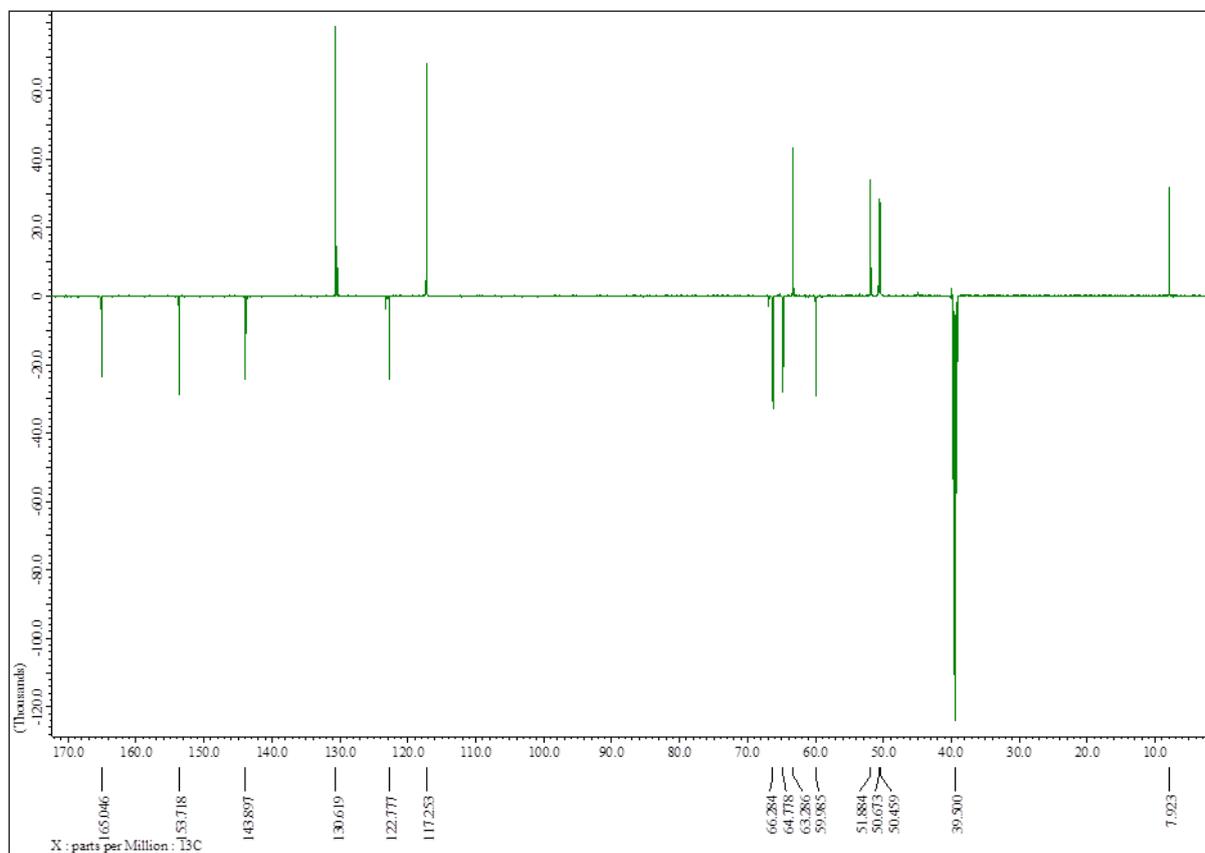


Figure S17. ¹³C-NMR (APT) spectrum of 6b

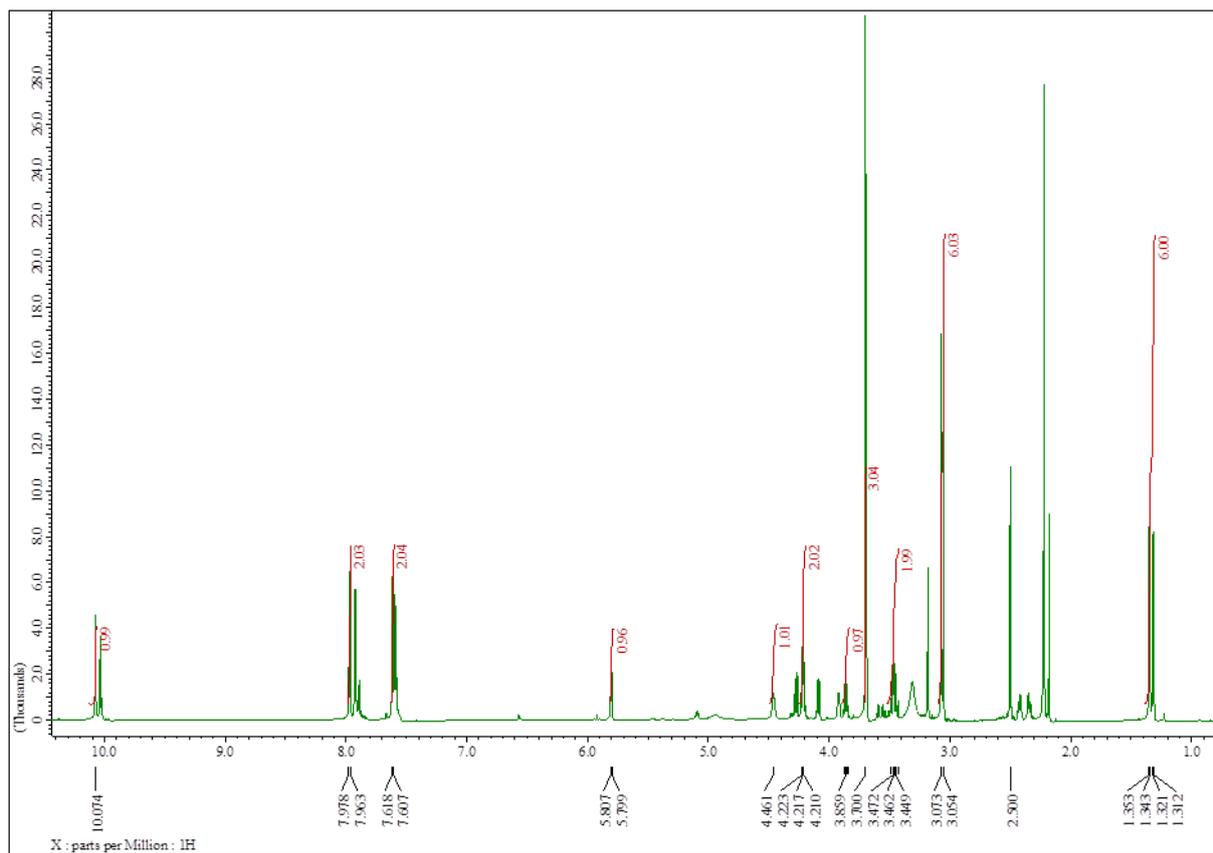


Figure S18. ¹H-NMR spectrum of 6c

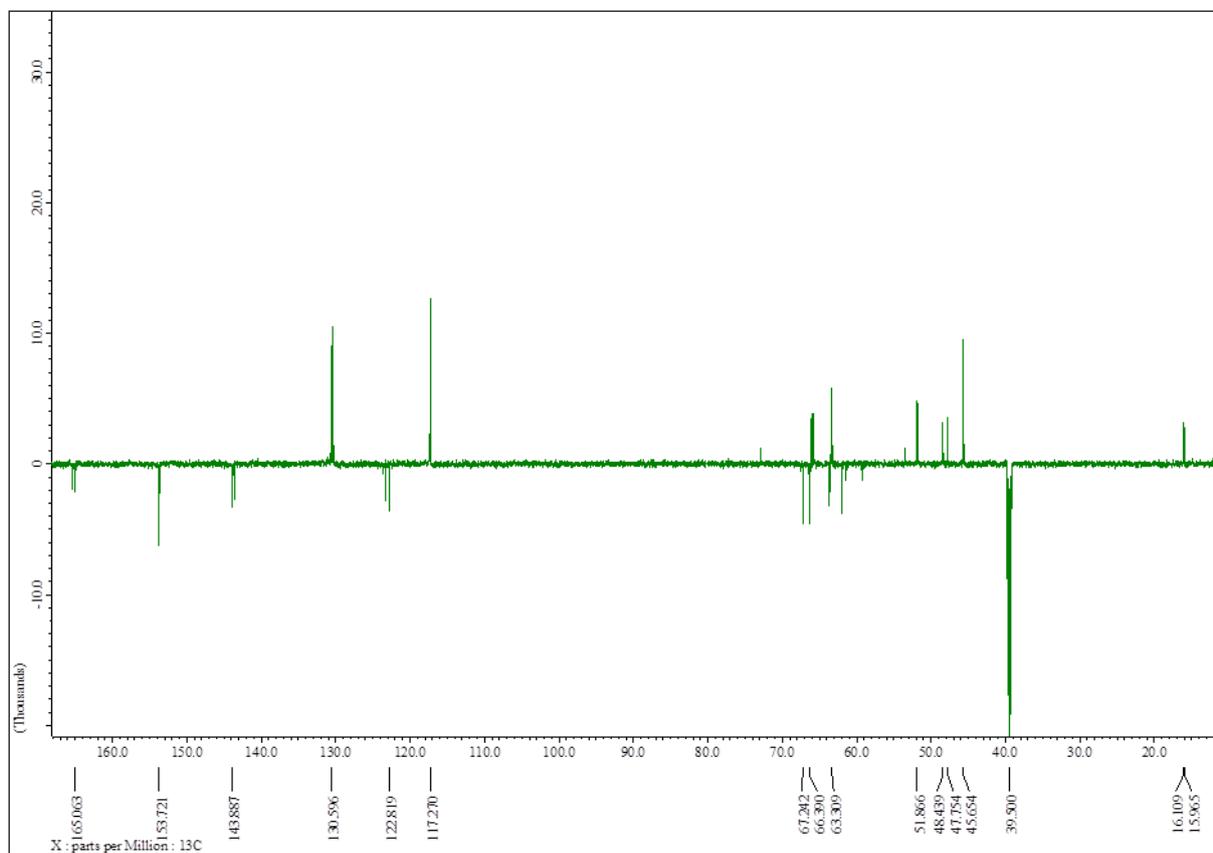


Figure S19. ¹³C-NMR (APT) spectrum of 6c

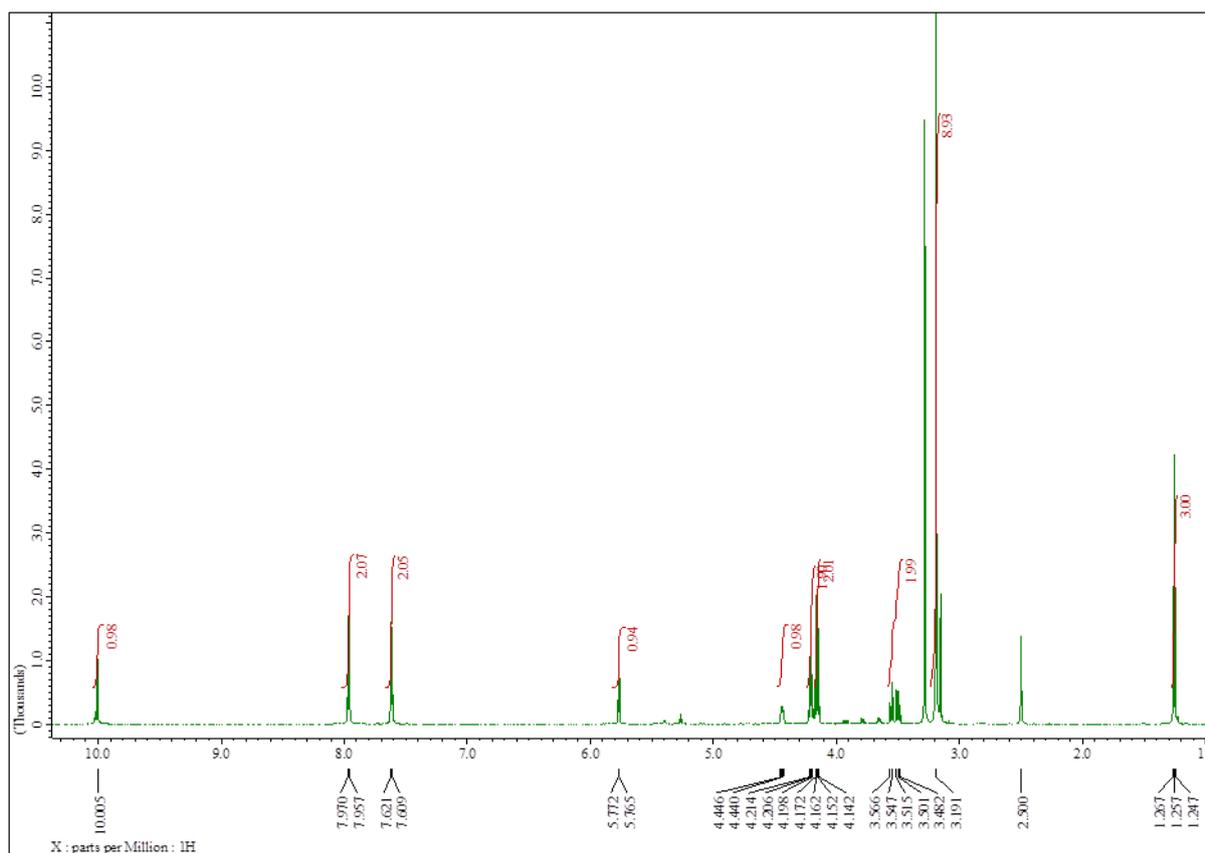


Figure S20. $^1\text{H-NMR}$ spectrum of 6d

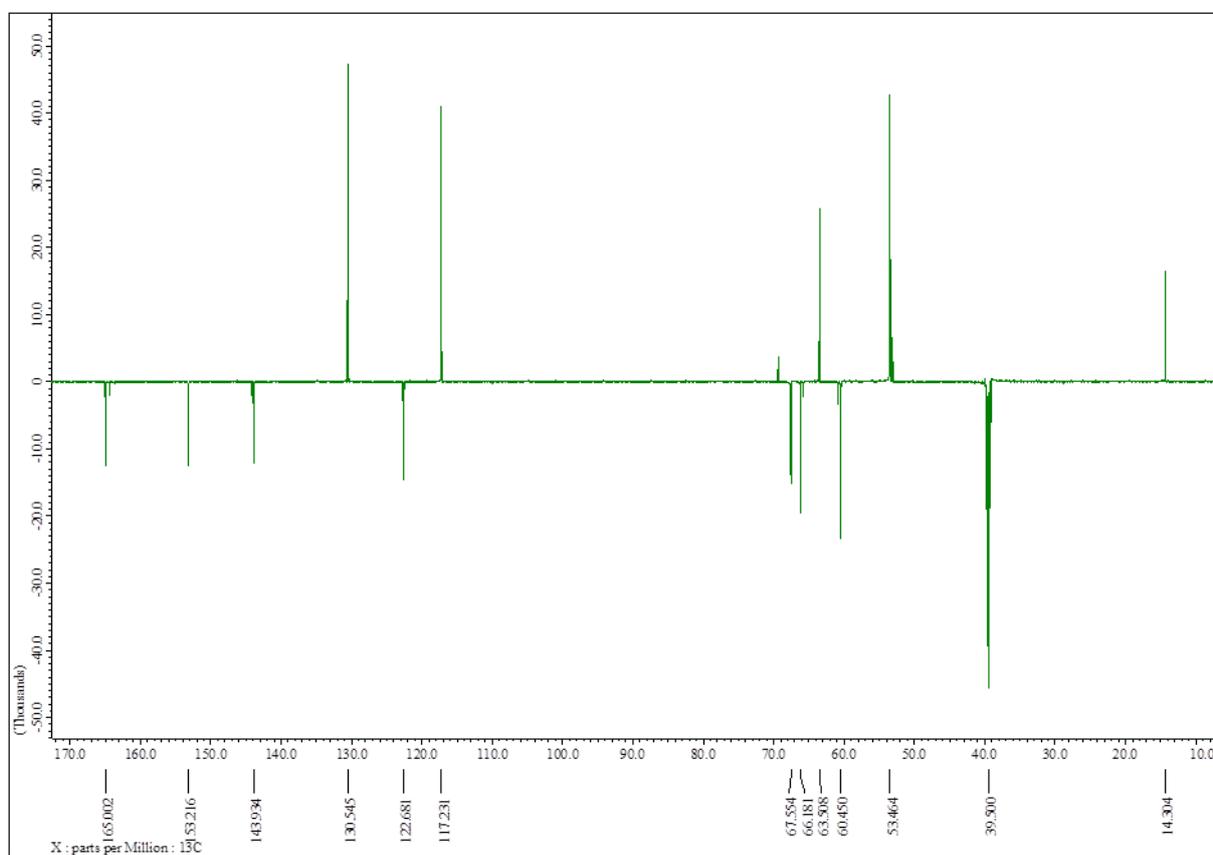


Figure S21. $^{13}\text{C-NMR}$ (APT) spectrum of 6d

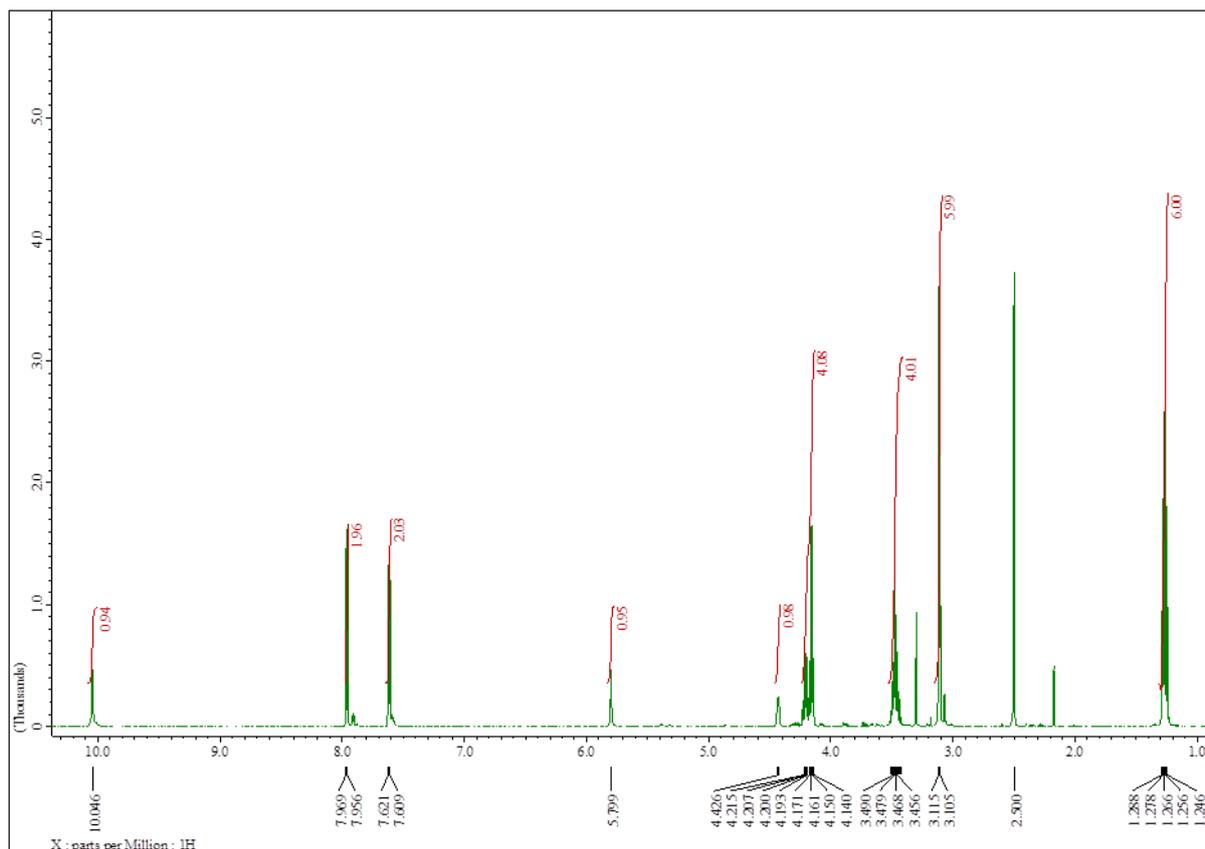


Figure S22. ¹H-NMR spectrum of 6e

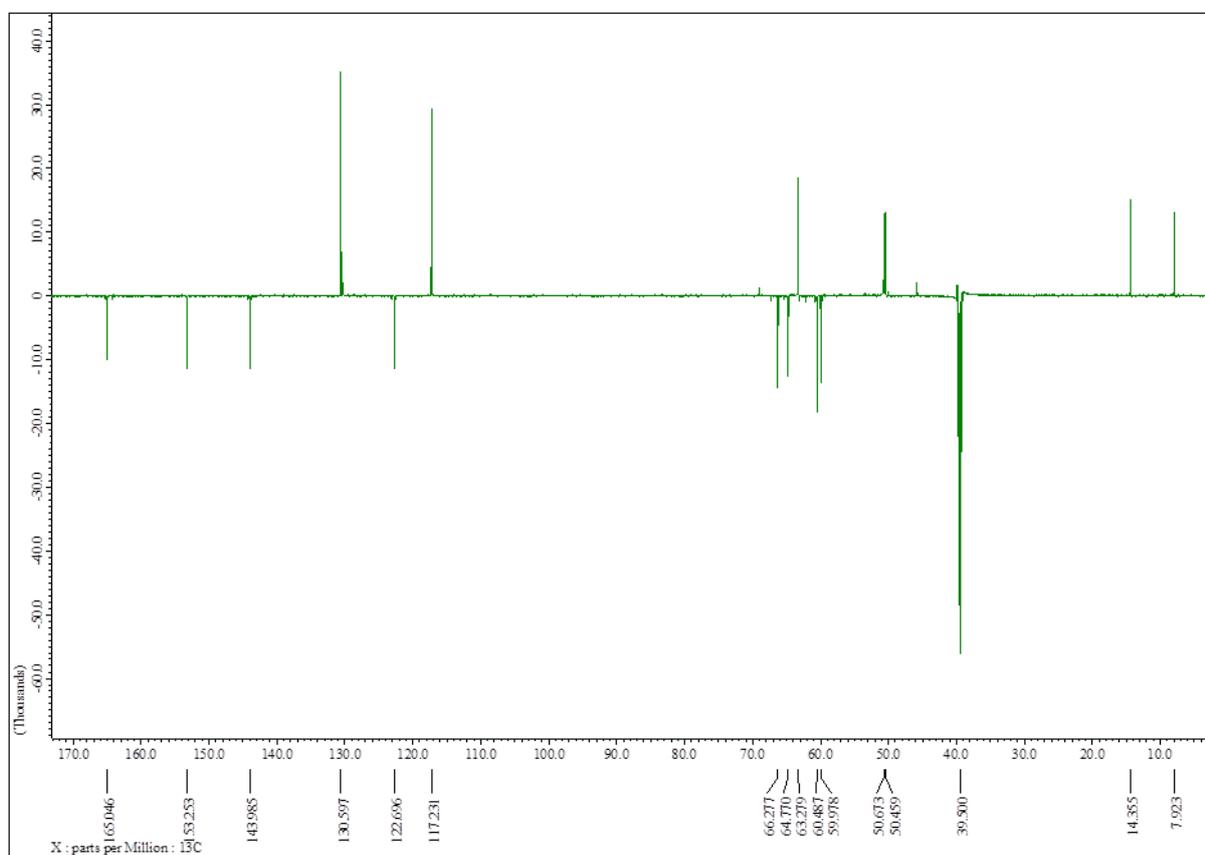


Figure S23. ¹³C-NMR (APT) spectrum of 6e

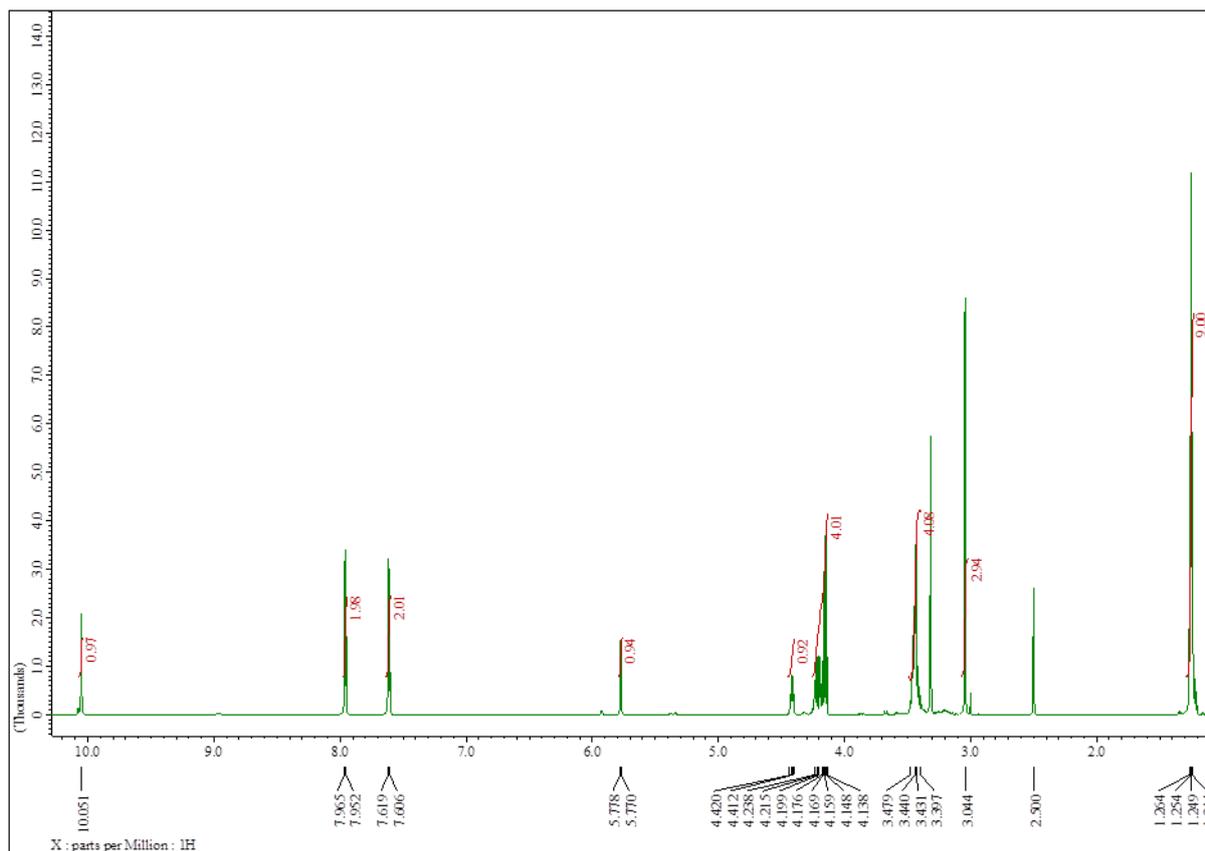


Figure S24. ¹H-NMR spectrum of **6f**

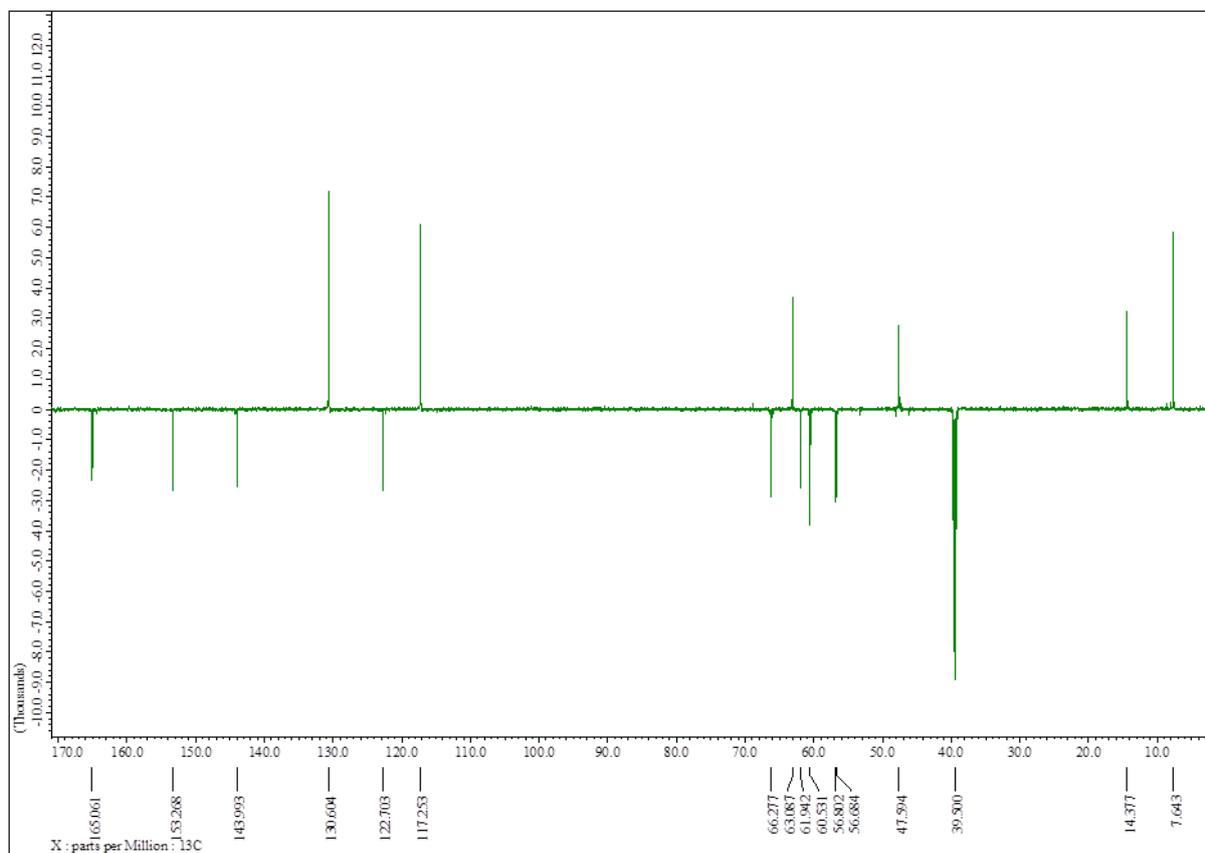


Figure S25. ¹³C-NMR (APT) spectrum of **6f**

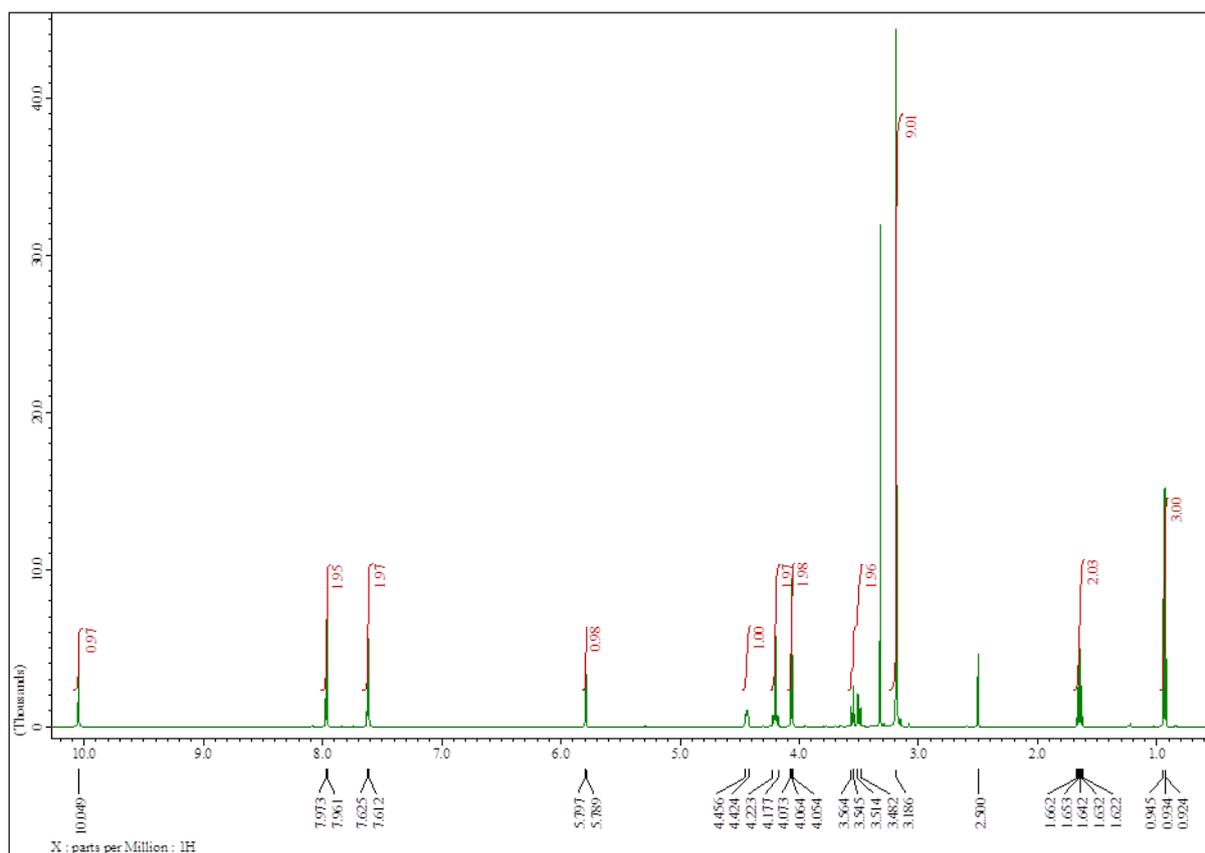


Figure S26. ¹H-NMR spectrum of **6g**

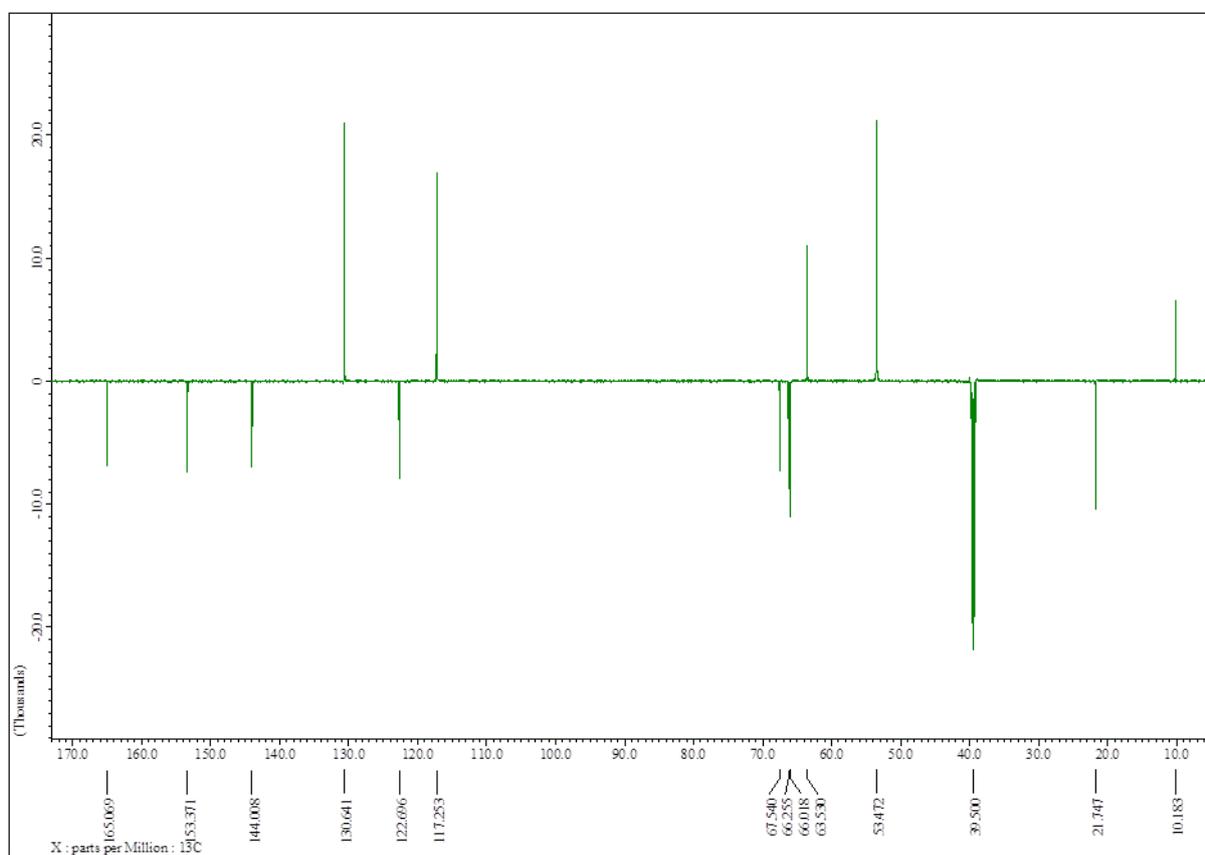


Figure S27. ¹³C-NMR (APT) spectrum of **6g**

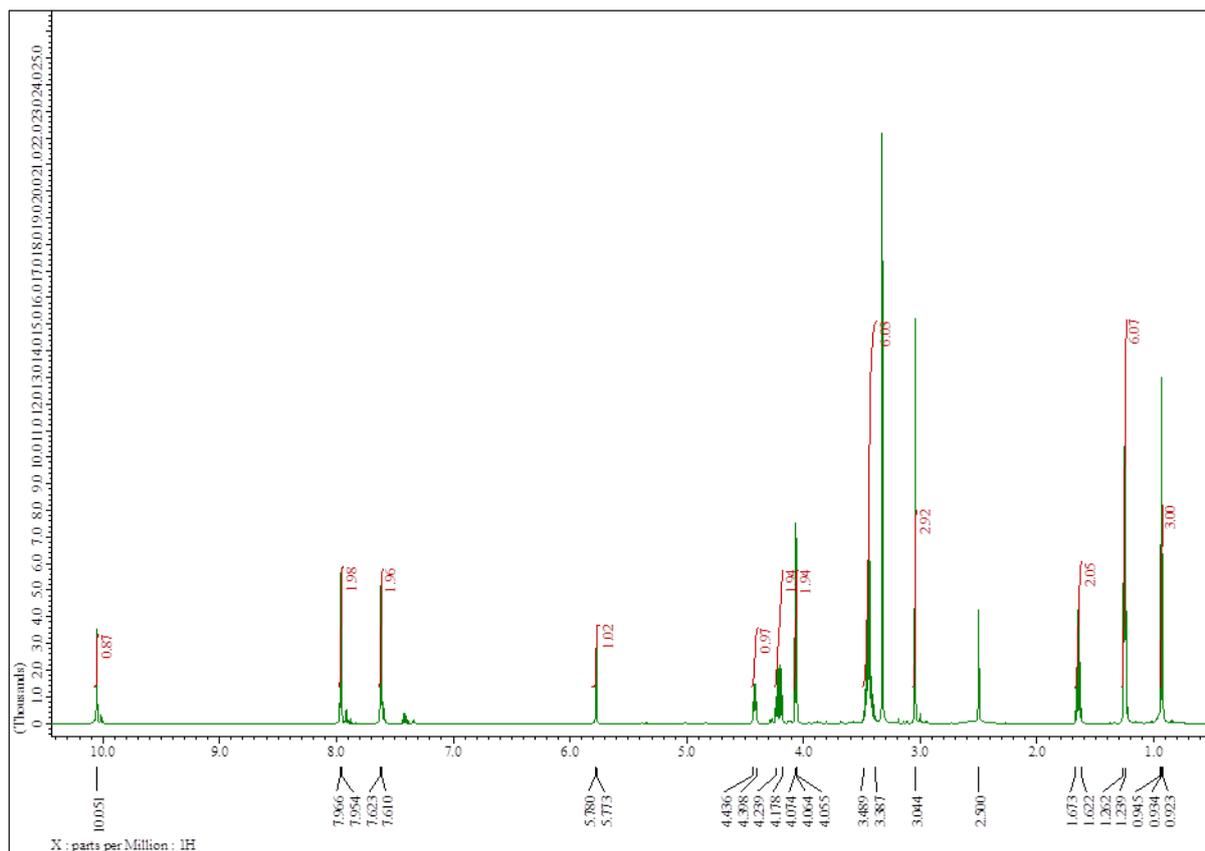


Figure S28. $^1\text{H-NMR}$ spectrum of **6h**

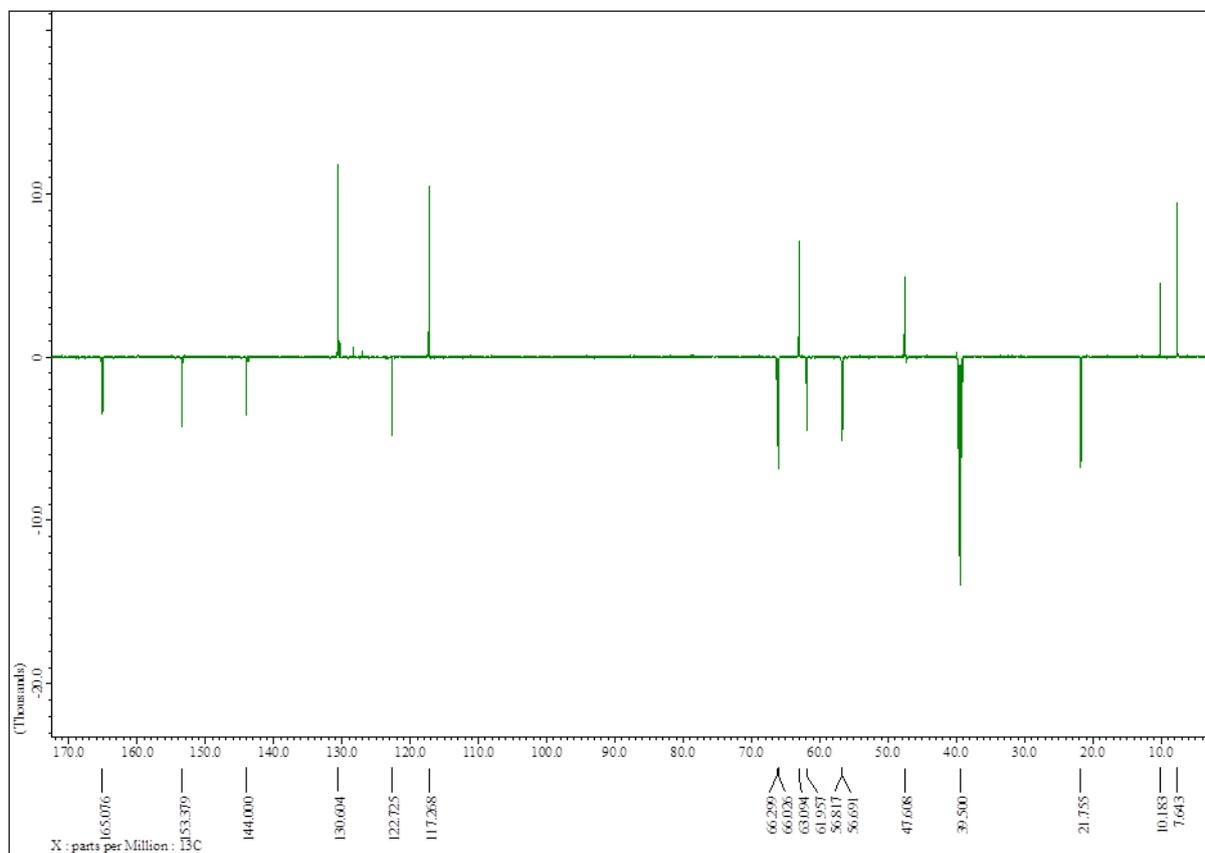


Figure S29. $^{13}\text{C-NMR}$ (APT) spectrum of **6h**

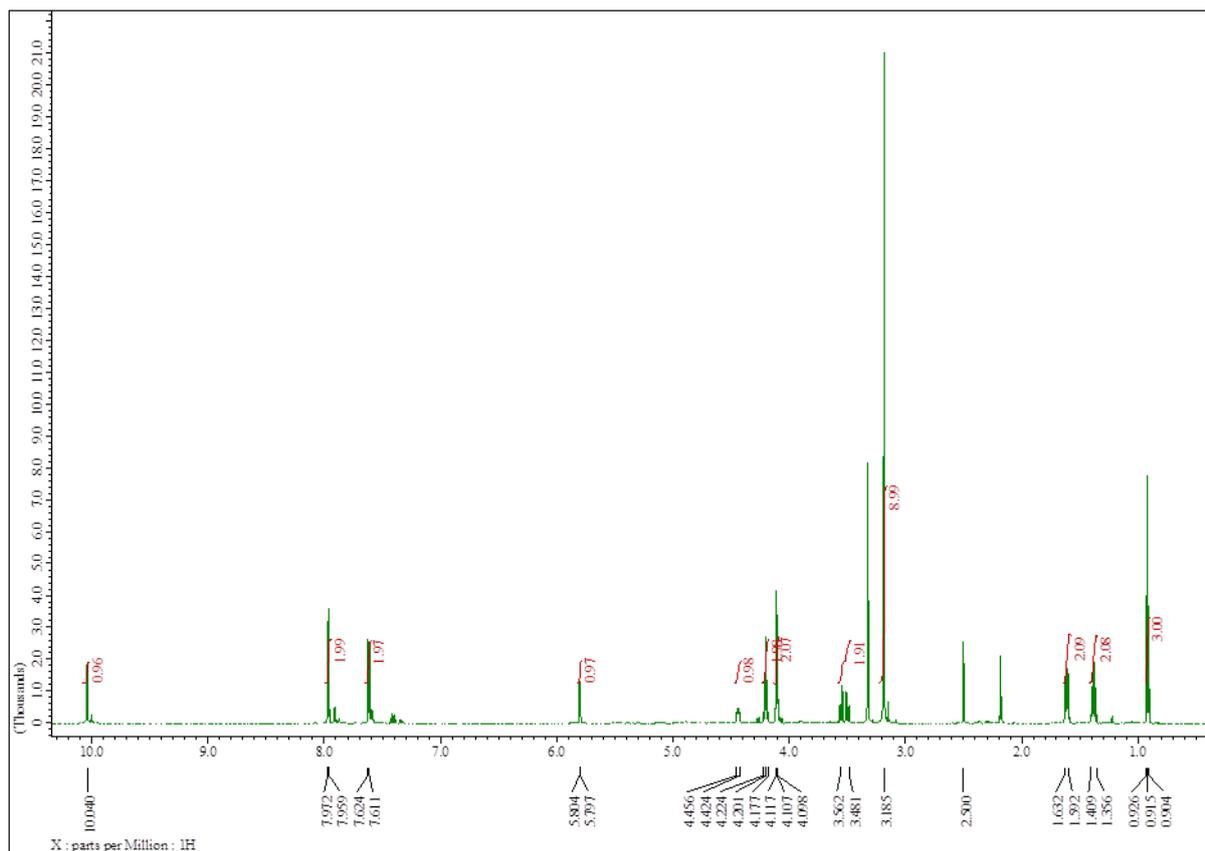


Figure S30. ¹H-NMR spectrum of **6i**

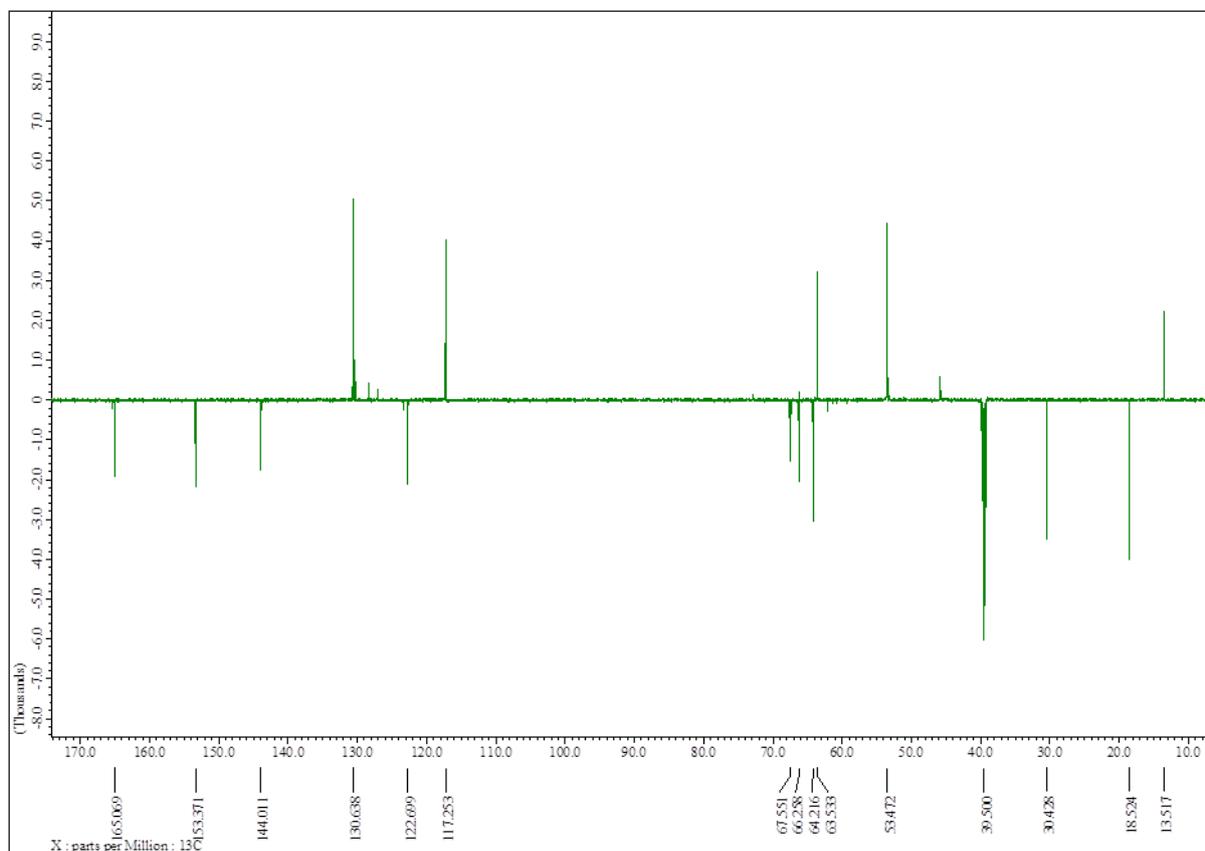


Figure S31. ¹³C-NMR (APT) spectrum of **6i**