

### Supplementary Data

This supplementary data is a part of a paper entitled “New Charge-Transfer Complexes of Organochalcogenide Compound Based on Aryl Acetamide Group with Quinones: Synthesis, Characterization, Antioxidant, and Computational Study”.

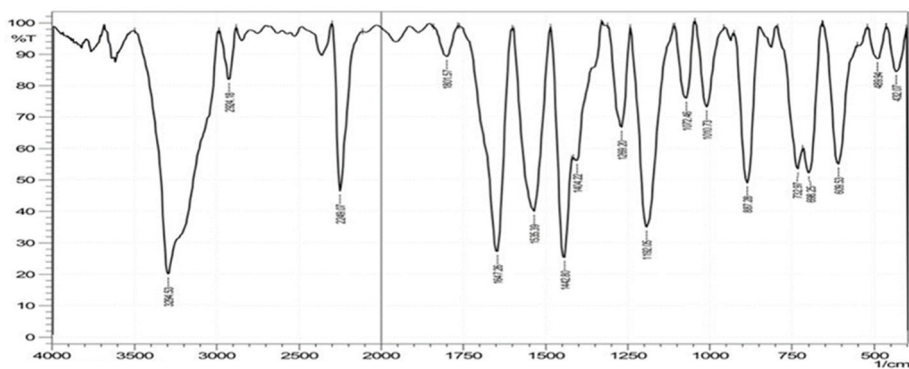


Fig S1. Infrared spectrum of compound I

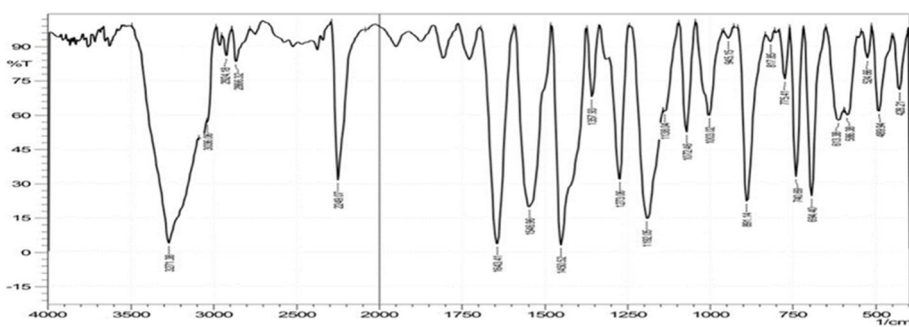


Fig S2. Infrared spectrum of compound II

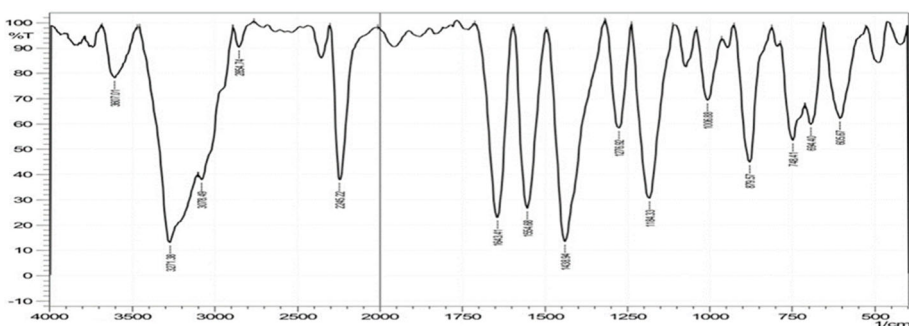


Fig S3. Infrared spectrum of compound III

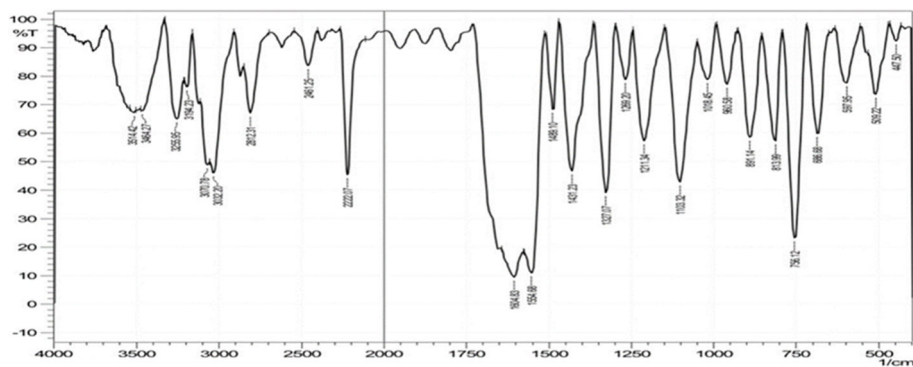


Fig S4. Infrared spectrum of compound IV

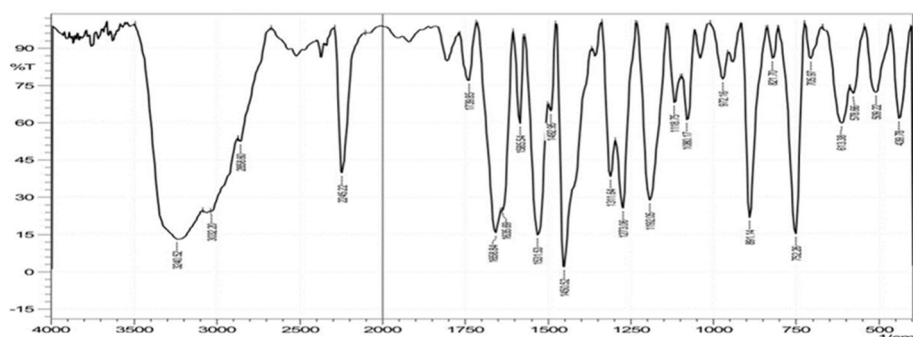


Fig S5. Infrared spectrum of compound V

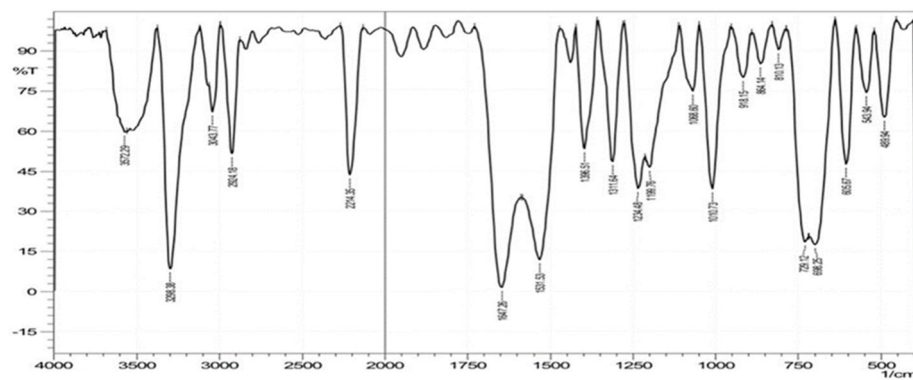


Fig S6. Infrared spectrum of compound VI

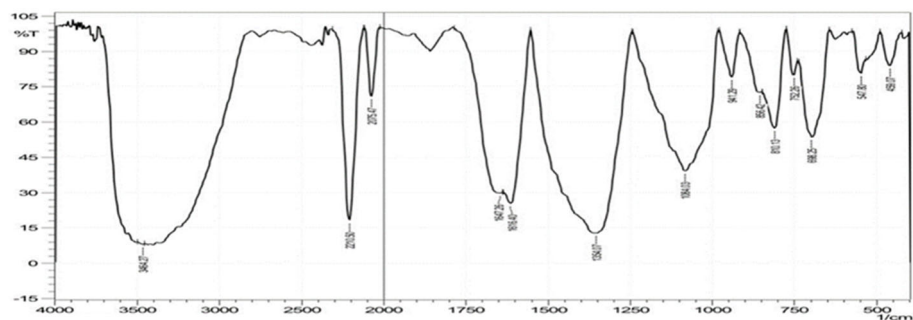


Fig S7. Infrared spectrum of compound VII

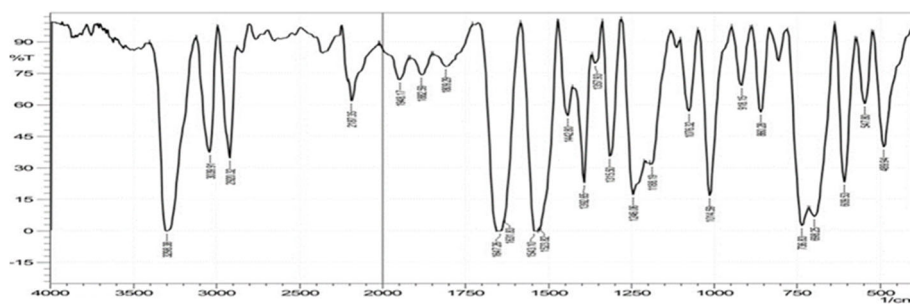


Fig S8. Infrared spectrum of compound VIII

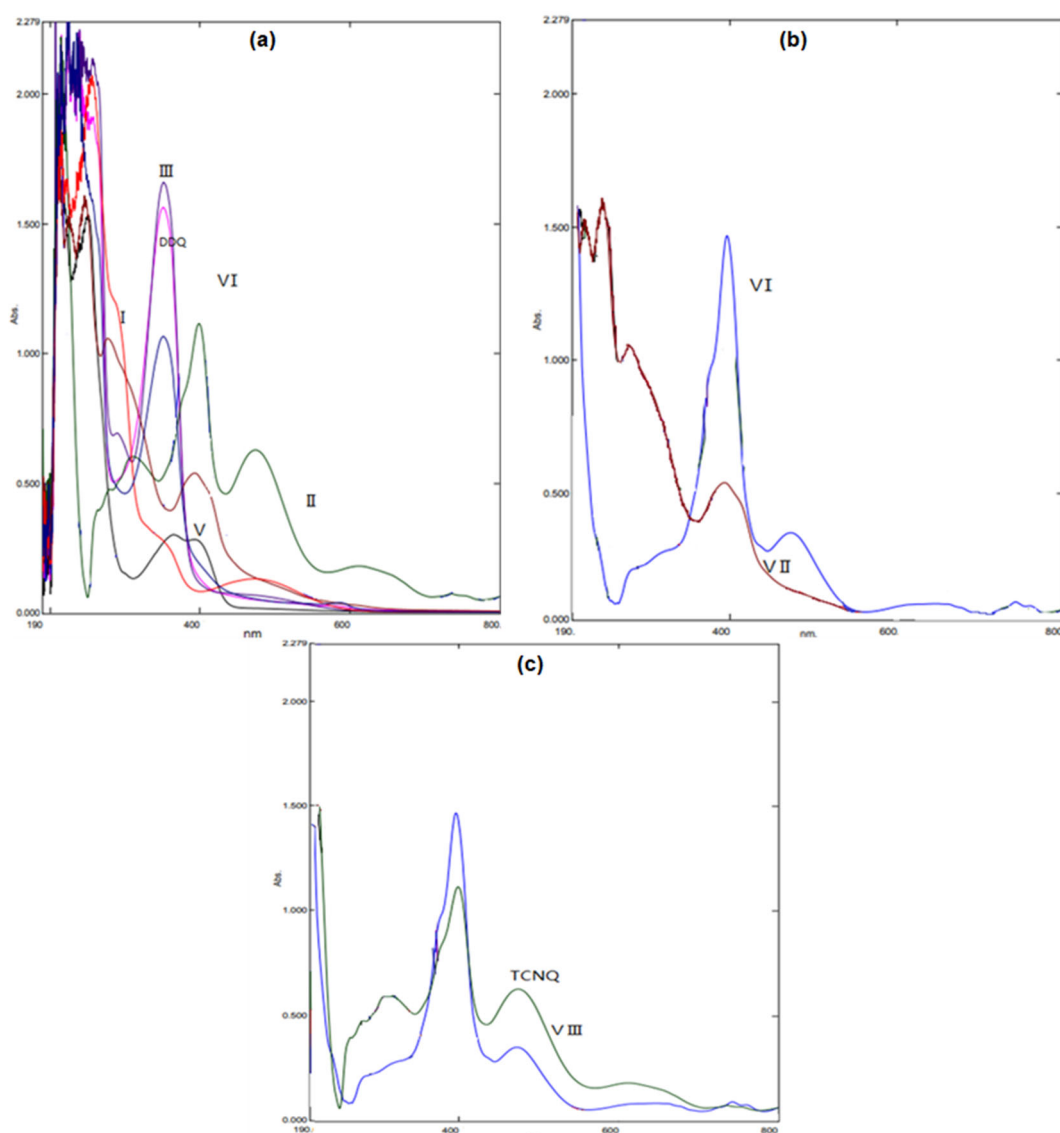
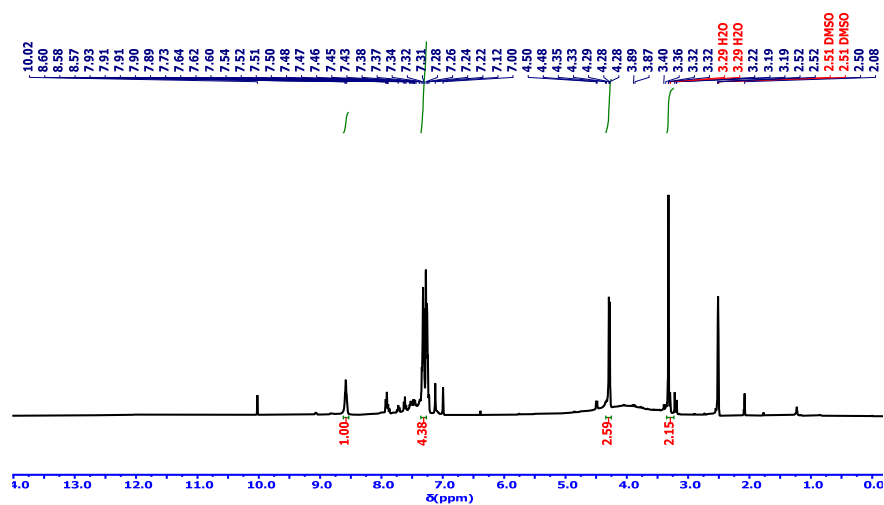
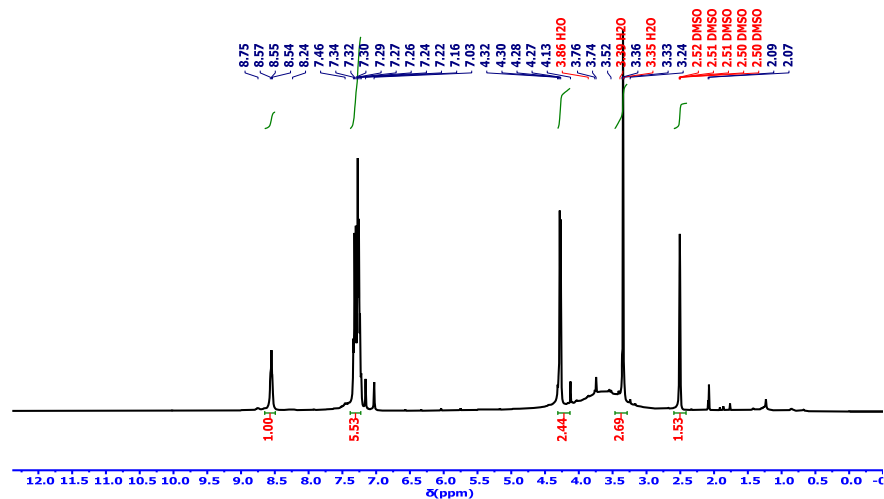
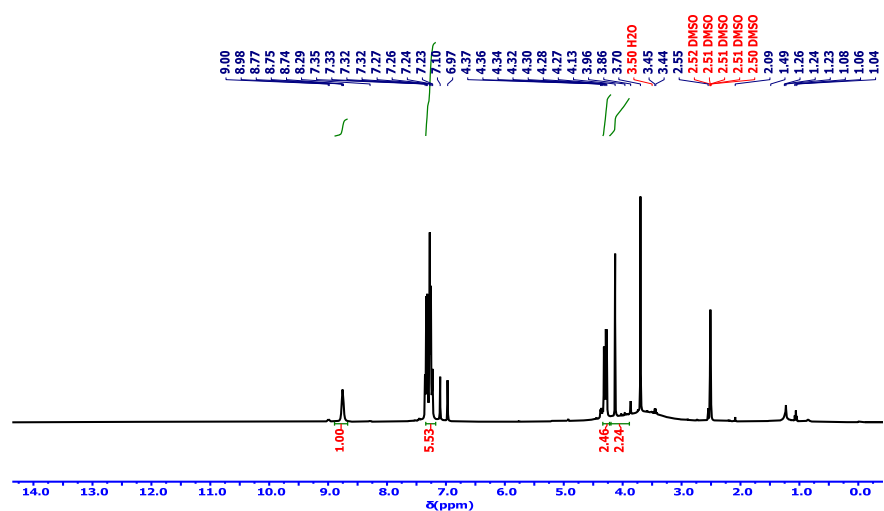


Fig S9. The UV-vis spectra for (a) CT complexes I-V, (b) CT complexes VI-VII, and (c) CT complex VIII

Fig S10. <sup>1</sup>H-NMR spectrum of compound IFig S11. <sup>1</sup>H-NMR spectrum of compound IIFig S12. <sup>1</sup>H-NMR spectrum of compound III

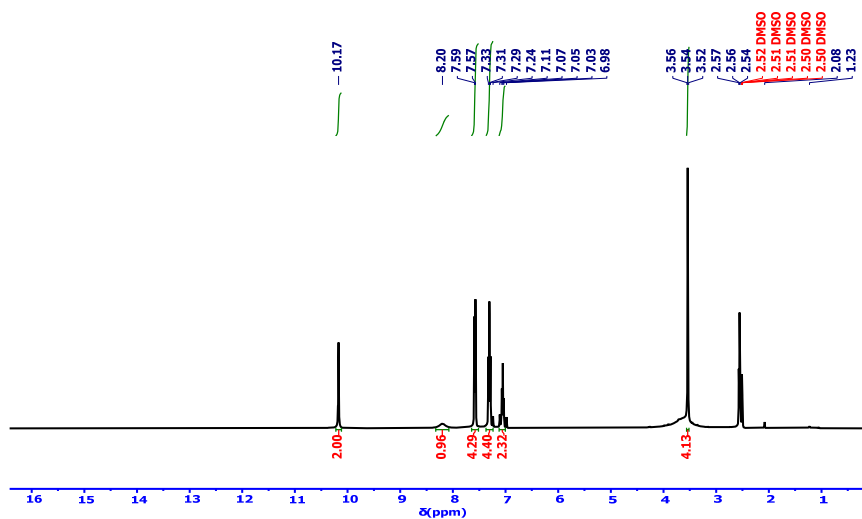


Fig S13. <sup>1</sup>H-NMR spectrum of compound IV

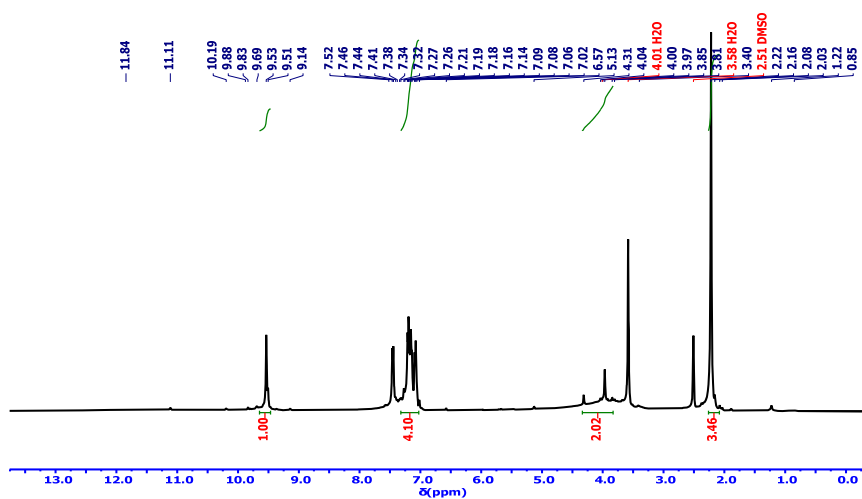


Fig S14. <sup>1</sup>H-NMR spectrum of compound V

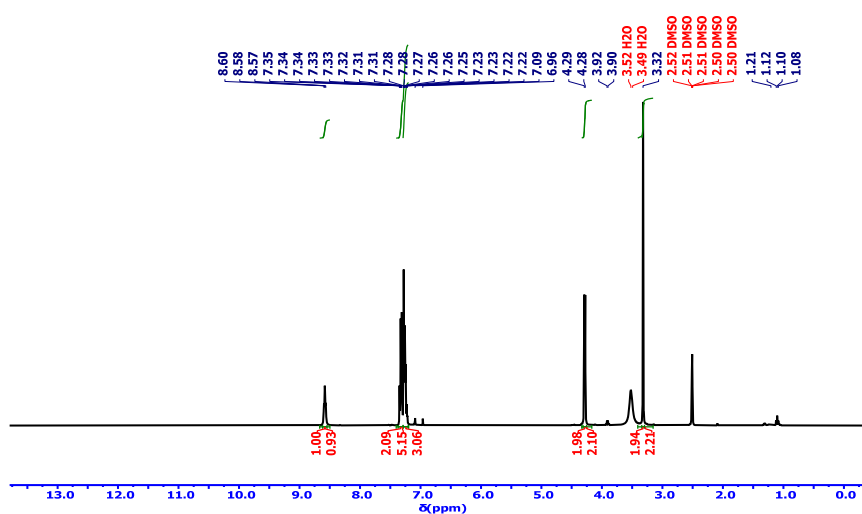
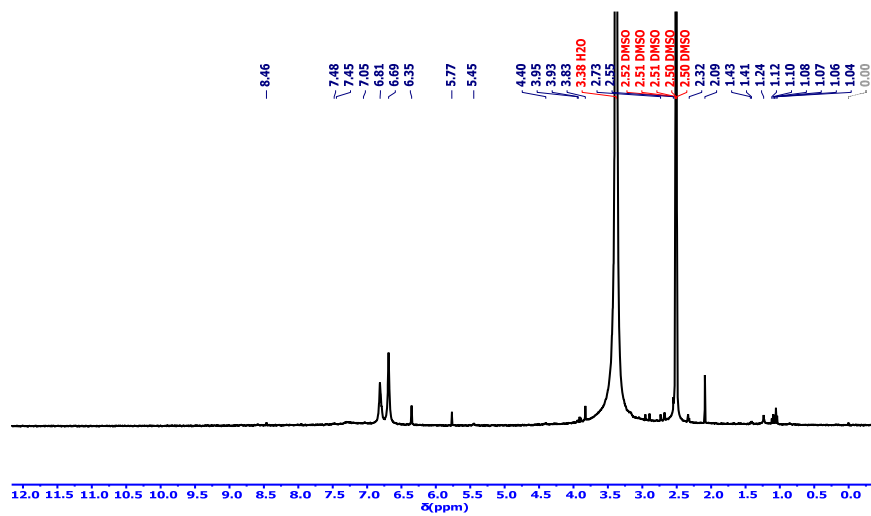
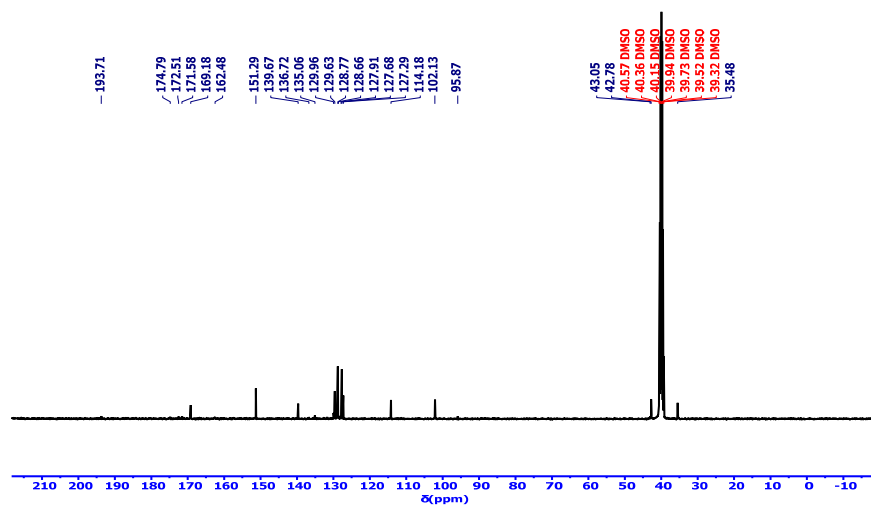
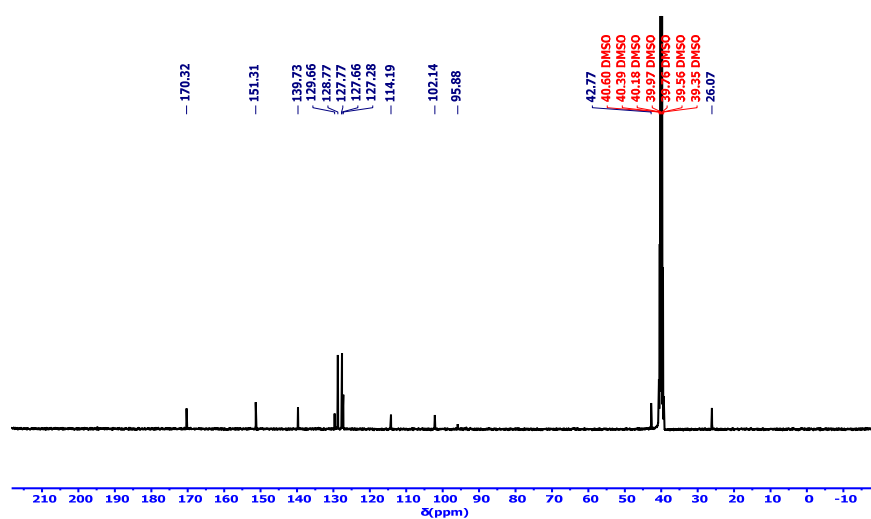
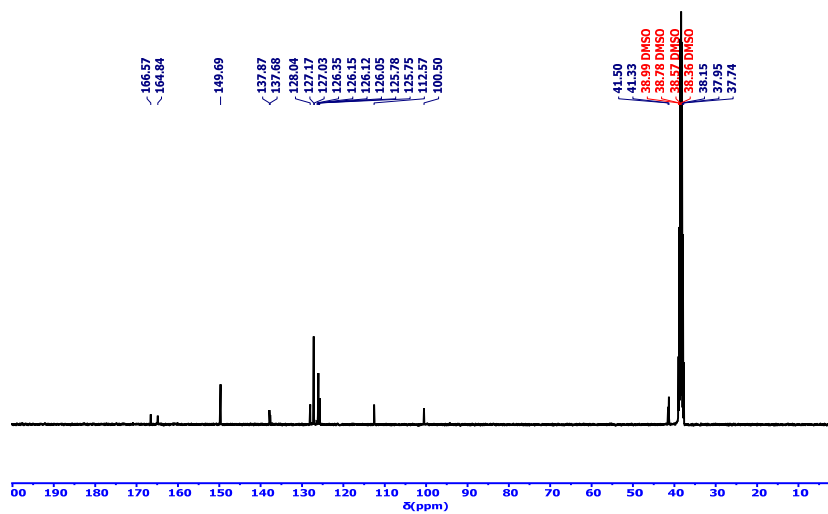
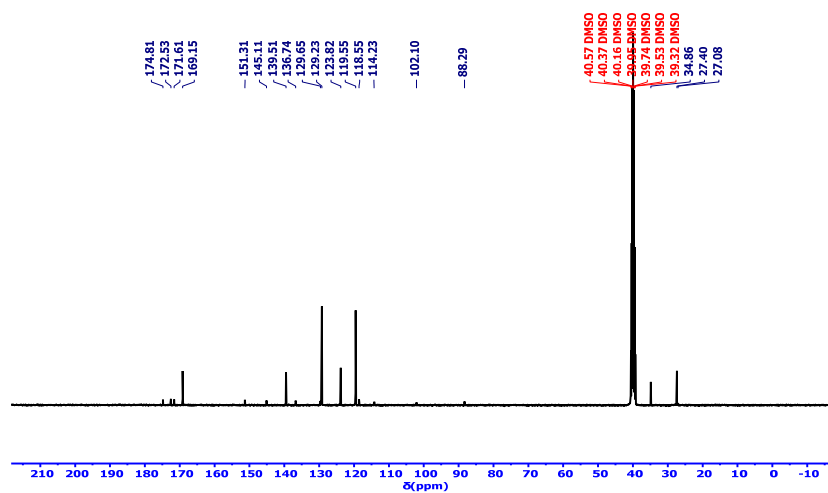
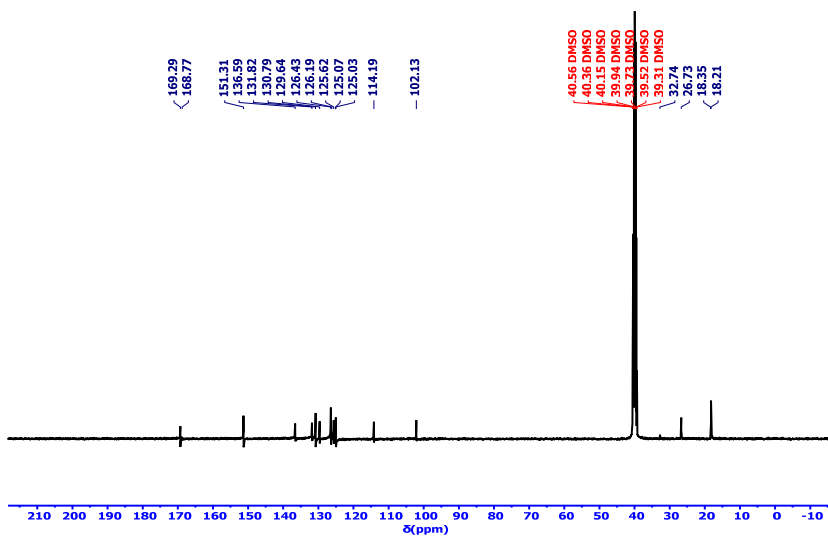


Fig S15. <sup>1</sup>H-NMR spectrum of compound VI

Fig S16. <sup>1</sup>H-NMR spectrum of compound VIIFig S17. <sup>13</sup>C-NMR spectrum of compound IFig S18. <sup>13</sup>C-NMR spectrum of compound II

Fig S19.  $^{13}\text{C-NMR}$  spectrum of compound IIIFig S20.  $^{13}\text{C-NMR}$  spectrum of compound IVFig S21.  $^{13}\text{C-NMR}$  spectrum of compound V

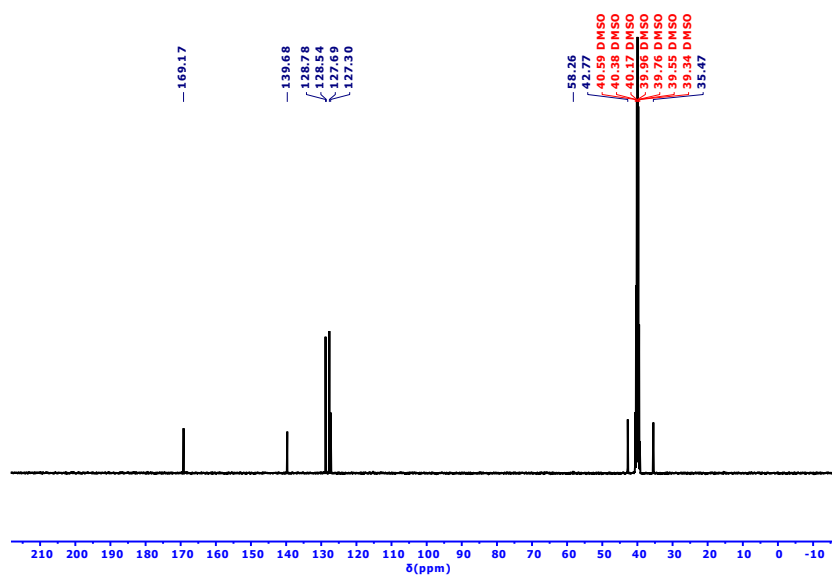
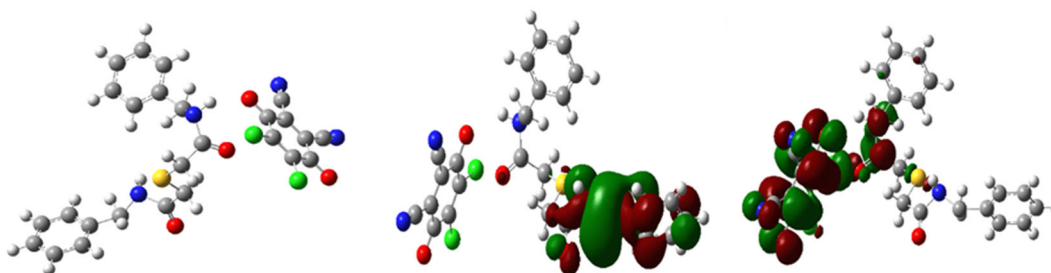
Fig S22.  $^{13}\text{C}$ -NMR spectrum of compound VI

Fig S23. Molecular structure and molecular orbitals (HOMO and LUMO) of compound I

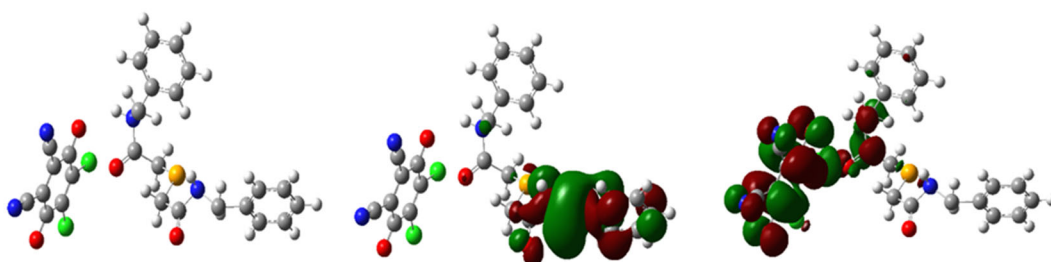


Fig S24. Molecular structure and molecular orbitals (HOMO and LUMO) of compound II

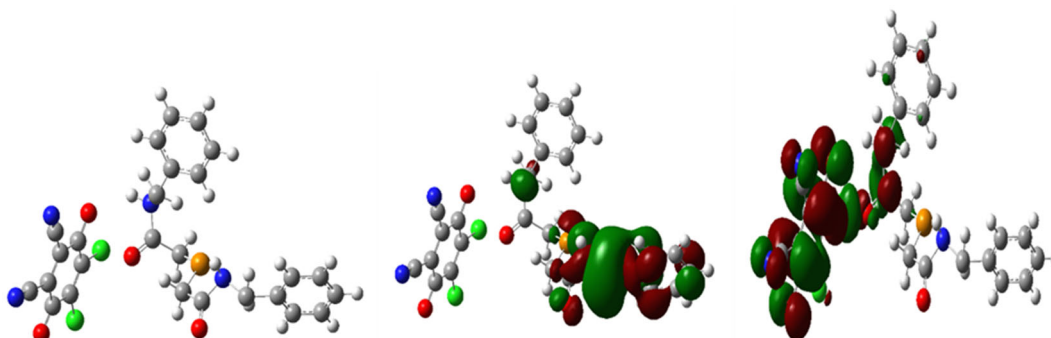
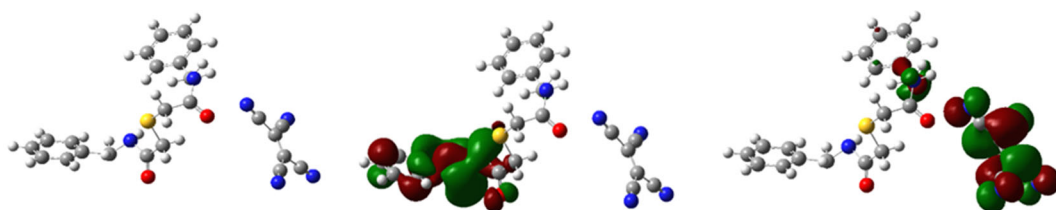
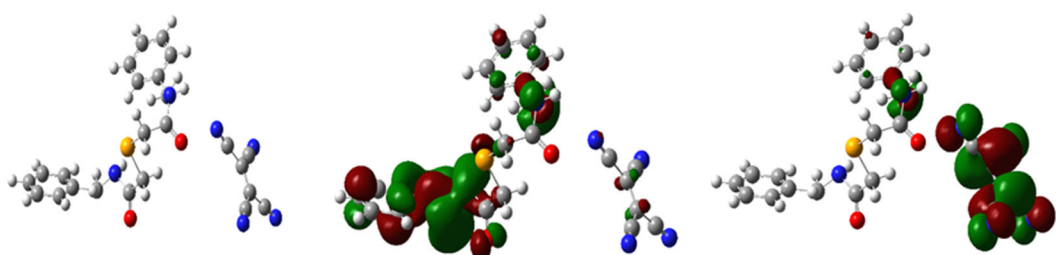


Fig S25. Molecular structure and molecular orbitals (HOMO and LUMO) of compound III

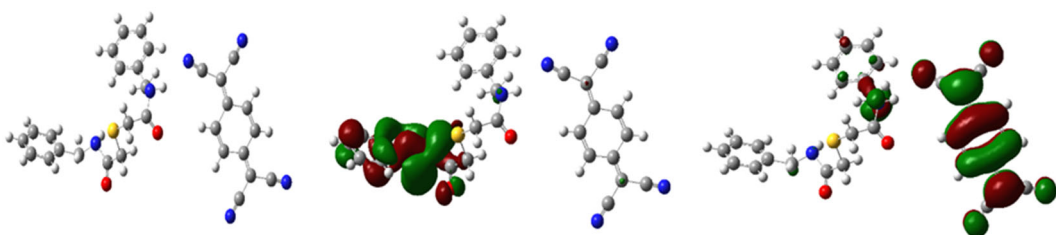




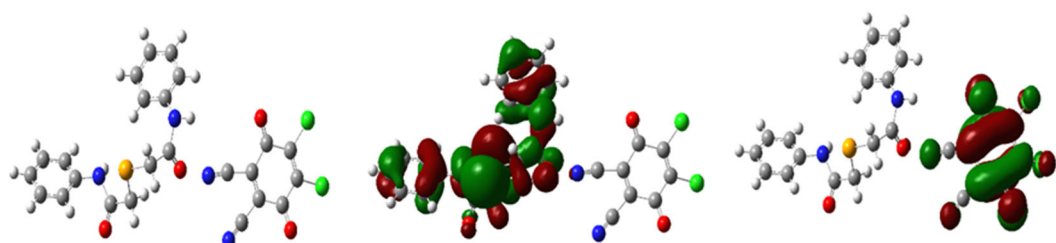
**Fig S26.** Molecular structure and molecular orbitals (HOMO and LUMO) of compound VI



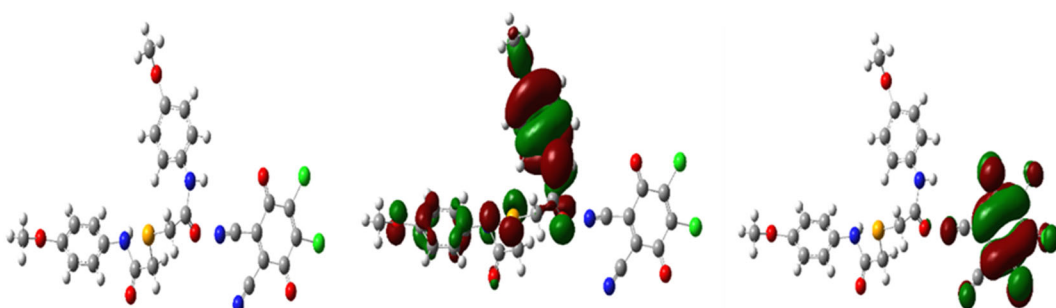
**Fig S27.** Molecular structure and molecular orbitals (HOMO and LUMO) of compound VII



**Fig S28.** Molecular structure and molecular orbitals (HOMO and LUMO) of compound VIII



**Fig S29.** Molecular structure and molecular orbitals (HOMO and LUMO) of compound IV



**Fig S30.** Molecular structure and molecular orbitals (HOMO and LUMO) of compound V