Electronic Supplementary Information

One-pot Preparation of Isocyanides from Amines and their Multicomponent Reactions: Crucial Role of Dehydrating agent and Base

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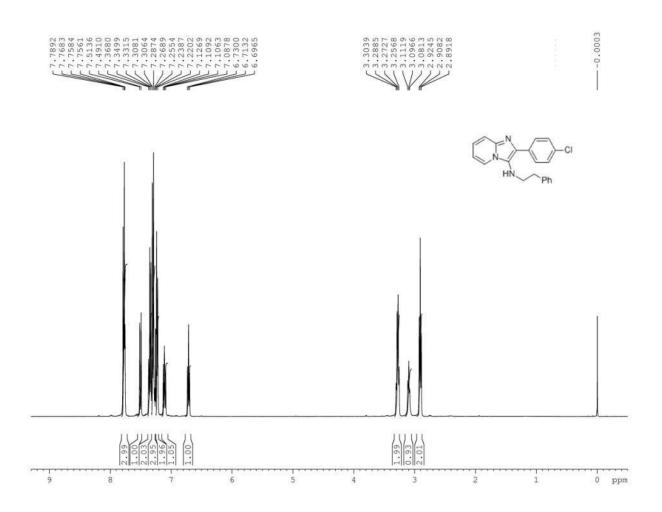
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General Information

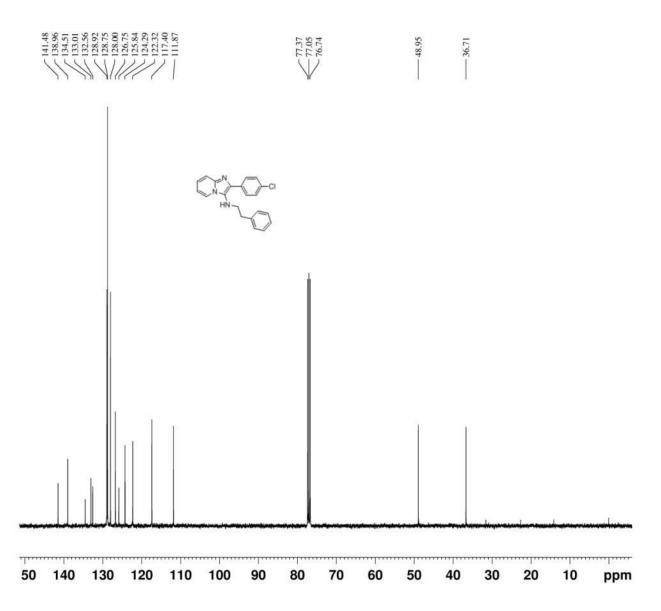
¹H NMR spectra were recorded on a Bruker Avance III-400 (400 MHz) spectrometer. Tetramethylsilane as an internal standard and NMR solvent CDCl₃, CD₃OD or DMSO-*d*₆ were used. Chemical shifts are in ppm. The ¹H NMR data includes the integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, td = triplet of doublet, dt = doublet of triplet, br = broad), and coupling constants (Hz). ¹³C NMR spectra were recorded on a Bruker Avance III-400 (100 MHz) spectrometer with complete proton decoupling. Chemical shifts are in ppm with NMR solvent as an internal standard. The acquisition of High-resolution mass spectra (HRMS) was performed on Bruker maxis Q-TOF. Infrared (IR) spectra were recorded on a Perkin Elmer FTIR with ATR and IR Microscope spectrometer. For thin layer chromatography (TLC) analysis, Merck precoated TLC plates (silica gel 60 GF 254, 0.25 mm) were used. The products were purified by column chromatography with silica gel 60-120 (Merck, silica gel 60-120 mesh, neutral, spherical) or preparative thin layer chromatography silica gel (Rankem, Silica Gel GF 254, 400 mesh). Melting points determined are uncorrected.

All commercially obtained reagents were used as received. Acetonitrile solvent was made anhydrous by distillation on calcium hydride.

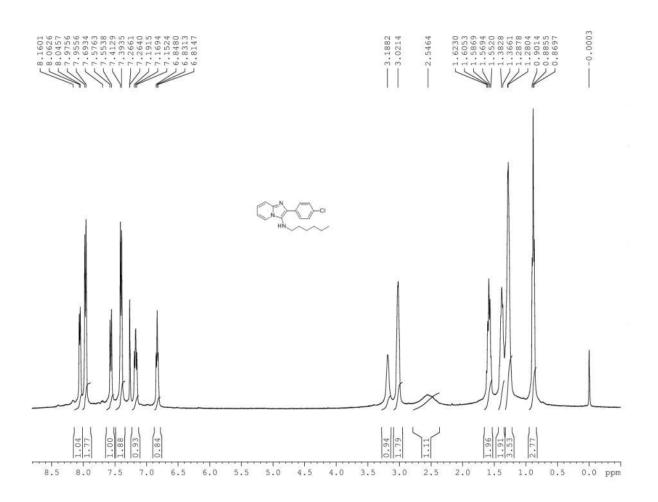
Spectra of compounds (6a-n) 6a: ¹H NMR



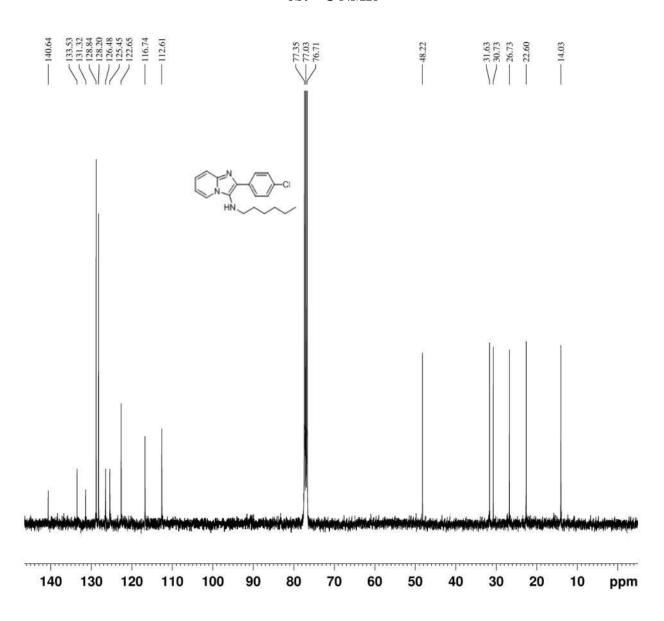




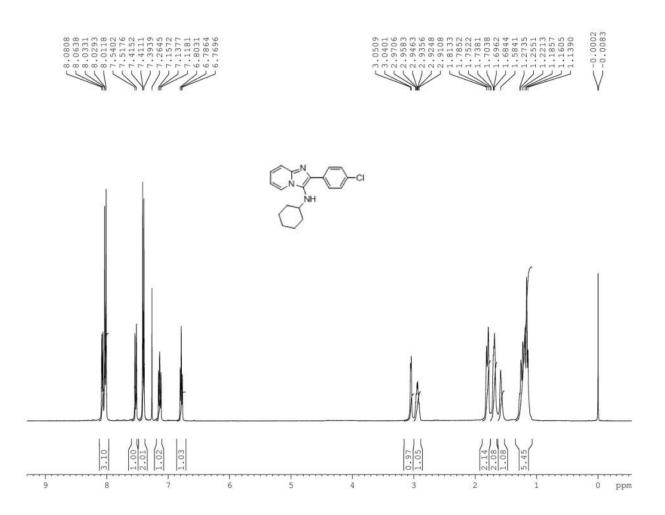
6b: ¹H NMR



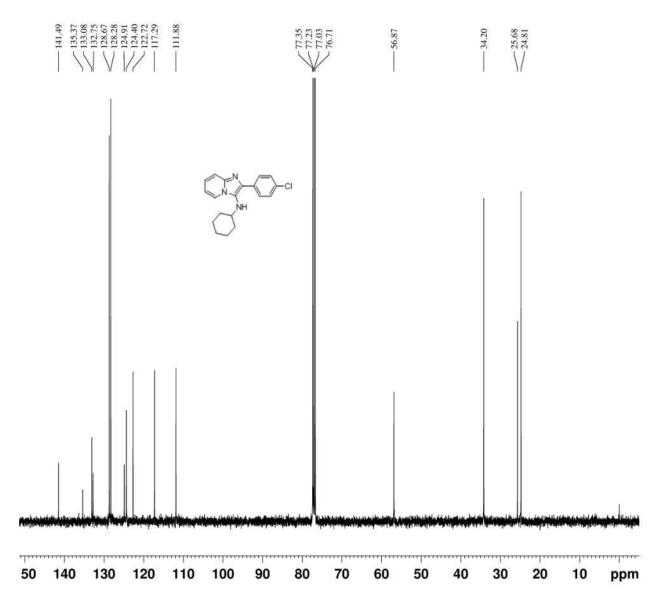
6b: ¹³C NMR



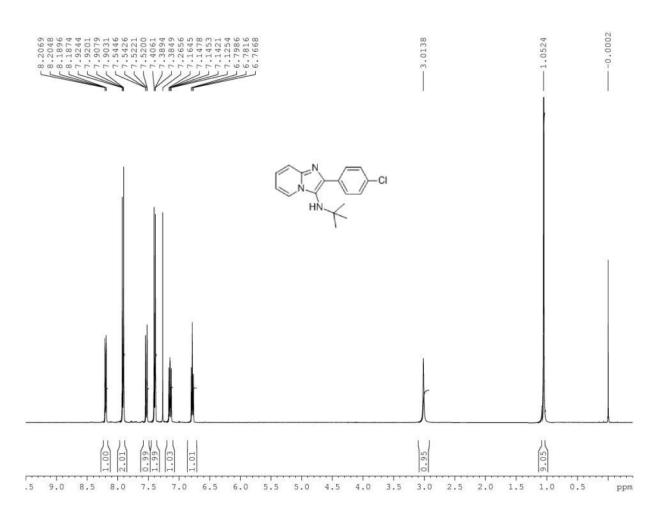
6c: ¹H NMR

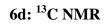


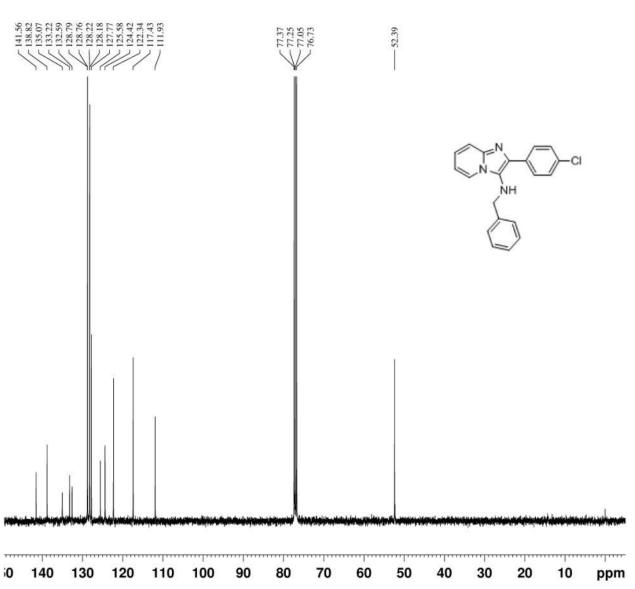




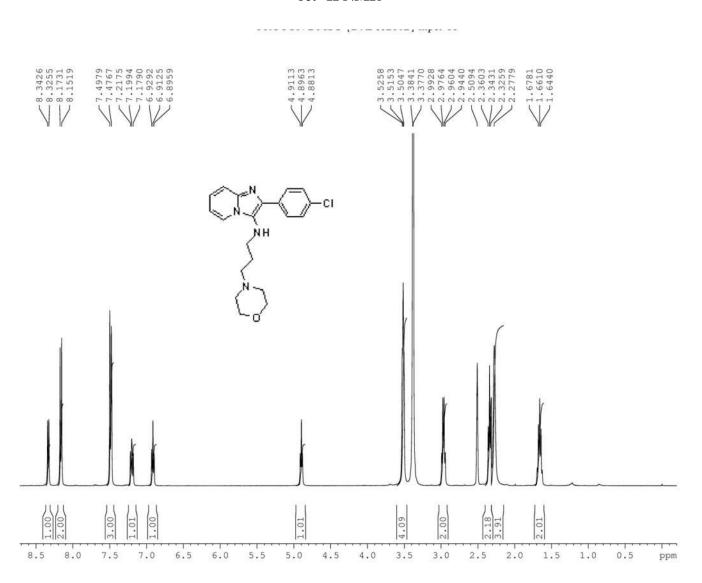
6d: ¹H NMR



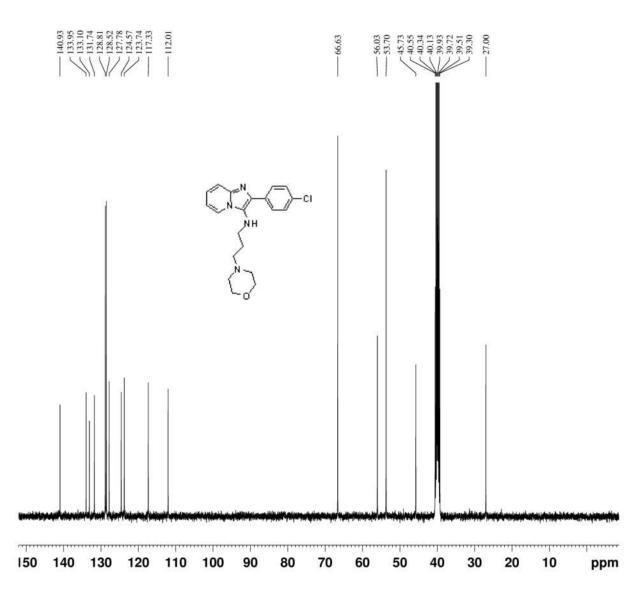




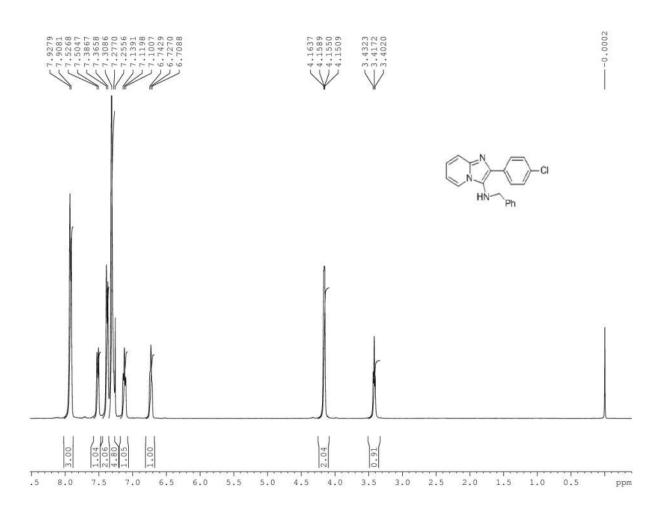
6e: ¹H NMR



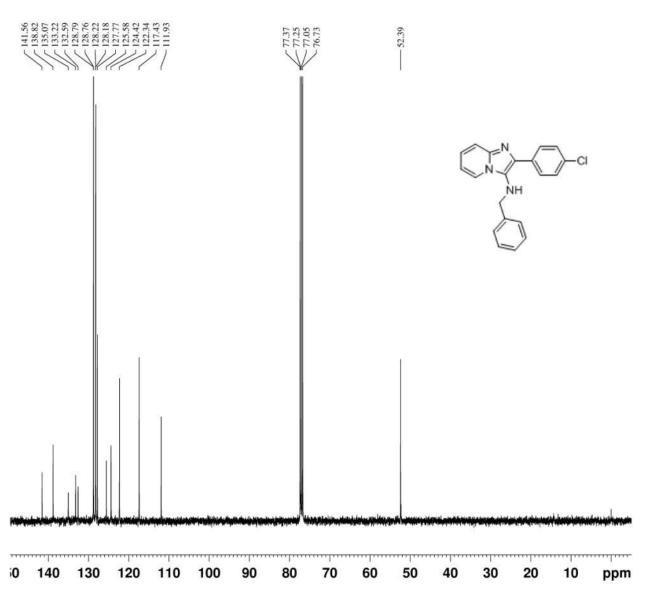
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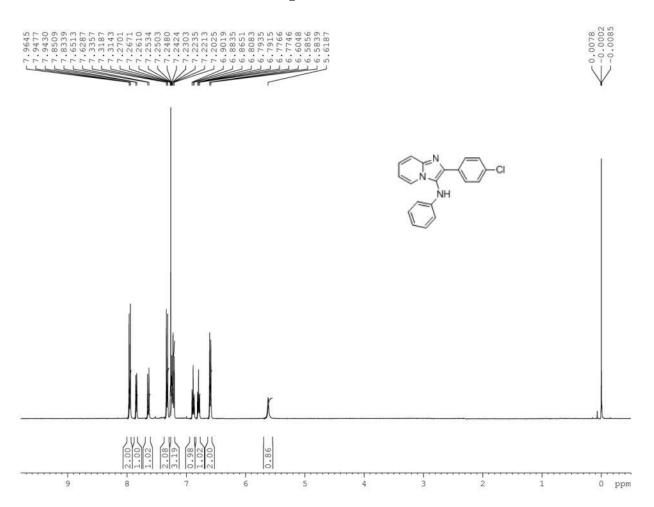
6f: ¹H NMR



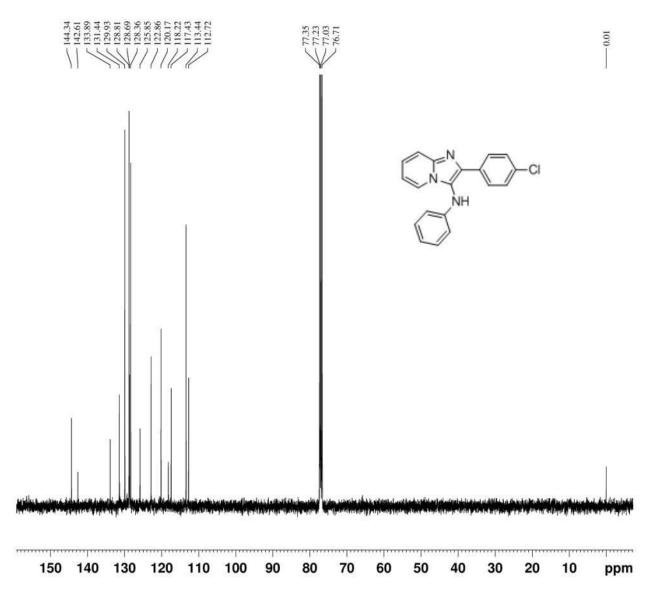




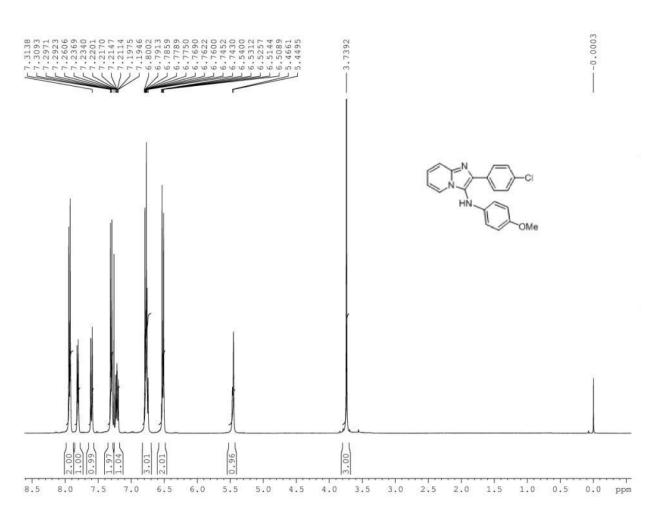
6g: ¹H NMR



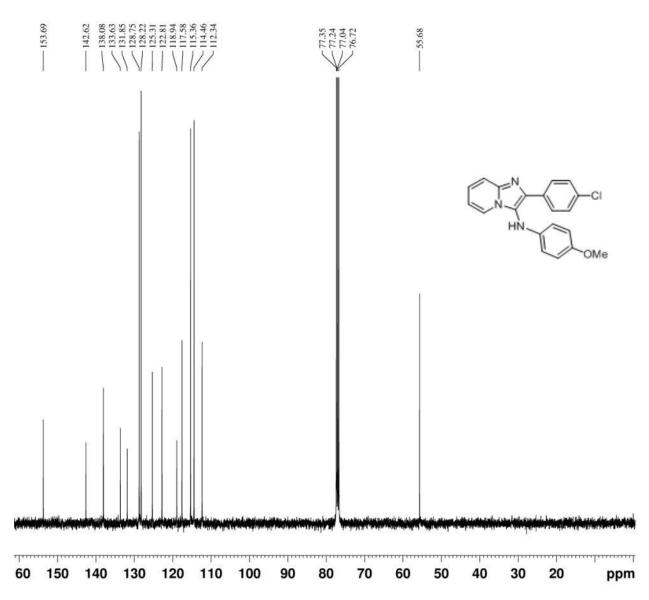
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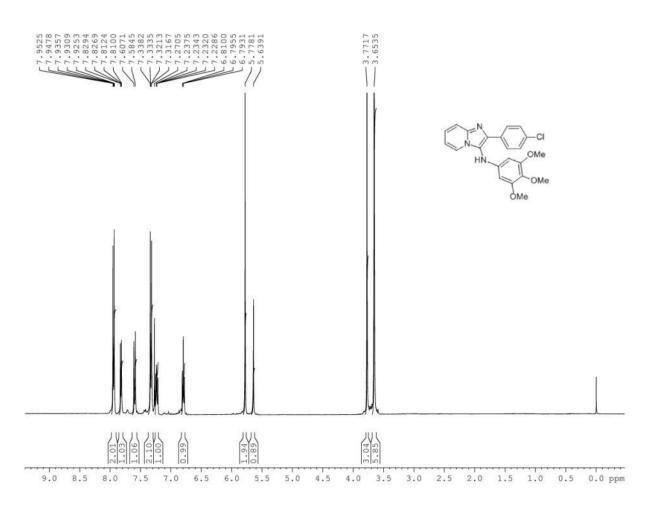
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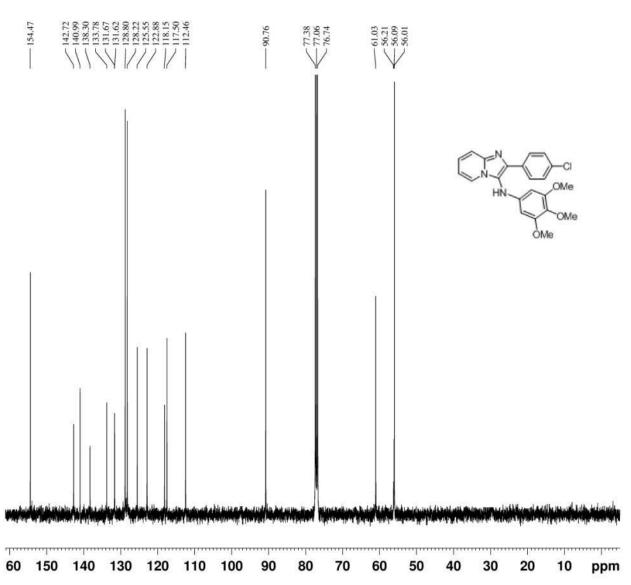




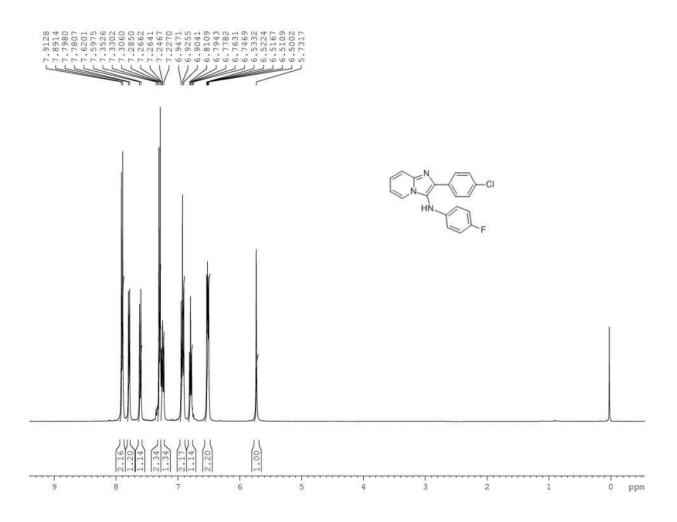
6i: ¹H NMR

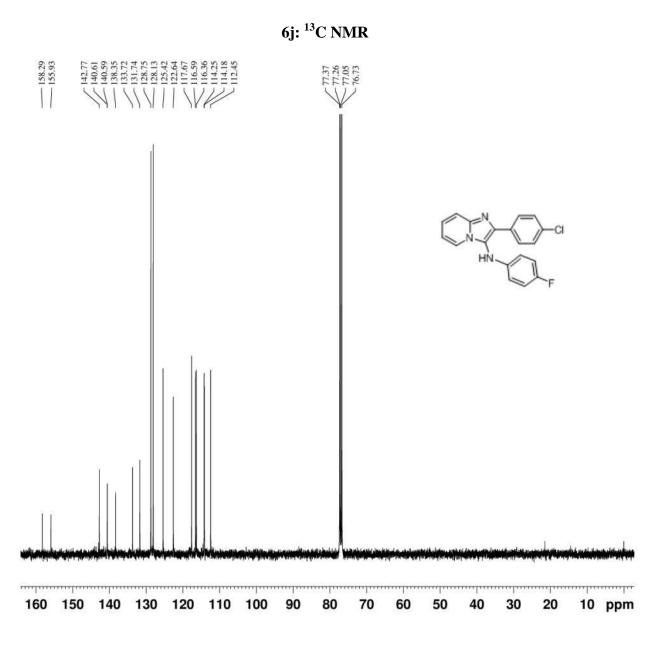




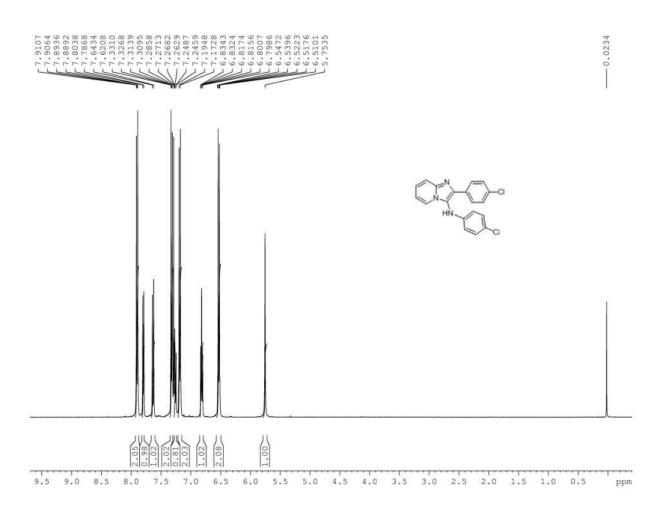


6j: ¹H NMR

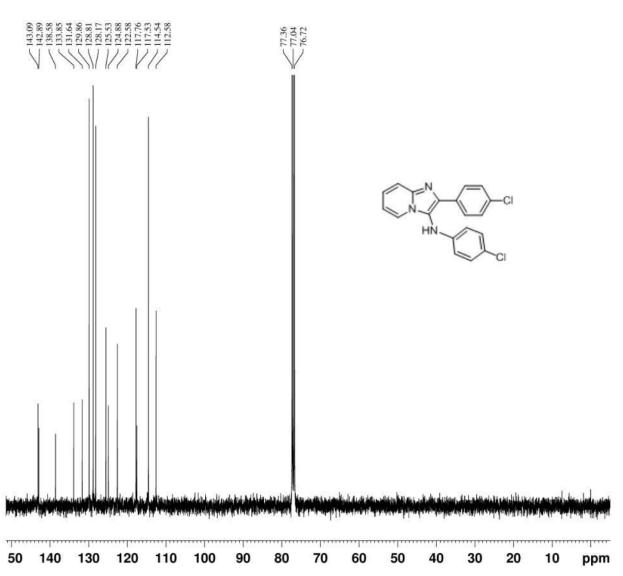




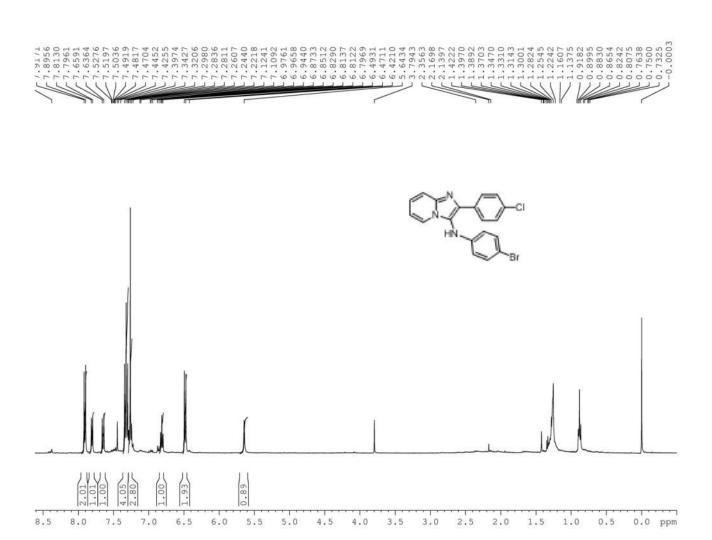
6k: ¹H NMR



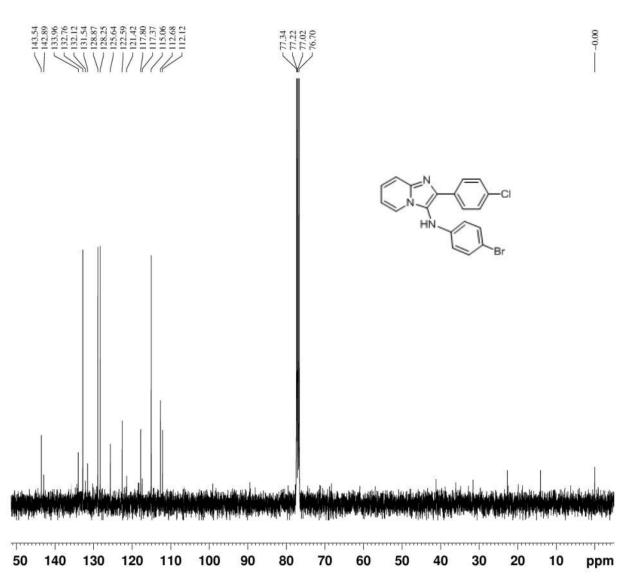




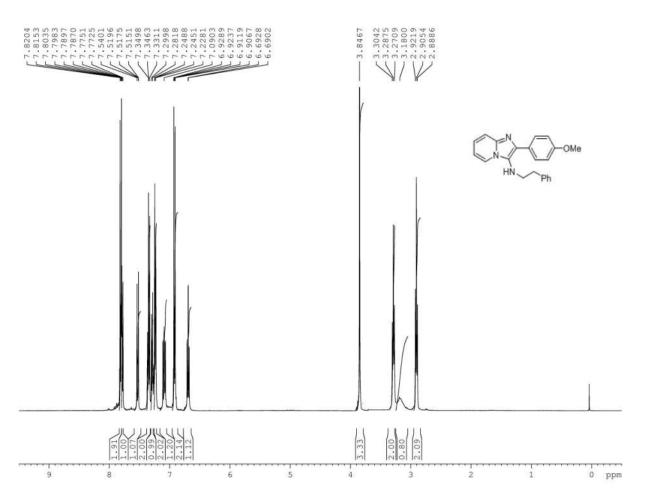
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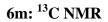


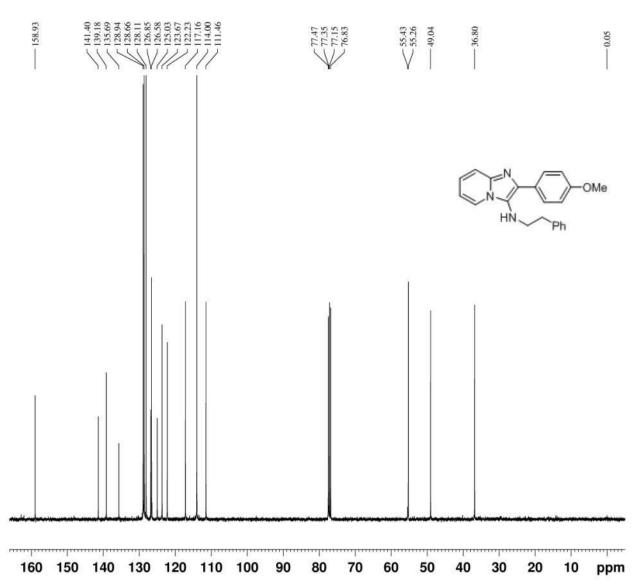
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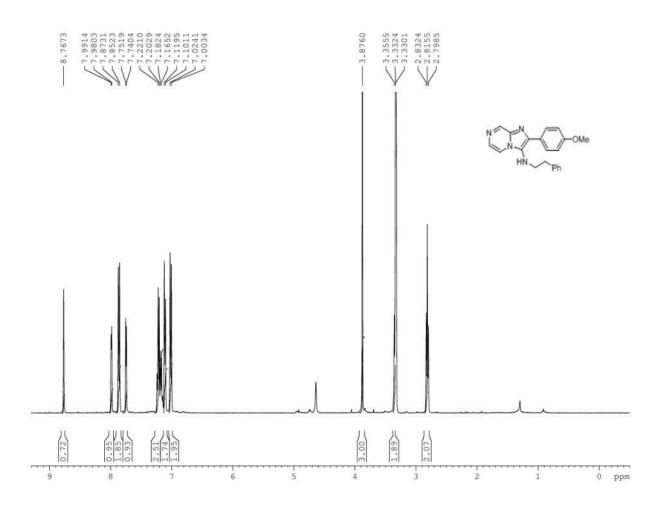
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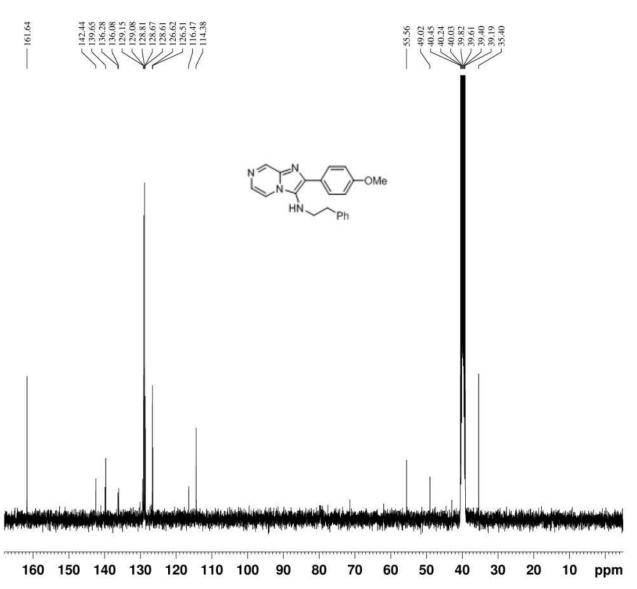




6n: ¹H NMR

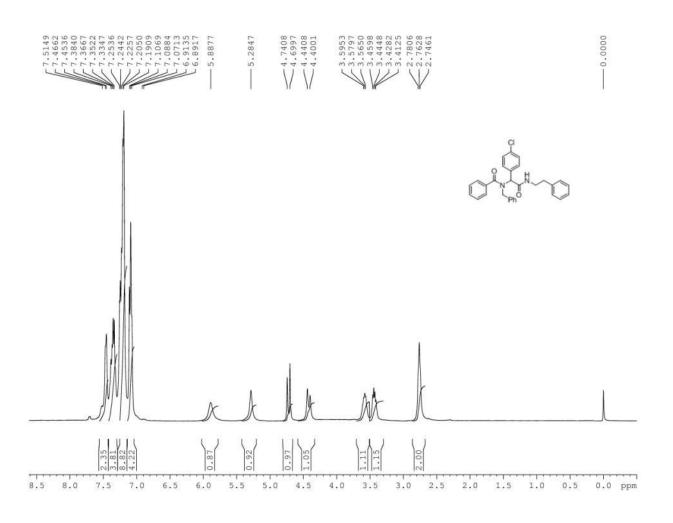


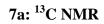


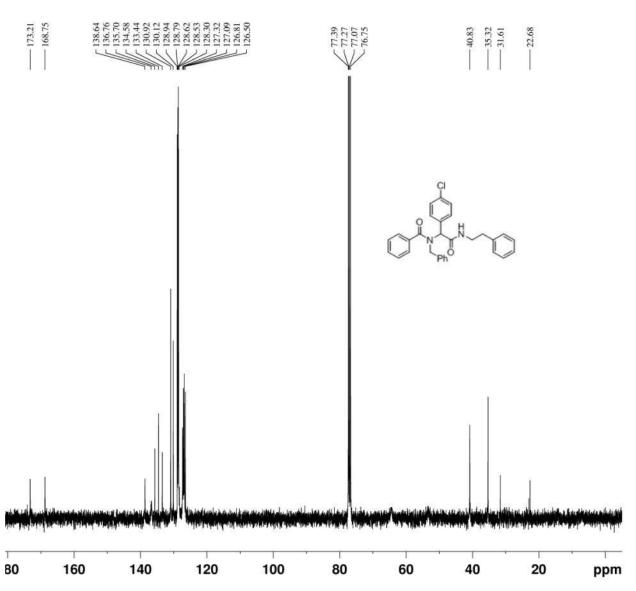


NMR Spectra of Compounds (7a-o)

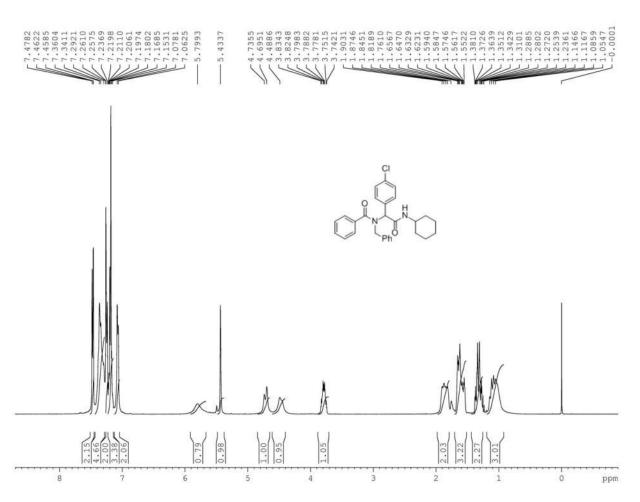
7a: ¹H NMR



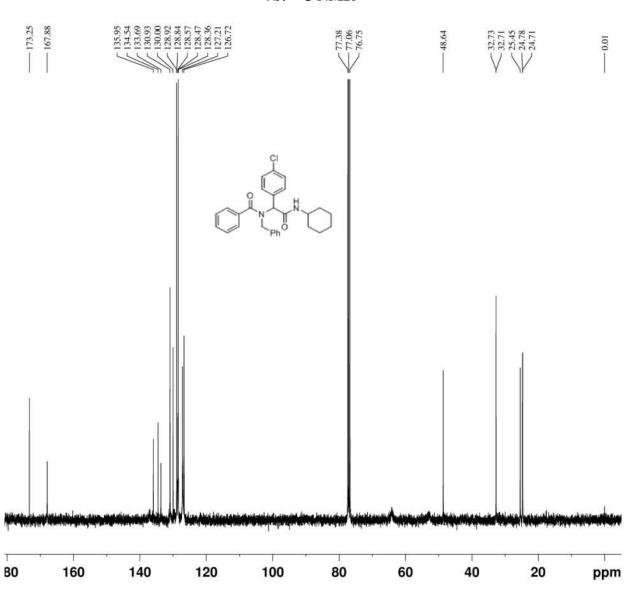




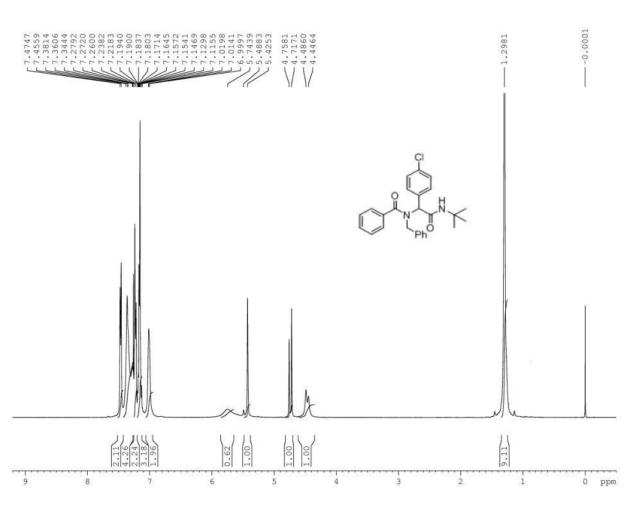
7b: ¹H NMR

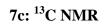


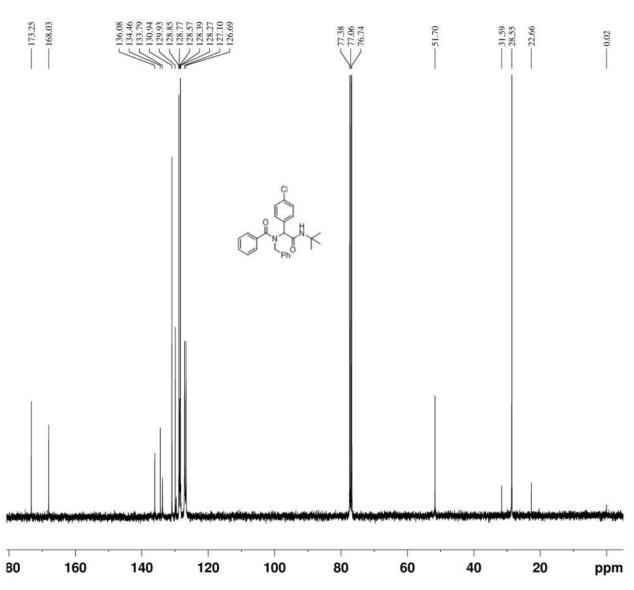
7b: ¹³C NMR

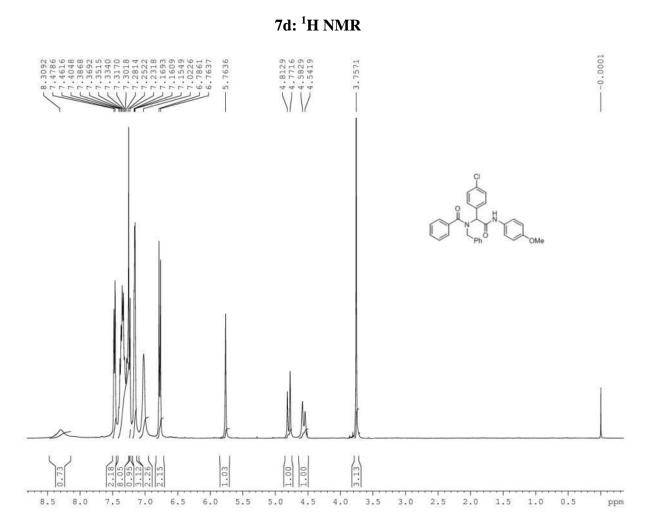


7c: ¹H NMR

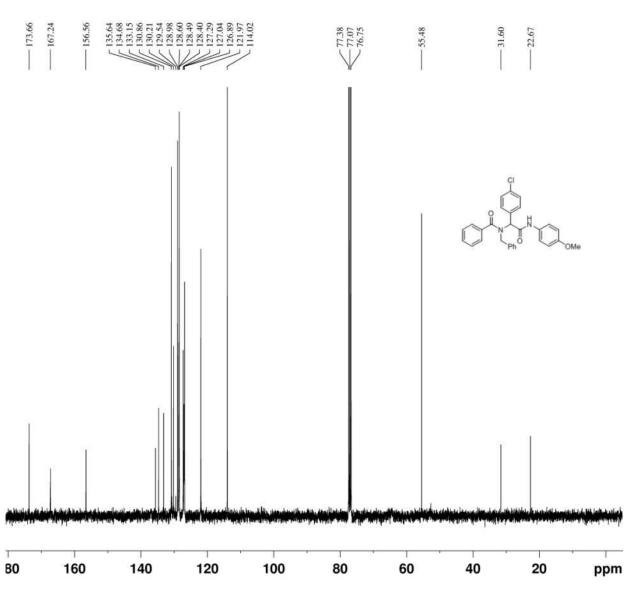




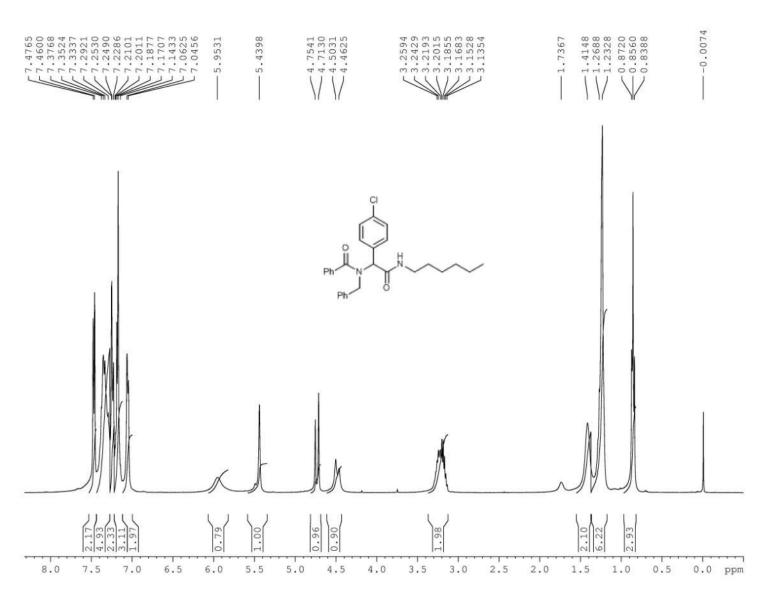


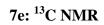


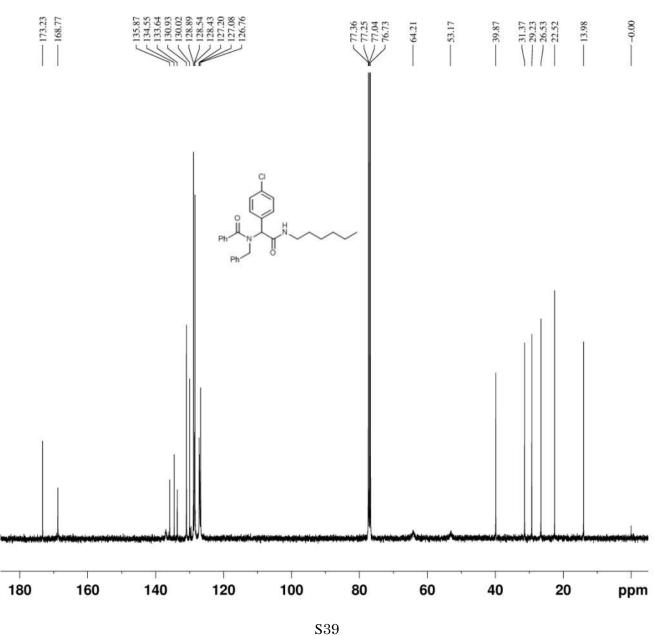




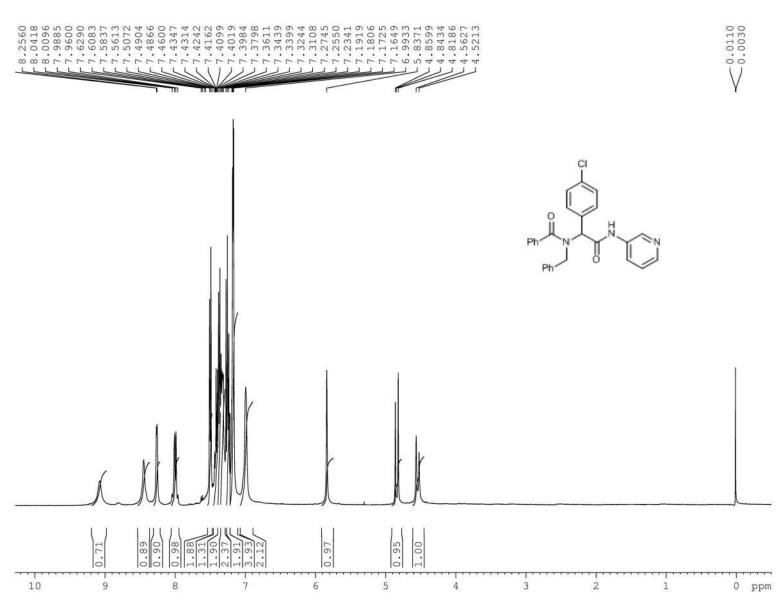
7e: ¹H NMR



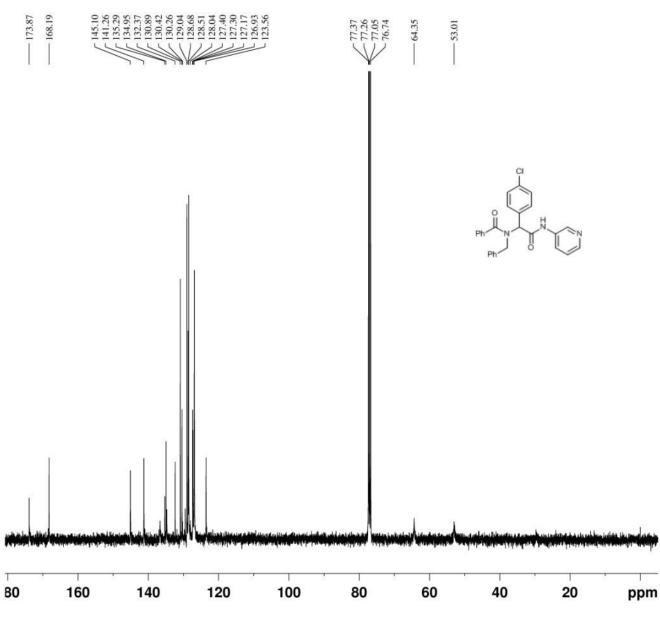




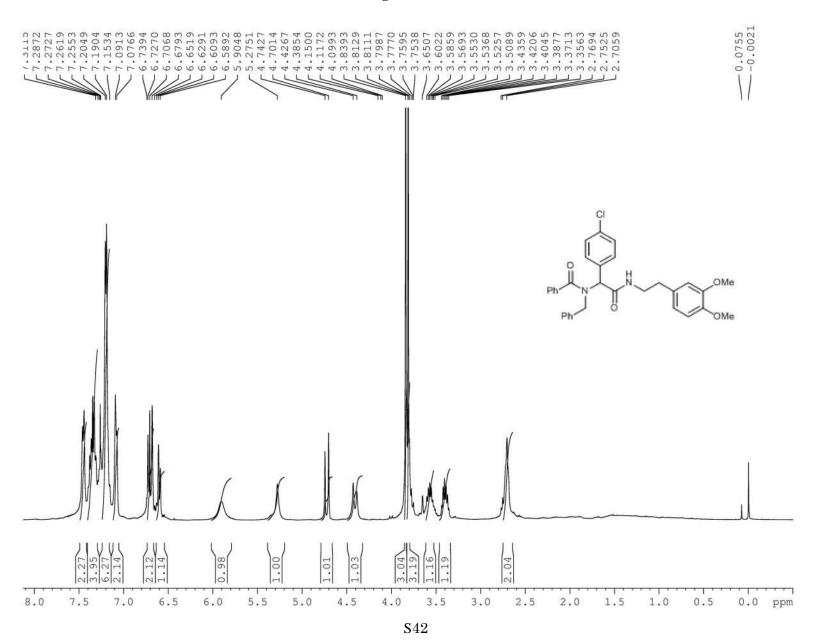
7f: ¹H NMR

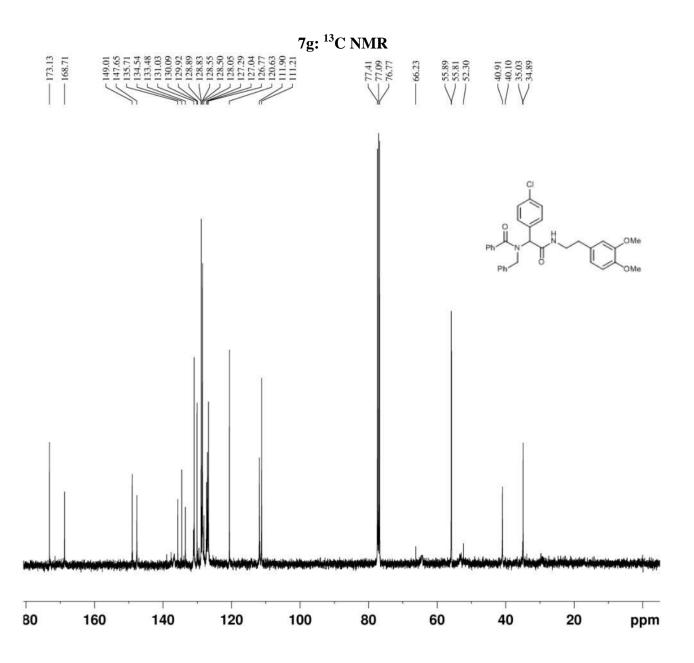




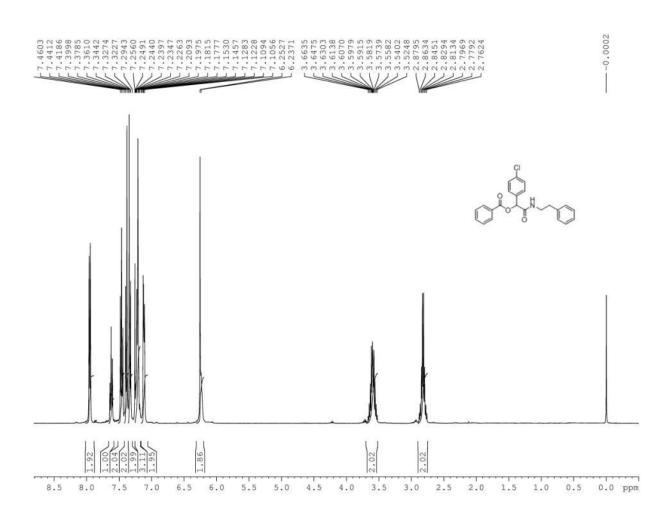


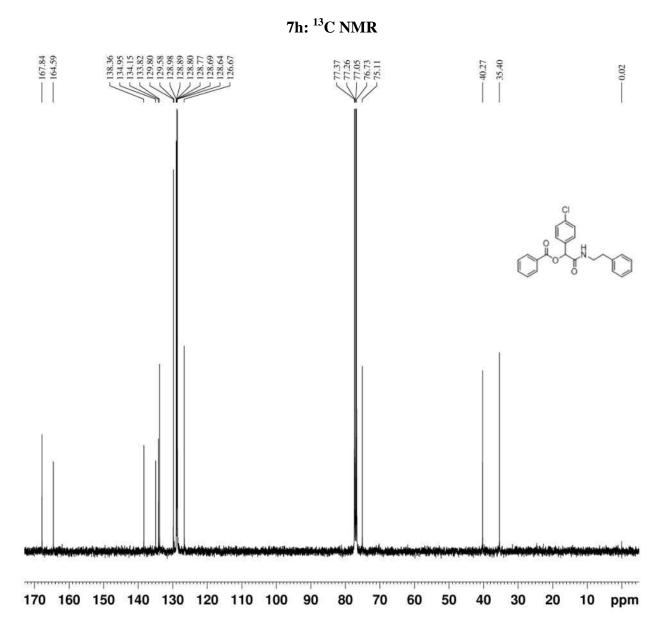
7g: ¹H NMR



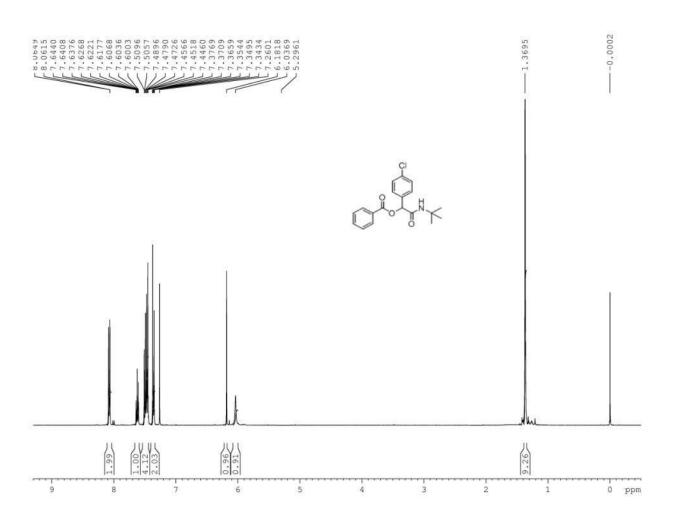


7h: ¹H NMR

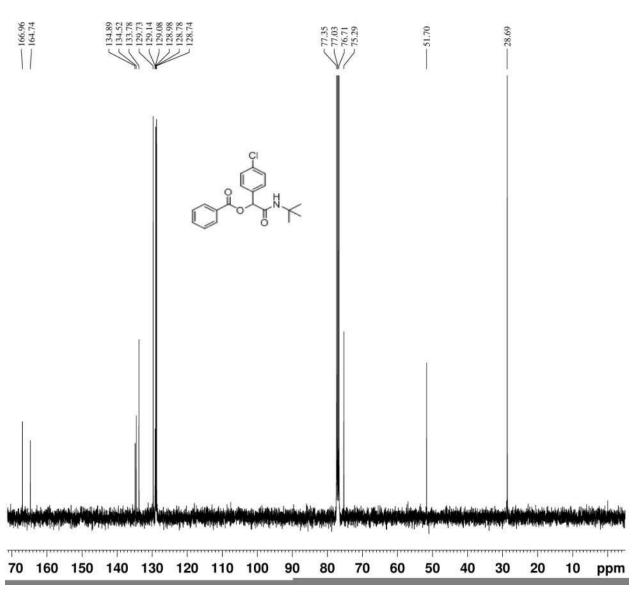




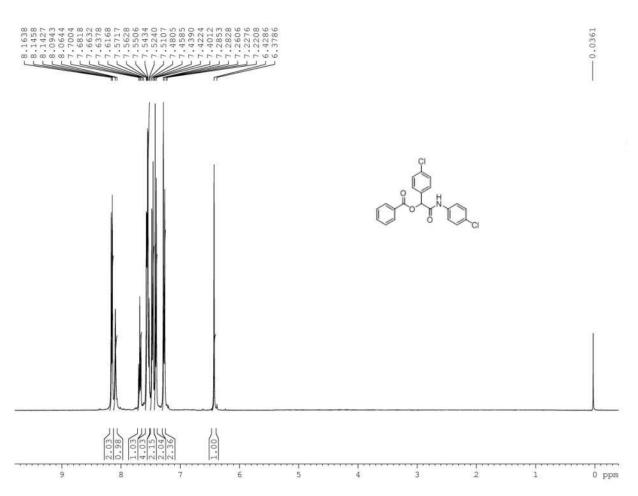
7i: ¹H NMR

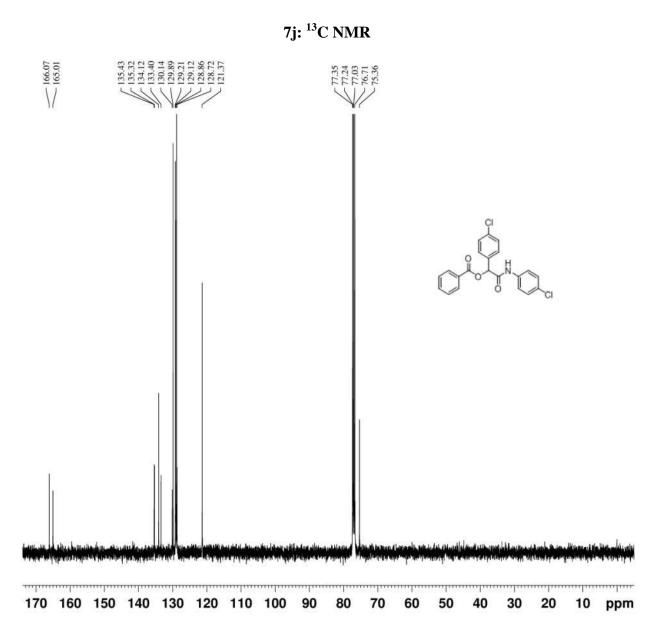




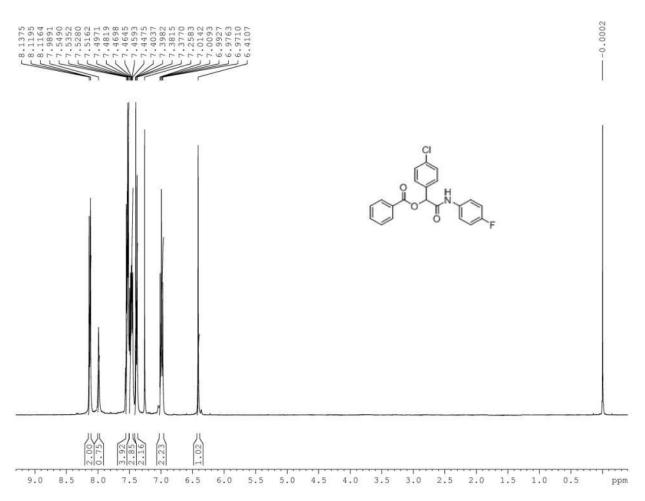


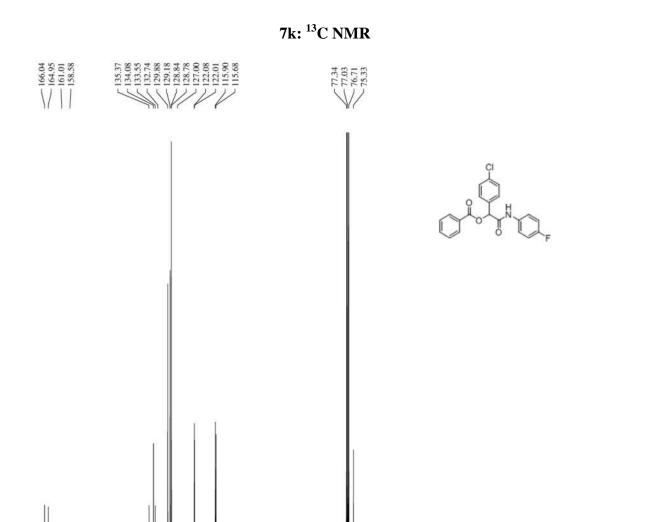
7j: ¹H NMR





7k: ¹H NMR

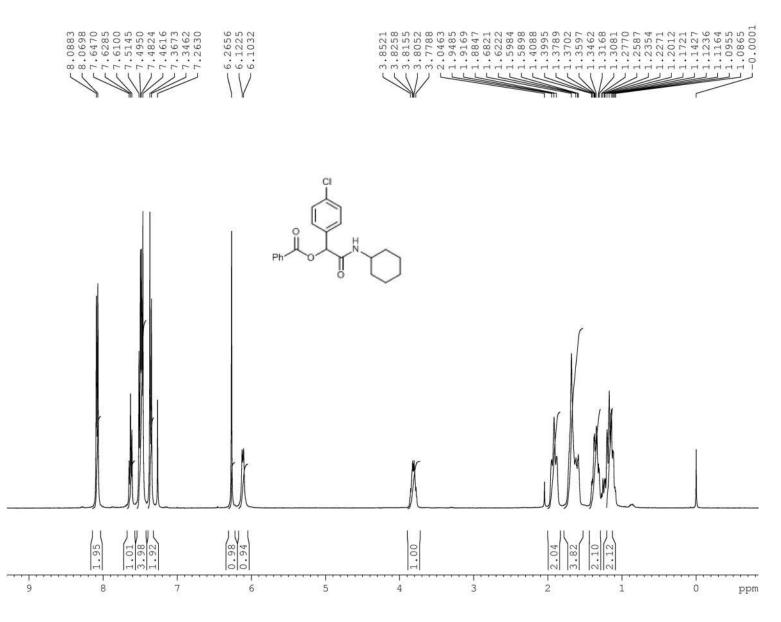


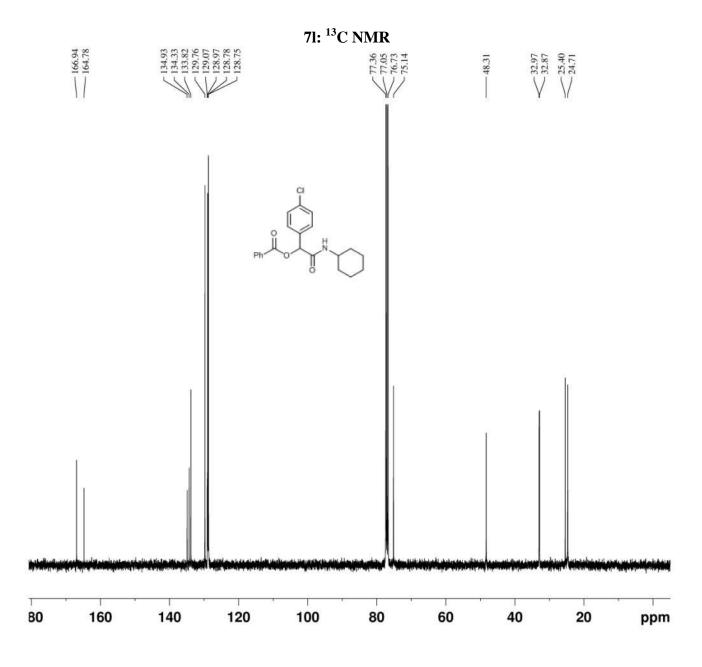


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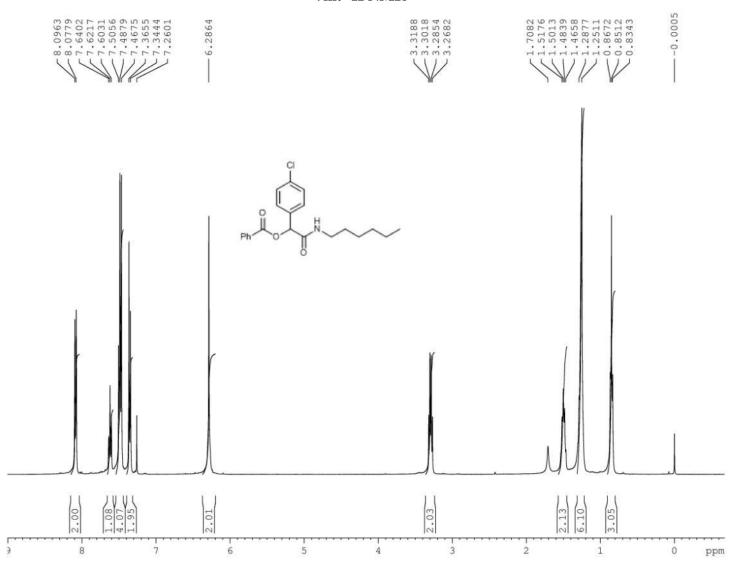
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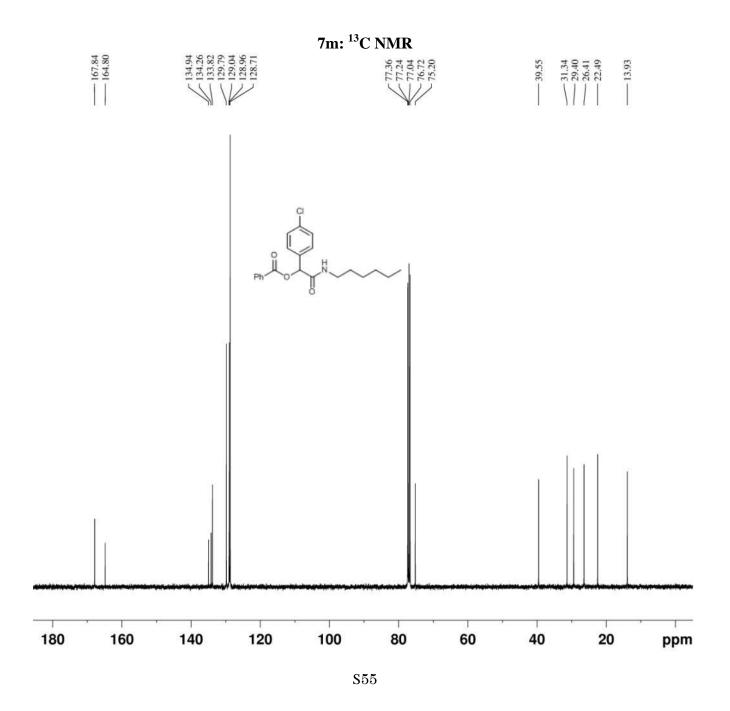
71: ¹H NMR











7n: ¹H NMR

