

Facile access to Fe(III)-complexing cyclic hydroxamic acids in a three-component format

Evgeny Chupakhin^{a,b}, Olga Bakulina^a, Dmitry Dar'in^a and Mikhail Krasavin^{a,b*}

^a Saint Petersburg State University, Saint Petersburg, 199034 Russian Federation

^b Immanuel Kant Baltic Federal University, Kaliningrad, 236016 Russian Federation

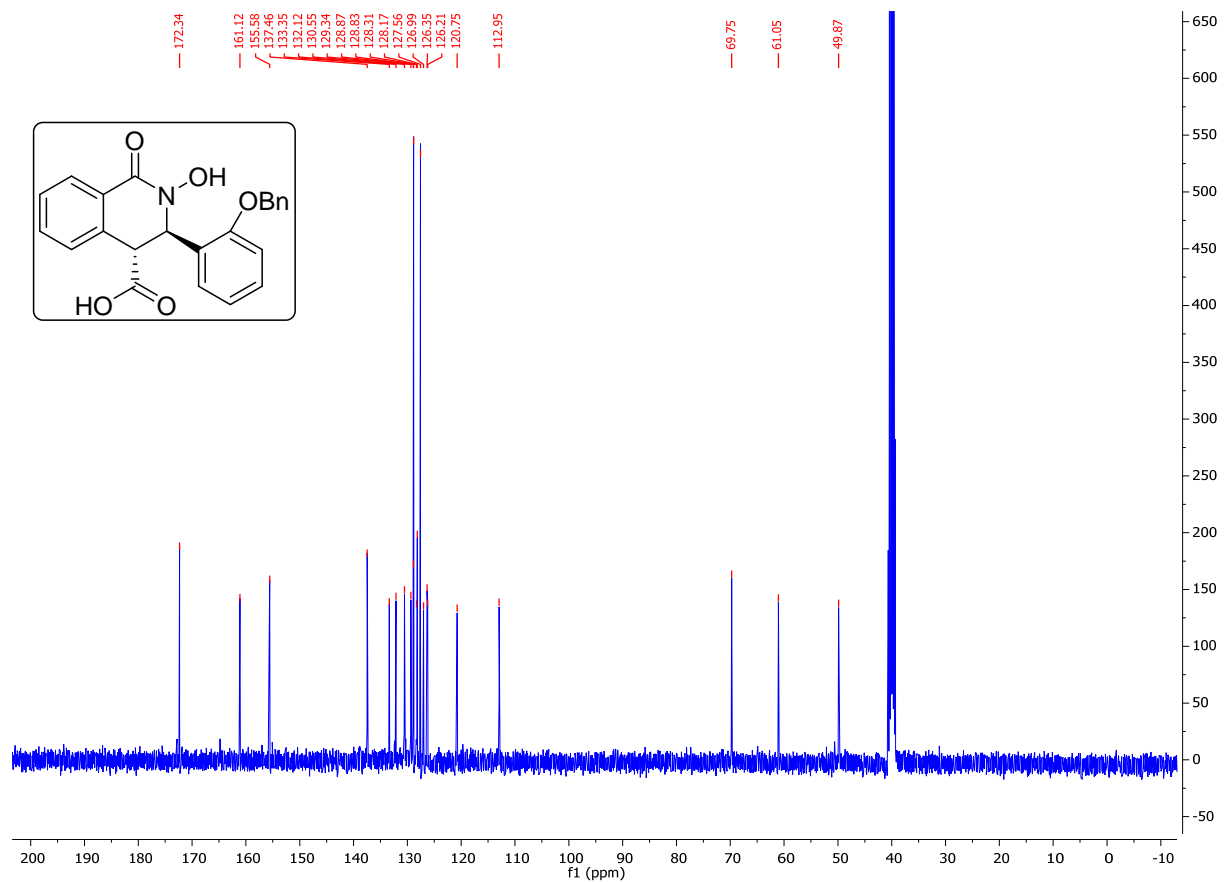
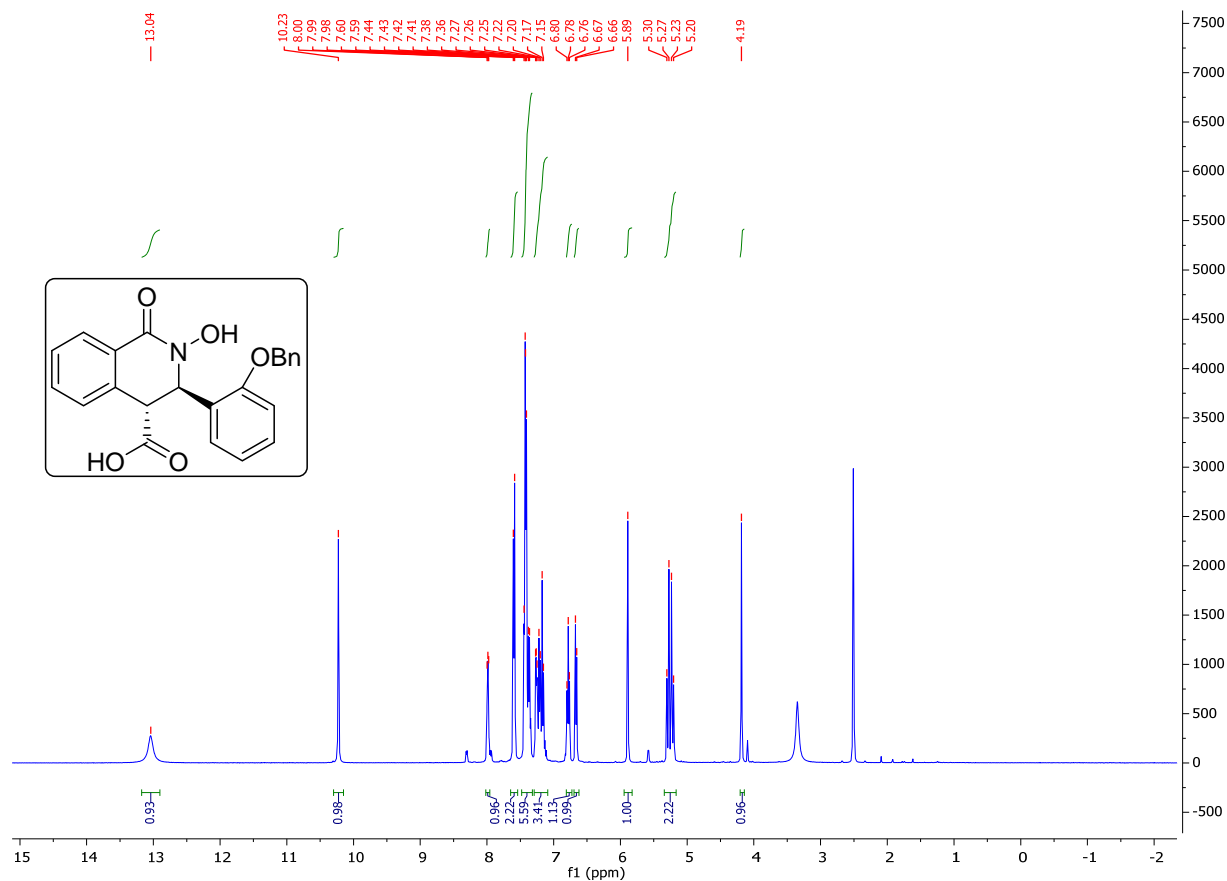
* Corresponding author at: Laboratory of Chemical Pharmacology, Institute of Chemistry, Saint Petersburg State University, 26 Universitetskyi prospekt, Peterhof 198504 Russian Federation

E-mail address: m.krasavin@spbu.ru (M. Krasavin)

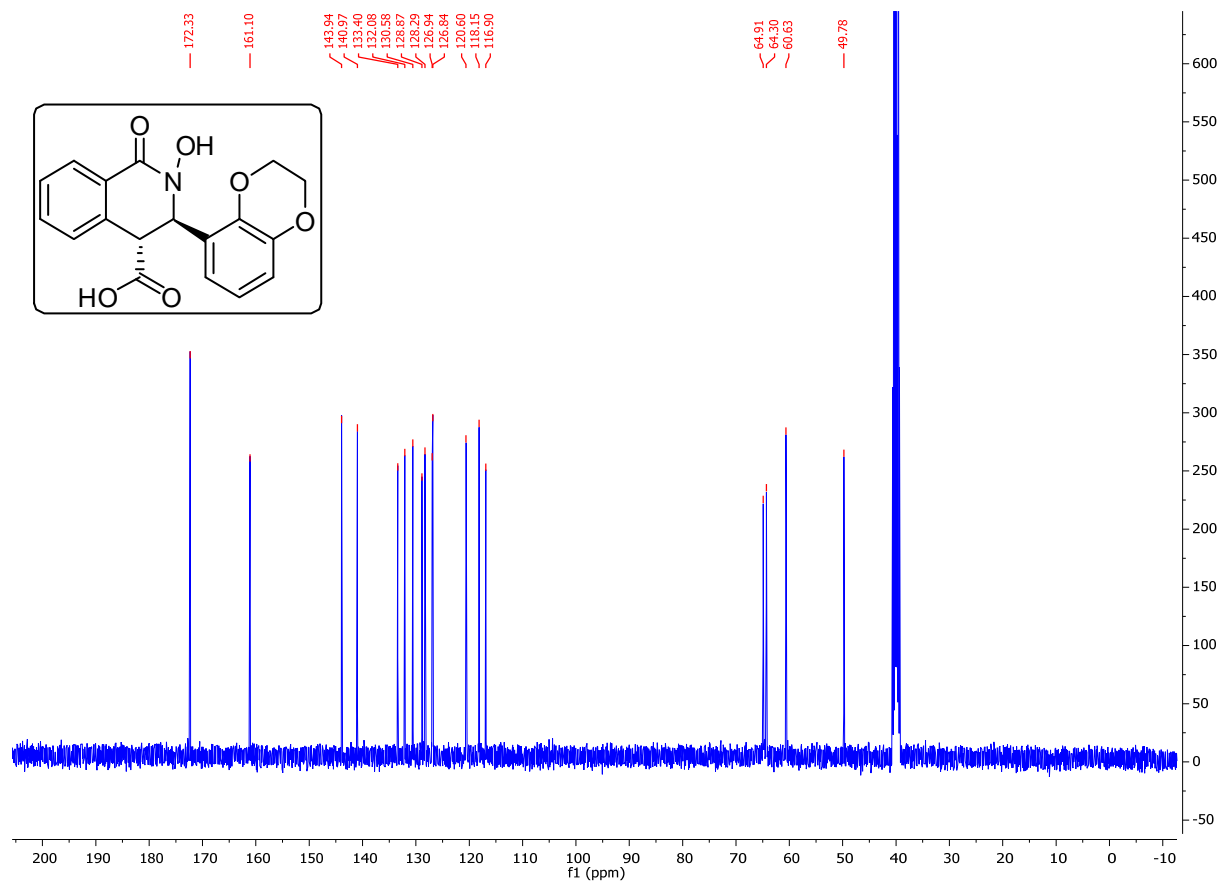
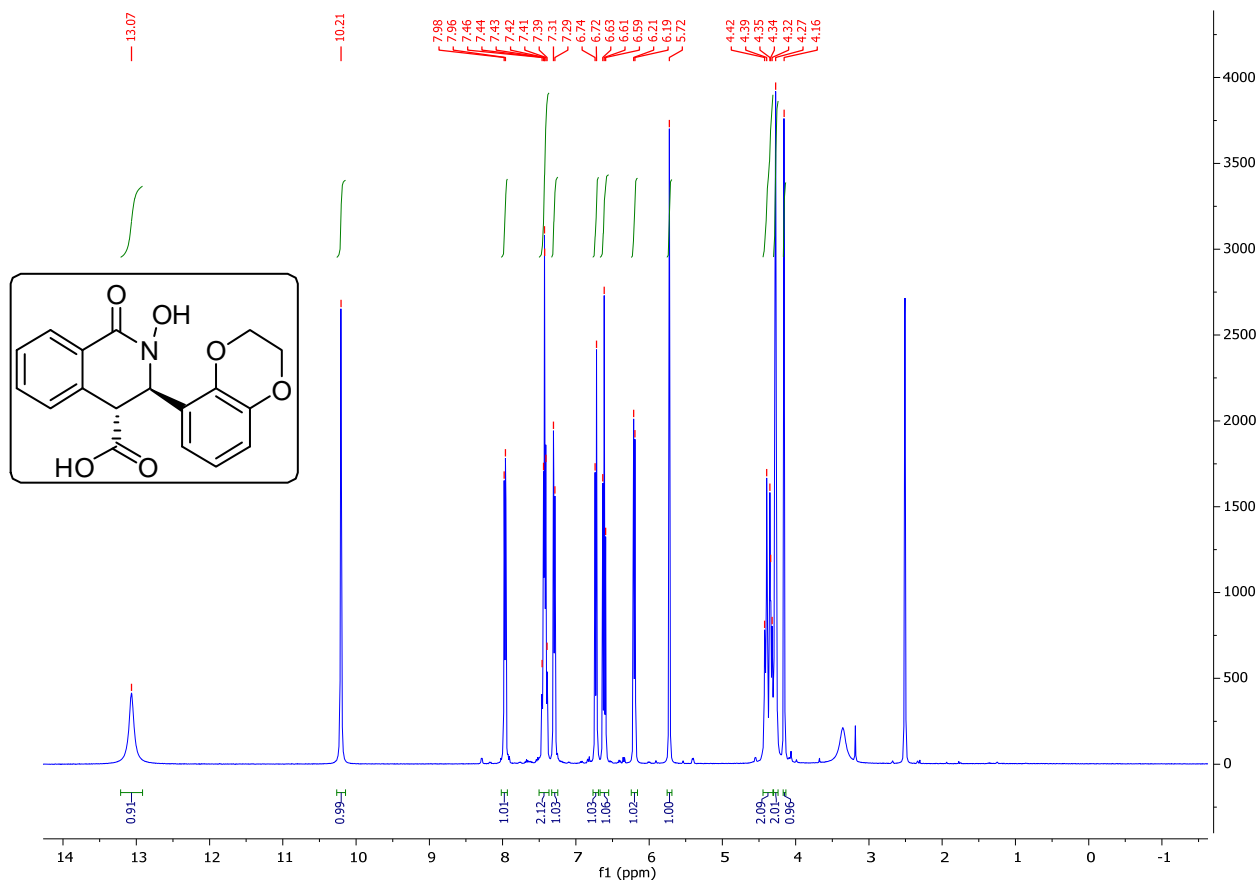
Contents

| | |
|---|--------|
| Copies of ¹ H and ¹³ C NMR spectra for compounds 7c-j,l,m , 8 , 9a-g and 10-12 | S2-21 |
| Electronic absorption spectra of free 7d,f,g,h,j ligands (Figures S1-S3) | S22 |
| Electronic absorption spectra of ligands 7 in the presence of increasing concentration of Fe ³⁺ and corresponding binding isotherms (Figures S4-S8) | S23-24 |

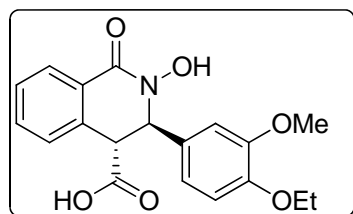
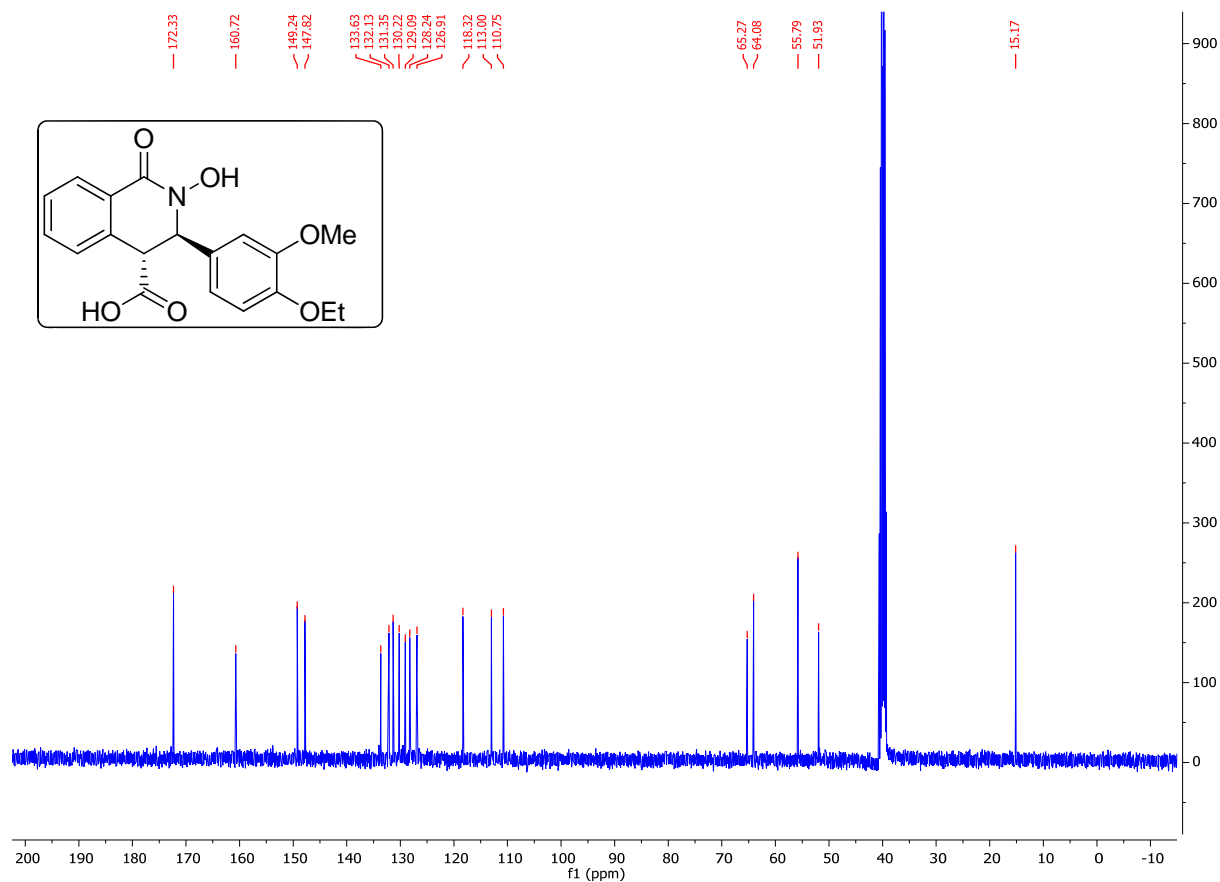
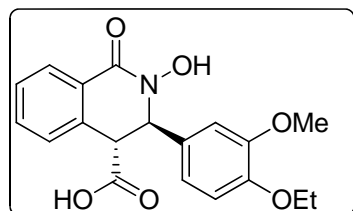
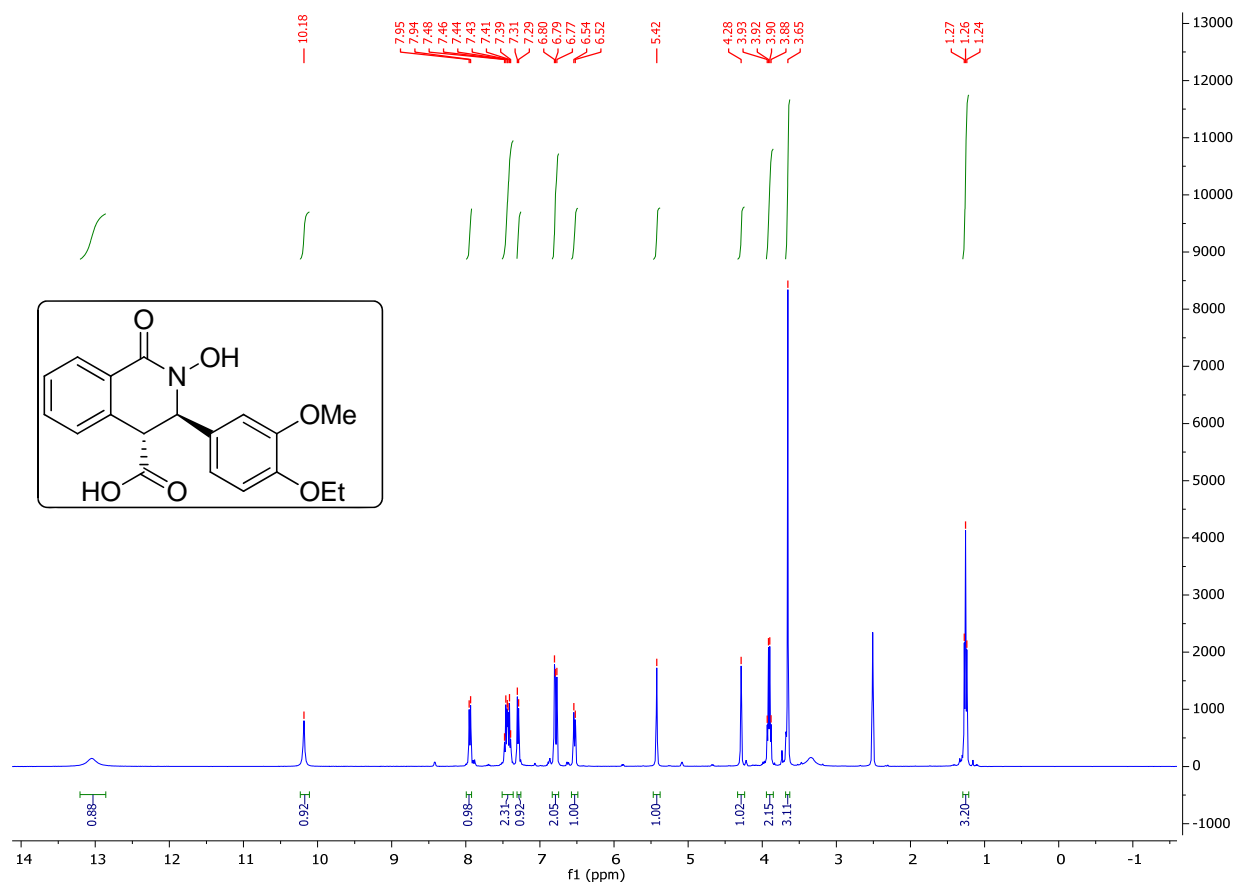
^1H and ^{13}C NMR of compound 7c



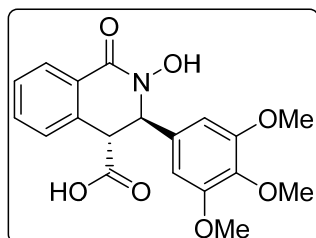
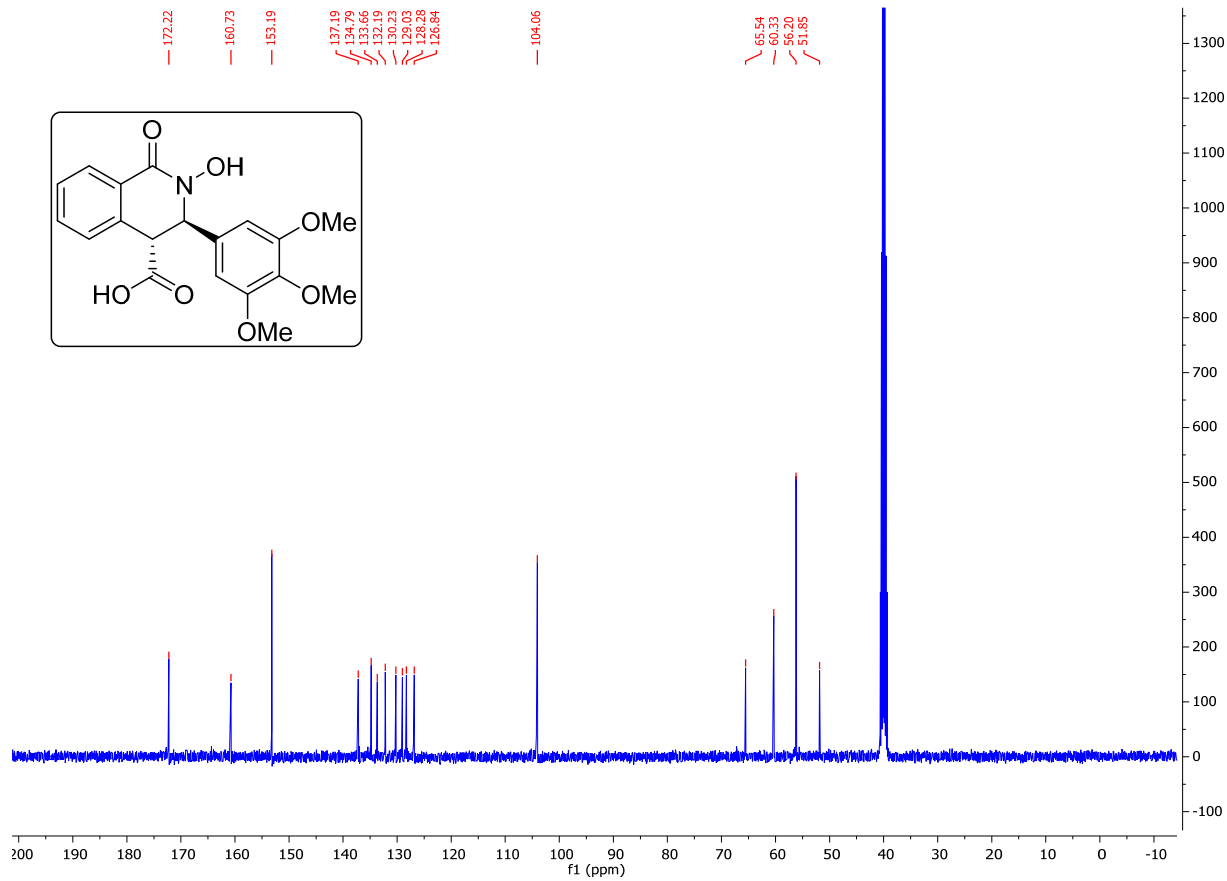
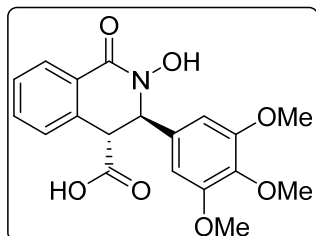
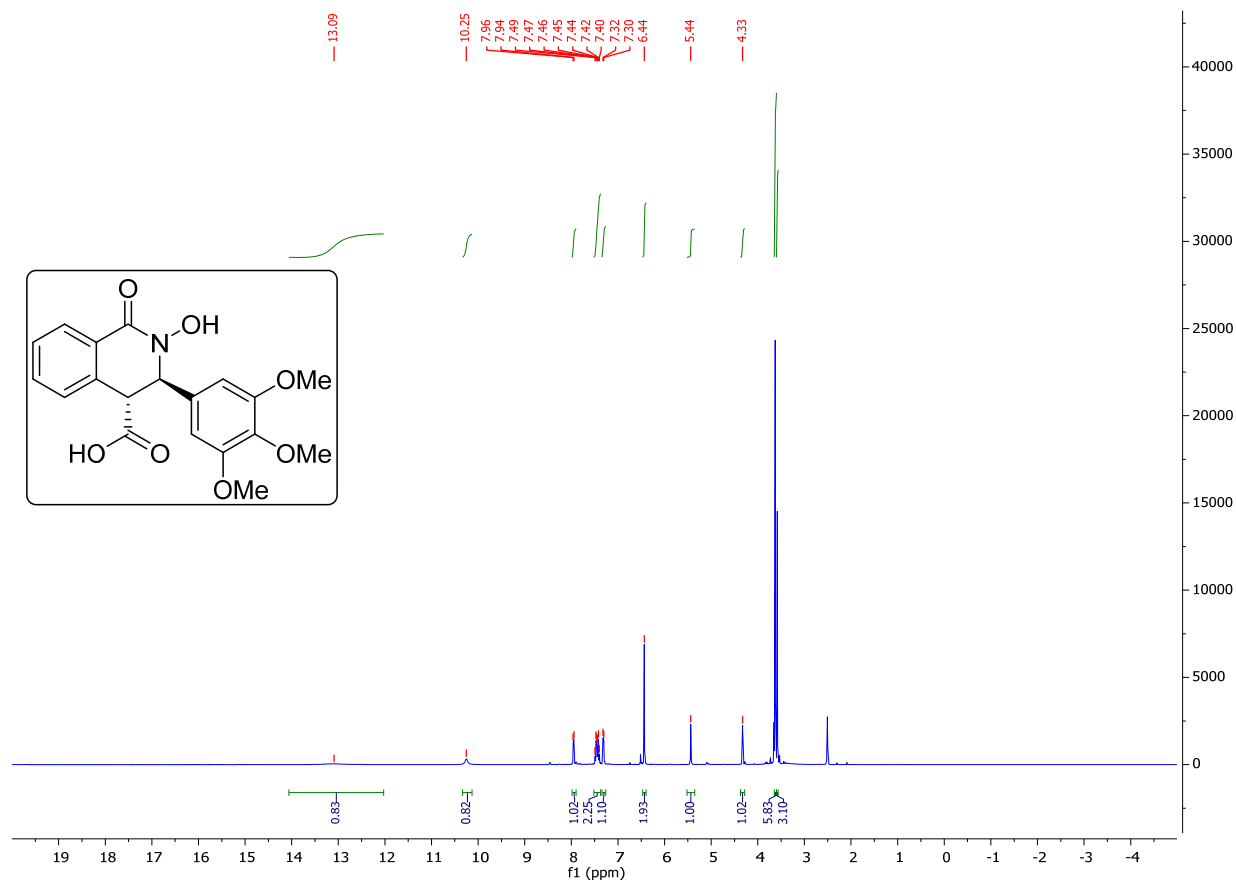
^1H and ^{13}C NMR of compound 7d



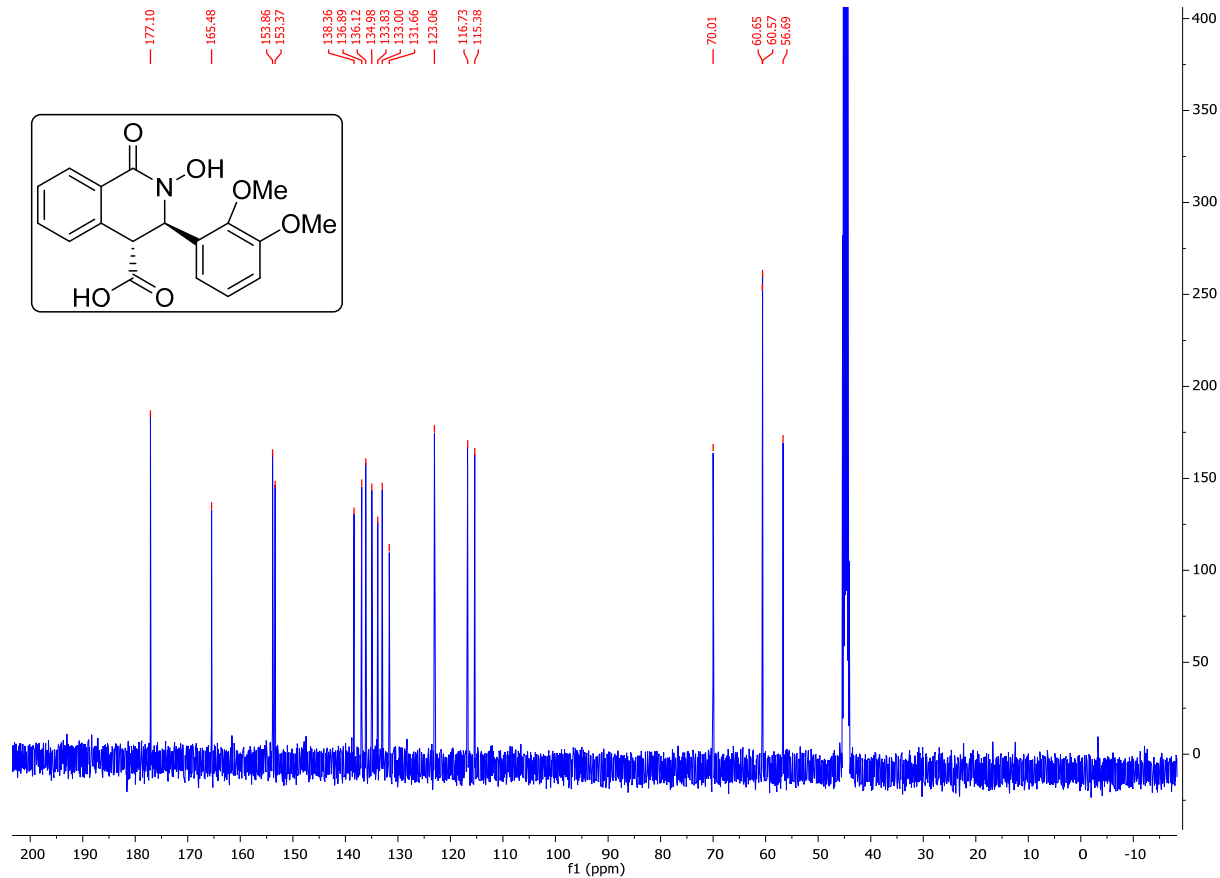
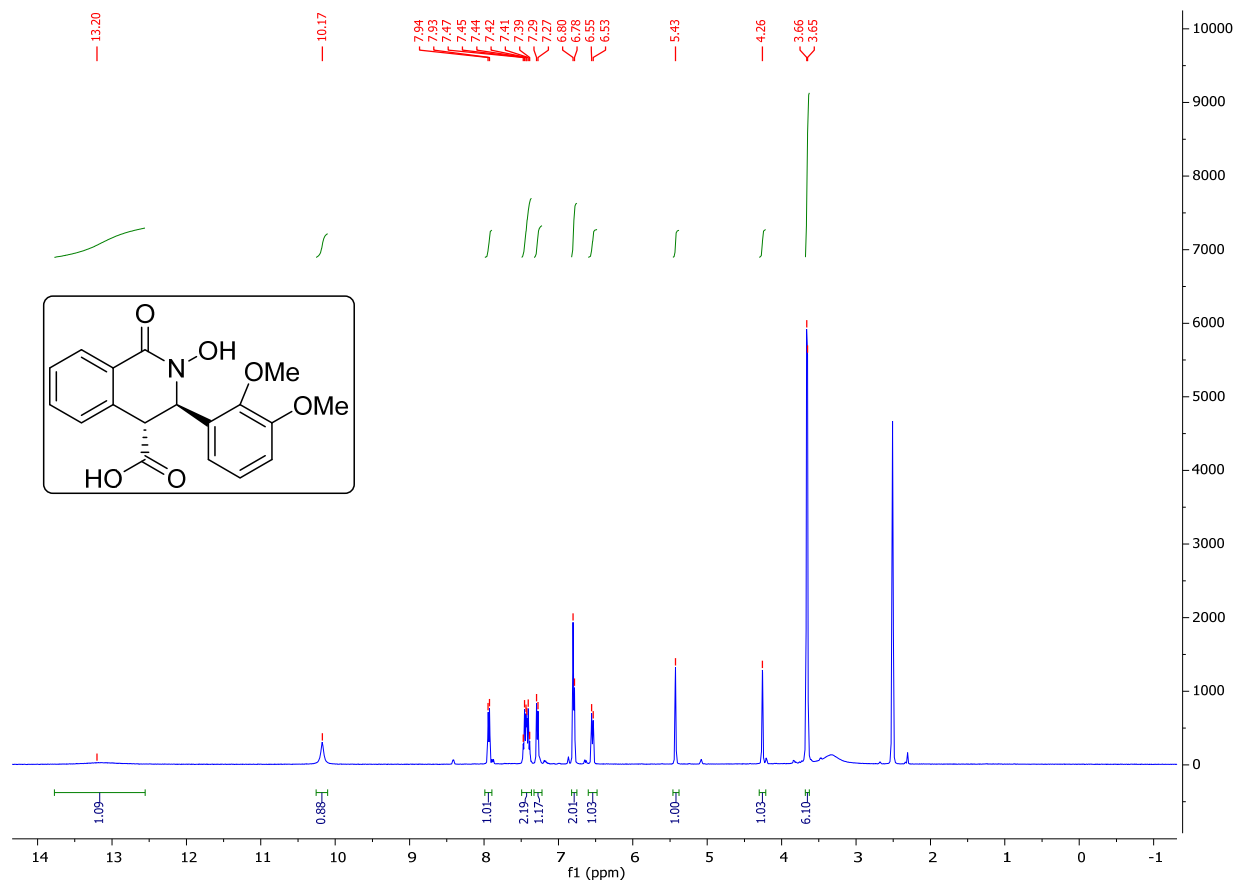
^1H and ^{13}C NMR of compound 7e



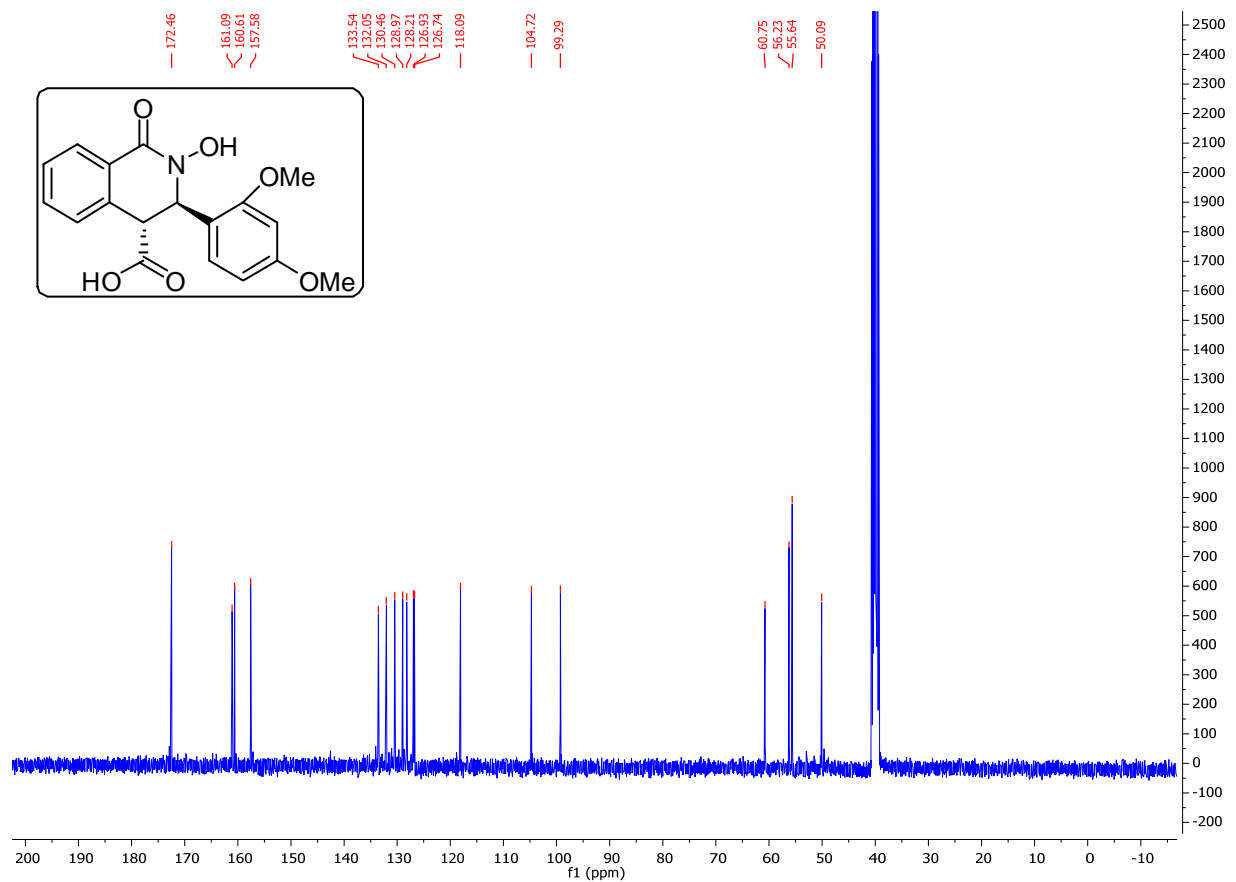
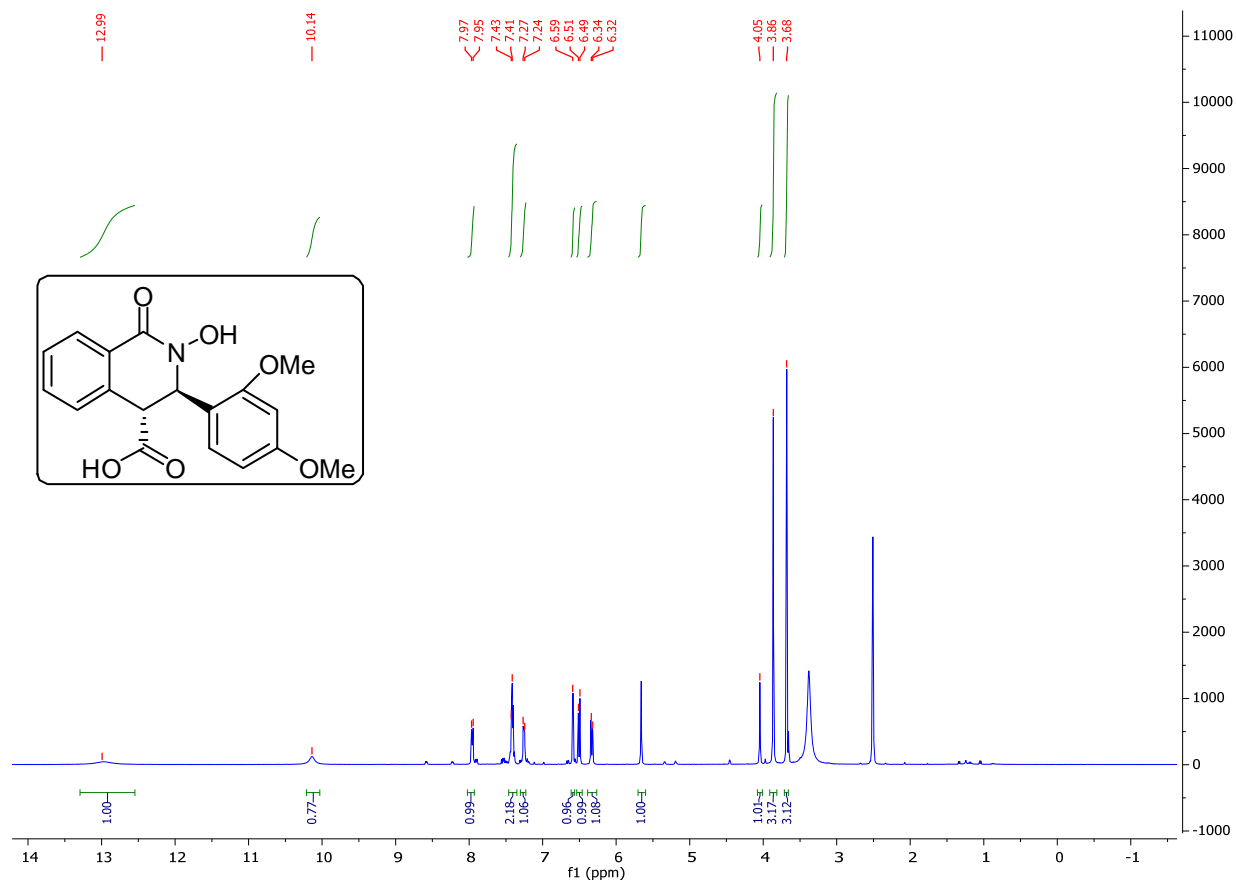
^1H and ^{13}C NMR of compound 7f



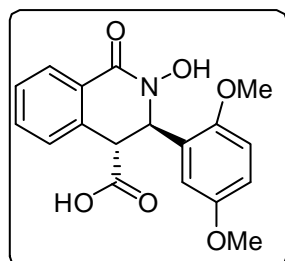
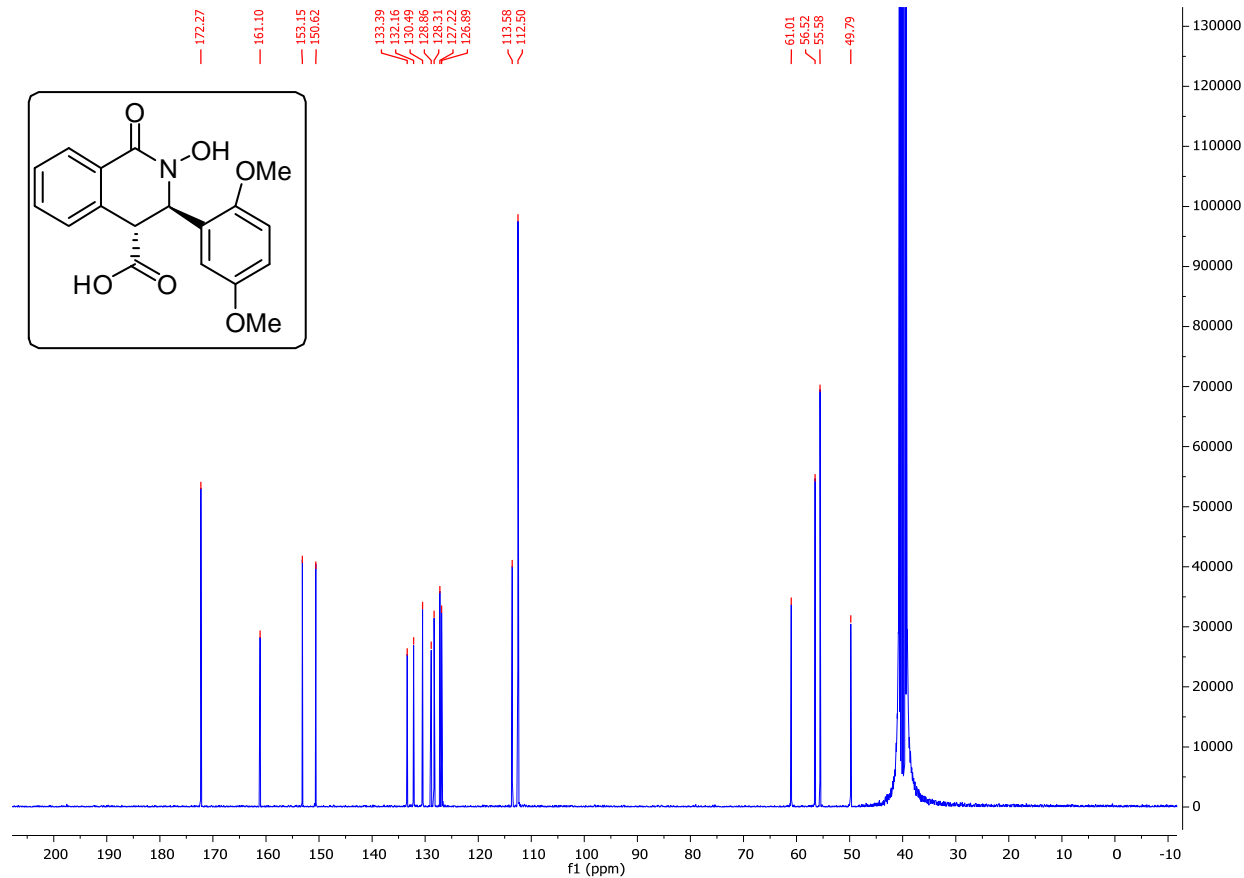
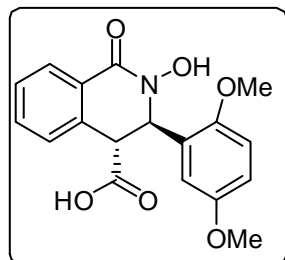
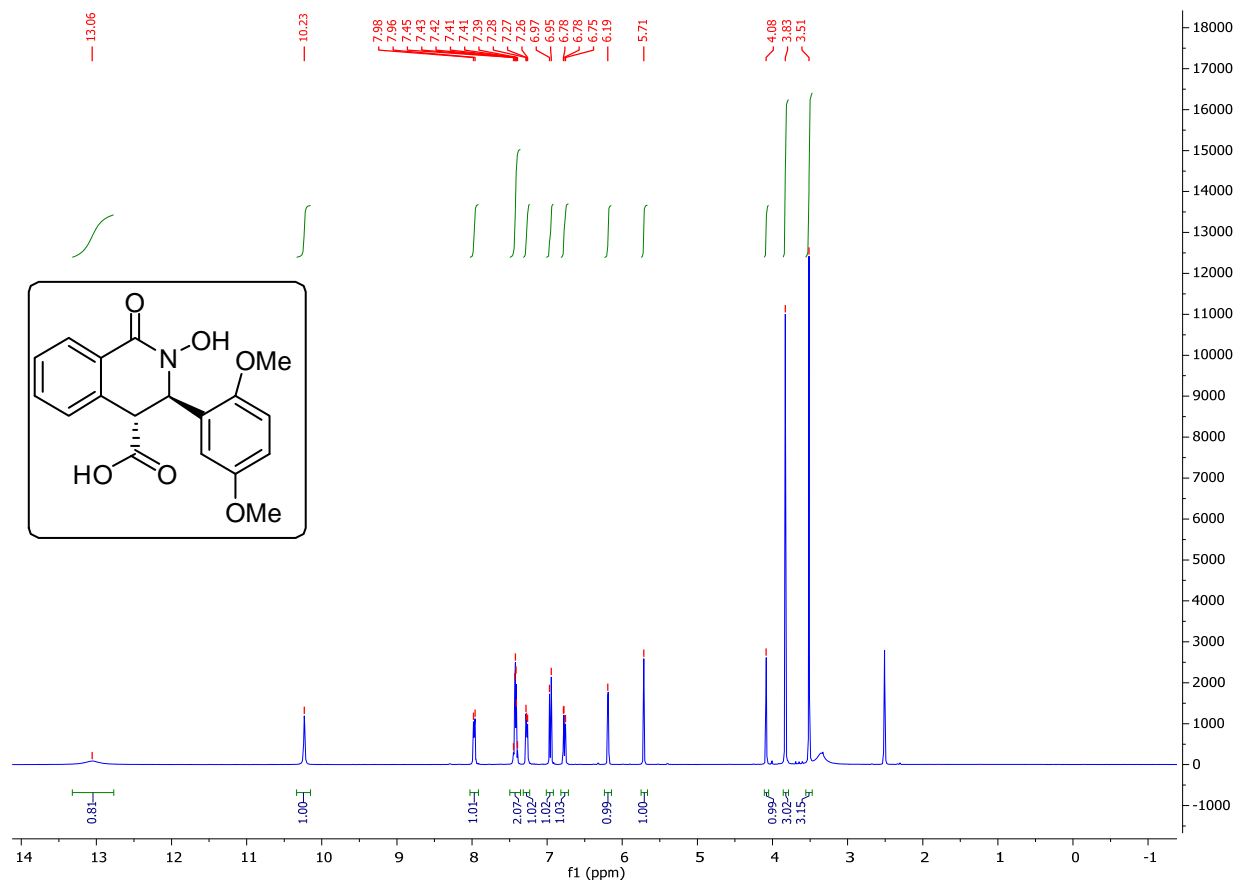
^1H and ^{13}C NMR of compound 7g



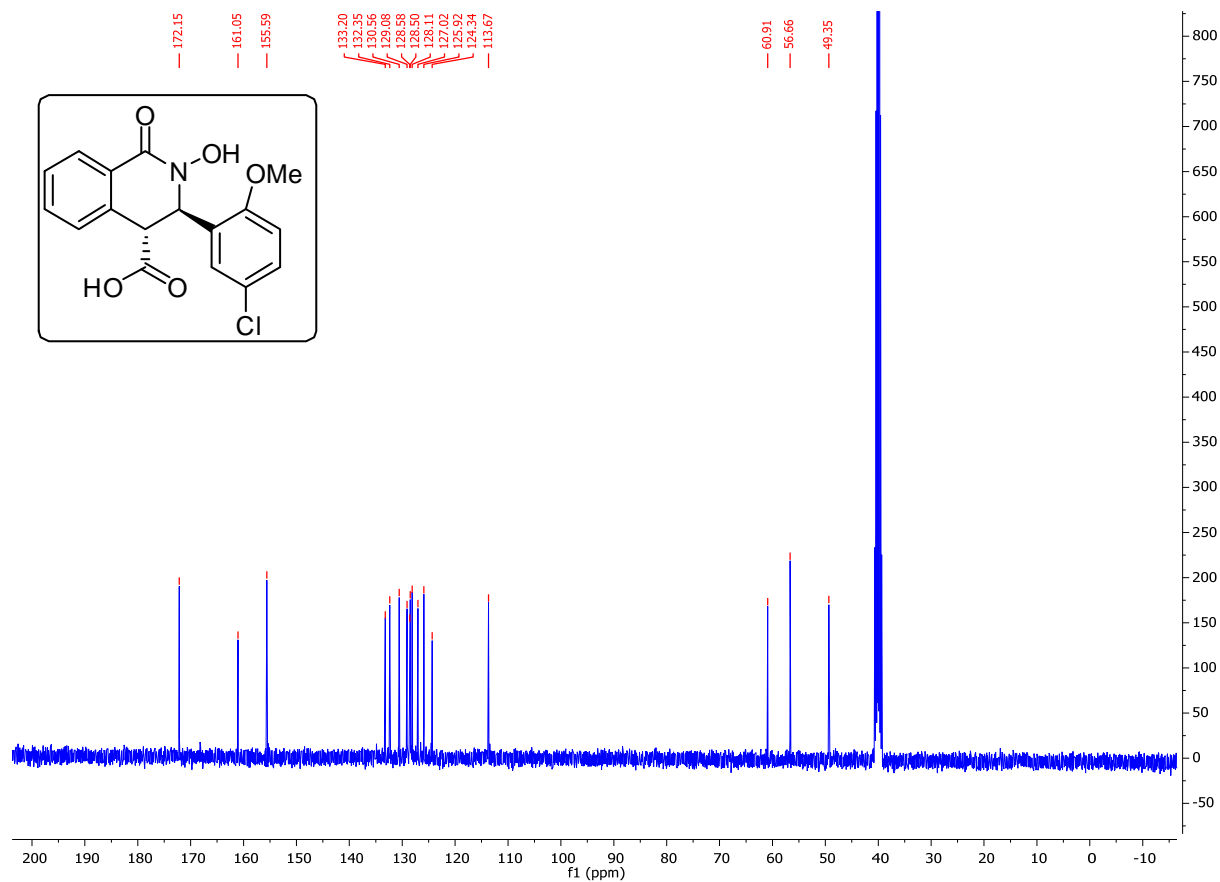
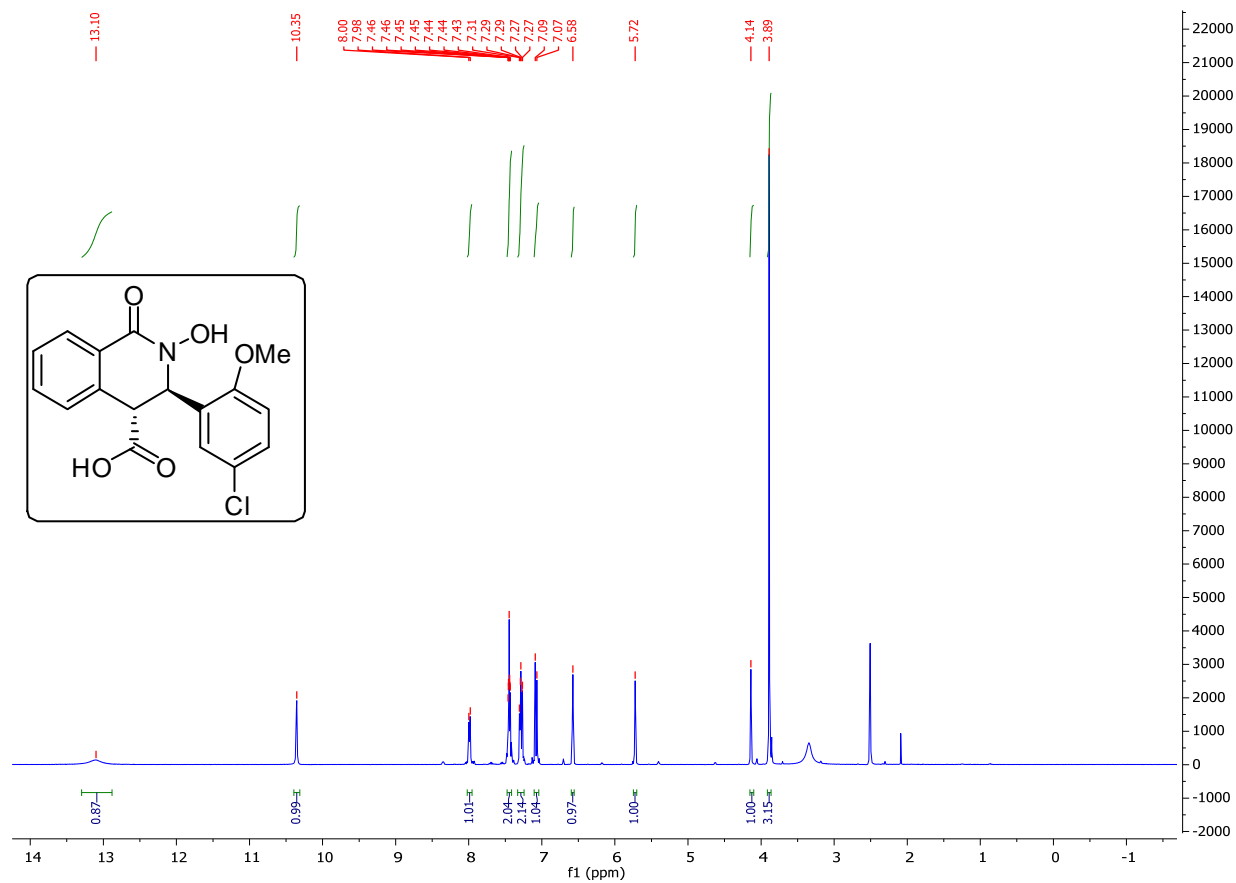
¹H and ¹³C NMR of compound 7h



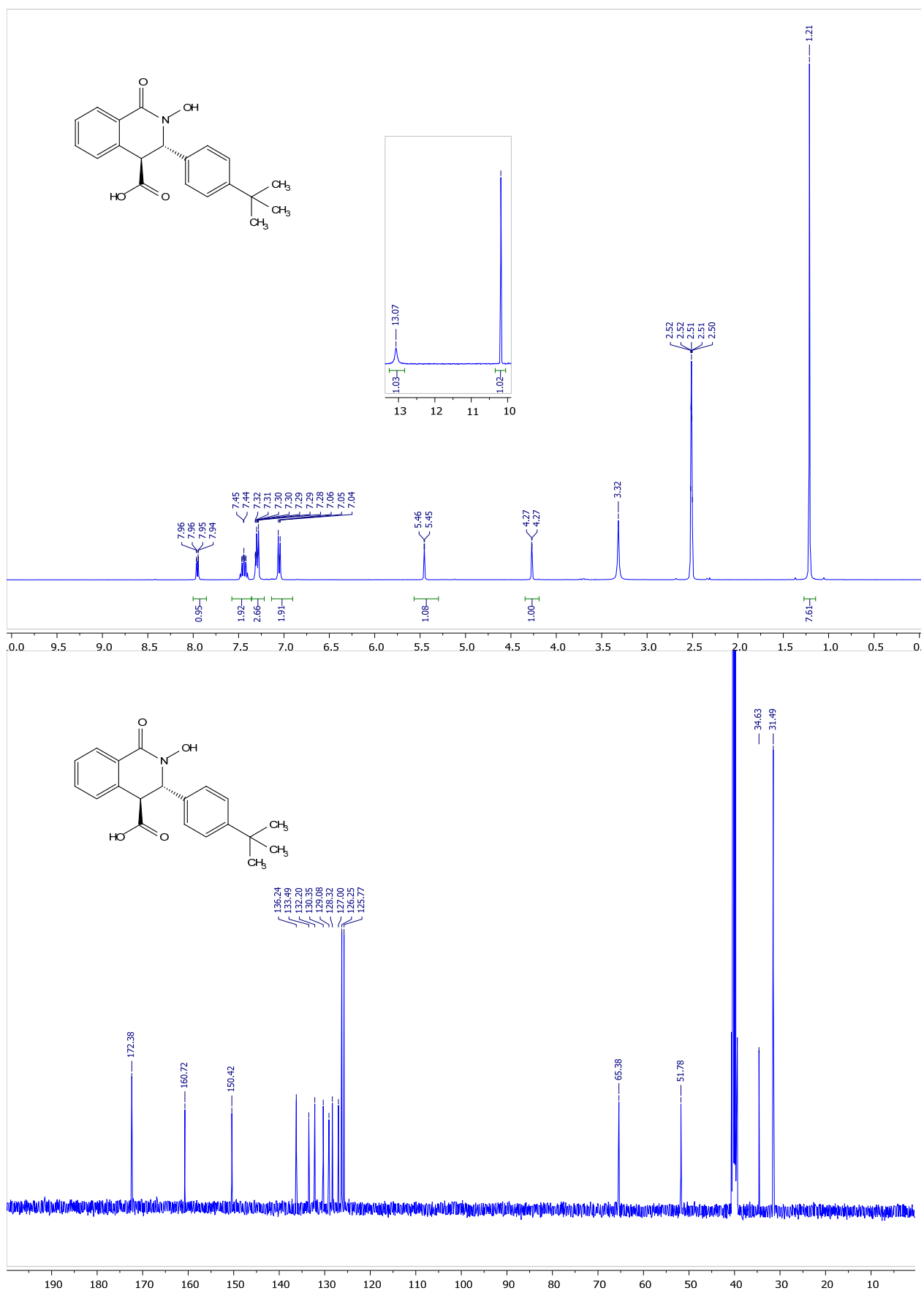
^1H and ^{13}C NMR of compound 7i



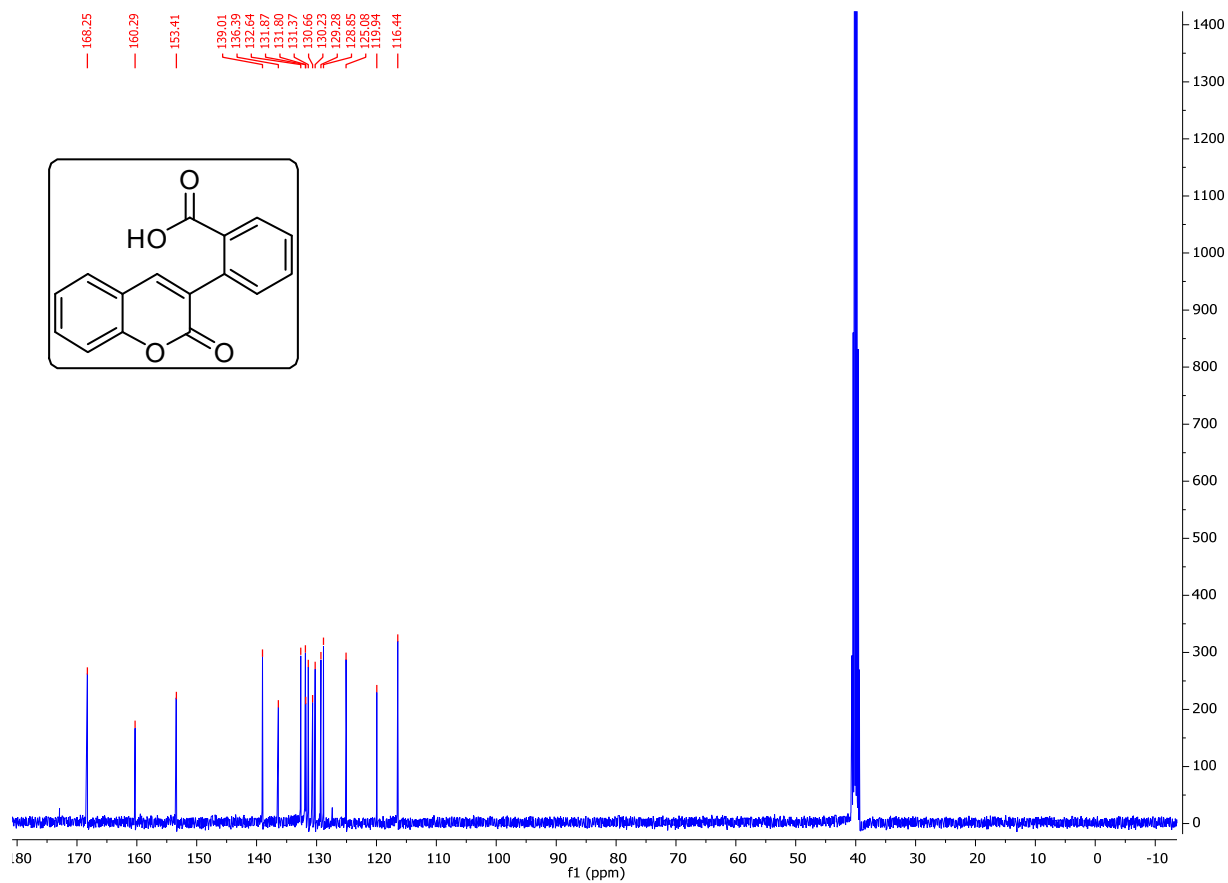
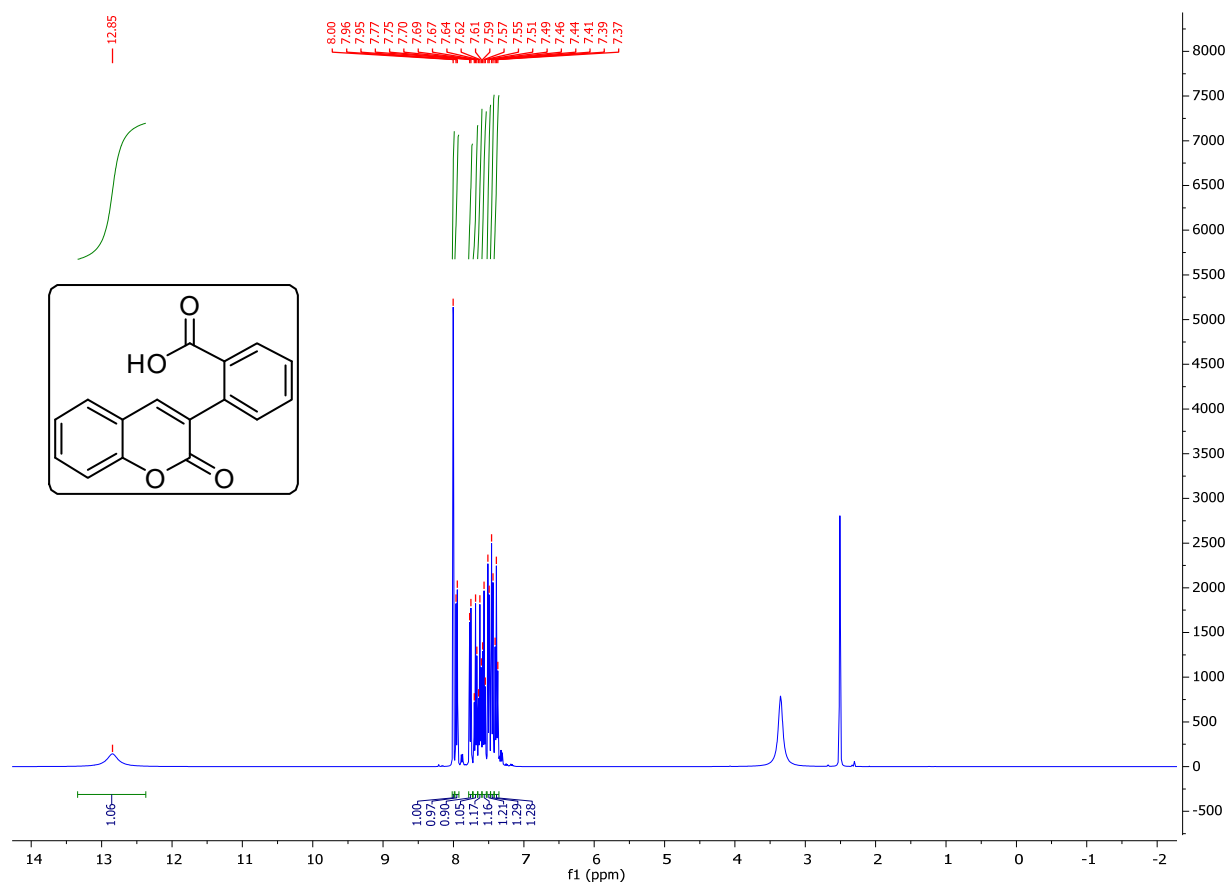
^1H and ^{13}C NMR of compound 7j



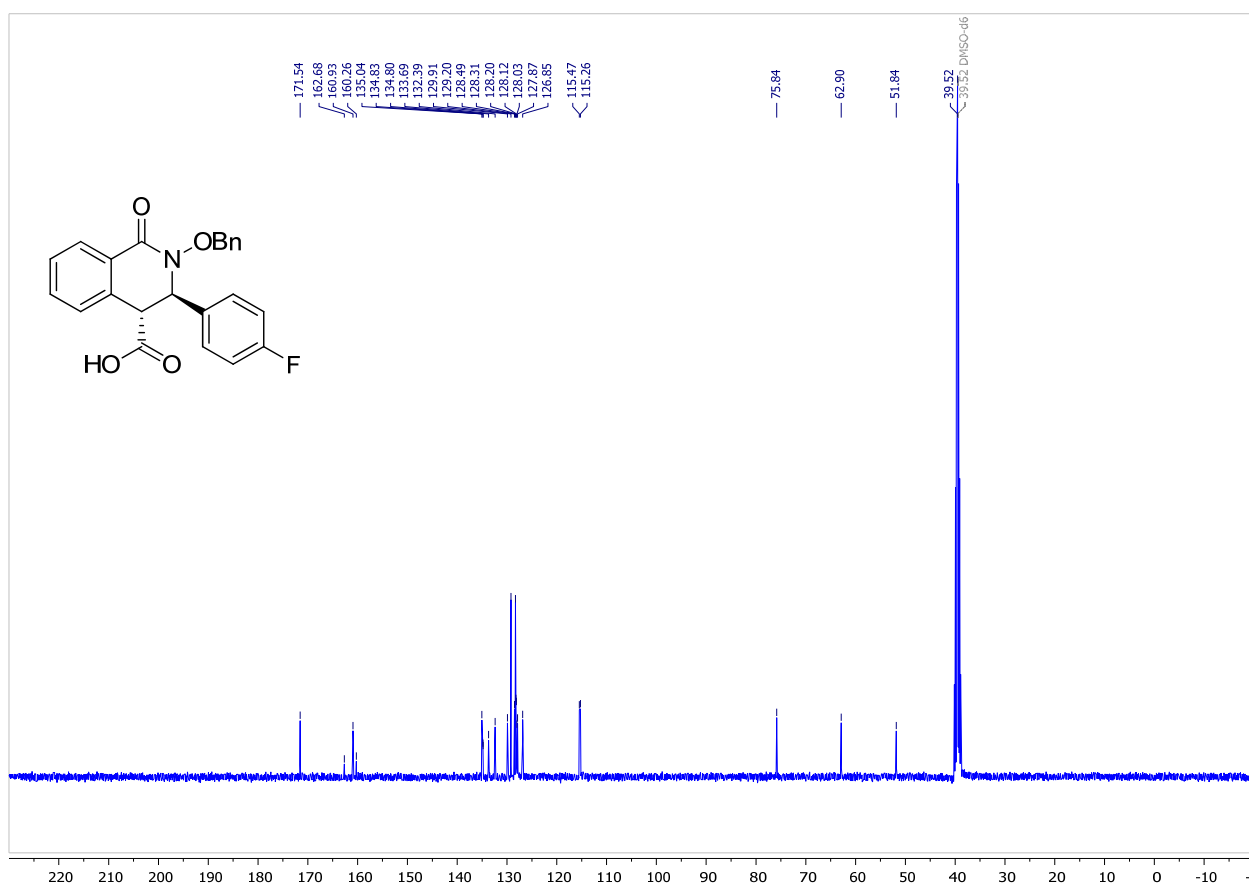
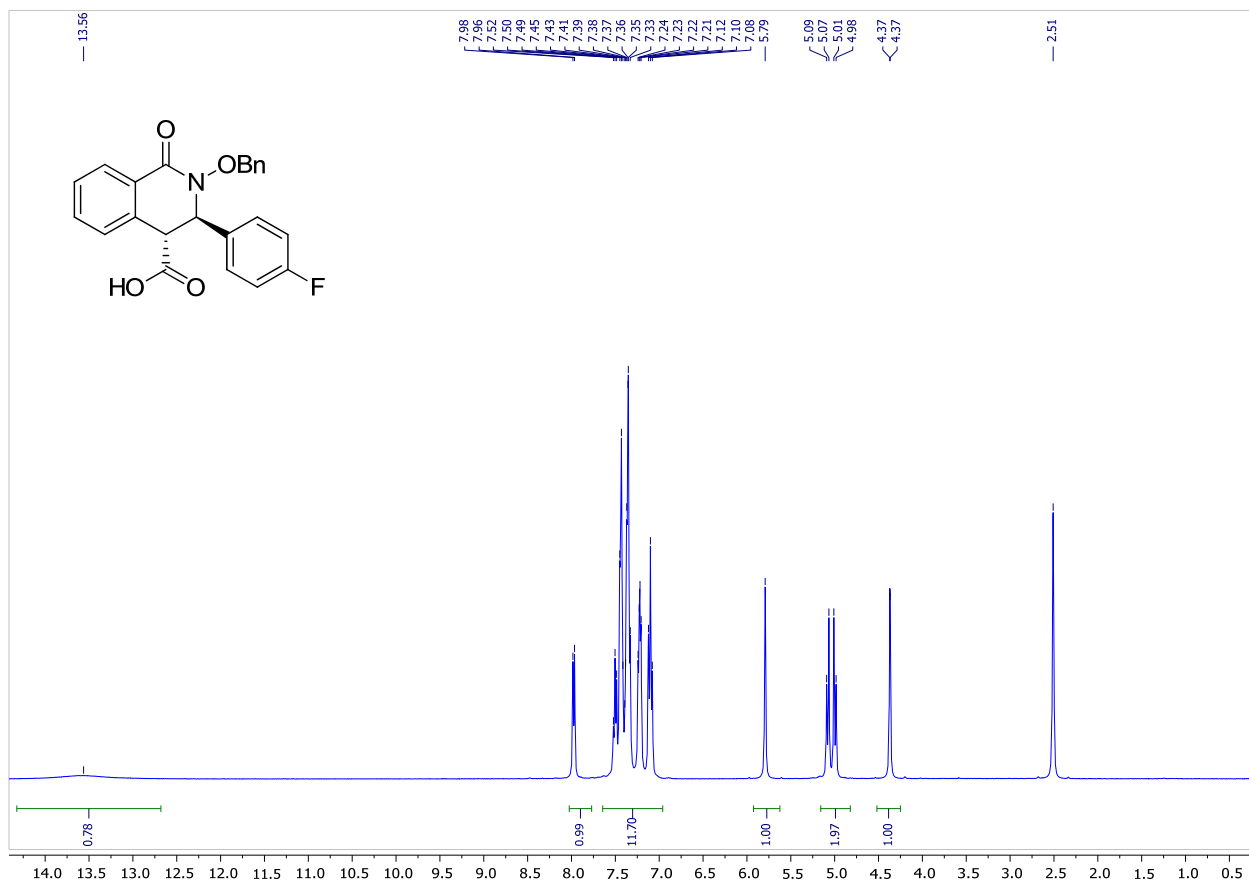
^1H and ^{13}C NMR of compound 71



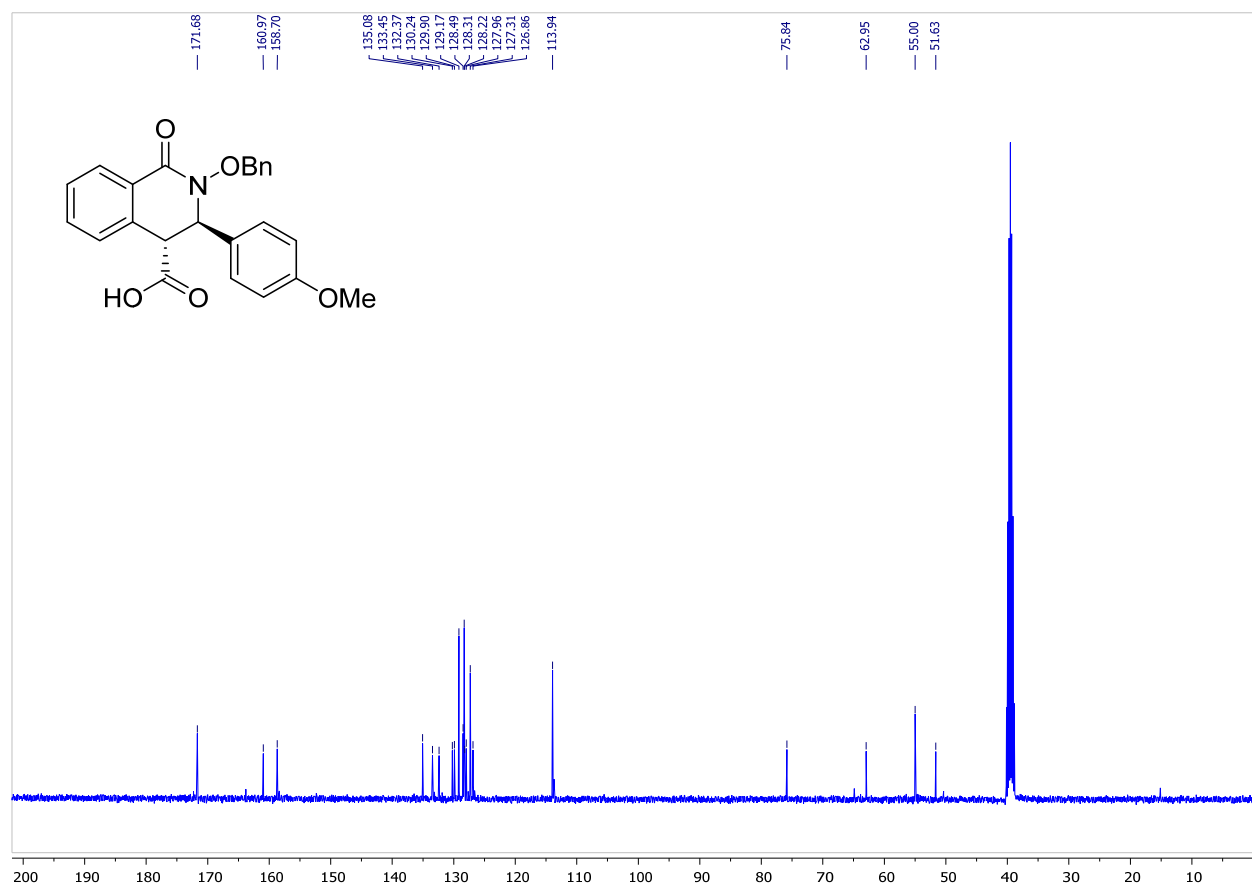
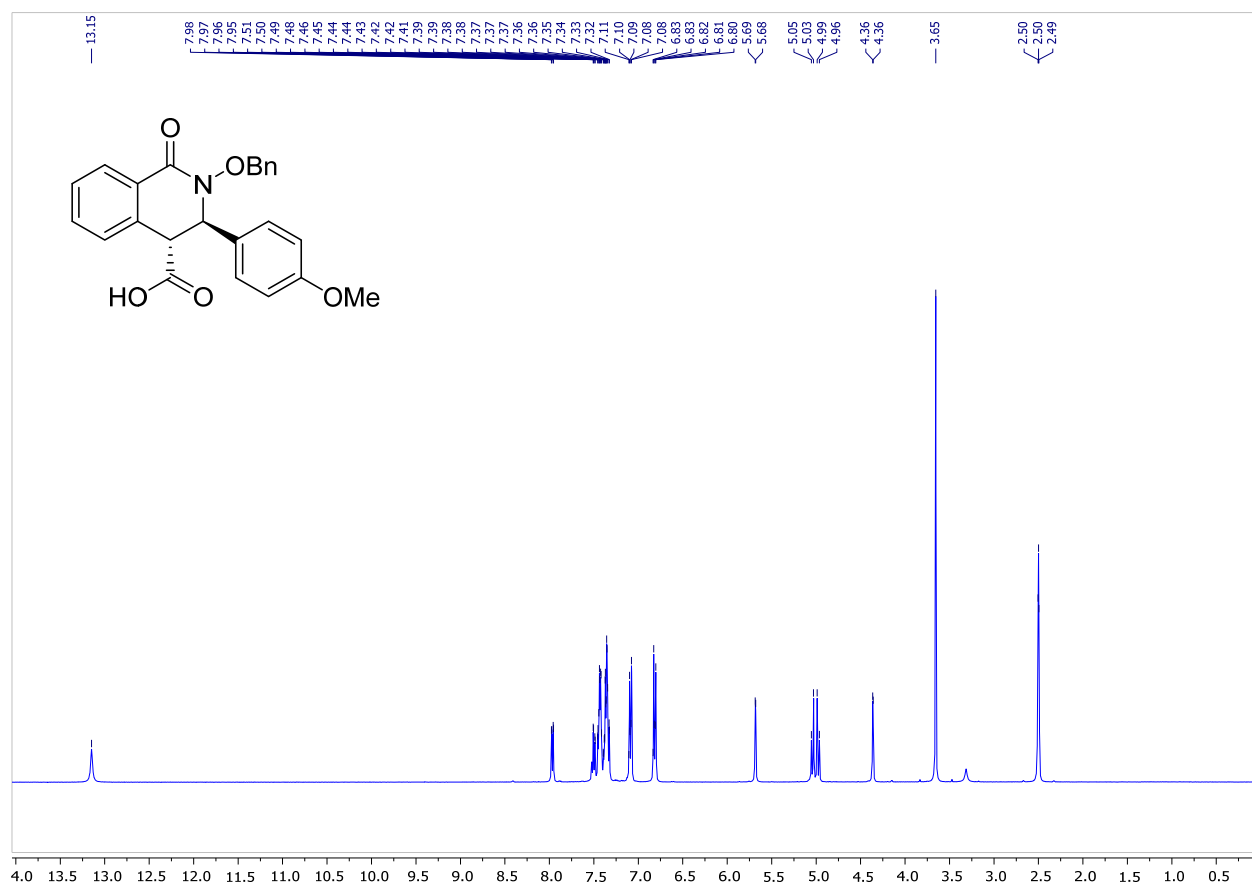
^1H and ^{13}C NMR of compound 8



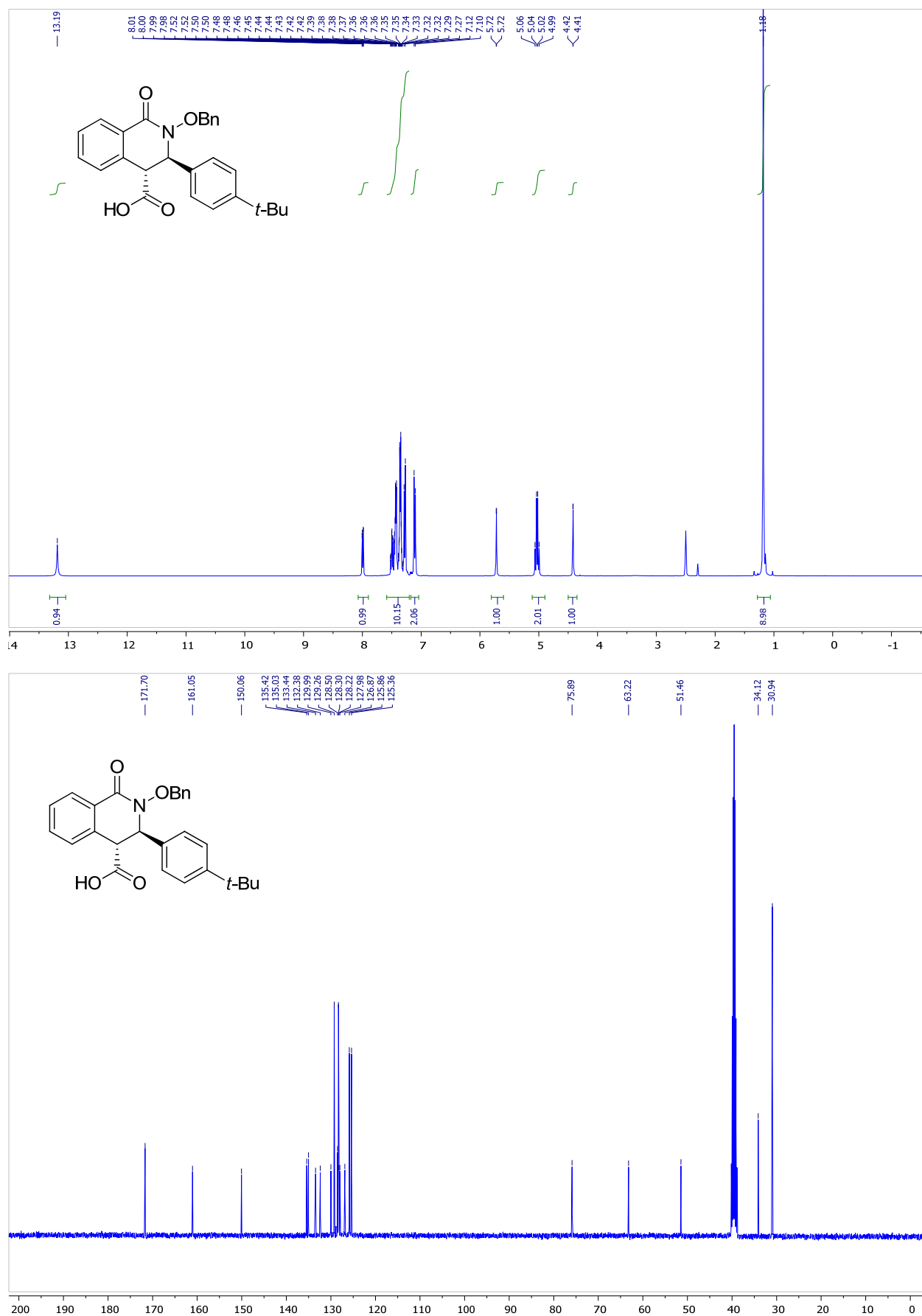
^1H and ^{13}C NMR of compound 9a



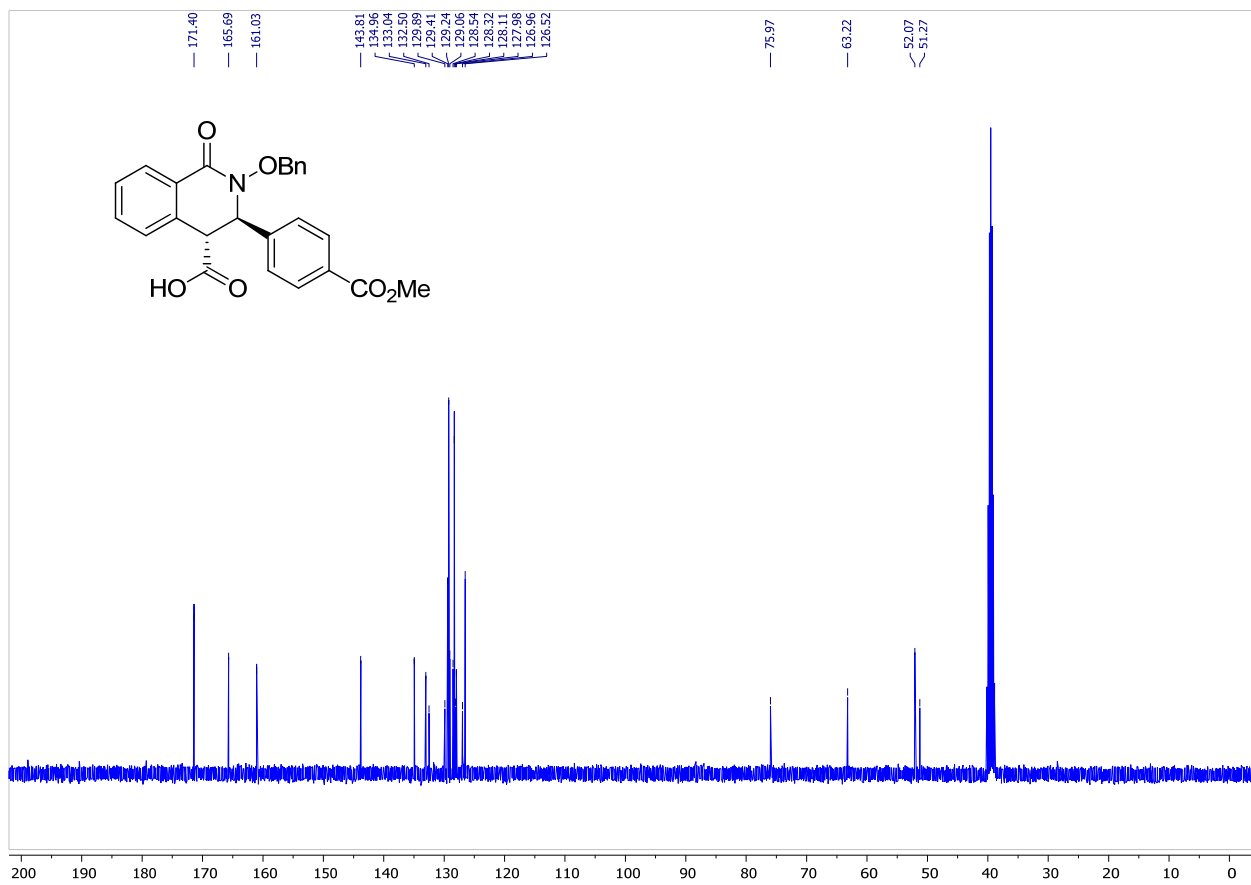
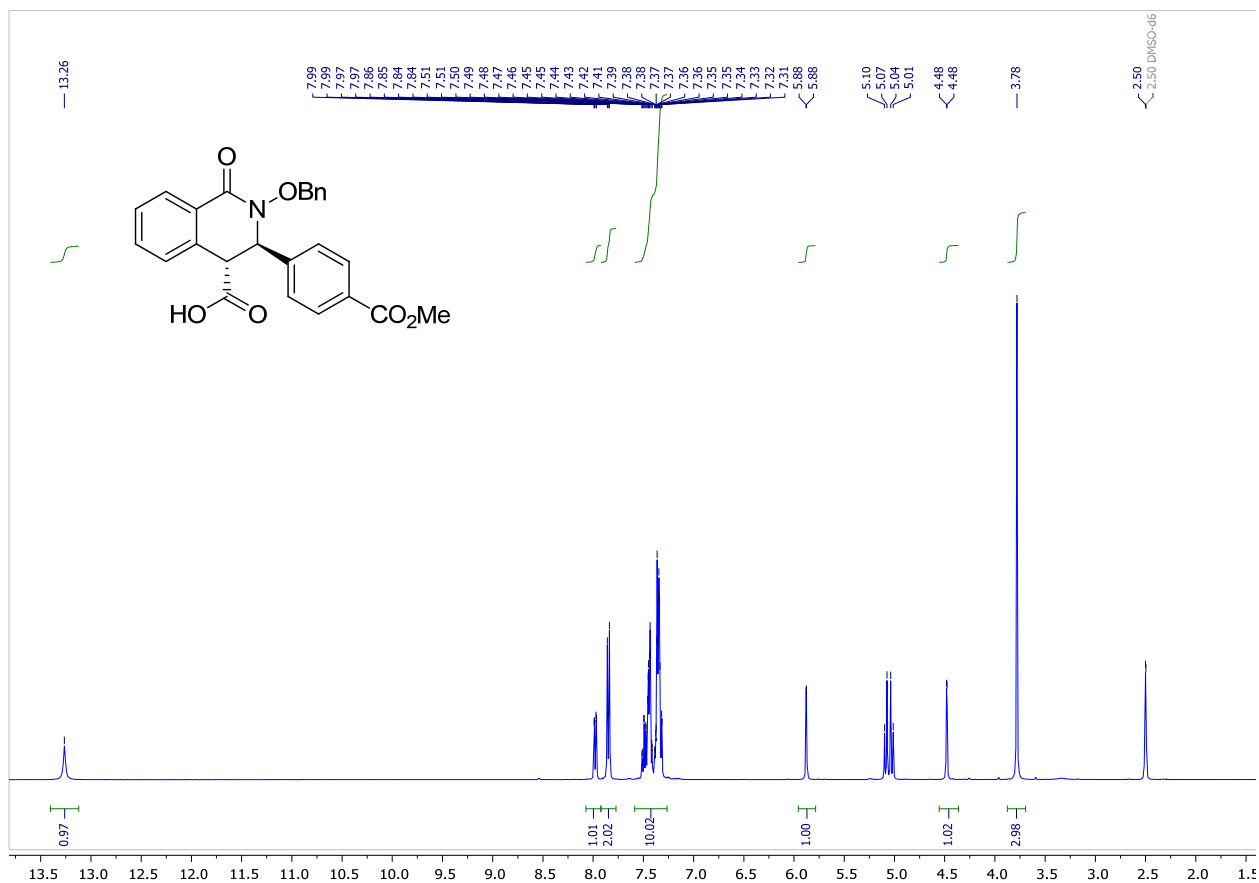
^1H and ^{13}C NMR of compound **9b**



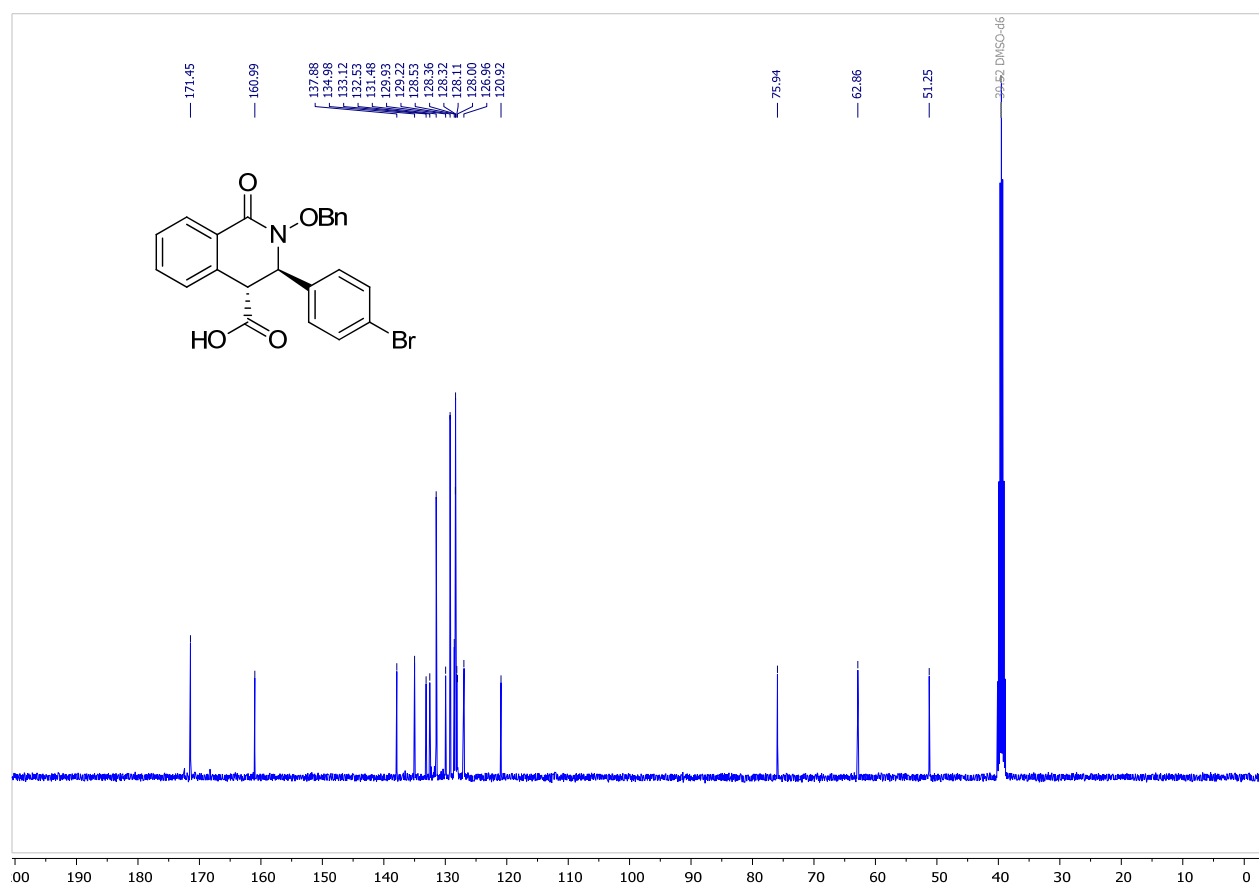
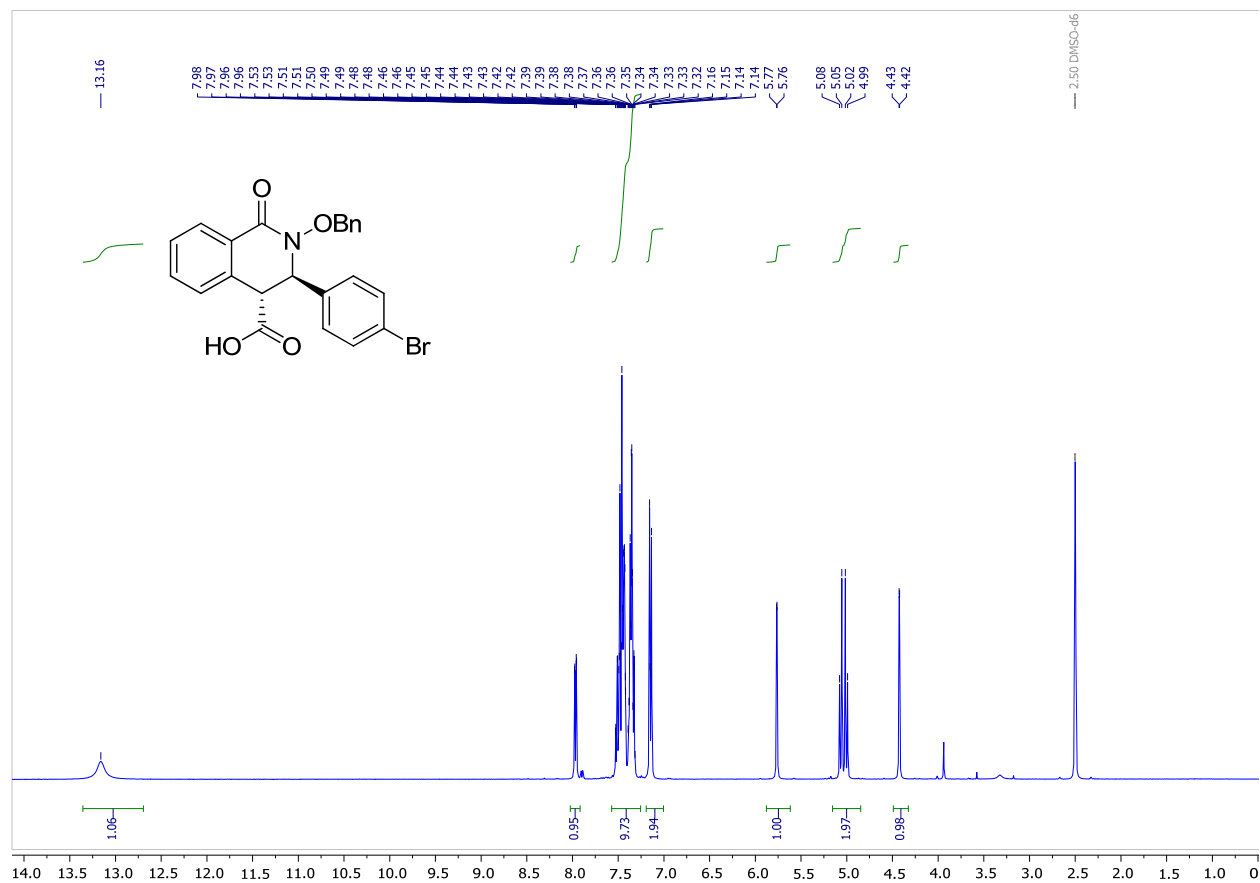
^1H and ^{13}C NMR of compound 9c



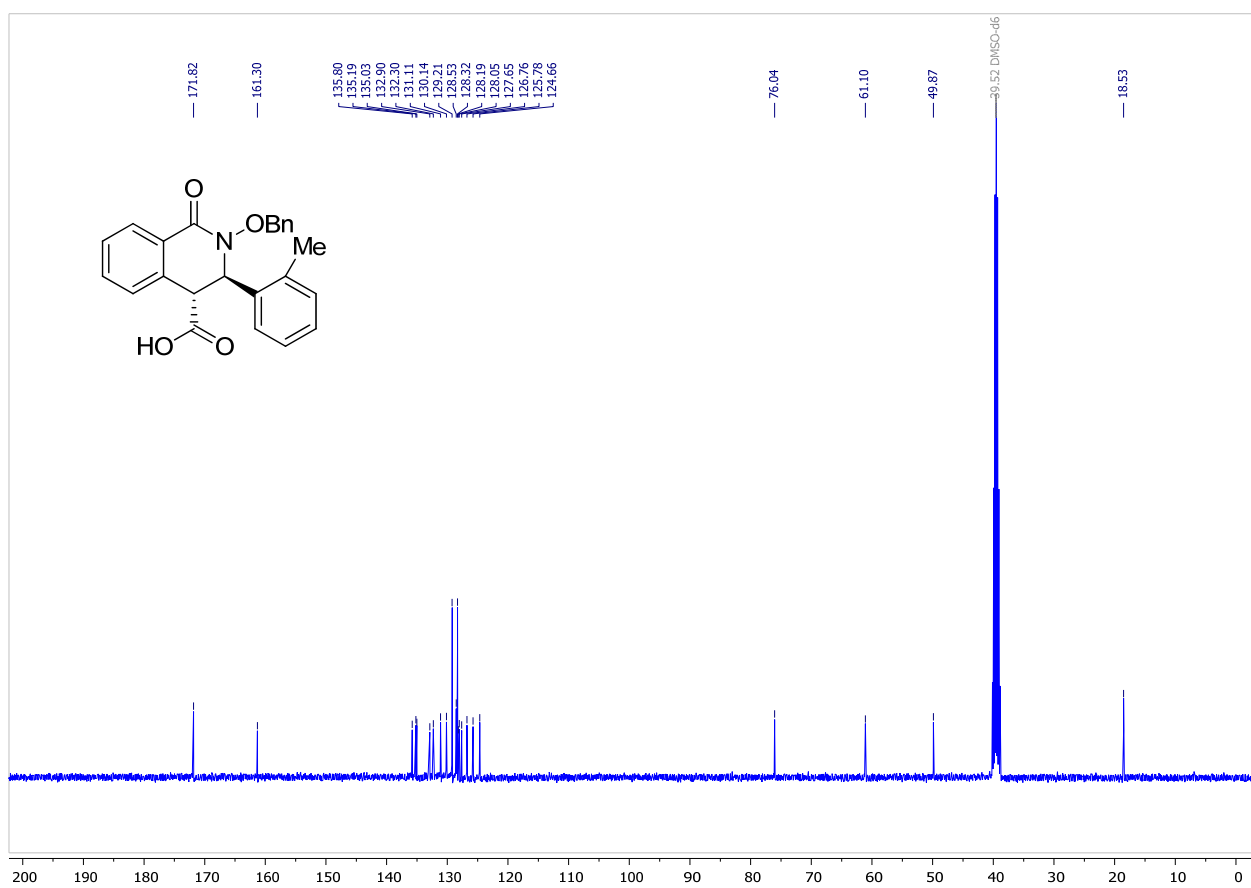
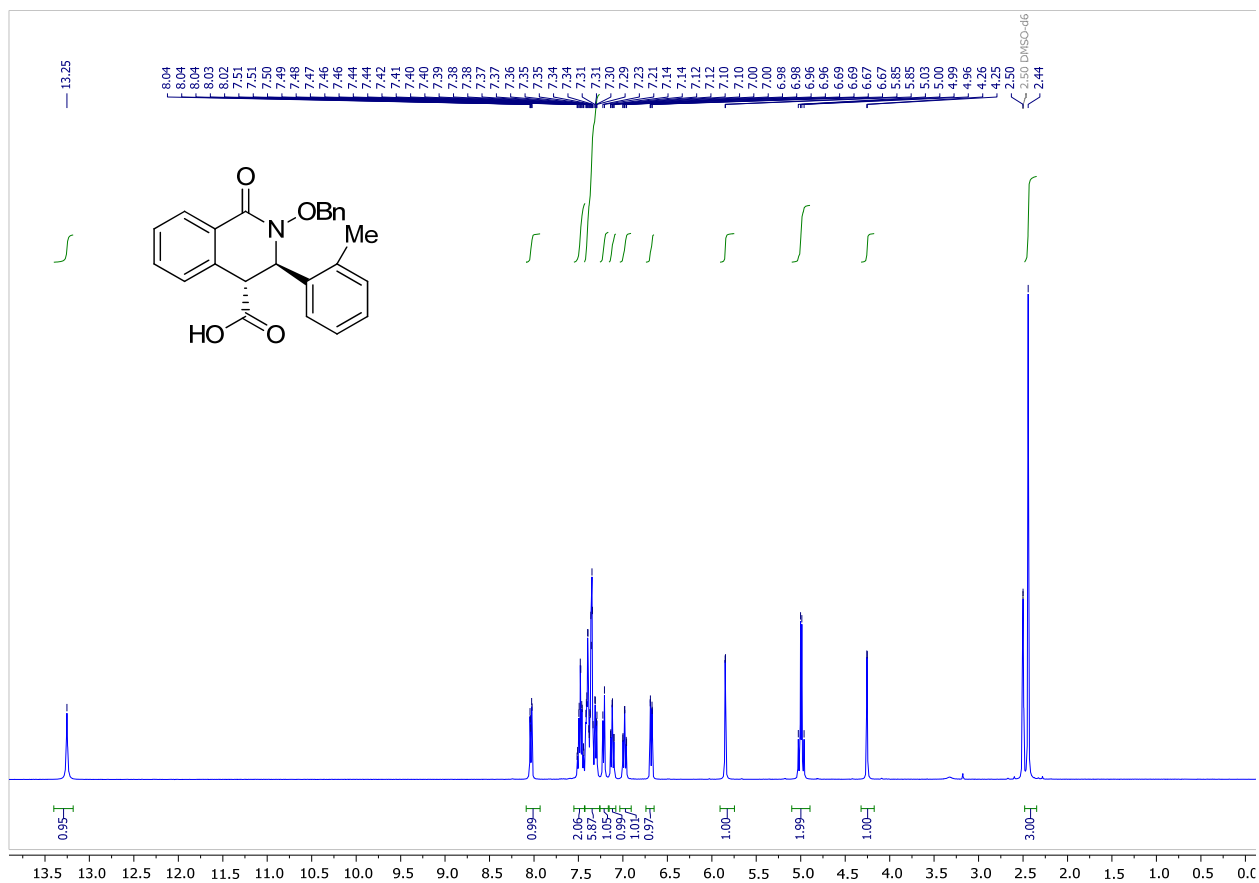
^1H and ^{13}C NMR of compound **9d**



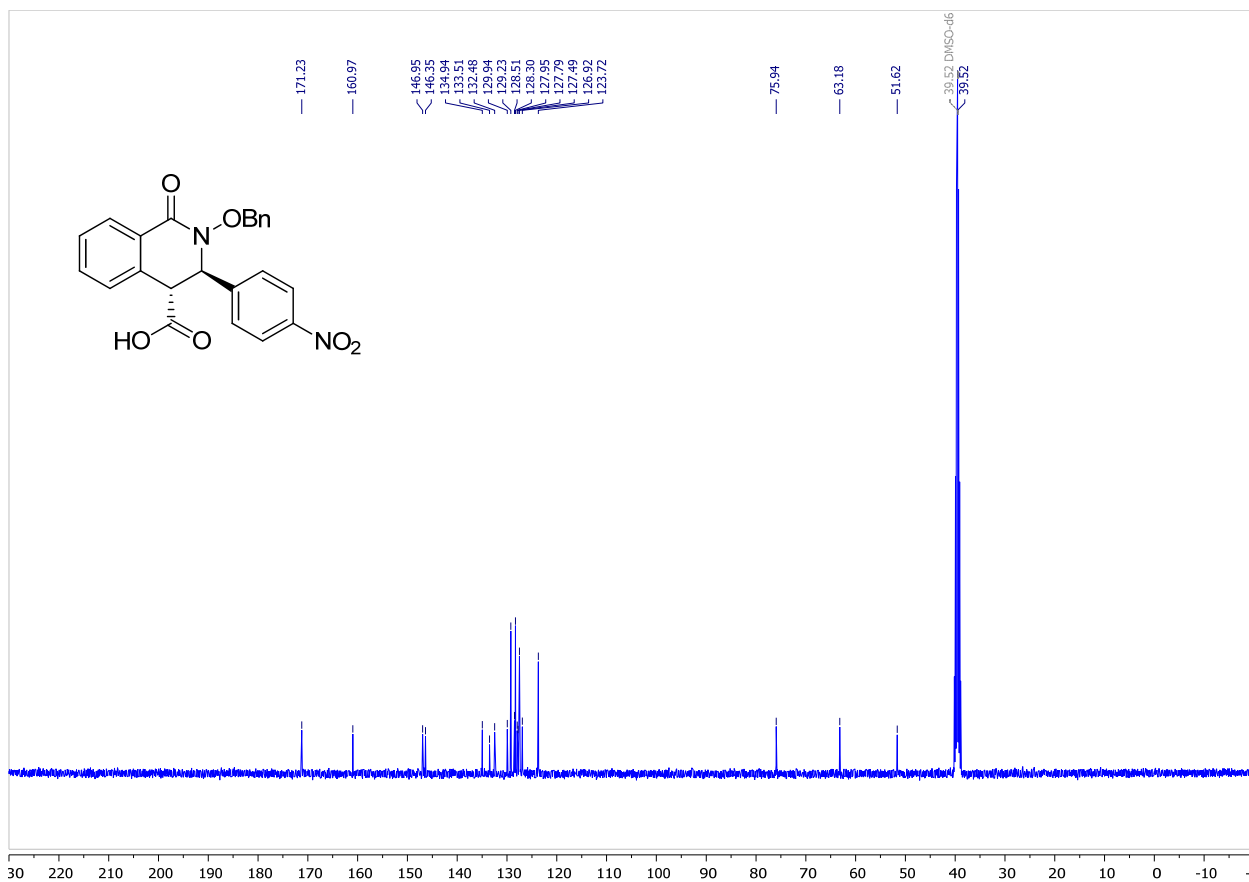
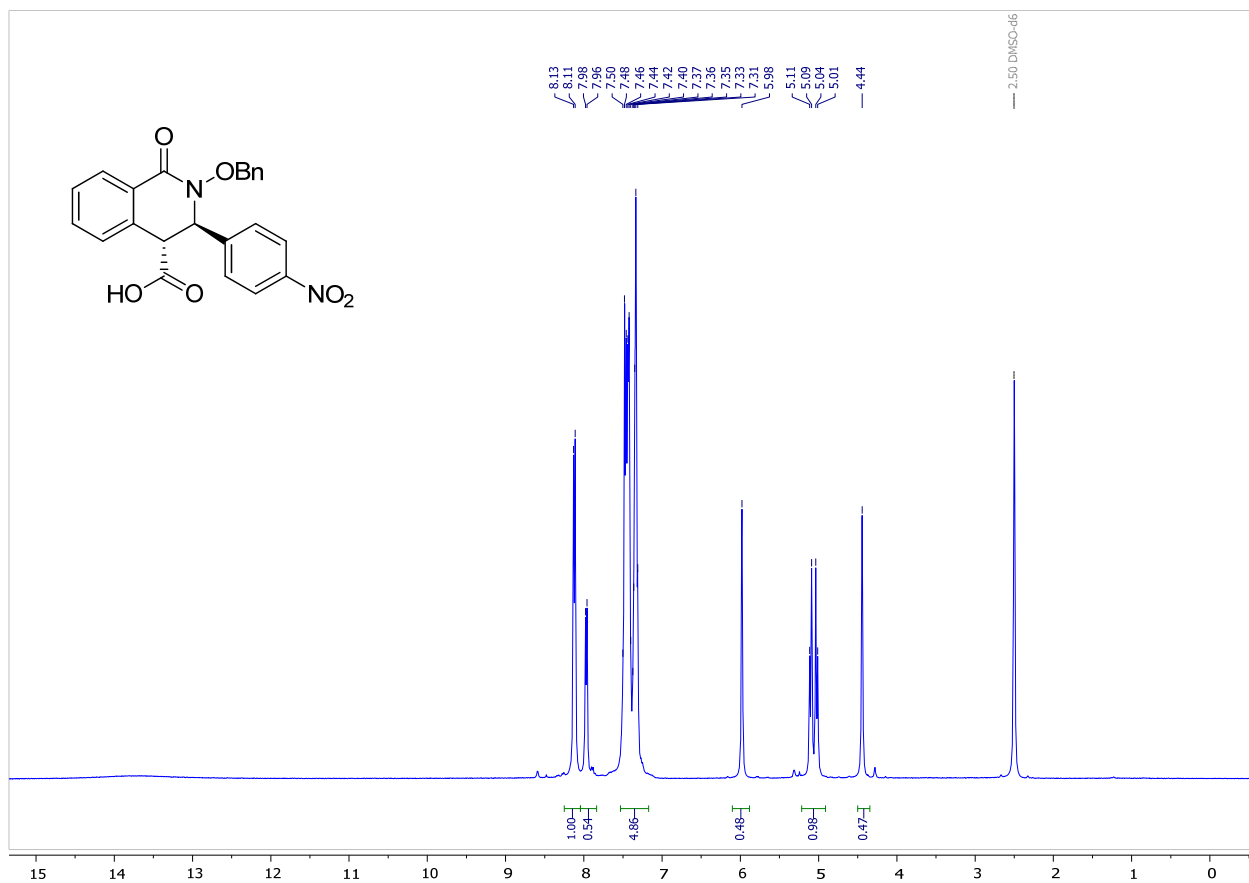
^1H and ^{13}C NMR of compound **9e**



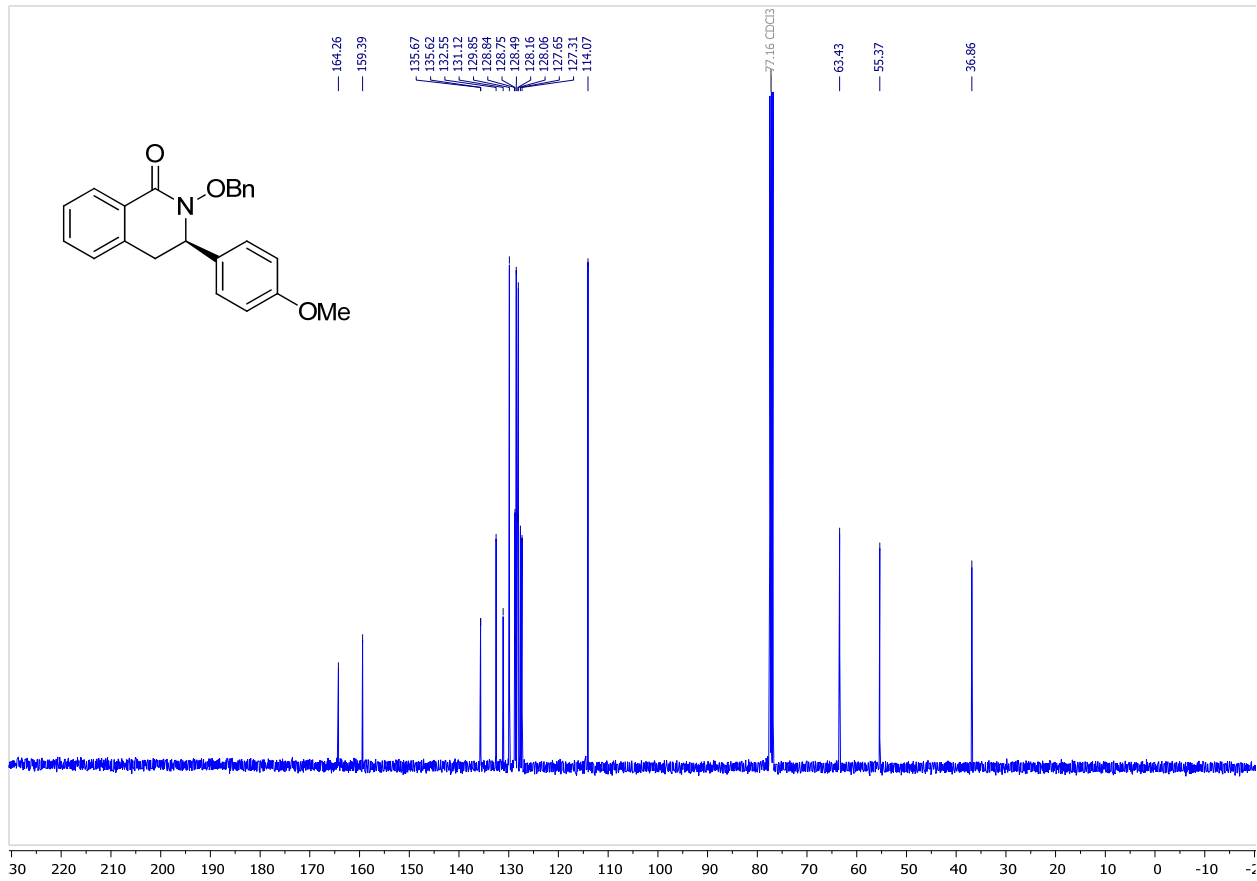
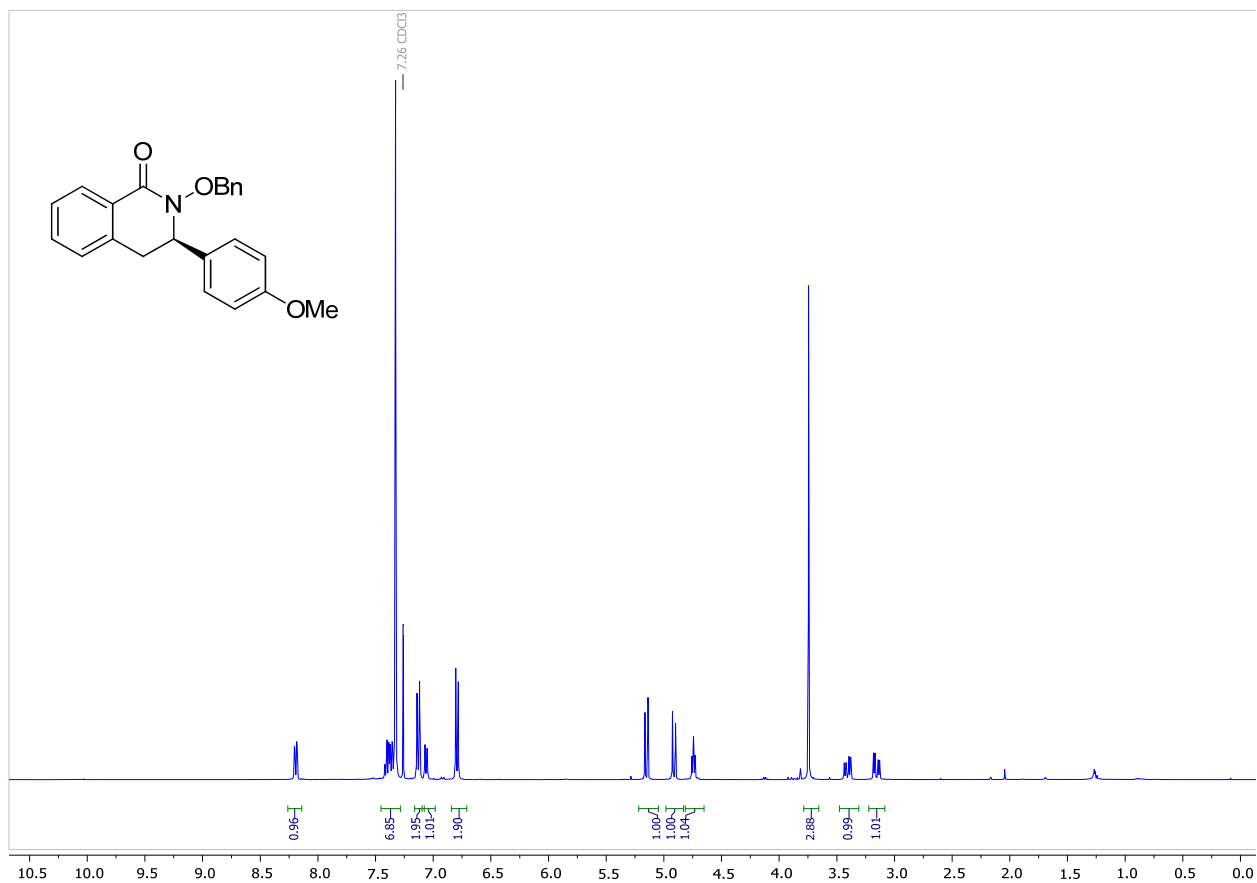
^1H and ^{13}C NMR of compound 9f



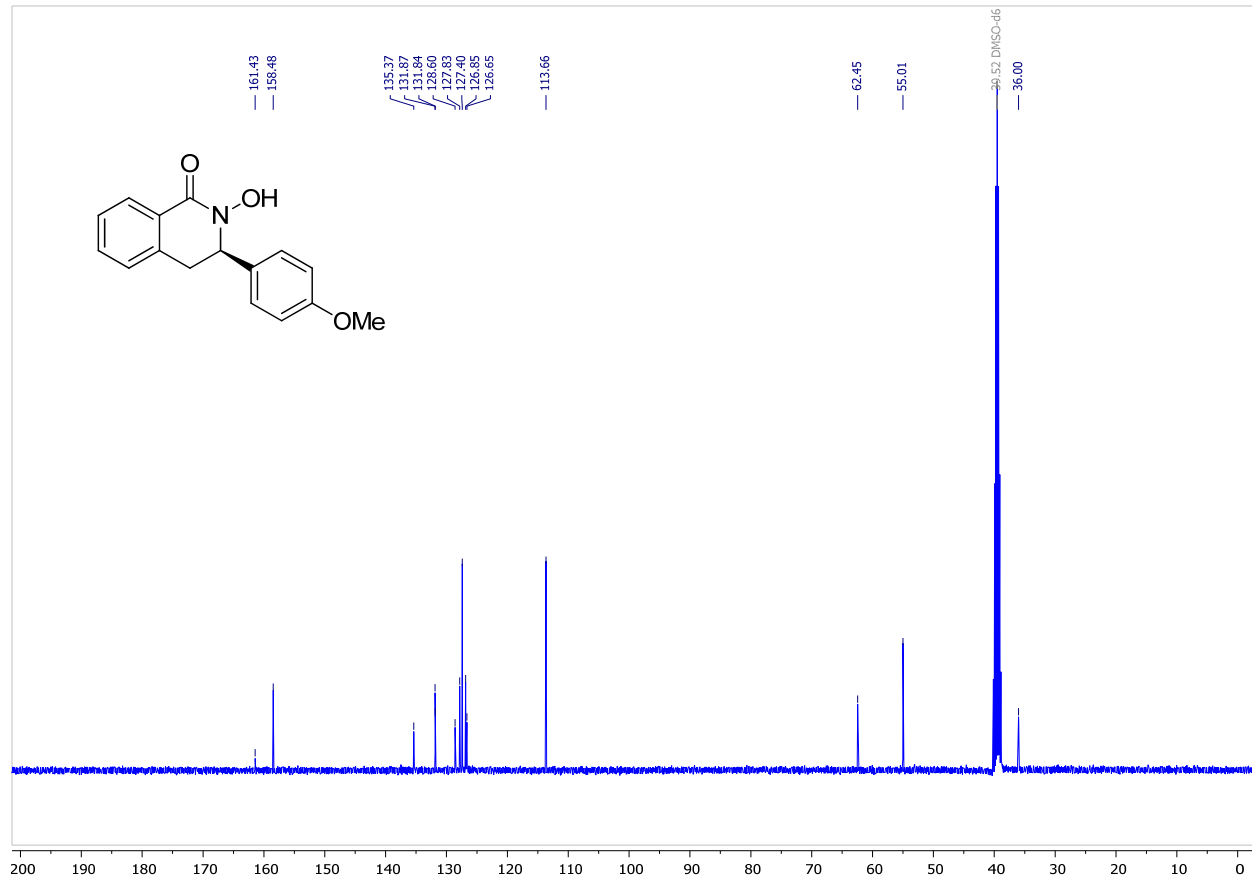
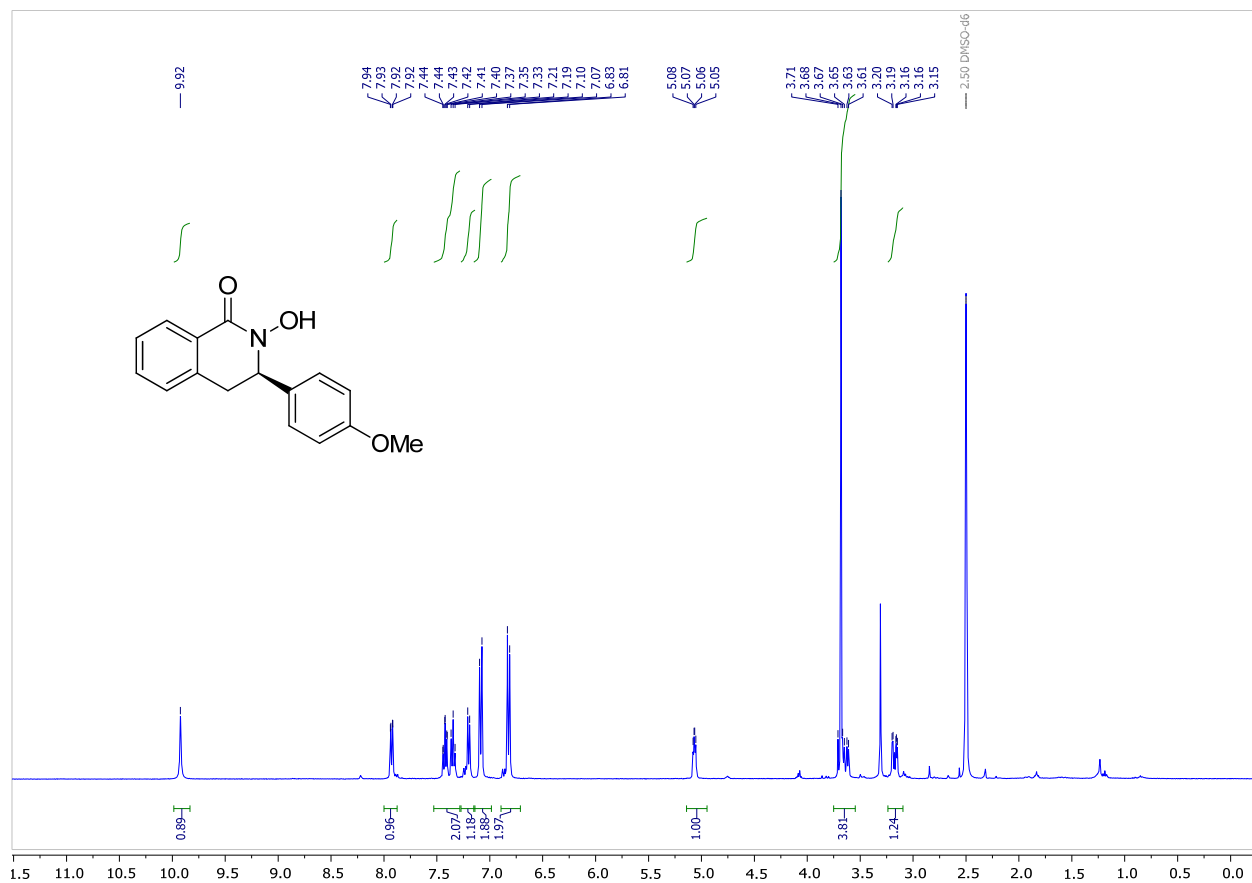
^1H and ^{13}C NMR of compound **9g**



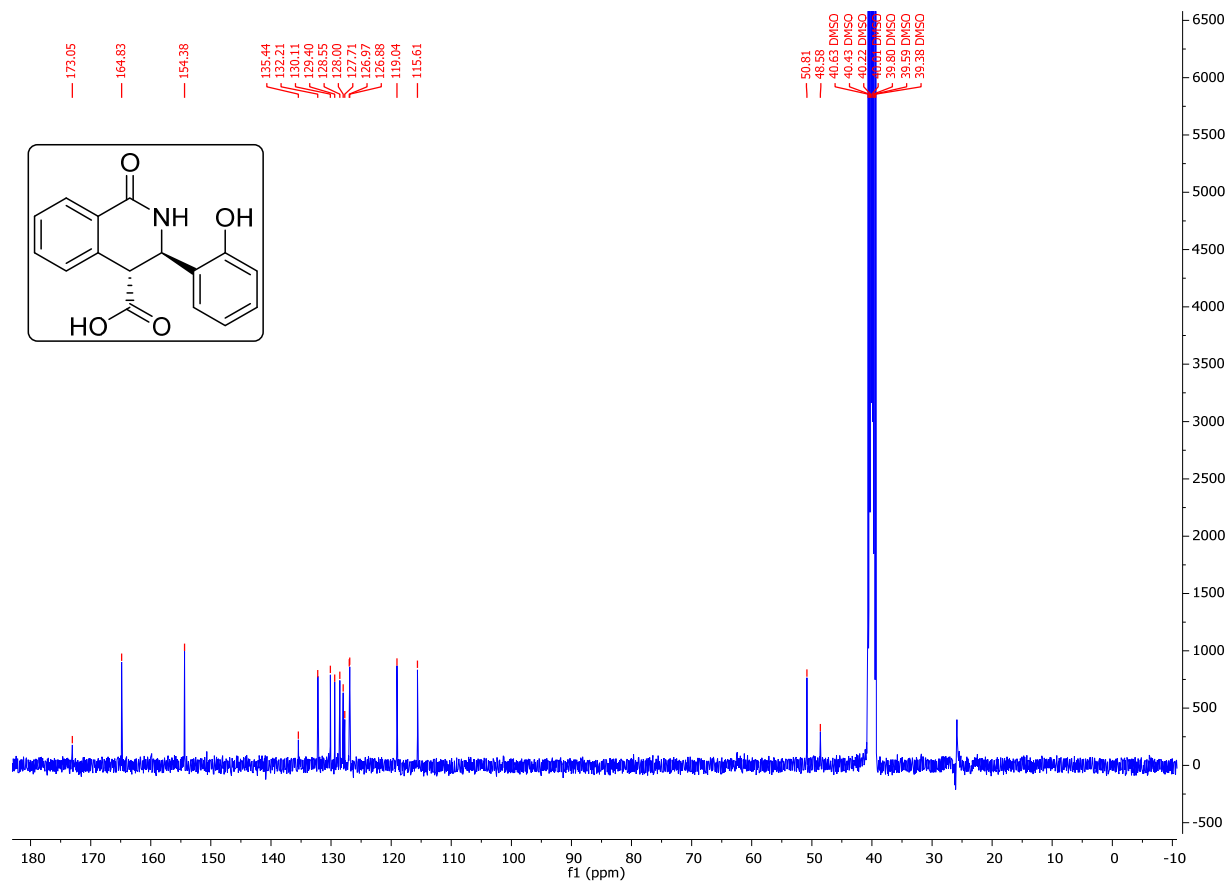
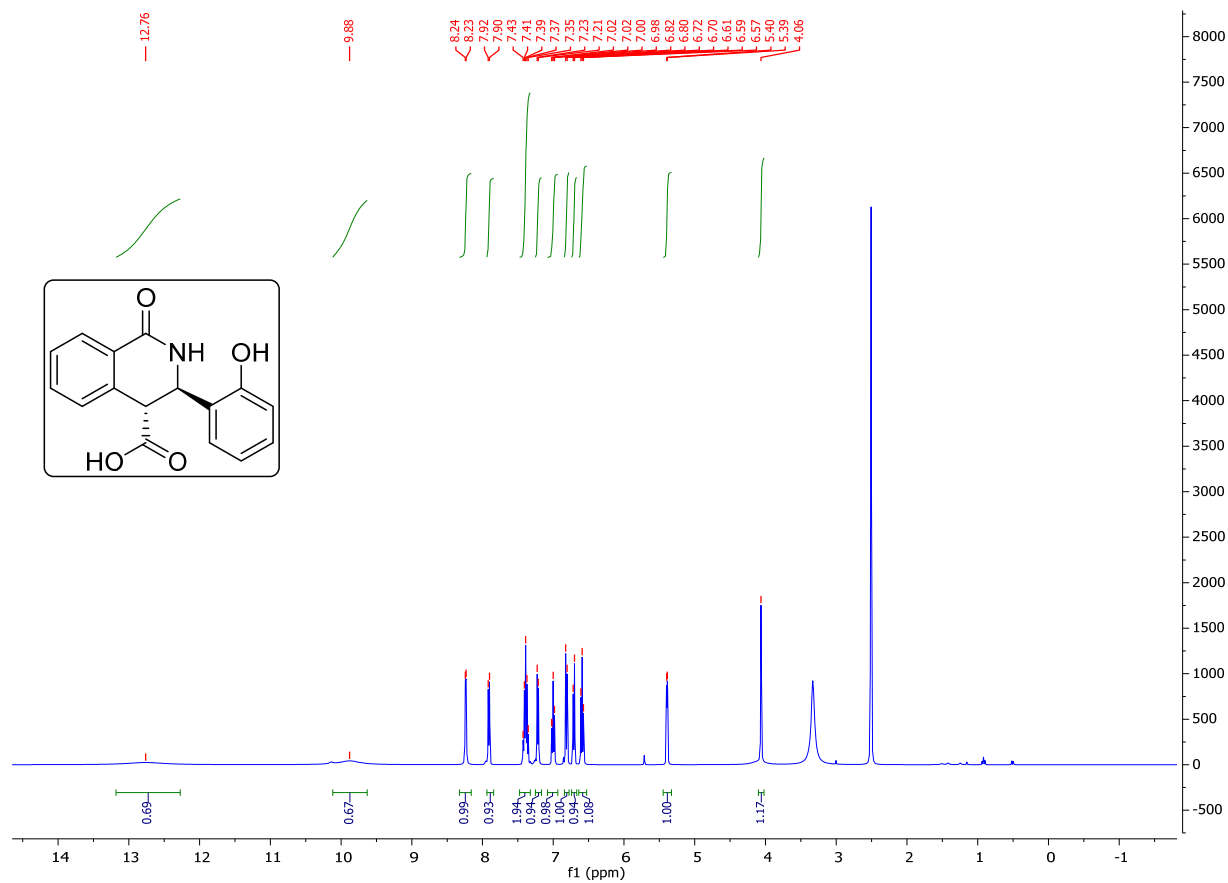
^1H and ^{13}C NMR of compound 10



^1H and ^{13}C NMR of compound 11



^1H and ^{13}C NMR of compound 12



Electronic absorption spectra of 7d,f,g,h,j ligands recorded in MeOH ($C = 5 \times 10^{-5}$ M).

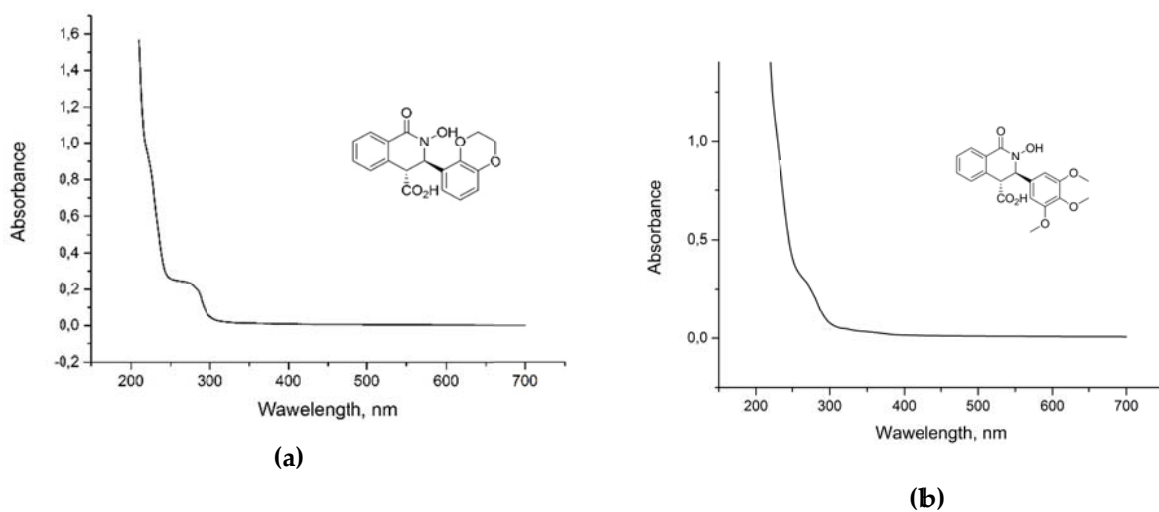


Figure S1. (a) UV-Vis spectrum of compound 7d; (b) UV-Vis spectrum of compound 7f;

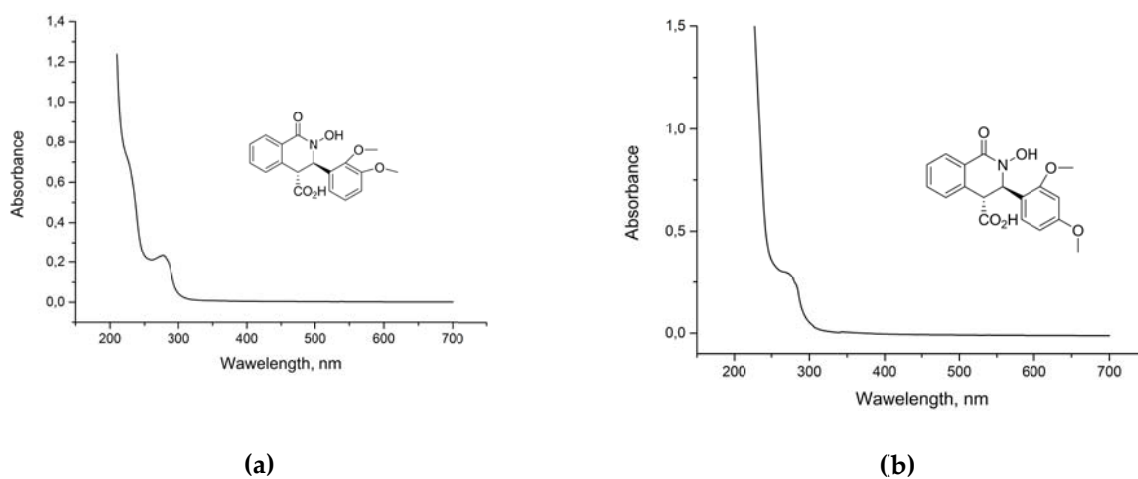


Figure S2. (a) UV-Vis spectrum of compound 7g; (b) UV-Vis spectrum of compound 7h;

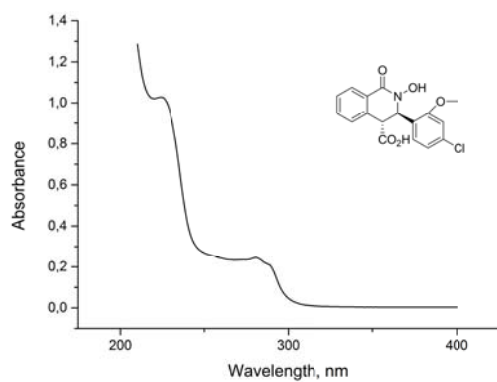


Figure S3. UV-Vis spectrum of compound 7j

Electronic absorption spectra of 7d,f,g,h,j ligands ($C_L = 5 \times 10^{-4}$ M) in the presence of increasing concentration of Fe^{3+} (left; $C_{Fe} = 0.25-5 \times 10^{-4}$ M) and corresponding binding isotherms plotted at selected wavelengths (right; red asterisks – experimental data, black line – nonlinear curve fitting according to eqn.3, Materials and Methods).

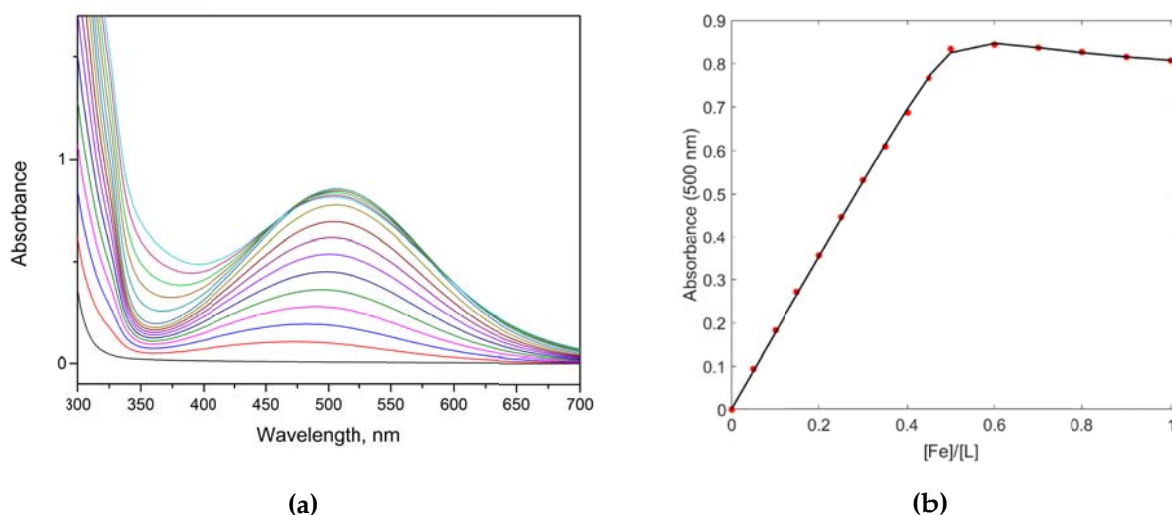


Figure S4. (a) Changes in UV-Vis spectrum of compound 7d upon addition of $Fe(NO_3)_3$; (b) corresponding mole ratio plot (500 nm), 7d+ Fe^{3+}

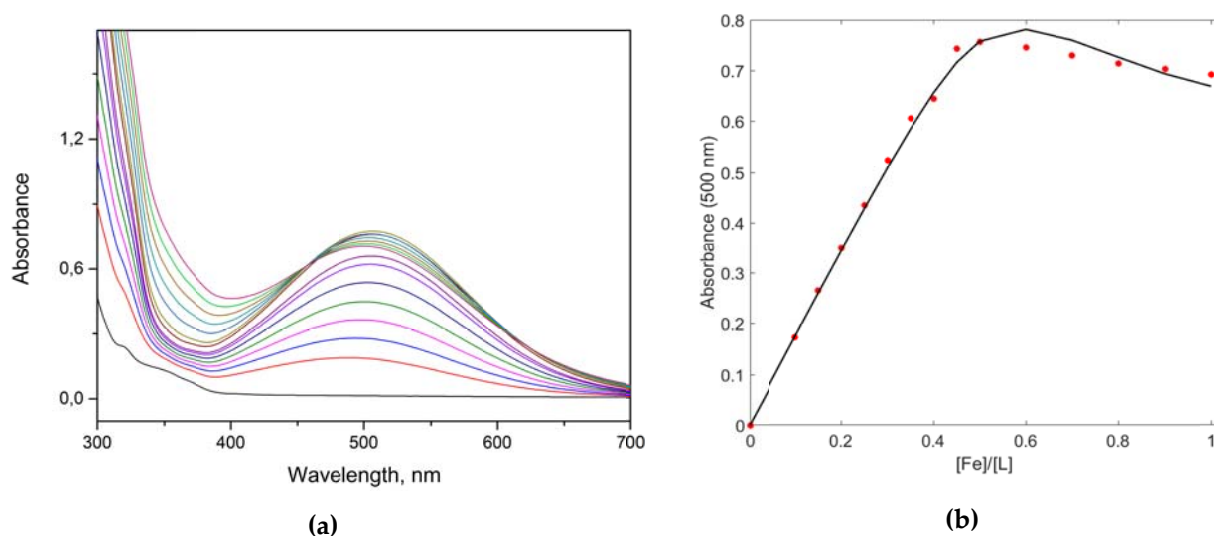
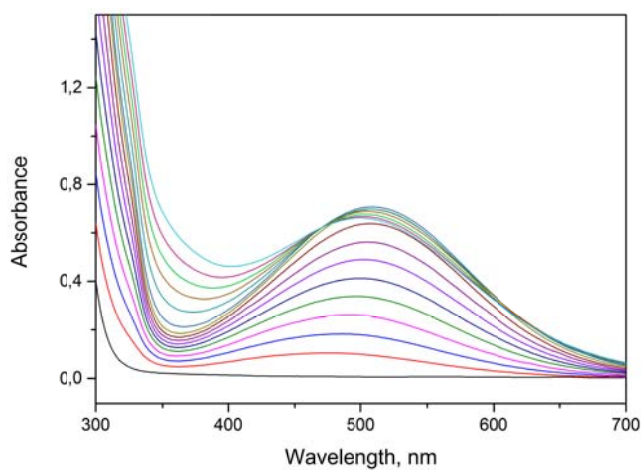
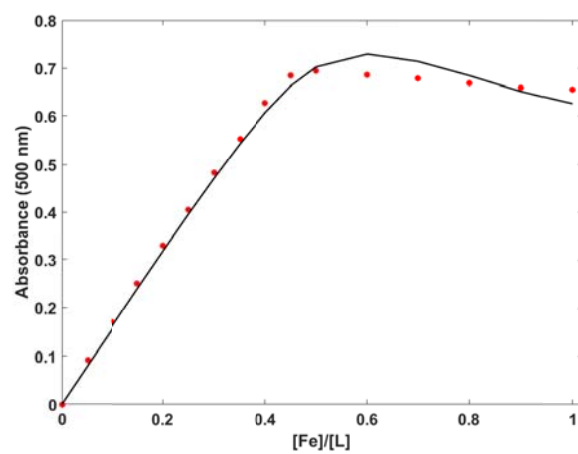


Figure S5. (a) Changes in UV-Vis spectrum of compound 7f upon addition of $Fe(NO_3)_3$; (b) corresponding mole ratio plot (500 nm), 7f+ Fe^{3+}

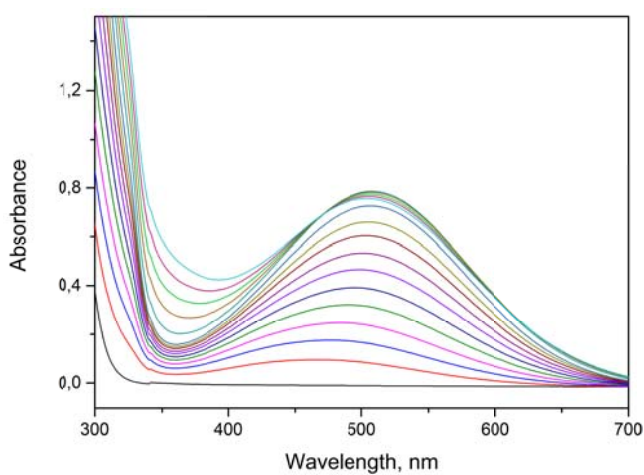


(a)

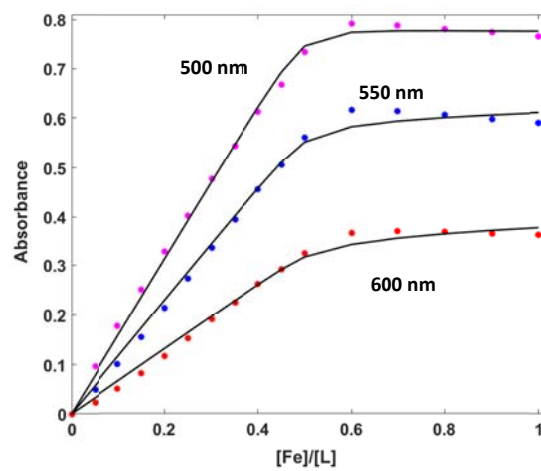


(b)

Figure S6. (a) Changes in UV-Vis spectrum of compound **7g** upon addition of $\text{Fe}(\text{NO}_3)_3$; (b) corresponding mole ratio plot (500 nm), $7\text{g}+\text{Fe}^{3+}$

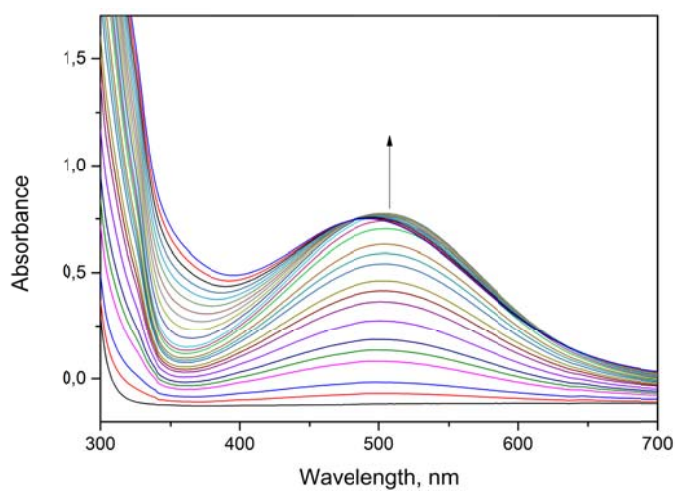


(a)

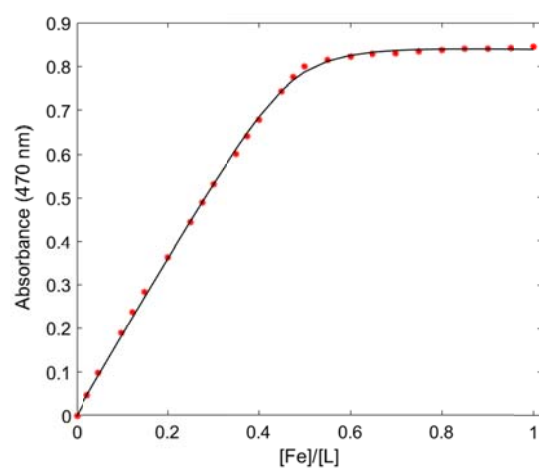


(b)

Figure S7. (a) Changes in UV-Vis spectrum of compound **7h** upon addition of $\text{Fe}(\text{NO}_3)_3$; (b) corresponding mole ratio plots (500, 550, 600 nm), $7\text{h}+\text{Fe}^{3+}$



(a)



(b)

Figure S8. (a) Changes in UV-Vis spectrum of compound **7j** upon addition of $\text{Fe}(\text{NO}_3)_3$; (b) corresponding mole ratio plot (470 nm), $7j+\text{Fe}^{3+}$