Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

A Tandem Reduction of Primary Amines, Carbonyl Compounds, CO_2, and Borane Catalyzed by in-situ Formed Frustrated Lewis Pairs

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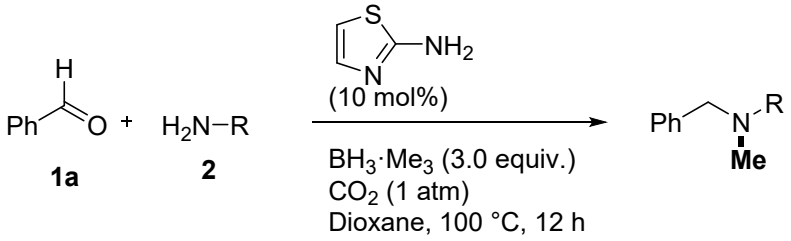
Table of Contents

1. General Information.

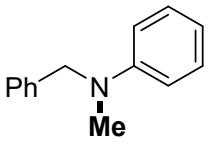
Unless otherwise noted, materials were purchased from Adamas, Energy-Chemical and other commercial suppliers and were used as received. Flash column chromatography was performed using 200-300 mesh silica gel. ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded on VARIAN-400 (400 MHz) or Bruker AV-400 (400 MHz) NMR spectrometers. Chemical shifts (δ) are reported in ppm from the resonance of tetramethyl silane as the internal standard (TMS: 0.00 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. Gas chromatographic (GC) analysis was performed on a Shimadzu GC-2010 system equipped with an FID detector and a capillary column, and the tridecane as the internal standard. High-resolution mass spectra (HRMS) were obtained with a MICROTOF-10454 Premier LC HR mass spectrometer. Enantiomeric ratio (ee) values were determined by chiral HPLC with chiral IC, AZ columns with n-hexane and *i*-PrOH as solvents. IR was measured with a Bruker TENSOR 27.

2. General Procedure and Spectral Data of Products.

2.1 General Procedure for the Reaction of Aldehydes

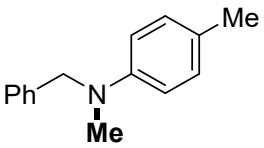


In a Schlenk tube was placed benzaldehyde (53.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol), $BH_3{\cdot}NMe_3$ (109.7 mg, 1.5 mmol), 2-aminothiazole (5.0 mg, 0.05 mmol), and dioxane (0.5 mL). The resulting mixture was stirred with a CO_2 balloon at 100 ºC (heating block) for 12 h, and then allowed to room temperature. The reaction was quenched by brine (1 mL). The aqueous layer was extracted with EtOAc (2 mL x 3). The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (silica gel, EtOAc/PE =200/1) to afford ***N*-Benzyl-*N*-methylaninline (3)** in 80% (78.9 mg) as a yellow oil.



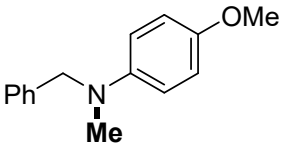
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.50 (d, J = 7.8 Hz, 2H), 7.38 (t, J = 7.2 Hz, 2H), 7.33-7.29 (m, 2H), 7.25 (d, J = 7.2 Hz, 2H), 6.57 (d, J = 7.9 Hz, 2H), 4.57 (s, 2H), 3.07 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.7, 139.0, 129.1, 128.5, 126.8, 126.7, 116.5, 112.3, 56.5, 38.4. The physical and spectral data were consistent with those previously reported.[1]

_N_-Benzyl-_N_,4-dimethylaniline (4)



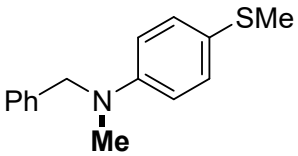
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), _p_-toluidine (54.0 mg, 0.5 mmol). Yield: 97.1 mg, 92 %, yellow oil; R_f = 0.8 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.38-7.34 (m, 2H), 7.30-7.29 (m, 3H), 7.09 (d, J = 8.4 Hz, 2H), 6.74 (d, J = 8.4 Hz, 2H), 4.54 (s, 2H), 3.02 (s, 3H), 2.31 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 147.8, 139.2, 129.7, 128.5, 126.8, 126.7, 125.7, 112.7, 57.0, 38.6, 20.2. The physical and spectral data were consistent with those previously reported.[3]

_N_-Benzyl-4-methoxy-_N_-methylaniline (5)



The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 4-methoxyaniline (62.0 mg, 0.5 mmol). Yield: 102.0 mg, 90 %, yellow oil; R_f= 0.8 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.33-7.30 (m, 2H), 7.26-7.24 (m, 3H), 6.83 (d, J = 9.0 Hz, 2H), 6.75 (d, J = 9.0 Hz, 2H), 4.43 (s, 2H), 3.75 (s, 3H), 2.92 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 151.7, 144.7, 139.2, 128.4, 127.1, 126.8, 114.7, 114.5, 57.9, 55.7, 39.0. The physical and spectral data were consistent with those previously reported.[2]

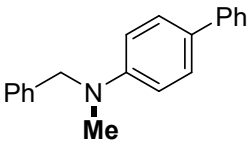
_N_-Benzyl-_N_-methyl-4-(methylthio)aniline (6)



The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 4-(methylthio)aniline (69.6 mg, 0.5 mmol). Yield: 97.3 mg, 80 %, yellow oil; R_f= 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.40-7.36 (m, 2H), 7.33-7.29 (m, 3H), 6.90 (d, J = 8.1 Hz, 2H), 6.82 (d, J = 8.1 Hz, 2H), 4.49 (s, 2H), 3.81 (s, 3H), 2.98 (s, 3H). ^{13}C{^{1}H} NMR

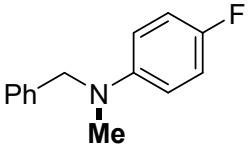
($CDCl_3$,100 MHz): δ 145.1, 139.9, 130.9, 128.2, 128.0, 126.8, 125.4, 115.5, 55.8, 35.8, 18.6. HRMS(ESI) m/z: [M + H]+ Calcd for $C_{15}H_{18}NS$ 244.1154; Found 244.1149; IR (KBr) v (cm^{-1}): 2917, 2799, 1584, 1561, 1490, 1346, 1104, 988, 955, 759, 685.

_N_-Benzyl-_N_-methyl-[1,1'-biphenyl]-4-amine (7)



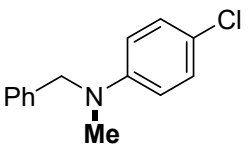
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), [1,1'-biphenyl]-4-amine (85.0 mg, 0.5 mmol). Yield: 122.0 mg, 89 %, yellow oil; R_f = 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.63-7.61 (m, 2H), 7.56 (d, J = 8.8 Hz, 2H), 7.47-7.38 (m, 4H), 7.33-7.31 (m, 4H), 6.88 (d, J = 8.8 Hz, 2H), 4.64 (s, 2H), 3.13 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.0, 141.1, 138.8, 129.2, 128.6, 128.5, 127.8, 126.9, 126.6, 125.9, 126.2, 112.5, 56.5, 38.6. The physical and spectral data were consistent with those previously reported.[4]

_N_-Benzyl-4-fluoro-_N_-methylaniline (8)



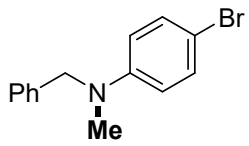
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 4-fluoroaniline (55.6 mg, 0.5 mmol). Yield: 85.0 mg, 79 %, yellow oil; R_f = 0.6 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.34-7.31 (m, 2H), 7.27-7.22 (m, 4H), 6.95-6.90 (m, 2H), 6.70-6.66 (m, 2H), 4.48 (s, 2H), 2.98 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 155.5 (d, $^1J_{C\text{-}F}$ = 234.0 Hz), 146.5, 138.8, 128.6, 126.9, 126.8, 115.5 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 113.6 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 57.5, 39.1. The physical and spectral data were consistent with those previously reported.[4]

_N_-Benzyl-4-chloro-_N_-methylaniline (9)



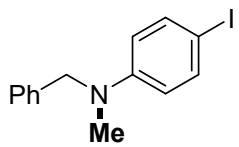
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 4-chloroaniline (64.0 mg, 0.5 mmol). Yield: 95.0 mg, 82 %, yellow oil; R_f = 0.8 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.31-7.27 (m, 2H), 7.24-7.18 (m, 1H), 7.18-7.16 (m, 2H), 7.12 (d, J = 9.1 Hz, 2H), 6.62 (d, J = 9.1 Hz, 2H), 4.48 (s, 2H), 2.97 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 148.2, 138.4, 128.9, 128.6, 126.9, 126.6, 121.2, 113.4, 56.6, 38.7. The physical and spectral data were consistent with those previously reported.[1]

***N*-Benzyl-4-bromo-*N*-methylaniline (10)**



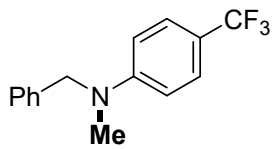
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 4-bromoaniline (86.0 mg, 0.5 mmol). Yield: 117.0 mg, 85 %, yellow oil; R_f = 0.8 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.31-7.28 (m, 2H), 7.23 (d, J = 9.1 Hz, 2H), 7.23-7.16 (m, 3H), 6.58 (d, J = 9.1 Hz, 2H), 4.48 (s, 2H), 2.98 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 148.5, 138.3, 131.7, 128.6, 127.0, 126.5, 113.9, 108.3, 56.5, 38.7. The physical and spectral data were consistent with those previously reported.[5]

***N*-Benzyl-4-iodo-*N*-methylaniline (11)**



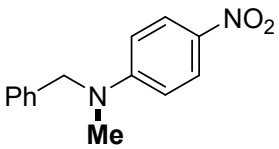
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 4-iodoaniline (110.0 mg, 0.5 mmol). Yield: 141.0 mg, 87 %, yellow oil; R_f = 0.8 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.43 (d, J = 9.0 Hz, 2H), 7.33-7.29 (m, 2H), 7.26-7.22 (m, 1H), 7.19-7.17 (m, 2H), 6.50 (d, J = 9.0 Hz, 2H), 4.50 (s, 2H), 3.00 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.0, 138.2, 137.6, 128.6, 127.0, 126.5, 114.5, 77.3, 56.3, 38.6. The physical and spectral data were consistent with those previously reported.[6]

***N*-Benzyl-*N*-methyl-4-(trifluoromethyl)aniline (12)**



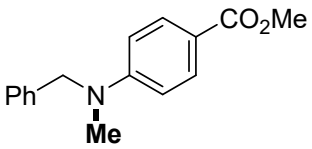
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 4-(trifluoromethyl)aniline (80.6 mg, 0.5 mmol). Yield: 104.5 mg, 79 %, yellow oil; R_f = 0.7 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.43 (d, J = 8.7 Hz, 2H), 7.33 (t, J = 7.3 Hz, 2H), 7.30-7.23 (m, 2H), 7.19 (d, J = 7.5 Hz, 2H), 6.73 (d, J = 8.7 Hz, 2H), 4.60 (s, 2H), 3.11 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 151.6, 137.9, 128.7, 127.1, 126.5 (q, $^3J_{C\text{-}F}$ = 4.0 Hz), 125.1 (q, $^1J_{C\text{-}F}$= 265.0 Hz), 117.8 (q, $^2J_{C\text{-}F}$ = 32.0 Hz), 56.1, 38.7. The physical and spectral data were consistent with those previously reported.[7]

***N*-Benzyl-*N*-methyl-4-nitroaniline (13)**



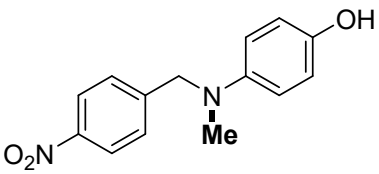
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 4-nitroaniline (69.0 mg, 0.5 mmol). Yield: 91.3 mg, 76 %, yellow oil; R_f = 0.4 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (100:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (d, J = 9.4 Hz, 2H), 7.36-7.28 (m, 3H), 7.17-7.15 (m, 2H), 6.67 (d, J = 9.4 Hz, 2H), 4.68 (s, 2H), 3.19 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 153.8, 137.4, 136.7, 129.0, 127.6, 126.3, 126.2, 110.6, 56.1, 39.2. The physical and spectral data were consistent with those previously reported.[7]

Methyl 4-(benzyl(methyl)amino)benzoate (14)



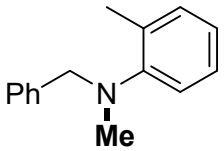
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), methyl 4-aminobenzoate (75.6 mg, 0.5 mmol). Yield: 102.0 mg, 80 %, yellow oil; R_f = 0.8 (PE/EtOAc = 5/1); purified by column chromatography eluting with PE/EtOAc (50:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.33-7.29 (m, 2H), 7.26-7.23 (m, 3H), 7.03 (d, J = 8.3 Hz, 2H), 6.69 (d, J = 8.2 Hz, 2H), 4.49 (s, 2H), 2.98 (s, 3H), 2.25 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 167.1, 151.0, 139.9, 131.4, 128.2, 128.0, 126.8, 119.2, 113.5, 55.9, 51.4, 35.8. The physical and spectral data were consistent with those previously reported[8]

4-(Methyl(4-nitrobenzyl)amino)phenol (15)



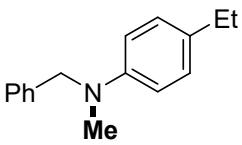
The typical procedure was applied to 4-nitrobenzaldehyde (76.0 mg, 0.5 mmol), 4-aminophenol (55.0 mg, 0.5 mmol). Yield: 104.6 mg, 81 %, yellow oil; R_f = 0.8 (PE/EtOAc = 1/1); purified by column chromatography eluting with PE/EtOAc (50:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.17 (d, J = 8.7 Hz, 2H), 7.41 (d, J = 8.7 Hz, 2H), 6.75 (d, J = 9.0 Hz, 2H), 6.65 (d, J = 9.0 Hz, 2H), 4.49 (s, 2H), 4.41 (br, 1H), 2.95 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 152.8, 139.9, 138.6, 128.3, 128.0, 126.8, 126.2, 113.0, 55.9, 35.8. The physical and spectral data were consistent with those previously reported. HRMS(ESI) m/z: [M + H]+ Calcd for $C_{14}H_{15}N_2O_3$ 259.1077; Found 259.1072; IR (KBr) v (cm^{-1}): 3425, 3324, 2912, 2754, 1520, 1516, 1456, 1358, 1018, 925, 890.

***N*-Benzyl-*N*,2-dimethylaniline (16)**



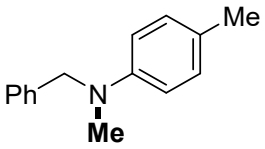
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), o-toluidine (53.6 mg, 0.5 mmol). Yield: 80.0 mg, 76 %, yellow oil; R_f = 0.6 (PE/EtOAc = 2/1); purified by column chromatography eluting with PE/EtOAc (20:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.39 (d, J = 7.6 Hz, 2H), 7.33 (t, J = 7.1 Hz, 2H), 7.28-7.26 (m, 2H), 7.22-7.16 (m, 2H), 7.09 (d, J = 7.9 Hz, 1H), 6.99 (t, J = 7.2 Hz, 1H), 4.04 (s, 2H), 2.59 (s, 3H), 2.42 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 152.4, 139.1, 132.9, 131.2, 128.4, 128.3, 127.0, 126.5, 123.0, 120.0, 60.8, 40.9, 18.4. The physical and spectral data were consistent with those previously reported.[3]

_N_-Benzyl-4-ethyl-_N_-methylaniline (17)



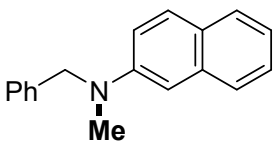
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 4-acetylaniline (68.0 mg, 0.5 mmol). Yield: 90.1 mg, 80 %, yellow oil; R_f = 0.8 (PE/EtOAc = 5/1); purified by column chromatography eluting with PE/EtOAc (100:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.41-7.38 (m, 2H), 7.34-7.30 (m, 3H), 7.15 (d, J = 8.4 Hz, 2H), 6.80 (d, J = 8.4 Hz, 2H), 4.57 (s, 2H), 3.06 (s, 3H), 2.65 (q, J =7.5 Hz, 2H), 1.31-1.28 (t, J = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 147.9, 139.3, 132.3, 128.5, 128.4, 126.8, 113.1, 112.6, 57.0, 38.6, 27.7, 15.9. IR (KBr) v (cm^{-1}): 2970, 2775, 1602, 1584, 1510, 1451, 737, 692.

_N_-Benzyl-_N_,4-dimethylaniline (4)



The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 4-aminobenzoic acid (68.6 mg, 0.5 mmol). Yield: 91.0 mg, 86 %, yellow oil; R_f = 0.8 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.38-7.34 (m, 2H), 7.30-7.29 (m, 3H), 7.09 (d, J = 8.4 Hz, 2H), 6.74 (d, J = 8.4 Hz, 2H), 4.54 (s, 2H), 3.02 (s, 3H), 2.31 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 147.8, 139.2, 129.7, 128.5, 126.8, 126.7, 125.7, 112.7, 57.0, 38.6, 20.2. The physical and spectral data were consistent with those previously reported.[3]

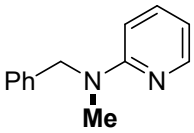
_N_-Benzyl-_N_-methylnaphthalen-2-amine (18)



The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), naphthalen-2-amine (72.0 mg, 0.5 mmol). Yield: 105.1

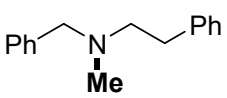
mg, 85 %, yellow oil; R_f = 0.6 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (100:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.60-7.55 (m, 3H), 7.50-7.48 (m, 2H), 7.27 (s, 1H), 7.15-7.11 (m, 3H), 6.88-6.82 (m, 3H), 4.59 (s, 2H), 2.54 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 144.1, 140.9, 134.9, 129.2, 128.6, 128.0, 127.7, 127.6, 127.0, 126.4, 125.8, 122.5, 118.3, 108.7, 65.4, 54.2. The physical and spectral data were consistent with those previously reported.[9]

_N_-Benzyl-_N_-methylpyridin-2-amine (19)



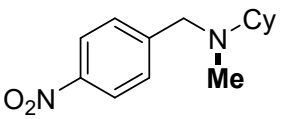
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), pyridin-2-amine (47.0 mg, 0.5 mmol). Yield: 161.0 mg, 81 %, yellow oil; R_f = 0.5 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (100:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.22-8.21 (m, 1H), 7.48-7.43 (m, 1H), 7.35-7.31 (m, 2H), 7.28-7.24 (m, 3H), 6.60-6.59 (m, 1H), 6.54-6.52 (m, 1H), 4.83 (s, 2H), 3.10 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 158.9, 148.0, 138.7, 137.3, 128.5, 127.0, 126.9, 111.8, 105.7, 53.2, 36.2. The physical and spectral data were consistent with those previously reported.[3]

_N_-Benzyl-_N_-methyl-2-phenylethan-1-amine (20)



The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 2-phenylethan-1-amine (60.6 mg, 0.5 mmol). Yield: 84.0 mg, 75 %, yellow oil; R_f = 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.29-7.26 (m, 2H), 7.24-7.04 (m, 8H), 3.53 (s, 2H), 2.80 (t, J = 8.4 Hz, 2H), 2.62 (t, J = 8.4 Hz, 2H), 2.25 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 140.5, 138.9, 129.0, 128.7, 128.3, 128.2, 126.9, 125.9, 62.2, 59.2, 42.2, 33.9. The physical and spectral data were consistent with those previously reported.[10]

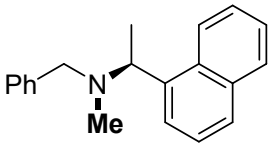
_N_-Methyl-_N_-(4-nitrobenzyl)cyclohexanamine (21)



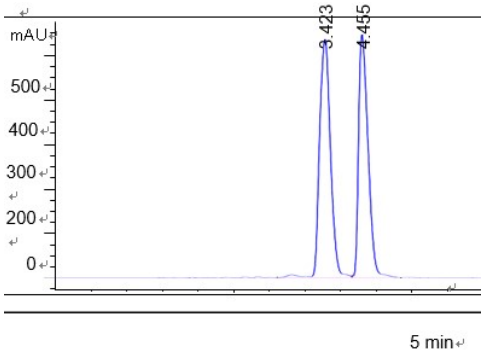
The typical procedure was applied to 4-nitrobenzaldehyde (76.0 mg, 0.5 mmol), cyclohexanamine (49.6 mg, 0.5 mmol). Yield: 111.7 mg, 90 %, yellow oil; R_f = 0.5 (PE/EtOAc = 5/1); purified by column chromatography eluting with PE/EtOAc (50:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 8.4 Hz, 2H), 3.89 (s, 2H), 2.62 (s, 3H), 2.44-2.39

(m, 1H), 1.88-1.85 (m, 2H), 1.70-1.68 (m, 2H), 1.58-1.56 (m, 1H), 1.22-1.05 (m, 5H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$,100 MHz): δ 148.9, 146.6, 128.4, 123.4, 56.2, 54.0, 50.1, 33.4, 25.9, 24.8. The physical and spectral data were consistent with those previously reported.[20]

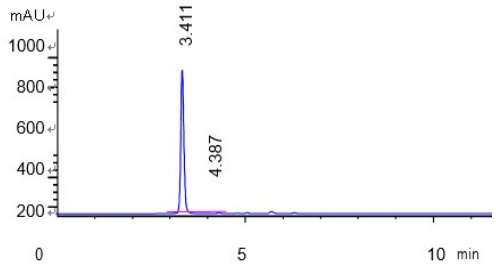
(*S*)-*N*-Benzyl-*N*-methyl-1-(naphthalen-1-yl)ethan-1-amine (22)



The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), (*S*)-1-(naphthalen-1-yl)ethan-1-amine (85.6 mg, 0.5 mmol). Yield: 118.3 mg, 86 %, yellow oil; R_f= 0.5 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); 98:2 ee, determined by HPLC analysis (Chiralpak AS column, hexane/i-PrOH, 95:5 v/v, flow rate 1 mL/min, λ = 220 nm, 25 ˚C), tR (major) = 3.411 min, tR (minor) = 4.387 min; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.47 (d, J = 8.2 Hz, 1H), 7.86 (d, J = 7.0 Hz, 1H), 7.76 (d, J = 8.2 Hz, 1H), 7.67 (d, J = 7.0 Hz, 1H), 7.53-7.44 (m, 3H), 7.27-7.26 (m, 4H), 7.24-7.18 (m, 1H), 4.42-3.37 (q, J =6.5 Hz, 1H), 3.66 (d, J = 13.2 Hz, 1H), 3.43 (d, J = 13.2 Hz, 1H), 2.21 (s, 3H), 1.57 (d, J = 7.0 Hz, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$,100 MHz): δ 140.8, 140.2, 134.2, 131.9, 128.8, 128.7, 128.2, 127.6, 126.7, 125.5, 125.4, 125.3, 124.7, 124.6, 60.7, 59.2, 38.5, 16.8. HRMS(ESI) m/z: [M + H]+ Calcd for $C_{20}H_{22}N$ 276.1748; Found 276.1743; IR (KBr) v (cm^{-1}): 2970, 2787, 1600, 1577, 1491, 1444, 1229, 796, 776, 736, 697.

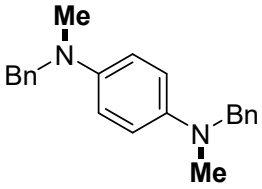


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.423	BB	0.0972	2613.33432	752.66867	48.5922
2	4.455	BB	0.0940	2764.76021	800.23354	51.4078



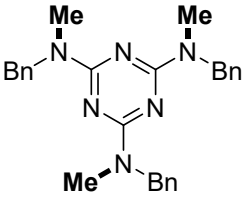
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.411	BB	0.0872	6506.74170	1129.00330	99.2119
2	4.387	BB	0.0940	51.68519	8.14864	0.7881

N^1,N^4-Dibenzyl-N^1,N^4-dimethylbenzene-1,4-diamine (23)



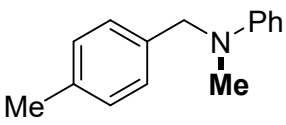
The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), benzene-1,4-diamine (27.0 mg, 0.25 mmol). Yield: 71.0 mg, 90 %, yellow oil; R_f = 0.5 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.31-7.20 (m, 10H), 6.75 (s, 4H), 4.36 (s, 4H). 2.85 (s, 6H). $^{13}C\{^1H\}$ NMR ($CDCl_3$,100 MHz): δ 142.9, 139.5, 128.4, 127.3, 126.7, 115.1, 58.3, 39.0. HRMS(ESI) m/z: [M + H]+ Calcd for $C_{22}H_{25}N_2$ 317.2012; Found 317.2015; IR (KBr) v (cm^{-1}): 3028, 2790, 1600, 1586, 1494, 1453, 1363, 1024, 736, 698.

N^2,N^4,N^6-Tribenzyl-N^2,N^4,N^6-trimethyl-1,3,5-triazine-2,4,6-triamine (24)



The typical procedure was applied to benzaldehyde (53.1 mg, 0.5 mmol), 1,3,5-triazine-2,4,6-triamine (21.0 mg, 0.17 mmol). Yield: 153.0 mg, 70 %, yellow oil; R_f= 0.4 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.35-7.32 (m, 6H), 7.29-7.28 (m, 5H), 7.22 (d, J = 3.6 Hz, 2H), 6.50 (d, J = 3.6 Hz, 2H), 4.71 (s, 6H), 3.06 (s, 9H). $^{13}C\{^1H\}$ NMR ($CDCl_3$,100 MHz): δ 163.9, 146.6, 138.2, 116.3, 110.7, 53.2, 52.9. HRMS(ESI) m/z: [M + H]+ Calcd for $C_{27}H_{31}N_6$ 439.2605; Found 439.2607; IR (KBr) v (cm^{-1}): 3426, 1602, 1541, 1496, 1450, 1212, 805.

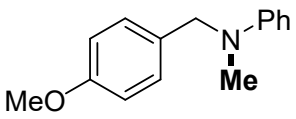
***N*-Methyl-*N*-(4-methylbenzyl)aniline (25)**



The typical procedure was applied to 4-methylbenzaldehyde (60.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 85.0

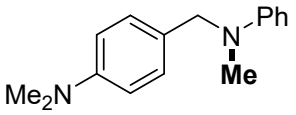
mg, 80 %, yellow oil; R_f = 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.40-7.34 (m, 2H), 7.31-7.26 (m, 4H), 6.90-6.83 (m, 3H), 4.62 (s, 2H), 3.12 (s, 3H), 2.47 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.7, 136.3, 135.8, 129.2, 129.1, 126.7, 116.4, 112.3, 56.2, 38.3, 21.0. The physical and spectral data were consistent with those previously reported.[11]

_N_-(4-Methoxybenzyl)-_N_-methylaniline (26)



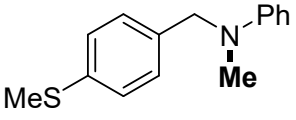
The typical procedure was applied to 4-methoxybenzaldehyde (68.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 97.0 mg, 85 %, yellow oil; R_f = 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.32-7.28 (m, 2H), 7.23 (d, J = 8.2 Hz, 2H), 6.93 (m, 2H), 6.84 (d, J = 8.2 Hz, 2H), 6.81-6.77 (m, 1H), 4.54 (s, 2H), 3.85 (s, 3H), 3.05 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 158.5, 149.7, 130.8, 129.1, 127.9, 116.5, 113.9, 112.4, 55.9, 55.2, 38.2. The physical and spectral data were consistent with those previously reported.[1]

_N_,_N_-Dimethyl-4-((methyl(phenyl)amino)methyl)aniline (27)



The typical procedure was applied to 4-(dimethylamino)benzaldehyde (75.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 108.0 mg, 90 %, yellow oil; R_f = 0.2 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (150:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.28-7.24 (m, 2H), 7.15 (d, J = 8.2 Hz, 2H), 6.83 (d, J = 8.2 Hz, 2H), 6.76-6.73 (m, 3H), 4.48 (s, 2H), 3.01 (s, 3H), 2.96 (s, 6H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 150.0, 149.7, 129.1, 127.8, 126.6, 116.2, 112.8, 112.5, 55.9, 40.7, 38.1. The physical and spectral data were consistent with those previously reported.[11]

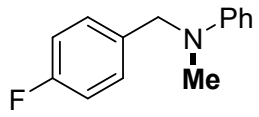
_N_-Methyl-_N_-(4-(methylthio)benzyl)aniline (28)



The typical procedure was applied to 4-(methylthio)benzaldehyde (76.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 103.0 mg, 85 %, yellow oil; R_f = 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.12-7.08 (m, 4H), 7.04-7.02 (m, 2H), 6.64-6.58 (m, 3H), 4.35 (s, 2H), 2.87 (s, 3H), 2.32 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.5, 136.6,

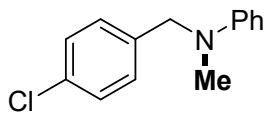
135.9, 129.1, 127.2, 126.9, 116.5, 112.3, 56.1, 38.3, 15.9. The physical and spectral data were consistent with those previously reported.[12]

_N_-(4-Fluorobenzyl)-_N_-methylaniline (29)



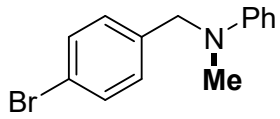
The typical procedure was applied to 4-fluorobenzaldehyde (62.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 101.0 mg, 94 %, yellow oil; R_f = 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.26-7.19 (m, 4H), 7.03-6.99 (m, 2H), 6.77-6.73 (m, 3H), 4.50 (s, 2H), 3.01 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 161.8 (d, $^1J_{C\text{-}F}$ = 243.0 Hz), 149.6, 134.5 ((d, $^4J_{C\text{-}F}$ = 3.0 Hz), 129.2, 128.2 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 116.8, 115.3 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 112.5, 56.0, 38.4. The physical and spectral data were consistent with those previously reported.[13]

_N_-(4-Chlorobenzyl)-_N_-methylaniline (30)



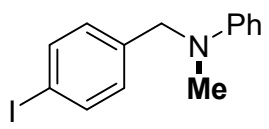
The typical procedure was applied to 4-chlorobenzaldehyde (70.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 105.0 mg, 91 %, yellow oil; R_f = 0.4 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.28-7.15 (m, 6H), 6.76-6.72 (m, 3H), 4.47 (s, 2H), 2.99 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.4, 137.5, 132.4, 129.2, 128.6, 128.0, 116.8, 112.4, 56.1, 38.5. The physical and spectral data were consistent with those previously reported.[1]

_N_-(4-Bromobenzyl)-_N_-methylaniline (31)



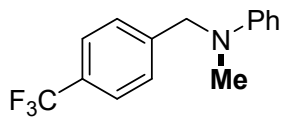
The typical procedure was applied to 4-bromobenzaldehyde (93.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 127.0 mg, 92 %, yellow oil; R_f = 0.4 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.44 (d, J = 8.2 Hz, 2H), 7.28-7.22 (m, 2H), 7.12 (d, J = 8.2 Hz, 2H), 6.77-6.73 (m, 3H), 4.48 (s, 2H), 3.01 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.4, 138.0, 131.6, 129.2, 128.4, 120.5, 116.8, 112.4, 56.1, 38.5. The physical and spectral data were consistent with those previously reported.[12]

_N_-(4-Iodobenzyl)-_N_-methylaniline (32)



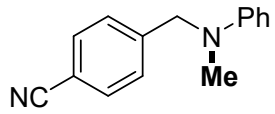
The typical procedure was applied to 4-iodobenzaldehyde (116.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 145.0 mg, 90 %, yellow oil; R_f = 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.68 (d, J = 8.2 Hz, 2H), 7.30-7.26 (m, 2H), 7.04 (d, J = 8.2 Hz, 2H), 6.81-6.77 (m, 3H), 4.51 (s, 2H), 3.05 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.4, 138.7, 137.5, 129.2, 128.7, 116.8, 112.4, 92.0, 56.2, 38.5. HRMS(ESI) m/z: [M + H]+ Calcd for $C_{14}H_{15}IN$ 324.0244; Found 324.0240; IR (KBr) v (cm^{-1}): 3027, 2817, 1599, 1576, 1507, 1452, 748, 502.

_N_-Methyl-_N_-(4-(trifluoromethyl)benzyl)aniline (33)



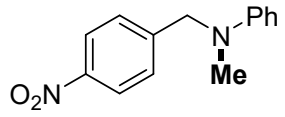
The typical procedure was applied to 4-(trifluoromethyl)benzaldehyde (87.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 110.0 mg, 83 %, yellow oil; R_f = 0.3 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58 (d, J = 8.0 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.26-7.22 (m, 2H), 6.77-6.73 (m, 3H), 4.59 (s, 2H), 3.05 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.4, 143.3, 129.3, 129.2 (q, $^2J_{C\text{-}F}$ = 21 Hz), 126.9, 125.5 (q, $^3J_{C\text{-}F}$ = 4 Hz), 124.2 (q, $^1J_{C\text{-}F}$ = 261 Hz), 117.0, 112.4, 56.4, 38.7. The physical and spectral data were consistent with those previously reported.[12]

4-((Methyl(phenyl)amino)methyl)benzonitrile (34)



The typical procedure was applied to 4-formylbenzonitrile (66.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 88.0 mg, 79 %, yellow oil; R_f = 0.2 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (100:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.61 (d, J = 8.0 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.27-7.23 (m, 2H), 6.79-6.77 (m, 1H), 6.75-6.71 (m, 2H), 4.59 (s, 2H), 3.06 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.1, 144.9, 132.4, 129.2, 127.3, 118.8, 117.1, 112.3, 110.7, 56.5, 38.8. The physical and spectral data were consistent with those previously reported.[13]

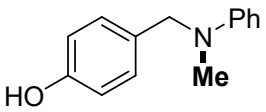
_N_-Methyl-_N_-(4-nitrobenzyl)aniline (35)



The typical procedure was applied to 4-nitrobenzaldehyde (76.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 97.0 mg, 80

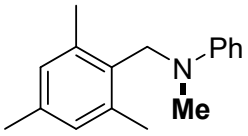
%, yellow oil; R_f = 0.3 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.22 (d, J = 8.2 Hz, 2H), 7.44 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 6.82-6.79 (m, 1H), 6.76 (d, J = 8.2 Hz, 2H), 4.66 (s, 2H), 3.11 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.1, 147.2, 147.1, 129.3, 127.3, 123.9, 117.3, 112.4, 56.5, 38.9. The physical and spectral data were consistent with those previously reported.[14]

4-((Methyl(phenyl)amino)methyl)phenol (36)



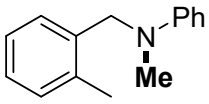
The typical procedure was applied to 4-hydroxybenzaldehyde (61.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 86.4 mg, 81 %, yellow oil; R_f = 0.5 (PE/EtOAc = 5/1); purified by column chromatography eluting with PE/EtOAc (100:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.27-7.23 (m, 2H), 7.11 (d, J = 9.0 Hz, 2H), 6.79 (d, J = 9.0 Hz, 2H), 6.77-6.75 (m, 3H), 5.06 (br, 1H), 4.47 (s, 2H), 2.99 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 154.4, 149.7, 130.9, 129.1, 128.2, 116.6, 115.3, 112.6, 56.1, 38.3. HRMS(ESI) m/z: [M + H]+ Calcd for $C_{14}H_{16}NO$ 214.1226; Found 214.1227; IR (KBr) v (cm^{-1}): 3362, 3039, 2856, 1613, 1591, 1508, 1281, 983, 920, 901, 857, 838, 819, 809, 750, 710, 693, 657.

***N*-Methyl-*N*-(2,4,6-trimethylbenzyl)aniline (37)**



The typical procedure was applied to 2,4,6-trimethylbenzaldehyde (74.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 97.0 mg, 81 %, yellow oil; R_f = 0.6 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.39 (t, J = 7.9 Hz, 2H), 7.01 (d, J = 8.1 Hz, 2H), 6.98 (s, 2H), 6.87 (t, J = 7.2 Hz, 1H), 4.42 (s, 2H), 2.68 (s, 3H), 2.38 (s, 9H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 150.7, 138.0, 136.8, 131.2, 129.1, 129.0, 116.9, 113.0, 48.7, 34.2, 20.9, 19.9. HRMS(ESI) m/z: [M + H]+ Calcd for $C_{17}H_{22}N$ 240.1752; Found 240.1750; IR (KBr) v (cm^{-1}): 1617, 1590, 1521, 1452, 1356, 1247, 1111, 945, 803, 733, 700.

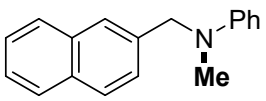
***N*-Methyl-*N*-(2-methylbenzyl)aniline (38)**



The typical procedure was applied to 2-methylbenzaldehyde (60.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 98.3 mg, 93 %, yellow

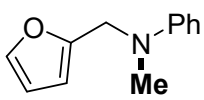
oil; R_f = 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.26-7.15 (m, 6H), 6.74-6.72 (m, 3H), 4.48 (s, 2H), 3.04 (s, 3H), 2.33 (s, 3H). $^{13}C\{^1H\}$ NMR ($CDCl_3$,100 MHz): δ 149.7, 136.2, 135.5, 130.2, 129.1, 126.7, 126.3, 126.0, 116.4, 112.1, 54.7, 38.3, 18.9. The physical and spectral data were consistent with those previously reported.[11]

_N_-Methyl-_N_-(naphthalen-2-ylmethyl)aniline (39)



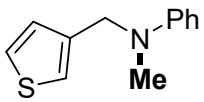
The typical procedure was applied to 2-naphthaldehyde (78.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 117.0 mg, 95 %, yellow oil; R_f= 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91-7.89 (m, 3H), 7.78 (s, 1H), 7.56-7.55 (m, 2H), 7.49-7.47 (m, 1H), 7.38-7.33 (m, 2H), 6.93 (s, 2H), 6.88-6.84 (m, 1H), 4.76 (s, 2H), 3.16 (s, 3H). $^{13}C\{^1H\}$ NMR ($CDCl_3$,100 MHz): δ 149.8, 136.6, 133.5, 132.6, 129.2, 128.3, 127.7, 127.6, 126.0, 125.5, 125.1, 125.1, 116.6, 112.4, 56.9, 38.4. The physical and spectral data were consistent with those previously reported.[11]

_N_-(Furan-2-ylmethyl)-_N_-methylaniline (40)



The typical procedure was applied to furan-2-carbaldehyde (48.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 86.0 mg, 92 %, yellow oil; R_f = 0.4 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.34 (s, 1H), 7.26-7.21 (m, 2H), 6.83 (d, J = 8.2 Hz, 2H), 6.76-6.73 (m, 1H), 6.28 (s, 1H), 6.14 (s, 1H), 4.45 (s, 2H), 2.98 (s, 3H). $^{13}C\{^1H\}$ NMR ($CDCl_3$,100 MHz): δ 152.3, 149.3, 141.8, 129.0, 117.1, 113.0, 110.1, 107.2, 49.8, 38.2. The physical and spectral data were consistent with those previously reported.[12]

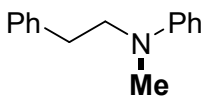
_N_-Methyl-_N_-(thiophen-3-ylmethyl)aniline (41)



The typical procedure was applied to thiophene-3-carbaldehyde (56.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 91.0 mg, 90 %, yellow oil; R_f = 0.6 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30-7.24 (m, 3H), 7.06 (s, 1H), 6.98 (d, J = 4.9 Hz, 1H), 6.81 (d, J = 8.2 Hz, 2H), 6.75 (t, J = 7.3 Hz, 1H), 4.54 (s, 2H), 3.00 (s, 3H). $^{13}C\{^1H\}$ NMR ($CDCl_3$,100 MHz): δ 149.5, 139.9, 129.1, 126.8, 126.0, 121.2, 116.7, 112.7, 52.4, 38.2. HRMS(ESI) m/z: [M + H]+ Calcd for

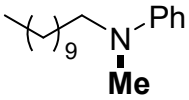
$C_{12}H_{14}NS$ 204.0841; Found 204.0838; IR (KBr) v (cm^{-1}): 3107, 3089, 2933, 1598, 1536, 1493, 1387, 1189, 1127, 1088, 945, 874, 746.

_N_-Methyl-_N_-phenethylaniline (42)



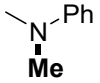
The typical procedure was applied to phenylacetaldehyde (60.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 82.0 mg, 78 %, yellow oil; R_f= 0.8 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.33-7.20 (m, 7H), 6.75-6.69 (m, 3H), 3.57 (t, J = 7.3 Hz, 2H), 2.89 (s, 3H), 2.85 (t, J = 7.3 Hz, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 148.8, 139.8, 129.3, 128.8, 128.6, 126.2, 116.1, 112.2, 54.8, 38.5, 32.9. The physical and spectral data were consistent with those previously reported.[15]

_N_-Methyl-_N_-undecylaniline (43)



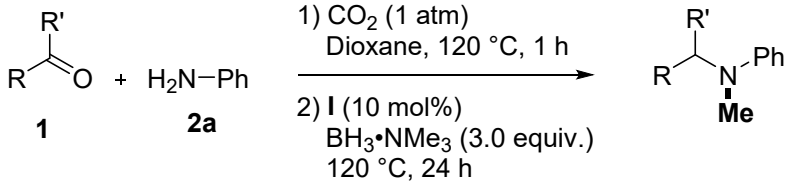
The typical procedure was applied to undecanal (85.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 98.0 mg, 75 %, yellow oil; R_f= 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.26-7.21 (m, 2H), 6.73-6.69 (m, 3H), 3.31 (t, J = 6.7 Hz, 2H), 2.94 (s, 3H), 1.60-1.57 (m, 2H), 1.33-1.29 (m, 16H), 0.90 (t, J = 6.7 Hz, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ148.8, 129.2, 116.9, 112.6, 47.5, 37.7, 32.2, 31.9, 31.8, 30.1, 29.7, 29.4, 29.3, 26.8, 22.7, 14.1. The physical and spectral data were consistent with those previously reported.[16]

_N_,_N_-Dimethylaniline (44)

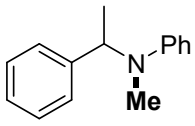


The typical procedure was applied to polyoxymethylene (30.0 mg, 0mmol), aniline (46.6 mg, 0.5 mmol). Yield: 58.0 mg, 96 %, yellow oil; R_f = 0.8 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.47-7.41 (m, 2H), 6.95-6.91 (m, 3H), 3.11 (s, 6H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 150.5, 128.9, 116.5, 112.5, 40.4. The physical and spectral data were consistent with those previously reported.[3]

2.2 General Procedure for the Reaction of Aldehydes

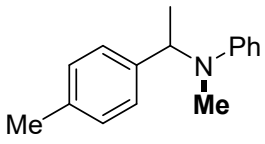


In a Schlenk tube was placed acetophenone (60.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol), and dioxane (0.5 mL). The resulting mixture was stirred with a CO_2 balloon at 120 ºC (heating block) for 1 h, then added $BH_3{\cdot}NMe_3$ (109.7 mg, 1.5 mmol) and 2-aminothiazole (5.0 mg, 0.05 mmol). The resulting mixture was stirred at 120 ºC (heating block) for 24 h, and then allowed to room temperature. The reaction was quenched by brine (1 mL). The aqueous layer was extracted with EtOAc (2 mL x 3). The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (silica gel, EtOAc/PE =300/1) to afford ***N*-Methyl-*N*-(1-phenylethyl)aniline (45)** in 86% (90.9 mg) as a yellow oil.



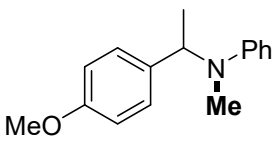
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.29-7.26 (m, 4H), 7.21-7.17 (m, 3H), 6.79-6.77 (m, 2H), 6.69-6.65 (m, 1H), 5.07 (q, J = 6.8 Hz,1H), 2.62 (s, 3H), 1.49 (d, J = 6.7 Hz, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 147.3, 145.2, 129.1, 128.6, 126.8, 125.8, 117.2, 113.3, 53.4, 29.7, 25.0. The physical and spectral data were consistent with those previously reported.[2]

***N*-Methyl-*N*-(1-(*p*-tolyl)ethyl)aniline (46)**



The typical procedure was applied to 1-(p-tolyl)ethan-1-one (67.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 87.0 mg, 77 %, yellow oil; R_f = 0.6 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.27 (d, J = 7.5 Hz, 2H), 7.15-7.08 (m, 4H), 6.67-6.63 (m, 1H), 6.53 (d, J = 7.5 Hz, 2H), 4.47 (q, J = 6.7 Hz, 1H), 2.33 (s, 3H), 1.51 (d, J = 6.7 Hz, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 147.3, 142.2, 136.4, 129.3, 129.1, 125.7, 117.2, 113.3, 53.1, 48.1, 25.0, 21.0. The physical and spectral data were consistent with those previously reported.[2]

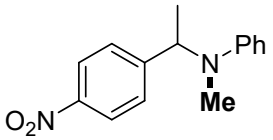
***N*-(1-(4-Methoxyphenyl)ethyl)-*N*-methylaniline (47)**



The typical procedure was applied to 1-(4-methoxyphenyl)ethan-1-one (75.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield:

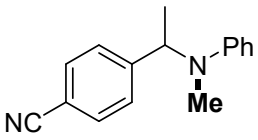
99.0 mg, 82 %, yellow oil; R_f = 0.6 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ7.66-7.61 (m, 4H), 7.26-7.23 (m, 4H), 7.12 (t, J = 7.5 Hz, 1H), 5.48 (q, J = 6.7 Hz, 1H), 4.19 (s, 3H), 3.03 (s, 3H), 1.90 (d, J = 6.7 Hz, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 158.5, 129.2, 128.1, 116.7, 113.7, 113.5, 113.3, 113.2, 56.0, 55.3, 31.7, 16.3. The physical and spectral data were consistent with those previously reported.[17]

***N*-Methyl-*N*-(1-(4-nitrophenyl)ethyl)aniline (48)**



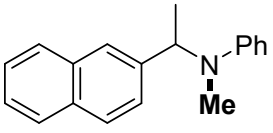
The typical procedure was applied to 1-(4-nitrophenyl)ethan-1-one (82.5 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 109.0 mg, 85 %, yellow oil; R_f = 0.5 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.18 (d, J = 8.5 Hz, 2H), 7.48 (d, J = 8.5 Hz, 2H), 7.26 (t, J = 6.7 Hz, 2H), 8.18 (d, J = 8.5 Hz, 2H), 6.78 (t, J = 6.7 Hz, 1H), 5.14 (q, J = 6.7 Hz, 1H), 2.72 (s, 3H), 1.60 (d, J = 6.7 Hz, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 161.7, 152.7, 140.2, 136.3, 129.1, 126.9, 126.3, 113.2, 53.4, 46.1, 20.9. The physical and spectral data were consistent with those previously reported.[17]

4-(1-(Methyl(phenyl)amino)ethyl)benzonitrile (49)



The typical procedure was applied to 4-acetylbenzonitrile (73.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 96.9 mg, 82 %, yellow oil; R_f = 0.4 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.62 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 8.4 Hz, 2H), 7.28-7.24 (m, 2H), 6.83-6.76 (m, 3H), 5.14-5.09 (q, J = 6.7 Hz, 1H), 2.70 (s, 3H), 1.58 (d, J = 6.9 Hz, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.8, 148.8, 132.3, 129.4, 127.6, 118.9, 117.5, 113.4, 110.8, 56.9, 32.2, 16.5. The physical and spectral data were consistent with those previously reported.[18]

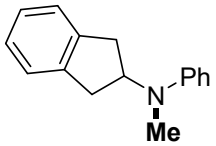
***N*-Methyl-*N*-(1-(naphthalen-2-yl)ethyl)aniline (50)**



The typical procedure was applied to 1-(naphthalen-2-yl)ethan-1-one (85.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 106.0 mg, 81 %, yellow solid; R_f= 0.6 (PE/EtOAc = 5/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz):

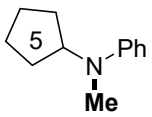
δ 7.84-7.81 (m, 2H), 7.77 (d, J = 13.5 Hz, 2H), 7.48-7.45 (m, 3H), 7.30-7.26 (m, 3H), 6.91 (d, J = 8.3 Hz, 1H), 6.76 (t, J = 7.2 Hz, 1H), 5.29 (q, J = 6.7 Hz, 1H), 2.70 (s, 3H), 1.66 (d, J = 6.8 Hz, 3H). $^{13}C\{^1H\}$ NMR ($CDCl_3$,100 MHz): δ 150.2, 140.4, 133.3, 132.5, 129.2, 128.0, 127.9, 127.5, 126.0, 125.9, 125.7, 124.9, 116.7, 113.0, 56.5, 31.8, 15.9. The physical and spectral data were consistent with those previously reported.[2]

_N_-Methyl-_N_-phenyl-2,3-dihydro-1_H_-inden-2-amine (51)



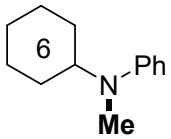
The typical procedure was applied to 1,3-dihydro-2_H_-inden-2-one (66.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 97.1 mg, 87 %, yellow oil; R_f = 0.6 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^1H NMR ($CDCl_3$, 400 MHz): δ 7.28-7.22 (m, 4H), 7.18-7.16 (m, 2H), 6.89 (d, J = 8.2 Hz, 2H), 6.77 (t, J = 7.2 Hz, 1H), 4.82-4.75 (m, 1H), 3.19 (dd, J = 16.3, 8.1 Hz, 2H), 3.06 (dd, J = 16.3, 8.1 Hz, 2H), 2.77 (s, 3H). $^{13}C\{^1H\}$ NMR ($CDCl_3$,100 MHz): δ 153.8, 149.3, 139.8, 128.0, 127.8, 126.5, 106.2, 55.7, 38.5, 35.6. The physical and spectral data were consistent with those previously reported.[19]

_N_-Cyclopentyl-_N_-methylaniline (52)



The typical procedure was applied to cyclopentanone (42.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 78.9 mg, 90 %, yellow oil; R_f = 0.4 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^1H NMR ($CDCl_3$, 400 MHz): δ 7.30-7.25 (t, J = 7.2 Hz, 2H), 6.88 (d, J = 8.2 Hz, 2H), 6.78-6.74 (t, J = 7.2 Hz, 1H), 4.25-4.17 (m, 1H), 2.84 (s, 3H), 1.95-1.90 (m, 2H), 1.82-1.72 (m, 2H), 1.68-1.60 (m, 4H). $^{13}C\{^1H\}$ NMR ($CDCl_3$,100 MHz): δ 151.1, 129.1, 116.8, 114.0, 60.3, 32.6, 28.7, 24.4. The physical and spectral data were consistent with those previously reported.[19]

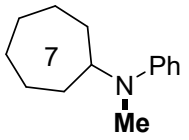
_N_-Cyclohexyl-_N_-methylaniline (53)



The typical procedure was applied to cyclohexanone (49.1 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 87.0 mg, 92 %, yellow oil; R_f = 0.6 (PE/EtOAc = 20/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^1H NMR ($CDCl_3$, 400 MHz): δ 7.22 (t, J = 7.7 Hz, 2H), 6.78 (d, J = 8.1 Hz, 2H), 6.68 (t, J = 7.2 Hz, 1H), 3.59-3.53 (m, 1H), 2.78 (s, 3H), 1.86–1.70 (m,

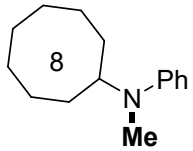
5H), 1.50–1.31 (m, 4H), 1.19-1.09 (m, 1H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$,100 MHz): δ 147.3, 129.2, 116.8, 113.1, 51.6, 33.4, 30.0, 25.9, 25.0. The physical and spectral data were consistent with those previously reported.[19]

_N_-Methyl-_N_-phenylcycloheptanamine (54)



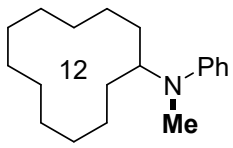
The typical procedure was applied to cycloheptanone (56.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 93.5 mg, 92 %, yellow oil; R_f = 0.6 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.26 (t, J = 7.2 Hz, 2H), 6.80 (d, J = 8.0 Hz, 2H), 6.72 (t, J = 7.2 Hz, 1H), 3.83-3.79 (m, 1H), 2.79 (s, 3H), 1.90-1.87 (m, 2H), 1.78-1.65 (m, 6H), 1.62-1.49 (m, 4H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$,100 MHz): δ 150.1, 129.2, 116.2, 113.1, 59.8, 32.1, 31.4, 27.8, 25.7. The physical and spectral data were consistent with those previously reported.[19]

_N_-Methyl-_N_-phenylcyclooctanamine (55)



The typical procedure was applied to cyclooctanone (63.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 90.2 mg, 83 %, yellow oil; R_f= 0.6 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.20-7.11 (m, 2H), 6.73-6.59 (m, 3H), 2.93 (s, 3H), 2.78-2.71 (m, 1H), 1.64-1.55 (m, 2H), 1.08-1.03 (m, 2H), 0.90-0.84 (m, 2H), 0.59-0.54 (m, 2H), 0.42-0.33 (m, 4H), 0.23-0.19 (m, 2H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$,100 MHz): δ 150.0, 129.2, 116.0, 112.9, 58.1, 31.6, 31.4, 26.6, 26.5, 25.5. HRMS(ESI) m/z: [M + H]+ Calcd for $C_{15}H_{24}N$ 218.1903; Found 218.1906; IR (KBr) v (cm^{-1}): 2933, 2921, 1617, 1590, 1521, 1483, 1364, 1297, 1260, 1175, 1088, 956, 854, 725, 691.

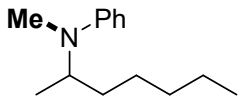
_N_-Methyl-_N_-phenylcyclododecanamine (56)



The typical procedure was applied to cyclododecanone (91.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 106.6 mg, 79 %, yellow oil; R_f= 0.8 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.23 (t, J = 7.9 Hz, 2H), 6.78 (d, J = 8.2 Hz, 2H), 6.67 (t, J = 7.1 Hz, 1H), 3.98-3.91 (m, 1H), 2.73 (s, 3H), 1.71-1.66 (m, 2H), 1.48-1.35 (m, 20H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$,100 MHz): δ 150.9, 129.1, 115.8, 112.6, 53.4, 30.9, 27.6, 24.1, 24.0, 23.2, 22.7, 22.6. HRMS(ESI) m/z:

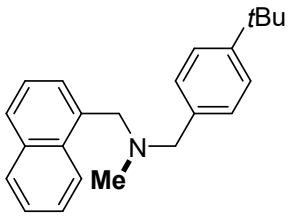
[M + Na]+ Calcd for $C_{19}H_{31}NNa$ 296.2349; Found 296.2355; IR (KBr) v (cm^{-1}): 2933, 2921, 1617, 1590, 1521, 1472, 1355, 1280, 1166, 1070, 946, 822, 710, 690.

_N_-(Heptan-2-yl)-_N_-methylaniline (57)



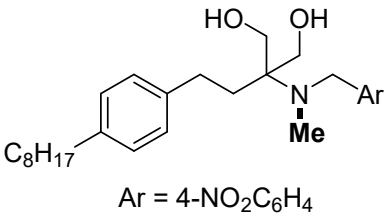
The typical procedure was applied to heptan-2-one (57.0 mg, 0.5 mmol), aniline (46.6 mg, 0.5 mmol). Yield: 67.8 mg, 66 %, yellow oil; R_f= 0.8 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (300:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30-7.26 (m, 2H), 6.83 (d, J = 8.2 Hz, 2H), 6.73 (t, J = 7.2 Hz, 1H), 3.99-3.91 (m, 1H), 2.76 (s, 3H), 1.68-1.61 (m, 2H), 1.52-1.45 (m, 2H), 1.36-1.33 (m, 4H), 1.16 (d, J = 6.6 Hz, 3H), 0.94-0.91 (m, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 150.6, 129.1, 116.0, 112.9, 53.3, 34.6, 31.9, 29.8, 26.6, 22.7, 17.1, 14.1. HRMS(ESI) m/z: [M + H]+ Calcd for $C_{14}H_{24}N$ 206.1903; Found 206.1904; IR (KBr) v (cm^{-1}): 1600, 1570, 1505, 1489, 1247, 945, 813, 732, 690.

_N_-(4-(Tert-butyl)benzyl)-_N_-methyl-1-(naphthalen-1-yl)methanamine (Butenafine) (58)



The typical procedure was applied to 4-(*tert*-butyl)benzaldehyde (811.0 mg, 5 mmol), naphthalen-1-ylmethanamine (786.0 mg, 5 mmol). Yield: 1.43 g, 90 %, yellow oil; R_f = 0.5 (PE/EtOAc = 10/1); purified by column chromatography eluting with PE/EtOAc (200:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.18-8.16 (m, 1H), 7.77-7,75 (m, 1H), 7.70-7.68 (m, 1H), 7.44-7.15 (m, 8H), 3.86 (s, 2H), 3.51 (s, 2H), 2.14 (s, 3H), 1.25 (s, 9H). ^{13}C{^{1}H} NMR ($CDCl_3$,100 MHz): δ 149.9, 136.4, 135.2, 134.0, 132.6, 128.8, 128.4, 127.9, 127.4, 125.7, 125.6, 125.1, 125.1, 125.0, 62.1, 60.5, 42.4, 34.5, 31.5. The physical and spectral data were consistent with those previously reported.[2]

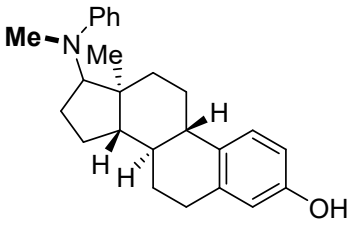
2-(Methyl(4-nitrobenzyl)amino)-2-(4-octylphenethyl)propane-1,3-diol (59)



The typical procedure was applied to 4-nitrobenzaldehyde (46.0 mg, 0.3 mmol), 2-amino-2-(4-octylphenethyl)propane-1,3-diol (Fingolimod) (92.0 mg, 0.3 mmol). Yield: 95.4 mg, 80 %, yellow oil; R_f = 0.5 (PE/EtOAc = 1/1); purified by column chromatography eluting with PE/EtOAc (10:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.15 (d, J = 6.7 Hz, 2H),

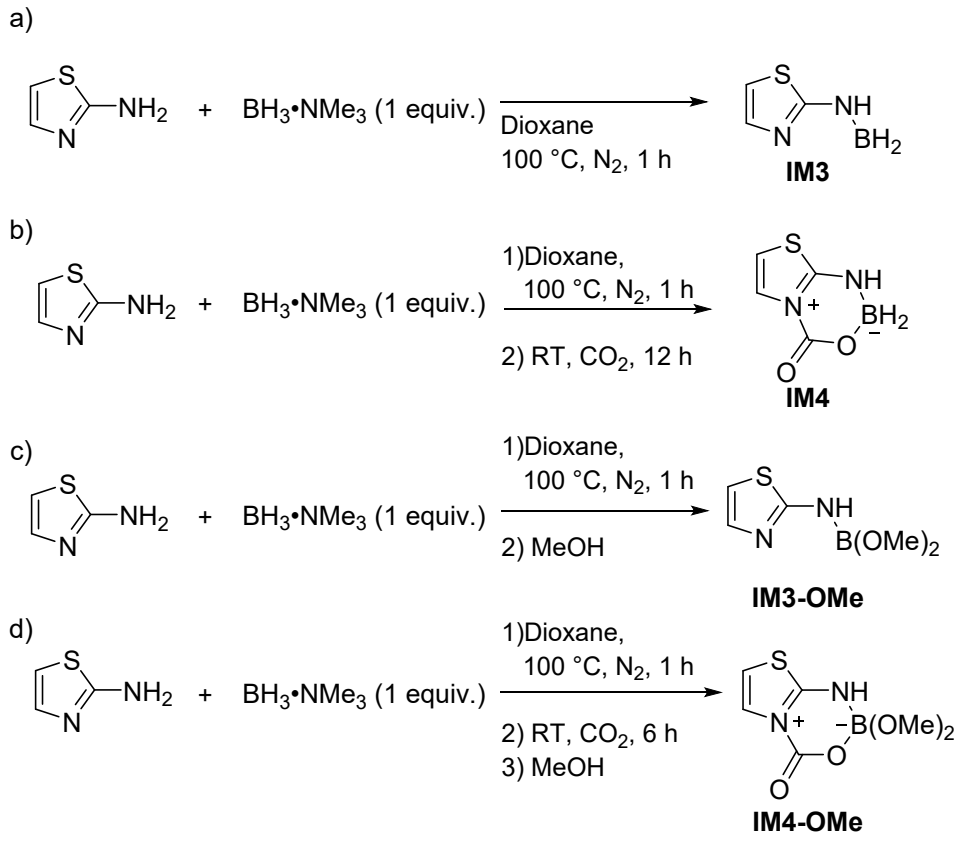
7.53 (d, J = 6.7 Hz, 2H), 7.09 (sr, 4H), 3.82 (s, 2H), 3.66 (s, 3H), 2.65-2.61 (m, 5H), 2.56 (t, J = 8.2 Hz, 2H), 1.74-1.70 (m, 2H), 1.61-1.54 (m, 2H), 1.30-1.27 (m, 11H), 0.88 (t, J = 8.2 Hz, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$,100 MHz): δ 148.0, 147.0, 140.7, 139.0, 128.8, 128.5, 127.9, 123.6, 65.2, 63.7, 59.2, 54.3, 44.9, 35.5, 33.1, 31.8, 31.5, 29.4, 29.3, 29.2, 28.8, 22.6, 14.0. HRMS(ESI) m/z: [M + Na]+ Calcd for $C_{27}H_{40}N_2O_4Na$ 479.2880; Found 479.2884; IR (KBr) v (cm^{-1}): 3435, 3351, 2926, 2854, 1524, 1513, 1466, 1348, 1018, 965, 920.

(8*R*,9*S*,13*S*,14*S*)-13-Methyl-17-(methyl(phenyl)amino)-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a]phenanthren-3-ol (60)



The typical procedure was applied to (8*R*,9*S*,13*S*,14*S*)-3-hydroxy-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[a]phenanthren-17-one (Estrone) (81.0 mg, 0.3 mmol), aniline (28.0 mg, 0.3 mmol). Yield: 86.8 mg, 80 %, yellow oil; R_f= 0.4 (PE/EtOAc = 5/1); purified by column chromatography eluting with PE/EtOAc (50:1); ^{1}H NMR ($CDCl_3$, 400 MHz): δ7.17-7.13 (m, 4H), 6.67-6.65 (m, 3H), 6.56 (s, 1H), 3.50 (t, J = 8.2 Hz, 1H), 2.82 (br, 1H), 2.27-2.25 (m, 2H), 2.18 (s, 3H), 1.92-1.90 (m, 4H), 1.43-1.42 (m, 2H), 1.39-1.36 (m, 4H), 1.26 (s, 3H), 0.80 (s, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz): δ 155.3, 148.5, 138.2, 132.6, 129.2, 126.5, 116.8, 115.2, 115.1, 113.2, 112.6, 63.6, 51.9, 43.9, 43.8, 39.0, 38.2, 30.0, 29.7, 29.6, 27.3, 26.4, 23.3, 14.1, 12.0. HRMS(ESI) m/z: [M + K]+ Calcd for $C_{25}H_{31}NOK$ 400.2037; Found 400.2034; IR (KBr) v (cm^{-1}): 3327, 1718, 1619, 1581, 1498, 1356, 1247, 942, 793, 682.

3. Mechanistic Studies:



Scheme S1. HRMS experiments.

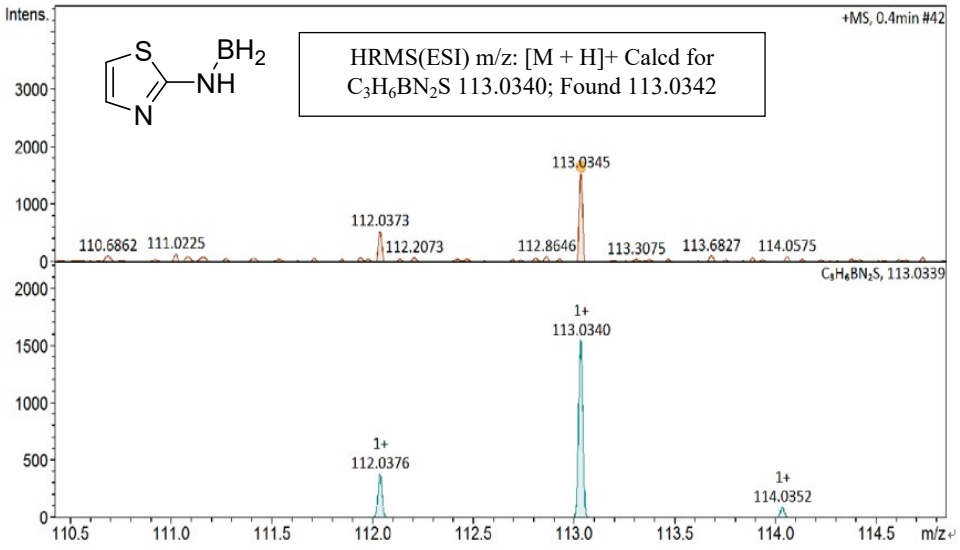
a) In a Schlenk tube was placed $BH_3{\cdot}NMe_3$ (14.7 mg, 0.2 mmol), 2-aminothiazole (20.0 mg, 0.2 mmol), dioxane (0.1 mL). The resulting mixture was stirred under N_2 atmosphere at 100 ºC (heating block) for 1 h, and then allowed to room temperature. The resulting mixture was added MeCN in glovebox for HRMS analysis.

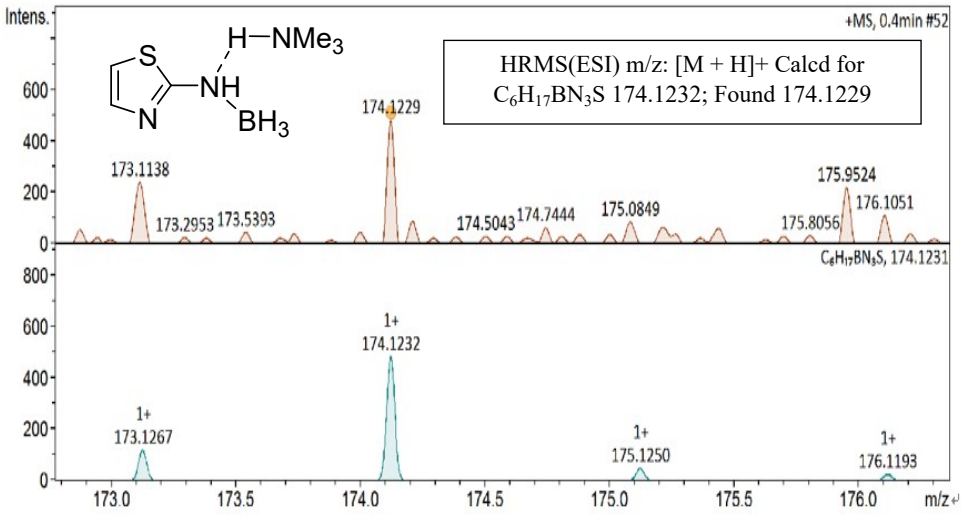
b) In a Schlenk tube was placed $BH_3{\cdot}NMe_3$ (14.7 mg, 0.2 mmol), 2-aminothiazole (20.0 mg, 0.2 mmol), dioxane (0.1 mL). The resulting mixture was stirred under N_2 atmosphere at 100 ºC (heating block) for 1 h, and then the Schlenk tube was attached to a CO_2 balloon at room temperature for 12 h. The resulting mixture was added dry MeCN in glovebox for HRMS analysis.

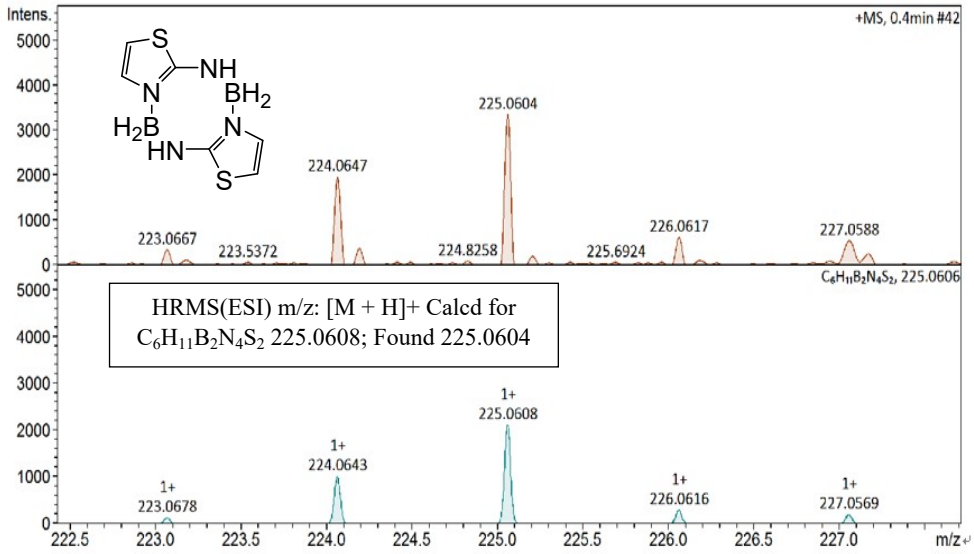
c) In a Schlenk tube was placed $BH_3{\cdot}NMe_3$ (14.7 mg, 0.2 mmol), 2-aminothiazole (20.0 mg, 0.2 mmol), dioxane (0.2 mL). The resulting mixture was stirred under N_2 atmosphere at 100 ºC (heating block) for 1 h, and then allowed to room temperature. Then MeOH (0.5 mL) was added. After stirred a few minutes, the resulting mixture was filtered.

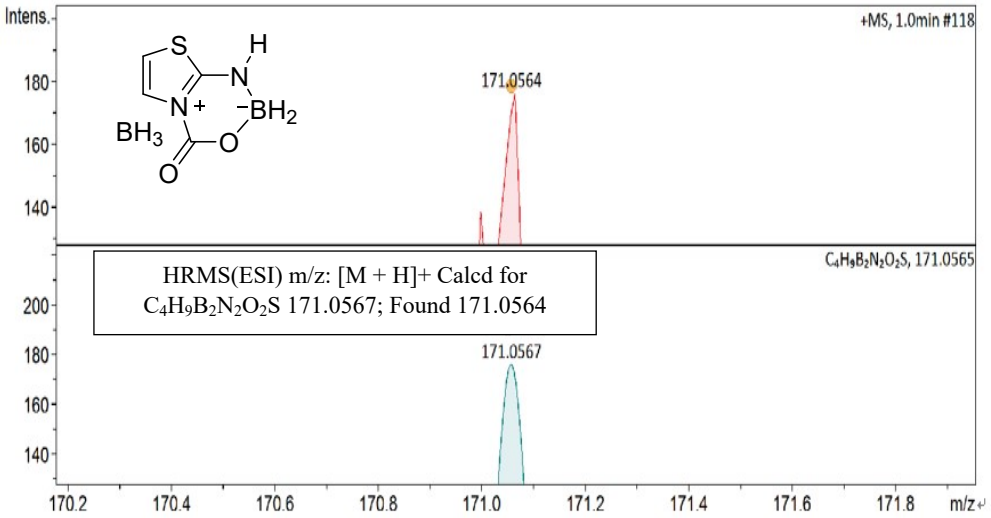
The filtrate was concentrated to dryness to afford **Dimethyl thiazol-2-ylboramidate (IM3-OMe)** in 56% (19.2 mg) as a pale yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.02 (d, J = 4.0 Hz, 1H), 6.46 (d, J = 4.0 Hz, 1H), 5.55 (br, 1H), 3.45 (s, 6H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$,100 MHz): δ 168.7, 138.4, 108.3, 51.1. $^{11}B\{^{1}H\}$ NMR ($CDCl_3$,128 MHz): δ 18.46. HRMS(ESI) m/z: [M+H]+ Calcd for $C_5H_{10}BN_2O_2S$ 172.0587; Found 172.0587.

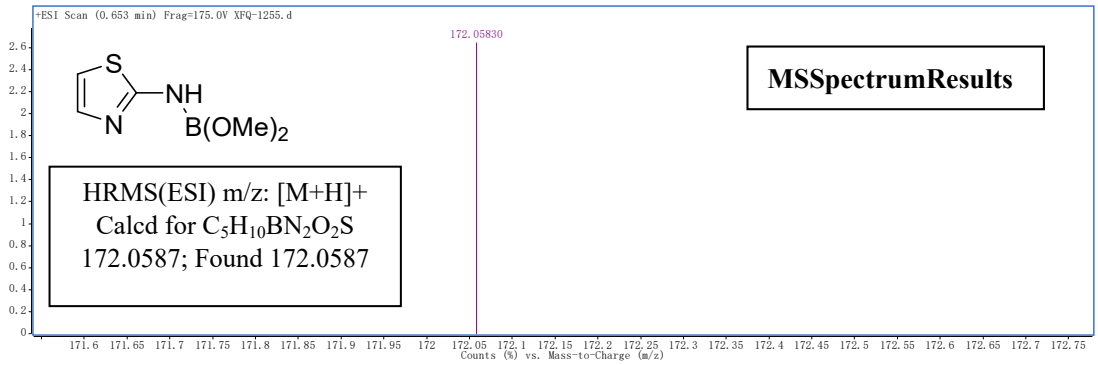
d) In a Schlenk tube was placed $BH_3{\cdot}NMe_3$ (14.7 mg, 0.2 mmol), 2-aminothiazole (20.0 mg, 0.2 mmol), dioxane (0.2 mL). The resulting mixture was stirred under N_2 atmosphere at 100 ºC (heating block) for 1 h, and then the Schlenk tube was attached to a CO_2 balloon at room temperature for 6 h, and then allowed to room temperature. Then MeOH (0.5 mL) was added. After stirring for a few minutes, the resulting mixture was added to dry MeCN in the glovebox for HRMS analysis.




Intens.
+MS, 0.4min #52
H—NMe3
S
NH
N
BH3
HRMS(ESI) m/z: [M + H]+ Calcd for
C6H17BN3S 174.1232; Found 174.1229
174.1229
173.1138
173.2953
173.5393
174.5043
174.7444
175.0849
175.8056
175.9524
176.1051
C6H17BN3S, 174.1231
1+
174.1232
1+
173.1267
1+
175.1250
1+
176.1193
m/z

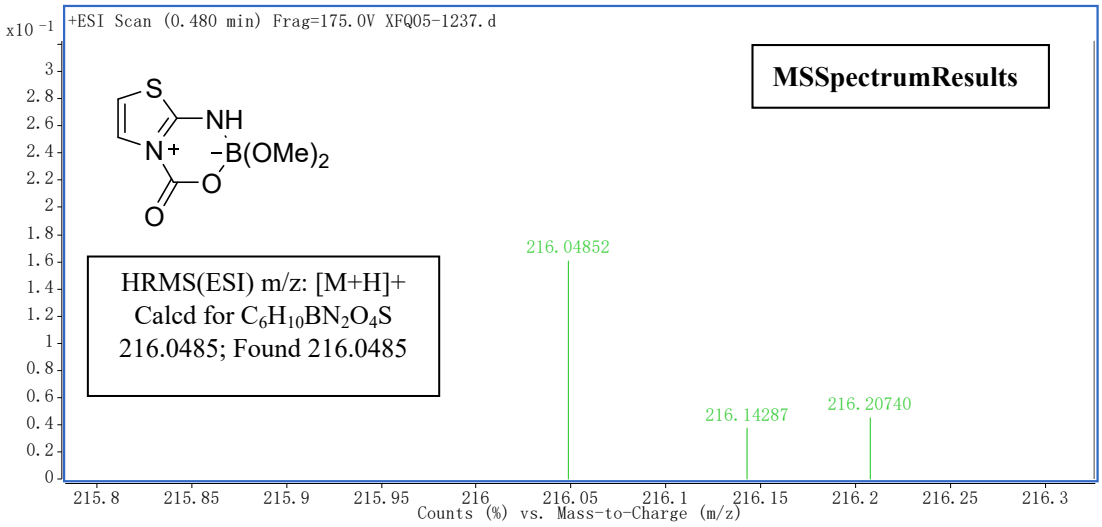

Intens.
+MS, 0.4min #42
S
NH
BH2
N
H2B
HN
N
S
HRMS(ESI) m/z: [M + H]+ Calcd for
C6H11B2N4S2 225.0608; Found 225.0604
225.0604
224.0647
223.0667
223.5372
224.8258
225.6924
226.0617
227.0588
C6H11B2N4S2, 225.0606
1+
225.0608
1+
224.0643
1+
223.0678
1+
226.0616
1+
227.0569
m/z


Intens.
+MS, 1.0min #118
S
H
N
N+
-BH2
BH3
O
O
HRMS(ESI) m/z: [M + H]+ Calcd for
C4H9B2N2O2S 171.0567; Found 171.0564
171.0564
C4H9B2N2O2S, 171.0565
171.0567
m/z



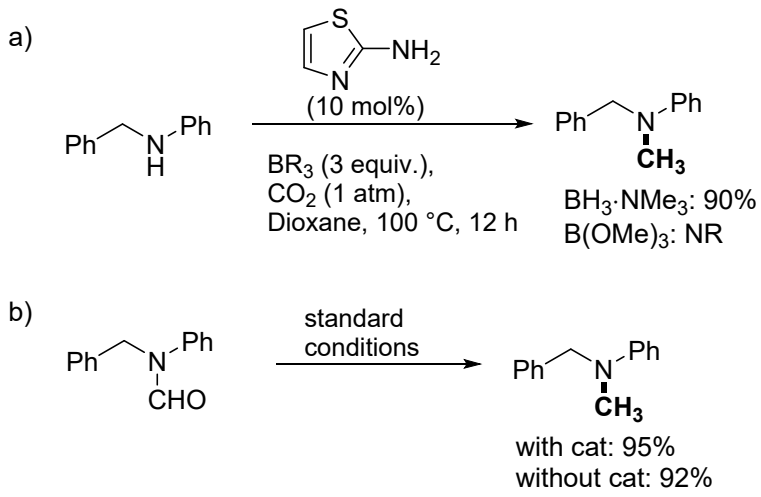
FormulaCalculate

Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	DBE	m/z
C5 H9 B N2 O2 S	**100**	**171.0514**	**171.0514**	**172.05869**	**-0.08**	**3**	**172.0587**
C13 H5 B	97.83	171.0514	171.0521	172.05934	3.73	12	172.0587
C7 H9 N O4	86.15	171.0514	171.0532	172.06043	10.14	4	172.0587
H9 N7 O2 S	76.77	171.0514	171.0538	172.06112	14.15		172.0587



FormulaCalculate

Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	DBE	m/z
C6 H9 B N2 O4 S	**100**	**215.0412**	**215.0412**	**216.04852**	**0.07**	**4**	**216.0485**
C14 H5 B O2	97.97	215.0412	215.0419	216.04917	3.11	13	216.0485
C12 H9 N O S	97.53	215.0412	215.0405	216.04776	-3.44	9	216.0485
C4 H13 N3 O3 S2	91.82	215.0412	215.0398	216.04711	-6.47	0	216.0485
C8 H9 N O6	87.56	215.0412	215.043	216.05026	8.2	5	216.0485
C9 H13 N O S2	76.63	215.0412	215.0439	216.05113	12.24	4	216.0485
C9 H5 N5 O2	71.05	215.0412	215.0443	216.0516	14.42	10	216.0485



Scheme S2. Control experiments.

a) In a Schlenk tube was placed $BH_3{\cdot}NMe_3$ (109.4 mg, 1.5 mmol) or $B(OMe)_3$ (155.9 mg, 1.5 mmol), 2-aminothiazole (5.0 mg, 0.05 mmol), *N*-benzylaniline (91.6 mg, 0.5 mmol), dioxane (0.5 mL). The resulting mixture was stirred with a CO_2 balloon at 100 ºC (heating block) for 12 h, and then allowed to room temperature. The reaction was quenched by brine (1 mL). The aqueous layer was extracted with EtOAc (2 mL x 3). The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The yield was determined by ^{1}H NMR with 1,1,2,2-tetrachloroethane as the internal standard.

b) In a Schlenk tube was placed *N*-benzyl-*N*-phenylformamide (105.6 mg, 0.5 mmol), $BH_3{\cdot}NMe_3$ (109.7 mg, 1.5 mmol), 2-aminothiazole (5.0 mg, 0.05 mmol) or no catalyst, dioxane (0.5 mL). The resulting mixture was stirred with a CO_2 balloon at 100 ºC (heating block) for 12 h, and then allowed to room temperature. The reaction was quenched by brine (1 mL). The aqueous layer was extracted with EtOAc (2 mL x 3). The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The yield was determined by ^{1}H NMR with 1,1,2,2-tetrachloroethane as the internal standard.

Computational Methods:

Density functional theory calculations were performed with the Gaussian 09 package[21]. Geometry optimizations and frequency calculations were performed at the B3LYP-D3(BJ)[22,23]/def2-SVP level in dioxane solution using the SMD solvation model,[24] in which the dispersion interaction correction D3(BJ) was added to the B3LYP functional to improve the computational accuracy. Frequency outcomes were examined to confirm stationary points as

minima (no imaginary frequencies) or transition states (only one imaginary frequency). Free energies (in kcal mol^{-1}) were utilized in the discussion.

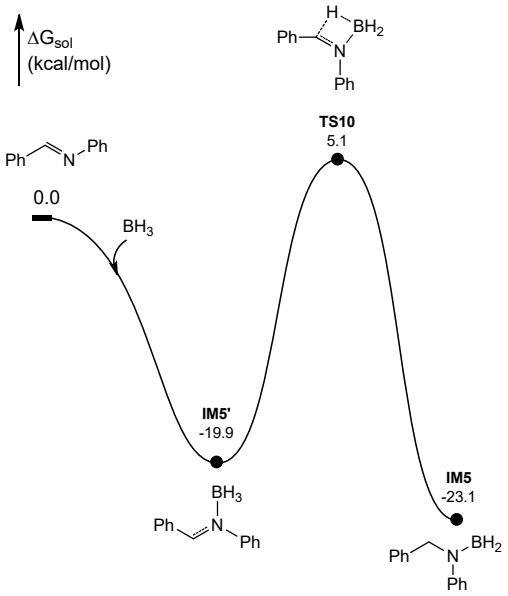


Figure S1. Free energy profile for the *in-situ*-generation of *N*-benzylideneaniline.

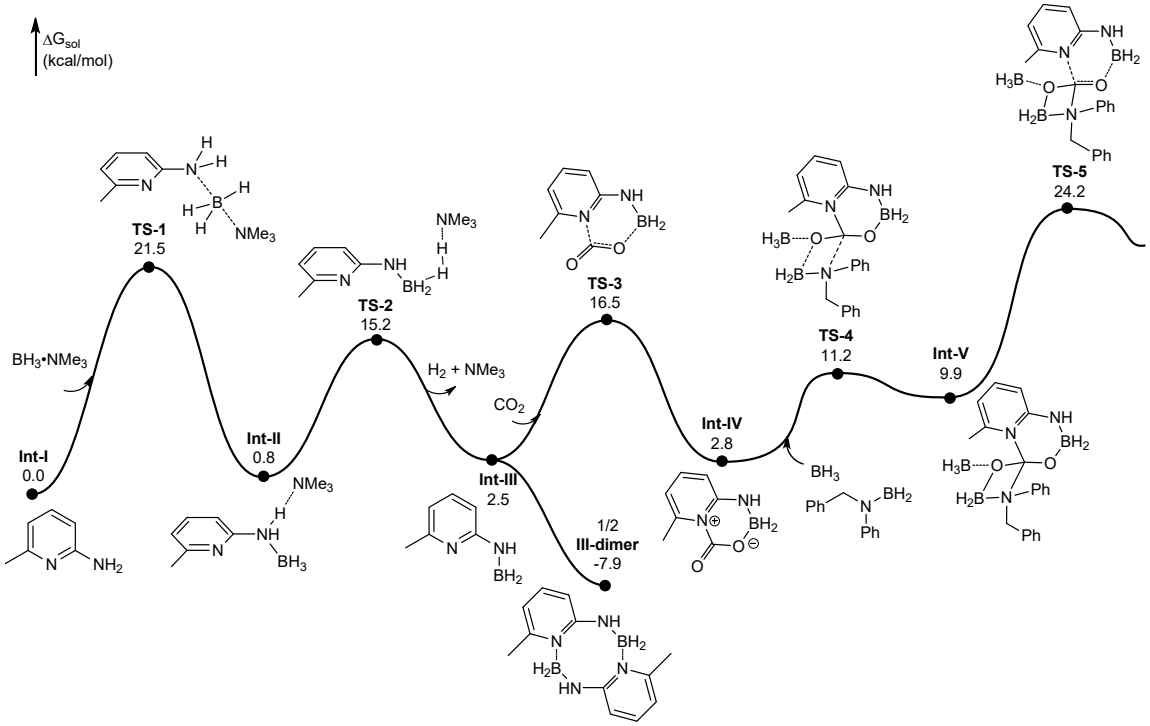


Figure S2. Free energy profile for the catalytic process by catalyst-**II**.

Cartesian Coordinates (Å) for the Optimized Structures

IM1 (1)

C	0.783935	0.220626	-0.004412
C	-1.216295	1.159407	0.003814
C	-1.645161	-0.135208	0.007876
S	-0.263839	-1.208623	-0.004734
H	-1.881942	2.025220	0.009821
H	-2.661414	-0.524309	0.020674
N	0.144348	1.356856	0.000926
N	2.141742	0.096957	-0.060019
H	2.659157	0.948409	0.135671
H	2.568119	-0.756994	0.279564

BH_3•NMe_3

B	0.000000	0.000000	1.647928
H	1.018318	0.587926	1.992666
H	-1.018318	0.587926	1.992666
H	0.000000	-1.175852	1.992666
N	0.000000	0.000000	0.007816
C	0.000000	1.397128	-0.490033
H	-0.891862	1.912090	-0.112810
H	0.891862	1.912090	-0.112810
H	0.000000	1.412251	-1.591632
C	1.209949	-0.698564	-0.490033
H	2.101850	-0.183670	-0.112810
H	1.209987	-1.728420	-0.112810
H	1.223045	-0.706125	-1.591632
C	-1.209949	-0.698564	-0.490033
H	-1.209987	-1.728420	-0.112810
H	-2.101850	-0.183670	-0.112810
H	-1.223045	-0.706125	-1.591632

TS1

C	1.940963	0.705315	-0.272485
C	3.555245	0.148080	1.120505
C	3.488943	-1.034869	0.440911
S	2.242085	-0.952168	-0.769634
H	4.248773	0.355530	1.937217
H	4.085242	-1.935888	0.574599
N	2.680711	1.125709	0.708525
N	0.898019	1.444558	-0.833743
H	0.923732	2.406797	-0.493973
H	0.876118	1.432264	-1.852951
B	-0.974153	0.719874	-0.366852
H	-1.540406	1.650578	-0.904061
H	-0.774961	0.743828	0.826542
H	-0.794687	-0.307745	-0.985756
N	-3.126223	-0.151021	0.158663
C	-3.768878	0.830624	1.010086
H	-3.158448	1.002904	1.909394
H	-3.860926	1.788249	0.475338
H	-4.785543	0.517870	1.336788
C	-3.828666	-0.340725	-1.094942
H	-3.927881	0.621806	-1.619637
H	-3.259549	-1.023475	-1.744241
H	-4.848134	-0.765206	-0.957831
C	-2.879049	-1.402661	0.847929
H	-2.315687	-2.085704	0.194184
H	-2.272364	-1.221314	1.747916
H	-3.816772	-1.914497	1.158749

IM2

C	-1.020252	0.213126	-0.558141
C	-2.373685	-1.521148	-0.472242
C	-2.944549	-0.779573	0.526972
S	-2.088381	0.714961	0.726349
H	-2.723649	-2.500355	-0.802855
H	-3.810542	-1.021250	1.141724
N	-1.278654	-0.951206	-1.073443

N	0.100959	1.002056	-0.942493
H	0.982647	0.502832	-0.538547
H	0.192236	0.937059	-1.961106
B	0.167623	2.545635	-0.460296
H	1.242332	2.972193	-0.866819
H	0.123957	2.521736	0.766562
H	-0.788989	3.138390	-0.943883
N	2.202118	-0.351401	0.165142
C	2.457329	-1.492605	-0.707894
H	1.526065	-2.058346	-0.860362
H	2.807771	-1.139576	-1.689928
H	3.225765	-2.176828	-0.293437
C	3.362640	0.524884	0.291883
H	3.668404	0.887331	-0.700858
H	3.103708	1.397984	0.907566
H	4.226961	0.007441	0.756626
C	1.685506	-0.764267	1.467326
H	1.403438	0.122083	2.054262
H	0.791249	-1.390430	1.333129
H	2.431722	-1.346465	2.045964

TS2

C	1.174810	0.587681	0.521135
C	2.252620	-1.323670	0.828857
C	2.570817	-1.159499	-0.487823
S	1.853234	0.316168	-1.090006
H	2.579469	-2.165633	1.442692
H	3.180208	-1.793650	-1.129274
N	1.459718	-0.350100	1.389872
N	0.381487	1.663134	0.785364
H	-1.601895	1.068971	-0.603331
H	0.065198	1.668318	1.750596
B	-0.208768	2.573134	-0.182685
H	-1.422199	1.863460	-0.955888
H	0.383898	2.735376	-1.224824
H	-0.870201	3.476960	0.269955
N	-2.175630	-0.356016	-0.125679
C	-2.123205	-0.500939	1.327351
H	-1.082127	-0.625672	1.656106
H	-2.546353	0.395612	1.805693
H	-2.704483	-1.380450	1.670597
C	-3.544870	-0.221584	-0.611438
H	-4.032455	0.635224	-0.122386
H	-3.539677	-0.040844	-1.696959
H	-4.146512	-1.129384	-0.409618
C	-1.454460	-1.421064	-0.817476
H	-1.386696	-1.188668	-1.890850
H	-0.436287	-1.508731	-0.417687
H	-1.961089	-2.399916	-0.701838

IM3

C	0.442852	-0.001101	-0.000030
C	-1.294471	1.355763	0.000069
C	-1.996991	0.182978	0.000057
S	-0.891345	-1.158911	-0.000091
H	-1.751698	2.346968	0.000130
H	-3.074392	0.027504	0.000087
N	0.072205	1.242399	0.000036
N	1.757425	-0.450179	-0.000058
H	1.845499	-1.462295	-0.000242
B	2.935545	0.323273	0.000133
H	2.869189	1.520334	0.000351
H	3.979448	-0.277679	0.000041

IM3-dimer

C	1.718325	-0.551672	0.045609
C	2.928177	1.364569	0.235351
C	3.858496	0.636278	-0.420186
S	3.242717	-0.969834	-0.740137
H	3.031674	2.397652	0.560067
H	4.853124	0.937686	-0.740292
N	1.727754	0.715667	0.489750
N	0.728422	-1.429832	0.137893
H	0.898424	-2.279150	-0.389924
B	-0.487578	-1.512255	1.105467
H	-0.835024	-2.682249	1.123160
H	-0.216545	-1.099123	2.209103
C	-1.718100	0.551460	0.044815
C	-2.928017	-1.364657	0.235228
C	-3.858450	-0.636391	-0.420216

S	-3.243056	0.969908	-0.739655
H	-3.031318	-2.397756	0.559930
H	-4.853086	-0.937947	-0.740173
N	-1.727502	-0.715748	0.489142
N	-0.728116	1.429630	0.137018
H	-0.898523	2.279239	-0.390212
B	0.487448	1.512640	1.105199
H	0.215886	1.100445	2.209034
H	0.834961	2.682566	1.122423

TS3

C	0.544700	0.655255	0.037070
C	0.834639	-1.549339	0.346550
C	2.126634	-1.229516	0.067112
S	2.274452	0.488890	-0.224156
H	0.453583	-2.549519	0.553191
H	2.993953	-1.884132	0.004665
N	-0.042612	-0.489767	0.323315
N	-0.144181	1.818227	-0.033220
H	0.225205	2.533379	-0.651159
B	-1.489099	1.926428	0.529043
H	-1.665612	1.451913	1.621402
H	-2.151788	2.852738	0.141039
C	-2.015143	-0.732728	-0.185697
O	-2.173339	-1.894401	-0.161828
O	-2.381474	0.391900	-0.381762

IM4

C	0.430698	-0.726393	0.014617
C	0.860917	1.549849	-0.139934
C	2.125327	1.101509	-0.059611
S	2.182405	-0.657604	0.079286
H	0.508310	2.575343	-0.217573
H	3.045924	1.680868	-0.071413
N	-0.093431	0.532756	-0.099092
N	-0.331227	-1.777435	0.051503
H	0.110306	-2.686062	0.155302
B	-1.876616	-1.657593	-0.220953
H	-2.080129	-1.839397	-1.416886
H	-2.471345	-2.439262	0.497481
C	-1.524439	0.813299	0.048309
O	-1.871321	1.964706	0.098133
O	-2.257539	-0.239541	0.157132

IM5

N	0.719802	-1.692484	-0.246374
C	-0.557769	-1.597942	-0.965582
H	-0.387188	-1.360095	-2.027362
C	-1.514171	-0.586698	-0.368817
C	-2.245445	0.274613	-1.195482
C	-1.697564	-0.508587	1.018974
C	-3.152263	1.188594	-0.651394
H	-2.101060	0.232117	-2.278812
C	-2.598500	0.406043	1.566141
H	-1.122420	-1.166153	1.675115
C	-3.330505	1.257316	0.732109
H	-3.714527	1.854660	-1.310722
H	-2.729645	0.456594	2.650007
H	-4.033962	1.975301	1.160851
C	1.471418	-0.481664	-0.135693
C	2.164533	-0.188672	1.048869
C	1.518439	0.440710	-1.192153
C	2.910833	0.984337	1.161892
H	2.103739	-0.881664	1.888798
C	2.260802	1.616822	-1.070761
H	0.981776	0.242339	-2.119939
C	2.964160	1.894881	0.103175
H	3.442825	1.193804	2.093274
H	2.287694	2.321393	-1.905739
H	3.540534	2.818139	0.196513
H	-1.007391	-2.600657	-0.942953
B	1.167176	-2.914340	0.273851
H	2.249143	-2.984977	0.794288
H	0.452177	-3.880224	0.174387

BH_3

B	0.000000	0.000000	0.000004
H	0.000000	1.204298	-0.000006
H	-1.042953	-0.602149	-0.000006
H	1.042953	-0.602149	-0.000006

TS4

N	0.536532	0.679664	-0.493636
C	1.546514	1.234608	0.420940
H	1.569460	2.319281	0.246441
C	2.936362	0.660942	0.234993
C	3.770939	0.484689	1.346317
C	3.423124	0.320928	-1.035202
C	5.069211	-0.009314	1.195081
H	3.398137	0.736456	2.343483
C	4.718396	-0.176990	-1.188485
H	2.782703	0.442357	-1.910722
C	5.546951	-0.342728	-0.074614
H	5.706389	-0.140964	2.073320
H	5.082650	-0.438538	-2.185195
H	6.559779	-0.734767	-0.195933
C	0.358510	-0.723082	-0.446489
C	-0.032274	-1.461836	-1.578213
C	0.527388	-1.420435	0.769344
C	-0.268477	-2.833665	-1.490554
H	-0.148430	-0.953563	-2.532523
C	0.294195	-2.792088	0.847266
H	0.834452	-0.886890	1.667398
C	-0.113527	-3.511170	-0.279435
H	-0.570548	-3.378902	-2.388410
H	0.433494	-3.302861	1.803480
H	-0.296391	-4.586100	-0.216026
H	1.236962	1.111171	1.469405
B	0.179275	1.578383	-1.698393
H	-0.321612	1.018930	-2.643197
H	1.017951	2.405022	-1.972669
C	-2.500799	-0.216378	1.029456
C	-2.773712	0.204195	-1.255972
C	-3.436143	-0.956510	-1.153960
S	-3.401023	-1.604279	0.486217
H	-2.636343	0.834225	-2.130684
H	-3.949810	-1.499528	-1.944082
N	-2.227439	0.624504	-0.030490
N	-2.114187	0.076340	2.234267
H	-2.308585	-0.601385	2.966988
B	-1.447266	1.437141	2.622707
H	-2.242685	2.155525	3.197275
H	-0.420710	1.235152	3.242138
C	-1.309936	1.678423	0.127137
O	-1.039803	2.398012	-0.951265
O	-1.081670	2.114755	1.281886
B	-2.159950	3.463262	-1.549961
H	-2.472733	2.988787	-2.631909
H	-1.576898	4.527628	-1.613107
H	-3.054065	3.420266	-0.718319

IM6

N	-0.424119	-0.662643	-0.167169
C	-1.417213	-1.164630	0.869423
H	-1.328313	-2.255523	0.881417
C	-2.828495	-0.731713	0.568691
C	-3.305707	0.505752	1.028816
C	-3.689460	-1.553154	-0.173802
C	-4.605501	0.921373	0.737017
H	-2.652015	1.150504	1.619546
C	-4.991281	-1.139353	-0.465485
H	-3.338363	-2.525691	-0.522434
C	-5.450449	0.101235	-0.016039
H	-4.960714	1.888084	1.102018
H	-5.650117	-1.791897	-1.043420
H	-6.468930	0.424911	-0.244598
C	-0.457367	0.793681	-0.253522
C	-1.049538	1.414157	-1.353601
C	0.038906	1.560240	0.806847
C	-1.124327	2.808324	-1.403130
H	-1.463817	0.811664	-2.160192
C	-0.025941	2.952185	0.743706
H	0.462453	1.074497	1.686725
C	-0.605632	3.580487	-0.362402
H	-1.595397	3.289277	-2.263141
H	0.372600	3.546543	1.568885
H	-0.659695	4.670544	-0.407958
H	-1.088592	-0.783891	1.843727
B	-0.431809	-1.564592	-1.531163
H	-0.203354	-0.910395	-2.520928

H	-1.361337	-2.325882	-1.606701
C	2.950367	0.051285	0.760266
C	2.354030	0.131517	-1.482999
C	3.416821	0.950912	-1.516035
S	4.150696	1.124663	0.075944
H	1.727967	-0.174780	-2.315351
H	3.842073	1.458309	-2.378602
N	2.082588	-0.371508	-0.206358
N	2.834601	-0.302455	2.008064
H	3.532083	0.039786	2.661772
B	1.666953	-1.225920	2.493864
H	2.095123	-2.058597	3.269655
H	0.789086	-0.526773	2.997877
C	1.016072	-1.337365	0.095592
O	0.836954	-2.216215	-0.966426
O	1.169189	-1.917905	1.252001
B	1.979150	-3.143217	-1.628848
H	2.896307	-3.125221	-0.824037
H	1.459340	-4.238498	-1.762101
H	2.258681	-2.603322	-2.692945

TS5

N	-0.522521	-0.650155	0.003000
C	-1.605070	-1.377965	0.819531
H	-1.404376	-2.450386	0.705899
C	-2.995470	-1.024032	0.376213
C	-3.674185	0.045819	0.979447
C	-3.627273	-1.737633	-0.652761
C	-4.953372	0.404868	0.554006
H	-3.190934	0.606928	1.782207
C	-4.907358	-1.378219	-1.079746
H	-3.114956	-2.580115	-1.120599
C	-5.570592	-0.303927	-0.480535
H	-5.469349	1.241064	1.031495
H	-5.390014	-1.942793	-1.880920
H	-6.572355	-0.023413	-0.815080
C	-0.740910	0.796837	0.057523
C	-1.408145	1.410347	-1.000841
C	-0.373842	1.516561	1.195011
C	-1.699522	2.774627	-0.925863
H	-1.711100	0.826966	-1.870023
C	-0.661578	2.880490	1.256444
H	0.150795	1.027289	2.014518
C	-1.323465	3.511727	0.198839
H	-2.225777	3.257868	-1.751716
H	-0.361833	3.451807	2.137607
H	-1.547712	4.579411	0.253632
H	-1.434870	-1.094594	1.865819
B	-0.174908	-1.369521	-1.438169
H	0.157574	-0.582640	-2.280101
H	-0.939660	-2.248133	-1.730256
C	3.390033	0.070967	0.369527
C	2.249294	1.138957	-1.238119
C	3.493062	1.285782	-1.765862
S	4.686388	0.550639	-0.722206
H	1.331529	1.520865	-1.681312
H	3.783469	1.781229	-2.690150
N	2.190364	0.450385	-0.043295
N	3.583166	-0.615843	1.512333
H	4.409541	-1.203322	1.549495
B	2.512979	-0.760769	2.522243
H	2.721517	-1.603608	3.360411
H	1.993401	0.277461	2.869758
C	0.813689	-1.193823	0.447488
O	1.053601	-1.927951	-0.636385
O	1.138748	-1.419891	1.601505
B	2.343178	-2.868019	-1.011332
H	2.738700	-3.278289	0.063985
H	3.112366	-2.107826	-1.572789
H	1.847960	-3.710715	-1.737346

IM7

N	-0.984728	-0.343176	-0.081502
C	-0.127117	-1.086108	-1.107453
H	-0.580512	-2.079448	-1.219379
C	1.310327	-1.173036	-0.683314
C	2.225232	-0.195002	-1.099832
C	1.747562	-2.200546	0.165366
C	3.552340	-0.237259	-0.670306
H	1.891366	0.610883	-1.757458

C	3.074786	-2.242218	0.596869
H	1.045182	-2.970523	0.489927
C	3.978108	-1.259026	0.182714
H	4.255037	0.530967	-1.001069
H	3.405579	-3.047973	1.256277
H	5.016540	-1.292853	0.521029
C	-0.471968	1.016446	0.163931
C	0.407724	1.214856	1.229398
C	-0.785527	2.056261	-0.713967
C	0.969113	2.476921	1.425248
H	0.662888	0.388587	1.891853
C	-0.224128	3.318161	-0.502061
H	-1.461258	1.889966	-1.552249
C	0.652530	3.530684	0.564040
H	1.659485	2.633056	2.256752
H	-0.476927	4.136908	-1.179106
H	1.090856	4.518407	0.723311
H	-0.233767	-0.537386	-2.052560
B	-1.486995	-1.218829	1.223191
H	-1.424832	-0.617294	2.258720
H	-1.115270	-2.360479	1.173005
C	-2.424351	-0.393260	-0.509559
O	-2.897053	-1.049032	0.535063
O	-2.929991	-0.007881	-1.508254
B	-4.419009	-1.685714	0.757498
H	-4.509993	-2.528397	-0.117982
H	-5.161019	-0.730826	0.627301
H	-4.331668	-2.124588	1.887763

TS6

N	0.757937	-0.509396	0.360967
C	-0.276572	-1.021665	1.305954
H	-0.013123	-2.066016	1.522497
C	-1.654504	-0.932465	0.706231
C	-2.550188	0.061864	1.116404
C	-2.035385	-1.816174	-0.314443
C	-3.807648	0.175267	0.517125
H	-2.255323	0.760005	1.903657
C	-3.288663	-1.702577	-0.917077
H	-1.340392	-2.592961	-0.642990
C	-4.177277	-0.704087	-0.502929
H	-4.497631	0.956314	0.845213
H	-3.575596	-2.396038	-1.711222
H	-5.158833	-0.614915	-0.974751
C	0.650313	0.908467	0.051671
C	-0.234639	1.329955	-0.945963
C	1.394409	1.842196	0.780307
C	-0.371854	2.692689	-1.211186
H	-0.807093	0.592949	-1.508035
C	1.265105	3.203818	0.494914
H	2.072983	1.509530	1.568847
C	0.379074	3.630966	-0.496358
H	-1.063884	3.021339	-1.989671
H	1.857112	3.930597	1.055586
H	0.275252	4.696158	-0.715180
H	-0.219855	-0.454152	2.248082
B	1.626933	-1.374233	-1.537456
H	1.440388	-0.593316	-2.421667
H	1.149560	-2.468948	-1.450925
C	2.072480	-0.956101	0.656825
O	2.682032	-1.049588	-0.564298
O	2.546494	-1.286597	1.695620
B	4.011896	-1.873077	-1.082331
H	4.100438	-2.849443	-0.369361
H	4.930723	-1.082669	-1.072329
H	3.589446	-2.129546	-2.214991

IM8

N	0.459915	0.610536	0.614147
C	-0.605618	0.058366	1.489518
H	-0.124612	-0.721884	2.091726
C	-1.775758	-0.512791	0.718370
C	-3.061201	0.022055	0.886056
C	-1.591115	-1.566845	-0.190790
C	-4.141156	-0.472765	0.146666
H	-3.221382	0.827742	1.606861
C	-2.667159	-2.056156	-0.931207
H	-0.599784	-2.005041	-0.322456
C	-3.944076	-1.507109	-0.768647
H	-5.135710	-0.042851	0.286028

H	-2.510149	-2.873660	-1.638964
H	-4.783933	-1.890810	-1.352570
C	1.583273	-0.234925	0.308303
C	1.785003	-0.664033	-1.005134
C	2.428681	-0.662465	1.335840
C	2.845798	-1.525593	-1.291250
H	1.117638	-0.321540	-1.797123
C	3.481157	-1.528643	1.043535
H	2.273528	-0.298942	2.353364
C	3.692247	-1.960880	-0.270032
H	3.010011	-1.854081	-2.319751
H	4.148521	-1.856664	1.843530
H	4.521890	-2.634162	-0.497035
H	-0.942712	0.847543	2.172753
C	0.279185	1.787355	-0.000559
O	1.091403	2.430766	-0.678004
O	-0.937806	2.342488	0.188648
B	-1.973300	2.195036	-0.702039
H	-1.804258	1.543673	-1.697946
H	-2.982329	2.784558	-0.435319
H	3.105618	2.113862	0.347252
H	3.043109	1.760610	-1.659513
H	2.921521	3.672839	-0.964787
B	2.705157	2.492083	-0.742812

TS7

N	-0.506402	0.522345	-0.575941
C	0.544998	0.106501	-1.516644
H	0.075600	-0.566950	-2.245290
C	1.701759	-0.589734	-0.829729
C	2.955537	0.032015	-0.721154
C	1.516489	-1.850843	-0.240582
C	4.000335	-0.586700	-0.022294
H	3.123947	0.996864	-1.206038
C	2.555254	-2.462667	0.460367
H	0.549912	-2.351290	-0.325576
C	3.798369	-1.829550	0.577302
H	4.969898	-0.089324	0.054305
H	2.396366	-3.441661	0.918927
H	4.608947	-2.311223	1.129005
C	-1.555908	-0.401614	-0.250148
C	-1.689300	-0.881949	1.055790
C	-2.423168	-0.840233	-1.255453
C	-2.697890	-1.799443	1.354751
H	-1.007441	-0.533661	1.832510
C	-3.416242	-1.773028	-0.955113
H	-2.327883	-0.435997	-2.265073
C	-3.558287	-2.251429	0.350659
H	-2.806500	-2.167224	2.377595
H	-4.094769	-2.111809	-1.741291
H	-4.344176	-2.972531	0.586685
H	0.892775	0.987465	-2.072004
C	-0.470566	1.732898	0.056146
O	-1.345677	2.135844	0.853301
O	0.955789	2.100417	0.539789
B	1.832368	1.445228	1.380218
H	1.425285	0.473699	1.945130
H	2.892297	1.975631	1.548994
B	0.882336	3.203736	-0.526379
H	1.668922	3.046526	-1.421406
H	0.597445	4.280318	-0.079950
H	-0.307154	2.687567	-0.938259
H	-3.205626	3.350420	1.246075
H	-2.422132	3.420144	-0.646797
H	-3.435154	1.764369	-0.022015
B	-2.745688	2.716402	0.311753

IM9

N	-0.768257	-0.782252	0.697878
C	0.437684	-0.902755	1.536608
H	0.322571	-0.228871	2.397753
C	1.692559	-0.568229	0.764518
C	2.161545	-1.445533	-0.224108
C	2.363360	0.641066	0.977796
C	3.285529	-1.119401	-0.983585
H	1.639400	-2.389379	-0.405960
C	3.491213	0.969158	0.219977
H	1.994670	1.335135	1.737433
C	3.952716	0.090578	-0.762361
H	3.644129	-1.810813	-1.749827

H	4.006616	1.916597	0.394621
H	4.832657	0.346673	-1.357364
C	-1.129874	0.529368	0.226544
C	-1.939985	1.341474	1.023823
C	-0.635917	0.987237	-0.997448
C	-2.260978	2.628397	0.587655
H	-2.319619	0.959515	1.973845
C	-0.962586	2.274809	-1.426860
H	-0.002781	0.336766	-1.602268
C	-1.772022	3.094978	-0.635898
H	-2.899215	3.265669	1.203778
H	-0.582180	2.637326	-2.384346
H	-2.025846	4.101729	-0.975832
H	0.470771	-1.934292	1.915575
C	-1.452630	-1.859541	0.327347
O	-2.446752	-1.809136	-0.424274
H	-1.103339	-2.827552	0.722651
B	-3.238492	-3.112514	-0.860408
H	-4.398053	-2.928775	-0.517405
H	-3.112664	-3.184711	-2.075763
H	-2.706523	-4.053229	-0.269838

TS8

N	0.789384	-1.032876	-0.093079
C	-0.397916	-1.512650	-0.799865
H	-0.296494	-1.366405	-1.889145
C	-1.672384	-0.869600	-0.302501
C	-1.899954	-0.715442	1.072156
C	-2.649515	-0.436925	-1.205781
C	-3.086801	-0.145018	1.533166
H	-1.133973	-1.035711	1.782411
C	-3.841714	0.130068	-0.746224
H	-2.474910	-0.540177	-2.280436
C	-4.062611	0.278102	0.624685
H	-3.251146	-0.026967	2.607102
H	-4.595517	0.465286	-1.462845
H	-4.990745	0.727511	0.986073
C	1.061315	0.371754	-0.080517
C	1.579648	0.973982	1.073970
C	0.775968	1.156891	-1.204522
C	1.828668	2.345983	1.090224
H	1.787359	0.362617	1.950733
C	1.015264	2.532142	-1.175242
H	0.369613	0.700290	-2.107199
C	1.546183	3.131303	-0.031337
H	2.237252	2.806246	1.992996
H	0.787340	3.135911	-2.056862
H	1.734587	4.207190	-0.011148
H	-0.444636	-2.602063	-0.641734
C	1.775241	-1.948195	0.162931
O	2.864482	-1.609612	0.821297
H	1.395799	-2.978877	0.262091
B	3.580377	-1.893578	-0.485528
H	2.496575	-2.260783	-1.152479
H	3.922297	-0.889984	-1.072890
H	4.284812	-2.883531	-0.464712

IM10

N	-0.668684	0.683521	-1.022293
C	0.657698	0.488720	-1.587920
H	0.624364	-0.296474	-2.362810
C	1.760720	0.159797	-0.595305
C	1.740068	0.663614	0.711322
C	2.837854	-0.642100	-0.995915
C	2.780364	0.373080	1.597263
H	0.902011	1.284824	1.031345
C	3.881666	-0.929155	-0.112955
H	2.857426	-1.051672	-2.010491
C	3.854791	-0.422386	1.189177
H	2.749416	0.770085	2.615156
H	4.713849	-1.557730	-0.440224
H	4.665947	-0.651112	1.884879
C	-1.351426	-0.395444	-0.445880
C	-2.587871	-0.219981	0.214708
C	-0.824632	-1.703857	-0.512563
C	-3.270613	-1.309404	0.755408
H	-3.030256	0.768931	0.320168
C	-1.518355	-2.782427	0.035654
H	0.138082	-1.889465	-0.983721
C	-2.748062	-2.601656	0.671998

H	-4.225910	-1.135392	1.257558
H	-1.079916	-3.781282	-0.035564
H	-3.283988	-3.449673	1.103490
H	0.921008	1.418427	-2.115597
C	-1.209367	1.992748	-0.974432
O	-0.972316	2.645957	0.293602
H	-0.717775	2.609784	-1.737962
B	-1.952019	3.212239	1.014397
H	-2.293415	1.989548	-1.166773
H	-3.097045	3.194057	0.615350
H	-1.641402	3.734347	2.057080

TS9

N	-0.572038	0.018441	1.416250
C	0.663497	-0.694185	1.849305
H	1.138852	-0.082639	2.629049
C	1.611641	-0.942536	0.704866
C	1.172152	-1.626735	-0.437382
C	2.934893	-0.490642	0.776242
C	2.053602	-1.851194	-1.495517
H	0.138740	-1.975851	-0.509222
C	3.818144	-0.726960	-0.280085
H	3.279048	0.049241	1.662677
C	3.376869	-1.405122	-1.418933
H	1.700425	-2.380049	-2.383750
H	4.850238	-0.374354	-0.215253
H	4.064517	-1.584855	-2.248974
C	-0.426101	1.180287	0.569195
C	-1.236996	1.292116	-0.563333
C	0.531754	2.148174	0.884674
C	-1.092276	2.412951	-1.382833
H	-1.951443	0.498986	-0.800087
C	0.661197	3.262321	0.056292
H	1.161465	2.047169	1.768748
C	-0.148536	3.396254	-1.076101
H	-1.716839	2.506620	-2.273551
H	1.400173	4.029140	0.297775
H	-0.037115	4.268045	-1.724621
H	0.327460	-1.632105	2.311638
C	-1.734419	-0.427260	1.738528
O	-3.283857	-1.221004	-0.407681
B	-4.560662	-0.947188	-0.612814
H	-4.935178	0.209747	-0.459861
H	-5.367414	-1.801431	-0.937013
B	-2.540423	-2.540376	-0.500722
H	-1.733064	-2.474867	-1.436111
H	-3.316649	-3.489025	-0.643801
H	-1.892689	-2.682516	0.560950
H	-2.626195	0.120599	1.439292
H	-1.816300	-1.339894	2.327983

3aa

N	0.614465	1.324803	-0.253702
C	-0.562085	1.114085	-1.067407
H	-0.283481	0.592927	-1.999112
C	-1.700201	0.358438	-0.395951
C	-2.831032	0.002416	-1.146227
C	-1.655367	0.016820	0.959854
C	-3.896205	-0.675933	-0.552172
H	-2.876018	0.258754	-2.209340
C	-2.720820	-0.664074	1.557376
H	-0.774026	0.280061	1.547502
C	-3.844610	-1.011709	0.805046
H	-4.770257	-0.946474	-1.150290
H	-2.668817	-0.926619	2.617166
H	-4.676524	-1.545077	1.271536
C	1.596011	0.352766	-0.158528
C	2.835900	0.624409	0.468908
C	1.396051	-0.951239	-0.675171
C	3.821351	-0.358615	0.560693
H	3.039709	1.612734	0.879017
C	2.394225	-1.918436	-0.577280
H	0.445522	-1.221306	-1.133430
C	3.617612	-1.638100	0.038880
H	4.768523	-0.111676	1.048352
H	2.203238	-2.915351	-0.984009
H	4.393506	-2.402905	0.114105
H	-0.934741	2.100625	-1.387785
C	0.780657	2.598568	0.410756
H	1.575527	3.219647	-0.046114

H	-0.160260	3.161326	0.356649
H	1.027908	2.473334	1.479002

NMe_3

N	0.000000	0.000000	0.353766
C	0.000000	1.387573	-0.056359
H	-0.890392	1.902967	0.338850
H	0.890392	1.902967	0.338850
H	0.000000	1.520001	-1.165001
C	1.201674	-0.693787	-0.056359
H	2.093214	-0.180381	0.338850
H	1.202822	-1.722586	0.338850
H	1.316360	-0.760001	-1.165001
C	-1.201674	-0.693787	-0.056359
H	-1.202822	-1.722586	0.338850
H	-2.093214	-0.180381	0.338850
H	-1.316360	-0.760001	-1.165001

H_2

H	0.000000	0.000000	0.380543
H	0.000000	0.000000	-0.380543

CO_2

C	0.000000	0.000000	-0.000003
O	0.000000	0.000000	-1.162902
O	0.000000	0.000000	1.162904

$B(OH_2)_2$

O	-0.000012	0.436938	0.000000
B	-0.000012	-0.178048	1.221410
H	0.000439	0.527328	2.199097
H	-0.000329	-1.384842	1.288676
B	-0.000012	-0.178048	-1.221410
H	0.000439	0.527328	-2.199097
H	-0.000329	-1.384842	-1.288676

TS4′

N	-0.463282	-0.622007	-0.629647
C	-1.531584	-1.307049	0.120613
H	-1.619245	-2.315701	-0.306435
C	-2.877870	-0.616419	0.072875
C	-3.763119	-0.772002	1.148753
C	-3.283253	0.153938	-1.026140
C	-5.029080	-0.182351	1.126376
H	-3.454560	-1.362263	2.016509
C	-4.546613	0.749226	-1.048015
H	-2.606486	0.294252	-1.869903
C	-5.425110	0.582511	0.026072
H	-5.705289	-0.315058	1.974803
H	-4.845374	1.348976	-1.911517
H	-6.412396	1.050673	0.007797
C	-0.204338	0.719736	-0.232269
C	0.209045	1.695326	-1.154479
C	-0.298937	1.087897	1.125412
C	0.537924	2.984168	-0.731239
H	0.268472	1.438040	-2.209089
C	0.027041	2.377545	1.540008
H	-0.616910	0.358899	1.869010
C	0.454756	3.335951	0.616700
H	0.857533	3.721945	-1.471601
H	-0.054372	2.633968	2.599364
H	0.710807	4.346141	0.944076
H	-1.231058	-1.455529	1.166818
B	-0.263328	-1.201072	-2.101436
H	0.201978	-0.399009	-2.886485
H	-1.256655	-1.762525	-2.519523
C	2.629267	-0.383955	0.774239
C	2.765259	-0.234812	-1.541070
C	3.616015	0.750833	-1.209505
S	3.741391	0.943870	0.538130
H	2.479298	-0.573238	-2.532356
H	4.181860	1.398734	-1.874751
N	2.198100	-0.864997	-0.431697
N	2.238141	-0.916503	1.894881
H	2.564585	-0.488839	2.756393
B	1.382126	-2.226417	1.966862
H	2.061189	-3.137100	2.413977
H	0.377584	-2.017287	2.630769
C	1.116335	-1.826217	-0.497616
O	0.812317	-2.250006	-1.688127

O	0.994890	-2.573865	0.533863

IM6′

N	-0.383198	-0.741274	-0.368090
C	-1.381472	-1.382294	0.569181
H	-1.361995	-2.456583	0.358249
C	-2.769295	-0.815590	0.405668
C	-3.168756	0.304027	1.152052
C	-3.680983	-1.381768	-0.497546
C	-4.440536	0.855278	0.988683
H	-2.473832	0.750802	1.865849
C	-4.954912	-0.832576	-0.661828
H	-3.389214	-2.259436	-1.076107
C	-5.336414	0.290508	0.076693
H	-4.733077	1.728142	1.577443
H	-5.653428	-1.287042	-1.368762
H	-6.332884	0.720467	-0.052503
C	-0.342644	0.699956	-0.183695
C	-0.907746	1.544333	-1.141274
C	0.202195	1.237938	0.988572
C	-0.907233	2.926273	-0.936289
H	-1.358857	1.118998	-2.036051
C	0.212652	2.619600	1.180909
H	0.605993	0.577679	1.756263
C	-0.339968	3.469089	0.218055
H	-1.358025	3.579795	-1.686641
H	0.649100	3.032020	2.093567
H	-0.335445	4.550574	0.372491
H	-1.019230	-1.231646	1.593518
B	-0.406746	-1.405854	-1.880037
H	-0.200316	-0.563838	-2.735880
H	-1.390765	-2.084207	-2.082110
C	3.002444	-0.320348	0.583046
C	2.449490	0.102394	-1.624297
C	3.532865	0.893264	-1.527985
S	4.241232	0.816839	0.083701
H	1.814393	-0.055408	-2.491599
H	3.975764	1.521514	-2.297064
N	2.143843	-0.568819	-0.442660
N	2.868037	-0.869980	1.757540
H	3.558049	-0.642339	2.466019
B	1.698617	-1.872498	2.061062
H	2.139484	-2.828111	2.678105
H	0.829552	-1.279178	2.701736
C	1.028196	-1.562490	-0.323719
O	0.816467	-2.188733	-1.491240
O	1.199482	-2.335631	0.728020

TS5′

N	0.488215	-0.902303	0.294997
C	1.561642	-1.471644	-0.635753
H	1.626473	-2.543526	-0.414021
C	2.890603	-0.790312	-0.460949
C	3.213169	0.334304	-1.235787
C	3.818038	-1.250920	0.484853
C	4.430338	0.993490	-1.060274
H	2.499041	0.701115	-1.976085
C	5.036844	-0.592135	0.661490
H	3.583311	-2.130731	1.086231
C	5.343523	0.533805	-0.107237
H	4.666193	1.869362	-1.669308
H	5.751045	-0.962750	1.400676
H	6.296972	1.049410	0.031764
C	0.356616	0.536273	0.091518
C	0.952718	1.405776	1.001475
C	-0.305629	1.020189	-1.039024
C	0.860817	2.783648	0.792147
H	1.485516	1.007362	1.864617
C	-0.410859	2.397664	-1.228850
H	-0.754186	0.327182	-1.750726
C	0.170527	3.281741	-0.314400
H	1.327829	3.468295	1.503441
H	-0.952642	2.781020	-2.096142
H	0.088767	4.359973	-0.469389
H	1.184774	-1.348483	-1.658634
B	0.508233	-1.594819	1.809784
H	0.141313	-0.817107	2.655481
H	1.523153	-2.207947	2.029618
C	-3.180848	-0.328644	-0.271622
C	-2.256474	0.575800	1.576205

C	-3.118237	1.584521	1.297028
S	-4.047539	1.209698	-0.145249
H	-1.572203	0.552142	2.421232
H	-3.284672	2.507523	1.847796
N	-2.271676	-0.483208	0.689009
N	-3.391212	-1.235399	-1.220483
H	-4.000629	-0.976192	-1.986825
B	-2.635359	-2.570732	-1.208189
H	-2.964826	-3.284873	-0.275610
H	-2.675872	-3.099872	-2.301952
C	-0.742729	-1.773118	0.182074
O	-0.615565	-2.483041	1.252271
O	-1.143278	-2.126405	-0.960794

Imine

N	0.457069	-0.481935	-0.104023
C	-0.404350	0.419065	0.178384
H	-0.101017	1.426555	0.523362
C	-1.851271	0.189731	0.087112
C	-2.739914	1.223228	0.428225
C	-2.368576	-1.048727	-0.337291
C	-4.119529	1.026583	0.347275
H	-2.341574	2.186623	0.758590
C	-3.744421	-1.243098	-0.416017
H	-1.666983	-1.843197	-0.598220
C	-4.623679	-0.206465	-0.074619
H	-4.802941	1.836226	0.614149
H	-4.140285	-2.206926	-0.745558
H	-5.703405	-0.362855	-0.138448
C	1.828999	-0.210370	-0.065829
C	2.690644	-1.229305	0.381617
C	2.385038	1.012392	-0.491217
C	4.066478	-1.015994	0.443889
H	2.251153	-2.181310	0.686492
C	3.765298	1.212407	-0.442287
H	1.733124	1.792270	-0.890744
C	4.611176	0.205598	0.032391
H	4.721304	-1.812230	0.806957
H	4.184572	2.161557	-0.786178
H	5.691208	0.366558	0.067963

IM5′

N	0.500453	0.617074	0.186432
C	-0.402084	-0.274567	-0.091901
H	-0.021243	-1.256638	-0.395015
C	-1.852518	-0.182729	-0.076668
C	-2.540425	-1.399949	-0.294766
C	-2.607247	0.996614	0.108169
C	-3.930017	-1.445811	-0.305771
H	-1.967605	-2.317363	-0.452862
C	-3.999769	0.943372	0.086093
H	-2.096911	1.943141	0.257269
C	-4.664139	-0.270161	-0.113563
H	-4.443960	-2.395726	-0.468348
H	-4.572418	1.862797	0.226773
H	-5.756466	-0.300350	-0.125057
C	1.868883	0.186074	0.076769
C	2.758946	0.922297	-0.714596
C	2.307193	-0.955931	0.756084
C	4.079798	0.495173	-0.842095
H	2.406742	1.817147	-1.228422
C	3.636153	-1.369701	0.631417
H	1.616577	-1.500142	1.403698
C	4.523528	-0.649338	-0.170100
H	4.769877	1.064047	-1.469575
H	3.977833	-2.254397	1.173777
H	5.562572	-0.972689	-0.265795
H	-0.522957	2.077581	1.611216
B	0.267245	2.124047	0.675909
H	1.348722	2.565059	1.017680
H	-0.209982	2.755721	-0.264349

TS10

N	0.500005	0.676130	-0.043955
C	-0.432587	-0.025233	-0.687791
C	1.824112	0.203472	0.021541
C	2.909640	1.095567	0.069564
C	2.072480	-1.176957	0.138108
C	4.208599	0.611651	0.206247
H	2.723254	2.166521	-0.013236

C	3.379431	-1.652382	0.264088
H	1.235489	-1.878842	0.166445
C	4.455499	-0.763533	0.296105
H	5.041357	1.318832	0.237666
H	3.552542	-2.728040	0.351399
H	5.477125	-1.135779	0.400174
H	-0.631800	1.491112	-1.927278
B	0.046807	1.962201	-0.979572
H	-0.623266	2.748243	-0.345301
H	1.063148	2.313507	-1.537711
C	-1.828897	-0.084009	-0.255241
C	-2.234123	0.509684	0.954318
C	-2.762914	-0.788157	-1.035136
C	-3.560822	0.411437	1.364061
H	-1.492079	1.032698	1.559509
C	-4.089426	-0.884002	-0.620225
H	-2.442796	-1.253063	-1.971111
C	-4.489322	-0.281561	0.577570
H	-3.875883	0.871575	2.303298
H	-4.814599	-1.429139	-1.228462
H	-5.529173	-0.358708	0.904465
H	-0.127404	-0.758703	-1.453564

Int-I

C	1.161853	-0.341602	-0.007029
C	1.279454	1.070113	-0.004609
C	0.113453	1.820020	0.002317
C	-1.130890	1.176204	0.005102
C	-1.151998	-0.222889	0.004146
H	2.263129	1.544750	-0.011521
H	0.167826	2.912083	0.005901
H	-2.061553	1.745922	0.009888
N	-0.028058	-0.954724	0.002804
N	2.270982	-1.147309	-0.056047
C	-2.444071	-0.995337	0.000218
H	-3.318840	-0.338882	0.111334
H	-2.549222	-1.560216	-0.941363
H	-2.447740	-1.737370	0.814582
H	3.163555	-0.764171	0.228626
H	2.115574	-2.126932	0.154389

TS-1

N	0.423615	-0.699179	1.654242
H	0.260045	-1.627921	2.035897
H	0.486745	0.001451	2.391142
B	-1.416902	-0.268743	0.740913
H	-2.017349	-0.425596	1.785552
H	-1.314492	-1.193773	-0.037511
H	-1.053260	0.838196	0.411670
N	-3.468416	0.224026	-0.258139
C	-4.308647	-0.947758	-0.103073
H	-3.830093	-1.817473	-0.578294
H	-4.440964	-1.175300	0.965541
H	-5.316050	-0.816830	-0.556257
C	-3.999531	1.378667	0.441274
H	-4.136007	1.141627	1.507228
H	-3.291807	2.218098	0.368805
H	-4.978533	1.713737	0.033323
C	-3.177213	0.511706	-1.649941
H	-2.476967	1.357576	-1.718675
H	-2.700131	-0.360611	-2.121626
H	-4.088911	0.766812	-2.233793
C	1.505954	-0.612699	0.765210
C	1.803111	-1.673806	-0.108618
C	3.163412	0.723944	-0.122591
C	2.842329	-1.489970	-1.012182
H	1.226628	-2.599728	-0.076155
C	3.537121	-0.275998	-1.028414
H	3.110453	-2.288607	-1.708431
H	4.354773	-0.106428	-1.731126
N	2.165400	0.542382	0.756460
C	3.859360	2.056181	-0.075120
H	4.293165	2.226258	0.923905
H	4.660790	2.129887	-0.823696
H	3.136909	2.870126	-0.249261

Int-II

N	0.388550	1.517557	-0.186238
H	1.162098	0.787891	-0.231310
H	0.487827	2.122162	-1.004831

B	0.669517	2.448534	1.130763
H	1.825256	2.844380	1.004131
H	0.523790	1.727205	2.108113
H	-0.141092	3.368818	1.103059
N	2.496849	-0.363905	-0.179153
C	2.217649	-1.413302	-1.148406
H	1.227641	-1.845955	-0.945048
H	2.207455	-0.993651	-2.166989
H	2.974386	-2.226421	-1.121770
C	3.749389	0.324175	-0.456245
H	3.733824	0.738856	-1.476606
H	3.883073	1.156239	0.250756
H	4.630703	-0.347733	-0.375081
C	2.435705	-0.863337	1.189789
H	2.625623	-0.041450	1.894538
H	1.428582	-1.256796	1.389285
H	3.180513	-1.666373	1.376196
C	-0.894288	0.864099	-0.204436
C	-2.054586	1.594532	-0.484032
C	-3.265948	0.910916	-0.439154
H	-2.001212	2.660153	-0.710218
C	-2.058873	-1.089946	0.153328
C	-3.274312	-0.447505	-0.112868
H	-4.201251	1.435408	-0.648591
H	-4.211670	-1.004478	-0.062454
N	-0.892380	-0.425635	0.097814
C	-1.985137	-2.548283	0.508070
H	-2.983061	-2.998634	0.602846
H	-1.424651	-3.104811	-0.261470
H	-1.444144	-2.681705	1.458385

TS-2

N	0.617986	2.210659	-0.298855
H	-2.044055	1.329960	0.052155
H	1.008977	3.052062	0.109003
B	-0.655481	2.334919	-1.002354
H	-1.797713	2.183039	0.058615
H	-0.944014	1.508308	-1.830620
H	-1.011425	3.479892	-1.193159
N	-2.688852	-0.137187	0.261639
C	-1.984810	-0.692509	1.410228
H	-0.911393	-0.749119	1.183400
H	-2.122792	-0.037793	2.284503
H	-2.351053	-1.705538	1.673973
C	-4.104540	0.078685	0.521175
H	-4.228893	0.723030	1.405127
H	-4.569508	0.582202	-0.340056
H	-4.647892	-0.870475	0.704241
C	-2.444407	-0.900778	-0.957871
H	-2.948118	-0.414679	-1.806112
H	-1.364584	-0.917731	-1.155102
H	-2.823937	-1.940348	-0.875697
C	1.398433	1.098751	-0.086149
C	2.670975	1.233954	0.528930
C	3.441237	0.099506	0.718623
H	3.028858	2.220580	0.832611
C	1.687357	-1.196477	-0.287251
C	2.954039	-1.146890	0.302063
H	4.425822	0.178846	1.187343
H	3.541485	-2.056921	0.434110
N	0.930975	-0.100475	-0.460670
C	1.090029	-2.498867	-0.750174
H	1.781837	-3.340787	-0.604831
H	0.159372	-2.718818	-0.201542
H	0.825786	-2.443529	-1.818440

Int-III

N	-2.249046	0.051713	-0.000029
H	-2.798555	0.906024	-0.000200
B	-2.936999	-1.172394	0.000078
H	-2.341575	-2.213580	0.000222
H	-4.142717	-1.118630	0.000036
C	-0.866352	0.301809	-0.000017
C	-0.402760	1.631215	0.000034
C	1.281631	-0.542322	-0.000044
C	0.971436	1.843389	0.000021
H	-1.106304	2.466862	0.000074
C	1.835217	0.745979	0.000011
H	1.369026	2.861307	0.000067
H	2.918045	0.881992	0.000039

N	-0.042680	-0.741899	-0.000110
C	2.142960	-1.775045	0.000021
H	3.214585	-1.530900	0.000061
H	1.920892	-2.394917	0.883869
H	1.920891	-2.395034	-0.883737

III-dimer

C	1.598724	-0.870938	-0.456919
C	3.212595	0.579389	0.506000
C	4.245731	-0.124567	-0.089891
H	5.277061	0.150086	0.131197
N	1.902602	0.260827	0.253999
N	0.341716	-1.335852	-0.487065
H	0.240390	-2.092651	-1.153556
B	-0.742913	-1.333930	0.605392
H	-1.275000	-2.428613	0.532578
H	-0.288256	-1.133447	1.714338
C	-1.598770	0.871036	-0.456830
C	-3.212560	-0.579390	0.506078
C	-4.245741	0.124451	-0.089873
H	-5.277053	-0.150367	0.131094
N	-1.902593	-0.260733	0.254102
N	-0.341752	1.335926	-0.487084
H	-0.240463	2.092707	-1.153600
B	0.742930	1.334042	0.605324
H	0.288322	1.133593	1.714295
H	1.274980	2.428731	0.532442
C	-2.637035	1.548904	-1.159177
H	-2.367263	2.402578	-1.783895
C	-3.945866	1.173005	-0.977756
H	-4.748809	1.709280	-1.489568
C	-3.518153	-1.710187	1.443272
H	-3.343214	-2.688309	0.969330
H	-2.882773	-1.671974	2.339791
H	-4.571841	-1.660016	1.750723
C	3.518302	1.710020	1.443359
H	3.343693	2.688227	0.969478
H	2.882760	1.671880	2.339765
H	4.571925	1.659555	1.750989
C	2.636941	-1.548820	-1.159315
C	3.945797	-1.173061	-0.977818
H	2.367134	-2.402560	-1.783926
H	4.748721	-1.709492	-1.489495

TS-3

N	-0.992572	-1.909977	0.120613
H	-1.015943	-2.805505	-0.353130
B	-2.175533	-1.391079	0.802436
H	-1.997760	-0.802187	1.842320
H	-3.189635	-2.025127	0.646210
C	-1.705972	1.009426	-0.416619
O	-1.381851	2.053751	-0.835946
O	-2.527772	0.159583	-0.216489
C	0.169251	-1.206285	0.001165
C	1.392469	-1.816664	-0.361255
C	1.224233	0.873729	0.281883
C	2.536453	-1.040787	-0.375608
H	1.415693	-2.883956	-0.588909
C	2.464463	0.314223	-0.019425
H	3.498319	-1.488585	-0.637626
H	3.362343	0.932337	0.021504
N	0.099864	0.121082	0.249491
C	1.104484	2.323341	0.659731
H	0.829177	2.941300	-0.208182
H	2.062182	2.694191	1.051765
H	0.326942	2.466624	1.423384

Int-IV

C	0.123887	-1.213827	-0.048631
C	-1.289510	0.743819	0.200009
C	-2.401997	-0.050481	0.074686
H	-3.385616	0.396599	0.215697
N	-0.028994	0.168022	0.055280
N	1.335873	-1.702336	0.086556
H	1.439604	-2.699267	-0.067837
B	2.488278	-0.821611	0.623620
H	2.355050	-0.653822	1.835279
H	3.568091	-1.289559	0.314515
C	1.144895	1.032394	-0.302668
O	0.929917	2.103828	-0.806880
O	2.292818	0.504070	-0.087859
C	-1.418423	2.196526	0.545916
H	-0.663556	2.503931	1.283621
H	-1.282129	2.837034	-0.335076
H	-2.418676	2.370410	0.965507
C	-1.037233	-2.007726	-0.292153
H	-0.900162	-3.075678	-0.467423
C	-2.273977	-1.428917	-0.229822
H	-3.169890	-2.035300	-0.381349

TS-4

N	-0.455389	-0.524929	-0.332506

C	-1.534105	-1.054945	0.522610
H	-1.488103	-2.149217	0.446057
C	-2.926841	-0.585007	0.158455
C	-3.931793	-0.652716	1.134509
C	-3.259496	-0.117113	-1.119474
C	-5.241650	-0.269906	0.840713
H	-3.683111	-1.011325	2.137627
C	-4.569501	0.269931	-1.413999
H	-2.494982	-0.046096	-1.893911
C	-5.565201	0.194447	-0.437436
H	-6.011444	-0.329610	1.614267
H	-4.811207	0.633478	-2.415837
H	-6.588677	0.498583	-0.669932
C	-0.314407	0.892835	-0.342937
C	0.298271	1.556490	-1.419469
C	-0.745136	1.667729	0.754068
C	0.485087	2.938004	-1.394415
H	0.627084	0.985571	-2.282986
C	-0.562146	3.049007	0.768246
H	-1.227027	1.194815	1.606911
C	0.058719	3.696423	-0.303021
H	0.966532	3.423980	-2.246489
H	-0.913014	3.623878	1.628786
H	0.199735	4.779466	-0.289962
H	-1.330341	-0.824463	1.577183
B	-0.177838	-1.434980	-1.593439
H	0.229235	-0.860209	-2.572936
H	-1.066730	-2.224408	-1.802665
N	1.497633	-0.110099	2.469838
H	1.386437	0.557343	3.226011
B	1.228941	-1.608575	2.722438
H	2.228947	-2.179271	3.133934
H	0.251200	-1.760989	3.429647
C	1.180055	-1.549437	0.254065
O	1.032068	-2.201456	-0.909632
O	0.921845	-2.162159	1.322947
B	1.369946	-3.805201	-1.079320
H	1.469527	-3.916012	-2.289225
H	0.427652	-4.403728	-0.592490
H	2.423529	-3.951370	-0.479433
C	2.101991	0.354049	1.396296
C	2.648670	1.661745	1.297497
C	3.382657	2.005361	0.197926
H	2.493653	2.343017	2.134006
C	3.003885	-0.174561	-0.809506
C	3.605304	1.058204	-0.829757
H	3.824468	3.000832	0.123428
H	4.265235	1.295696	-1.663013
N	2.178327	-0.490956	0.281185
C	3.289605	-1.170494	-1.890374
H	4.165009	-0.819688	-2.451973
H	3.501070	-2.168160	-1.484048
H	2.450970	-1.277792	-2.591474

Int-V

N	-0.461936	-0.604280	-0.146214
C	-1.440335	-1.021304	0.933384
H	-1.377056	-2.109546	1.009692
C	-2.846976	-0.576850	0.615772
C	-3.287973	0.709267	0.966492
C	-3.741687	-1.442348	-0.031042
C	-4.584931	1.126001	0.662664
H	-2.610964	1.391373	1.483852
C	-5.040182	-1.027085	-0.334876
H	-3.419362	-2.450726	-0.295065
C	-5.463509	0.259849	0.006050
H	-4.911371	2.130231	0.943851
H	-5.724625	-1.715043	-0.836970
H	-6.479571	0.584450	-0.231770
C	-0.376820	0.854142	-0.213357
C	-0.827002	1.555903	-1.331710
C	0.108626	1.557012	0.898047
C	-0.756129	2.951604	-1.352936
H	-1.243473	1.015108	-2.178160
C	0.188870	2.947773	0.867249
H	0.416515	1.022213	1.795896
C	-0.239384	3.651404	-0.262532
H	-1.114629	3.490674	-2.232598
H	0.582391	3.482664	1.734374
H	-0.180283	4.741849	-0.285810
H	-1.103090	-0.595697	1.884207
B	-0.636456	-1.500457	-1.506695
H	-0.787999	-0.879648	-2.527294
H	-1.409591	-2.406355	-1.331384
C	2.680335	-0.171937	1.260828
C	2.552161	0.295111	-1.121479
C	3.467565	1.306492	-0.956789
H	3.791986	1.854684	-1.839258
N	2.121628	-0.425480	0.005506
N	2.293522	-0.857284	2.316063
H	2.746771	-0.577901	3.180208
B	1.358682	-2.077973	2.345869

H	1.952996	-3.065616	2.754079
H	0.370068	-1.834599	3.033808
C	0.978410	-1.400601	-0.032588
O	0.815773	-1.941599	-1.295073
O	0.999187	-2.296267	0.901179
B	1.592513	-3.245514	-1.832349
H	2.756463	-3.069947	-1.498016
H	1.072315	-4.220964	-1.318549
H	1.419704	-3.175889	-3.041138
C	3.632444	0.884183	1.395083
C	4.006861	1.617598	0.310419
H	4.728831	2.430472	0.413548
H	4.033455	1.070941	2.391937
C	2.106931	-0.013048	-2.519385
H	2.428706	-1.017591	-2.826848
H	1.023011	0.033630	-2.661902
H	2.569273	0.724180	-3.186910

TS-5

N	-0.654731	-0.728842	-0.210490
C	-1.661774	-1.395788	0.741263
H	-1.575347	-2.474956	0.569031
C	-3.063993	-0.910810	0.514630
C	-3.563162	0.167049	1.260584
C	-3.881062	-1.502891	-0.459624
C	-4.850949	0.652195	1.030805
H	-2.931793	0.636005	2.018322
C	-5.169076	-1.016221	-0.691943
H	-3.507387	-2.348881	-1.039301
C	-5.654542	0.064355	0.049912
H	-5.226997	1.493304	1.617707
H	-5.797258	-1.485878	-1.452427
H	-6.662768	0.444250	-0.132199
C	-0.740985	0.742474	-0.092117
C	-1.570092	1.417784	-0.989806
C	-0.124269	1.424062	0.954999
C	-1.750935	2.794946	-0.859519
H	-2.082499	0.876399	-1.782489
C	-0.303390	2.804014	1.072561
H	0.496417	0.890054	1.666482
C	-1.109841	3.494468	0.165266
H	-2.399857	3.318211	-1.564747
H	0.196949	3.337380	1.883585
H	-1.245532	4.574079	0.261574
H	-1.316063	-1.167789	1.756618
B	-0.633192	-1.308159	-1.770914
H	-0.624187	-0.471121	-2.623821
H	-1.349389	-2.265905	-1.883659
N	2.949989	-1.007085	2.081431
H	3.708015	-1.472395	2.567221
B	1.581911	-1.484067	2.371001
H	1.556278	-2.452915	3.097834
H	0.725025	-0.659225	2.599902
C	0.663664	-1.461975	-0.104280
O	0.819474	-1.761275	-1.372608
O	1.087849	-2.099067	0.841081
B	1.896687	-2.824998	-2.064473
H	2.980238	-2.422708	-1.692361
H	1.657211	-2.659722	-3.245185
H	1.564370	-3.907573	-1.614991
C	3.381673	-0.226088	1.046056
C	4.757121	0.114030	0.952079
C	2.917779	0.953836	-0.915723
C	5.183012	0.896810	-0.101119
H	5.450894	-0.248913	1.713369
C	4.251972	1.334618	-1.052754
H	6.237063	1.171645	-0.191238
H	4.556509	1.957898	-1.894310
C	1.900266	1.412924	-1.920986
H	1.323099	0.570324	-2.322835
H	1.187780	2.116045	-1.464519
H	2.388920	1.920953	-2.763441
N	2.495625	0.184718	0.113104

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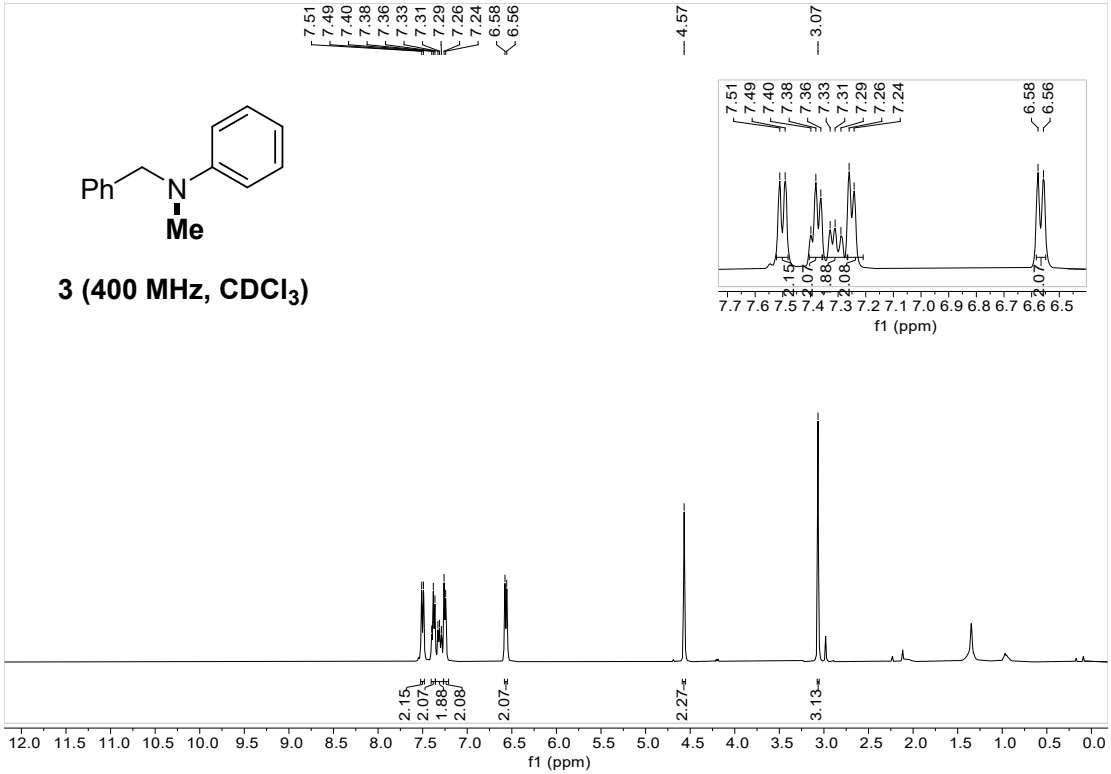
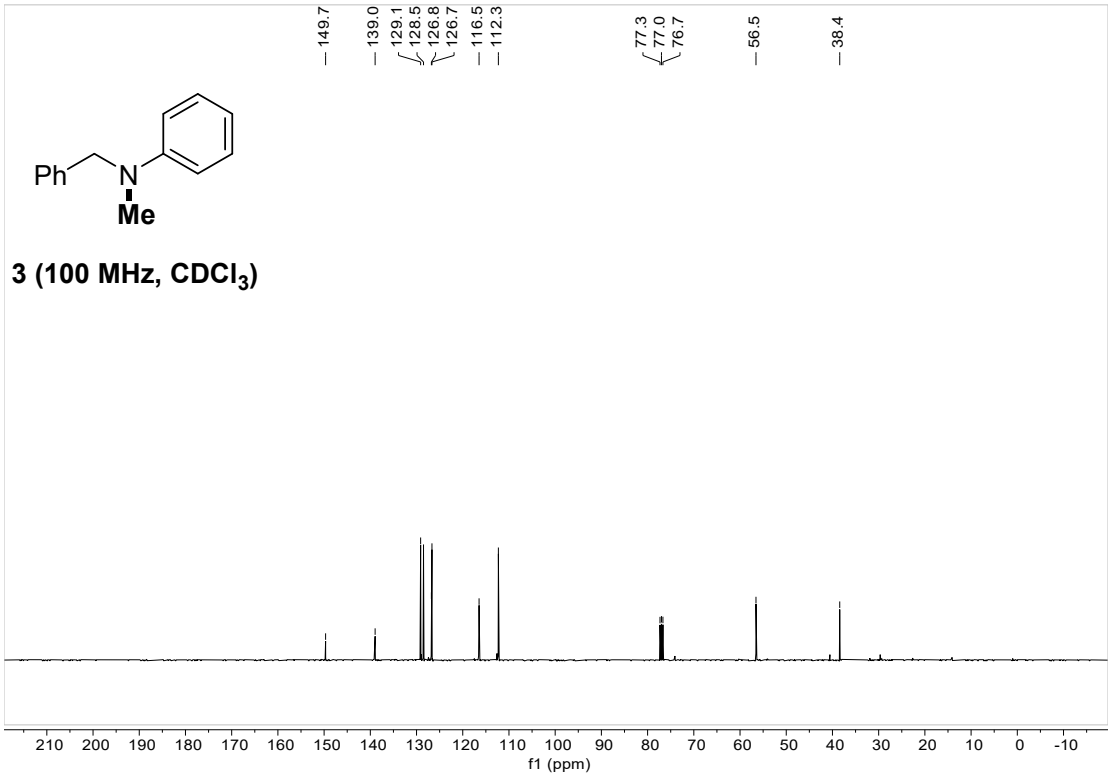
5. ^{1}H and ^{13}C NMR Spectra



3 (400 MHz, $CDCl_3$)



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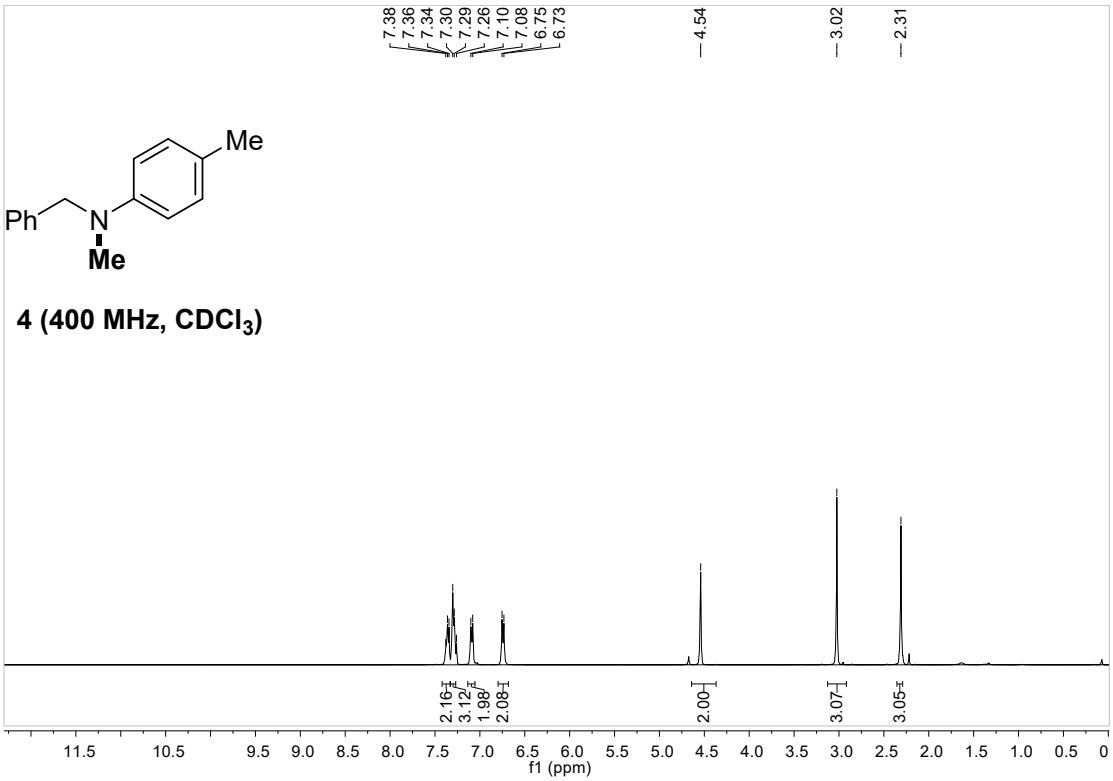

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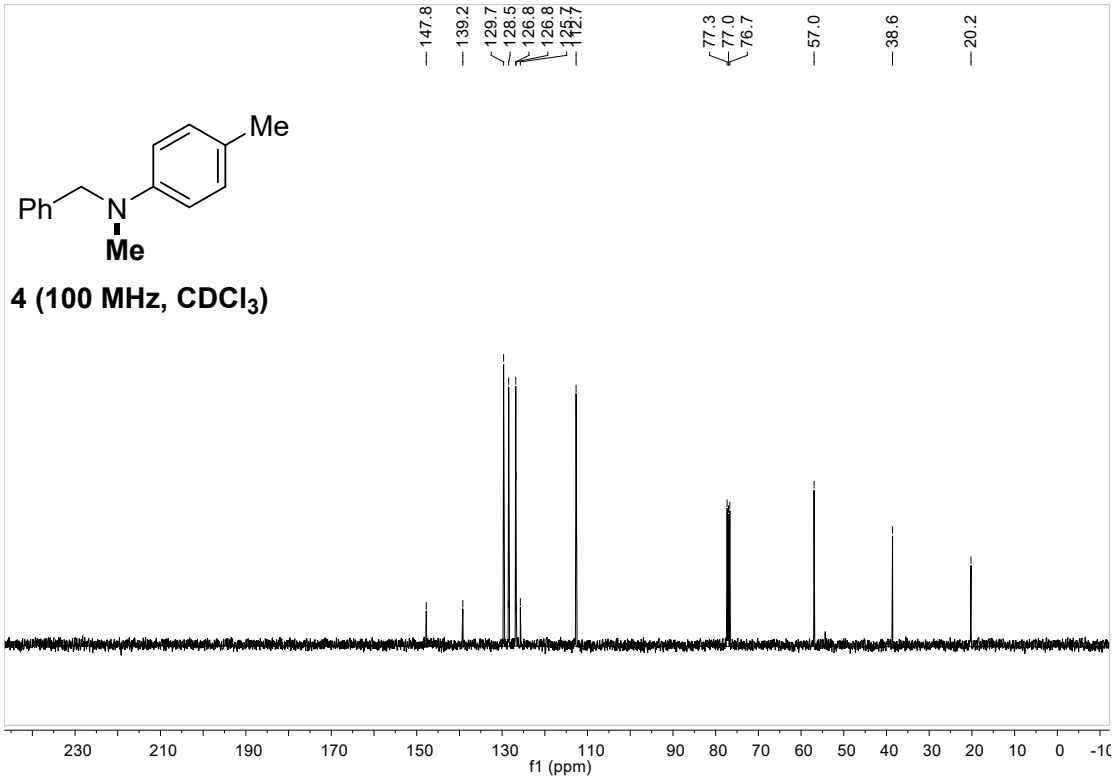

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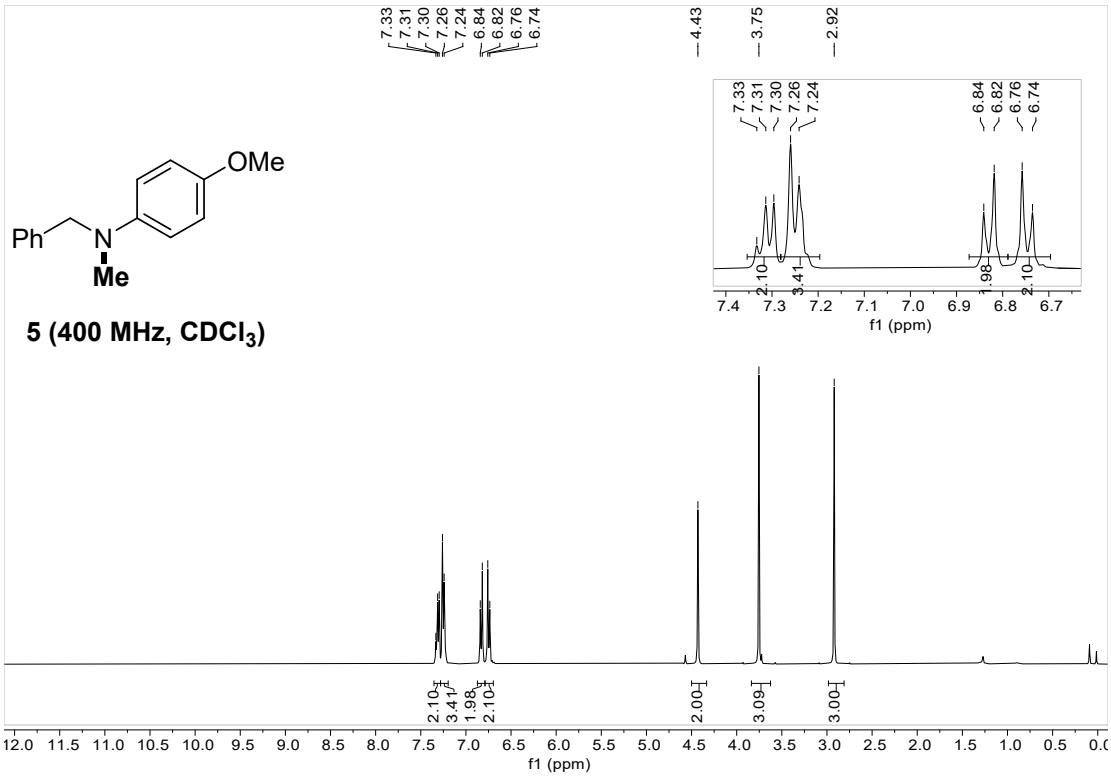

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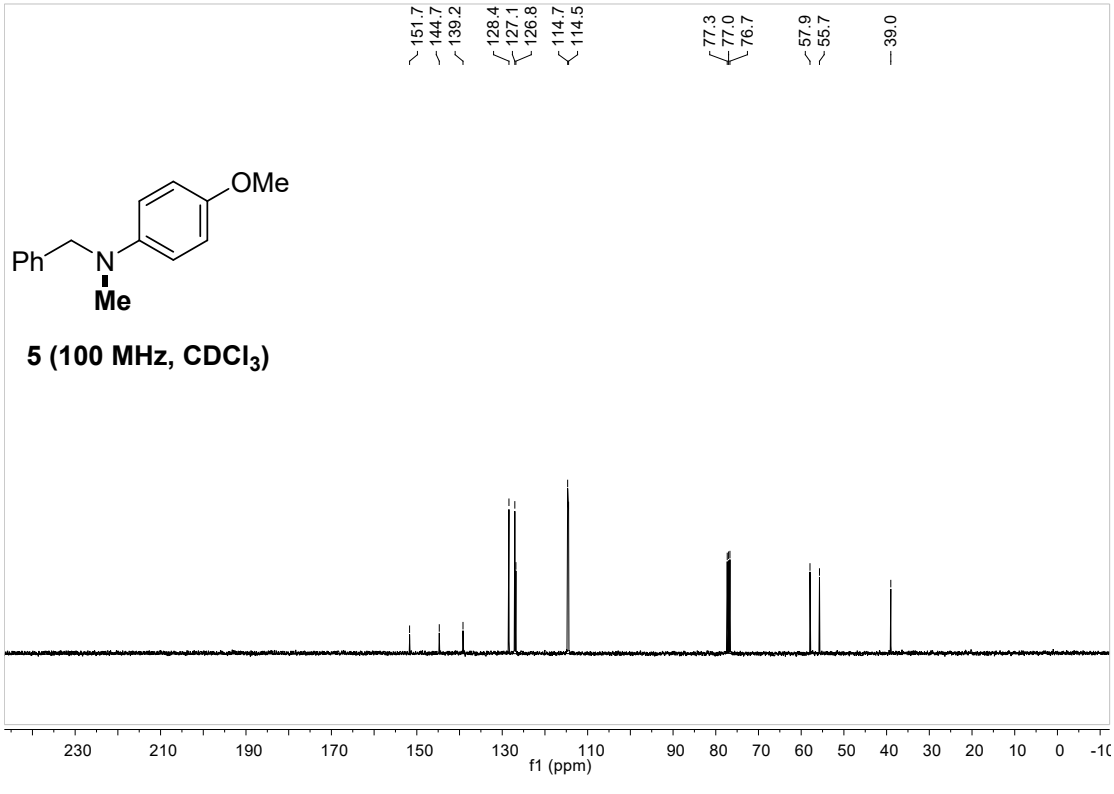

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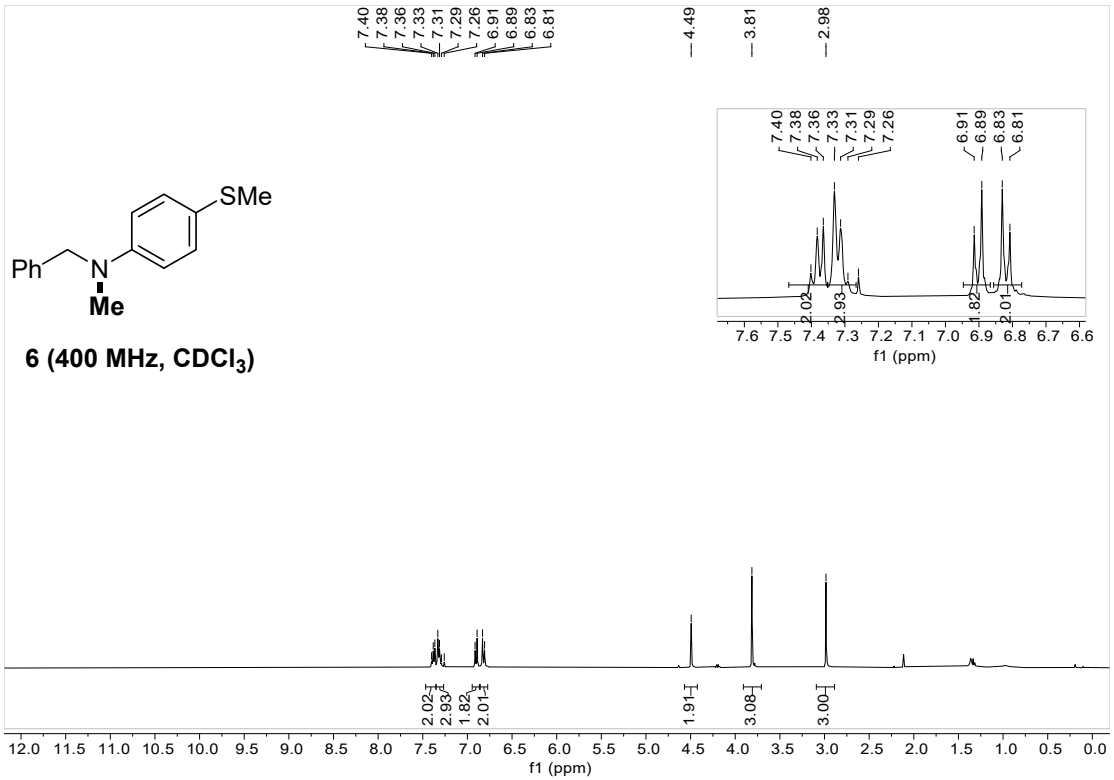

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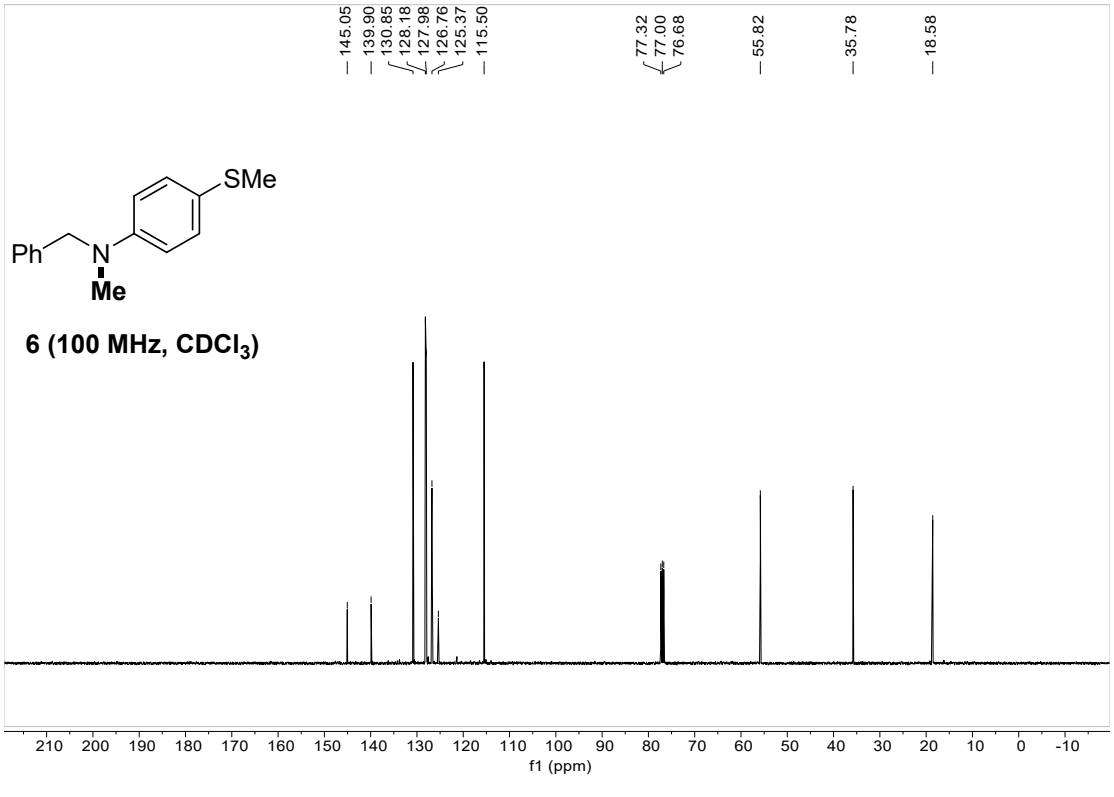

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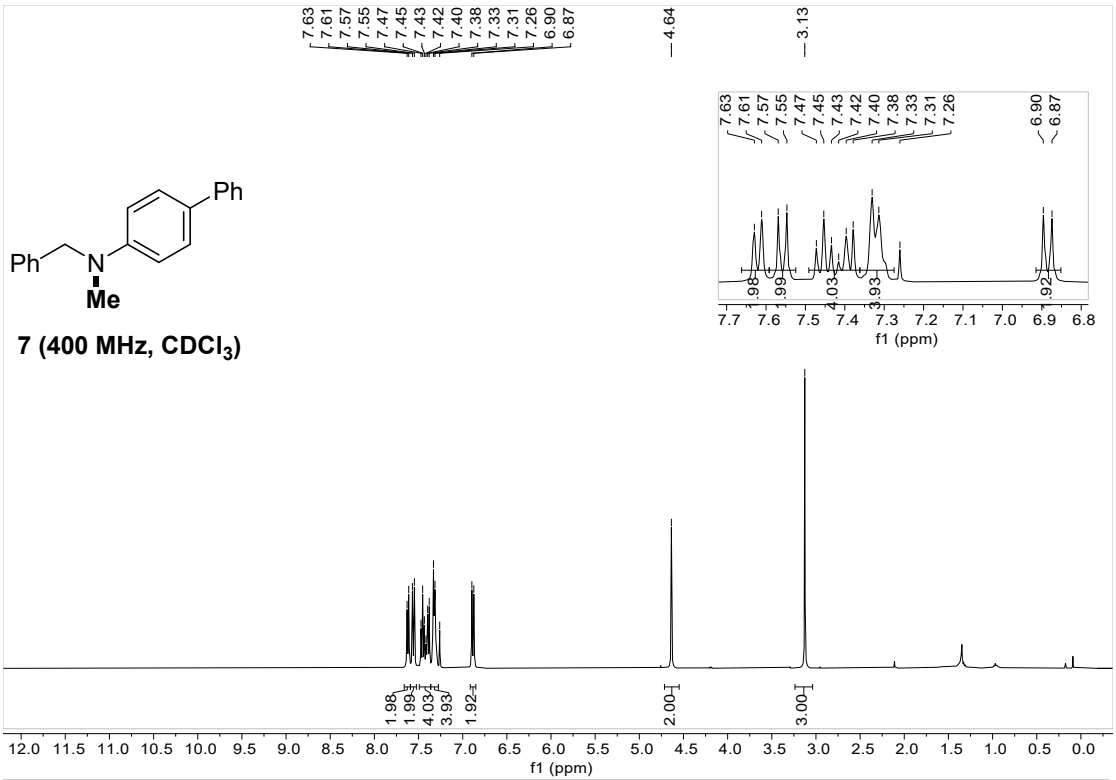

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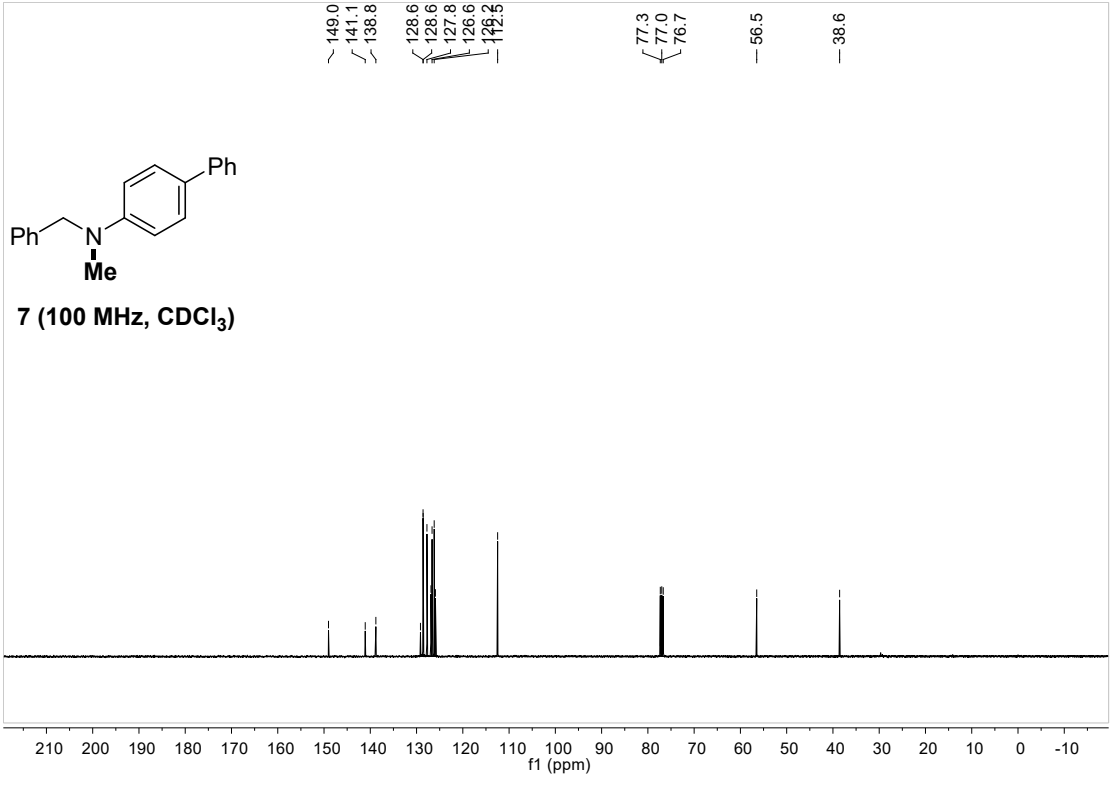

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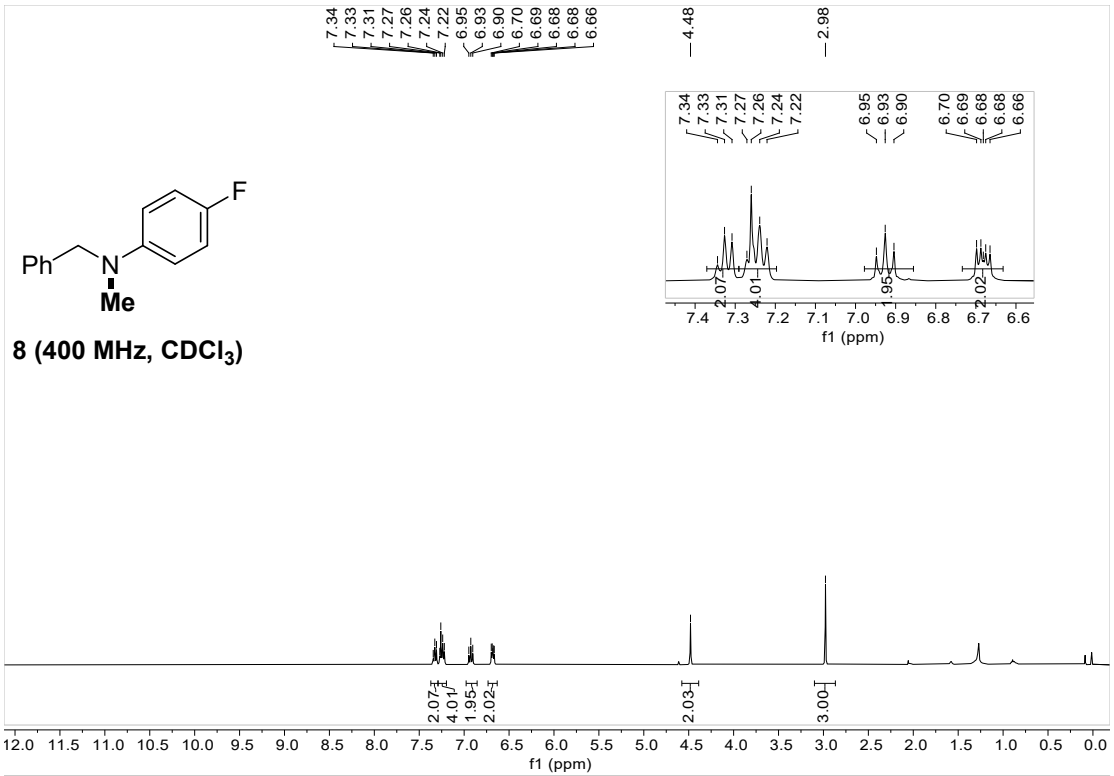
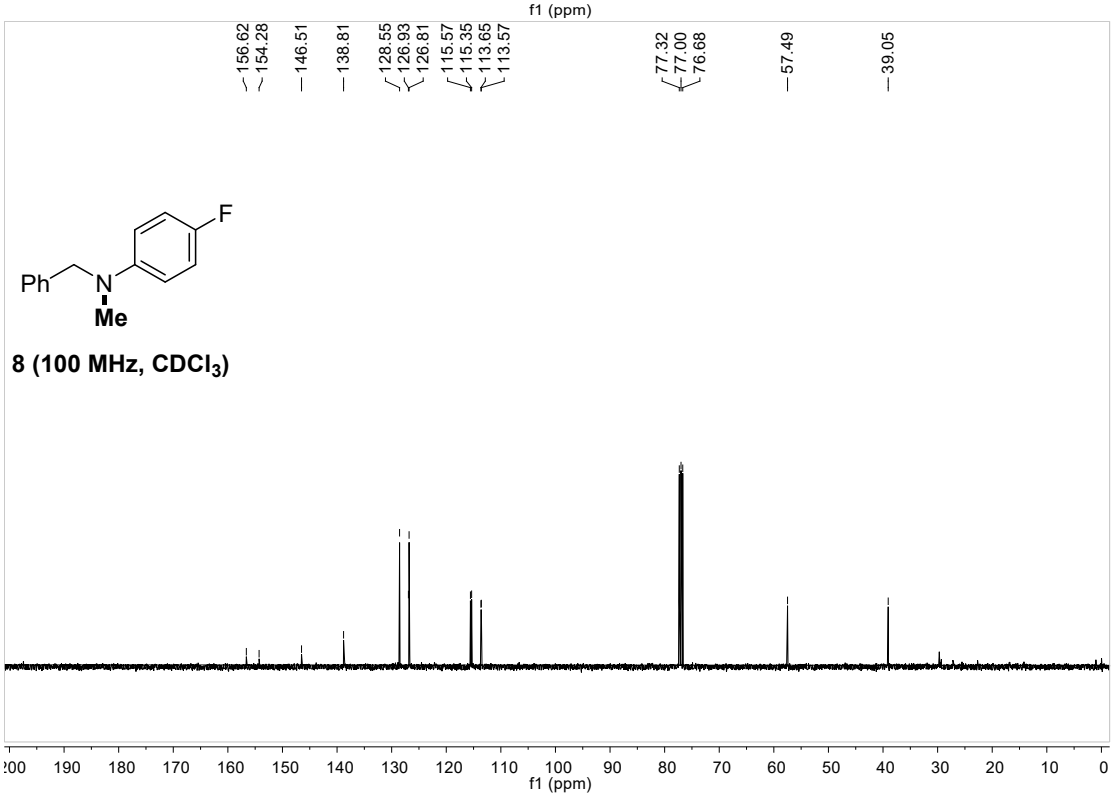


8 (400 MHz, $CDCl_3$)



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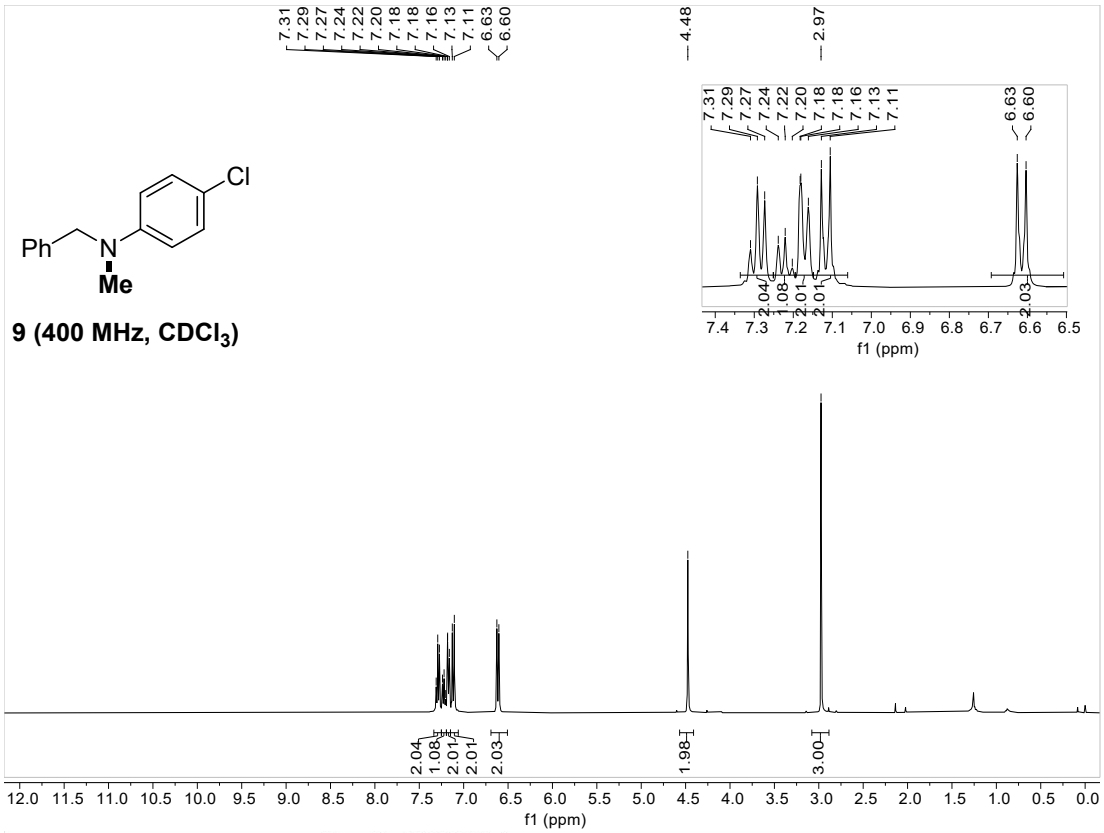

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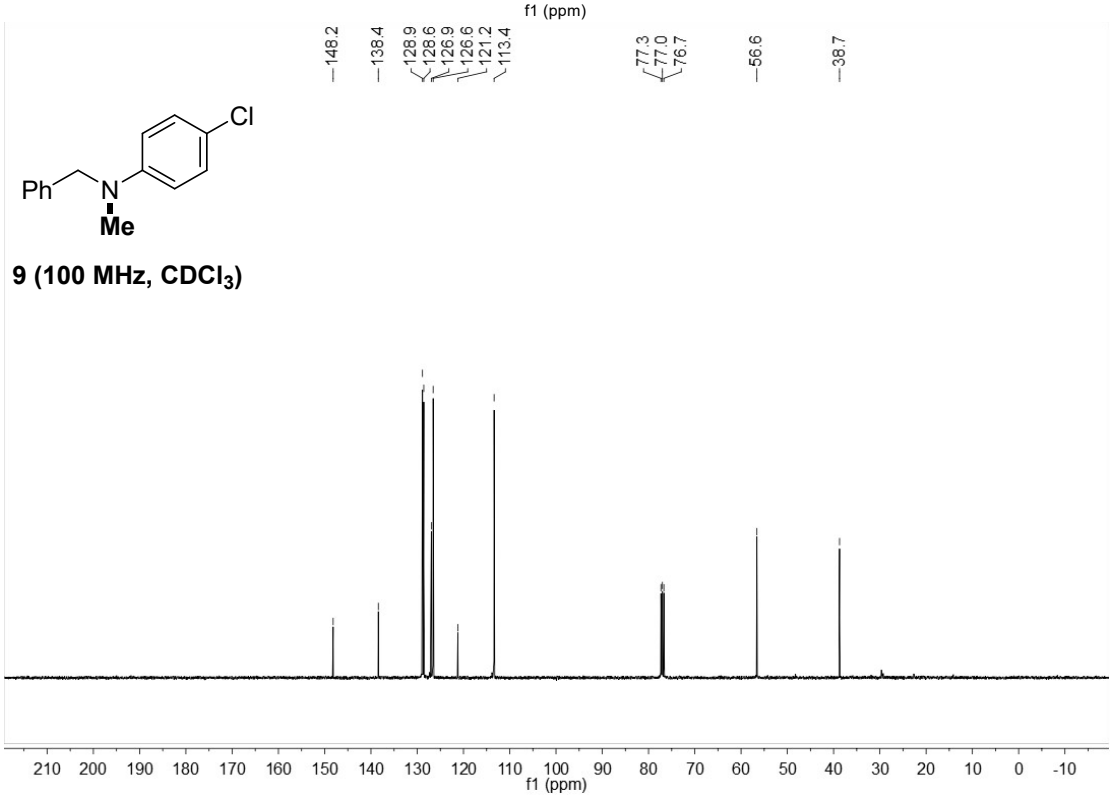

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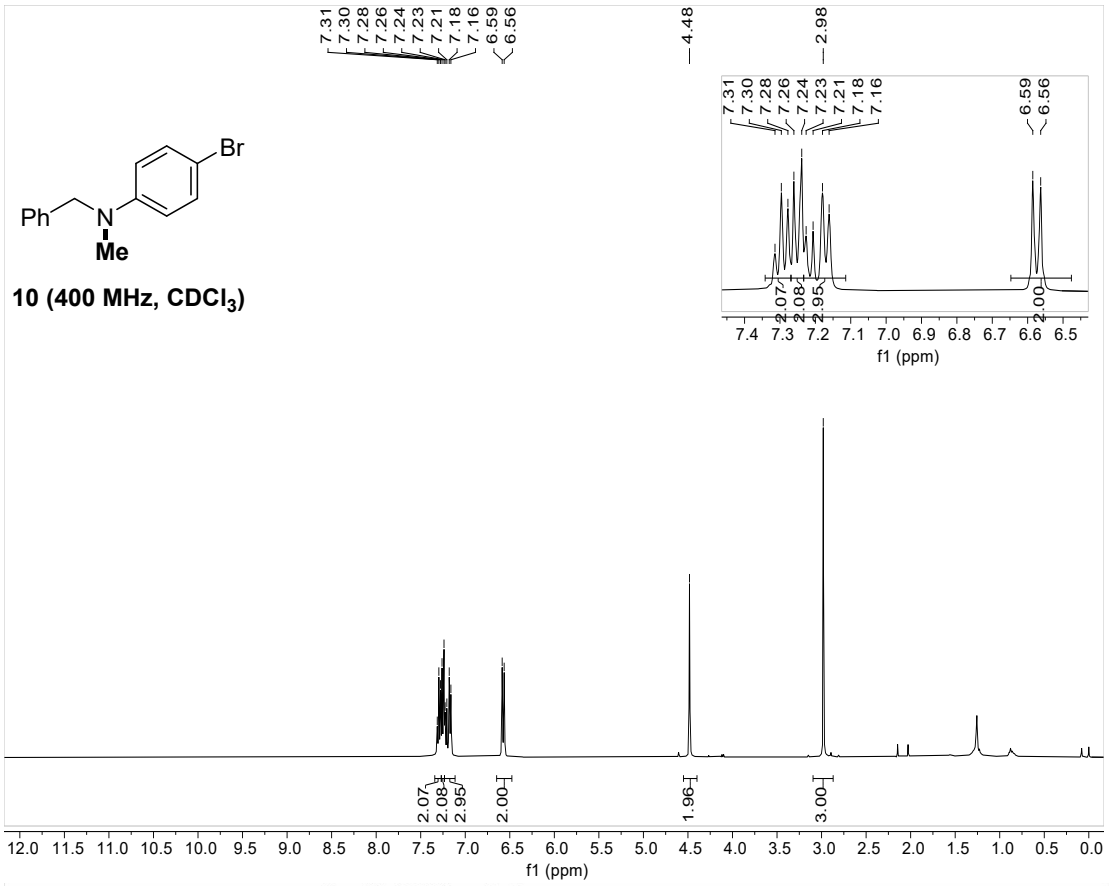

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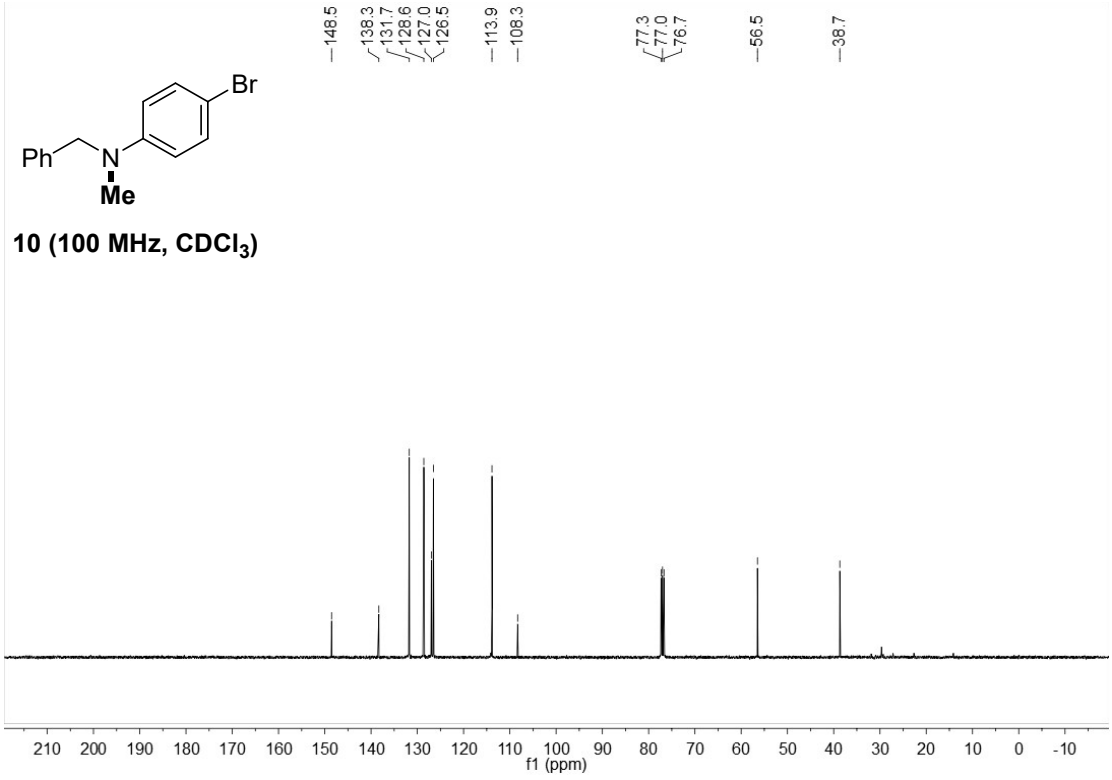

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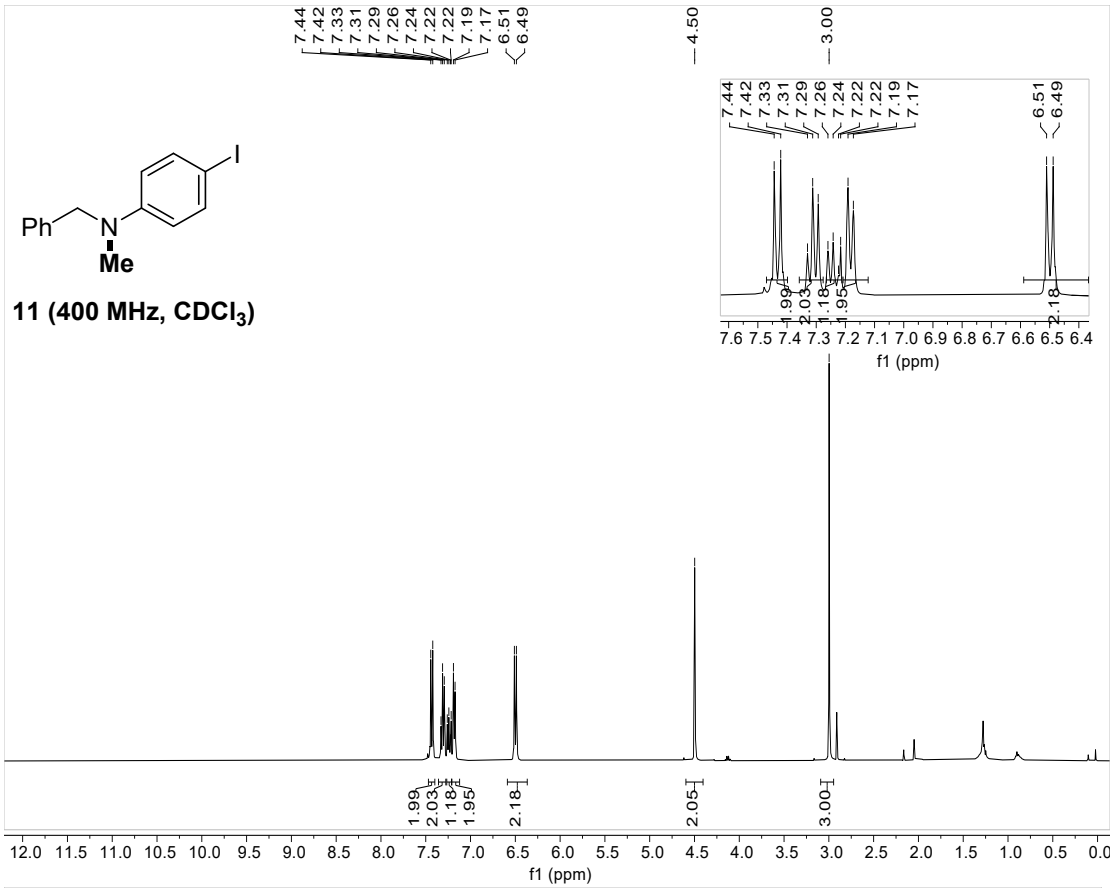
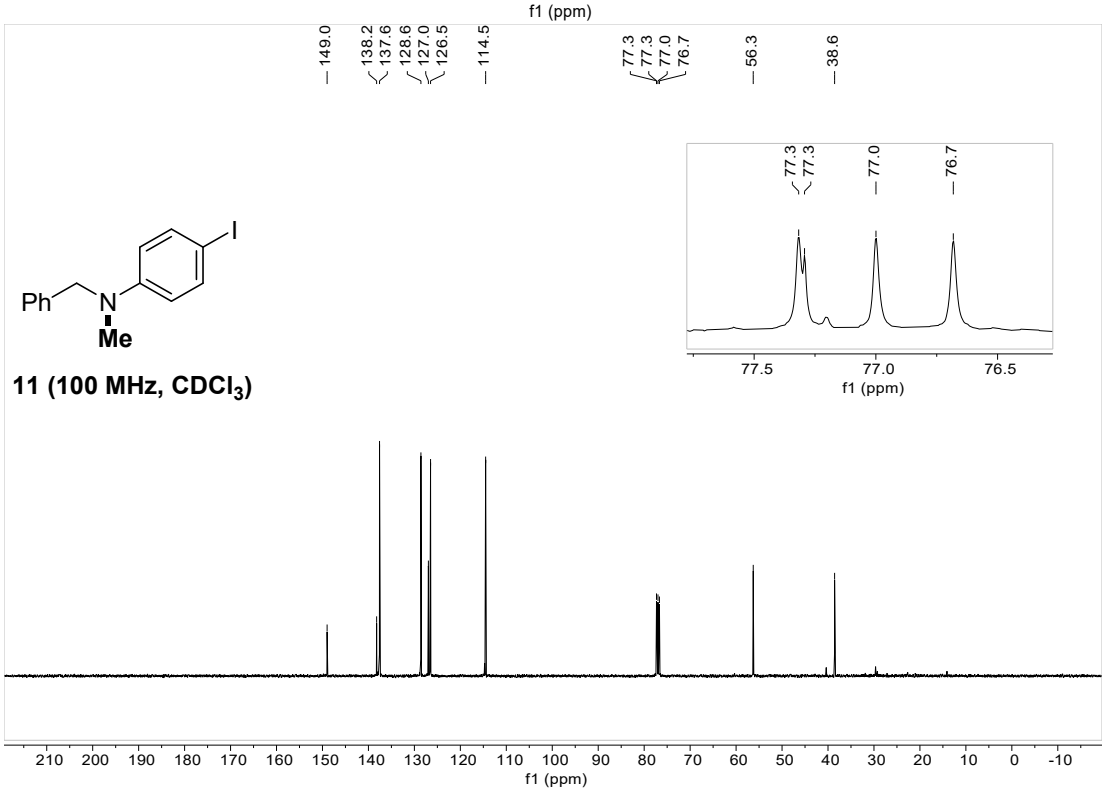
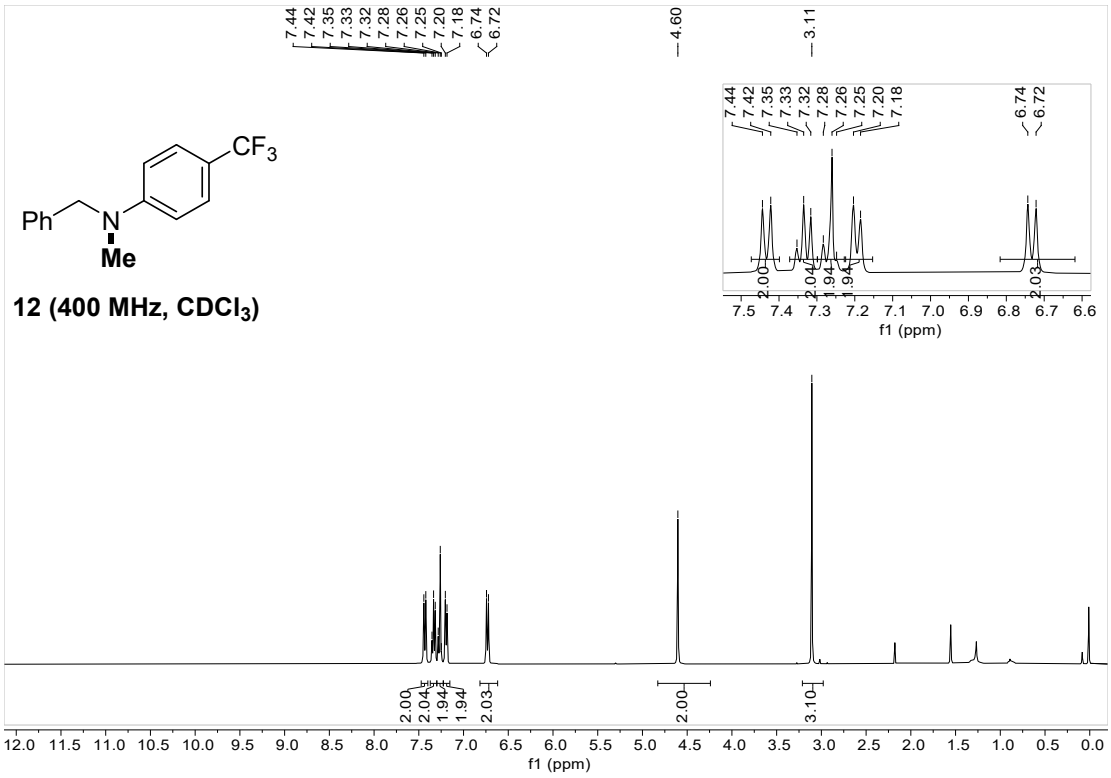
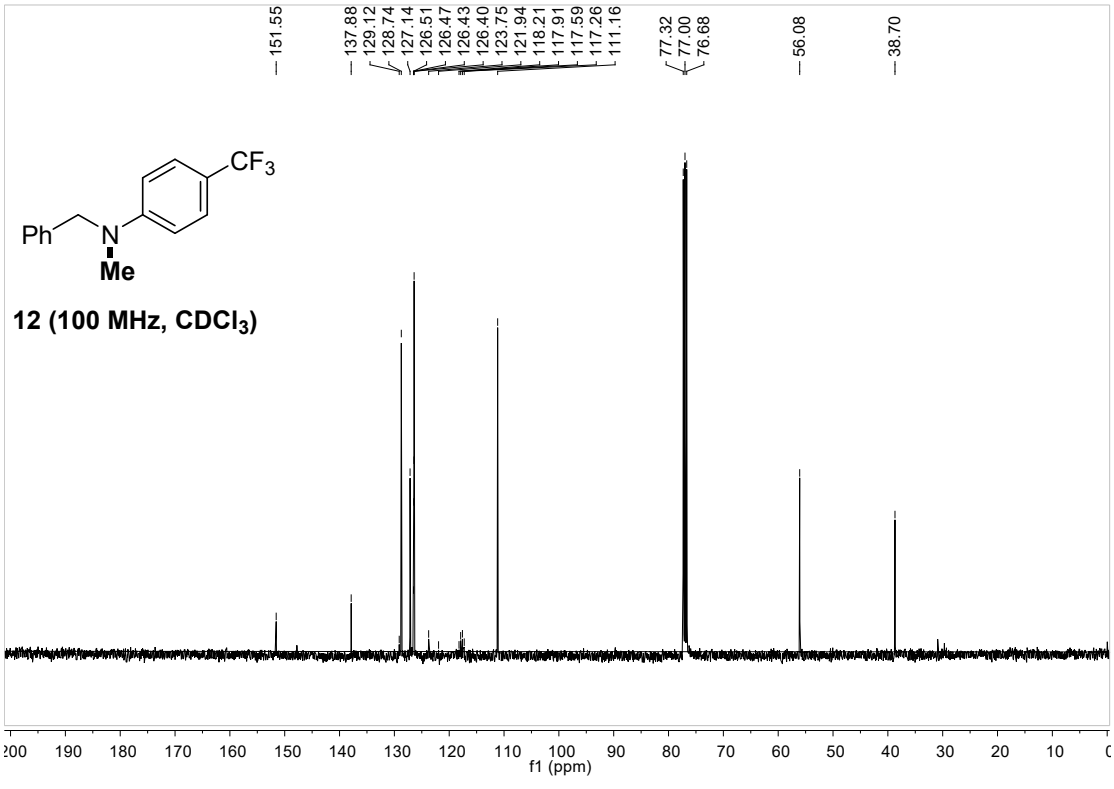


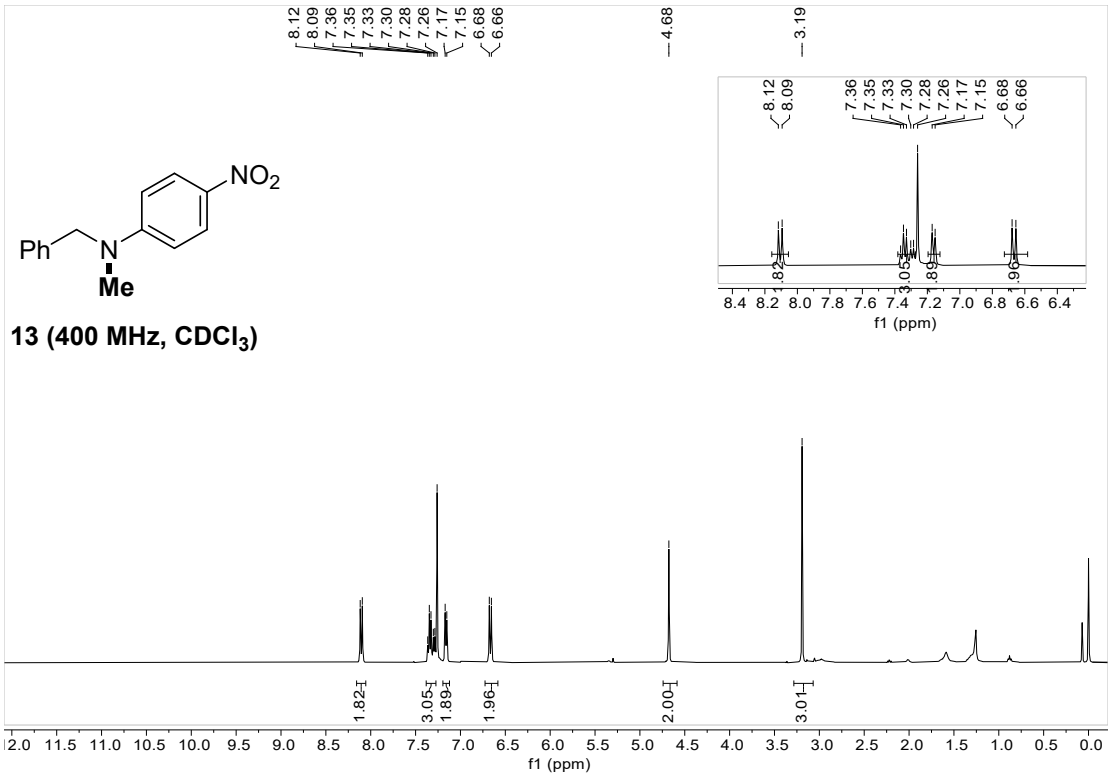
11 (400 MHz, $CDCl_3$)



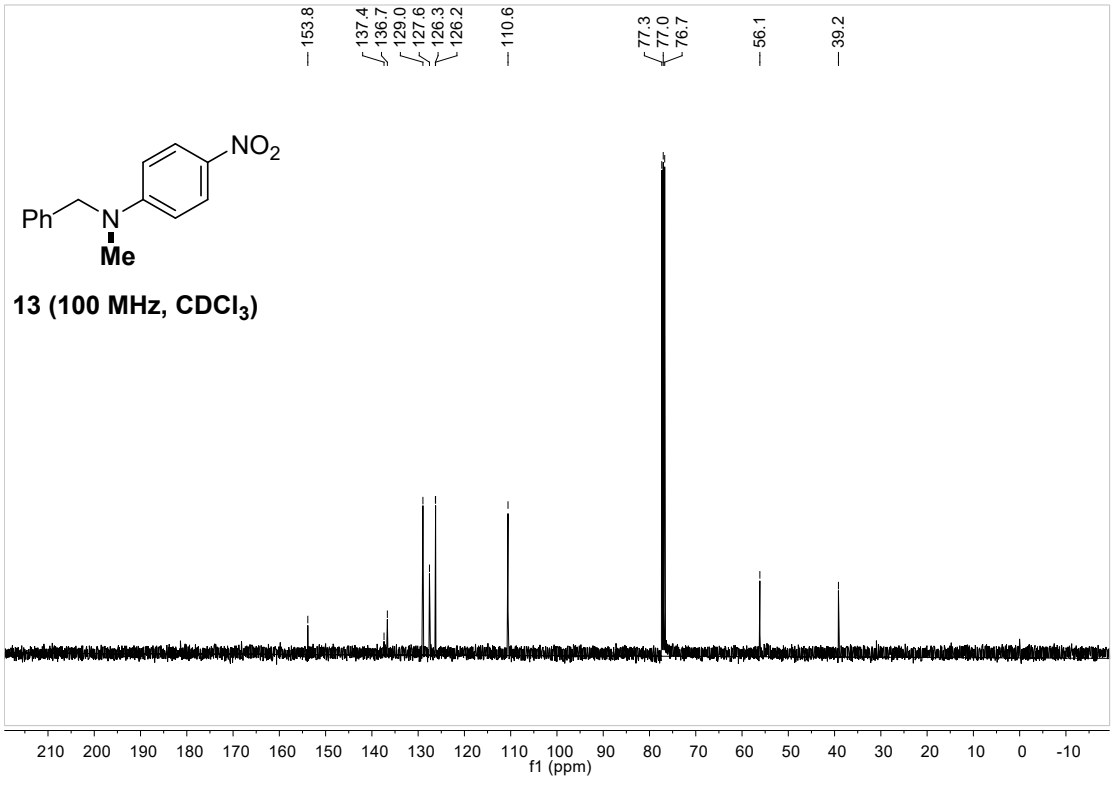
11 (100 MHz, $CDCl_3$)


7.44
7.42
7.35
7.33
7.32
7.28
7.26
7.25
7.20
7.18
6.74
6.72
4.60
3.11
CF3
Ph
N
Me
12 (400 MHz, CDCl3)
2.00
2.04
1.94
1.94
2.03
2.00
3.10
f1 (ppm)

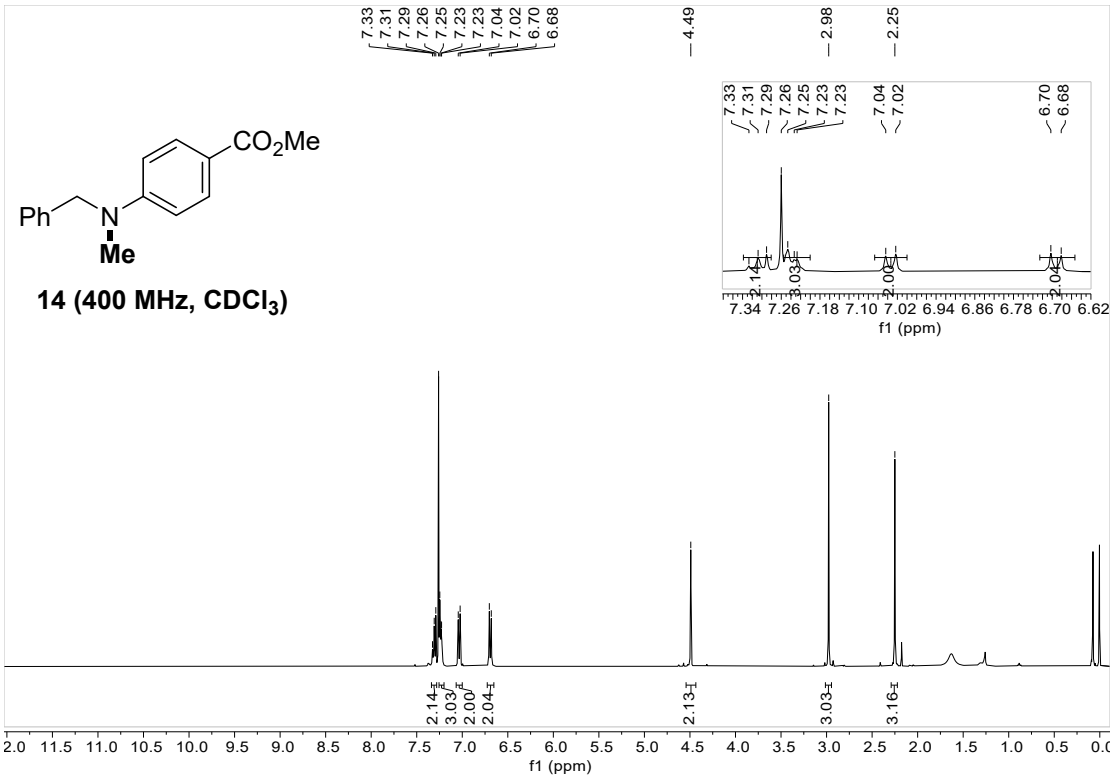

151.55
137.88
129.12
128.74
127.14
126.51
126.47
126.43
126.40
123.75
121.94
118.21
117.91
117.59
117.26
111.16
77.32
77.00
76.68
56.08
38.70
CF3
Ph
N
Me
12 (100 MHz, CDCl3)
f1 (ppm)

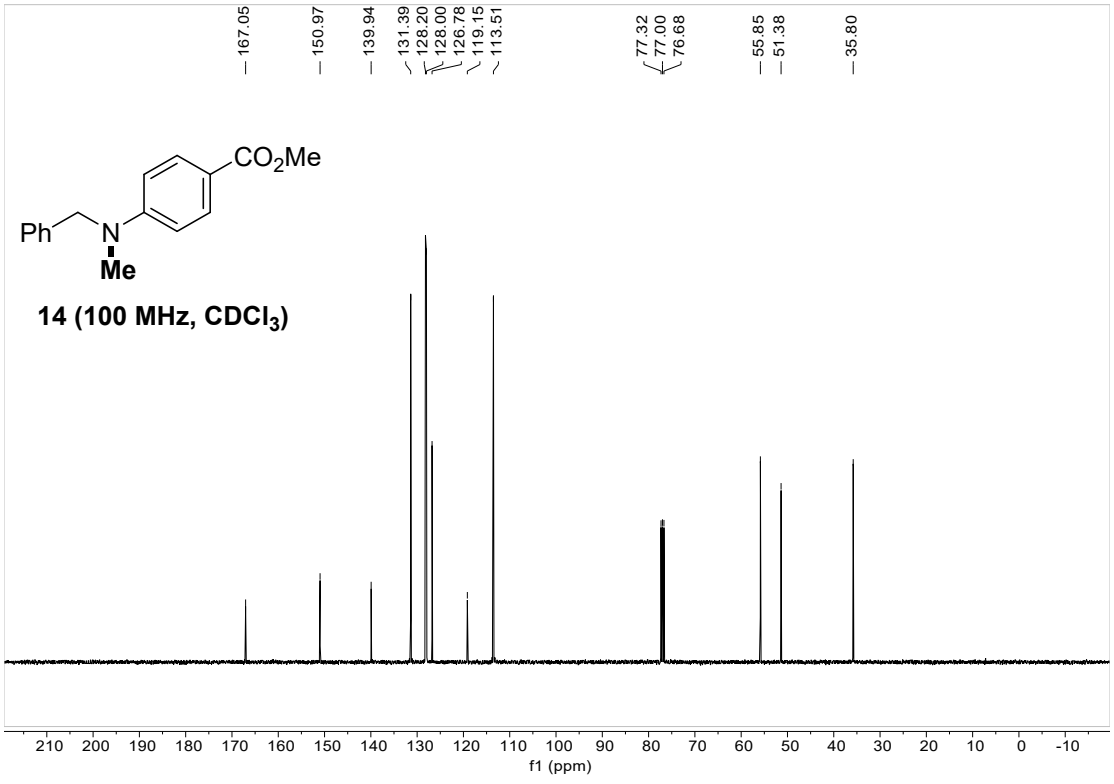


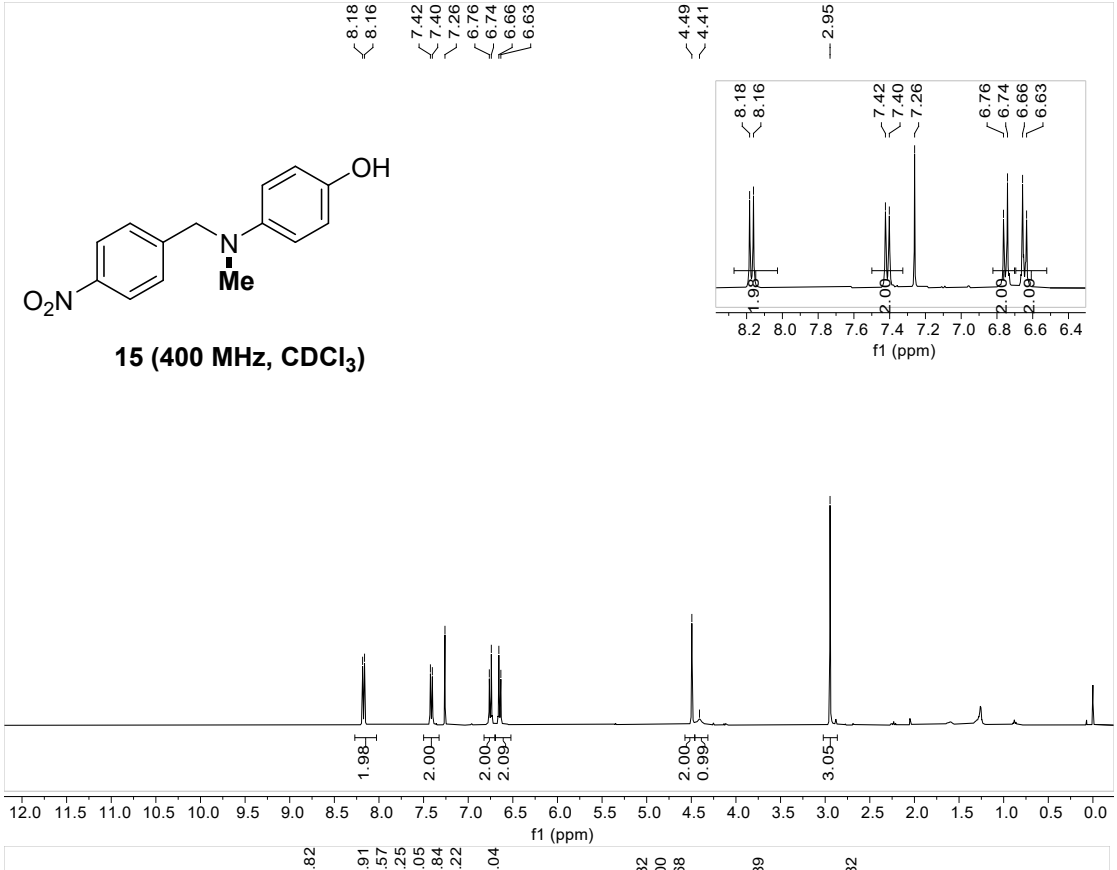
13 (400 MHz, $CDCl_3$)



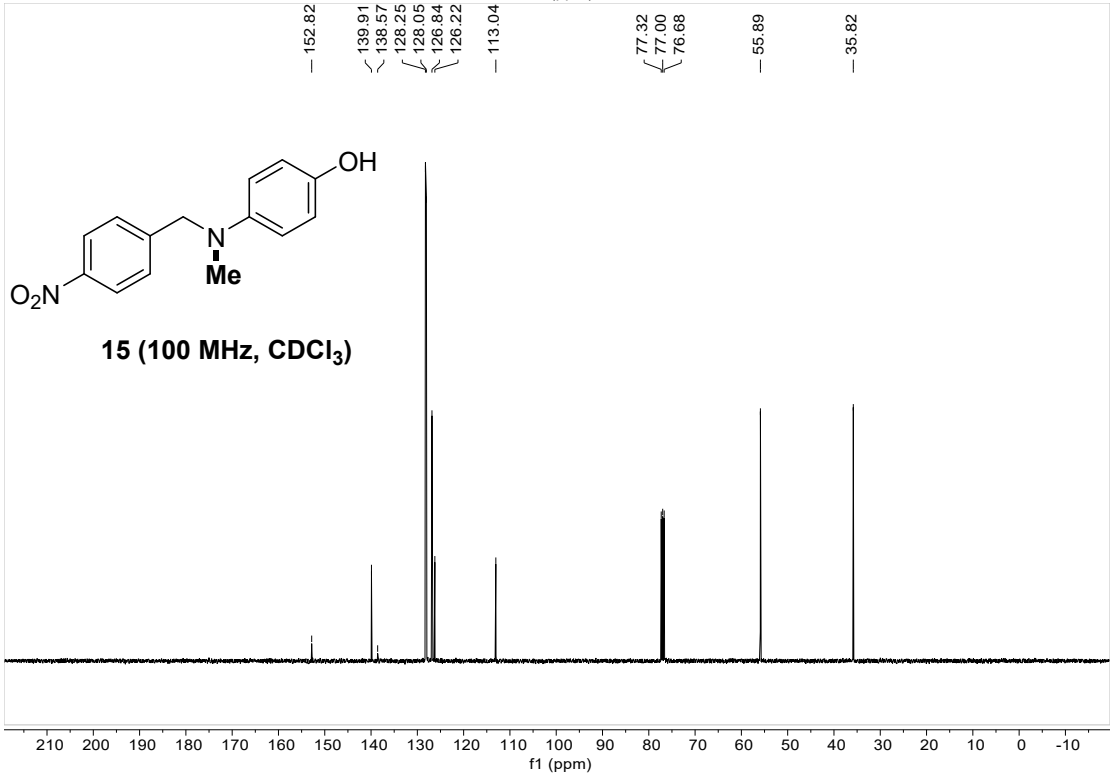
13 (100 MHz, $CDCl_3$)


7.33
7.31
7.29
7.26
7.25
7.23
7.23
7.04
7.02
6.70
6.68
4.49
2.98
2.25
CO2Me
Ph
N
Me
14 (400 MHz, CDCl3)
2.14
3.03
2.00
2.04
2.13
3.03
3.16
f1 (ppm)

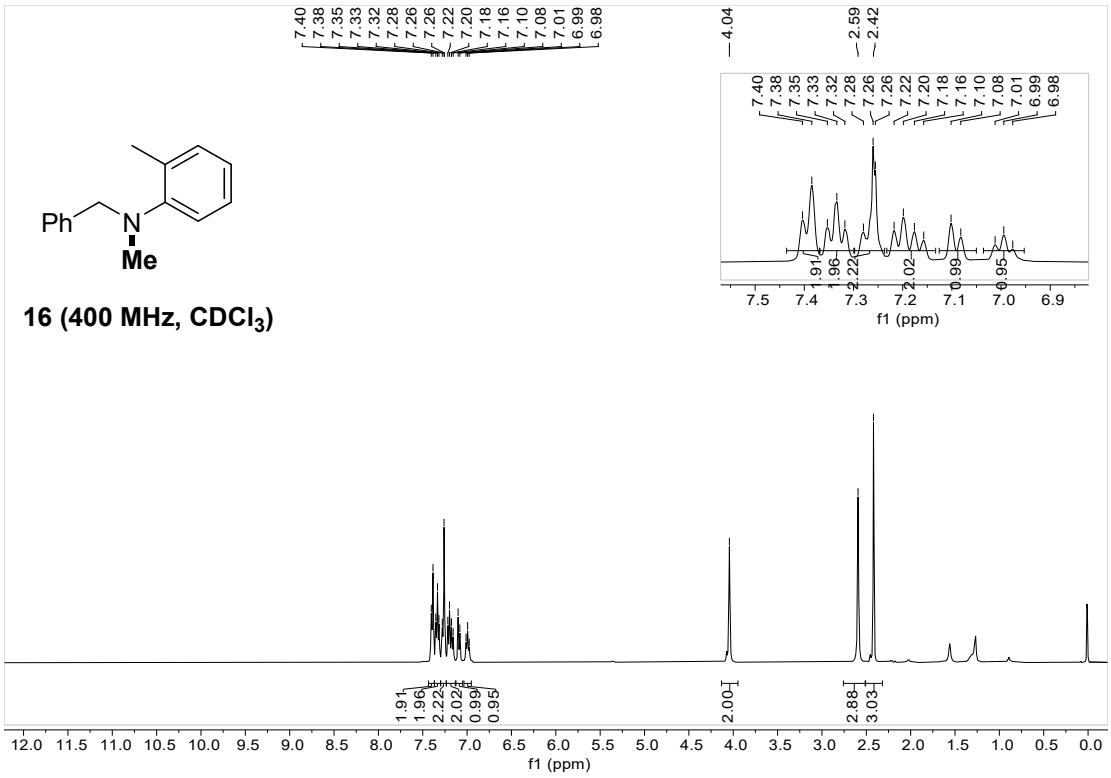

167.05
150.97
139.94
131.39
128.20
128.00
126.78
119.15
113.51
77.32
77.00
76.68
55.85
51.38
35.80
CO2Me
Ph
N
Me
14 (100 MHz, CDCl3)
f1 (ppm)

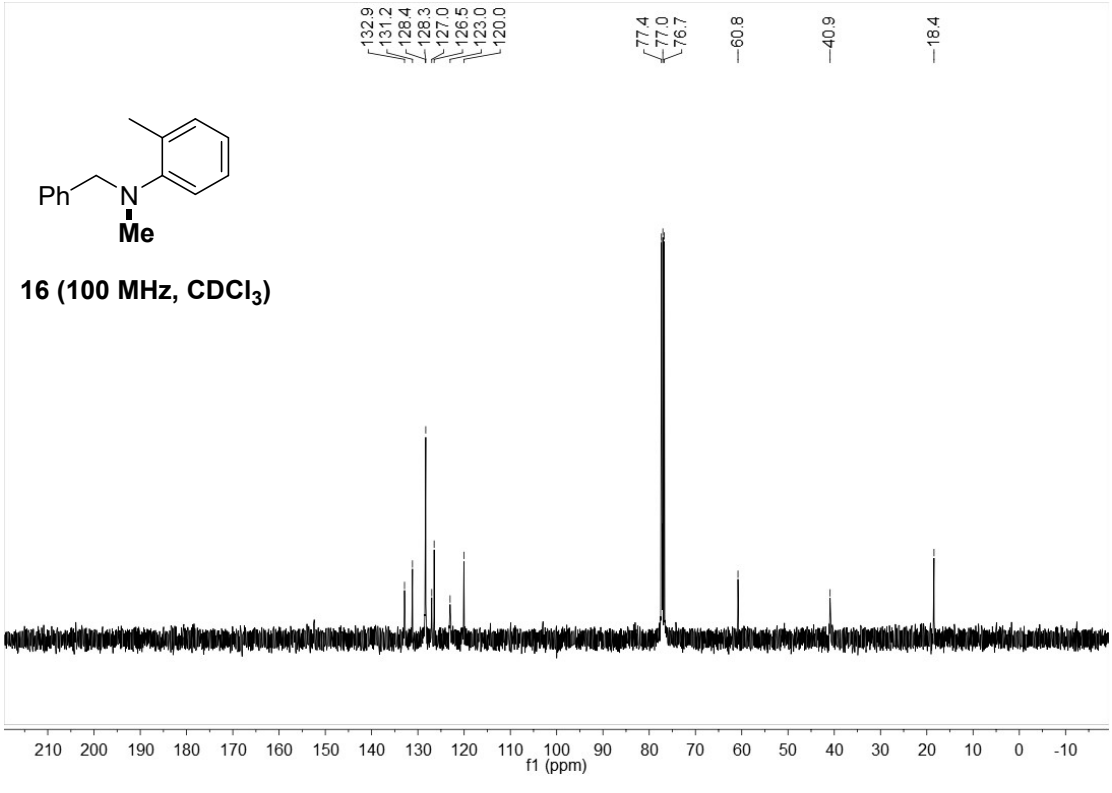


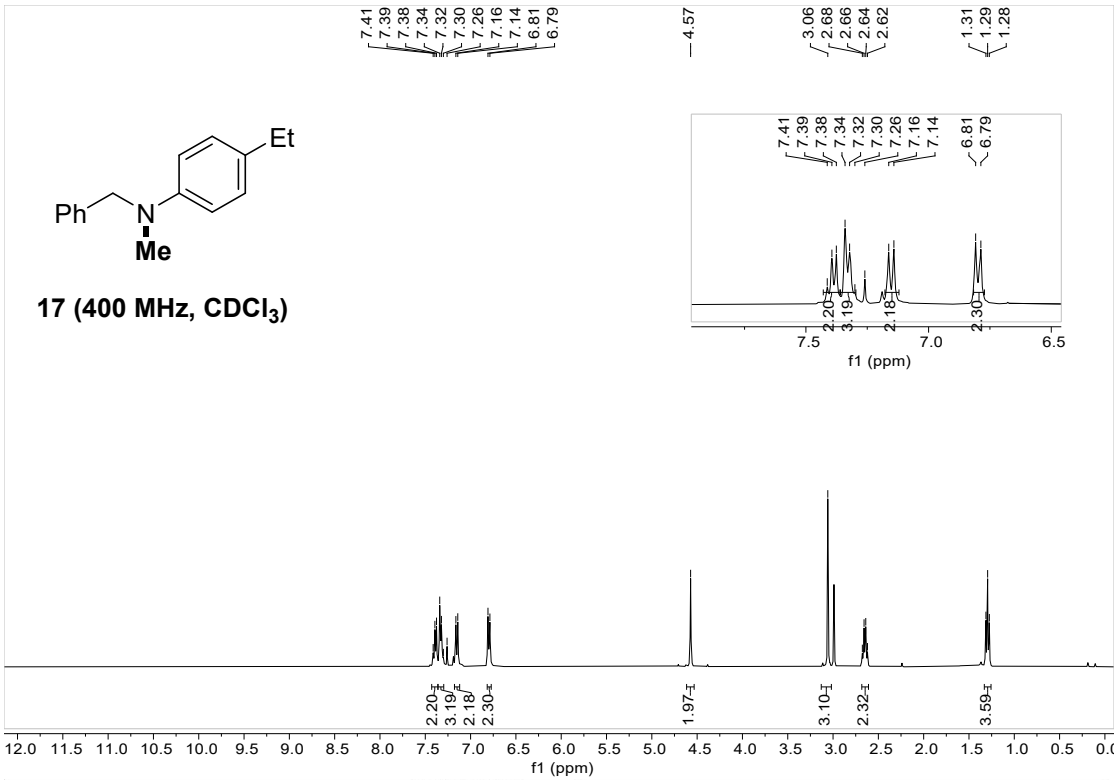
15 (400 MHz, $CDCl_3$)

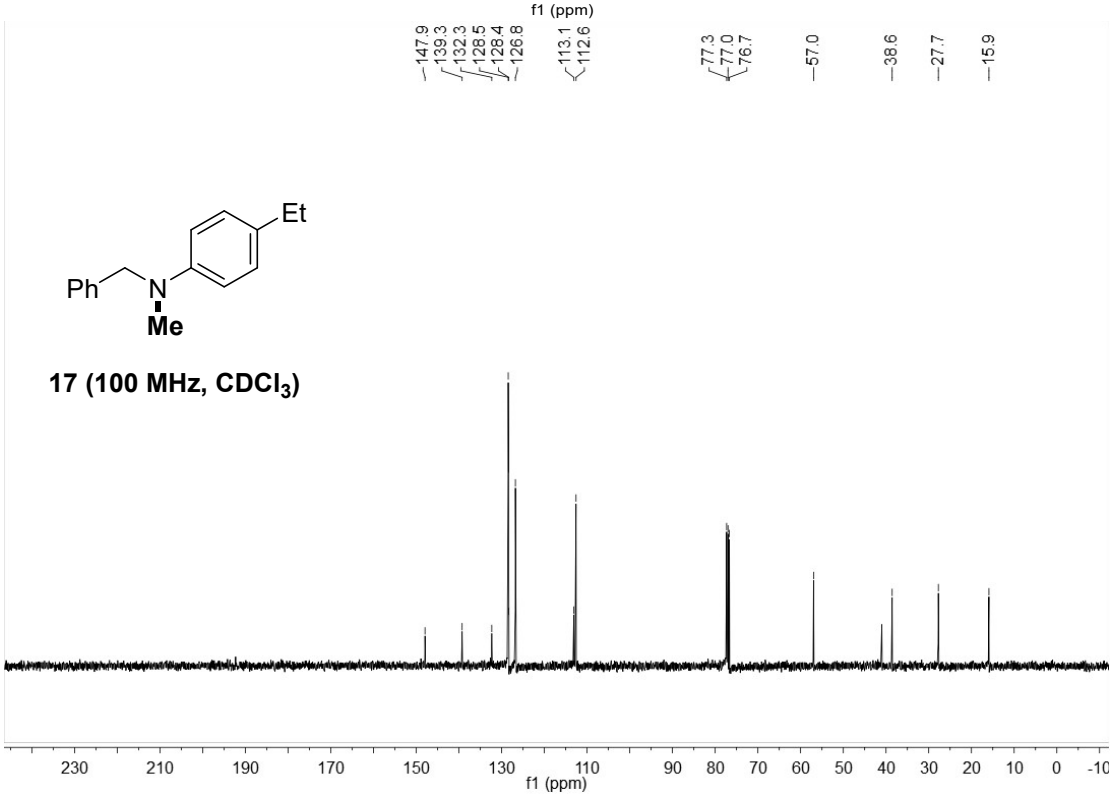


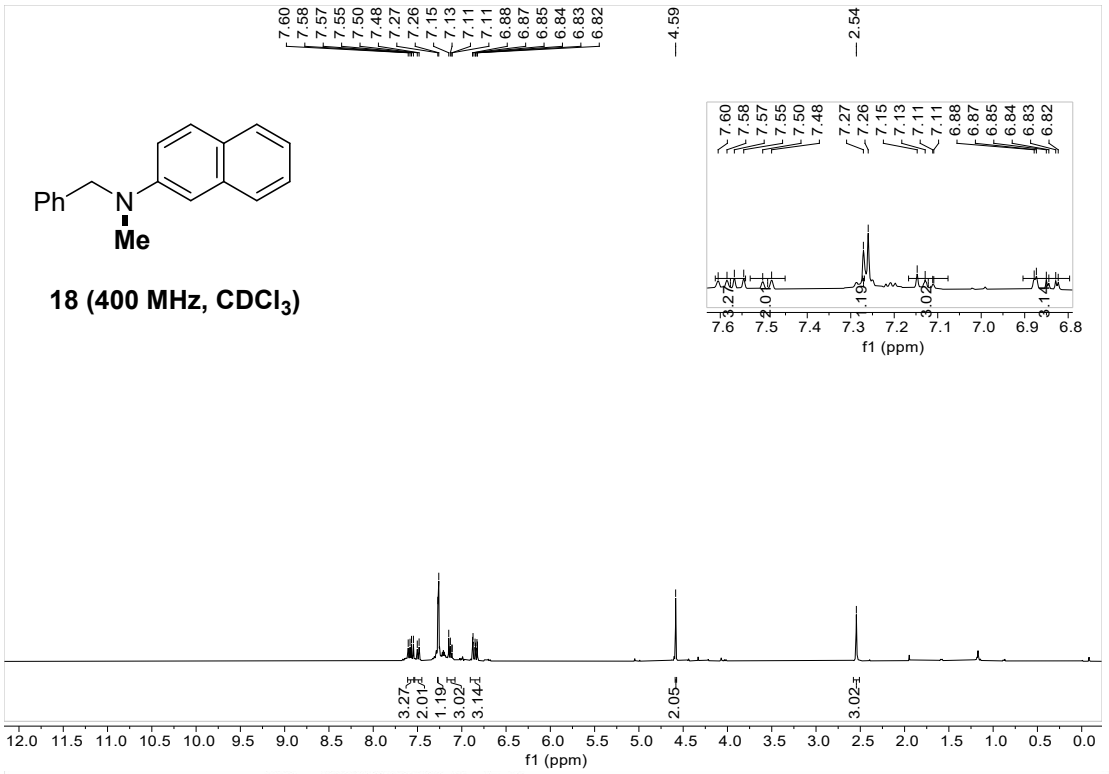
15 (100 MHz, $CDCl_3$)

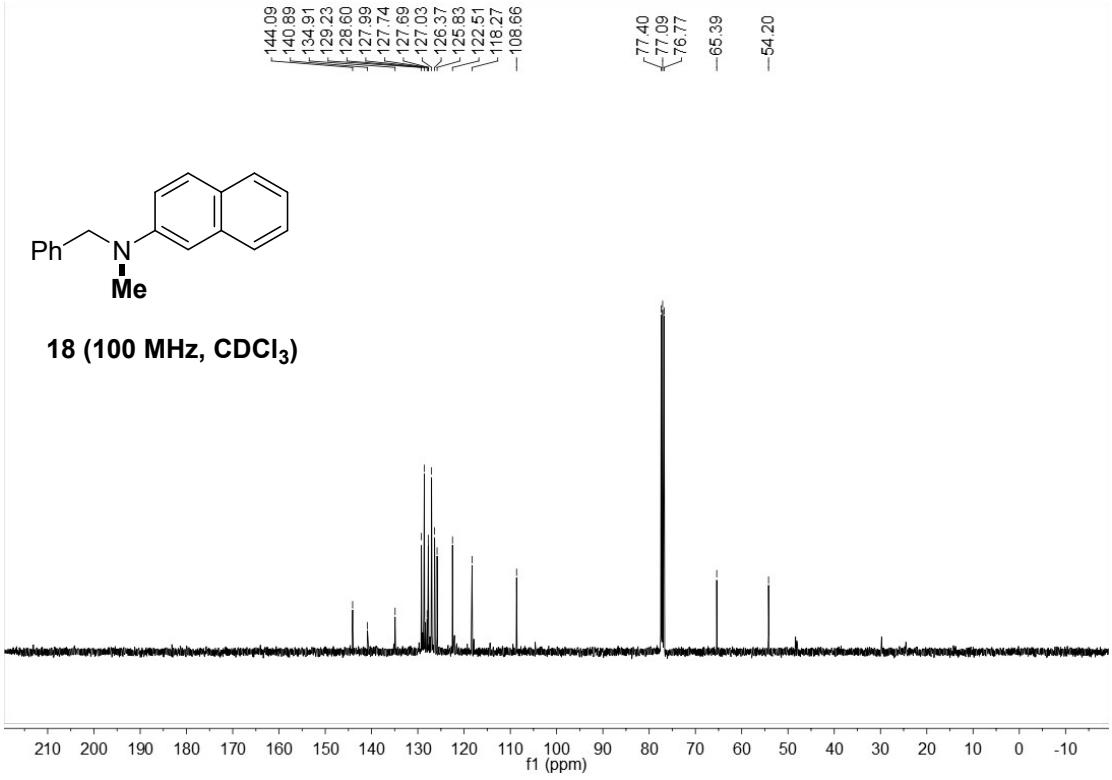

Ph
N
Me
16 (400 MHz, CDCl3)
f1 (ppm)

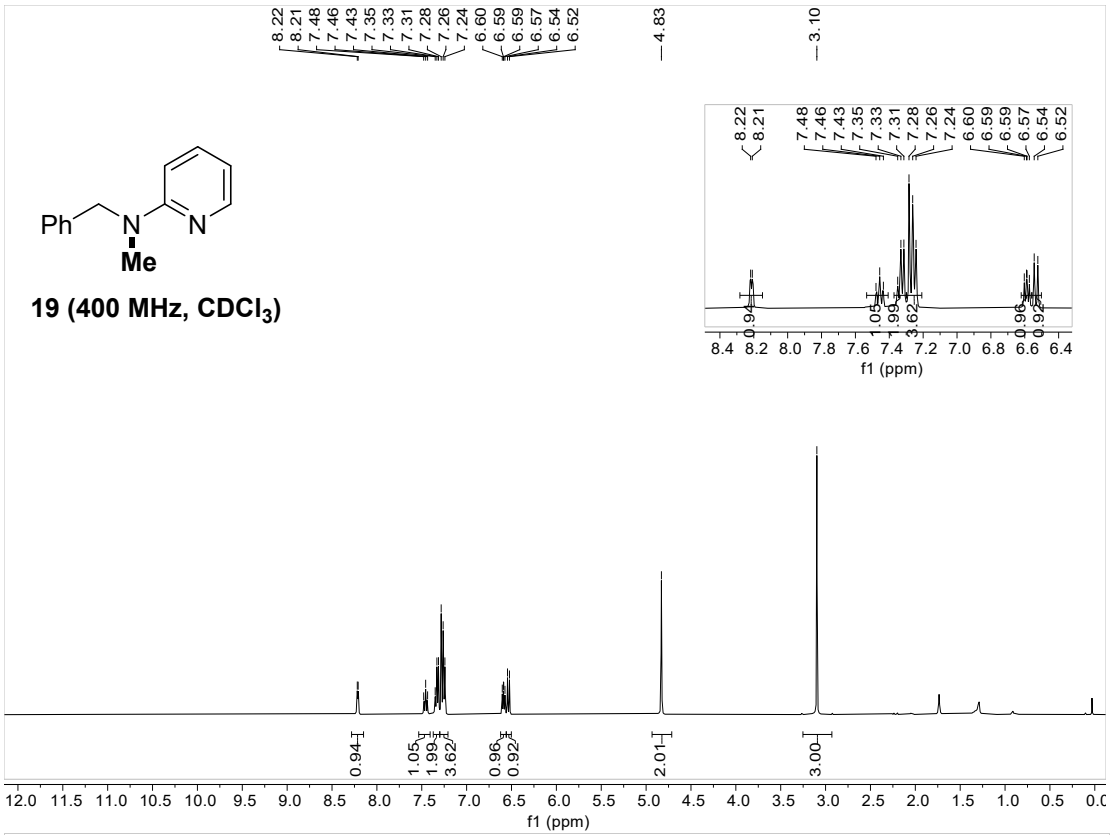

Ph
N
Me
16 (100 MHz, CDCl3)
f1 (ppm)


Et
Ph
N
Me
17 (400 MHz, CDCl3)
f1 (ppm)

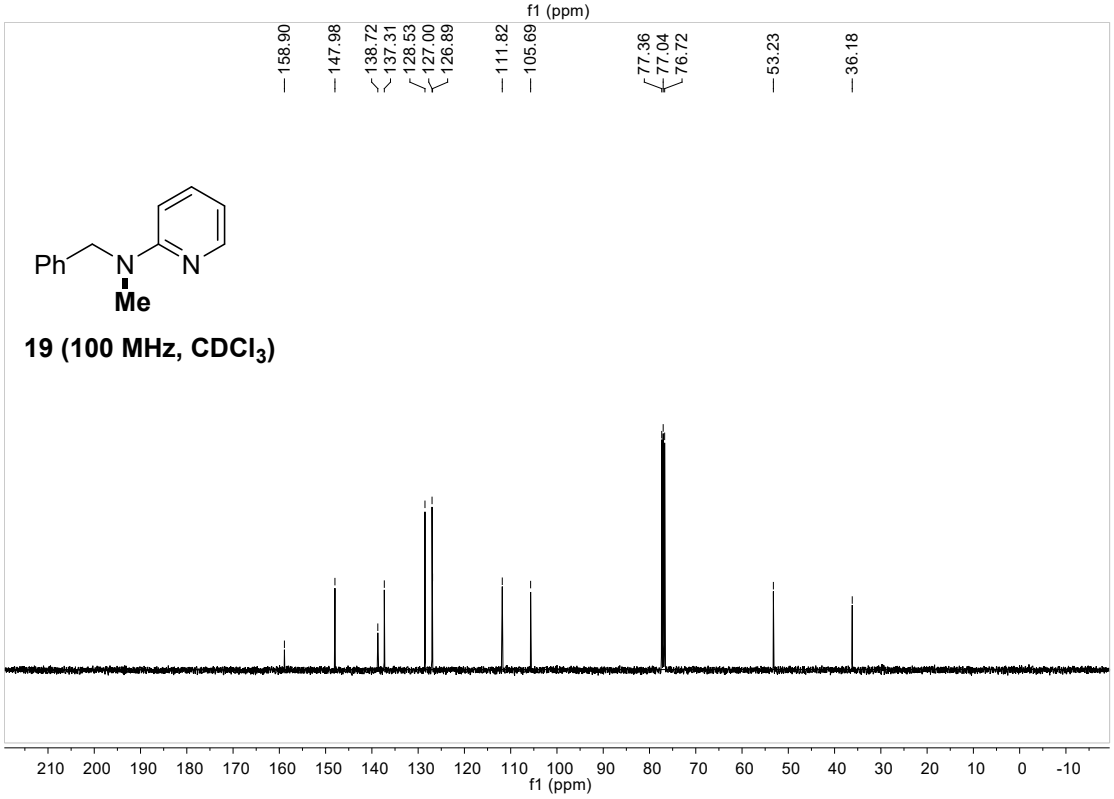

Et
Ph
N
Me
17 (100 MHz, CDCl3)
f1 (ppm)


7.60
7.58
7.57
7.55
7.50
7.48
7.27
7.26
7.15
7.13
7.11
7.11
6.88
6.87
6.85
6.84
6.83
6.82
4.59
2.54
Ph
N
Me
18 (400 MHz, CDCl3)
3.27
2.01
1.19
3.02
3.14
2.05
3.02
f1 (ppm)

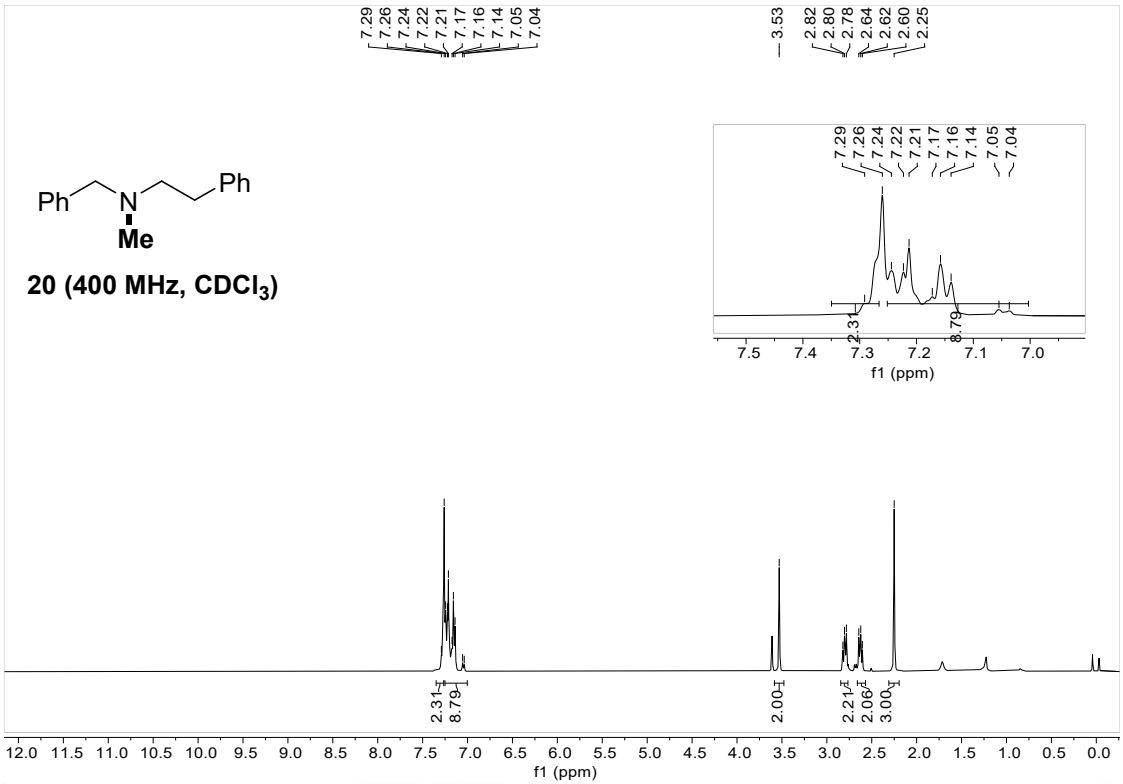

144.09
140.89
134.91
129.23
128.60
127.99
127.74
127.69
127.03
126.37
125.83
122.51
118.27
108.66
77.40
77.09
76.77
65.39
54.20
Ph
N
Me
18 (100 MHz, CDCl3)
f1 (ppm)



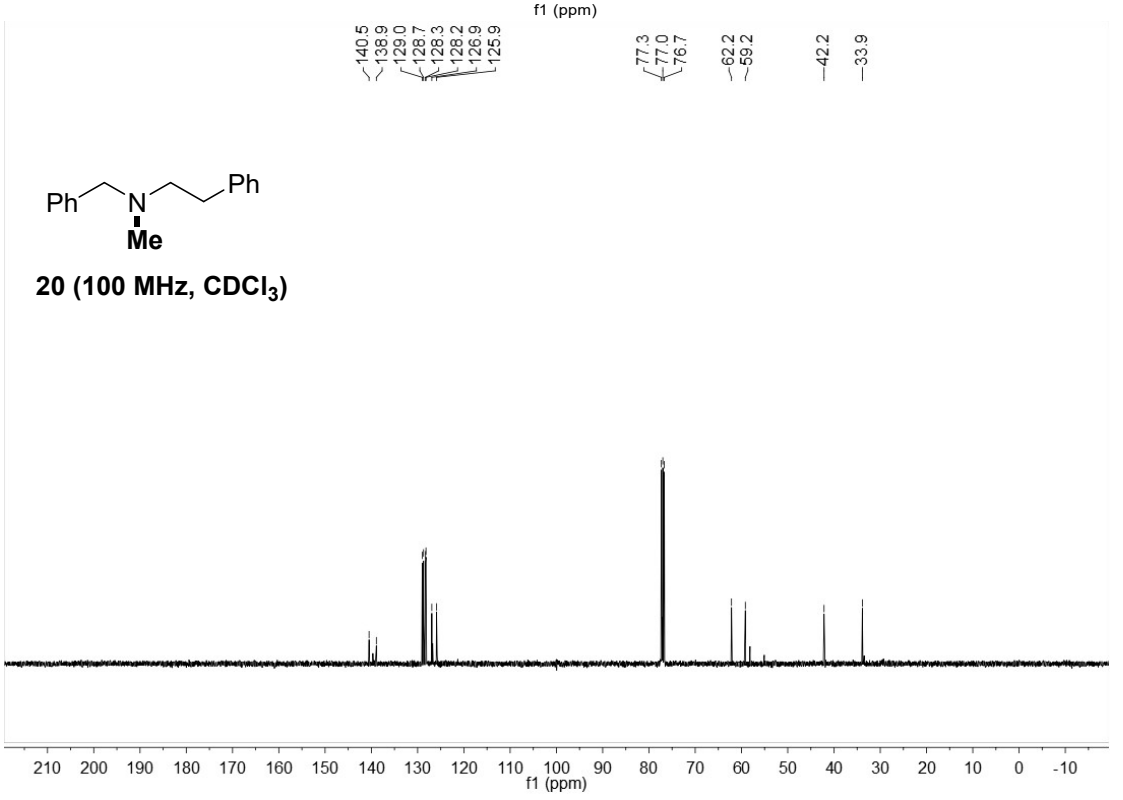
19 (400 MHz, $CDCl_3$)



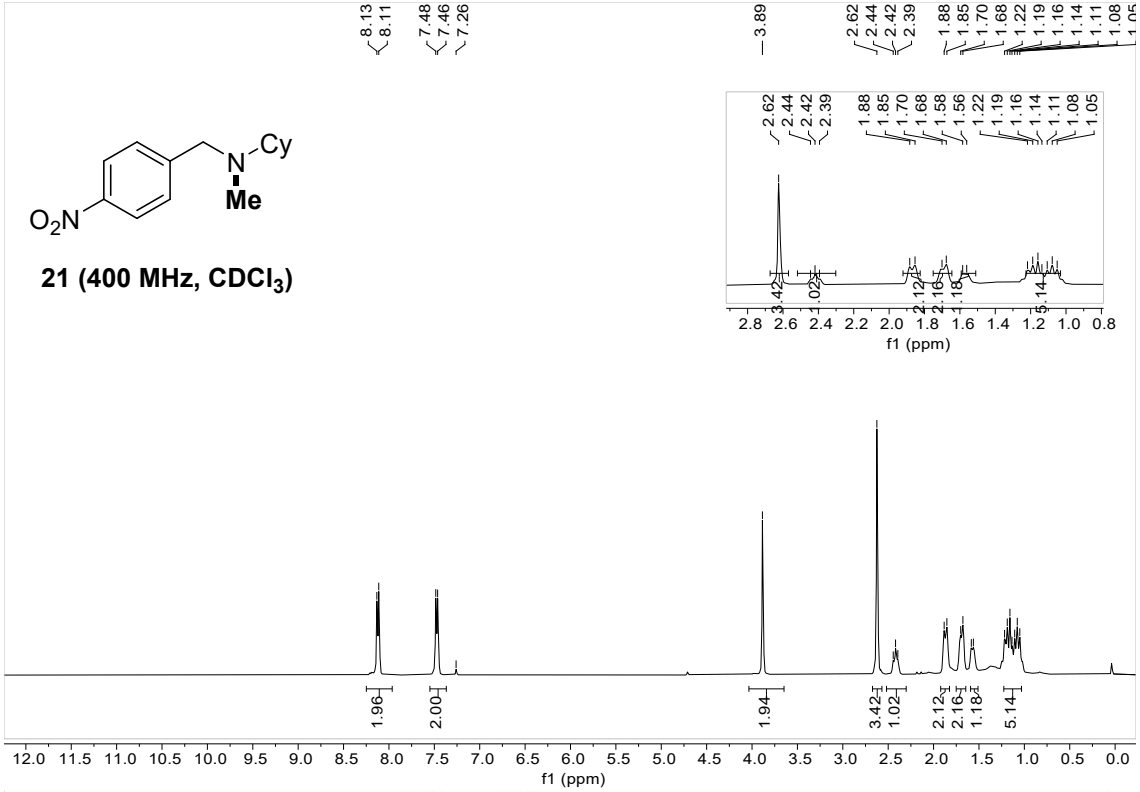
19 (100 MHz, $CDCl_3$)



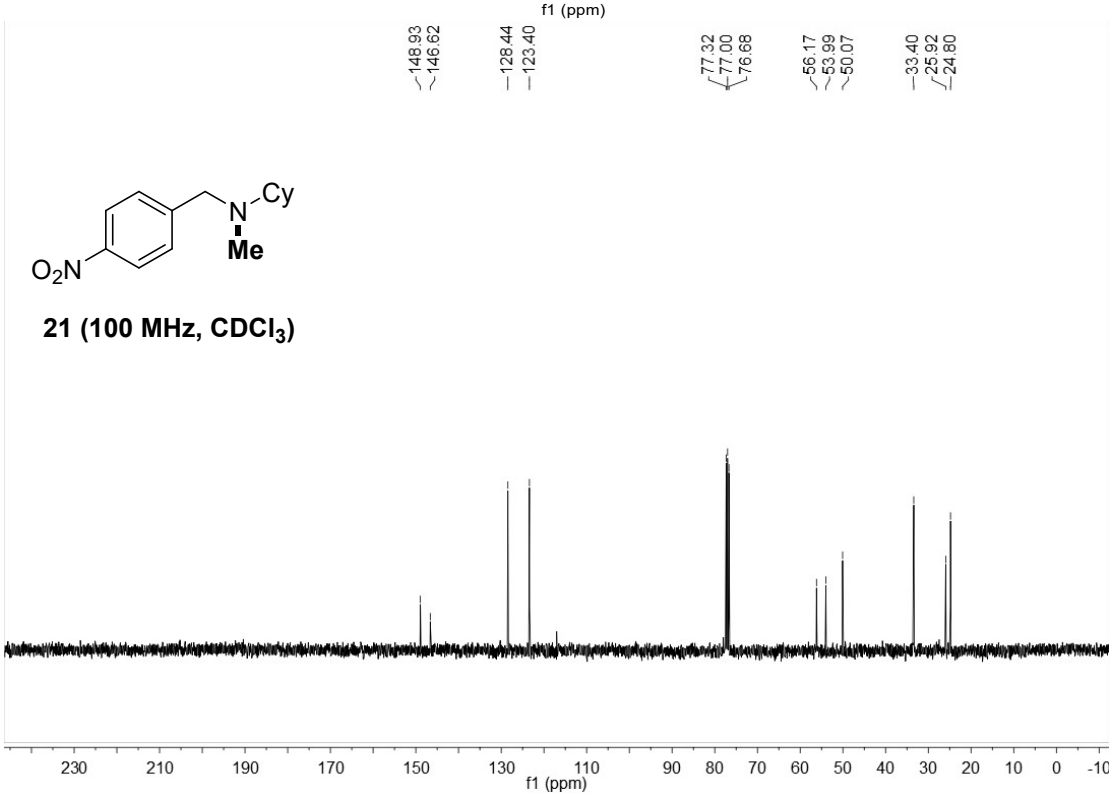
20 (400 MHz, $CDCl_3$)



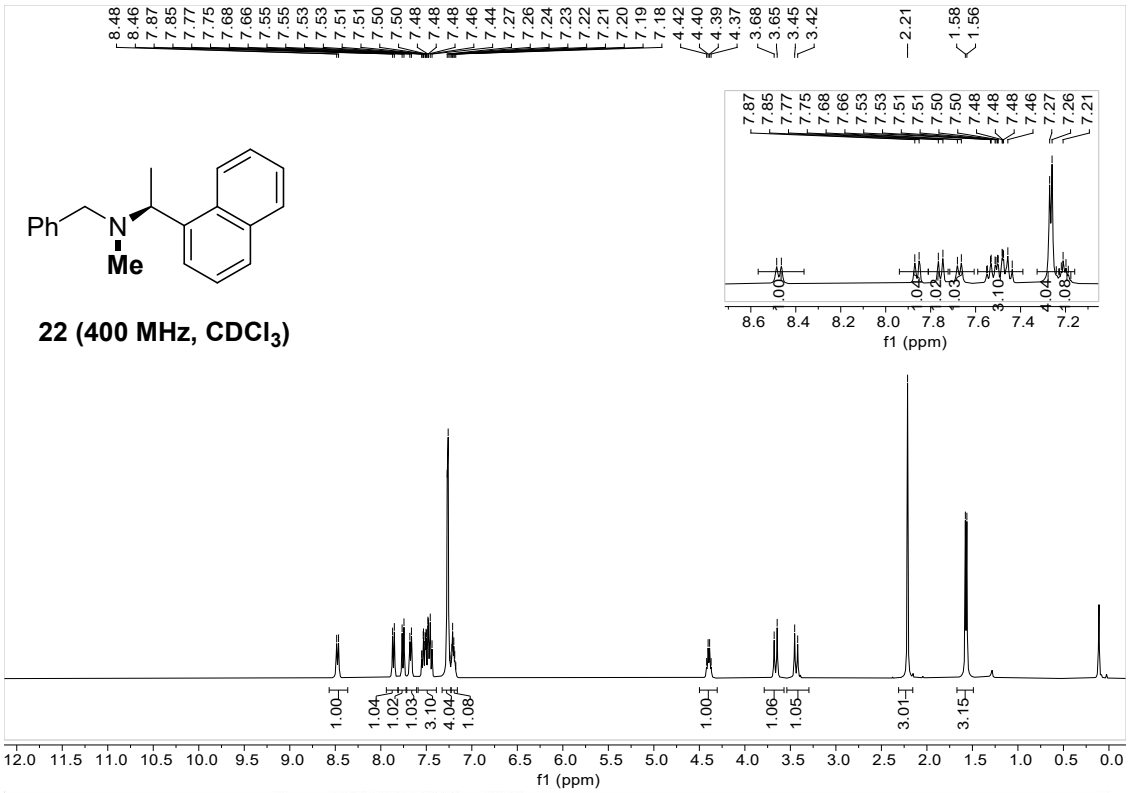
20 (100 MHz, $CDCl_3$)



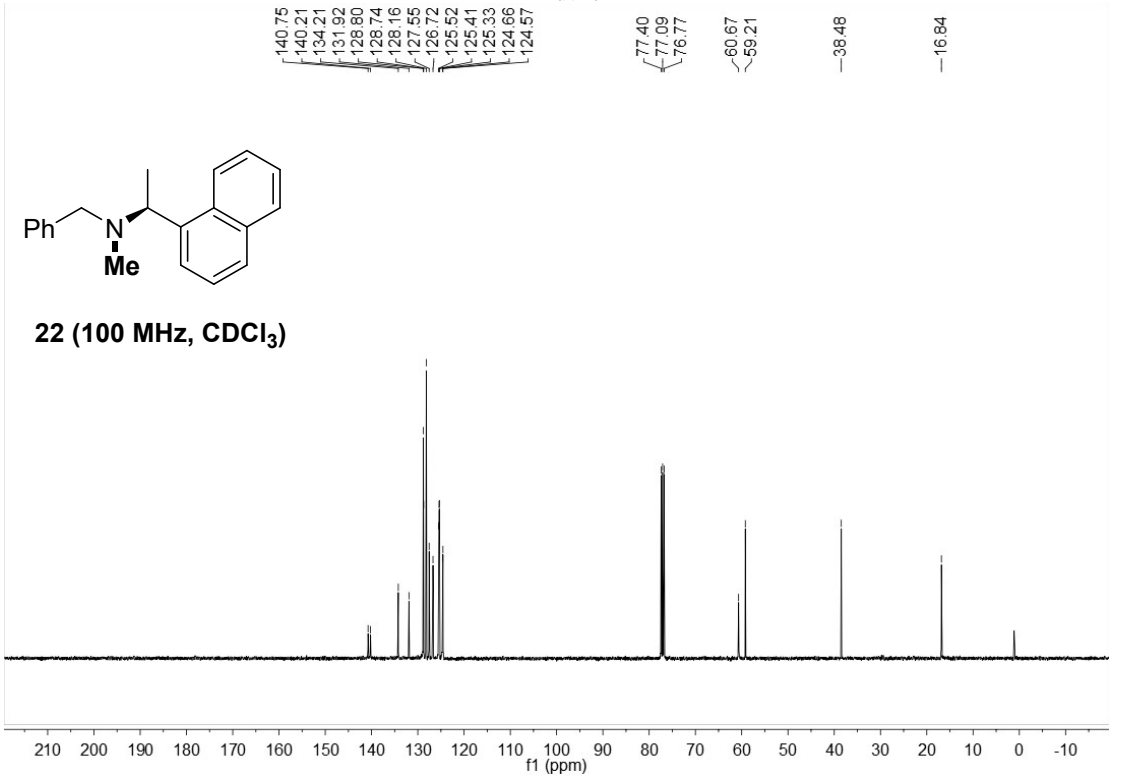
21 (400 MHz, $CDCl_3$)



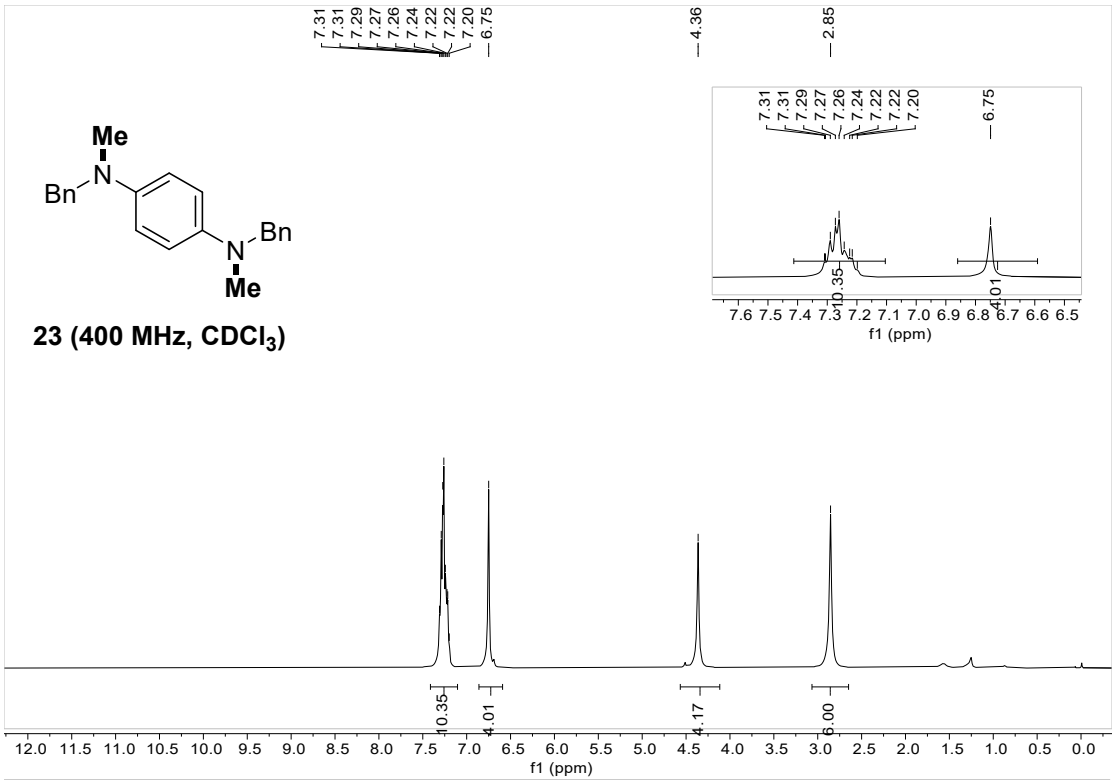
21 (100 MHz, $CDCl_3$)



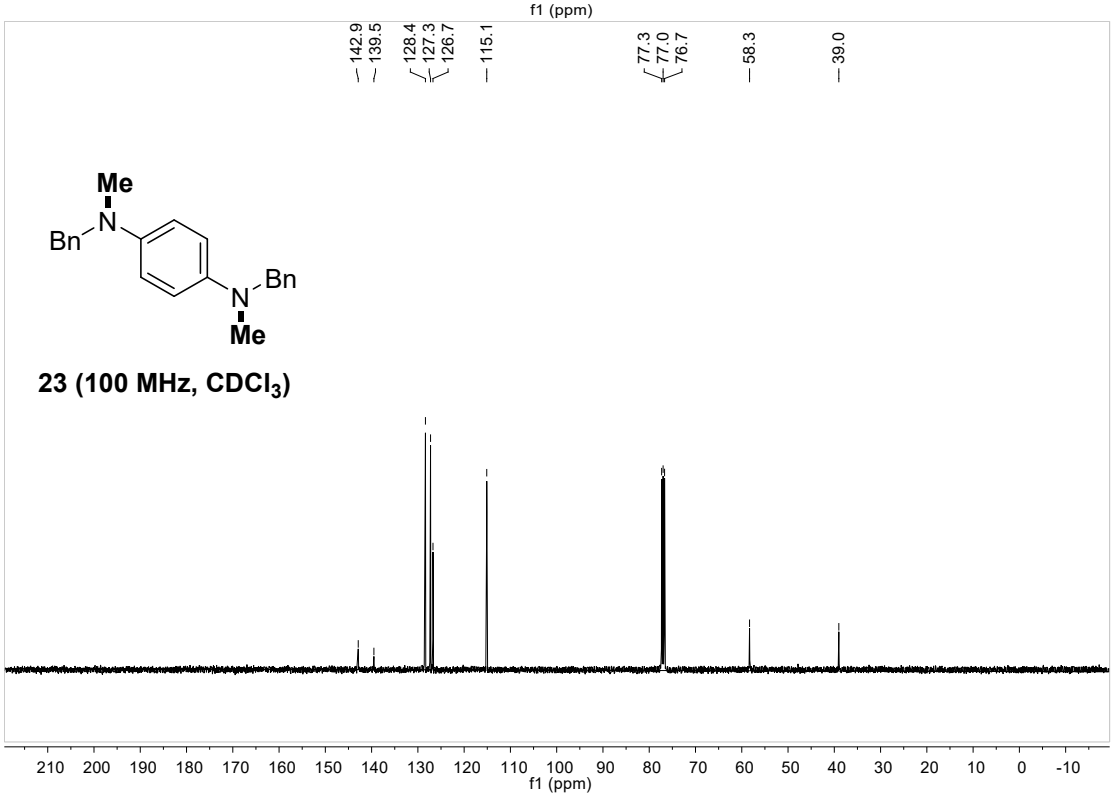
22 (400 MHz, $CDCl_3$)



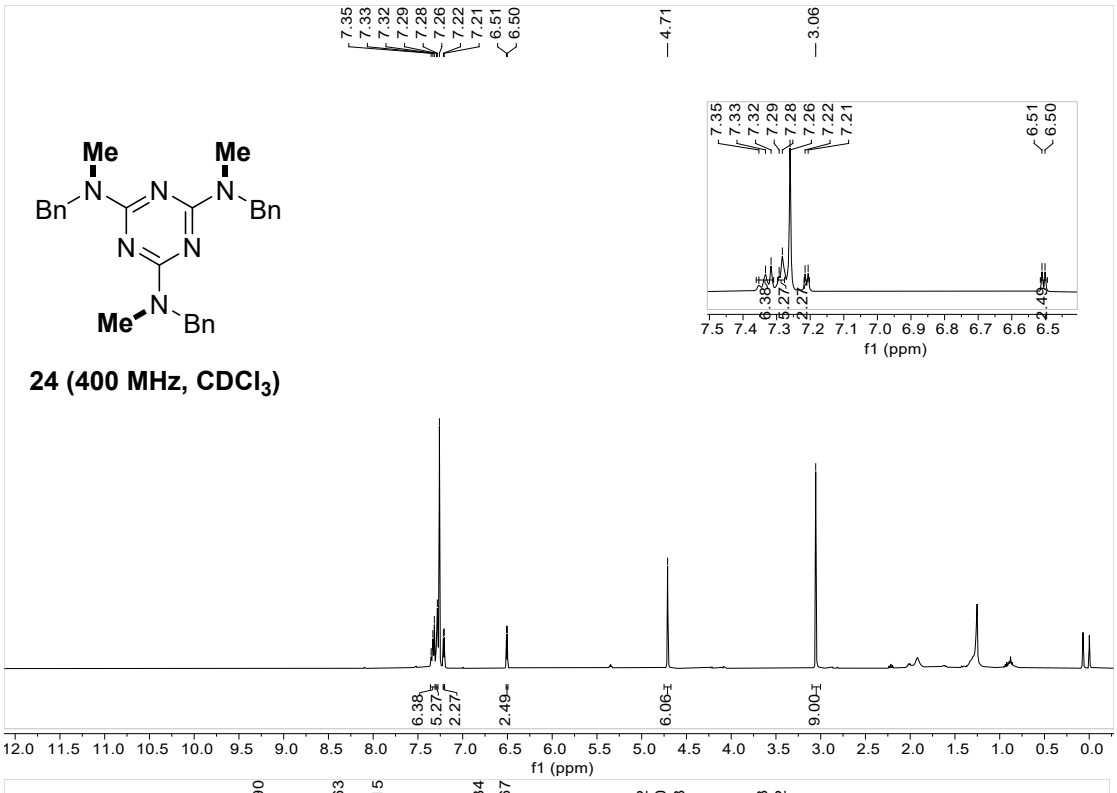
22 (100 MHz, $CDCl_3$)



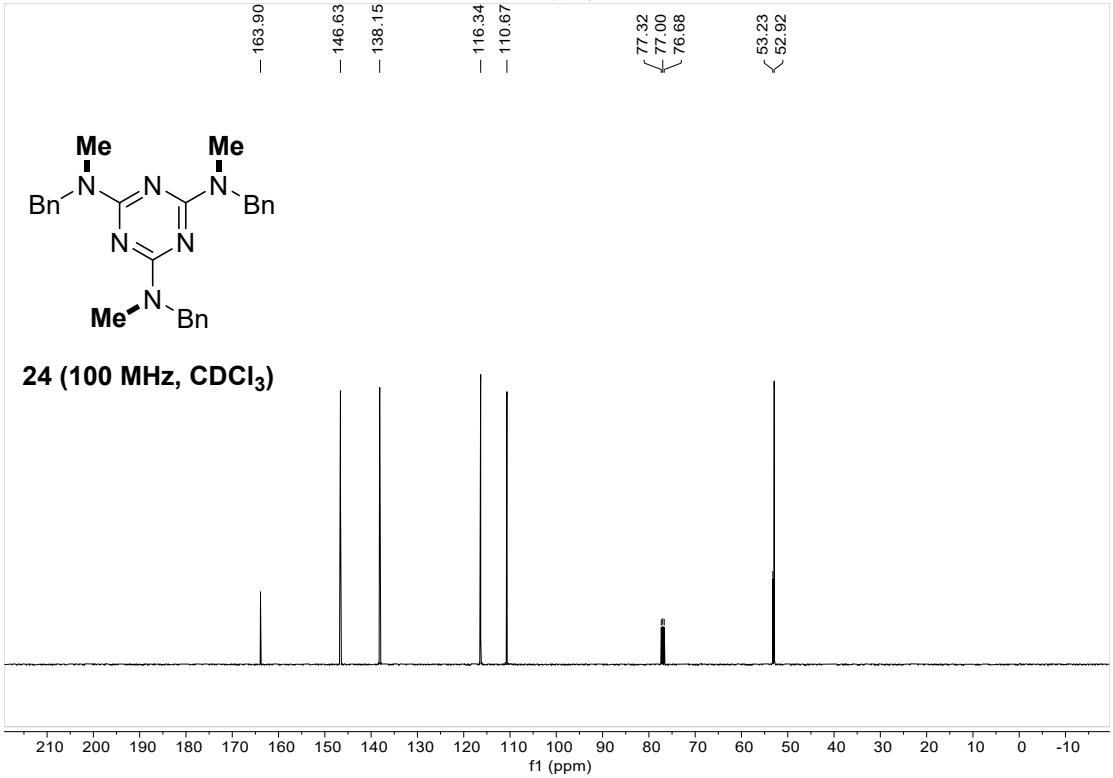
23 (400 MHz, $CDCl_3$)



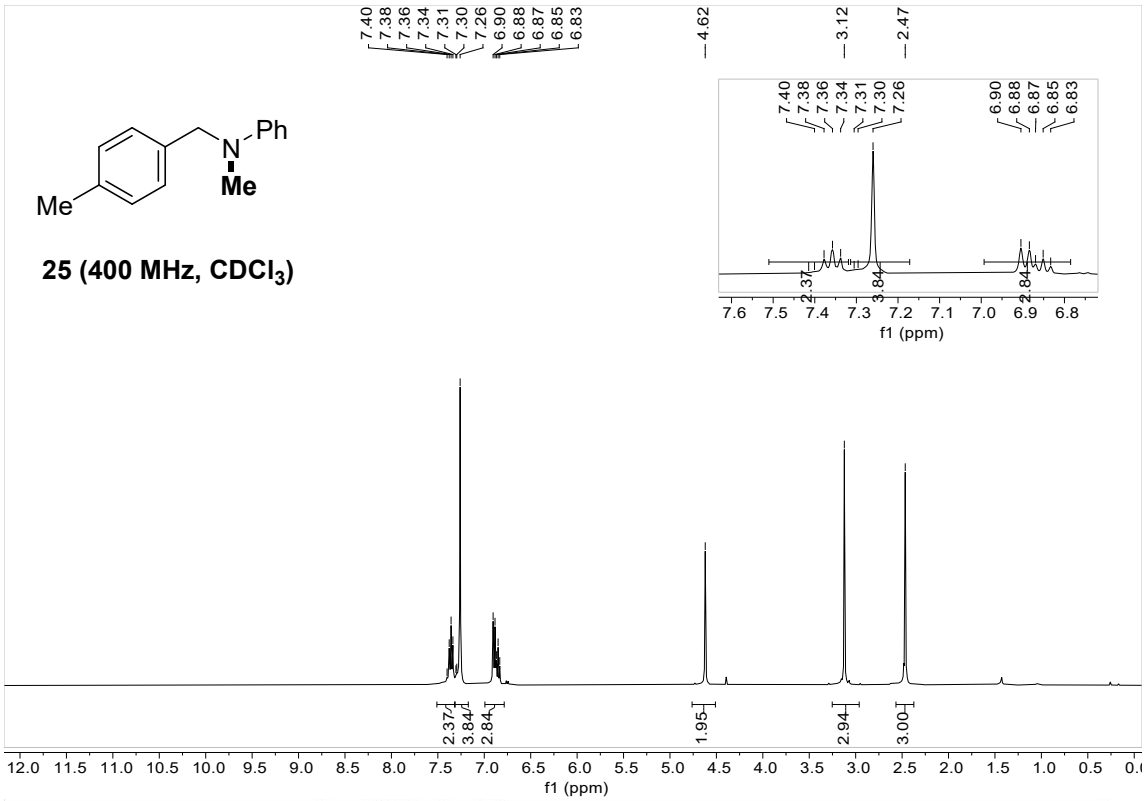
23 (100 MHz, $CDCl_3$)



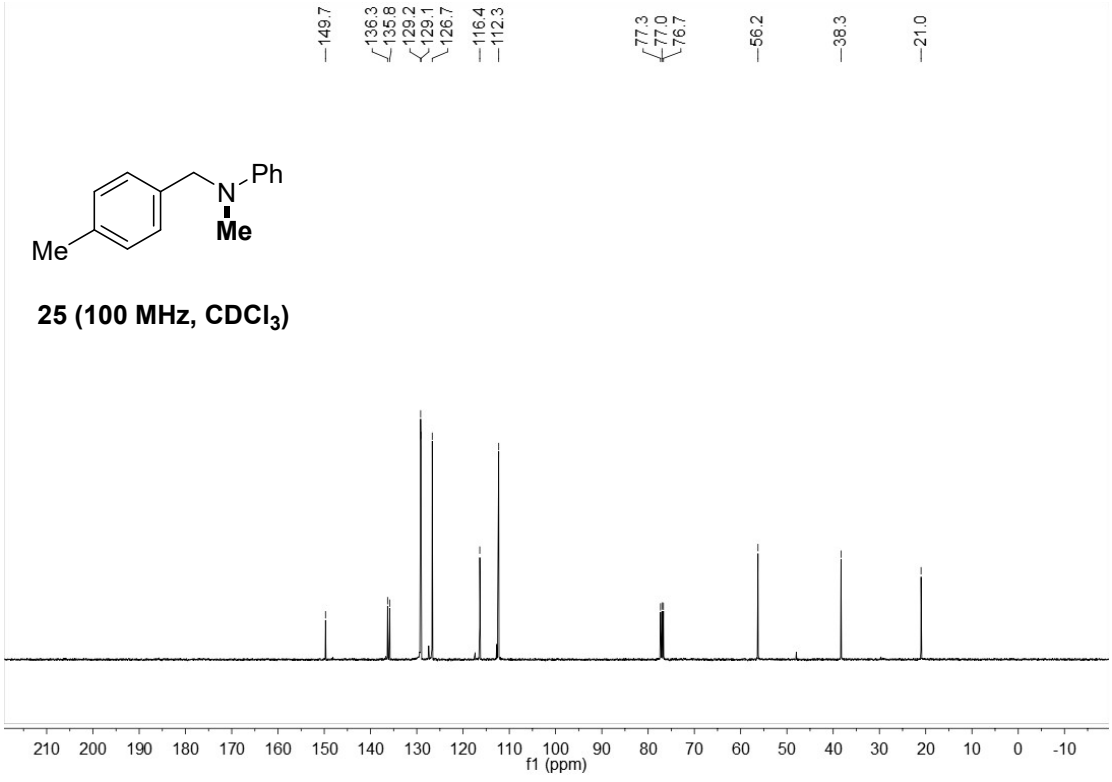
24 (400 MHz, $CDCl_3$)



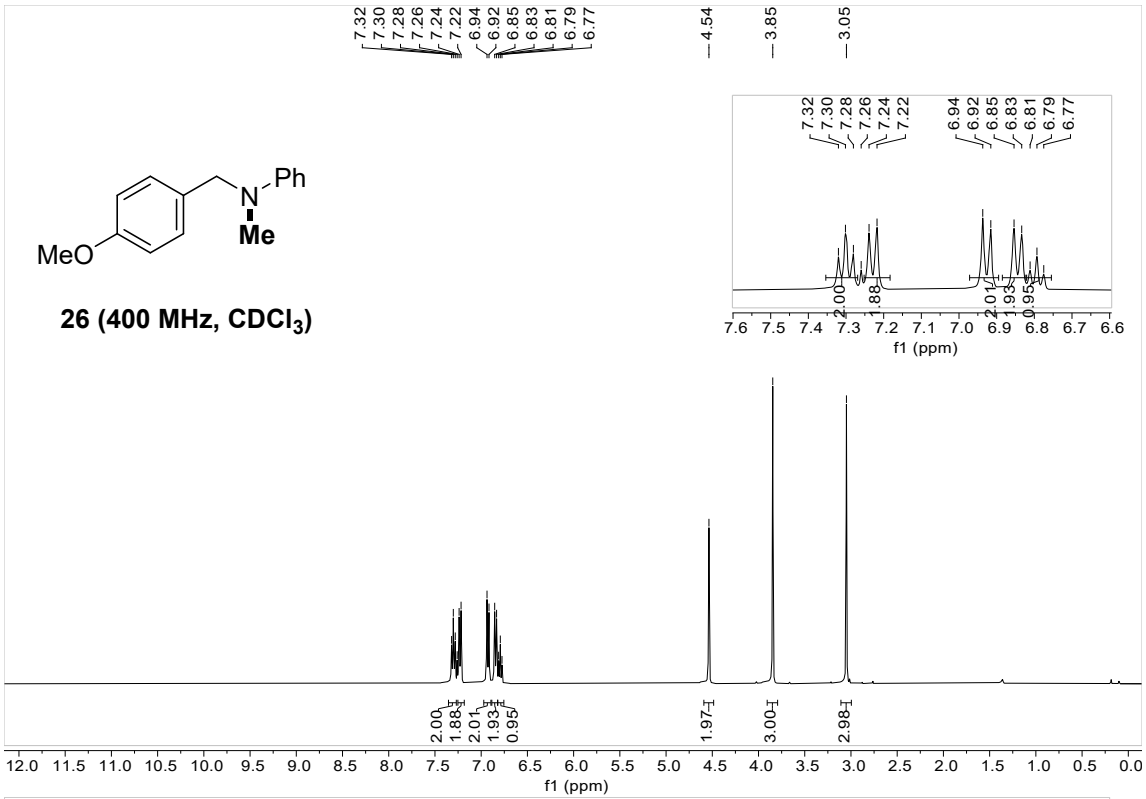
24 (100 MHz, $CDCl_3$)



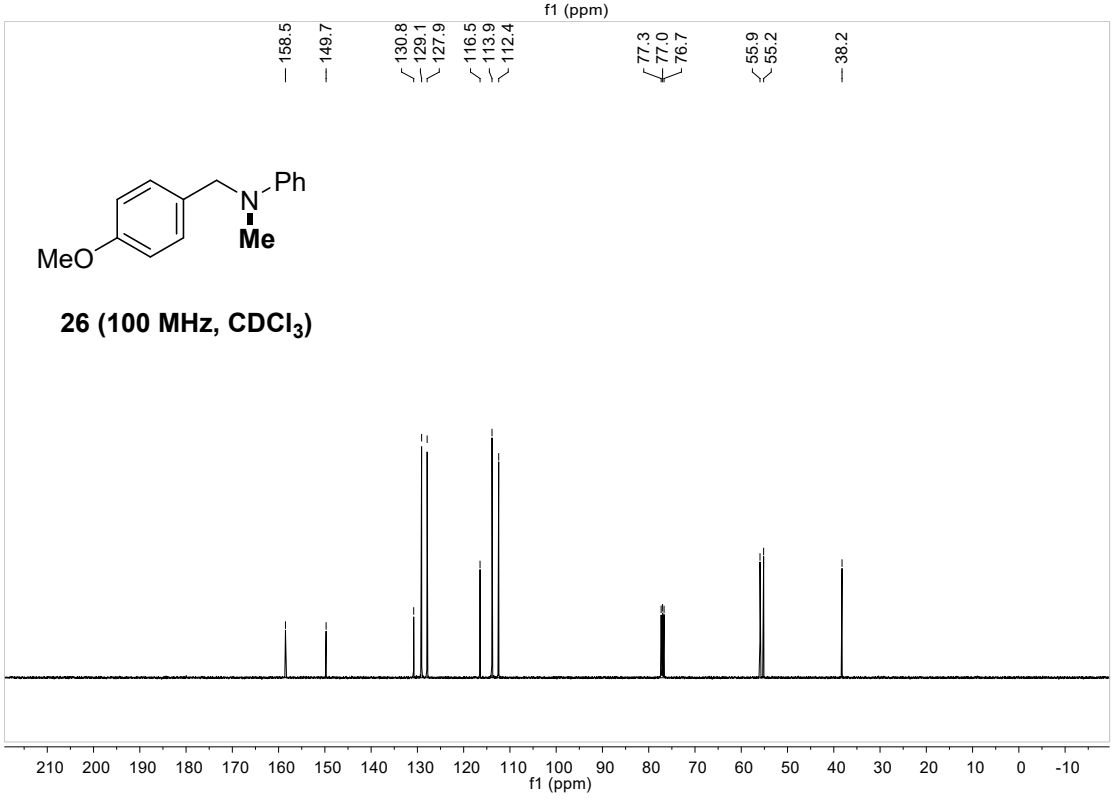
25 (400 MHz, $CDCl_3$)



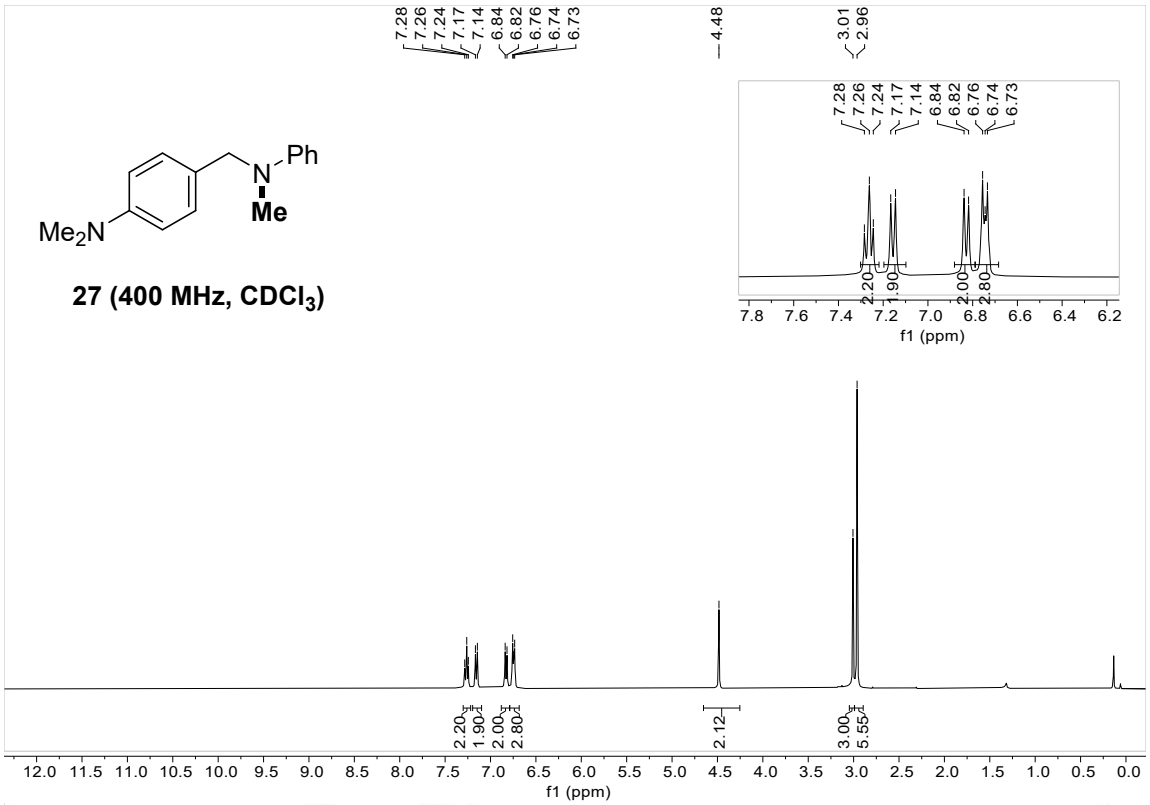
25 (100 MHz, $CDCl_3$)



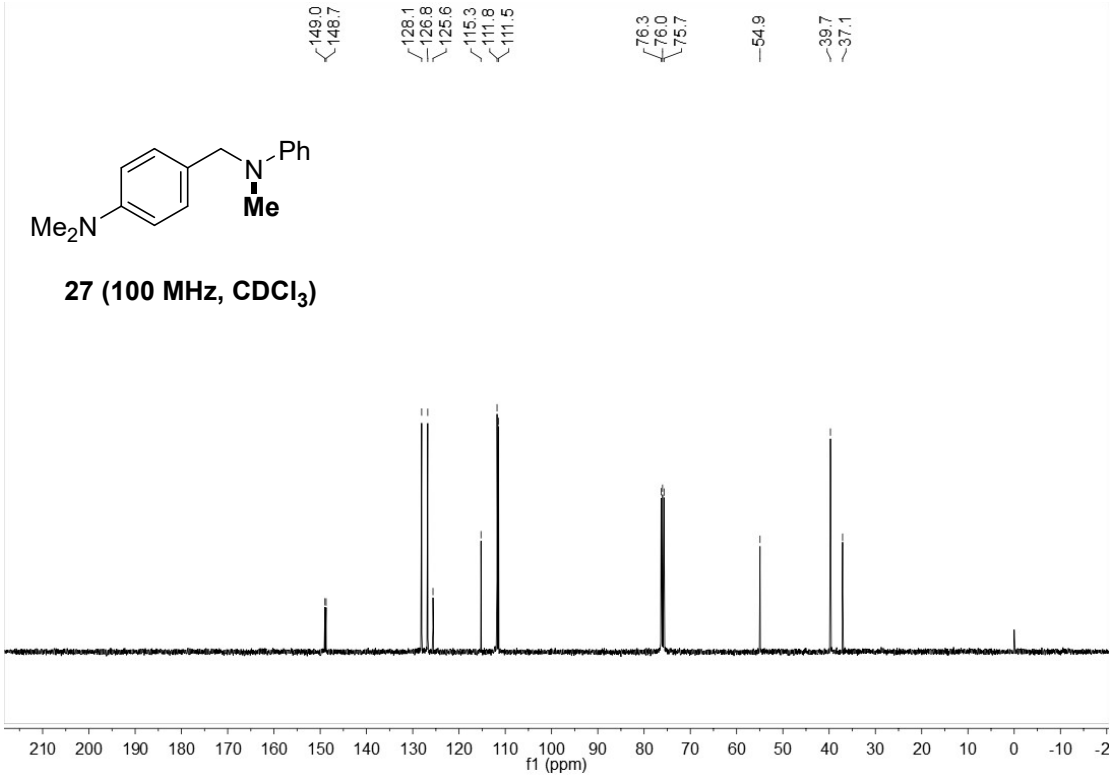
26 (400 MHz, $CDCl_3$)



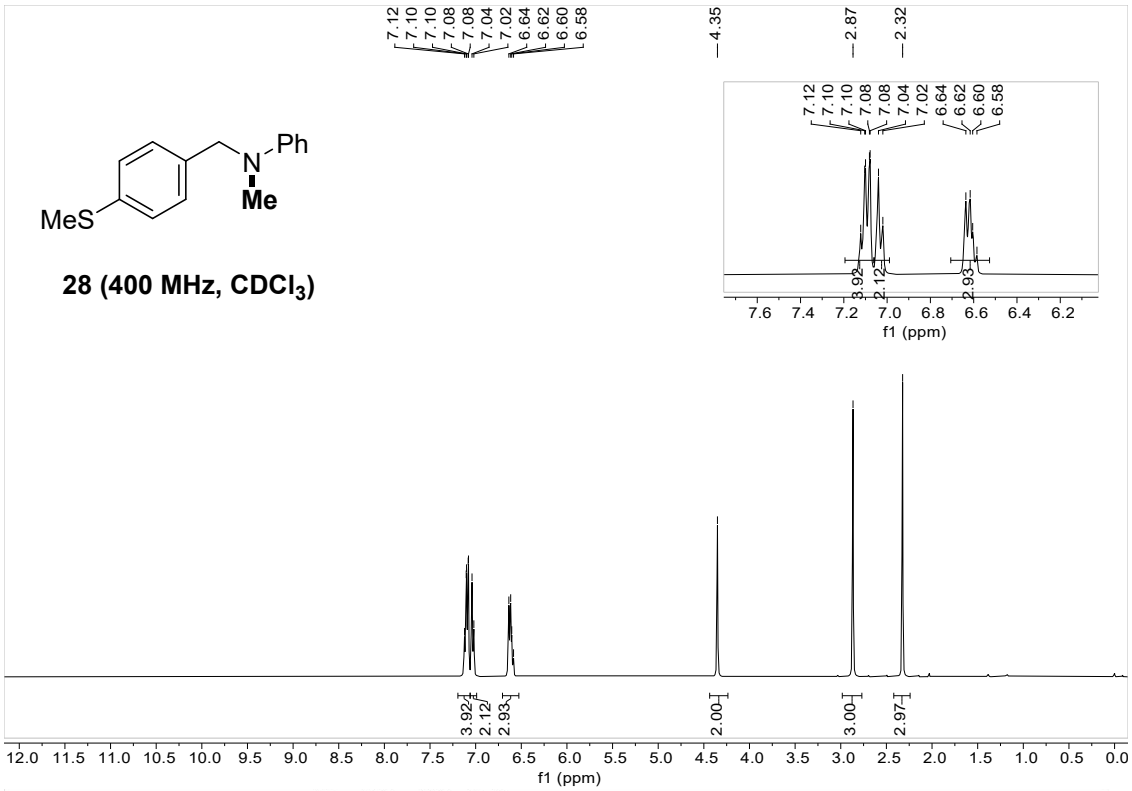
26 (100 MHz, $CDCl_3$)



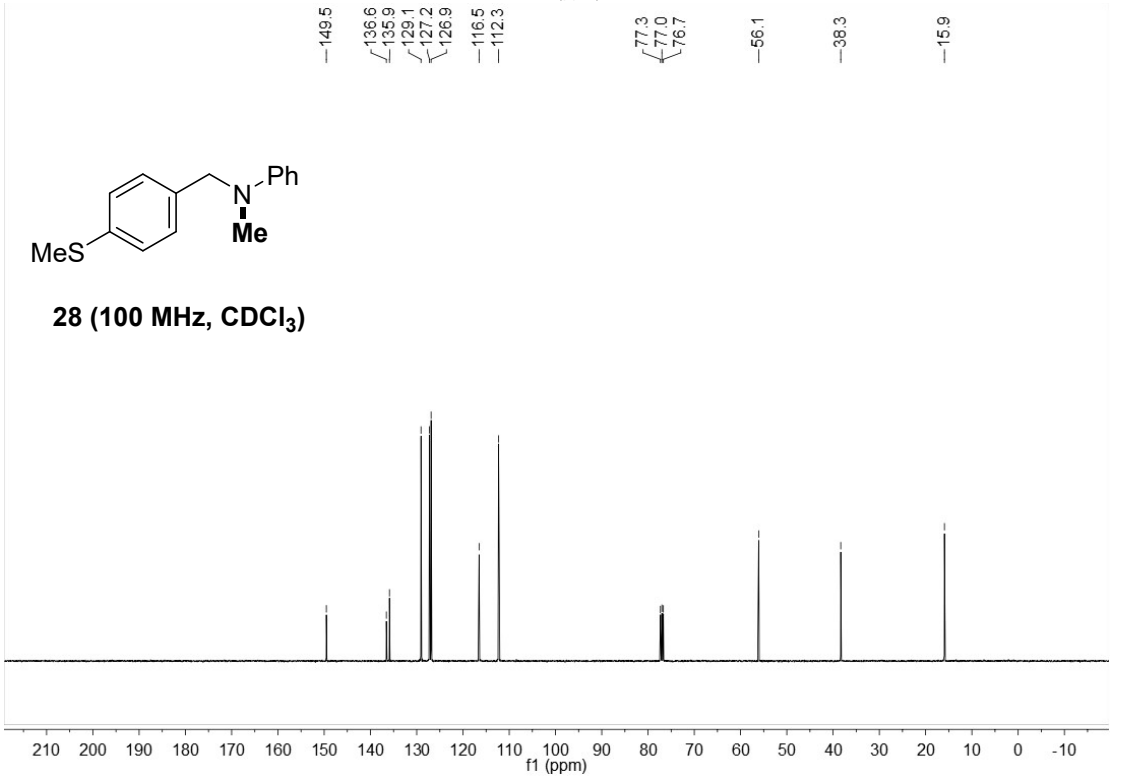
27 (400 MHz, $CDCl_3$)



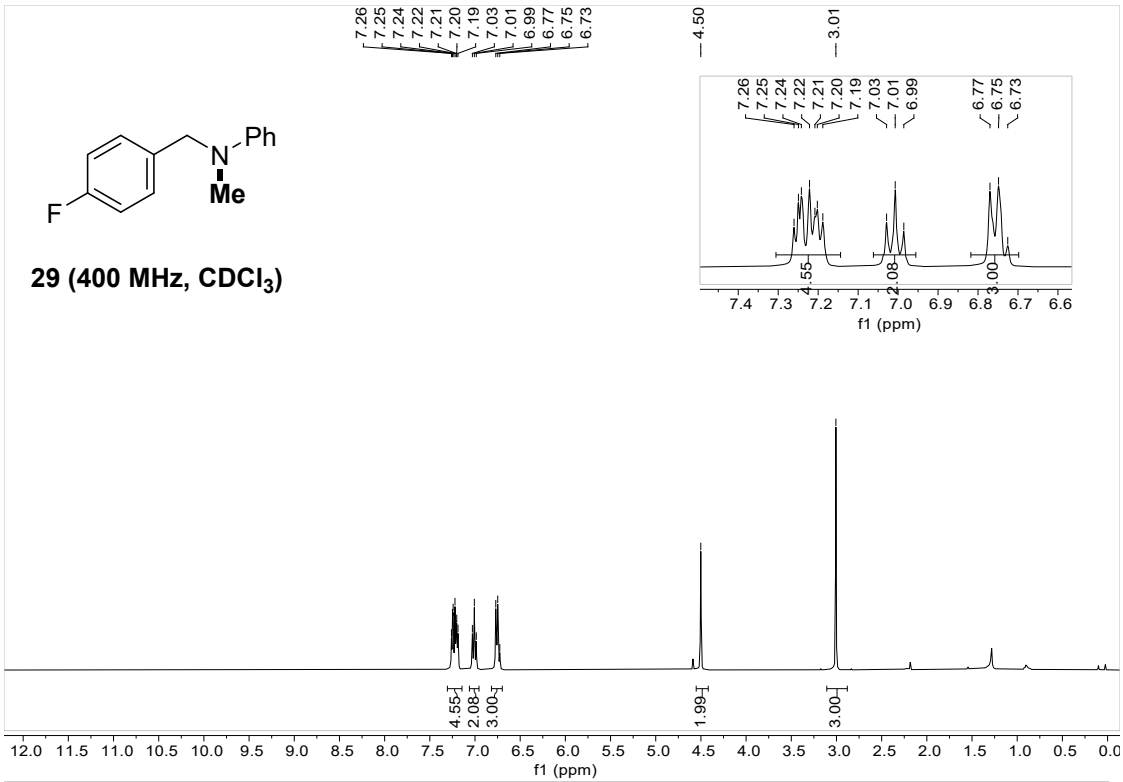
27 (100 MHz, $CDCl_3$)



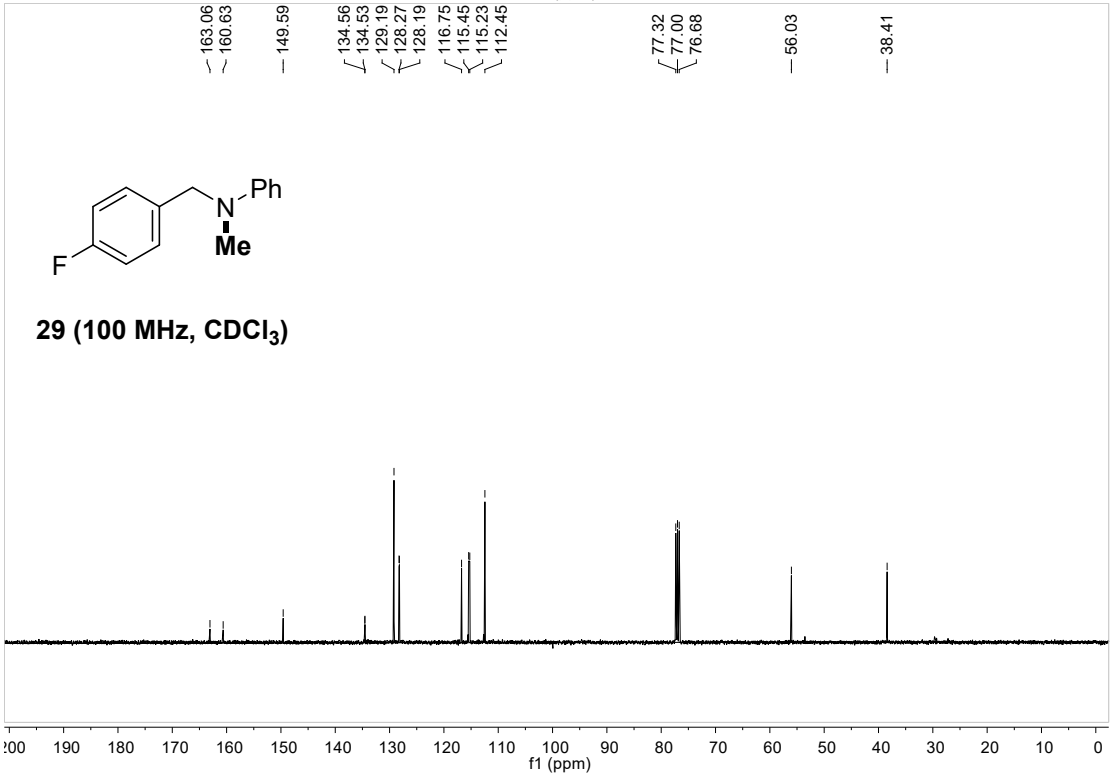
28 (400 MHz, $CDCl_3$)



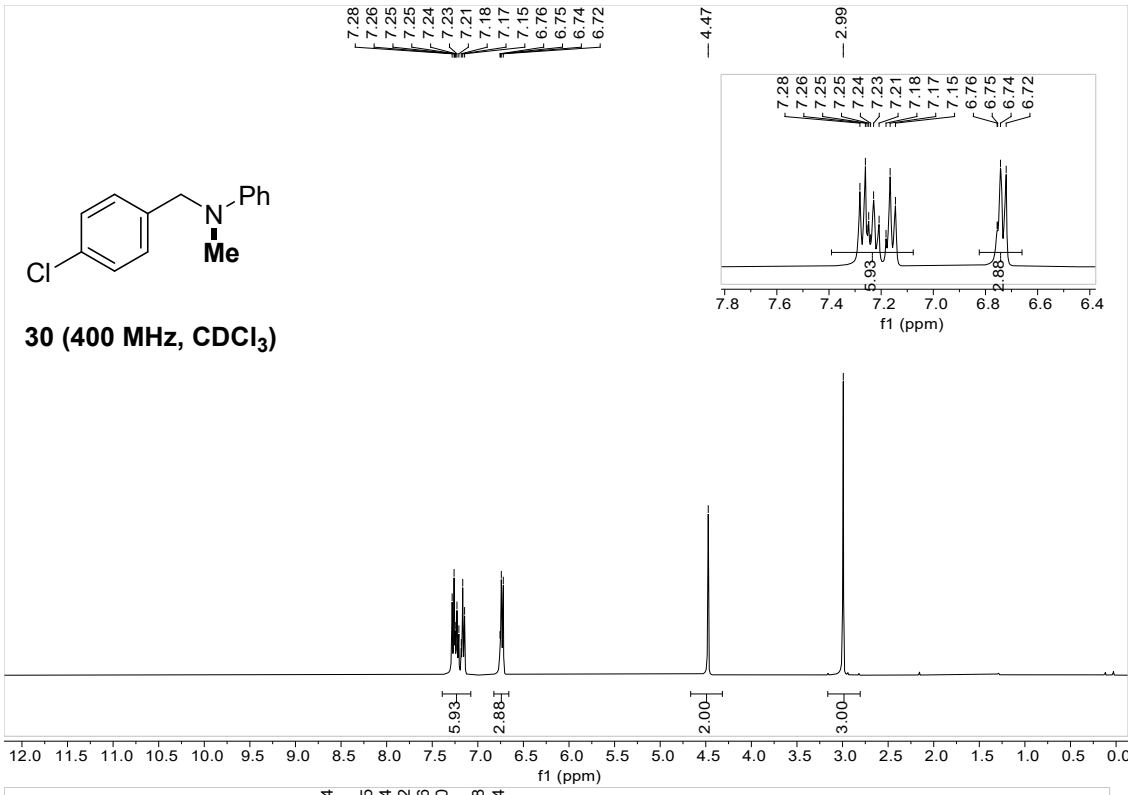
28 (100 MHz, $CDCl_3$)



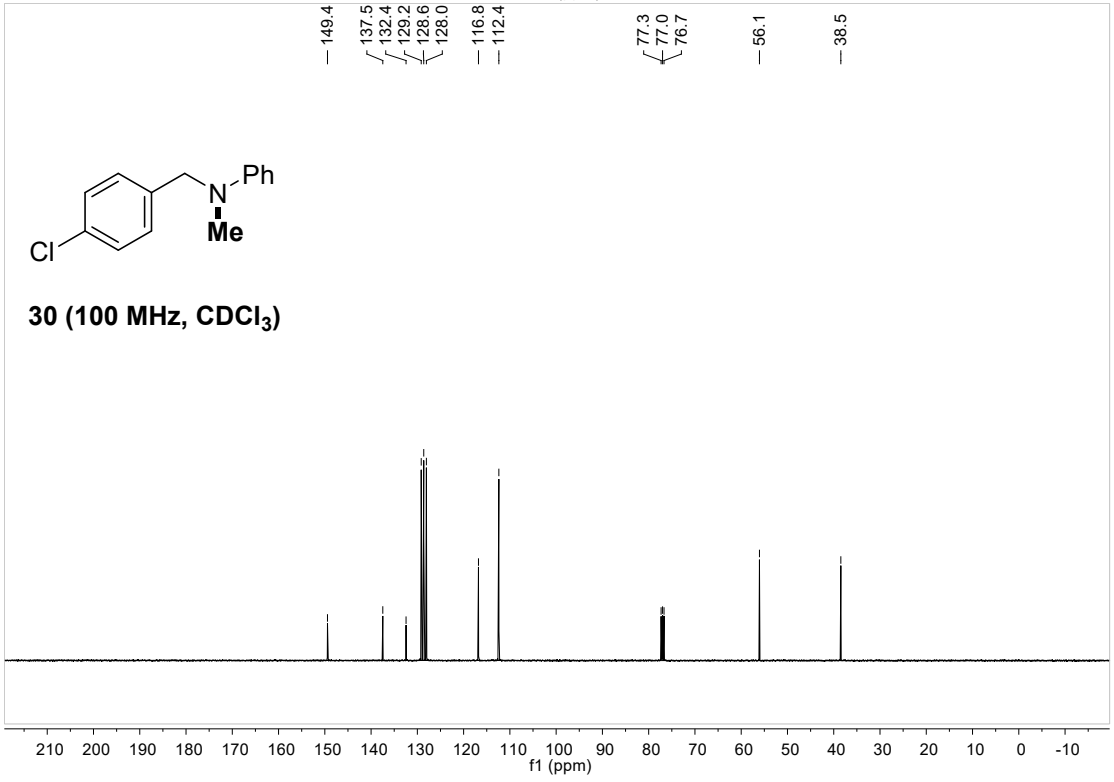
29 (400 MHz, $CDCl_3$)



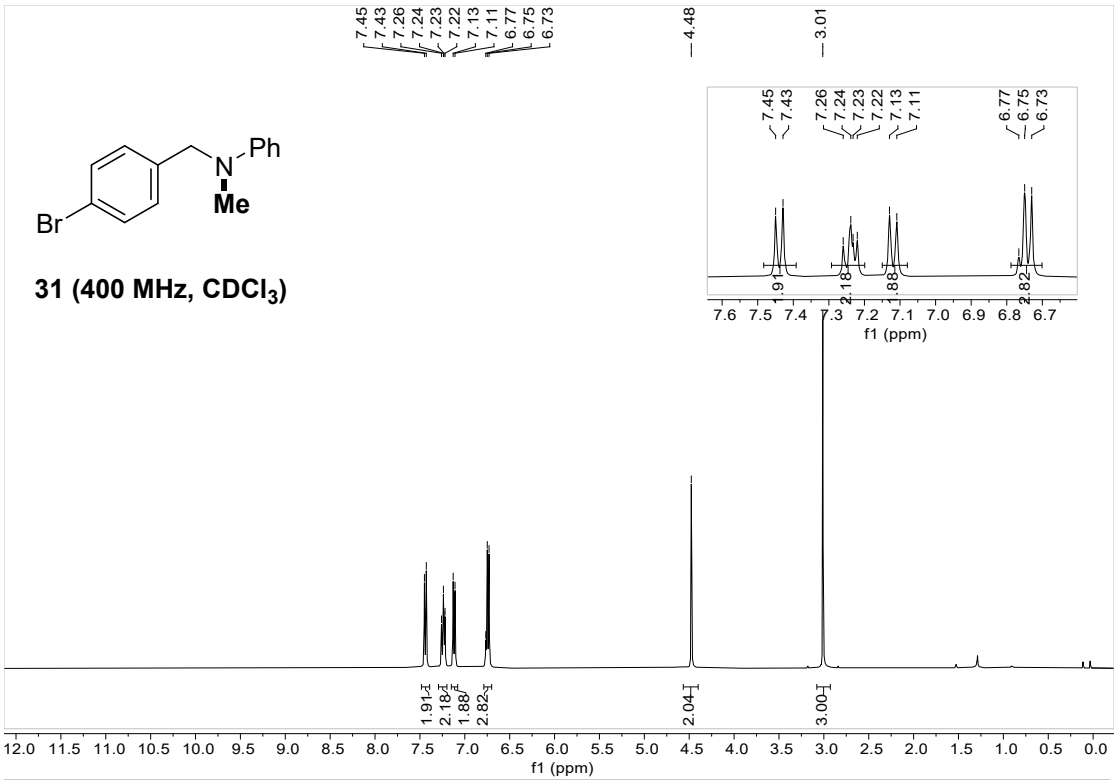
29 (100 MHz, $CDCl_3$)



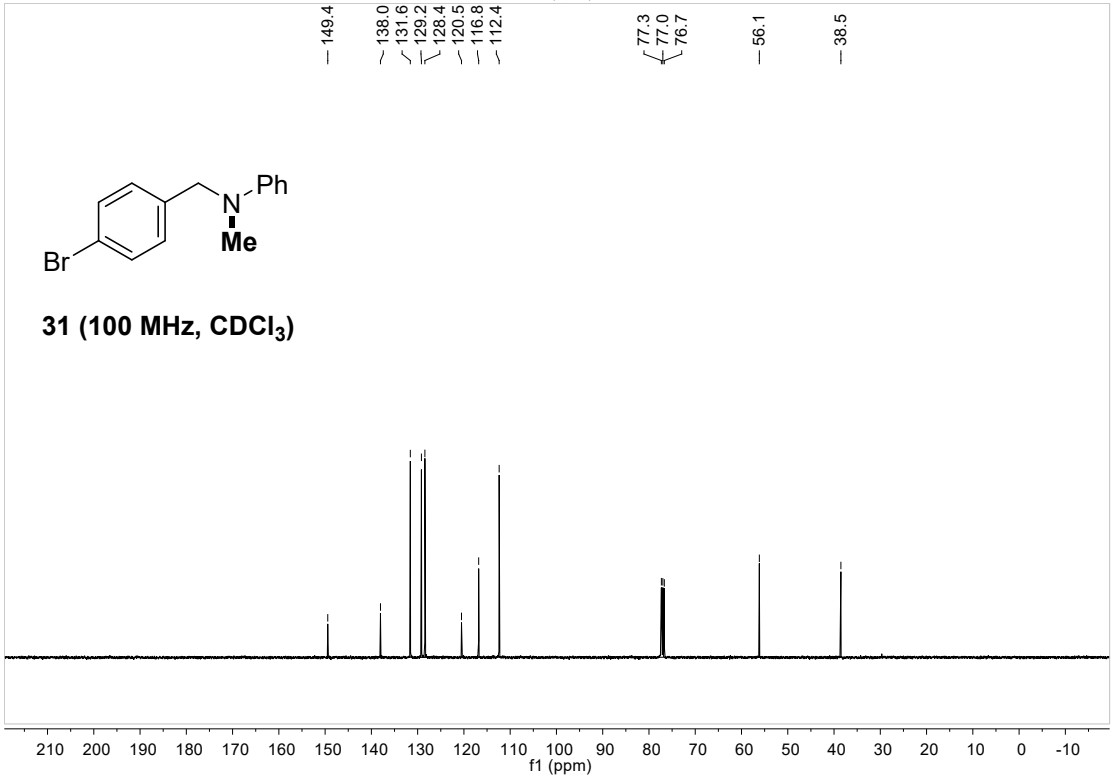
30 (400 MHz, $CDCl_3$)



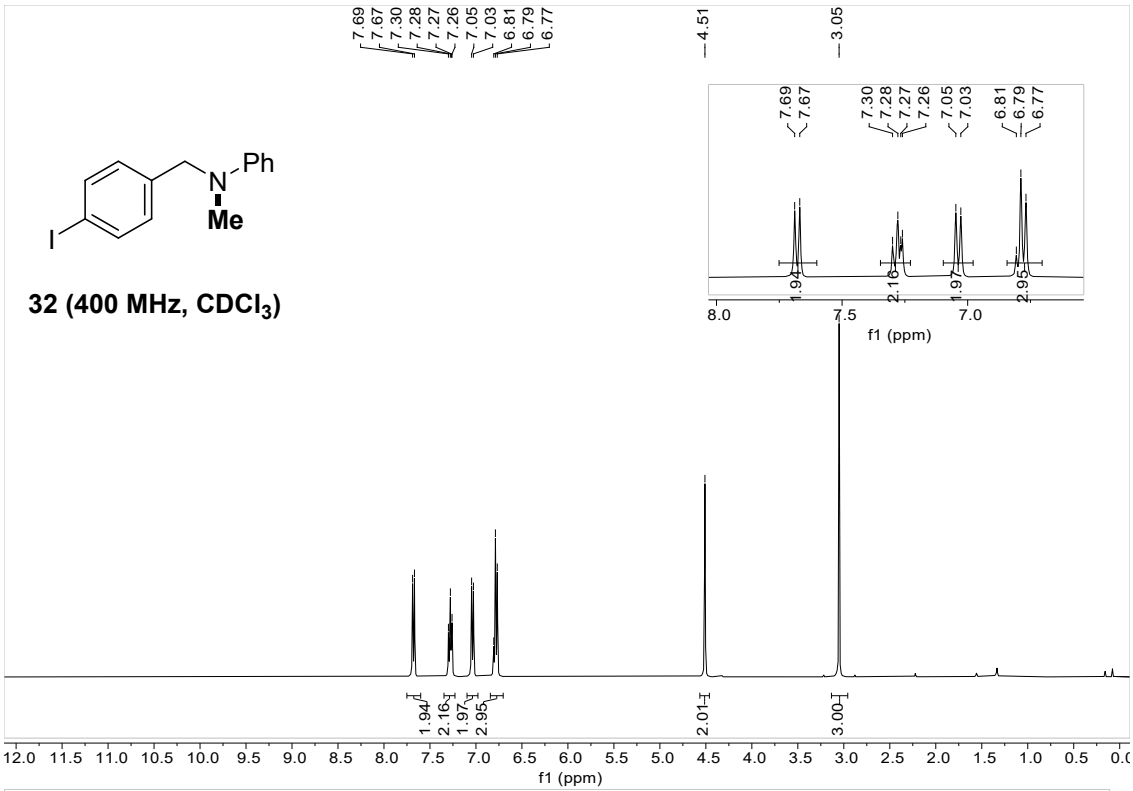
30 (100 MHz, $CDCl_3$)



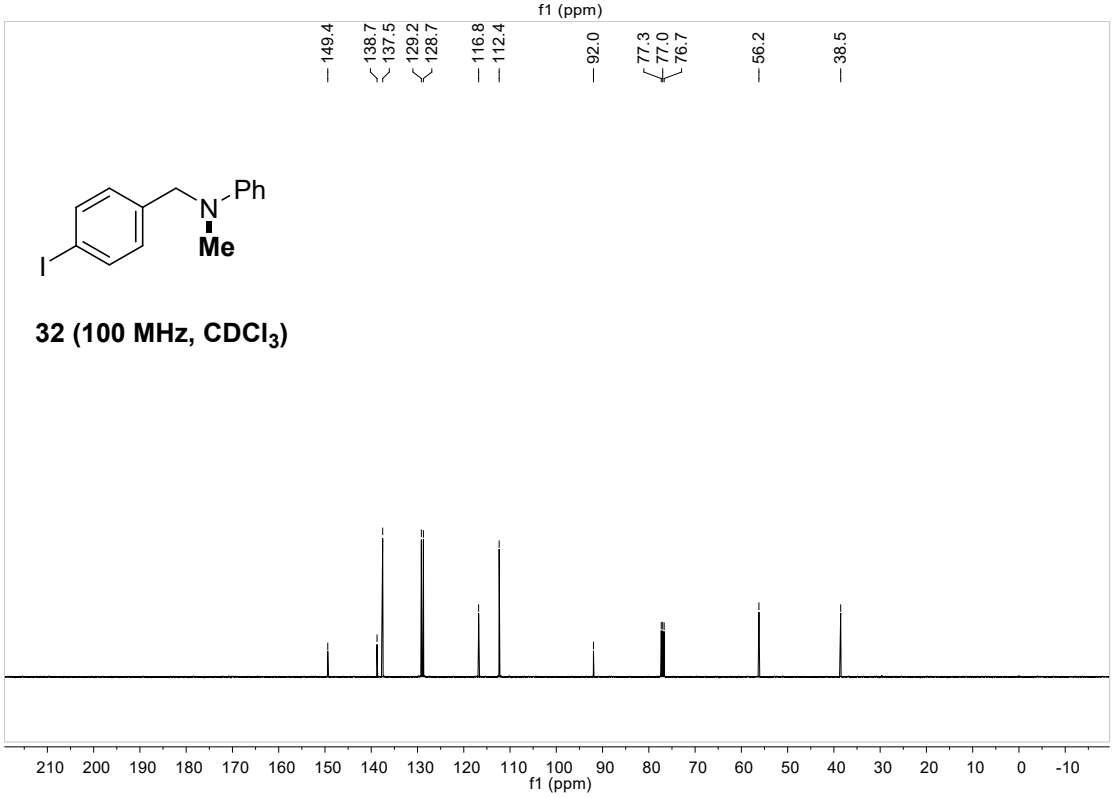
31 (400 MHz, $CDCl_3$)



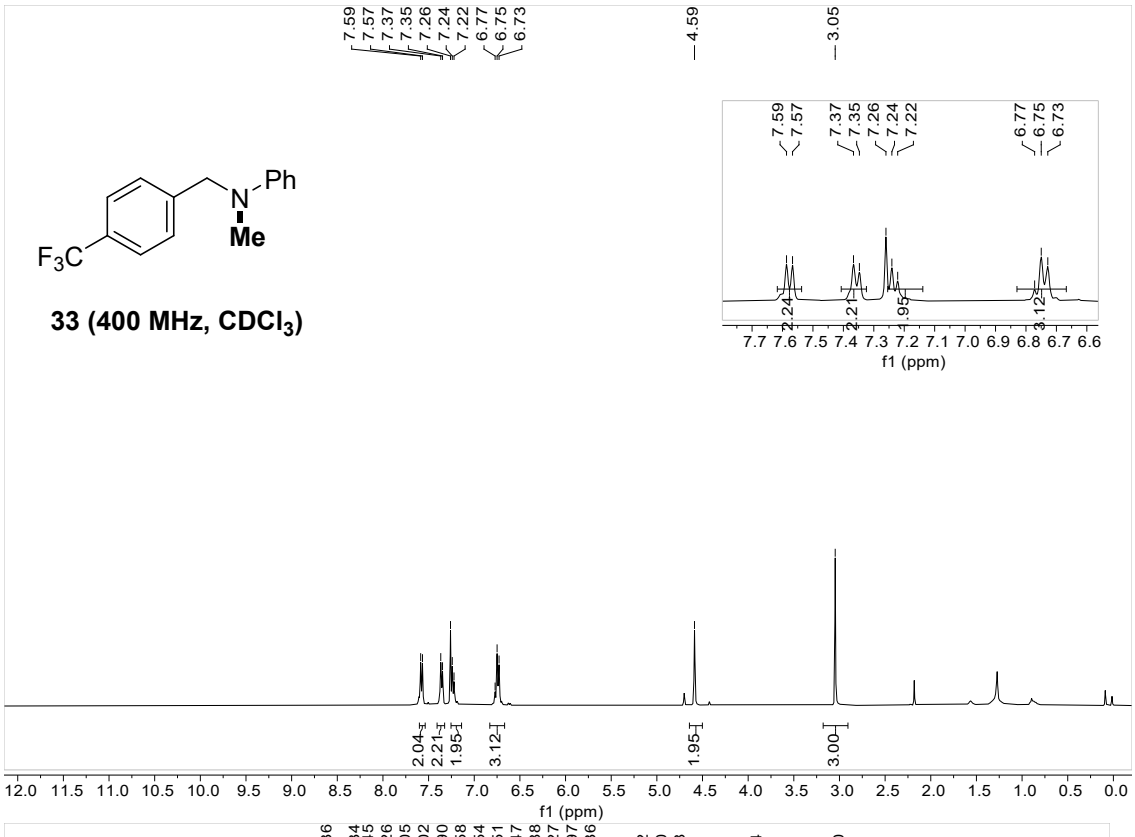
31 (100 MHz, $CDCl_3$)

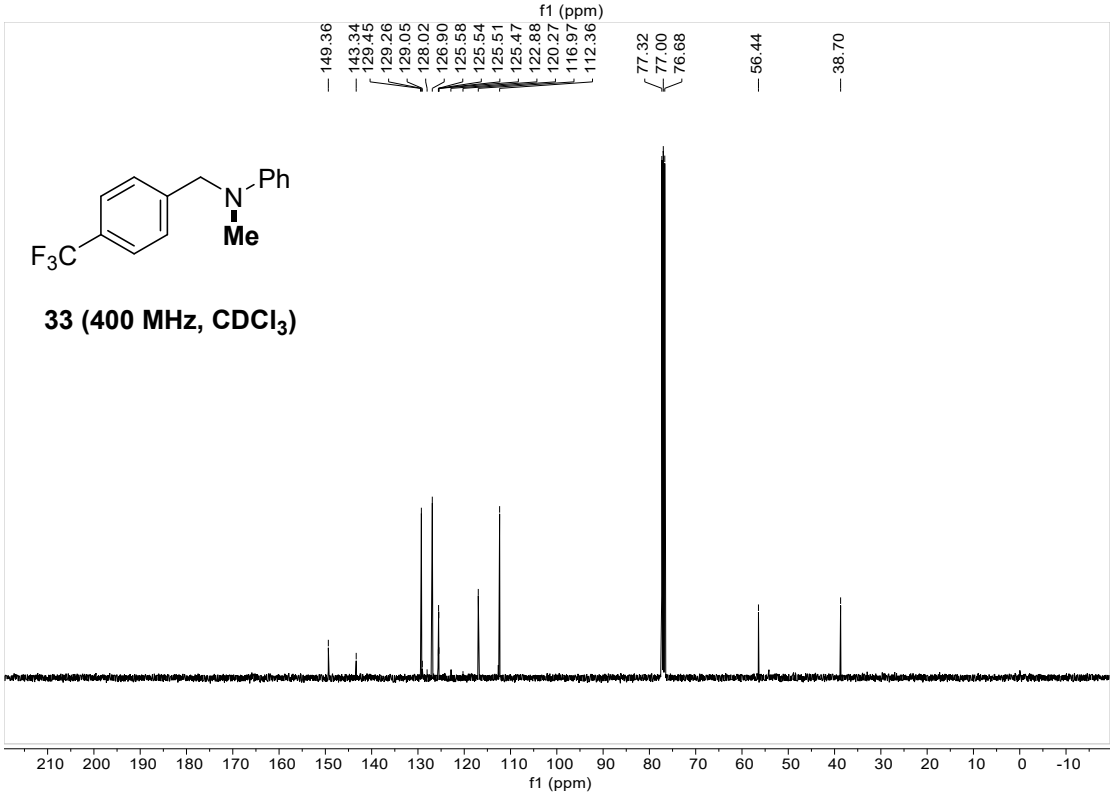


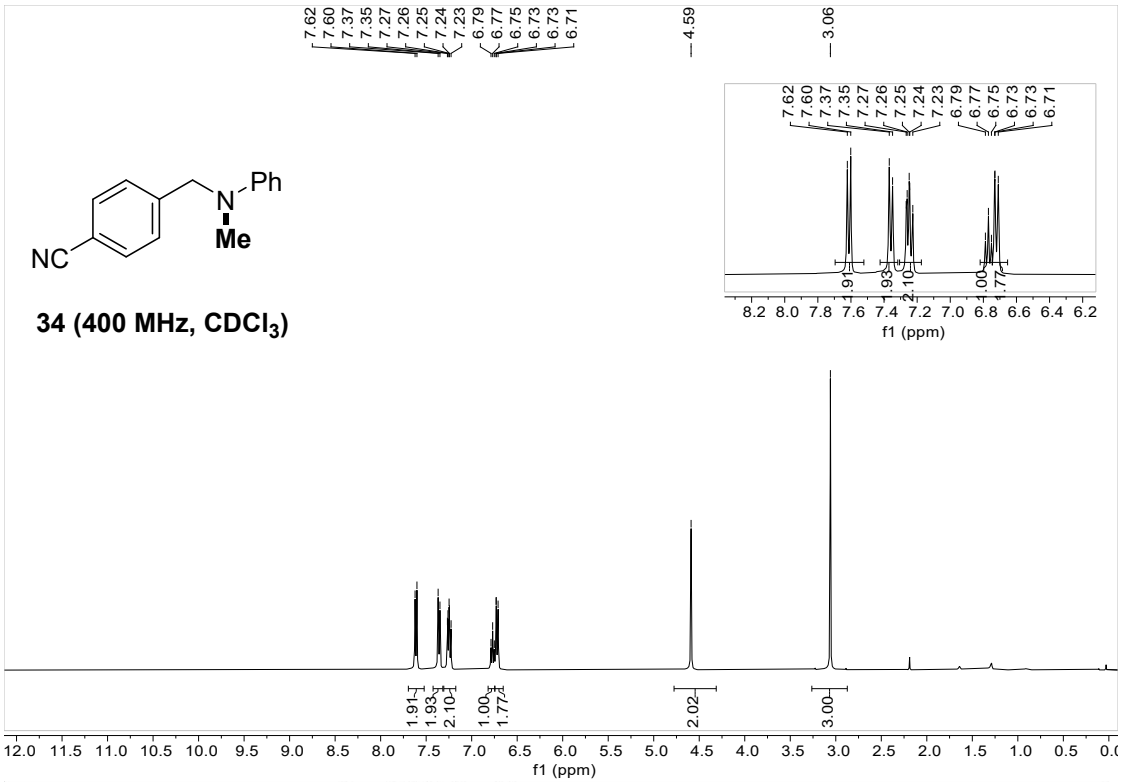
32 (400 MHz, $CDCl_3$)



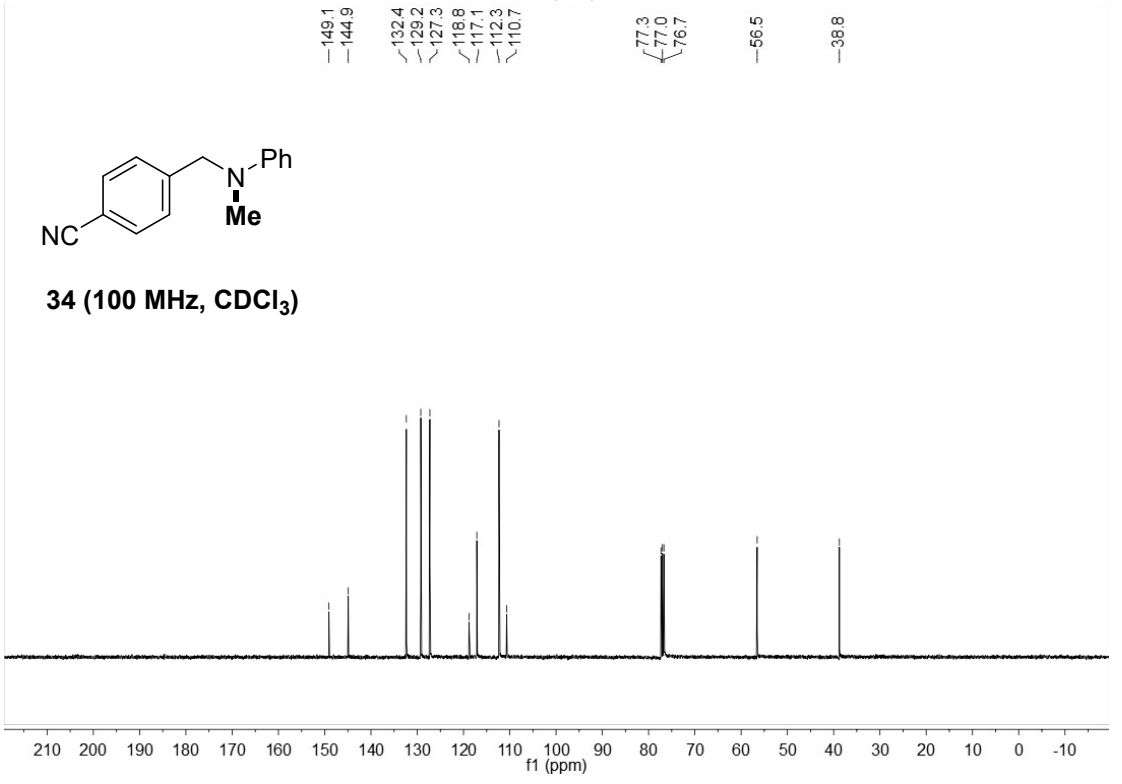
32 (100 MHz, $CDCl_3$)


7.59
7.57
7.37
7.35
7.26
7.24
7.22
6.77
6.75
6.73
4.59
3.05
Ph
N
Me
F3C
33 (400 MHz, CDCl3)
2.04
2.21
1.95
3.12
1.95
3.00
f1 (ppm)

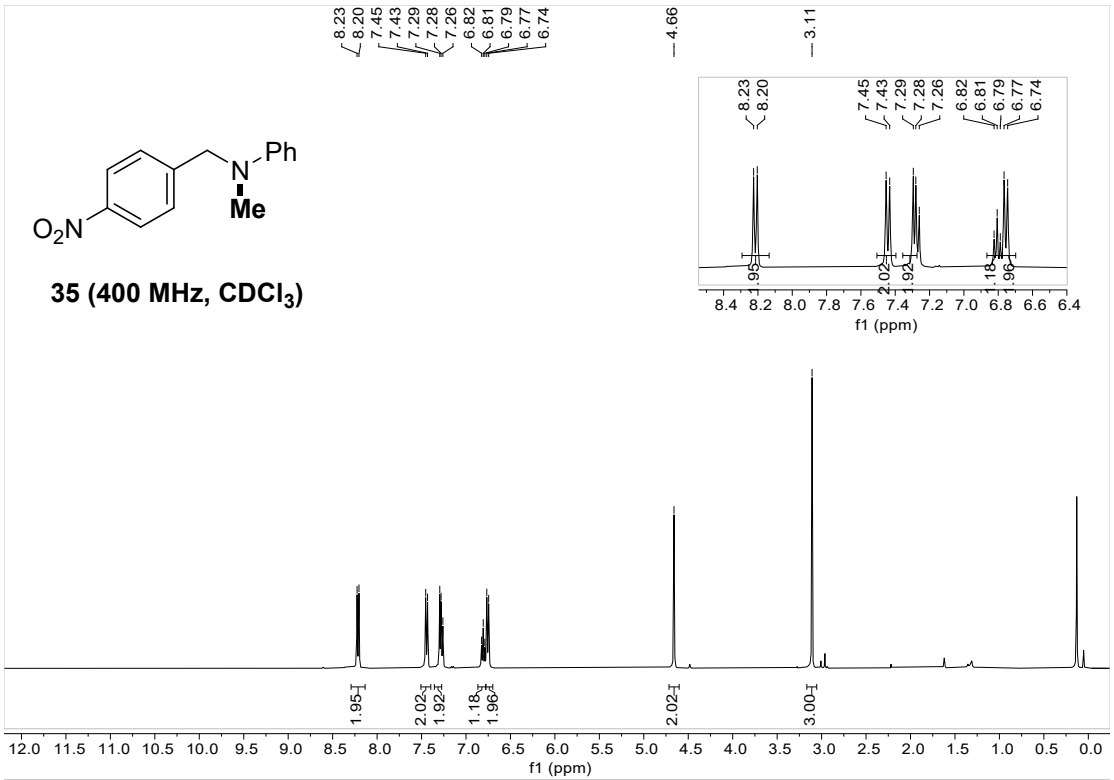

149.36
143.34
129.45
129.26
129.05
128.02
126.90
125.58
125.54
125.51
125.47
122.88
120.27
116.97
112.36
77.32
77.00
76.68
56.44
38.70
Ph
N
Me
F3C
33 (400 MHz, CDCl3)
f1 (ppm)

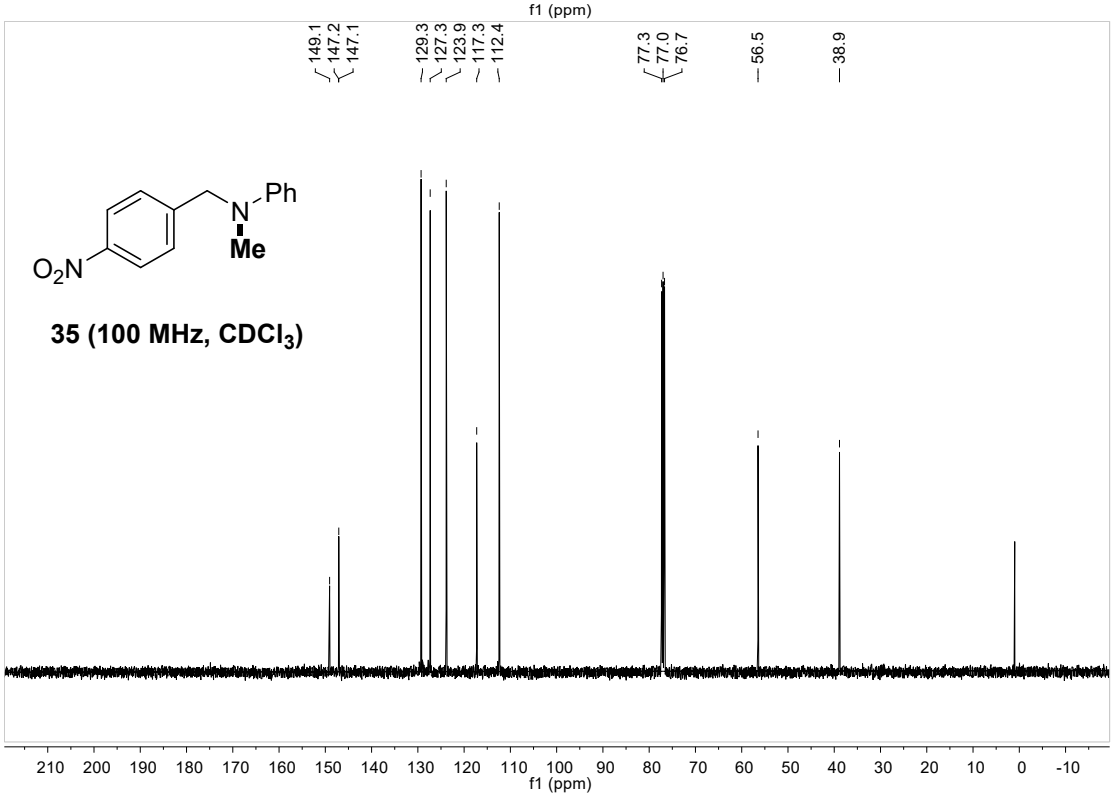


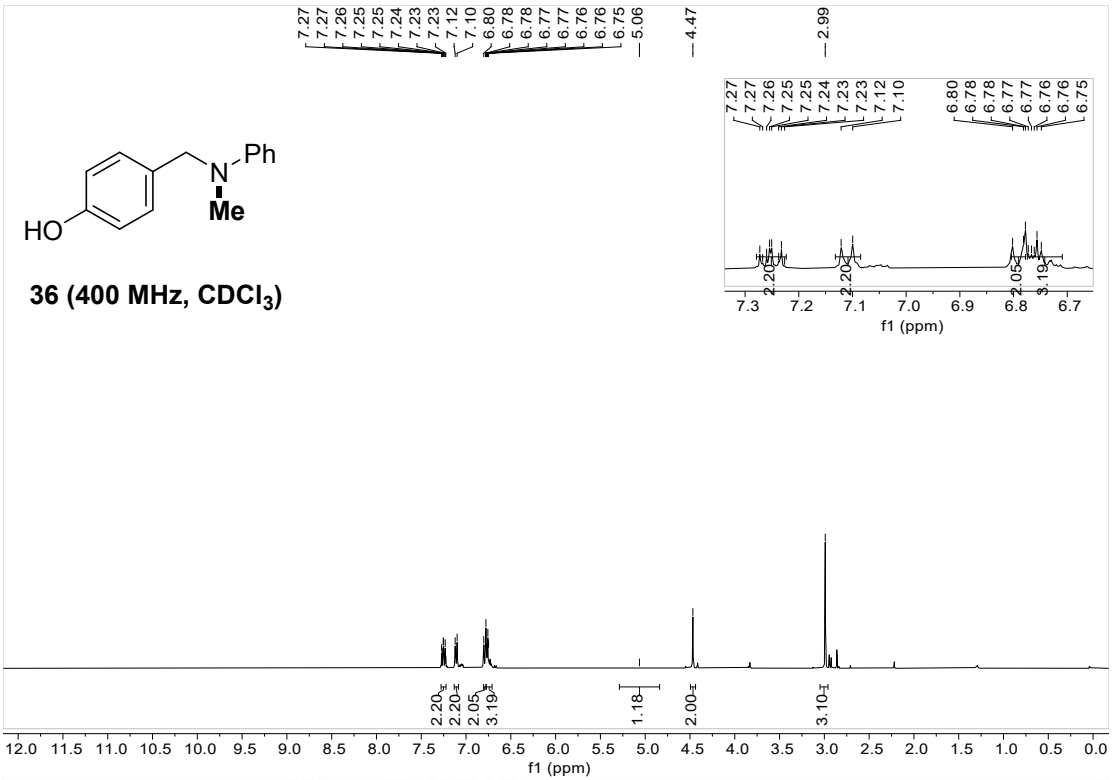
34 (400 MHz, $CDCl_3$)



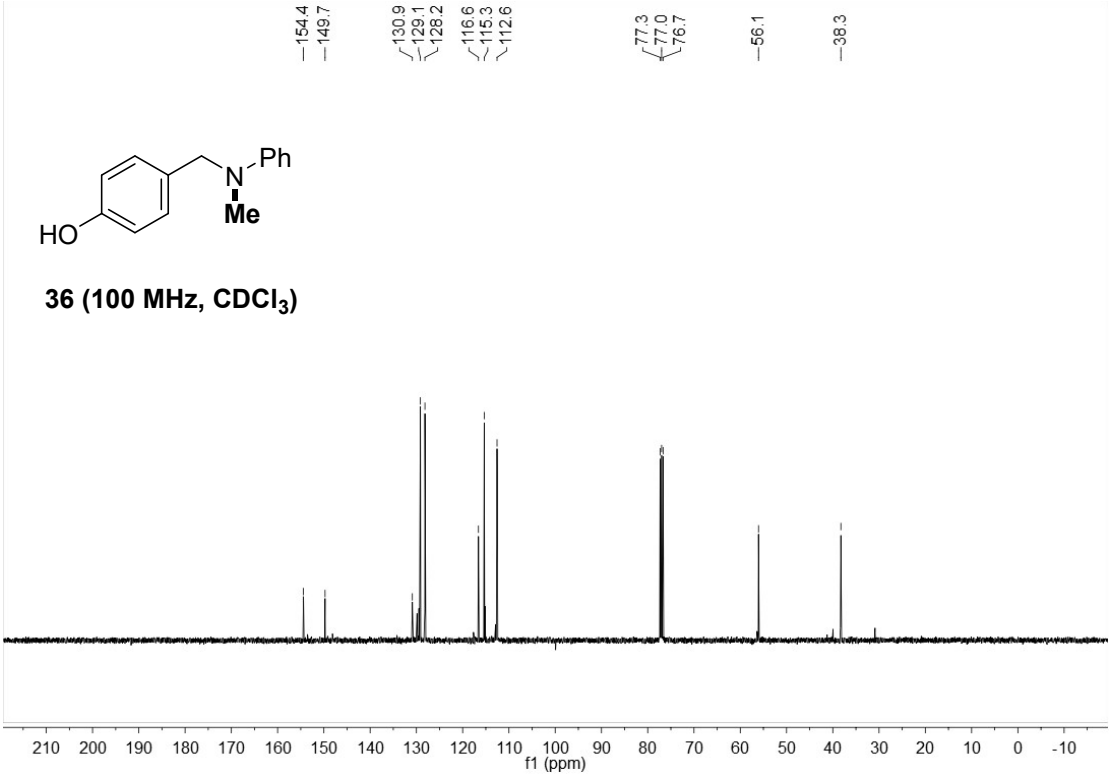
34 (100 MHz, $CDCl_3$)


8.23
8.20
7.45
7.43
7.29
7.28
7.26
6.82
6.81
6.79
6.77
6.74
4.66
3.11
Ph
N
Me
O2N
35 (400 MHz, CDCl3)
1.95
2.02
1.92
1.18
1.96
2.02
3.00
f1 (ppm)

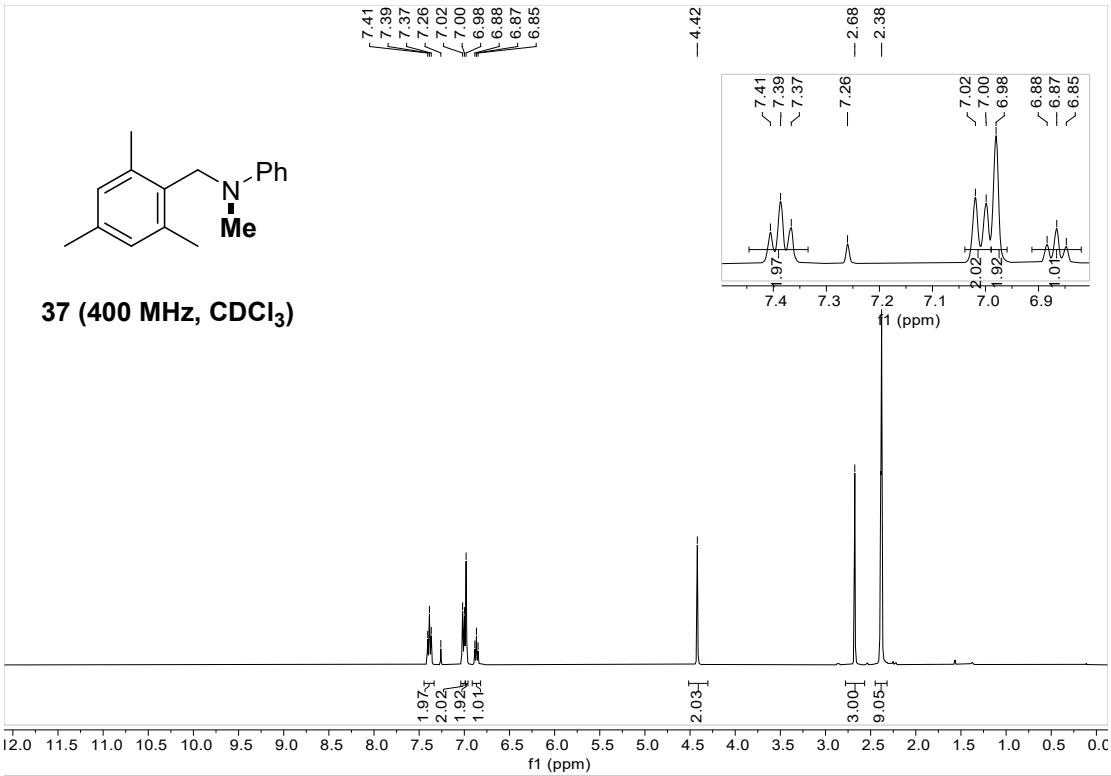

149.1
147.2
147.1
129.3
127.3
123.9
117.3
112.4
77.3
77.0
76.7
56.5
38.9
Ph
N
Me
O2N
35 (100 MHz, CDCl3)
f1 (ppm)



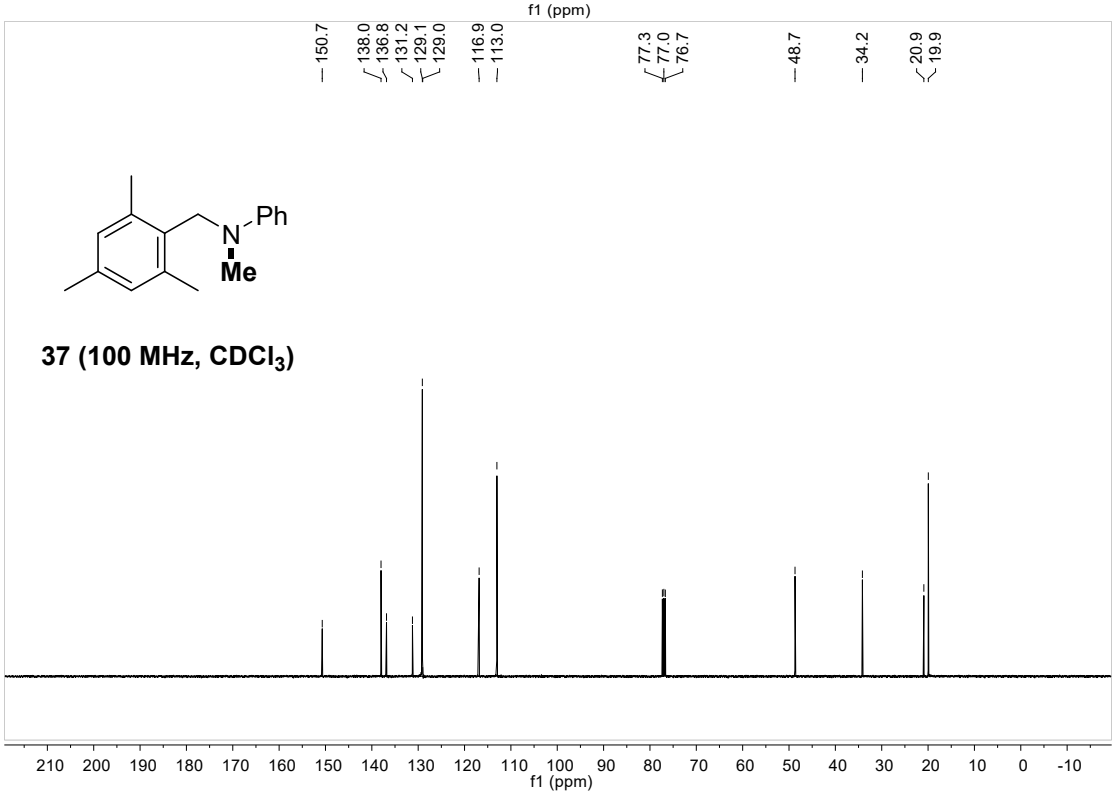
36 (400 MHz, $CDCl_3$)



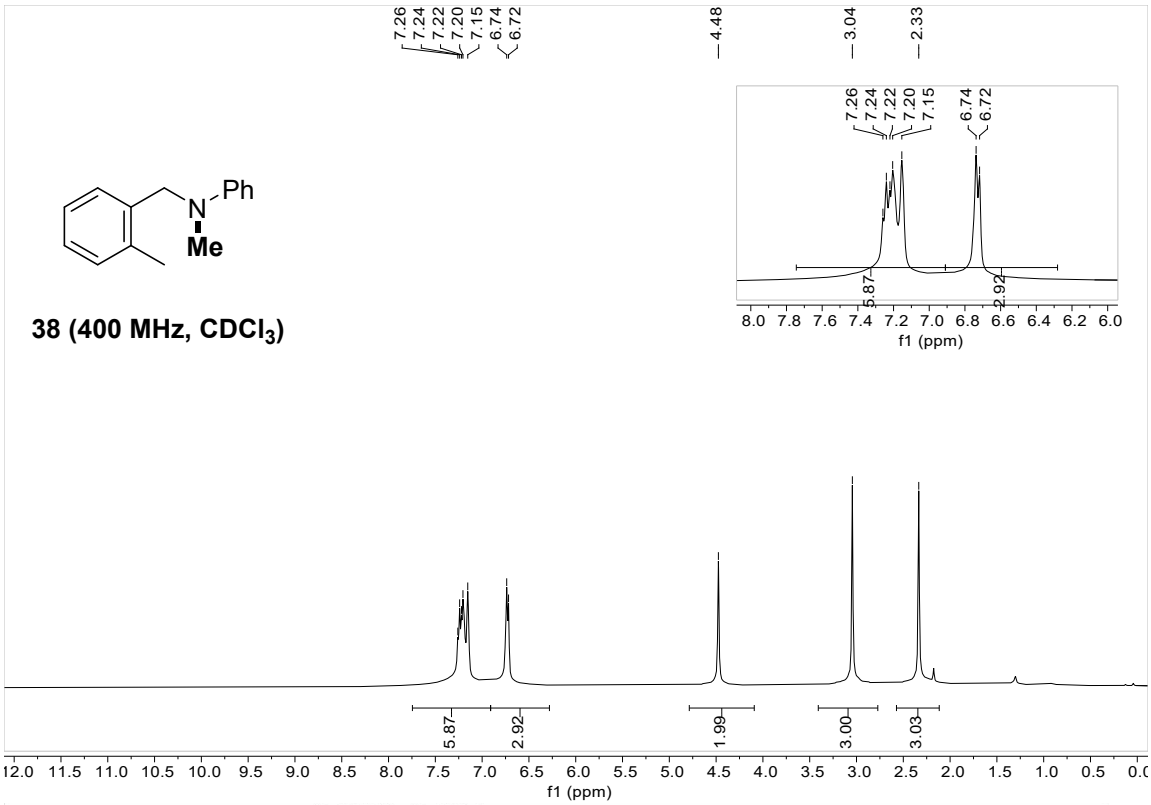
36 (100 MHz, $CDCl_3$)



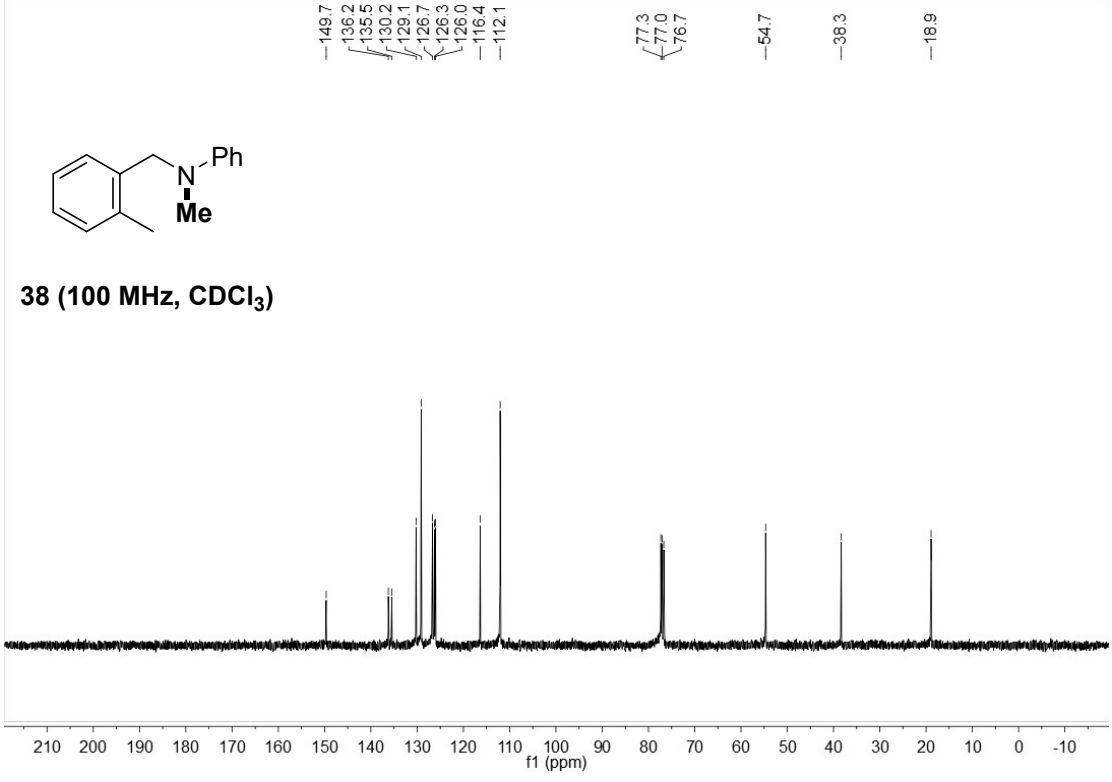
37 (400 MHz, $CDCl_3$)



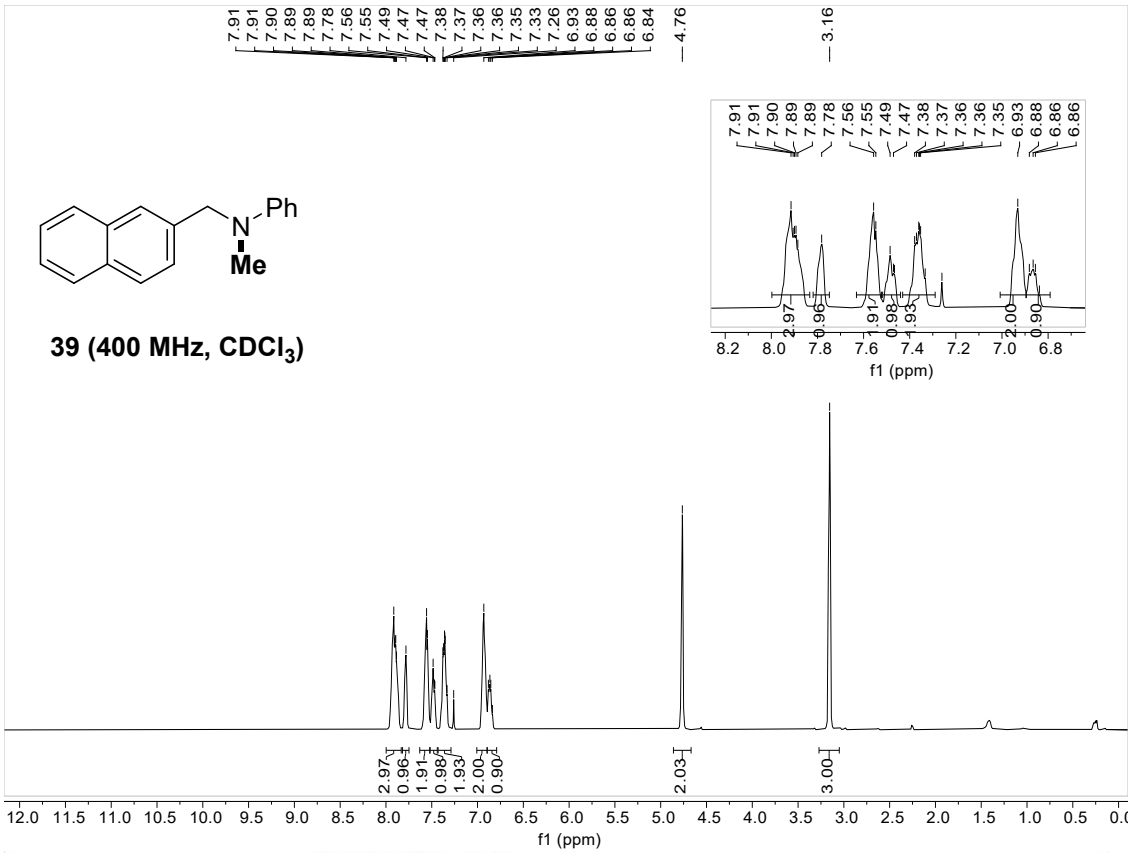
37 (100 MHz, $CDCl_3$)



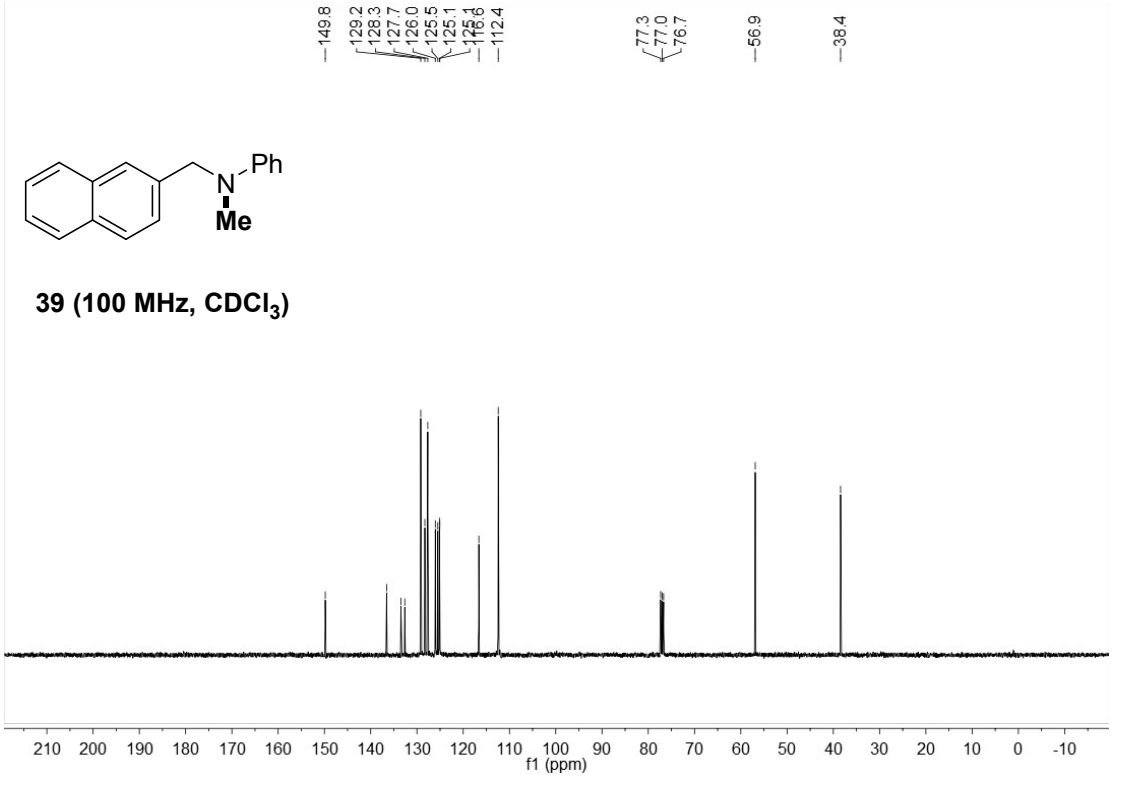
38 (400 MHz, $CDCl_3$)



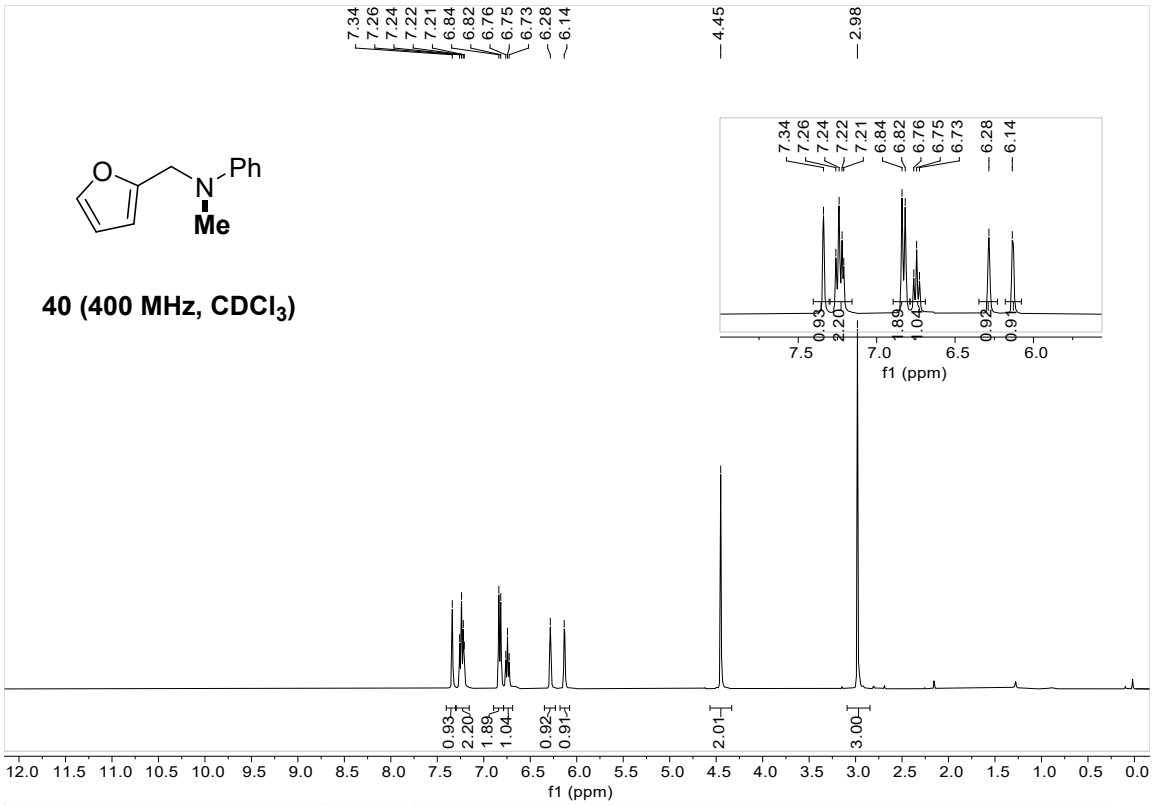
38 (100 MHz, $CDCl_3$)



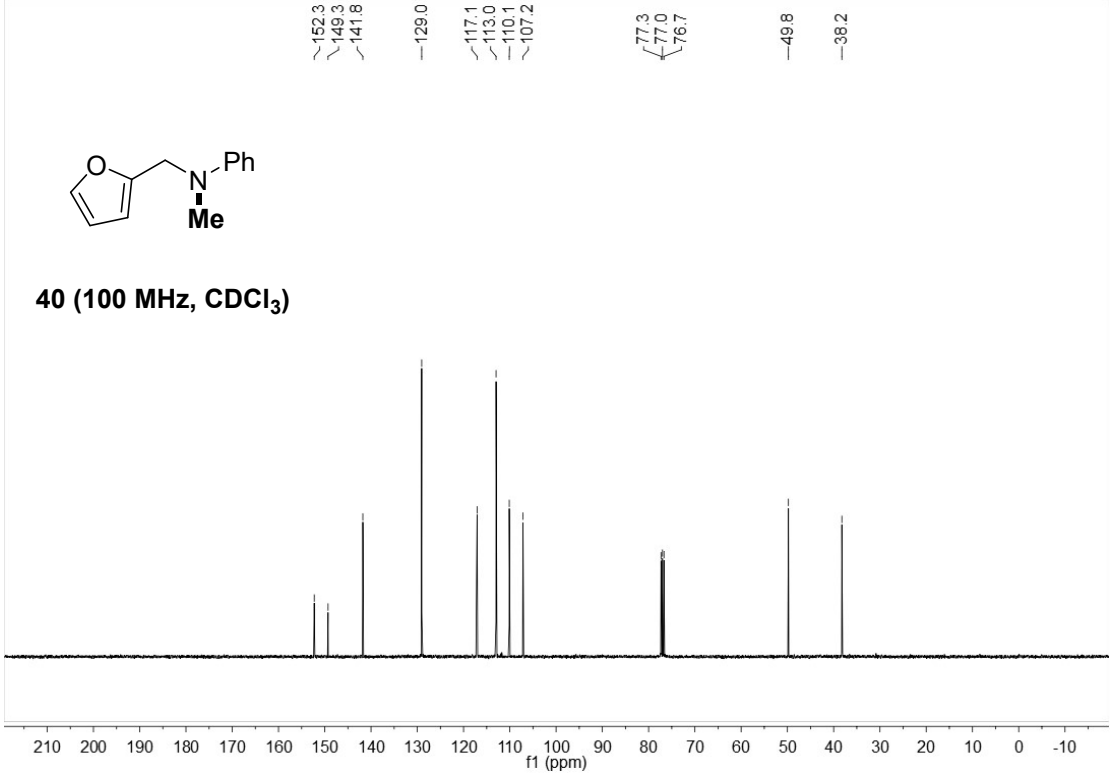
39 (400 MHz, $CDCl_3$)



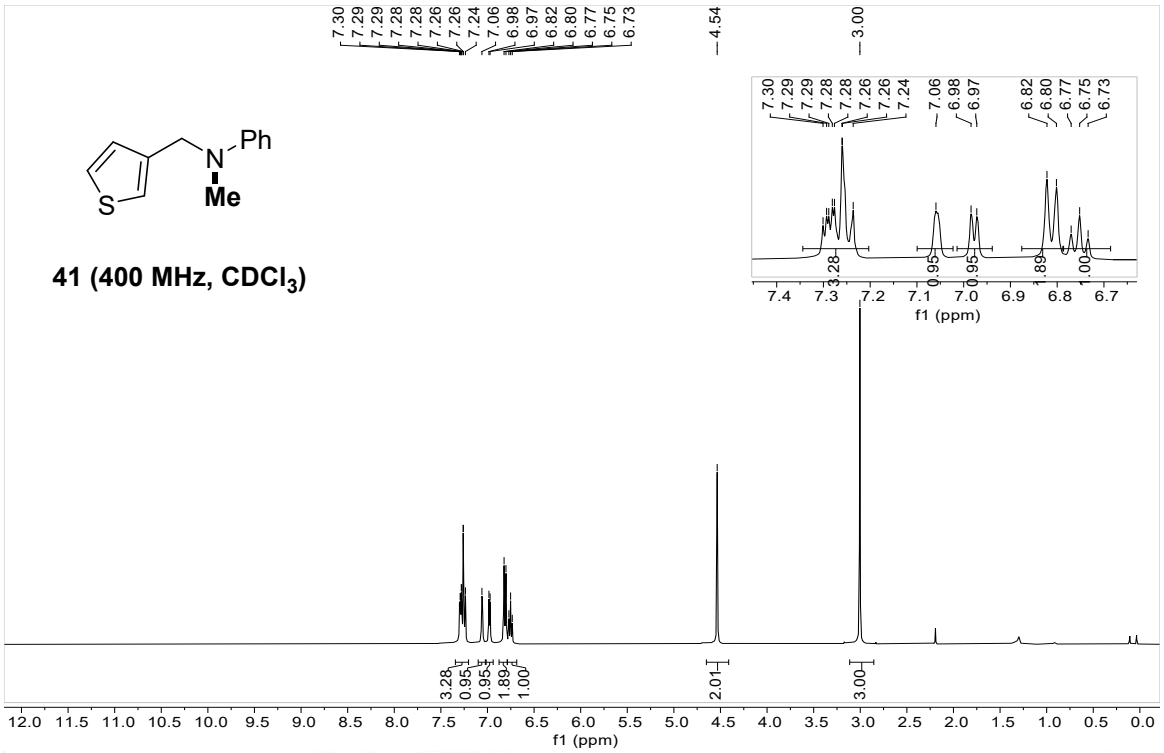
39 (100 MHz, $CDCl_3$)



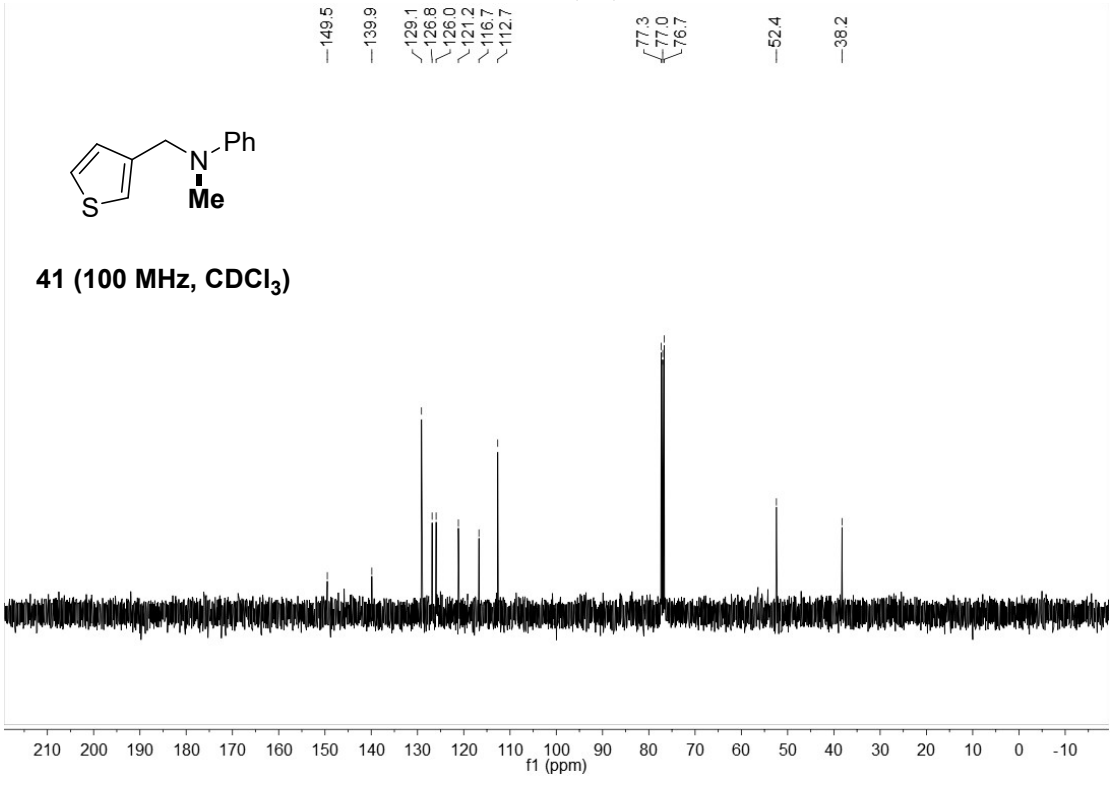
40 (400 MHz, $CDCl_3$)



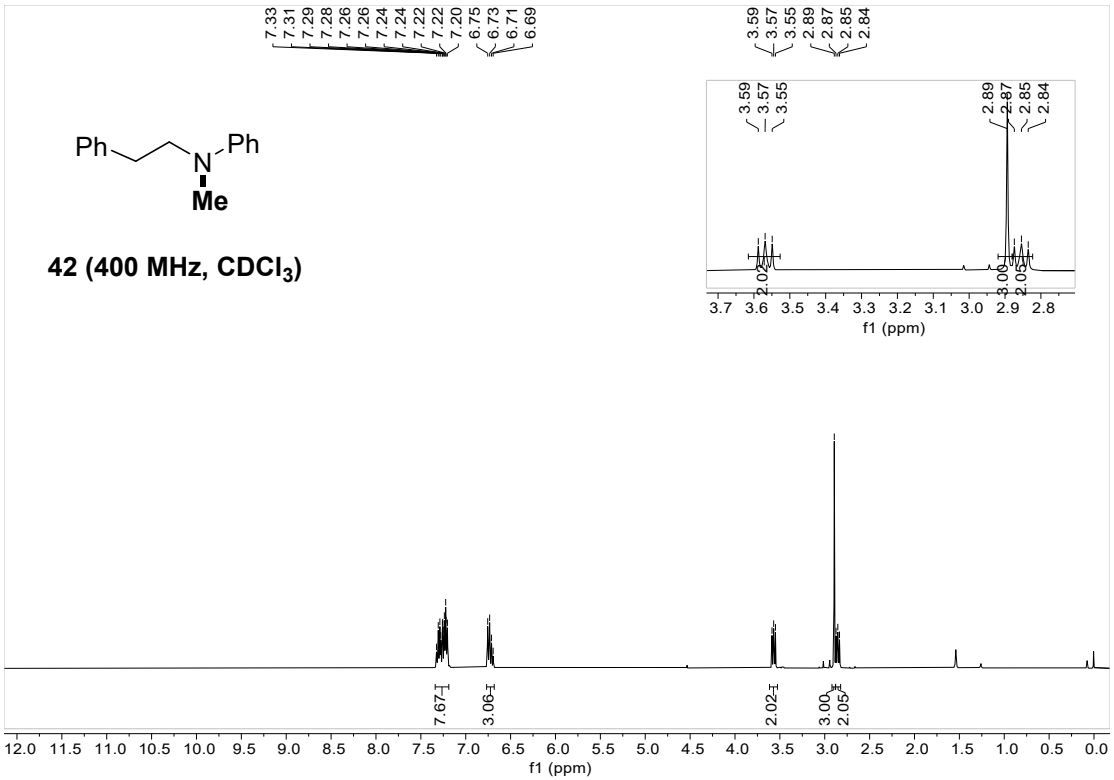
40 (100 MHz, $CDCl_3$)

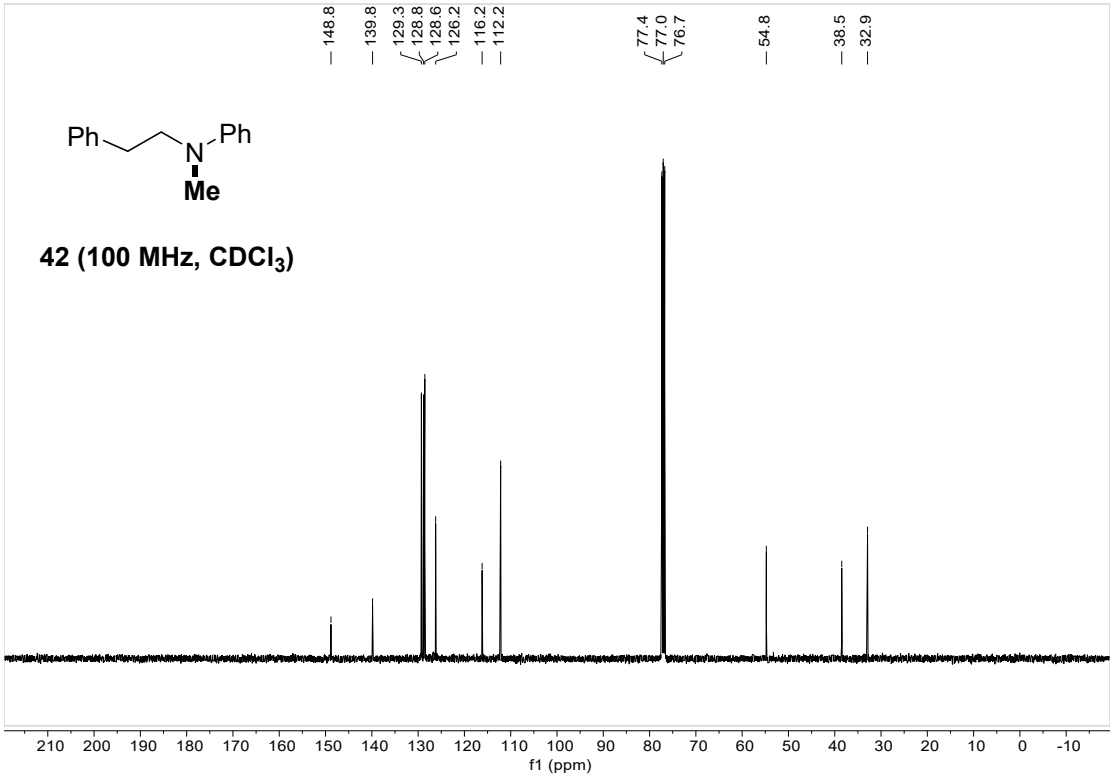


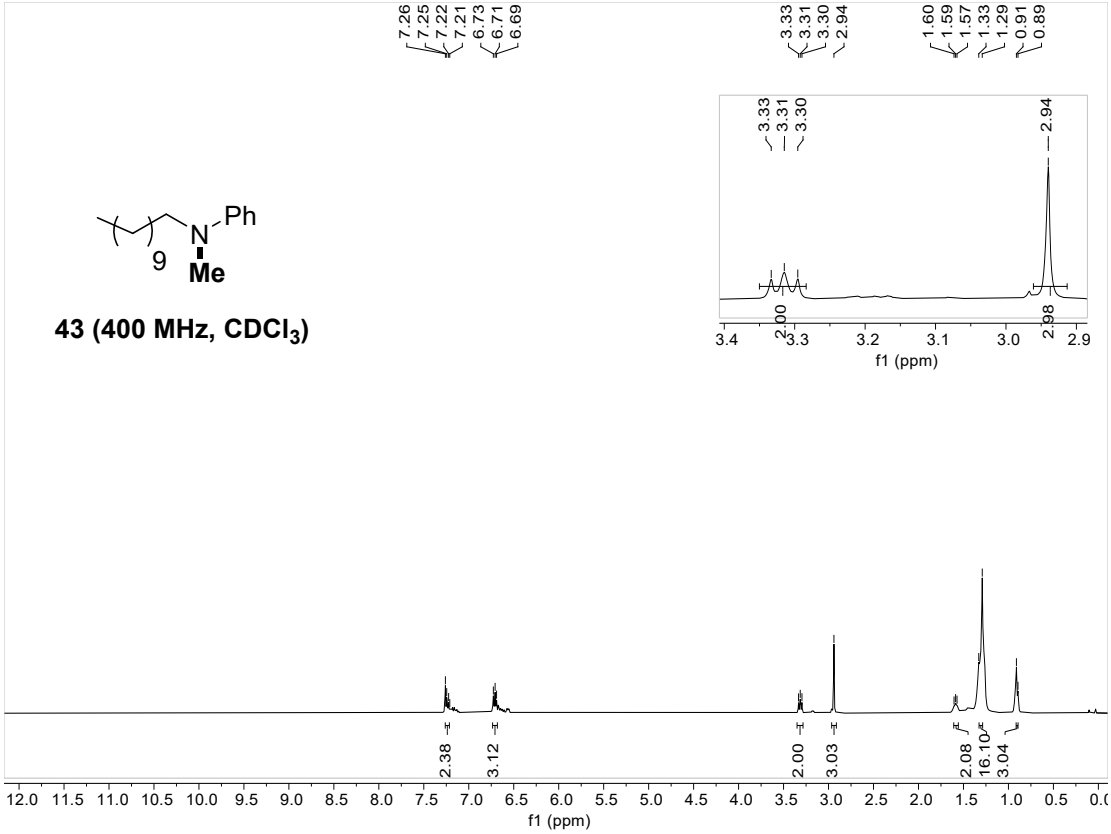
41 (400 MHz, $CDCl_3$)



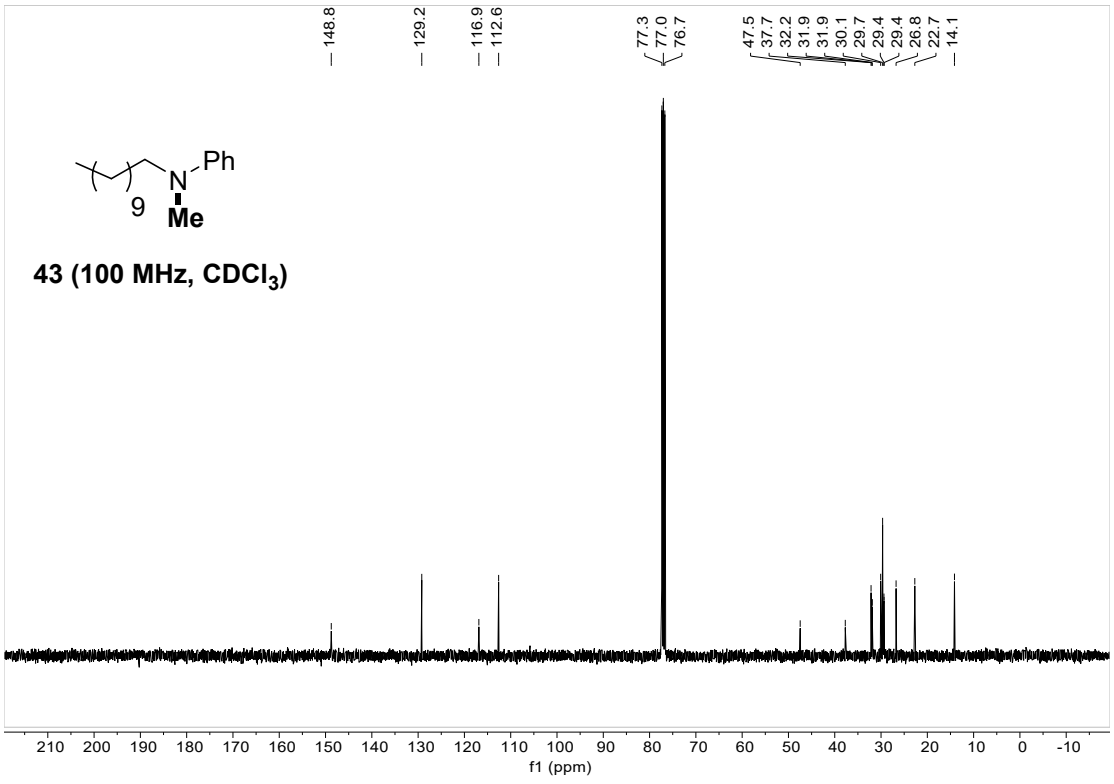
41 (100 MHz, $CDCl_3$)


7.33
7.31
7.29
7.28
7.26
7.26
7.24
7.24
7.22
7.22
7.20
6.75
6.73
6.71
6.69
3.59
3.57
3.55
2.89
2.87
2.85
2.84
Ph
N
Ph
Me
42 (400 MHz, CDCl3)
7.67
3.06
2.02
3.00
2.05
f1 (ppm)

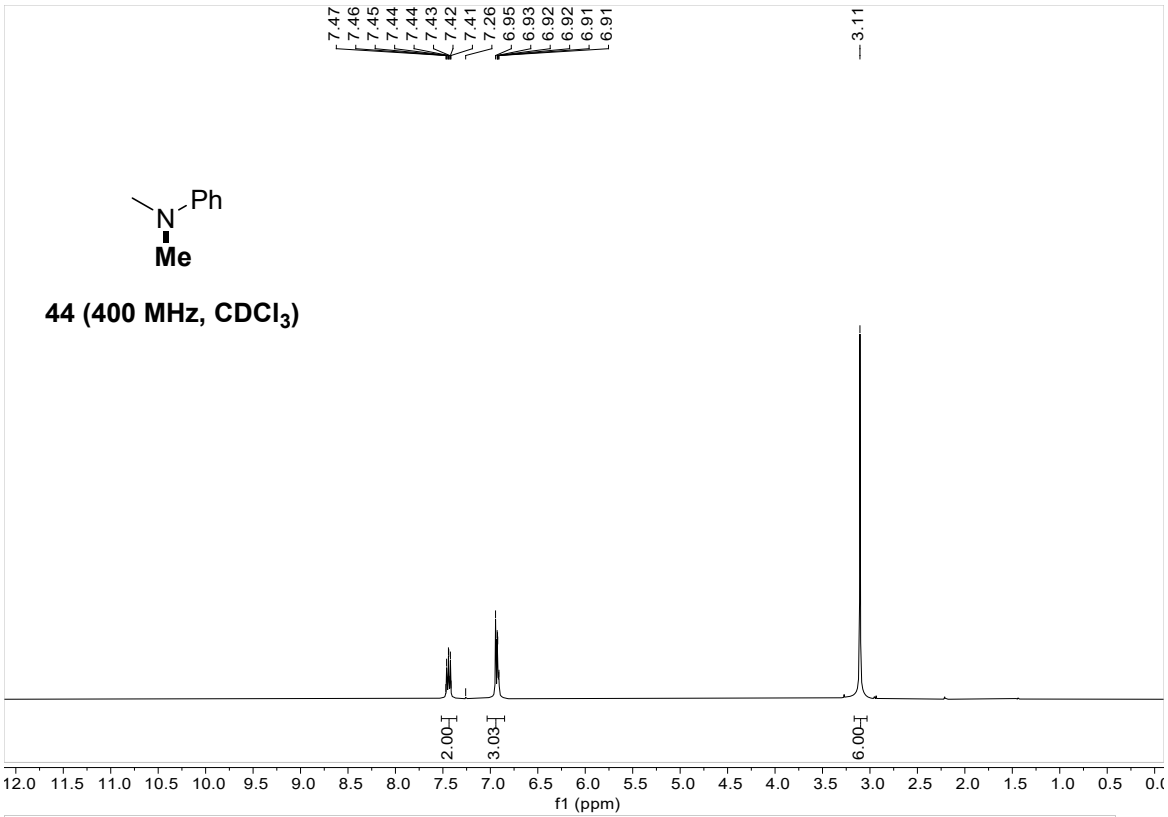

148.8
139.8
129.3
128.8
128.6
126.2
116.2
112.2
77.4
77.0
76.7
54.8
38.5
32.9
Ph
N
Ph
Me
42 (100 MHz, CDCl3)
f1 (ppm)



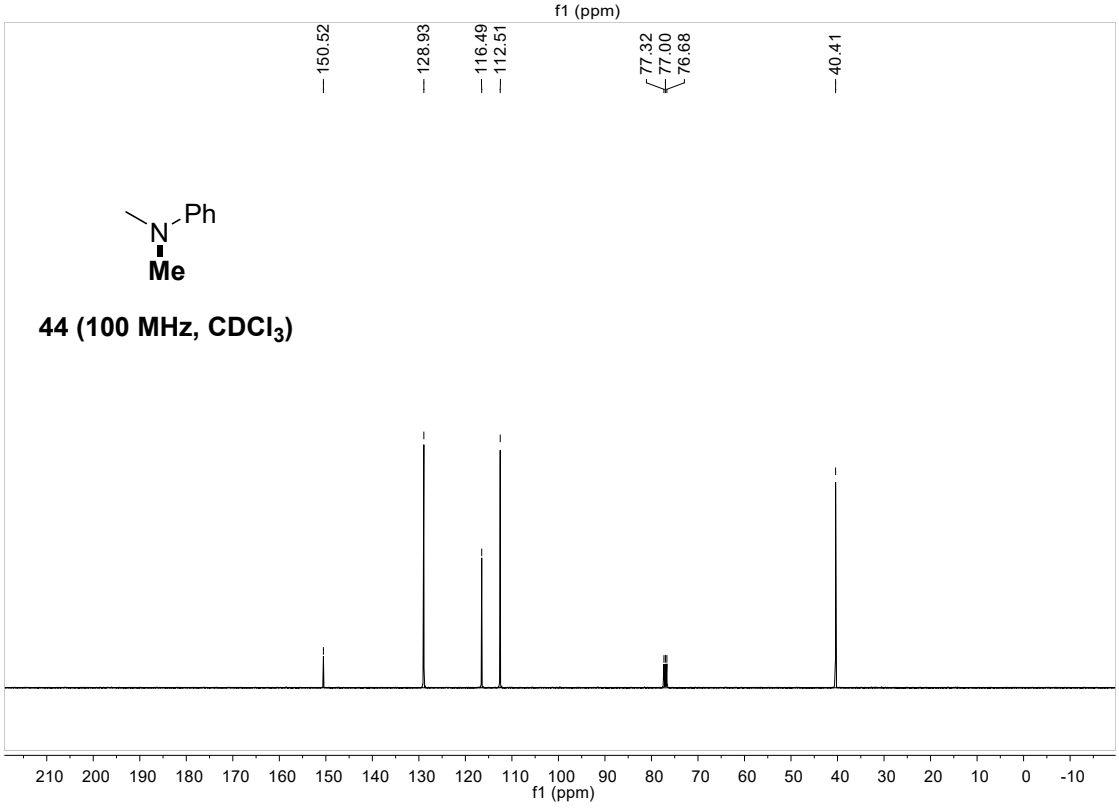
43 (400 MHz, $CDCl_3$)



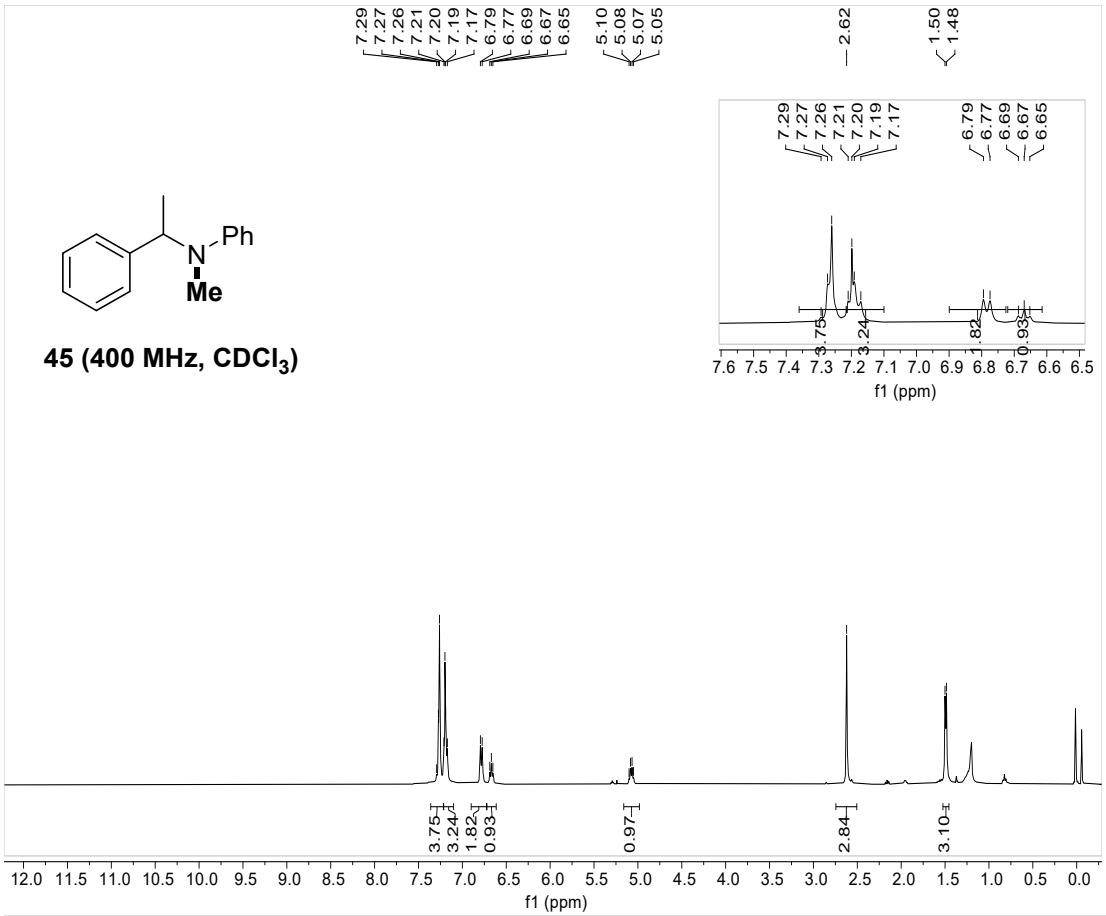
43 (100 MHz, $CDCl_3$)



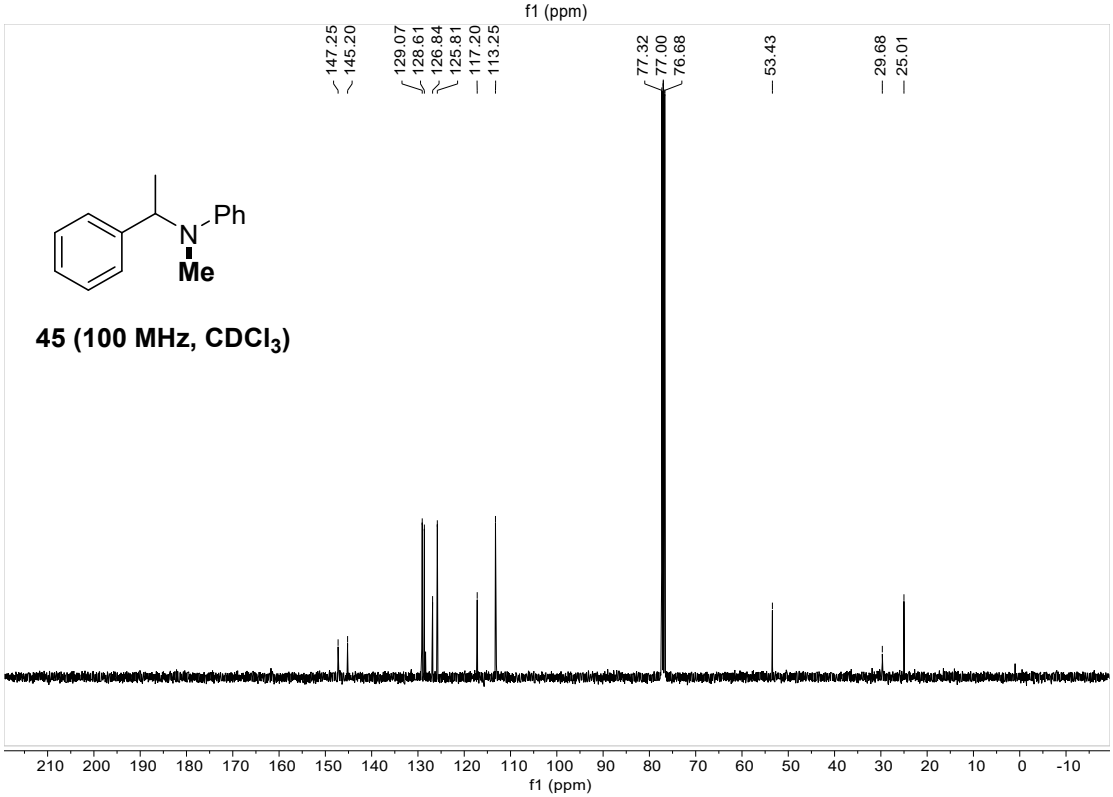
44 (400 MHz, $CDCl_3$)



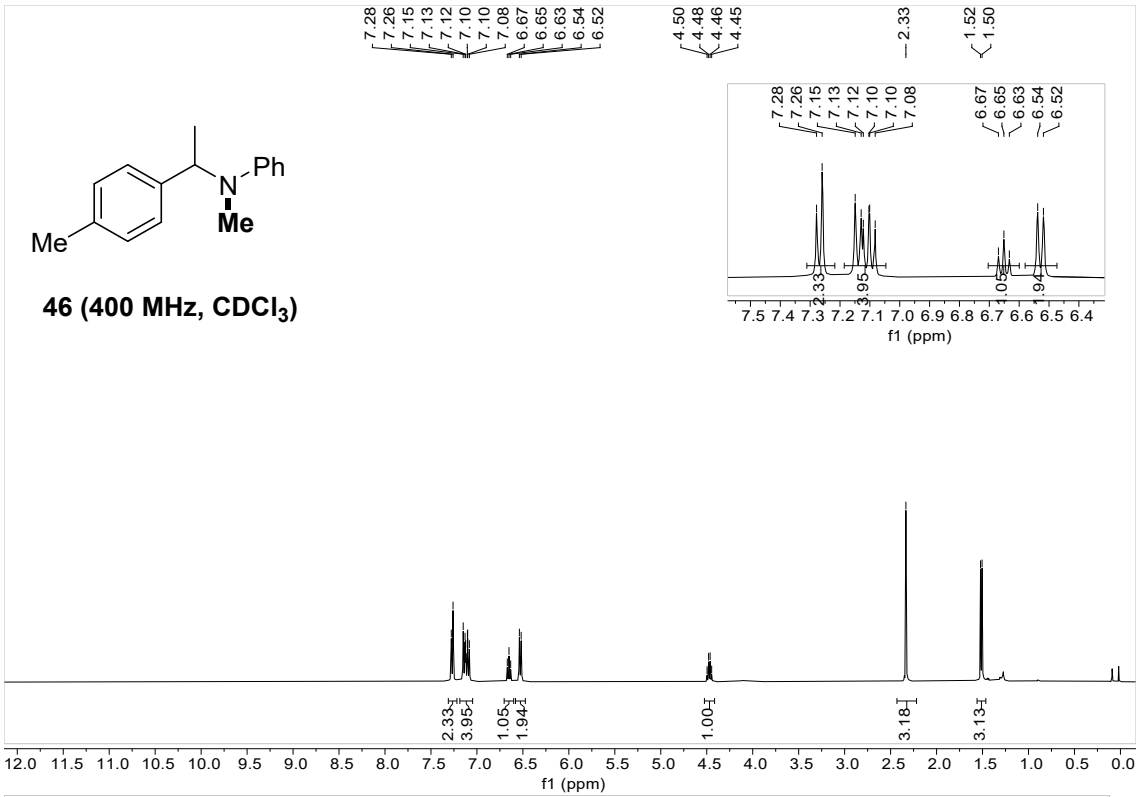
44 (100 MHz, $CDCl_3$)

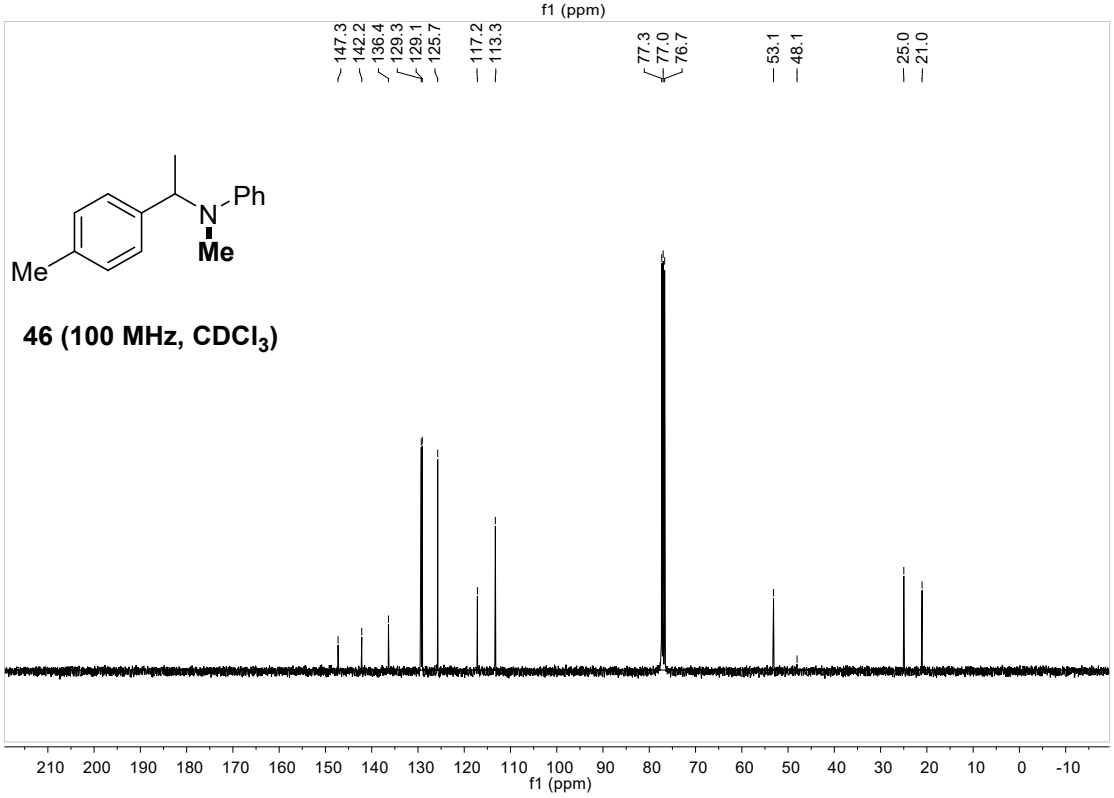


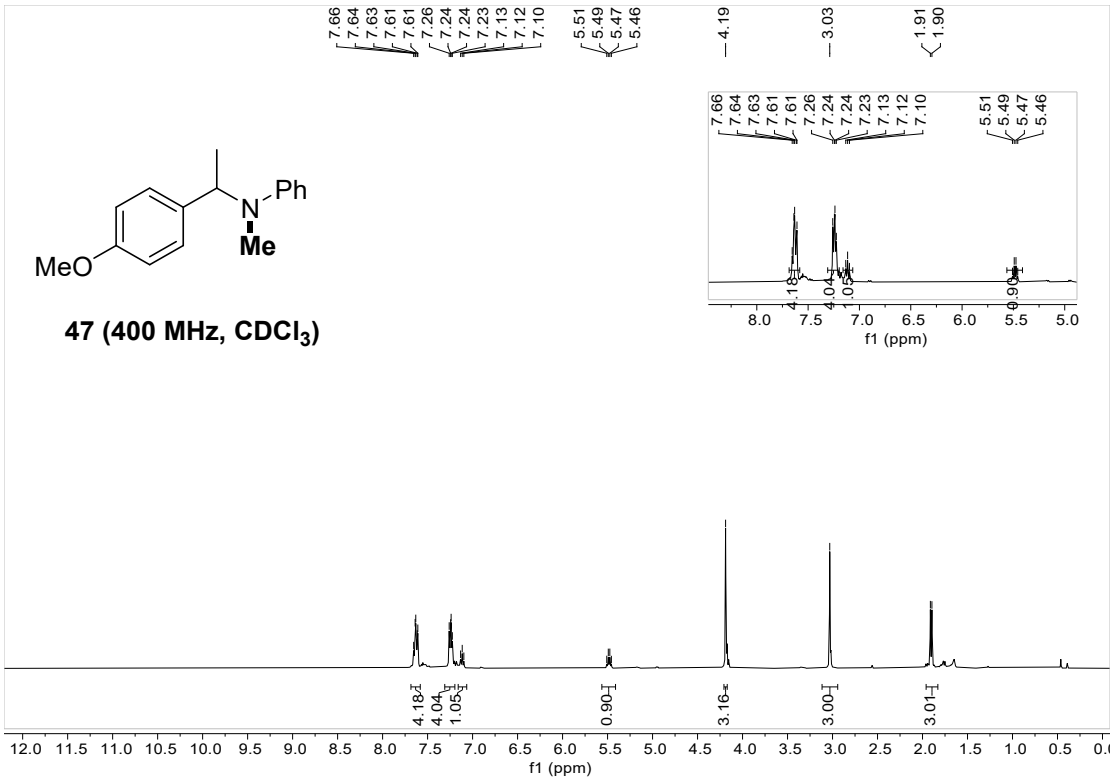
45 (400 MHz, $CDCl_3$)



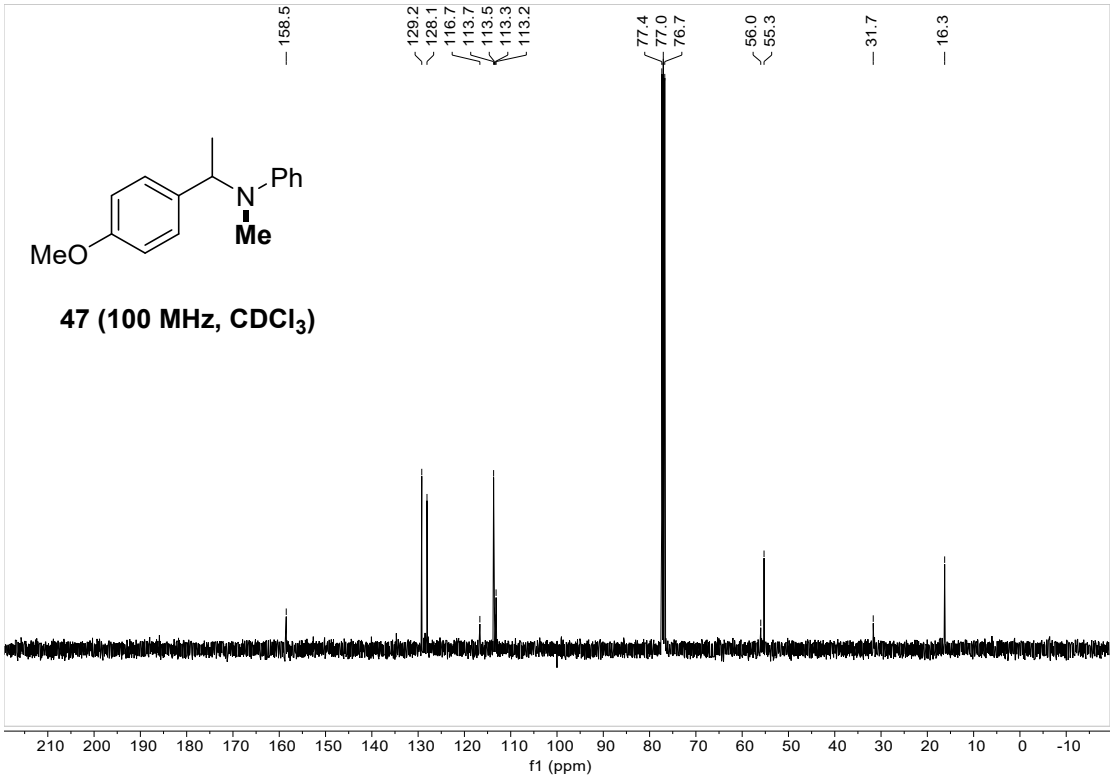
45 (100 MHz, $CDCl_3$)


7.28
7.26
7.15
7.13
7.12
7.10
7.10
7.08
6.67
6.65
6.63
6.54
6.52
4.50
4.48
4.46
4.45
2.33
1.52
1.50
Ph
N
Me
Me
46 (400 MHz, CDCl3)
2.33
3.95
1.05
1.94
1.00
3.18
3.13
f1 (ppm)

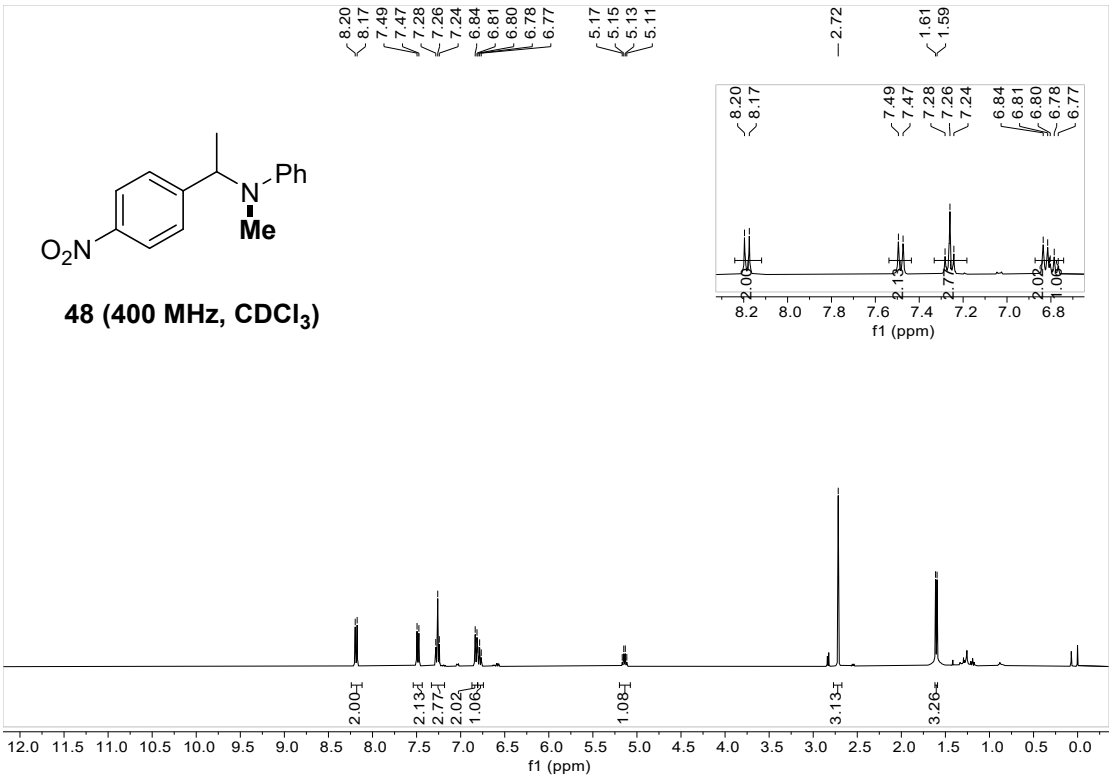

147.3
142.2
136.4
129.3
129.1
125.7
117.2
113.3
77.3
77.0
76.7
53.1
48.1
25.0
21.0
Ph
N
Me
Me
46 (100 MHz, CDCl3)
f1 (ppm)



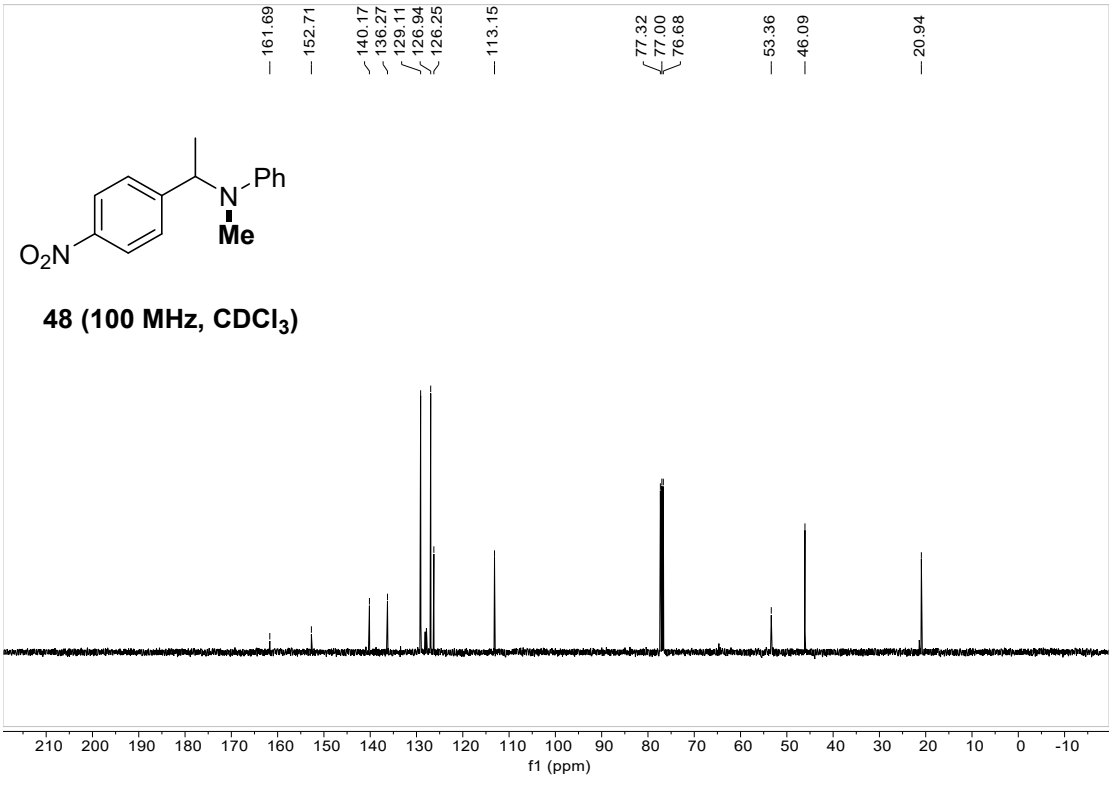
47 (400 MHz, $CDCl_3$)



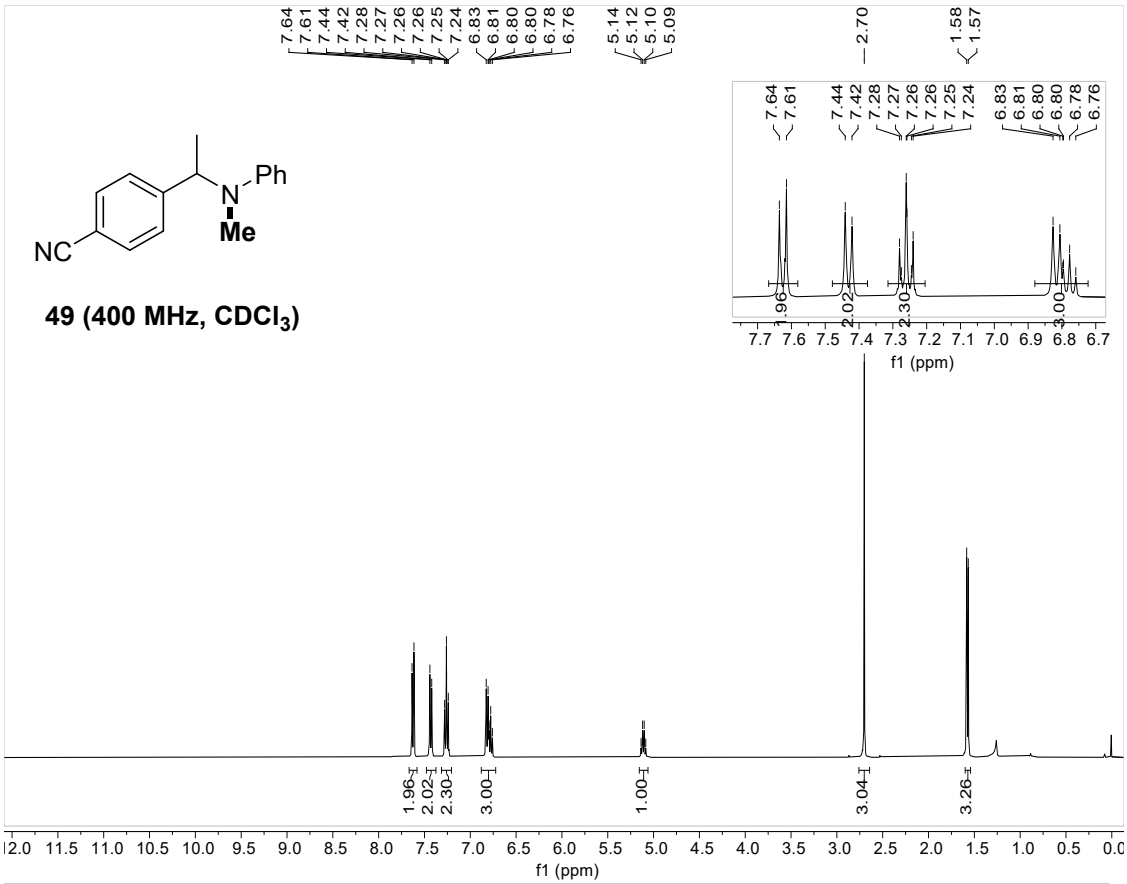
47 (100 MHz, $CDCl_3$)



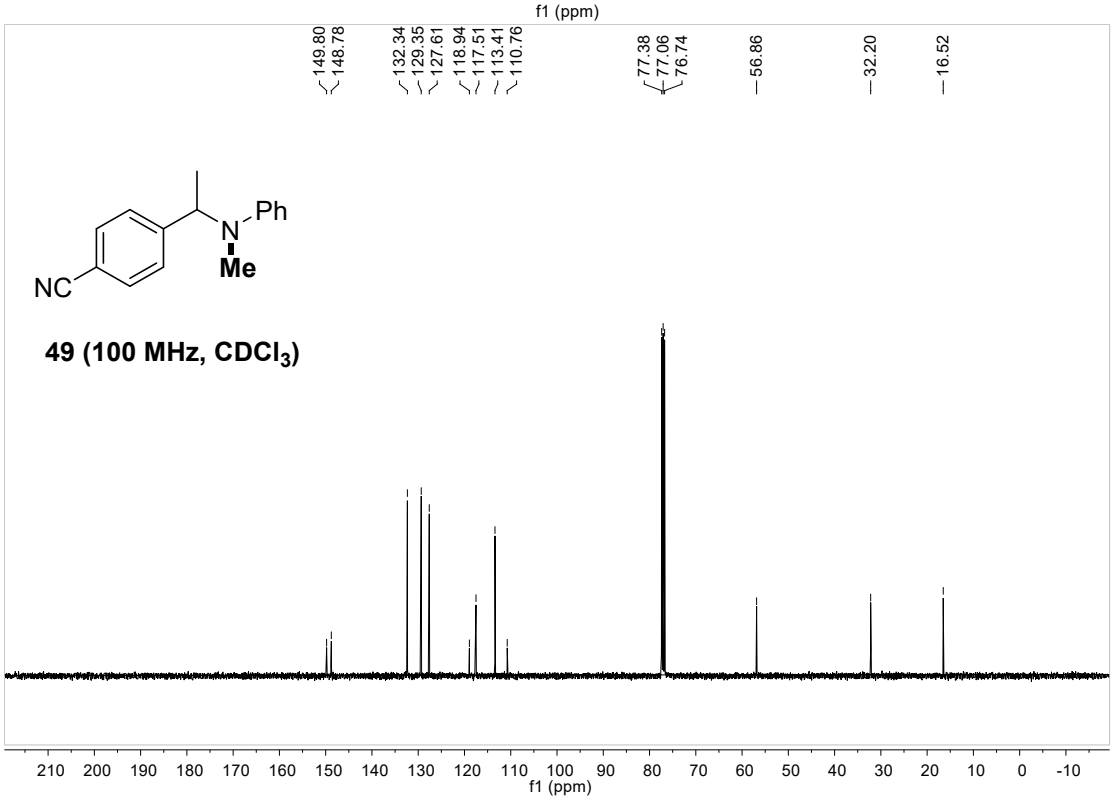
48 (400 MHz, $CDCl_3$)



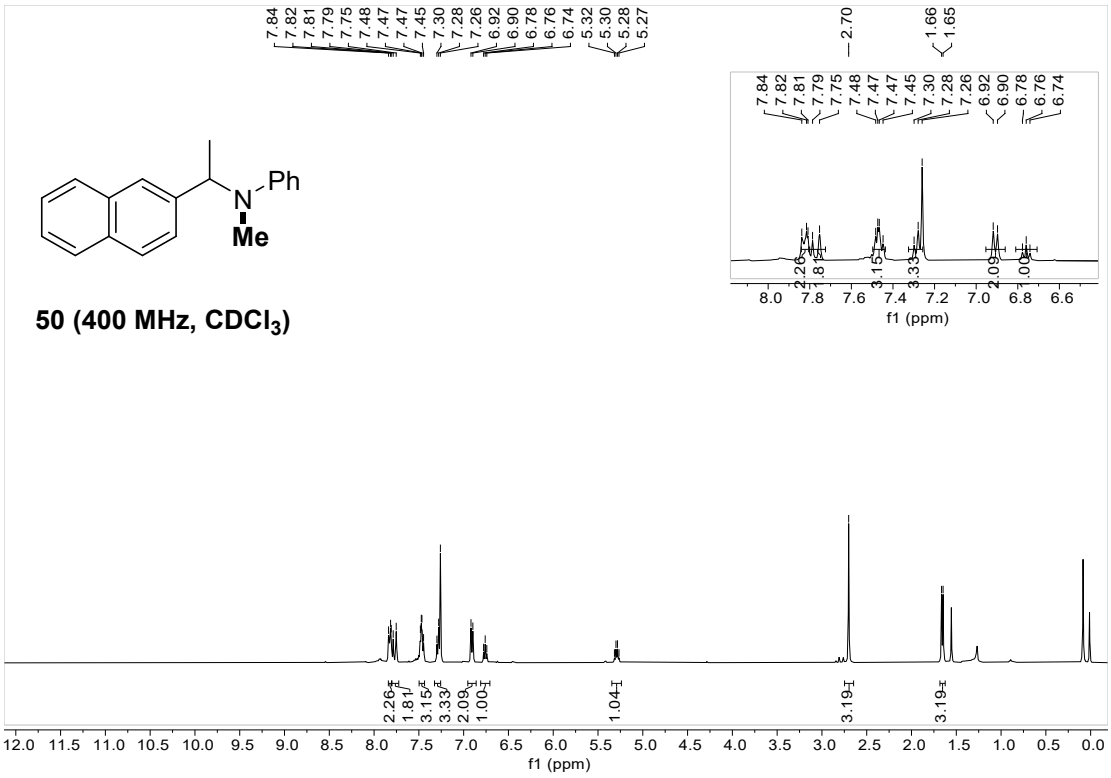
48 (100 MHz, $CDCl_3$)



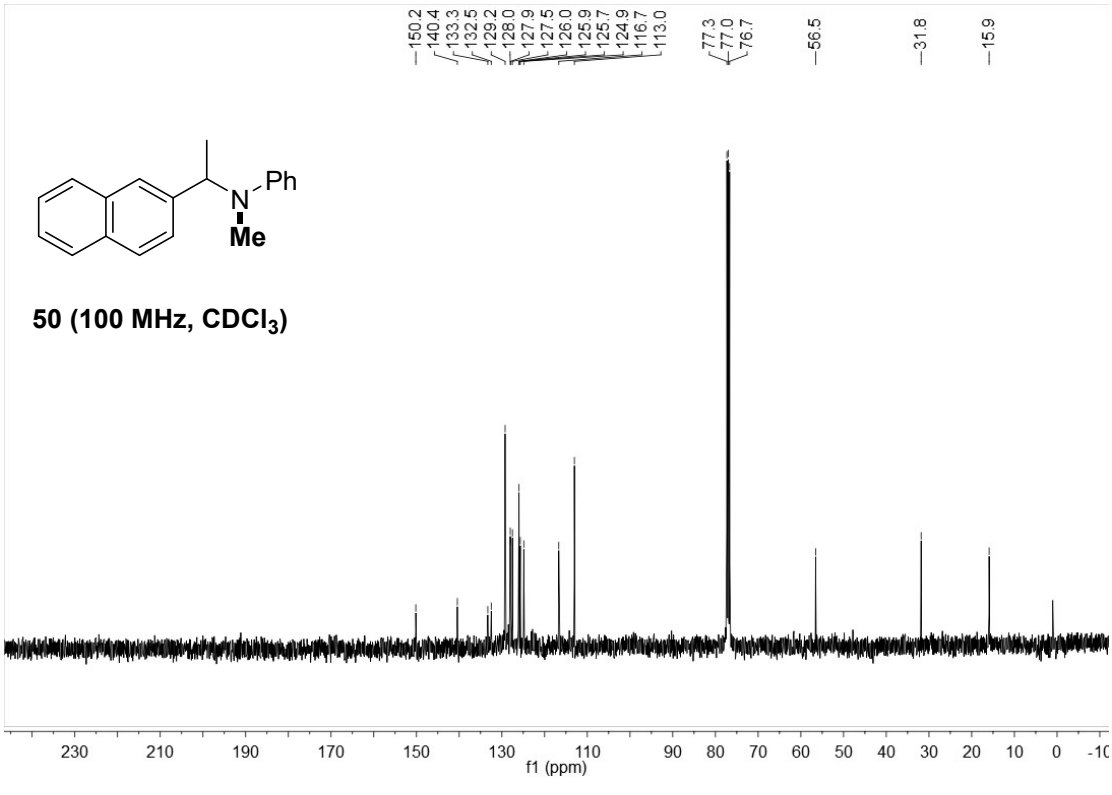
49 (400 MHz, $CDCl_3$)



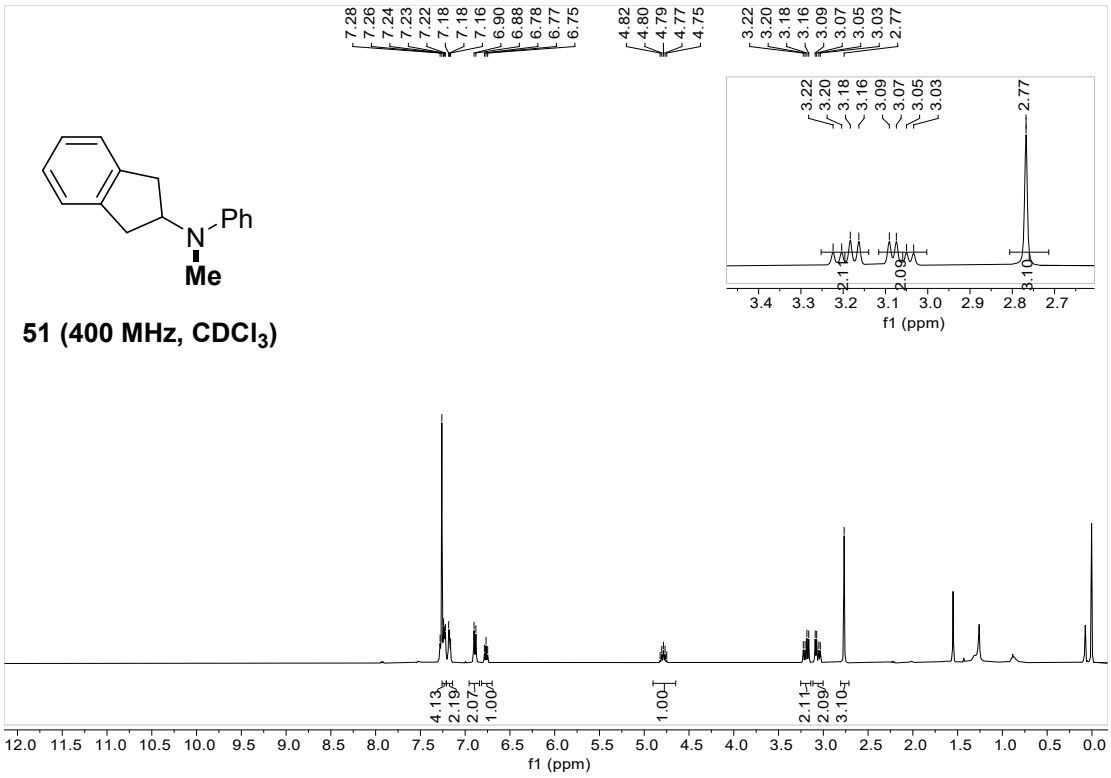
49 (100 MHz, $CDCl_3$)

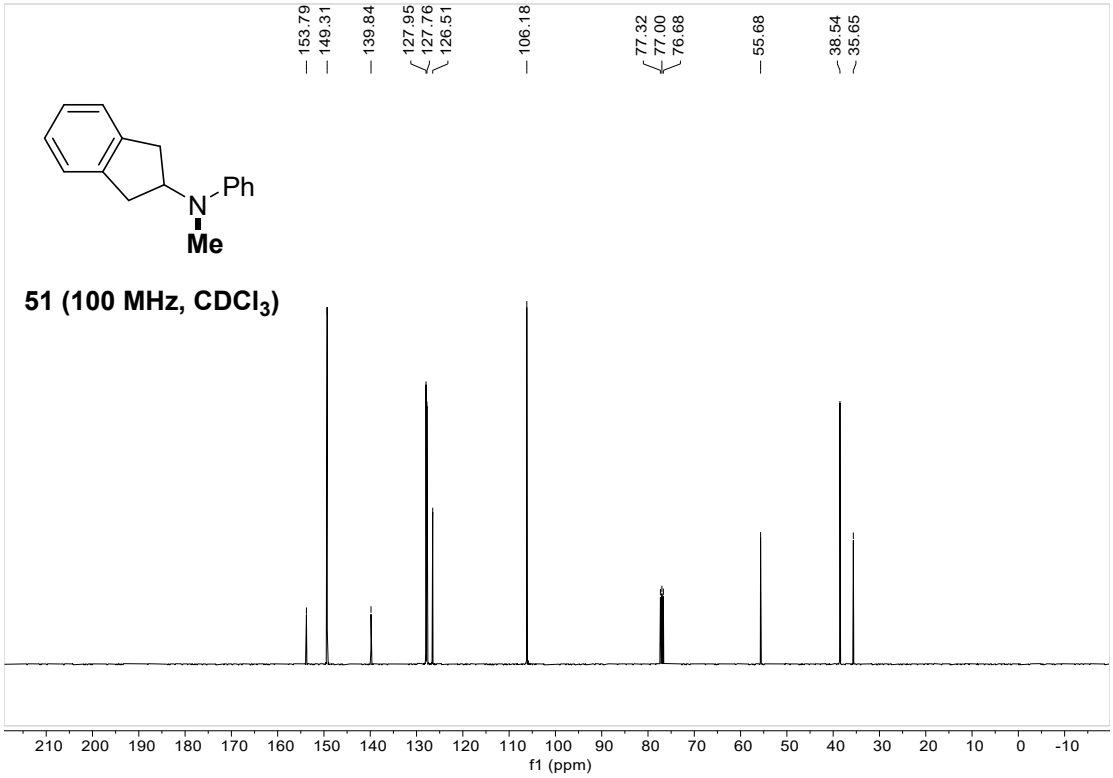


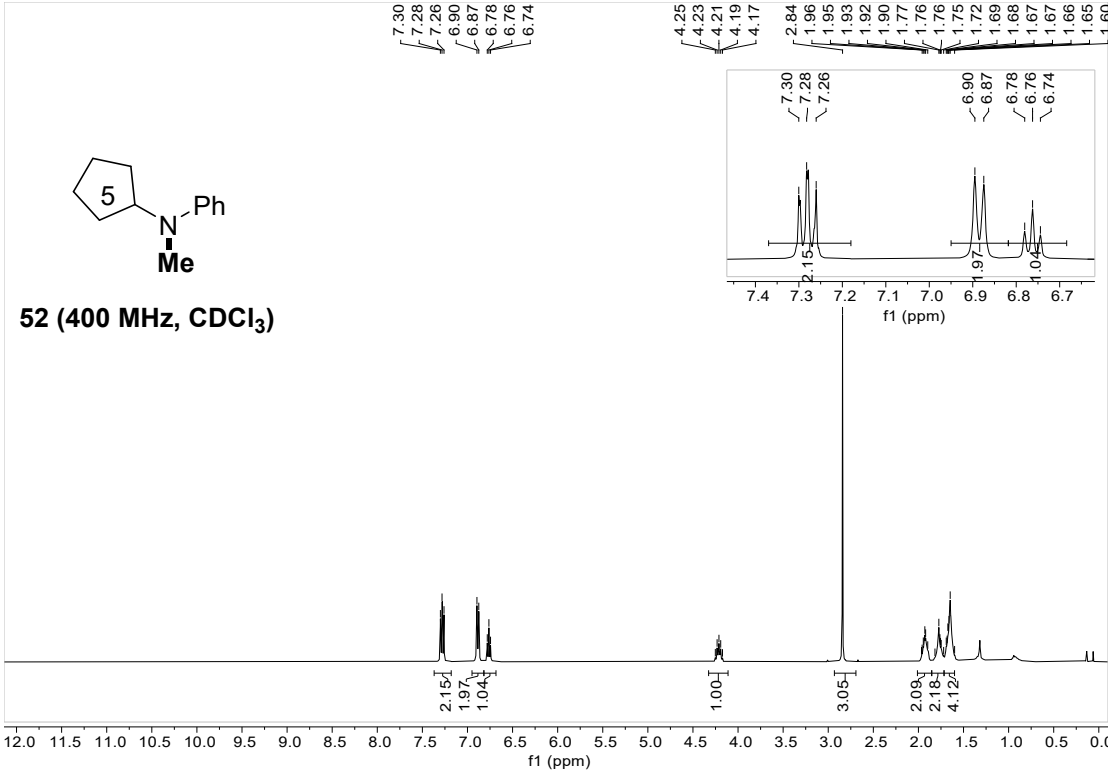
50 (400 MHz, $CDCl_3$)



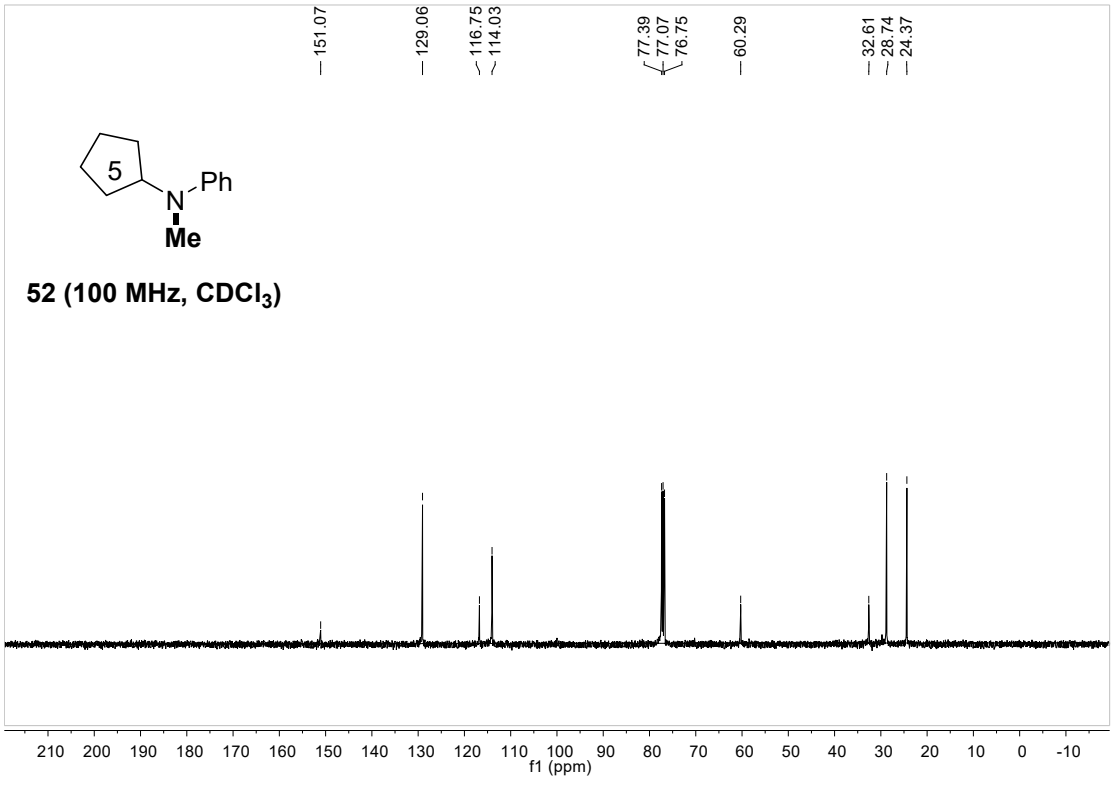
50 (100 MHz, $CDCl_3$)


7.28
7.26
7.24
7.23
7.22
7.18
7.18
7.16
6.90
6.88
6.78
6.77
6.75
4.82
4.80
4.79
4.77
4.75
3.22
3.20
3.18
3.16
3.09
3.07
3.05
3.03
2.77
Ph
N
Me
51 (400 MHz, CDCl3)
4.13
2.19
2.07
1.00
1.00
2.11
2.09
3.10
f1 (ppm)

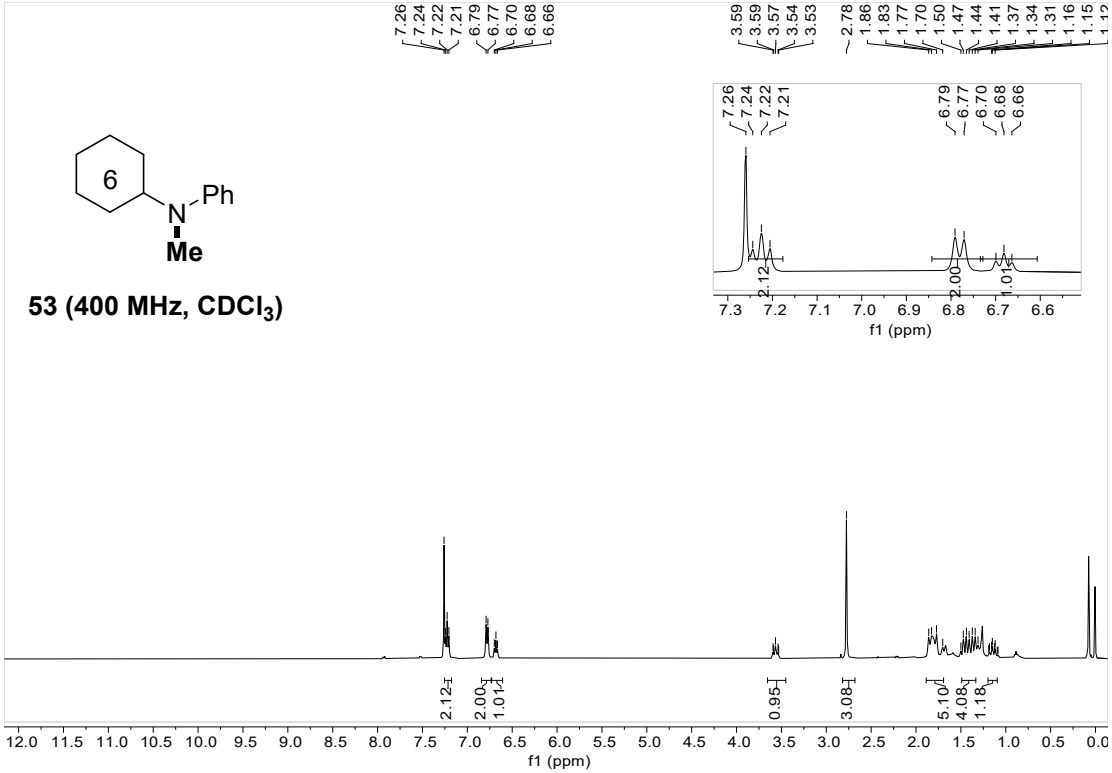

153.79
149.31
139.84
127.95
127.76
126.51
106.18
77.32
77.00
76.68
55.68
38.54
35.65
Ph
N
Me
51 (100 MHz, CDCl3)
f1 (ppm)



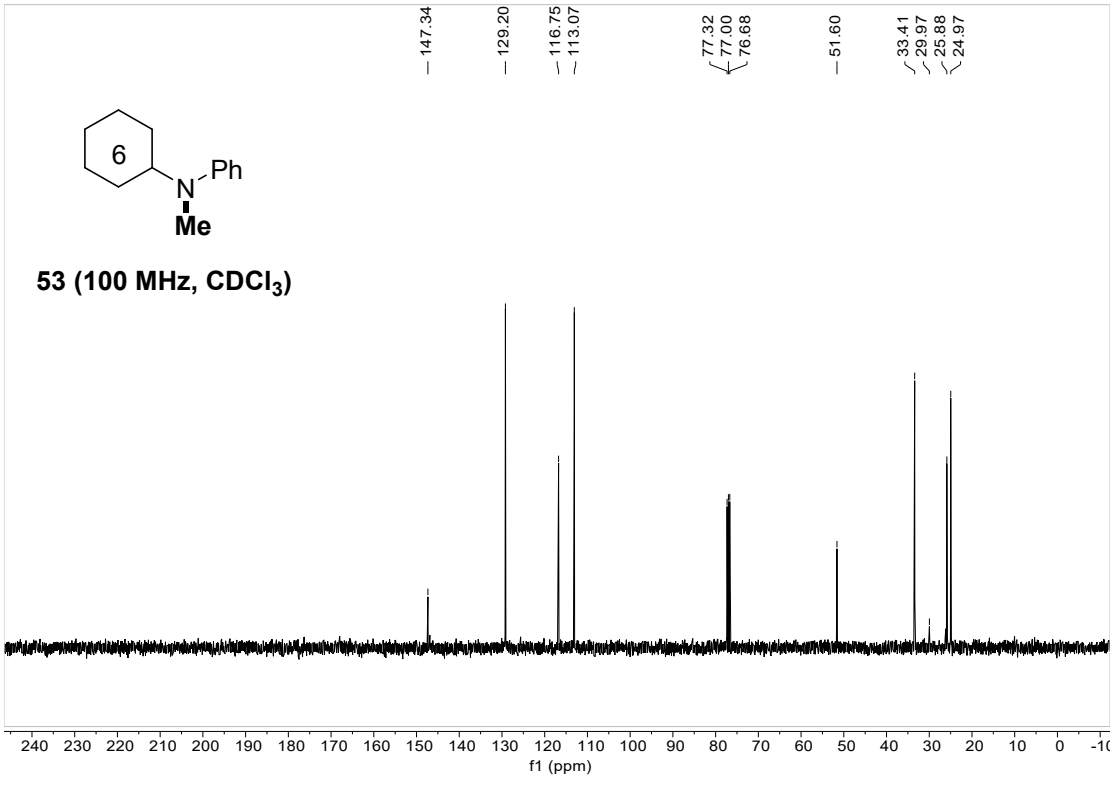
52 (400 MHz, $CDCl_3$)



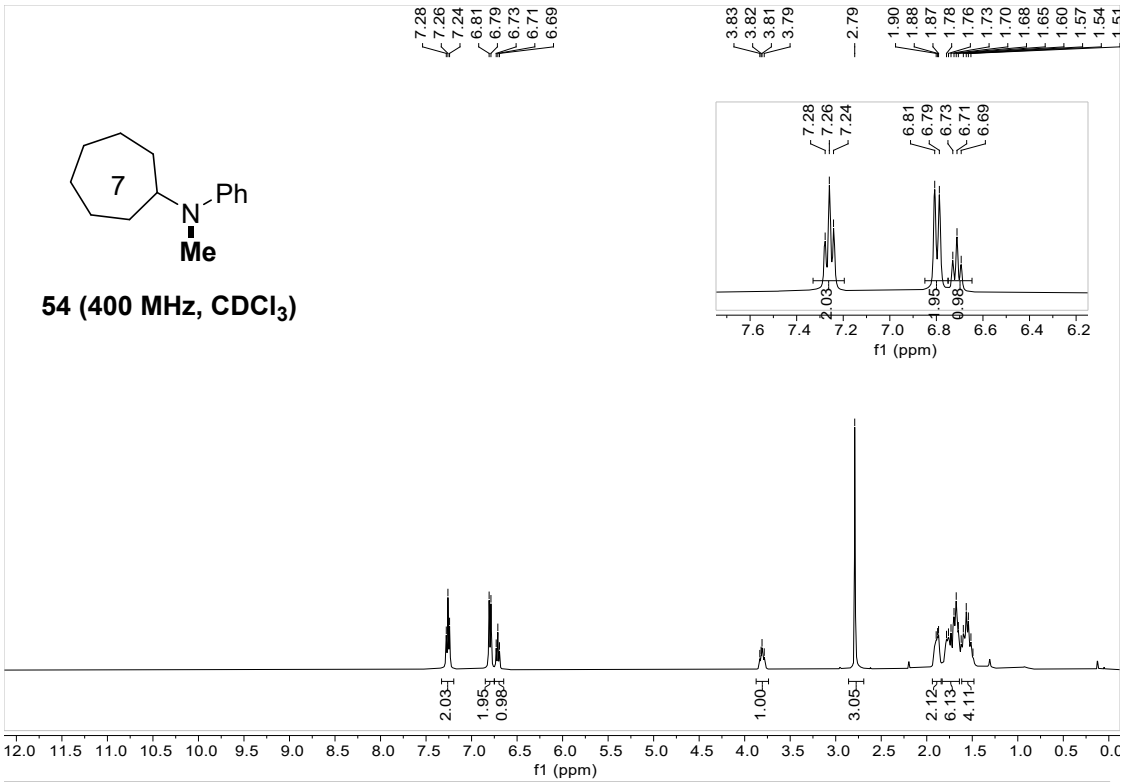
52 (100 MHz, $CDCl_3$)



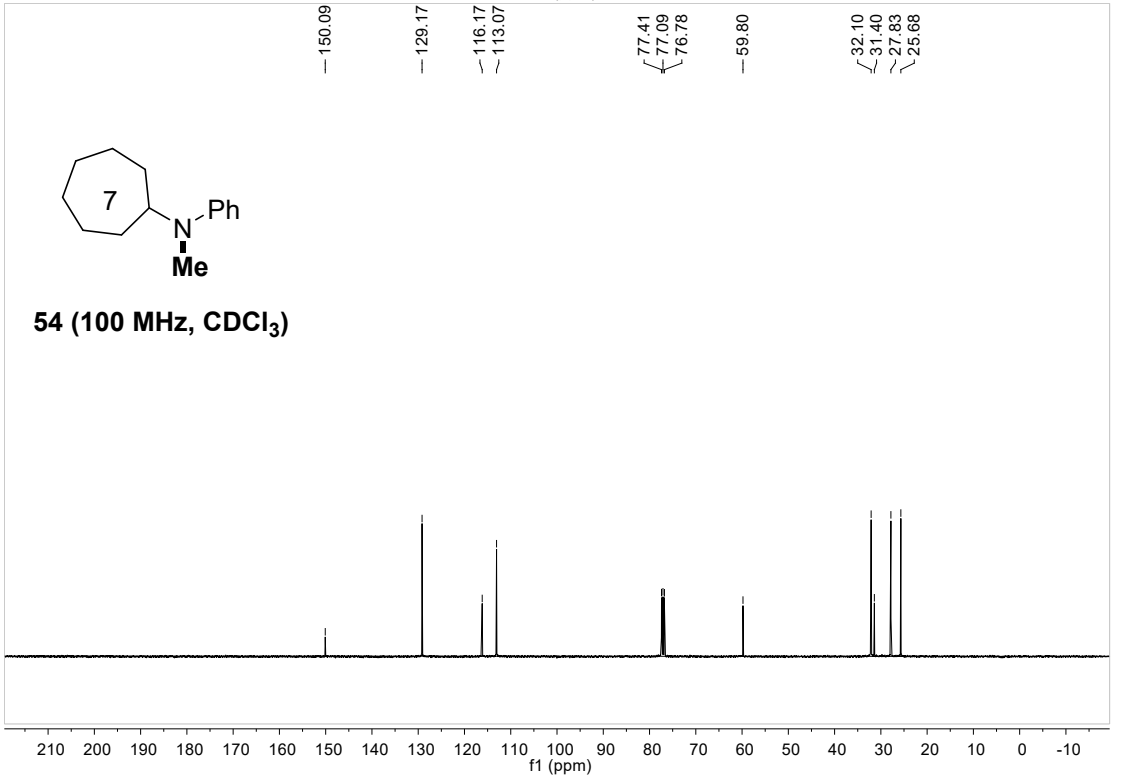
53 (400 MHz, $CDCl_3$)



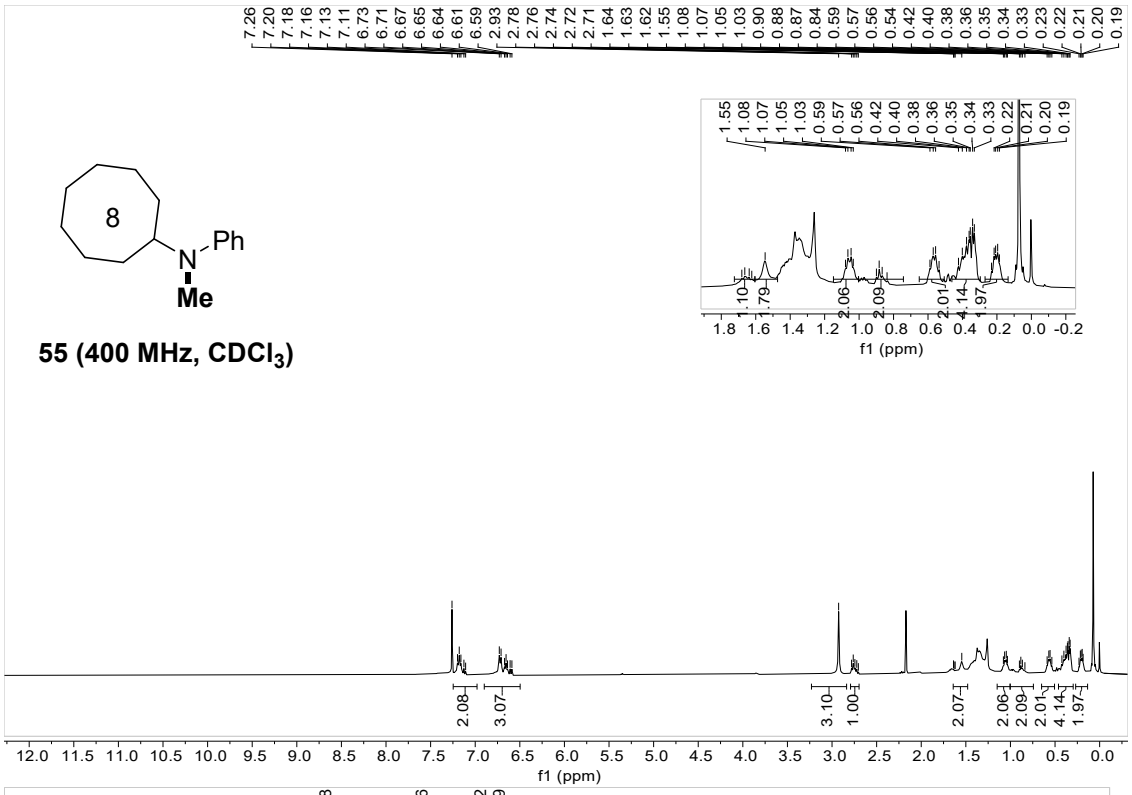
53 (100 MHz, $CDCl_3$)



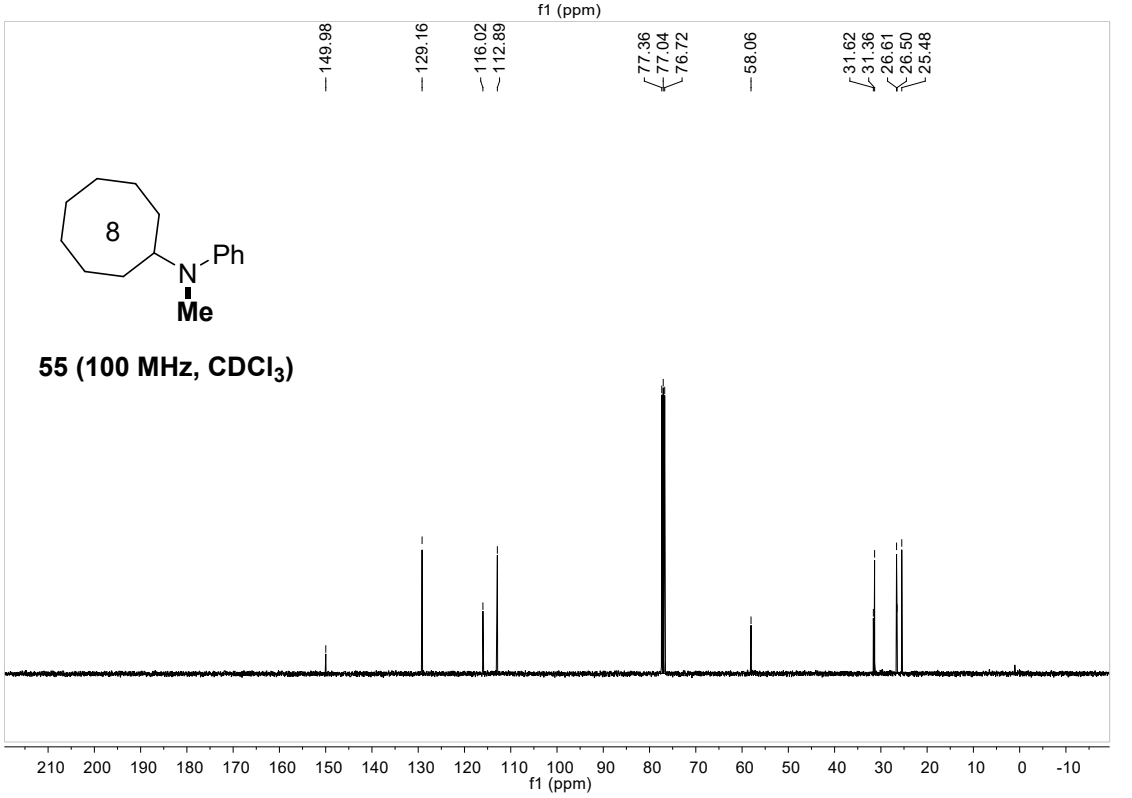
54 (400 MHz, $CDCl_3$)



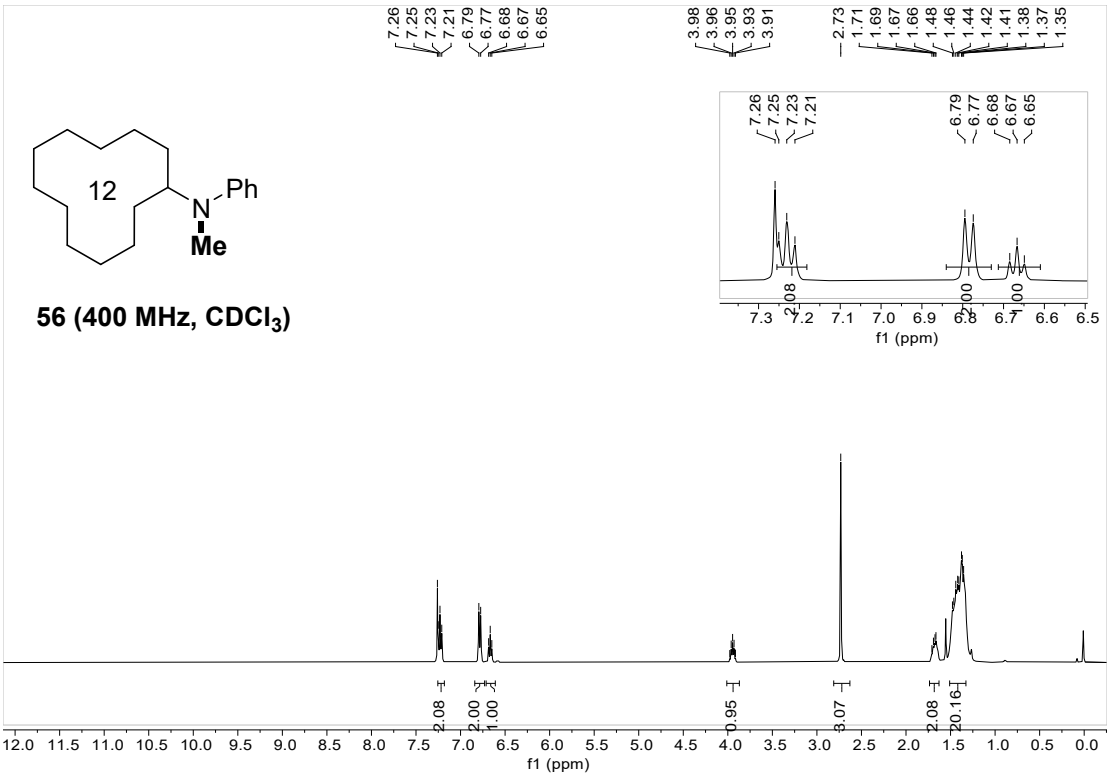
54 (100 MHz, $CDCl_3$)



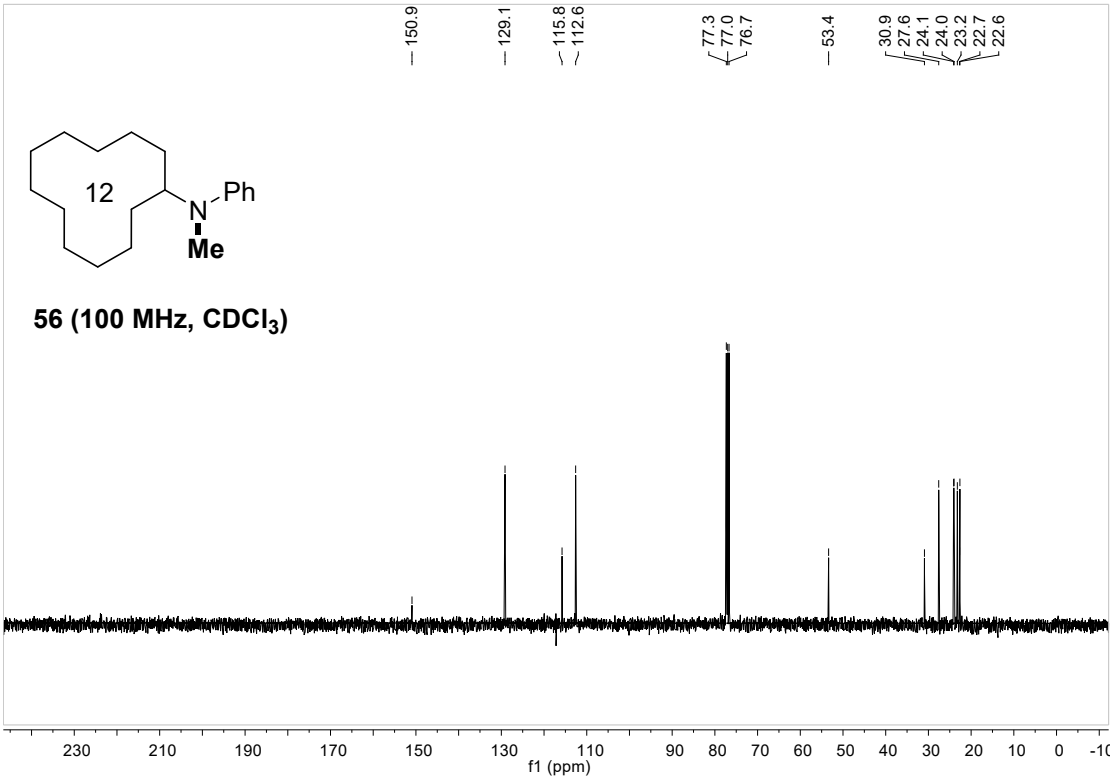
55 (400 MHz, $CDCl_3$)



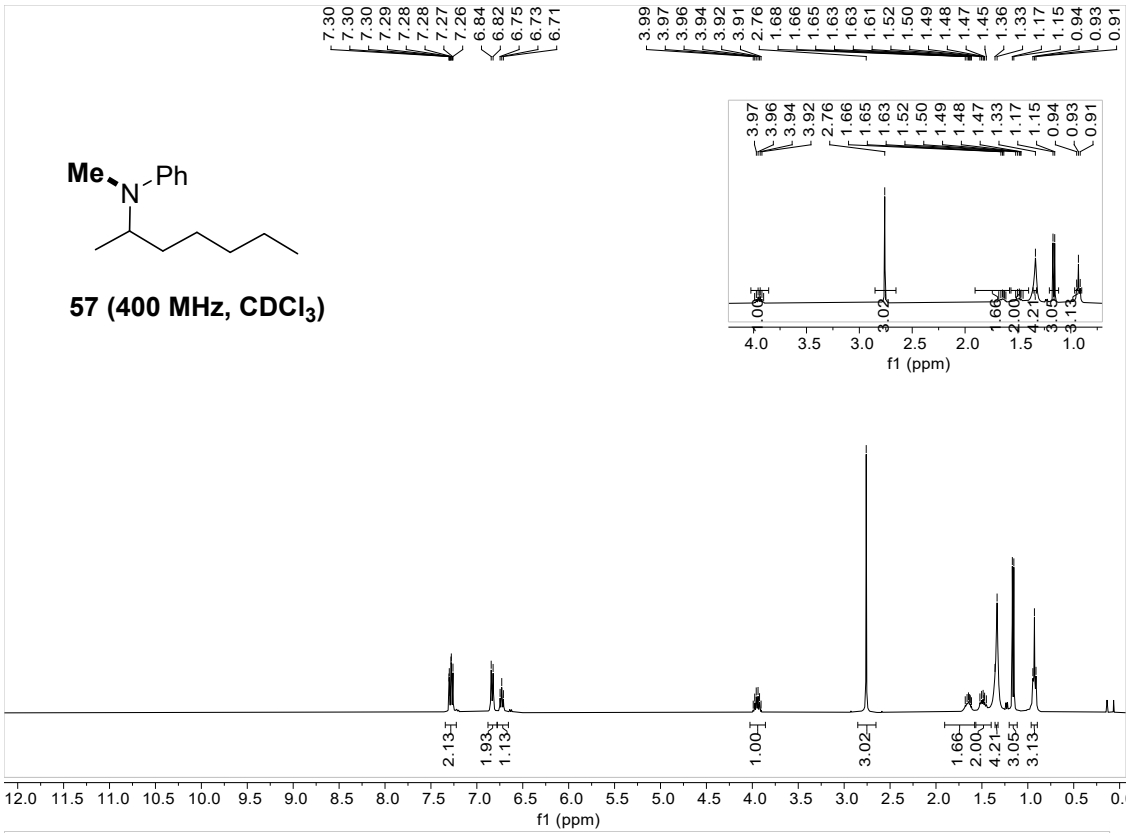
55 (100 MHz, $CDCl_3$)

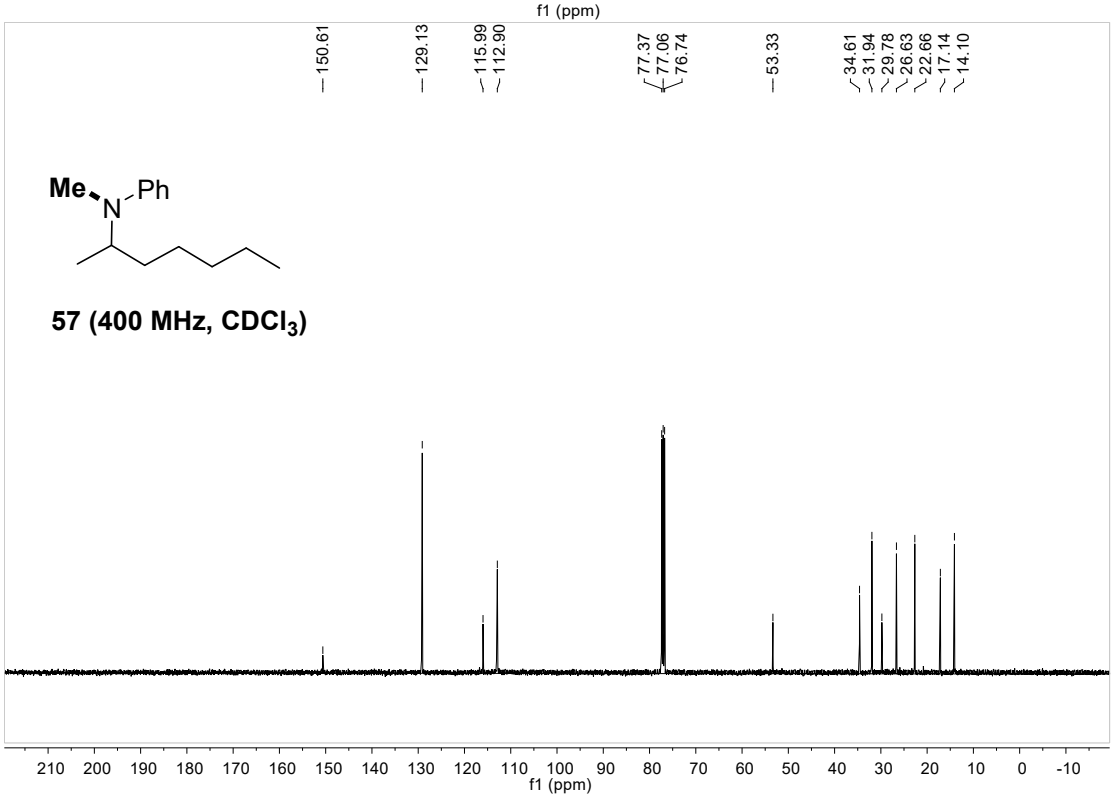


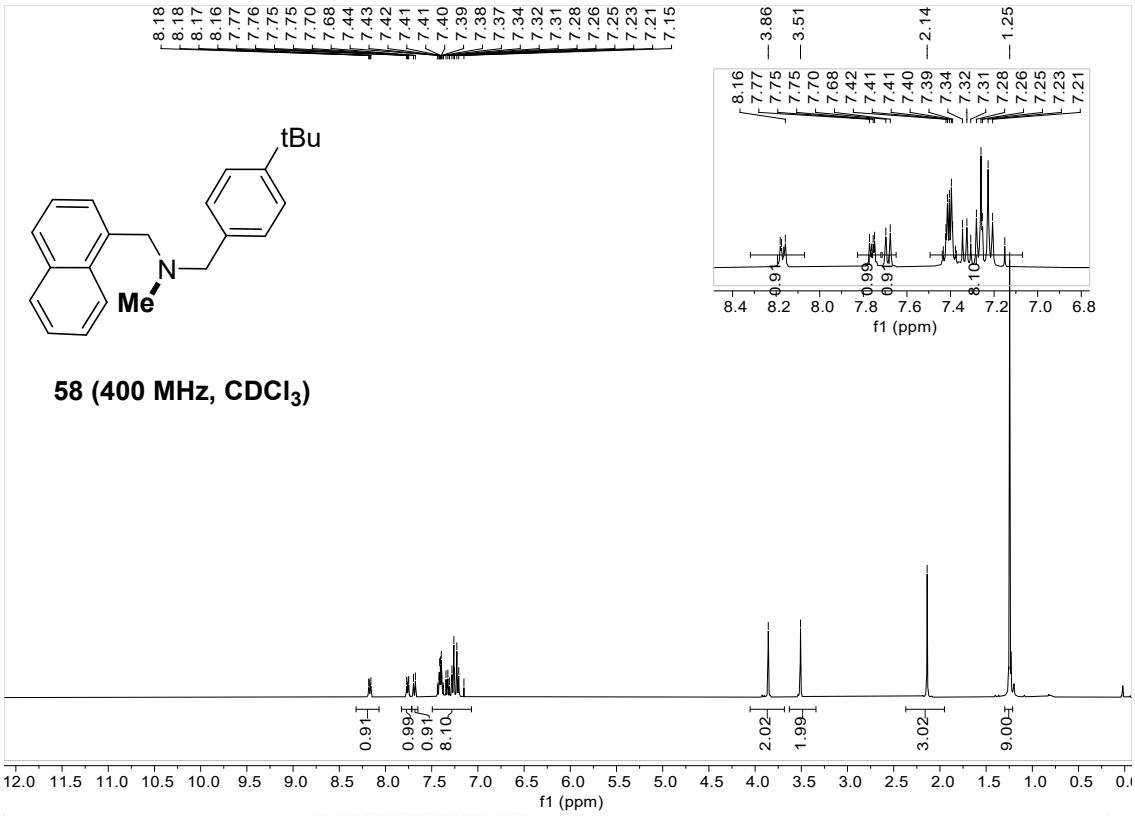
56 (400 MHz, $CDCl_3$)

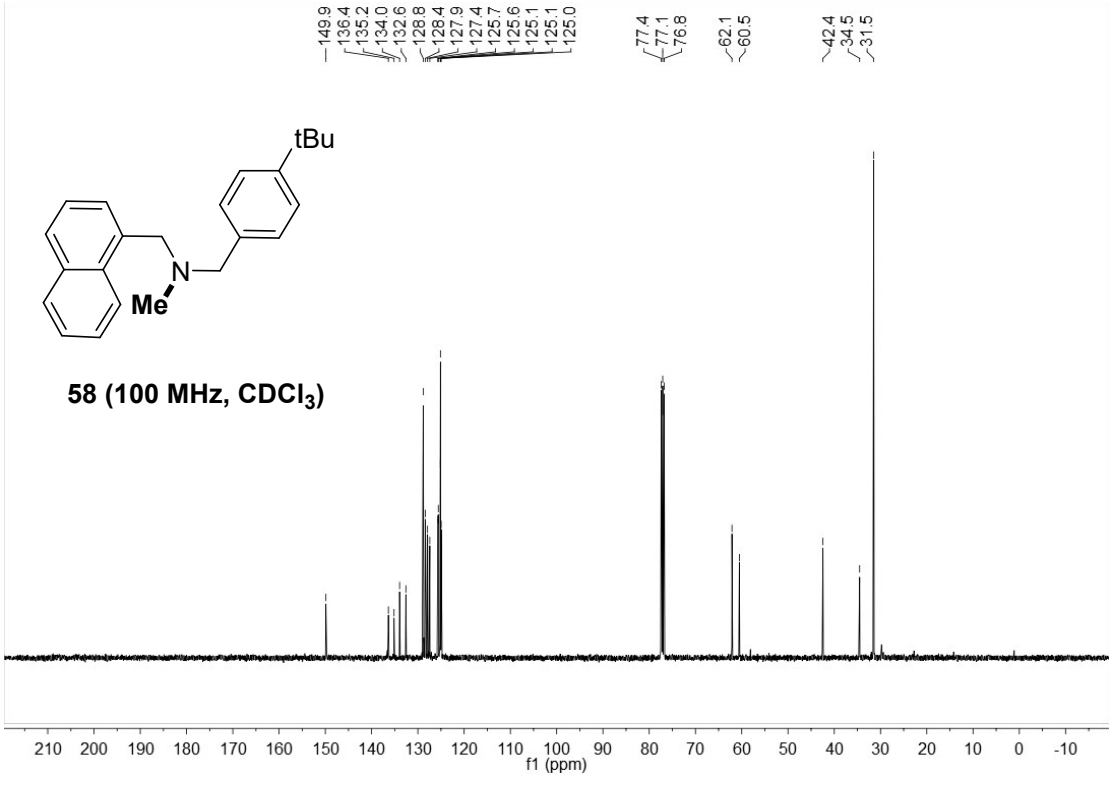


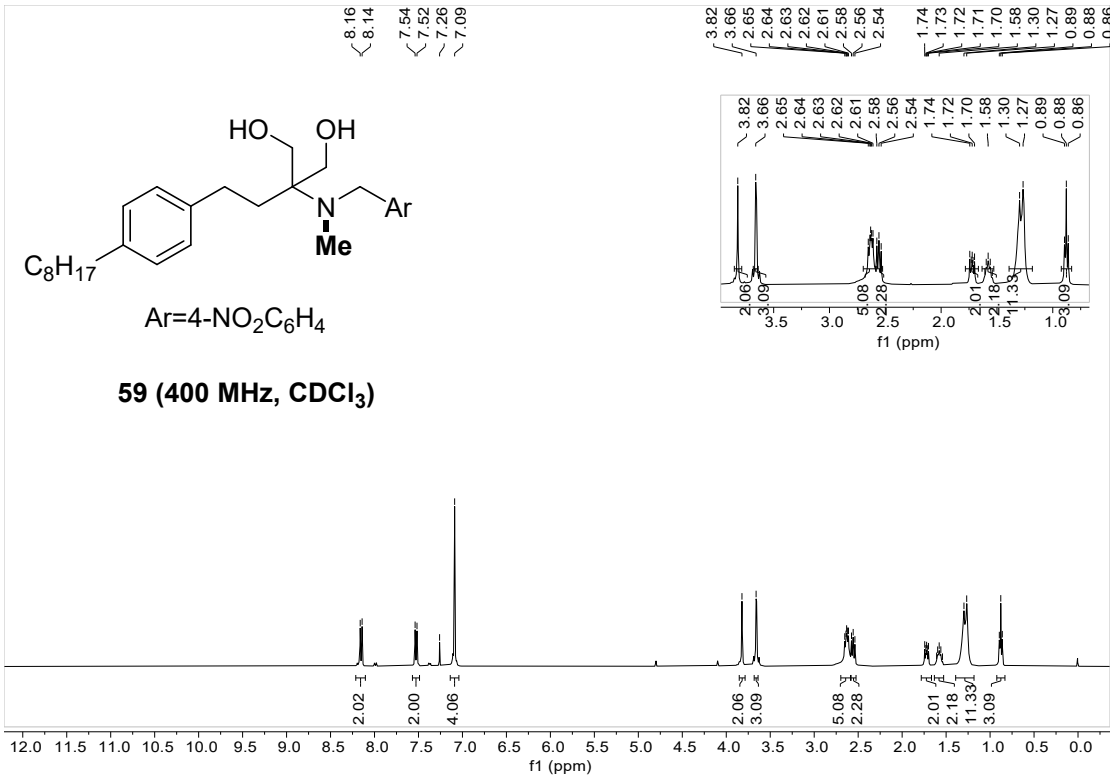
56 (100 MHz, $CDCl_3$)


Me
N
Ph
57 (400 MHz, CDCl3)
f1 (ppm)

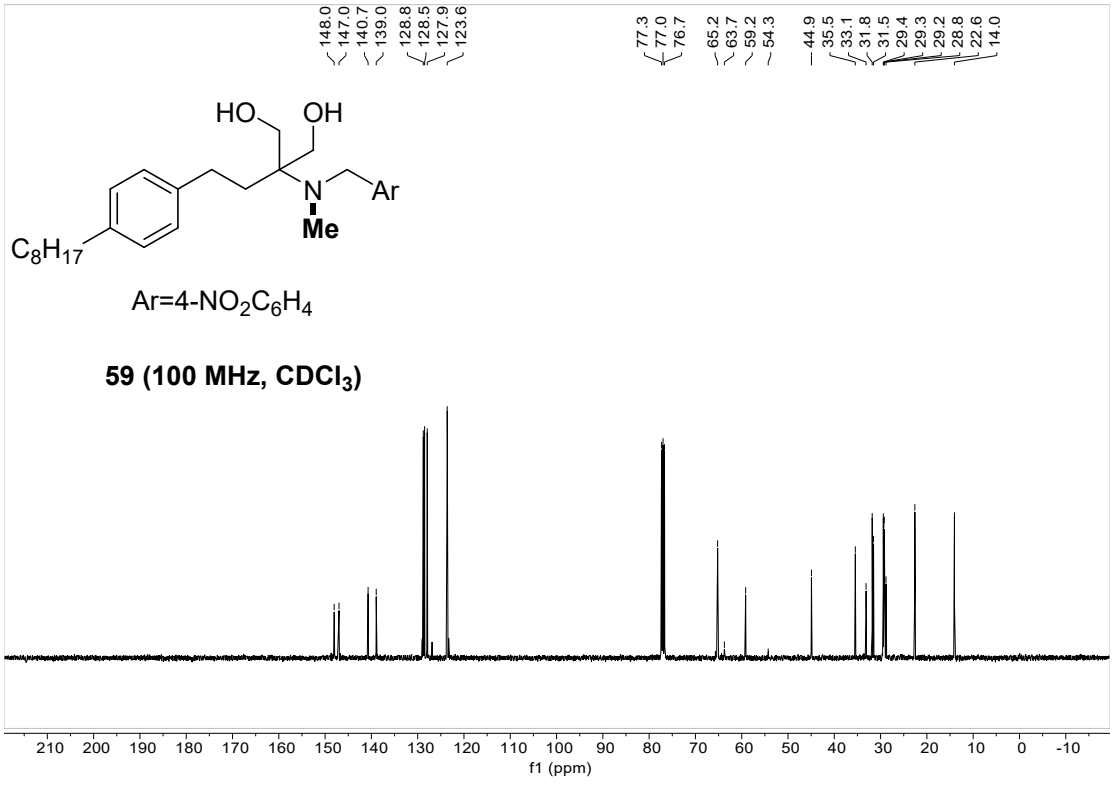

Me
N
Ph
57 (400 MHz, CDCl3)
f1 (ppm)


tBu
N
Me
58 (400 MHz, CDCl3)
f1 (ppm)

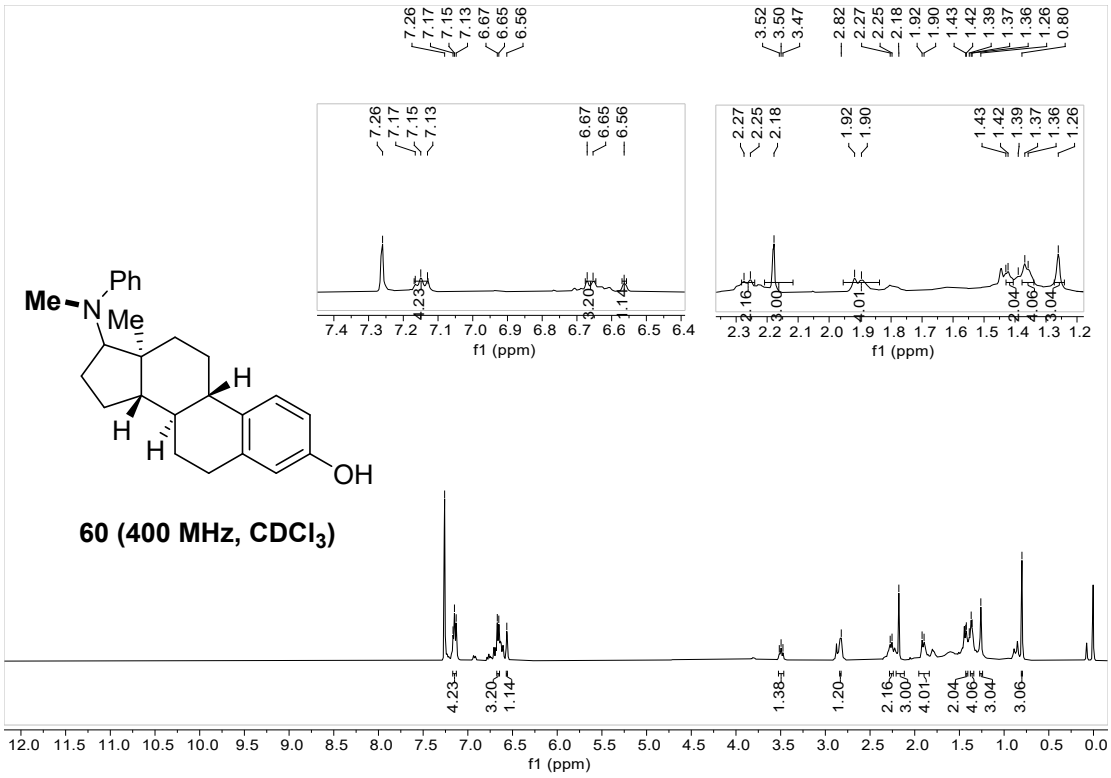

tBu
N
Me
58 (100 MHz, CDCl3)
f1 (ppm)

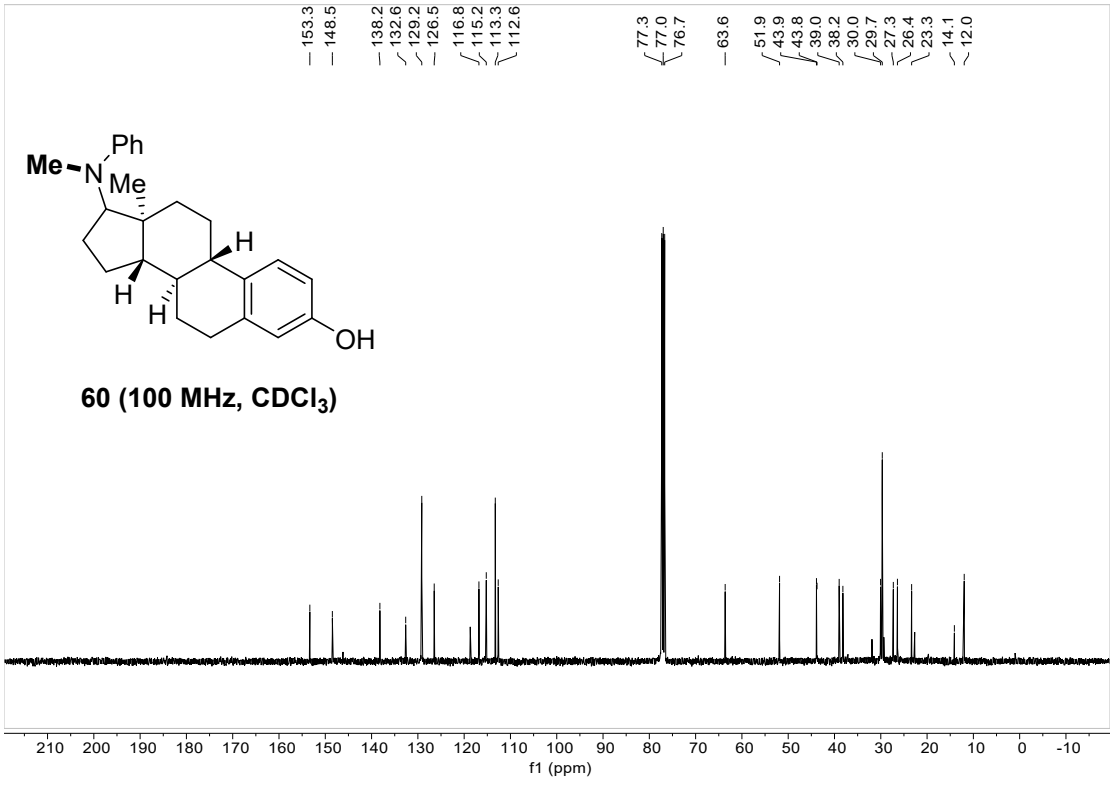


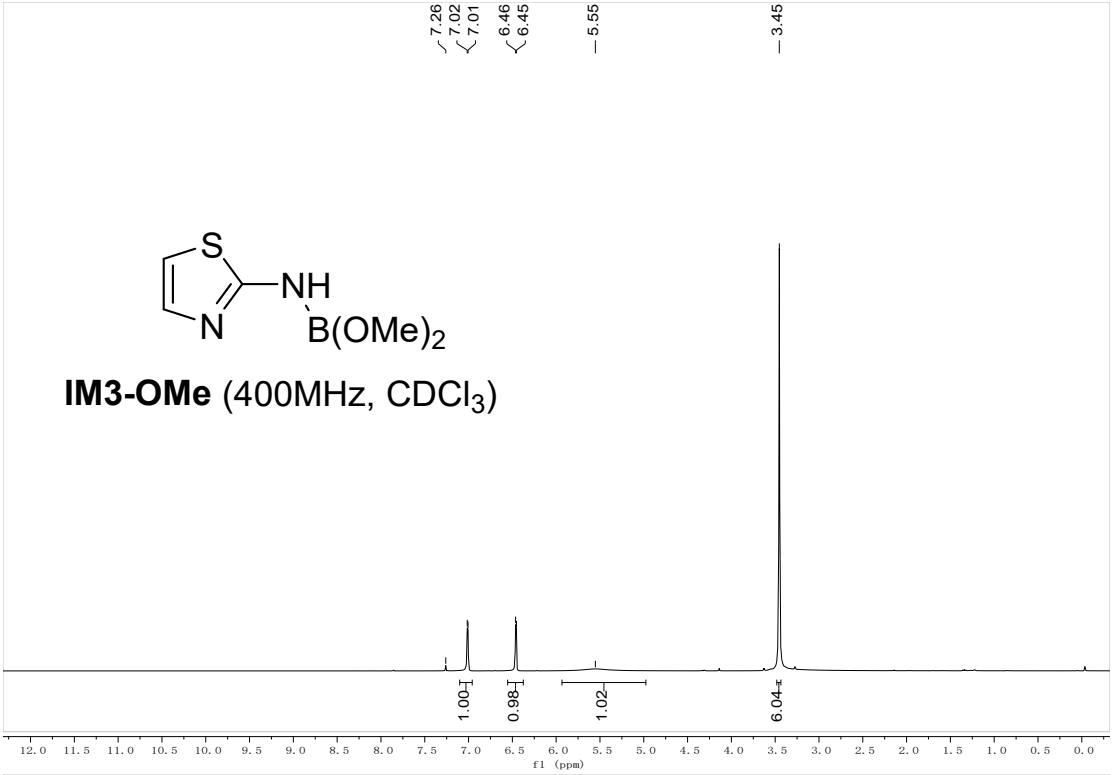
59 (400 MHz, $CDCl_3$)

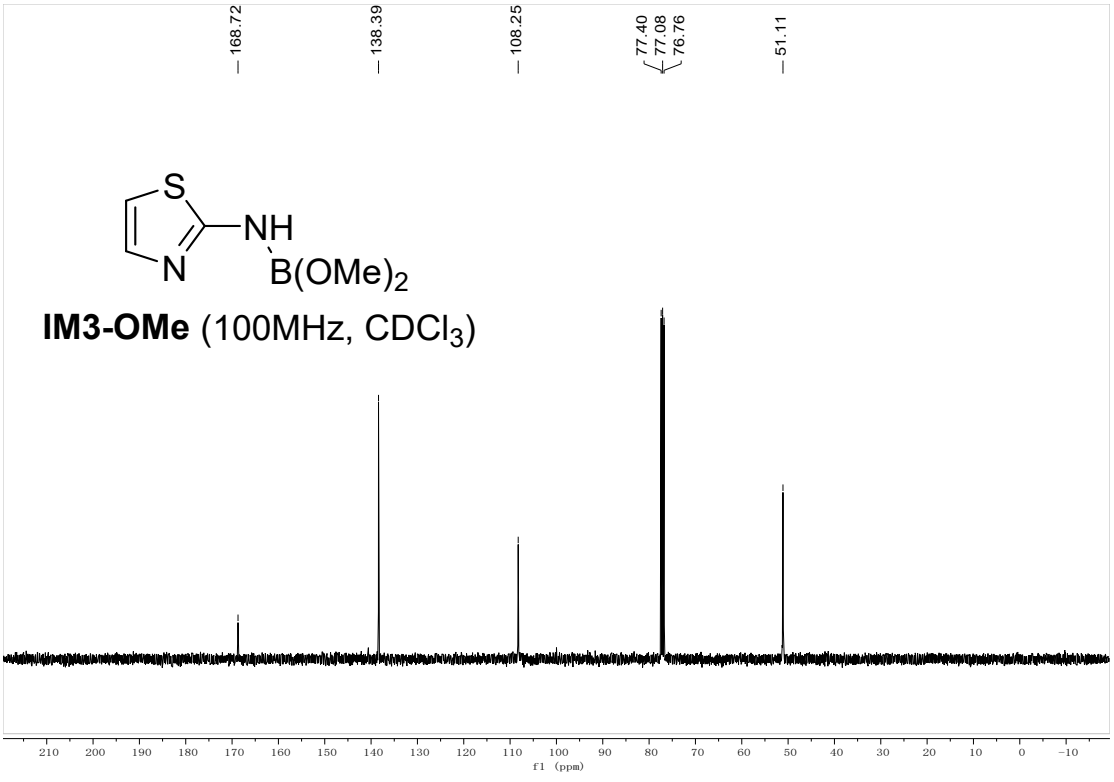


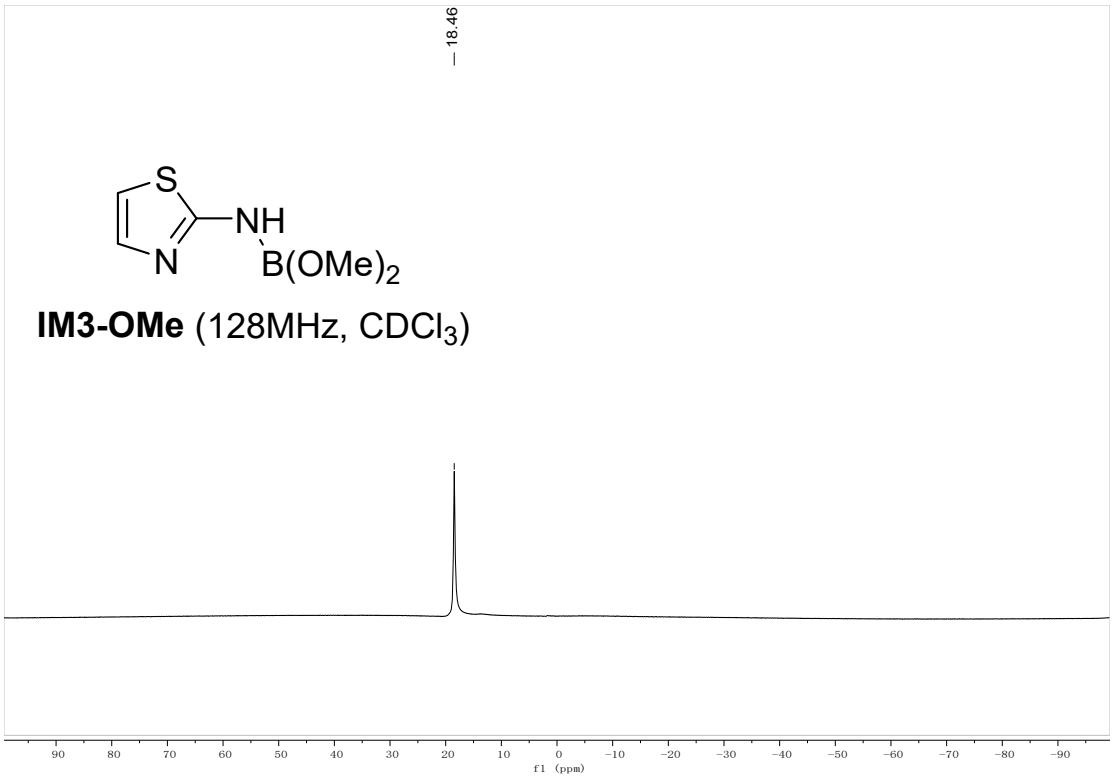
59 (100 MHz, $CDCl_3$)


Me
N
Ph
Me
H
H
H
OH
60 (400 MHz, CDCl3)
f1 (ppm)


Me
N
Ph
Me
H
H
H
OH
60 (100 MHz, CDCl3)
f1 (ppm)


7.26
7.02
7.01
6.46
6.45
5.55
3.45
S
NH
N
B(OMe)2
IM3-OMe (400MHz, CDCl3)
1.00
0.98
1.02
6.04
f1 (ppm)


168.72
138.39
108.25
77.40
77.08
76.76
51.11
S
NH
N
B(OMe)2
IM3-OMe (100MHz, CDCl3)
f1 (ppm)



IM3-OMe (128MHz, $CDCl_3$)