

Supporting Information

A convenient one-pot synthesis of *N*-substituted amidoximes and their application toward 1,2,4-oxadiazol-5-ones

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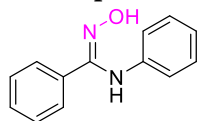
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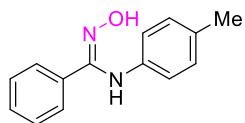
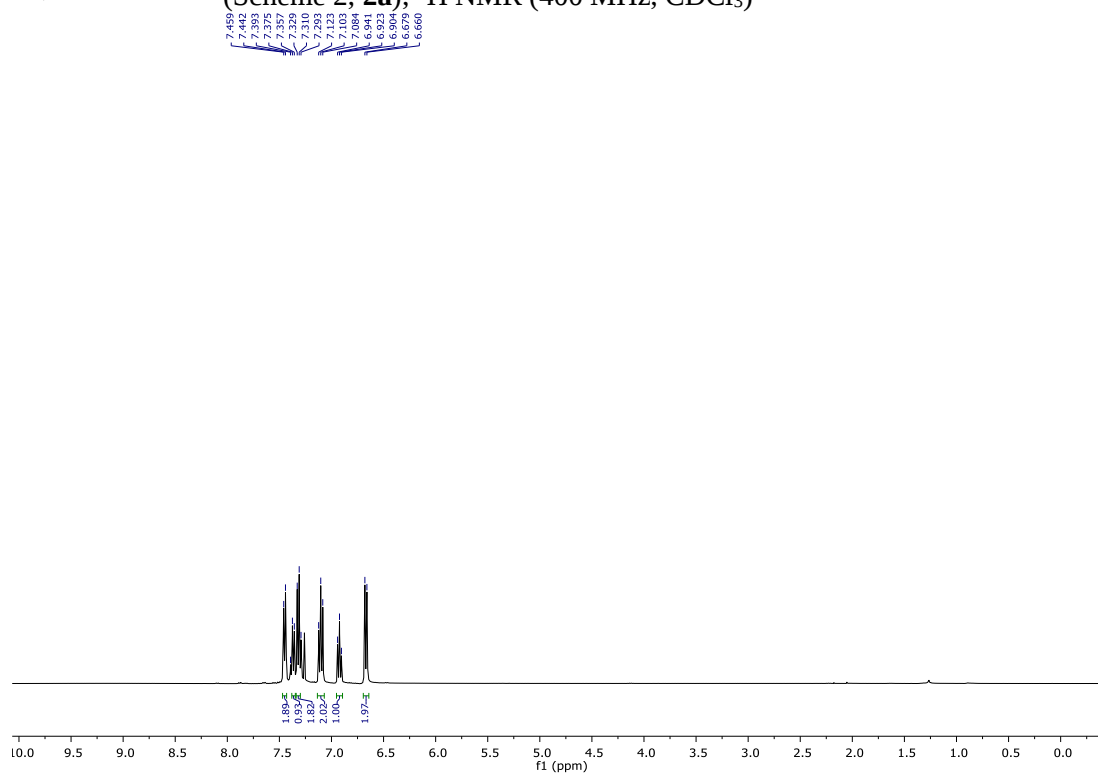
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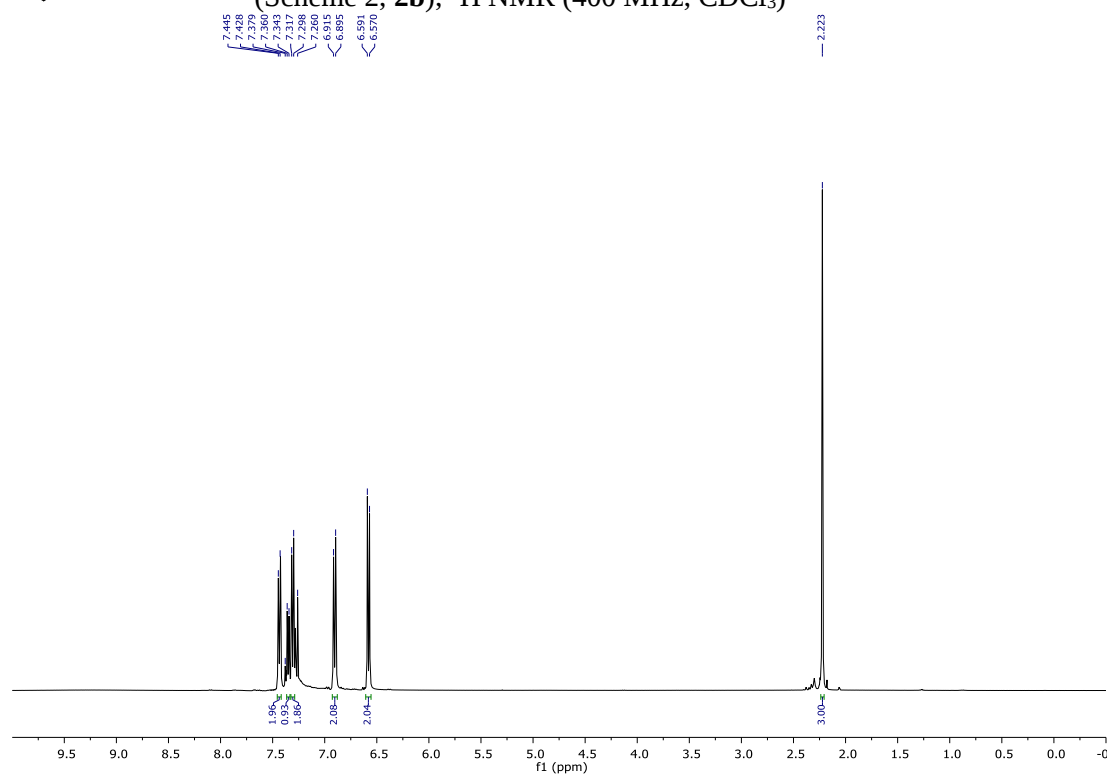
NMR spectra of all products

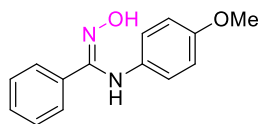


(Scheme 2, **2a**); ^1H NMR (400 MHz, CDCl_3)

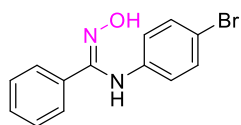
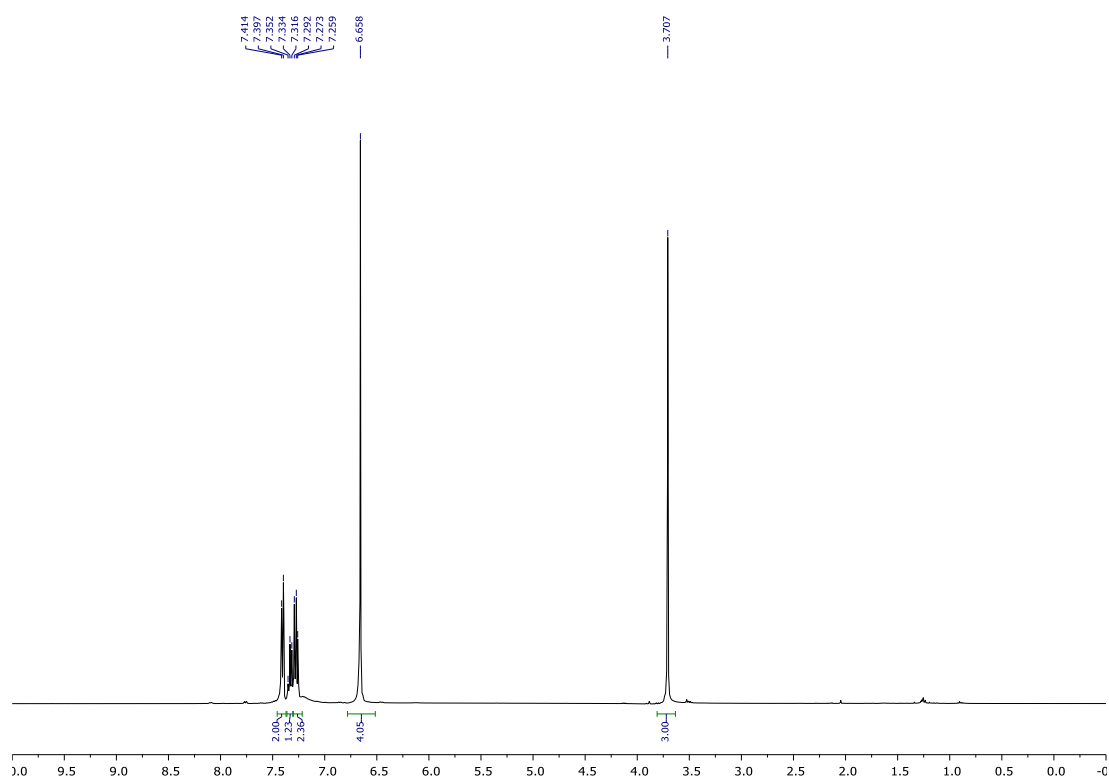


(Scheme 2, **2b**); ^1H NMR (400 MHz, CDCl_3)

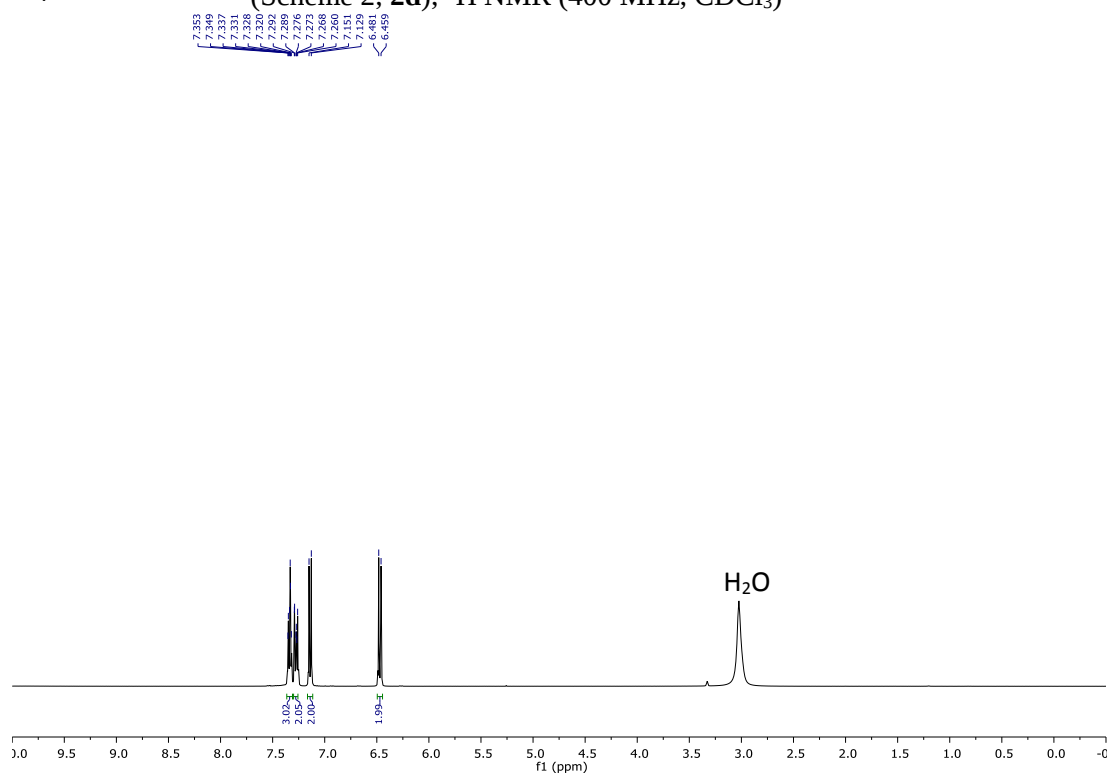


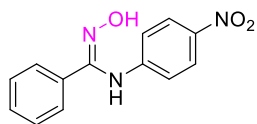


(Scheme 2, 2c); ^1H NMR (400 MHz, CDCl_3)

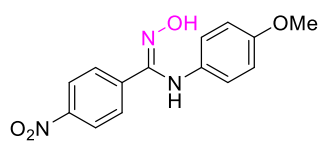
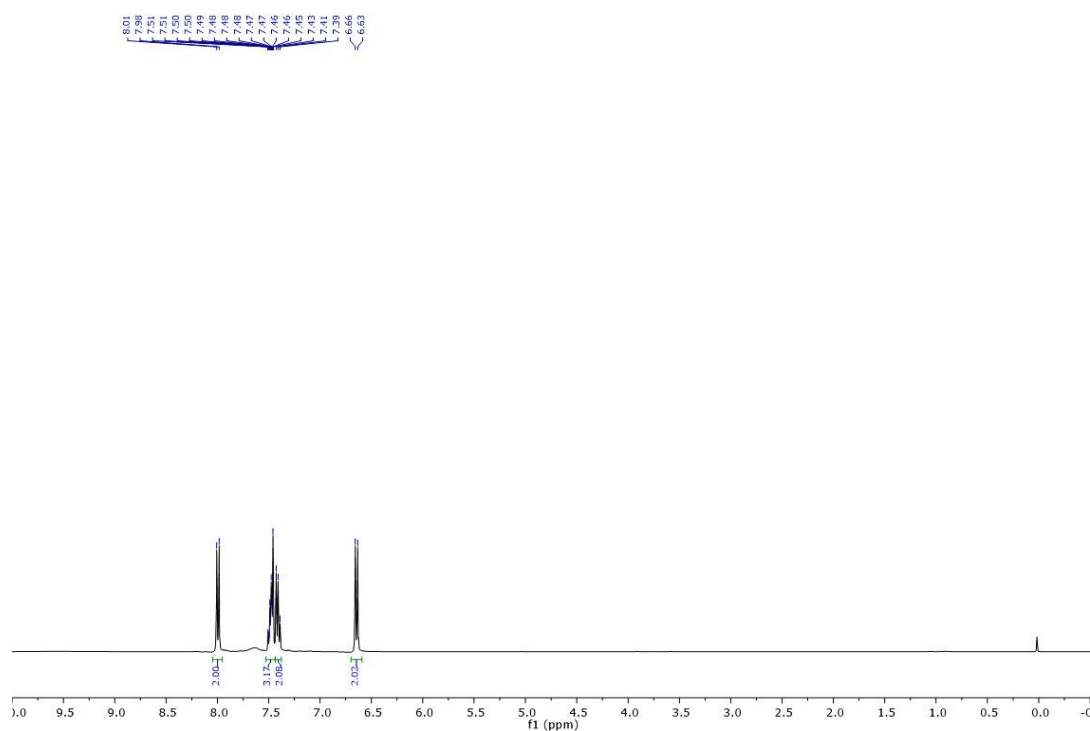


(Scheme 2, 2d); ^1H NMR (400 MHz, CDCl_3)

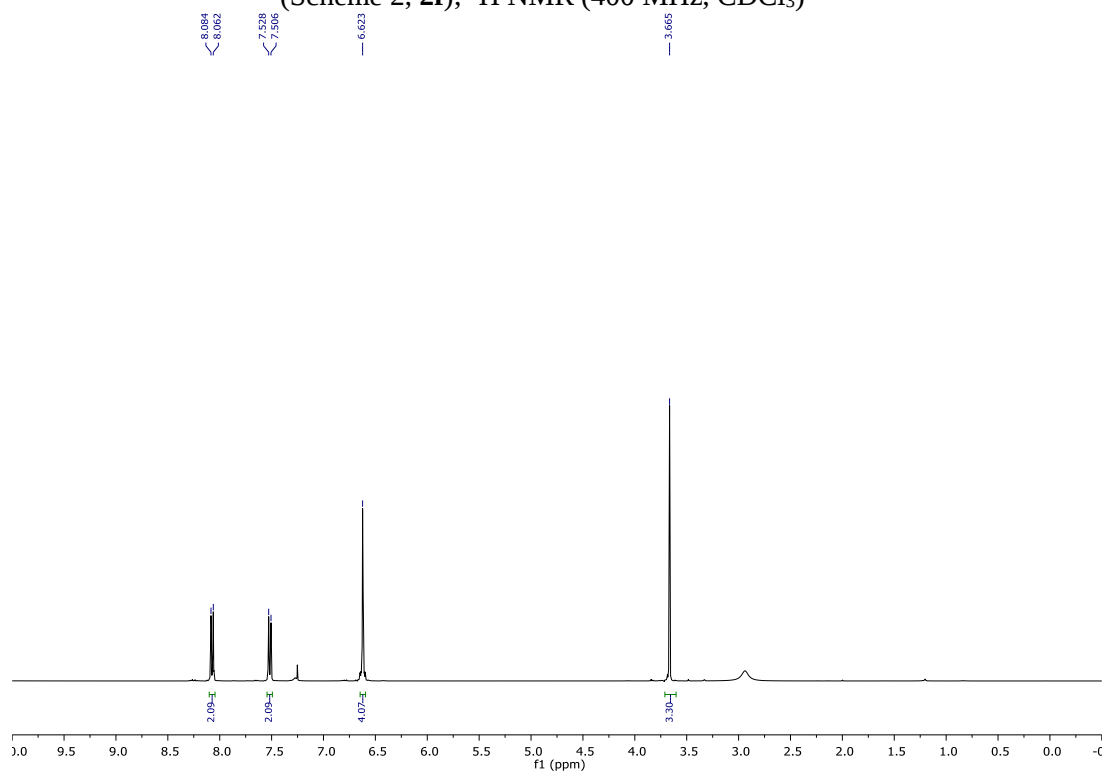


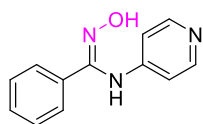


(Scheme 2, **2e**); ^1H NMR (400 MHz, CDCl_3)

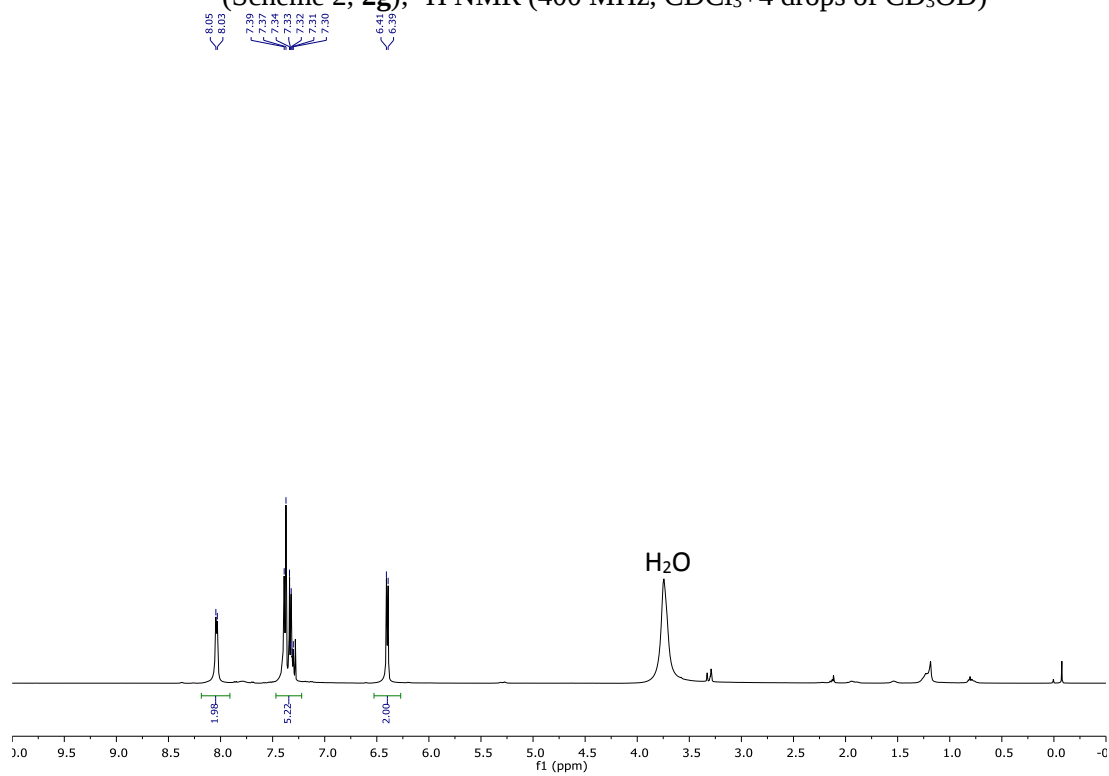


(Scheme 2, **2f**); ^1H NMR (400 MHz, CDCl_3)

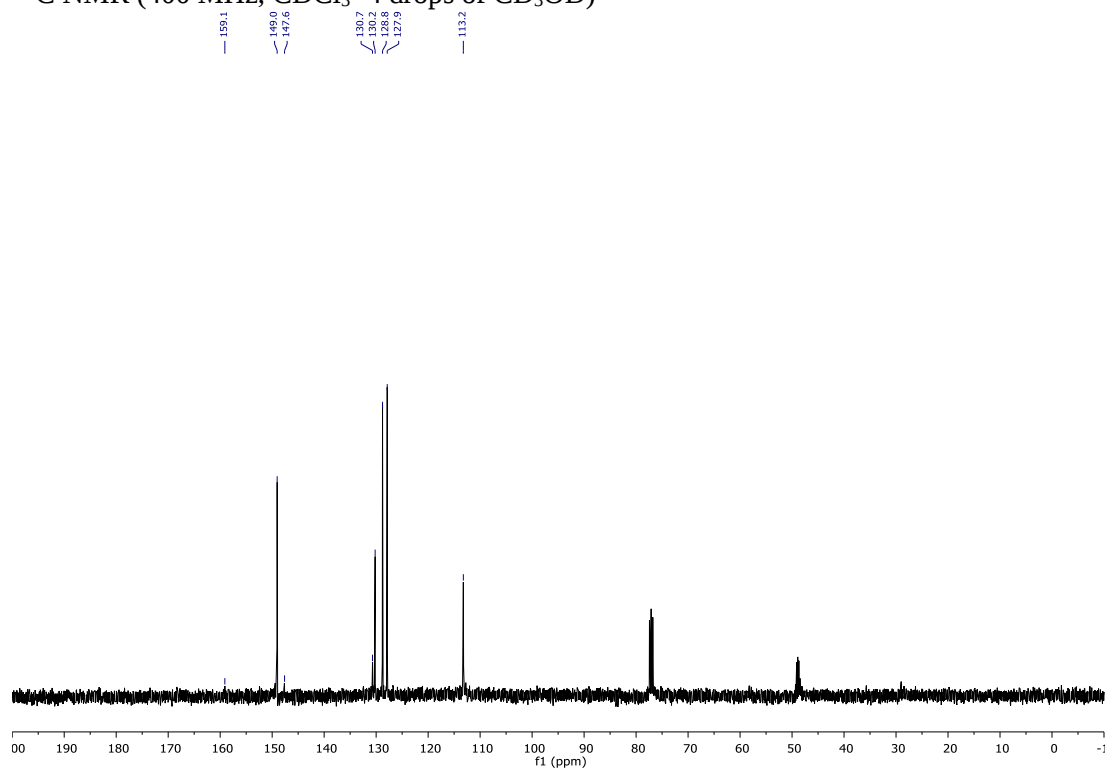


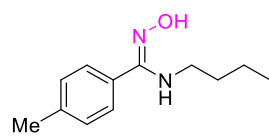


(Scheme 2, **2g**); ^1H NMR (400 MHz, CDCl_3 +4 drops of CD_3OD)

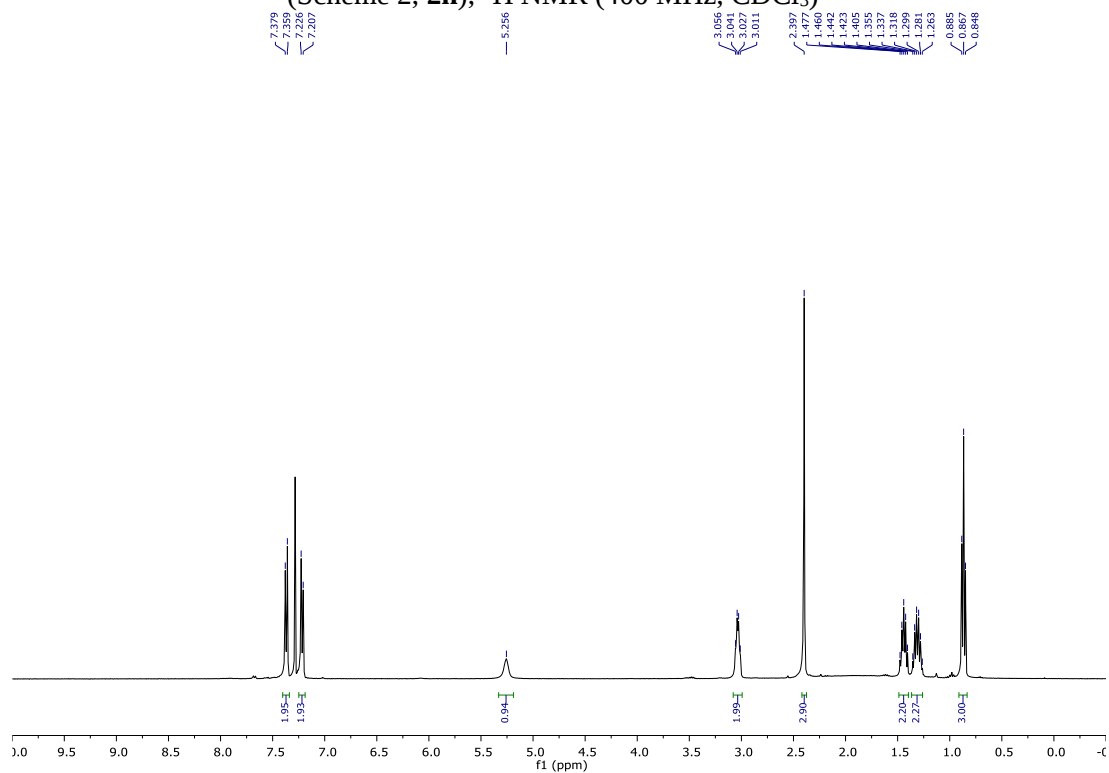


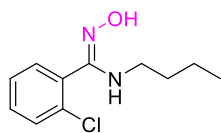
^{13}C NMR (400 MHz, CDCl_3 +4 drops of CD_3OD)



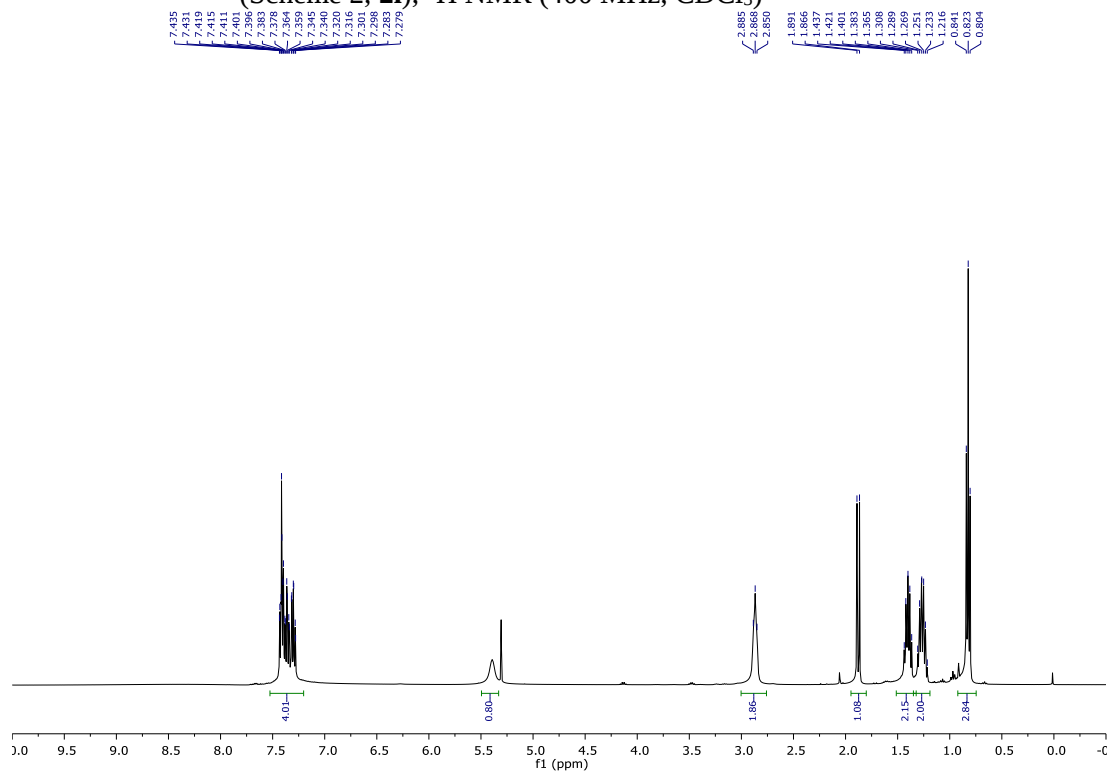


(Scheme 2, **2h**); ^1H NMR (400 MHz, CDCl_3)

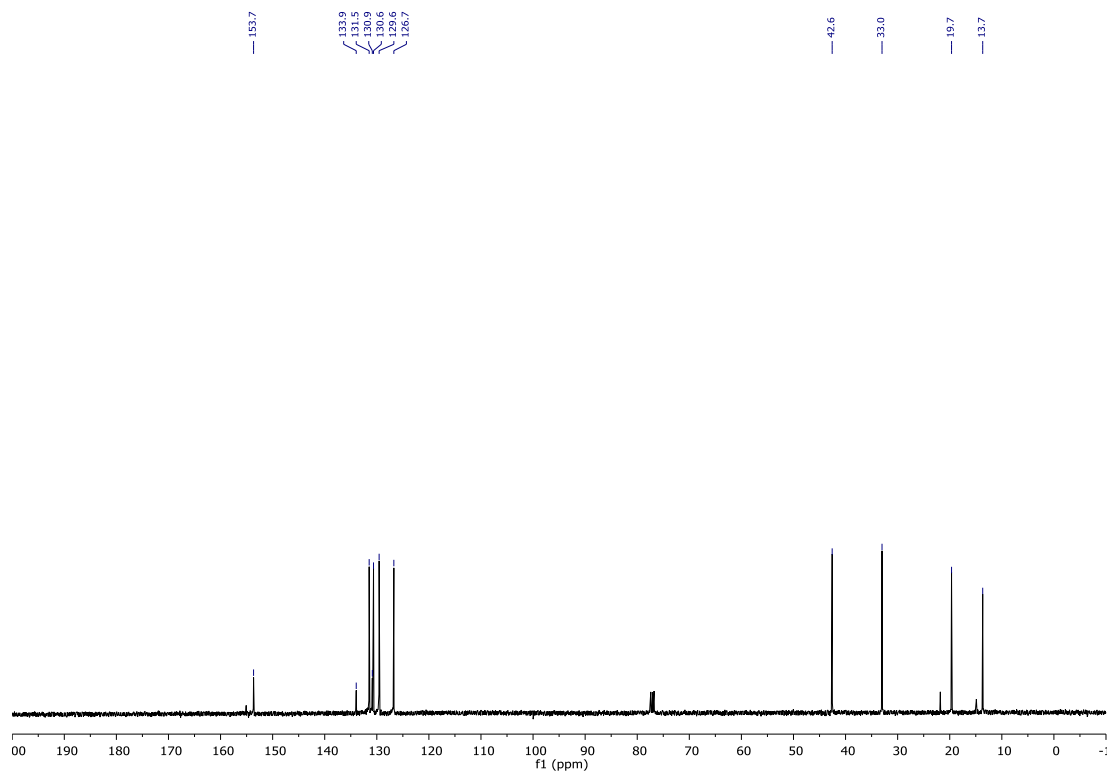


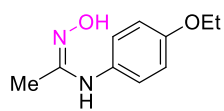


(Scheme 2, 2i); ^1H NMR (400 MHz, CDCl_3)

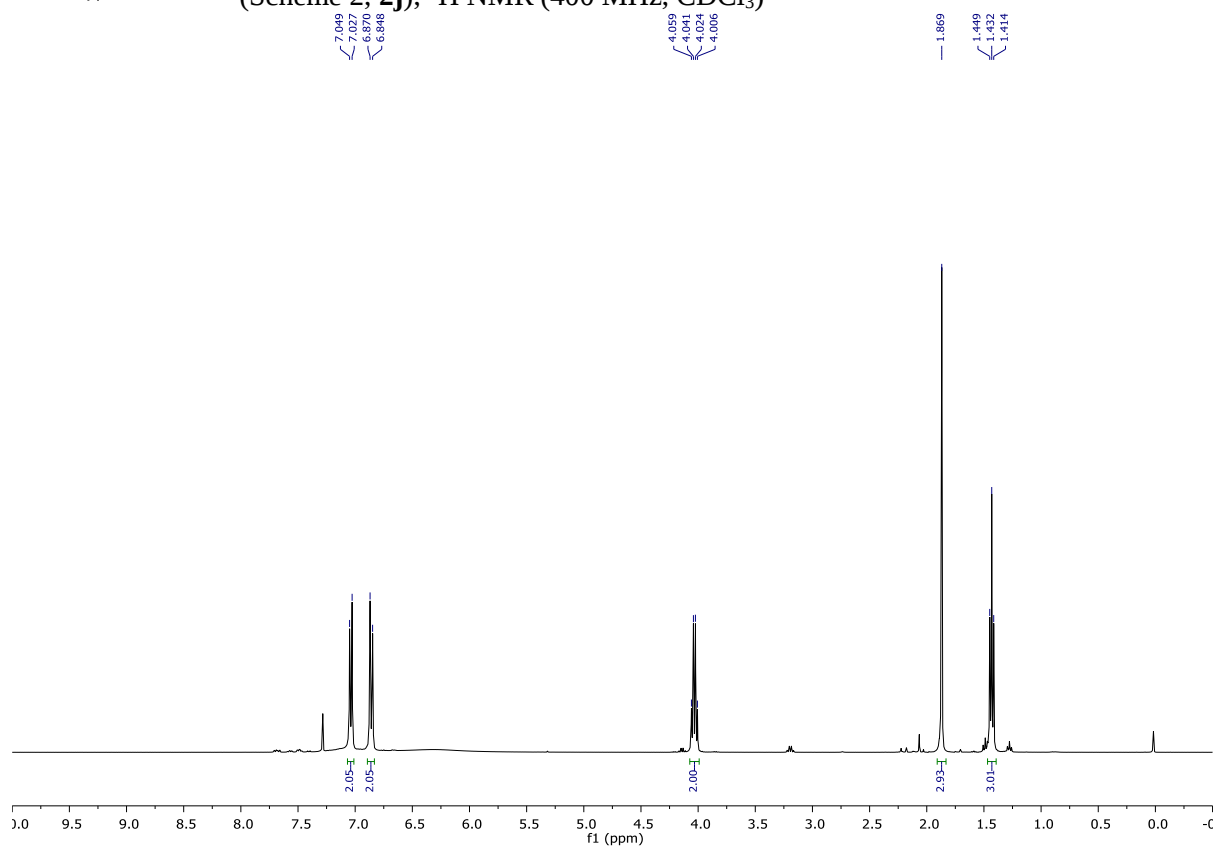


^{13}C NMR (400 MHz, CDCl_3)

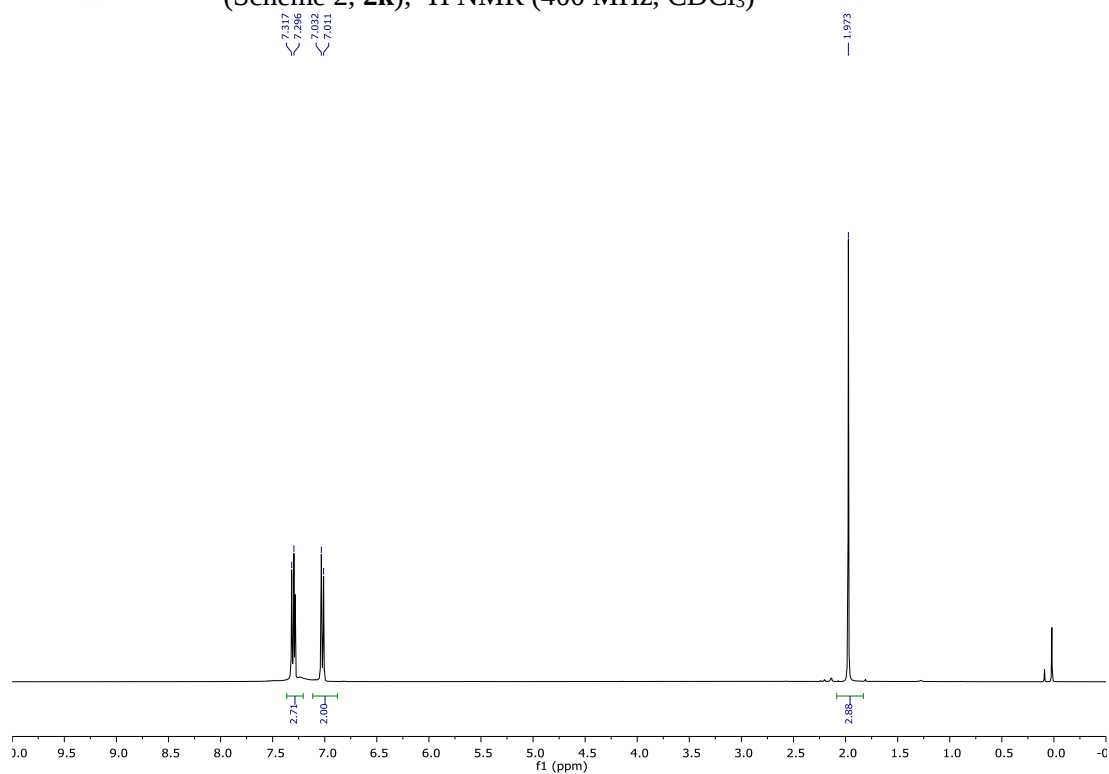


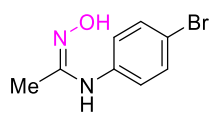


(Scheme 2, **2j**); ^1H NMR (400 MHz, CDCl_3)

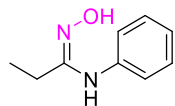
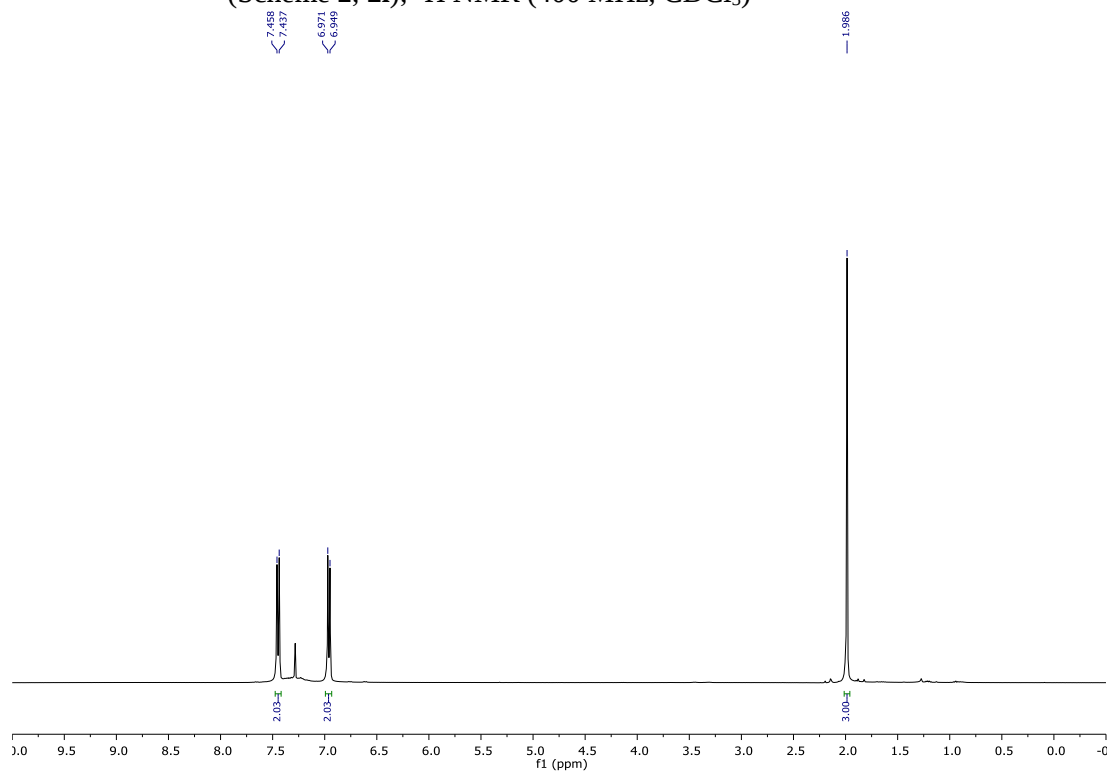


(Scheme 2, **2k**); ^1H NMR (400 MHz, CDCl_3)

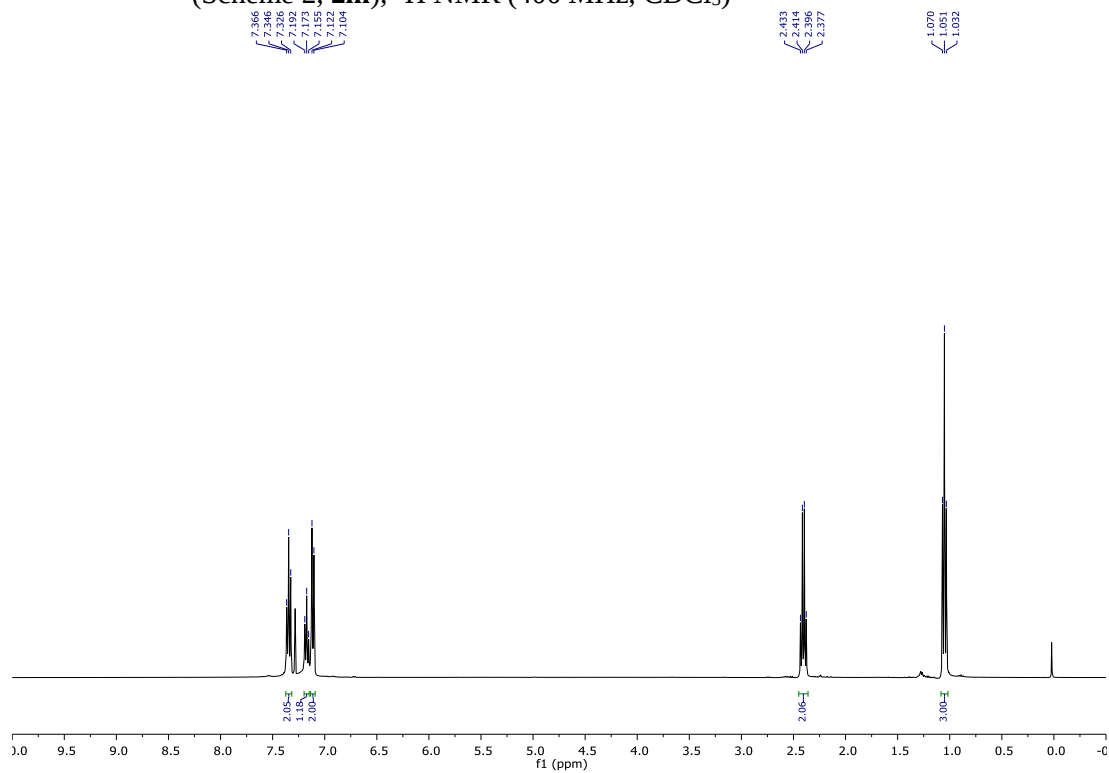


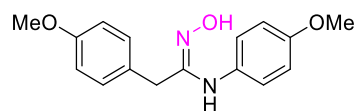


(Scheme 2, **2l**); ^1H NMR (400 MHz, CDCl_3)

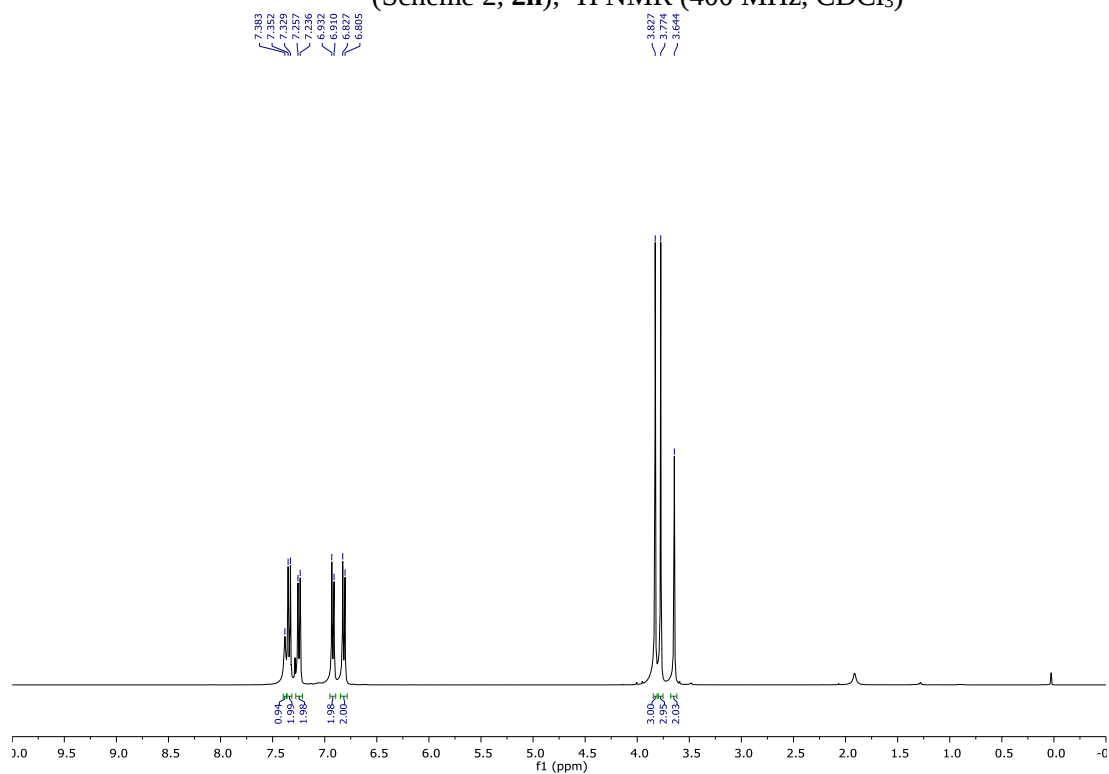


(Scheme 2, **2m**); ^1H NMR (400 MHz, CDCl_3)

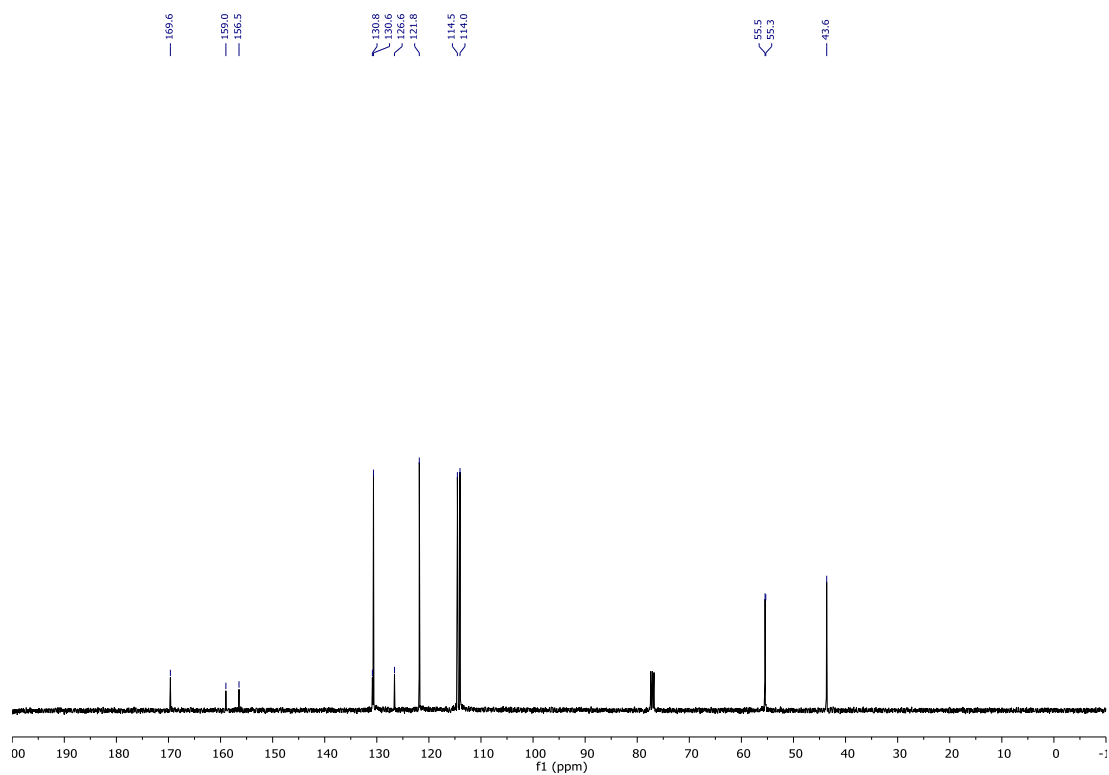


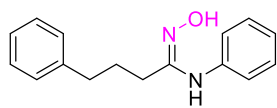


(Scheme 2, **2n**); ^1H NMR (400 MHz, CDCl_3)

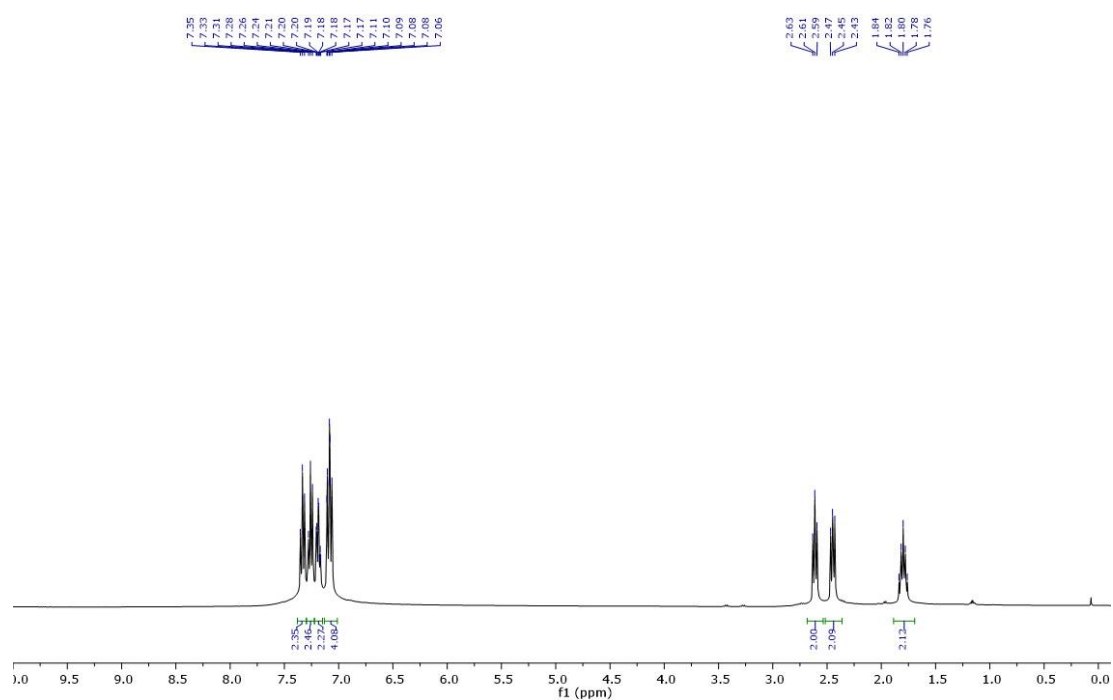


^{13}C NMR (400 MHz, CDCl_3)

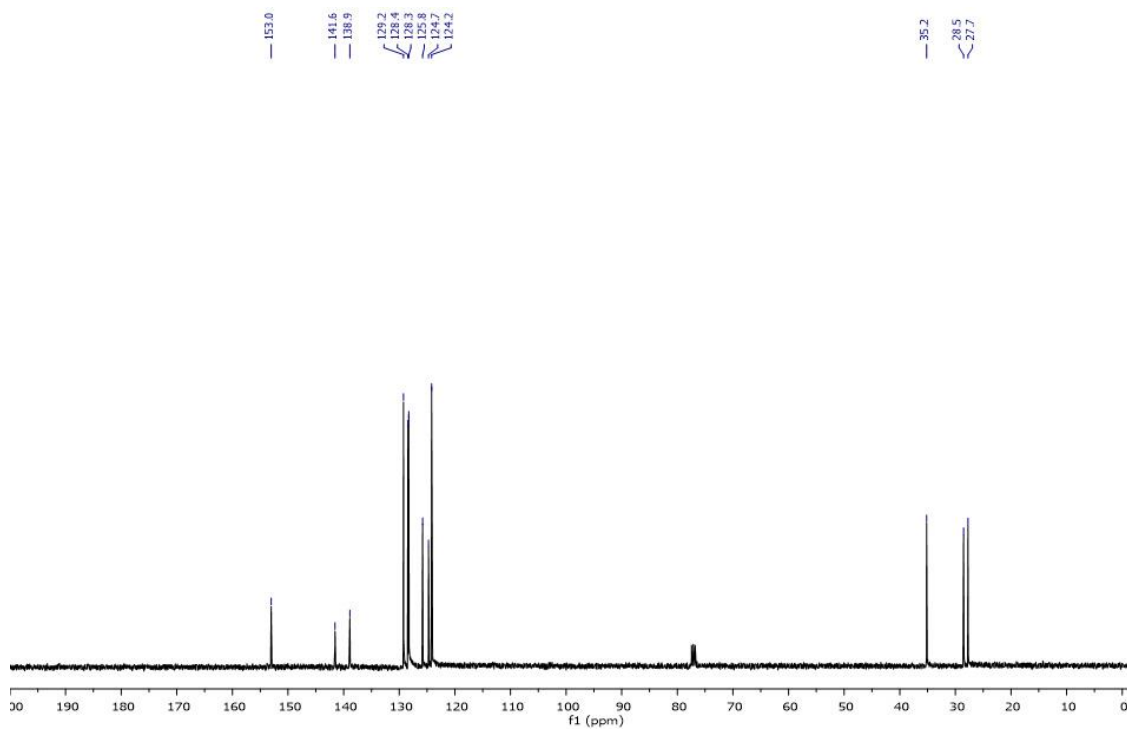


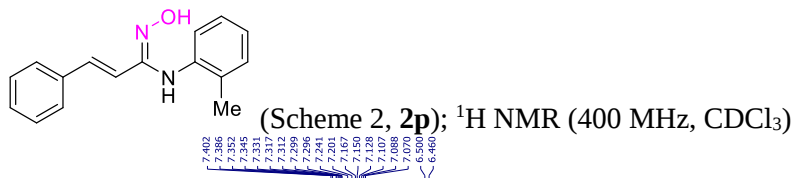


(Scheme 2, **2o**); ^1H NMR (400 MHz, CDCl_3)

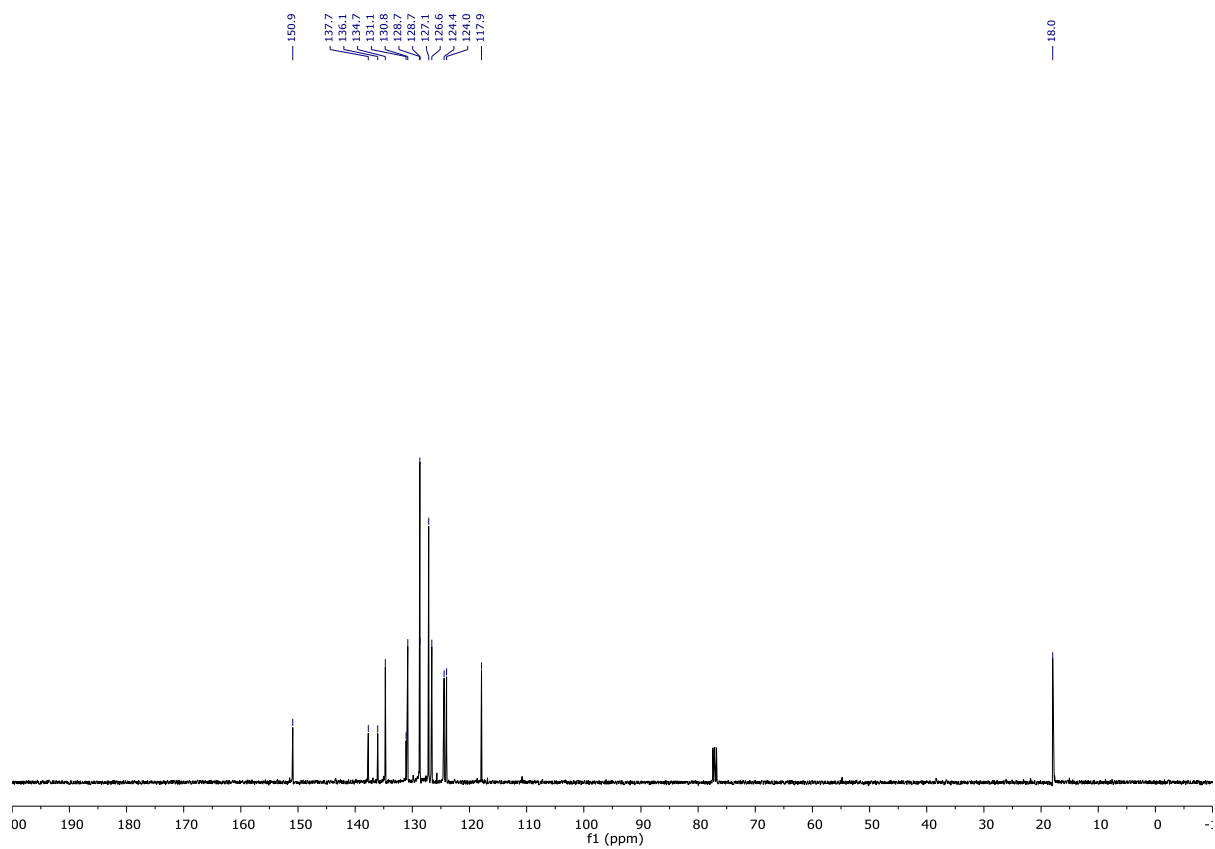


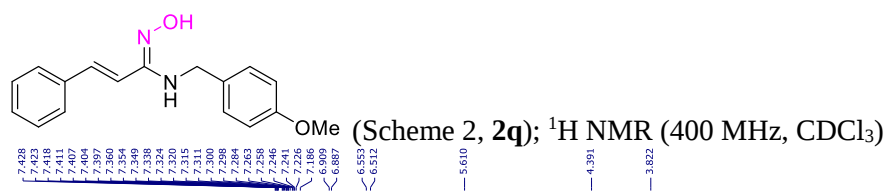
^{13}C NMR (400 MHz, CDCl_3)



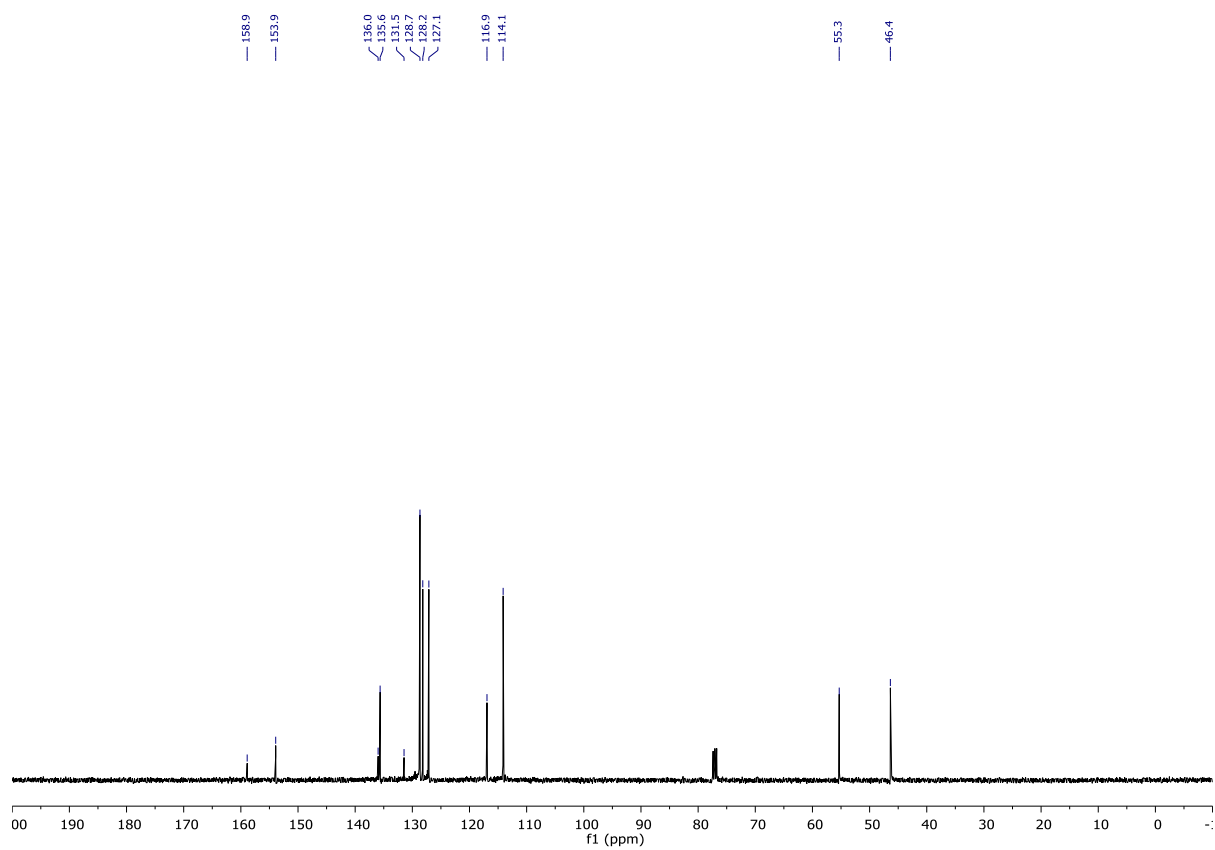


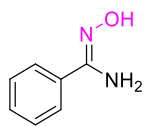
^{13}C NMR (400 MHz, CDCl_3)



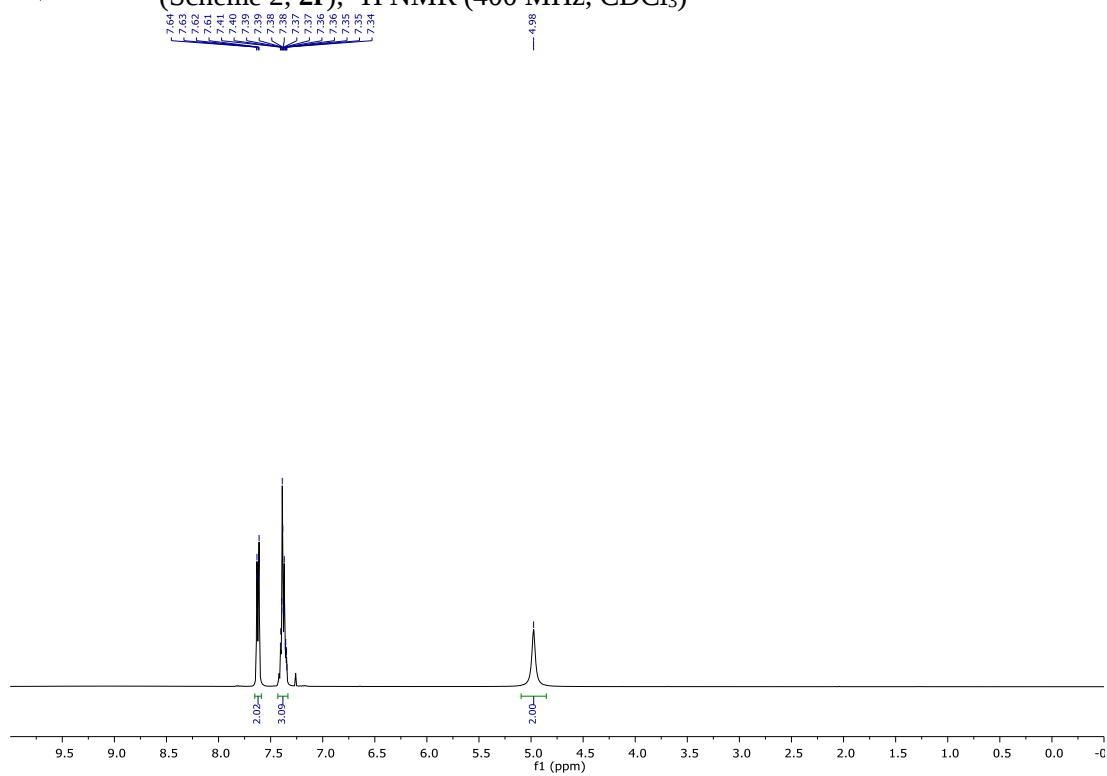


^{13}C NMR (400 MHz, CDCl_3)

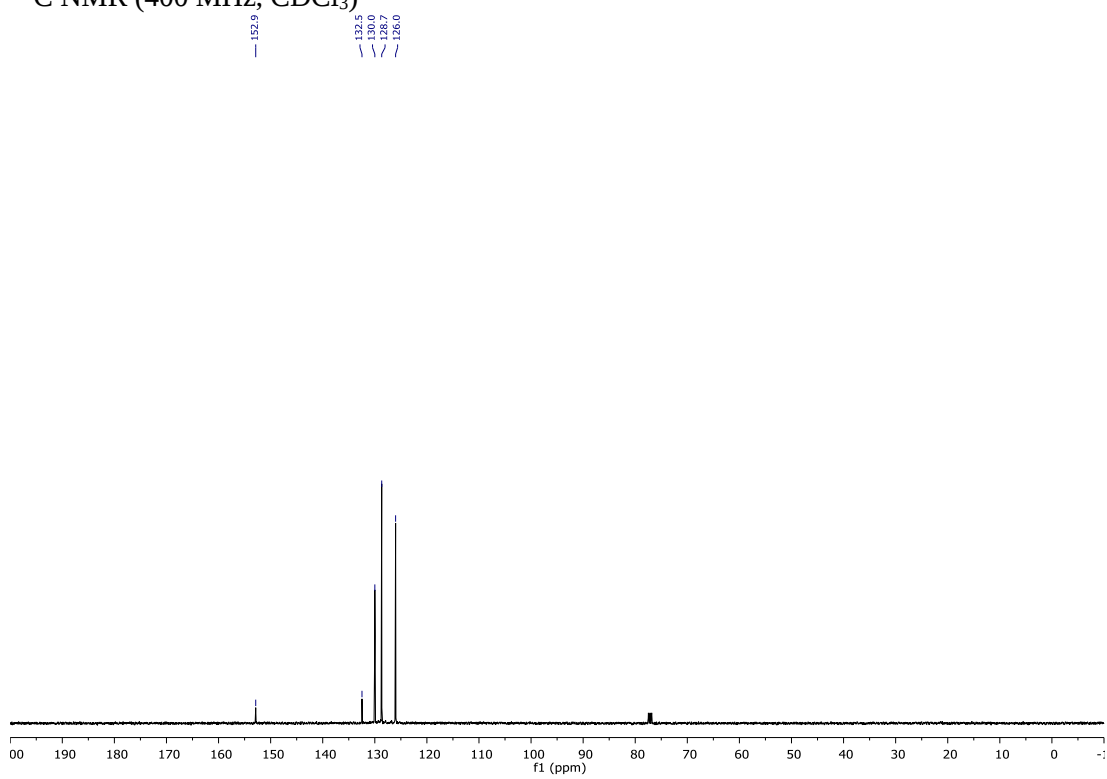


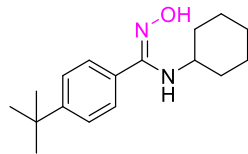


(Scheme 2, **2r**); ^1H NMR (400 MHz, CDCl_3)

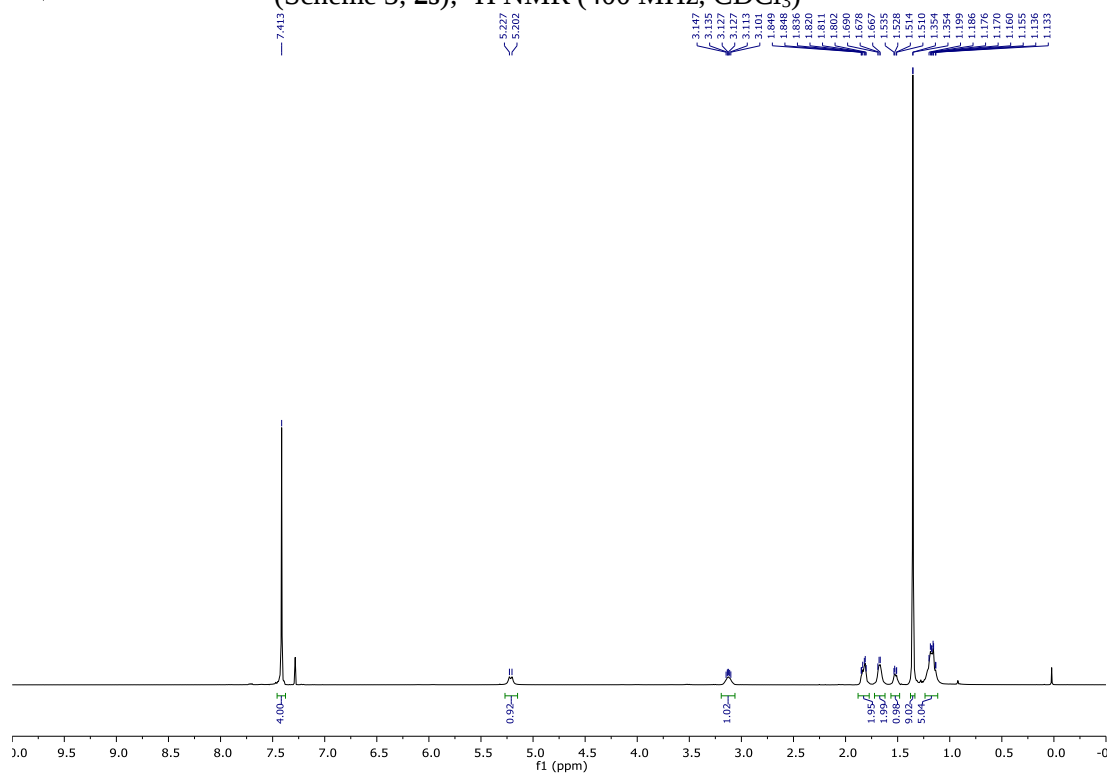


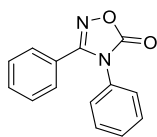
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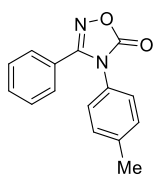
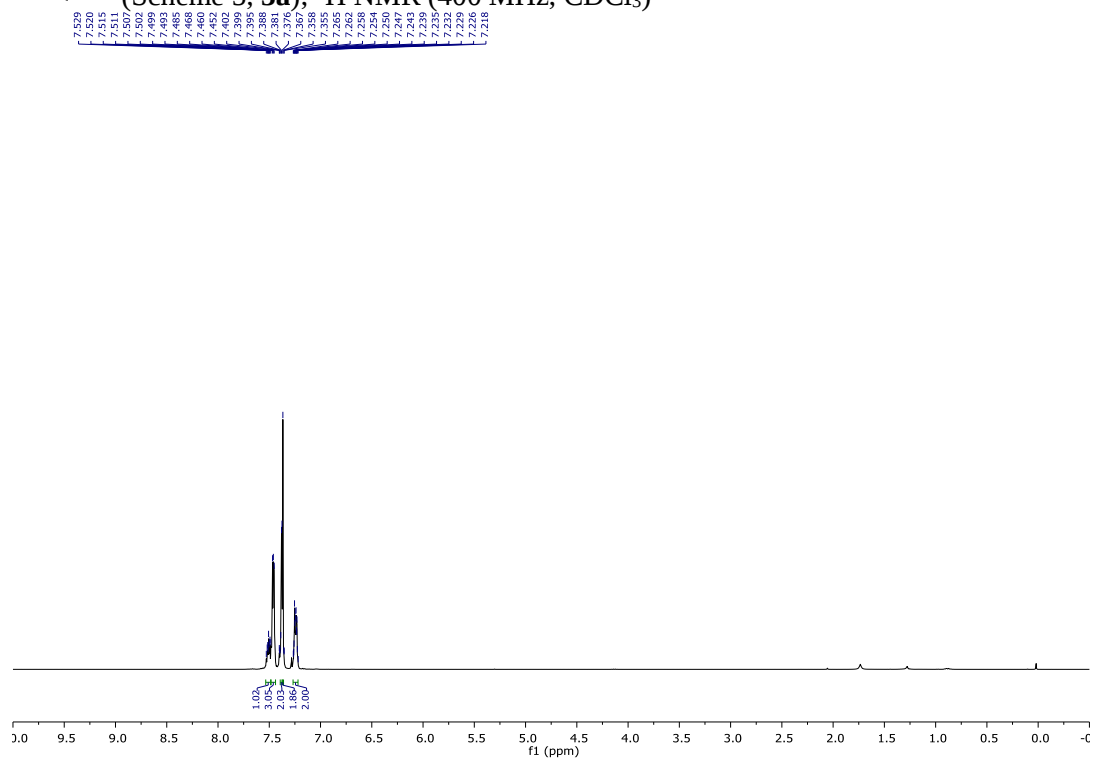


(Scheme 3, 2s); ^1H NMR (400 MHz, CDCl_3)

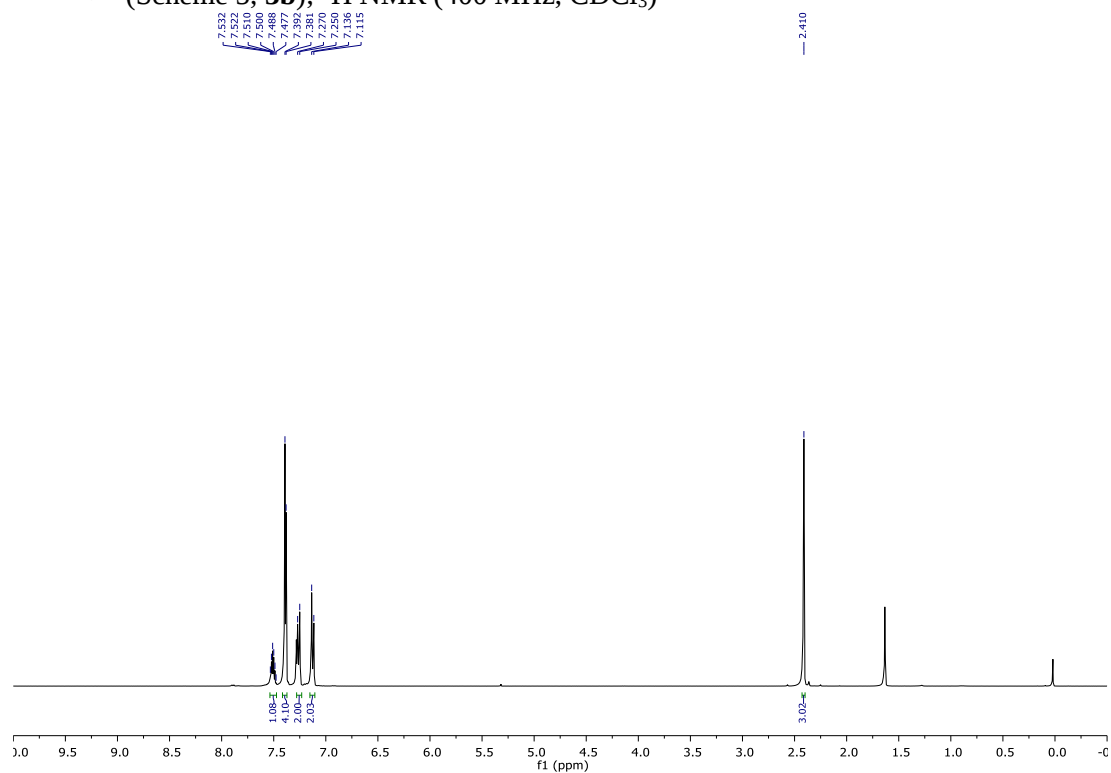


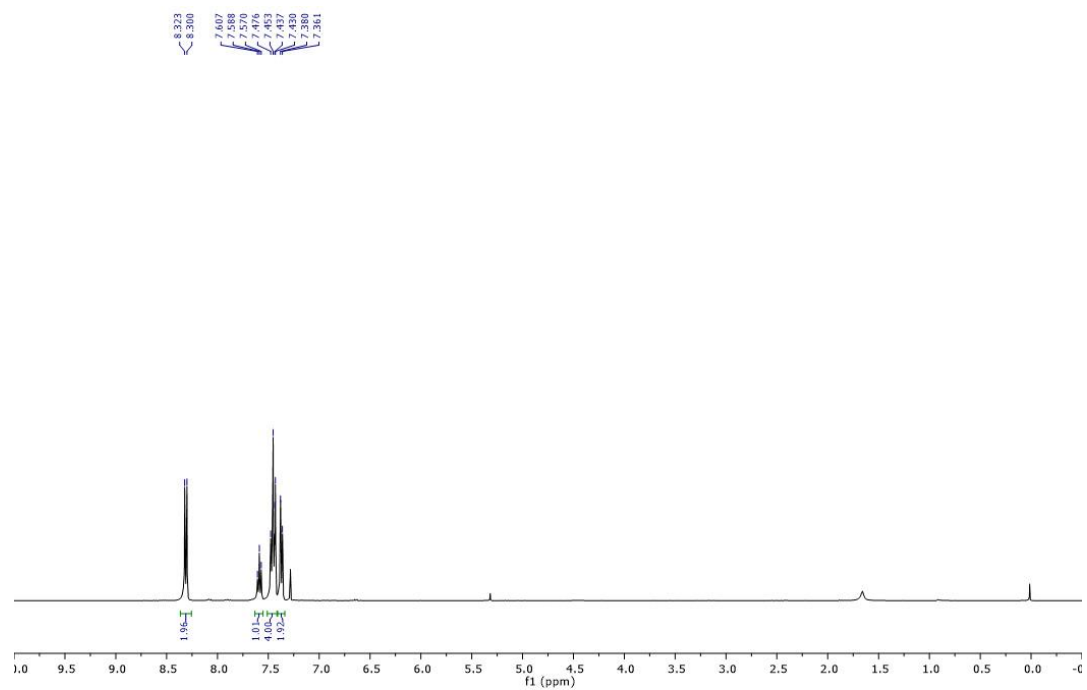
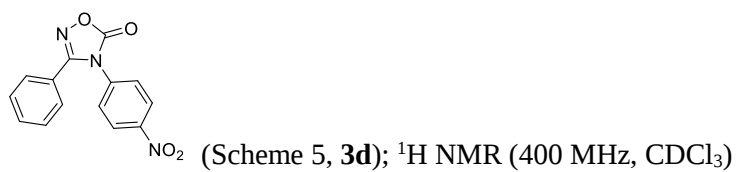
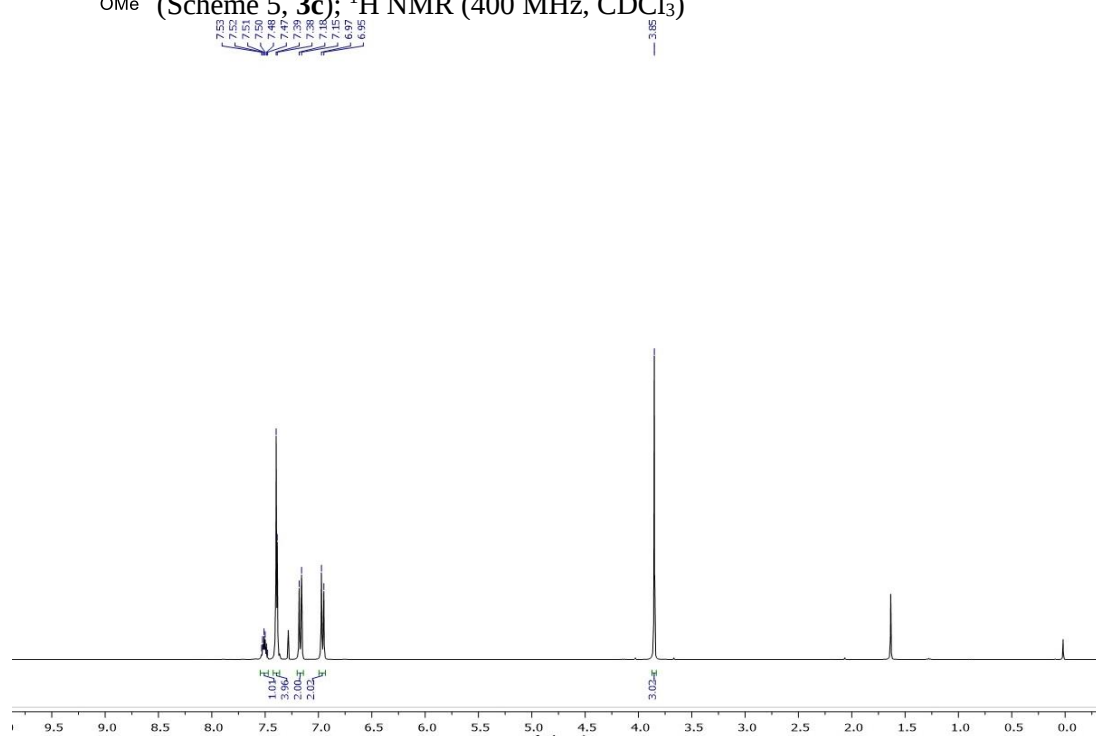
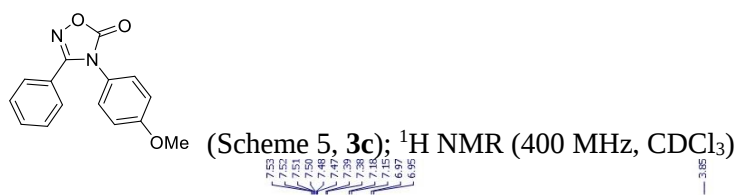


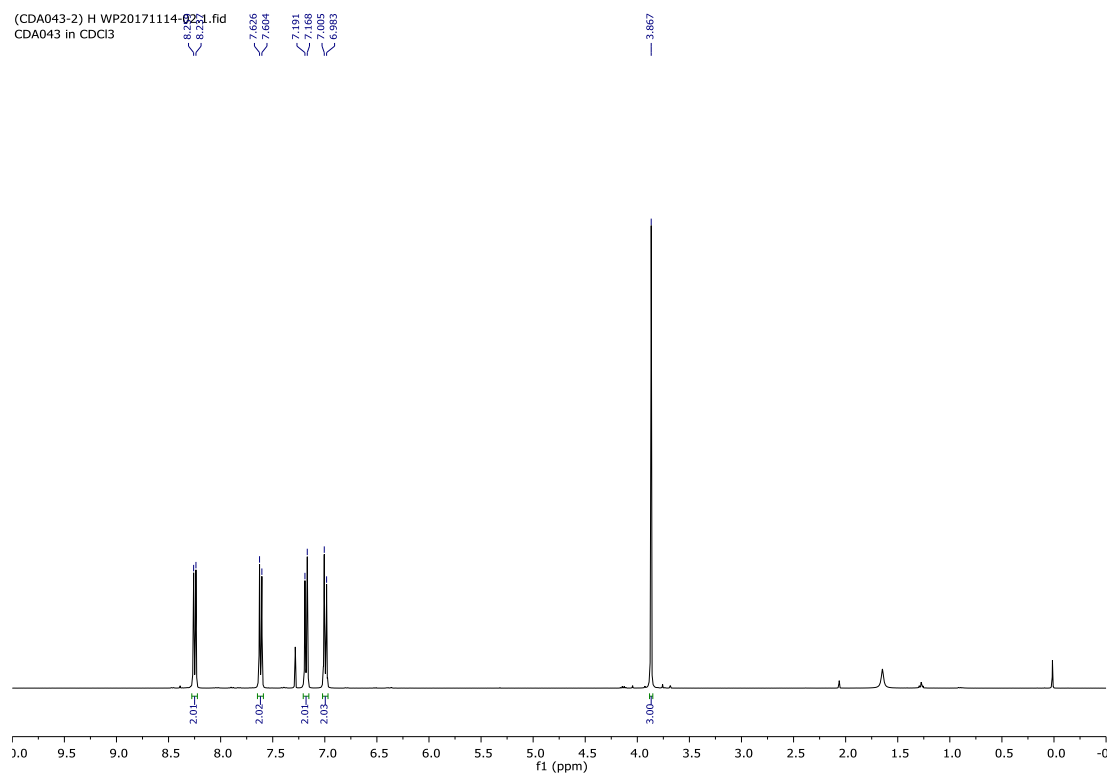
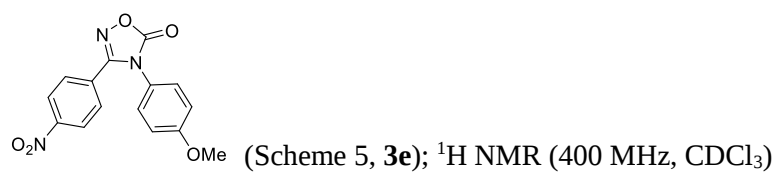
(Scheme 5, **3a**); ^1H NMR (400 MHz, CDCl_3)

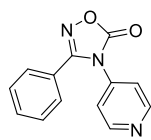


(Scheme 5, **3b**); ^1H NMR (400 MHz, CDCl_3)

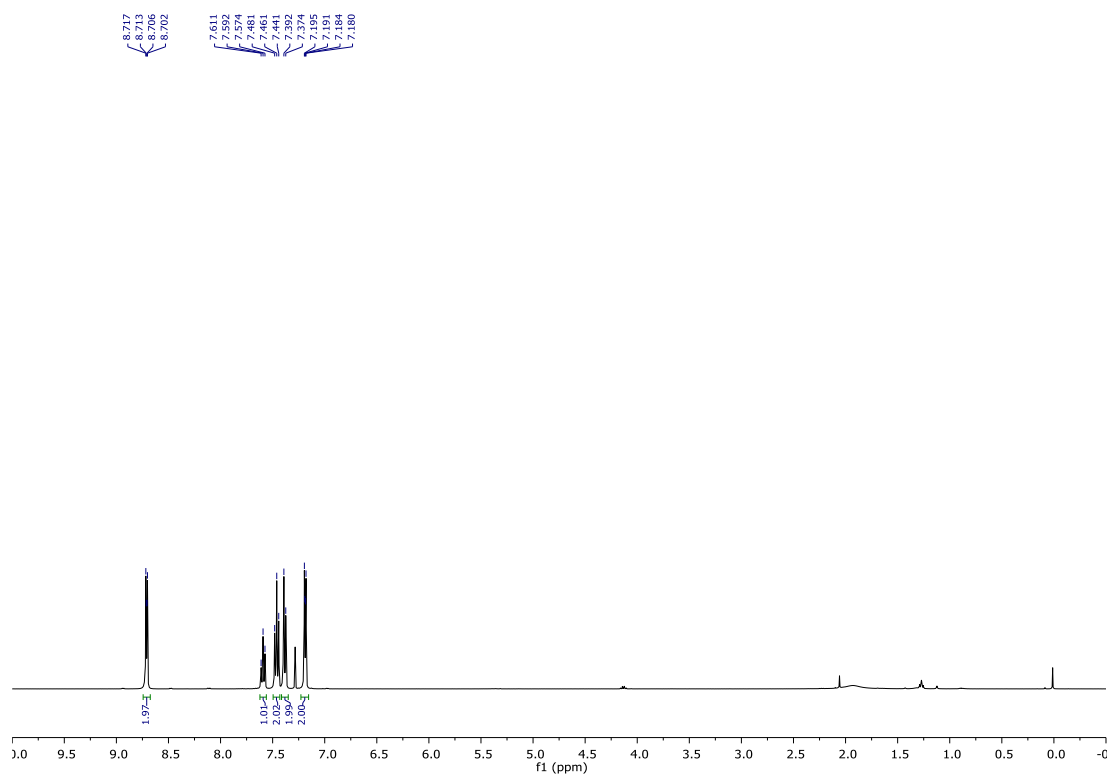




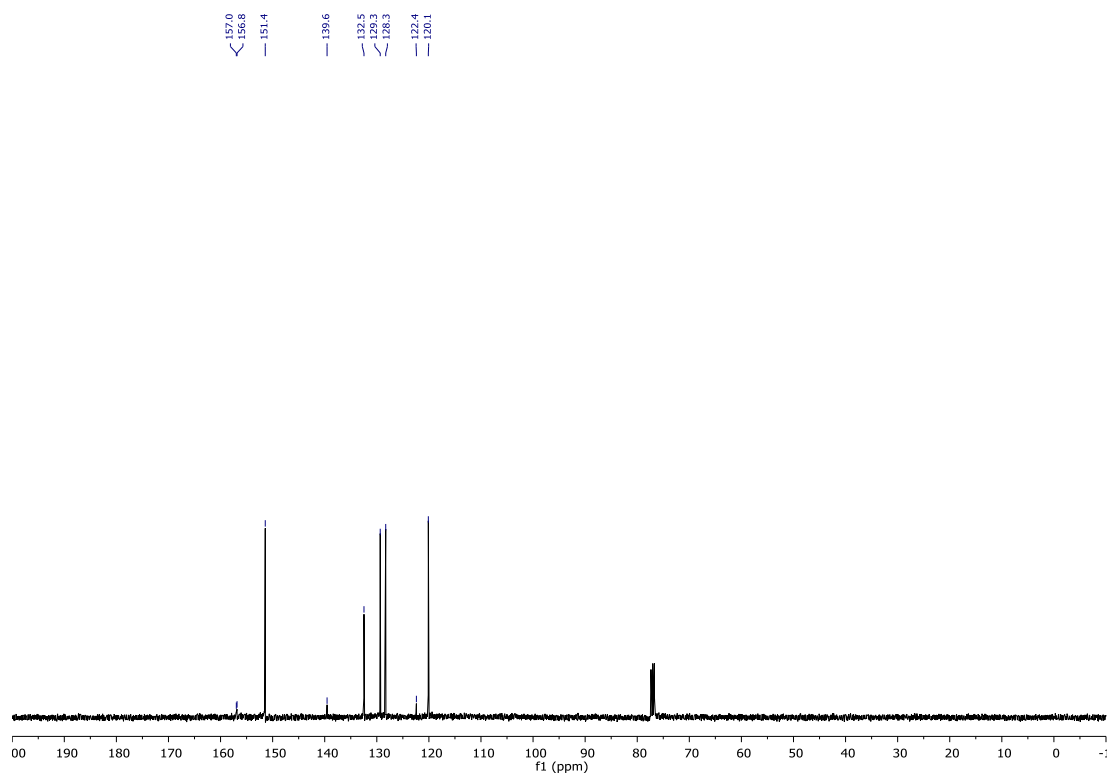


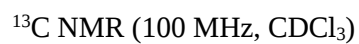


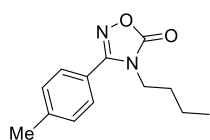
(Scheme 5, **3f**); ^1H NMR (400 MHz, CDCl_3)



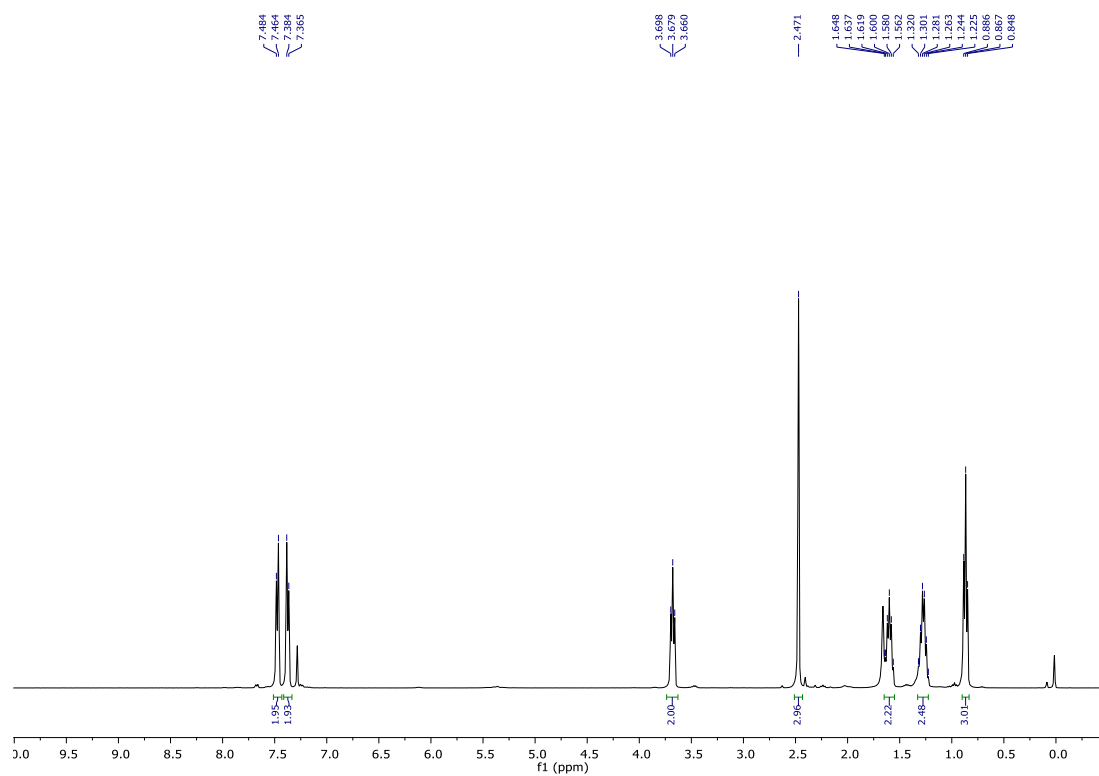
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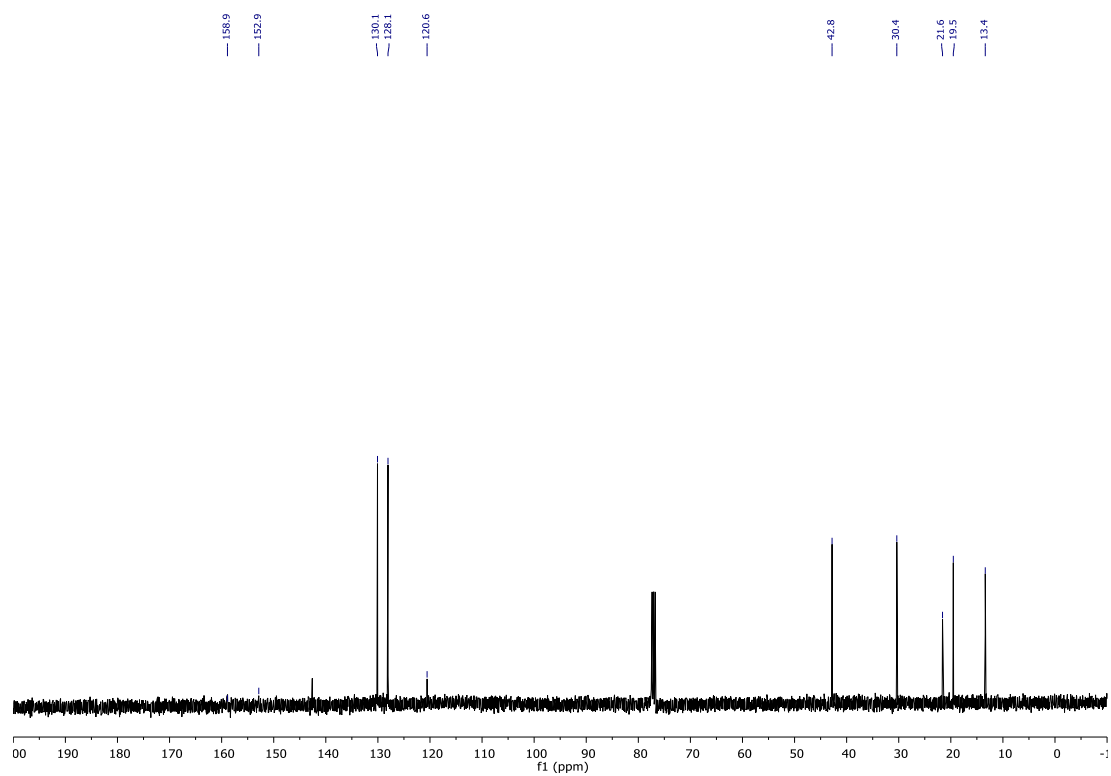


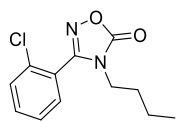


(Scheme 5, **3h**); ^1H NMR (400 MHz, CDCl_3)

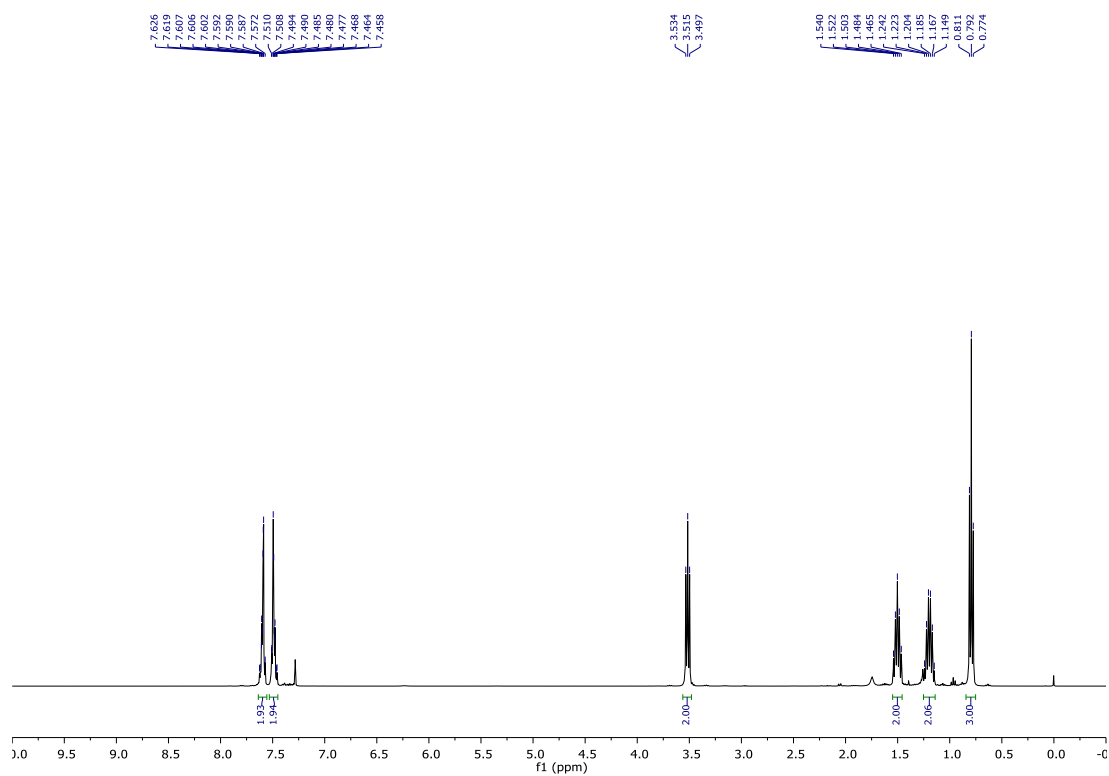


^{13}C NMR (100 MHz, CDCl_3)

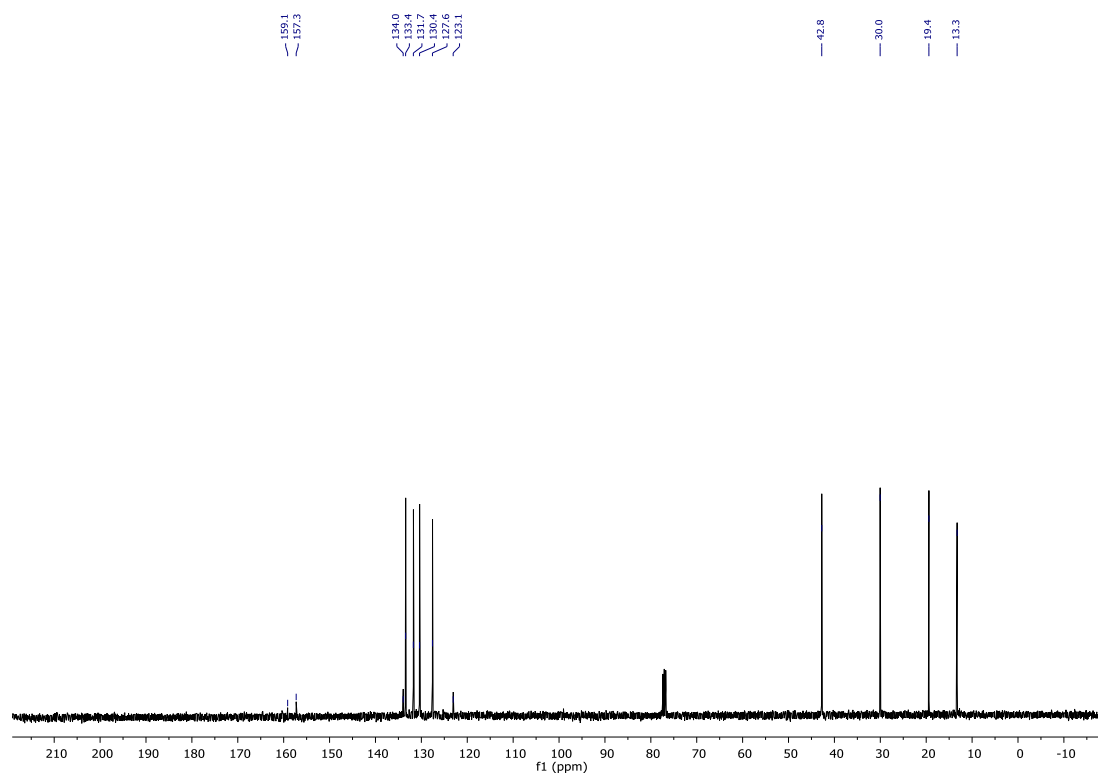


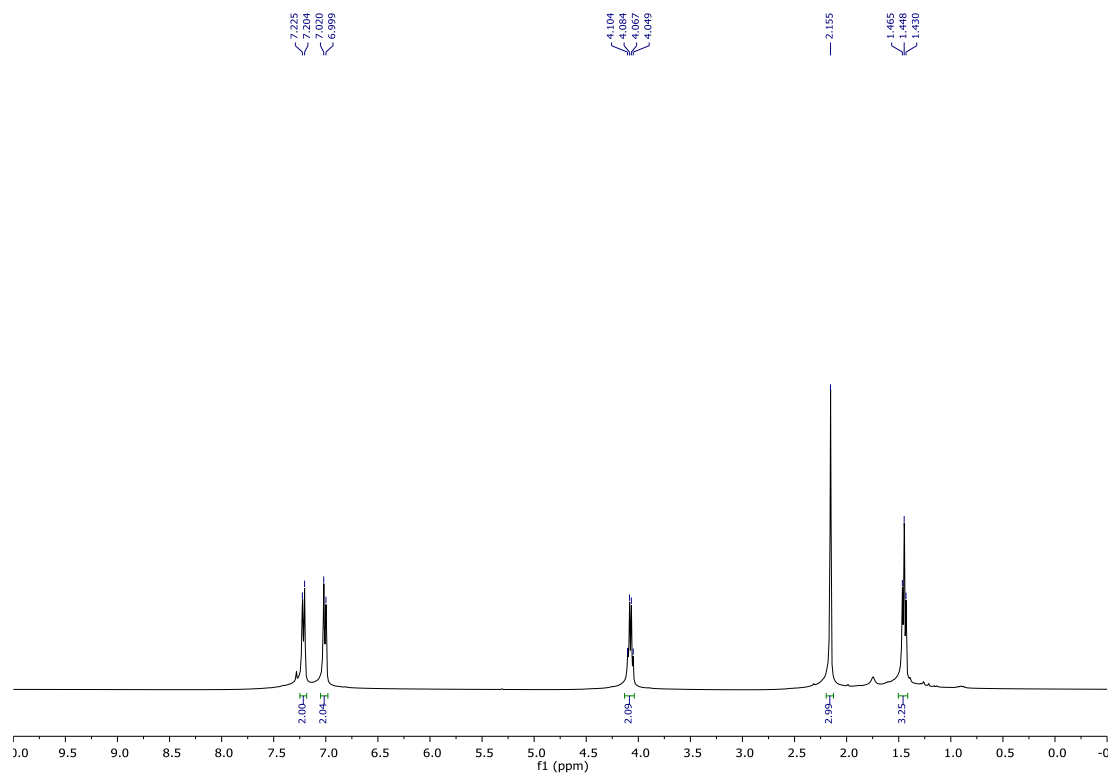
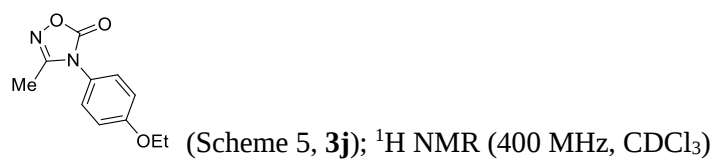


(Scheme 5, **3i**); ^1H NMR (400 MHz, CDCl_3)

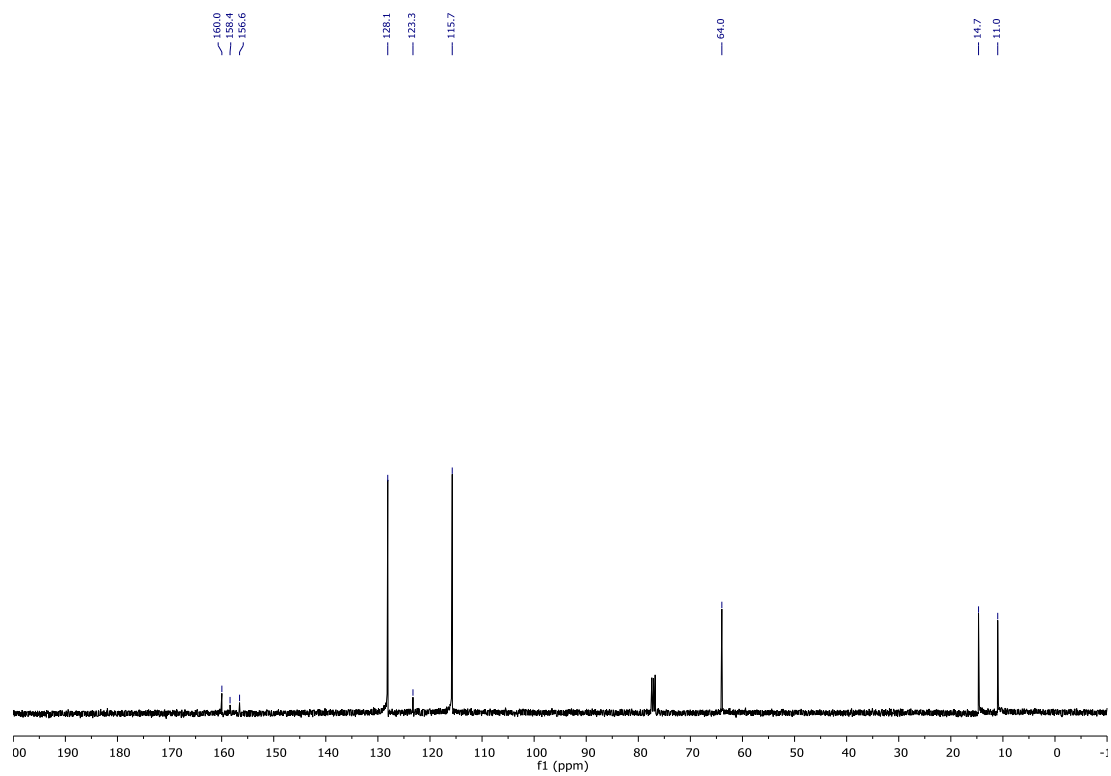


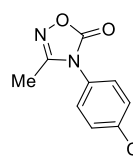
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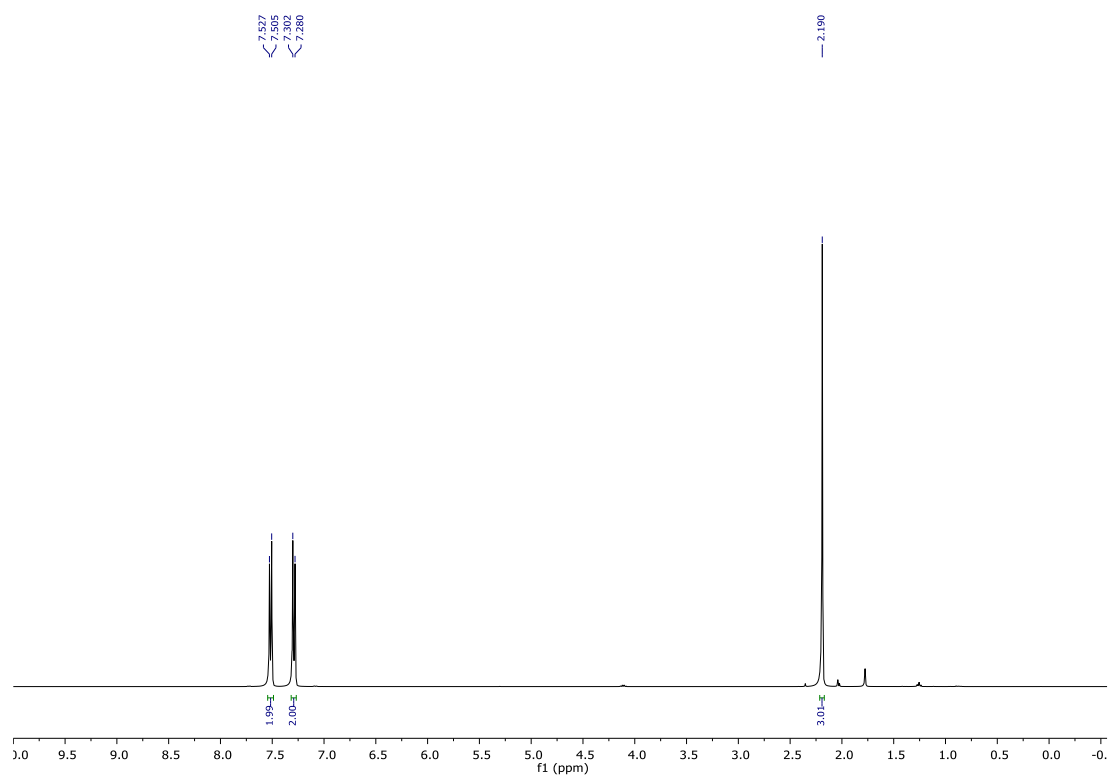


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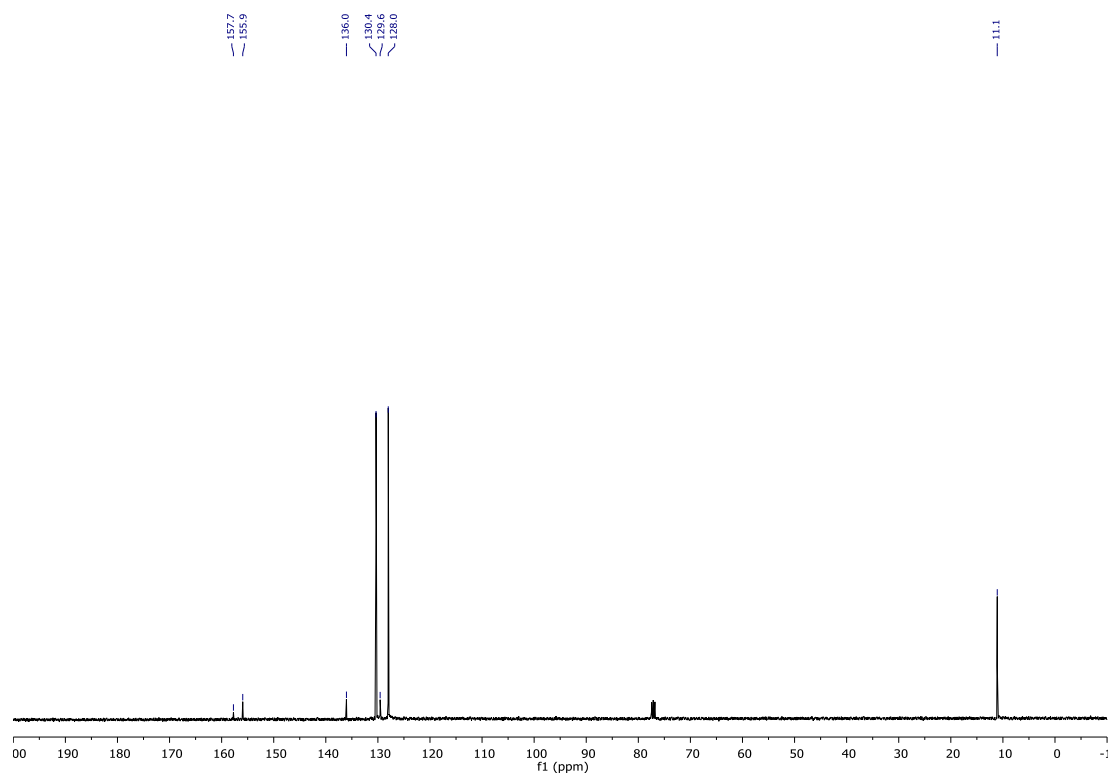


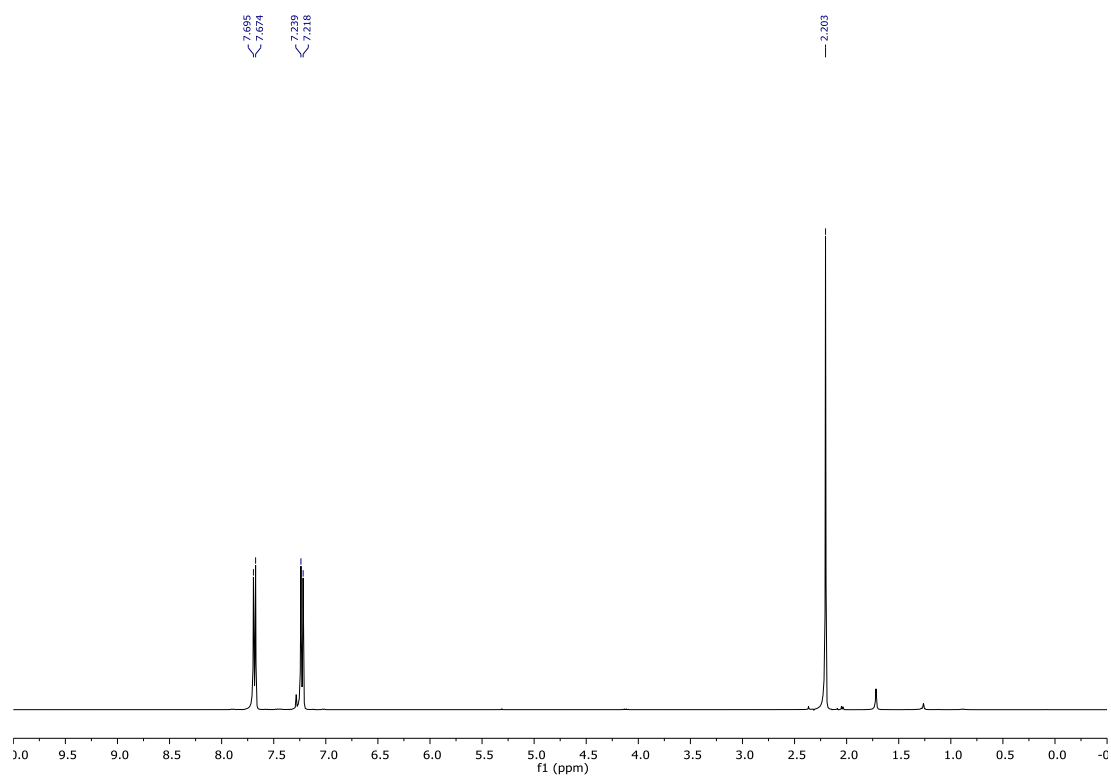
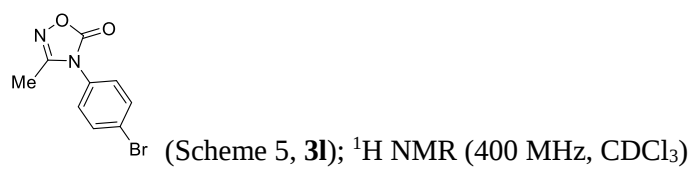


(Scheme 5, **3k**); ^1H NMR (400 MHz, CDCl_3)

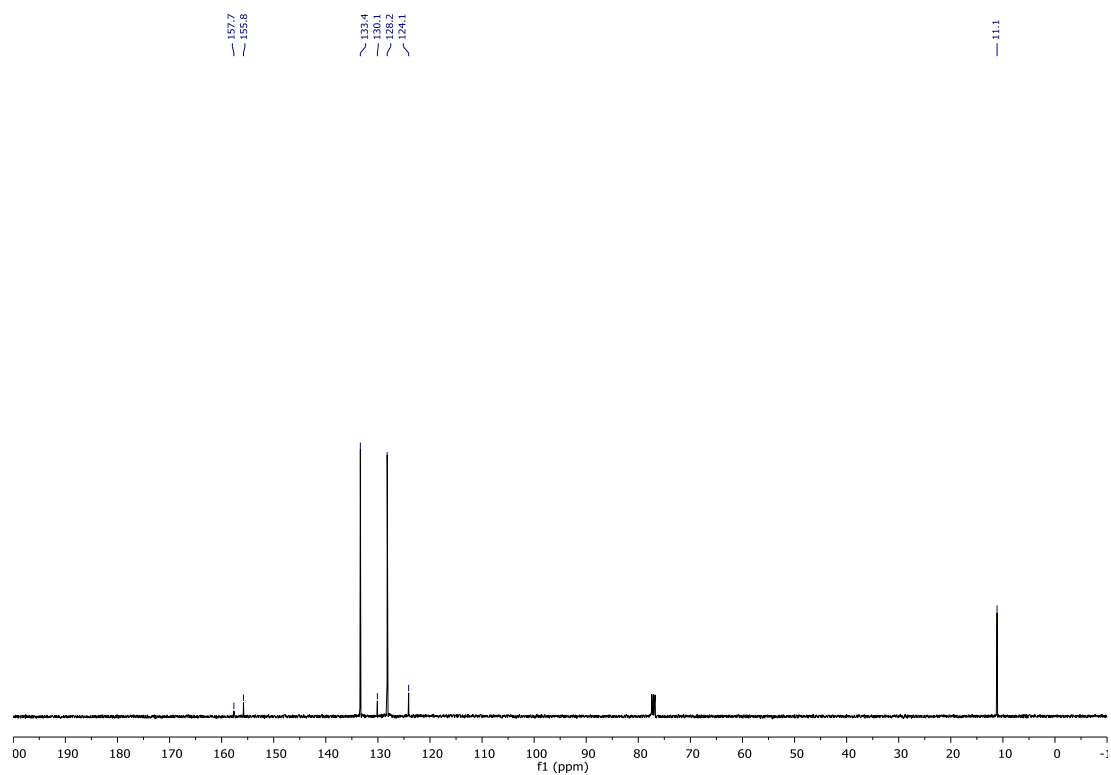


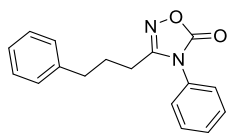
^{13}C NMR (100 MHz, CDCl_3)



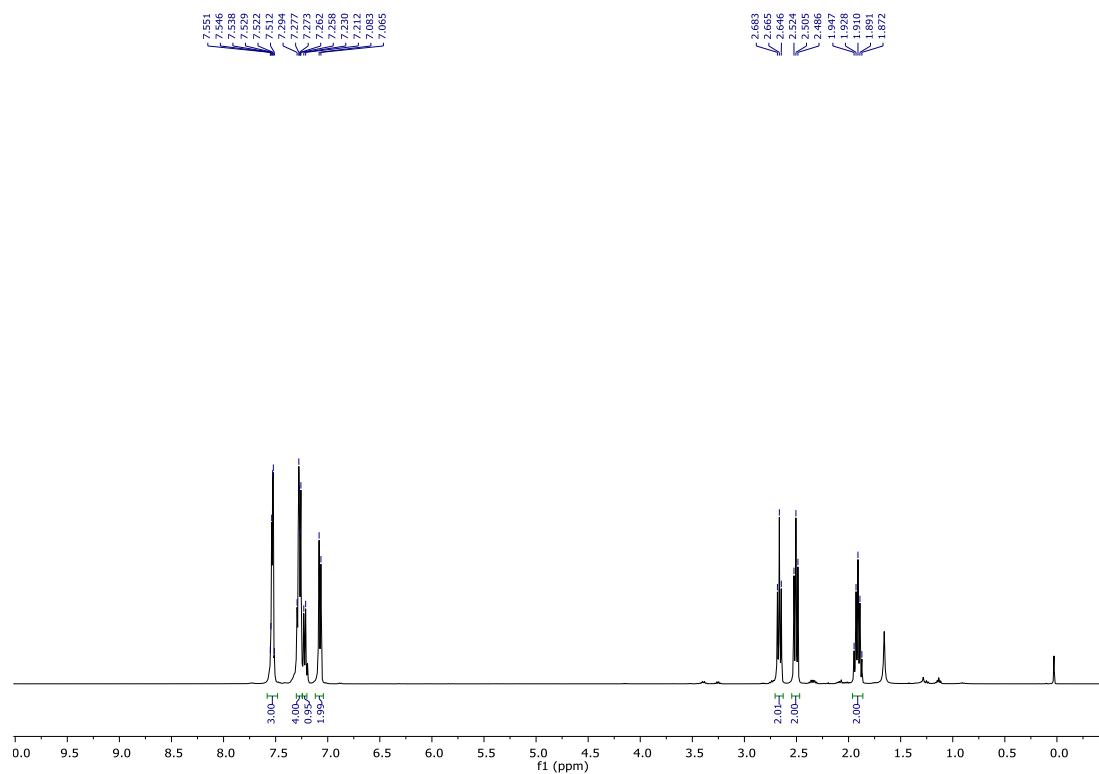


^{13}C NMR (100 MHz, CDCl_3)

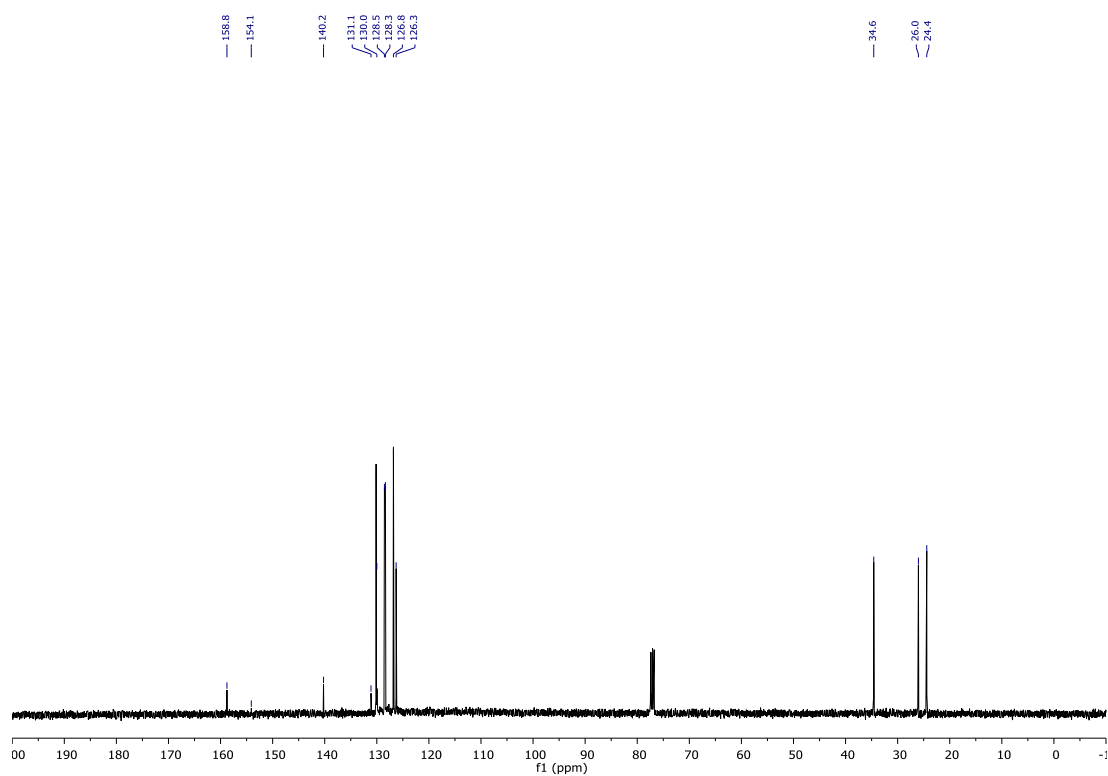


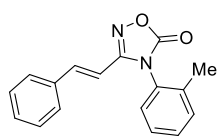


(Scheme 5, **3m**); ^1H NMR (400 MHz, CDCl_3)

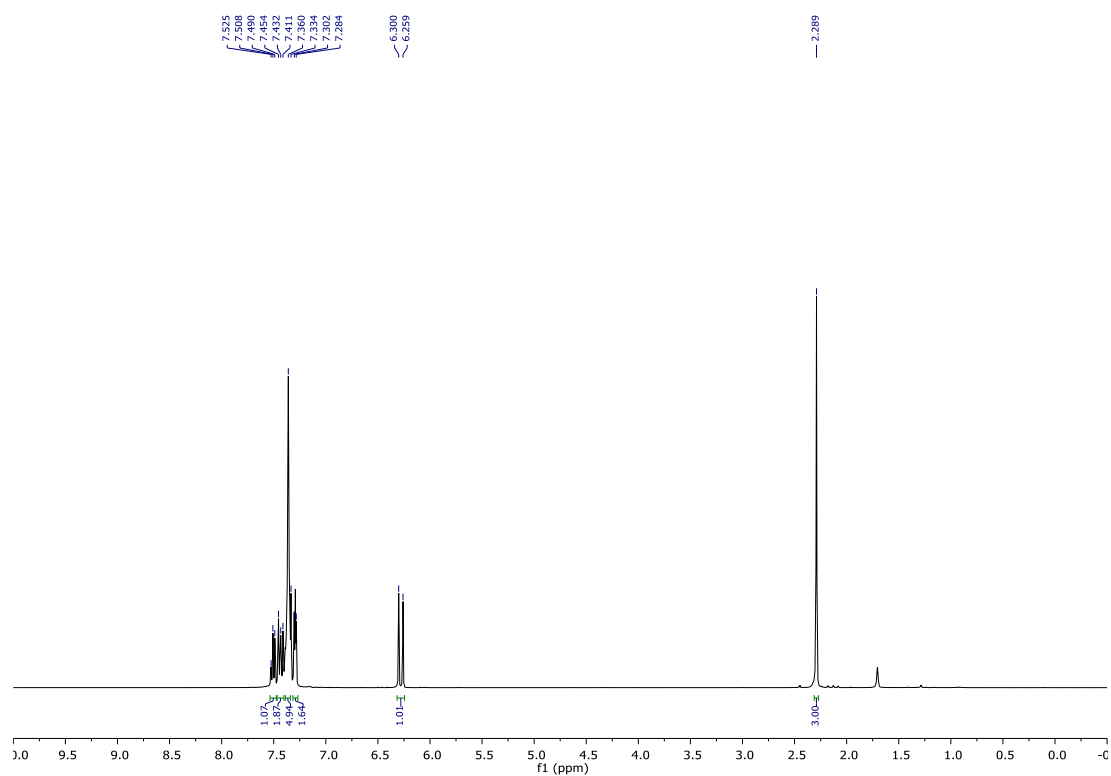


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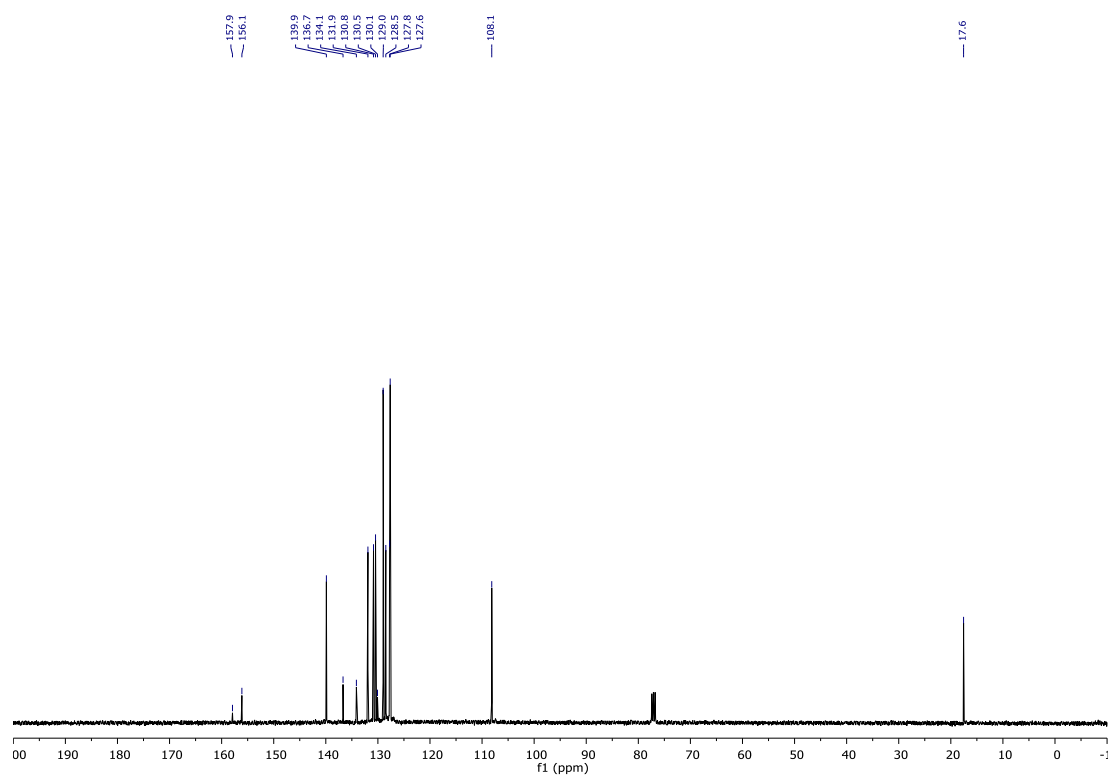


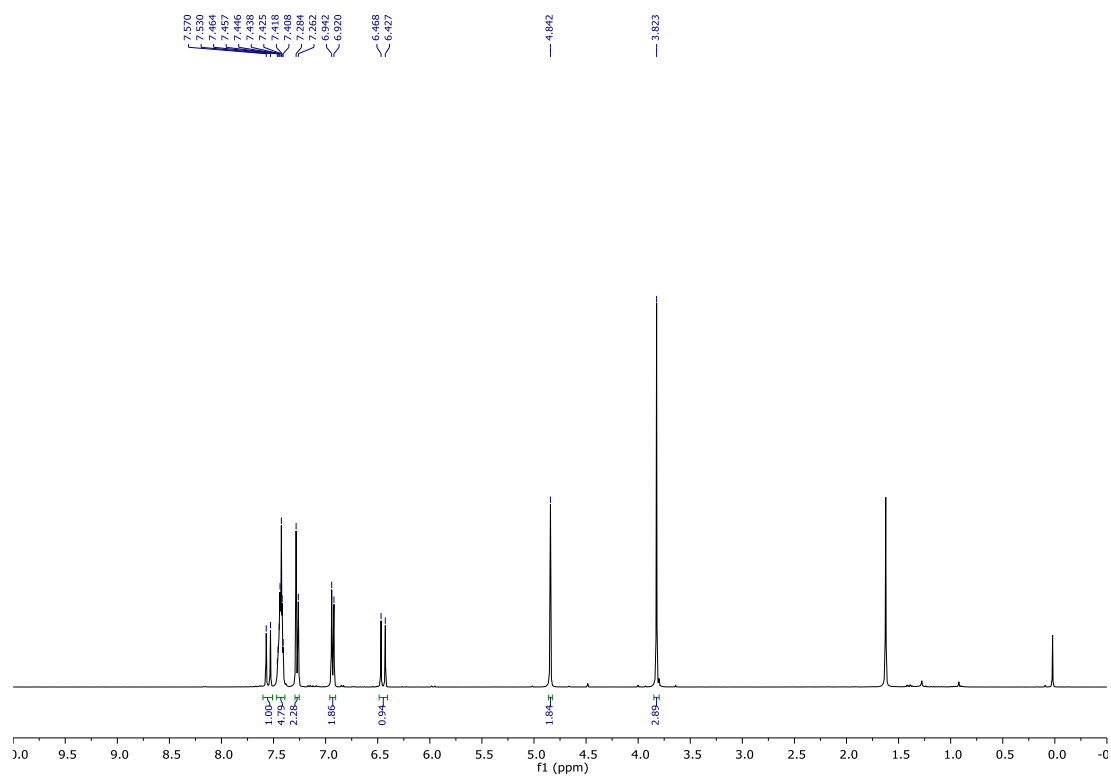
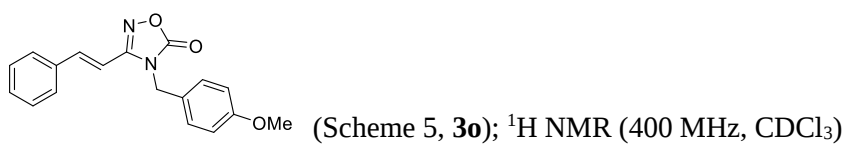


(Scheme 5, **3n**); ^1H NMR (400 MHz, CDCl_3)

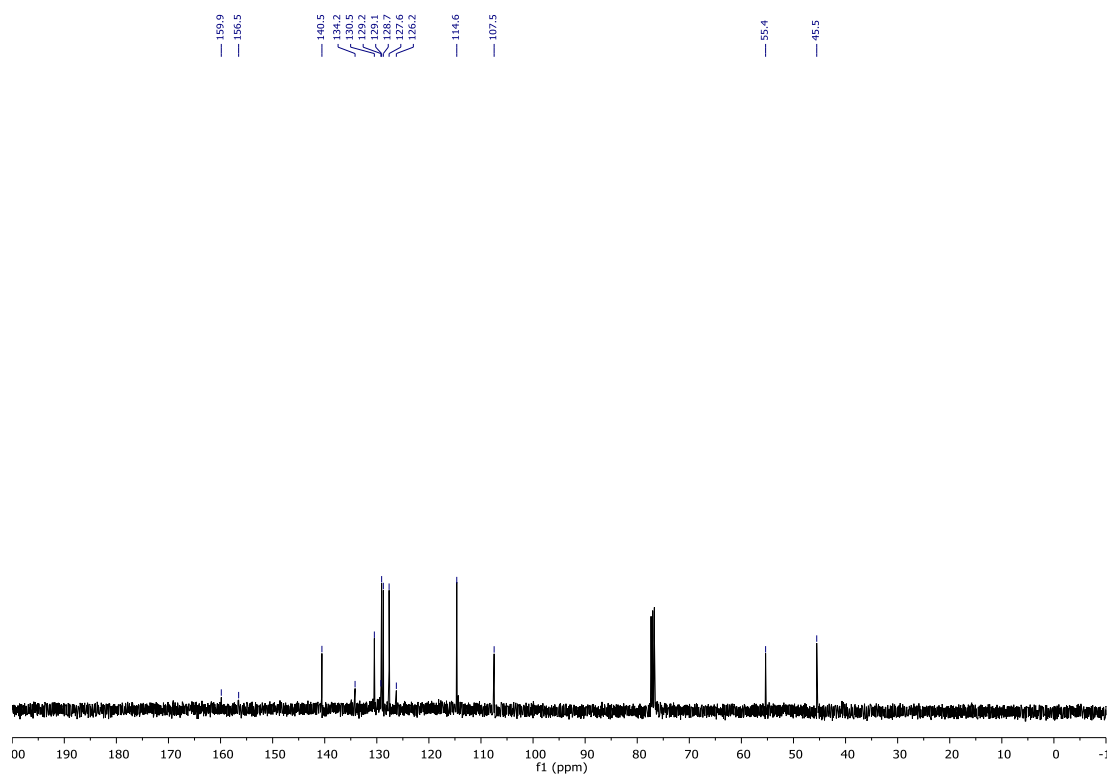


^{13}C NMR (100 MHz, CDCl_3)





^{13}C NMR (100 MHz, CDCl_3)



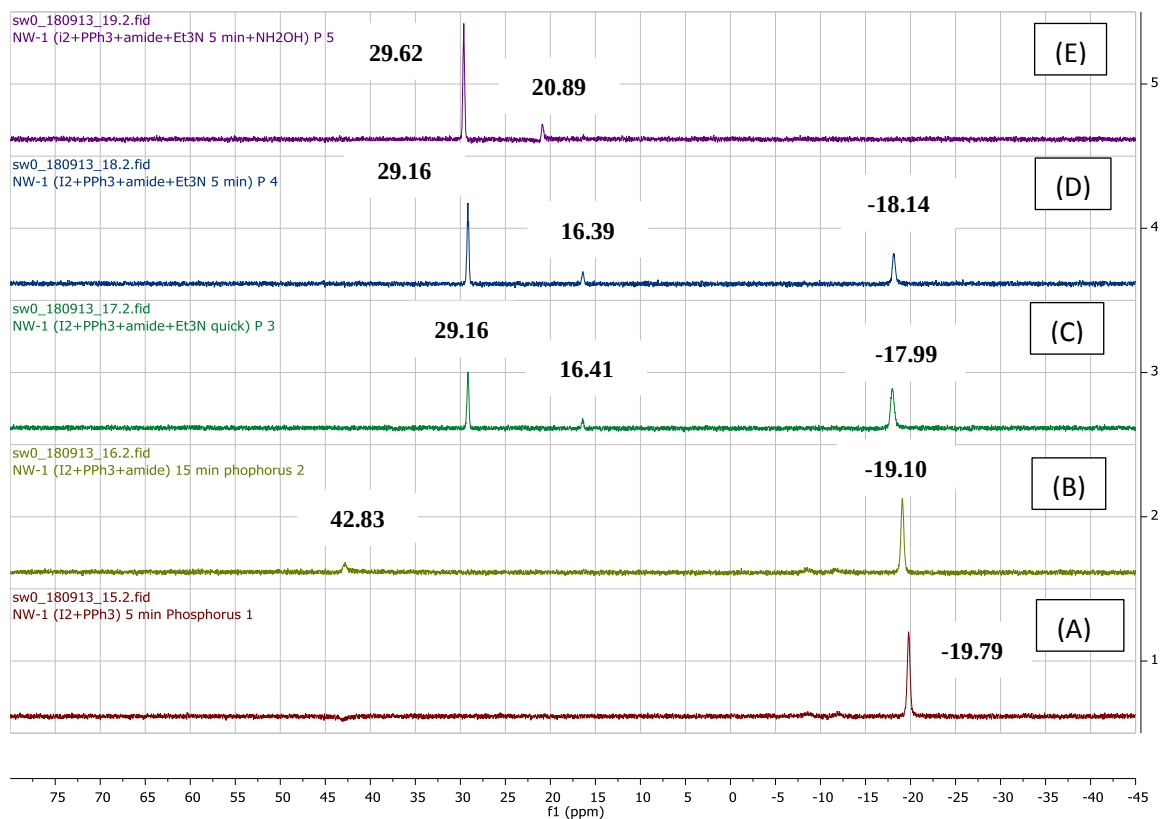
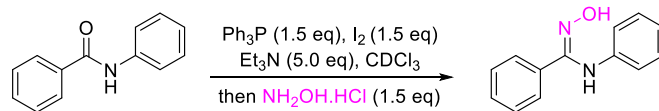


FIGURE S1. $^{31}\text{P}\{^1\text{H}\}$ NMR monitoring the progress of the reaction between *N*-phenylbenzamide and hydroxylamine hydrochloride in the presence of Ph_3P , I_2 , and Et_3N in CDCl_3 : (A) 5 min after mixing a stoichiometric amount of I_2 with Ph_3P at rt; (B) 15 min after addition of the amide; (C) 1 min after addition of Et_3N ; (D) solution (C) after mixing for 5 min; (E) 30 min after addition of $\text{NH}_2\text{OH}\cdot\text{HCl}$.

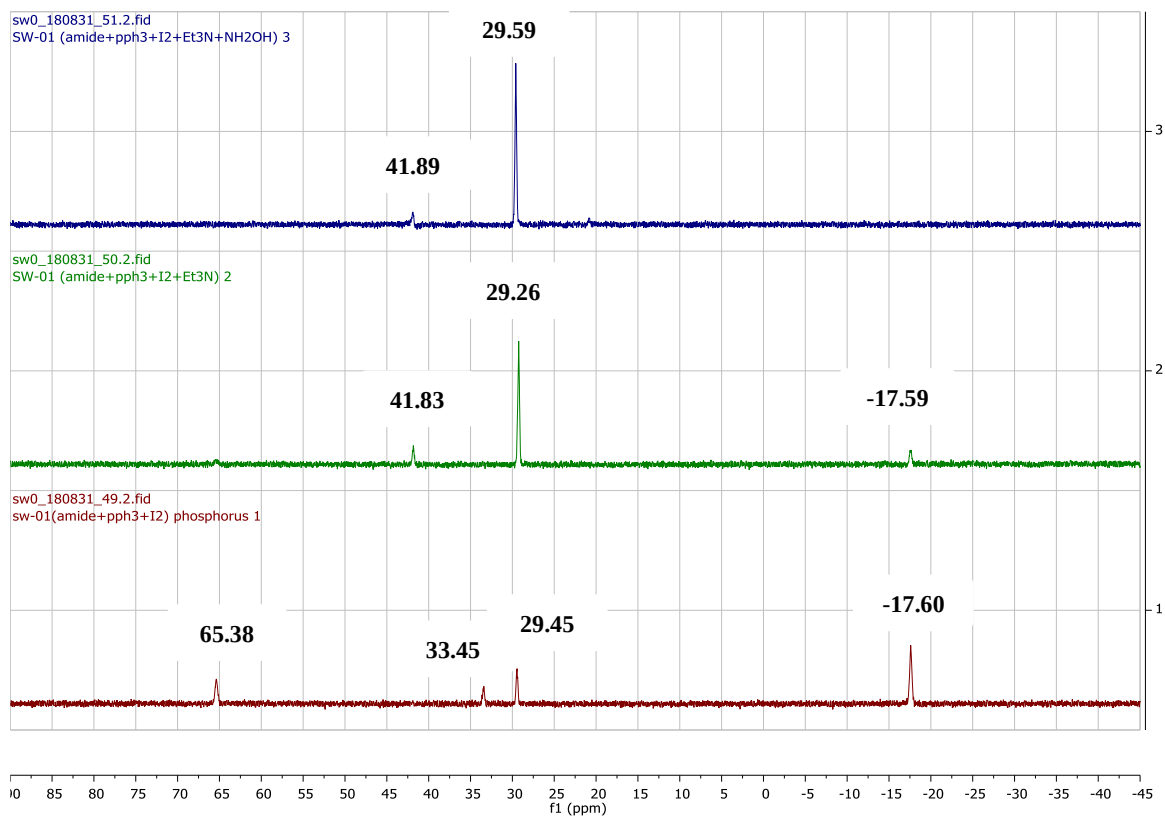
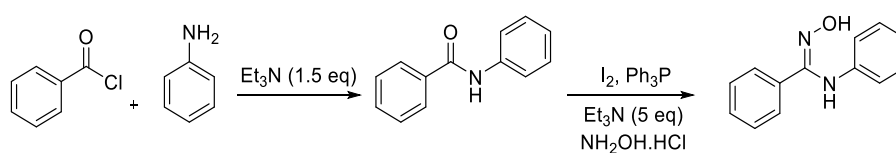


FIGURE S2. $^{31}\text{P}\{^1\text{H}\}$ NMR monitoring the progress of the reaction between benzoyl chloride, aniline, and hydroxylamine hydrochloride in the presence of Ph_3P , I_2 , and Et_3N in CDCl_3 : (A) 5 min after mixing preformed *N*-phenylbenzamide with a stoichiometric amount of I_2 with Ph_3P at rt; (B) 5 min after addition of Et_3N ; (C) 30 min after addition of $\text{NH}_2\text{OH.HCl}$.