Electronic Supplementary Material (ESI) for Green Chemistry

Engaging Isatins in Solvent-Free, Sterically Congested Passerini Reaction

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Supporting Information

1. General Information

Unless otherwise specified, all reactions were carried out under air in flame-dried reaction vessels with Teflon screw caps. Reaction temperatures are reported as the temperature of the bath surrounding the reaction vessel. Dry CH_2Cl_2, $CHCl_3$, $(CH_2Cl)_2$, and CH_3CN were purchased from commercial sources and stored under argon over 4 Å molecular sieves. THF was purified by distillation over Na-benzophenone and was transferred under argon. The carboxylic acids and 2-nitrophenol were purchased from commercial sources and used as received without any further purification. The isocyanides were purchased from Sigma Aldrich and used as received, without any further purification. The isatin derivatives were purchased from Sigma Aldrich or Acros and the *N*-alkylation was carried out by treating with the corresponding alkyl halides under basic condition following the known procedure.[1]

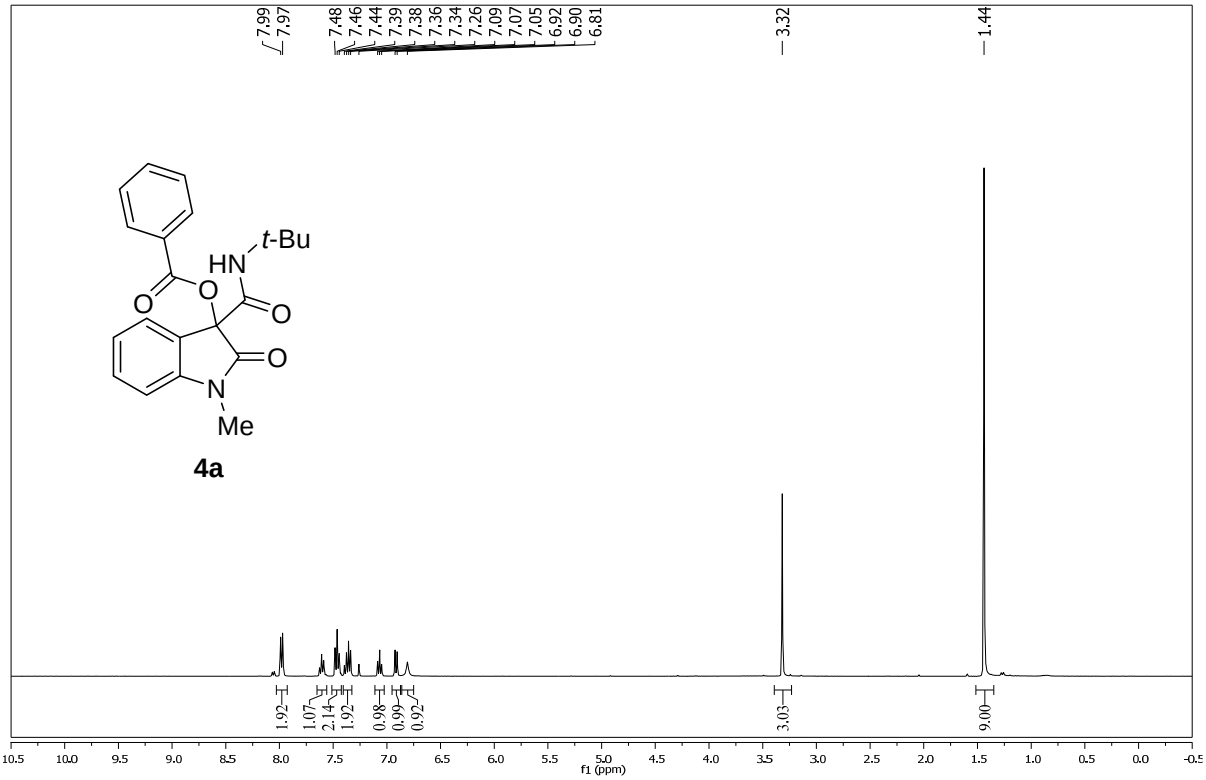
Analytical thin layer chromatography was performed on TLC Silica gel 60 F_{254}. Visualization was accomplished with short wave UV light or $KMnO_4$ staining solutions followed by heating. Chromatography was performed on silica gel (230-400 mesh) by standard techniques eluting with solvents as indicated.

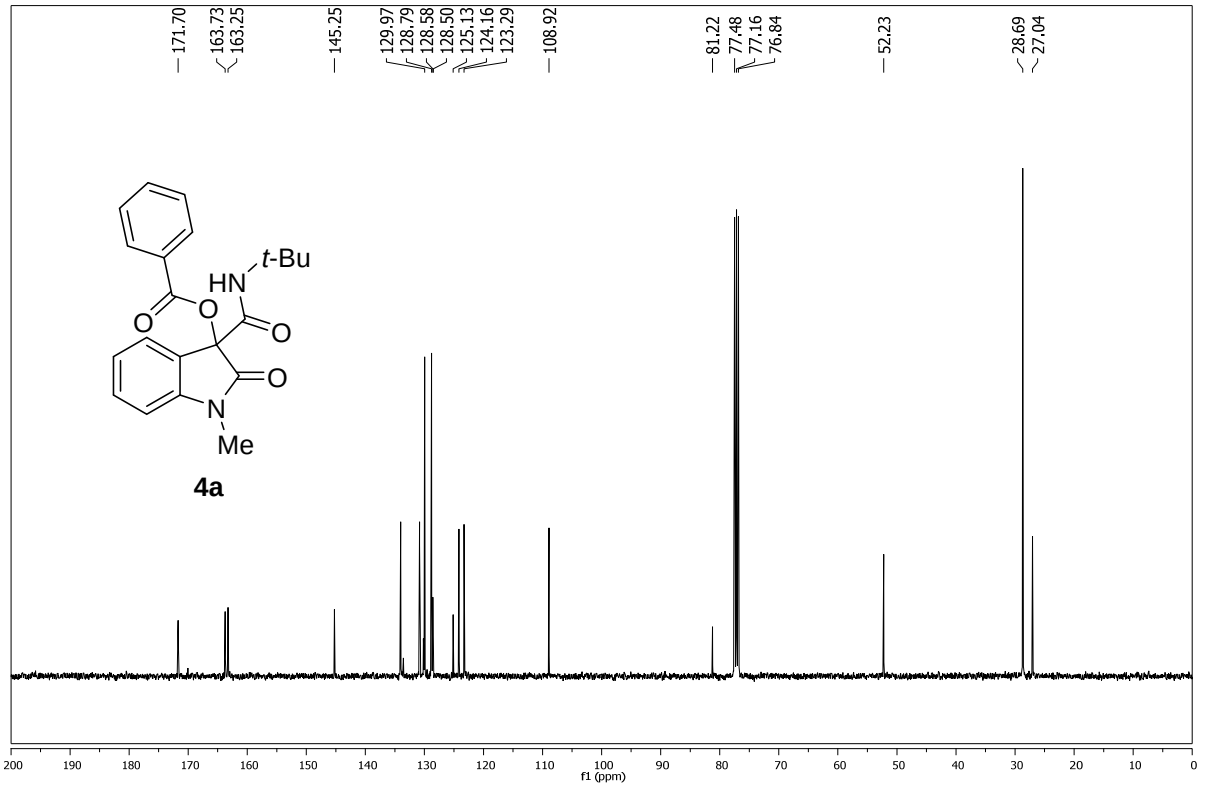
All compounds were fully characterized. ^1H and ^{13}C NMR spectra were recorded on Bruker AV 400, in solvents as indicated. Chemical shifts (δ) are given in ppm. The residual solvent signals were used as references and the chemical shifts converted to the TMS scale ($CDCl_3$: δH = 7.26 ppm, δC = 77.16 ppm). Infrared spectra were recorded on a Perkin-Elmer 1615 FT Infrared Spectrophotometer Model 60B. The wave numbers (n) of recorded IR-signals are quoted in cm^{-1}. HRMS data were recorded on a Thermo Scientific Q-Exactive, Accela 1250 pump.

[1] B. M. Trost, Y. Zhang, *J. Am. Chem. Soc.*, 2007, **129**, 14548.

2. ^{1}H and ^{13}C NMR Spectra of Oxindole Derivatives

3-(*tert*-Butylcarbamoyl)-1-methyl-2-oxoindolin-3-yl benzoate (4a)





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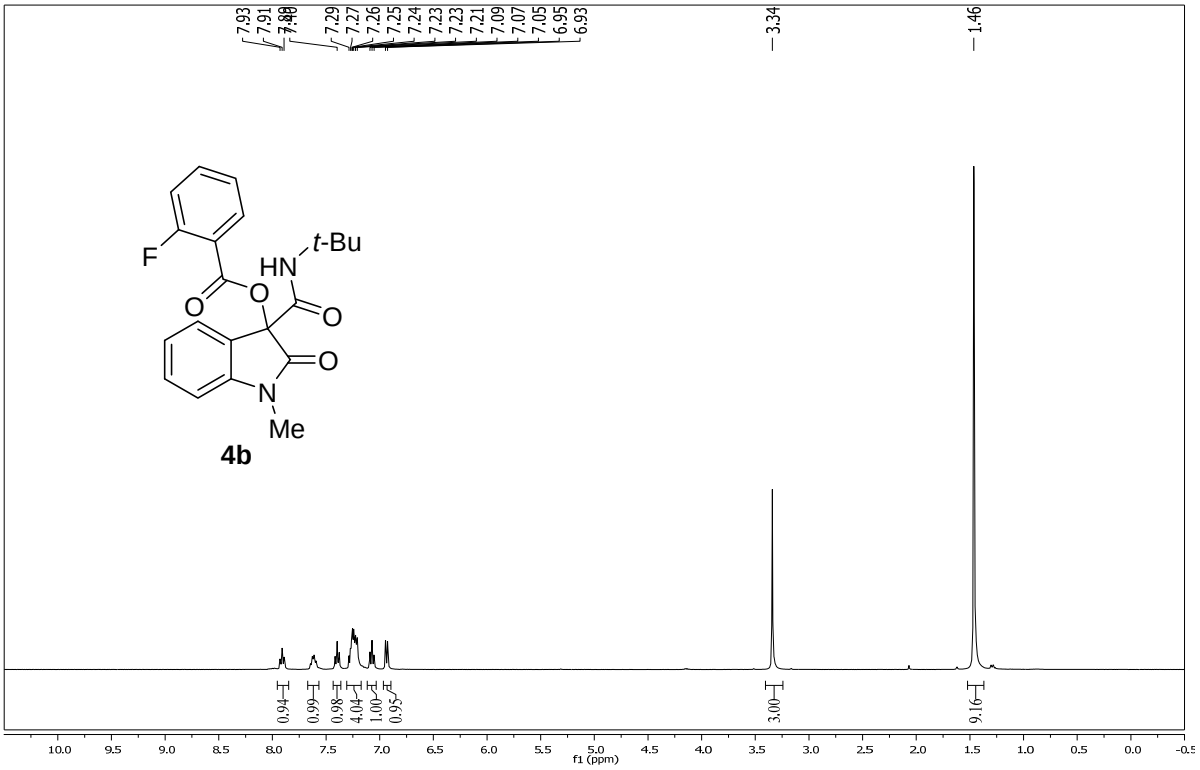

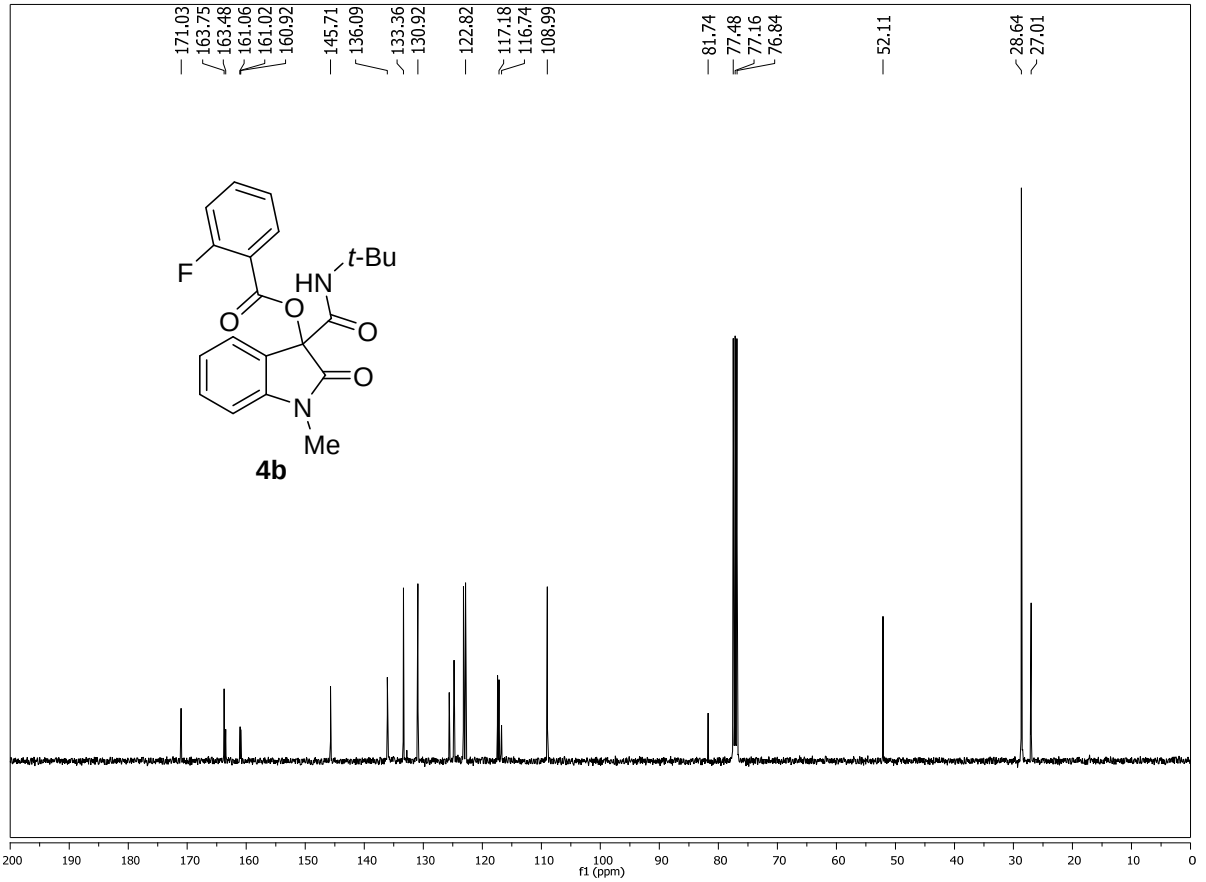

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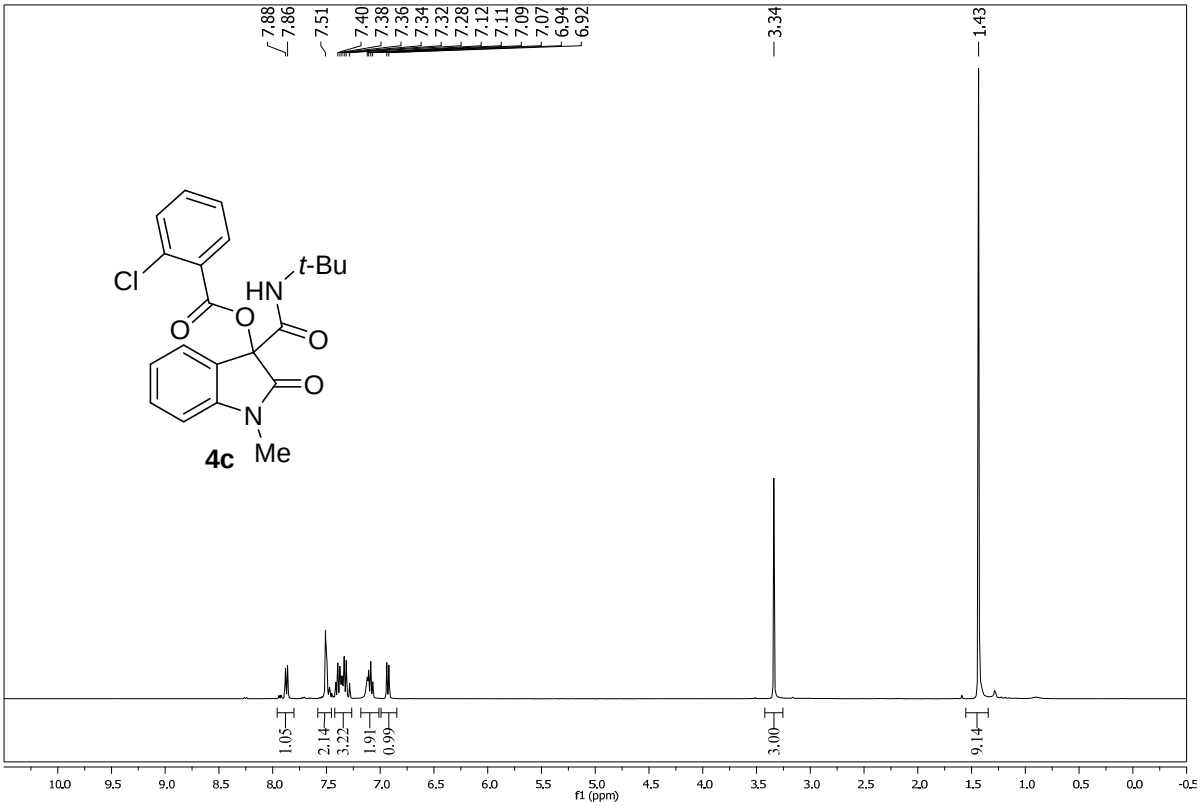

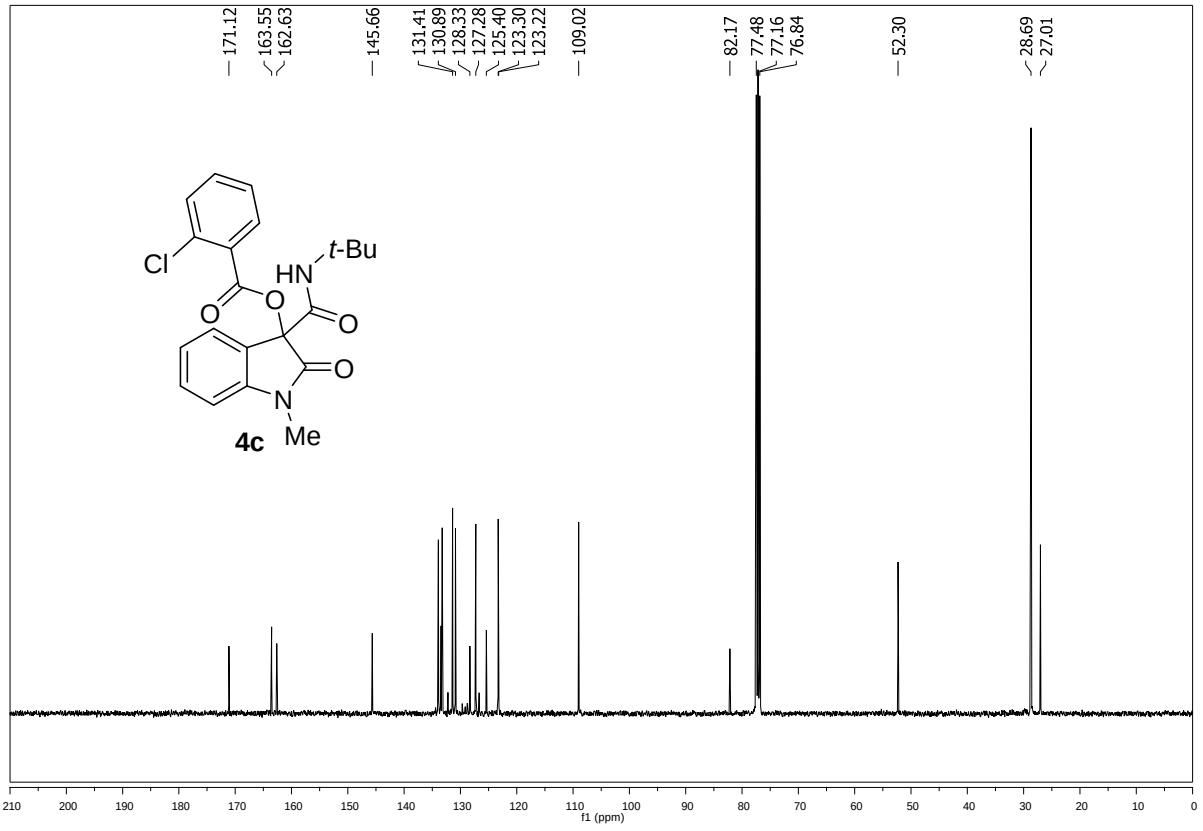

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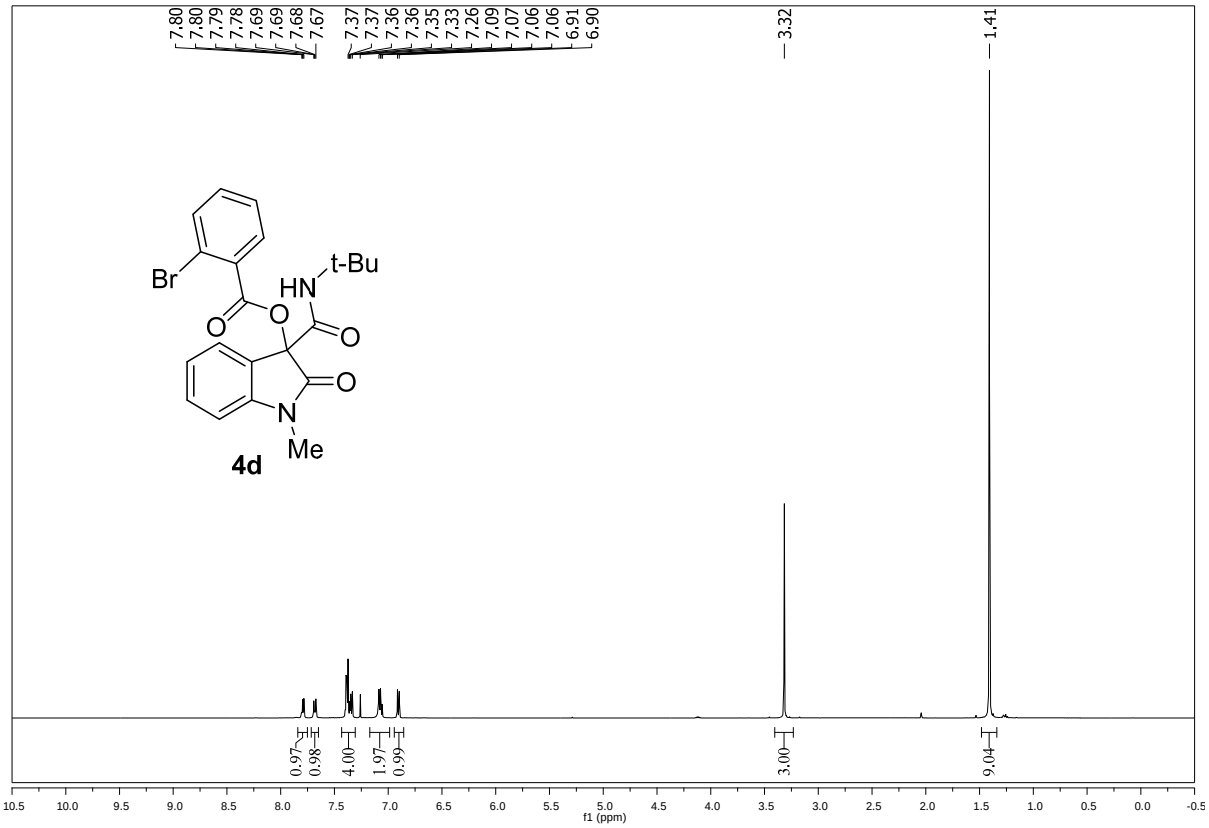

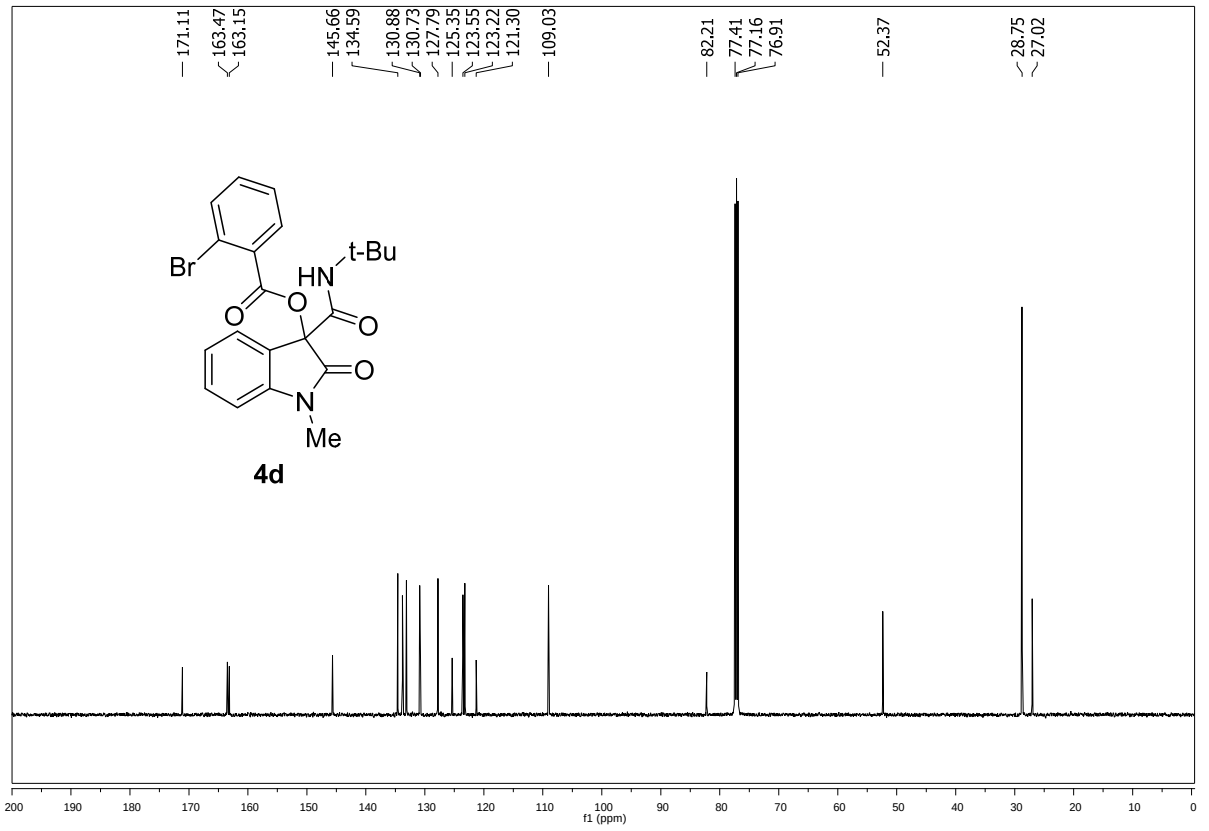

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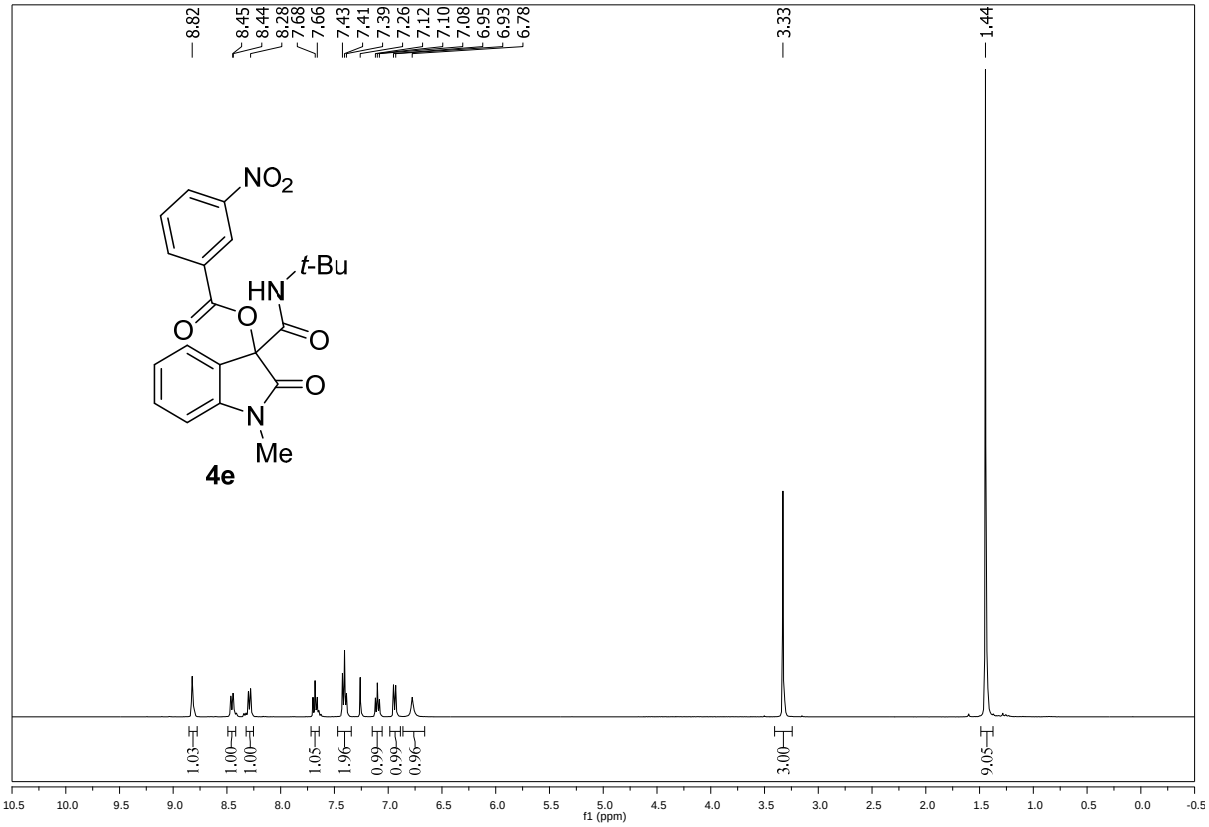

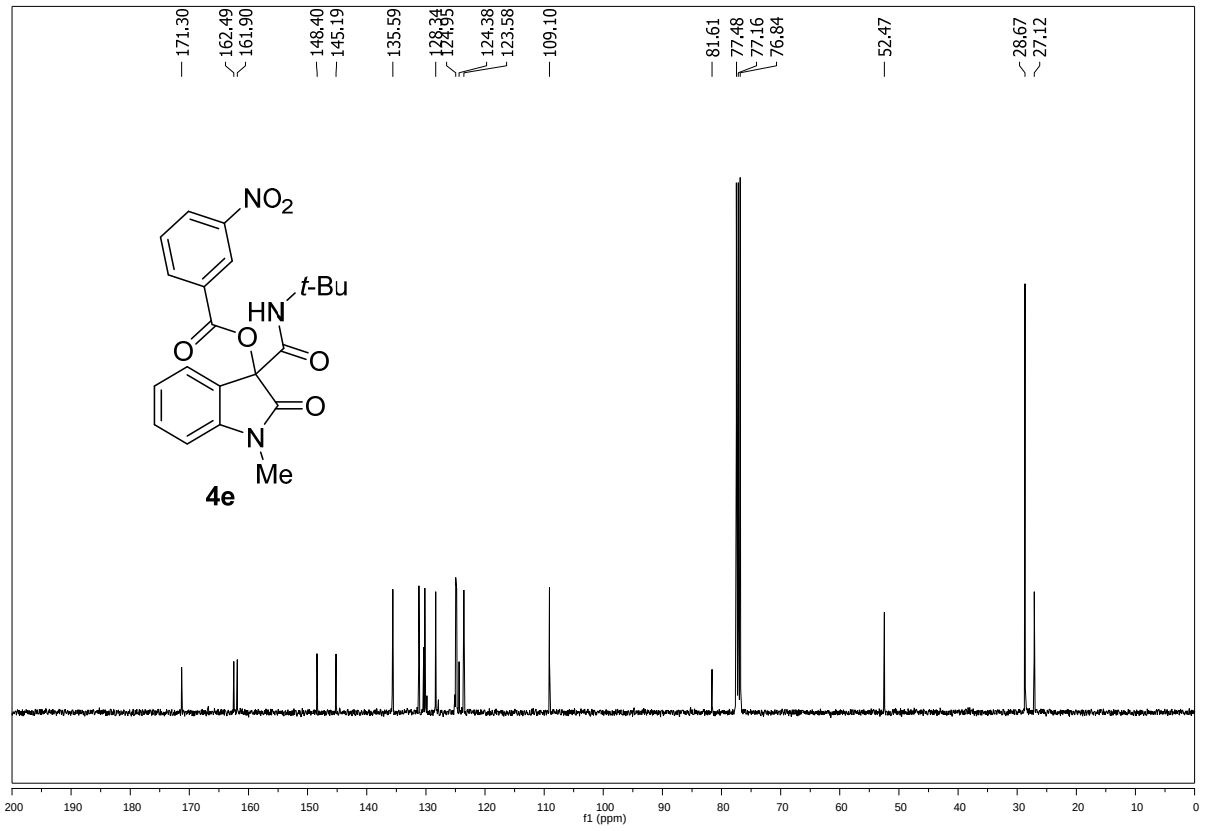

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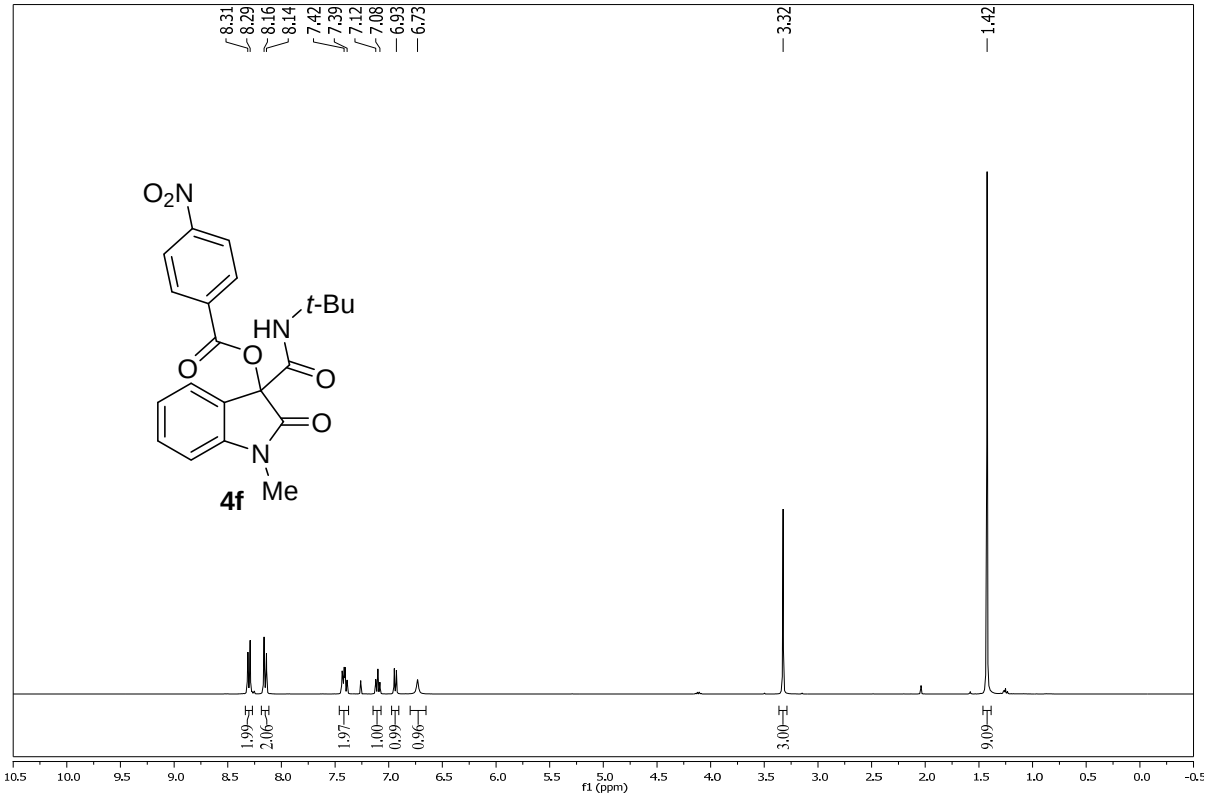

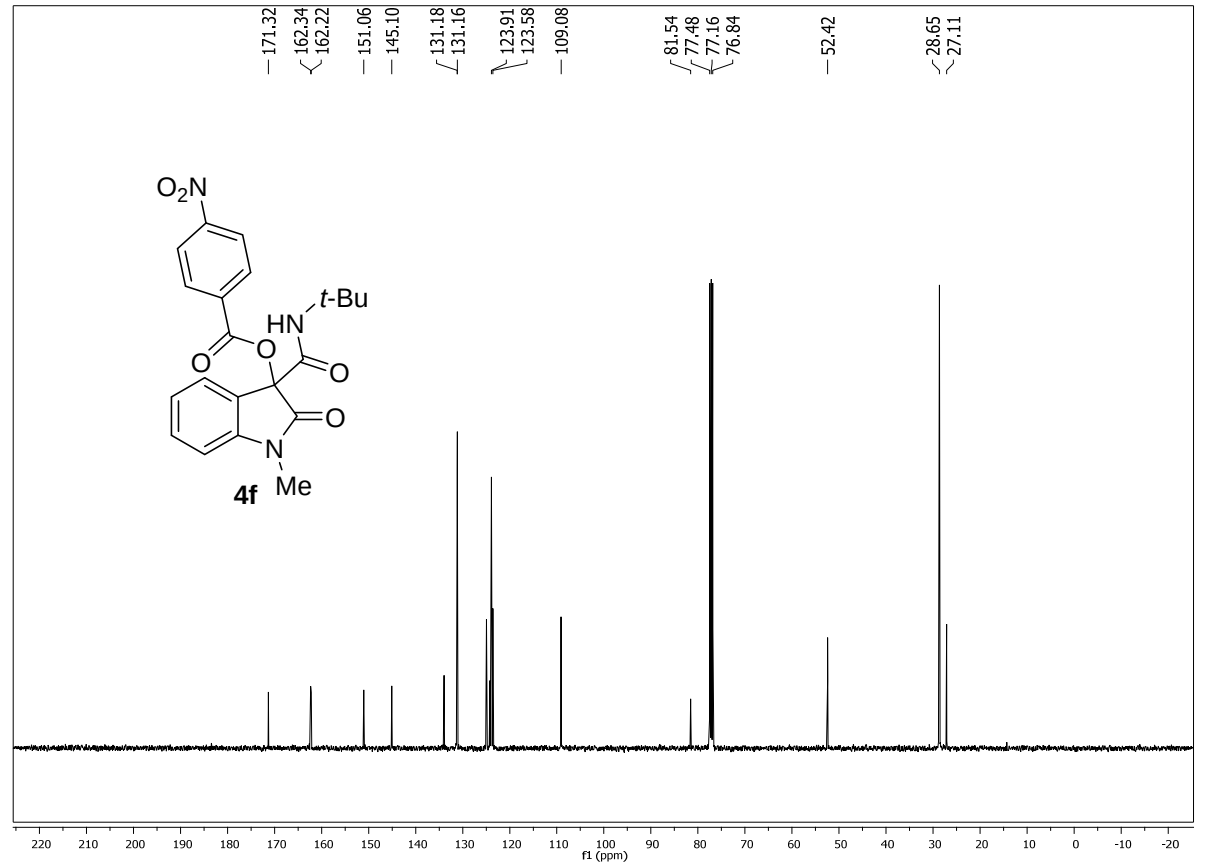

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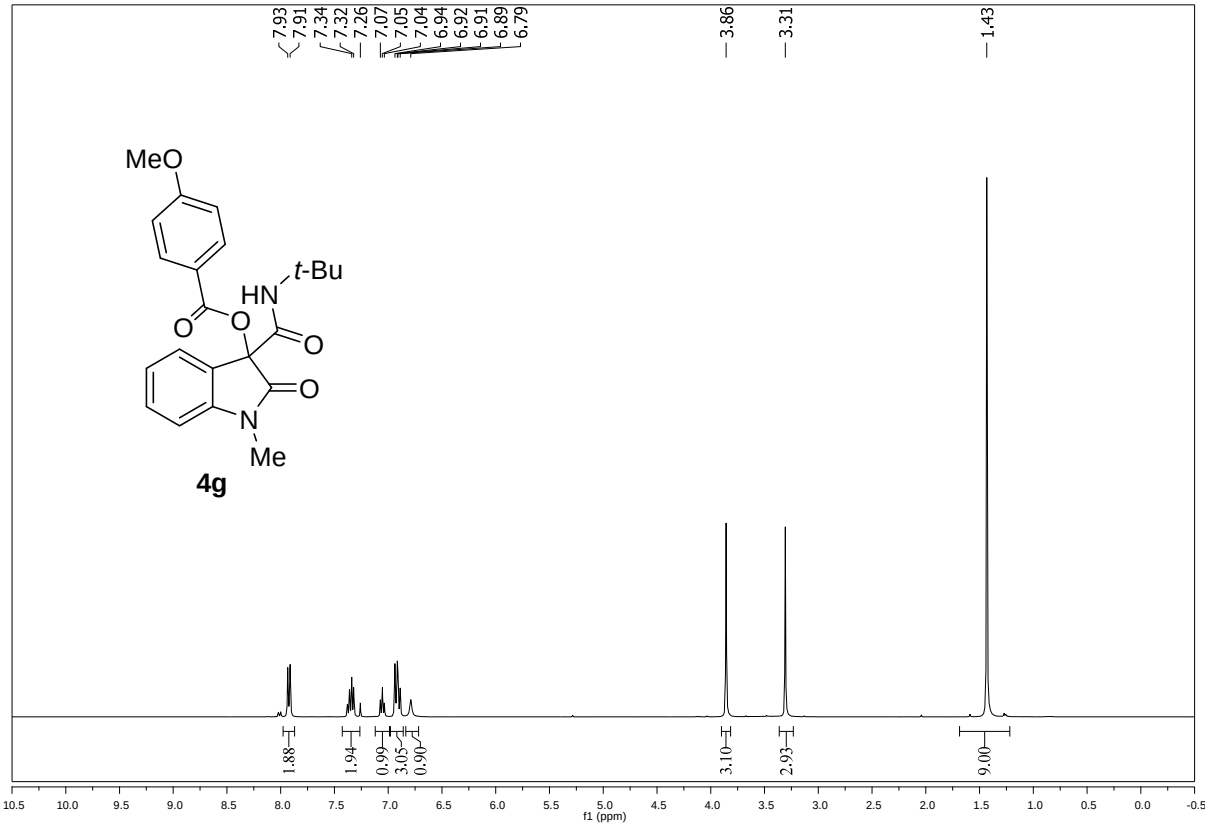
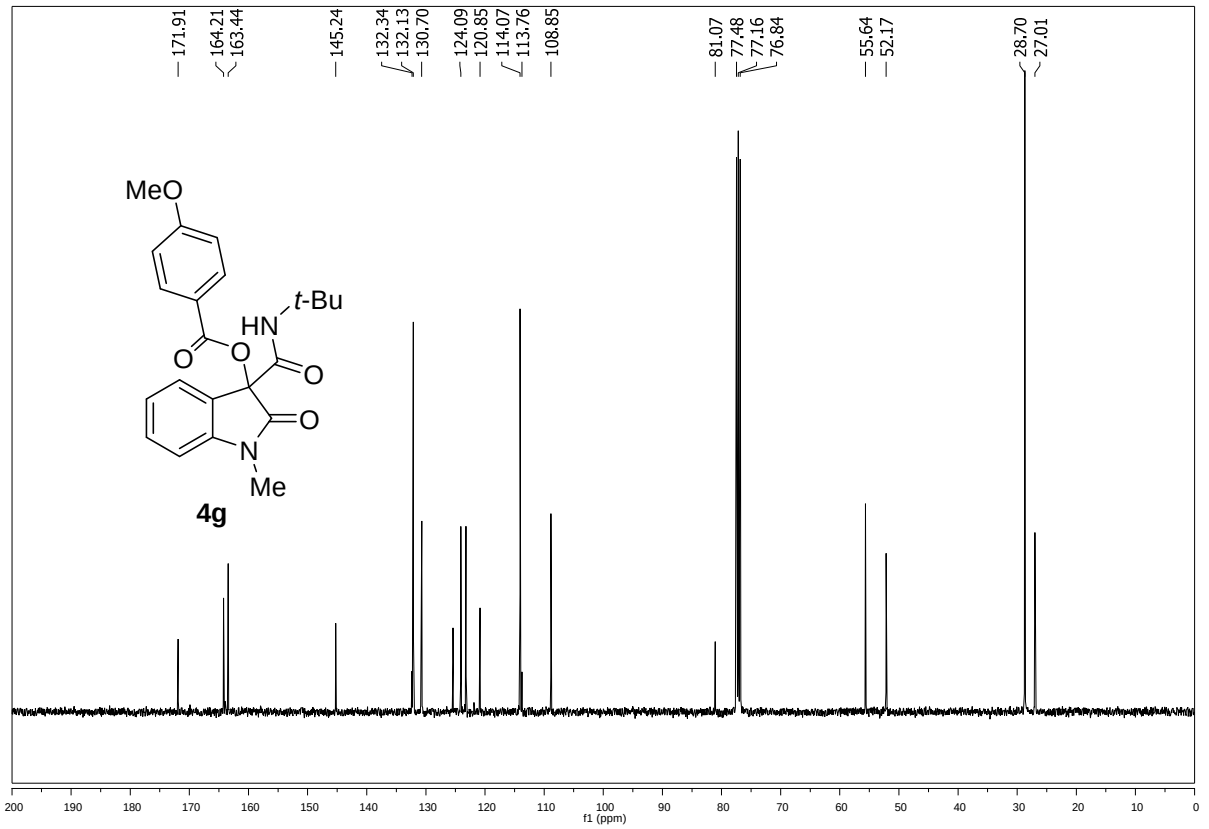
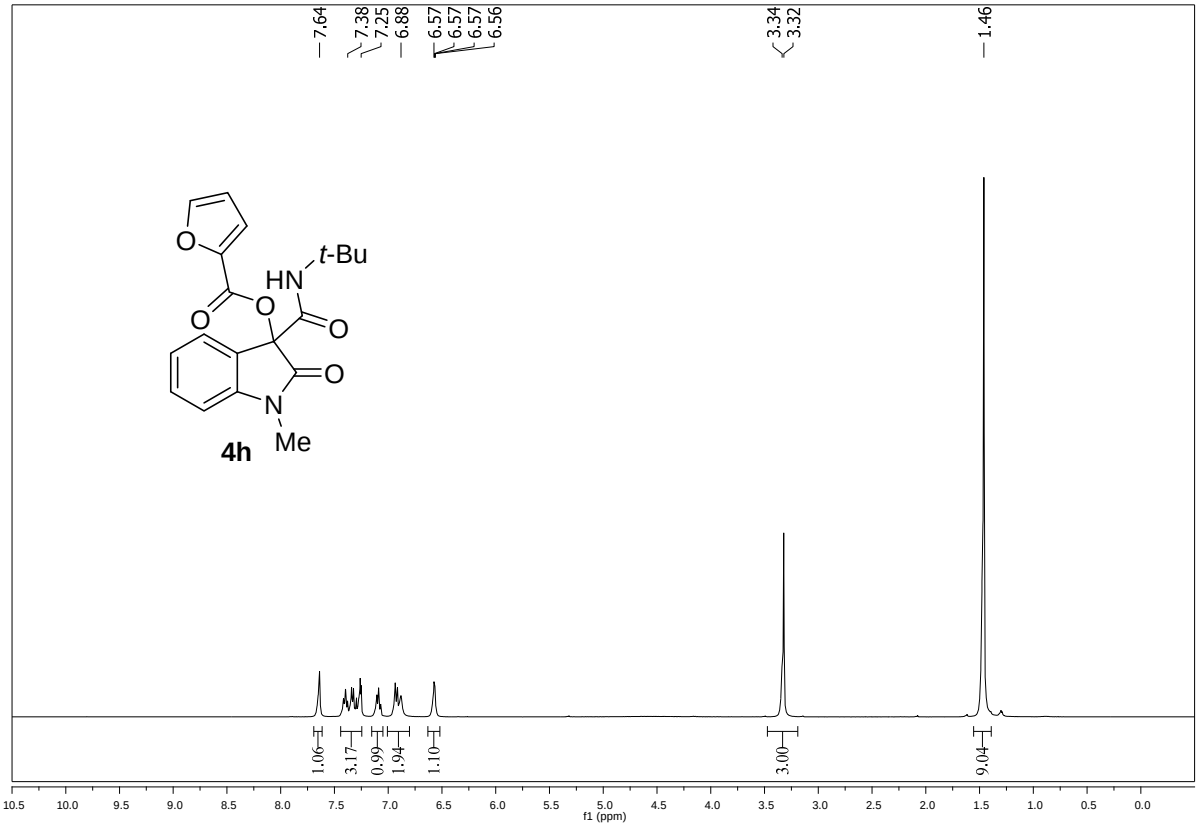
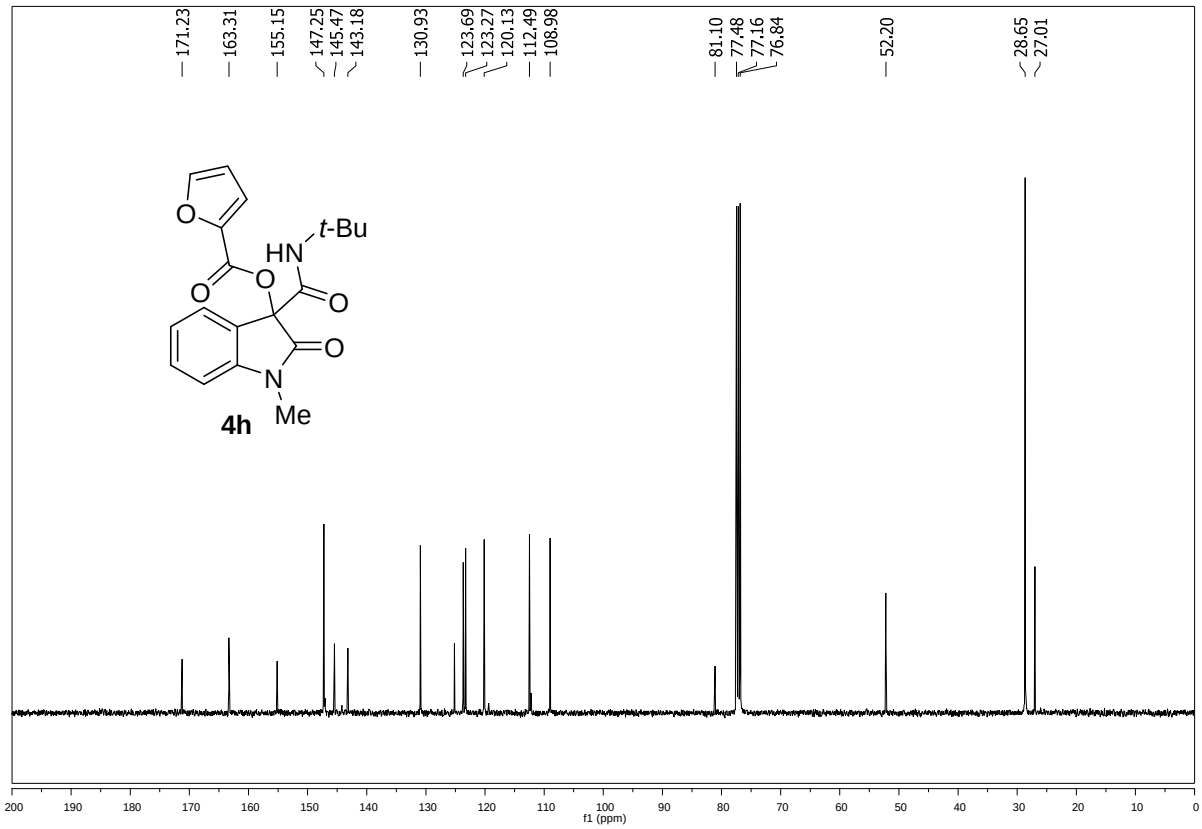


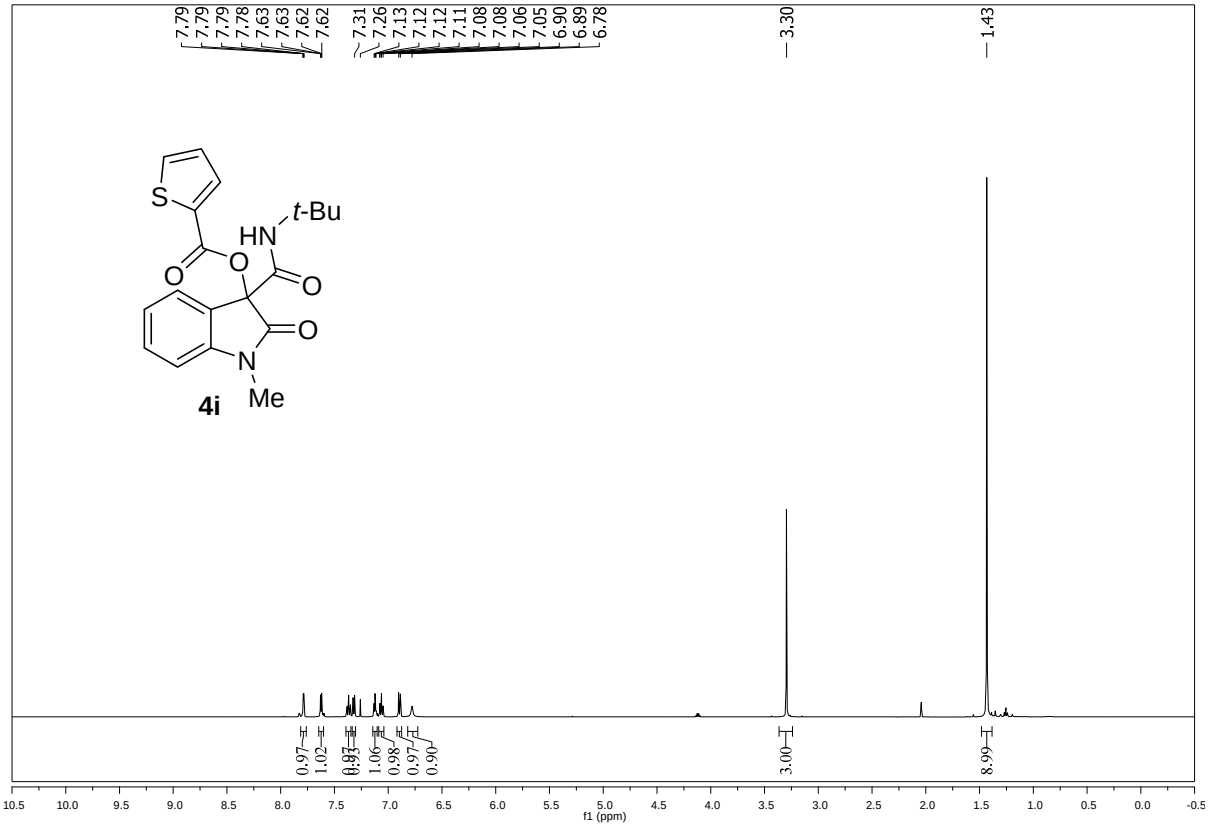


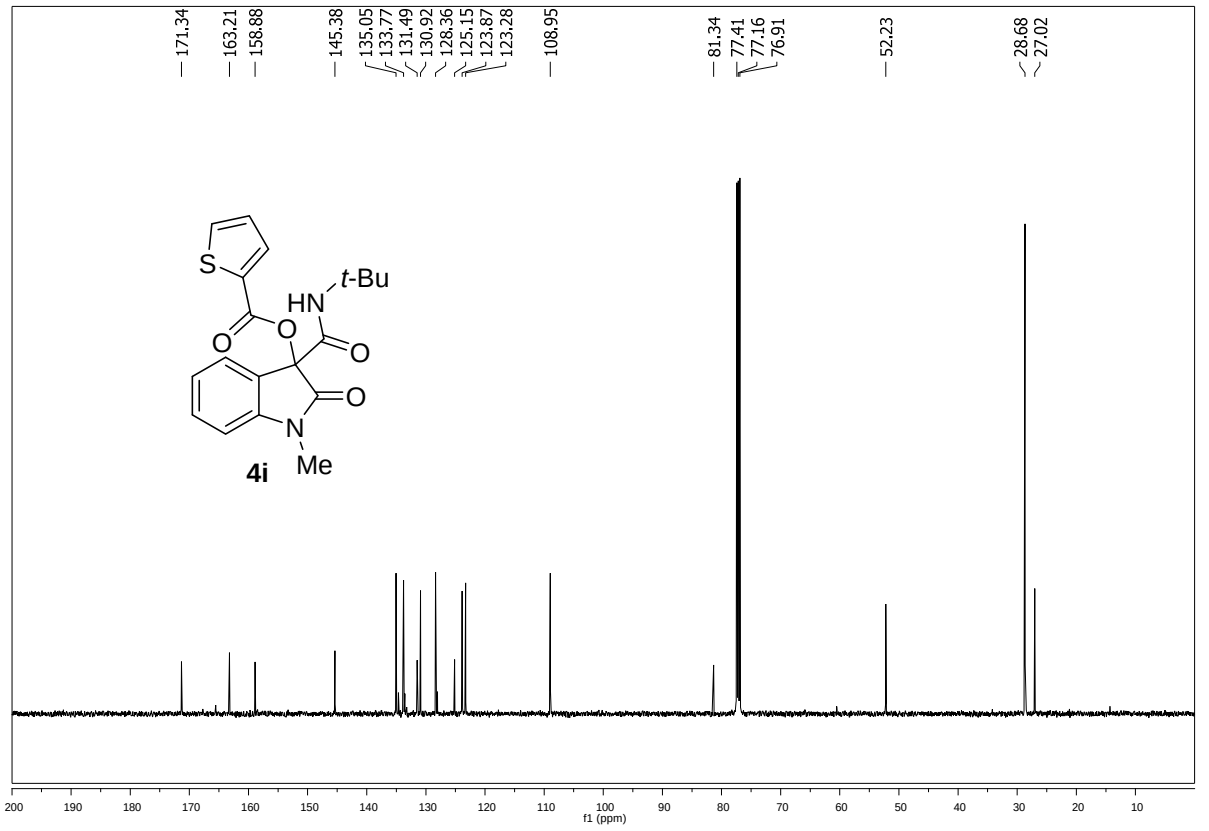
3-(*tert*-Butylcarbamoyl)-1-methyl-2-oxoindolin-3-yl furan-2-carboxylate (4h)



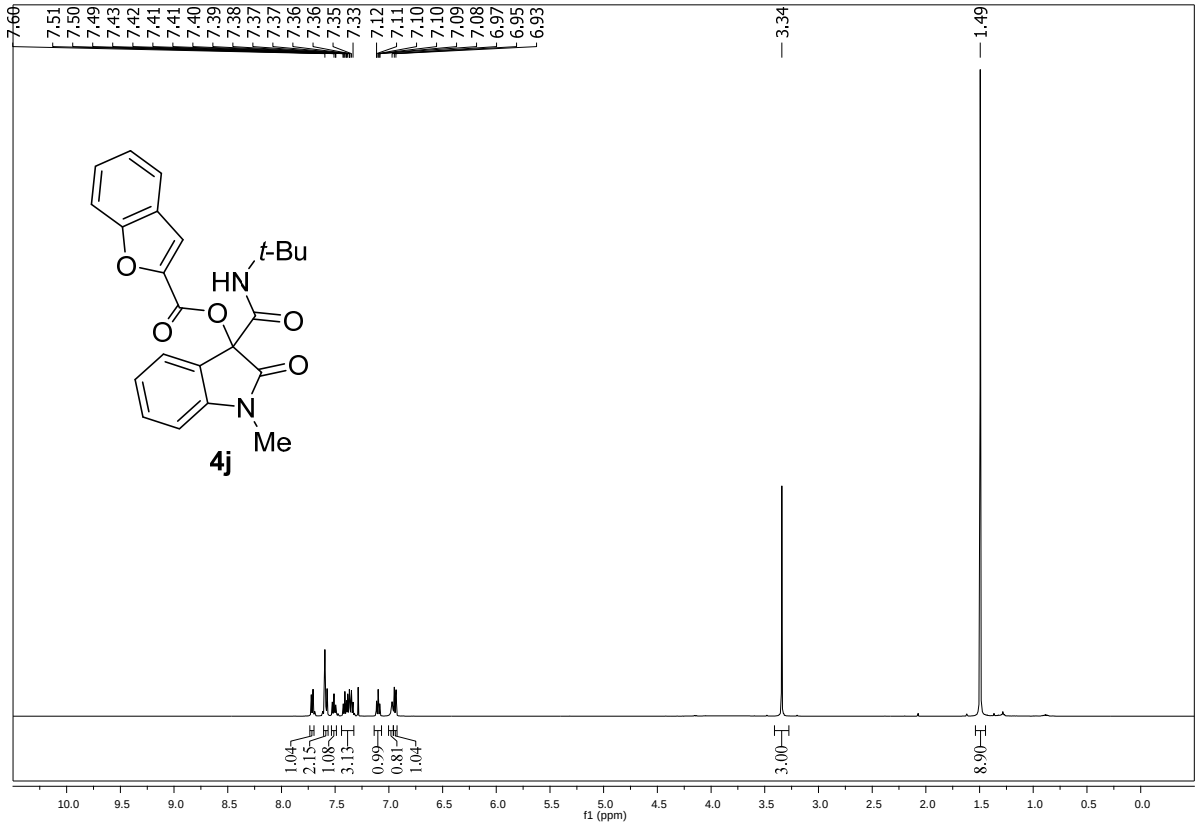


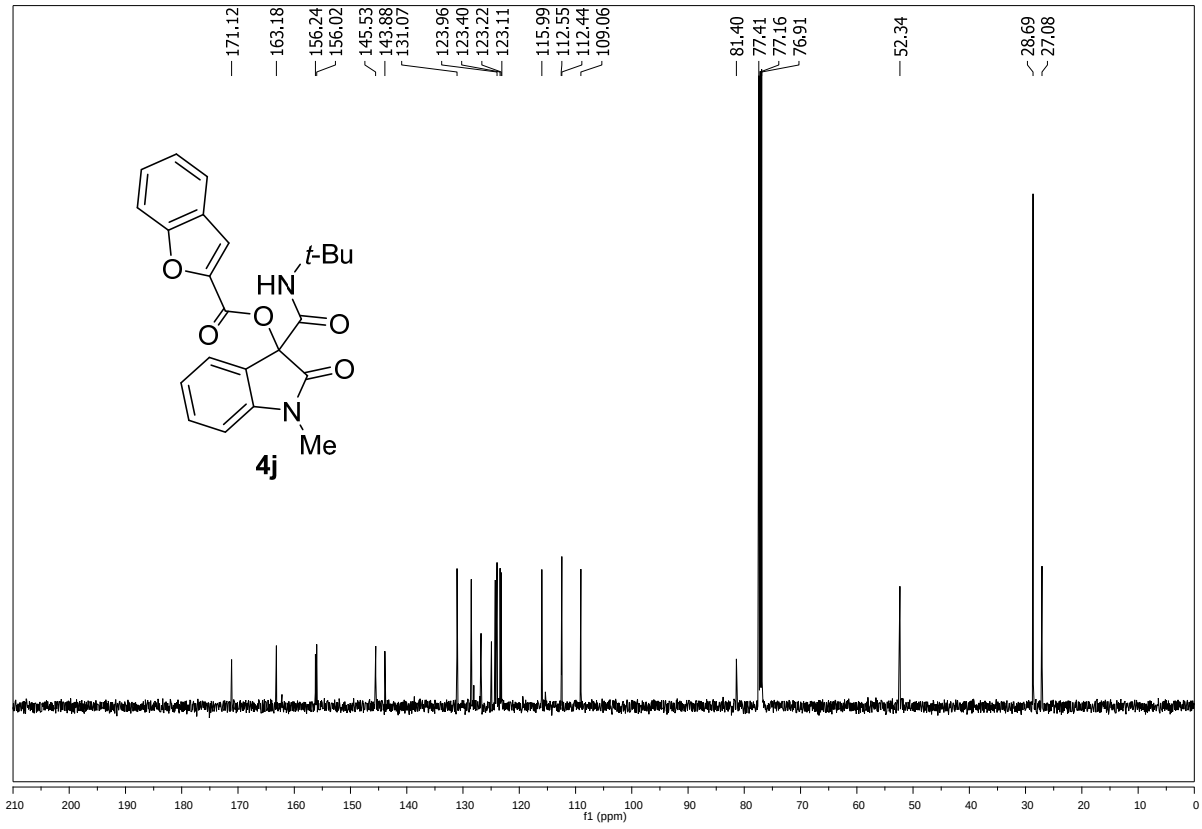
3-(*tert*-Butylcarbamoyl)-1-methyl-2-oxoindolin-3-yl thiophene-2-carboxylate (4i)





3-(*tert*-Butylcarbamoyl)-1-methyl-2-oxoindolin-3-yl benzofuran-2-carboxylate (4j)





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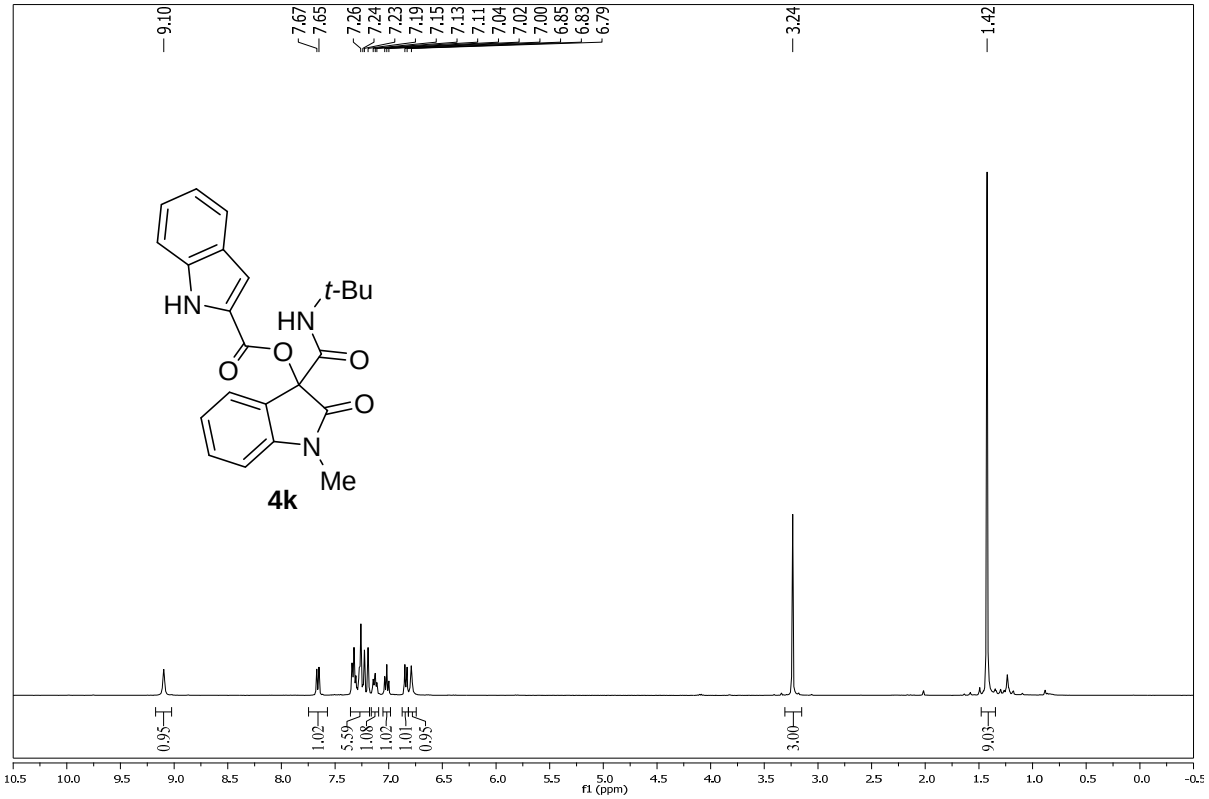
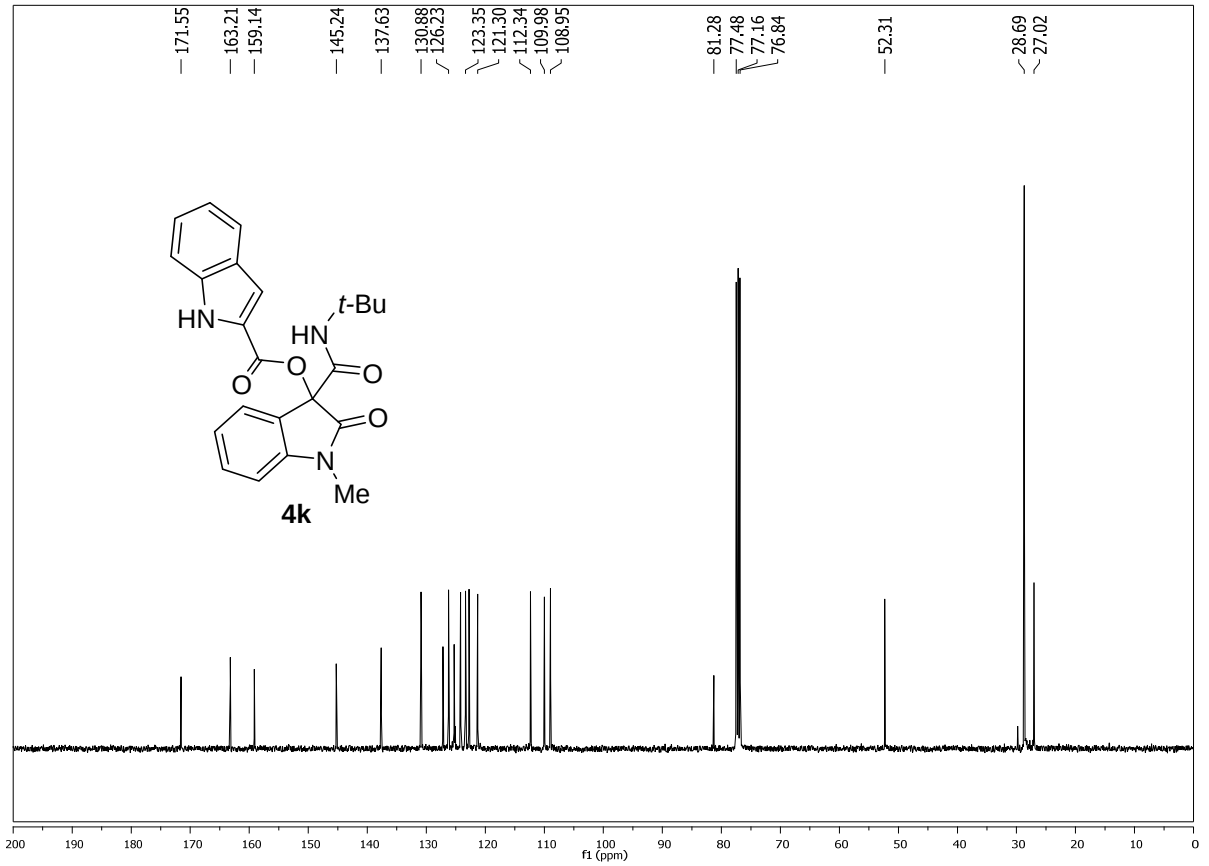
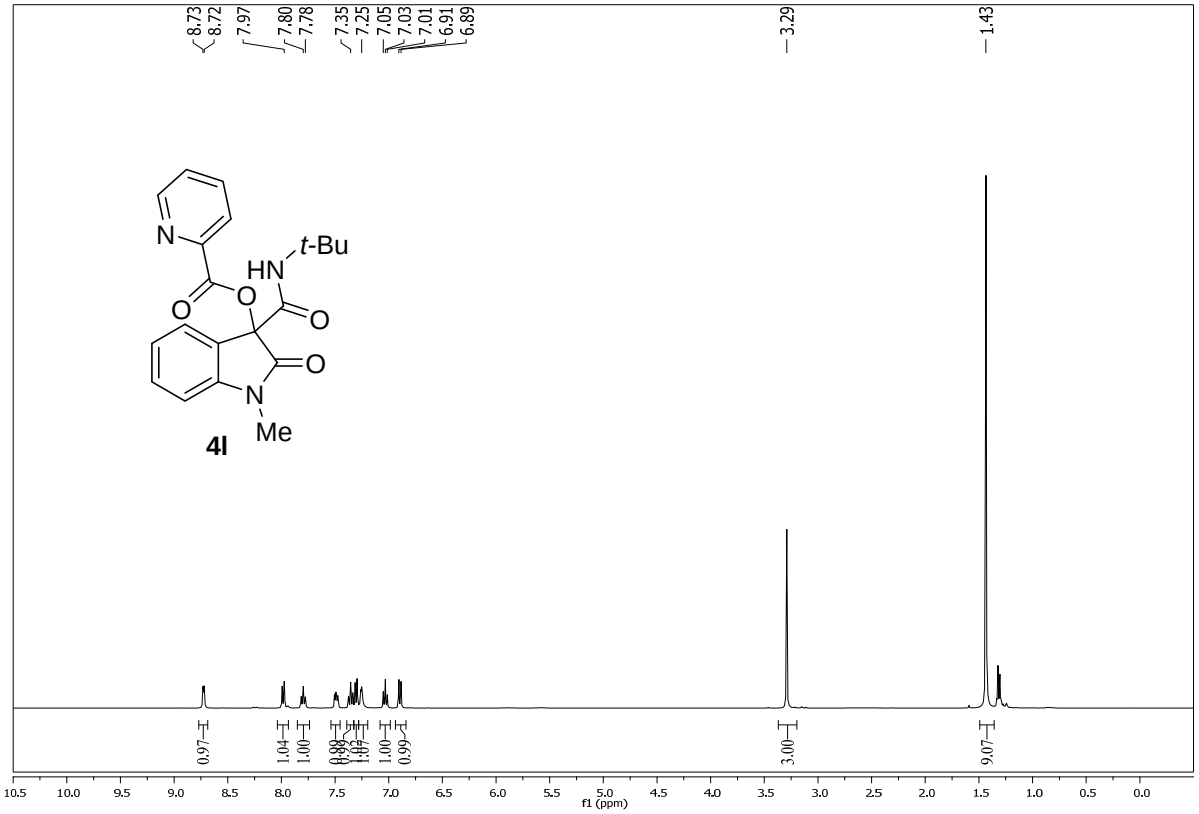
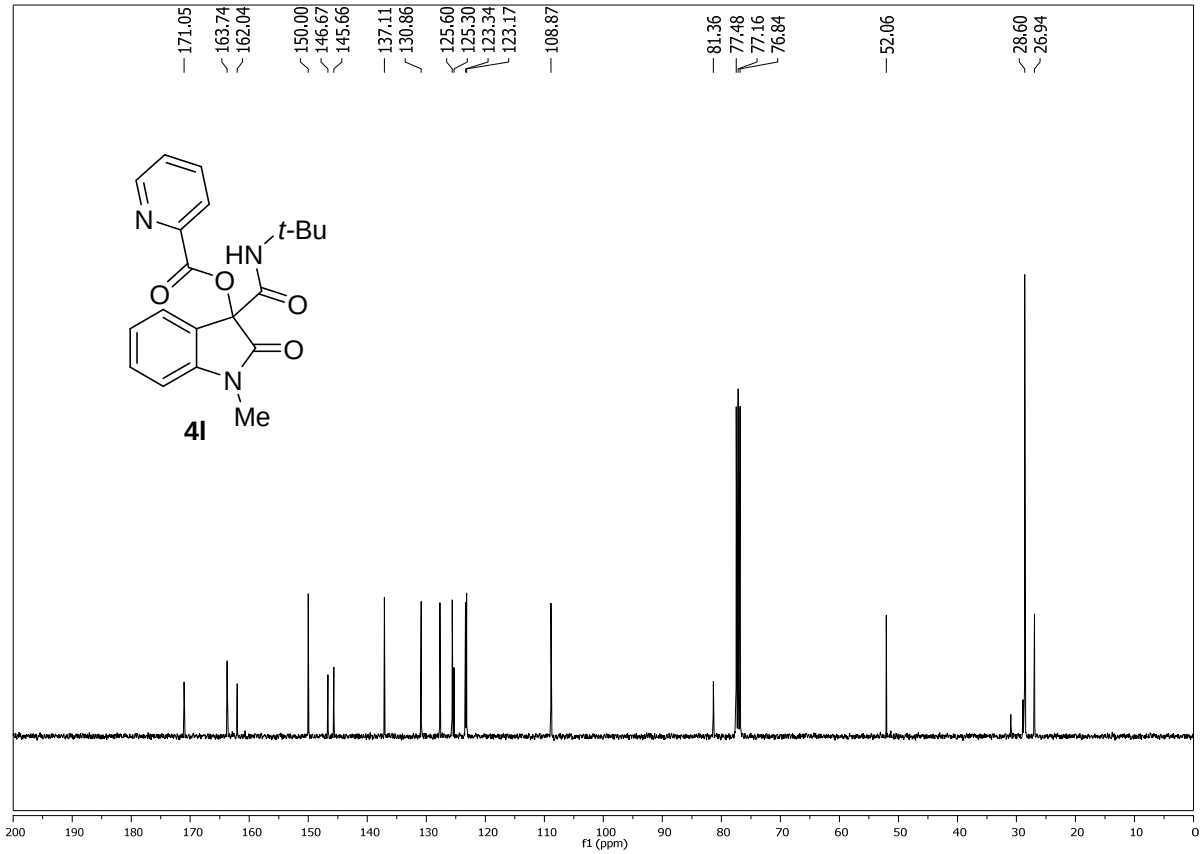




3-(*tert*-Butylcarbamoyl)-1-methyl-2-oxoindolin-3-yl picolinate (4l)





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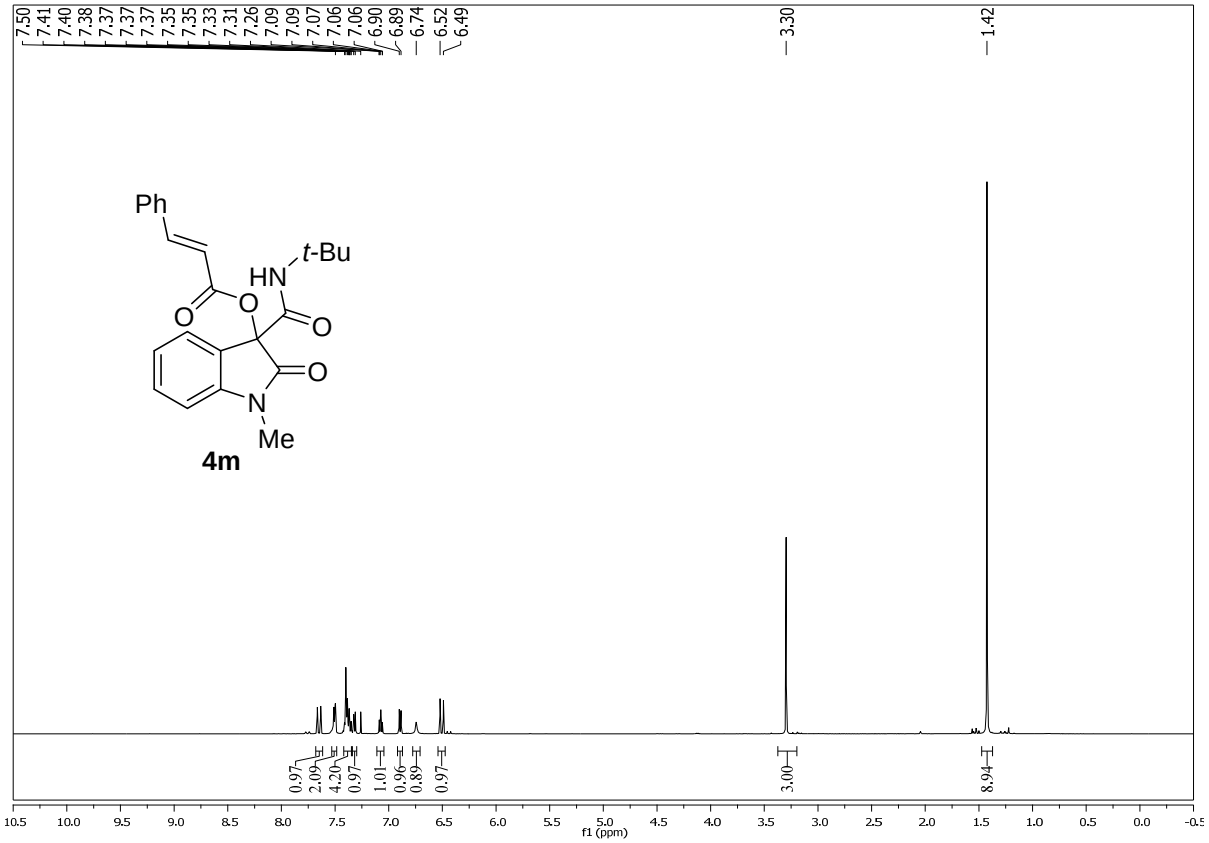

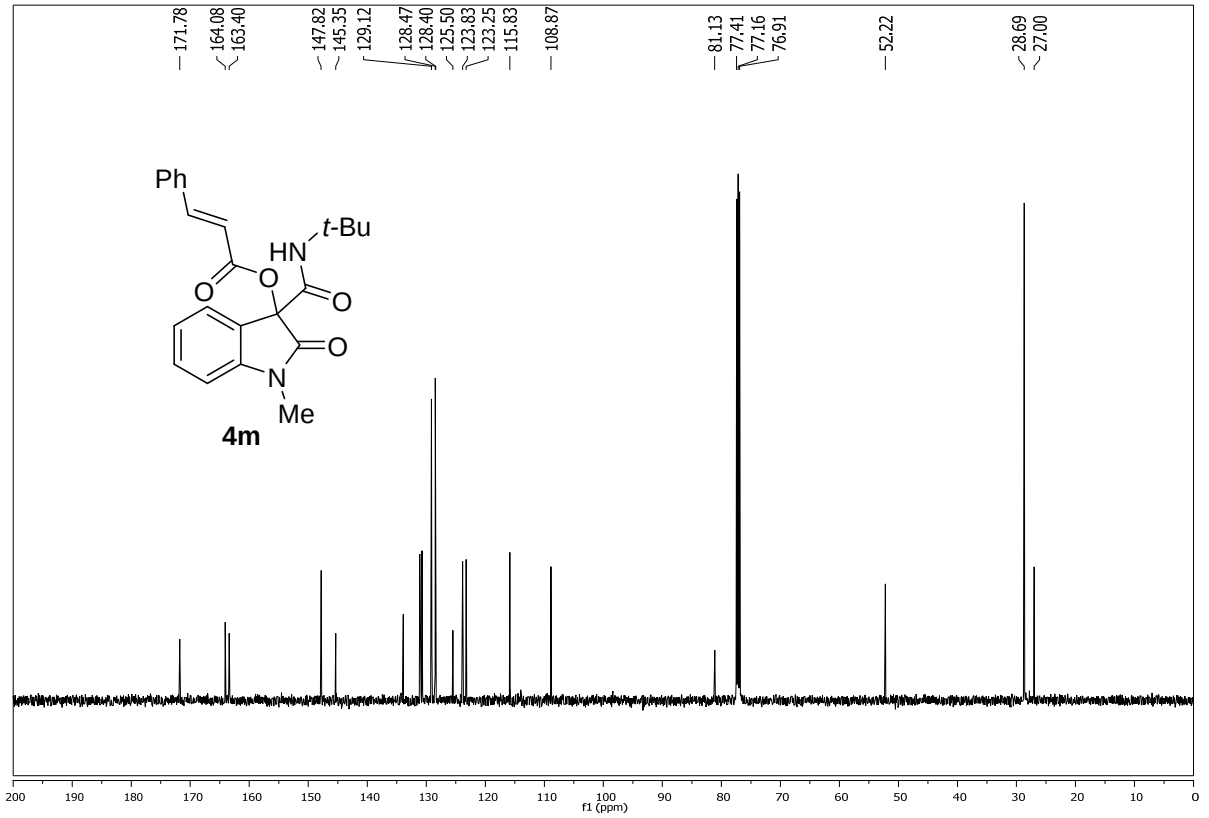

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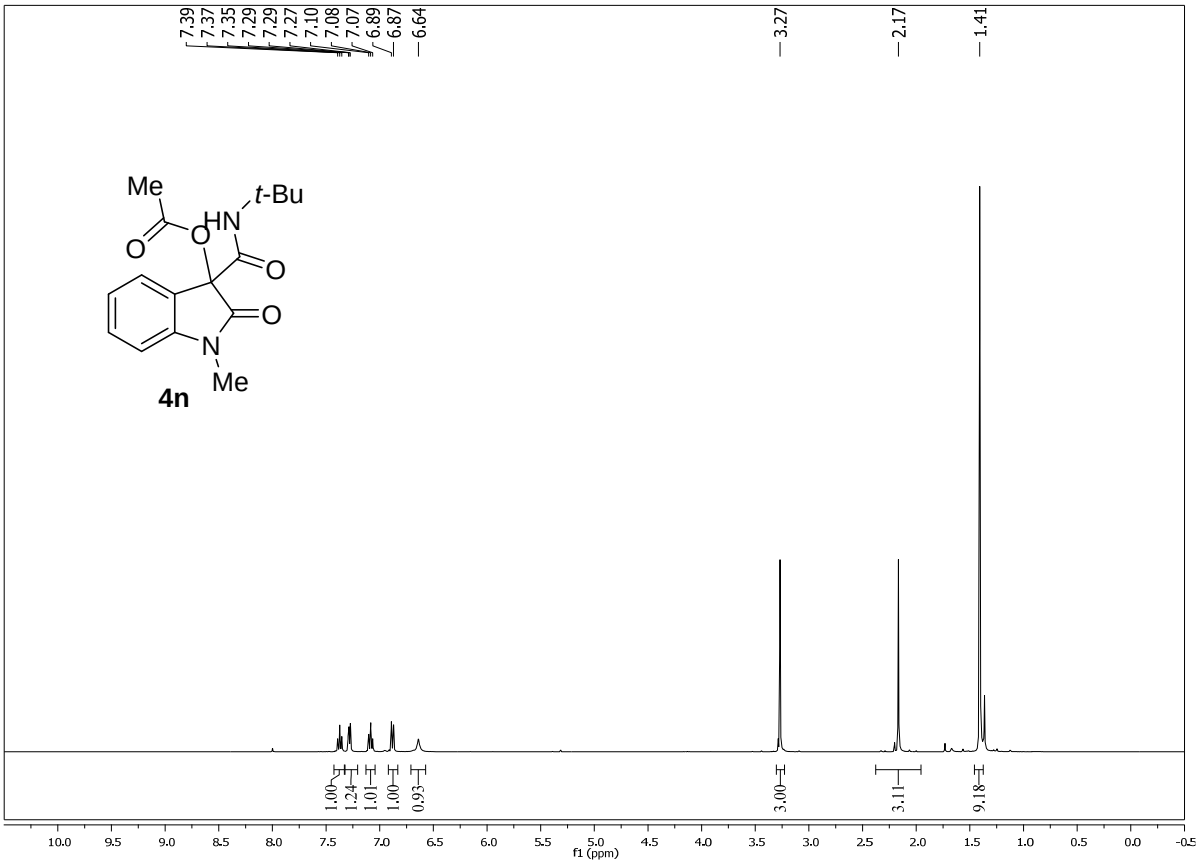

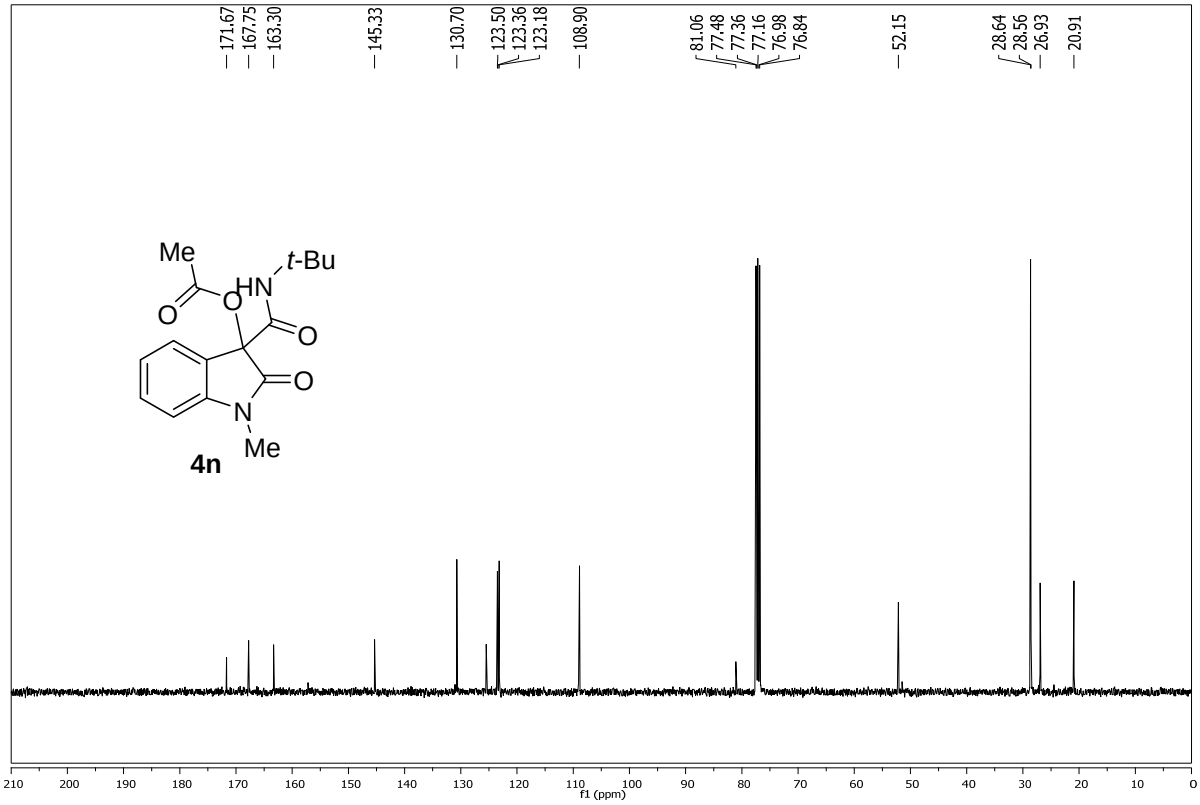

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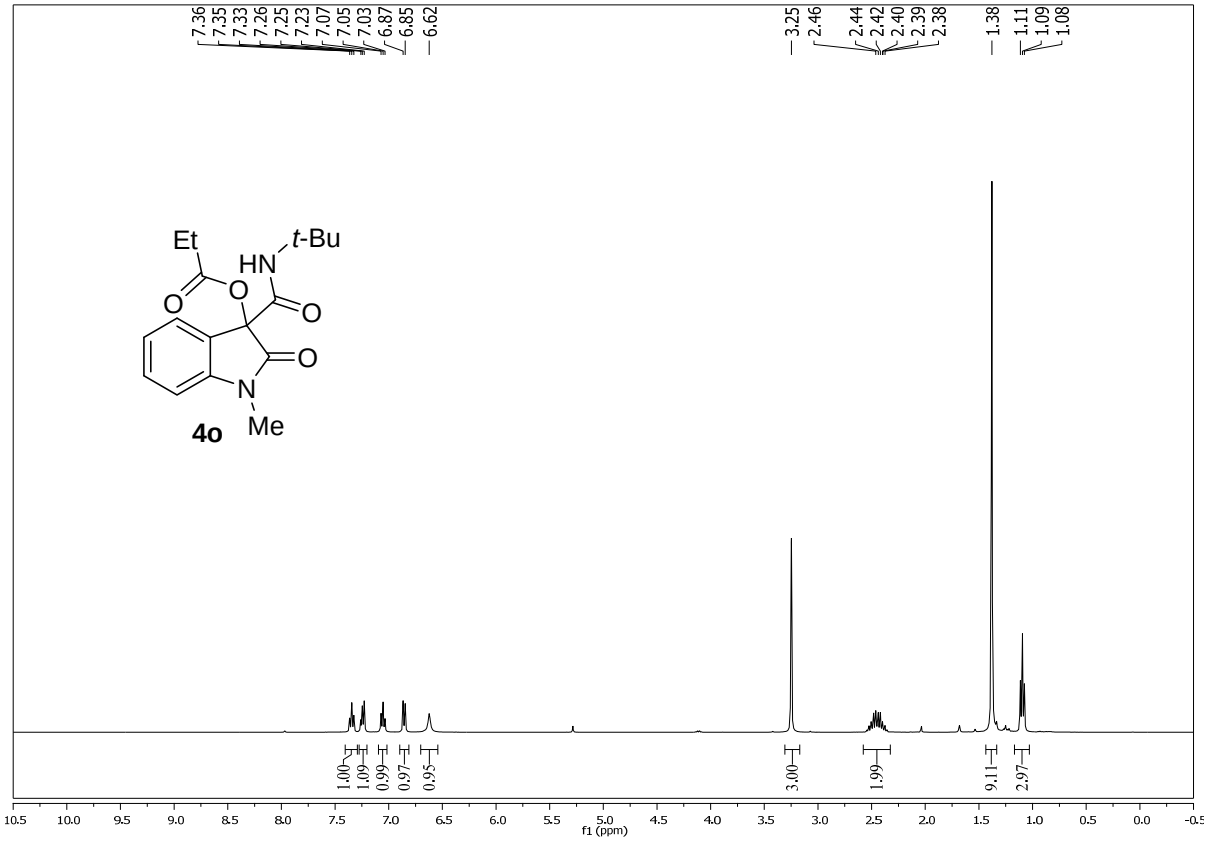
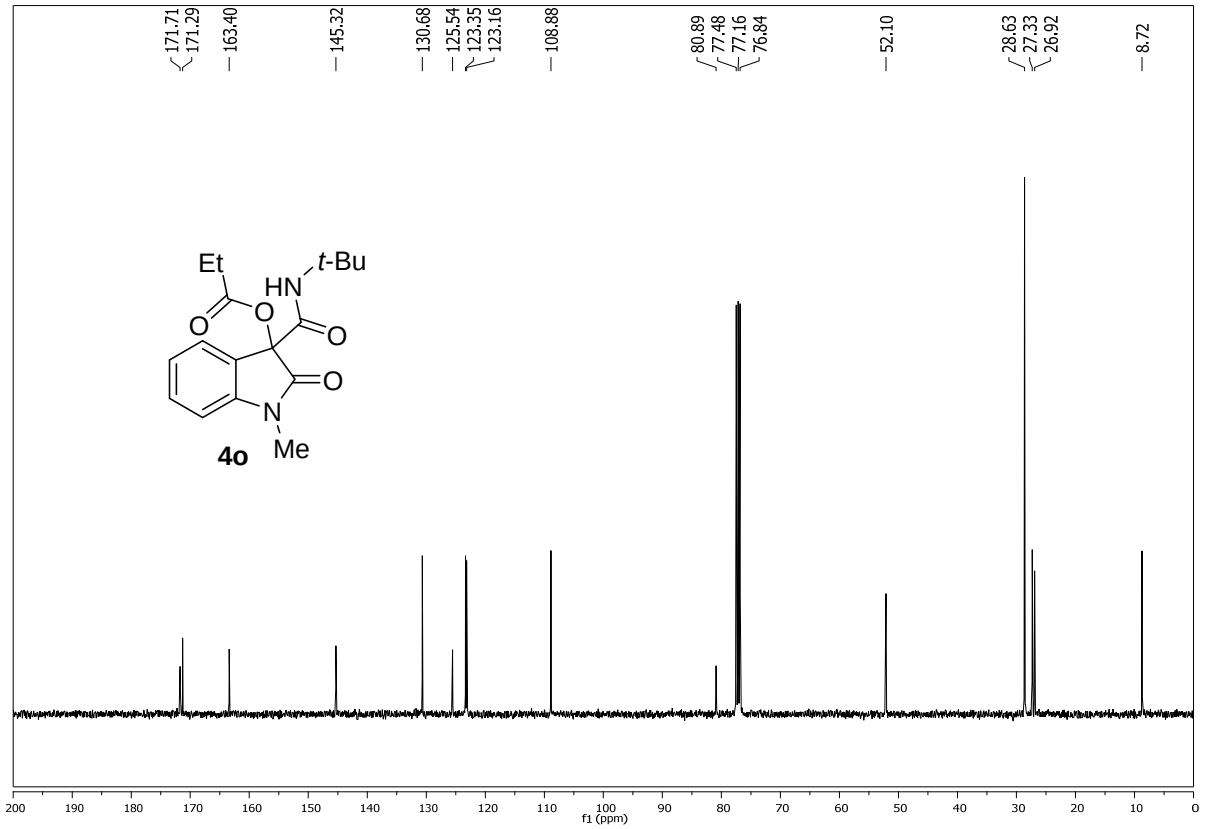
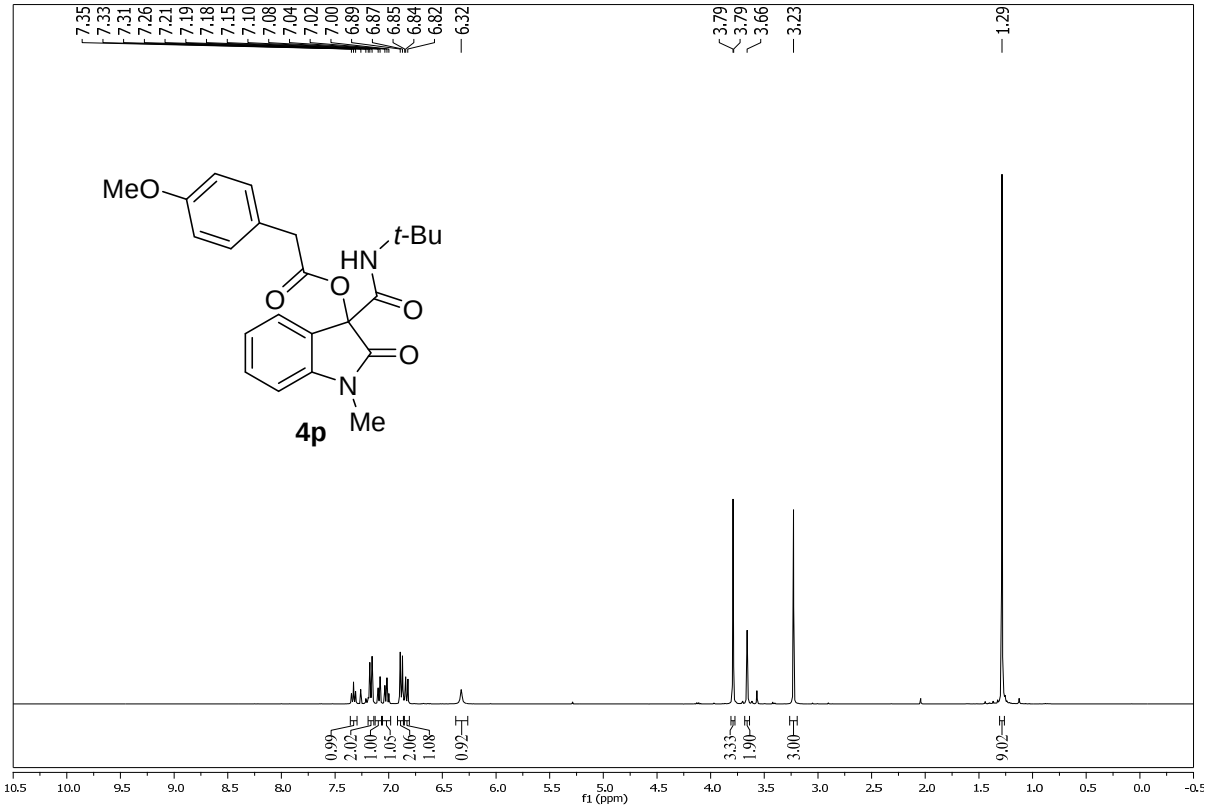
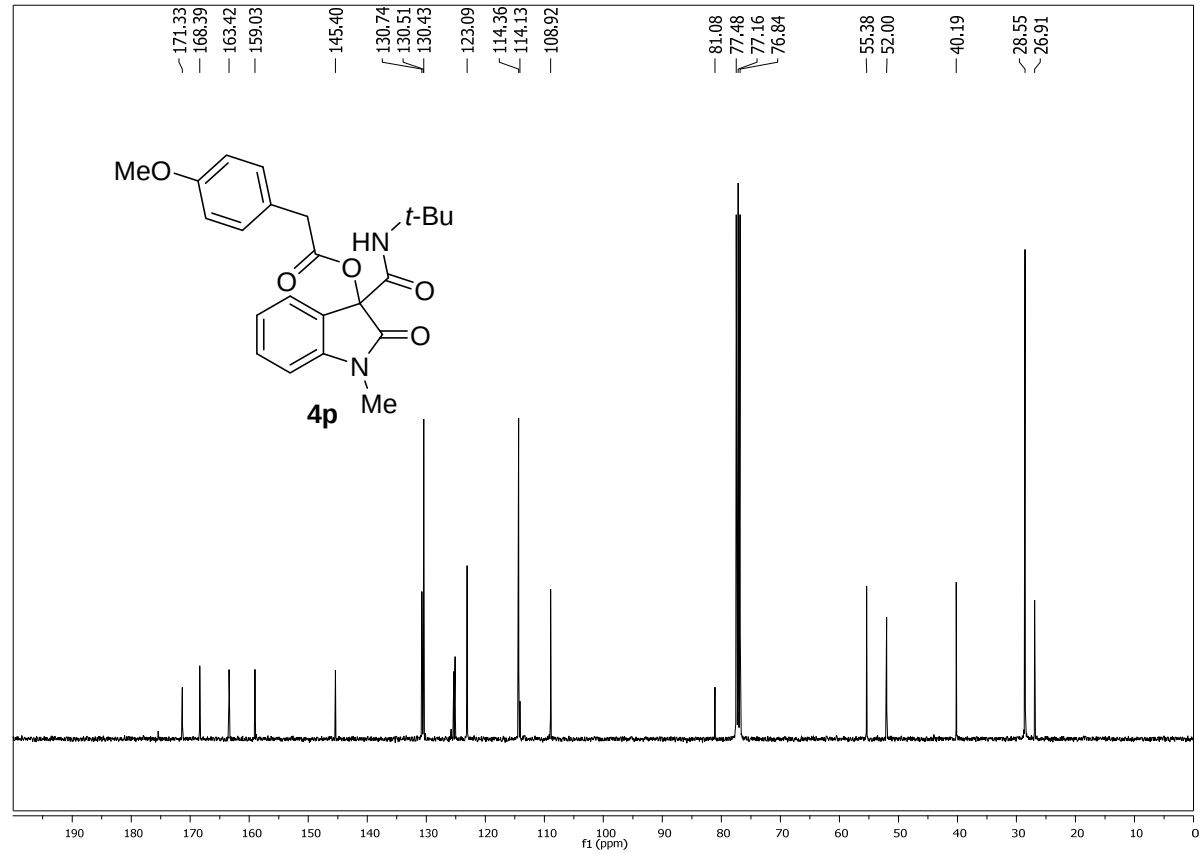




3-(*tert*-Butylcarbamoyl)-1-methyl-2-oxoindolin-3-yl 2-(4-methoxyphenyl)acetate (4p)





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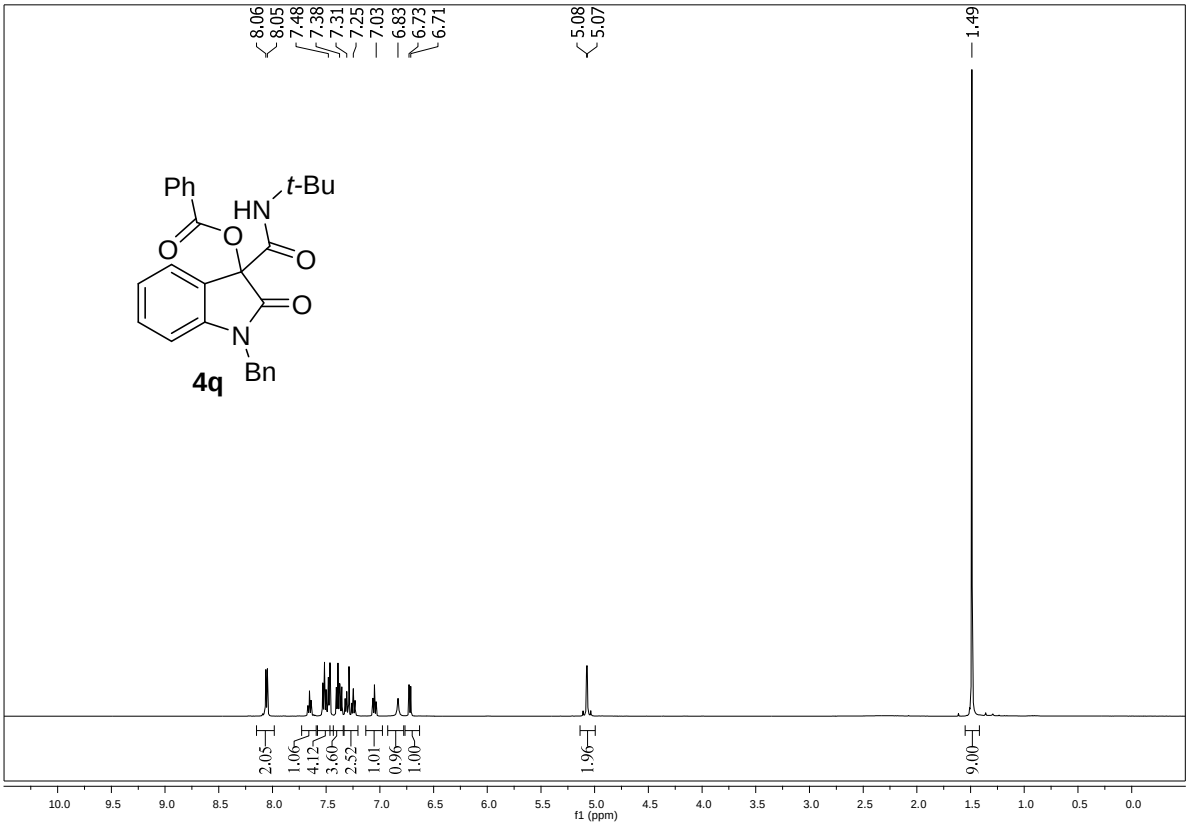

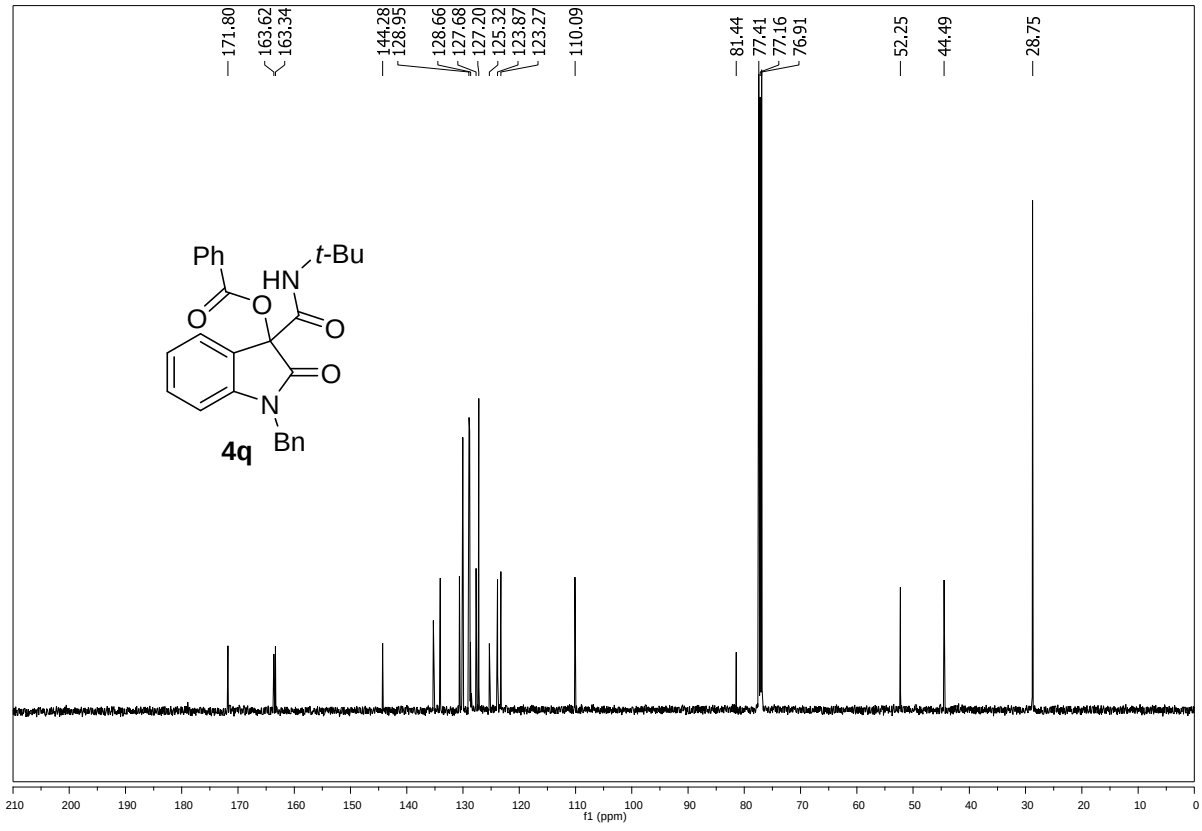

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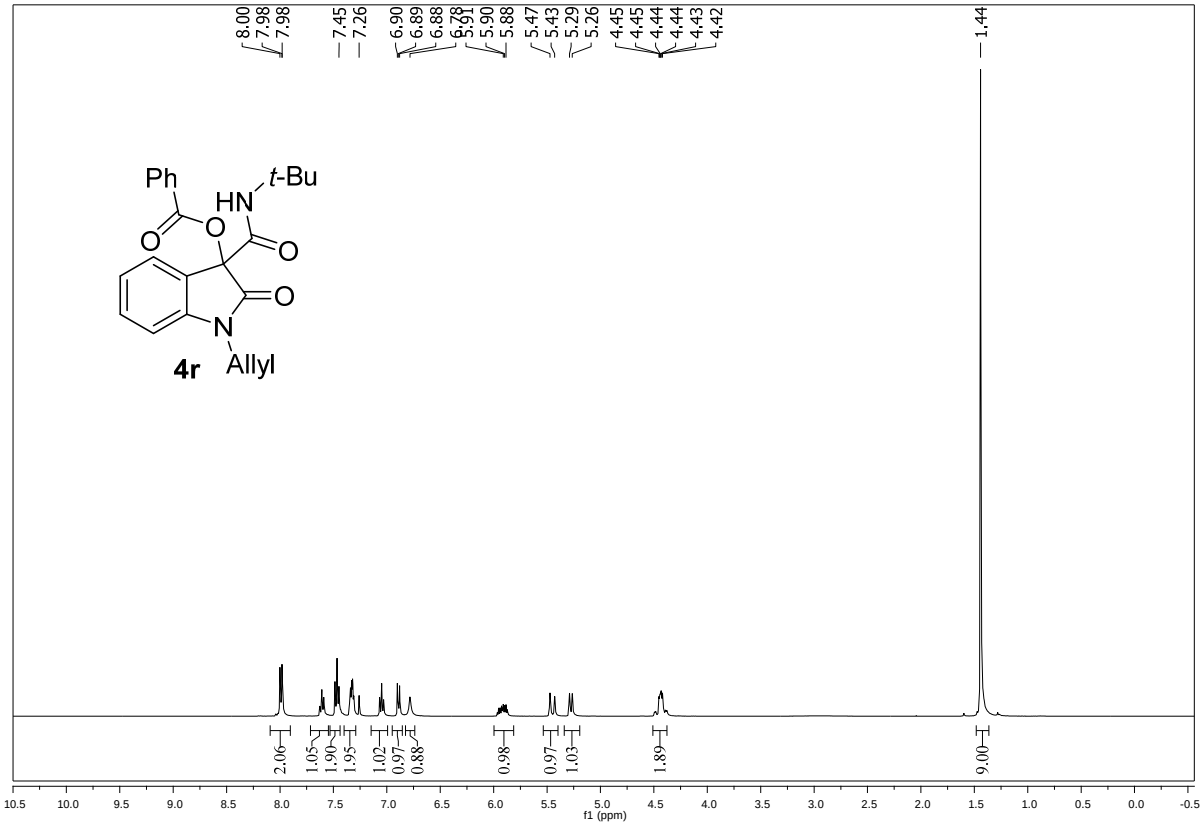

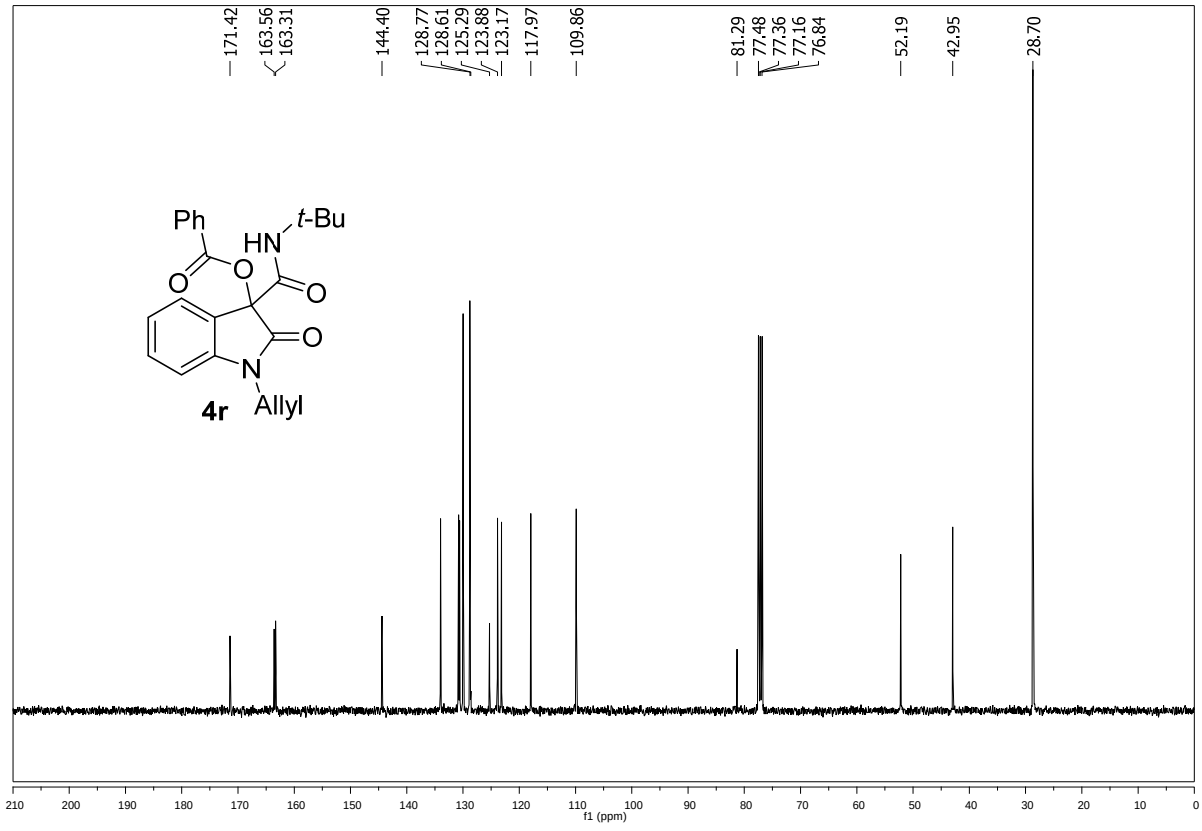

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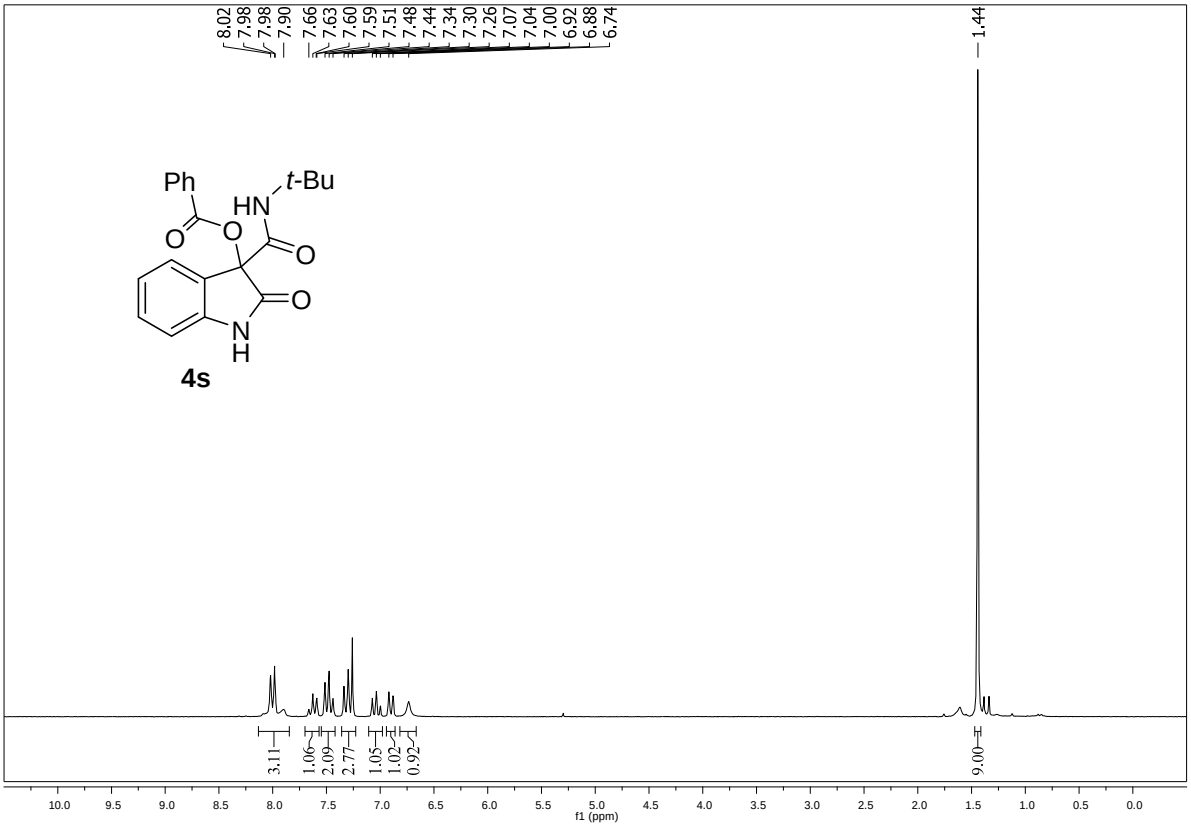

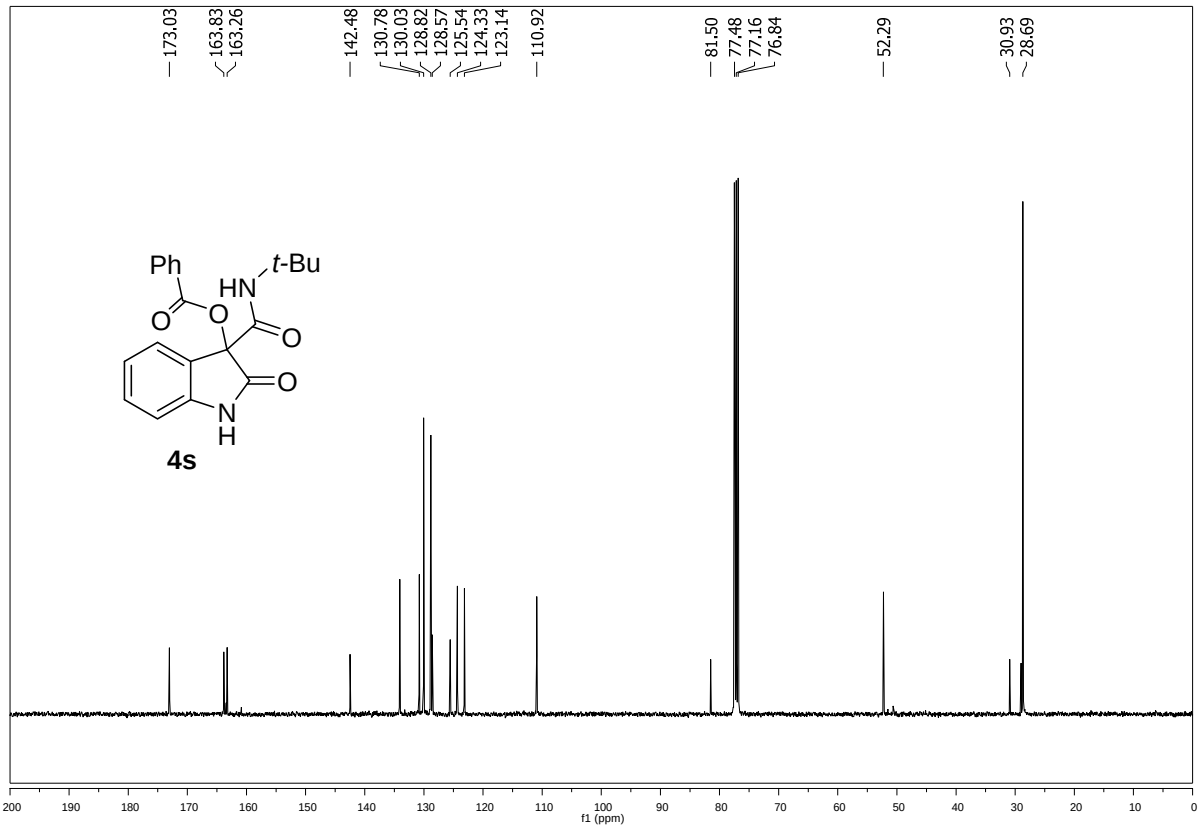

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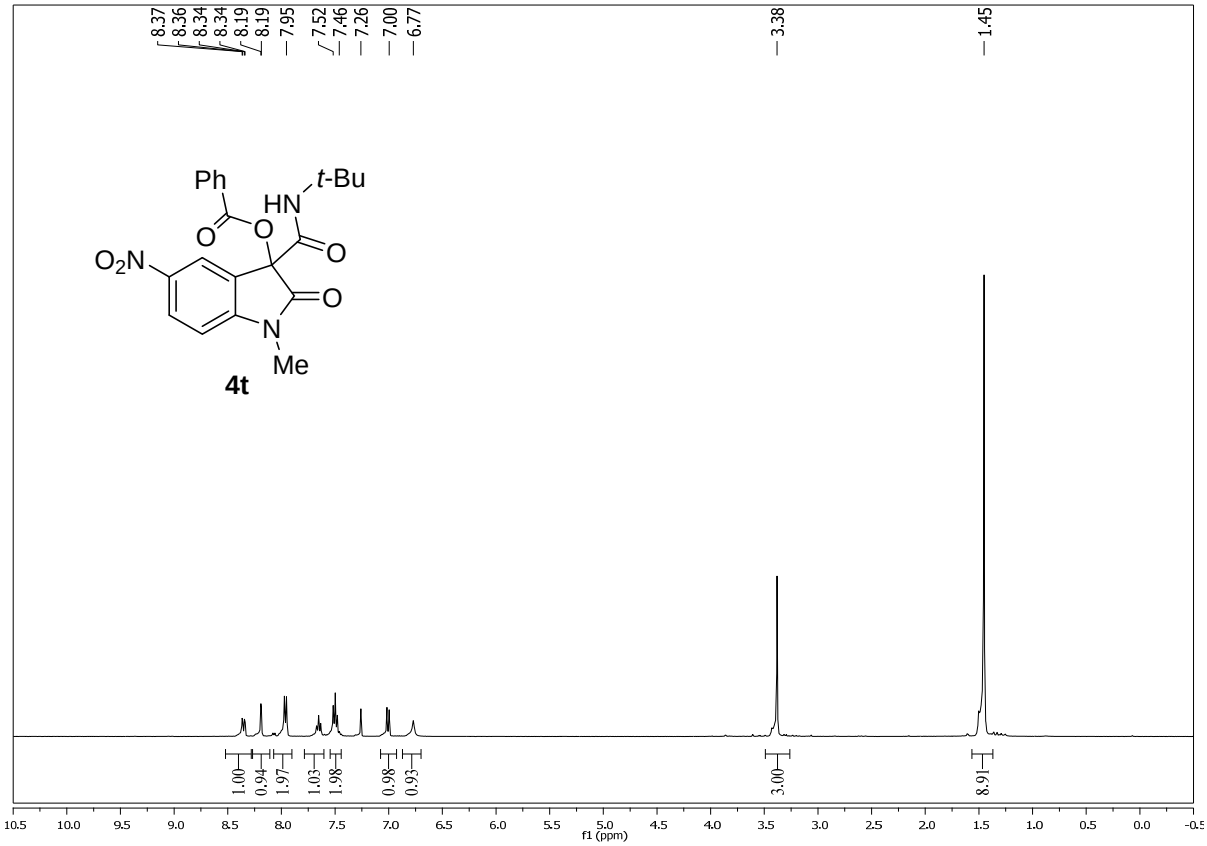

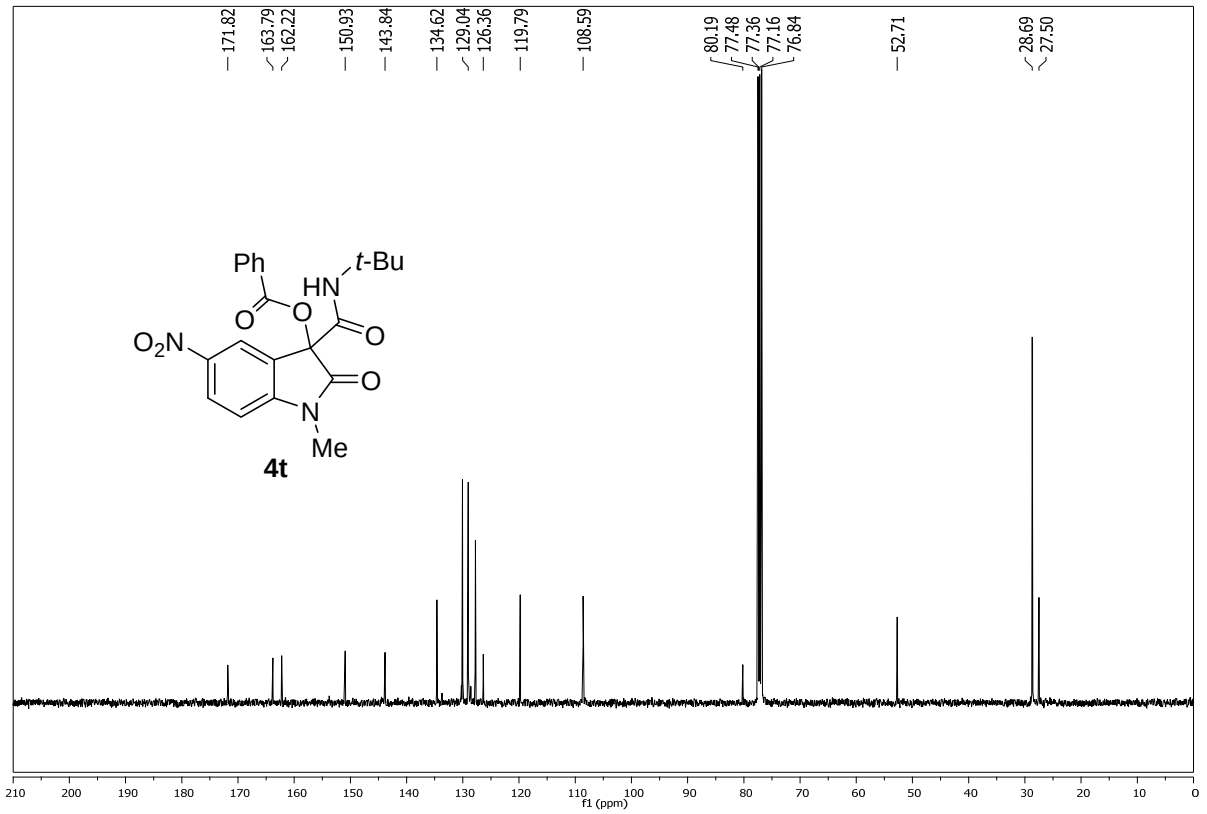

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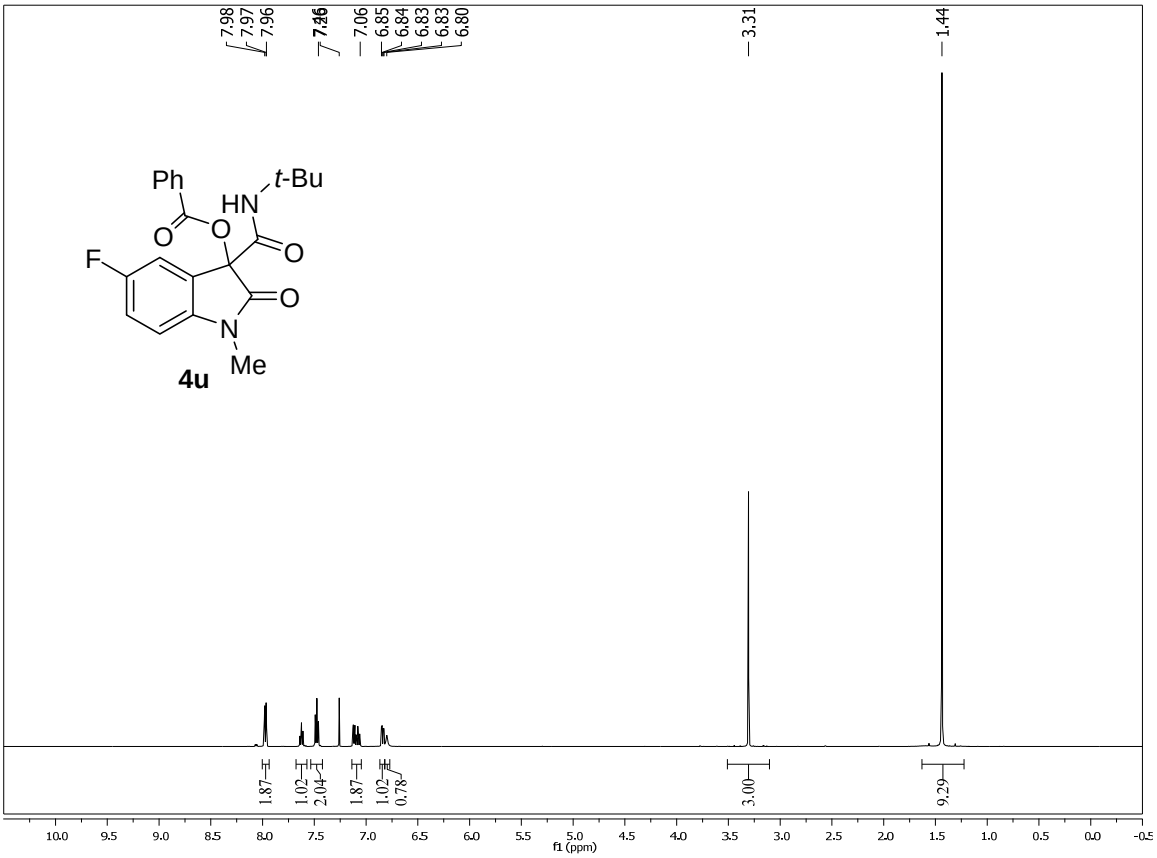

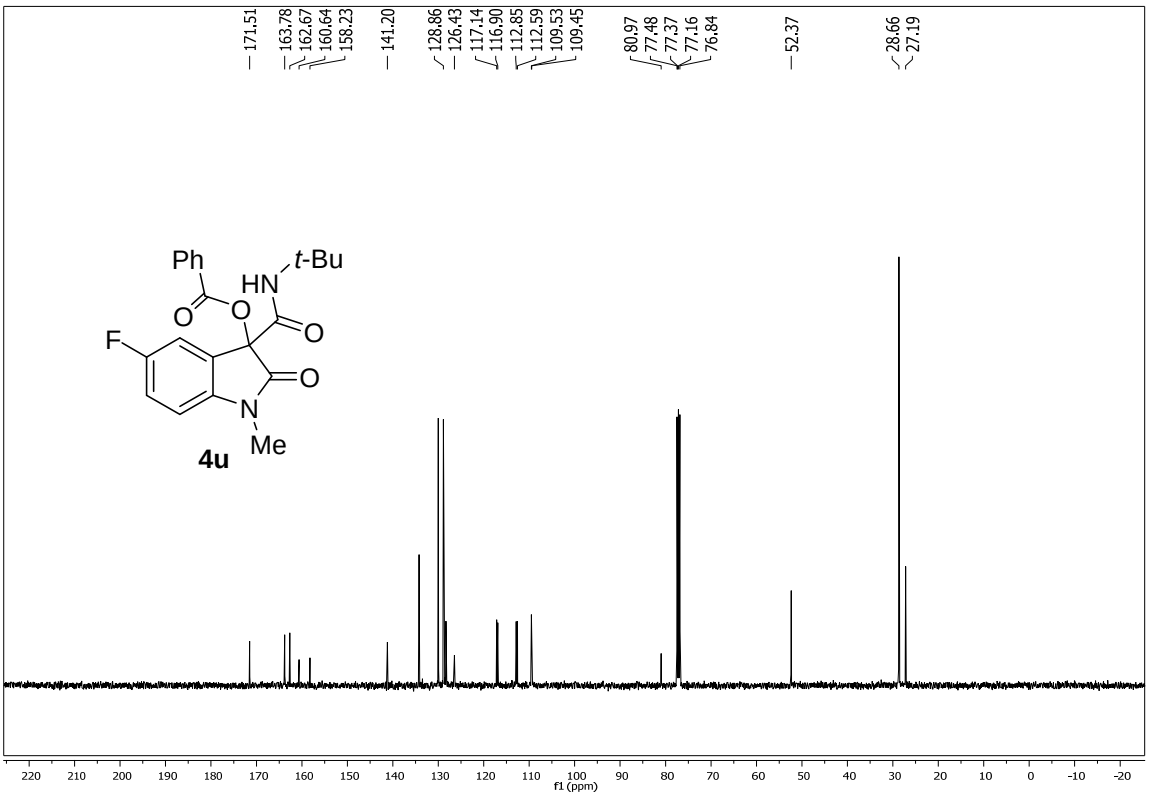

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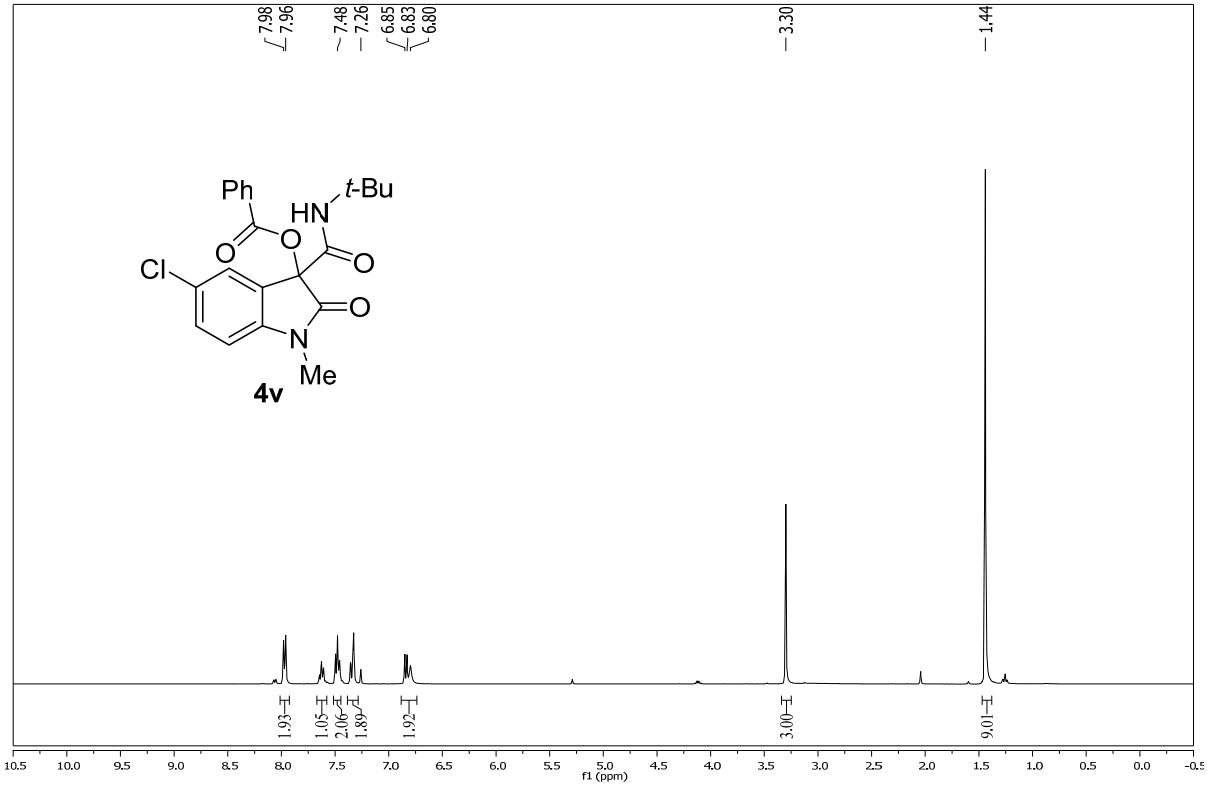

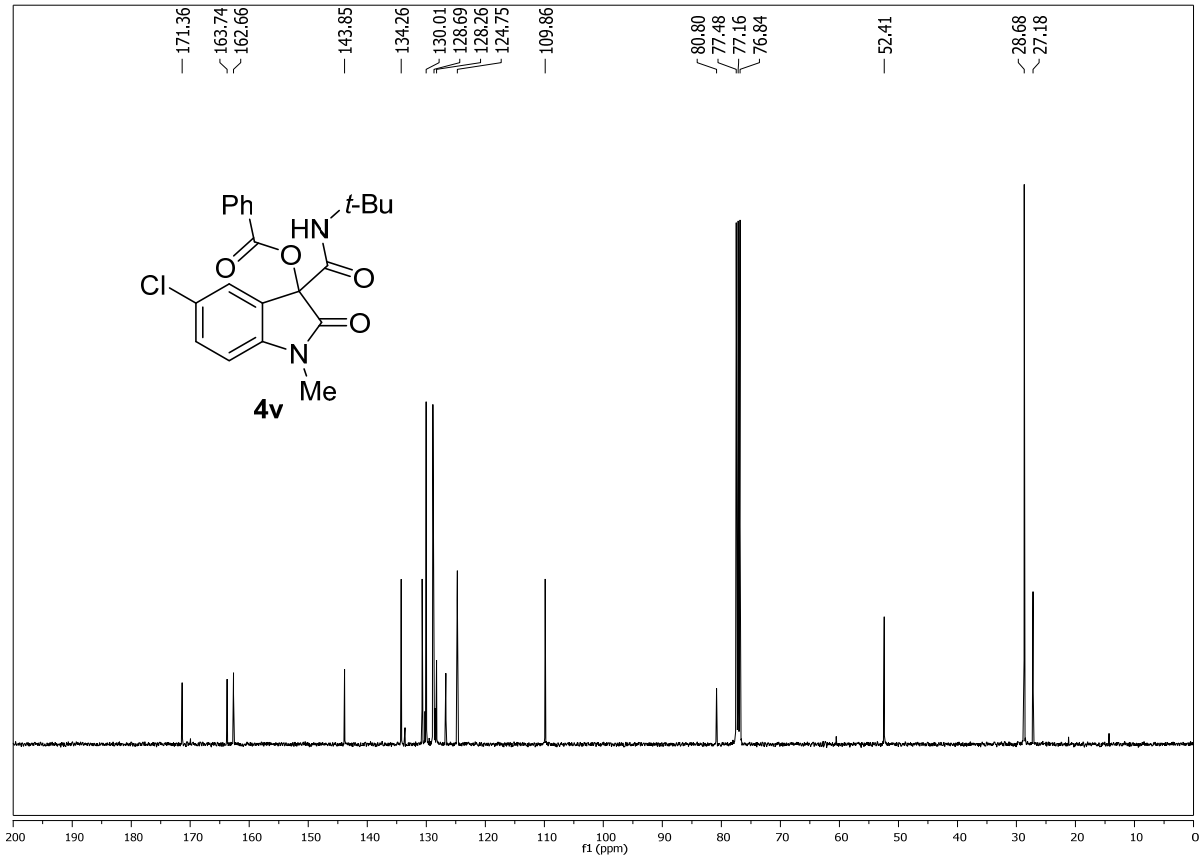

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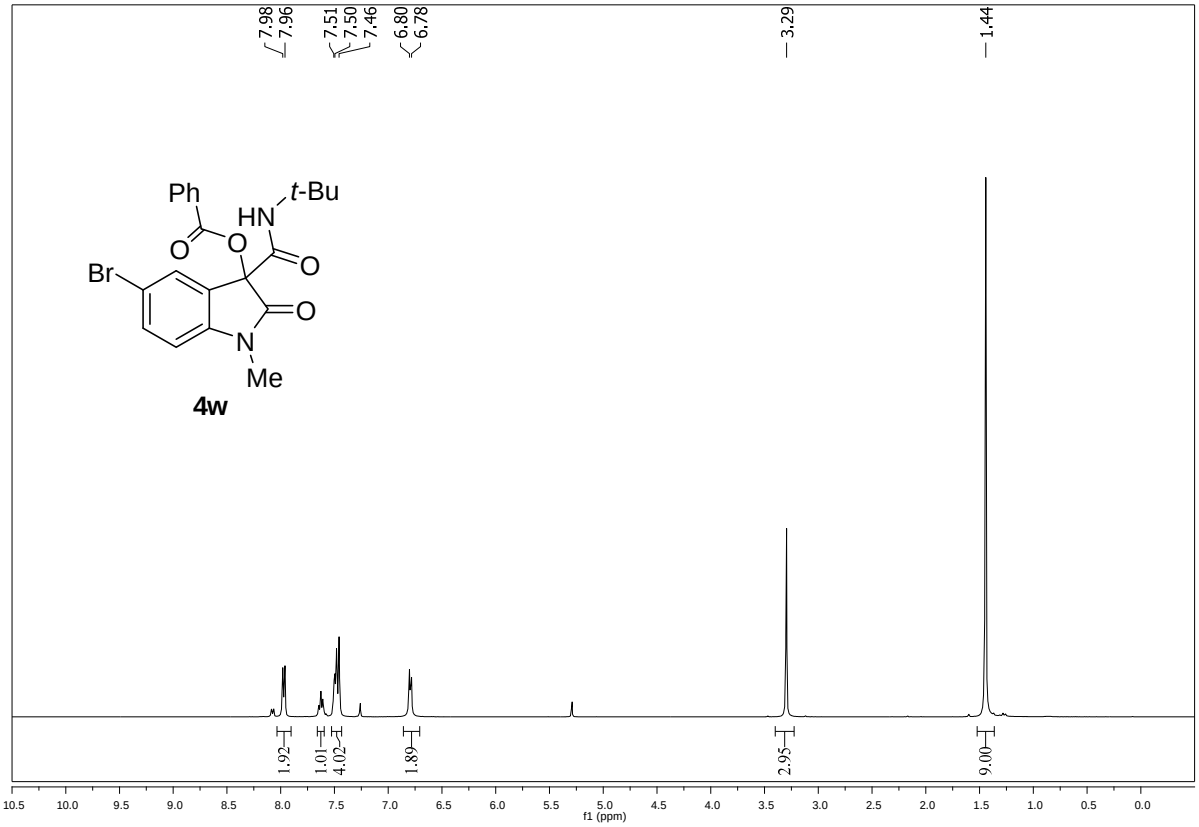

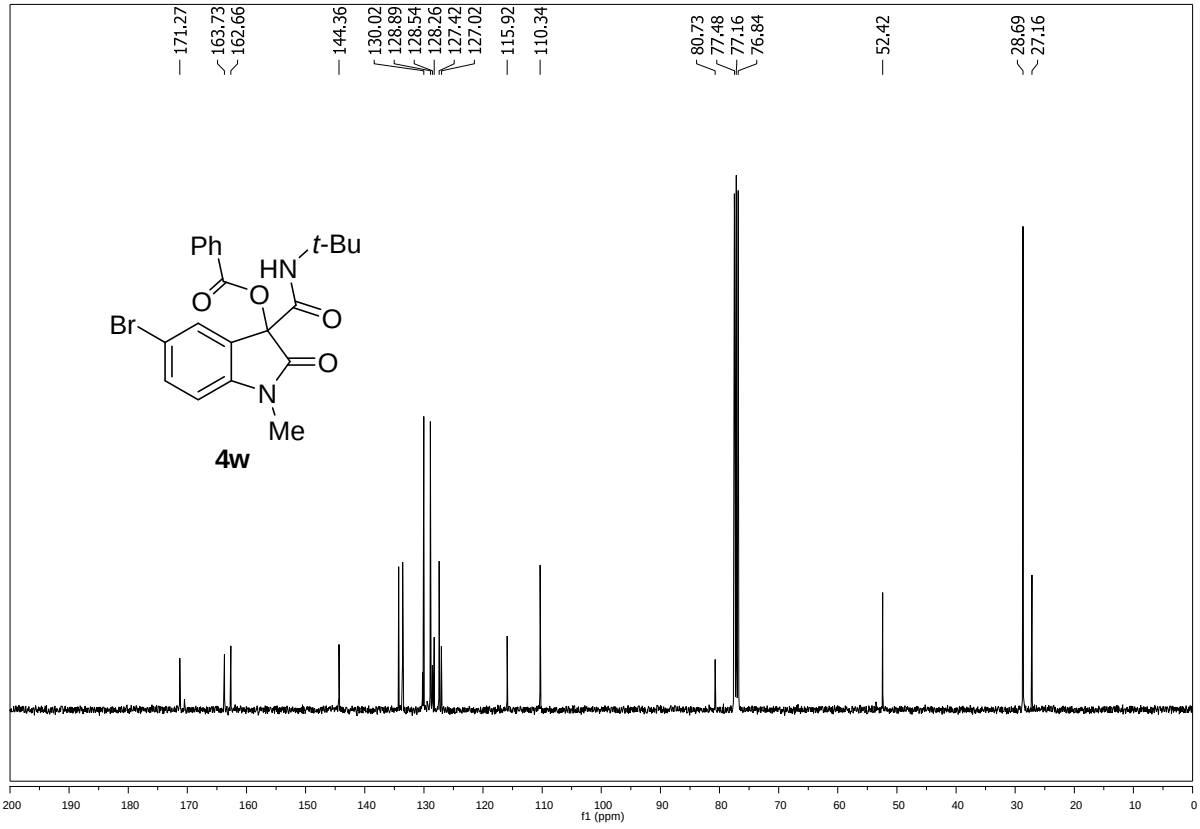

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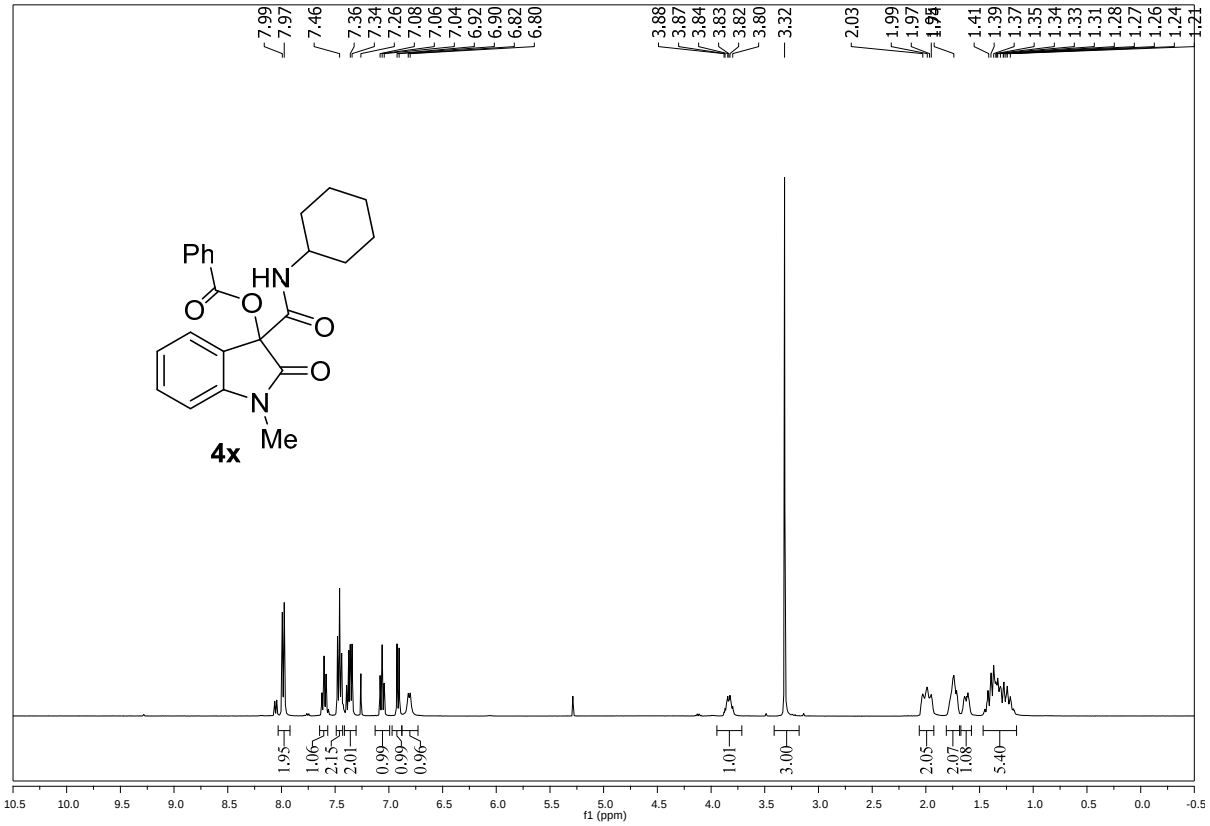

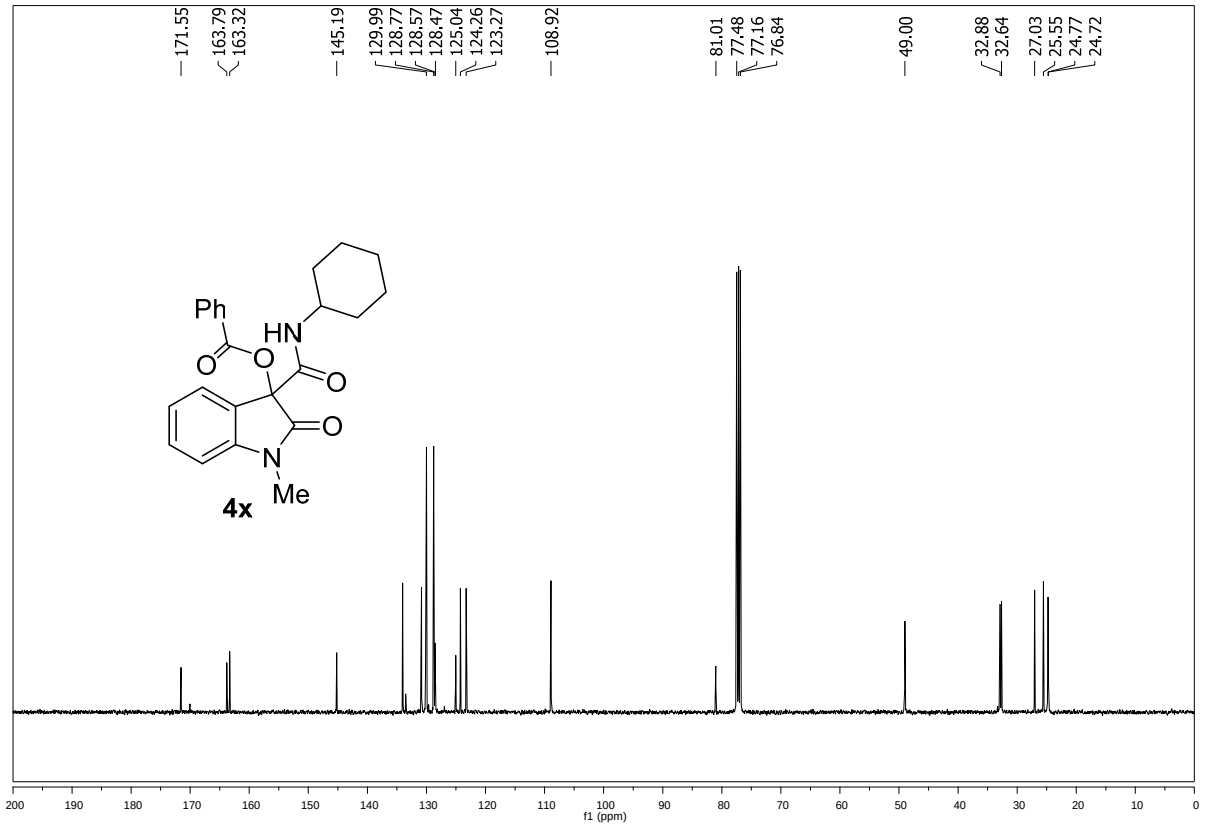

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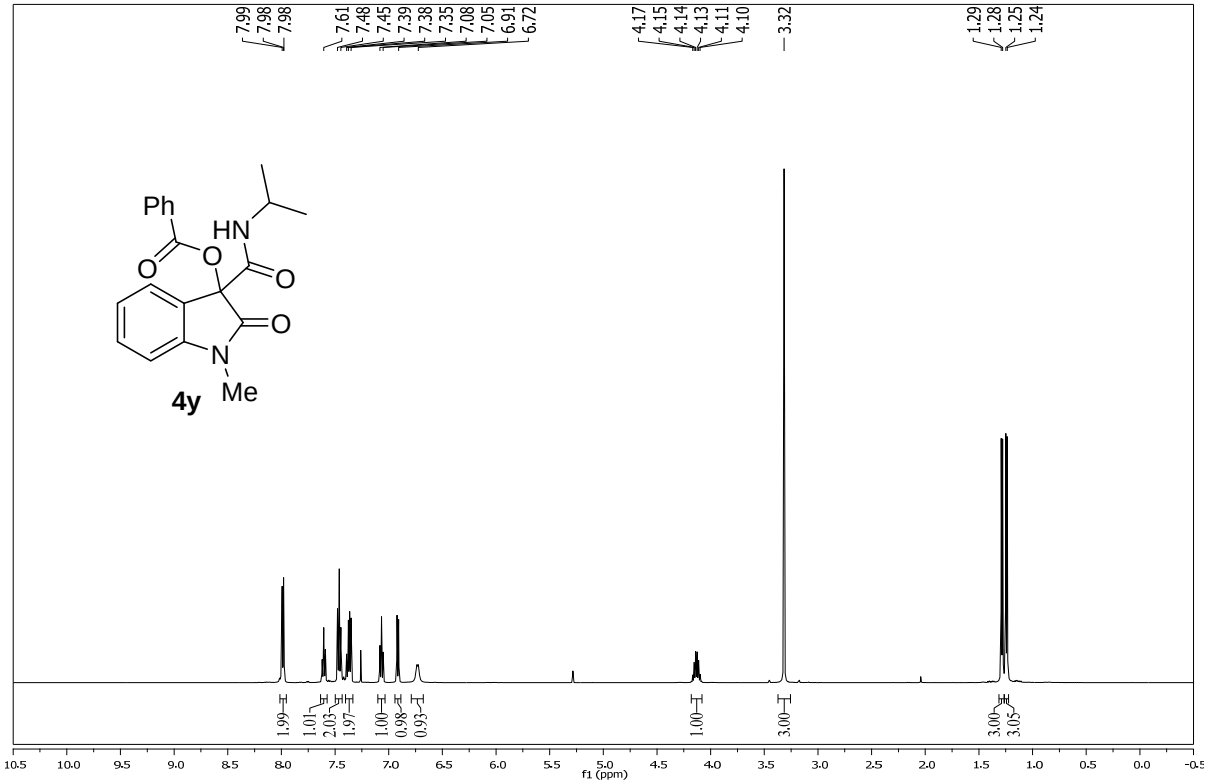
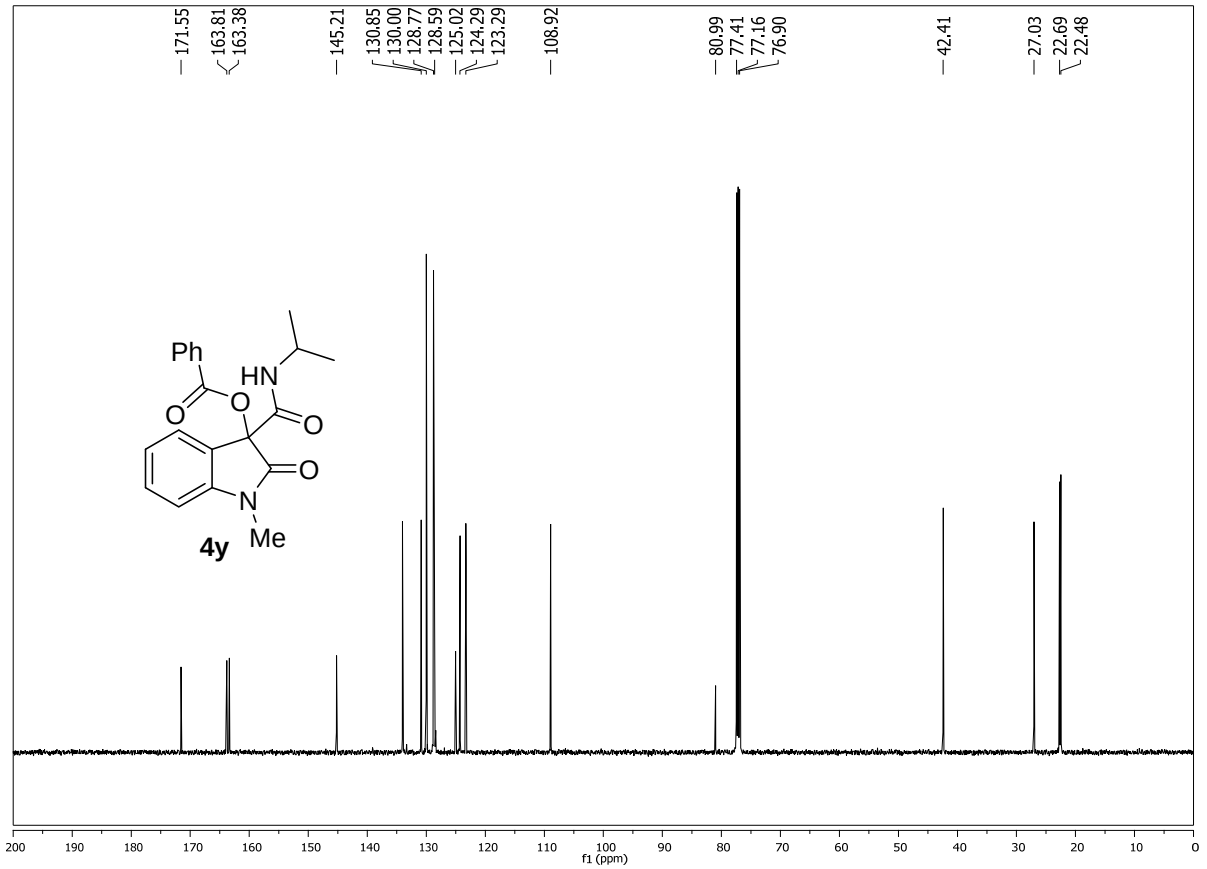
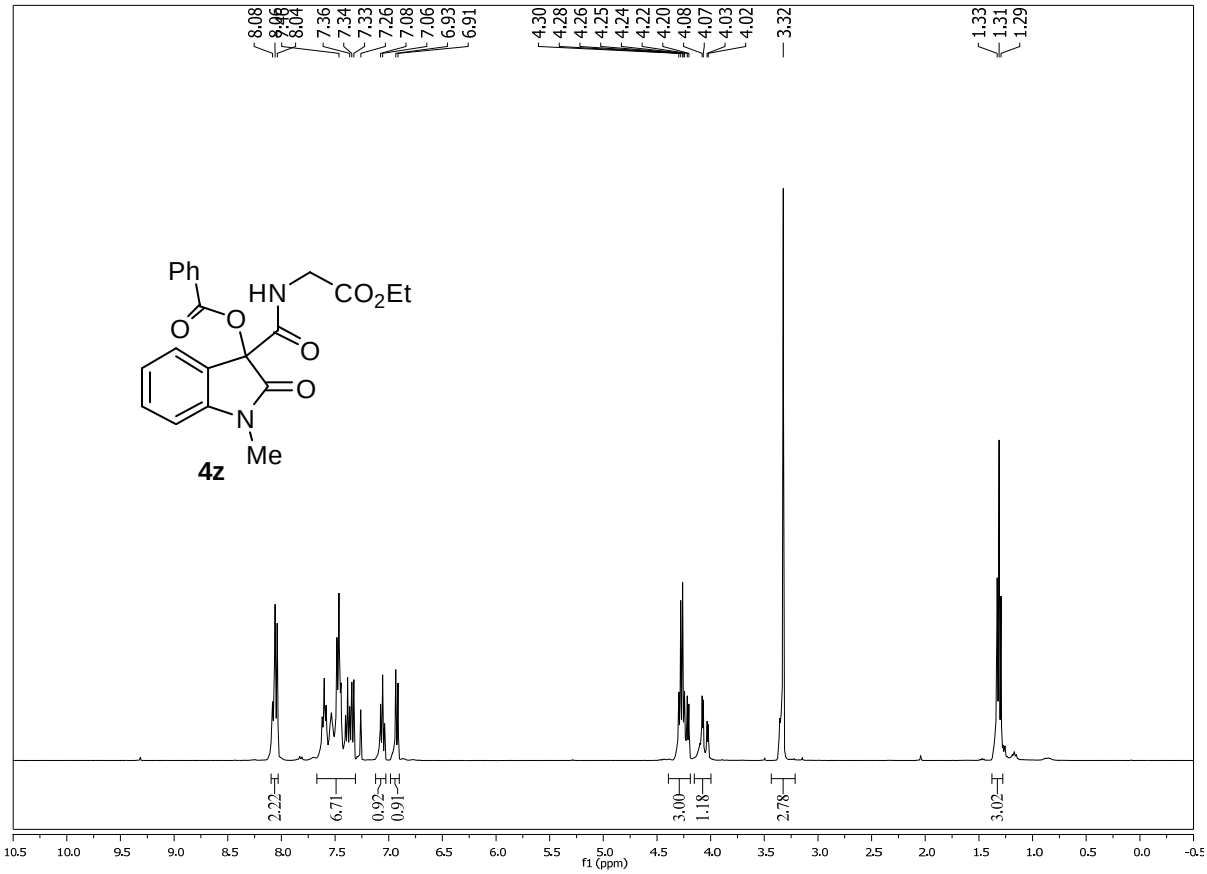
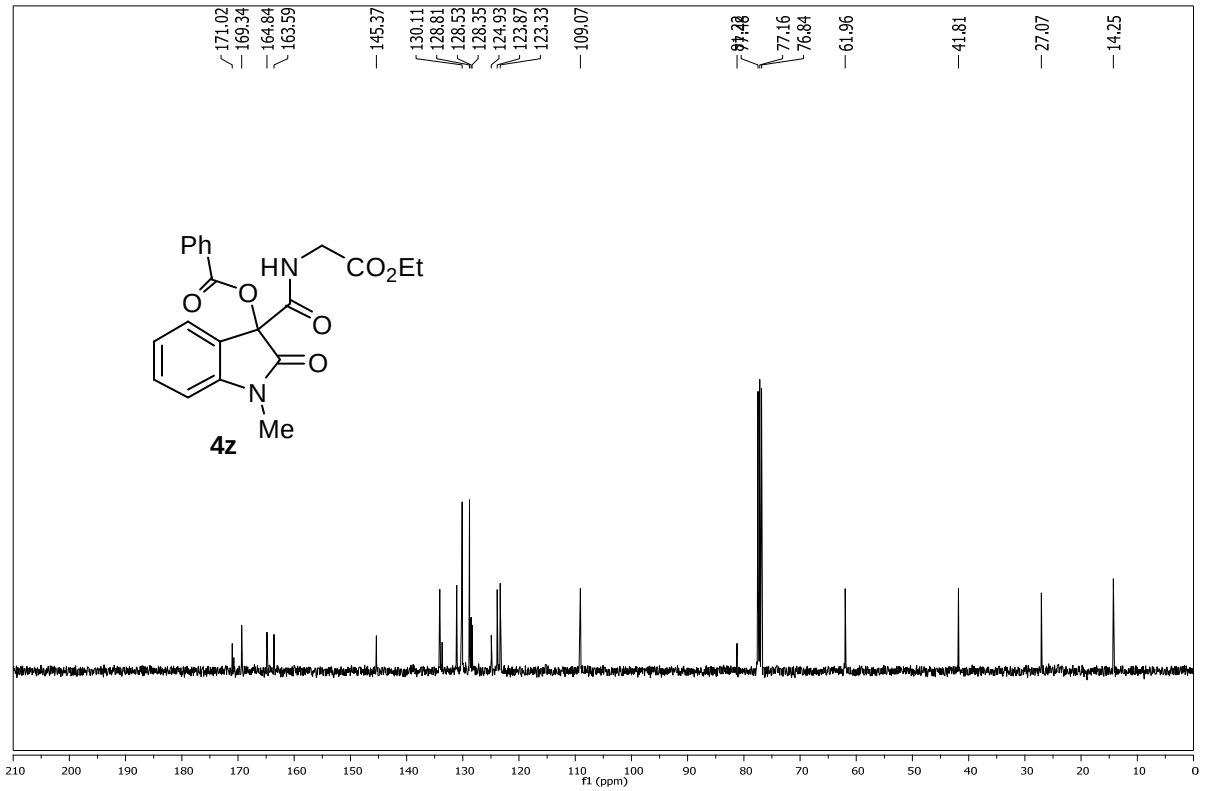


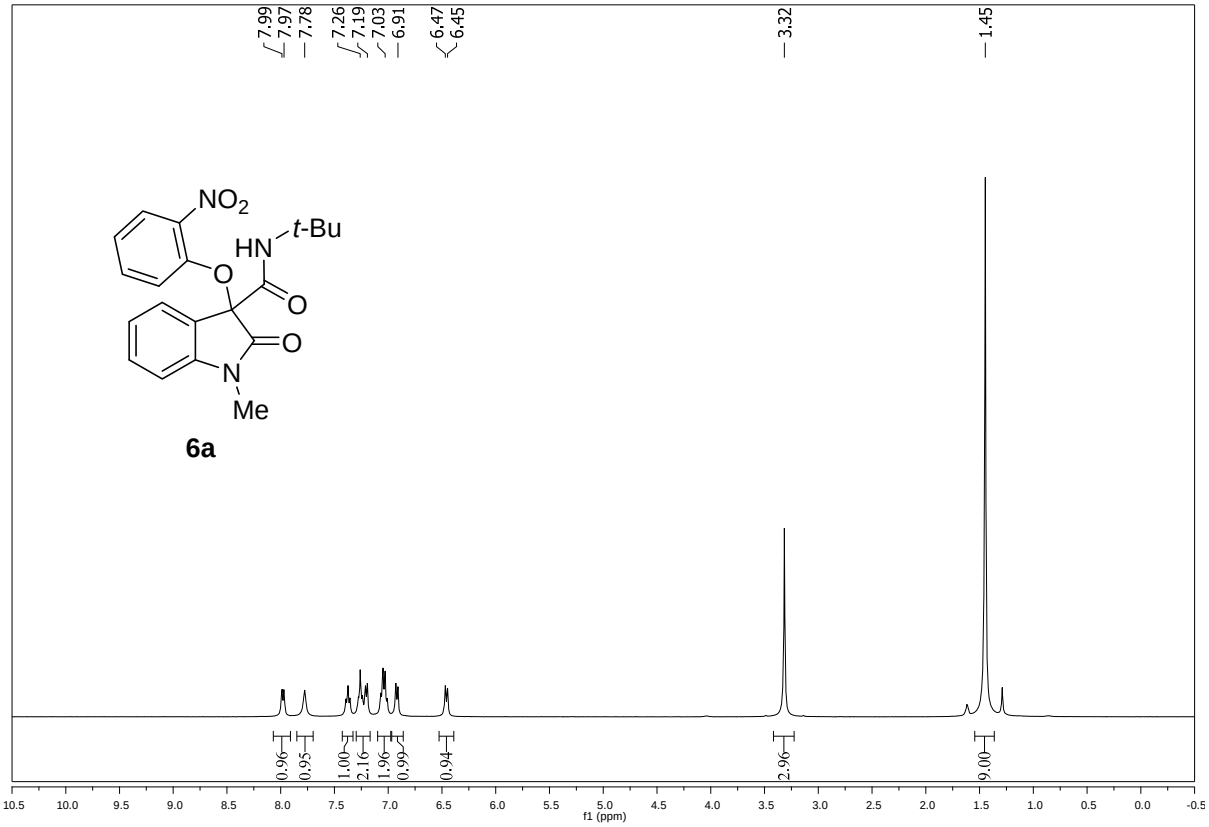


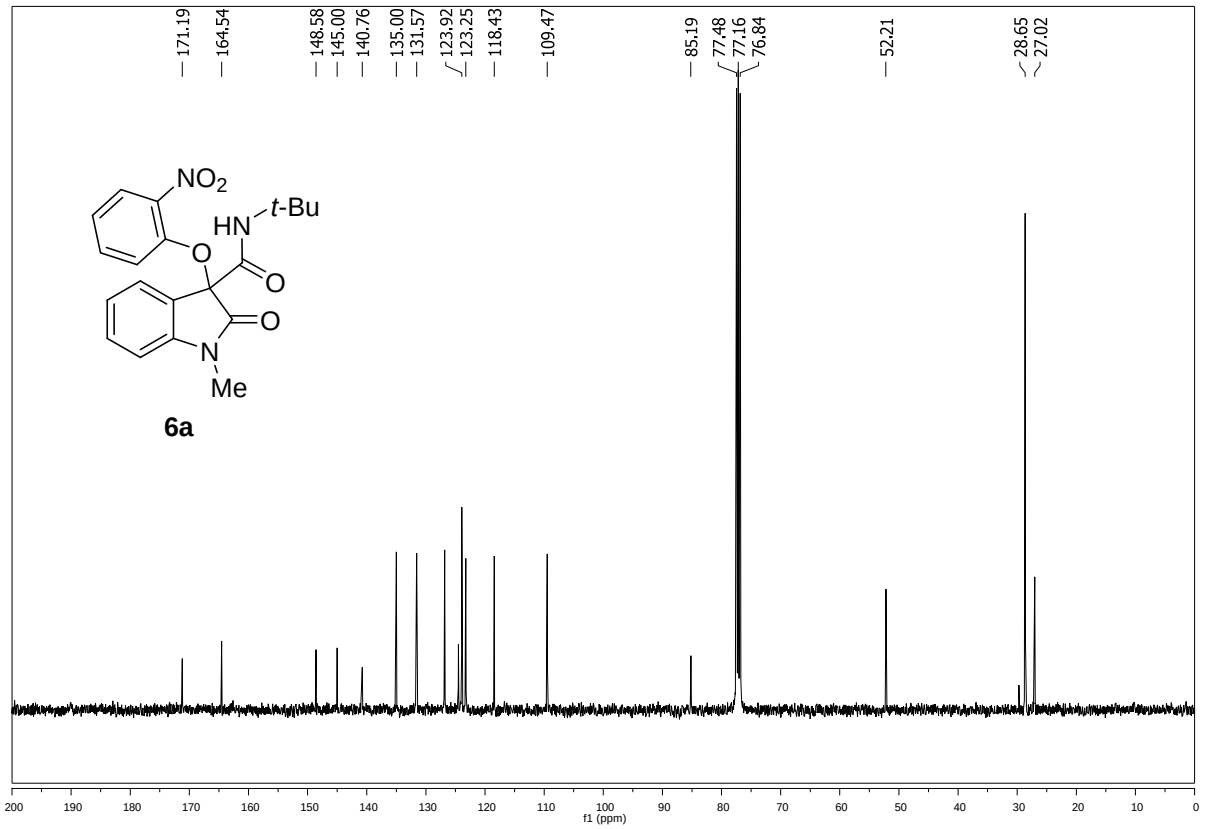
3-((2-Ethoxy-2-oxoethyl)carbamoyl)-1-methyl-2-oxoindolin-3-yl benzoate (4z)



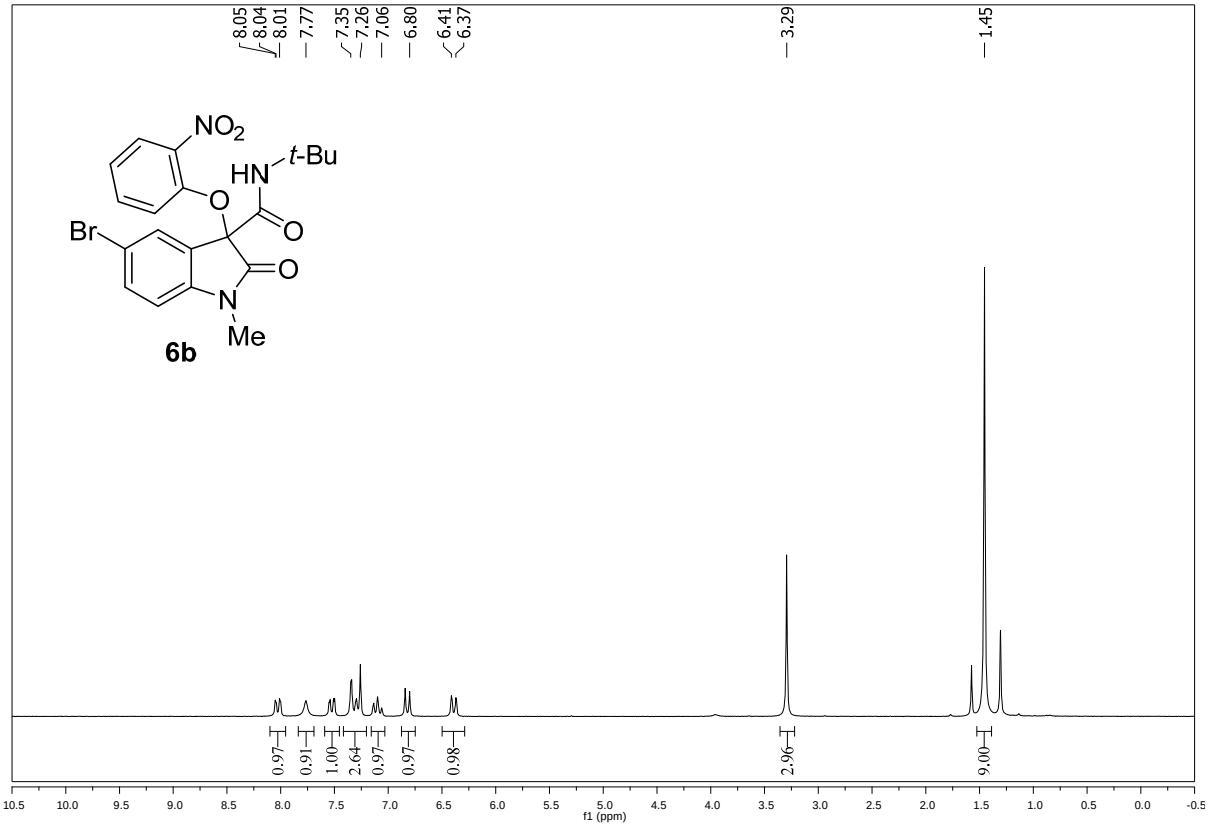


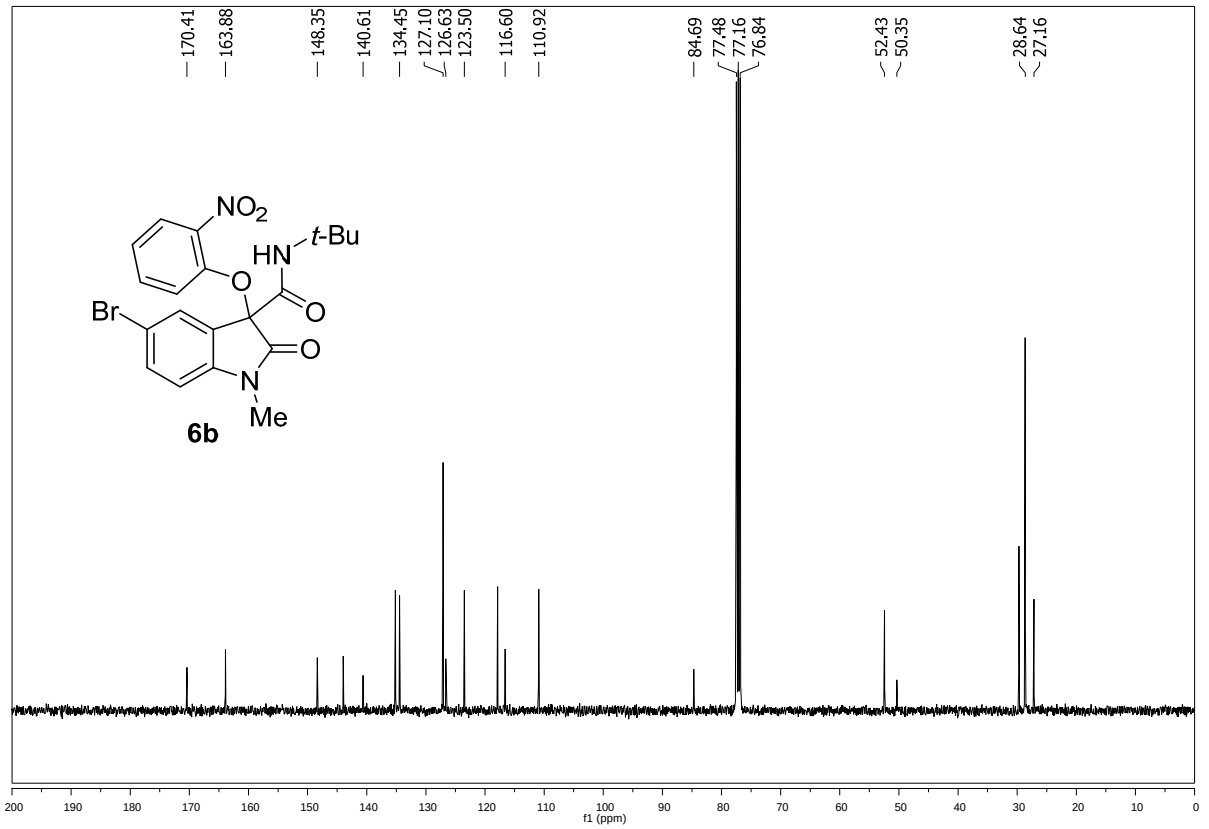
_N_-(_tert_-Butyl)-1-methyl-3-(2-nitrophenoxy)-2-oxoindoline-3-carboxamide (6a)



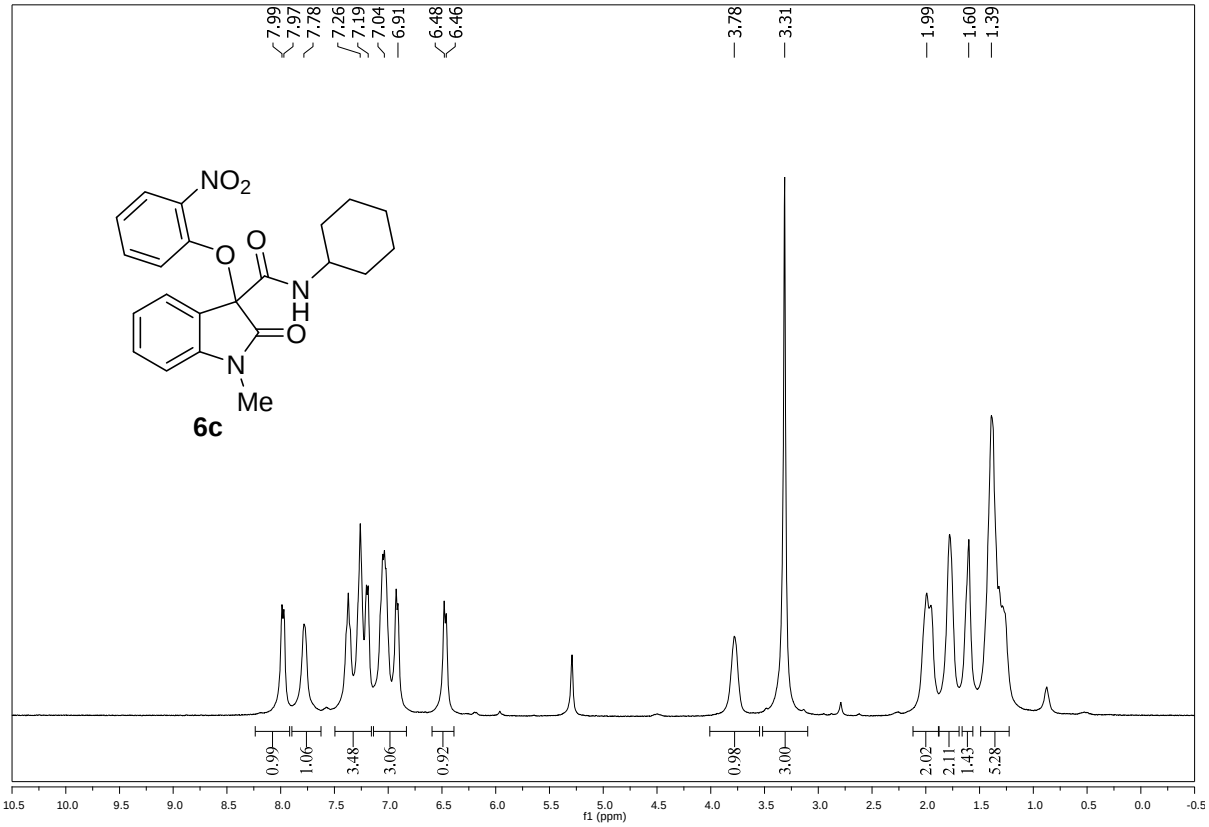


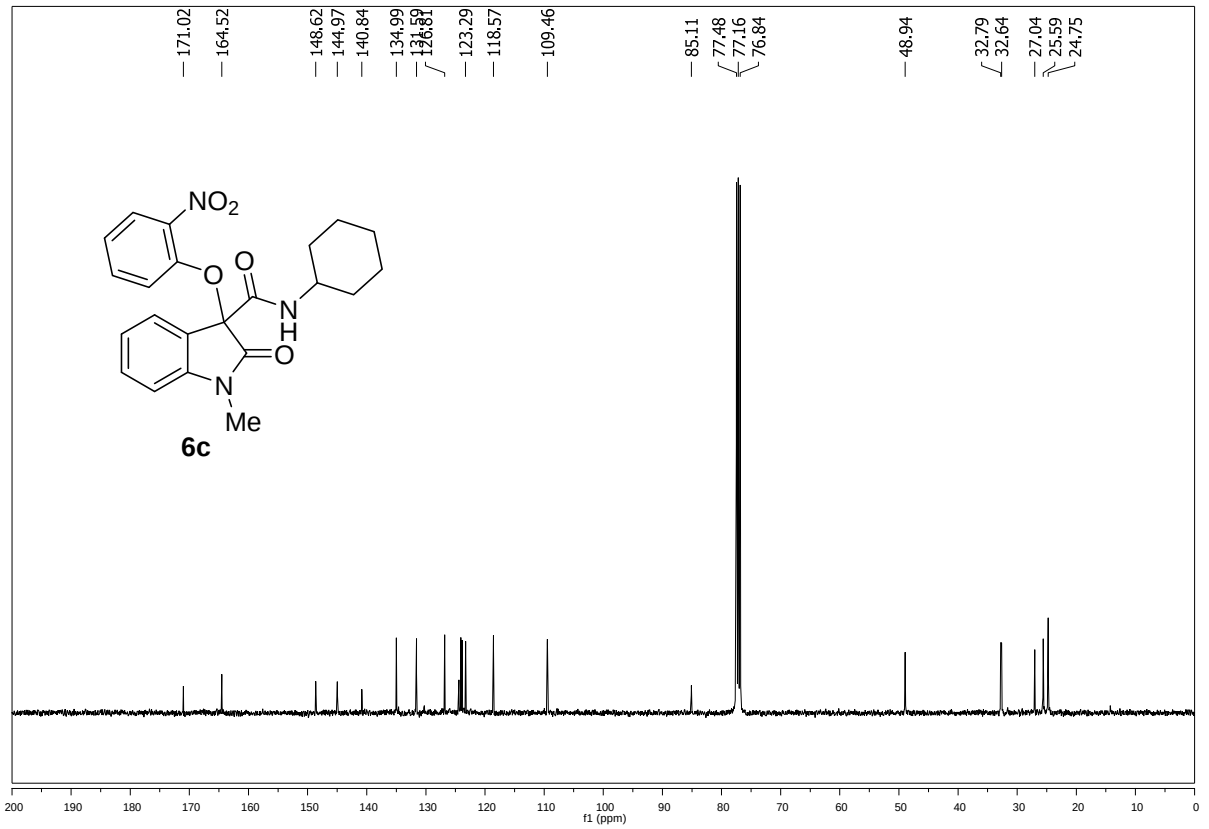
5-Bromo-N-(*tert*-butyl)-1-methyl-3-(2-nitrophenoxy)-2-oxoindoline-3-carboxamide (6b)





N-Cyclohexyl-1-methyl-3-(2-nitrophenoxy)-2-oxoindoline-3-carboxamide (6c)





5-Bromo-*N*-(*tert*-Butyl)-3-hydroxy-1-methyl-2-oxoindoline-3-carboxamide (7)