

Supplementary Materials

Crystalline Derivatives of Dipyrazolo-1,5-diazocine and Dipyrazolopyrimidine: A Case of Unexpected Synthesis and Isostructural Polymorphism

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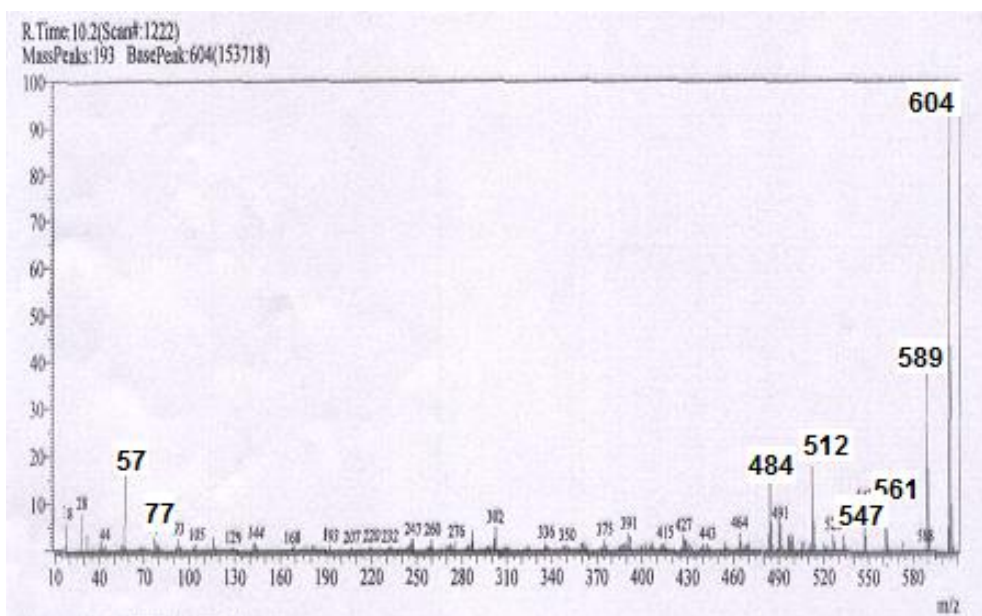


Figure S1. Electron-impact mass fragmentation spectrum of Dipyrzolo-1,5-diazocine derivative (8).

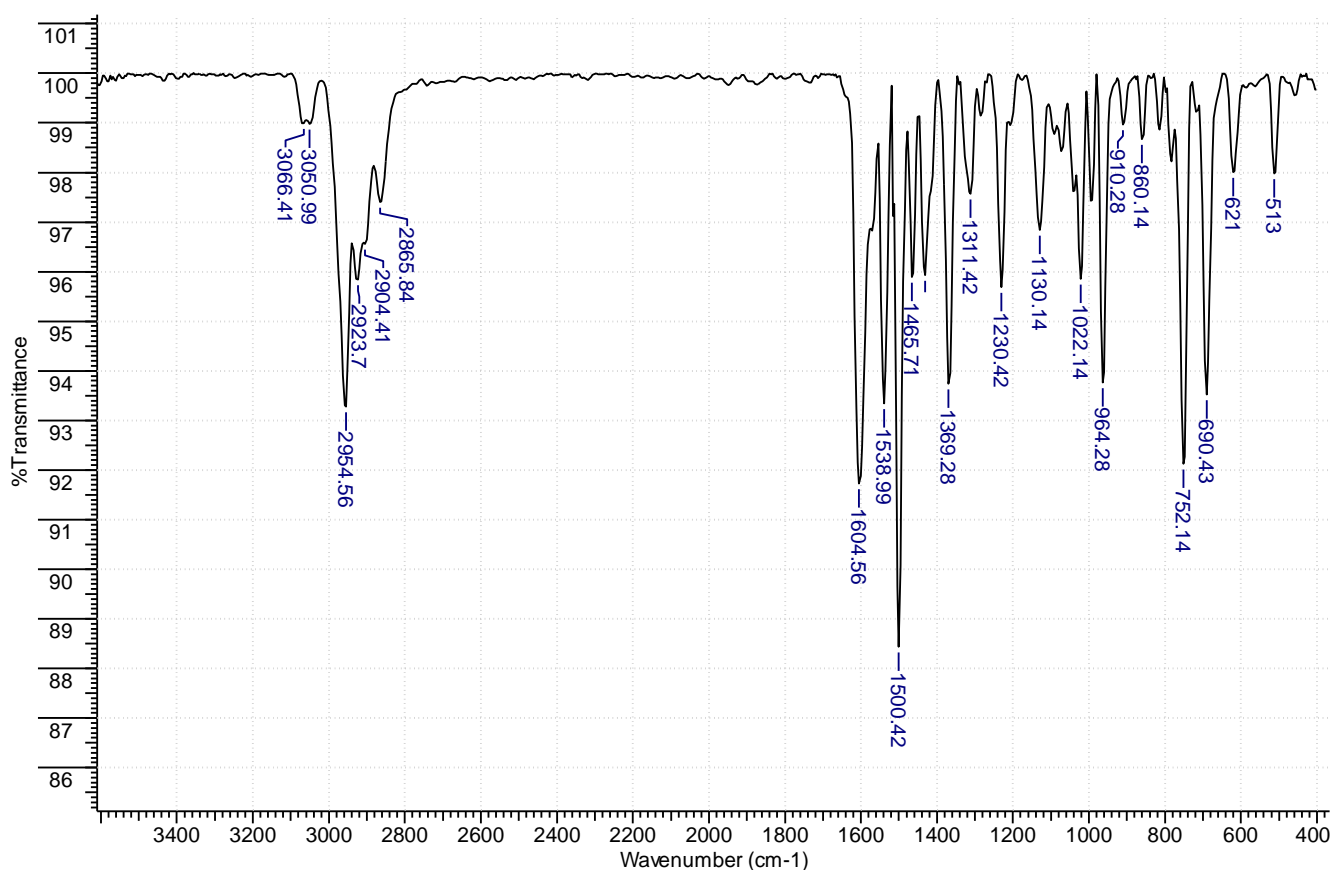


Figure S2. FTIR spectrum of the dipyrzolo-1,5-diazocine derivative (8) measured using the KBr disk technique.

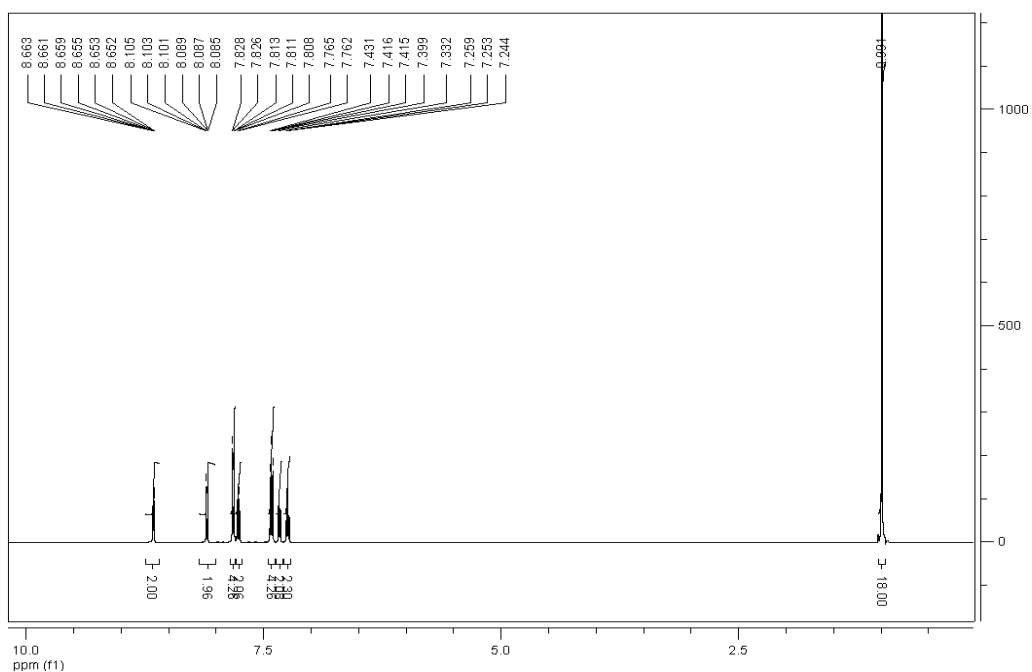


Figure S3. ¹H 1D-NMR spectrum of dipyrazolo-1,5-diazocine derivative (8) in deuterated chloroform.

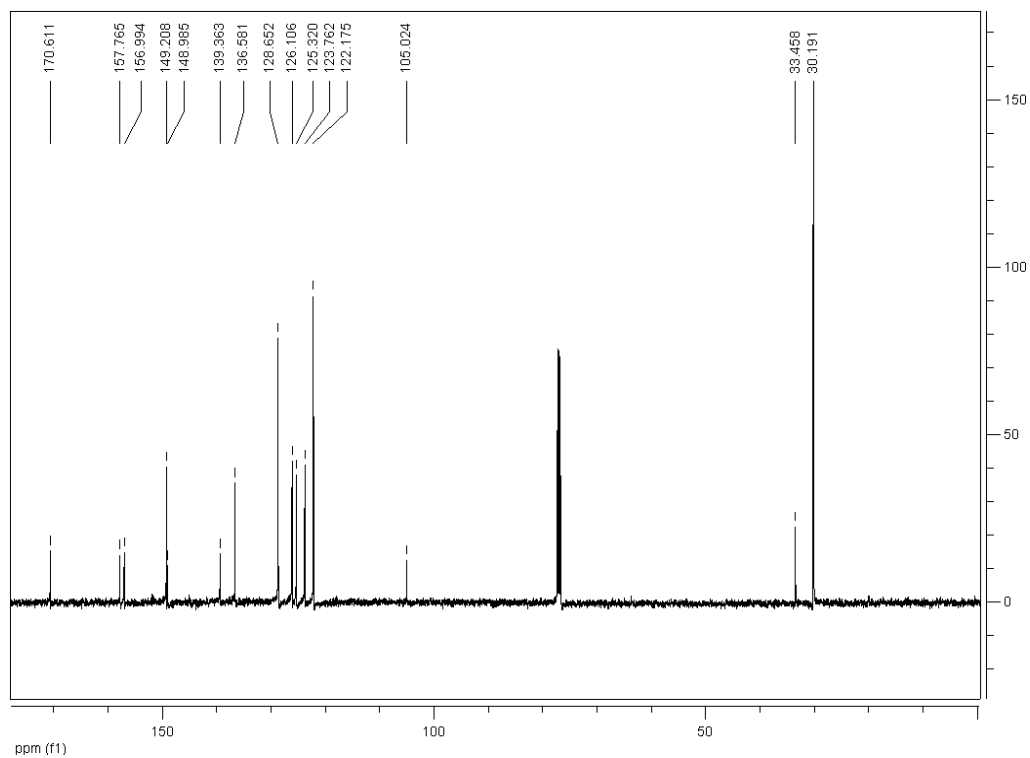


Figure S4. ¹³C 1D-NMR spectrum of dipyrazolo-1,5-diazocine derivative (8) in deuterated chloroform.

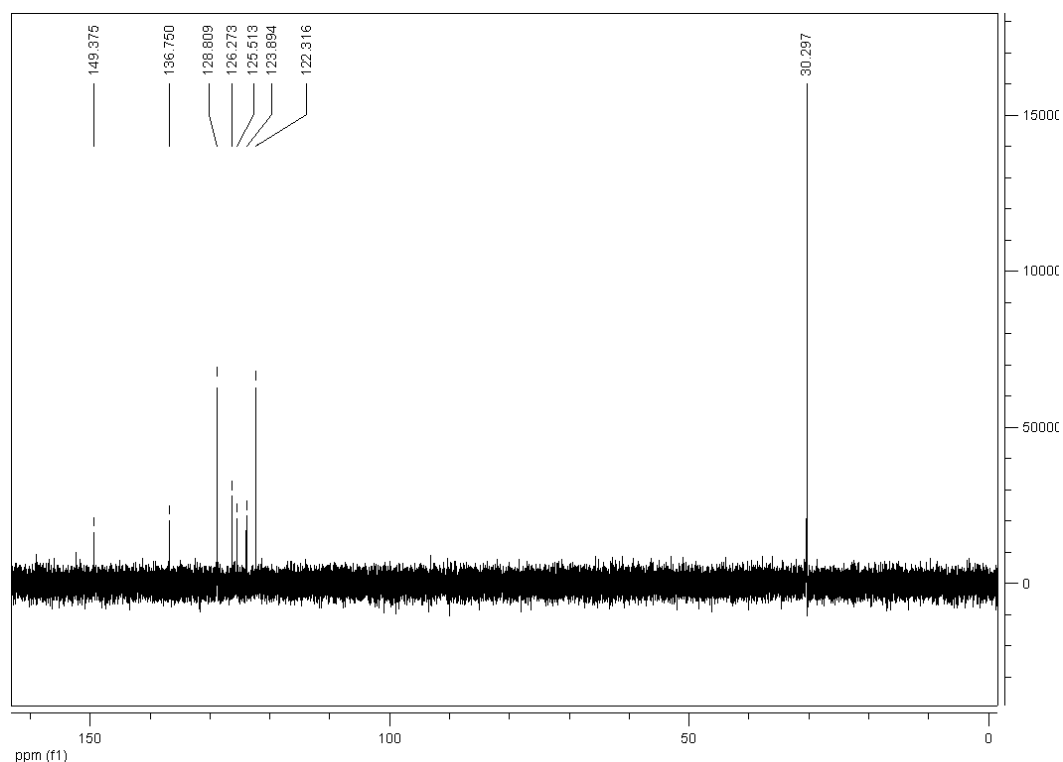


Figure S5. DEPT NMR spectrum of dipyrzolo-1,5-diazocine derivative (8) in deuterated chloroform.

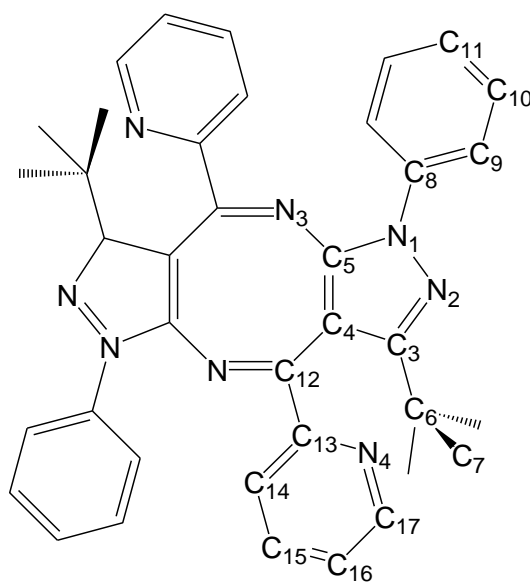


Figure S6. 2D-molecular representation of dipyrzolo-1,5-diazocine derivative (8) showing atomic numbering used for NMR assignments.

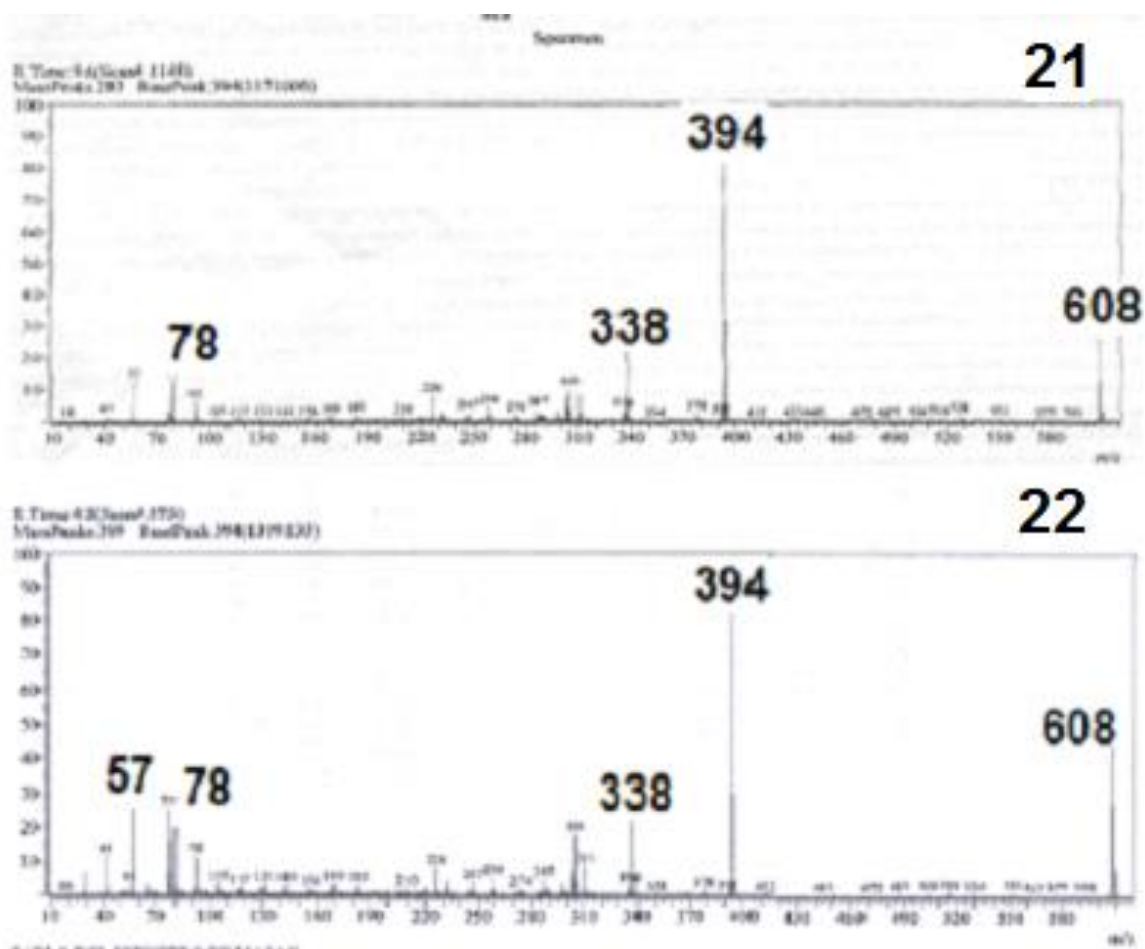


Figure S7. Electron-impact mass fragmentation impact of dipyrzolopyrimidine derivative (9). Polymorph 9a (top) and polymorph 9b (bottom).

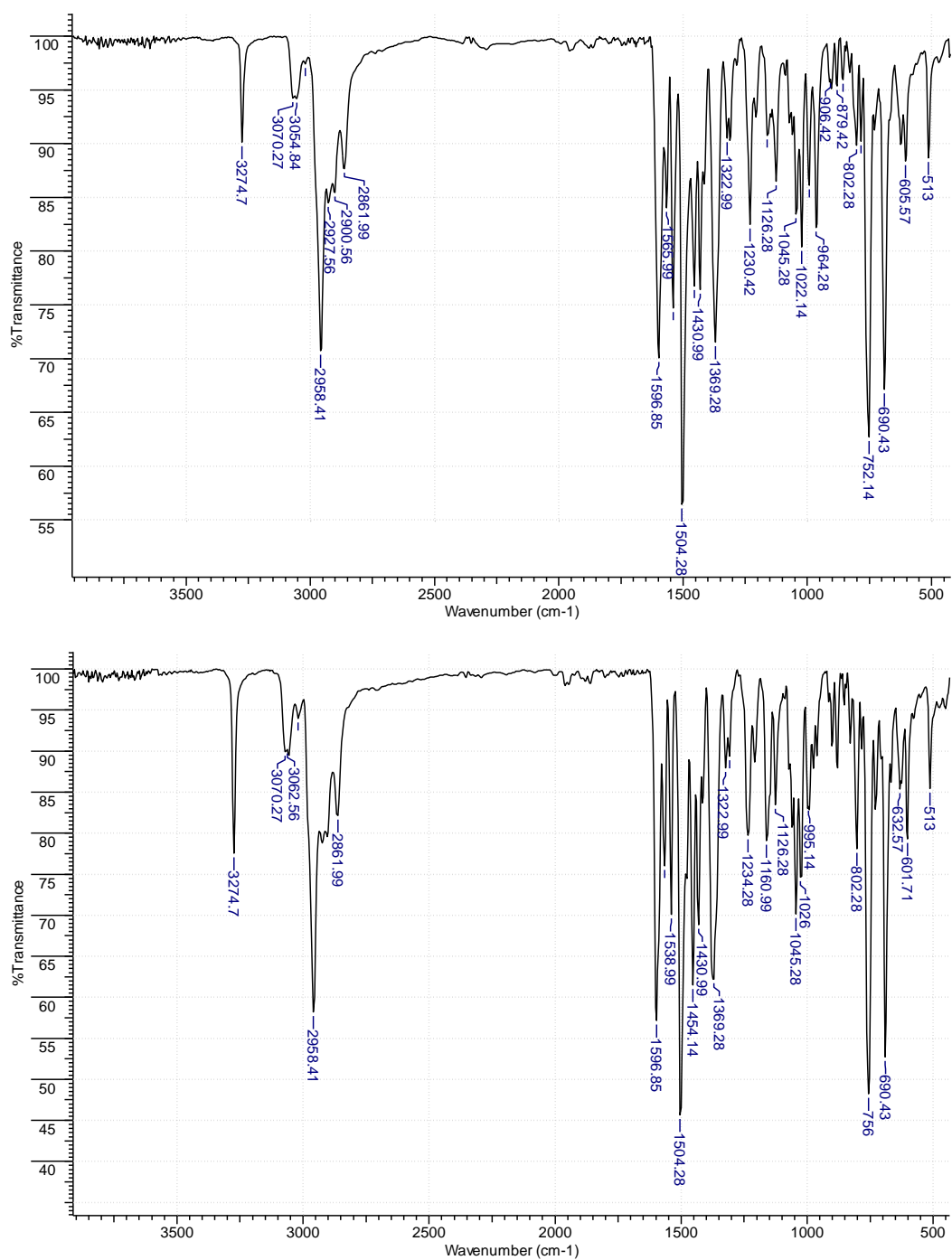


Figure S8. FTIR spectrum of dipyrzolopyrimidine derivative (9) measured using the KBr disk technique. Polymorph 9a (top) and polymorph 9b (bottom).

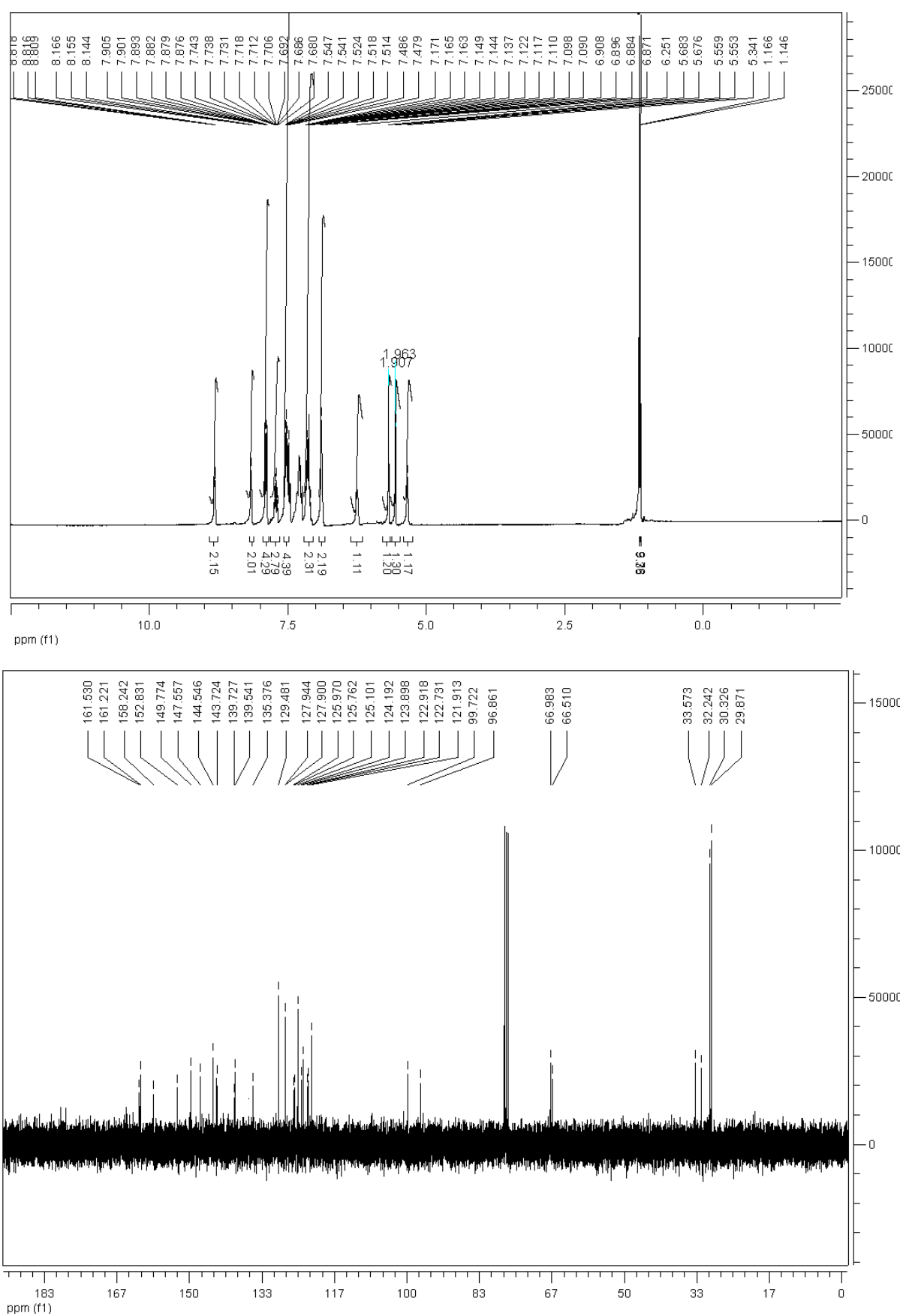


Figure S9. ¹H (top) and ¹³C (bottom) 1D-NMR spectra of dipyrazolopyrimidine derivative (**9**) in deuterated chloroform. These NMR spectra corresponds to polymorph **9a**.