Supporting Information

Regioselective Synthesis, Structural Characterization, and Antiproliferative Activity of Novel Tetra-Substituted Phenylaminopyrazole Derivatives

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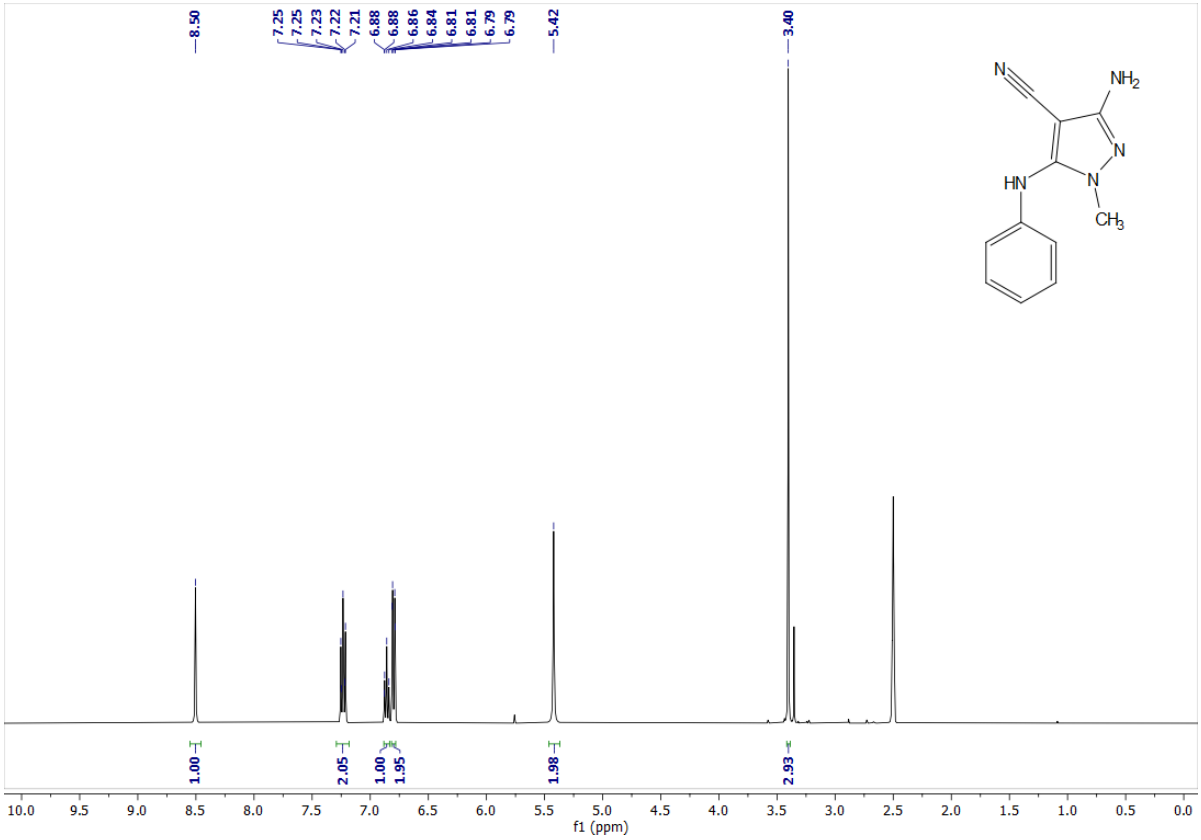


Figure S1. ^{1}H-NMR (400 MHz, d_6-DMSO) spectrum of compound **1**

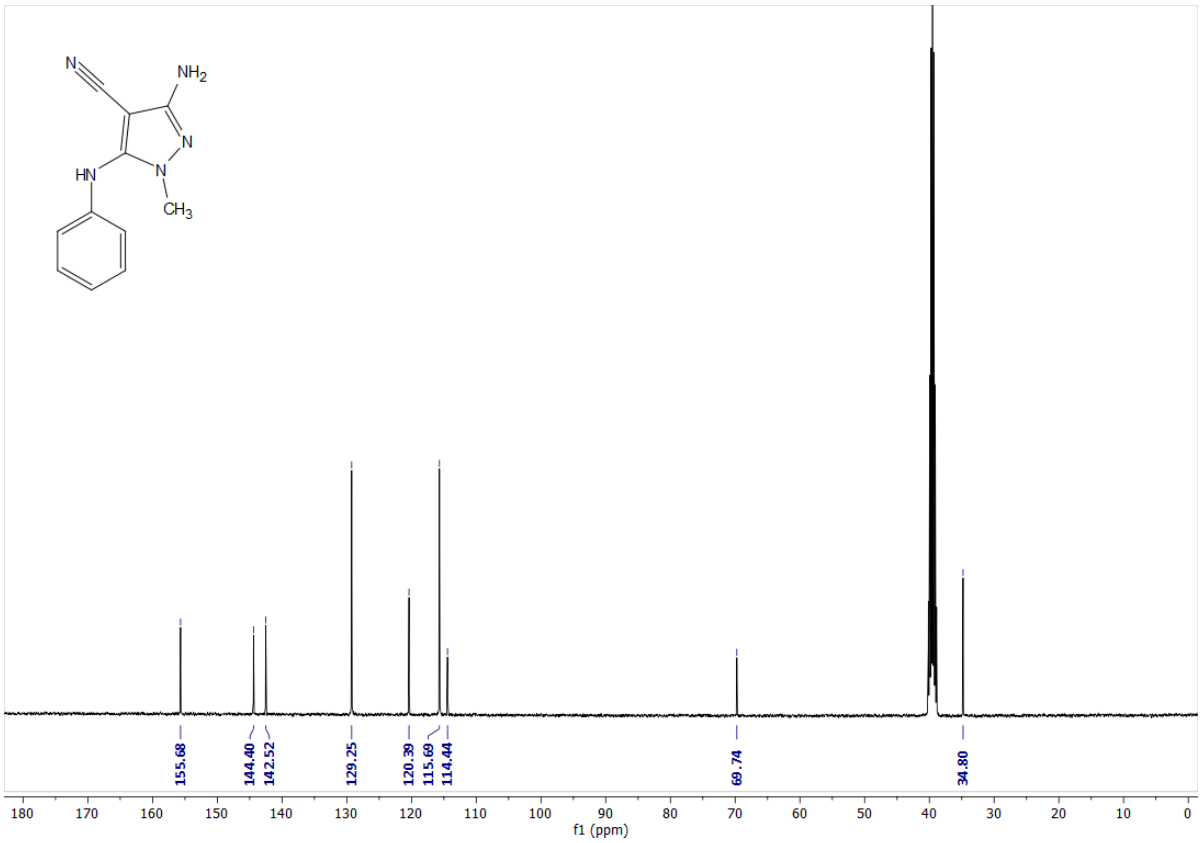


Figure S2. ^{13}C-NMR (101 MHz, d_6-DMSO) spectrum of compound **1**

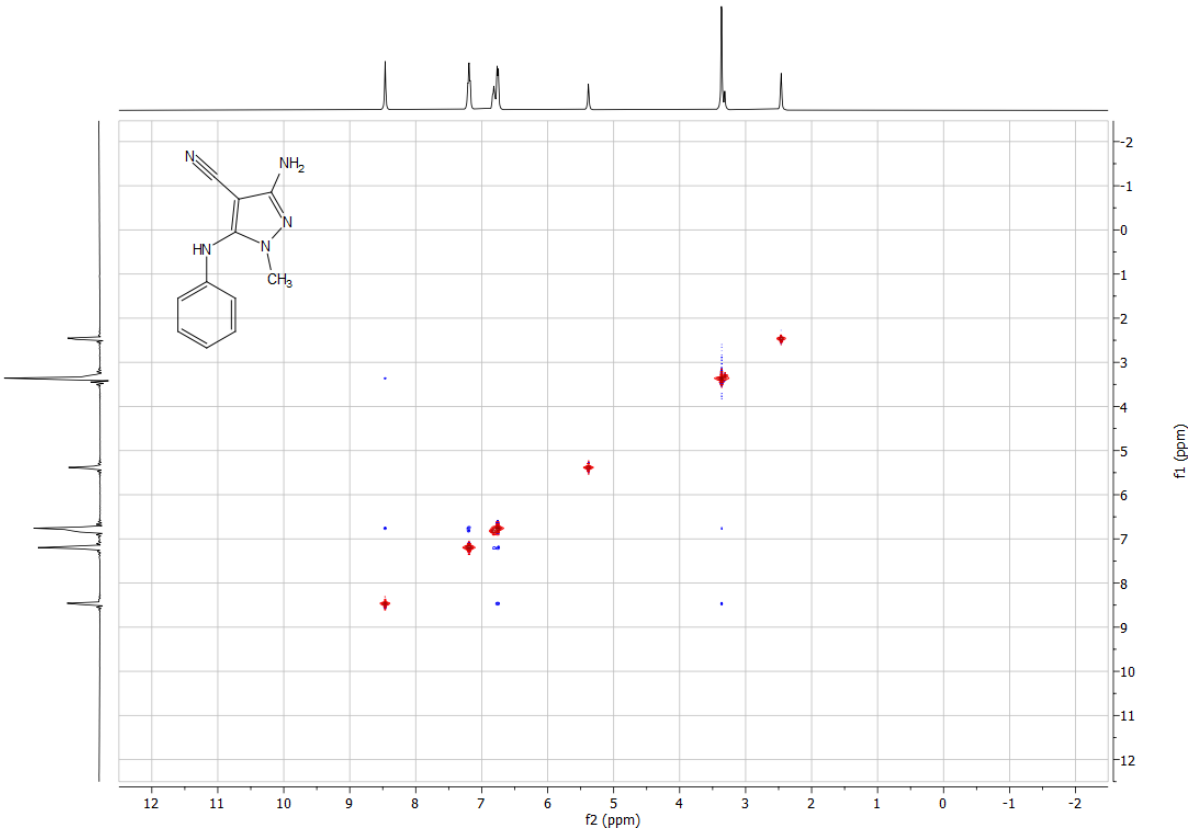


Figure S3. 2D NOESY (d_6-DMSO) spectrum of compound **1**

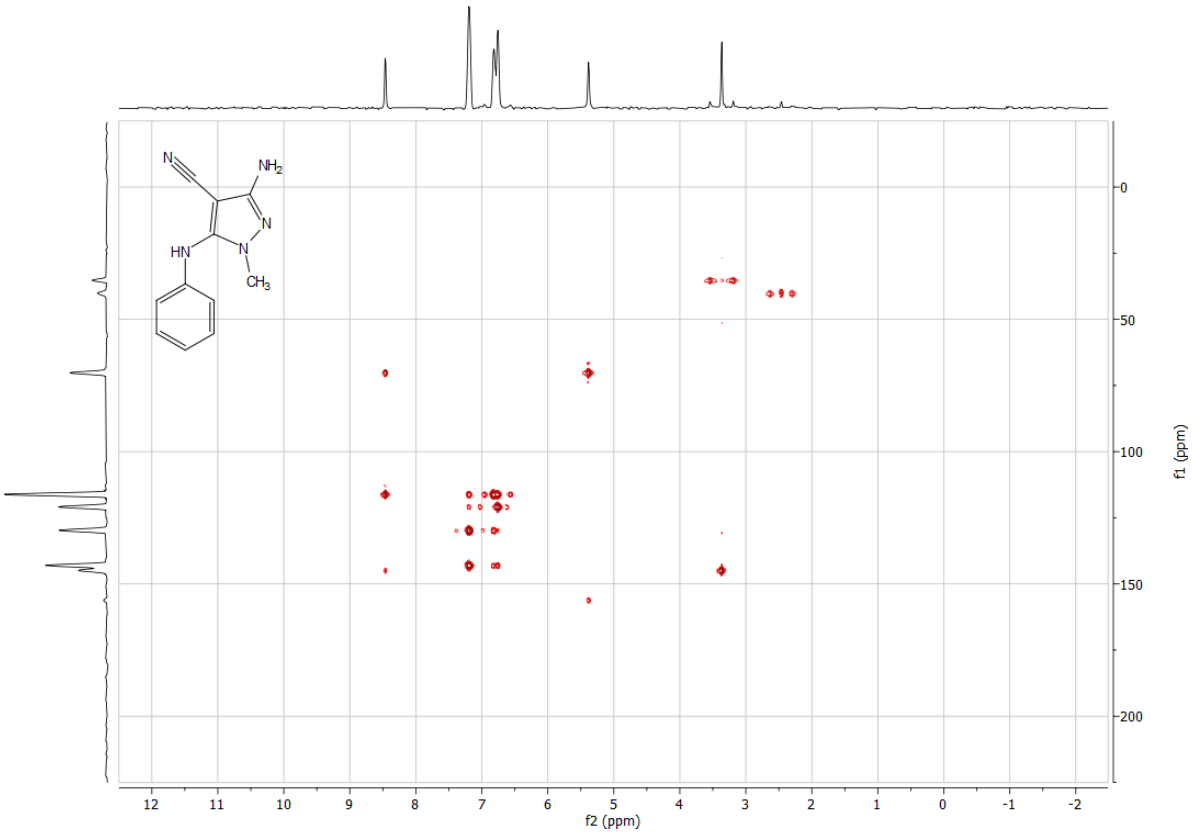


Figure S4. 2D HMBC (d_6-DMSO) spectrum of compound **1**

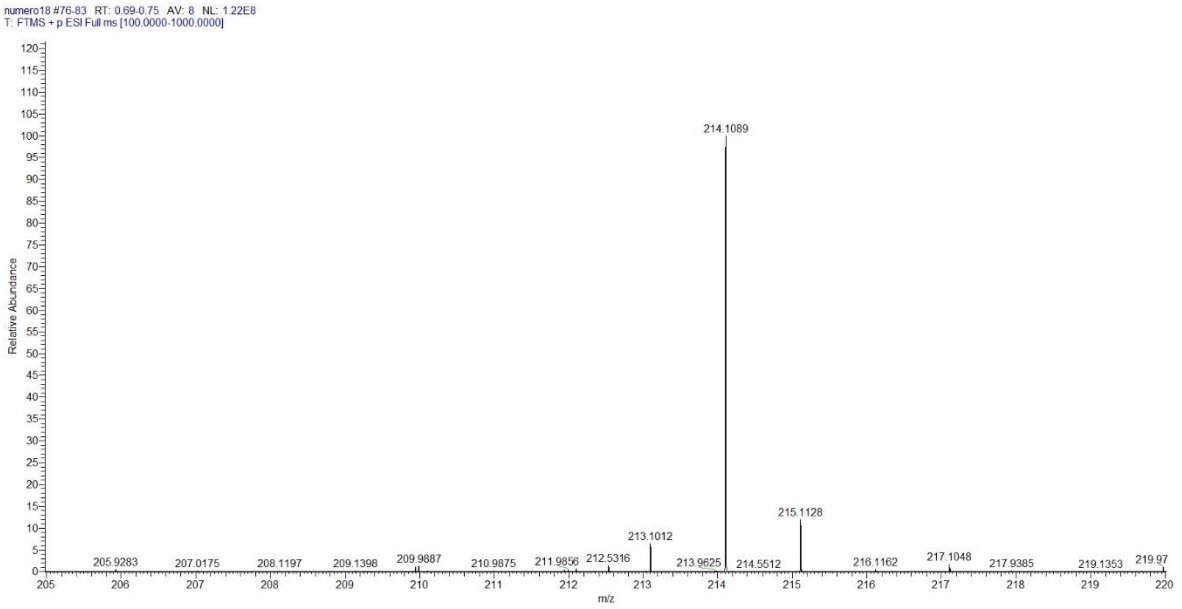


Figure S5. Fullscan analysis of compound **1**

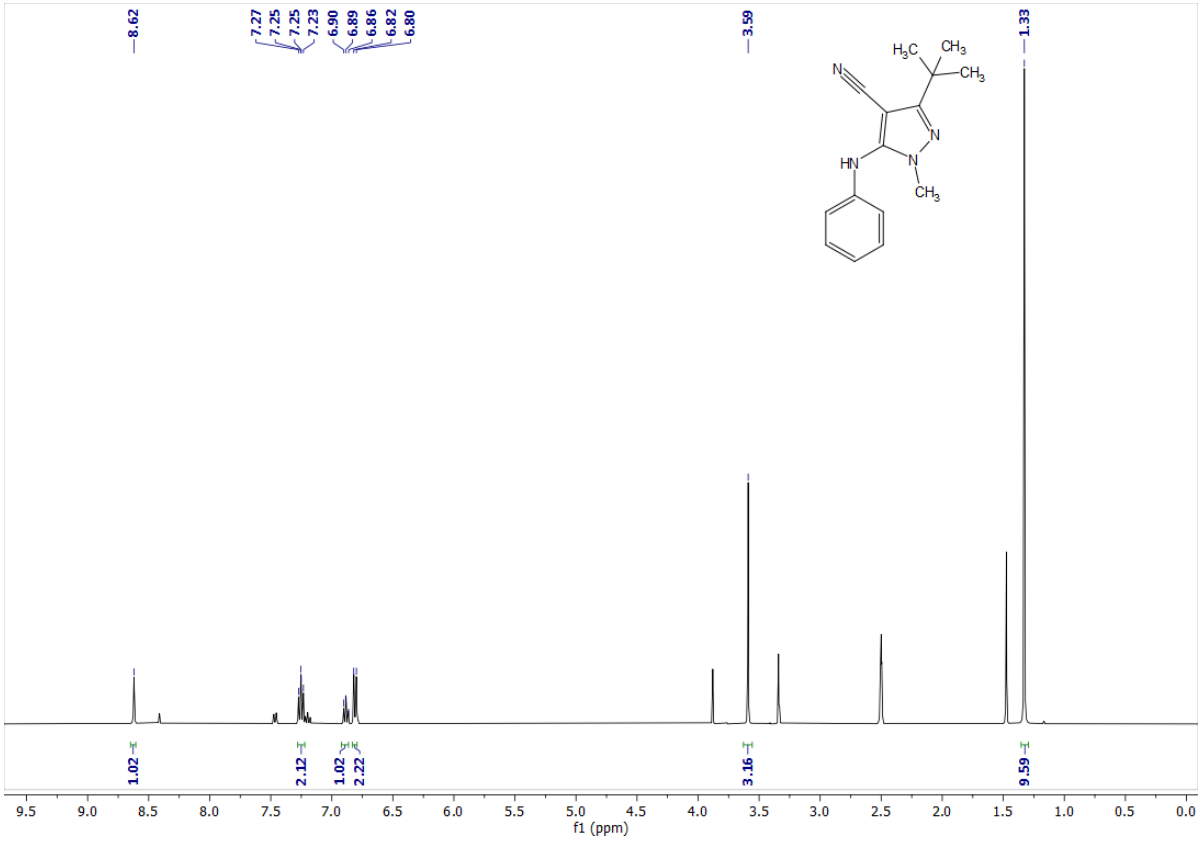


Figure S6. ^{1}H-NMR (400 MHz, d_6-DMSO) spectrum of compound **2**

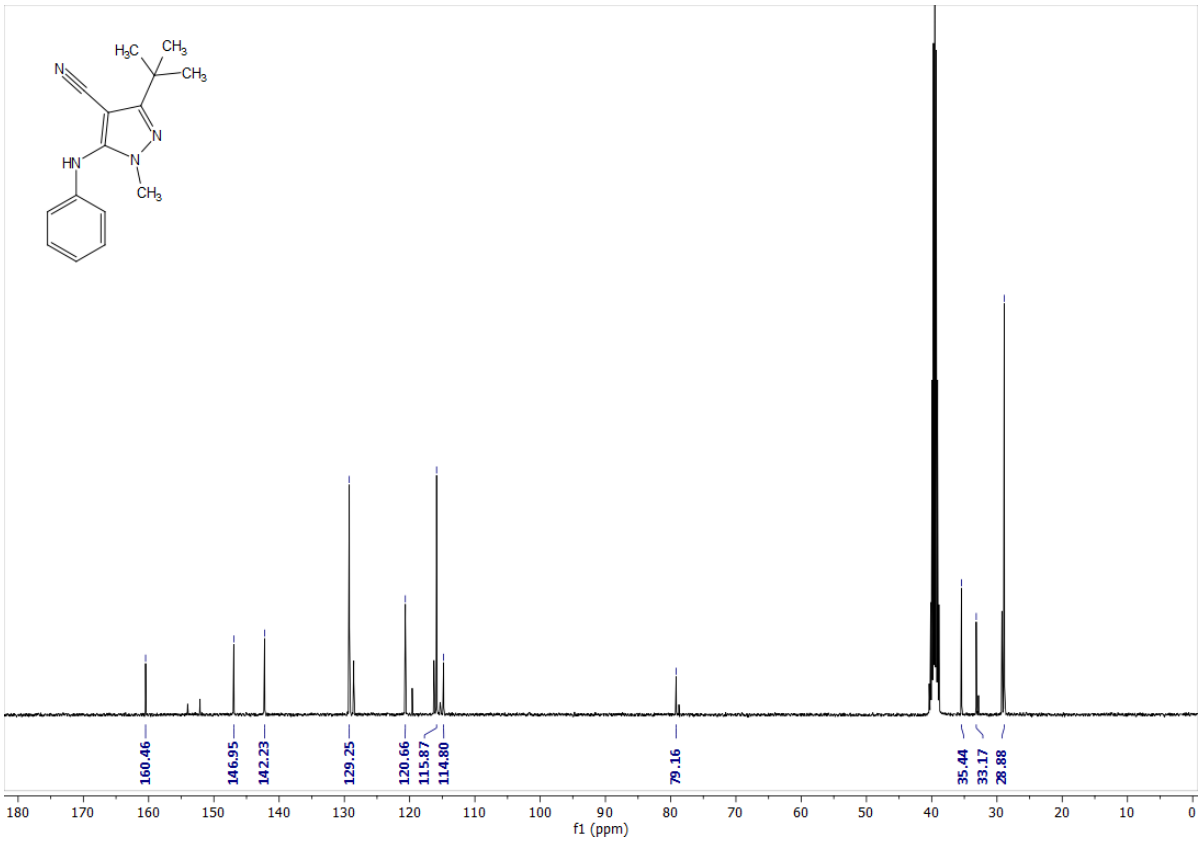


Figure S7. ^{13}C-NMR (101 MHz, d_6-DMSO) spectrum of compound **2**

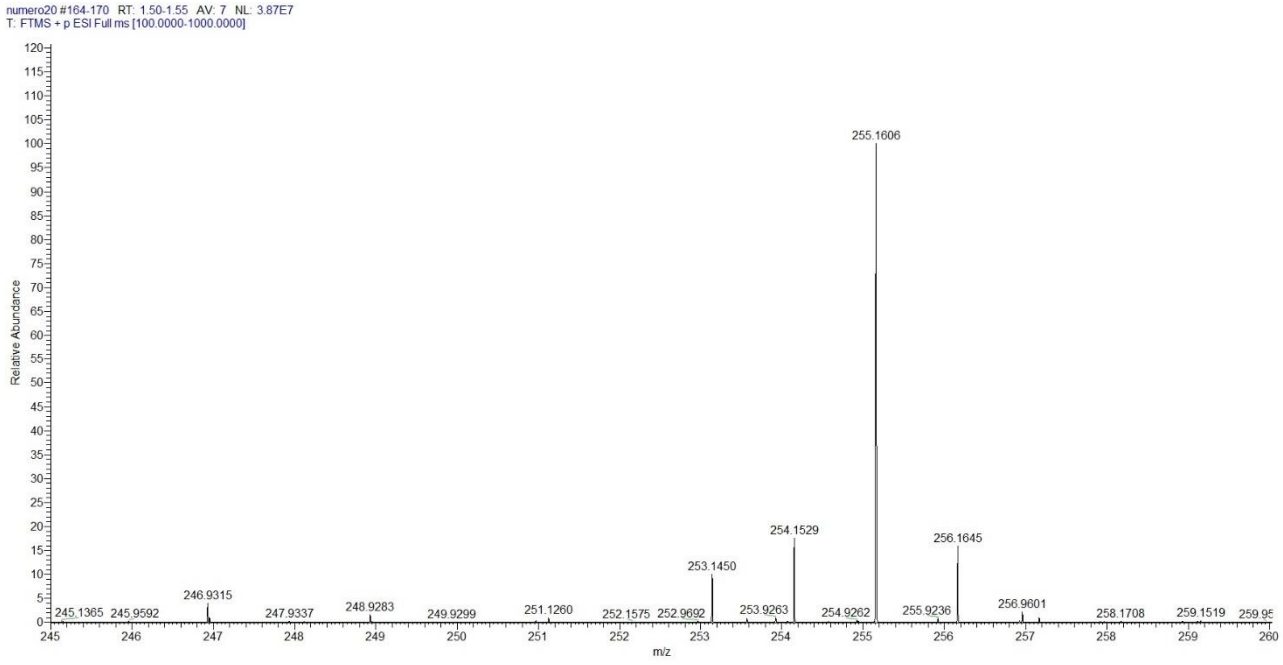


Figure S8. Fullscan analysis of compound **2**

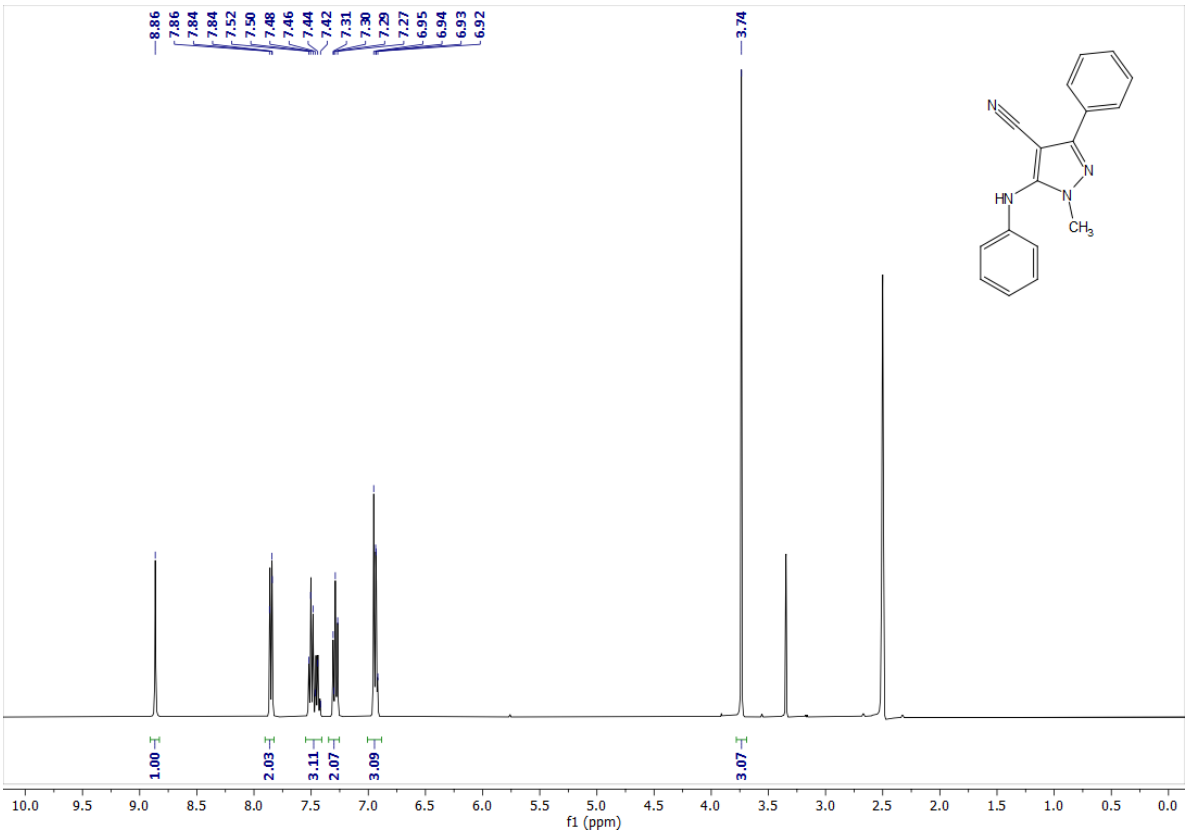


Figure S9. ^{1}H-NMR (400 MHz, d_6-DMSO) spectrum of compound **3**

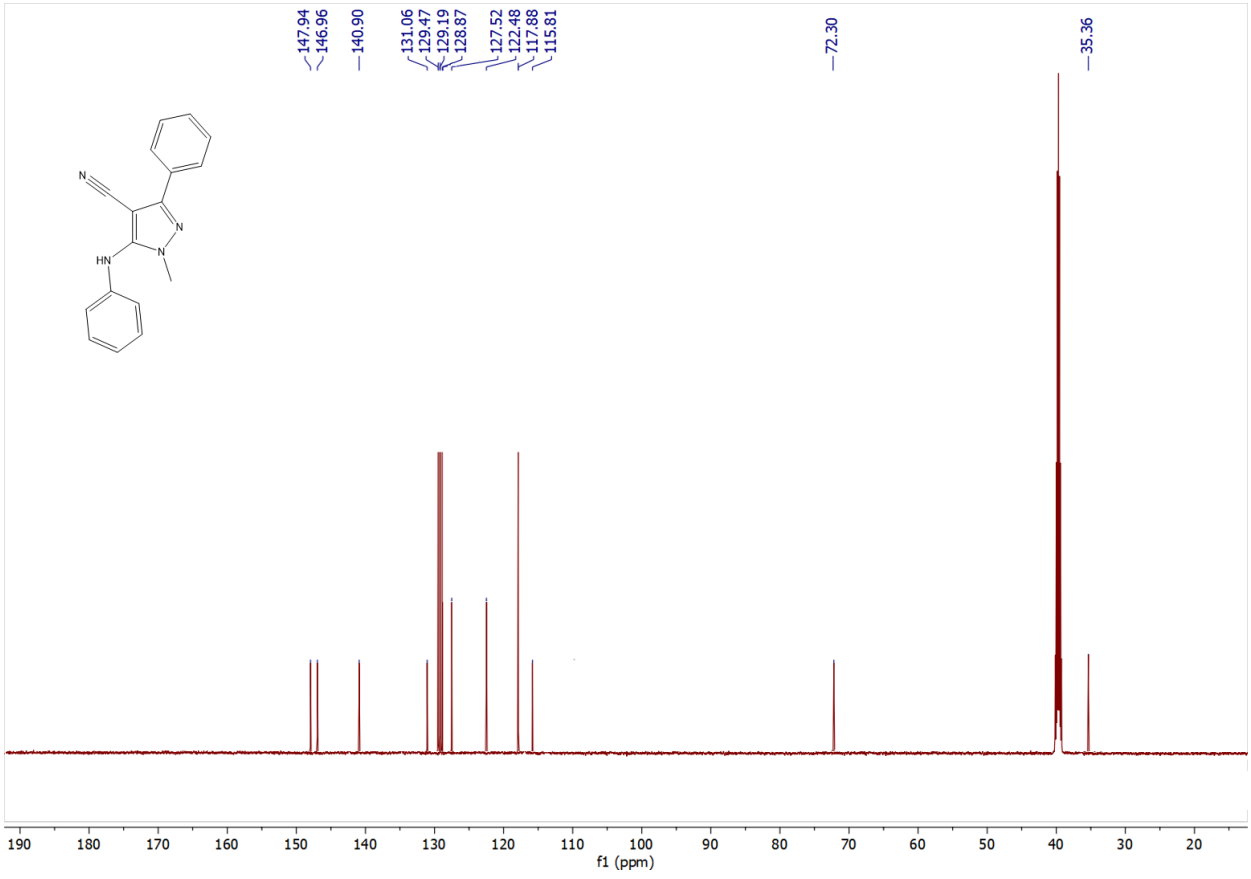


Figure S10. ^{13}C-NMR (101 MHz, d_6-DMSO) spectrum of compound **3**

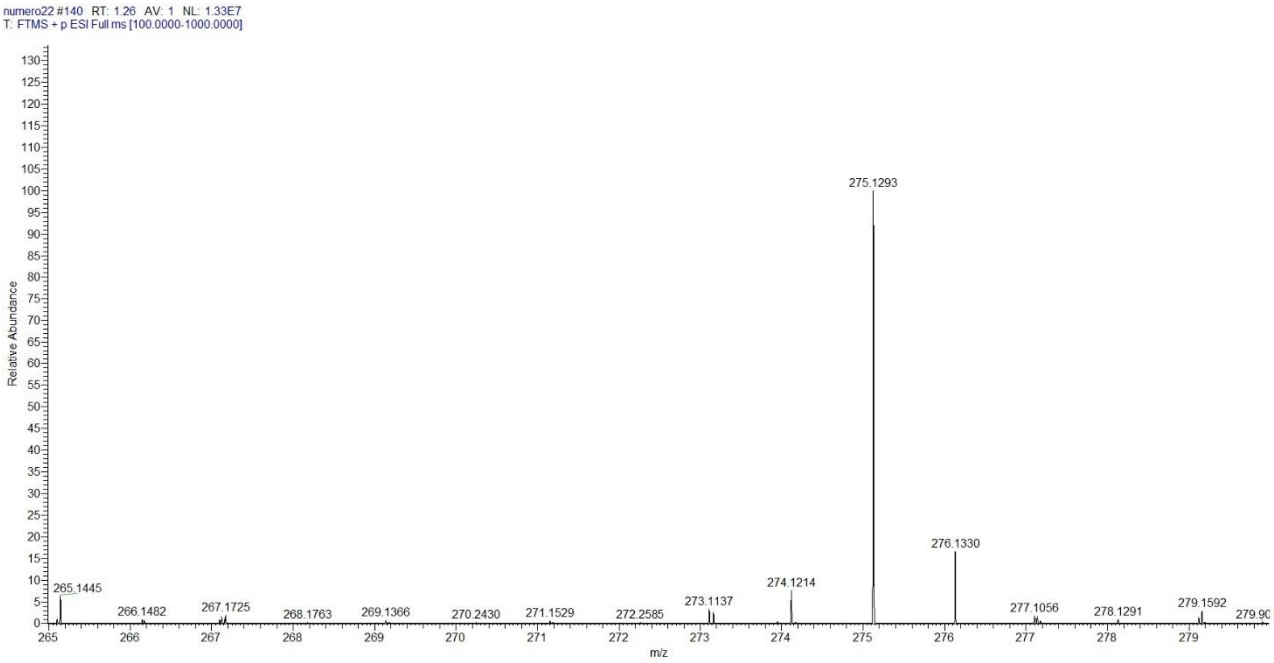


Figure S11. Fullscan analysis of compound **3**

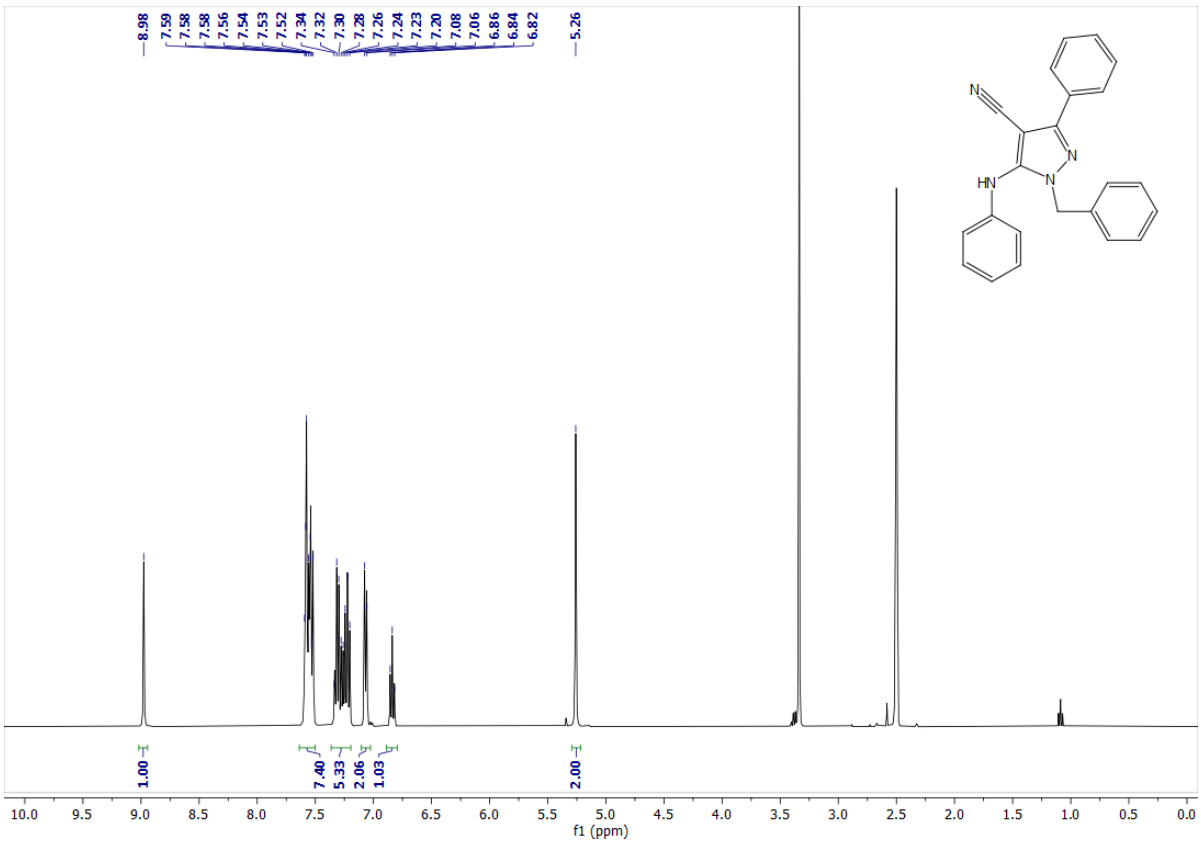


Figure S12. ^{1}H-NMR (400 MHz, d_6-DMSO) spectrum of compound **4**

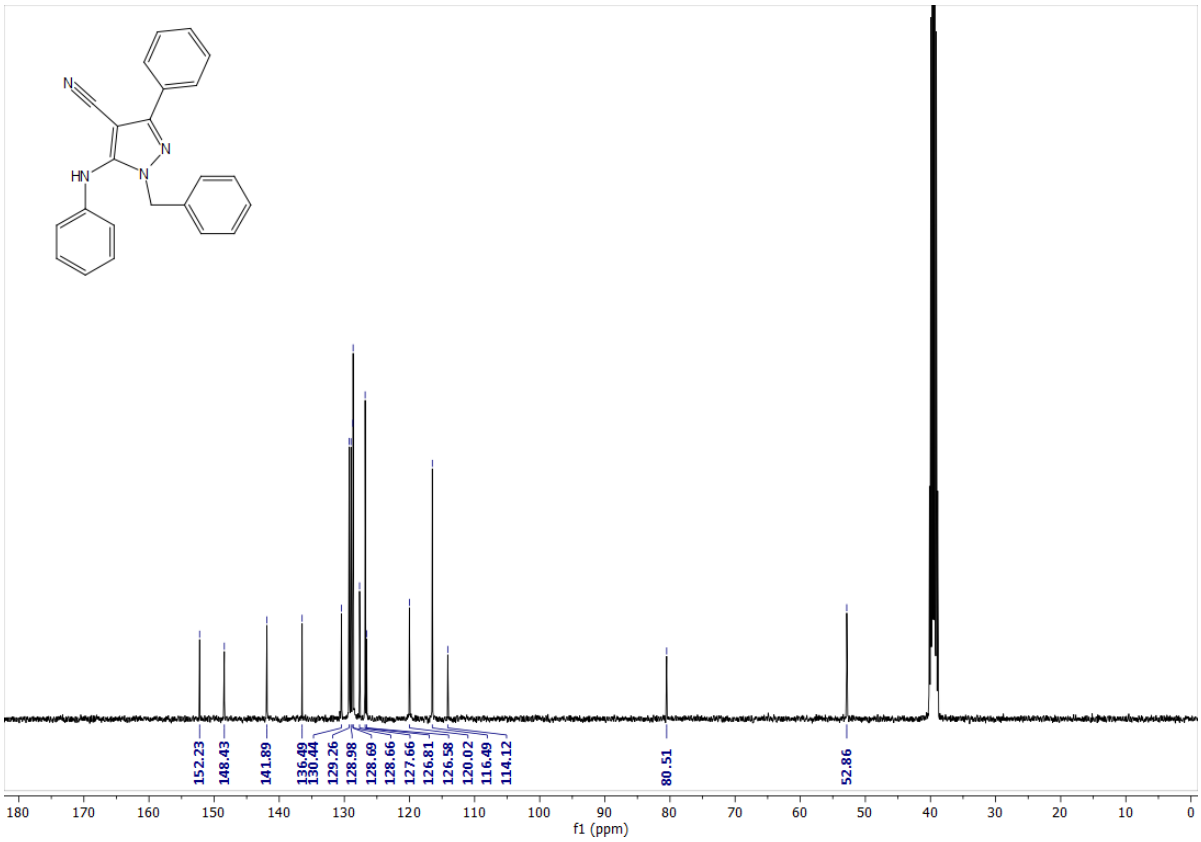


Figure S13. ^{13}C-NMR (101 MHz, d_6-DMSO) spectrum of compound **4**

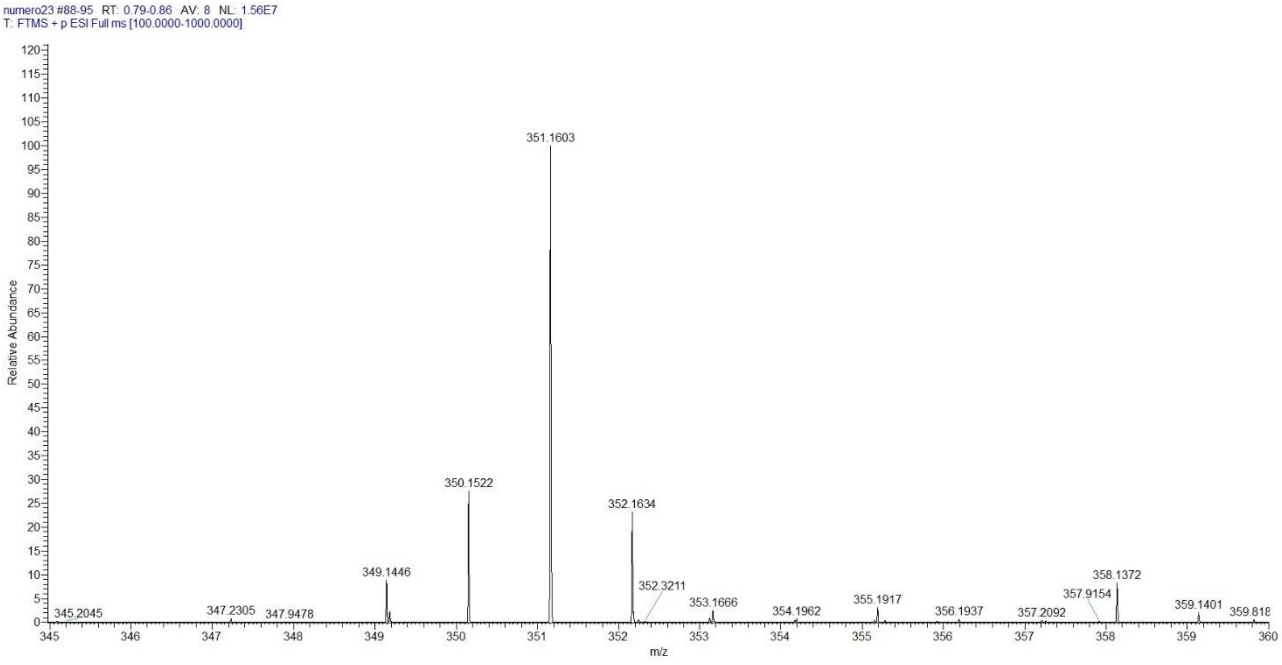


Figure S14. Fullscan analysis of compound **4**

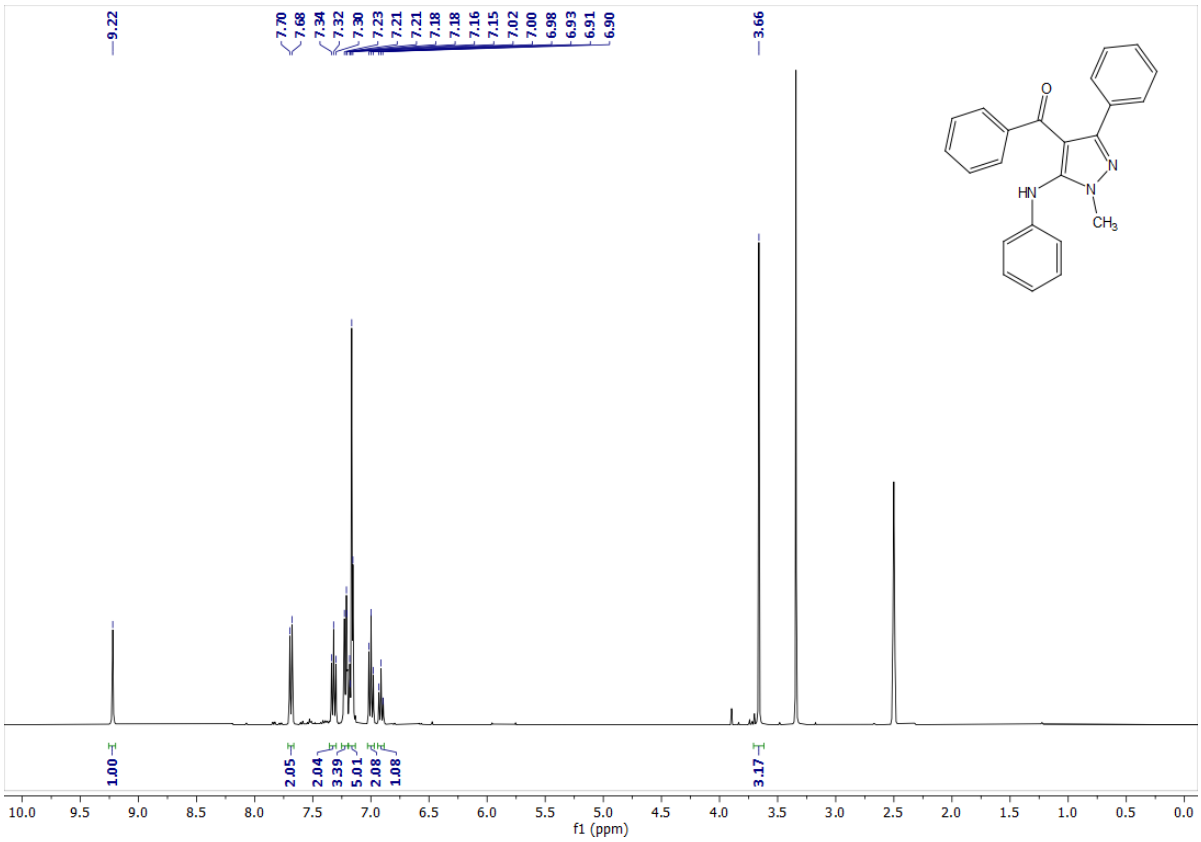


Figure S15. ^{1}H-NMR (400 MHz, d_6-DMSO) spectrum of compound **5**

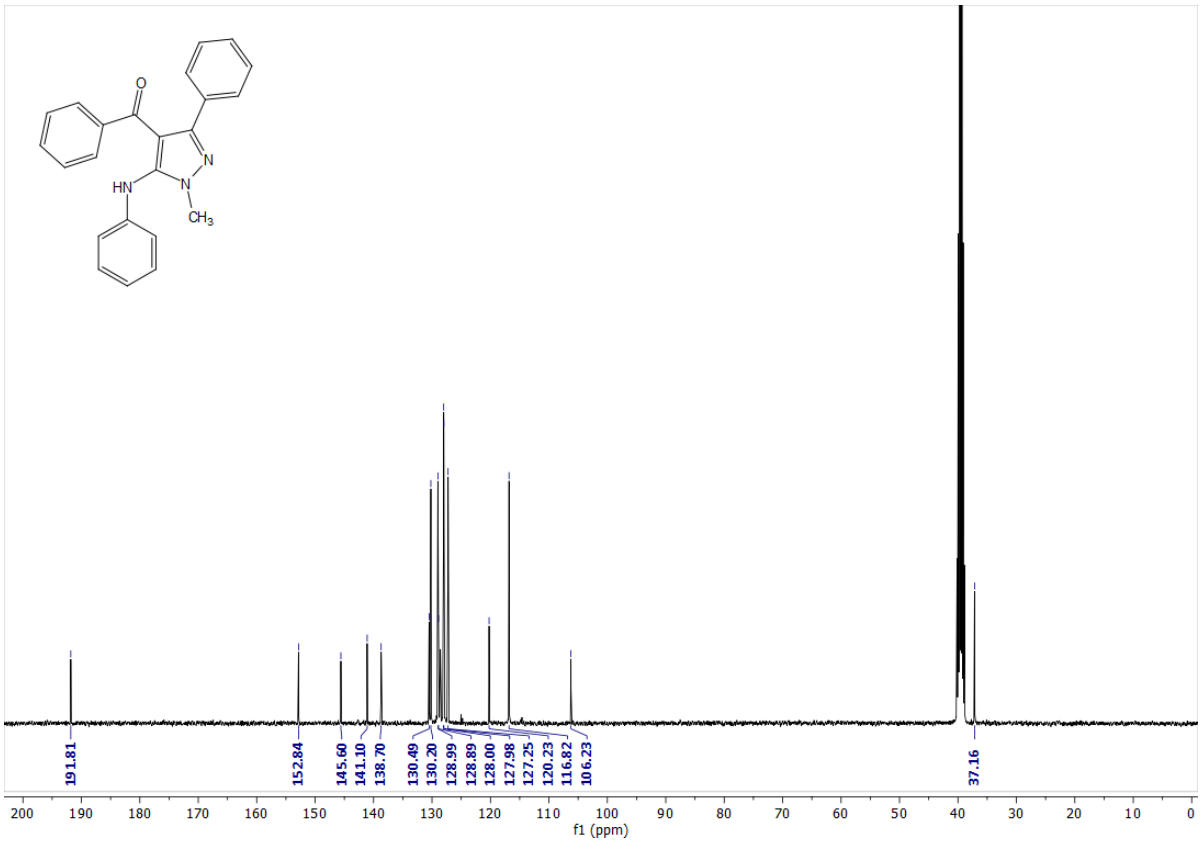


Figure S16. ^{13}C-NMR (101 MHz, d_6-DMSO) spectrum of compound **5**

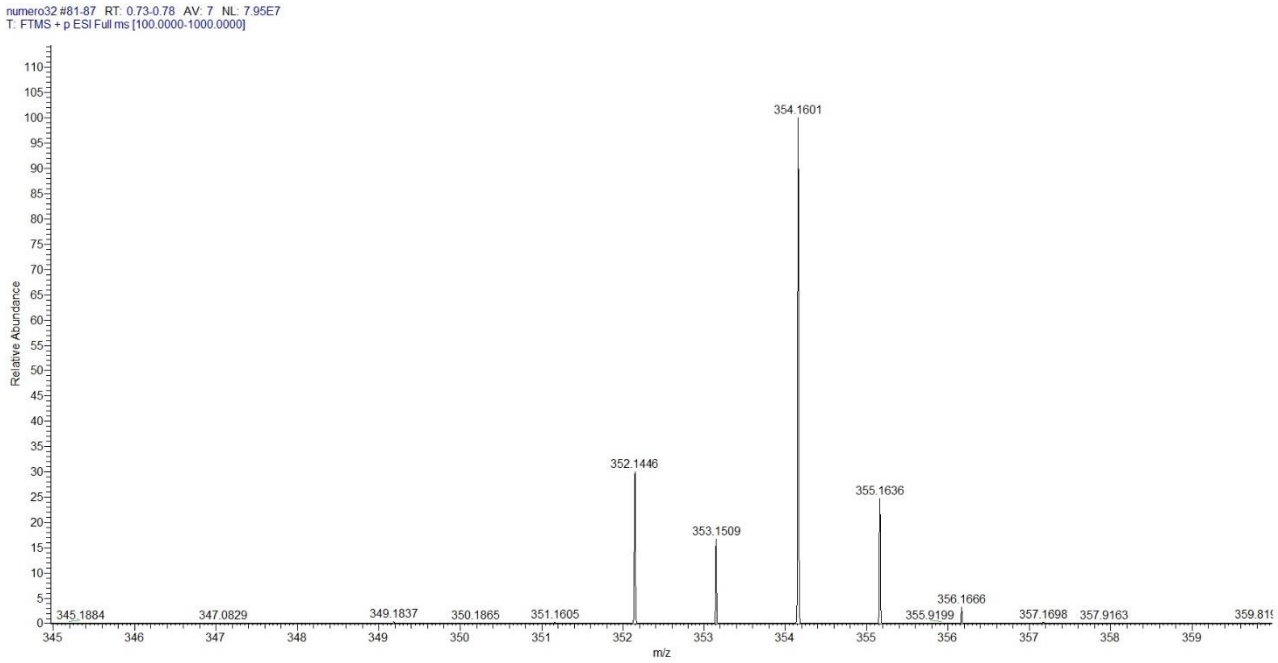


Figure S17. Fullscan analysis of compound **5**

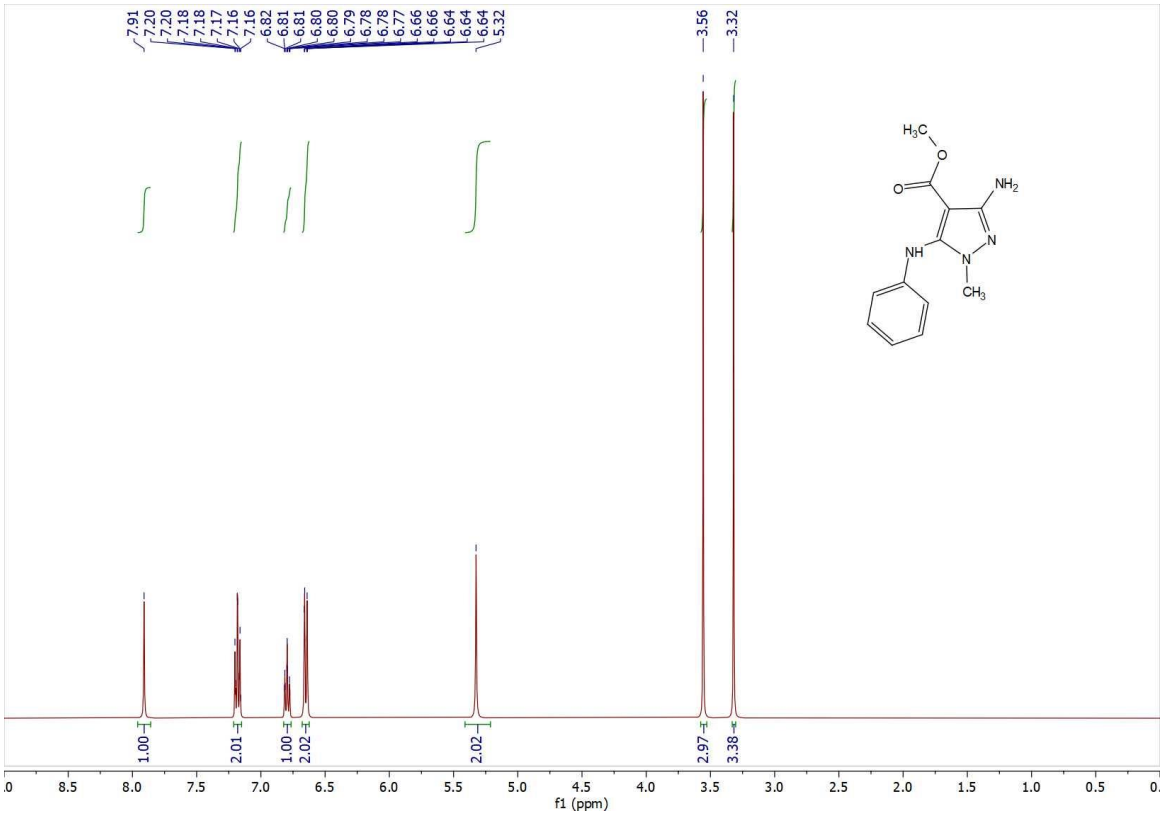


Figure S18. ^{1}H-NMR (400 MHz, d_6-DMSO) spectrum of compound **6**

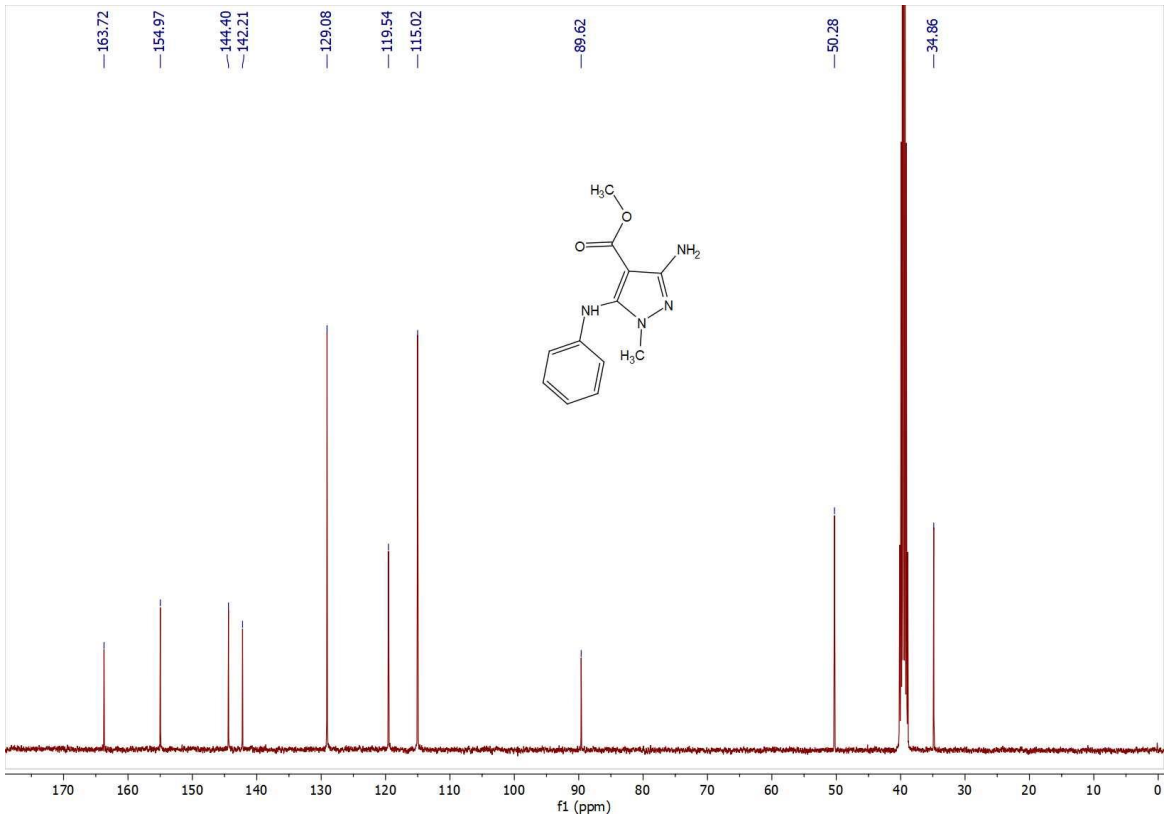


Figure S19. ^{13}C-NMR (101 MHz, d_6-DMSO) spectrum of compound **6**

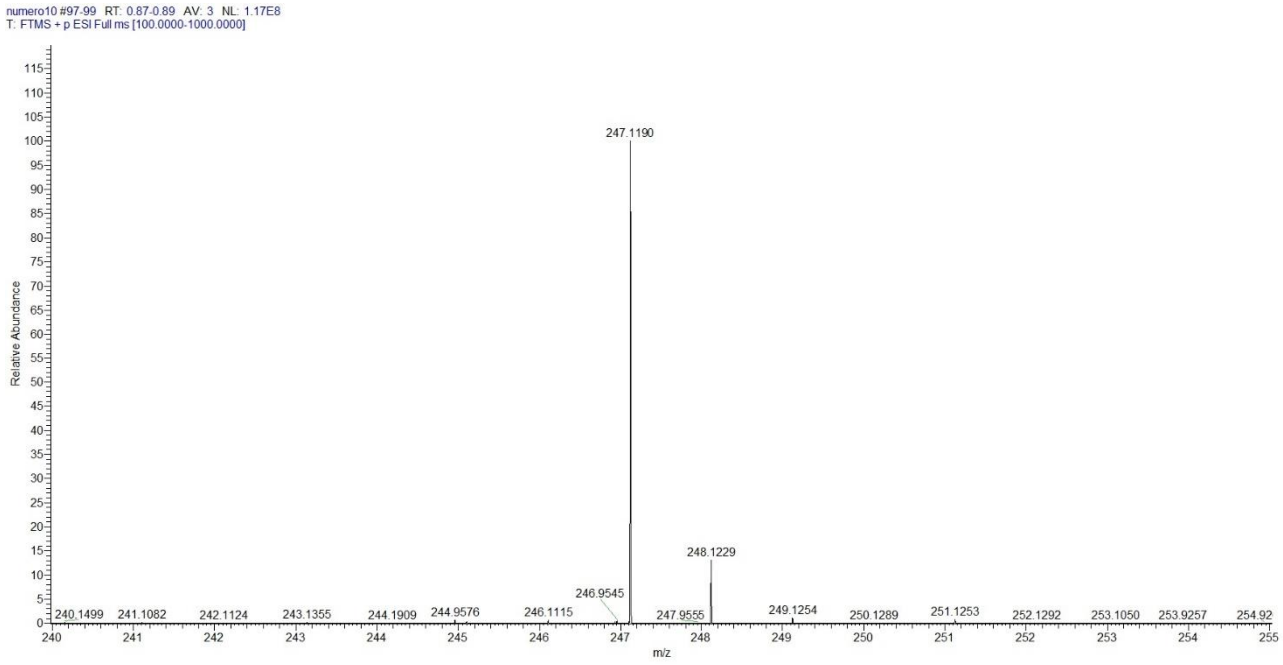


Figure S20. Fullscan analysis of compound **6**

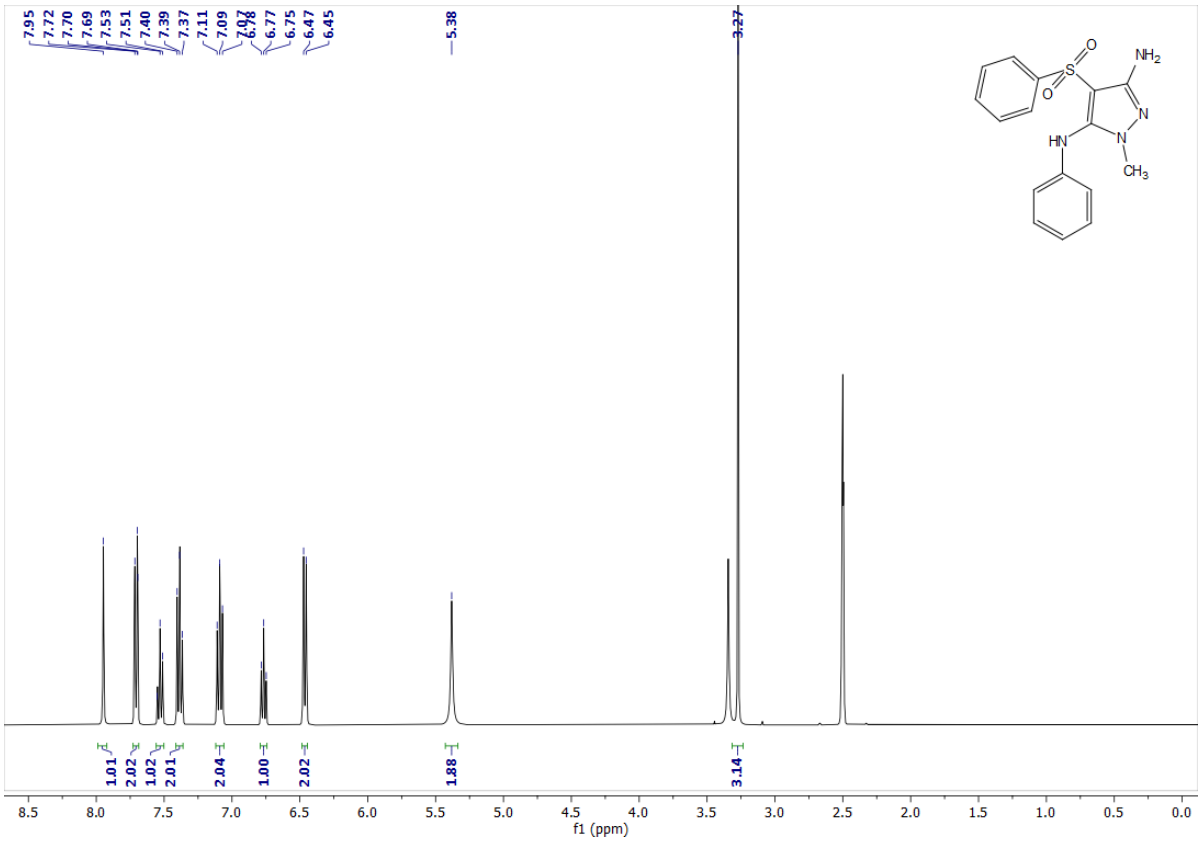


Figure S21. ^{1}H-NMR (400 MHz, d_6-DMSO) spectrum of compound **7**

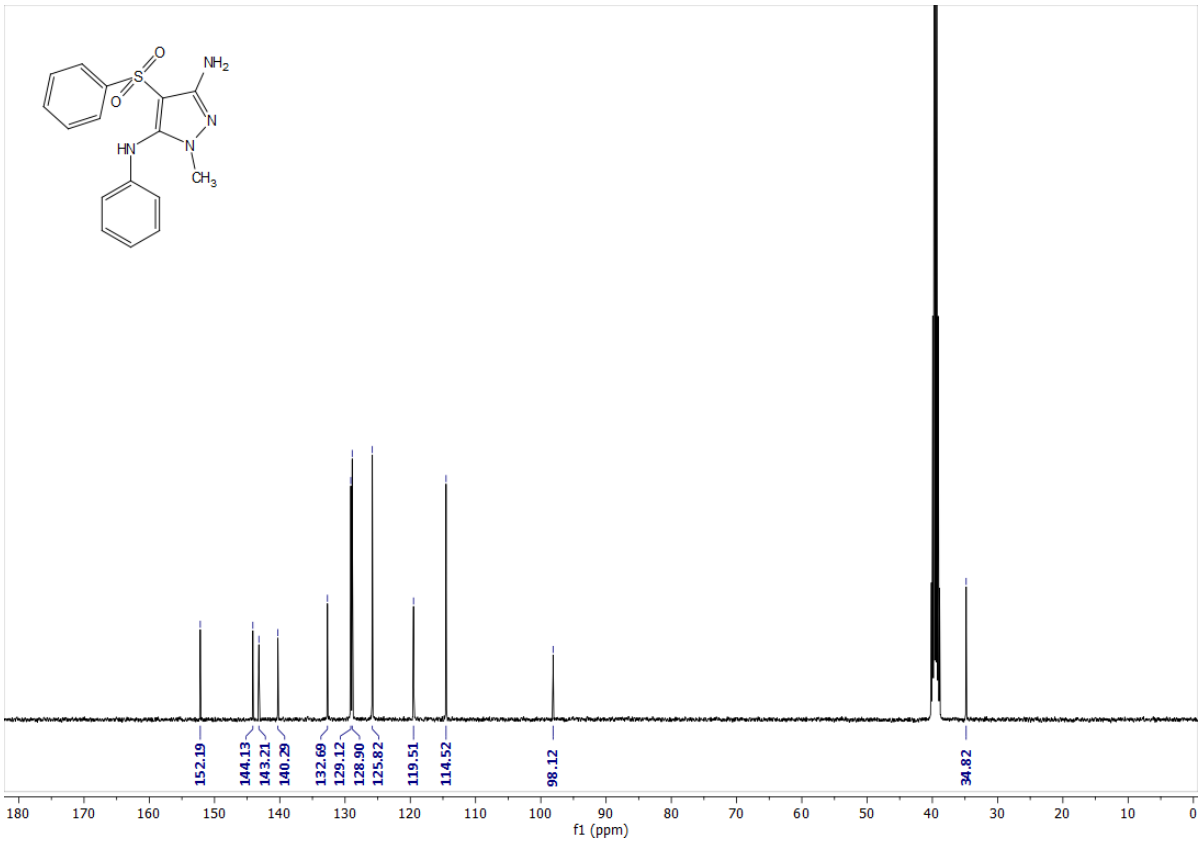


Figure S22. ^{13}C-NMR (101 MHz, d_6-DMSO) spectrum of compound **7**

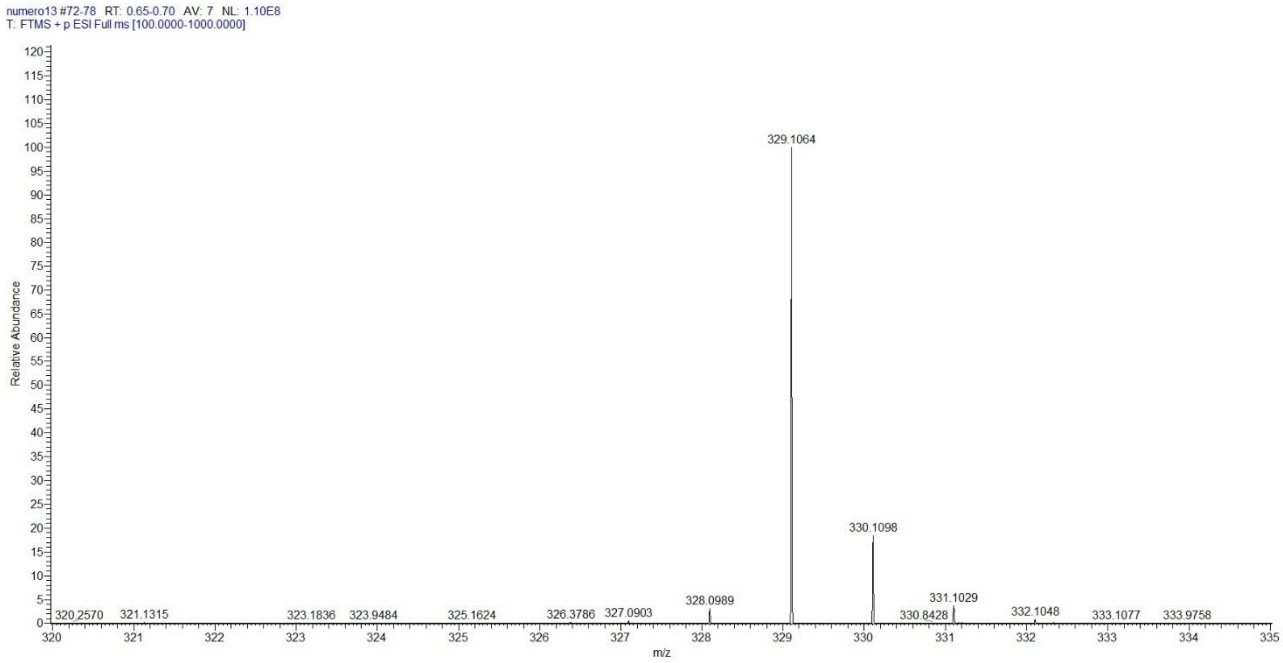


Figure S23. Fullscan analysis of compound **7**

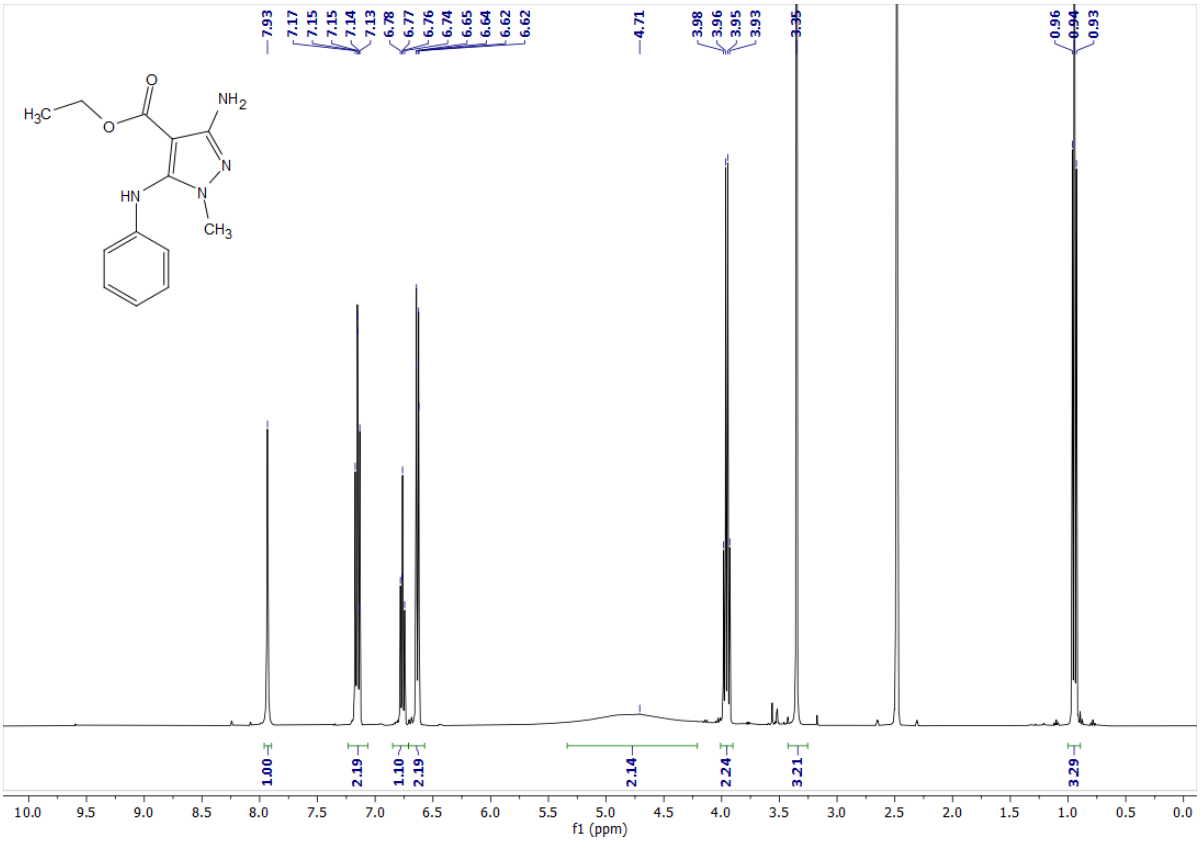


Figure S24. ^{1}H-NMR (400 MHz, d_6-DMSO) spectrum of compound **8a**

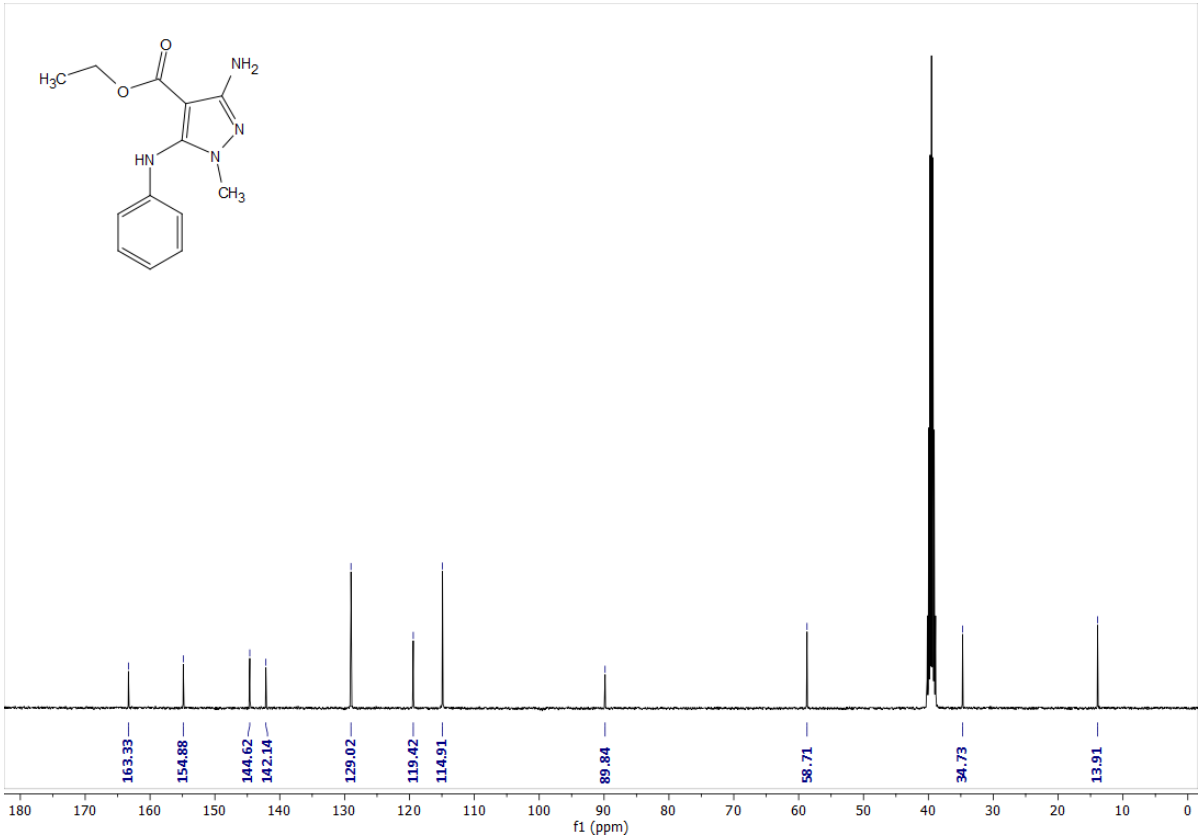


Figure S25. ^{13}C-NMR (101 MHz, d_6-DMSO) spectrum of compound **8a**

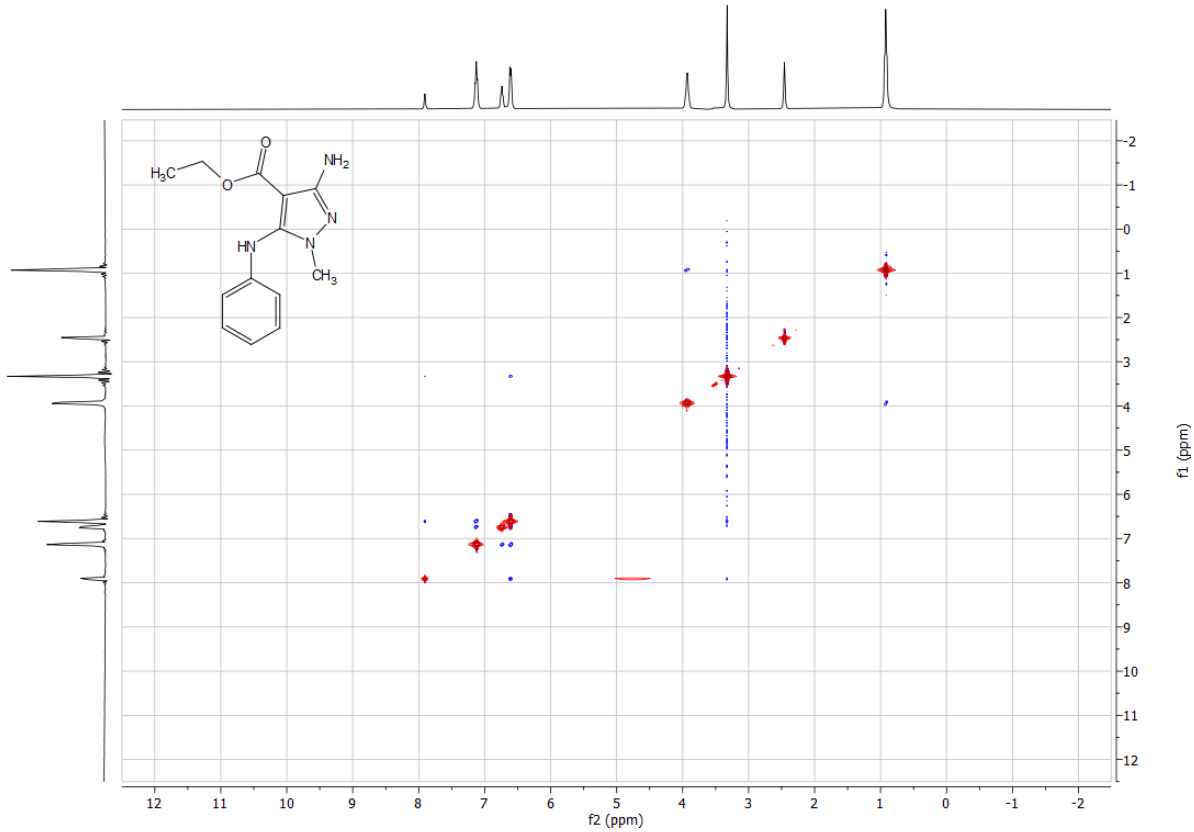


Figure S26. 2D NOESY (d_6-DMSO) spectrum of compound **8a**

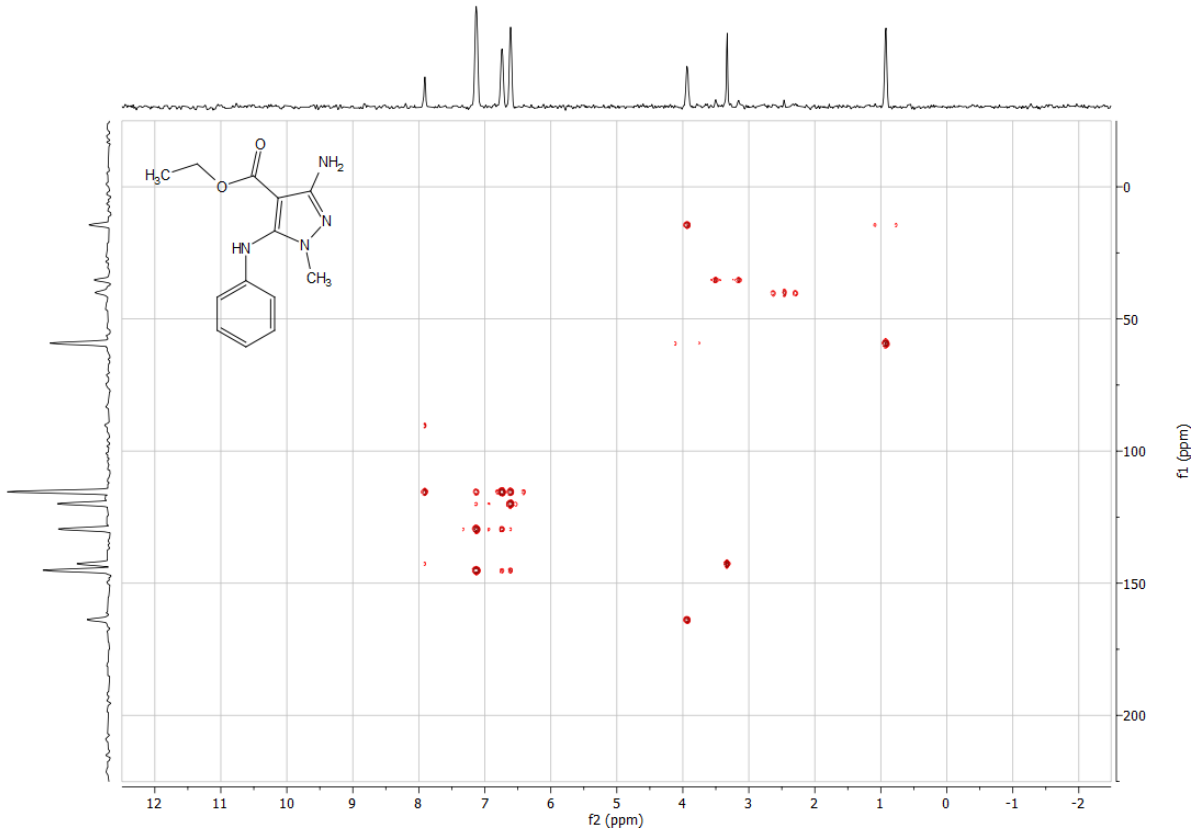


Figure S27. 2D HMBC (d_6-DMSO) spectrum of compound **8a**

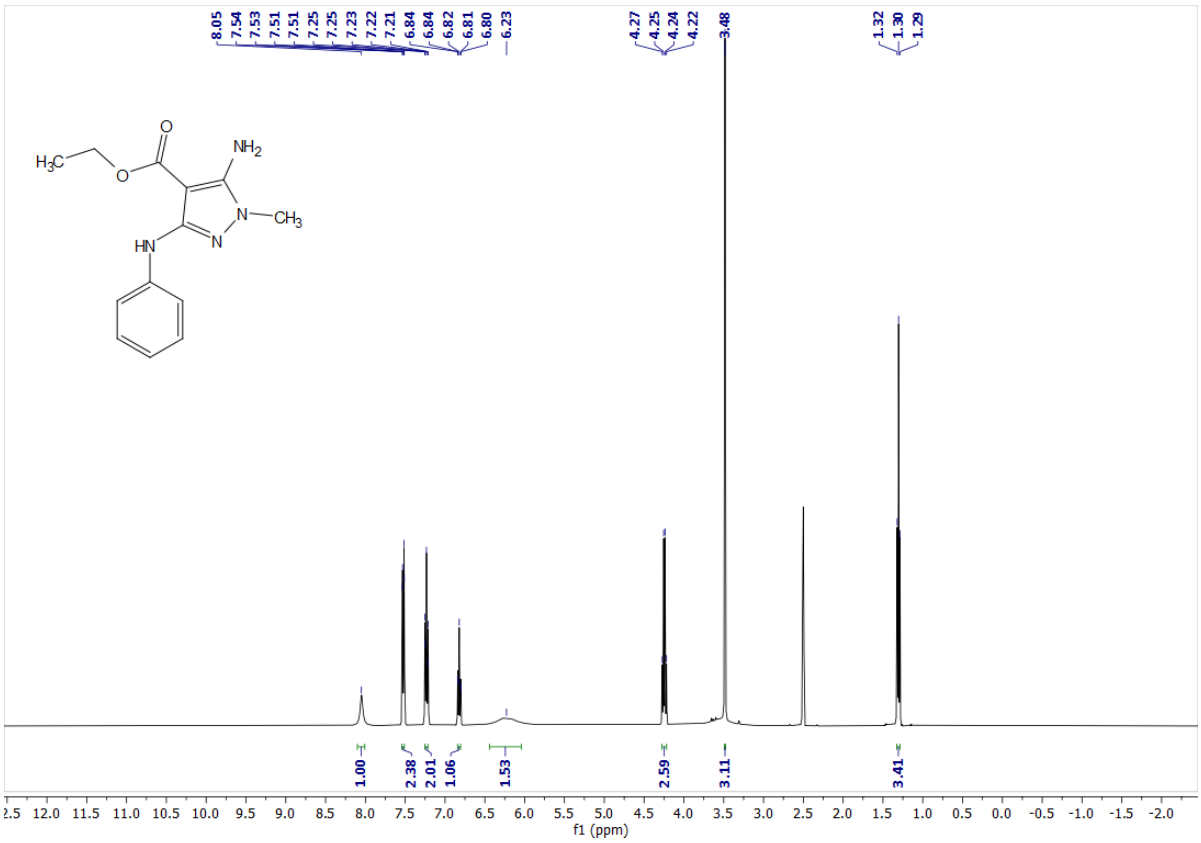


Figure S28. ^{1}H-NMR (400 MHz, d_6-DMSO) spectrum of compound **8b**

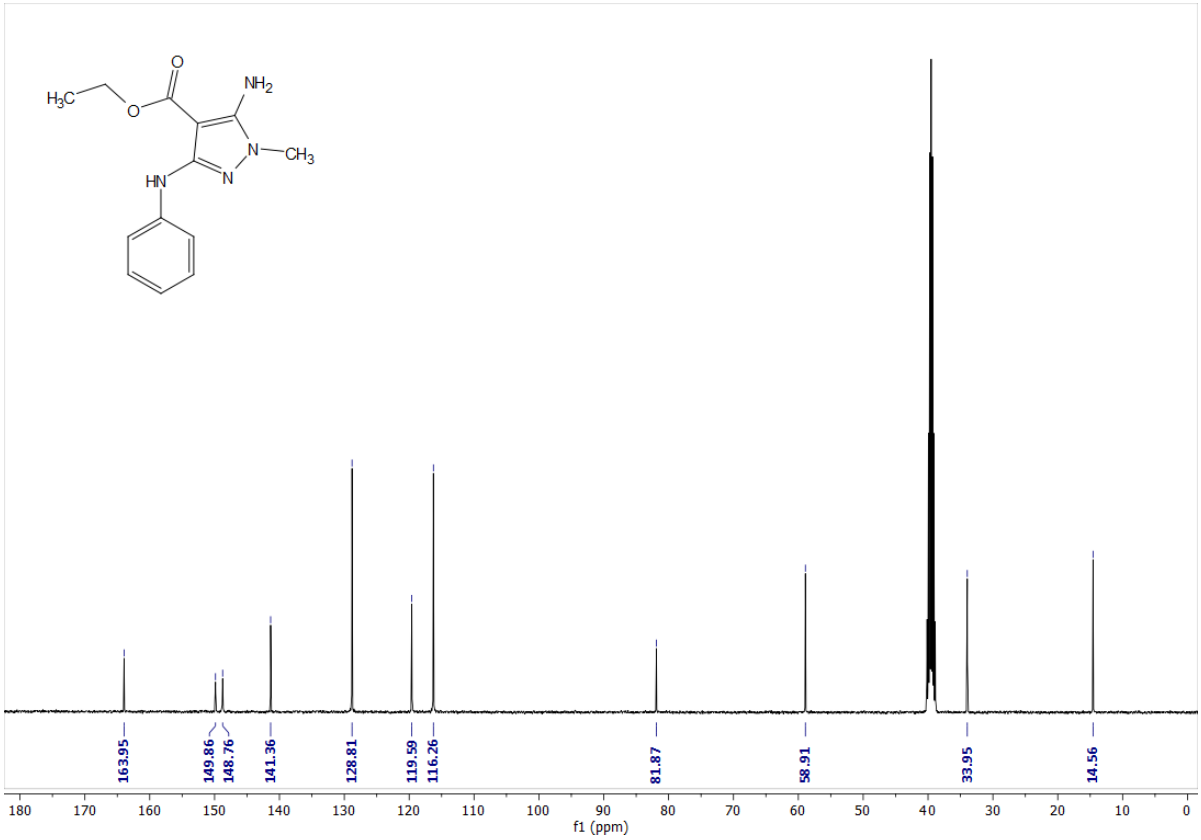


Figure S29. ^{13}C-NMR (101 MHz, d_6-DMSO) spectrum of compound **8b**

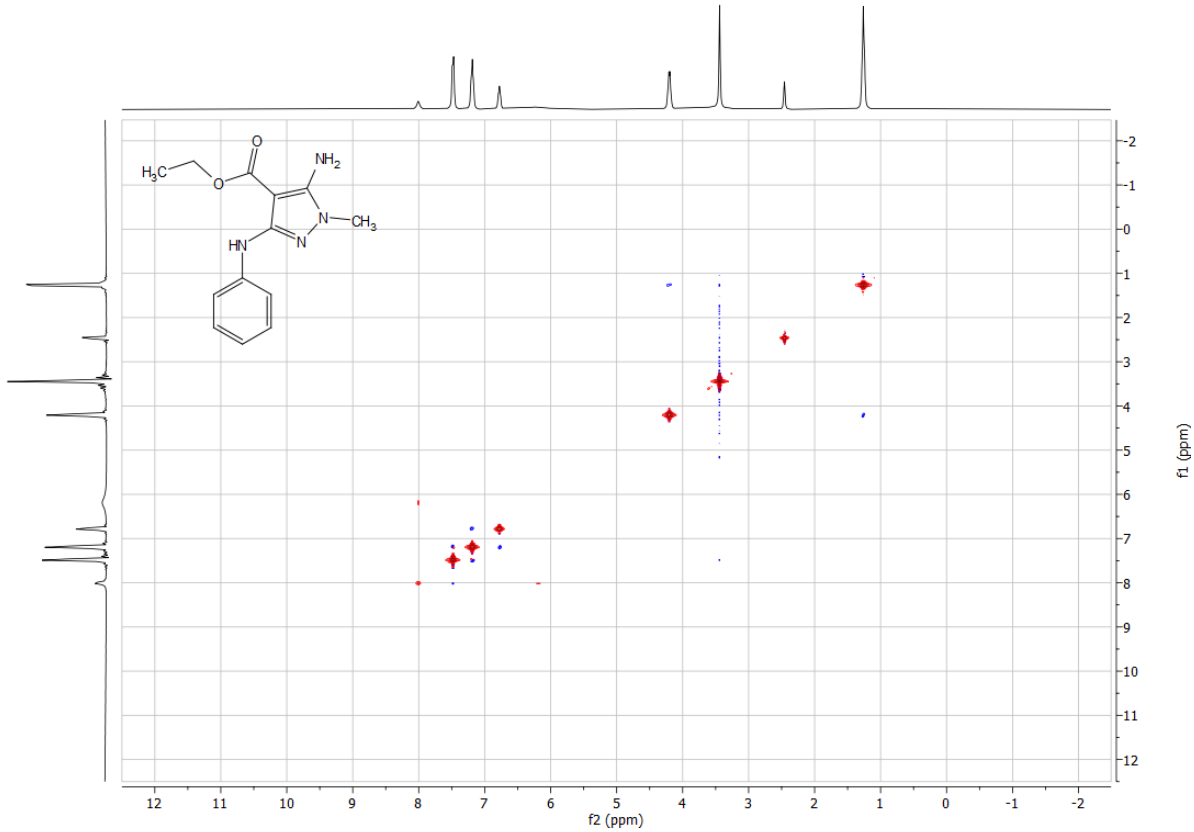


Figure S30. 2D NOESY (d_6-DMSO) spectrum of compound **8b**

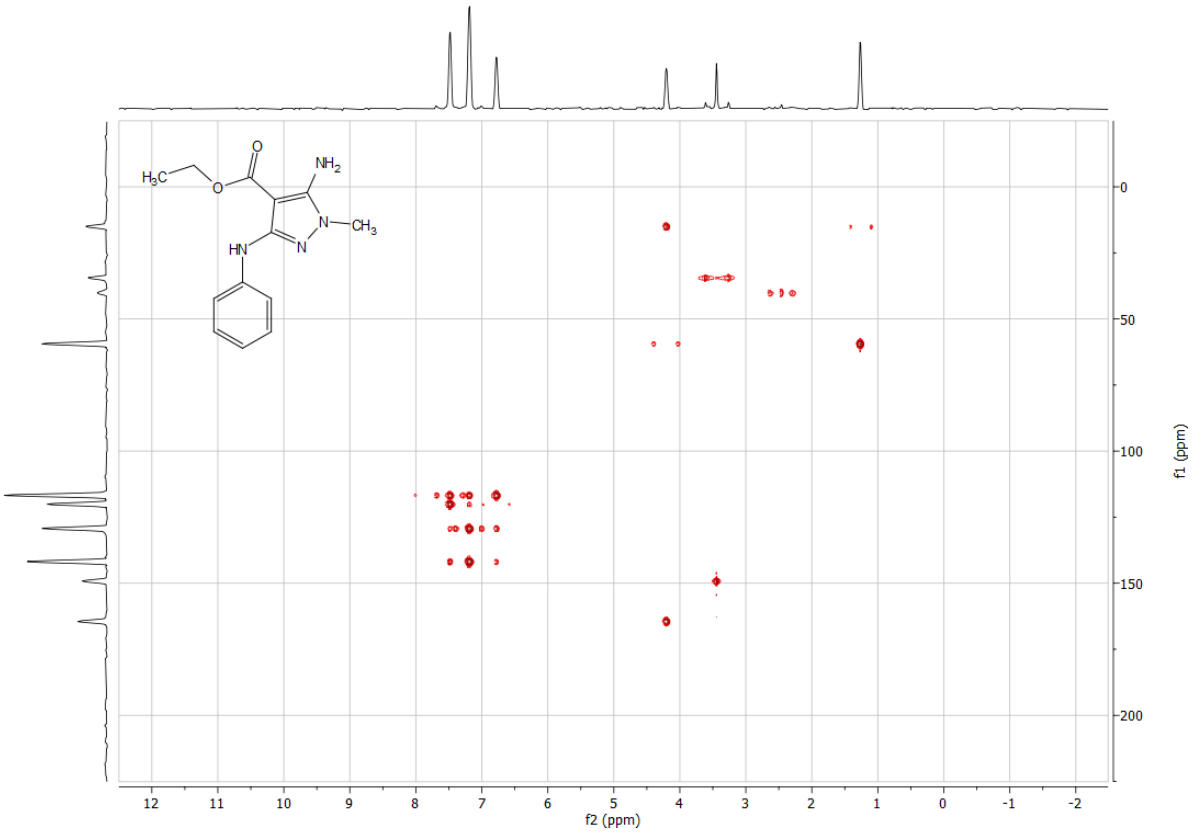


Figure S31. 2D HMBC (d_6-DMSO) spectrum of compound **8b**

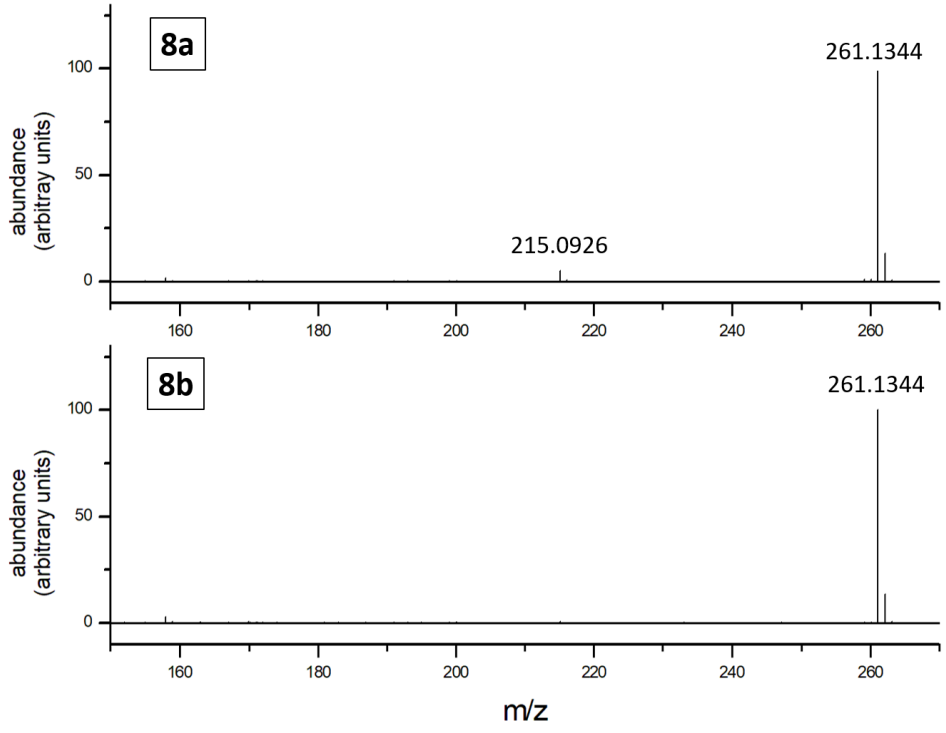


Figure S32. Fullscan analysis of isomers **8a** and **8b**

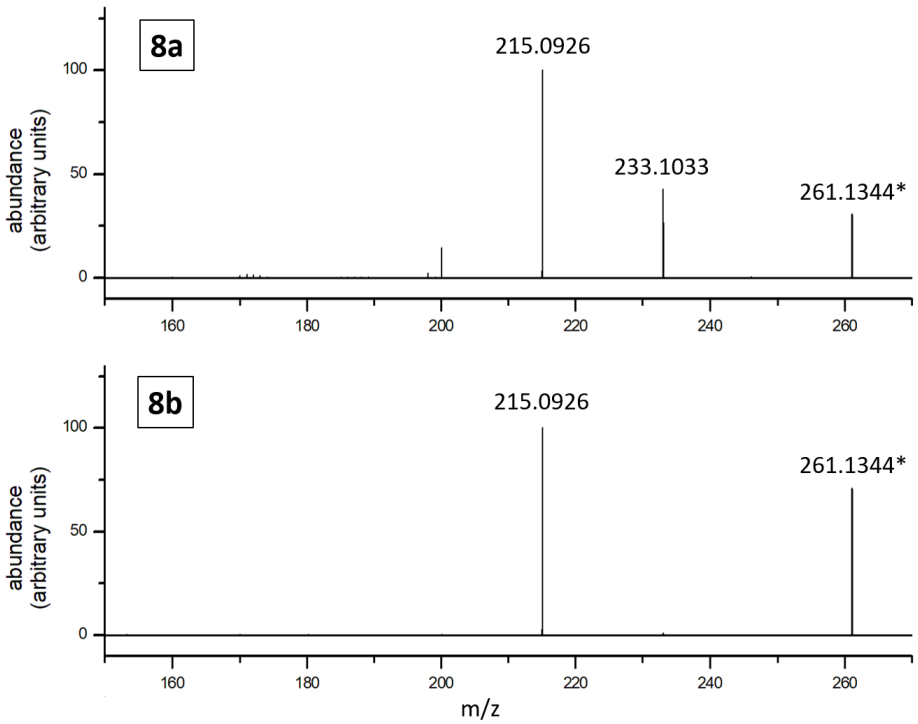


Figure S33. Fragmentation spectra of precursor ion m/z 261.1344 for isomers **8a** and **8b**. The precursor ion is marked by an asterisk. In sample **8a** a transient intermediate fragment (m/z 233.1033) is evidenced.

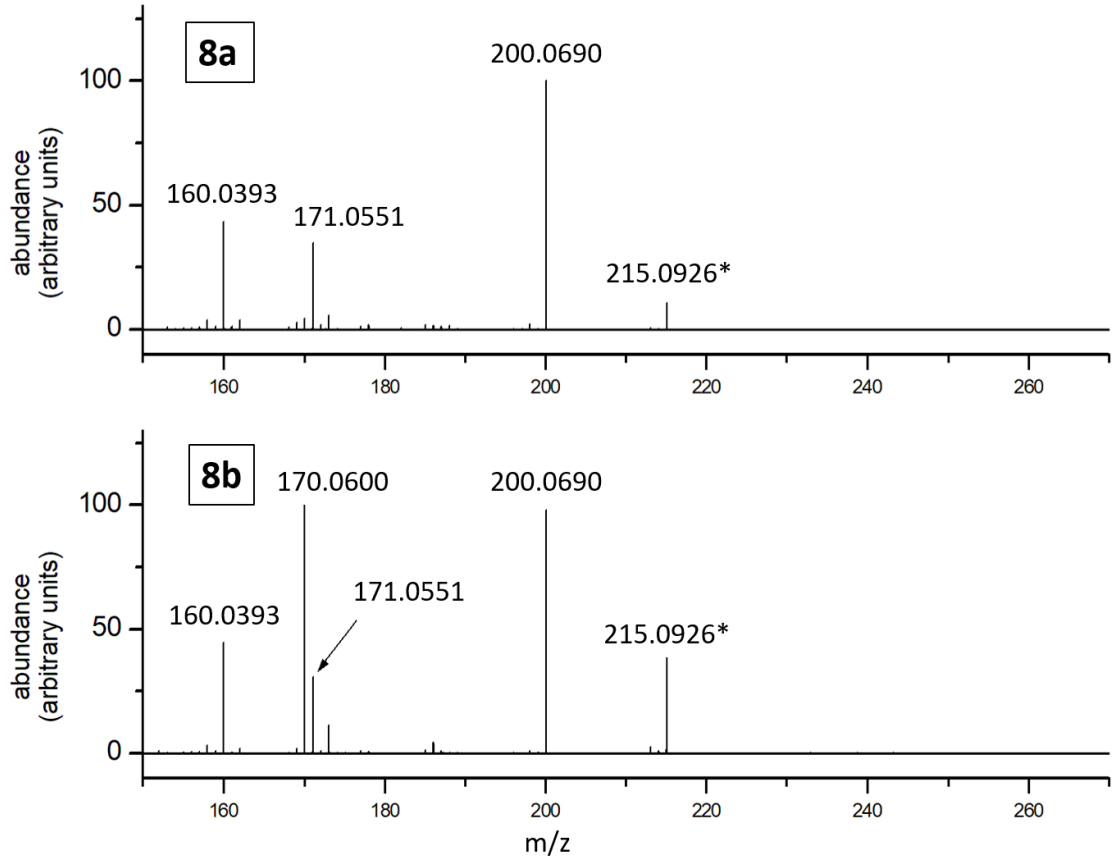


Figure S34. Fragmentation spectra of precursor ion m/z 215.0926 for isomers **8a** and **8b**. The precursor ion is marked by an asterisk. In sample **8b** the precursor ion 215.0926 evidenced an alternative fragmentation leading to the formation of fragment m/z 170.0600 which did not appear in **8a**.