

Supporting Information

Chemo- and Regioselective Magnesium-Catalyzed ortho-Alkenylation of Anilines

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1. General information:

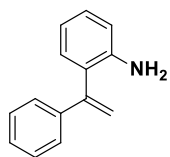
Unless otherwise noted, all commercially available compounds were used as provided without further purification. Solvents for chromatography were technical grade and distilled prior to use. Analytical thin-layer chromatography (TLC) was performed on Merck silica gel aluminium plates with F-254 indicator, visualised by irradiation with UV light. Column chromatography was performed using silica gel (Macherey Nagel, particle size 0.040-0.063 mm). Solvent mixtures are understood as volume/volume. ^1H -NMR and ^{13}C -NMR were recorded on a Varian AV400 or AV600 spectrometer in CDCl_3 and are reported relative to the solvents residual ^1H -signal (CHCl_3 , $\delta(\text{H})$ 7.26). Data are reported in the following order: chemical shift (δ) in ppm; multiplicities as indicated: s (singlet), bs (broad singlet), d (doublet), t (triplet), m (multiplet); coupling constants (J) are in Hertz (Hz). Mass spectra (MS-EI, 70eV) were conducted on a Finnigan SSQ 7000 mass spectrometer. HRMS were measured on Finnigan MAT 95 or LTQ Orbitrap XL spectrometer.

2. General procedure for the $\text{Mg}(\text{NTf}_2)_2$ catalyzed *ortho*-alkenylation of aniline (**3a** – **3ah**):

A screw cap sealed tube was charged with corresponding alkyne **1** (66.1 mg, 0.5 mmol, 1 equiv.), aniline **2** (140 mg, 1.5 mmol, 3 equiv.) in HFIP (1 mL). Then, $\text{Mg}(\text{NTf}_2)_2$ (5 mol%) was added to the reaction at room temperature and the reaction mixture was stirred at the optimal temperature until the reaction was completed. After completion, the solvent was evaporated to obtain the crude reaction. The corresponding products **3a-3ah** were obtained after column chromatography (SiO_2 , 40:1 hexane: EtOAc). Compound **3s** was obtained after column chromatography (SiO_2 , 2:1 hexane: EtOAc).

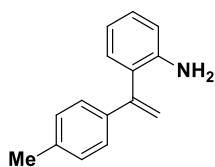
3. Characterization of compounds 3a-ah:

2-(1-phenylvinyl)aniline (3a)



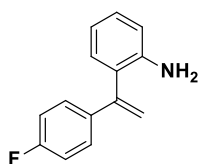
The title compound was prepared according to the general procedure, and isolated as a white solid (74%, 73 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.43 – 7.37 (m, 2H), 7.35 – 7.28 (m, 3H), 7.21 – 7.16 (m, 1H), 7.15 – 7.09 (m, 1H), 6.83 – 6.78 (m, 1H), 6.74 – 6.68 (m, 1H), 5.81 (d, J = 1.2 Hz, 1H), 5.37 (d, J = 1.2 Hz, 1H), 3.57 (brs, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ = 147.1, 143.9, 139.6, 130.8, 128.7, 128.5, 128.0, 127.3, 126.6, 118.3, 116.1, 115.6. **EI-MS**: m/z = 196 (M^+ + 1, 19), 195 (M^+ , 81), 194 (100), 180 (50). The data are in agreement with the reported spectroscopic data.¹

2-(1-(4-tolyl)vinyl)aniline (3b)



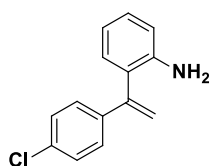
The title compound was prepared according to the general procedure, and isolated as yellow oil (62%, 65 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.35 – 7.26 (m, 2H), 7.21 – 7.09 (m, 4H), 6.85 – 6.78 (m, 1H), 6.77 – 6.67 (m, 1H), 5.78 (s, 1H), 5.32 (s, 1H), 3.57 (brs, 2H), 2.36 (s, 3H). **¹³C NMR** (151 MHz, CDCl₃): δ = 146.9, 143.9, 137.9, 136.7, 130.8, 129.3, 128.7, 127.5, 126.5, 118.3, 115.6, 115.3, 21.2. **EI-MS**: m/z = 209 (M^+ , 67), 208 (58), 194 (100). The data are in agreement with the reported spectroscopic data.¹

2-(1-(4-fluoro)vinyl)aniline (3c)



The title compound was prepared according to the general procedure, and isolated as yellow oil (75%, 80 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.44 – 7.33 (m, 2H), 7.25 – 7.15 (m, 1H), 7.15 – 7.08 (m, 1H), 7.07 – 6.98 (m, 2H), 6.87 – 6.78 (m, 1H), 6.76 – 6.68 (m, 1H), 5.77 (s, 1H), 5.36 (s, 1H), 3.49 (brs, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ = 162.7 (d, J = 248 Hz), 146.1, 143.8, 135.7 (d, J = 3 Hz), 130.7, 128.9, 128.4 (d, J = 8 Hz), 127.1, 118.4, 115.9, 115.7, 115.4 (d, J = 21 Hz). **EI-MS**: m/z = 213 (M^+ , 75), 212 (100), 198 (87). The data are in agreement with the reported spectroscopic data.¹

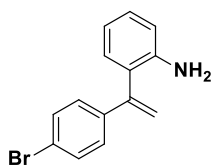
2-(1-(4-chloro)vinyl)aniline (3d)



The title compound was prepared according to the general procedure, and isolated as yellow oil (80%, 92 mg). **¹H NMR** (600 MHz, CDCl₃): δ 7.39 – 7.27 (m, 4H), 7.24 – 7.16 (m, 1H), 7.16 – 7.06 (m, 1H), 6.87 – 6.77 (m,

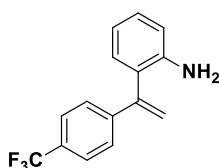
1H), 6.76 – 6.62 (m, 1H), 5.82 (s, 1H), 5.40 (s, 1H), 3.47 (brs, 2H). ¹³C NMR (151 MHz, CDCl₃): δ = 146.1, 143.8, 138.1, 133.9, 130.8, 129.0, 128.7, 127.9, 126.7, 118.4, 116.5, 115.7. **EI-MS**: *m/z* = 230 (*M*⁺ + 1, 49), 229 (*M*⁺, 100), 228 (89), 214 (93), 194 (63), 165 (34). The data are in agreement with the reported spectroscopic data.¹

2-(1-(4-bromo)vinyl)aniline (3e)



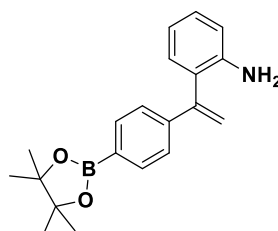
The title compound was prepared according to the general procedure, and isolated as blown oil (79%, 108 mg). ¹H NMR (600 MHz, CDCl₃): δ = 7.51 – 7.39 (m, 2H), 7.30 – 7.24 (m, 2H), 7.22 – 7.16 (m, 1H), 7.14 – 7.07 (m, 1H), 6.85 – 6.79 (m, 1H), 6.76 – 6.66 (m, 1H), 5.82 (s, 1H), 5.40 (s, 1H), 3.46 (brs, 2H). ¹³C NMR (151 MHz, CDCl₃): δ = 146.1, 143.8, 138.6, 131.7, 131.5, 130.8, 129.0, 128.3, 128.1, 126.6, 122.2, 118.4, 116.6, 115.7. **EI-MS**: *m/z* = 275 (*M*⁺ + 2, 60), 274 (*M*⁺ + 1, 67), 273 (*M*⁺, 62), 272 (59), 260 (58), 258 (56), 194 (100), 193 (59). The data are in agreement with the reported spectroscopic data.¹

2-(1-(4-trifluoromethyl)vinyl)aniline (3f)



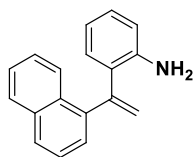
The title compound was prepared according to the general procedure, and isolated as yellow oil (52%, 69 mg). ¹H NMR (600 MHz, CDCl₃): δ = 7.57 (d, *J* = 8.3 Hz, 2H), 7.50 – 7.43 (m, 2H), 7.23 – 7.16 (m, 1H), 7.12 – 7.05 (m, 1H), 6.85 – 6.77 (m, 1H), 6.75 – 6.63 (m, 1H), 5.89 (s, 1H), 5.48 (s, 1H), 3.57 (brs, 2H). ¹³C NMR (151 MHz, CDCl₃): δ = 146.0, 143.8, 143.2, 130.8, 129.9 (q, *J* = 33 Hz), 129.1, 126.9, 126.4 (q, *J* = 4 Hz), 125.5 (q, *J* = 270 Hz), 118.5, 118.1, 115.7. **EI-MS**: *m/z* = 263 (*M*⁺, 100), 262 (88), 248 (69), 194 (60). The data are in agreement with the reported spectroscopic data.²

2-(1-(4-(4,4,5,5-tetramethyl-1,2-oxaborolan-2-yl)phenyl)vinyl)aniline (3g)



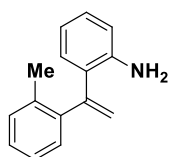
The title compound was prepared according to the general procedure, and isolated as a yellow solid (64%, 103 mg). ¹H NMR (400 MHz, CDCl₃): δ = 7.85 – 7.71 (m, 2H), 7.42 – 7.30 (m, 2H), 7.19 – 7.07 (m, 2H), 6.84 – 6.74 (m, 1H), 6.72 – 6.64 (m, 1H), 5.82 (s, 1H), 5.39 (s, 1H), 3.35 (brs, 2H), 1.33 (s, 12H). ¹³C NMR (101 MHz, CDCl₃): δ = 147.2, 143.9, 142.4, 135.0, 130.8, 128.8, 127.1, 125.9, 125.8, 118.3, 116.9, 115.6, 83.8, 24.8. **EI-MS**: *m/z* = 321 (*M*⁺, 72), 320 (64), 306 (72), 220 (100), 206 (51), 194 (91). **HRMS** (EI⁺) calcd for [C₂₀H₂₅BNO₂]: *m/z* 322.1978; found, 322.1972.

2-(1-(naphthalen-1-yl)vinyl)aniline (3h)



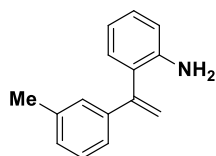
The title compound was prepared according to the general procedure, and isolated as yellow oil (72%, 88 mg). **¹H NMR** (400 MHz, CDCl₃): δ = 8.08 (d, *J* = 7.9 Hz, 1H), 7.84 (dd, *J* = 15.1, 7.9 Hz, 2H), 7.50 – 7.36 (m, 3H), 7.17 – 7.03 (m, 2H), 6.78 – 6.62 (m, 2H), 5.82 (d, *J* = 1.8 Hz, 1H), 5.65 (d, *J* = 1.8 Hz, 1H), 3.63 (brs, 2H). **¹³C NMR** (100 MHz, CDCl₃): δ = 146.8, 143.6, 140.1, 133.9, 131.2, 130.2, 128.6, 128.4, 128.0, 126.7, 126.2, 125.8, 125.6, 125.4, 125.2, 120.0, 118.4, 116.0. **EI-MS**: *m/z* = 245 (*M*⁺, 100), 244 (55), 230 (48). The data are in agreement with the reported spectroscopic data.²

2-(1-(2-tolyl)vinyl)aniline (3i)



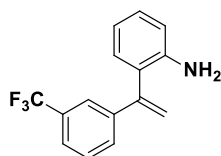
The title compound was prepared according to the general procedure, and isolated as yellow oil (79%, 83 mg). **¹H NMR** (400 MHz, CDCl₃): δ = 7.34 – 7.30 (m, 1H), 7.24 – 7.18 (m, 2H), 7.06 (dt, *J* = 5.7, 2.8 Hz, 1H), 7.02 – 6.96 (m, 1H), 6.73 – 6.62 (m, 2H), 5.60 (d, *J* = 1.9 Hz, 1H), 5.45 (d, *J* = 1.9 Hz, 1H), 3.49 (brs, 2H), 2.11 (s, 3H). **¹³C NMR** (100 MHz, CDCl₃): δ = 148.2, 143.6, 141.8, 135.8, 130.6, 130.1, 129.5, 128.4, 127.7, 127.3, 125.9, 118.6, 118.3, 115.9, 20.3. **EI-MS**: *m/z* = 209 (*M*⁺, 100), 208 (28), 194 (100). The data are in agreement with the reported spectroscopic data.²

2-(1-(3-tolyl)vinyl)aniline (3j)



The title compound was prepared according to the general procedure, and isolated as yellow oil (78%, 82 mg). **¹H NMR** (400 MHz, CDCl₃): δ = 7.27 – 7.10 (m, 6H), 6.85 – 6.77 (m, 1H), 6.74 – 6.67 (m, 1H), 5.79 (d, *J* = 1.3 Hz, 1H), 5.36 (d, *J* = 1.3 Hz, 1H), 3.41 (brs, 2H), 2.35 (s, 3H). **¹³C NMR** (100 MHz, CDCl₃): δ = 147.3, 143.9, 139.7, 138.1, 130.8, 128.9, 128.7, 128.5, 127.5, 127.2, 123.9, 118.3, 116.0, 115.6, 21.5. **EI-MS**: *m/z* = 209 (*M*⁺, 77), 208 (51), 194 (100). The data are in agreement with the reported spectroscopic data.²

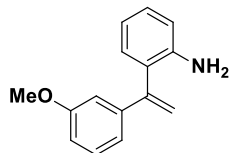
2-(1-(3-(trifluoromethyl)phenyl)vinyl)aniline (3k)



The title compound was prepared according to the general procedure, and isolated as yellow oil (74%, 97 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.68 (s, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.46 – 7.37 (m, 1H), 7.23 – 7.15 (m, 1H), 7.09 (dd, *J* = 7.6, 1.3 Hz, 1H), 6.86 – 6.78 (m, 1H), 6.73 (d, *J* = 8.1 Hz, 1H), 5.88 (s, 1H), 5.47 (s, 1H), 3.48 (brs, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ = 145.9, 143.8, 140.6, 130.9 (q, *J* = 32 Hz), 130.8, 130.1, 129.0, 124.0 (q, *J* = 270 Hz), 123.2, (q, *J* = 5

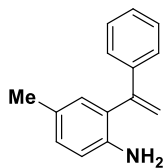
Hz), 123.1 (q, $J = 5$ Hz), 118.5, 117.7, 115.7. **EI-MS**: $m/z = 263$ (M^+ , 100), 262 (79), 248 (70), 242 (34), 194 (86). The data are in agreement with the reported spectroscopic data.²

2-(1-(3-(methoxy)phenyl)vinyl)aniline (3l)



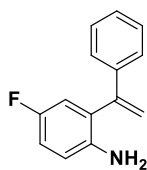
The title compound was prepared according to the general procedure, and isolated as a yellow oil (72%, 81 mg). **¹H NMR** (600 MHz, $CDCl_3$): $\delta = 7.26 - 7.21$ (m, 1H), 7.19 – 7.13 (m, 1H), 7.12 (d, $J = 7.6$ Hz, 1H), 6.96 (d, $J = 7.6$ Hz, 1H), 6.93 (d, $J = 1.8$ Hz, 1H), 6.85 (dd, $J = 8.1, 1.8$ Hz, 1H), 6.81 – 6.75 (m, 1H), 6.69 (d, $J = 8.1$ Hz, 1H), 5.79 (d, $J = 1.1$ Hz, 1H), 5.36 (d, $J = 1.1$ Hz, 1H), 3.78 (s, 3H), 3.56 (brs, 2H). **¹³C NMR** (151 MHz, $CDCl_3$) $\delta = 159.7, 147.1, 143.9, 141.2, 130.8, 129.5, 128.8, 127.2, 119.2, 118.3, 116.4, 116.4, 115.6, 113.3, 112.4, 55.2$. **EI-MS**: $m/z = 225.2$ (M^+ , 100), 224 (65), 210 (40), 194(72). The data are in agreement with the reported spectroscopic data.³

4-methyl-2-(1-phenylvinyl)aniline (3m)



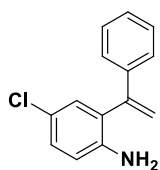
The title compound was prepared according to the general procedure, and isolated as red oil (90%, 94 mg). **¹H NMR** (600 MHz, $CDCl_3$): $\delta = 7.46 - 7.41$ (m, 2H), 7.41 – 7.33 (m, 3H), 7.06 – 6.97 (m, 2H), 6.66 (dd, $J = 8.0, 2.1$ Hz, 1H), 5.84 (d, $J = 3.4$ Hz, 1H), 5.40 (d, $J = 3.7$ Hz, 1H), 3.37 (brs, 2H), 2.32 (s, 3H). **¹³C NMR** (151 MHz, $CDCl_3$): $\delta = 147.3, 141.4, 139.8, 131.3, 129.4, 128.6, 128.1, 127.6, 127.5, 126.7, 116.0, 115.8, 20.5$. **EI-MS**: $m/z = 209$ (M^+ , 100), 208 (89), 194 (51). The data are in agreement with the reported spectroscopic data.⁴

4-fluoro-2-(1-phenylvinyl)aniline (3n)



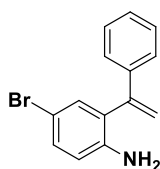
The title compound was prepared according to the general procedure, and isolated as green oil (84%, 82 mg). **¹H NMR** (600 MHz, $CDCl_3$): $\delta = 7.43 - 7.32$ (m, 5H), 6.96 – 6.86 (m, 2H), 6.69 – 6.60 (m, 1H), 5.84 (s, 1H), 5.39 (s, 1H), 3.33 (brs, 2H). **¹³C NMR** (151 MHz, $CDCl_3$): $\delta = 156.1$ (d, $J = 237$ Hz), 146.4 (d, $J = 2$ Hz), 140.1 (d, $J = 2$ Hz), 139.0, 128.7, 128.4, 127.4, 126.6, 121.4, 117.1, 116.9, 116.7, 116.5 (d, $J = 8$ Hz), 115.2 (d, $J = 23$ Hz). **EI-MS**: $m/z = 213$ (M^+ , 89), 212 (100), 198 (68). The data are in agreement with the reported spectroscopic data.⁵

4-chloro-2-(1-phenylvinyl)aniline (3o)



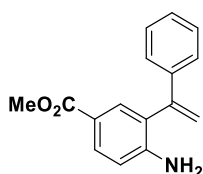
The title compound was prepared according to the general procedure, and isolated as yellow oil (84%, 96 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.44 – 7.31 (m, 5H), 7.19 – 7.11 (m, 2H), 6.66 – 6.58 (m, 1H), 5.83 (s, 1H), 5.38 (s, 1H), 3.57 (brs, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ = 146.1, 142.7, 138.9, 130.3, 128.7, 128.6, 128.6, 128.4, 126.6, 122.8, 122.7, 116.8, 116.7. **EI-MS**: m/z = 231 (M^+ + 2, 34), 230 (M^+ + 1, 52), 229 (M^+ , 84), 228 (100), 214 (50). The data are in agreement with the reported spectroscopic data.⁴

4-bromo-2-(1-phenylvinyl)aniline (3p)



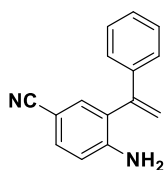
The title compound was prepared according to the general procedure, and isolated as green oil (87%, 119 mg). **¹H NMR** (400 MHz, CDCl₃): δ = 7.42 – 7.29 (m, 5H), 7.28 – 7.21 (m, 2H), 6.61 – 6.50 (m, 1H), 5.81 (d, J = 0.6 Hz, 1H), 5.36 (d, J = 0.6 Hz, 1H), 3.44 (brs, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ = 146.0, 143.1, 138.9, 133.0, 131.4, 129.1, 128.7, 128.8, 126.6, 117.1, 116.8, 109.9. **EI-MS**: m/z = 276 (M^+ + 3, 22), 275 (M^+ + 2, 95), 274 (M^+ + 1, 94), 273 (M^+ , 100), 272 (66), 260 (27), 258 (27), 193 (22). The data are in agreement with the reported spectroscopic data.⁵

Methyl 4-amino-3-(1-phenylvinyl)benzoate (3q)



The title compound was prepared according to the general procedure, and isolated as yellow oil (61%, 77 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.89 – 7.81 (m, 2H), 7.38 – 7.27 (m, 5H), 6.65 (d, J = 8.3 Hz, 1H), 5.83 (d, J = 0.8 Hz, 1H), 5.39 (d, J = 0.8 Hz, 1H), 3.99 (brs, 2H), 3.85 (s, 3H). **¹³C NMR** (151 MHz, CDCl₃): δ = 167.2, 148.4, 146.2, 138.9, 132.7, 130.8, 128.7, 128.3, 126.5, 126.1, 119.5, 116.9, 114.4, 51.6. **EI-MS**: m/z = 253 (M^+ , 86), 252 (100), 238 (53). **HRMS** (EI⁺) calcd for [C₁₆H₁₅NO₂Na]: m/z 276.0995; found, 276.0991.

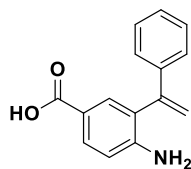
4-amino-3-(1-phenylvinyl)benzonitrile (3r)



The title compound was prepared according to the general procedure, and isolated as brown oil (58%, 64 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.44 – 7.39 (m, 2H), 7.38 – 7.31 (m, 5H), 6.66 (d, J = 8.3 Hz, 1H), 5.85 (s, 1H), 5.38 (s, 1H), 4.06 (brs, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ = 143.3,

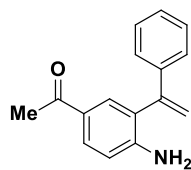
140.5, 133.6, 130.1, 128.2, 124.1, 123.9, 122.1, 121.7, 115.2, 112.7, 110.2, 95.4. **EI-MS**: m/z = 220 (M^+ , 80), 219 (100), 205 (45). **HRMS** (EI^+) calcd for $[C_{15}H_{12}N_2Na]$: m/z 243.0893; found, 243.0890.

4-amino-3-(1-phenylvinyl)benzoic acid (3s)



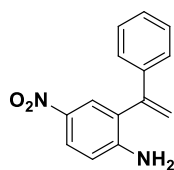
The title compound was prepared according to the general procedure, and isolated as brown oil (72%, 86 mg). **1H NMR** (600 MHz, $CDCl_3$): δ = 7.98 – 7.88 (m, 2H), 7.40 – 7.29 (m, 5H), 6.67 (d, J = 8.1 Hz, 1H), 5.84 (d, J = 0.8 Hz, 1H), 5.41 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$): δ = 172.1, 149.1, 146.0, 138.8, 133.5, 131.6, 128.7, 128.4, 126.5, 126.1, 118.5, 117.1, 114.4. **EI-MS**: m/z = 239 (M^+ , 91), 238 (100), 224 (50). **HRMS** (EI^+) calcd for $[C_{15}H_{13}NO_2Na]$: m/z 262.0838; found, 262.0830.

1-(4-amino-3-(1-phenylvinyl)phenyl)ethanone (3t)



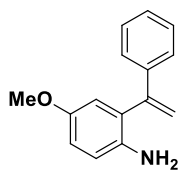
The title compound was prepared according to the general procedure, and isolated as red oil (62%, 74 mg). **1H NMR** (600 MHz, $CDCl_3$): δ = 7.82 (dd, J = 8.4, 2.0 Hz, 1H), 7.78 (d, J = 2.0 Hz, 1H), 7.40 – 7.29 (m, 5H), 6.67 (d, J = 8.4 Hz, 1H), 5.85 (s, 1H), 5.40 (s, 1H), 4.03 (brs, 2H), 2.52 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$): δ = 196.6, 148.7, 146.2, 138.8, 131.9, 130.0, 128.7, 128.4, 127.7, 126.5, 125.9, 117.0, 114.4, 26.1. **EI-MS**: m/z = 237 (M^+ , 70), 236 (60), 222 (100), 193 (37). **HRMS** (EI^+) calcd for $[C_{16}H_{15}NONa]$: m/z 260.1046; found, 260.1043.

4-nitro-2-(1-phenylvinyl)aniline (3u)



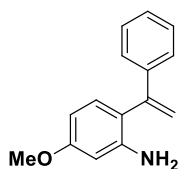
The title compound was prepared according to the general procedure, and isolated as yellow oil (52%, 62 mg). **1H NMR** (600 MHz, $CDCl_3$): δ = 8.10 – 8.05 (m, 2H), 7.37 – 7.32 (m, 5H), 6.66 – 6.63 (m, 1H), 5.89 (d, J = 0.6 Hz, 1H), 5.44 (s, 1H), 4.28 (brs, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$): δ = 150.1, 145.1, 138.9, 138.1, 128.9, 128.7, 127.2, 126.5, 125.8, 125.5, 117.9, 113.9. **EI-MS**: m/z = 240 (M^+ , 100), 239 (95), 225 (48), 193 (70). The data are in agreement with the reported spectroscopic data.¹

4-methoxy-2-(1-phenylvinyl)aniline (3v)



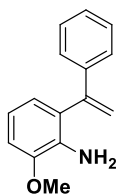
The title compound was prepared according to the general procedure, and isolated as red oil (82%, 92 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.42 – 7.37 (m, 2H), 7.36 – 7.29 (m, 3H), 6.79 (dd, J = 8.6, 2.9 Hz, 1H), 6.74 (d, J = 2.8 Hz, 1H), 6.67 (d, J = 8.6 Hz, 1H), 5.82 (s, 1H), 5.37 (s, 1H), 3.77 (s, 3H), 3.11 (brs, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ = 152.5, 147.1, 139.4, 137.6, 128.8, 128.6, 128.1, 127.5, 126.6, 126.4, 116.9, 116.2, 116.1, 114.6, 55.8. **EI-MS**: m/z = 225 (M^+ , 100), 224 (74), 210 (34), 165 (25). The data are in agreement with the reported spectroscopic data.¹

3-methoxy-2-(1-phenylvinyl)aniline (3w)



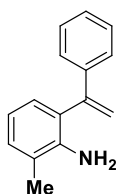
The title compound was prepared according to the general procedure, and isolated as red oil (82%, 92 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.42 – 7.37 (m, 2H), 7.34 – 7.24 (m, 3H), 7.16 – 7.10 (m, 1H), 6.43 (d, J = 8.0 Hz, 1H), 6.38 (d, J = 8.2 Hz, 1H), 6.05 (d, J = 1.2 Hz, 1H), 5.33 (d, J = 1.1 Hz, 1H), 3.66 (s, 3H). **¹³C NMR** (151 MHz, CDCl₃): δ = 157.9, 145.2, 142.4, 139.3, 128.8, 128.4, 127.8, 125.9, 116.6, 116.0, 108.4, 100.9, 55.8. **EI-MS**: m/z = 225 (M^+ , 100), 224 (54), 210 (77), 165 (19). The data are in agreement with the reported spectroscopic data.²

2-methoxy-6-(1-phenylvinyl)aniline (3x)



The title compound was prepared according to the general procedure, and isolated as red oil (76%, 86 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.43 – 7.37 (m, 2H), 7.36 – 7.26 (m, 4H), 7.09 (d, J = 7.4 Hz, 1H), 7.02 (d, J = 7.7 Hz, 1H), 6.79 – 6.70 (m, 1H), 5.84 (d, J = 1.1 Hz, 1H), 5.38 (d, J = 1.2 Hz, 1H), 3.48 (brs, 2H), 2.20 (s, 3H). **¹³C NMR** (151 MHz, CDCl₃): δ = 147.1, 146.9, 139.7, 133.9, 128.5, 128.0, 127.2, 126.7, 122.9, 117.3, 115.9, 109.4, 55.6. **EI-MS**: m/z = 225 (M^+ , 100), 224 (76), 210 (50), 165 (16). The data are in agreement with the reported spectroscopic data.¹

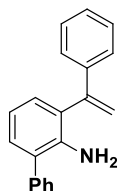
2-methyl-6-(1-phenylvinyl)aniline (3y)



The title compound was prepared according to the general procedure, and isolated as yellow oil (72%, 75 mg). **¹H NMR** (400 MHz, CDCl₃): δ = 7.45 – 7.37 (m, 2H), 7.36 – 7.25 (m, 3H), 6.86 – 6.71 (m, 3H), 5.82 (d, J = 1.4 Hz, 1H), 5.39 (d, J = 1.4 Hz, 1H), 3.88 (s, 3H), 3.77 (brs, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ =

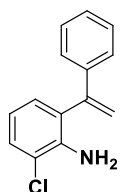
147.4, 142.0, 139.7, 129.9, 128.6, 128.5, 128.1, 126.6, 122.4, 117.8, 116.1, 17.8. **EI-MS**: m/z = 209 (M^+ , 100), 208 (98), 194 (68). The data are in agreement with the reported spectroscopic data.¹

2-phenyl-6-(1-phenylvinyl)aniline (3z)



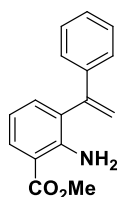
The title compound was prepared according to the general procedure, and isolated as brown oil (72%, 98 mg). **¹H NMR** (600 MHz, $CDCl_3$): δ = 7.55 – 7.40 (m, 6H), 7.39 – 7.28 (m, 4H), 7.20 – 7.13 (m, 2H), 6.93 – 6.86 (m, 1H), 5.88 (s, 1H), 5.46 (s, 1H), 3.74 (brs, 2H). **¹³C NMR** (151 MHz, $CDCl_3$): δ = 147.4, 141.1, 139.6, 139.6, 130.1, 129.9, 129.3, 128.8, 128.6, 128.1, 127.8, 127.5, 127.2, 126.6, 117.9, 116.4. **EI-MS**: m/z = 271 (M^+ , 100), 270 (93), 254 (59). **HRMS** (EI^+) calcd for $[C_{20}H_{18}N]$: m/z 272.1434; found, 272.1435.

2-chloro-6-(1-phenylvinyl)aniline (3aa)



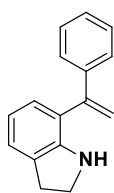
The title compound was prepared according to the general procedure, and isolated as yellow oil (94%, 74 mg). **¹H NMR** (600 MHz, $CDCl_3$): δ = 7.40 – 7.32 (m, 5H), 7.28 (dd, J = 8.0, 1.4 Hz, 1H), 7.04 (dd, J = 7.5, 1.4 Hz, 1H), 6.76 – 6.70 (m, 1H), 5.85 (d, J = 1.0 Hz, 1H), 5.39 (d, J = 1.0 Hz, 1H), 4.01 (brs, 2H). **¹³C NMR** (151 MHz, $CDCl_3$): δ = 147.4, 141.1, 139.6, 139.6, 130.1, 129.9, 129.3, 128.8, 128.6, 128.1, 127.8, 127.5, 127.2, 126.6, 117.9, 116.4. **EI-MS**: m/z = 230 (M^+ + 1, 50), 229 (M^+ , 89), 228 (100), 214 (53). The data are in agreement with the reported spectroscopic data.⁵

methyl 2-amino-3-(1-phenylvinyl)benzoate (3ab)



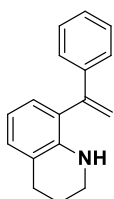
The title compound was prepared according to the general procedure, and isolated as brown oil (54%, 68 mg). **¹H NMR** (600 MHz, $CDCl_3$): δ = 7.90 (dd, J = 8.1, 1.5 Hz, 1H), 7.39 – 7.35 (m, 2H), 7.35 – 7.29 (m, 3H), 7.24 (dd, J = 7.2, 1.6 Hz, 1H), 6.70 – 6.65 (m, 1H), 5.87 (d, J = 0.9 Hz, 1H), 5.81 (brs, 2H), 5.37 (d, J = 1.0 Hz, 1H), 3.86 (s, 3H). **¹³C NMR** (151 MHz, $CDCl_3$): δ = 168.8, 148.1, 146.2, 138.9, 135.4, 130.9, 128.6, 128.3, 126.4, 116.9, 115.5, 110.6, 51.6. **EI-MS**: m/z = 254 (M^+ + 1, 43), 253 (M^+ , 76), 221 (51), 220 (59), 193 (100), 165 (41). **HRMS** (EI^+) calcd for $[C_{16}H_{16}NO_2]$: m/z 254.1175; found, 254.1175.

7-(1-phenylvinyl)indoline (3ac)



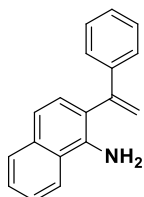
The title compound was prepared according to the general procedure, and isolated as yellow oil (71%, 78 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.39 – 7.35 (m, 2H), 7.35 – 7.29 (m, 3H), 7.11 (d, *J* = 7.2 Hz, 1H), 6.98 (d, *J* = 7.7 Hz, 1H), 6.77 – 6.71 (m, 1H), 5.62 (d, *J* = 1.2 Hz, 1H), 5.42 (d, *J* = 1.1 Hz, 1H), 3.44 (t, *J* = 8.4 Hz, 2H), 3.03 (t, *J* = 8.3 Hz, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ = 147.3, 140.3, 129.7, 128.5, 128.3, 127.9, 127.2, 124.1, 118.7, 115.6, 47.1, 29.7. **EI-MS**: *m/z* = 221 (*M*⁺, 14), 220 (19), 115 (26), 78 (67), 77 (100). **HRMS** (EI⁺) calcd for [C₁₆H₁₆N]: *m/z* 222.1277; found, 222.1277.

8-(1-phenylvinyl)-1,2,3,4-tetrahydroquinoline (3ad)



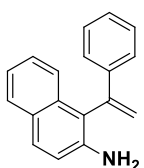
The title compound was prepared according to the general procedure, and isolated as red oil (62%, 76 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.42 – 7.38 (m, 2H), 7.35 – 7.28 (m, 3H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 7.4 Hz, 1H), 6.66 – 6.62 (m, 1H), 5.82 (d, *J* = 1.4 Hz, 1H), 5.35 (d, *J* = 1.3 Hz, 1H), 3.84 (brs, 1H), 3.21 – 3.15 (m, 2H), 2.82 (t, *J* = 6.4 Hz, 2H), 1.94 – 1.85 (m, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ = 147.0, 142.1, 139.6, 128.9, 128.5, 128.4, 128.0, 126.5, 126.1, 121.2, 116.0, 115.9, 41.9, 27.4, 21.9. **EI-MS**: *m/z* = 235 (*M*⁺, 100), 234 (86), 220 (66), 206.1 (38). The data are in agreement with the reported spectroscopic data.⁶

2-(1-phenylvinyl)naphthalen-1-amine (3ae)



The title compound was prepared according to the general procedure, and isolated as red oil (65%, 80 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.88 – 7.81 (m, 2H), 7.54 – 7.47 (m, 2H), 7.46 – 7.42 (m, 2H), 7.40 – 7.32 (m, 4H), 7.30 – 7.24 (m, 1H), 6.00 (s, 1H), 5.49 (s, 1H), 4.07 (brs, 2H). **¹³C NMR** (151 MHz, CDCl₃): δ = 147.4, 139.9, 139.1, 133.9, 128.9, 128.6, 128.5, 128.2, 126.9, 125.8, 125.2, 123.7, 121.6, 121.1, 118.2, 116.7. **EI-MS**: *m/z* = 245 (*M*⁺, 100), 244 (99), 230 (56). The data are in agreement with the reported spectroscopic data.⁵

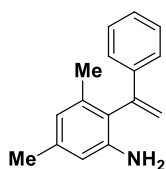
2-(1-phenylvinyl)naphthalen-1-amine (3af)



The title compound was prepared according to the general procedure, and isolated as red oil (75%, 92 mg). **¹H NMR** (600 MHz, CDCl₃): δ = 7.78 – 7.69 (m, 2H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.46 – 7.38 (m, 2H), 7.37 – 7.21 (m, 5H),

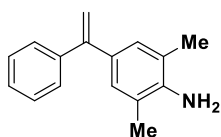
7.04 (d, $J = 8.7$ Hz, 1H), 6.27 (d, $J = 1.3$ Hz, 1H), 5.43 (d, $J = 1.2$ Hz, 1H), 3.68 (brs, 2H). **^{13}C NMR** (151 MHz, CDCl_3): $\delta = 144.0, 140.9, 139.1, 133.5, 128.8, 128.7, 128.1, 127.9, 127.9, 126.5, 126.2, 124.3, 122.2, 119.2, 118.1, 117.8$. **EI-MS**: $m/z = 245$ (M^+ , 100), 244 (64), 230 (20), 167 (25). **HRMS** (EI^+) calcd for $[\text{C}_{18}\text{H}_{16}\text{N}]$: m/z 246.1277; found, 246.1276.

3,5-dimethyl-2-(1-phenylvinyl)aniline (3ag)



The title compound was prepared according to the general procedure, and isolated as brown oil (74%, 82 mg). **^1H NMR** (600 MHz, CDCl_3): $\delta = 7.50 - 7.41$ (m, 2H), 7.41 – 7.31 (m, 3H), 6.60 (s, 1H), 6.52 (s, 1H), 6.11 (d, $J = 1.3$ Hz, 1H), 5.35 (d, $J = 1.3$ Hz, 1H), 3.61 (brs, 2H), 2.36 (s, 3H), 2.14 (s, 3H). **^{13}C NMR** (151 MHz, CDCl_3): $\delta = 145.0, 144.0, 139.1, 137.7, 137.1, 128.7, 128.0, 125.9, 124.5, 120.9, 116.3, 113.6, 21.3, 20.1$. **EI-MS**: $m/z = 223$ (M^+ , 94), 222.2 (60), 208 (100), 193 (29). The data are in agreement with the reported spectroscopic data.⁵

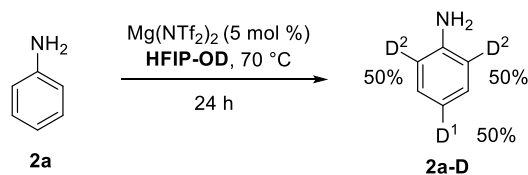
2,6-dimethyl-4-(1-phenylvinyl)aniline (3ah)



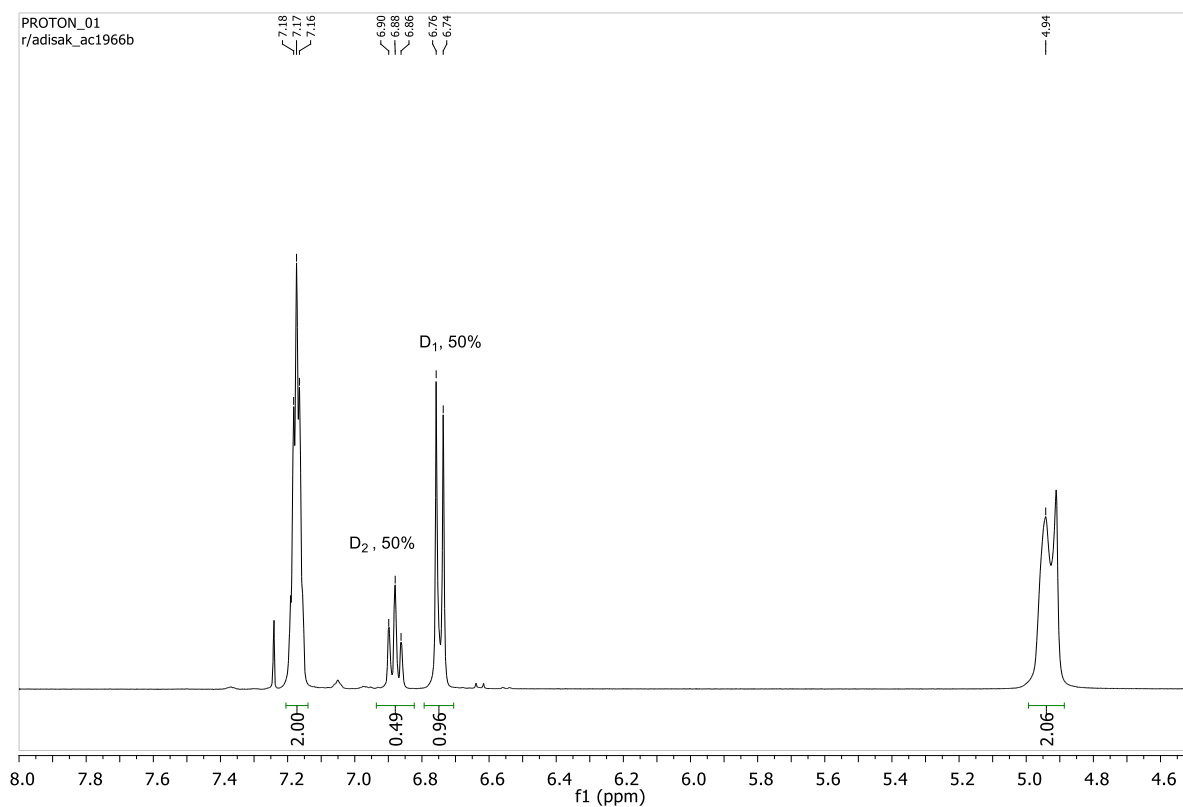
The title compound was prepared according to the general procedure, and isolated as brown oil (71%, 79 mg). **^1H NMR** (600 MHz, CDCl_3): $\delta = 7.36 - 7.23$ (m, 5H), 7.00 (d, $J = 7.6$ Hz, 1H), 6.68 (d, $J = 7.5$ Hz, 1H), 5.80 (d, $J = 1.4$ Hz, 1H), 5.22 (d, $J = 1.4$ Hz, 1H), 3.63 (brs, 2H), 2.25 (s, 3H), 1.95 (s, 3H). **^{13}C NMR** (151 MHz, CDCl_3): $\delta = 149.8, 142.8, 140.9, 140.4, 128.3, 127.5, 127.4, 126.5, 121.1, 120.2, 119.7, 114.4, 17.8, 14.6$. **EI-MS**: $m/z = 223$ (M^+ , 100), 208 (64), 193 (47). **HRMS** (EI^+) calcd for $[\text{C}_{16}\text{H}_{18}\text{N}]$: m/z 224.1434; found, 224.1434.

4. Deuterium labelling experiments.

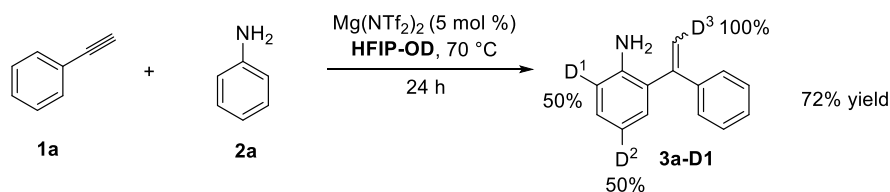
Control experiment



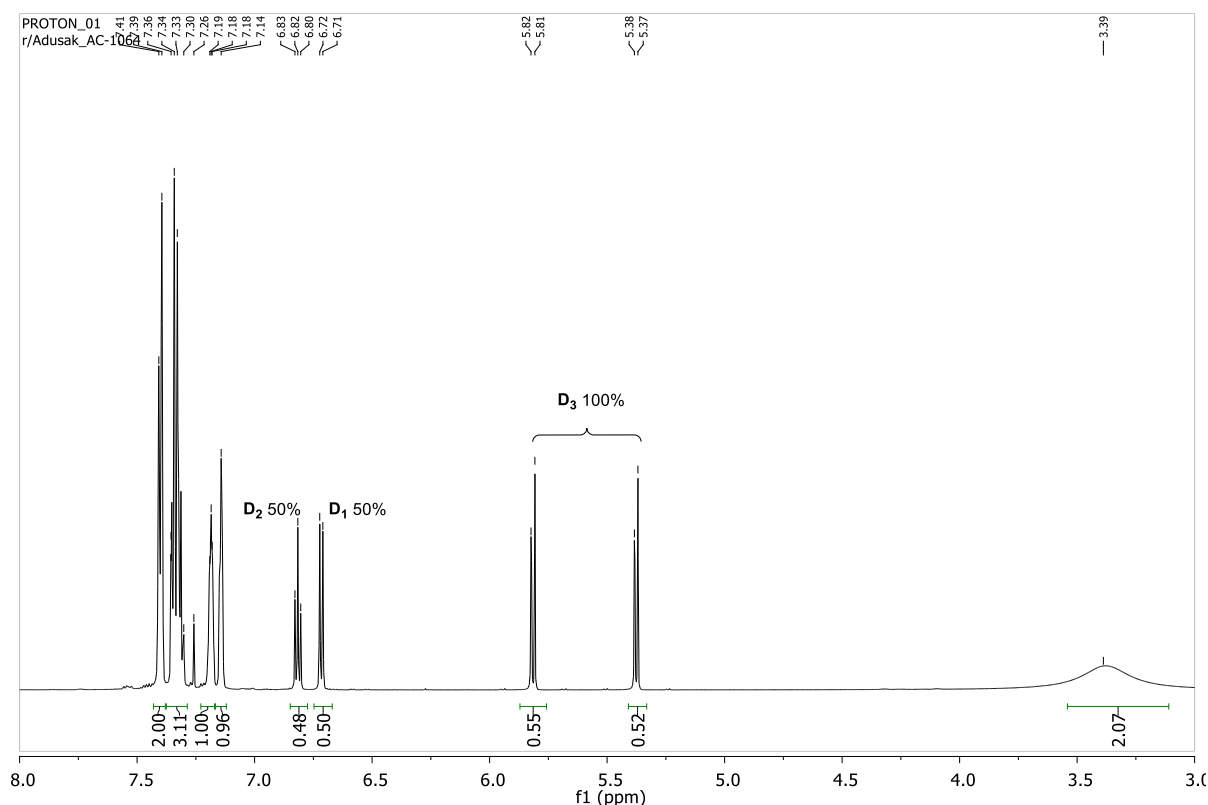
A screw cap sealed tube was charged with aniline **2a** (70 mg, 0.75 mmol, 1 equiv.) and HFIP-OD (0.5 mL). $\text{Mg}(\text{NTf}_2)_2$ was added to the reaction at room temperature and the reaction mixture was stirred continuously at 70 °C for 24 h. Then, the solvent was evaporated to obtain the corresponding product **2a-D** as yellow liquid; ^1H NMR (400 MHz, CDCl_3): δ = 7.21 – 7.14 (m, 2H), 6.88 (H/D = 50%; t, J = 7.3 Hz, 1H), 6.75 (H/D = 50%; d, J = 8.4 Hz, 2H), 4.94 (s, 2H). Deuterium incorporation was calculated by integration of ^1H NMR.

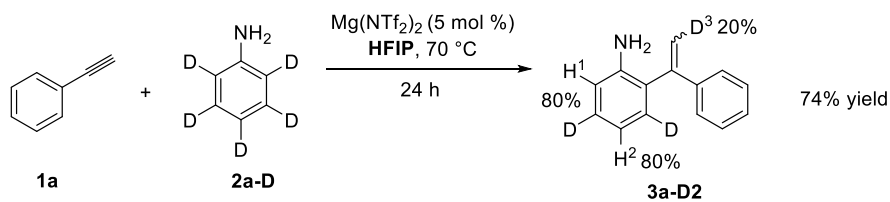


Deuterium incorporation

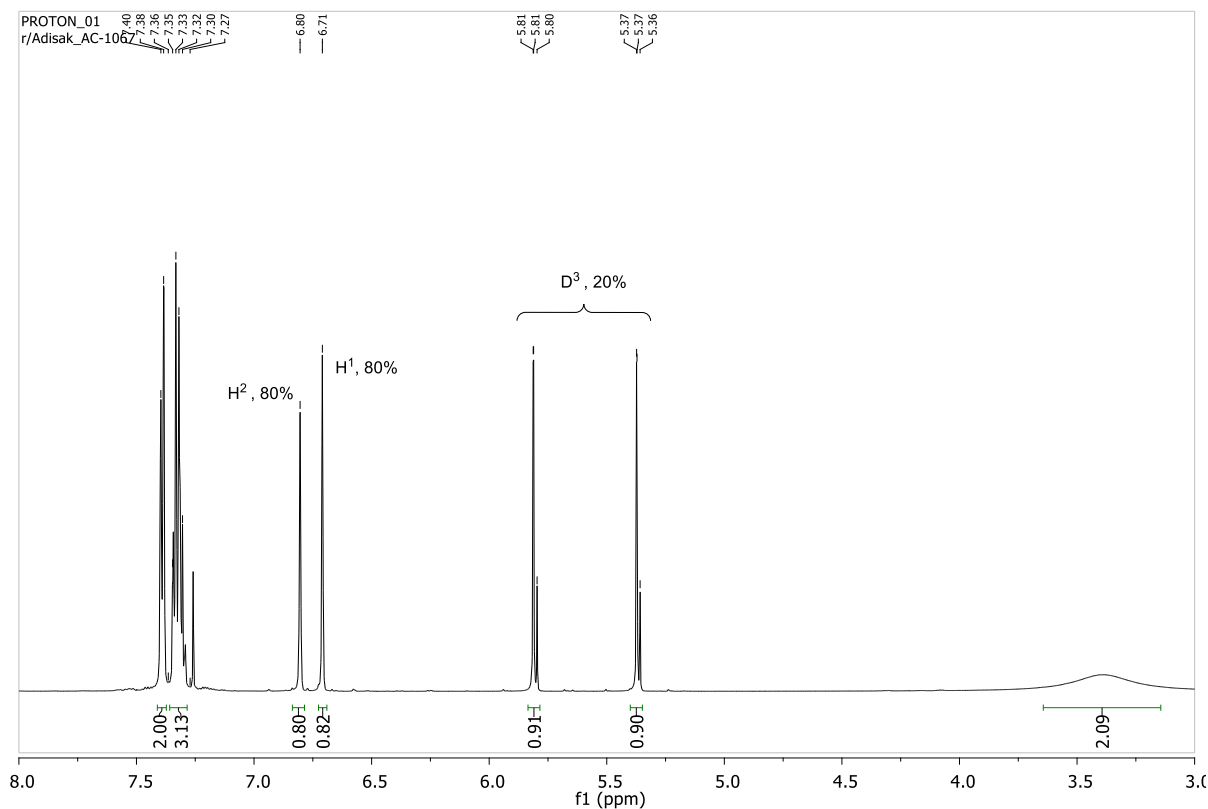


A screw cap sealed tube was charged with phenylacetylene **1a** (33.1 mg, 0.25 mmol, 1 equiv.), aniline **2** (70 mg, 0.75 mmol, 3 equiv.) and HFIP-OD (0.5 mL). $\text{Mg}(\text{NTf}_2)_2$ was added to the reaction at room temperature and the reaction mixture was stirred continuously at 70 °C for 24 h. Then, solvent was evaporated to obtain the crude reaction mixture. The corresponding product **3a-D1** was obtained after column chromatography (SiO_2 , 50:1 hexane: EtOAc as a colourless solid; ^1H NMR (600 MHz, CDCl_3) δ = 7.44 – 7.38 (m, 2H), 7.36 – 7.29 (m, 3H), 7.21 – 7.16 (m, 1H), 7.14 (s, 1H), 6.82 (H/D = 50%; t, J = 7.4 Hz, 1H), 6.72 (H/D = 50%; d, J = 8.0 Hz, 1H), 5.85 – 5.78 (H/D = 50%, m, 1H), 5.42 – 5.33 (H/D = 50%, m, 1H), 3.39 (bs, 2H). Deuterium incorporation was calculated by integration of ^1H NMR.





A screw cap sealed tube was charged with phenylacetylene **1a** (33.1 mg, 0.25 mmol, 1 equiv.), deuterated aniline **2a-D** (70 mg, 0.75 mmol, 3 equiv.) and HFIP (0.5 mL). $\text{Mg}(\text{NTf}_2)_2$ was added to the reaction at room temperature and the reaction mixture was stirred continuously at 70 °C for 24 h. Then, the solvent was evaporated to obtain the crude reaction mixture. The corresponding product **3a-D1** was obtained after column chromatography (SiO_2 , 50:1 hexane: EtOAc) as a colourless solid; ^1H NMR (600 MHz, CDCl_3) δ = 7.44 – 7.37 (m, 2H), 7.37 – 7.28 (m, 3H), 6.80 (D/H = 80%; s, 1H), 6.71 (D/H = 80%; s, 1H), 5.86 – 5.75 (H/D = 10%, m, 1H), 5.44 – 5.32 (H/D = 10%, m, 1H), 3.38 (s, 2H). Deuterium incorporation was calculated by integration of ^1H NMR.

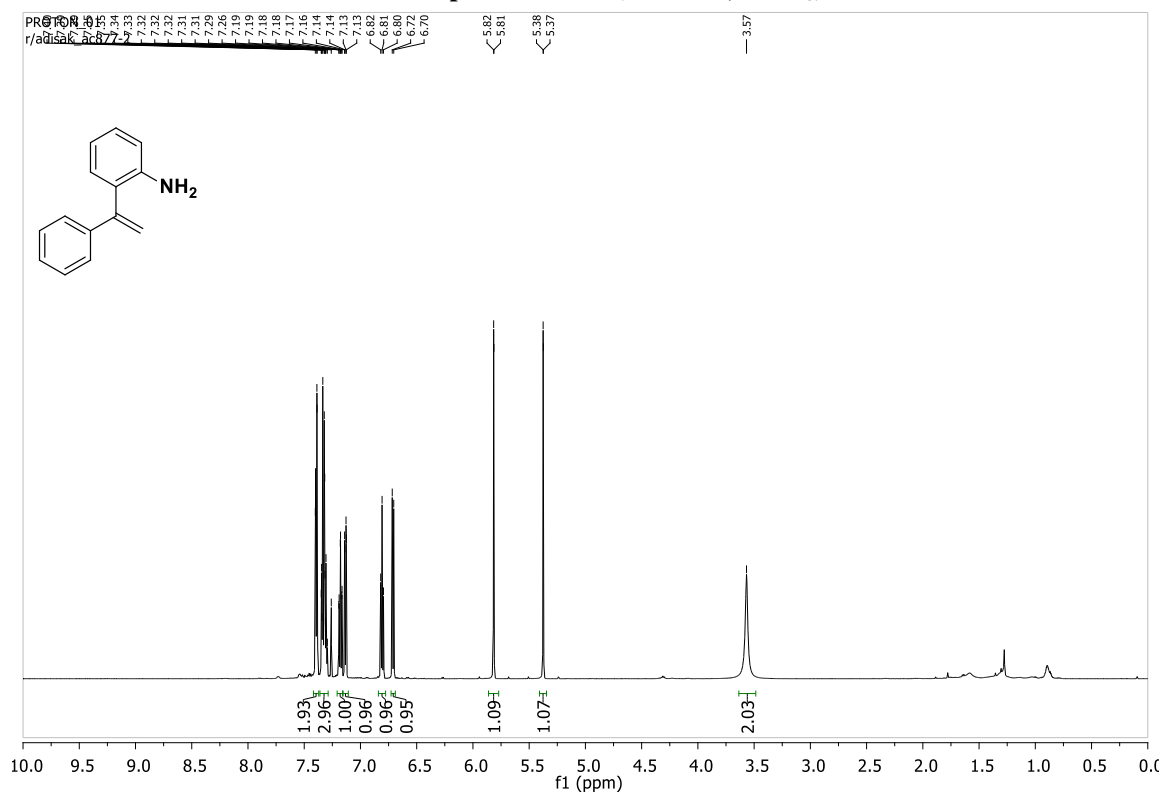


5. References

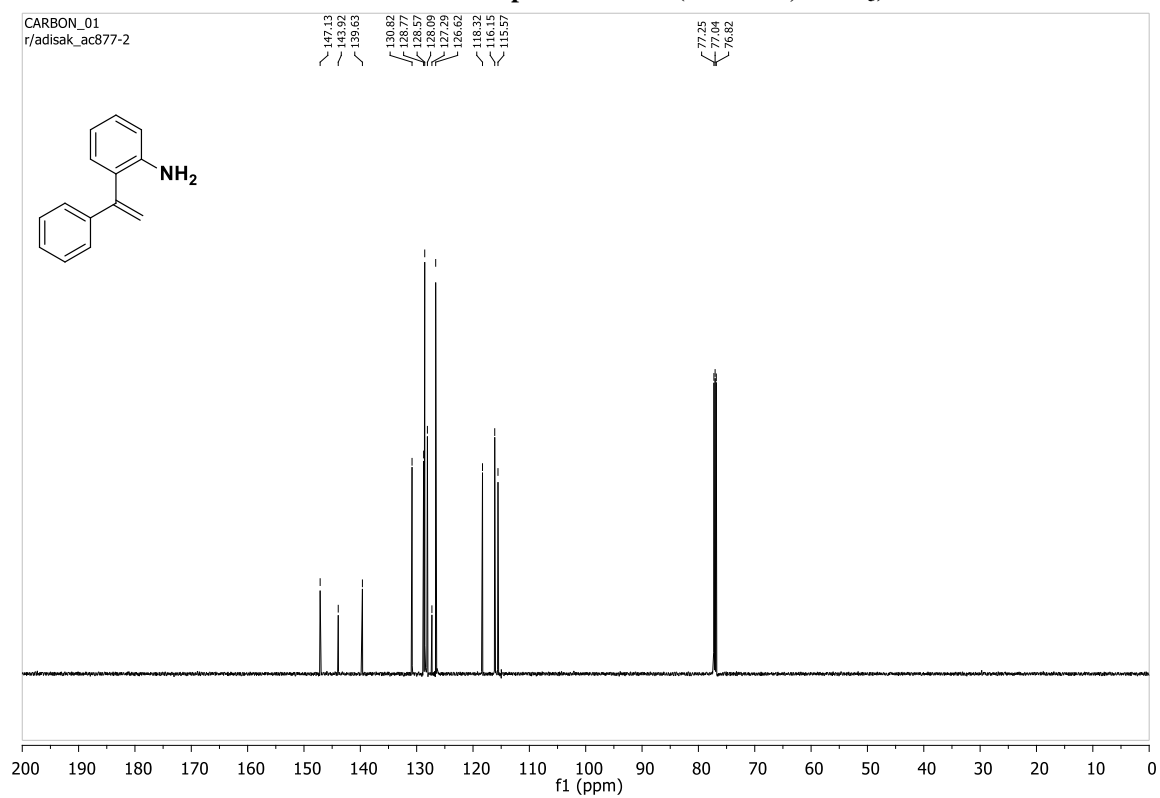
- (1) Mamede, N.; Peraka, S.; Kodumuri, Srujana.; Chevella, D.; Marri, M. R.; Nama, N. *RSC Adv.* **2015**, *5*, 78374.
- (2) Huang, Y.-N.; Li, Y.-L.; Li, J.; Deng, J. *J. Org. Chem.* **2016**, *81*, 4645.
- (3) Caspers, L. D.; Finkbeiner, P.; Nachtsheim, B. J. *Chem. Eur. J.* **2017**, *23*, 2748.
- (4) Ferguson, J.; Zeng, F.; Alwis, N.; Alper, H. *Org. Lett.* **2013**, *15*, 1998.
- (5) Ni, J.; Jiang, Y.; An, Z.; Yan, R. *Org. Lett.* **2018**, *20*, 1534.
- (6) Ghorai, J.; Reddy, A. C. S.; Anbarasan, P. *Chem. Eur. J.* **2016**, *22*, 16042.

6. ^1H and ^{13}C -NMR Spectra of compounds 3a-3ah

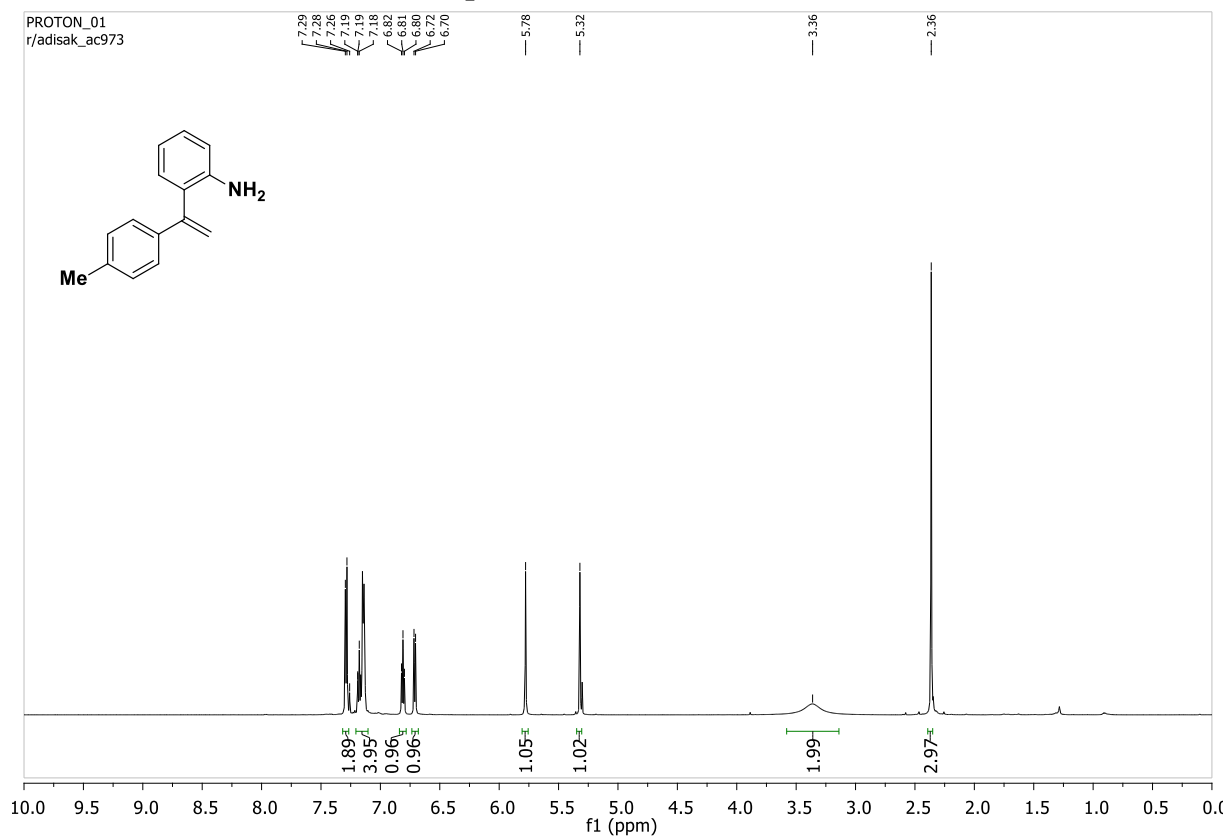
^1H NMR Spectrum of 3a (600 MHz, CDCl_3)



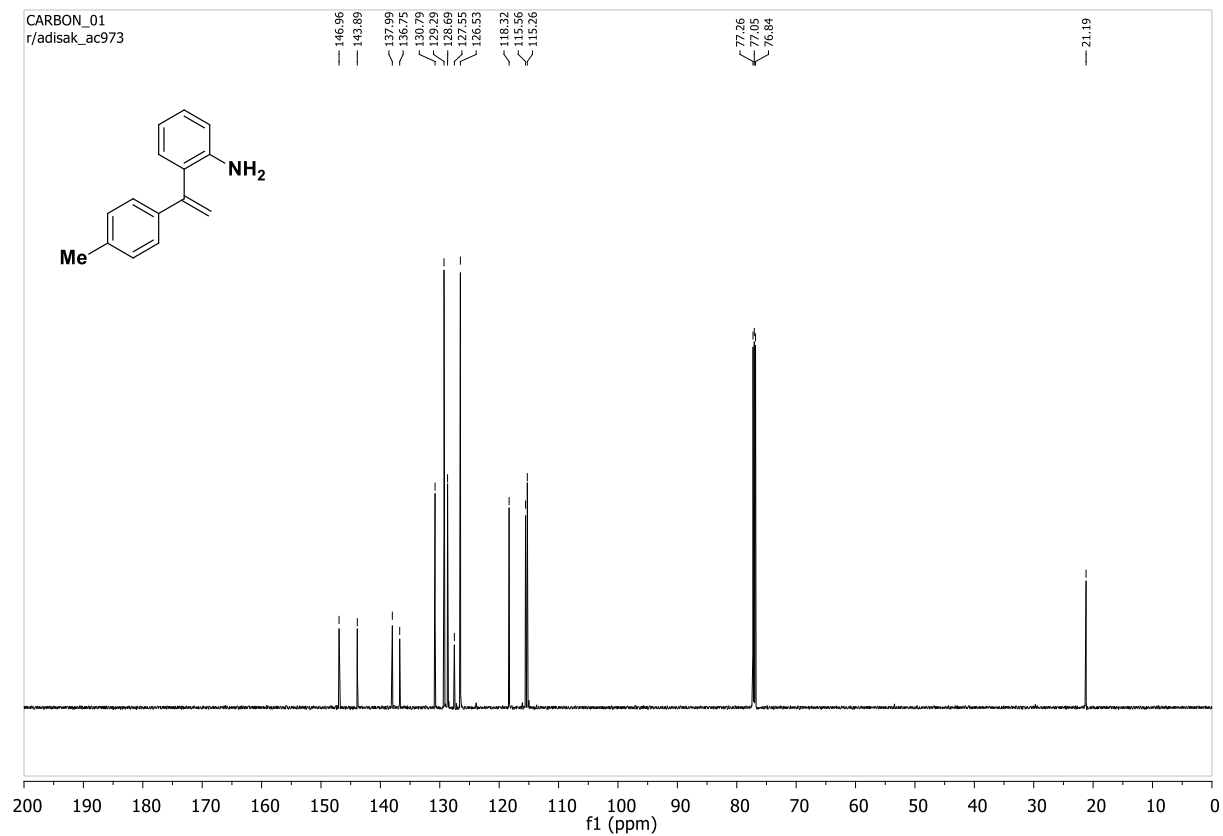
^{13}C NMR Spectrum of 3a (151 MHz, CDCl_3)



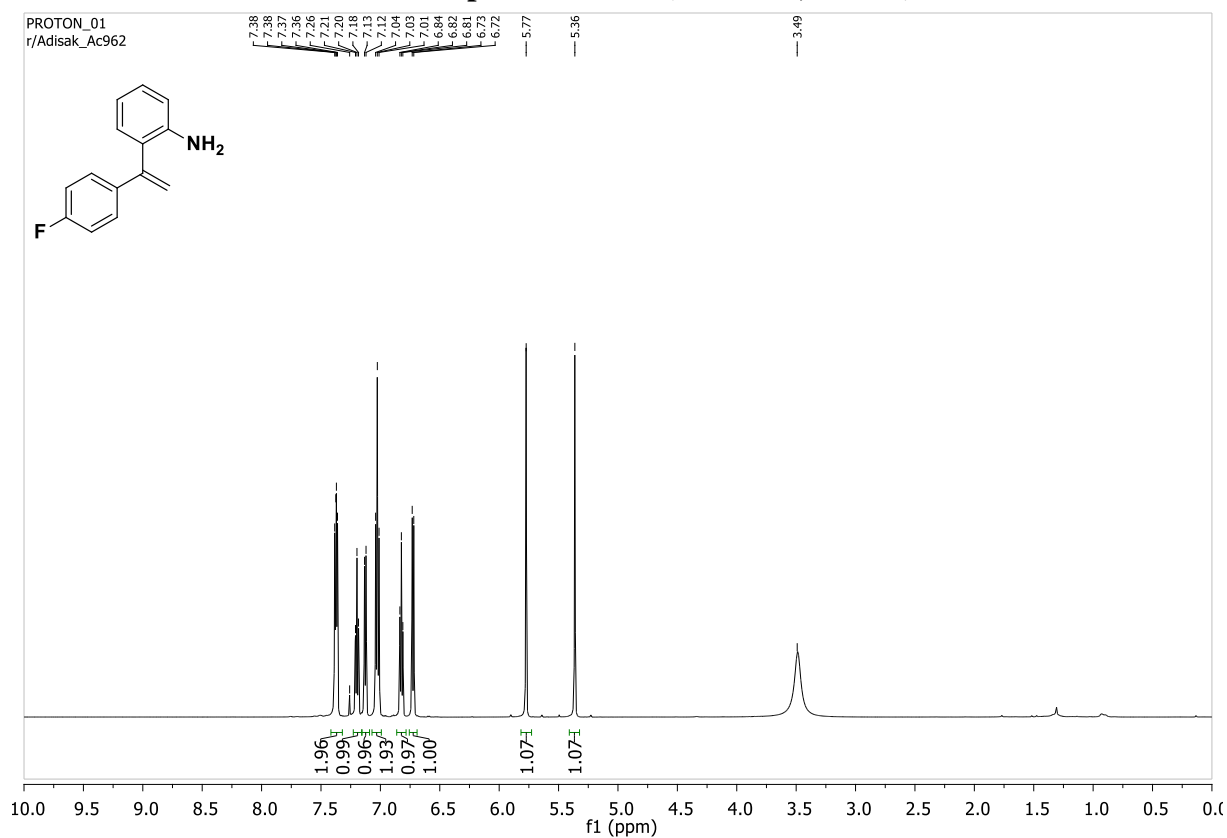
¹H NMR Spectrum of 3b (600 MHz, CDCl₃)



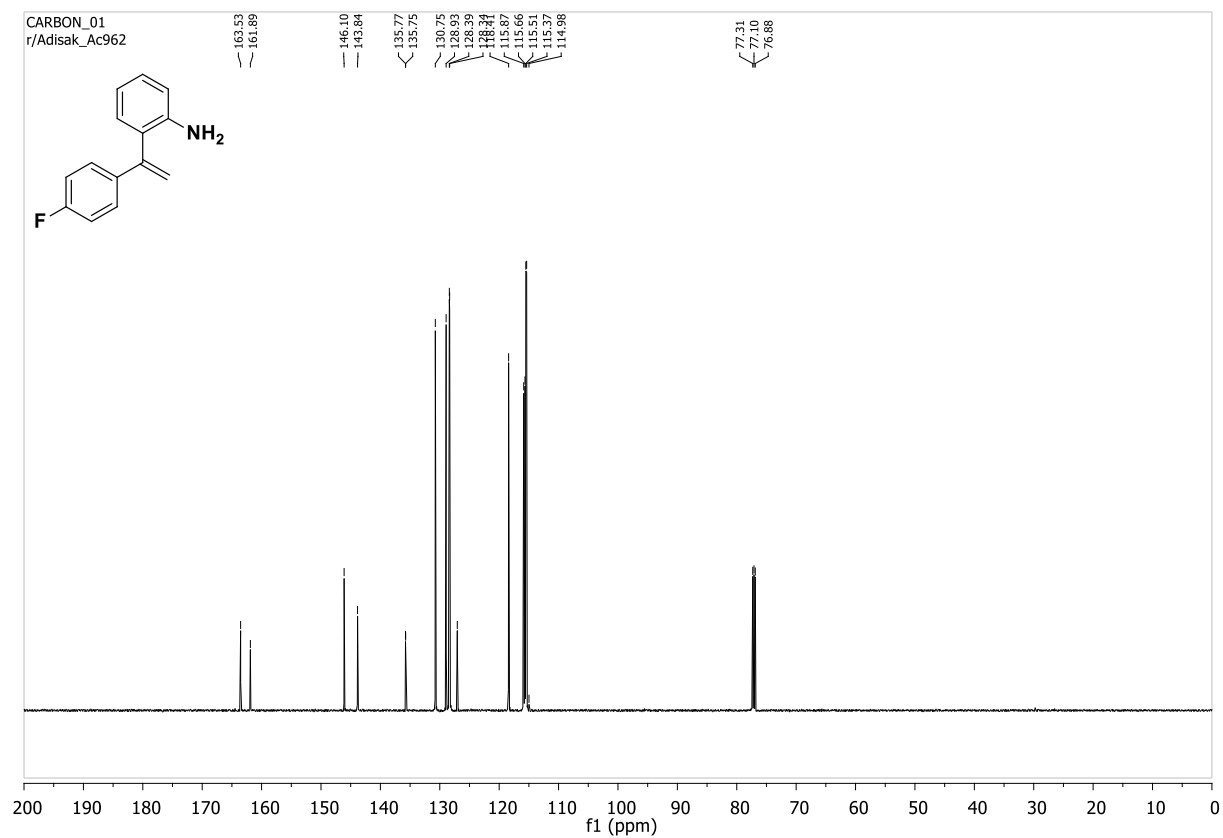
¹³C NMR Spectrum of 3b (151 MHz, CDCl₃)



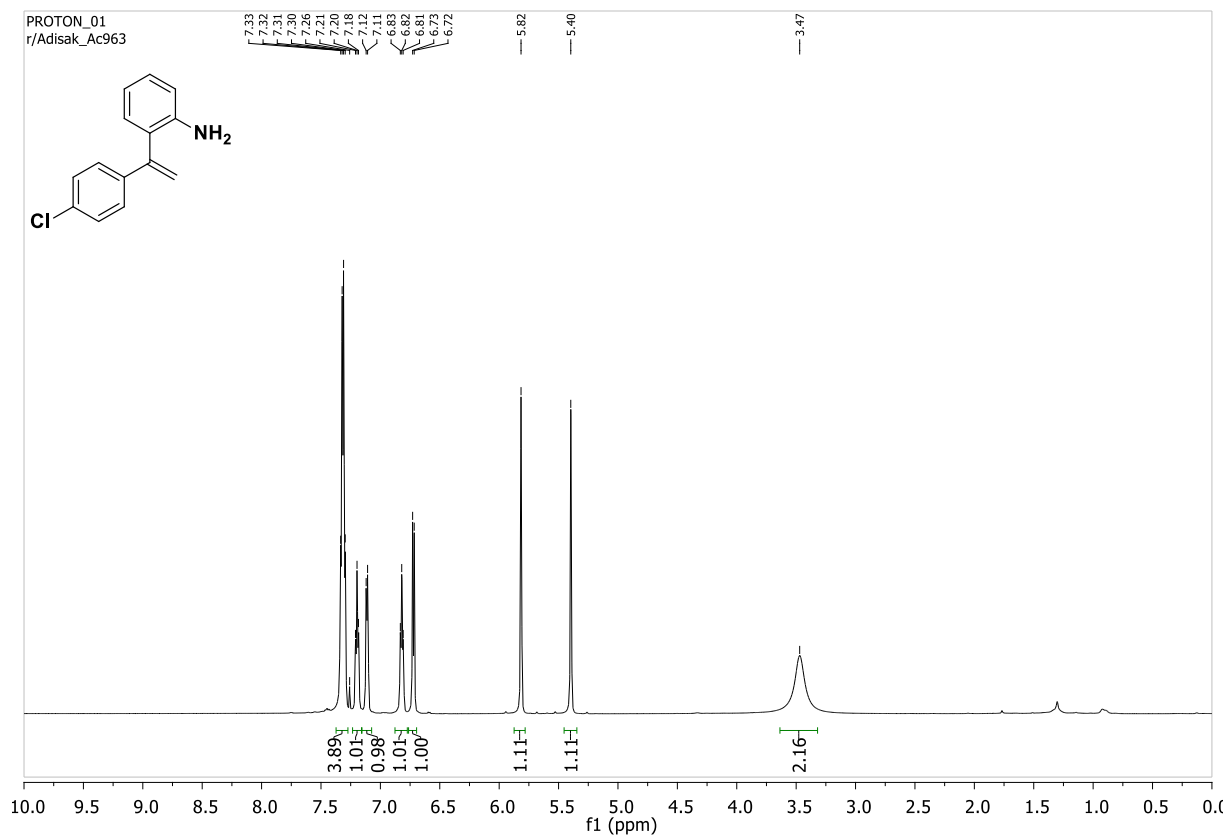
¹H NMR Spectrum of 3c (600 MHz, CDCl₃)



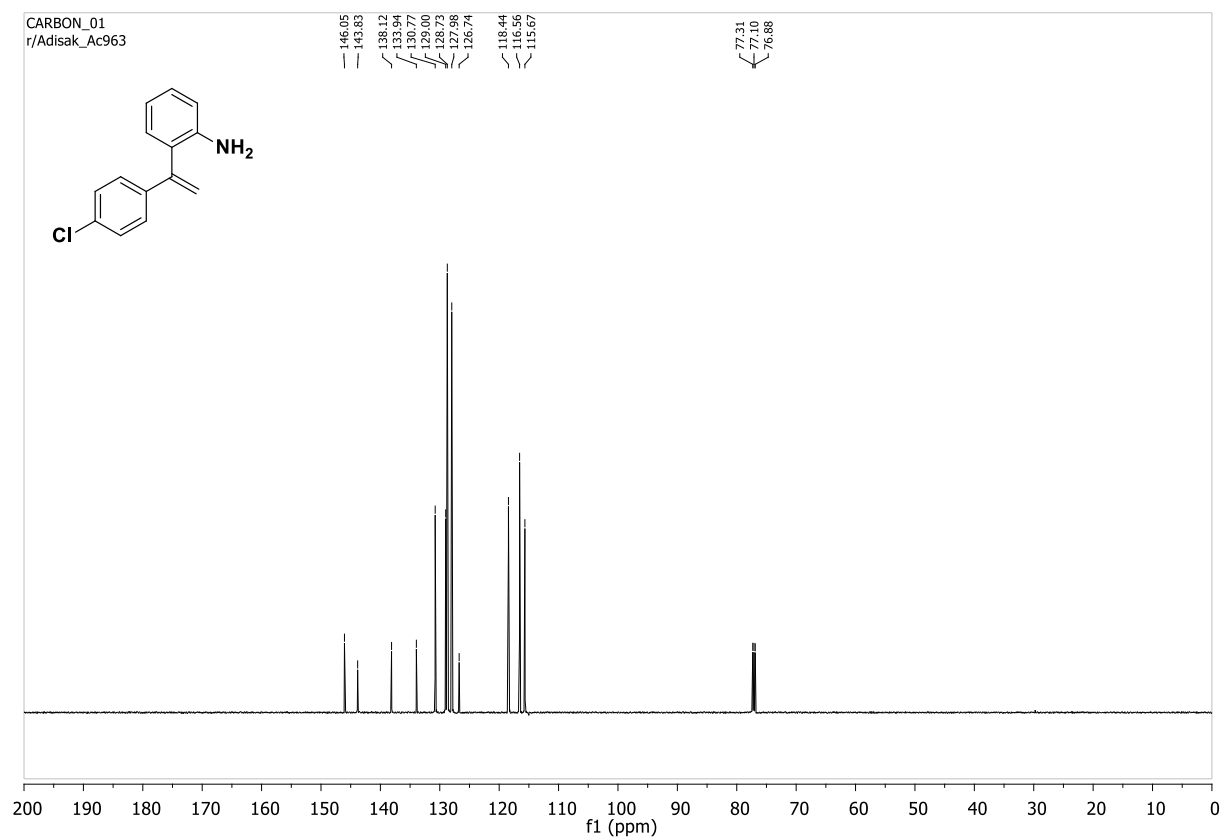
¹³C NMR Spectrum of 3c (151 MHz, CDCl₃)



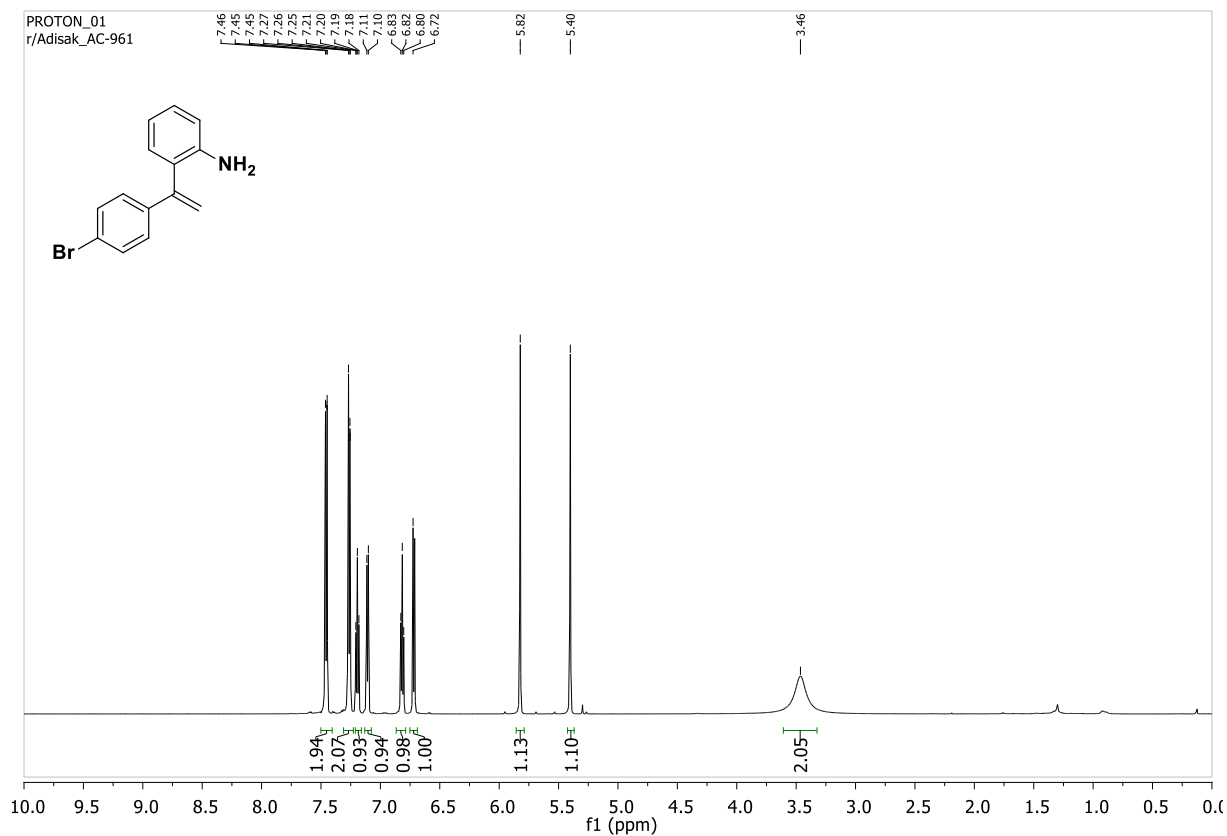
¹H NMR Spectrum of 3d (600 MHz, CDCl₃)



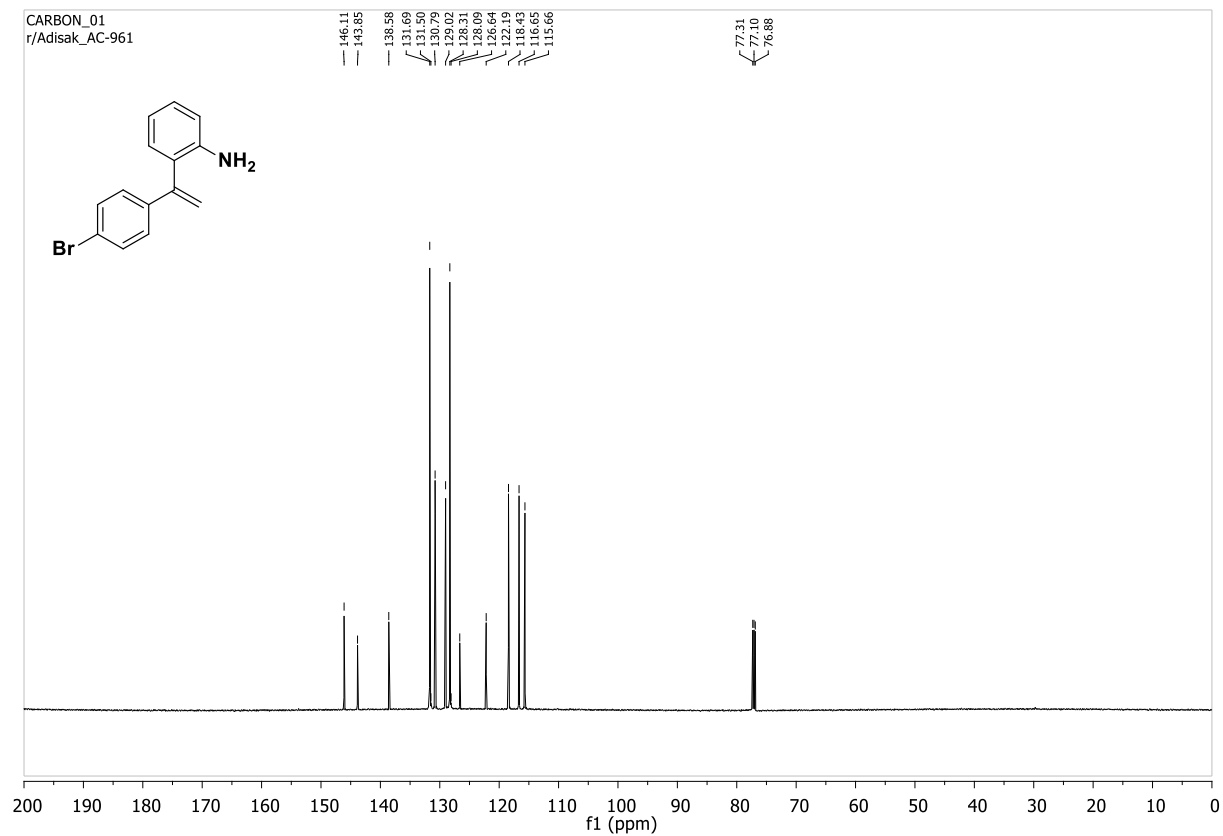
¹³C NMR Spectrum of 3d (151 MHz, CDCl₃)



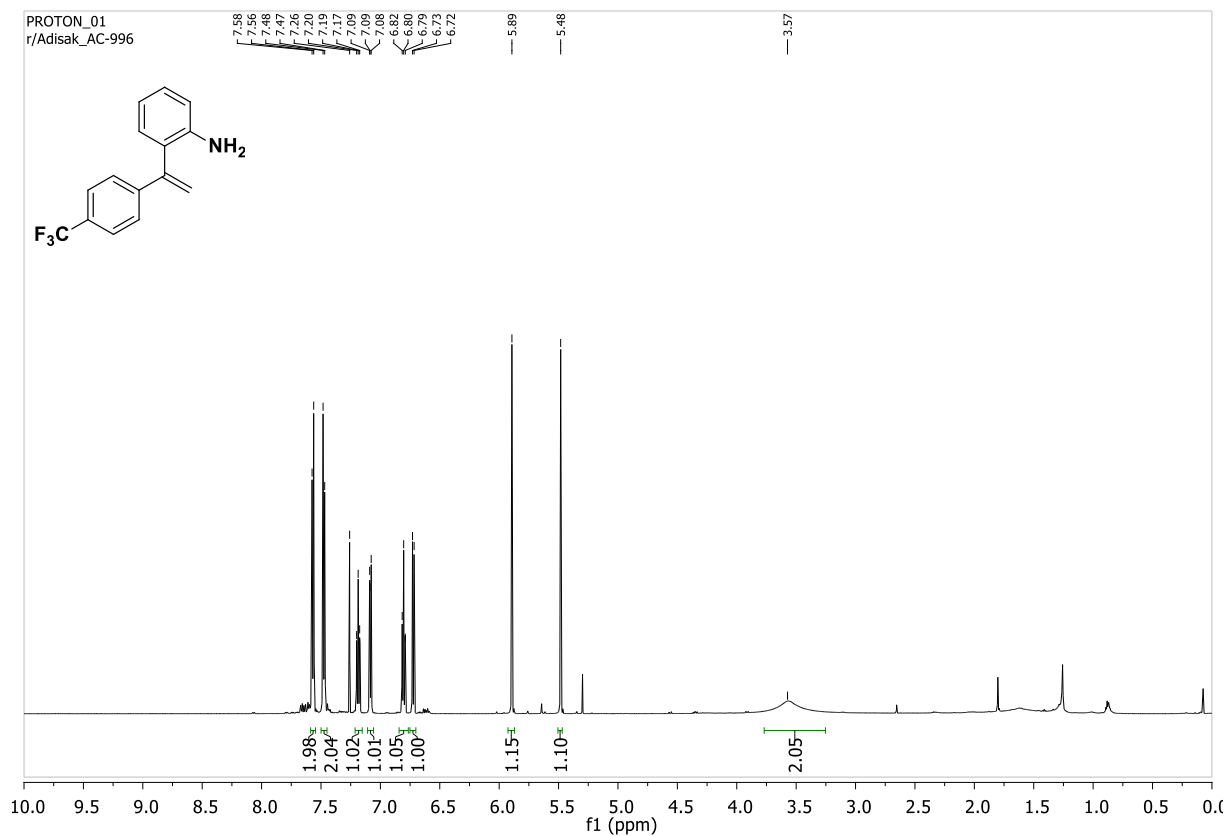
¹H NMR Spectrum of 3e (600 MHz, CDCl₃)



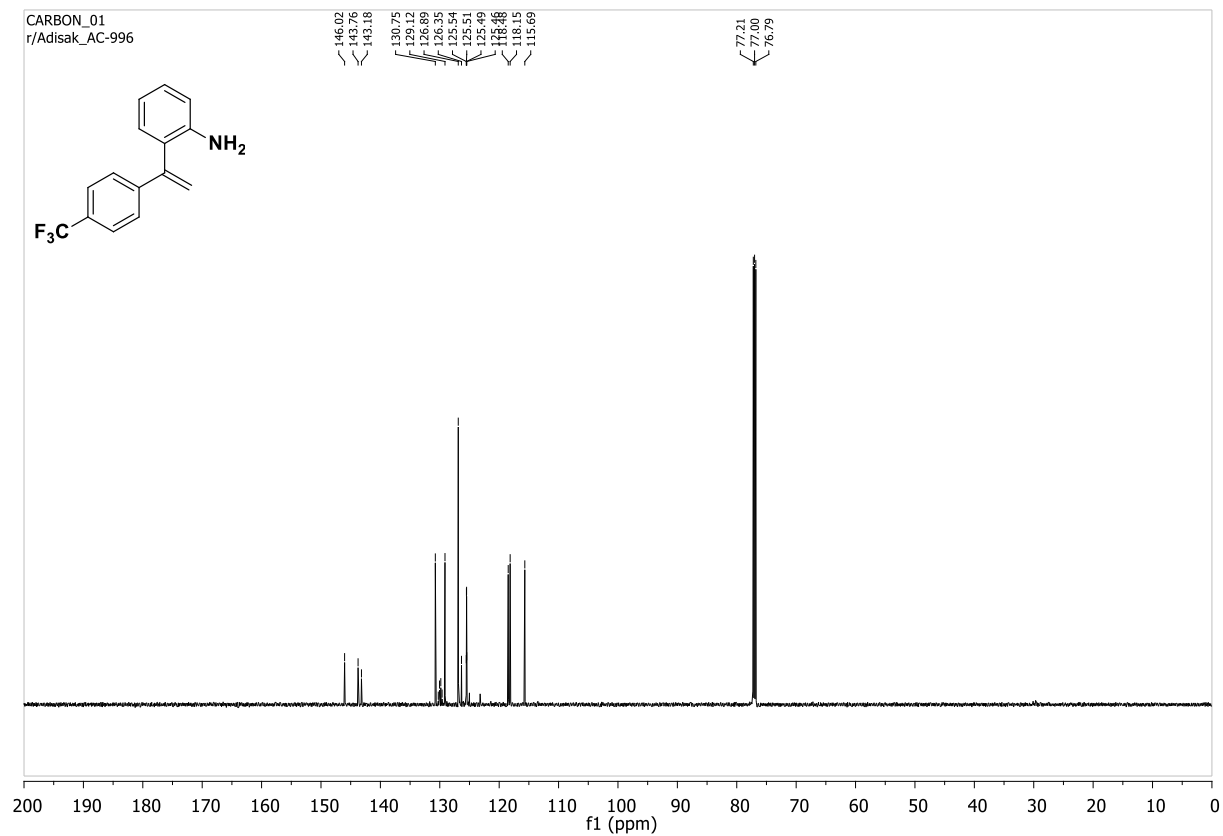
¹³C NMR Spectrum of 3e (151 MHz, CDCl₃)



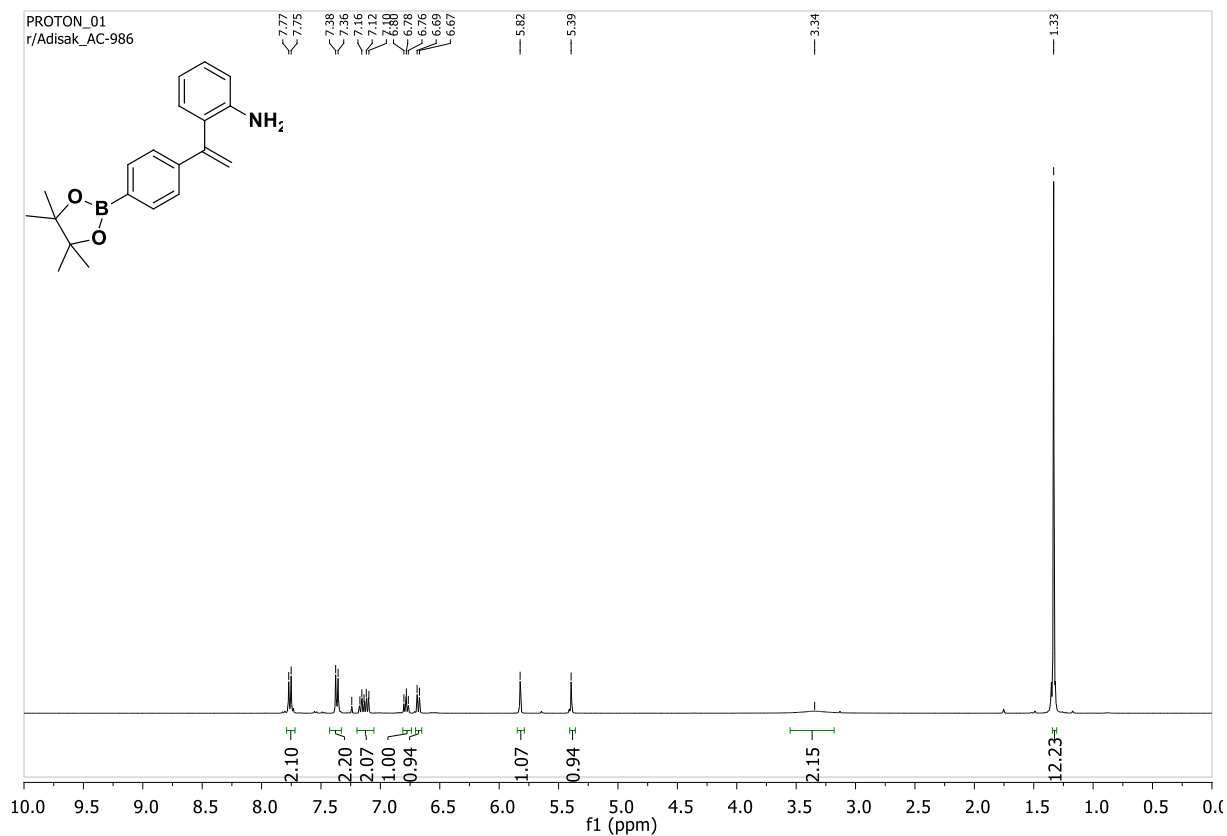
¹H NMR Spectrum of 3f (600 MHz, CDCl₃)



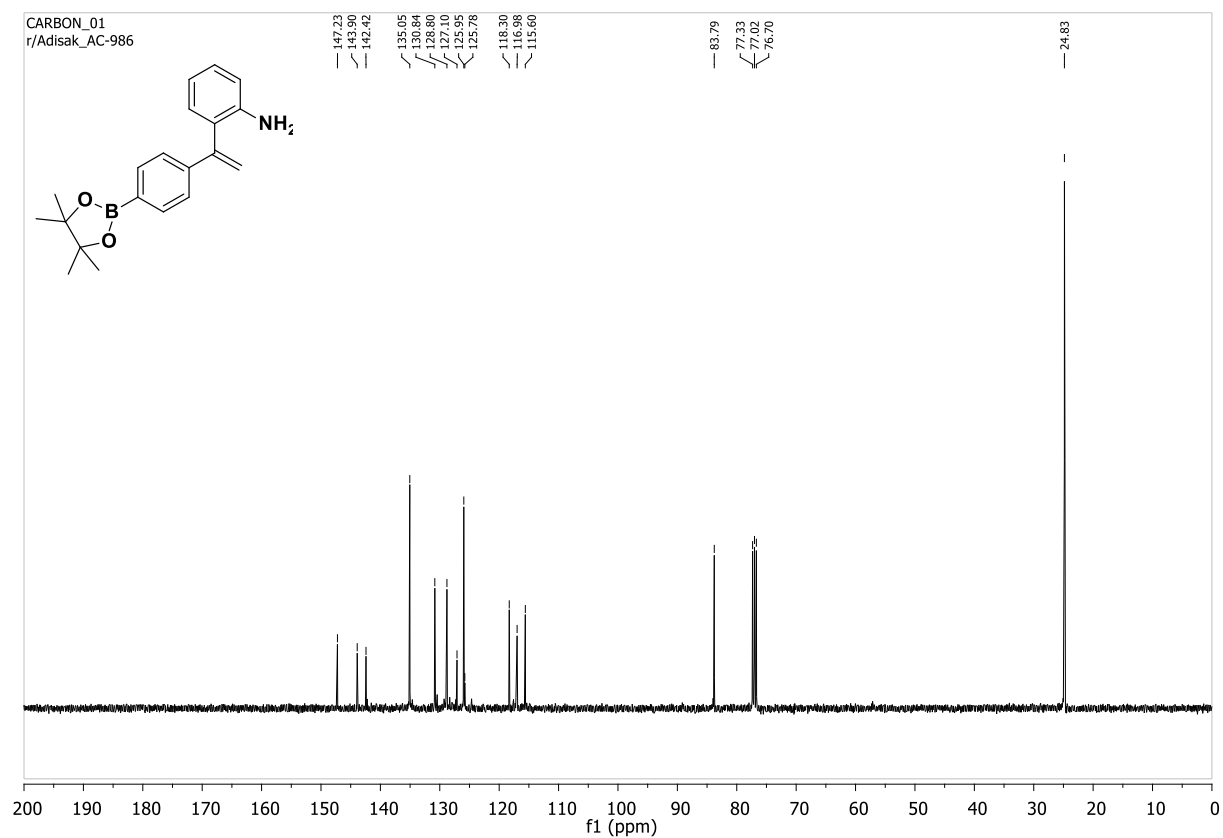
¹³C NMR Spectrum of 3f (151 MHz, CDCl₃)



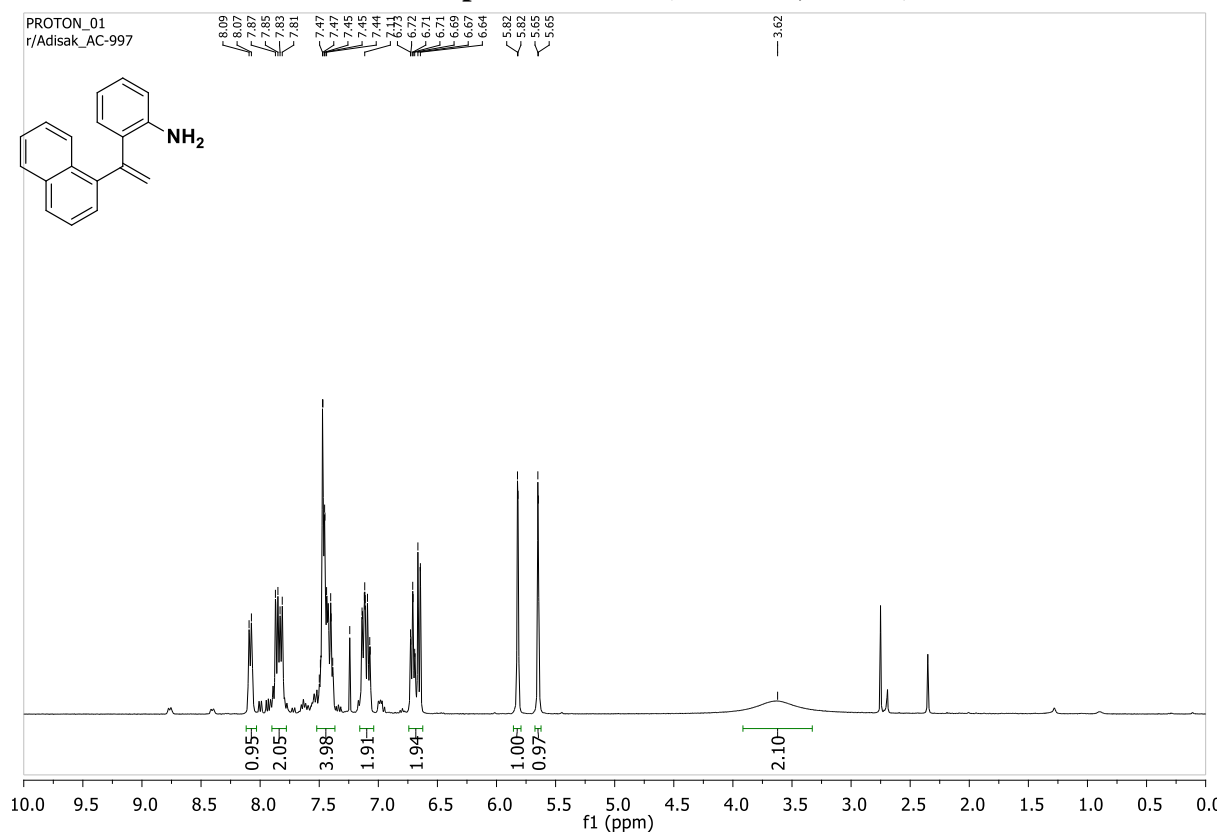
¹H NMR Spectrum of 3g (400 MHz, CDCl₃)



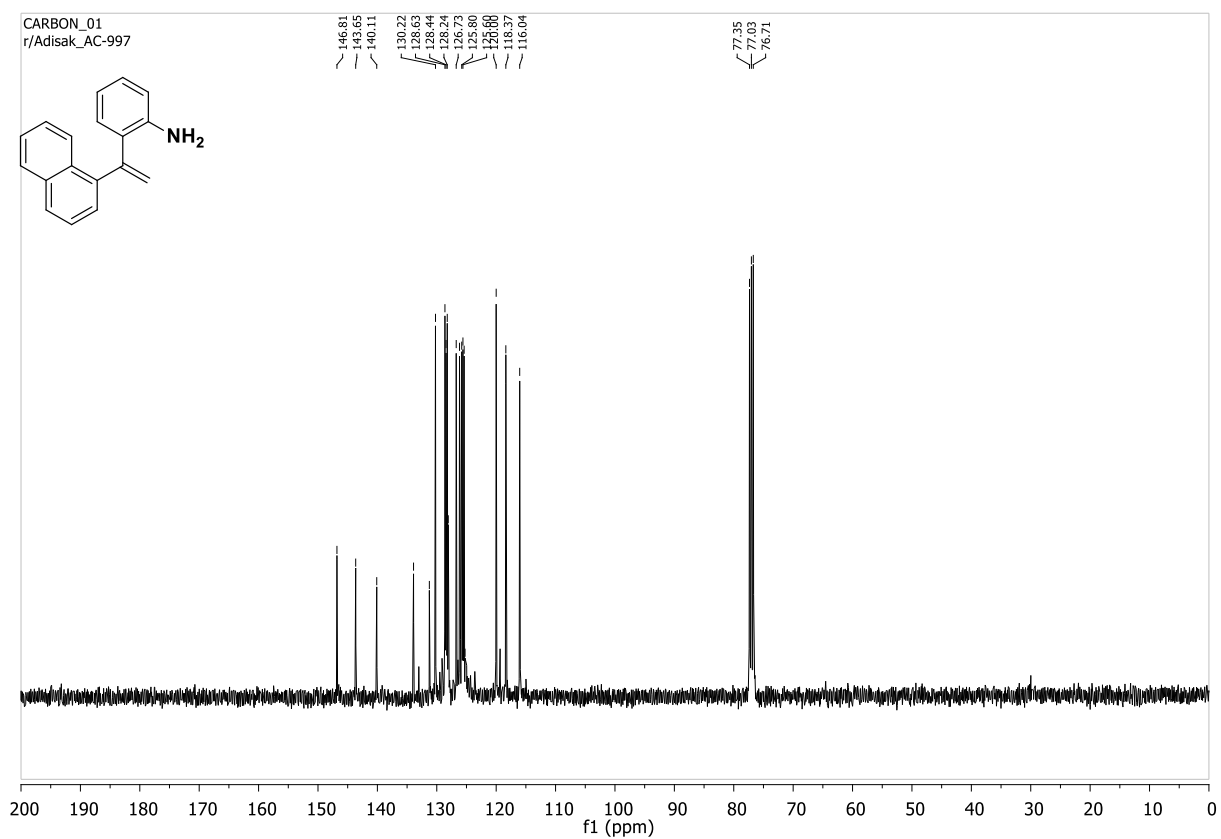
¹³C NMR Spectrum of 3g (100 MHz, CDCl₃)



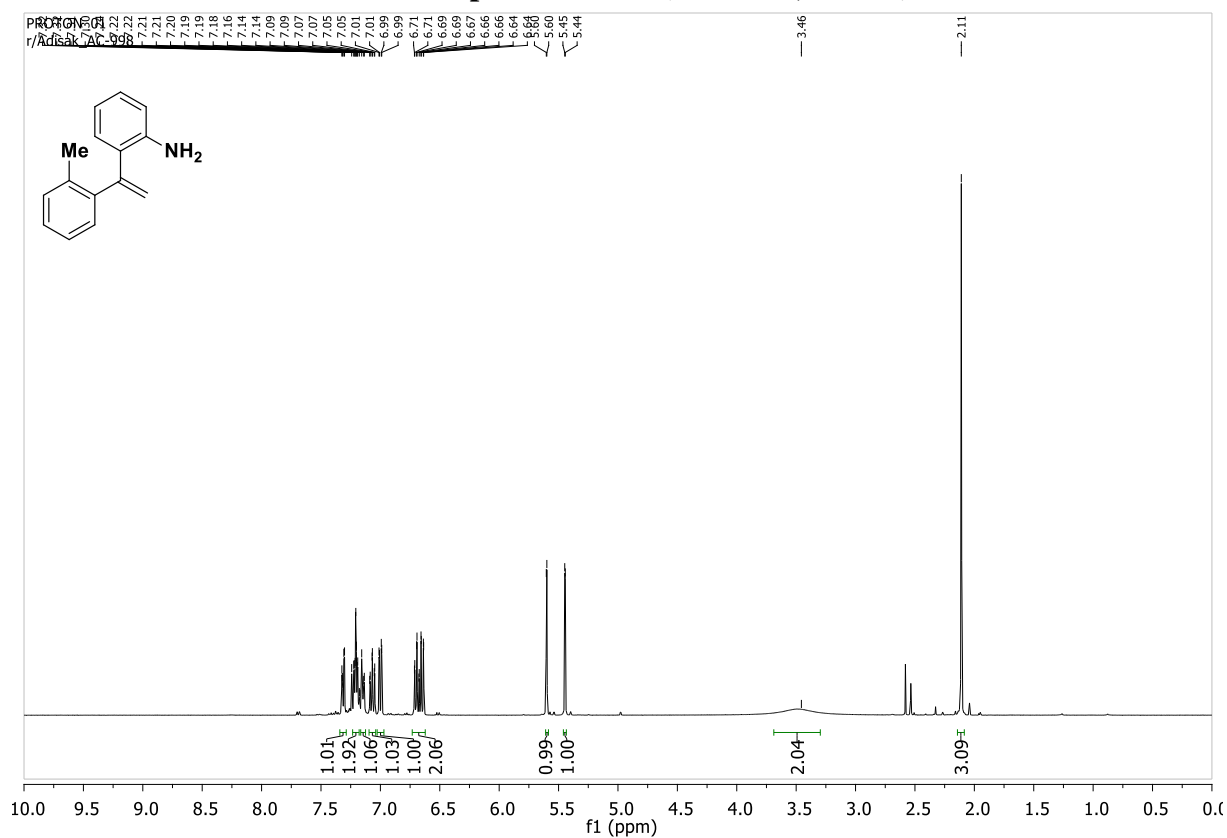
¹H NMR Spectrum of 3h (400 MHz, CDCl₃)



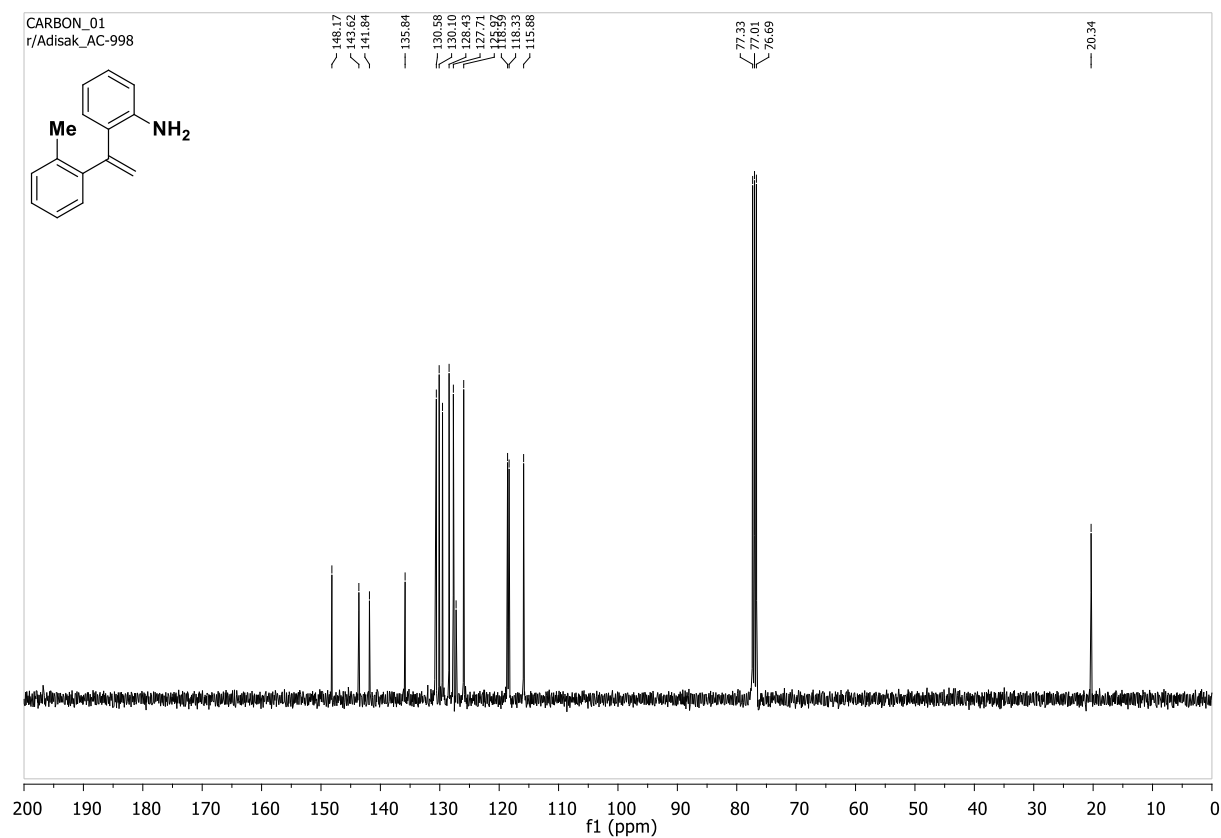
¹³C NMR Spectrum of 3h (101 MHz, CDCl₃)



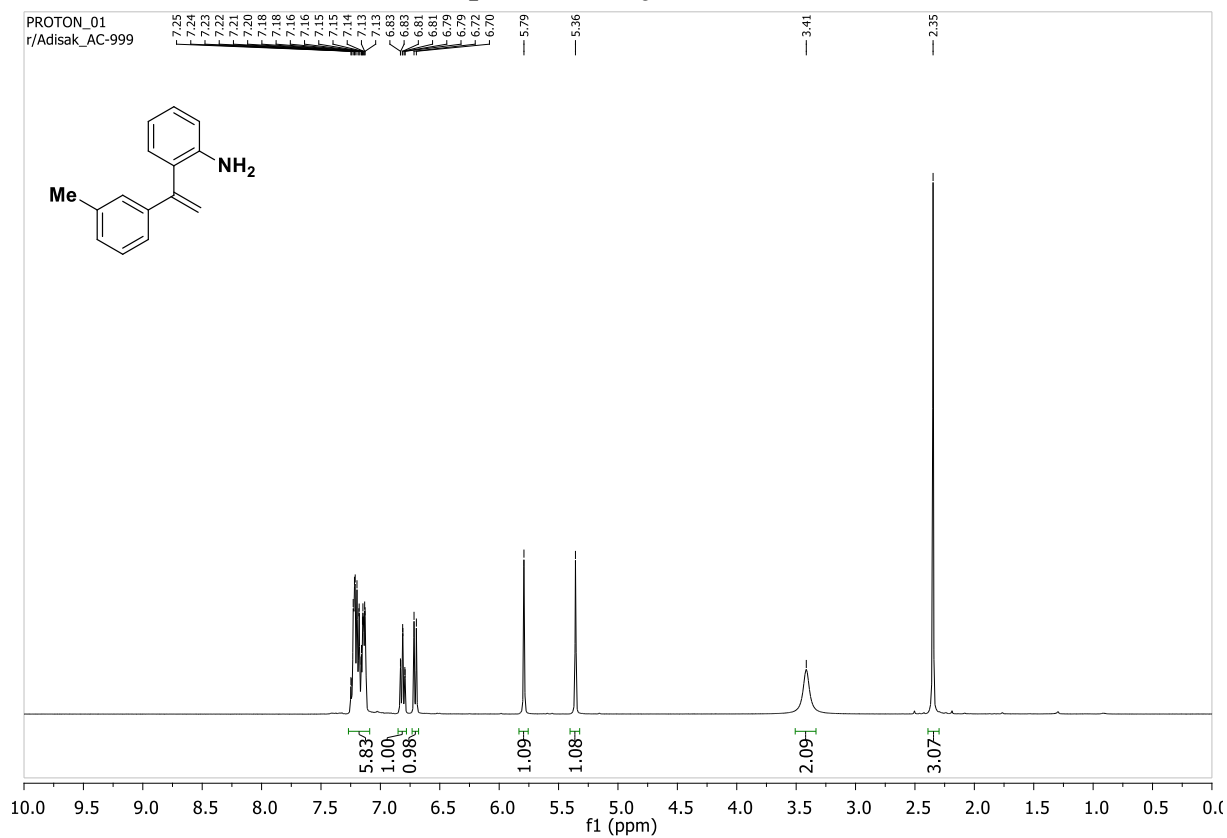
¹H NMR Spectrum of 3i (400 MHz, CDCl₃)



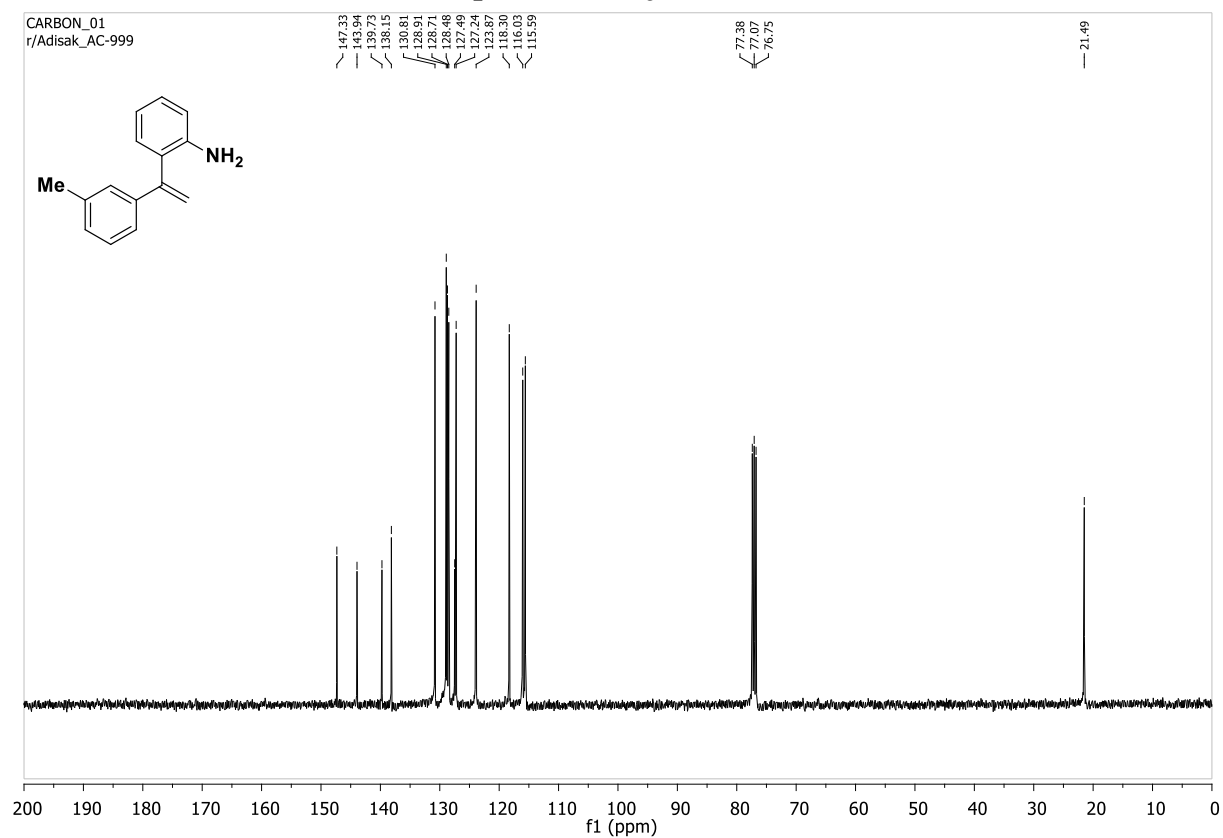
¹³C NMR Spectrum of 3i (101 MHz, CDCl₃)



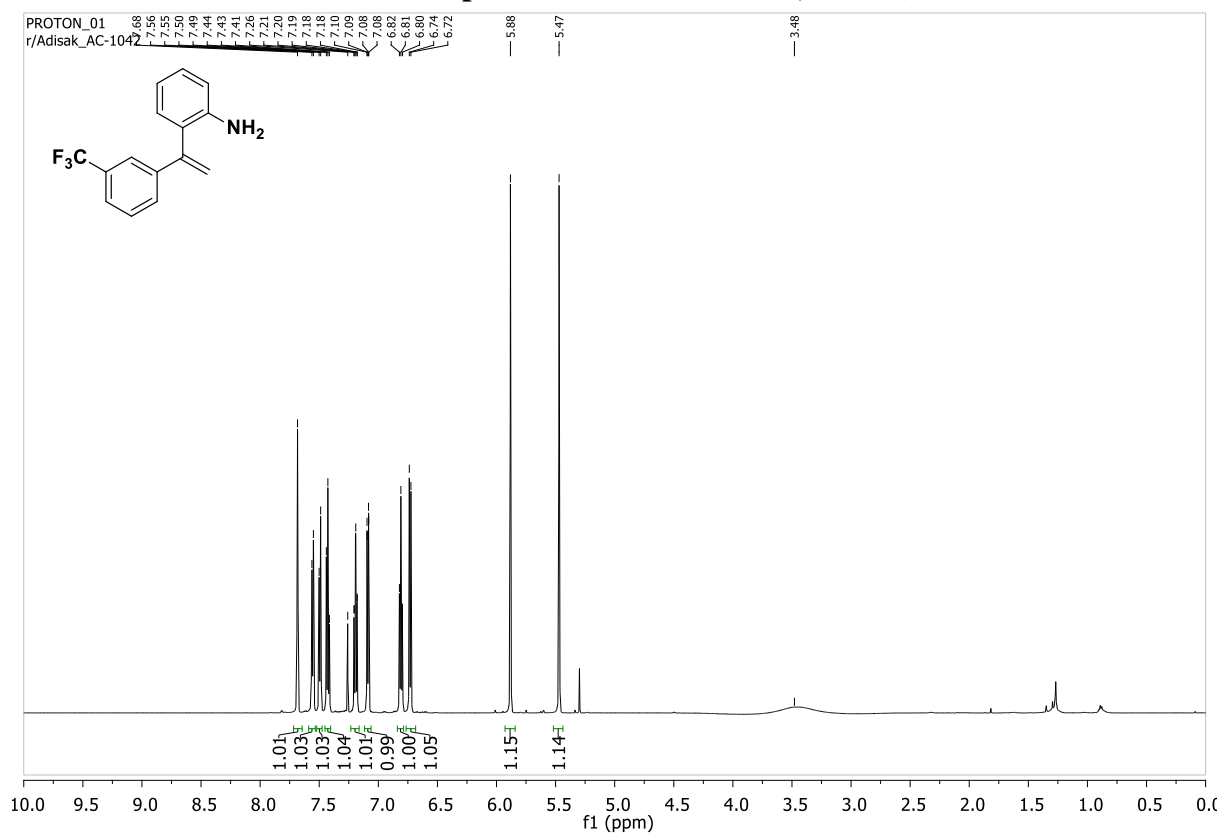
¹H NMR Spectrum of 3j (400 MHz, CDCl₃)



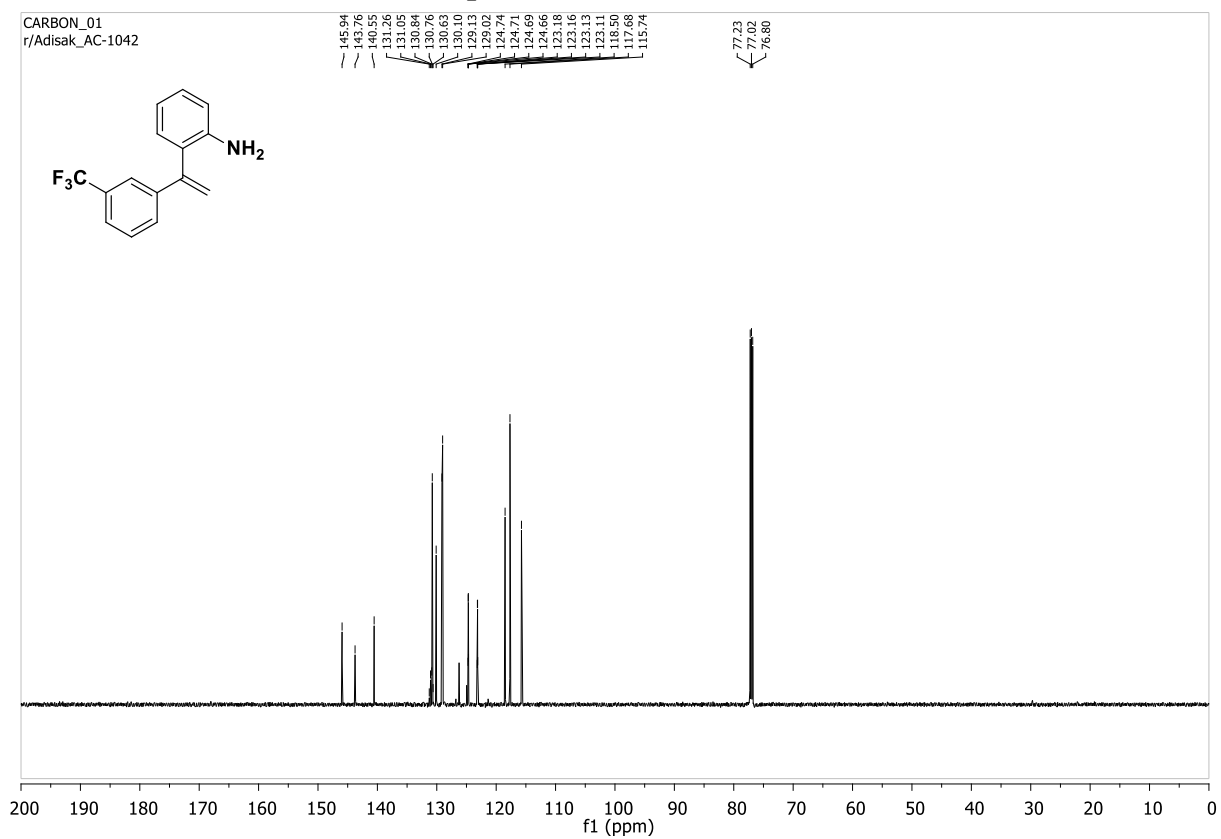
¹³C NMR Spectrum of 3j (101 MHz, CDCl₃)



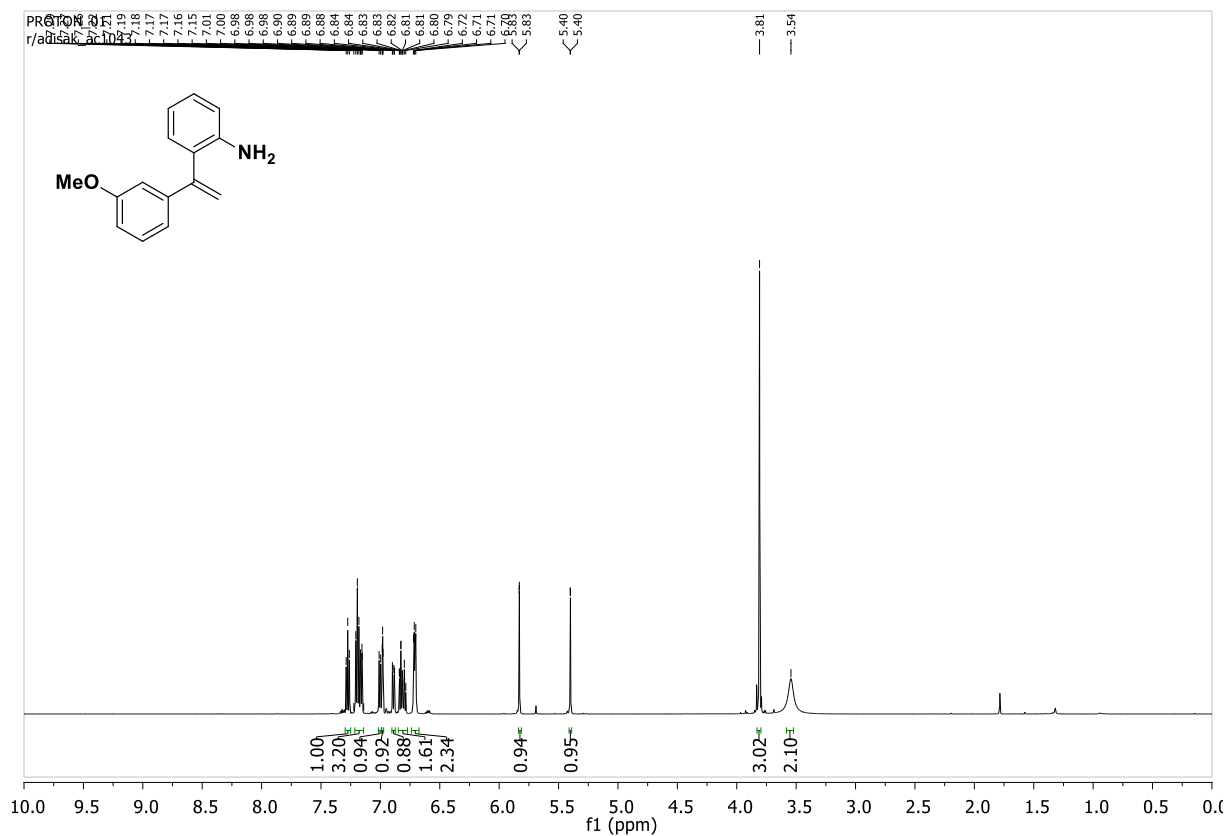
¹H NMR Spectrum of 3k (600 MHz, CDCl₃)



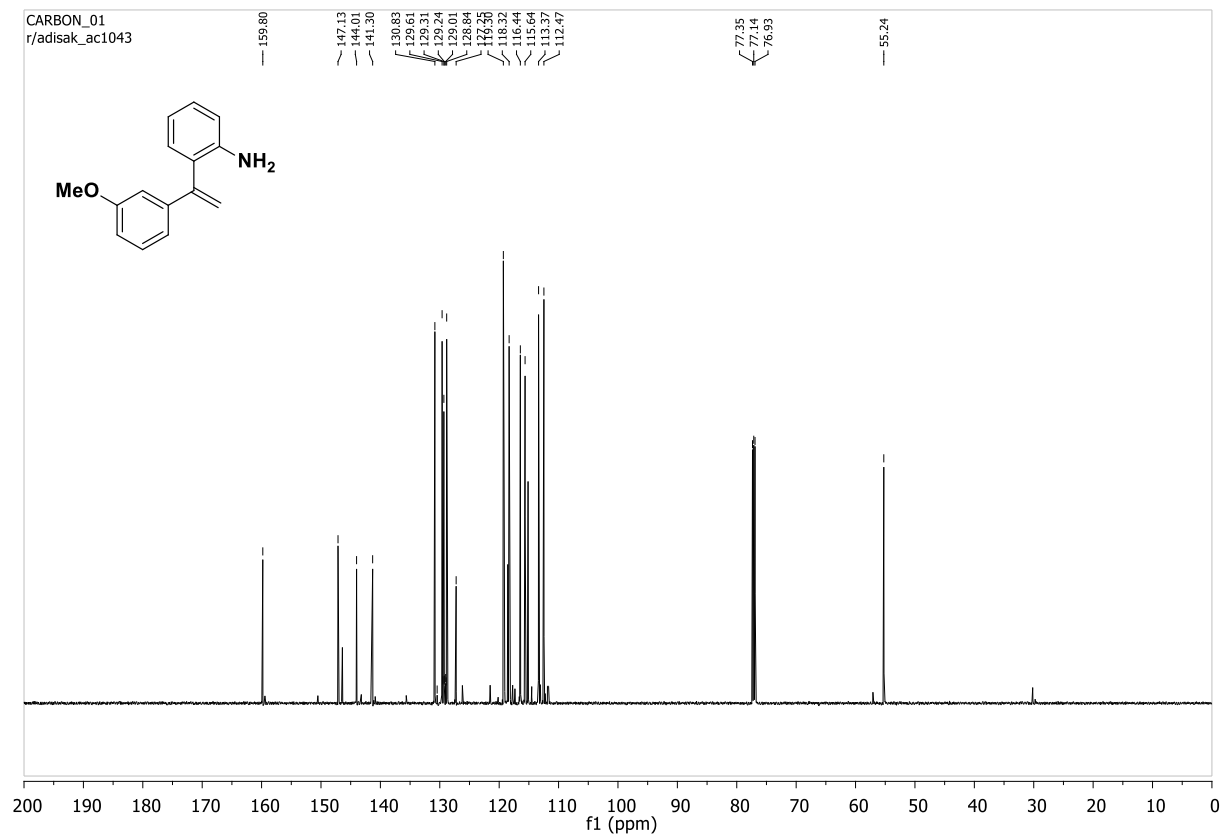
¹³C NMR Spectrum of 3k (151 MHz, CDCl₃)



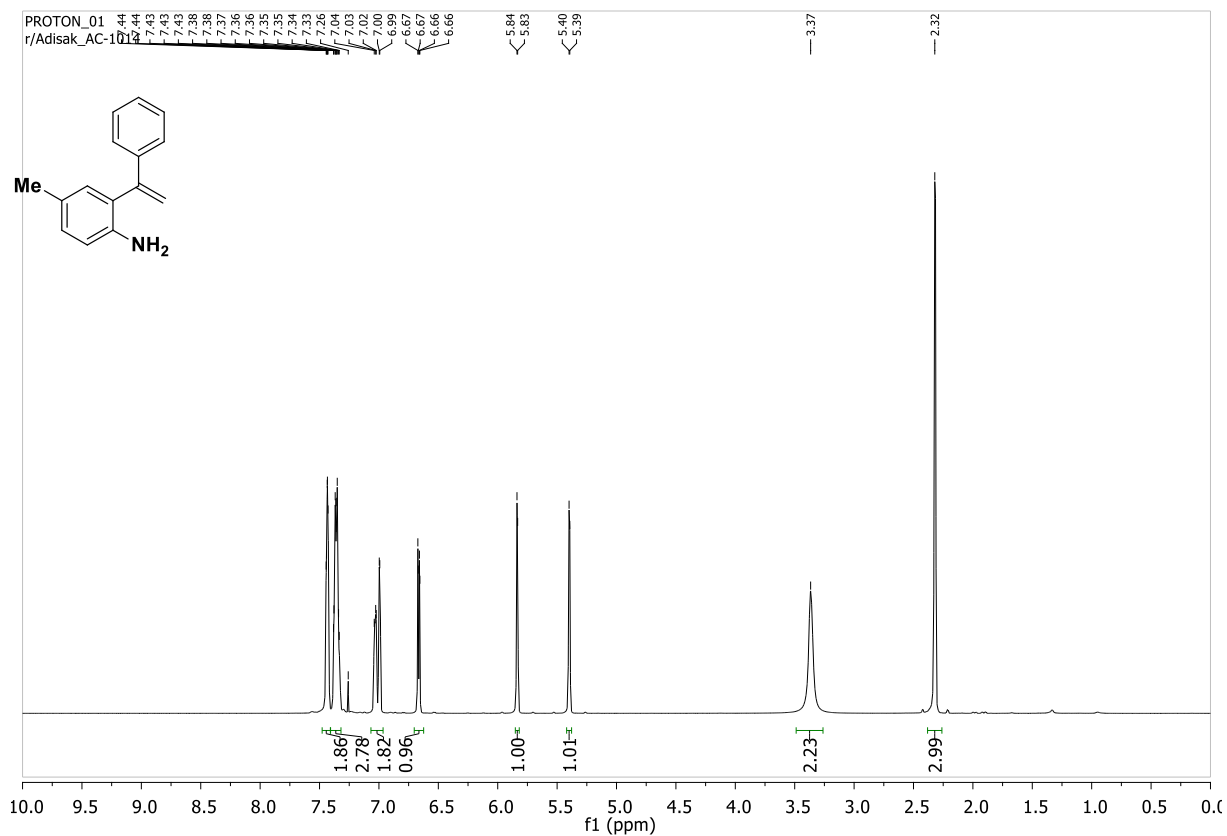
¹H NMR Spectrum of 3l (600 MHz, CDCl₃)



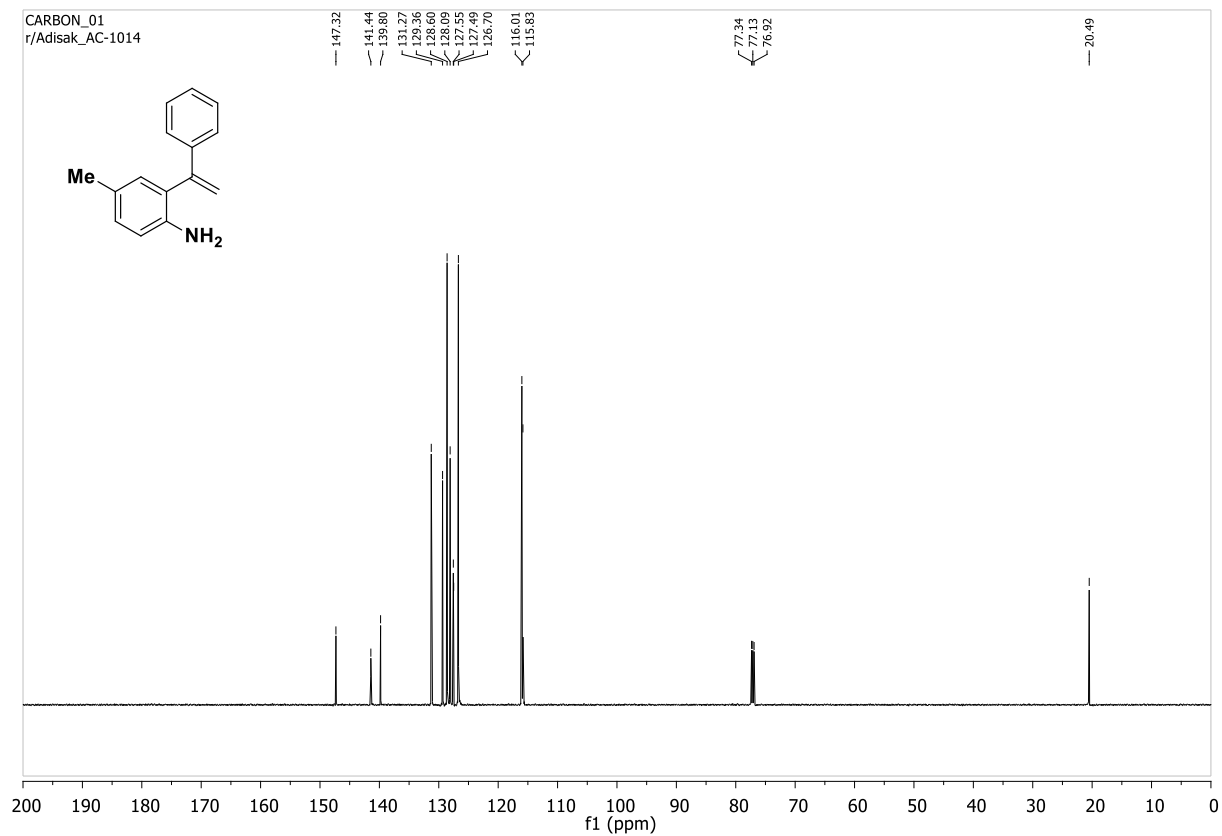
¹³C NMR Spectrum of 3l (151 MHz, CDCl₃)



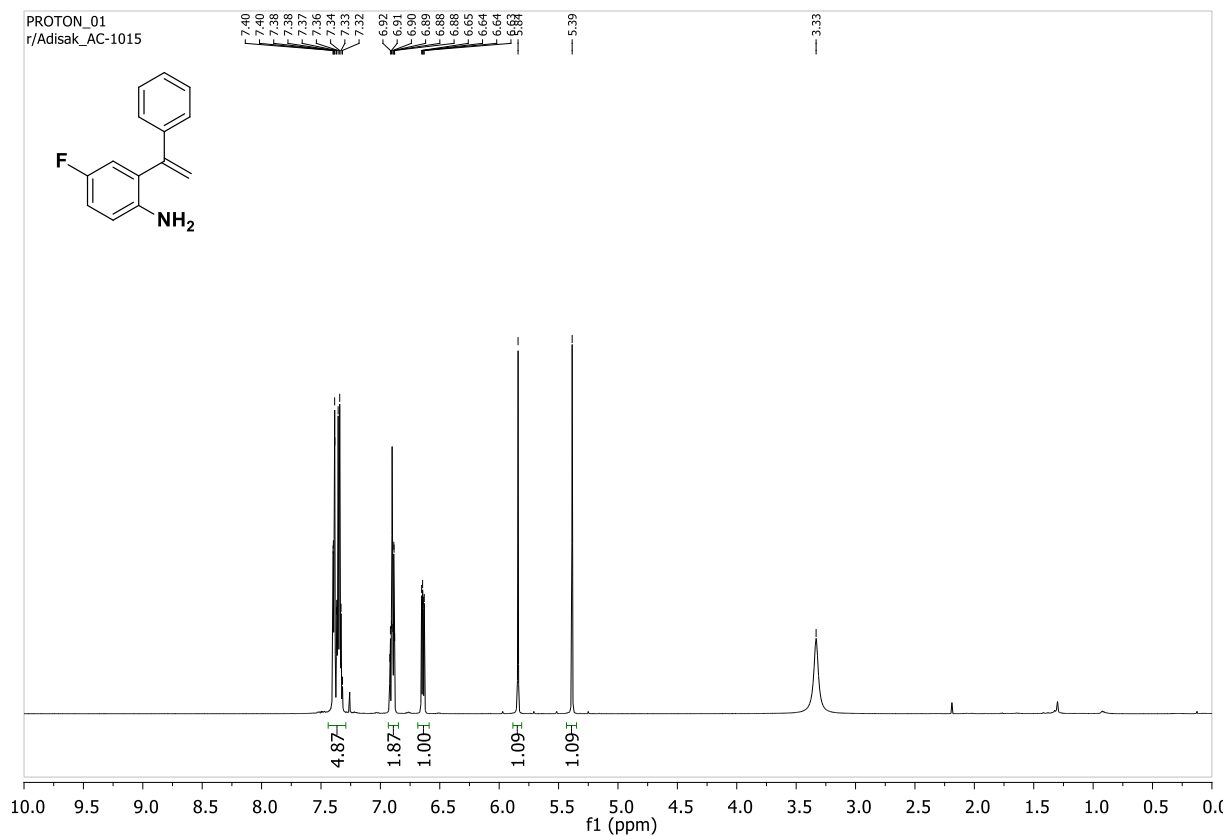
¹H NMR Spectrum of 3m (600 MHz, CDCl₃)



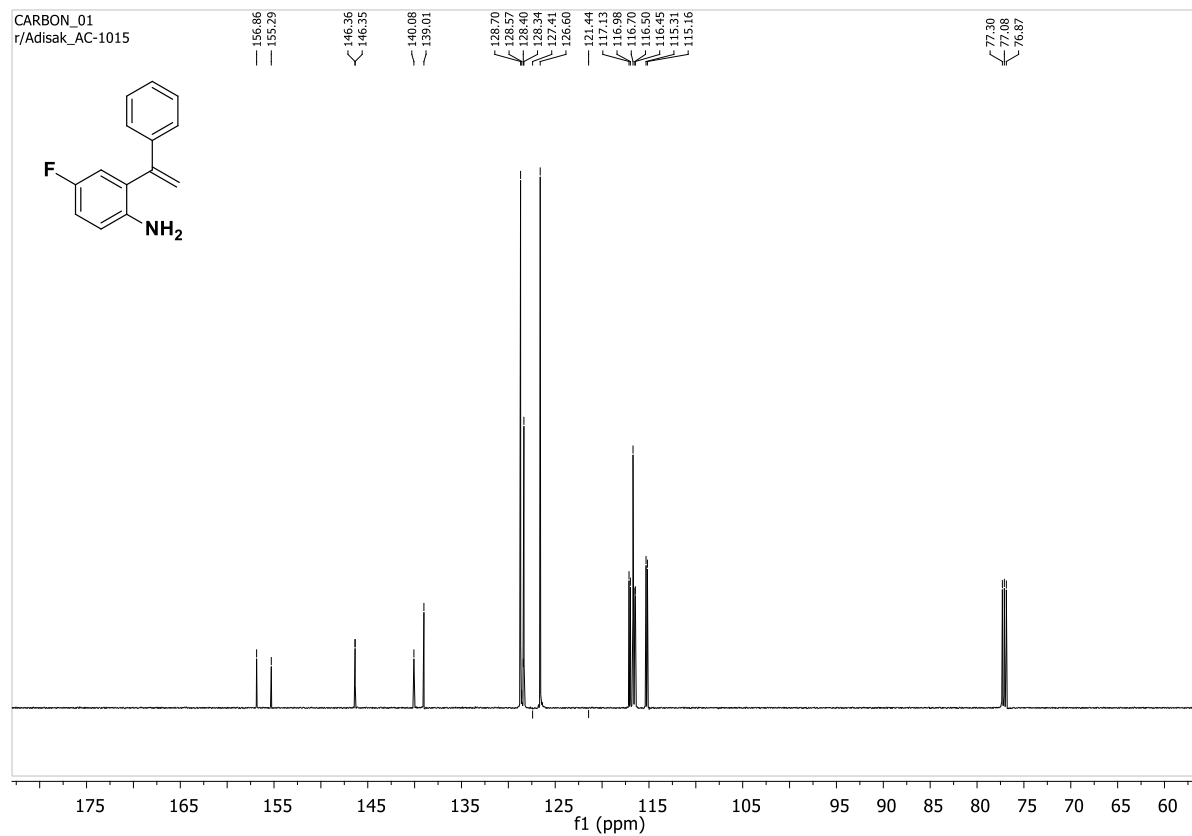
¹³C NMR Spectrum of 3m (151 MHz, CDCl₃)



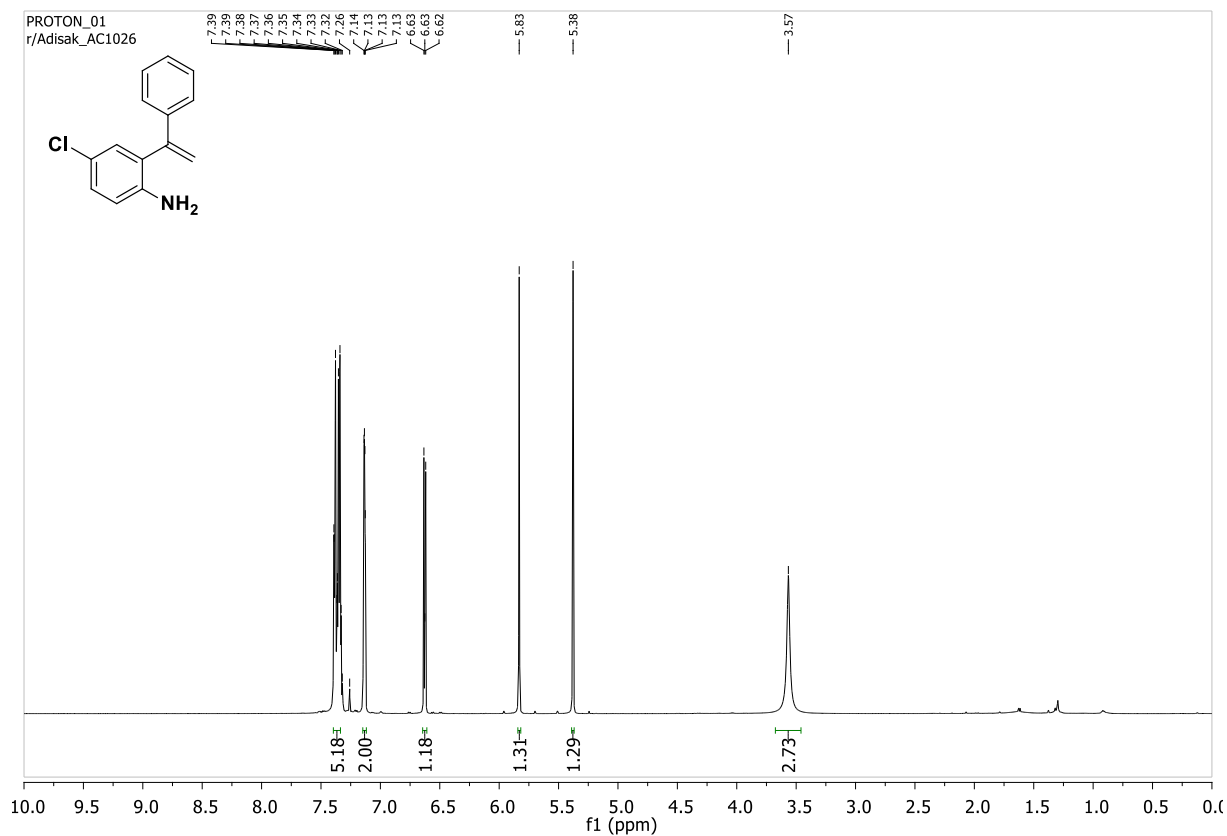
¹H NMR Spectrum of 3n (600 MHz, CDCl₃)



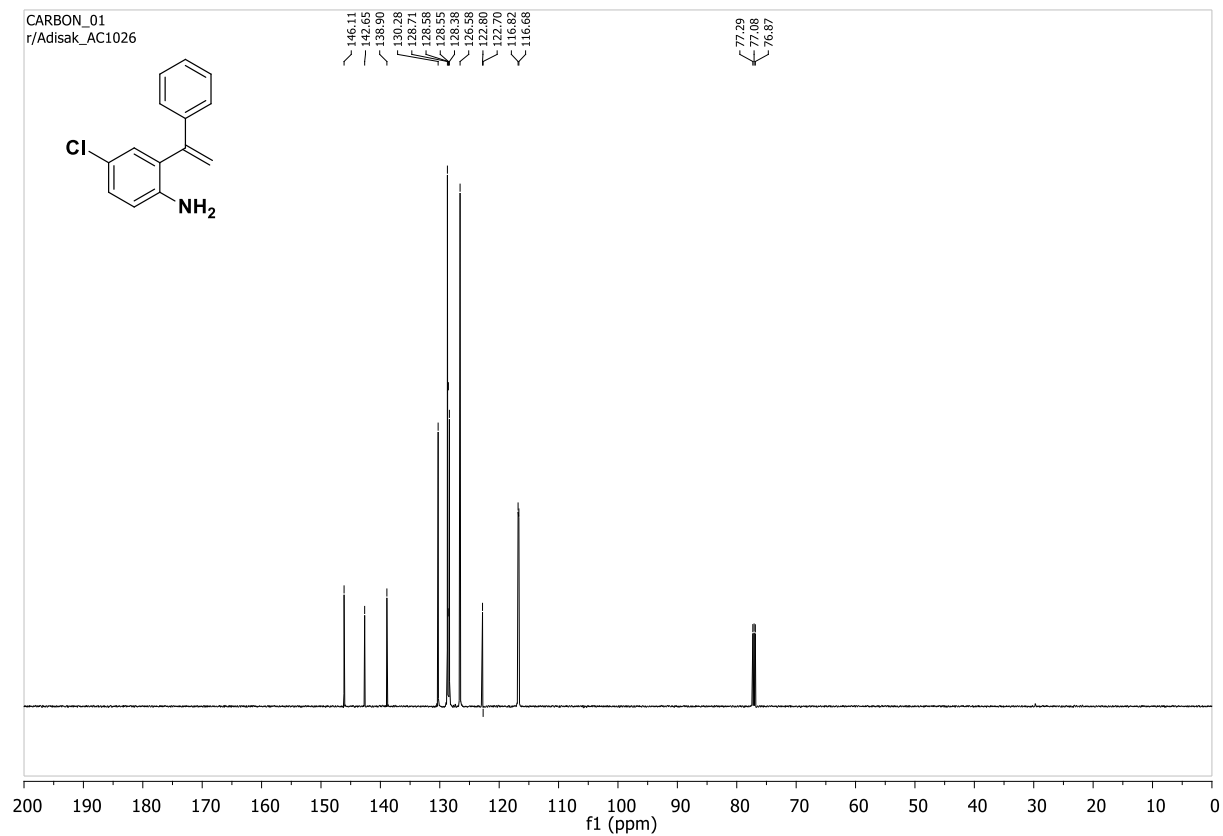
¹³C NMR Spectrum of 3n (151 MHz, CDCl₃)



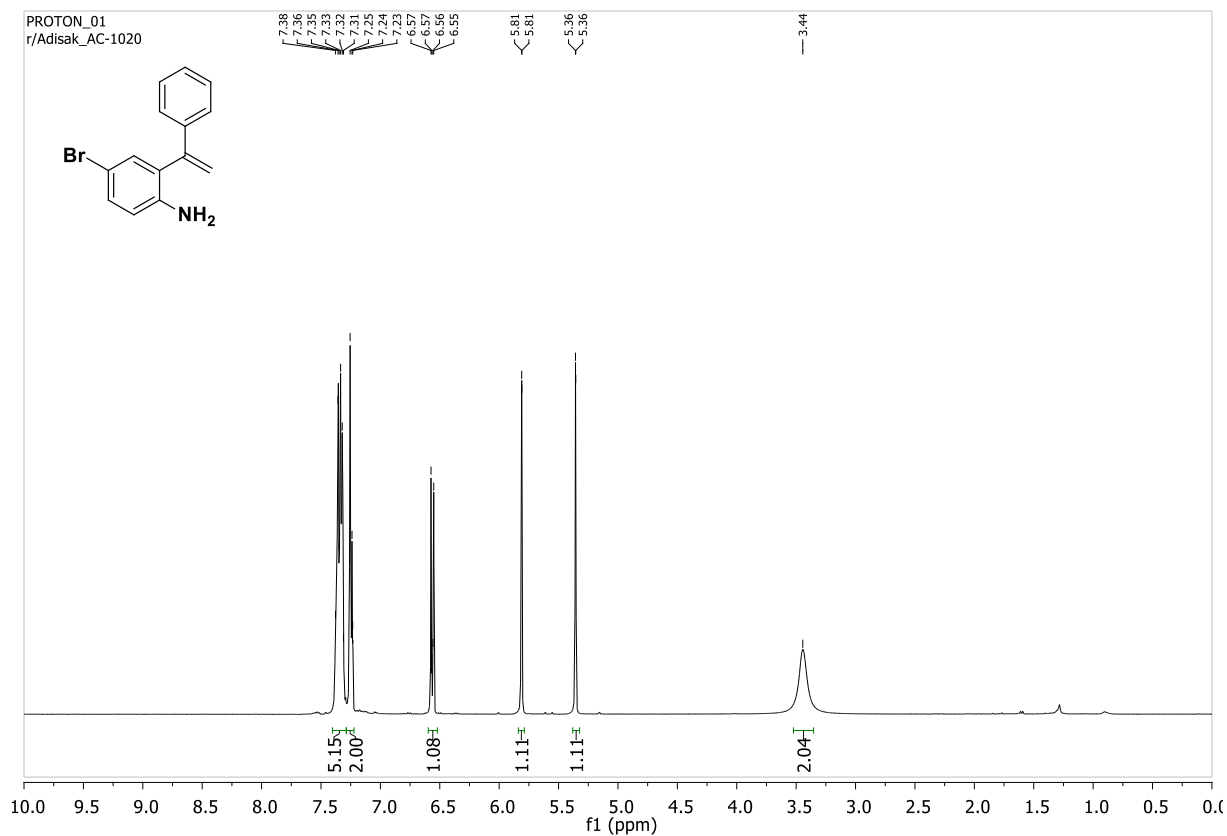
¹H NMR Spectrum of 3o (600 MHz, CDCl₃)



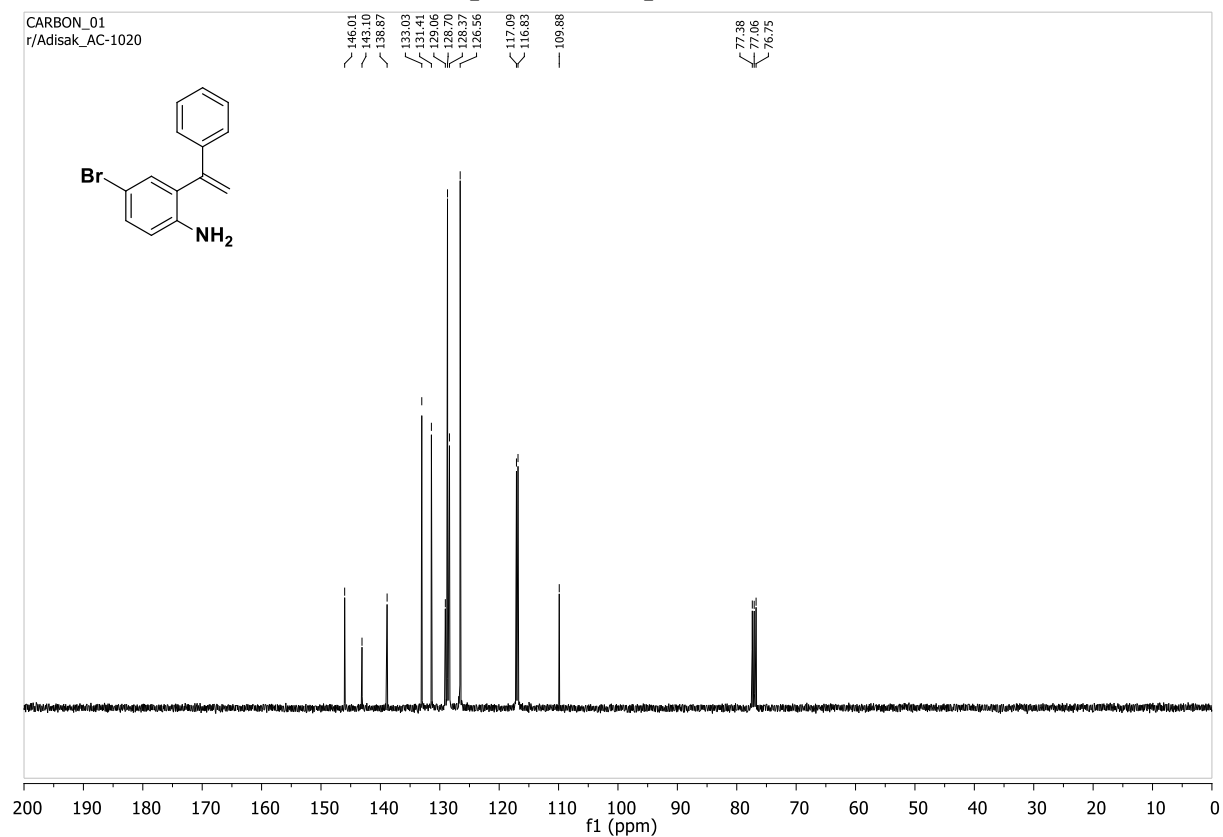
¹³C NMR Spectrum of 3o (151 MHz, CDCl₃)



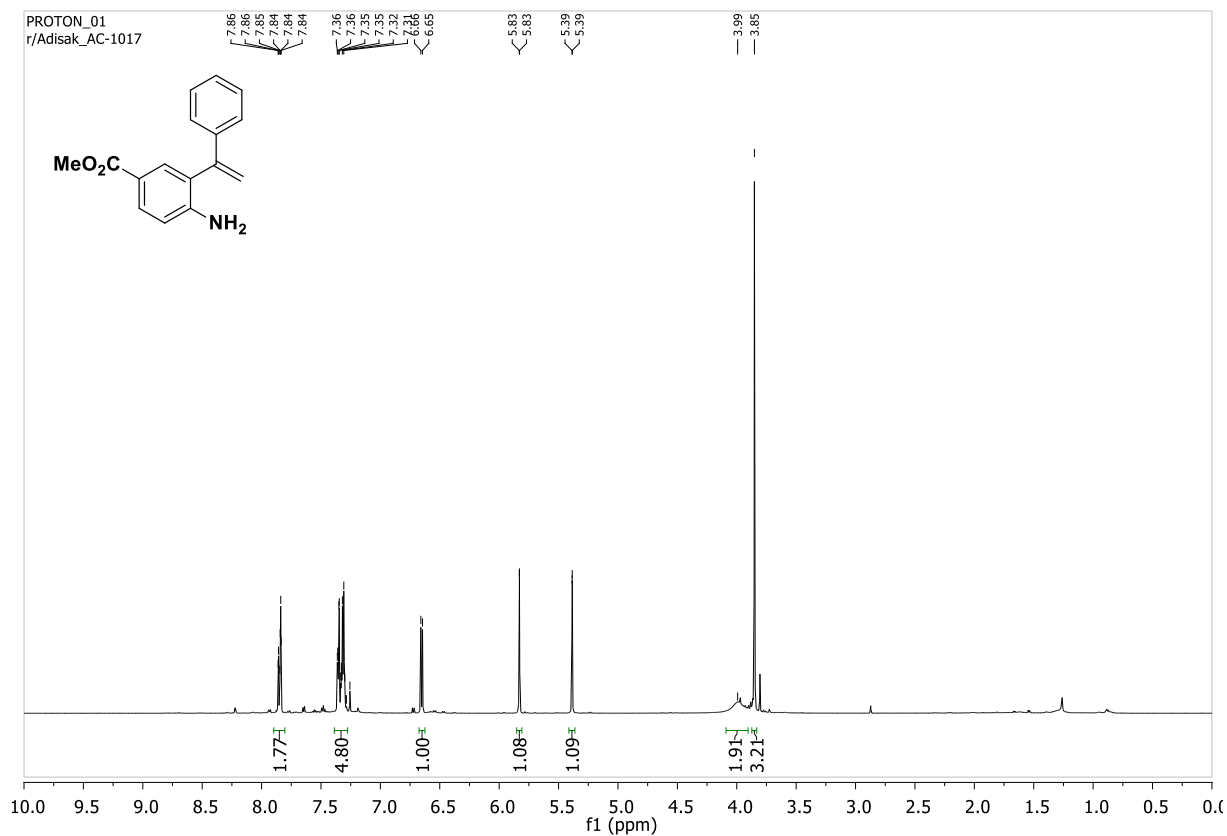
¹H NMR Spectrum of 3p (400 MHz, CDCl₃)



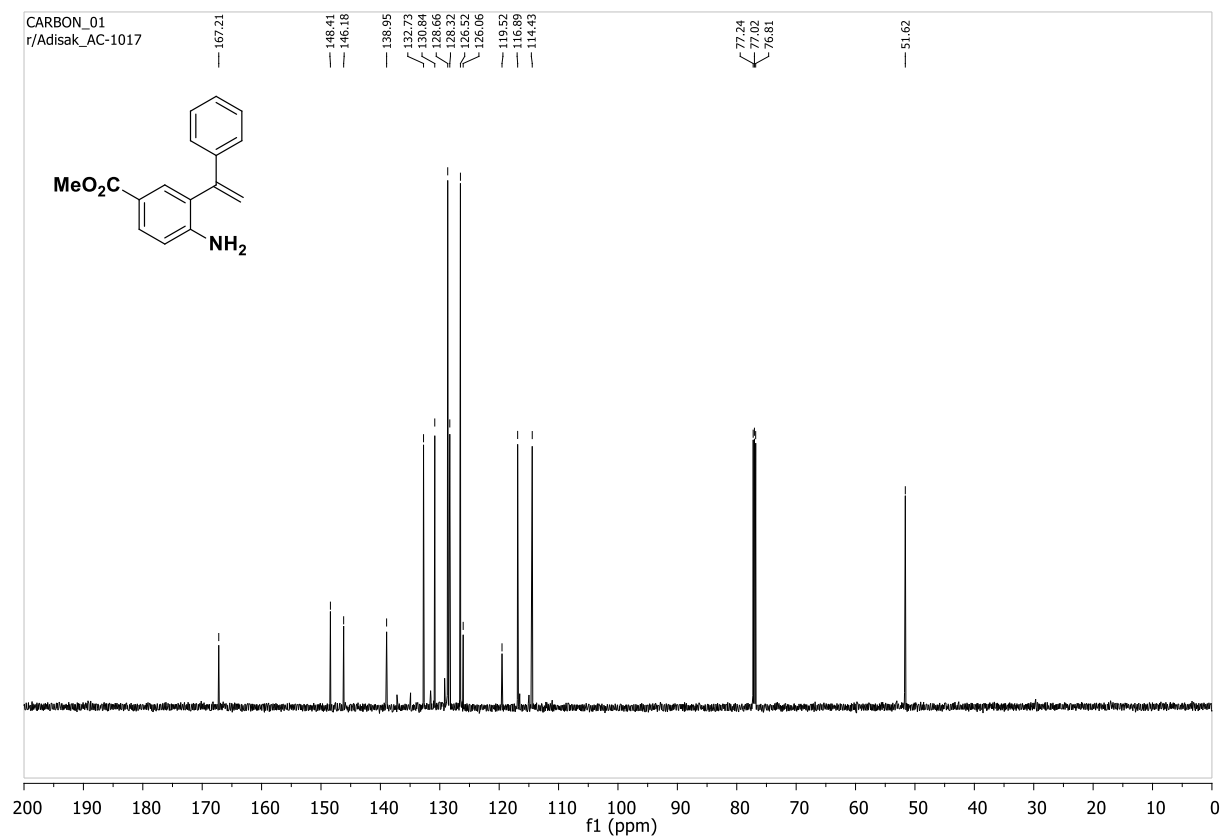
¹³C NMR Spectrum of 3p (101 MHz, CDCl₃)



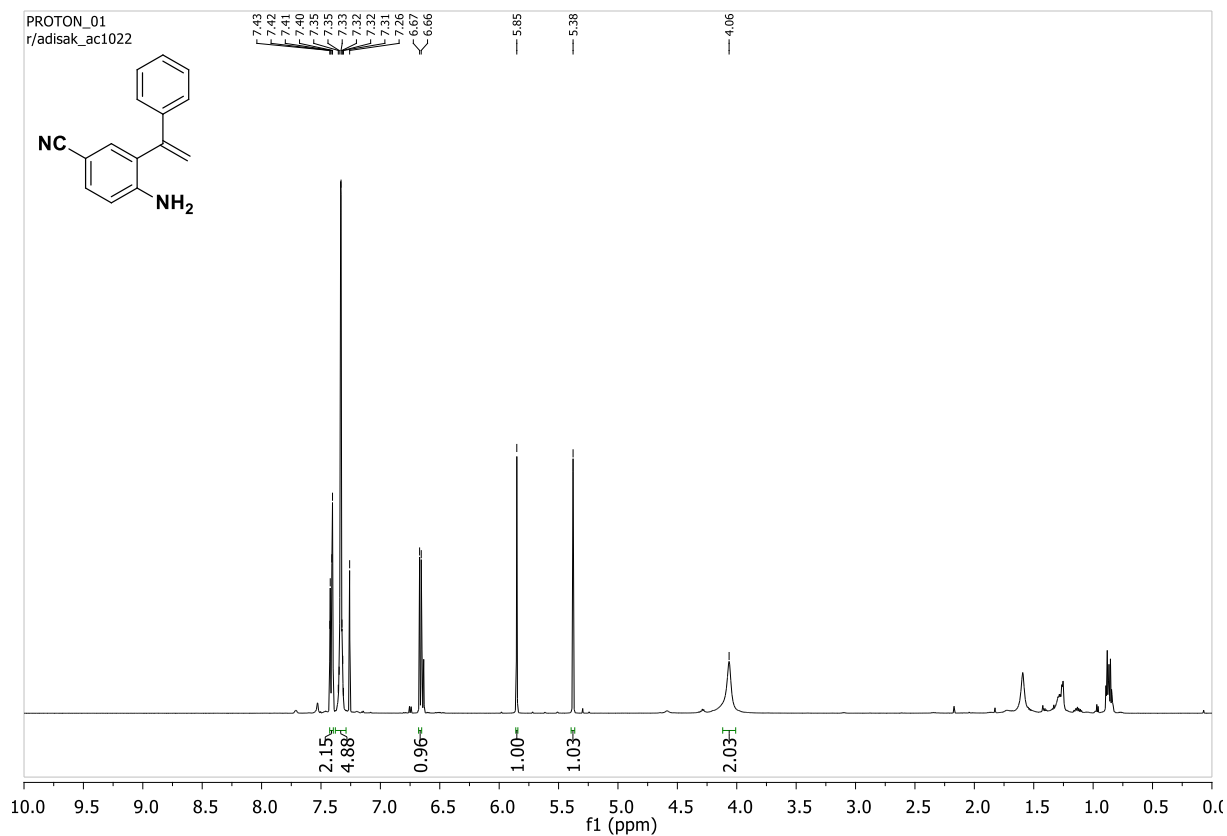
¹H NMR Spectrum of 3q (600 MHz, CDCl₃)



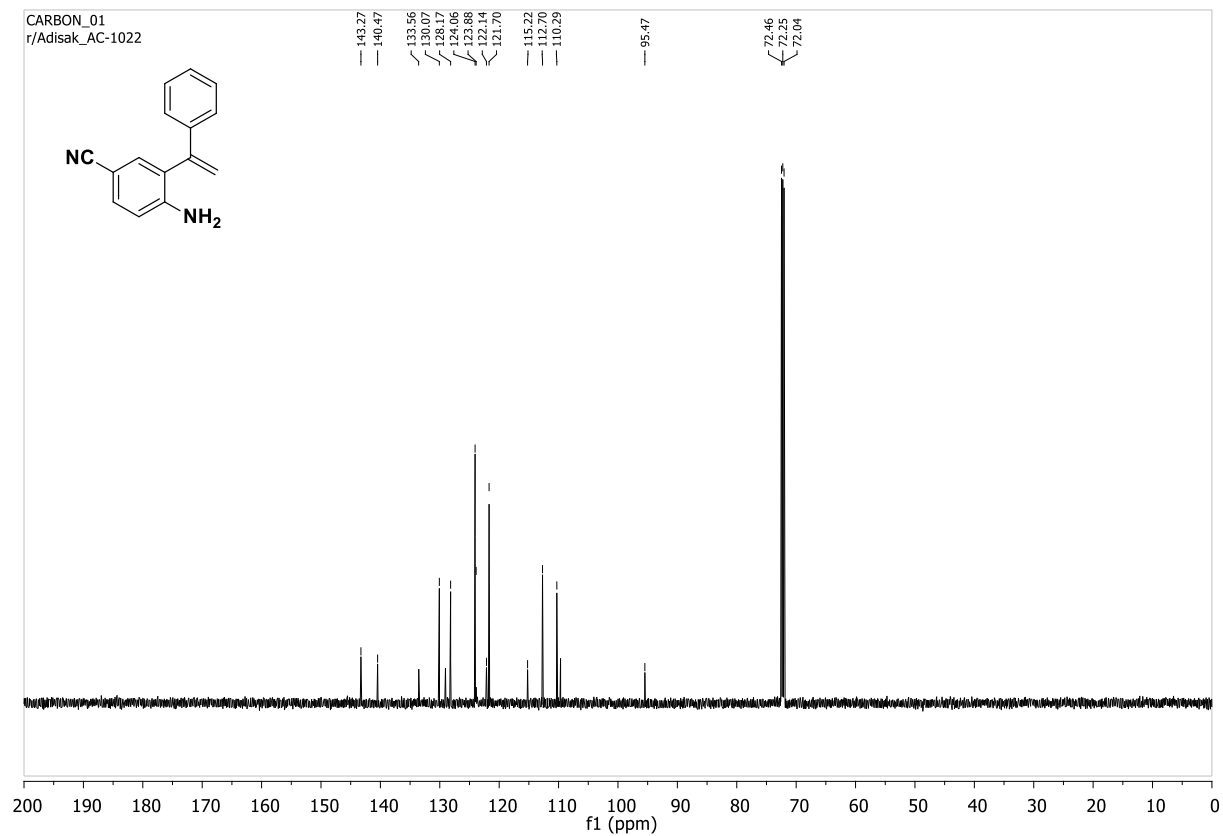
¹³C NMR Spectrum of 3q (151 MHz, CDCl₃)



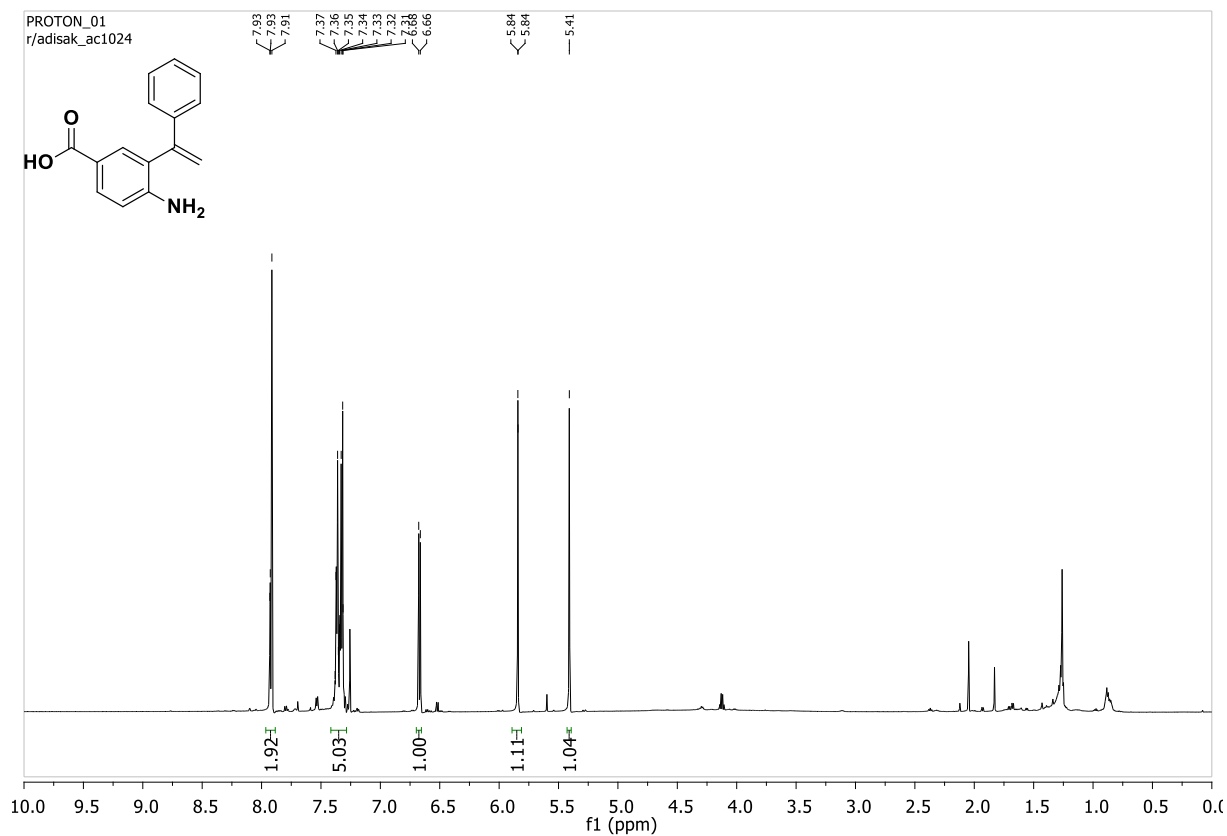
¹H NMR Spectrum of 3r (600 MHz, CDCl₃)



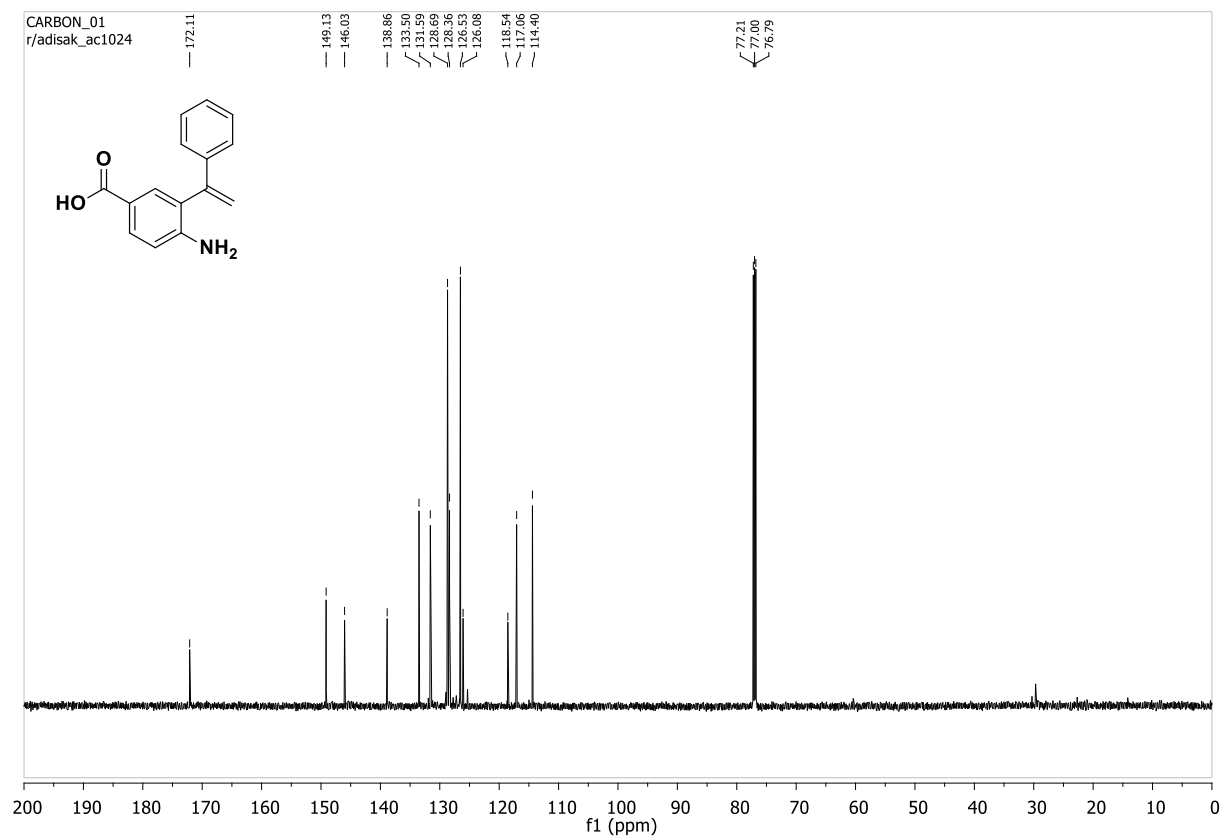
¹³C NMR Spectrum of 3r (151 MHz, CDCl₃)



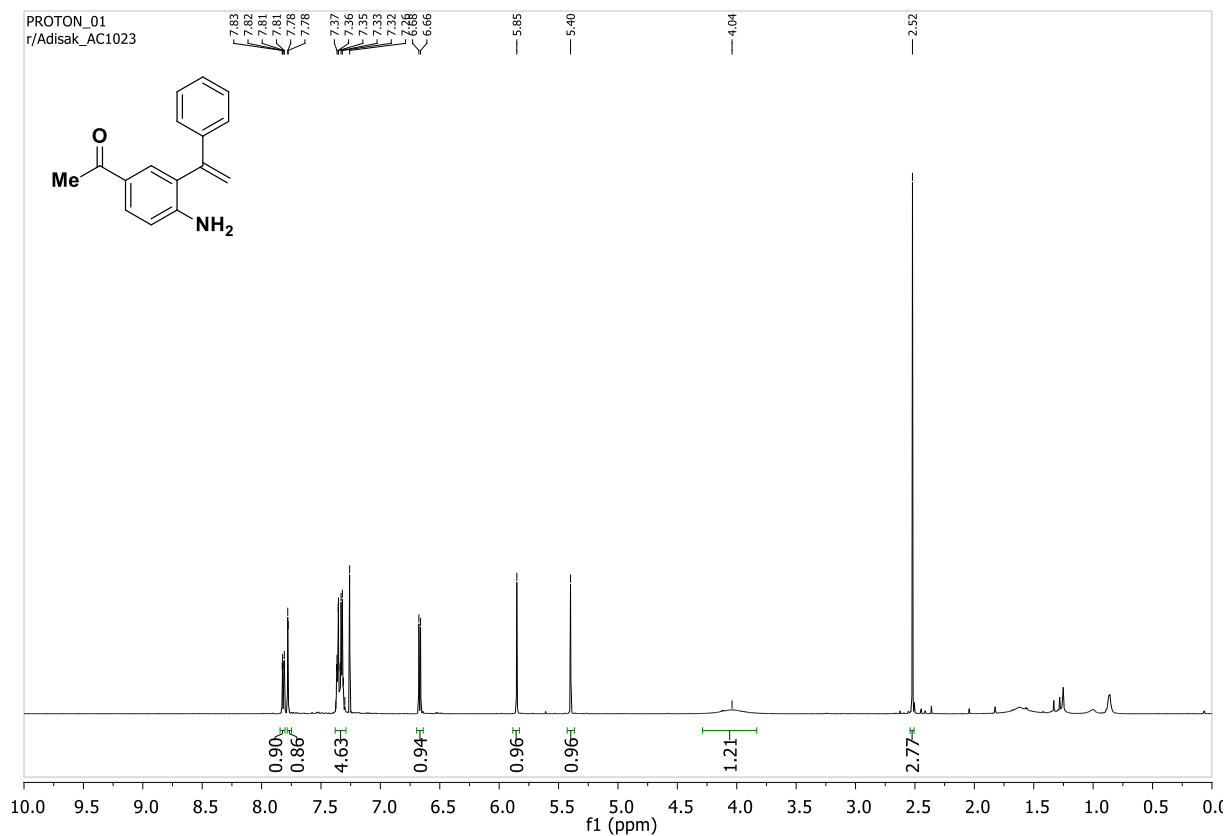
¹H NMR Spectrum of 3s (600 MHz, CDCl₃)



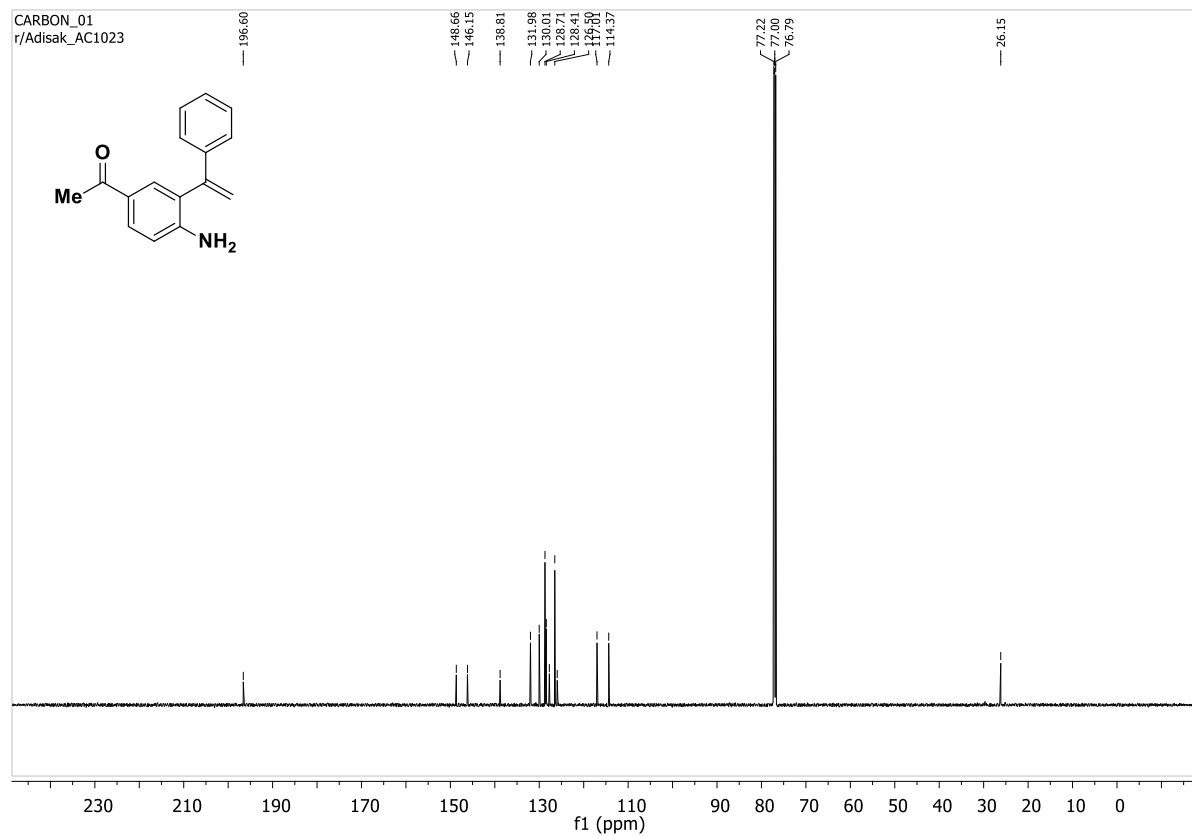
¹³C NMR Spectrum of 3s (151 MHz, CDCl₃)



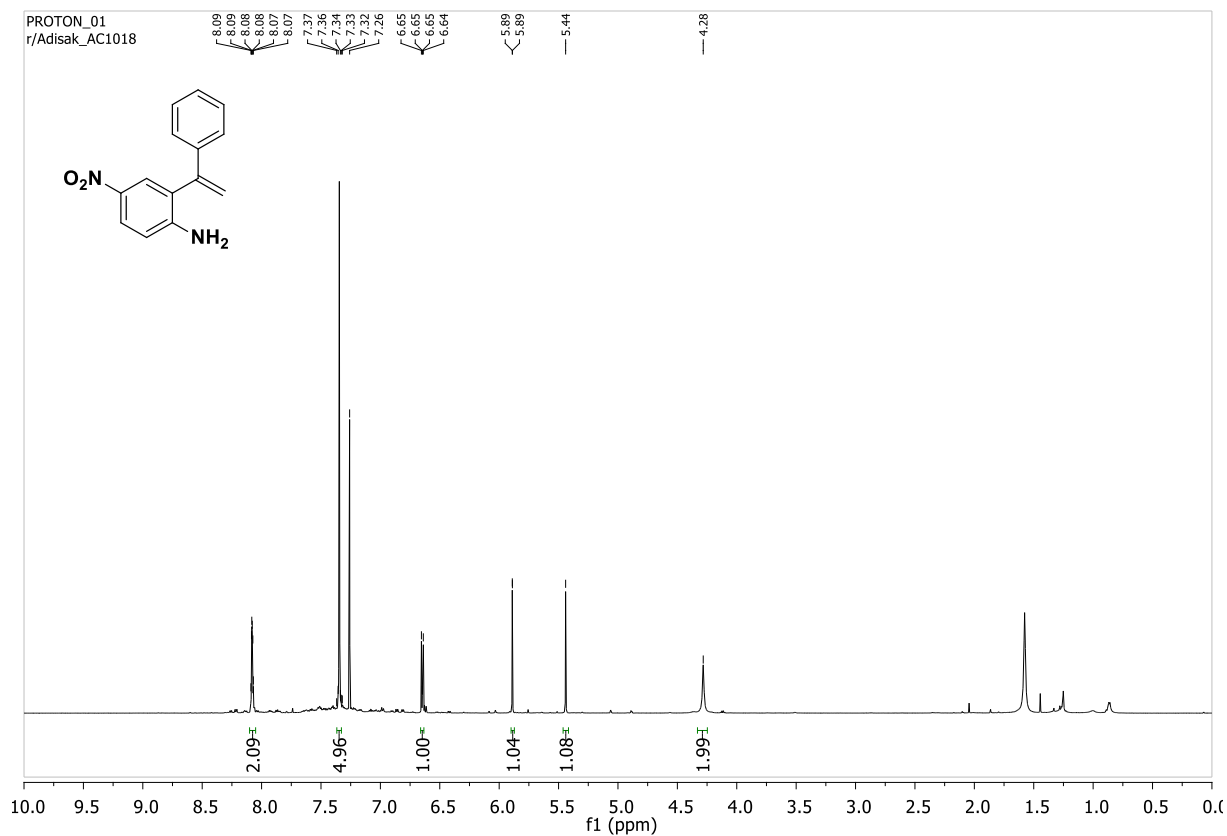
¹H NMR Spectrum of 3t (600 MHz, CDCl₃)



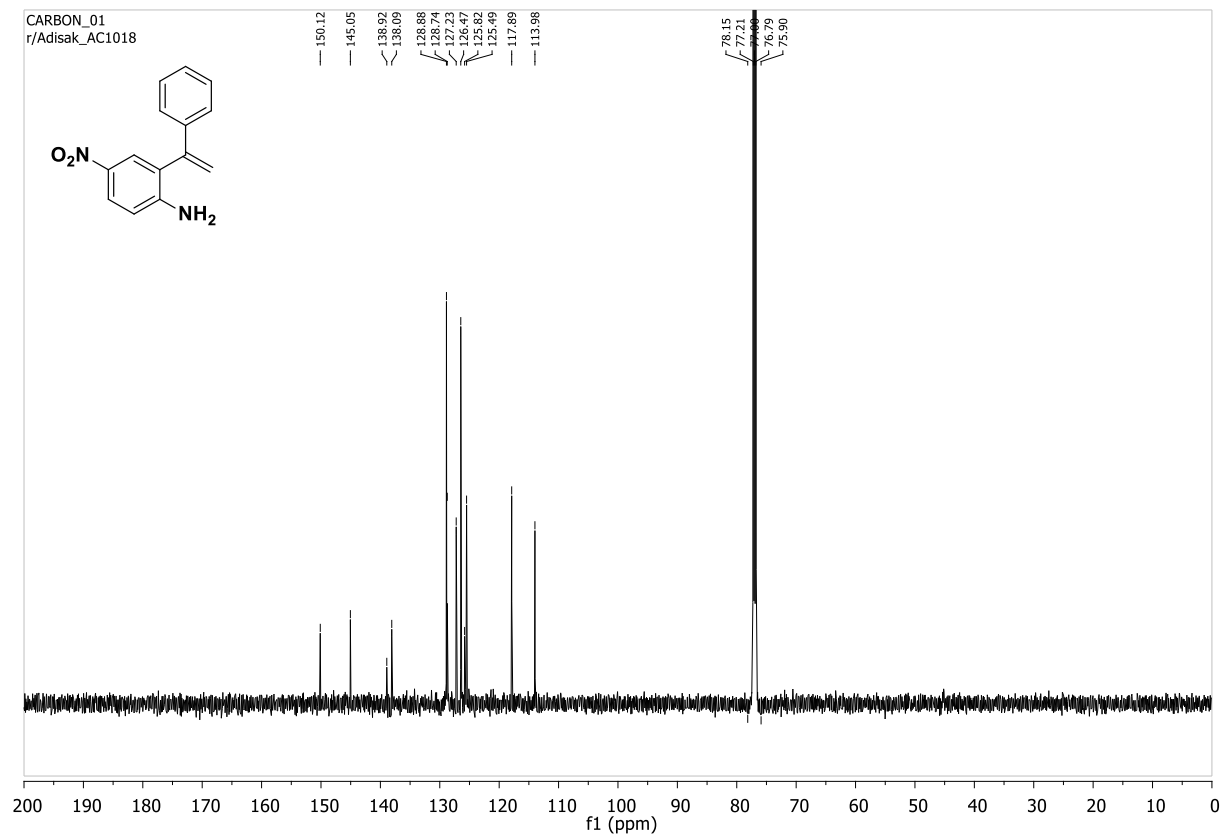
¹³C NMR Spectrum of 3t (151 MHz, CDCl₃)



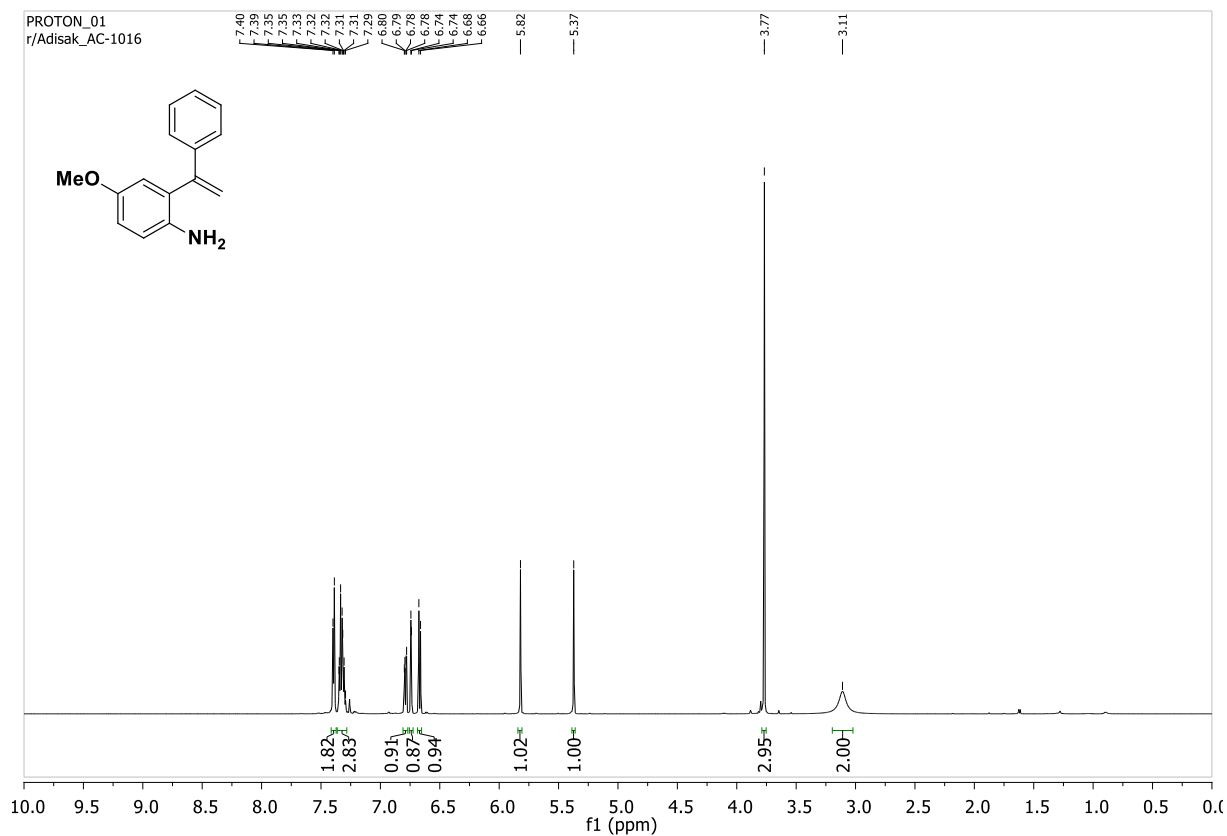
¹H NMR Spectrum of 3u (600 MHz, CDCl₃)



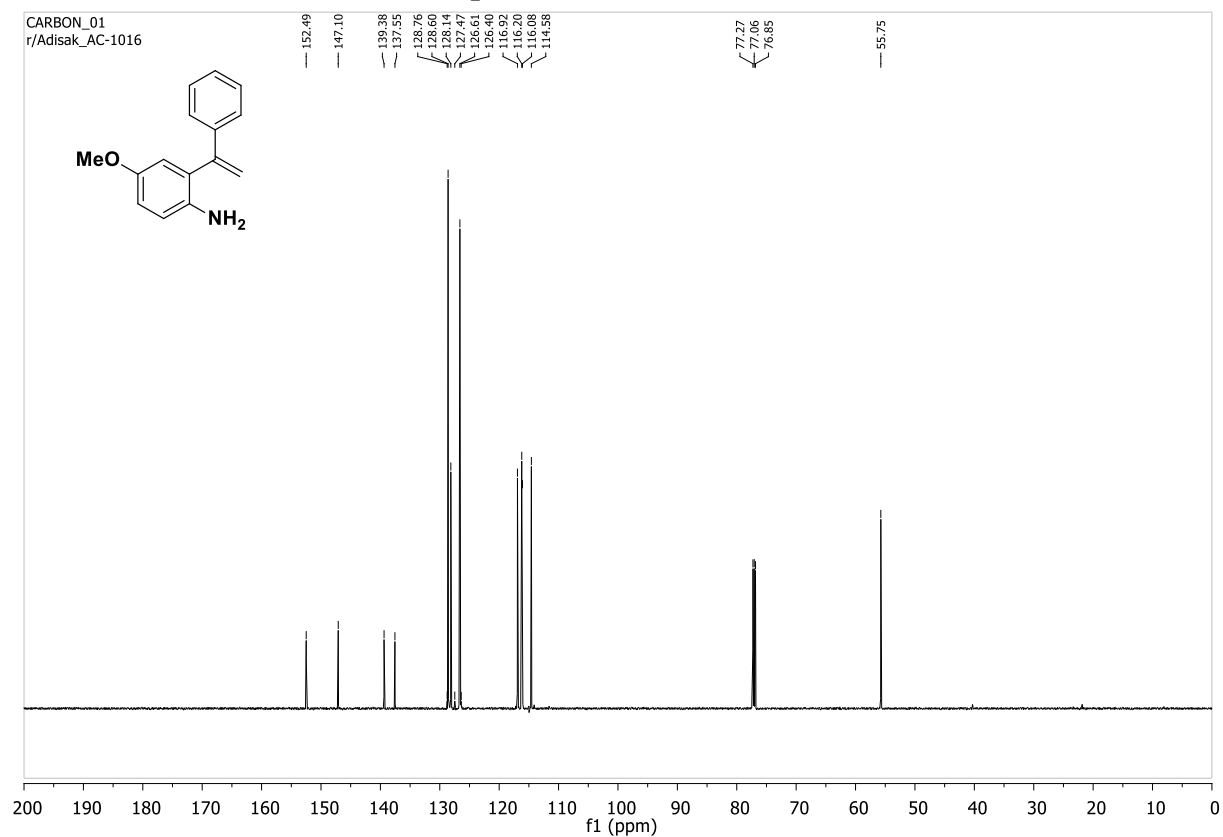
¹³C NMR Spectrum of 3u (151 MHz, CDCl₃)



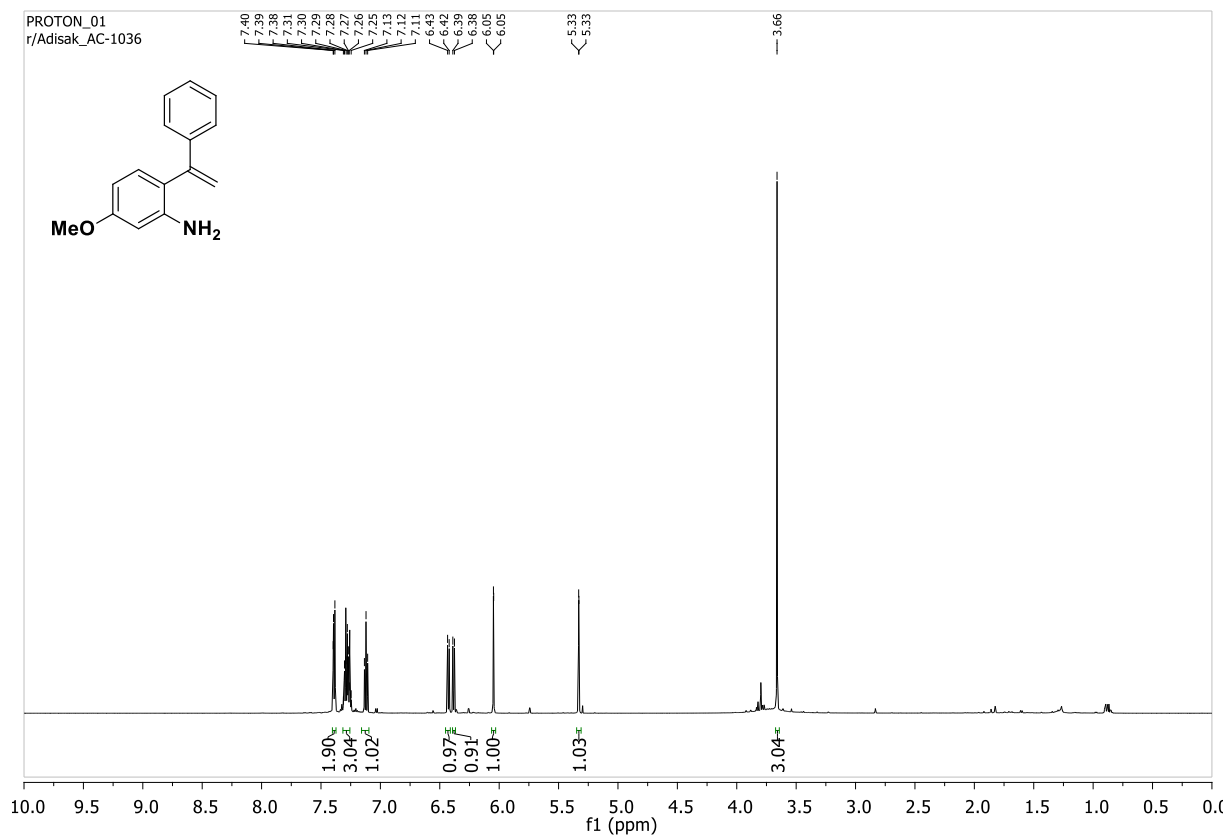
¹H NMR Spectrum of 3v (600 MHz, CDCl₃)



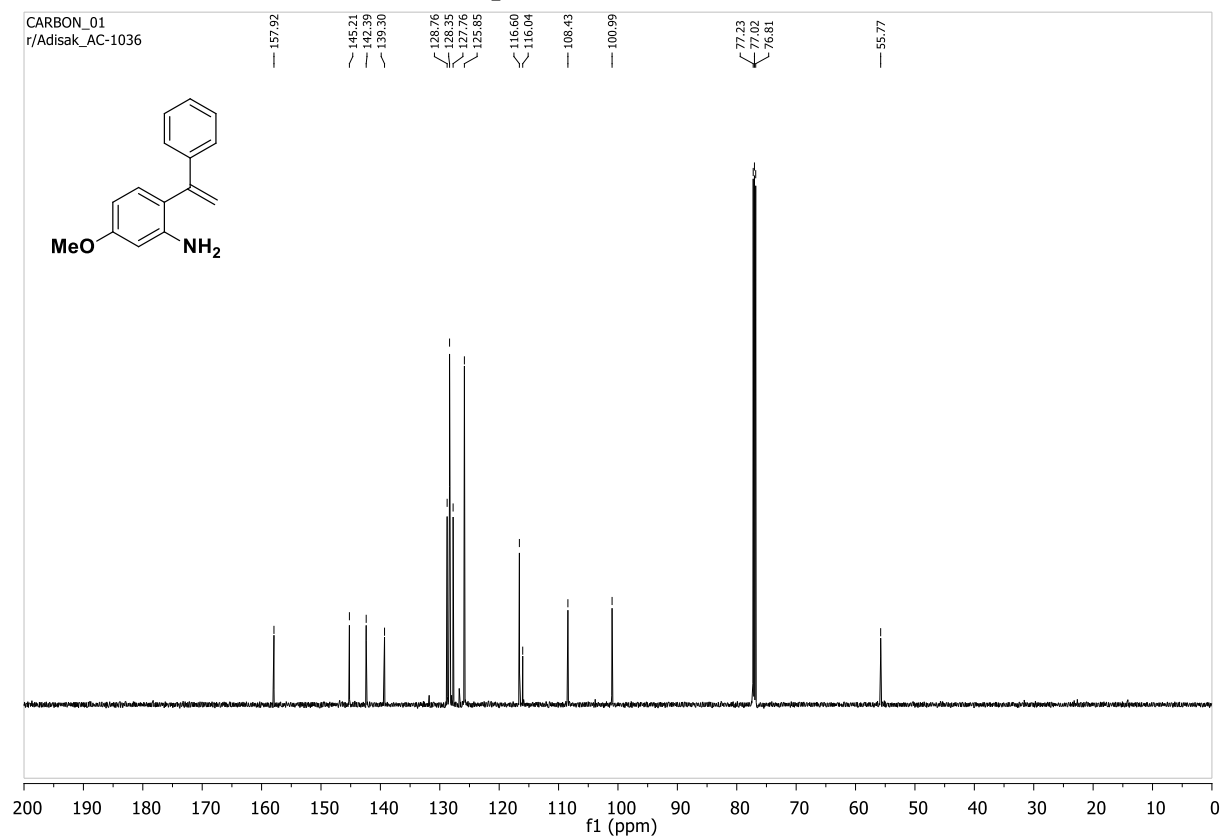
¹³C NMR Spectrum of 3v (151 MHz, CDCl₃)



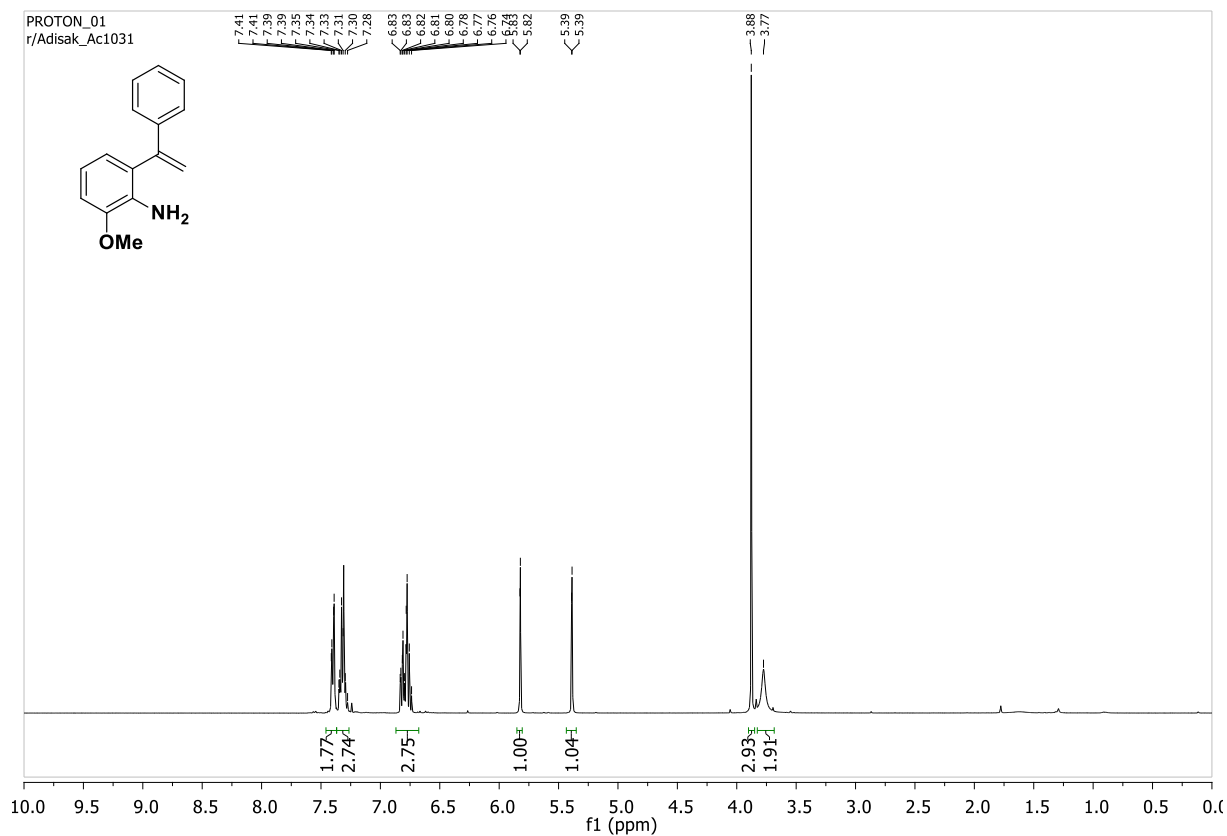
¹H NMR Spectrum of 3w (600 MHz, CDCl₃)



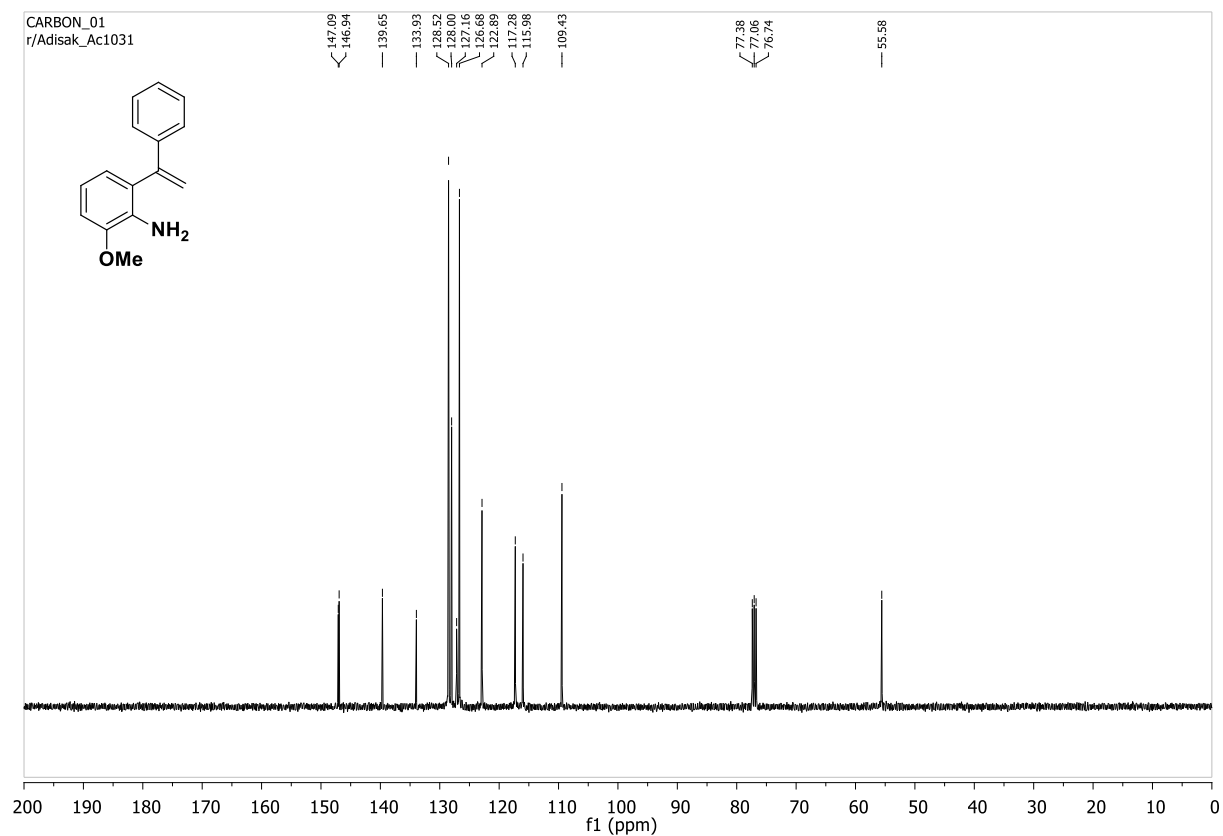
¹³C NMR Spectrum of 3w (151 MHz, CDCl₃)



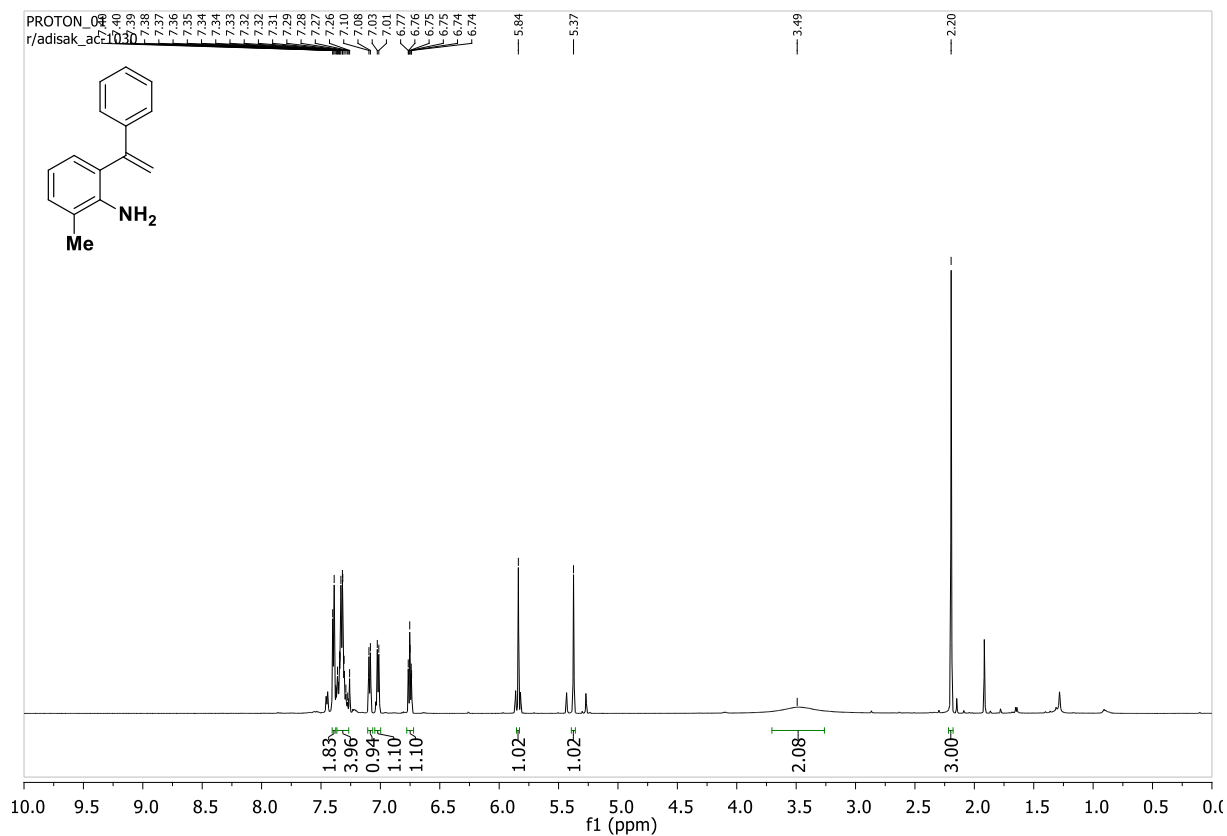
¹H NMR Spectrum of 3x (400 MHz, CDCl₃)



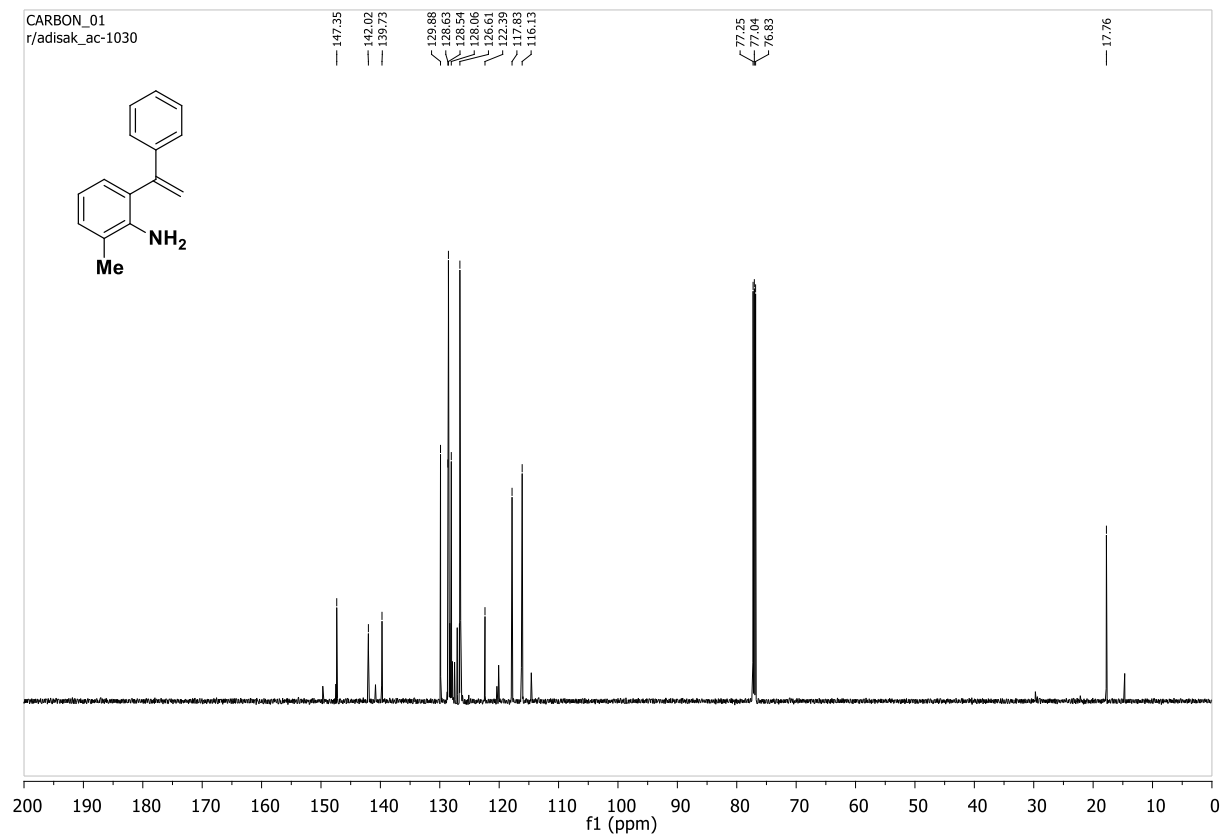
¹³C NMR Spectrum of 3x (101 MHz, CDCl₃)



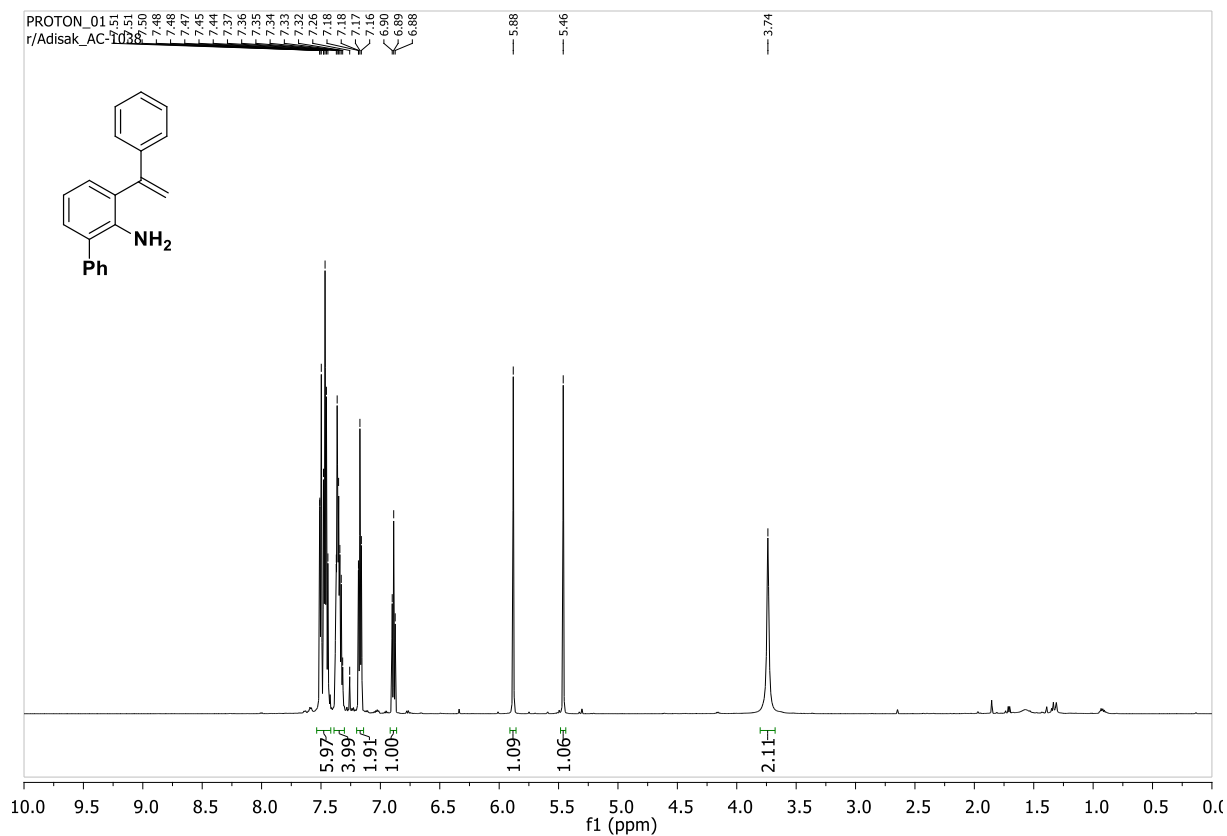
¹H NMR Spectrum of 3y (600 MHz, CDCl₃)



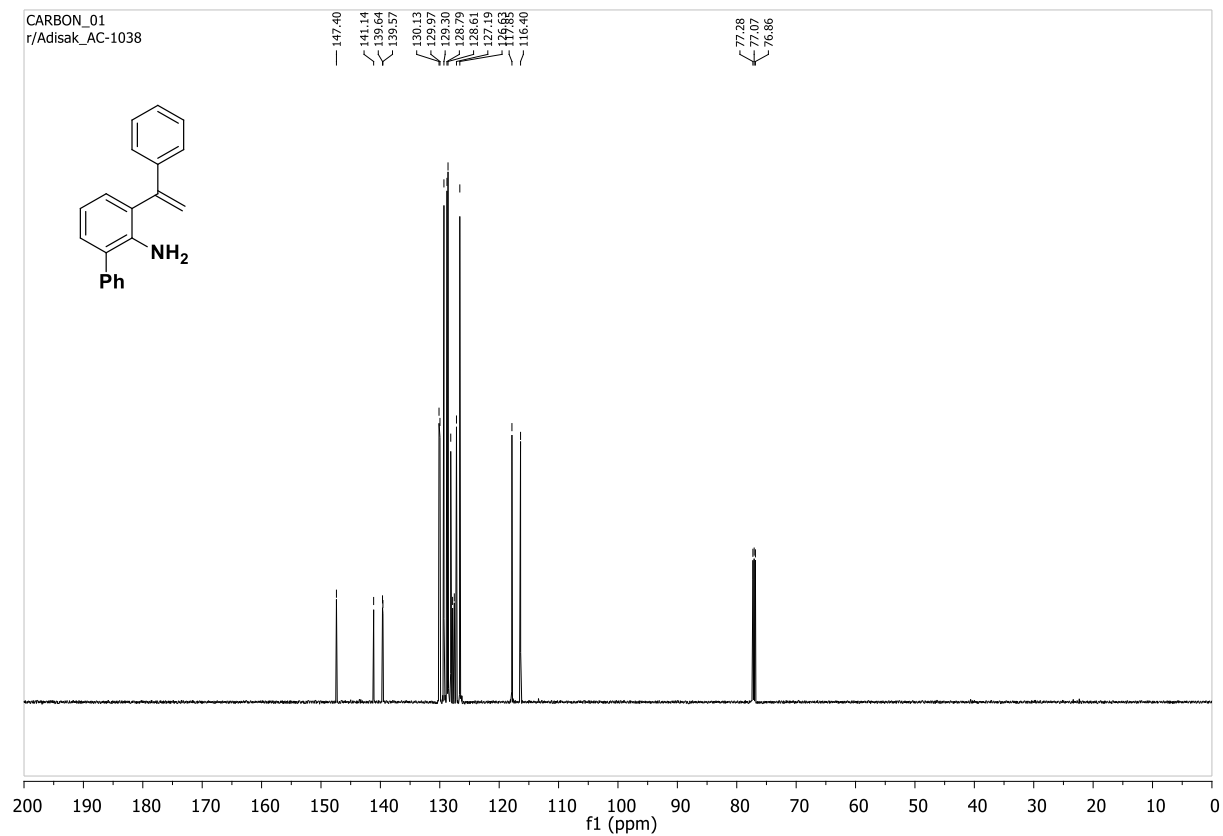
¹³C NMR Spectrum of 3y (151 MHz, CDCl₃)



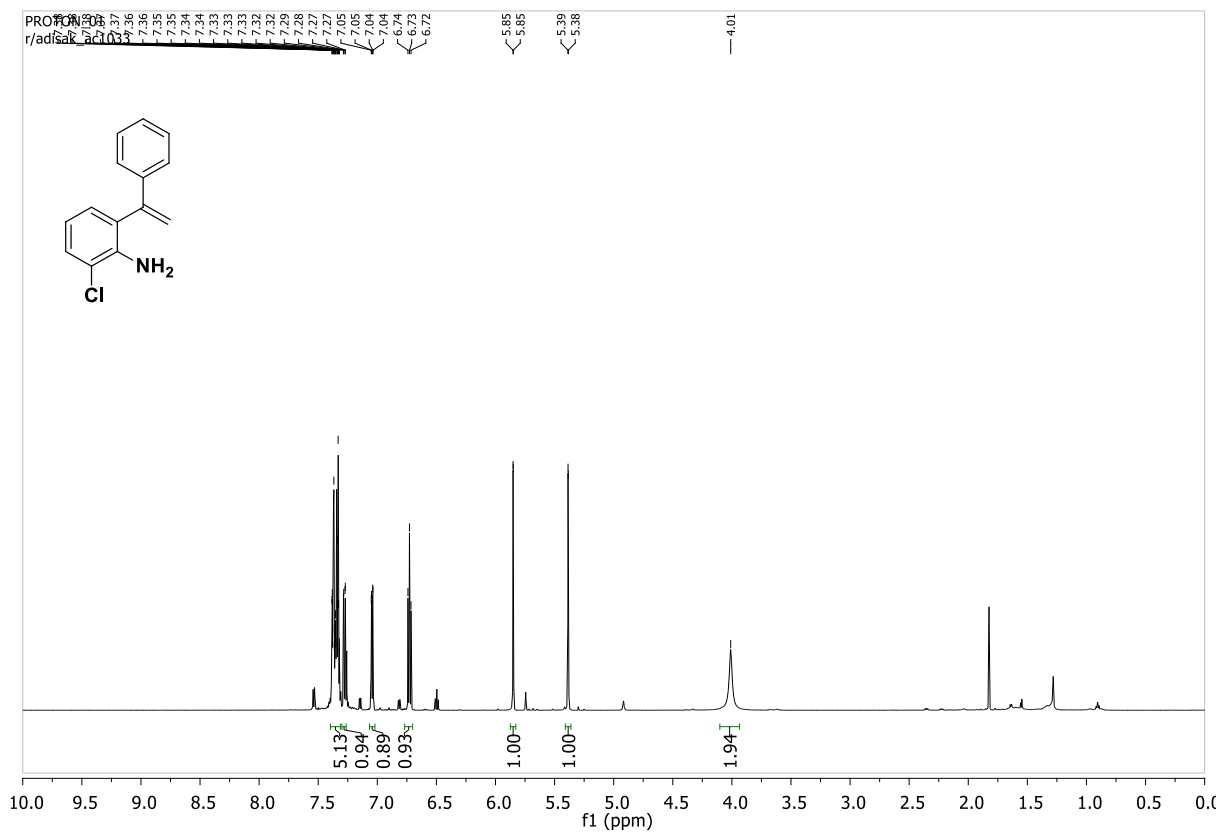
¹H NMR Spectrum of 3z (600 MHz, CDCl₃)



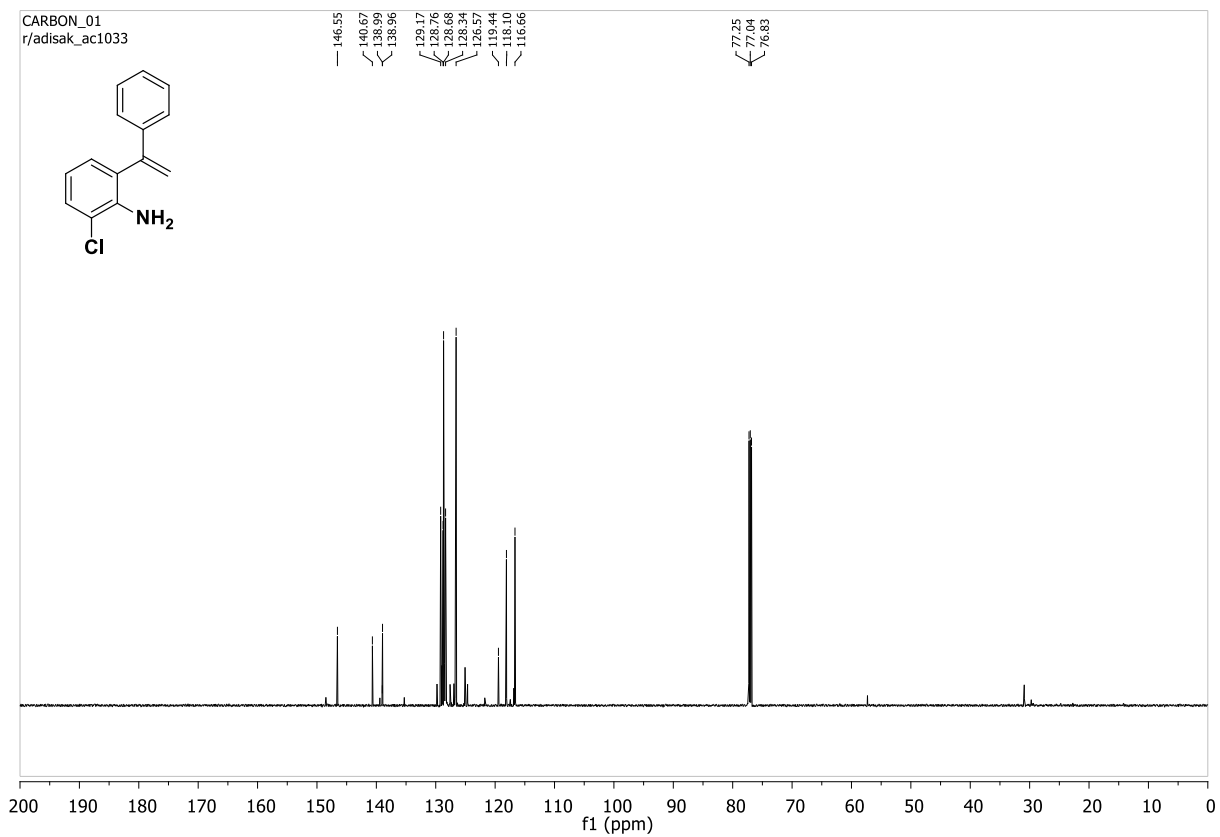
¹³C NMR Spectrum of 3z (151 MHz, CDCl₃)



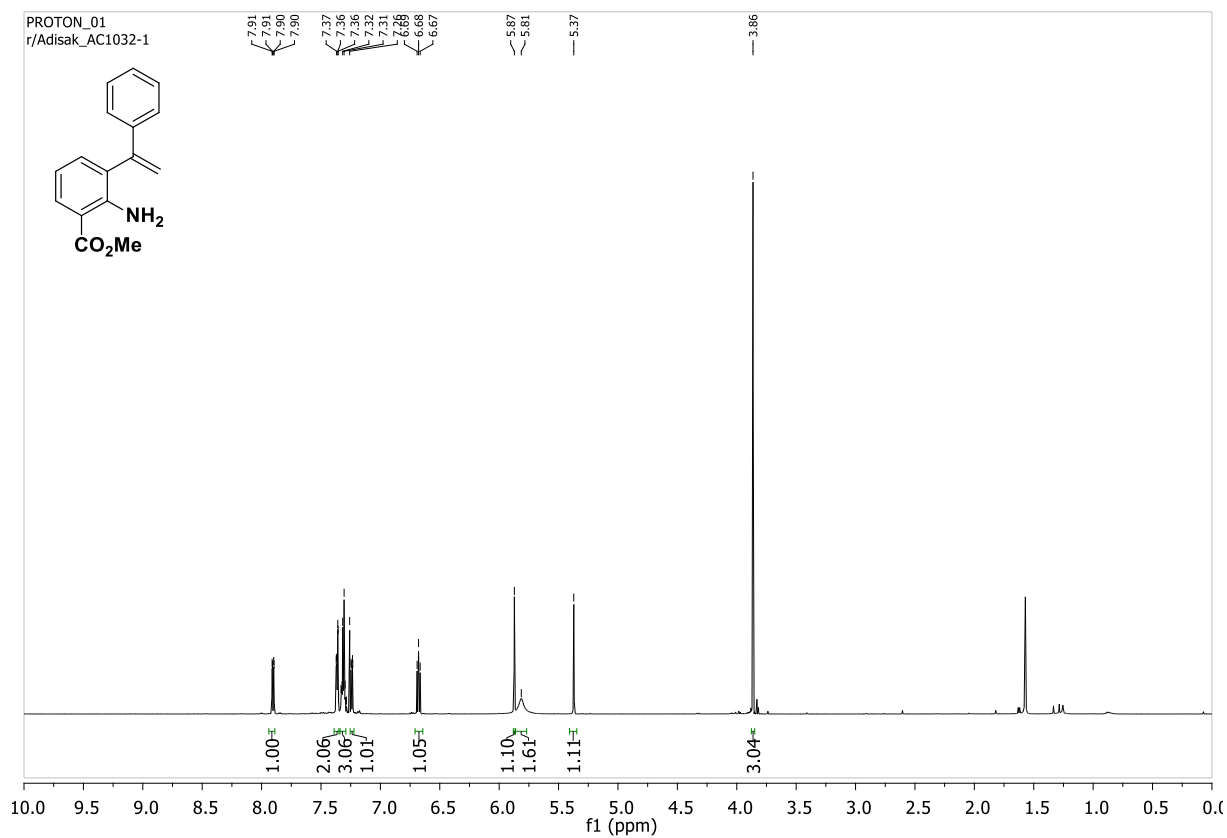
¹H NMR Spectrum of 3aa (600 MHz, CDCl₃)



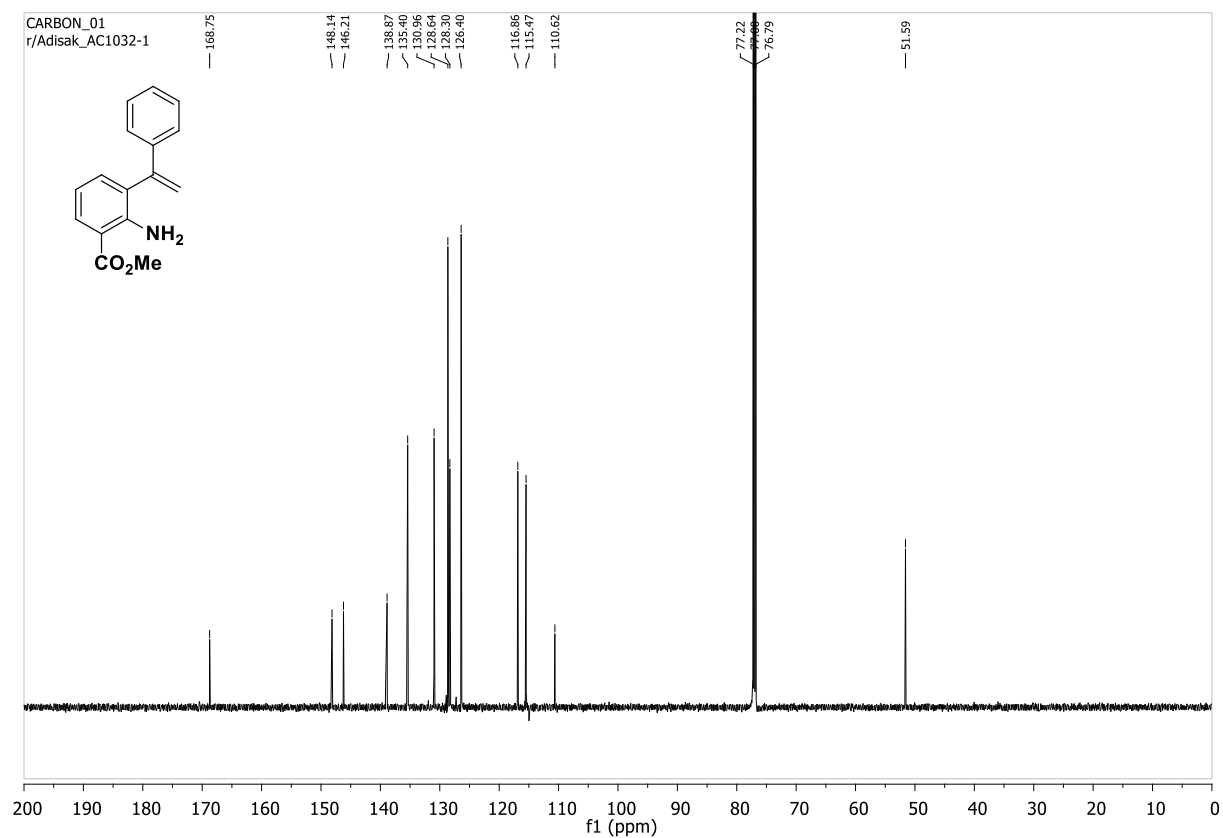
¹³C NMR Spectrum of 3aa (151 MHz, CDCl₃)



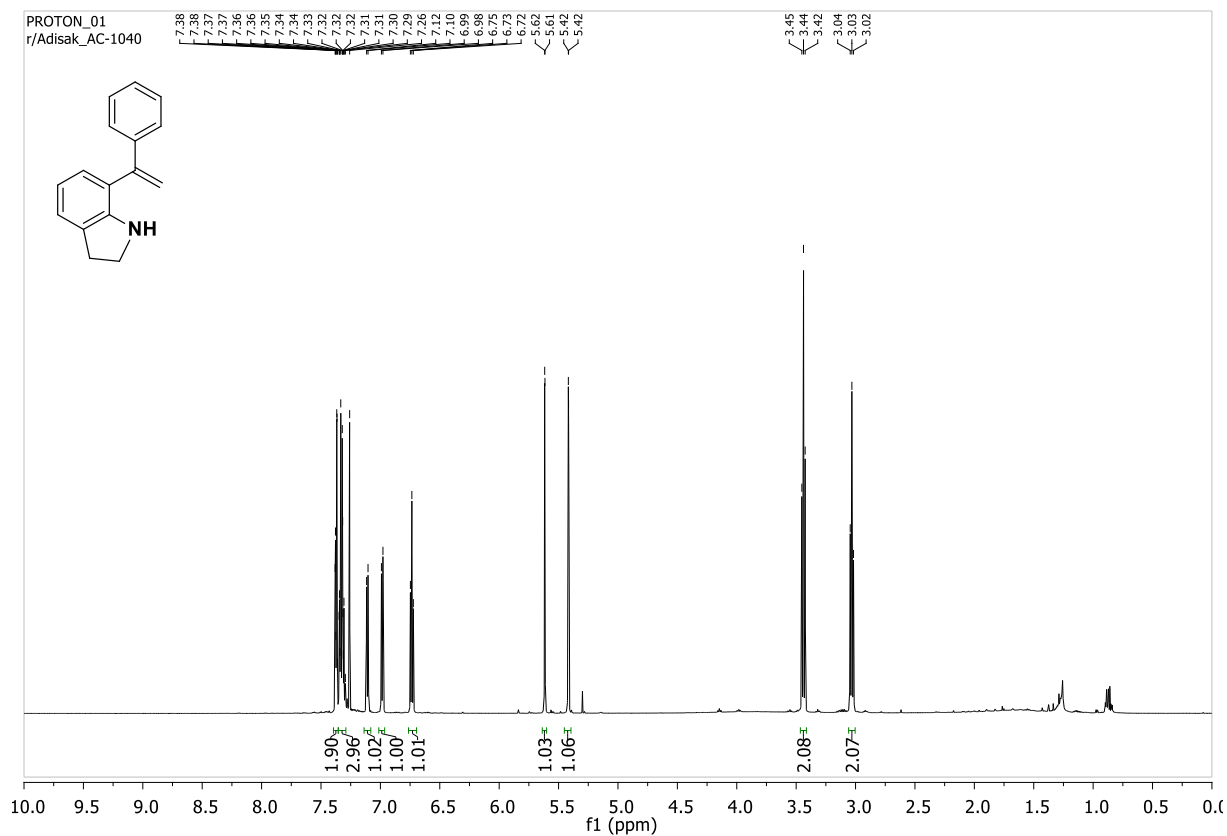
¹H NMR Spectrum of 3ab (600 MHz, CDCl₃)



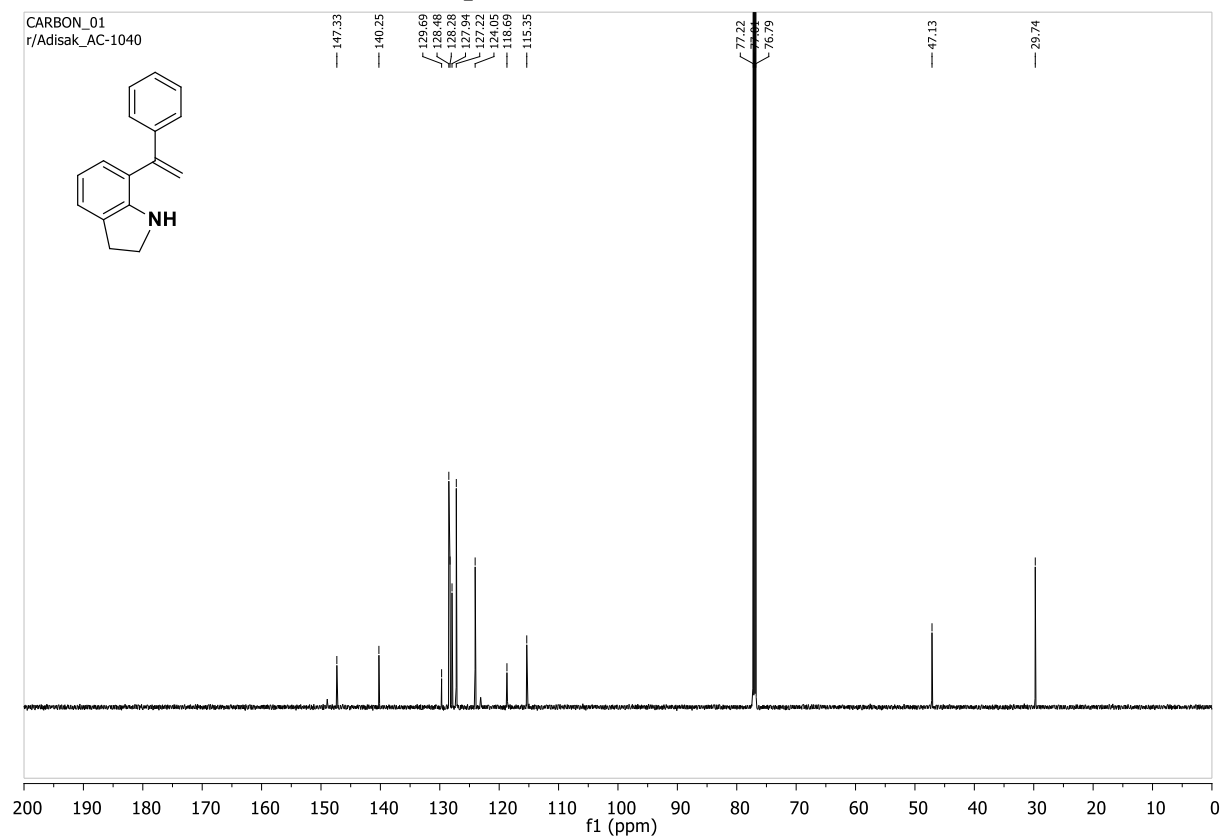
¹³C NMR Spectrum of 3ab (151 MHz, CDCl₃)



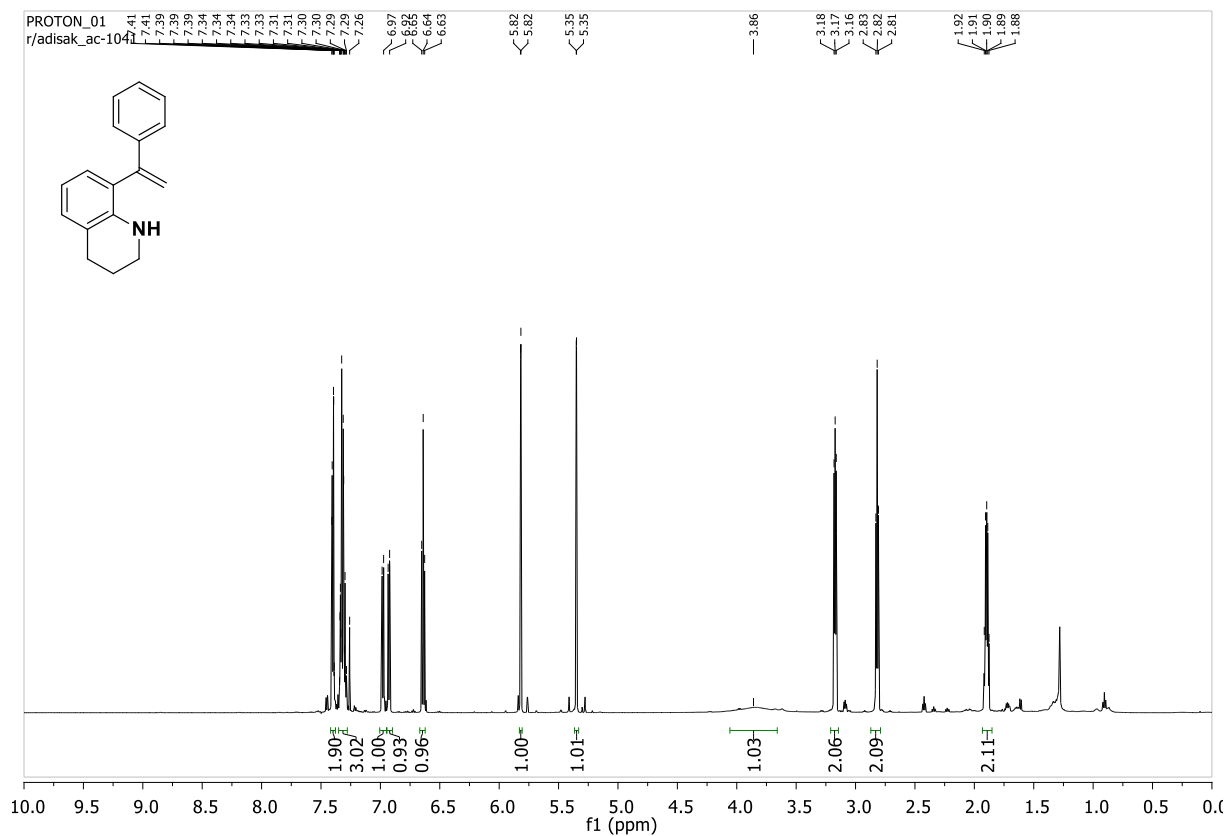
¹H NMR Spectrum of 3ac (600 MHz, CDCl₃)



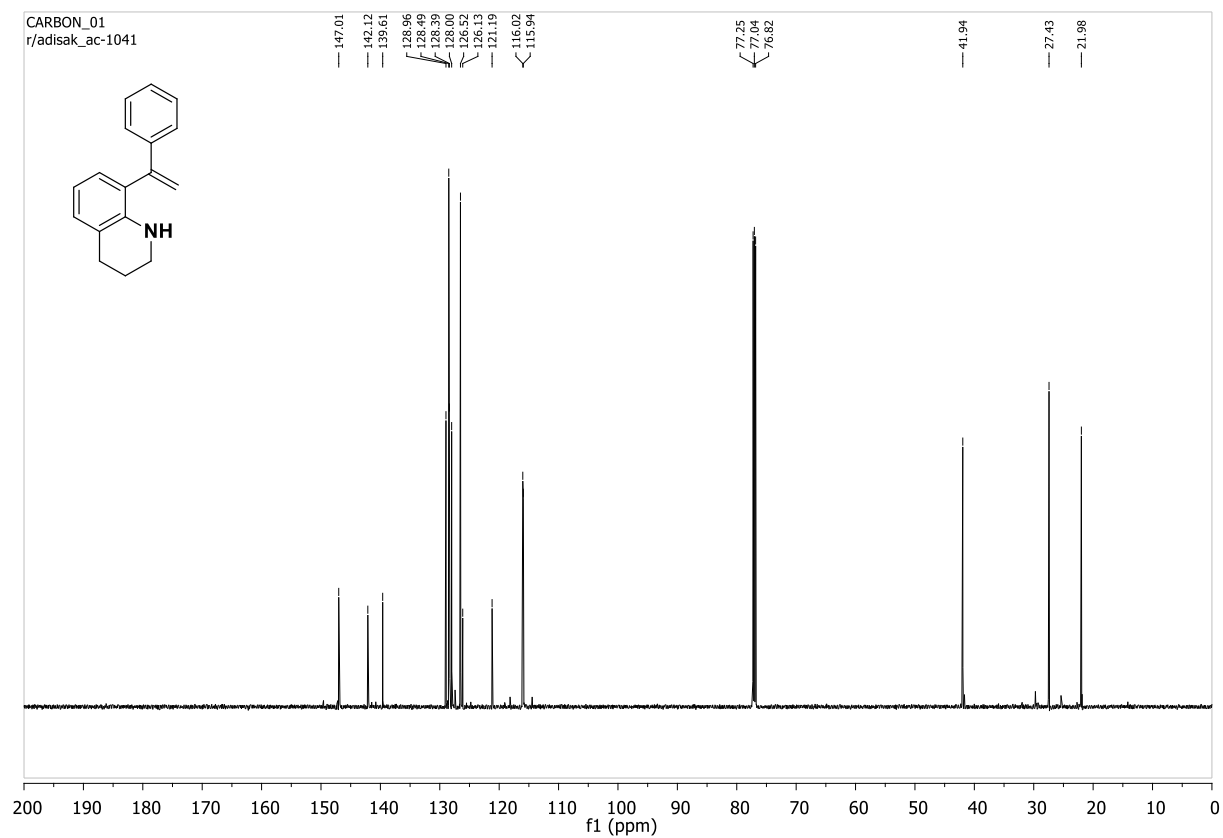
¹³C NMR Spectrum of 3ac (151 MHz, CDCl₃)



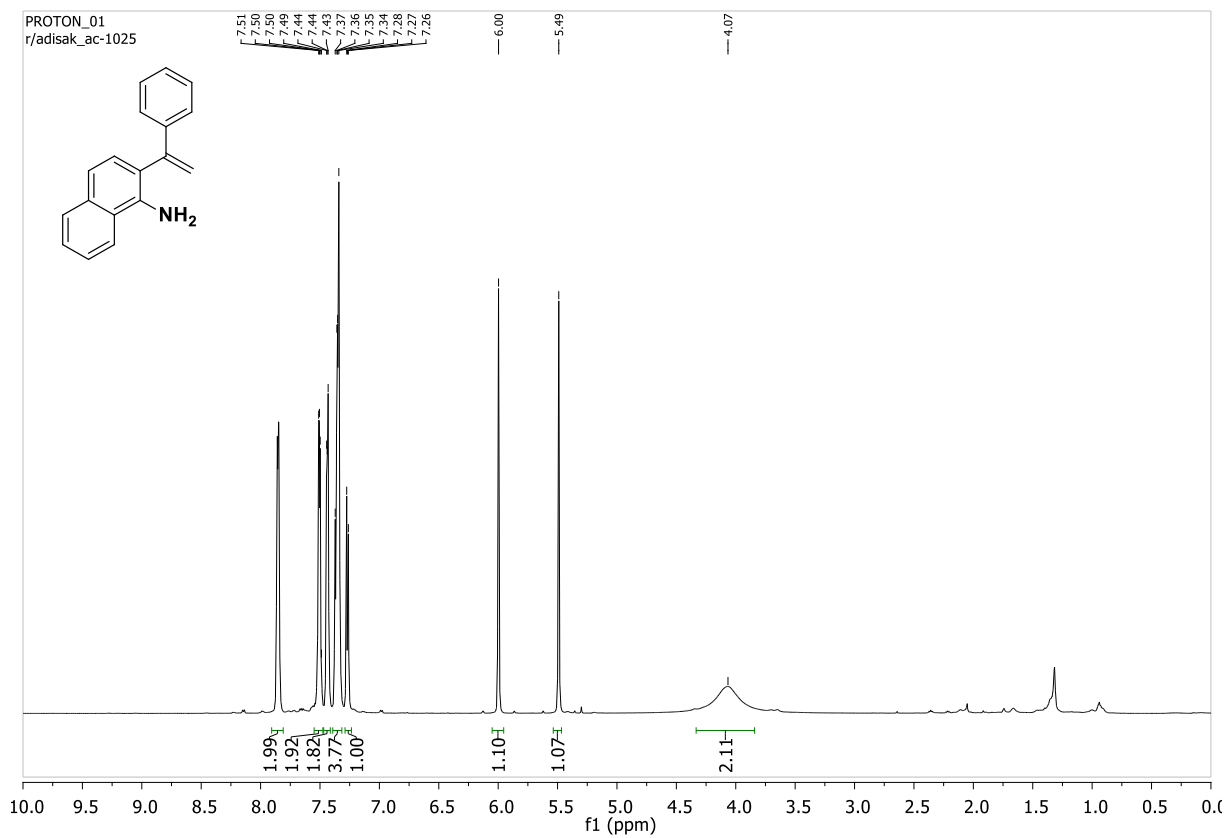
¹H NMR Spectrum of 3ad (600 MHz, CDCl₃)



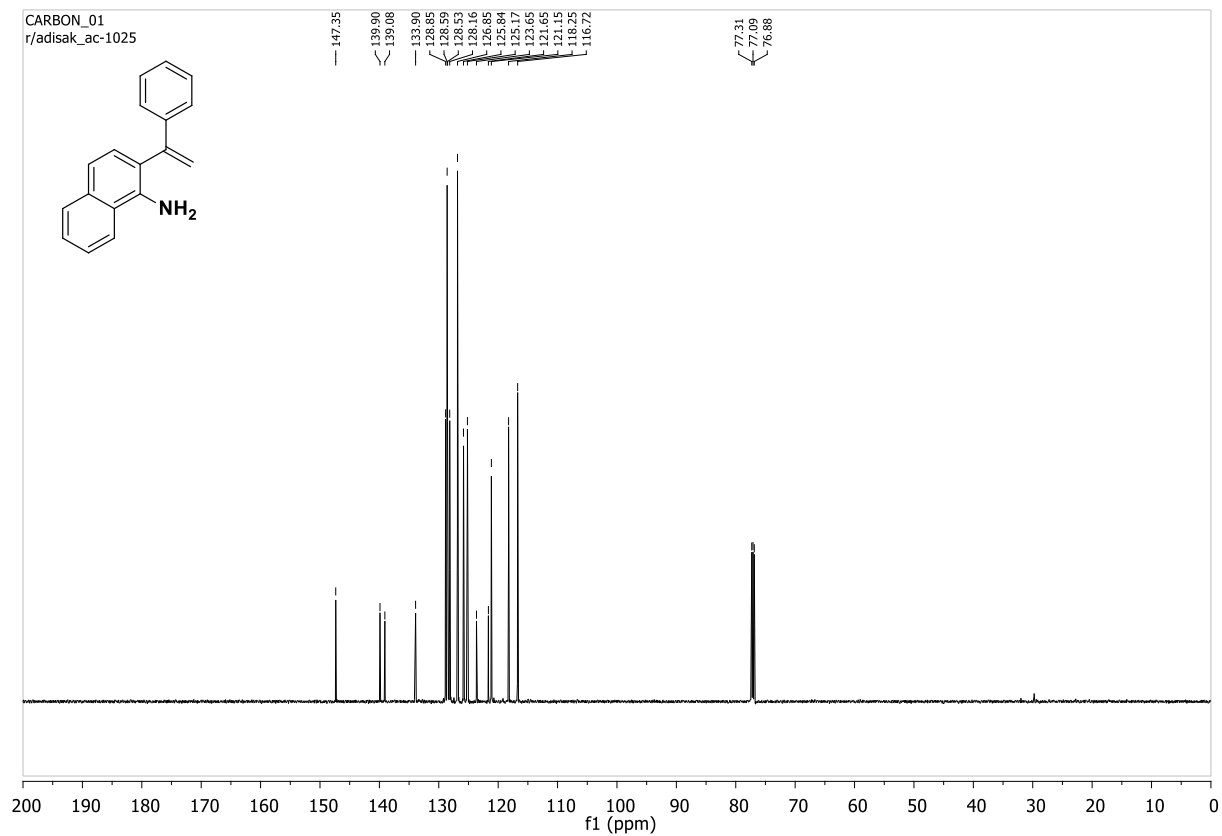
¹³C NMR Spectrum of 3ad (151 MHz, CDCl₃)



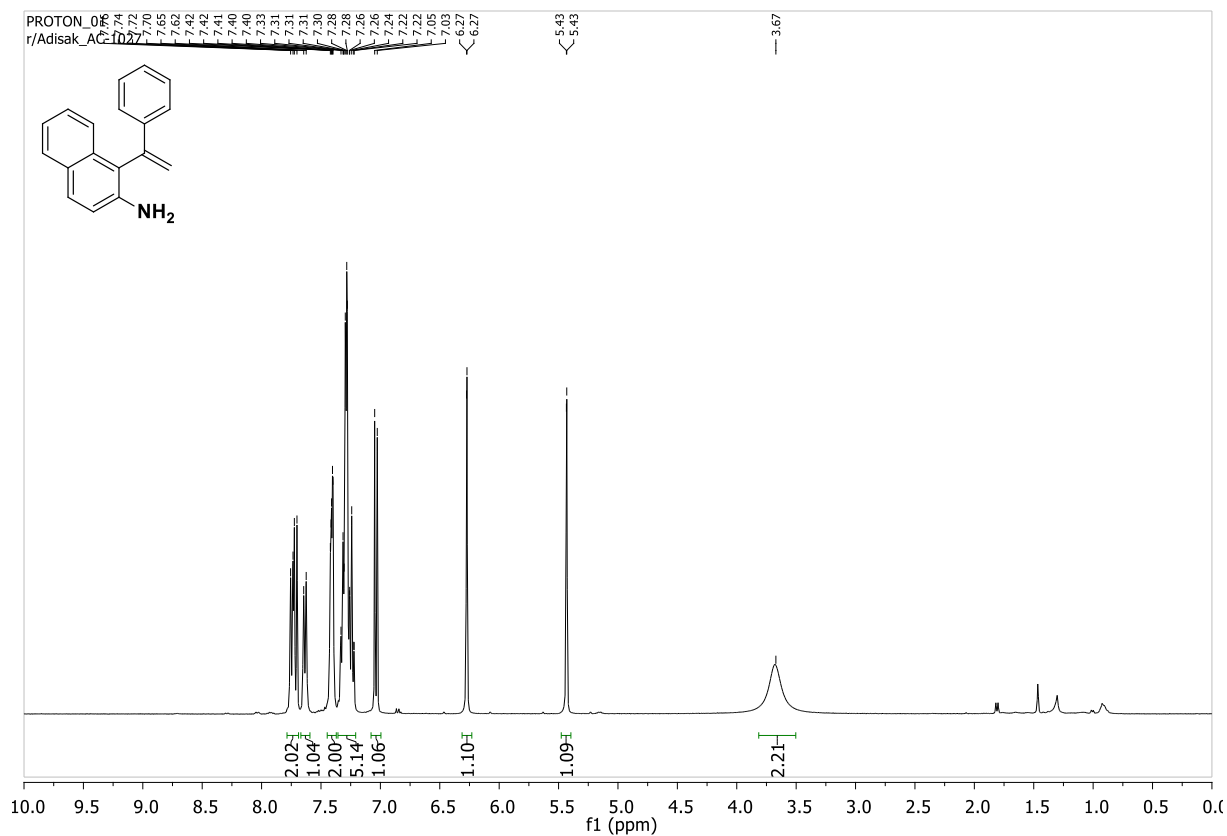
¹H NMR Spectrum of 3ae (600 MHz, CDCl₃)



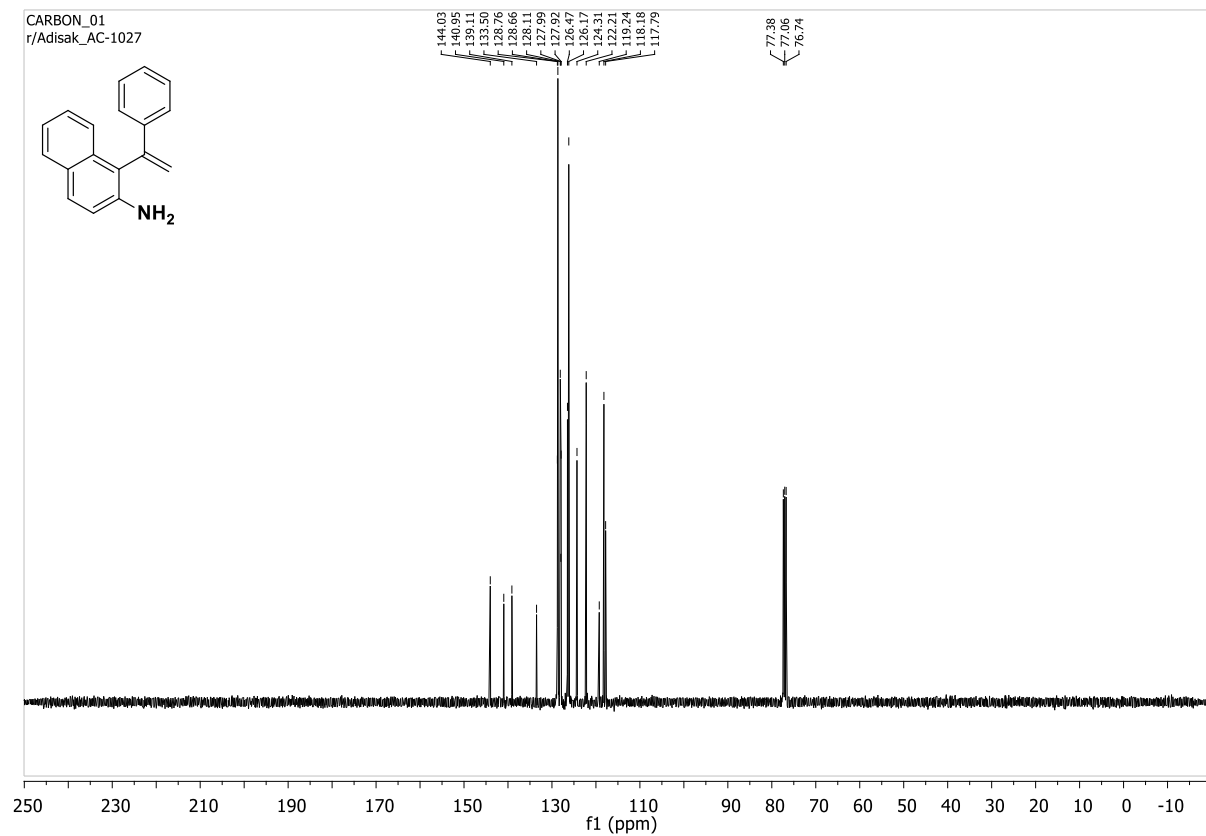
¹³C NMR Spectrum of 3ae (151 MHz, CDCl₃)

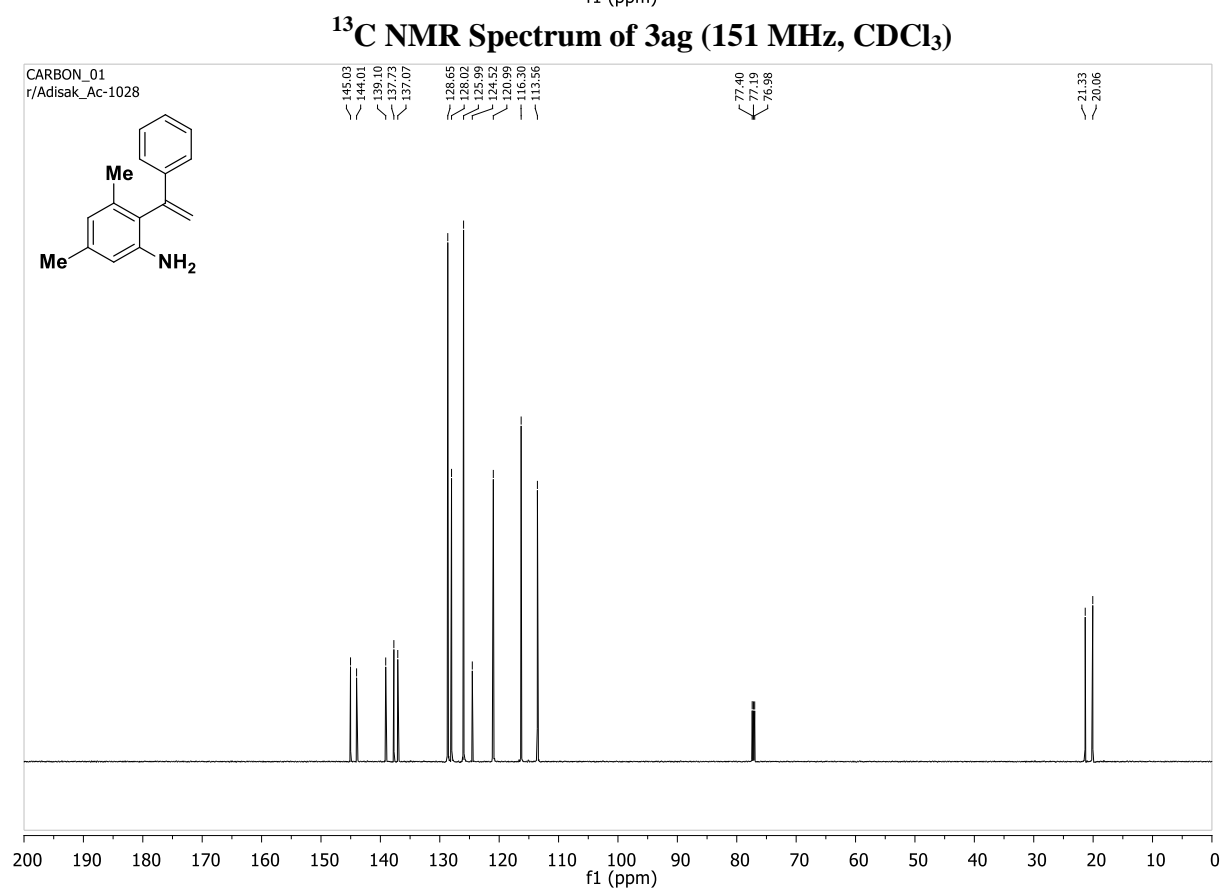
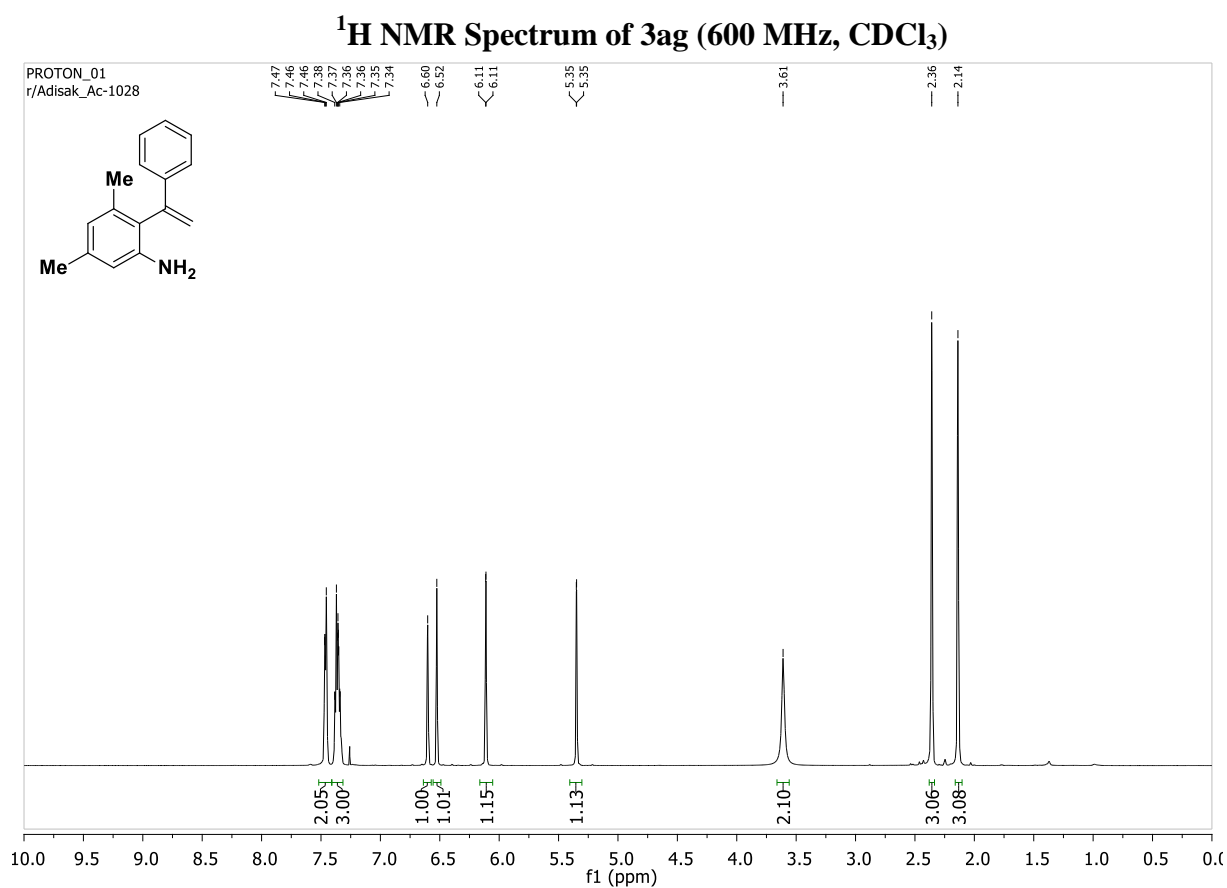


¹H NMR Spectrum of 3af (600 MHz, CDCl₃)

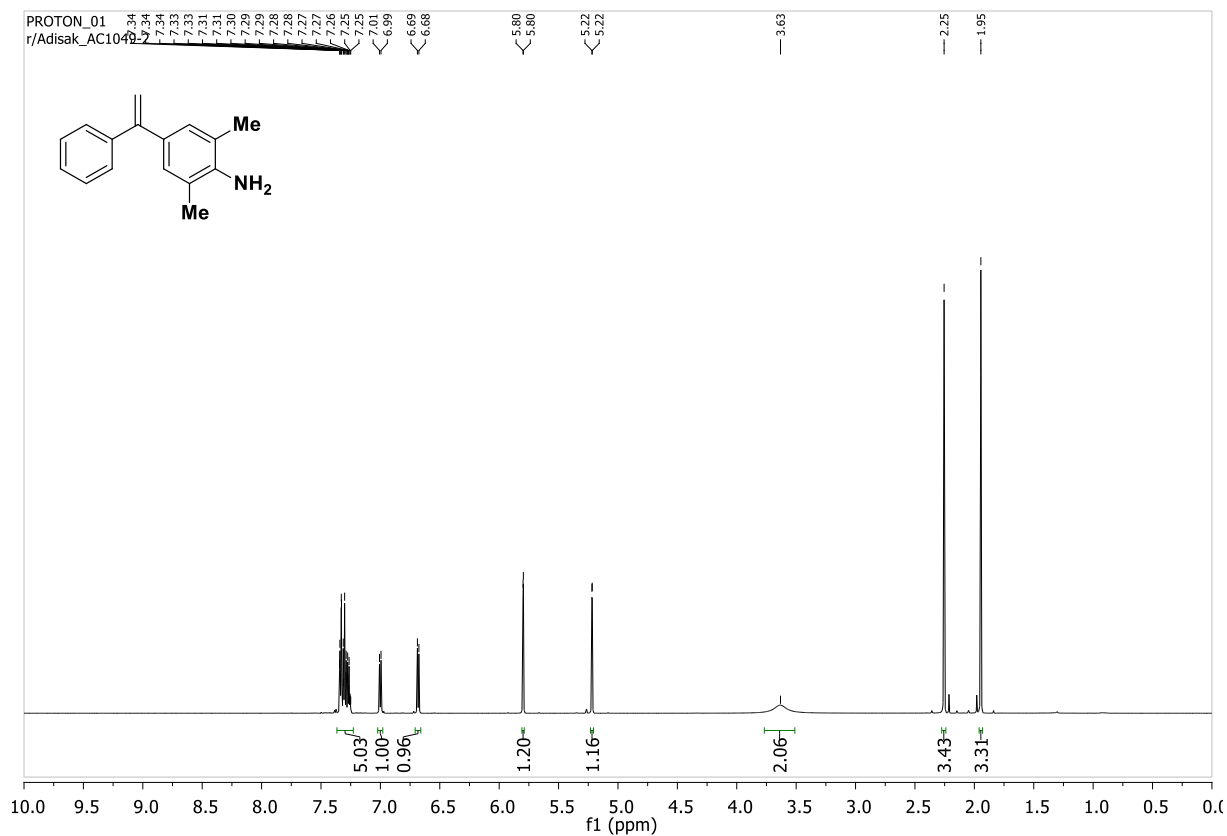


¹³C NMR Spectrum of 3af (151 MHz, CDCl₃)





¹H NMR Spectrum of 3ah (600 MHz, CDCl₃)



¹³C NMR Spectrum of 3ah (151 MHz, CDCl₃)

