

Supporting Information for

**Thienopyrimidine Scaffolds as Promising Antimicrobial Agents: Synthesis, Biological
Evaluation, DFT Analysis, and Molecular Docking**

Mostafa Sayed^{1#}, Menna A. Naguib^{1#}, Ahmed A.K. Mohammed², Reda Hassanien¹,
Mahmoud S. Tolba^{1*}, Mostafa Ahmed^{1*}

¹Chemistry Department, Faculty of Science, New Valley University, El-Kharja 72511, Egypt

²Chemistry Department, Faculty of Science, Assiut University, Assiut 71516 , Egypt

#Theses authors contributed equally to this work.

Corresponding authors: Mahmoud S. Tolba (Mahmoud.Tolba@sci.nvu.edu.eg) and Mostafa Ahmed (drmostafa@scinv.au.edu.eg)

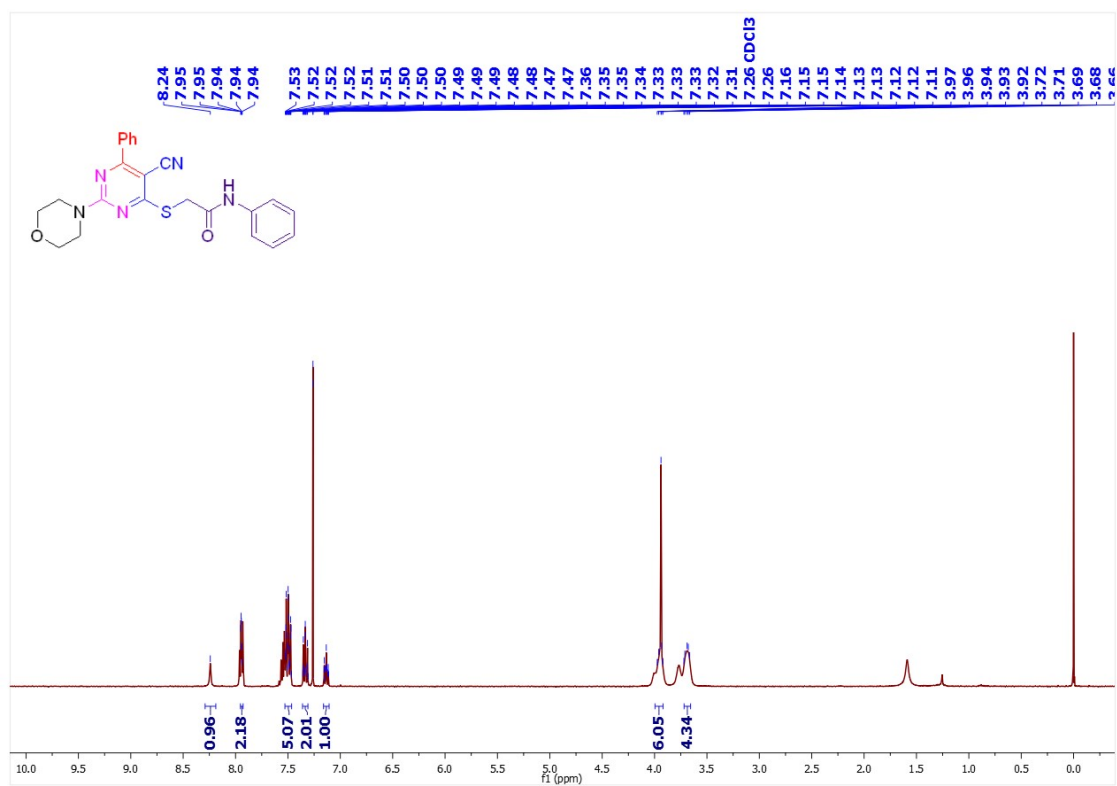


Figure S1. ¹H NMR Spectrum of Compound 9.

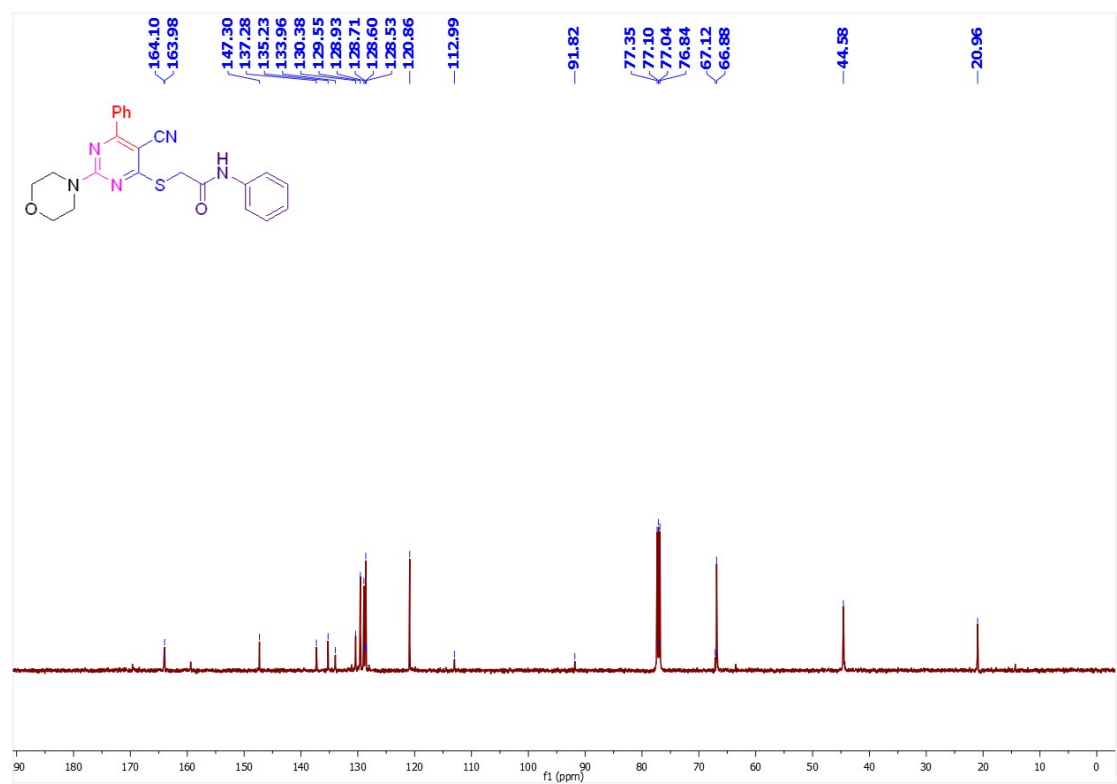


Figure S2. ¹³C NMR Spectrum of Compound 9.

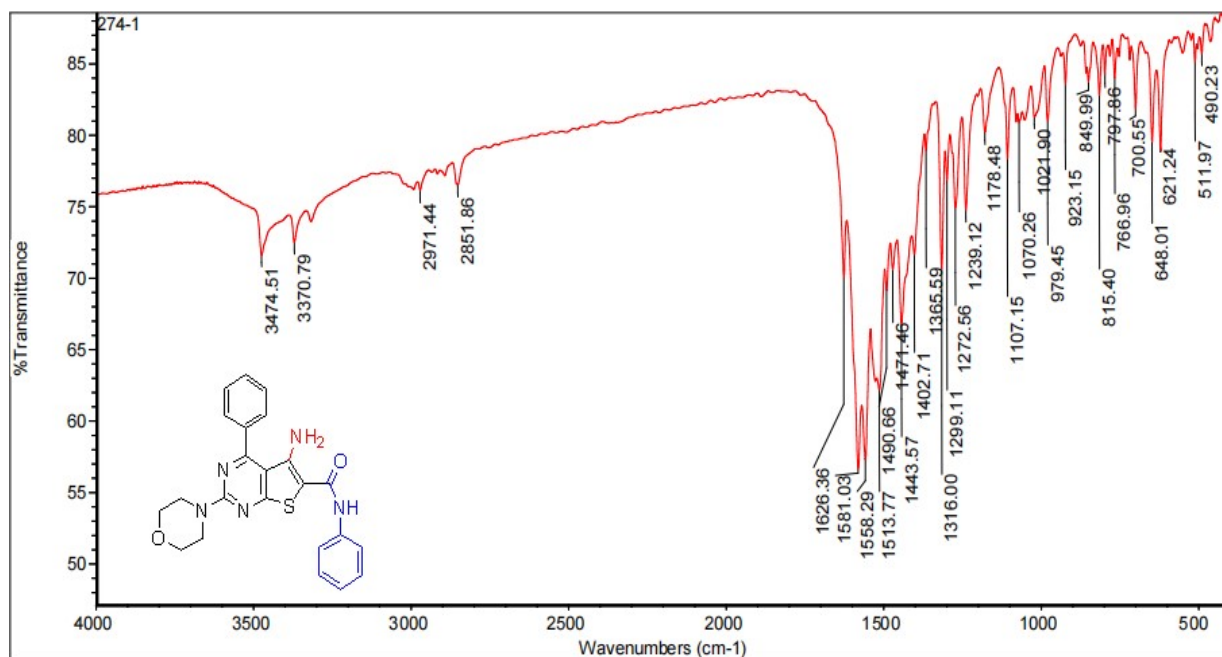


Figure S3. FTIR Spectrum of Compound 10.

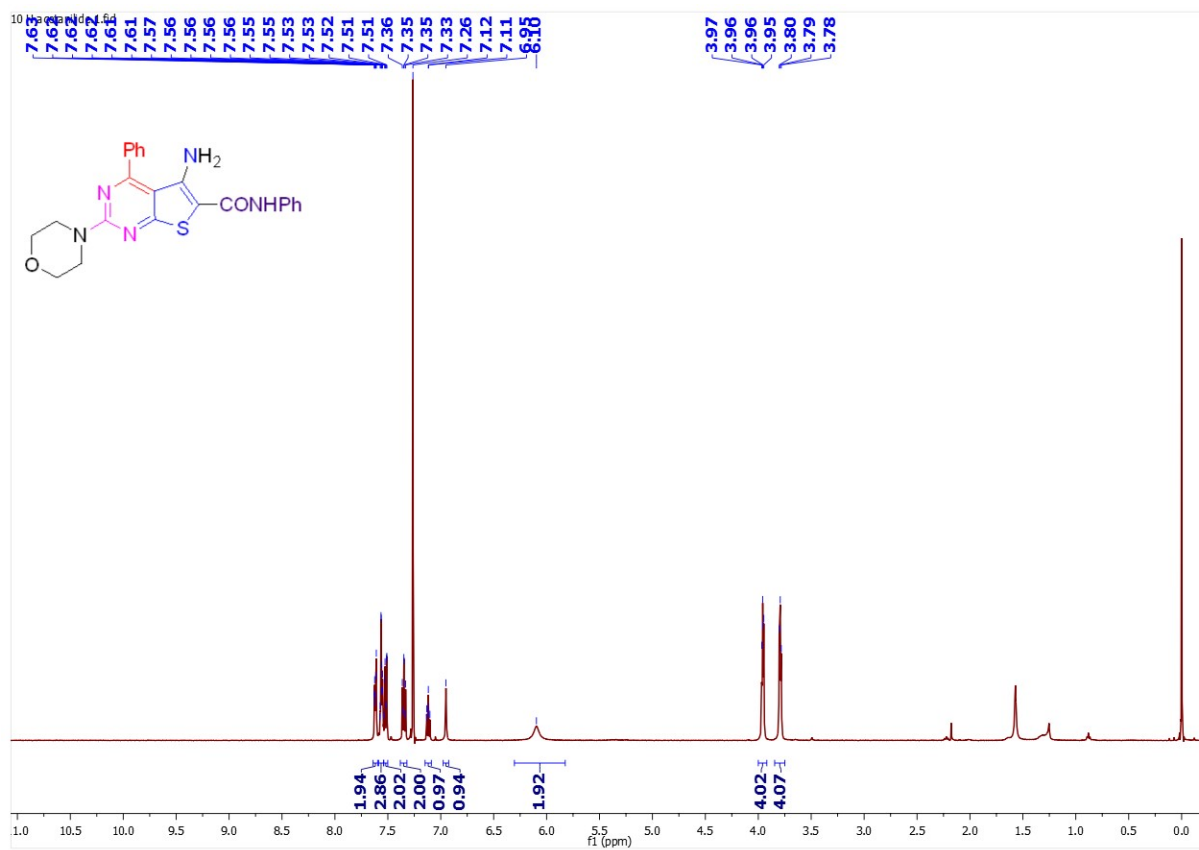


Figure S4. ^1H NMR Spectrum of Compound 10.

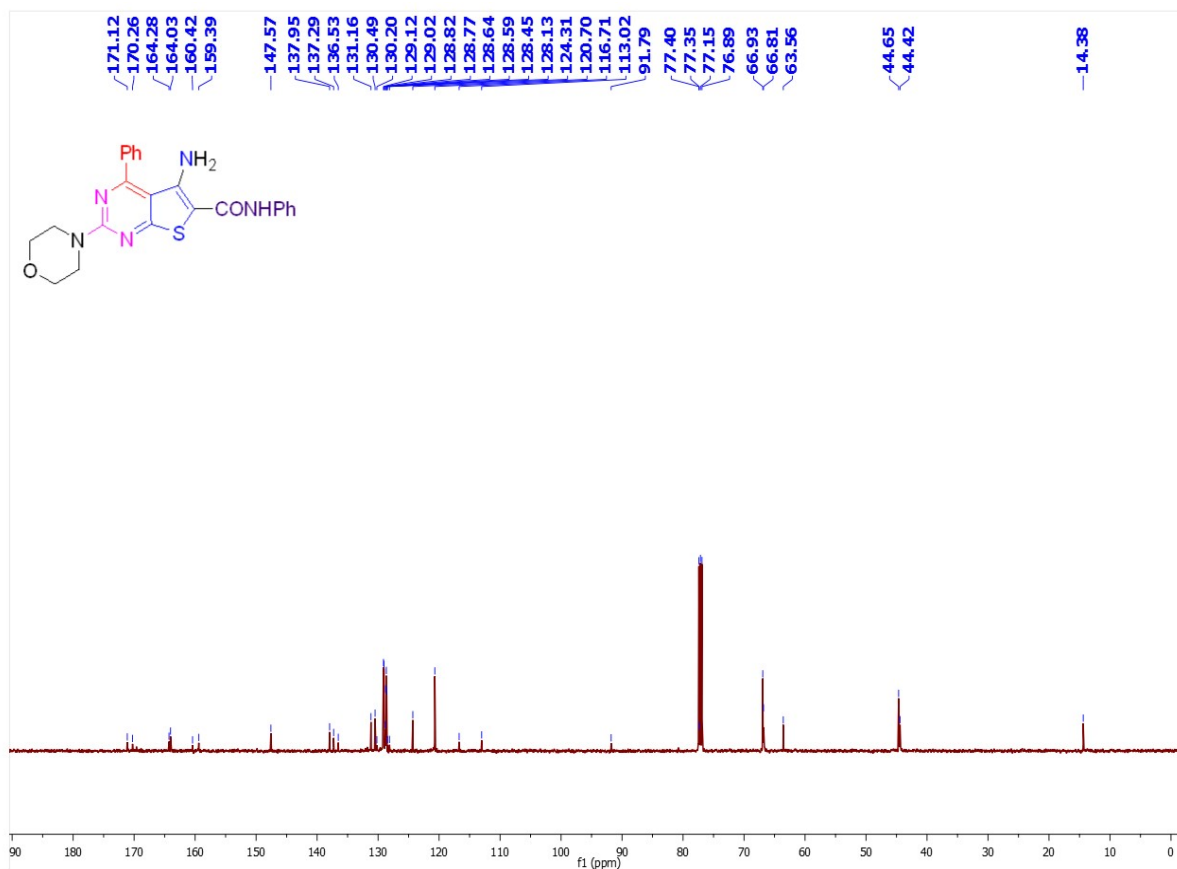


Figure S5. ¹³C NMR Spectrum of Compound 10.

Sample-8 #6307 RT: 21.48 AV: 1 NL: 1.13E3
T: + c EI Full ms [30.00-650.00]

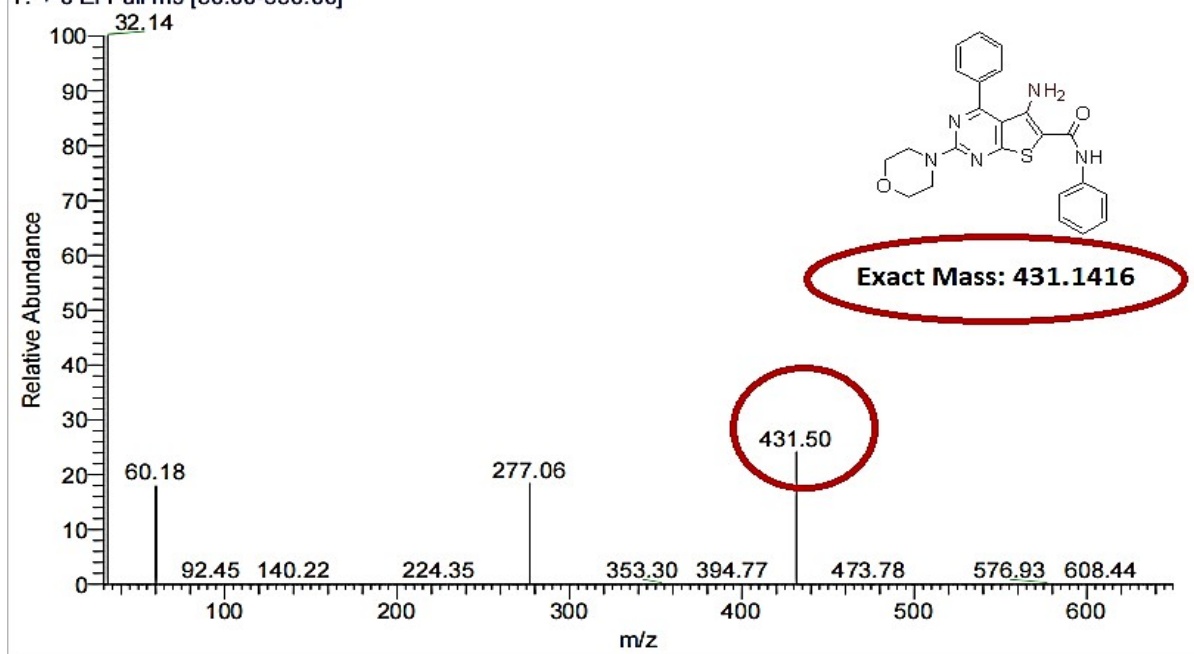


Figure S6. Mass Spectrum of Compound 10.

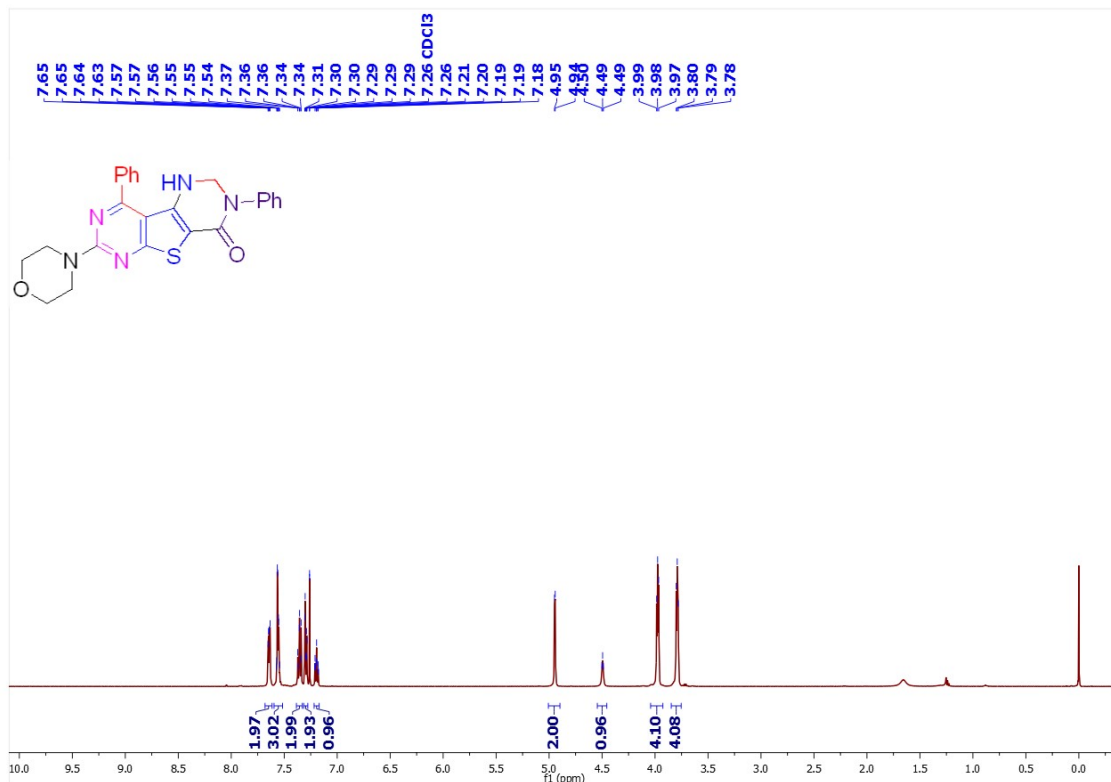


Figure S7. ¹H NMR Spectrum of Compound 11.

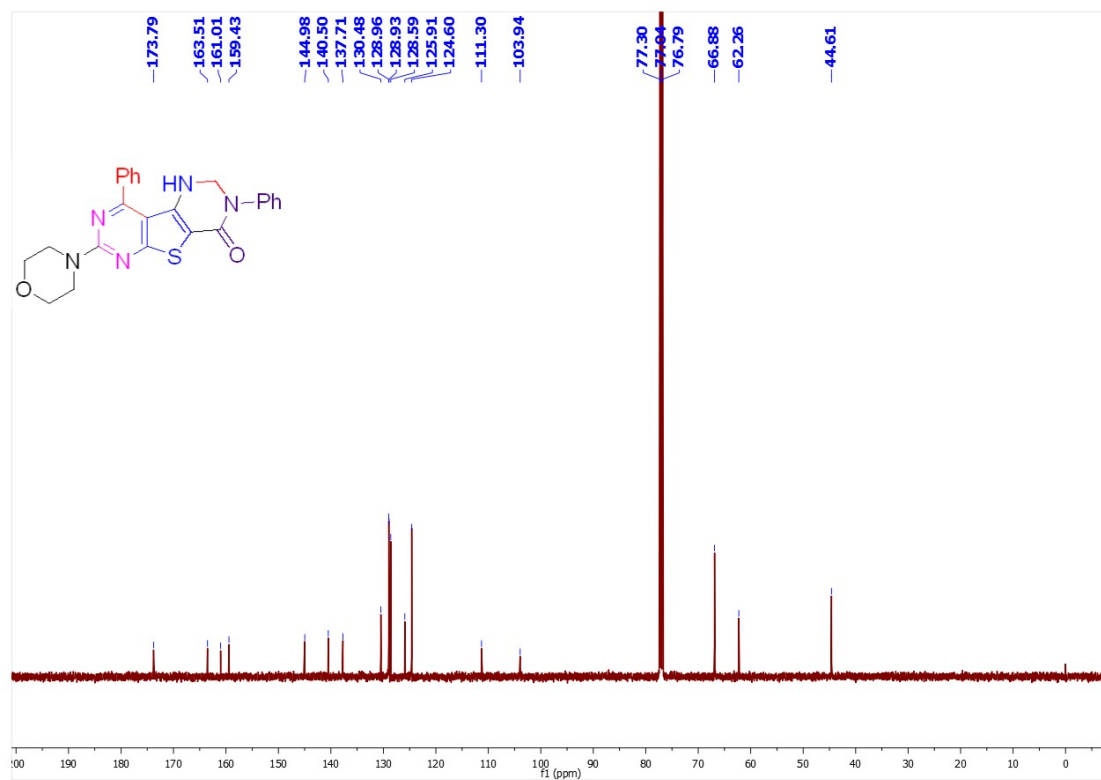


Figure S8. ¹³C NMR Spectrum of Compound 11.

Sample-11 #8310 RT: 28.29 AV: 1 NL: 8.77E3
T: + c EI Full ms [30.00-650.00]

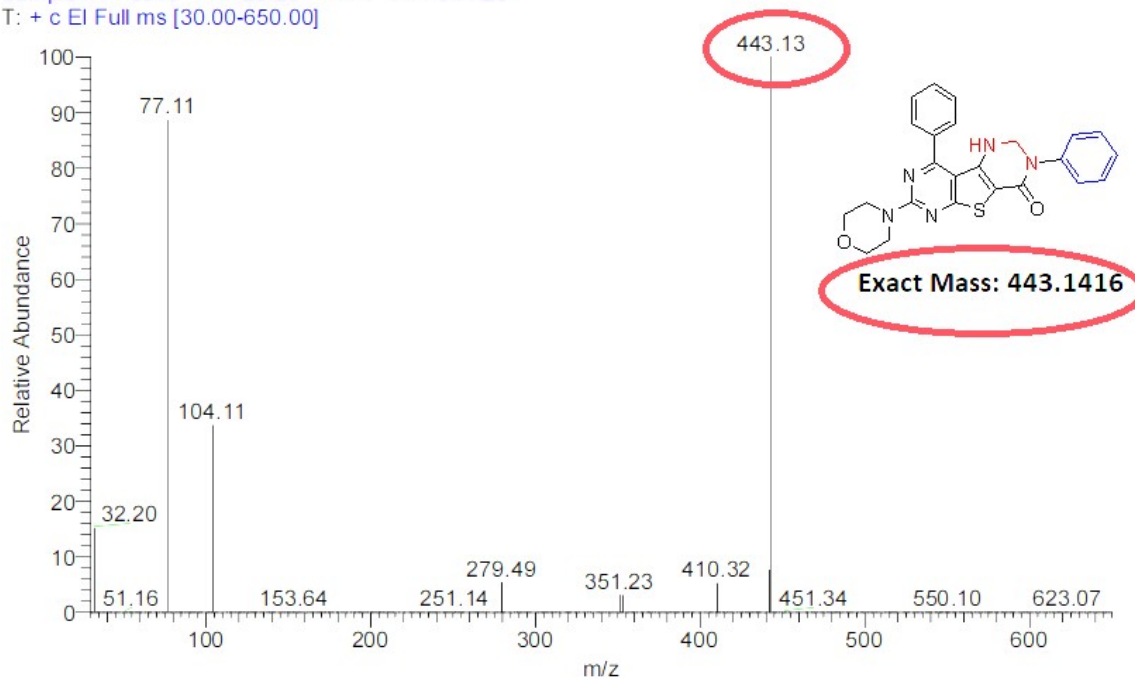


Figure S9. Mass Spectrum of Compound 11.

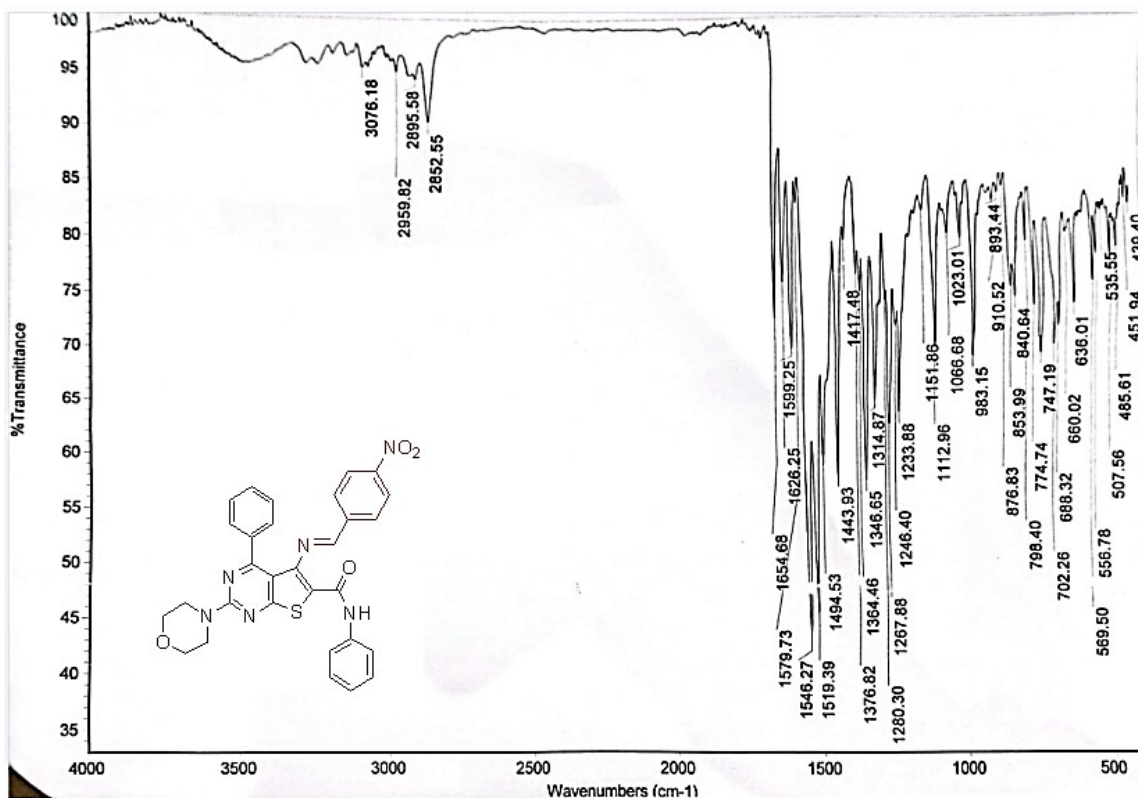


Figure S10. FTIR Spectrum of Compound 12.

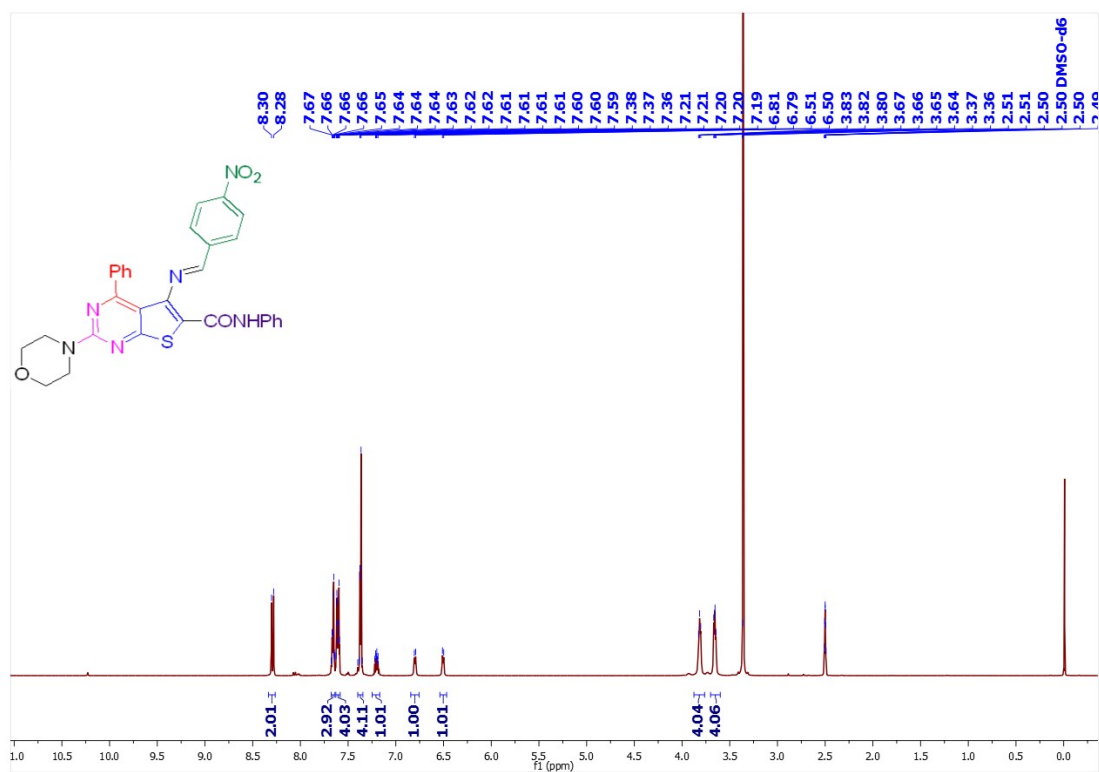


Figure S11. ¹H NMR Spectrum of Compound 12.

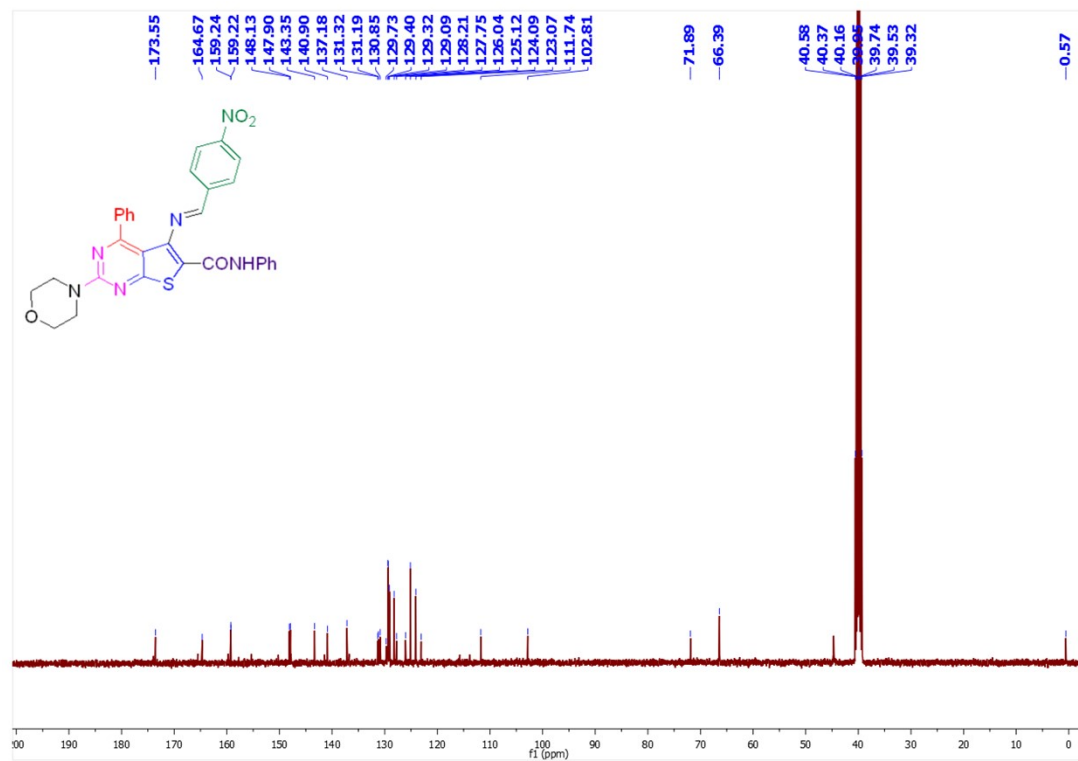


Figure S12. ¹³C NMR Spectrum of Compound 12.

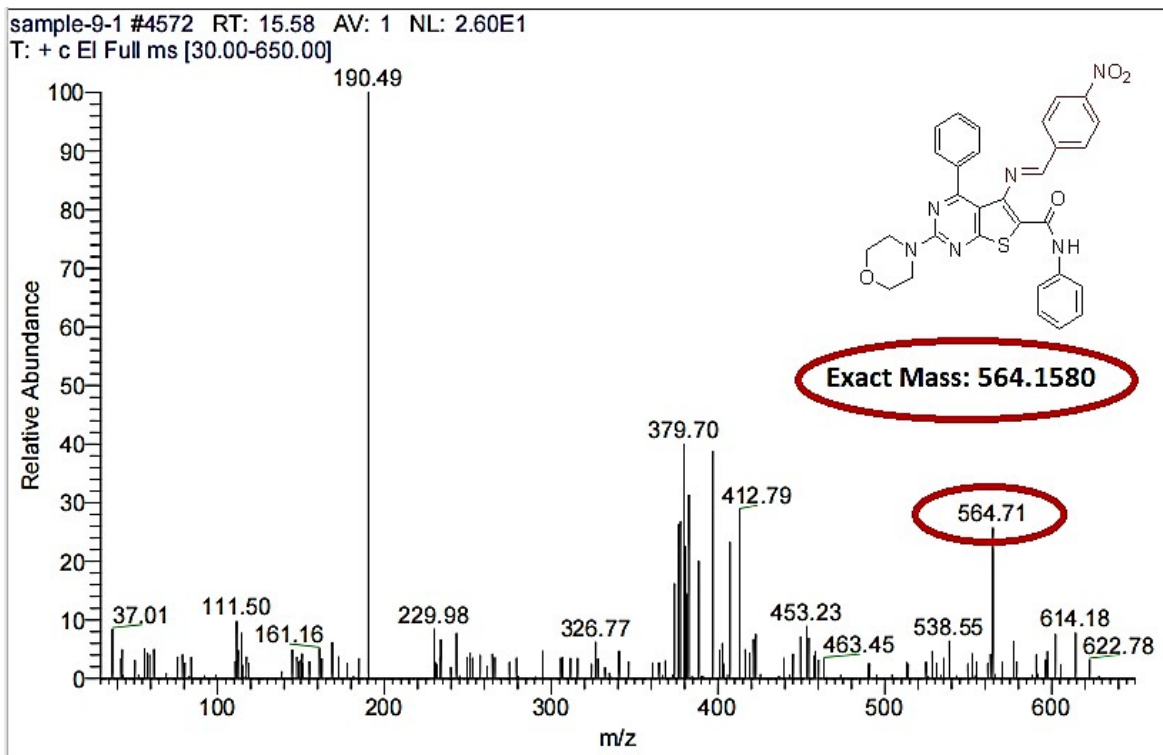


Figure S13. Mass Spectrum of Compound 12.

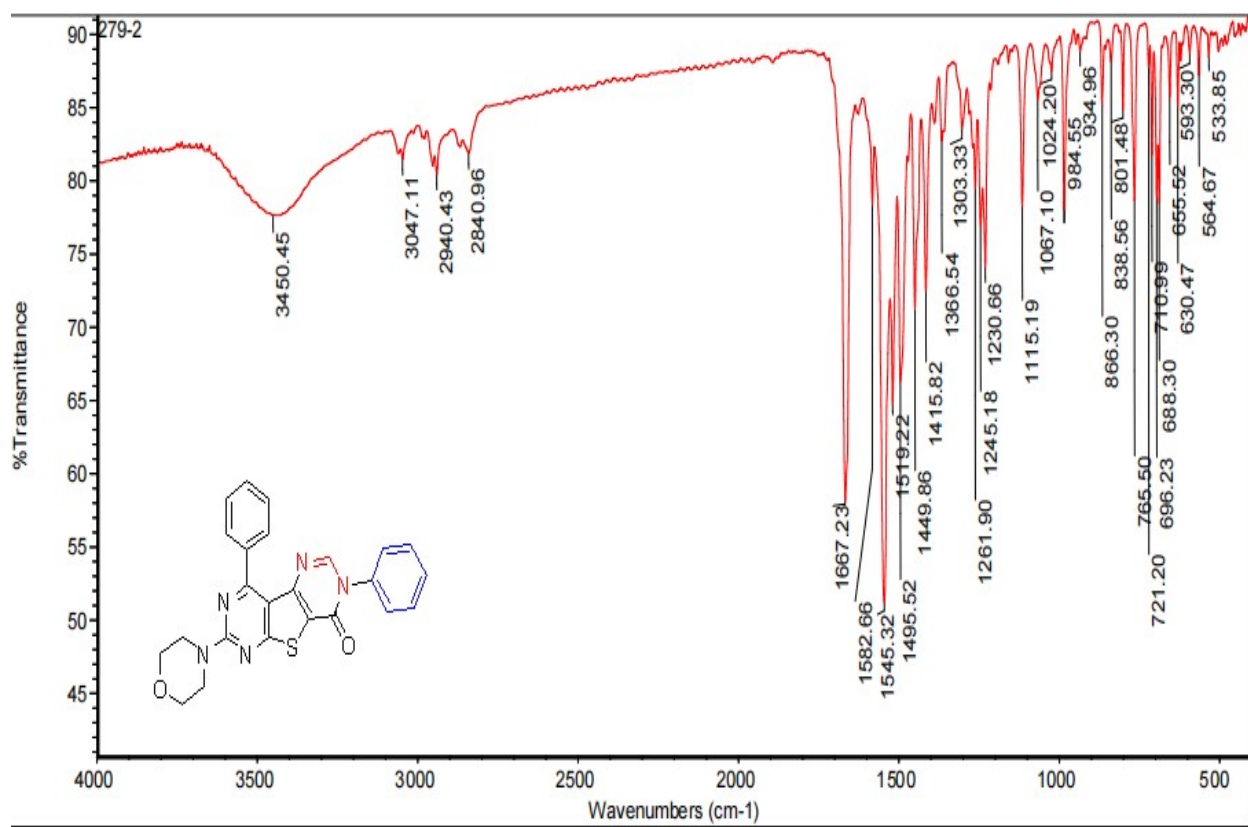


Figure S14. FTIR Spectrum of Compound 13.

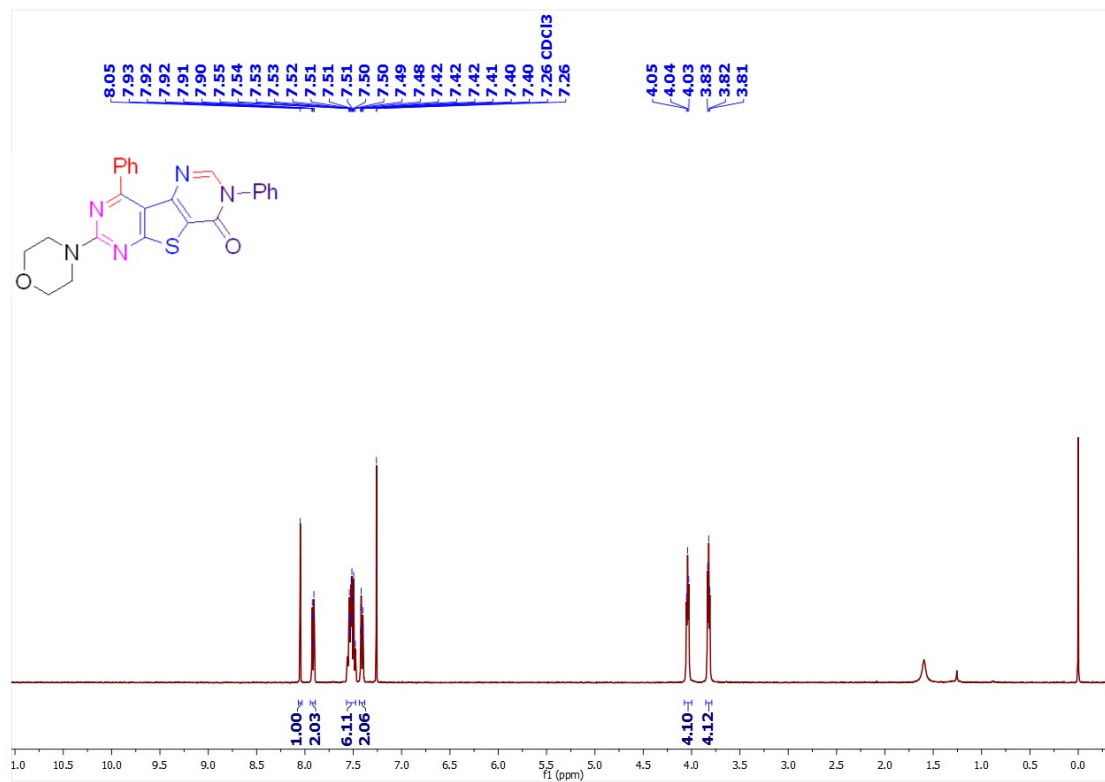


Figure S15. ¹H NMR Spectrum of Compound 13

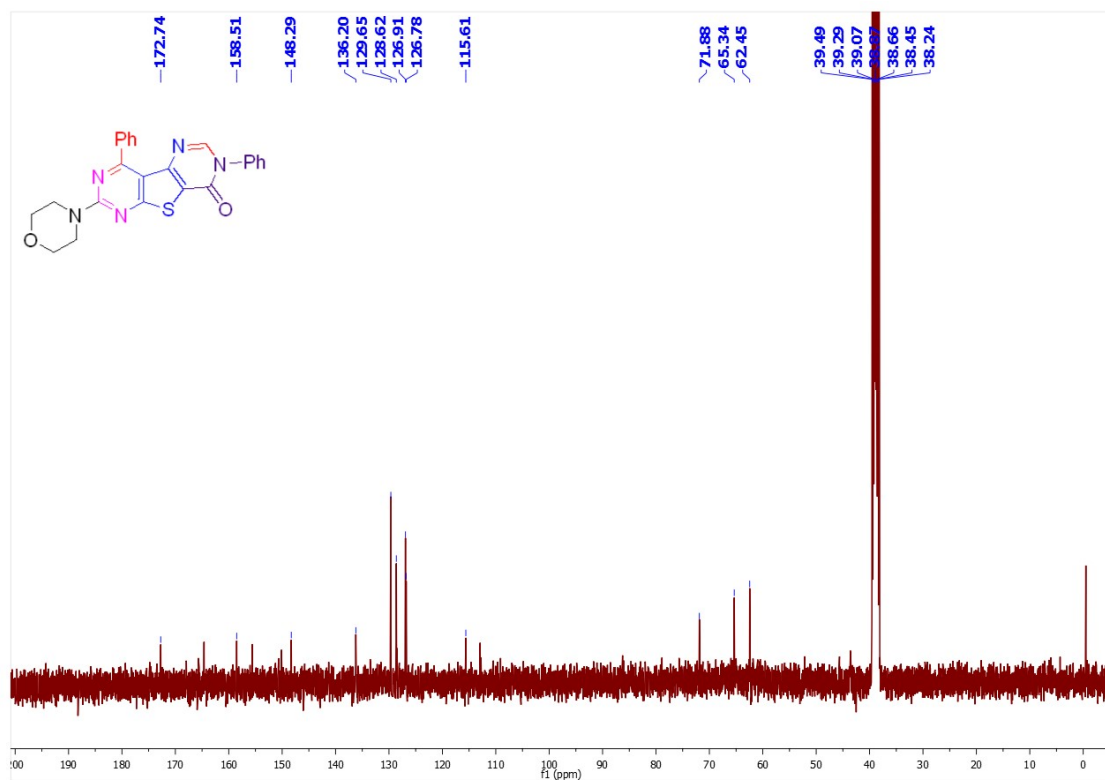


Figure S16. ¹³C NMR Spectrum of Compound 13.

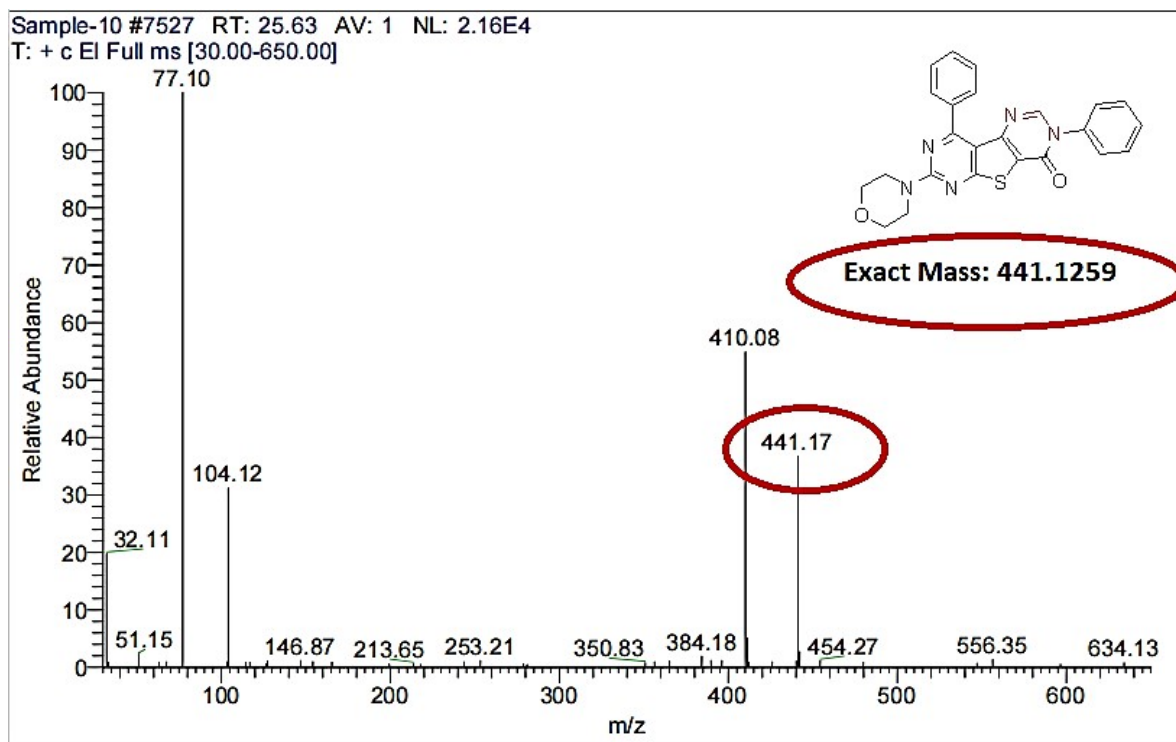


Figure S17. Mass Spectrum of Compound 13.

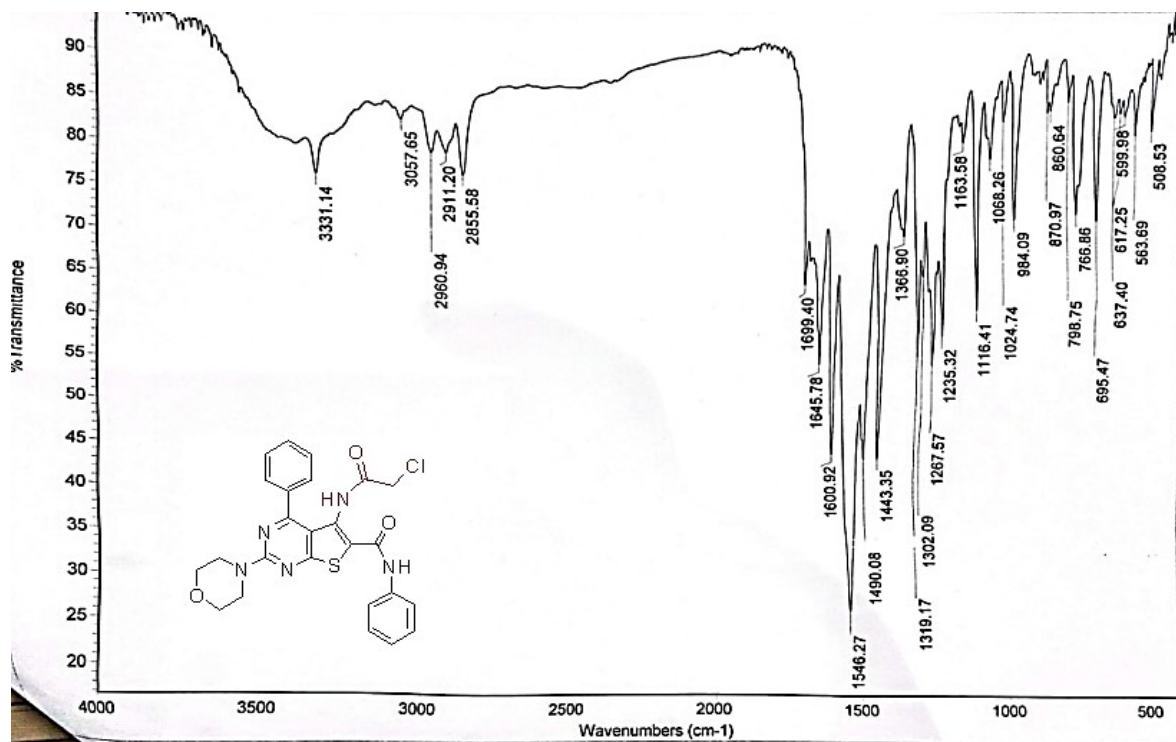


Figure S18. FTIR Spectrum of Compound 14.

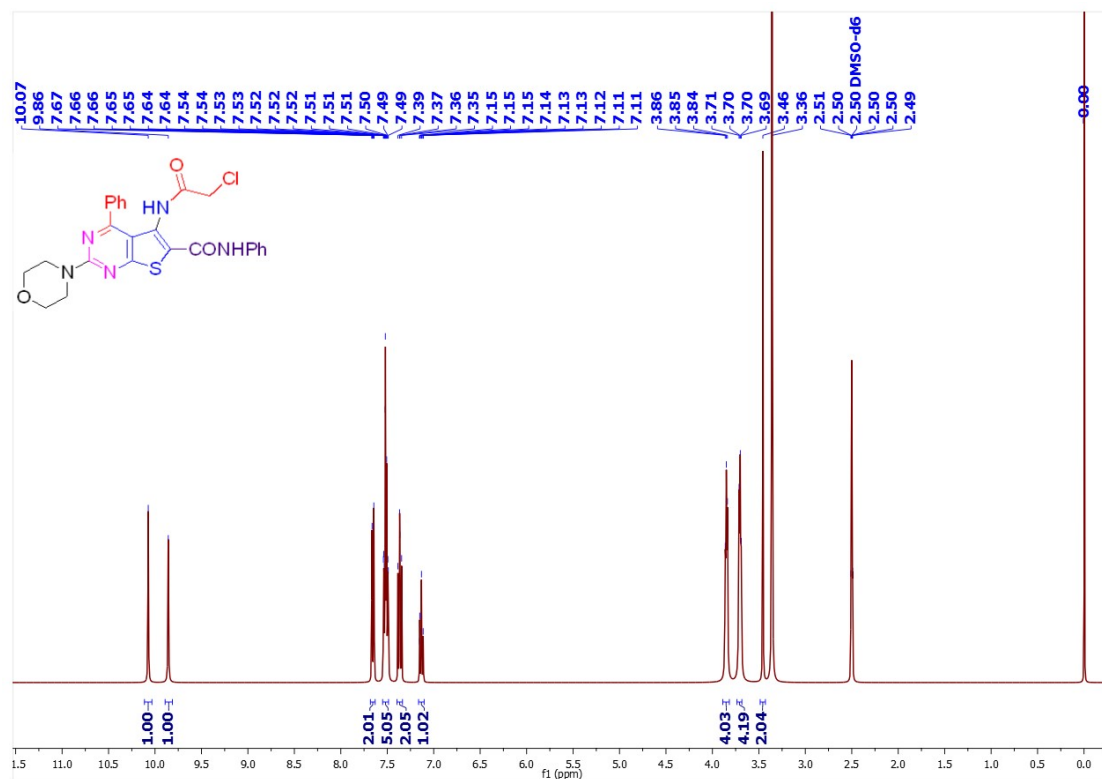


Figure S19. ¹H NMR Spectrum of Compound 14.

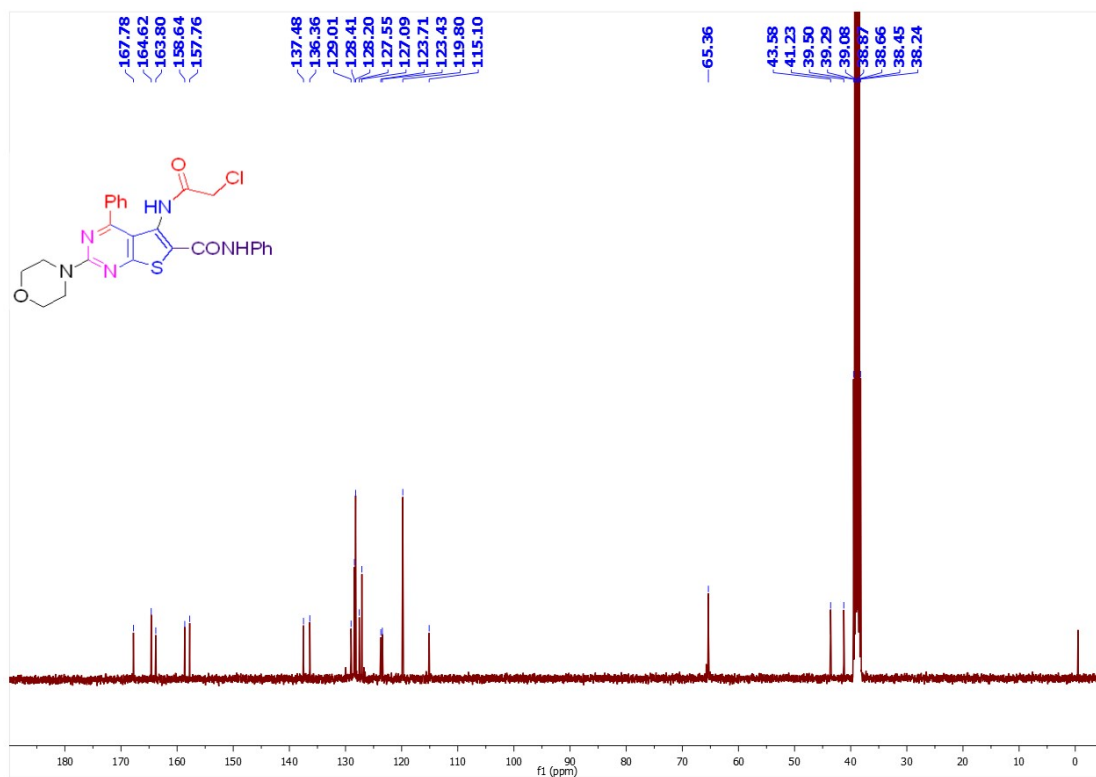


Figure S20. ¹³C NMR Spectrum of Compound 14.

Sample-12 #10638 RT: 36.21 AV: 1 NL: 2.73E2
T: + c EI Full ms [30.00-650.00]

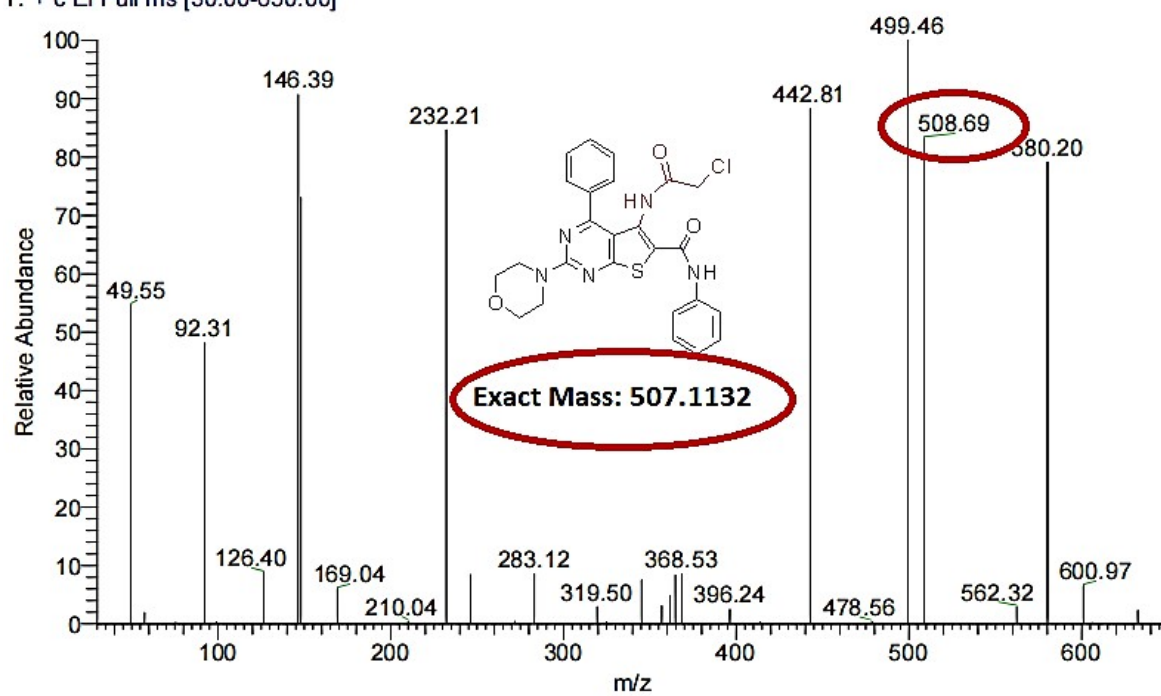


Figure S21. Mass Spectrum of Compound 14.