Supporting Information

Ruthenium Catalyzed β-Selective Alkylation of Vinylpyridines with Aldehydes/Ketones via N_2H_4 Mediated Deoxygenative Couplings

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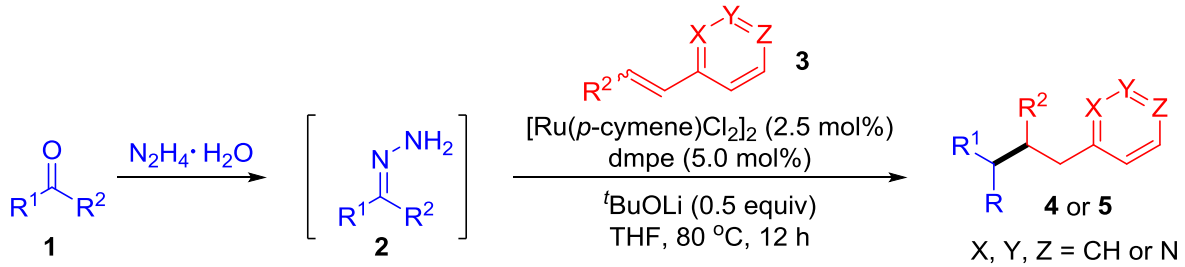
1. General information

^{1}H NMR spectra were recorded on Bruker 400 or 500 MHz spectrometer and the chemical shifts were reported in parts per million (δ) relative to internal standard TMS (0 ppm) for $CDCl_3$. The peak patterns are indicated as follows: s, singlet; d, doublet; dd, doublet of doublet; t, triplet; q, quartet; m, multiplet. The coupling constants, *J*, are reported in Hertz (Hz). ^{1}H NMR spectra were obtained at Bruker 400 or 500 MHz and referenced to the internal solvent signals. ^{13}C NMR spectra were obtained at Bruker 100 or 125 MHz and referenced to the internal solvent signals. $CDCl_3$ was used as the NMR solvent. APEX II (Bruker Inc.) was used for HR-MS and APCI-MS. Flash column chromatography was performed over silica gel 200-300. All other reagents were purchased from Alfa, Acros, Aldrich, TCI and used without further purification.

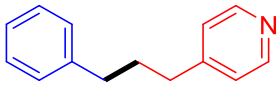
2. General procedure and characterization data for products 4 and 5



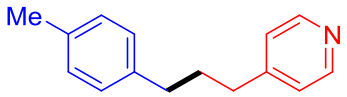
Preparation of hydrazone **2**: a mixture of aldehydes **1** (0.4 mmol, 2.0 equiv) and hydrazine monohydrate (24 μL, 0.48mmol, 64–65 wt%, 2.4 equiv) in THF (1.0 mL) solution was stirred for 30 min at room temperature. After that, 50 mg of anhydrous Na_2SO_4 was added. The resulting mixture was filtered and the filtrate was evaporated *in vacuo* before use.

A flame-dried V-shape reaction vial (10 cm^3) equipped with a magnetic stir bar was charged with [Ru(*p*-cymene)Cl_2]$_2$ (3.1 mg, 2.5 mol%). The vial was transferred to the glovebox and charged with THF (0.1 mL) and dmpe (1.8 μl, 5.0 mol%) before being sealed with a rubber septum. The reaction mixture was stirred at room temperature for 30 min. Then vinylpyridine **3** (0.2 mmol, 1.0 equiv), hydrazone **2** (0.4 mmol, dissolved in 0.2 mL THF) and ^{t}BuOLi (0.1 mmol, 8.0 mg) was added sequentially. After that, the reaction mixture was sealed with aluminum cap, moved out of glovebox, and stirred at 80 ℃ for 12 hour. After the mixture was cooled to room temperature, the resulting solution was directly filtered through a pad of celite by EtOAc (3.0 mL). The crude mixture was analyzed by GC-MS. The solvent was evaporated *in vacuo* to give the crude product. NMR yield was determined by ^{1}H NMR using mesitylene as an internal standard. The residue was purified by preparative TLC (ethyl acetate/petroleum ether) to give the pure product **4** or **5**.

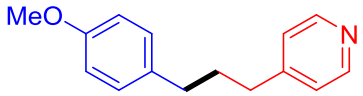
Note: Use of the glovebox is not necessary unless to store and manipulate air-sensitive dmpe ligand. The other operations can be successfully performed outside the glovebox with standard Schlenk line procedure.



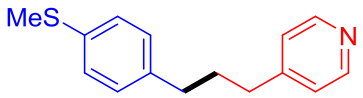
4-(3-Phenylpropyl)pyridine (4aa).[1] (37 mg, 95%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.61 (br, 2H), 7.33-7.30 (m, 2H), 7.24-7.19 (m, 5H), 2.68 (t, J = 7.8 Hz, 2H), 2.66 (t, J = 8.0 Hz, 2H), 2.03-1.97 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.4, 149.4, 141.6, 128.5, 128.4, 126.0, 124.4, 35.3, 34.7, 31.7.



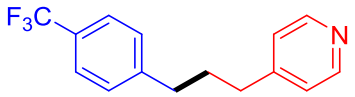
4-(3-(*p*-Tolyl)propyl)pyridine (4ab).[2] (41 mg, 97%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (br, 2H), 7.14-7.12 (m, 4H), 7.09 (d, J = 8.0 Hz, 2H), 2.65 (t, J = 7.6 Hz, 2H), 2.64 (t, J = 7.6 Hz, 2H), 2.35 (s, 3H), 2.01-1.95 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.2, 149.7, 138.5, 135.4, 129.1, 128.3, 123.9, 34.8, 34.6, 31.9, 21.0.



4-(3-(4-Methoxyphenyl)propyl)pyridine (4ac).[3] (43 mg, 95%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (br, 2H), 7.13 (br, 2H), 7.11 (d, J = 8.6 Hz, 2H), 6.86 (d, J = 8.6 Hz, 2H), 3.81 (s, 3H), 2.64 (t, J = 7.6 Hz, 2H), 2.62 (t, J = 7.6 Hz, 2H), 1.99-1.92 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.9, 151.3, 149.7, 133.7, 129.3, 123.9, 113.8, 55.3, 34.6, 34.4, 32.0.

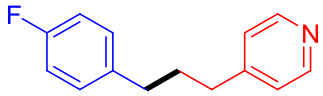


4-(3-(4-(Methylthio)phenyl)propyl)pyridine (4ad). (44 mg, 92%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (br, 2H), 7.22 (d, J = 8.4 Hz, 2H), 7.12 (br, 2H), 7.11 (d, J = 8.4 Hz, 2H), 2.64-2.61 (m, 4H), 2.49 (s, 3H), 1.99-1.93 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.1, 149.7, 138.7, 135.6, 129.0, 127.2, 123.9, 34.7, 34.6, 31.7, 16.3; HRMS (ESI) calcd for $C_{15}H_{18}NS$ [M + H^+], 244.1154; found: 244.1154.

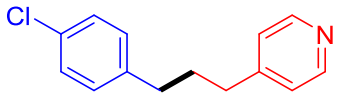


4-(3-(4-(Trifluoromethyl)phenyl)propyl)pyridine (4ae). (51 mg, 97%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (br, 2H), 7.56 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.2 Hz, 2H), 7.13 (br, 2H), 2.72 (t, J = 7.8 Hz, 2H), 2.66 (t, J = 7.8 Hz, 2H), 2.03-1.97 (m, 2H); ^{13}C NMR (125 MHz,

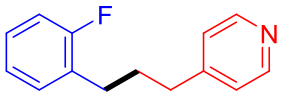
$CDCl_3$) δ 150.8, 149.7, 145.7, 128.7, 128.4 (q, $J_{C\text{-}F}$ = 32.3 Hz), 125.4 (q, $J_{C\text{-}F}$ = 3.9 Hz), 124.3 (q, $J_{C\text{-}F}$ = 272.4 Hz), 124.0, 35.0, 34.5, 31.4; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.3; HRMS (ESI) calcd for $C_{15}H_{15}F_3N$ [M + H^+], 266.1151; found: 266.1148.



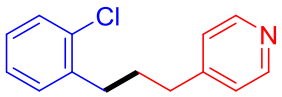
4-(3-(4-Fluorophenyl)propyl)pyridine (4af).[2] (42 mg, 97%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (br, 2H), 7.15-7.11 (m, 4H), 7.01-6.96 (m, 2H), 2.64 (t, J = 7.8 Hz, 4H), 1.99-1.93 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3 (d, $J_{C\text{-}F}$ = 243.8 Hz), 151.0, 149.8, 137.2 (d, $J_{C\text{-}F}$ = 2.9 Hz), 129.7 (d, $J_{C\text{-}F}$ = 8.0 Hz), 123.9, 115.2 (d, $J_{C\text{-}F}$ = 21.2 Hz), 34.5, 34.4, 31.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.5.



4-(3-(4-Chlorophenyl)propyl)pyridine (4ag).[4] (44 mg, 96%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (br, 2H), 7.28-7.26 (m, 2H), 7.13-7.10 (m, 4H), 2.65-2.62 (m, 4H), 1.99-1.93 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.1, 149.6, 140.0, 131.7, 129.7, 128.5, 124.0, 34.6, 34.5, 31.6.

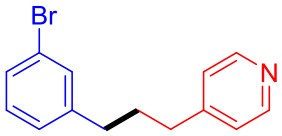


4-(3-(2-Fluorophenyl)propyl)pyridine (4ah). (42 mg, 98%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (br, 2H), 7.22-7.17 (m, 2H), 7.13 (d, J = 5.4 Hz, 2H), 7.08 (dt, J = 7.4, 1.0 Hz, 1H), 7.03 (dt, J = 8.2, 1.0 Hz, 1H), 2.71 (t, J = 7.6 Hz, 2H), 2.67 (t, J = 7.8 Hz, 2H), 2.00-1.95 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.1 (d, $J_{C\text{-}F}$ = 244.0 Hz), 151.0, 149.7, 130.6 (d, $J_{C\text{-}F}$ = 5.4 Hz), 128.4 (d, $J_{C\text{-}F}$ = 15.8 Hz), 127.8 (d, $J_{C\text{-}F}$ = 8.2 Hz), 124.0 (d, $J_{C\text{-}F}$ = 3.4 Hz), 123.9, 115.3 (d, $J_{C\text{-}F}$ = 22.2 Hz), 34.7, 30.5, 28.6 (d, $J_{C\text{-}F}$ = 2.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.8; HRMS (ESI) calcd for $C_{14}H_{15}FN$ [M + H^+], 216.1183; found: 216.1183.

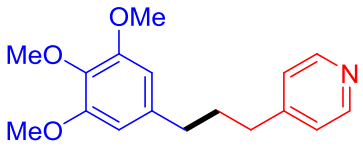


4-(3-(2-Chlorophenyl)propyl)pyridine (4ai).[4] (45 mg, 97%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (br, 2H), 7.36-7.35 (m, 1H), 7.21-7.19 (m, 2H), 7.18-7.14 (m, 3H), 2.79 (t, J = 7.8 Hz, 2H), 2.70 (t, J = 7.8 Hz, 2H), 2.02-1.96 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.1,

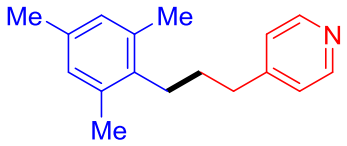
149.6, 139.2, 133.9, 130.4, 129.6, 127.5, 126.8, 124.0, 34.8, 33.1, 30.1.



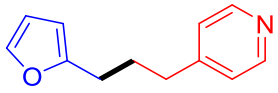
4-(3-(3-Bromophenyl)propyl)pyridine (4aj). (53 mg, 97%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 (br, 2H), 7.35-7.33 (m, 2H), 7.18-7.09 (m, 4H), 2.66-2.61 (m, 4H), 2.00-1.94 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.1, 149.5, 143.9, 131.5, 130.0, 129.2, 127.1, 124.1, 122.5, 34.9, 34.6, 31.5; HRMS (ESI) calcd for $C_{14}H_{15}BrN$ [M + H^+], 276.0382; found: 276.0374.



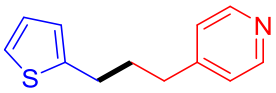
4-(3-(3,4,5-Trimethoxyphenyl)propyl)pyridine (4ak). (57 mg, 99%). Isolated by preparative TLC (hexane: ethyl acetate = 2:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (br, 2H), 7.13 (br, 2H), 6.39 (s, 2H), 3.85 (s, 6H), 3.84 (s ,3H), 2.66 (t, J = 7.6 Hz, 2H), 2.61 (t, J = 7.6 Hz, 2H), 2.00-1.94 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.2, 151.0, 149.7, 137.4, 136.2, 123.9, 105.3, 60.9, 56.1, 35.7, 34.7, 31.8; HRMS (APCI) calcd for $C_{17}H_{22}NO_3$ [M + H^+], 288.1594; found: 288.1592.



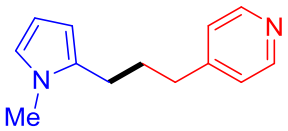
4-(3-Mesitylpropyl)pyridine (4al). (26 mg, 54%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (br, 2H), 7.20 (br, 2H), 6.85 (s, 2H), 2.76 (t, J = 7.6 Hz, 2H), 2.64-2.61 (m, 2H), 2.27 (s, 3H), 2.25 (s, 6H), 1.85-1.79 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.2, 149.7, 135.8, 135.5, 135.2, 129.0, 124.1, 35.6, 29.6, 28.8, 20.8, 19.7; HRMS (ESI) calcd for $C_{17}H_{22}N$ [M + H^+], 240.1747; found: 240.1737.



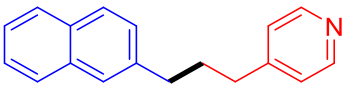
4-(3-(Furan-2-yl)propyl)pyridine (4am). (33 mg, 87%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (d, J = 5.8 Hz, 2H), 7.33 (d, J = 1.4 Hz, 1H), 7.12 (d, J = 5.8 Hz, 2H), 6.30 (dd, J = 3.0, 1.4 Hz, 1H), 6.01 (d, J = 3.0 Hz, 1H), 2.69-2.64 (m, 4H), 2.03-1.97 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.3, 150.8, 149.7, 141.0, 123.9, 110.1, 105.2, 34.4, 28.6, 27.3; HRMS (ESI) calcd for $C_{12}H_{14}NO$ [M + H^+], 188.1070; found: 188.1067.



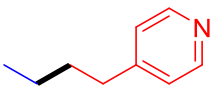
4-(3-(Thiophen-2-yl)propyl)pyridine (4an). (28 mg, 69%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (d, J = 5.8 Hz, 2H), 7.16 (dd, J = 5.2, 1.2 Hz, 1H), 7.14 (d, J = 5.8 Hz, 2H), 6.95 (dd, J = 5.2, 3.4 Hz, 1H), 6.82 (dq, J = 3.4, 1.2 Hz, 1H), 2.89 (t, J = 7.6 Hz, 2H), 2.69 (t, J = 7.6 Hz, 2H), 2.08-2.02 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.8, 149.8, 144.4, 126.8, 124.4, 123.9, 123.2, 34.3, 32.1, 29.2; HRMS (ESI) calcd for $C_{12}H_{14}NS$ [M + H^+], 204.0841; found: 204.0838.



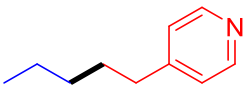
4-(3-(Thiophen-2-yl)propyl)pyridine (4ao). (36 mg, 91%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53 (br, 2H), 7.16 (d, J = 5.8 Hz, 2H), 6.58 (t, J = 2.2 Hz, 1H), 6.09 (t, J = 3.0 Hz, 1H), 5.94-5.93 (m, 1H), 3.52 (s, 3H), 2.74 (t, J = 7.6 Hz, 2H), 2.60 (t, J = 7.6 Hz, 2H), 2.04-1.98 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.0, 149.8, 132.4, 123.9, 121.3, 106.6, 105.7, 34.7, 33.5, 29.1, 25.6; HRMS (ESI) calcd for $C_{13}H_{17}N_2$ [M + H^+], 201.1386; found: 201.1391.



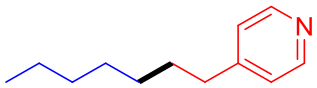
4-(3-(Naphthalen-2-yl)propyl)pyridine (4ap). (49 mg, 99%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (br, 2H), 7.85 (d, J = 7.8 Hz, 1H), 7.82 (d, J = 8.2 Hz, 2H), 7.64 (s, 1H), 7.50 (dt, J = 6.8, 1.2 Hz, 1H), 7.46 (dt, J = 6.8, 1.2 Hz, 1H), 7.35 (dd, J = 8.4, 1.6 Hz, 1H), 7.14 (d, J = 5.6 Hz, 2H), 2.85 (t, J = 7.6 Hz, 2H), 2.69 (t, J = 7.8 Hz, 2H), 2.12-2.06 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.1, 149.8, 139.1, 133.6, 132.1, 128.1, 127.7, 127.4, 127.2, 126.6, 126.0, 125.3, 124.0, 35.4, 34.6, 31.6; HRMS (ESI) calcd for $C_{18}H_{18}N$ [M + H^+], 248.1434; found: 248.1433.



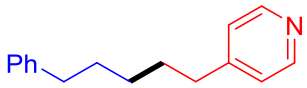
4-Butylpyridine (4aq).[5] (22 mg, 82%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53 (br, 2H), 7.13 (br, 2H), 2.61 (t, J = 7.8 Hz, 2H), 1.65-1.59 (m, 2H), 1.40-1.33 (m, 2H), 0.94 (t, J = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 149.5, 124.1, 34.9, 32.4, 22.2, 13.8.



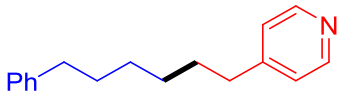
4-Pentylpyridine (4ar).[5] (23 mg, 78%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (br, 2H), 7.13 (br, 2H), 2.60 (t, J = 7.8 Hz, 2H), 1.67-1.61 (m, 2H), 1.37-1.28 (m, 4H), 0.91 (t, J = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 149.5, 124.1, 35.2, 31.3, 30.0, 22.4, 13.9.



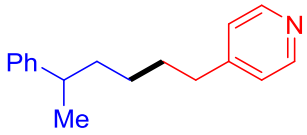
4-Heptylpyridine (4as). (29 mg, 83%).[6] Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 (br, 2H), 7.14 (br, 2H), 2.60 (t, J = 7.8 Hz, 2H), 1.65-1.62 (m, 2H), 1.33-1.28 (m, 8H), 0.89 (t, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 149.4, 124.2, 35.3, 31.7, 30.3, 29.1, 29.0, 22.6, 14.1.



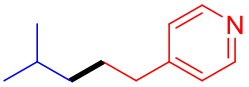
4-(5-Phenylpentyl)pyridine (4at).[4] (39 mg, 87%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (br, 2H), 7.32-7.29 (m, 2H), 7.22-7.18 (m, 3H), 7.12 (br, 2H), 2.65-2.60 (m, 4H), 1.71-1.65 (m, 4H), 1.44-1.38 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 149.5, 142.5, 128.4, 128.3, 125.7, 124.0, 35.8, 35.2, 31.2, 30.2, 28.8.



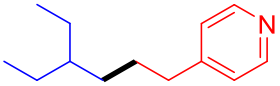
4-(6-Phenylhexyl)pyridine (4au).[4] (45 mg, 95%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.50 (br, 2H), 7.33-7.30 (m, 2H), 7.23-7.18 (m, 3H), 7.08 (br, 2H), 2.73-2.66 (m, 1H), 2.61-2.52 (m, 2H), 1.69-1.55 (m, 4H), 1.37-1.19 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.6, 149.6, 147.5, 128.3, 127.0, 125.9, 124.0, 39.9, 38.1, 35.1, 30.3, 27.2, 22.3.



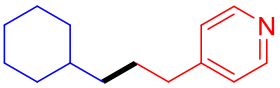
4-(5-Phenylhexyl)pyridine (4av). (40 mg, 84%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (br, 2H), 7.33-7.30 (m, 2H), 7.23-7.18 (m, 3H), 7.07 (d, J = 5.8 Hz, 2H), 2.73-2.66 (m, 1H), 2.62-2.53 (m, 2H), 1.67-1.55 (m, 4H), 1.34-1.20 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 149.6, 147.5, 128.3, 127.0, 125.9, 123.9, 39.9, 38.1, 35.1, 30.3, 27.2, 22.3; HRMS (ESI) calcd for $C_{17}H_{22}N$ [M + H^+], 240.1747; found: 240.1749.



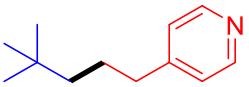
4-(4-Methylpentyl)pyridine (4aw).[7] (25 mg, 76%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 (br, 2H), 7.15 (br, 2H), 2.60 (t, J = 7.8 Hz, 2H), 1.68-1.61 (m, 2H), 1.60-1.54 (m, 1H), 1.26-1.21 (m, 2H), 0.89 (d, J = 6.6 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 149.3, 124.2, 38.4, 35.5, 28.1, 27.8, 22.5.



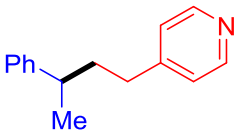
4-(4-Ethylhexyl)pyridine (4ax). (29 mg, 77%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (br, 2H), 7.14 (br, 2H), 2.60 (t, J = 7.8 Hz, 2H), 1.65-1.59 (m, 2H), 1.31-1.27 (m, 7H), 0.84 (t, J = 7.4 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 149.5, 124.1, 40.2, 35.7, 32.3, 27.5, 25.3, 10.9; HRMS (ESI) calcd for $C_{13}H_{22}N$ [M + H^+], 192.1747; found: 192.1744.



4-(3-Cyclohexylpropyl)pyridine (4ay).[8] (32 mg, 79%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 (br, 2H), 7.13 (br, 2H), 2.59 (t, J = 7.8 Hz, 2H), 1.71-1.61 (m, 7H), 1.27-1.12 (m, 6H), 0.91-0.85 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.0, 149.4, 124.1, 37.5, 37.0, 35.6, 33.3, 27.6, 26.7, 26.4.

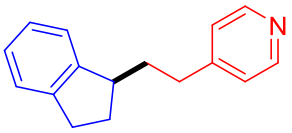


4-(4,4-Dimethylpentyl)pyridine (4az).[9] (27 mg, 75%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (br, 2H), 7.13 (d, J = 5.2 Hz, 2H), 2.59 (t, J = 7.6 Hz, 2H), 1.65-1.58 (m, 2H), 1.25-1.21 (m, 2H), 0.89 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 149.6, 124.0, 43.7, 36.1, 30.3, 29.3, 25.5.

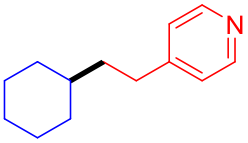


4-(3-Phenylbutyl)pyridine (4ba).[4] (33 mg, 78%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (br, 2H), 7.36-7.32 (m, 2H), 7.26-7.20 (m, 3H), 7.09 (br, 2H), 2.78-2.69 (m, 1H), 2.58-2.46 (m, 2H), 1.98-1.91 (m, 2H), 1.31 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.6,

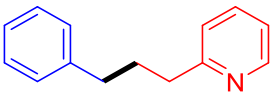
149.5, 146.6, 128.5, 127.0, 126.2, 124.0, 39.5, 38.7, 33.3, 22.5.



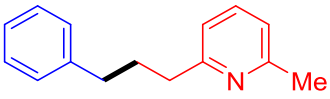
4-(2-(2,3-Dihydro-1H-inden-1-yl)ethyl)pyridine (4bb). (43 mg, 96%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.3); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53 (br, 2H), 7.27-7.25 (m, 1H), 7.24-7.17 (m, 5H), 3.21-3.15 (m, 1H), 3.02-2.96 (m, 1H), 2.92-2.86 (m, 1H), 2.81-2.69 (m, 2H), 2.41-2.34 (m, 1H), 2.24-2.17 (m, 1H), 1.83-1.74 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.4, 149.8, 146.7, 144.0, 126.6, 126.2, 124.6, 123.9, 123.5, 44.4, 35.6, 33.2, 32.0, 31.4; HRMS (ESI) calcd for $C_{16}H_{18}N$ [M + H^+], 224.1434; found: 224.1433.



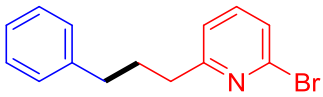
4-(2-Cyclohexylethyl)pyridine (4bc).[10] (32 mg, 86%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 (br, 2H), 7.15 (br, 2H), 2.62 (t, *J* = 8.0 Hz, 2H), 1.78-1.67 (m, 5H), 1.55-1.51 (m, 2H), 1.31-1.16 (m, 4H), 0.99-0.92 (m, 2H), ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 149.5, 124.1, 38.1, 37.2, 33.2, 32.6, 26.6, 26.3.



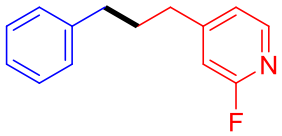
2-(3-Phenylpropyl)pyridine (5a).[1] (38 mg, 96%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 (d, *J* = 4.2 Hz, 1H), 7.60 (dt, *J* = 7.6, 1.8 Hz, 1H), 7.32-7.29 (m, 2H), 7.23-7.19 (m, 3H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.13-7.11 (m, 1H), 2.86 (t, *J* = 7.8 Hz, 2H), 2.72 (t, *J* = 7.8 Hz, 2H), 2.14-2.07 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.0, 149.3, 142.2, 136.3, 128.5, 128.3, 125.8, 122.8, 121.0, 37.9, 35.6, 31.5.



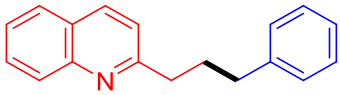
2-Methyl-6-(3-phenylpropyl)pyridine (5b).[11] (40 mg, 96%). Isolated by preparative TLC (hexane: ethyl acetate = 10:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (t, *J* = 7.6 Hz, 1H), 7.32-7.29 (m, 2H), 7.23-7.18 (m, 3H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 1H), 2.83 (t, *J* = 7.6 Hz, 2H), 2.72 (t, *J* = 7.6 Hz, 2H), 2.56 (s, 3H), 2.11-2.04 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.4, 157.8, 142.3, 136.5, 128.5, 128.3, 125.7, 120.5, 119.5, 38.1, 35.7, 31.8, 24.6.



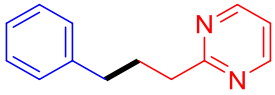
2-Bromo-6-(3-phenylpropyl)pyridine (5c). (48 mg, 88%). Isolated by preparative TLC (hexane: ethyl acetate = 10:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (t, J = 7.6 Hz, 1H), 7.33-7.28 (m, 3H), 7.27-7.20 (m, 3H), 7.10 (d, J = 7.6 Hz, 1H), 2.83 (t, J = 7.6 Hz, 2H), 2.71 (t, J = 7.8 Hz, 2H), 2.11-2.05 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.7, 141.9, 141.6, 138.6, 128.5, 128.4, 125.9, 125.3, 121.6, 37.5, 35.5, 31.3; HRMS (ESI) calcd for $C_{14}H_{15}BrN$ [M + H^+], 276.0382; found: 276.0374.



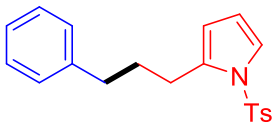
2-Fluoro-4-(3-phenylpropyl)pyridine (5d).[1] (40 mg, 92%). Isolated by preparative TLC (hexane: ethyl acetate = 10:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, J = 5.2 Hz, 1H), 7.34-7.31 (m, 2H), 7.25-7.22 (m, 1H), 7.21-7.19 (m, 2H), 7.02 (d, J = 5.2 Hz, 1H), 6.76 (s, 1H), 2.71-2.68 (m, 4H), 2.04-1.98 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.1 (d, $J_{C\text{-}F}$ = 237.4 Hz), 157.3 (d, $J_{C\text{-}F}$ = 7.5 Hz), 147.3 (d, $J_{C\text{-}F}$ = 15.2 Hz), 141.3, 128.5, 128.4, 126.1, 121.6 (d, $J_{C\text{-}F}$ = 4.0 Hz), 109.1 (d, $J_{C\text{-}F}$ = 36.7 Hz), 35.2, 34.5 (d, $J_{C\text{-}F}$ = 2.9 Hz), 31.6; ^{19}F NMR (470 MHz, $CDCl_3$) δ -69.1.



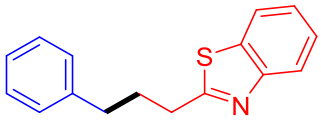
2-(3-Phenylpropyl)quinoline (5f).[12] (48 mg, 97%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, J = 8.4 Hz, 1H), 8.08 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 8.2 Hz, 1H), 7.72 (dt, J = 7.6, 1.4 Hz, 1H), 7.51 (dt, J = 7.6, 1.0 Hz, 1H), 7.35-7.30 (m, 3H), 7.26-7.21 (m, 3H), 3.06 (t, J = 7.8 Hz, 2H), 2.78 (t, J = 7.8 Hz, 2H), 2.24-2.17 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.5, 148.0, 142.1, 136.3, 129.4, 128.9, 128.5, 128.4, 127.5, 126.8, 125.8, 125.7, 121.4, 38.8, 35.7, 31.6.



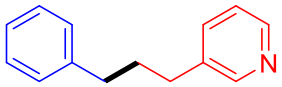
2-(3-phenylpropyl)pyrimidine (5g).[1] (37 mg, 94%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.69 (d, J = 4.8 Hz, 2H), 7.31-7.28 (m, 2H), 7.24-7.23 (m, 2H), 7.21-7.18 (m, 1H), 7.14 (t, J = 4.8 Hz, 1H), 3.03 (t, J = 7.8 Hz, 2H), 2.74 (t, J = 7.6 Hz, 2H), 2.22-2.16 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.3, 157.0, 142.0, 128.5, 128.3, 125.8, 118.5, 39.1, 35.6, 30.3.



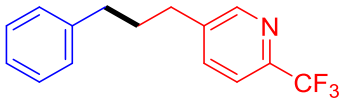
2-(3-Phenylpropyl)-1-tosyl-1H-pyrrole (5h). (49 mg, 72%). Isolated by preparative TLC (hexane: ethyl acetate = 10:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, J = 8.4 Hz, 2H), 7.32-7.29 (m, 3H), 7.26 (d, J = 8.4 Hz, 2H), 7.24-7.21 (m, 1H), 7.18-7.16 (m, 2H), 2.71 (t, J = 7.8 Hz, 2H), 2.67 (t, J = 7.6 Hz, 2H), 2.42 (s, 3H), 1.93-1.87 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.7, 141.9, 136.4, 135.4, 130.0, 128.5, 128.3, 126.8, 125.8, 122.2, 118.8, 111.2, 35.4, 30.2, 26.7, 21.6; HRMS (ESI) calcd for $C_{20}H_{22}NO_2S$ [M + H^+], 340.1366; found: 340.1365.



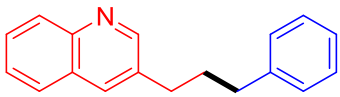
2-(3-Phenylpropyl)benzo[d]thiazole (5i). (38 mg, 76%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, J = 8.2 Hz, 1H), 7.87 (d, J = 8.0 Hz, 1H), 7.48 (td, J = 7.8, 1.2 Hz, 1H), 7.38 (td, J = 7.8, 1.2 Hz, 1H), 7.34-7.31 (m, 2H), 7.26-7.22 (m, 3H), 3.17 (t, J = 7.8 Hz, 2H), 2.80 (t, J = 7.8 Hz, 2H), 2.29-2.23 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.8, 153.3, 141.3, 135.2, 128.5, 128.4, 126.1, 126.0, 124.7, 122.6, 121.5, 35.2, 33.7, 31.2; HRMS (ESI) calcd for $C_{16}H_{16}NS$ [M + H^+], 254.0998; found: 254.1996.



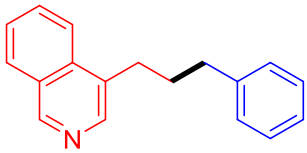
3-(3-Phenylpropyl)pyridine (5j).[1] (37 mg, 94%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (br, 2H), 7.51 (dt, J = 7.8, 1.8 Hz, 1H), 7.33-7.30 (m, 2H), 7.24-7.20 (m, 4H), 2.70-2.66 (m, 4H), 2.02-1.96 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.0, 147.4, 141.7, 137.4, 135.8, 128.4, 125.9, 123.3, 35.3, 32.6, 32.5.



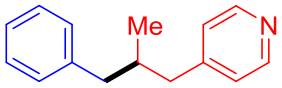
5-(3-Phenylpropyl)-2-(trifluoromethyl)pyridine (5k). (51 mg, 97%). Isolated by preparative TLC (hexane: ethyl acetate = 10:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.58 (s, 1H), 7.68 (dd, J = 8.0, 1.4 Hz, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.34 (m, 2H), 7.25-7.20 (m, 3H), 2.75 (t, J = 7.6 Hz, 2H), 2.71 (t, J = 7.6 Hz, 2H), 2.06-2.00 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.2, 146.0 (q, J_{C-F} = 34.4 Hz), 141.3, 140.9, 136.9, 128.5, 128.4, 126.1, 121.6 (q, J_{C-F} = 273.7 Hz), 120.1 (q, J_{C-F} = 2.6 Hz), 35.2, 32.3, 32.2; ^{19}F NMR (470 MHz, $CDCl_3$) δ -67.6; HRMS (ESI) calcd for $C_{15}H_{15}F_3N$ [M + H^+], 266.1151; found: 266.1148.



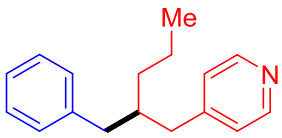
3-(3-Phenylpropyl)quinoline (5l). (48 mg, 98%). Isolated by preparative TLC (hexane: ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, J = 1.4 Hz, 1H), 8.13 (d, J = 8.4 Hz, 1H), 7.93 (s, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.69 (t, J = 7.4 Hz, 1H), 7.55 (t, J = 7.4 Hz, 1H), 7.35-7.32 (m, 2H), 7.25-7.22 (m, 3H), 2.86 (t, J = 7.6 Hz, 2H), 2.74 (t, J = 7.6 Hz, 2H), 2.14-2.06 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 146.9, 141.7, 134.8, 134.2, 129.2, 128.6, 128.5, 128.4, 128.2, 127.3, 126.6, 126.0, 35.3, 32.6, 32.5; HRMS (ESI) calcd for $C_{18}H_{18}N$ [M + H^+], 248.1434; found: 248.1427.



4-(3-Phenylpropyl)isoquinoline (5m). (45 mg, 92%). Isolated by preparative TLC (hexane: ethyl acetate = 10:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.42 (s, 1H), 7.99 (d, J = 8.2 Hz, 1H), 7.92 (d, J = 8.2 Hz, 1H), 7.72 (dt, J = 7.6, 1.2 Hz, 1H), 7.61 (dt, J = 7.6, 0.8 Hz, 1H), 7.35-7.32 (m, 2H), 7.25-7.22 (m, 3H), 3.07 (t, J = 8.0 Hz, 2H), 2.79 (t, J = 7.6 Hz, 2H), 2.15-2.09 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.3, 142.7, 141.8, 134.6, 130.2, 128.5, 128.4, 128.3, 126.8, 126.0, 122.9, 35.7, 32.1, 29.5; HRMS (ESI) calcd for $C_{18}H_{18}N$ [M + H^+], 248.1434; found: 248.1427.

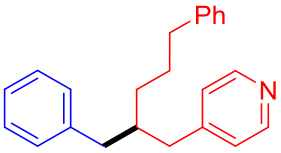


4-(2-Methyl-3-phenylpropyl)pyridine (5n).[2] (39 mg, 93%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 (br, 2H), 7.33-7.30 (m, 2H), 7.24-7.21 (m, 1H), 7.18-7.16 (m, 2H), 7.11 (br, 2H), 2.70 (dd, J = 13.4, 5.8 Hz, 1H), 2.67 (dd, J = 13.4, 6.4 Hz, 1H), 2.50 (dd, J = 13.4, 8.0 Hz, 1H), 2.40 (dd, J = 13.4, 8.6 Hz, 1H), 2.14-2.07 (m, 1H), 0.87 (d, J = 6.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.3, 149.6, 140.6, 129.1, 128.3, 126.0, 124.8, 43.3, 42.5, 36.5, 19.2.

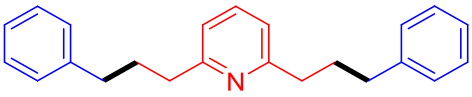


4-(2-Benzylpentyl)pyridine (5o). (43 mg, 90%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.50 (br, 2H), 7.32-7.29 (m, 2H), 7.23-7.20 (m, 1H), 7.16-7.14 (m, 2H), 7.07 (d, J = 5.6 Hz, 2H), 2.66 (dd, J = 13.6, 7.0 Hz, 1H), 2.59-2.48 (m, 3H), 2.07-1.98 (m, 1H), 1.43-1.34 (m, 2H),

1.29-1.23 (m, 2H), 0.86 (t, J = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.6, 149.6, 140.7, 129.1, 128.3, 126.0, 124.7, 41.0, 40.2, 39.5, 35.2, 19.7, 14.2; HRMS (ESI) calcd for $C_{17}H_{22}N$ [M + H^+], 240.1747; found: 240.1749.

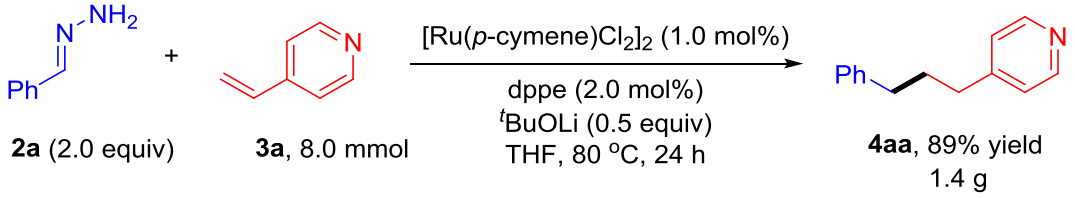


4-(2-Benzyl-5-phenylpentyl)pyridine (5p). (53 mg, 85%). Isolated by preparative TLC (hexane: ethyl acetate = 5:1, R_f = 0.4); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (br, 2H), 7.32-7.26 (m, 4H), 7.24-7.19 (m, 2H), 7.14-7.10 (m, 6H), 2.68-2.63 (m, 1H), 2.57-2.49 (m, 5H), 2.10-2.00 (m, 1H), 1.74-1.66 (m, 2H), 1.36-1.31 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 149.1, 142.3, 140.5, 129.1, 128.4, 128.3, 128.2, 126.0, 125.8, 41.1, 40.2, 39.5, 35.9, 32.3, 28.4; HRMS (ESI) calcd for $C_{23}H_{26}N$ [M + H^+], 316.2060; found: 316.2059.



2,6-Bis(3-phenylpropyl)pyridine (5r).[13] (29 mg, 92%). Isolated by preparative TLC (hexane: ethyl acetate = 4:1, R_f = 0.4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (t, J = 7.2 Hz, 1H), 7.32-7.29 (m, 4H), 7.24-7.20 (m, 6H), 6.98 (d, J = 7.2 Hz, 2H), 2.85 (t, J = 7.4 Hz, 4H), 2.72 (t, J = 7.4 Hz, 4H), 2.13-2.06 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.4, 142.3, 136.5, 128.5, 128.3, 125.7, 119.9, 38.1, 35.6, 31.8.

3. Gram-scale synthesis of product 4aa



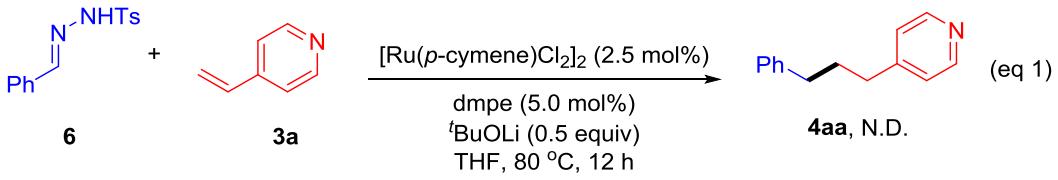
Preparation of hydrazone **2a**: a mixture of benzaldehydes **1** (16.0 mmol, 2.0 equiv) and hydrazine monohydrate (1.0 mL, 19.2 mmol, 64–65 wt%, 2.4 equiv) in THF (30.0 mL) solution was stirred for 120 min at room temperature. After that, 1.0 g of anhydrous Na_2SO_4 was added. The resulting mixture was filtered and the filtrate was evaporated *in vacuo* before use.

A flame-dried Schlenk tube (25 cm^3) equipped with a magnetic stir bar was charged with [Ru(*p*-cymene)Cl_2]$_2$ (50 mg, 1.0 mol%) and dppe (64 mg, 2.0 mol%). The tube was transferred to the glovebox and charged with THF (1.0 mL) before being sealed with Teflon septum. The reaction mixture was stirred at room temperature for 60 min. Then vinylpyridine **3a** (8.0 mmol, 1.0 equiv), hydrazone **2a** (16.0 mmol, dissolved in 6.0 mL THF) and ^{t}BuOLi (4.0 mmol, 320 mg) was added sequentially. After that, the reaction mixture was sealed with Teflon septum, moved out of glovebox, and stirred at 80 ℃ for 24 hour. After the mixture was cooled to room temperature, the Teflon septum was removed carefully. [***Caution: N_2 was generated in the reaction and should be released slowly***]. Water (5.0 mL)

and ether (30.0 mL) were added to the resulting mixture. The aqueous solution was separated and extracted with ether (2 x 25.0 mL). The organic layer was then washed with brine and dried over anhydrous Na_2SO_4. Evaporation and column chromatography on silica gel (ethyl acetate/hexane = 1:5 to 1:3) to give the pure product **4ae** (1.4 g, 89%).

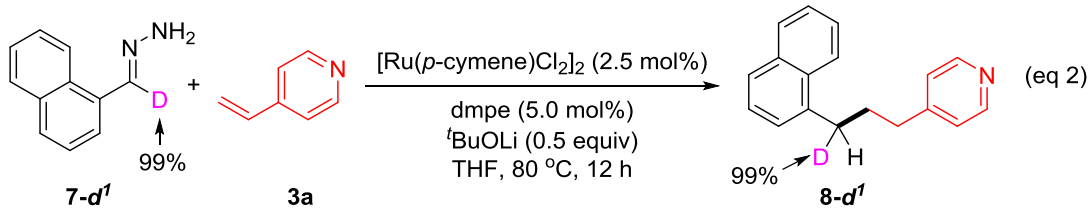
4. Control experiments

Reaction of *N*-Ts hydrazone with vinylpyridine



N-Ts hydrazone **6** was used in the place of **2a**, and the other operations were following the general procedure. No desired product **4aa** was detected under the standard conditions.

Deuterium experiment



The deuterated aldehyde **7-*d*^{1}** was synthesized according to the literature.[14] **7-*d*^{1}** was used in the place of **2a**, and the other operations were following the general procedure. No H/D loss or scrambling among benzylic moiety and other positions. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (br, 2H), 7.98 (d, J = 7.8 Hz, 1H), 7.89 (dd, J = 8.2, 1.6 Hz, 1H), 7.76 (d, J = 8.2 Hz, 1H), 7.55-7.48 (m, 2H), 7.43 (t, J = 7.6 Hz, 1H), 7.34 (d, J = 6.8 Hz, 1H), 7.16 (br, 2H), 3.12 (t, J = 7.4 Hz, 1H), 2.75 (t, J = 7.8 Hz, 2H), 2.16-2.10 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 141.7, 137.7, 134.0, 131.8, 128.9, 126.8, 126.0, 125.9, 125.5, 124.0, 123.6, 35.1, 32.0 ($J_{C\text{-}D}$ = 19.5 Hz), 31.0; ^{2}H NMR (61 MHz, $CDCl_3$) δ 3.12. HRMS (APCI) calcd for $C_{18}H_{17}DN$ [M + H$^+$], 249.1497; found: 249.1495.

5. References

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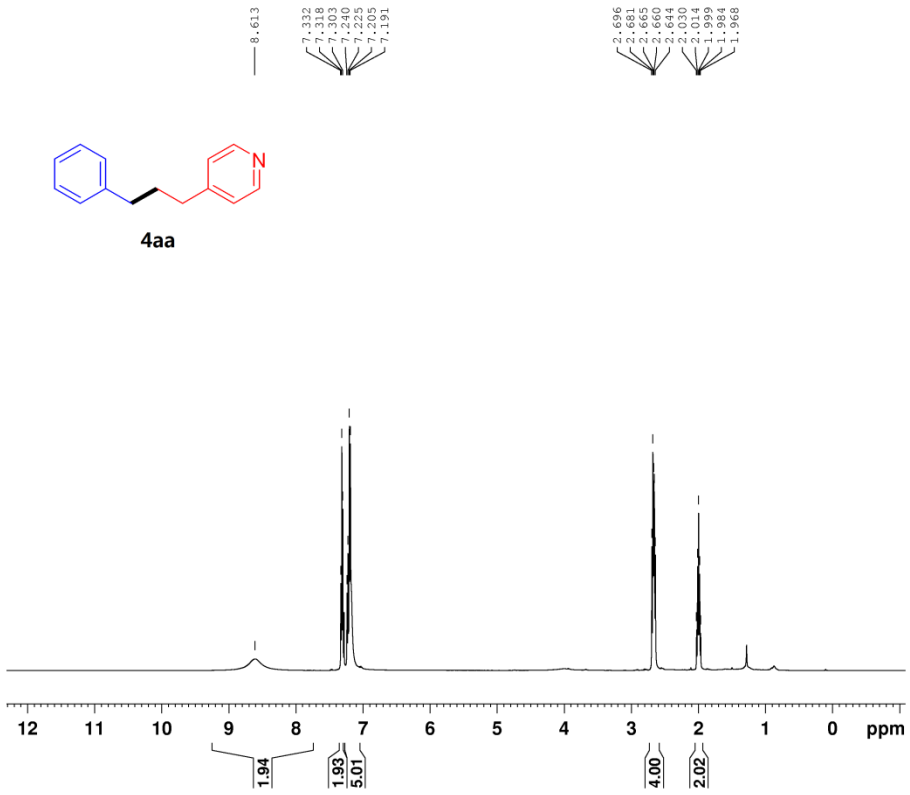
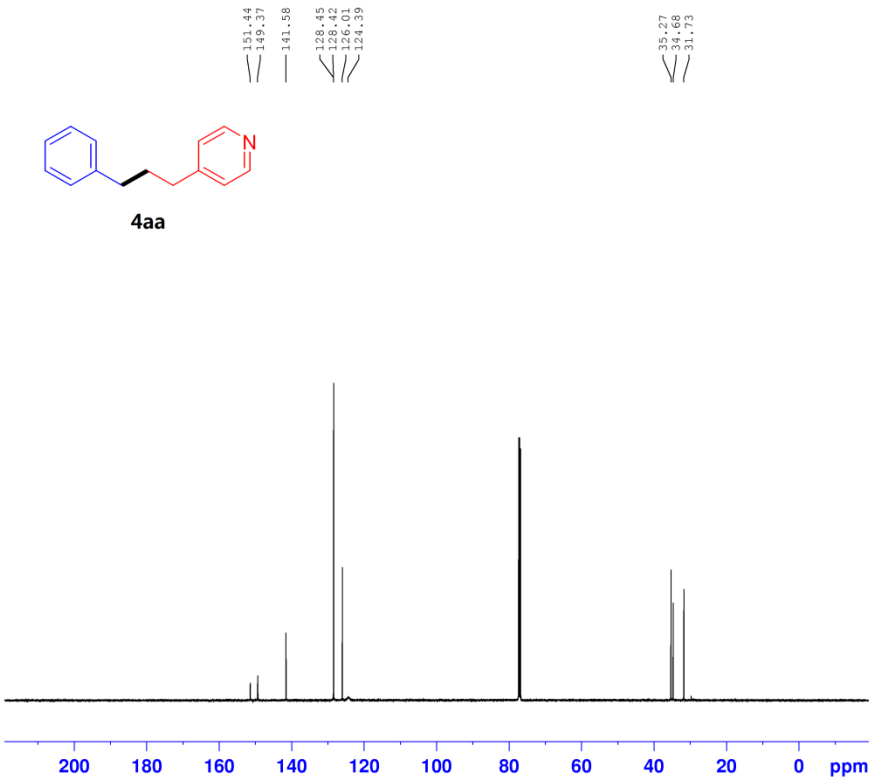
6. Copies of ^{1}H NMR and ^{13}C NMR spectra for all products

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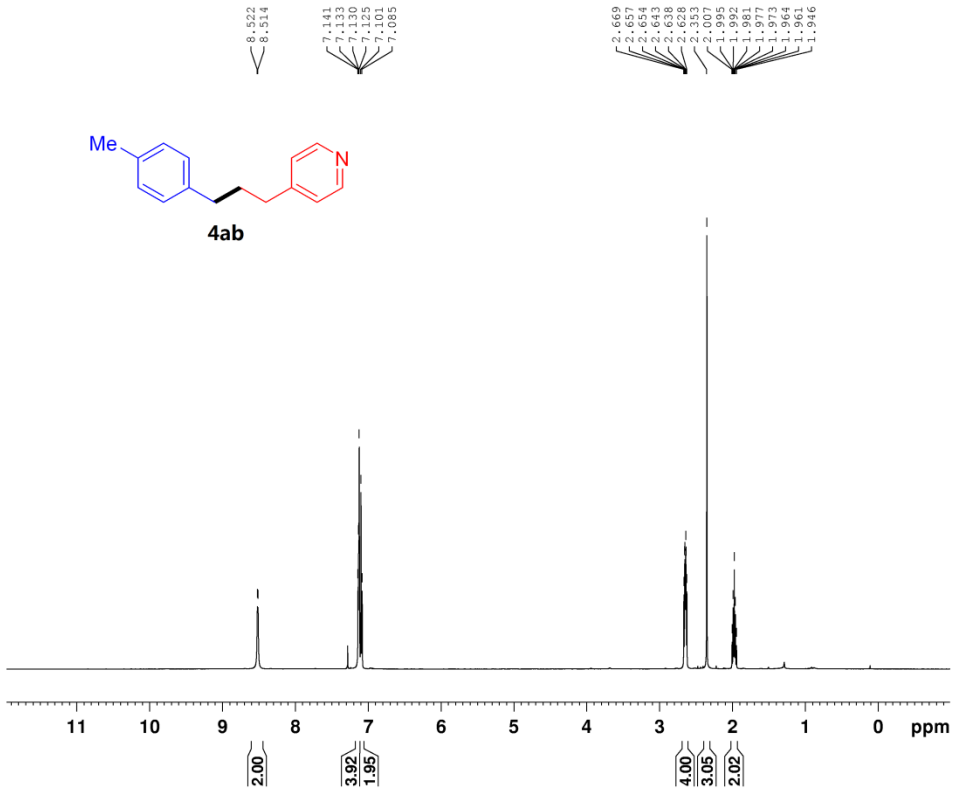
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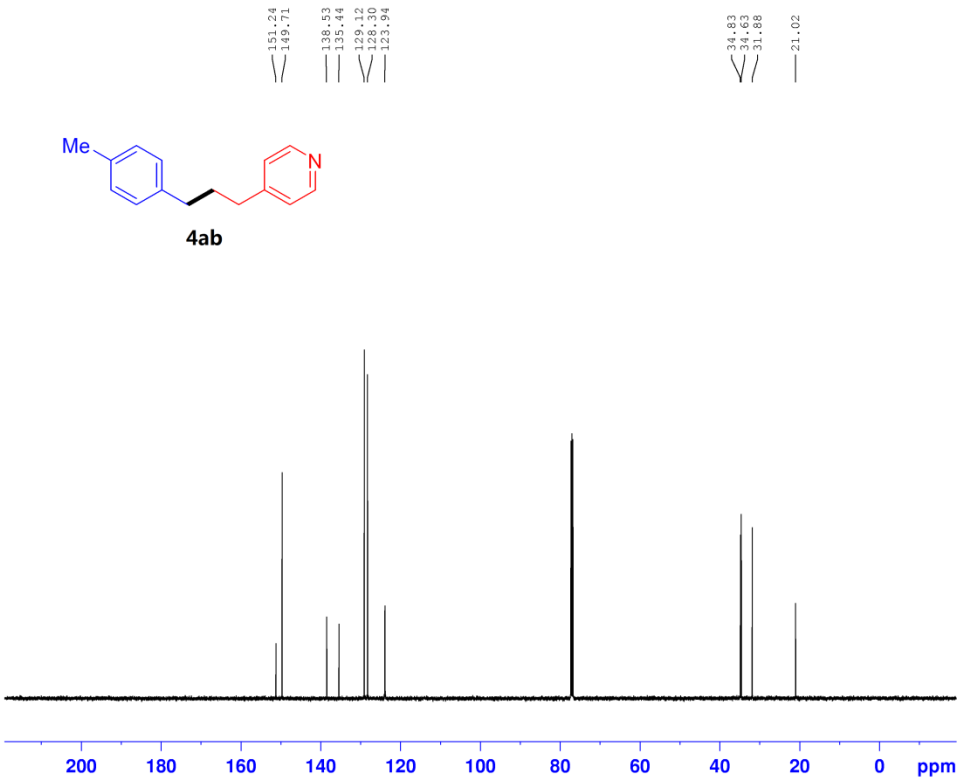
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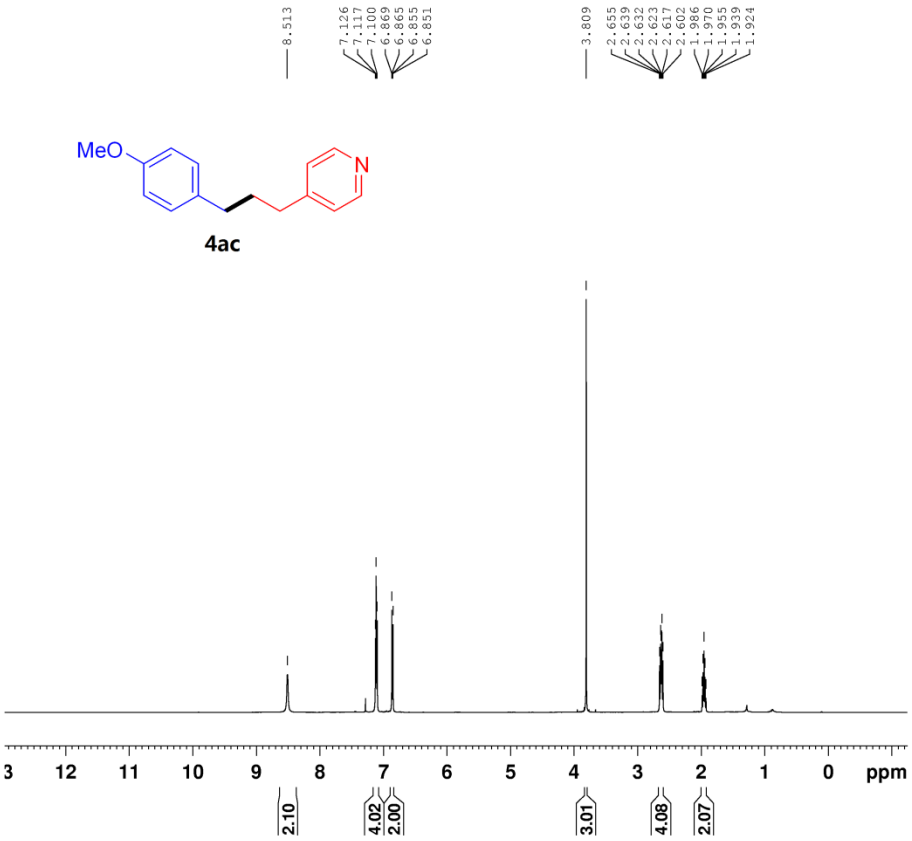
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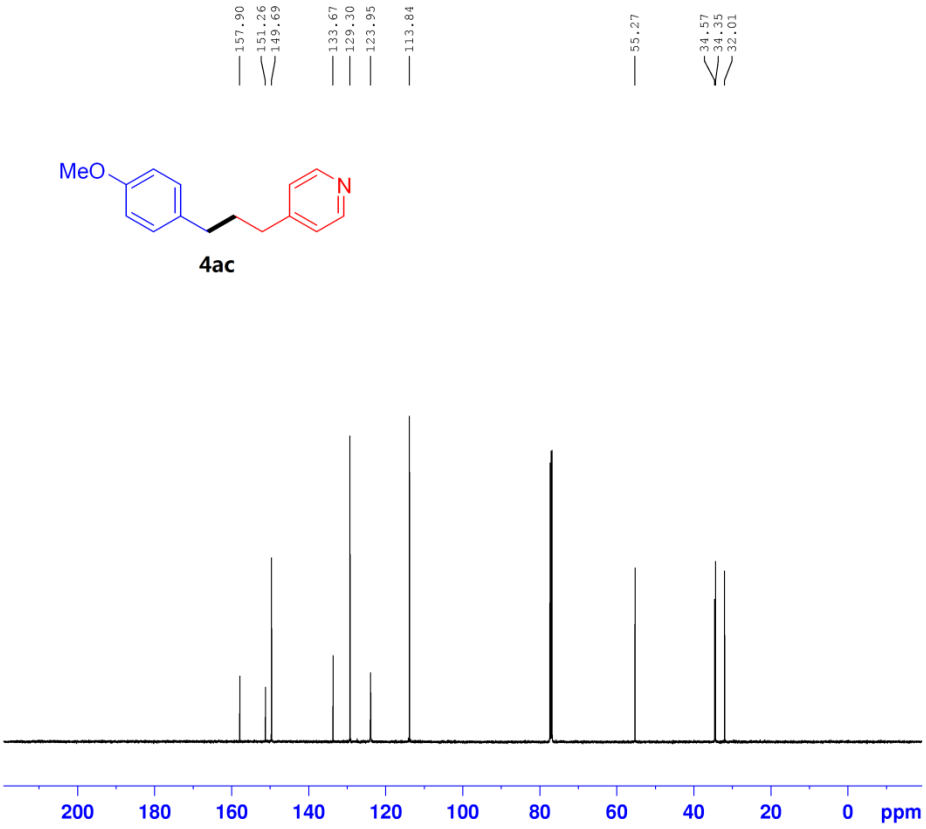
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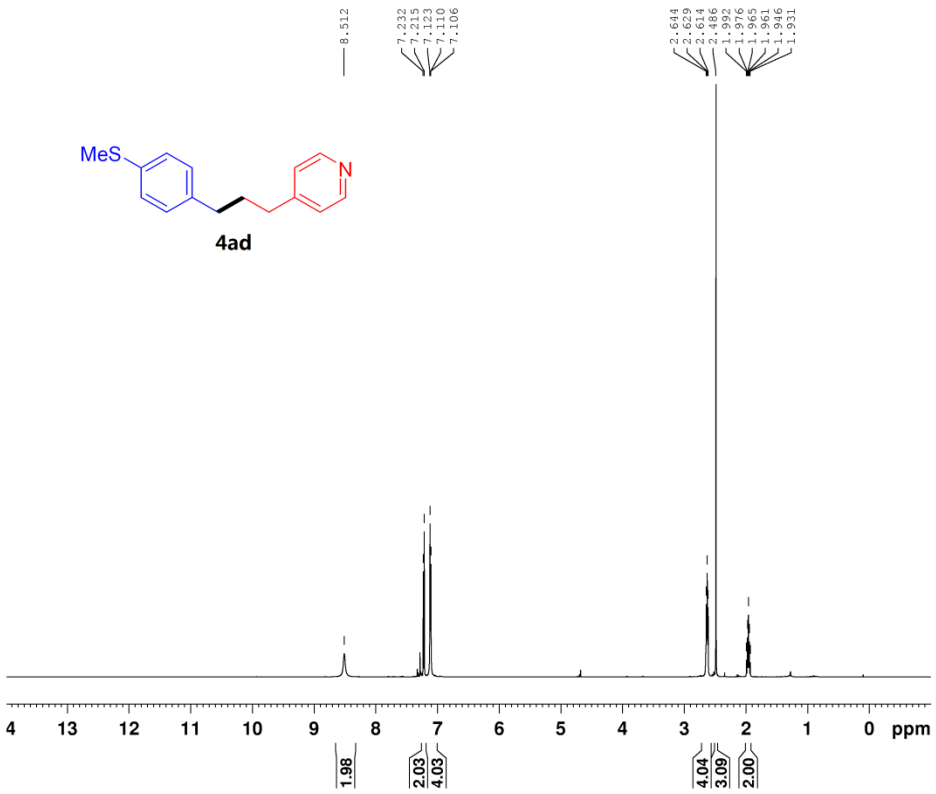
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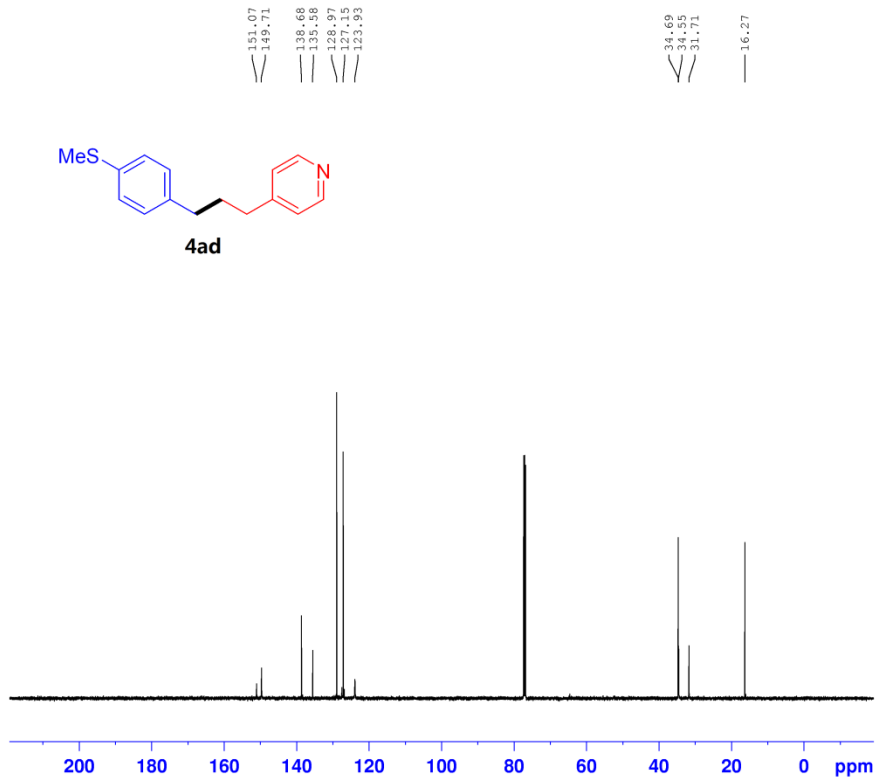
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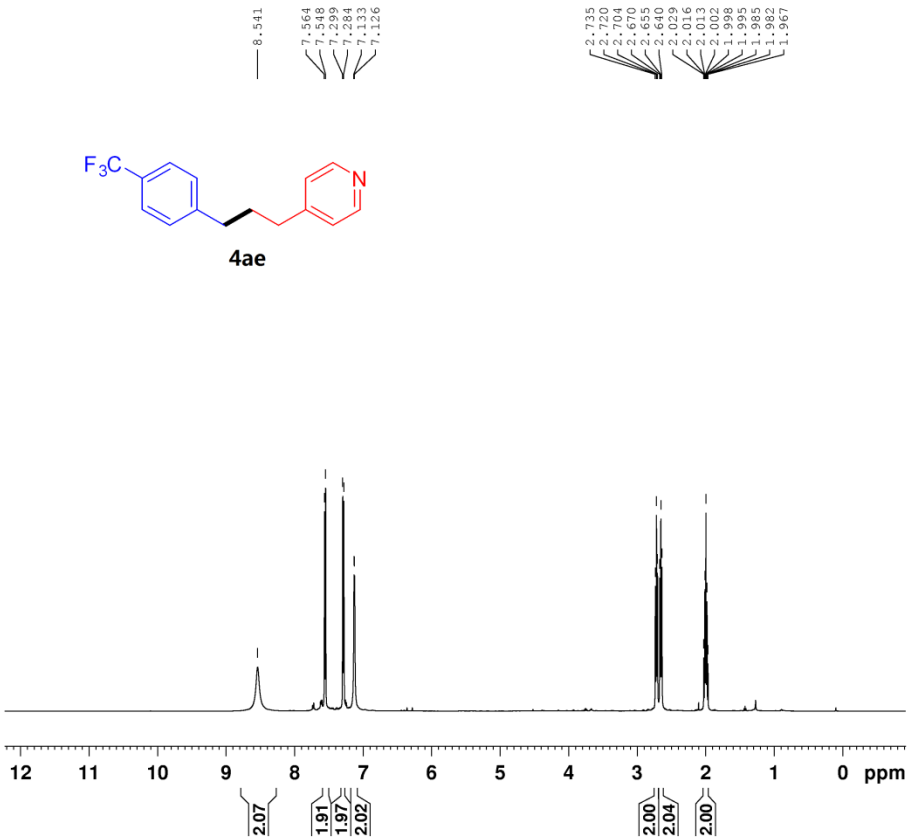
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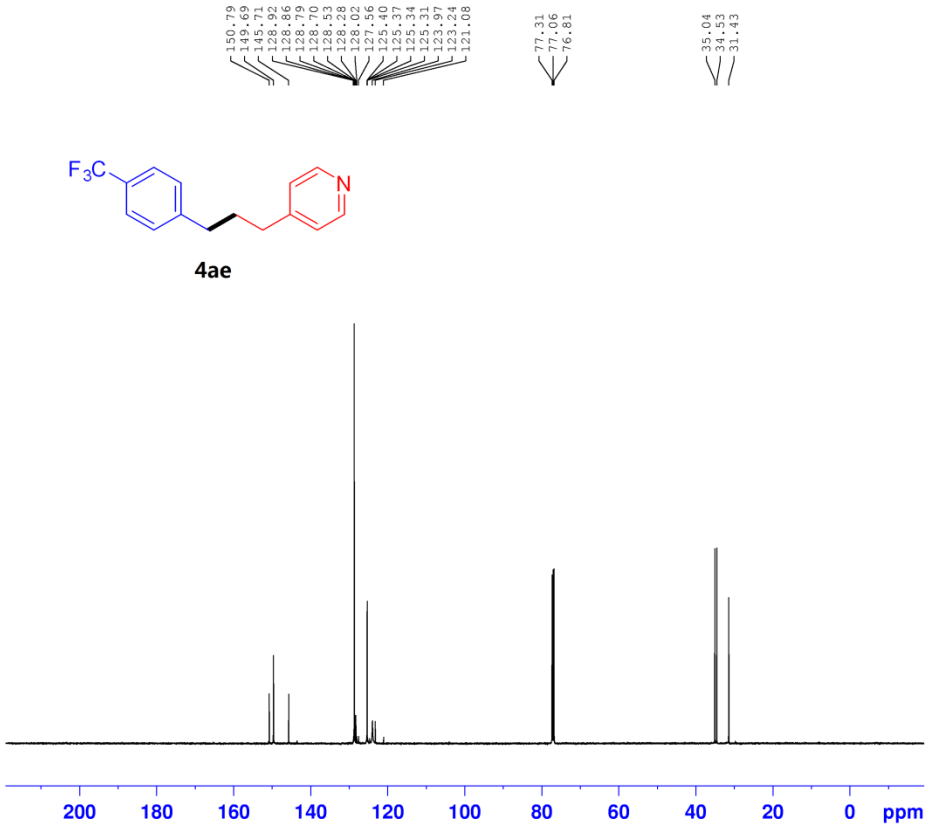
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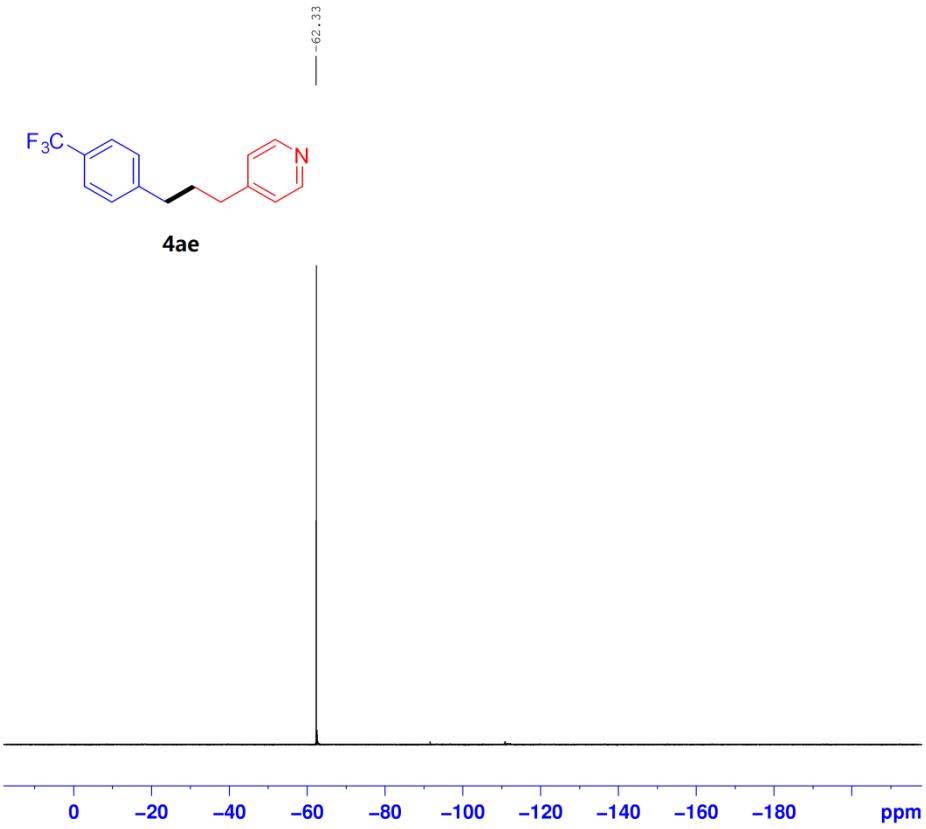
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−180
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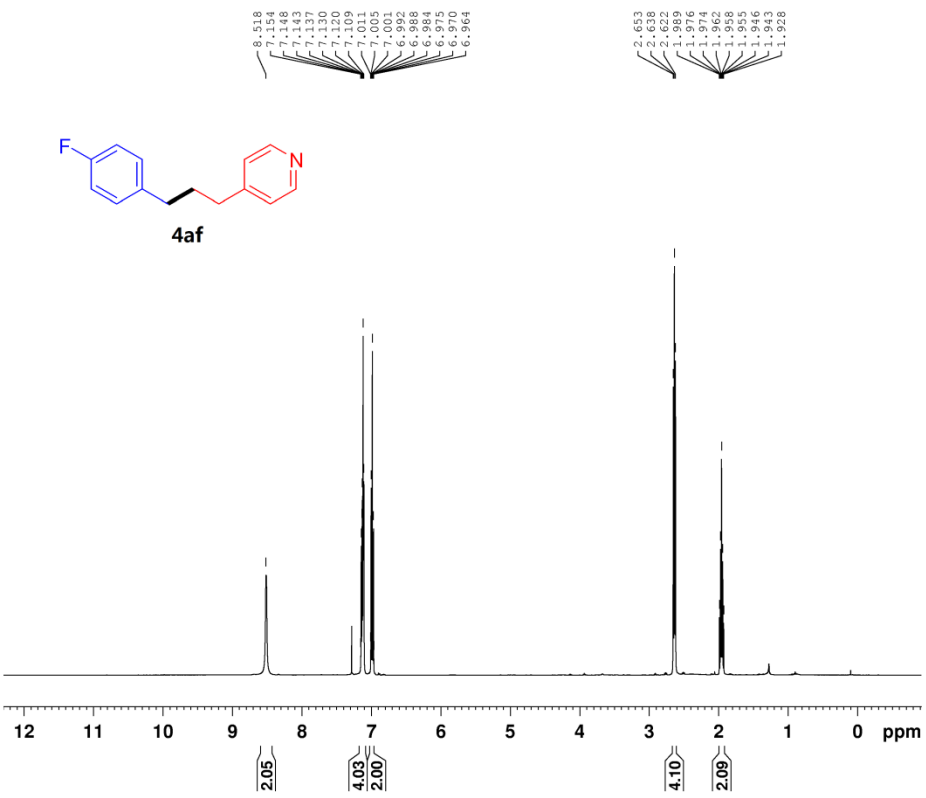
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7.109
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7.005
7.001
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6.975
6.970
6.964
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2.622
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1.974
1.962
1.958
1.955
1.946
1.943
1.928
F
N
4af
12
11
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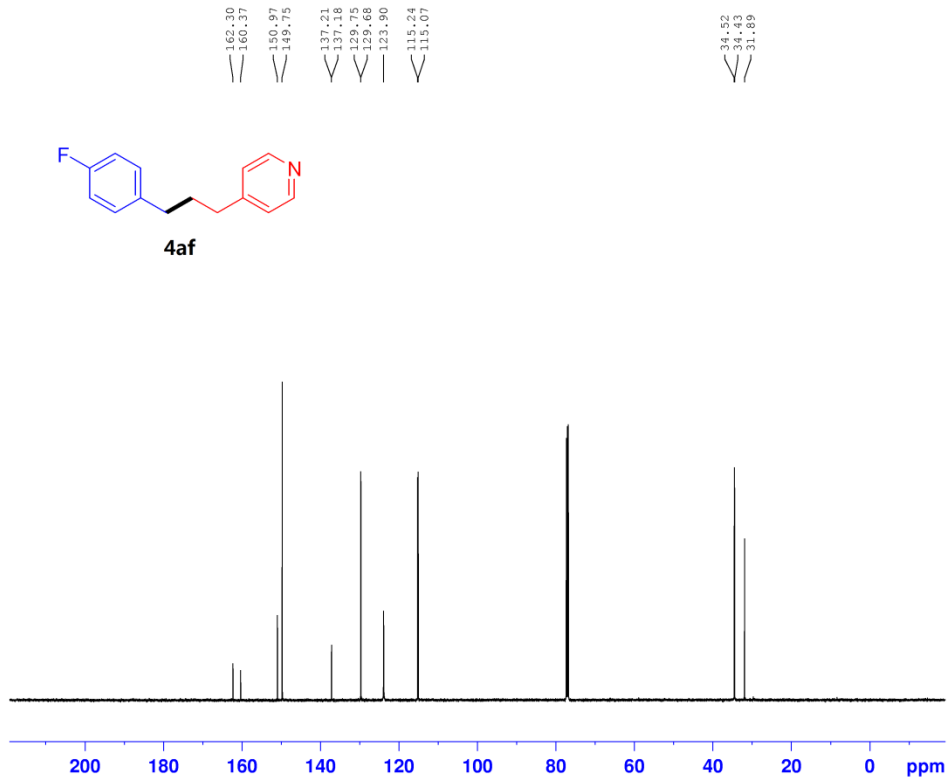
2.00
4.10
2.09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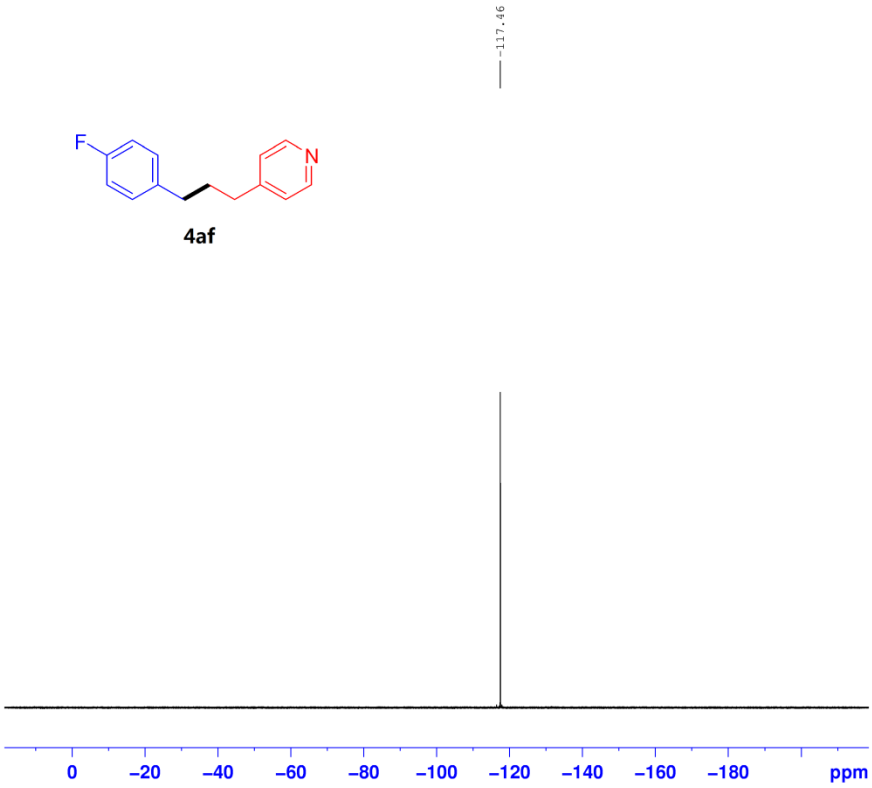
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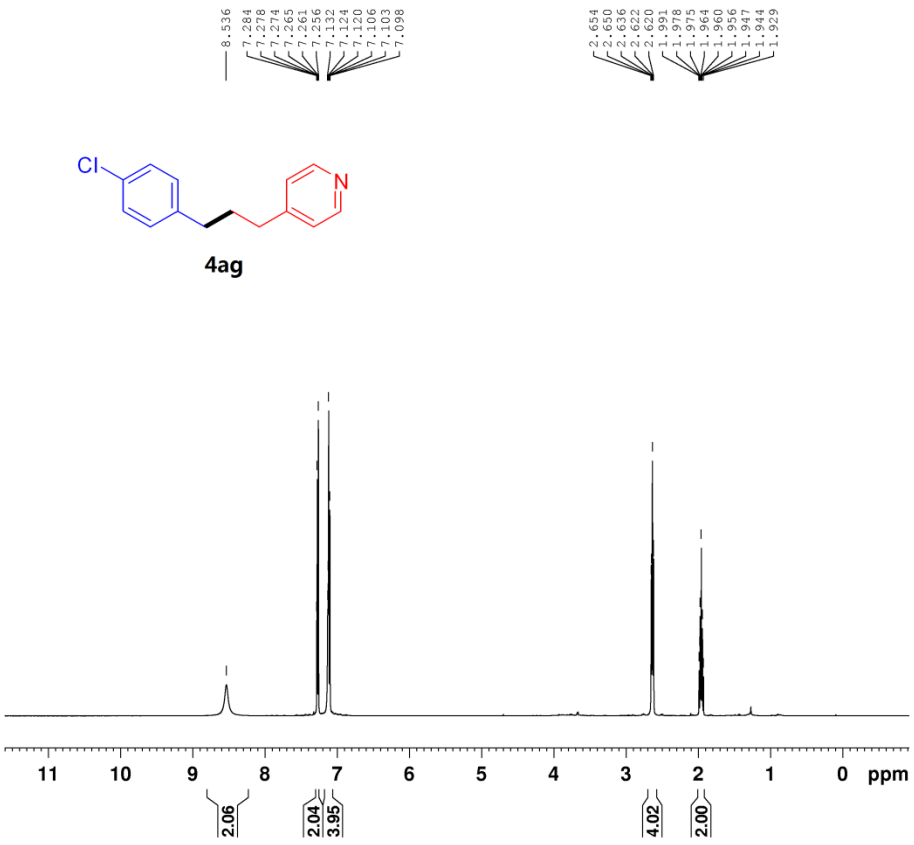
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7.106
7.103
7.098
2.654
2.650
2.636
2.622
2.620
1.991
1.978
1.975
1.964
1.960
1.956
1.947
1.944
1.929
Cl
N
4ag
11
10
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6
5
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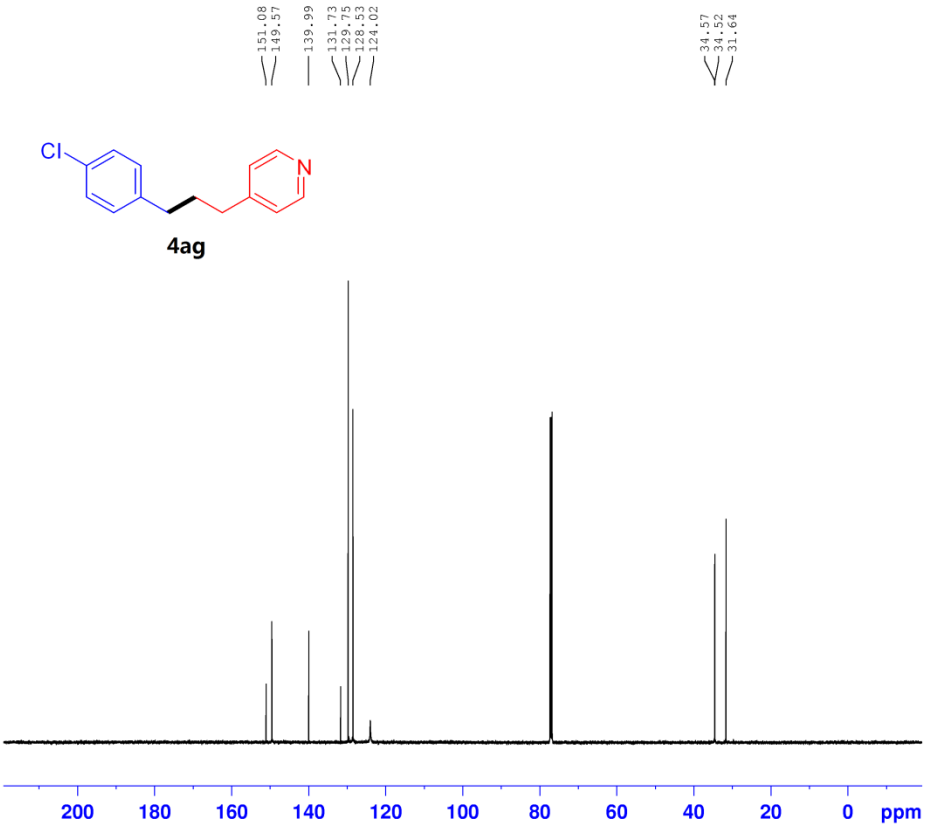
4.02
2.00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4ag
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160
140
120
100
80
60
40
20
0
ppm


8.515
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7.215
7.208
7.204
7.199
7.197
7.193
7.189
7.185
7.181
7.178
7.175
7.166
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7.092
7.090
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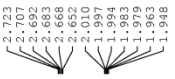
7.076
7.063
7.060
7.048
7.039
7.012
7.011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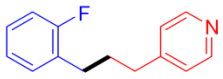
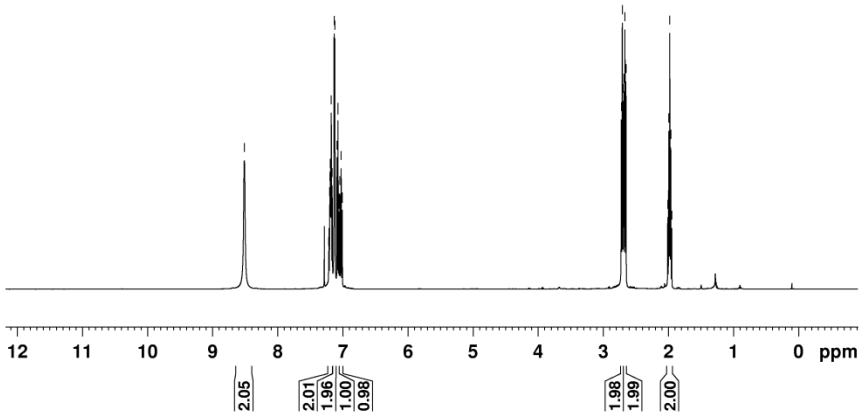
1.979
1.963
1.948


F
N

4ah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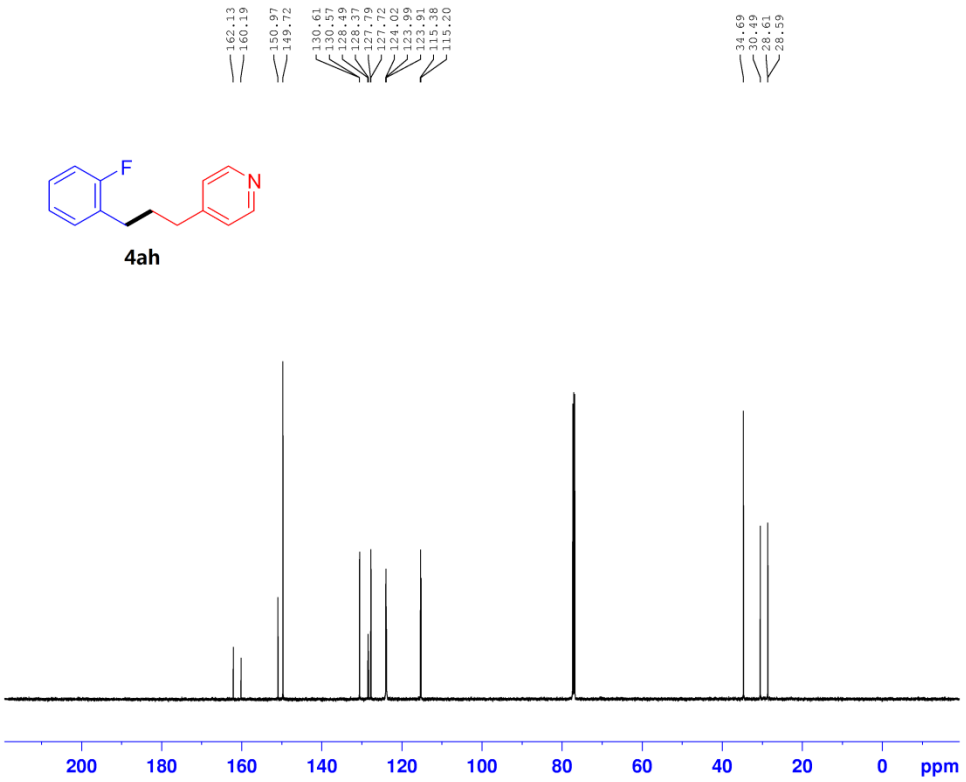
1.99
2.00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128.49
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127.79
127.72
124.02
123.99
123.91
115.38
115.20
34.69
30.49
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N
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120
100
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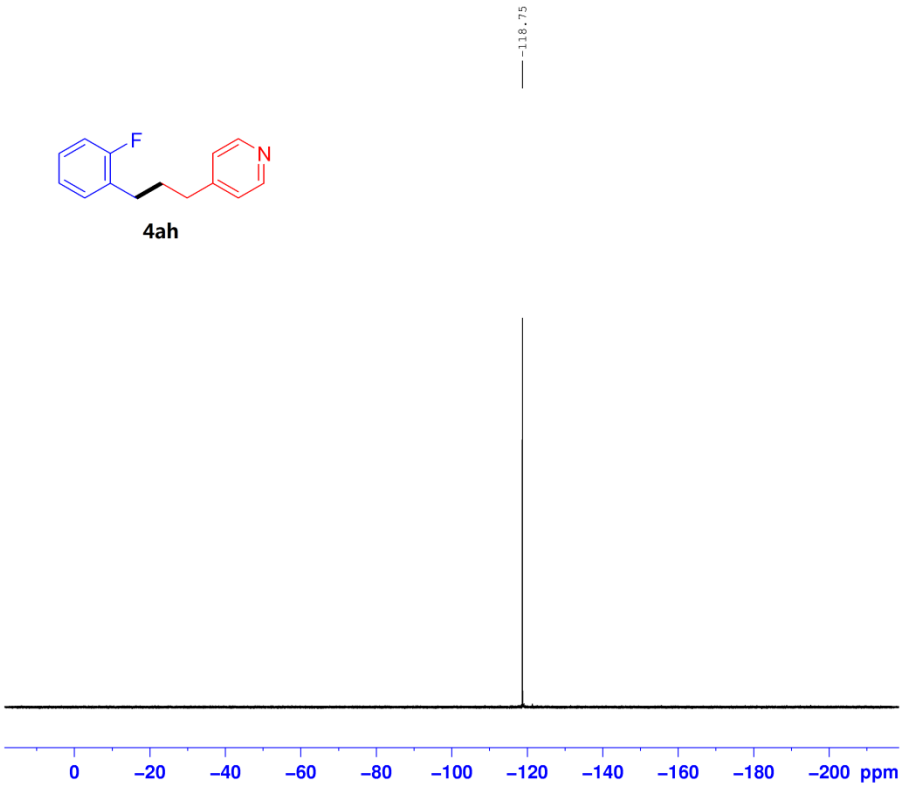
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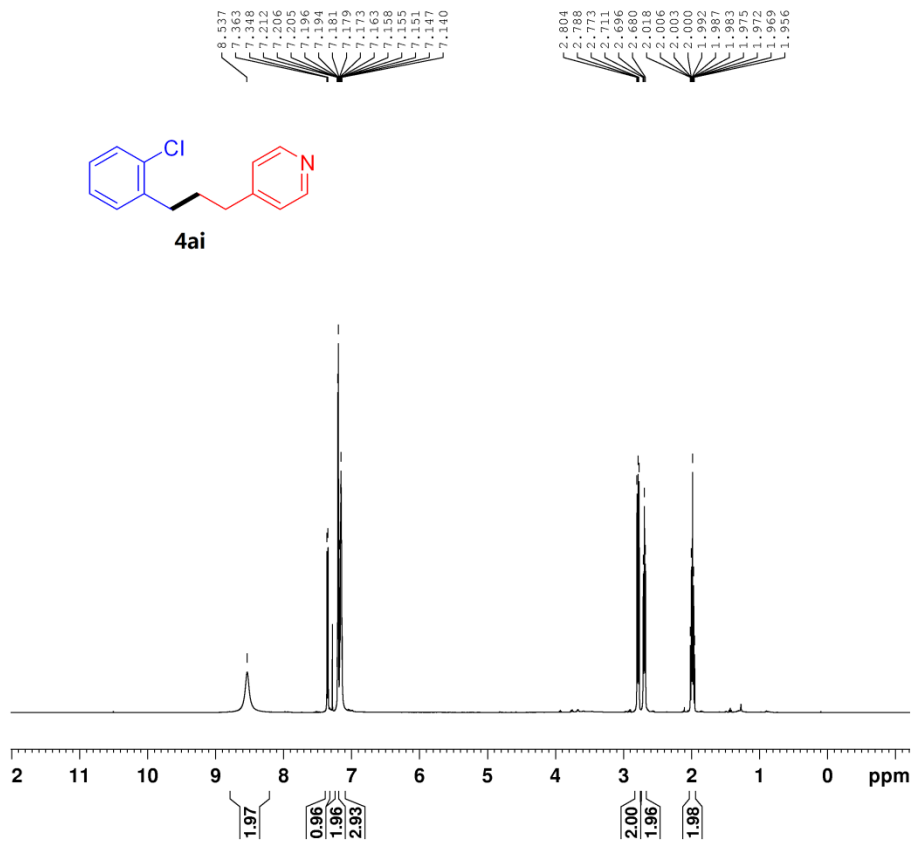
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7.173
7.163
7.158
7.155
7.151
7.147
7.140
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2.696
2.680
2.018
2.006
2.003
2.000
1.992
1.987
1.983
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1.972
1.969
1.956
Cl
N
4ai
2
11
10
9
8
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1.96
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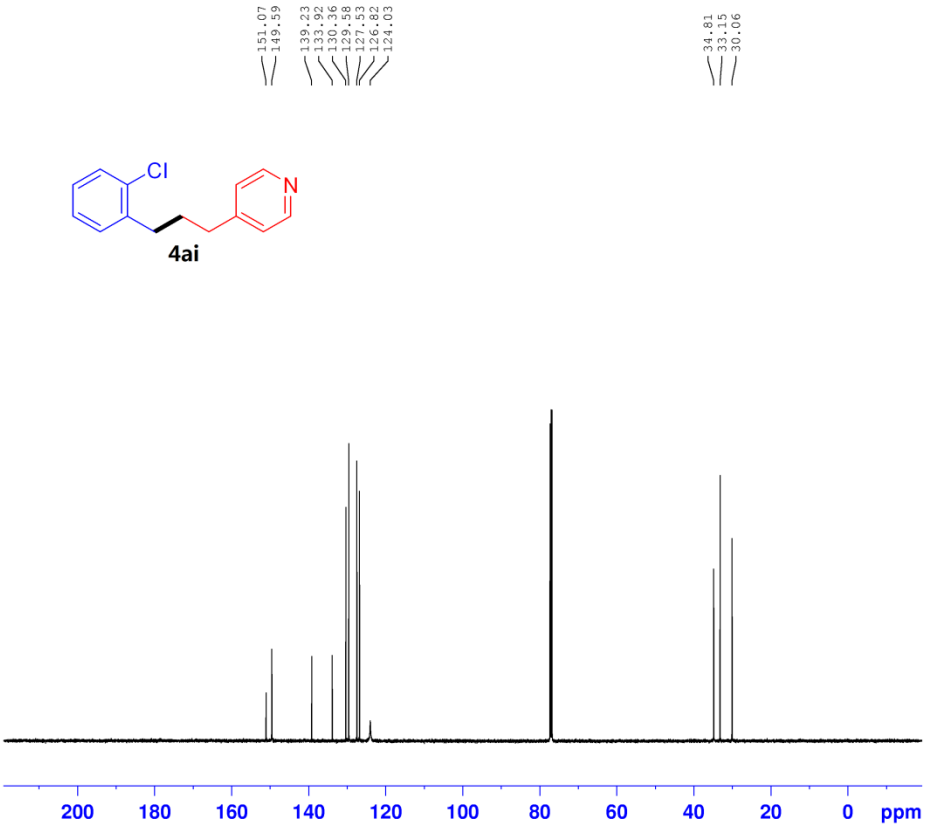
1.96
1.98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129.58
127.53
126.82
124.03
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30.06
Cl
N
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120
100
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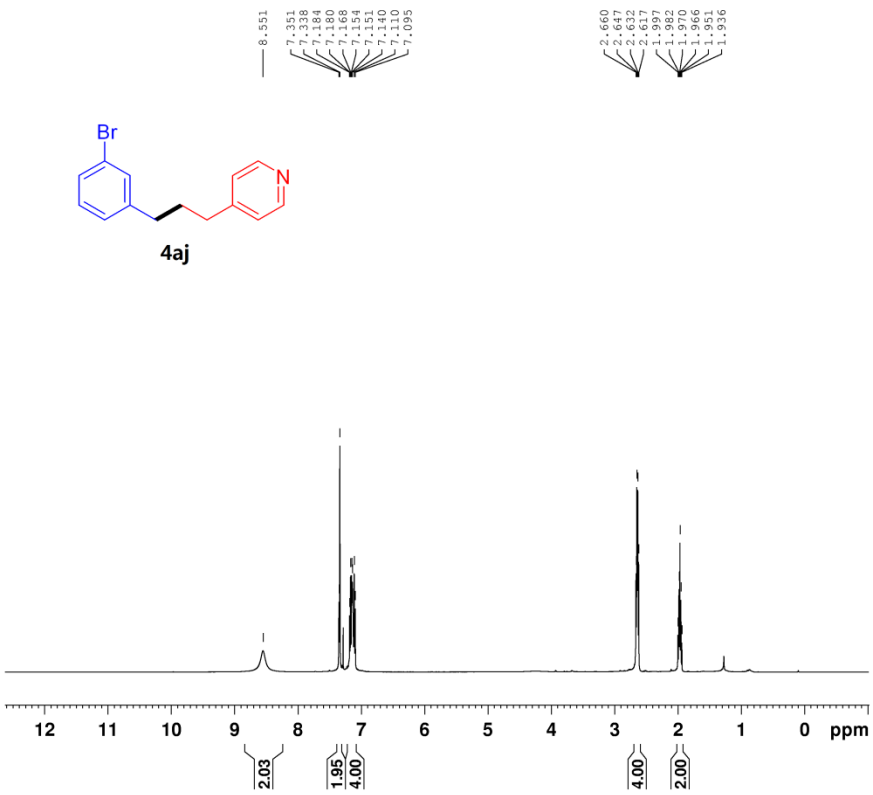
60
40
20
0
ppm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7.151
7.140
7.110
7.095
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2.647
2.632
2.617
1.997
1.982
1.970
1.966
1.951
1.936
Br
N
4aj
12
11
10
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8
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6
5
4
3
2
1
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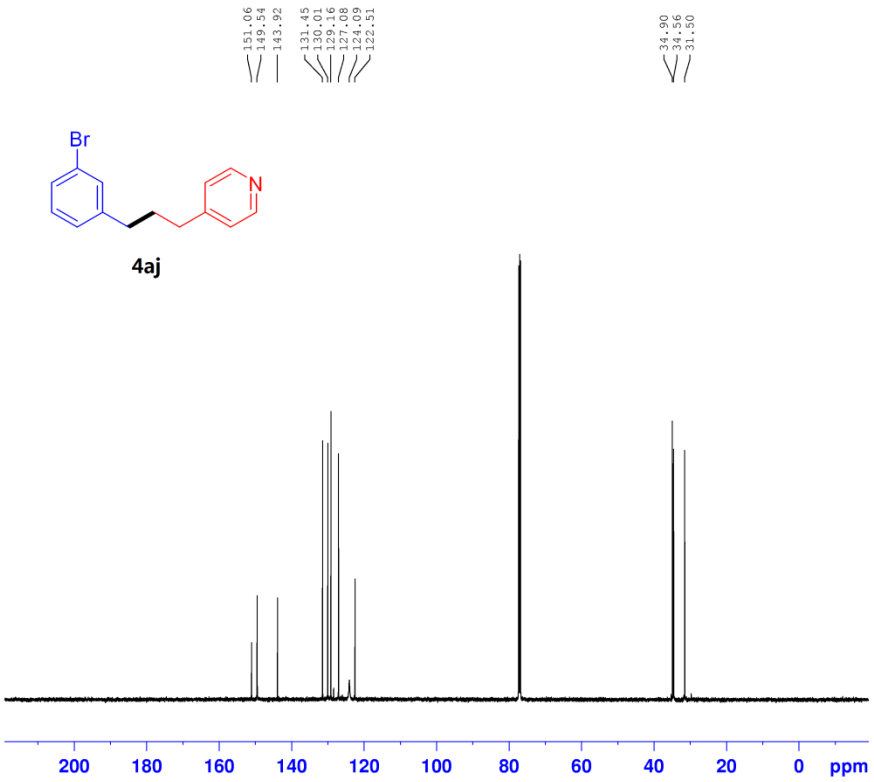
ppm
2.03
1.95
4.00
4.00
2.00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122.51
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Br
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120
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40
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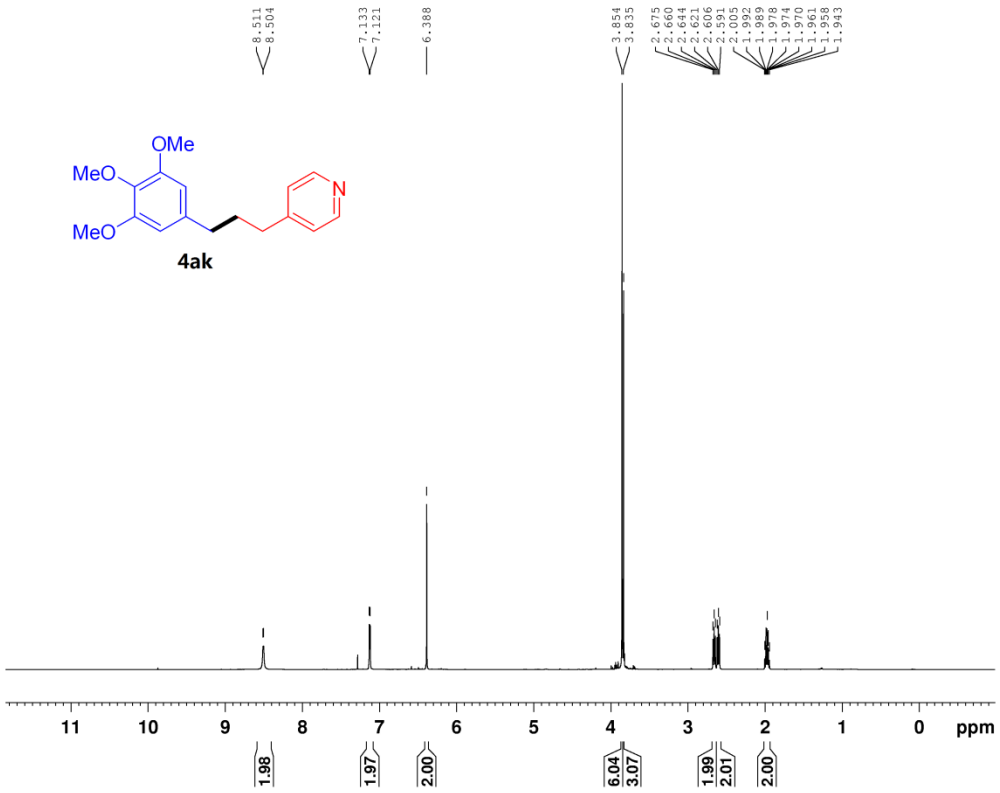
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2.644
2.621
2.606
2.591
2.055
1.993
1.989
1.978
1.974
1.970
1.961
1.958
1.943
OMe
MeO
MeO
N
4ak
11
10
9
8
7
6
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6.04
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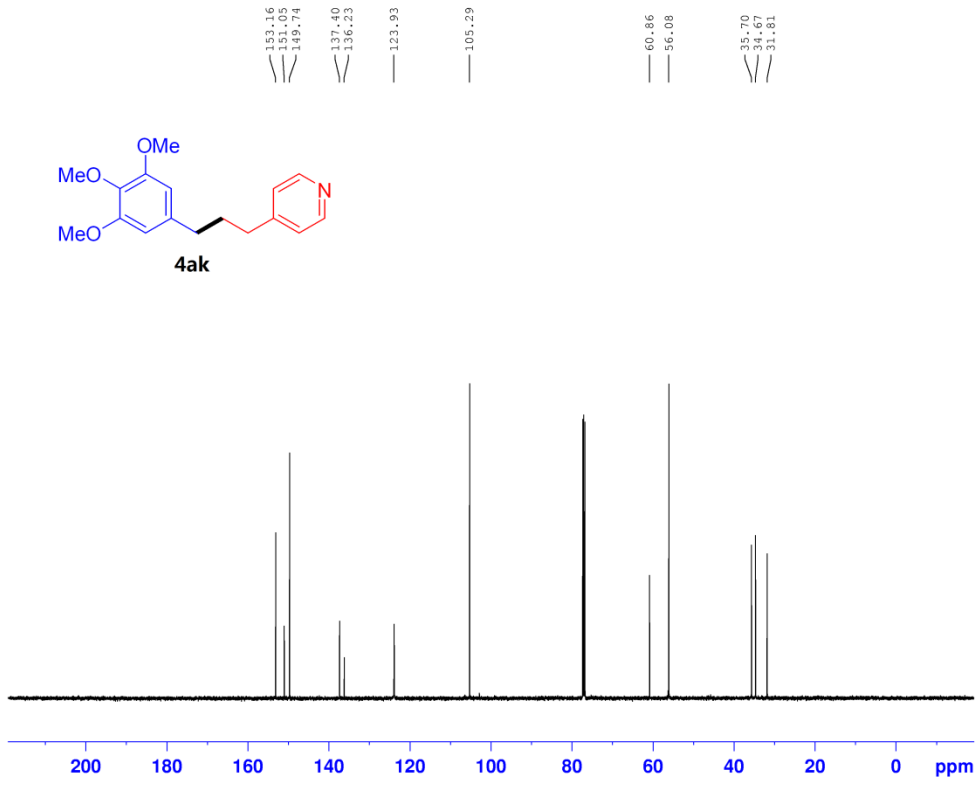
2.01
2.00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35.70
34.67
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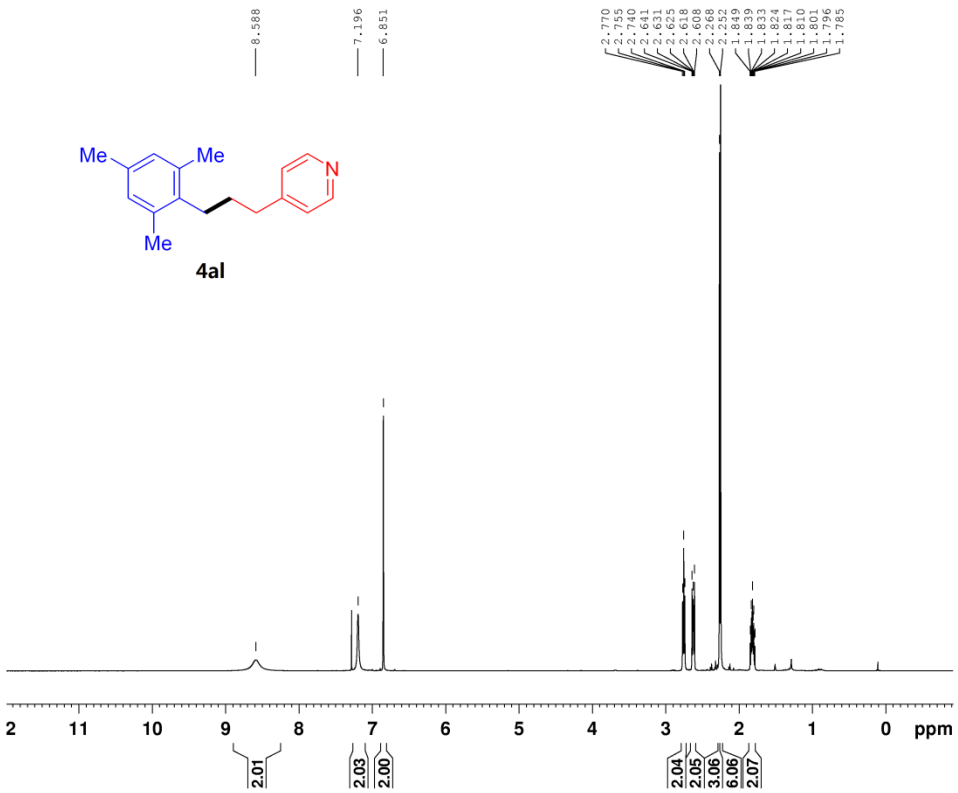
MeO
MeO
N
4ak
200
180
160
140
120
100
80
60
40
20
0
ppm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2.252
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1.839
1.833
1.824
1.817
1.810
1.801
1.796
1.785
Me
Me
Me
N
4al
2
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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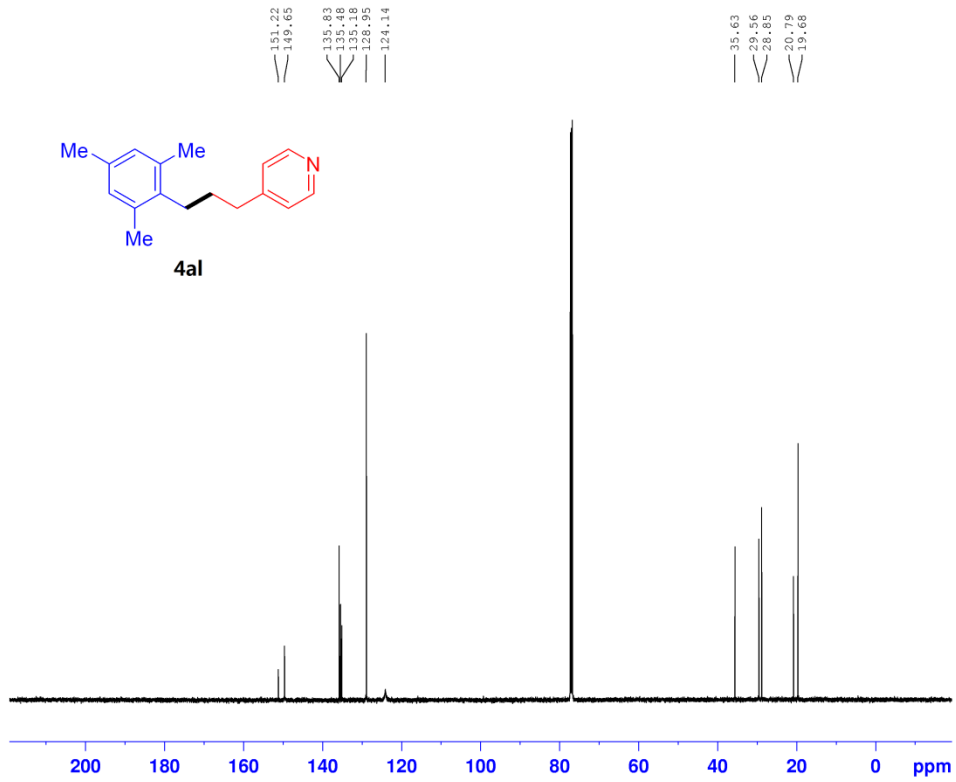
2.03
2.00
2.04
2.05
3.06
6.06
2.07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28.85
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Me
Me
N
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20
0
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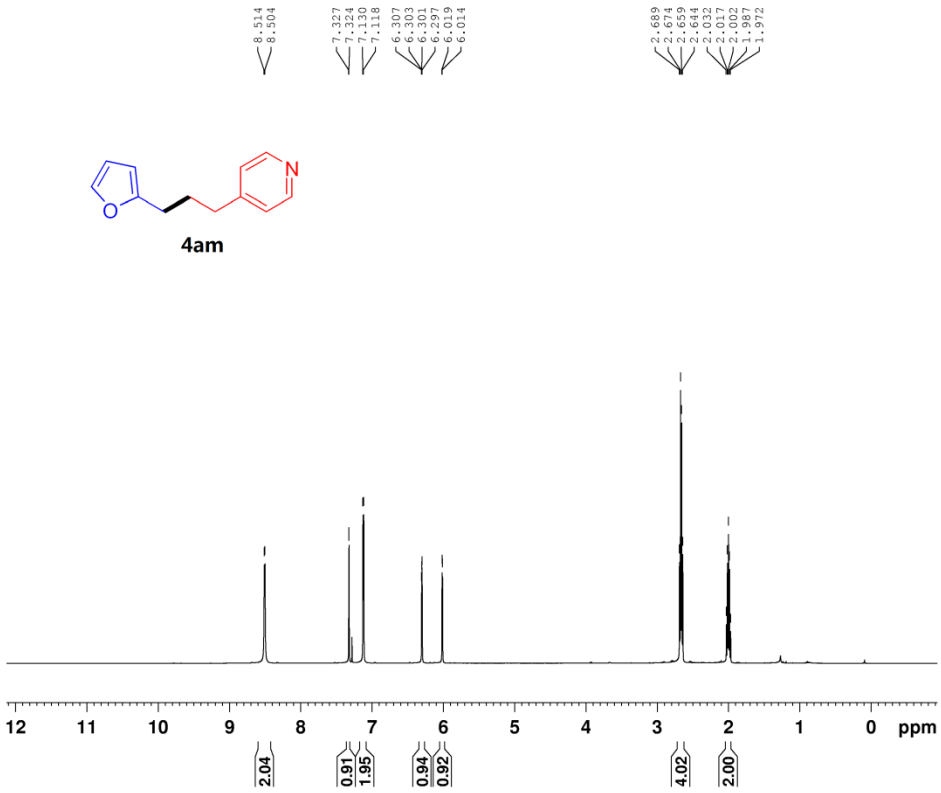
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2.002
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1.972
N
O
4am
12
11
10
9
8
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1.95
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0.92
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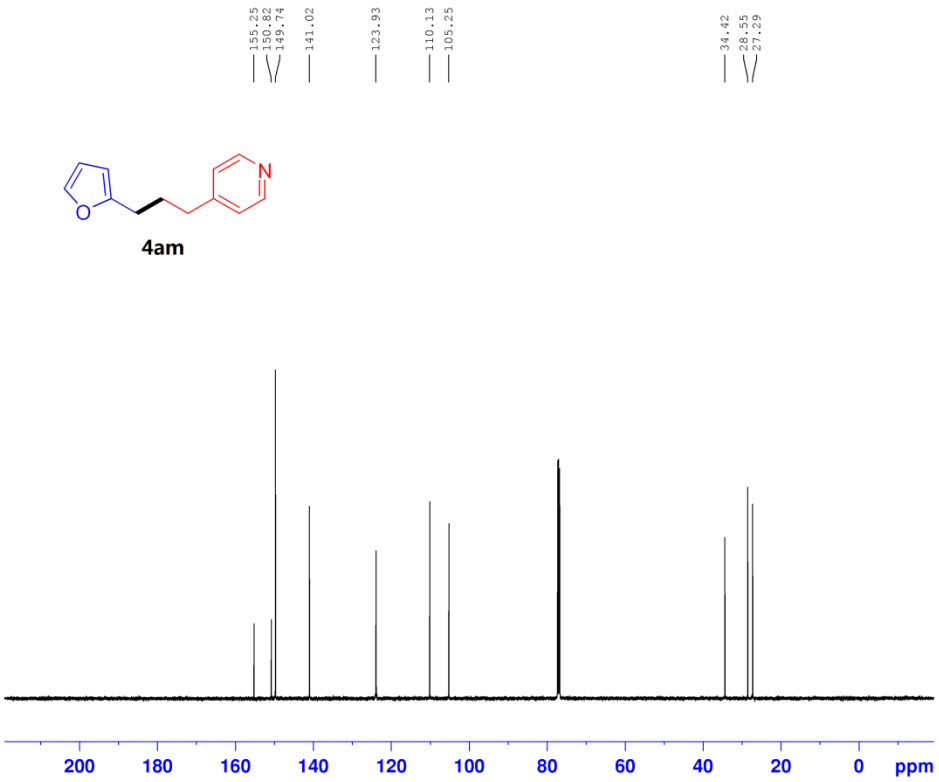
2.00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110.13
105.25
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140
120
100
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0
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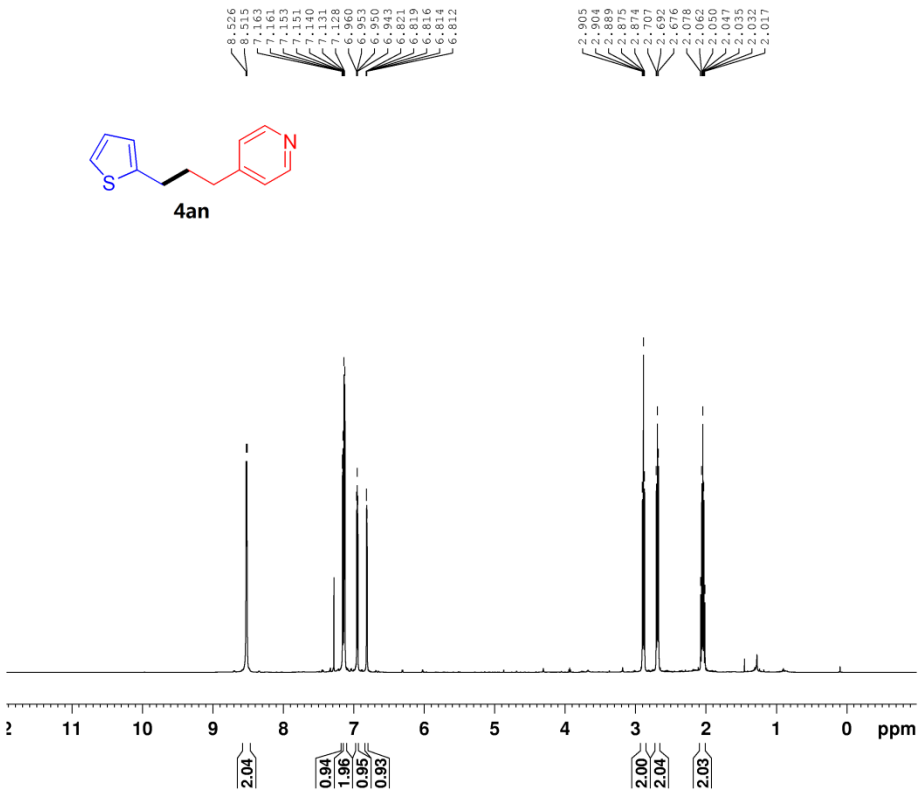
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6.943
6.821
6.819
6.816
6.814
6.812
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2.904
2.889
2.875
2.874
2.707
2.692
2.676
2.078
2.062
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2.047
2.035
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2.017
N
S
4an
11
10
9
8
7
6
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1
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ppm
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1.96
0.95
0.93
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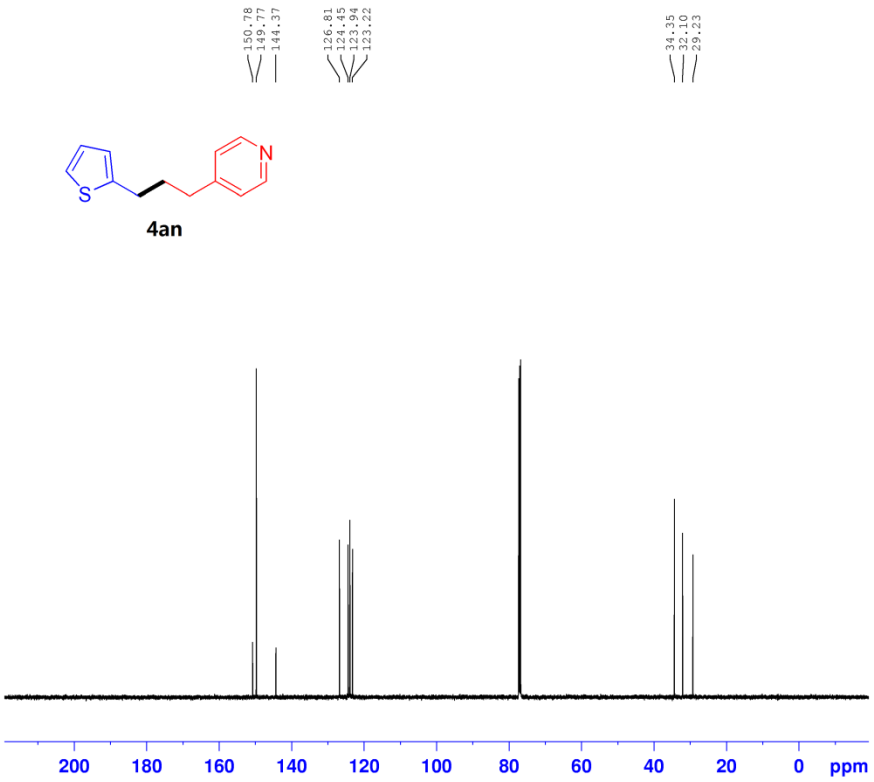
2.04
2.03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N
S
4an
200
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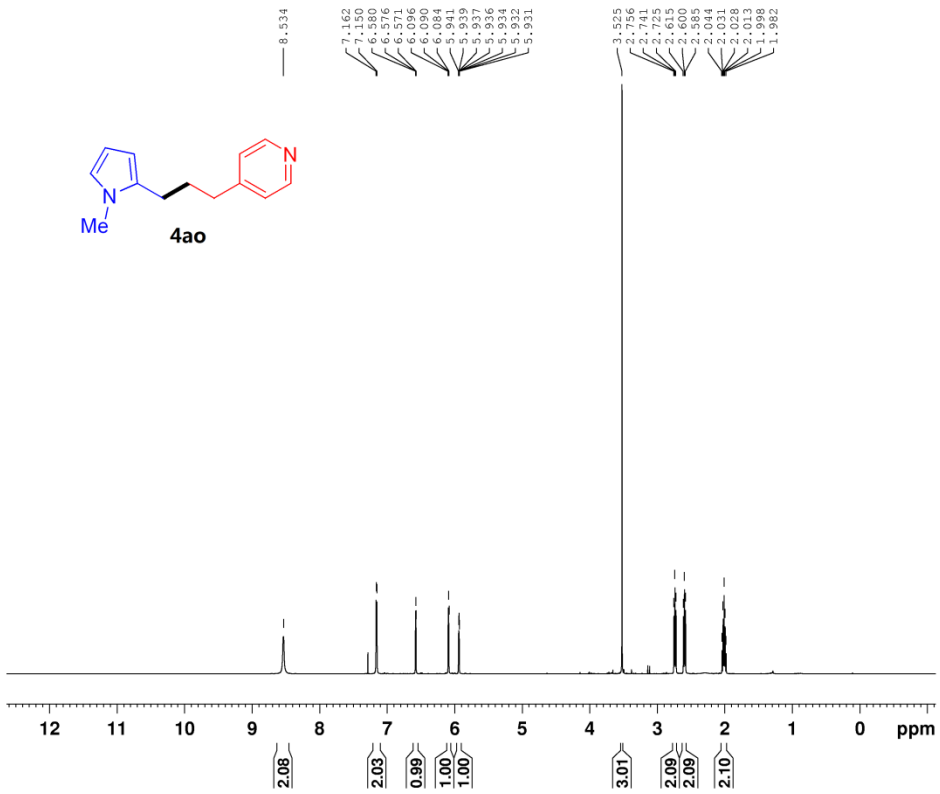
160
140
120
100
80
60
40
20
0
ppm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5.936
5.934
5.932
5.931
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2.741
2.725
2.615
2.600
2.585
2.044
2.031
2.028
2.013
1.998
1.982
N
N
Me
4ao
12
11
10
9
8
7
6
5
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ppm
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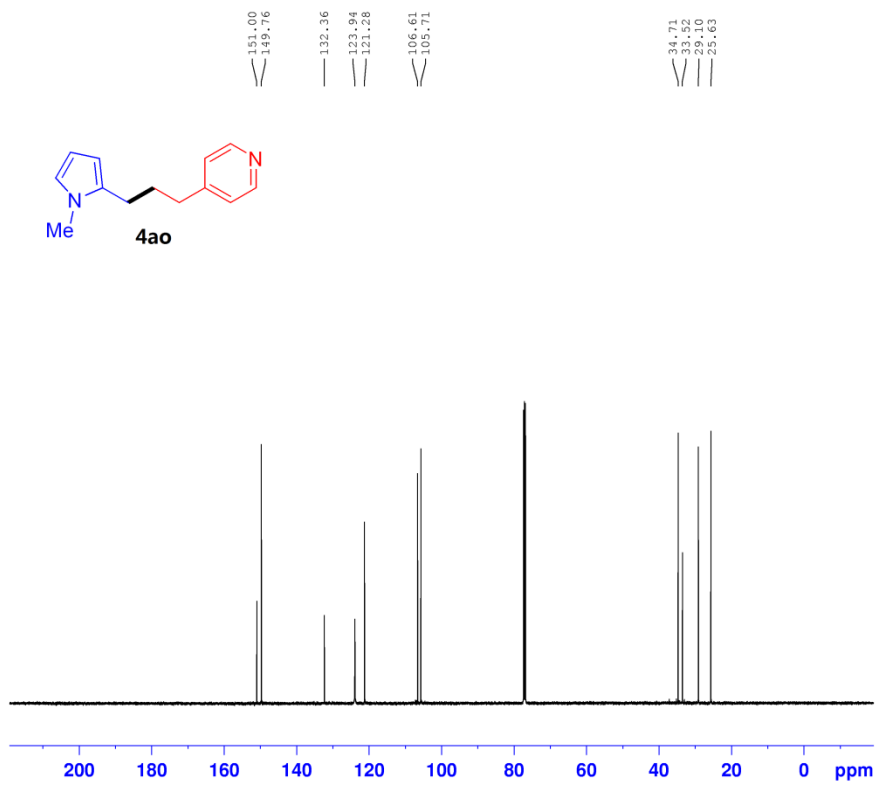
0.99
1.00
1.00
3.01
2.09
2.09
2.10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34.71
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29.10
25.63
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N
Me
4ao
200
180
160
140
120
100
80
60
40
20
0
ppm


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7.840
7.827
7.810
7.641
7.513
7.511
7.500
7.497
7.484
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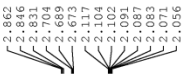
7.143
7.132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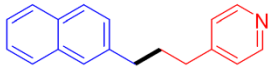
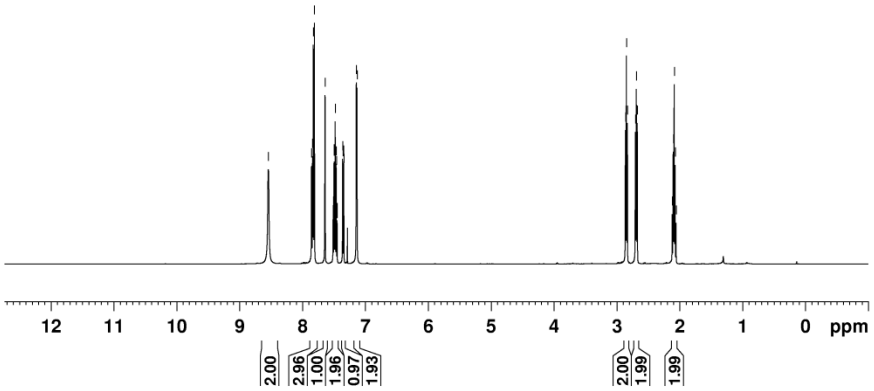

N

4ap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6
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ppm
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0.97
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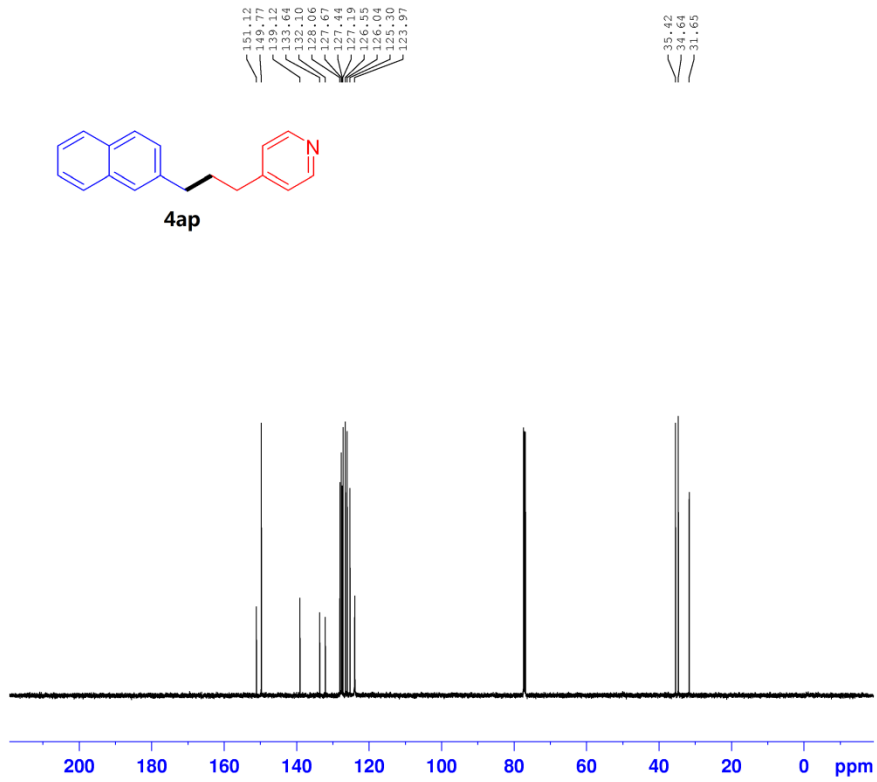
1.99
1.99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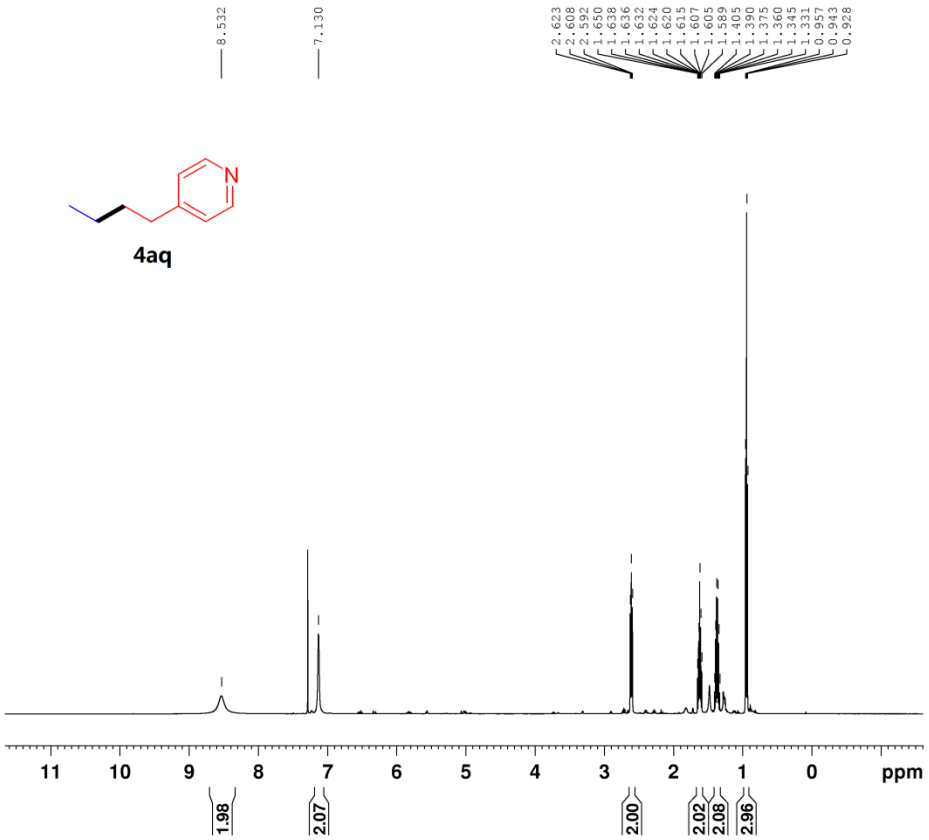
ppm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1.405
1.390
1.375
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0.928
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10
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2
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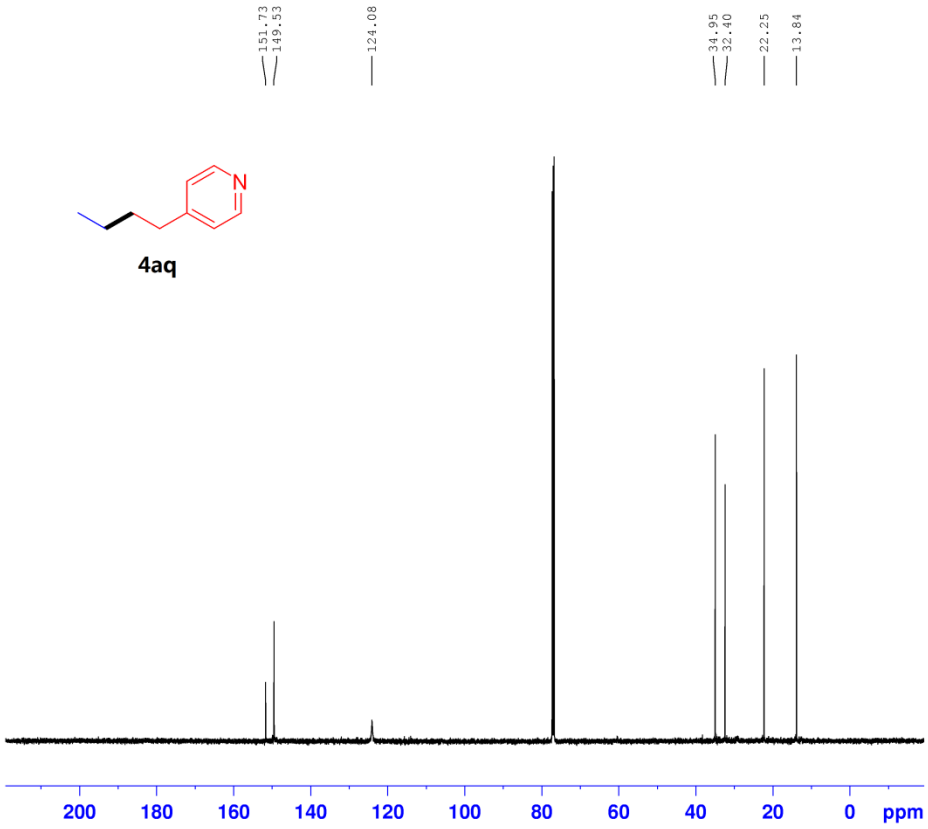
2.96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180
160
140
120
100
80
60
40
20
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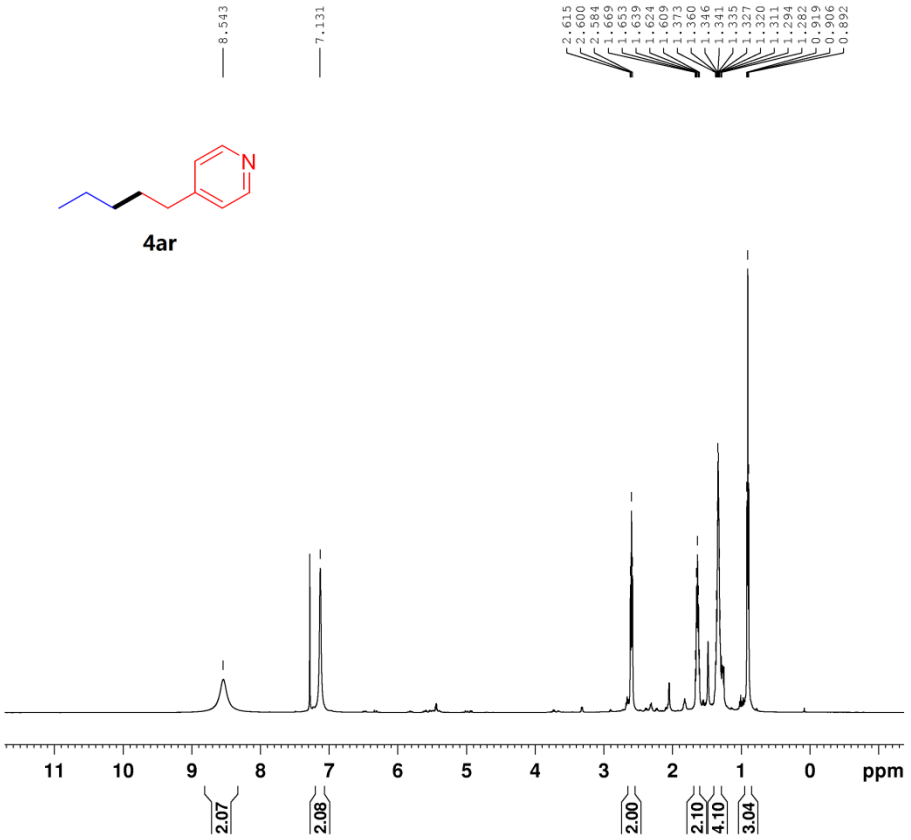
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1.320
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1.294
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0.906
0.892
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4ar
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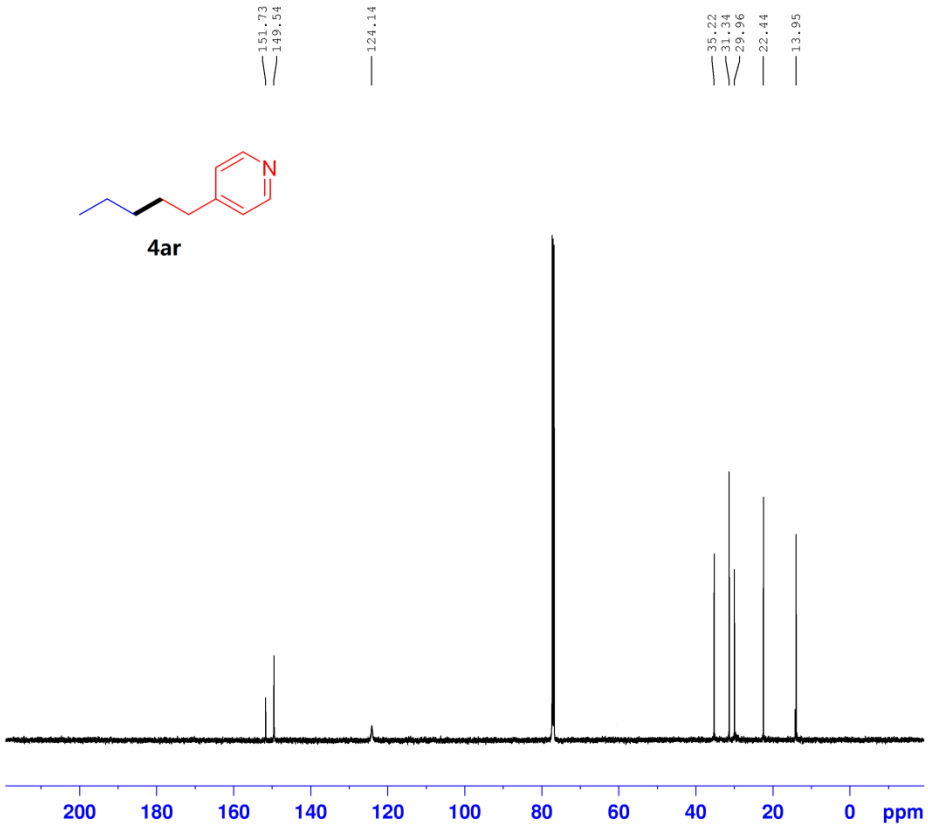
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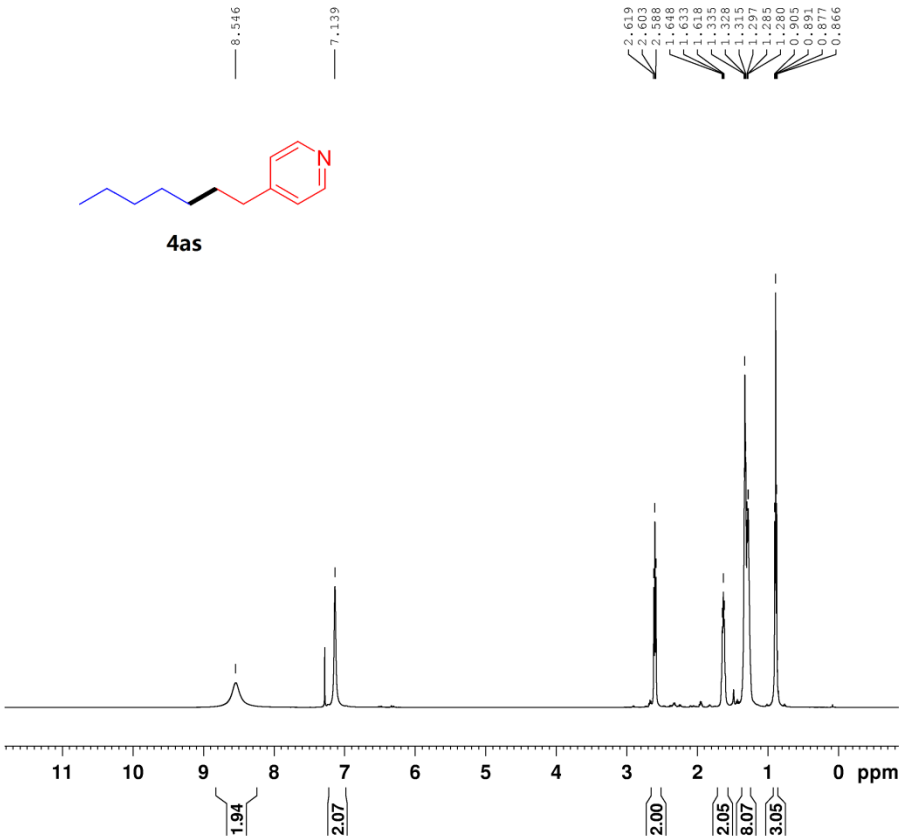
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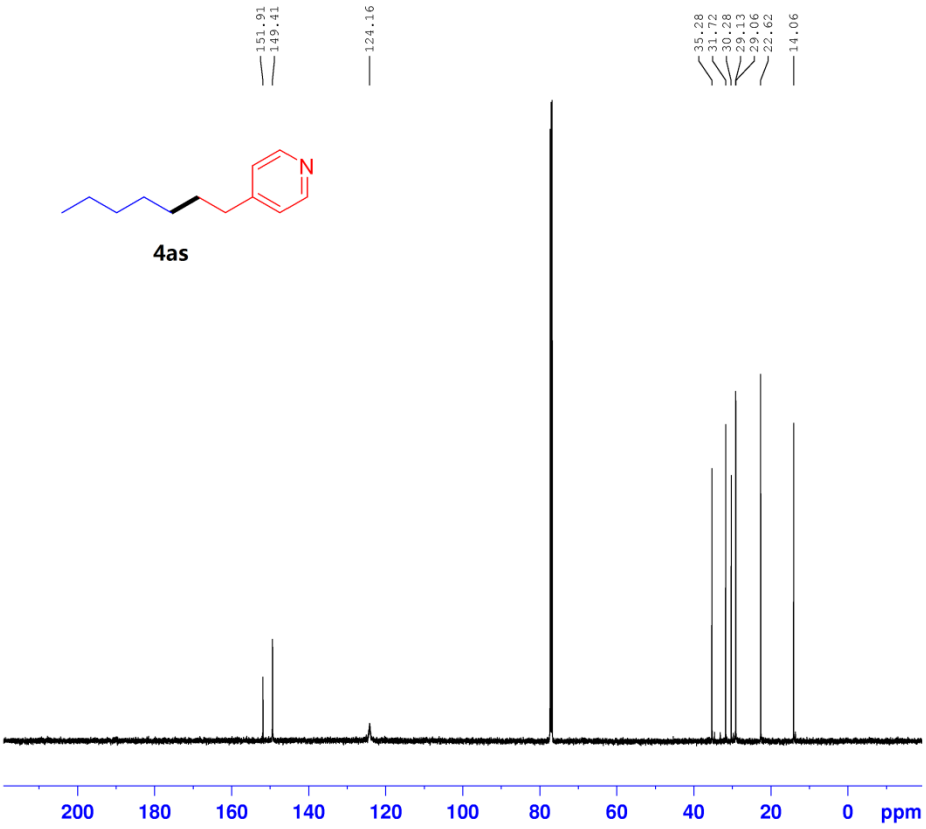
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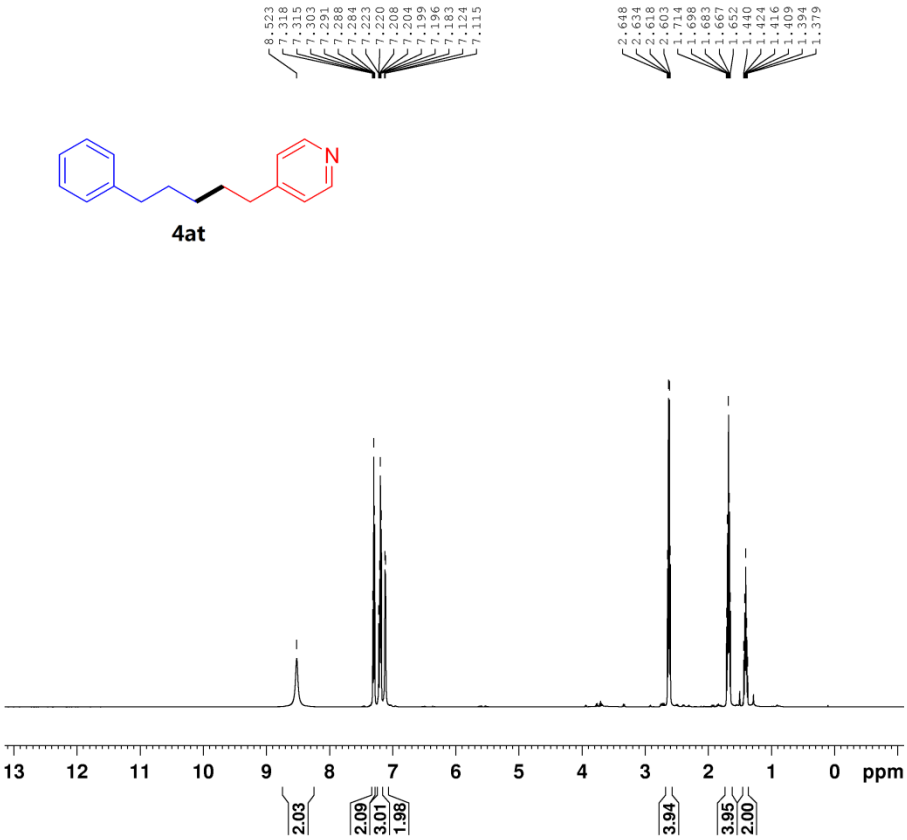
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8
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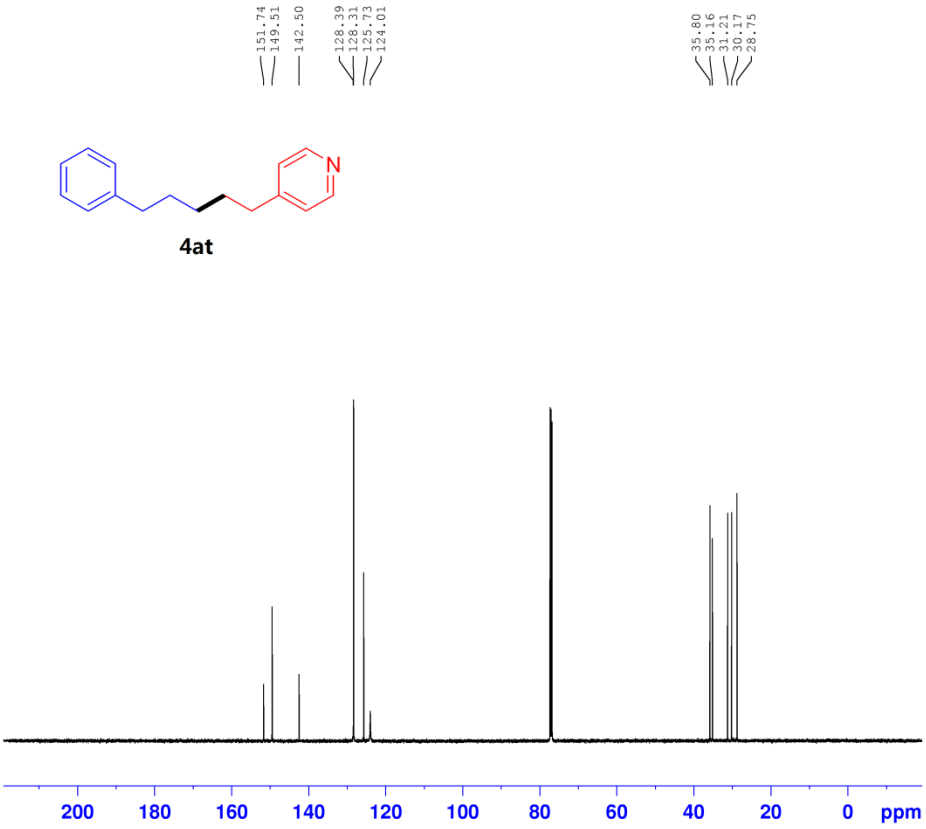
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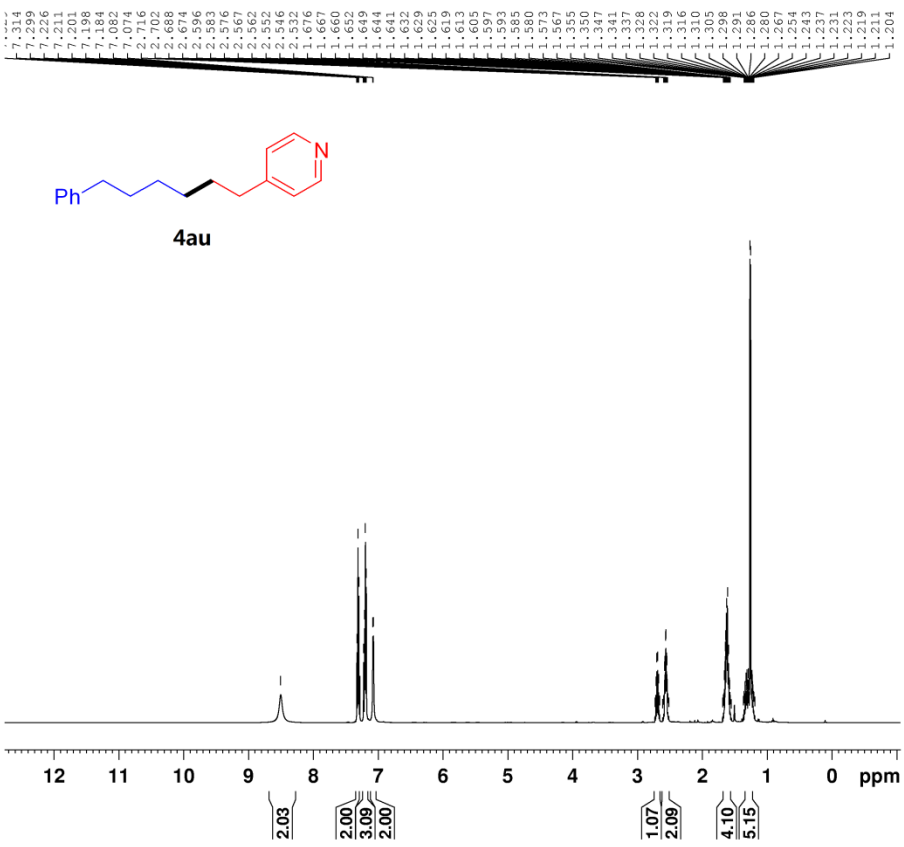
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2.552
2.546
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Ph
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11
10
9
8
7
6
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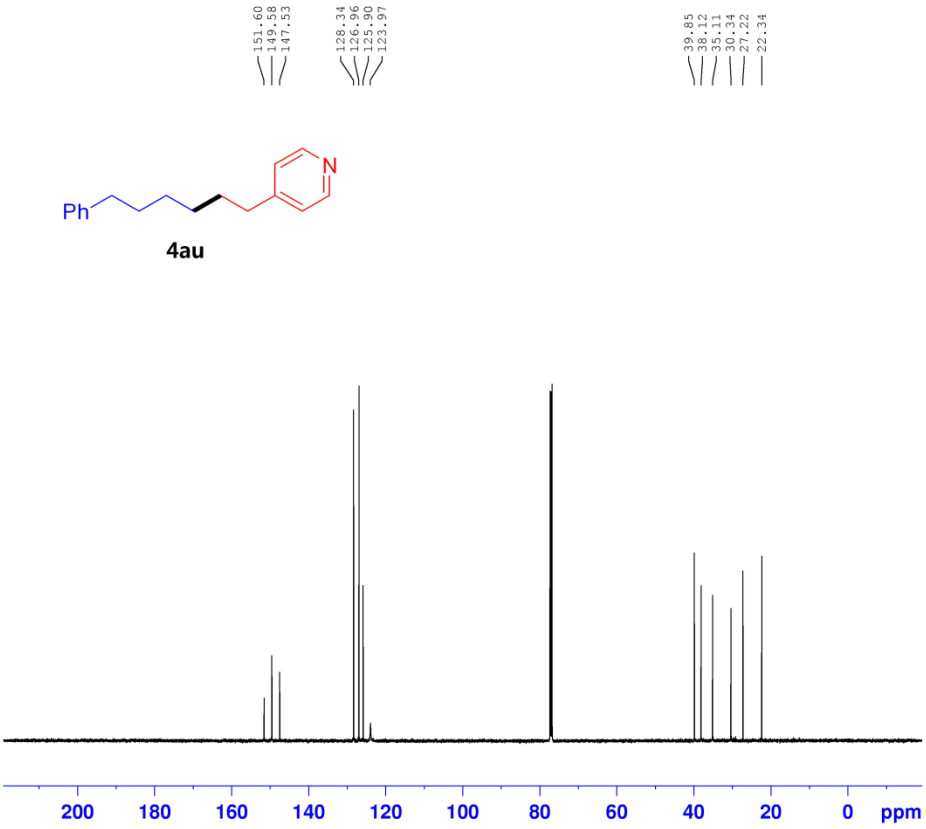
2.00
3.09
2.00
1.07
2.09
4.10
5.15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Ph
4au
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120
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40
20
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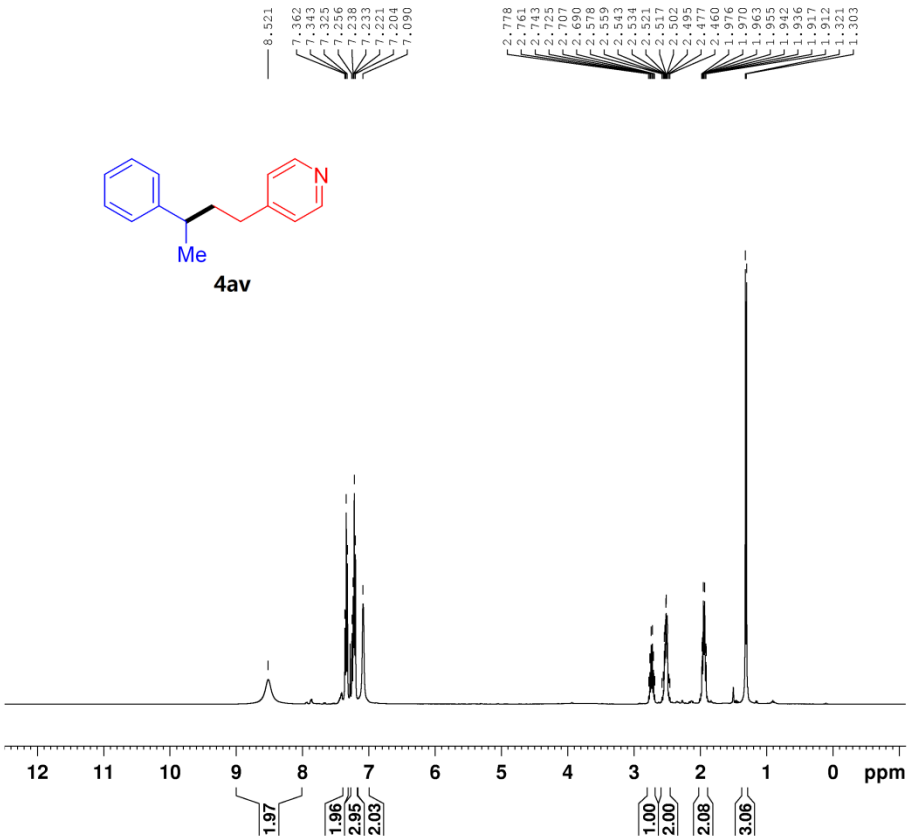
ppm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2.707
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2.543
2.534
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1.303
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Me
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11
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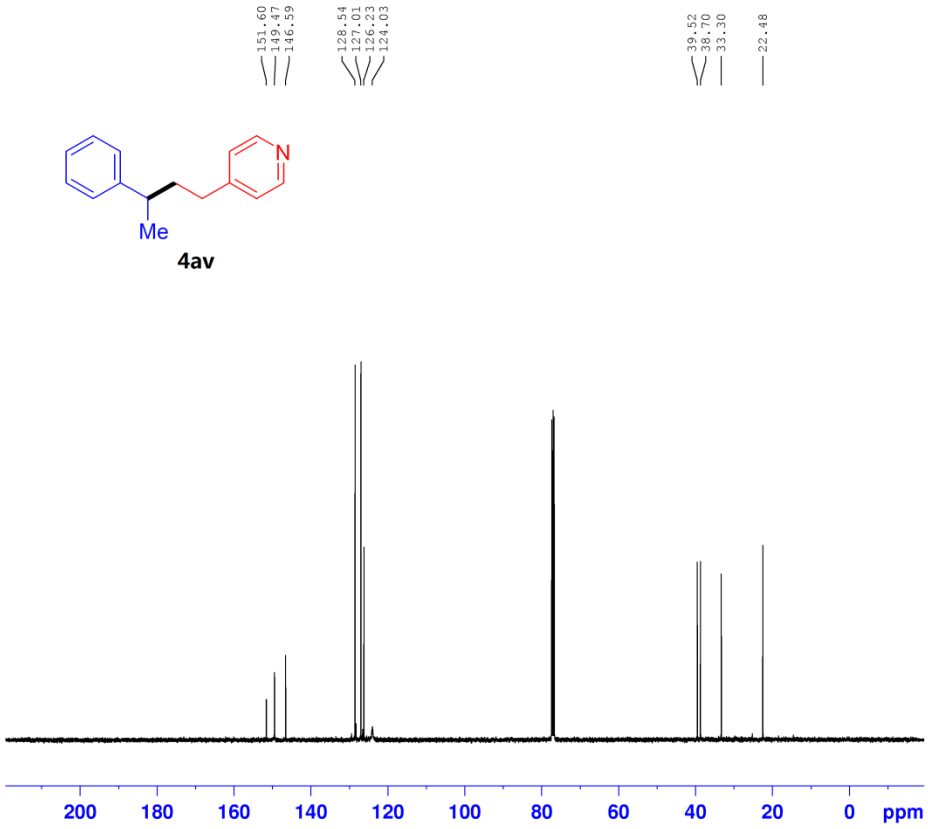
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40
20
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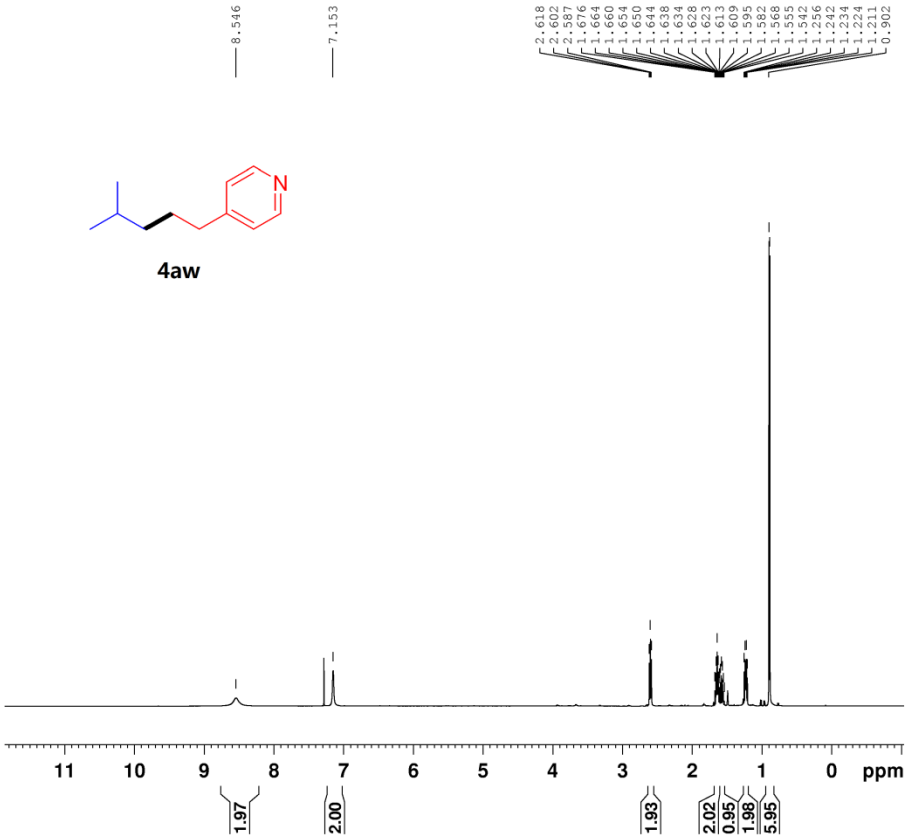
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1.634
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1.609
1.595
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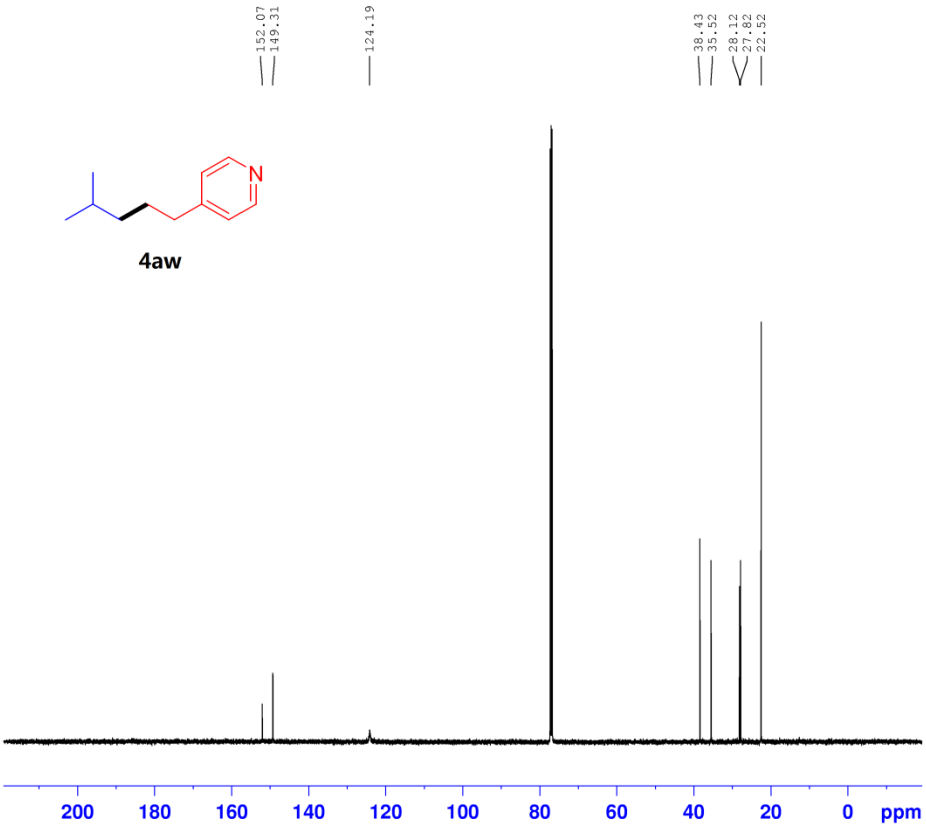
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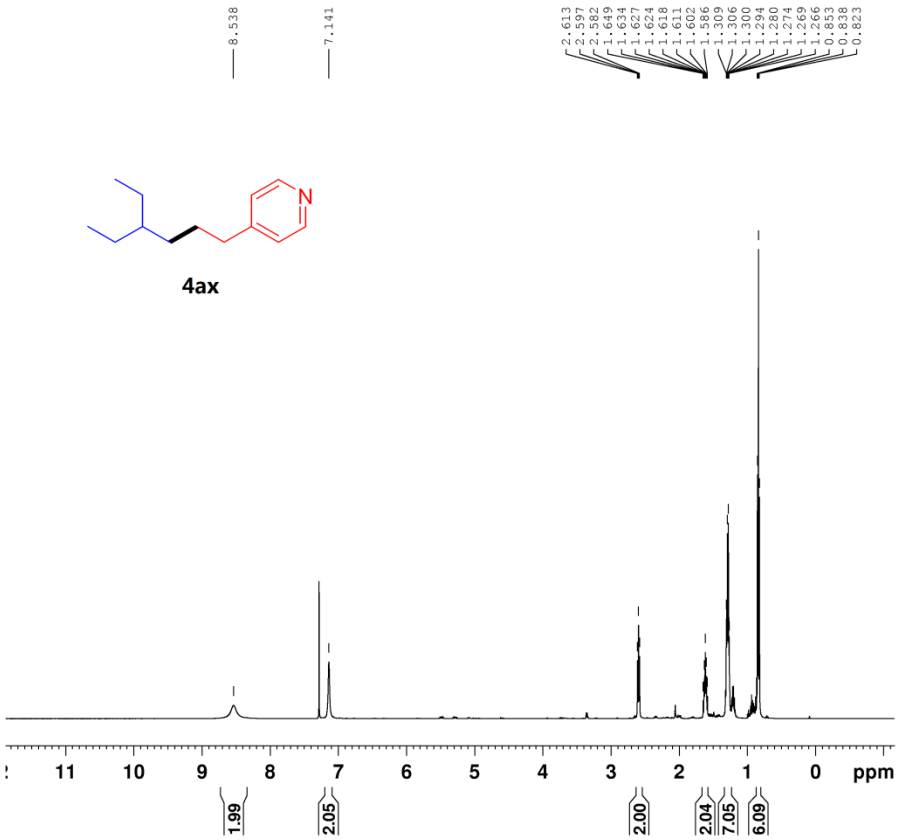
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0.823
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10
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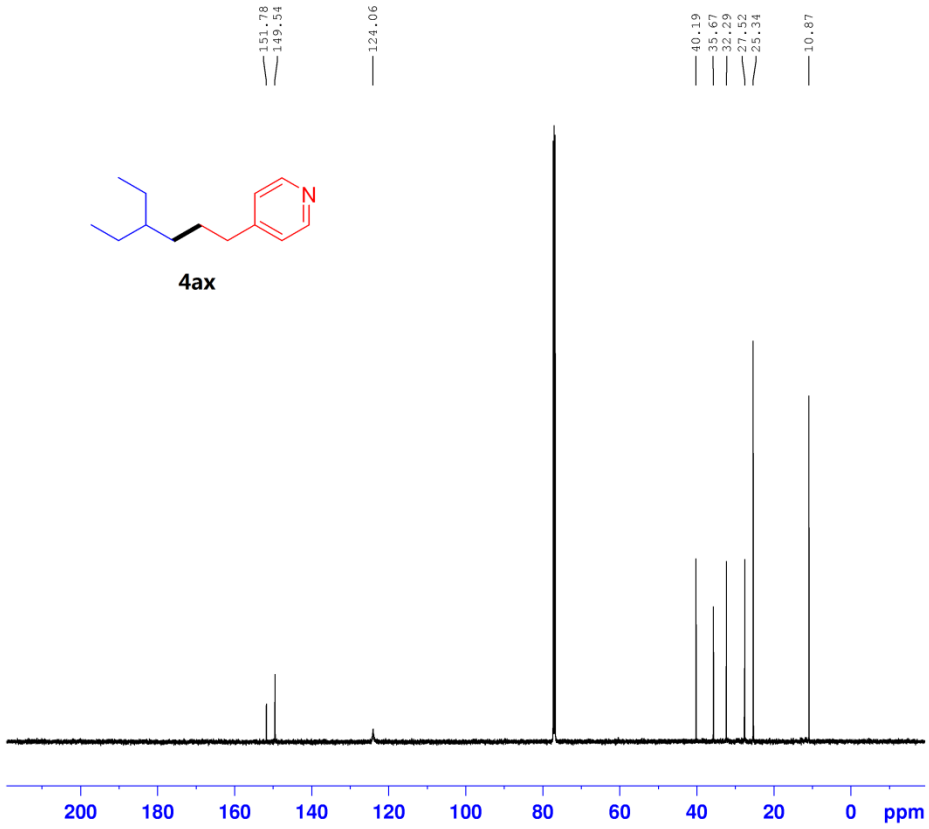
6.09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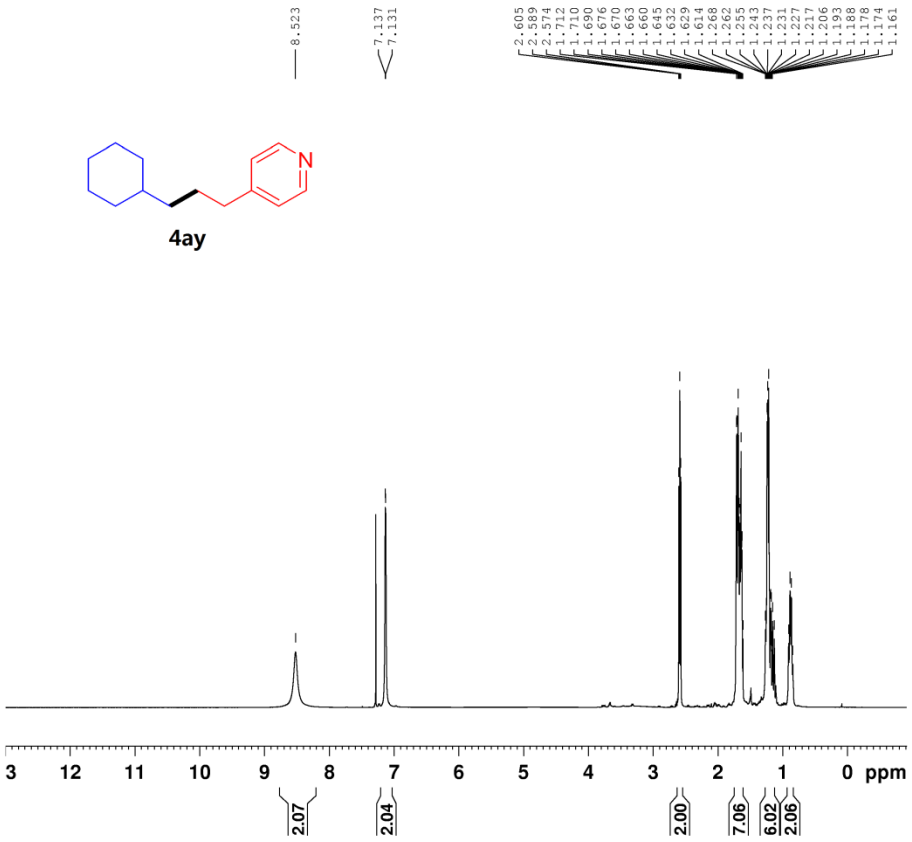
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1.237
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1.227
1.217
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1.193
1.188
1.178
1.174
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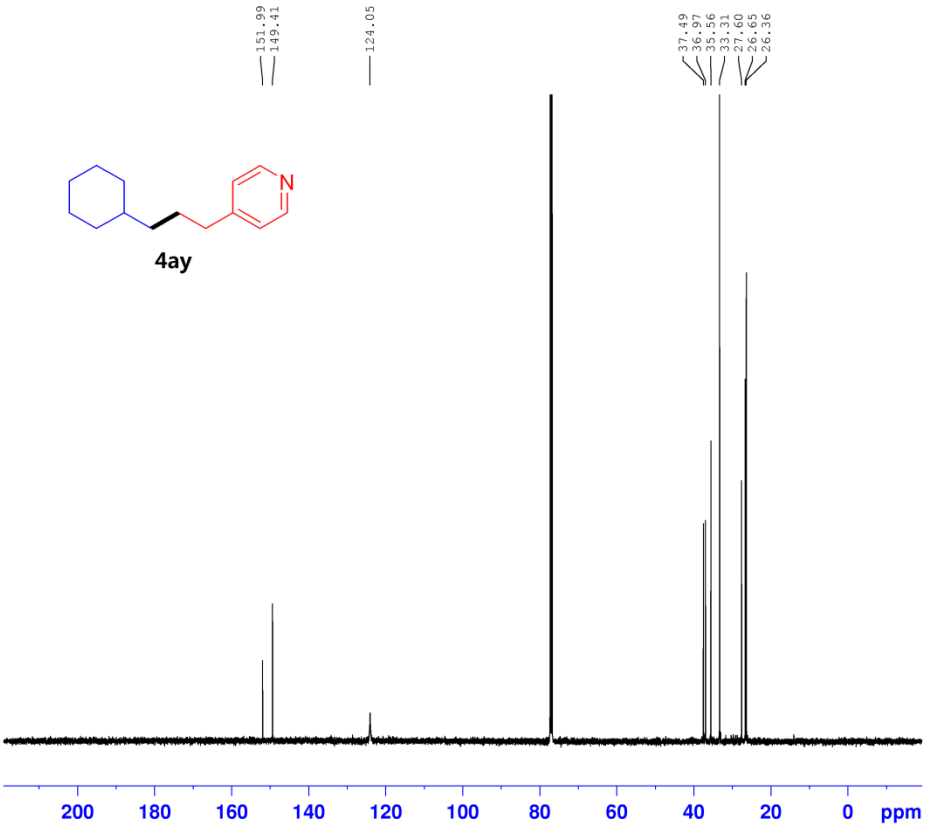
2.04
2.00
7.06
6.02
2.06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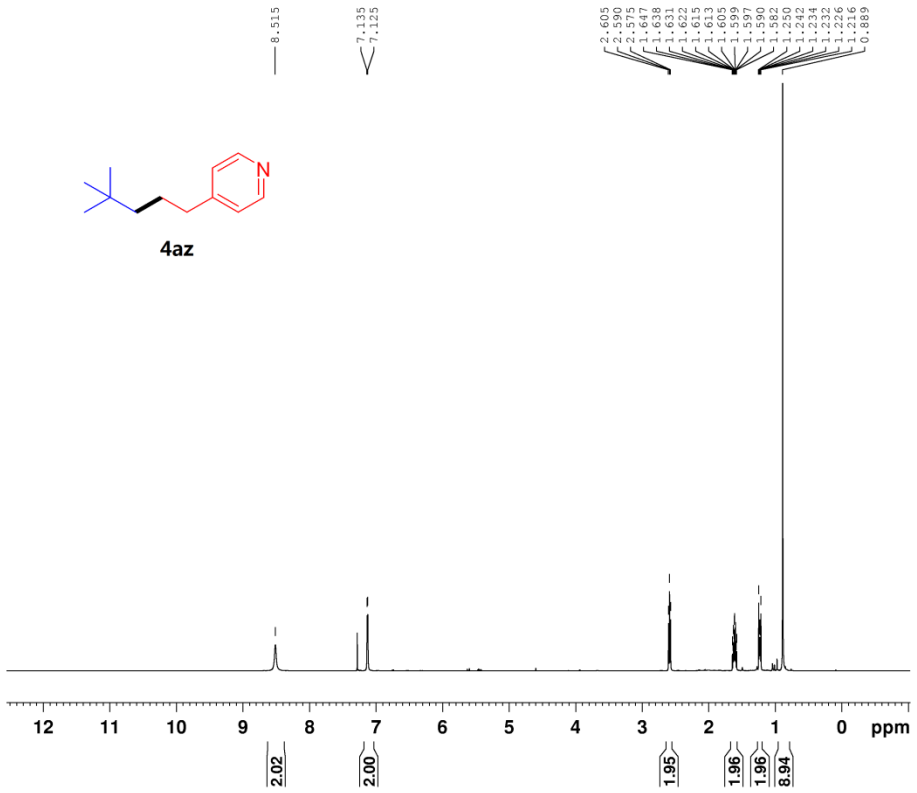
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11
10
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3
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2.00
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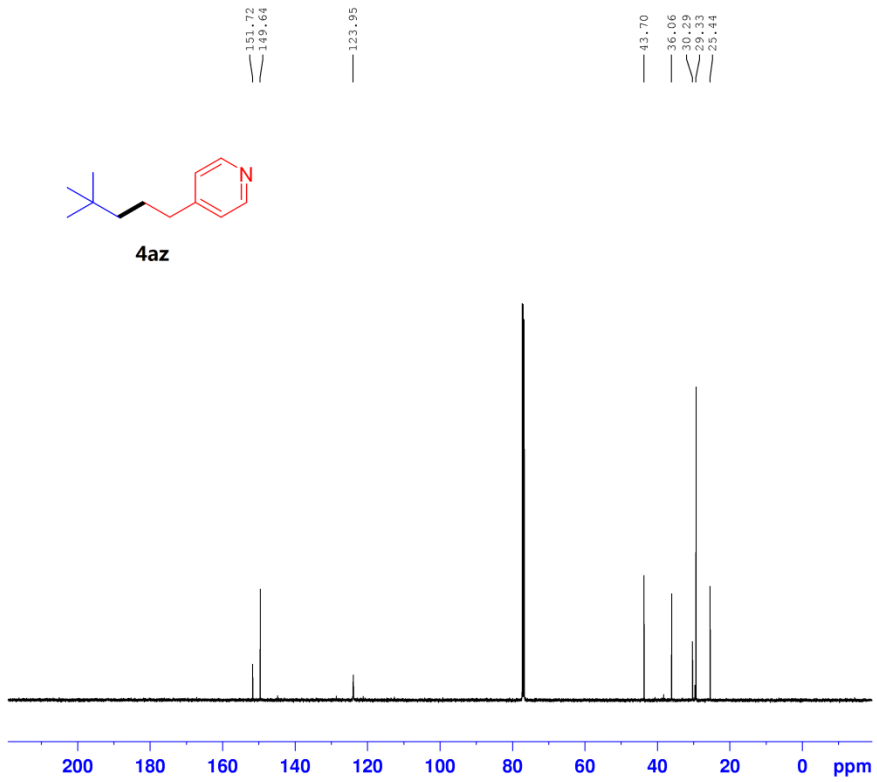
1.96
8.94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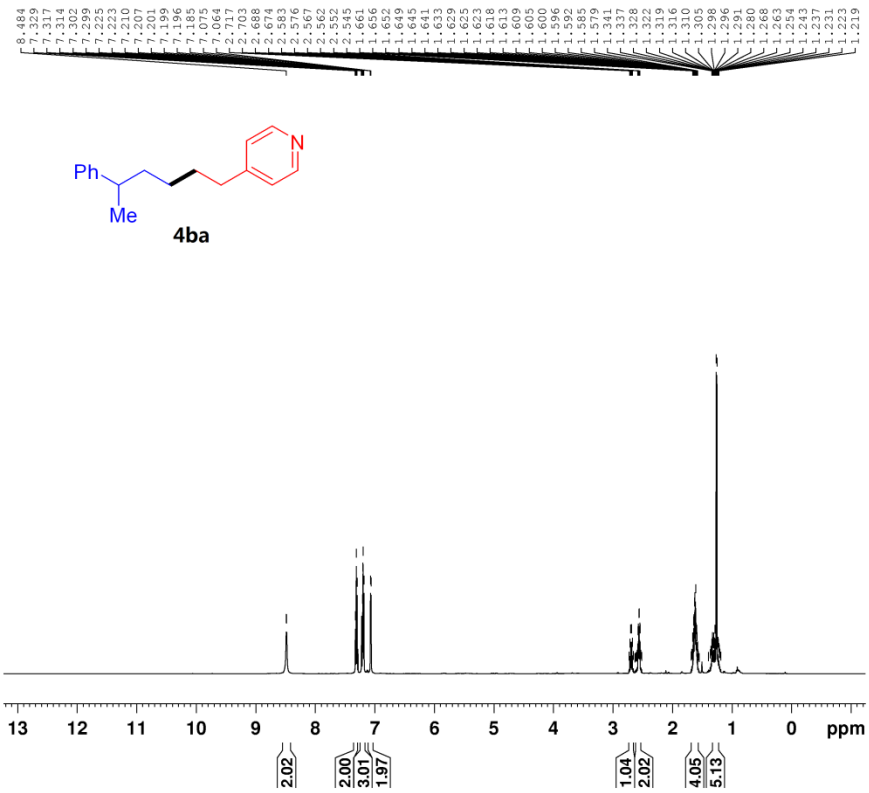
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1.231
1.223
1.219
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Me
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6
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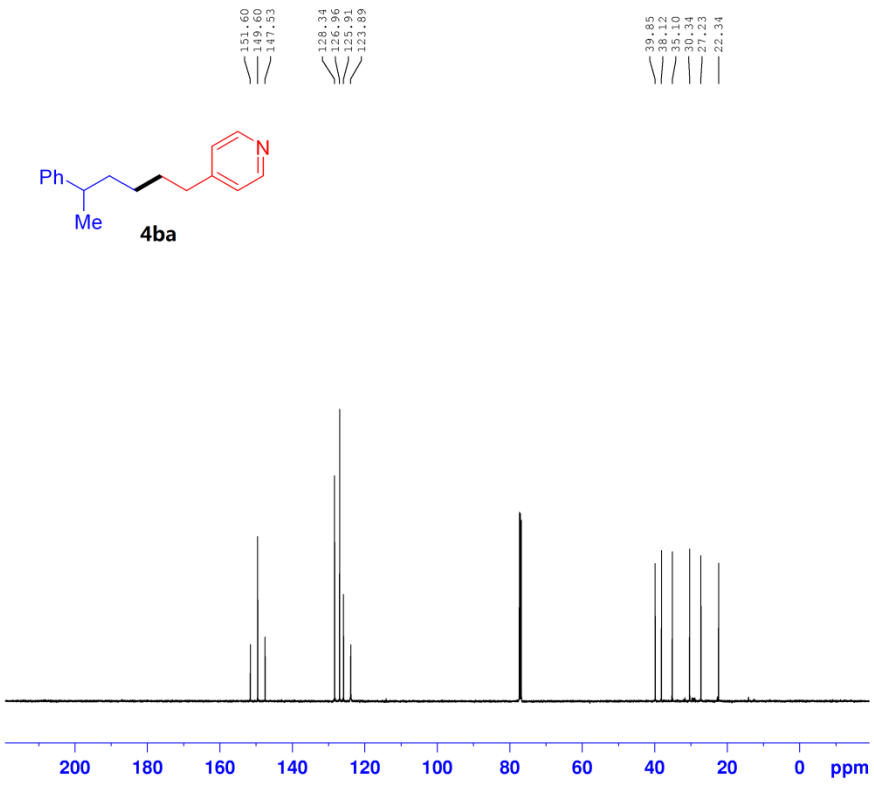
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Ph
Me
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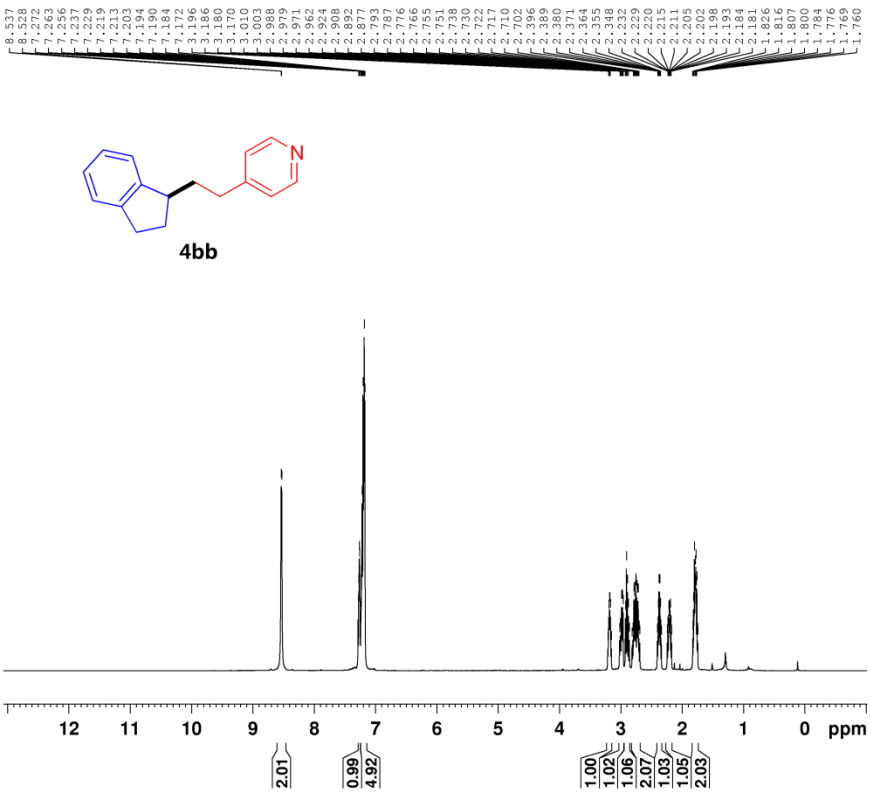
ppm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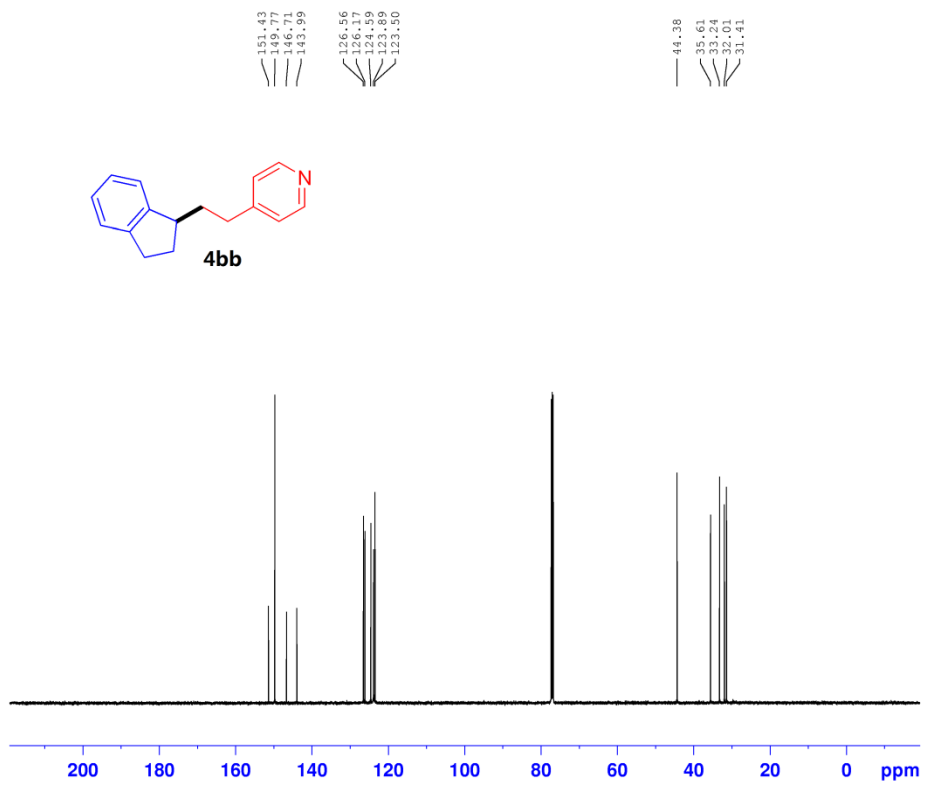
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120
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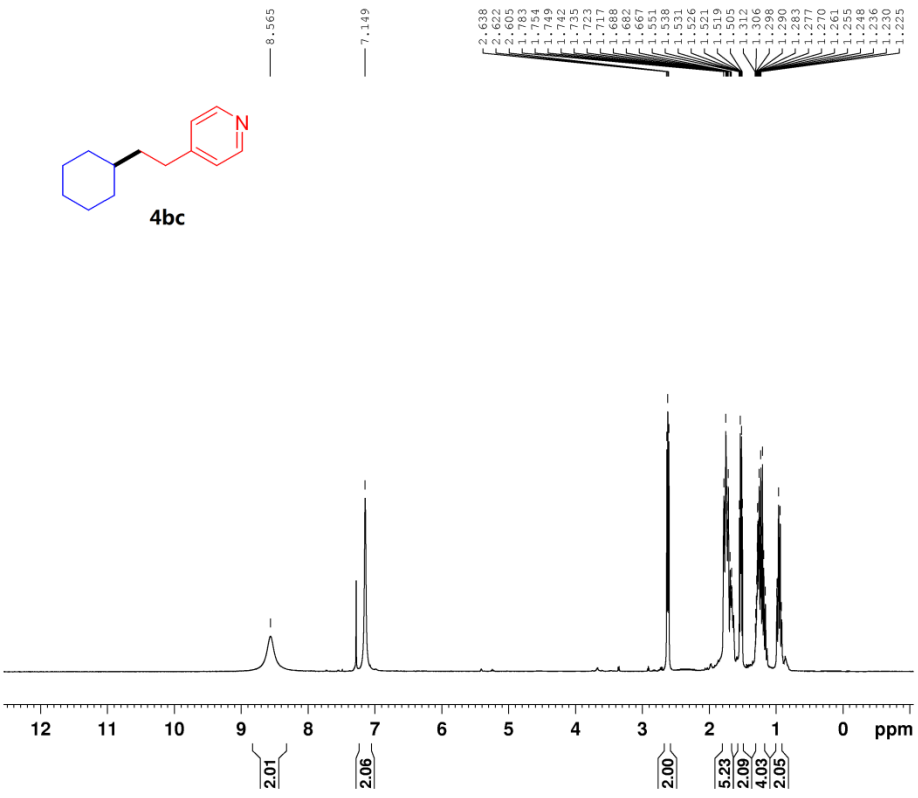
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1.283
1.277
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1.261
1.255
1.248
1.236
1.230
1.225
N
4bc
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11
10
9
8
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ppm
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2.00
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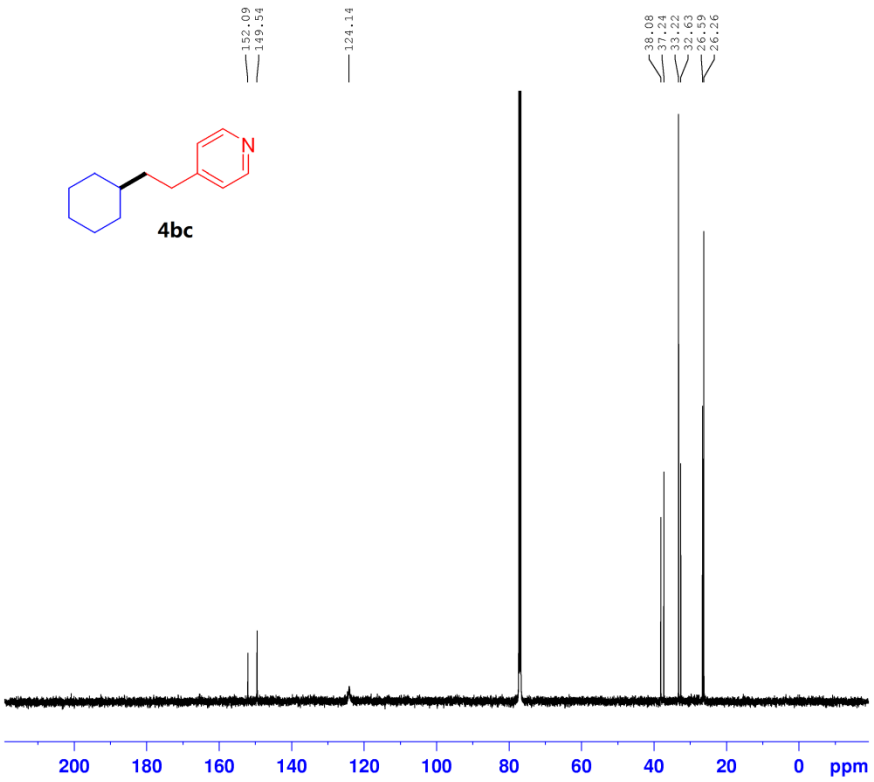
4.03
2.05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26.26
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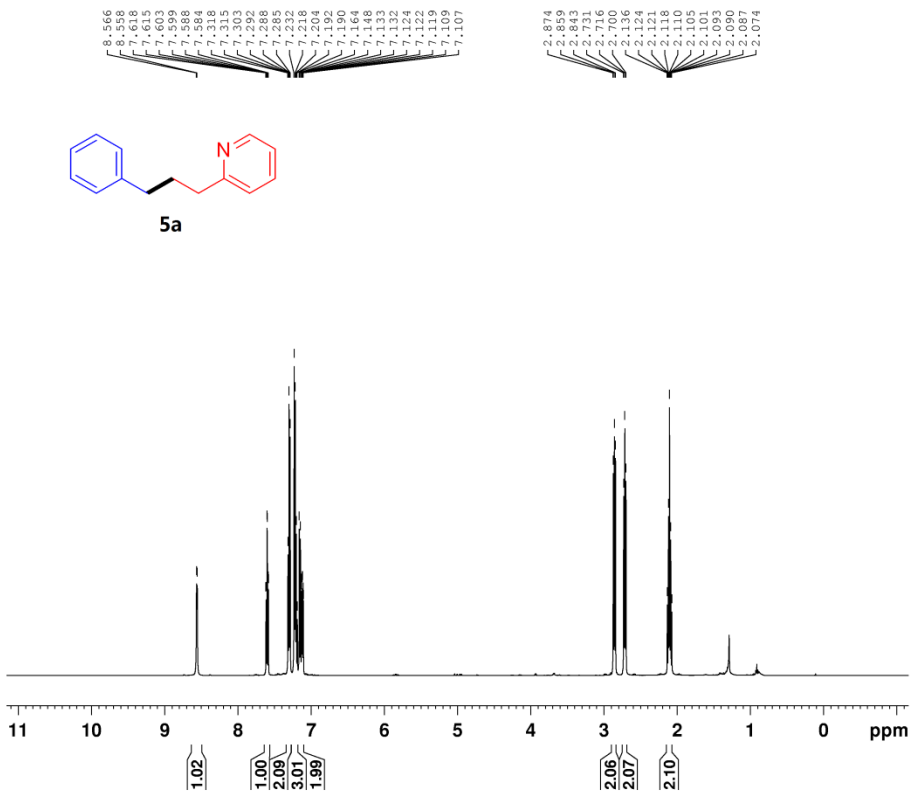
ppm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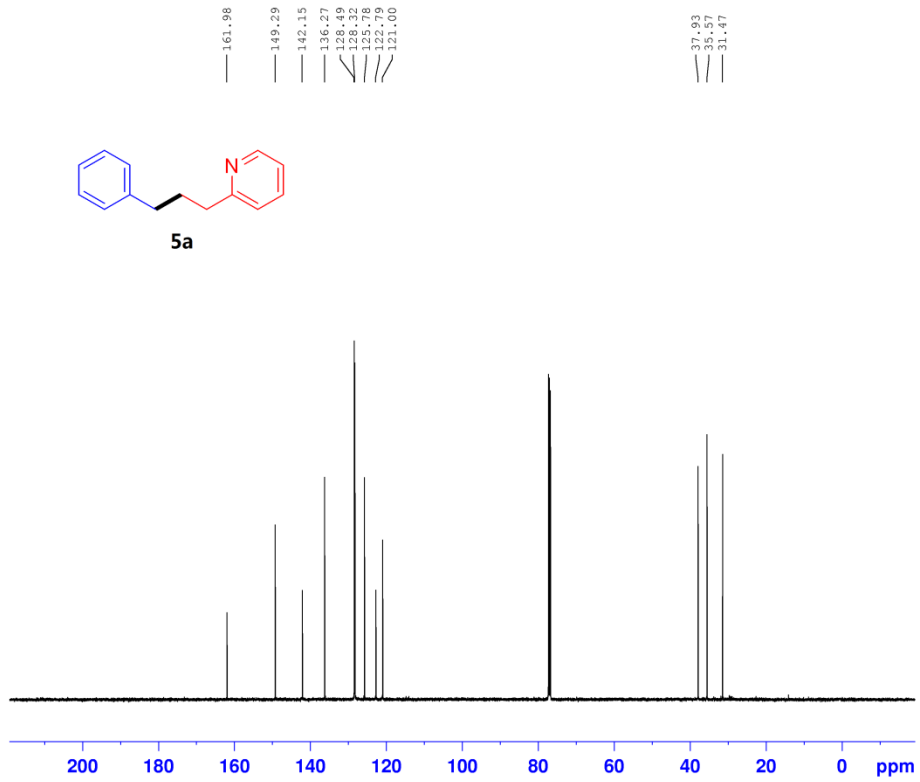
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122.79
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31.47
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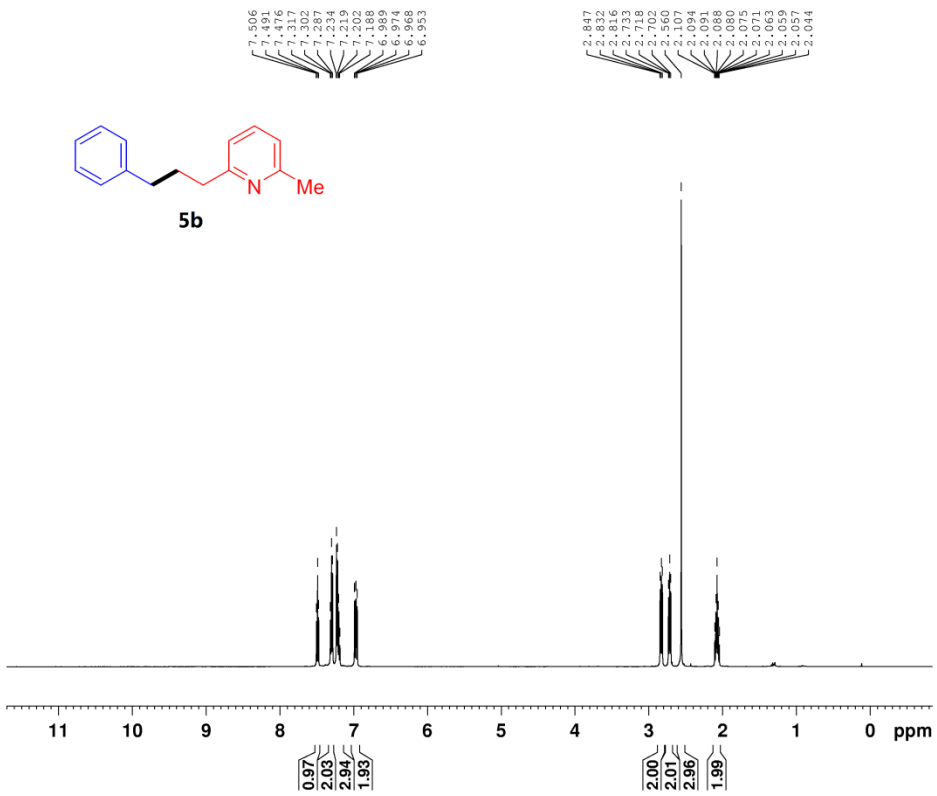
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7.219
7.202
7.188
6.989
6.974
6.968
6.953
2.847
2.832
2.816
2.733
2.718
2.702
2.560
2.107
2.094
2.091
2.088
2.080
2.075
2.071
2.063
2.059
2.057
2.044
N
Me
5b
11
10
9
8
7
6
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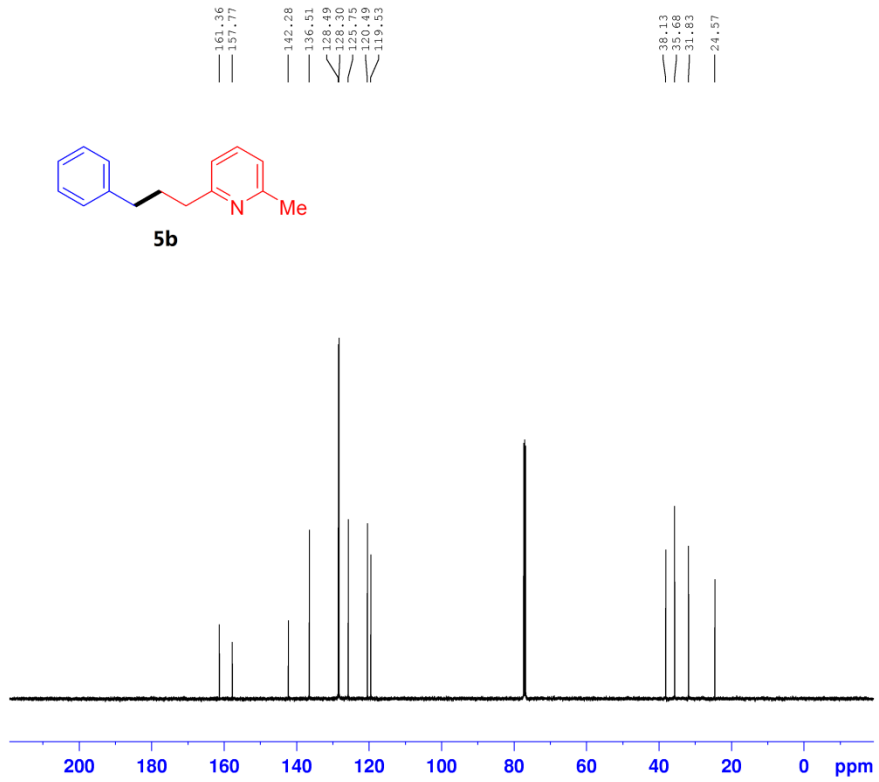
2.96
1.99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120.49
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38.13
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Me
5b
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120
100
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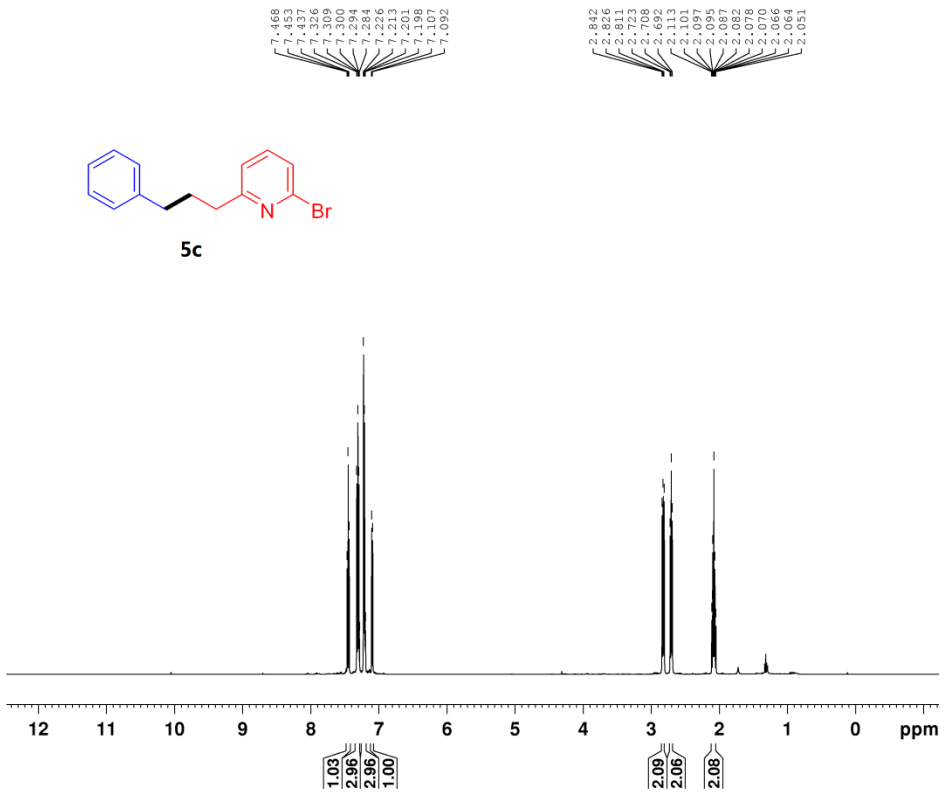
ppm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7.294
7.284
7.226
7.213
7.201
7.198
7.107
7.092
2.842
2.826
2.811
2.723
2.708
2.692
2.113
2.101
2.097
2.095
2.087
2.082
2.078
2.070
2.066
2.064
2.051
N
Br
5c
12
11
10
9
8
7
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2.96
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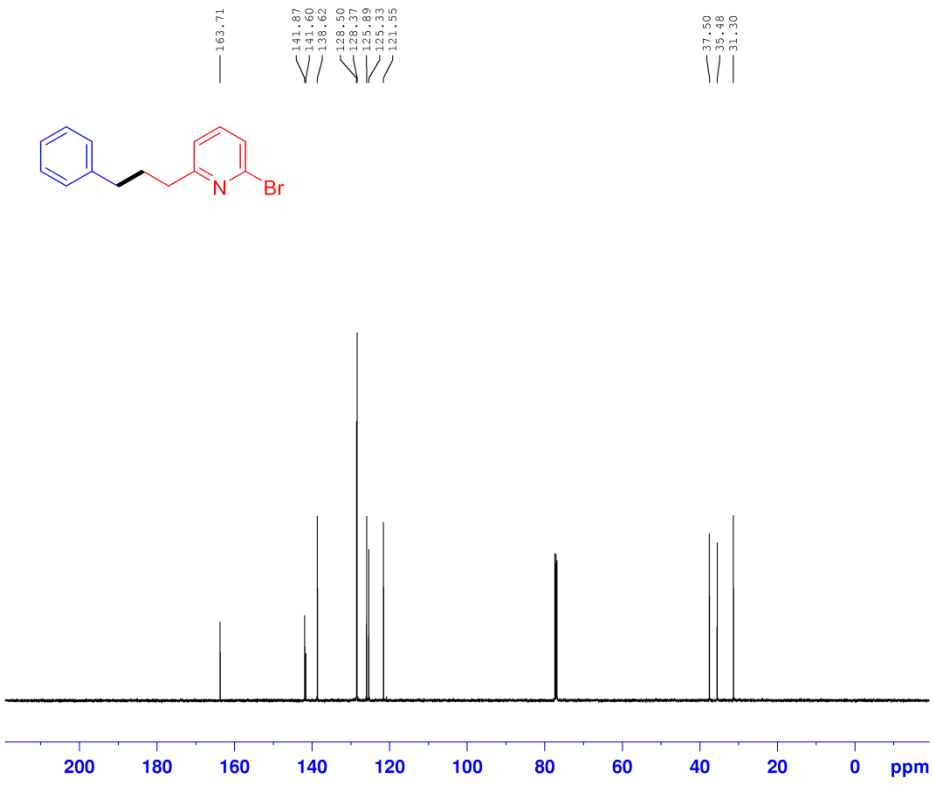
2.06
2.08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125.33
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Br
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120
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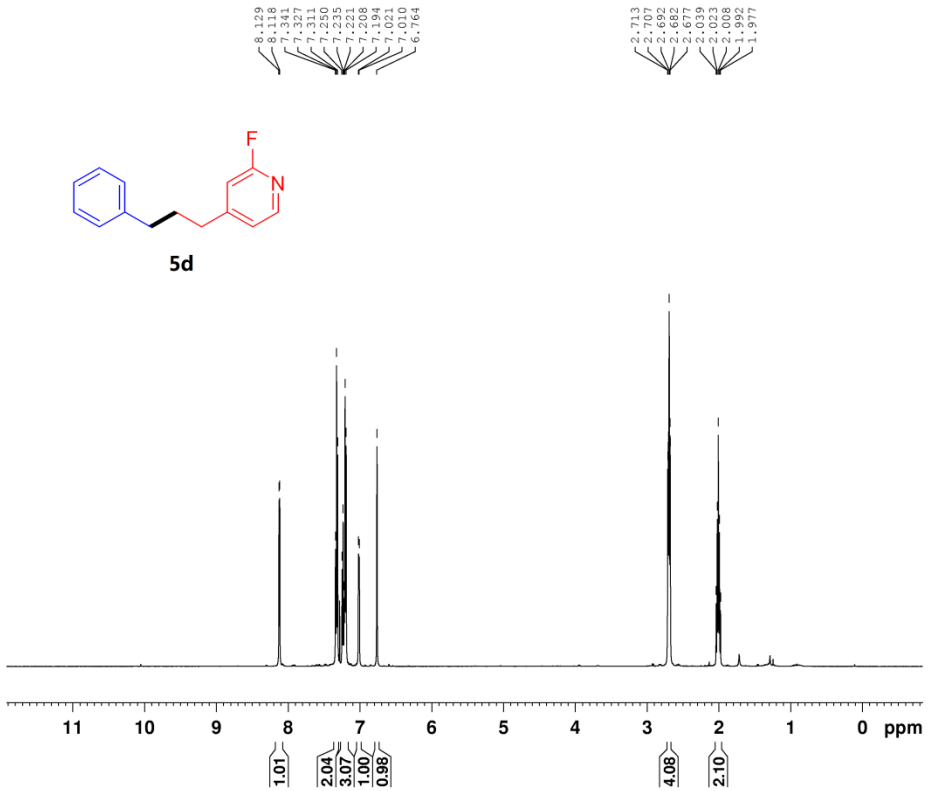
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7.221
7.208
7.194
7.021
7.010
6.764
2.713
2.707
2.692
2.682
2.677
2.039
2.023
2.008
1.992
1.977
F
N
5d
11
10
9
8
7
6
5
4
3
2
1
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ppm
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2.04
3.07
1.00
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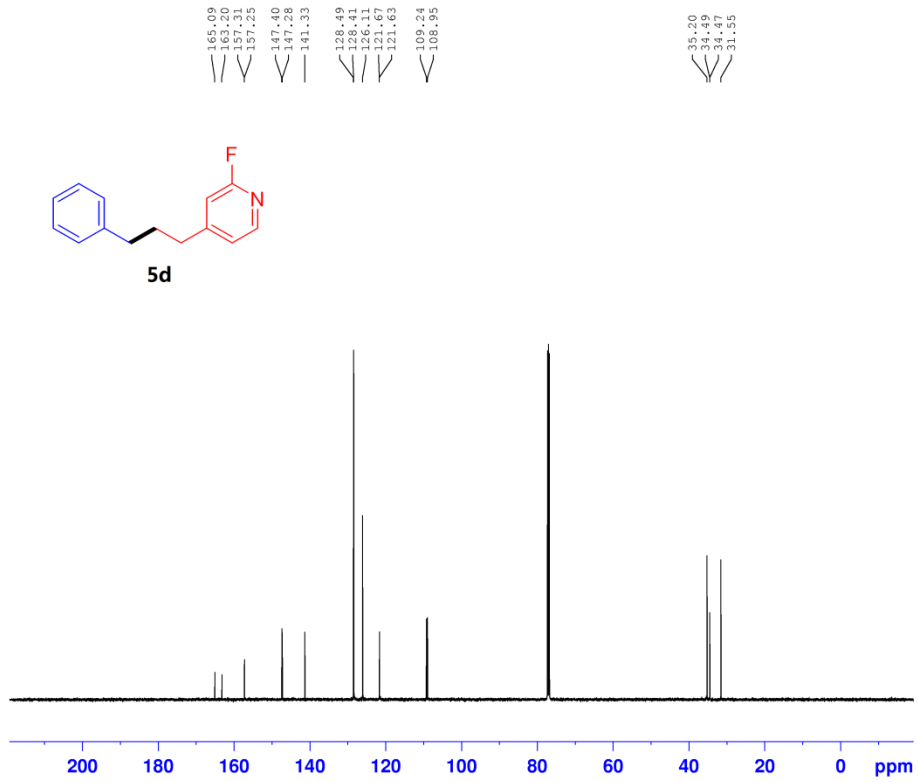
4.08
2.10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128.49
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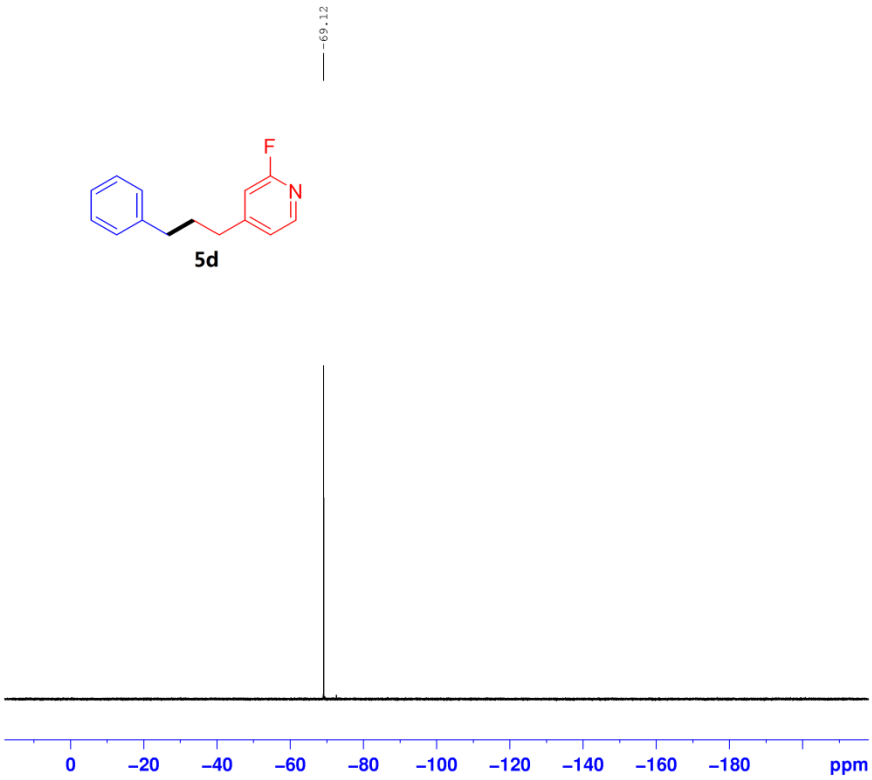
126.11
121.67
121.63
109.24
108.95
35.20
34.49
34.47
31.55
F
N
5d
200
180
160
140
120
100
80
60
40
20
0
ppm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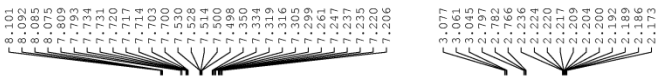
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7.720
7.717
7.714
7.703
7.700
7.530
7.528
7.514
7.500
7.498
7.350
7.334
7.319
7.316
7.305
7.299
7.261
7.247
7.237
7.235
7.220
7.206
3.077
3.061
3.045
2.797
2.782
2.766
2.236
2.224
2.220
2.217
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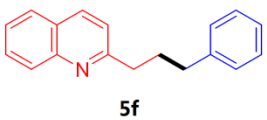
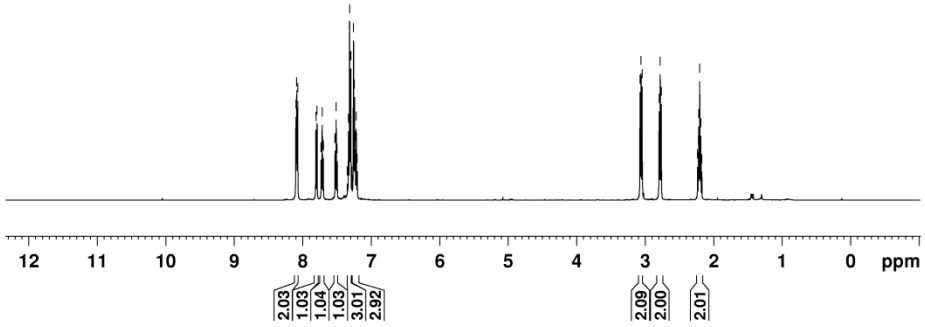
2.204
2.200
2.192
2.189
2.186
2.173


N

5f


12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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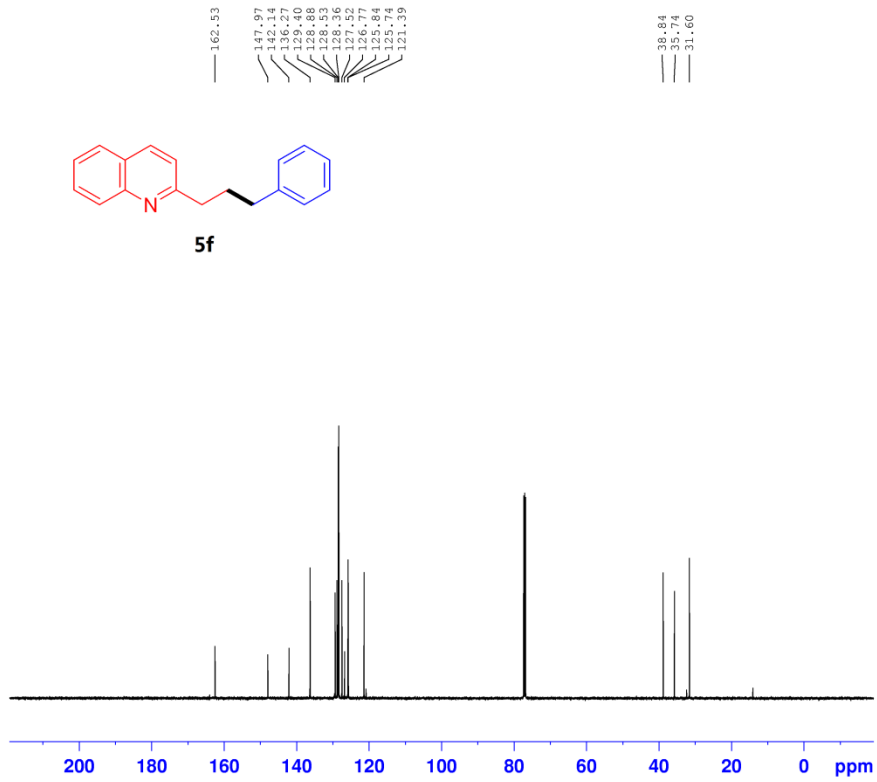
1.03
1.04
1.03
3.01
2.92
2.09
2.00
2.01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128.36
127.52
126.77
125.84
125.74
121.39
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31.60
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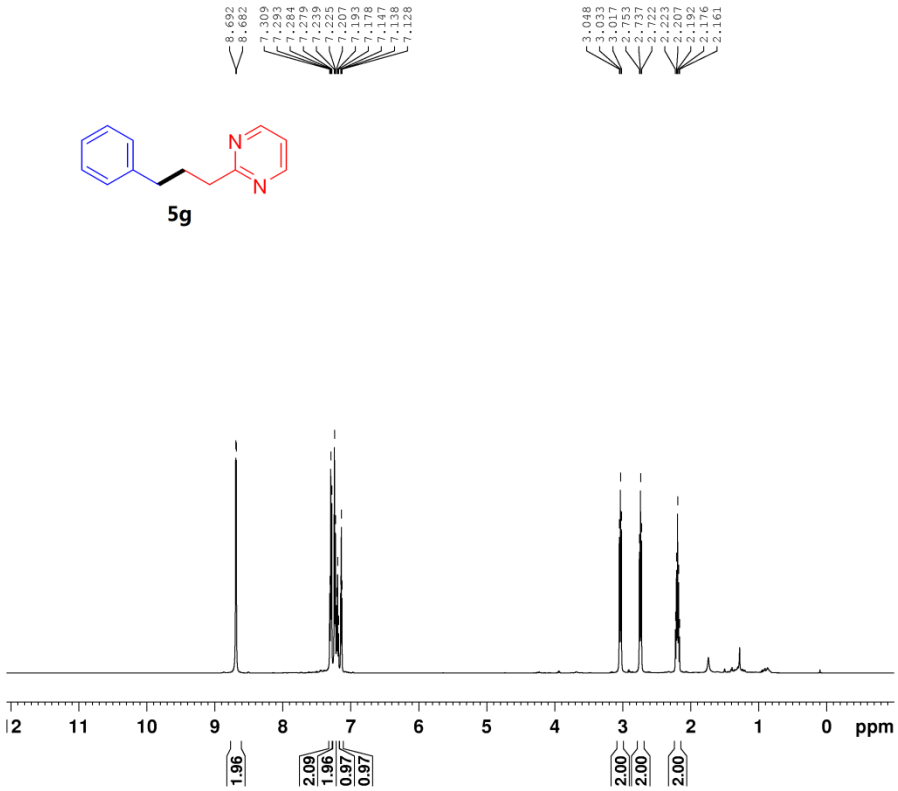
180
160
140
120
100
80
60
40
20
0
ppm

5f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7.284
7.279
7.239
7.225
7.207
7.193
7.178
7.147
7.138
7.128
3.048
3.033
3.017
2.753
2.737
2.722
2.223
2.207
2.192
2.176
2.161
N
N
5g
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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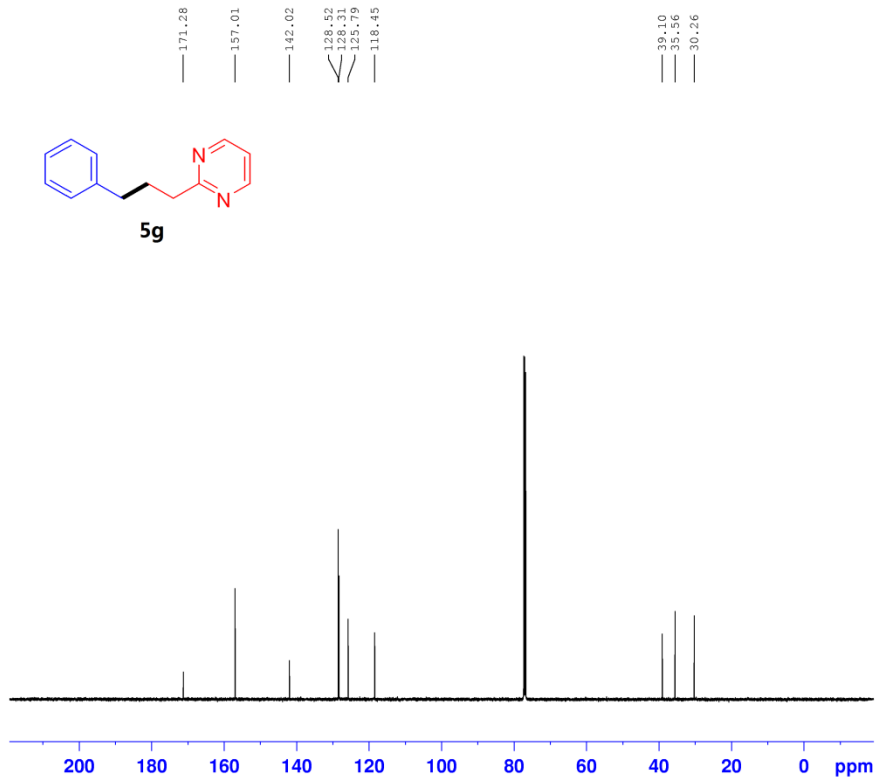
2.09
1.96
0.97
0.97
2.00
2.00
2.00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157.01
142.02
128.52
128.31
125.79
118.45
39.10
35.56
30.26
N
N
5g
200
180
160
140
120
100
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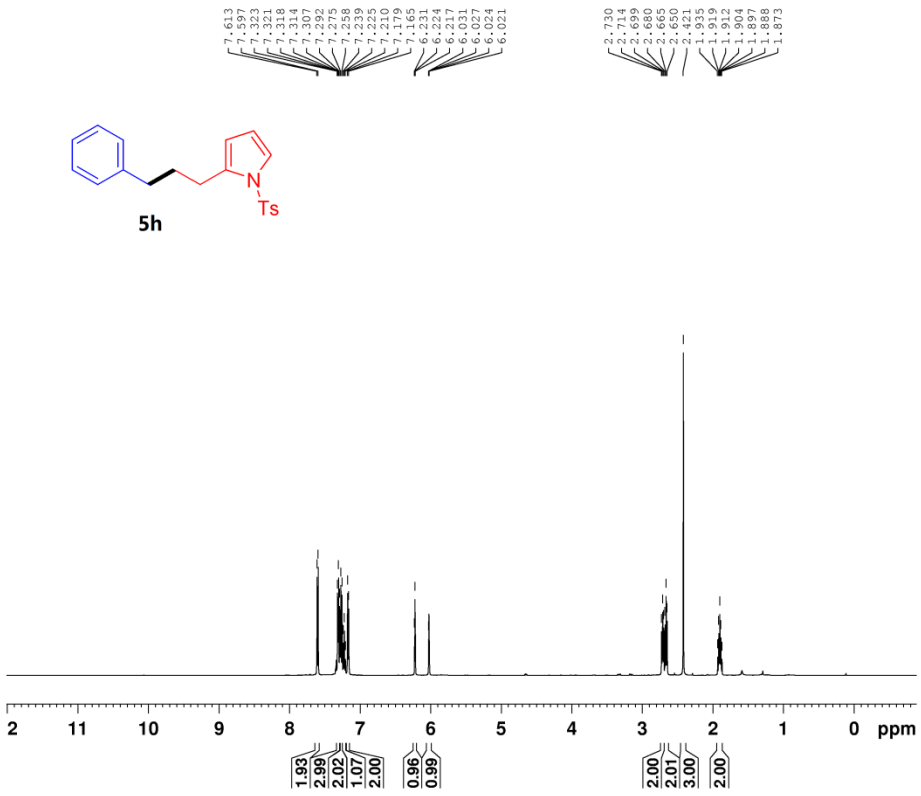
60
40
20
0
ppm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7.275
7.258
7.239
7.225
7.210
7.179
7.165
6.231
6.224
6.217
6.031
6.027
6.024
6.021
2.730
2.714
2.699
2.680
2.665
2.650
2.421
1.935
1.919
1.912
1.904
1.897
1.888
1.873
N
Ts
5h
2
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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2.02
1.07
2.00
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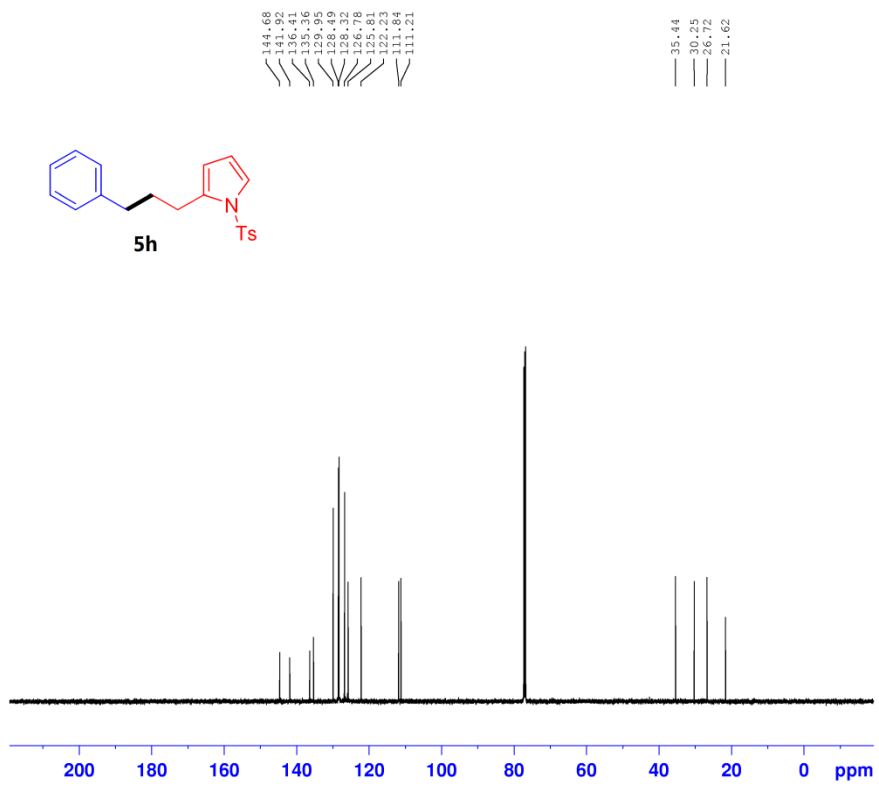
0.99
2.00
2.01
3.00
2.00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129.49
128.32
126.78
125.81
122.23
111.84
111.21
35.44
30.25
26.72
21.62
N
Ts
5h
200
180
160
140
120
100
80
60
40
20
0
ppm


8.017
8.001
7.880
7.864
7.500
7.497
7.485
7.483
7.469
7.467
7.396
7.394
7.380
7.365
7.363
7.343
7.340
7.328
7.317
7.314
7.256
7.249
7.242
7.231
7.236
7.233
7.221
7.218
3.188
3.173
3.158
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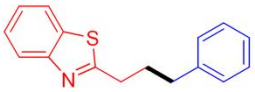
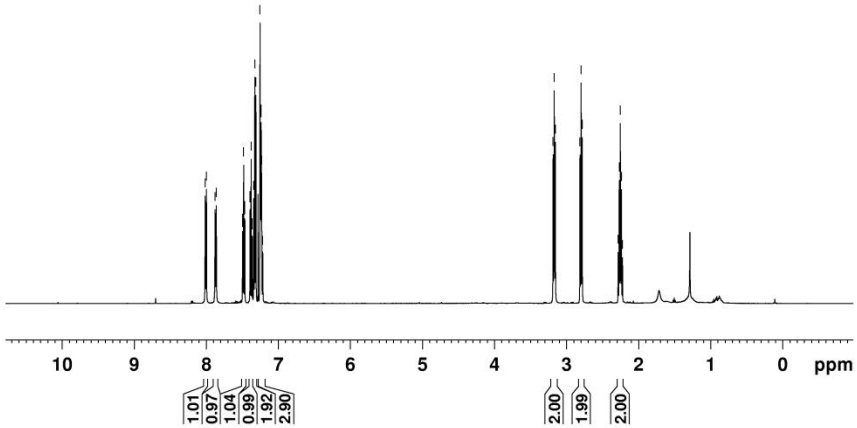
2.800
2.785
2.286
2.271
2.256
2.240
2.225


S
N

5i


10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
0.97
1.04
0.99
1.92
2.90
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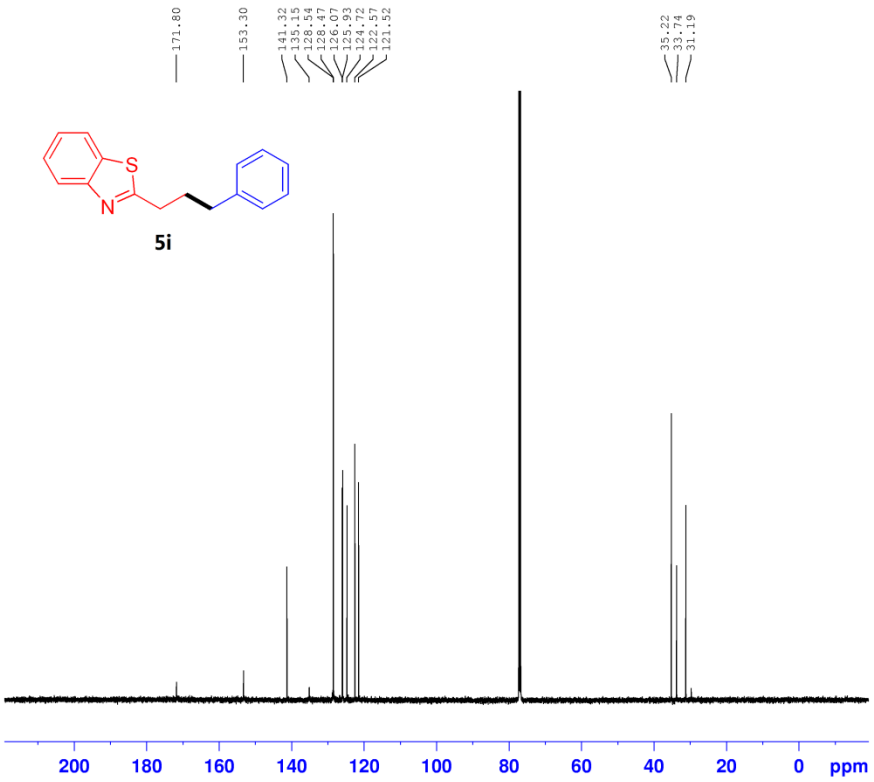
2.00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128.47
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125.93
124.72
122.57
121.52
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33.74
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S
N
5i
200
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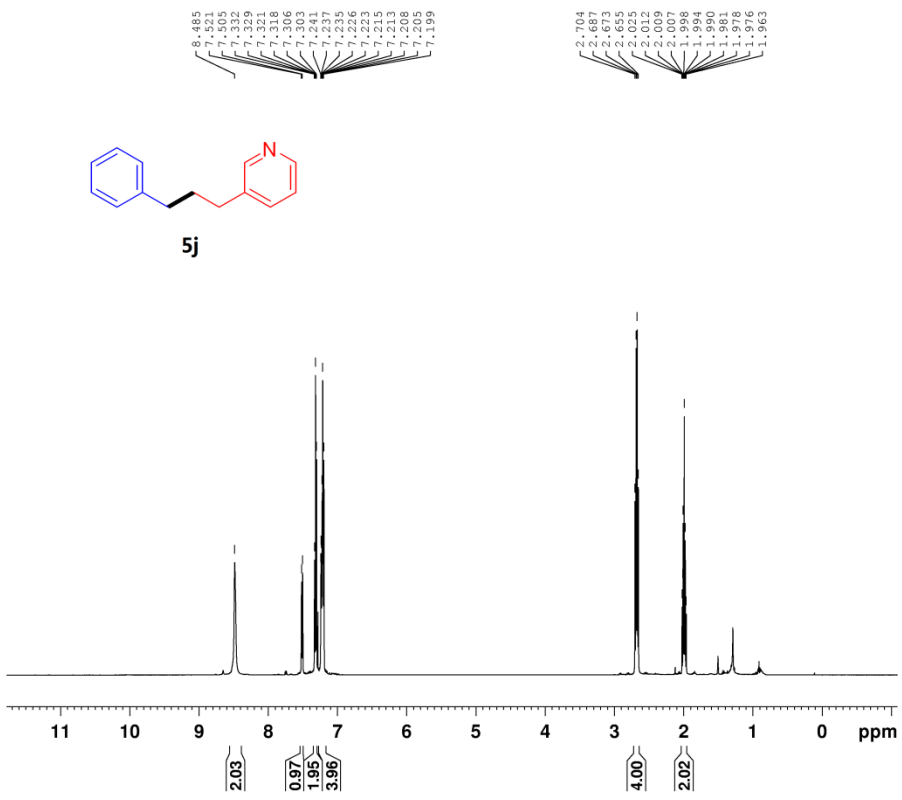
140
120
100
80
60
40
20
0
ppm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7.332
7.329
7.321
7.318
7.306
7.303
7.241
7.237
7.235
7.226
7.223
7.215
7.213
7.208
7.205
7.199
2.704
2.687
2.673
2.655
2.025
2.012
2.009
2.007
1.998
1.994
1.990
1.981
1.978
1.976
1.963
N
5j
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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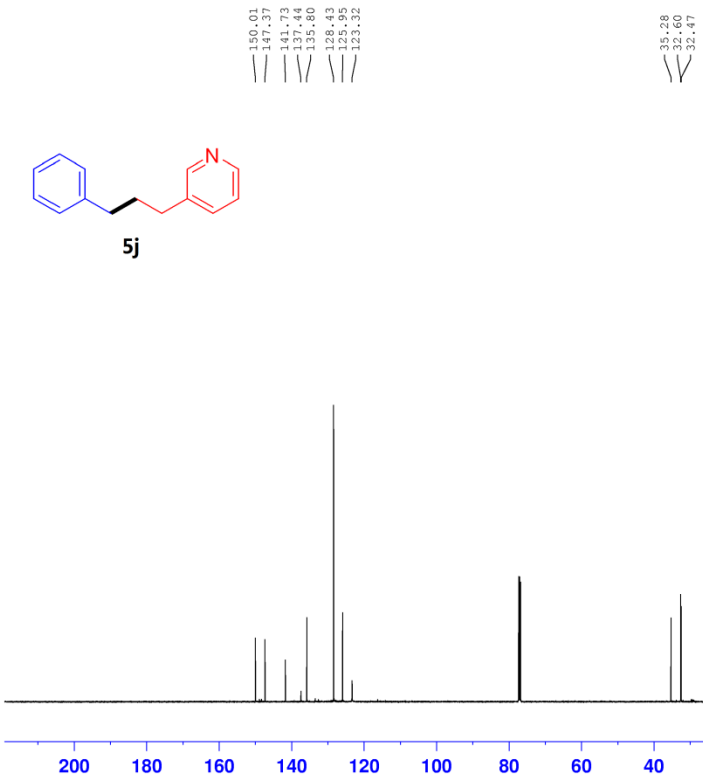
0.97
1.95
3.96
4.00
2.02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147.37
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137.44
135.80
128.43
125.95
123.32
35.28
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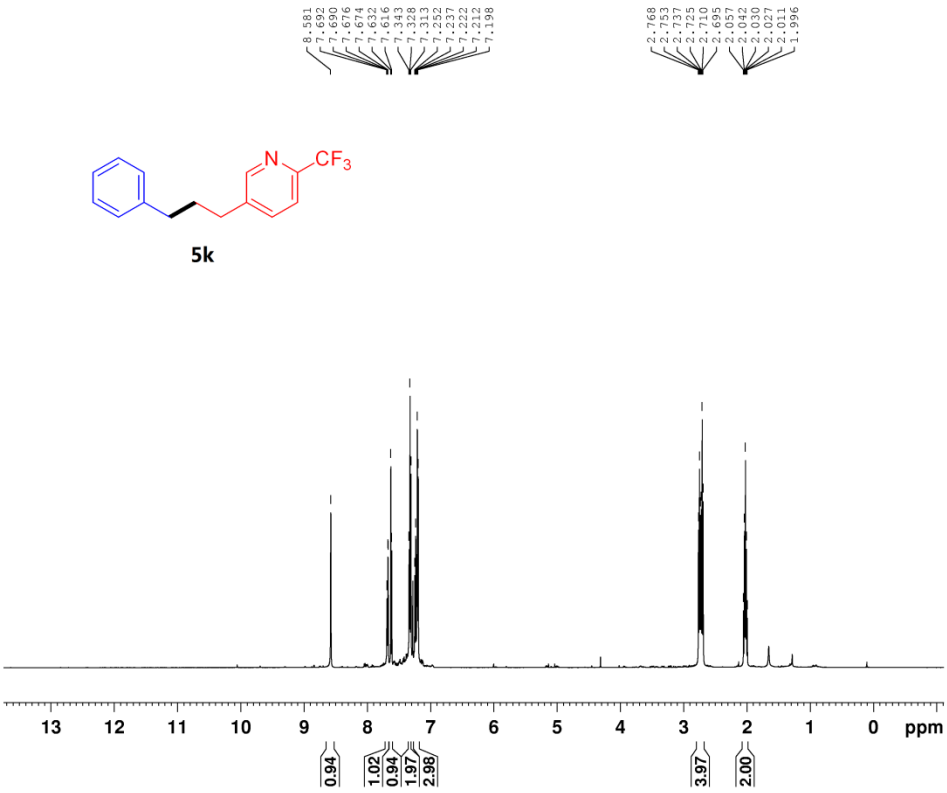
32.47
N
5j
200
180
160
140
120
100
80
60
40
20
0
ppm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7.690
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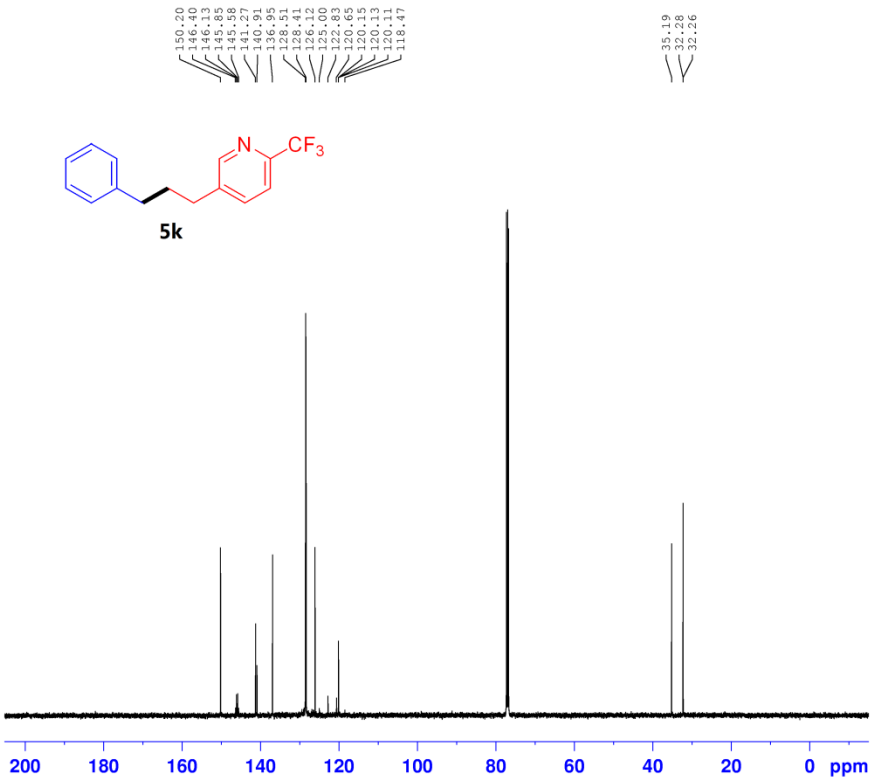
7.674
7.632
7.616
7.343
7.328
7.313
7.152
7.237
7.222
7.212
7.198
2.768
2.753
2.737
2.725
2.710
2.695
2.057
2.042
2.030
2.027
2.011
1.996
N
CF3
5k
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.94
1.02
0.94
1.97
2.98
3.97
2.00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136.95
128.51
128.41
126.12
125.00
122.83
120.65
120.15
120.13
120.11
118.47
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32.28
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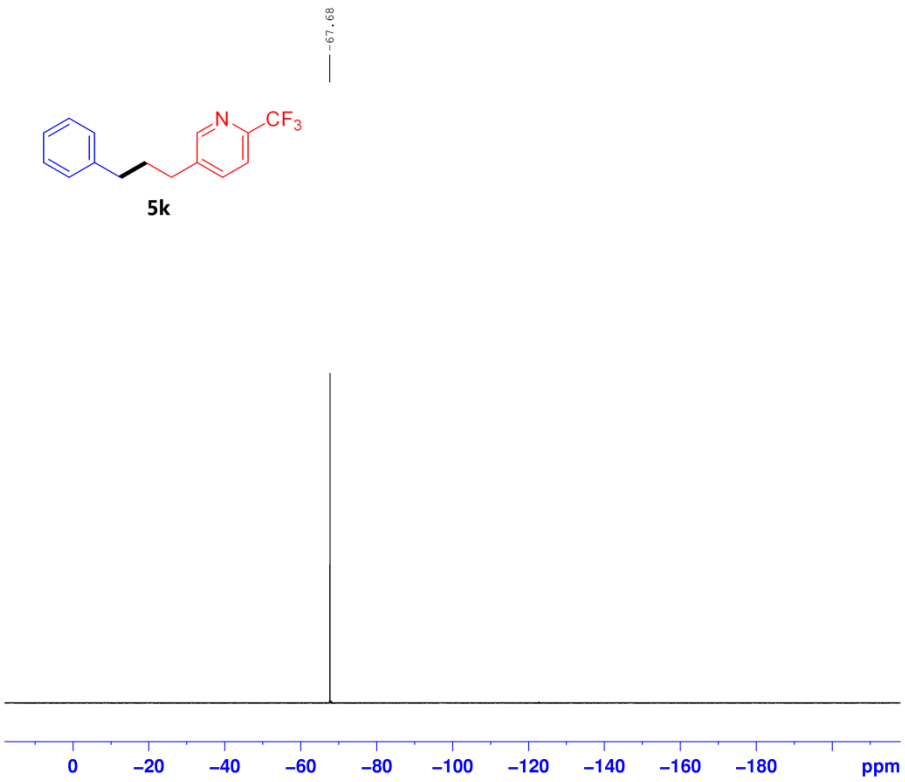
N
CF3
5k
200
180
160
140
120
100
80
60
40
20
0
ppm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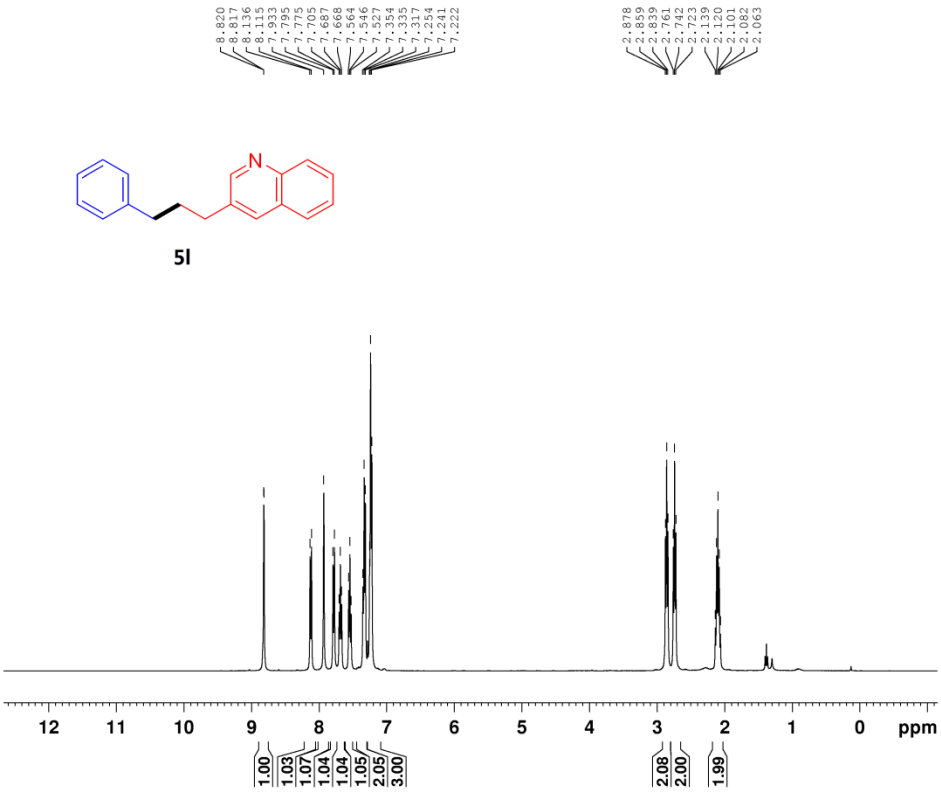
−160
−180
ppm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7.668
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7.527
7.354
7.335
7.317
7.254
7.241
7.222
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2.859
2.839
2.761
2.742
2.723
2.139
2.120
2.101
2.082
2.063
N
5l
12
11
10
9
8
7
6
5
4
3
2
1
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ppm
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1.07
1.04
1.04
1.05
2.05
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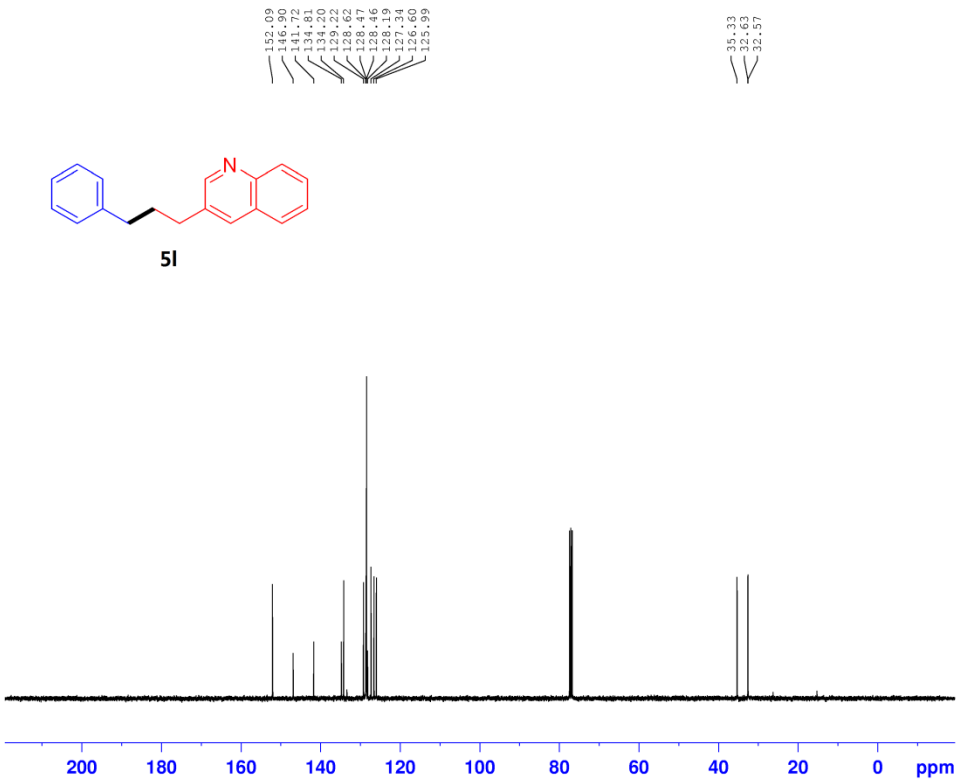
2.08
2.00
1.99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128.47
128.46
128.19
127.34
126.60
125.99
35.33
32.63
32.57
N
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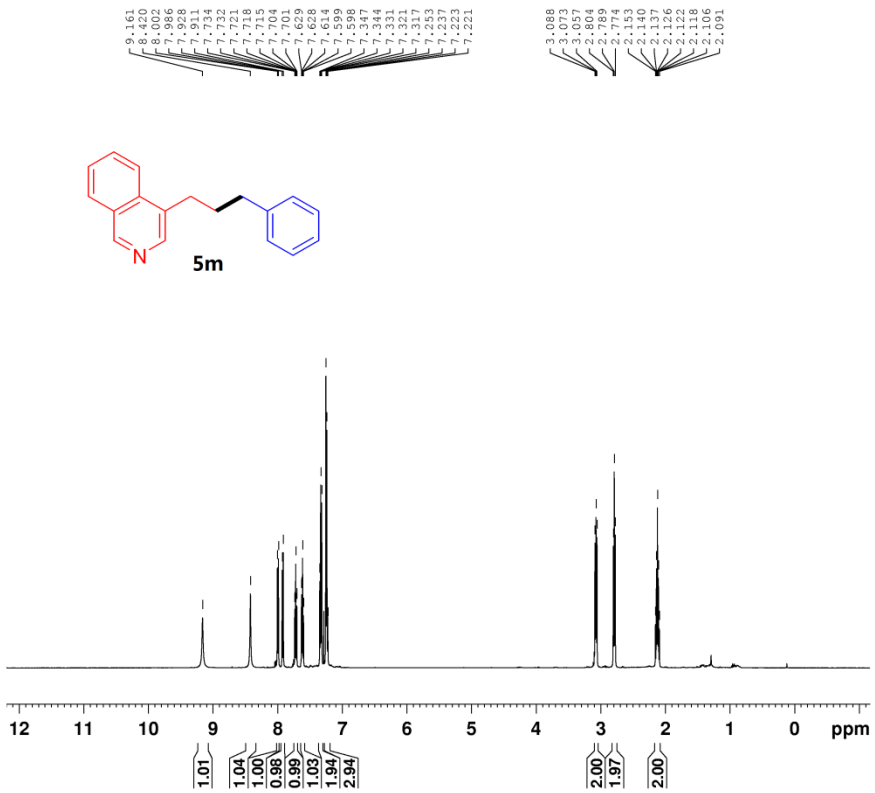
180
160
140
120
100
80
60
40
20
0
ppm

5l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7.732
7.721
7.718
7.715
7.704
7.701
7.629
7.628
7.614
7.599
7.598
7.347
7.344
7.331
7.321
7.317
7.253
7.237
7.223
7.221
3.088
3.073
3.057
2.804
2.789
2.774
2.153
2.140
2.137
2.126
2.122
2.118
2.106
2.091
N
5m
12
11
10
9
8
7
6
5
4
3
2
1
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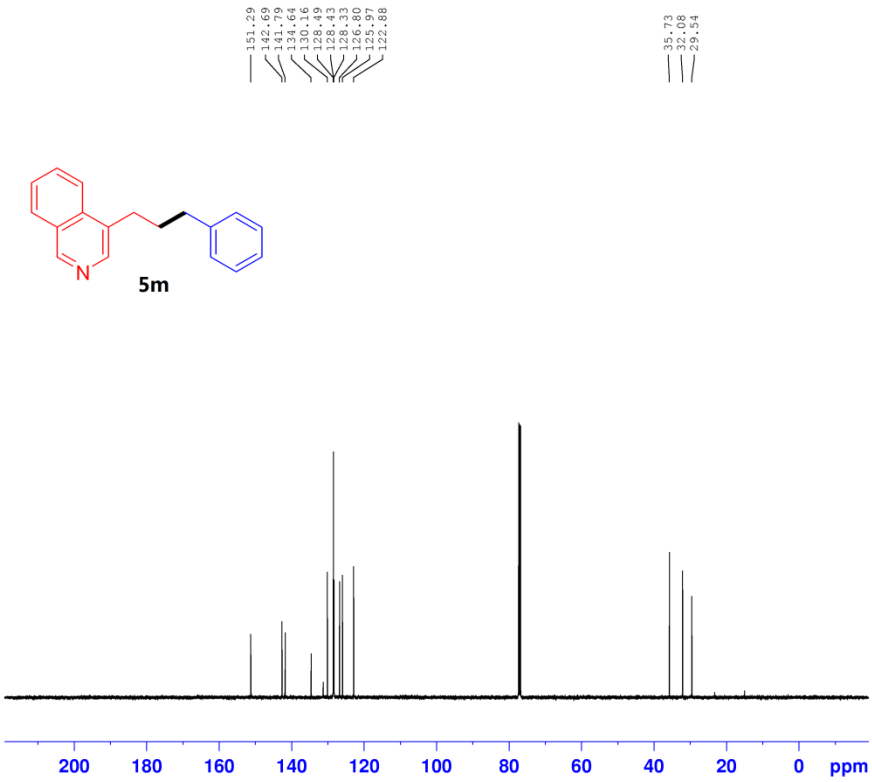
1.97
2.00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128.49
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128.33
126.80
125.97
122.88
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29.54
N
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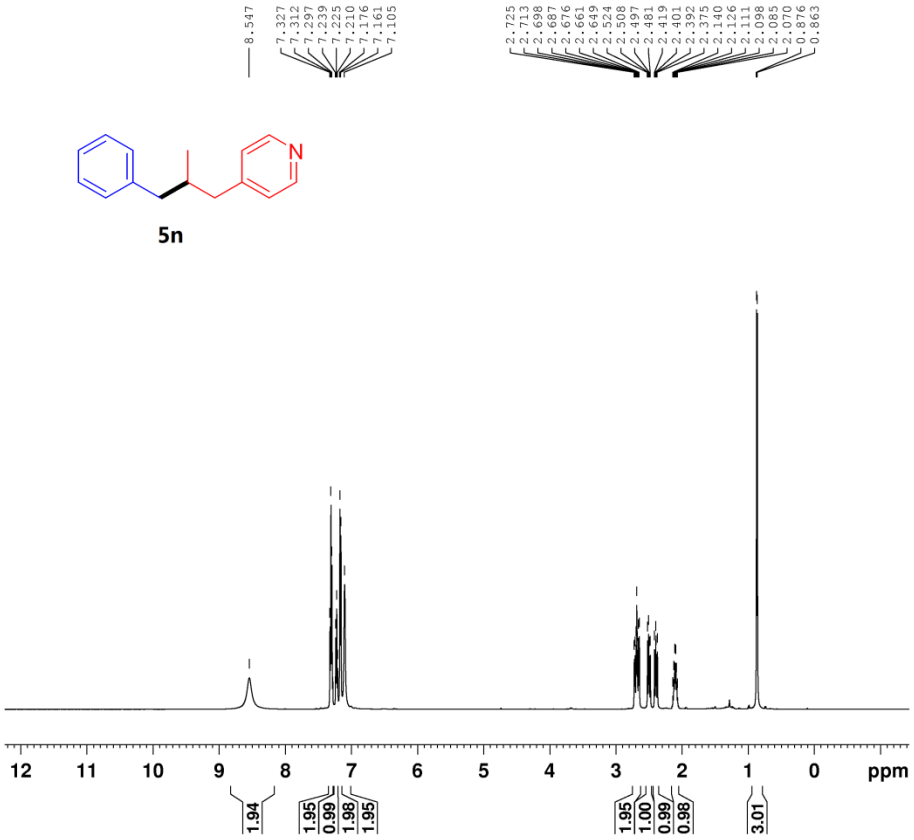
200
180
160
140
120
100
80
60
40
20
0
ppm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7.247
7.239
7.225
7.210
7.176
7.161
7.105
2.725
2.713
2.698
2.687
2.676
2.661
2.649
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2.497
2.481
2.419
2.401
2.392
2.375
2.140
2.126
2.111
2.098
2.085
2.070
0.876
0.863
N
5n
12
11
10
9
8
7
6
5
4
3
2
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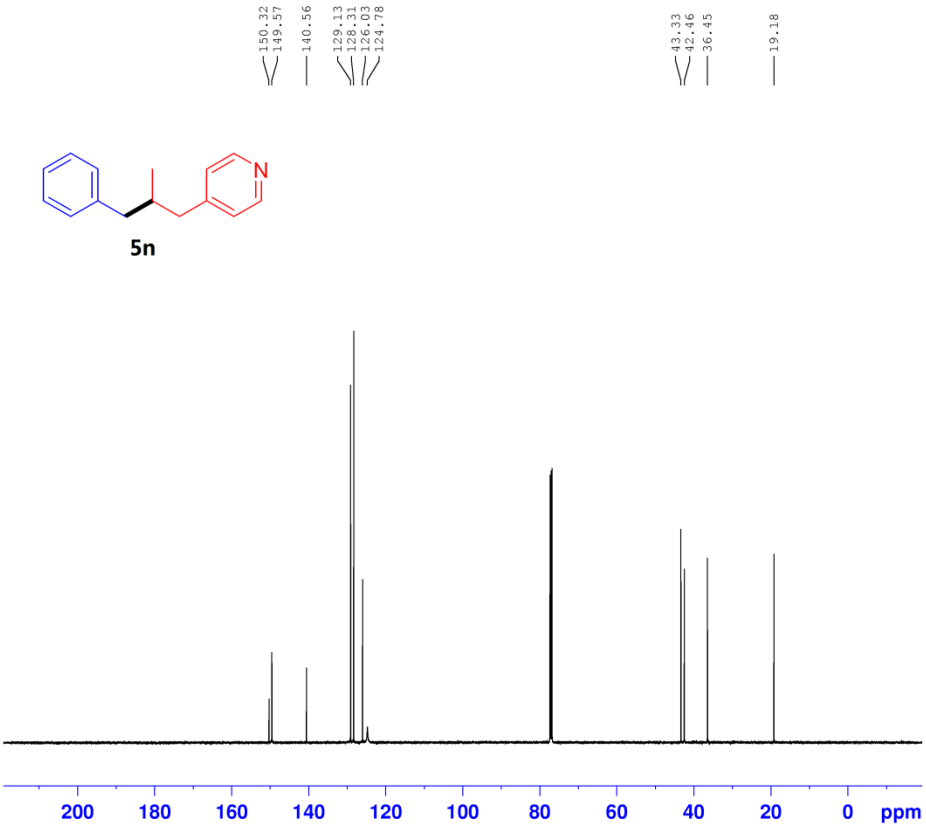
1.95
0.99
1.98
1.95
1.95
1.00
0.99
0.98
3.01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149.57
140.56
129.13
128.31
126.03
124.78
43.33
42.46
36.45
19.18
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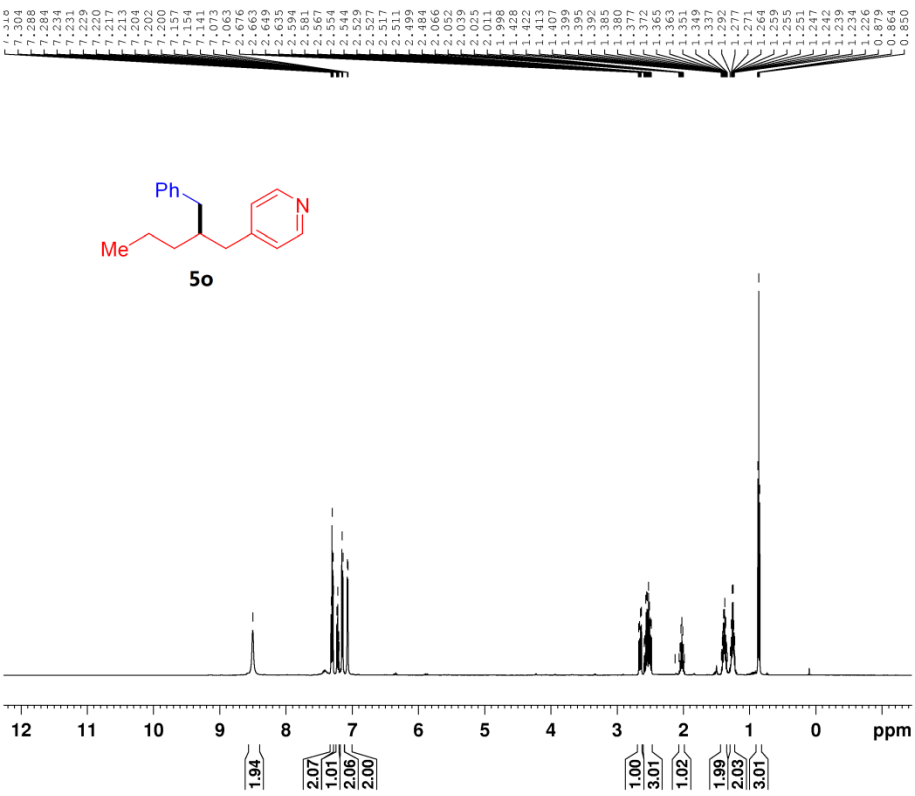
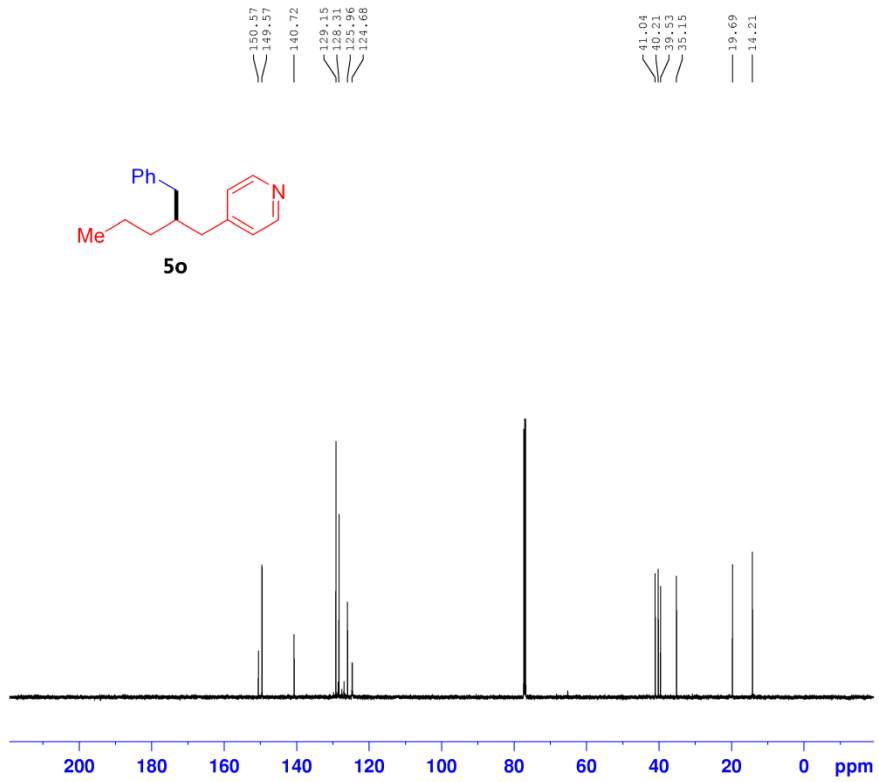
5n
200
180
160
140
120
100
80
60
40
20
0
ppm


Ph
N
Me
5o
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.94
2.07
1.01
2.06
2.00
1.00
3.01
1.02
1.99
2.03
3.01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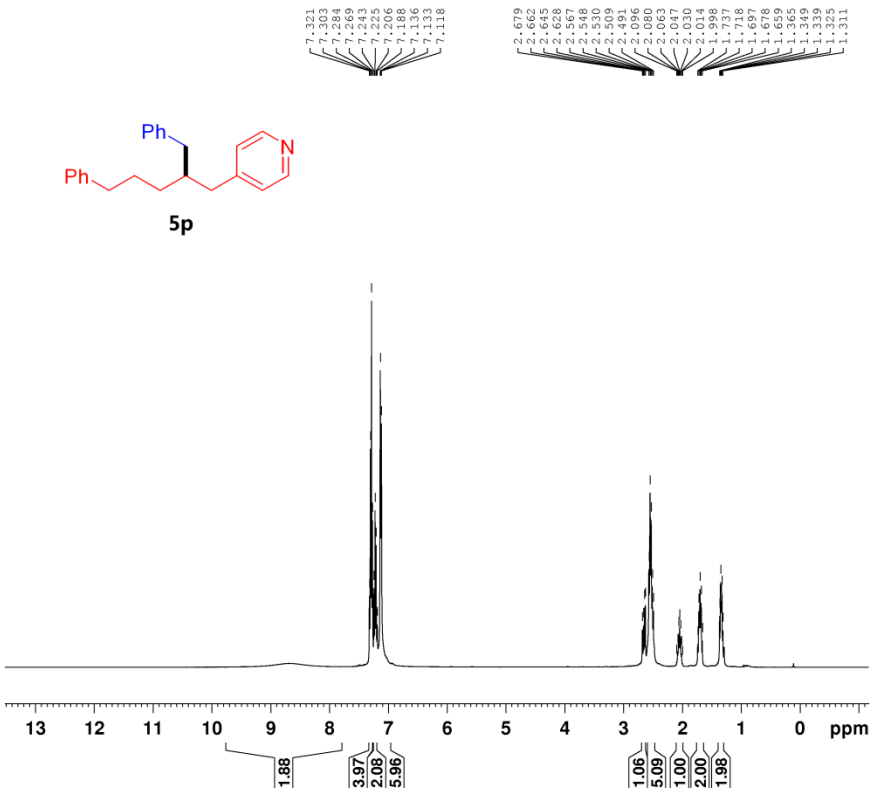
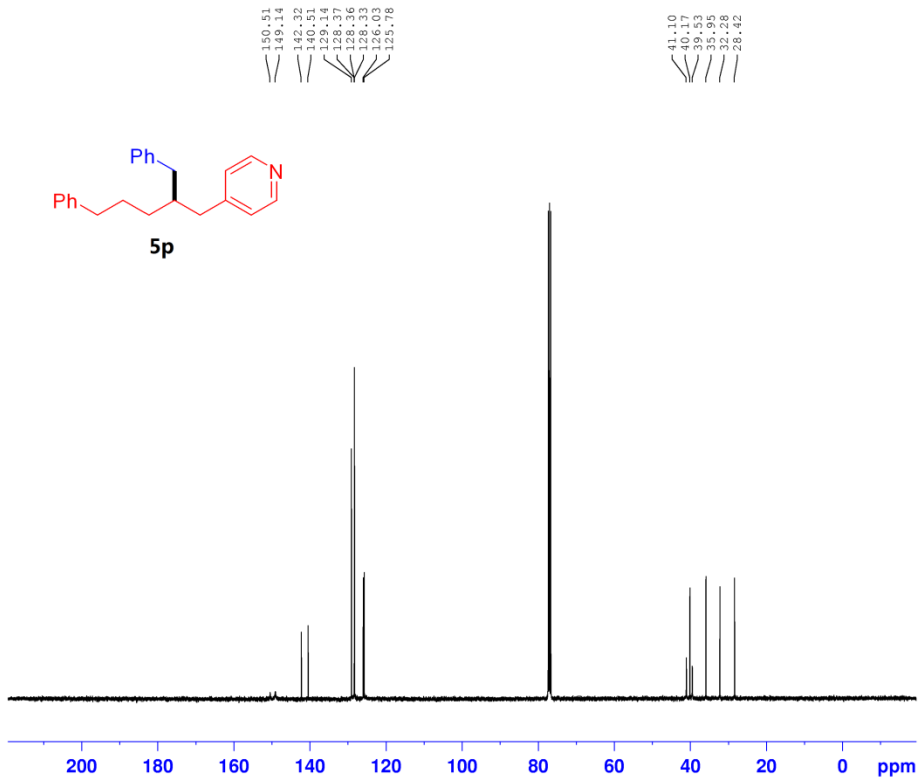
149.57
140.72
129.15
128.31
125.96
124.68
41.04
40.21
39.53
35.15
19.69
14.21
Ph
N
Me
5o
200
180
160
140
120
100
80
60
40
20
0
ppm


7.321
7.303
7.284
7.269
7.243
7.225
7.206
7.188
7.136
7.133
7.118
2.679
2.662
2.645
2.628
2.567
2.548
2.530
2.509
2.491
2.096
2.080
2.063
2.047
2.030
2.014
1.998
1.737
1.718
1.697
1.678
1.659
1.365
1.349
1.339
1.325
1.311
Ph
Ph
N
5p
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.88
3.97
2.08
5.96
1.06
5.09
1.00
2.00
1.98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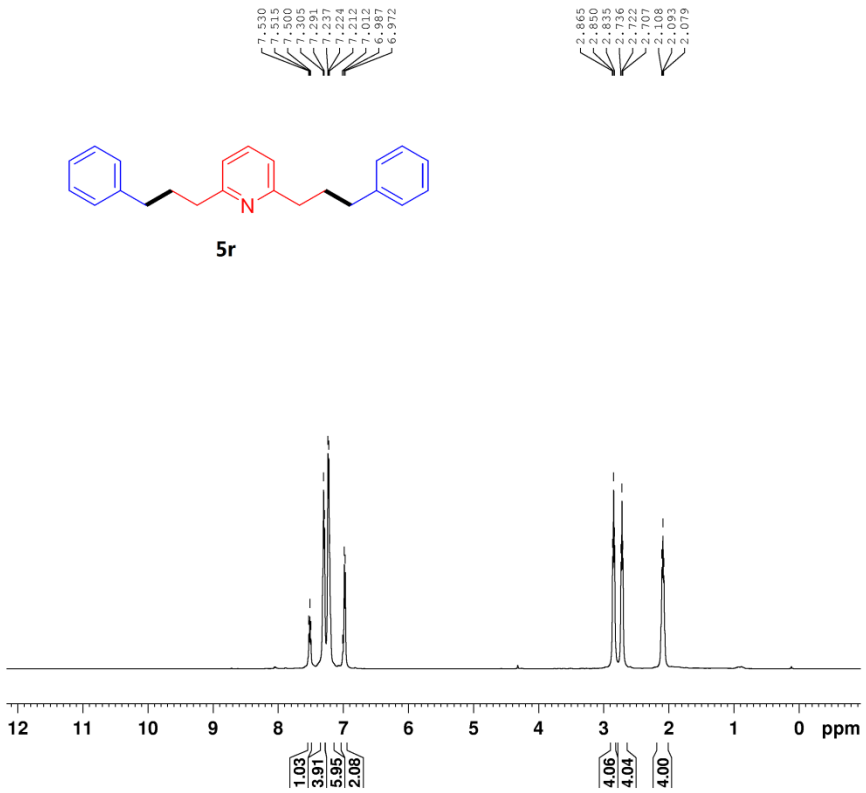
142.32
140.51
129.14
128.37
128.36
128.33
126.03
125.78
41.10
40.17
39.53
35.95
32.28
28.42
Ph
Ph
N
5p
200
180
160
140
120
100
80
60
40
20
0
ppm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7.515
7.500
7.305
7.291
7.237
7.224
7.212
7.012
6.987
6.972
2.865
2.850
2.835
2.736
2.722
2.707
2.108
2.093
2.079
N
5r
12
11
10
9
8
7
6
5
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3
2
1
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ppm
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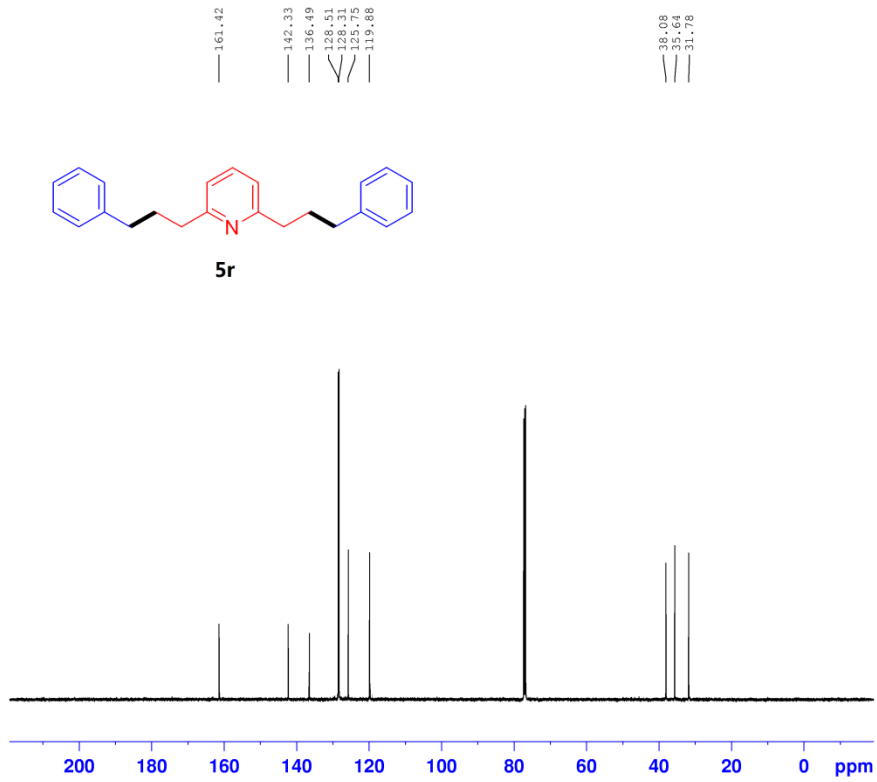
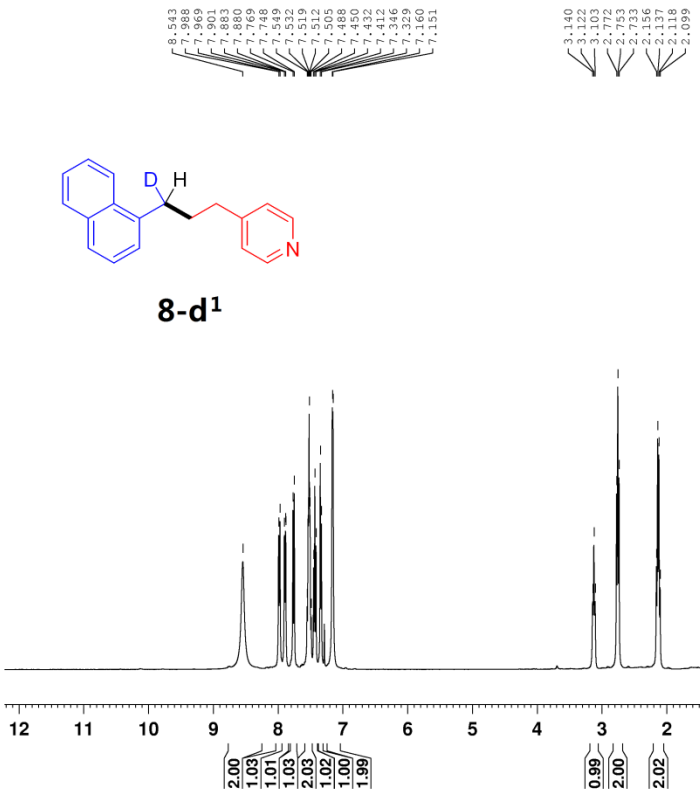
3.91
5.95
2.08
4.06
4.04
4.00


161.42
142.33
136.49
128.51
128.31
125.75
119.88
38.08
35.64
31.78
N
200
180
160
140
120
100
80
60
40
20
0
ppm

5r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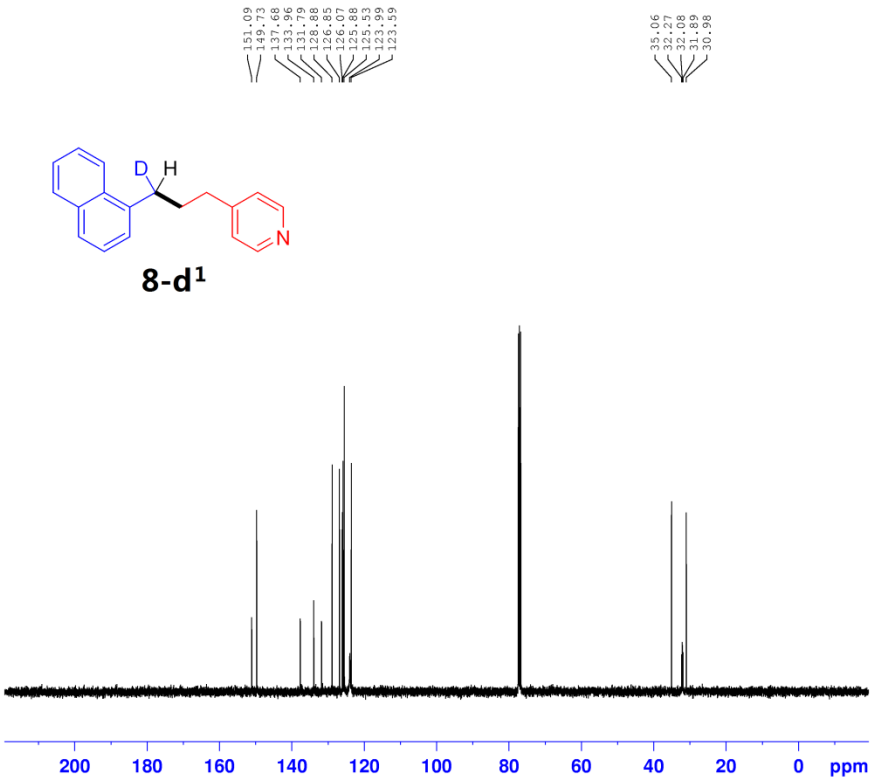
7.988
7.969
7.959
7.901
7.883
7.880
7.769
7.748
7.549
7.532
7.519
7.512
7.505
7.488
7.450
7.432
7.312
7.246
7.229
7.160
7.151
3.140
3.122
3.103
2.772
2.753
2.733
2.156
2.137
2.118
2.099
D
H
N
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.03
1.01
1.03
2.03
1.02
1.00
1.99
0.99
2.00
2.02

8-d^1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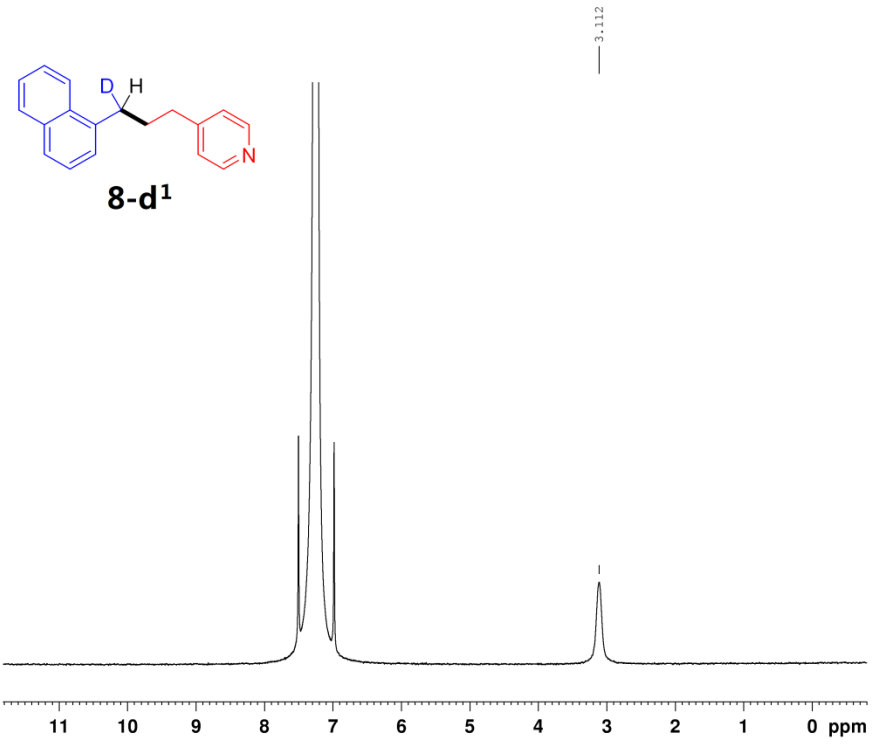
149.73
137.68
133.96
131.79
128.88
126.85
126.07
125.88
125.53
123.99
123.59
35.06
32.27
32.08
31.89
30.98
D
H
N
200
180
160
140
120
100
80
60
40
20
0
ppm

8-d¹


D
H
N
8-d1
3.112
11
10
9
8
7
6
5
4
3
2
1
0 ppm