

Supplementary Information

New Derivatives of the Multi-Stage Active Malaria Box Compound MMV030666 and Their Antiplasmodial Potencies

Theresa Hermann ^{1,*}, Robin Wallner ¹, Johanna Dolensky ¹, Werner Seebacher ¹, Eva-Maria Pferschy-Wenzig ², Marcel Kaiser ^{3,4}, Pascal Mäser ^{3,4} and Robert Weis ¹

¹ Pharmaceutical Chemistry, Institute of Pharmaceutical Sciences, University of Graz, Schubertstraße 1, 8010 Graz, Austria

² Pharmacognosy, Institute of Pharmaceutical Sciences, University of Graz, Beethovenstraße 8, 8010 Graz, Austria

³ Swiss Tropical and Public Health Institute, Kreuzstraße 2, Allschwil, CH-4123 Basel, Switzerland

⁴ Faculty of Philosophy and Natural Sciences, Swiss Tropical and Public Health Institute Petersplatz 1, University of Basel, CH-4003 Basel, Switzerland

* Correspondence: theresa.hermann@uni-graz.at; Tel.: +43-316-380-5381; Fax: +43-316-380-9846

NMR spectra data of compounds 10, 11, 13-15 and 26-47

Figure S1. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound **10** (CDCl₃)

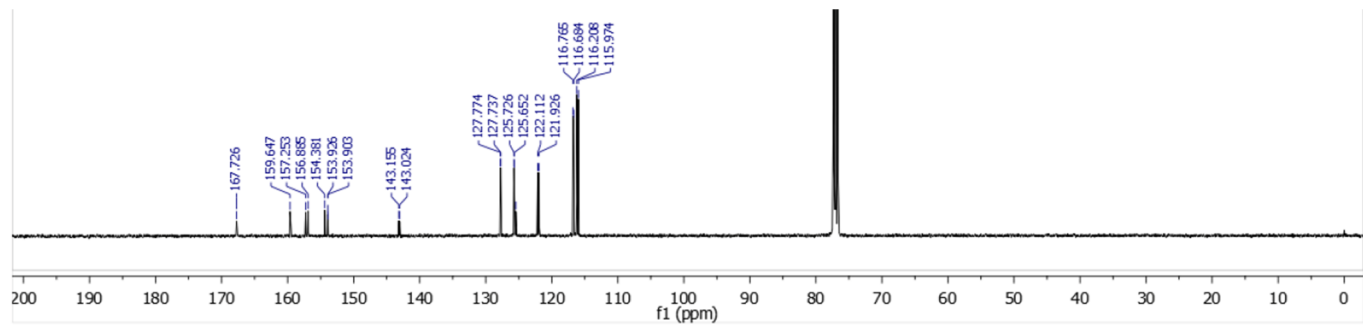
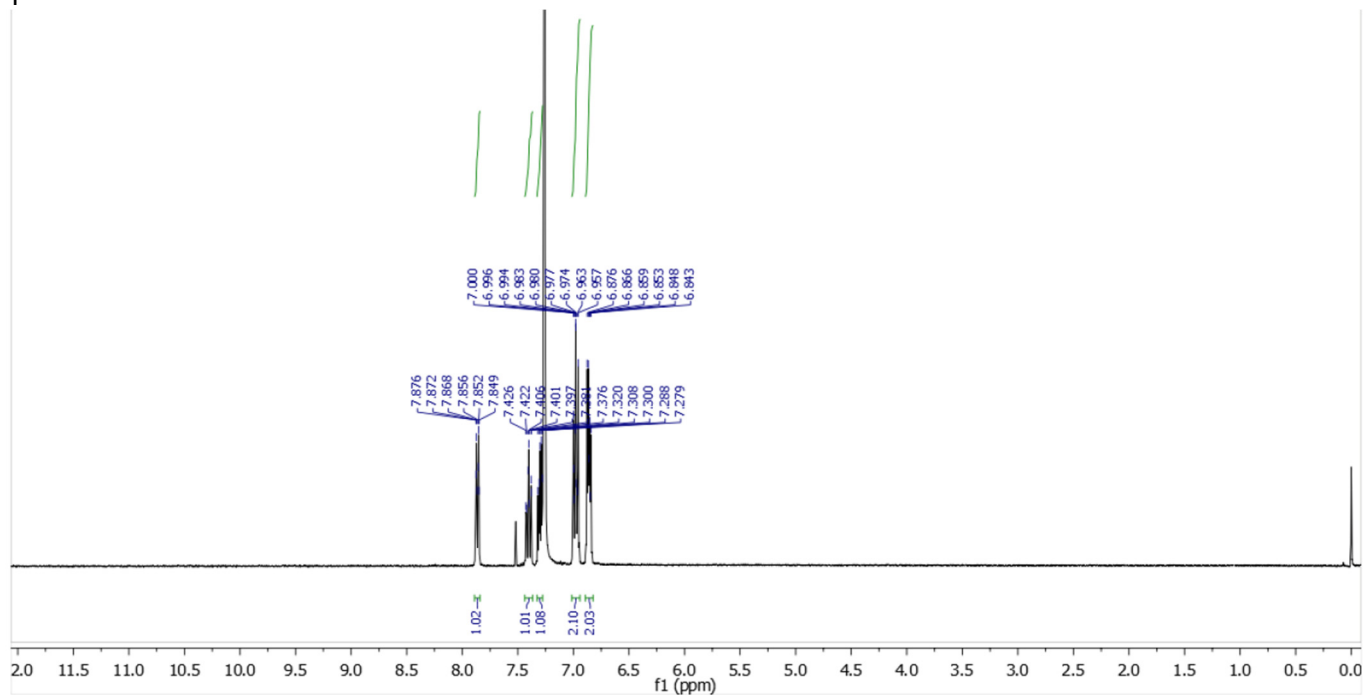
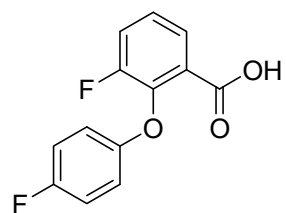


Figure S2. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound 11 (CDCl₃)

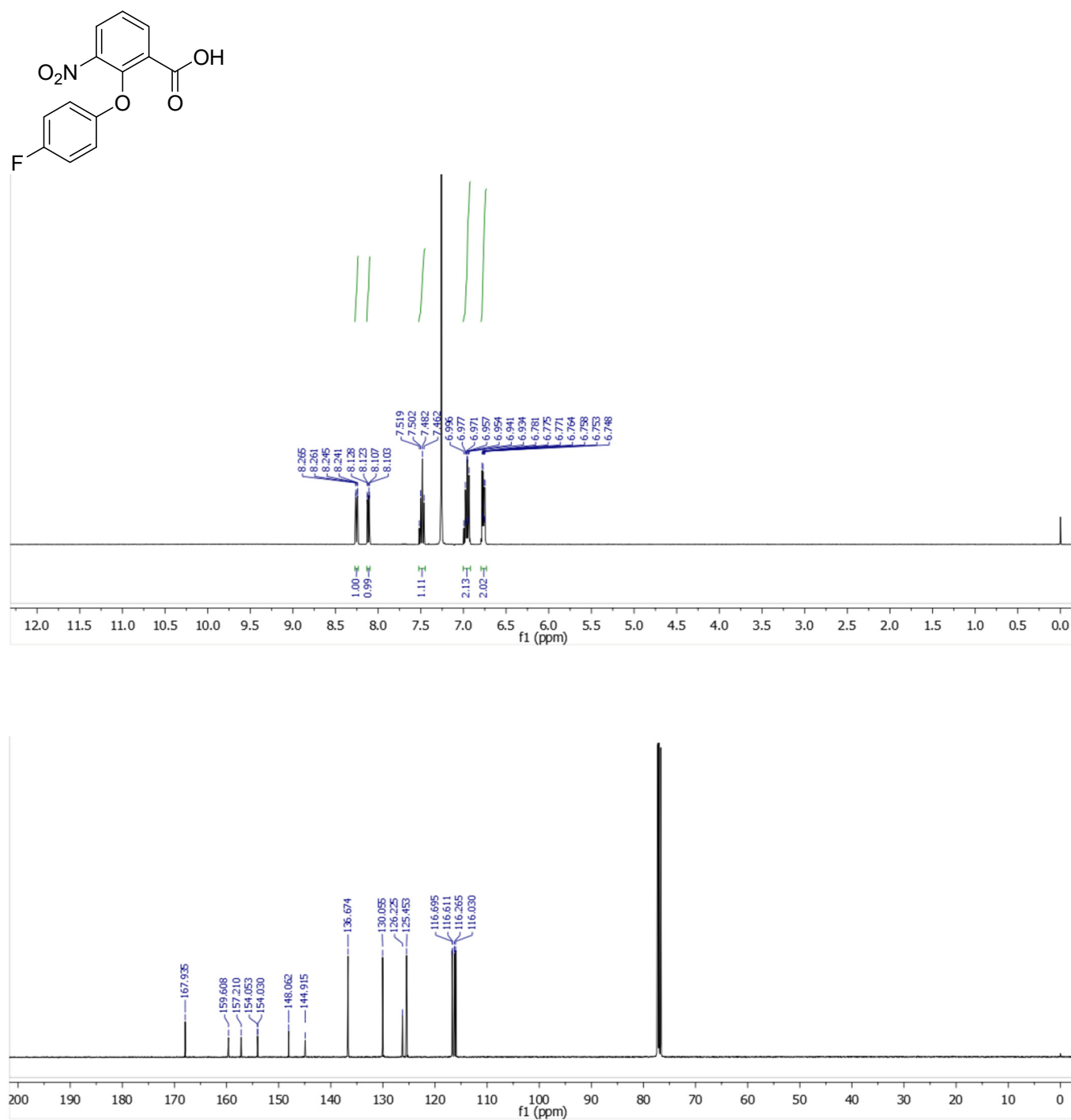


Figure S3. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **13** (CDCl_3)

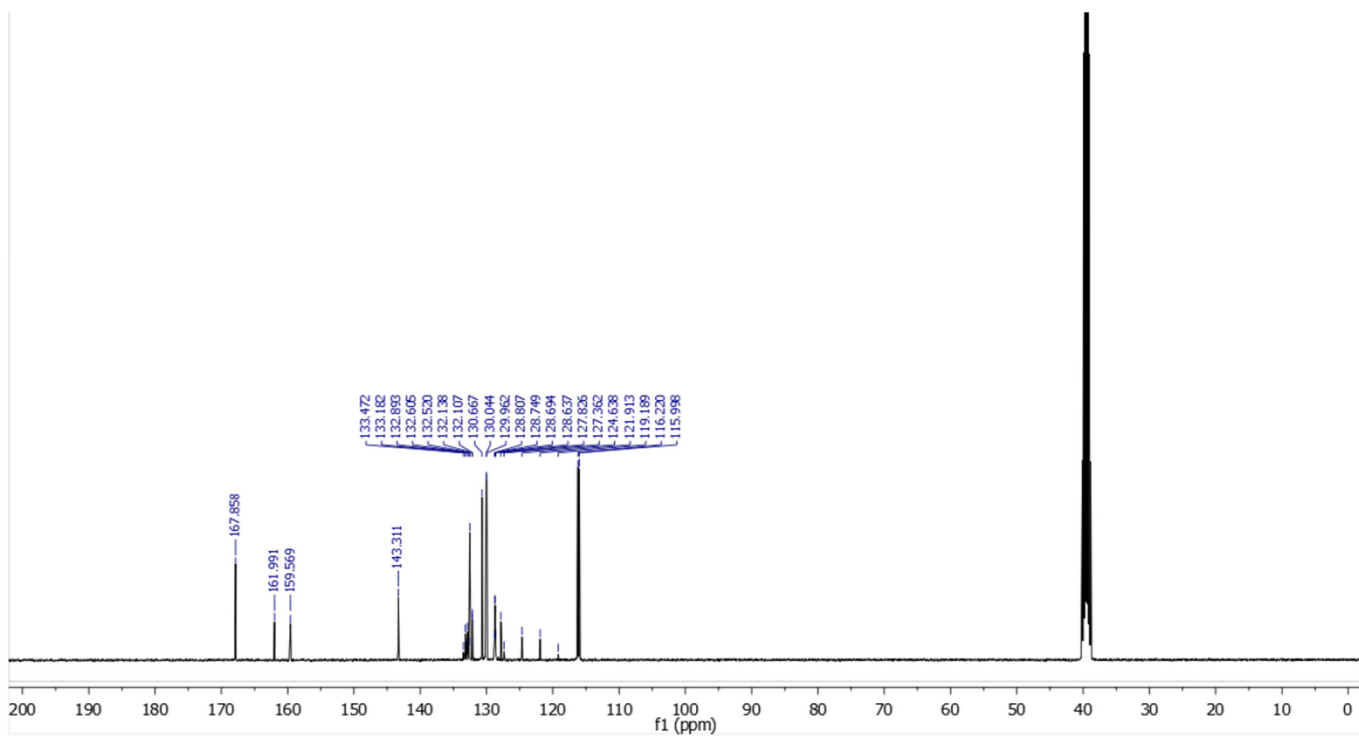
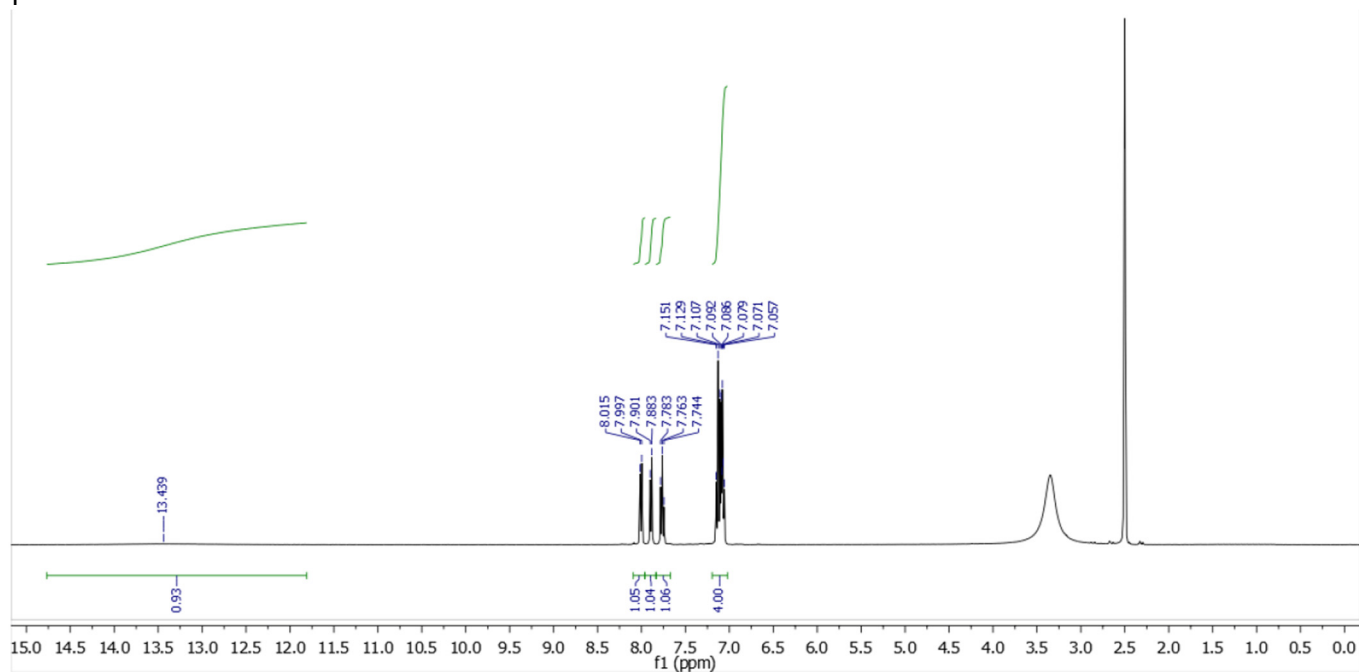
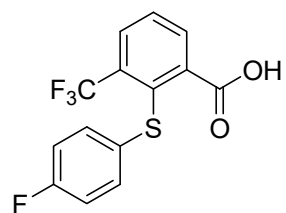


Figure S4. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound **14** (CDCl₃)

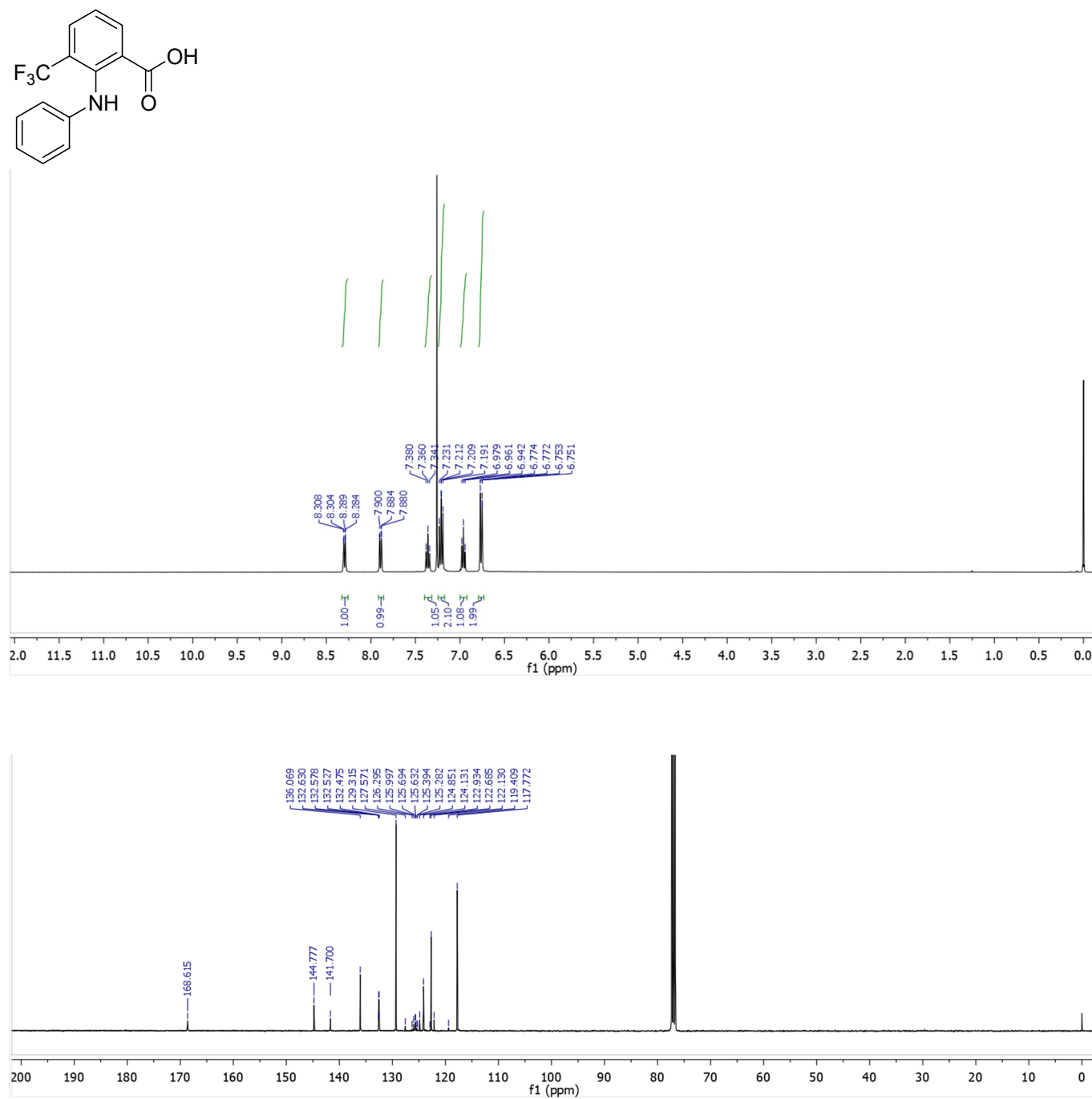


Figure S5. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound 15 (CDCl₃)

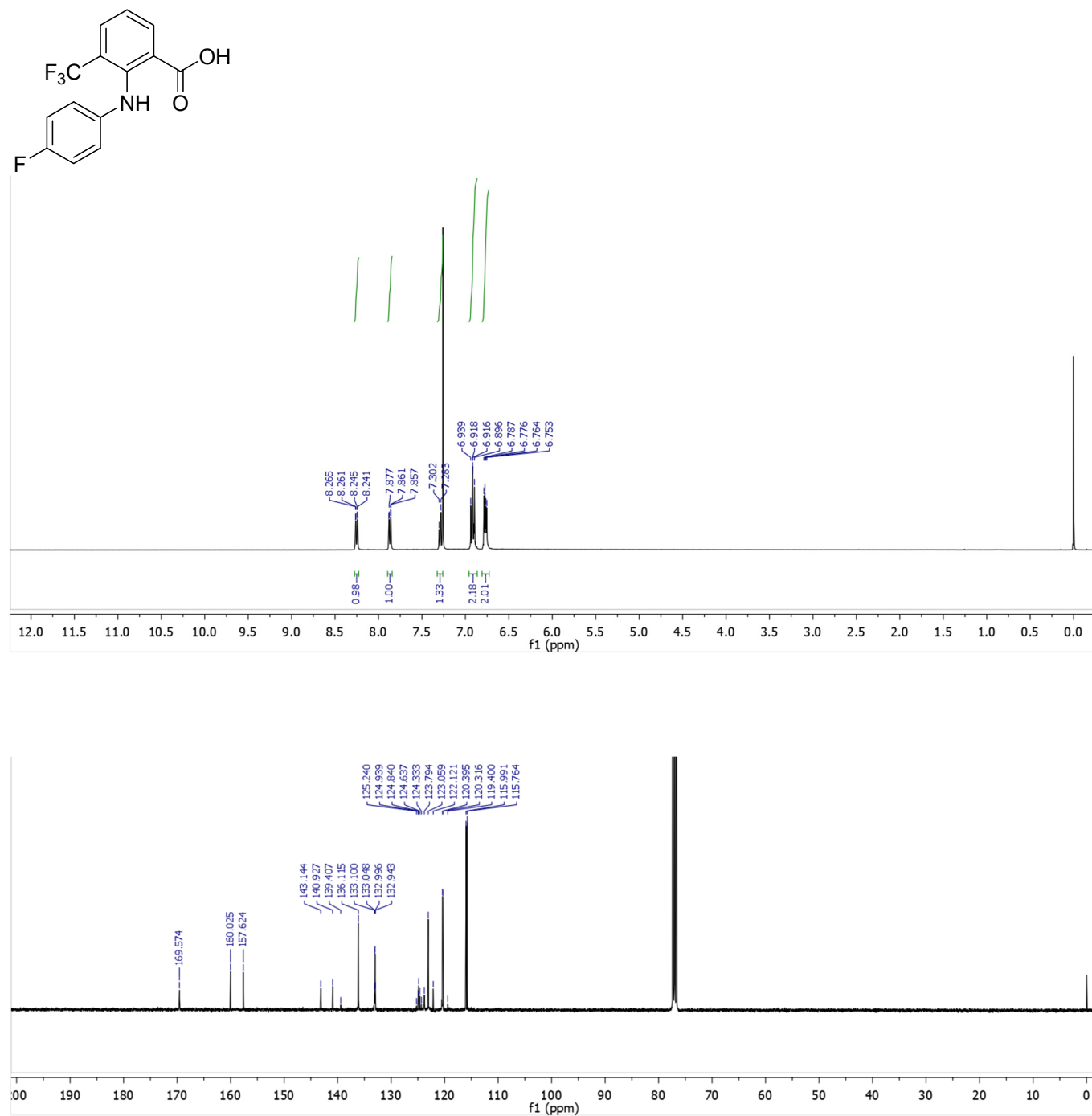


Figure S6. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **26** (CDCl_3)

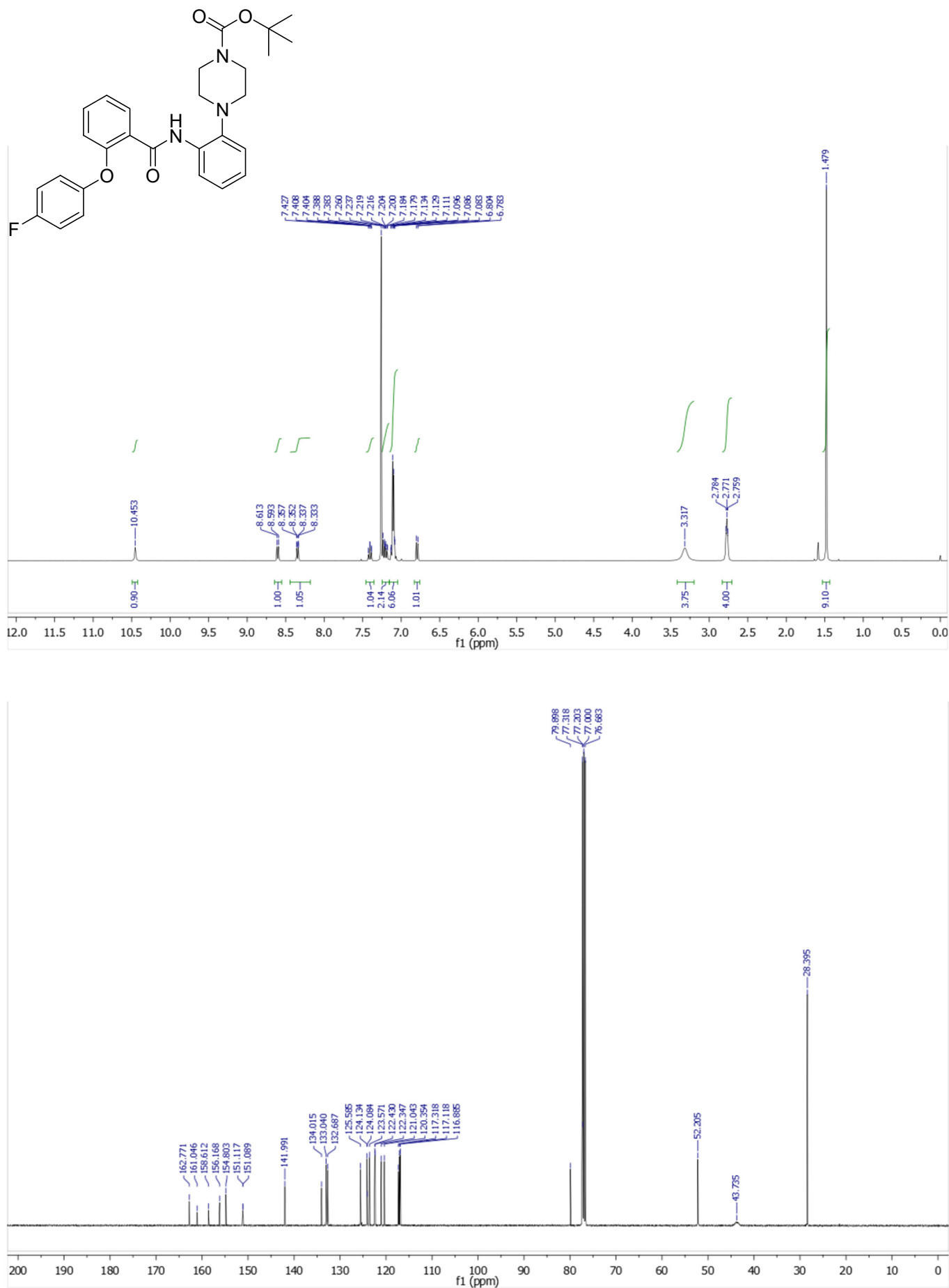


Figure S7. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound 27 (CDCl₃)

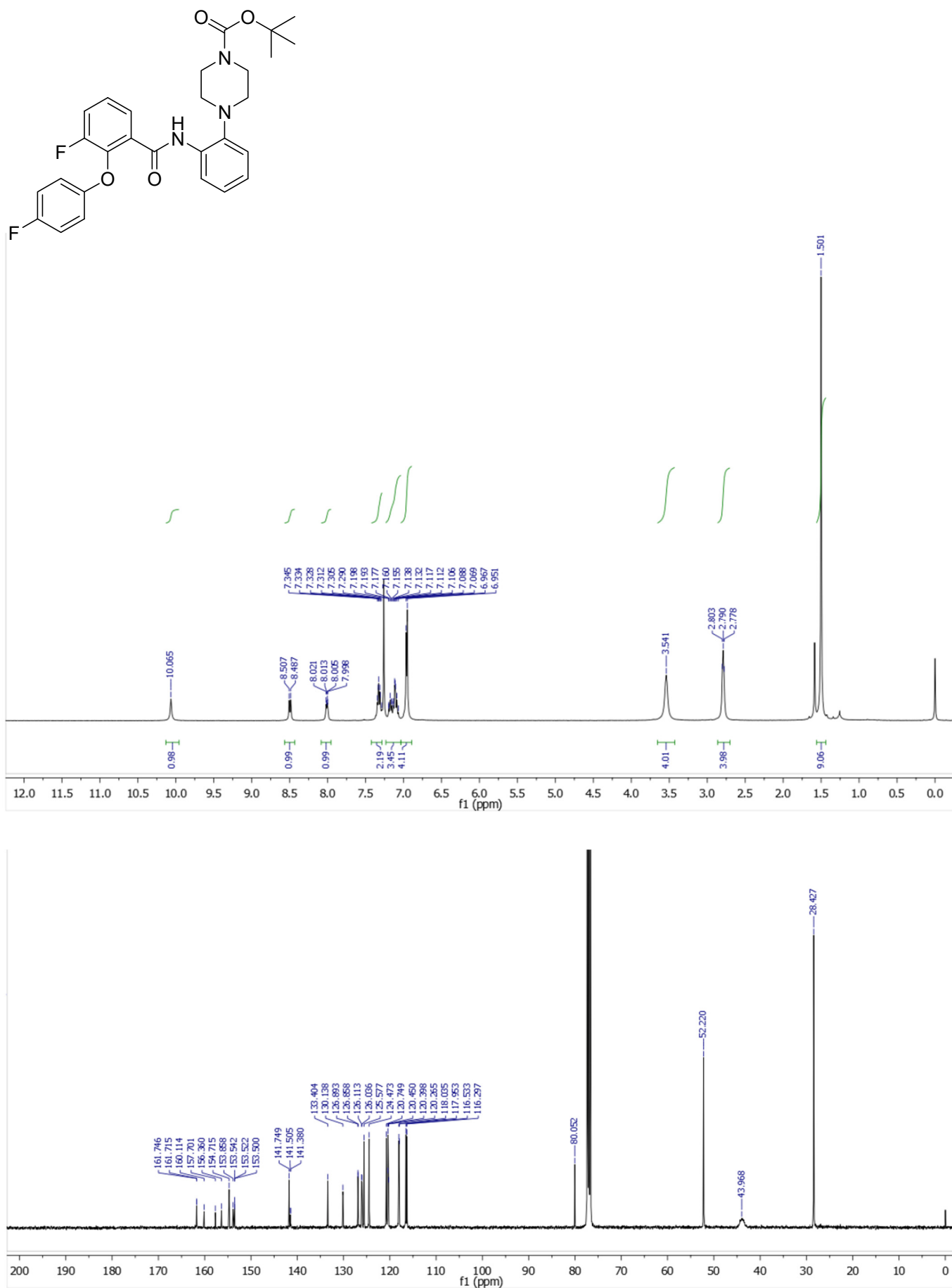


Figure S8. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound 28 (CDCl₃)

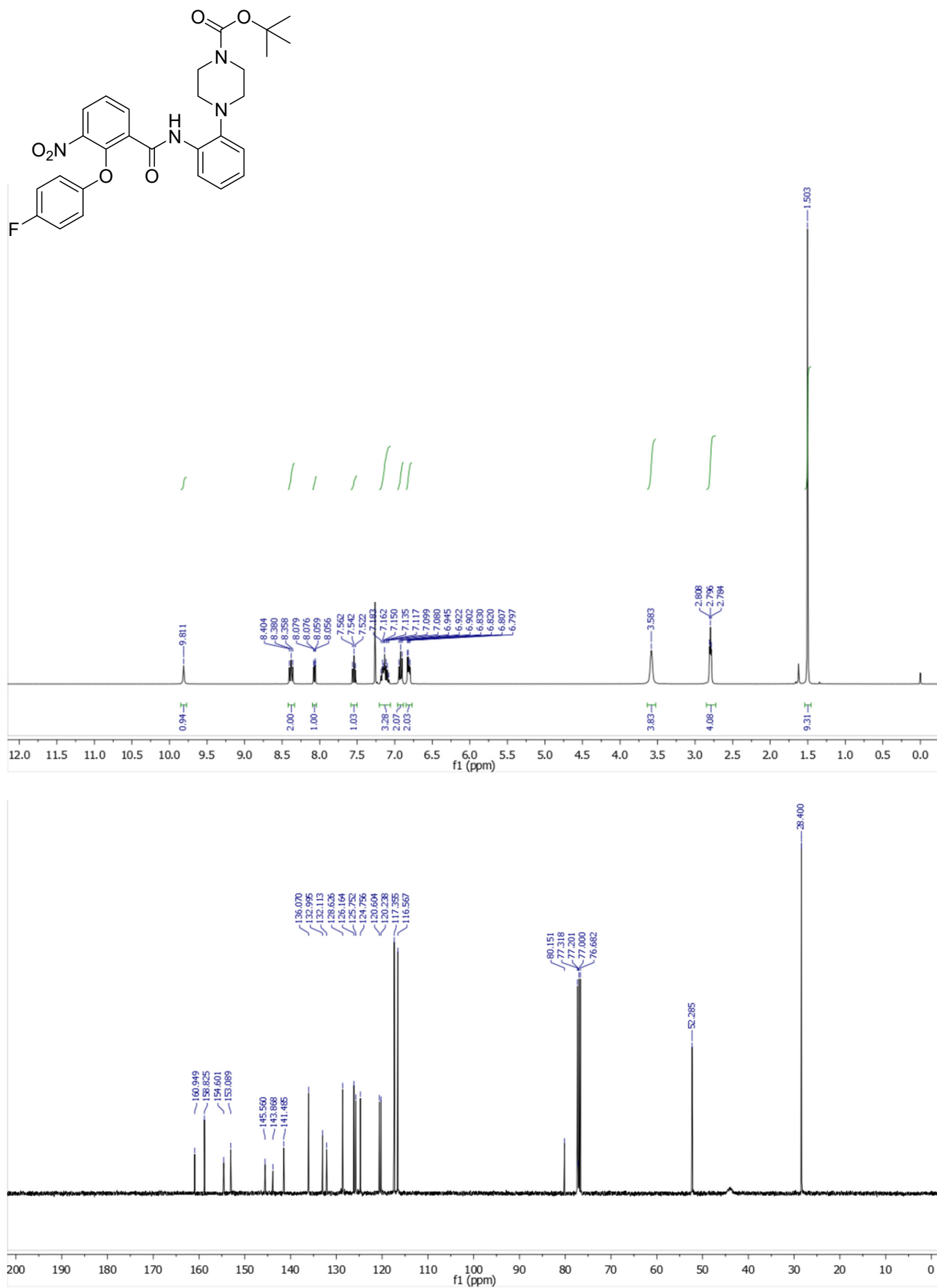


Figure S9. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound **29** (CDCl₃)

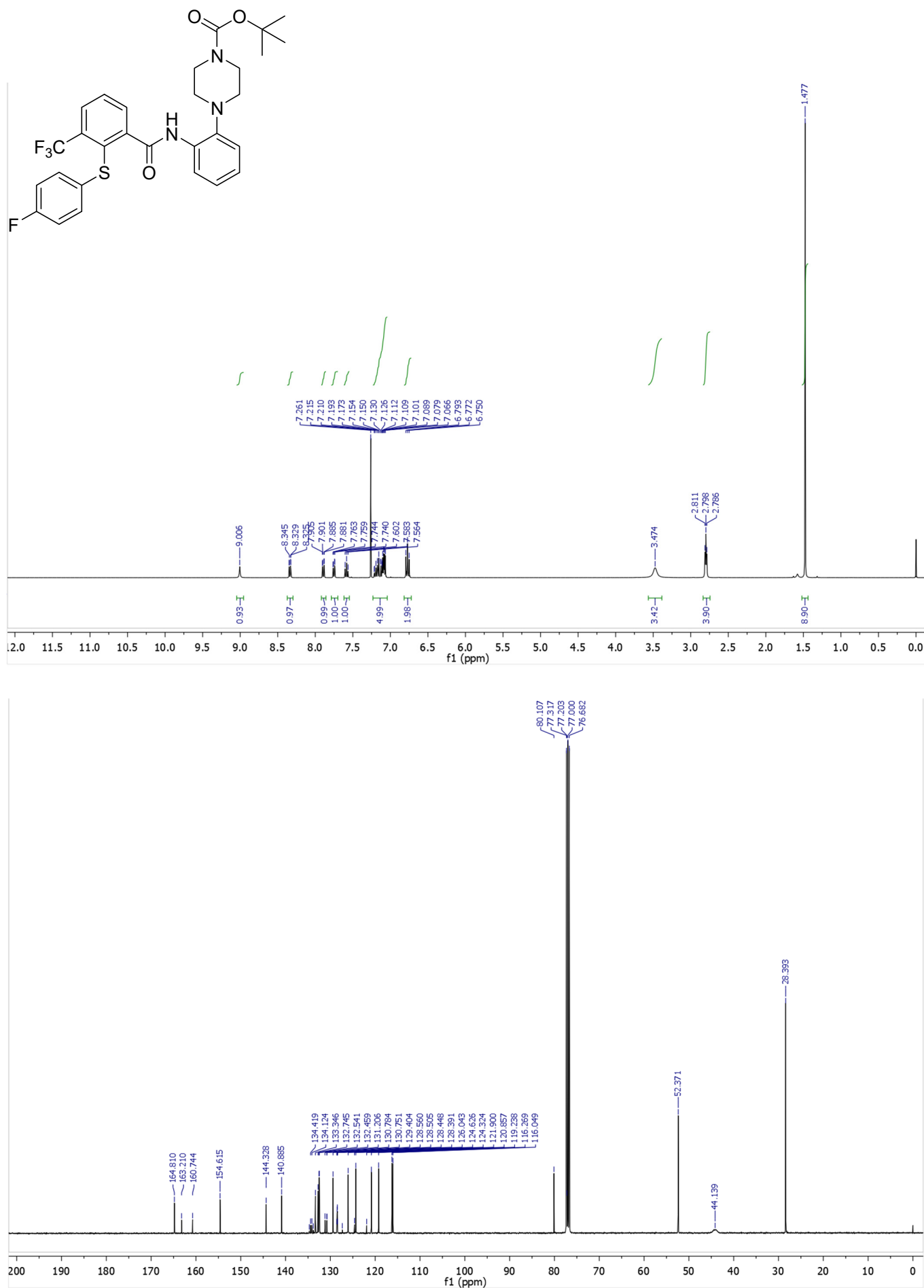


Figure S10. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **30** (CDCl_3)

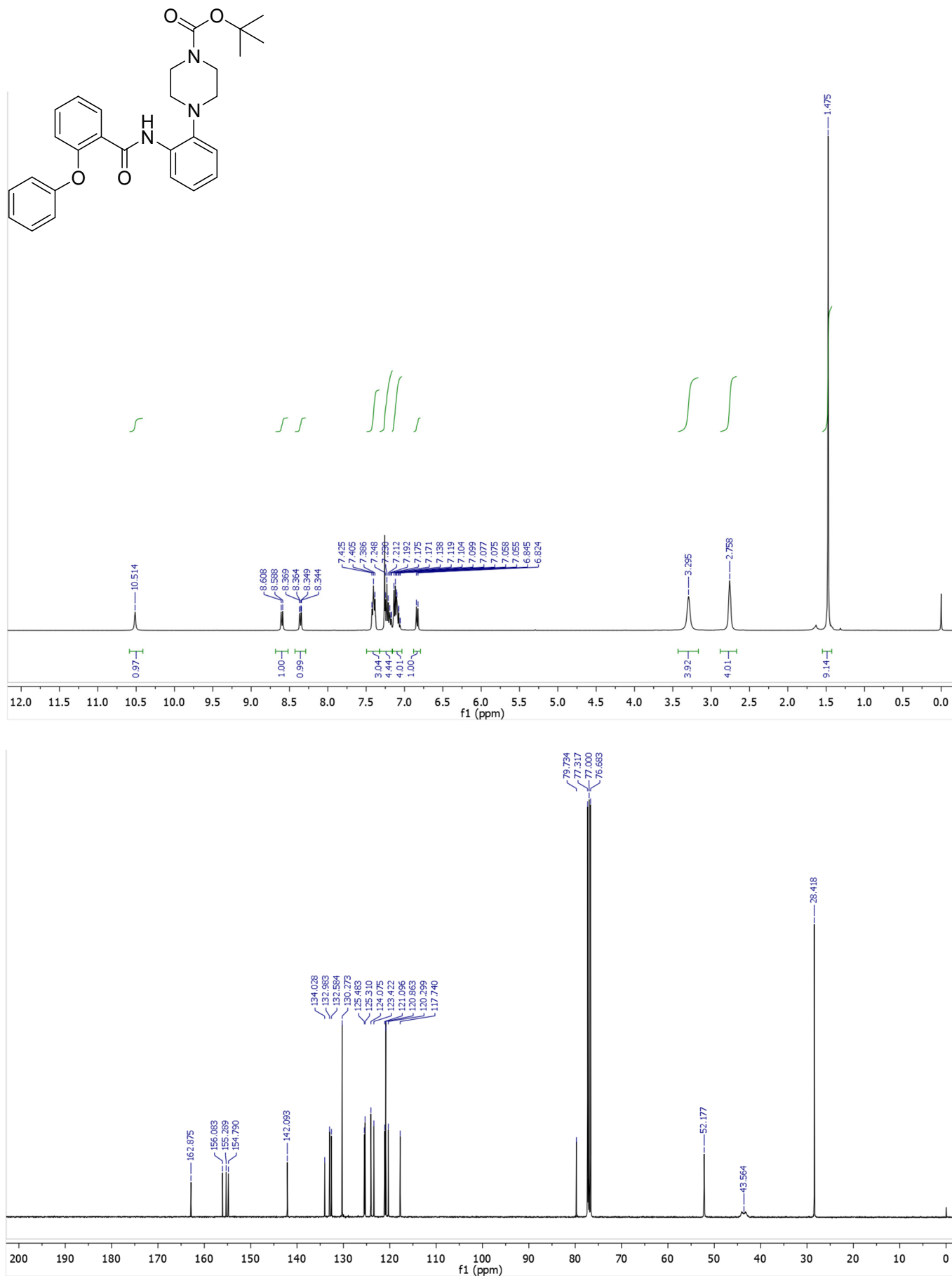


Figure S11. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **31** (CDCl_3)

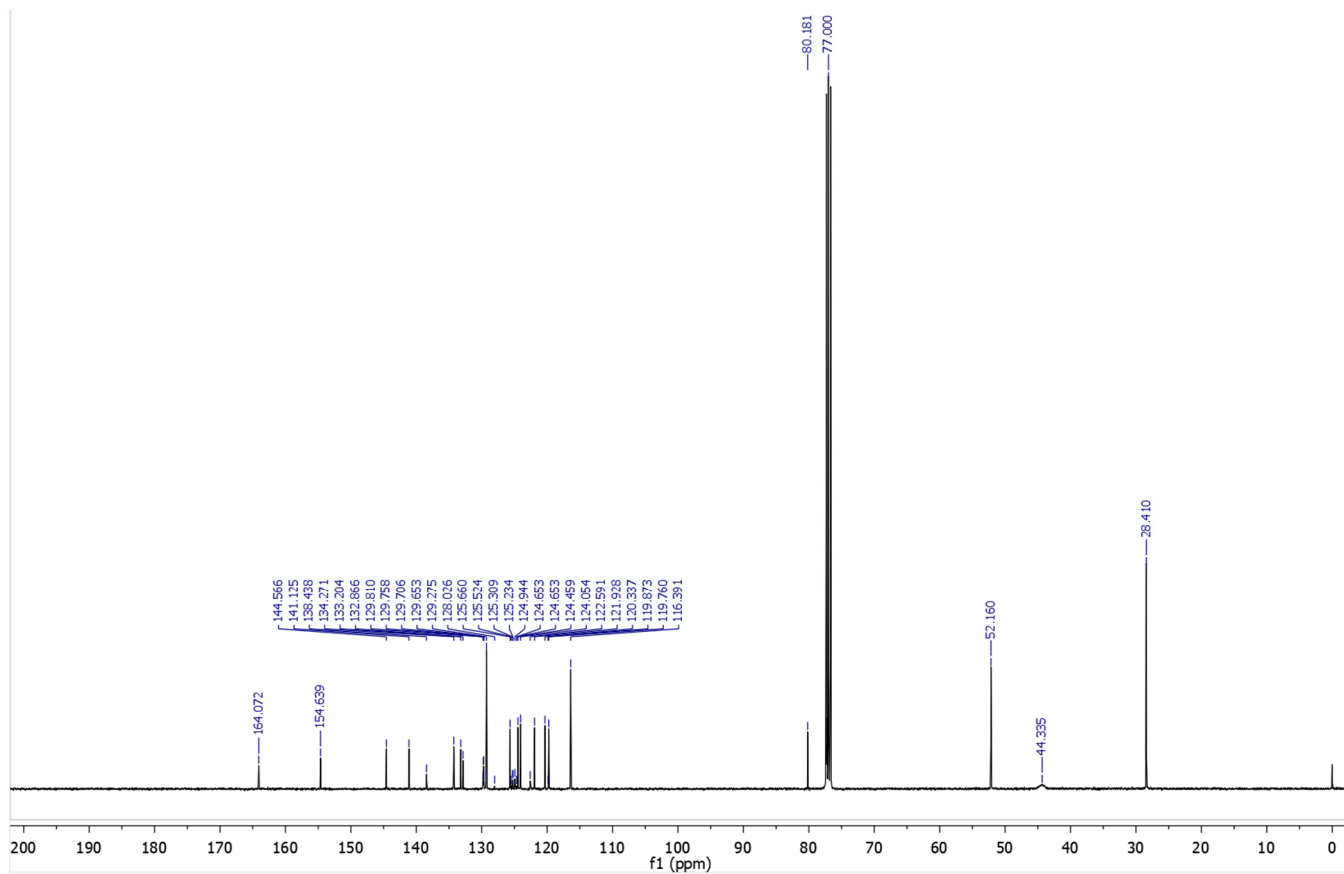
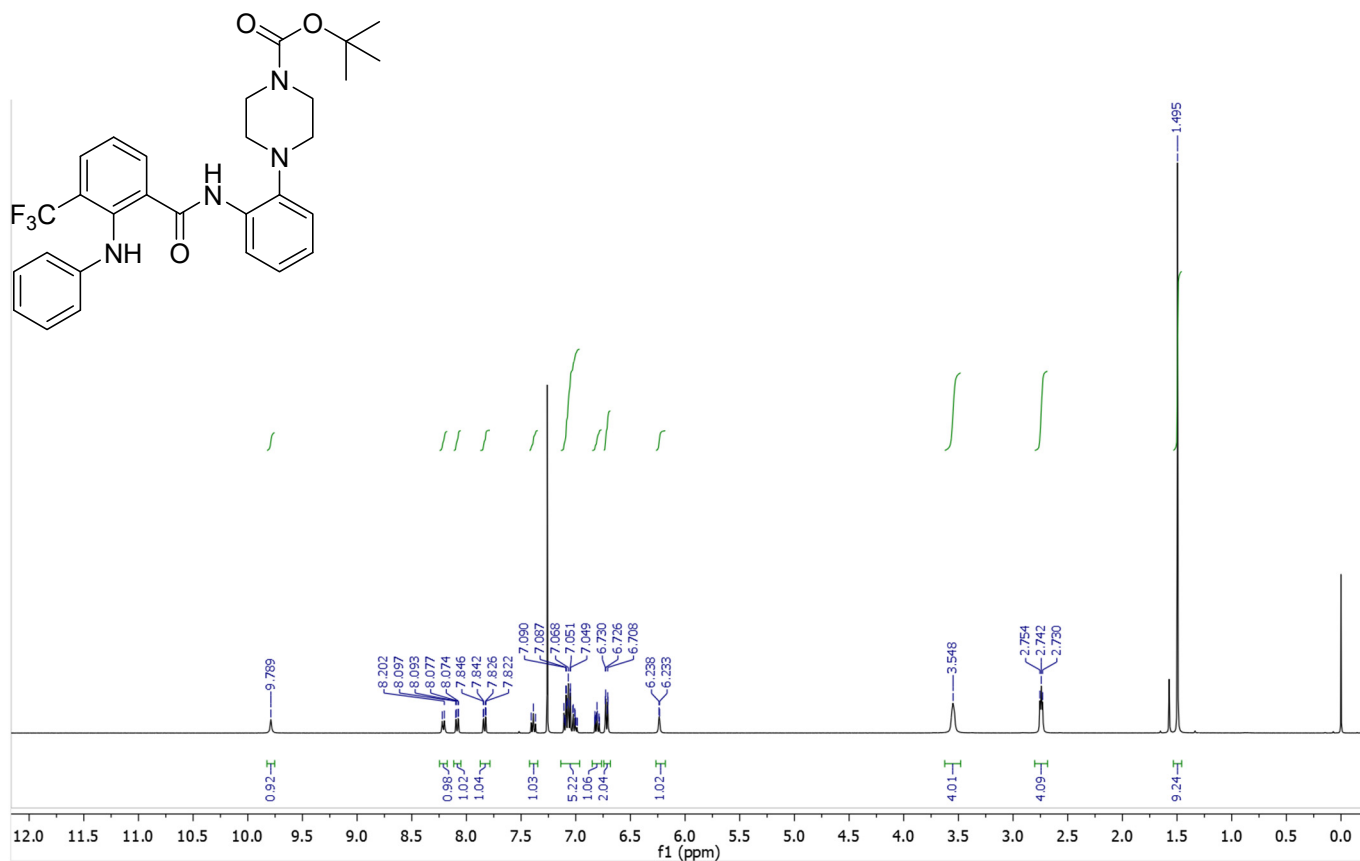


Figure S12. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **32** (CDCl_3)

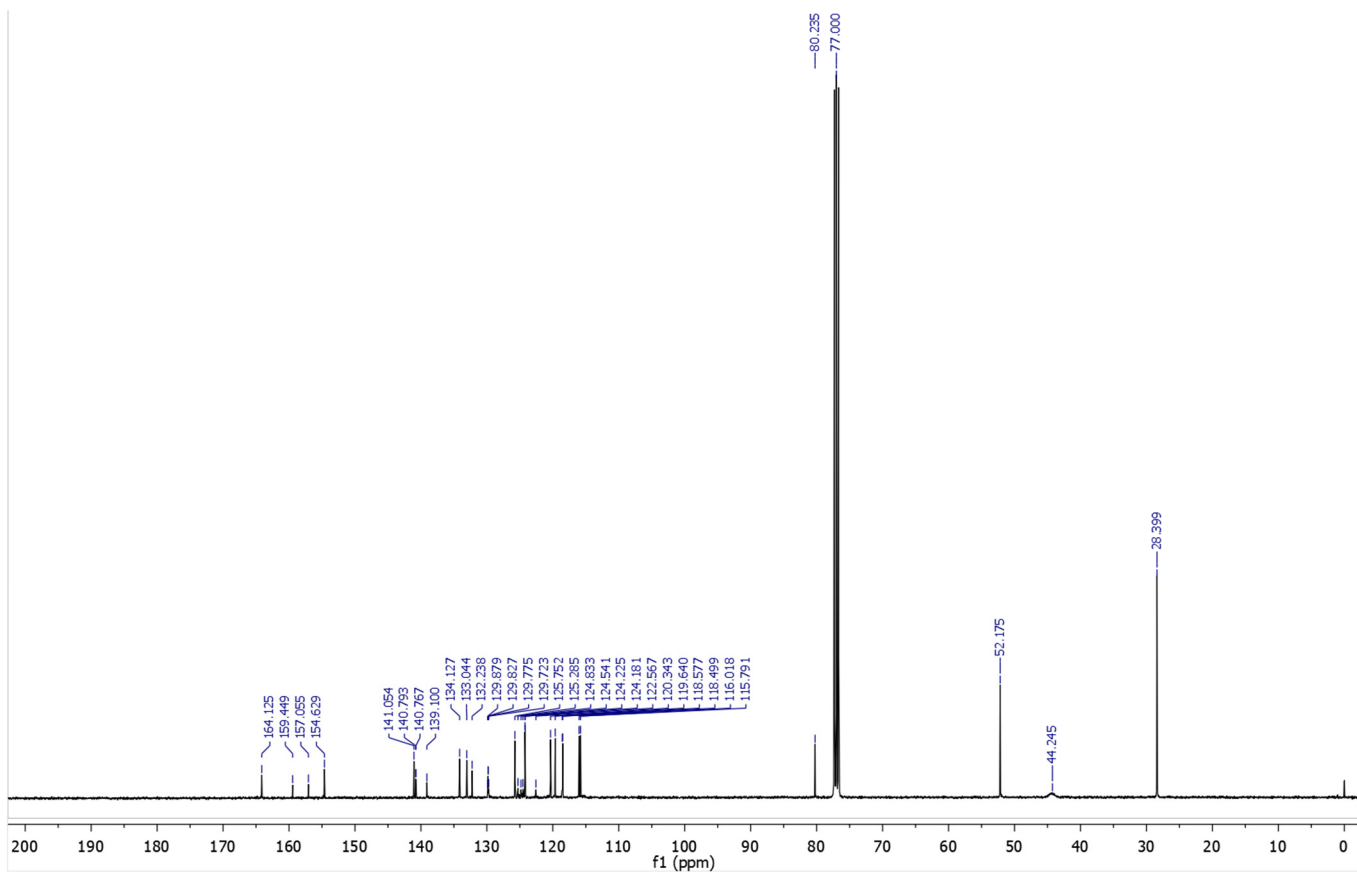
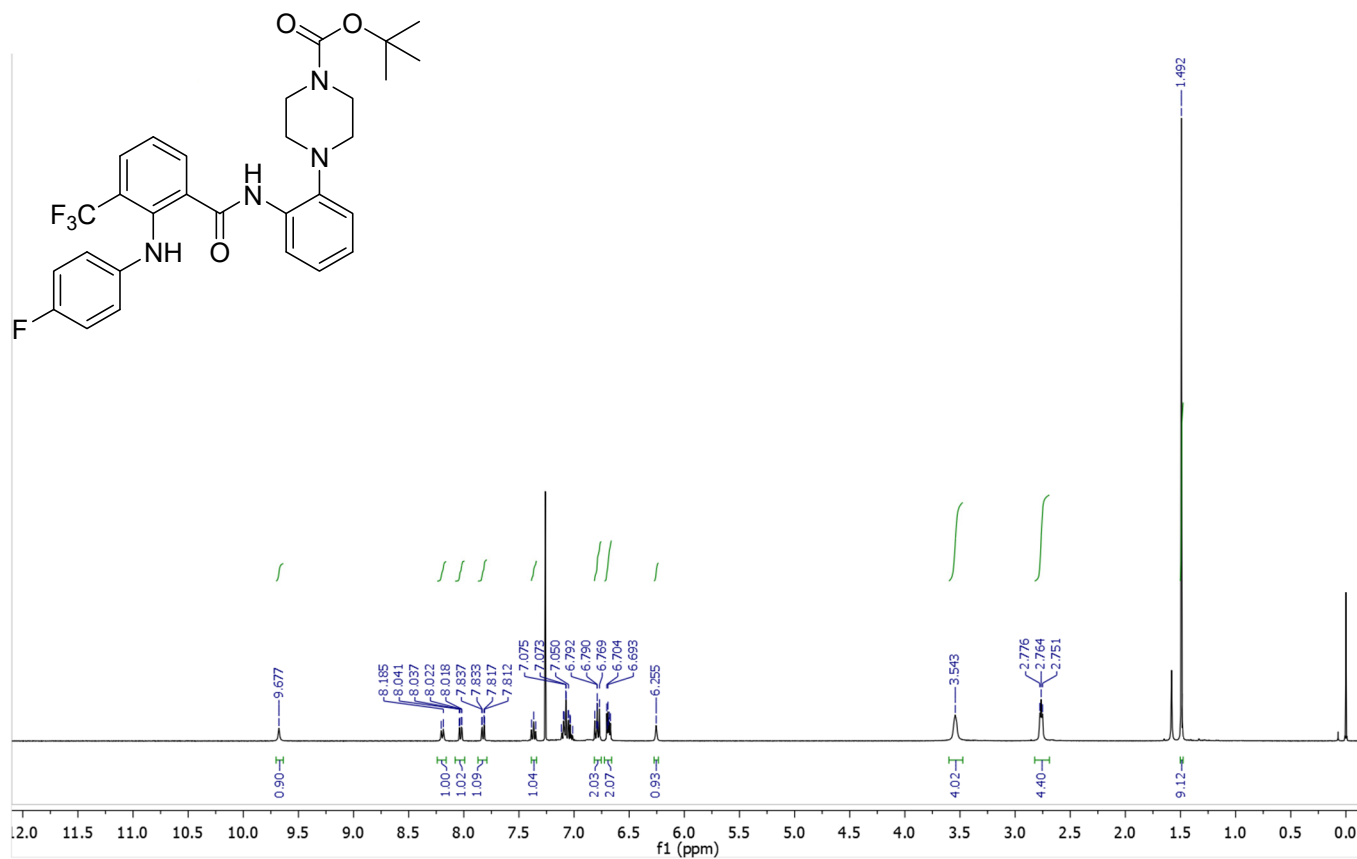


Figure S13. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **33** (CDCl_3)

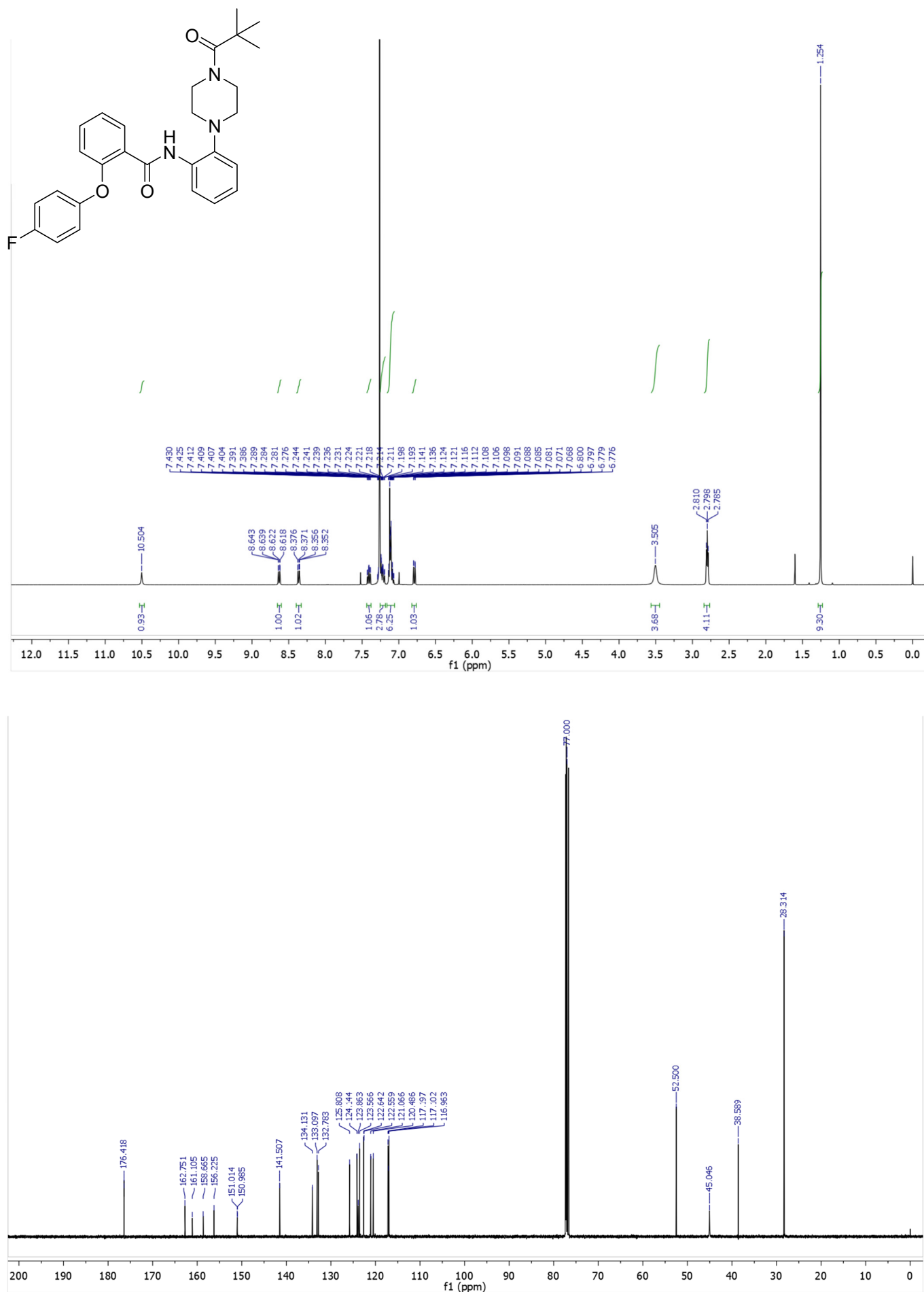


Figure S14. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **34** (CDCl_3)

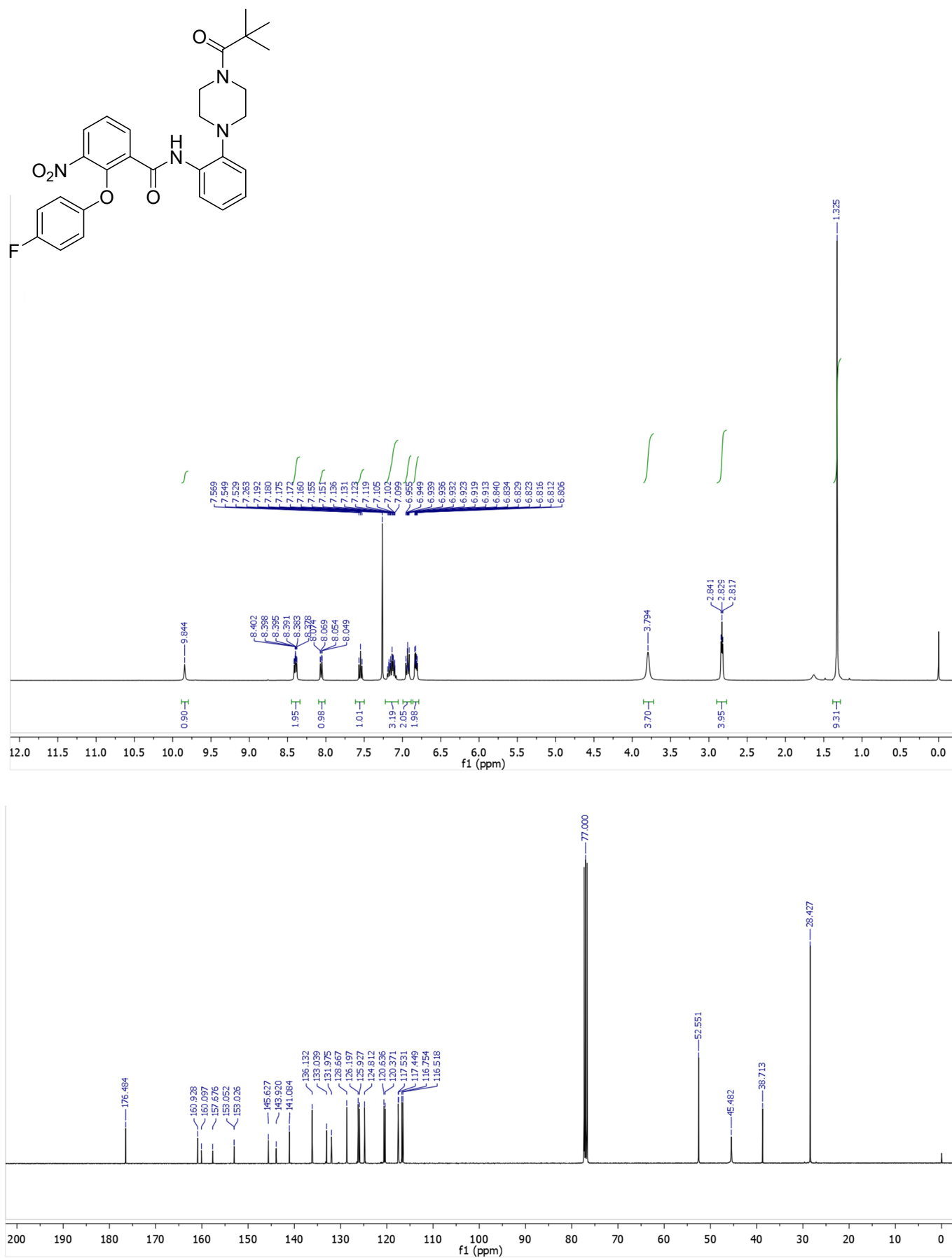


Figure S15. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound 35 (CDCl₃)

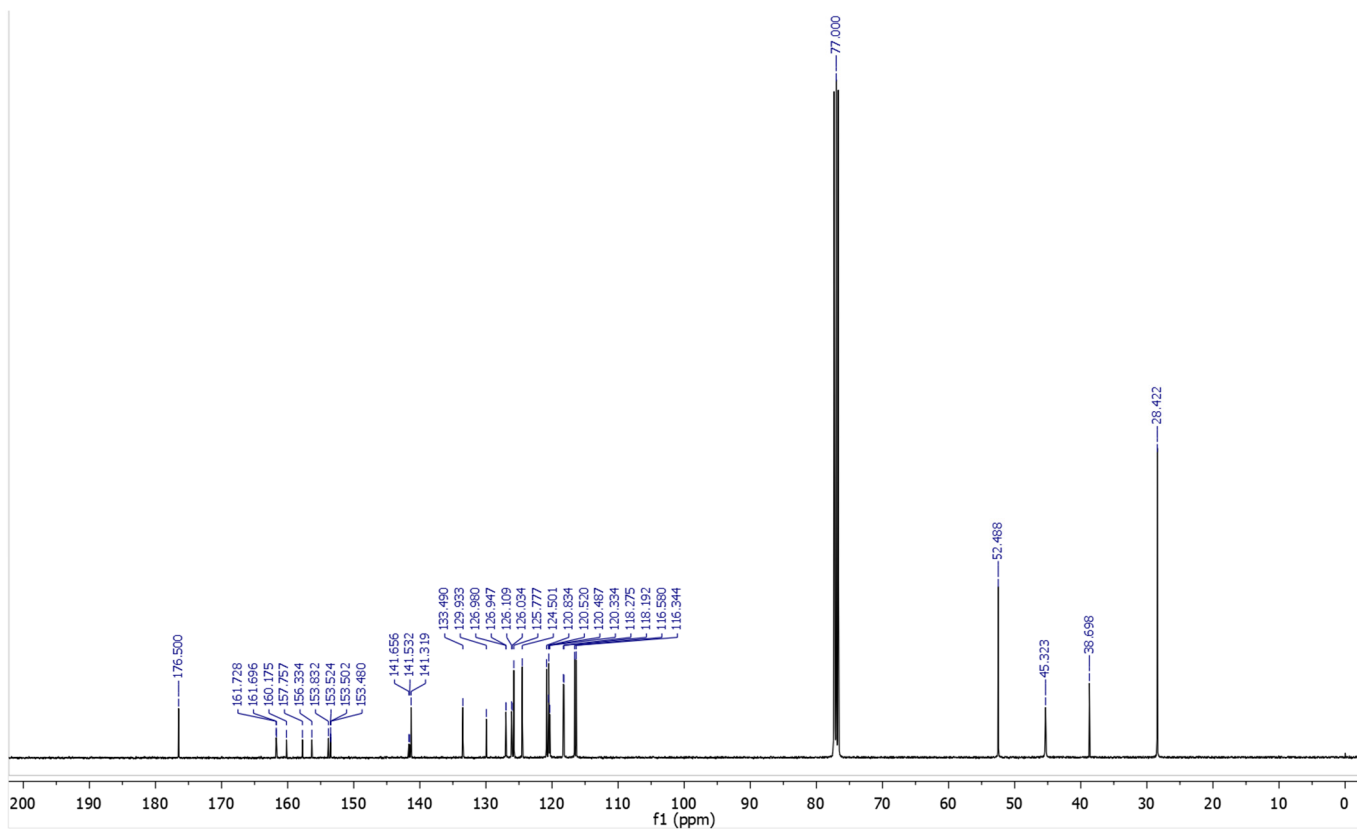
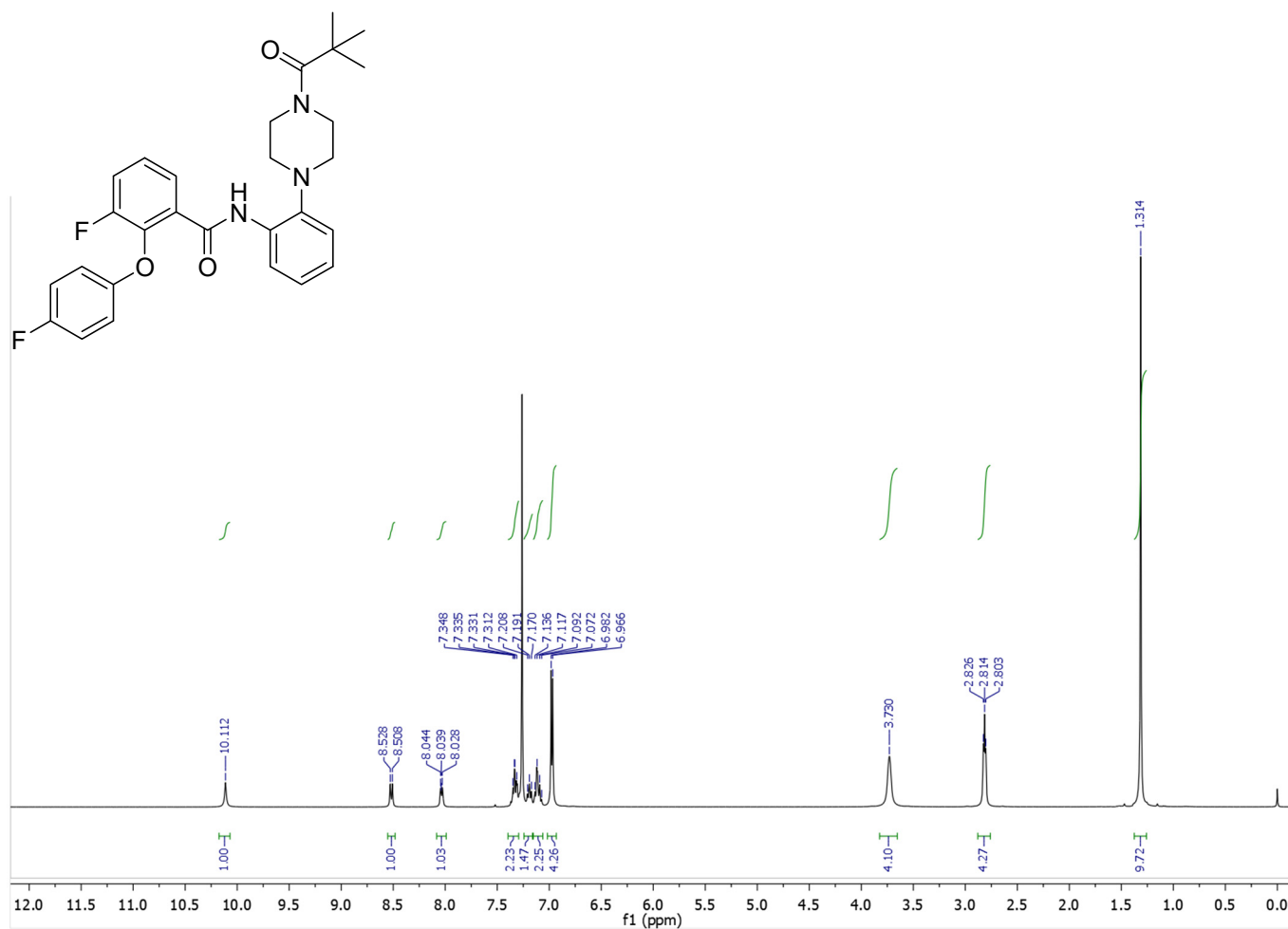


Figure S16. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **36** (CDCl_3)

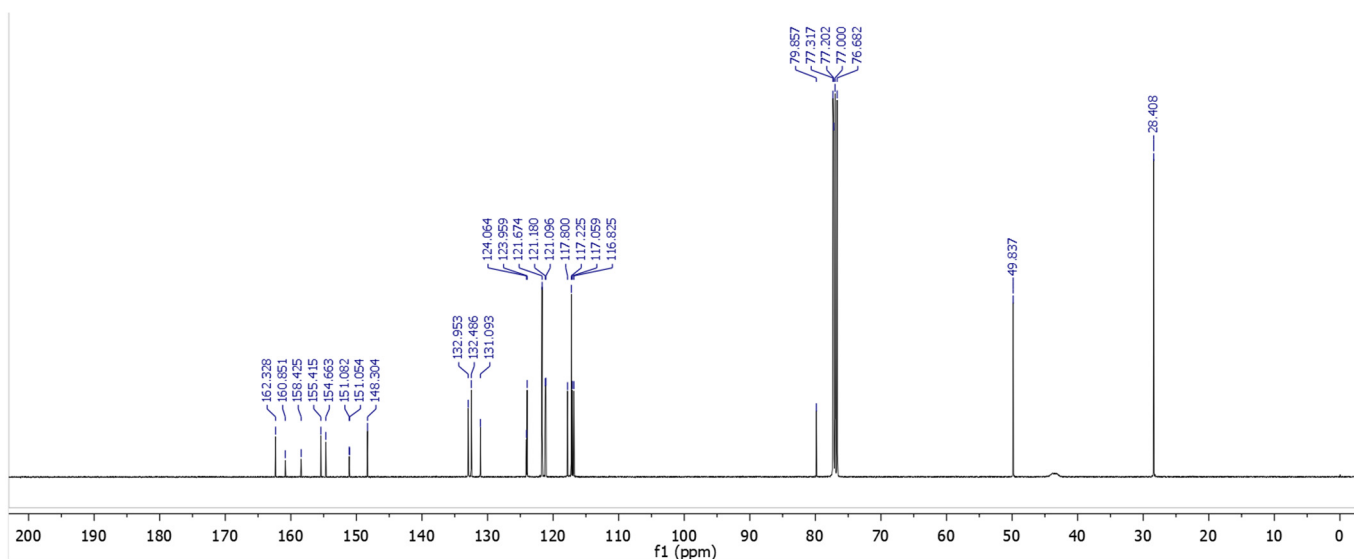
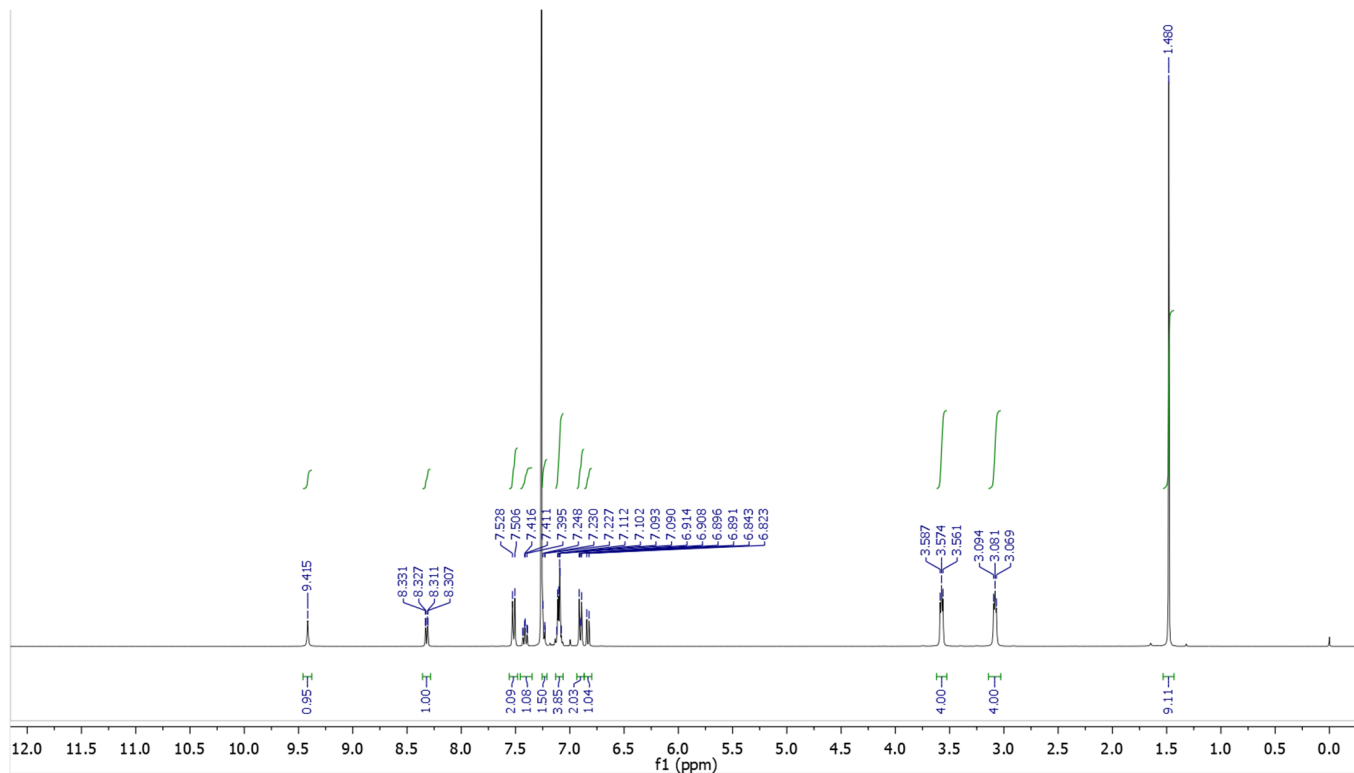
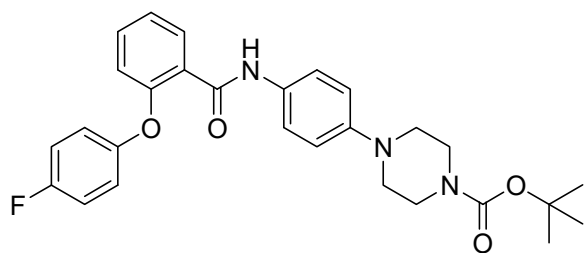


Figure S17. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **37** (CDCl_3)

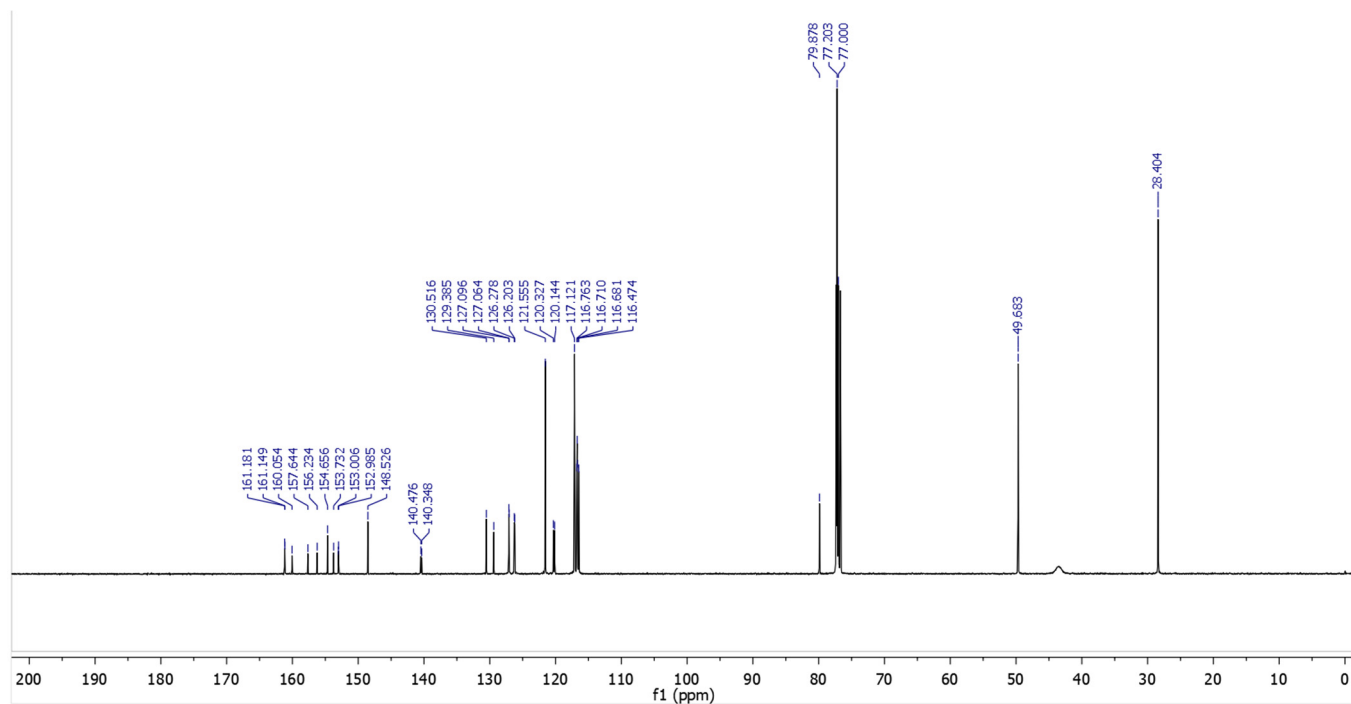
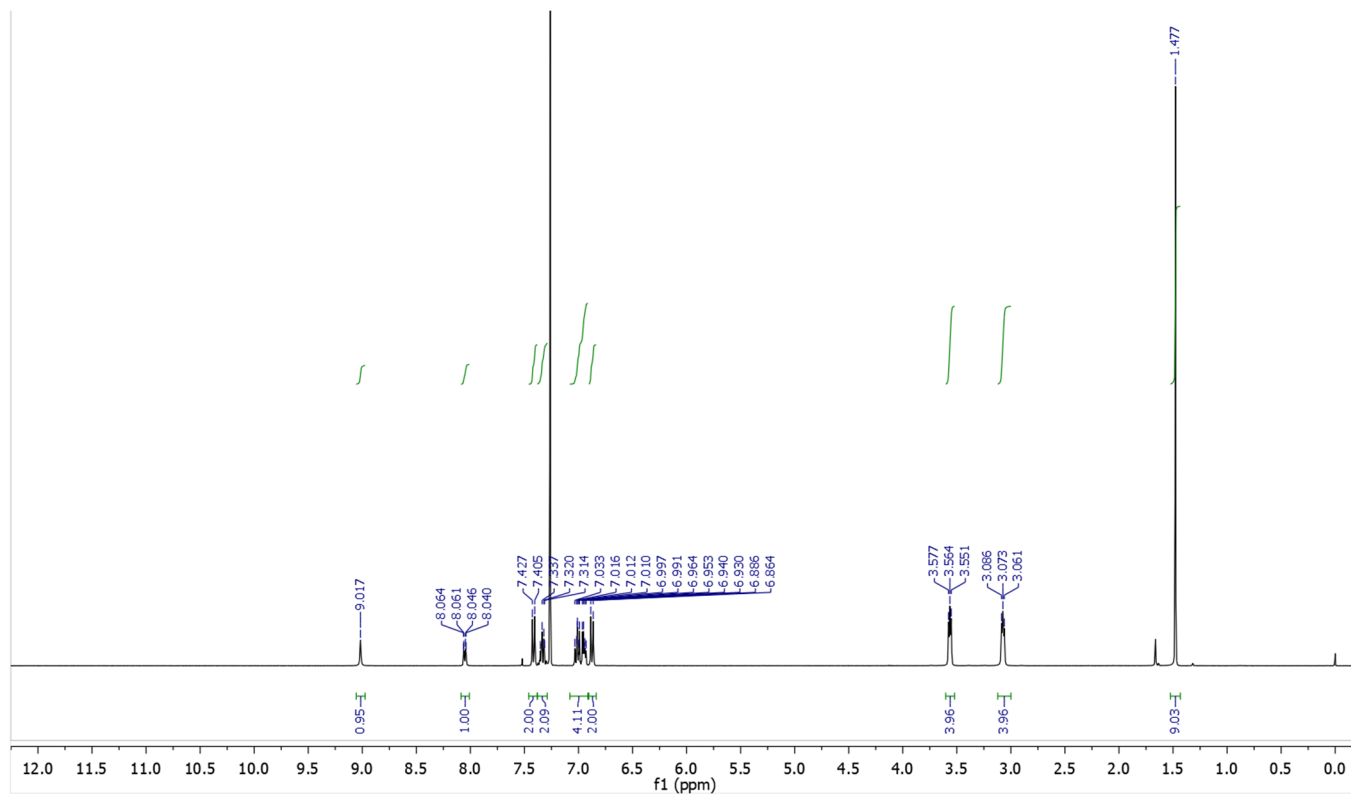
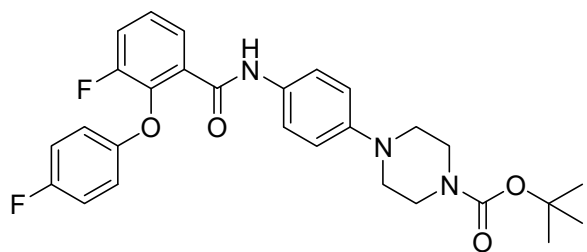


Figure S18. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **38** (CDCl_3)

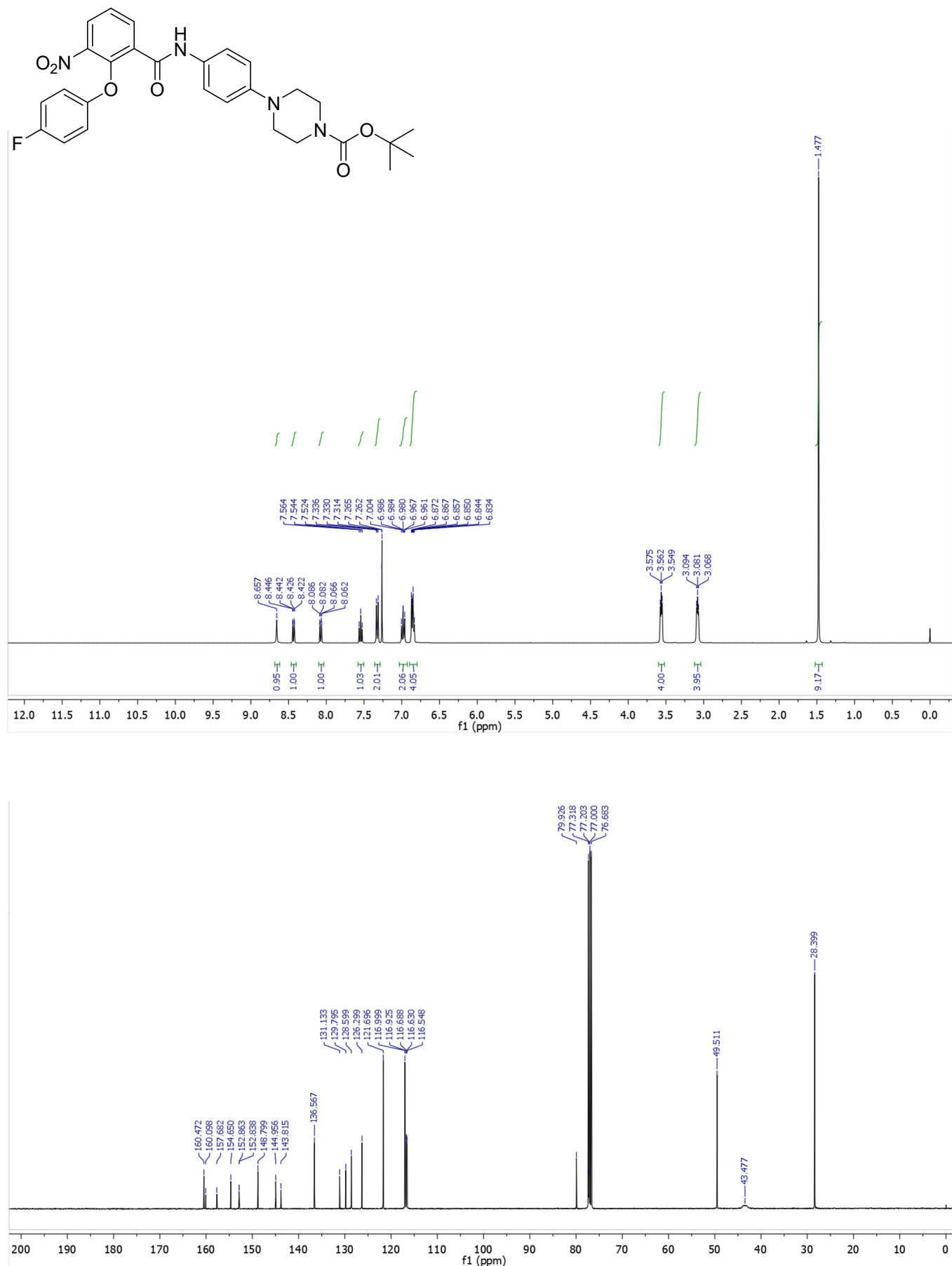


Figure S19. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **39** (CDCl_3)

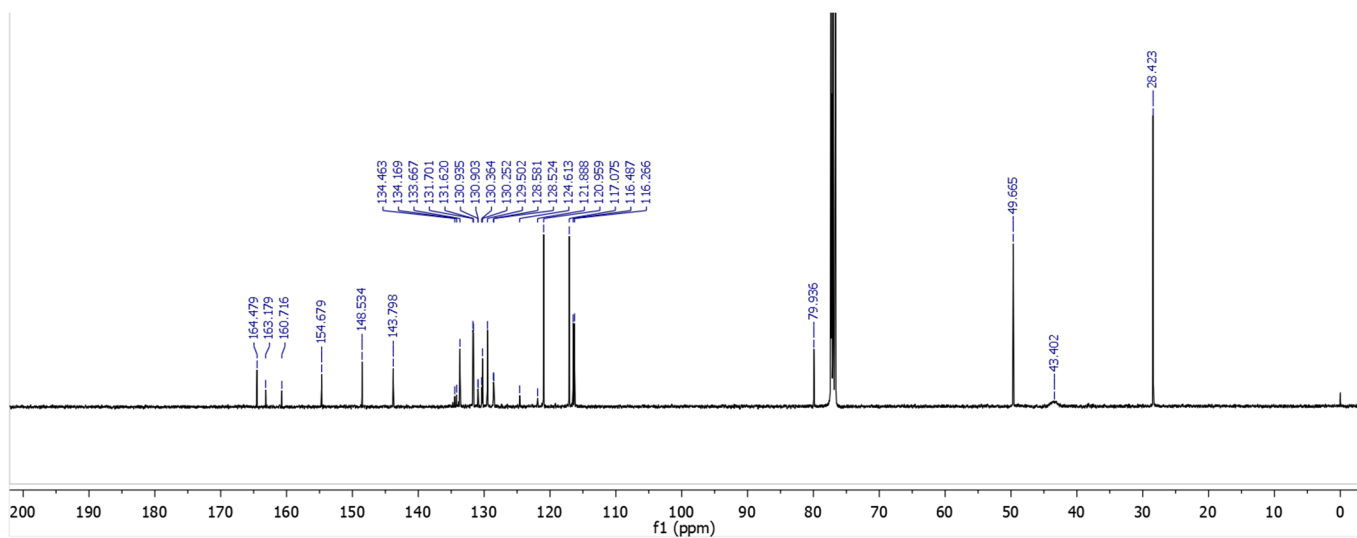
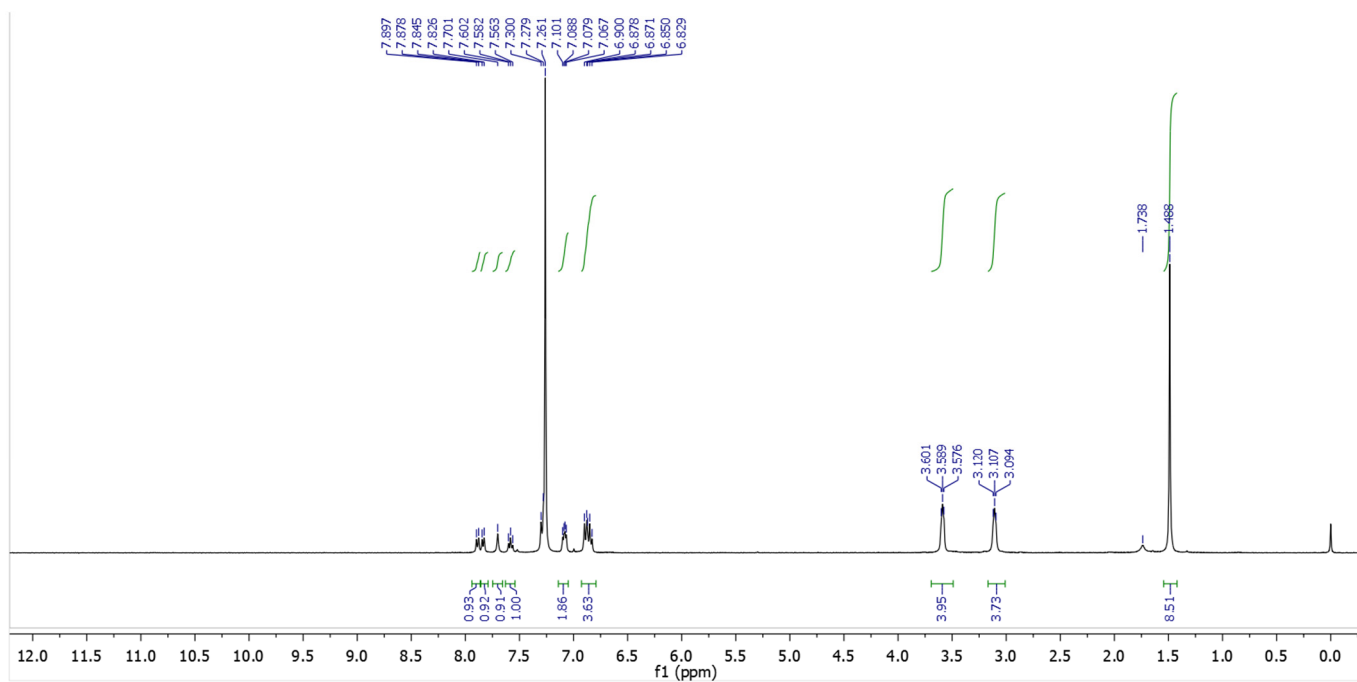
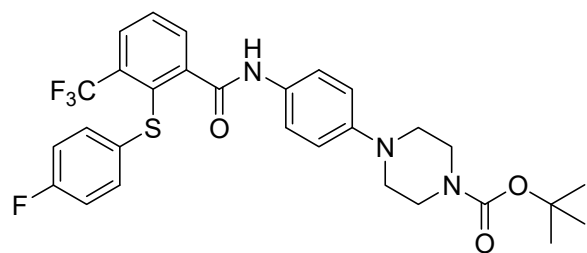


Figure S20. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **40** (CDCl_3)

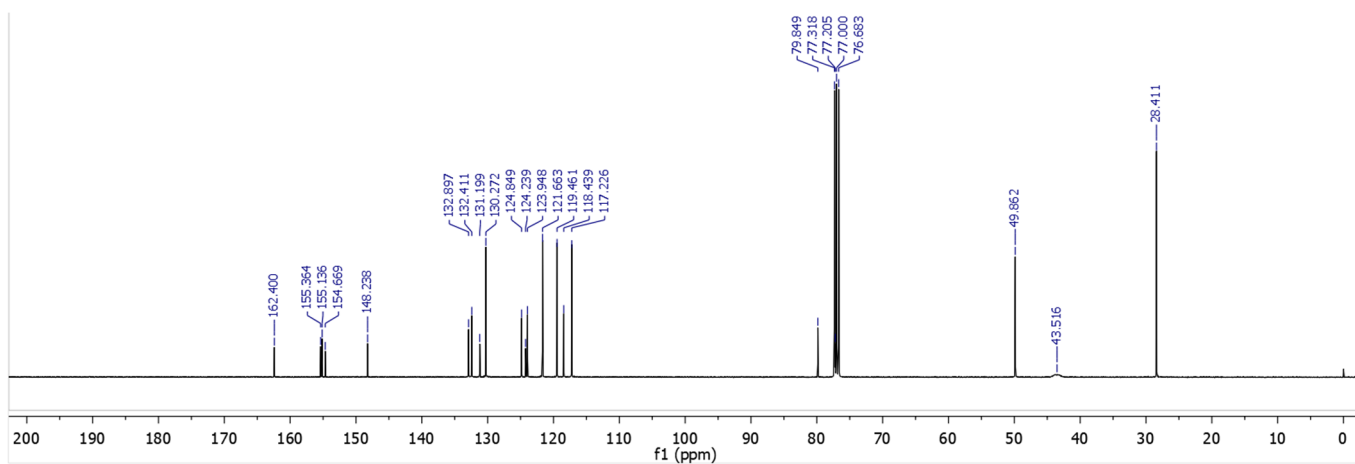
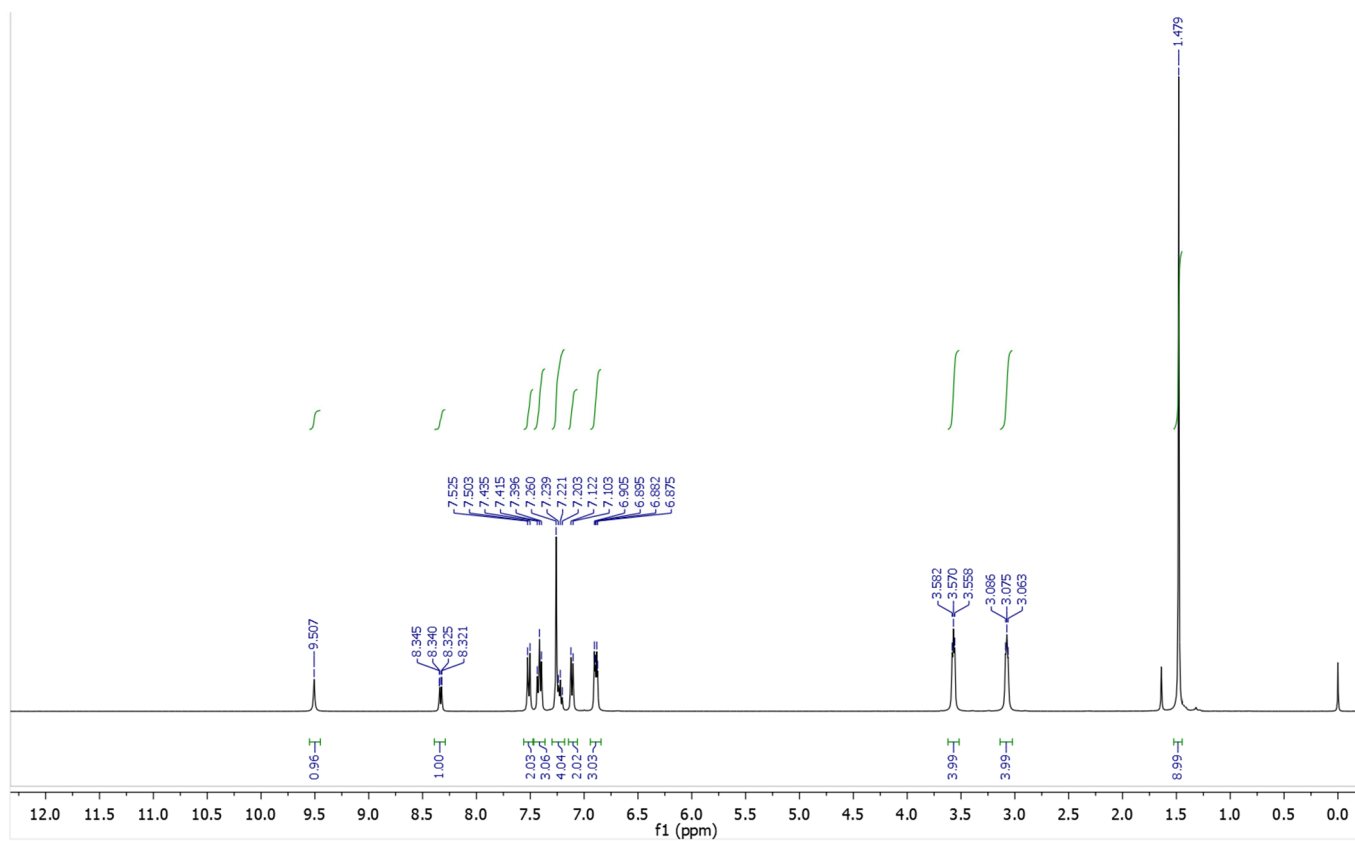
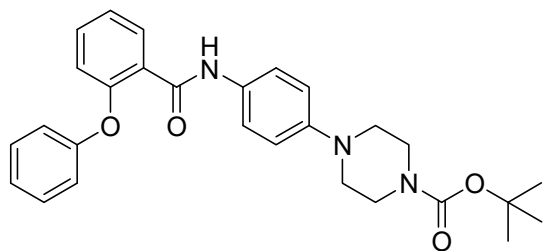
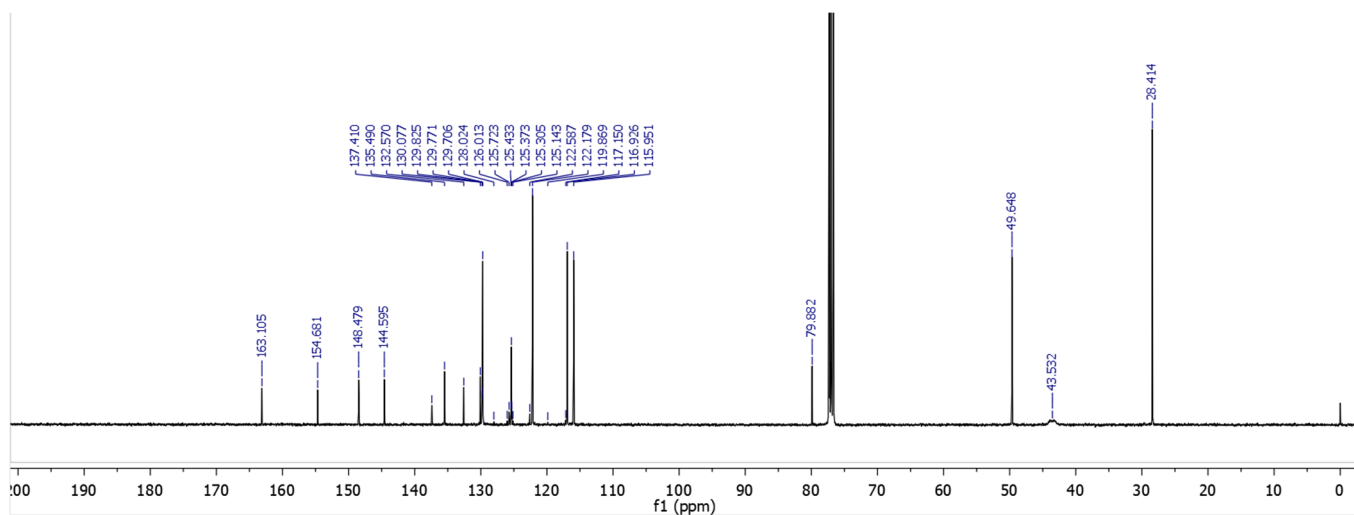
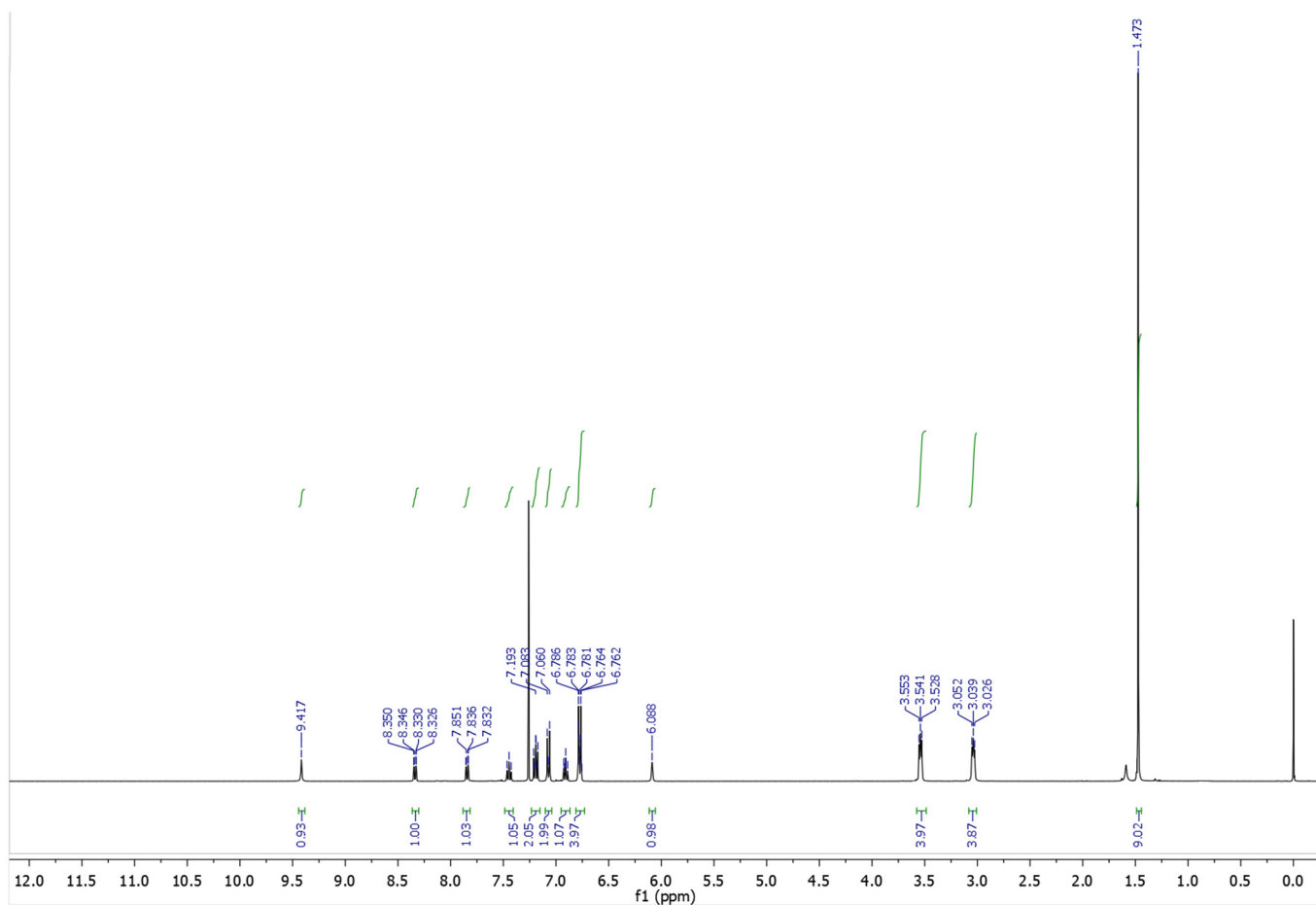
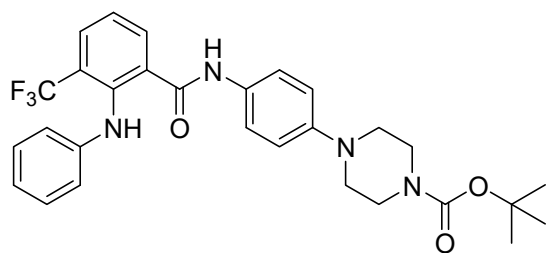


Figure S21. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound **41** (CDCl₃)



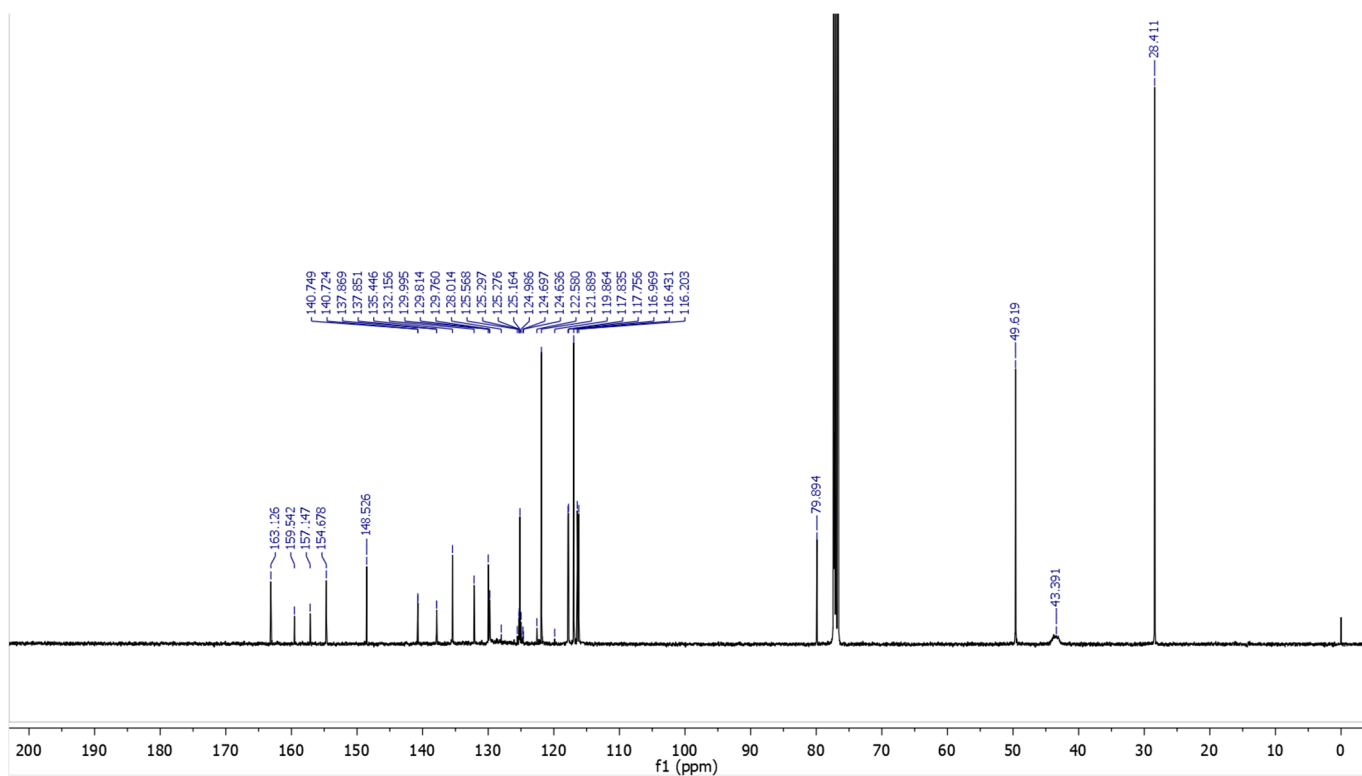
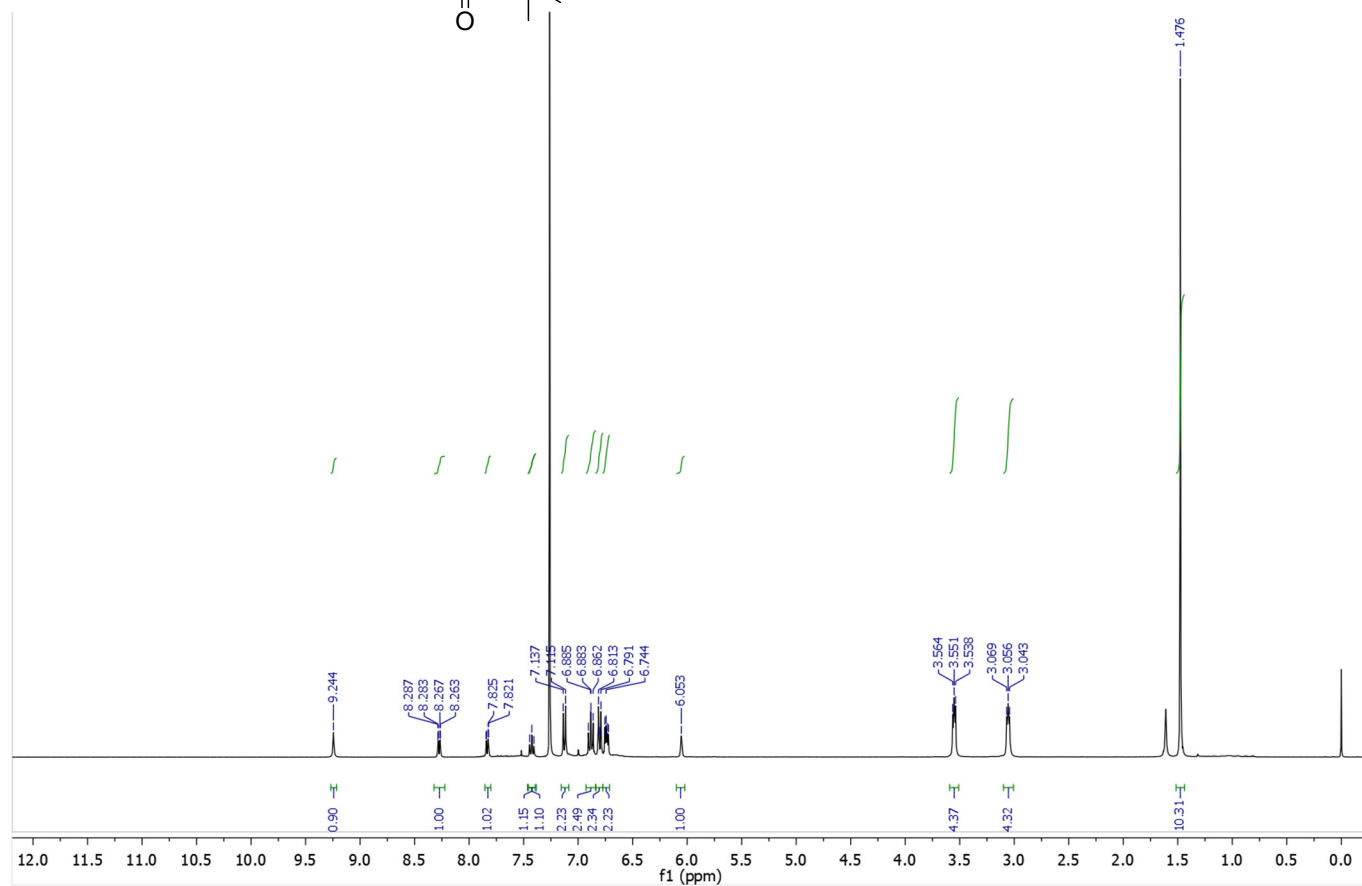
CC(C)(C)OC(=O)N1CCN(CC1)C2=CC=C(NC(=O)N3C(=CC(=C3)C(F)(F)F)NC4=CC=C(C=C4)F)C=C2

Figure S23. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **43** (CDCl_3)

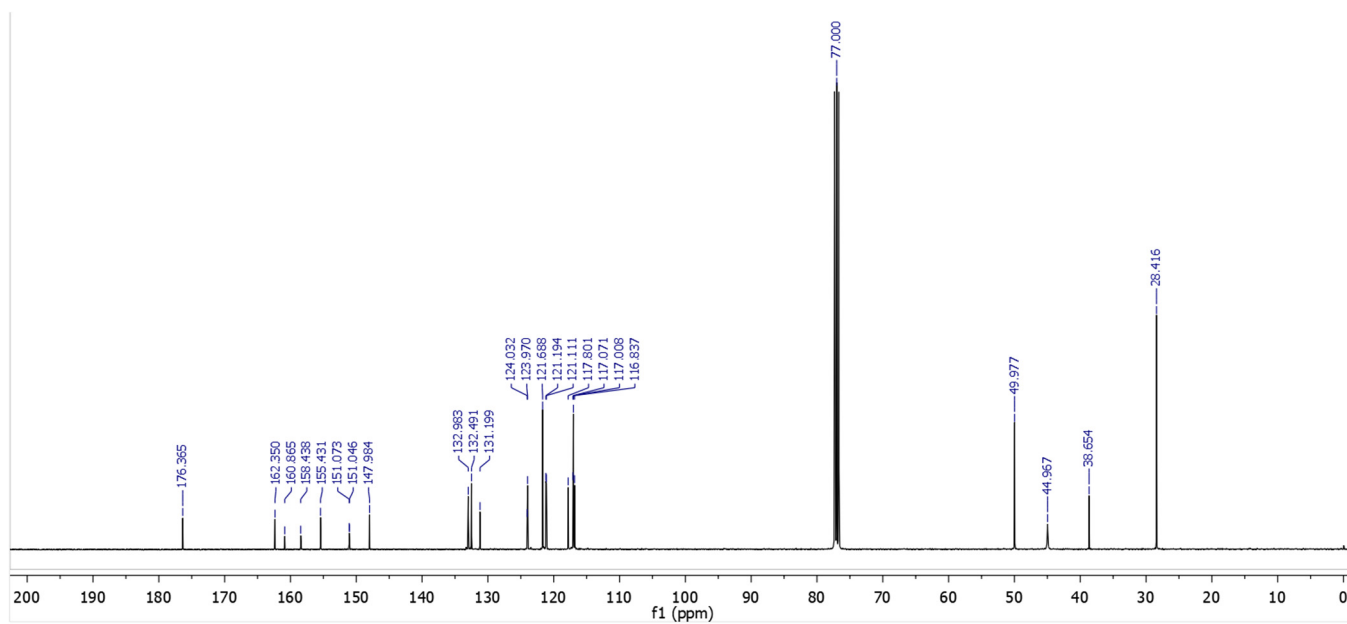
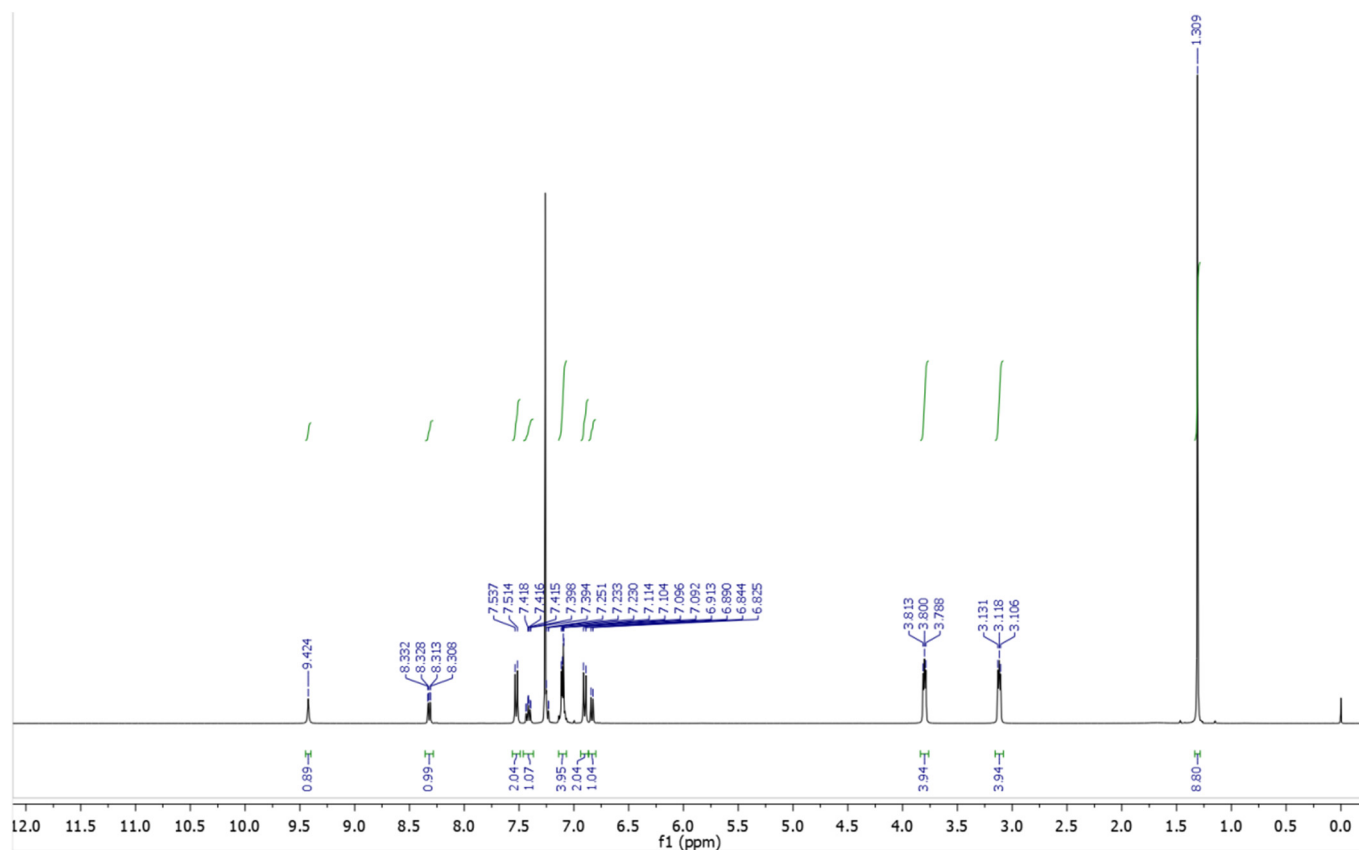
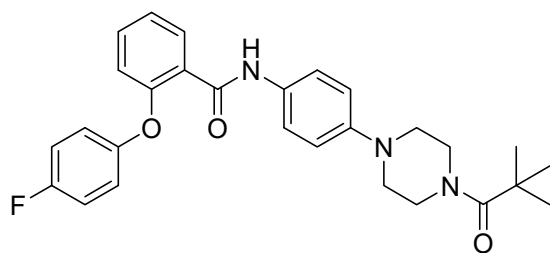


Figure S24. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound **44** (CDCl₃)

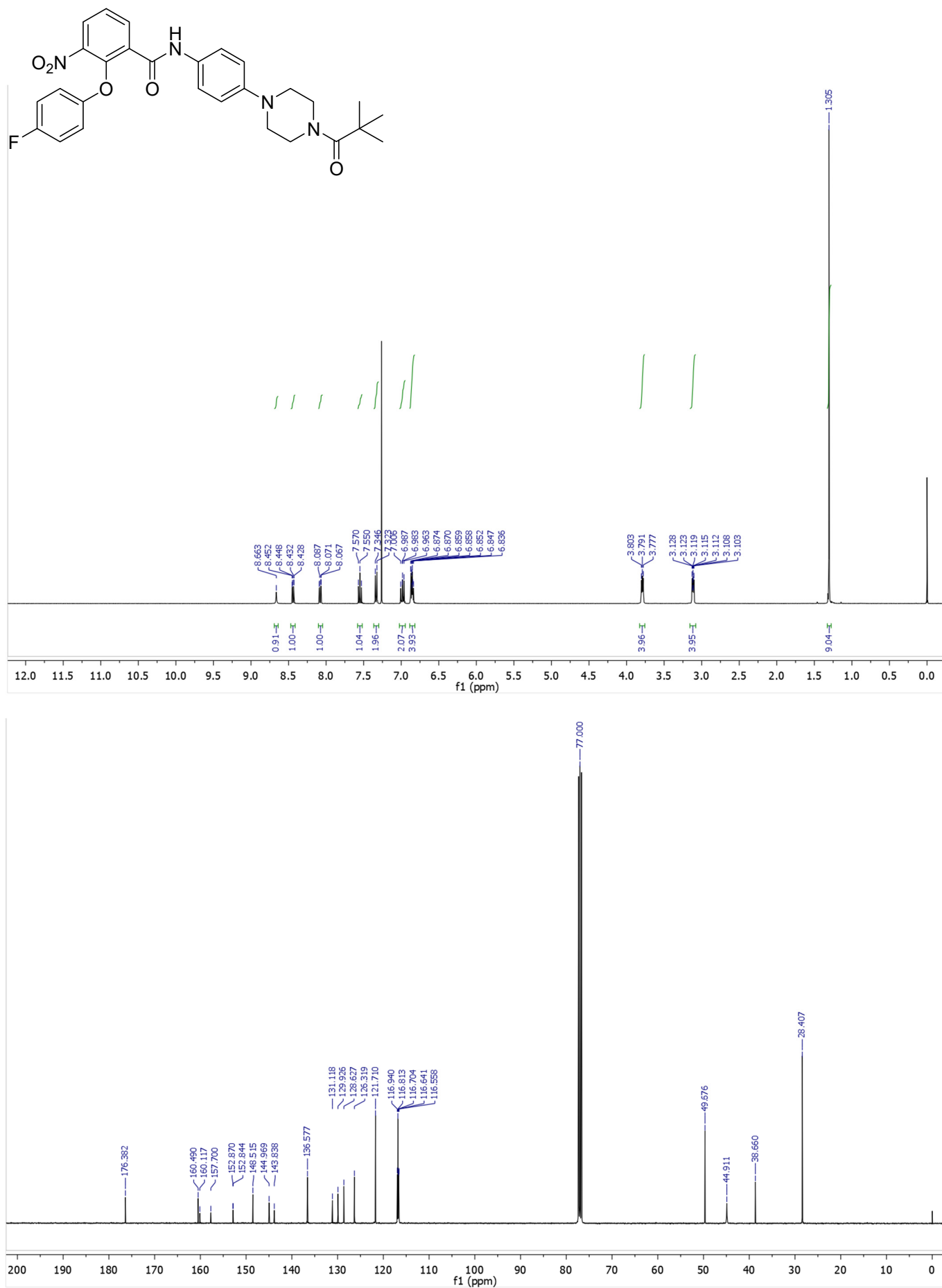


Figure S25. ¹H NMR at 400 MHz and ¹³C NMR at 100 MHz spectra for compound **45** (CDCl₃)

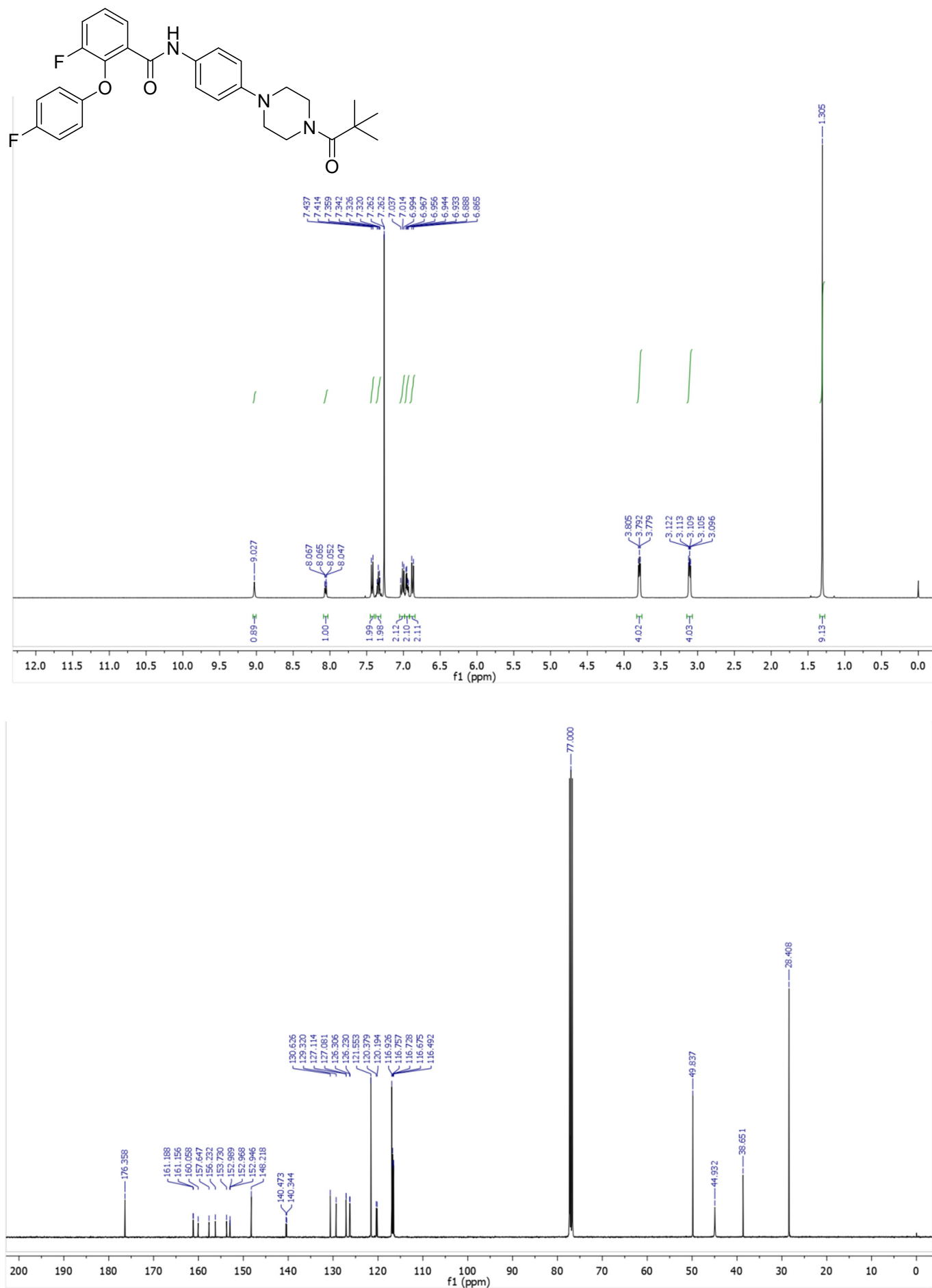


Figure S26. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **46** (CDCl_3)

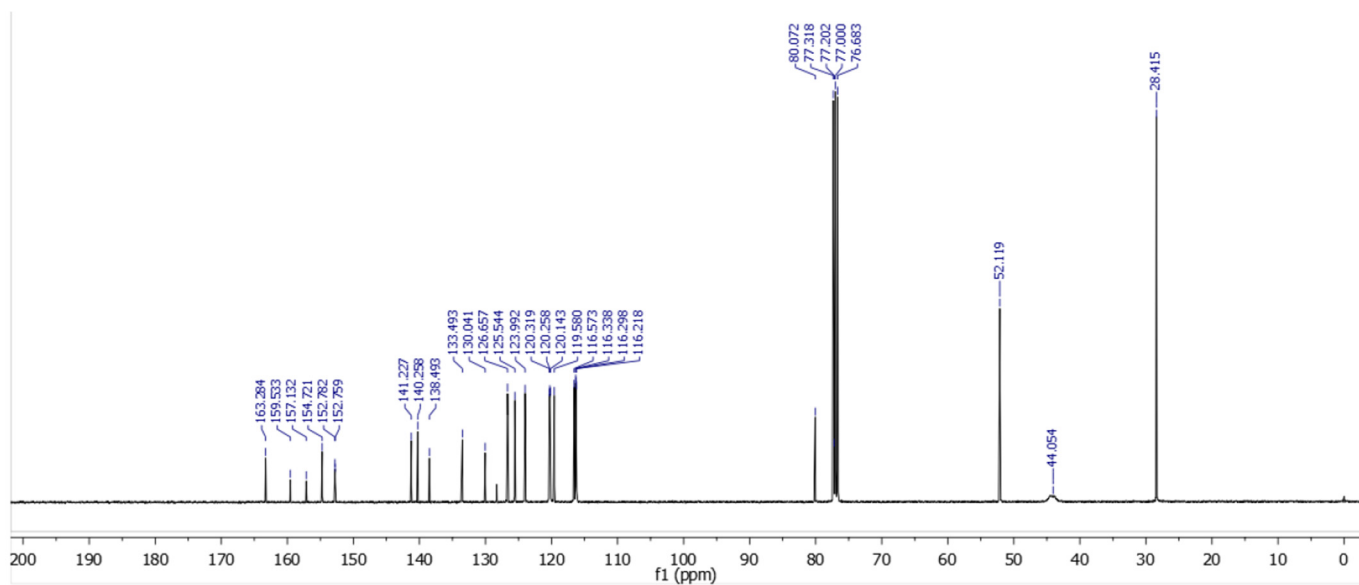
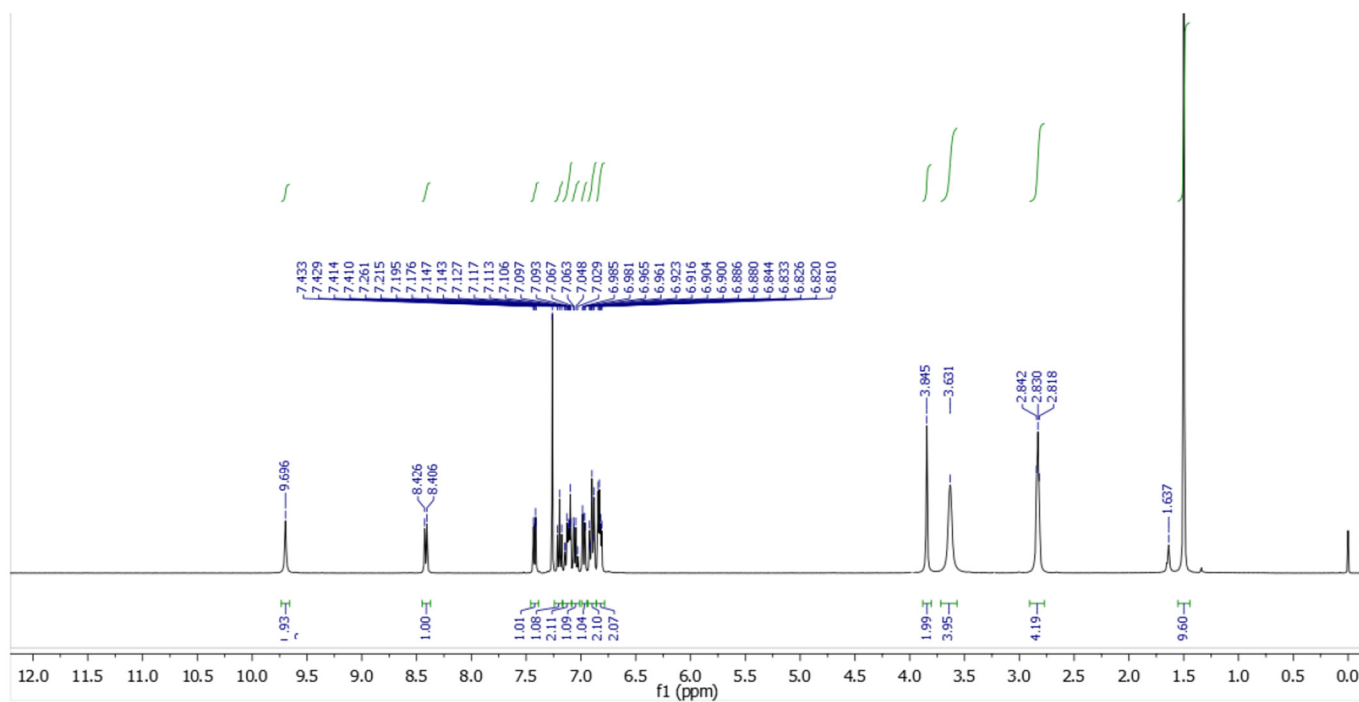
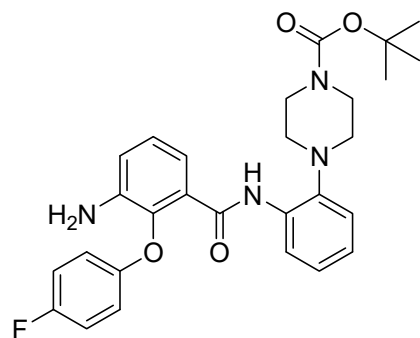


Figure S27. ^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz spectra for compound **47** (CDCl_3)

