Supporting Information

Efficient Three-Component Strecker Reaction of Aldehydes/Ketones *via* NHC-Amidate Palladium (II) Complex Catalysis

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General Information. All commercially available reagents and solvents were used as received by Aldrich and Acros chemical without further purification. ^{1}H and ^{13}C NMR spectra were recorded on a 250 and 63MHz Bruker or 400 and 100MHz Varian instrument. Thin-layer chromatography (TLC) was performed using commercially prepared 60 mesh silica gel plates visualized with short-wavelength UV light (254 nm). Silica gel 60 (9385, 230-400 mesh) was used for column chromatography. The reported conversions are based upon consumption of amine substrate and yields are isolated yields and are the average of two runs. MS analysis was performed using a Thermo Scientific DSQ II GC-MS (ESI) instrument (He gas, 25 minute run time, the first 5 minutes at 40 degrees Celsius, an increase of 15 degrees/min for the next 15 minutes, and the final 5 minutes at 250 degrees Celsius, with a constant flow of 1.5 mL per minute).

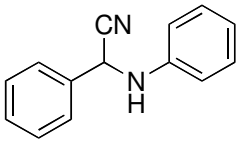
Preparation of Ligand

Methyl 2-[2-(1*H*-benzo[*d*]imidazol-1-yl)acetamido]-3-methylbutanoate (5) To a solution of benzimidazole (500 mg, 4.23 mmol) in DMF (10 mL) was added methyl 2-(2-bromoacetamido)-3-methylbutanoate **4** (1.06 g, 4.23 mmol) followed by KOH (356 mg, 6.35 mmol). After stirring the reaction mixture for 16 h at room temperature, EtOAc (50 mL) was added. Subsequently, a precipitated solid was removed by filtration. The filtrated organic layers were washed with brine twice, dried over anhydrous Na_2SO_4 and then concentrated under reduced pressure to give a crude oil, which was purified by column chromatography on silica gel using EtOAc followed by MeOH as an eluent to afford **5** as a white solid (991 mg, 81% yield). ^{1}H-NMR ($CDCl_3$): δ 7.95 (s, 1H), 7.76-7.80 (m, 1H), 7.52 (d, J = 7.5 Hz, 1H, NH), 7.35-7.39 (m, 1H), 7.24-7.32 (m, 2H), 4.86 (s, 2H), 4.53 (dd, J = 8.5 and 5.7 Hz, 1H), 3.68 (s, 3H), 2.06-2.19 (m, 1H), 0.87 (d, J = 7 Hz, 3H), 0.79 (d, J = 7 Hz, 3H); ^{13}C-NMR ($CDCl_3$): δ 17.7, 18.8, 30.5, 47.5, 52.0, 57.5, 109.5, 120.0, 122.3, 122.6, 123.4, 133.6, 143.5, 166.6, 171.8; Anal. calcd. for $C_{15}H_{19}N_3O_3$: C 62.27, H 6.62, N 14.52, found: C 62.09, H 6.74, N, 14.07; HRMS-ESI (m/z) [$M+H^+$] calcd. for $C_{15}H_{20}N_3O_3$: 290.1505, found: 290.1557

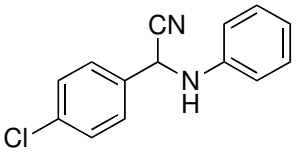
1-[2-(1-methoxy-3-methyl-1-oxobutan-2-ylamino)-2-oxoethyl]-3-methyl-1*H*-benzo[*d*] imidazol-3-ium iodide (6) To a 300 mL round-bottom flask **5** (900 mg, 3.11 mmol), iodomethane

(1.32 g, 9.33 mmol), and THF (100 mL) were added. The reaction mixture was stirred under refluxing for 16 h. After cooling the solution at room temperature, a white solid, which is the desired product **6**, was filtrated and then washed with THF (1.19 g, 89% yield). ^{1}H-NMR ($CDCl_3$): δ 10.16 (s, 1H), 8.32 (d, *J* = 7.2 Hz, 1H, NH), 7.98-8.02 (m, 1H), 7.67-7.70 (m, 1H), 7.56-7.59 (m, 2H), 5.95 (d, *J* = 16.3 Hz, 1H), 5.77 (d, *J* = 16.3 Hz, 1H), 4.31 (dd, *J* = 7.5 and 6.0 Hz, 1H), 4.17 (s, 3H), 3.63 (s, 3H), 2.19-2.33 (m, 1H), 1.03 (d, *J* = 6.7 Hz, 3H), 0.96 (d, *J* = 6.7 Hz, 3H); ^{13}C-NMR ($CDCl_3$): δ 18.8, 19.1, 30.2, 34.2, 49.8, 52.0, 58.9, 112.4, 114.1, 127.2, 127.4, 131.3, 142.5, 164.7, 171.5; HRMS-ESI (m/z) [M+H$^+$] calcd. for $C_{16}H_{23}IN_3O_3$: 432.0784, found: 432.0736

Typical procedure for synthesis of α-aminonitrile compounds

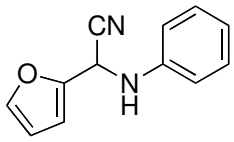


To a mixture of $Pd(OAc)_2$ (6 mg, 0.025 mmol), sodium sulfate (100 mg, 2 mmol), benzaldehyde (0.053 mL, 0.5 mmol), and aniline (0.046 mL, 0.5 mmol) in 1 mL CH_2Cl_2 in a pressure tube was added dropwise TMSCN (0.133 mL, 1 mmol). The pressure tube was closed and stirred for 24 h at 23 °C and reaction progress was monitored by TLC. The mixture was then filtered and the residue was washed with CH_2Cl_2 (10 mL). The filtrate was collected and the solvent was removed under reduced pressure. If necessary, column chromatography on silica gel with an ethyl acetate/hexanes gradient elution was performed to obtain 2-phenyl-2-(phenylamino)acetonitrile **13a** (33 mg, 79%) as a light yellow solid m.p. 76-79 °C. ^{1}H NMR (250 MHz) δ 4.67 (br s, 1H), 5.36 (s, 1H), 6.72 (d, *J* = 7.8Hz, 2H), 6.84 (t, *J* = 7.4 Hz, 1H), 7.22 (t, *J* = 8.0 Hz, 2 H), 7.37-7.44 (m, 3H), 7.52-7.55 (m, 2H); ^{13}C NMR (63 MHz) δ 50.1, 114.1, 118.1, 120.2, 127.2, 128.4, 129.2, 129.4, 134.0, 144.7. This compound is known.[1]

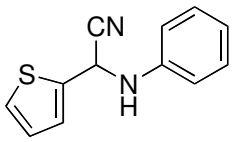


13b: Synthesized according to the general procedure to obtain 2-(4-chlorophenyl)-2-(phenylamino)acetonitrile as a white solid (20 mg, 42%). m.p. 95-97 °C. ^{1}H NMR ($CDCl_3$, 250 MHz) δ 4.04 (br s, 1H),

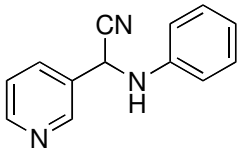
5.43 (s, 1H), 6.77 (d, *J* = 7.5 Hz, 2H), 6.92 (t, *J* = 7.5 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.44 (d, *J* = 5 Hz), 7.55 (d *J* = 7.5 Hz). This compound is known.[1]



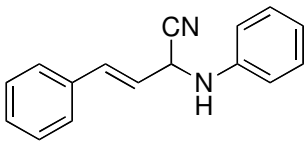
13c: Synthesized according to the general procedure to obtain 2-(furan-2-yl)-2-(phenylamino)acetonitrile as a light yellow solid (31 mg, 79%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 4.19 (br s, 1H), 5.51 (s, 1H), 6.44-6.46 (m, 1H), 6.61 (d, *J* = 2.5 Hz, 1H), 6.80 (d, *J* = 10.0 Hz, 2H), 6.94 (t, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.50-7.51 (m, 1 H). This compound is known.[1]



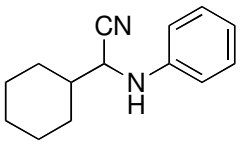
13d: Synthesized according to the general procedure to obtain 2-(phenylamino)-2-(thiophen-2-yl)acetonitrile as a white solid (39 mg, 91%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.65 (s, 1H), 6.81 (d, *J* = 8.0 Hz, 2H), 6.94 (t, *J* = 8.0 Hz, 1H), 7.05-7.07 (m, 1H), 7.26-7.32 (m, 3H), 7.39-7.40 (m, 2H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 46.2, 114.7, 117.6, 120.8, 125.5, 127.1, 127.2, 127.3, 130.0, 144.2. This compound is known.[1]



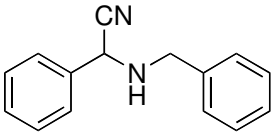
13e: Synthesized according to the general procedure to obtain 2-(phenylamino)-2-(pyridin-3-yl)acetonitrile as a light yellow solid (40 mg, 95%). m.p. 74-83 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.16 (br s, 1H), 5.53 (d, *J* = 8.0 Hz, 1H), 6.81, (d, *J* = 8.0 Hz, 2H), 6.96, (t, *J* = 8.0 Hz, 1H), 7.28-7.34 (m, 3H), 7.42-7.45 (m, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 8.71 (d, *J* = 4.0 Hz, 1H), 8.88 (s, 1H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 48.3, 114.5, 117.3, 120.9, 123.9, 129.7, 134.9, 144.3, 148.7, 150.8. This compound is known.[2]



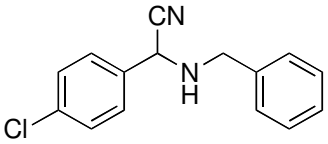
13f: Synthesized according to the general procedure to obtain (E)-4-phenyl-2-(phenylamino)but-3-enenitrile as a yellow solid (39 mg, 83%). m.p. 55-61 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.50 (br s, 1H), 5.08 (dd, *J* = 8.0 Hz, 1H), 6.30 (dd, *J* = 16.0 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 2H), 6.93 (t, *J* = 8.0 Hz, 1H), 7.07 (d, *J* = 16.0 Hz, 1H), 7.27-7.32 (m, 2H), 7.34-7.40 (m, 3H), 7.44-7.46 (m, 2H). This compound is known.[1]



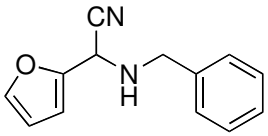
13g: Synthesized according to the general procedure to obtain 2-cyclohexyl-2-(phenylamino)acetonitrile as a white solid (38 mg, 88%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 1.17-1.35 (m, 5H), 1.74 (d, *J* = 5.0 Hz, 1H), 1.82-1.88 (m, 3H), 1.96-2.01 (m, 2H), 3.79 (br s, 1H), 4.04-4.08 (m, 1H), 6.72 (d, *J* = 5.0 Hz, 2H), 6.86 (t, *J* = 5.0 Hz, 1H), 7.23-7.27 (t, *J* = 5.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 25.7, 29.7, 30.4, 40.8, 51.8, 114.1, 118.9. 119.9, 129.5, 145.3. This compound is known.[3]



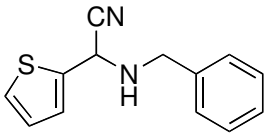
13h: Synthesized according to the general procedure to obtain 2-(benzylamino)-2-phenylacetonitrile as a white solid (35 mg, 79%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.99 (AB, q, *J* = 11.0 Hz, 2H), 4.77 (s, 1H), 7.31-7.45 (m, 8H), 7.55 (d, *J* = 4.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 51.1, 53.3, 118.5, 127.2, 127.5, 128.3, 128.5, 128.8, 128.9, 134.6, 137.9. This compound is known.[1]



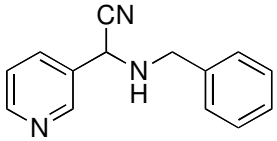
13i: Synthesized according to the general procedure to obtain 2-(benzylamino)-2-(4-chlorophenyl)acetonitrile as a white solid (46 mg, 90%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 1.89(br s, 1H), 4.00 (AB, q, *J*= 12.5 Hz, 2H), 4.74 (s, 1H), 7.32-7.51 (m, 9H). This compound is known.[4]



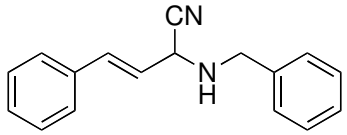
13j: Synthesized according to the general procedure to obtain 2-(benzylamino)-2-(furan-2-yl)acetonitrile as a light brown oil (36 mg, 86%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 2.03 (br s, 1H), 3.99 (AB, q, *J* = 15.0 Hz, 2H), 4.80 (s, 1H), 6.38-6.40 (m, 1H), 6.48-6.50 (m, 1H), 7.29-7.41 (m, 5H), 7.44-7.45 (m, 1H). This compound is known.[5]



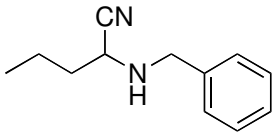
13k: Synthesized according to the general procedure to obtain 2-(benzylamino)-2-(thiophen-2-yl)acetonitrile as a white solid (42 mg, 91%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 2.47 (br s, 1H), 4.03 (AB, q, *J* = 17.5 Hz, 2H), 4.97, (s, 1H), 6.99-7.02 (m, 1H), 7.25-7.43 (m, 6H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 49.3, 50.9, 118.1, 126.5, 126.9, 127.8, 128.4, 128.8, 137.9, 138.2; MS Anal. Calcd [-CN]: 228.07 Found: 228.10. This compound is known.[5]



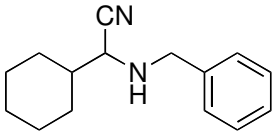
13l: Synthesized according to the general procedure to obtain 2-(benzylamino)-2-(pyridin-3-yl)acetonitrile as a yellow solid (39 mg, 87%). m.p. 103-105 °C. ^{1}H NMR ($CDCl_3$, 250 MHz) δ 2.47 (br s, 1H), 4.03 (AB, q, *J* = 15.0 Hz, 2H), 4.81 (s, 1H), 7.27-7.44 (m, 6H), 7.88-7.93 (m, 1H), 8.63-8.65 (m, 1H), 8.80 (d, *J* = 5.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 51.0, 117.5, 123.4, 127.6, 128.1, 128.5, 130.5, 134.8, 137.4, 148.5, 150.1. This compound is known.[6]



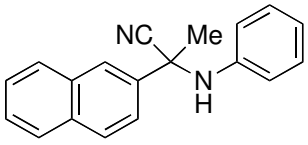
13m: Synthesized according to the general procedure to obtain (E)-2-(benzylamino)-4-phenylbut-3-enenitrile as a yellow solid (49 mg, 98%). m.p. 109-115 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.62 (br s, 1H), 4.01 (AB, q, *J* = 14.0 Hz, 2H), 4.40 (dd, *J* = 8.0 Hz, 1H), 6.19 (dd, *J* = 12.0 Hz, 1H), 6.93 (d, *J* = 20.0 Hz), 7.28-7.42 (m, 10H). This compound is known.[7]



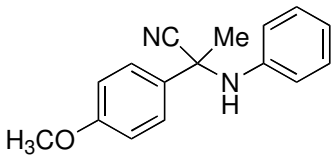
13n: Synthesized according to the general procedure to obtain 2-(benzylamino)pentanenitrile as a white oil (27 mg, 70%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 0.94 (t, *J* = 7.5 Hz, 3H), 1.46-1.61 (m, 2H), 1.71-1.80 (m, 2H), 3.50 (t, *J* = 7.5 Hz, 1H), 3.95 (AB, q, *J* = 12.5 Hz, 2H), 7.27-7.36 (m, 5H). This compound is known.[8]



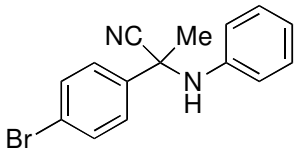
13o: Synthesized according to the general procedure to obtain 2-(benzylamino)-2-cyclohexylacetonitrile as a white solid (28 mg, 62%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 1.09-1.30 (m, 5H), 1.67-1.92 (m, 6H), 3.31 (d, *J* = 5.0 Hz, 1H), 3.96 (AB, q, *J* = 12.5 Hz, 2H), 7.27-7.38 (m, 5H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 25.9, 26.3, 29.2, 30.0, 51.8, 55.8, 119.9, 128.6, 128.8, 138.8.



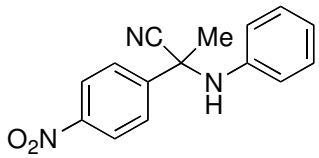
15a: Synthesized according to the general procedure to obtain 2-(naphthalen-2-yl)-2-(phenylamino)propanenitrile as an orange solid (50 mg, 92%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 2.02 (s, 3H), 4.37 (br s, 1H), 6.57 (d, *J* = 7.5 Hz, 2H), 6.76 (t, *J* = 7.5 Hz, 1H), 7.09 (t, *J* = 7.5 Hz, 2H), 7.51-7.56 (m, 2H), 7.68 (d, *J* = 7.5 Hz, 1H), 7.86-7.90 (m, 3H), 8.15 (s, 1H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 33.2, 57.3, 113.2, 115.8, 120.0, 122.0, 124.3, 126.6, 127.6, 128.2, 129.0, 129.3, 133.1, 143.6. This compound is known.[1]



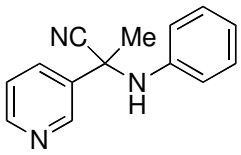
15b: Synthesized according to the general procedure to obtain 2-(4-methoxyphenyl)-2-(phenylamino)propanenitrile as a white solid (22 mg, 44%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 1.92 (s, 3H), 3.82 (s, 3H), 4.26 (br s, 1H), 6.56 (d, *J* = 7.5 Hz, 2 H), 6.80 (t, *J* = 10.0 Hz, 1H), 6.92 (d, *J* = 10.0 Hz, 2H), 7.13 (t, *J* = 7.5 Hz, 2H), 7.52 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 33.4, 55.3, 56.7, 114.5, 115.9, 119.9, 126.2, 129.0, 143.6, 159.6; MS Anal. Calcd [-CN]: 225.12 Found: 225.00.



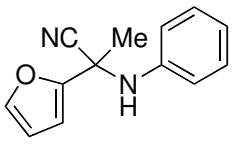
15c: Synthesized according to the general procedure to obtain 2-(4-bromophenyl)-2-(phenylamino)propanenitrile as a white solid (55 mg, 88%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 1.92 (s, 3H), 4.30 (br s, 1H), 6.53 (d, *J* = 7.5 Hz, 2H), 6.77-6.86 (m, 1H), 7.14 (t, *J* = 5.0 Hz, 2H), 7.52-7.63 (m, 3H), 7.84 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 33.4, 56.8, 115.8, 120.4, 126.8, 129.2, 132.5, 143.2. This compound is known.[9]



15d: Synthesized according to the general procedure to obtain 2-(4-nitrophenyl)-2-(phenylamino)propanenitrile as a yellow solid (8 mg, 15%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.98 (s, 3H), 4.39 (br s, 1H), 6.49 (d, *J* = 8.0 Hz, 2H), 6.85 (t, *J* = 8.0 Hz, 1H), 7.14 (t, *J* = 8.0 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 2H), 8.27 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 32.7, 56.4, 115.3, 119.3, 120.4, 123.5, 124.3, 125.8, 128.8, 142.3, 147.7. This compound is known.[1]

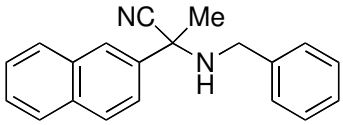


15e: Synthesized according to the general procedure to obtain 2-(phenylamino)-2-(pyridin-3-yl)propanenitrile as an orange solid (18 mg, 40%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.00 (s, 3H), 4.33 (br s, 1H), 6.55 (d, *J* = 8.0 Hz, 2H), 6.85 (t, *J* = 8.0 Hz), 1H), 7.15 (t, *J* = 8.0 Hz, 2H), 7.35-7.38 (m, 1H), 7.93 (d, *J* = 8 Hz, 1H), 8.65 (d, *J* = 4.0 Hz, 1H), 8.93 (s, 1H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 33.0, 55.4, 116.1, 120.5, 124.0, 129.3, 133.2, 135.6, 143.1, 147.2, 150.1, 153.5. This compound is known.[10]

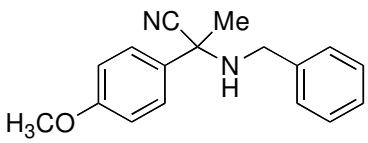


15f: Synthesized according to the general procedure to obtain 2-(furan-2-yl)-2-(phenylamino)propanenitrile as a light yellow solid (35 mg, 83%). m.p. 83-85 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.02 (s, 3H), 4.11 (br s, 1H), 6.37-6.38 (m, 1H), 6.48 (d, *J* = 4.0 Hz, 1H), 6.75 (d, *J* = 8.0 Hz,

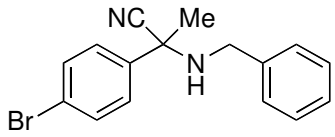
2H), 6.90 (t, *J* = 8.0 Hz, 1 H), 7.20 (t, *J* = 4.0 Hz, 2H), 7.43 (s, 1H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 28.8, 52.8, 108.4, 110.9, 117.2, 119.3, 121.3, 129.4, 143.4, 150.8, 152.2, 156.6. This compound is known.[10]



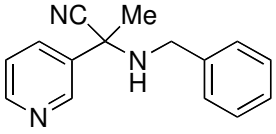
15g: Synthesized according to the general procedure to obtain 2-(benzylamino)-2-(naphthalen-2-yl)propanenitrile as a white solid (19 mg, 33%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.87 (s, 3H), 3.76 (AB, q, *J* = 12.0 Hz, 2H), 7.25-7.38 (m, 6H), 7.51-7.56 (m, 2H), 7.76-7.79 (m, 1H), 7.85-7.93 (m, 3H), 8.19 (s, 1H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 31.0, 49.6, 60.6, 122.6, 125.2, 126.5, 126.6, 127.3, 127.5, 128.1, 128.2, 128.4, 129.0, 132.9, 133.2, 136.9; MS Anal. Calcd [-CN]: 259.14 Found: 258.11.



15h: Synthesized according to the general procedure to obtain 2-(benzylamino)-2-(4-methoxyphenyl)propanenitrile as a light brown solid (11 mg, 35%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 1.80 (s, 3H), 3.76 (AB, q, *J* = 7.5 Hz, 2H), 3.85 (s, 3H), 6.98 (d, *J* = 7.5Hz, 2H), 7.27-7.41 (m, 5H), 7.65 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 31.2, 49.4, 55.3, 59.9, 114.1, 126.7, 127.3, 128.2, 128.4, 139.0, 159.7; MS Anal. Calcd [-CN]: 239.13 Found: 238.08. This compound is known.[11]



15i: Synthesized according to the general procedure to obtain 2-(benzylamino)-2-(4-bromophenyl)propanenitrile as a white solid (35 mg, 55%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.61 (br s, 1H), 1.75 (s, 3H), 3.71 (AB, q, *J* = 12.0 Hz, 2H), 7.27-7.36 (m, 5H), 7.53-7.63 (m, 3H), 8.39-8.42 (m, 1H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 31.3, 49.6, 60.1, 122.7, 127.4, 127.5, 128.2, 128.6, 132.1. This compound is known.[11]



15j: Synthesized according to the general procedure to obtain 2-(benzylamino)-2-(pyridin-3-yl)propanenitrile as a white solid (28 mg, 60%). ^{1}H NMR ($CDCl_3$, 250 MHz) δ 1.84 (s, 3H), 2.86 (br s,

1H), 3.75 (AB, q, J = 7.5 Hz, 2H), 7.28-7.47 (m, 6H), 7.99-8.04 (m, 1H), 8.62-8.65 (m, 1H), 8.98 (d, J = 2.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 63 MHz) δ 31.2, 49.7, 59.0, 123.6, 127.7, 128.3, 133.6, 135.6, 147.6, 150.2.

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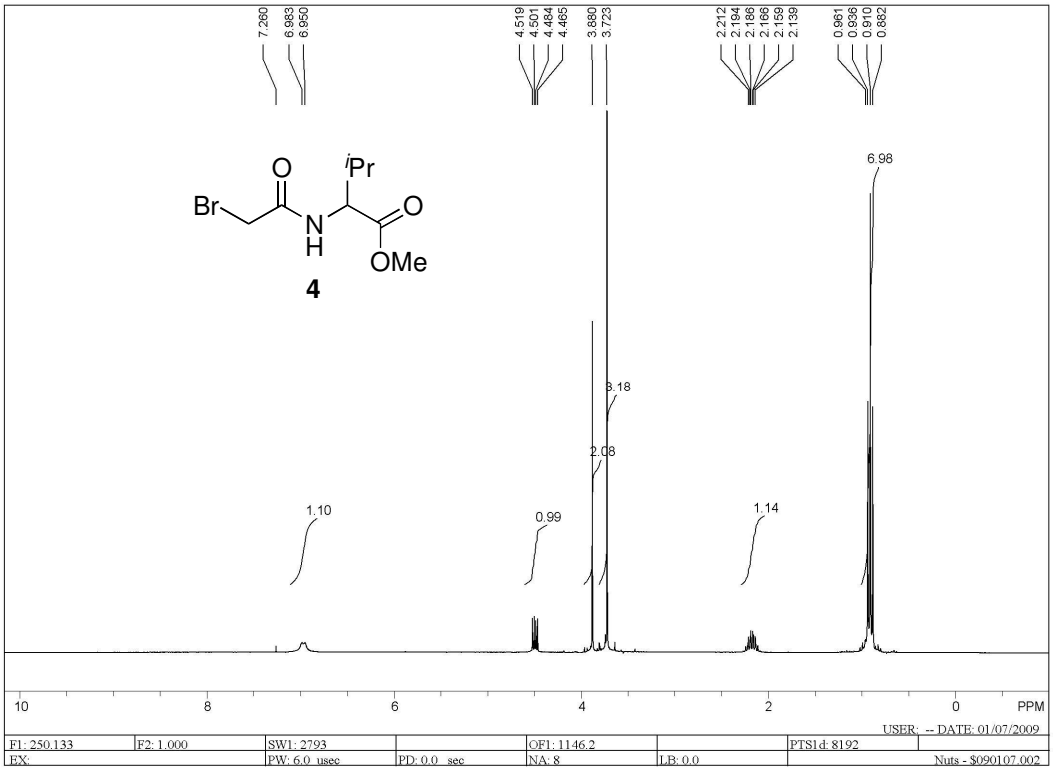
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2.166
2.159
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2.08
1.10
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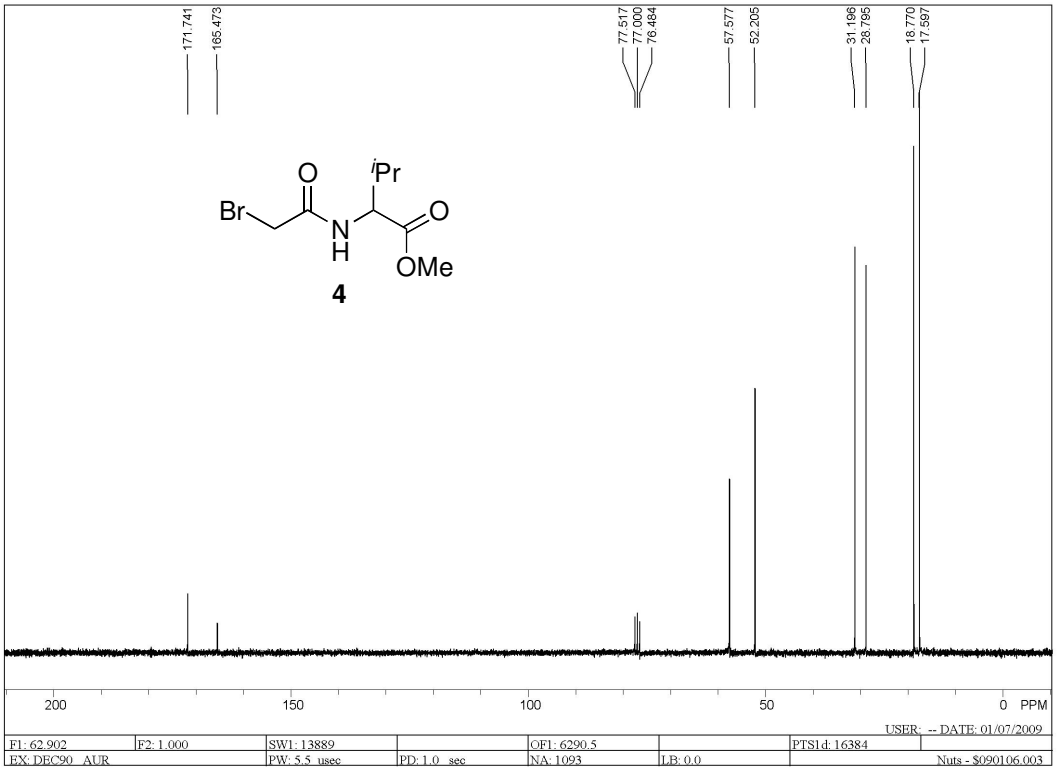
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OMe
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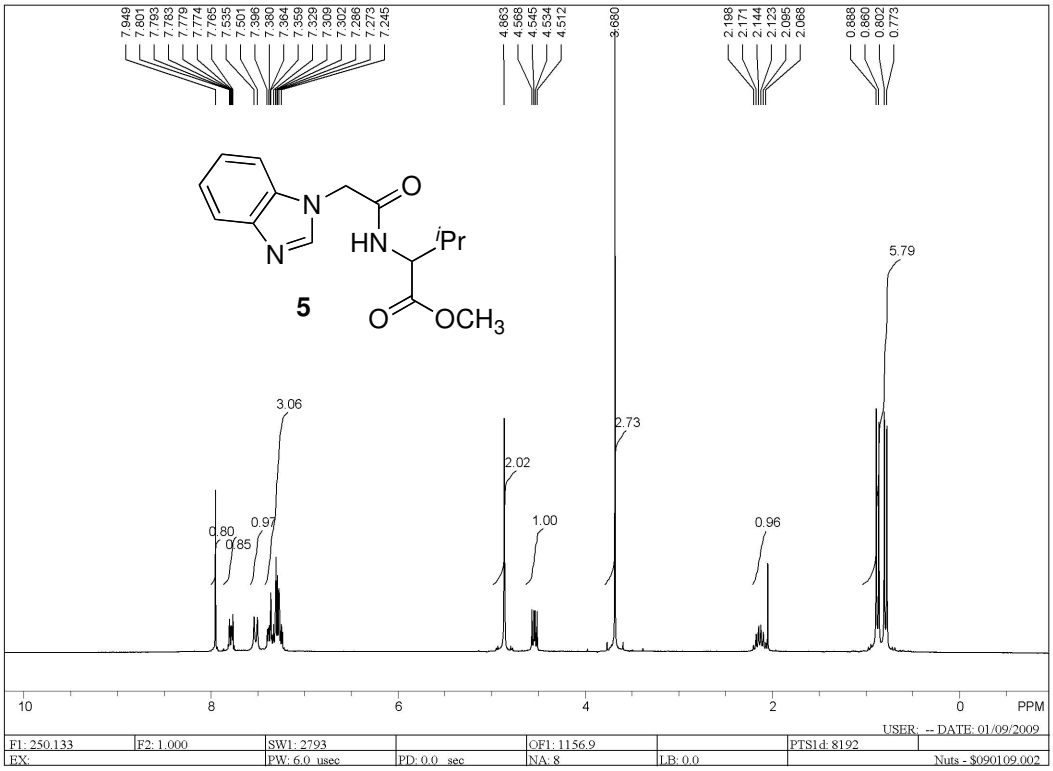
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7.302
7.286
7.273
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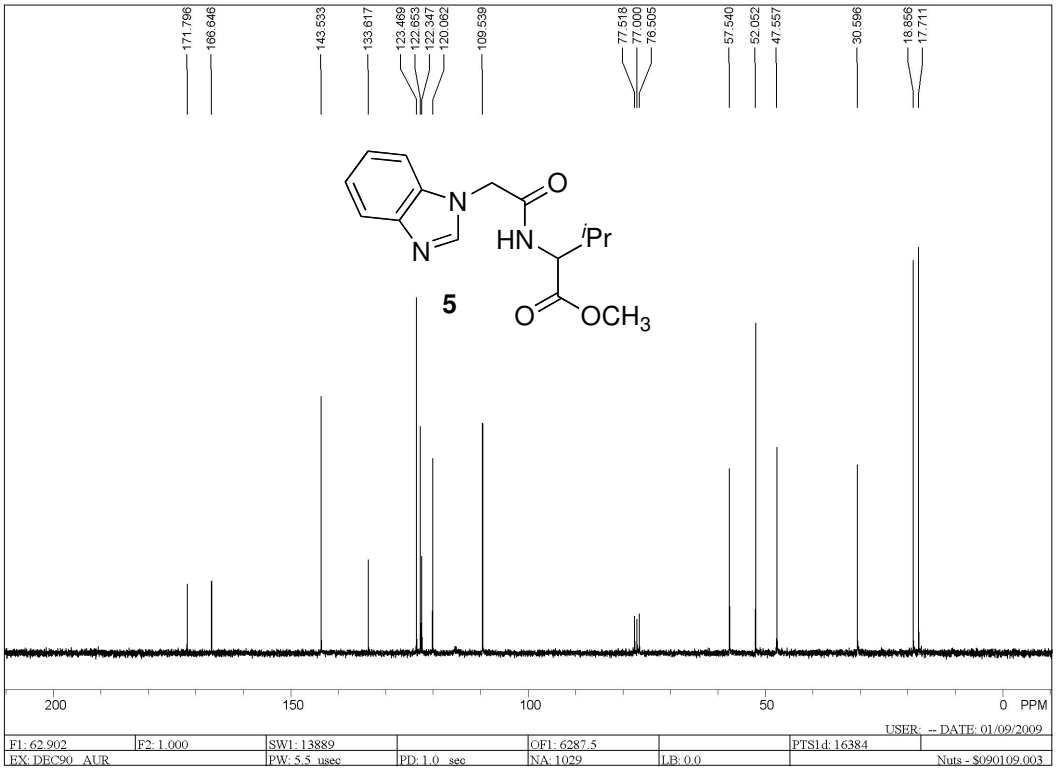
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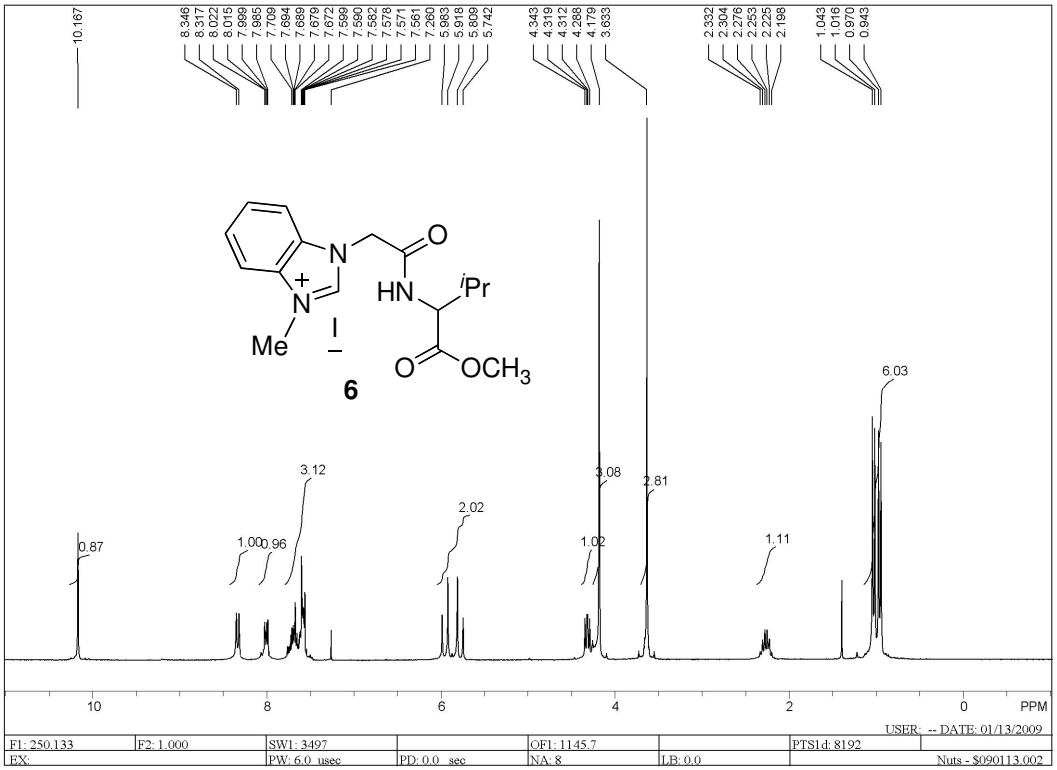
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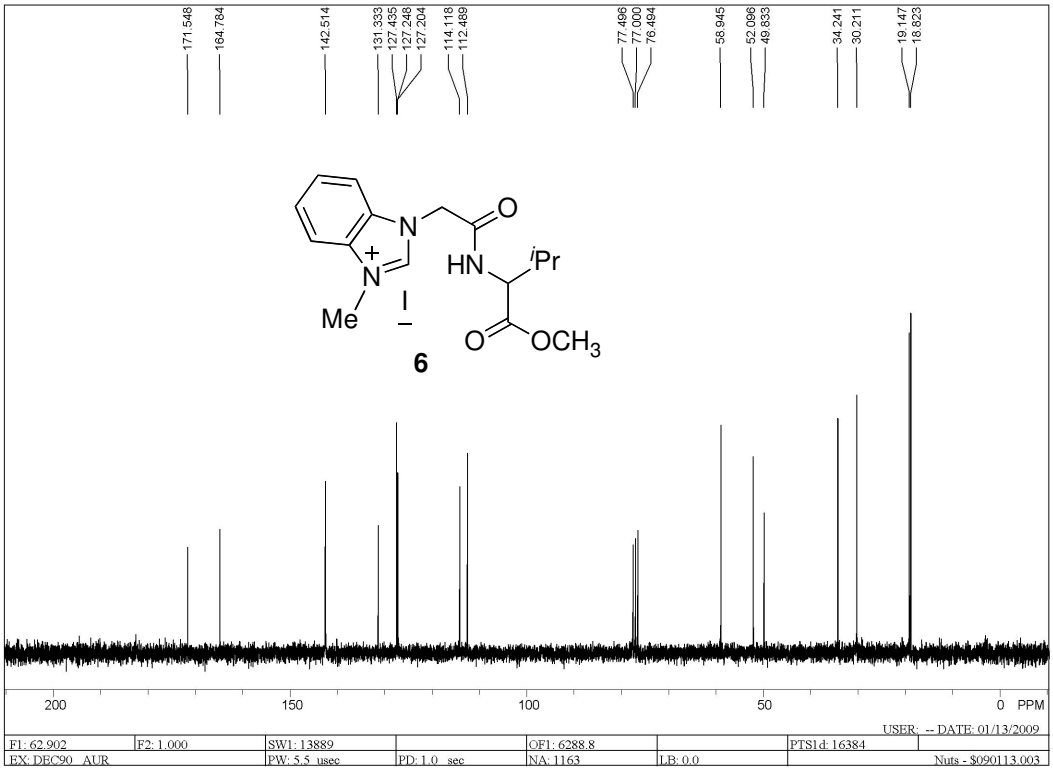
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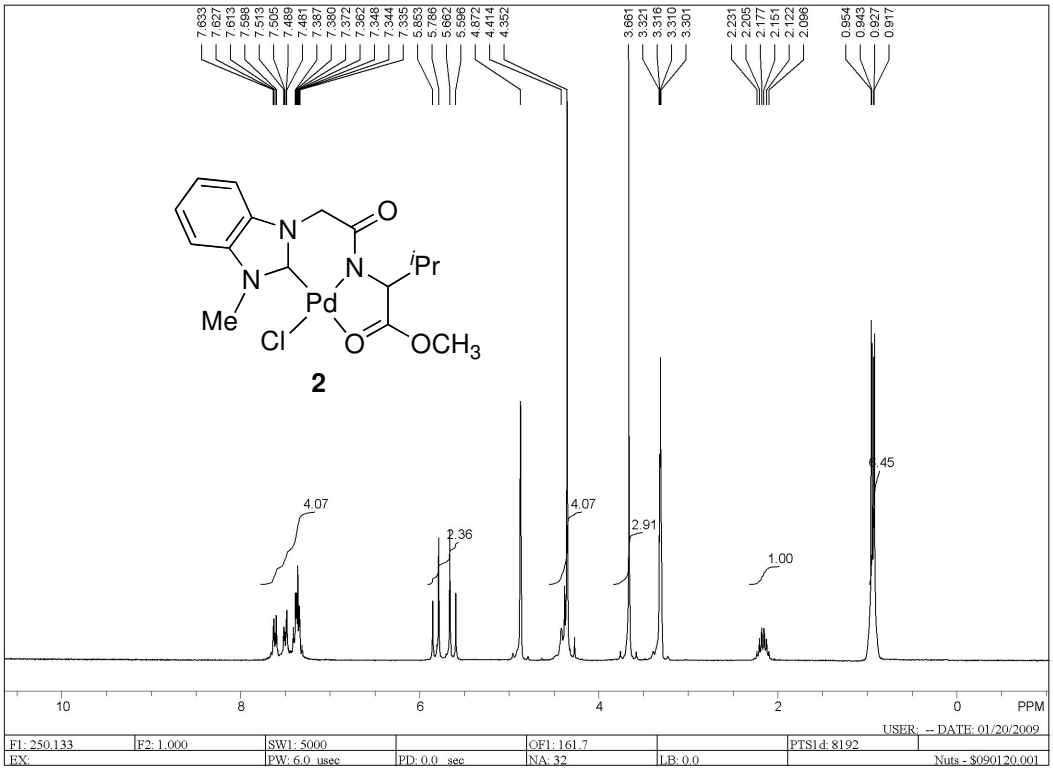
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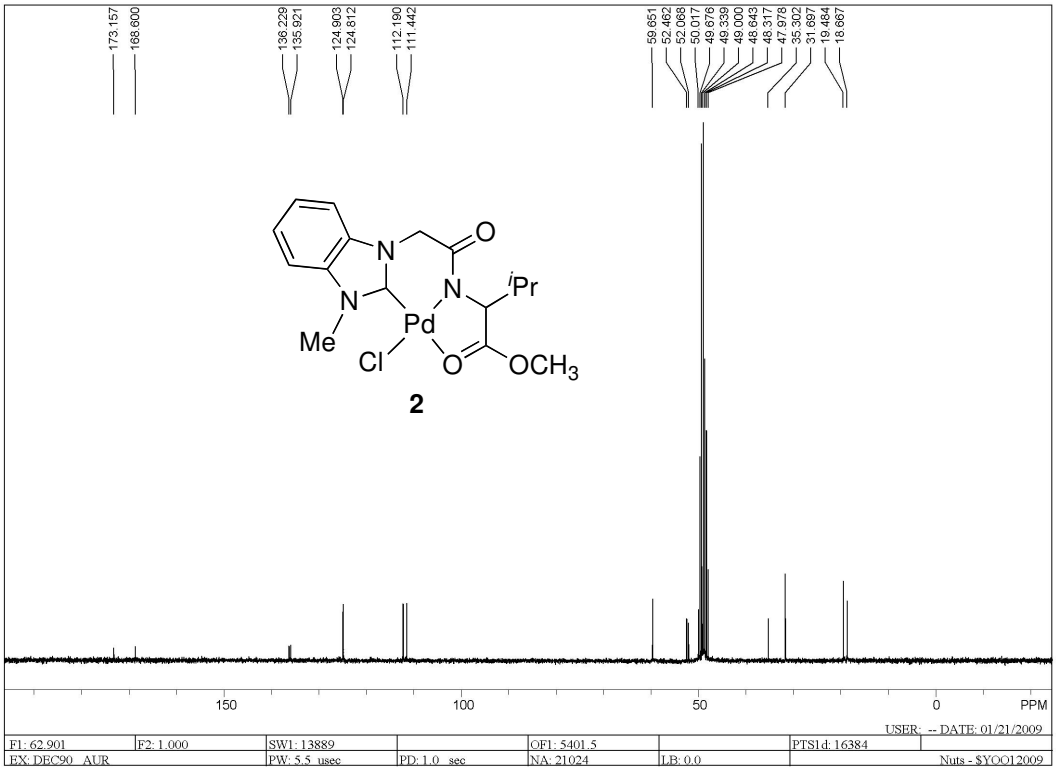
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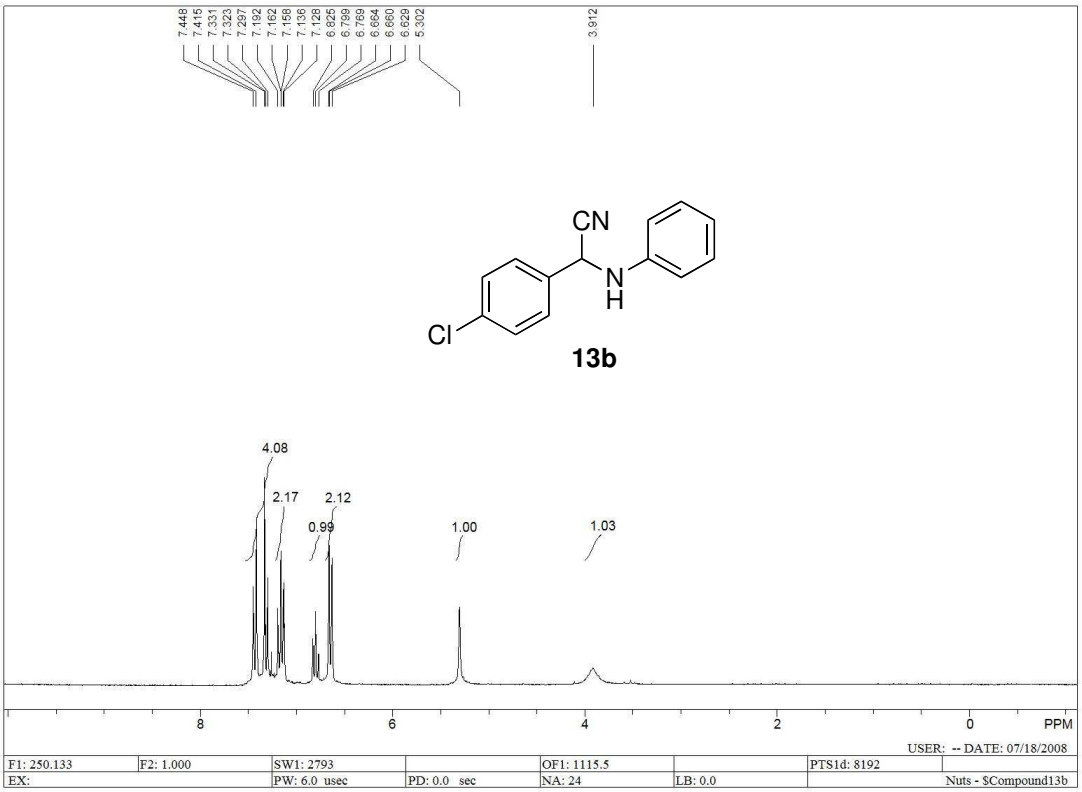
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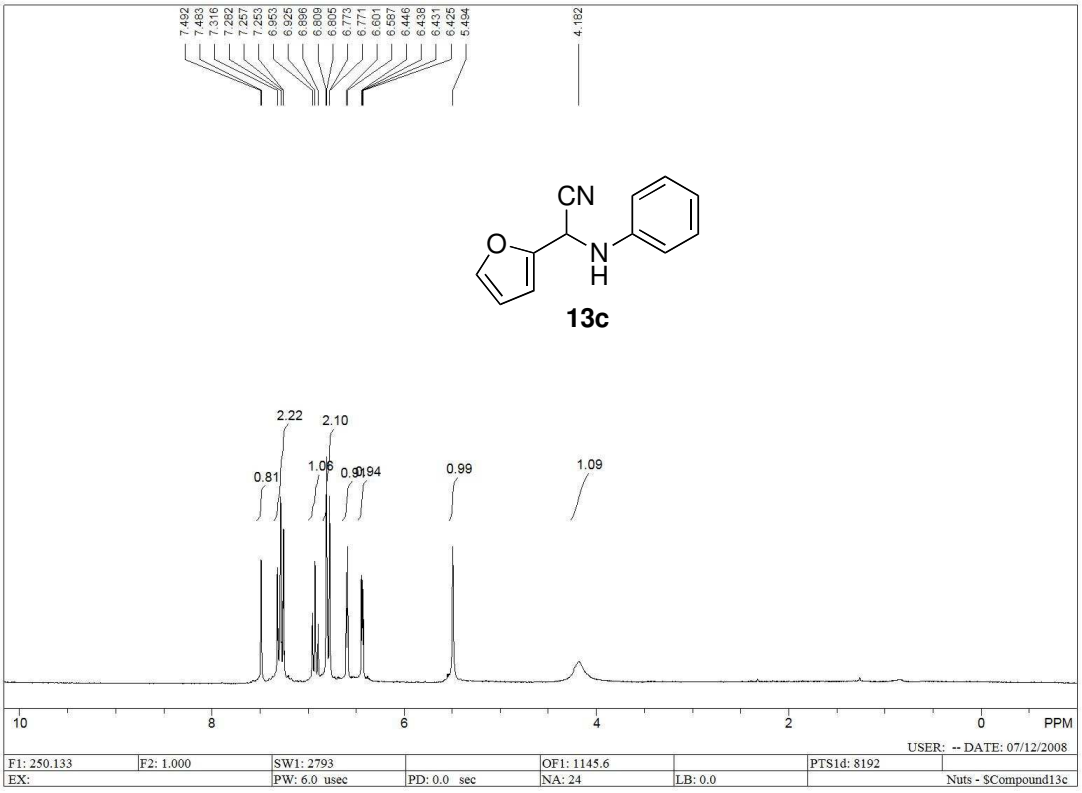
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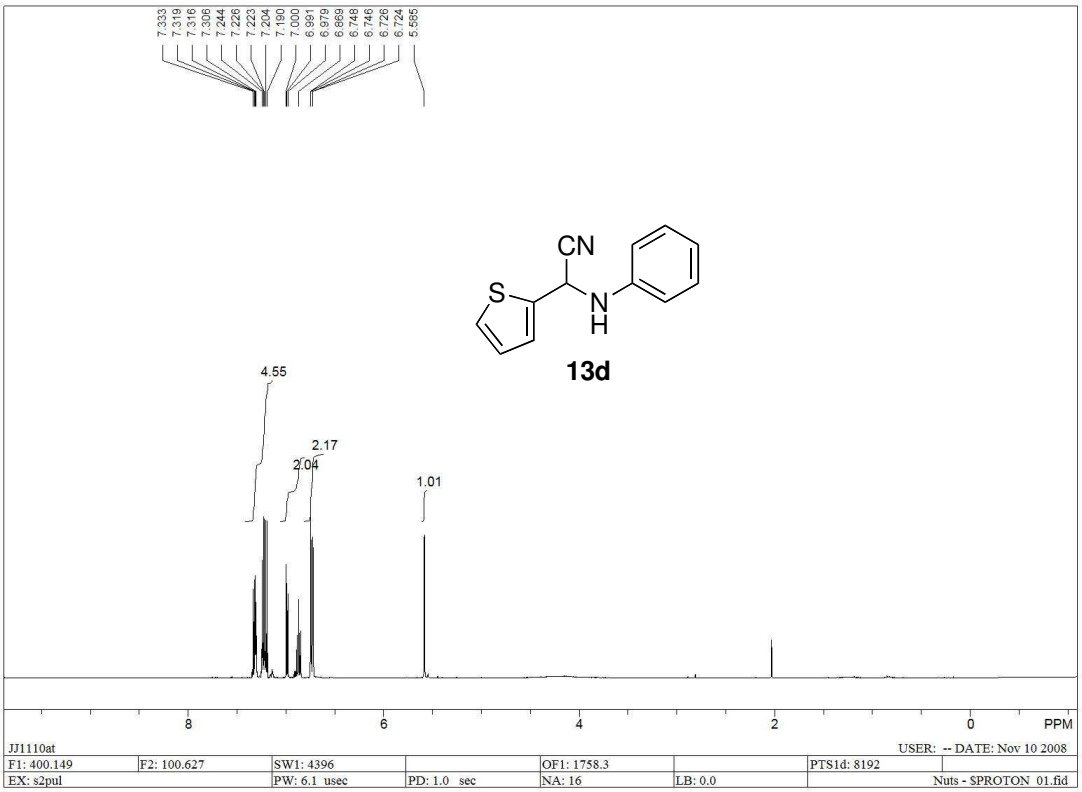
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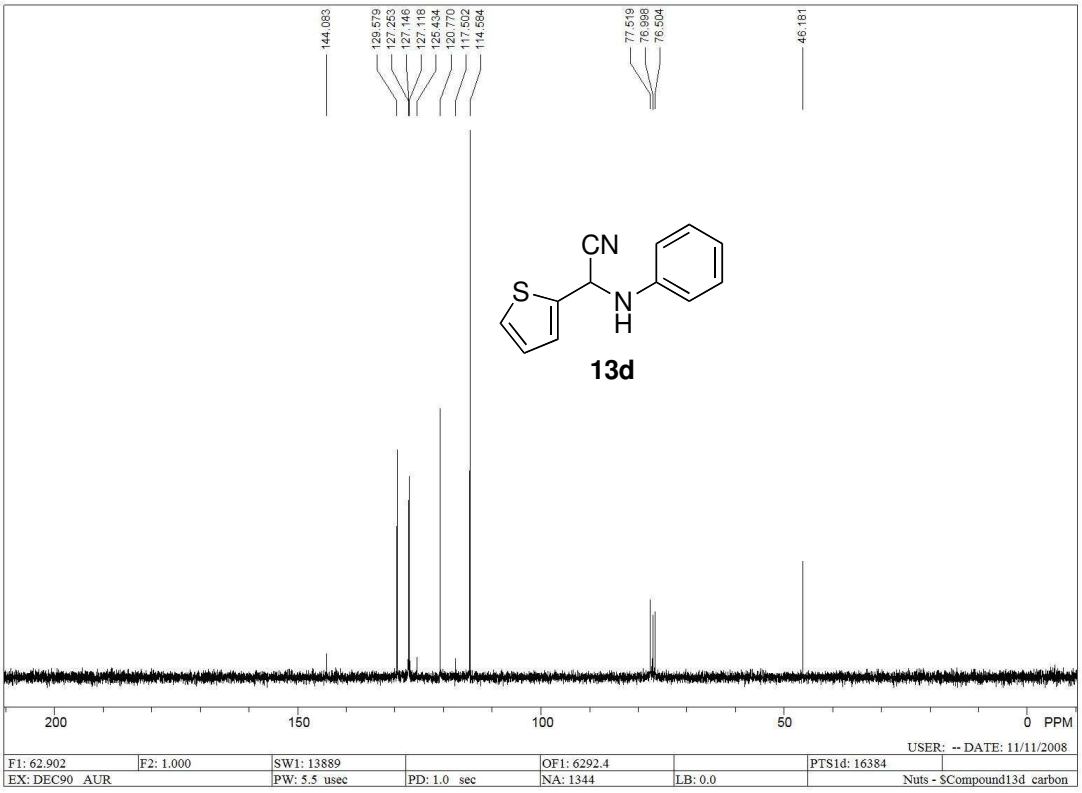
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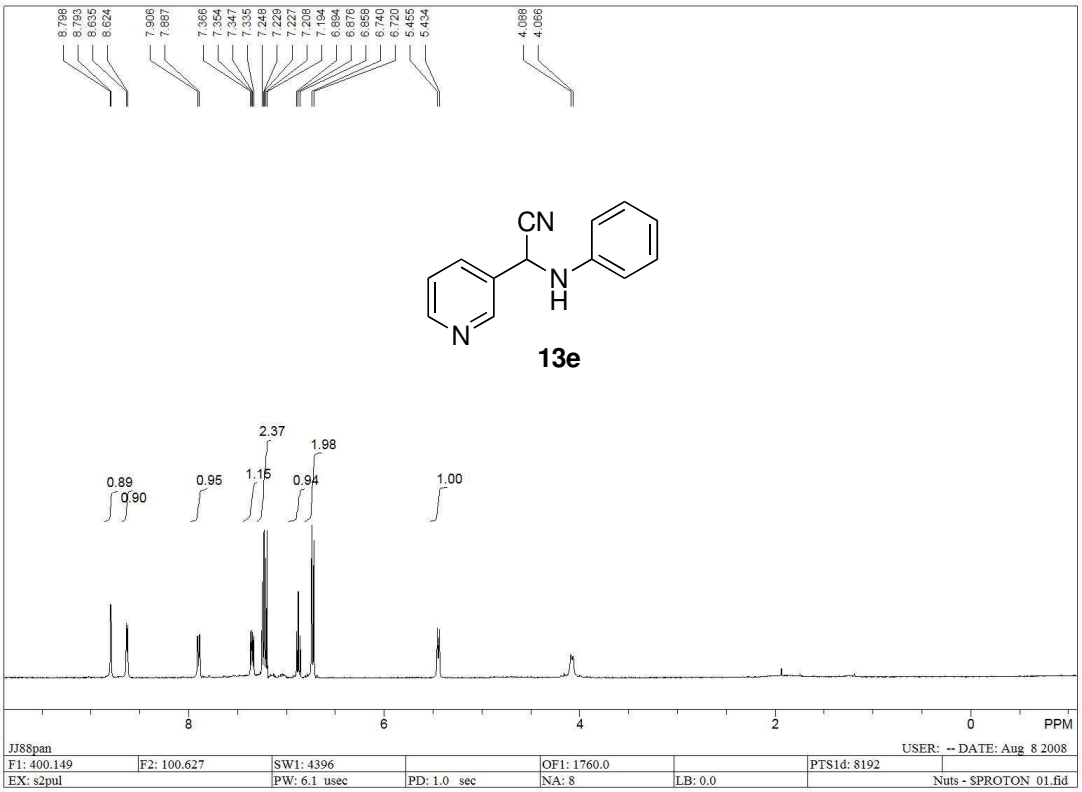
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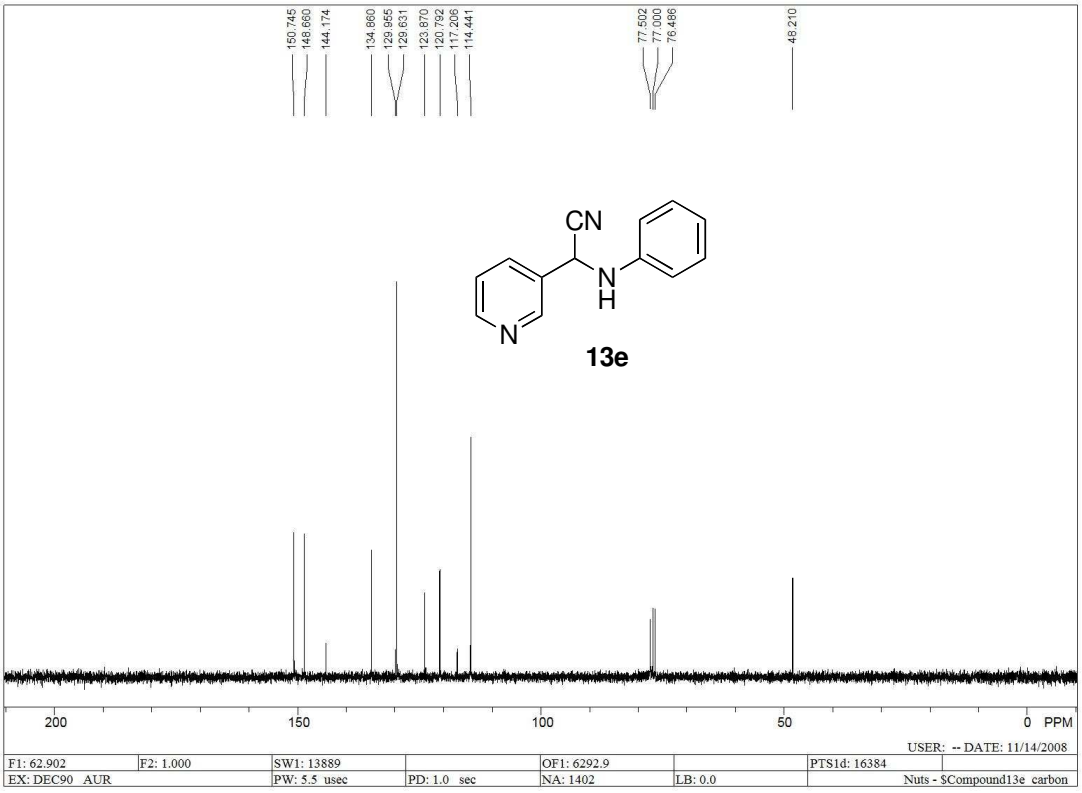
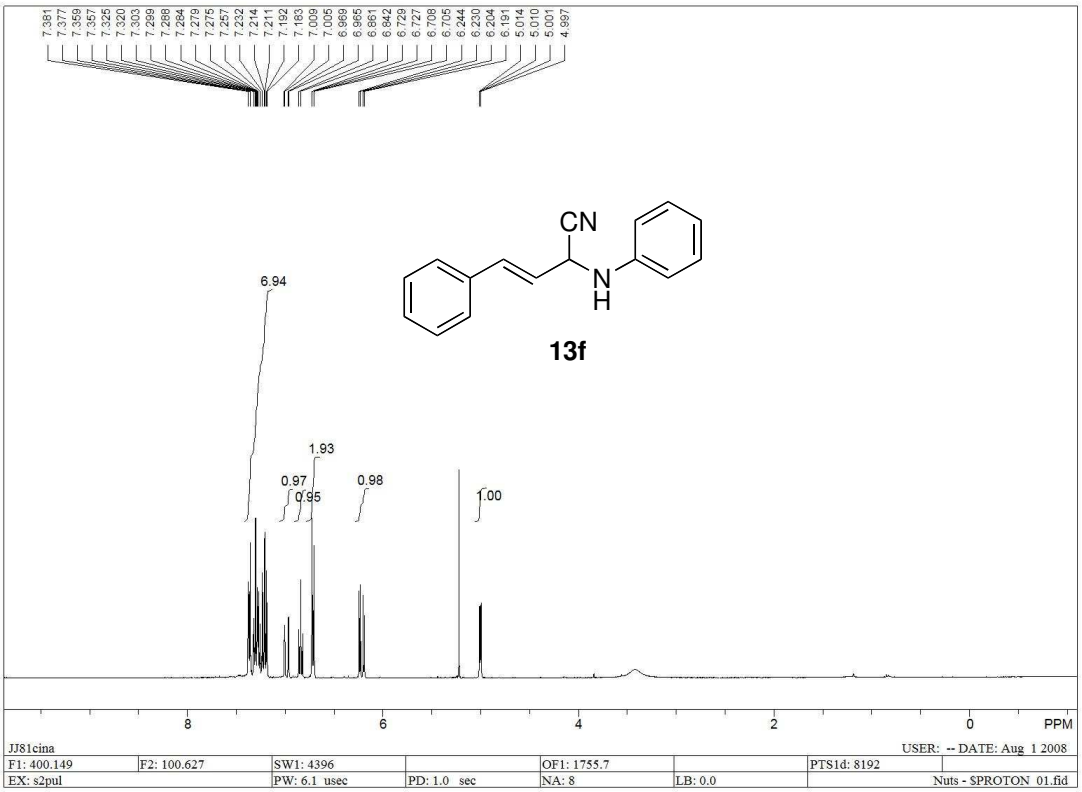
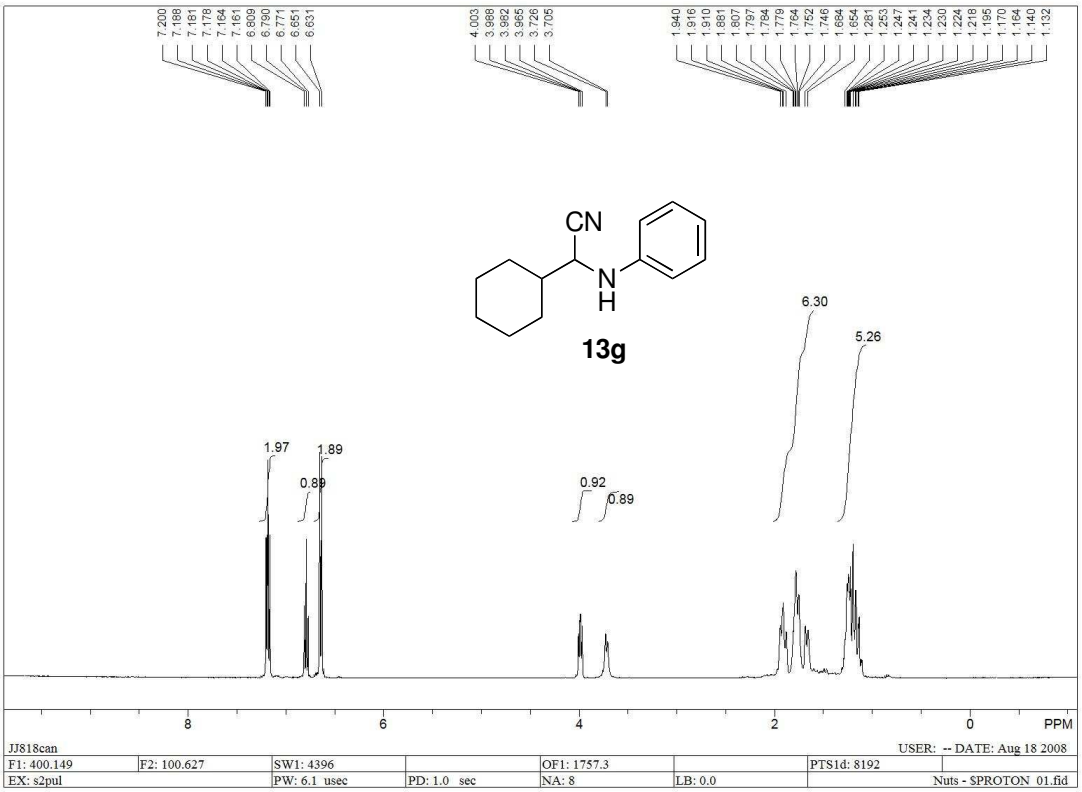
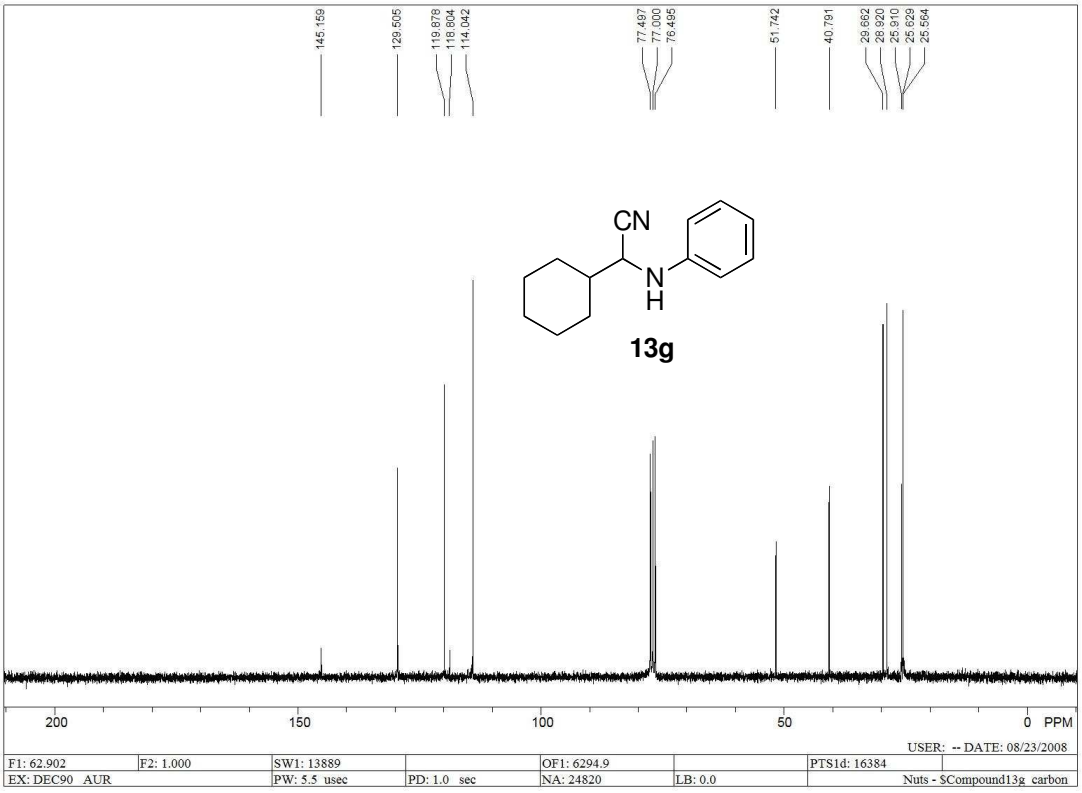
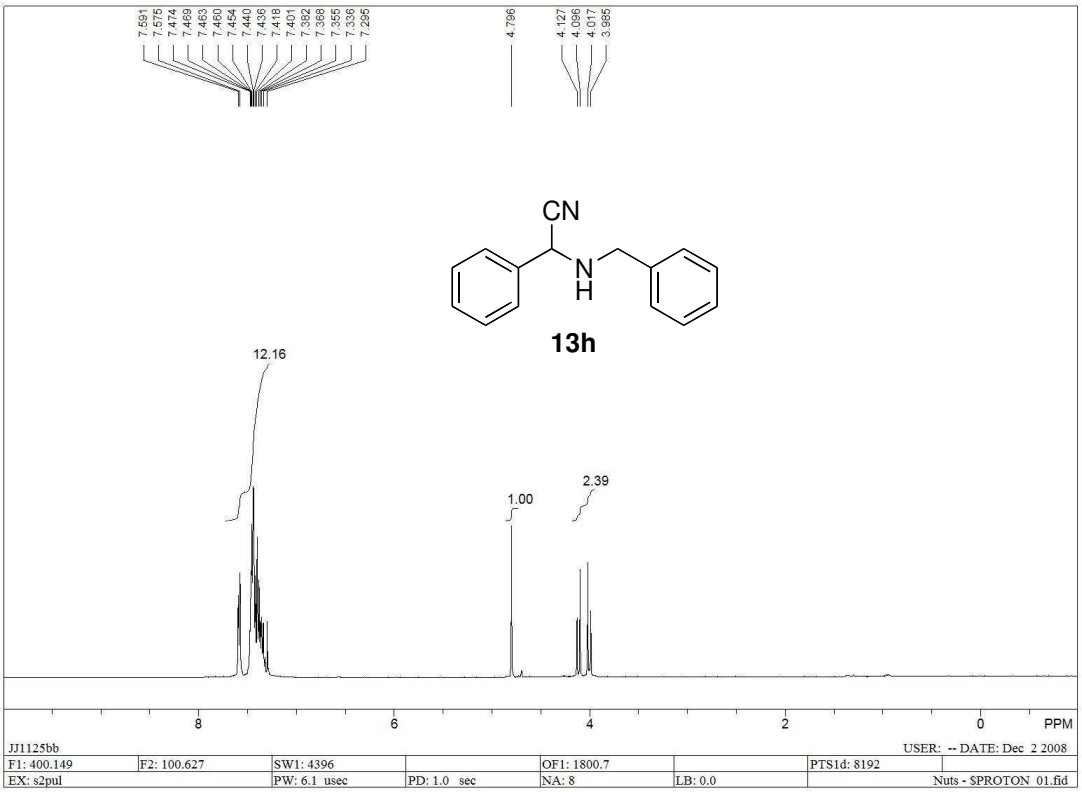
PW: 6.1 usec
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON 01.fid

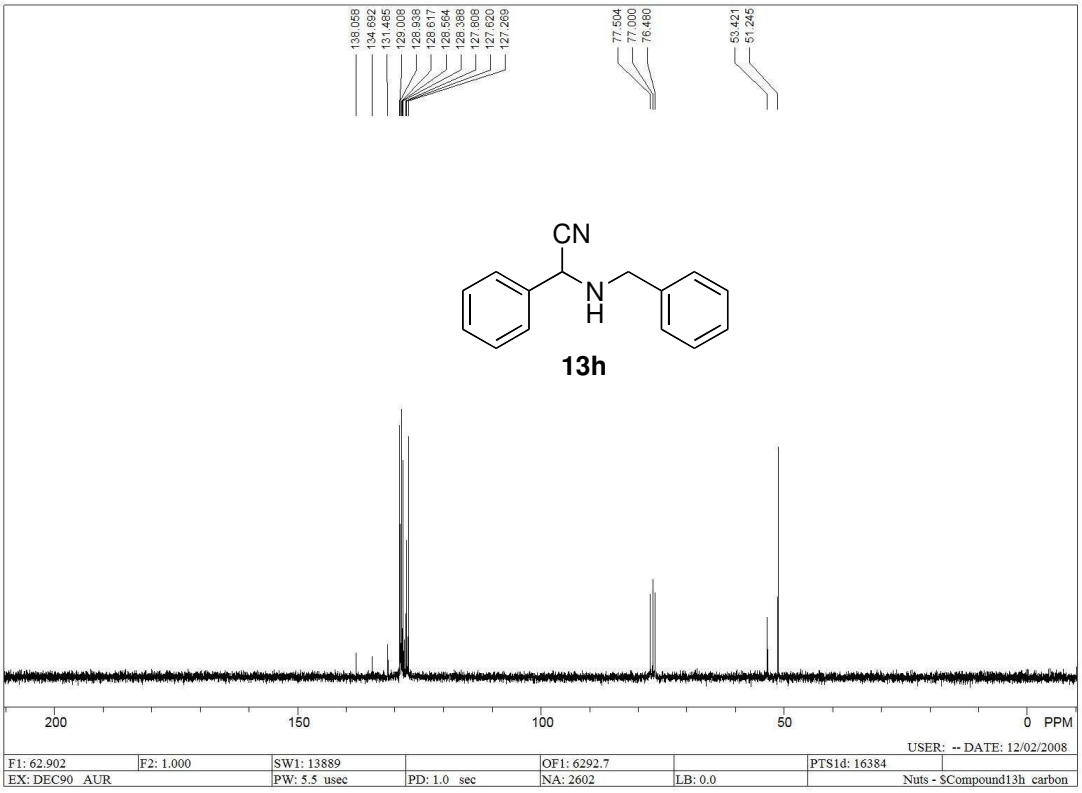

150.745
148.660
144.174
134.860
129.955
129.631
123.870
120.792
117.206
114.441
77.502
77.000
76.486
48.210
CN
N
H
N
13e
200
150
100
50
0
PPM
USER: -- DATE: 11/14/2008
F1: 62.902
F2: 1.000
SW1: 13889
OF1: 6292.9
PTS1d: 16384
EX: DEC90 AUR
PW: 5.5 usec
PD: 1.0 sec
NA: 1402
LB: 0.0
Nuts - $Compound13e carbon

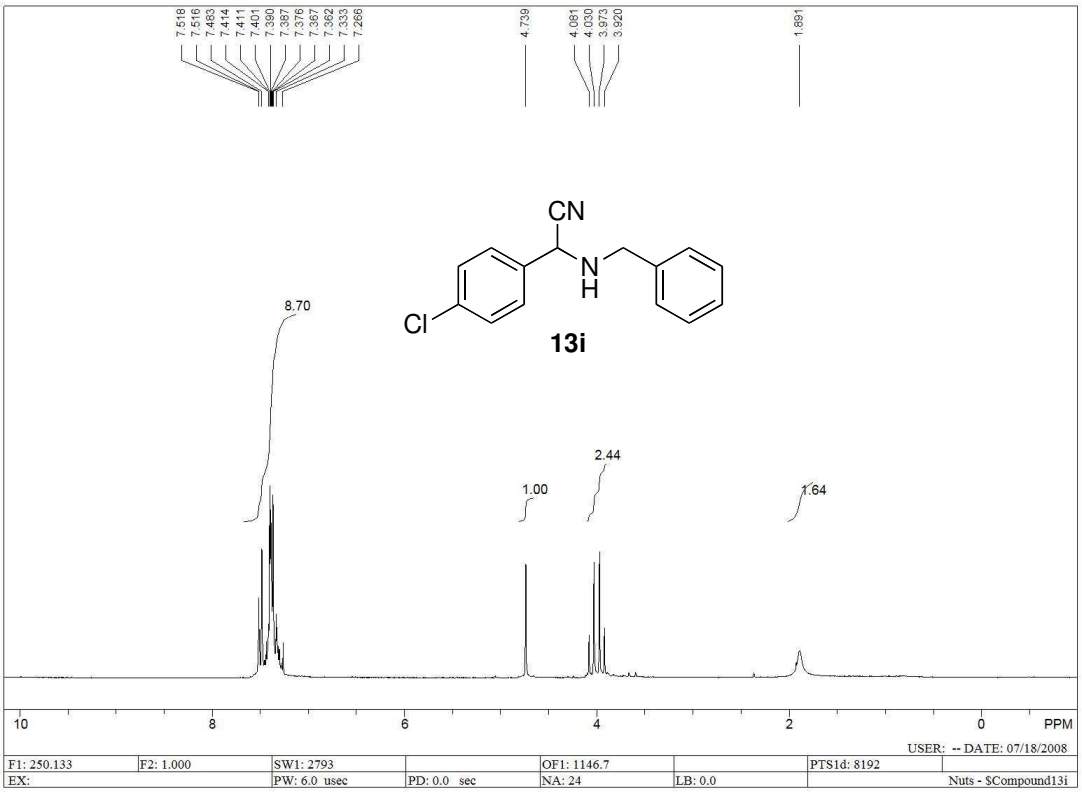

7.381
7.377
7.359
7.357
7.325
7.320
7.303
7.299
7.288
7.284
7.279
7.275
7.257
7.232
7.214
7.211
7.192
7.183
7.009
7.005
6.969
6.965
6.861
6.842
6.729
6.727
6.708
6.705
6.244
6.230
6.204
6.191
5.014
5.010
5.001
4.997
CN
N
H
13f
6.94
1.93
0.97
0.95
0.98
1.00
8
6
4
2
0
PPM
JJ81cina
USER: -- DATE: Aug 1 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1755.7
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON 01.fid

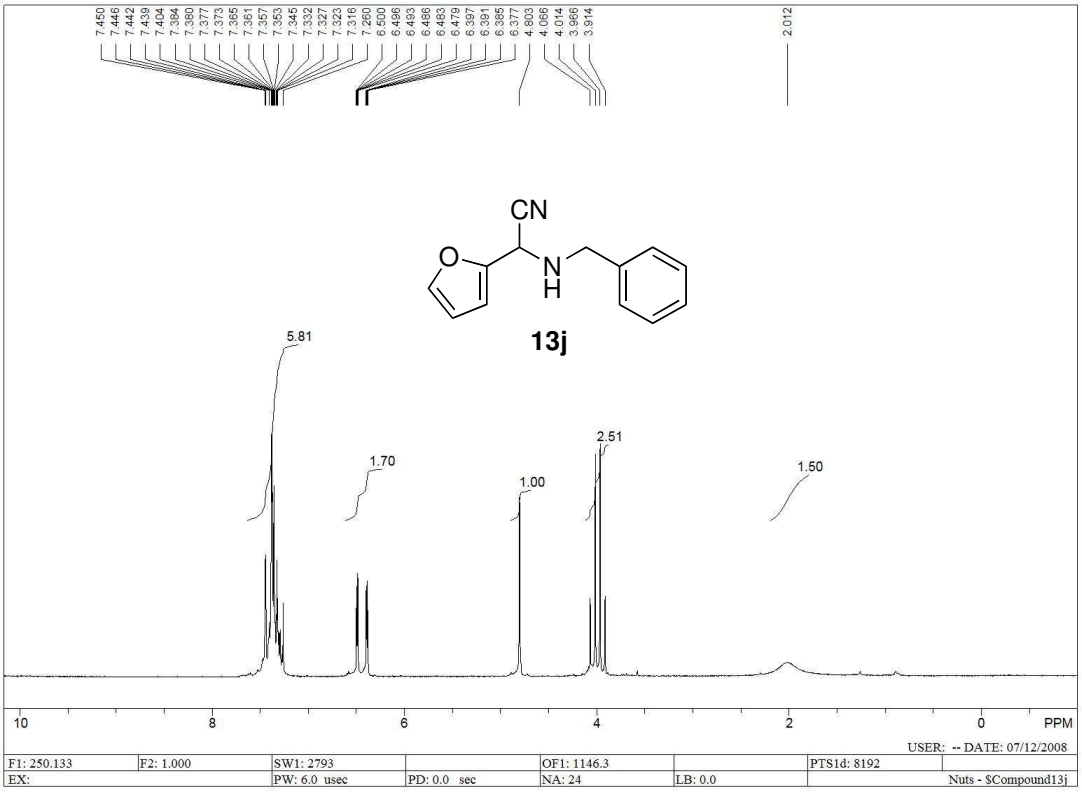

7.200
7.188
7.181
7.178
7.164
7.161
6.809
6.790
6.771
6.651
6.631
4.003
3.988
3.982
3.965
3.726
3.705
1.940
1.916
1.910
1.881
1.807
1.797
1.784
1.779
1.764
1.752
1.746
1.684
1.654
1.281
1.253
1.247
1.241
1.234
1.230
1.224
1.218
1.195
1.170
1.164
1.140
1.132
CN
N
H
13g
6.30
5.26
1.97
1.89
0.89
0.92
0.89
8
6
4
2
0
PPM
JJ818can
USER: -- DATE: Aug 18 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1757.3
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

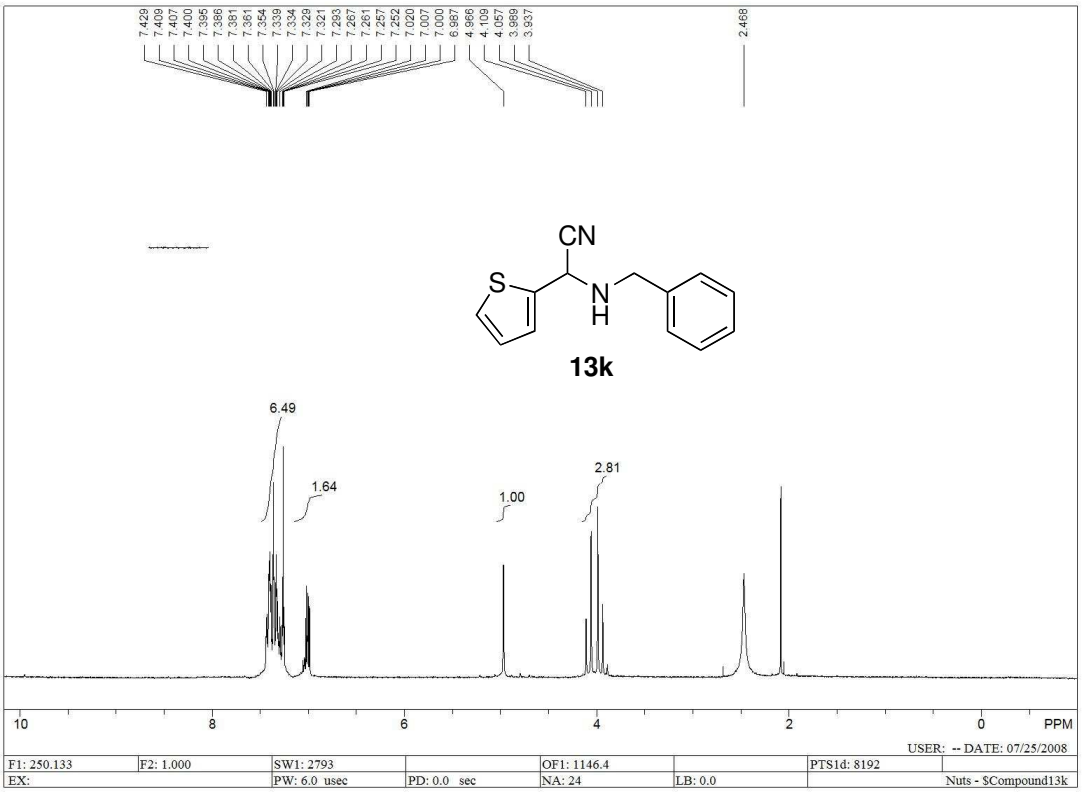

145.159
129.505
119.878
118.804
114.042
77.497
77.000
76.495
51.742
40.791
29.662
28.920
25.910
25.629
25.564
CN
N
H
13g
200
150
100
50
0
PPM
USER: -- DATE: 08/23/2008
F1: 62.902
F2: 1.000
SW1: 13889
OF1: 6294.9
PTS1d: 16384
EX: DEC90_AUR
PW: 5.5 usec
PD: 1.0 sec
NA: 24820
LB: 0.0
Nuts - $Compound13g_carbon

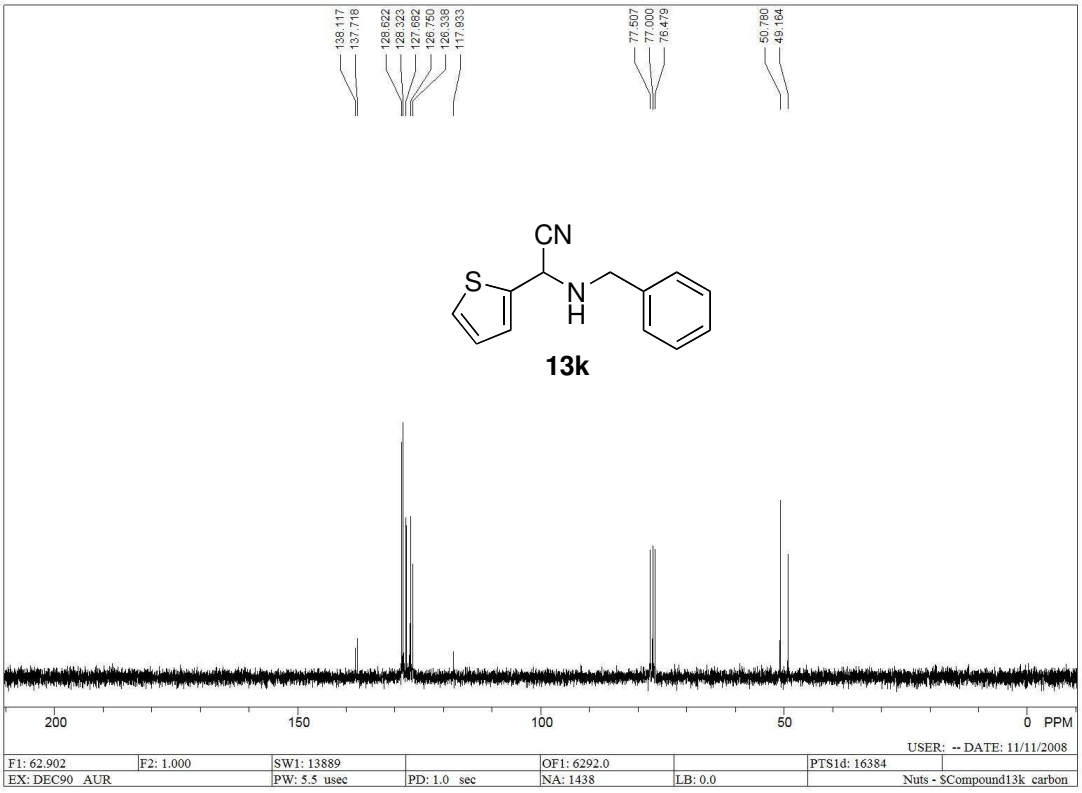

7.591
7.575
7.474
7.469
7.463
7.460
7.454
7.440
7.436
7.418
7.401
7.382
7.368
7.355
7.336
7.295
4.796
4.127
4.096
4.017
3.985
CN
N
H
13h
12.16
1.00
2.39
8
6
4
2
0
PPM
JJ1125bb
USER: -- DATE: Dec 2 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1800.7
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

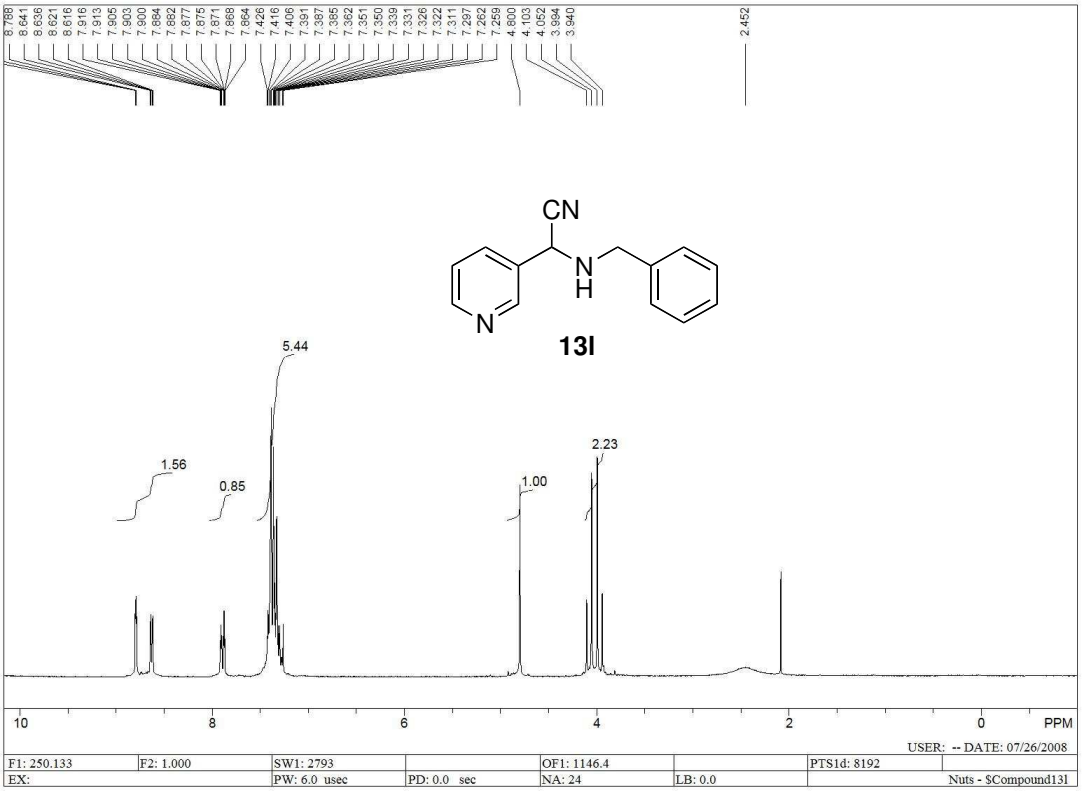

138.058
134.692
131.485
129.008
128.938
128.617
128.564
128.386
127.808
127.620
127.269
77.504
77.000
76.480
53.421
51.245
CN
N
H
13h
200
150
100
50
0
PPM
USER: -- DATE: 12/02/2008
F1: 62.902
F2: 1.000
SW1: 13889
OF1: 6292.7
PTS1d: 16384
EX: DEC90_AUR
PW: 5.5 usec
PD: 1.0 sec
NA: 2602
LB: 0.0
Nuts - $Compound13h_carbon

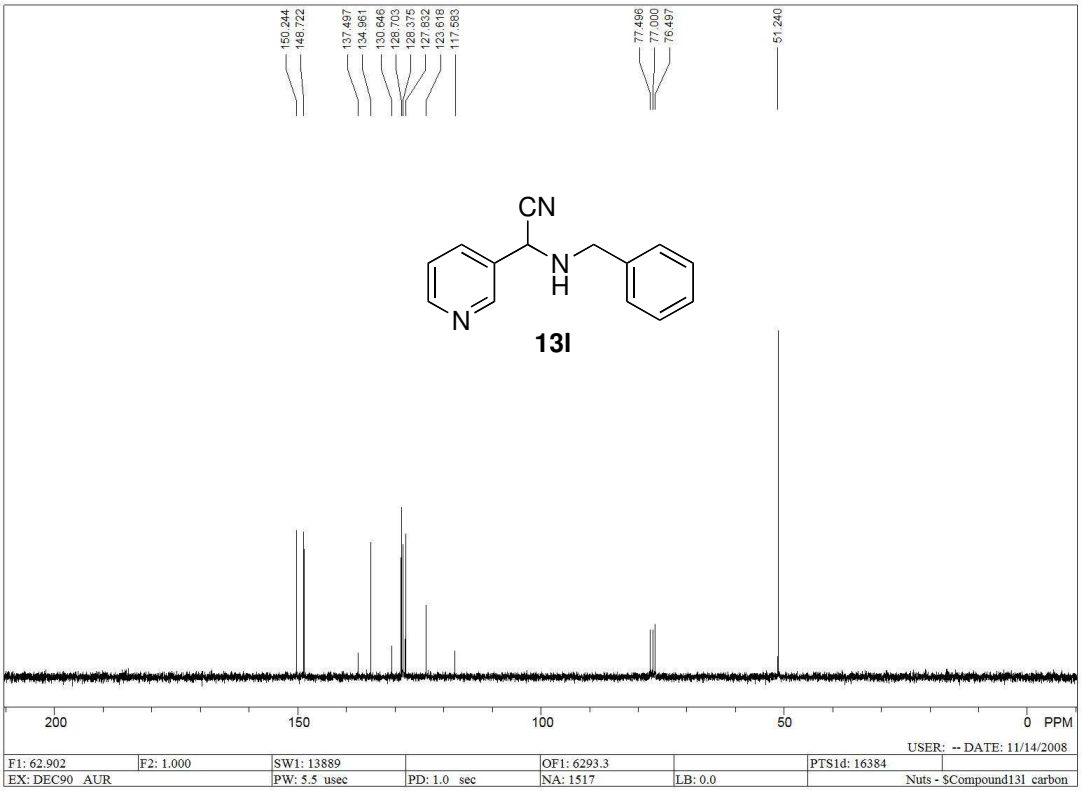

7.518
7.516
7.483
7.414
7.411
7.401
7.390
7.387
7.376
7.367
7.362
7.333
7.266
4.739
4.081
4.030
3.973
3.920
1.891
CN
N
H
Cl
13i
8.70
2.44
1.00
1.64
10
8
6
4
2
0
PPM
USER: -- DATE: 07/18/2008
F1: 250.133
F2: 1.000
SW1: 2793
OF1: 1146.7
PTS1d: 8192
EX:
PW: 6.0 usec
PD: 0.0 sec
NA: 24
LB: 0.0
Nuts - $Compound13i

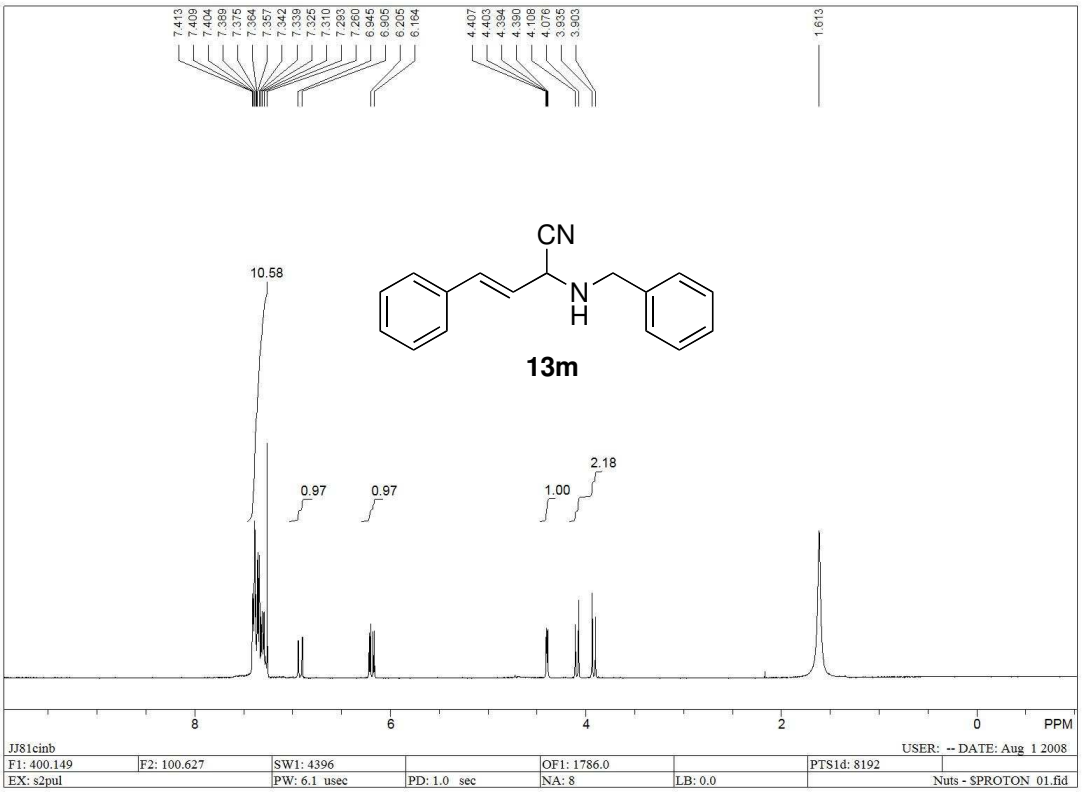

7.450
7.446
7.442
7.439
7.404
7.384
7.380
7.377
7.373
7.365
7.361
7.357
7.353
7.345
7.332
7.327
7.323
7.316
7.260
6.500
6.496
6.493
6.486
6.483
6.479
6.397
6.391
6.385
6.377
4.803
4.066
4.014
3.966
3.914
2.012
CN
O
N
H
13j
5.81
1.70
1.00
2.51
1.50
10
8
6
4
2
0
PPM
USER: -- DATE: 07/12/2008
F1: 250.133
F2: 1.000
SW1: 2793
OF1: 1146.3
PTS1d: 8192
EX:
PW: 6.0 usec
PD: 0.0 sec
NA: 24
LB: 0.0
Nuts - $Compound13j

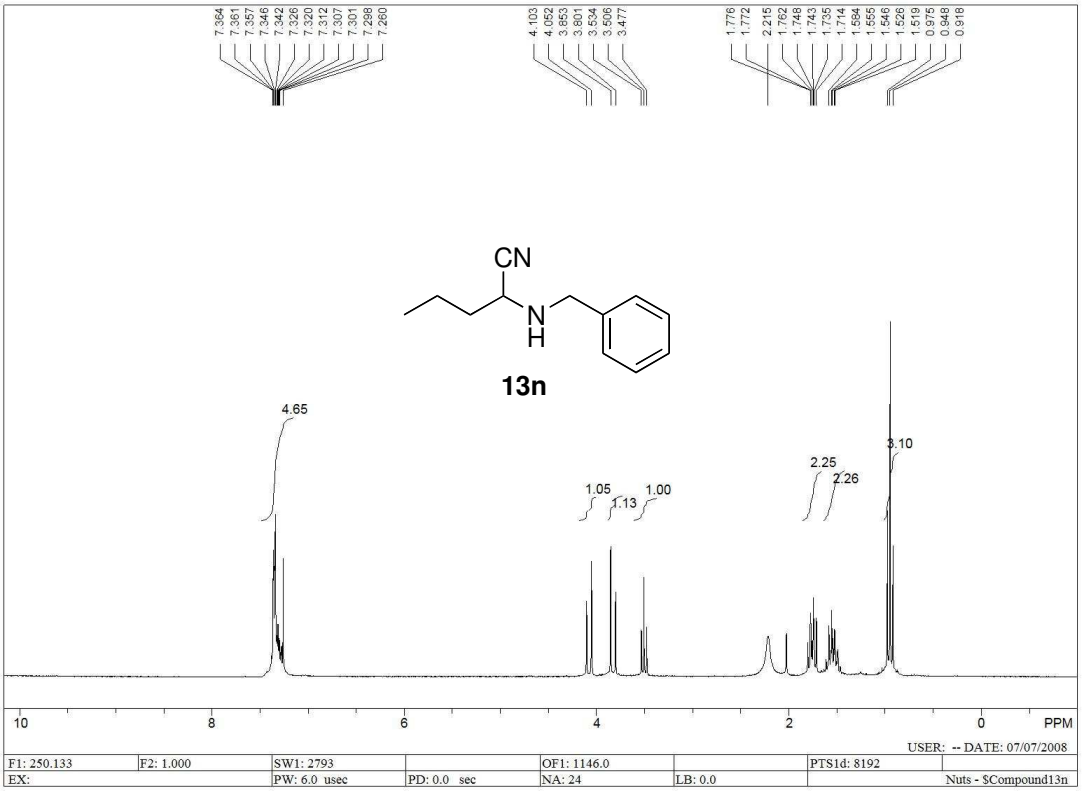

7.429
7.409
7.407
7.400
7.395
7.386
7.381
7.361
7.354
7.339
7.334
7.329
7.321
7.293
7.267
7.261
7.257
7.252
7.020
7.007
7.000
6.987
4.966
4.109
4.057
3.989
3.937
2.468
CN
S
N
H
13k
6.49
1.64
1.00
2.81
10
8
6
4
2
0
PPM
USER: -- DATE: 07/25/2008
F1: 250.133
F2: 1.000
SW1: 2793
OF1: 1146.4
PTS1d: 8192
EX:
PW: 6.0 usec
PD: 0.0 sec
NA: 24
LB: 0.0
Nuts - $Compound13k

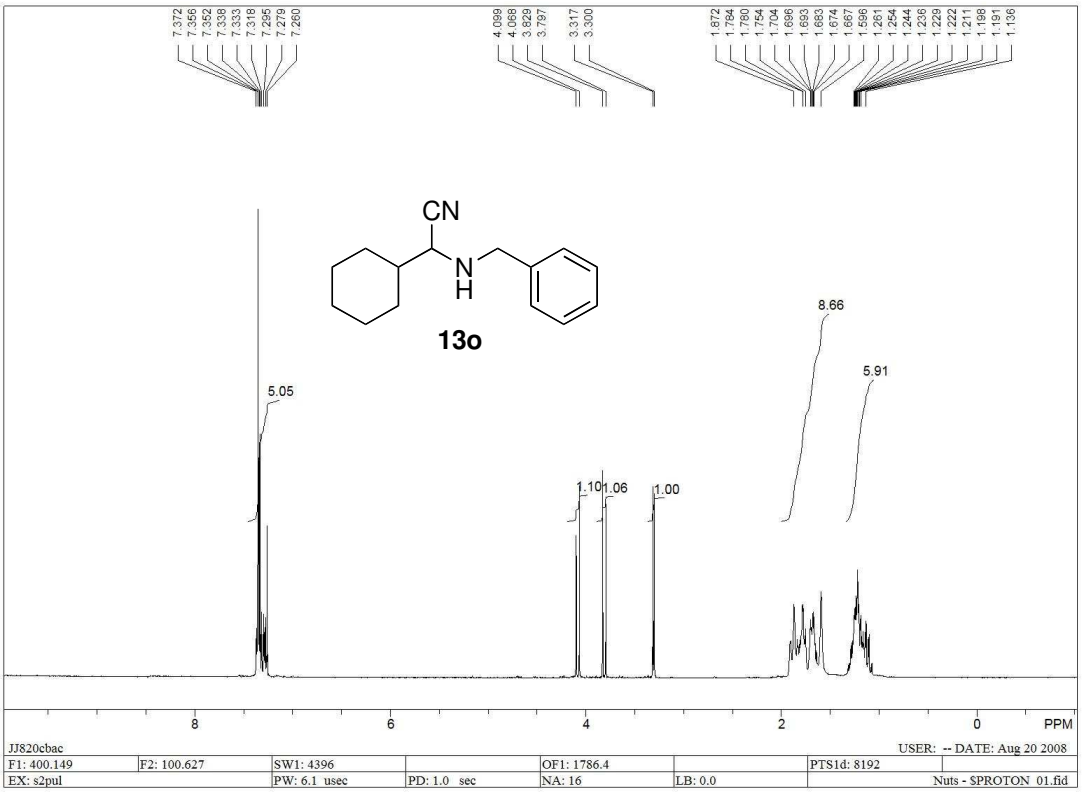

138.117
137.716
128.622
128.323
127.682
126.750
126.338
117.933
77.507
77.000
76.479
50.780
49.164
CN
S
N
H
13k
200
150
100
50
0
PPM
USER: -- DATE: 11/11/2008
F1: 62.902
F2: 1.000
SW1: 13889
OF1: 6292.0
PTS1d: 16384
EX: DEC90_AUR
PW: 5.5 usec
PD: 1.0 sec
NA: 1438
LB: 0.0
Nuts - $Compound13k_carbon

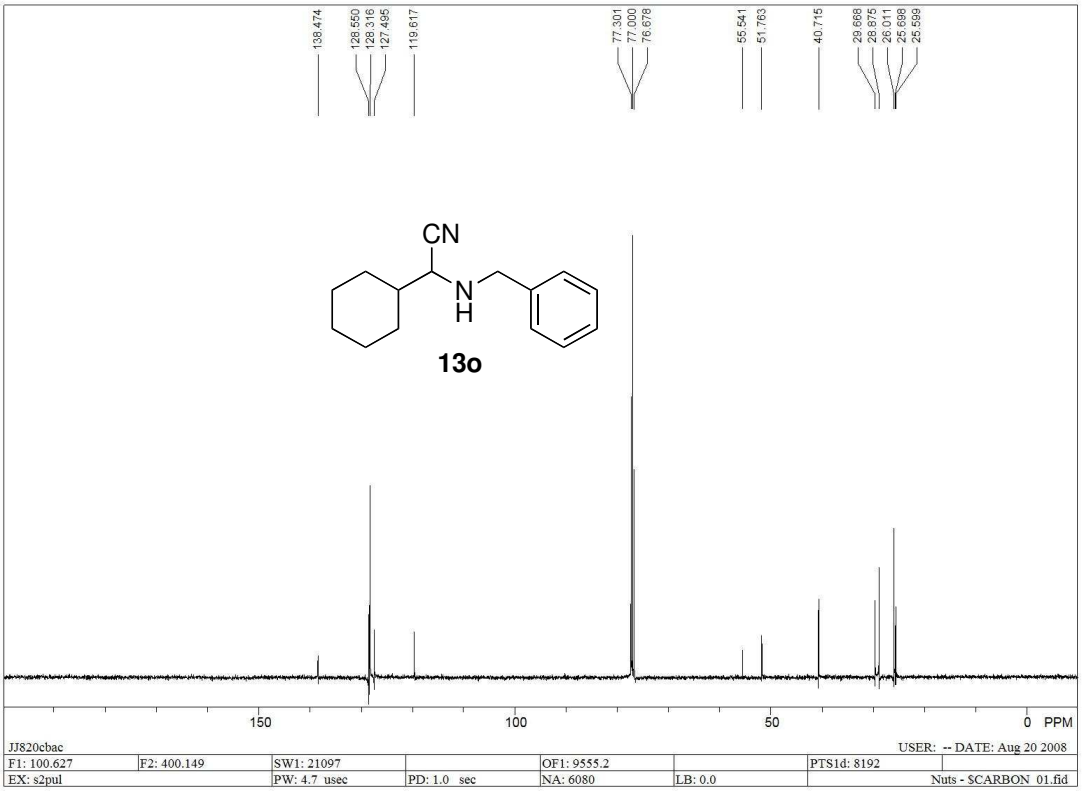

8.788
8.641
8.636
8.621
8.616
7.916
7.913
7.905
7.903
7.900
7.884
7.882
7.877
7.875
7.871
7.868
7.864
7.426
7.416
7.406
7.391
7.387
7.385
7.362
7.351
7.350
7.339
7.331
7.326
7.322
7.311
7.297
7.282
7.258
4.600
4.103
4.052
3.994
3.940
2.452
CN
N
H
N
13l
5.44
1.56
0.85
1.00
2.23
10
8
6
4
2
0
PPM
USER: -- DATE: 07/26/2008
F1: 250.133
F2: 1.000
SW1: 2793
OF1: 1146.4
PTS1d: 8192
EX:
PW: 6.0 usec
PD: 0.0 sec
NA: 24
LB: 0.0
Nuts - $Compound13l

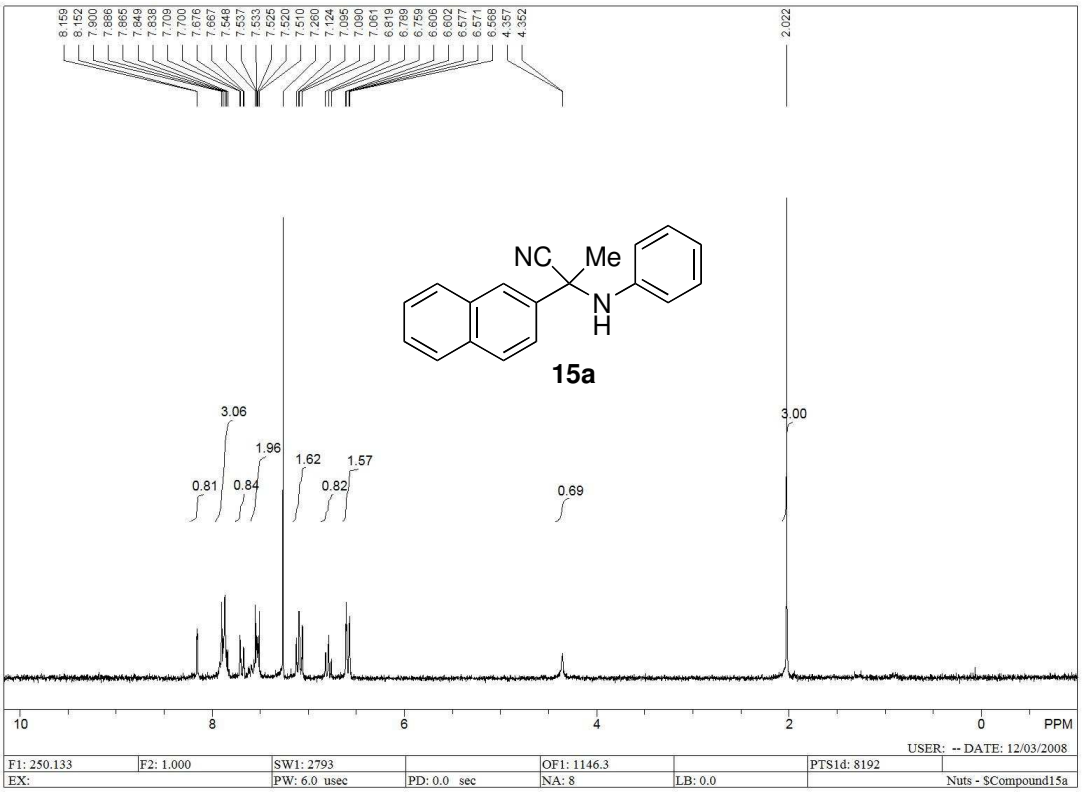

150.244
148.722
137.497
134.961
130.646
128.703
128.375
127.832
123.618
117.583
77.496
77.000
76.497
51.240
CN
N
H
N
13l
200
150
100
50
0
PPM
USER: -- DATE: 11/14/2008
F1: 62.902
F2: 1.000
SW1: 13889
OF1: 6293.3
PTS1d: 16384
EX: DEC90_AUR
PW: 5.5 usec
PD: 1.0 sec
NA: 1517
LB: 0.0
Nuts - $Compound13l carbon

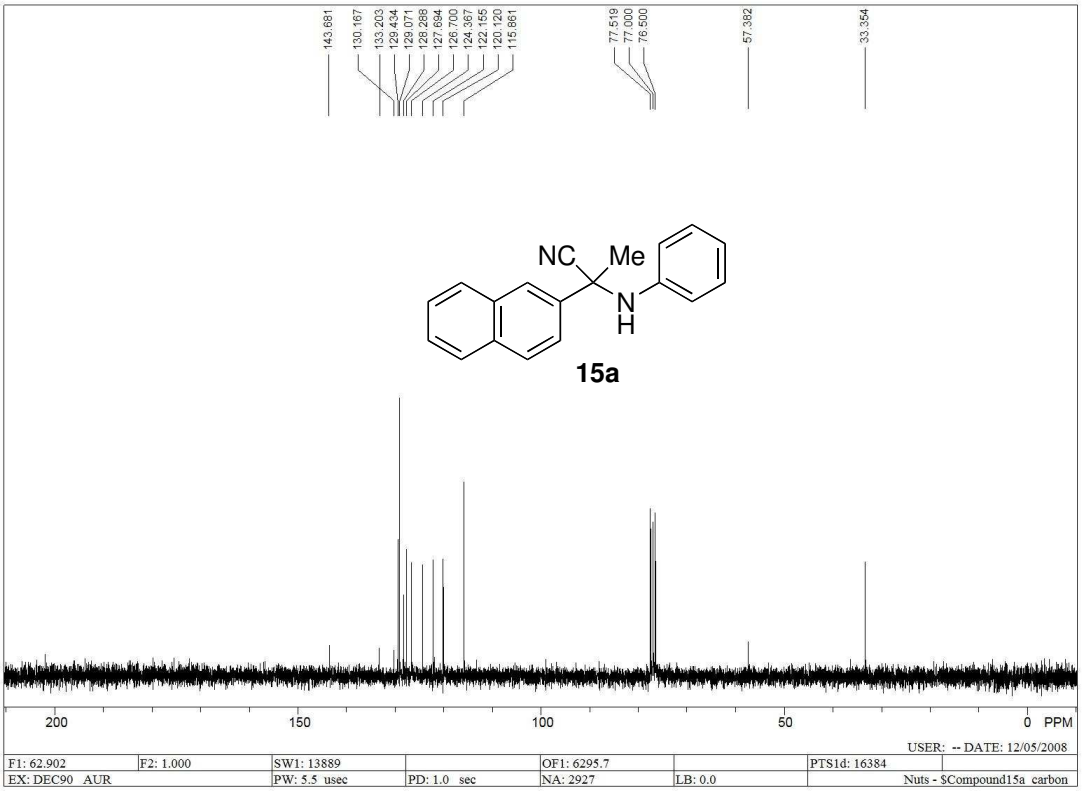

7.413
7.409
7.404
7.389
7.375
7.364
7.357
7.342
7.339
7.325
7.310
7.283
7.260
6.945
6.905
6.205
6.164
4.407
4.403
4.394
4.390
4.108
4.076
3.935
3.903
1.613
CN
N
H
13m
10.58
0.97
0.97
1.00
2.18
8
6
4
2
0
PPM
JJ81cinb
USER: -- DATE: Aug 1 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1786.0
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON 01.fid

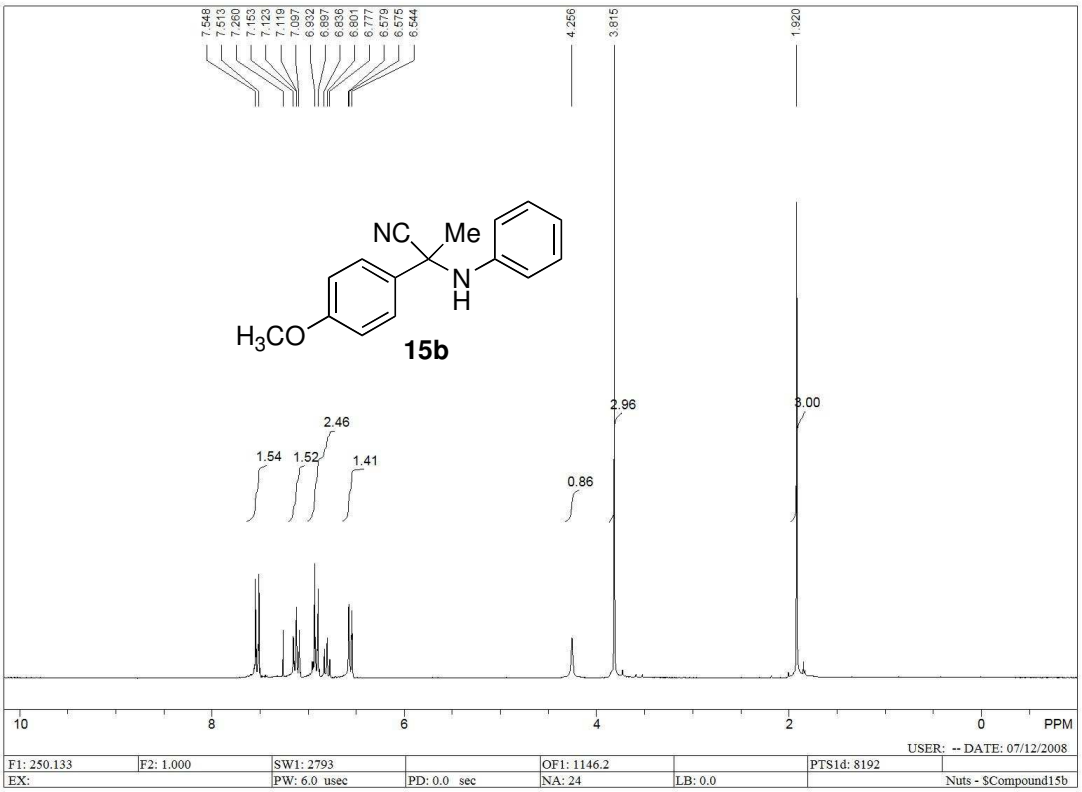

7.364
7.361
7.357
7.346
7.342
7.326
7.320
7.312
7.307
7.301
7.298
7.260
4.103
4.052
3.853
3.801
3.534
3.506
3.477
1.776
1.772
2.215
1.762
1.748
1.743
1.735
1.714
1.584
1.555
1.546
1.526
1.519
0.975
0.948
0.918
CN
N
H
13n
4.65
1.05
1.13
1.00
2.25
2.26
3.10
10
8
6
4
2
0
PPM
USER: -- DATE: 07/07/2008
F1: 250.133
F2: 1.000
SW1: 2793
OF1: 1146.0
PTS1d: 8192
EX:
PW: 6.0 usec
PD: 0.0 sec
NA: 24
LB: 0.0
Nuts - $Compound13n

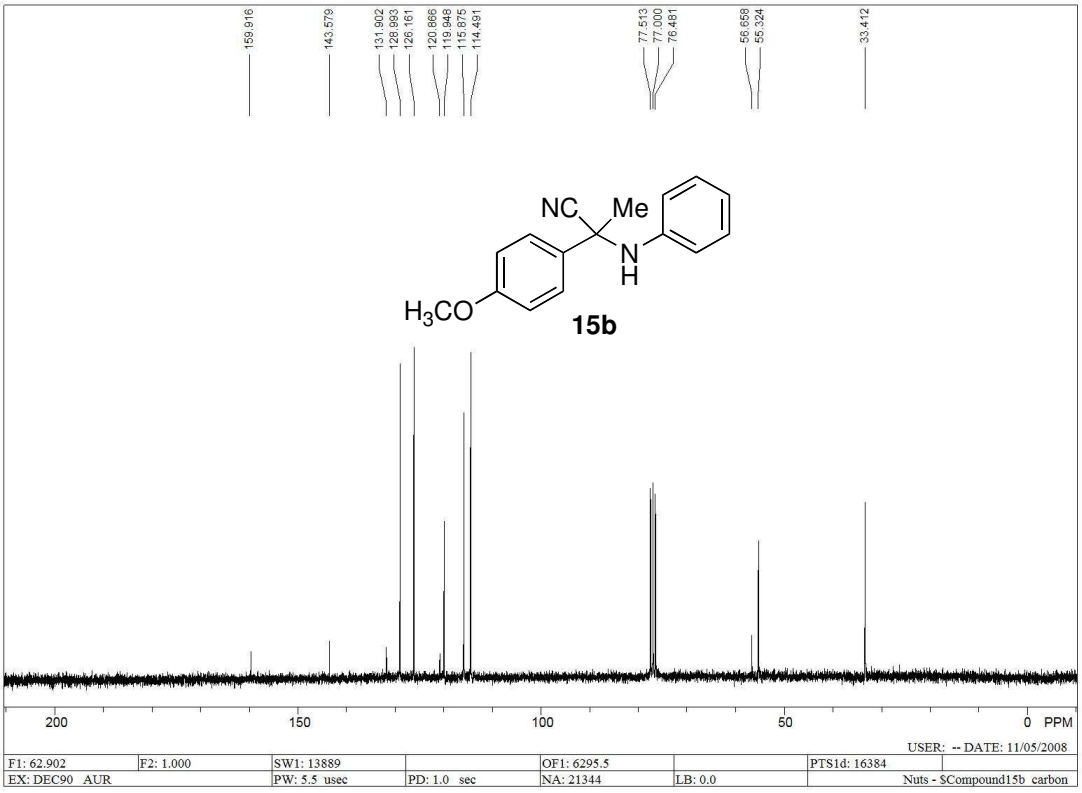

7.372
7.356
7.352
7.338
7.333
7.318
7.295
7.279
7.260
4.099
4.068
3.829
3.797
3.317
3.300
1.872
1.784
1.780
1.754
1.704
1.696
1.693
1.683
1.674
1.667
1.596
1.261
1.254
1.244
1.236
1.229
1.222
1.211
1.198
1.191
1.136
CN
N
H
13o
8.66
5.91
5.05
1.10
1.06
1.00
8
6
4
2
0
PPM
JJ820cbac
USER: -- DATE: Aug 20 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1786.4
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $PROTON_01.fid

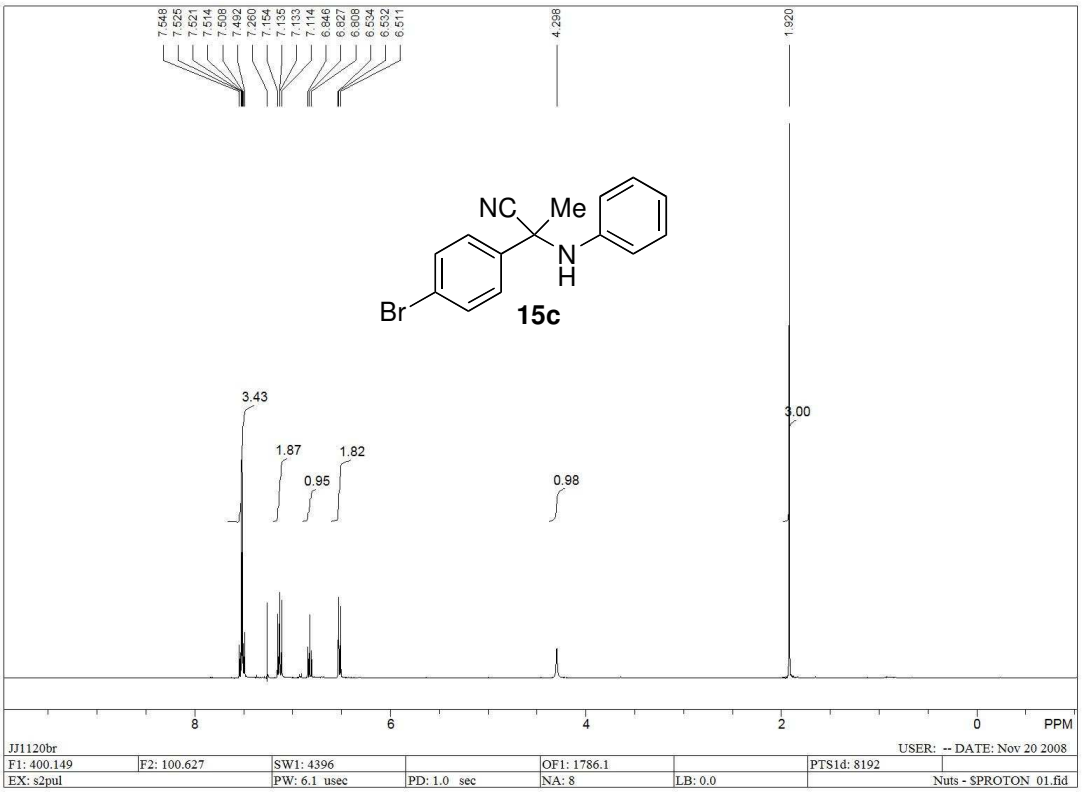

138.474
128.550
128.316
127.495
119.617
77.301
77.000
76.678
55.541
51.763
40.715
29.668
28.875
26.011
25.698
25.599
CN
N
H
13o
150
100
50
0
PPM
JJ820cbac
USER: -- DATE: Aug 20 2008
F1: 100.627
F2: 400.149
SW1: 21097
OF1: 9555.2
PTS1d: 8192
EX: s2pul
PW: 4.7 usec
PD: 1.0 sec
NA: 6080
LB: 0.0
Nuts - $CARBON_01.fid

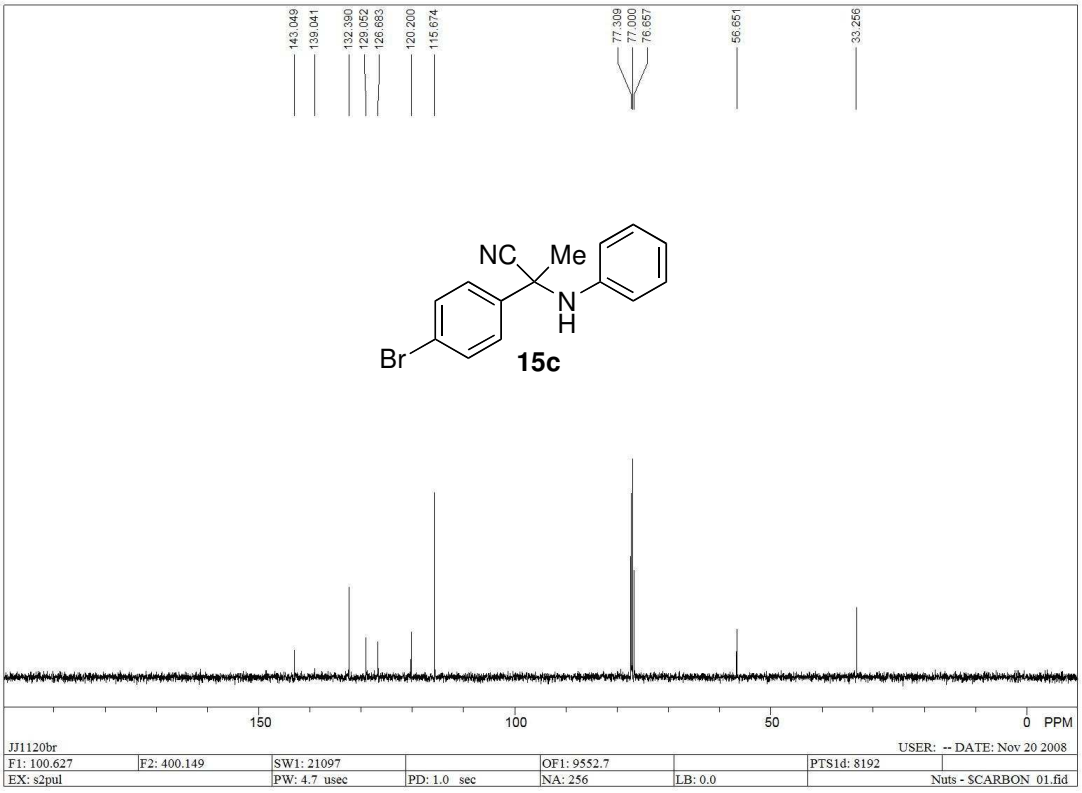

8.159
8.152
7.900
7.886
7.865
7.849
7.838
7.709
7.700
7.676
7.667
7.548
7.537
7.533
7.525
7.520
7.510
7.260
7.124
7.095
7.080
7.061
6.819
6.789
6.759
6.606
6.602
6.577
6.571
6.568
4.357
4.352
2.022
NC
Me
N
H
15a
3.06
1.96
1.62
1.57
0.81
0.84
0.82
0.69
3.00
10
8
6
4
2
0
PPM
USER: -- DATE: 12/03/2008
F1: 250.133
F2: 1.000
SW1: 2793
OF1: 1146.3
PTS1d: 8192
EX:
PW: 6.0 usec
PD: 0.0 sec
NA: 8
LB: 0.0
Nuts - $Compound15a

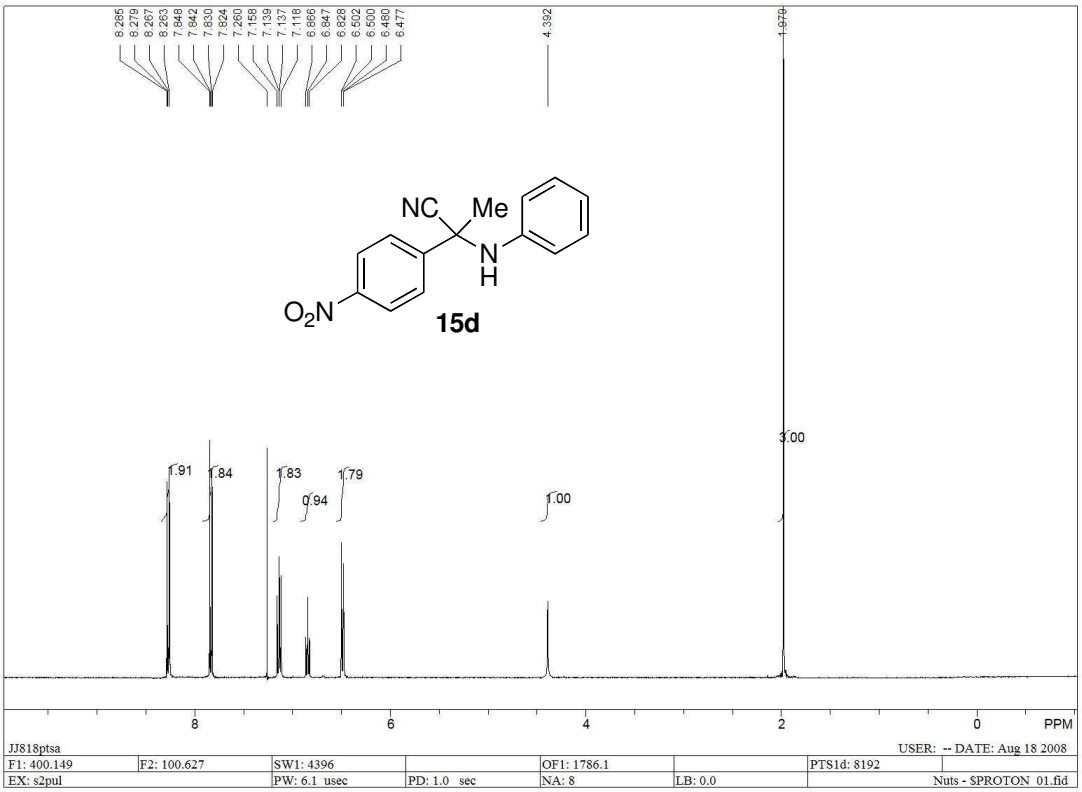

143.681
130.167
133.203
129.434
129.071
128.288
127.694
126.700
124.367
122.155
120.120
115.861
77.519
77.000
76.500
57.382
33.354
NC
Me
N
H
15a
200
150
100
50
0
PPM
USER: -- DATE: 12/05/2008
F1: 62.902
F2: 1.000
SW1: 13889
OF1: 6295.7
PTS1d: 16384
EX: DEC90_AUR
PW: 5.5 usec
PD: 1.0 sec
NA: 2927
LB: 0.0
Nuts - $Compound15a_carbon

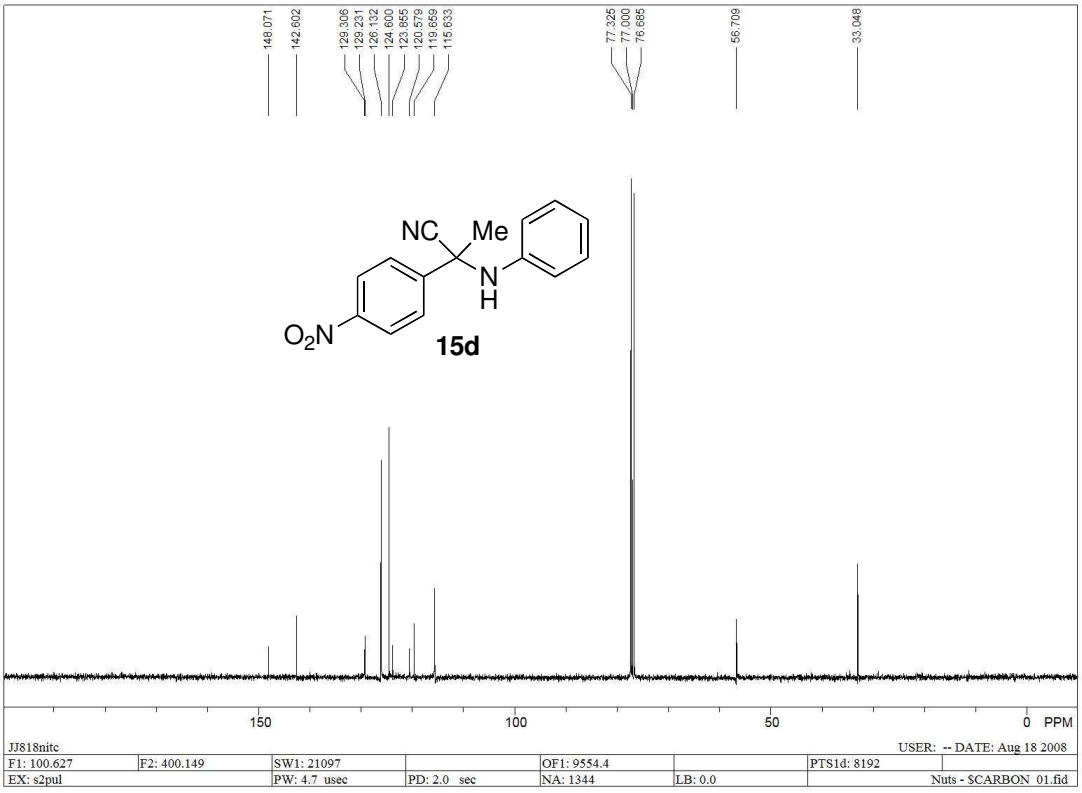

7.548
7.513
7.260
7.153
7.123
7.119
7.097
6.932
6.897
6.836
6.801
6.777
6.578
6.575
6.544
4.256
3.815
1.920
NC
Me
N
H
H3CO
15b
2.96
3.00
2.46
1.54
1.52
1.41
0.86
10
8
6
4
2
0
PPM
USER: -- DATE: 07/12/2008
F1: 250.133
F2: 1.000
SW1: 2793
OF1: 1146.2
PTS1d: 8192
EX:
PW: 6.0 usec
PD: 0.0 sec
NA: 24
LB: 0.0
Nuts - $Compound15b

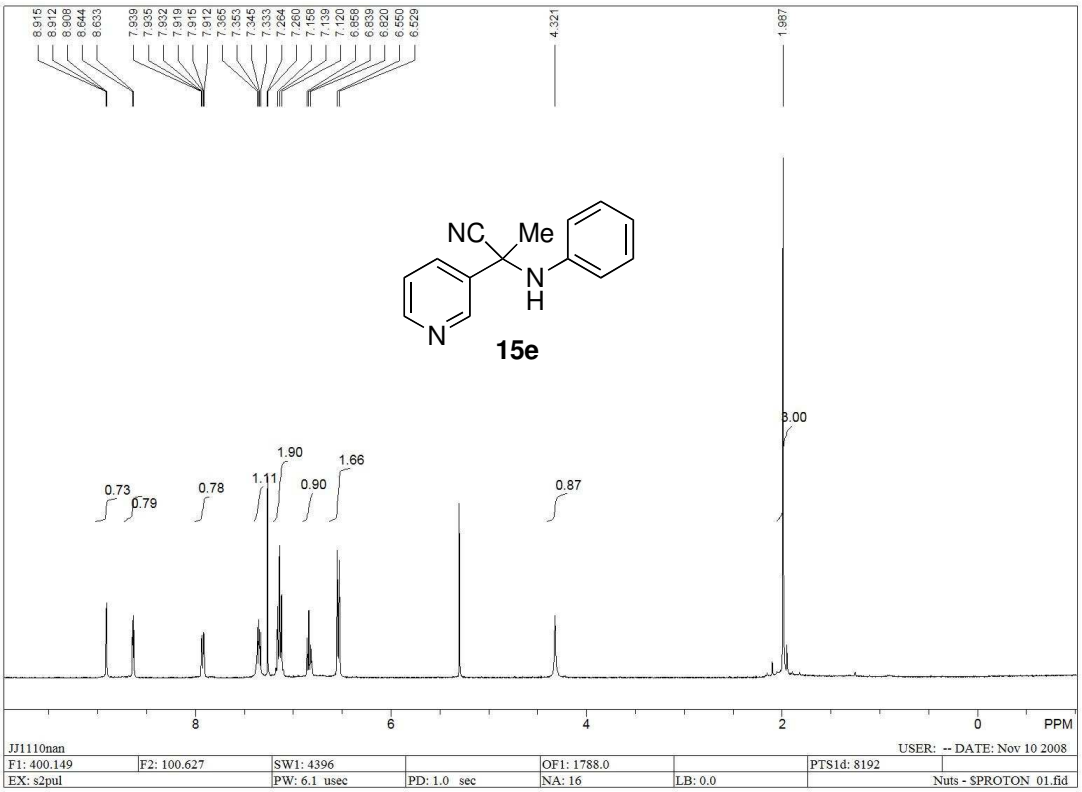

159.916
143.579
131.902
128.993
126.161
120.866
119.948
115.875
114.491
77.513
77.000
76.481
56.658
55.324
33.412
NC
Me
N
H
H3CO
15b
200
150
100
50
0
PPM
USER: -- DATE: 11/05/2008
F1: 62.902
F2: 1.000
SW1: 13889
OF1: 6295.5
PTS1d: 16384
EX: DEC90_AUR
PW: 5.5 usec
PD: 1.0 sec
NA: 21344
LB: 0.0
Nuts - $Compound15b_carbon

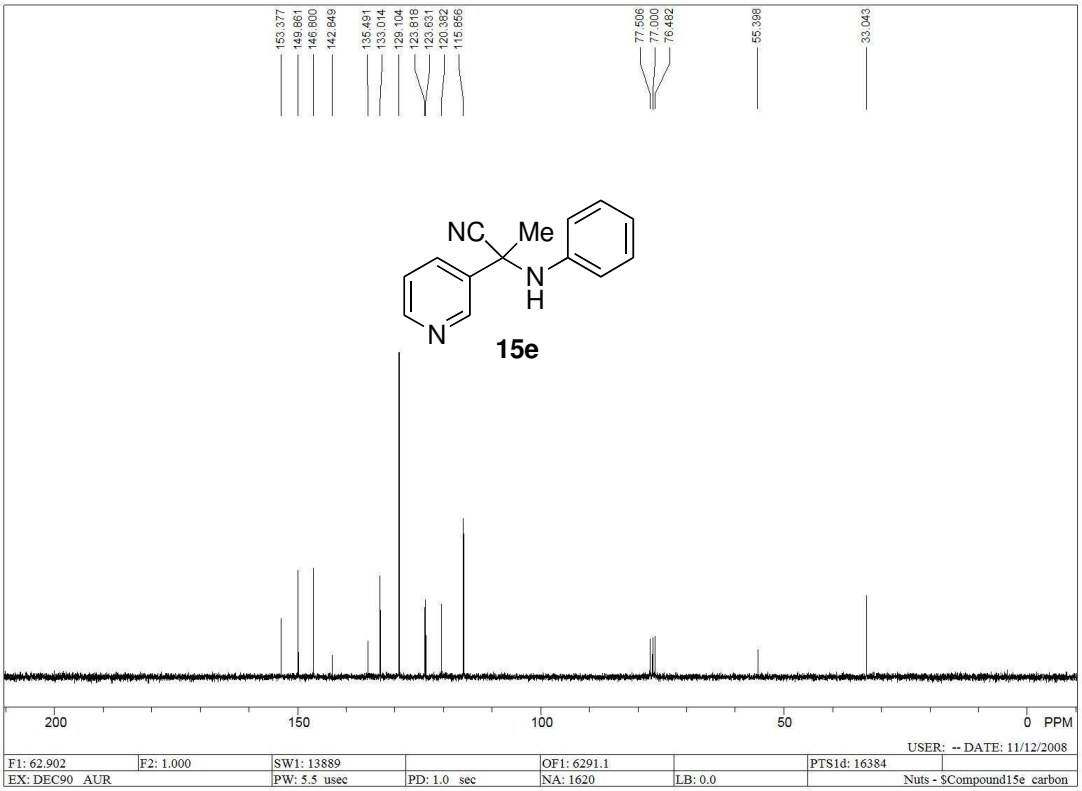

7.548
7.525
7.521
7.514
7.508
7.492
7.260
7.154
7.135
7.133
7.114
6.846
6.827
6.808
6.634
6.532
6.511
4.298
1.920
NC
Me
N
H
Br
15c
3.43
1.87
1.82
0.95
0.98
3.00
8
6
4
2
0
PPM
JJ1120br
USER: -- DATE: Nov 20 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1786.1
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

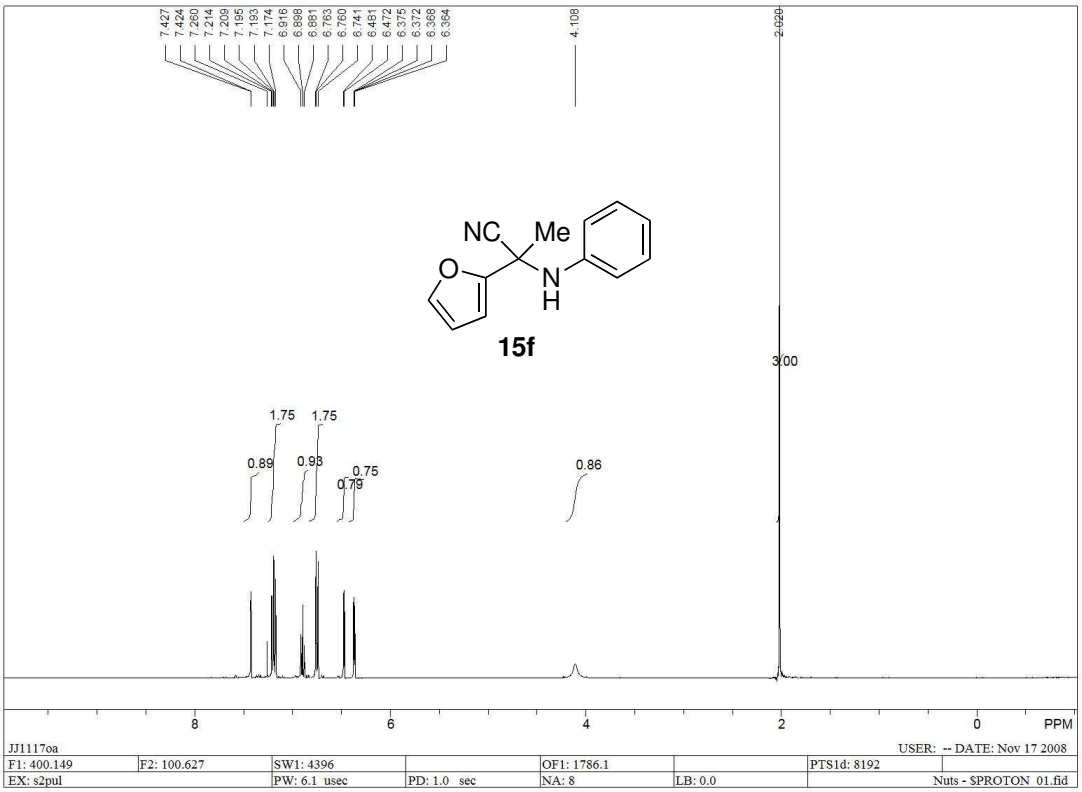

143.049
139.041
132.390
129.052
126.683
120.200
115.674
77.309
77.000
76.657
56.651
33.256
NC
Me
N
H
Br
15c
150
100
50
0
PPM
JJ1120br
USER: -- DATE: Nov 20 2008
F1: 100.627
F2: 400.149
SW1: 21097
OF1: 9552.7
PTS1d: 8192
EX: s2pul
PW: 4.7 usec
PD: 1.0 sec
NA: 256
LB: 0.0
Nuts - $CARBON_01.fid

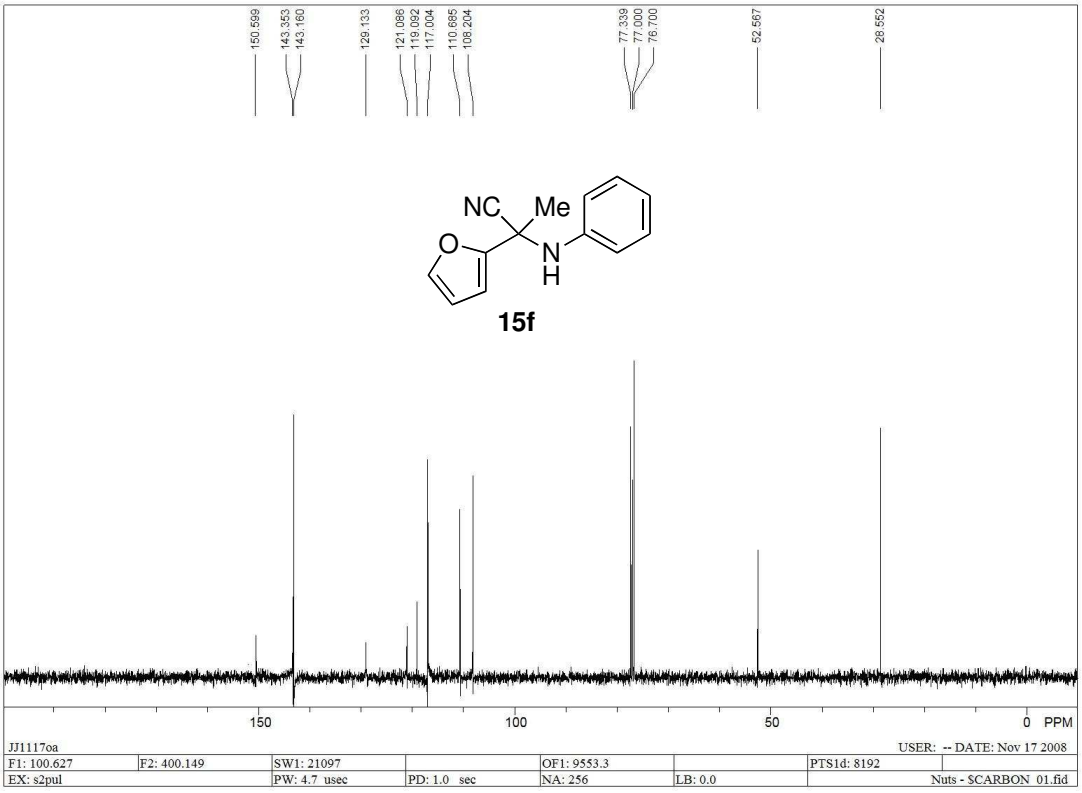

8.285
8.279
8.267
8.263
7.848
7.842
7.830
7.824
7.260
7.158
7.139
7.137
7.118
6.866
6.847
6.628
6.502
6.500
6.480
6.477
4.392
1.979
NC
Me
N
H
O2N
15d
3.00
1.91
1.84
1.83
1.79
0.94
1.00
8
6
4
2
0
PPM
JJ818ptsa
USER: -- DATE: Aug 18 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1786.1
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

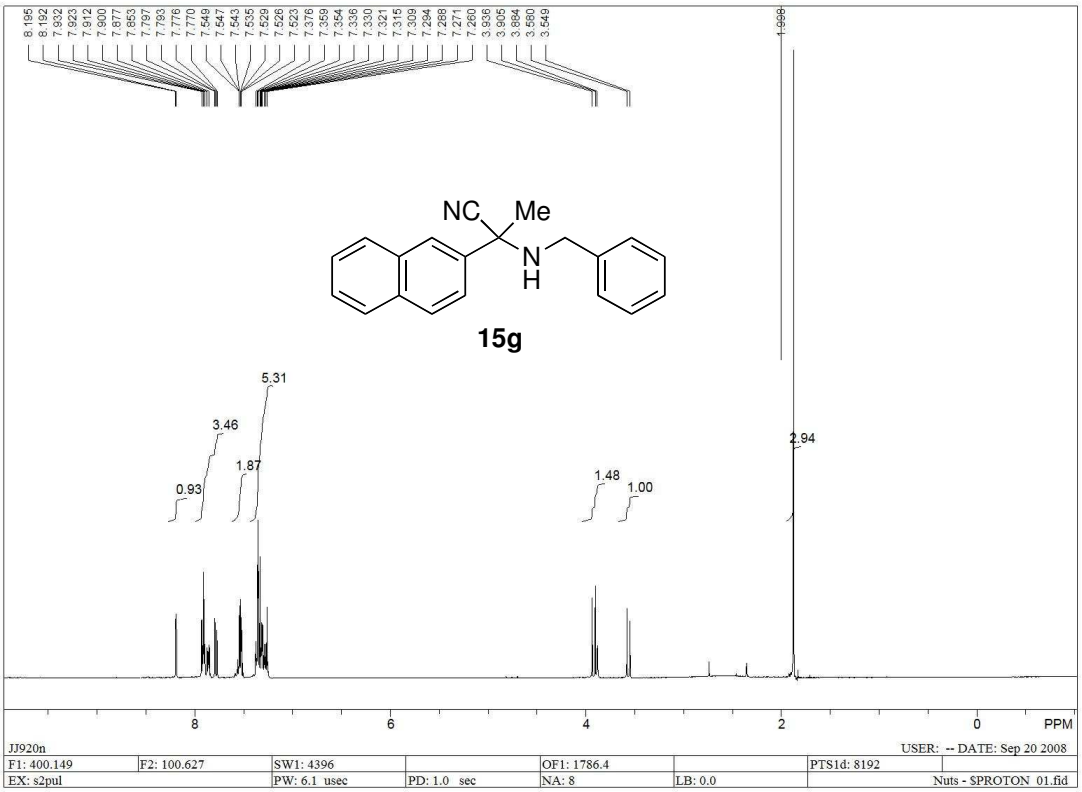

148.071
142.602
129.306
129.231
126.132
124.600
123.855
120.579
119.659
115.633
77.325
77.000
76.685
56.709
33.048
NC
Me
N
H
O2N
15d
150
100
50
0
PPM
JJ818nitc
USER: -- DATE: Aug 18 2008
F1: 100.627
F2: 400.149
SW1: 21097
OF1: 9554.4
PTS1d: 8192
EX: s2pul
PW: 4.7 usec
PD: 2.0 sec
NA: 1344
LB: 0.0
Nuts - $CARBON_01.fid

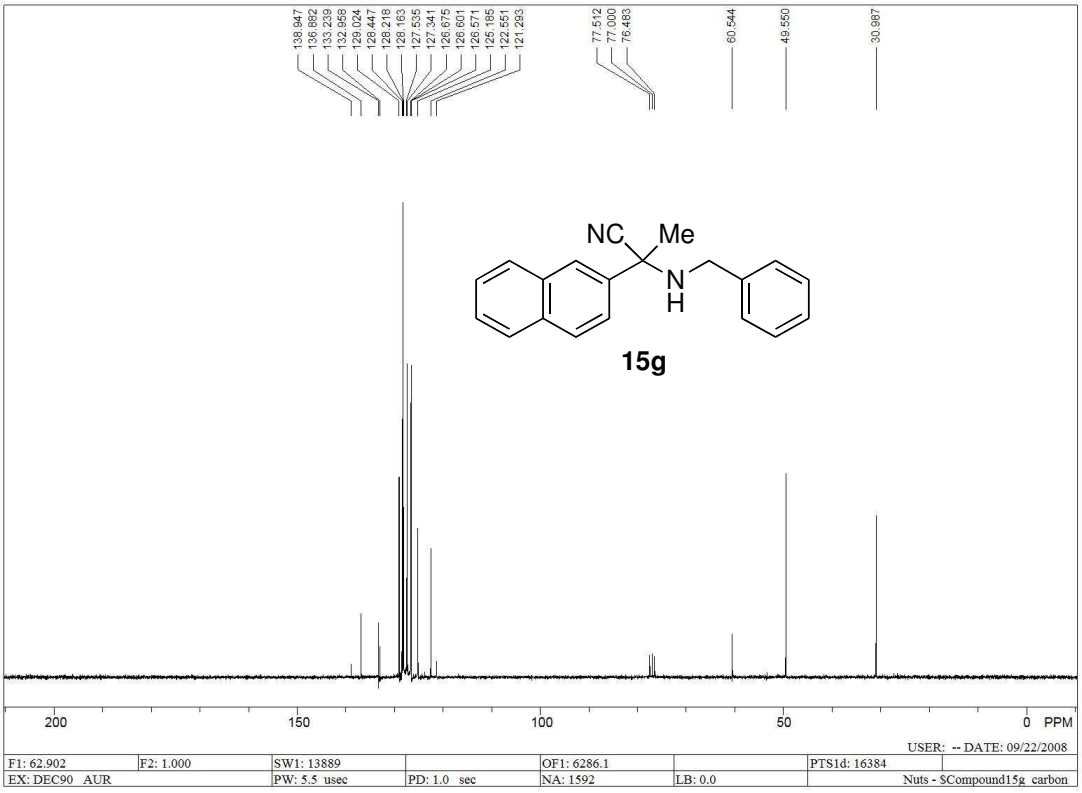

8.915
8.912
8.908
8.644
8.633
7.939
7.935
7.932
7.919
7.915
7.912
7.365
7.353
7.345
7.333
7.264
7.260
7.158
7.139
7.120
6.858
6.839
6.620
6.550
6.529
4.321
1.987
NC
Me
N
H
N
15e
3.00
1.90
1.66
1.11
0.90
0.73
0.79
0.78
0.87
8
6
4
2
0
PPM
JJ1110nan
USER: -- DATE: Nov 10 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1788.0
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $PROTON_01.fid

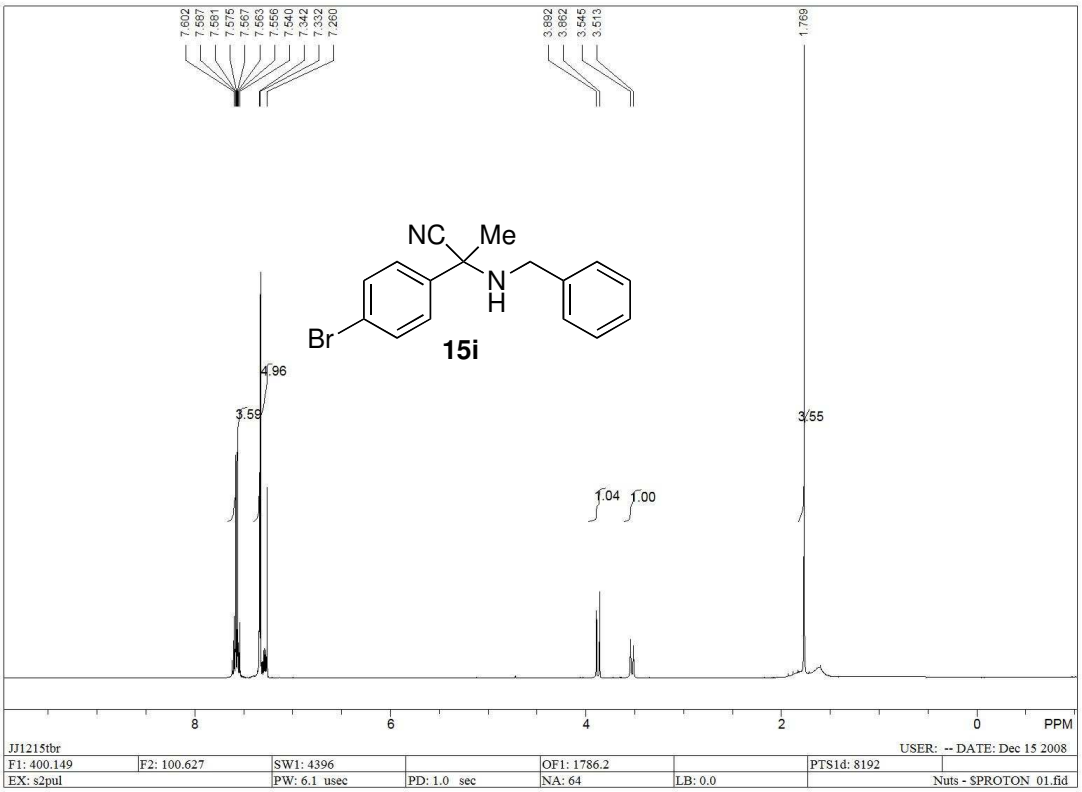

153.377
149.861
146.800
142.849
135.491
133.014
129.104
123.818
123.631
120.382
115.856
77.506
77.000
76.482
55.398
33.043
NC
Me
N
H
N
15e
200
150
100
50
0
PPM
USER: -- DATE: 11/12/2008
F1: 62.902
F2: 1.000
SW1: 13889
OF1: 6291.1
PTS1d: 16384
EX: DEC90_AUR
PW: 5.5 usec
PD: 1.0 sec
NA: 1620
LB: 0.0
Nuts - $Compound15e_carbon

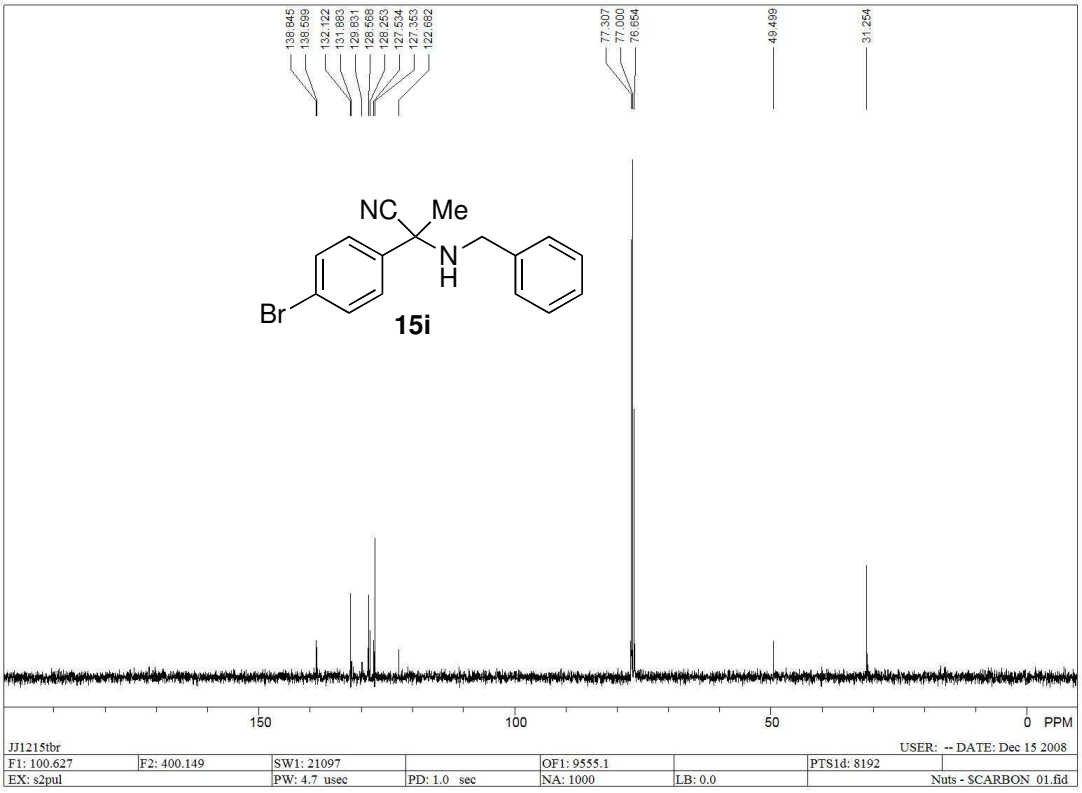

7.427
7.424
7.260
7.214
7.209
7.195
7.193
7.174
6.916
6.898
6.881
6.763
6.760
6.741
6.481
6.472
6.375
6.372
6.368
6.364
4.108
2.020
NC
Me
O
N
H
15f
3.00
1.75
1.75
0.89
0.93
0.75
0.79
0.86
8
6
4
2
0
PPM
JJ1117oa
USER: -- DATE: Nov 17 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1786.1
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

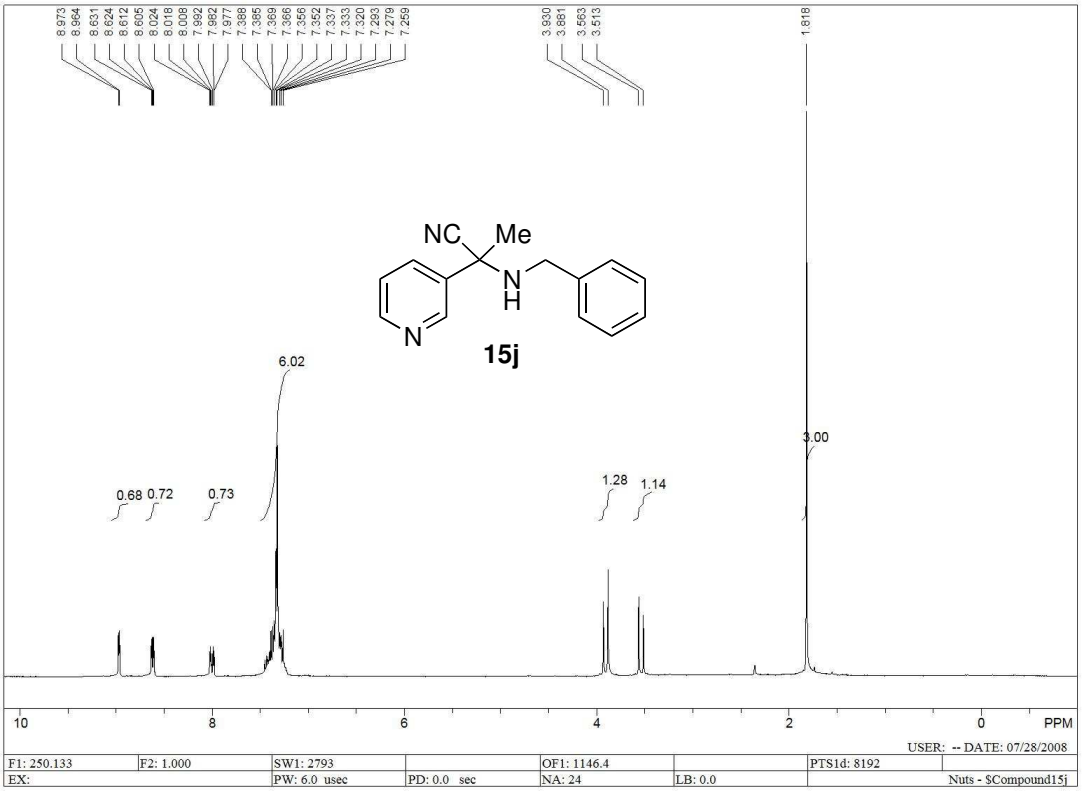

150.599
143.353
143.160
129.133
121.086
119.092
117.004
110.685
108.204
77.339
77.000
76.700
52.567
28.552
NC
Me
O
N
H
15f
150
100
50
0
PPM
JJ1117oa
USER: -- DATE: Nov 17 2008
F1: 100.627
F2: 400.149
SW1: 21097
OF1: 9553.3
PTS1d: 8192
EX: s2pul
PW: 4.7 usec
PD: 1.0 sec
NA: 256
LB: 0.0
Nuts - $CARBON_01.fid

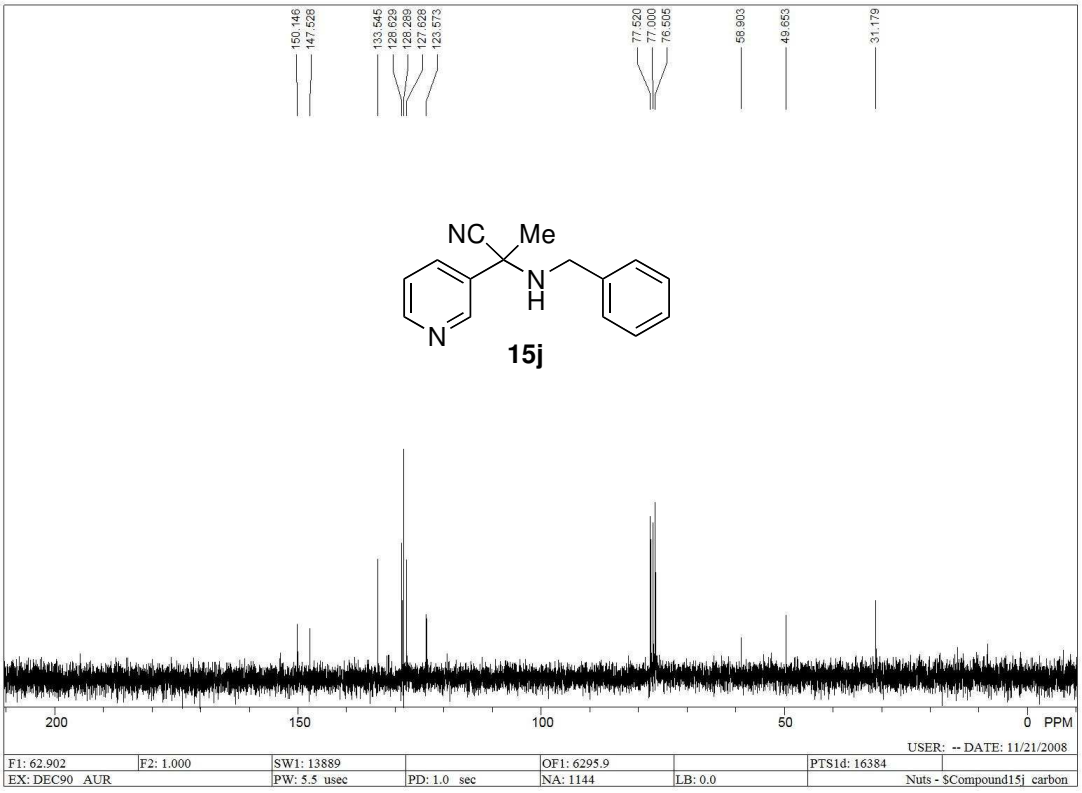

8.195
8.192
7.932
7.923
7.912
7.900
7.877
7.865
7.797
7.793
7.776
7.770
7.549
7.547
7.543
7.535
7.529
7.526
7.523
7.376
7.359
7.354
7.336
7.330
7.321
7.315
7.308
7.294
7.288
7.271
7.260
3.936
3.905
3.884
3.580
3.549
1.988
NC
Me
N
H
15g
5.31
3.46
1.87
0.93
1.48
1.00
2.94
8
6
4
2
0
PPM
JJ920n
USER: -- DATE: Sep 20 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1786.4
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid


138.947
136.882
133.239
132.958
129.024
128.447
128.218
128.163
127.535
127.341
126.675
126.601
126.571
125.185
122.551
121.293
77.512
77.000
76.483
60.544
49.550
30.987
NC
Me
N
H
15g
200
150
100
50
0
PPM
USER: -- DATE: 09/22/2008
F1: 62.902
F2: 1.000
SW1: 13889
OF1: 6286.1
PTS1d: 16384
EX: DEC90_AUR
PW: 5.5 usec
PD: 1.0 sec
NA: 1592
LB: 0.0
Nuts - $Compound15g_carbon


7.602
7.587
7.581
7.575
7.567
7.563
7.556
7.540
7.342
7.332
7.260
3.892
3.862
3.545
3.513
1.769
NC
Me
N
H
Br
15i
4.96
3.59
3.55
1.04
1.00
8
6
4
2
0
PPM
JJ1215tbr
USER: -- DATE: Dec 15 2008
F1: 400.149
F2: 100.627
SW1: 4396
OF1: 1786.2
PTS1d: 8192
EX: s2pul
PW: 6.1 usec
PD: 1.0 sec
NA: 64
LB: 0.0
Nuts - $PROTON_01.fid


138.845
138.599
132.122
131.883
129.831
128.568
128.253
127.534
127.353
122.682
77.307
77.000
76.654
49.499
31.254
NC
Me
N
H
Br
15i
150
100
50
0
PPM
JJ1215tbr
USER: -- DATE: Dec 15 2008
F1: 100.627
F2: 400.149
SW1: 21097
OF1: 9555.1
PTS1d: 8192
EX: s2pul
PW: 4.7 usec
PD: 1.0 sec
NA: 1000
LB: 0.0
Nuts - $CARBON_01.fid


8.973
8.964
8.631
8.624
8.612
8.605
8.024
8.018
8.008
7.992
7.982
7.977
7.388
7.385
7.368
7.366
7.356
7.352
7.337
7.333
7.320
7.293
7.279
7.259
3.930
3.881
3.563
3.513
1.818
NC
Me
N
H
N
15j
6.02
3.00
0.68
0.72
0.73
1.28
1.14
10
8
6
4
2
0
PPM
USER: -- DATE: 07/28/2008
F1: 250.133
F2: 1.000
SW1: 2793
OF1: 1146.4
PTS1d: 8192
EX:
PW: 6.0 usec
PD: 0.0 sec
NA: 24
LB: 0.0
Nuts - $Compound15j


150.146
147.528
133.545
128.629
128.289
127.628
123.573
77.520
77.000
76.505
58.903
49.653
31.179
NC
Me
N
H
N
15j
200
150
100
50
0
PPM
USER: -- DATE: 11/21/2008
F1: 62.902
F2: 1.000
SW1: 13889
OF1: 6295.9
PTS1d: 16384
EX: DEC90_AUR
PW: 5.5 usec
PD: 1.0 sec
NA: 1144
LB: 0.0
Nuts - $Compound15j_carbon