A new proton transfer complex between 3,4-diaminopyridine drug and 2,6-dichloro-4-nitrophenol: Synthesis, spectroscopic characterization, DFT studies, DNA binding analysis, and antitumor activity.

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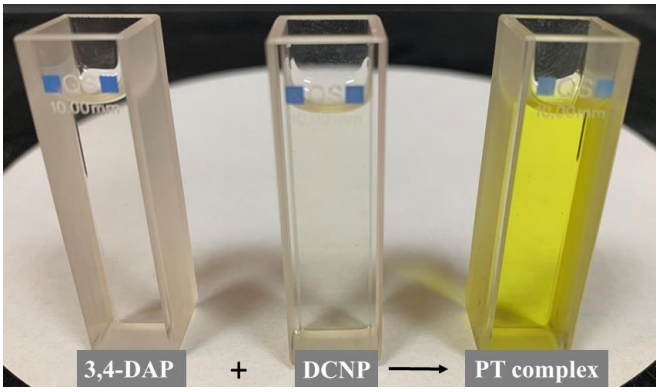


Figure S1. Naked-eye visible color change in the solution when adding DCNP (1.0×10^{-4} mol L^{-1}) to 3,4-DAP (1.0×10^{-4} mol L^{-1}) in EtOH.

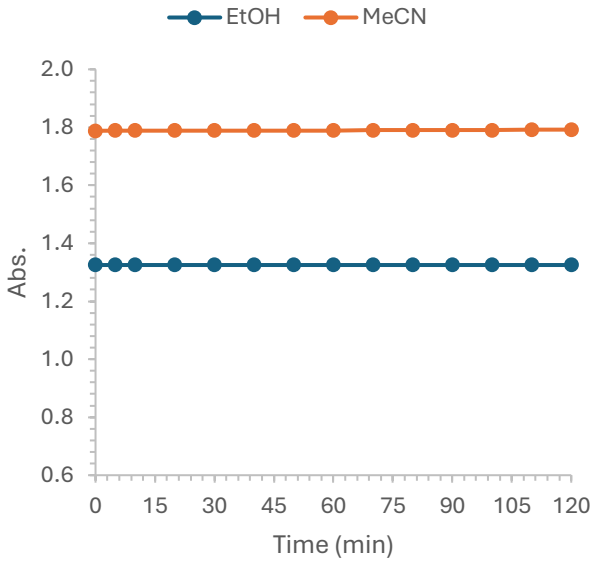


Figure S2. Effect of time on the stability of PT complex in different solvents.

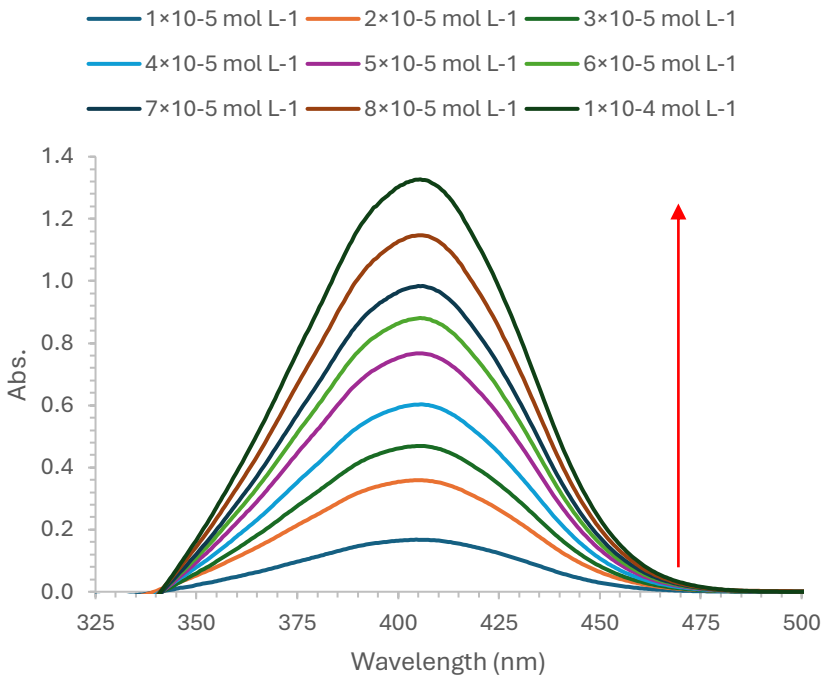


Figure S3. Electronic absorption spectra of PT complex at different concentrations of 3,4-DAP with 1.0 × 10^{-4} mol L^{-1} in EtOH at room temperature.

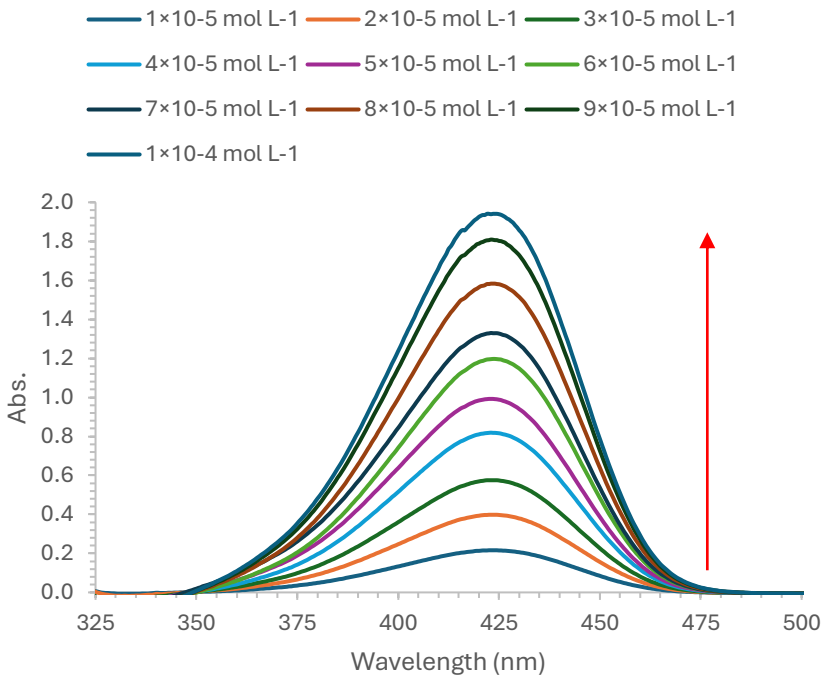


Figure S4. Electronic absorption spectra of PT complex at different concentrations of 3,4-DAP with 1.0 × 10^{-4} mol L^{-1} in MeCN at room temperature.

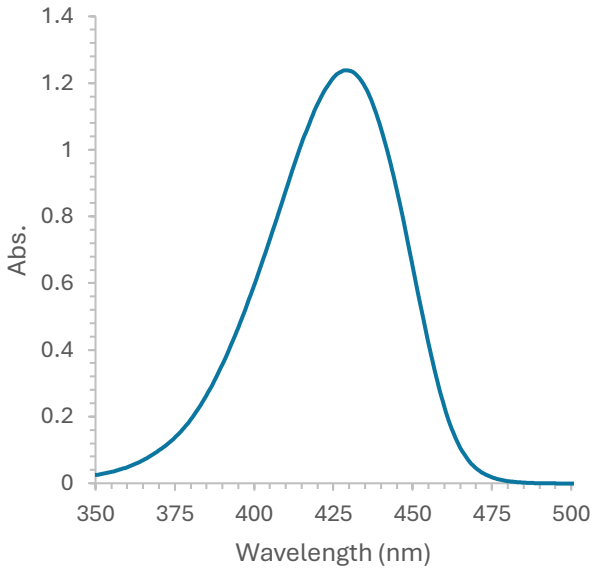


Figure S5. Electronic absorption spectra of the solid PT complex in DMF.

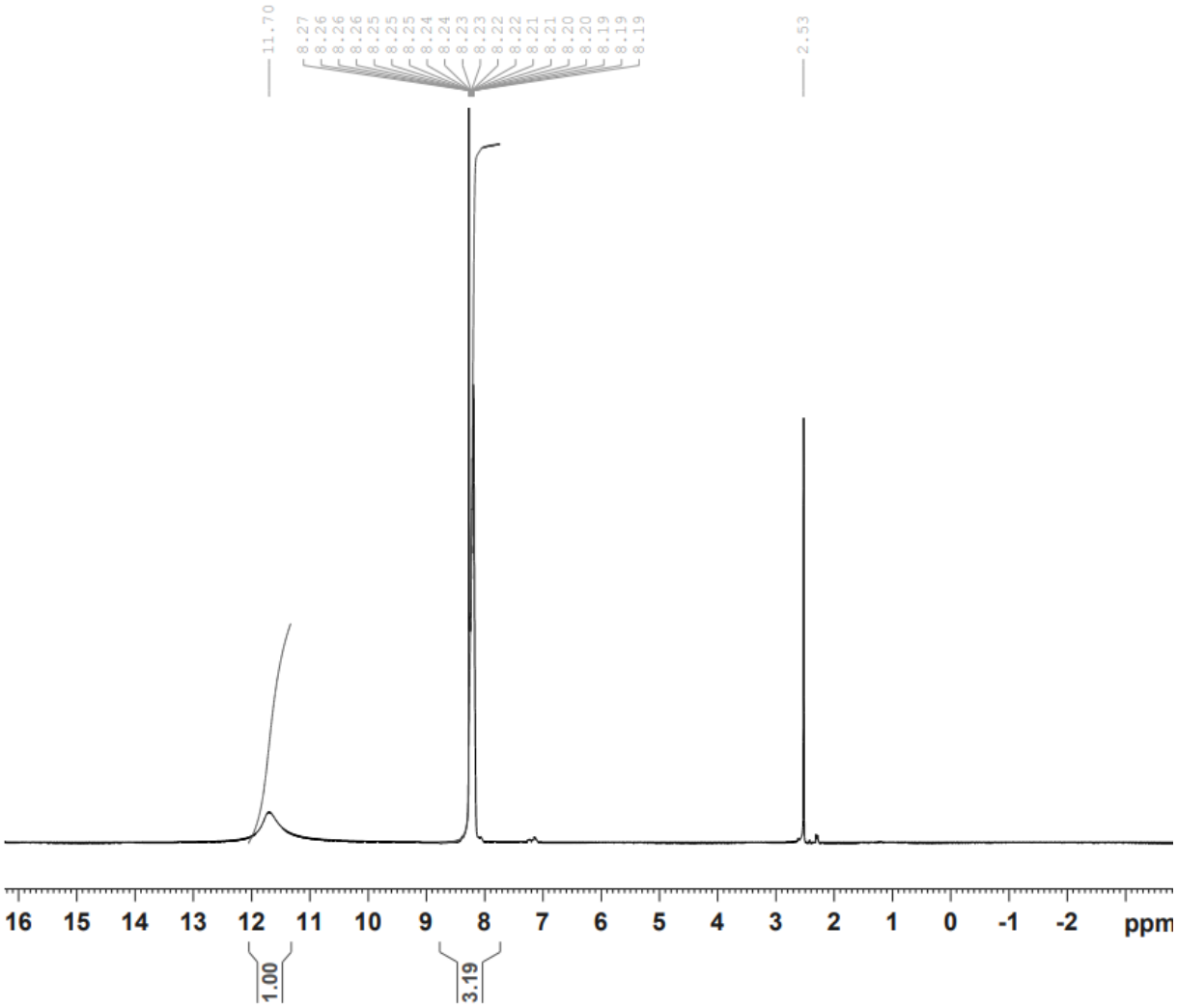


Figure S6.[1]H NMR spectrum of the free DCNP.

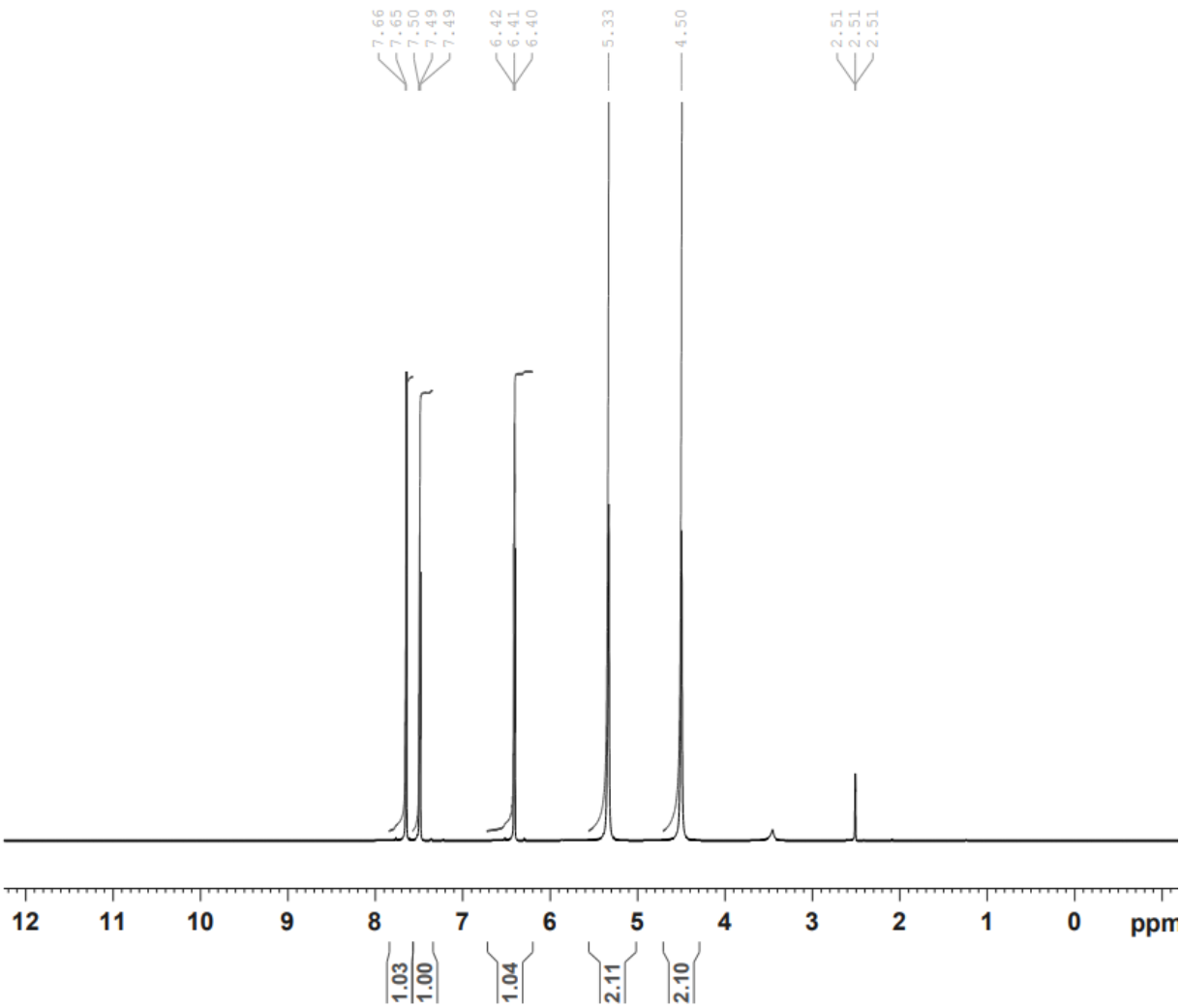


Figure S7.[1]H NMR spectrum of the free 3,4-DAP.

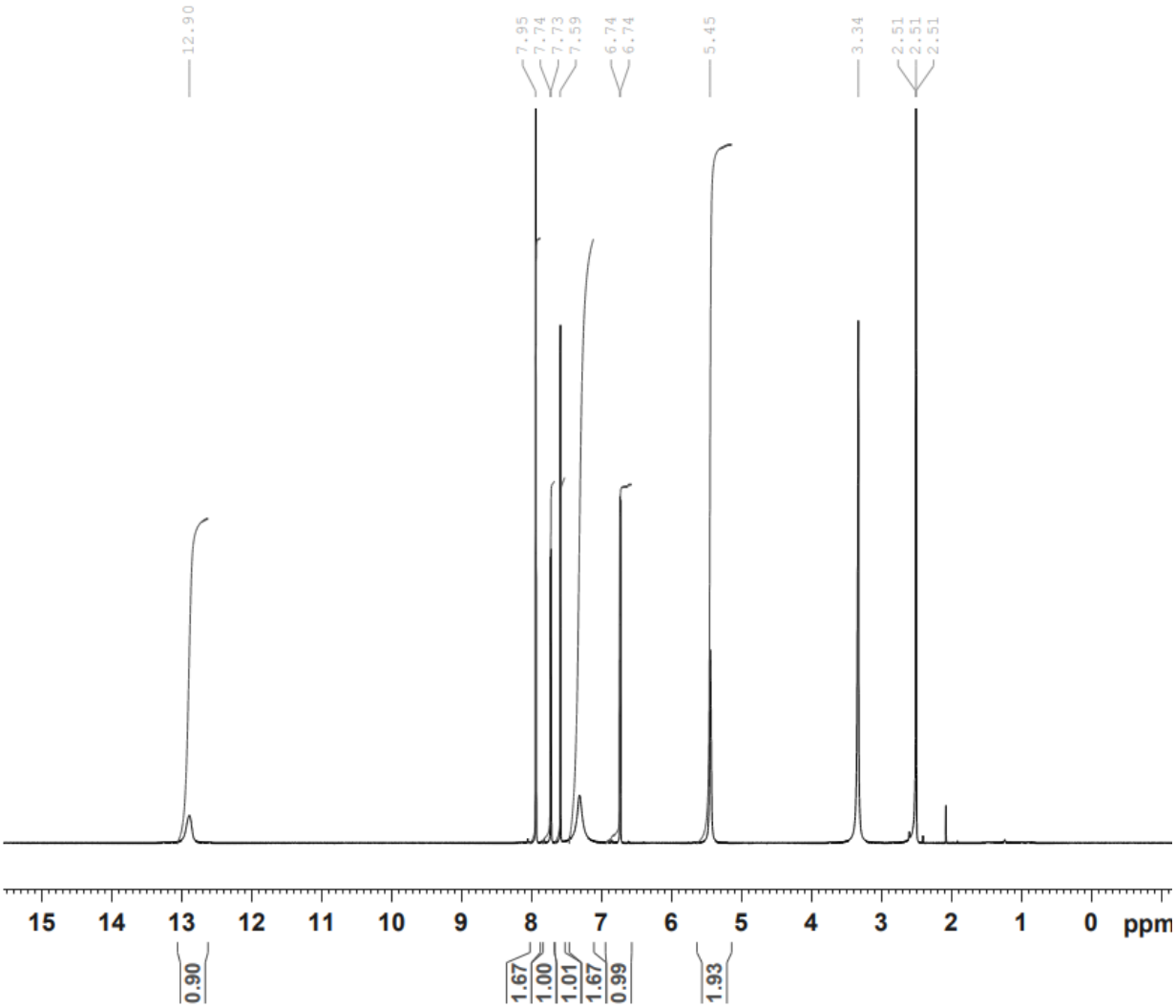


Figure S8.[1]H NMR spectrum of PT complex.

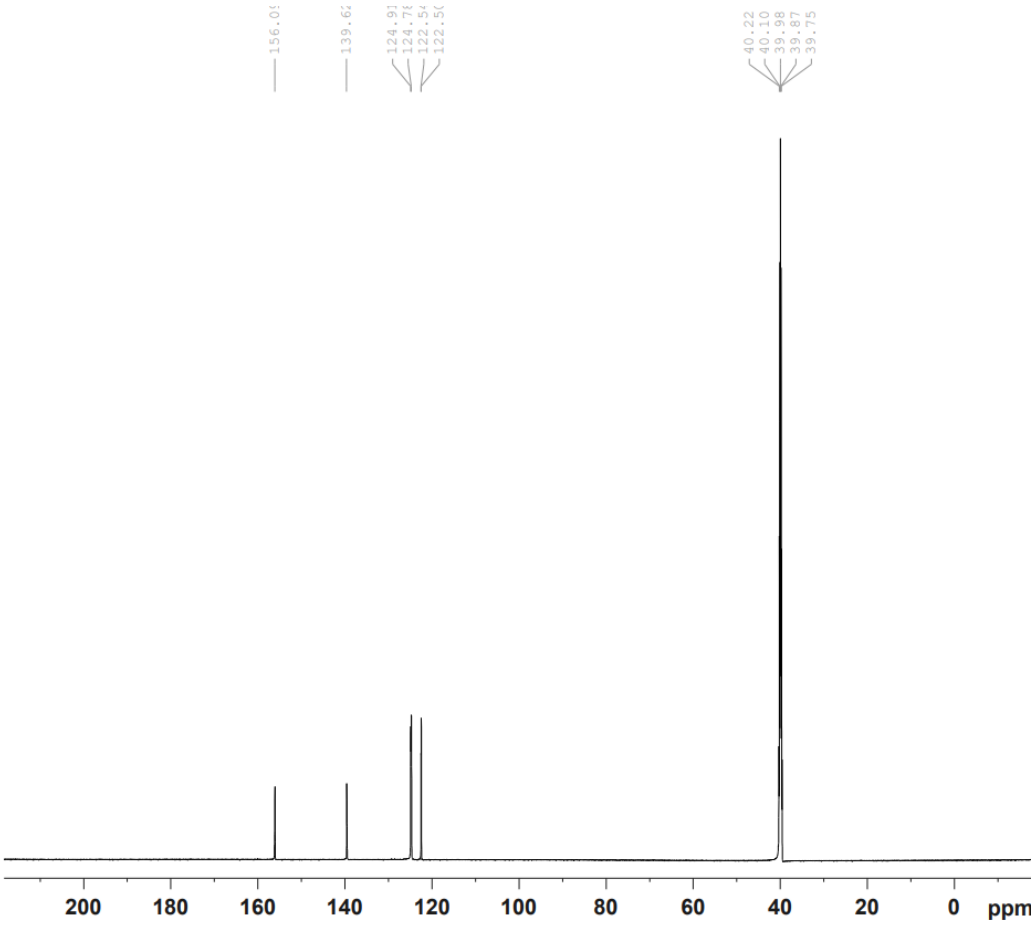


Figure S9. ^{13}C NMR spectrum of the free DCNP.

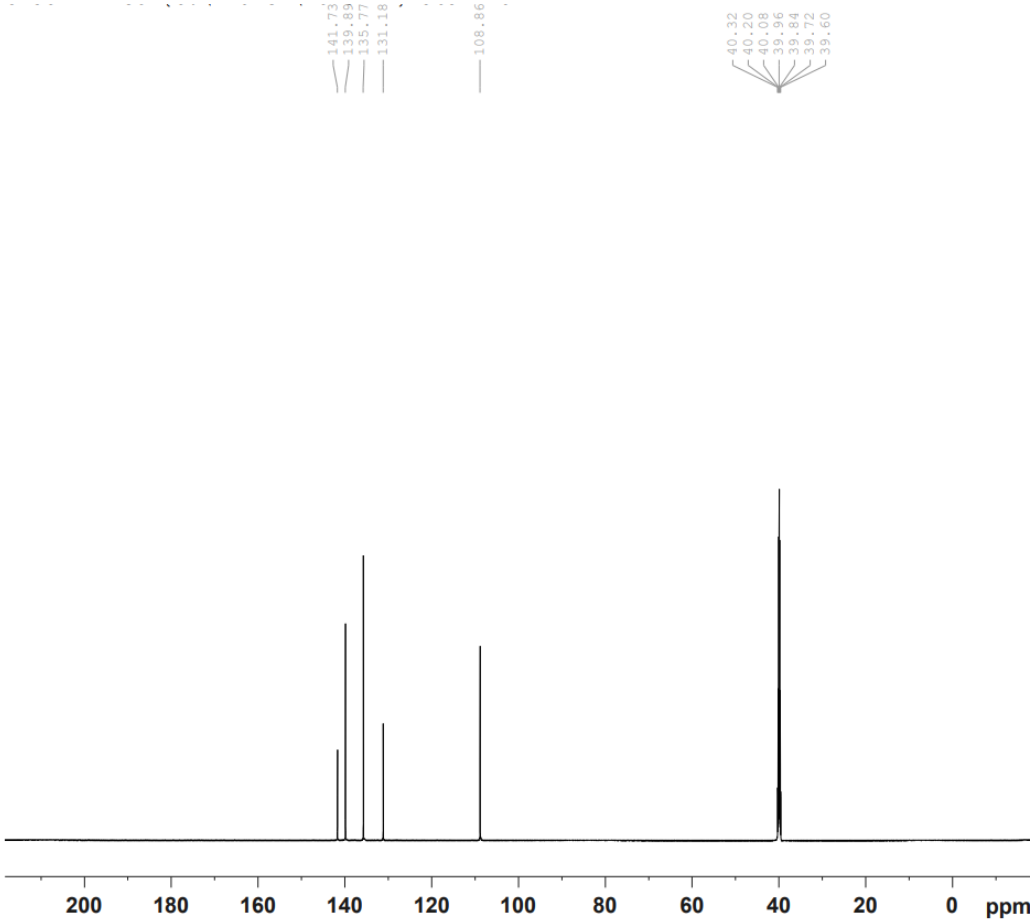


Figure S10. ^{13}C NMR spectrum of the free 3,4-DAP.

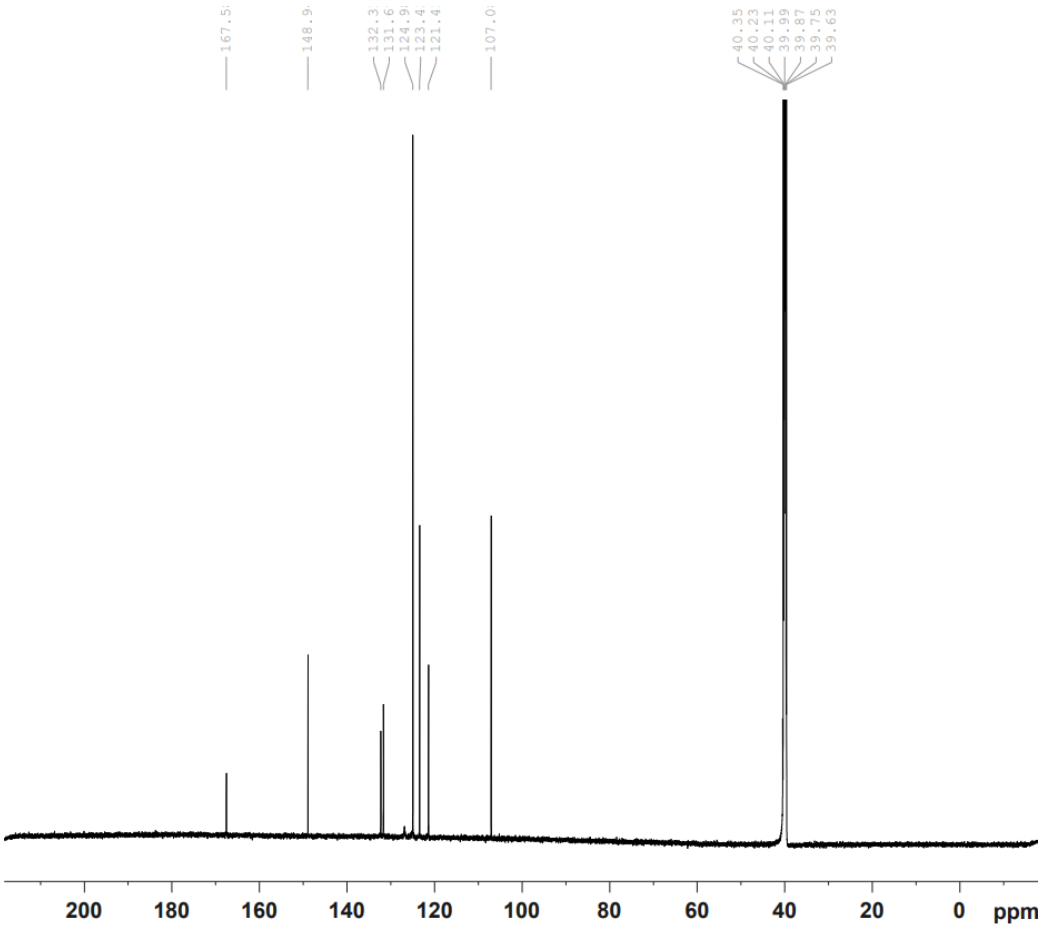


Figure S11. ^{13}C NMR spectrum of PT complex.