

# New pyrroles derivatives as promising biological agents: Design, Synthesis, Characterization, *In Silico* and Cytotoxicity Evaluation

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## Supplementary Material

### 1. The IR spectra

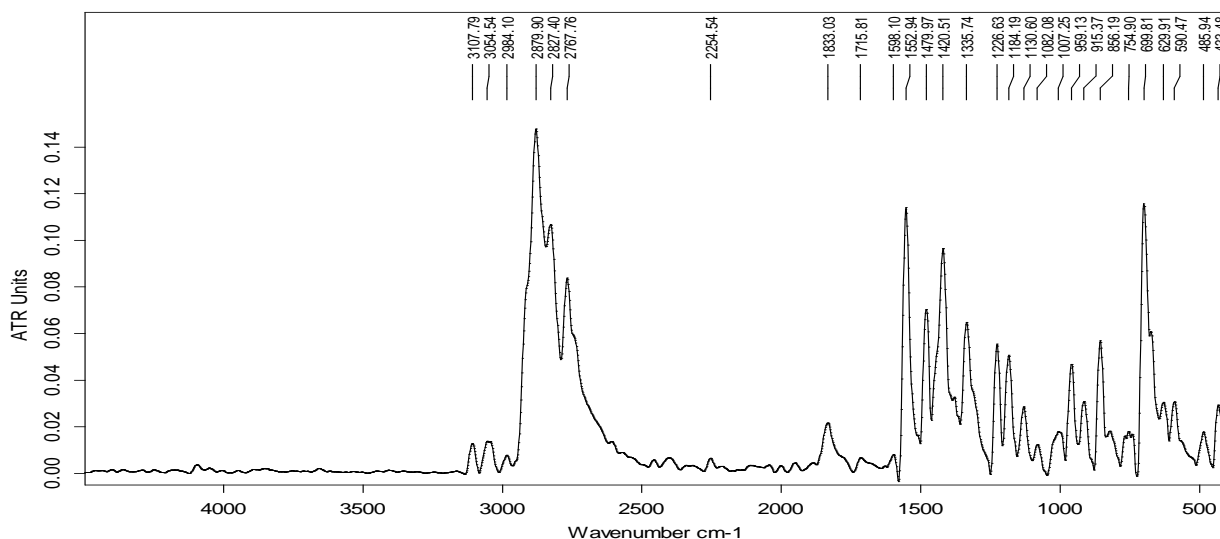


Figure S1. The IR spectrum of salt **2c**

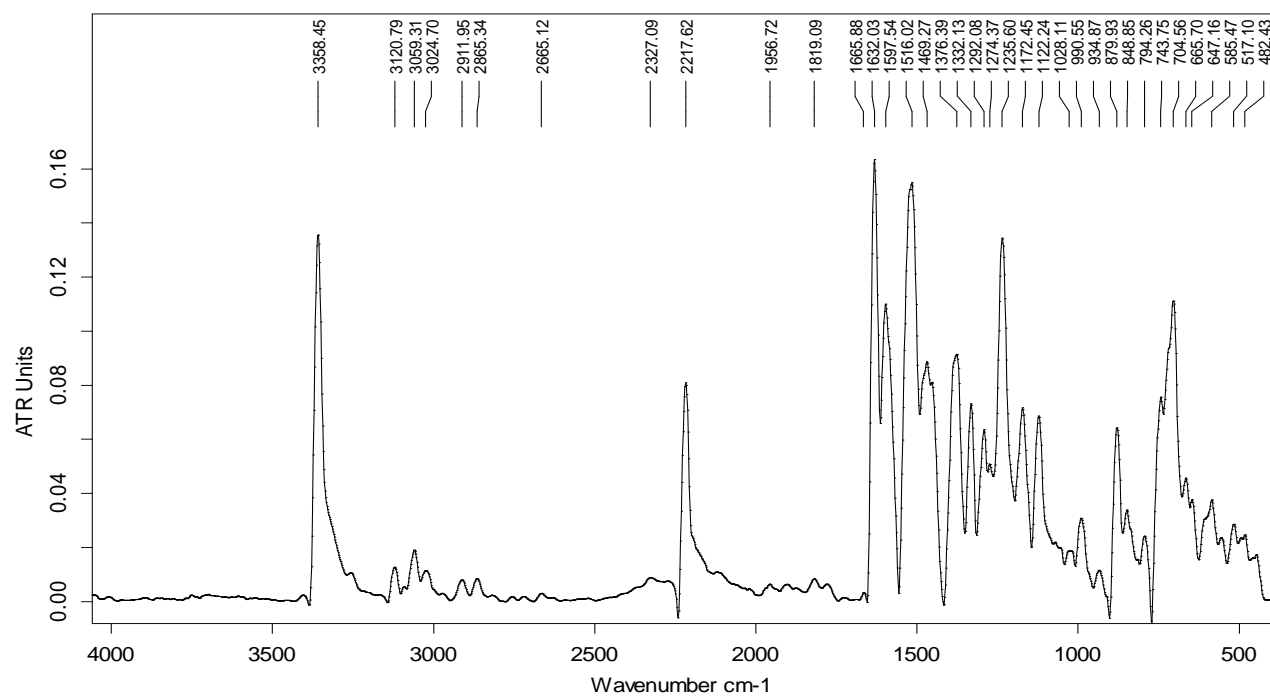


Figure S2. The IR spectrum of pyrrole **4a**

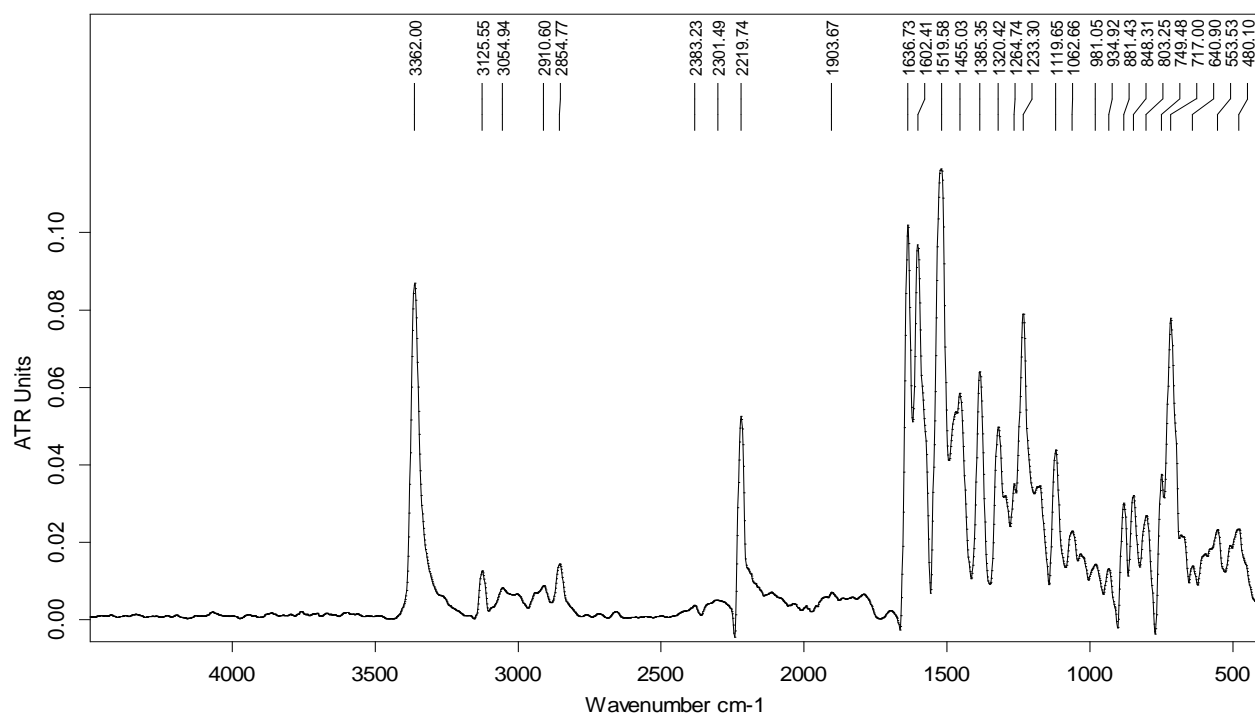


Figure S3. The IR spectrum of pyrrole **4b**

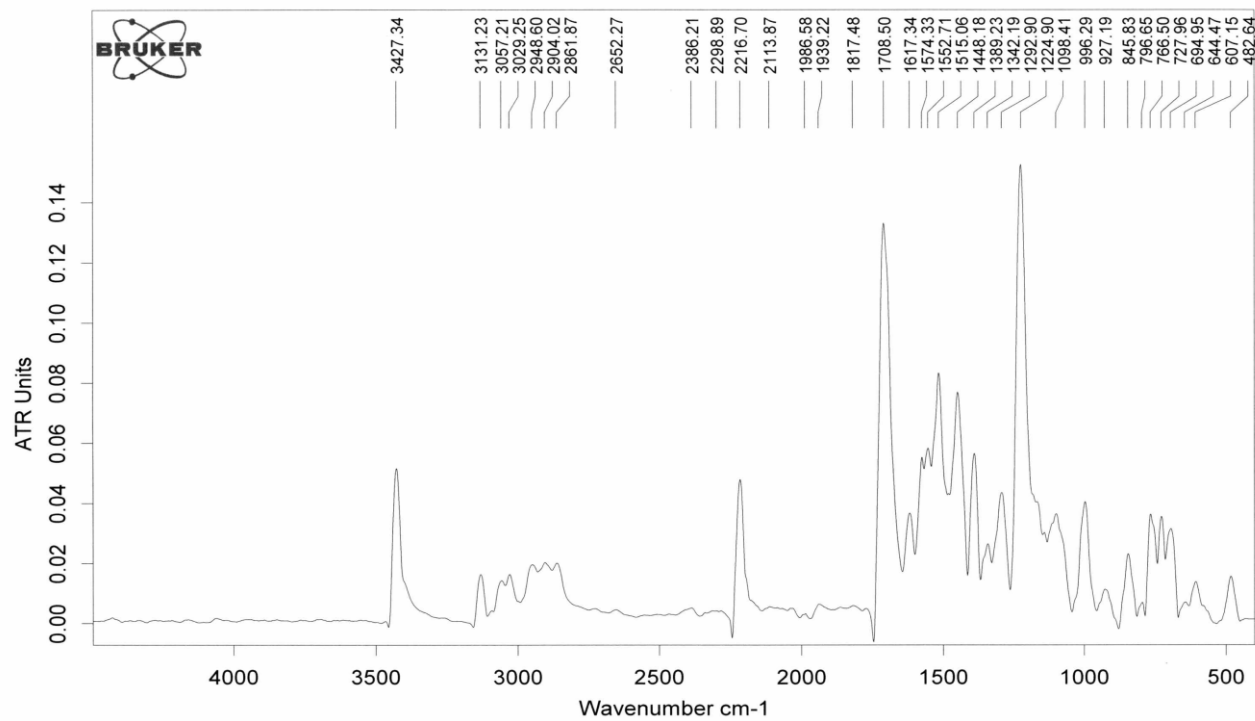


Figure S4. The IR spectrum of pyrrole **4c**

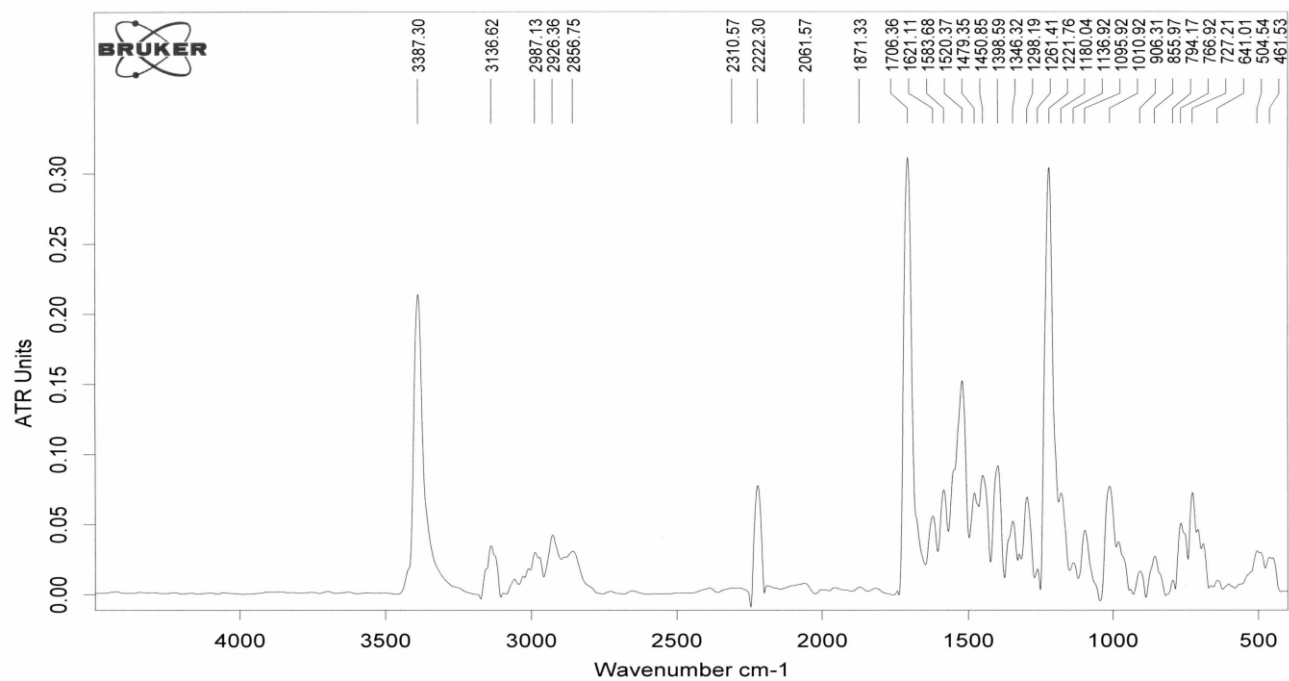


Figure S5. The IR spectrum of pyrrole **4d**

## 2. The $^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR spectra

The NMR spectrum of 1-benzyl-5,6-dimethyl-3-cyanomethylbenzimidazolium bromide (**2c**)

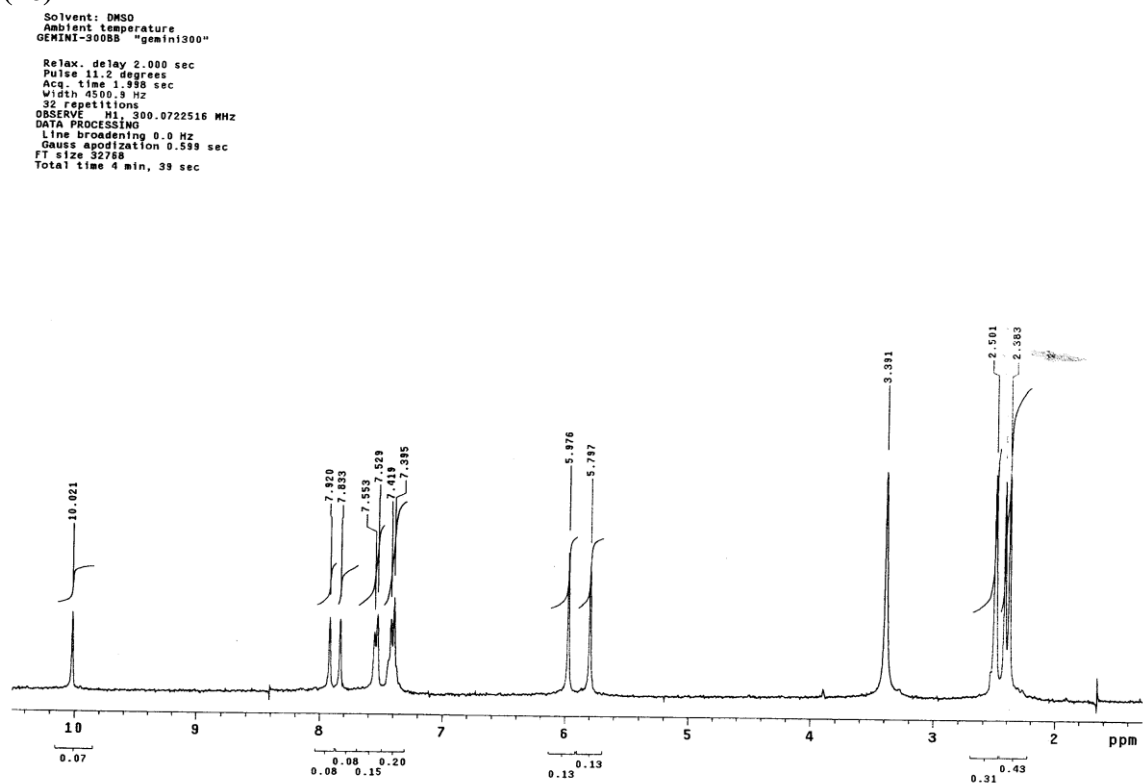


Figure S6. The  $^1\text{H}$ -NMR spectrum of salt **2c**

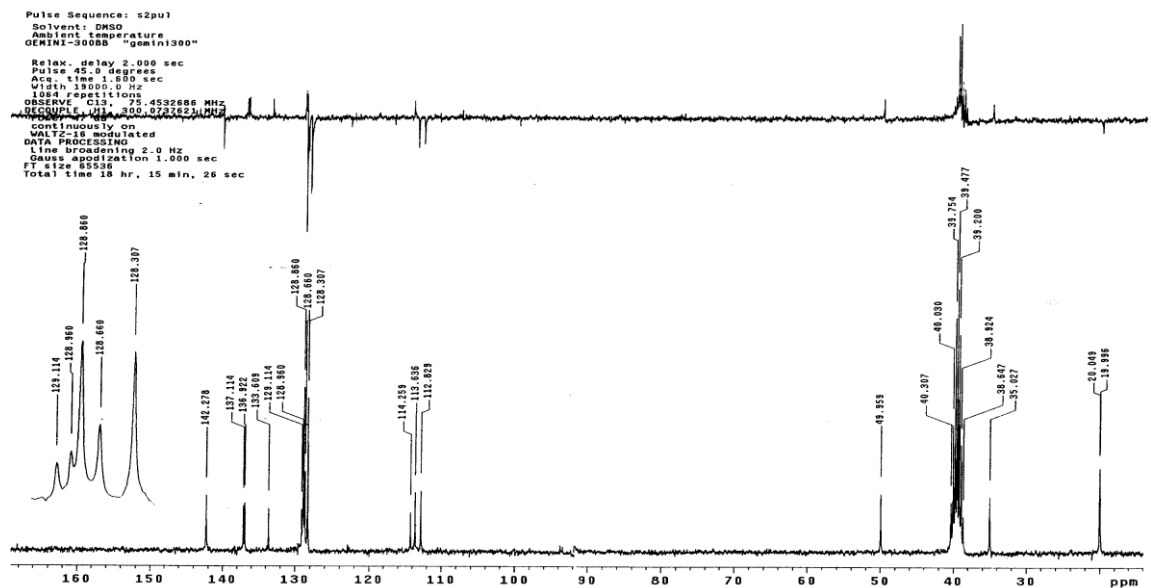


Figure S7. The  $^{13}\text{C}$ -NMR spectrum of salt **2c**

## OpenVnmrJ



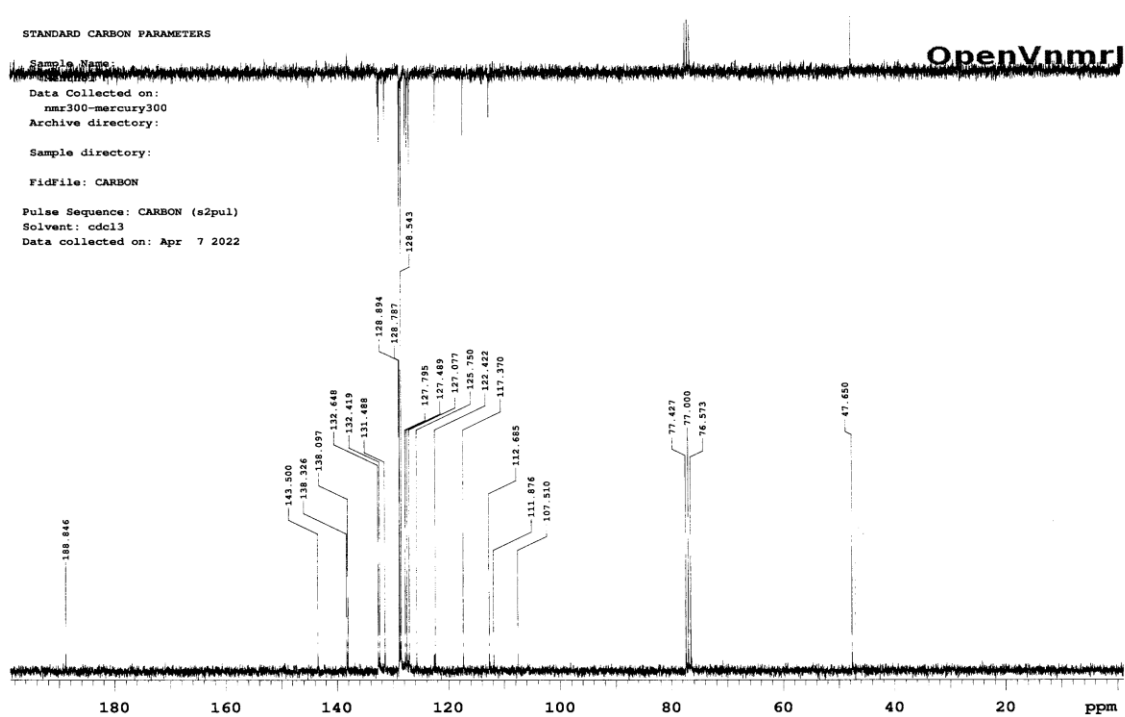


Figure S10. The  $^{13}\text{C}$ -NMR spectrum of pyrrole **4a**

The NMR spectrum of 4-benzoyl-2-cyano-1-[2-(4-methylbenzylamino)phenyl]pyrrole (**4b**)

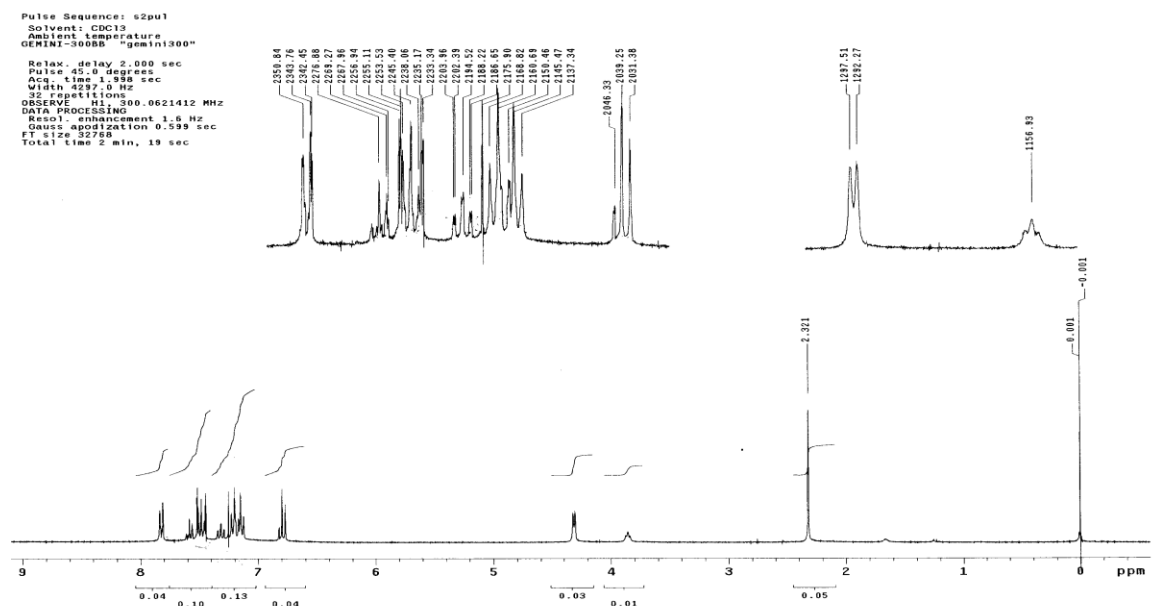


Figure S11. The <sup>1</sup>H-NMR spectrum of pyrrole **4b**

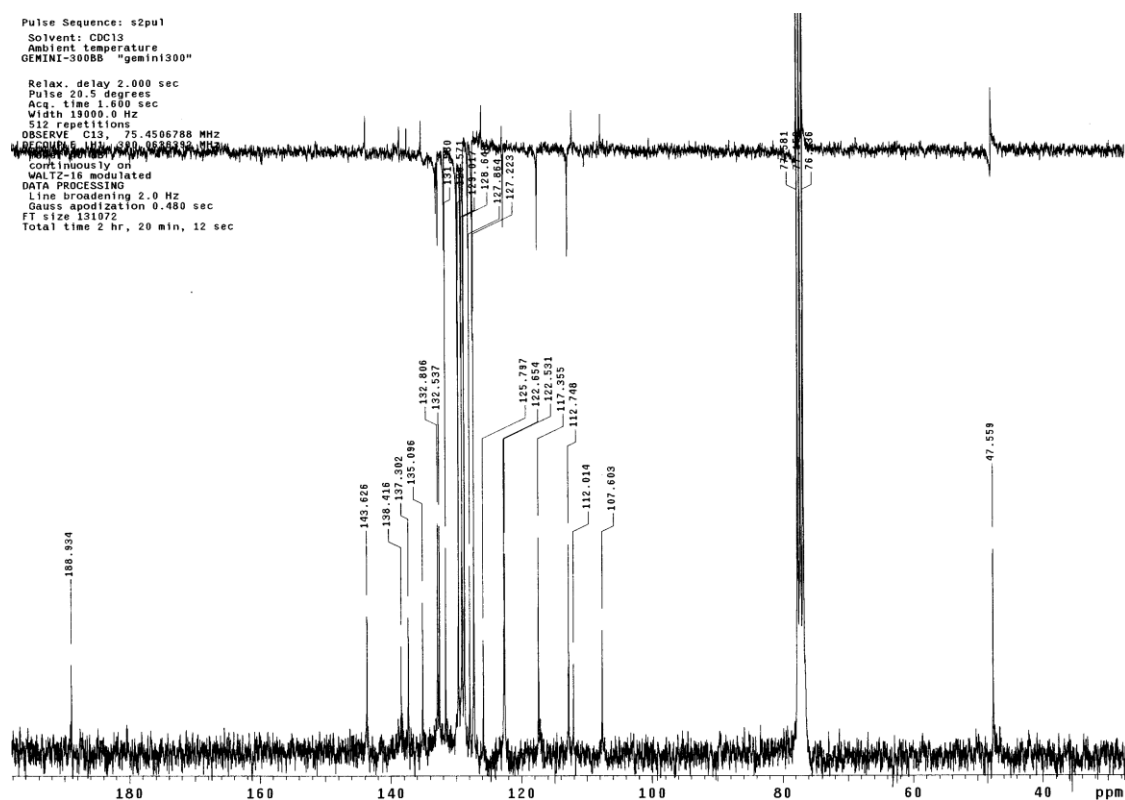


Figure S12. The <sup>13</sup>C-NMR spectrum of pyrrole **4b**

The NMR spectrum of methyl 1- [(2-benzylamino-4,5-dimethyl)phenyl]-2-cyanopyrrole-4-carboxylate (**4c**)

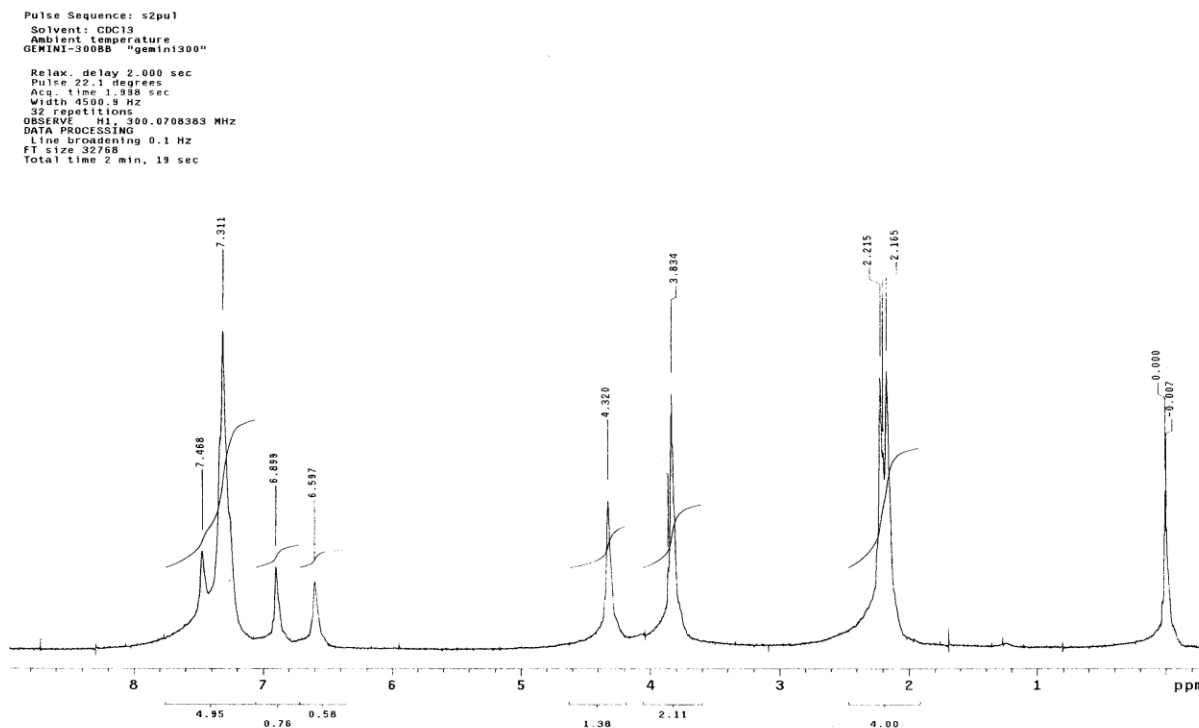


Figure S13. The <sup>1</sup>H-NMR spectrum of pyrrole **4c**

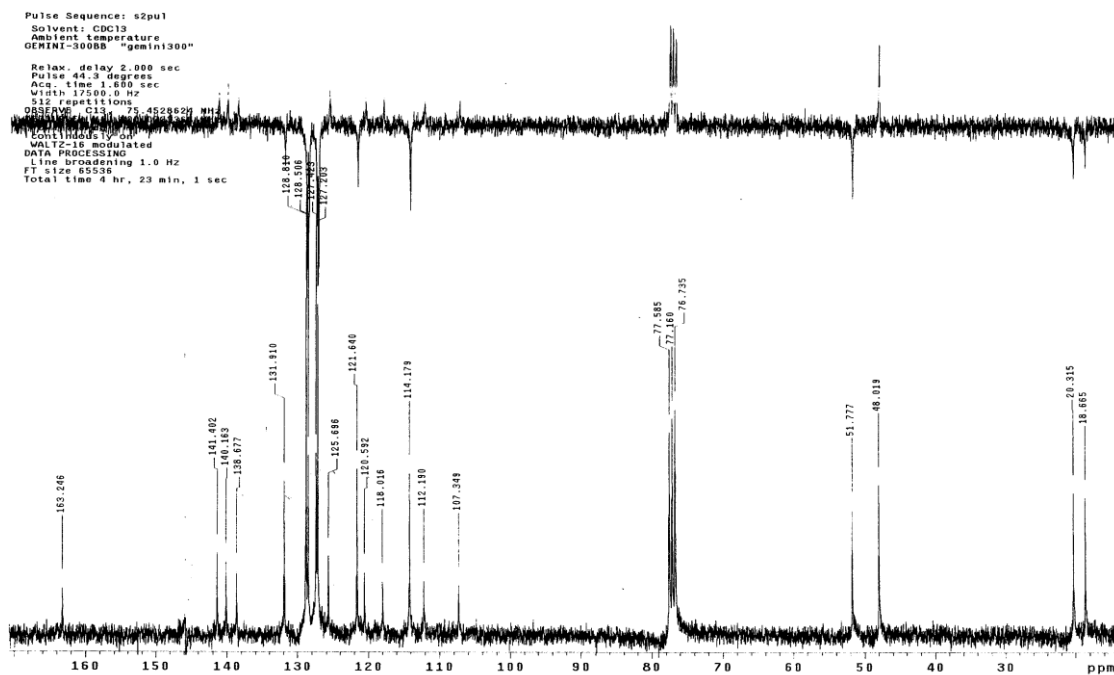


Figure S14. The <sup>13</sup>C-NMR spectrum of pyrrole **4c**



The NMR spectrum of ethyl 1- [(2-benzylamino-4,5-dimethyl)phenyl]-2-cyanopyrrole-4-carboxylate (**4d**)

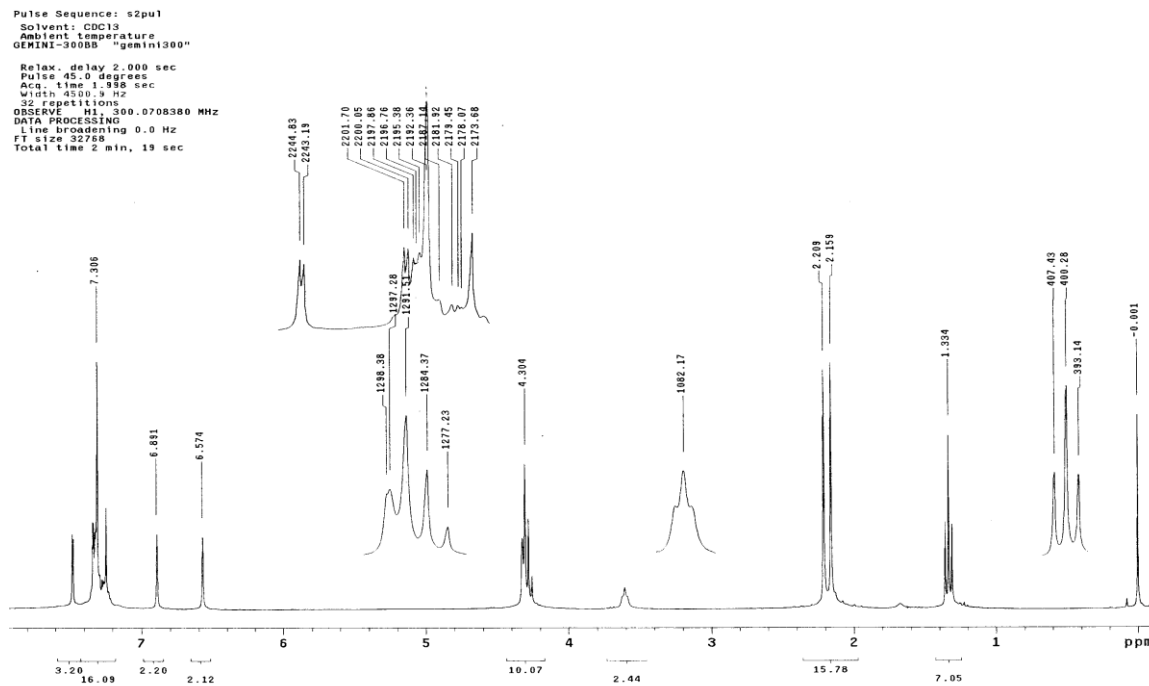


Figure S15. The  $^1\text{H}$ -NMR spectrum of pyrrole **4d**

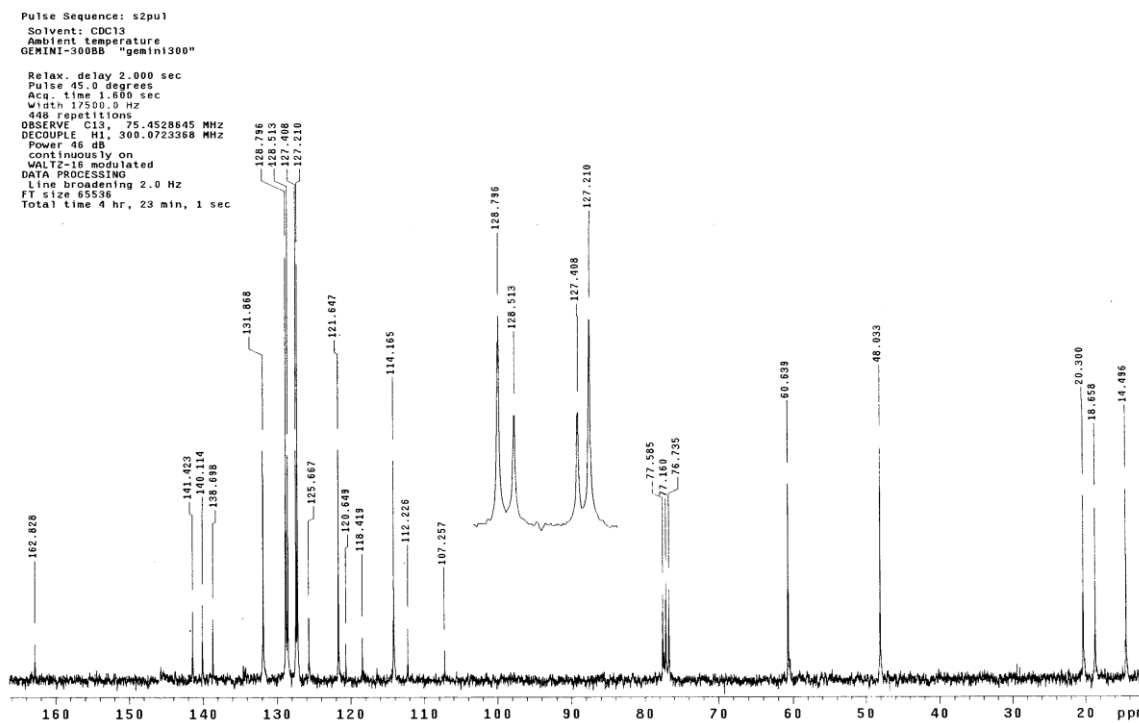


Figure S16. The  $^{13}\text{C}$ -NMR spectrum of pyrrole **4d**