

Identification of unusual C–Cl... π contacts in 2-(alkylamino)-3-chloro-1,4-naphthoquinones: Effect of *N*-substituents on crystal packings, fluorescence, redox and anti-microbial properties

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Supplementary Information

1. **IR spectra:** The IR spectra of secondary amines summarized below as Fig. S1 to S7.

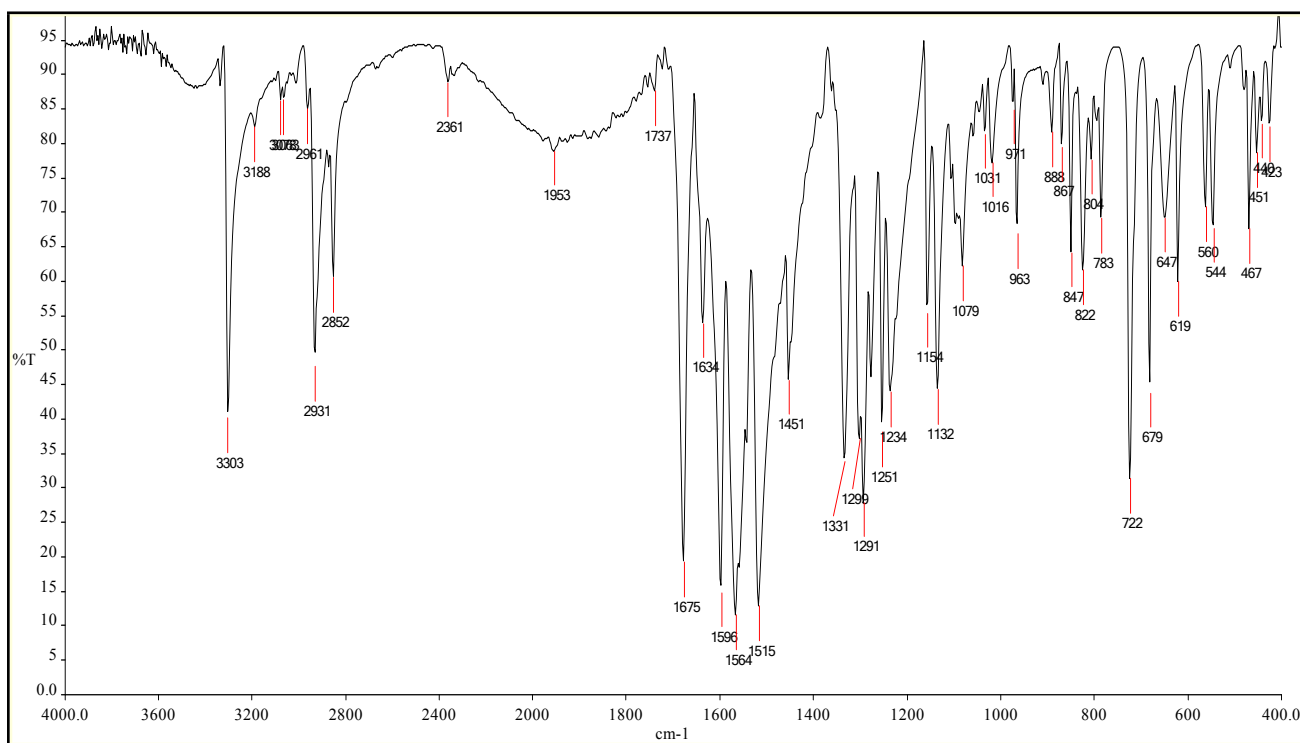


Fig. S1: IR Spectrum of compound 1

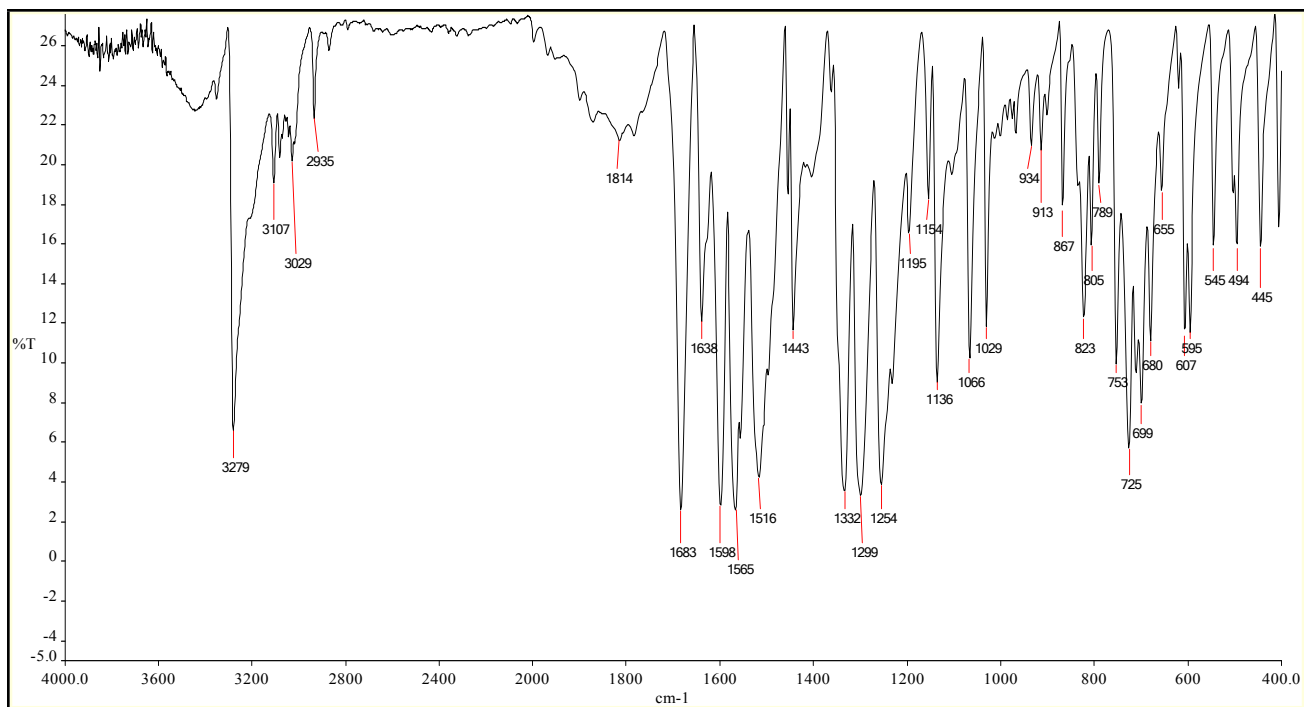


Fig. S2: IR Spectrum of compound 2

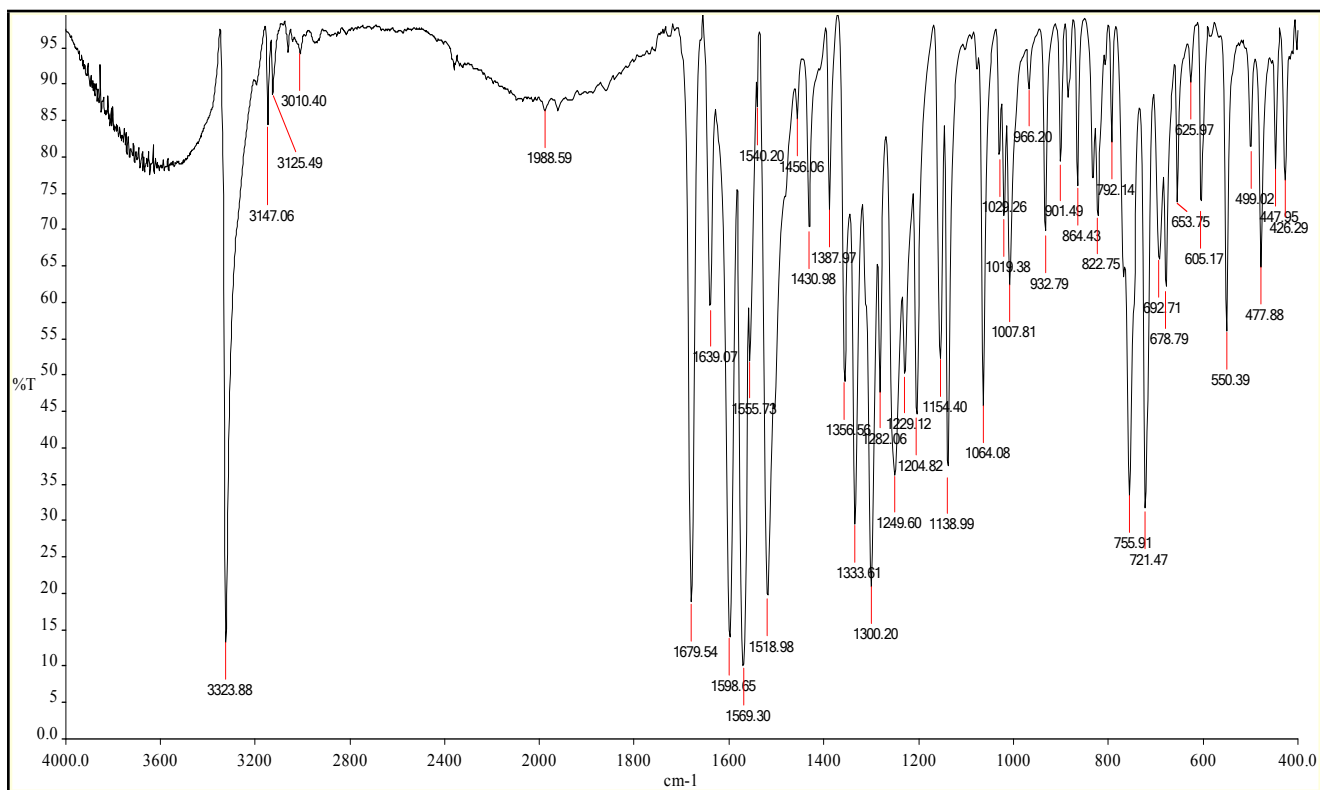


Fig. S3: IR Spectrum of compound 3

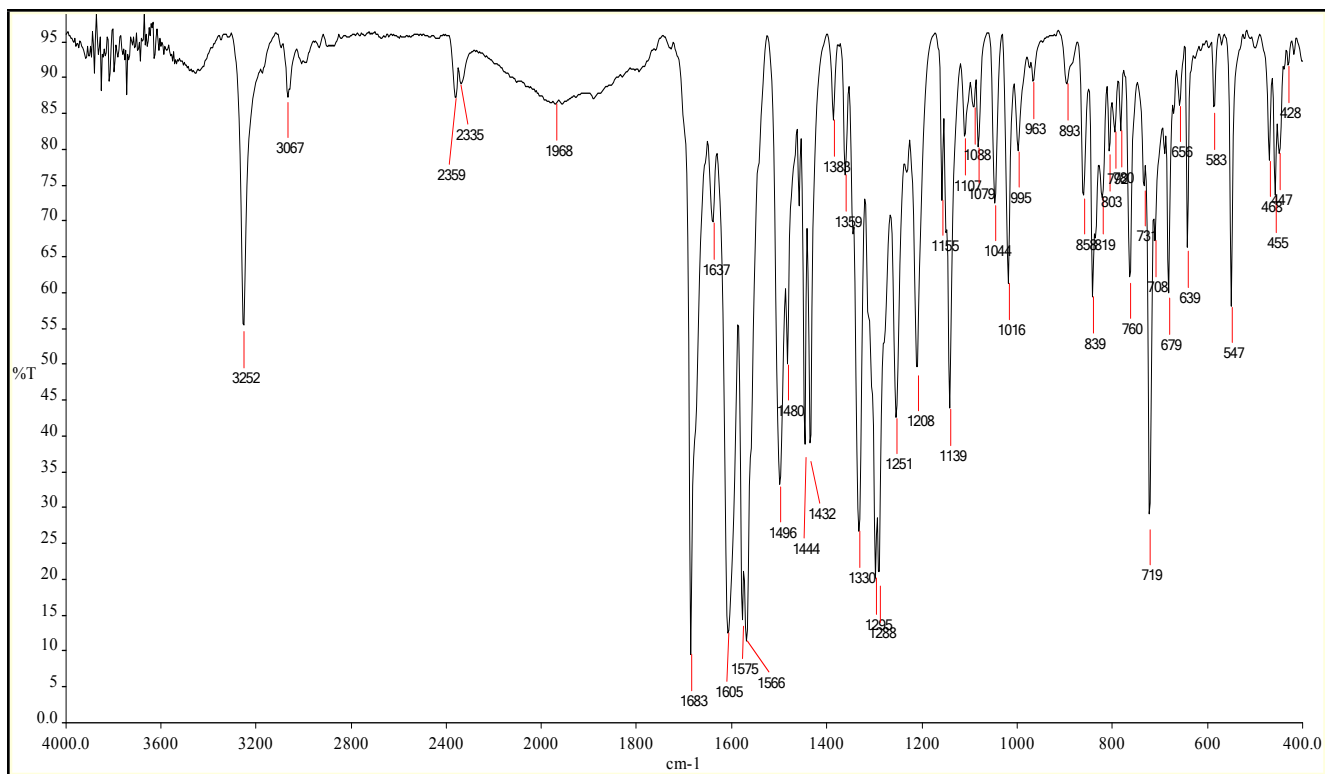


Fig. S4: IR Spectrum of compound 4

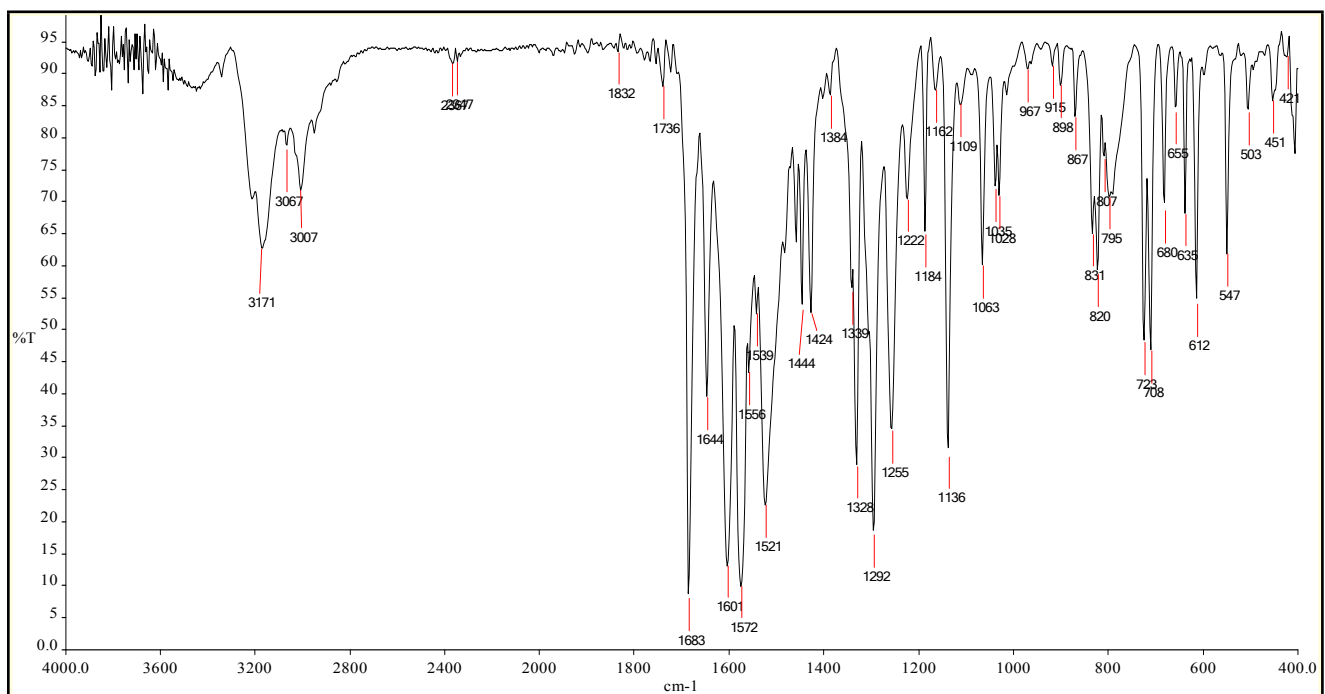


Fig. S5: IR Spectrum of compound 5

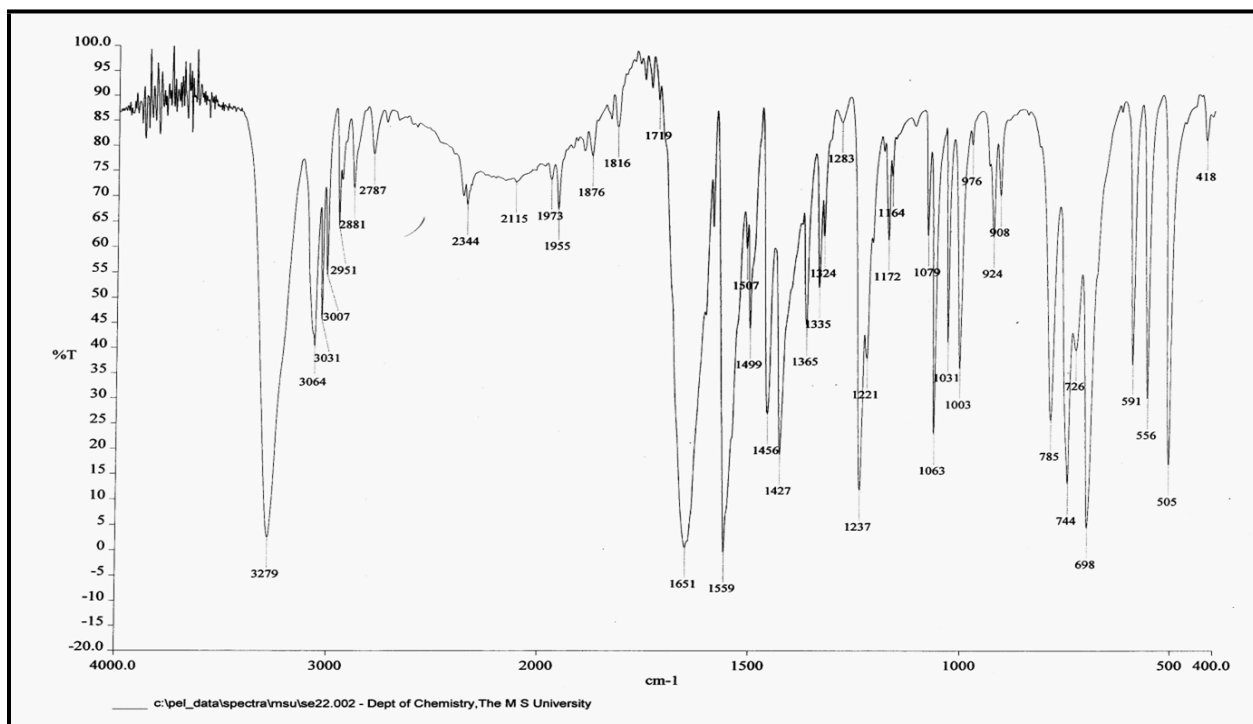


Fig. S6: IR Spectrum of compound 6

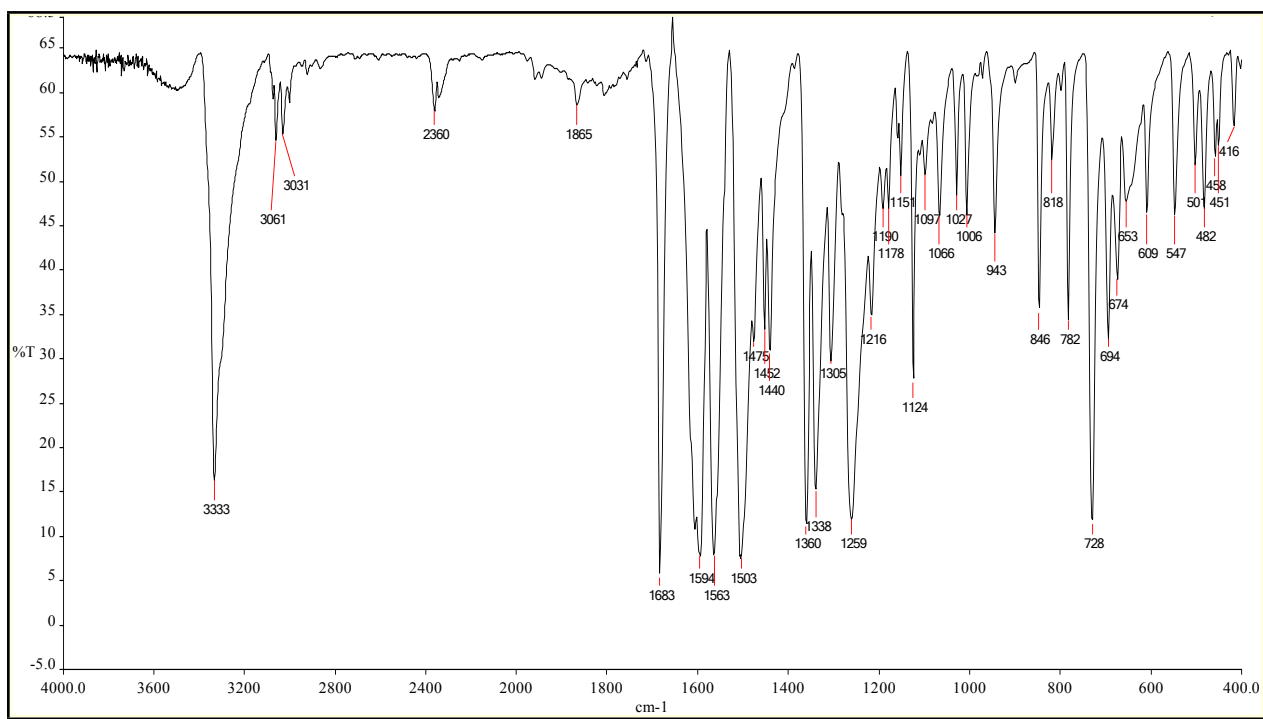


Fig. S7: IR Spectrum of compound 7

2. **NMR spectra:** The NMR spectra of secondary amines summarized below as Fig. S8 to S21.

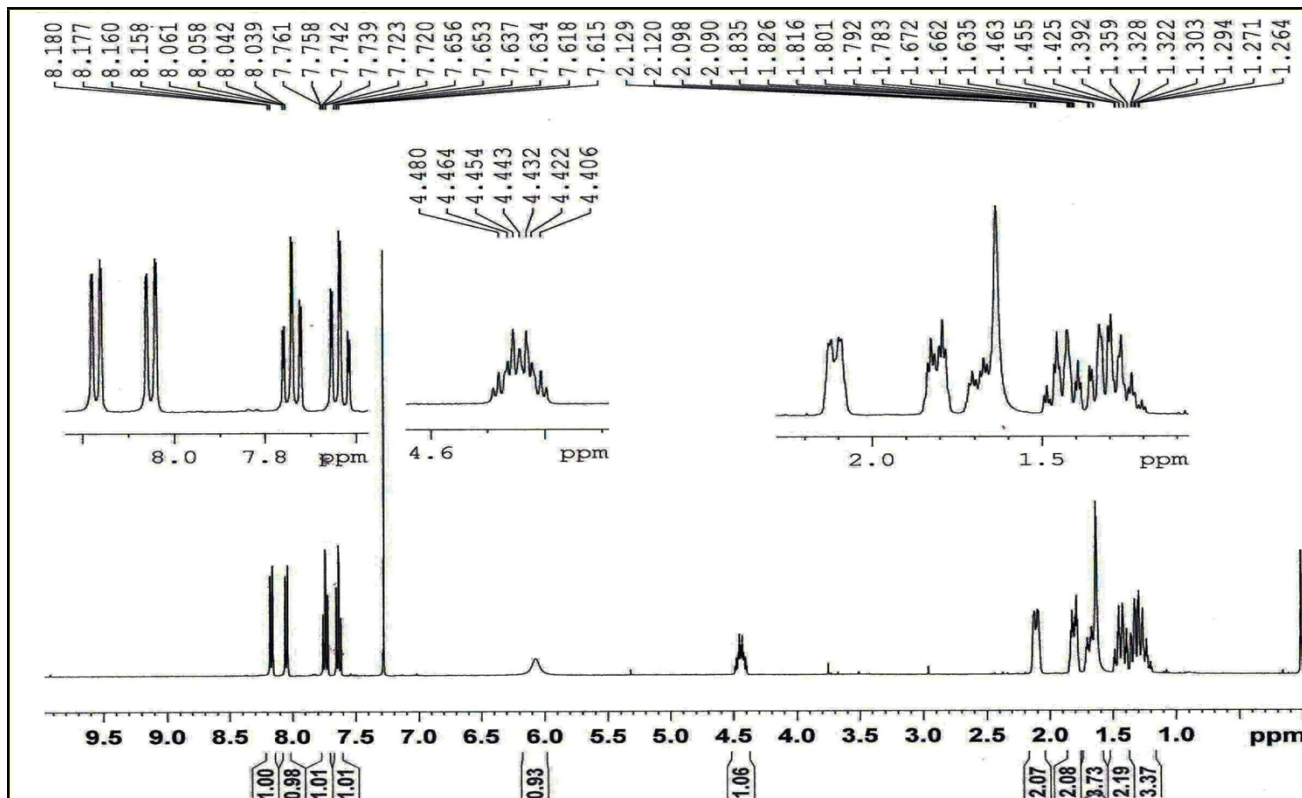


Fig. S8: ¹H NMR spectrum of compound 1

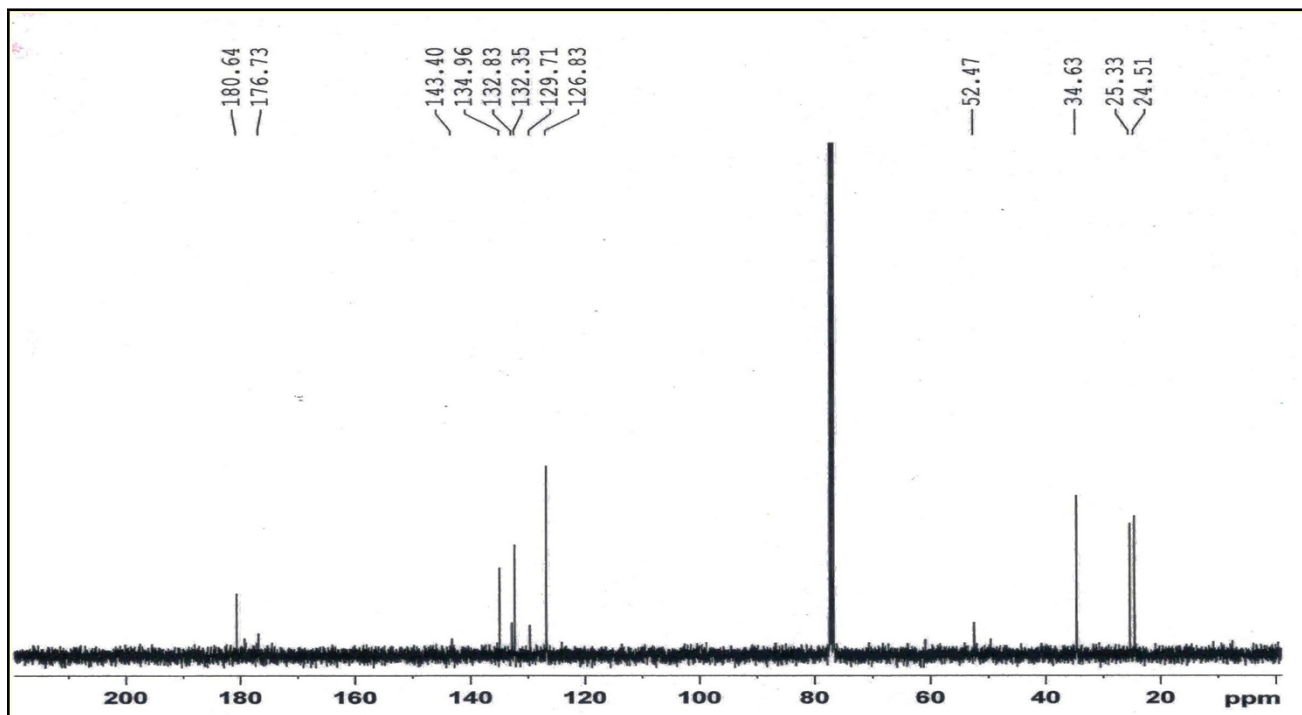


Fig. S11: ^{13}C NMR spectrum of compound 2

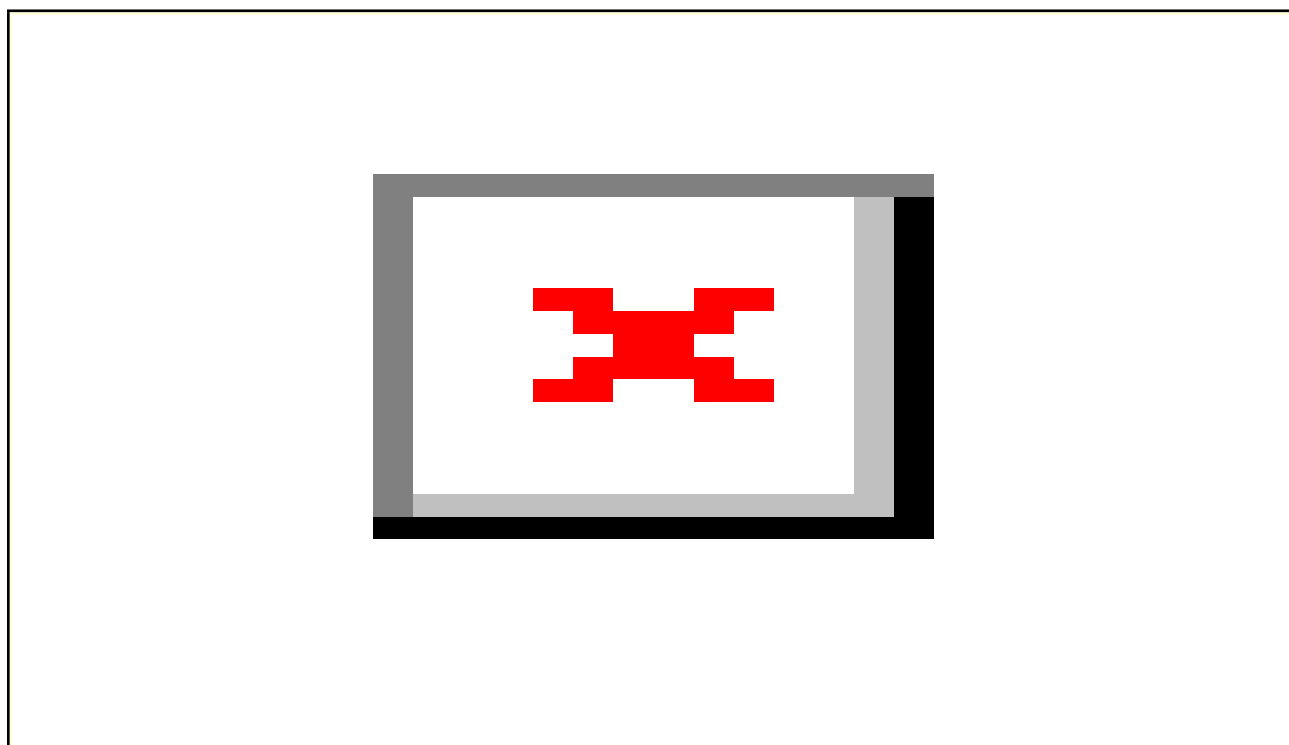


Fig. S12: ^1H NMR spectrum of compound 3

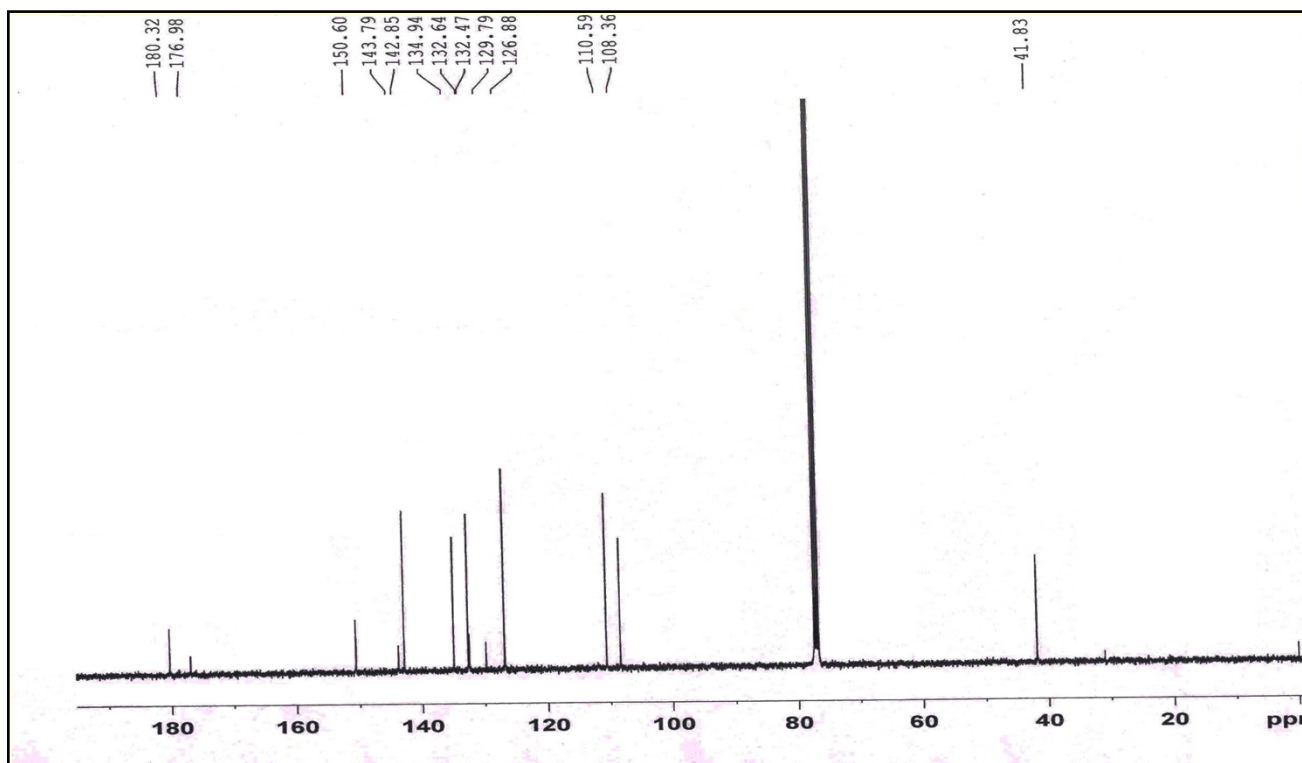


Fig. S13: ^{13}C NMR spectrum of compound 3

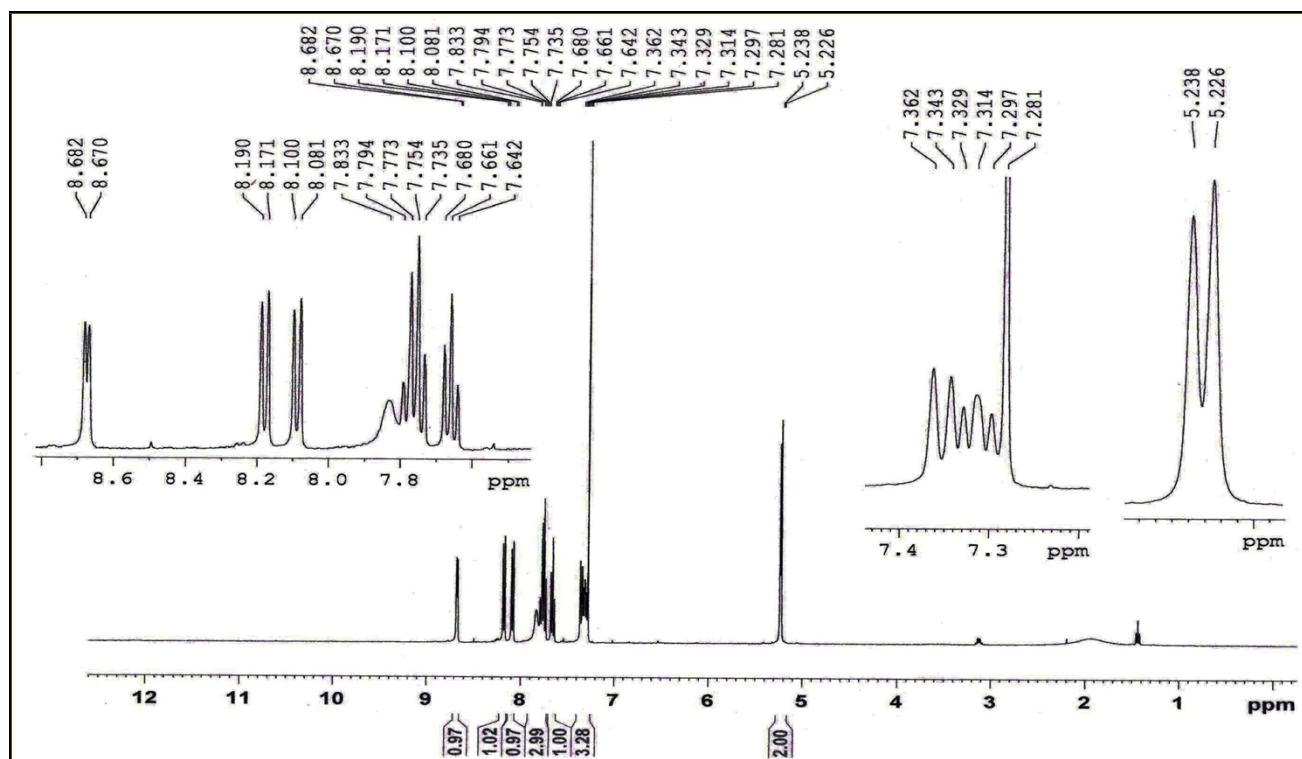


Fig. S14: ^1H NMR spectrum of compound 4

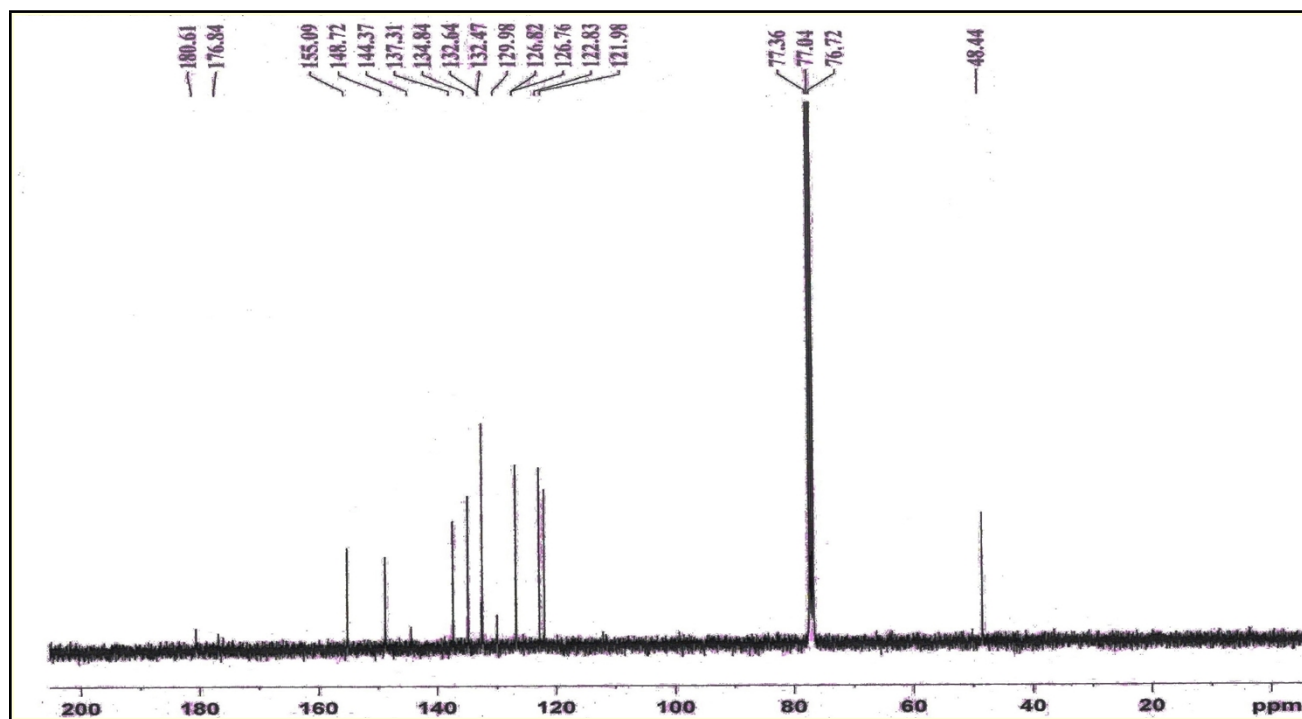


Fig. S15: ^{13}C NMR spectrum of compound 4

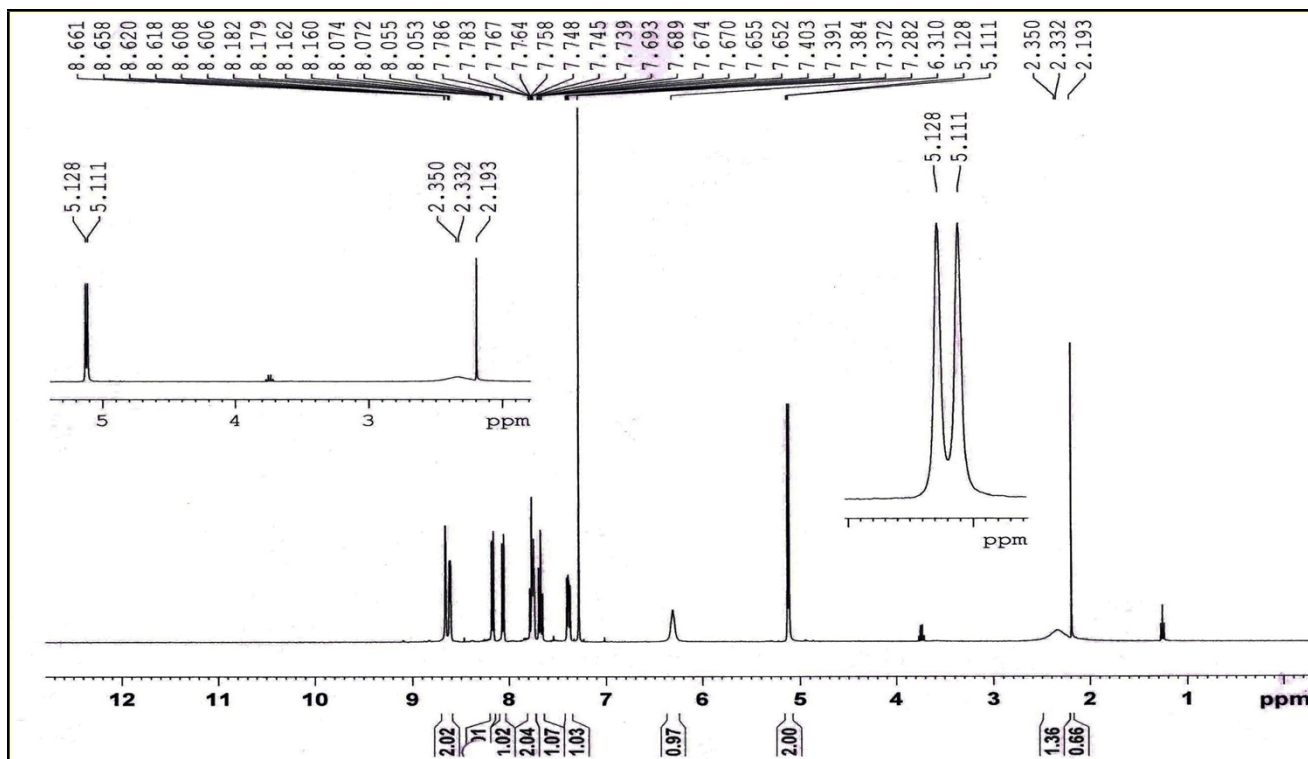


Fig. S16: ^1H NMR spectrum of compound 5

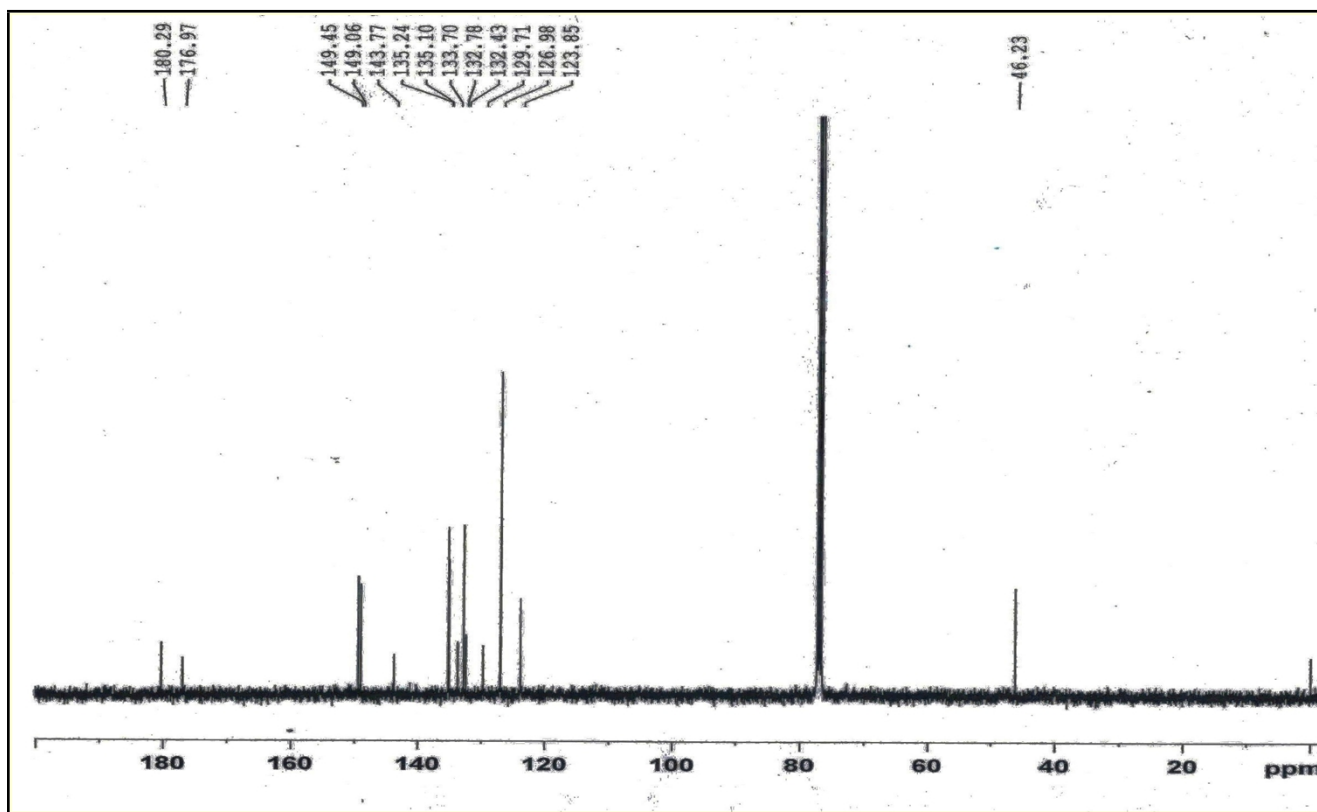


Fig. S17: ^{13}C NMR spectrum of compound 5

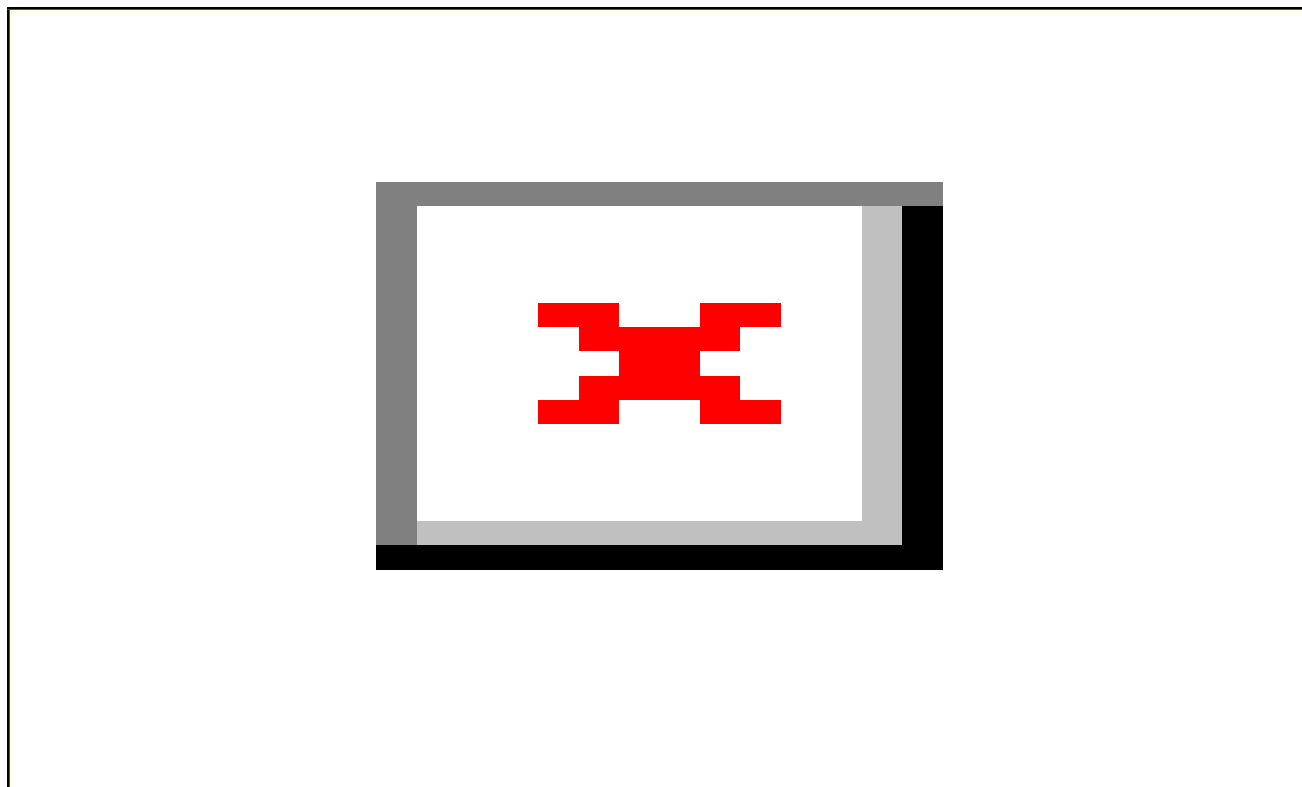


Fig. S18: ^1H NMR spectrum of compound 6

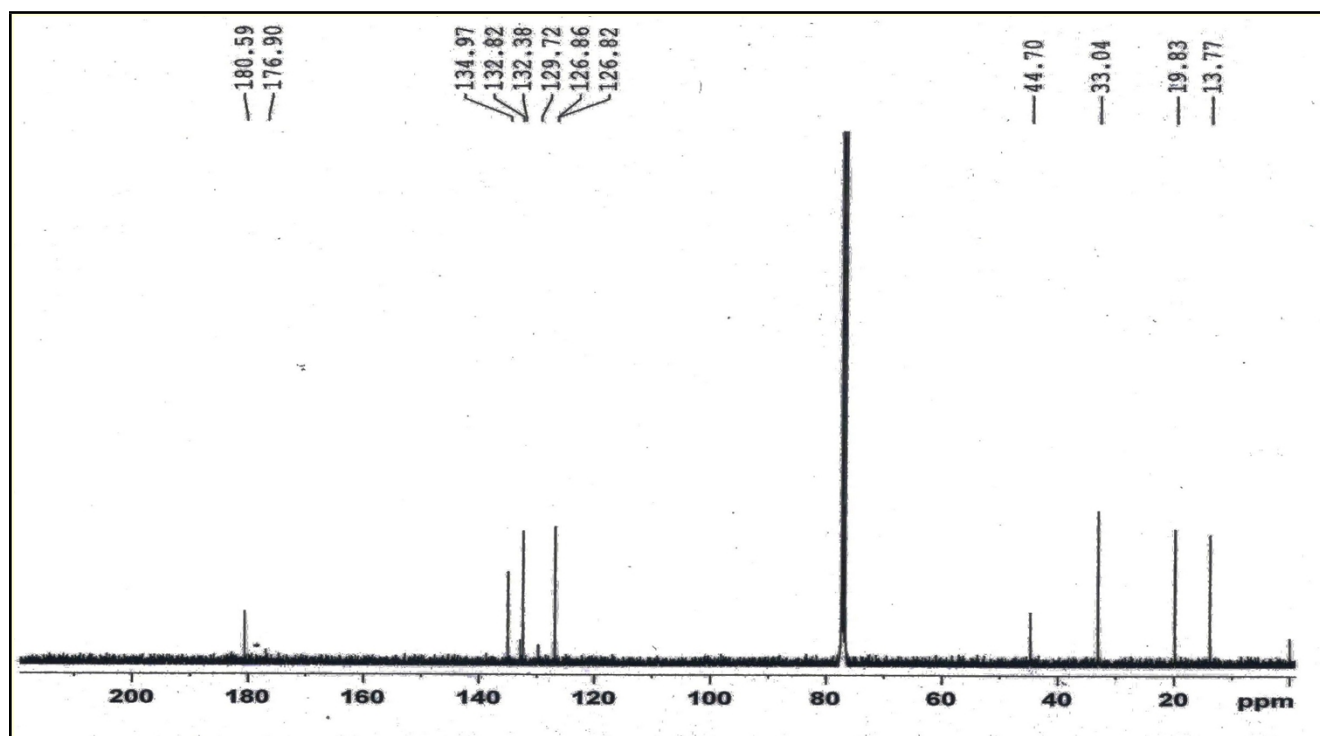


Fig. S19: ^{13}C NMR spectrum of compound 6

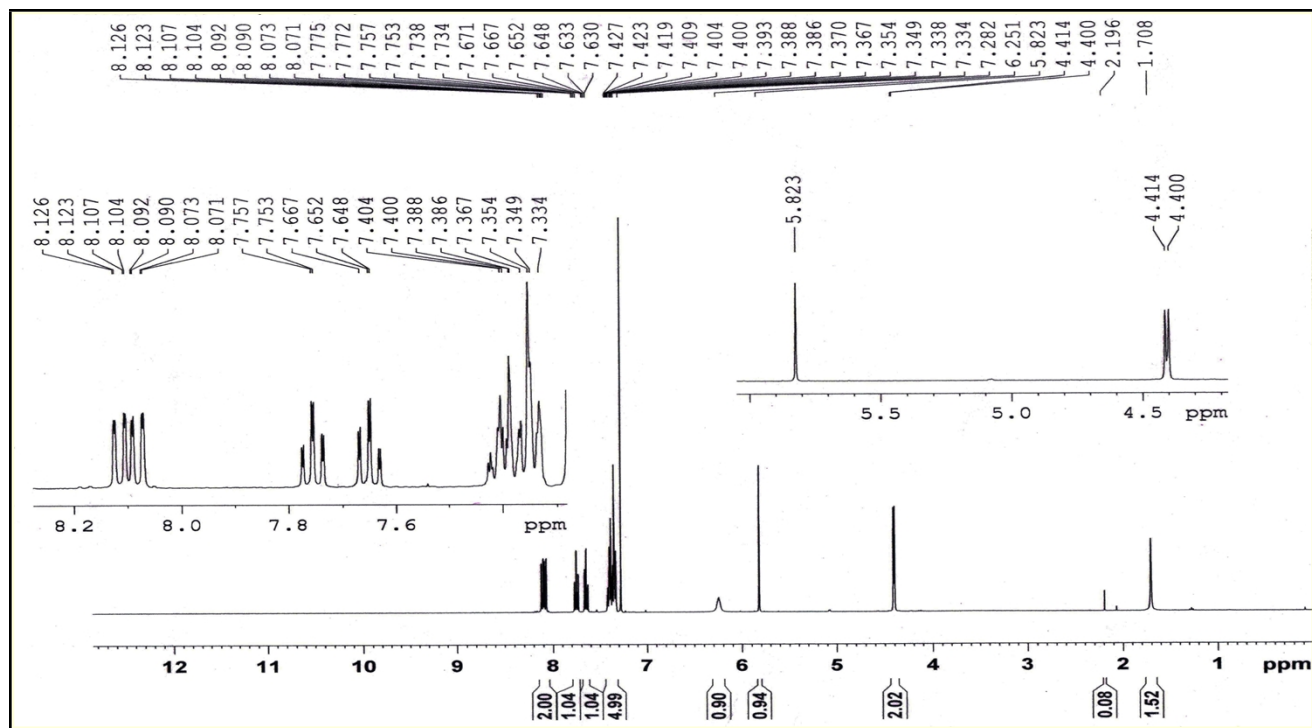


Fig. S20: ^1H NMR spectrum of compound 7

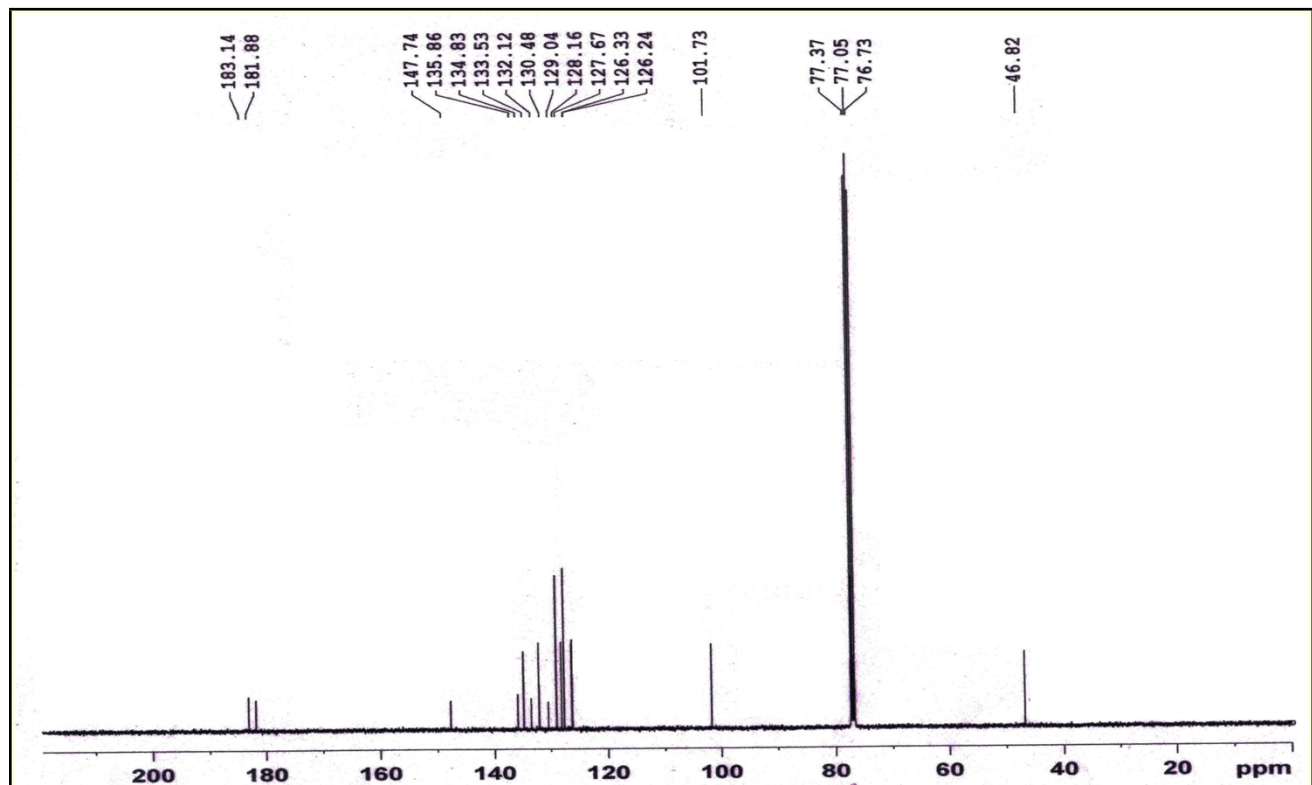


Fig. S21: ^{13}C NMR spectrum of compound 7

3. GC MS spectra: The GC MS spectra of compounds are summarized below as Fig. S22 to S28

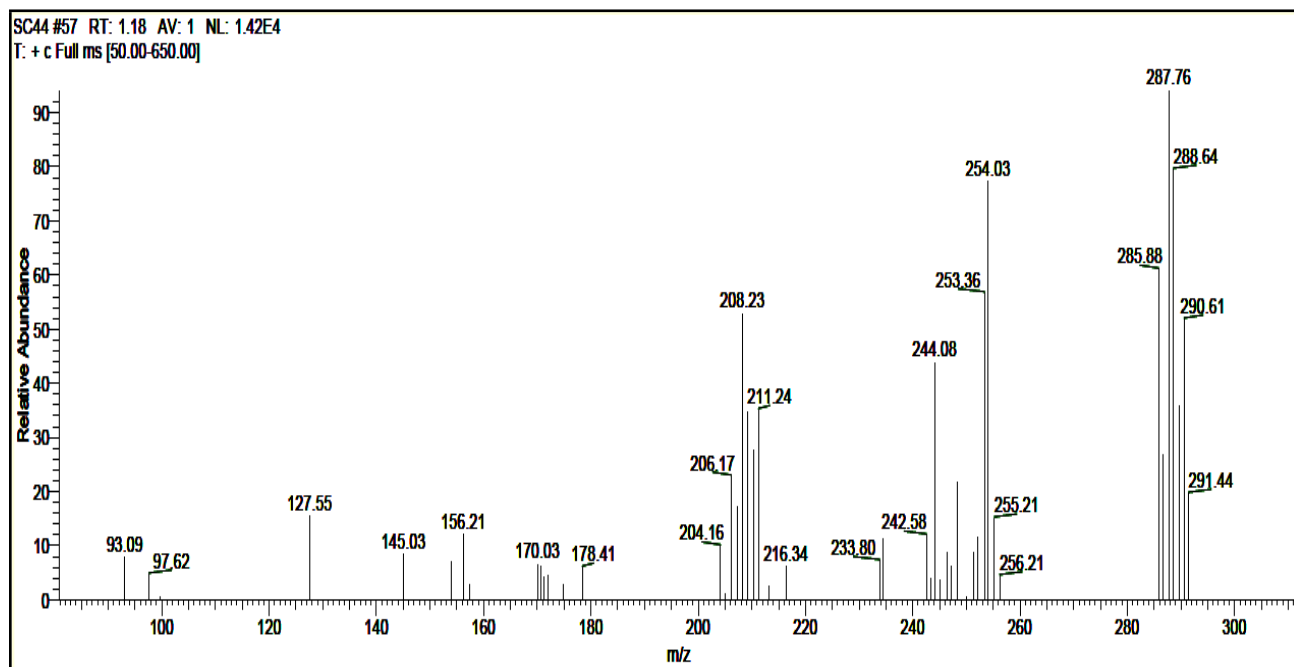


Fig. S22: GC MS spectra of compound 1

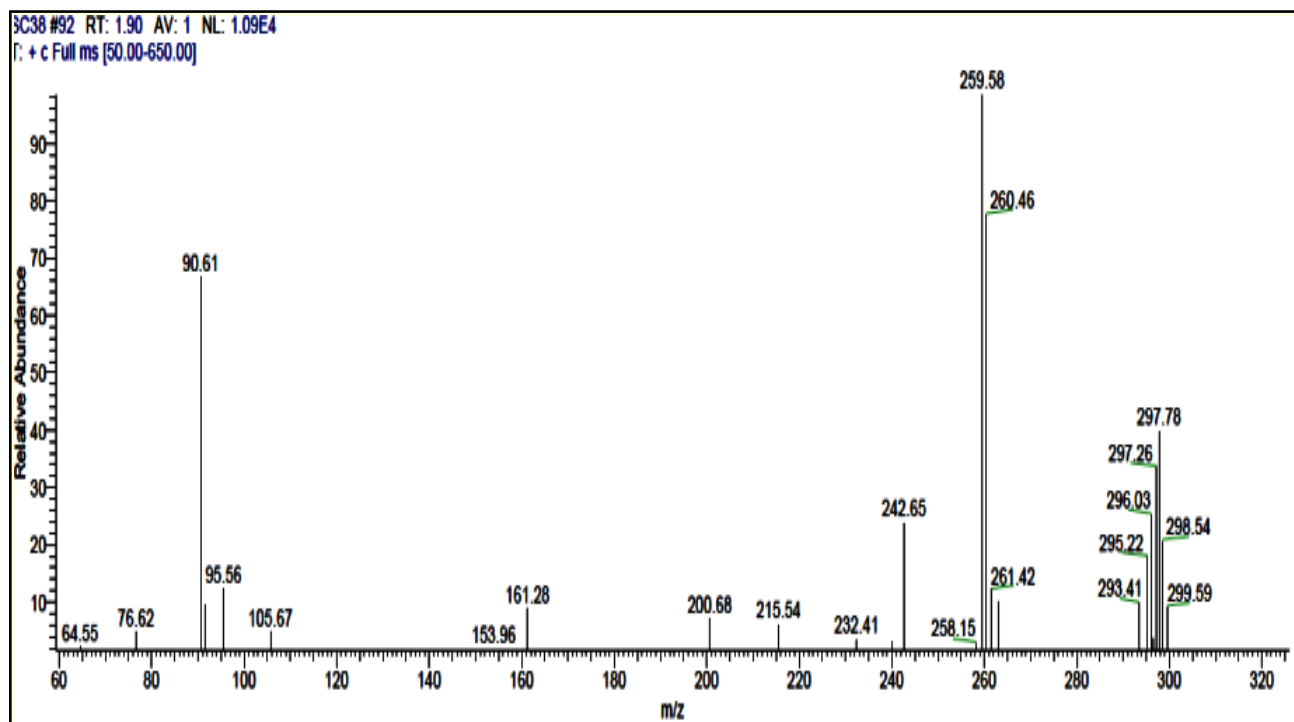


Fig. S23: GC MS spectra of compound 2

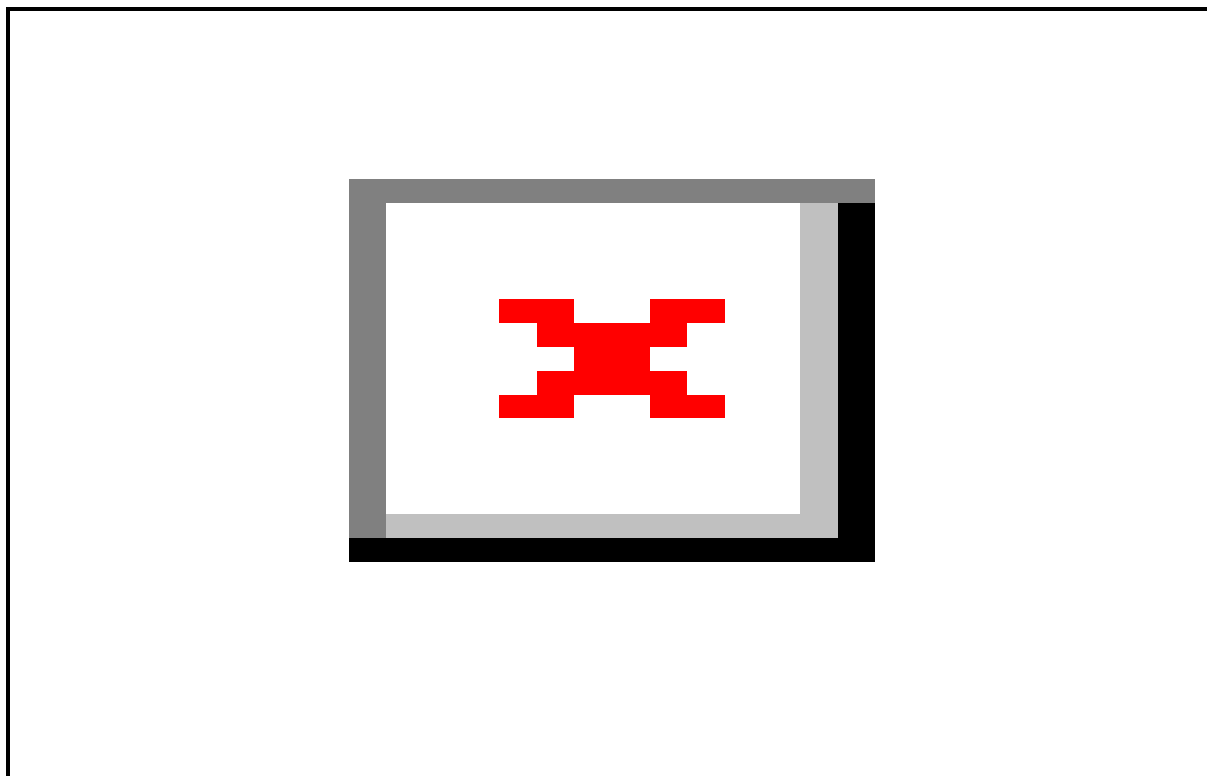


Fig. S24: GC MS spectra of compound 3

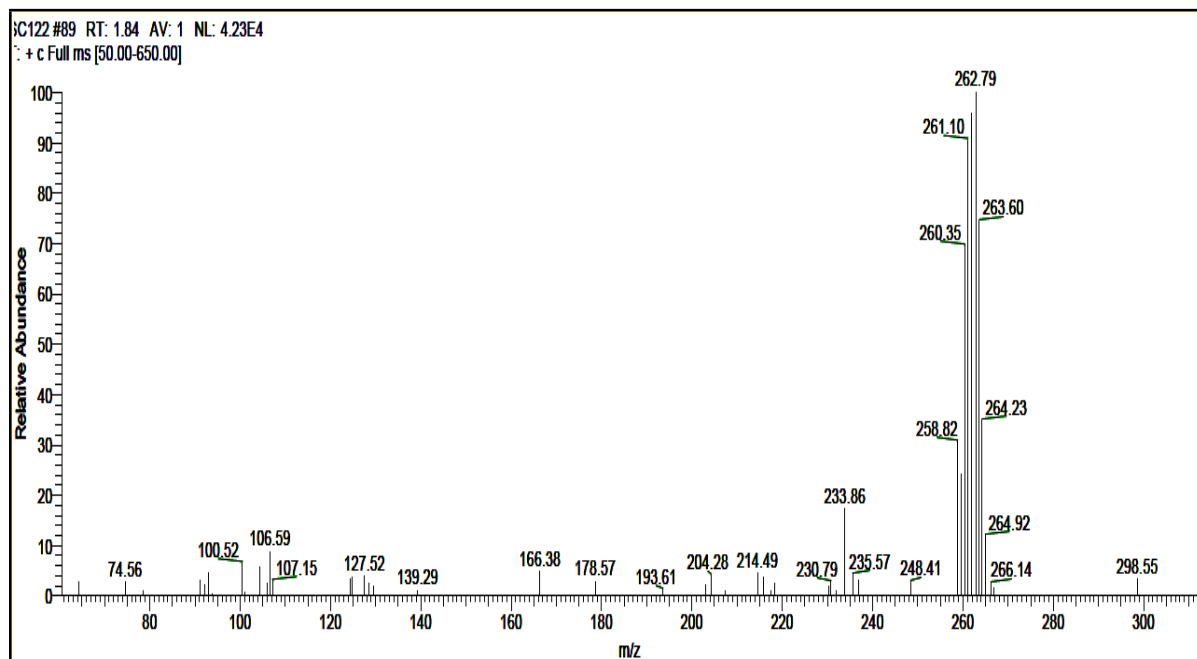


Fig. S25: GC MS spectra of compound 4

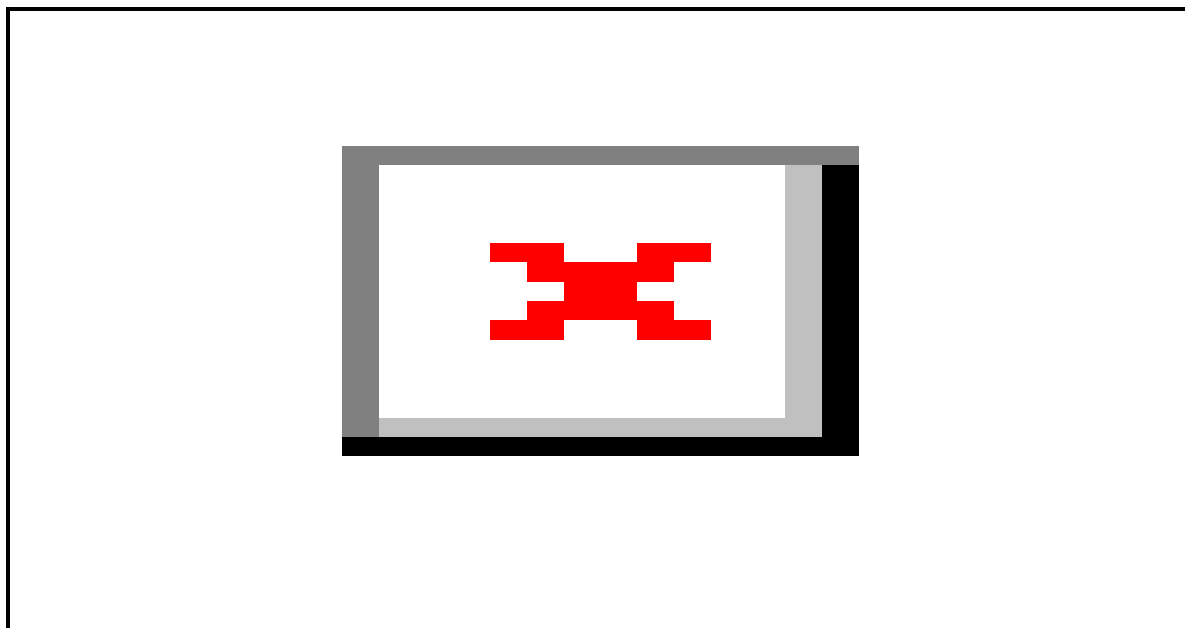


Fig. S26: GC MS spectra of compound 5

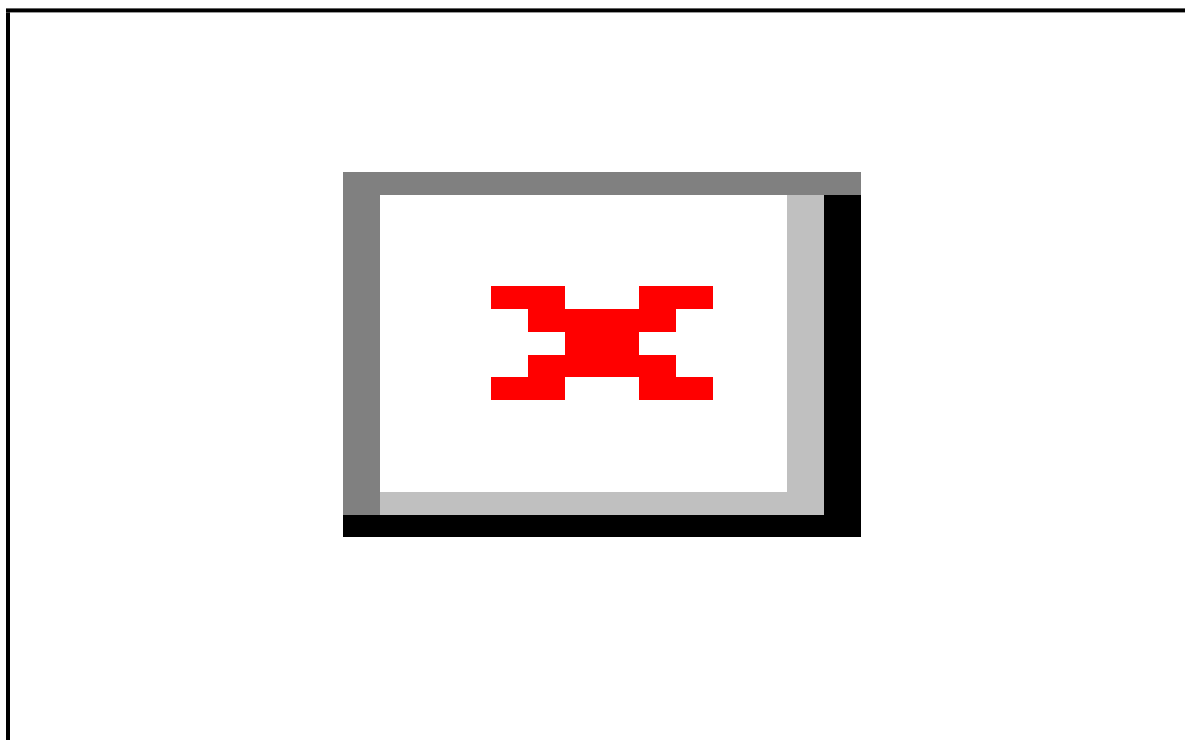


Fig. S27: GC MS spectra of compound 6

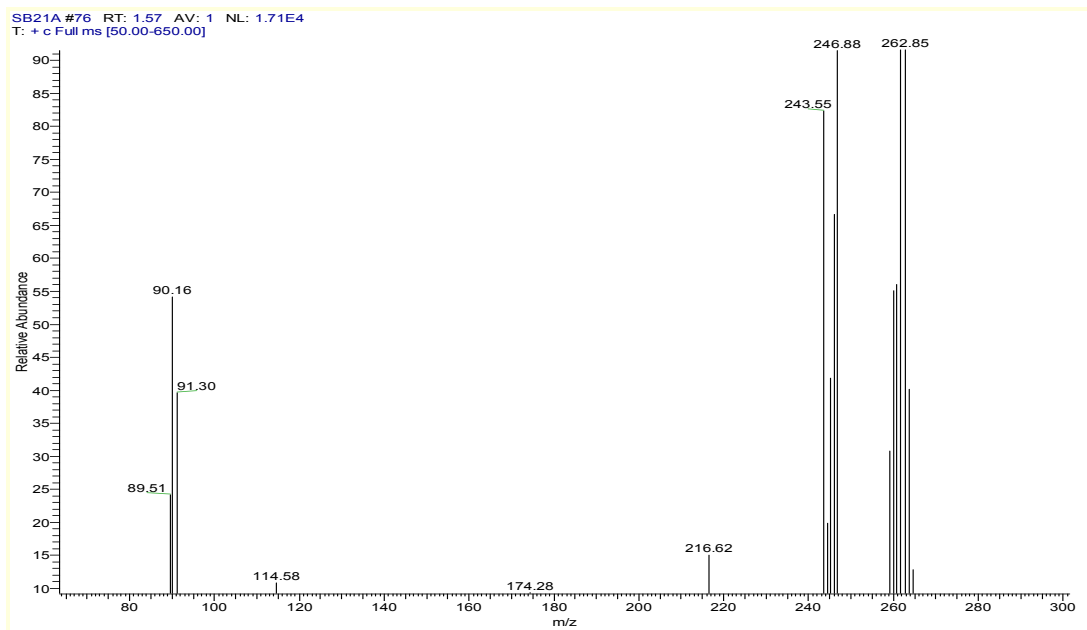
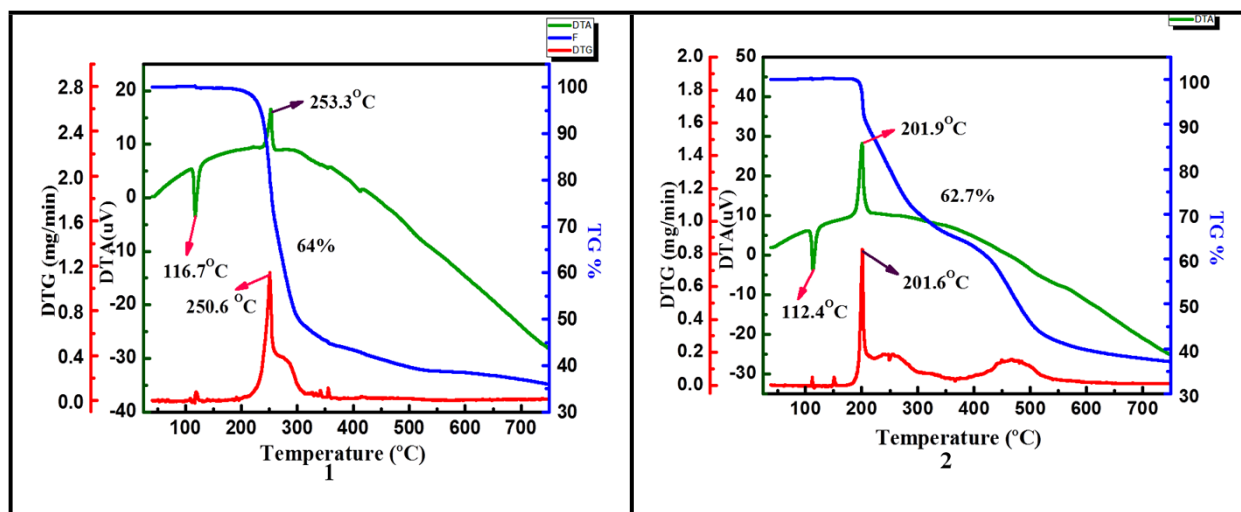


Fig. S28: GC MS spectra of compound 7

4. **Figures:** TG/DTA of the compounds is summarized below as Fig. S29



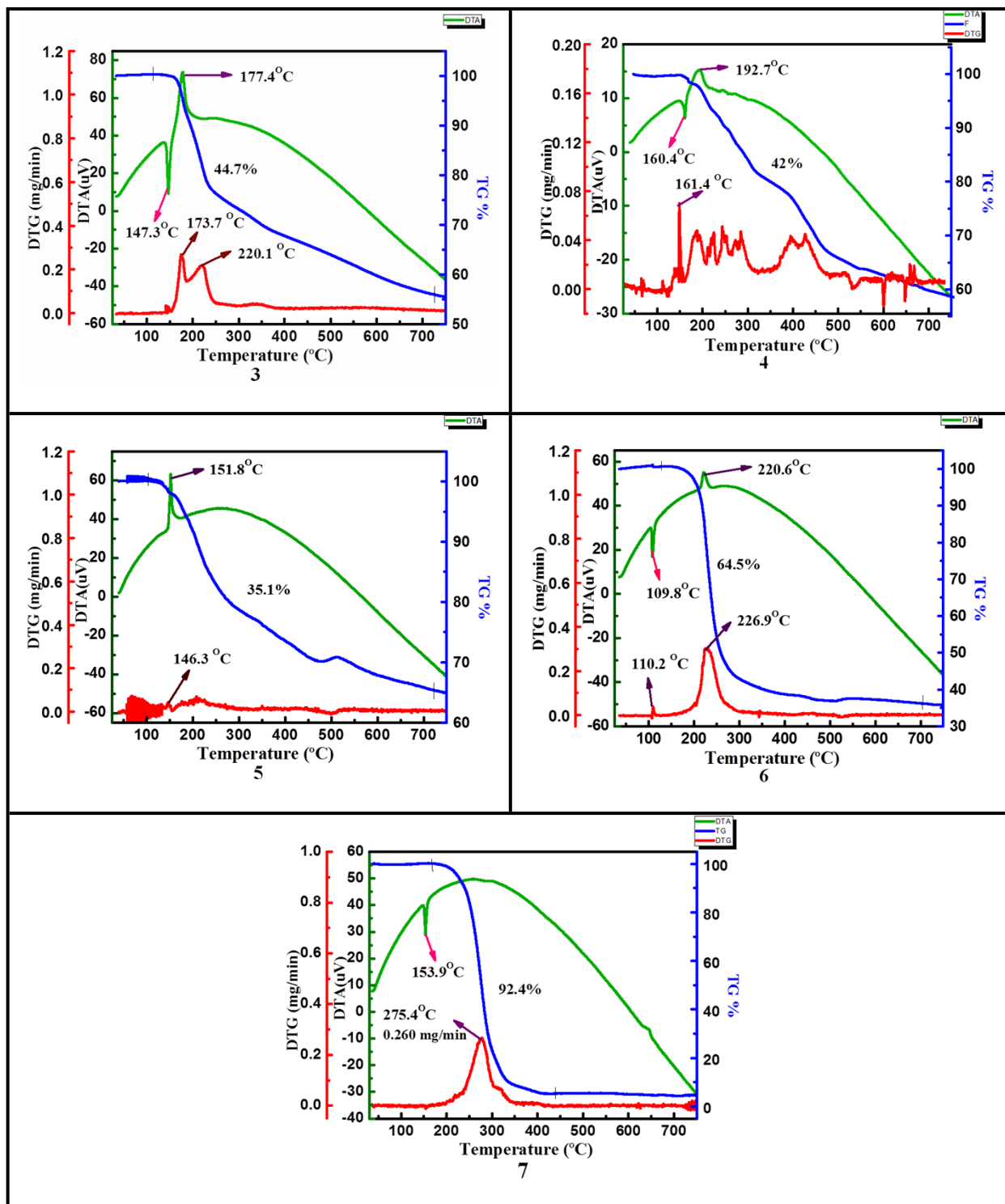


Fig. S29: TG/DTA of the compounds 1-7.