Supporting Information

Lithium bromide: an inexpensive and efficient catalyst for hydroboration of imines with pinacolborane at room temperature

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1. Experimental Section

General Information

All glassware used was dried thoroughly in an oven, assembled hot, and cooled under a stream of dry nitrogen prior to use. All reactions and manipulations of air- and moisture-sensitive materials were carried out using standard techniques for the handling of such materials. All chemicals were commercial products of the highest purity which were further purified before use by using standard methods. Lithium bromide, HBpin, aldehydes, ketones and amines were purchased from Aldrich Chemical Company, Alfa Aesar, and Tokyo Chemical Industry Company (TCI). Imines were synthesized using amine, aldehyde, and ketone. ^{1}H NMR spectra were measured at 400 MHz with $CDCl_3$ as a solvent at ambient temperature unless otherwise indicated and the chemical shifts were recorded in parts per million downfield from tetramethylsilane (δ = 0 ppm) or based on residual $CDCl_3$ (δ = 7.26 ppm) as the internal standard. ^{13}C NMR spectra were recorded at 100 MHz with $CDCl_3$ as a solvent and referenced to the central line of the solvent (δ = 77.0 ppm). The coupling constants (*J*) are reported in hertz. Analytical thin-layer chromatography (TLC) was performed on glass precoated with silica gel (Merck, silica gel 60 F254). Column chromatography was carried out using 70–230 mesh silica gel (Merck) at normal pressure. GC analyses were performed on a Younglin Acme 6100M and 6500GC FID chromatography, using an HP-5 capillary column (30m). All GC yields were determined with the use of naphthalene as the internal standard and the authentic sample.

Catalytic hydroboration of aldimines (Table 3)

The following experimental procedure for the synthesis of *N*-benzylaniline (2a) is representative. A dry and argon-flushed flask, equipped with a magnetic stirring bar was charged with lithium bromide (0.0026 g, 3 mol%), N-benzylidenaniline (0.1812 g, 1.0 mmol) and 0.5 mL of THF at room temperature. To this, pinacolborane (0.22 mL, 1.5 mmol) was added dropwise under nitrogen atmosphere and stirred for 1 h. After completion of the reaction, unreacted substrates were quenched by the addition of 2 drops of water. The crude mixture was extracted with ethyl acetate and combined organic layers were dried over $MgSO_4$. Solvents (volatiles) were evaporated under reduced presser, residue mixture was subjected to column chromatography using silica gel. Isolated compounds were analyzed by spectroscopic data.

Catalytic hydroboration of ketimines (Table 5)

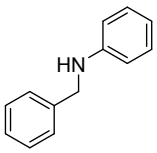
The following experimental procedure for the synthesis of *N*-(1-phenylethyl)aniline (4a) is representative. A dry and argon-flushed flask, equipped with a magnetic stirring bar was charged with lithium bromide (0.0026 g, 3 mol%), *N*,1-diphenylethan-1-imine (0.1953 g, 1.0 mmol) and 0.5 mL of THF at room temperature. To this, pinacolborane (0.29 mL, 2.0 mmol) was added dropwise under nitrogen atmosphere and stirred for 30 min. After completion of the reaction, unreacted substrates were quenched by the addition of 2 drops of water. The crude mixture was extracted with ethyl acetate and combined organic layers were dried over $MgSO_4$. Solvents (volatiles) were evaporated under reduced presser, residue mixture was subjected to column chromatography using silica gel. Isolated compounds were analyzed by spectroscopic data.

Chemoselective catalytic hydroboration of imine over various functional groups (Table 6)

The following experimental procedure for the reaction of *N*-benzylidenaniline over ester is representative. A dry and argon-flushed flask, equipped with a magnetic stirring bar was charged with lithium bromide (0.0026 g, 3 mol%), *N*-benzylidenaniline (0.1812 g, 1.0 mmol), ethyl benzoate (0.14 ml, 1.0 mmol), ethyl hexanoate (0.17 ml, 1.0 mmol) and 0.5 mL of THF at room temperature. To this, pinacolborane (0.22 mL, 1.5 mmol) was added dropwise under nitrogen atmosphere and stirred for 1 h. The reaction was stopped by H_2O. To the reaction mixture was added 1 *N* NaOH (2 mL) with stirring for 1 h at room temperature. After all products in Table 3 were confirmed through comparison with GC data of the authentic sample.

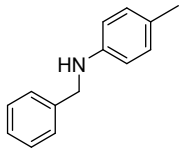
2. Characterization of the products.

***N*-Benzylaniline (2a)**



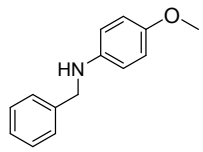
White solid. Yield. 178 mg (97%). ^{1}H NMR(400 MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 4H), 7.31 – 7.25 (m, 1H), 7.21 – 7.14 (m, 2H), 6.72 (tt, *J* = 7.4, 1.1 Hz, 1H), 6.64 (dd, *J* = 8.6, 1.0 Hz, 2H), 4.33 (s, 2H), 4.03 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.23, 139.50, 129.37, 128.73, 127.61, 127.33, 117.65, 112.92, 48.41 ppm. NMR data was in accordance with reported literature[S1]

***N*-Benzyl-4-methylaniline (2b)**



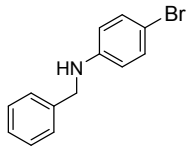
Pale yellow oil. Yield. 187 mg (95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.30 (m, 4H), 7.29 – 7.24 (m, 1H), 6.99 (d, *J* = 8.5 Hz, 2H), 6.59 – 6.54 (m, 2H), 4.31 (s, 2H), 3.91 (bs, 1H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.01, 139.74, 129.84, 128.69, 127.59, 127.25, 126.84, 113.07, 48.72, 20.50 ppm. NMR data was in accordance with reported literature[S1]

***N*-Benzyl-4-methoxyaniline (2c)**



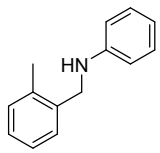
Pale yellow solid. Yield. 202 mg (95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 4H), 7.28 (dd, *J* = 6.4, 2.1 Hz, 1H), 6.80 – 6.74 (m, 2H), 6.64 – 6.57 (m, 2H), 4.28 (s, 2H), 3.83 (bs, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.28, 142.46, 139.71, 128.69, 127.66, 127.28, 114.97, 114.22, 55.89, 49.35 ppm. NMR data was in accordance with reported literature[S1]

***N*-Benzyl-4-bromoaniline (2d)**



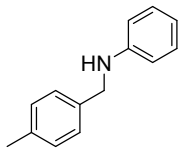
Pale yellow solid. Yield. 254 mg (97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 4.5 Hz, 4H), 7.31 – 7.26 (m, 1H), 7.25 – 7.21 (m, 2H), 6.52 – 6.48 (m, 2H), 4.30 (s, 2H), 4.08 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.12, 138.94, 132.03, 128.81, 127.50, 127.48, 114.50, 109.20, 48.30 ppm. NMR data was in accordance with reported literature[S1]

***N*-(2-Methylbenzyl)aniline (2e)**



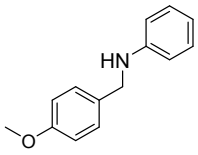
Pale yellow solid. Yield. 193 mg (98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 6.7 Hz, 1H), 7.23 – 7.14 (m, 5H), 6.72 (tt, *J* = 7.4, 1.0 Hz, 1H), 6.63 (dd, *J* = 8.6, 1.0 Hz, 2H), 4.26 (s, 2H), 3.84 (bs, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.37, 137.08, 136.45, 130.51, 129.38, 128.35, 127.52, 126.26, 117.54, 112.76, 46.47, 19.05 ppm. NMR data was in accordance with reported literature[S2]

_N_-(4-Methylbenzyl)aniline (2f)



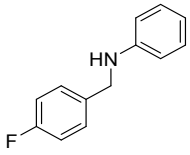
Pale yellow solid. Yield. 195 mg (99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.24 (m, 2H), 7.18 – 7.12 (m, 4H), 6.70 (td, *J* = 7.4, 0.9 Hz, 1H), 6.65 – 6.60 (m, 2H), 4.27 (s, 2H), 3.99 (bs, 1H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.26, 136.98, 136.38, 129.39, 129.34, 127.61, 117.58, 112.91, 48.16, 21.21 ppm. NMR data was in accordance with reported literature[S1]

_N_-(4-Methoxybenzyl)aniline (2g)



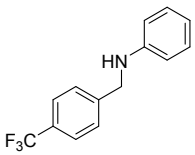
Pale yellow solid. Yield. 209 mg (98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.8 Hz, 2H), 7.23 – 7.13 (m, 2H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.71 (tt, *J* = 7.3, 1.1 Hz, 1H), 6.64 (dt, *J* = 7.7, 1.1 Hz, 2H), 4.25 (s, 2H), 3.95 (bs, 1H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) 158.93, 148.28, 131.47, 129.35, 128.92, 117.59, 114.10, 112.91, 55.40, 47.88 ppm. NMR data was in accordance with reported literature[S1]

_N_-(4-Fluorobenzyl)aniline (2h)



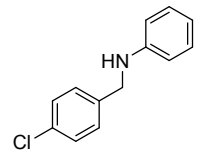
Pale yellow oil. Yield. 191 mg (95%). ^{1}H NMR(400 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 8.5, 5.7 Hz, 2H), 7.20 – 7.14 (m, 2H), 7.06 – 6.98 (m, 2H), 6.75 – 6.69 (m, 1H), 6.64 – 6.59 (m, 2H), 4.30 (s, 2H), 4.02 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.13, (d, J_{C-F} = 245.43 Hz), 148.00, 135.17 (d, J_{C-F} = 3.03 Hz), 129.38, 129.09 (d, J_{C-F} = 8.08 Hz), 117.83, 115.54 (d, J_{C-F} = 21.21 Hz), 112.95, 47.70 ppm. NMR data was in accordance with reported literature[S3]

_N_-(4-(Trifluoromethyl)benzyl)aniline (2i)



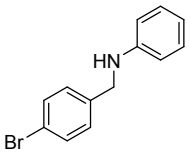
Pale yellow oil. Yield. 246 mg (98%). ^{1}H NMR(400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.1 Hz, 2H), 7.48 (d, *J* = 8.1 Hz, 2H), 7.17 (t, *J* = 8.0 Hz, 2H), 6.73 (t, *J* = 7.8 Hz, 1H), 6.60 (d, *J* = 8.5 Hz, 2H), 4.41 (s, 2H), 4.14 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.72, 143.82, 129.44, 127.52, 125.66 (q, *J* = 4.04 Hz),118.05, 112.97, 47.86 ppm. NMR data was in accordance with reported literature[S4]

_N_-(4-Chlorobenzyl)aniline (2j)



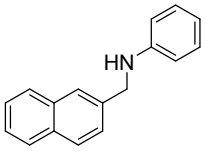
Pale yellow solid. Yield. 209 mg (96%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (s, 4H), 7.19 – 7.13 (m, 2H), 6.72 (td, *J* = 7.4, 0.8 Hz, 1H), 6.60 (dd, *J* = 8.5, 0.8 Hz, 2H), 4.30 (s, 2H), 4.06 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.87, 138.05, 132.95, 129.39, 128.84, 128.78, 117.90, 112.97, 47.70 ppm. NMR data was in accordance with reported literature[S1]

***N*-(4-Bromobenzyl)aniline (2k)**



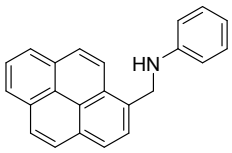
Pale yellow solid. Yield. 257 mg (98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.38 (m, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.20 – 7.13 (m, 2H), 6.72 (tt, *J* = 7.4, 1.0 Hz, 1H), 6.60 (dd, *J* = 8.6, 1.0 Hz, 2H), 4.29 (s, 2H), 4.07 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.85, 138.60, 131.79, 129.40, 129.14, 121.01, 117.91, 112.96, 47.73 ppm. NMR data was in accordance with reported literature[S1]

***N*-(Naphthalen-2-ylmethyl)aniline (2l)**



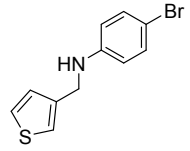
Pale yellow solid. Yield. 226 mg (97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.78 (m, 4H), 7.53 – 7.42 (m, 3H), 7.21 – 7.14 (m, 2H), 6.72 (tt, *J* = 7.4, 1.0 Hz, 1H), 6.70 – 6.64 (m, 2H), 4.50 (s, 2H), 4.16 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.23, 137.01, 133.57, 132.84, 129.39, 128.47, 127.85, 127.79, 126.26, 126.01, 125.82, 117.74, 113.03, 48.61 ppm. NMR data was in accordance with reported literature[S1]

***N*-(Pyren-1-ylmethyl)aniline (2m)**



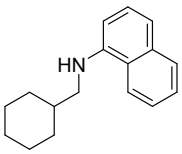
Yellow solid. Yield. 301 mg (98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 9.2 Hz, 1H), 8.20 (d, *J* = 7.6 Hz, 2H), 8.17 – 8.10 (m, 2H), 8.10 – 8.04 (m, 3H), 8.02 (td, *J* = 7.7, 0.9 Hz, 1H), 7.25 – 7.19 (m, 2H), 6.77 (dd, *J* = 12.3, 8.4 Hz, 3H), 4.99 (s, 2H), 4.10 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.37, 132.21, 131.39, 131.11, 130.90, 129.49, 129.09, 128.05, 127.54, 127.46, 126.83, 126.15, 125.41, 125.34, 125.15, 124.95, 123.11, 117.80, 112.91, 46.86 ppm.NMR data was in accordance with reported literature[S5]

4-Bromo-*N*-(thiophen-3-ylmethyl)aniline (2n)



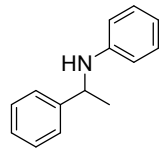
Pale yellow solid. Yield. 263 mg (98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.25 – 7.22 (m, 2H), 7.16 (dq, *J* = 3.0, 0.9 Hz, 1H), 7.05 (dd, *J* = 5.0, 1.3 Hz, 1H), 6.52 – 6.49 (m, 2H), 4.30 (s, 2H), 4.02 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.00, 139.97, 132.04, 127.09, 126.45, 121.93, 114.56, 109.36, 43.79 ppm. NMR data was in accordance with reported literature[S6]

***N*-(Cyclohexylmethyl)naphthalen-1-amine (2o)**



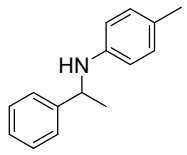
Pale yellow liquid. Yield. 227 mg (95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.72 (m, 2H), 7.49 – 7.38 (m, 2H), 7.39 – 7.28 (m, 1H), 7.21 (d, *J* = 8.2 Hz, 1H), 6.60 (d, *J* = 7.5 Hz, 1H), 4.45 (bs, 1H), 3.12 (d, *J* = 6.7 Hz, 7H), 1.92 (d, *J* = 13.2 Hz, 2H), 1.81 – 1.65 (m, 4H), 1.36 – 1.17 (m, 3H), 1.08 (qd, *J* = 12.2, 3.0 Hz, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.69, 134.41, 128.79, 126.77, 125.74, 124.67, 123.39, 119.85, 116.99, 104.25, 50.96, 37.49, 31.65, 26.69, 26.12. ppm. NMR data was in accordance with reported literature[S6]

***N*-(1-Phenylethyl)aniline (4a)**



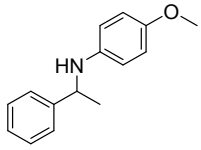
Pale yellow oil. Yield. 195 mg (99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.31 (td, *J* = 6.8, 6.3, 1.8 Hz, 2H), 7.24 – 7.18 (m, 1H), 7.12 – 7.04 (m, 2H), 6.63 (tt, *J* = 7.4, 1.0 Hz, 1H), 6.50 (dd, *J* = 8.6, 1.0 Hz, 2H), 4.48 (q, *J* = 6.7 Hz, 1H), 4.03 (bs, 1H), 1.51 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.41, 145.36, 129.24, 128.78, 127.01, 125.98, 117.36, 113.41, 53.58, 25.19 ppm. NMR data was in accordance with reported literature[S8]

4-Methyl-*N*-(1-phenylethyl)aniline (4b)



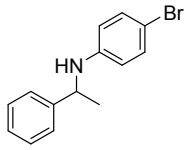
Pale yellow solid. Yield. 205 mg (97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.23 (t, *J* = 7.1 Hz, 1H), 6.91 (d, *J* = 8.1 Hz, 2H), 6.44 (d, *J* = 8.1 Hz, 2H), 4.46 (q, *J* = 6.7 Hz, 1H), 3.94 (bs, 1H), 2.19 (s, 3H), 1.52 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.51, 145.10, 129.69, 128.70, 126.89, 126.45, 125.95, 113.49, 53.77, 25.18, 20.45 ppm. NMR data was in accordance with reported literature[S9]

4-Methoxy-*N*-(1-phenylethyl)aniline (4c)



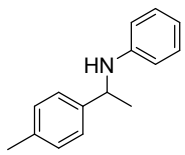
Pale yellow solid. Yield. 220 mg (97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.28 (m, 4H), 7.25 – 7.19 (m, 1H), 6.72 – 6.66 (m, 2H), 6.51 – 6.44 (m, 2H), 4.41 (q, *J* = 6.7 Hz, 1H), 3.81 (bs, 1H), 3.69 (s, 3H), 1.50 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.99, 145.58, 141.65, 128.72, 126.93, 126.00, 114.85, 114.64, 55.83, 54.36, 25.25 ppm. NMR data was in accordance with reported literature[S10]

4-Bromo-*N*-(1-phenylethyl)aniline (4d)



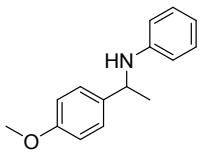
Pale yellow solid. Yield. 268 mg (97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.27 (m, 4H), 7.25 – 7.19 (m, 1H), 7.19 – 7.09 (m, 2H), 6.40 – 6.33 (m, 2H), 4.43 (q, *J* = 6.7 Hz, 1H), 4.06 (bs, 1H), 1.50 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.26, 144.70, 131.88, 128.83, 127.15, 125.85, 114.97, 108.96, 53.58, 25.08. ppm. NMR data was in accordance with reported literature[S7]

***N*-(1-(*p*-Tolyl)ethyl)aniline (4e)**



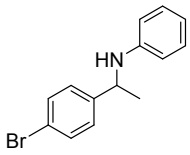
Pale yellow oil. Yield. 203 mg (96%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.23 (m, 2H), 7.15 – 7.04 (m, 4H), 6.63 (tt, *J* = 7.4, 1.0 Hz, 1H), 6.50 (dd, *J* = 8.6, 1.0 Hz, 2H), 4.45 (q, *J* = 6.7 Hz, 1H), 4.00 (bs, 1H), 2.31 (s, 3H), 1.49 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.47, 142.35, 136.52, 129.45, 129.22, 125.88, 117.27, 113.39, 53.26, 25.18, 21.21 ppm. NMR data was in accordance with reported literature[S11]

***N*-(1-(4-Methoxyphenyl)ethyl)aniline (4f)**



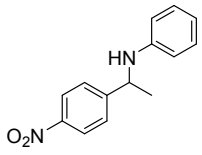
Pale yellow oil. Yield. 223 mg (98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.7 Hz, 2H), 7.12 (t, *J* = 7.9 Hz, 2H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.67 (t, *J* = 7.8 Hz, 1H), 6.54 (d, *J* = 8.5 Hz, 2H), 4.47 (q, *J* = 6.7 Hz, 1H), 4.02 (bs, 1H), 3.80 (s, 3H), 1.52 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.58, 147.47, 137.38, 129.22, 127.01, 117.28, 114.11, 113.42, 55.36, 52.93, 25.15 ppm. NMR data was in accordance with reported literature[S12]

***N*-(1-(4-Bromophenyl)ethyl)aniline (4g)**



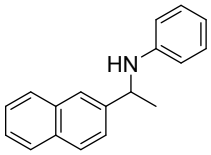
Pale yellow oil. Yield. 268 mg (97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.38 (m, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 7.08 (tt, *J* = 7.4, 1.0 Hz, 2H), 6.65 (td, *J* = 7.3, 1.0 Hz, 1H), 6.46 (dd, *J* = 7.6, 1.0 Hz, 2H), 4.42 (q, *J* = 6.7 Hz, 1H), 3.99 (bs, 1H), 1.47 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.04, 144.48, 131.85, 129.25, 127.74, 120.58, 117.63, 113.40, 53.14, 25.19 ppm. NMR data was in accordance with reported literature[S12]

***N*-(1-(4-Nitrophenyl)ethyl)aniline (4h)**



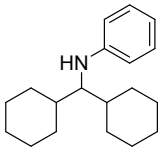
Orange oil. Yield. 235 mg (97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.13 (m, 2H), 7.58 – 7.51 (m, 2H), 7.09 (tt, *J* = 7.4, 2.1 Hz, 2H), 6.73 – 6.64 (m, 1H), 6.44 (dd, *J* = 8.6, 1.0 Hz, 2H), 4.56 (q, *J* = 6.7 Hz, 1H), 4.08 (bs, 1H), 1.54 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.26, 147.15, 146.59, 129.34, 126.79, 124.20, 118.07, 113.37, 53.41, 25.08 ppm. NMR data was in accordance with reported literature[S13]

***N*-(1-(Naphthalen-2-yl)ethyl)aniline (4i)**



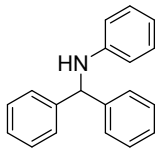
Pale yellow oil. Yield. 242 mg (98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.77 (m, 4H), 7.53 – 7.42 (m, 3H), 7.09 (t, *J* = 7.8 Hz, 2H), 6.65 (t, *J* = 7.3 Hz, 1H), 6.57 (d, *J* = 8.0 Hz, 2H), 4.65 (q, *J* = 6.7 Hz, 1H), 4.15 (bs, 1H), 1.60 (s, 3H);^{13}C NMR (100 MHz, $CDCl_3$) δ 147.37, 142.84, 133.68, 132.84, 129.23, 128.59, 127.94, 127.77, 126.11, 125.61, 124.52, 124.36, 117.46, 113.50, 53.87, 25.16 ppm. NMR data was in accordance with reported literature[S11]

***N*-(Dicyclohexylmethyl)aniline (4j)**



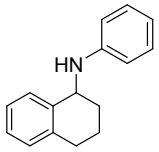
White solid. Yield. 5263 mg (97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (dd, *J* = 8.4, 7.4 Hz, 2H), 6.55 (t, *J* = 8.1 Hz, 3H), 3.35 (bs, 1H), 2.98 (s, 1H), 1.80 – 1.56 (m, 10H), 1.52 – 1.42 (m, 2H), 1.29 – 0.86 (m, 11H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.37, 129.28, 115.79, 112.27, 62.65, 40.76, 31.20, 28.34, 26.63, 26.57, 26.48 ppm. HRMS(EI-MS) Calcd for $C_{19}H_{29}N$: 271.2300. Found: 271.2298.

_N_-Benzhydrylaniline (4k)



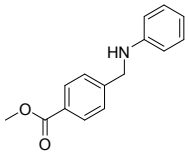
Yellow oil. Yield. 246 mg (95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.28 (m, 8H), 7.28 – 7.25 (m, 1H), 7.25 – 7.22 (m, 1H), 7.13 – 7.08 (m, 2H), 6.68 (t, *J* = 7.3 Hz, 1H), 6.53 (dd, *J* = 8.6, 1.0 Hz, 2H), 5.49 (s, 1H), 4.22 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$). δ 147.46, 143.04, 129.23, 128.86, 127.56, 127.47, 117.76, 113.58, 63.15 ppm. NMR data was in accordance with reported literature[S14]

_N_ -Phenyl-1,2,3,4-tetrahydronaphthalen-1-amine (4l)



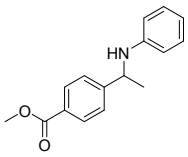
Pale yellow oil. Yield. 216 mg (97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.0 Hz, 1H), 7.24 – 7.08 (m, 5H), 6.74 – 6.62 (m, 3H), 4.63 (t, *J* = 4.9 Hz, 1H), 3.87 (bs, 1H), 2.90 – 2.67 (m, 2H), 2.01 – 1.74 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.56, 138.30, 137.77, 129.53, 129.41, 129.18, 127.28, 126.24, 117.21, 112.94, 51.12, 29.47, 28.83, 19.51 ppm. NMR data was in accordance with reported literature[S15]

Methyl 4-((phenylamino)methyl)benzoate (6a)



Pale yellow oil. Yield. 236 mg (98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.17 (dd, *J* = 8.6, 7.4 Hz, 2H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.61 (d, *J* = 7.6 Hz, 2H), 4.40 (s, 2H), 4.17 (bs, 1H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.08, 147.90, 145.13, 130.07, 129.43, 129.17, 127.25, 117.93, 113.00, 52.21, 48.06 ppm. NMR data was in accordance with reported literature[S16]

Methyl 4-((phenylamino)ethyl)benzoate (6b)



White solid. Yield. 247 mg (97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.3 Hz, 2H), 7.43 (d, *J* = 8.3 Hz, 2H), 7.11 – 7.02 (m, 2H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.46 (d, *J* = 8.5 Hz, 2H), 4.51 (q, *J* = 6.7 Hz, 1H), 4.04 (bs, 1H), 3.89 (s, 3H), 1.51 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.09, 150.86, 147.00, 130.19, 129.24, 128.98, 125.96, 117.66, 113.38, 53.55, 52.13, 25.06 ppm.

HRMS(EI-MS)

Calcd for $C_{16}H_{17}NO_2$: 255.1259. Found: 255.1261.

3. Copies of NMR spectra

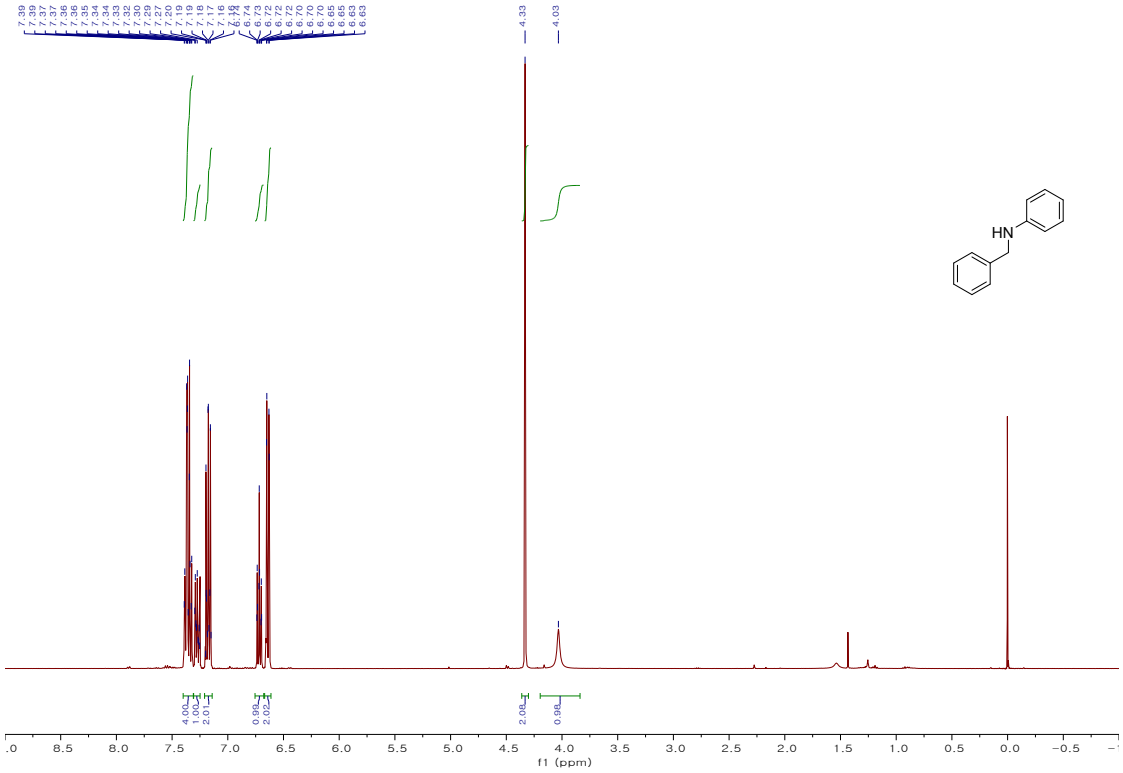


Figure S1: ^{1}H NMR of *N*-benzylaniline (**2a**)

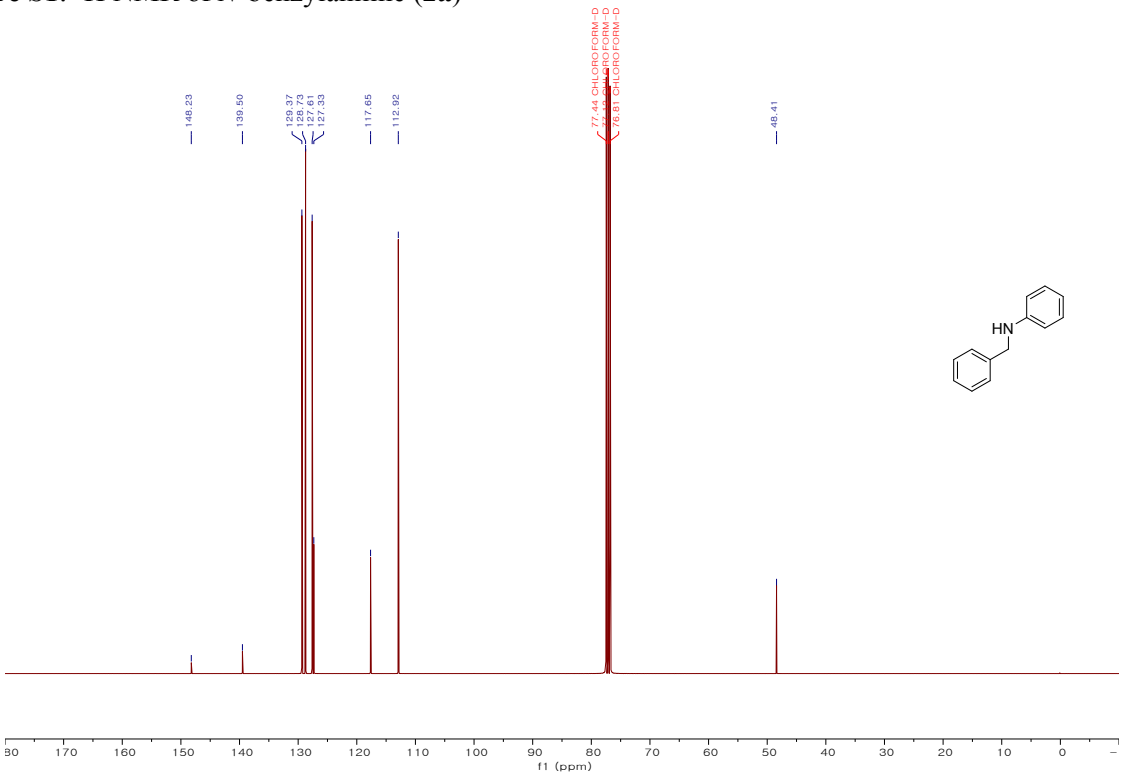


Figure S2: ^{13}C NMR of *N*-benzylaniline (**2a**)

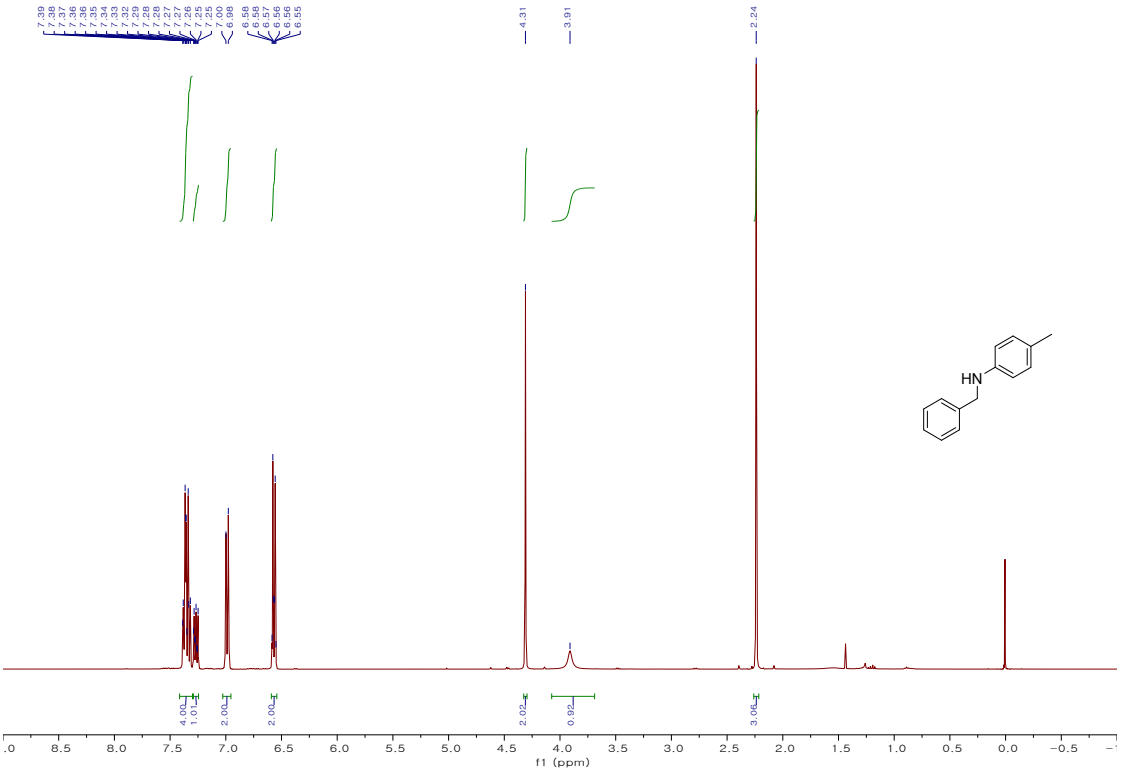


Figure S3: ^{1}H NMR of *N*-benzyl-4-methylaniline (**2b**)

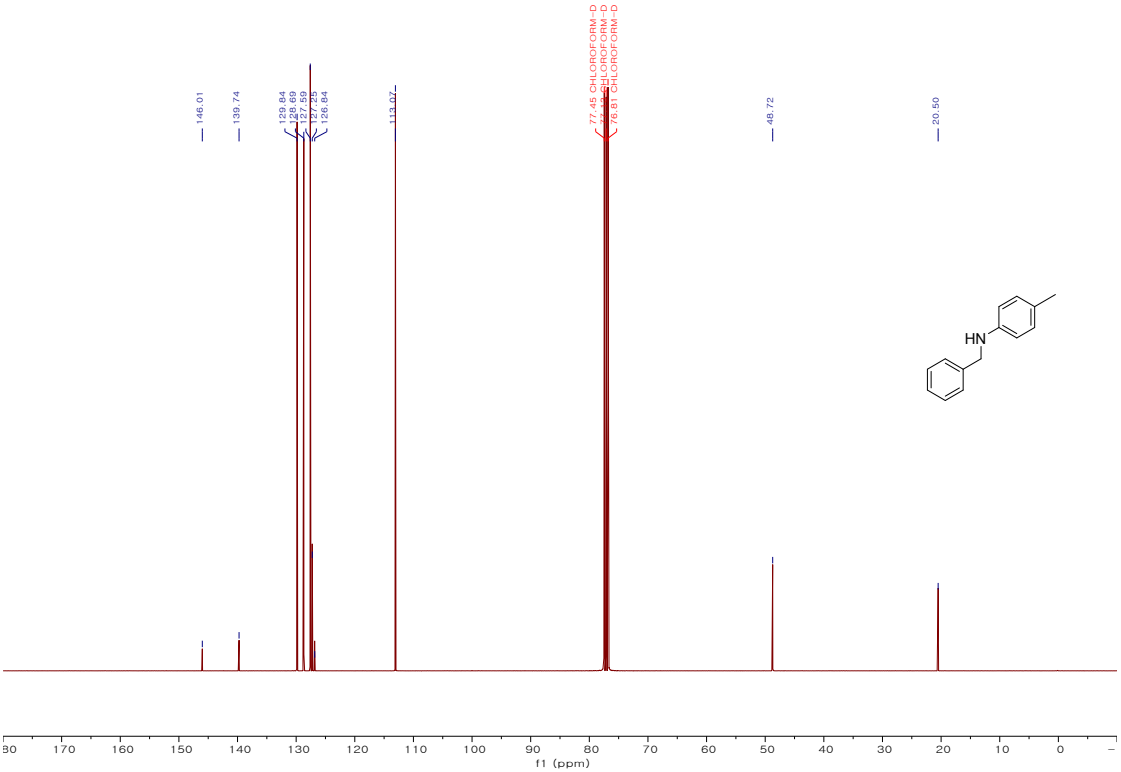


Figure S4: ^{13}C NMR of *N*-benzyl-4-methylaniline (**2b**)

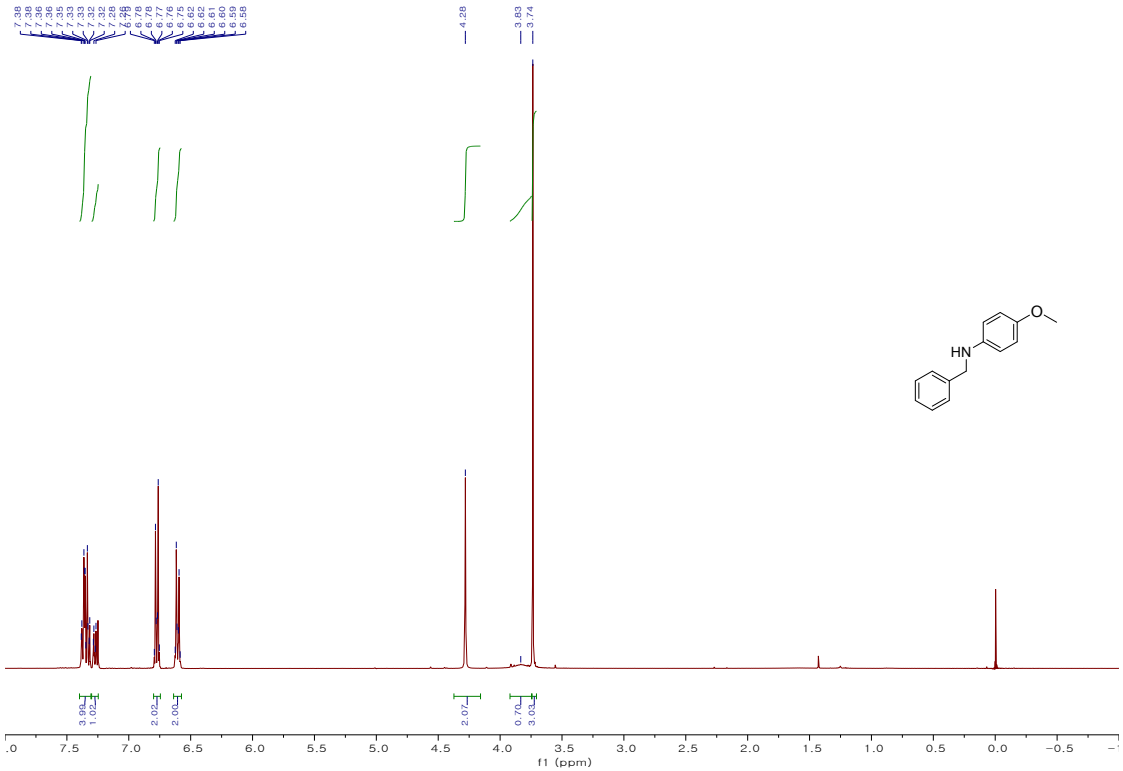


Figure S5: [1]H NMR of *N*-benzyl-4-methoxyaniline (**2c**)

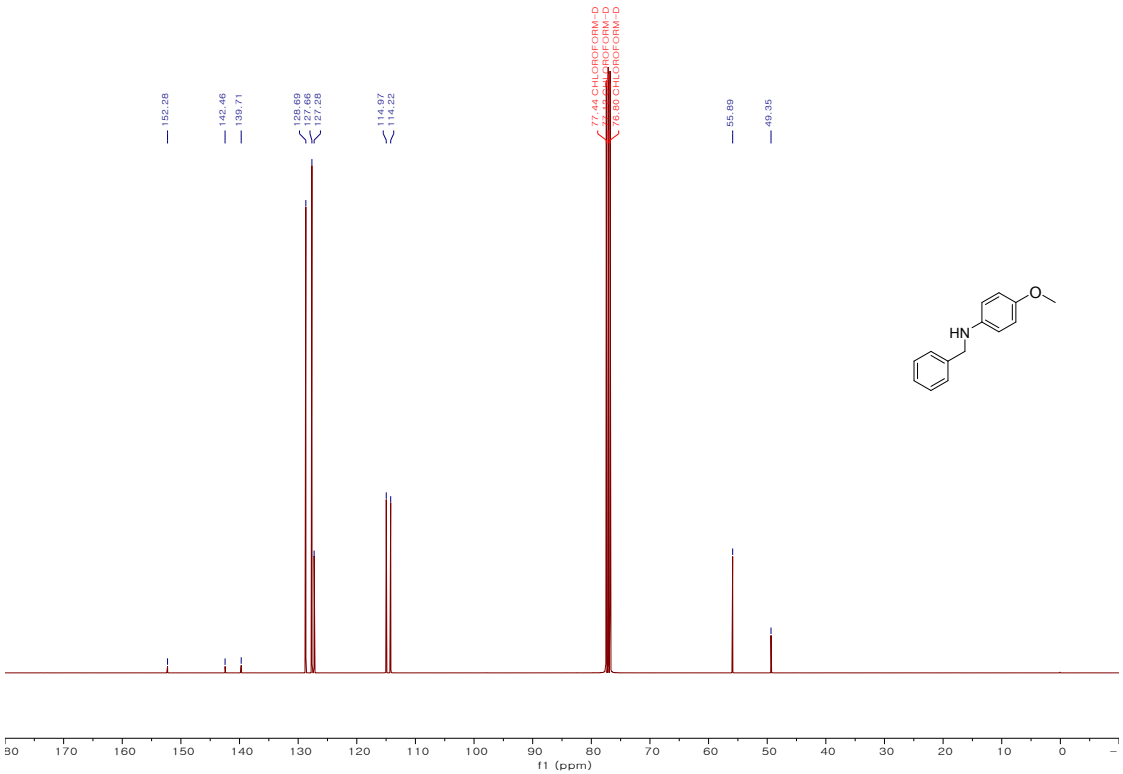


Figure S6: [13]C NMR of *N*-benzyl-4-methoxyaniline (**2c**)

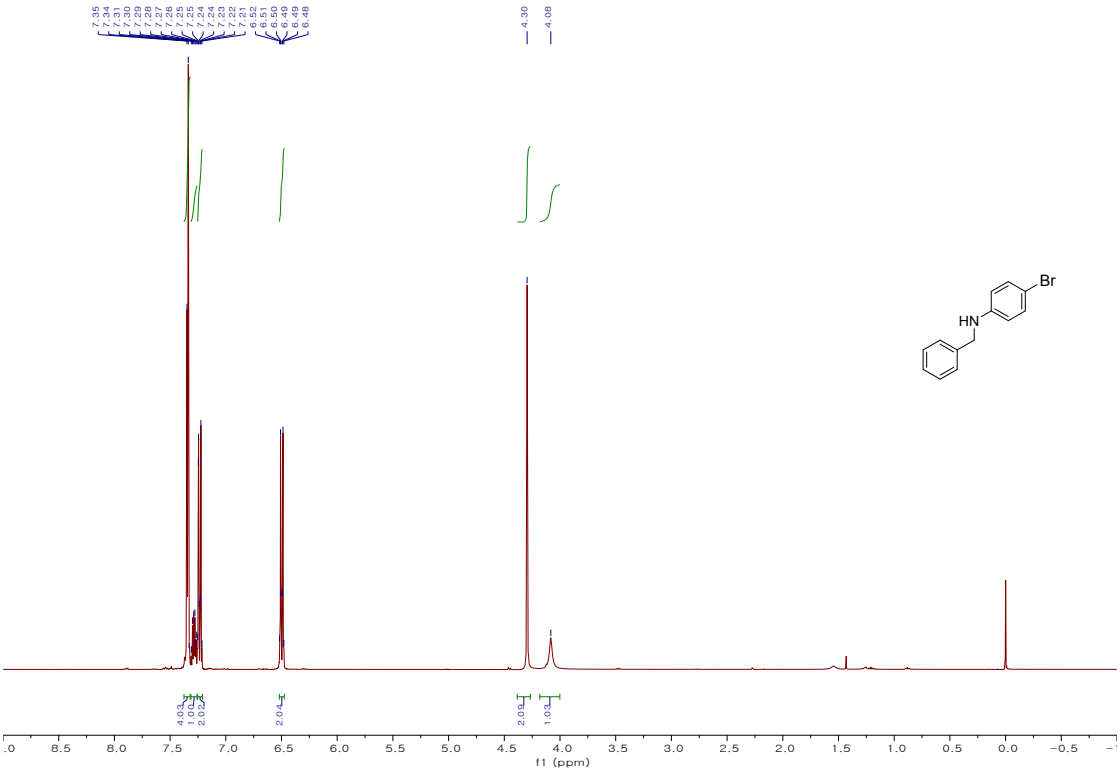


Figure S7: [1]H NMR of *N*-benzyl-4-bromoaniline (**2d**)

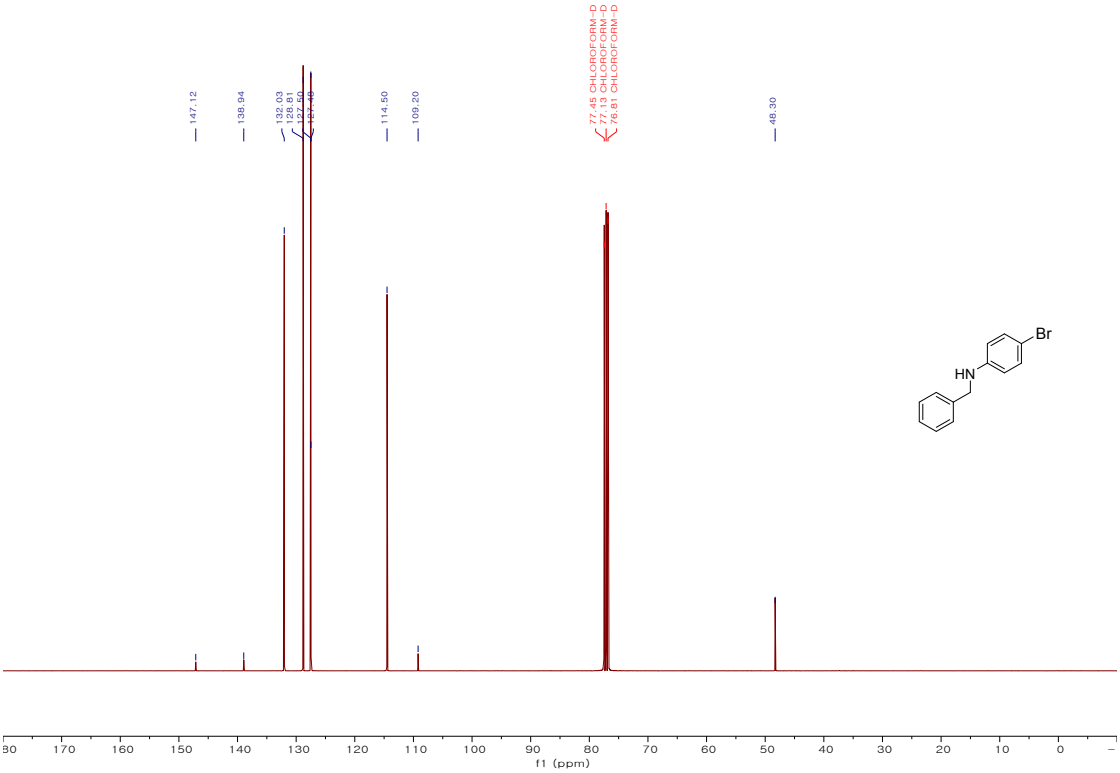


Figure S8: [13]C NMR of *N*-benzyl-4-bromoaniline (**2d**)

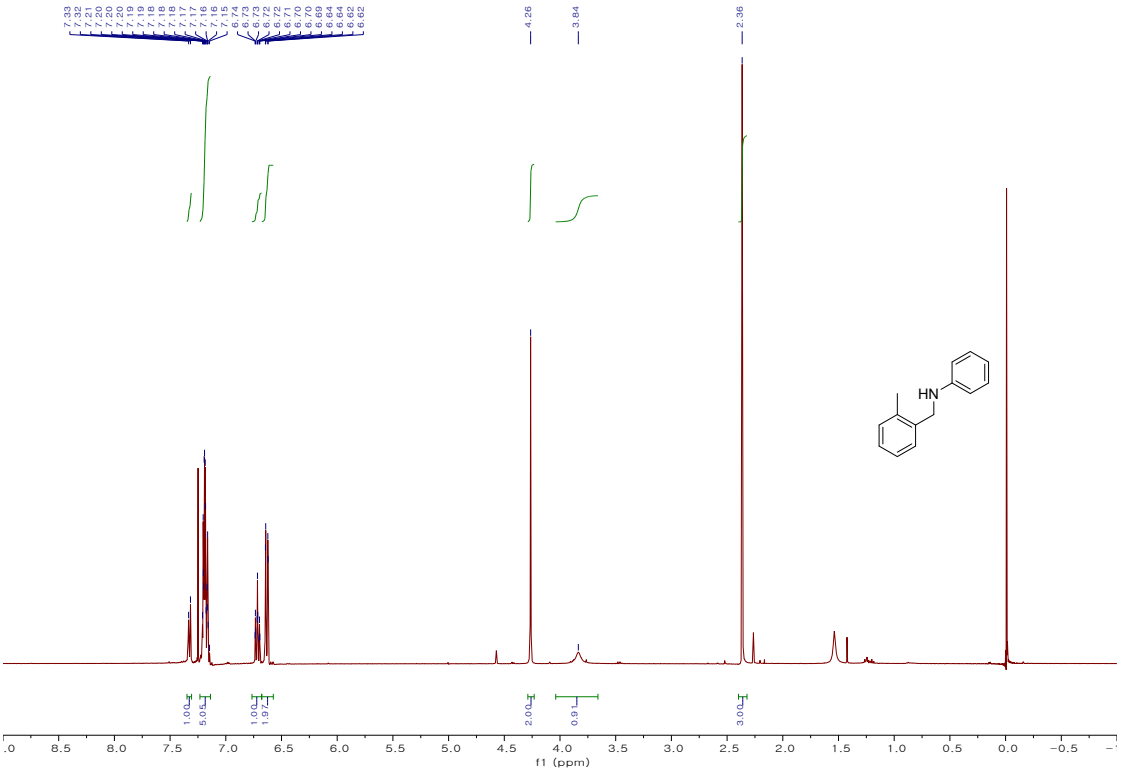


Figure S9: [1]H NMR of *N*-(2-methylbenzyl)aniline (**2e**)

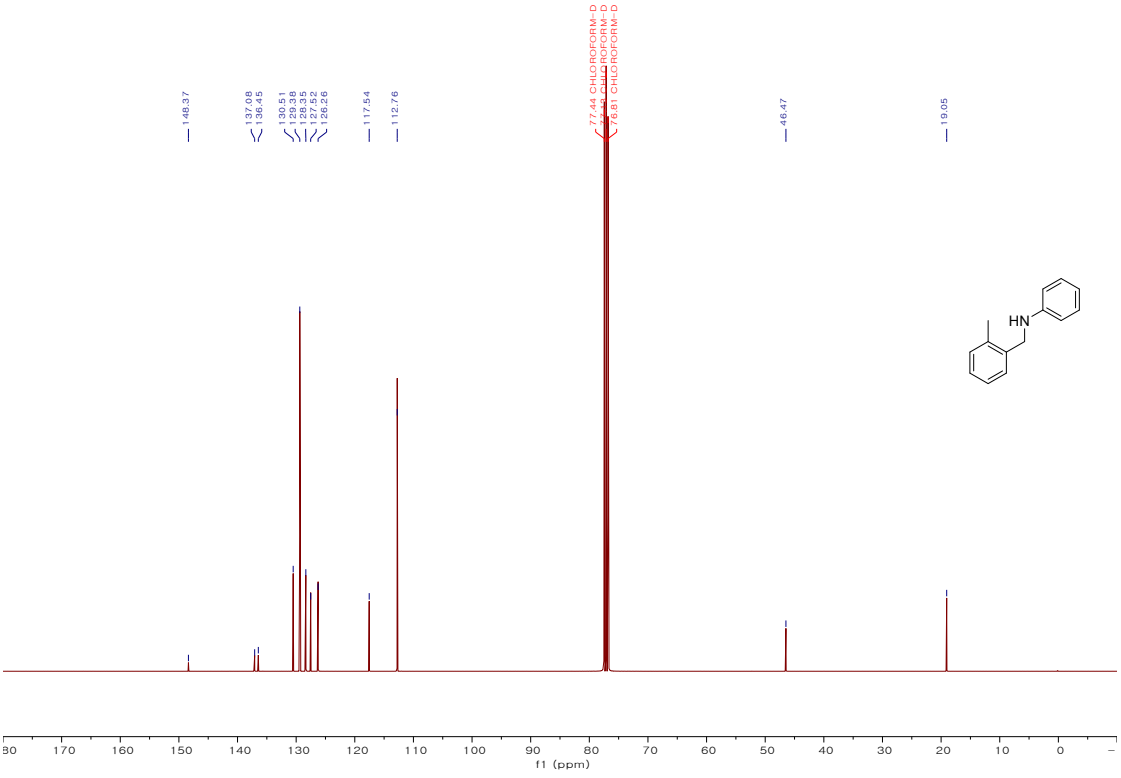


Figure S10: [13]C NMR of *N*-(2-methylbenzyl)aniline (**2e**)

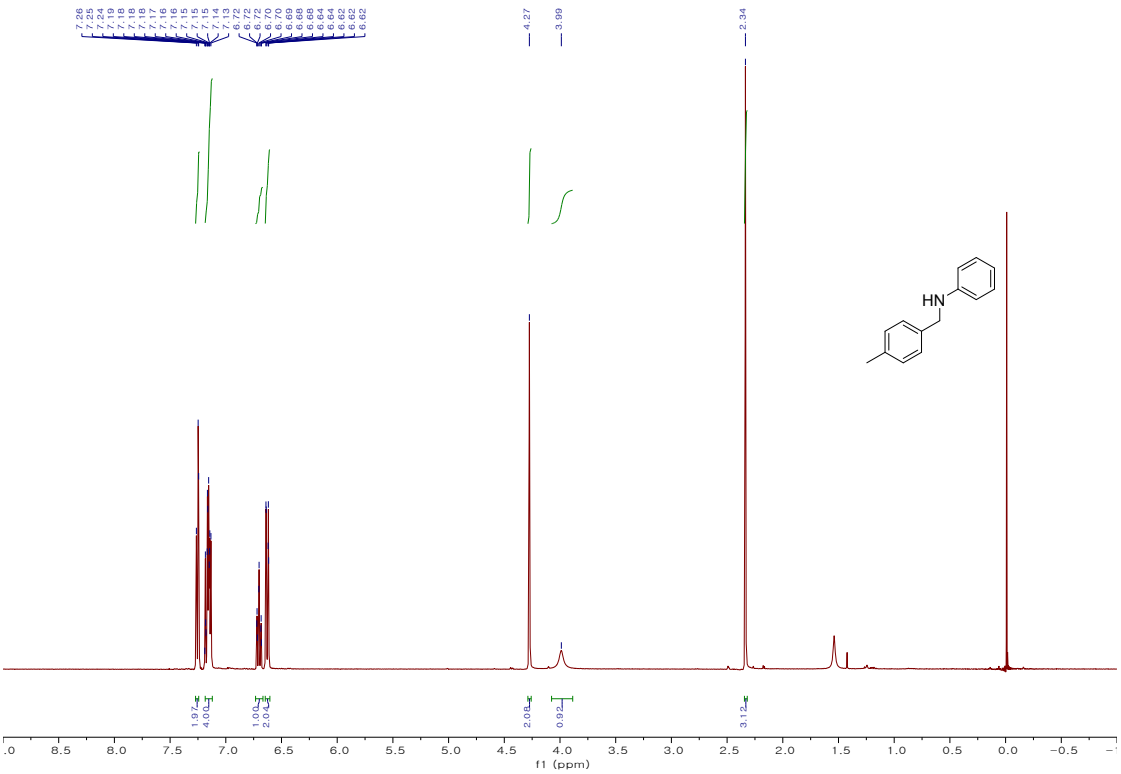


Figure S11: [1]H NMR of *N*-(4-methylbenzyl)aniline (**2f**)

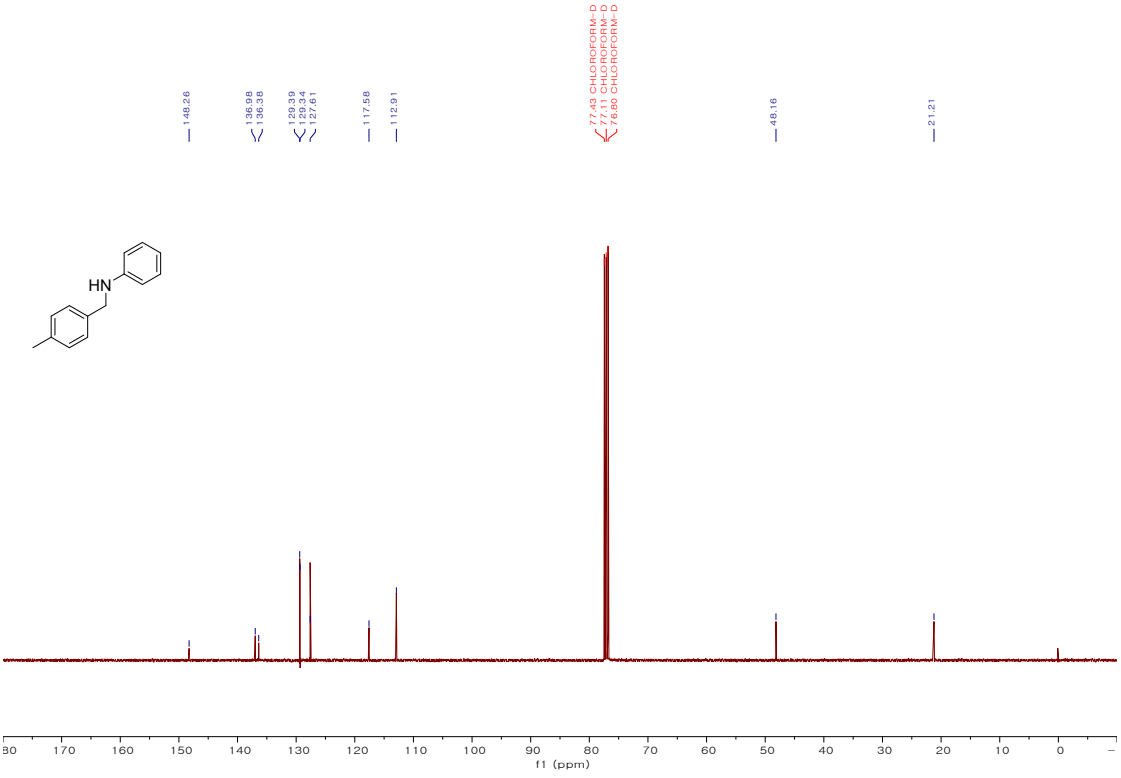


Figure S12: [13]C NMR of *N*-(4-methylbenzyl)aniline (**2f**)

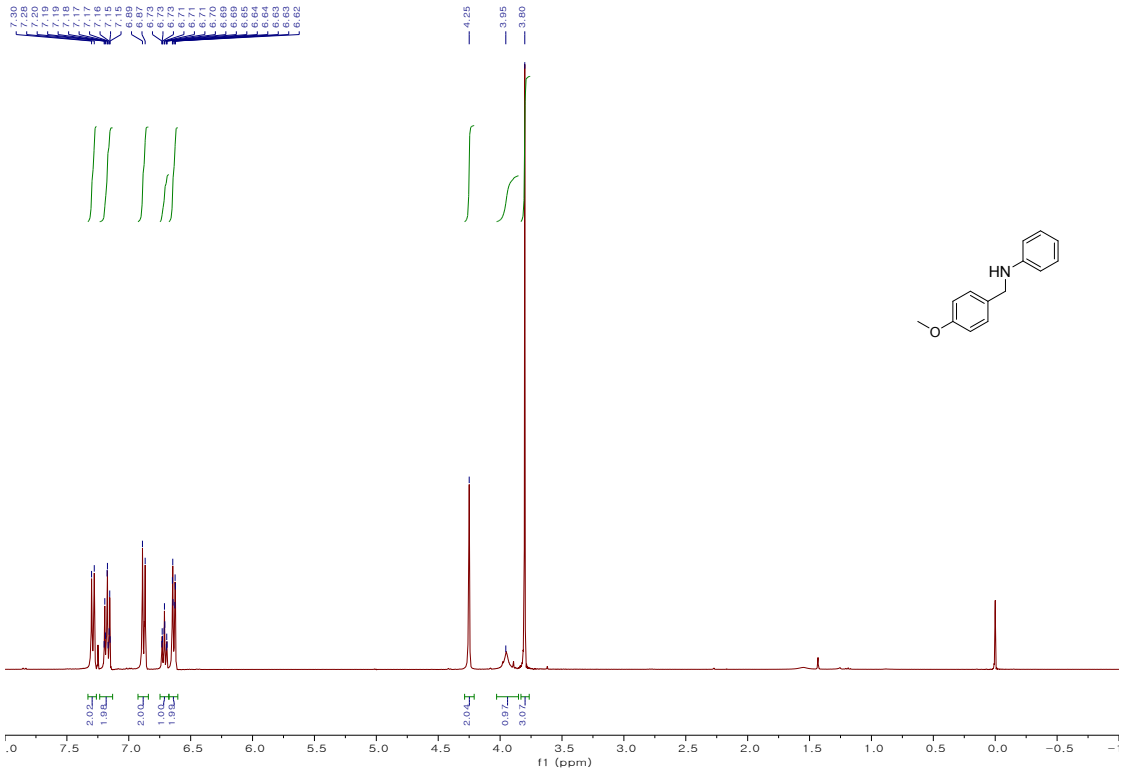


Figure S13: [1]H NMR of *N*-(4-methoxybenzyl)aniline (**2g**)

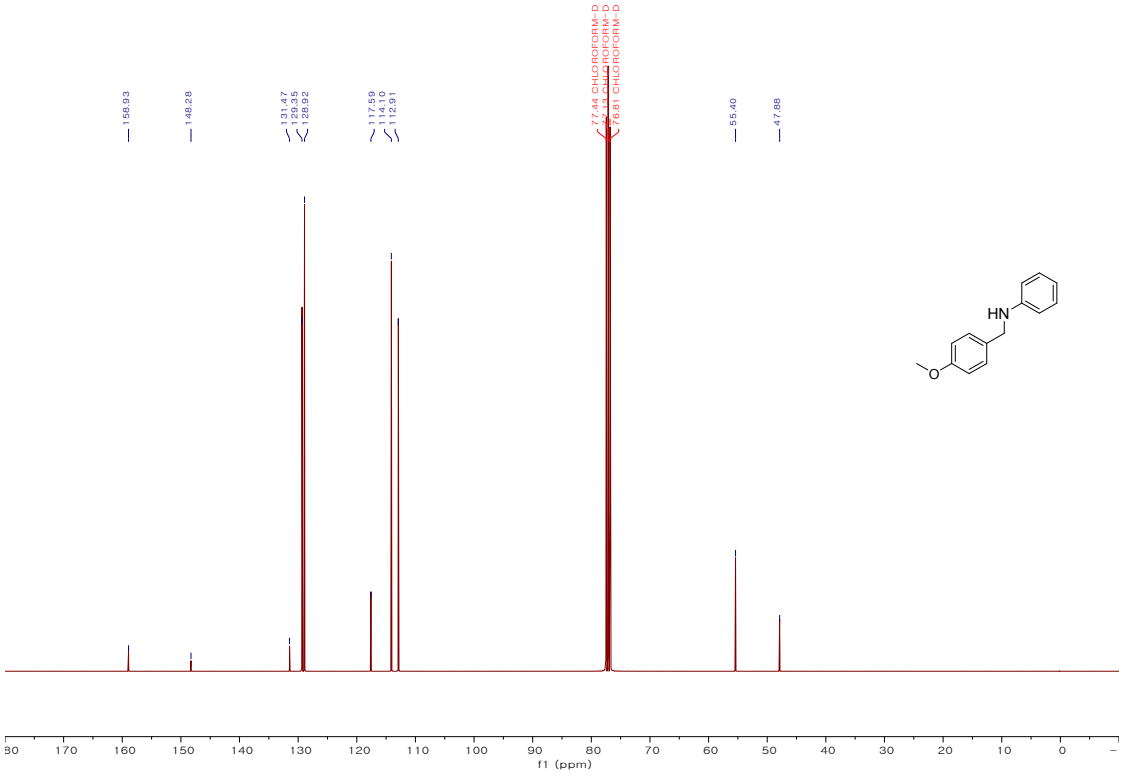


Figure S14: [13]C NMR of *N*-(4-methoxybenzyl)aniline (**2g**)

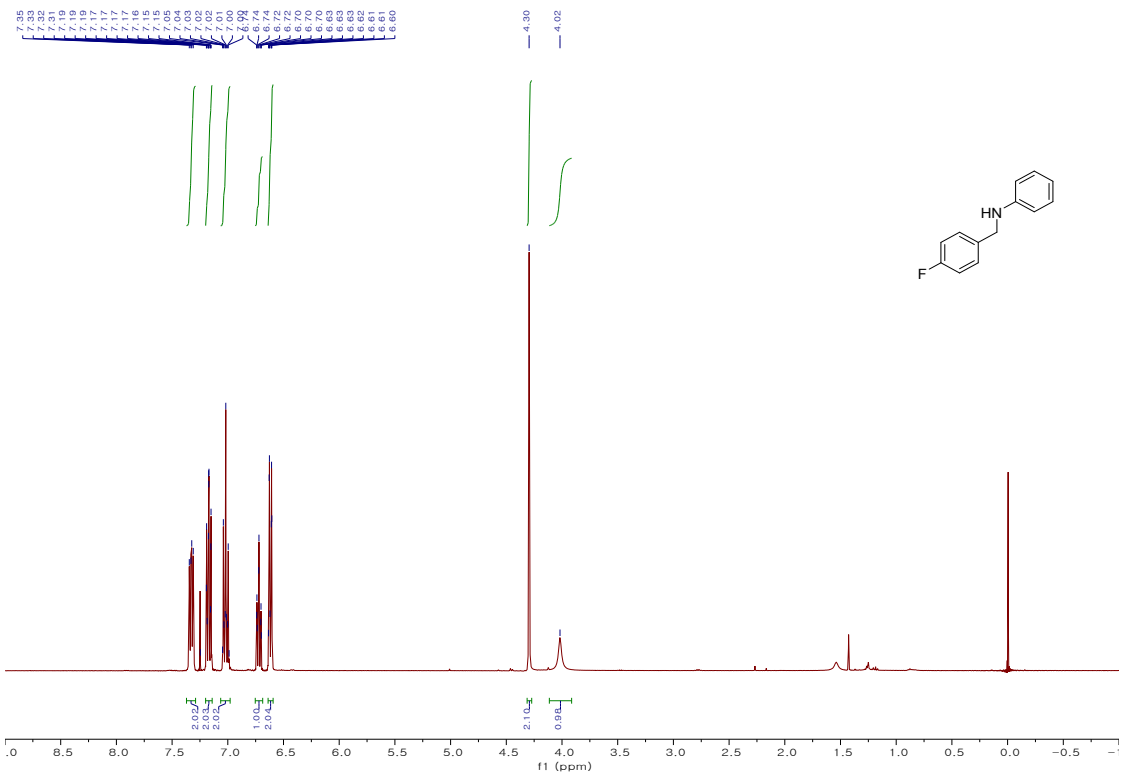


Figure S15: ^{1}H NMR of *N*-(4-fluorobenzyl)aniline (**2h**)

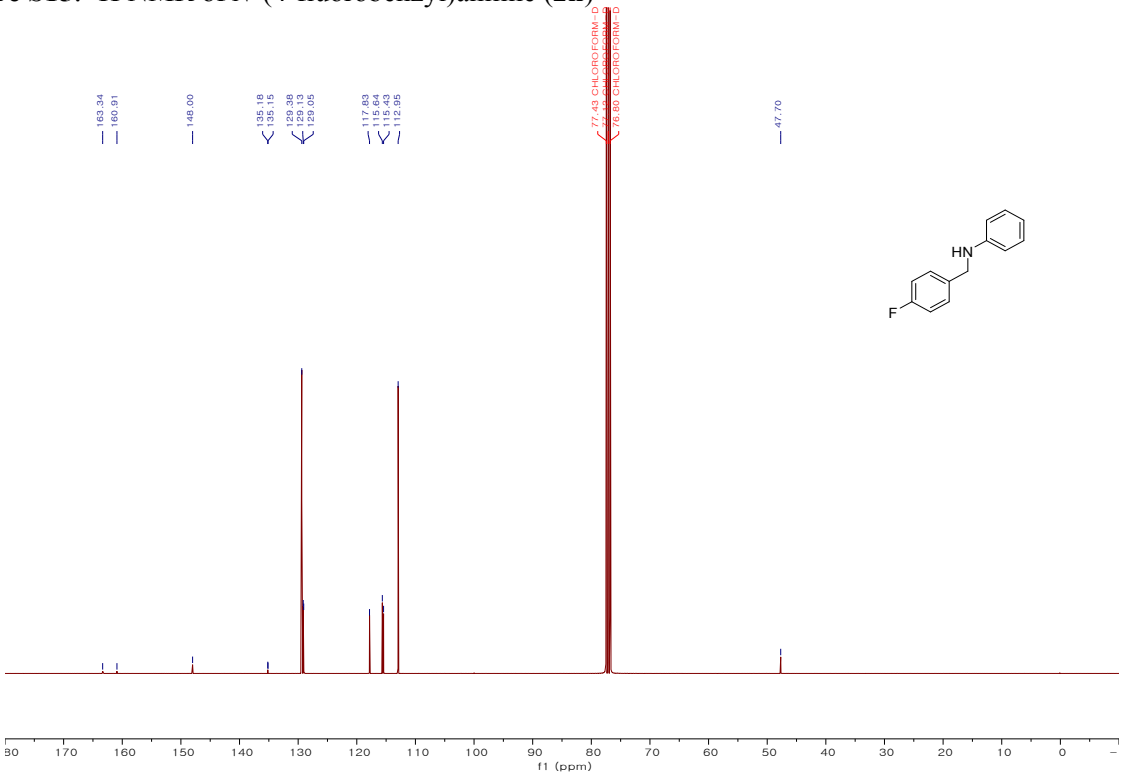


Figure S16: ^{13}C NMR of *N* -(4-fluorobenzyl)aniline (**2h**)

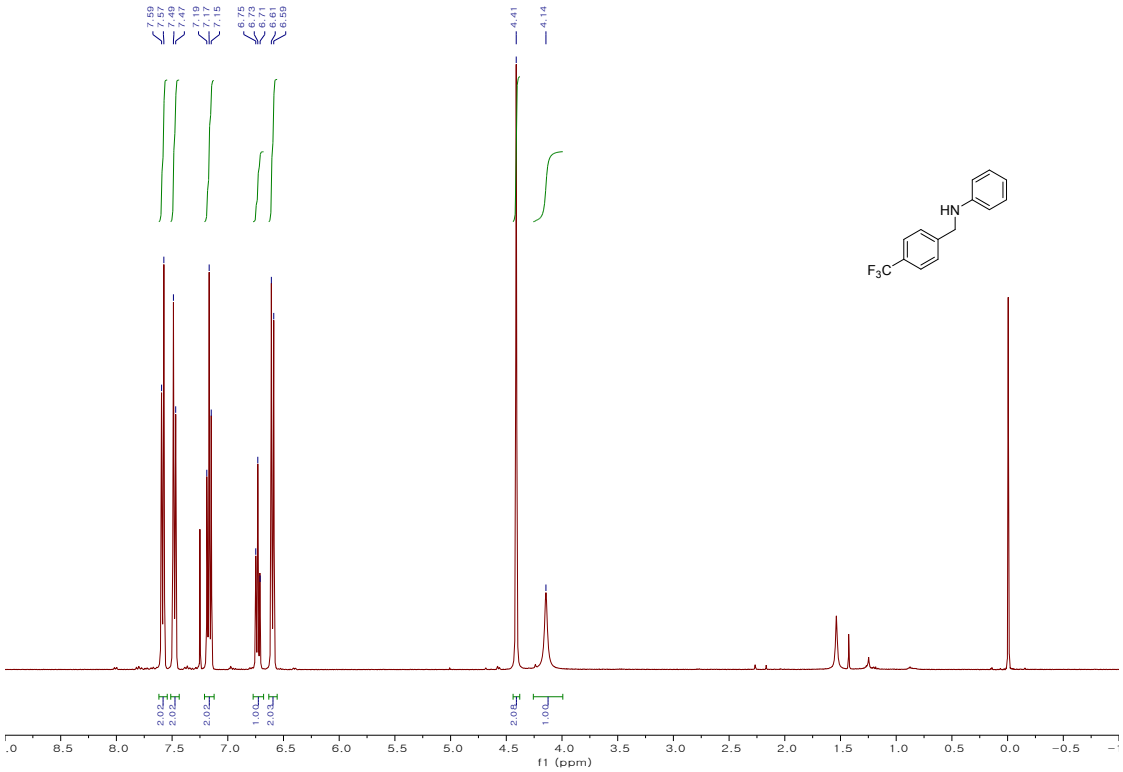


Figure S17: ^{1}H NMR of *N* -(4-(trifluoromethyl)benzyl)aniline (**2i**)

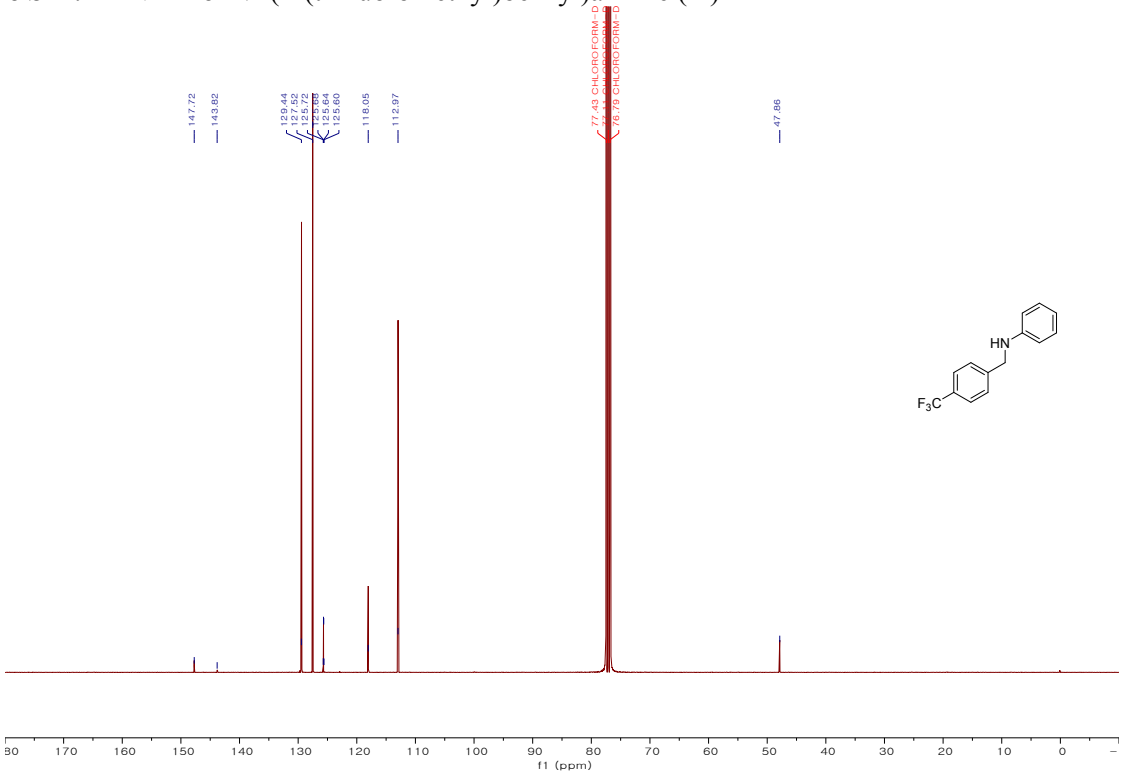


Figure S18: ^{13}C NMR of *N* -(4-(trifluoromethyl)benzyl)aniline (**2i**)

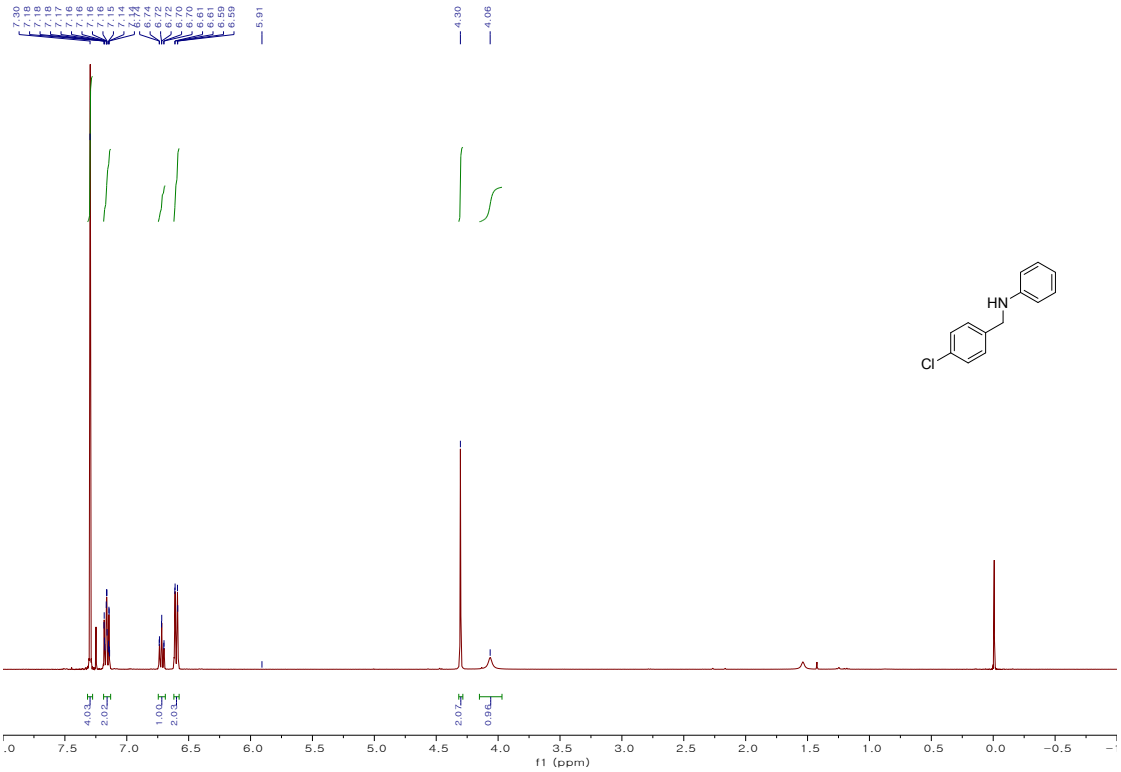


Figure S19: ^{1}H NMR of *N*-(4-chlorobenzyl)aniline (**2j**)

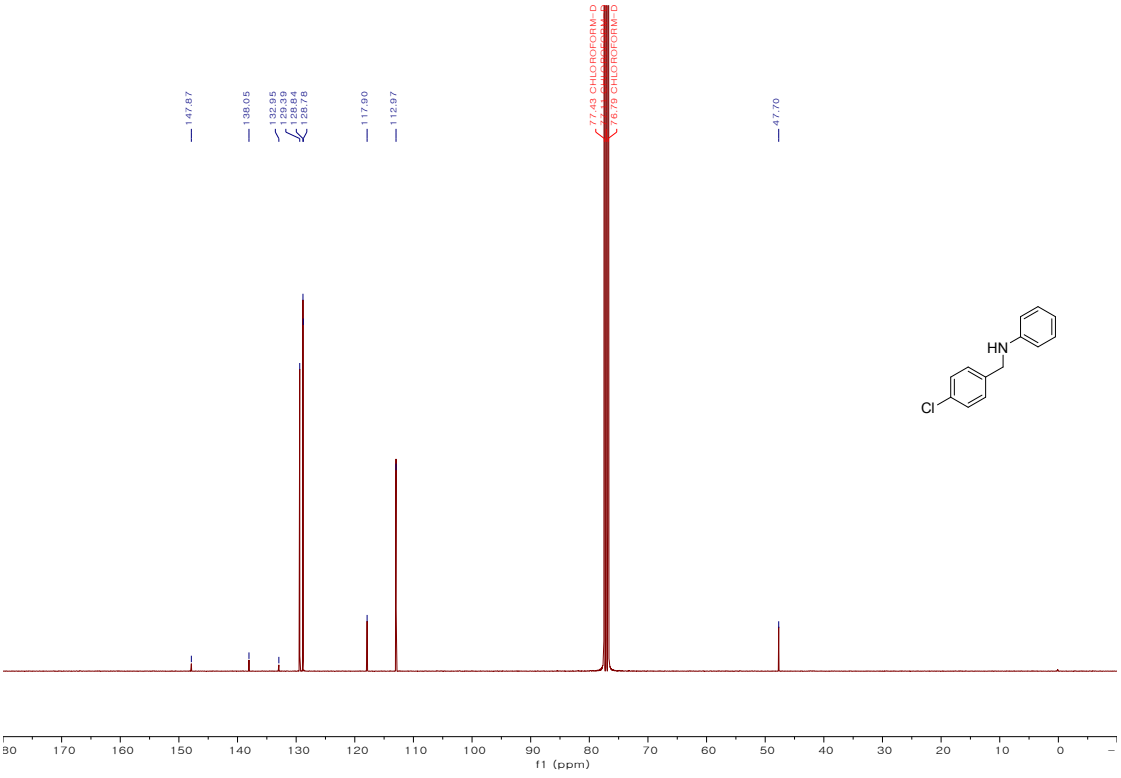


Figure S20: ^{13}C NMR of *N*-(4-chlorobenzyl)aniline (**2j**)

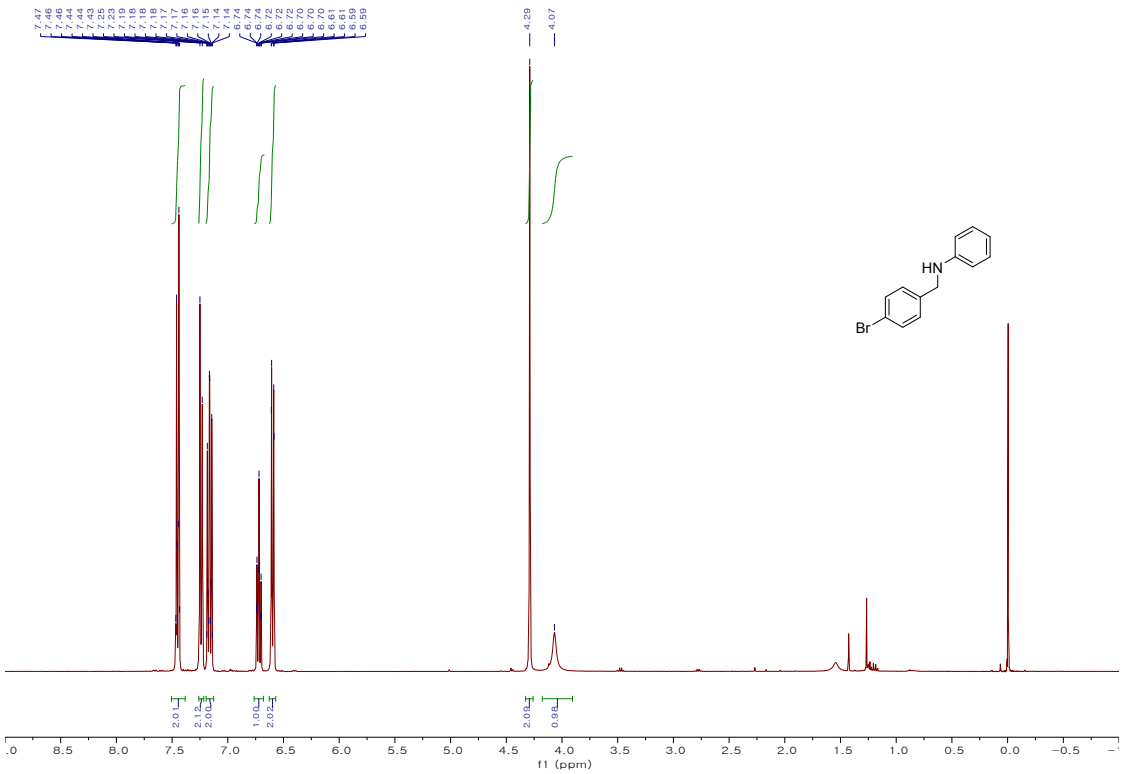


Figure S21: ^{1}H NMR of *N*-(4-bromobenzyl)aniline (**2k**)

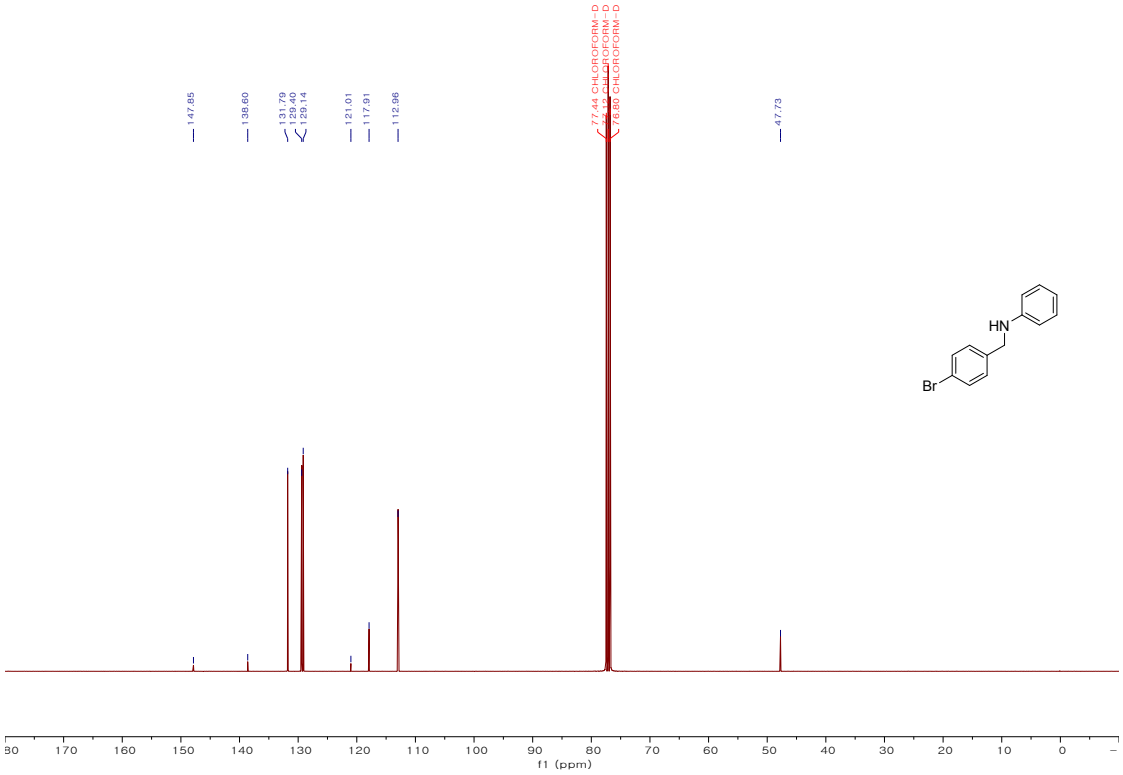


Figure S22: ^{13}C NMR of *N*-(4-bromobenzyl)aniline (**2k**)

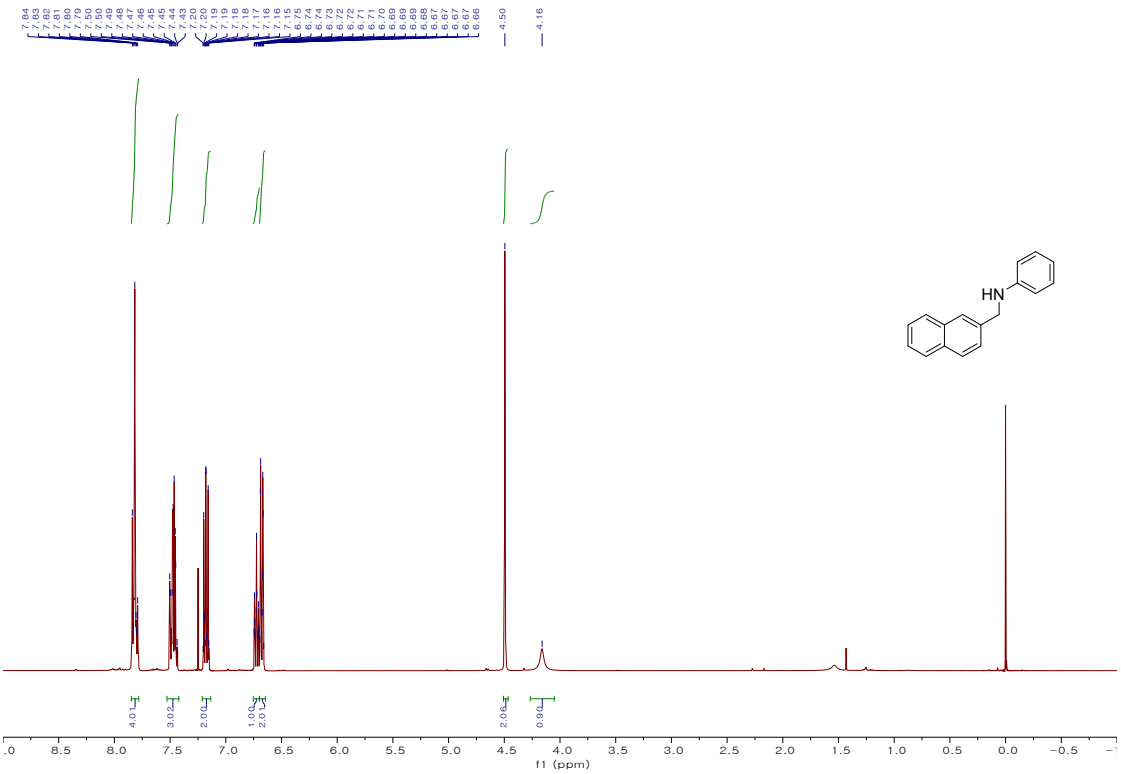


Figure S23: ^{1}H NMR of *N*-(naphthalen-2-ylmethyl)aniline (**2l**)

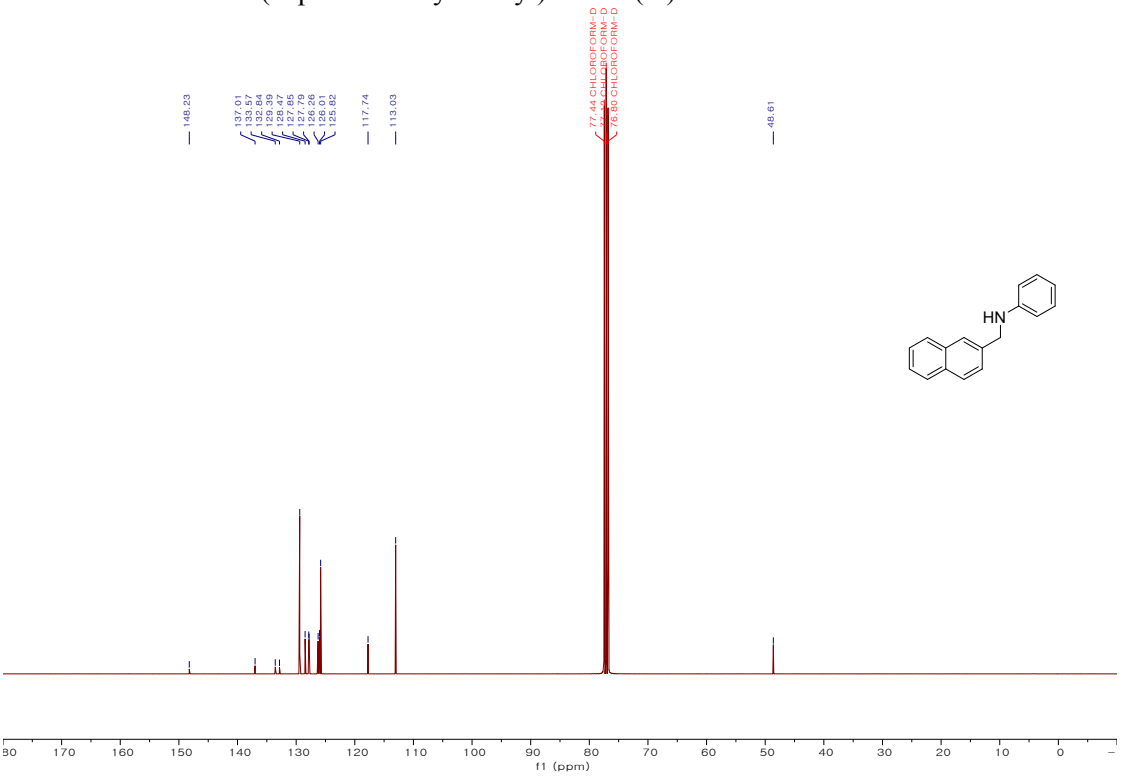


Figure S24: ^{13}C NMR of *N*-(naphthalen-2-ylmethyl)aniline (**2l**)

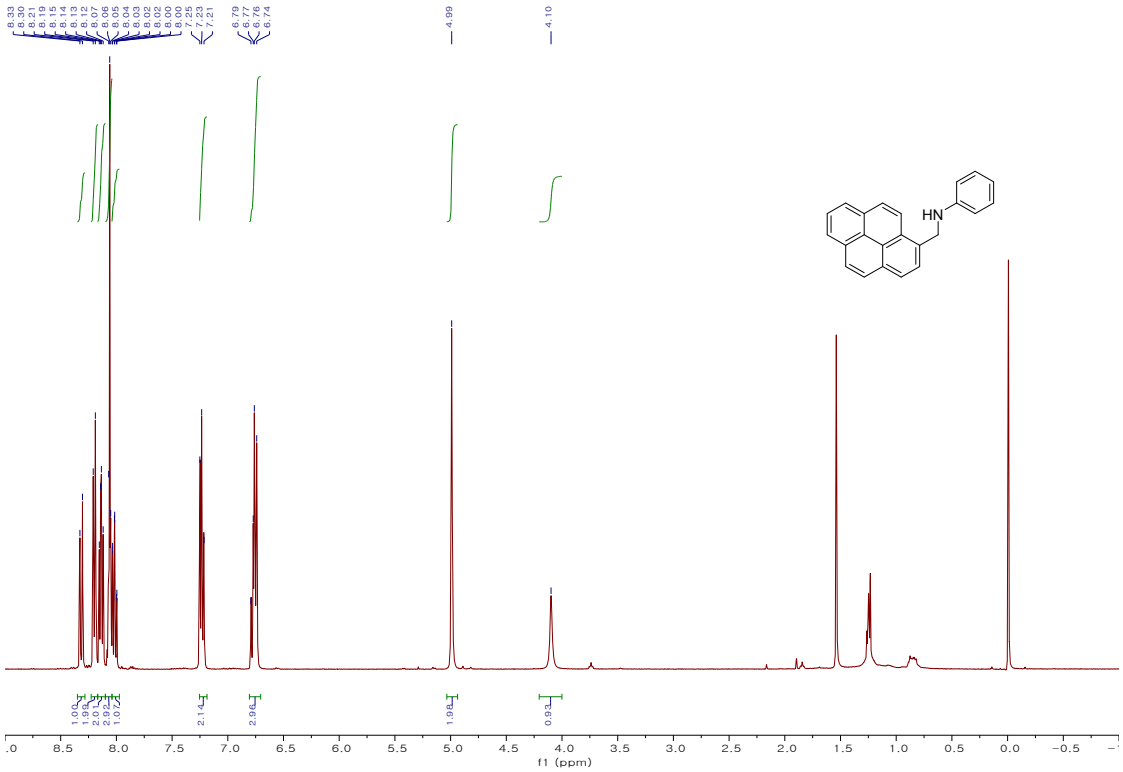


Figure S25: ^{1}H NMR of *N* -(pyren-1-ylmethyl)aniline (**2m**)

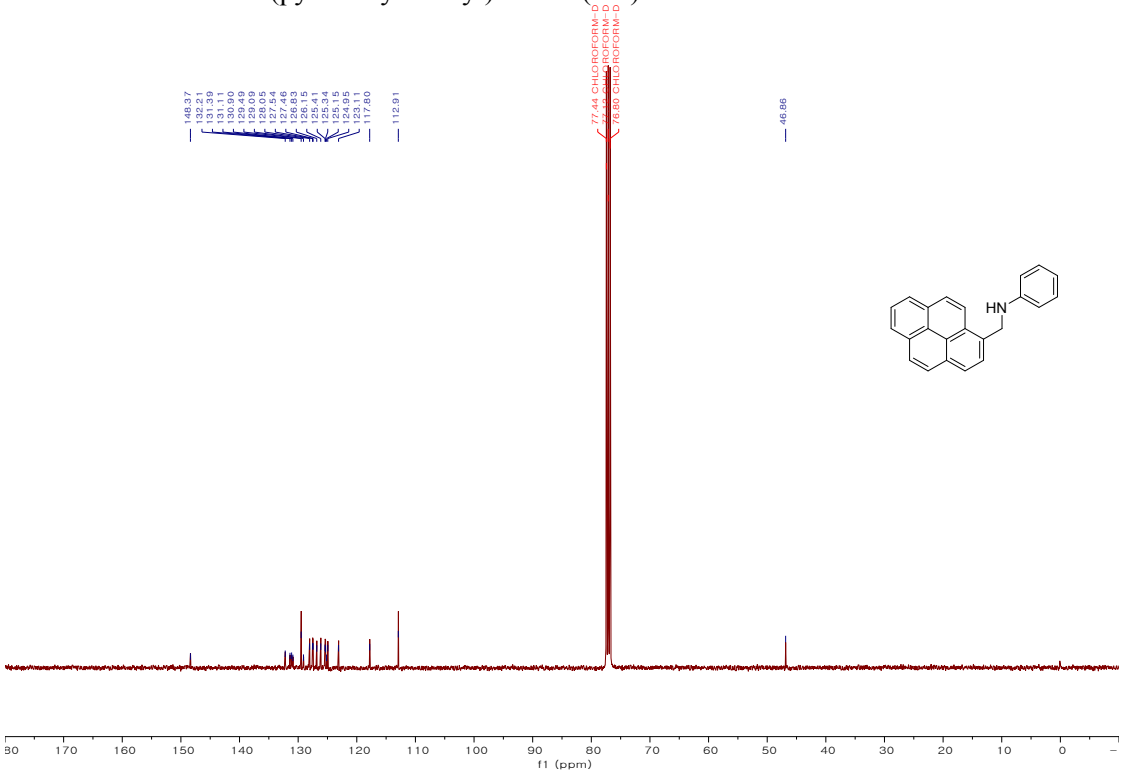


Figure S26: ^{13}C NMR of *N*-(pyren-1-ylmethyl)aniline (**2m**)

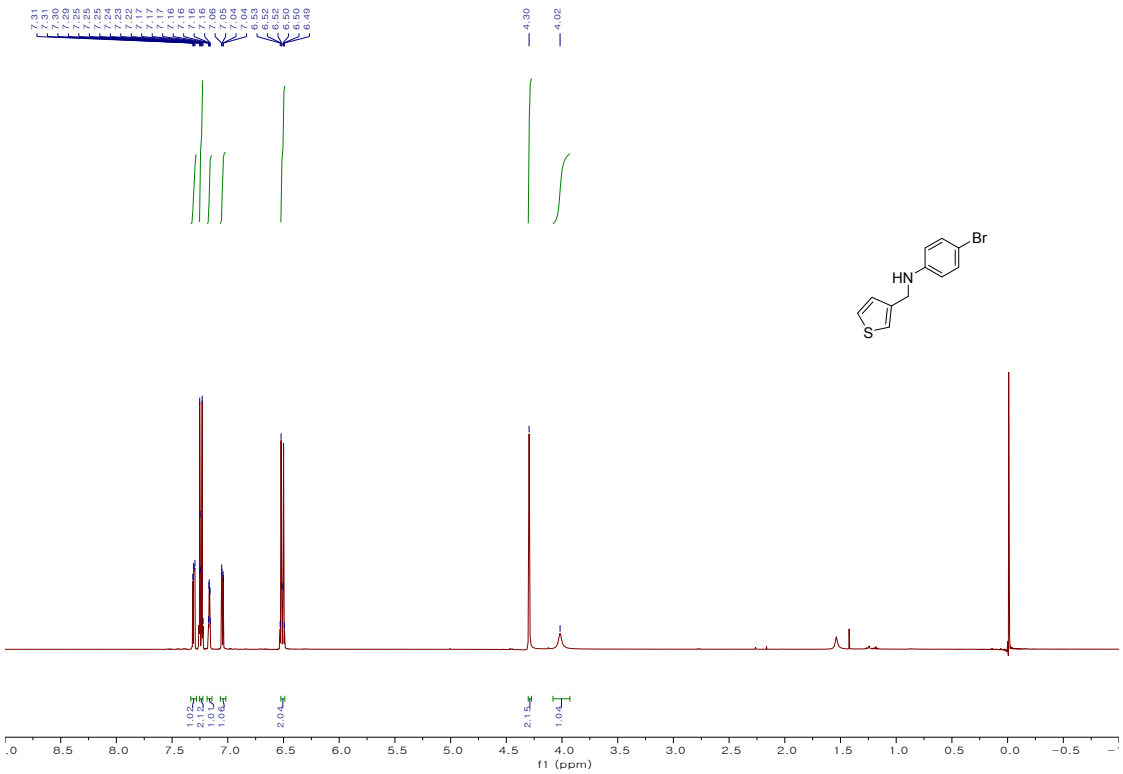


Figure S27: ^{1}H NMR of 4-bromo-*N*-(thiophen-3-ylmethyl)aniline (**2n**)

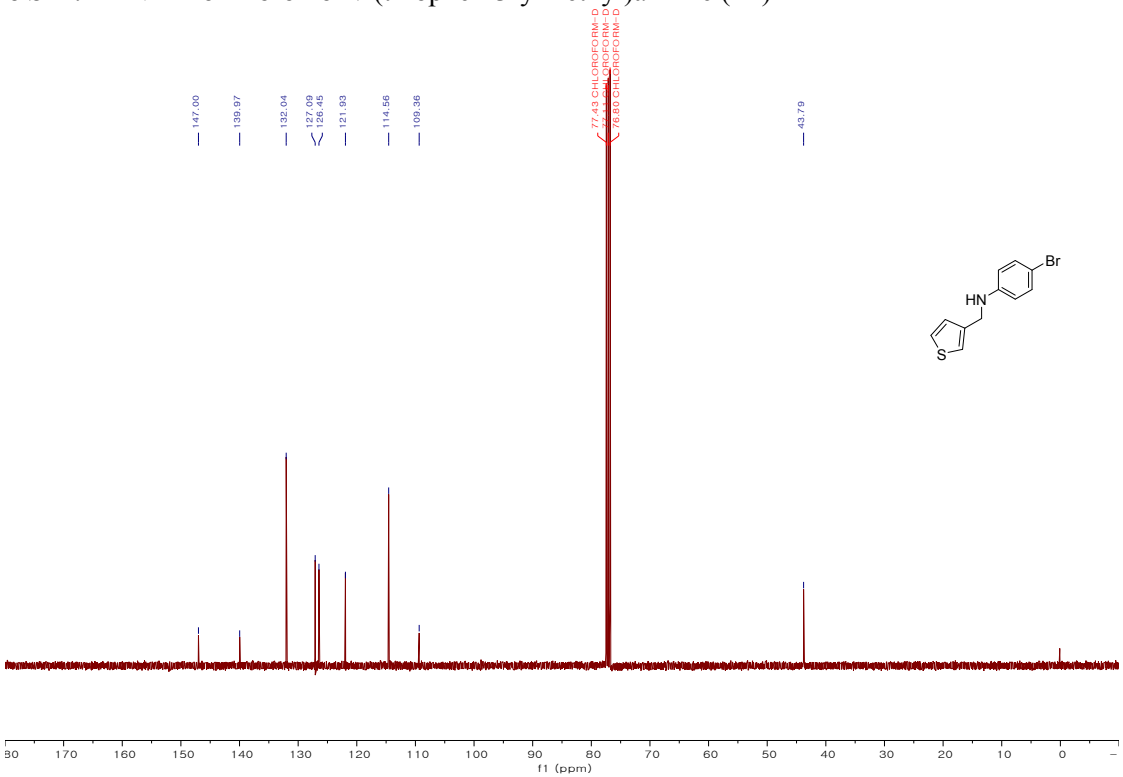


Figure S28: ^{13}C NMR of 4-bromo-*N*-(thiophen-3-ylmethyl)aniline (**2n**)

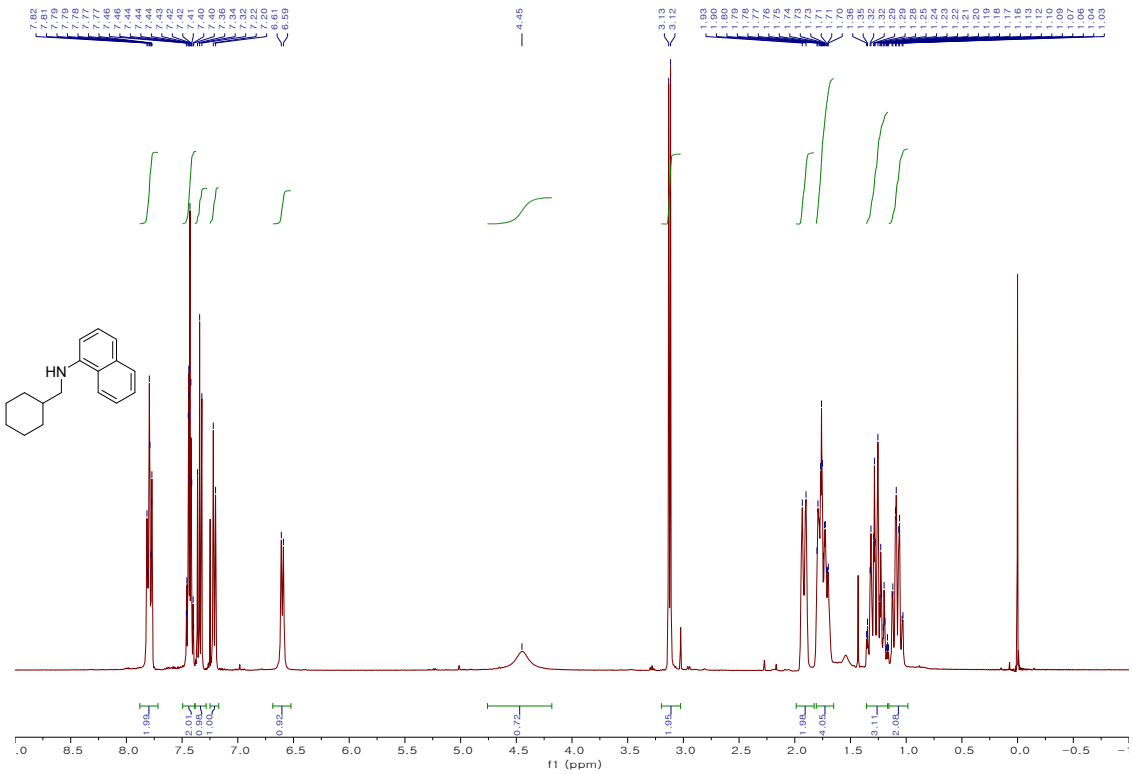


Figure S29: ^{1}H NMR of *N*-(cyclohexylmethyl)naphthalen-1-amine (**2o**)

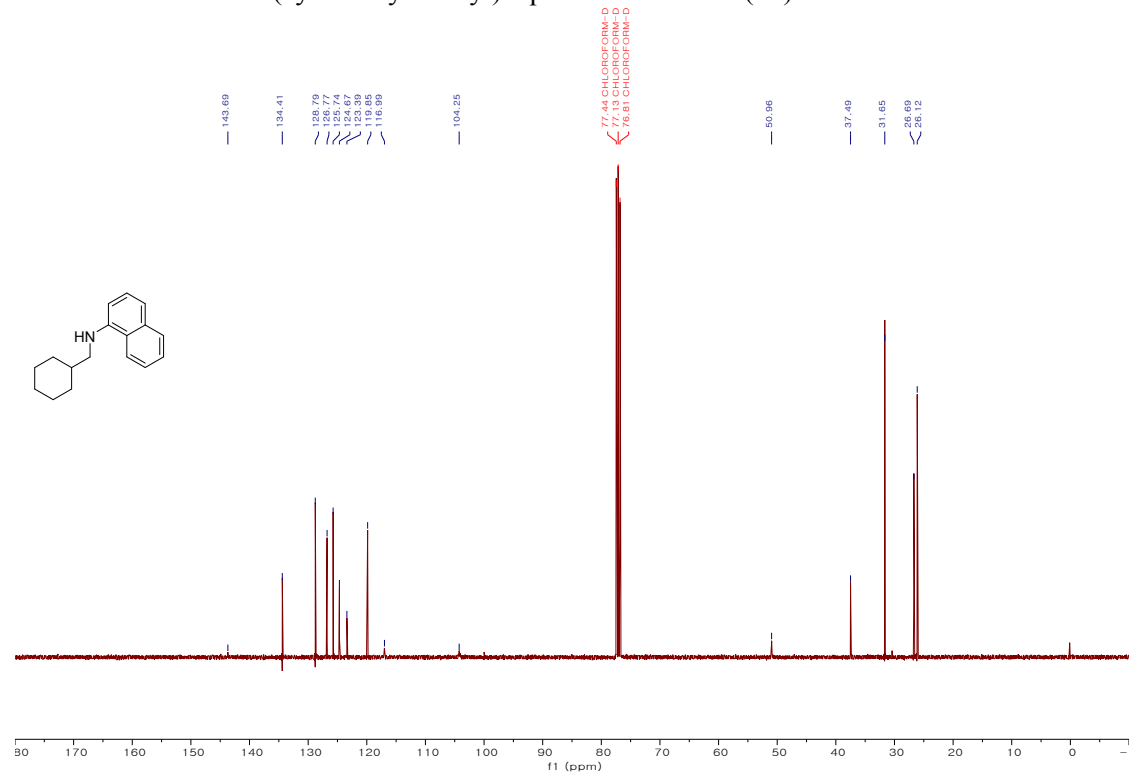


Figure S30: ^{13}C NMR of *N*-(cyclohexylmethyl)naphthalen-1-amine (**2o**)

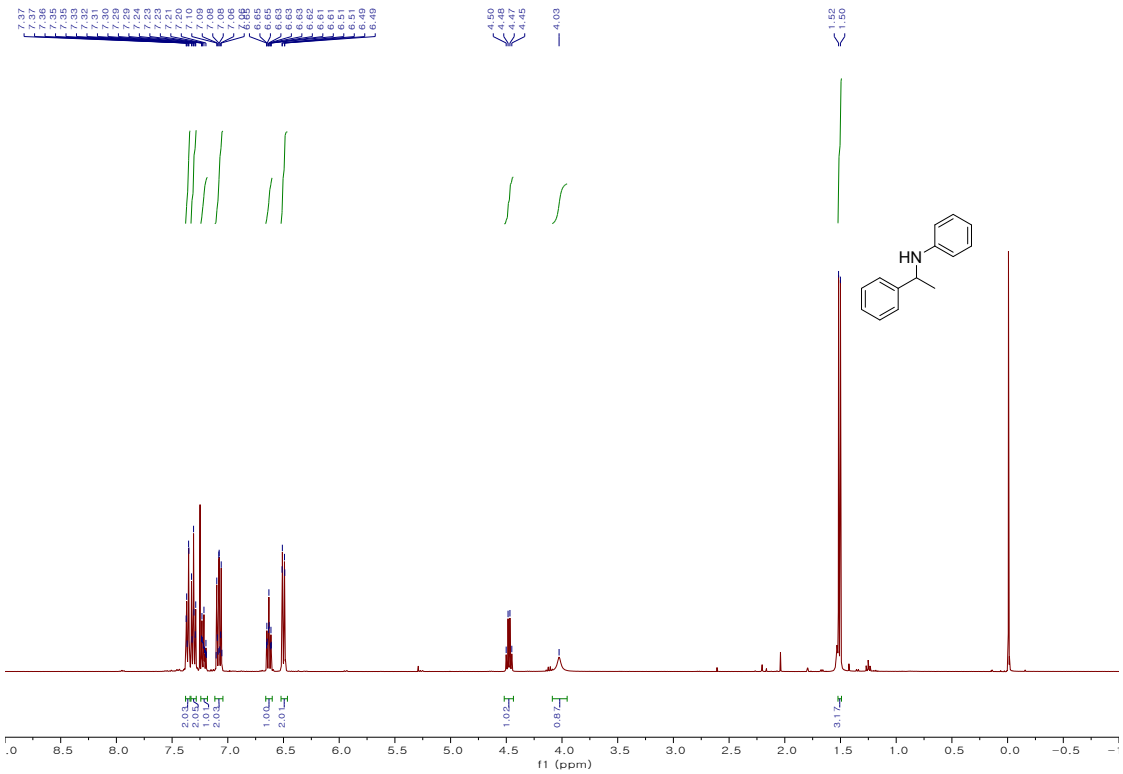


Figure S31: ^{1}H NMR of *N*-(1-phenylethyl)aniline (**4a**)

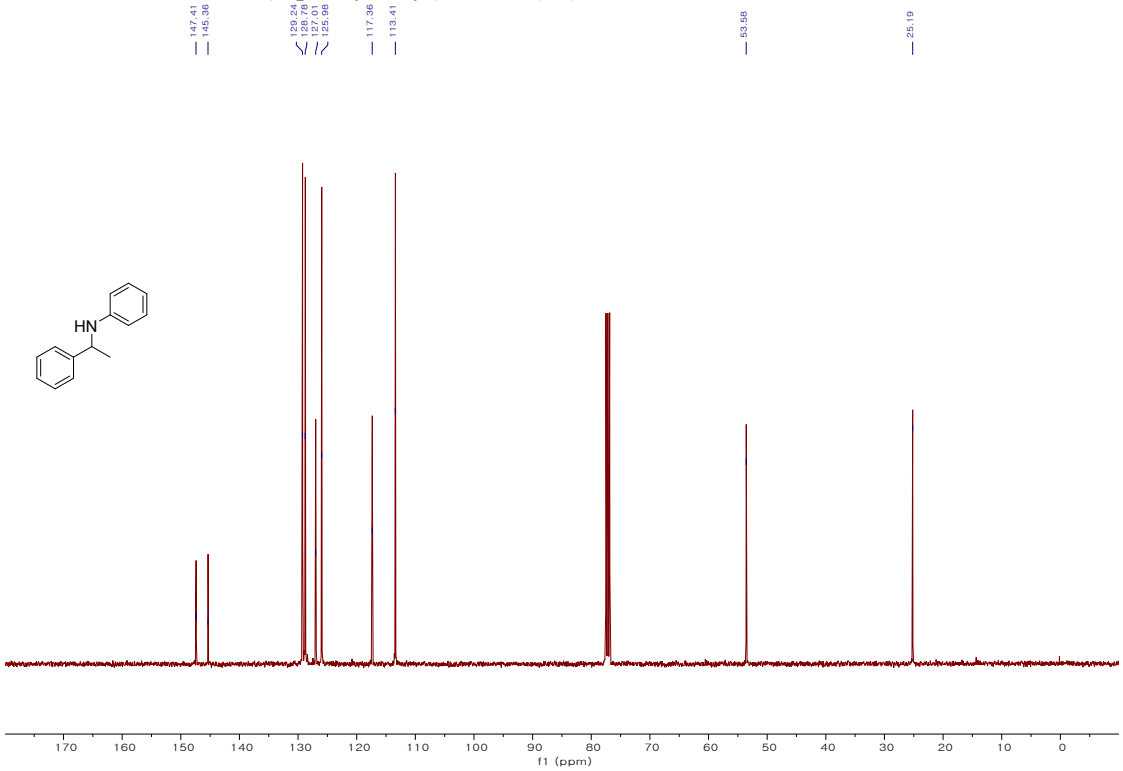


Figure S32: ^{13}C NMR of *N*-(1-phenylethyl)aniline (**4a**)

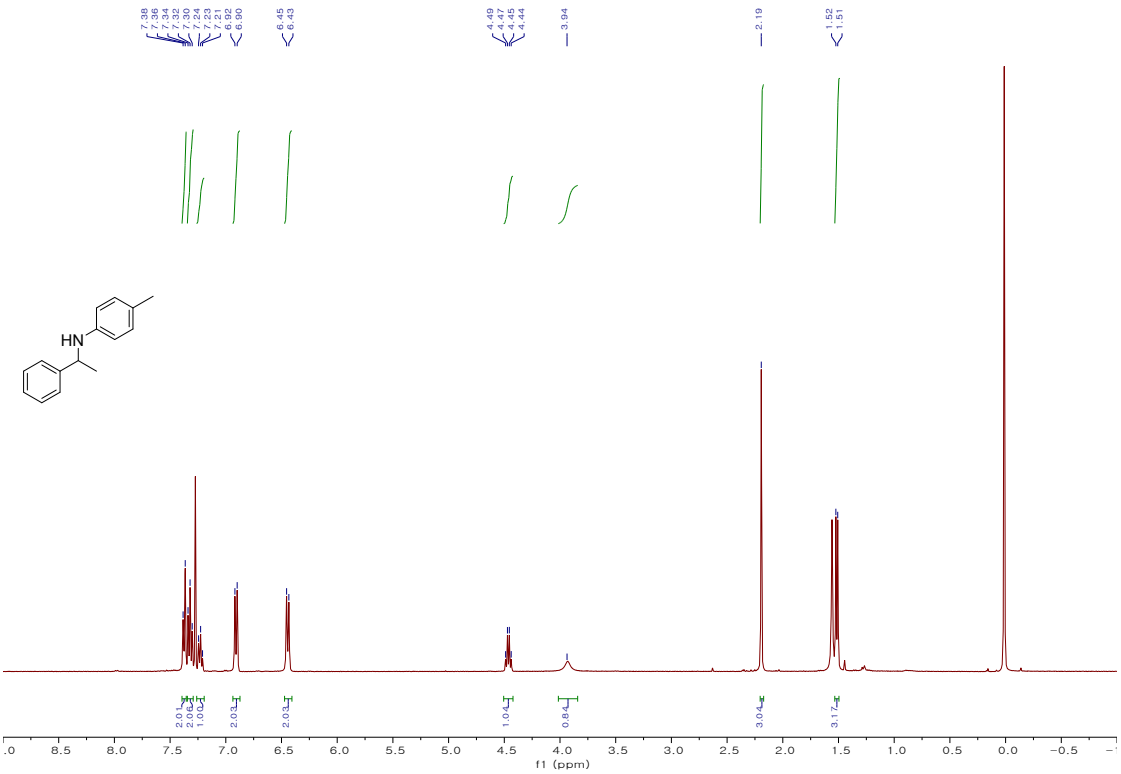


Figure S33: ^{1}H NMR of 4-methyl-*N*-(1-phenylethyl)aniline **(4b)**

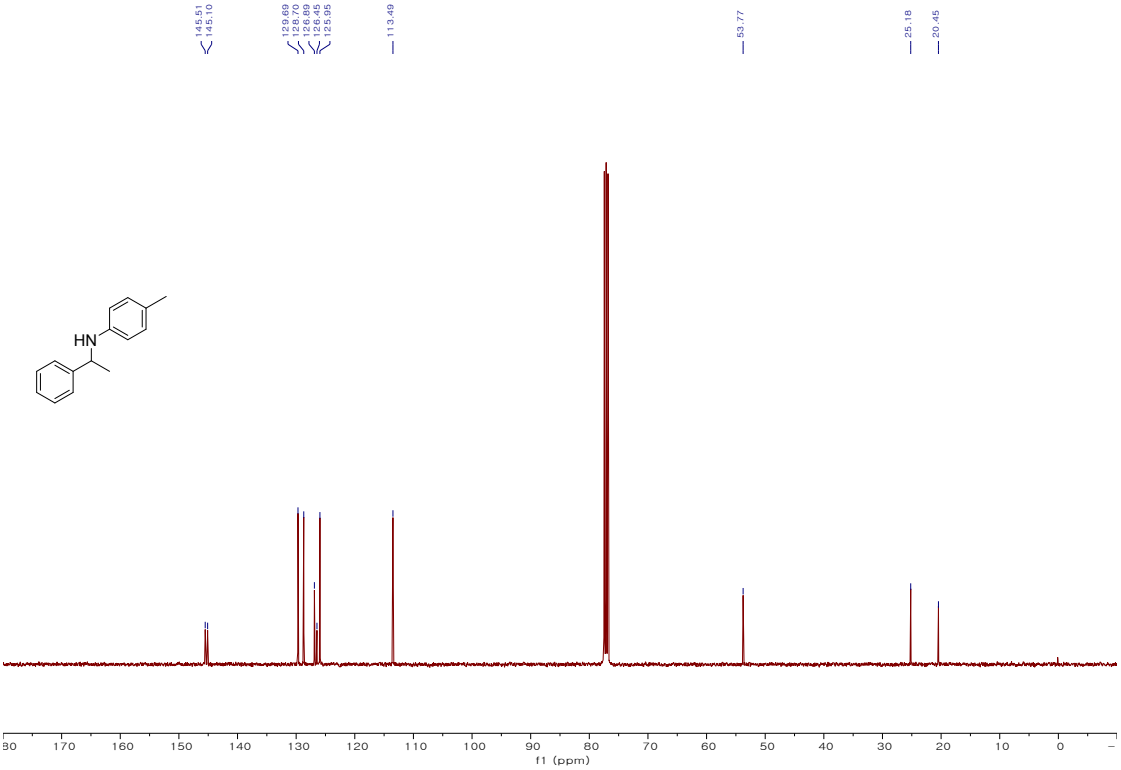


Figure S34: ^{13}C NMR of 4-methyl-*N*-(1-phenylethyl)aniline **(4b)**

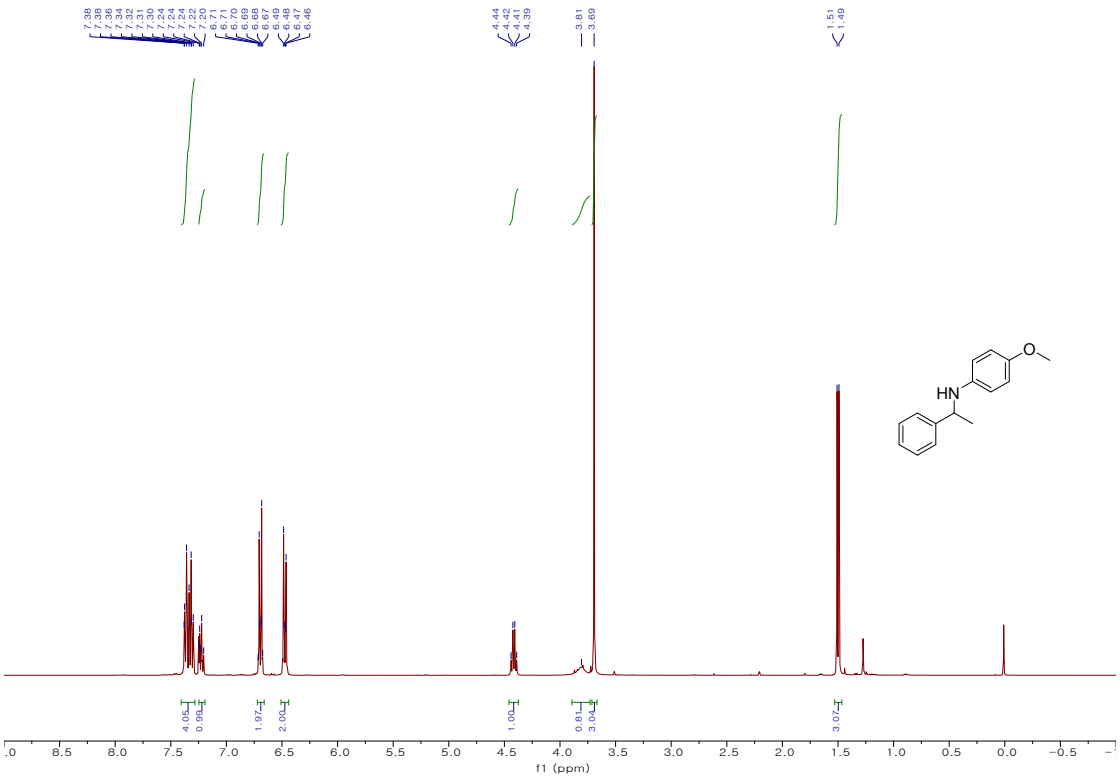


Figure S35: ^{1}H NMR of 4-methoxy-*N*-(1-phenylethyl)aniline **(4c)**

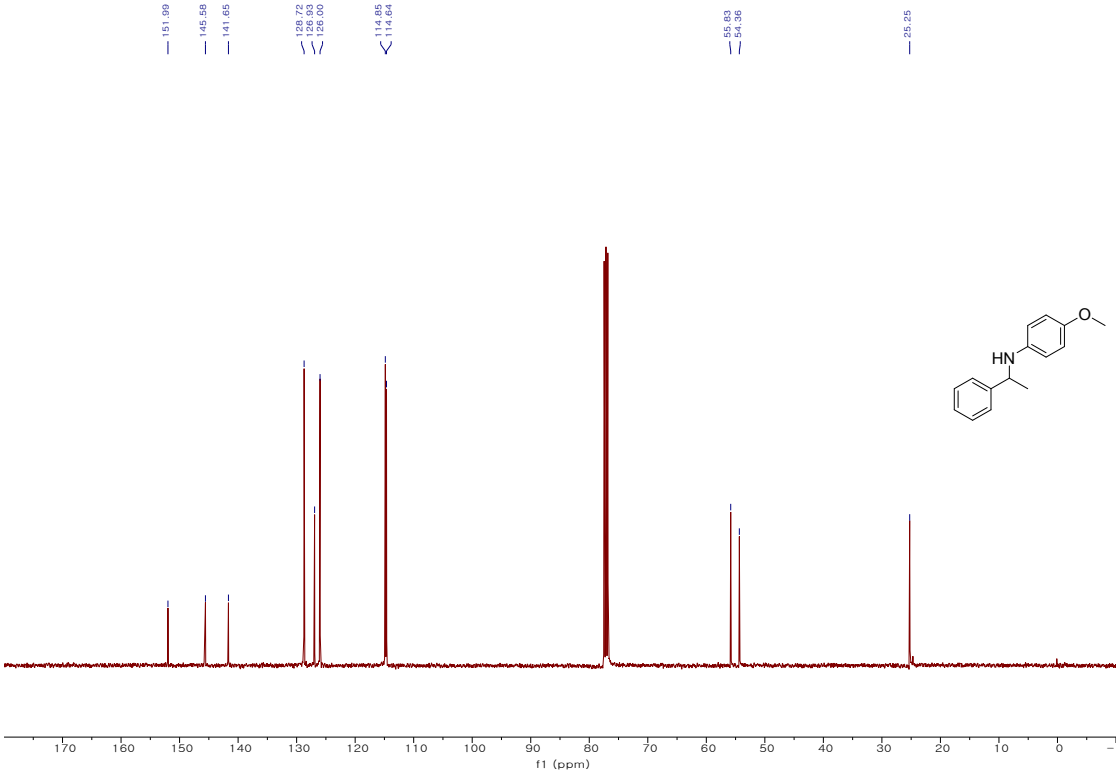


Figure S36: ^{13}C NMR of 4-methoxy-*N*-(1-phenylethyl)aniline **(4c)**

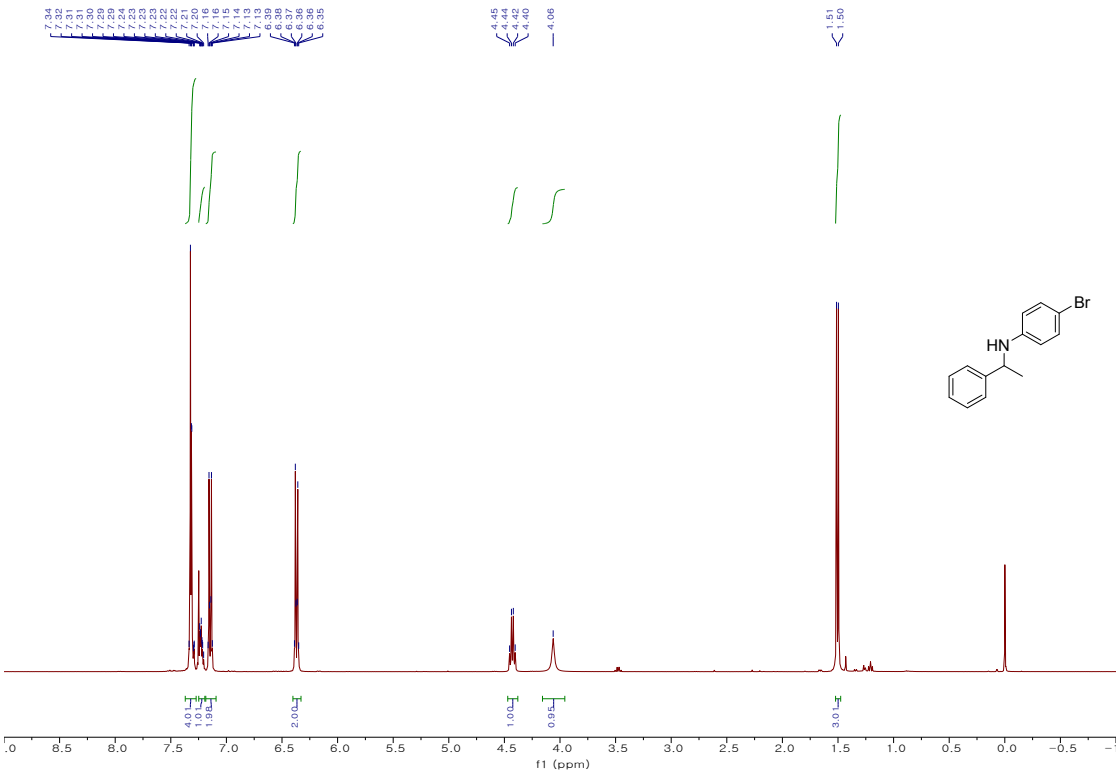


Figure S37: ^{1}H NMR of 4-bromo-*N*-(1-phenylethyl)aniline **(4d)**

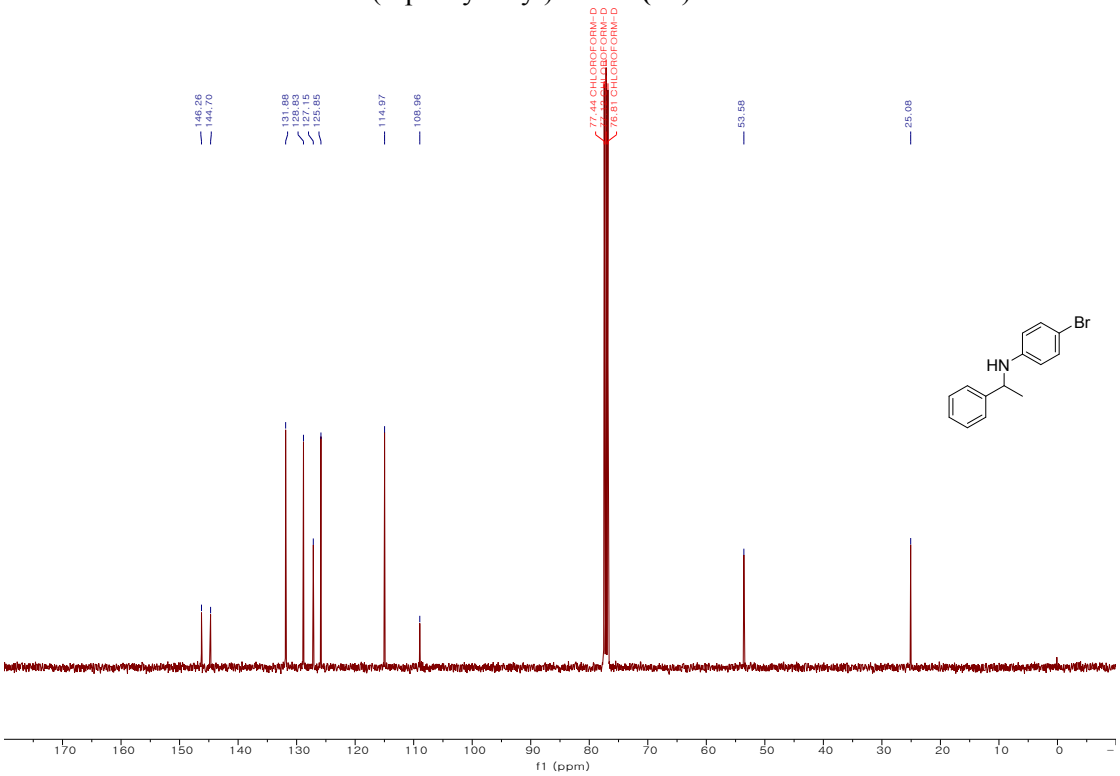


Figure S38: ^{13}C NMR of 4-bromo-*N*-(1-phenylethyl)aniline **(4d)**

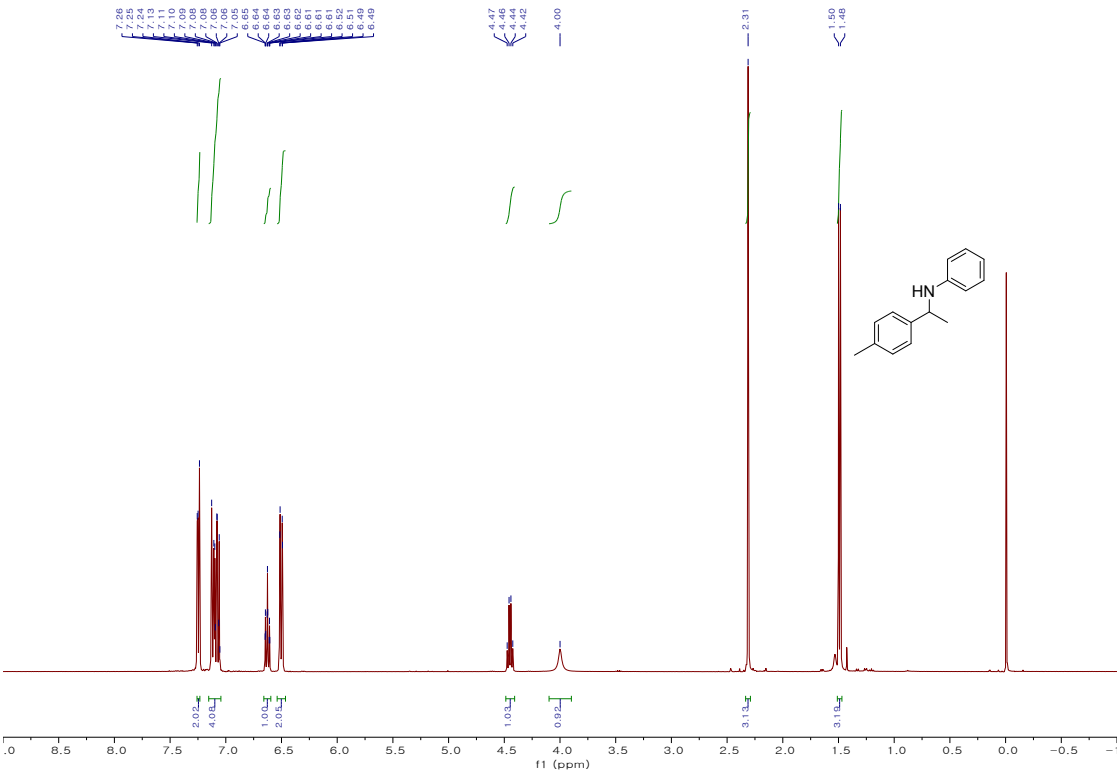


Figure S39: ^{1}H NMR of *N*-(1-(*p*-tolyl)ethyl)aniline **(4e)**

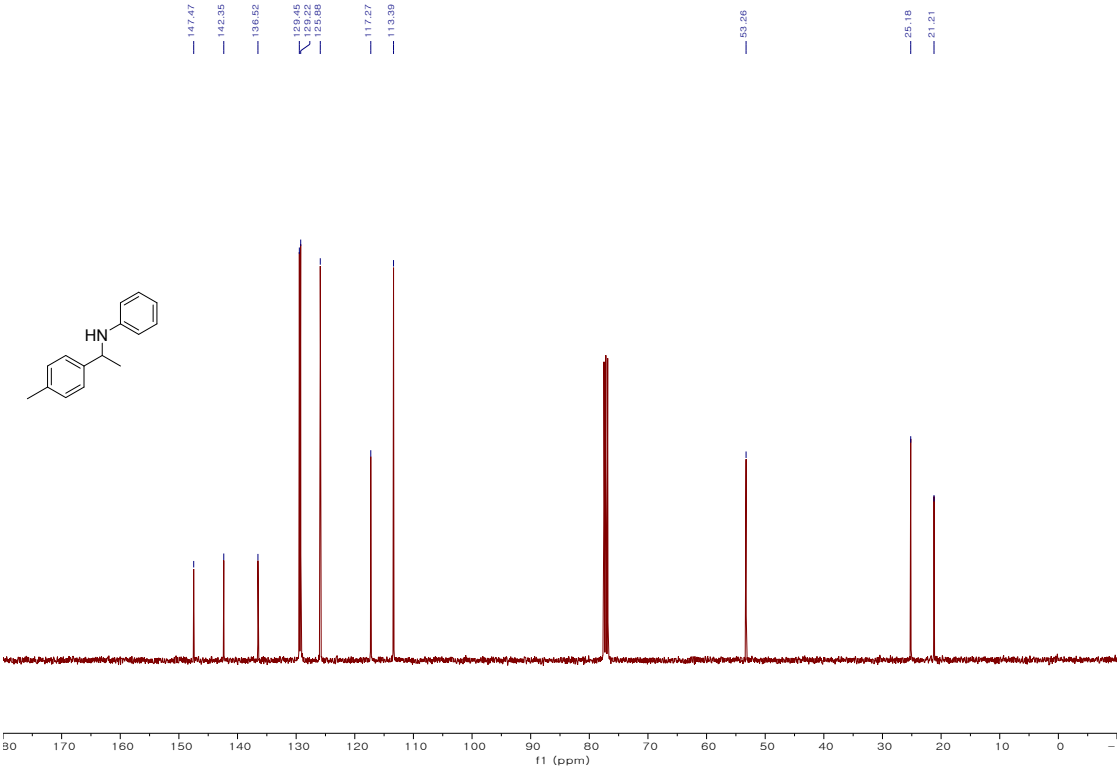


Figure S40: ^{13}C NMR of *N*-(1-(*p*-tolyl)ethyl)aniline **(4e)**

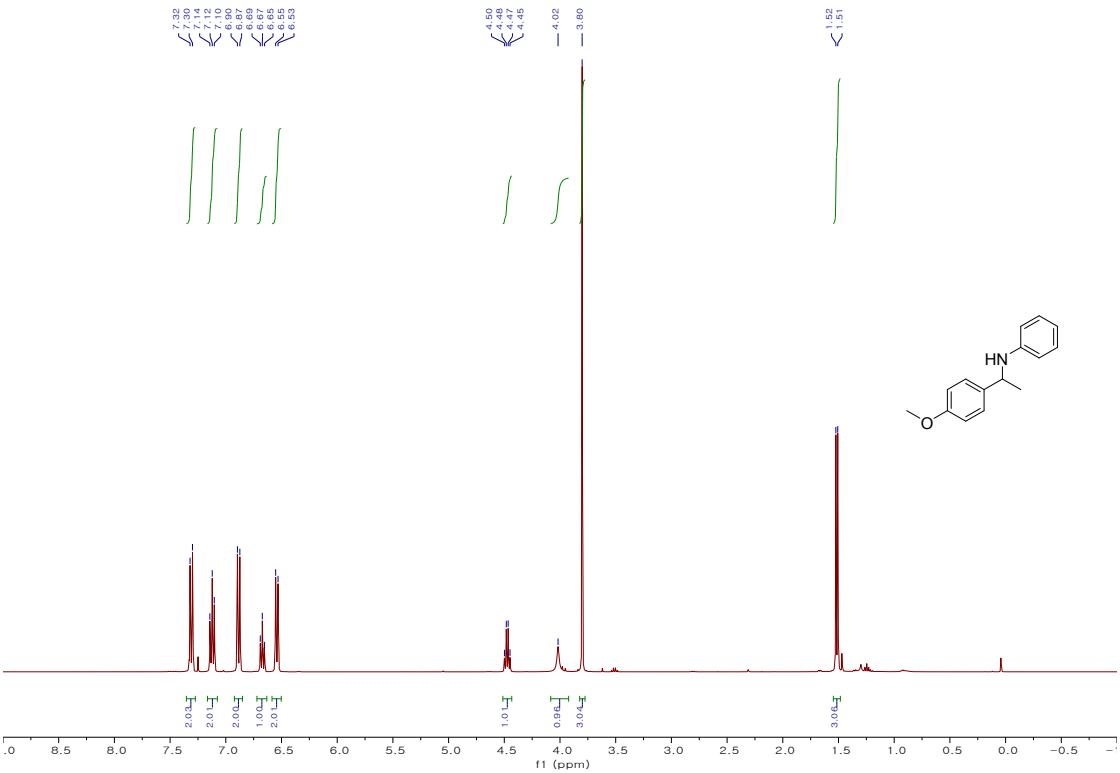


Figure S41: ^{1}H NMR of *N*-(1-(4-methoxyphenyl)ethyl)aniline **(4f)**

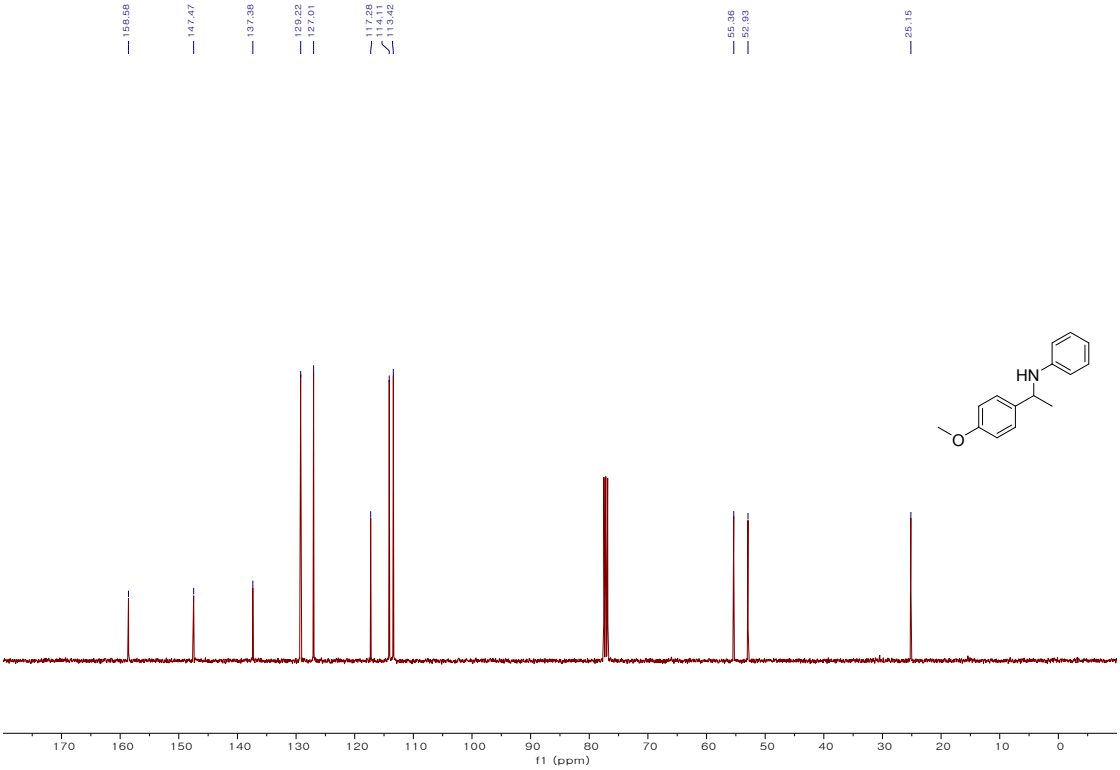


Figure S42: ^{13}C NMR of *N*-(1-(4-methoxyphenyl)ethyl)aniline **(4f)**

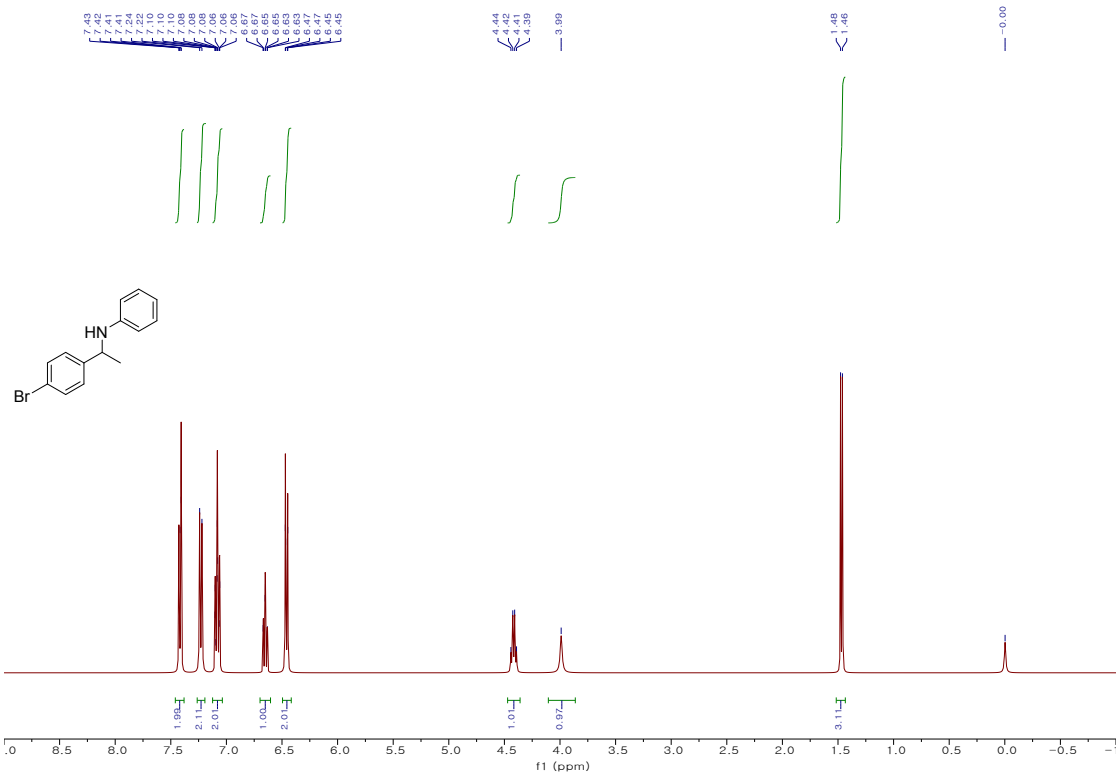


Figure S43: ^{1}H NMR of *N*-(1-(4-bromophenyl)ethyl)aniline **(4g)**

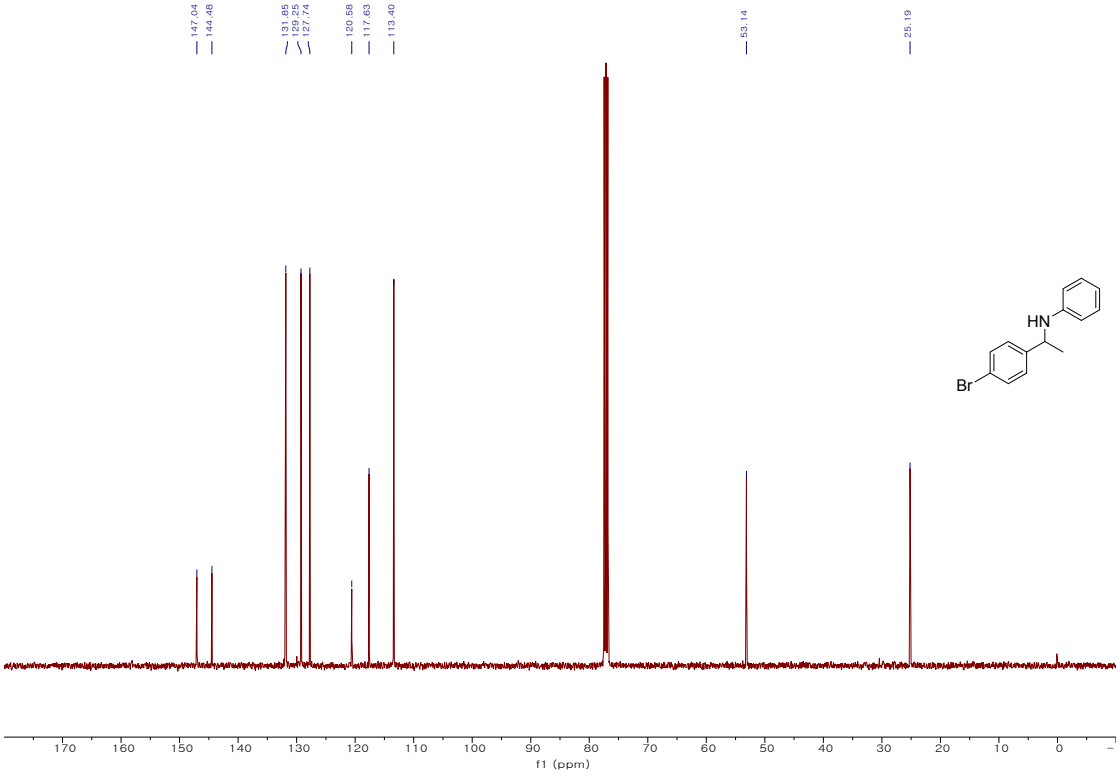


Figure S44: ^{13}C NMR of *N*-(1-(4-bromophenyl)ethyl)aniline **(4g)**

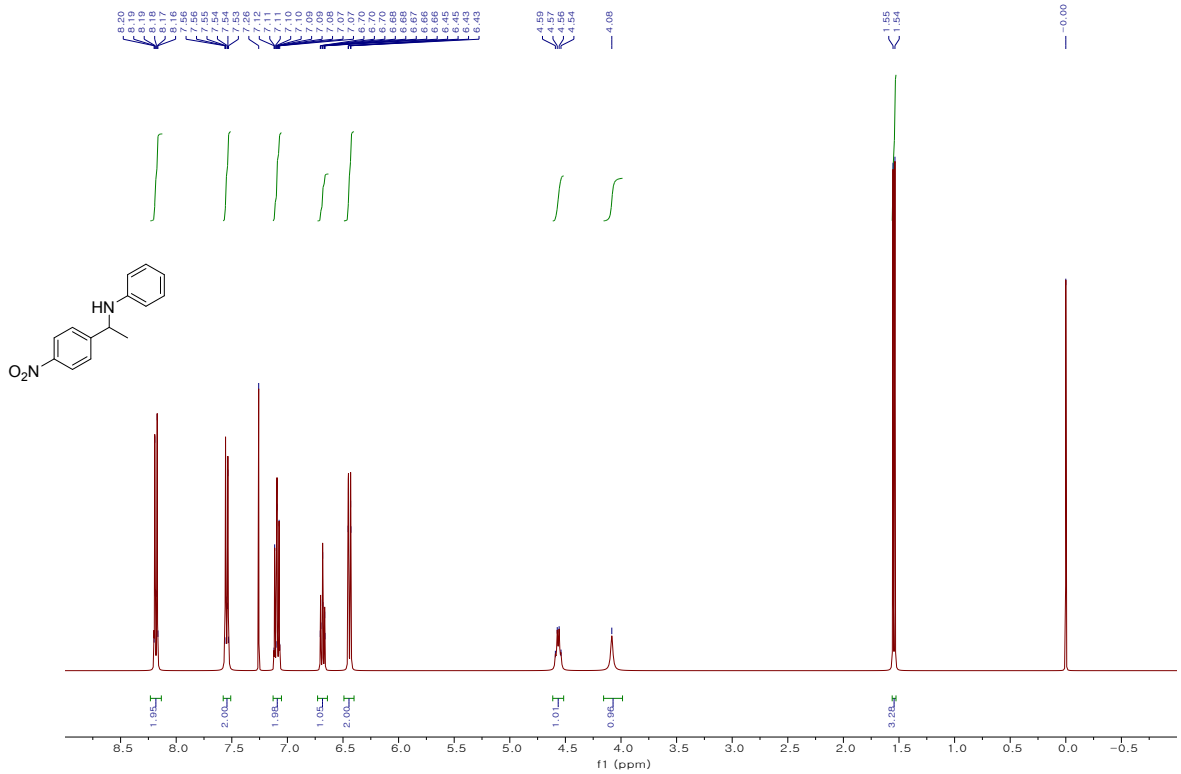


Figure S45: ^{1}H NMR of *N*-(1-(4-nitrophenyl)ethyl)aniline **(4h)**

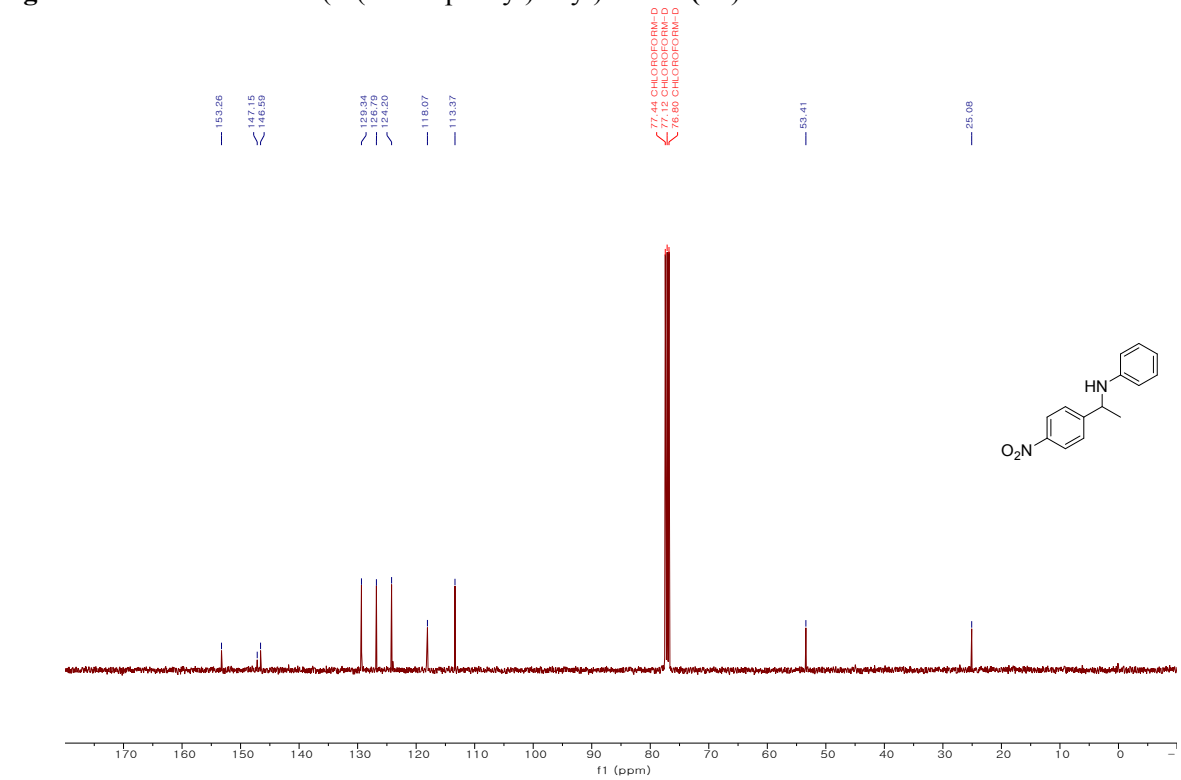


Figure S46: ^{13}C NMR of *N*-(1-(4-nitrophenyl)ethyl)aniline **(4h)**

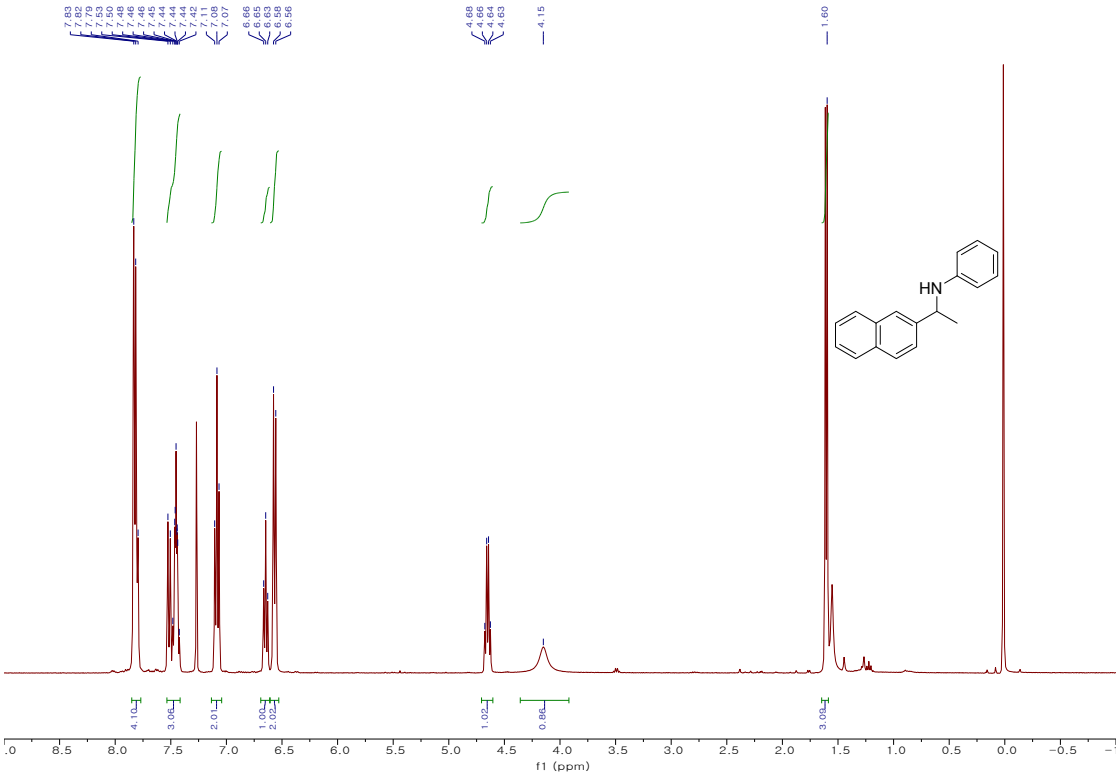


Figure S47: ^{1}H NMR of *N*-(1-(naphthalen-2-yl)ethyl)aniline **(4i)**

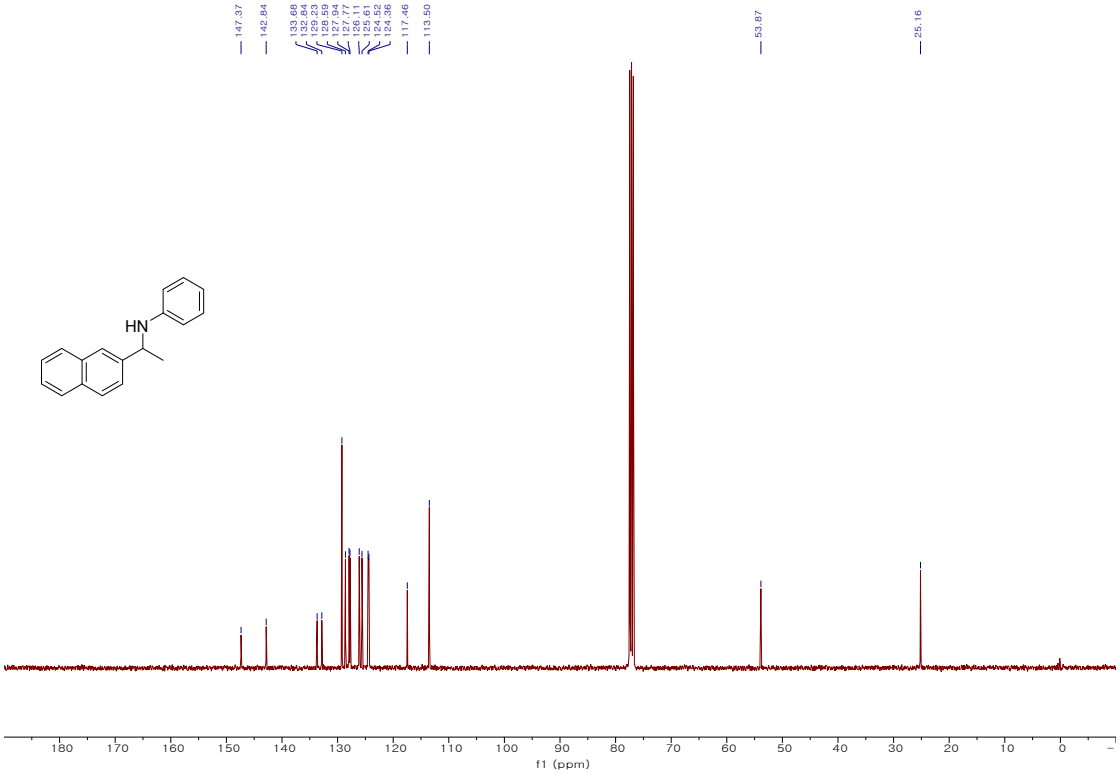


Figure S48: ^{13}C NMR of *N*-(1-(naphthalen-2-yl)ethyl)aniline **(4i)**

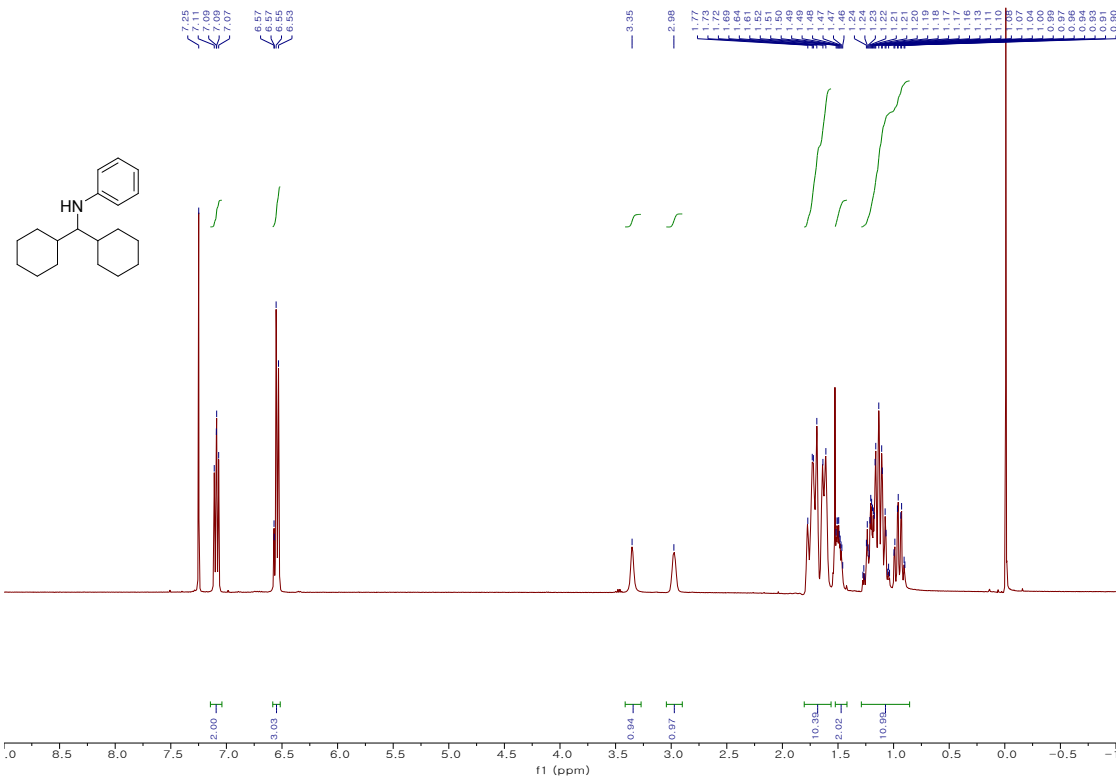


Figure S49: ^{1}H NMR of *N*-(dicyclohexylmethyl)aniline **(4j)**

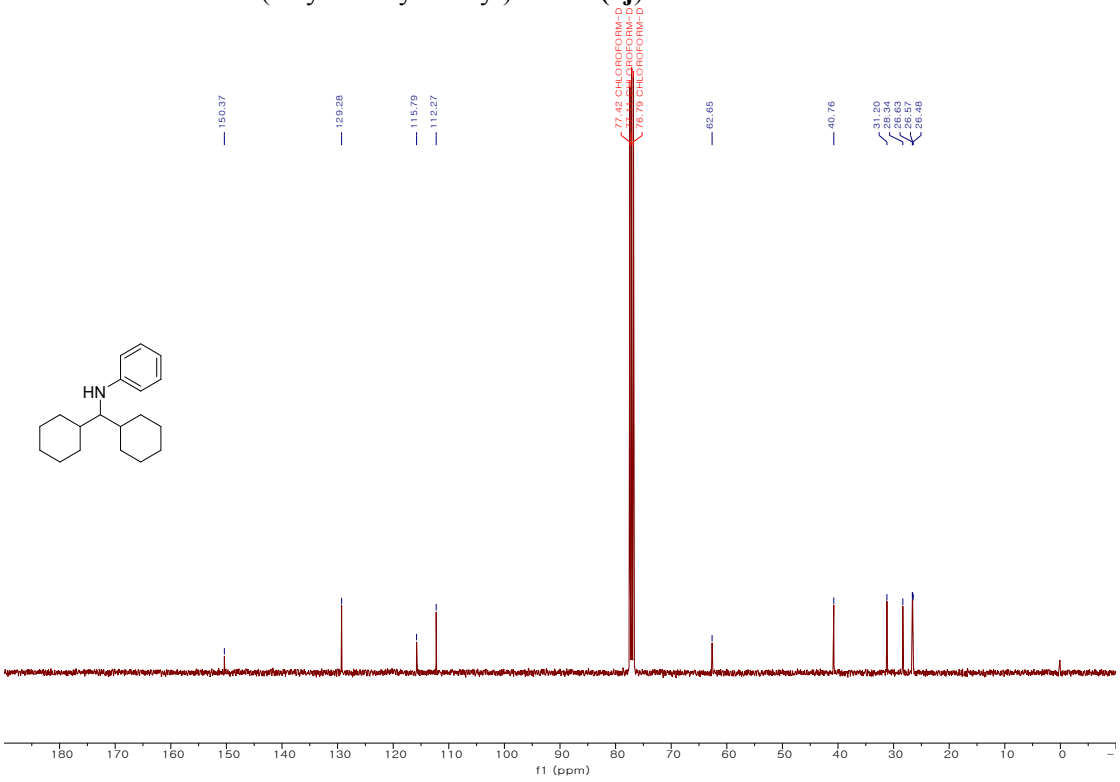


Figure S50: ^{13}C NMR of *N*-(dicyclohexylmethyl)aniline **(4j)**

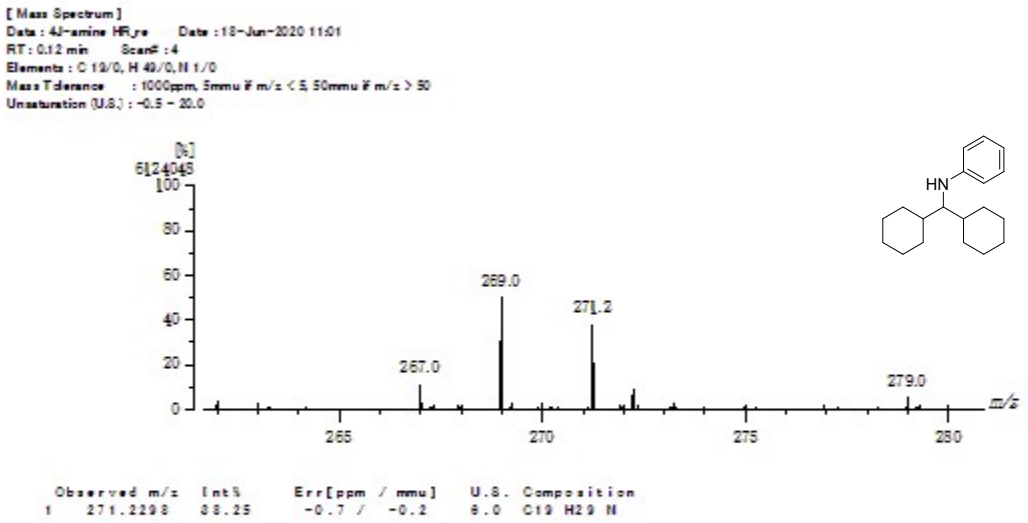


Figure S51: HRMS of *N*-(dicyclohexylmethyl)aniline **(4j)**

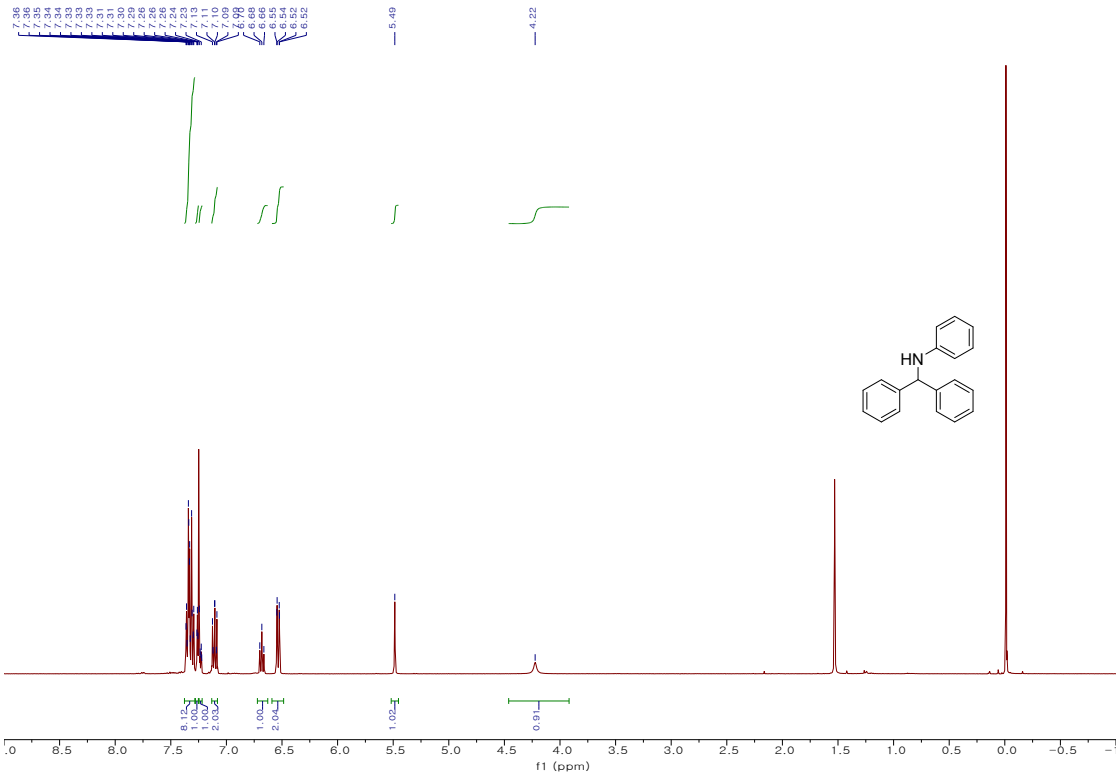


Figure S52: ^{1}H NMR of *N*-benzhydrylaniline **(4k)**

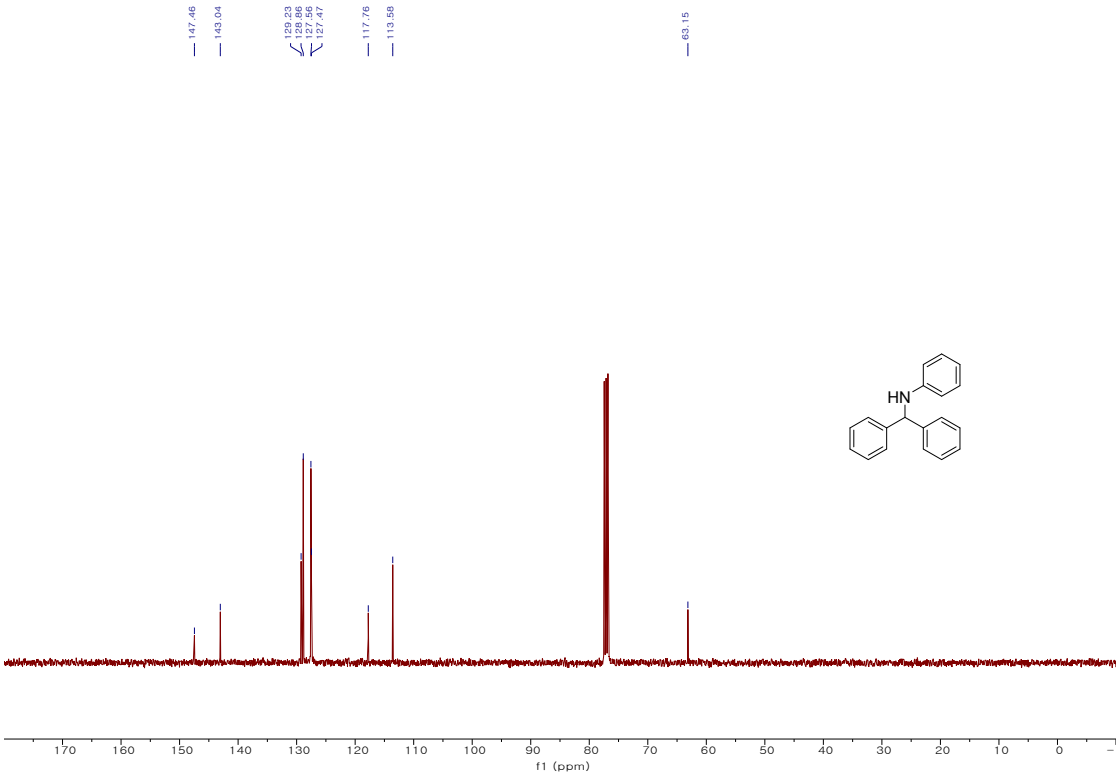


Figure S53: ^{13}C NMR of *N*-benzhydrylaniline **(4k)**

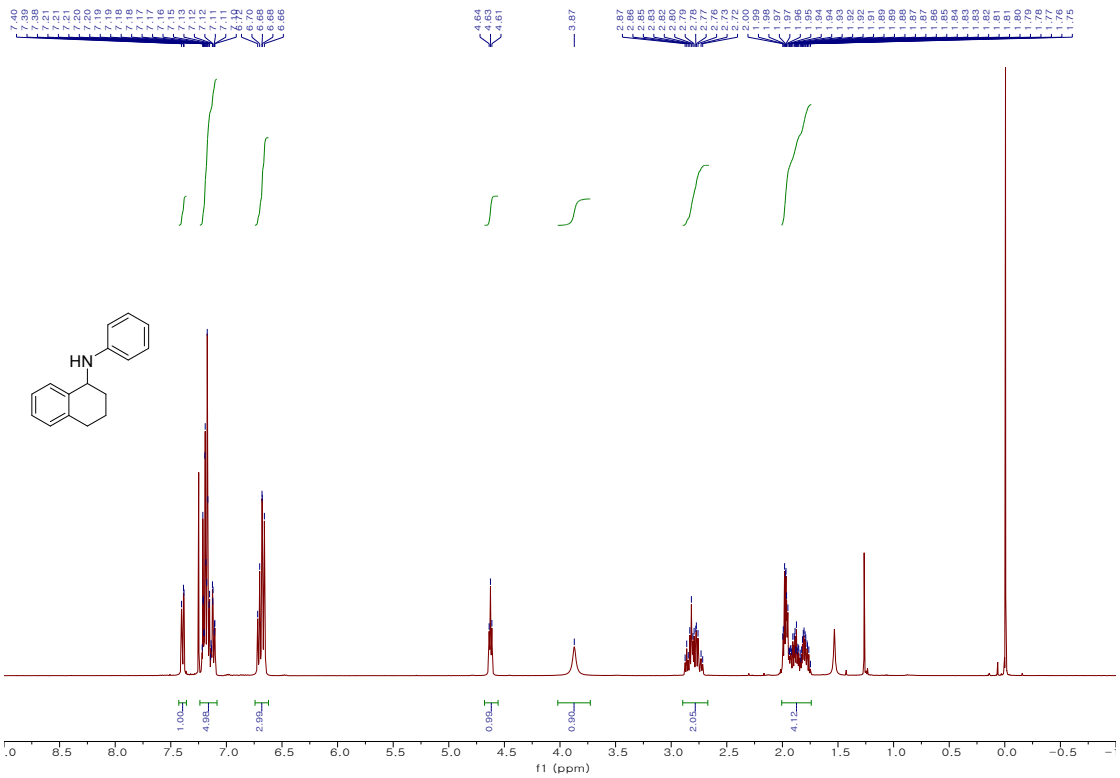


Figure S54: ^{1}H NMR of *N*-phenyl-1,2,3,4-tetrahydronaphthalen-1-amine **(4l)**

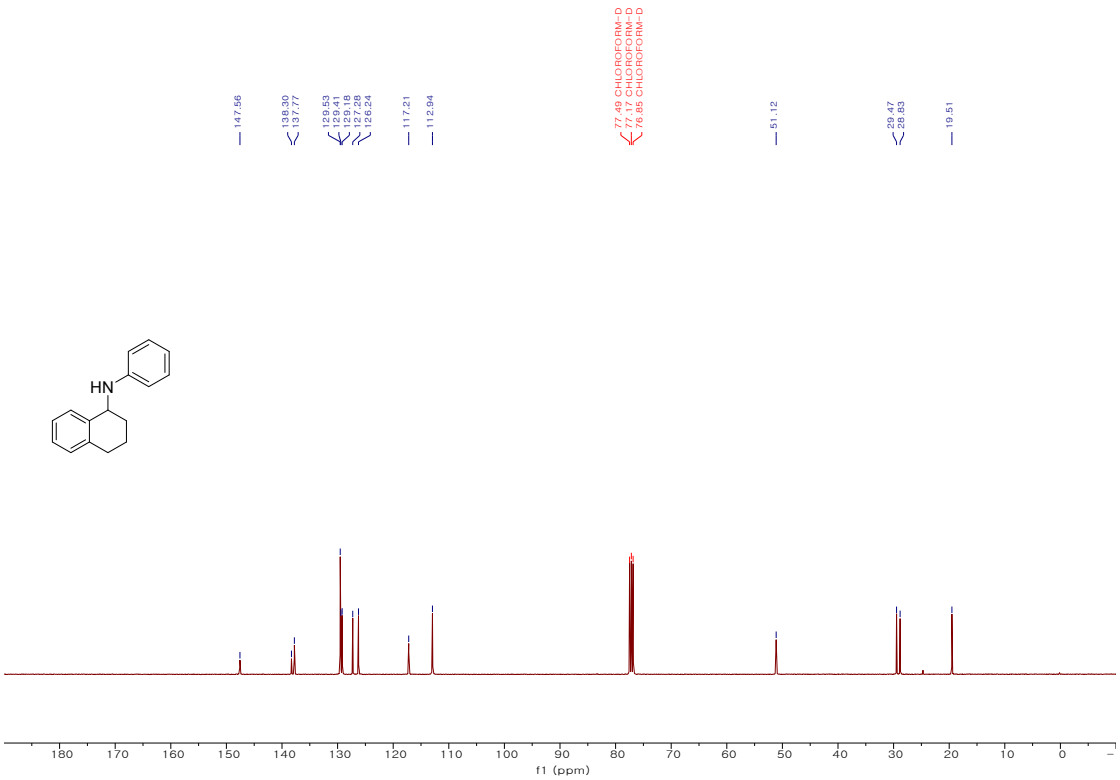


Figure S55: ^{13}C NMR of *N*-phenyl-1,2,3,4-tetrahydronaphthalen-1-amine **(4l)**

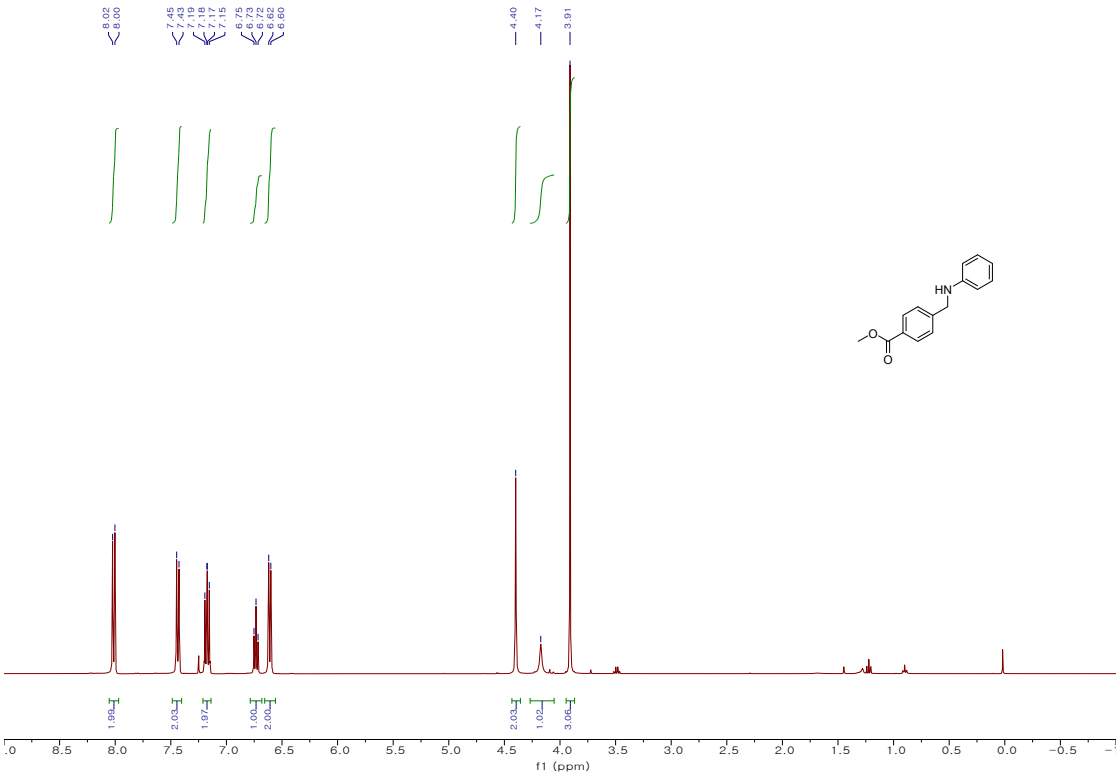


Figure S56: ^{1}H NMR of methyl 4-((phenylamino)methyl)benzoate **(6a)**

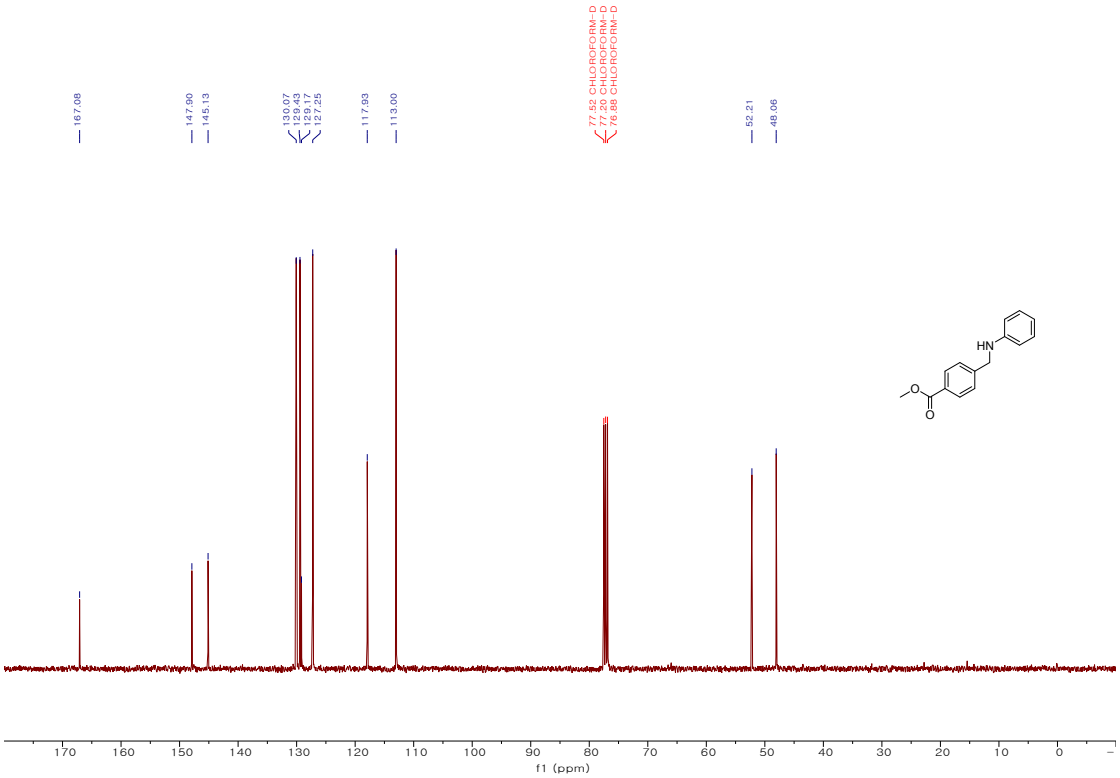


Figure S57: ^{13}C NMR of methyl 4-((phenylamino)methyl)benzoate **(6a)**

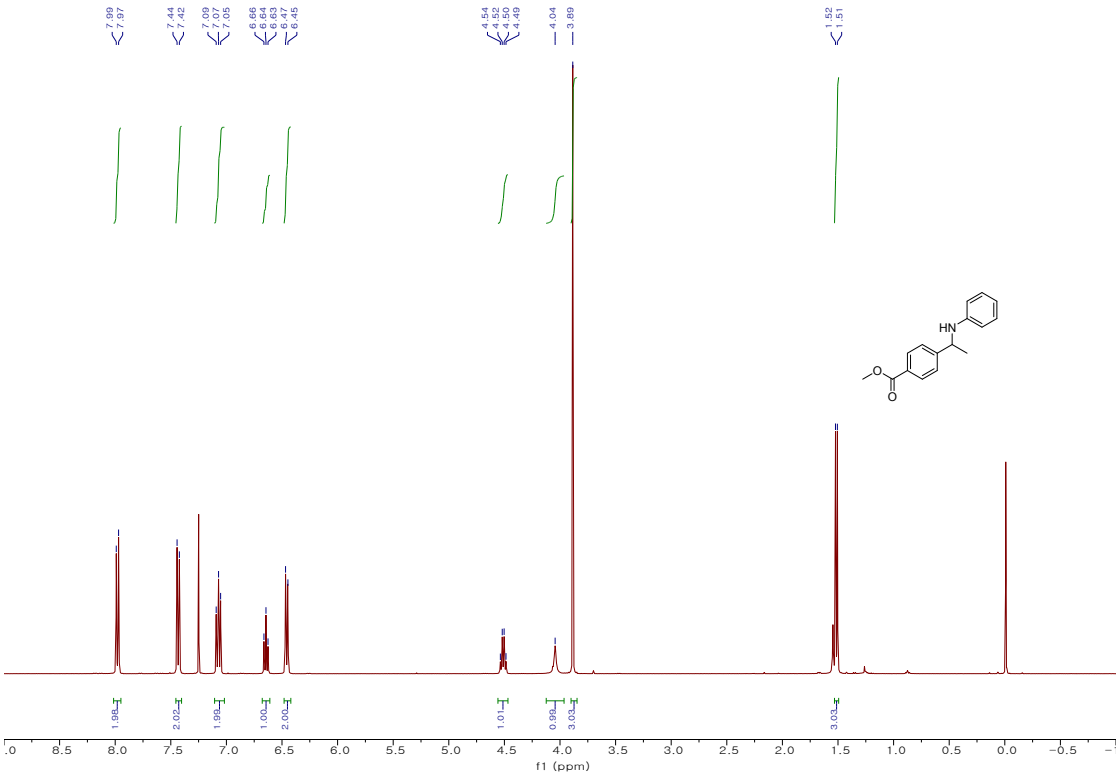


Figure S58: ^{1}H NMR of methyl 4-((phenylamino)ethyl)benzoate **(6b)**

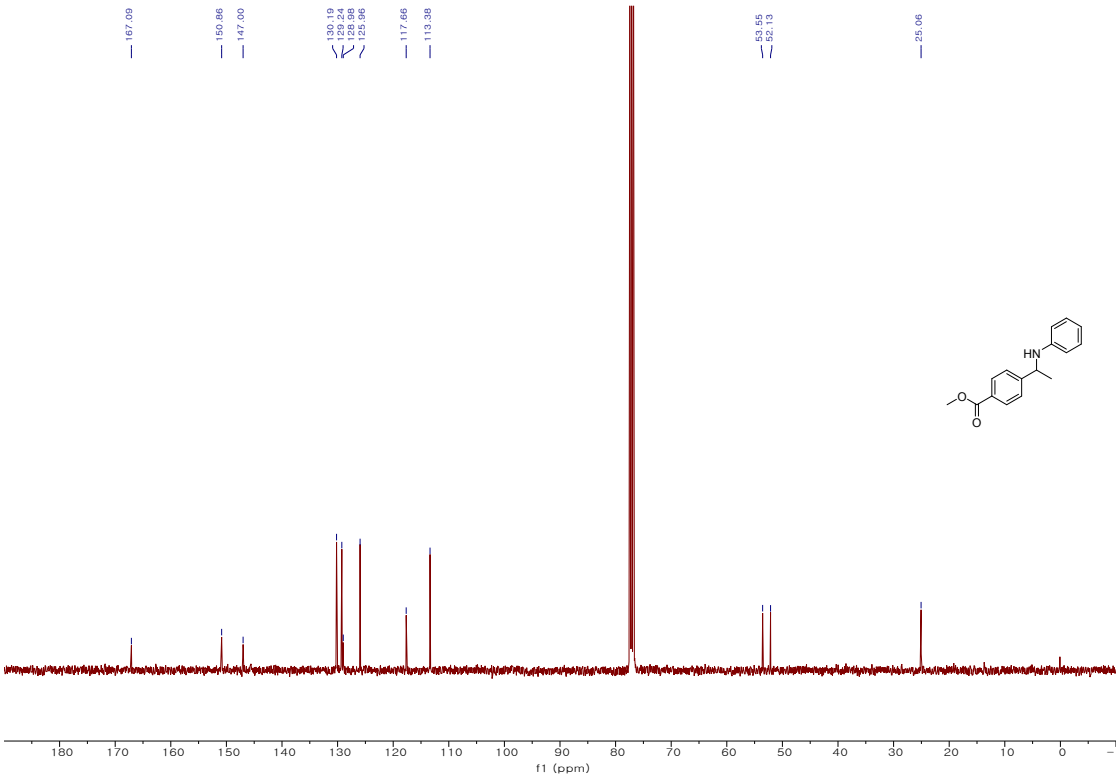


Figure S59: ^{13}C NMR of methyl 4-((phenylamino)ethyl)benzoate **(6b)**

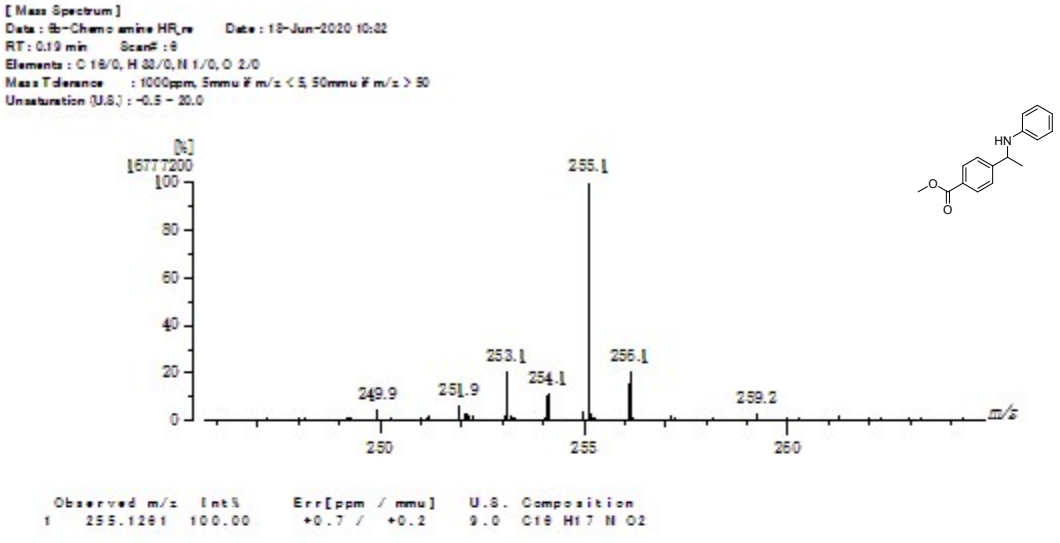


Figure S60: HRMS of methyl 4-((phenylamino)ethyl)benzoate **(6b)**

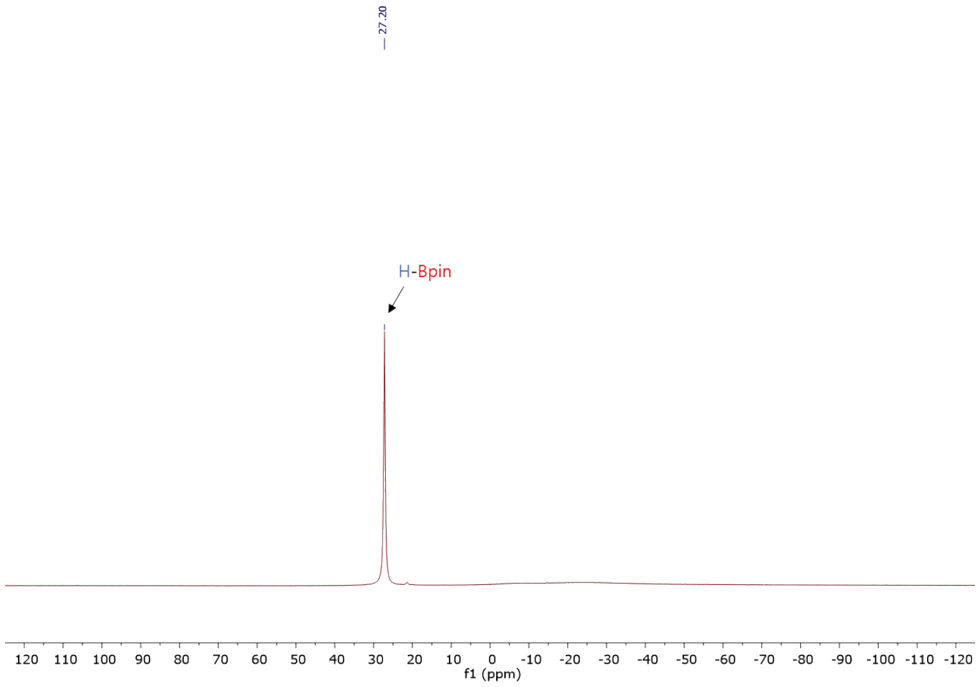


Figure S61: ^{11}B NMR of HBpin

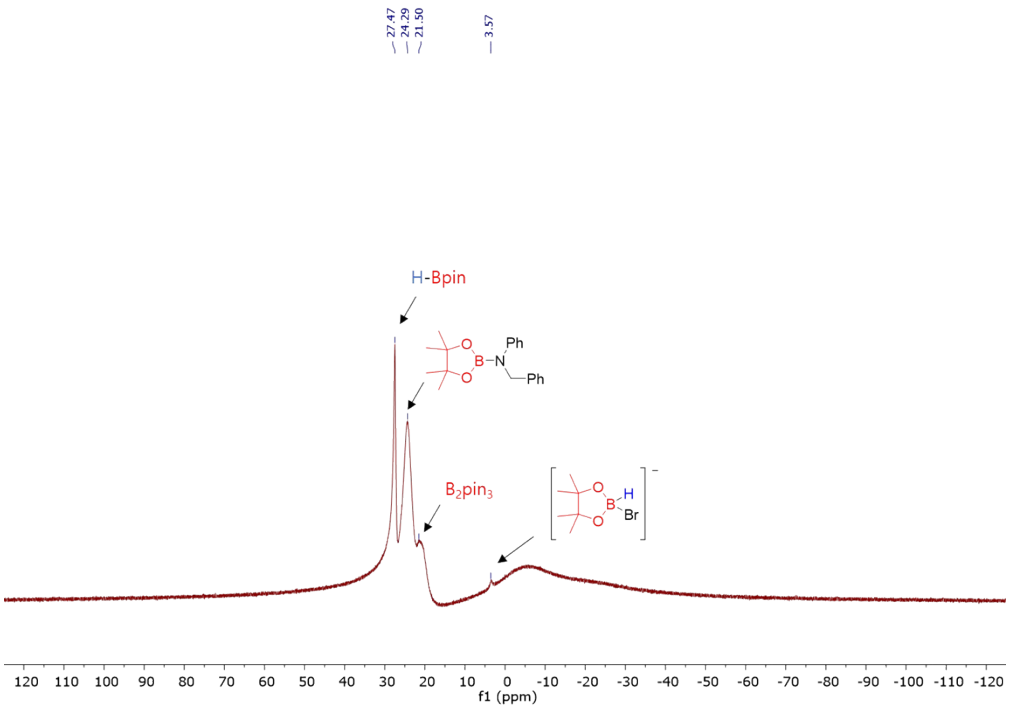


Figure S62: ^{11}B NMR of crude reaction mixture (HBpin:Imine:LiBr=1:1:1)[S17]

4. Computational method

All calculation results were obtained using the density functional theory (DFT) method as implemented in the Gaussian 16 program. [S18] Geometry optimizations and energy evaluations for all the compounds were conducted at the M06-2X/6-31G+(d,p) level of theory. Frequency calculations were performed at the same level of theory to confirm the optimized geometries with no imaginary frequency and transition states with one imaginary frequency. Intrinsic reaction coordinate (IRC) calculations were also employed to validate the transition states.

LiBr

Atom	X	Y	Z
Li	0.000000	0.000000	-2.024813
Br	0.000000	0.000000	0.173555

HBpin

Atom	X	Y	Z
C	0.780457	-0.186075	-0.054508
O	1.063449	1.186189	-0.416319
C	-0.780456	-0.186079	0.054505
B	-0.000004	1.939173	-0.000002
O	-1.063455	1.186186	0.416311
H	-0.000008	3.124660	-0.000011
C	-1.471678	-0.440687	-1.283974
H	-1.355259	-1.481015	-1.601261
H	-2.537391	-0.225307	-1.173424
H	-1.069586	0.211776	-2.064820
C	-1.346139	-1.105593	1.124701
H	-0.984963	-0.831953	2.117382
H	-2.436882	-1.033783	1.125453
H	-1.069659	-2.145403	0.920240
C	1.346152	-1.105596	-1.124693
H	2.436895	-1.033793	-1.125427
H	1.069662	-2.145404	-0.920234
H	0.984995	-0.831956	-2.117380
C	1.471672	-0.440671	1.283976
H	1.069578	0.211804	2.064812
H	1.355246	-1.480994	1.601276

H	2.537386	-0.225296	1.173428

INT1

Atom	X	Y	Z
B	-0.589805	-0.000045	-0.668776
O	0.063540	1.126827	0.030635
O	0.063548	-1.126818	0.030821
C	1.462729	0.803808	0.005433
C	1.462734	-0.803802	0.005489
C	2.096990	-1.437287	1.241638
H	1.958931	-2.520243	1.191621
H	3.168832	-1.225022	1.295052
H	1.640174	-1.088354	2.174371
C	2.096864	1.437380	1.241602
H	3.168709	1.225164	1.295120
H	1.958759	2.520328	1.191519
H	1.639988	1.088475	2.174319
C	2.089735	-1.428043	-1.241251
H	3.153843	-1.185318	-1.317672
H	1.985496	-2.514137	-1.176232
H	1.586234	-1.097123	-2.150993
C	2.089834	1.427962	-1.241292
H	1.985630	2.514063	-1.176348
H	3.153939	1.185194	-1.317628
H	1.586381	1.097001	-2.151047
Li	-0.683027	0.000078	1.472519
Br	-2.577214	-0.000002	0.005660
H	-0.596345	-0.000157	-1.865232

Aldimine (PhHCNPh)

Atom	X	Y	Z
N	-0.451520	0.529056	0.140300
C	0.386461	-0.379835	-0.166746
H	0.059068	-1.367350	-0.525713
C	-1.828128	0.233305	0.081694
C	-2.361885	-0.973248	0.552947
C	-2.688928	1.214272	-0.424452

C	-3.734188	-1.203184	0.484894
H	-1.704107	-1.711727	1.001887
C	-4.055706	0.971258	-0.505144
H	-2.262656	2.154680	-0.758677
C	-4.584604	-0.238256	-0.051498
H	-4.140076	-2.136756	0.862342
H	-4.713156	1.732396	-0.913682
H	-5.653185	-0.420130	-0.102129
C	1.841703	-0.172891	-0.083414
C	2.376766	1.036984	0.378207
C	2.701759	-1.204494	-0.471057
C	3.753899	1.205237	0.446761
H	1.694638	1.826731	0.676162
C	4.082946	-1.034556	-0.401253
H	2.285117	-2.142846	-0.829279
C	4.609605	0.170665	0.057793
H	4.166670	2.143156	0.804740
H	4.744936	-1.839467	-0.704018
H	5.685191	0.306386	0.113881

INT2

Atom	X	Y	Z
C	-1.621271	-0.154624	1.506625
C	-1.880181	-1.508998	0.696591
O	-1.626611	-1.132247	-0.666515
C	-0.403363	-0.196986	2.432545
H	-0.259689	0.796741	2.866662
H	-0.542489	-0.914154	3.247017
H	0.517225	-0.462426	1.900047
C	-2.827419	0.337925	2.305955
H	-3.080381	-0.365506	3.106101
H	-2.575636	1.300947	2.758676
H	-3.698620	0.483164	1.666948
C	-3.306733	-2.049905	0.813933
H	-3.398927	-2.919494	0.157436
H	-3.520463	-2.366781	1.839910
H	-4.048327	-1.314875	0.503183

C	-0.910334	-2.640092	1.039000
H	-1.056722	-2.987541	2.066494
H	-1.095692	-3.477602	0.360673
H	0.138918	-2.350061	0.925082
O	-1.315415	0.798064	0.476657
Li	0.116373	-0.173204	-0.591417
N	2.082706	-0.254270	-0.405246
C	2.470903	-1.621096	-0.454666
C	1.870561	-2.440390	-1.416387
C	3.356331	-2.171118	0.477495
C	2.185860	-3.793937	-1.468668
H	1.162278	-2.013778	-2.122810
C	3.659769	-3.529681	0.423667
H	3.770967	-1.544499	1.261865
C	3.081186	-4.342128	-0.549913
H	1.722463	-4.422487	-2.221850
H	4.338611	-3.955813	1.155349
H	3.315334	-5.400883	-0.583907
C	2.982935	0.638779	-0.219163
H	4.038369	0.340551	-0.182229
C	2.716808	2.072320	-0.078545
C	3.808091	2.946876	-0.169610
C	1.430196	2.588280	0.139891
C	3.619457	4.321564	-0.071703
H	4.805707	2.544597	-0.327430
C	1.247676	3.962409	0.239845
H	0.567913	1.938367	0.265096
C	2.336928	4.829411	0.130338
H	4.467824	4.993141	-0.150778
H	0.250080	4.354023	0.408734
H	2.185248	5.901318	0.209064
B	-1.847320	0.313541	-0.802968
Br	-3.768801	0.886071	-1.197450
H	-1.155605	0.744168	-1.717271

TS1

Atom	X	Y	Z

B	0.389773	-1.015445	-0.512282
H	0.032092	0.261085	-0.799067
O	-0.170798	-1.237292	0.808269
O	1.773966	-1.189271	-0.444485
C	2.154734	-1.348085	0.927749
C	0.855973	-1.940455	1.558505
C	0.663919	-1.642873	3.038202
H	1.477301	-2.080318	3.625214
H	0.660560	-0.566554	3.244972
H	-0.273490	-2.085268	3.392041
C	0.684461	-3.432030	1.283875
H	1.386378	-4.023743	1.878754
H	-0.334728	-3.727952	1.546345
H	0.841623	-3.652664	0.224703
C	2.508141	0.021697	1.506275
H	3.246722	0.500600	0.856963
H	1.635427	0.681975	1.540066
H	2.926988	-0.066077	2.514119
C	3.357131	-2.277820	0.991390
H	4.222728	-1.778028	0.549057
H	3.599280	-2.529098	2.029940
H	3.171589	-3.197263	0.433759
C	-0.368043	1.554035	-0.609478
H	-0.846859	1.583917	-1.600180
C	-2.501905	1.344935	0.359771
C	-3.038772	0.502056	-0.636915
C	-3.363193	1.776209	1.392849
C	-4.390850	0.163938	-0.621312
H	-2.399161	0.084628	-1.408495
C	-4.708759	1.425351	1.401254
H	-2.952016	2.430892	2.157456
C	-5.235234	0.622071	0.388171
H	-4.778913	-0.484452	-1.401272
H	-5.351446	1.788810	2.197695
H	-6.285076	0.348792	0.392813
N	-1.148847	1.686812	0.480075
C	0.983650	2.201719	-0.584729
C	1.953113	1.822098	-1.517989

C	1.280080	3.185280	0.359413
C	3.205385	2.427496	-1.512016
H	1.731449	1.029241	-2.228976
C	2.539741	3.783383	0.371603
H	0.512751	3.468257	1.072645
C	3.503668	3.406266	-0.562132
H	3.953707	2.126126	-2.238251
H	2.766575	4.548621	1.107711
H	4.483218	3.874421	-0.553007
Br	-0.493305	-1.936521	-2.065152
Li	-1.130910	0.117568	1.609670

INT3

Atom	X	Y	Z
C	-1.292091	-1.901169	1.010785
C	-2.361523	-0.889831	1.560462
O	-3.077216	-0.476969	0.348108
C	-1.801803	-3.332569	0.908711
H	-1.076836	-3.931680	0.352000
H	-1.918771	-3.771706	1.902859
H	-2.763382	-3.378231	0.389120
C	0.061692	-1.830564	1.694939
H	-0.046656	-2.046078	2.762724
H	0.739157	-2.574398	1.265946
H	0.521727	-0.846647	1.568903
C	-1.739586	0.380268	2.123000
H	-2.531057	1.110533	2.307763
H	-1.213405	0.184539	3.061397
H	-1.030575	0.822146	1.415672
C	-3.361288	-1.495817	2.527199
H	-2.841244	-1.879449	3.410829
H	-4.062126	-0.723142	2.851358
H	-3.928746	-2.307335	2.068995
B	-2.209970	-0.643152	-0.660782
O	-1.124274	-1.428069	-0.371841
Li	0.318636	-1.028480	-1.535029
N	1.732564	0.078090	-1.228278

C	2.923757	-0.370039	-0.742446
C	3.117597	-1.778061	-0.624494
C	4.025690	0.429077	-0.330028
C	4.287761	-2.333730	-0.135847
H	2.314562	-2.441088	-0.953688
C	5.201648	-0.142400	0.150210
H	3.958791	1.511450	-0.374801
C	5.356704	-1.522690	0.261956
H	4.375236	-3.415791	-0.073254
H	6.013787	0.515562	0.450248
H	6.275803	-1.955040	0.641462
C	1.523781	1.502140	-1.383476
H	2.453426	2.041010	-1.627452
C	0.867794	2.176794	-0.186632
C	-0.275297	2.965989	-0.351082
C	1.391391	2.030319	1.107107
C	-0.861341	3.625165	0.732362
H	-0.703116	3.078016	-1.345283
C	0.814917	2.692735	2.188362
H	2.259092	1.394669	1.260796
C	-0.311729	3.498339	2.005345
H	-1.745954	4.236198	0.577897
H	1.246010	2.579884	3.179217
H	-0.758655	4.015202	2.849267
H	0.861365	1.670531	-2.245976
Br	-2.292256	0.139485	-2.402794

TS2

Atom	X	Y	Z
C	2.390146	-1.118025	1.356412
C	2.235502	-1.918870	0.019144
O	2.365929	-0.874521	-0.980906
C	3.841075	-0.910470	1.776313
H	3.874987	-0.188658	2.595921
H	4.289852	-1.847939	2.115291
H	4.437044	-0.516309	0.948017
C	1.559951	-1.645877	2.514472

H	1.875432	-2.661292	2.773045
H	1.706878	-1.014191	3.395430
H	0.493283	-1.686491	2.271018
C	0.855769	-2.542985	-0.149368
H	0.747814	-2.886989	-1.181417
H	0.723536	-3.400214	0.517558
H	0.060542	-1.818865	0.044627
C	3.326233	-2.949698	-0.220737
H	3.320578	-3.701038	0.575835
H	3.138453	-3.456581	-1.170163
H	4.313582	-2.487667	-0.267795
B	2.069087	0.308230	-0.397664
O	1.880397	0.202866	0.981285
Li	0.046776	0.671240	1.261255
N	-0.806769	0.631779	-0.375999
C	-1.485208	1.746862	0.022136
C	-0.769365	2.729859	0.775885
C	-2.873670	2.006486	-0.173698
C	-1.405692	3.829980	1.346265
H	0.321083	2.686615	0.806069
C	-3.480593	3.122524	0.382391
H	-3.472911	1.305074	-0.746153
C	-2.769792	4.038321	1.168503
H	-0.813485	4.550661	1.904476
H	-4.543325	3.276608	0.212458
H	-3.264181	4.900534	1.601637
C	-1.439567	-0.226471	-1.343748
H	-2.027387	0.355598	-2.073374
C	-2.334832	-1.328712	-0.785203
C	-2.658380	-2.429164	-1.587014
C	-2.826051	-1.293641	0.521689
C	-3.447463	-3.467562	-1.099026
H	-2.275283	-2.473154	-2.605020
C	-3.619943	-2.330221	1.016000
H	-2.598886	-0.435314	1.149083
C	-3.931427	-3.422325	0.209275
H	-3.681616	-4.315135	-1.736516
H	-4.000696	-2.279479	2.032030

H	-4.546597	-4.229979	0.593565
H	-0.652488	-0.718971	-1.933879
Br	2.193276	1.974258	-1.299611

INT4

Atom	X	Y	Z
B	0.238532	-0.581903	-0.168176
O	0.170477	-1.130140	1.197598
O	-1.145970	-0.671704	-0.587319
C	-0.797312	-2.190185	1.218485
C	-1.759896	-1.826101	-0.006065
C	-3.169468	-1.391232	0.402946
H	-3.712527	-1.084529	-0.494987
H	-3.722297	-2.200860	0.888328
H	-3.164460	-0.528309	1.081084
C	-1.475601	-2.141592	2.588014
H	-2.236784	-2.921718	2.682742
H	-0.719503	-2.300948	3.361016
H	-1.960715	-1.179053	2.787173
C	-1.871577	-2.928135	-1.058789
H	-2.349555	-3.820664	-0.641993
H	-2.486862	-2.560878	-1.884767
H	-0.893770	-3.198033	-1.458801
C	-0.079937	-3.534526	1.087097
H	0.606079	-3.642919	1.931584
H	-0.794171	-4.363444	1.111739
H	0.505987	-3.590990	0.170258
Li	-0.893718	0.558560	1.183264
Br	1.536993	-1.565987	-1.433178
C	-0.011786	1.748464	-1.115793
H	0.592444	2.649251	-1.252911
H	-0.072762	1.231947	-2.082593
C	1.976483	1.190275	0.237851
C	2.855871	1.784235	-0.674382
C	2.462766	0.837662	1.503603
C	4.170968	2.065747	-0.308843
H	2.526927	2.005256	-1.684287

C	3.780826	1.106306	1.857439
H	1.803084	0.331048	2.200890
C	4.642203	1.733678	0.958231
H	4.834990	2.529430	-1.032078
H	4.134658	0.825052	2.844726
H	5.668145	1.949763	1.237661
C	-1.396794	2.182043	-0.663603
C	-1.542063	2.815251	0.579742
C	-2.539881	1.930961	-1.424239
C	-2.804997	3.172837	1.059455
H	-0.649079	3.051781	1.159803
C	-3.799429	2.296744	-0.954002
H	-2.438244	1.414361	-2.374331
C	-3.938631	2.908741	0.292195
H	-2.899213	3.669919	2.020357
H	-4.679619	2.086224	-1.553939
H	-4.922211	3.182920	0.659686
N	0.616668	0.908072	-0.083191

Dioxolan amine

Atom	X	Y	Z
C	-2.917998	0.119014	0.682222
C	-2.890492	-0.952467	-0.455838
O	-1.488253	-1.001187	-0.789023
C	-2.573010	-0.467065	2.050621
H	-2.396943	0.355068	2.748813
H	-3.387242	-1.087461	2.436318
H	-1.664492	-1.075634	1.997807
C	-4.195864	0.937665	0.758458
H	-5.056727	0.286076	0.942030
H	-4.123623	1.651281	1.583448
H	-4.364979	1.495836	-0.164019
C	-3.639817	-0.501801	-1.708863
H	-3.406307	-1.192093	-2.523437
H	-4.722060	-0.503199	-1.549355
H	-3.330854	0.503733	-2.010540
C	-3.344855	-2.340153	-0.033528

H	-4.377151	-2.310893	0.331170
H	-3.303289	-3.014834	-0.892664
H	-2.702307	-2.745473	0.749821
B	-0.946836	0.216842	-0.423672
O	-1.826946	0.988818	0.306584
N	0.391537	0.560054	-0.772412
C	1.046404	1.752818	-0.384014
C	0.312364	2.925621	-0.145790
C	2.442790	1.800577	-0.260217
C	0.960773	4.100489	0.217656
H	-0.765639	2.911699	-0.248134
C	3.081415	2.987714	0.094427
H	3.039184	0.908949	-0.418873
C	2.349449	4.145138	0.339353
H	0.370433	4.994463	0.395078
H	4.163357	2.996348	0.185492
H	2.850099	5.066674	0.617246
C	1.175189	-0.468597	-1.447300
H	0.489816	-1.057005	-2.063700
C	1.921665	-1.422182	-0.526964
C	2.756413	-2.390562	-1.093321
C	1.790894	-1.374308	0.860428
C	3.442376	-3.297567	-0.290626
H	2.866799	-2.434280	-2.175037
C	2.478029	-2.281148	1.668150
H	1.160726	-0.613153	1.312990
C	3.303703	-3.246022	1.096814
H	4.085576	-4.044081	-0.746547
H	2.369922	-2.227844	2.747215
H	3.838545	-3.950635	1.725742
H	1.885597	0.017838	-2.126108

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