

Regioselective Halogenation of Arenes and Heterocycles in Hexafluoroisopropanol

Ren-Jin Tang, Thierry Milcent, Benoit Crousse*

Faculty of Pharmacy, Fluorinated Molecules and Medicinal Chemistry UMR 8076, BioCIS, Univ.

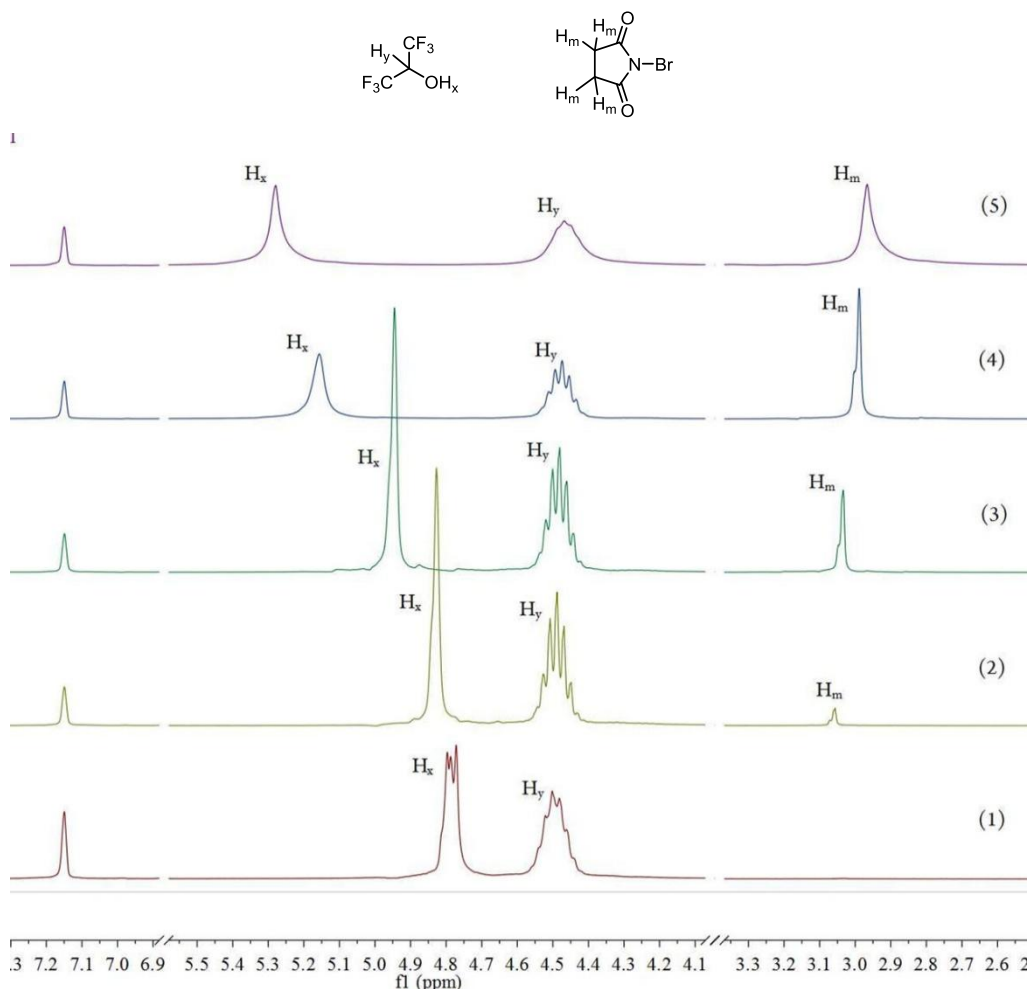
Paris-Sud, CNRS, Université Paris-Saclay, 92290, Châtenay-Malabry, FRANCE

Table of Contents

1	¹H NMR titration of a mixture of HFIP and NBS	S2
2	¹H NMR and ¹³C NMR Spectral for Purified Products	S3
3	Spectral for Yield of Products Determined by ¹H NMR	S60

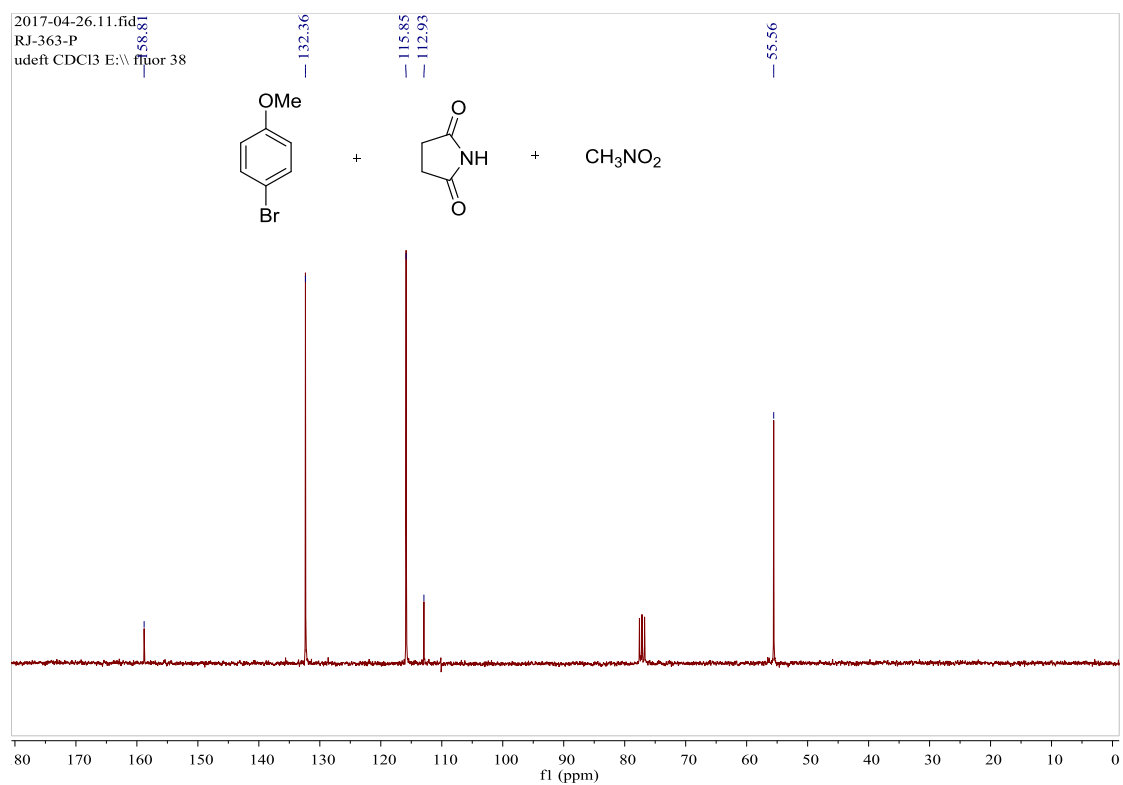
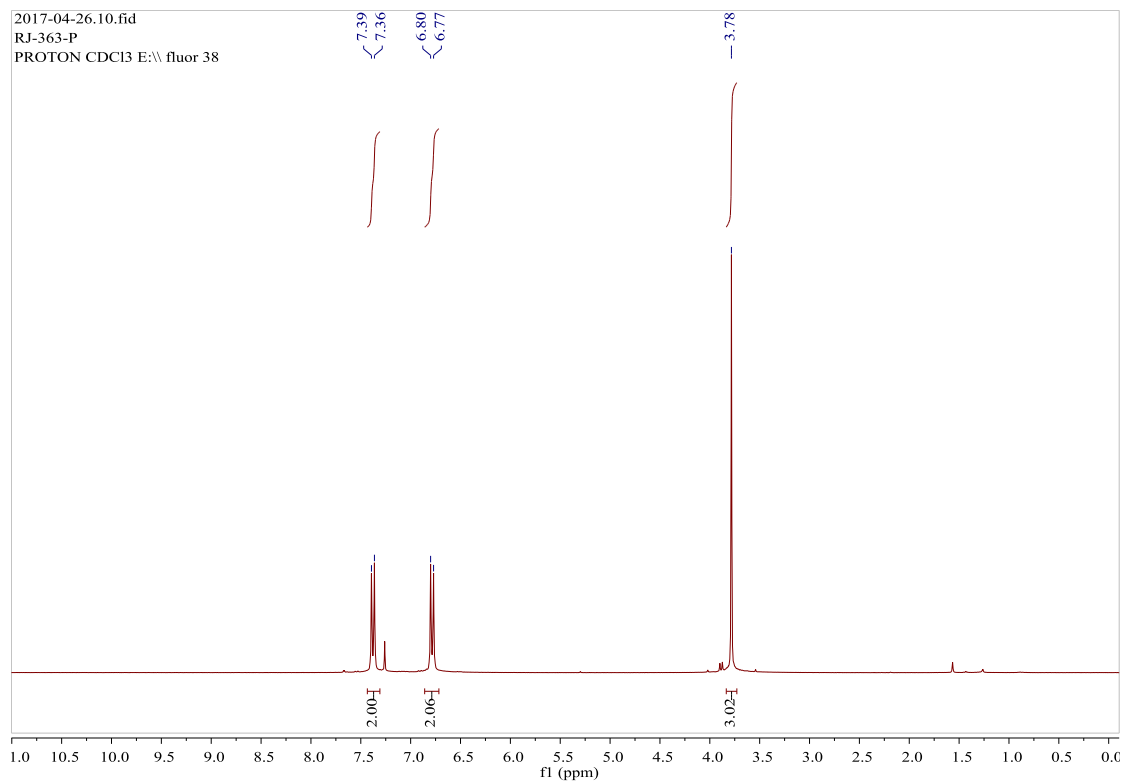
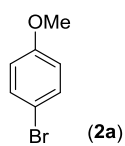
1. ^1H NMR titration of a mixture of HFIP and NBS ^a

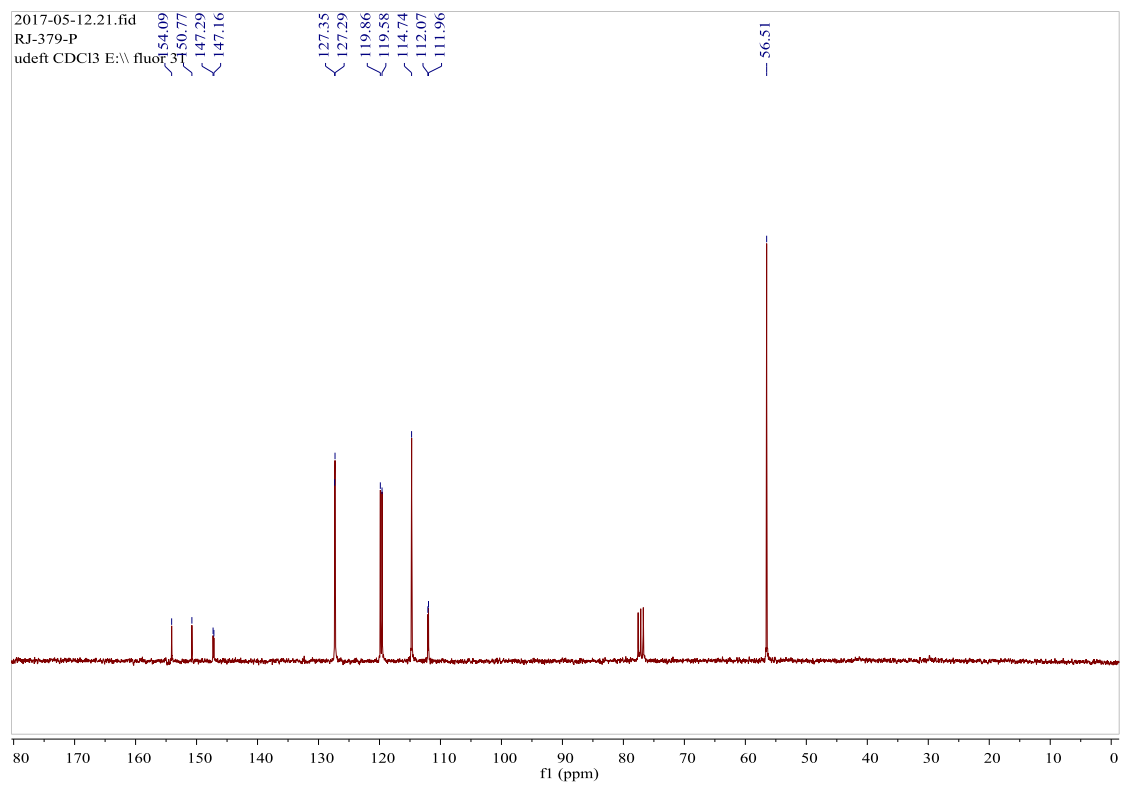
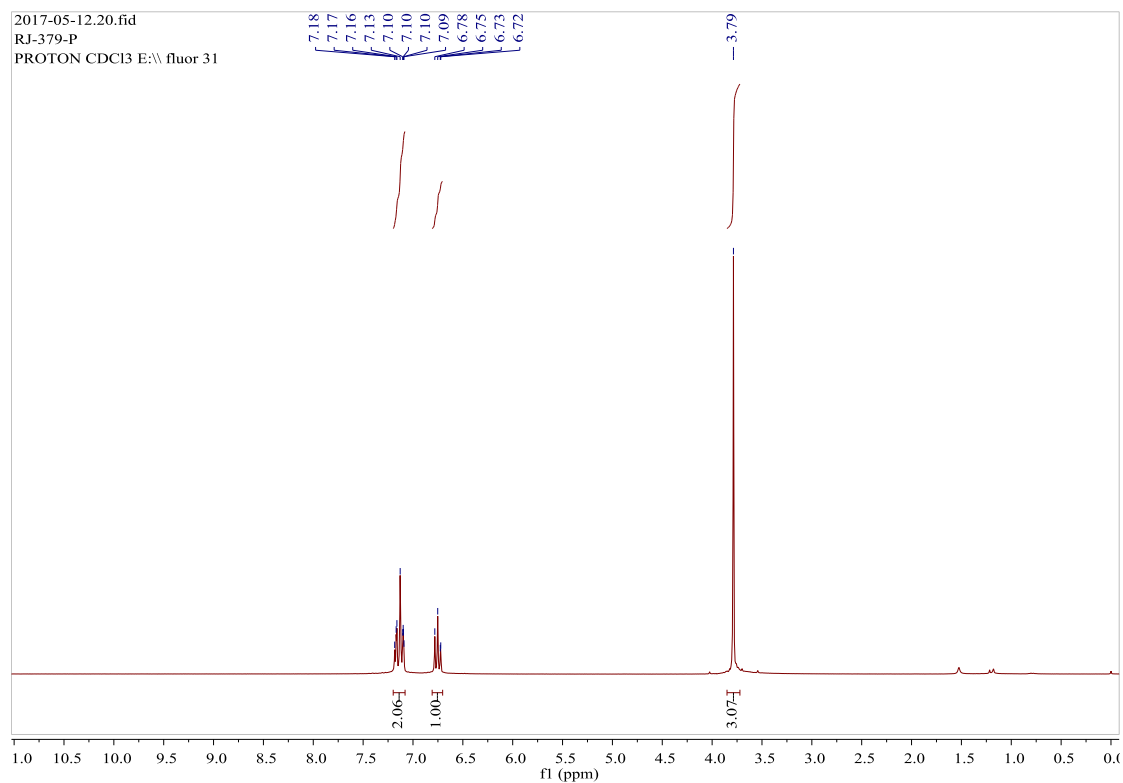
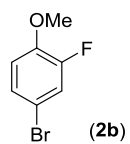
In the NMR tube, different amounts of NBS (**2a**) were dissolved in 1.0 mmol of HFIP, containing a capillary with C_6D_6 (external standard). Then, the NMR spectra (1-5) were measured. A downfield shift of the OH proton (H_x) of HFIP was observed with increasing concentrations of NBS.

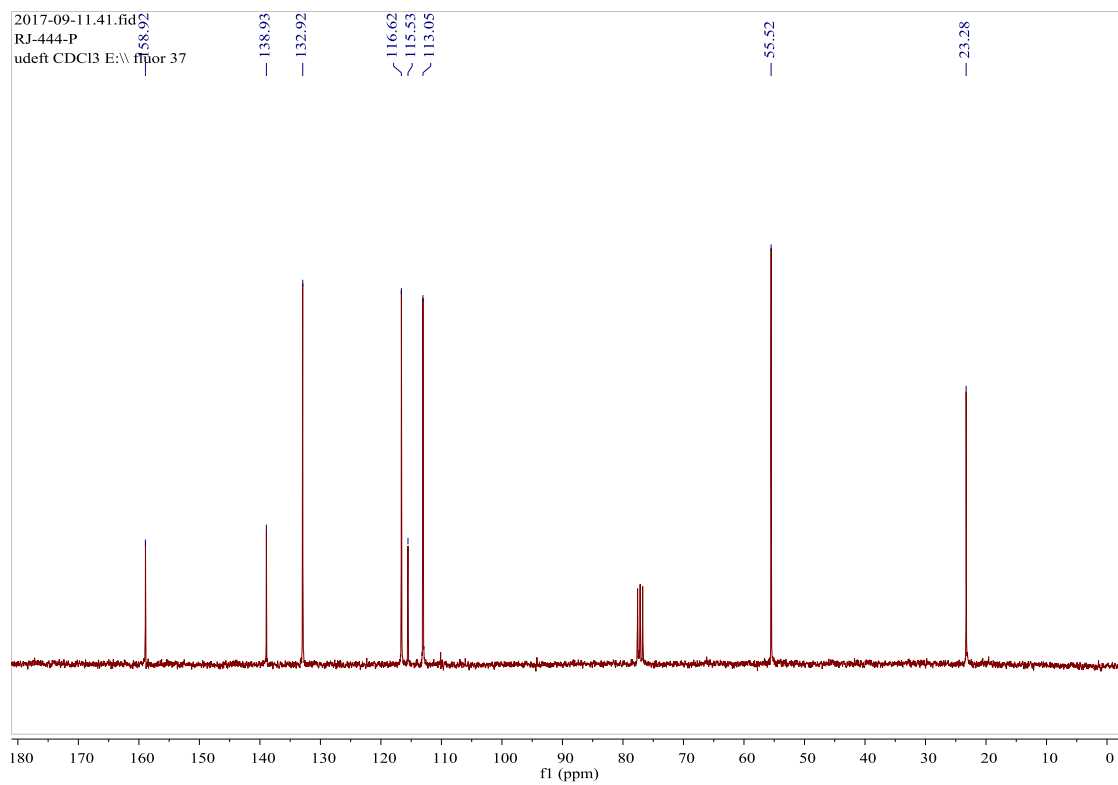
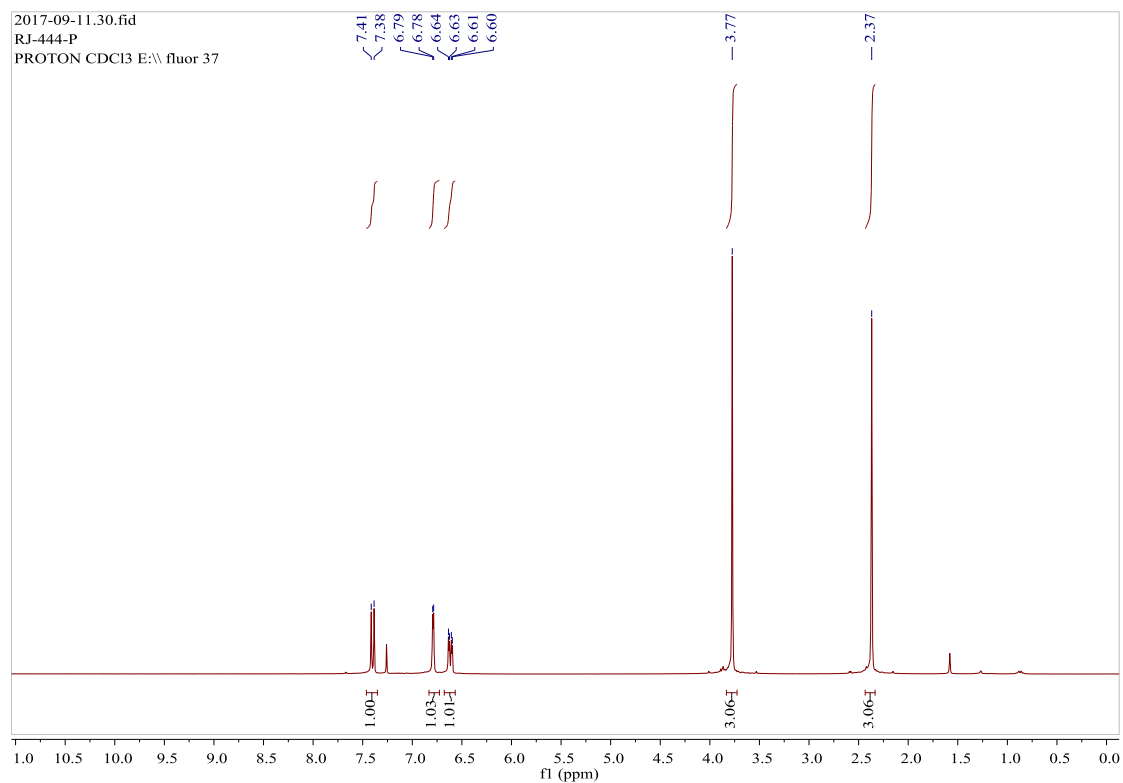
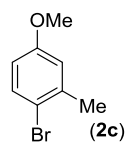


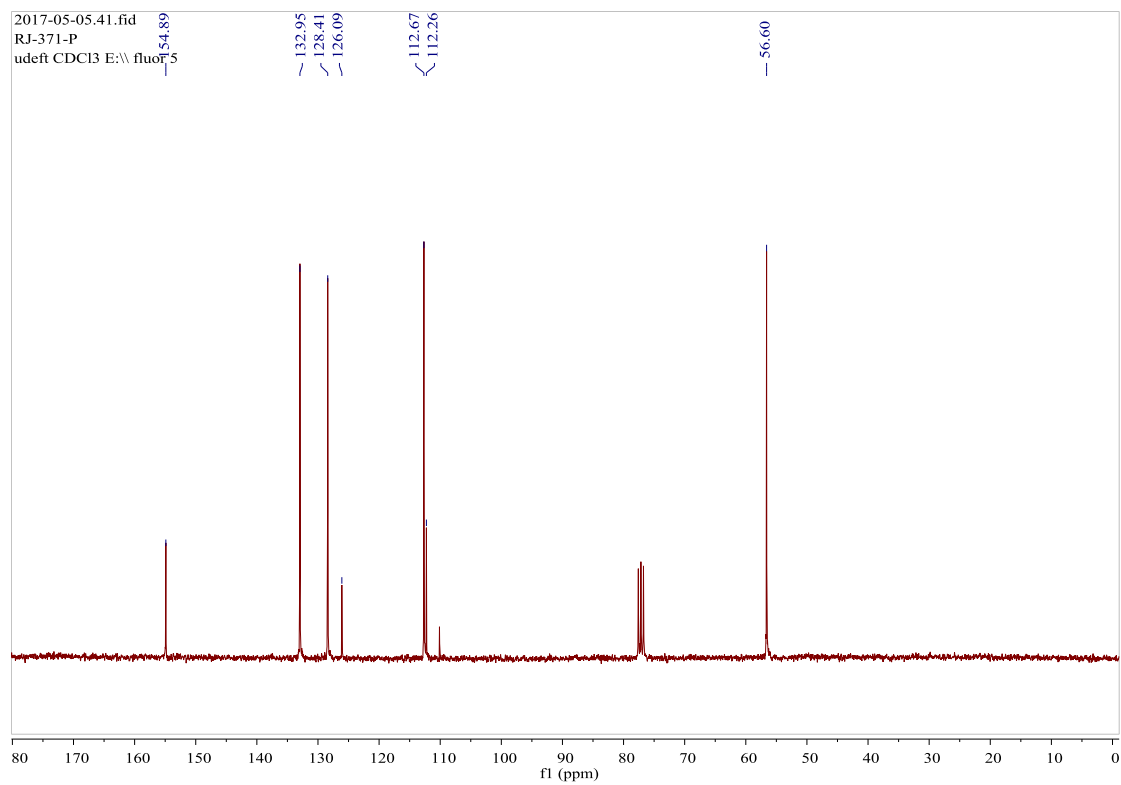
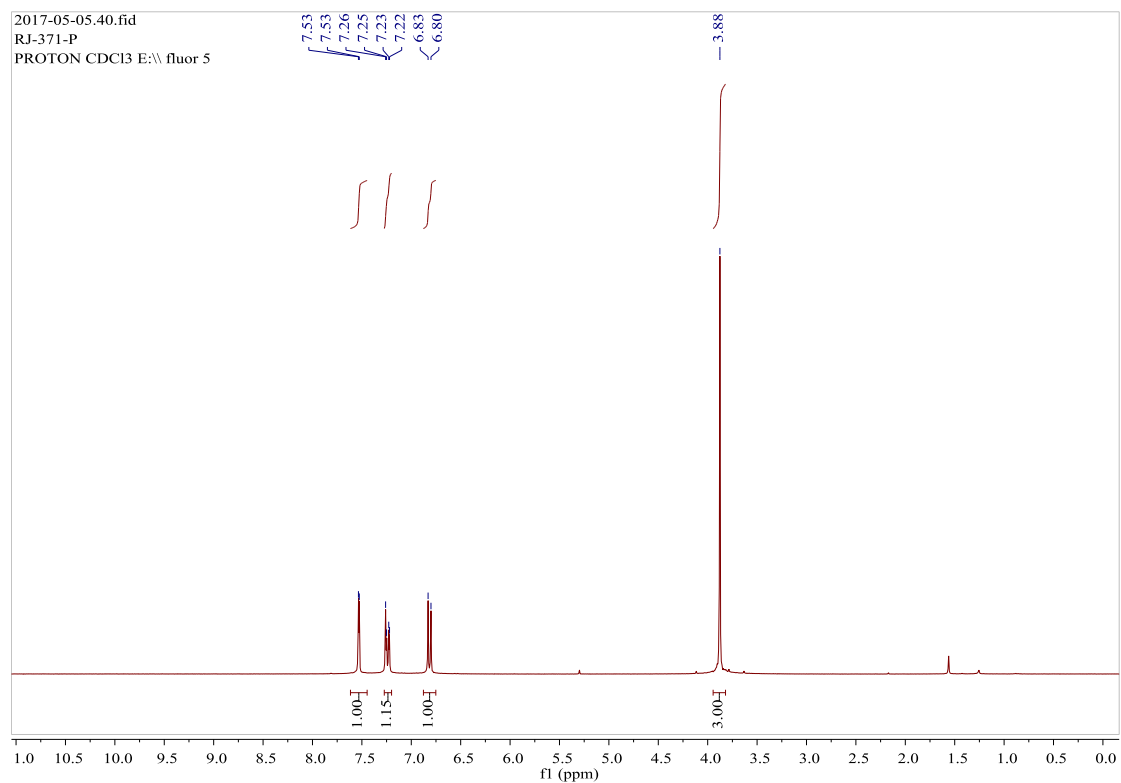
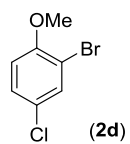
^a Spectra were acquired in the presence of the following quantities of NBS: (1) 0 mol%; (2) 1 mol%; (3) 5 mol%; (4) 20 mol%; (5) 20 - 50 mol% (because 50% of NBS can not be completely dissolved in HFIP).

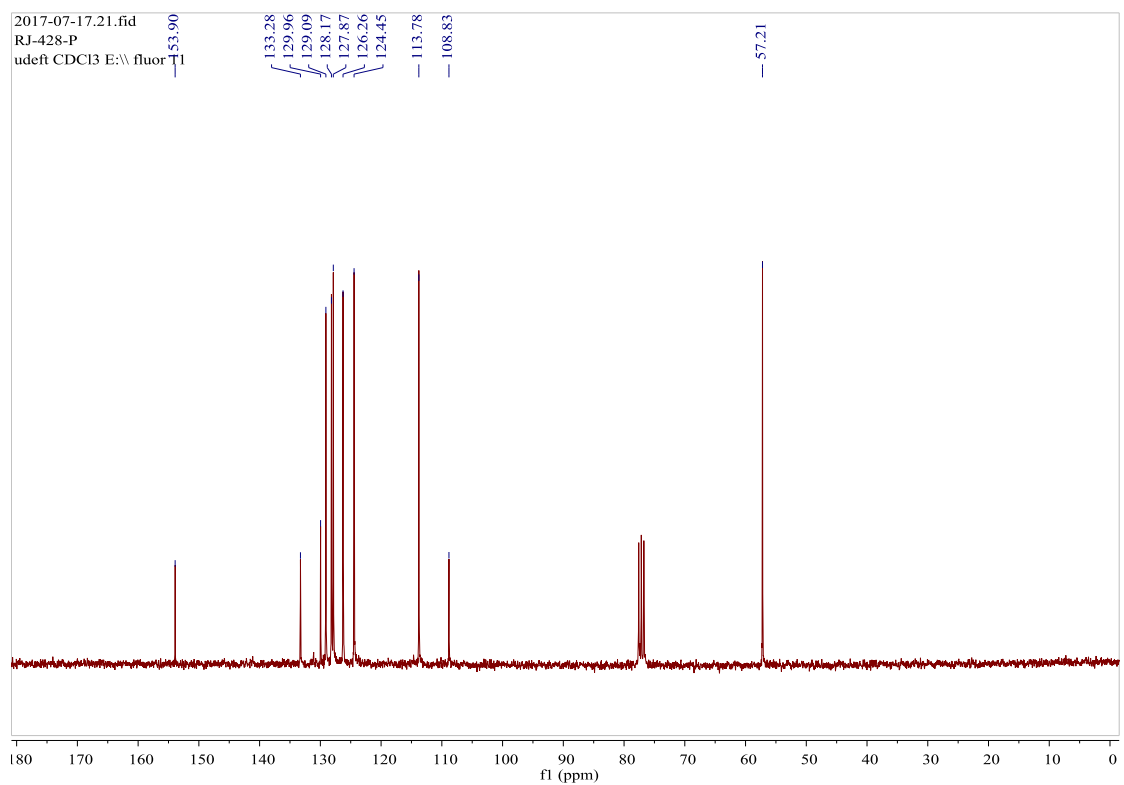
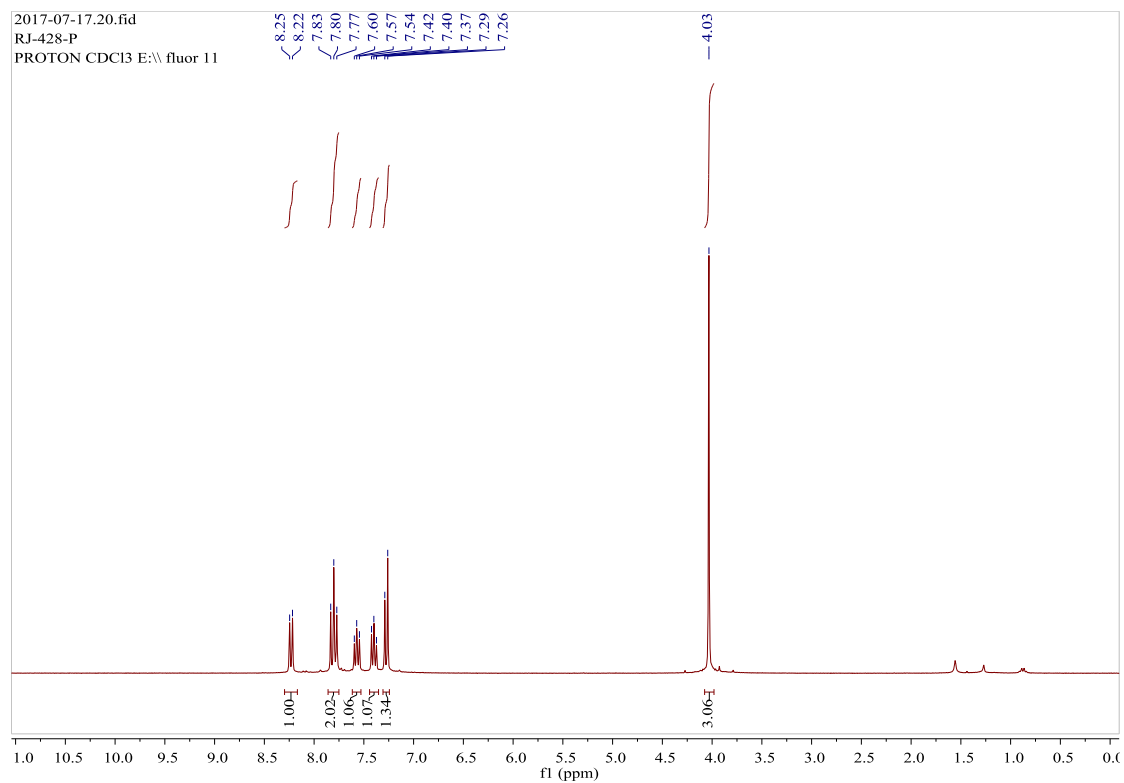
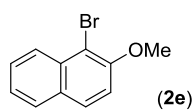
1. ^1H NMR and ^{13}C NMR spectral for Purified Products:

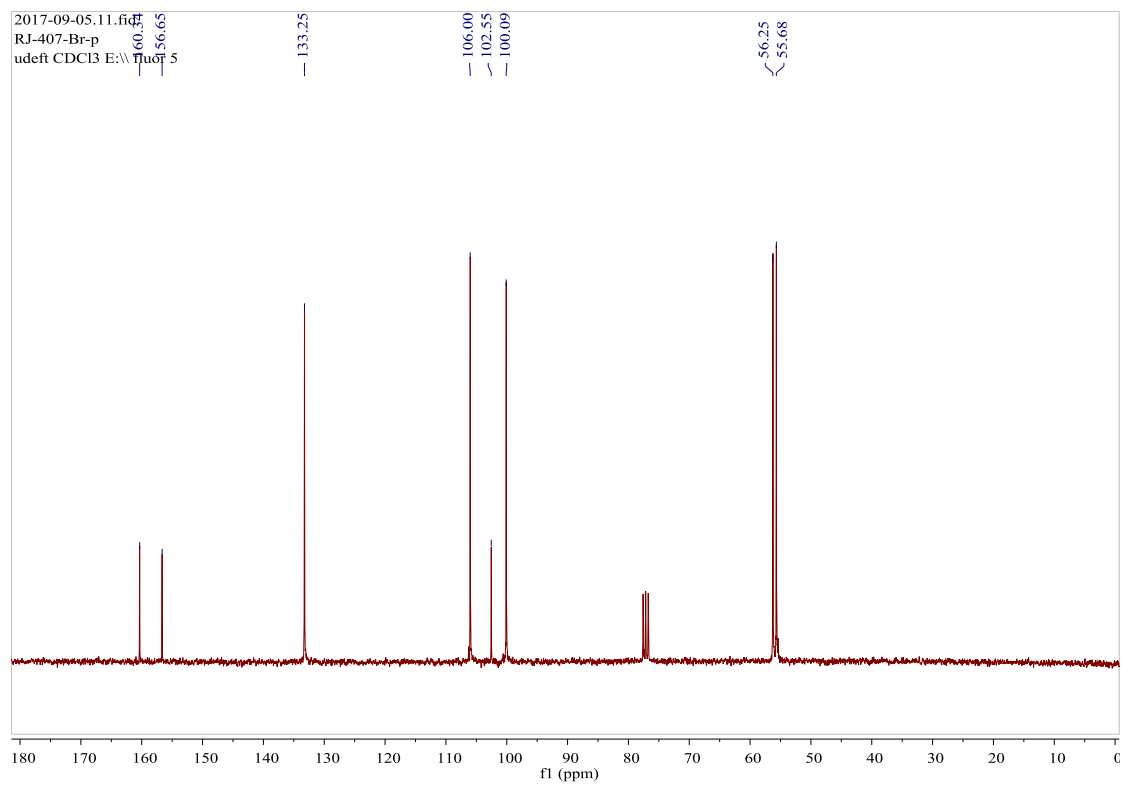
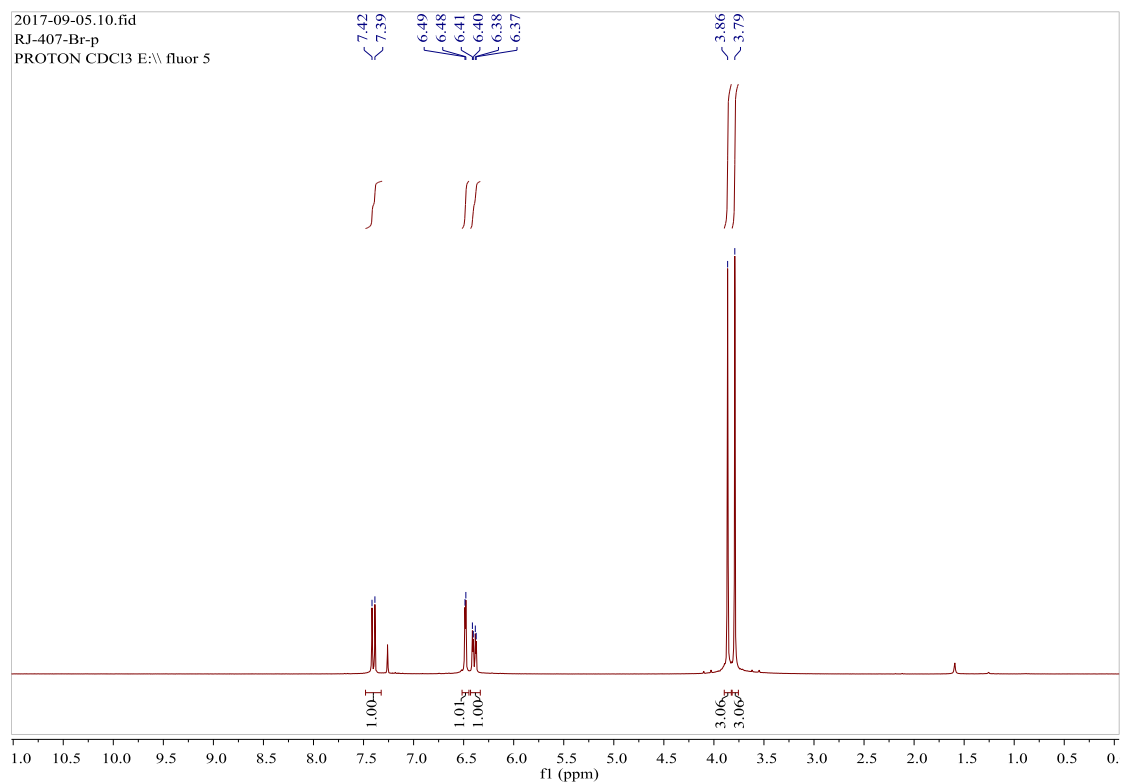
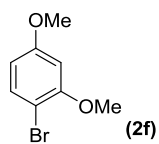


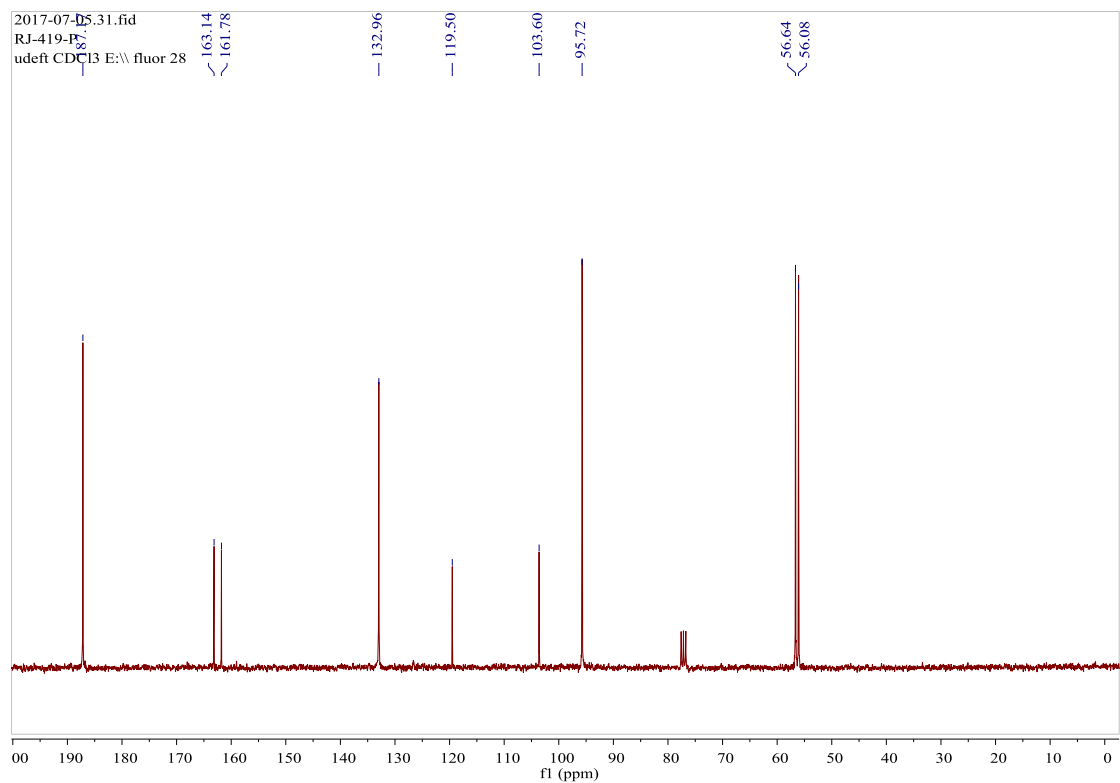
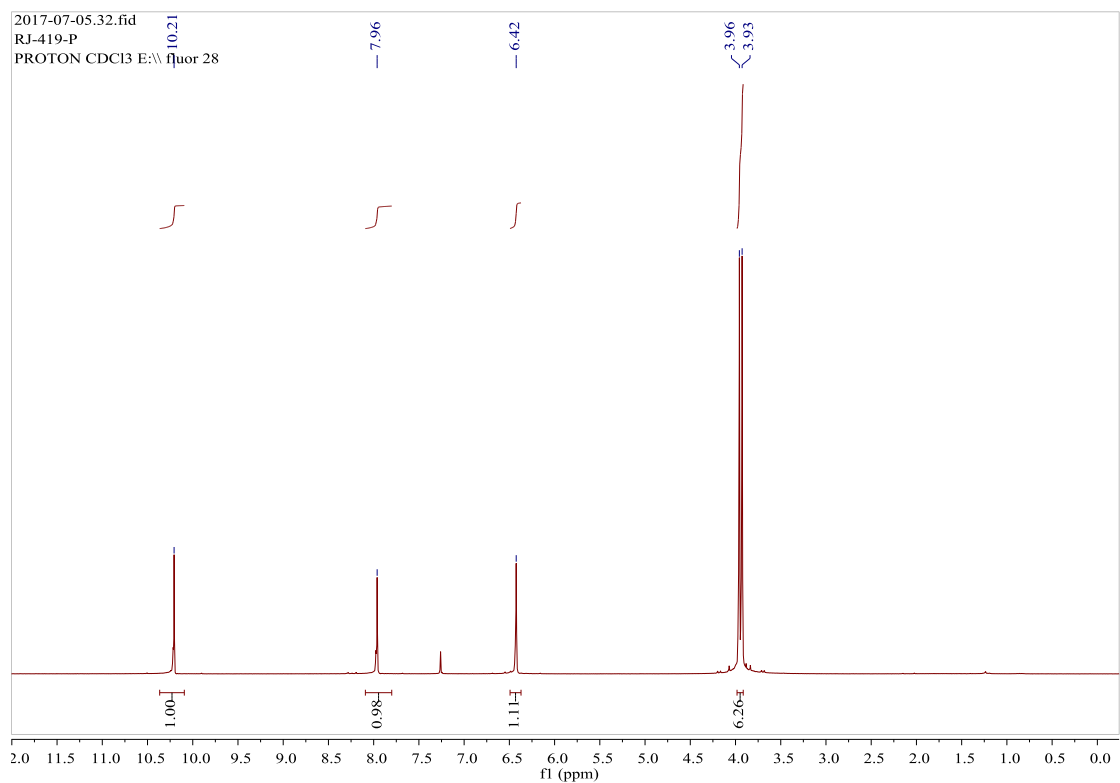
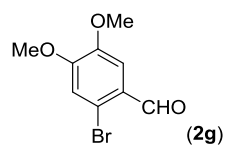


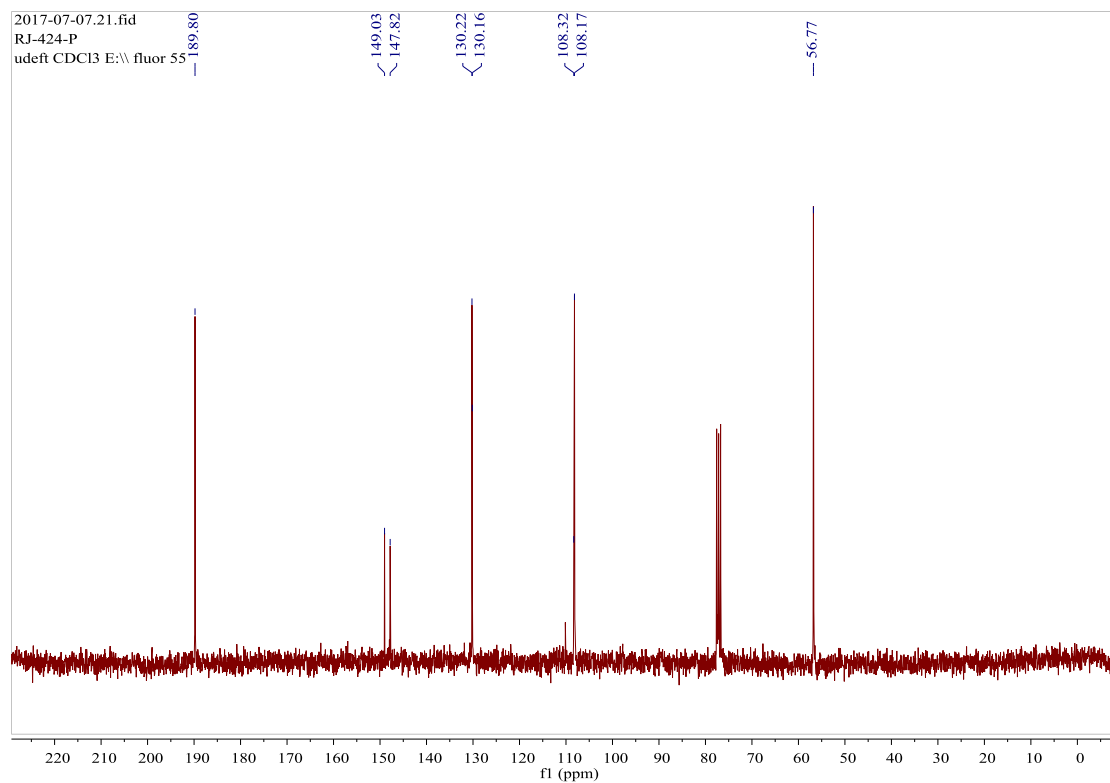
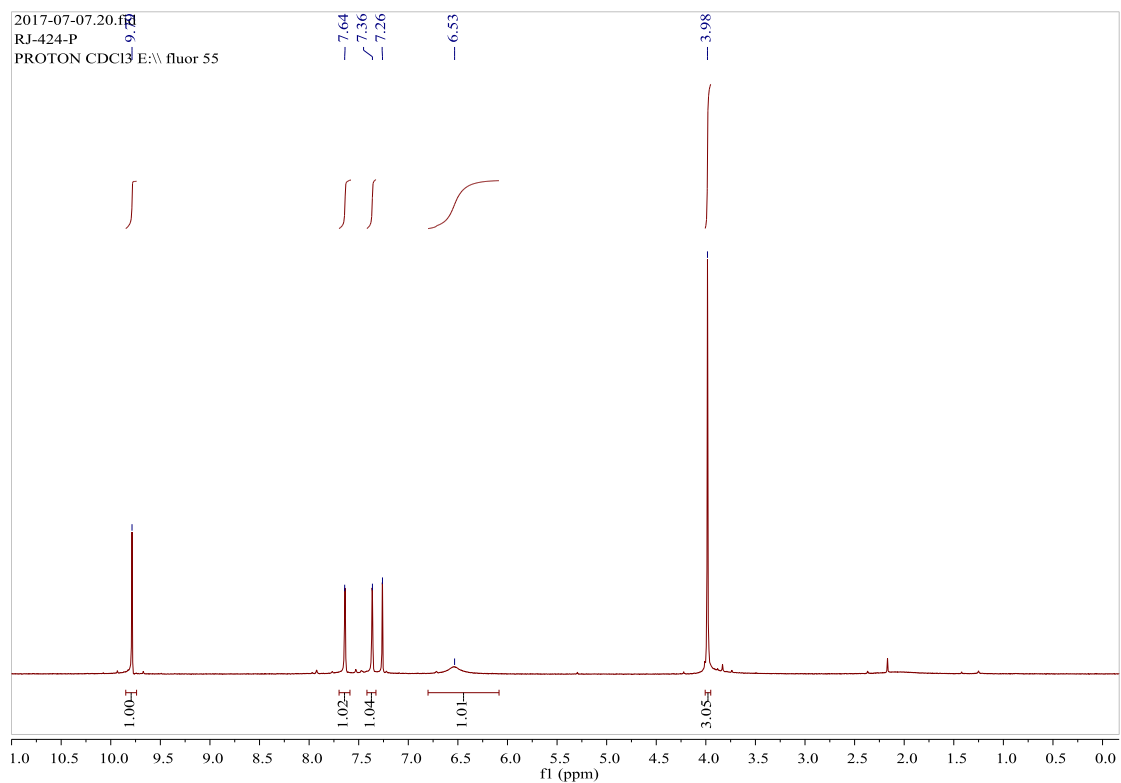
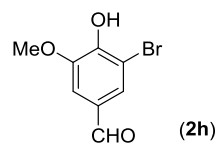


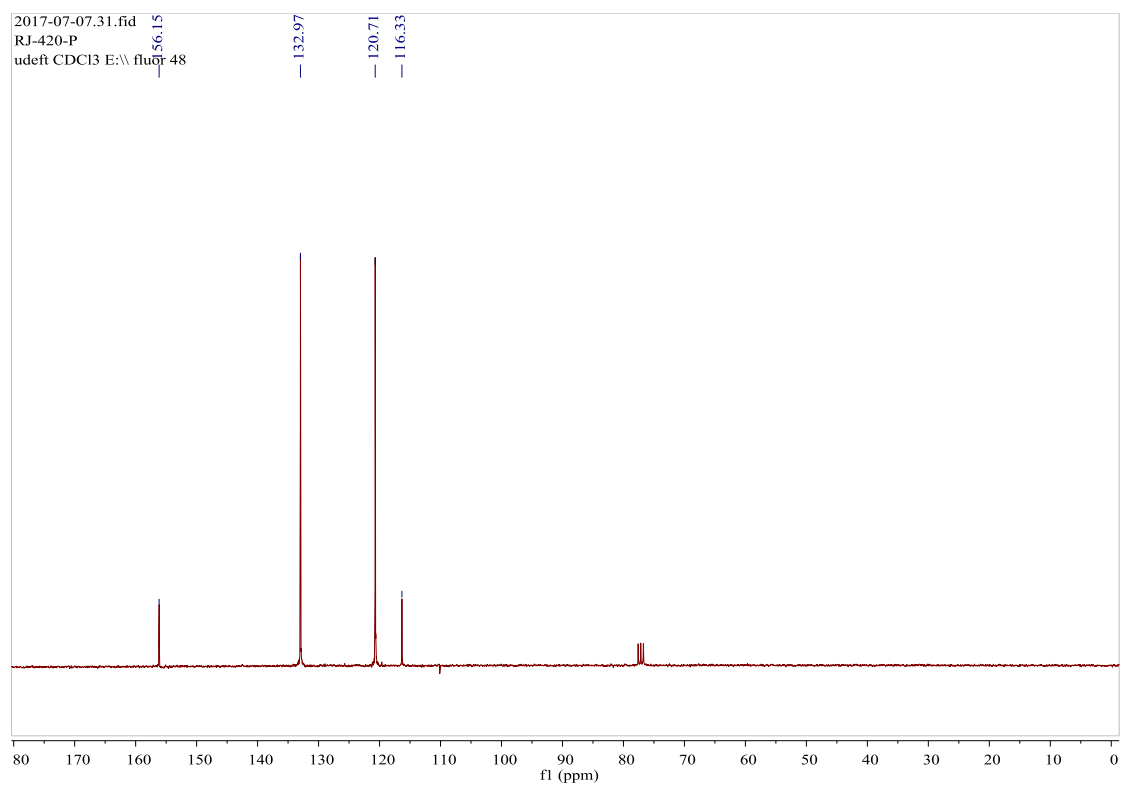
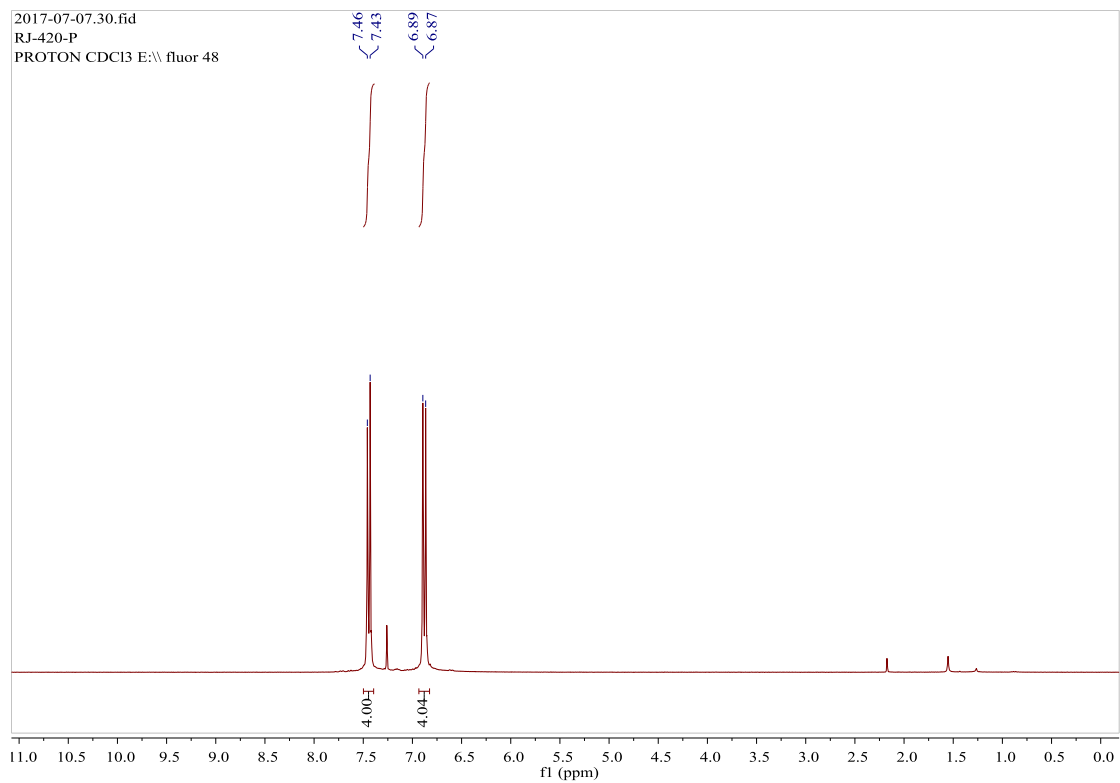
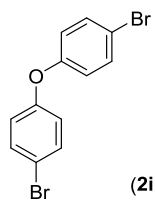


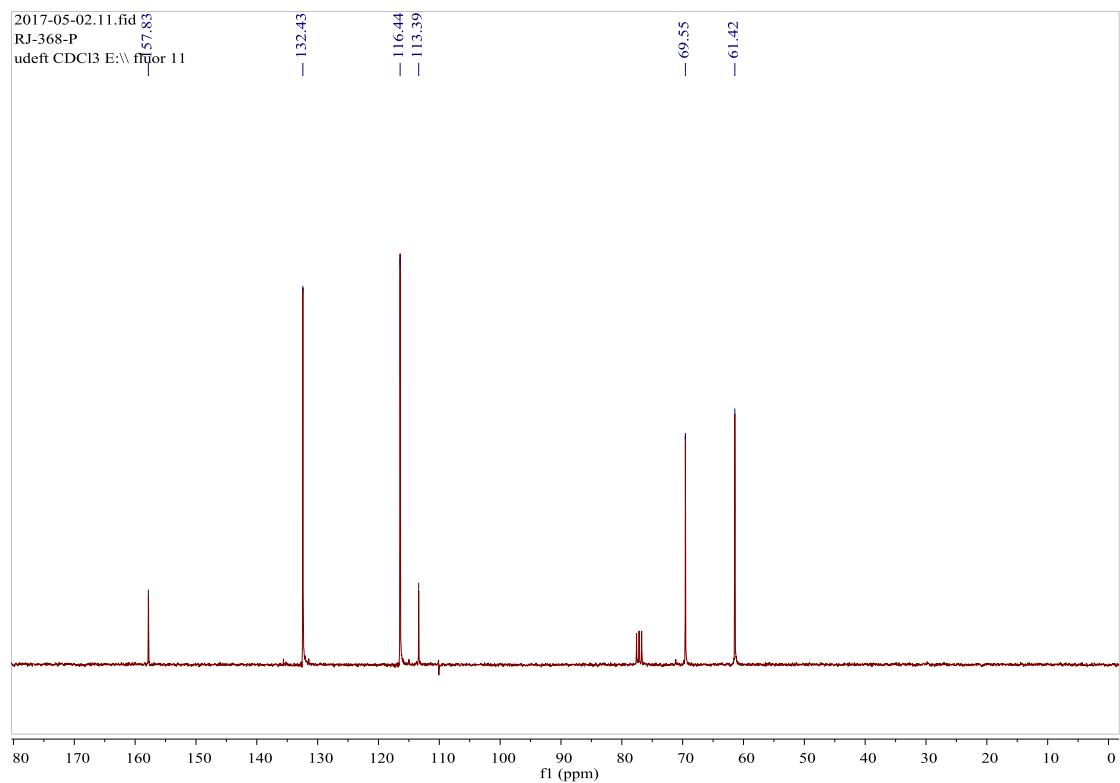
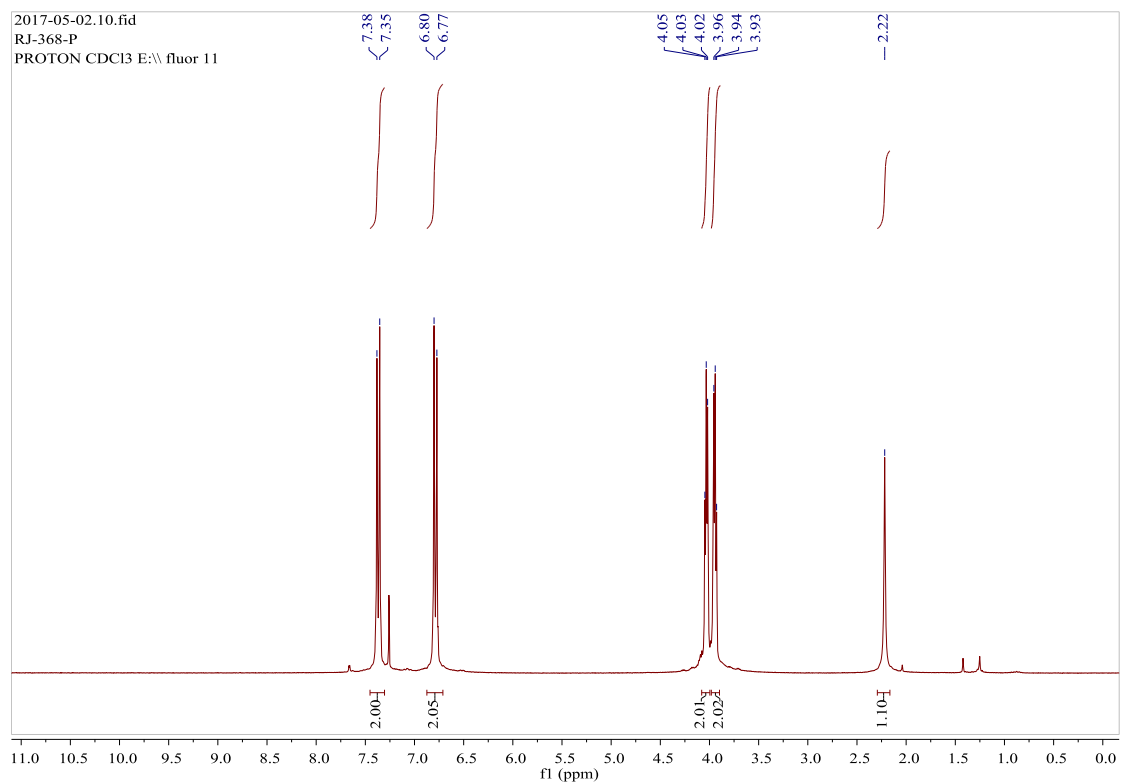
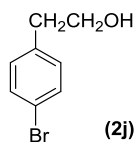


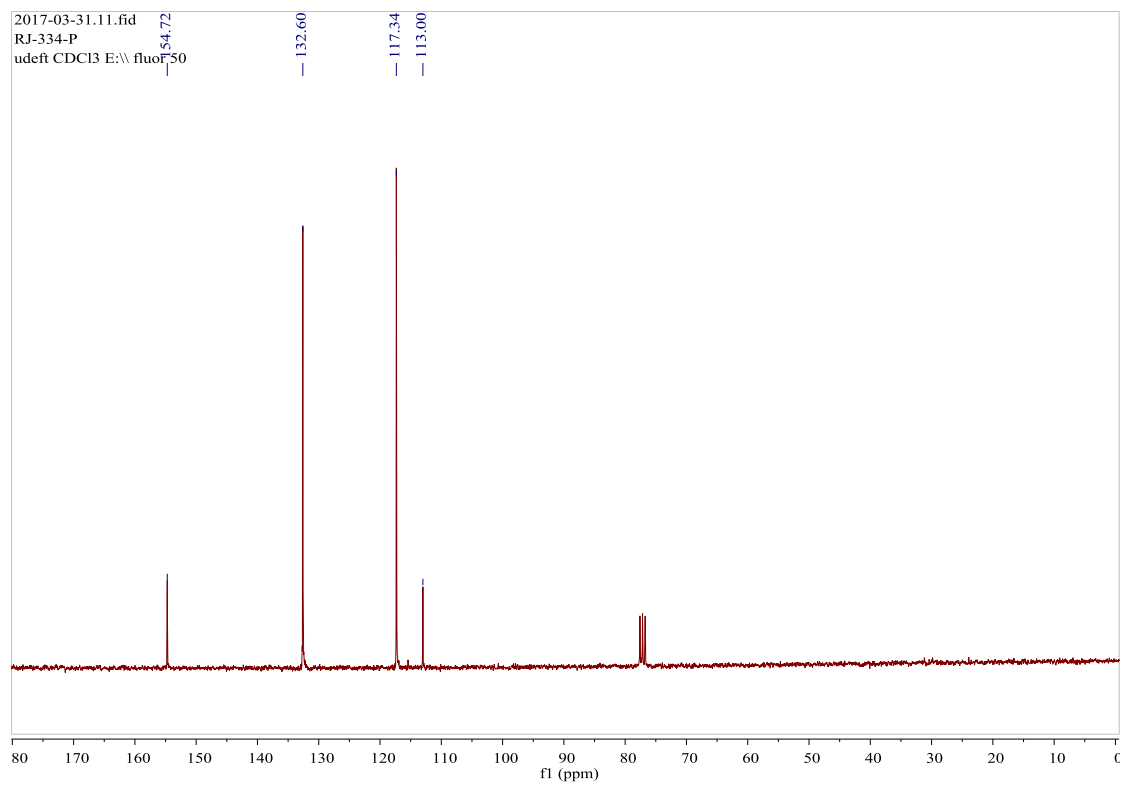
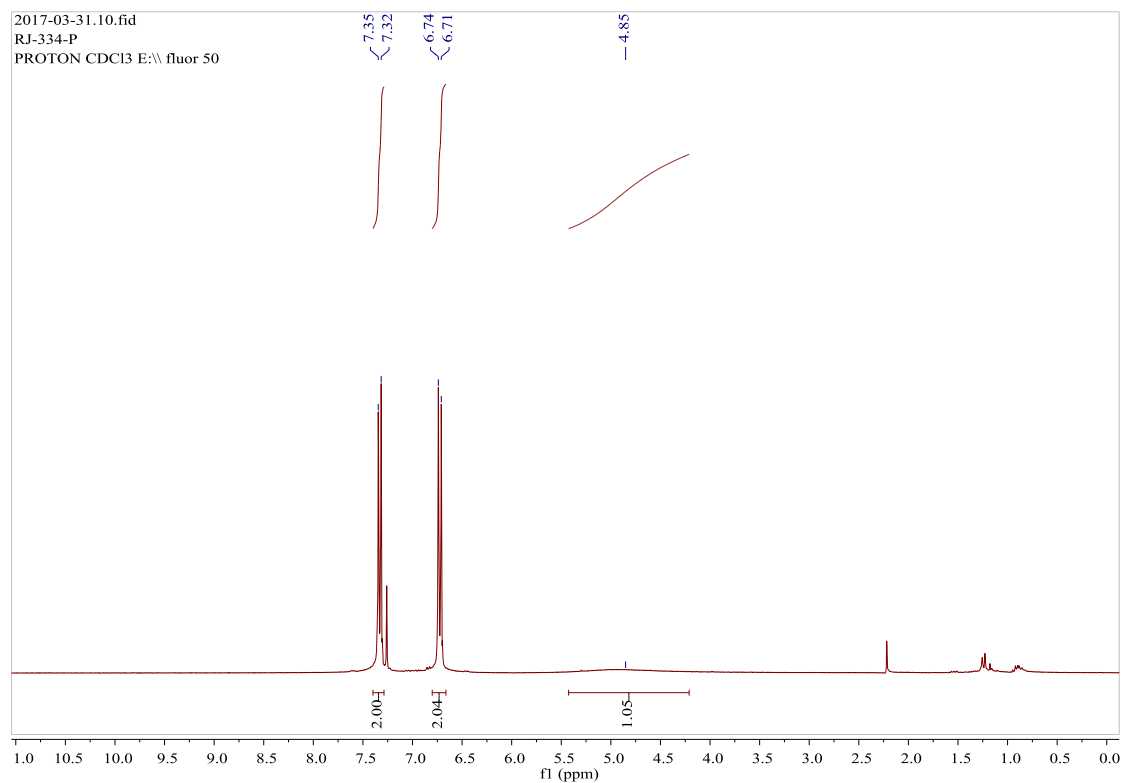
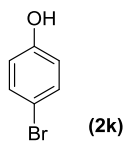


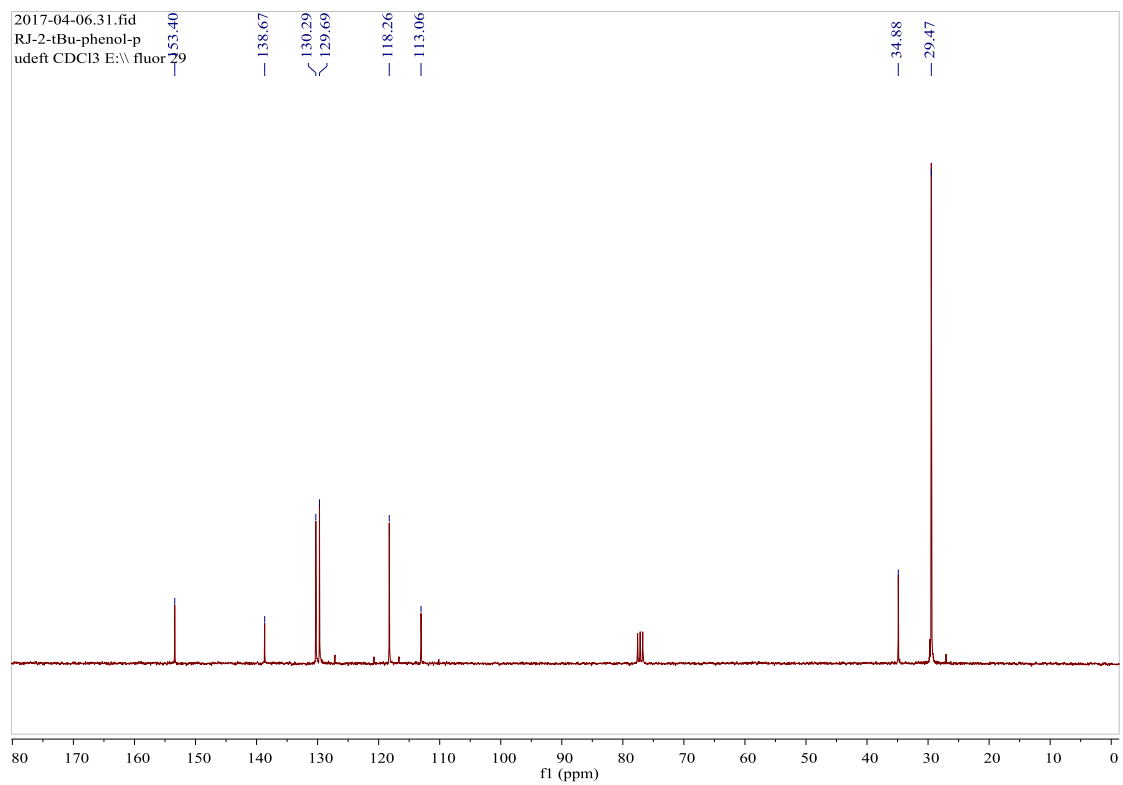
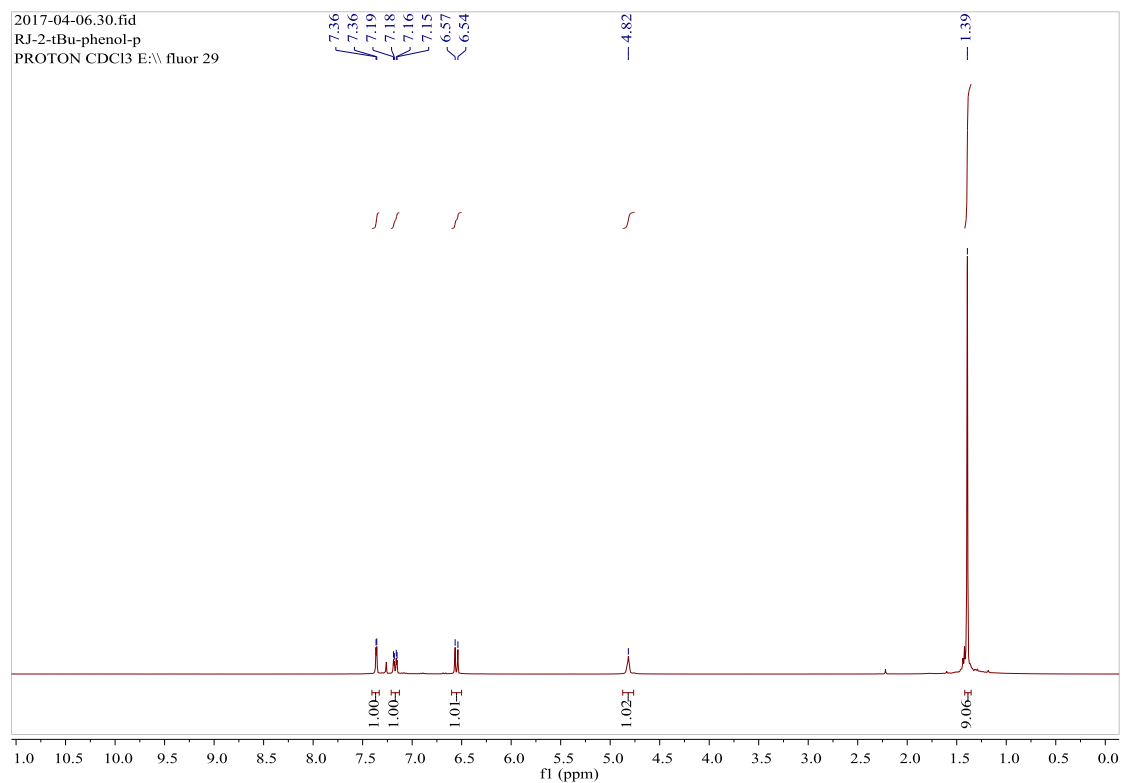
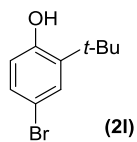


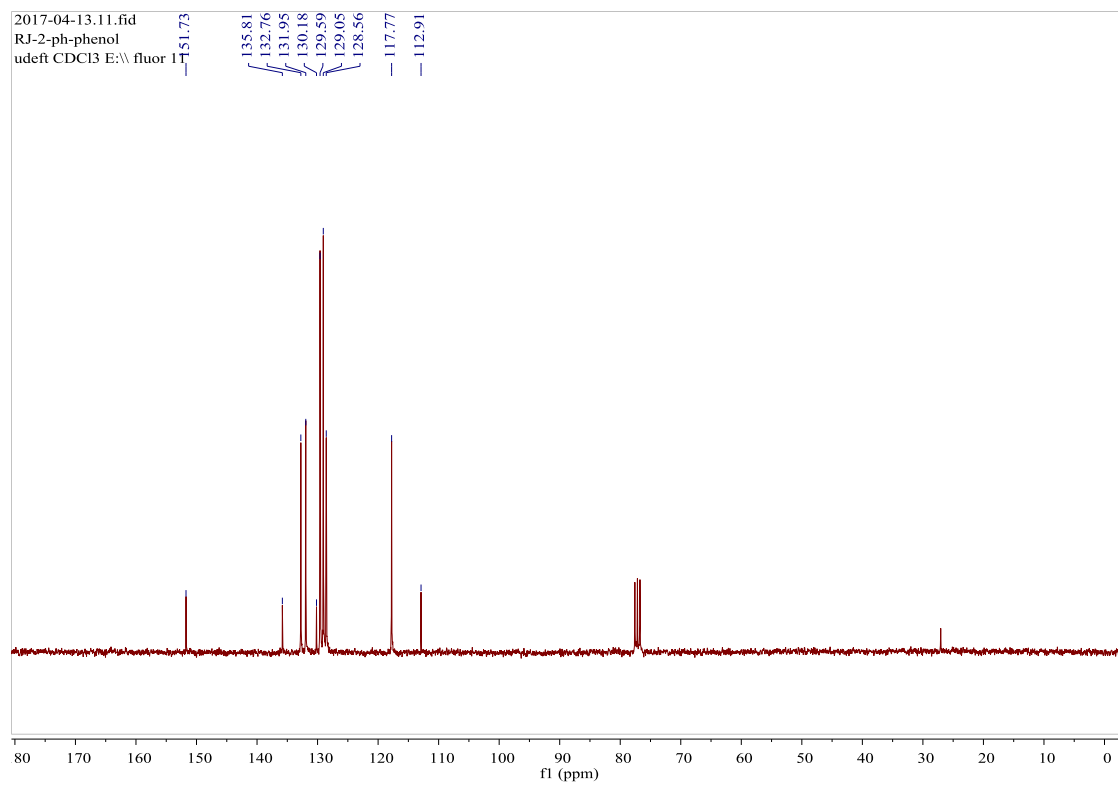
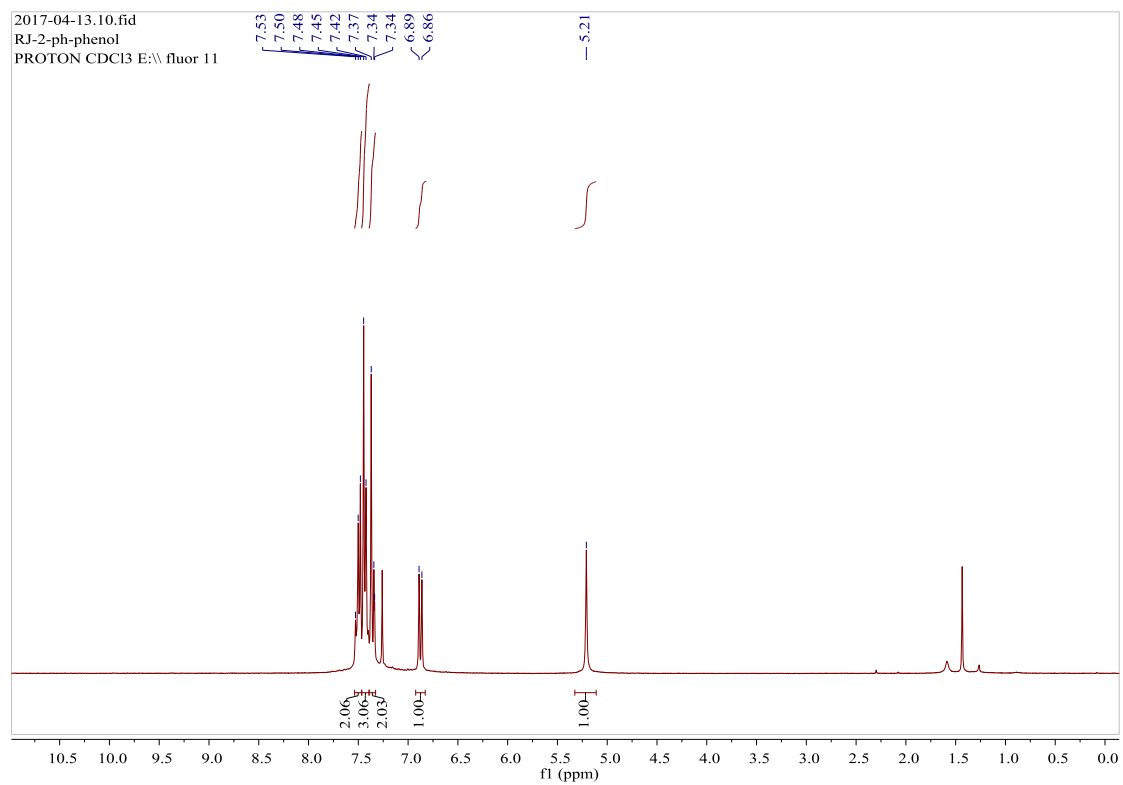
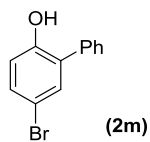


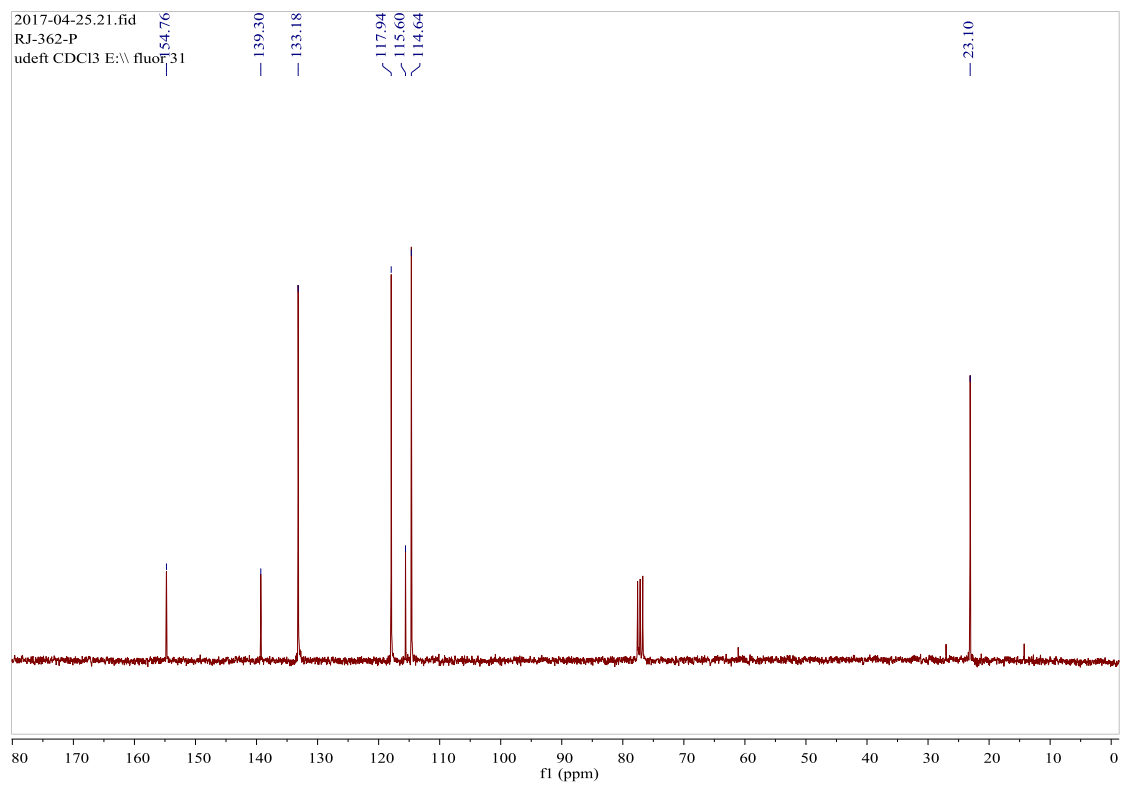
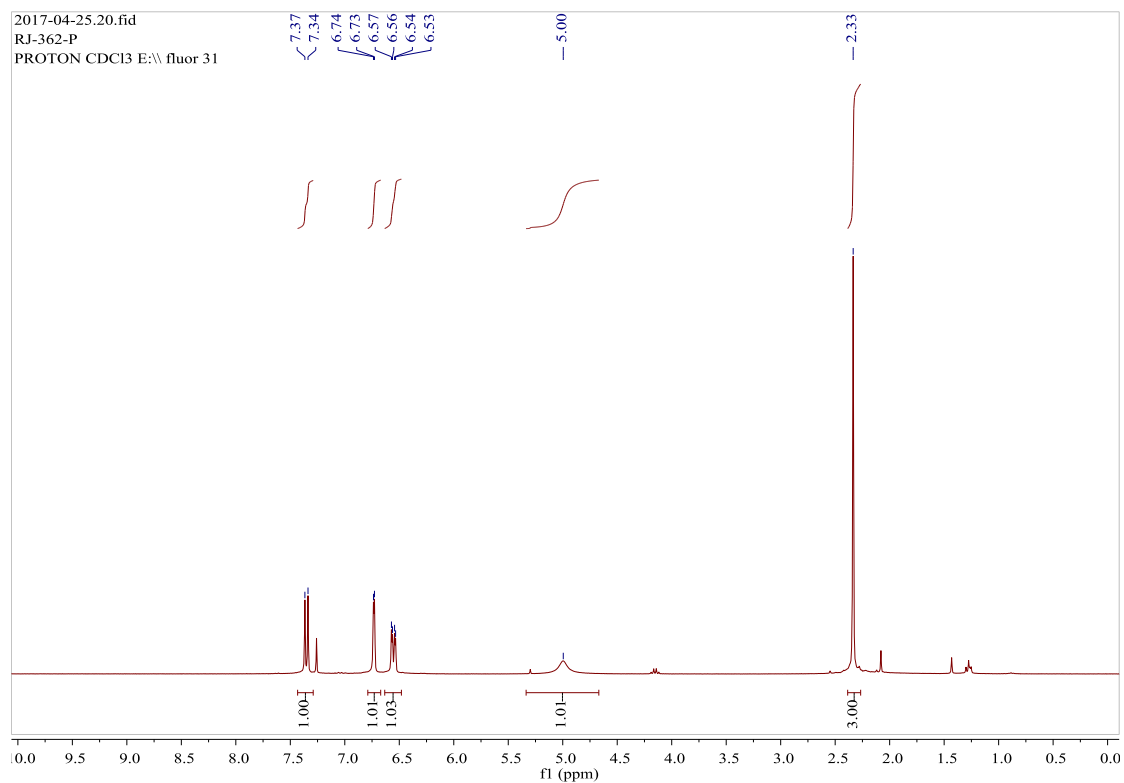
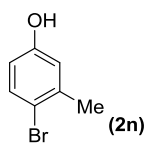


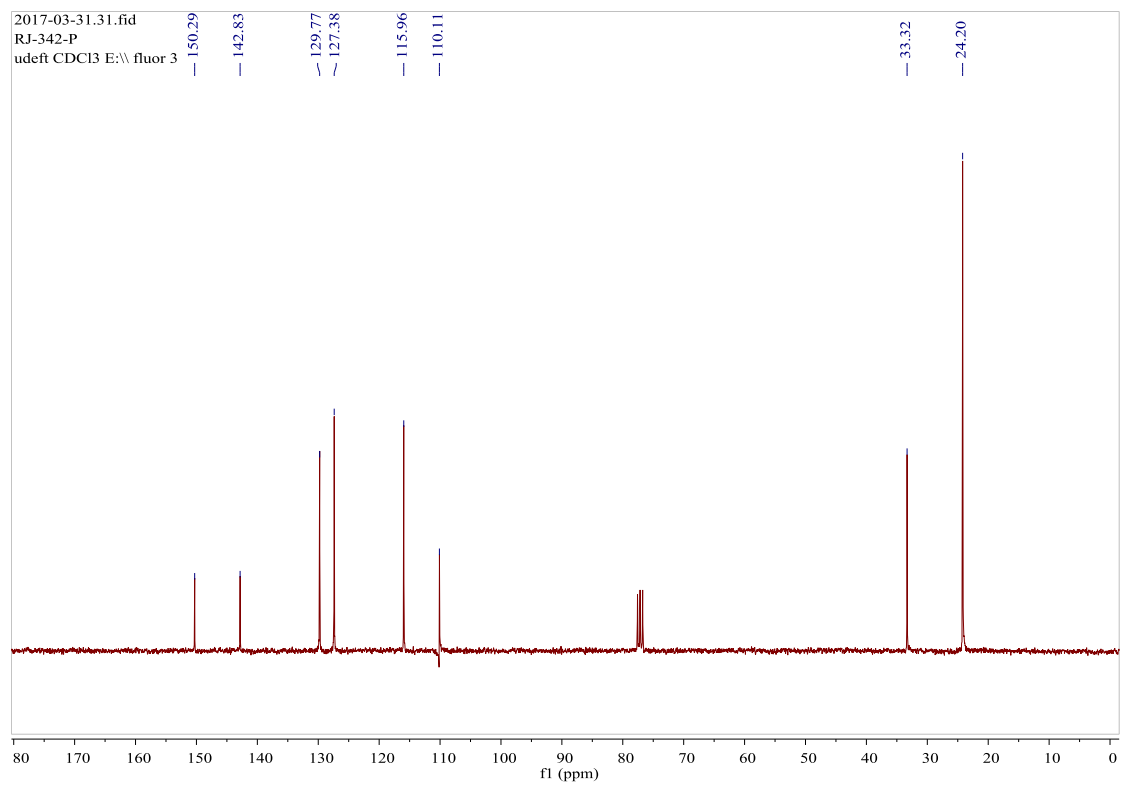
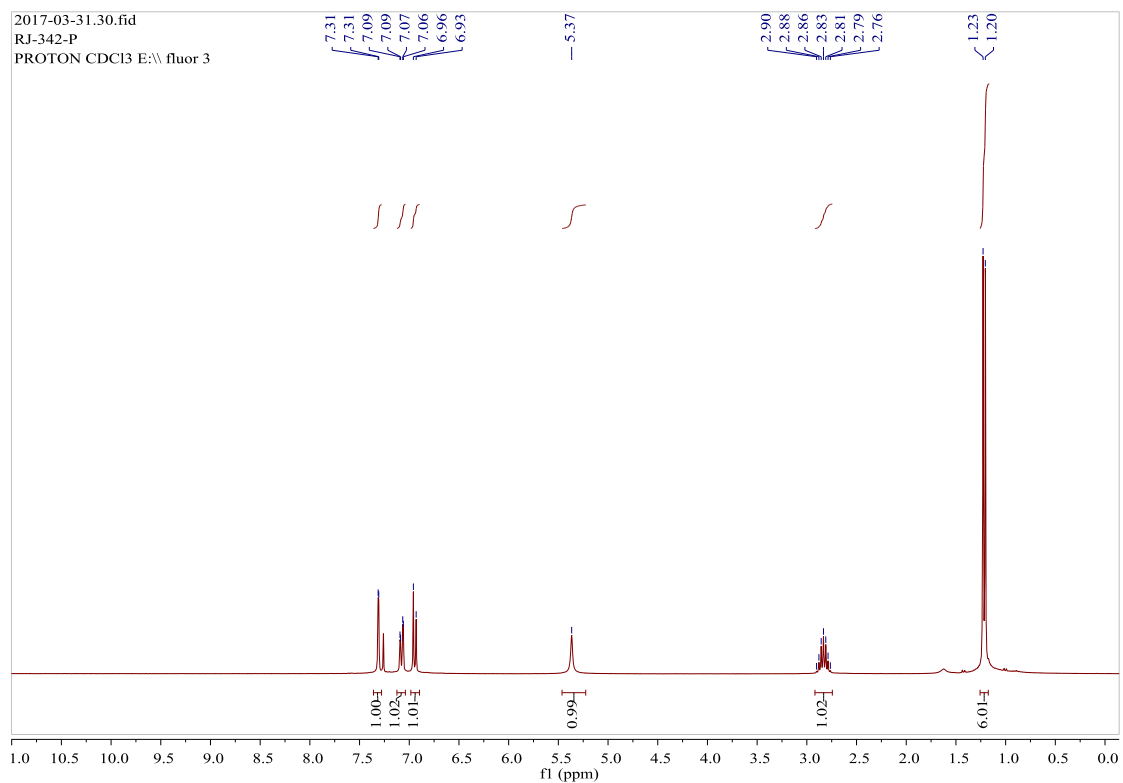
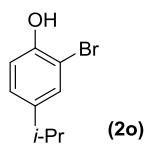


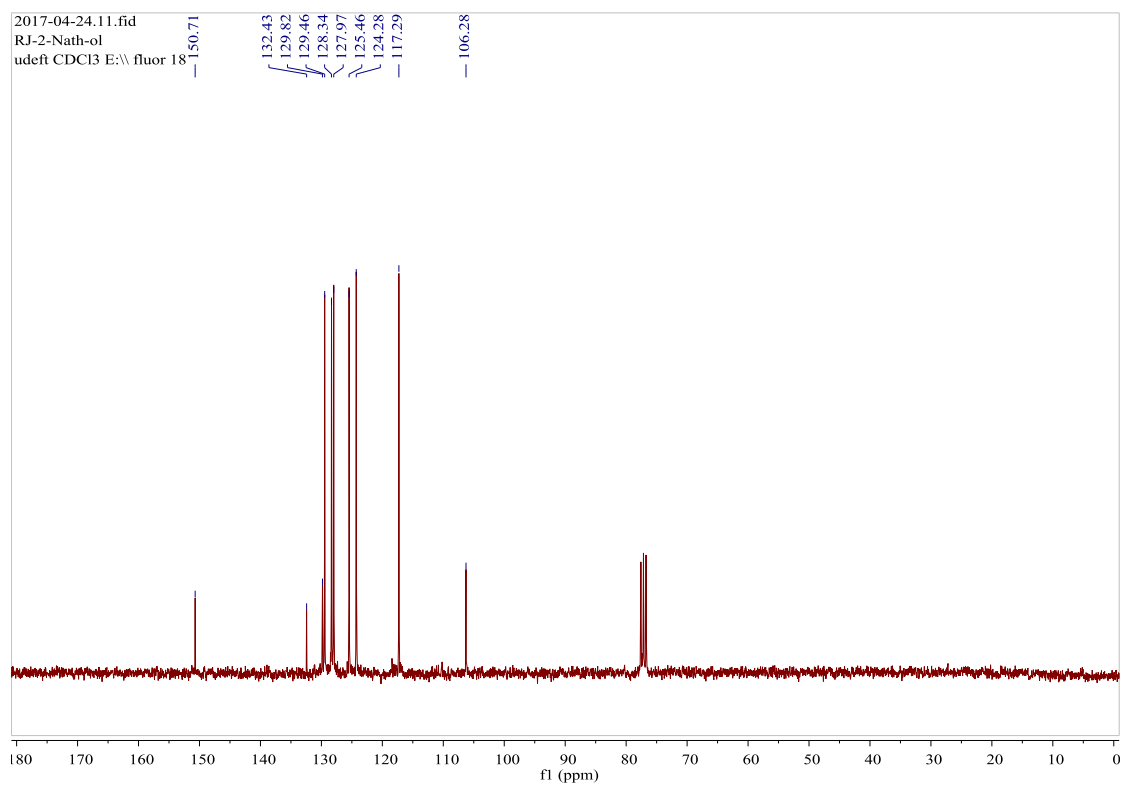
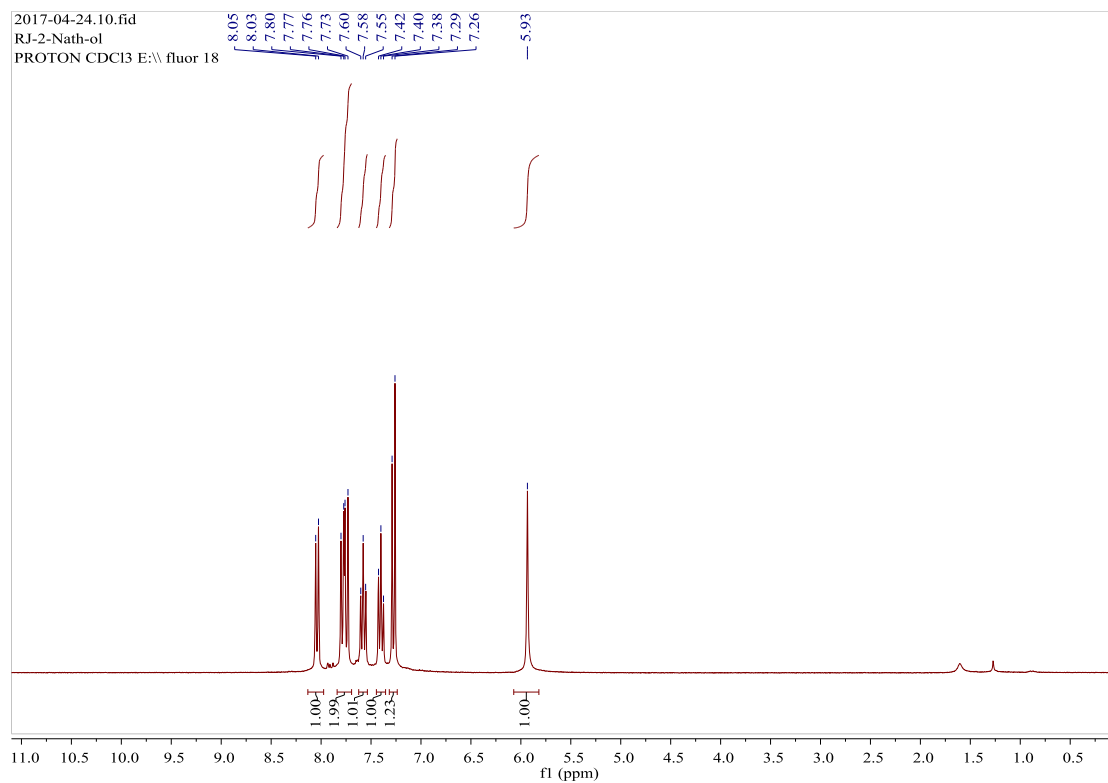
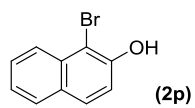


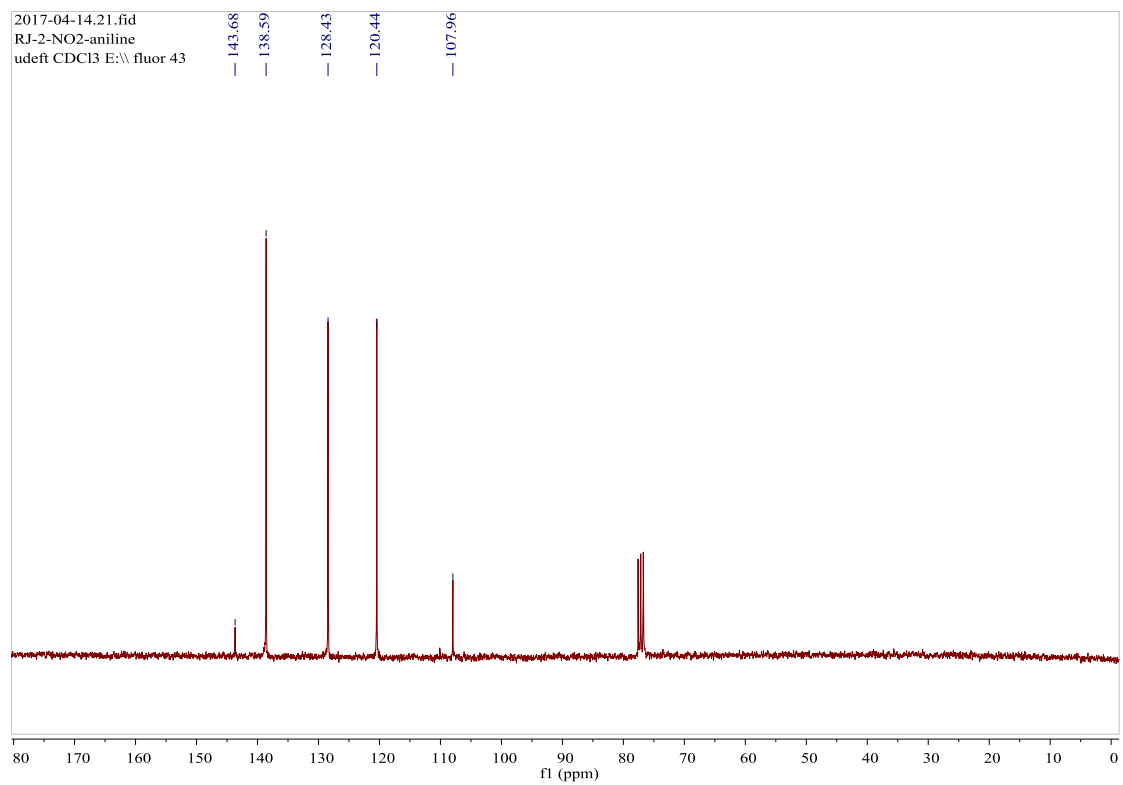
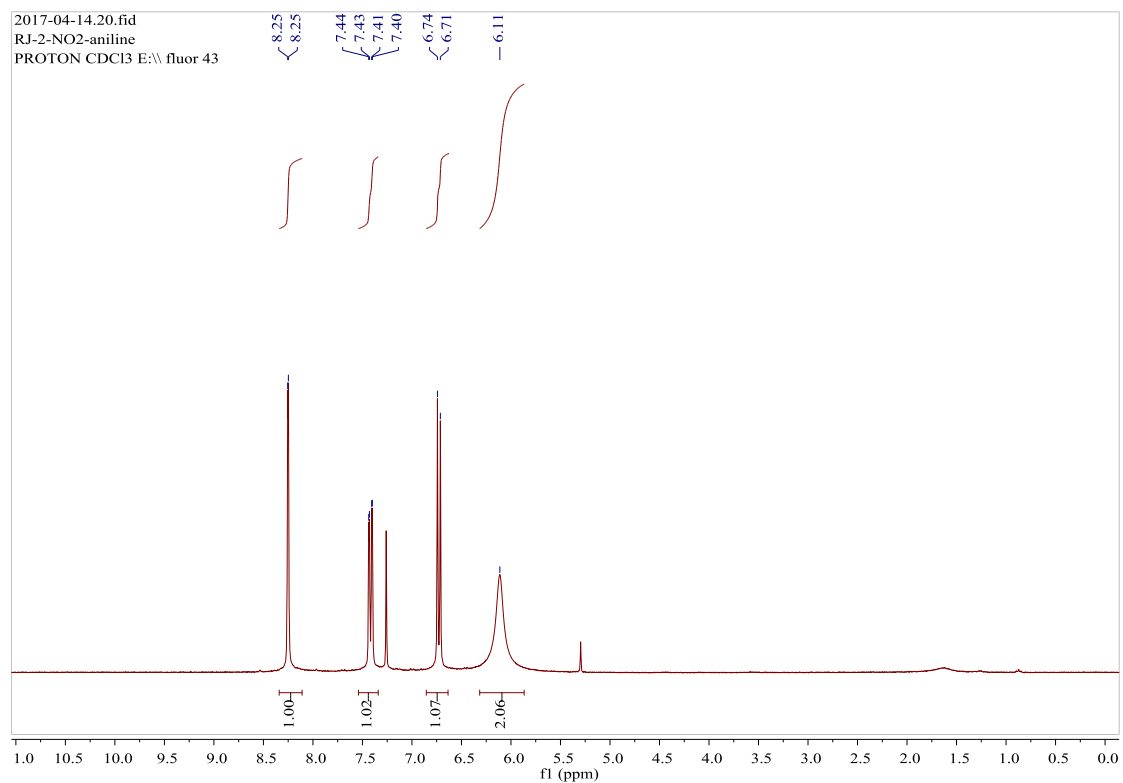
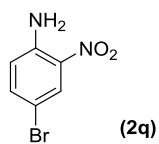


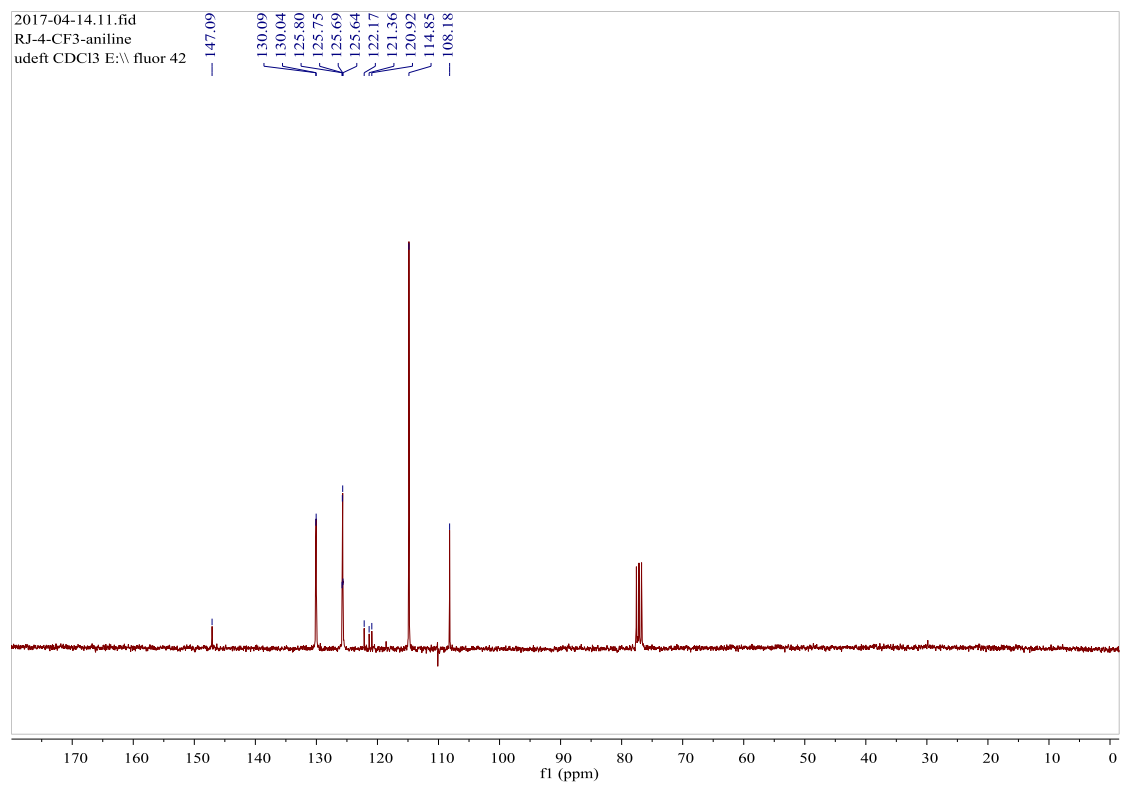
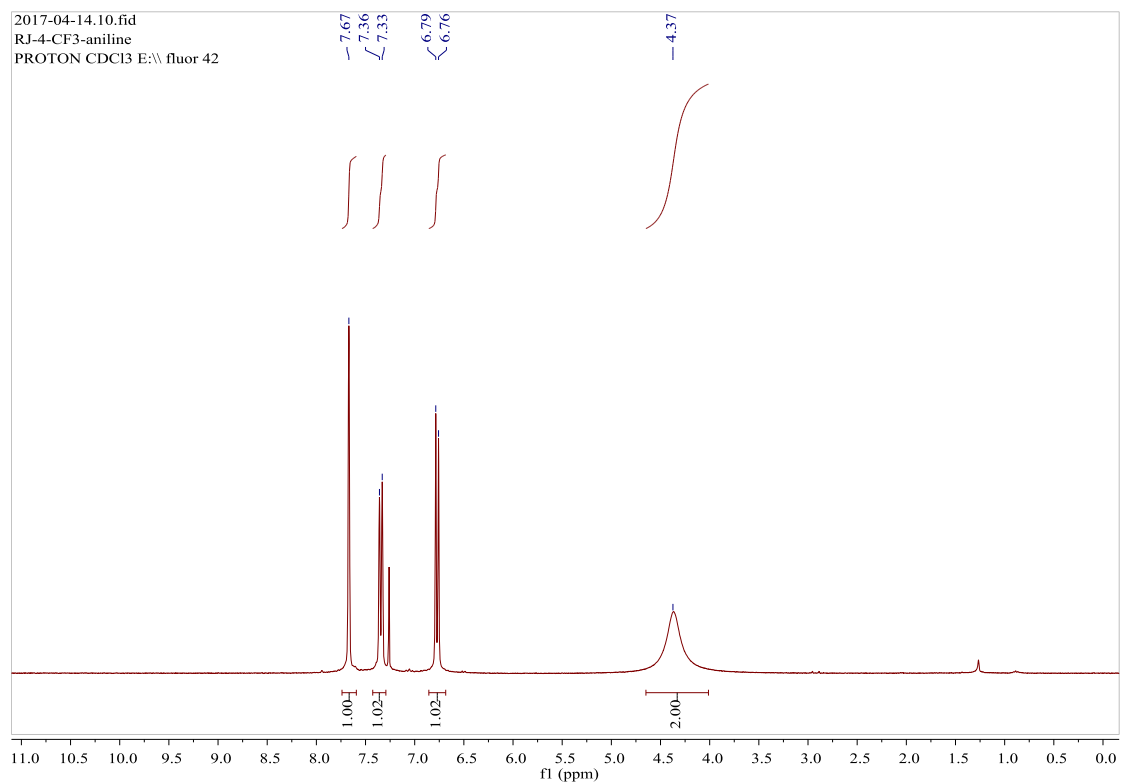
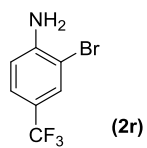


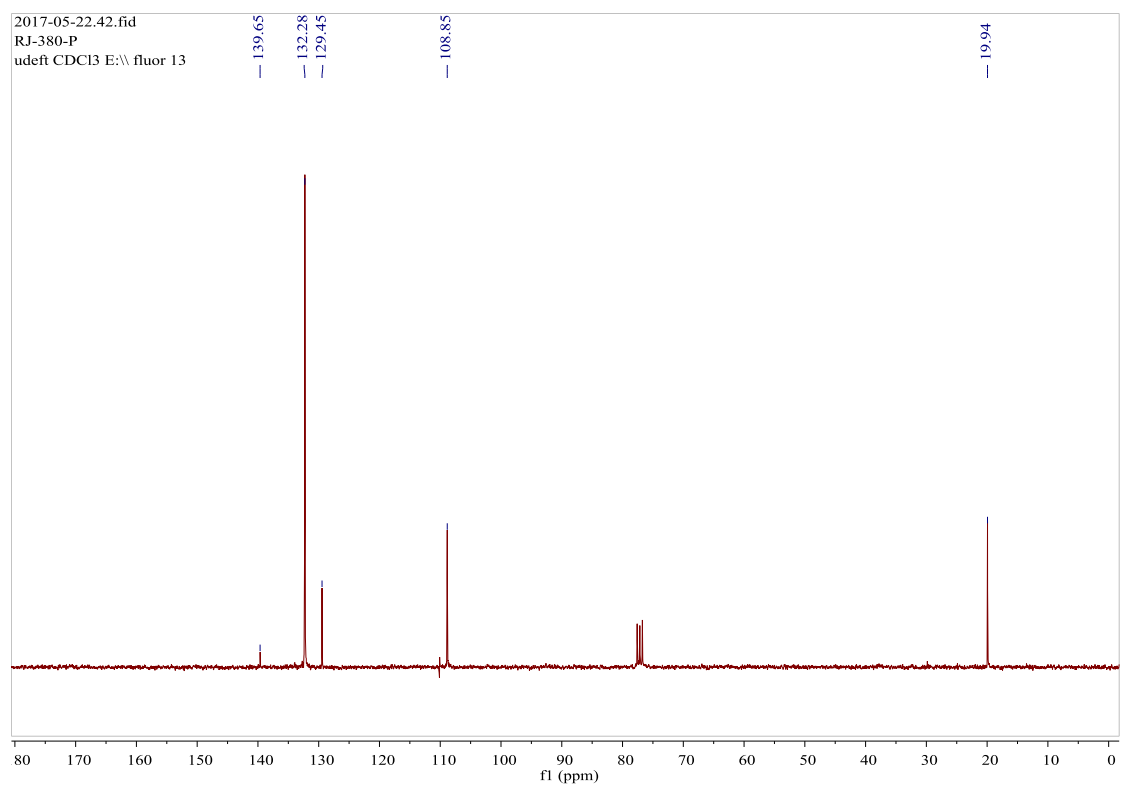
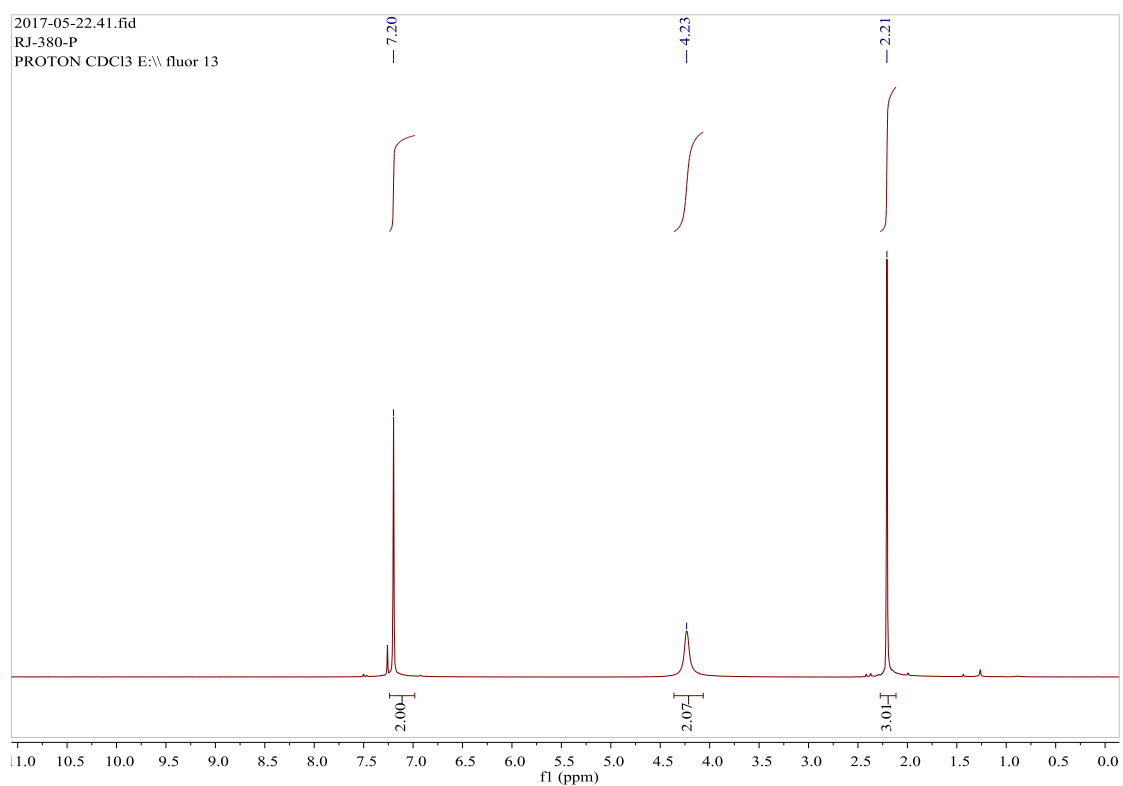
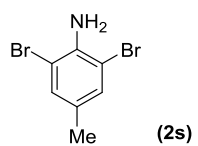


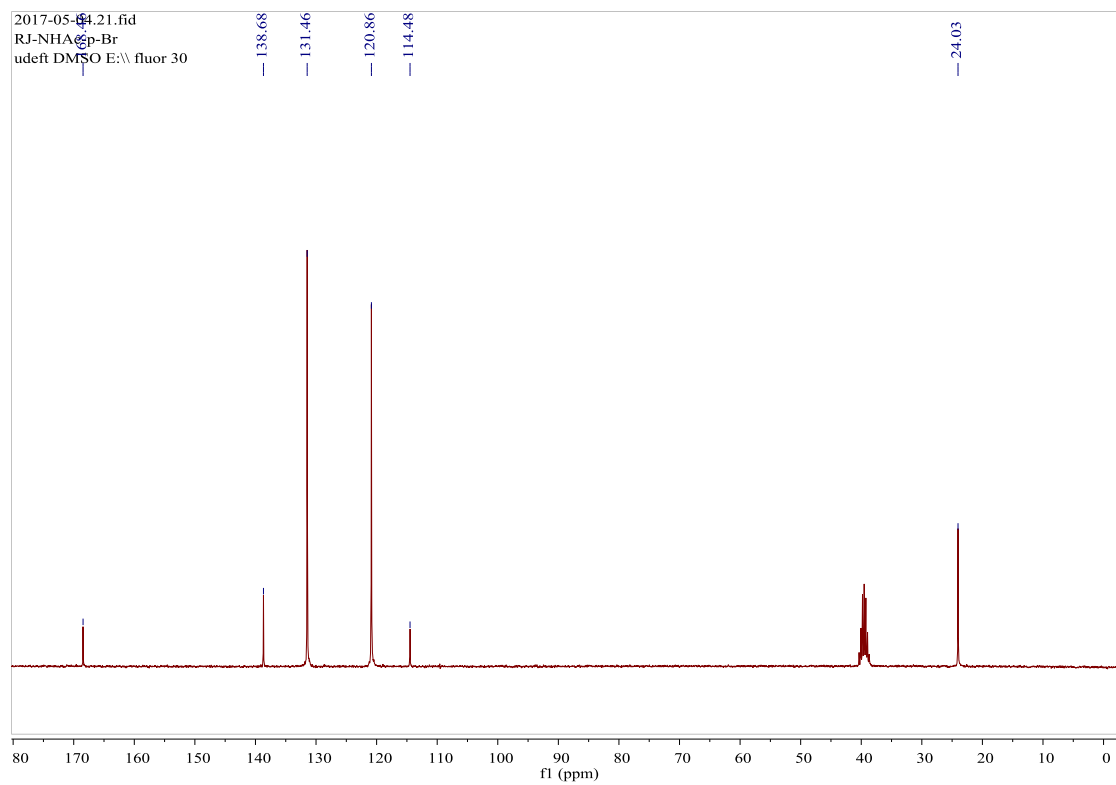
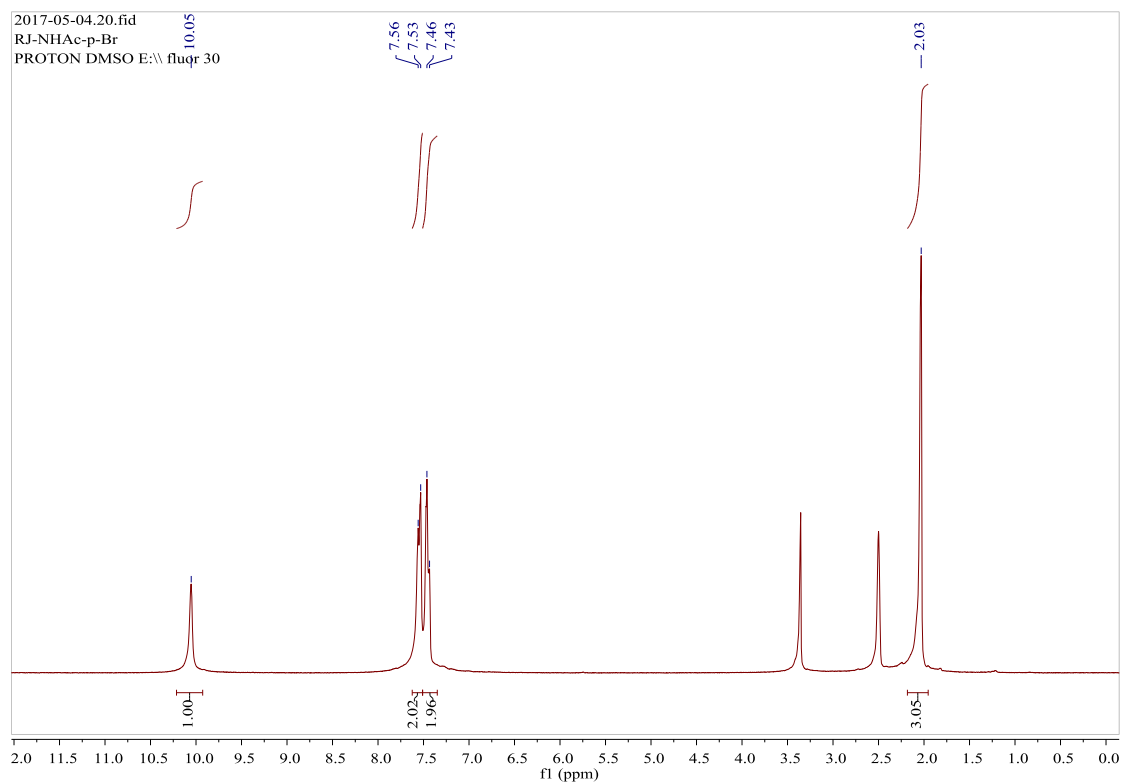
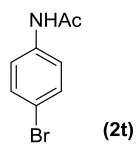


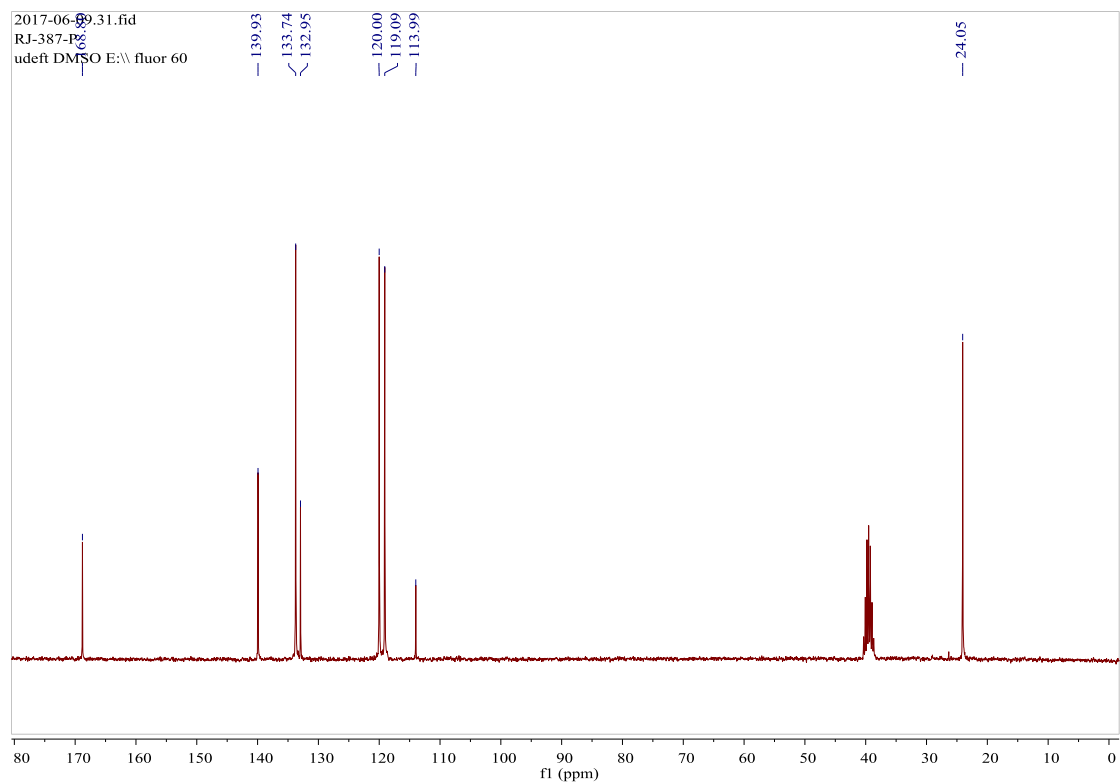
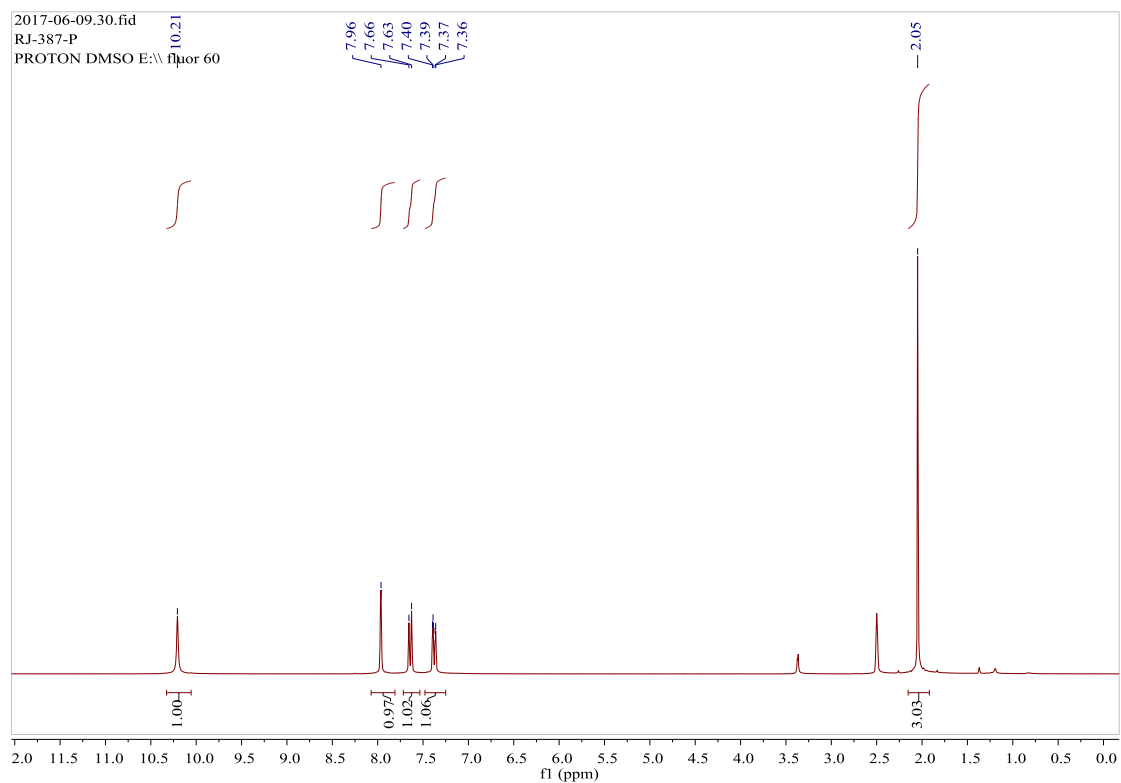
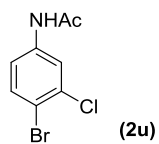


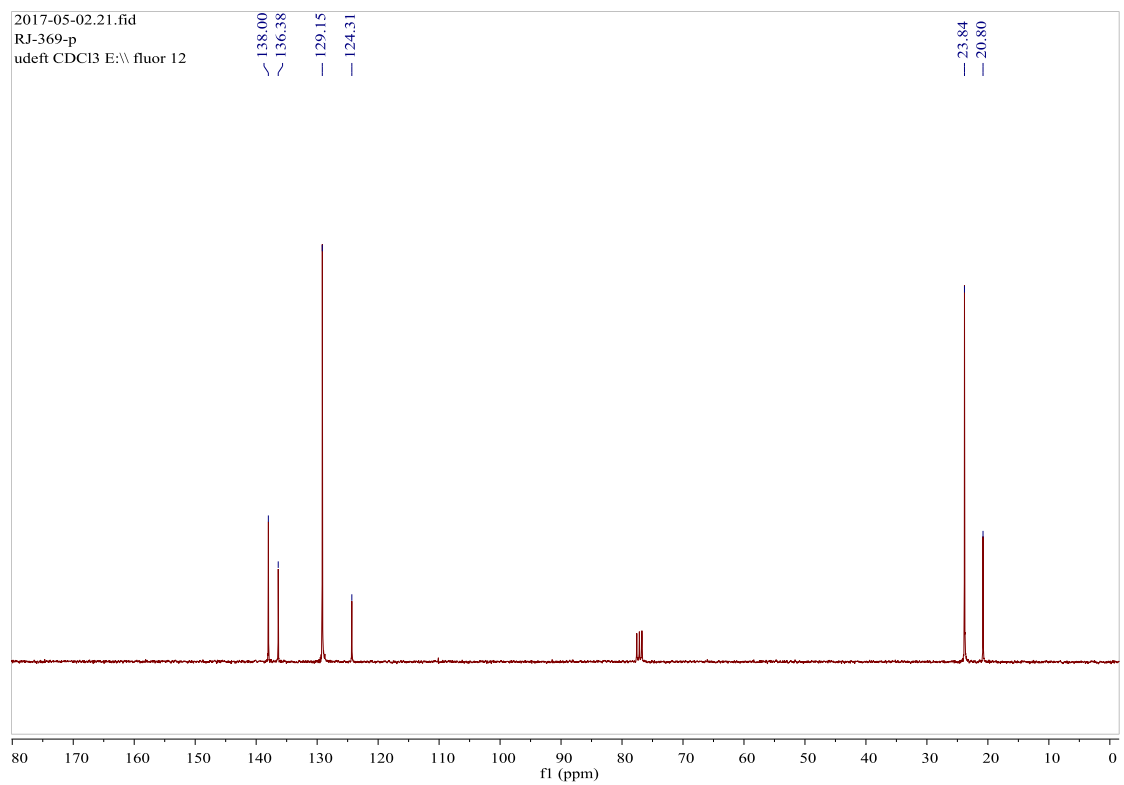
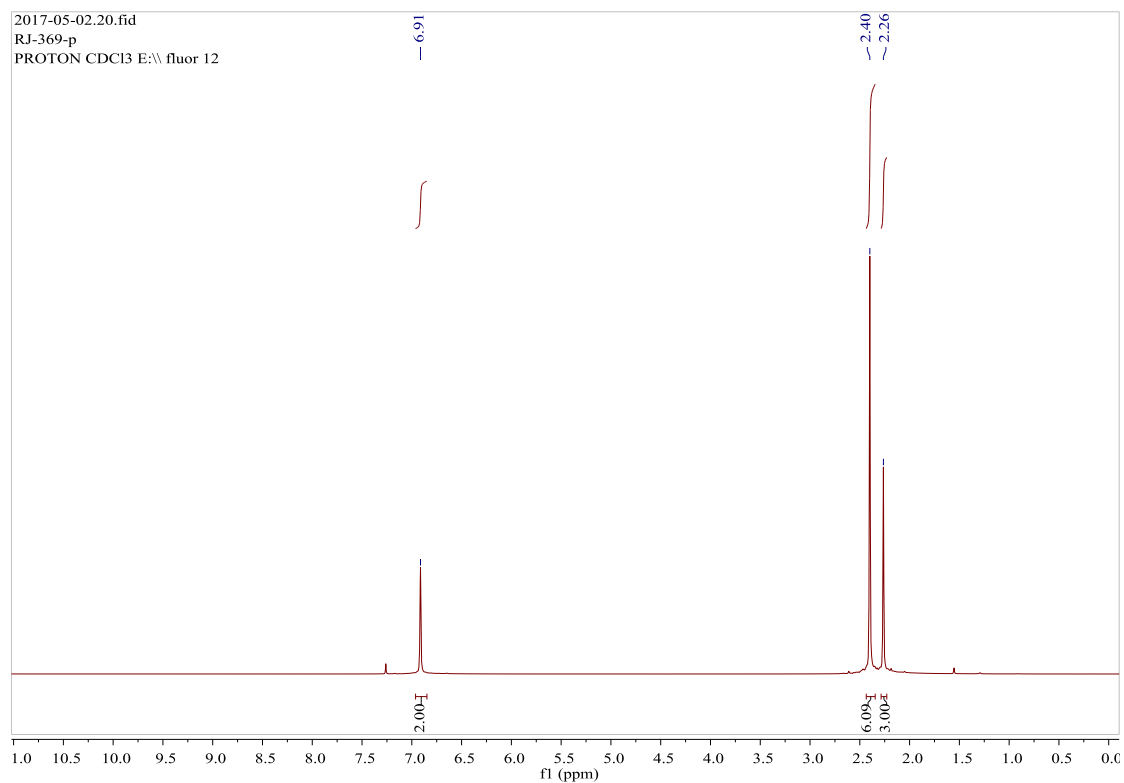
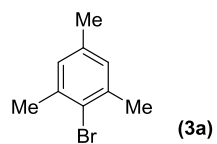


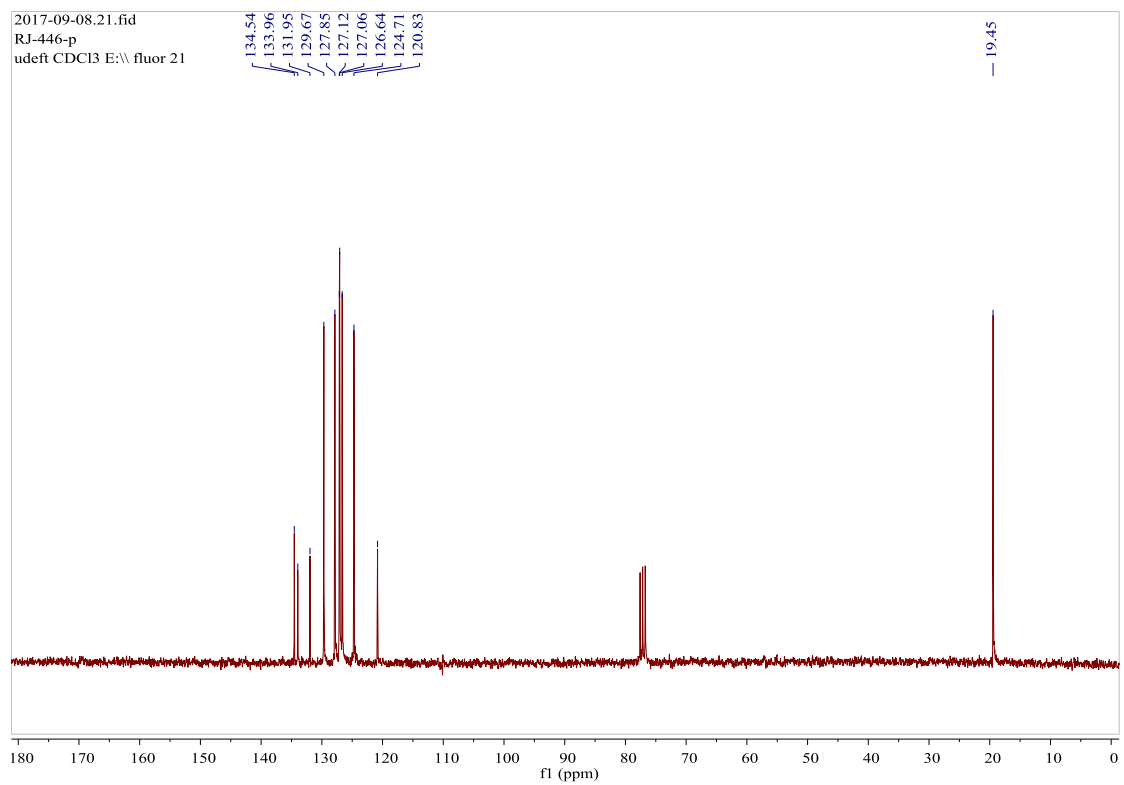
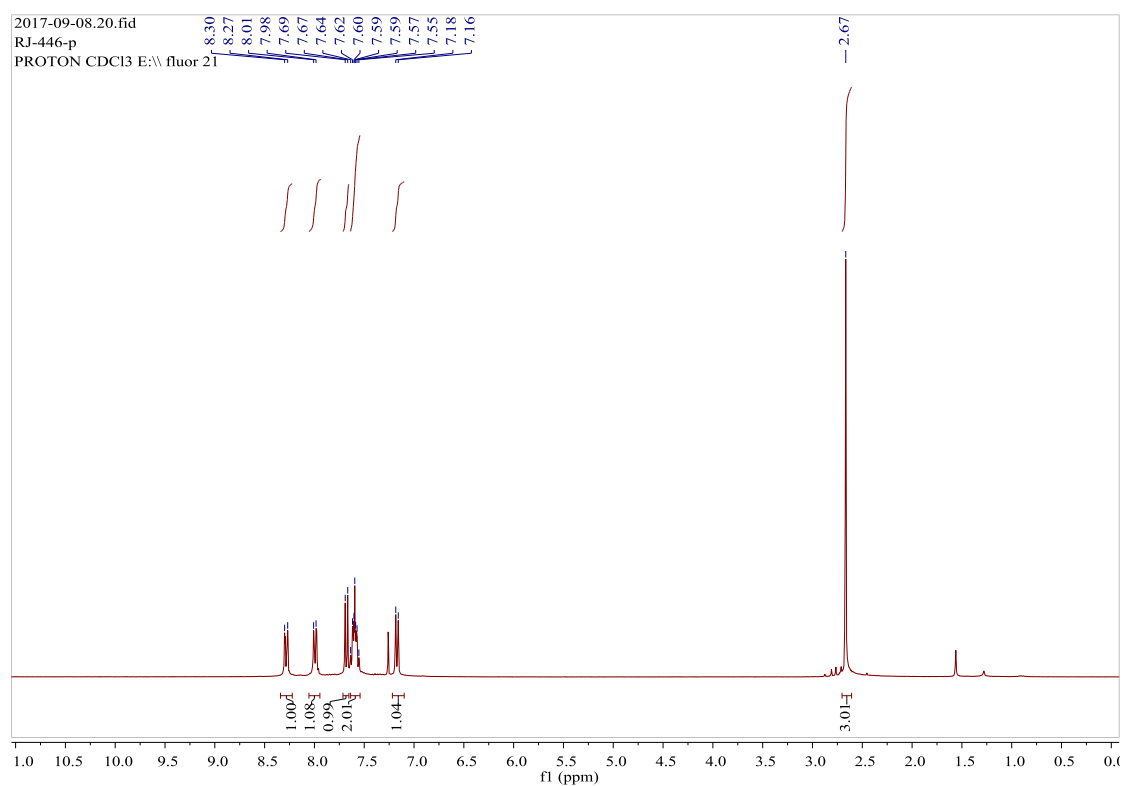
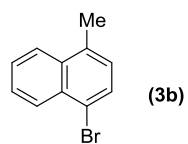


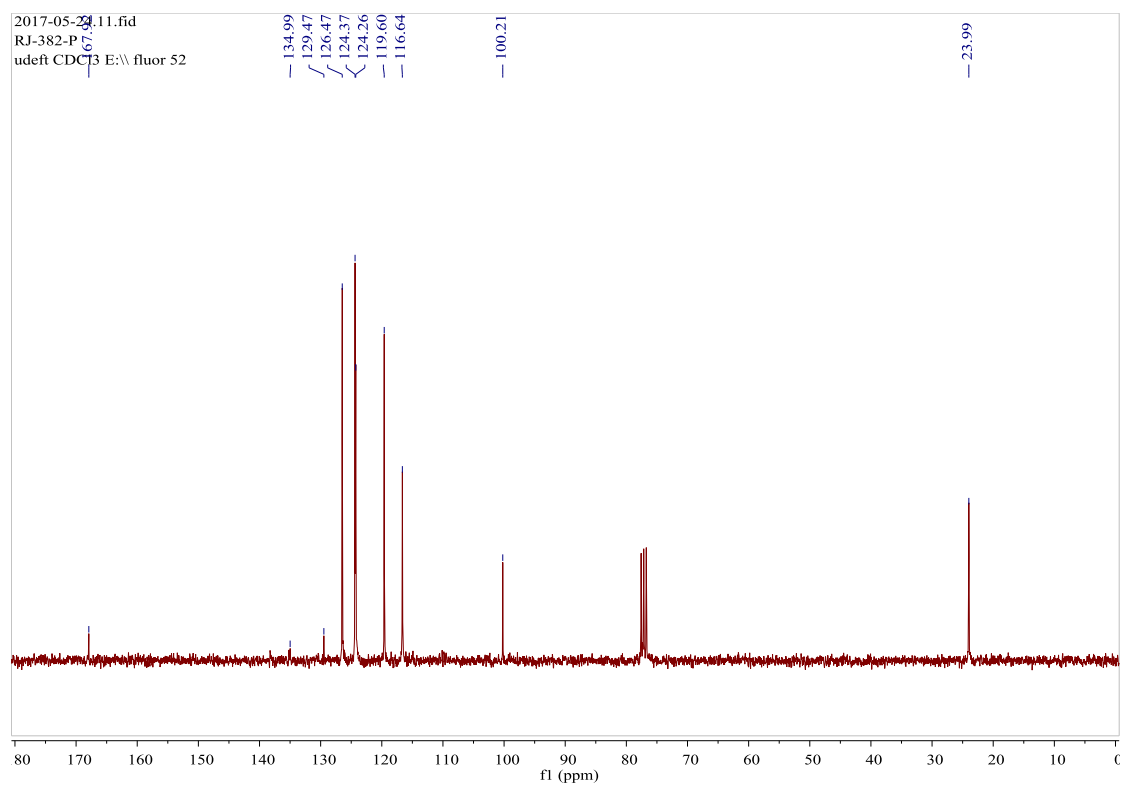
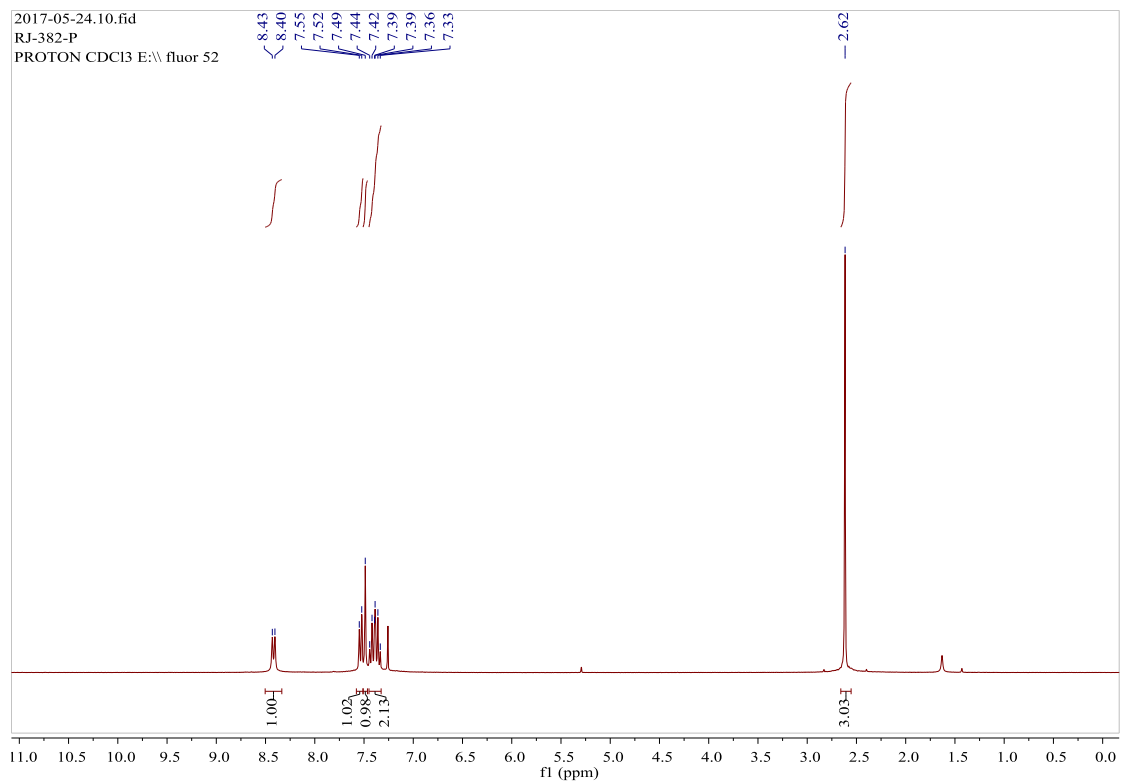
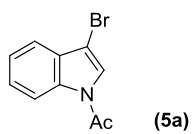


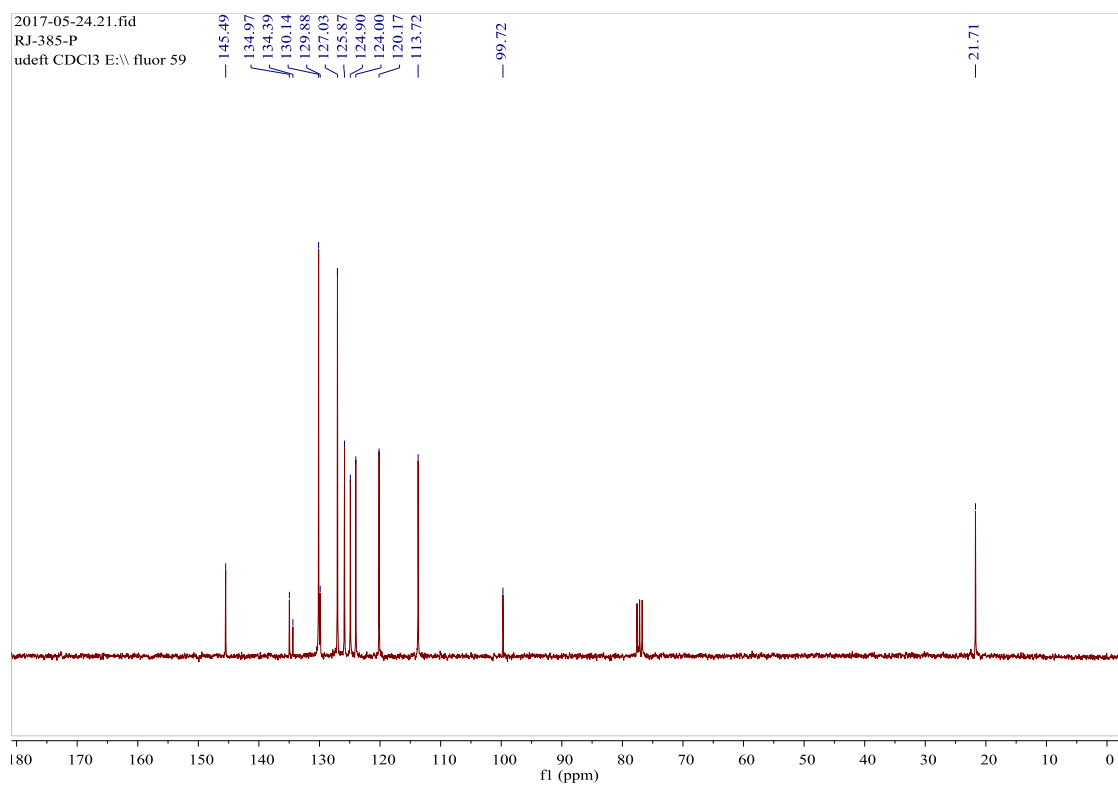
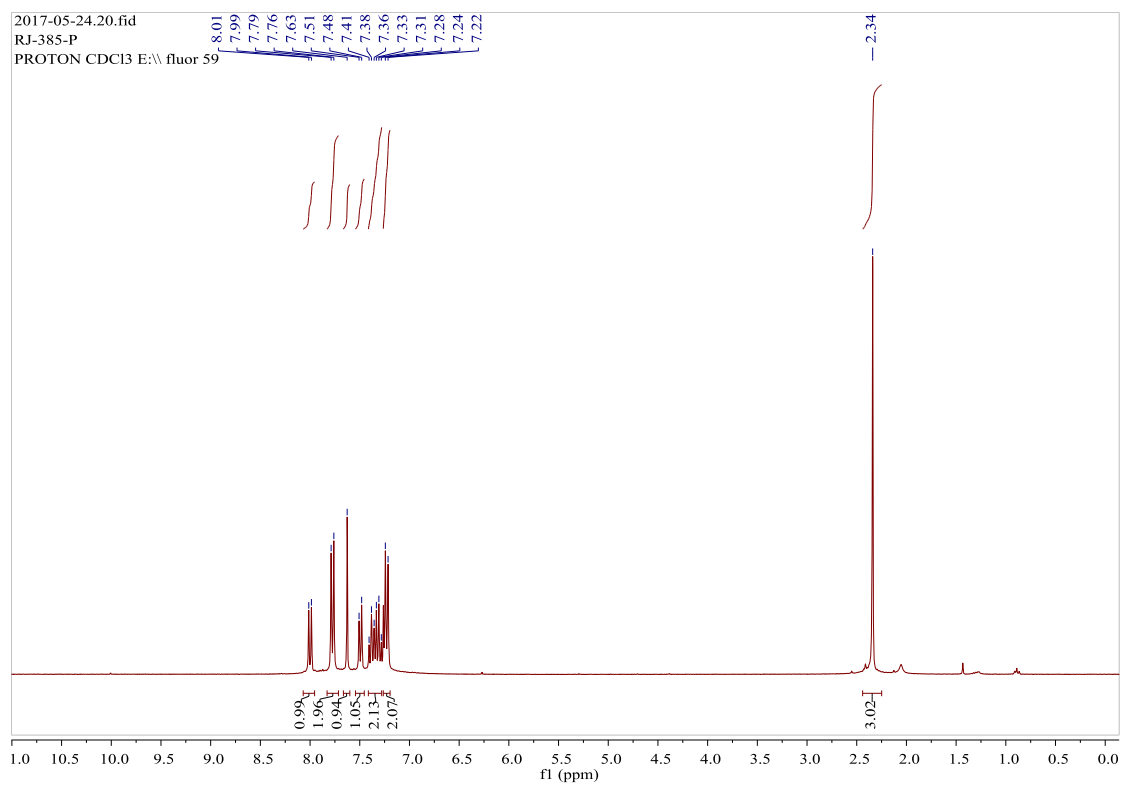
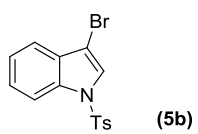


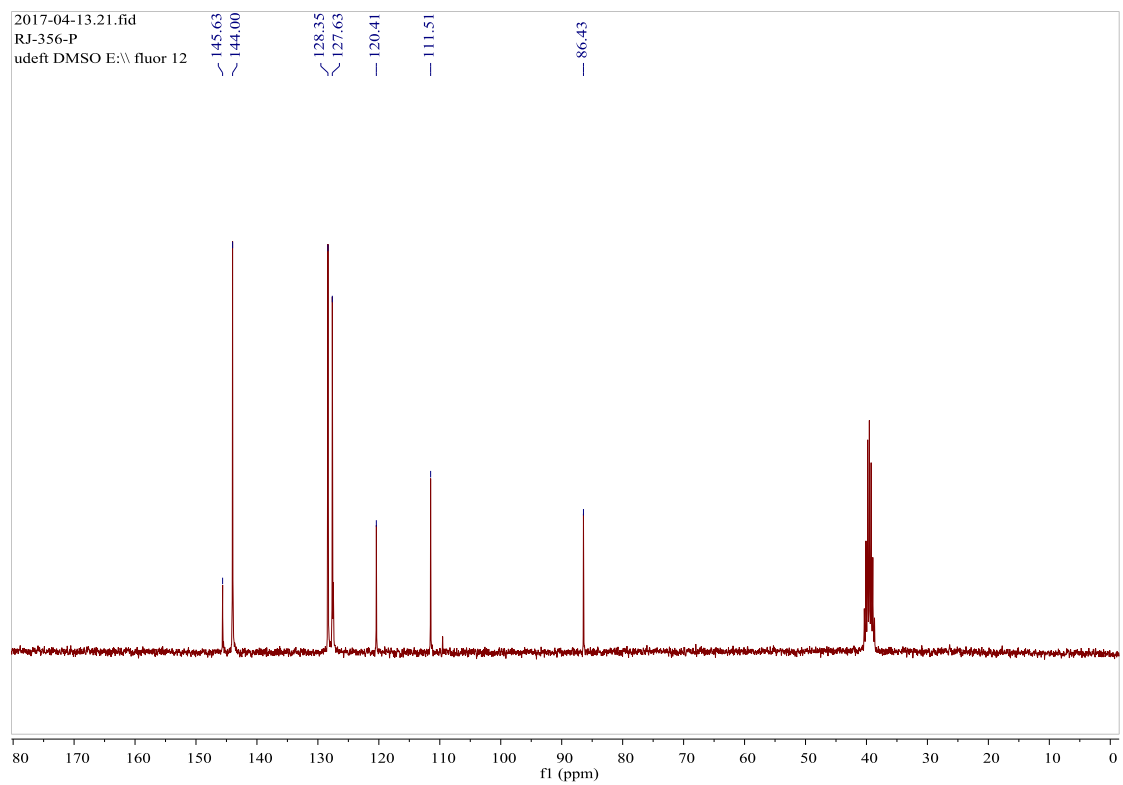
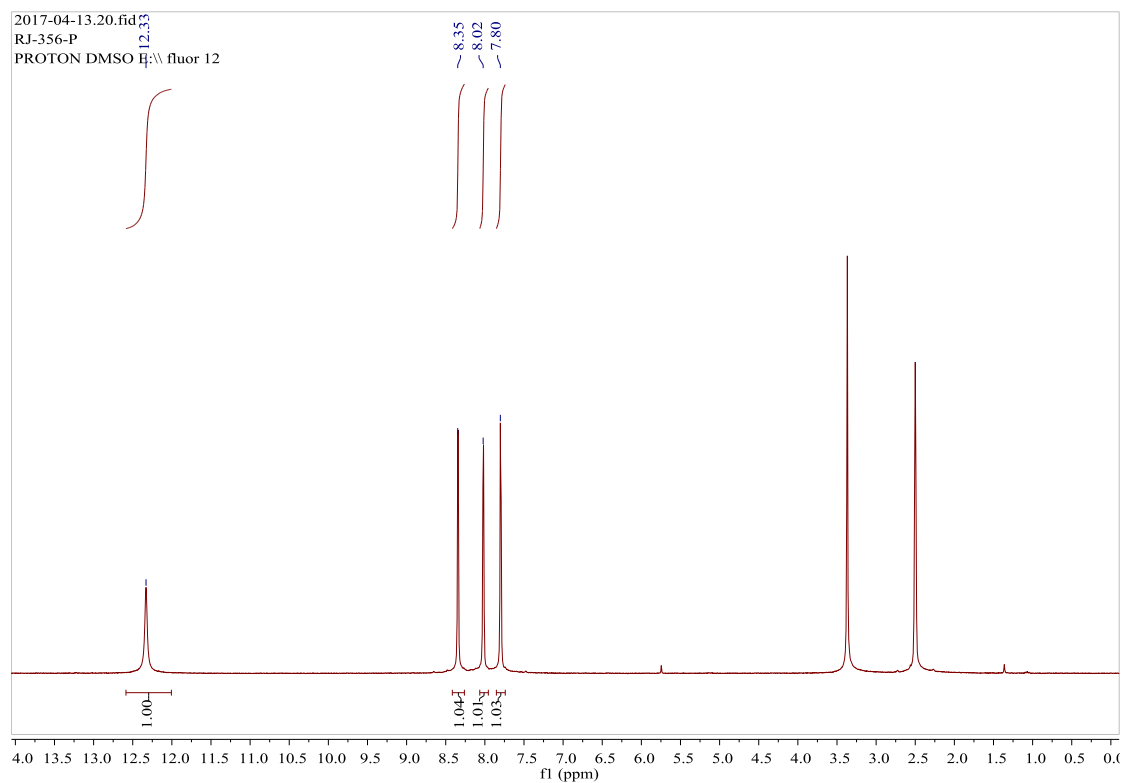
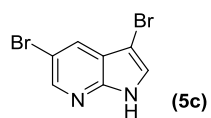


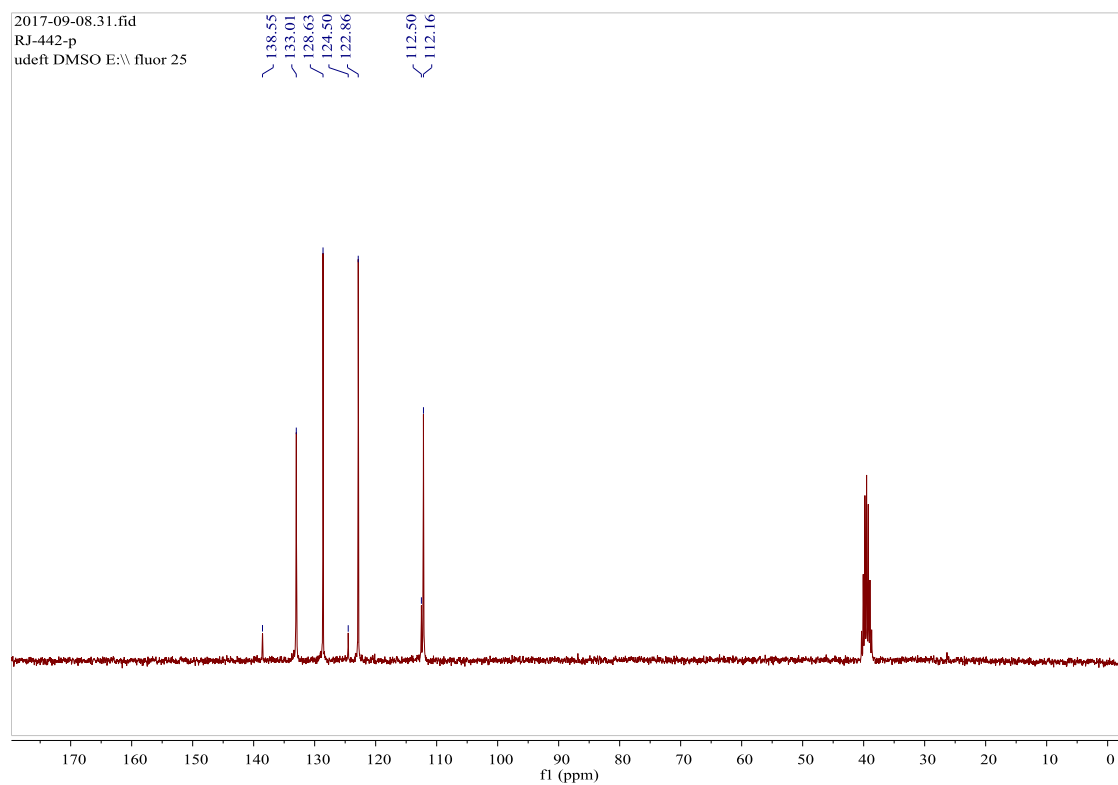
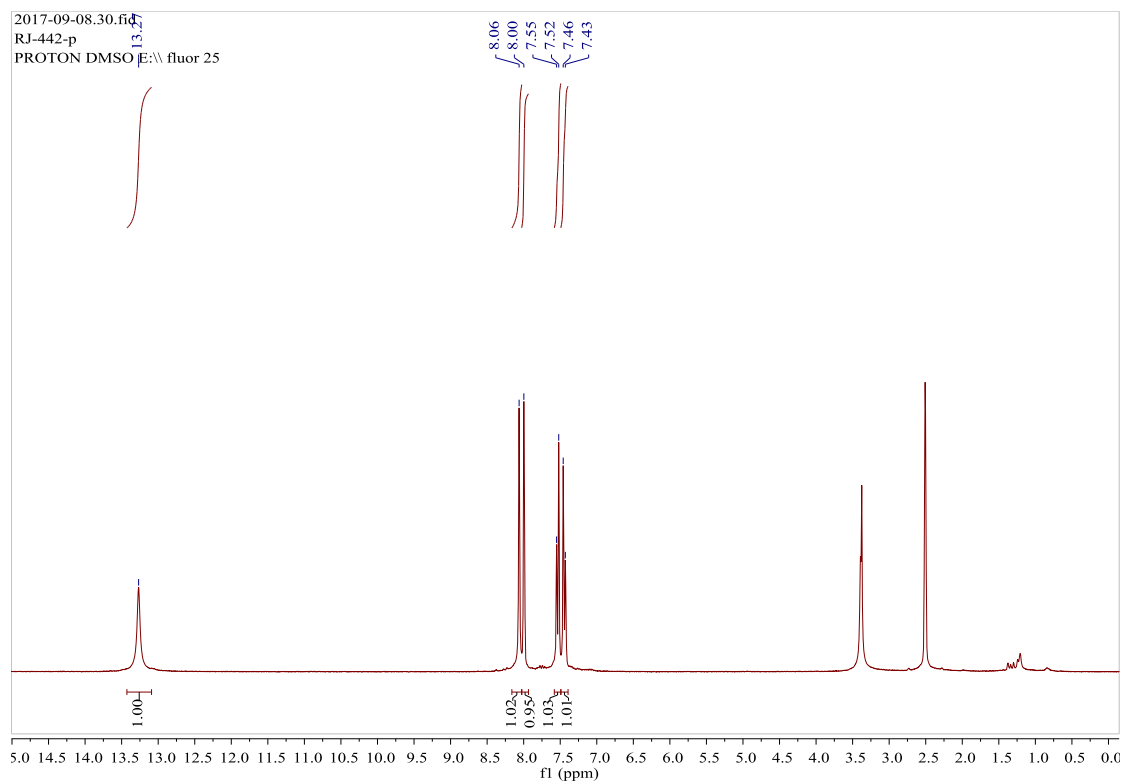
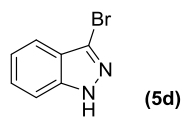


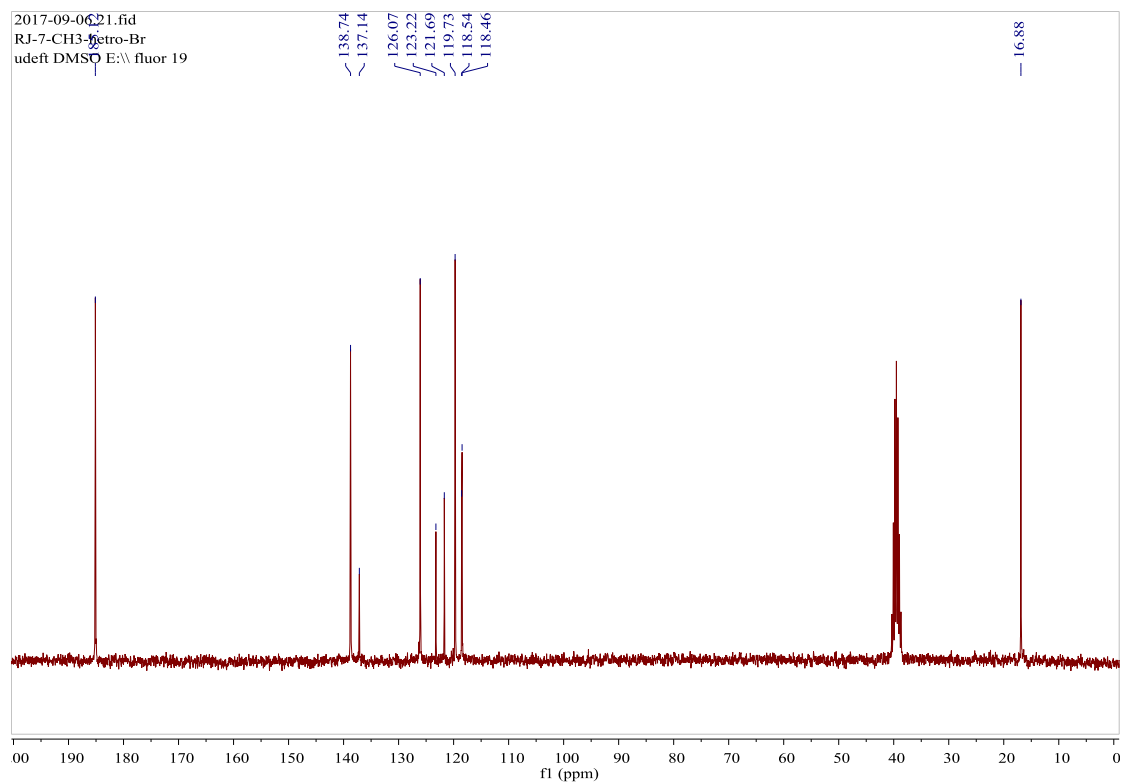
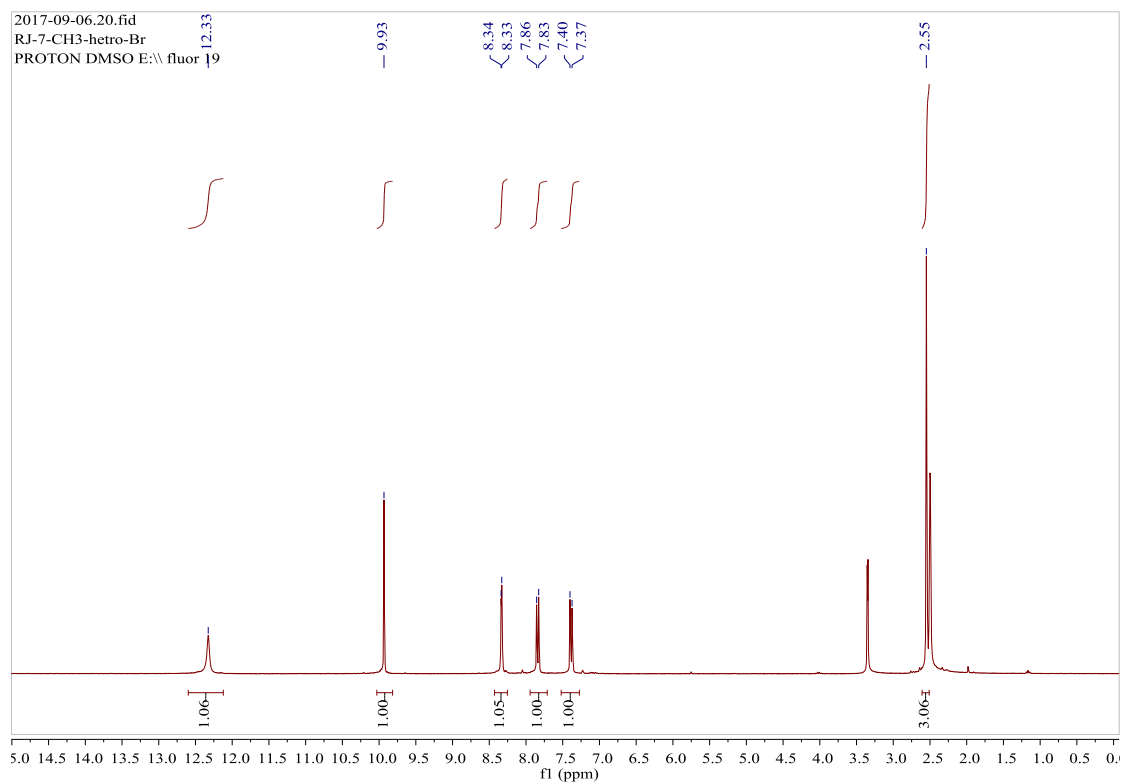
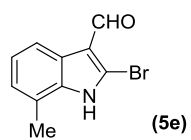


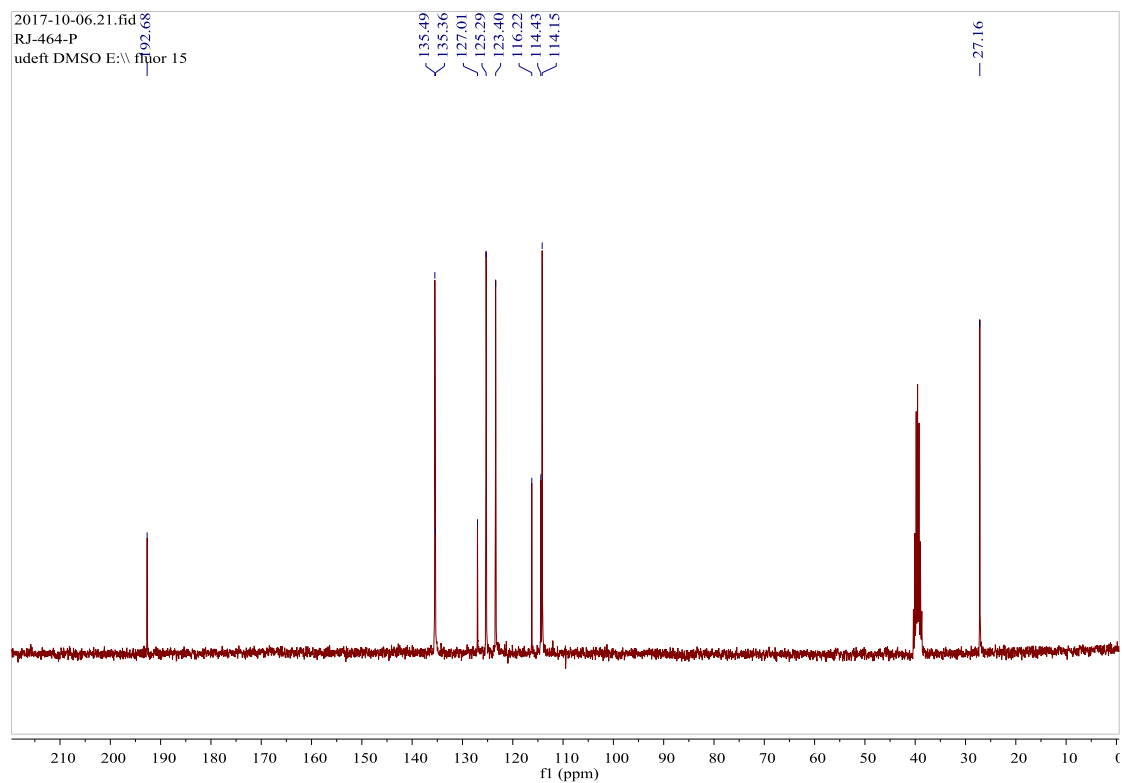
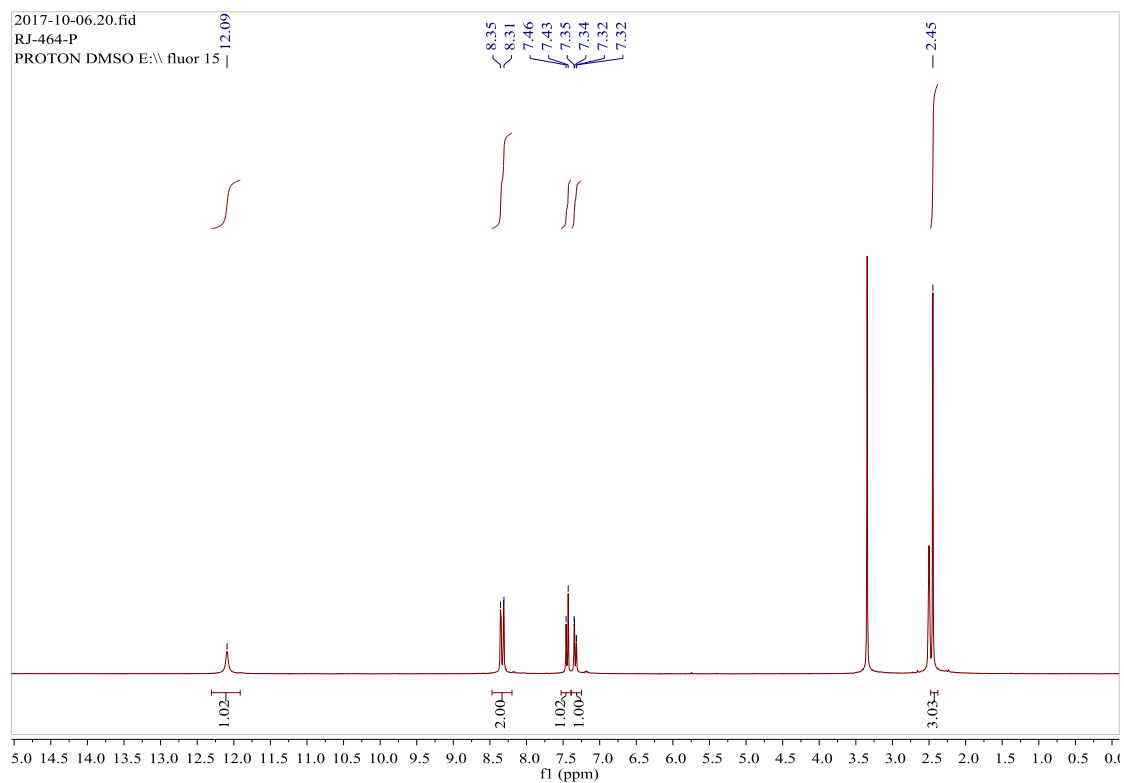
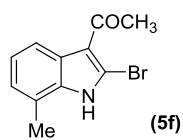


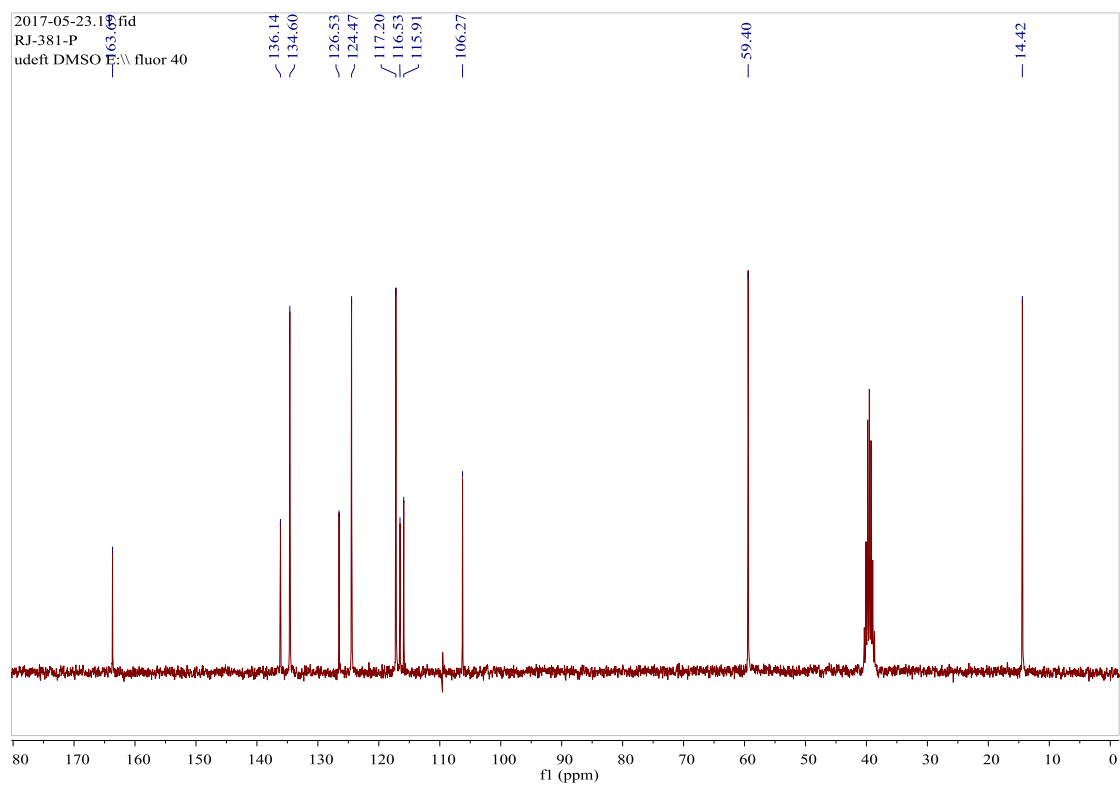
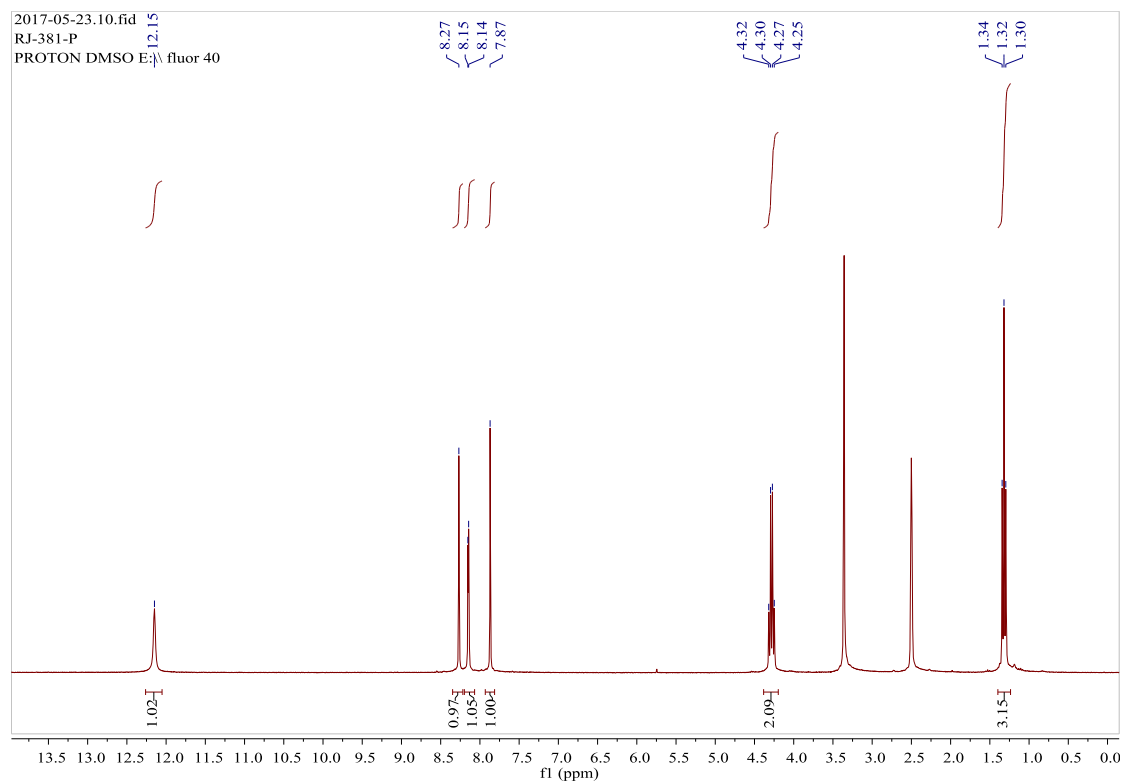
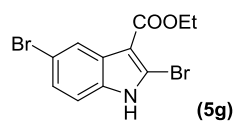


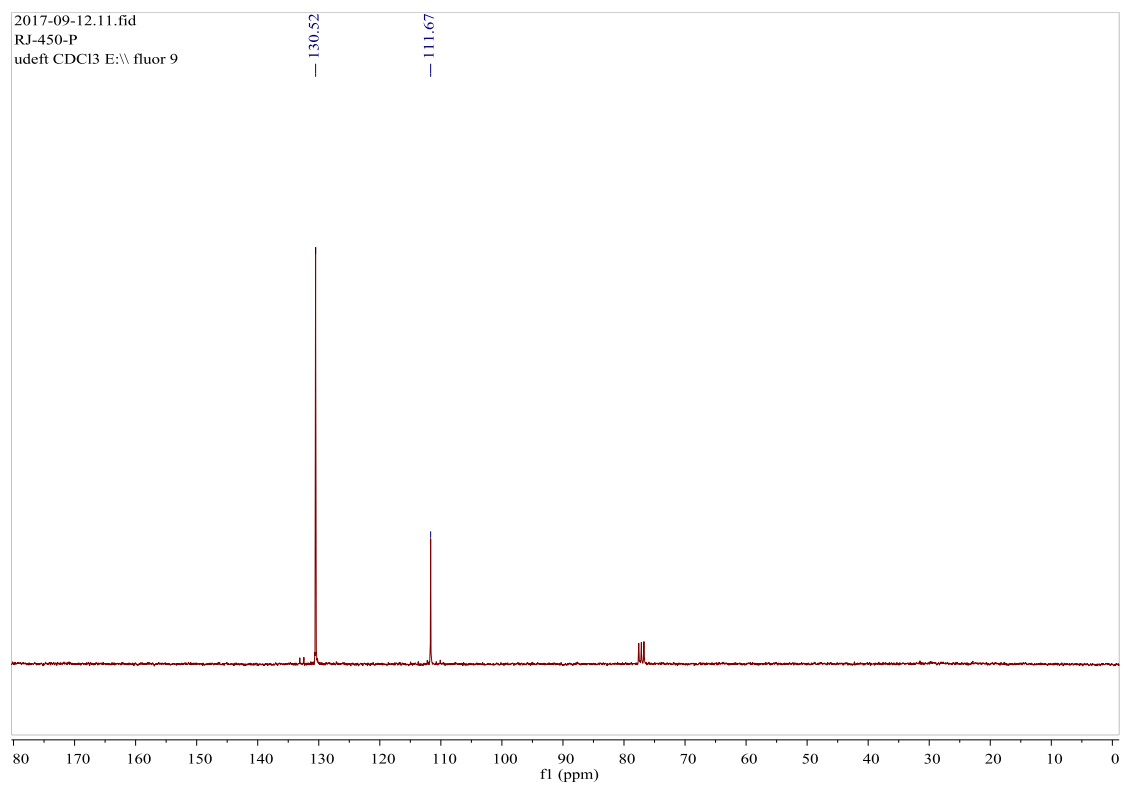
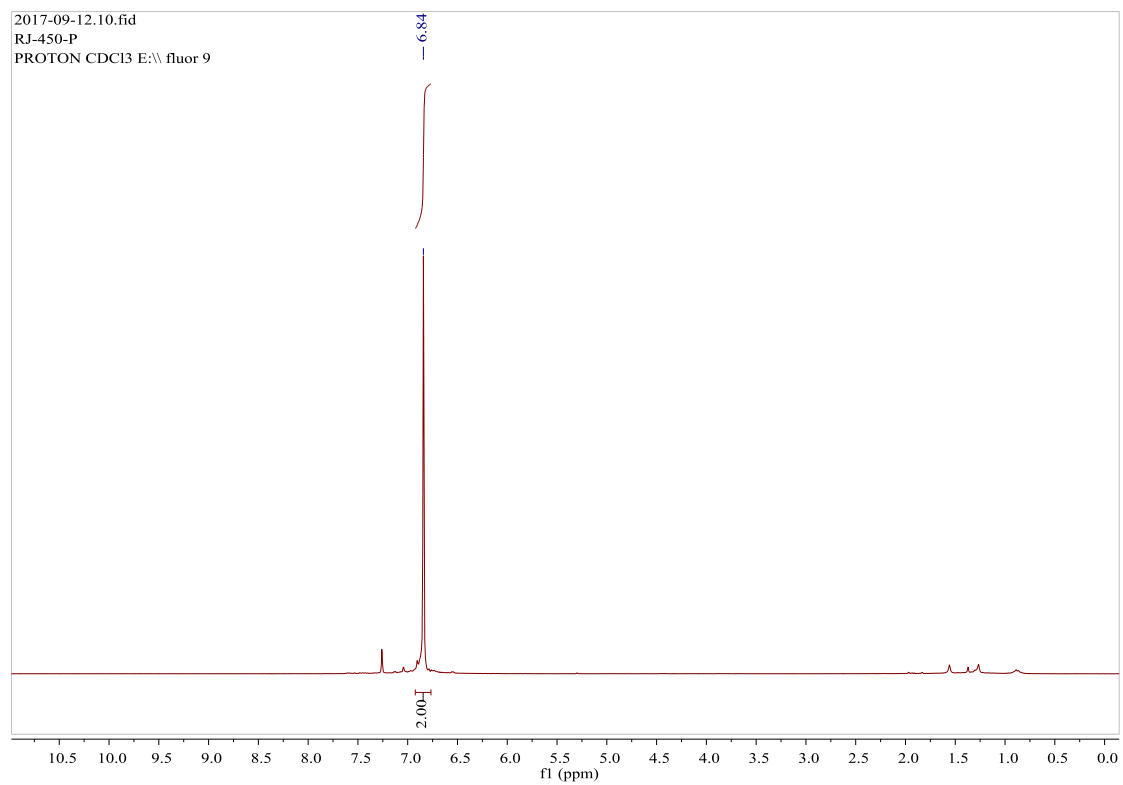
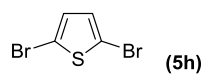


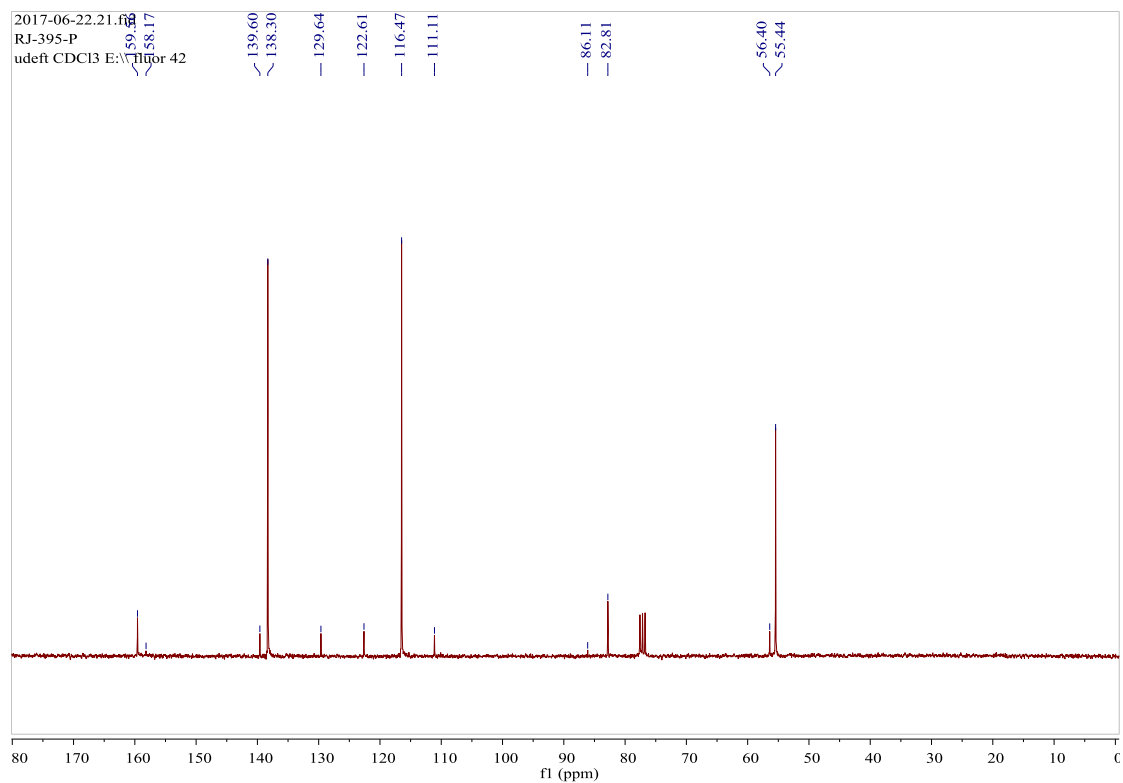
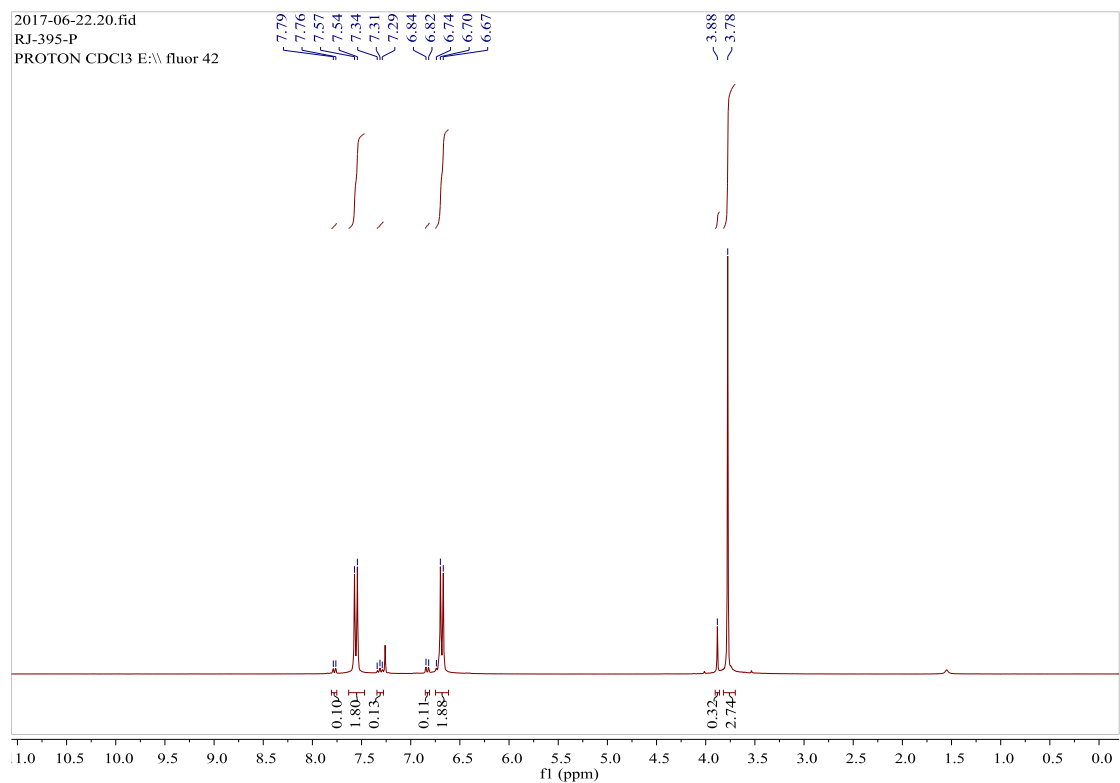
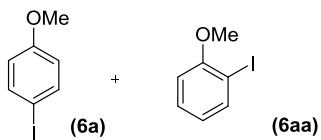


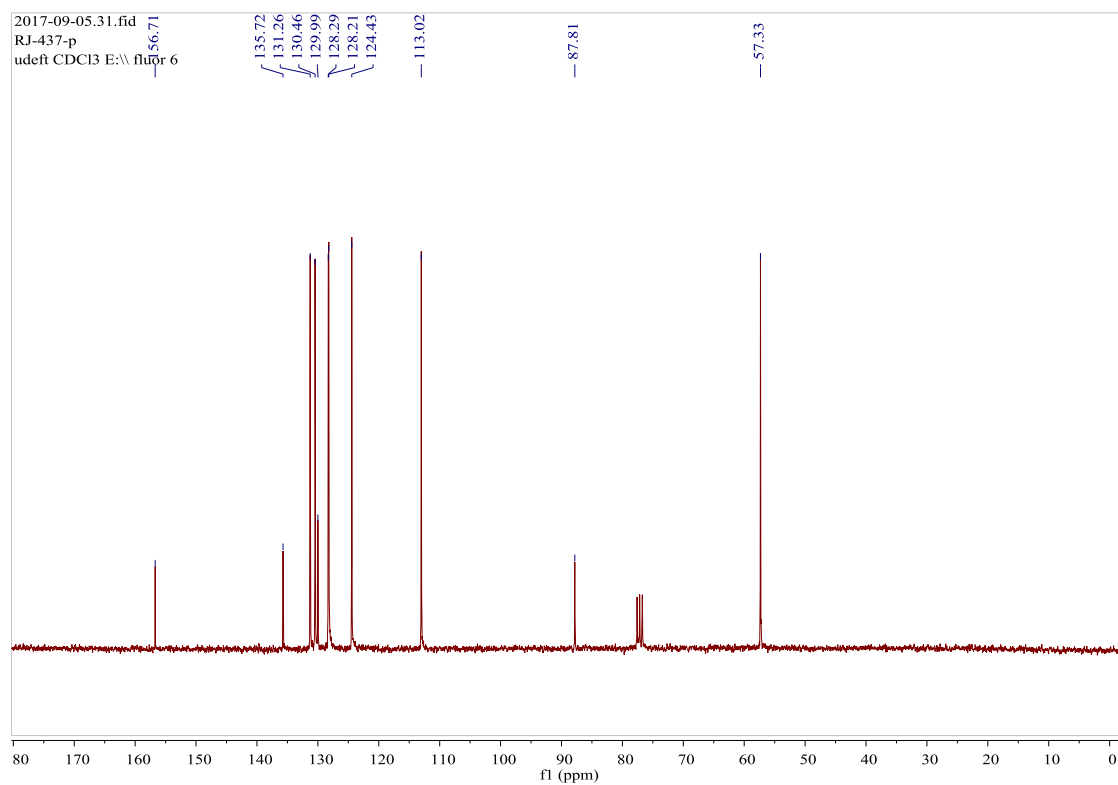
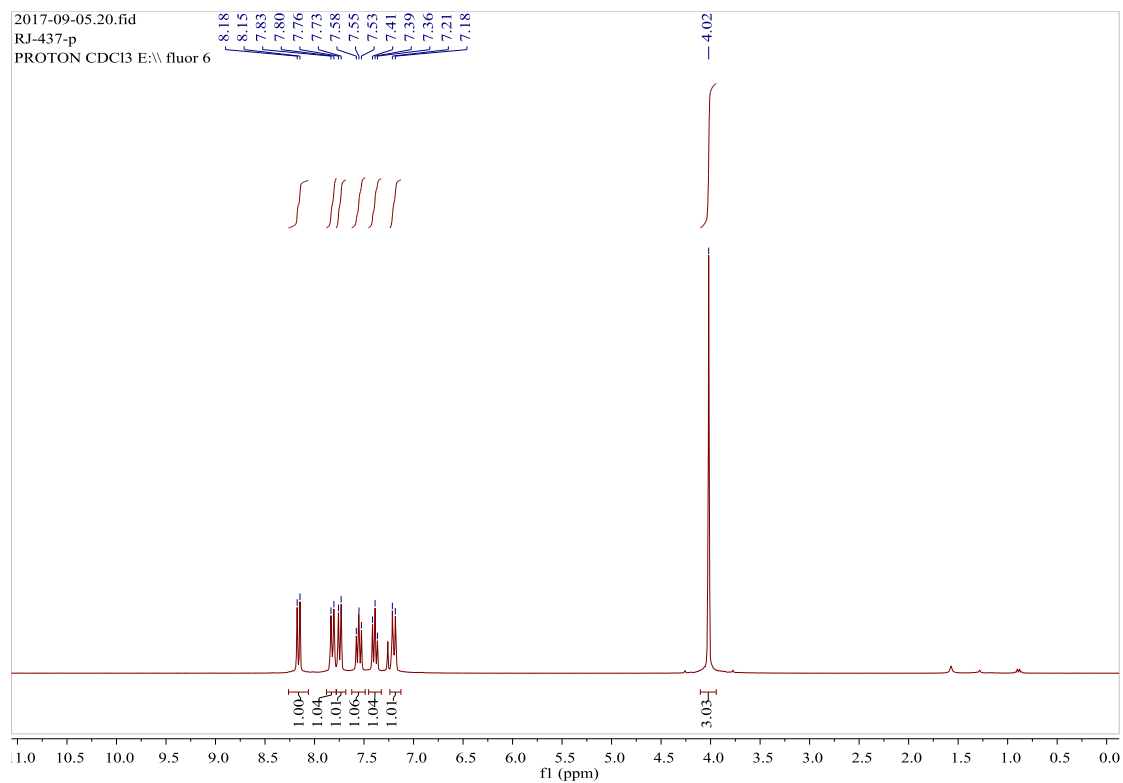
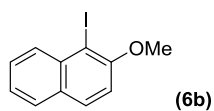


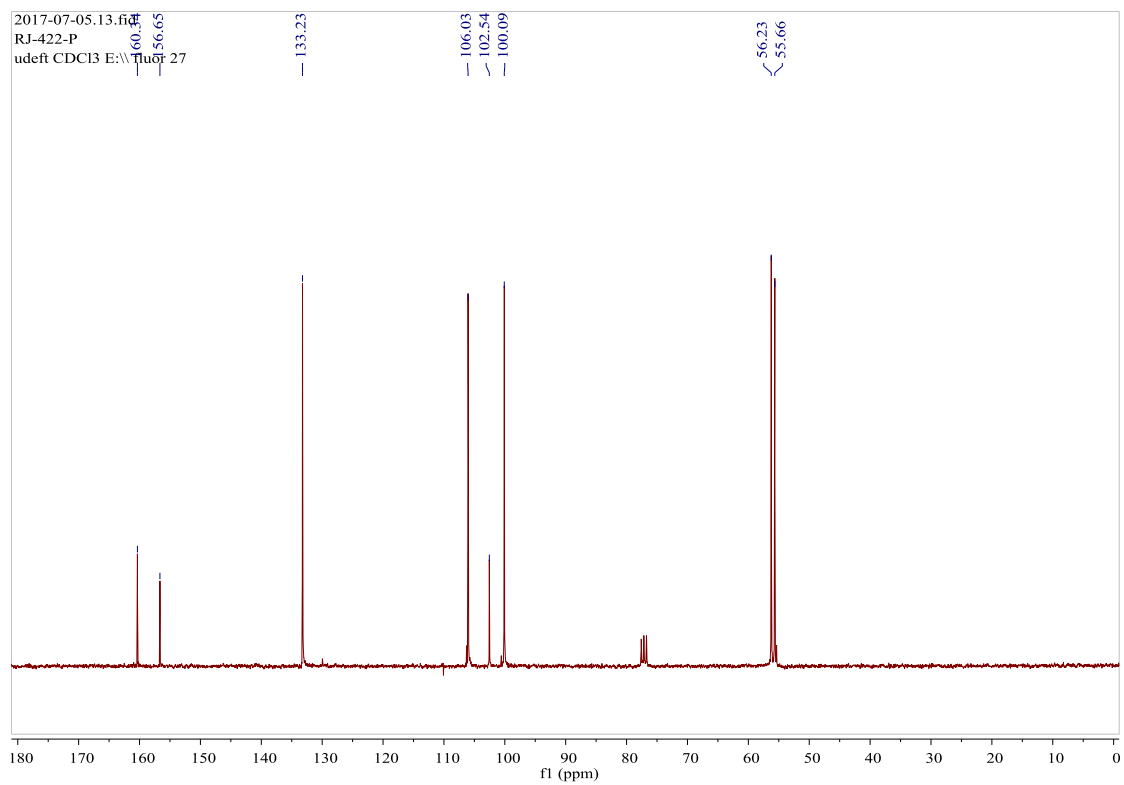
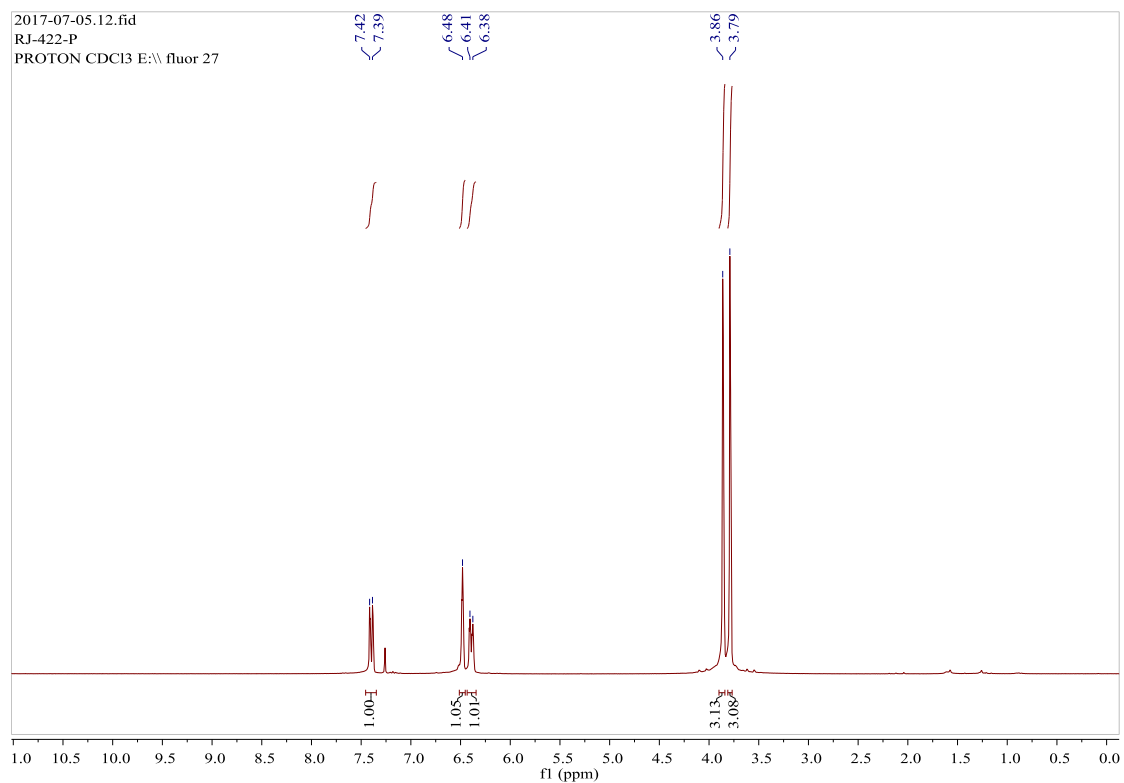
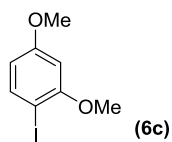


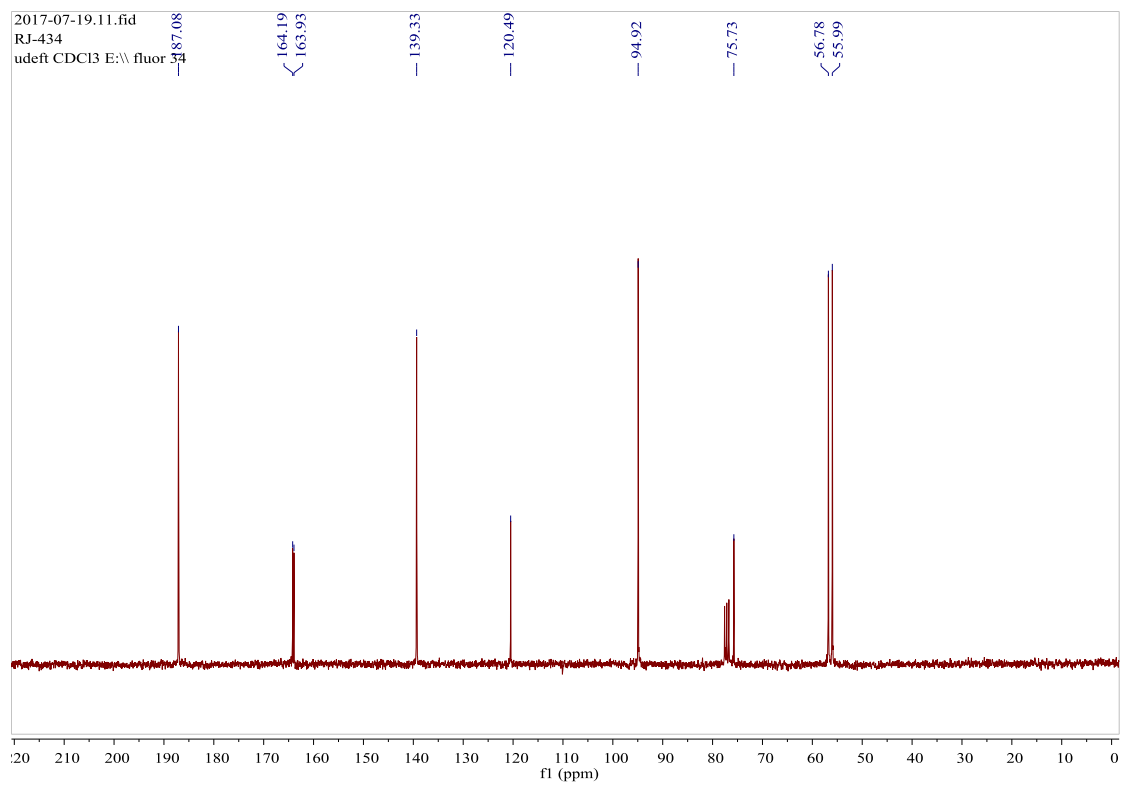
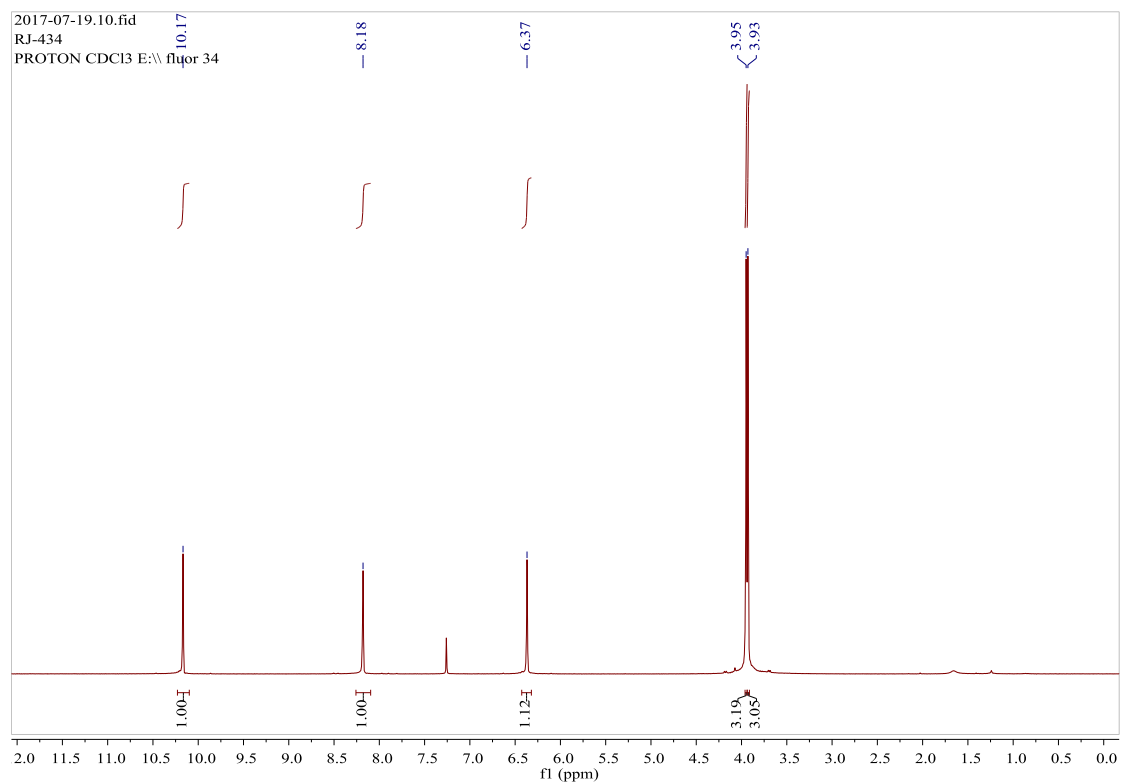
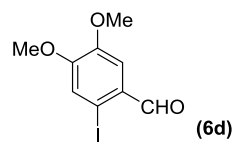


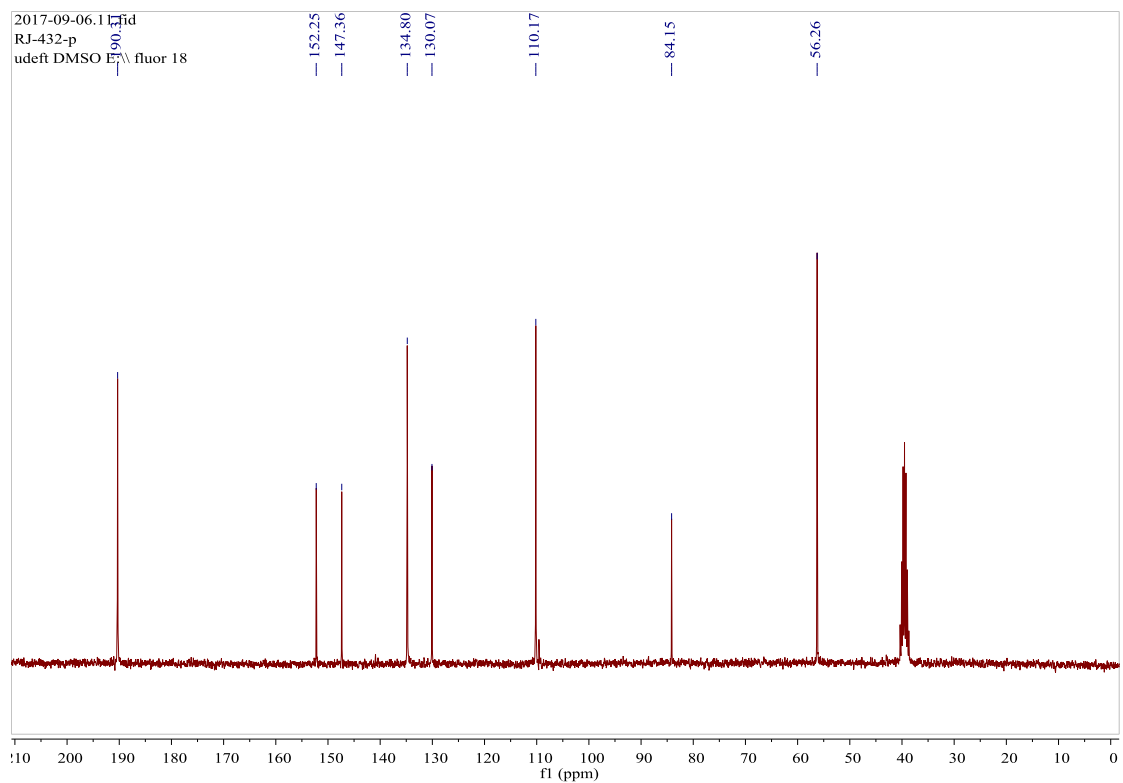
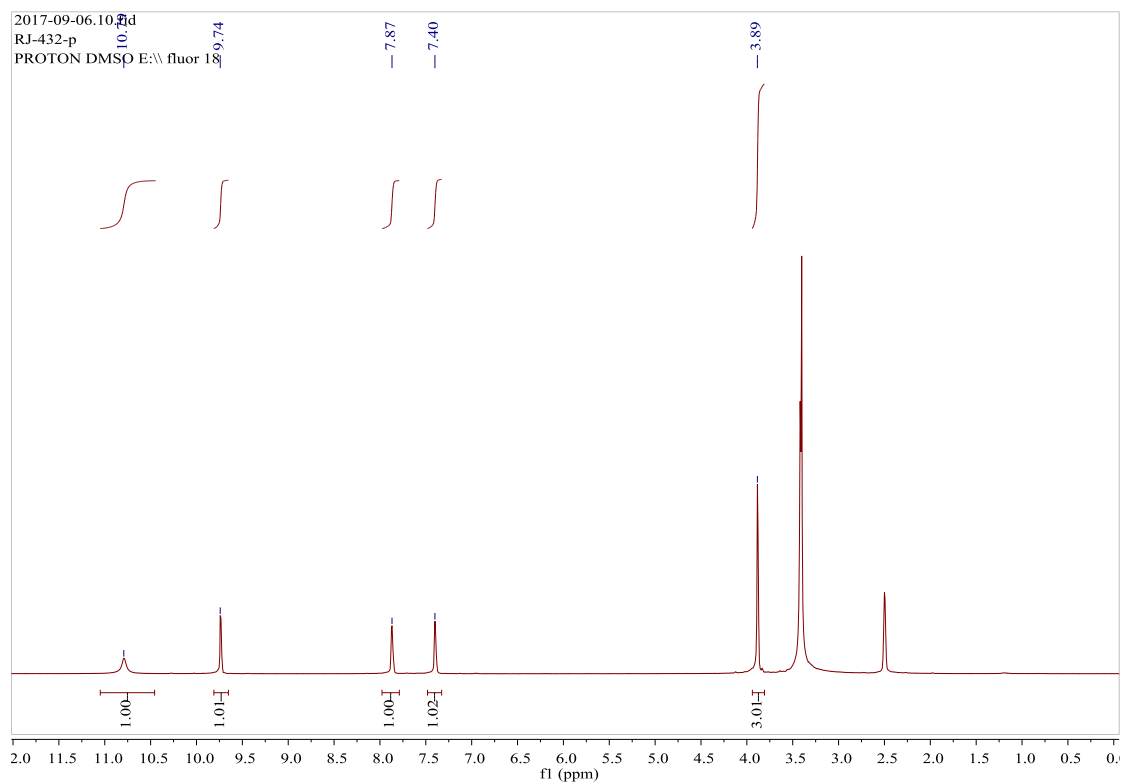
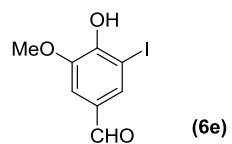


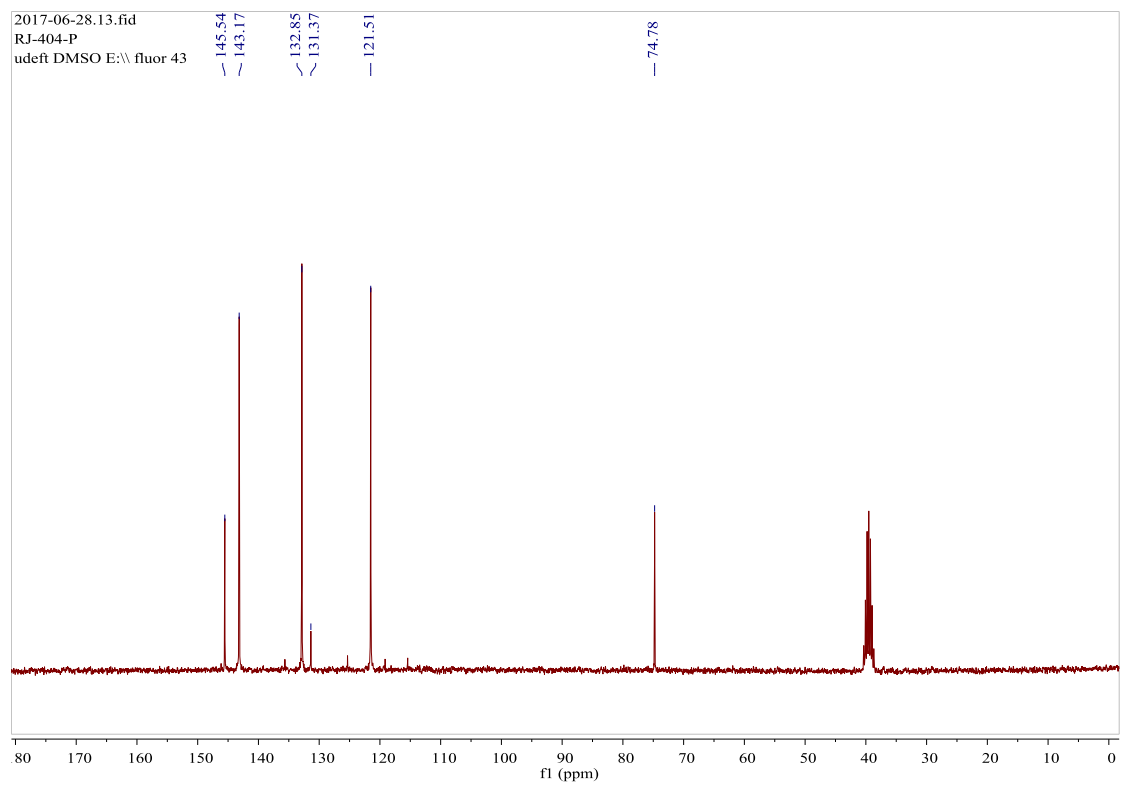
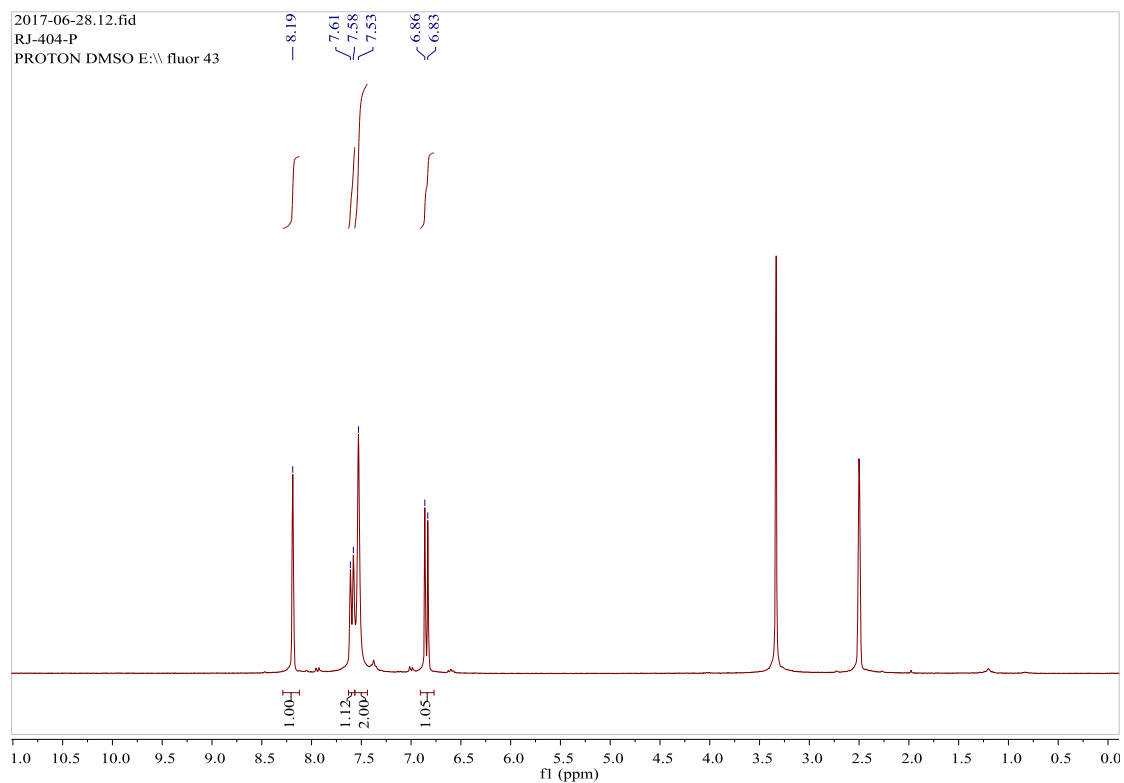
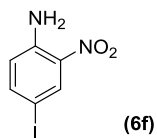


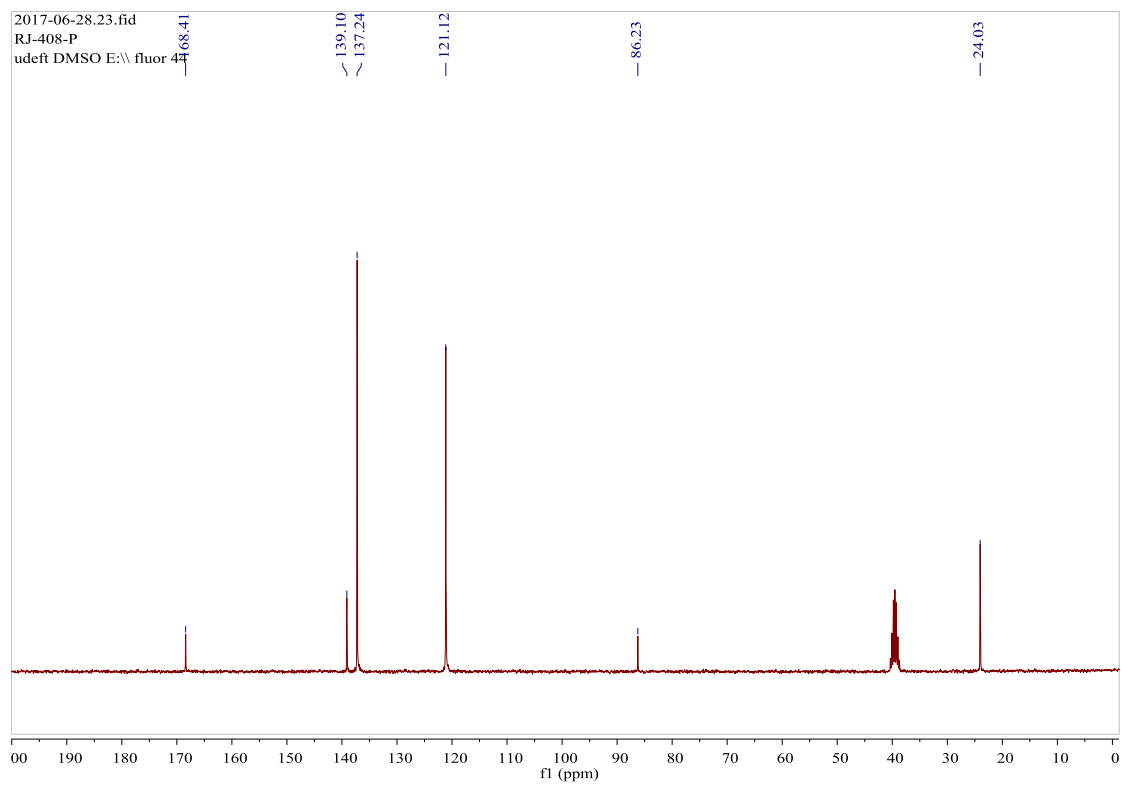
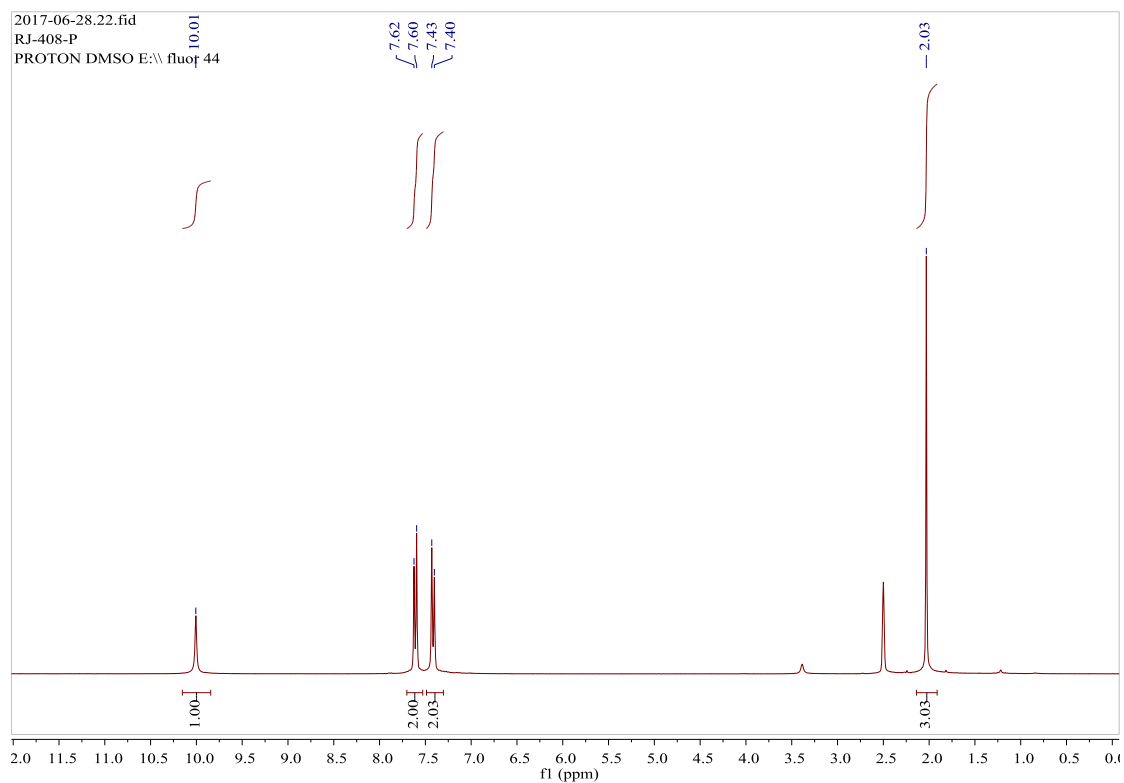
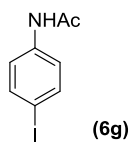


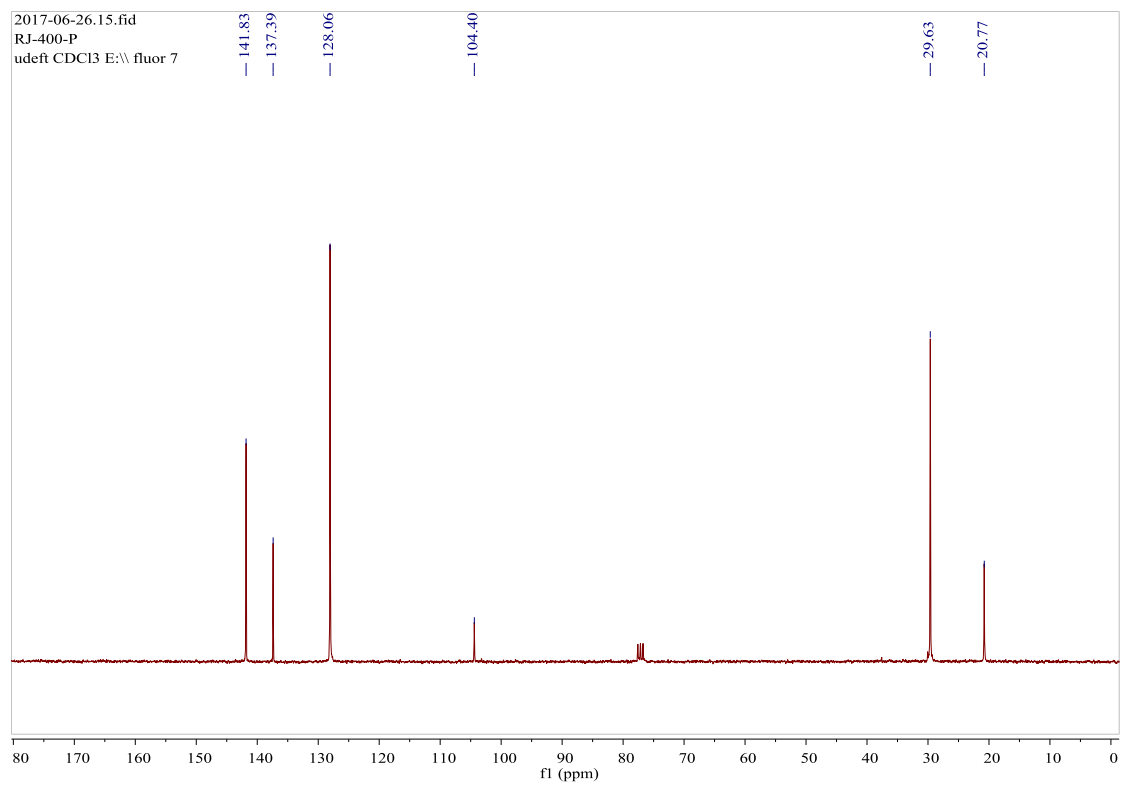
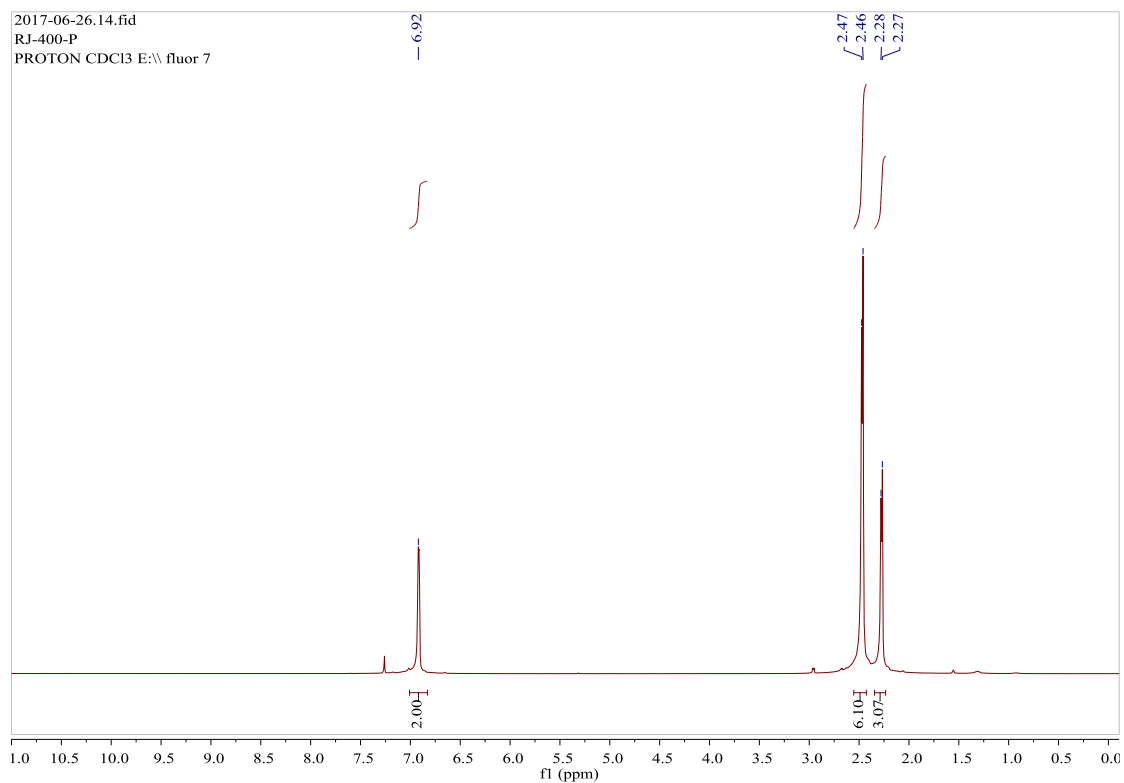
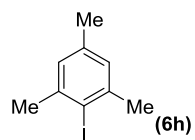


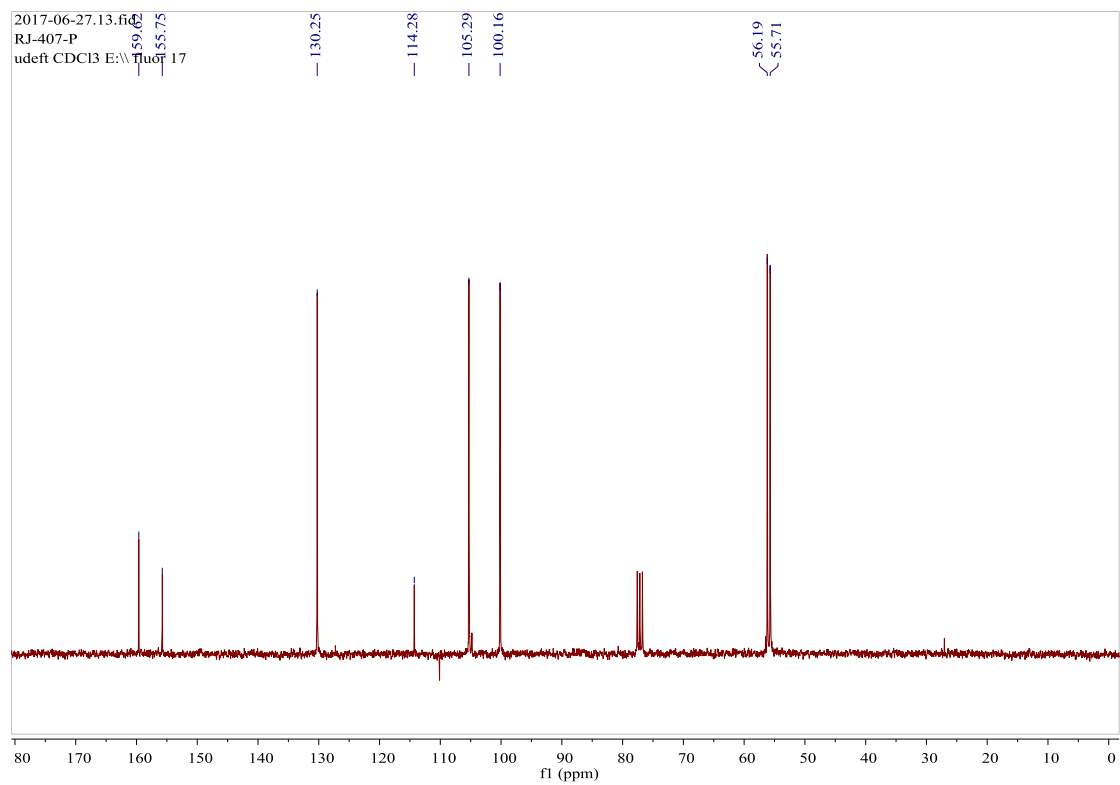
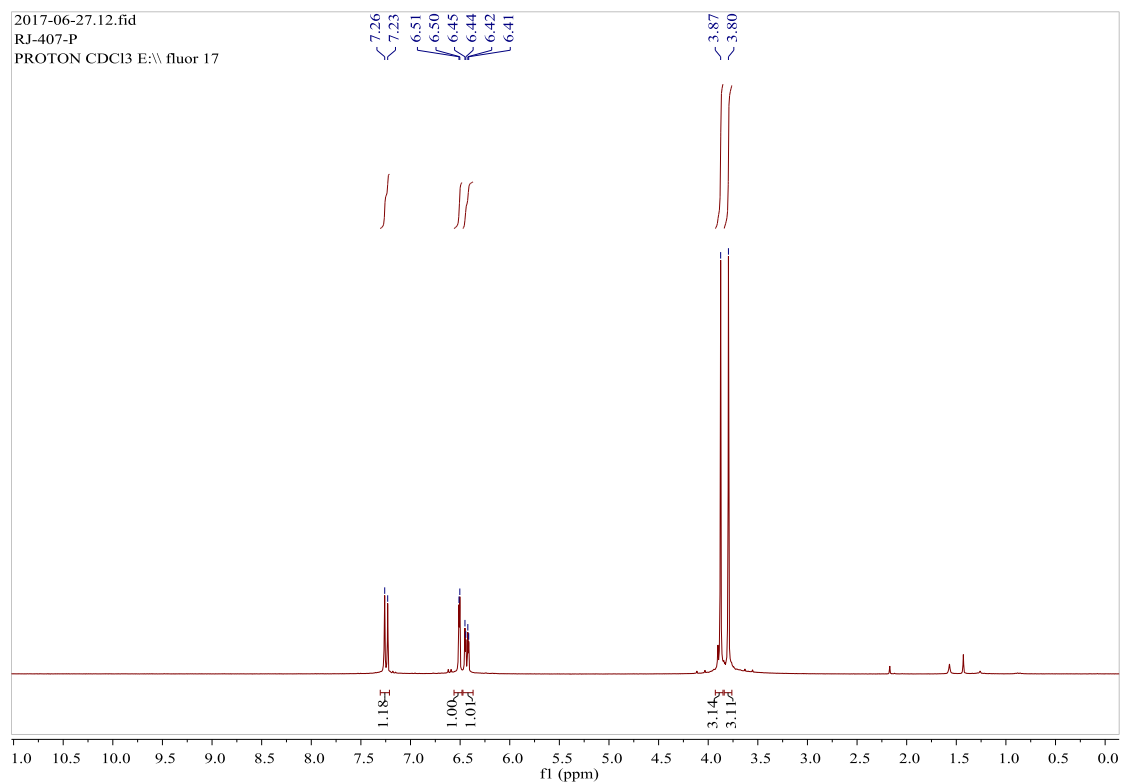
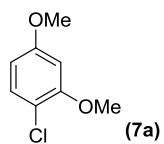


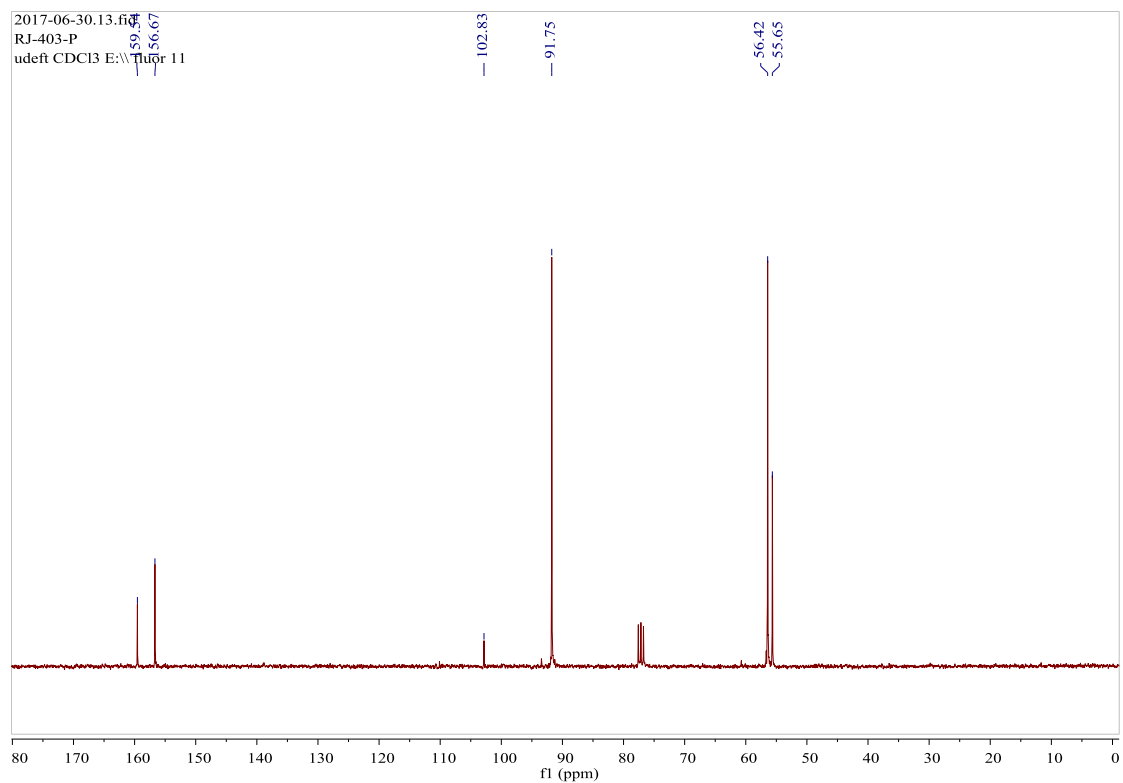
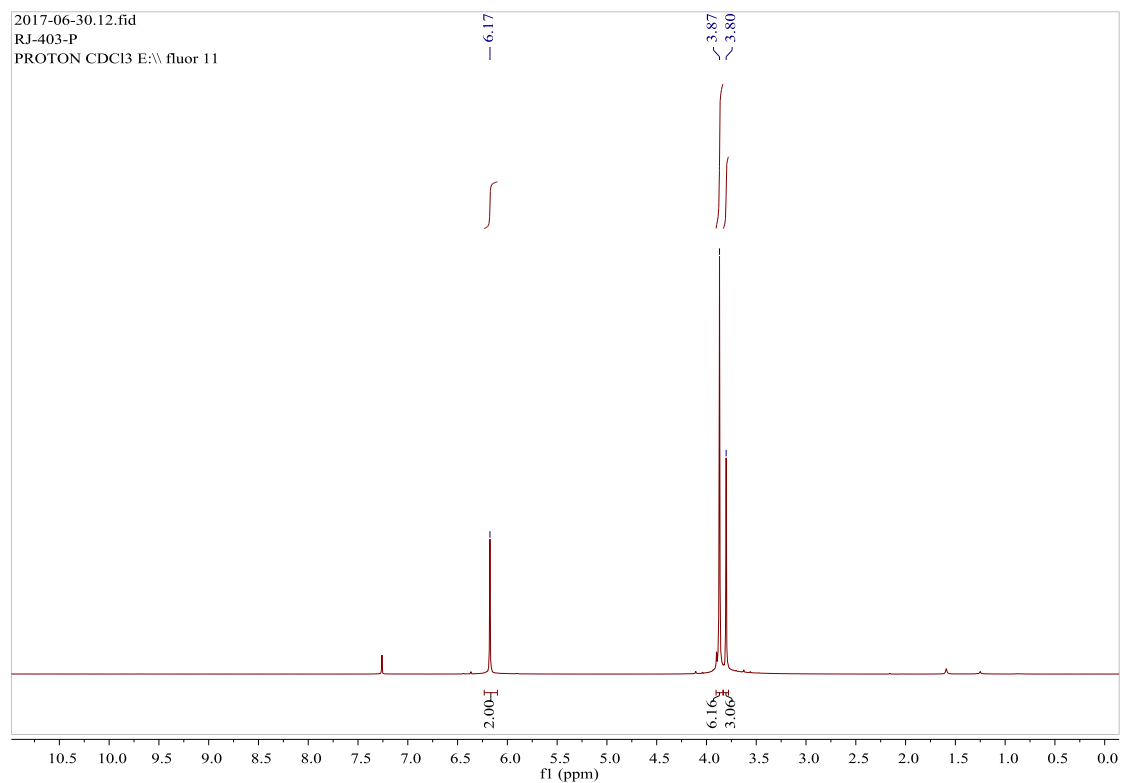
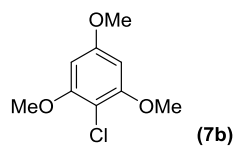


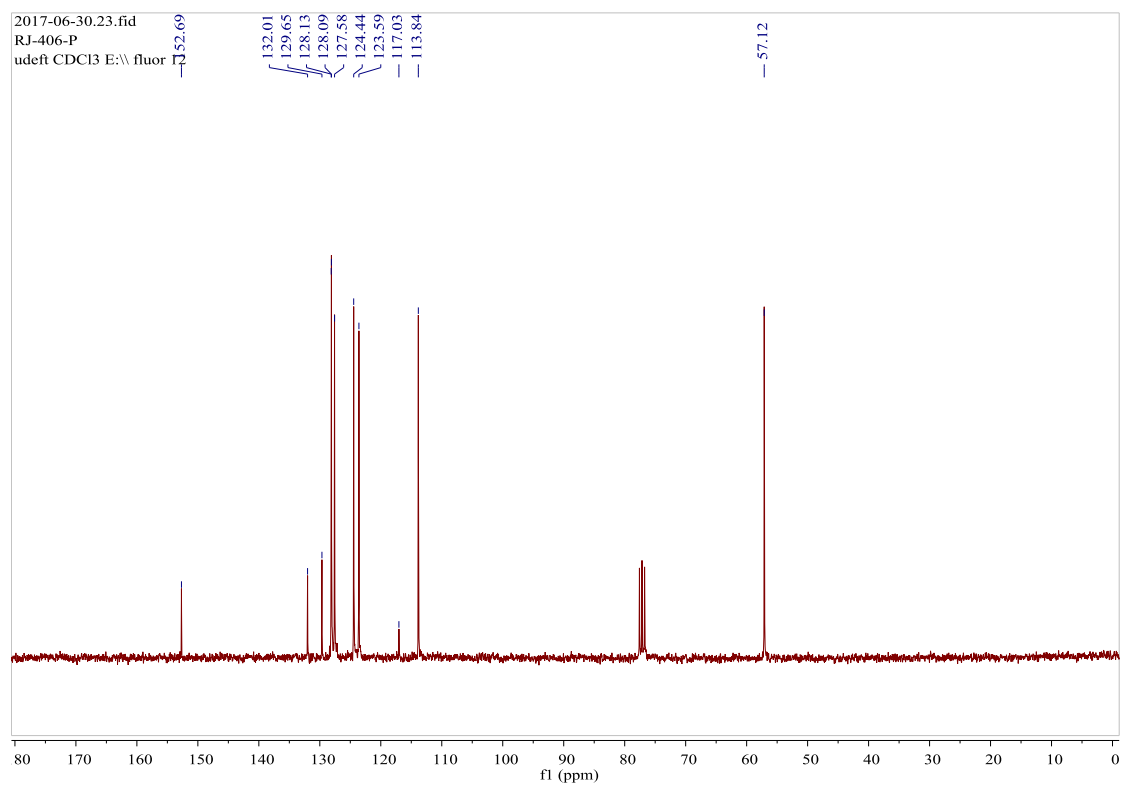
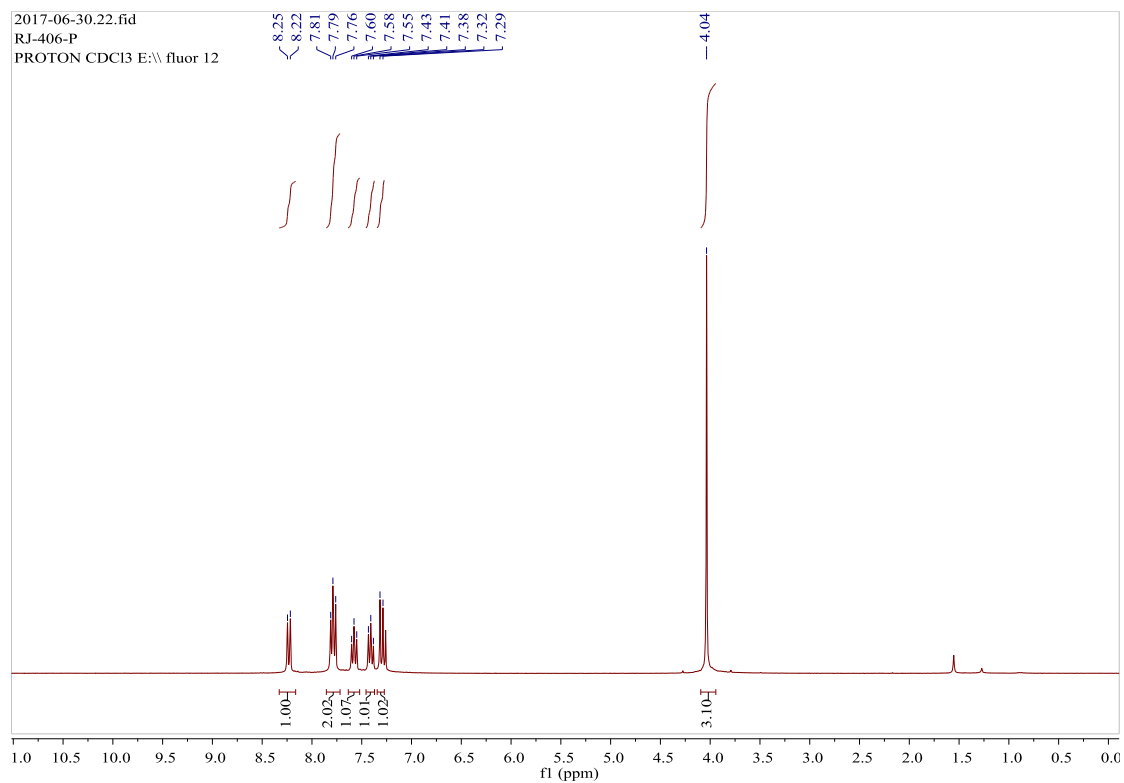
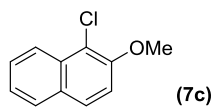


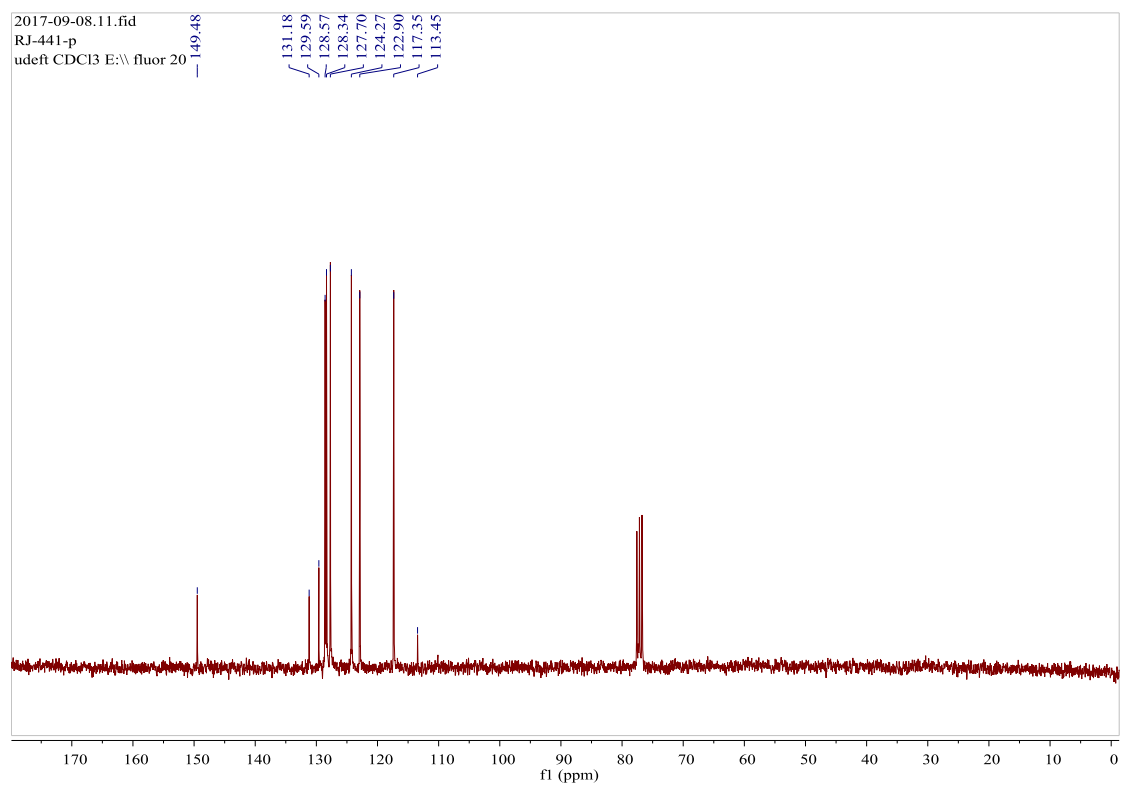
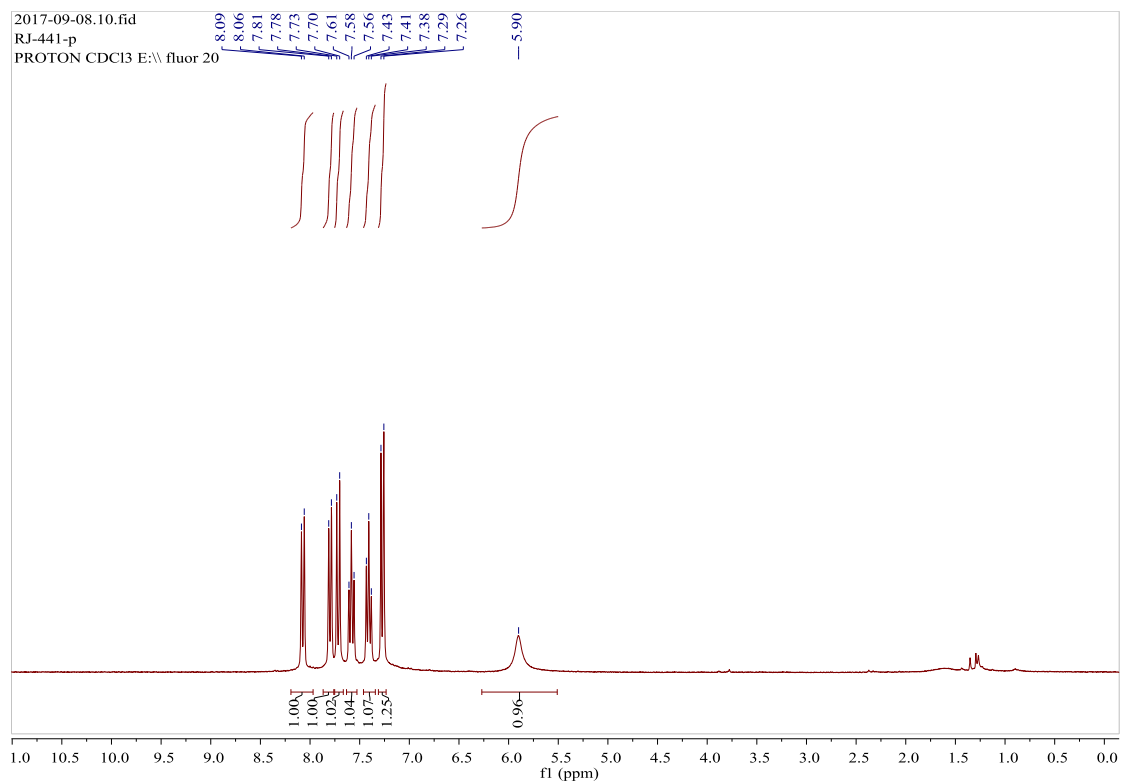
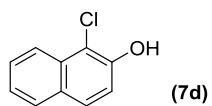


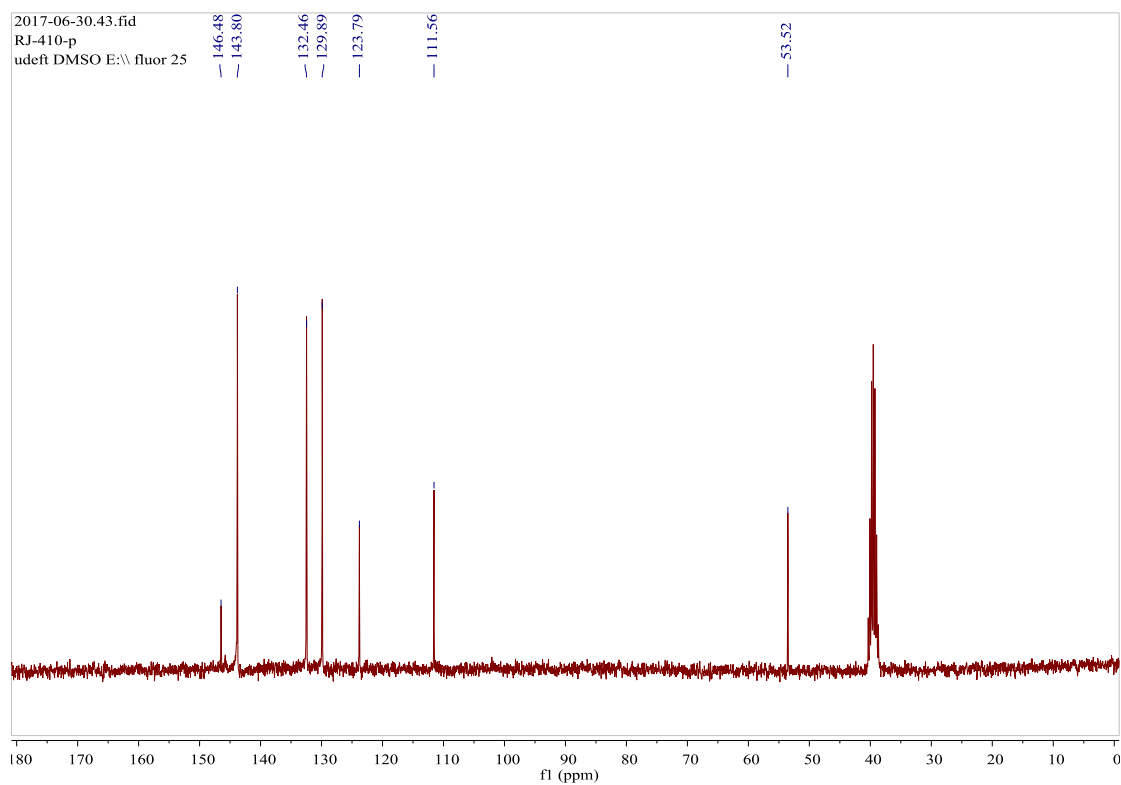
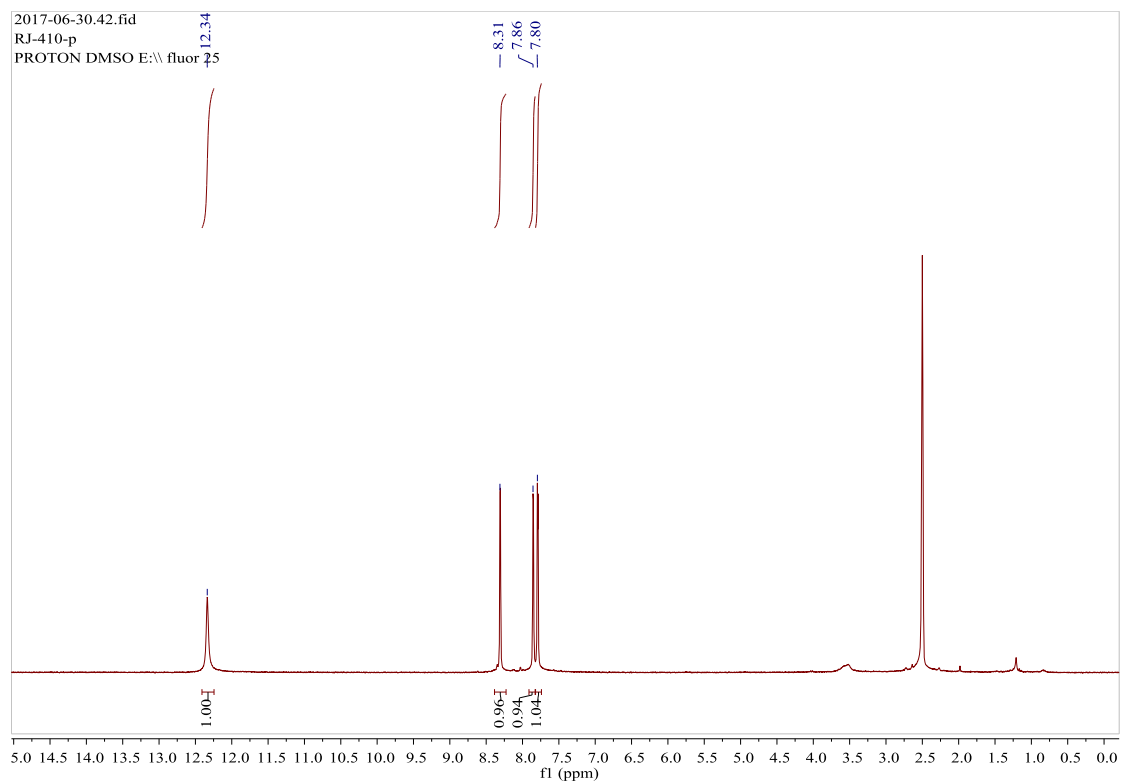
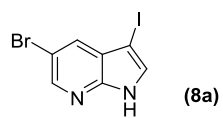


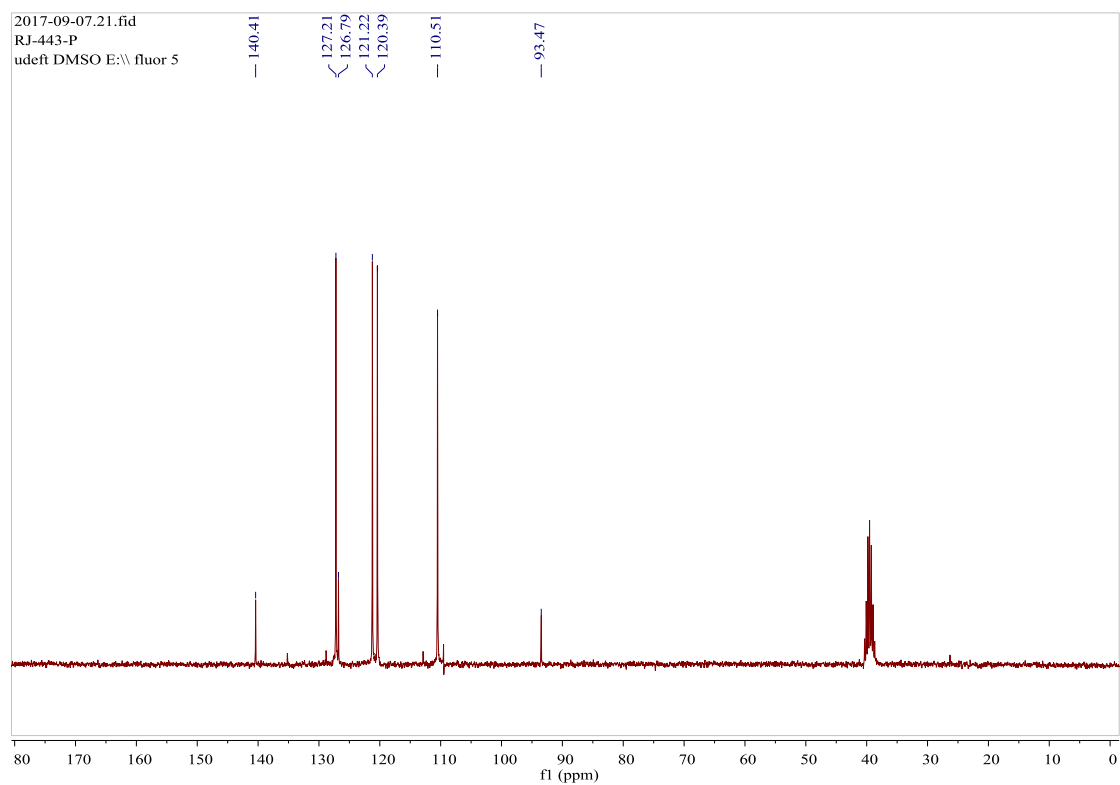
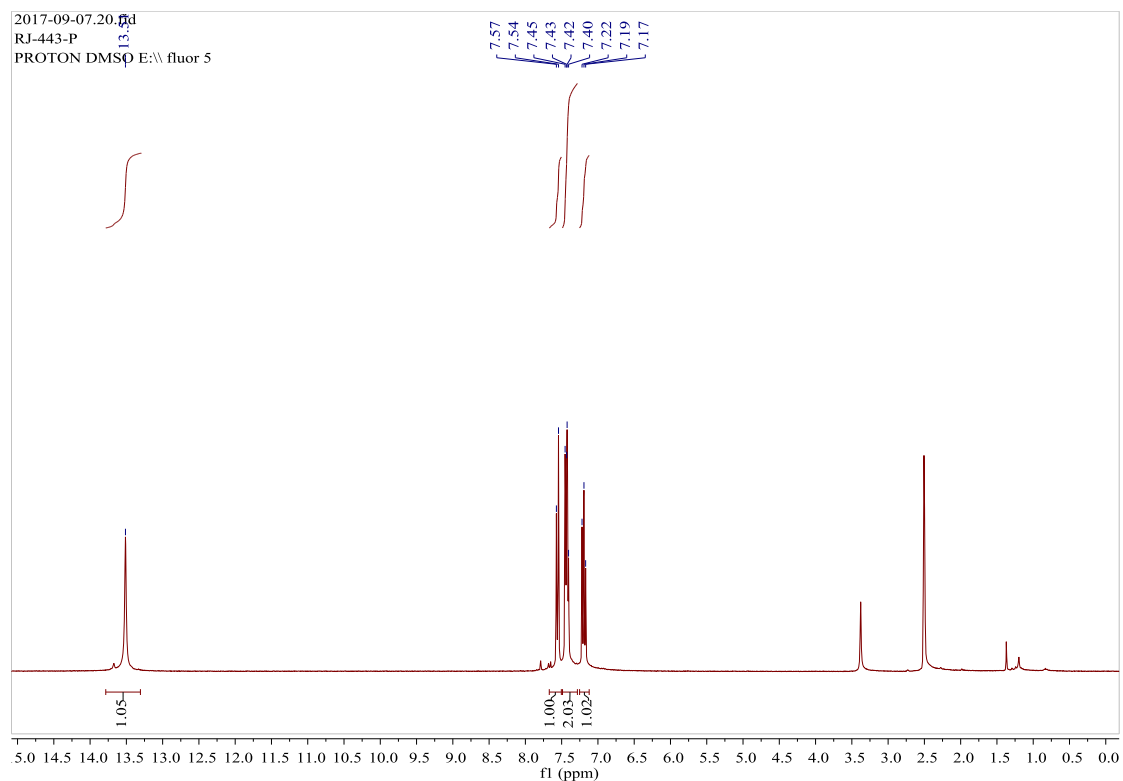
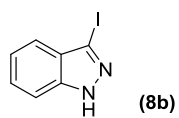


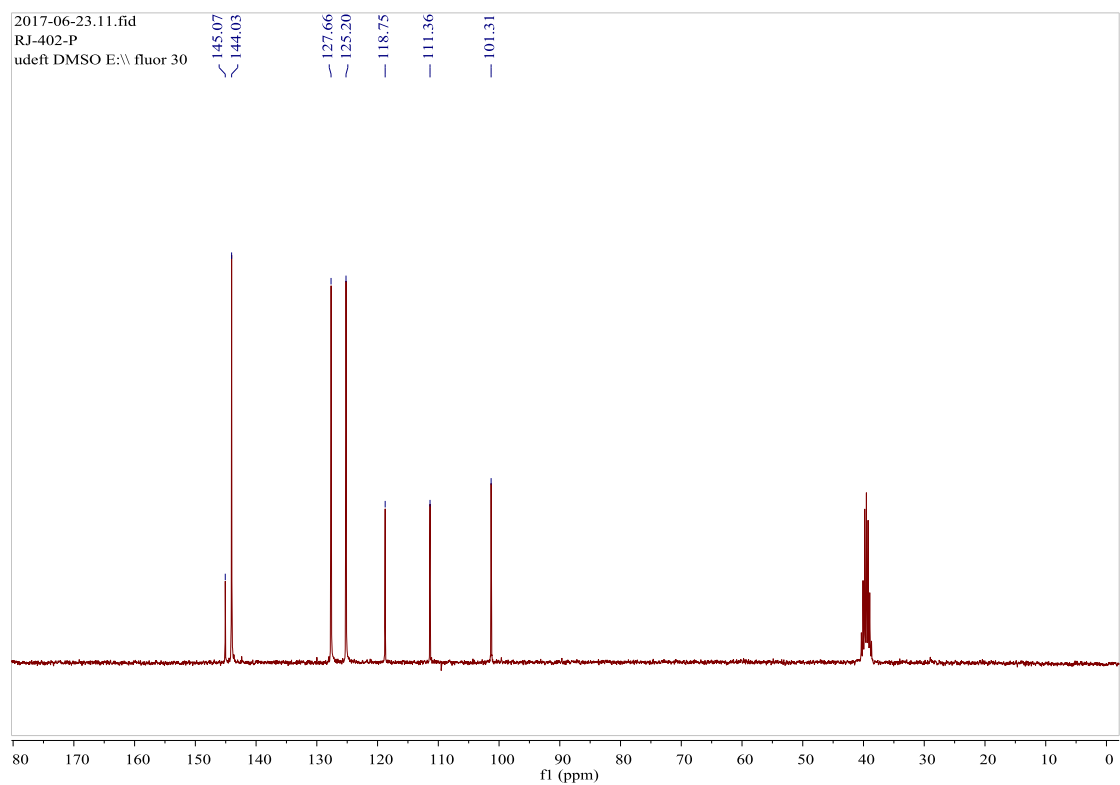
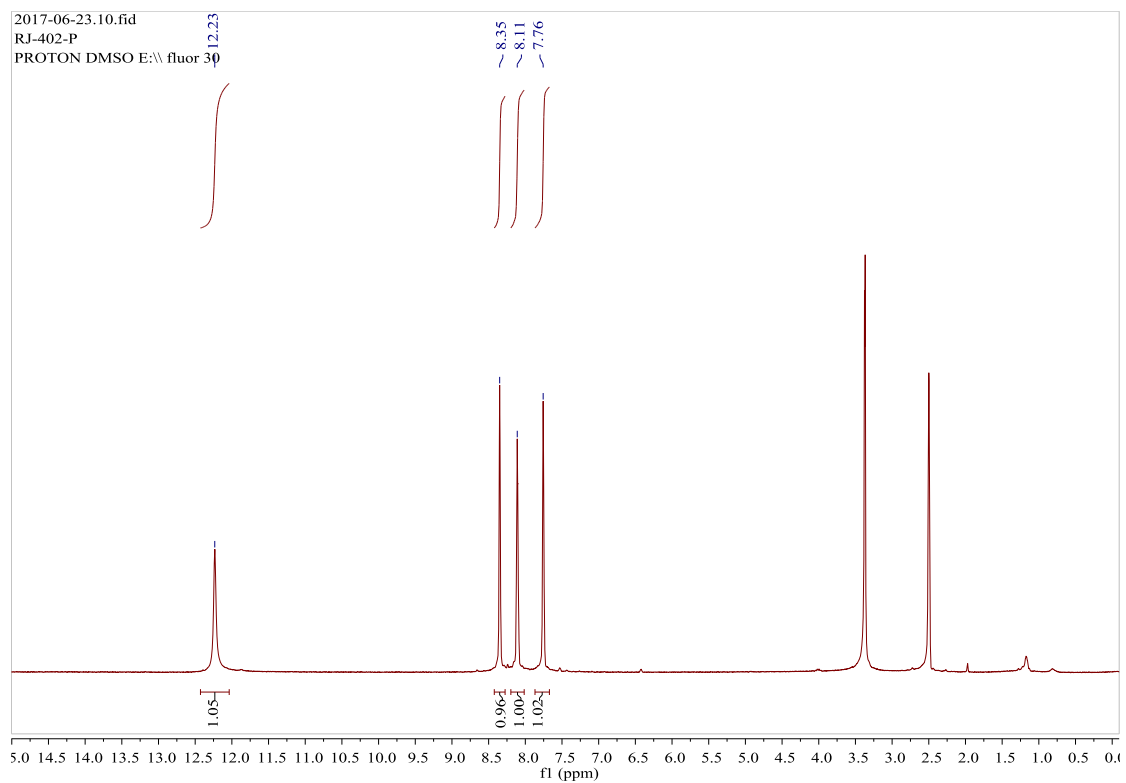
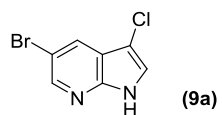


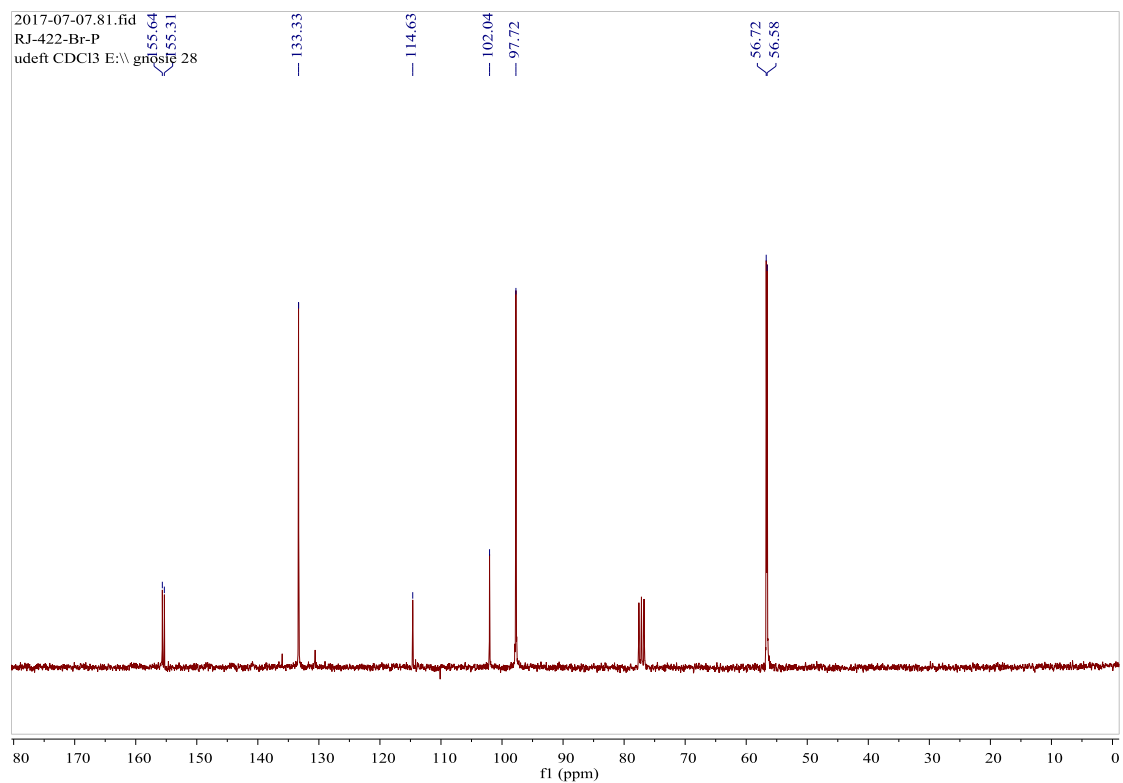
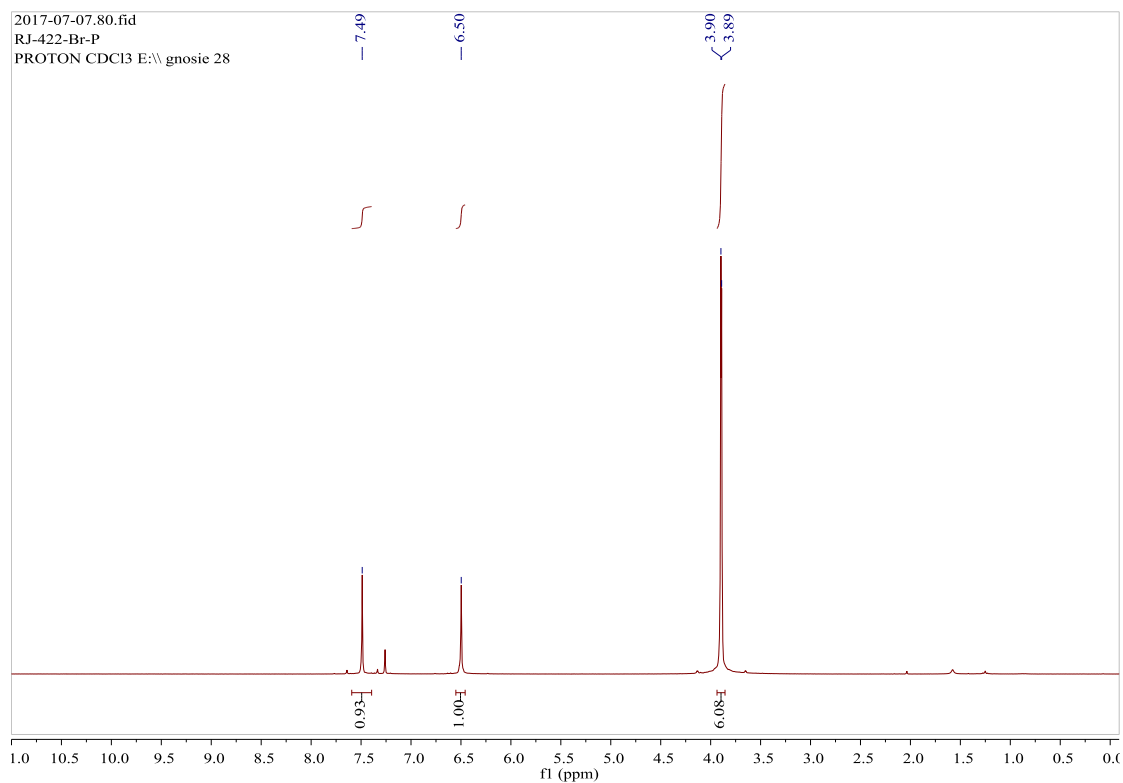
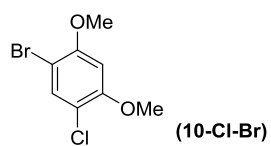


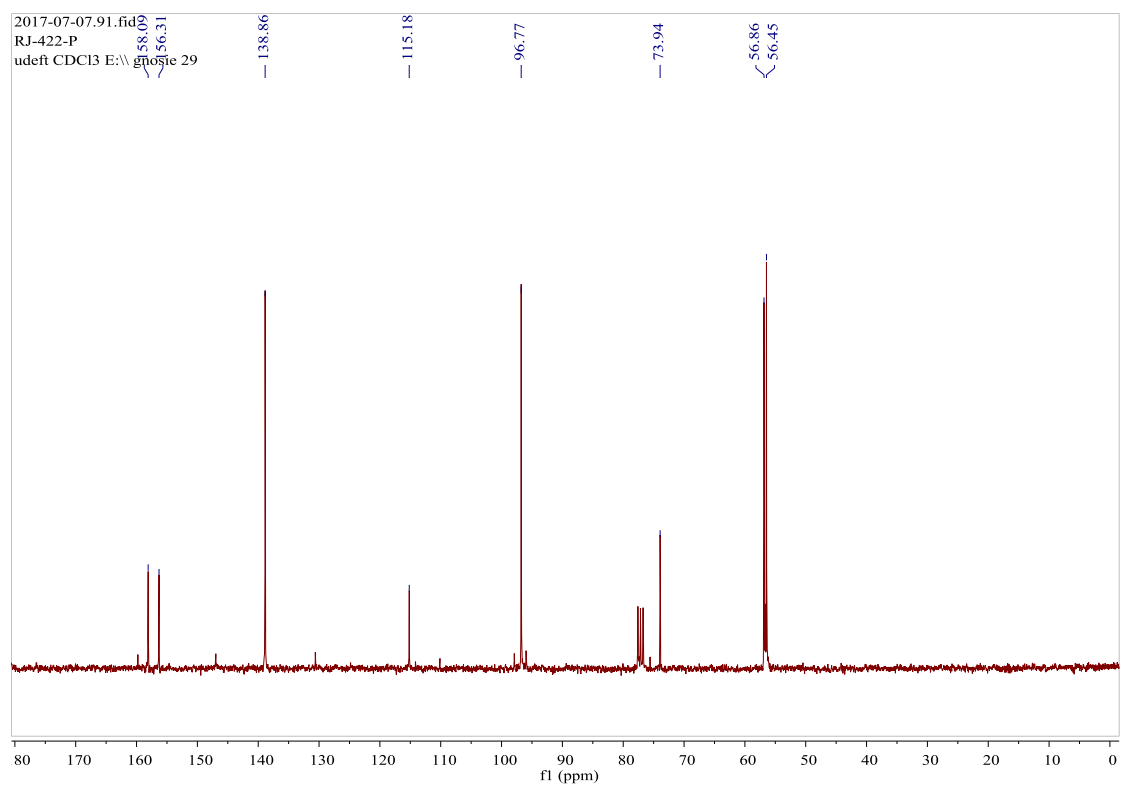
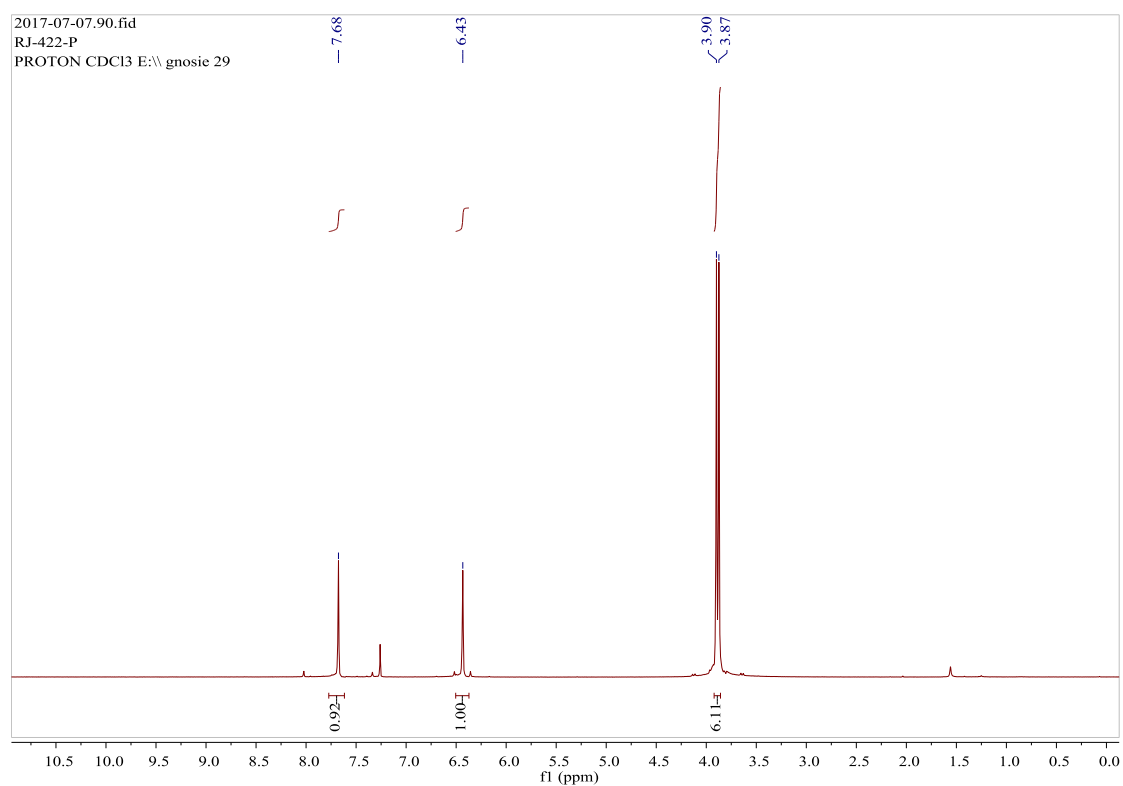
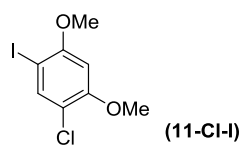


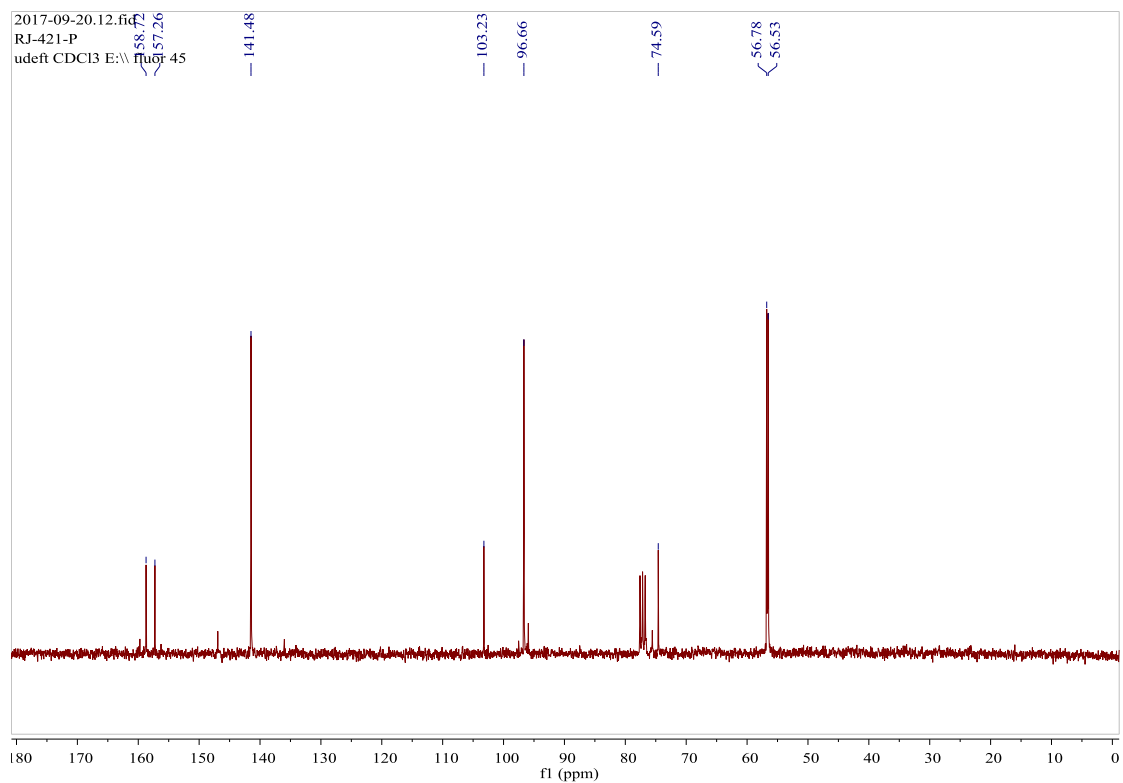
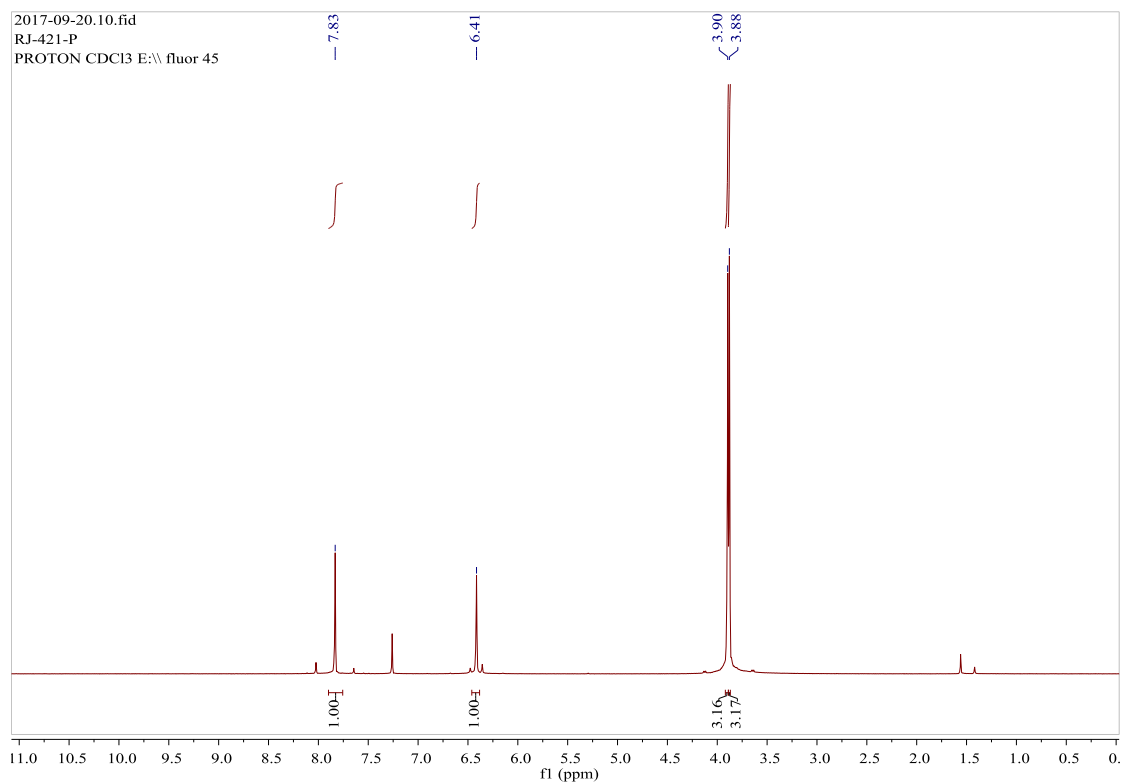
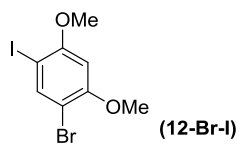


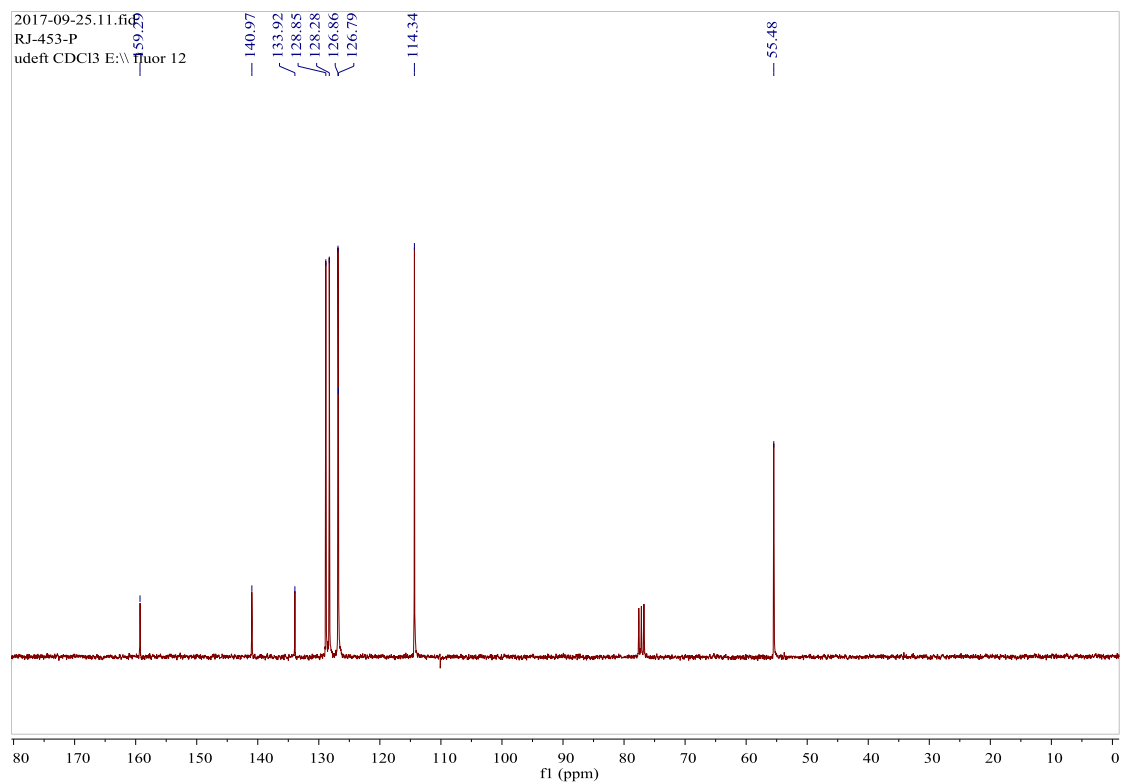
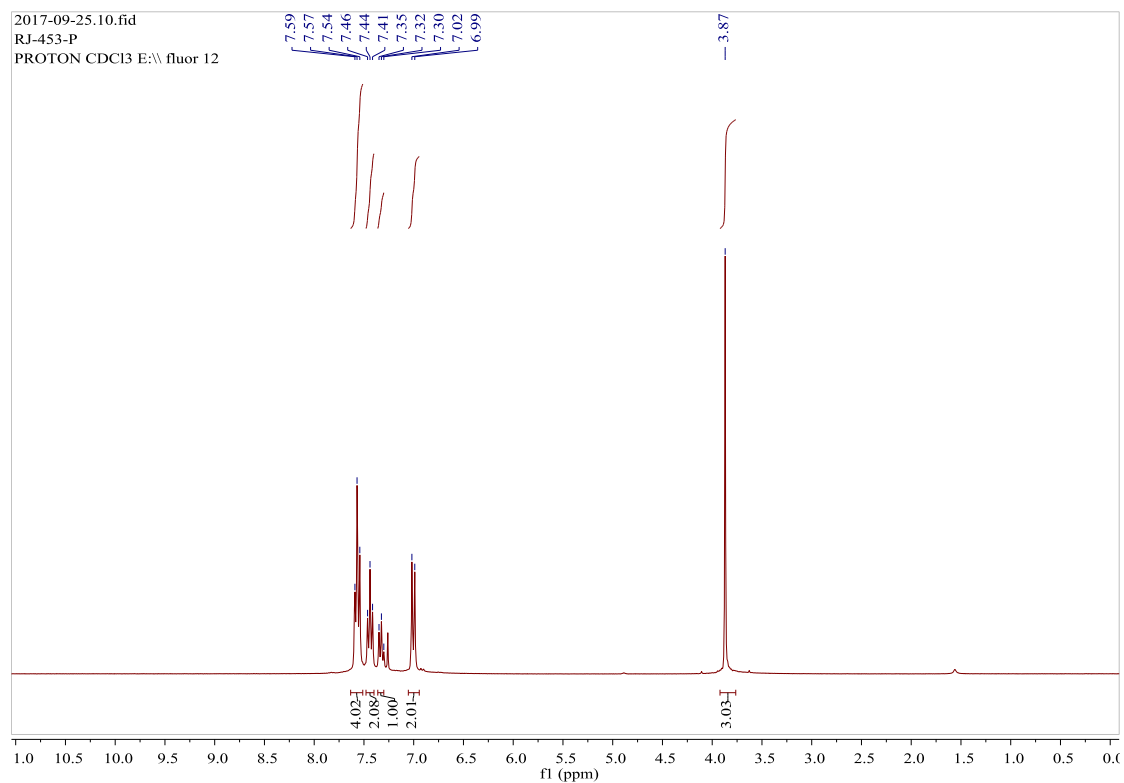
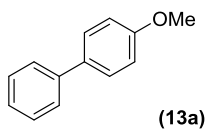


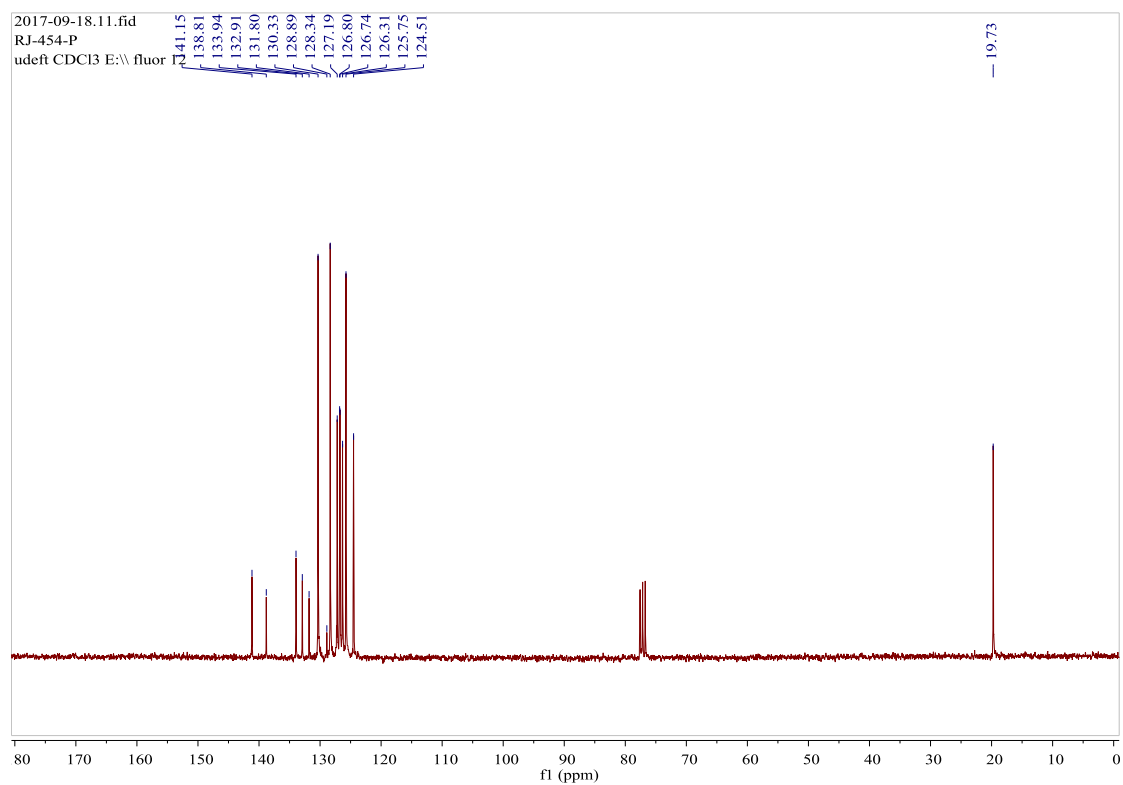
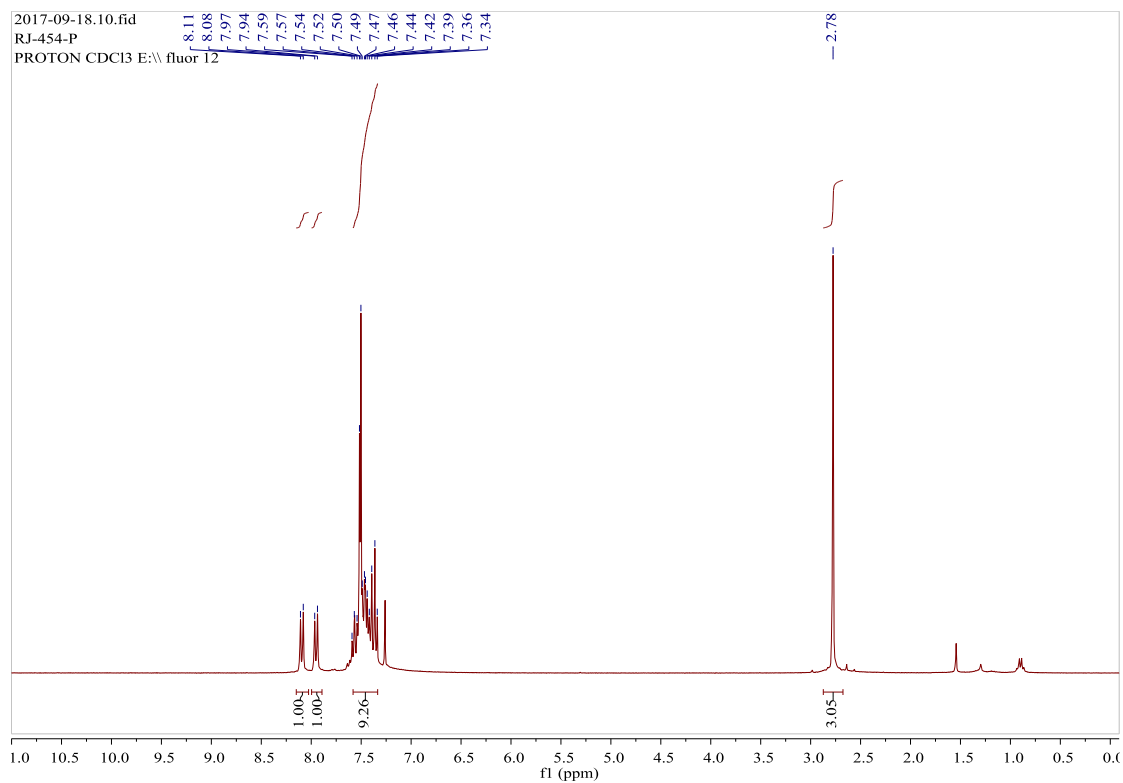
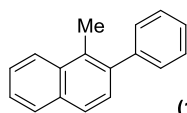


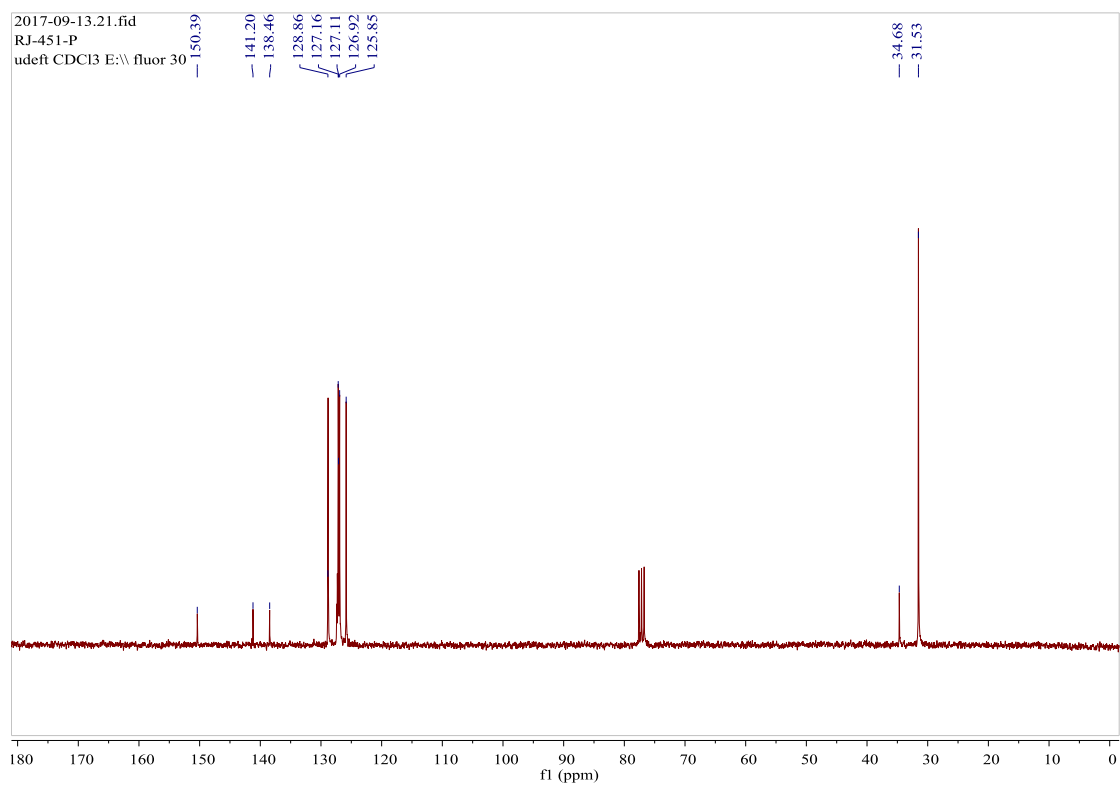
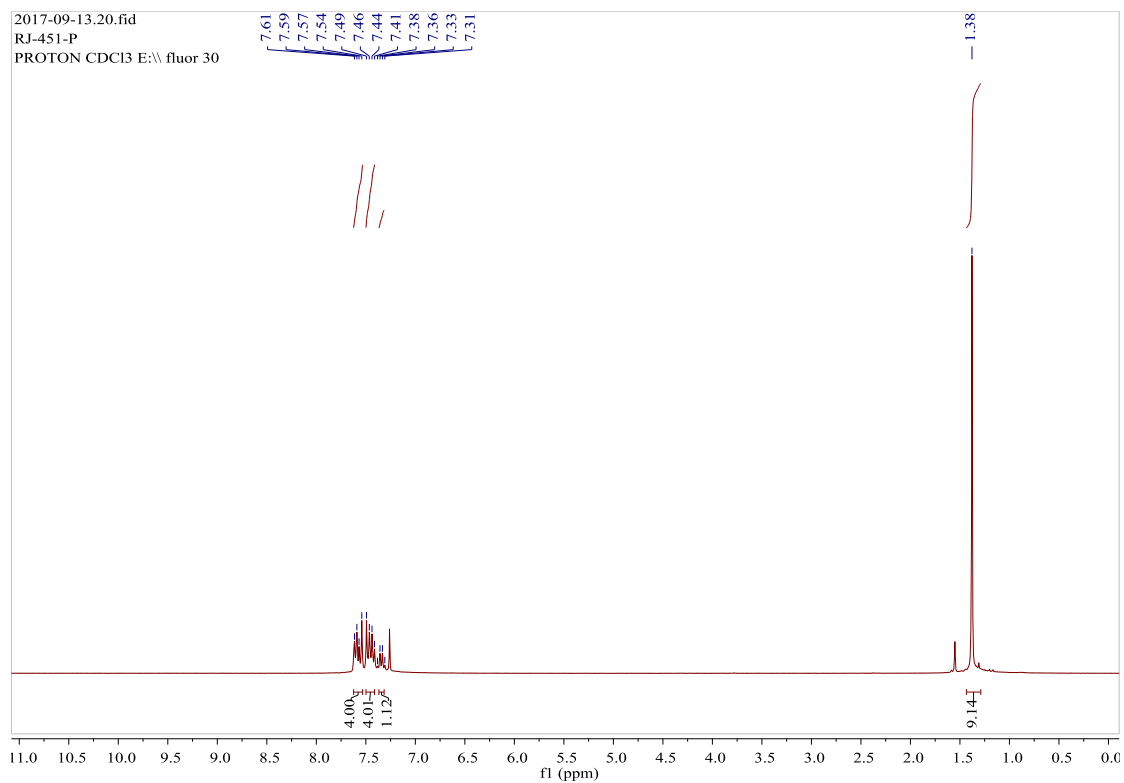
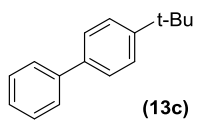


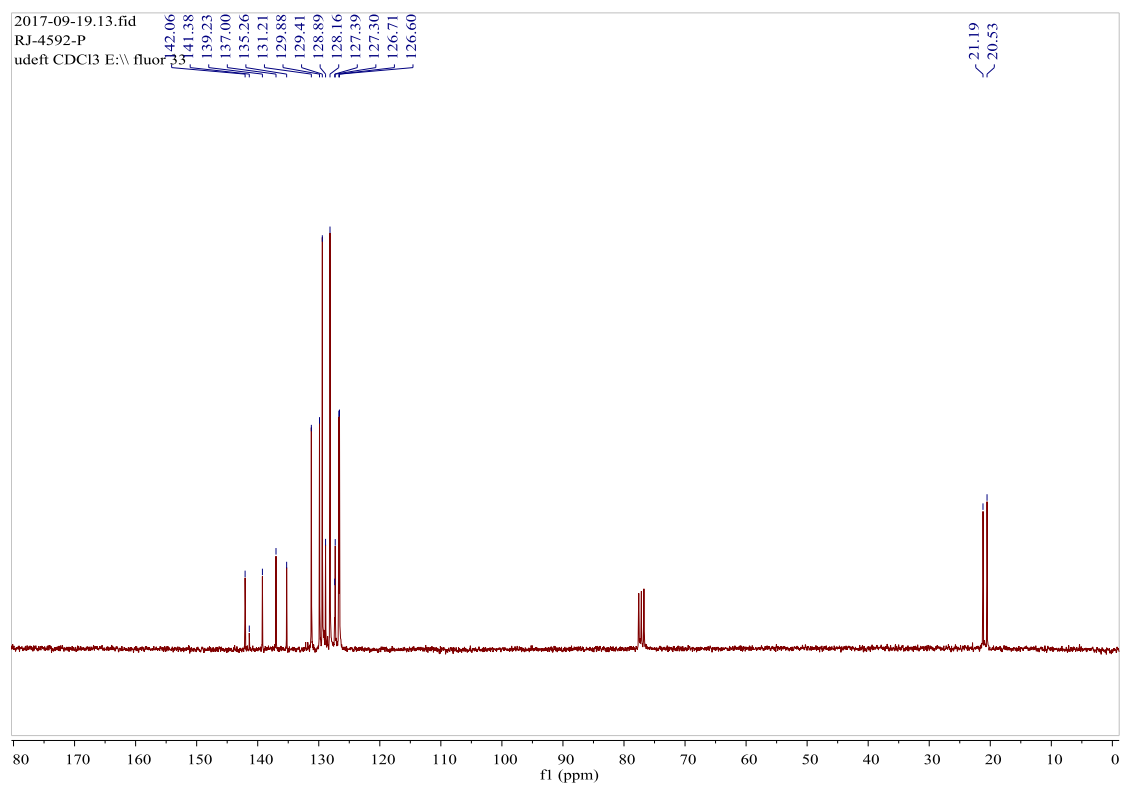
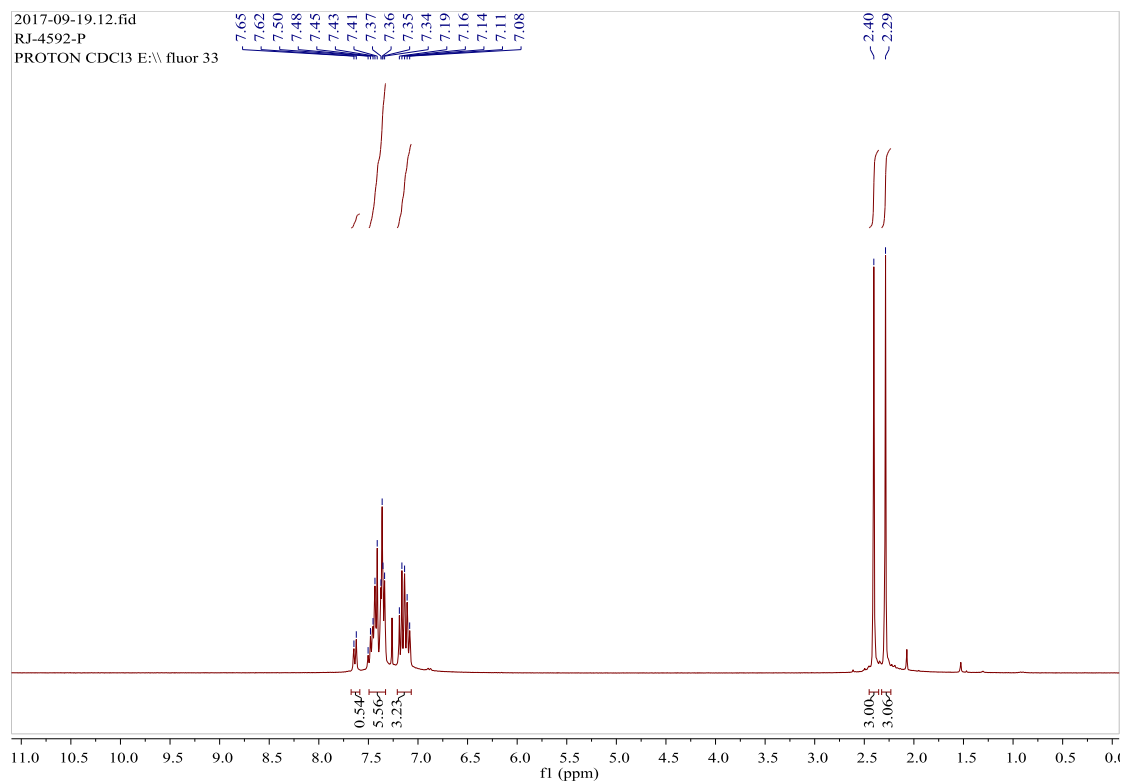
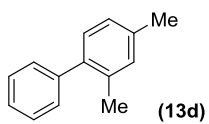


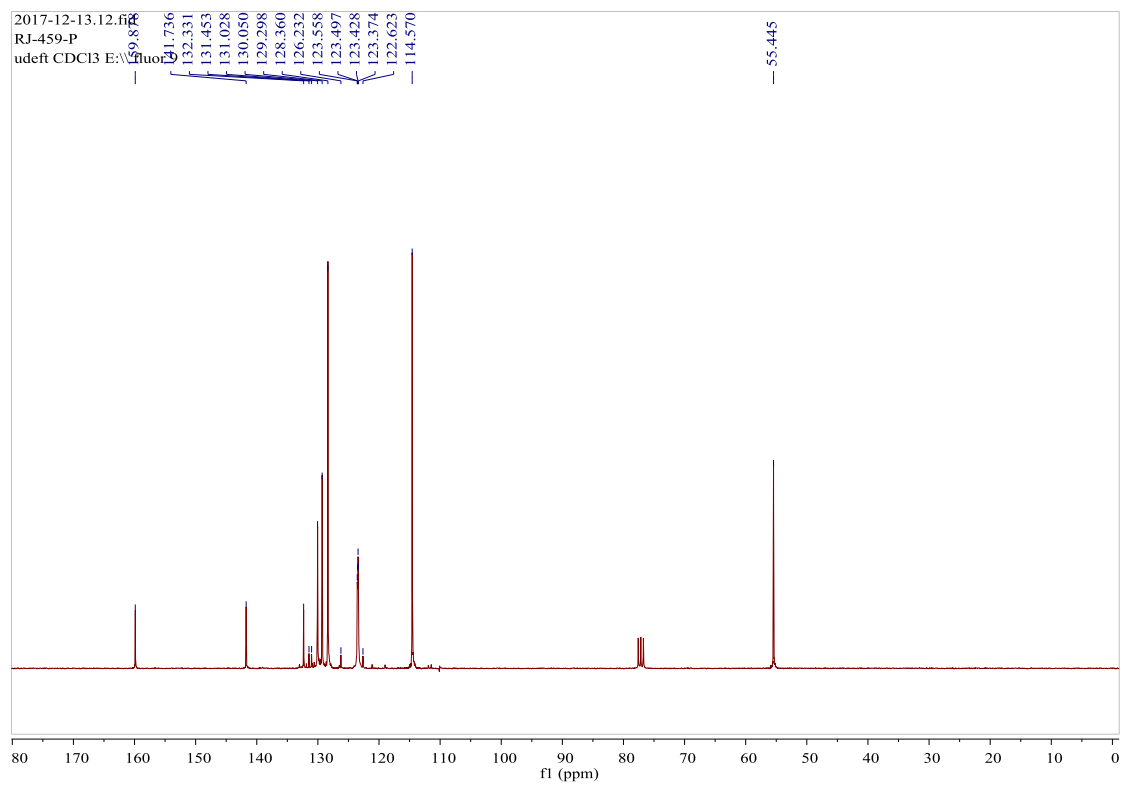
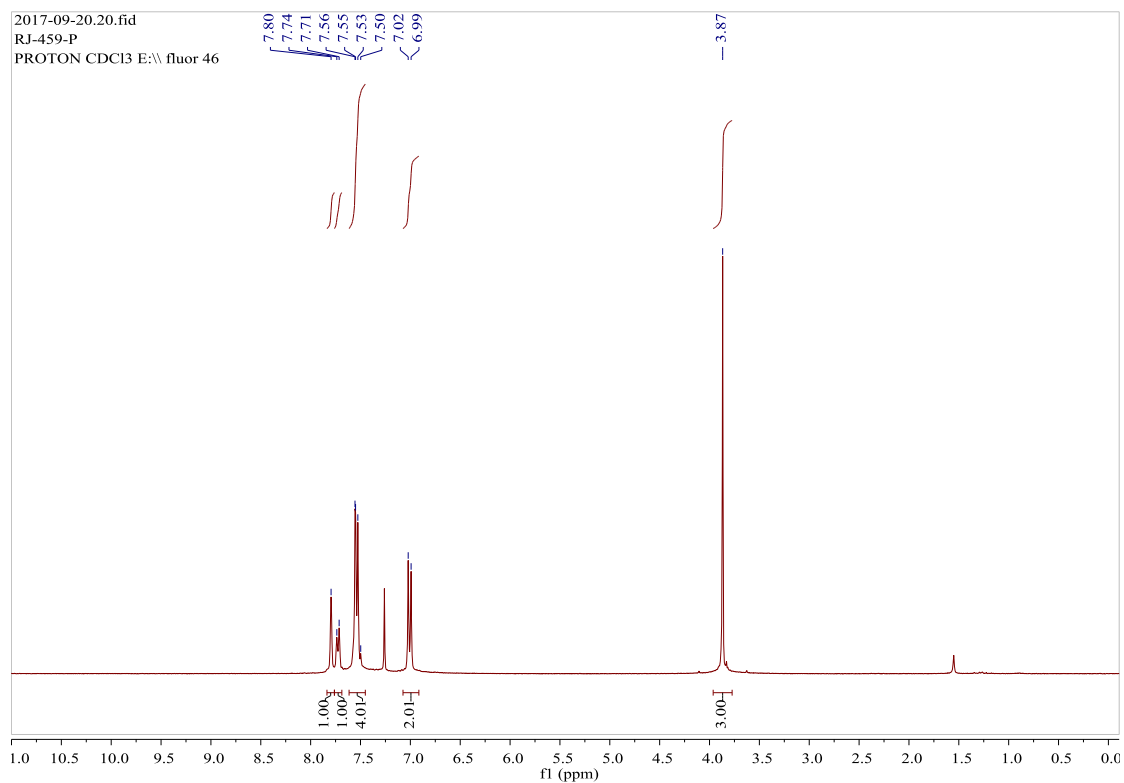
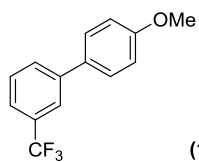


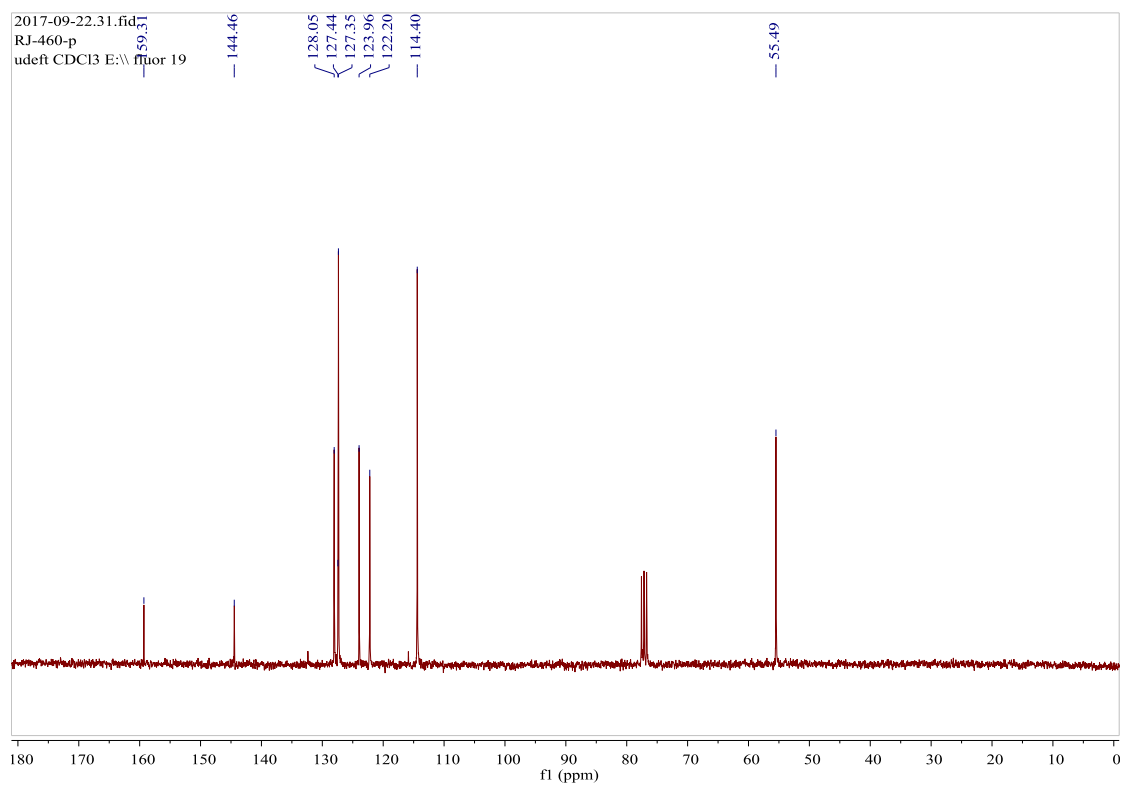
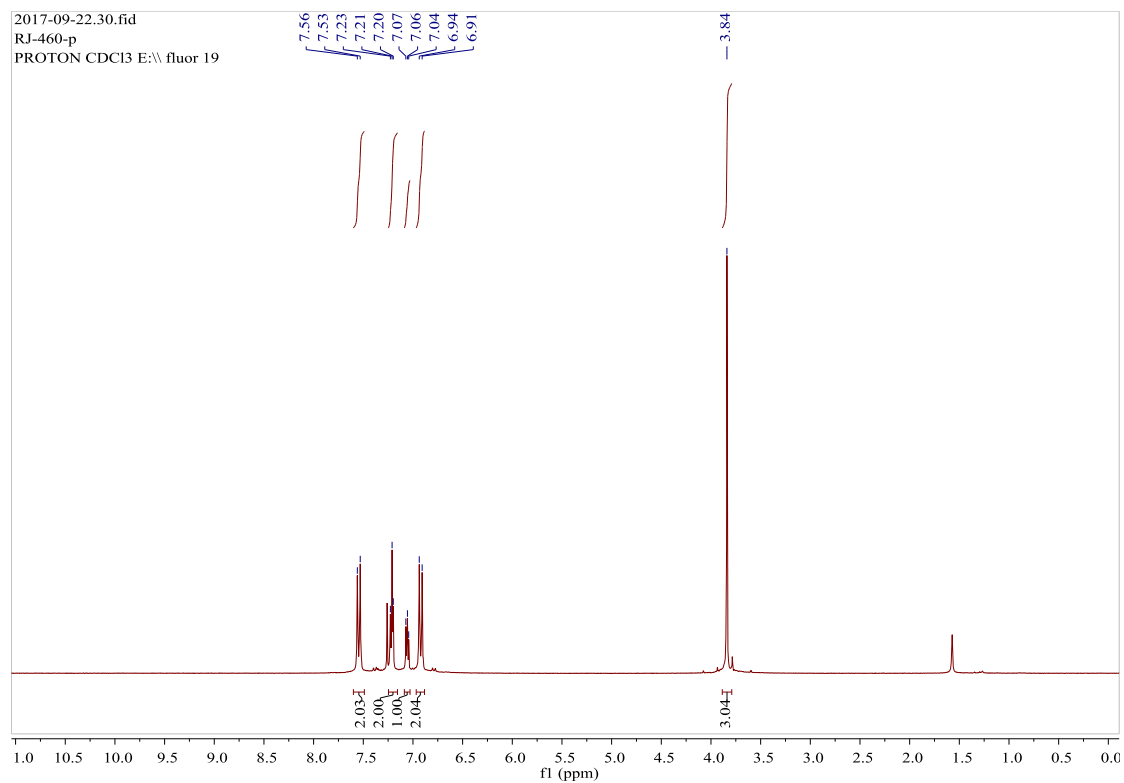
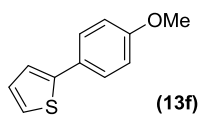


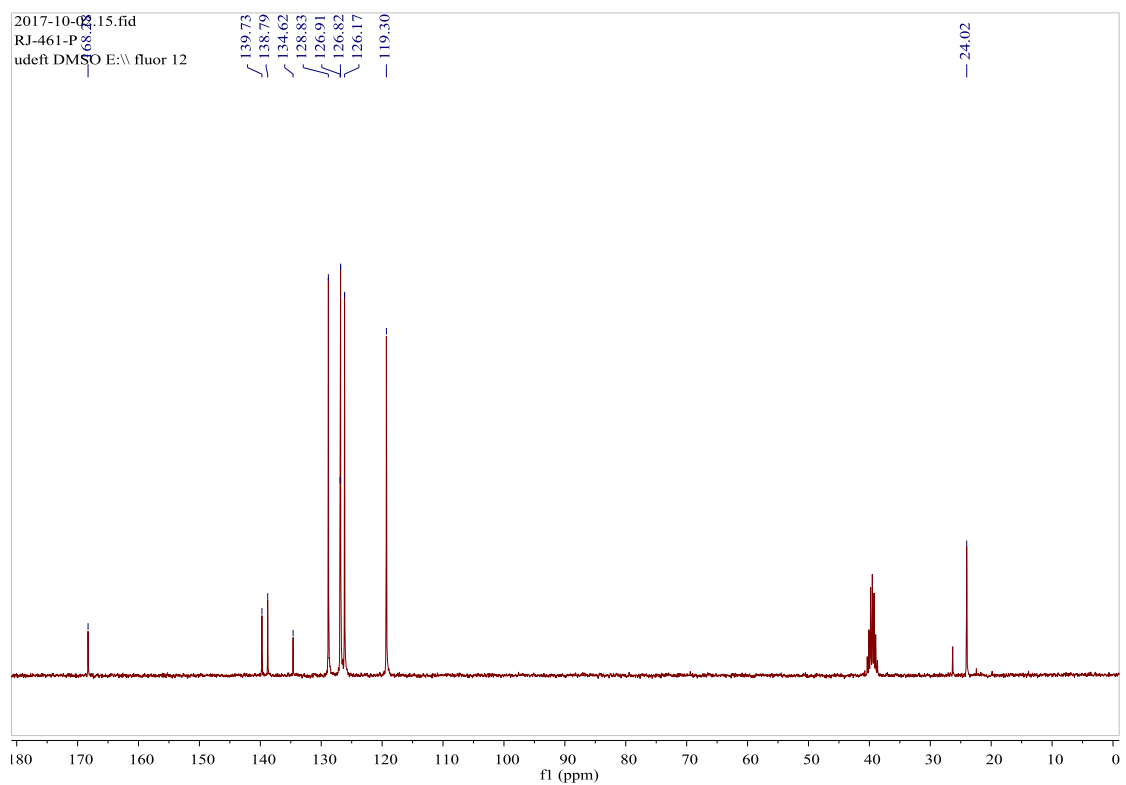
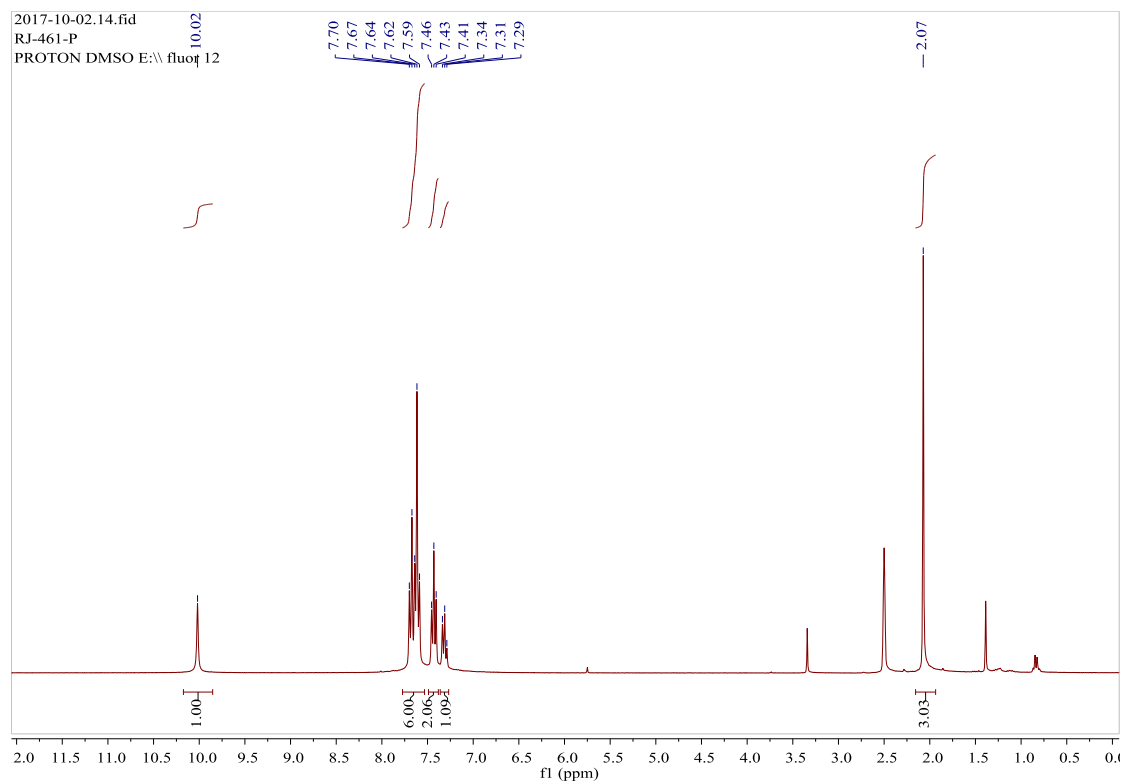
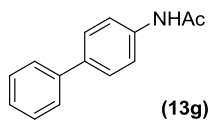


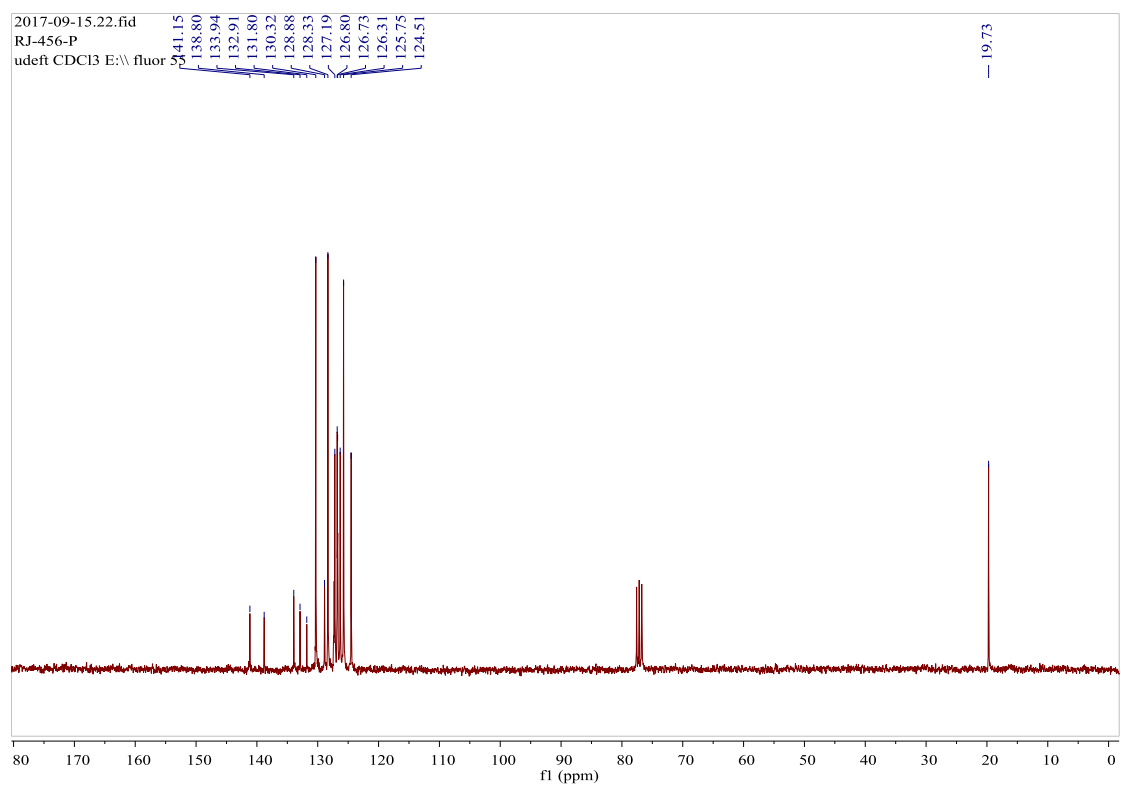
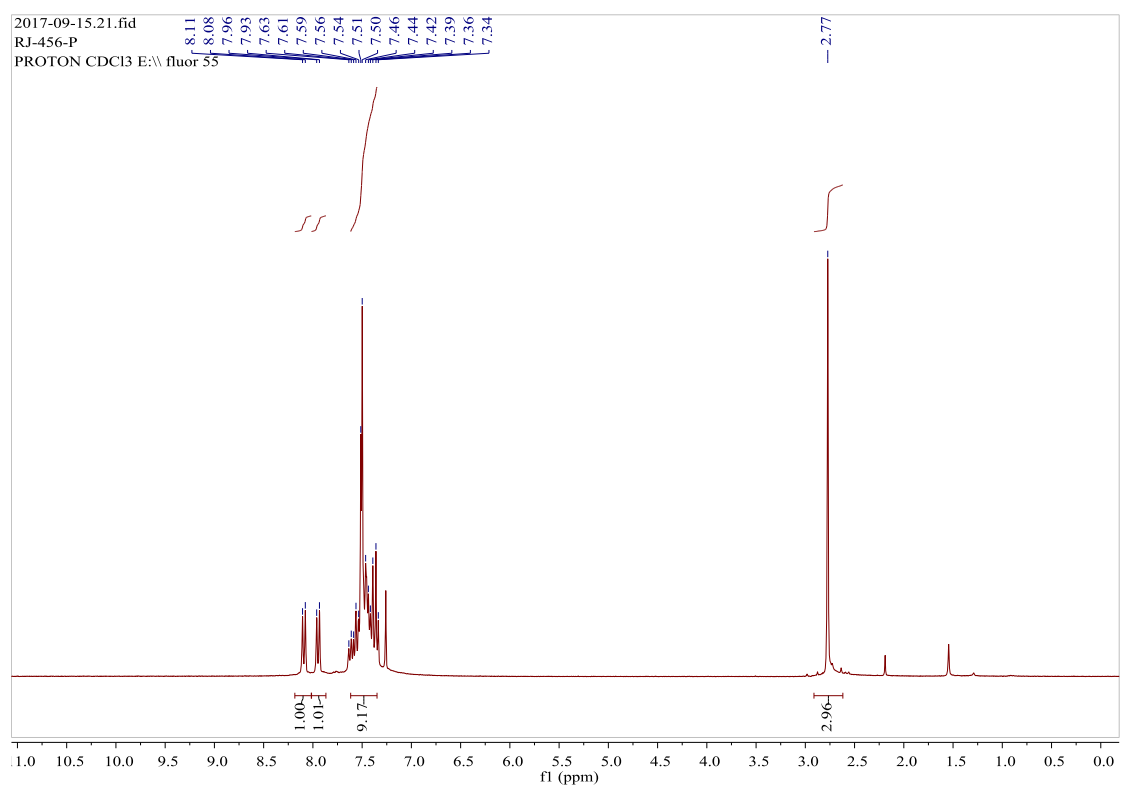
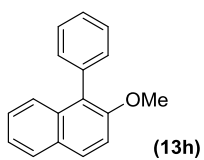




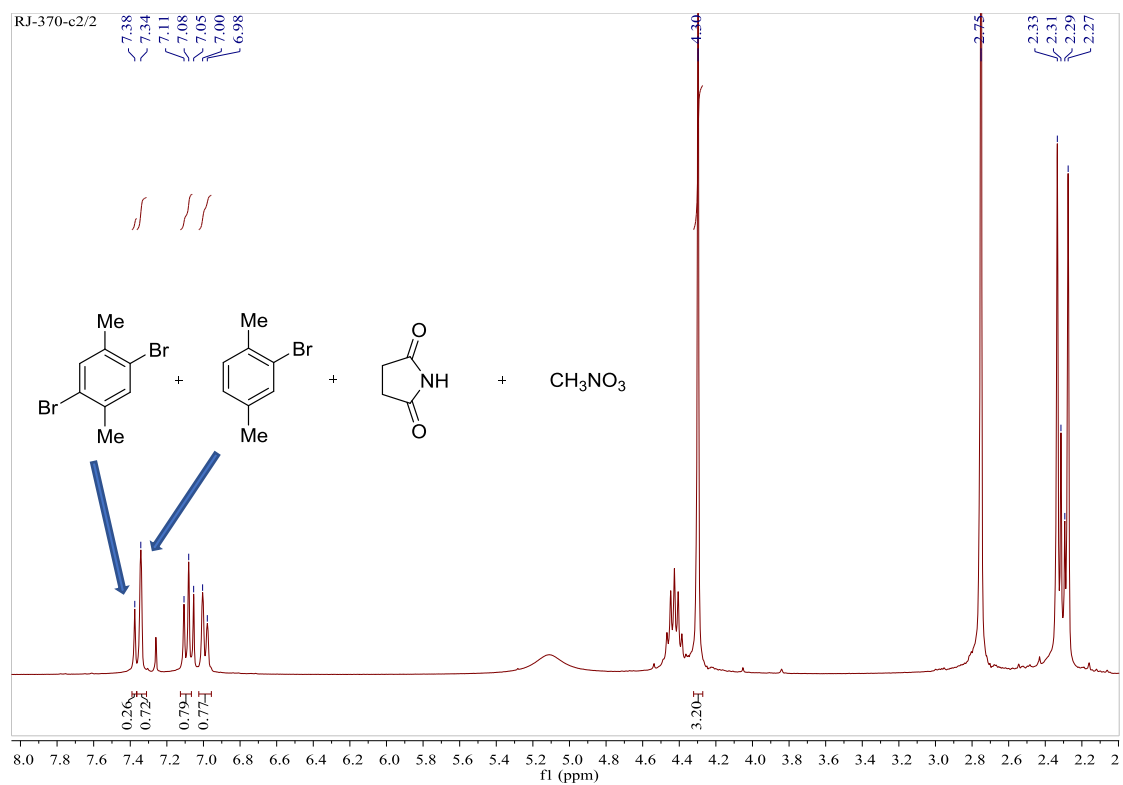
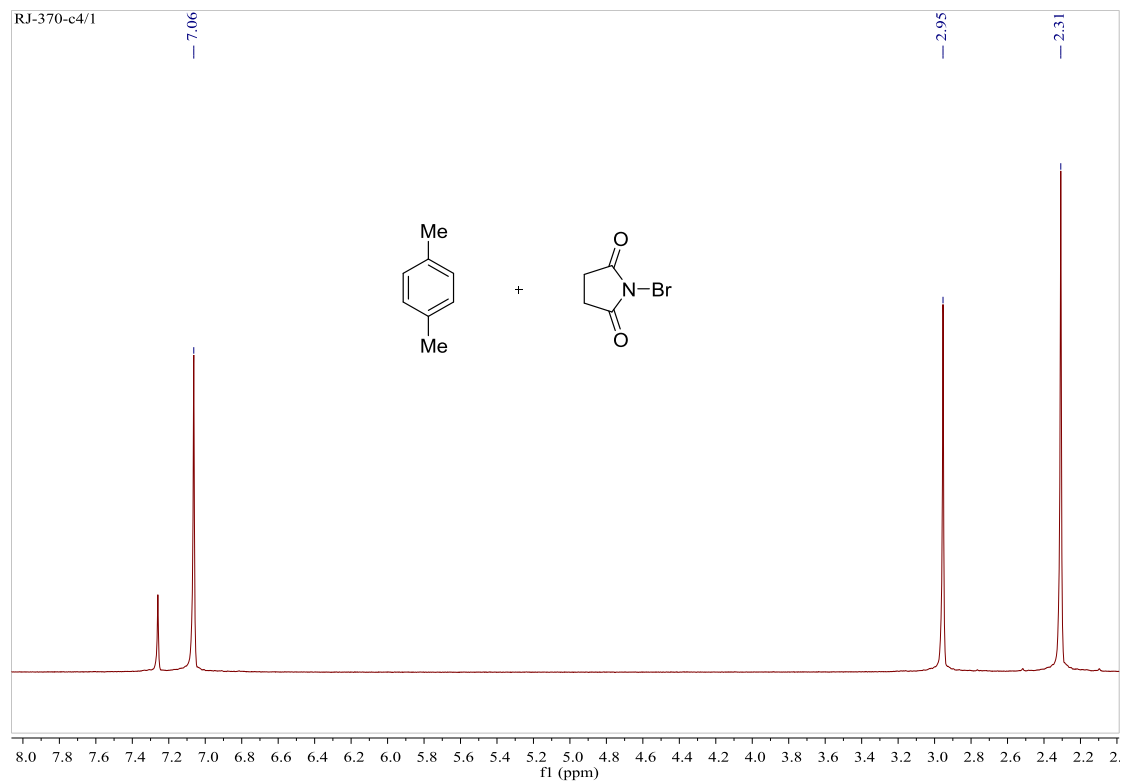
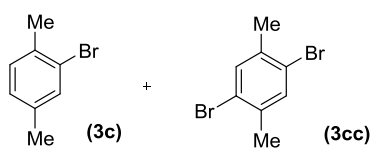




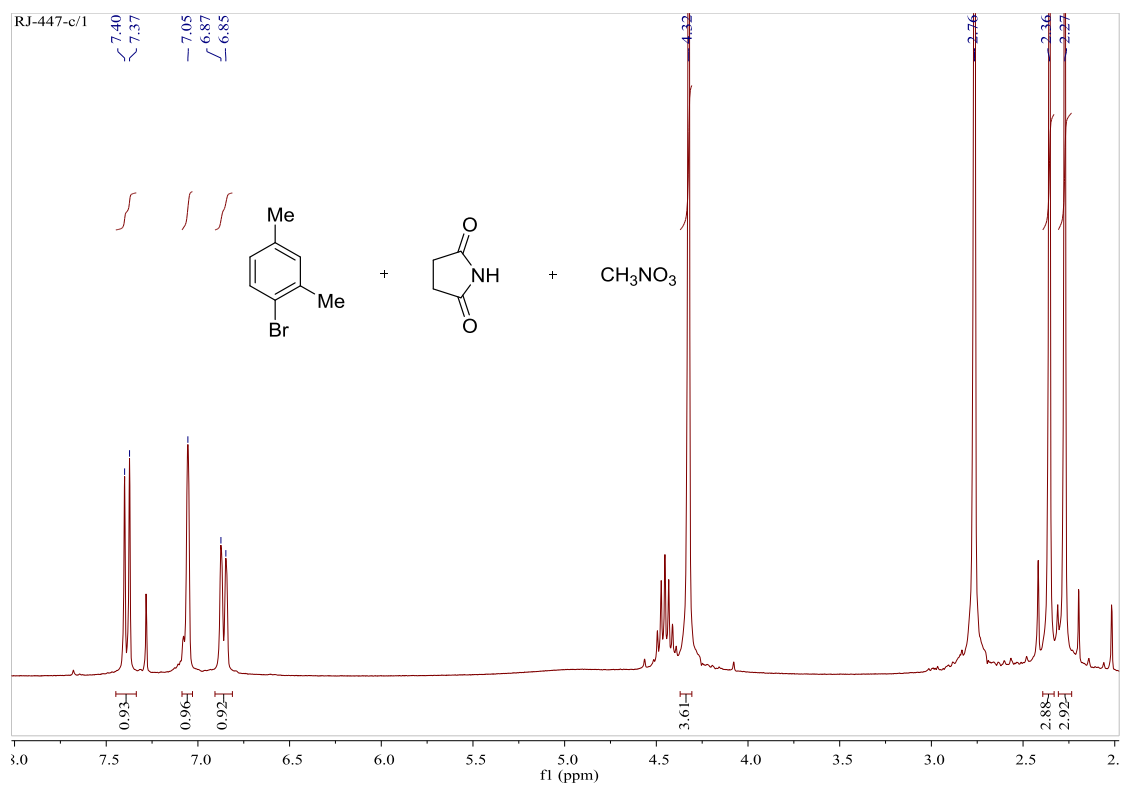
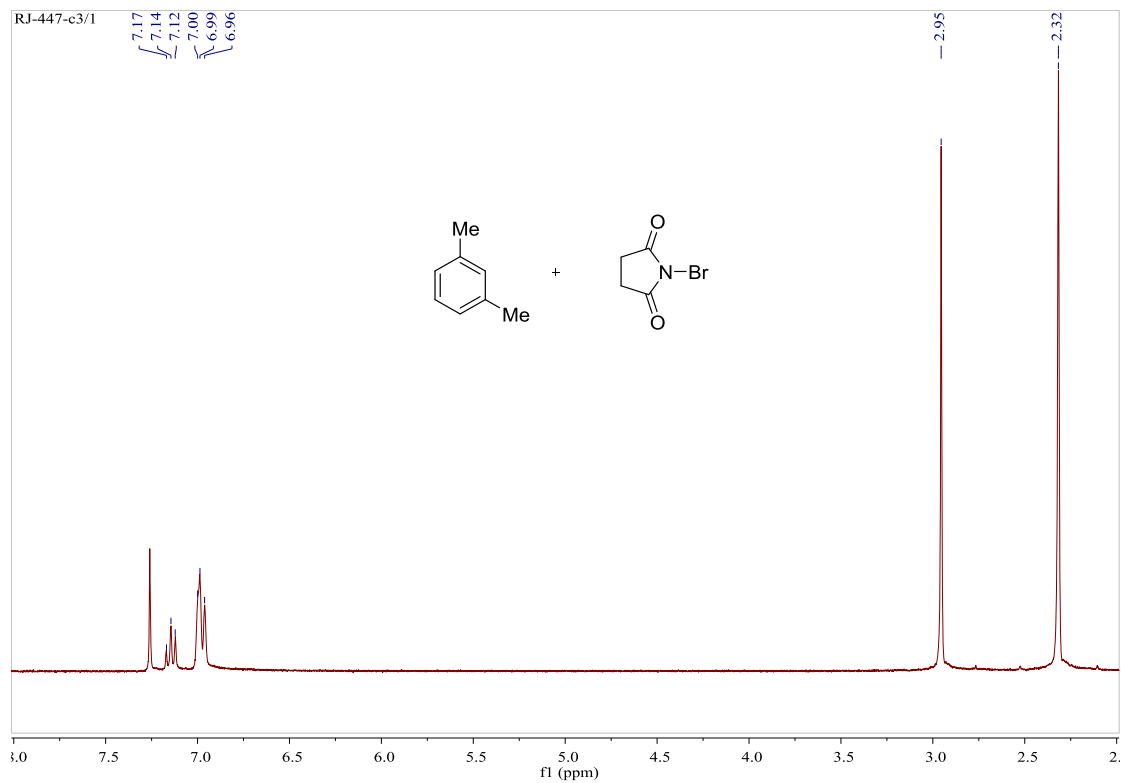
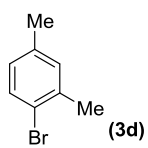




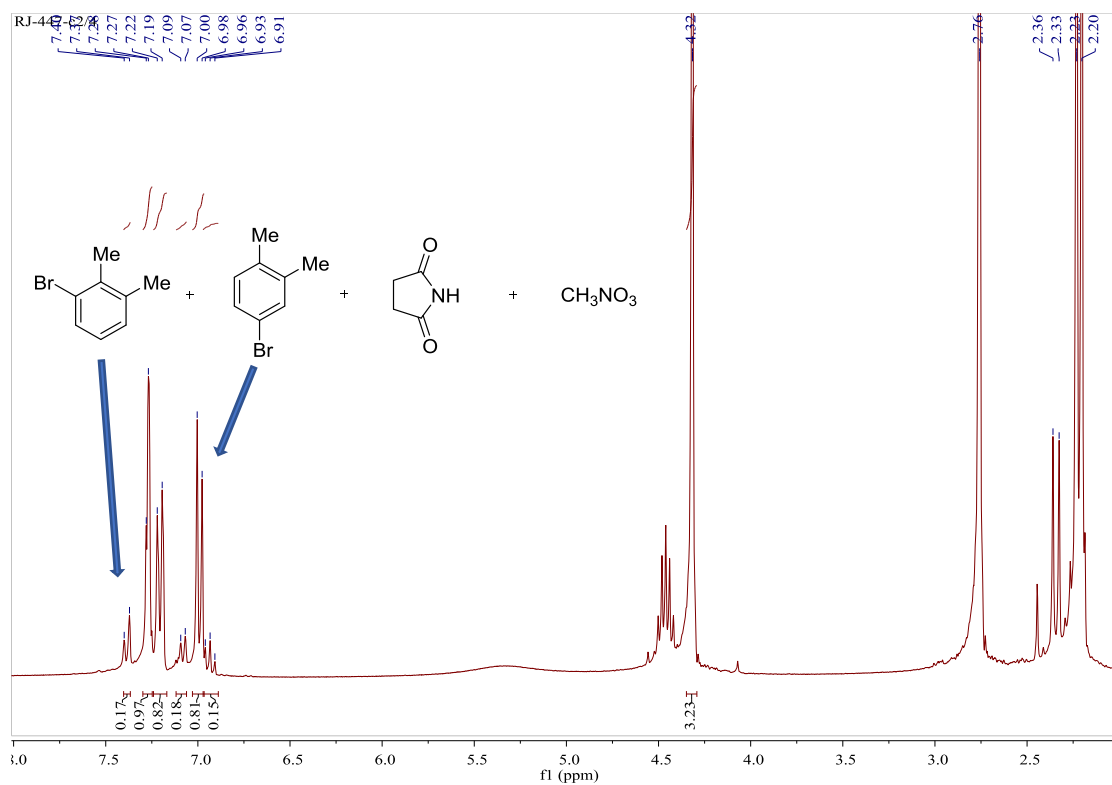
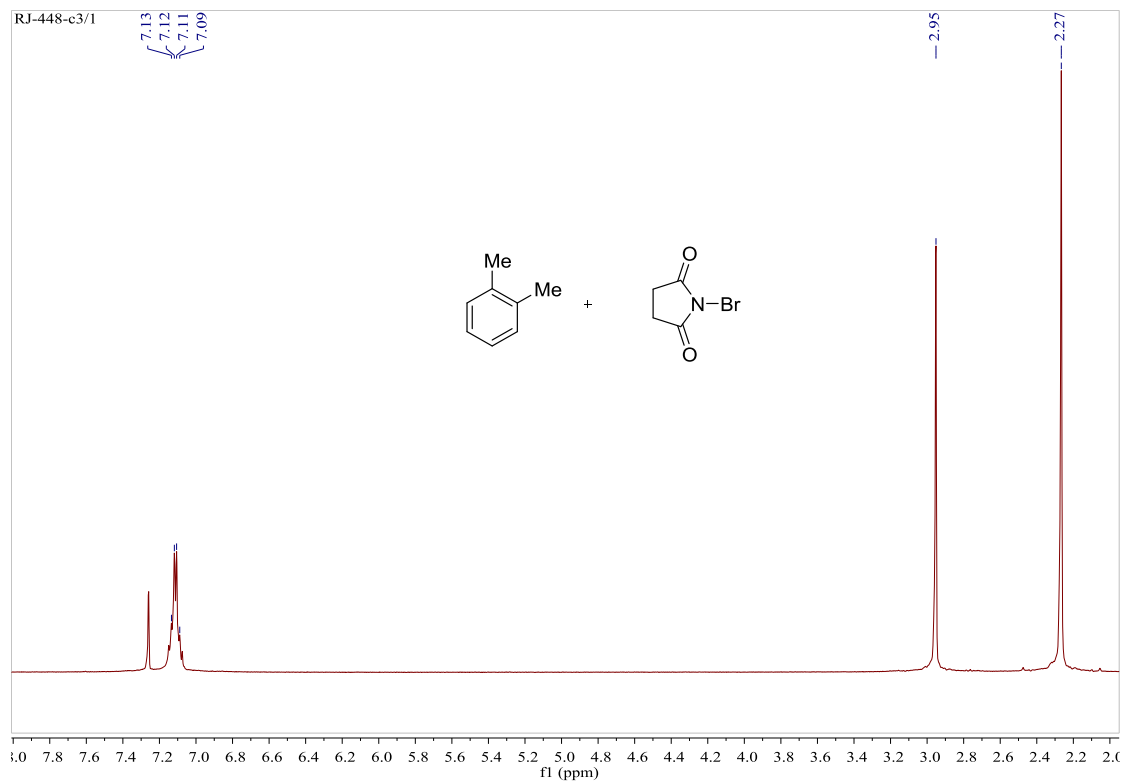
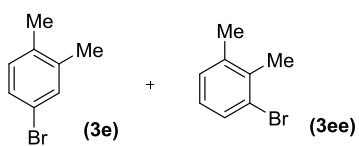
1,4-dibromo-2,5-dimethylbenzene and 2-bromo-1,4-dimethylbenzene (5.9:1)



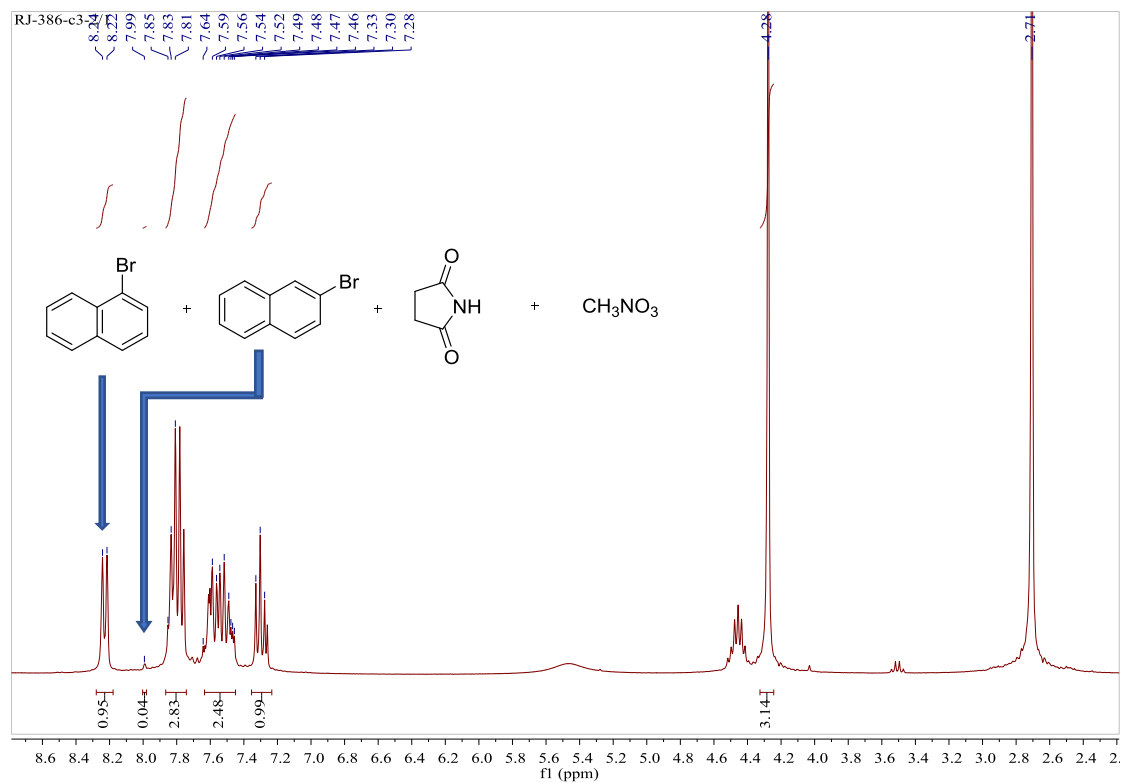
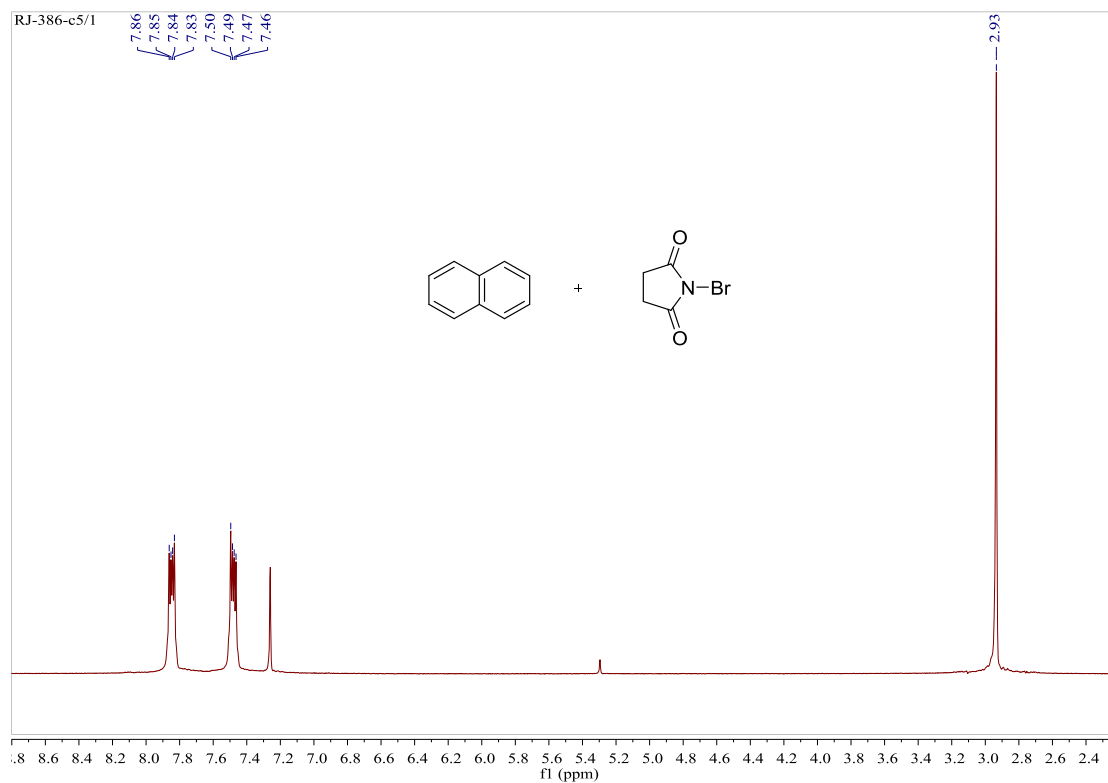
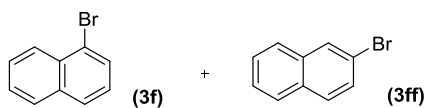
1-bromo-2,4-dimethylbenzene



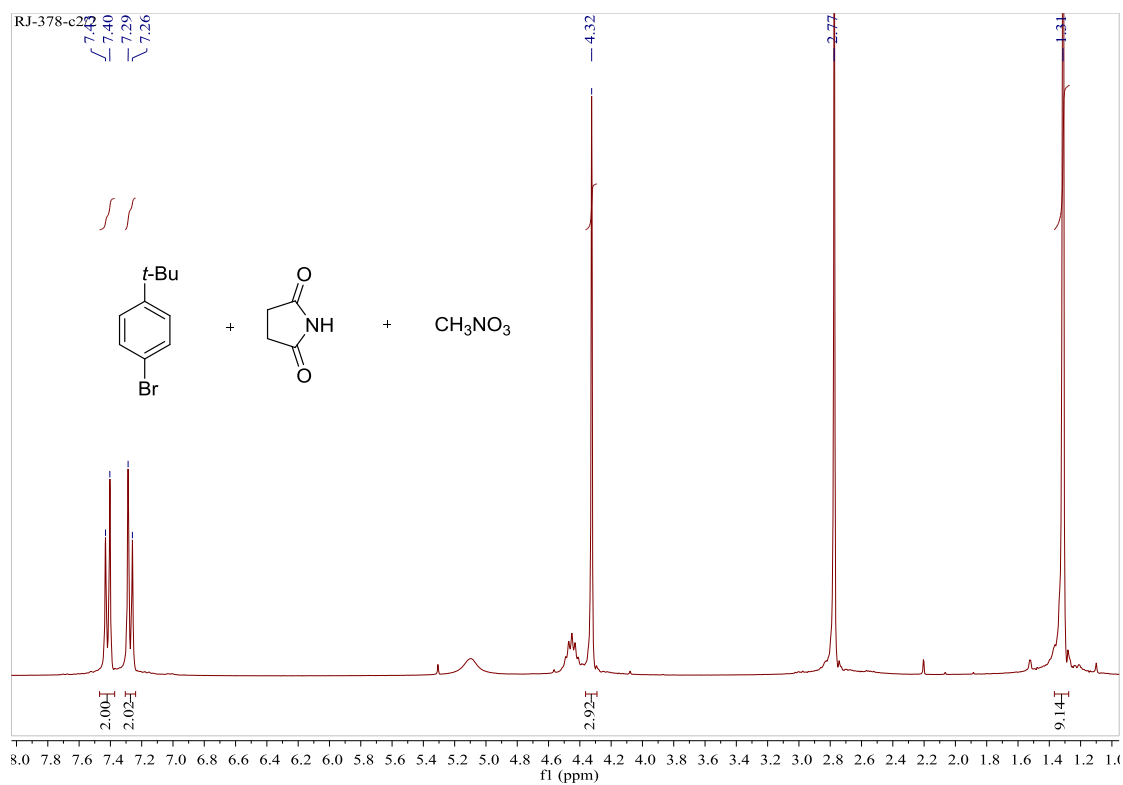
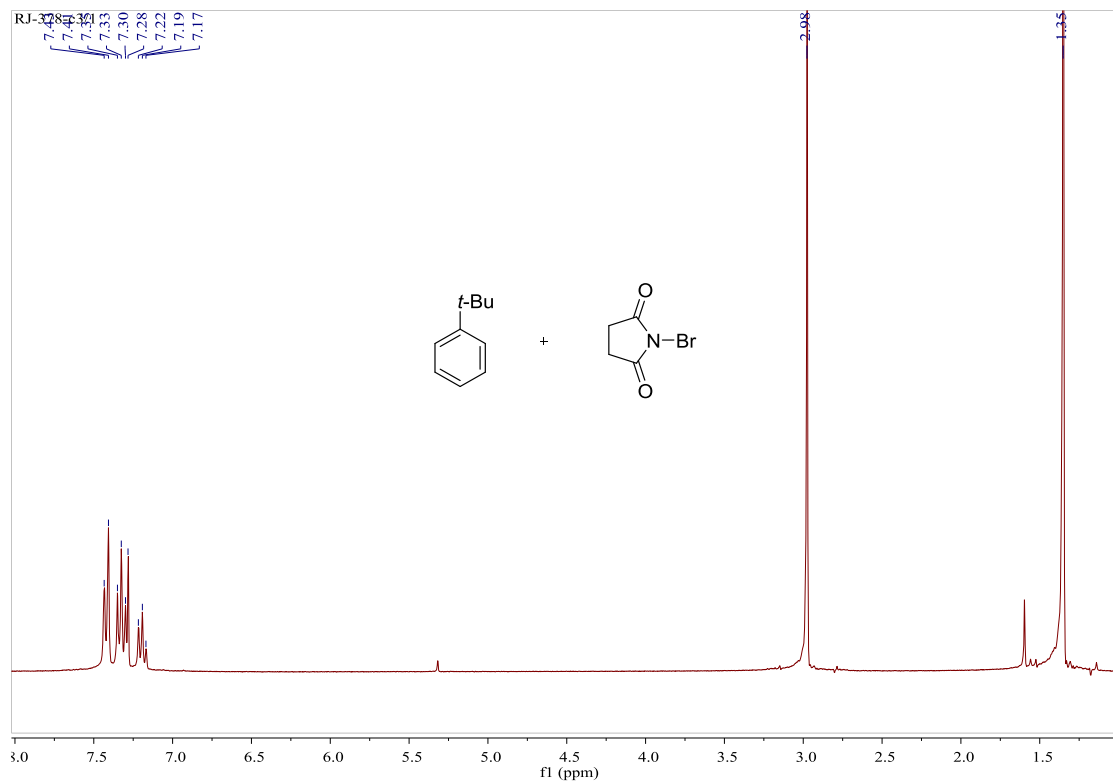
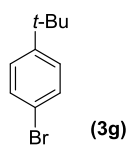
1-bromo-2,3-dimethylbenzene and 4-bromo-1,2-dimethylbenzene (4.8:1)



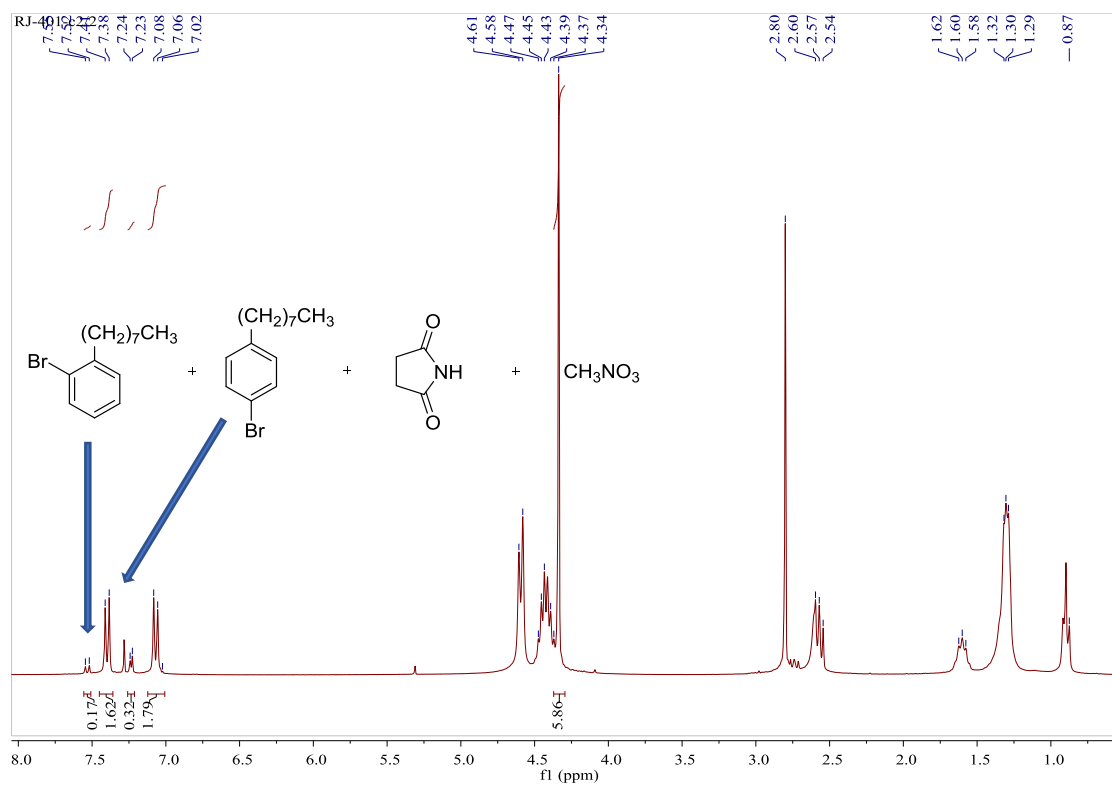
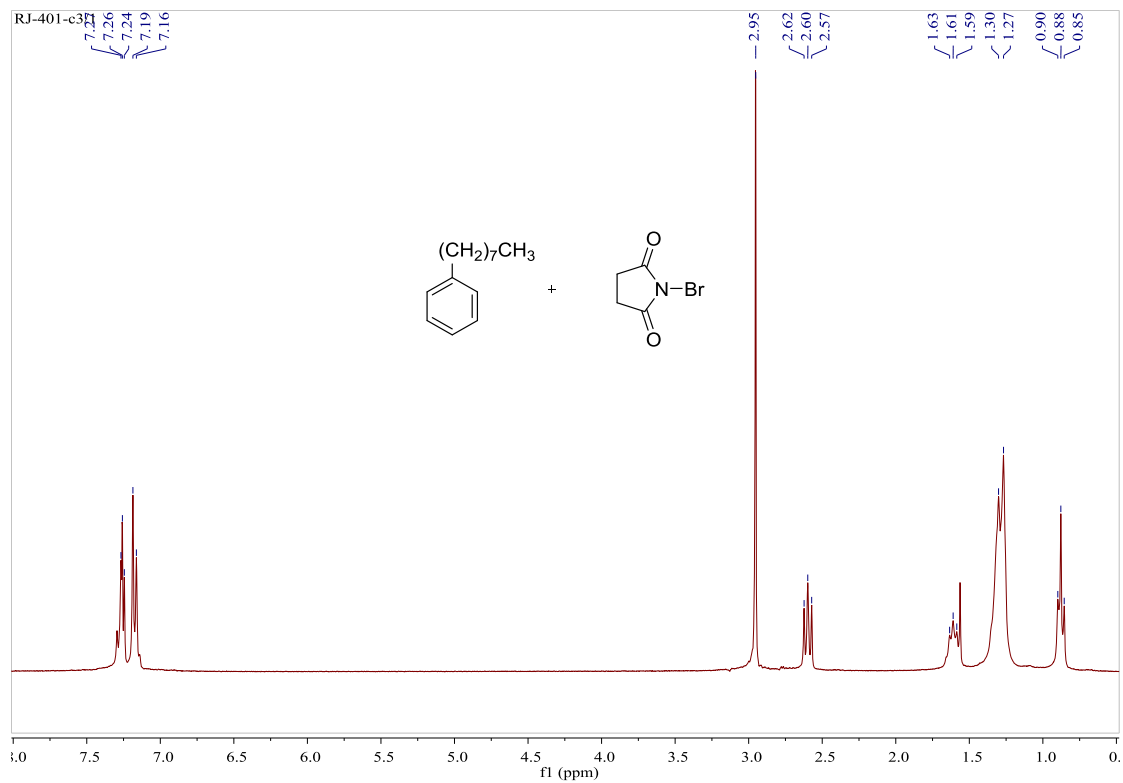
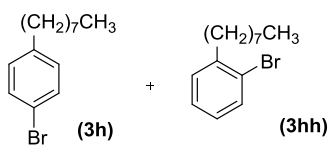
1-bromonaphthalene compound with 2-bromonaphthalene (24:1)



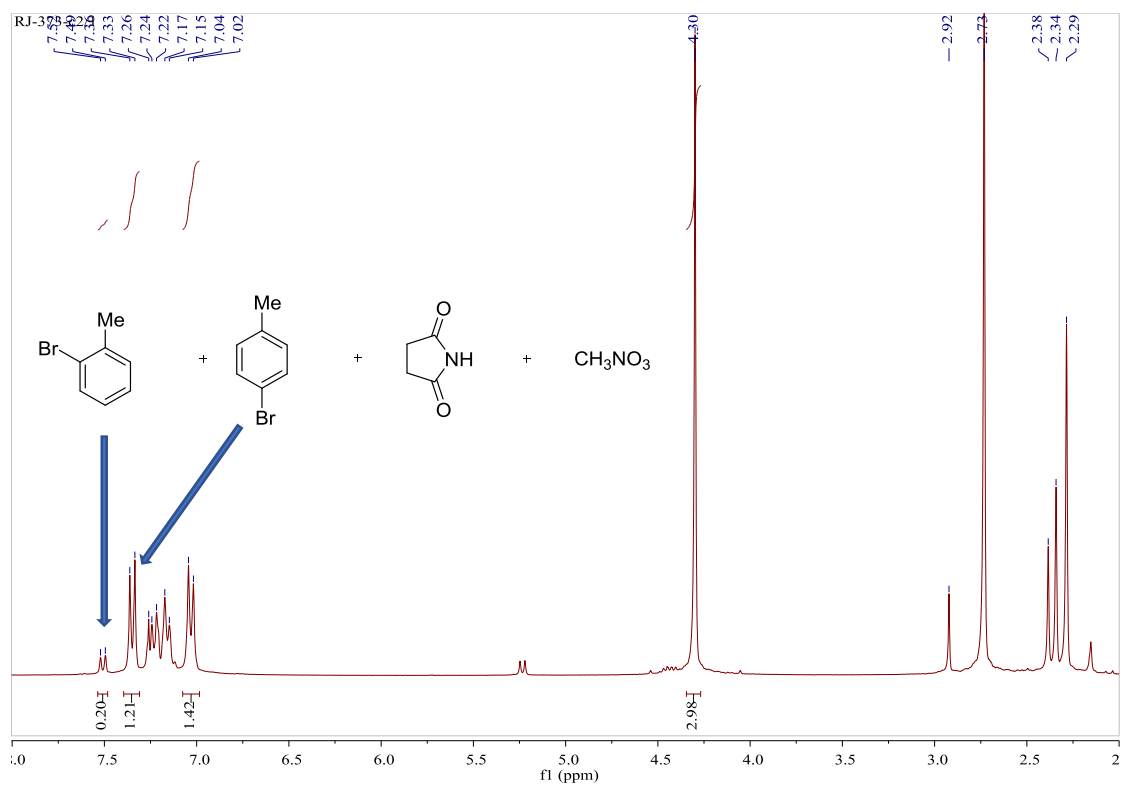
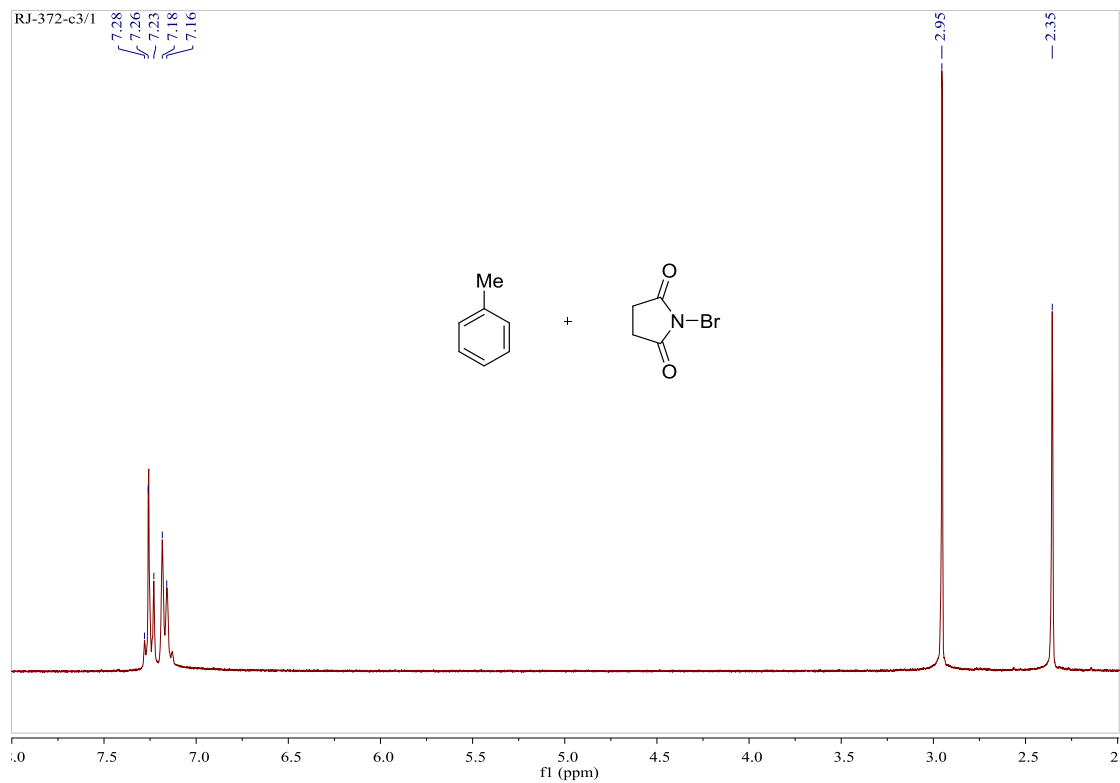
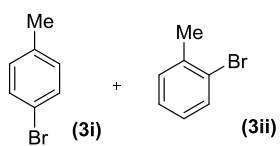
1-bromo-4-(tert-butyl)benzene



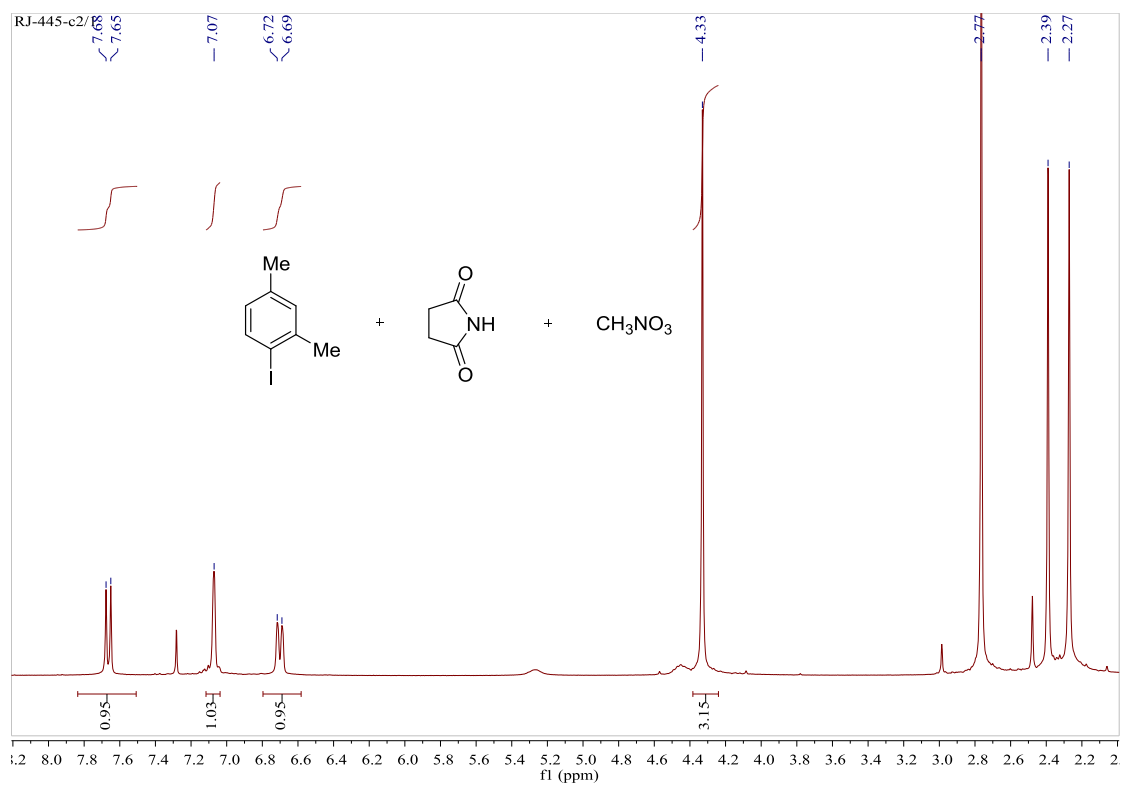
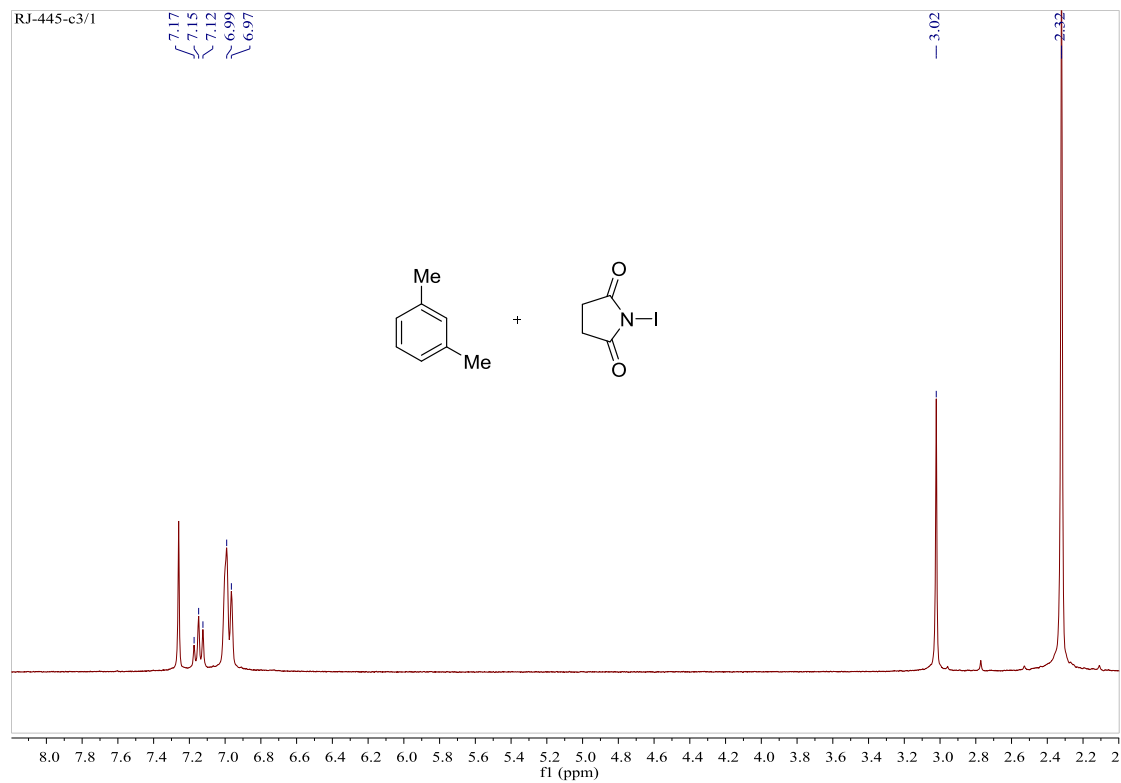
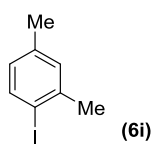
1-bromo-2-octylbenzene and 1-bromo-4-octylbenzene (4.8:1)



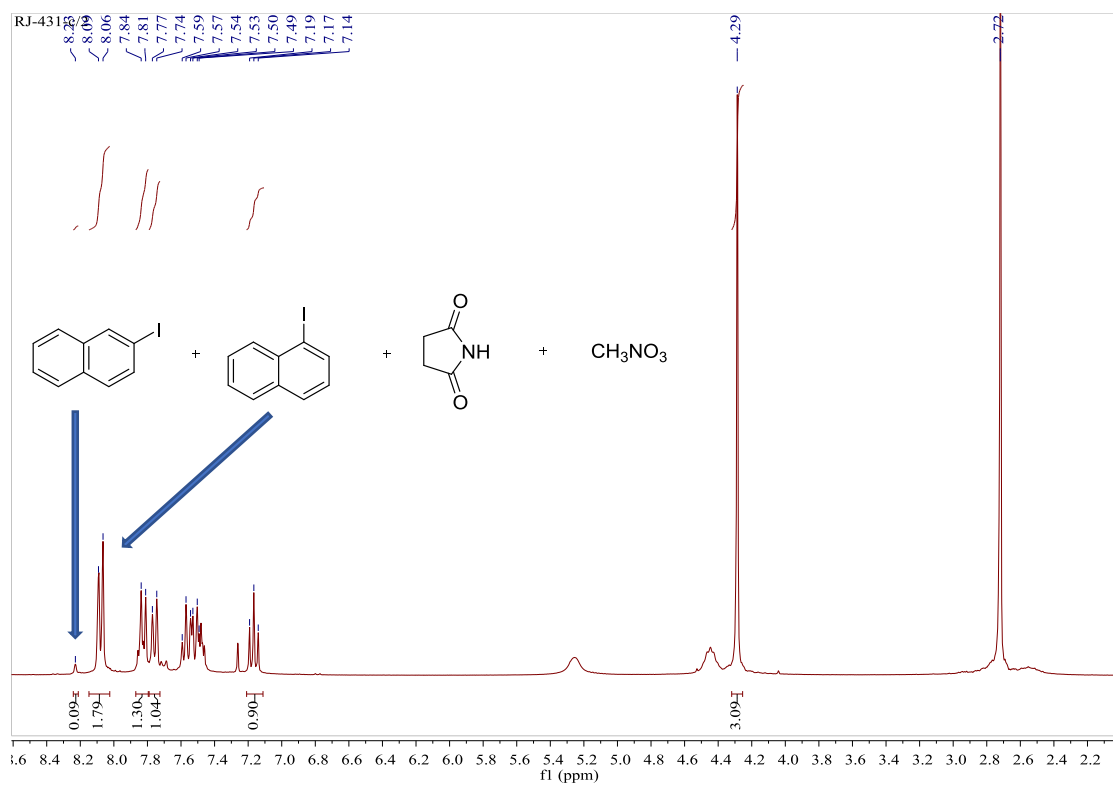
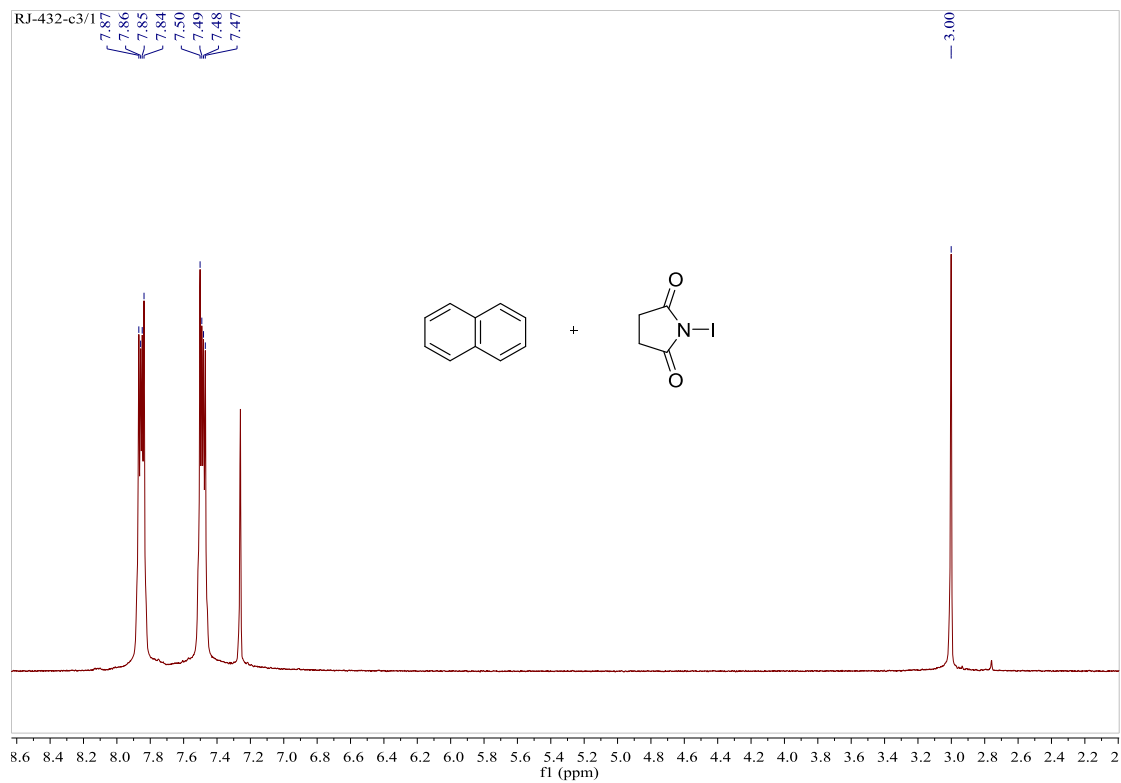
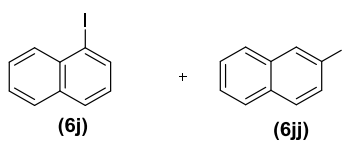
1-bromo-2-methylbenzene and 1-bromo-4-methylbenzene (3.0:1)



1-iodo-2,4-dimethylbenzene



iodonaphthalene and 2-iodonaphthalene (10:1)



2-chloro-1,3,5-trimethylbenzene

