Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Asymmetric hydrogenations of imines with chiral alkene-derived boron Lewis acids

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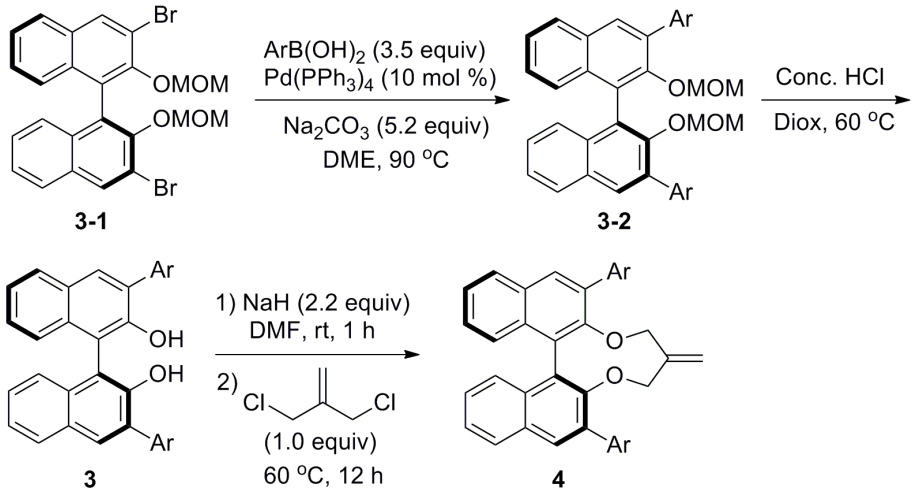
Supporting Information

General consideration: All air-sensitive compounds were handled under an atmosphere of argon or in a nitrogen-filled glovebox. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AV 300/400/500 at ambient temperature with $CDCl_3$ as solvent and TMS as internal standard. Chemical shifts (δ) were given in ppm, referenced to the residual proton resonance of TMS (0), to the carbon resonance of the $CDCl_3$ (77.23). Coupling constants (*J*) were given in Hertz (Hz). IR spectrums were recorded on Perkin-Elmer-983 spectrometer. Optical rotations were measured with PerkinElmer 341 polarimeter. Flash column chromatography was performed on silica gel (200-300 mesh). All solvents were purified by conventional methods, distilled before use. Commercially available reagents were used without further purification.

General procedure for the synthesis of chiral alkenes 4



Synthesis of compounds 3-2: To a solution of compound **3-1** (0.2661 g, 0.5 mmol) and $Pd(PPh_3)_4$ (0.058 g, 0.05 mmol) in DME (3.0 mL), arylboronic acid (1.75 mmol) and aqueous Na_2CO_3 (5.2 mmol, 2 M, 2.6 mL) were added under argon atmosphere. The resulting mixture was was stirred at room temperature for 15 min and then at 90 °C for another 12 h. After being cooled to room temperature, the reaction mixture was passed through a pad of Celite. After removal of the solvent, the residue was dissolved in DCM (20 mL). The organic phase was washed with saturated aqueous NH_4Cl (10 mL), water (10 mL), and brine (10 mL). The organic phase was dried over sodium sulfate, filtered, and concentrated. The crude residue was purified by column chromatography on silica gel using hexanes/DCM (2/1) to afford compounds **3-2**.

T. R. Wu, L. Shen and J. M. Chong, *Org. Lett.*, 2004, **6**, 2701.

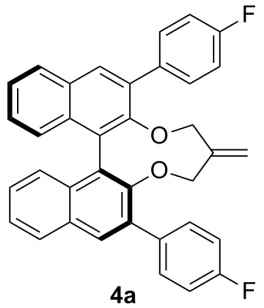
Synthesis of compounds 3: To a flask containing a stir bar were charged with compound **3-2**, conc. HCl (0.2 mL), and dioxane (3 mL). The resulting mixture was stirred at 60 °C for 12 h. After being cooled to the room temperature, the mixture was poured into a mixture of Et_2O (20 mL) and water (20 mL). The organic phase was separated, and the aqueous layer was extracted with Et_2O (2 x 20 mL). The combined organic layers were dried over sodium sulfate, filtered, and concentrated. The residue was purified by column chromatography on silica gel with hexanes/ethyl acetate (10/1) to afford compound **3.**

Synthesis of compounds 4: To a flask containing a stir bar were charged with compound **3**, NaH (60% dispersion in mineral oil, 2.5 equiv), and in DMF (10 mL). The mixture was stirred for at room temperature1 h. Then 3-cholro-2-(chloromethyl)prop-1-ene (1.0 equiv) was added, the result mixture was stirred at 60 °C for 12 h. After being cooled to the room temperature, the reaction mixture was quenched by saturated aqueous NH_4Cl (10 mL). The aqueous phase was extracted with DCM (3 x 10 mL), and the combined organic layers were dried over sodium sulfate. After being filtered and concentrated, the residue was concentrated and purified by column chromatography on silica gel with petroleum ether/ethyl acetate (100/1) to afford compounds **4.**

C. Song, Y. Kim, K. Lee, S.-G. Lee and B. Jin, *Tetrahedron: Asymmetry*, 1997, **8**, 2921.

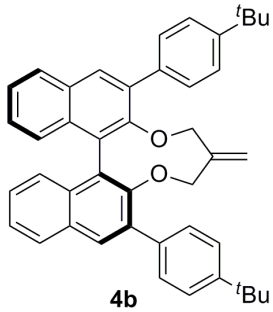
General procedure for the asymmetric hydrogenation of imines (Scheme 3): To a glass test tube (10 mL) in a nitrogen atmosphere glovebox, $HB(C_6F_5)_2$ (0.0104 g, 0.03 mmol), chiral alkene **4i** (0.0104 g, 0.03 mmol) , and dry *p*-xylene (0.75 mL) were added. The resulting mixture was stirred at room temperature for 5 min, followed by the addition of imine **6** (0.3 mmol). Then the tube was moved to a stainless-steel autoclave, and the autoclave was purged three times with H_2 and the final pressure of H_2 was adjusted to 30 bar. The reaction was stirred at 30 °C for 12 h. The solvent was removed under reduced pressure, and the crude residue was purified by flash chromatography on silica with petroleum ether/ethyl acetate (50/1) to afford amines **7**.

Characterization of chiral alkenes 4



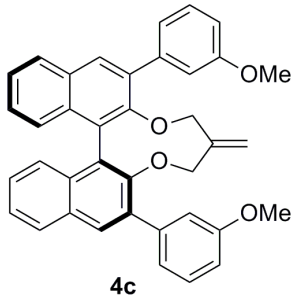
4a

4a: Yellow solid, 0.196 g, 75% yield; m.p. 120-122 °C; $[\alpha]_D^{20}$ = +107.6 (*c* 1.10, $CHCl_3$); IR (film): 1509, 1222, 1005, 837, 751 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.95-7.86 (m, 4H), 7.78-7.68 (m, 4H), 7.45-7.36 (m, 2H), 7.32-7.23 (m, 3H), 7.20-7.09 (m, 5H), 4.84 (s, 2H), 4.00 (d, *J* = 12.4 Hz, 2H), 3.85 (d, *J* = 12.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 162.6 (d, $J_{C\text{-}F}$ = 245.3 Hz), 152.2, 141.5, 135.5 (d, $J_{C\text{-}F}$ = 3.4 Hz), 133.2, 131.0, 130.9, 130.8 (d, $J_{C\text{-}F}$ = 20.3 Hz), 128.3, 126.8, 126.7, 126.3, 125.4, 123.8, 115.9 (d, $J_{C\text{-}F}$ = 21.2 Hz), 77.4, 76.0; ^{19}F NMR (377 MHz, $CDCl_3$, ppm) δ -114.8; HRMS (APCI) calcd. for $C_{36}H_{25}O_2F_2$ $[M+H]^+$: 527.1817, Found: 527.1811.



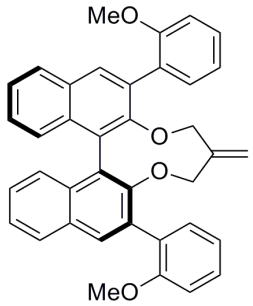
4b

4b: Yellow solid, 0.220 g, 73% yield; m.p. 170-172 °C; $[\alpha]_D^{20}$ = +88.1 (*c* 1.21, $CHCl_3$); IR (film): 2961, 1258, 1194, 1005, 836, 749 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.93 (s, 2H), 7.89 (d, *J* = 8.2 Hz, 2H), 7.72-7.65 (m, 4H), 7.50-7.44 (m, 4H), 7.42-7.34 (m, 2H), 7.26-7.20 (m, 4H), 4.85 (s, 2H), 4.01 (d, *J* = 12.4 Hz, 2H), 3.89 (d, *J* = 12.4 Hz, 2H), 1.37 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 152.5, 150.6, 141.8, 136.6, 134.1, 133.2, 131.1, 130.7, 128.8, 128.3, 126.6, 126.5, 126.4, 125.7, 125.1, 123.6, 76.0, 34.8, 31.6; HRMS (ESI) calcd. for $C_{44}H_{42}O_2Na$ $[M+Na]^+$: 625.3077, Found: 625.3068.



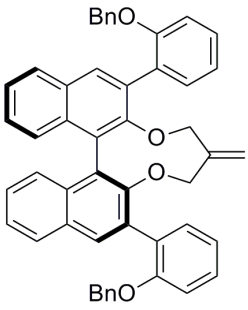
4c

4c: White solid, 0.115 g, 55% yield; m.p. 119-122 °C; $[\alpha]_D^{20}$ = +82.3 (*c* 0.83, $CHCl_3$); IR (film): 1599, 1416, 1259, 1009, 911, 734 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.94 (s, 2H), 7.90 (d, *J* = 8.2 Hz, 2H), 7.45-7.35 (m, 4H), 7.35-7.28 (m, 4H), 7.28-7.20 (m, 4H), 6.97-6.90 (m, 2H), 4.87 (s, 2H), 4.04 (d, *J* = 12.4 Hz, 2H), 3.93 (d, *J* = 12.4 Hz, 2H), 3.84 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 160.1, 152.3, 141.7, 141.1, 134.1, 133.2, 131.0, 130.8, 129.9, 128.4, 126.7, 126.6, 126.4, 125.2, 123.6, 121.8, 114.4, 113.6, 76.0, 55.6; HRMS (ESI) calcd. for $C_{38}H_{30}O_4Na$ $[M+Na]^+$: 573.2036, Found:573.2029.



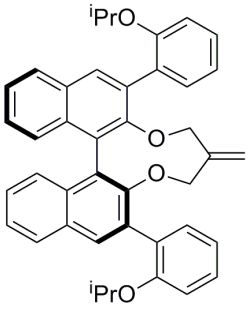
4d

4d: Yellow solid, 0.104 g, 38% yield; m.p. 146-147 °C; $[\alpha]_D^{20}$ = +16.7 (*c* 0.91, $CHCl_3$); IR (film): 1494, 1462, 1421, 1248, 910, 751, 732 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.95-7.80 (m, 4H), 7.53-7.44 (m, 2H), 7.42-7.30 (m, 4H), 7.28-7.18 (m, 4H), 7.10-6.95 (m, 4H), 4.83 (s, 2H), 3.96-3.85 (m, 4H), 3.76 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 162.7, 157.2, 153.1, 142.0, 133.4, 131.5, 130.8, 129.2, 128.2, 126.4, 126.3, 126.0, 124.7, 122.8, 120.8, 111.3, 75.9, 55.9, 36.7, 31.6; HRMS (ESI) calcd. for $C_{38}H_{30}O_4Na$ $[M+Na]^+$: 573.2036, Found: 573.2032.



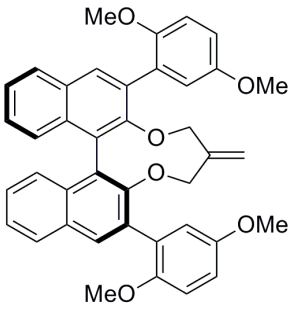
4e

4e: Yellow solid, 0.211 g, 64% yield; m.p. 111-112 °C; $[\alpha]_D^{20}$ = +2.3 (*c* 1.24, $CHCl_3$); IR (film): 1492, 1448, 1421, 1005, 911, 750 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.05-7.90 (m, 2H), 7.89-7.81 (m, 2H), 7.59-7.50 (m, 2H), 7.41-7.32 (m, 4H), 7.30-7.16 (m, 8H), 7.15-6.95 (m, 10H), 5.20-5.00 (m, 4H), 4.82 (s, 2H), 4.05-3.85 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 156.5, 153.2, 142.1, 137.3, 133.5, 131.9, 131.5, 130.7, 129.2, 128.5, 128.3, 128.2, 127.5, 127.0, 126.6, 126.4, 126.1, 124.6, 122.7, 121.3, 113.2, 75.9, 70.6, 29.9, 27.1; HRMS (ESI) calcd. for $C_{50}H_{38}O_4Na$ $[M+Na]^+$: 725.2662, Found: 725.2654.



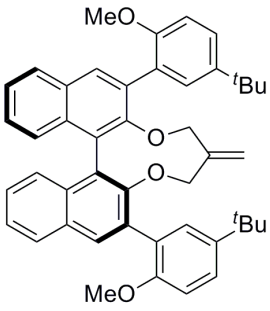
4f

4f: Yellow foam, 0.084 g, 86% yield; m.p. 110-112 °C; $[\alpha]_D^{20}$ = +6.8 (*c* 0.90, $CHCl_3$); IR (film): 1490, 1120, 1005, 749, 733 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.90 (s, 2H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.54-7.46 (m, 2H), 7.40-7.28 (m, 4H), 7.24-7.18 (m, 4H), 7.06-6.96 (m, 4H), 4.85 (s, 2H), 4.58-4.39 (m, 2H), 3.95-3.84(m, 4H), 1.32-1.18 (m, 6H), 1.13 (d, *J* = 5.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.6, 153.3, 142.3, 133.4, 131.8, 131.3, 130.7, 128.9, 128.1, 126.4, 126.1(3), 126.0(8), 124.6, 122.9, 120.7, 114.7, 75.9, 70.7, 29.9, 22.5, 22.1; HRMS (ESI) calcd. for $C_{42}H_{38}O_4Na$ $[M+Na]^+$:629.2662, Found: 629.2651.



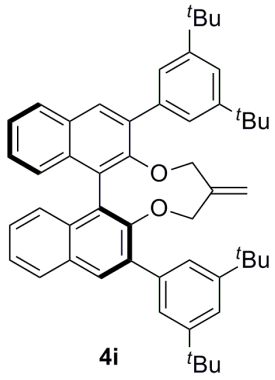
4g

4g: White solid, 0.169 g, 69% yield; m.p. 149-150 °C; $[\alpha]_D^{20}$ = -5.9 (*c* 0.92, $CHCl_3$); IR (film): 1502, 1219, 1046, 1009, 730 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.95-7.80 (m, 4H), 7.41-7.31 (m, 2H), 7.25-7.20 (m, 4H), 7.10-7.05 (m, 2H), 7.00-6.87 (m, 4H), 4.87 (s, 2H), 4.02-3.92 (m, 4H), 3.79 (s, 6H), 3.72 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 153.8, 153.0, 151.7, 142.1, 133.4, 131.6, 130.7, 128.3, 126.5, 126.4, 126.0, 124.8, 122.9, 117.0, 114.3, 112.7, 77.4, 75.9, 56.6(1), 56.5(8), 56.1; HRMS (ESI) calcd. for $C_{40}H_{34}O_6Na$ $[M+Na]^+$: 633.2248, Found:633.2241.



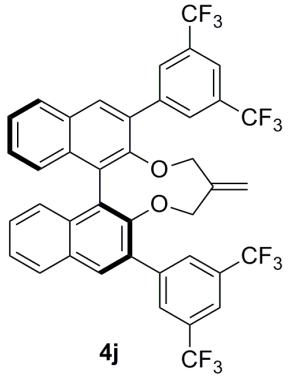
4h

4h: White solid, 0.265 g, 85% yield; m.p. 149-151 °C; $[\alpha]_D^{20}$ = +18.8 (*c* 1.16, $CHCl_3$); IR (film): 2960, 1504, 1252, 1010, 750 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.95-7.84 (m, 4H), 7.55-7.49 (m, 2H), 7.42-7.33 (m, 4H), 7.29-7.18 (m, 4H), 6.95 (s, 1H), 6.94 (s, 1H), 4.82 (s, 2H), 3.94-3.88 (m, 4H), 3.74 (s, 6H), 1.32 (s, 18H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 155.0, 153.2, 143.6, 142.3, 133.3, 131.8, 130.7, 129.4, 129.0, 128.2, 126.7, 126.4, 126.2，126.0, 125.6, 124.7, 122.4, 110.8, 75.8, 56.0, 34.4, 31.8; HRMS (ESI) calcd. for $C_{46}H_{46}O_4Na$ $[M+Na]^+$: 685.3288, Found: 685.3278.



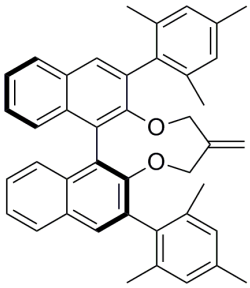
4i

4i: Yellow solid, 1.227 g, 89% yield; m.p. 172-175 °C; $[\alpha]_D^{20}$ = +75.1 (*c* 1.11, $CHCl_3$); IR (film): 2963, 1594, 1014, 876, 750, 716 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.97-7.83 (m, 4H), 7.60-7.55 (m, 4H), 7.47-7.43 (m, 2H), 7.42-7.36 (m, 2H), 7.31-7.25 (m, 4H), 4.78 (s, 2H), 3.96 (d, *J* = 12.4 Hz, 2H), 3.84 (d, *J* = 12.4 Hz, 2H), 1.37 (s, 36H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 152.6, 151.2, 142.1, 138.9, 135.2, 133.1, 131.0, 130.8, 128.3, 126.7, 126.5, 126.4, 125.0, 123.8, 122.9, 121.2, 75.7, 35.2, 31.8; HRMS (ESI) calcd. for $C_{52}H_{58}O_2Na$ $[M+Na]^+$: 737.4340, Found: 737.4329.



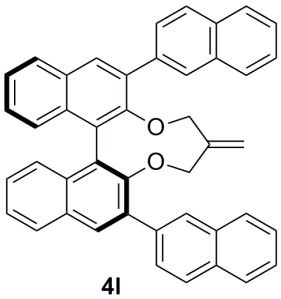
4j

4j: Yellow solid, 0.259 g, 68% yield; m.p. 170-172 °C; $[\alpha]_D^{20}$ = +74.9 (*c* 1.07, $CHCl_3$); IR (film): 2926, 1379, 1278, 1135 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.25 (s, 4H), 8.01 (s, 2H), 7.99 (s, 1H), 7.87 (s, 1H), 7.92 (s, 2H), 7.53-7.45 (m, 2H), 7.40-7.32 (m, 2H), 7.25-7.20 (m, 2H), 4.87 (s, 2H), 4.06 (d, *J* = 12.3 Hz, 2H), 3.76 (d, *J* = 12.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 151.5, 141.5, 140.5, 132.5 (q, $J_{C\text{-}F}$ = 33.4 Hz), 132.4 (q, $J_{C\text{-}F}$ = 277.7 Hz), 131.4, 129.3 (d, $J_{C\text{-}F}$ = 2.9 Hz), 128.7, 127.9, 127.1, 126.2 (d, $J_{C\text{-}F}$ = 20.0 Hz), 125.0, 124.9, 122.2, 121.5, 119.5, 76.4, 29.9; ^{19}F NMR (377 MHz, $CDCl_3$, ppm) δ -62.7; HRMS (ESI) calcd. for $C_{40}H_{23}O_2F_{12}$ $[M+H]^+$: 763.1501, Found: 763.1495.



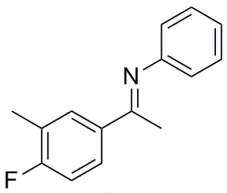
4k

4k: White solid, 0.198 g, 69% yield; m.p. 163-165 °C; $[\alpha]_D^{20}$ = -81.5 (*c* 0.82, $CHCl_3$); IR (film): 2920, 2851, 1258, 1007, 750 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.84 (d, *J* = 8.1 Hz, 2H), 7.71 (s, 2H), 7.40-7.33 (m, 2H), 7.23-7.16 (m, 2H), 7.12-7.06 (m, 2H), 7.03 (s, 2H), 6.97 (s, 2H), 4.87 (s, 2H), 3.99-3.86 (m, 4H), 2.34 (d, *J* = 11.4 Hz, 12H), 2.08 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 153.3, 143.1, 137.8, 137.2, 135.8, 135.5, 133.3, 133.0, 131.3, 130.9, 128.7(3), 128.6(7), 128.1, 126.3(4), 126.2(9), 126.1, 124.7, 121.9, 77.4, 76.0, 21.8, 21.3, 20.5; HRMS (ESI) calcd. for $C_{42}H_{38}O_2Na$ $[M+Na]^+$: 597.2775, Found: 597.2763.



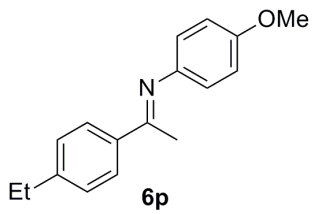
4l

4l: Yellow solid, 0.139 g, 47% yield; m.p. 103-105 °C; $[\alpha]_D^{20}$ = +74.6 (*c* 1.00, $CHCl_3$); IR (film): 2923, 1009, 913, 749 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.24 (s, 2H), 8.07 (s, 2H), 8.00-7.85 (m, 10H), 7.55-7.48 (m, 4H), 7.47-7.40 (m, 2H), 7.35-7.29 (m, 4H), 4.78 (s, 2H), 3.96 (d, *J* = 12.4 Hz, 2H), 3.86 (d, *J* = 12.4 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 152.5, 141.5, 137.1, 134.2, 133.9, 133.3, 132.8, 131.2, 131.1, 128.4(4), 128.3(9), 127.9(4), 127.9(1), 127.6, 126.9, 126.8, 126.5, 126.4(1), 126.3(7), 125.3, 123.7, 76.2, 29.9; HRMS (ESI) calcd. for $C_{44}H_{31}O_2$ $[M+H]^+$: 591.2319, Found: 591.2314.



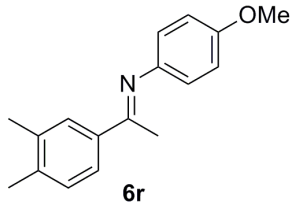
6k

(*E*)-*N*-(1-(4-fluoro-3-methylphenyl)ethylidene)aniline: Yellow solid, m.p. 46-47 °C; IR (film): 1630, 1447, 1114, 831, 708 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.90-7.82 (m, 1H), 7.78-7.69 (m, 1H), 7.39-7.30 (m, 2H), 7.12-7.01 (m, 2H), 6.82-6.74 (m, 2H), 2.33 (d, J = 1.7 Hz, 3H), 2.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 164.7, 163.1 (d, J_{C-F} = 248.0 Hz), 151.8, 135.6 (d, J_{C-F} = 3.3 Hz), 130.8 (d, J_{C-F} = 5.8 Hz), 129.2, 126.8 (d, J_{C-F} = 8.6 Hz), 125.1 (d, J_{C-F} = 17.5 Hz), 123.5, 119.6, 115.0 (d, J_{C-F} = 22.6 Hz), 17.5, 14.8 (d, J_{C-F} = 3.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$, ppm) δ -114.7; HRMS (APCI) calcd. for $C_{15}H_{15}NF$ $[M+H]^+$: 228.1183, Found: 228.1180.



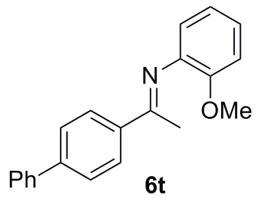
6p

(*E*)-*N*-(1-(4-ethylphenyl)ethylidene)-4-methoxyaniline: Yellow solid, m.p. 66-67 °C; IR (film): 2961, 1502, 1367, 1033, 845, 830 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ7.95-7.84 (m, 2H), 7.35-7.20 (m, 2H), 6.95-6.85 (m, 2H), 6.78-6.70 (m, 2H), 3.81 (s, 3H), 2.70 (q, J = 7.6 Hz, 2H), 2.23 (s, 3H), 1.26 (t, J = 7.6 Hz, 3H);^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.8, 156.1, 147.1, 145.2, 137.5, 128.0, 127.4, 121.0, 114.4, 55.7, 28.9, 17.4, 15.7; HRMS (ESI) calcd. for $C_{17}H_{20}ON$ $[M+H]^+$: 254.1539, Found: 254.1540.



6r

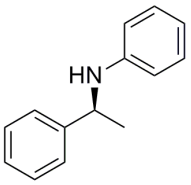
(*E*)-*N*-(1-(3,4-dimethylphenyl)ethylidene)-4-methoxyaniline: Red solid, m.p. 72-73 °C; IR (film): 1627, 1502, 1240, 1034, 846, 755 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.78 (s, 1H), 7.68-7.62 (m, 1H), 7.18 (d, J = 7.9 Hz, 1H), 6.94-6.85 (m, 2H), 6.79-6.70 (m, 2H), 3.79 (s, 3H), 2.31 (s, 3H), 2.30 (s, 3H), 2.21 (s, 3H);^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 165.9, 156.0, 145.2, 139.4, 137.6, 136.7, 129.7, 128.3, 124.9, 120.9, 114.4, 55.6, 20.0, 19.9, 17.4; HRMS (ESI) calcd. for $C_{17}H_{20}ON$ $[M+H]^+$: 254.1539, Found: 254.1538.



6t

(*E*)-*N*-(1-([1,1'-biphenyl]-4-yl)ethylidene)-2-methoxyaniline: Yellow solid, m.p. 141-143 °C; IR (film): 1630, 1487, 1240, 766, 756 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ8.14-8.04 (m, 2H), 7.72-7.60 (m, 4H), 7.52-7.41 (m, 2H), 7.40-7.33 (m, 1H), 7.12-7.03 (m, 1H), 7.01-6.90 (m, 2H), 6.85-6.75 (m, 1H), 3.79 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ166.8, 149.2, 143.3, 140.8, 140.7, 138.5, 129.0, 128.0, 127.9, 127.3, 127.2, 124.4, 121.1, 120.8, 111.8, 55.8, 17.9; HRMS (ESI) calcd. for $C_{21}H_{20}ON$ $[M+H]^+$: 302.1539, Found: 302.1538.

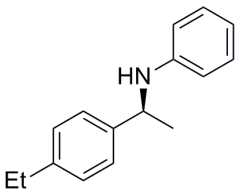
Characterization of amine products 7



7a

(*S*)-*N*-(1-phenylethyl)aniline: Colorless liquid, 0.0573 g, 97% yield, 65% ee, $[\alpha]_D^{20}$ = +3.2 (*c* 1.33, $CHCl_3$); ^1H NMR (300 MHz, $CDCl_3$, ppm) δ 7.42-7.25 (m, 4H), 7.25-7.16 (m, 1H), 7.08 (t, *J* = 8.3 Hz, 2H), 6.63 (t, *J* = 7.3 Hz, 1H), 6.50 (d, *J* = 7.8 Hz, 2H), 4.48 (q, *J* = 6.7 Hz, 1H), 4.00 (br s, 1H), 1.50 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 147.5, 145.4, 129.3, 128.8, 127.0, 126.0, 117.4, 113.5, 53.6, 25.2.

W. Li, G. Hou, M. Chang and X. Zhang, *Adv. Synth. Catal.*, 2009, **351**, 3123.

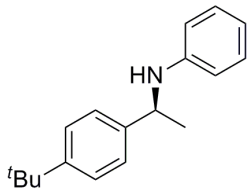


7b

(*S*)-*N*-(1-(4-ethylphenyl)ethyl)aniline: Colorless liquid, 0.0650 g, 96% yield, 78% ee, $[\alpha]_D^{20}$

= +0.6 (*c* 1.09, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.26 (d, *J* = 8.0 Hz, 2H), 7.17-7.02 (m, 4H), 6.67-6.57 (m, 1H), 6.54-6.45 (m, 2H), 4.44 (q, *J* = 6.7 Hz, 1H), 3.96 (br s, 1H), 2.60 (q, *J* = 7.6 Hz, 2H), 1.47 (d, *J* = 6.7 Hz, 3H), 1.21 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 147.6, 142.9, 142.6, 129.3, 128.3, 126.0, 117.3, 113.4, 53.3, 28.6, 25.1, 15.7.

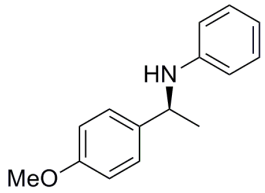
Y. Liu and H. Du, *J. Am. Chem. Soc.*, 2013, **135**, 12968.



7c

(*S*)-*N*-(1-(4-(*tert*-butyl)phenyl)ethyl)aniline: Colorless liquid, 0.0697 g, 92% yield, 79% ee, $[\alpha]_D^{20}$ = -9.1 (*c* 0.86, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.36-7.24 (m, 4H), 7.13-7.03 (m, 2H), 6.68-6.58 (m, 1H), 6.57-6.46 (m, 2H), 4.47 (q, *J* = 6.7 Hz, 1H), 3.97 (br s, 1H), 1.49 (d, *J* = 6.7 Hz, 3H), 1.30 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 149.8, 147.6, 142.2, 129.3, 125.7(1), 125.6(6), 117.3, 113.4, 53.1, 34.6, 31.6, 24.9.

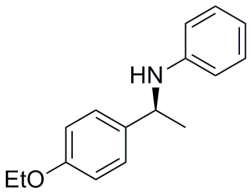
Y. Liu and H. Du, *J. Am. Chem. Soc.*, 2013, **135**, 12968.



7d

(*S*)-*N*-(1-(4-methoxyphenyl)ethyl)aniline: Colorless liquid, 0.0570 g, 84% yield, 67% ee, $[\alpha]_D^{20}$ = +8.2 (*c* 1.01, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.26 (d, *J* = 8.5 Hz, 2H), 7.08 (t, *J* = 7.7 Hz, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 6.62 (t, *J* = 7.3 Hz, 1H), 6.50 (d, *J* = 7.9 Hz, 2H), 4.43 (q, *J* = 6.7 Hz, 1H), 3.96 (br s, 1H), 3.75 (s, 3H), 1.47 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 158.7, 147.5, 137.4, 129.3, 127.1, 117.3, 114.2, 113.5, 55.4, 53.0, 25.1.

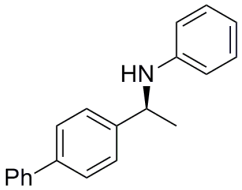
W. Li, G. Hou, M. Chang and X. Zhang, *Adv. Synth. Catal.*, 2009, **351**, 3123.



7e

(*S*)-*N*-(1-(4-ethoxyphenyl)ethyl)aniline: Colorless liquid, 0.0609 g, 84% yield, 65% ee, $[\alpha]_D^{20}$ = +5.4 (*c* 0.88, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.31-7.20 (m, 2H), 7.13-7.03 (m, 2H), 6.87-6.79 (m, 2H), 6.67-6.59 (m, 1H), 6.55-6.46 (m, 2H), 4.43 (q, *J* = 6.6 Hz, 1H), 4.00 (q, *J* = 7.0 Hz, 2H), 3.95 (br s, 1H), 1.48 (d, *J* = 6.7 Hz, 3H), 1.38 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 158.0, 147.6, 137.3, 129.2, 127.0, 117.3, 114.7, 113.5, 63.5, 53.0, 25.1, 15.1.

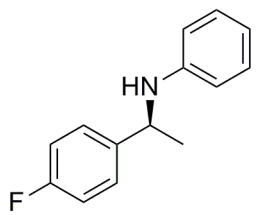
Y. Liu and H. Du, *J. Am. Chem. Soc.*, 2013, **135**, 12968.



7f

(*S*)-*N*-(1-([1,1'-biphenyl]-4-yl)ethyl)aniline: White solid, 0.0781 g, 95% yield, 66% ee, $[\alpha]_D^{20}$ = -20.5 (*c* 0.89, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.62-7.49 (m, 4H), 7.48-7.36 (m, 4H), 7.35-7.27 (m, 1H), 7.16-7.03 (m, 2H), 6.65 (t, *J* = 7.3 Hz, 1H), 6.54 (d, *J* = 8.0 Hz, 2H), 4.53 (q, *J* = 6.6 Hz, 1H), 4.03 (br s, 1H), 1.54 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 147.5, 144.5, 141.1, 140.0, 129.3, 128.9, 127.6, 127.3, 127.2, 126.5, 117.5, 113.5, 53.4, 25.2.

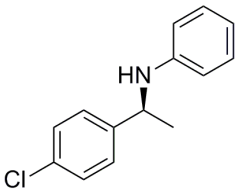
Y. Liu and H. Du, *J. Am. Chem. Soc.*, 2013, **135**, 12968.



7g

(*S*)-*N*-(1-(4-fluorophenyl)ethyl)aniline: Colorless liquid, 0.0656 g, 99% yield, 60% ee, $[\alpha]_D^{20}$ = +27.9 (*c* 0.99, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.37-7.25 (m, 2H), 7.13-7.03 (m, 2H), 7.02-6.92 (m, 2H), 6.64 (t, *J*= 7.3 Hz, 1H), 6.47 (d, *J* = 7.8 Hz, 2H), 4.44 (q, *J* = 6.7 Hz, 1H), 3.97 (br s, 1H), 1.46 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 161.9 (d, J_{C-F} = 242.8 Hz), 147.3, 141.1(d, J_{C-F} = 3.0 Hz), 129.3, 127.5 (d, J_{C-F} = 8.0 Hz), 117.6, 115.6 (d, J_{C-F} = 21.2 Hz), 113.5, 53.1, 25.3; ^{19}F NMR (377 MHz, $CDCl_3$, ppm) δ -116.9.

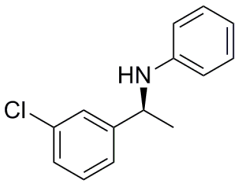
W. Pan, Y. Deng, J. He, B. Bai and H. Zhu, *Tetrahedron*, 2013, **69**, 7253.



7h

(*S*)-*N*-(1-(4-chlorophenyl)ethyl)aniline: Colorless liquid, 0.0645 g, 93% yield, 58% ee, $[\alpha]_D^{20}$ = +5.8 (*c* 0.86, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.32-7.21 (m, 4H), 7.13-7.02 (m, 2H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.46 (d, *J* = 7.8 Hz, 2H), 4.43 (q, *J* = 6.7 Hz, 1H), 3.97 (br s, 1H), 1.46 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 147.2, 144.0, 132.6, 129.3, 129.0, 127.4, 117.7, 113.5, 53.1, 25.2.

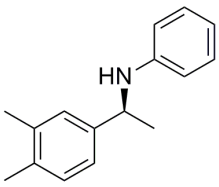
A. Baeza and A. Pfaltz, *Chem. Eur. J.*, 2010, **16**, 4003.



7i

(*S*)-*N*-(1-(3-chlorophenyl)ethyl)aniline: Colorless liquid, 0.0662 g, 95% yield, 45% ee, $[\alpha]_D^{20}$ = +10.6 (*c* 1.02, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.46 (s, 1H), 7.38-7.26 (m, 3H), 7.25-7.13 (m, 2H), 6.77 (t, *J* = 7.3 Hz, 1H), 6.59 (d, *J* = 7.9 Hz, 2H), 4.53 (q, *J* = 6.7 Hz, 1H), 4.08 (br s, 1H), 1.58 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 147.8, 147.1, 134.7, 130.1, 129.3, 127.3, 126.2, 124.2, 117.7, 113.5, 53.4, 25.2.

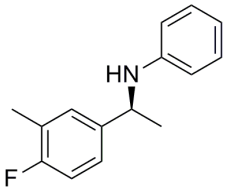
S. Zhu, J. Xie, Y. Zhang, S. Li and Q. Zhou, *J. Am. Chem. Soc.*, 2006, **128**, 12886.



7j

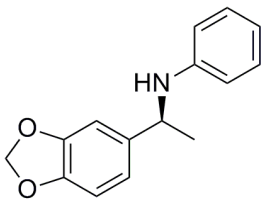
(*S*)-*N*-(1-(3,4-dimethylphenyl)ethyl)aniline: Colorless liquid, 0.0659 g, 97% yield, 83% ee, $[\alpha]_D^{20}$ = +7.3 (*c* 0.87, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.15-7.02 (m, 5H), 6.62 (t, *J* = 7.3 Hz, 1H), 6.51 (d, *J* = 7.9 Hz, 2H), 4.41 (q, *J* = 6.7 Hz, 1H), 3.96 (br s, 1H), 2.23 (s, 3H), 2.22 (s, 3H), 1.48 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 147.7, 142.9, 136.9, 135.2, 130.0, 129.3, 127.3, 123.4, 117.3, 113.5, 53.4, 25.2, 20.1, 19.6.

S. Zhu, J. Xie, Y. Zhang, S. Li and Q. Zhou, *J. Am. Chem. Soc.*, 2006, **128**, 12886.



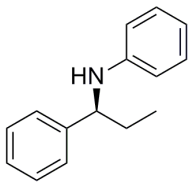
7k

(*S*)-*N*-(1-(4-fluoro-3-methylphenyl)ethyl)aniline: Yellow liquid, 0.0664 g, 96% yield, 89% ee, $[\alpha]_D^{20}$ = +23.6 (*c* 0.56, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.19-7.04 (m, 4H), 6.91 (t, *J* = 9.0 Hz, 1H), 6.69-6.60 (m, 1H), 6.55-6.45 (m, 2H), 4.40 (q, *J* = 6.6 Hz, 1H), 3.96 (brs, 1H), 2.23 (s, 3H), 1.46 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 160.3 (d, $J_{C\text{-}F}$ = 241.6 Hz), 147.4, 140.8 (d, $J_{C\text{-}F}$ = 3.4 Hz), 129.3, 129.0 (d, $J_{C\text{-}F}$ = 5.1 Hz), 125.0 (d, $J_{C\text{-}F}$ = 17.4 Hz), 124.7 (d, $J_{C\text{-}F}$ = 8.0 Hz), 117.5, 115.2 (d, $J_{C\text{-}F}$ = 22.3 Hz), 113.5, 53.1, 25.4, 14.9 (d, $J_{C\text{-}F}$ = 3.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$, ppm) δ -120.5; HRMS (ESI) calcd. for $C_{15}H_{15}NF$ $[M\text{-}H]^-$: 228.1194, Found: 228.1187.



7l

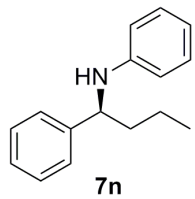
(*S*)-*N*-(1-(benzo[*d*][1,3]dioxol-5-yl)ethyl)aniline: Colorless liquid, 0.0659 g, 91% yield, 72% ee, $[\alpha]_D^{20}$ = +0.8 (*c* 0.77, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.08 (t, *J* = 7.8 Hz, 2H), 6.90-6.77 (m, 2H), 6.76-6.69 (m, 1H), 6.63 (t, *J* = 7.3 Hz, 1H), 6.49 (d, *J* = 7.8 Hz, 2H), 5.93-5.82 (m, 2H), 4.37 (q, *J* = 6.7 Hz, 1H), 3.95 (br s, 1H), 1.45 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 148.1, 147.4, 146.5, 139.7, 129.3, 119.0, 117.5, 113.5, 108.5, 106.4, 101.1, 53.5, 25.4; HRMS (ESI) calcd. for $C_{15}H_{14}O_2N$ $[M-H]^-$: 240.1030, Found: 240.1024.



7m

(*S*)-*N*-(1-phenylpropyl)aniline: Colorless liquid, 0.0645 g, 99% yield, 66% ee, $[\alpha]_D^{20}$ = +3.3 (*c* 0.95, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.38-7.24 (m, 4H), 7.23-7.15 (m, 1H), 7.06 (t, *J* = 7.8 Hz, 2H), 6.61 (t, *J* = 7.3 Hz, 1H), 6.50 (d, *J* = 7.9 Hz, 2H), 4.21 (t, *J* = 6.7 Hz, 1H), 4.03 (br s, 1H), 1.90-1.72 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 147.7, 144.1, 129.3, 128.7, 127.1, 126.7, 117.3, 113.4, 59.9, 31.8, 11.0.

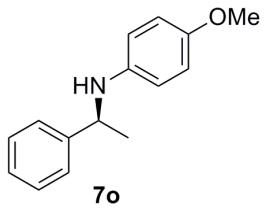
A. Baeza and A. Pfaltz, *Chem. Eur. J.*, 2010, **16**, 4003.



7n

(*S*)-*N*-(1-(3,4-dimethylphenyl)ethyl)-4-methoxyaniline: Yellow liquid, 0.0618 g, 91% yield, 65% ee, $[\alpha]_D^{20}$ = -0.9 (*c* 0.78, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ7.40-7.25 (m, 4H), 7.24-7.15 (m, 1H), 7.11-7.02 (m, 2H), 6.66-6.57 (m, 1H), 6.55-6.45(m, 2H), 4.29 (t, *J* = 6.8 Hz, 1H), 4.03 (br s, 1H), 1.85-1.66 (m, 2H), 1.50-1.28 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.7, 144.5, 129.3, 128.7, 127.0, 126.6, 117.3, 113.4, 58.2, 41.3, 19.7, 14.2.

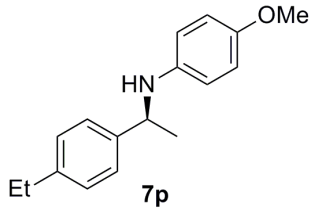
D. Pei, Y. Zhang, S. Wei, M. Wang and J. Sun, *Adv. Synth. Catal.*, 2008, **350**, 619 .



7o

(*S*)-4-methoxy-*N*-(1-phenylethyl)aniline: Colorless liquid, 0.0725 g, 99% yield, 73% ee, $[\alpha]_D^{20}$ = +7.5 (*c* 1.01, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.39-7.23 (m, 4H), 7.23-7.13 (m, 1H), 6.72-6.62 (m, 2H), 6.50-6.39 (m,2H), 4.38 (q, *J* = 6.7 Hz, 1H), 3.73 (br s, 1H), 3.65 (s, 3H), 1.46 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 152.0, 145.7, 141.7, 128.7, 126.9, 126.0, 114.9, 114.7, 55.8, 54.4, 25.2.

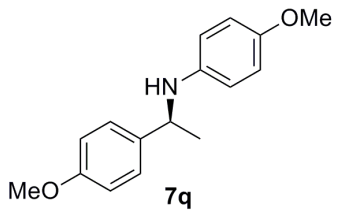
Y. Chi, Y. Zhou and X. Zhang, *J. Org. Chem.,* 2003, **68**, 4120.



7p

(*S*)-*N*-(1-(4-ethylphenyl)ethyl)-4-methoxyaniline: Yellow liquid, 0.0775 g, 99% yield, 70% ee, $[\alpha]_D^{20}$ = -3.7 (*c* 1.14, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.26 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 7.9 Hz, 2H), 6.72-6.65(m, 2H), 6.52-6.43 (m, 2H), 4.38 (q, *J* = 5.8 Hz, 1H), 3.72 (br s, 1H), 3.67 (s, 3H), 2.61 (q, *J* = 7.6 Hz, 2H), 1.47 (d, *J* = 6.7 Hz, 3H), 1.21 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 152.0, 142.8, 141.9, 128.2, 126.0, 114.9, 114.7, 55.9, 54.1, 28.6, 25.2, 15.7.

H. F. Zhou, S. S. Liu, P. Cui, H. Liu and Q. X. Liu, CN 108358793 A 20180803.

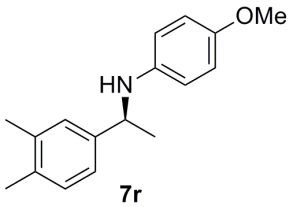


7q

(*S*)-4-methoxy-*N*-(1-(4-methoxyphenyl)ethyl)aniline: Colorless liquid, 0.0770 g, 99% yield, 73% ee, $[\alpha]_D^{20}$ = -5.1 (*c*1.01, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.31-7.21 (m, 2H), 6.90-6.79 (m, 2H), 6.76-6.61(m, 2H), 6.52-6.40 (m, 2H), 4.36 (q, *J* = 6.7 Hz, 1H), 3.75(s, 3H),

3.72 (br s, 1H), 3.67 (s, 3H), 1.45 (d, J = 6.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ158.6, 152.0, 141.8, 137.7, 127.1, 114.9, 114.7, 114.1, 55.9, 55.4, 53.8, 25.2.

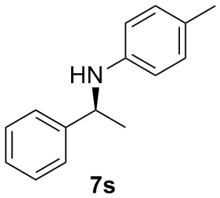
C. Li, B. Villa-Marcos and J. Xiao, *J. Am. Chem. Soc.*, 2009, **131**, 6967.



7r

(*S*)-*N*-(1-(3,4-dimethylphenyl)ethyl)-4-methoxyaniline: Yellow liquid, 0.0777 g, 99% yield, 71% ee, $[\alpha]_D^{20}$ = -0.9 (*c* 0.78, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.18-7.02 (m, 3H), 6.80-6.64 (m, 2H), 6.55-6.43(m, 2H), 4.34 (q, J = 6.6 Hz, 1H), 3.72 (br s, 1H), 3.67 (s, 3H), 2.23 (s, 3H), 2.21 (s, 3H), 1.46 (d, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 152.0, 143.2, 142.0, 136.9, 135.2, 130.0, 127.4, 123.4, 114.9, 114.7, 55.9, 54.2, 25.3, 20.1, 19.6.

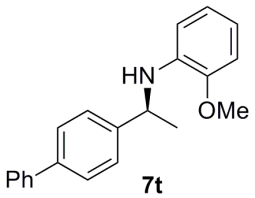
X. Zhu and H. Du, *Org. Biomol. Chem.*, 2015, **13**, 1013.



7s

(*S*)-4-methyl-*N*-(1-phenylethyl)aniline: Colorless liquid, 0.0636 g, 99% yield, 63% ee, $[\alpha]_D^{20}$ = +11.7 (*c* 1.14, CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.40-7.24 (m, 4H), 7.23-7.14 (m, 1H), 6.88 (d, J = 8.1 Hz, 2H), 6.48-6.36 (m,2H), 4.43 (q, J = 6.7 Hz, 1H), 3.86 (br s, 1H), 2.17 (s, 3H), 1.47 (d, J = 6.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 145.6, 145.2, 129.8, 128.8, 127.0, 126.5, 126.0, 113.6, 53.8, 25.2, 20.5.

D. Pei, Z. Wang, S. Wei, Y. Zhang and J. Sun, *Org. Lett.,* 2006, **8**, 5913.



7t

(*S*)-*N*-(1-([1,1'-biphenyl]-4-yl)ethyl)-2-methoxyaniline: White solid, 0.0904 g, 99% yield, 55% ee, $[\alpha]_D^{20}$ = +16.8 (*c* 1.20, CH_2Cl_2); IR (film): 1602, 1511, 1224, 734 cm^{-1}; ^{1}H NMR

(400 MHz, $CDCl_3$, ppm) δ7.61-7.50 (m, 4H), 7.47-7.37 (m, 4H), 7.35-7.28 (m, 1H), 6.82-6.75 (m, 1H), 6.75-6.68 (m, 1H), 6.66-6.57 (m, 1H), 6.43-6.35 (m, 1H), 4.65 (br s, 1H), 4.57-4.46 (m, 1H), 3.89 (s, 3H), 1.58 (d, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 146.8, 144.8, 141.2, 139.9, 137.4, 128.9, 127.6, 127.3, 127.2, 126.5, 121.4, 116.6, 111.3, 109.5, 55.7, 53.3, 25.4; HRMS (ESI) calcd. for $C_{21}H_{22}ON$ $[M+H]^+$: 304.1696, Found: 304.1697.

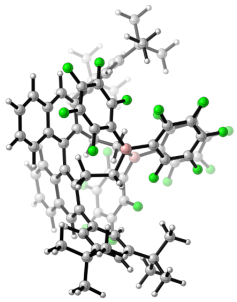
Computational Details: All calculations were performed with the Gaussian 09 program.[1] Geometry optimizations of all stationary points were performed with the M06-2X functional,[2] which has been proven to be suitable to describe the dispersion effects. The 6-31G(d) basis set was applied for all elements in the catalyst. Frequency calculations at the same level were performed to confirm each stationary point to be either a minimum structure. All figures of structures were prepared using CYLView.[3]

(1) Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2013.

(2) (a) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157. (b) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.

(3) Legault, C. Y. CYLview, 1.0b; Université de Sherbrooke: Sherbrooke, Québec, Canada, 2009; http://www.cylview.org.

Coordinates of All Stationary Points



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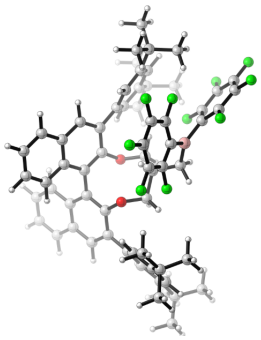

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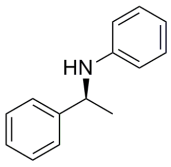
C	1.23897300	-3.19511400	2.41226900	C	6.87035800	2.24464800	-3.34343500
C	2.37563000	-3.49098200	3.21365800	C	7.01459900	1.06956100	-4.31563000
C	2.22881500	-3.89542400	4.51646900	C	6.09437700	3.36506300	-4.05538400
C	0.94225600	-4.03150800	5.09084200	C	8.27835100	2.74744700	-2.98344700
C	-0.17106700	-3.74972500	4.34372300	H	7.57766800	0.24337400	-3.86853700
C	-0.05098200	-3.31998800	2.99586300	H	6.03903900	0.68897700	-4.63631300
C	-1.19057200	-3.03152100	2.20983800	H	7.55551100	1.39816300	-5.20916100
C	-1.09845400	-2.60514900	0.90378100	H	6.00002000	4.25438200	-3.42464200
C	0.20984300	-2.43269100	0.34419500	H	6.61273000	3.65836400	-4.97531800
C	-0.17516500	-0.75552200	-1.32748600	H	5.08605200	3.02992400	-4.31983200
H	2.24458300	1.54510000	-0.43613200	H	8.82163900	3.03427300	-3.89097300
H	2.29538400	0.17149900	-1.55991800	H	8.23894700	3.61994600	-2.32413200
H	6.22364700	-2.11710500	-1.15456800	H	8.84910000	1.96502700	-2.47274000
H	6.52616700	-4.53920500	-1.27964800	C	4.99891000	3.63497100	1.14671400
H	5.70000800	-6.82998500	-0.85182700	C	4.08718500	4.69646100	0.50768200
H	3.45072400	-7.16866500	0.16436200	C	4.30735000	3.11534400	2.41196400
H	2.04946700	-5.23960500	0.76070800	C	6.33284800	4.28134300	1.55256500
H	3.36604500	-3.38469900	2.78377500	H	4.53257500	5.12166800	-0.39750200
H	3.10816400	-4.11463600	5.11409500	H	3.11955100	4.25821900	0.23797000

H	0.84295900	-4.35763400	H	3.90646500	5.51456100	1.21436600
H	-1.16583500	-3.84818500	4.77067200	H	4.91091000	2.35357200	2.91691000
H	-2.17474600	-3.19546400	2.64242900	H	4.15826500	3.94312900	3.11337200
H	0.07418000	-0.65900500	-2.39061300	H	3.32336900	2.68746700	2.19347300
H	-1.26298800	-0.77746300	-1.24456000	H	6.15906700	5.07712800	2.28547900
C	-2.34831200	-2.41215400	0.11817300	H	7.00143400	3.54003100	2.00214700
C	-3.44989700	-1.77568000	0.69844700	H	6.84833600	4.72421400	0.69456800
C	-2.44912000	-2.90106500	-1.18966900	H	0.11592300	0.32060600	0.49726400
C	-4.65370200	-1.63495200	0.00114500	C	-0.33757500	1.70953800	-1.12029400
H	-3.35528100	-1.39850800	1.71200800	H	-0.55469300	1.59051100	-2.18651000
C	-3.61151900	-2.72178400	-1.93621900	H	0.34863700	2.56551200	-1.04206900
H	-1.58509700	-3.39492800	-1.61922100	B	-1.61670600	2.11285000	-0.29510900
C	-4.69586800	-2.08546800	-1.32064000	C	-1.49925600	2.29116000	1.26690300
H	-5.61383600	-1.95417100	-1.88881800	C	-2.59298800	2.13169800	2.12405700
C	4.98625700	0.23142400	-0.65025600	C	-0.28457900	2.55638900	1.91141300
C	5.65154200	0.55619100	-1.83521500	C	-2.50157700	2.20053200	3.50511100
C	4.80767700	1.21612500	0.32783700	C	-0.15502600	2.65891400	3.28820700
C	6.13343900	1.84794300	-2.06055800	C	-1.27240200	2.47239600	4.09077100
H	5.76529500	-0.21412500	-2.59095900	C	-2.99762000	2.35668800	-1.00823500
C	5.25036100	2.52144900	0.12592700	C	-3.84548400	3.40591200	-0.64457500
H	4.29194800	0.94609700	1.24058300	C	-3.44898200	1.54886500	-2.05419300
C	5.91211200	2.81037100	-1.07178100	C	-5.05167300	3.65971500	-1.27765300
H	6.26127300	3.82599200	-1.24416500	C	-4.66162900	1.75721900	-2.69500500
C	-5.91425700	-1.03459200	0.63398200	C	-5.46206200	2.82198200	-2.30733100
C	-5.73903900	-0.75865300	2.13147700	F	0.83646400	2.74318100	1.20755500
C	-6.26477800	0.28287800	-0.07460000	F	1.02268000	2.92900800	3.84030500
C	-7.08239800	-2.02379100	0.47568200	F	-1.16780300	2.55831500	5.40670900
H	-5.47962100	-1.67340600	2.67545500	F	-3.57576300	2.01329000	4.26453100
H	-4.96906500	-0.00759700	2.32500400	F	-3.80854100	1.87344800	1.63365400
H	-6.67964100	-0.37894900	2.54365000	F	-3.49685700	4.23040200	0.34649500
H	-6.42386500	0.12786200	-1.14829700	F	-5.81887600	4.67938900	-0.90648400
H	-7.18221300	0.71147200	0.34529700	F	-6.62426100	3.02890800	-2.90823300
H	-5.45618500	1.01057200	0.05302600	F	-5.08007400	0.93370700	-3.65212000
H	-7.98333300	-1.61660600	0.94804800	F	-2.72683700	0.50179000	-2.46415400

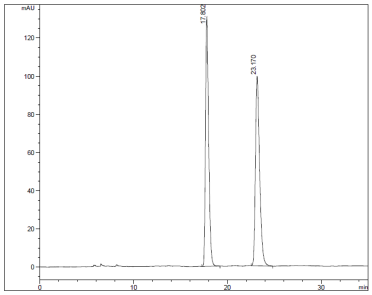
The chromatography for the determination of enantiomeric excess



7a

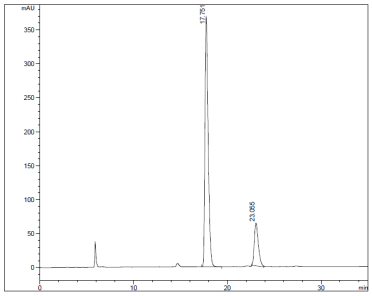
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

Racemic

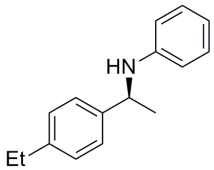


Peak #	RT [min]	Area	Area %
1	17.802	3.055e3	49.789
2	23.170	3.081e3	50.211

Chiral



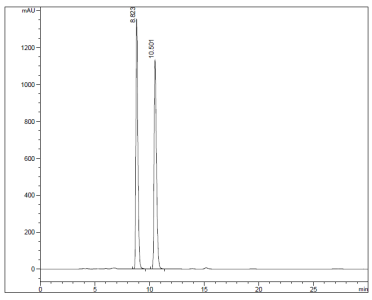
Peak #	RT [min]	Area	Area %
1	17.751	8.717e3	82.256
2	23.055	1.880e3	17.744



7b

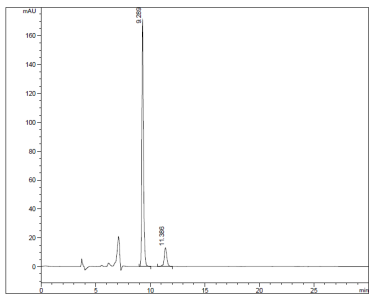
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.8 mL/min; **Detection:** UV 254 nm

Racemic

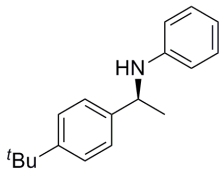


Peak #	RT [min]	Area	Area %
1	8.823	1.719e4	49.825
2	10.501	1.731e4	50.175

Chiral



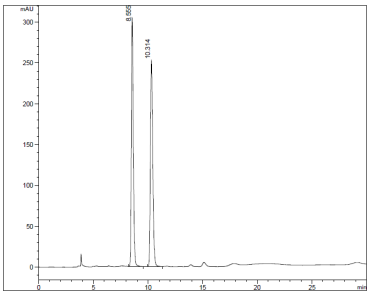
Peak #	RT [min]	Area	Area %
1	9.289	1.754e3	88.996
2	11.386	216.865	11.004



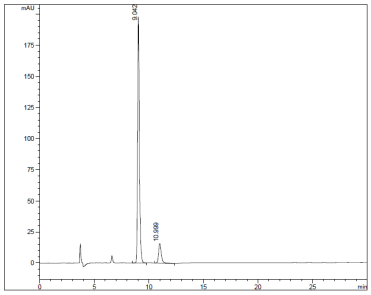
7c

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.8 mL/min; **Detection:** UV 254 nm

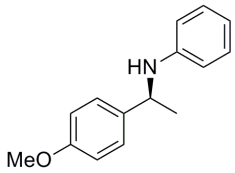
Racemic **Chiral**



Peak #	RT [min]	Area	Area %
1	8.555	3.808e3	50.111
2	10.314	3.791e3	49.889



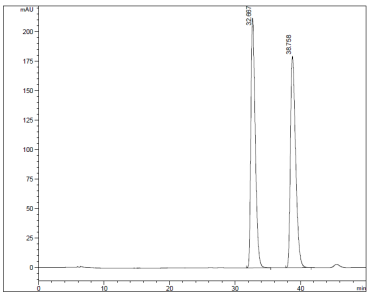
Peak #	RT [min]	Area	Area %
1	9.042	2.217e3	89.158
2	10.999	269.552	10.842



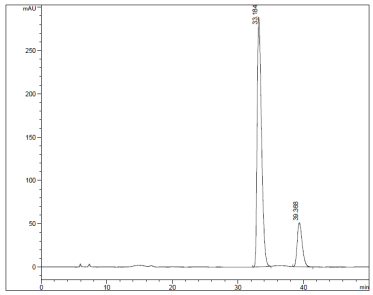
7d

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (99/1); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

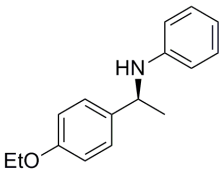
Racemic **Chiral**



Peak #	RT [min]	Area	Area %
1	32.667	9.840e3	49.991
2	38.758	9.844e3	50.009



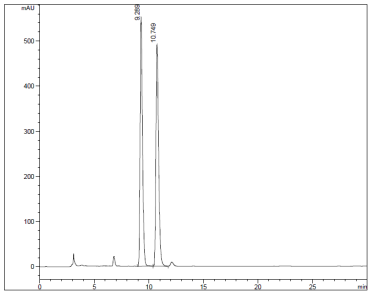
Peak #	RT [min]	Area	Area %
1	33.184	1.340e4	83.285
2	39.368	2.689e3	16.715



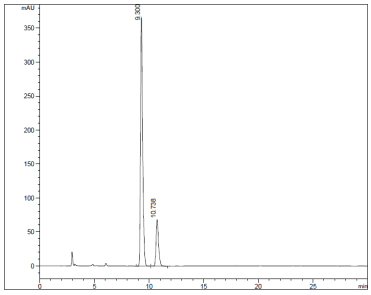
7e

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

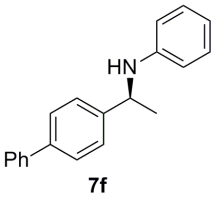
Racemic **Chiral**



Peak #	RT [min]	Area	Area %
1	9.289	8.391e3	49.926
2	10.749	8.416e3	50.074



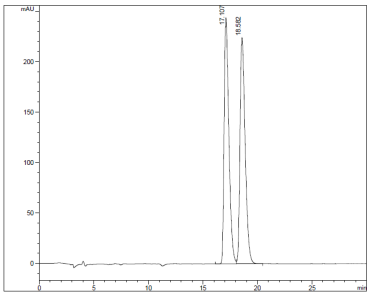
Peak #	RT [min]	Area	Area %
1	9.300	4.998e3	82.286
2	10.738	1.076e3	17.714



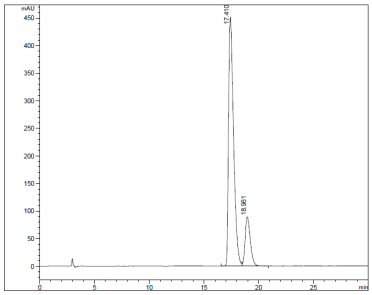
7f

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

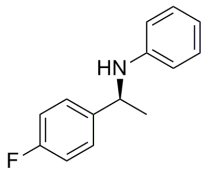
Racemic **Chiral**



Peak #	RT [min]	Area	Area %
1	17.107	7.374e3	49.889
2	18.582	7.407e3	50.111



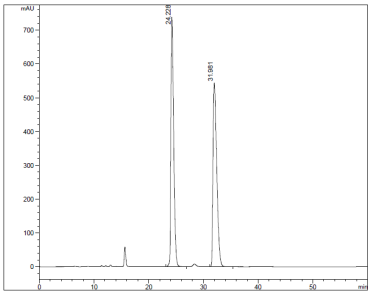
Peak #	RT [min]	Area	Area %
1	17.410	1.435e4	83.032
2	18.961	2.933e3	16.968



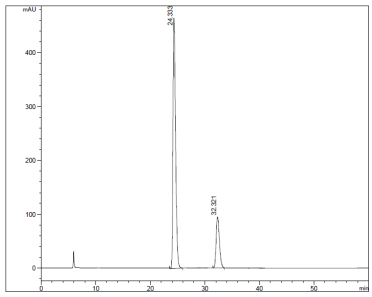
7g

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

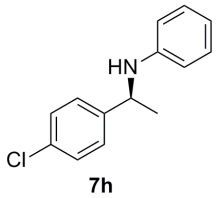
Racemic **Chiral**



Peak #	RT [min]	Area	Area %
1	24.228	2.619e4	50.301
2	31.981	2.588e4	49.699



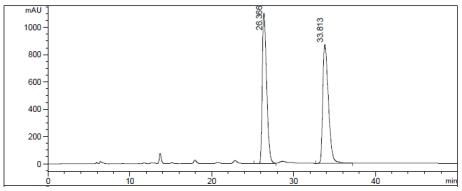
Peak #	RT [min]	Area	Area %
1	24.333	1.550e4	79.750
2	32.321	3.935e3	20.250



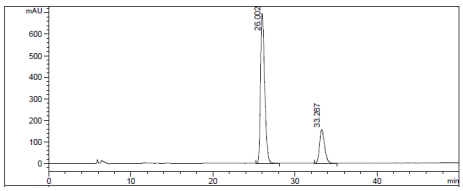
7h

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

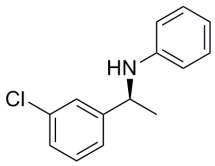
Racemic **Chiral**



Peak #	RT [min]	Area	Area %
1	26.366	4.051e4	49.342
2	33.813	4.159e4	50.658



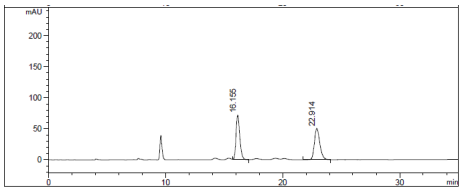
Peak #	RT [min]	Area	Area %
1	26.002	2.427e4	78.663
2	33.267	6.583e3	21.337



7i

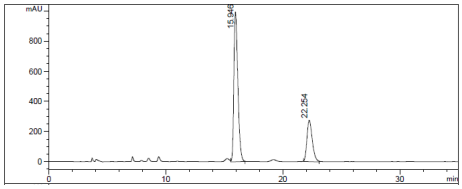
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

Racemic

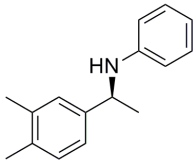


Peak #	RT [min]	Area	Area %
1	16.155	1.607e3	49.861
2	22.914	1.616e3	50.139

Chiral



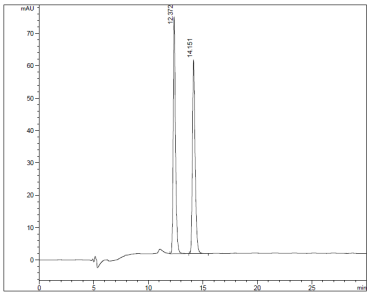
Peak #	RT [min]	Area	Area %
1	15.946	2.346e4	73.027
2	22.254	8.666e3	26.973



7j

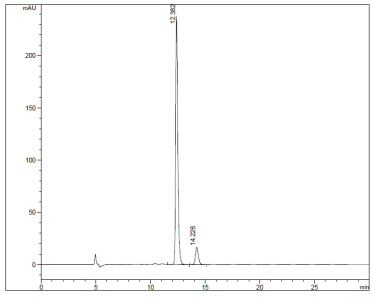
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

Racemic

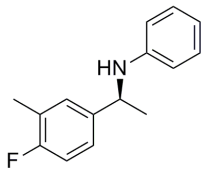


Peak #	RT [min]	Area	Area %
1	12.372	1.073e3	51.161
2	14.151	1.024e3	48.839

Chiral



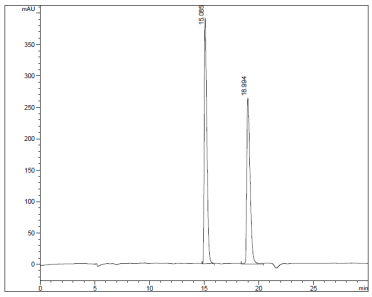
Peak #	RT [min]	Area	Area %
1	12.382	3.257e3	91.347
2	14.226	308.512	8.653



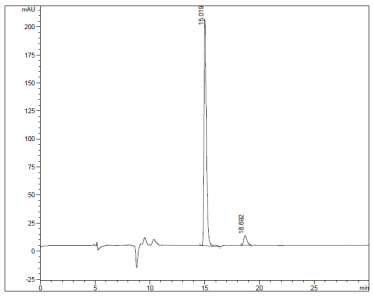
7k

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.6 mL/min; **Detection:** UV 254 nm

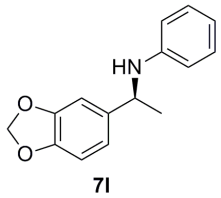
Racemic **Chiral**



Peak #	RT [min]	Area	Area %
1	15.085	6.500e3	53.746
2	18.994	5.594e3	46.254



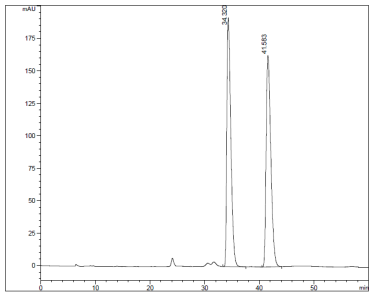
Peak #	RT [min]	Area	Area %
1	15.019	3.152e3	94.598
2	18.692	179.999	5.402



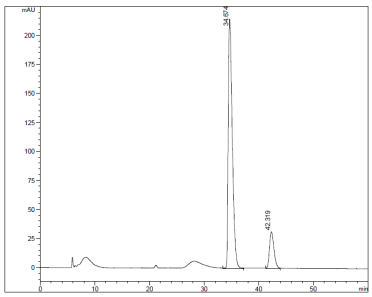
7l

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254nm

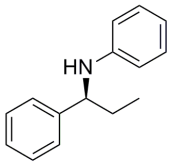
Racemic **Chiral**



Peak #	RT [min]	Area	Area %
1	34.320	9.738e3	50.043
2	41.583	9.721e3	49.957



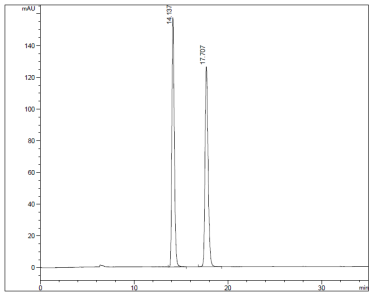
Peak #	RT [min]	Area	Area %
1	34.674	1.114e4	86.185
2	42.319	1.785e3	13.815

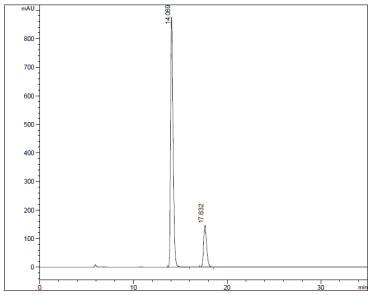


7m

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

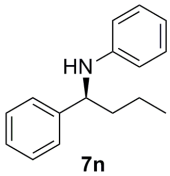
Racemic **Chiral**





Peak #	RT [min]	Area	Area %
1	14.137	2.864e3	50.043
2	17.707	2.859e3	49.957

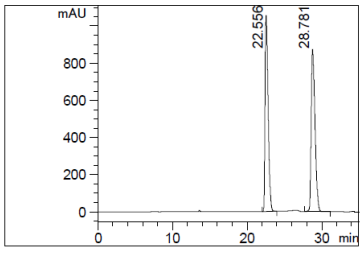
Peak #	RT [min]	Area	Area %
1	14.069	1.654e4	83.396
2	17.632	3.292e3	16.604

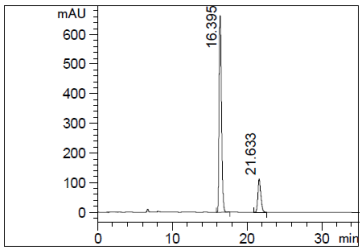


7n

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA(98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

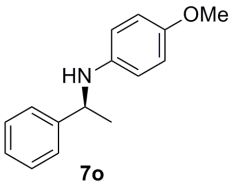
Racemic **Chiral**





Peak #	RT [min]	Area %	Area
1	22.556	49.641	3.071e4
2	28.781	50.359	3.115e4

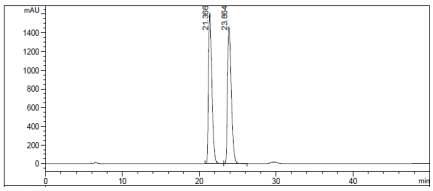
Peak #	RT [min]	Area %	Area
1	16.395	82.667	1.470e4
2	21.633	17.333	3.081e3

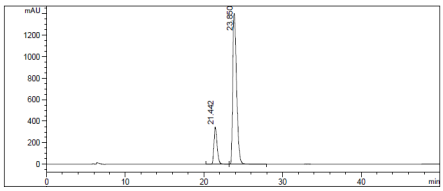


7o

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA(98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

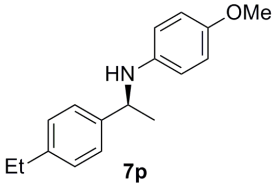
Racemic **Chiral**





Peak #	RT [min]	Area	Area %
1	21.366	4.941e4	49.731
2	23.864	4.994e4	50.269

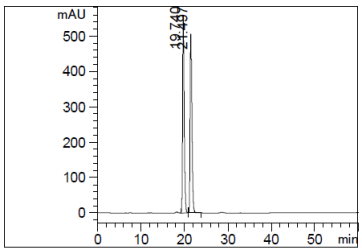
Peak #	RT [min]	Area	Area %
1	21.442	9.662e3	16.872
2	23.850	4.760e4	83.128

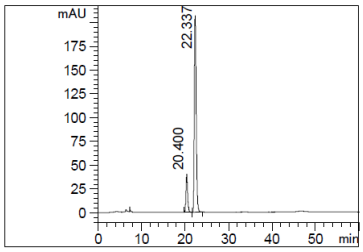


7p

HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA(98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

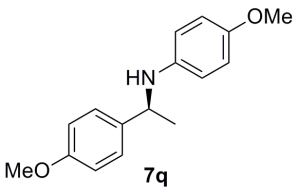
Racemic **Chiral**





Peak #	RT [min]	Area %	Area
1	19.740	49.952	1.482e4
2	21.497	50.048	1.485e4

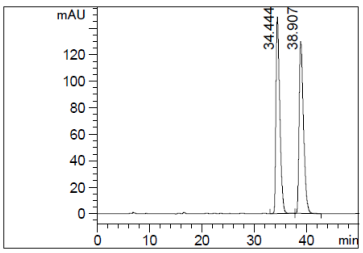
Peak #	RT [min]	Area %	Area
1	20.400	14.780	1.071e3
2	22.337	85.220	6.174e3



7q

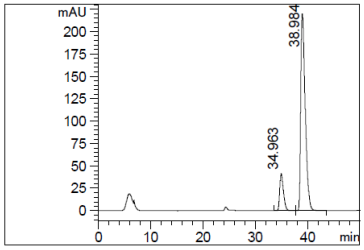
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA(98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

Racemic

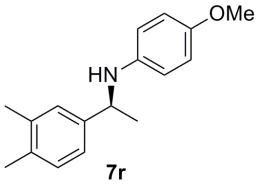


Peak #	RT [min]	Area %	Area
1	34.444	50.003	7.563e3
2	38.907	49.997	7.562e3

Chiral



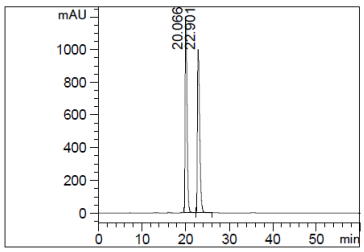
Peak #	RT [min]	Area %	Area
1	34.963	13.375	2.031e3
2	38.984	86.625	1.315e4



7r

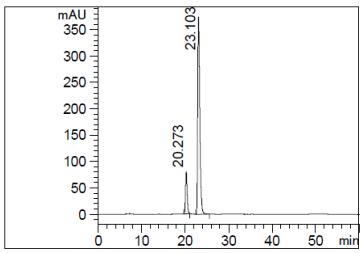
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA(98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

Racemic

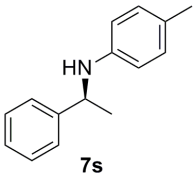


Peak #	RT [min]	Area %	Area
1	20.066	49.856	3.584e4
2	22.901	50.144	3.604e4

Chiral



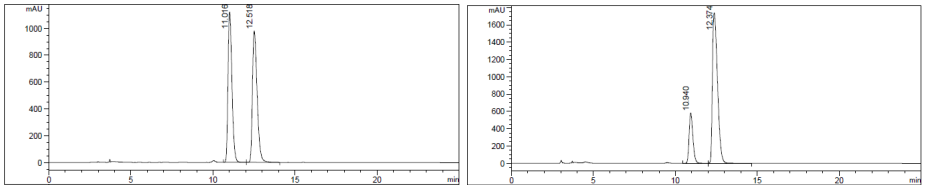
Peak #	RT [min]	Area %	Area
1	20.273	14.533	2.140e3
2	23.103	85.467	1.259e4



7s

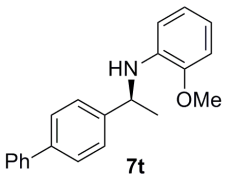
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA(99/1); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic **Chiral**



Peak #	RT [min]	Area	Area %
1	11.016	1.873e4	49.092
2	12.518	1.943e4	50.908

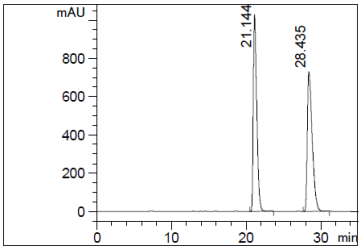
Peak #	RT [min]	Area	Area %
1	10.940	9.276e3	19.913
2	12.374	3.731e4	80.087



7t

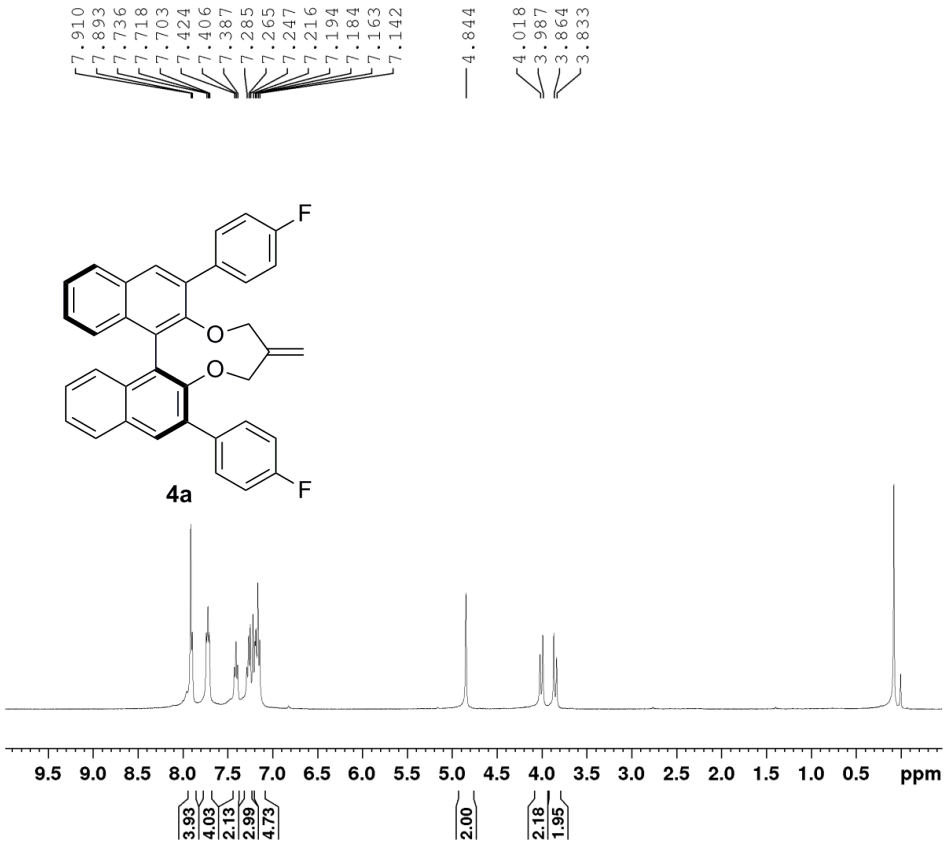
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA(98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

Racemic **Chiral**

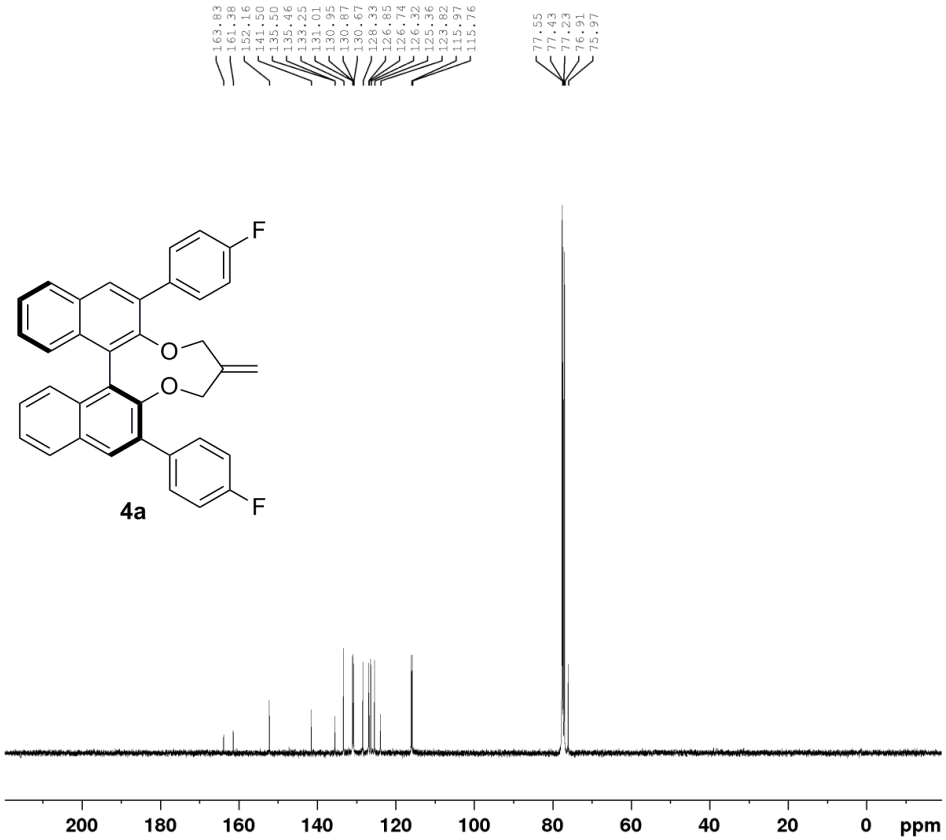


Peak #	RT [min]	Area %	Area
1	21.144	49.846	3.311e4
2	28.435	50.154	3.332e4

Peak #	RT [min]	Area %	Area
1	21.319	77.538	8.416e3
2	28.806	22.462	2.438e3

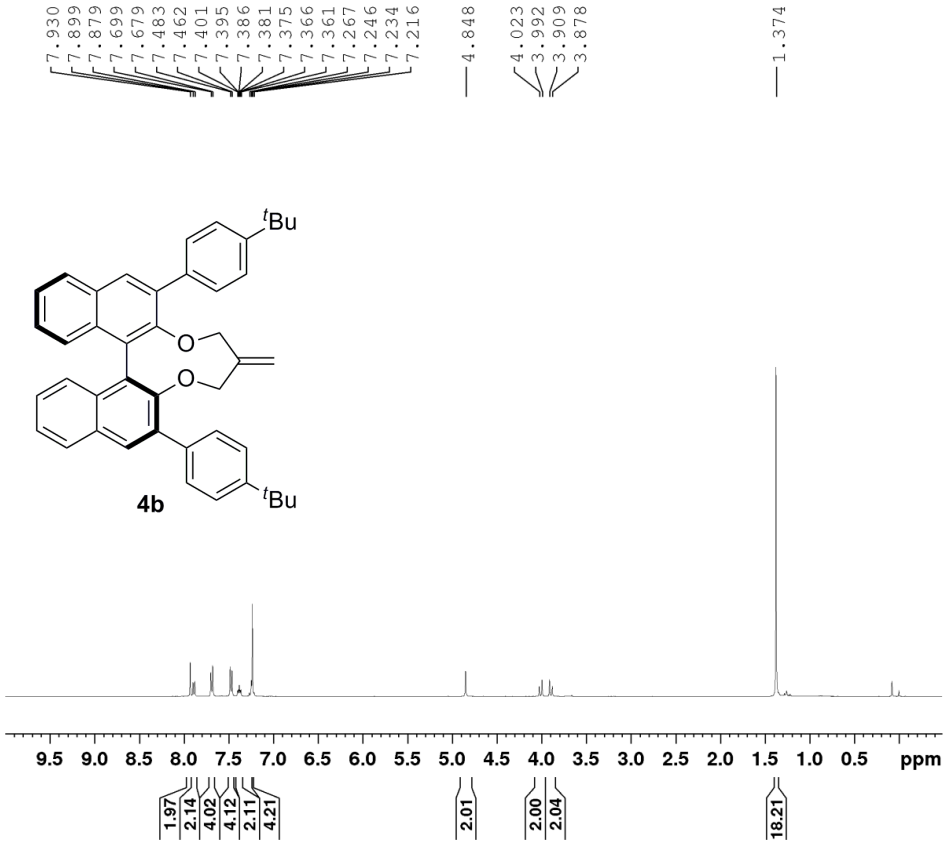



```
Current Data Parameters
NAME            400-2018
EXPNO                357
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180925
Time               15.47 h
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     5
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                162.77
DW                62.400 usec
DE                 6.50 usec
TE                298.1 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                  1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400158 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

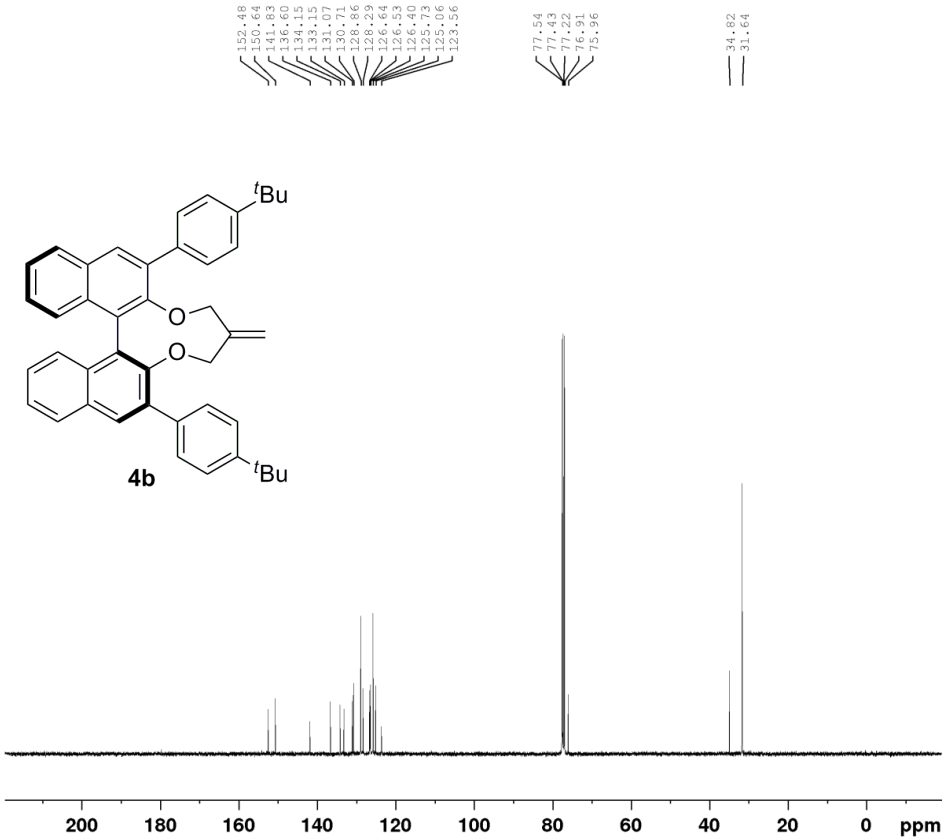



```
Current Data Parameters
NAME            400-2018
EXPNO                109
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180406
Time                5.07 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404098 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

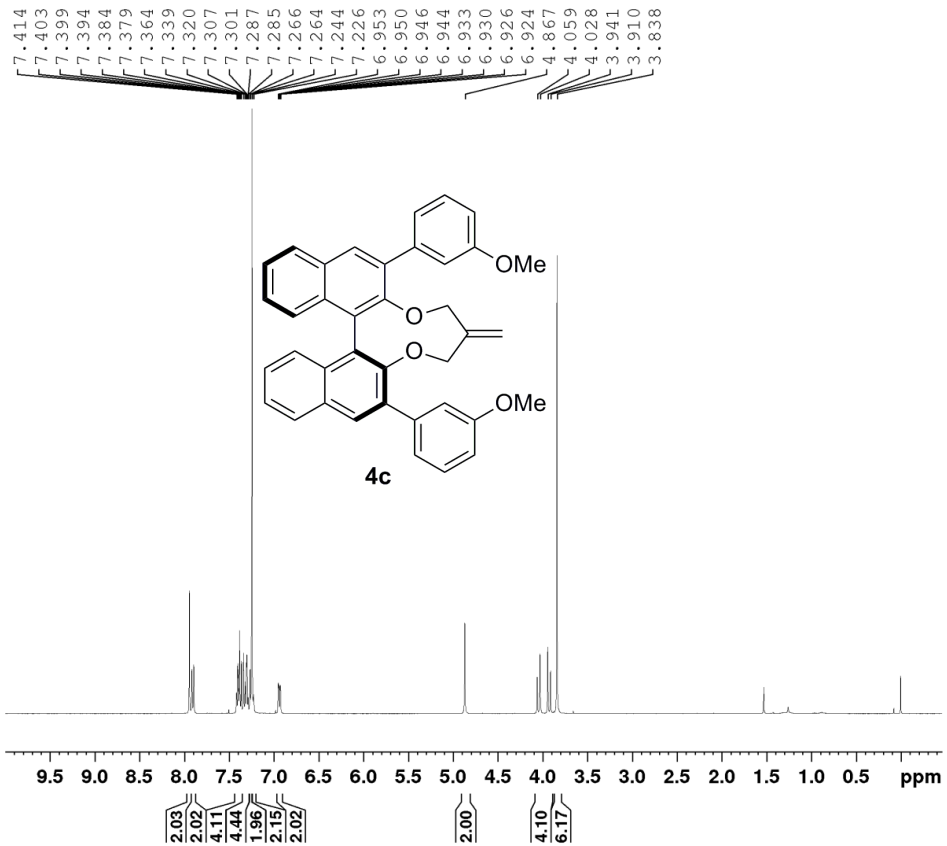

```
Current Data Parameters
NAME            400-2018
EXPNO                129
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180408
Time               21.25 h
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH             89285.711 Hz
FIDRES          1.362392 Hz
AQ              0.7340032 sec
RG                 206.33
DW                  5.600 usec
DE                  6.50 usec
TE                 298.1 K
D1              1.00000000 sec
d11             0.03000000 sec
d12             0.00002000 sec
TD0                    1
rde1            0.00000650 sec
SFO1          376.5642094 MHz
NUC1                  19F
P1                 14.50 usec
PLW1          17.98900032 W
SFO2          400.2416010 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W

F2 - Processing parameters
SI                 65536
SF            376.6018696 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



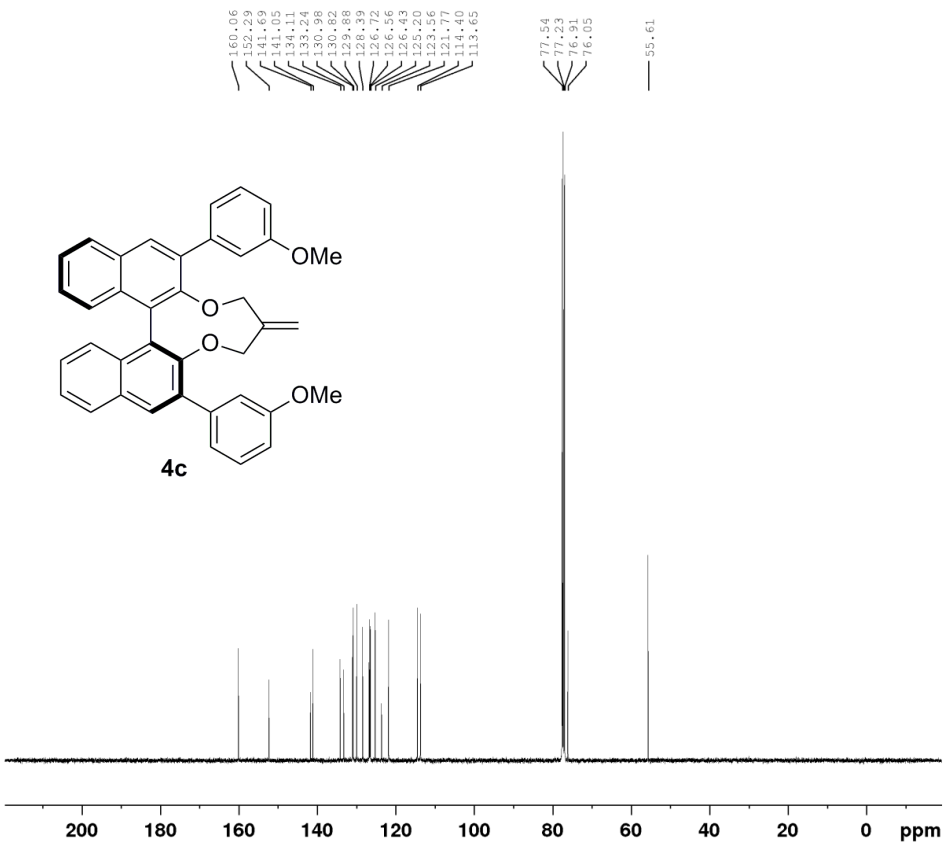

```
Current Data Parameters
NAME            400-2018
EXPNO                110
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180406
Time                5.10 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                  73.9
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400199 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



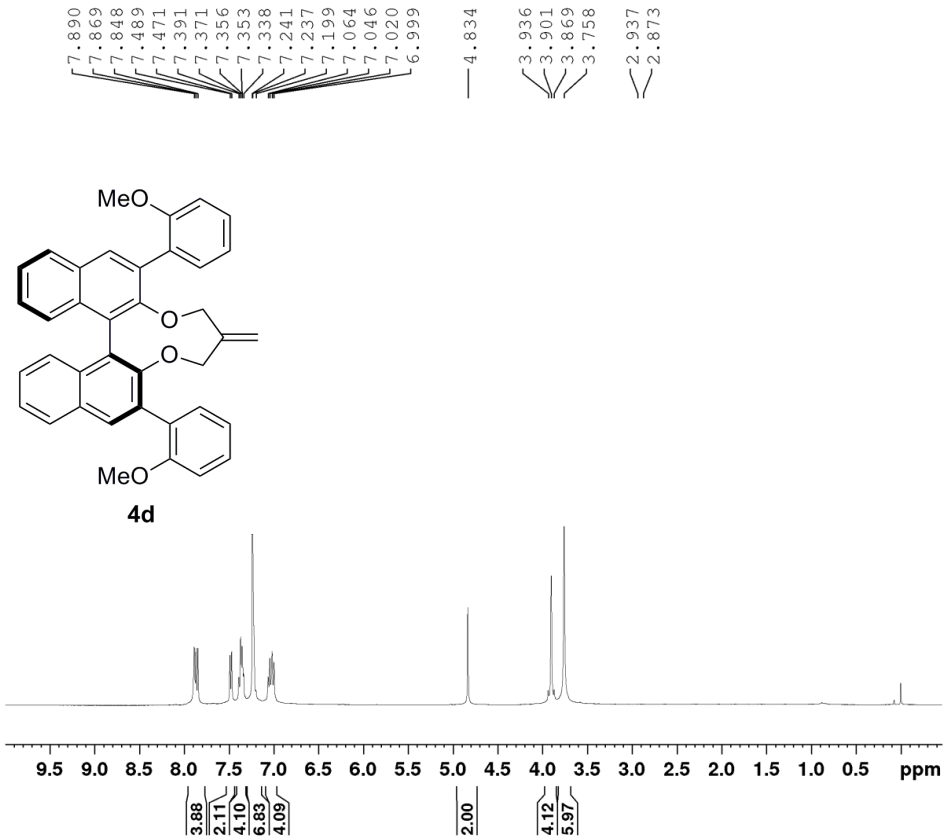

```
Current Data Parameters
NAME            400-2018
EXPNO                111
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180406
Time                6.09 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404105 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



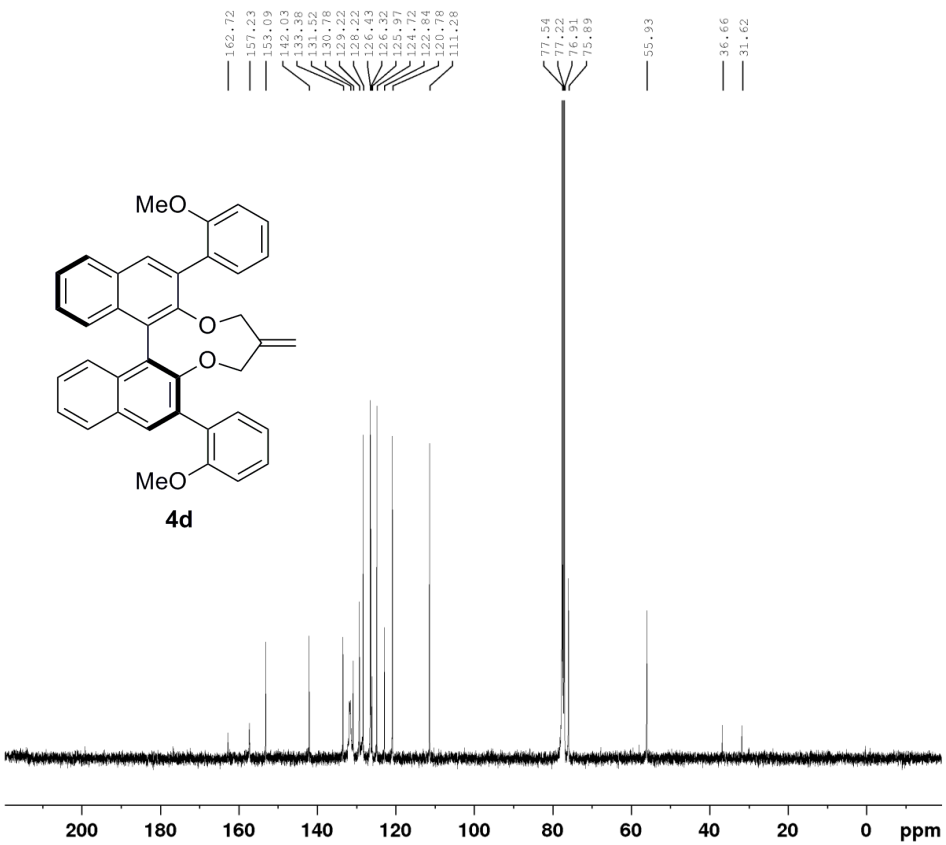

```
Current Data Parameters
NAME            400-2018
EXPNO                 91
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180404
Time                5.07 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                125.02
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                  1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400161 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```




```
Current Data Parameters
NAME            400-2018
EXPNO                 92
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180404
Time                6.06 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                298.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404098 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

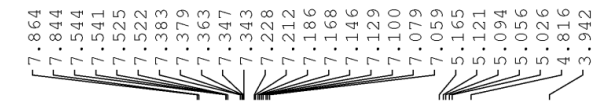


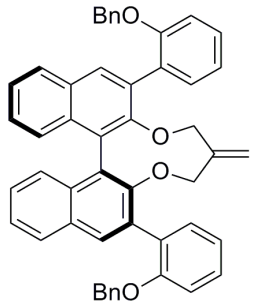

```
Current Data Parameters
NAME                  400-2018
EXPNO                       85
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180404
Time                      1.03 h
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      32768
SOLVENT                  CDCl3
NS                          16
DS                           0
SWH                  8012.820 Hz
FIDRES               0.489064 Hz
AQ                   2.0447233 sec
RG                      125.02
DW                      62.400 usec
DE                       6.50 usec
TE                      298.0 K
D1                   2.00000000 sec
TD0                          1
SFO1               400.2424716 MHz
NUC1                        1H
P1                      14.80 usec
PLW1              12.00000000 W

F2 - Processing parameters
SI                       65536
SF                 400.2400175 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```



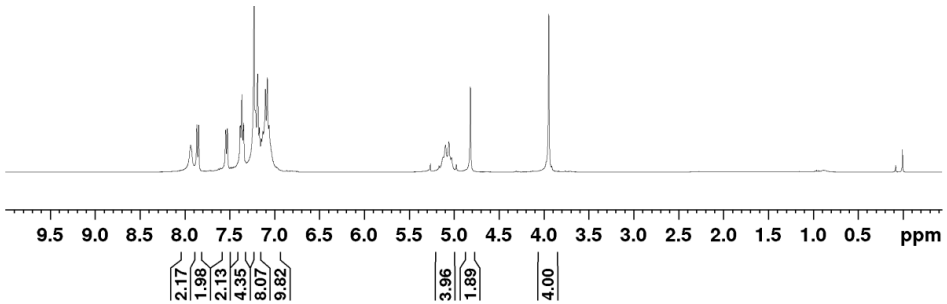
4d

```
Current Data Parameters
NAME            400-2018
EXPNO                 86
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180404
Time                2.02 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                298.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404112 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

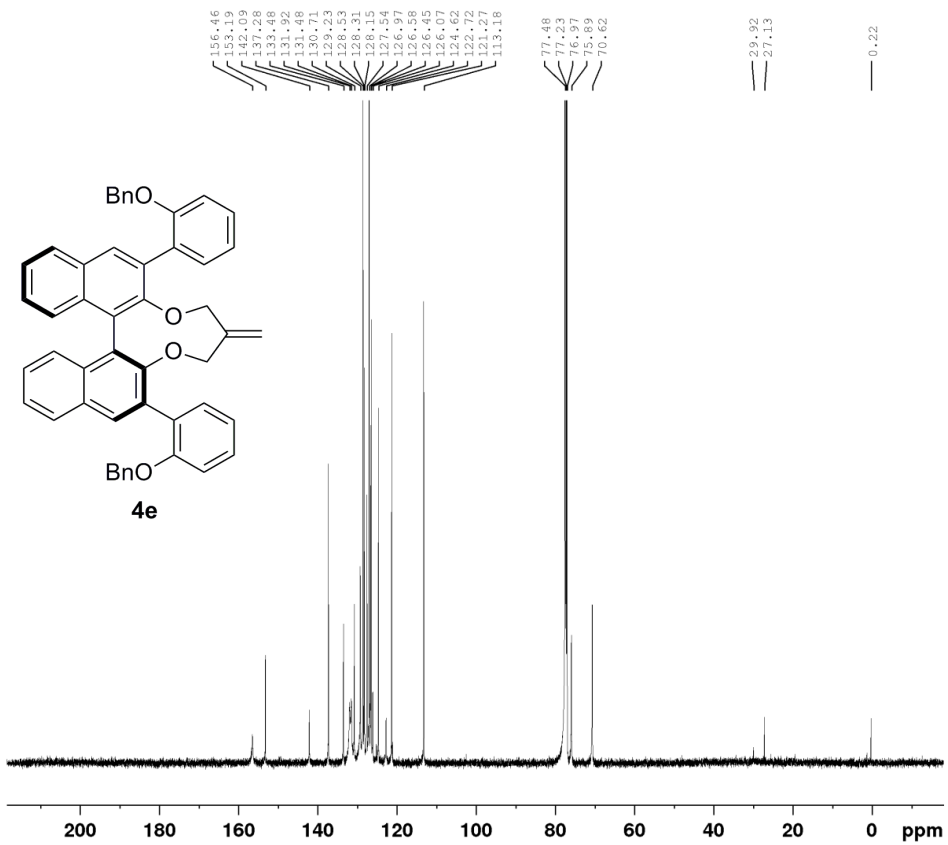




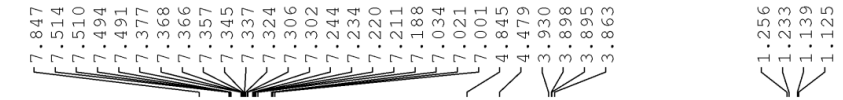
4e

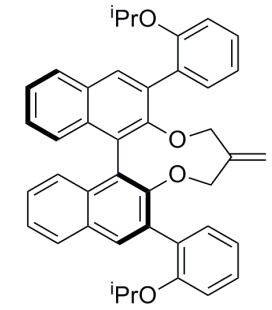



```
Current Data Parameters
NAME            400-2018
EXPNO                106
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180406
Time                3.06 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH              8012.820 Hz
FIDRES           0.489064 Hz
AQ              2.0447233 sec
RG                  73.9
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400222 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

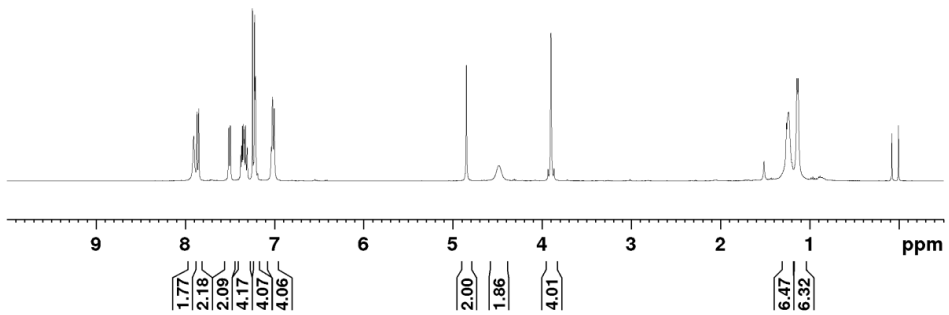



```
Current Data Parameters
NAME                  500-2018
EXPNO                      151
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180925
Time                     17.20 h
INSTRUM                  spect
PROBHD    5 mm CPPBBO BB
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1500
DS                           4
SWH                  29761.904 Hz
FIDRES                0.908261 Hz
AQ                    1.1010048 sec
RG                       192.89
DW                       16.800 usec
DE                       18.00 usec
TE                       298.2 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                          1
SFO1                125.7703637 MHz
NUC1                        13C
P1                        9.80 usec
PLW1                57.00000000 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2                20.00000000 W
PLW12                0.35778001 W
PLW13                0.22898000 W

F2 - Processing parameters
SI                       32768
SF                  125.7577659 MHz
WDW                         EM
SSB       0
LB                        1.00 Hz
GB        0
PC                        1.40
```

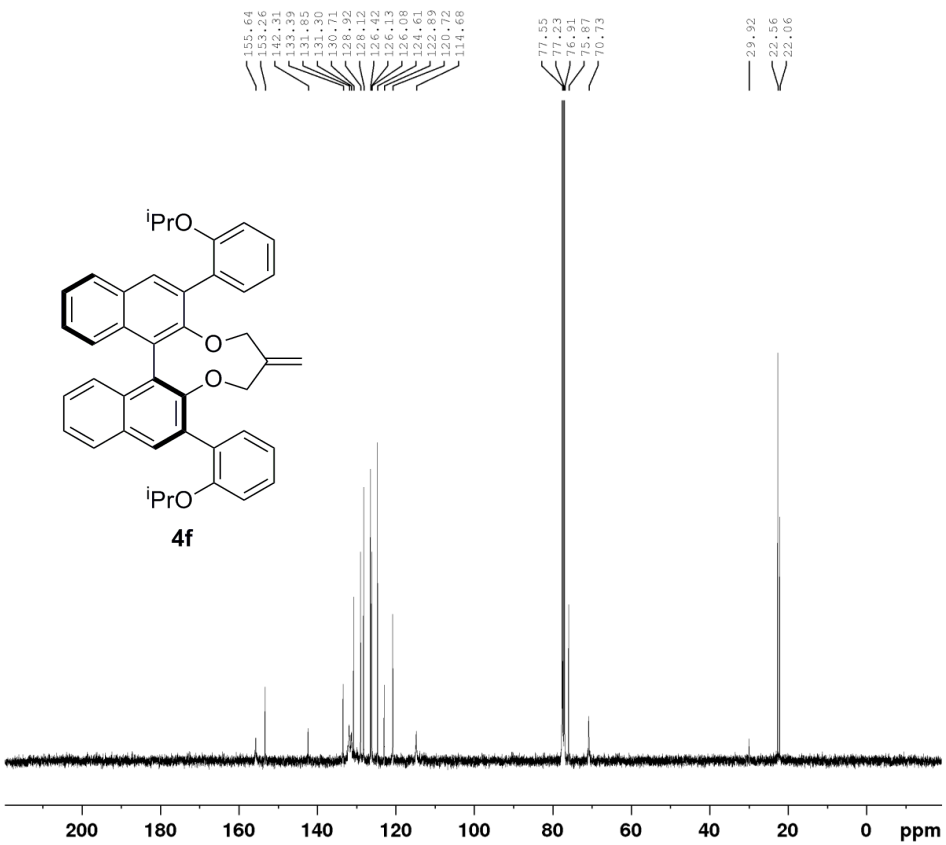




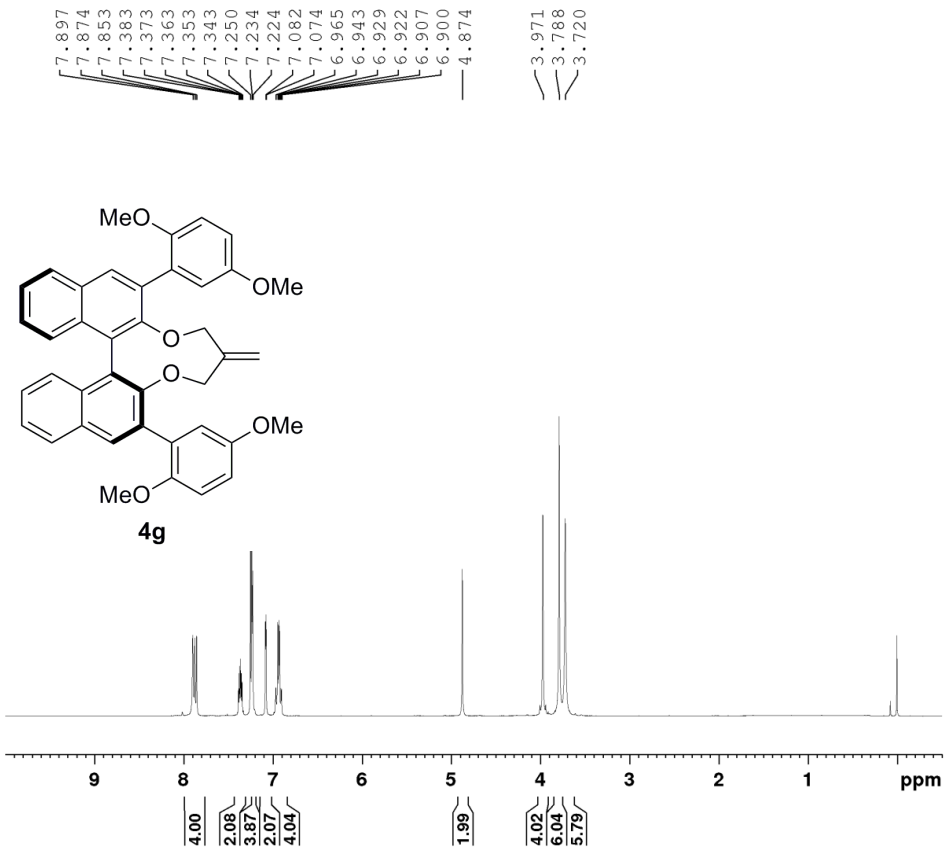
4f



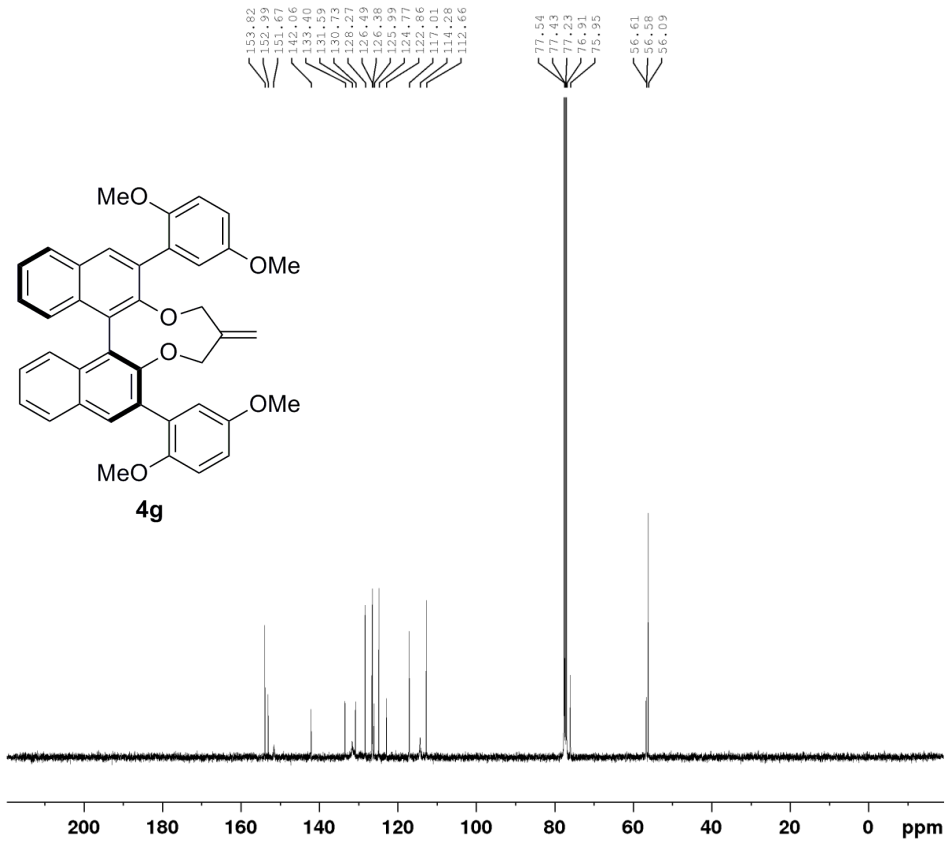

```
Current Data Parameters
NAME            400-2018
EXPNO                 83
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180404
Time      0 h
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              8012.820 Hz
FIDRES           0.489064 Hz
AQ              2.0447233 sec
RG                 125.02
DW                 62.400 usec
DE                  6.50 usec
TE                 298.0 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                  1H
P1                 14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                  65536
SF           400.2400159 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



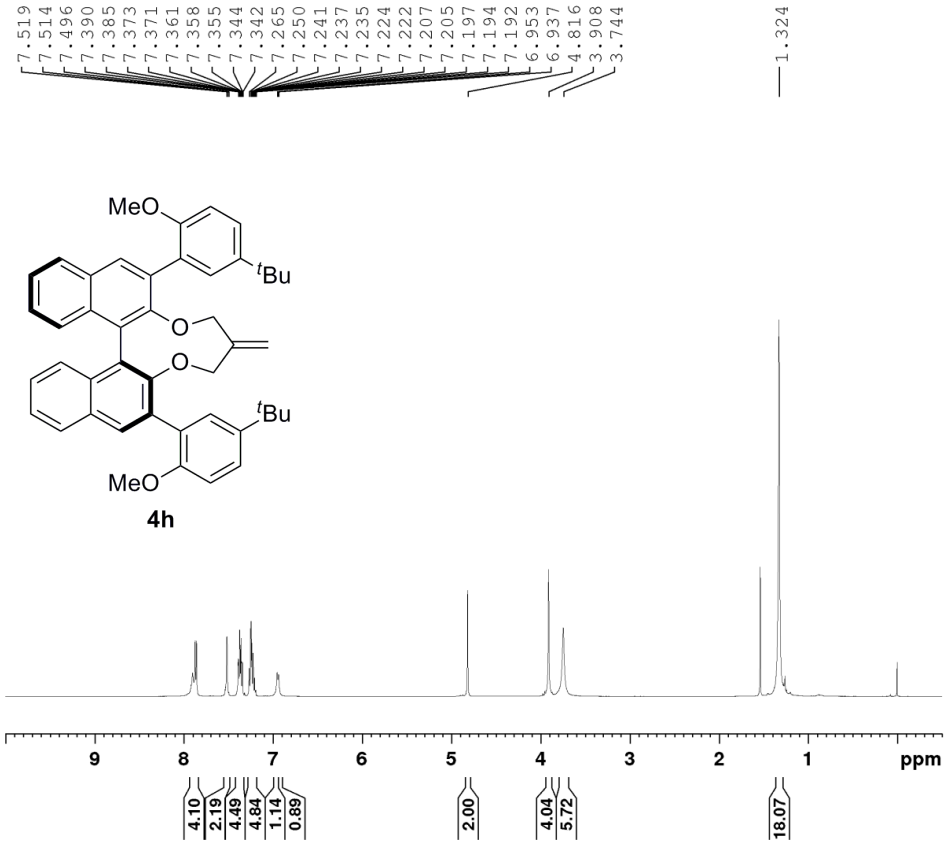

```
Current Data Parameters
NAME            400-2018
EXPNO                 84
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180404
Time                0.59 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                 206.33
DW                 20.800 usec
DE                  6.50 usec
TE                 298.4 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                 13C
P1                 10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404091 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



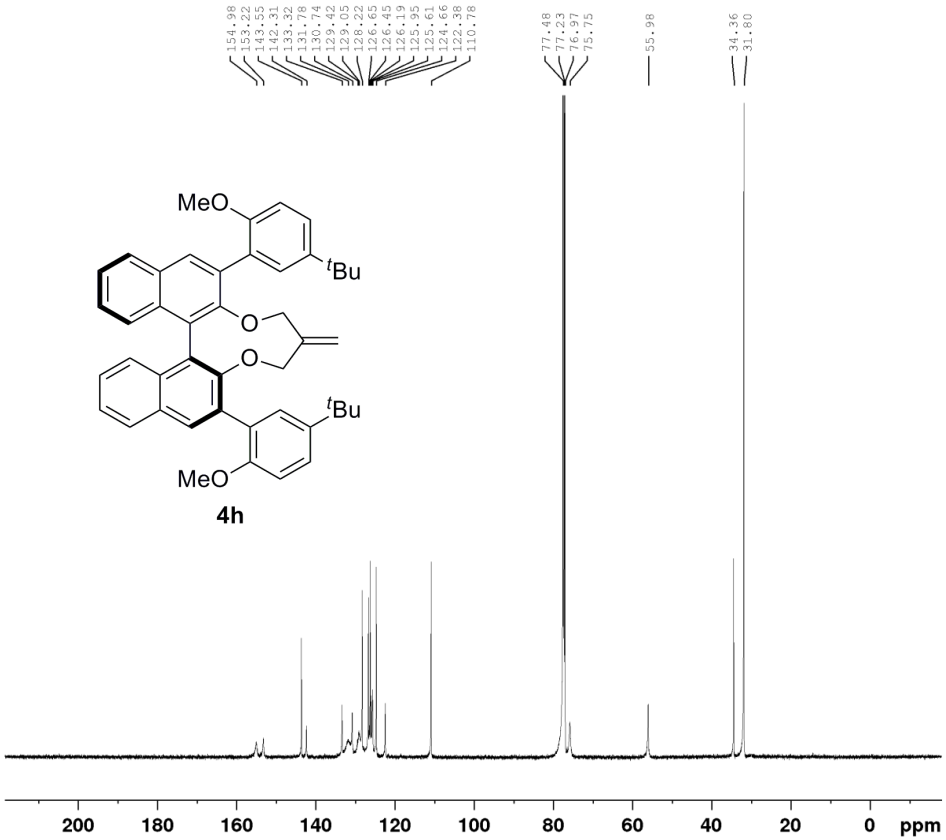

```
Current Data Parameters
NAME                  400-2018
EXPNO                       81
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180403
Time                     22.58 h
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      32768
SOLVENT                  CDCl3
NS                          16
DS                           0
SWH                   8012.820 Hz
FIDRES                0.489064 Hz
AQ                    2.0447233 sec
RG                      182.09
DW                      62.400 usec
DE                       6.50 usec
TE                      298.0 K
D1                    2.00000000 sec
TD0                          1
SFO1                400.2424716 MHz
NUC1                        1H
P1                      14.80 usec
PLW1                12.00000000 W

F2 - Processing parameters
SI                          65536
SF                  400.2400137 MHz
WDW                            EM
SSB       0
LB                       0.30 Hz
GB        0
PC                       1.00
```



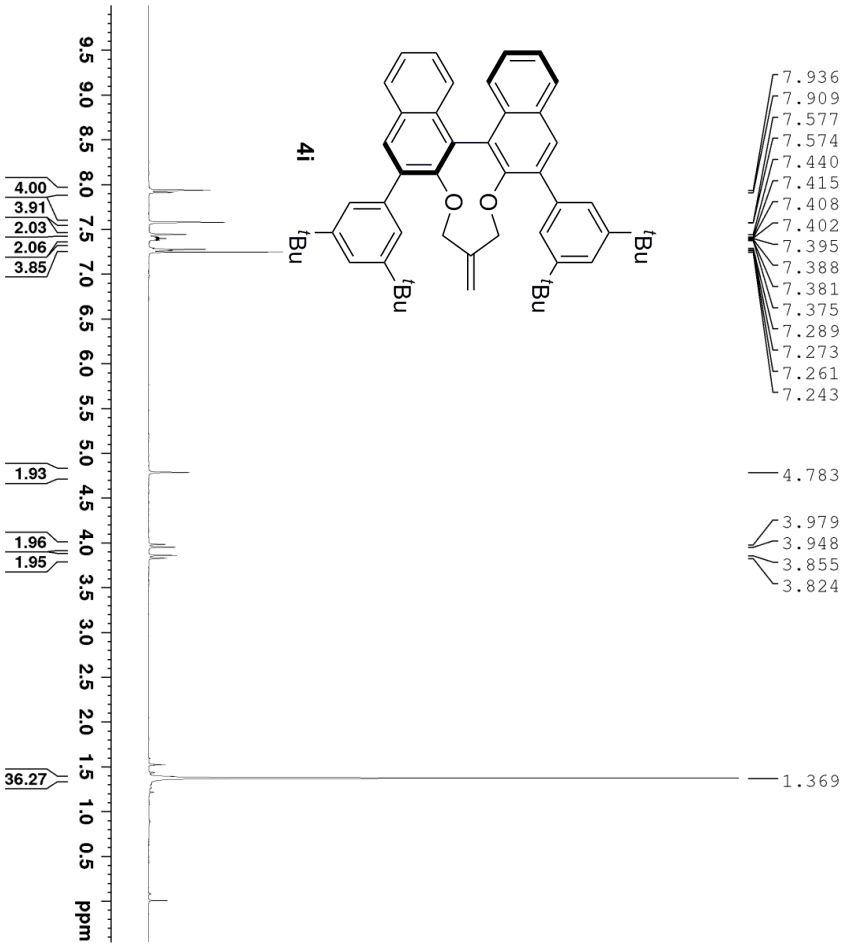

```
Current Data Parameters
NAME                  400-2018
EXPNO                       82
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180403
Time                     23.57 h
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  24038.461 Hz
FIDRES                0.733596 Hz
AQ                    1.3631488 sec
RG                       206.33
DW                       20.800 usec
DE                        6.50 usec
TE                       298.1 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                          1
SFO1               100.6504916 MHz
NUC1                        13C
P1                       10.00 usec
PLW1                54.00000000 W
SFO2               400.2416010 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                12.00000000 W
PLW12                0.34680000 W
PLW13                0.28090999 W

F2 - Processing parameters
SI                       32768
SF                 100.6404091 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```



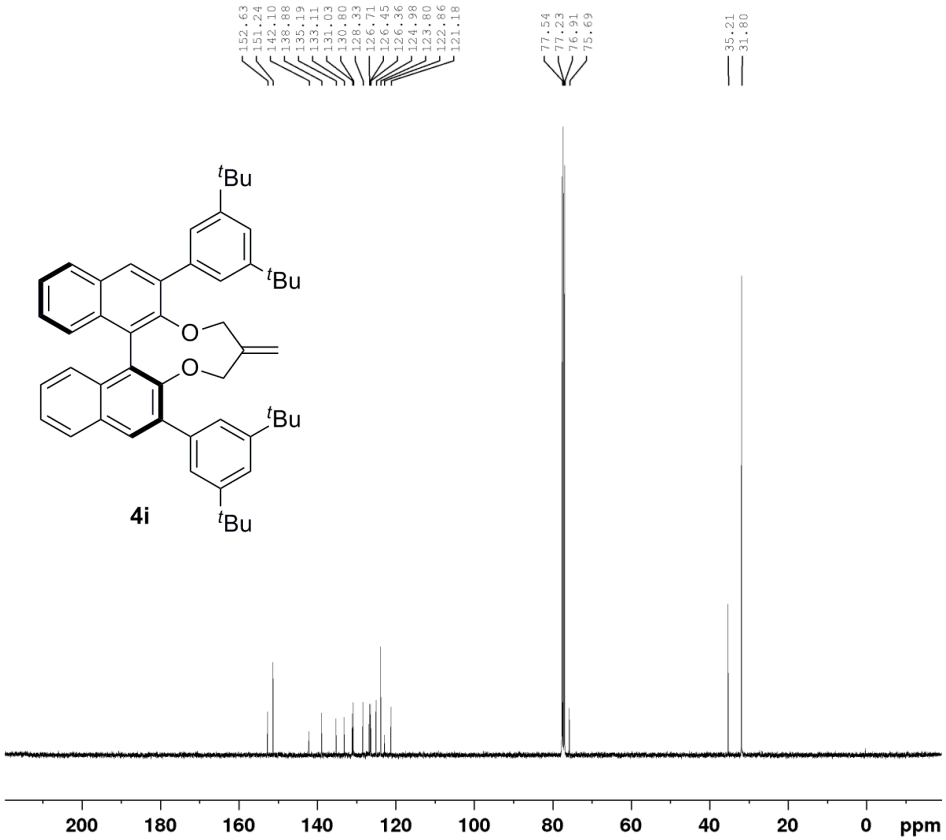

```
Current Data Parameters
NAME                  500-2018
EXPNO                      139
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180801
Time                     22.25 h
INSTRUM                  spect
PROBHD    5 mm CPPBBO BB
PULPROG                  zg30
TD                      65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES                0.305176 Hz
AQ                    3.2767999 sec
RG                       31.72
DW                      50.000 usec
DE                       6.50 usec
TE                      298.1 K
D1                    1.00000000 sec
TD0                          1
SFO1                500.1330885 MHz
NUC1                        1H
P1                      11.50 usec
PLW1                20.00000000 W

F2 - Processing parameters
SI                      65536
SF                  500.1300218 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```



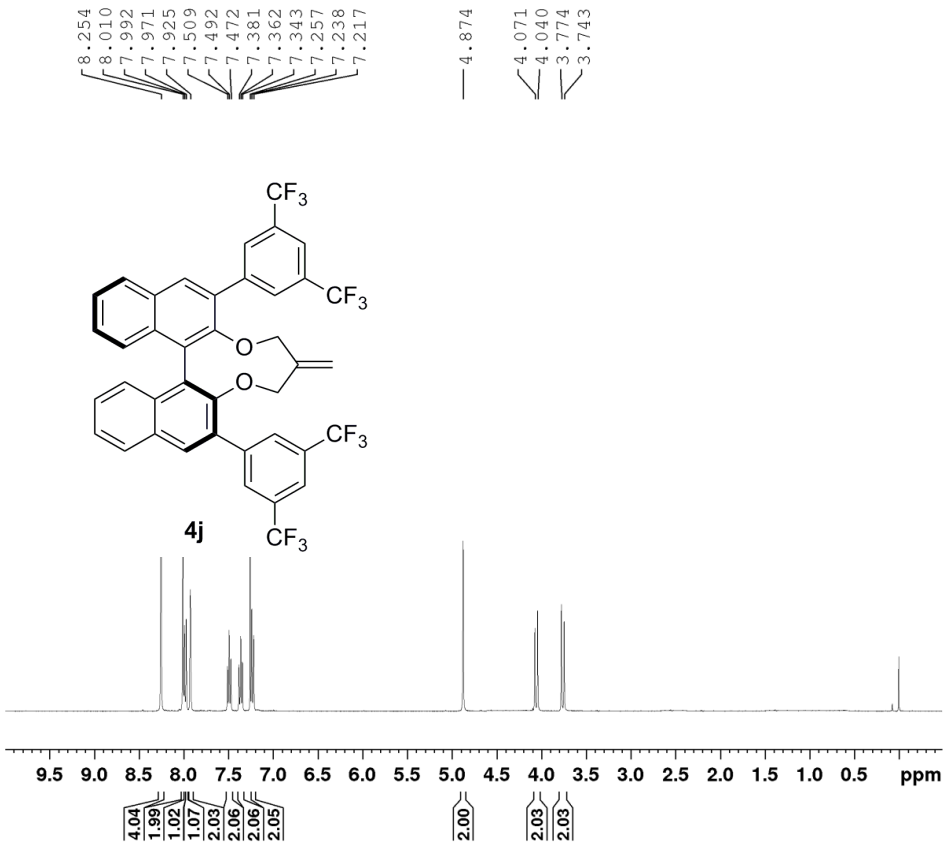

```
Current Data Parameters
NAME                  500-2018
EXPNO                      132
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180726
Time                      2.24 h
INSTRUM                  spect
PROBHD    5 mm CPPBBO BB
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        3000
DS                           4
SWH                  29761.904 Hz
FIDRES                0.908261 Hz
AQ                    1.1010048 sec
RG                       192.89
DW                       16.800 usec
DE                       18.00 usec
TE                       298.2 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                          1
SFO1                125.7703637 MHz
NUC1                        13C
P1                        9.80 usec
PLW1                57.00000000 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2                20.00000000 W
PLW12                0.35778001 W
PLW13                0.22898000 W

F2 - Processing parameters
SI                       32768
SF                  125.7577668 MHz
WDW                         EM
SSB       0
LB                        1.00 Hz
GB        0
PC                        1.40
```



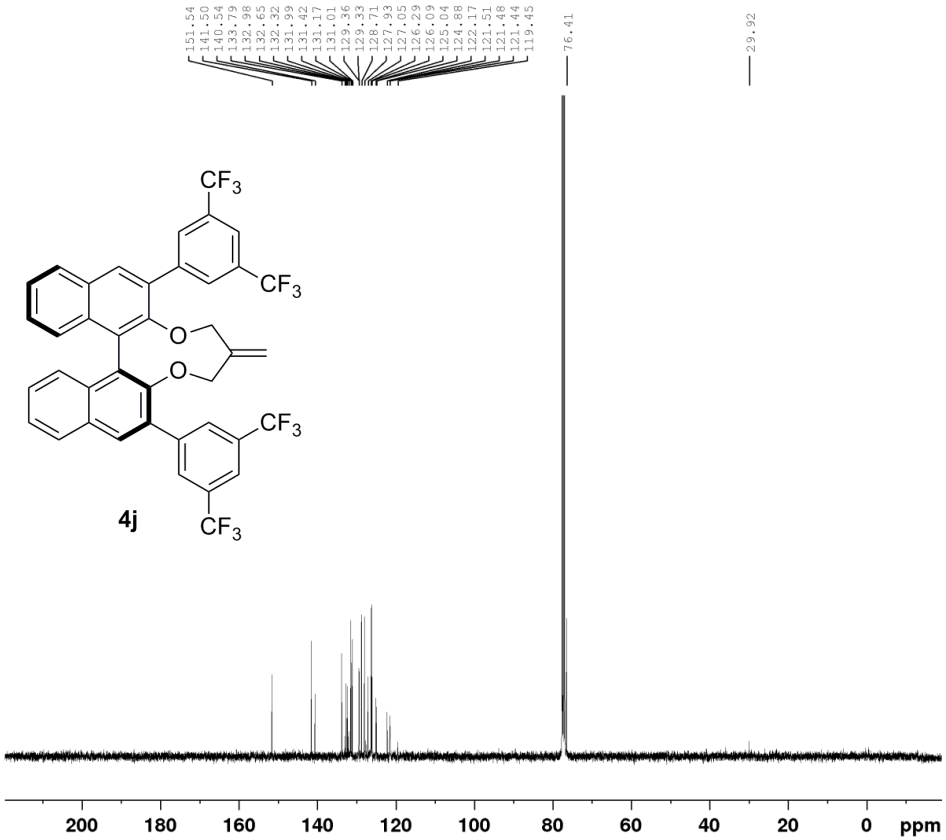

```
Current Data Parameters
NAME                  400-2018
EXPNO                       98
PROCNO                       1

F2 - Acquisition Parameters
Date_              20180405
Time                   22.57 h
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                 2.0447233 sec
RG                    116.67
DW                    62.400 usec
DE                     6.50 usec
TE                    298.0 K
D1                 2.00000000 sec
TD0                       1
SFO1           400.2424716 MHz
NUC1                      1H
P1                    14.80 usec
PLW1           12.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.2400164 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



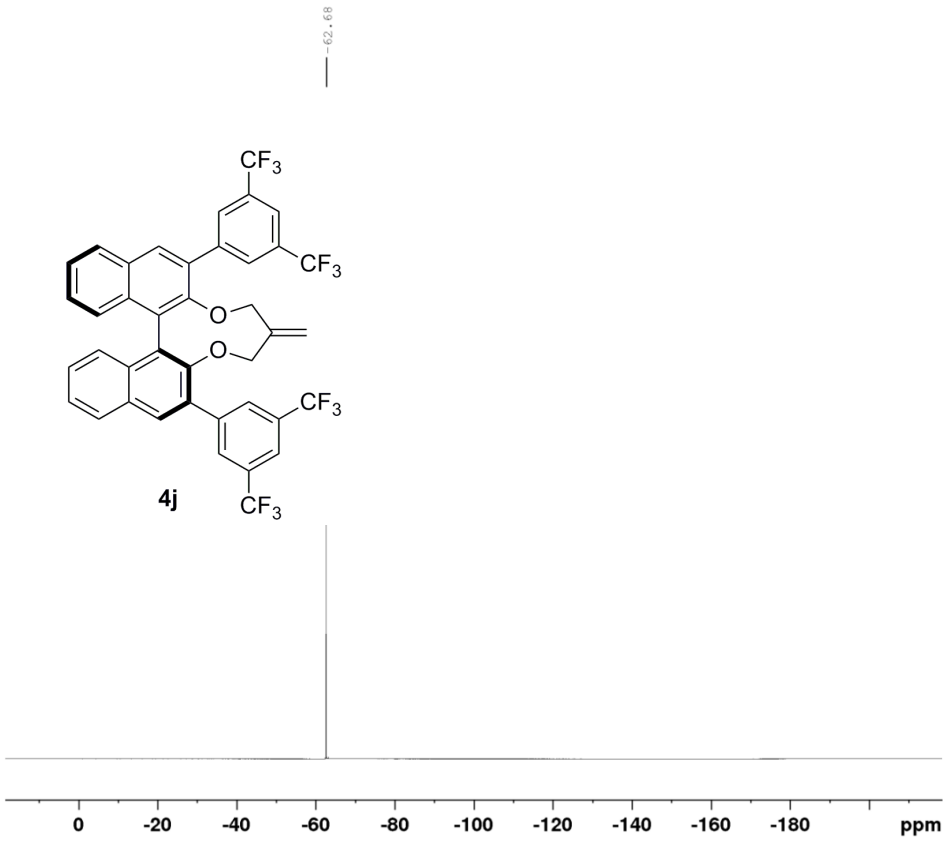

```
Current Data Parameters
NAME            400-2018
EXPNO                118
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180405
Time               23.56 h
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                 13C
P1                10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404091 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



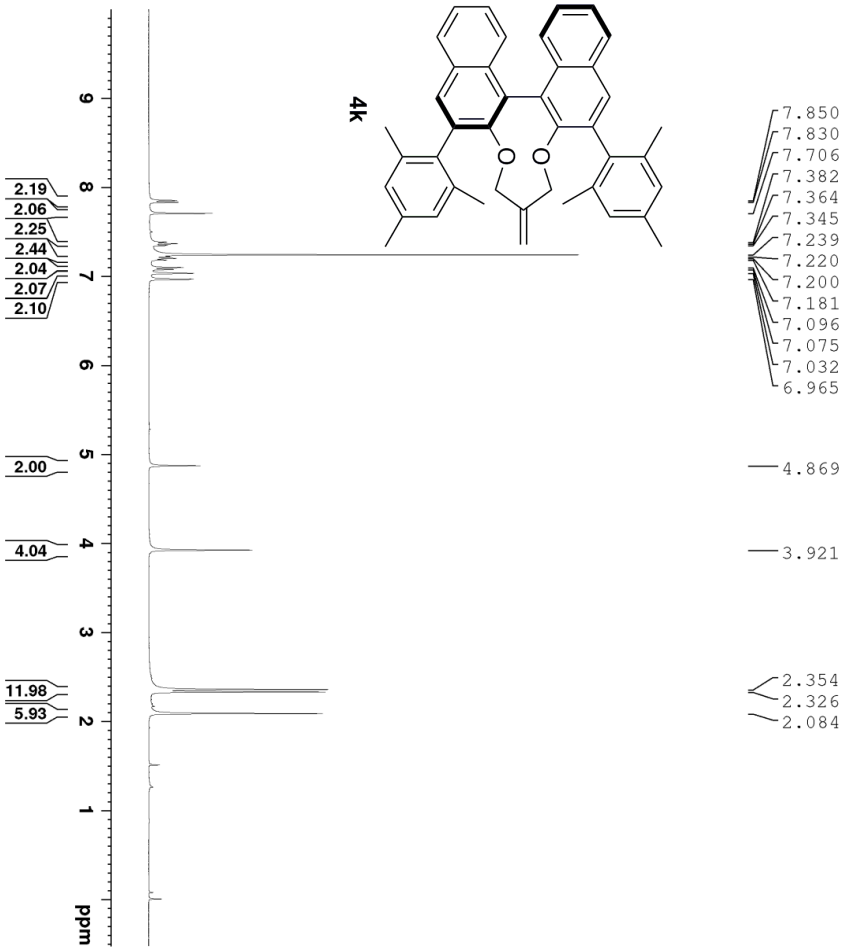

```
Current Data Parameters
NAME            400-2018
EXPNO                214
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180701
Time                0.57 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ              2.0447233 sec
RG                206.33
DW                62.400 usec
DE                 6.50 usec
TE                299.2 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400111 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



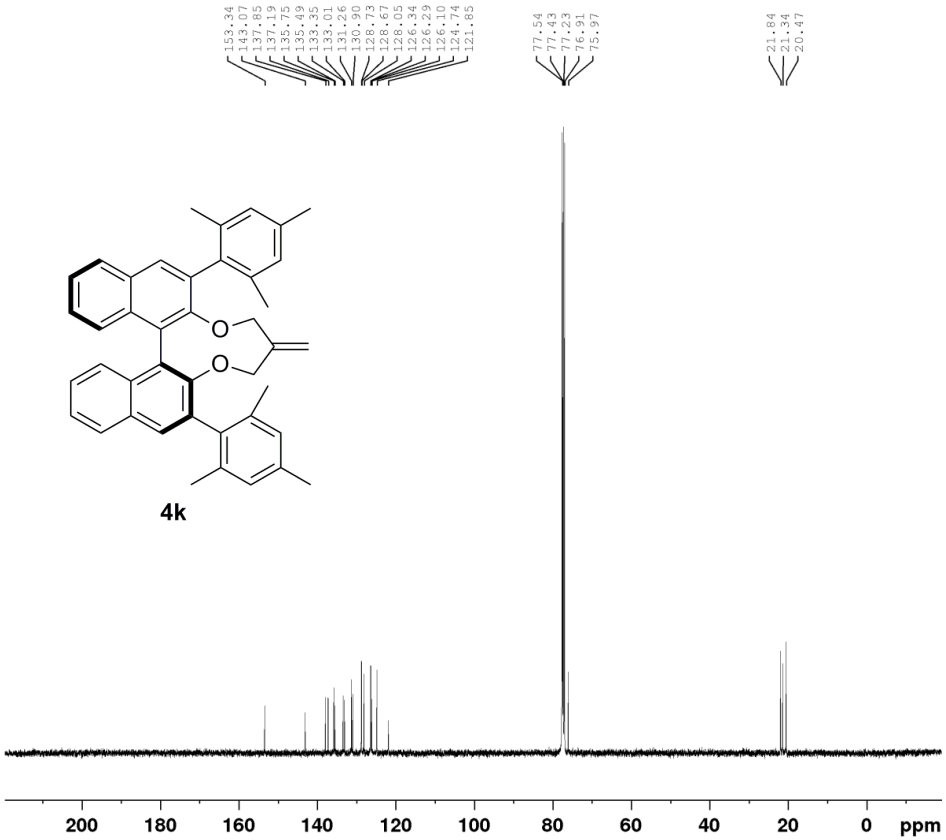

```
Current Data Parameters
NAME            400-2018
EXPNO                215
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180701
Time                2.55 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2048
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                 300.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                 13C
P1                10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404065 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



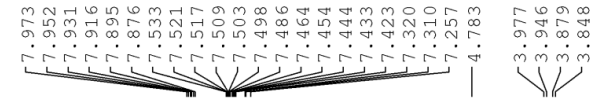

```
Current Data Parameters
NAME            400-2018
EXPNO                130
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180408
Time               21.30 h
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH             89285.711 Hz
FIDRES          1.362392 Hz
AQ              0.7340032 sec
RG                 206.33
DW                  5.600 usec
DE                  6.50 usec
TE                 298.1 K
D1              1.00000000 sec
d11             0.03000000 sec
d12             0.00002000 sec
TD0                    1
rde1            0.00000650 sec
SFO1          376.5642094 MHz
NUC1                  19F
P1                 14.50 usec
PLW1          17.98900032 W
SFO2          400.2416010 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W

F2 - Processing parameters
SI                 65536
SF            376.6018696 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

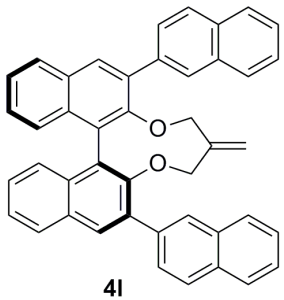



```
Current Data Parameters
NAME                  400-2018
EXPNO                      102
PROCNO                       1

F2 - Acquisition Parameters
Date_              20180406
Time                   1.01 h
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                 2.0447233 sec
RG                      73.9
DW                   62.400 usec
DE                    6.50 usec
TE                   298.0 K
D1                 2.00000000 sec
TD0                       1
SFO1           400.2424716 MHz
NUC1                     1H
P1                    14.80 usec
PLW1           12.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.2400180 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

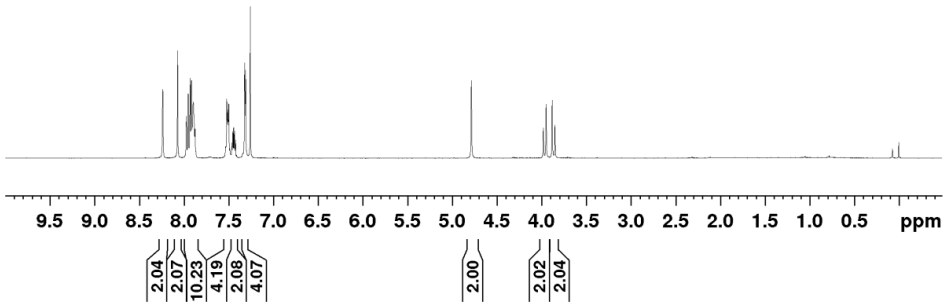



```
Current Data Parameters
NAME            400-2018
EXPNO                103
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180406
Time                2.00 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404098 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

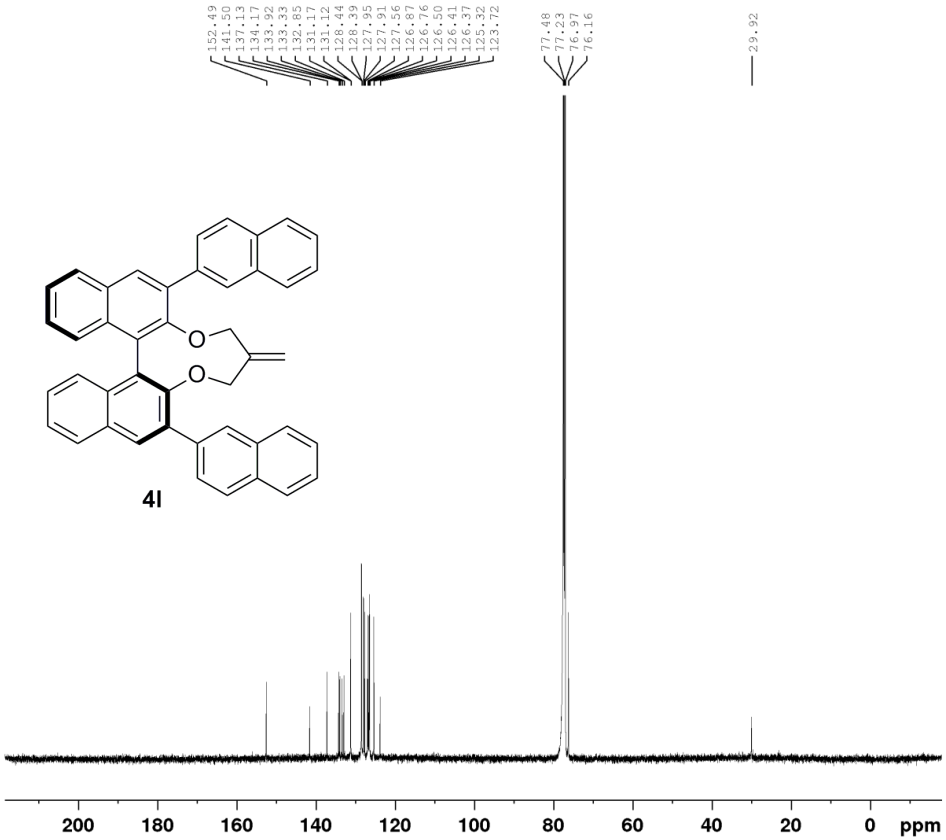




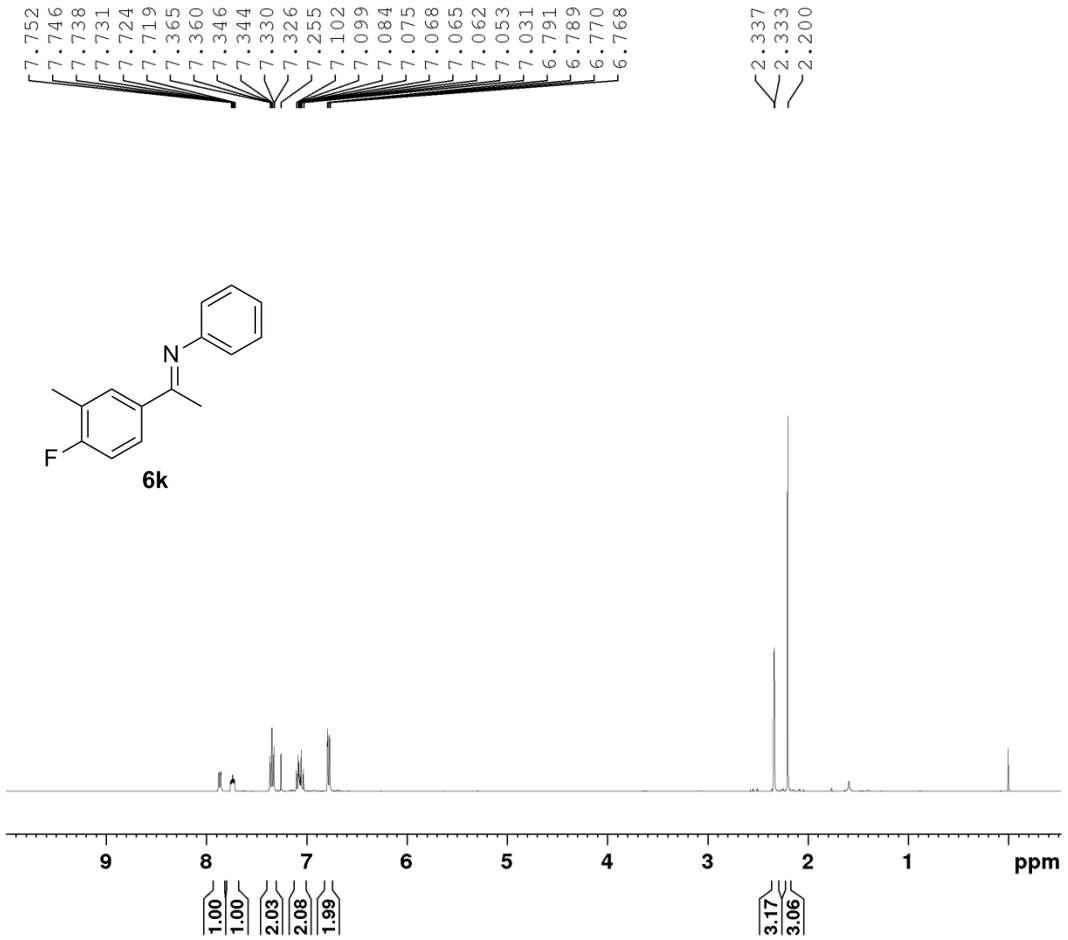
4l



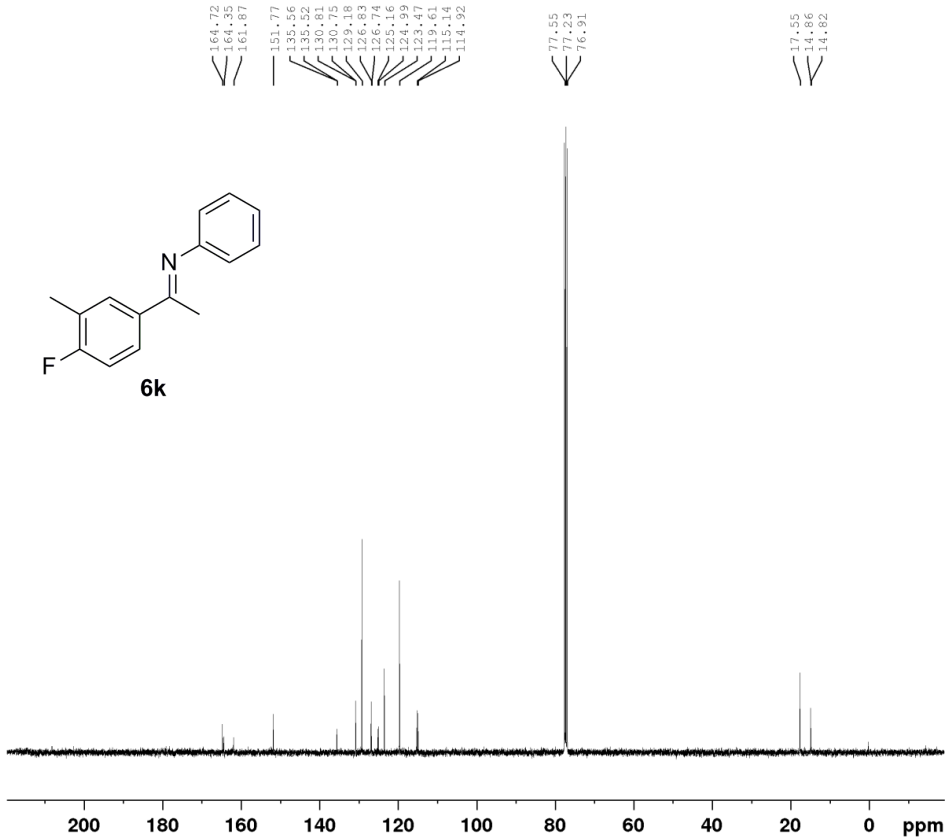

```
Current Data Parameters
NAME            400-2018
EXPNO                223
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180716
Time               22.10 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ              2.0447233 sec
RG                206.33
DW                62.400 usec
DE                 6.50 usec
TE                298.7 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                  1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400109 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



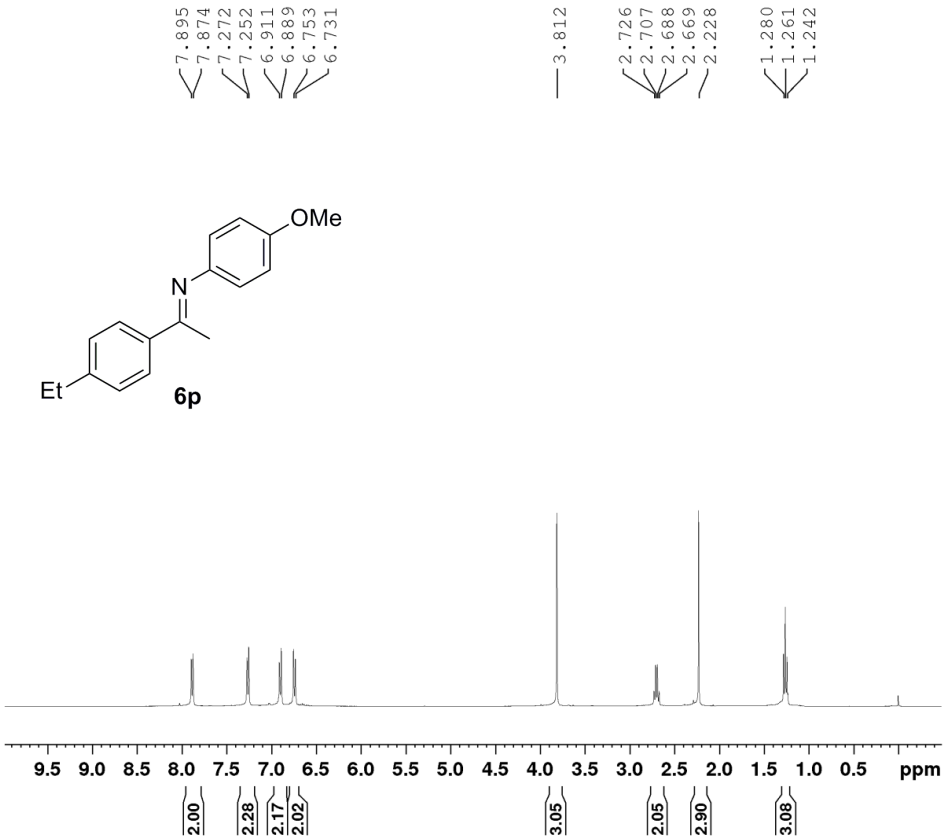

```
Current Data Parameters
NAME                  500-2018
EXPNO                      131
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180725
Time                      22.31 h
INSTRUM                   spect
PROBHD    5 mm CPPBBO BB
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        3000
DS                           4
SWH                  29761.904 Hz
FIDRES                0.908261 Hz
AQ                    1.1010048 sec
RG                       192.89
DW                       16.800 usec
DE                       18.00 usec
TE                       298.2 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                          1
SFO1               125.7703637 MHz
NUC1                        13C
P1                        9.80 usec
PLW1               57.00000000 W
SFO2               500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2               20.00000000 W
PLW12               0.35778001 W
PLW13               0.22898000 W

F2 - Processing parameters
SI                       32768
SF                 125.7577632 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```



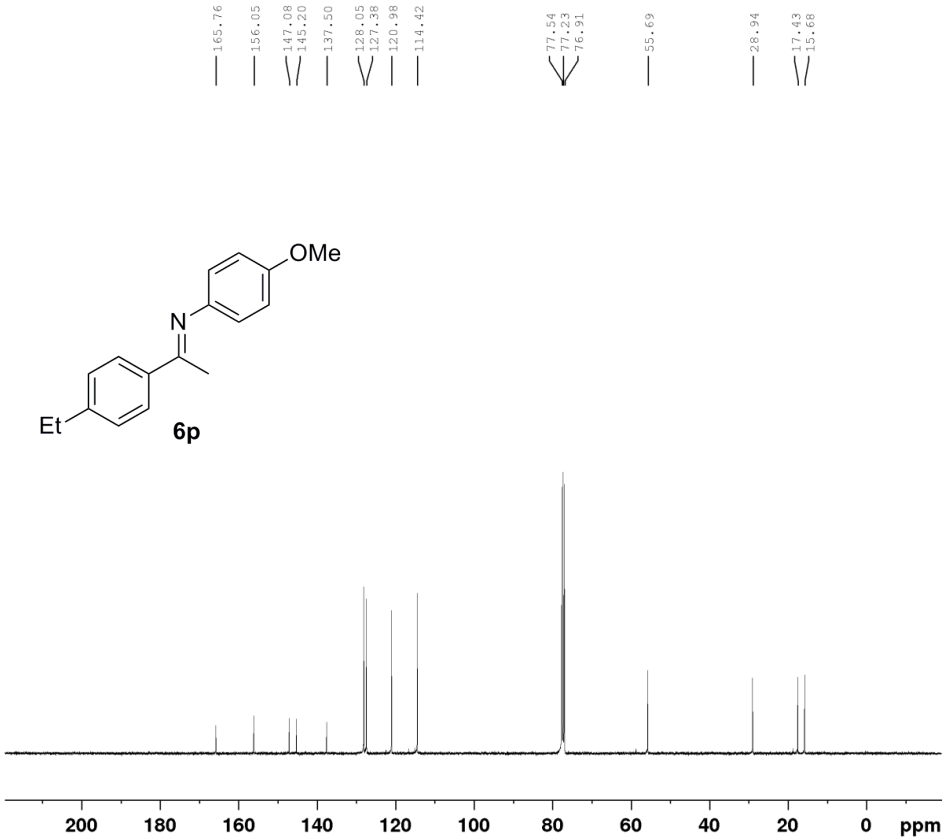

```
Current Data Parameters
NAME            400-2018
EXPNO                268
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180801
Time                6.48 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH              8012.820 Hz
FIDRES           0.489064 Hz
AQ              2.0447233 sec
RG                 206.33
DW                62.400 usec
DE                 6.50 usec
TE                299.0 K
D1             2.00000000 sec
TD0                    1
SFO1          400.2424716 MHz
NUC1                  1H
P1                 14.80 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF            400.24000116 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



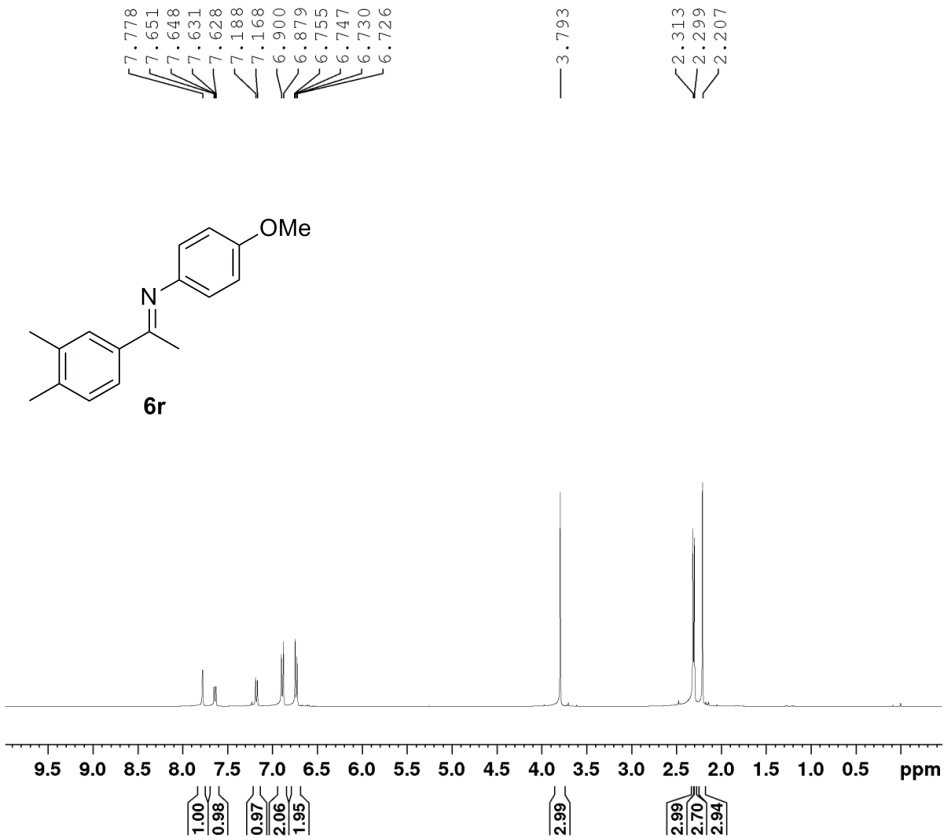

```
Current Data Parameters
NAME            400-2018
EXPNO                269
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180801
Time                7.17 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   500
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                 206.33
DW                20.800 usec
DE                 6.50 usec
TE                299.9 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                 13c
P1                10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404083 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



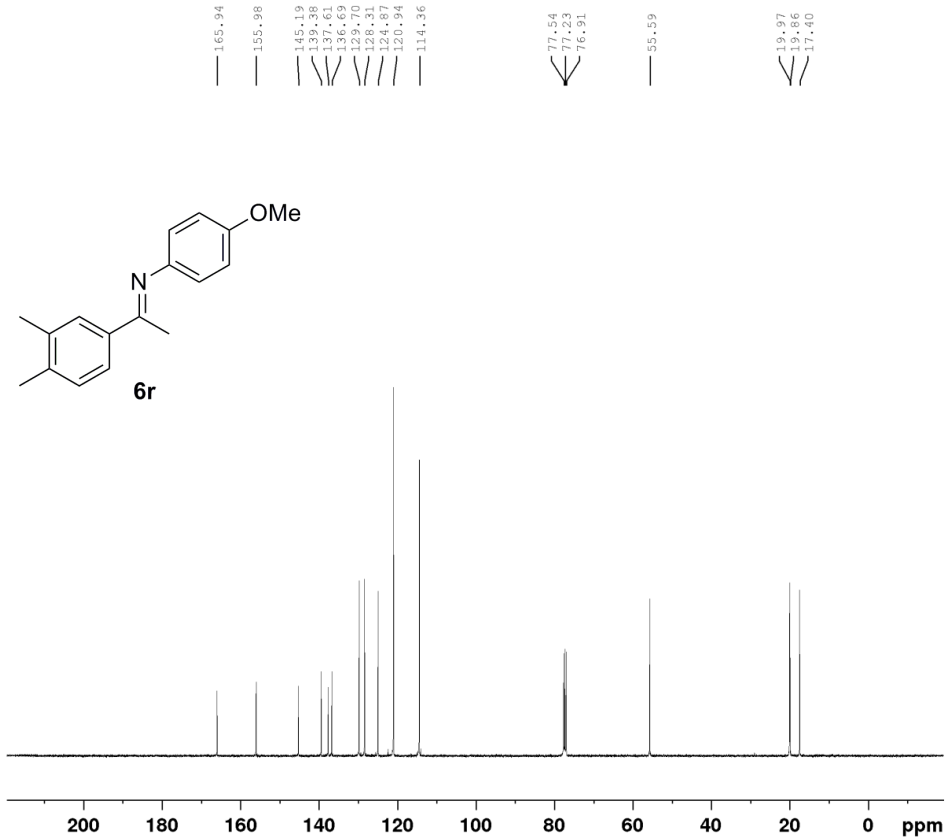

```
Current Data Parameters
NAME            400-2018
EXPNO                373
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181017
Time               22.27 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                140.59
DW                62.400 usec
DE                 6.50 usec
TE                299.1 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400134 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



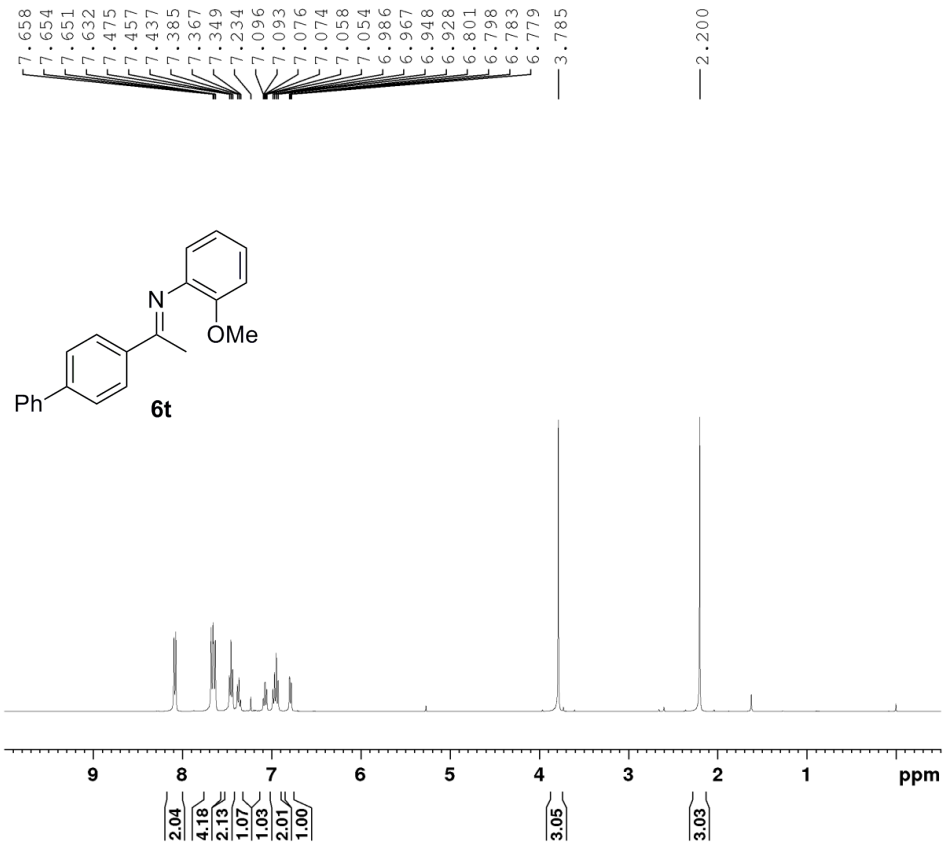

```
Current Data Parameters
NAME            400-2018
EXPNO                374
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181017
Time              23.54 h
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1500
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                300.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                 13C
P1                10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404091 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



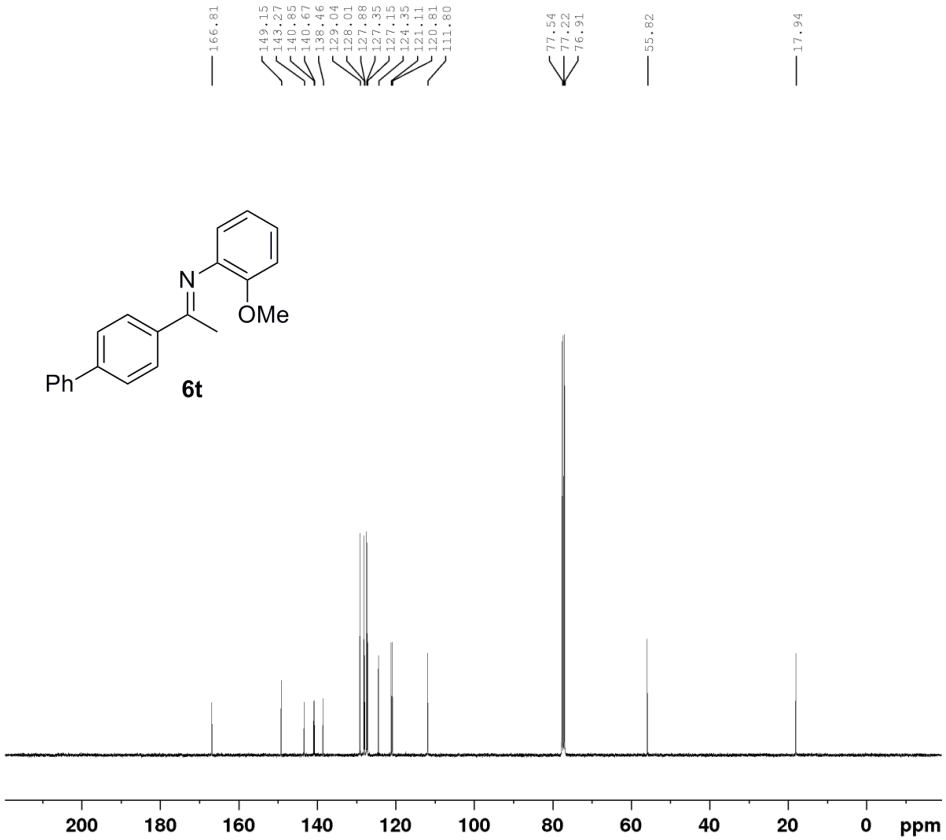

```
Current Data Parameters
NAME            400-2018
EXPNO                375
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181017
Time               23.57 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ              2.0447233 sec
RG                 39.92
DW                 62.400 usec
DE                  6.50 usec
TE                 299.2 K
D1              2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                1H
P1                 14.80 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400222 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



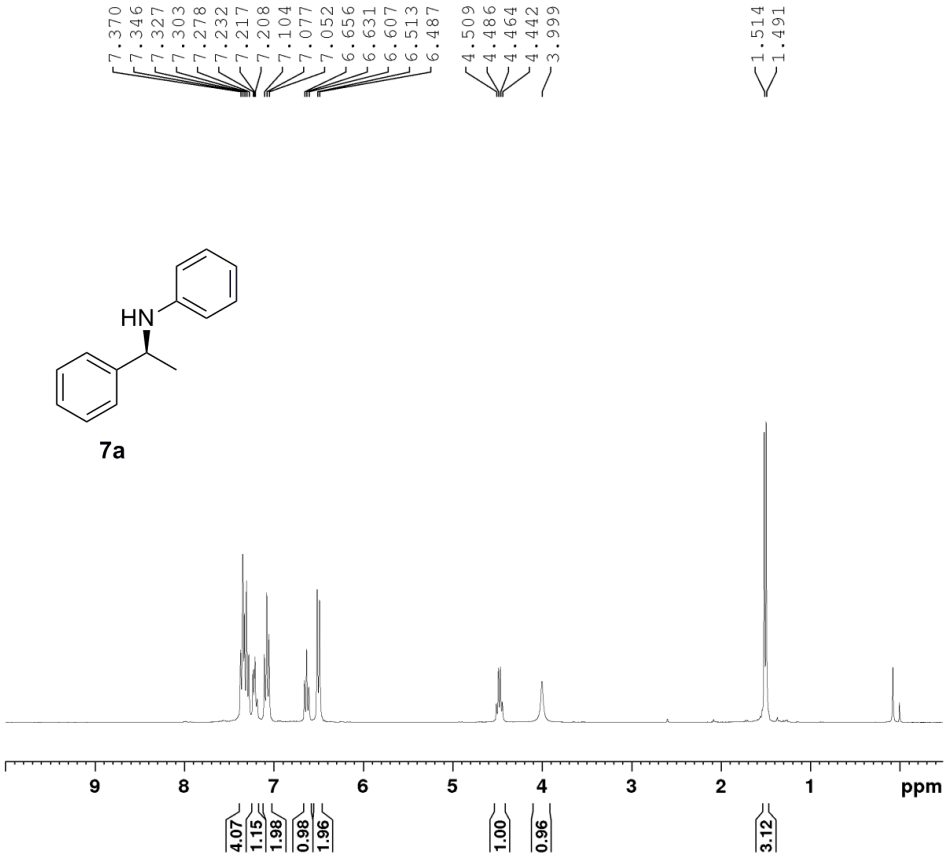

```
Current Data Parameters
NAME            400-2018
EXPNO                376
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181018
Time                0.26 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   500
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                 206.33
DW                20.800 usec
DE                 6.50 usec
TE                 300.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1
SFO1        100.6504916 MHz
NUC1                 13C
P1                10.00 usec
PLW1         54.00000000 W
SFO2        400.2416010 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.34680000 W
PLW13         0.28090999 W

F2 - Processing parameters
SI                 32768
SF          100.6404164 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



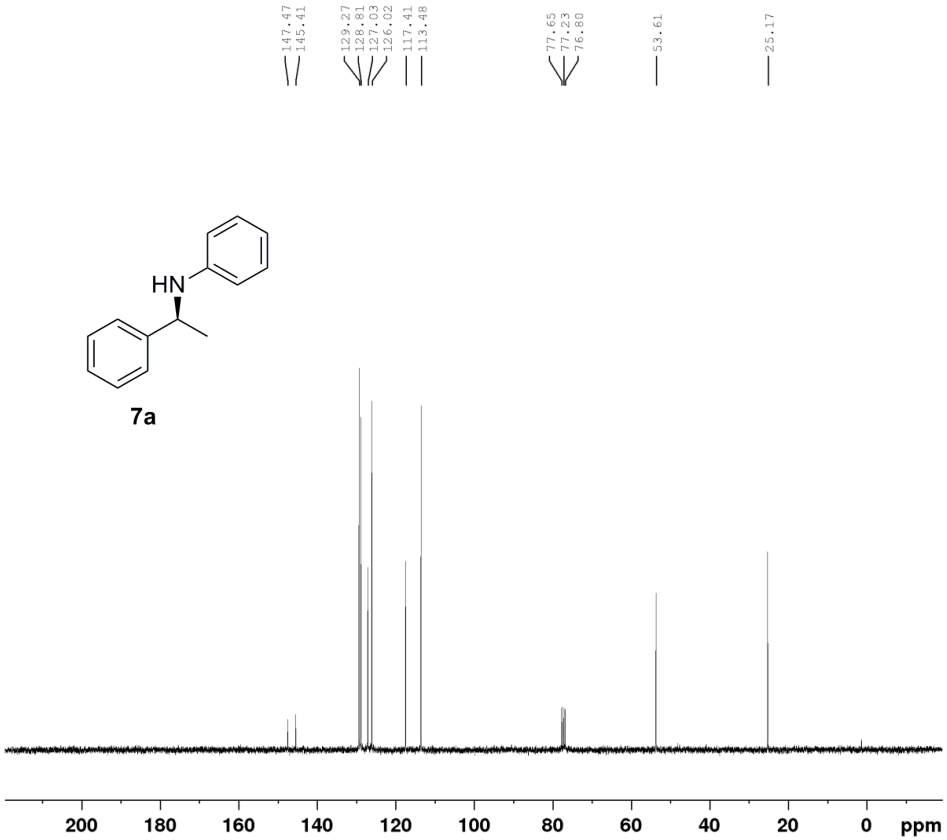

```
Current Data Parameters
NAME            400-2018
EXPNO                383
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181021
Time               22.29 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ              2.0447233 sec
RG                 80.72
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400202 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



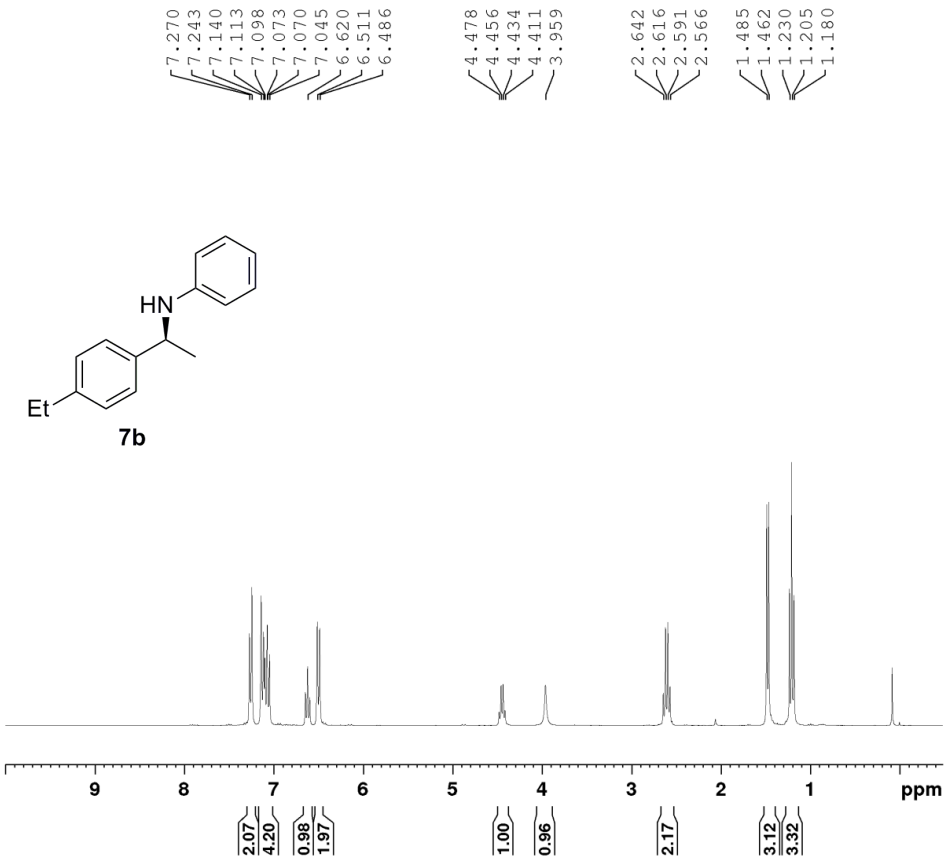

```
Current Data Parameters
NAME                  400-2018
EXPNO                      384
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20181021
Time                     23.55 h
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                        65536
SOLVENT                  CDCl3
NS                        1500
DS                           4
SWH                  24038.461 Hz
FIDRES                0.733596 Hz
AQ                    1.3631488 sec
RG                       206.33
DW                       20.800 usec
DE                        6.50 usec
TE                       298.8 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                          1
SFO1                100.6504916 MHz
NUC1                        13C
P1                       10.00 usec
PLW1                54.00000000 W
SFO2                400.2416010 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                12.00000000 W
PLW12                0.34680000 W
PLW13                0.28090999 W

F2 - Processing parameters
SI                        32768
SF                  100.6404127 MHz
WDW                          EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```




```
Current Data Parameters
NAME                du-1t
EXPNO                 225
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180516
Time                15.47 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               5.4525952 sec
RG                 142.81
DW                 83.200 usec
DE                   6.50 usec
TE                 301.2 K
D1              1.00000000 sec
TD0                    1
SFO1          300.1318534 MHz
NUC1                  1H
P1                   8.00 usec
PLW1          18.00000000 W

F2 - Processing parameters
SI                 65536
SF            300.1300206 MHz
WDW                   EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

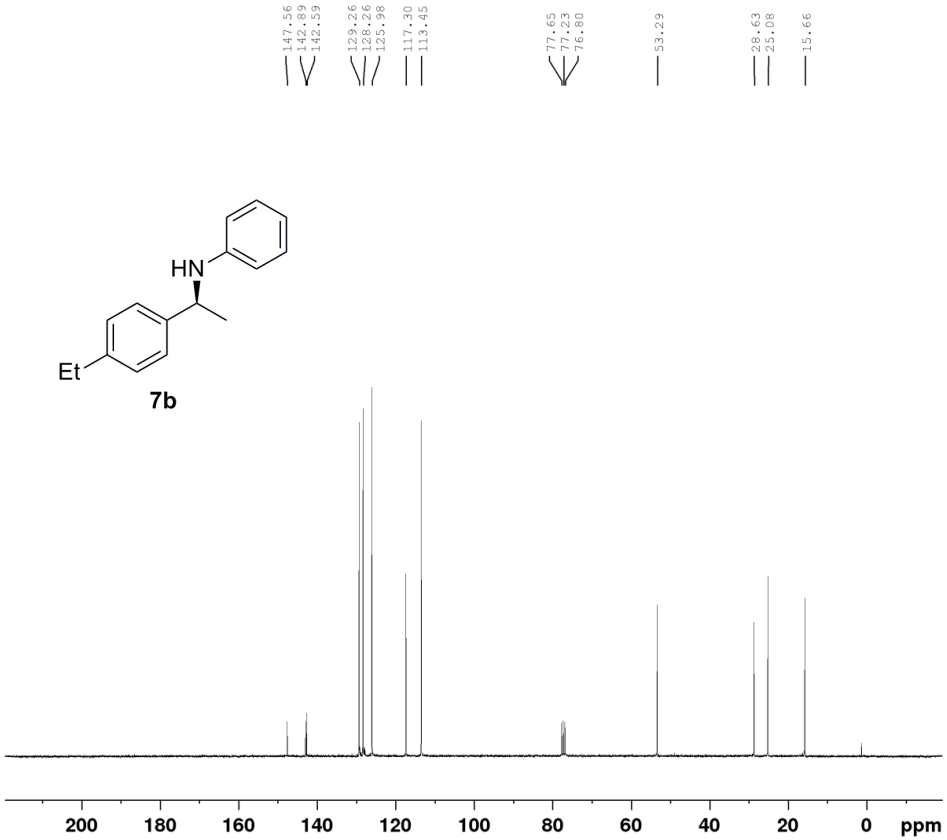



```
Current Data Parameters
NAME                  du-lt
EXPNO                   229
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180516
Time                  16.32 h
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        36
DS                         4
SWH                18028.846 Hz
FIDRES                0.550197 Hz
AQ                    1.8175317 sec
RG                      209.09
DW                     27.733 usec
DE                       6.50 usec
TE                      301.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1
SFO1              75.4752949 MHz
NUC1                      13C
P1                     11.00 usec
PLW1             195.00000000 W
SFO2             300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                  90.00 usec
PLW2              14.00000000 W
PLW12              0.17284000 W
PLW13              0.14000000 W

F2 - Processing parameters
SI                        32768
SF                75.4677422 MHz
WDW                        EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

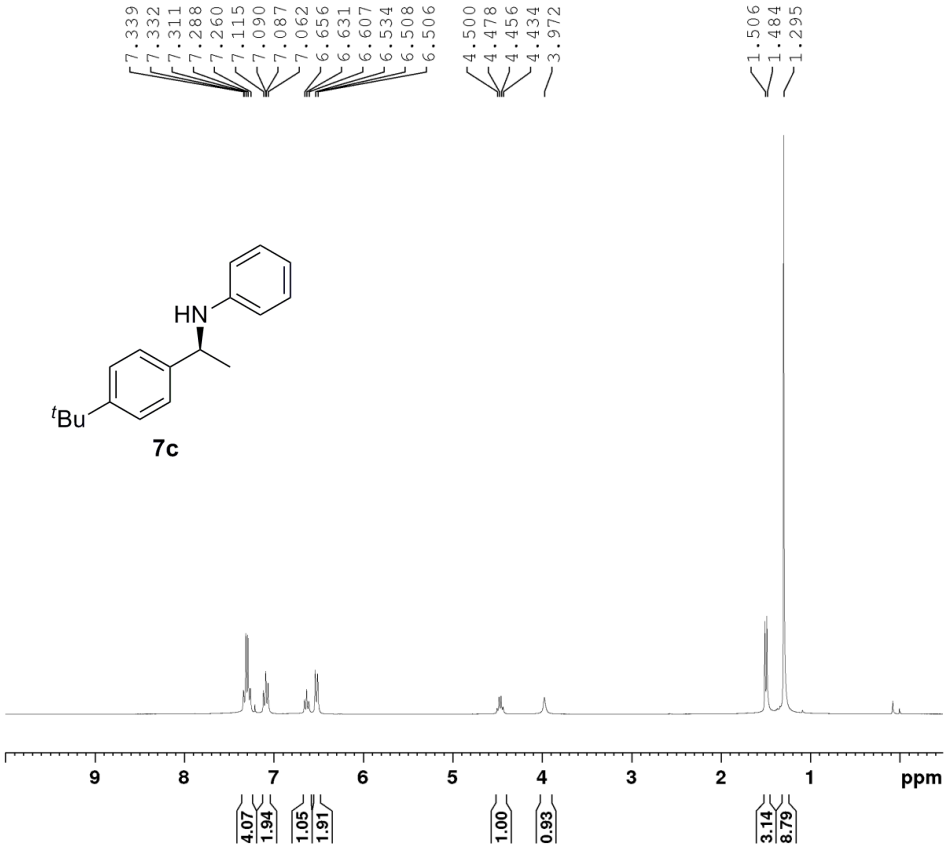


7b

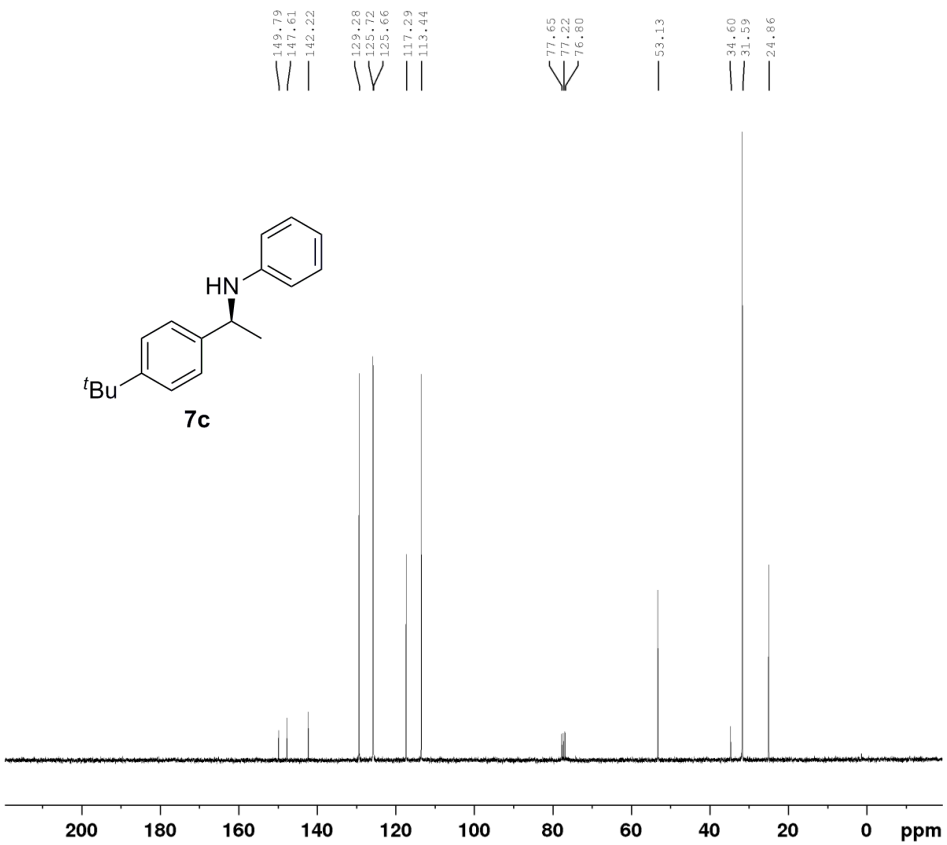
```
Current Data Parameters
NAME                  du-lt
EXPNO                   260
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180524
Time                 14.02 h
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               5.4525952 sec
RG                  74.53
DW                 83.200 usec
DE                  6.50 usec
TE                 299.3 K
D1              1.00000000 sec
TD0                     1
SFO1           300.1318534 MHz
NUC1                   1H
P1                  8.00 usec
PLW1           18.00000000 W

F2 - Processing parameters
SI                  65536
SF             300.1300409 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



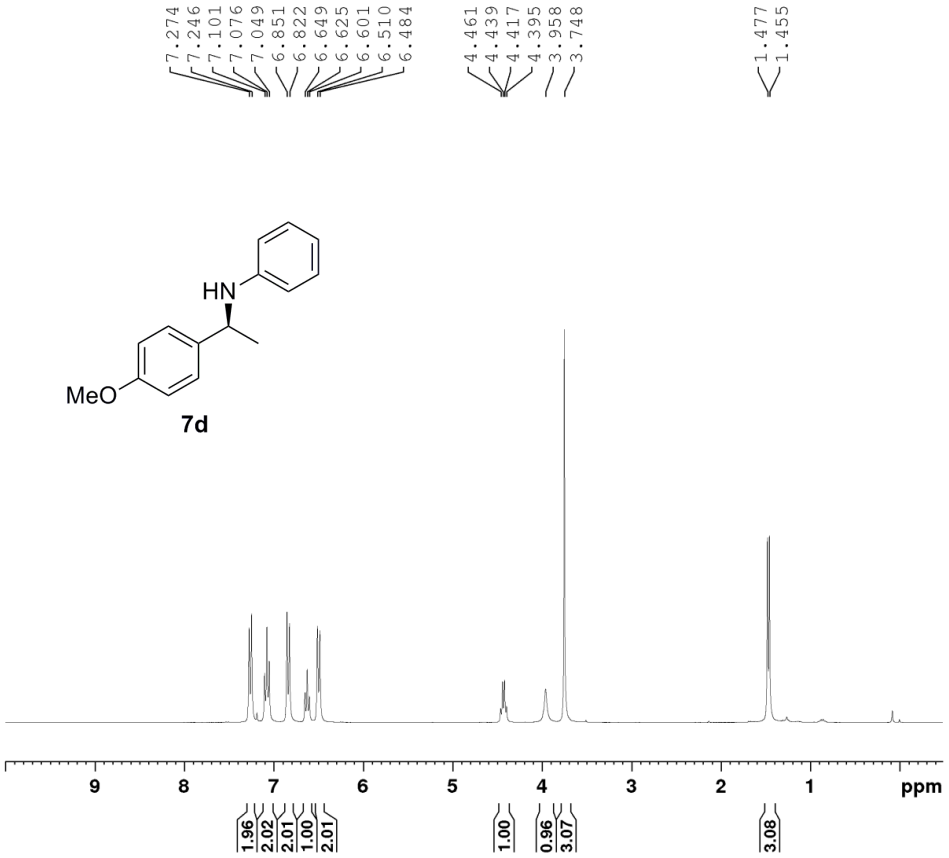

```
Current Data Parameters
NAME                  du-lt
EXPNO                   261
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180524
Time                   14.23 h
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      189
DS                        4
SWH                18028.846 Hz
FIDRES                0.550197 Hz
AQ                    1.8175317 sec
RG                      209.09
DW                     27.733 usec
DE                      6.50 usec
TE                     299.9 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                       1
SFO1               75.4752949 MHz
NUC1                     13C
P1                     11.00 usec
PLW1              195.00000000 W
SFO2              300.1312005 MHz
NUC2                     1H
CPDPRG[2               waltz16
PCPD2                  90.00 usec
PLW2               14.00000000 W
PLW12               0.17284000 W
PLW13               0.14000000 W

F2 - Processing parameters
SI                        32768
SF                 75.4677434 MHz
WDW                        EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



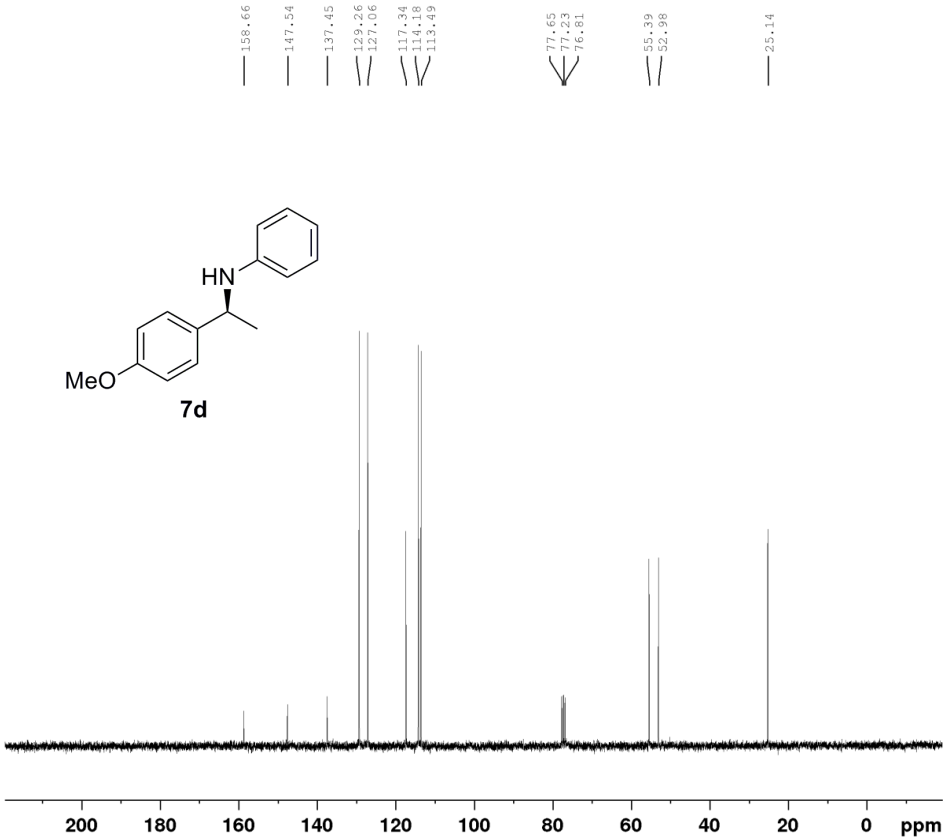

```
Current Data Parameters
NAME                  du-1t
EXPNO                   224
PROCNO                    1

F2 - Acquisition Parameters
Date_           20180516
Time                15.25 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             5.4525952 sec
RG                142.81
DW                83.200 usec
DE                 6.50 usec
TE                301.2 K
D1             1.00000000 sec
TD0                    1
SFO1         300.1318534 MHz
NUC1                  1H
P1                 8.00 usec
PLW1         18.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300231 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



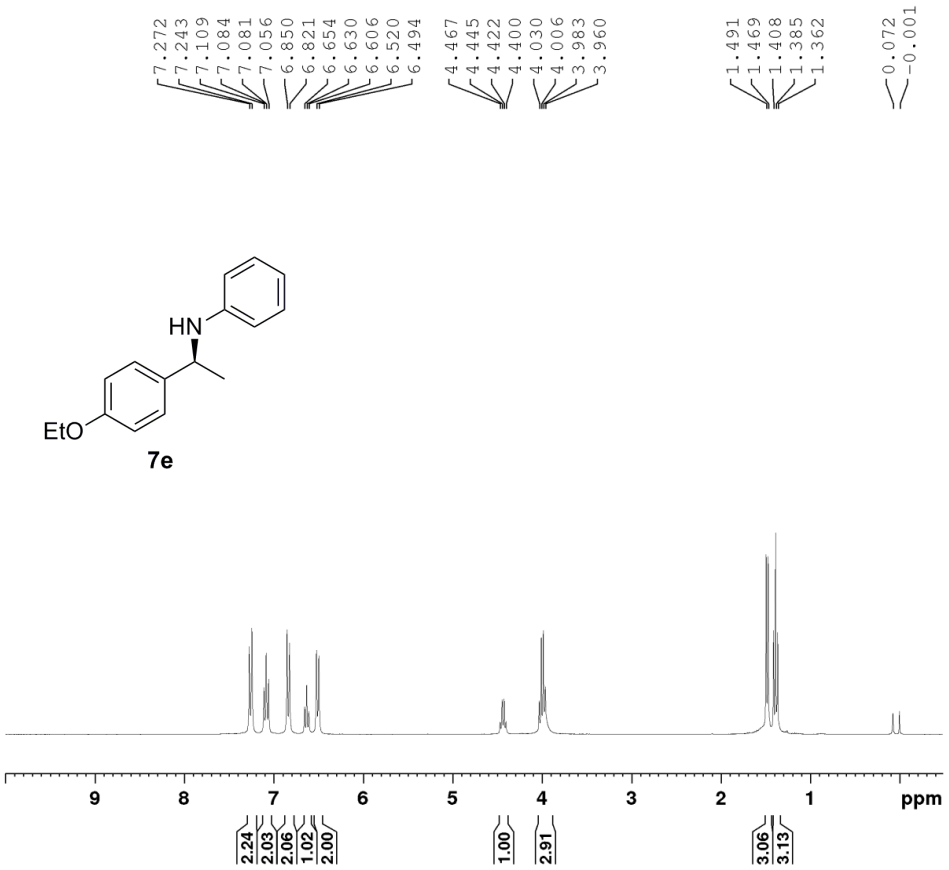

```
Current Data Parameters
NAME                  du-lt
EXPNO                   228
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180516
Time                  16.15 h
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        44
DS                         4
SWH                18028.846 Hz
FIDRES                0.550197 Hz
AQ                 1.8175317 sec
RG                    209.09
DW                    27.733 usec
DE                      6.50 usec
TE                     301.1 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1
SFO1              75.4752949 MHz
NUC1                      13C
P1                     11.00 usec
PLW1             195.00000000 W
SFO2             300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                  90.00 usec
PLW2              14.00000000 W
PLW12              0.17284000 W
PLW13              0.14000000 W

F2 - Processing parameters
SI                     32768
SF                75.4677428 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



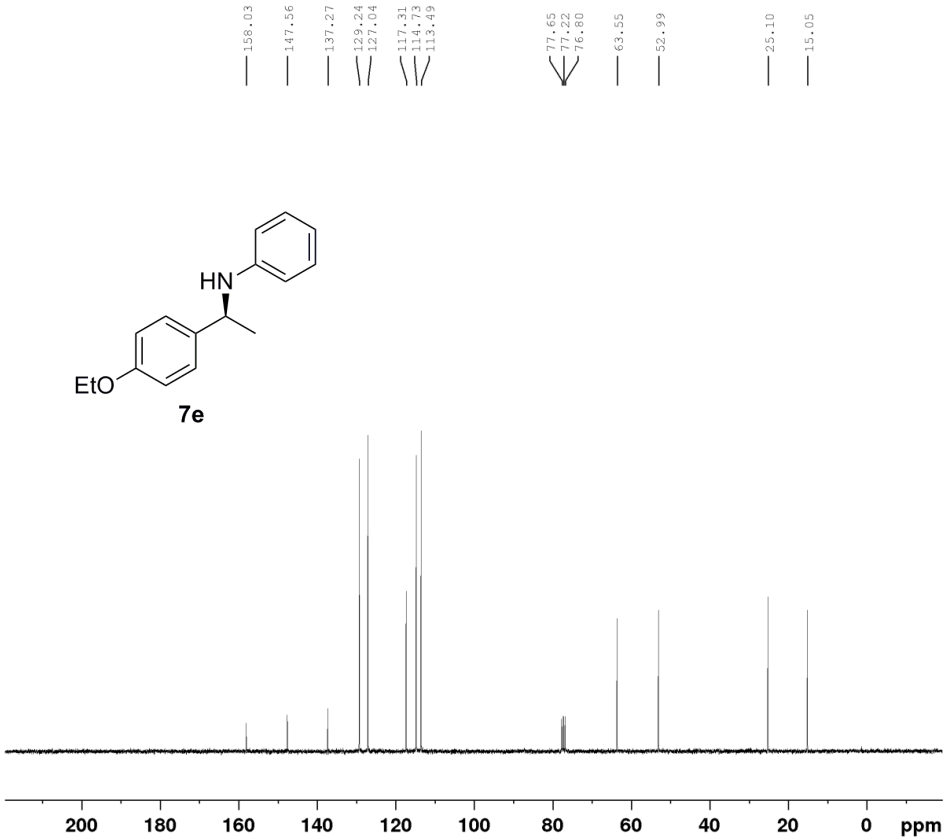

```
Current Data Parameters
NAME                du-lt
EXPNO                 239
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180517
Time                15.51 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     7
DS                     2
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              5.4525952 sec
RG                 103.37
DW                 83.200 usec
DE                  6.50 usec
TE                 300.9 K
D1              1.00000000 sec
TD0                    1
SFO1         300.1318534 MHz
NUC1                 1H
P1                  8.00 usec
PLW1        18.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300291 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



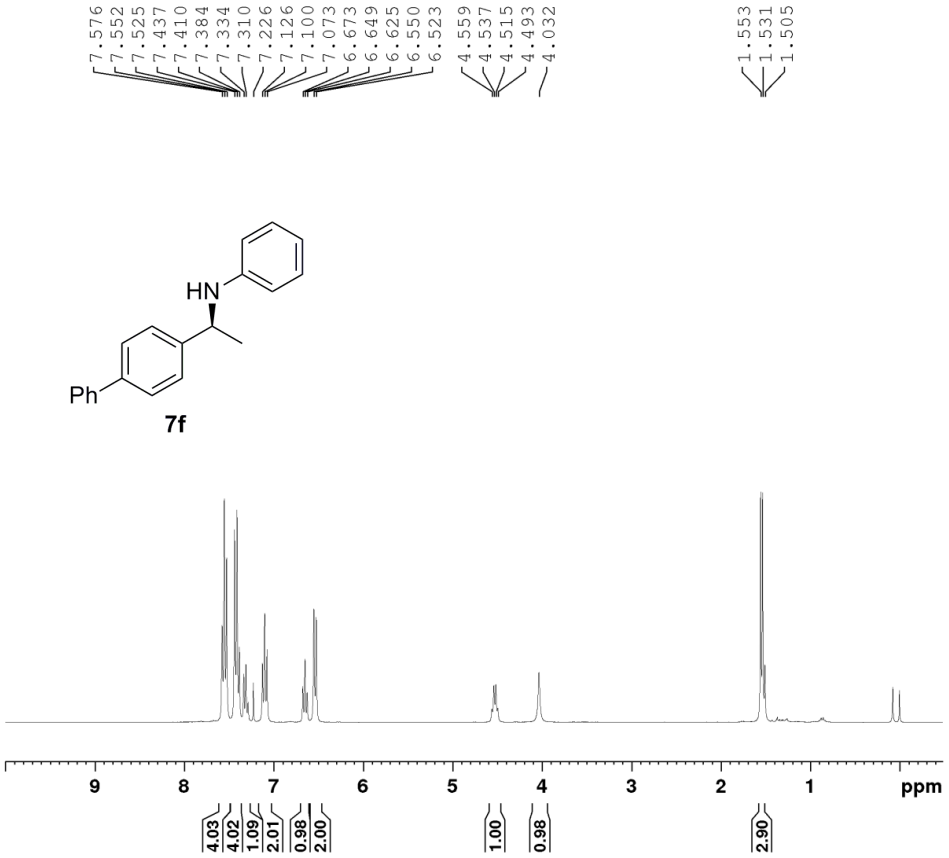

```
Current Data Parameters
NAME                  du-lt
EXPNO                   240
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180517
Time                  15.54 h
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT               CDCl3
NS                        25
DS                         4
SWH               18028.846 Hz
FIDRES             0.550197 Hz
AQ                 1.8175317 sec
RG                    209.09
DW                    27.733 usec
DE                      6.50 usec
TE                     301.1 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1             75.4752949 MHz
NUC1                     13C
P1                    11.00 usec
PLW1            195.00000000 W
SFO2            300.1312005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             14.00000000 W
PLW12             0.17284000 W
PLW13             0.14000000 W

F2 - Processing parameters
SI                     32768
SF               75.4677406 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```




```
Current Data Parameters
NAME                  du-lt
EXPNO                   226
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180516
Time                  15.52 h
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6009.615 Hz
FIDRES            0.183399 Hz
AQ                5.4525952 sec
RG                   209.09
DW                   83.200 usec
DE                    6.50 usec
TE                   301.0 K
D1                1.00000000 sec
TD0                       1
SFO1           300.1318534 MHz
NUC1                    1H
P1                    8.00 usec
PLW1           18.00000000 W

F2 - Processing parameters
SI                    65536
SF             300.1300138 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

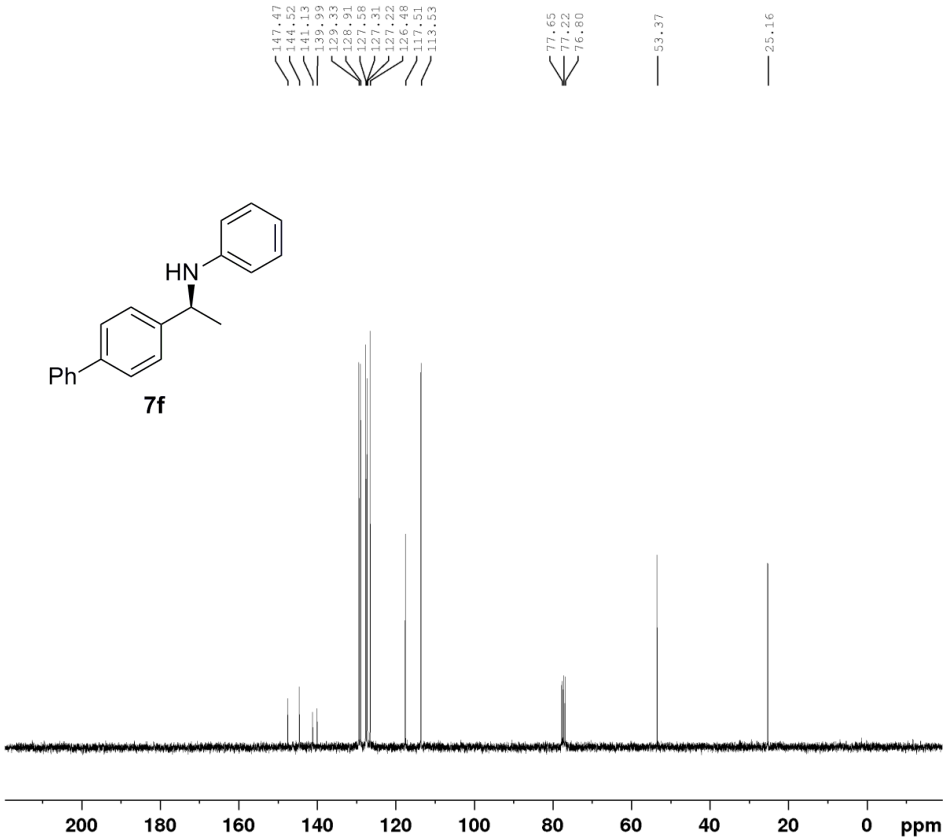



```
Current Data Parameters
NAME                  du-lt
EXPNO                   231
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180516
Time                  16.37 h
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT               CDCl3
NS                        51
DS                         4
SWH               18028.846 Hz
FIDRES             0.550197 Hz
AQ                 1.8175317 sec
RG                    209.09
DW                   27.733 usec
DE                     6.50 usec
TE                    301.1 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1             75.4752949 MHz
NUC1                    13C
P1                    11.00 usec
PLW1            195.00000000 W
SFO2            300.1312005 MHz
NUC2                    1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             14.00000000 W
PLW12             0.17284000 W
PLW13             0.14000000 W

F2 - Processing parameters
SI                     32768
SF               75.4677412 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

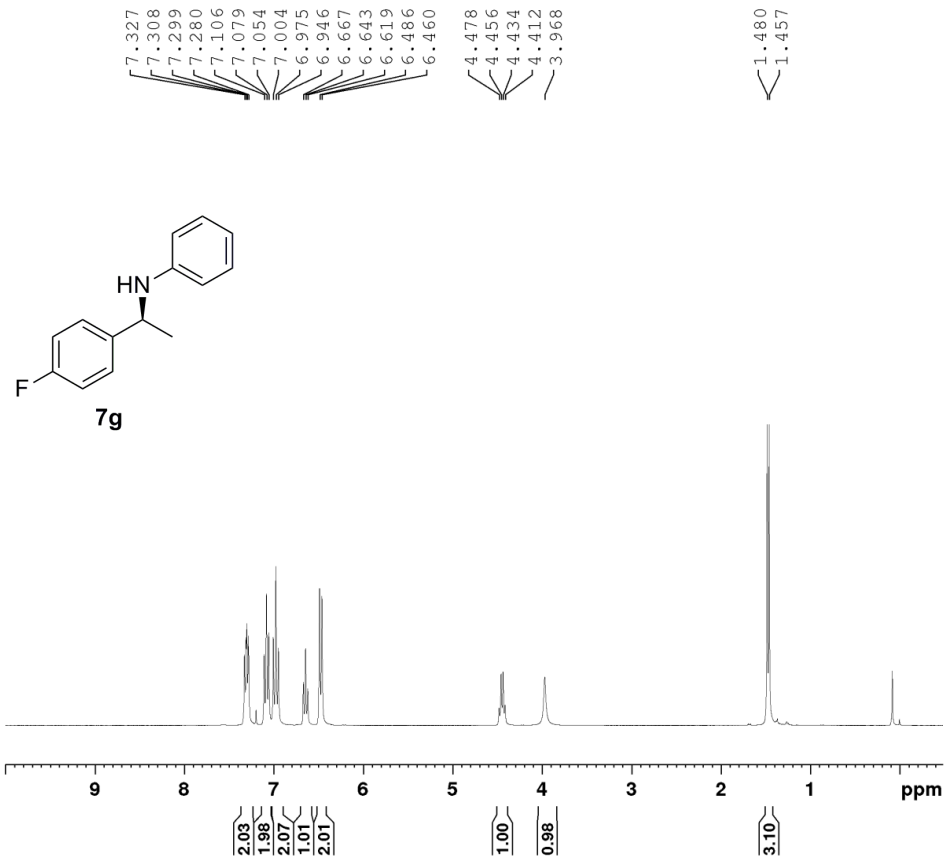


7f

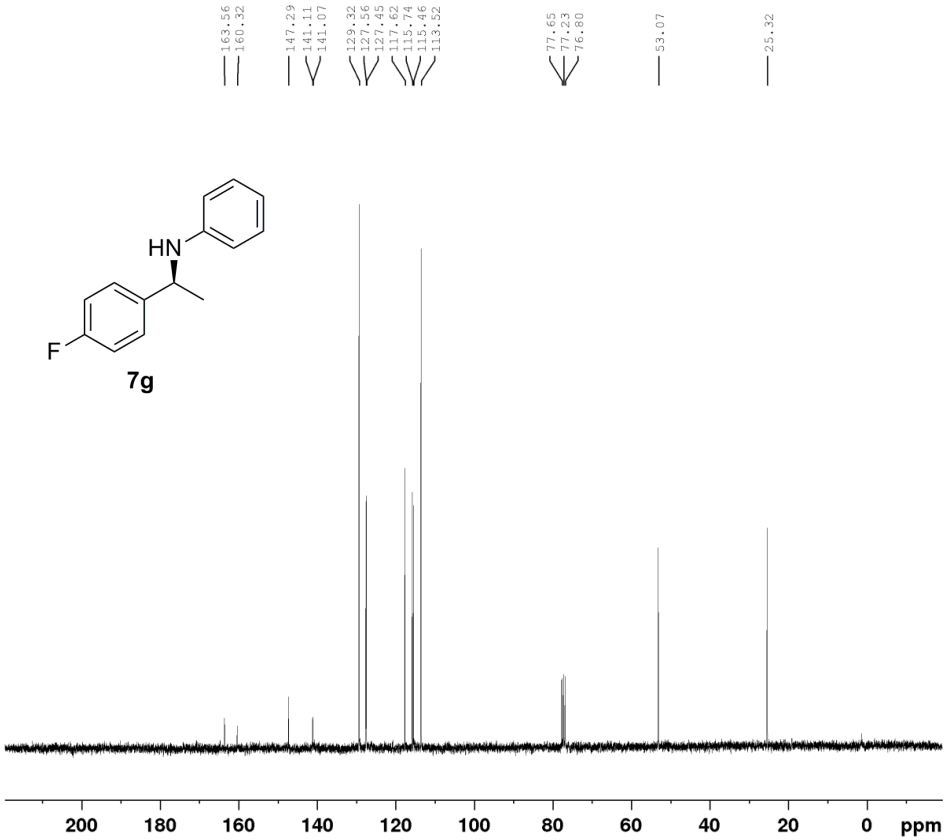
```
Current Data Parameters
NAME                  du-lt
EXPNO                   221
PROCNO                    1

F2 - Acquisition Parameters
Date_           20180515
Time                13.45 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              5.4525952 sec
RG                 209.09
DW                 83.200 usec
DE                  6.50 usec
TE                 301.1 K
D1              1.00000000 sec
TD0                    1
SFO1         300.1318534 MHz
NUC1                 1H
P1                  8.00 usec
PLW1        18.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300172 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



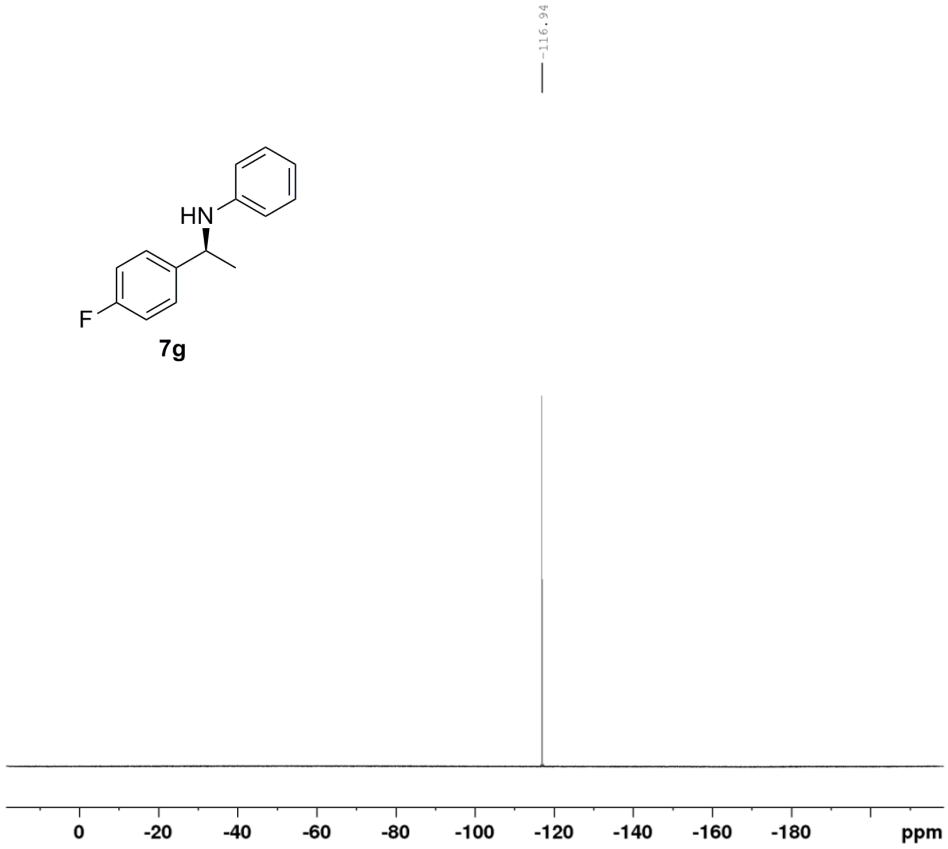

```
Current Data Parameters
NAME                  du-lt
EXPNO                   223
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180515
Time                   17.15 h
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        54
DS                         4
SWH                18028.846 Hz
FIDRES                 0.550197 Hz
AQ                     1.8175317 sec
RG                       209.09
DW                        27.733 usec
DE                         6.50 usec
TE                       301.7 K
D1                     2.00000000 sec
d11                    0.03000000 sec
DELTA                  1.89999998 sec
TD0                           1
SFO1                  75.4752949 MHz
NUC1                         13C
P1                        11.00 usec
PLW1                195.00000000 W
SFO2                300.1312005 MHz
NUC2                         1H
CPDPRG[2                 waltz16
PCPD2                     90.00 usec
PLW2                 14.00000000 W
PLW12                 0.17284000 W
PLW13                 0.14000000 W

F2 - Processing parameters
SI                        32768
SF                    75.4677390 MHz
WDW                          EM
SSB       0
LB                         1.00 Hz
GB        0
PC                         1.40
```



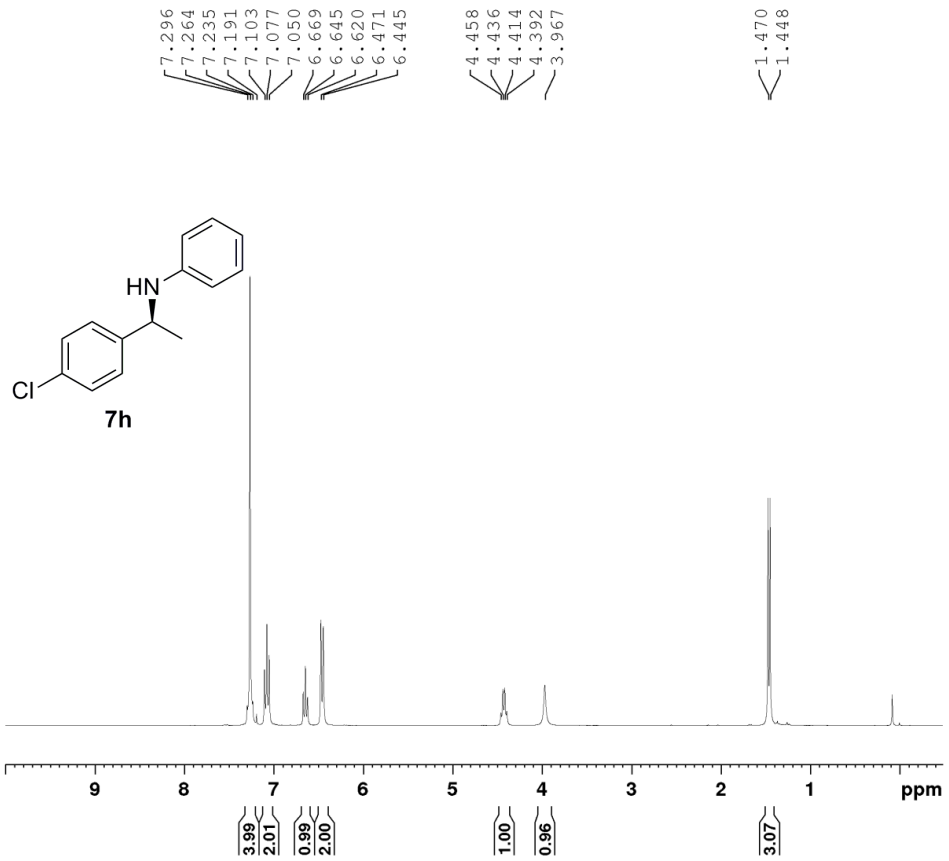

```
Current Data Parameters
NAME                  du-lt
EXPNO                   243
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180518
Time                  17.08 h
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        9
DS                        2
SWH                6009.615 Hz
FIDRES            0.183399 Hz
AQ                5.4525952 sec
RG                   117.72
DW                   83.200 usec
DE                    6.50 usec
TE                   301.3 K
D1                1.00000000 sec
TD0                       1
SFO1           300.1318534 MHz
NUC1                    1H
P1                    8.00 usec
PLW1           18.00000000 W

F2 - Processing parameters
SI                    65536
SF             300.1300261 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```



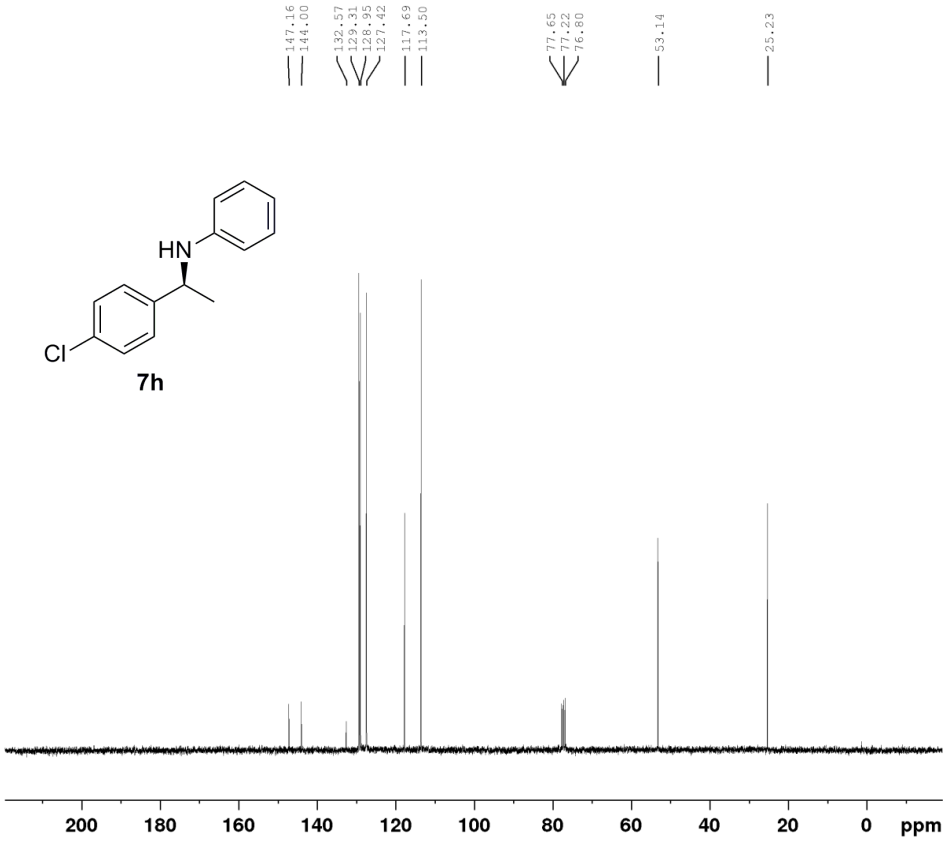

```
Current Data Parameters
NAME                  du-lt
EXPNO                   244
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180518
Time                  17.11 h
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       38
DS                        4
SWH               18028.846 Hz
FIDRES             0.550197 Hz
AQ                 1.8175317 sec
RG                    209.09
DW                    27.733 usec
DE                      6.50 usec
TE                     301.4 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1             75.4752949 MHz
NUC1                    13C
P1                     11.00 usec
PLW1            195.00000000 W
SFO2            300.1312005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2             14.00000000 W
PLW12             0.17284000 W
PLW13             0.14000000 W

F2 - Processing parameters
SI                     32768
SF               75.4677384 MHz
WDW                       EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```



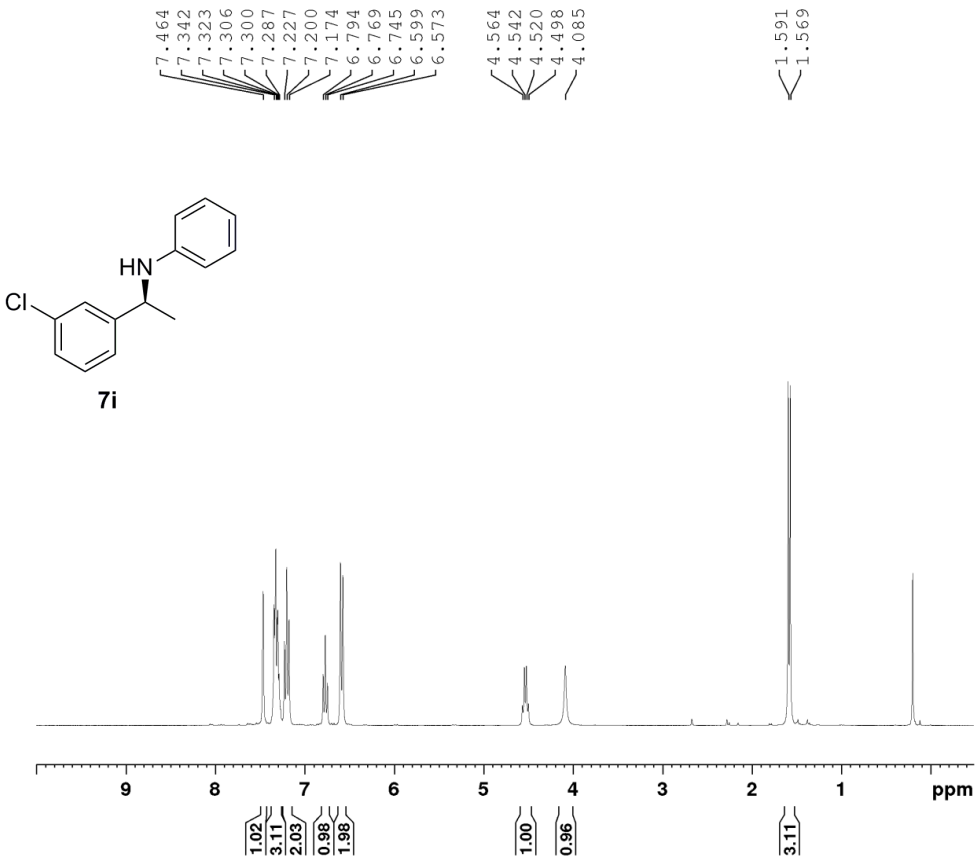

```
Current Data Parameters
NAME            400-2018
EXPNO                218
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180707
Time               10.09 h
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                      9
DS                      4
SWH             89285.711 Hz
FIDRES          1.362392 Hz
AQ              0.7340032 sec
RG                 206.33
DW                  5.600 usec
DE                  6.50 usec
TE                298.9 K
D1             1.00000000 sec
d11            0.03000000 sec
d12            0.00002000 sec
TD0                     1
rde1           0.00000650 sec
SFO1          376.5642094 MHz
NUC1                  19F
P1                 14.50 usec
PLW1          17.98900032 W
SFO2          400.2416010 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W

F2 - Processing parameters
SI                  65536
SF            376.6018696 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



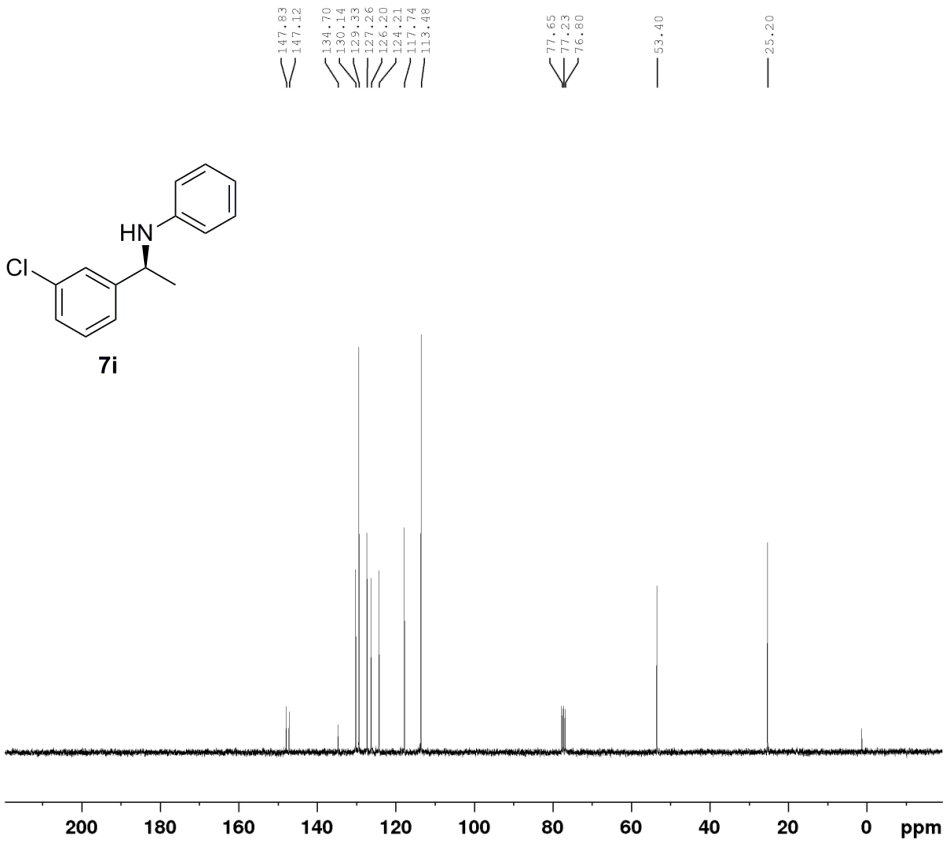

```
Current Data Parameters
NAME                  du-lt
EXPNO                   247
PROCNO                    1

F2 - Acquisition Parameters
Date_           20180519
Time                13.49 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              5.4525952 sec
RG                 117.72
DW                 83.200 usec
DE                  6.50 usec
TE                 300.2 K
D1              1.00000000 sec
TD0                    1
SFO1         300.1318534 MHz
NUC1                 1H
P1                  8.00 usec
PLW1        18.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300278 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



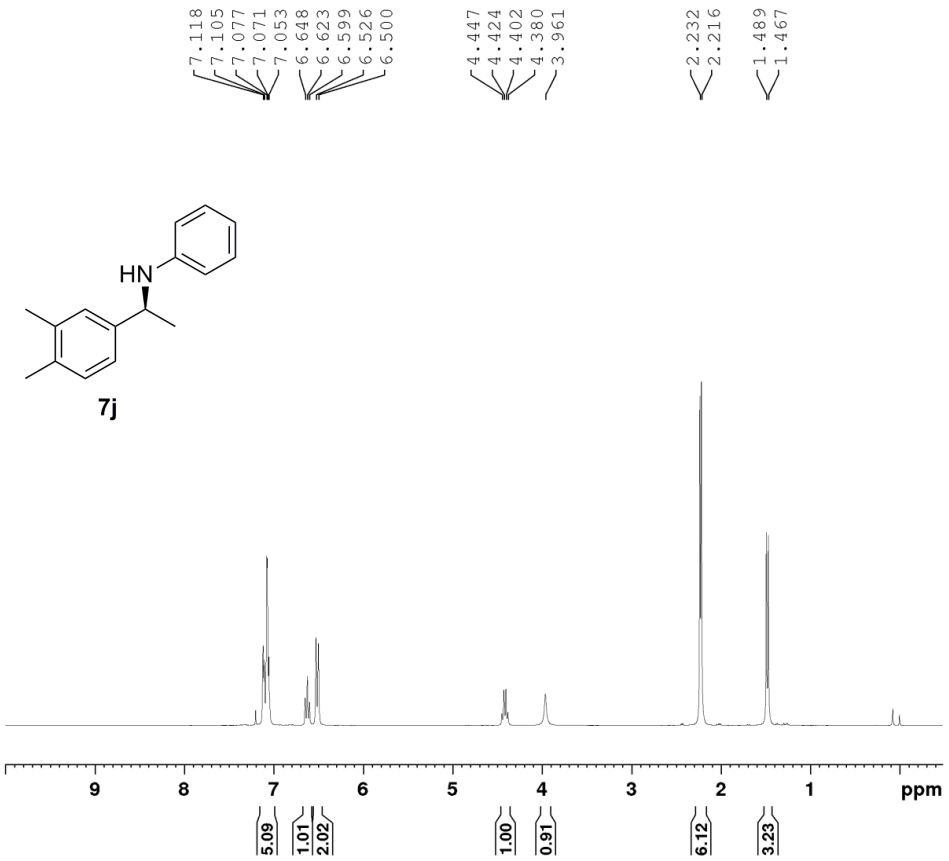

```
Current Data Parameters
NAME                  du-lt
EXPNO                   248
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180519
Time                 13.51 h
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT              CDCl3
NS                       42
DS                        4
SWH               18028.846 Hz
FIDRES             0.550197 Hz
AQ                1.8175317 sec
RG                   209.09
DW                  27.733 usec
DE                    6.50 usec
TE                   300.4 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1             75.4752949 MHz
NUC1                    13C
P1                   11.00 usec
PLW1            195.00000000 W
SFO2            300.1312005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2             14.00000000 W
PLW12             0.17284000 W
PLW13             0.14000000 W

F2 - Processing parameters
SI                    32768
SF               75.4677406 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



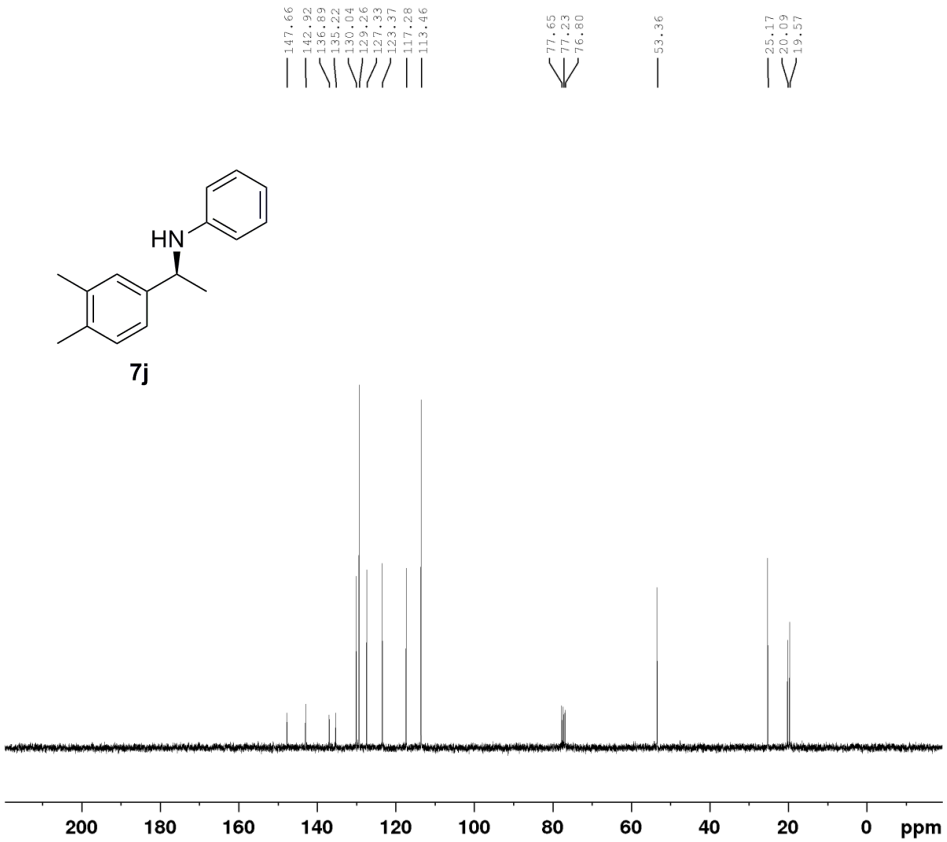

```
Current Data Parameters
NAME                du-1t
EXPNO                 237
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180517
Time                15.45 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     7
DS                     2
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               5.4525952 sec
RG                 103.37
DW                 83.200 usec
DE                  6.50 usec
TE                 301.0 K
D1              1.00000000 sec
TD0                    1
SFO1          300.1318534 MHz
NUC1                  1H
P1                  8.00 usec
PLW1          18.00000000 W

F2 - Processing parameters
SI                 65536
SF            300.1299934 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



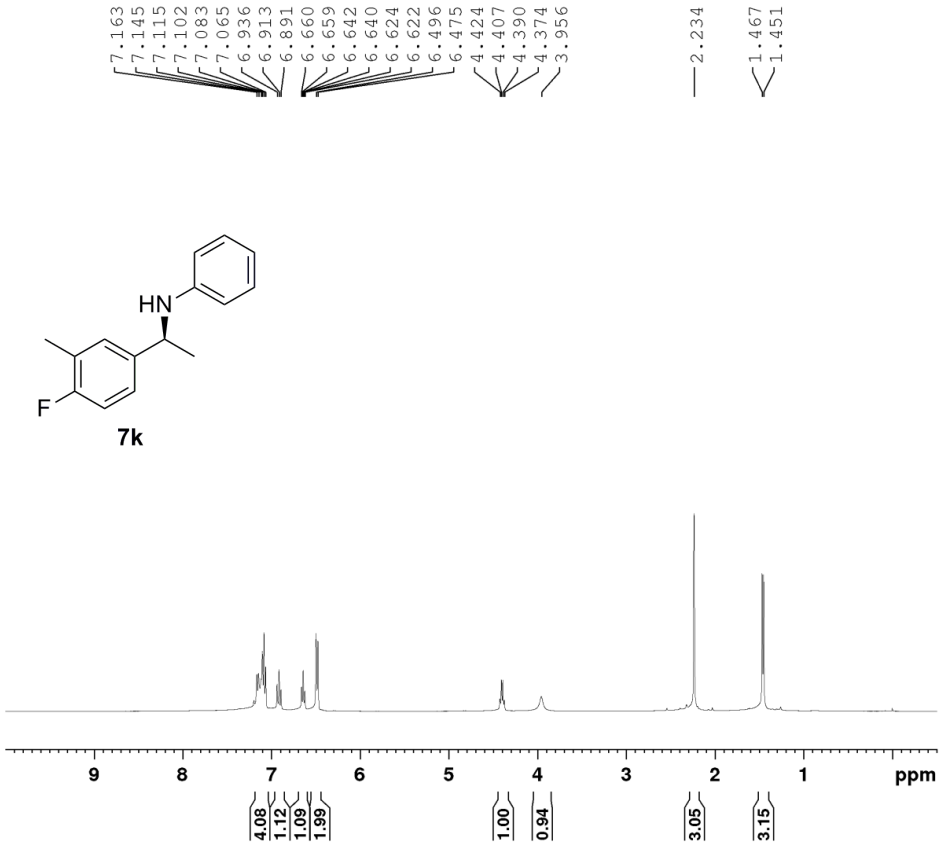

```
Current Data Parameters
NAME                  du-lt
EXPNO                   238
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180517
Time                  15.48 h
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT               CDCl3
NS                        34
DS                         4
SWH               18028.846 Hz
FIDRES             0.550197 Hz
AQ                 1.8175317 sec
RG                    209.09
DW                    27.733 usec
DE                      6.50 usec
TE                     301.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1             75.4752949 MHz
NUC1                     13C
P1                    11.00 usec
PLW1            195.00000000 W
SFO2            300.1312005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             14.00000000 W
PLW12             0.17284000 W
PLW13             0.14000000 W

F2 - Processing parameters
SI                     32768
SF               75.4677406 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



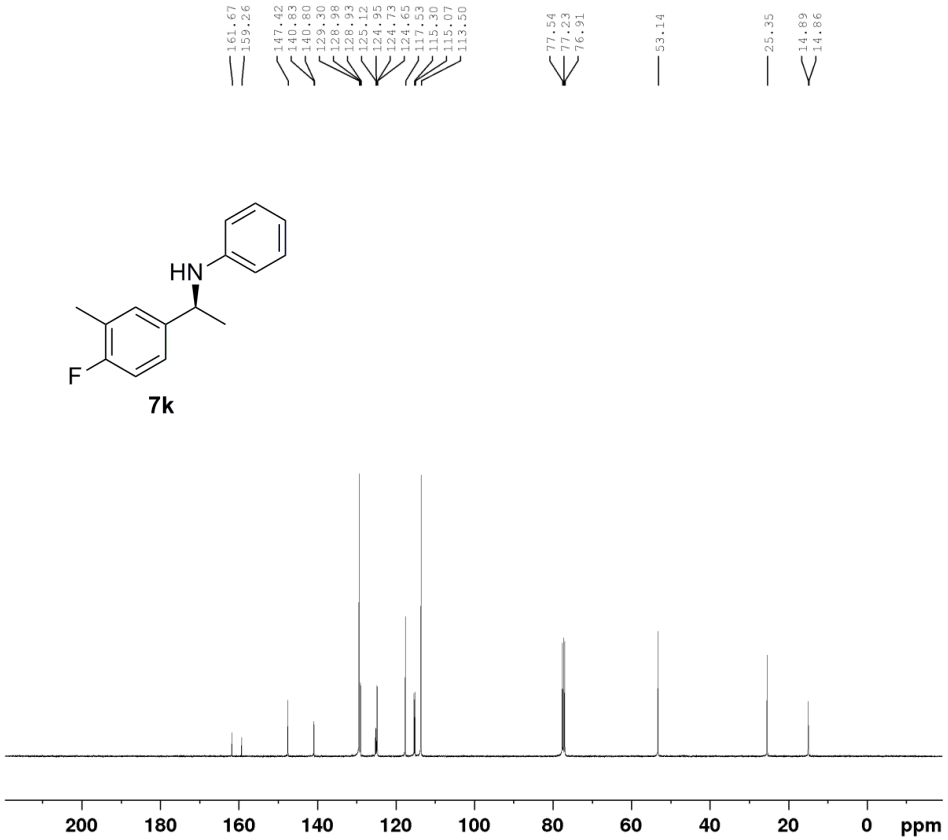

```
Current Data Parameters
NAME                du-1t
EXPNO                 227
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180516
Time                15.59 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               5.4525952 sec
RG                 142.81
DW                 83.200 usec
DE                  6.50 usec
TE                 301.0 K
D1              1.00000000 sec
TD0                    1
SFO1          300.1318534 MHz
NUC1                  1H
P1                  8.00 usec
PLW1          18.00000000 W

F2 - Processing parameters
SI                 65536
SF            300.1300245 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



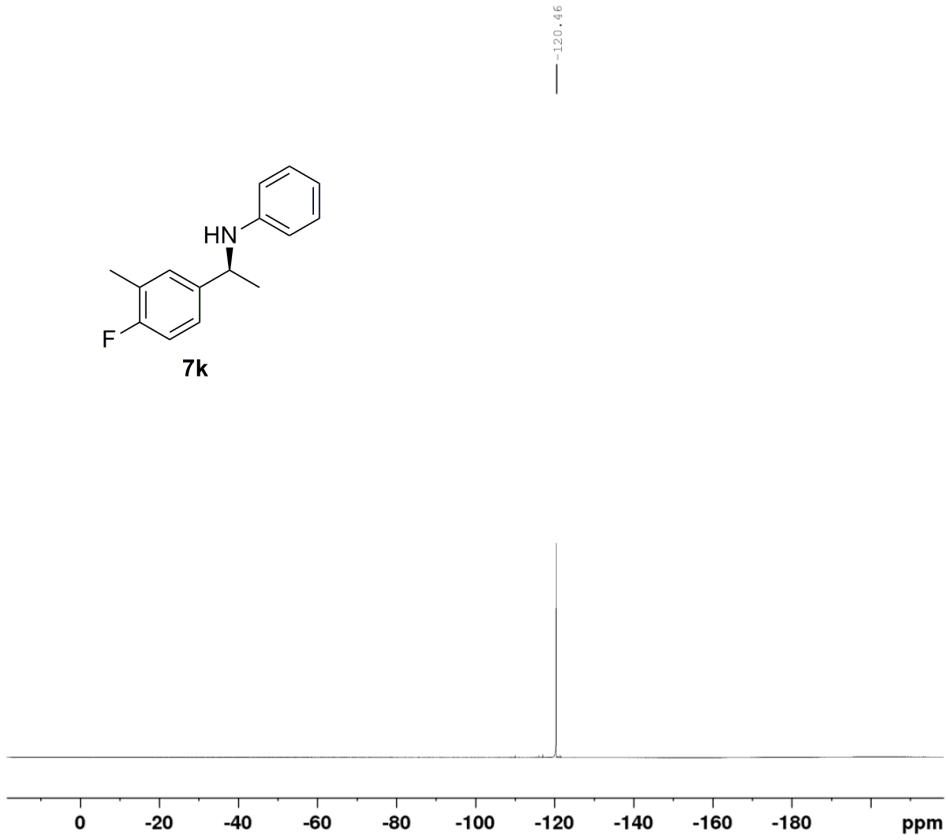

```
Current Data Parameters
NAME                  du-lt
EXPNO                   230
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180516
Time                  16.44 h
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT               CDCl3
NS                        21
DS                         4
SWH               18028.846 Hz
FIDRES             0.550197 Hz
AQ                 1.8175317 sec
RG                    209.09
DW                    27.733 usec
DE                     6.50 usec
TE                    301.1 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1             75.4752949 MHz
NUC1                     13C
P1                    11.00 usec
PLW1            195.00000000 W
SFO2            300.1312005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             14.00000000 W
PLW12             0.17284000 W
PLW13             0.14000000 W

F2 - Processing parameters
SI                     32768
SF               75.4677423 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



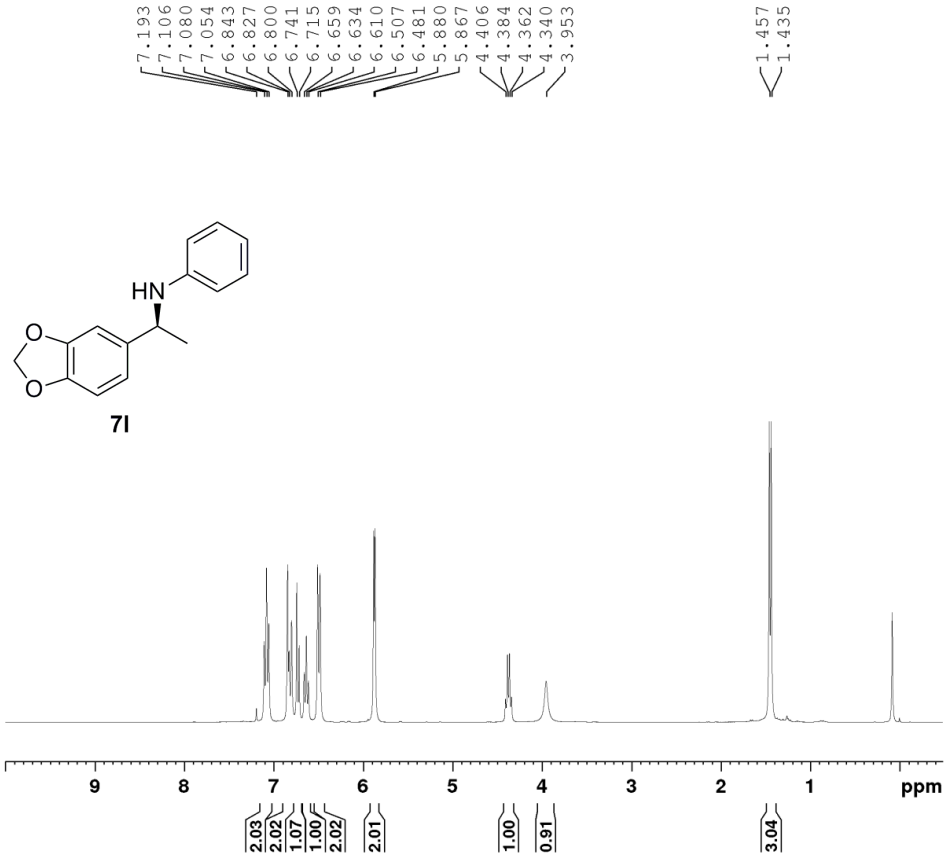

```
Current Data Parameters
NAME            400-2018
EXPNO                303
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180802
Time               23.15 h
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                  43.5
DW                62.400 usec
DE                 6.50 usec
TE                301.0 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400346 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



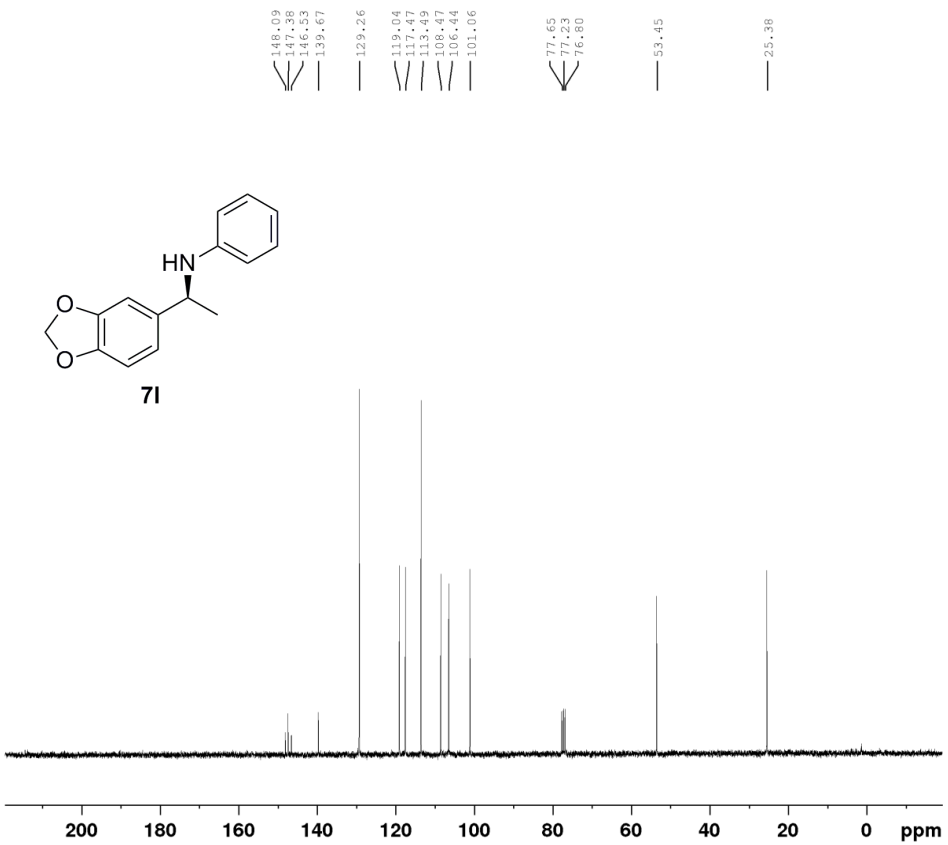

```
Current Data Parameters
NAME            400-2018
EXPNO                304
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180803
Time                0.14 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                301.3 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                  13c
P1                 10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404149 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



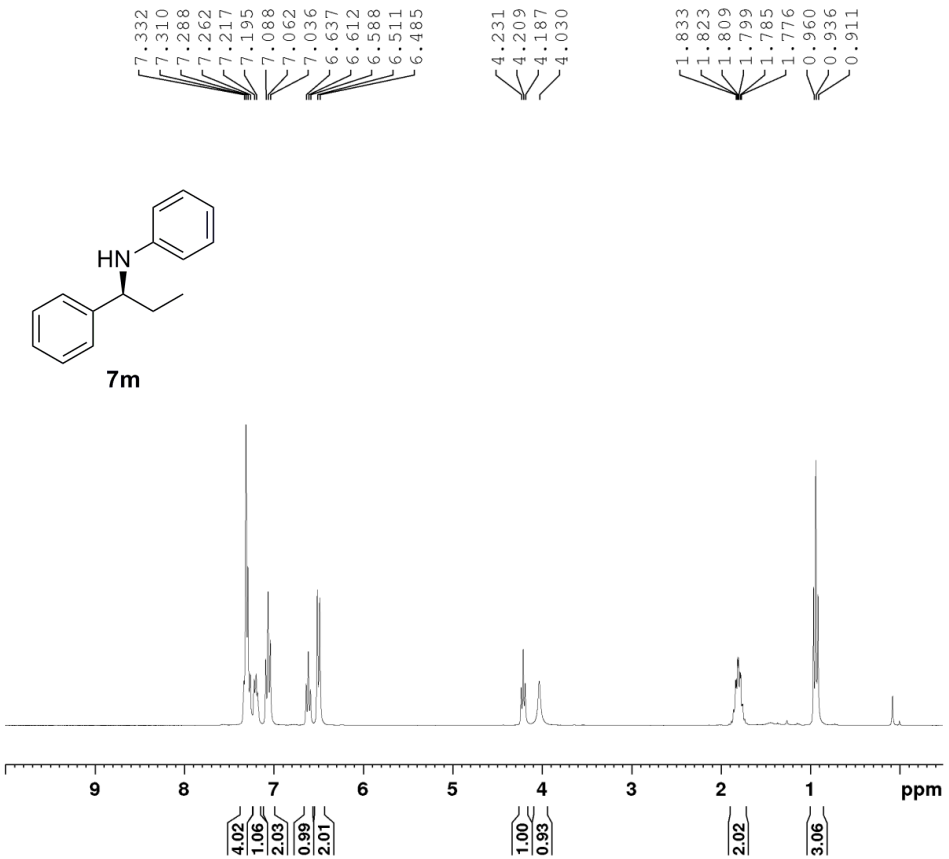

```
Current Data Parameters
NAME            400-2018
EXPNO                333
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180827
Time               21.45 h
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG       zgfhigqn.2
TD                131072
SOLVENT              CDCl3
NS                       8
DS                       4
SWH             89285.711 Hz
FIDRES           1.362392 Hz
AQ              0.7340032 sec
RG                  206.33
DW                   5.600 usec
DE                   6.50 usec
TE                  298.2 K
D1              1.00000000 sec
d11             0.03000000 sec
d12             0.00002000 sec
TD0                      1
rde1            0.00000650 sec
SFO1           376.5642094 MHz
NUC1                   19F
P1                  14.50 usec
PLW1           17.98900032 W
SFO2           400.2416010 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2           12.00000000 W
PLW12           0.34680000 W

F2 - Processing parameters
SI                   65536
SF             376.6018696 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```



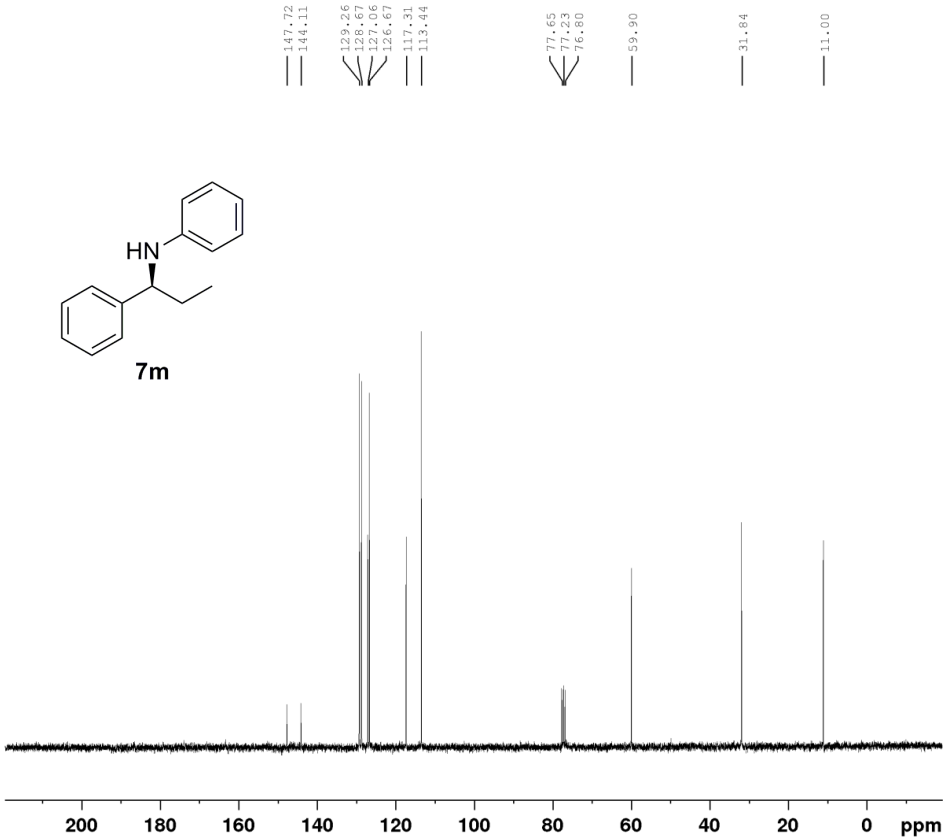

```
Current Data Parameters
NAME                du-lt
EXPNO                 241
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180518
Time                17.05 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     9
DS                     2
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             5.4525952 sec
RG                 103.37
DW                 83.200 usec
DE                  6.50 usec
TE                 301.4 K
D1             1.00000000 sec
TD0                    1
SFO1         300.1318534 MHz
NUC1                 1H
P1                  8.00 usec
PLW1        18.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300272 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



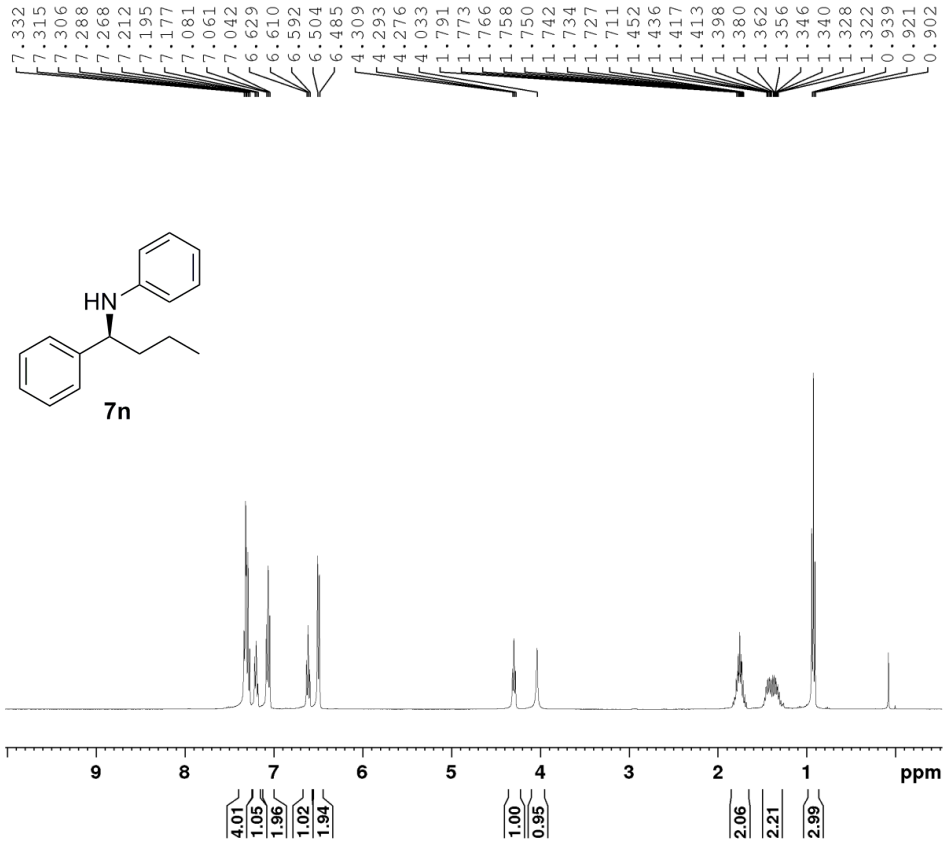

```
Current Data Parameters
NAME                  du-lt
EXPNO                   242
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180518
Time                  17.01 h
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        39
DS                         4
SWH                18028.846 Hz
FIDRES              0.550197 Hz
AQ                  1.8175317 sec
RG                     209.09
DW                     27.733 usec
DE                       6.50 usec
TE                      301.4 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1
SFO1               75.4752949 MHz
NUC1                      13C
P1                     11.00 usec
PLW1              195.00000000 W
SFO2              300.1312005 MHz
NUC2                       1H
CPDPRG[2               waltz16
PCPD2                  90.00 usec
PLW2               14.00000000 W
PLW12               0.17284000 W
PLW13               0.14000000 W

F2 - Processing parameters
SI                        32768
SF                 75.4677406 MHz
WDW                          EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```



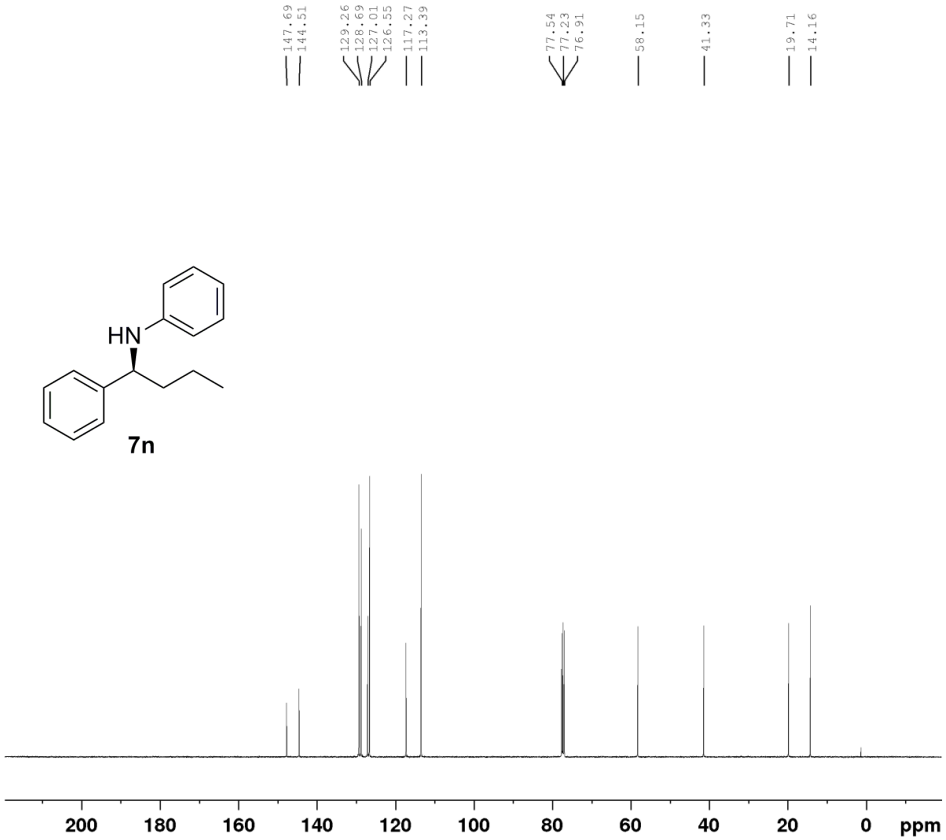

```
Current Data Parameters
NAME                du-lt
EXPNO                 232
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180517
Time                15.33 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     9
DS                     2
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               5.4525952 sec
RG                 103.37
DW                 83.200 usec
DE                   6.50 usec
TE                  300.8 K
D1              1.00000000 sec
TD0                    1
SFO1          300.1318534 MHz
NUC1                  1H
P1                   8.00 usec
PLW1          18.00000000 W

F2 - Processing parameters
SI                 65536
SF            300.1300308 MHz
WDW                   EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```



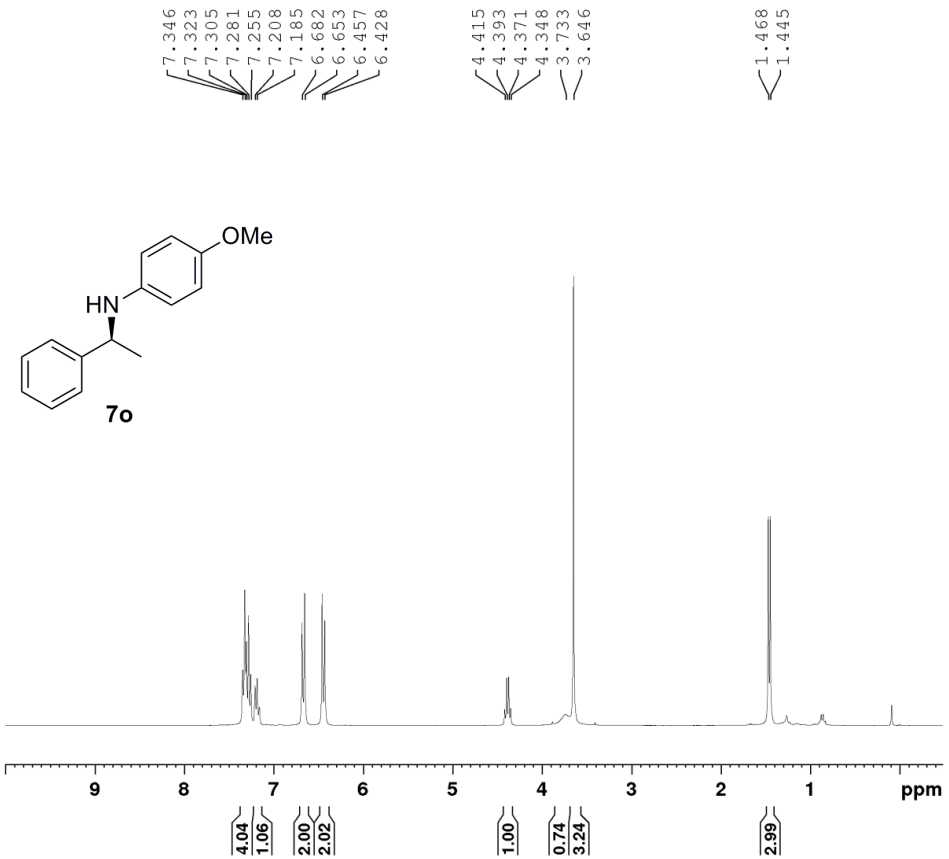

```
Current Data Parameters
NAME                  du-lt
EXPNO                   234
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180517
Time                  15.36 h
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                18028.846 Hz
FIDRES              0.550197 Hz
AQ                  1.8175317 sec
RG                     209.09
DW                     27.733 usec
DE                       6.50 usec
TE                      301.1 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1
SFO1               75.4752949 MHz
NUC1                      13C
P1                     11.00 usec
PLW1              195.00000000 W
SFO2              300.1312005 MHz
NUC2                       1H
CPDPRG[2               waltz16
PCPD2                  90.00 usec
PLW2               14.00000000 W
PLW12               0.17284000 W
PLW13               0.14000000 W

F2 - Processing parameters
SI                        32768
SF                 75.4677401 MHz
WDW                          EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```



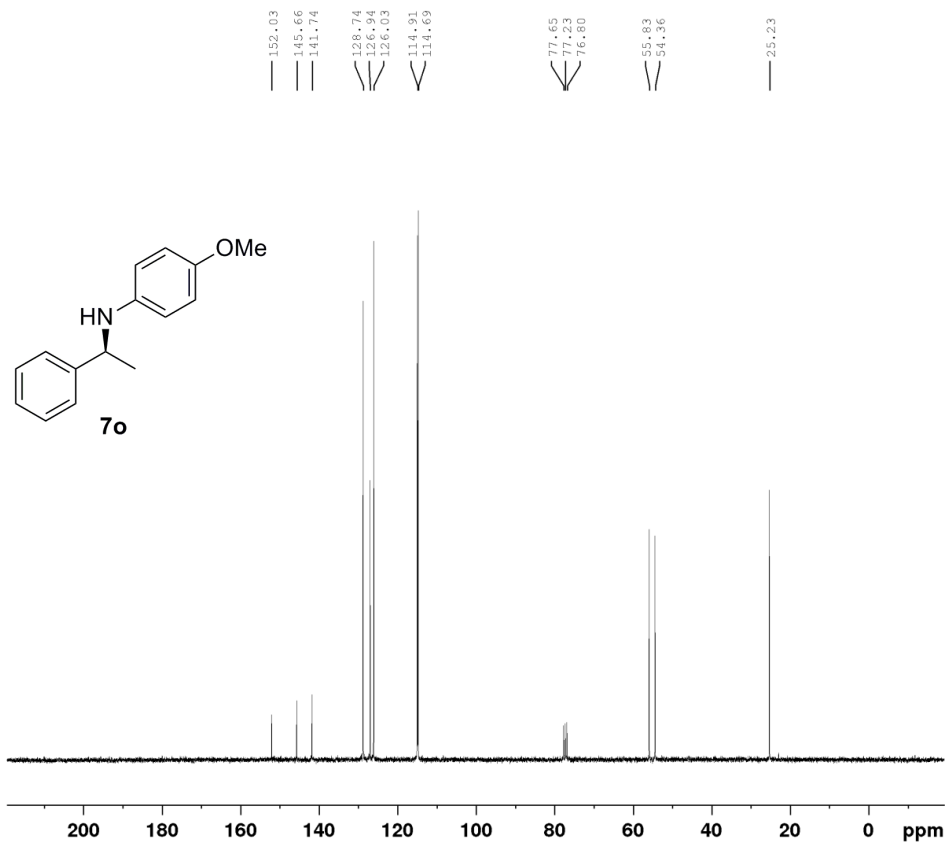

```
Current Data Parameters
NAME            400-2018
EXPNO                385
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181021
Time               13.16 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                  43.5
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400374 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



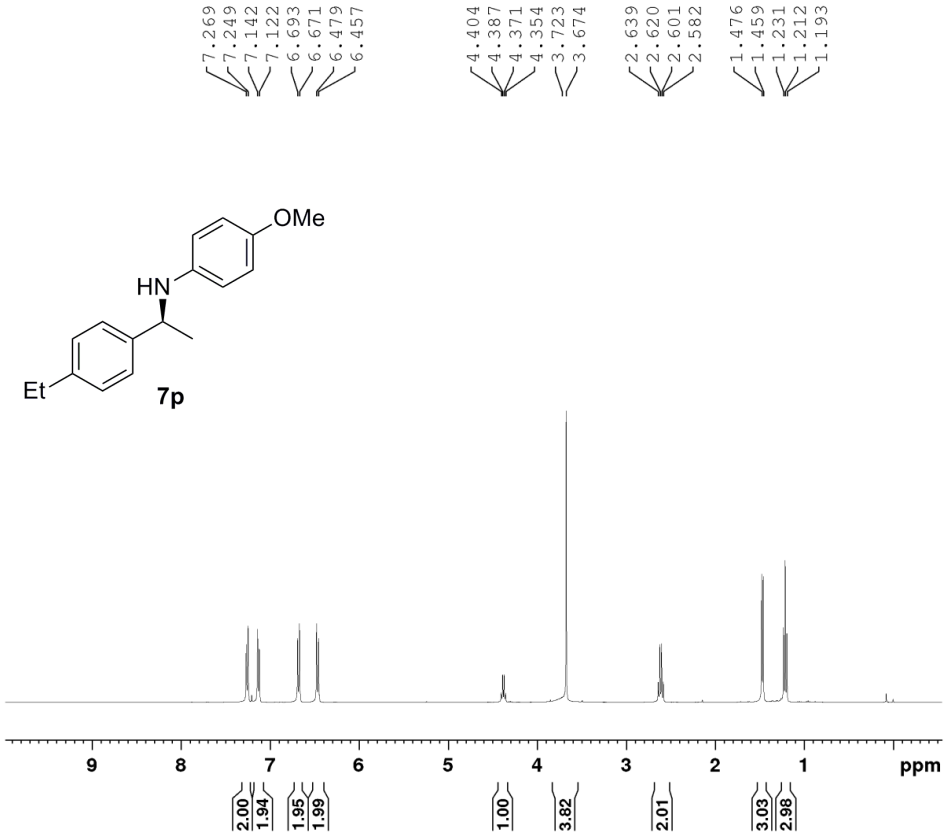

```
Current Data Parameters
NAME                  400-2018
EXPNO                      386
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20181021
Time                     14.15 h
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  24038.461 Hz
FIDRES                0.733596 Hz
AQ                    1.3631488 sec
RG                       206.33
DW                       20.800 usec
DE                        6.50 usec
TE                       298.6 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                          1
SFO1               100.6504916 MHz
NUC1                        13C
P1                       10.00 usec
PLW1                54.00000000 W
SFO2                400.2416010 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                12.00000000 W
PLW12                0.34680000 W
PLW13                0.28090999 W

F2 - Processing parameters
SI                       32768
SF                 100.6404164 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```



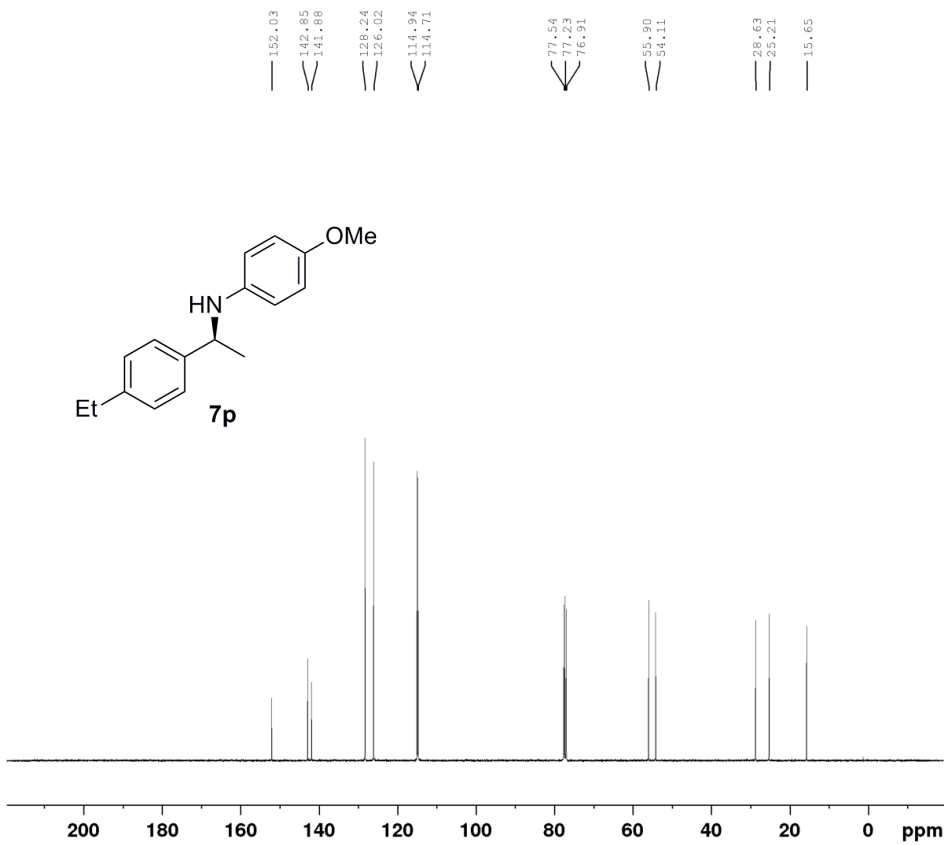

```
Current Data Parameters
NAME                du-lt
EXPNO                 249
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180519
Time                13.57 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     2
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              5.4525952 sec
RG                  66.2
DW                83.200 usec
DE                 6.50 usec
TE                300.1 K
D1             1.00000000 sec
TD0                    1
SFO1         300.1318534 MHz
NUC1                 1H
P1                 8.00 usec
PLW1        18.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300386 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



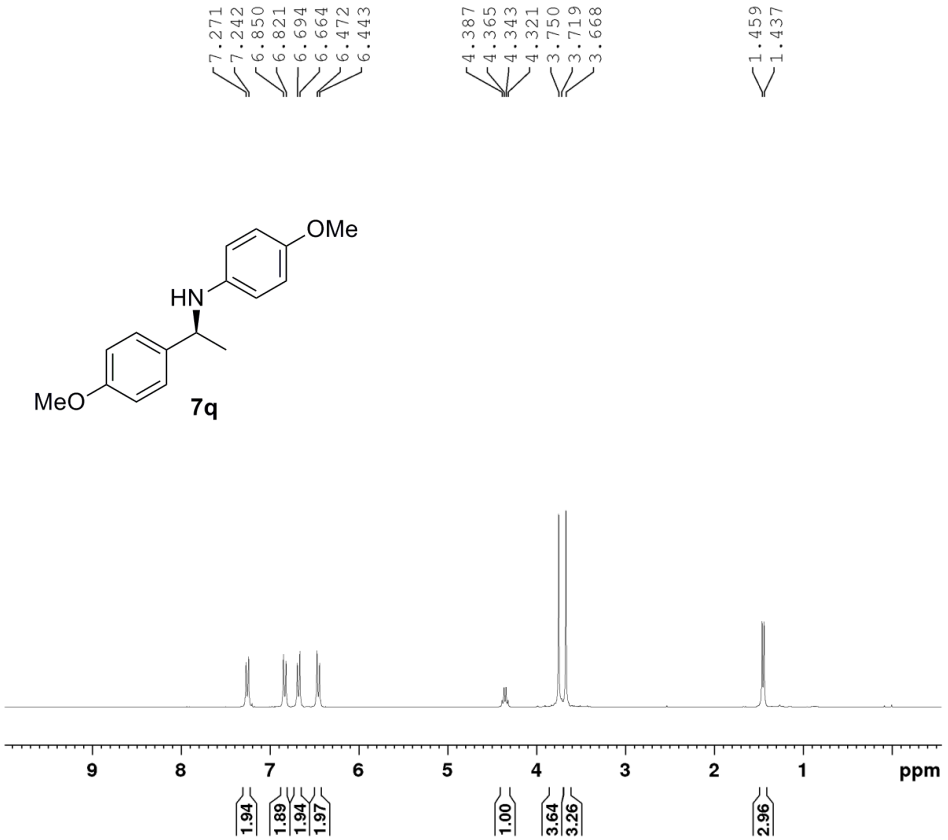

```
Current Data Parameters
NAME                  du-lt
EXPNO                   250
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180519
Time                  14.01 h
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        51
DS                         4
SWH               18028.846 Hz
FIDRES             0.550197 Hz
AQ                 1.8175317 sec
RG                    209.09
DW                    27.733 usec
DE                      6.50 usec
TE                     300.4 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1             75.4752949 MHz
NUC1                     13C
P1                     11.00 usec
PLW1            195.00000000 W
SFO2            300.1312005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2             14.00000000 W
PLW12             0.17284000 W
PLW13             0.14000000 W

F2 - Processing parameters
SI                     32768
SF               75.4677456 MHz
WDW                       EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```



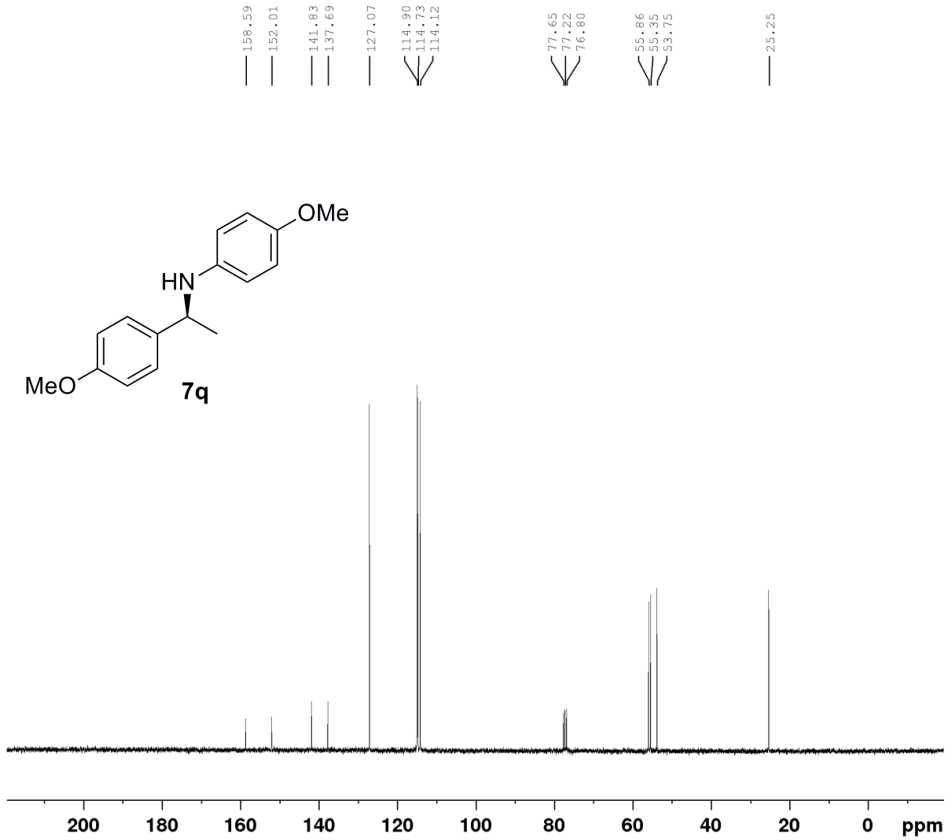

```
Current Data Parameters
NAME            400-2018
EXPNO                379
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181018
Time                1.58 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                  43.5
DW                62.400 usec
DE                 6.50 usec
TE                299.0 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400308 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



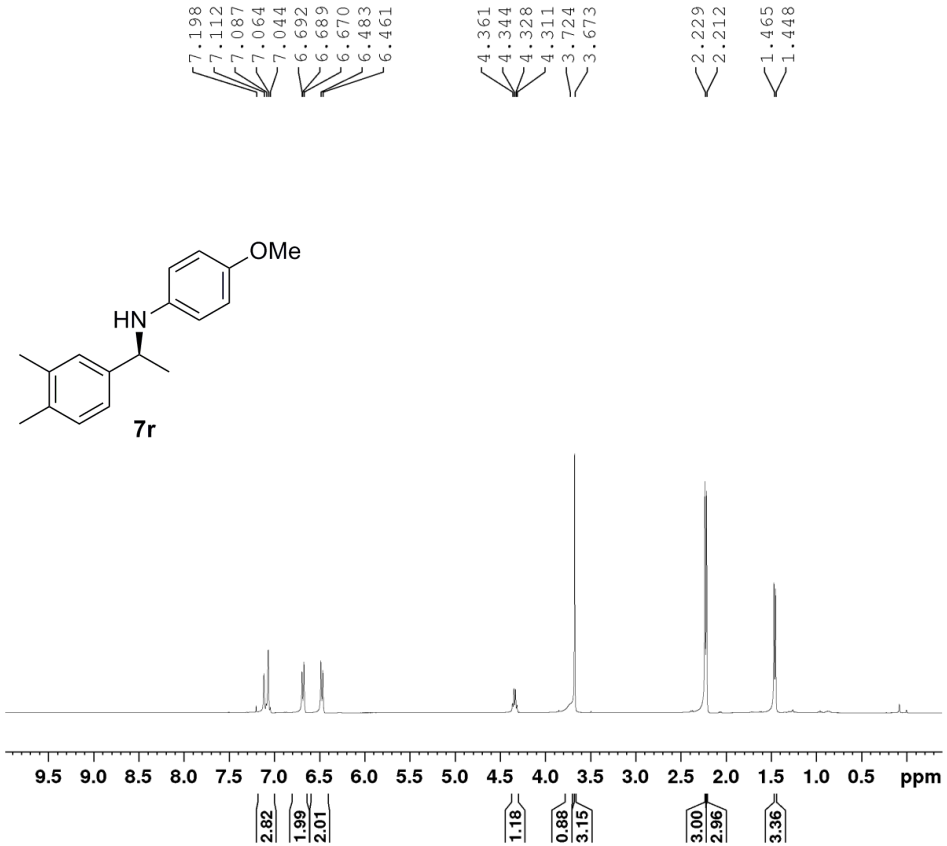

```
Current Data Parameters
NAME            400-2018
EXPNO                380
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181018
Time                2.28 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   500
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                 206.33
DW                20.800 usec
DE                 6.50 usec
TE                299.8 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         100.6504916 MHz
NUC1                 13C
P1                10.00 usec
PLW1          54.00000000 W
SFO2         400.2416010 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          12.00000000 W
PLW12          0.34680000 W
PLW13          0.28090999 W

F2 - Processing parameters
SI                 32768
SF           100.6404149 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



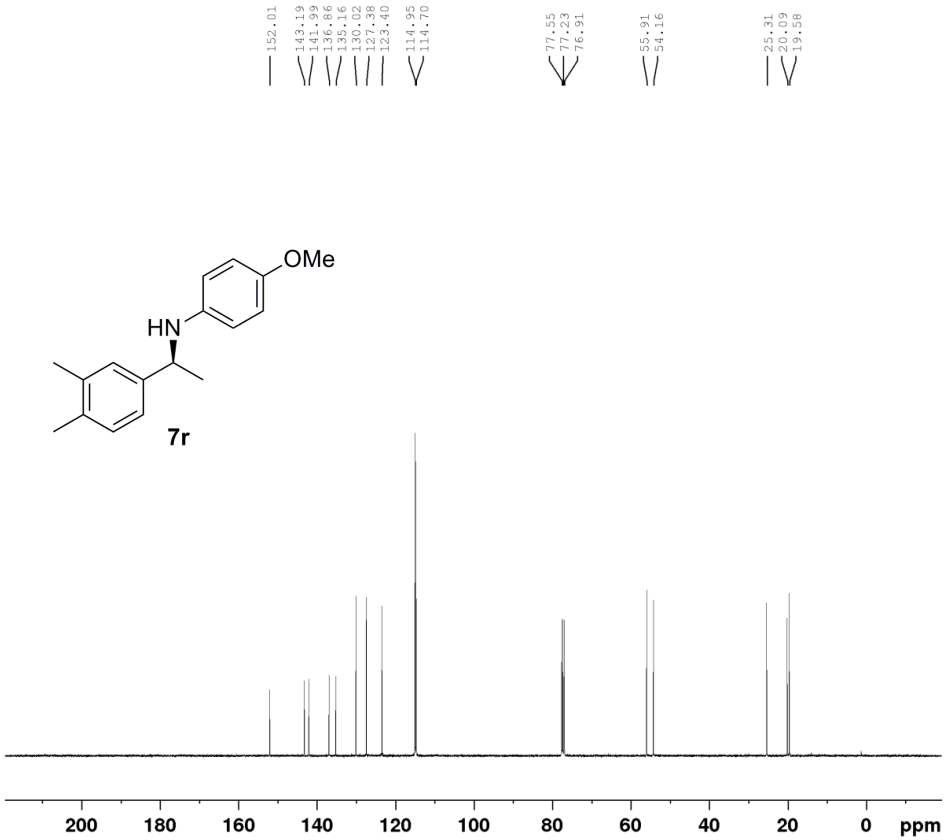

```
Current Data Parameters
NAME                du-1t
EXPNO                 274
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180530
Time                14.03 h
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      7
DS                      2
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               5.4525952 sec
RG                  82.09
DW                 83.200 usec
DE                  6.50 usec
TE                 299.1 K
D1              1.00000000 sec
TD0                     1
SFO1         300.1318534 MHz
NUC1                 1H
P1                  8.00 usec
PLW1         18.00000000 W

F2 - Processing parameters
SI                  65536
SF           300.1300243 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



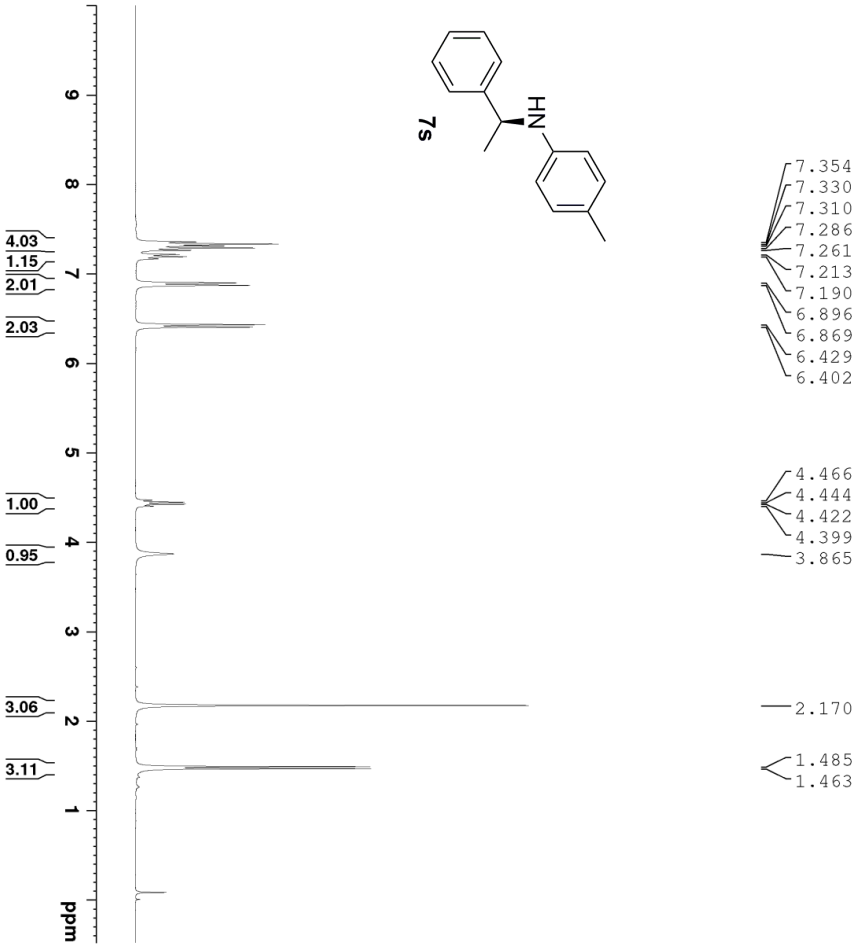

```
Current Data Parameters
NAME                  du-lt
EXPNO                   275
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180530
Time                   14.05 h
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       40
DS                        4
SWH                18028.846 Hz
FIDRES                0.550197 Hz
AQ                    1.8175317 sec
RG                      209.09
DW                     27.733 usec
DE                      6.50 usec
TE                     299.4 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                       1
SFO1               75.4752949 MHz
NUC1                     13C
P1                     11.00 usec
PLW1              195.00000000 W
SFO2               300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                  90.00 usec
PLW2               14.00000000 W
PLW12               0.17284000 W
PLW13               0.14000000 W

F2 - Processing parameters
SI                        32768
SF                 75.4677417 MHz
WDW                        EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



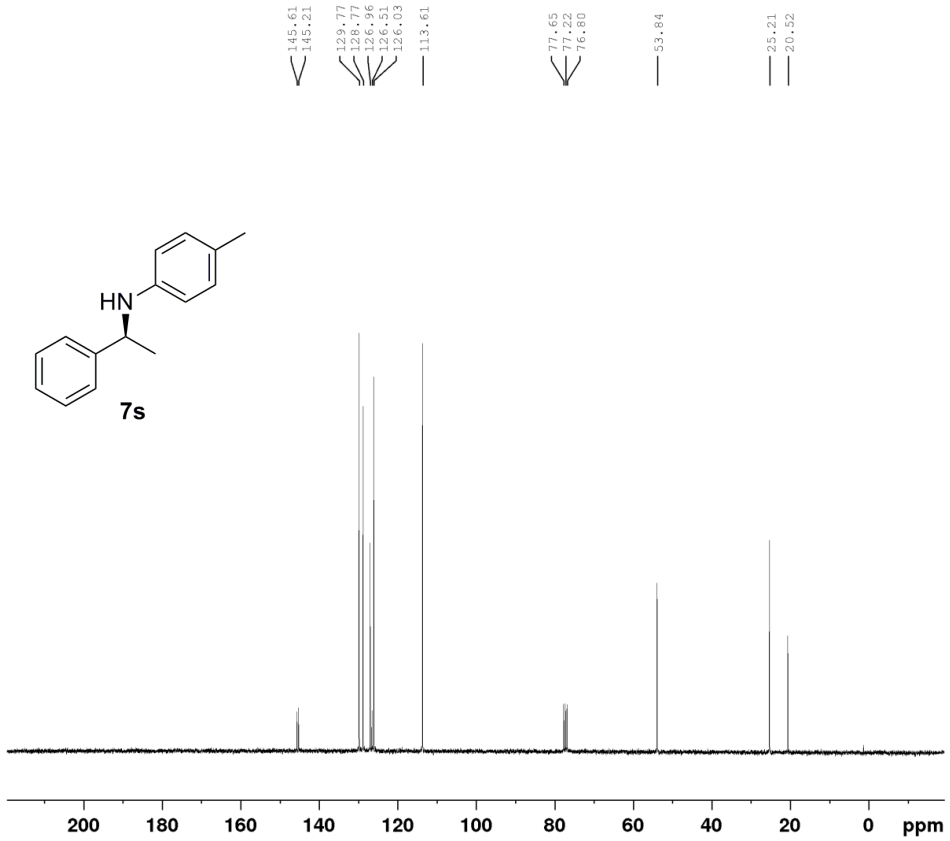

```
Current Data Parameters
NAME            400-2018
EXPNO                381
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181018
Time                2.31 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                  43.5
DW                62.400 usec
DE                 6.50 usec
TE                298.9 K
D1             2.00000000 sec
TD0                    1
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2400345 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



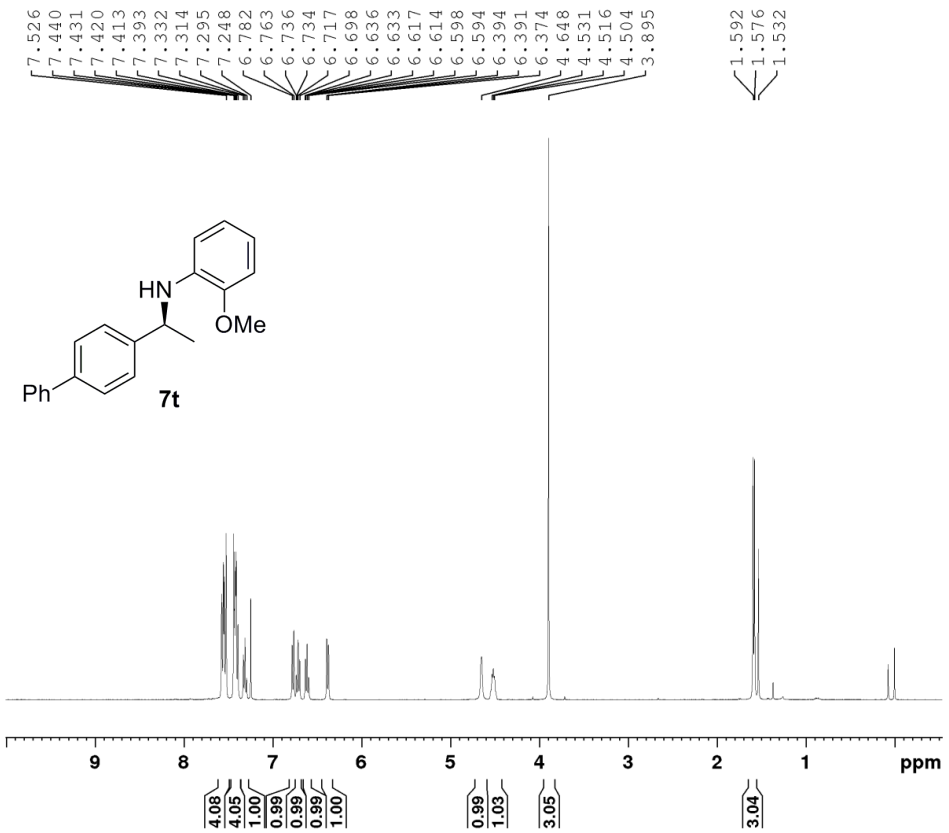

```
Current Data Parameters
NAME                  400-2018
EXPNO                      382
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20181018
Time                      3.00 h
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         500
DS                           4
SWH                  24038.461 Hz
FIDRES                0.733596 Hz
AQ                    1.3631488 sec
RG                       206.33
DW                       20.800 usec
DE                        6.50 usec
TE                       299.8 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                          1
SFO1               100.6504916 MHz
NUC1                        13C
P1                       10.00 usec
PLW1                54.00000000 W
SFO2               400.2416010 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                12.00000000 W
PLW12                0.34680000 W
PLW13                0.28090999 W

F2 - Processing parameters
SI                       32768
SF                 100.6404157 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```



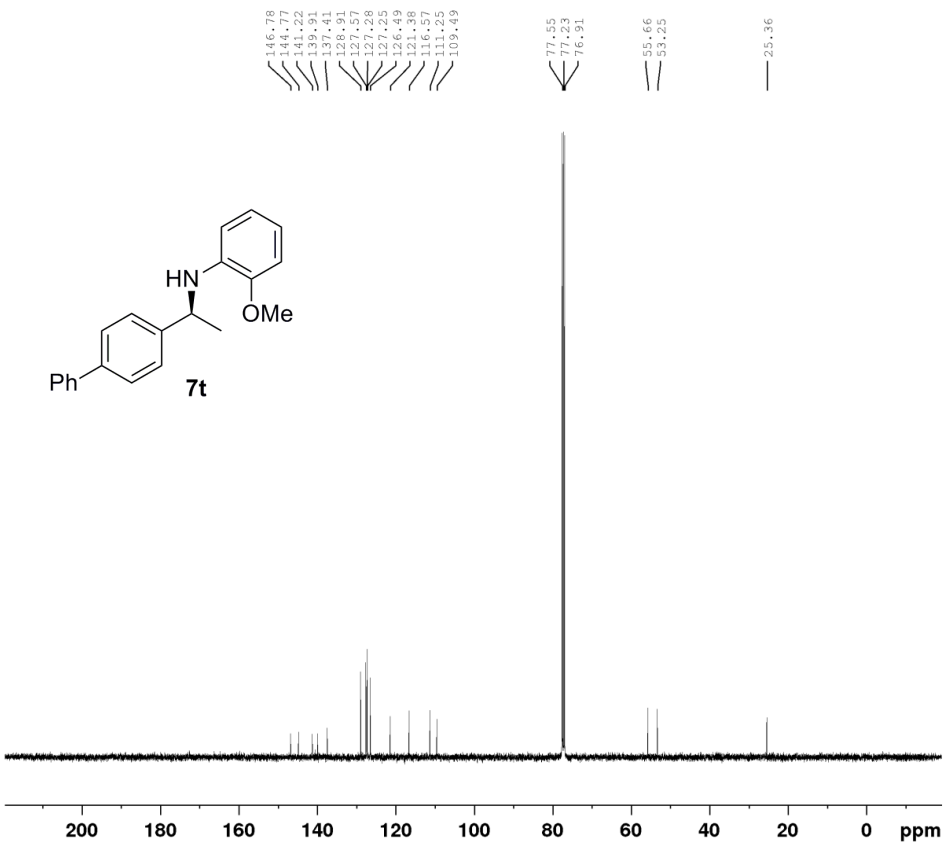

```
Current Data Parameters
NAME                  du-lt
EXPNO                    256
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180524
Time                   13.39 h
INSTRUM                spect
PROBHD      5 mm DUL 13C-1
PULPROG             zg30
TD                    65536
SOLVENT             CDCl3
NS                       16
DS                        2
SWH                6009.615 Hz
FIDRES             0.183399 Hz
AQ                 5.452592 sec
RG                    56.57
DW                   83.200 usec
DE                    6.50 usec
TE                   299.3 K
D1                1.00000000 sec
TD0                       1
SFO1       300.1318534 MHz
NUC1                    1H
P1                    8.00 usec
PLW1         18.00000000 W

F2 - Processing parameters
SI                    65536
SF         300.1300360 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




```
Current Data Parameters
NAME                  du-lt
EXPNO                   257
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180524
Time                   13.43 h
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        80
DS                         4
SWH                18028.846 Hz
FIDRES              0.550197 Hz
AQ                  1.8175317 sec
RG                     209.09
DW                     27.733 usec
DE                       6.50 usec
TE                      299.5 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1
SFO1               75.4752949 MHz
NUC1                      13C
P1                     11.00 usec
PLW1              195.00000000 W
SFO2              300.1312005 MHz
NUC2                       1H
CPDPRG[2               waltz16
PCPD2                  90.00 usec
PLW2               14.00000000 W
PLW12               0.17284000 W
PLW13               0.14000000 W

F2 - Processing parameters
SI                         32768
SF                 75.4677423 MHz
WDW                           EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```




```
Current Data Parameters
NAME            400-2018
EXPNO                391
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181022
Time                9.32 h
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ              2.0447233 sec
RG                206.33
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1
SFO1          400.2424716 MHz
NUC1                  1H
P1                 14.80 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF            400.2400143 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```




```
Current Data Parameters
NAME            400-2018
EXPNO                392
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181022
Time                10.02 h
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   500
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                 206.33
DW                 20.800 usec
DE                  6.50 usec
TE                 298.7 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                    1
SFO1          100.6504916 MHz
NUC1                  13C
P1                 10.00 usec
PLW1           54.00000000 W
SFO2          400.2416010 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2           12.00000000 W
PLW12           0.34680000 W
PLW13           0.28090999 W

F2 - Processing parameters
SI                 32768
SF            100.6404083 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```