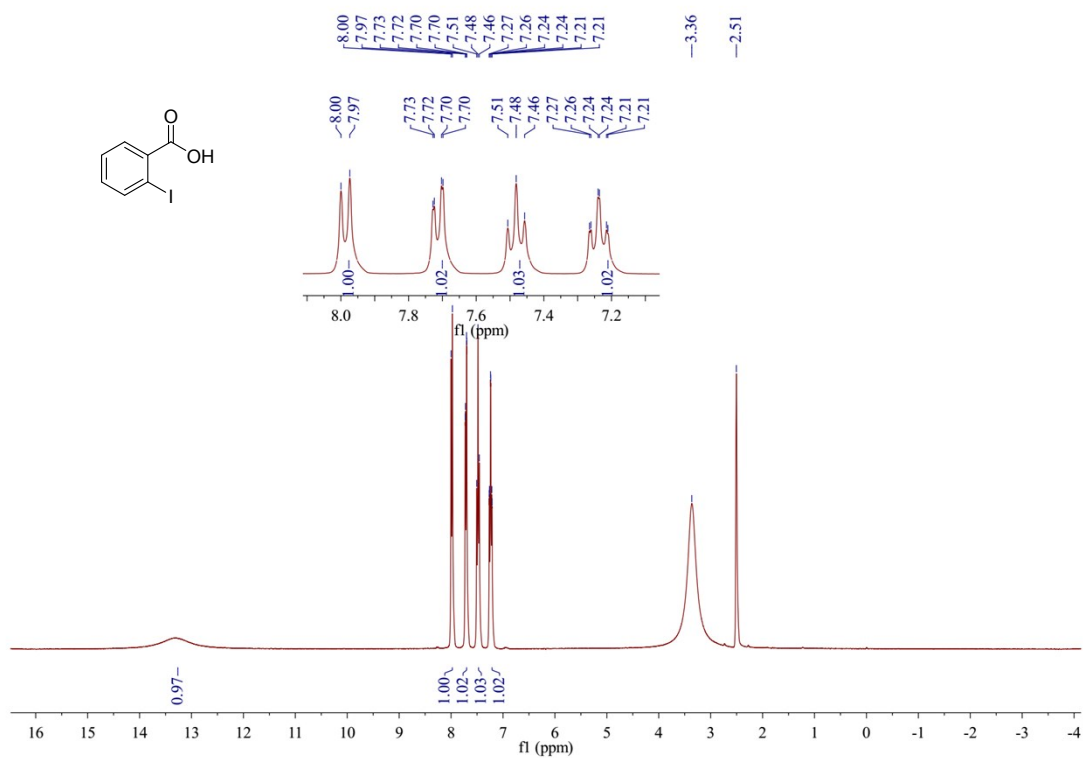
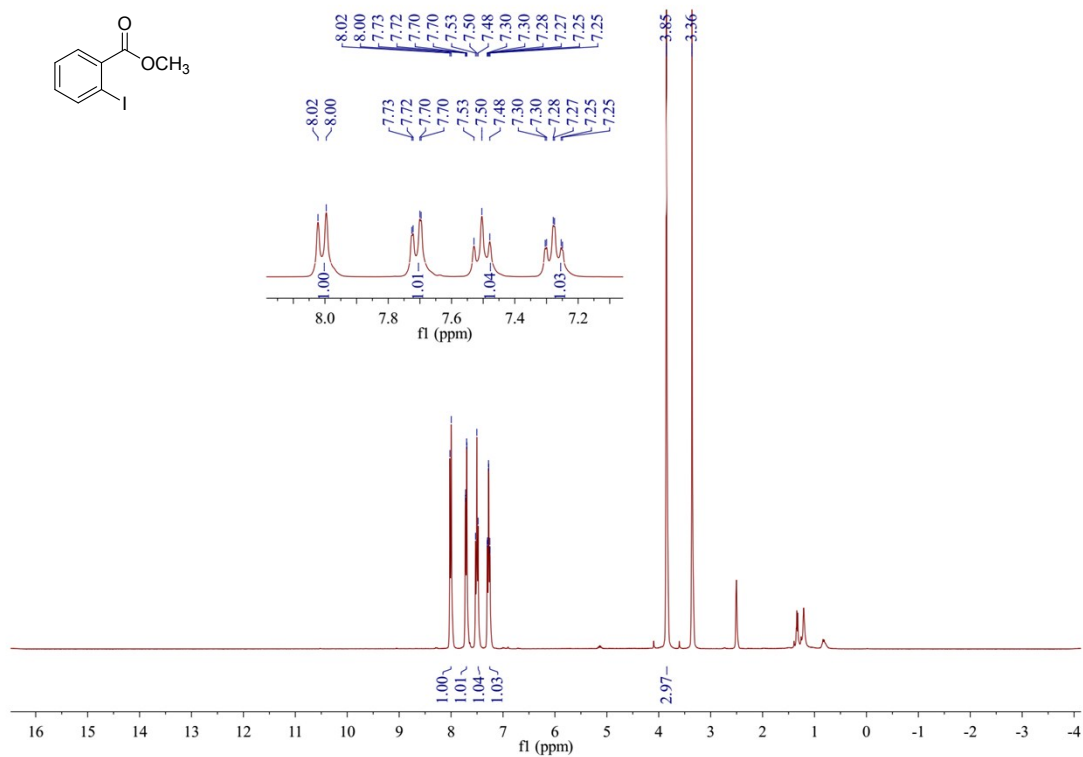


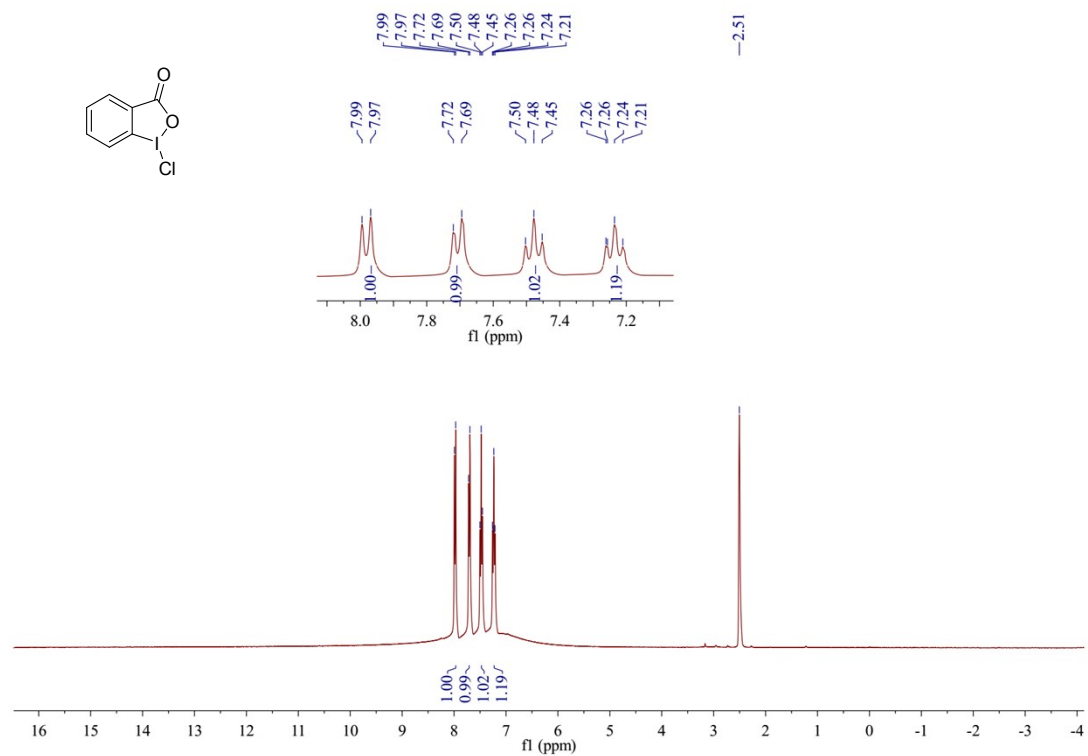
2-Iodobenzoic acid (300 MHz, DMSO-*d*<sub>6</sub>)



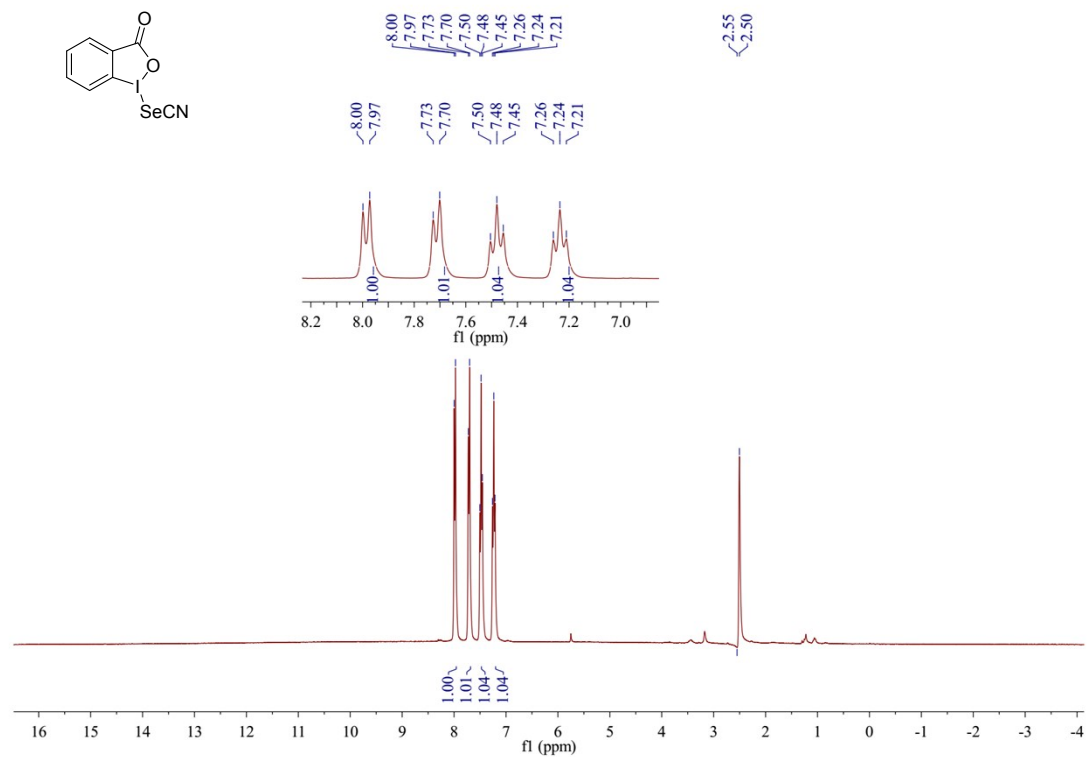
Methyl 2-Iodobenzoate ester (300 MHz, DMSO-*d*<sub>6</sub>)



BI-Cl (300 MHz, DMSO-*d*<sub>6</sub>)

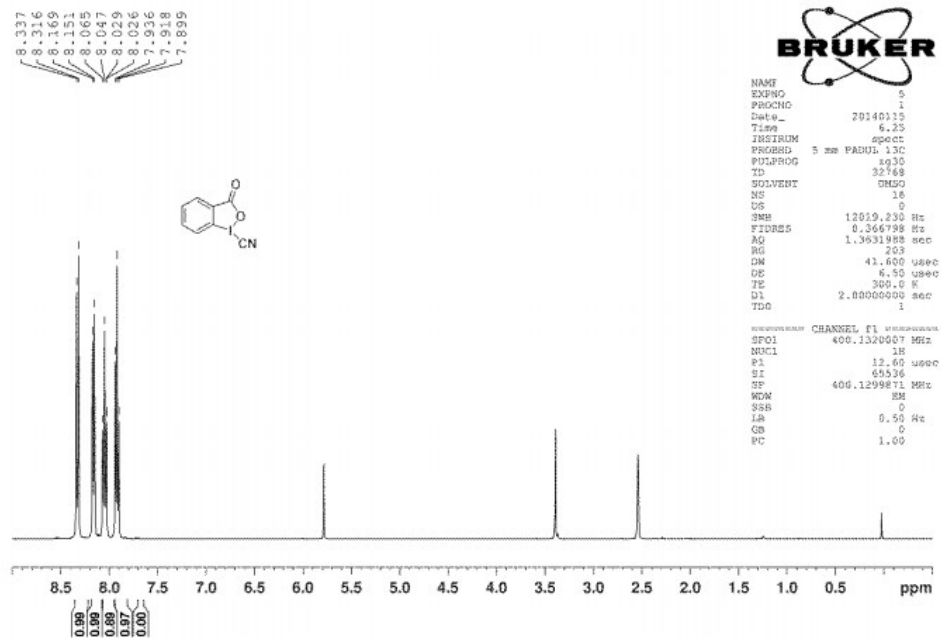


BI-SeCN (300 MHz, DMSO-*d*<sub>6</sub>)

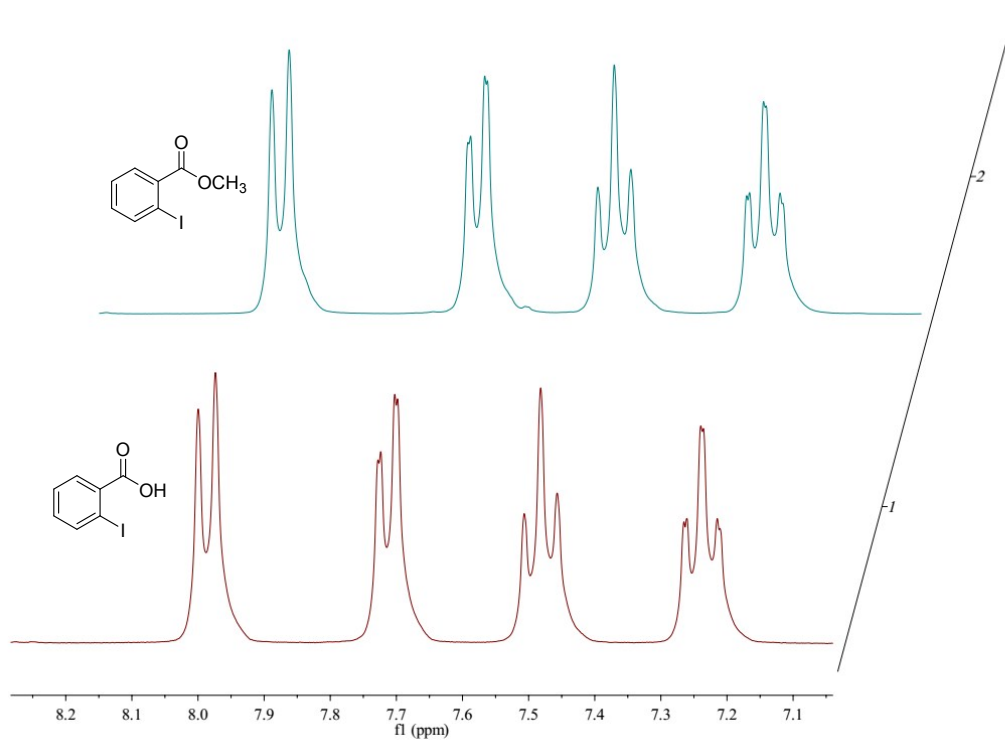


BI-CN (400 MHz, DMSO-*d*<sub>6</sub>) (Q.-Y. Zheng et al, *Org. Biomol. Chem.*, 2015, 13(33):8812-8816)

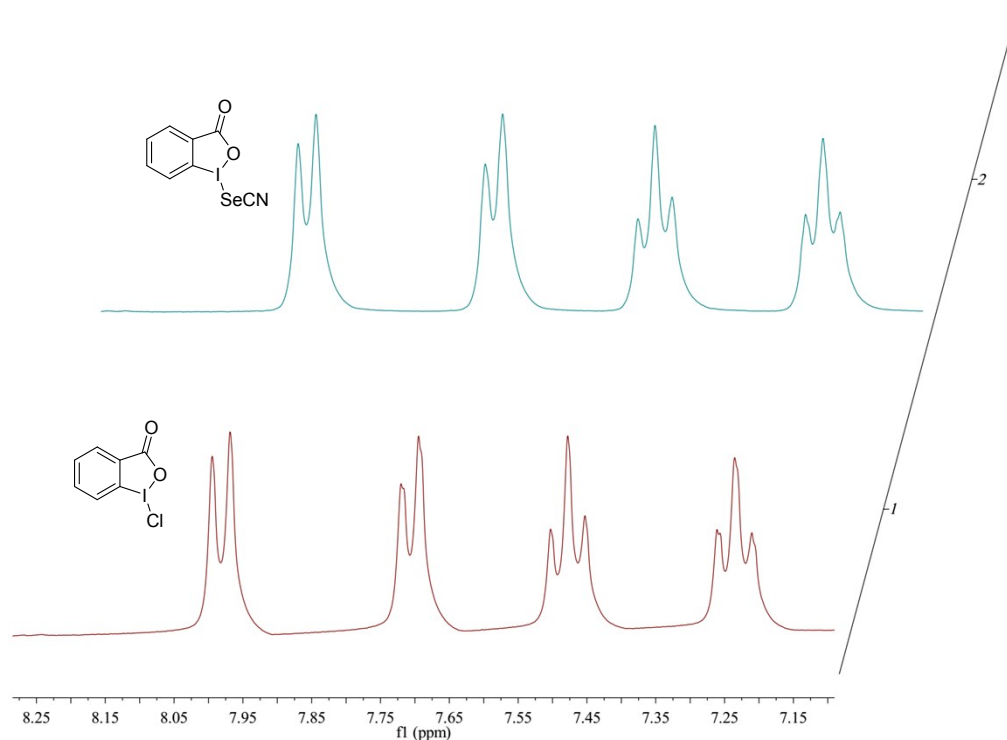
### 1-Cyano-1,2-benziodoxol-3-(1H)-one



<sup>1</sup>H NMR comparison of 2-Iodobenzoic acid and Methyl 2-Iodobenzoate ester



# <sup>1</sup>H NMR comparison of BI-Cl and BI-SeCN



## XRD analysis of the selenocyanation reagent BI-SeCN

Cell: Space group : Triclinic P-1  
 a = 2.27(1)                      b = 3.81(6)                      c = 6.51(1)  
 alpha = 107(1)                      beta = 94(3)                      gamma = 99(3)  
 Volume = 53(3)  
 N = 13                      min = 0.86 Å                      max = 6.17 Å  
 I/Sig = 1.0                      obs = 7.7%                      I/SigO = 4.4

