Supplementary Materials

Structure-based design of potent pyrazolo[1,5-*a*]pyrimidine CDK4/6 inhibitors: Biological evaluation and computational validation

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Content

Docking Studies

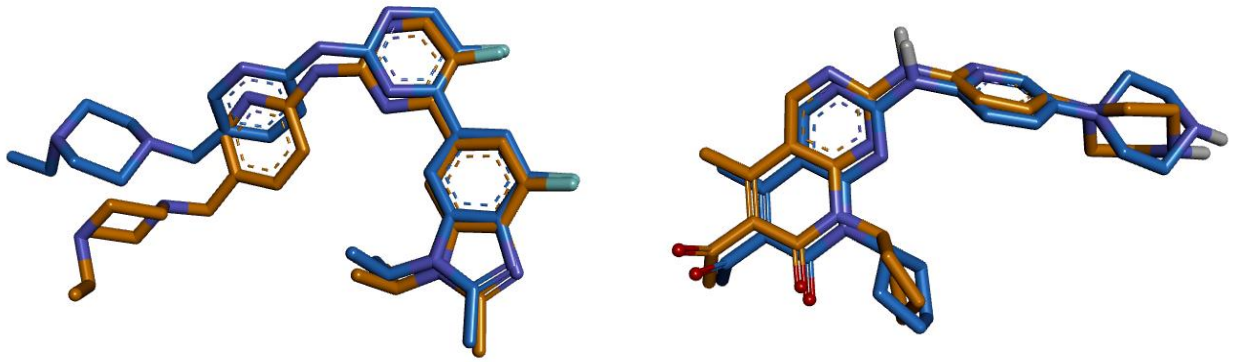

Figure S1. Docking protocol validation for CDK4 and CDK6. Superposition of the co-crystallized ligand (**orange**) and the redocked pose (**blue**) within the active site of CDK4 (**left**) and CDK6 (**right**), demonstrating the reliability of the applied docking protocol through the close overlap of binding conformations.

^{1}HNMR and ^{13}CNMR Spectra

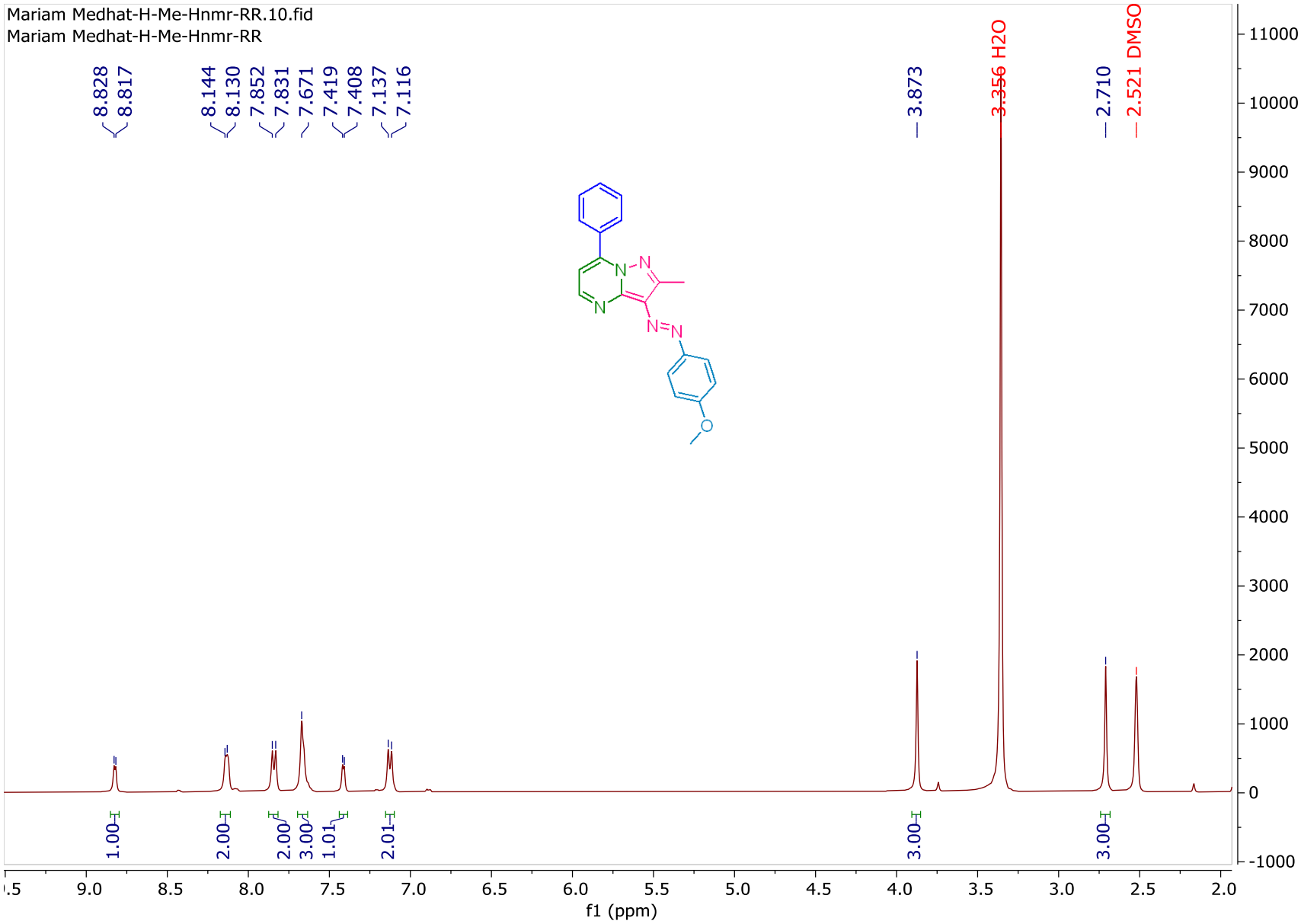

Figure S2. ^{1}H NMR of compound 19a

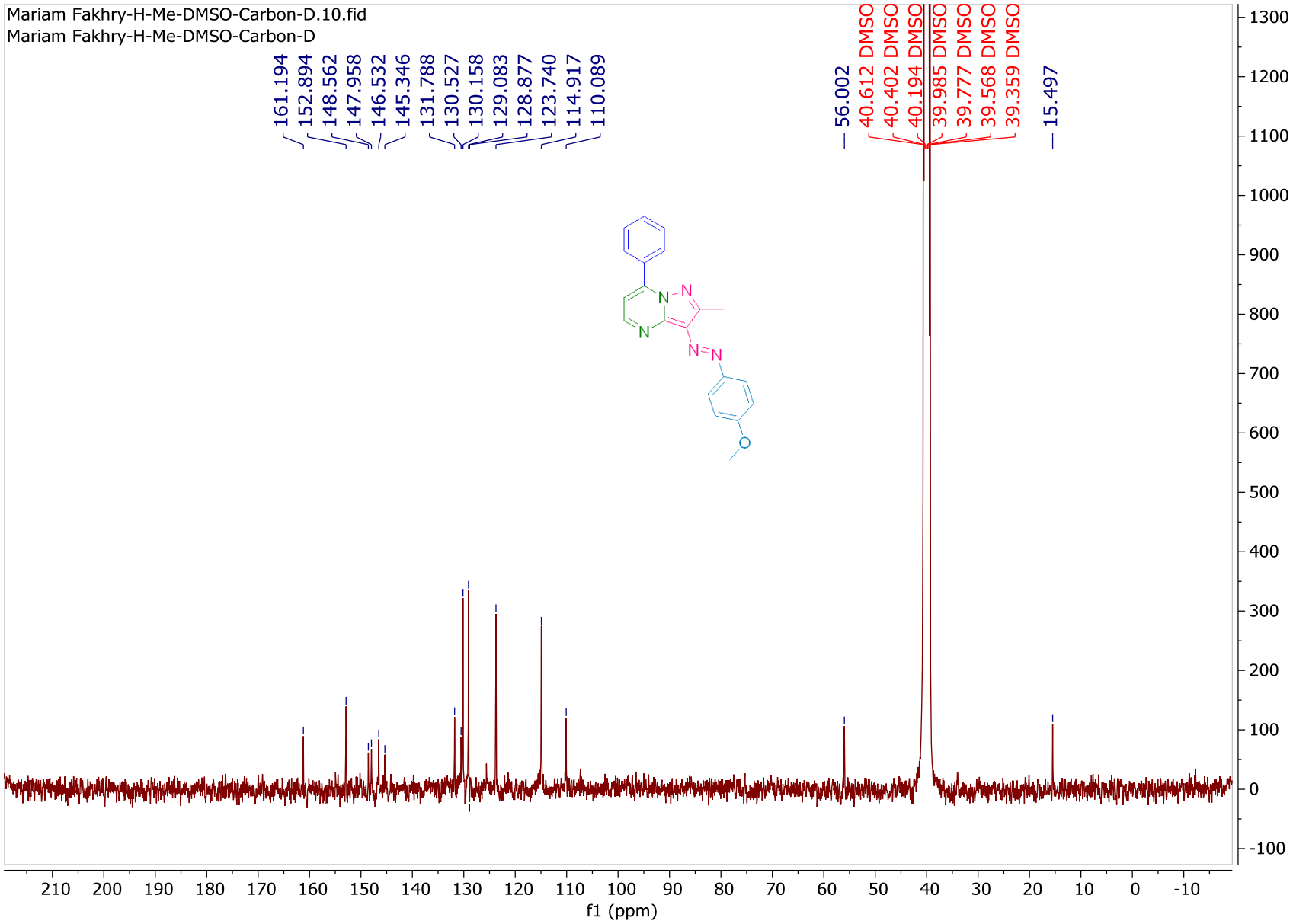

Figure S3. ^{13}C NMR of compound 19a

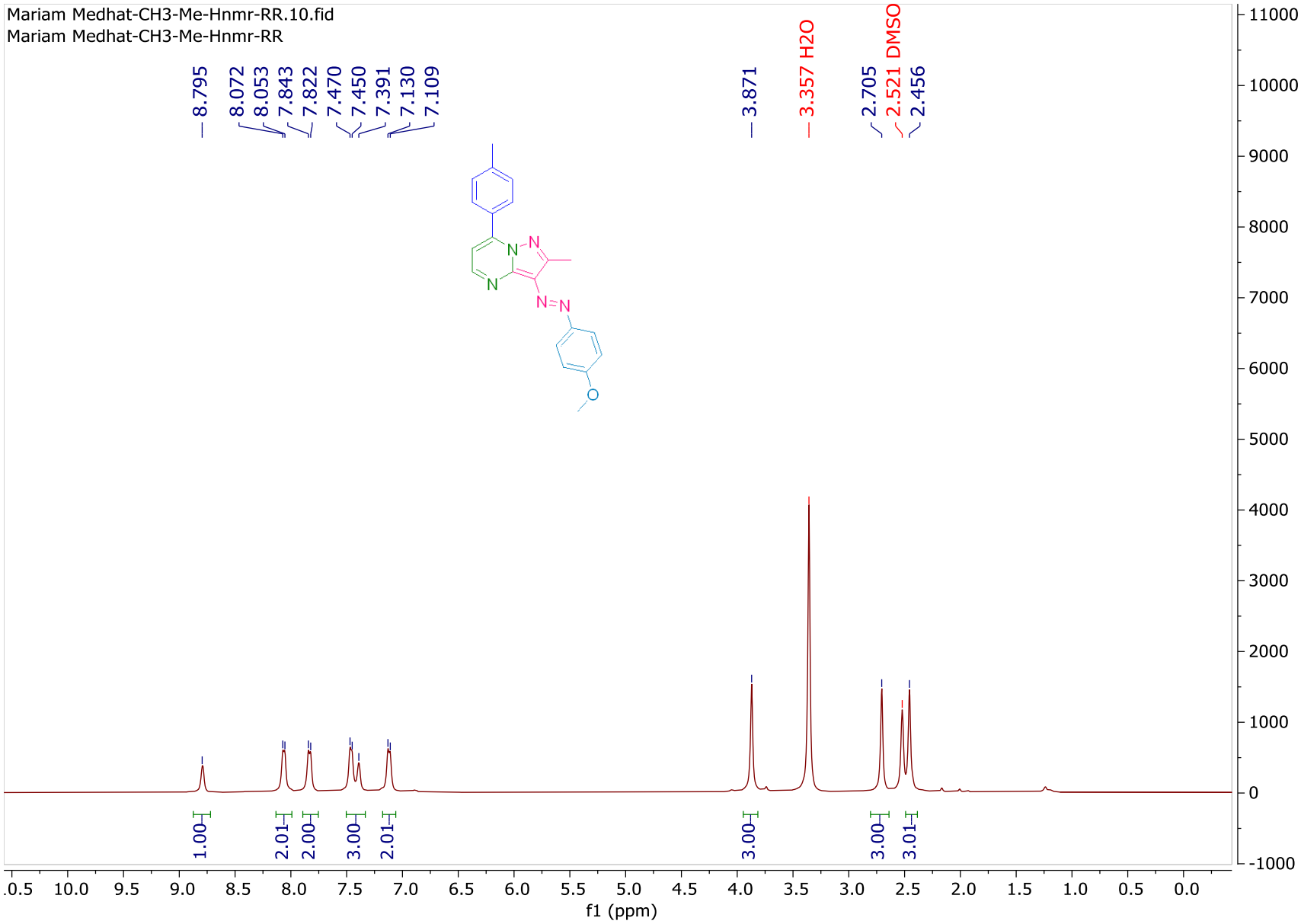

Figure S4. ^{1}H NMR of compound 19b

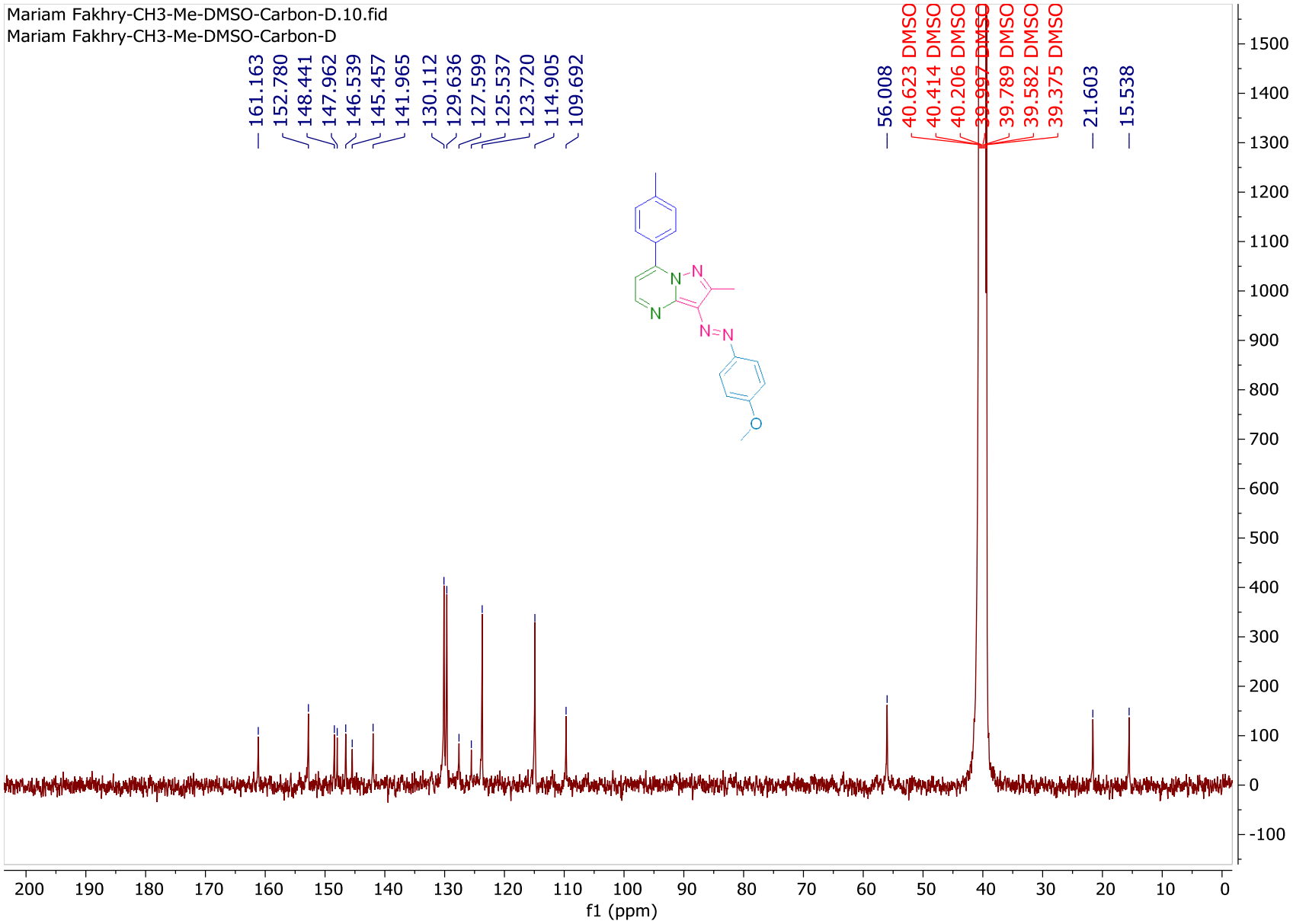

Figure S5. ^{13}C NMR of compound 19b

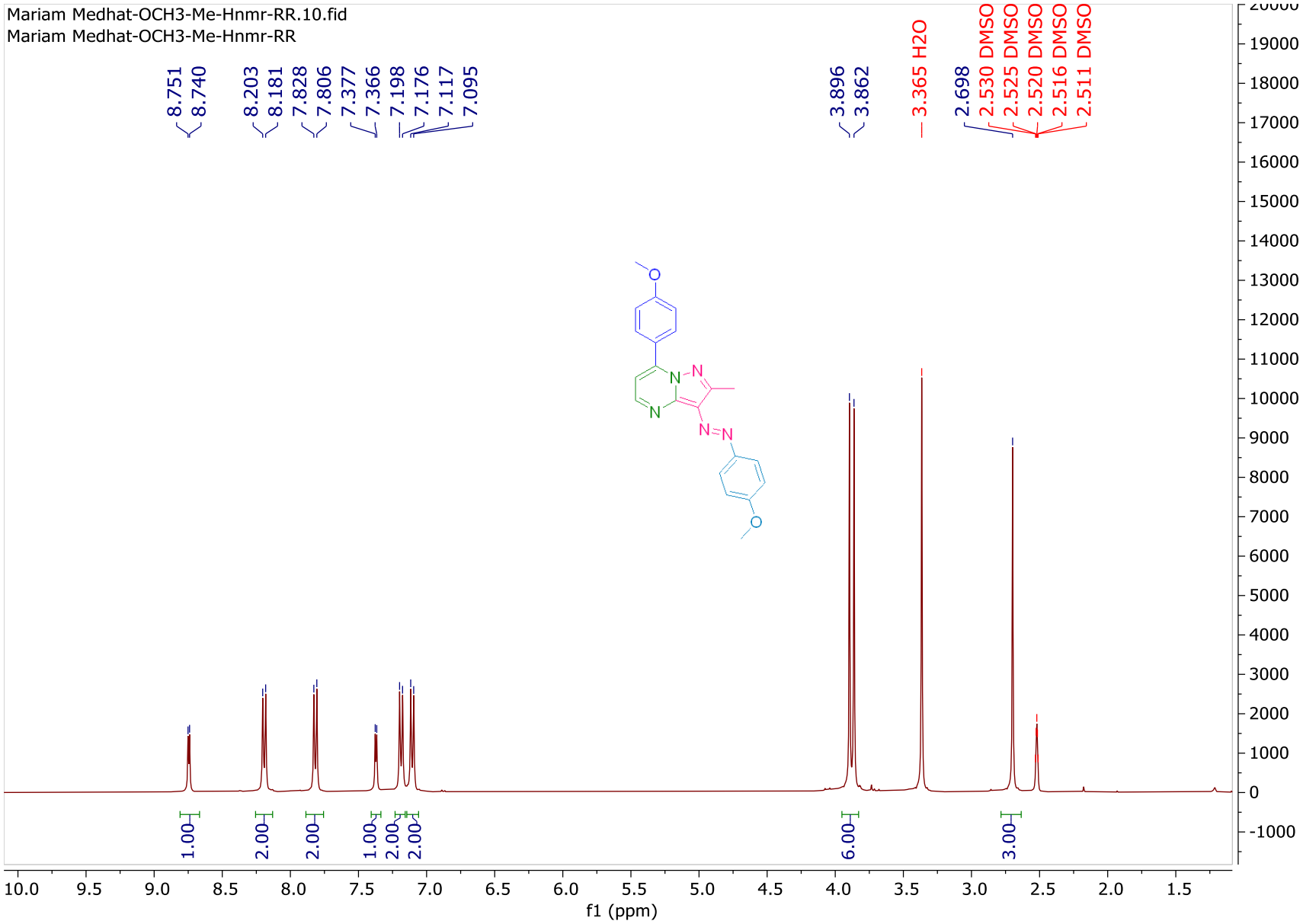

Figure S6. ^{1}H NMR of compound 19c

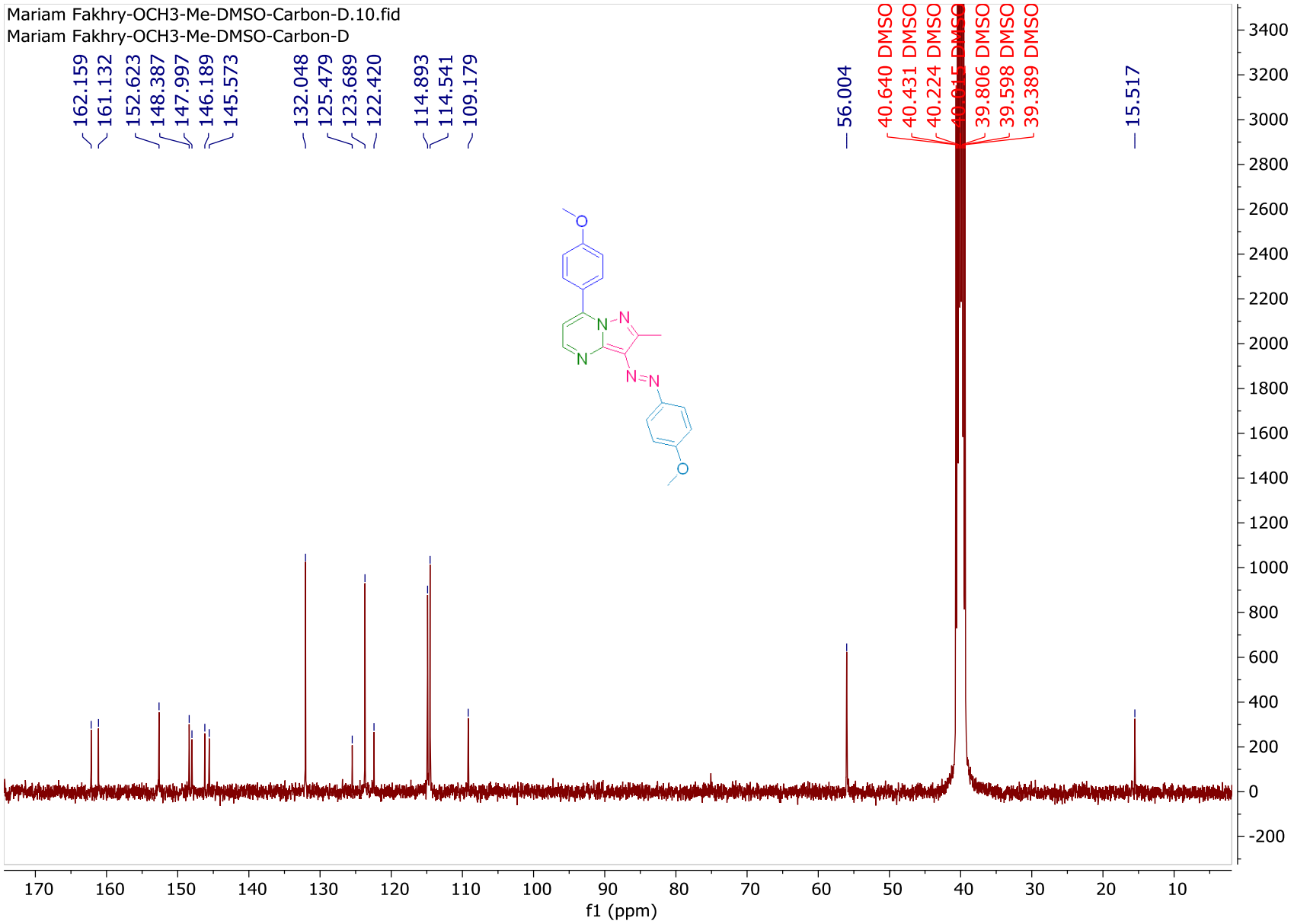

Figure S7. ^{13}C NMR of compound 19c

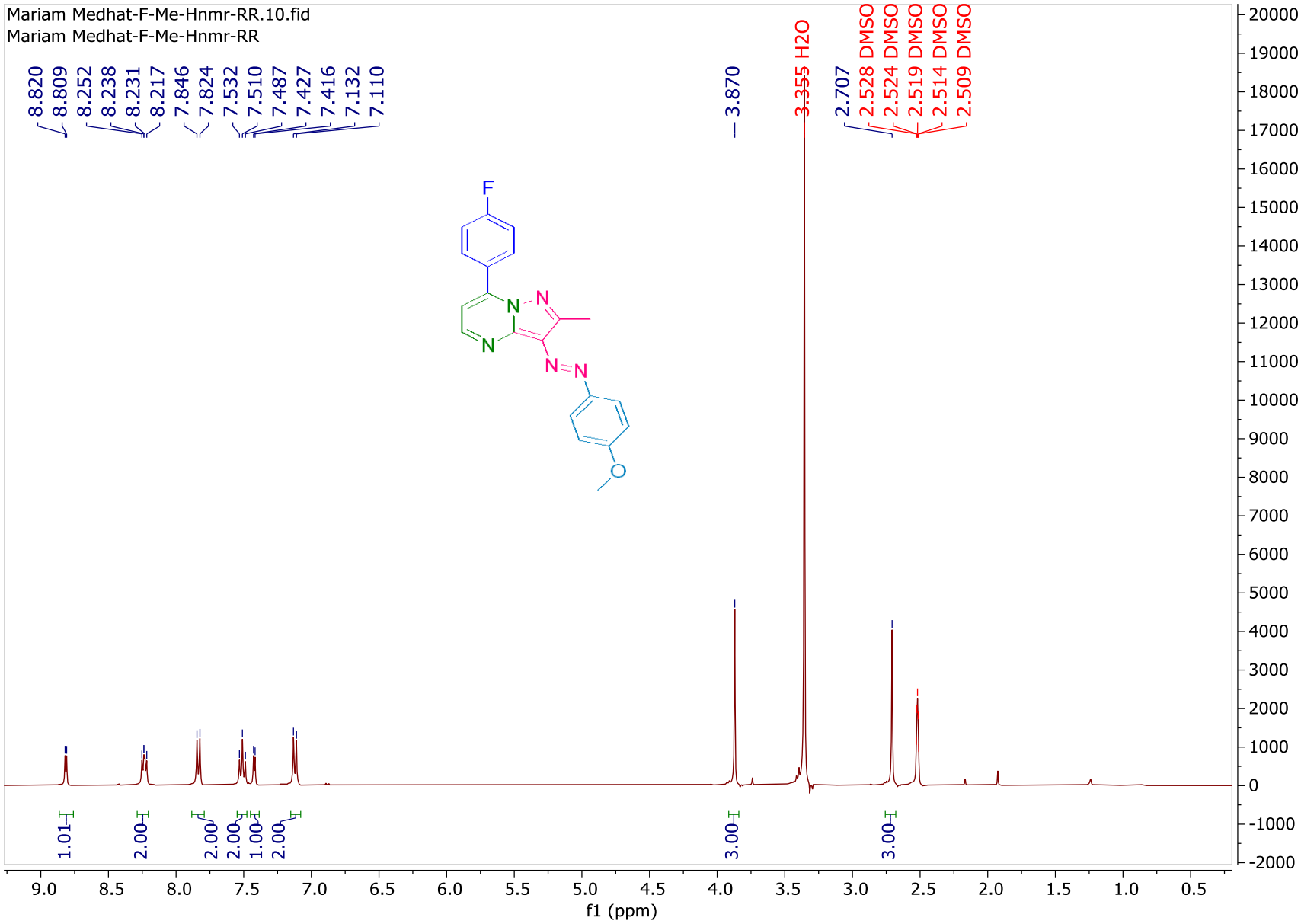

Figure S8. ^{1}H NMR of compound 19d

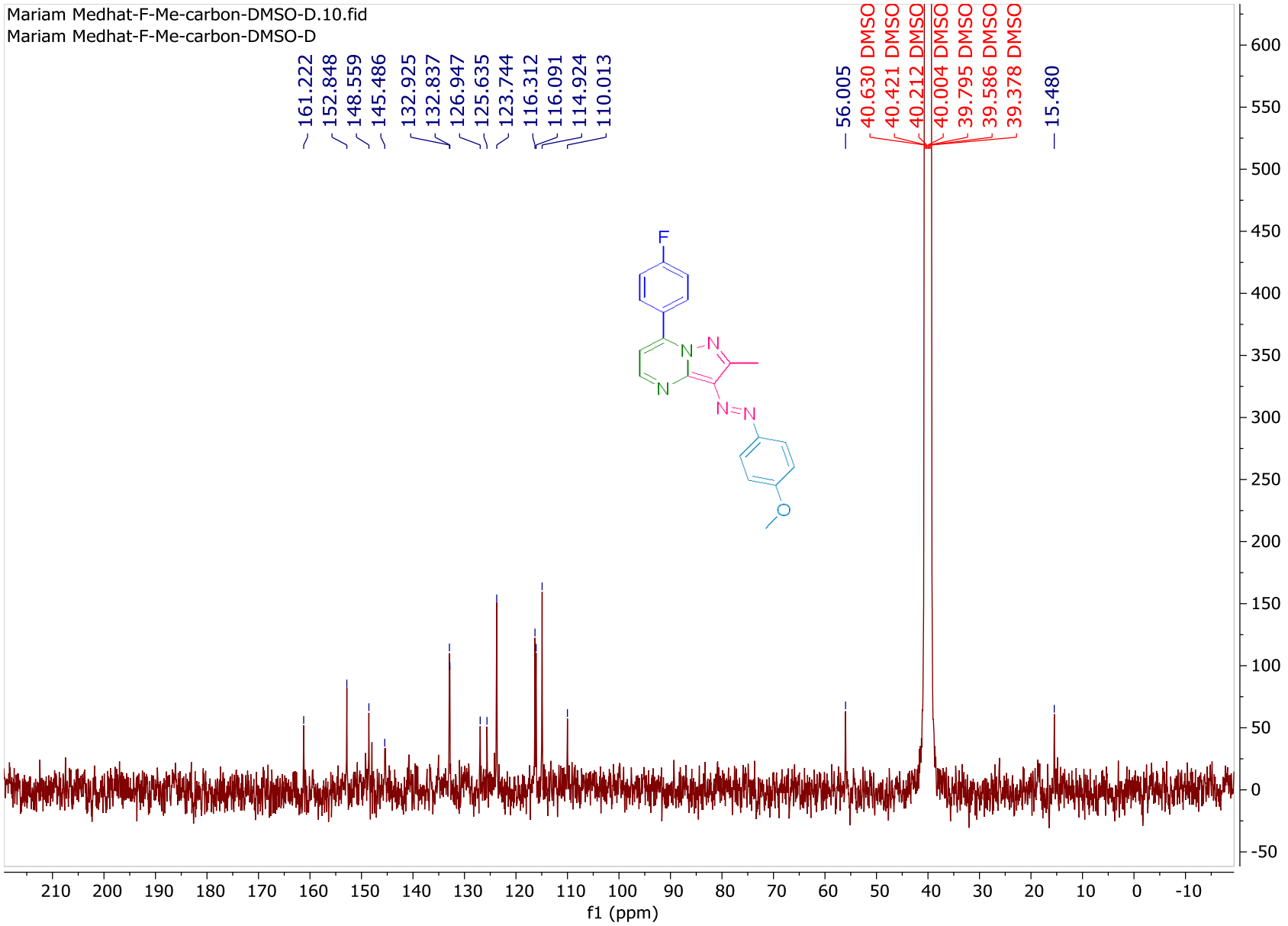

Figure S9. ^{13}C NMR of compound 19d

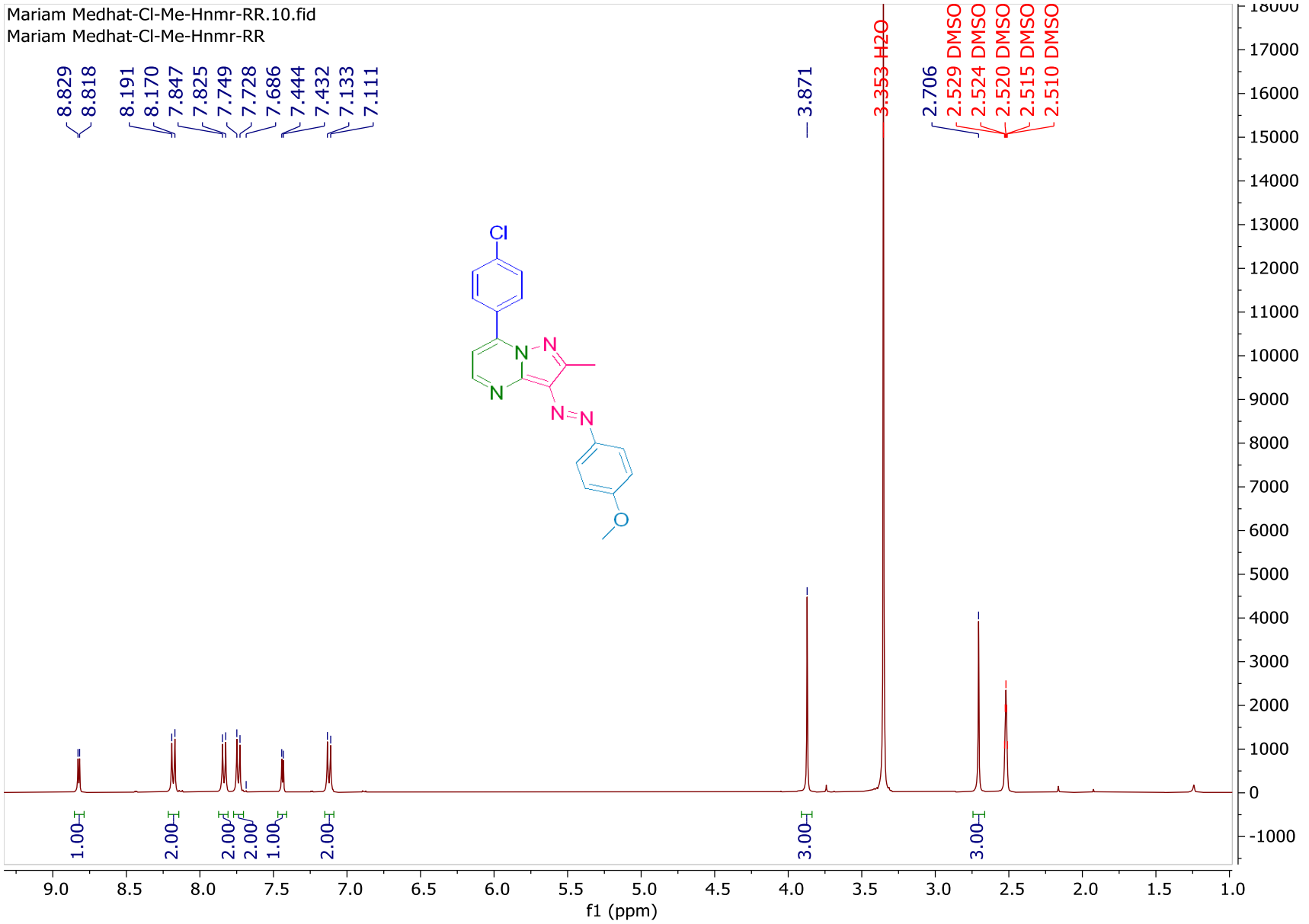

Figure S10. ^{1}H NMR of compound 19e

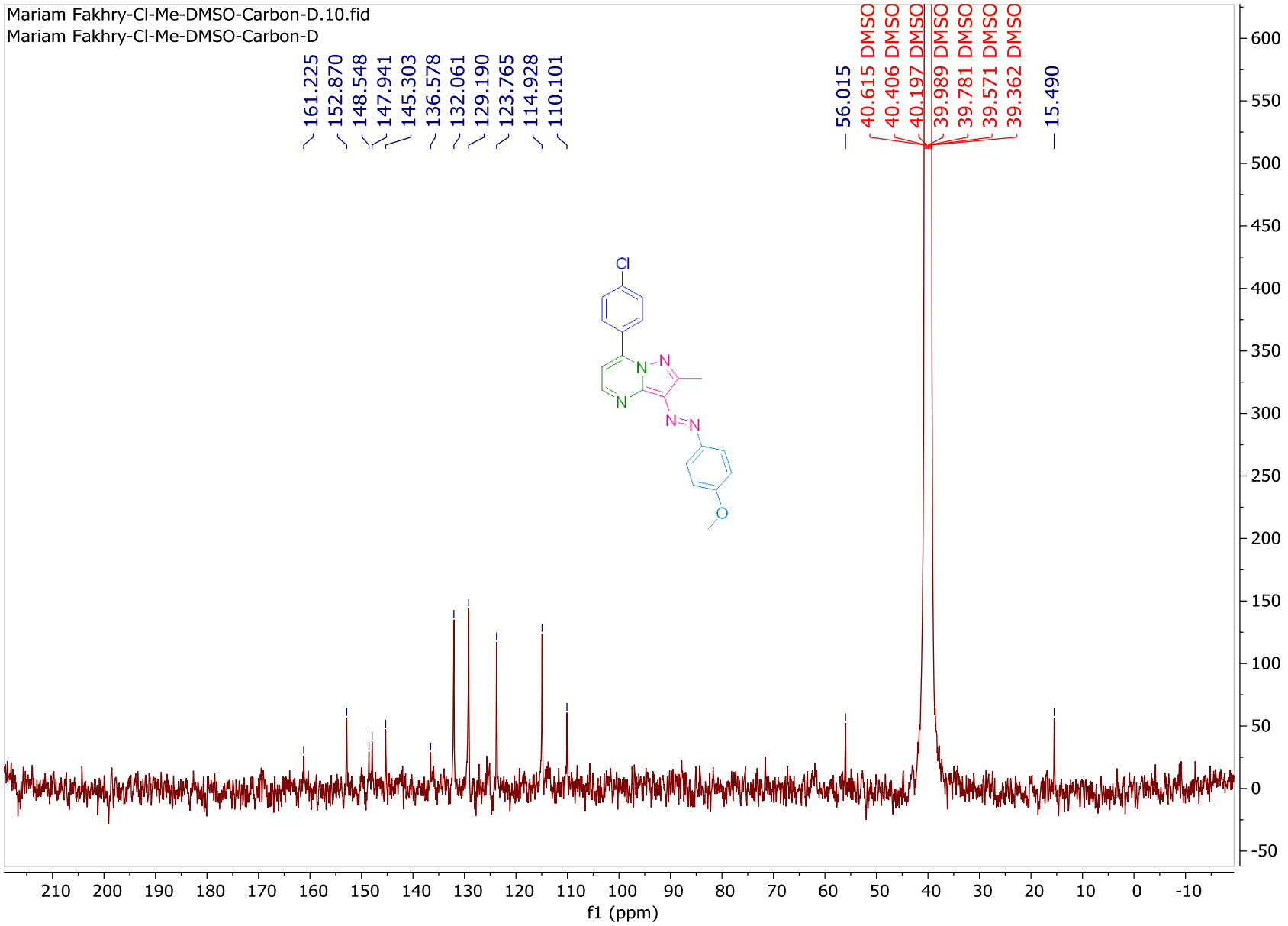

Figure S11. ^{13}C NMR of compound 19e

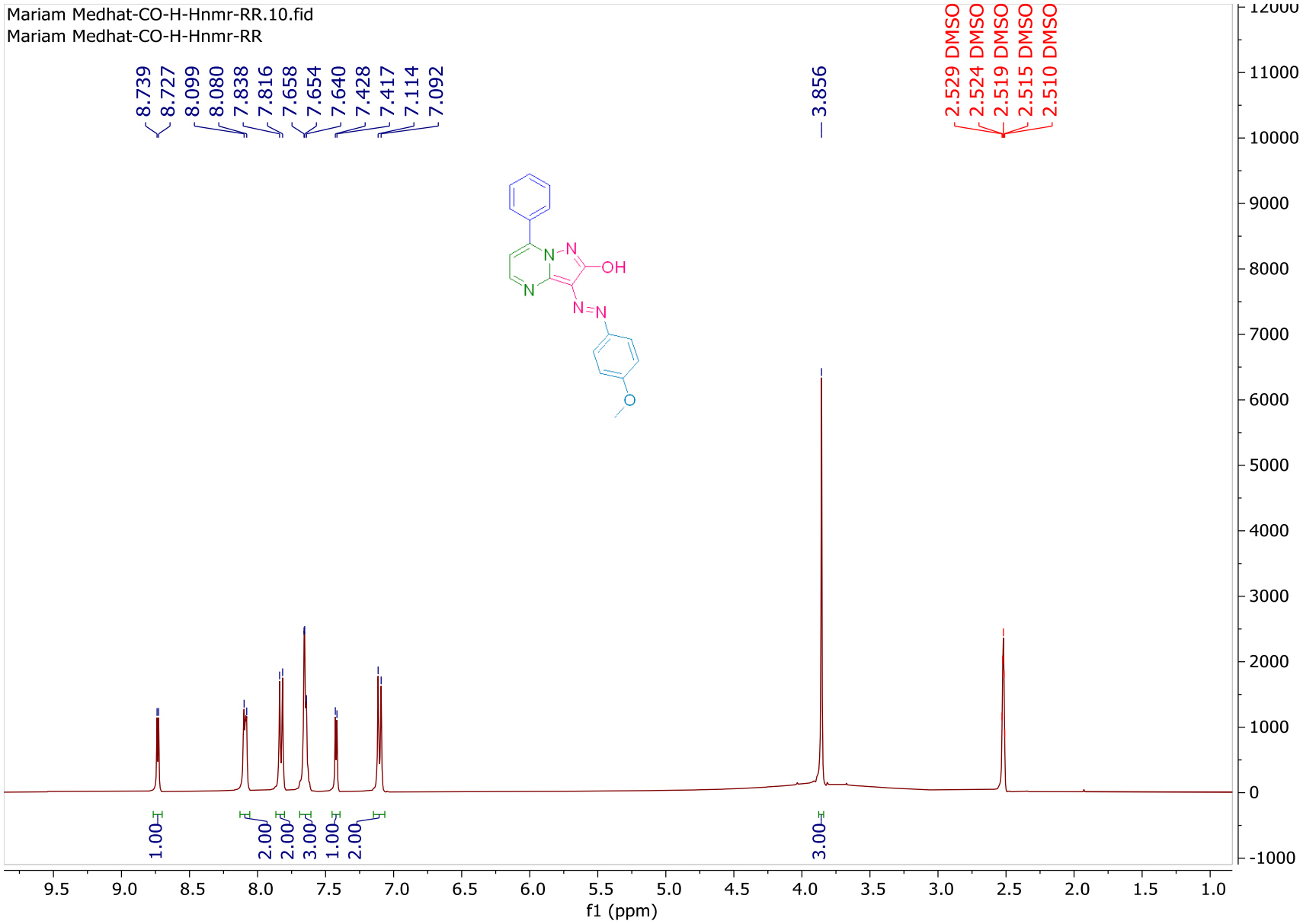

Figure S12. ^{1}H NMR of compound 19f

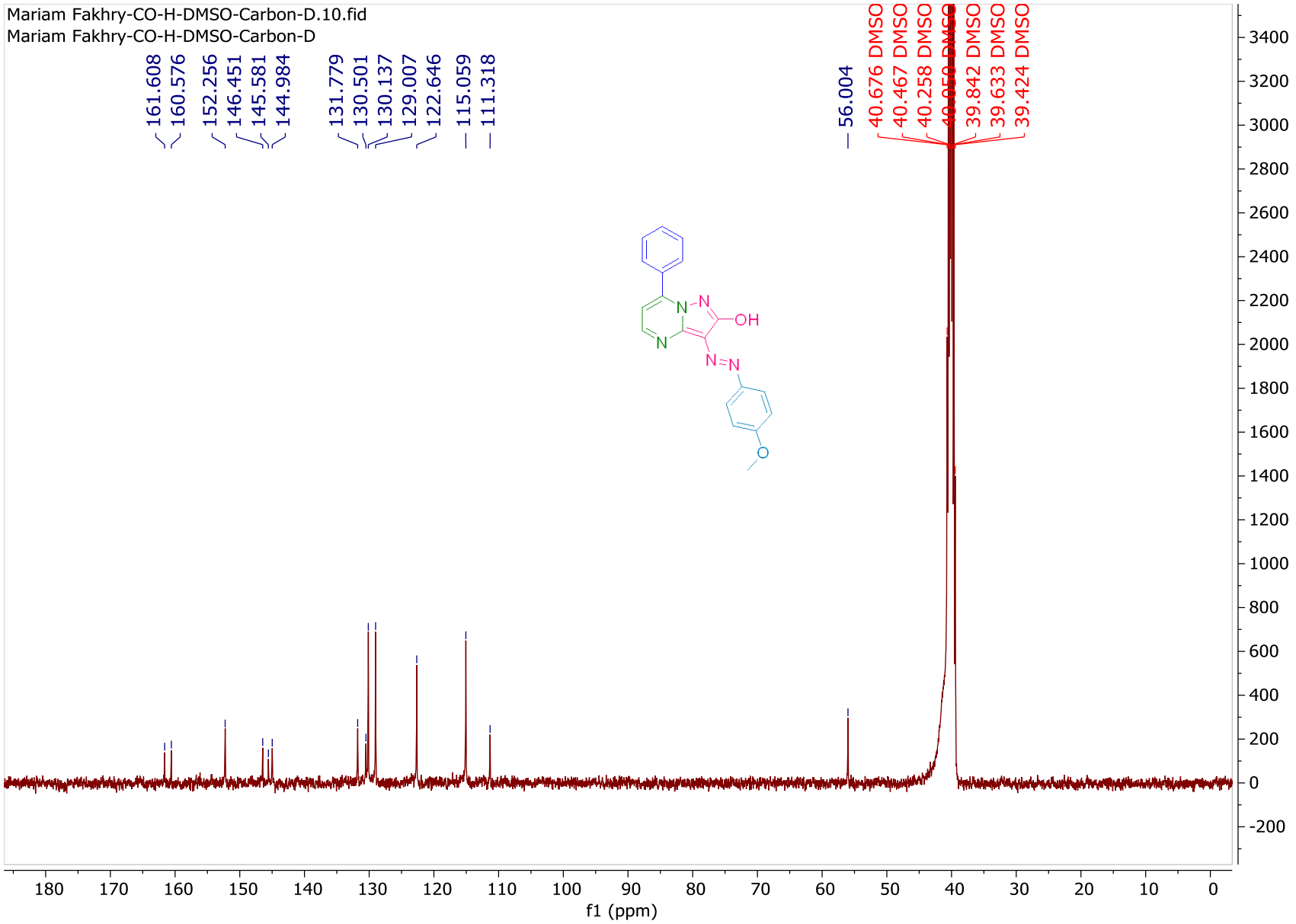

Figure S13. ^{13}C NMR of compound 19f

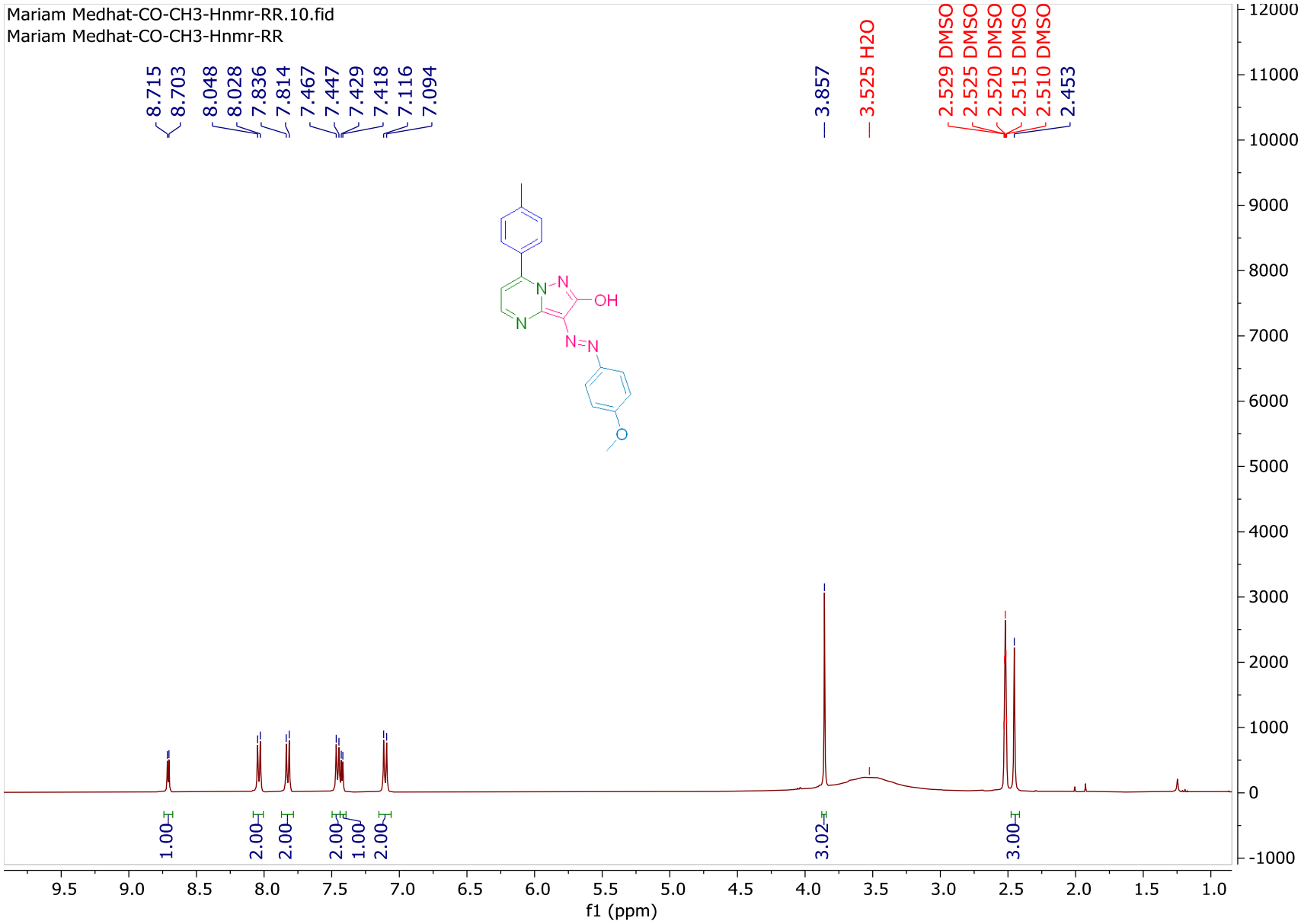

Figure S14. ^{1}H NMR of compound 19g

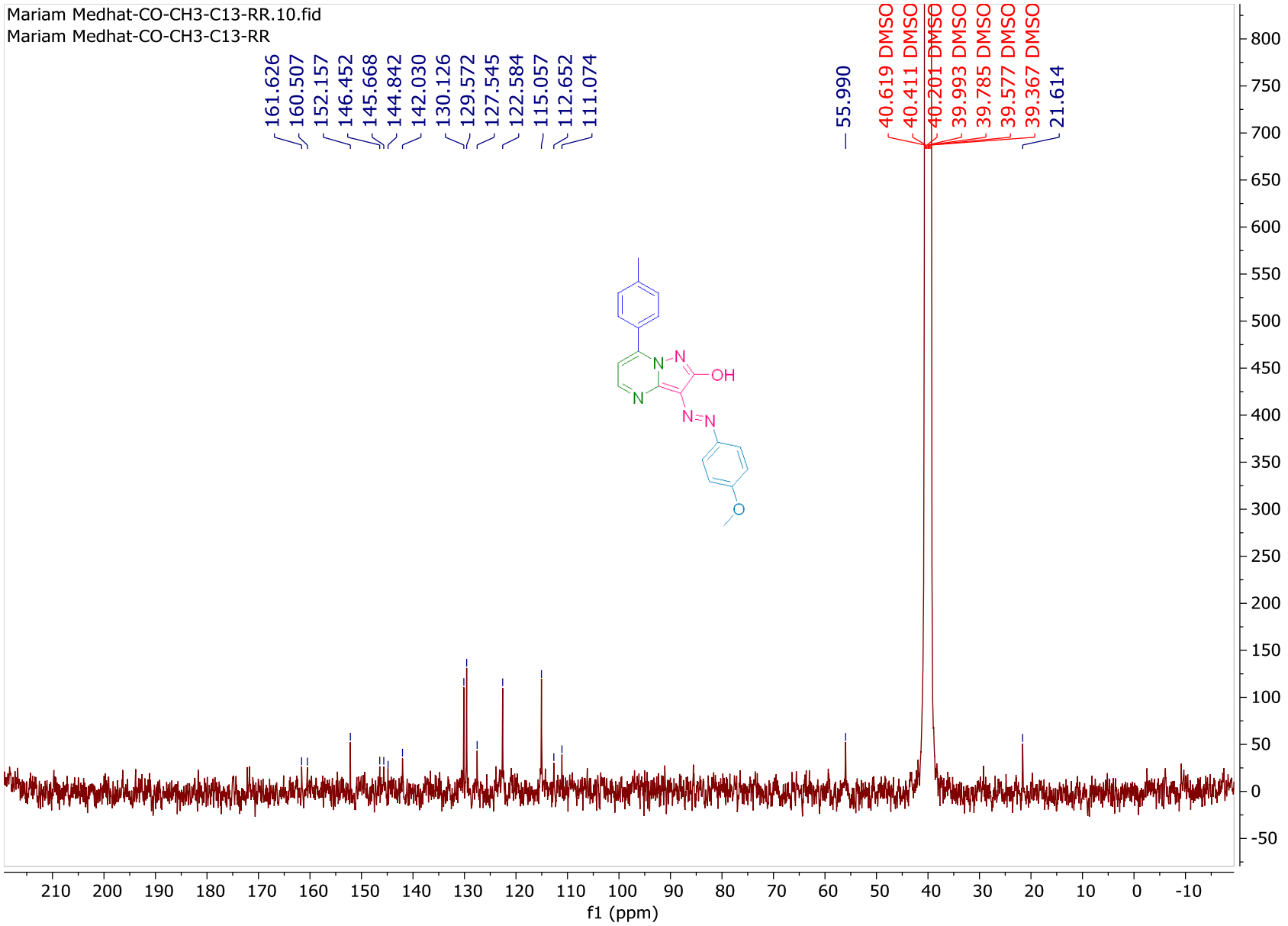

Figure S15. ^{13}C NMR of compound 19g

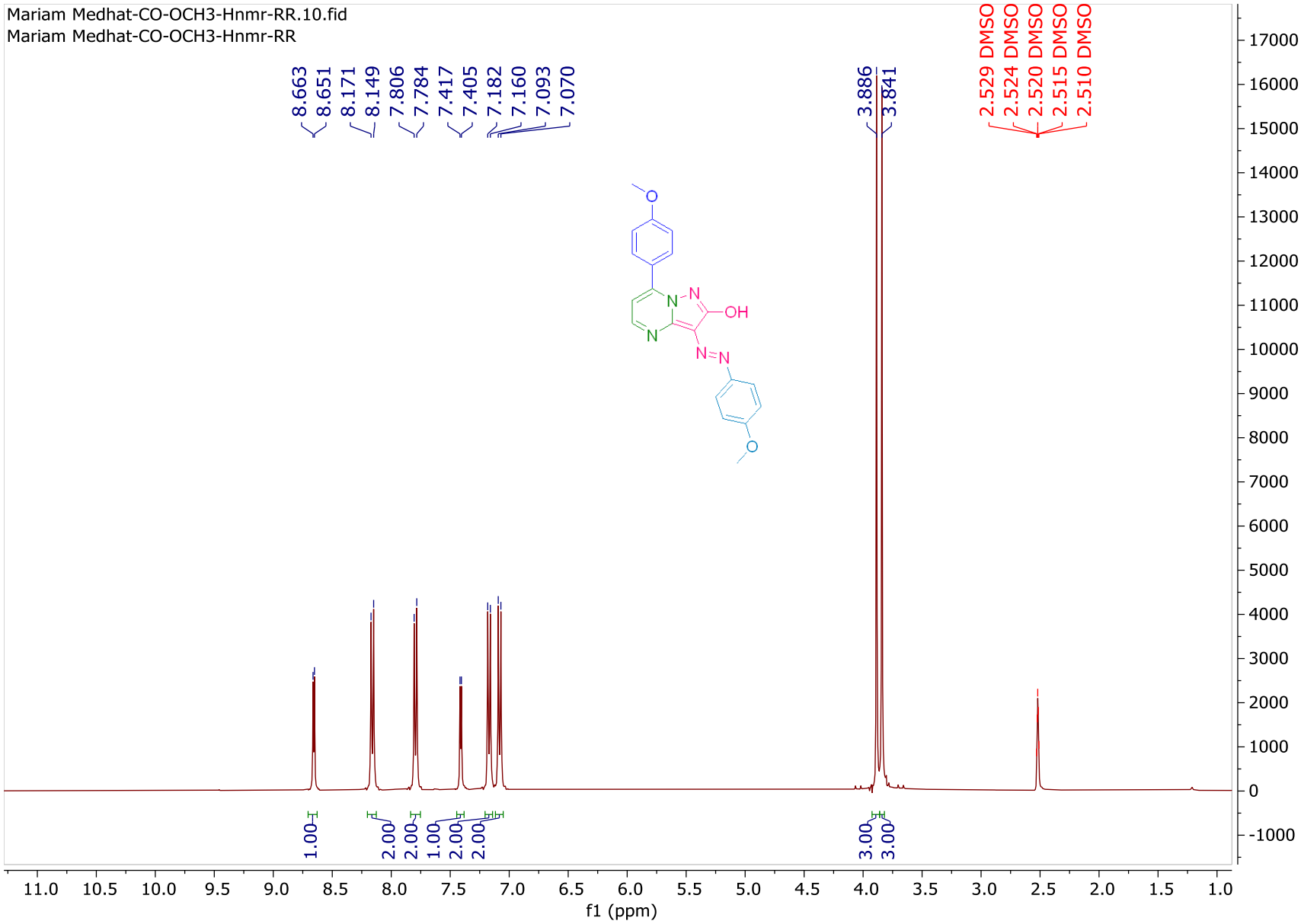

Figure S16. ^{1}H NMR of compound 19h

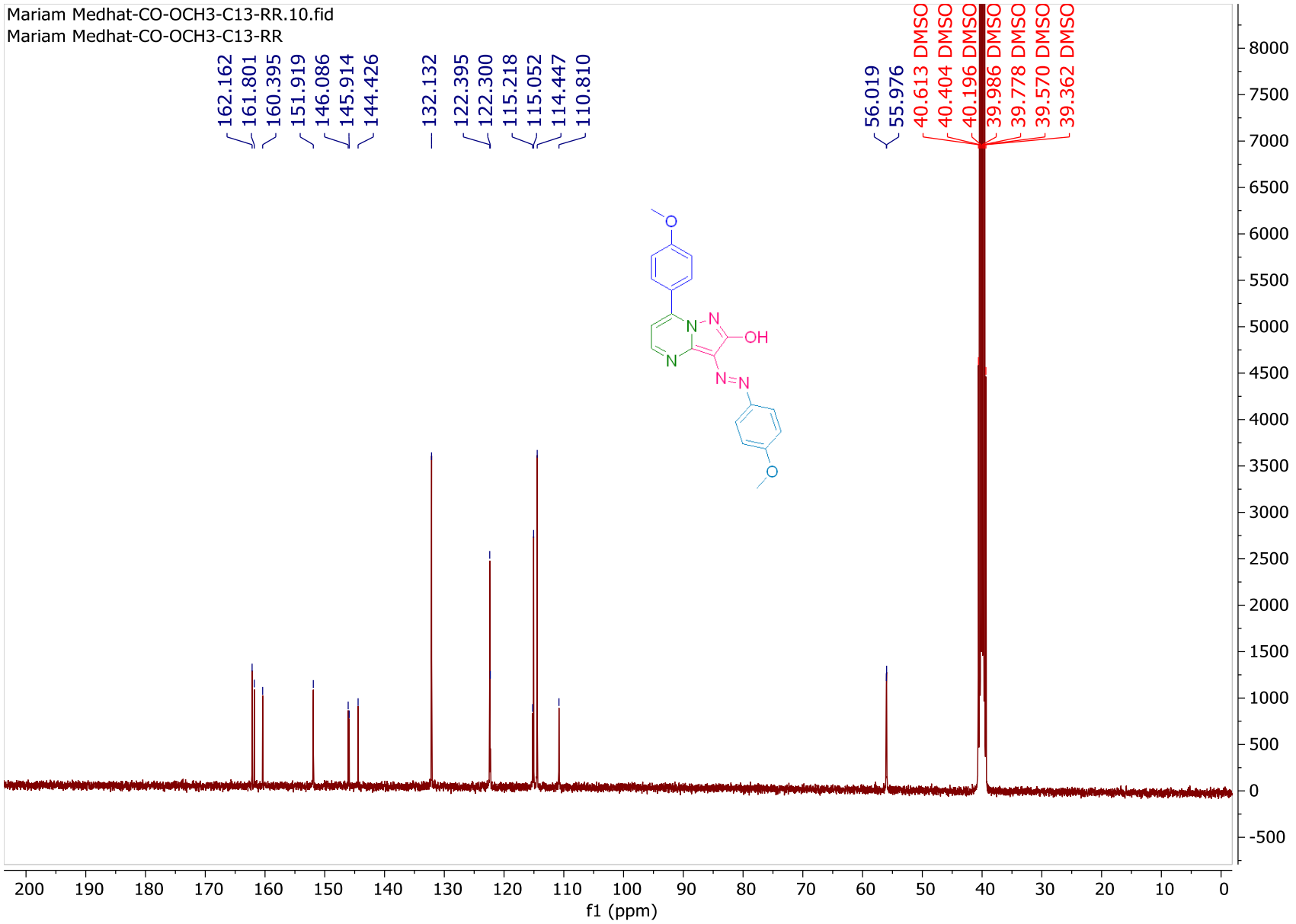

Figure S17. ^{13}C NMR of compound 19h

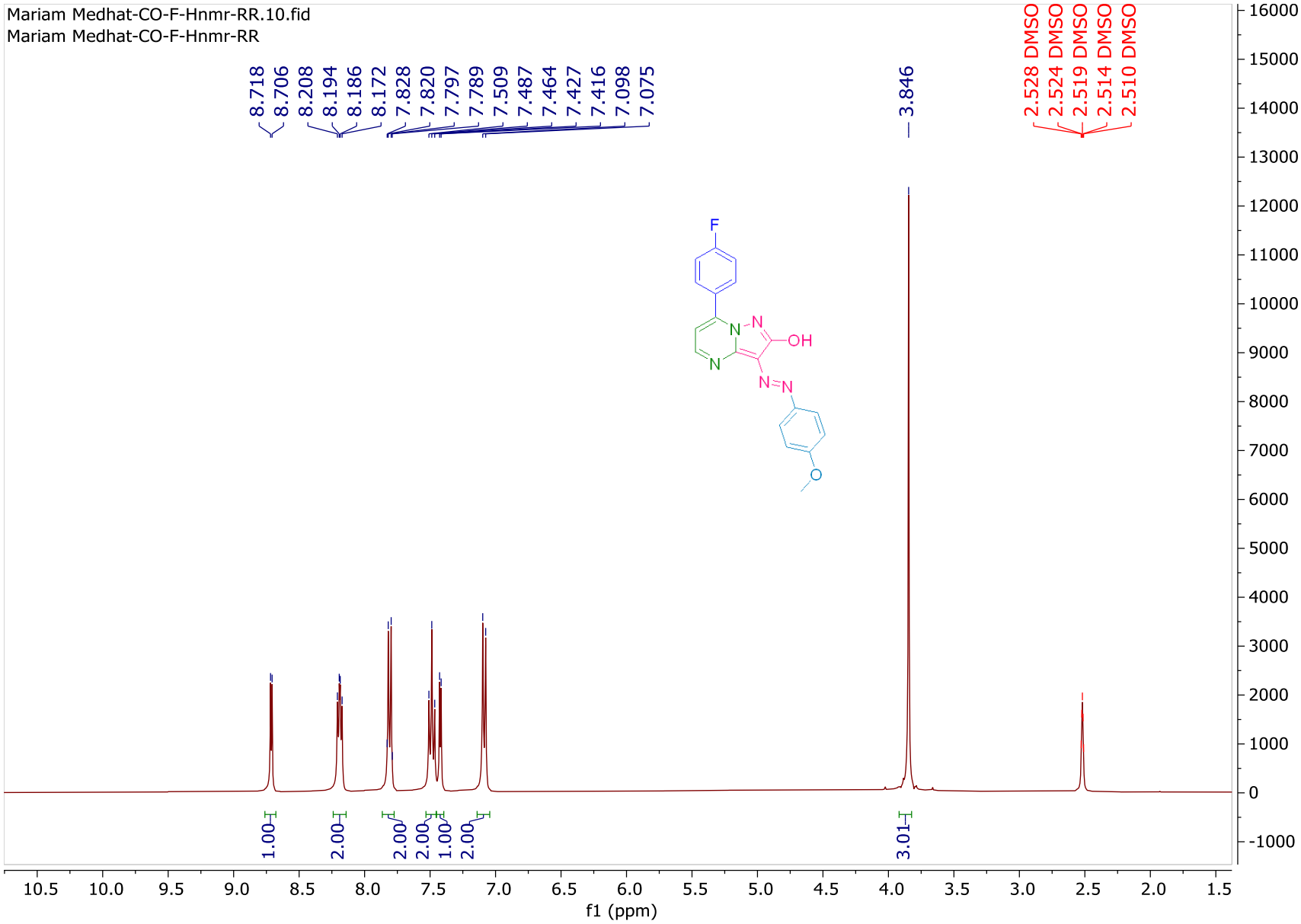

Figure S18. ^{1}H NMR of compound 19i

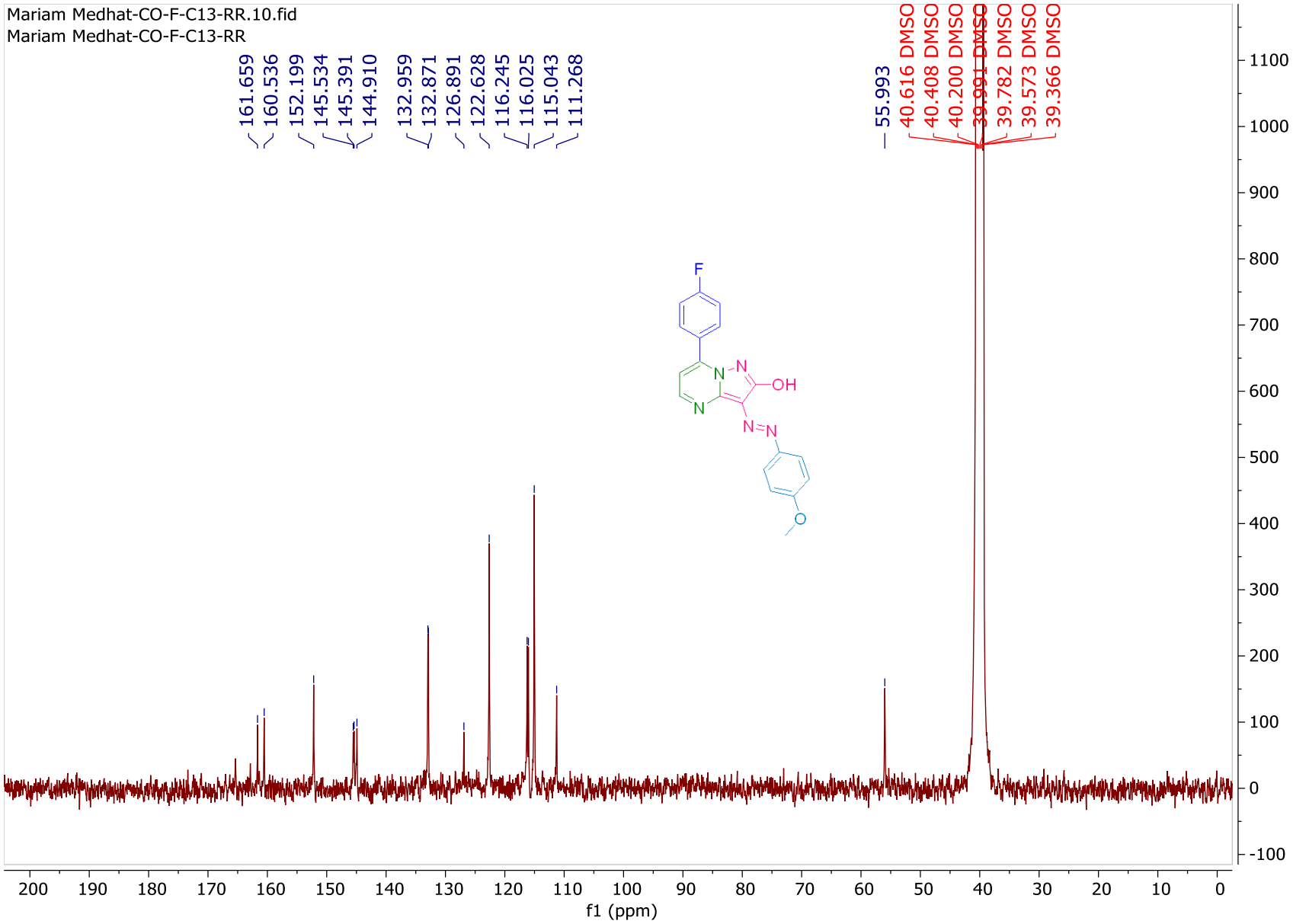

Figure S19. ^{13}C NMR of compound 19i

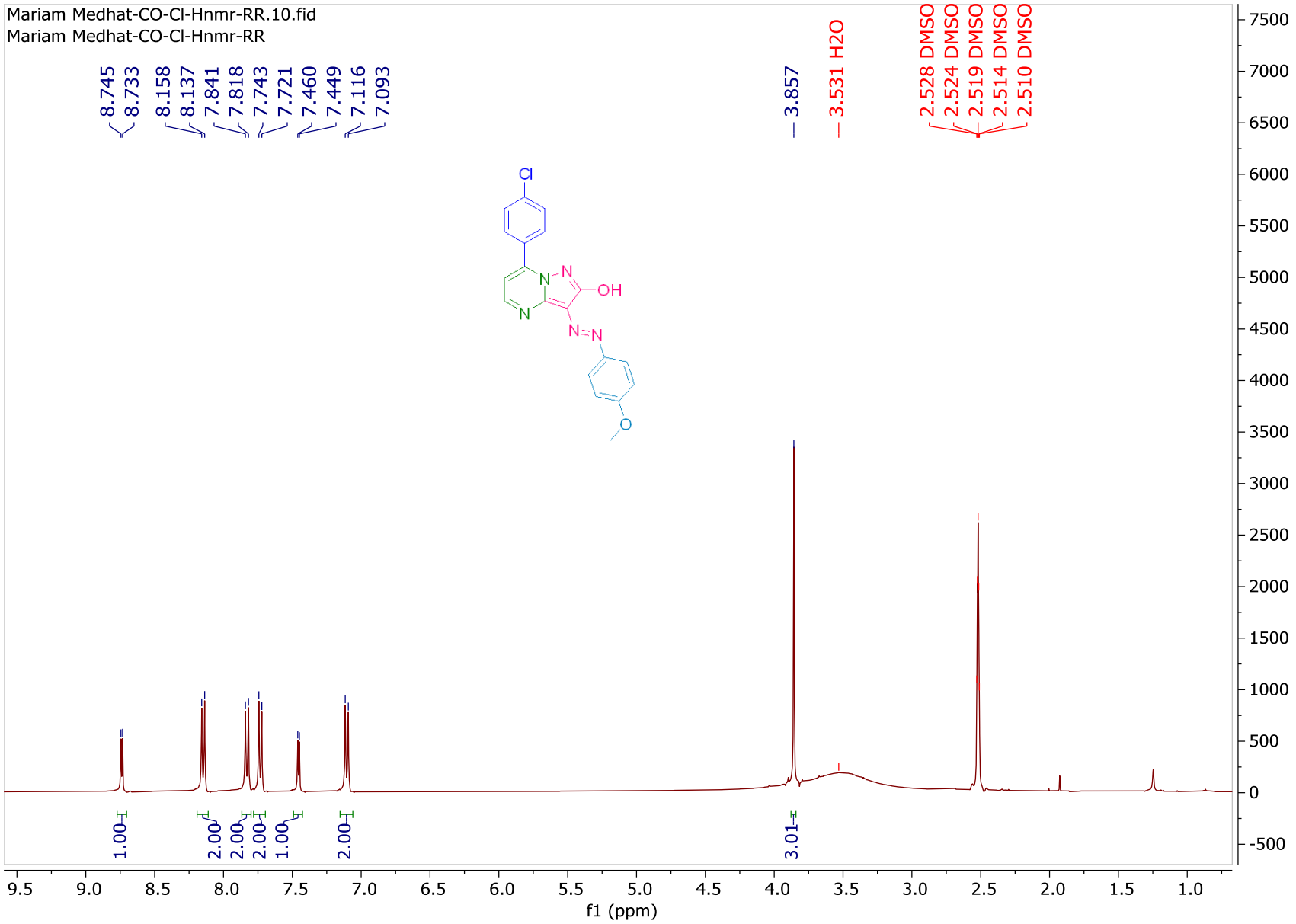

Figure S20. ^{1}H NMR of compound 19j

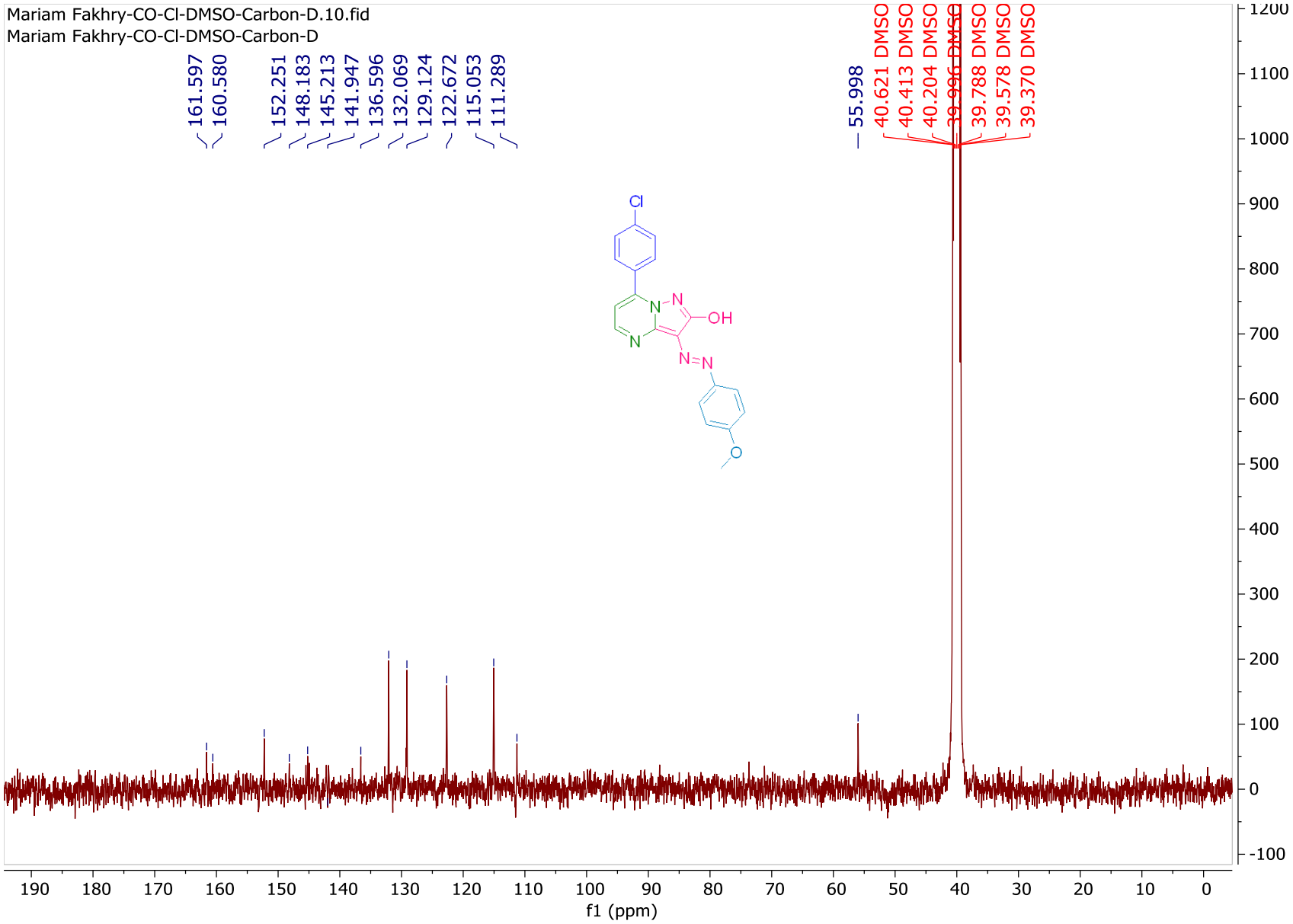

Figure S21. ^{13}C NMR of compound 19j

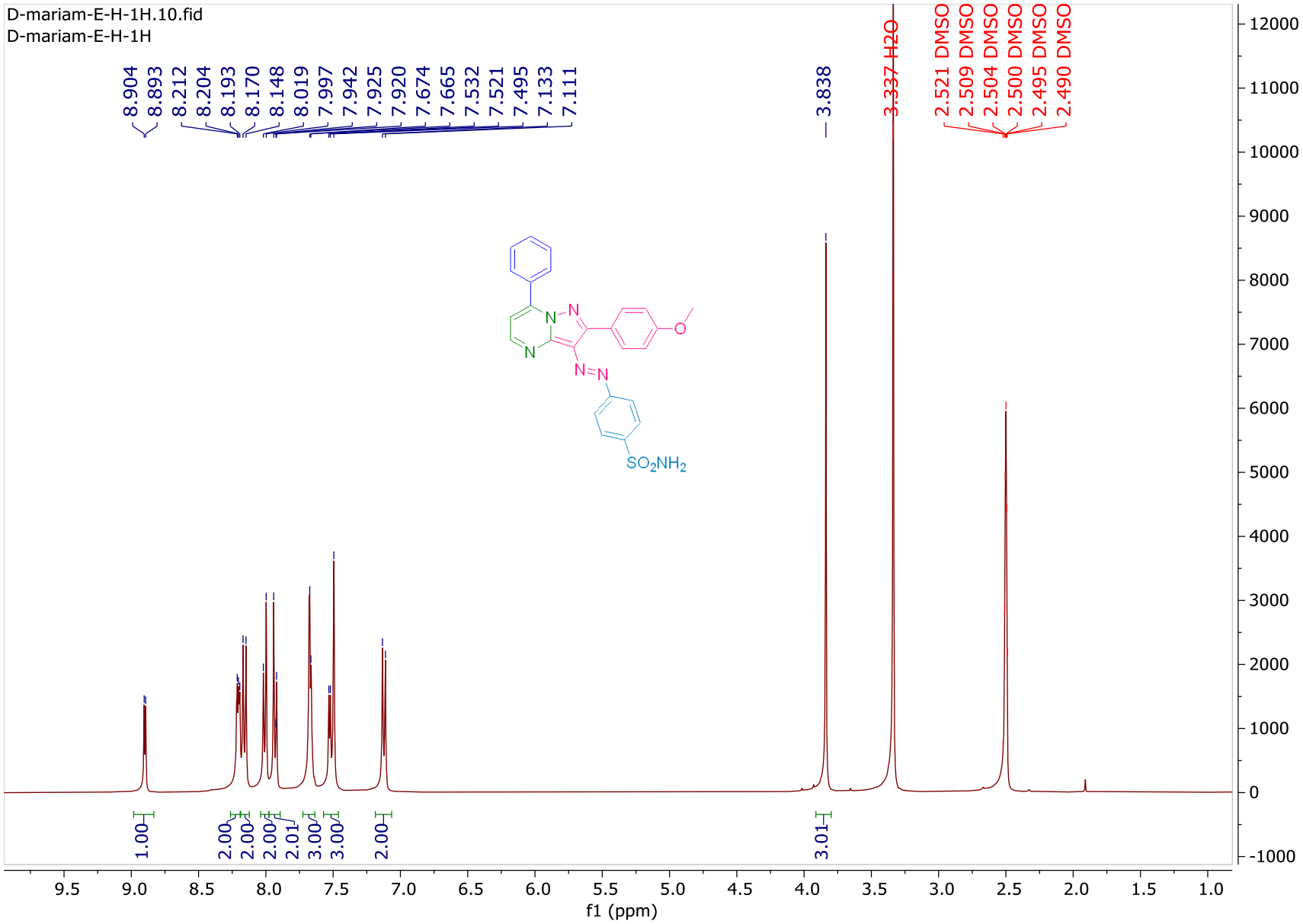

Figure S22. ^{1}H NMR of compound 19k

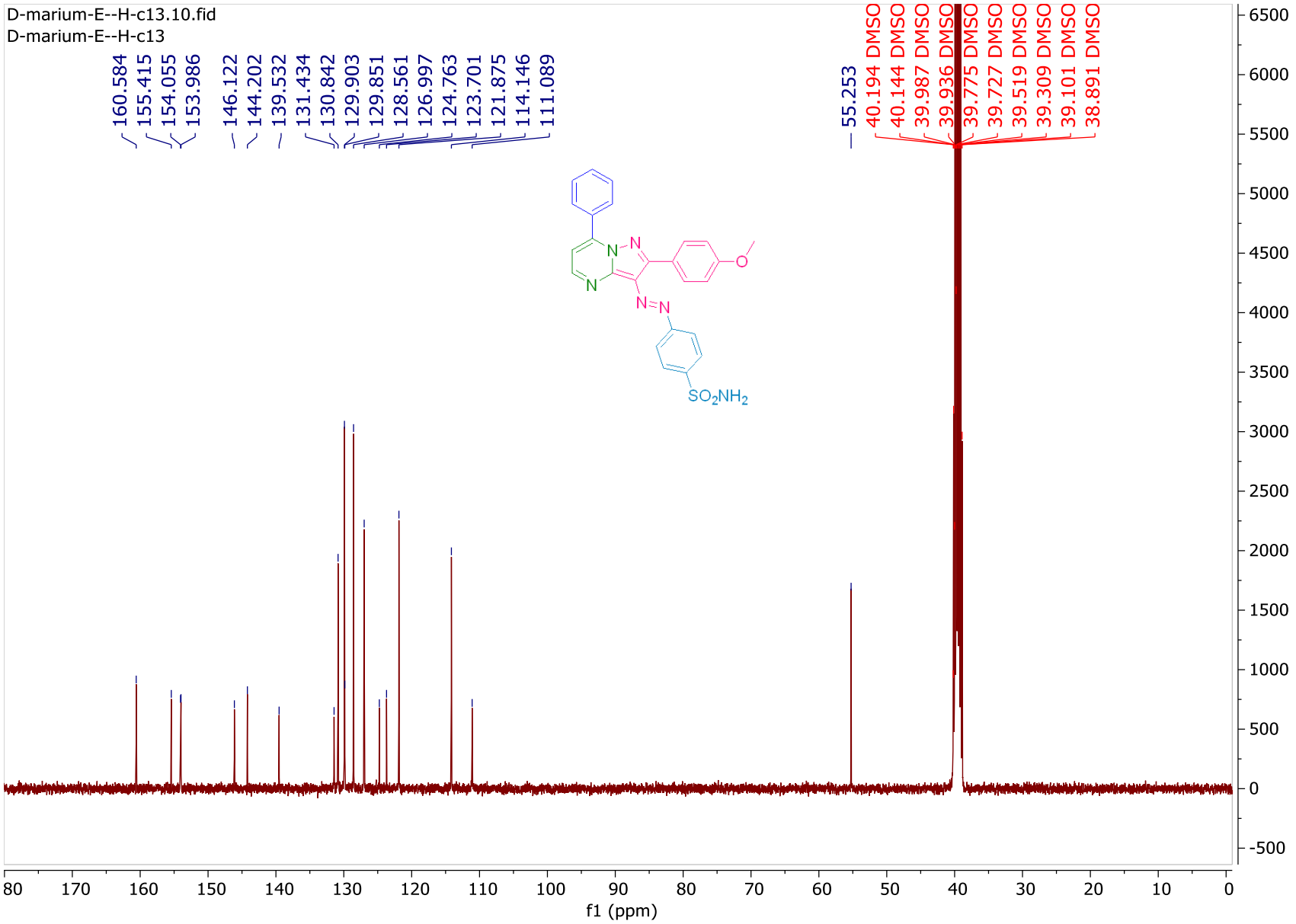

Figure S23. ^{13}C NMR of compound 19k

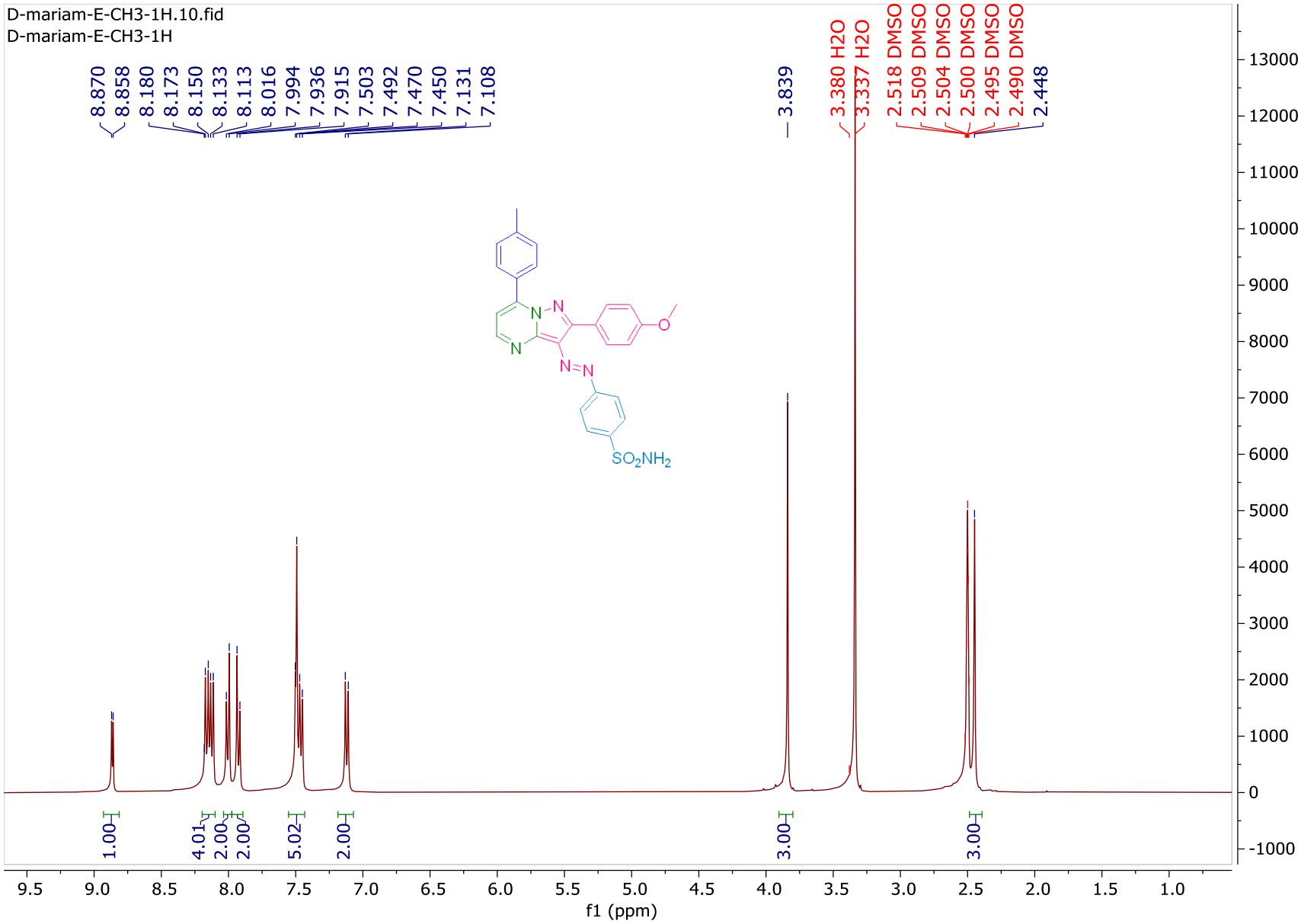

Figure S24. ^{1}H NMR of compound 19l

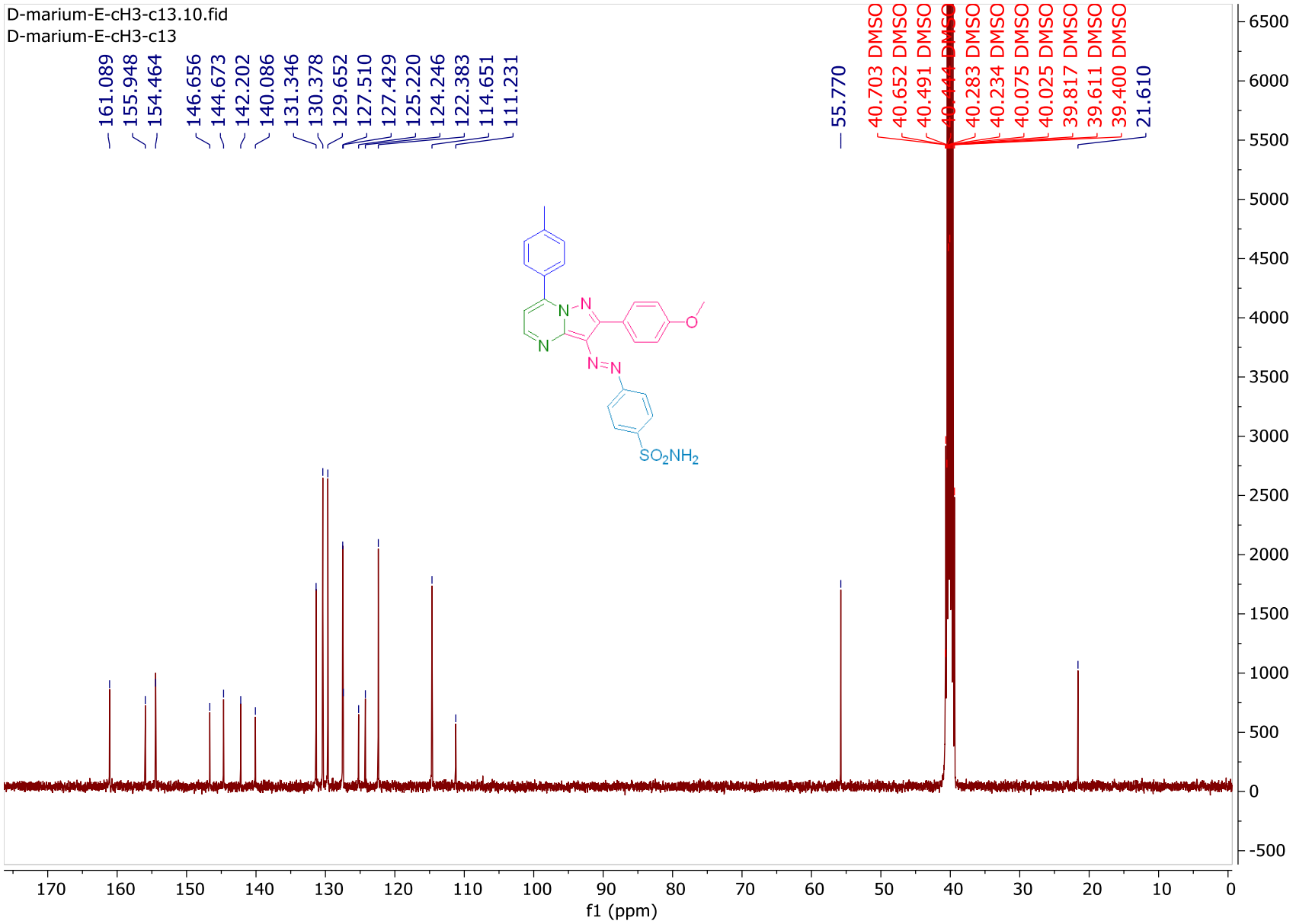

Figure S25. ^{13}C NMR of compound 19l

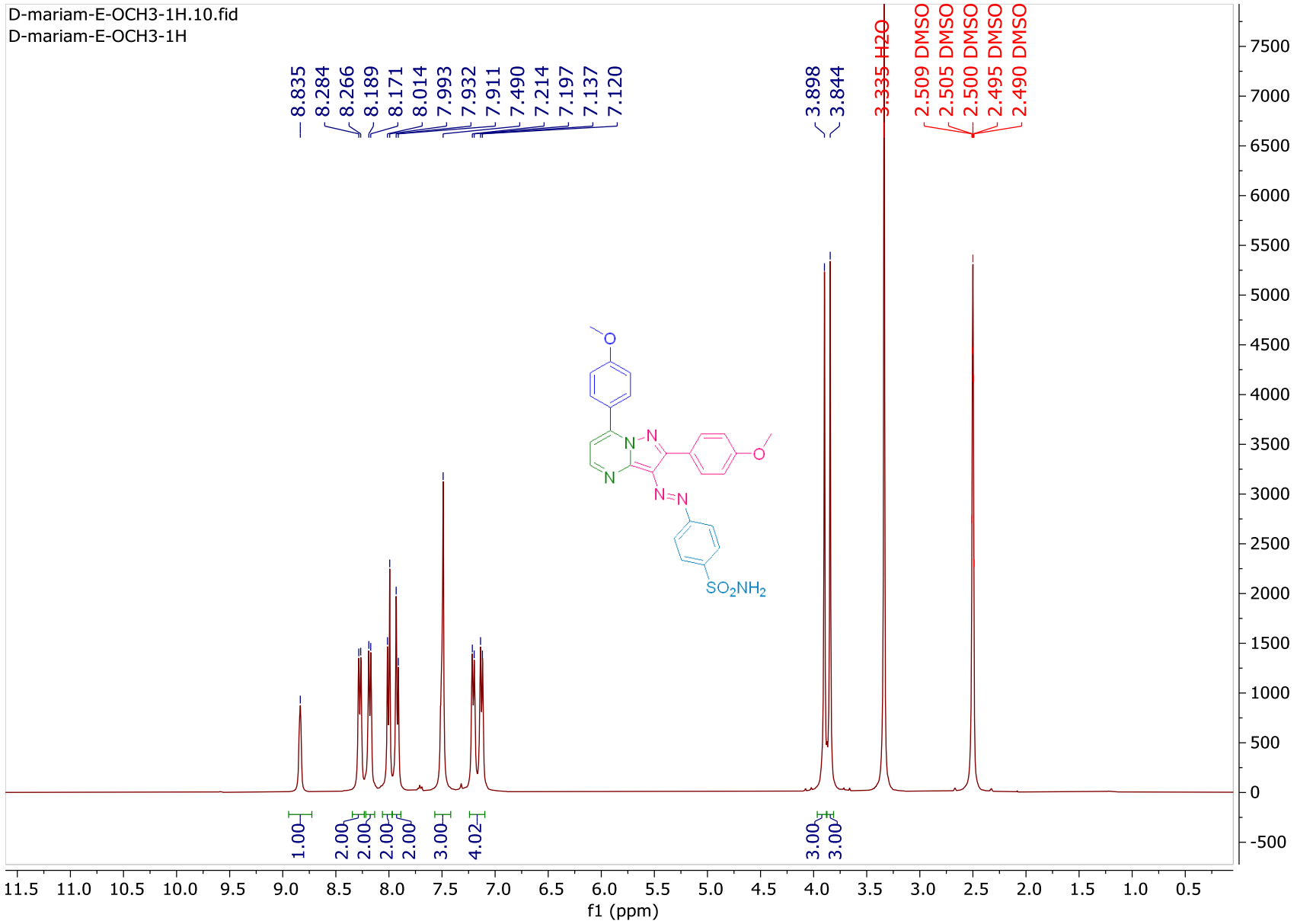

Figure S26. ^{1}H NMR of compound 19m

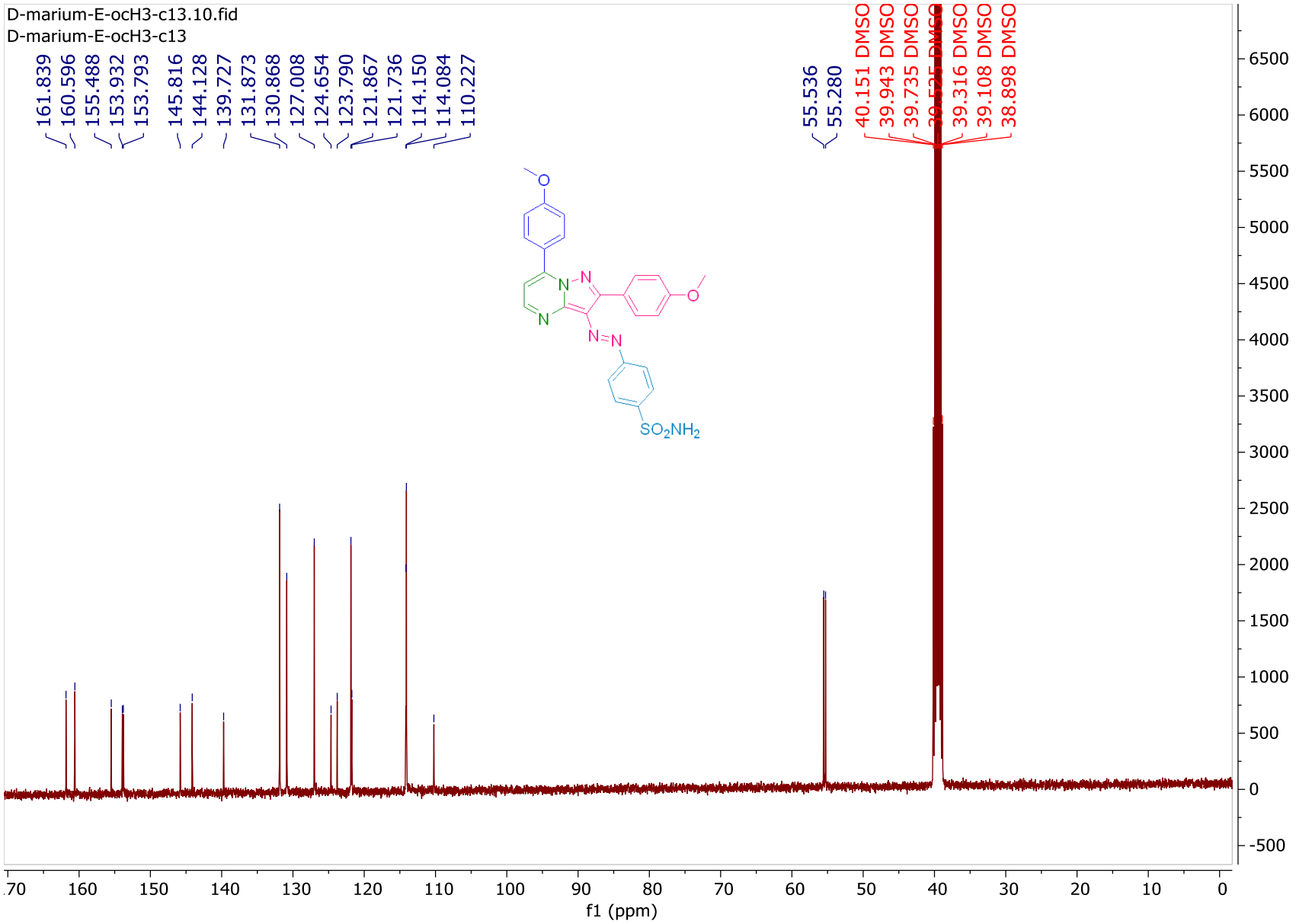

Figure S27. ^{13}C NMR of compound 19m

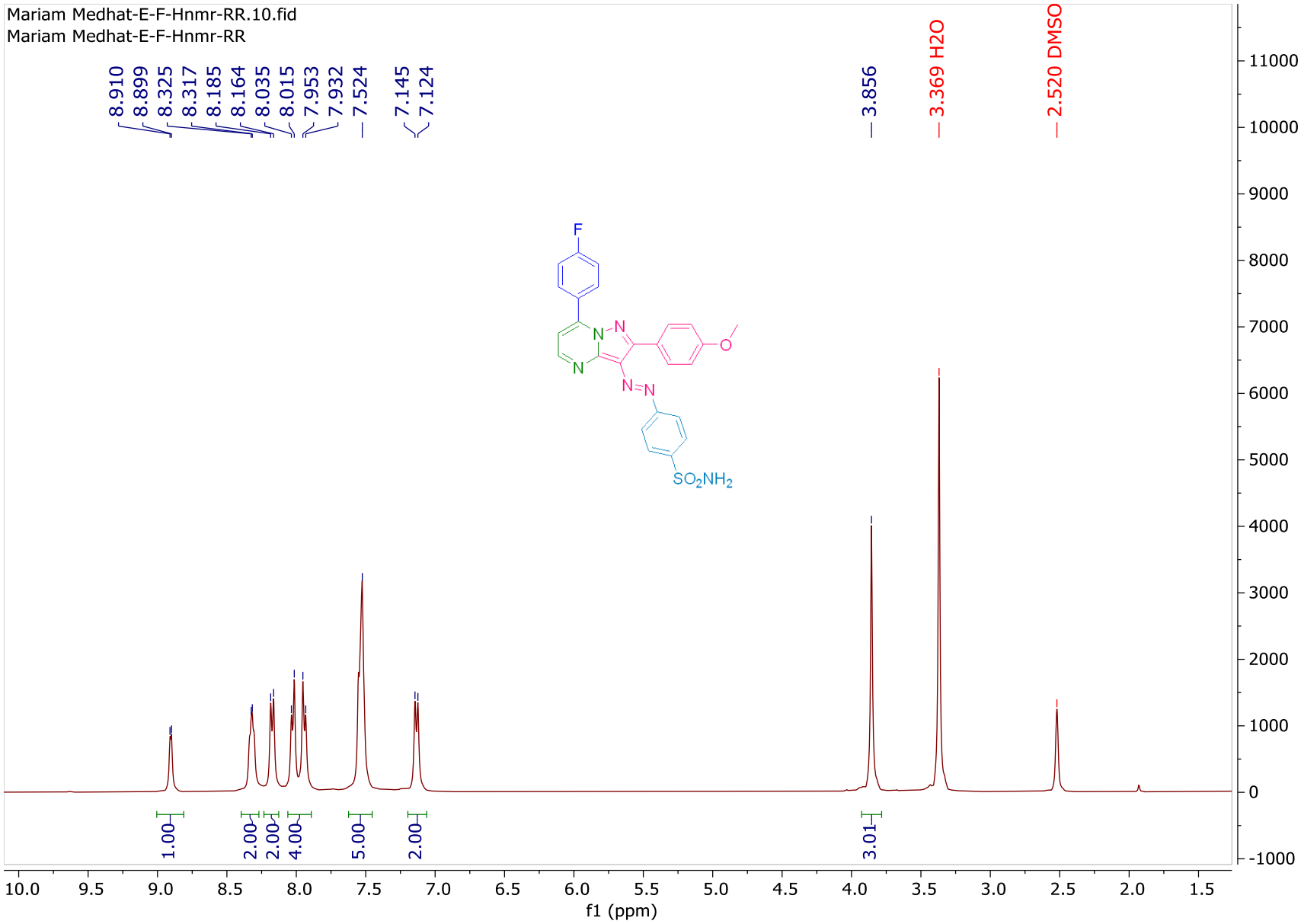

Figure S28. ^{1}H NMR of compound 19n

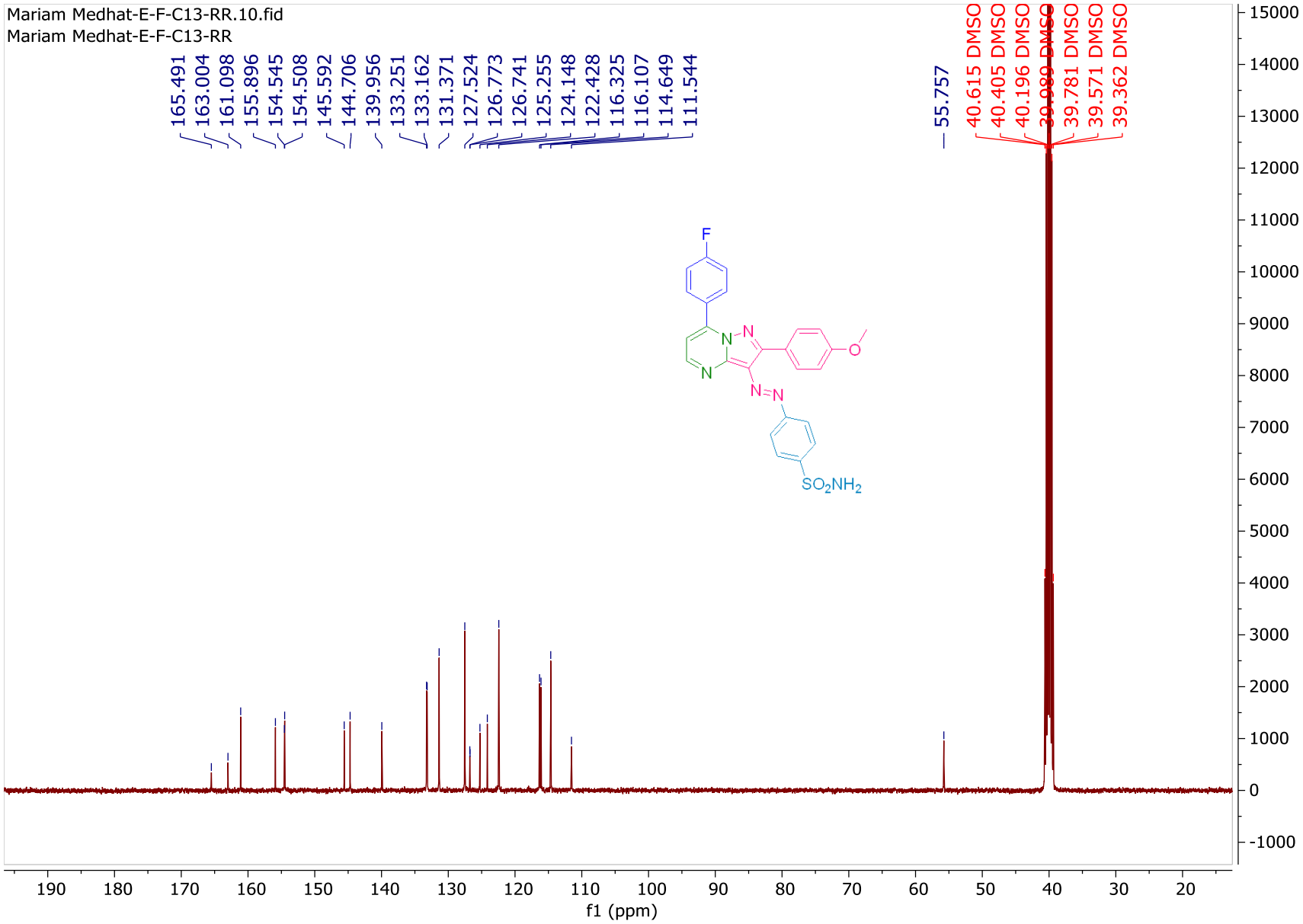

Figure S29. ^{13}C NMR of compound 19n

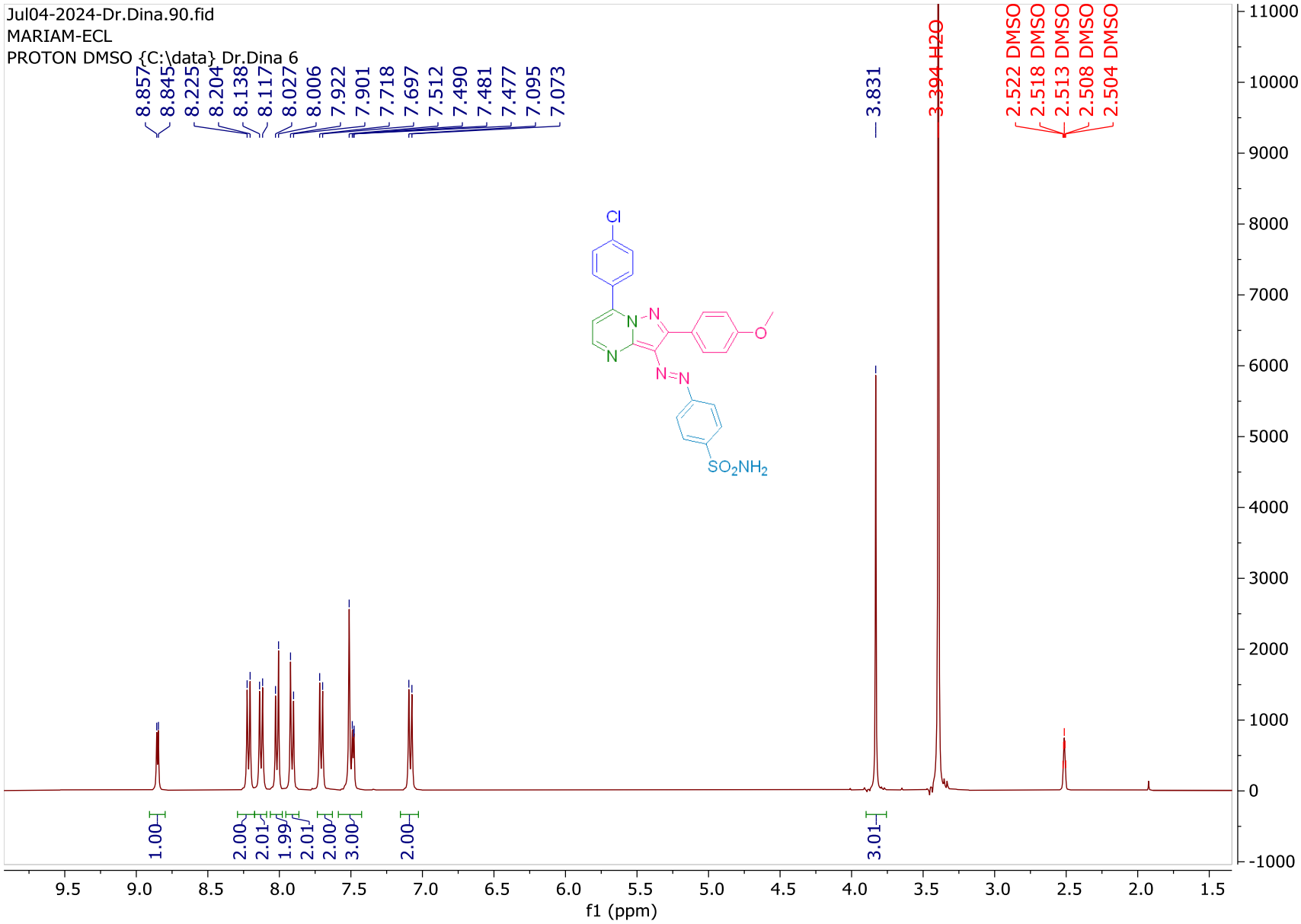

Figure S30. ^{1}H NMR of compound 19o