

SUPPORTING INFORMATION:

Room temperature reduction of titanium tetrachloride-activated nitriles to primary amines with ammonia-borane

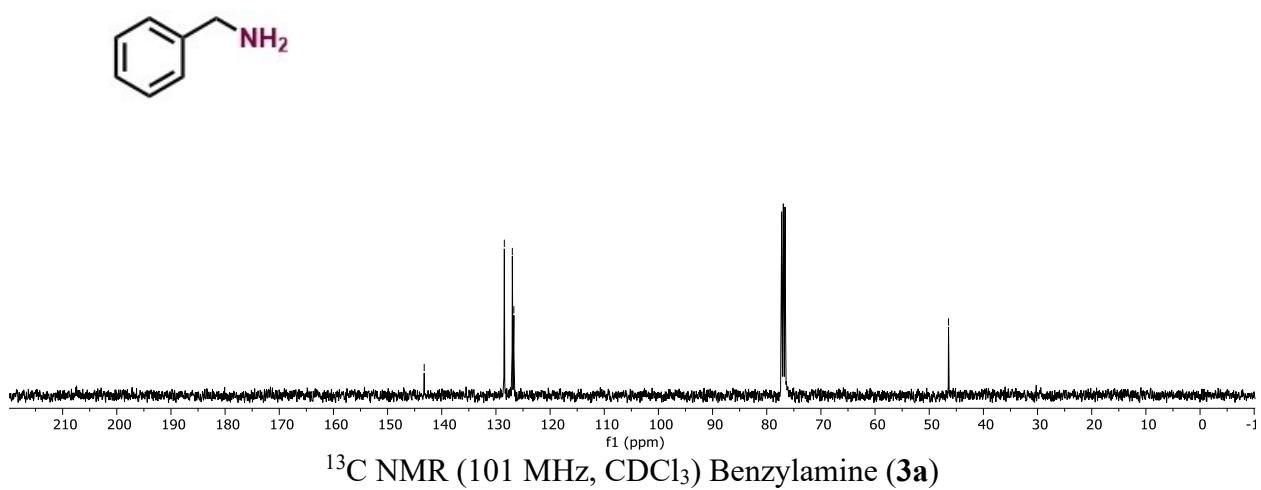
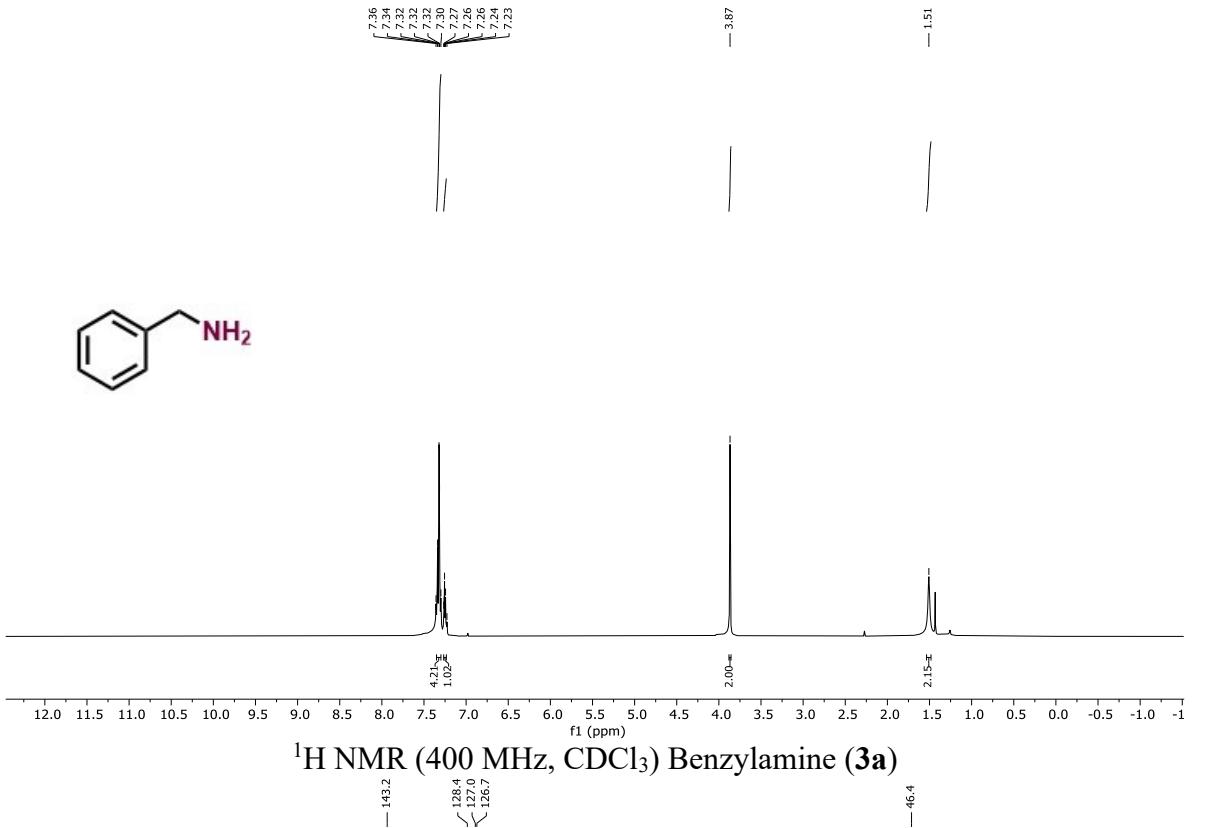
P. Veeraraghavan Ramachandran,* Abdulkhalil A. Alawaed

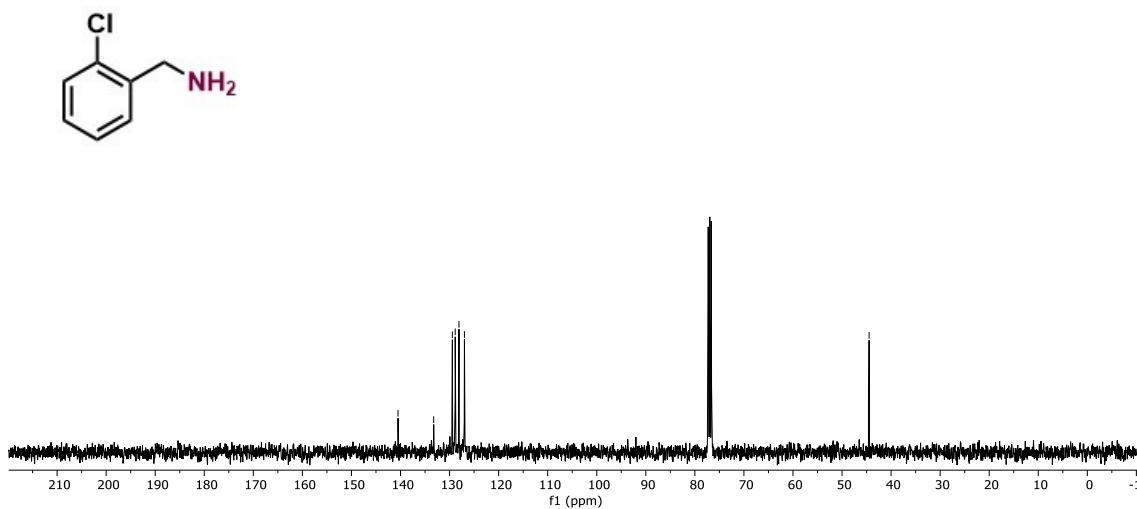
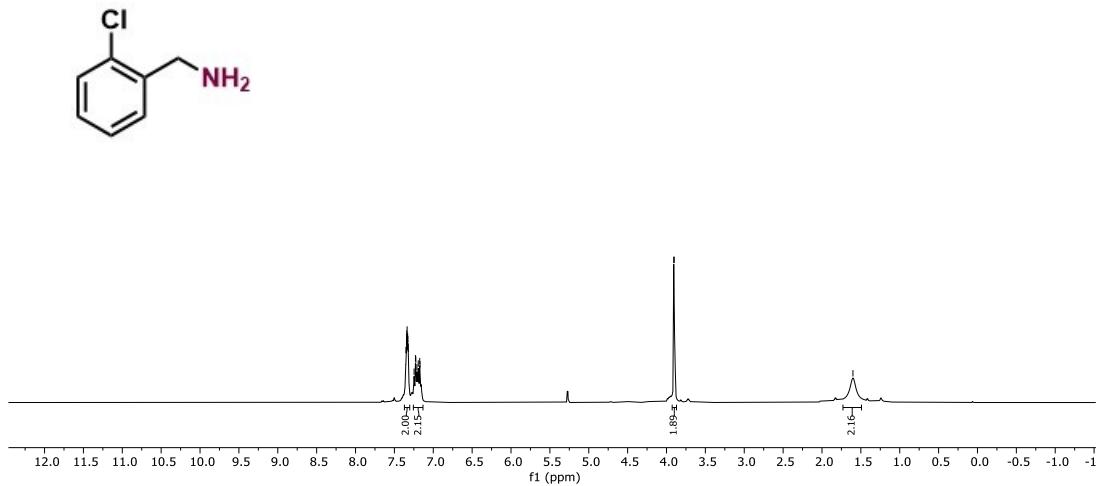
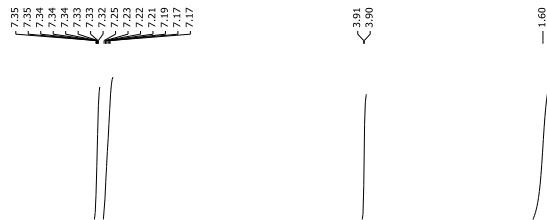
† Herbert C. Brown Center for Borane Research, Department of Chemistry, Purdue University,
West Lafayette, Indiana 47907, United States

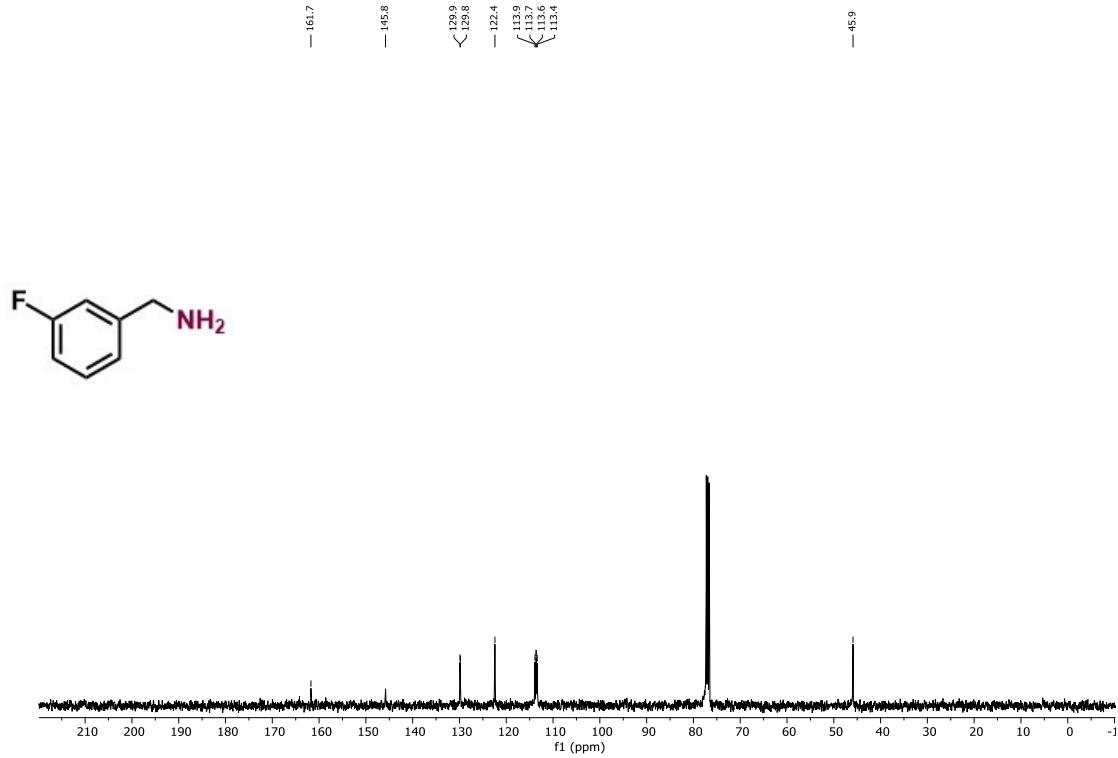
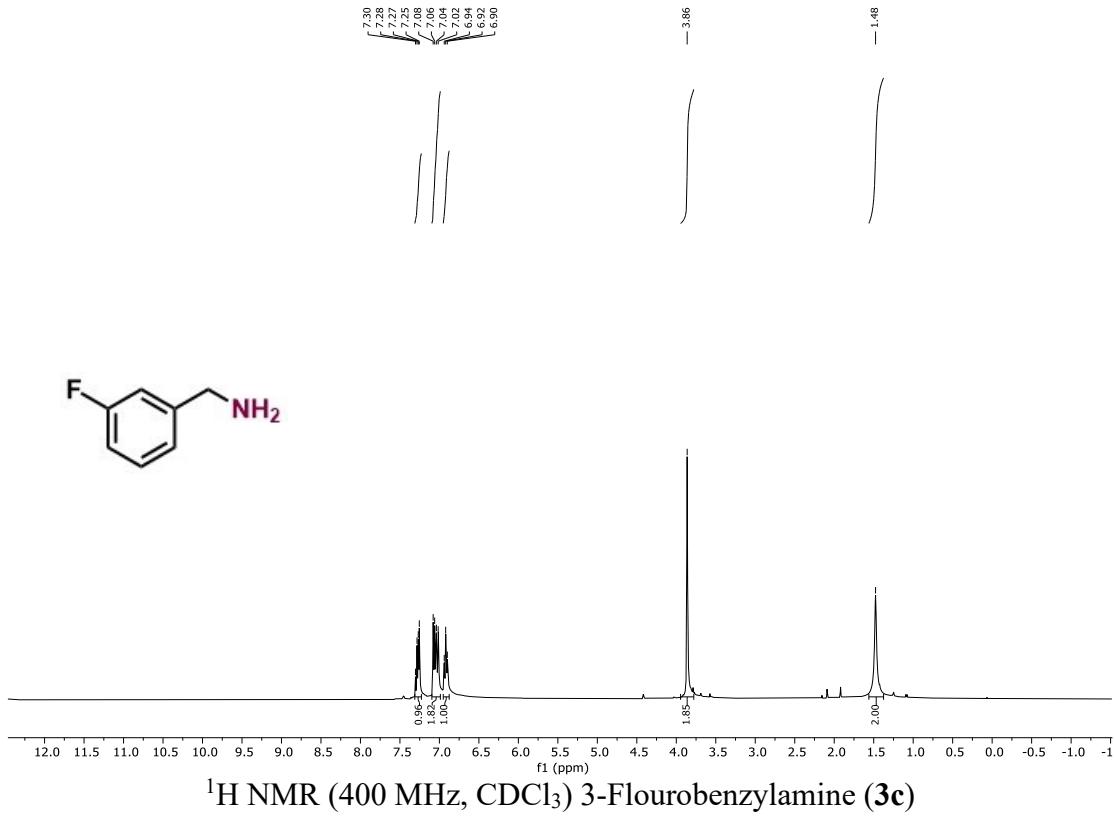
E-mail: chandran@purdue.edu

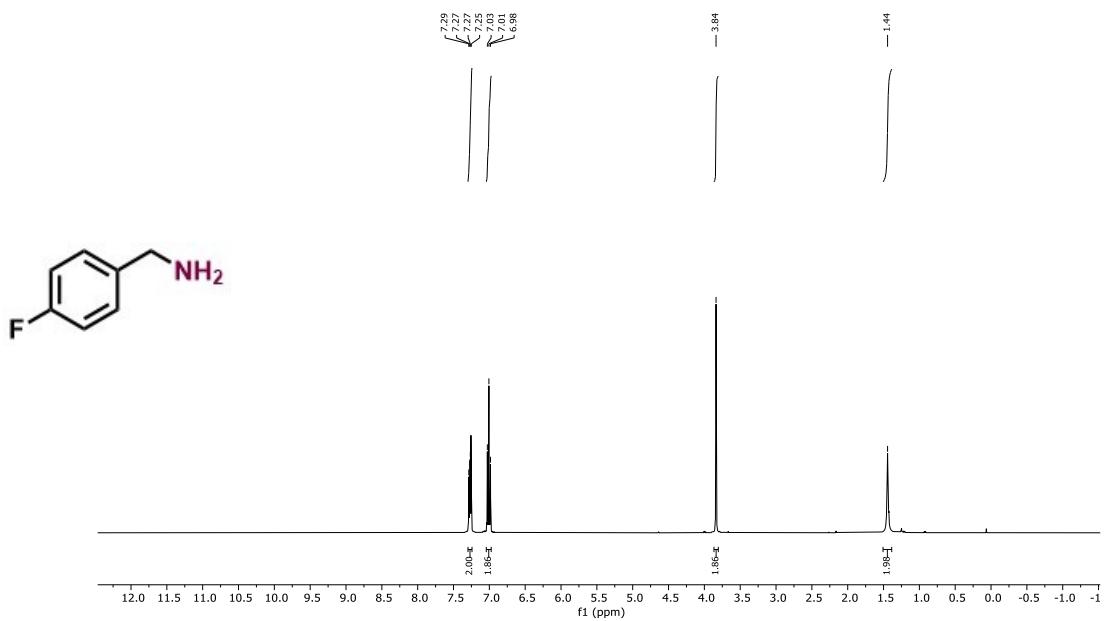
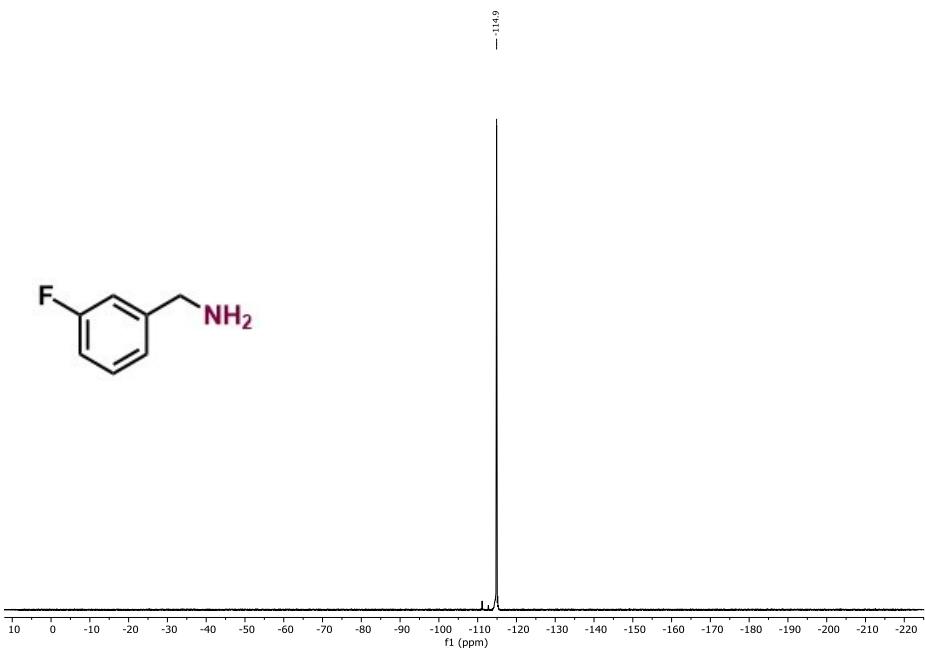
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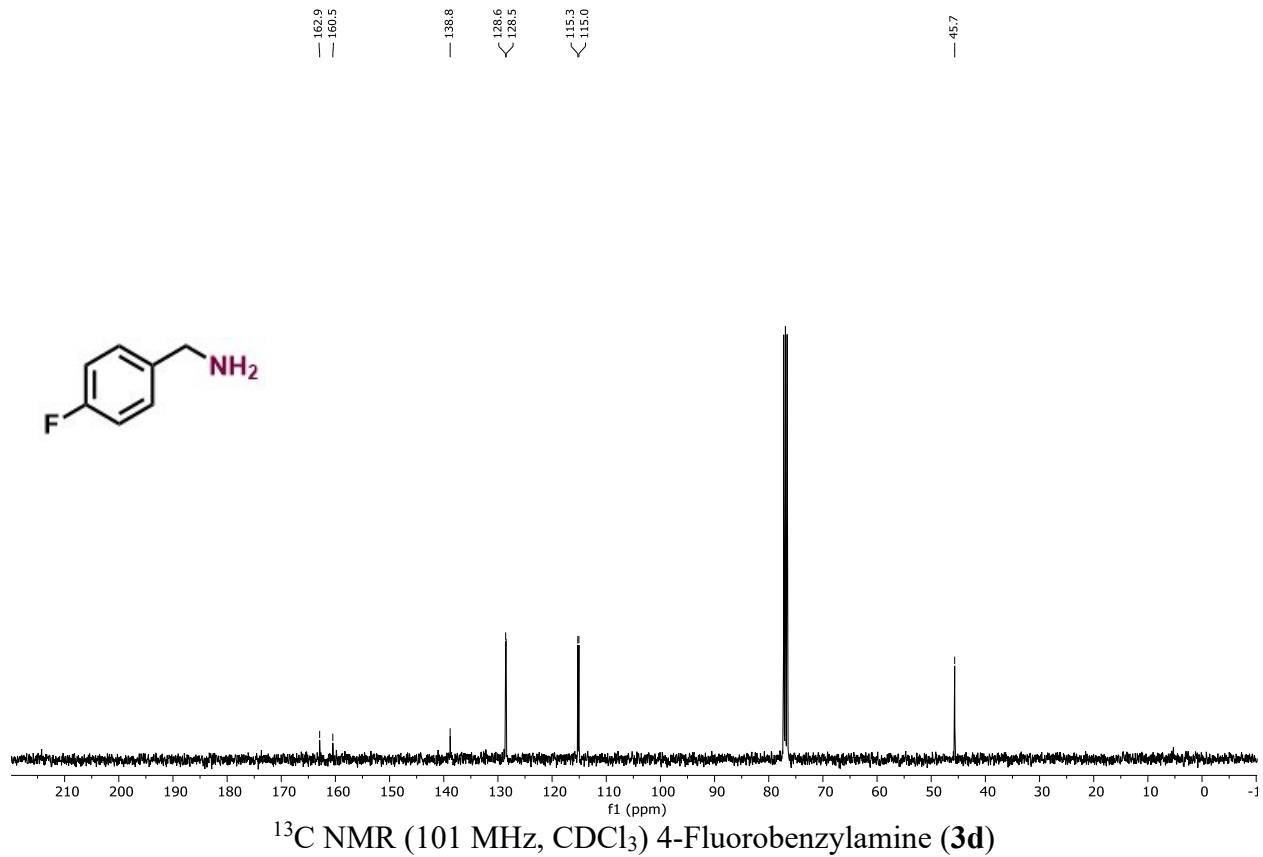


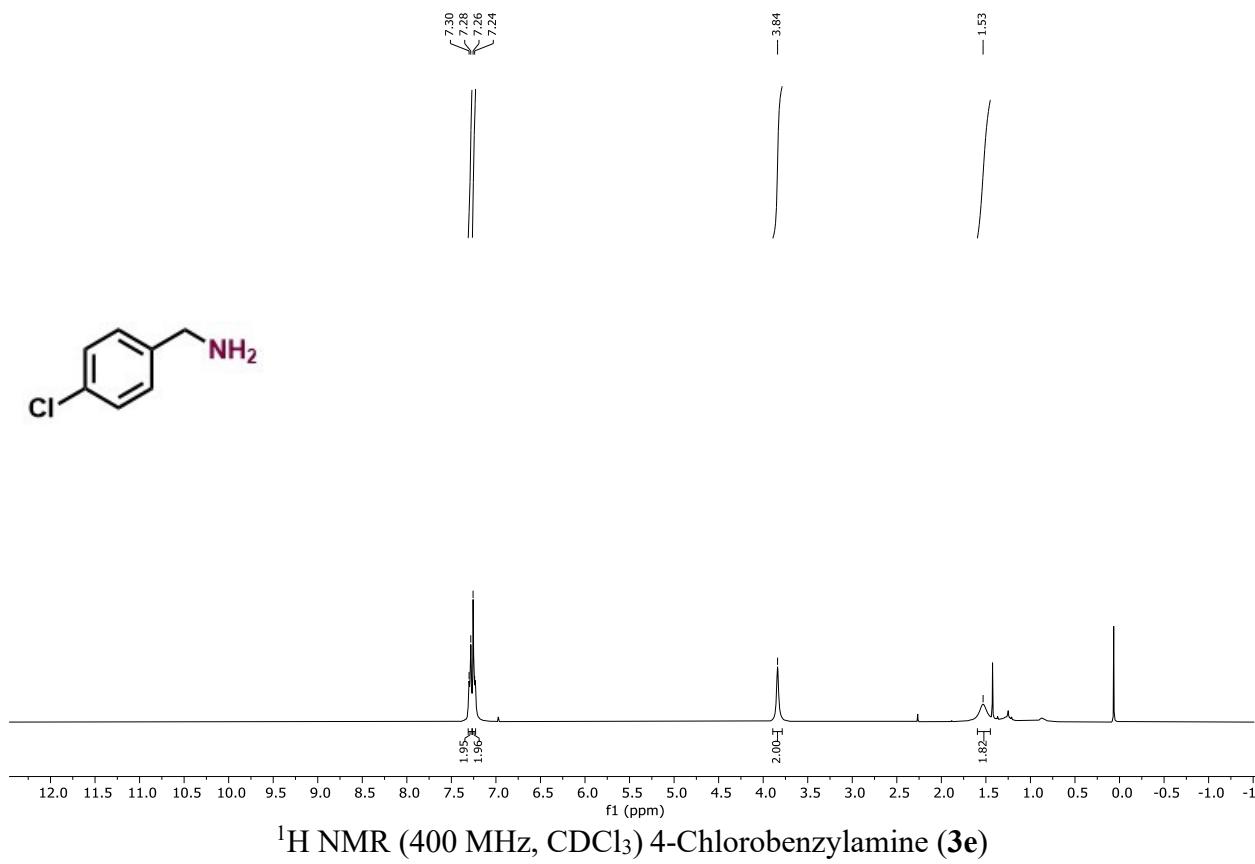
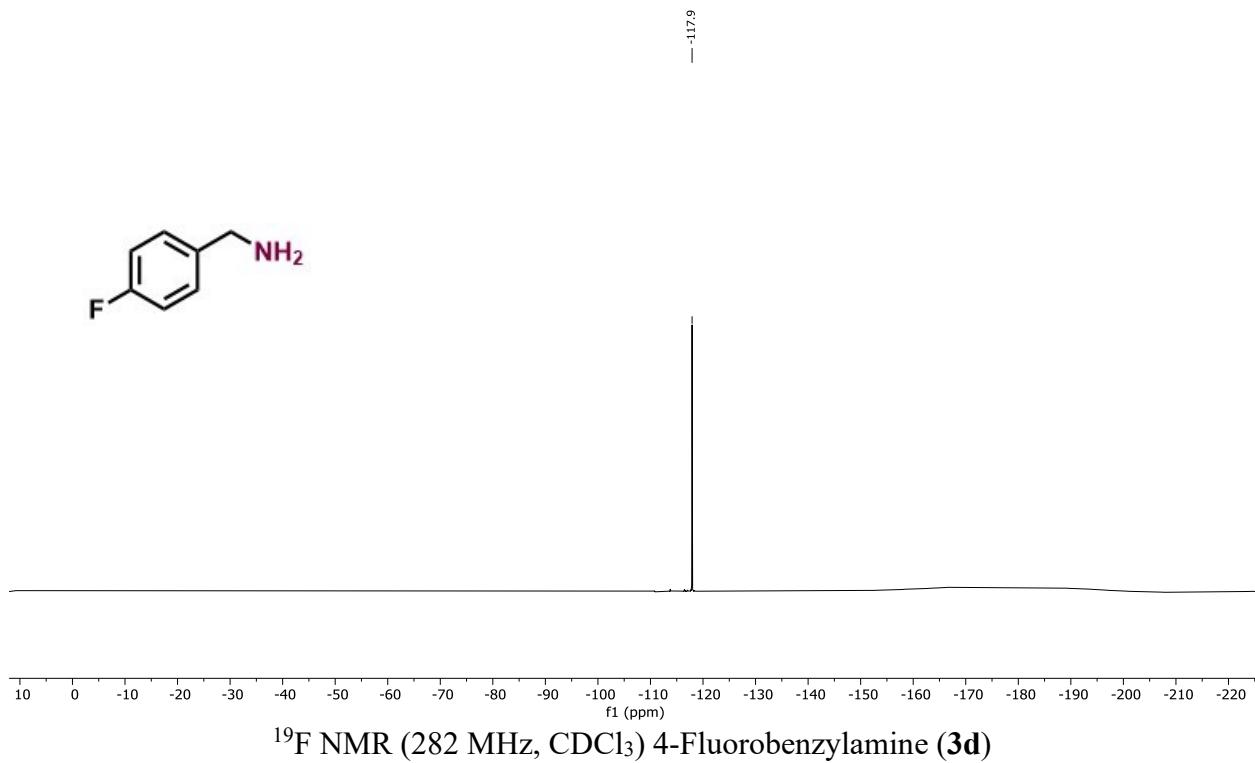


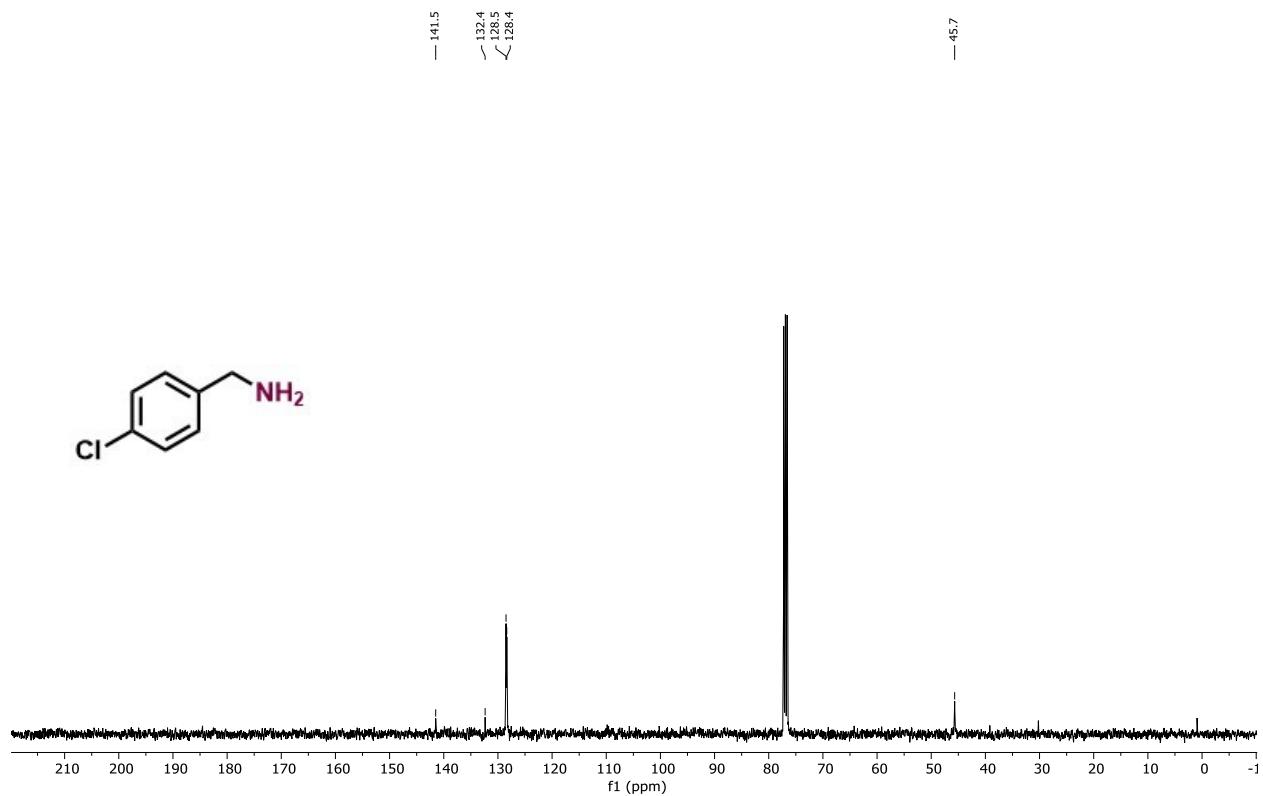




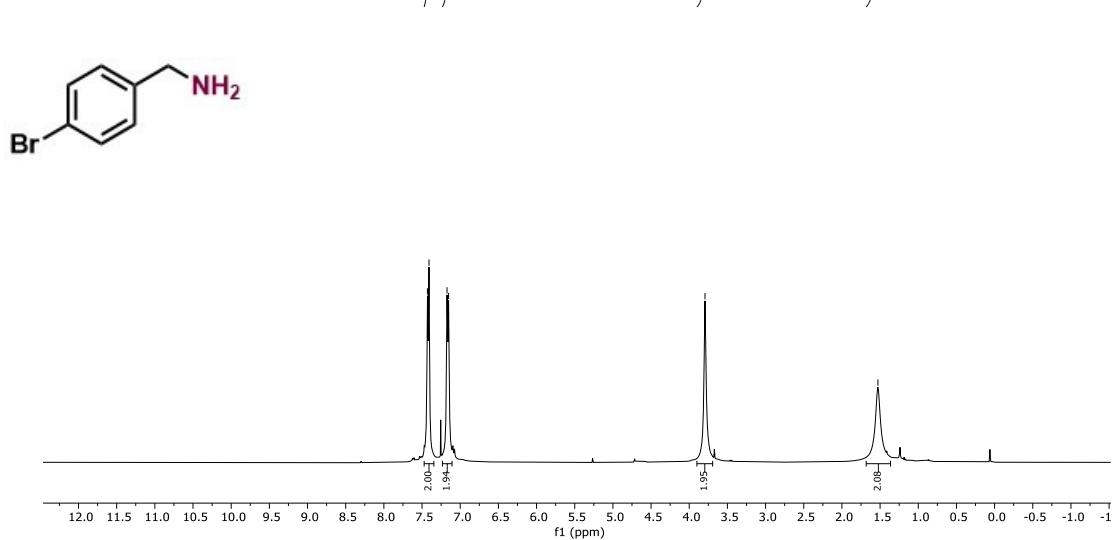
¹H NMR (400 MHz, CDCl₃) 4-Fluorobenzylamine (**3d**)



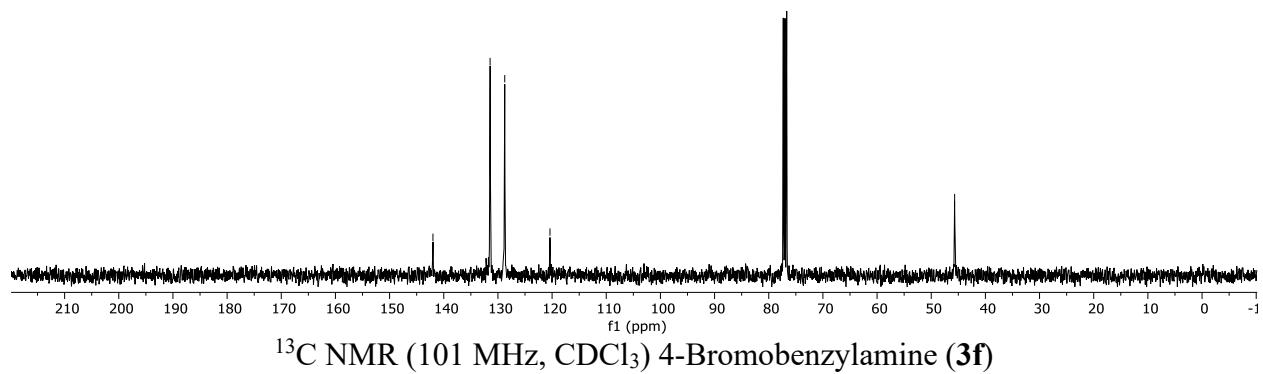
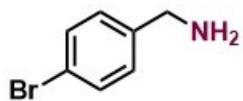


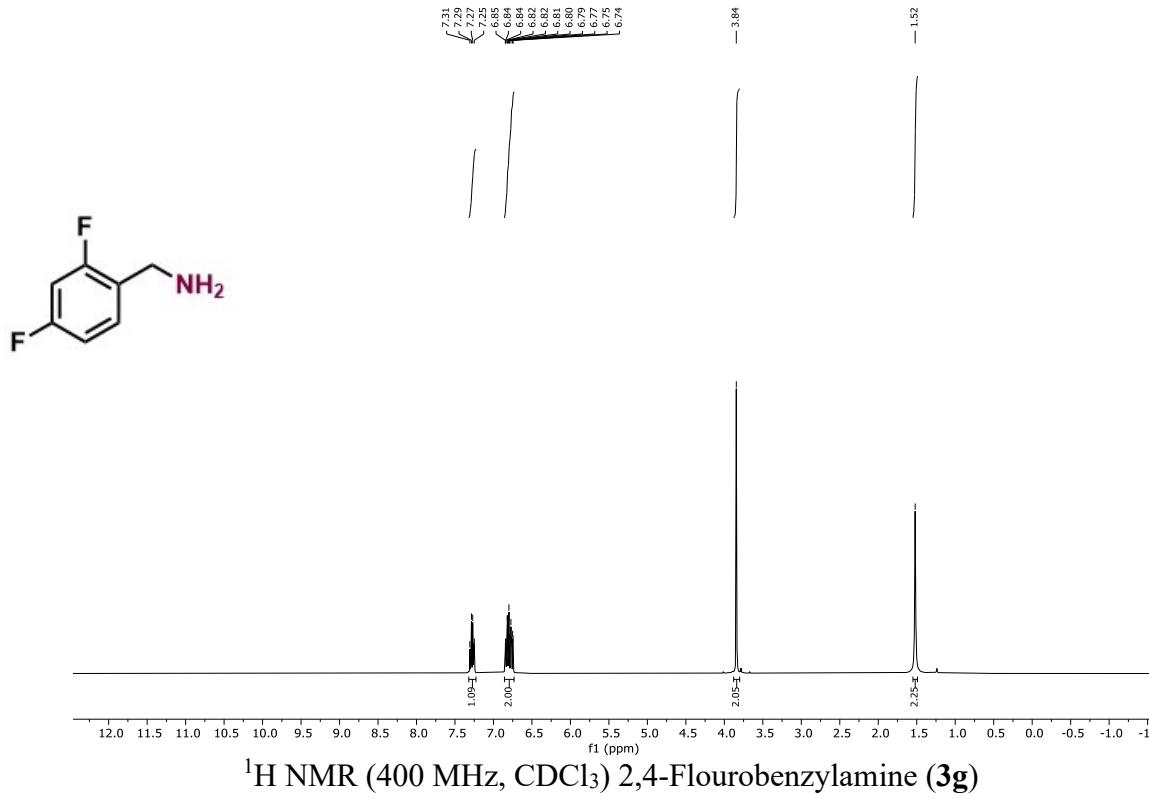


¹³C NMR (101 MHz, CDCl₃) 4-Chlorobenzylamine (**3e**)

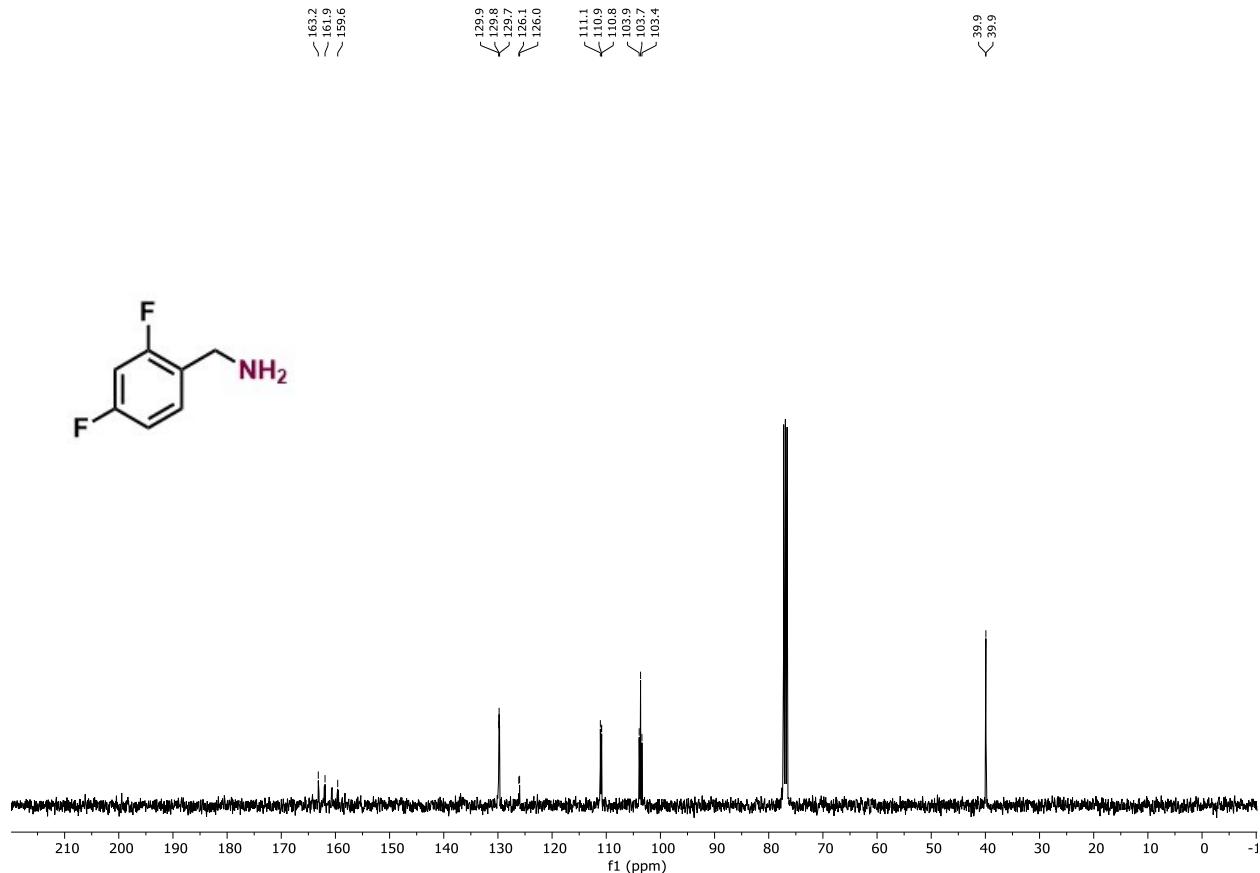


¹H NMR (400 MHz, CDCl₃) 4-Bromobenzylamine (**3f**)





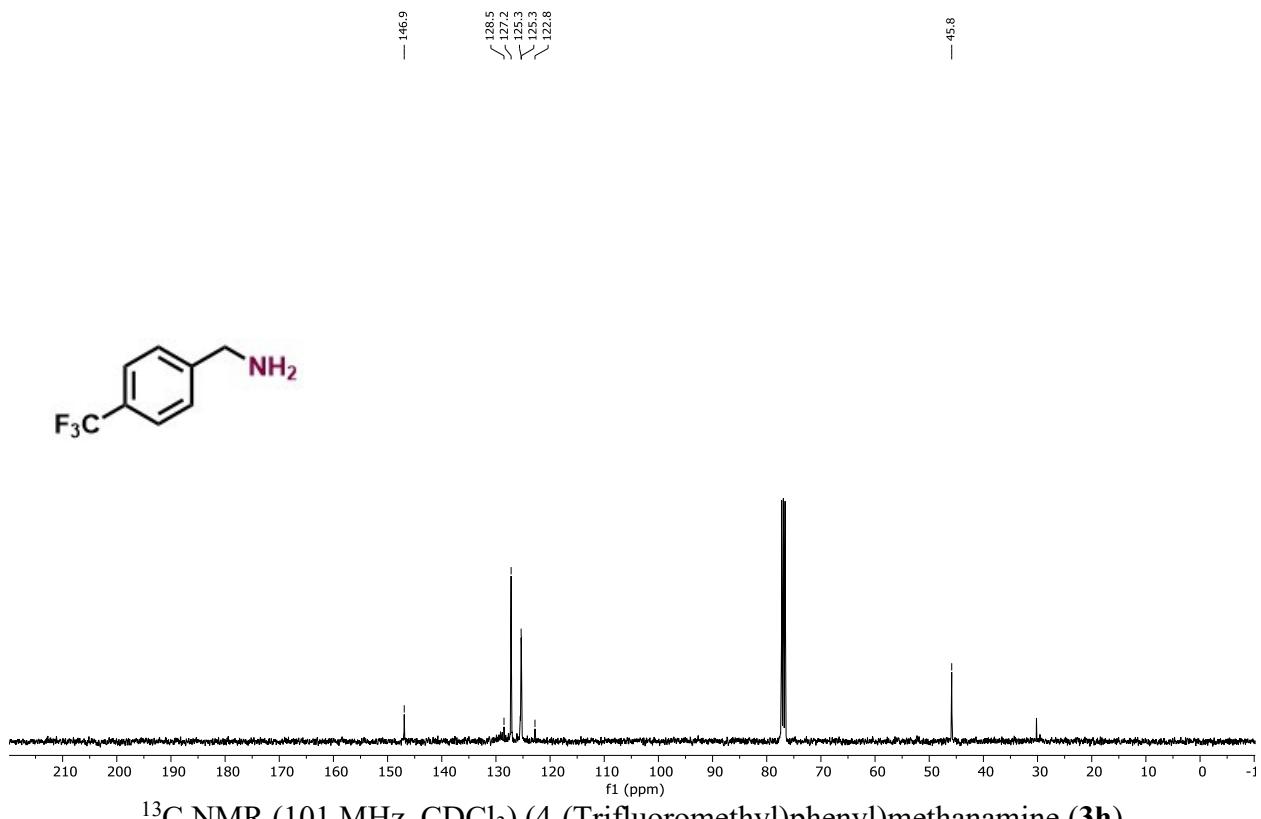
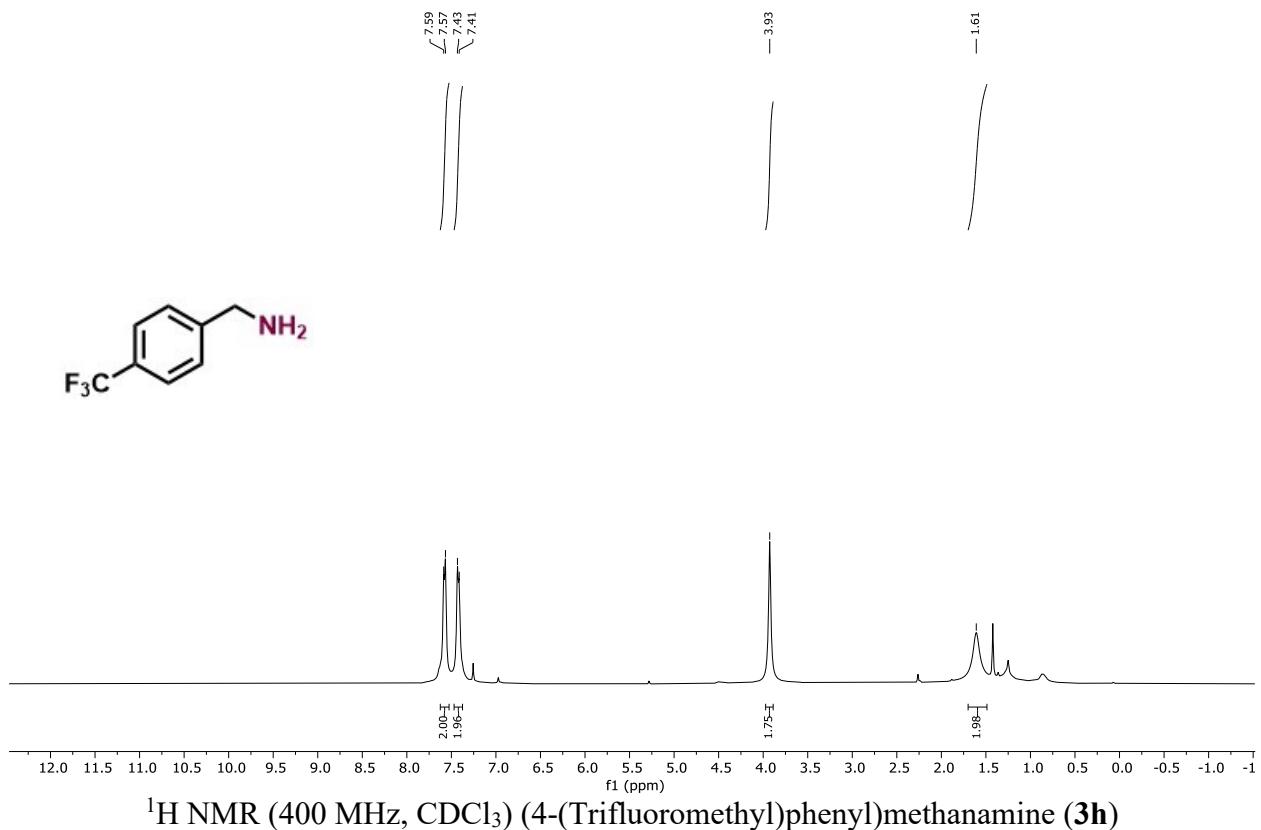
¹H NMR (400 MHz, CDCl₃) 2,4-Fluorobenzylamine (3g)

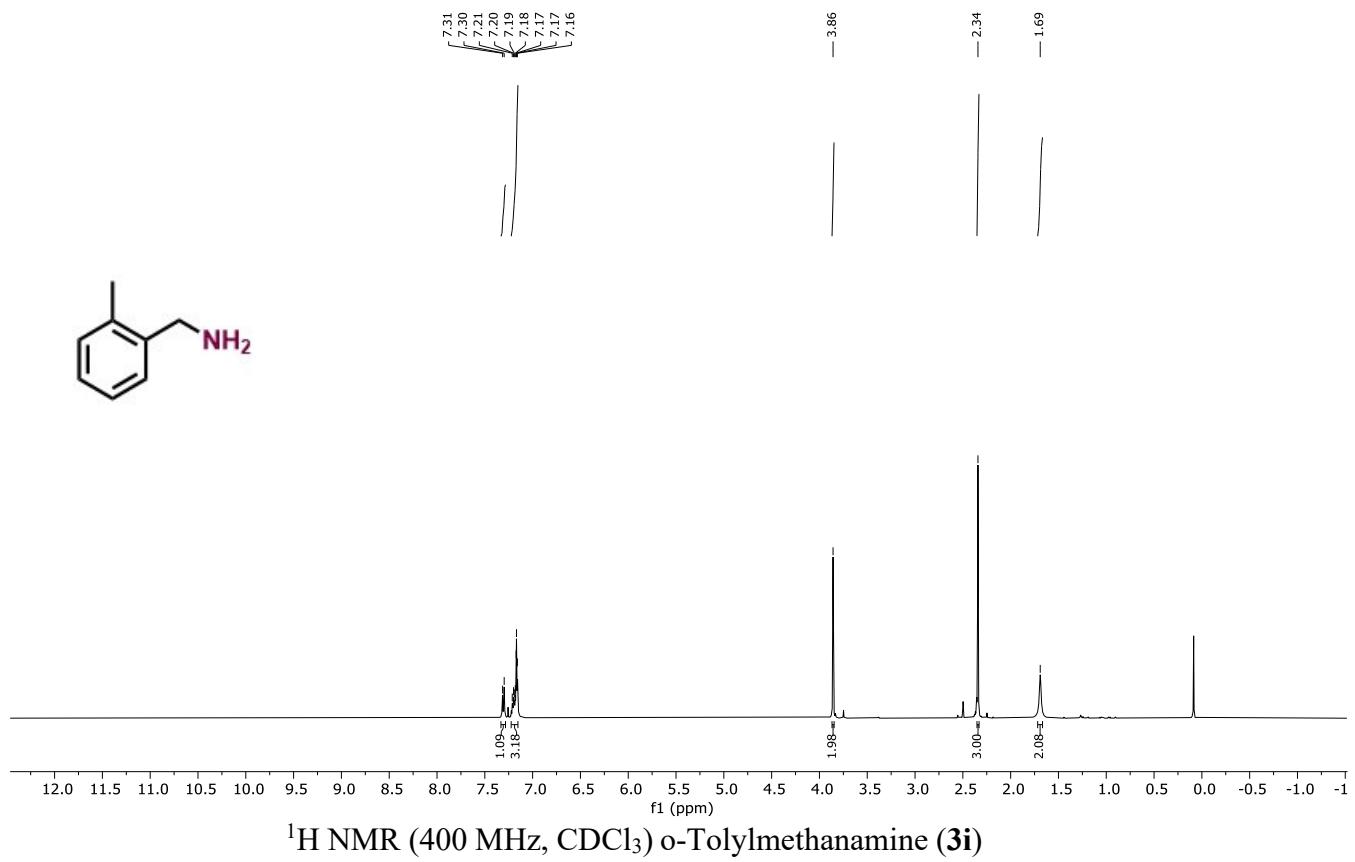
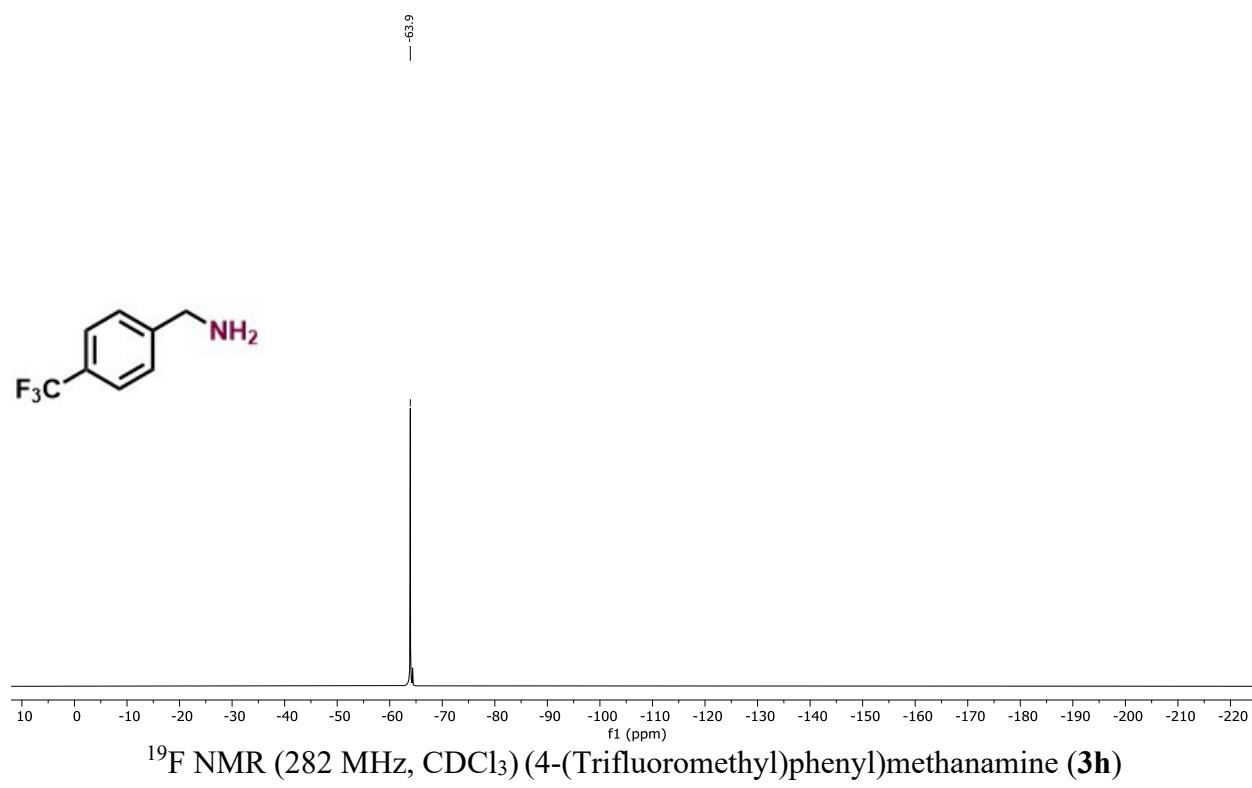


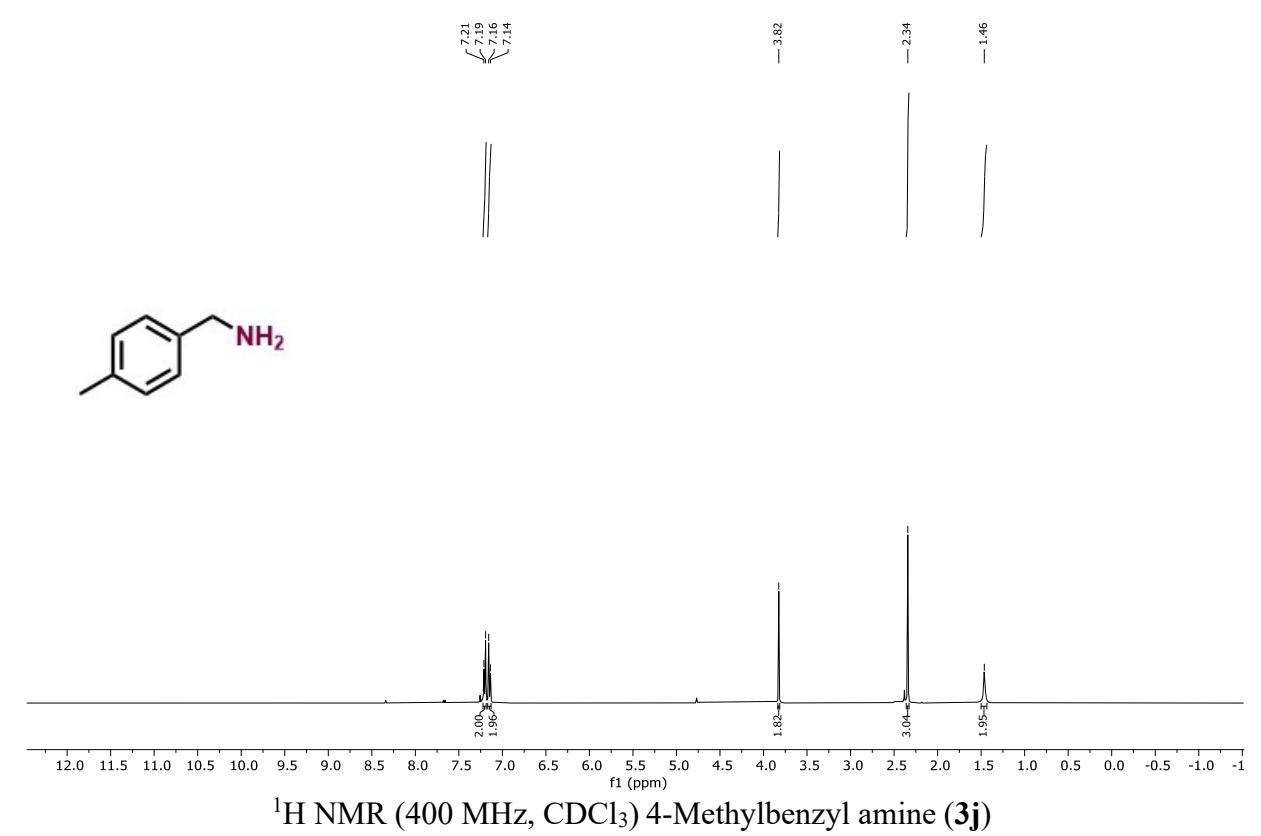
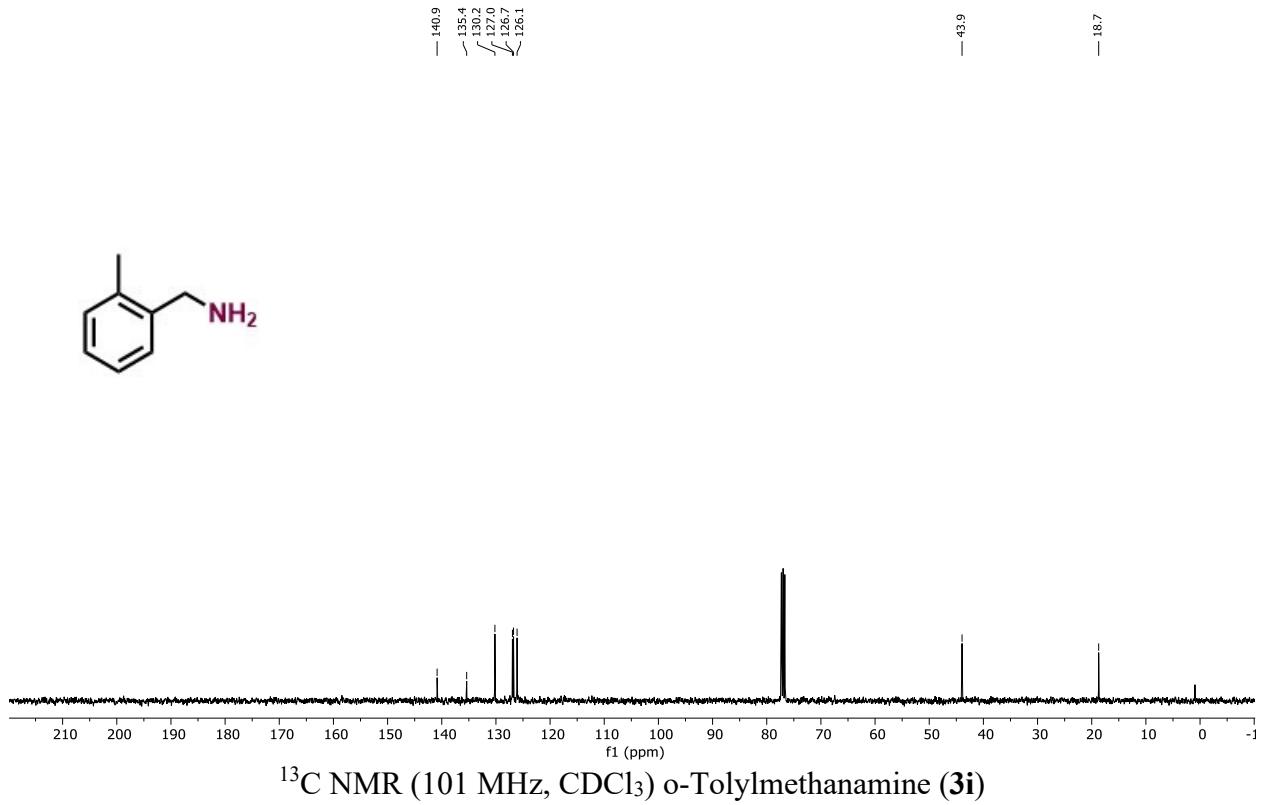
^{13}C NMR (101 MHz, CDCl_3) 2,4-Fluorobenzylamine (**3g**)



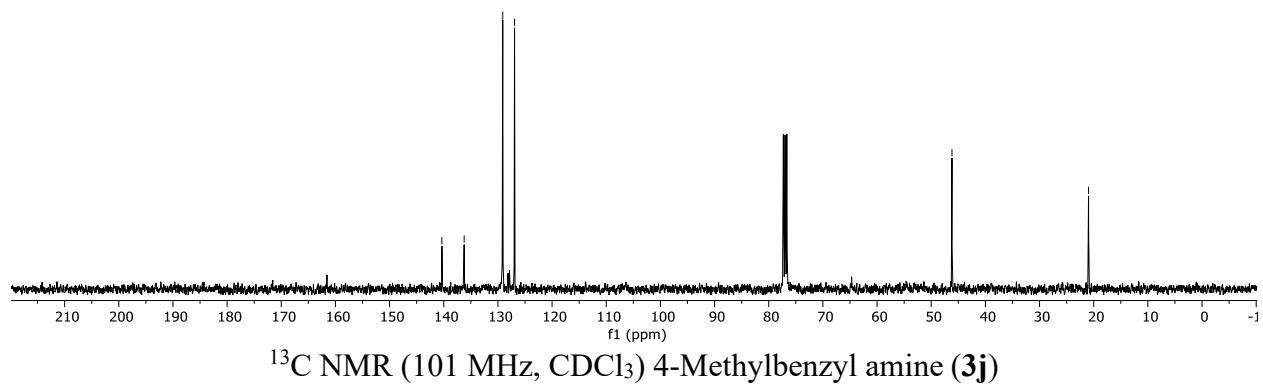
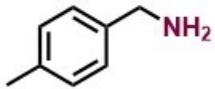
^{19}F NMR (282 MHz, CDCl_3) 2,4-Fluorobenzylamine (**3g**)



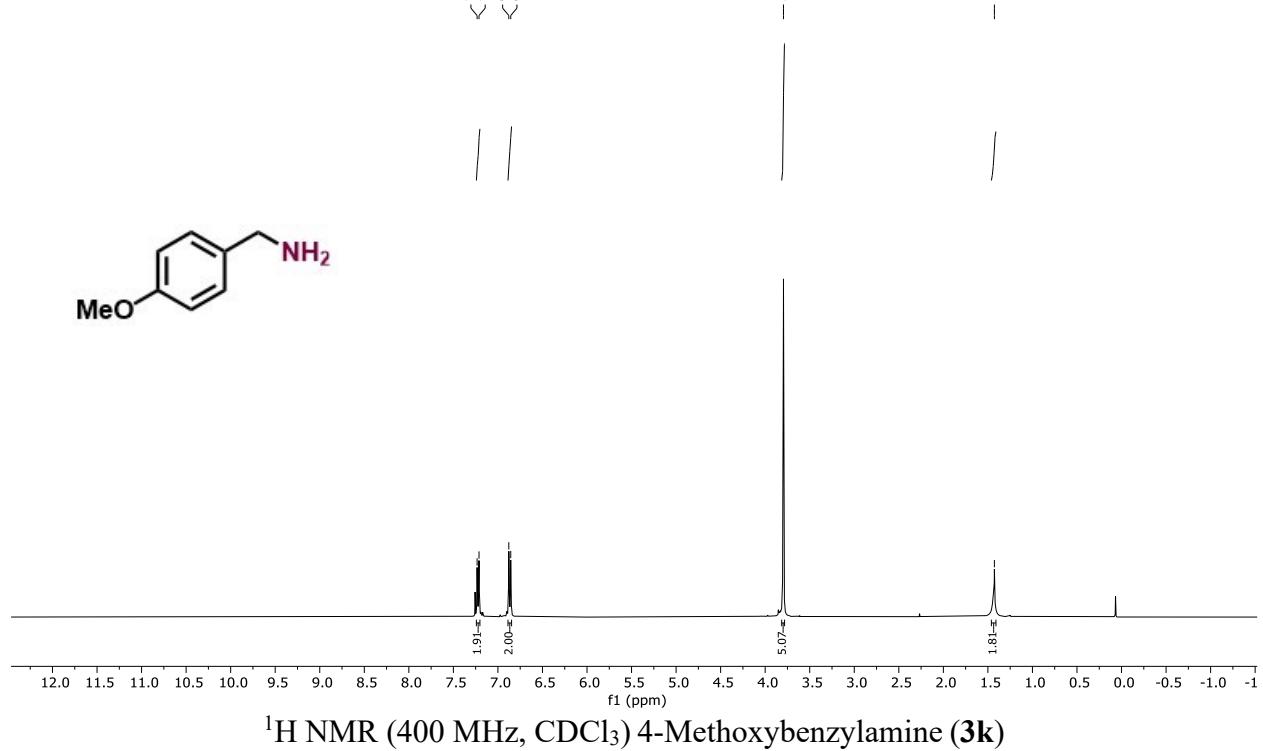
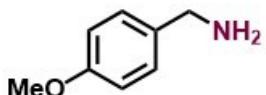


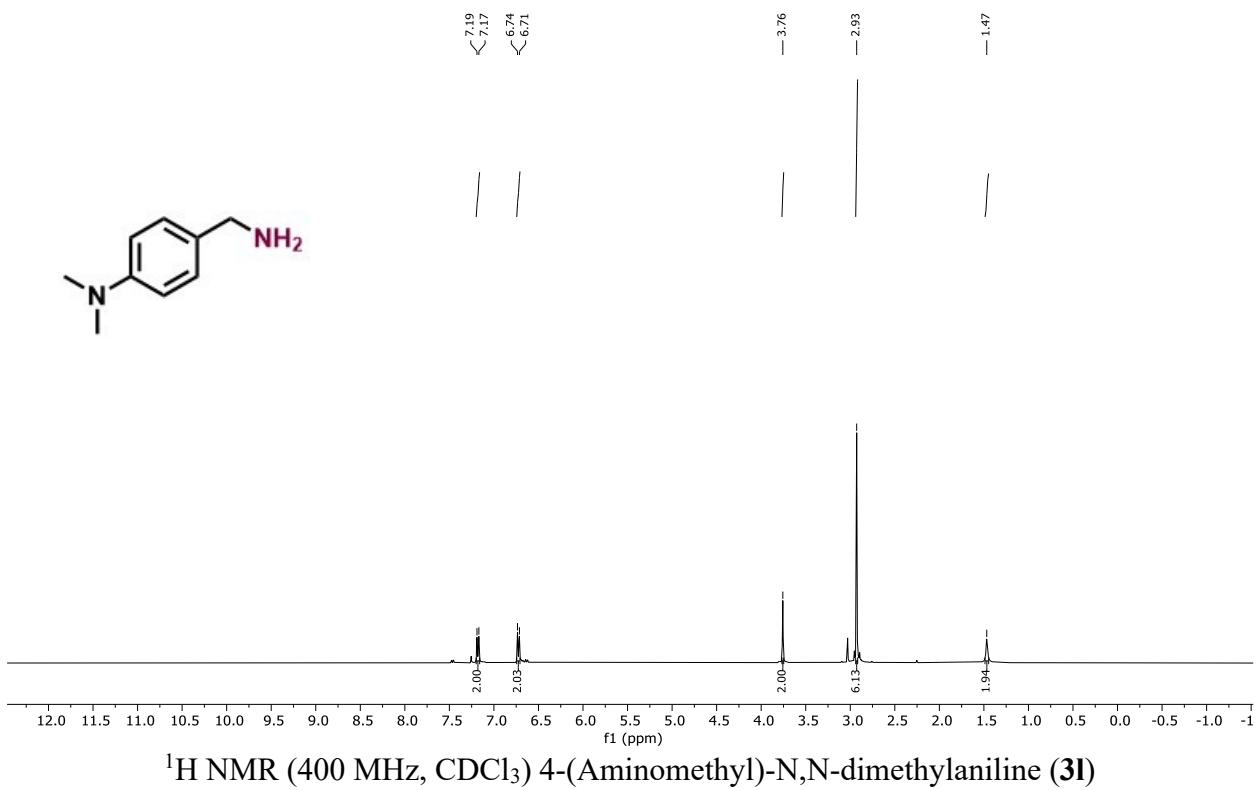
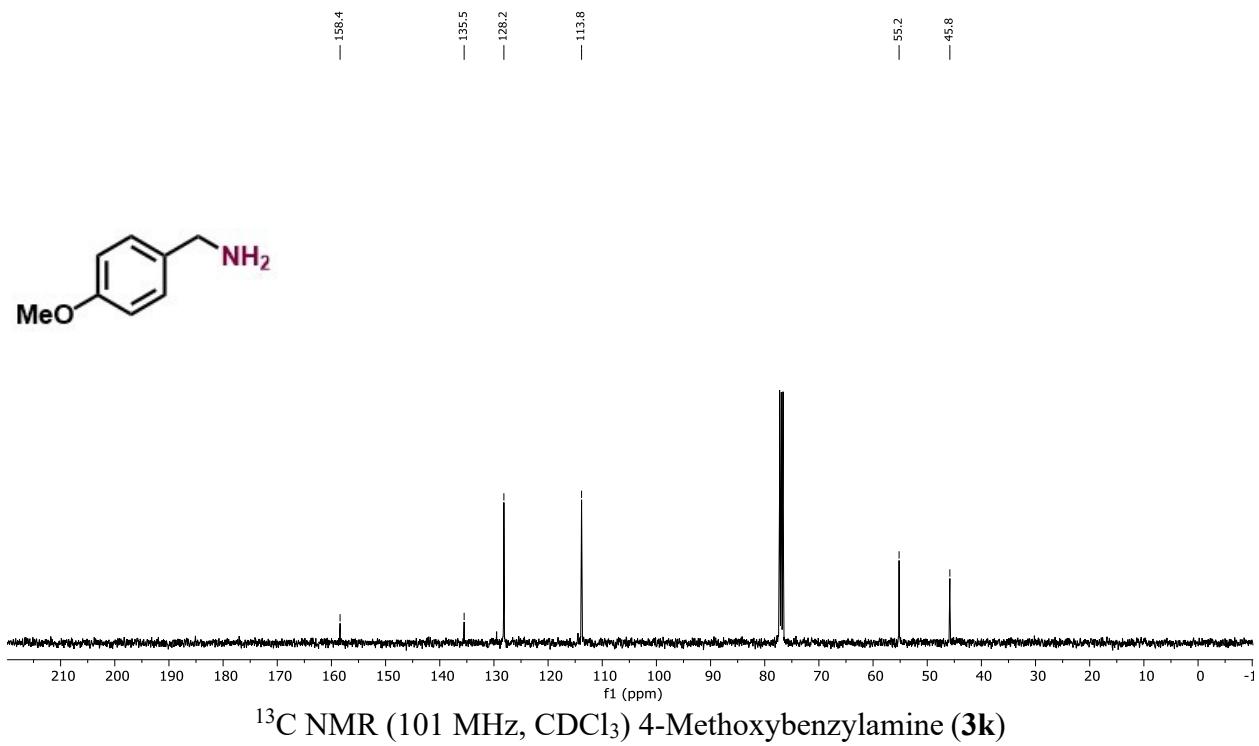


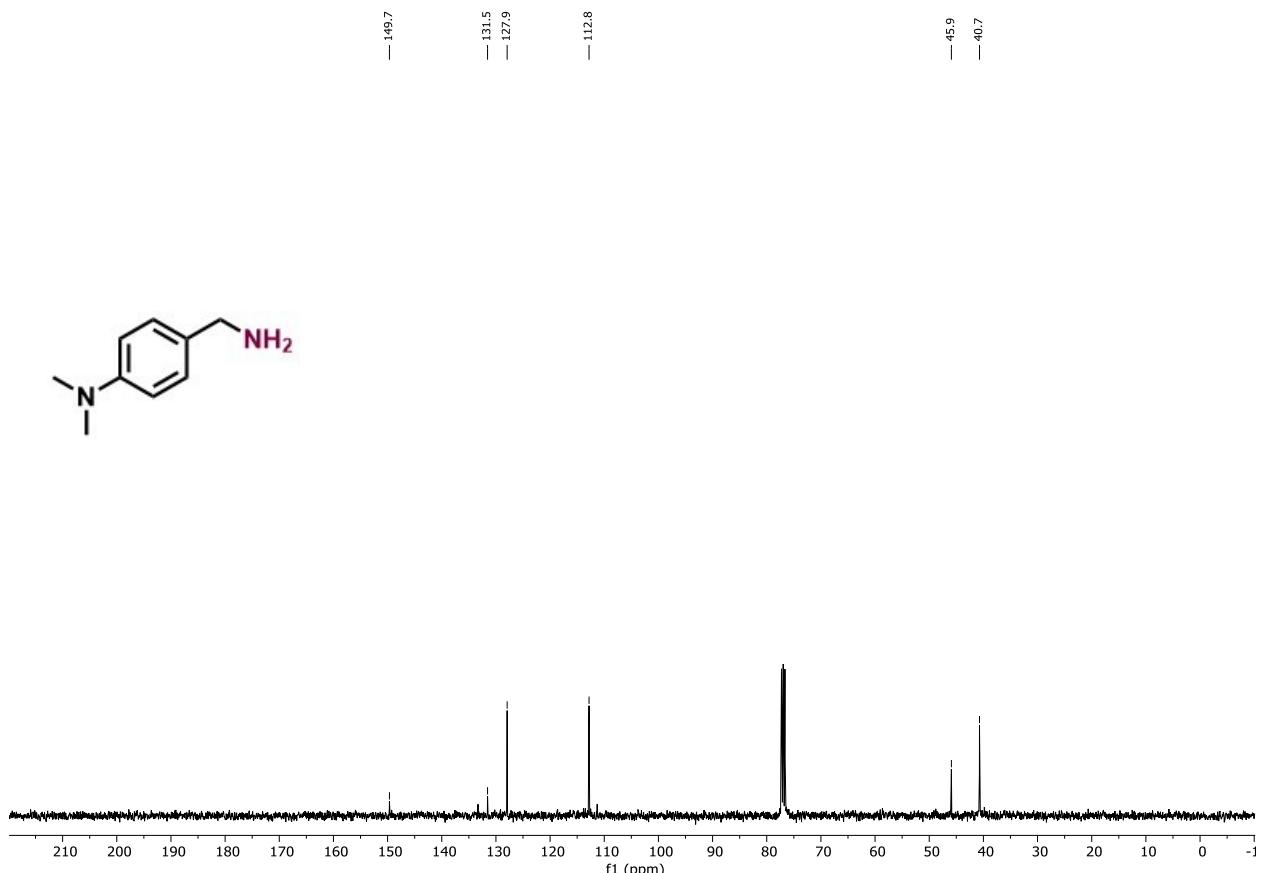
— 140.3
— 136.2
— 129.1
— 126.9
— 46.2
— 21.0



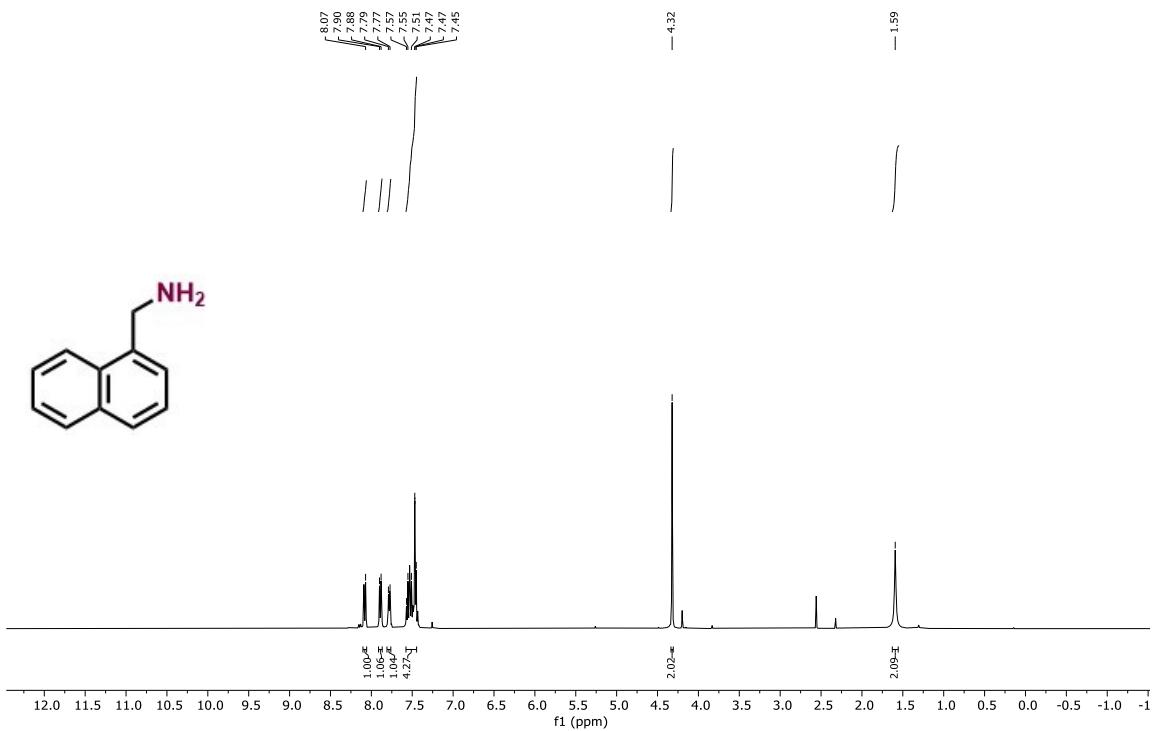
< 7.23
< 7.21
< 6.88
< 6.86
— 3.79
— 1.43



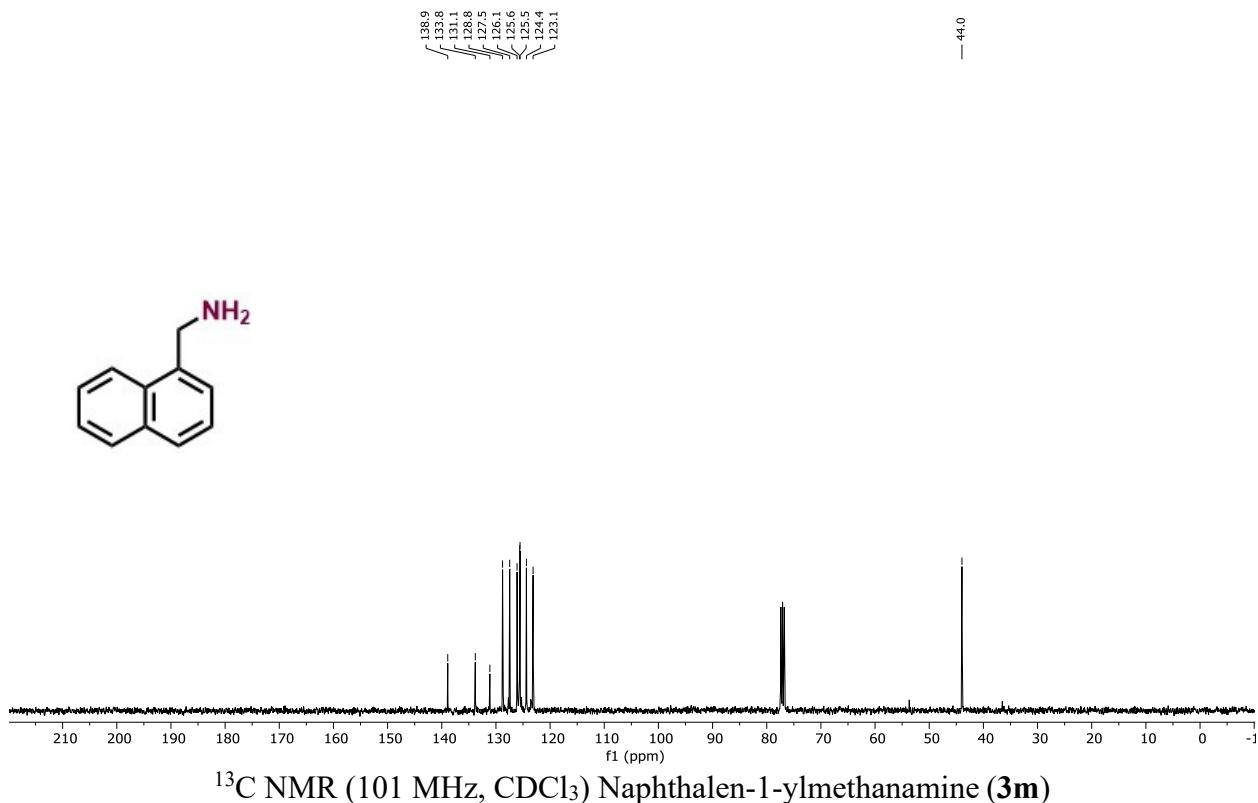




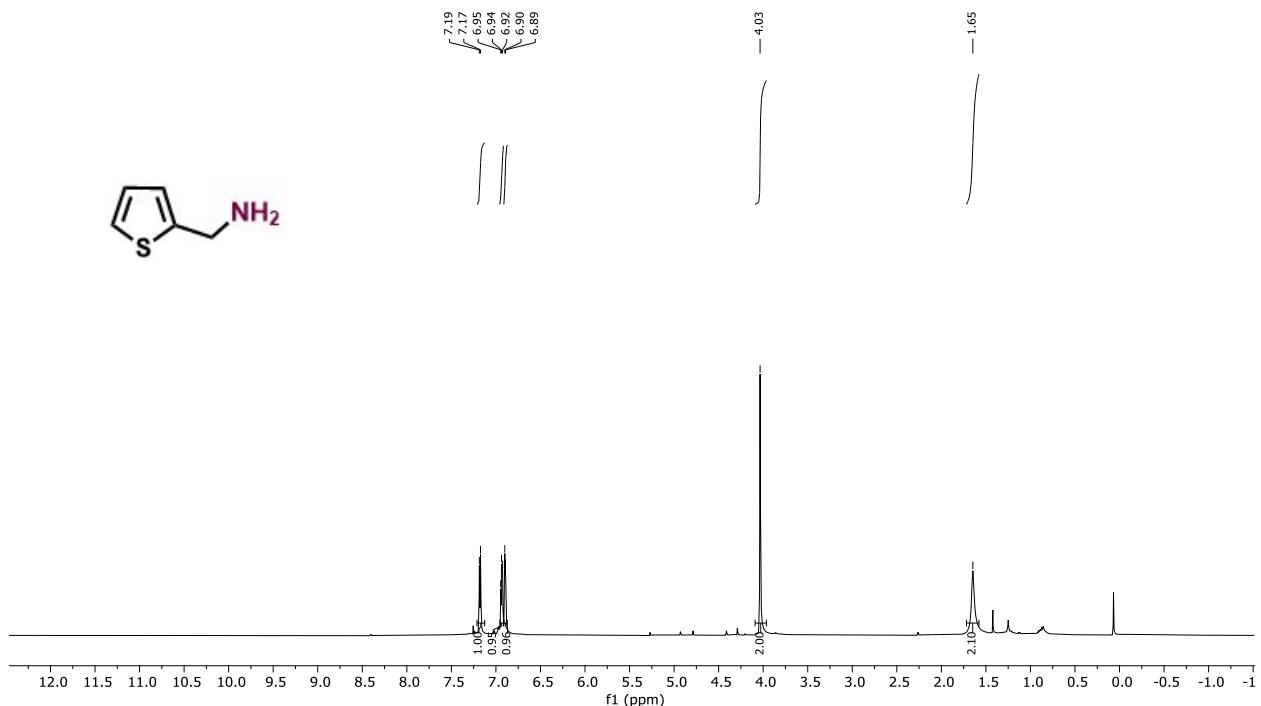
^{13}C NMR (101 MHz, CDCl_3) 4-(Aminomethyl)-N,N-dimethylaniline (**3l**)



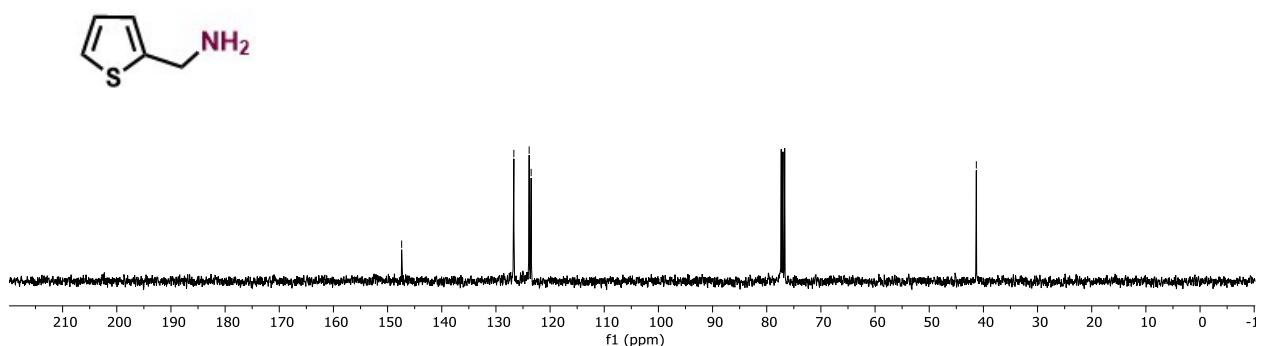
¹H NMR (400 MHz, CDCl₃) Naphthalen-1-ylmethanamine (**3m**)



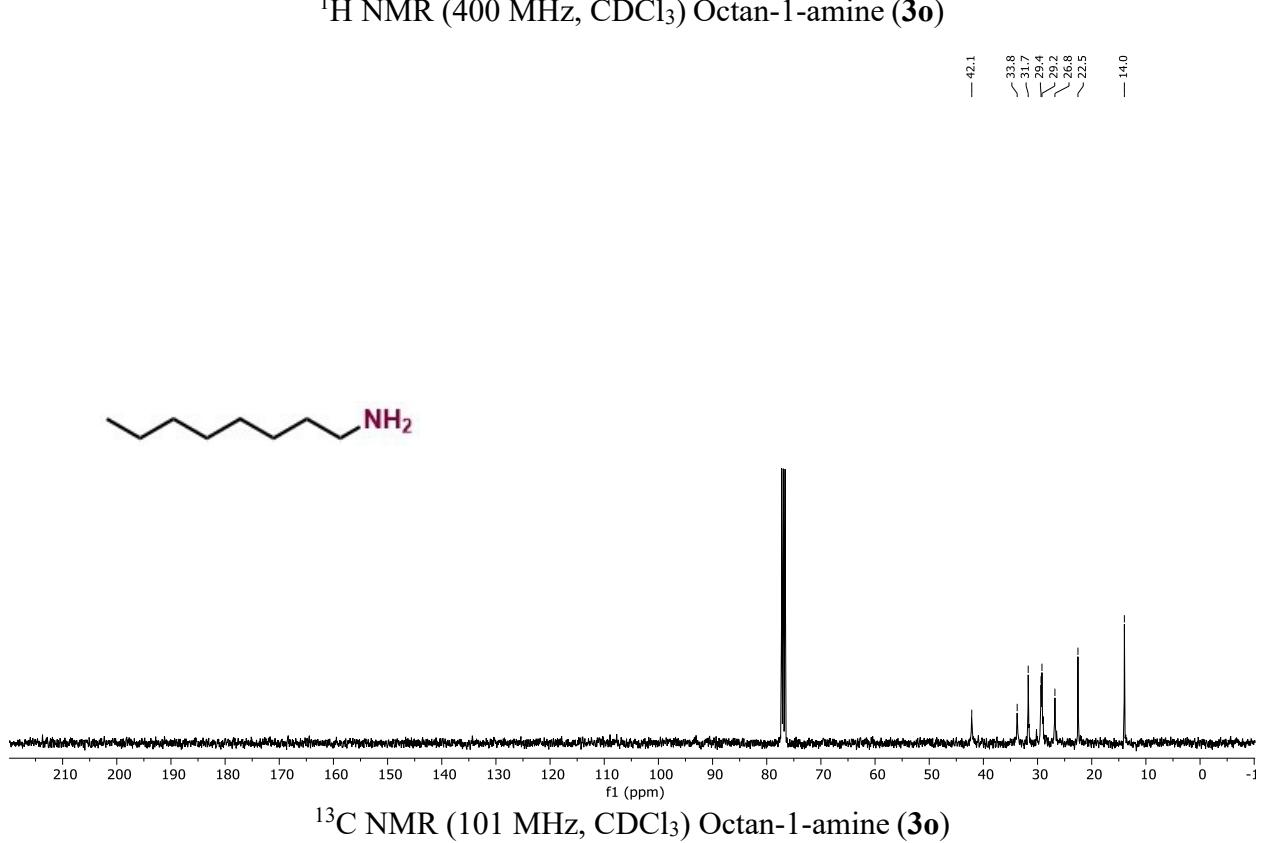
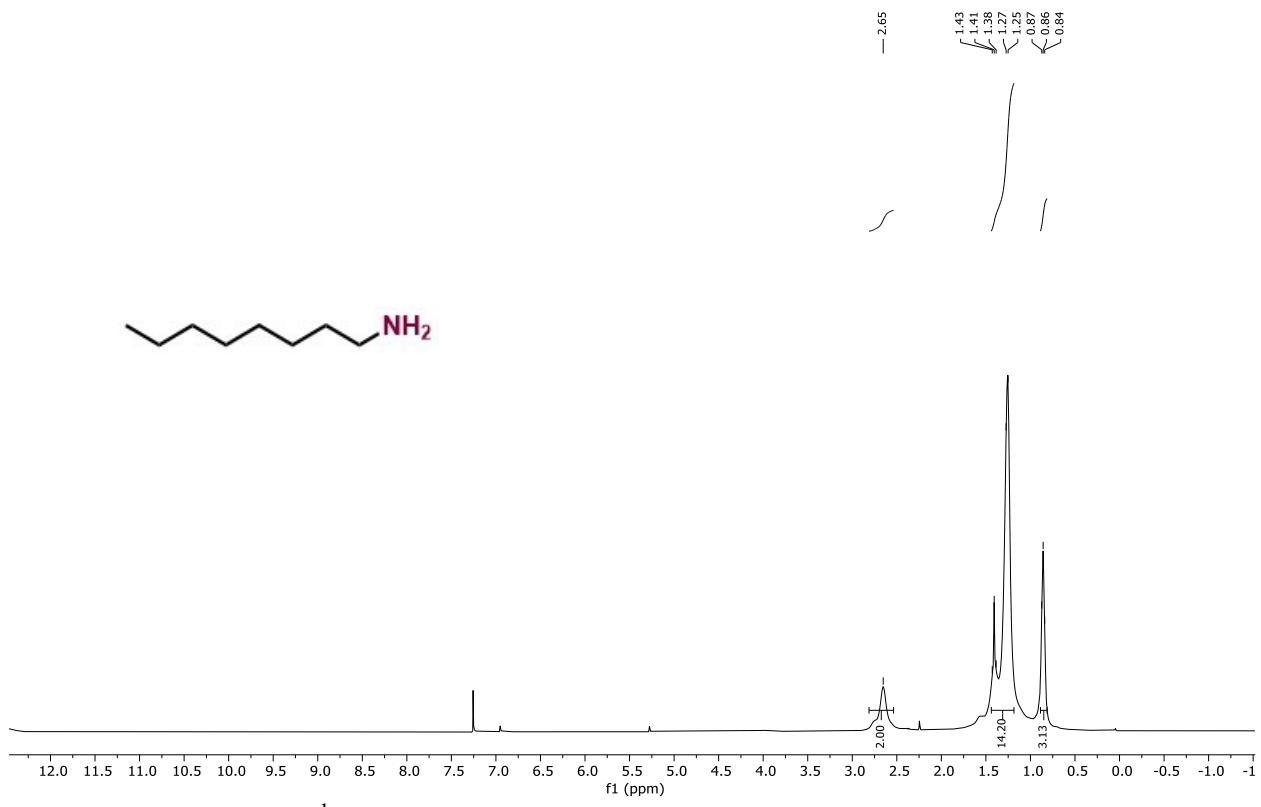
¹³C NMR (101 MHz, CDCl₃) Naphthalen-1-ylmethanamine (**3m**)

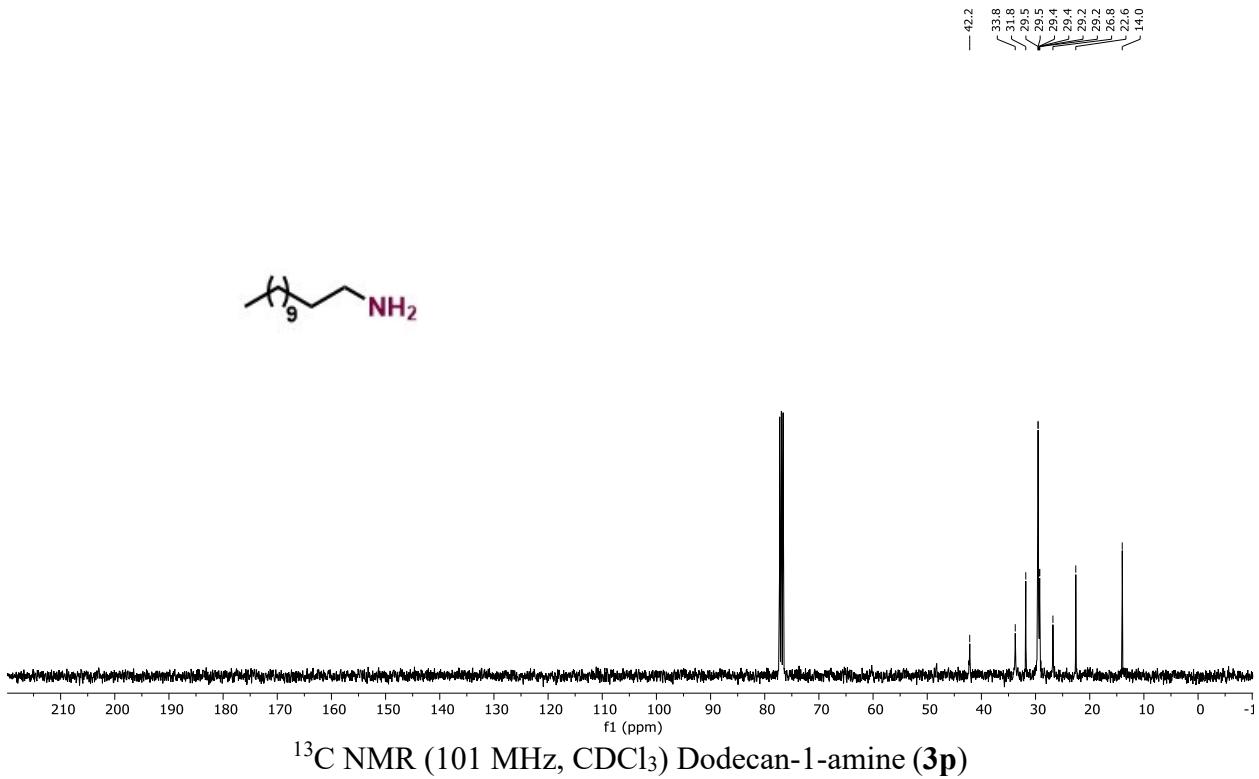
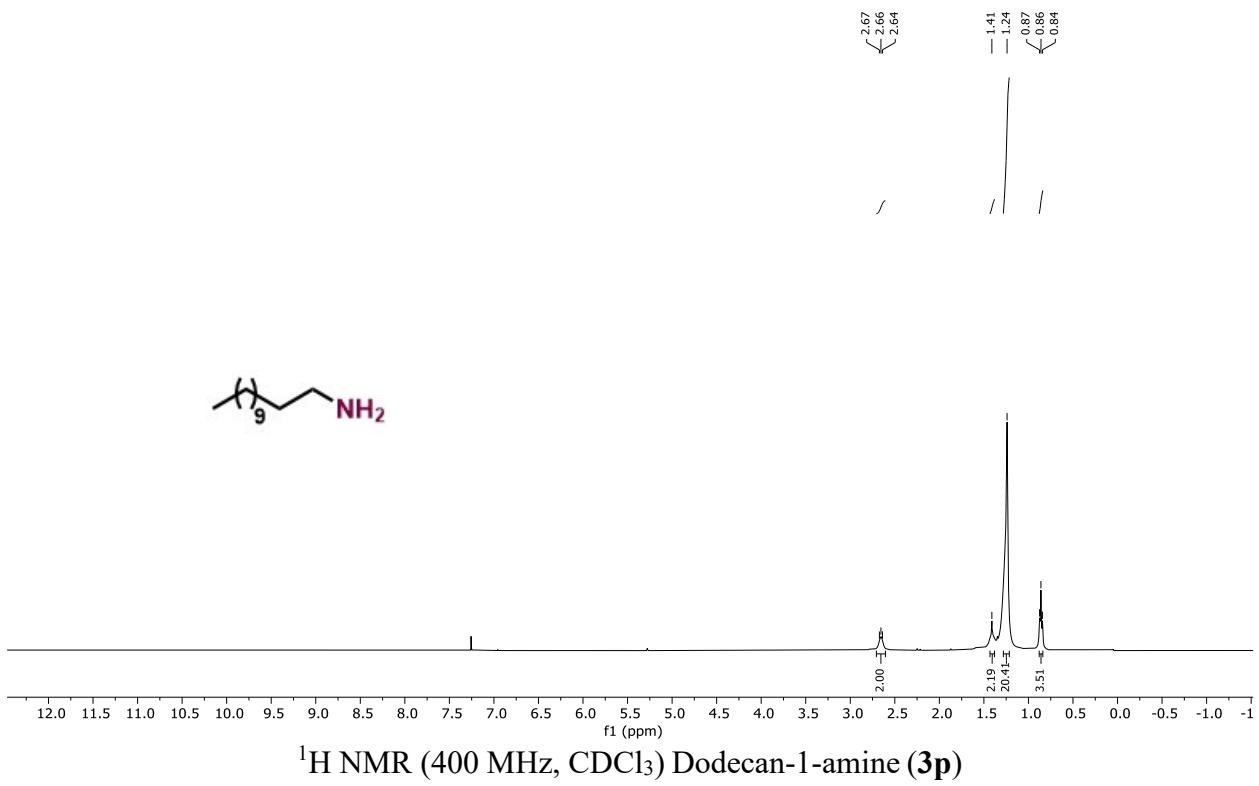


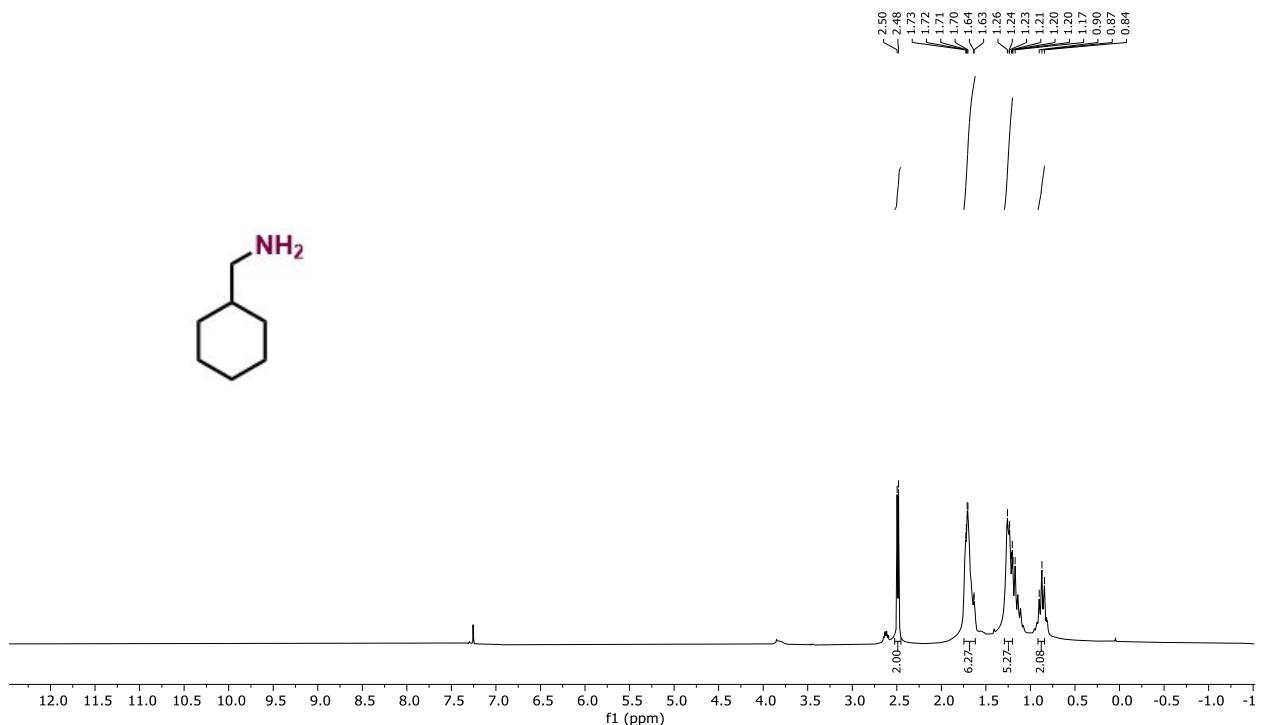
¹H NMR (400 MHz, CDCl₃) Thiophen-2-ylmethanamine (**3n**)



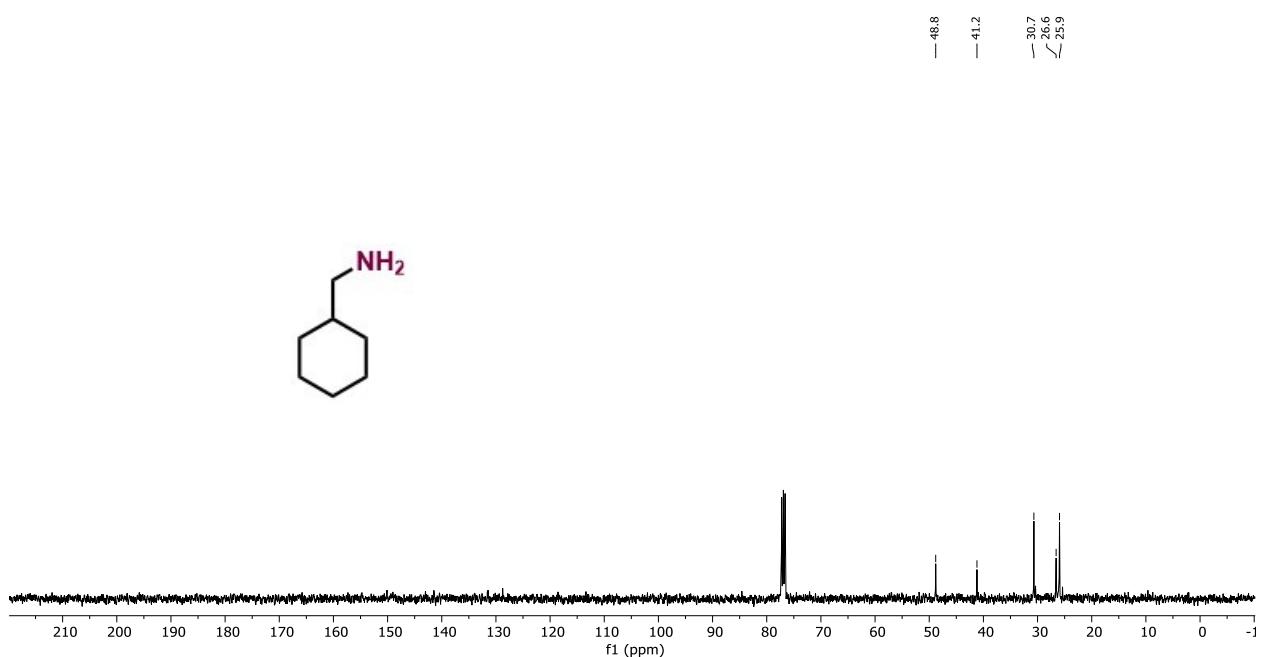
¹³C NMR (101 MHz, CDCl₃) Thiophen-2-ylmethanamine (**3n**)



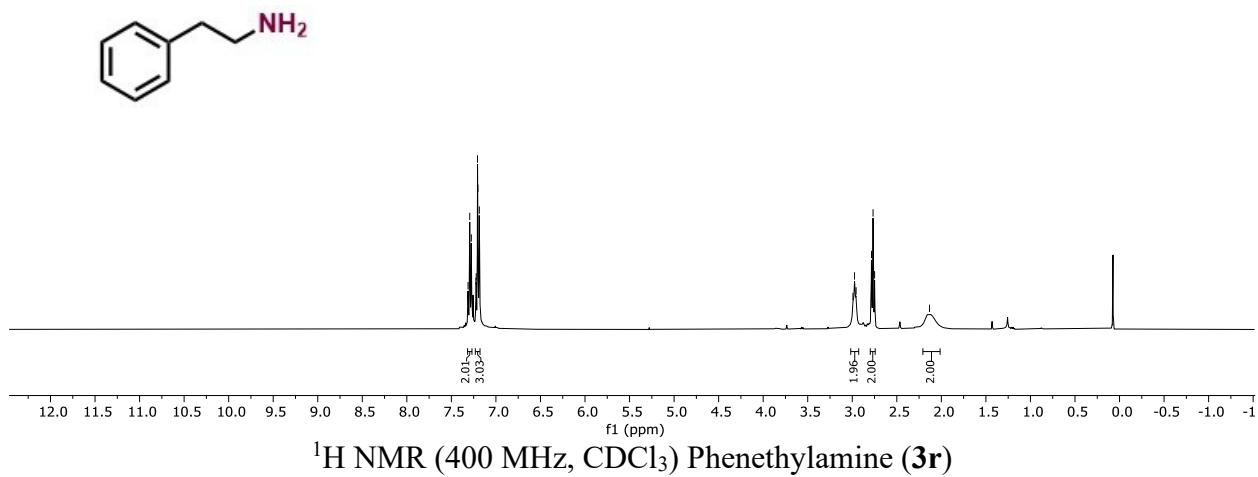




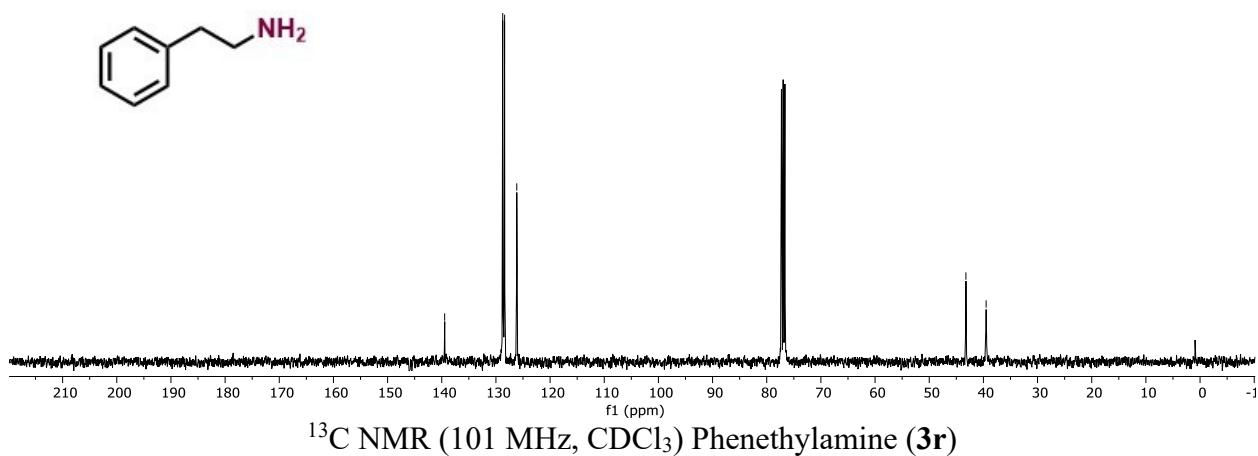
¹H NMR (400 MHz, CDCl₃) Cyclohexylmethanamine (**3q**)

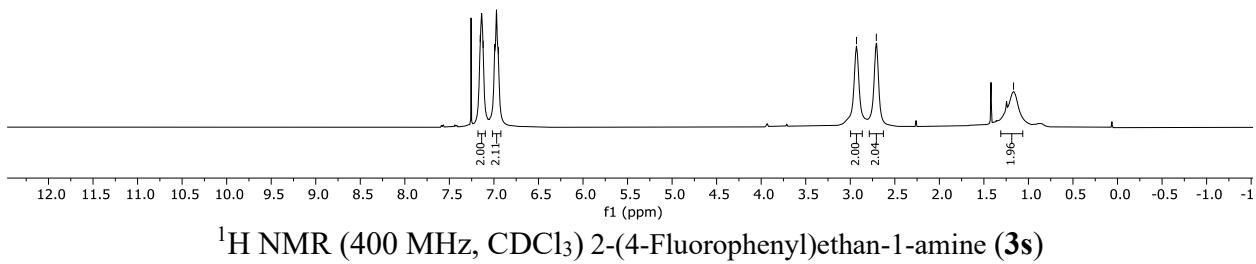
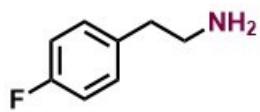
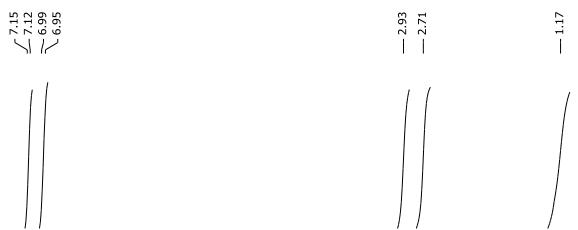


¹³C NMR (101 MHz, CDCl₃) Cyclohexylmethanamine (**3q**)

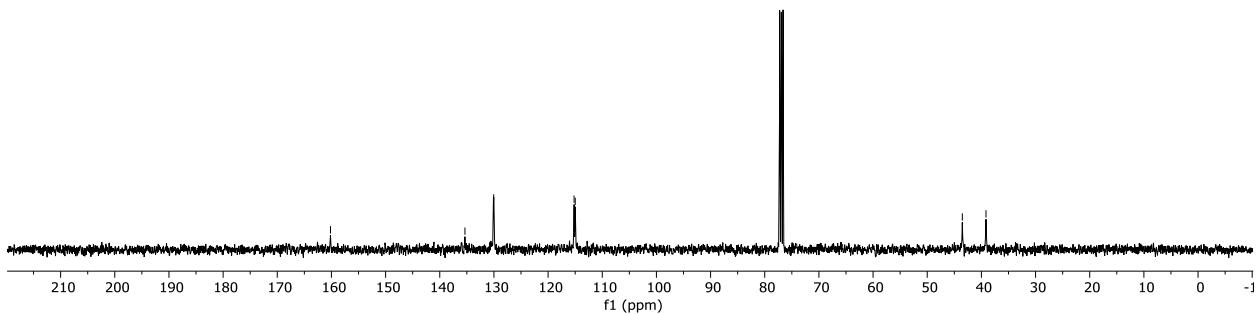
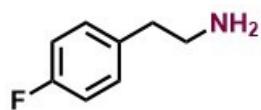


— 139.5 < 128.4 > 126.1 — 43.2 — 39.5

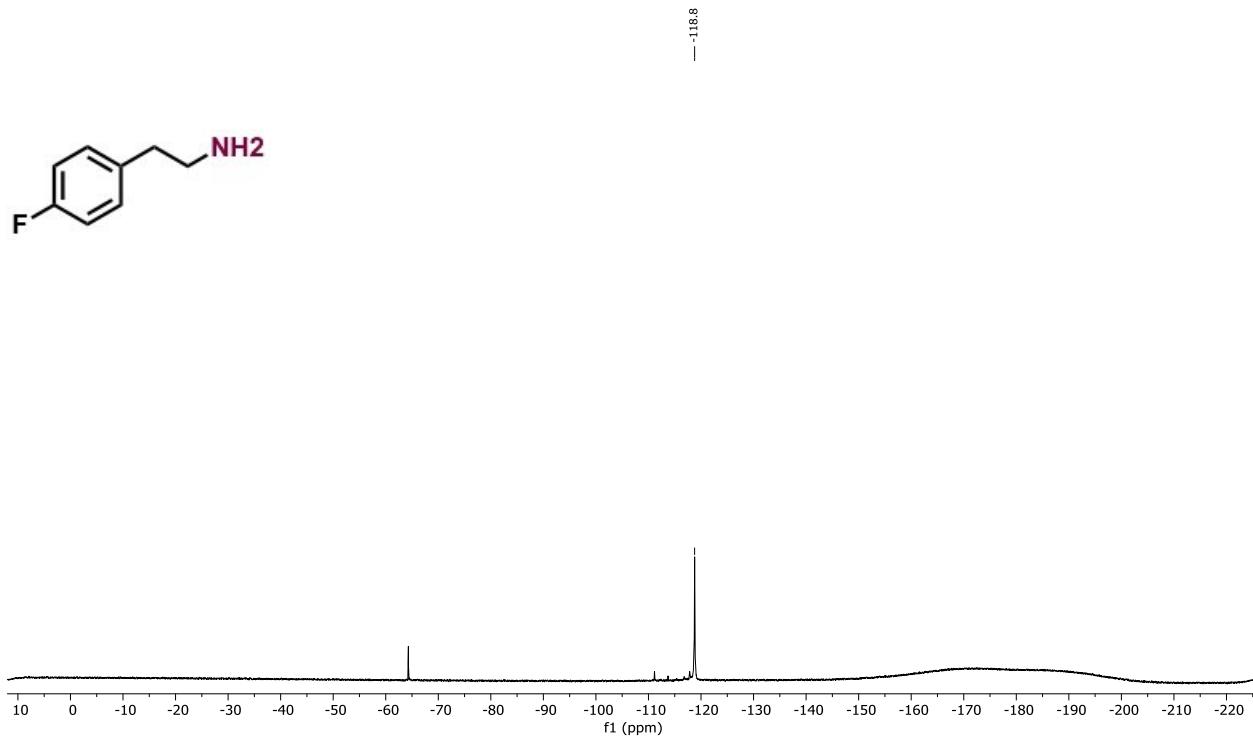




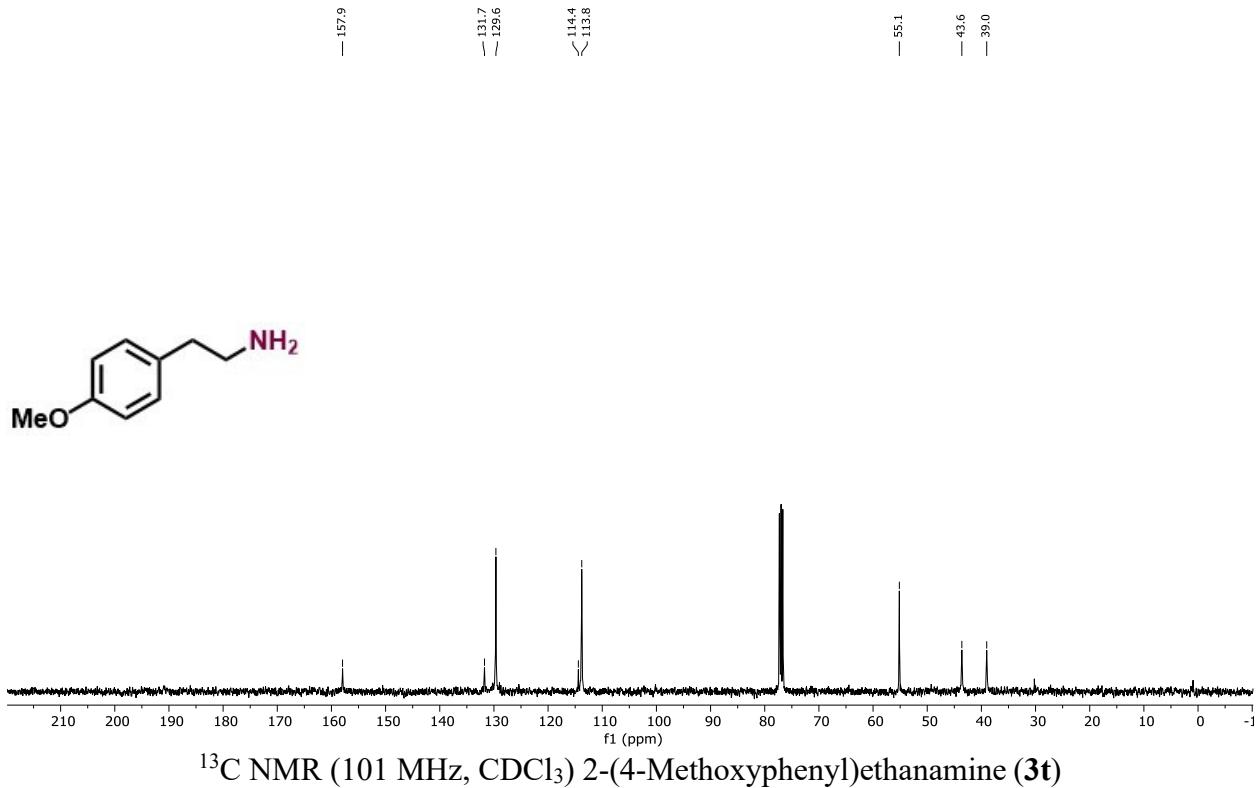
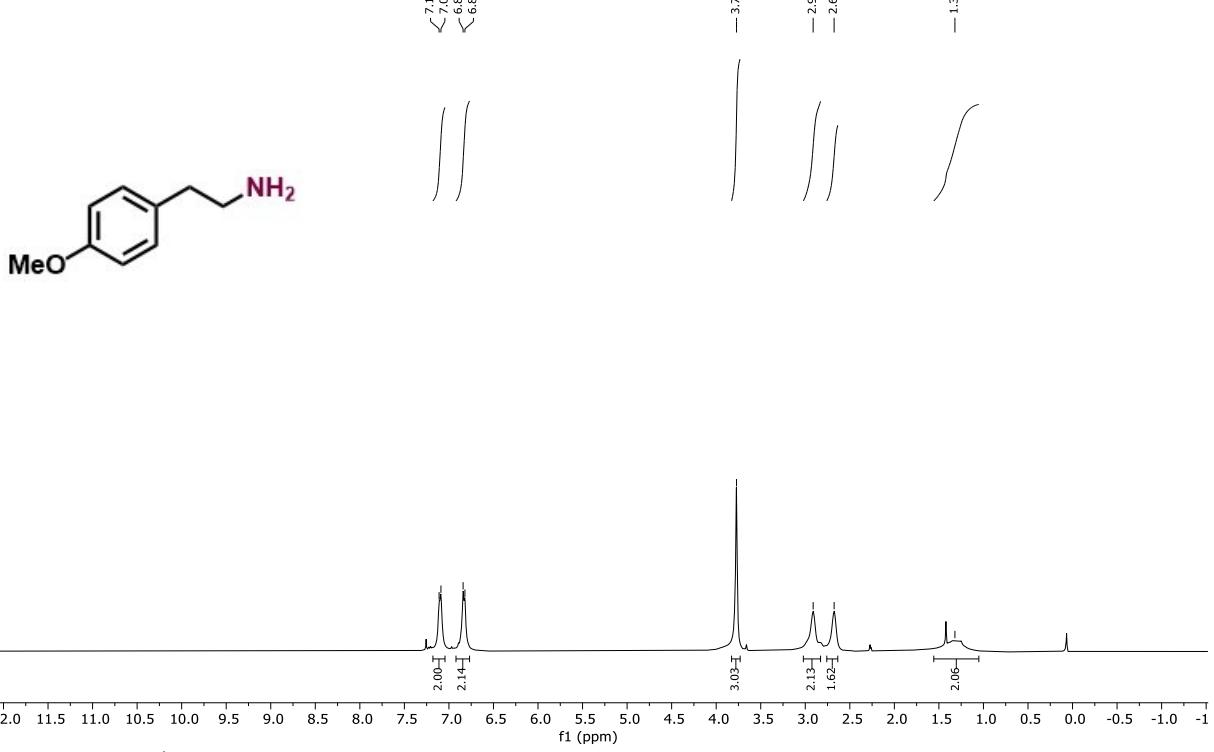
— 160.2 — 135.4 — 130.0 < 115.2 < 115.0 — 43.5 — 39.1

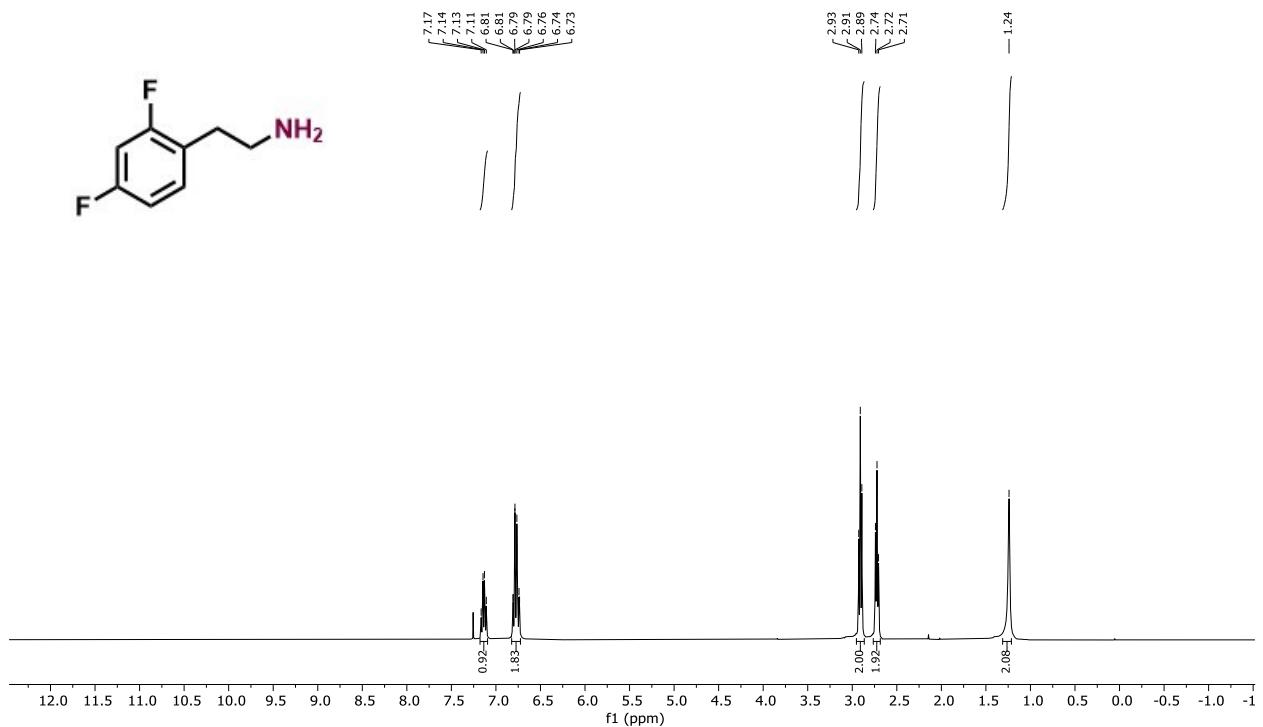


¹³C NMR (101 MHz, CDCl₃) 2-(4-Fluorophenyl)ethan-1-amine (**3s**)

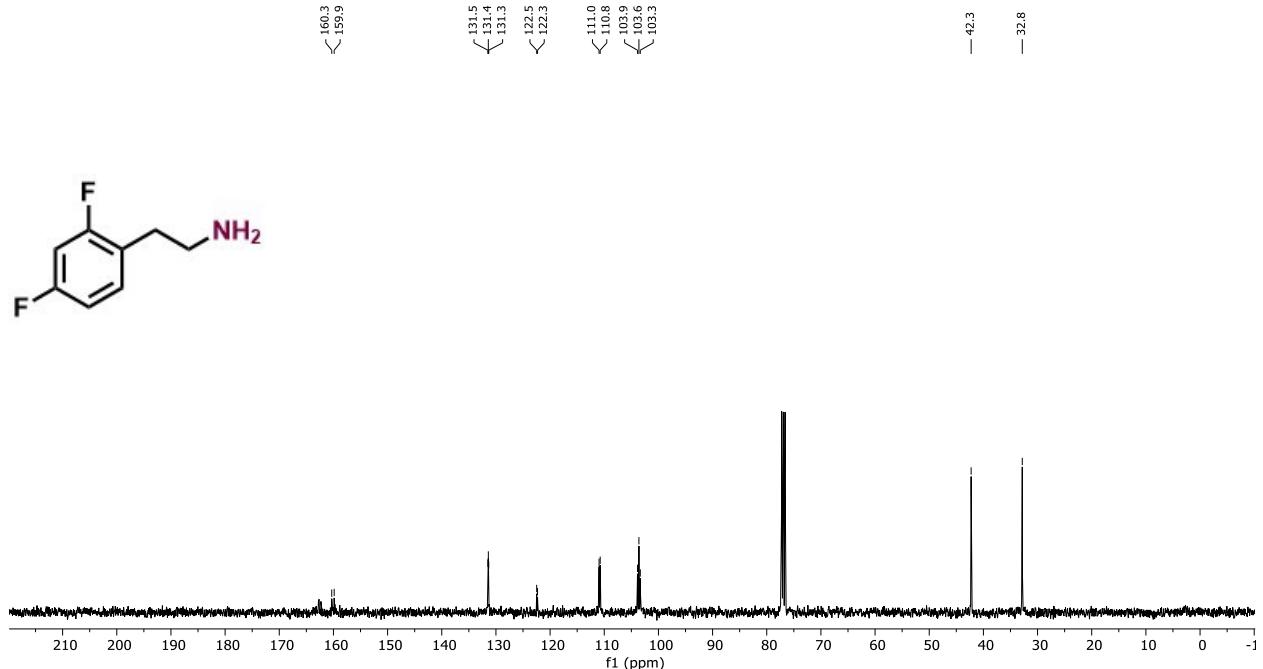


¹⁹F NMR (282 MHz, CDCl₃) 2-(4-Fluorophenyl)ethan-1-amine (**3s**)

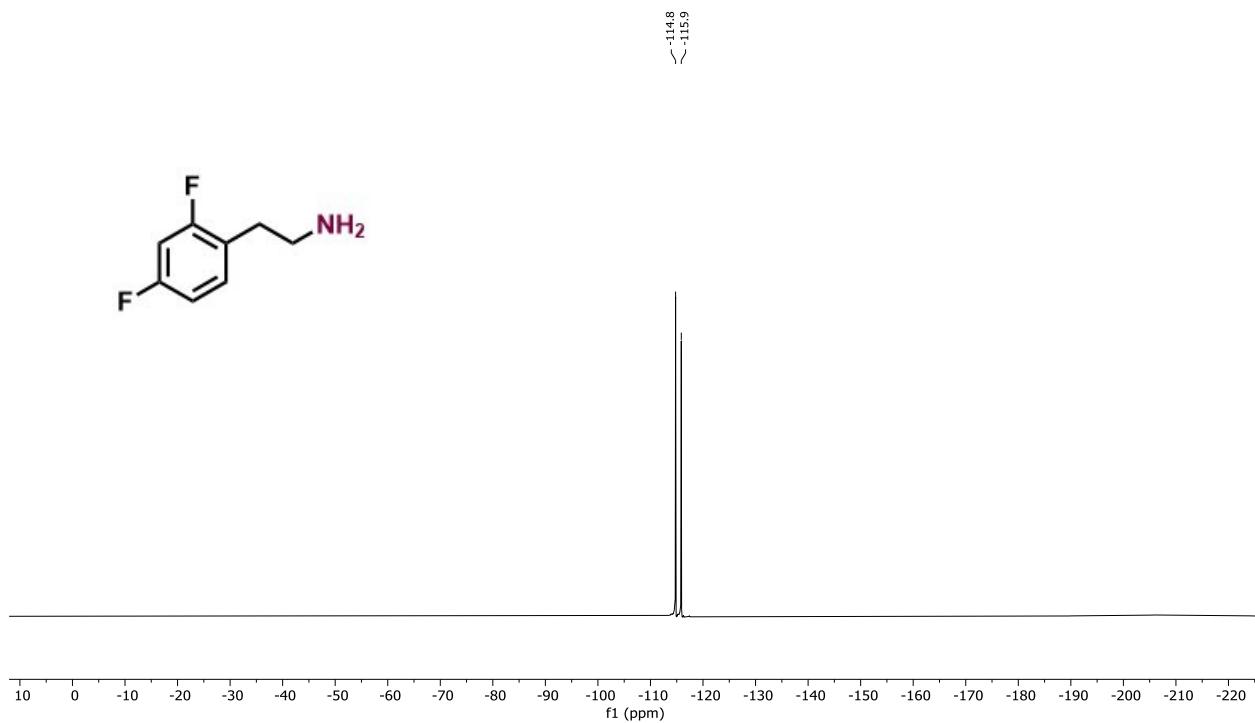




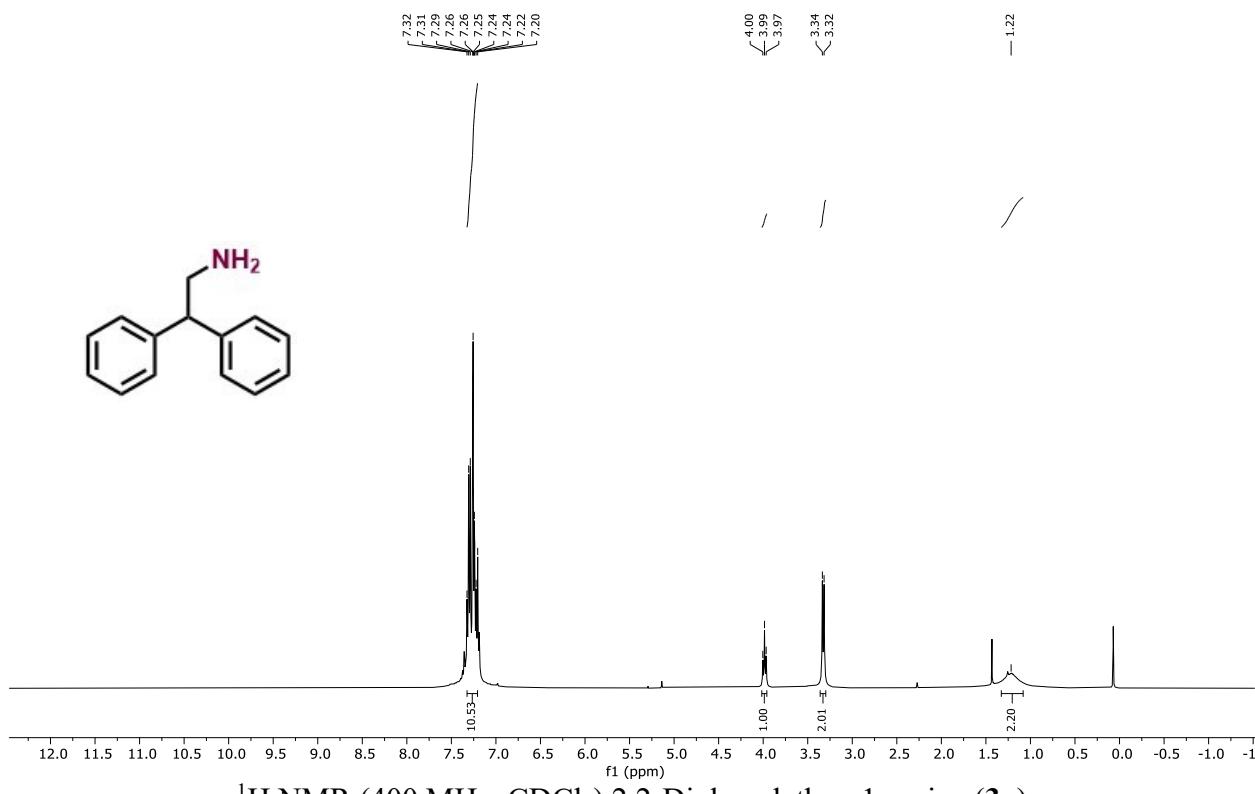
¹H NMR (400 MHz, CDCl₃) 2-(2,4-difluorophenyl)ethan-1-amine (**3u**)



¹³C NMR (101 MHz, CDCl₃) 2-(2,4-difluorophenyl)ethan-1-amine (**3u**)



^{19}F NMR (282 MHz, CDCl_3) 2-(2,4-difluorophenyl)ethan-1-amine (**3u**)



^1H NMR (400 MHz, CDCl_3) 2,2-Diphenylethan-1-amine (**3v**)

