

Supporting Information

for

Application of heterocyclic aldehydes as components in Ugi–Smiles couplings

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Experimental procedures and analytical data for Ugi–Smiles and US-IMDA products

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General experimental details

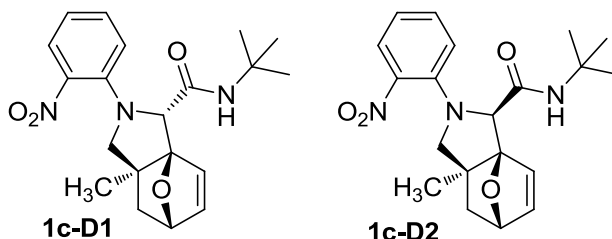
Methanol was distilled from CaH₂ under N₂ immediately before use. 2-Furaldehyde was distilled under reduced pressure (62 °C, 18 mm). Cyclohex-1-en-1-ylmethyl amine and 1-cyclohex-1-en-1-ylethyl amine were purchased as hydrochloride salts and converted to the free base form via 1.0 M NaOH prior to use. All other reagents and solvents were commercial grade (Aldrich or Acros) and used without purification. Characterization data for compounds **1a-D1**, **1a-D2**, **1b-D1**, and **1b-D2** have been reported previously [1]. Novel Ugi-Smiles and tandem US-IMDA products in this work were prepared in a similar manner to experimental procedures previously reported for known US-IMDA products [1].

1. Richey, B.; Mason, K. M.; Meyers, M. S.; Luesse, S. B. *Tetrahedron Lett.* **2016**, *57*, 492-494.

Thin layer chromatography (TLC) was performed using plastic-backed silica gel (225 μm) plates and flash chromatography utilized 230–400 mesh silica gel from Sigma-Aldrich. Some compounds were purified via automated chromatography on the Biotage IsoleraTM Flash Purification system using a gradient method with SNAP Ultra cartridges. Products were visualized by UV light, and/or the use of ceric ammonium molybdate, *p*-anisaldehyde, and potassium iodoplatinate solutions.

IR spectra were recorded on a NicoletTM iS5 FT-IR Spectrometer and are reported in wavenumbers (cm^{-1}). Liquids and oils were analyzed as neat films on a NaCl plate (transmission), whereas solids were applied to a diamond plate (ATR). Nuclear magnetic resonance spectra (NMR) were acquired on a Varian Unity Plus (300 MHz) or a Bruker Ascend (400 MHz) Spectrometer and processed with TopSpin 3.2. Chemical shifts are measured relative to residual solvent peaks as an internal standard set to δ 7.26 and δ 77.1 (CDCl_3). HRMS FAB data was collected from a JEOL MStation [JMS-700] Mass Spectrometer at the University of Missouri-St Louis. Direct infusion mass spectrometry (DIMS) was used to verify accurate masses for several compounds, using a Triversa Nanomate nanospray direct infusion robot (Advion) attached to a Q-Exactive Mass Spectrometer. These samples were analyzed at the Proteomics & Mass Spectrometry Facility at the Danforth Plant Science Center (St Louis, MO).

Synthesis of *N*-(*tert*-butyl)-7*a*-methyl-2-(2-nitrophenyl)-1,2,3,6,7,7*a*-hexahydro-3*a*,6-epoxyisoindole-3-carboxamide (**1c**).



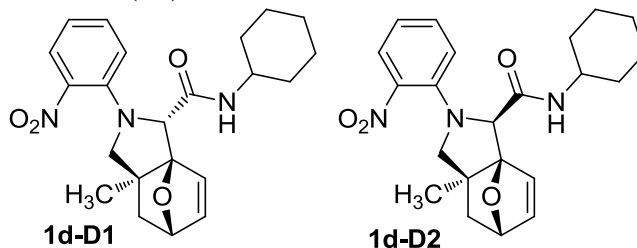
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-furaldehyde (41.4 μL , 0.5 mmol, 1 equiv), 2-methylallylamine (45.6 μL , 0.5 mmol, 1 equiv), and *tert*-butyl isocyanide (114 μL , 1.0 mmol, 2 equiv). The reaction mixture was warmed at 50 $^{\circ}\text{C}$ for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (10% ethyl acetate in hexanes) to afford epoxyisoindolines **1c-D1** (26.0 mg, 14%) and **1c-D2** (53.9 mg, 29%).

1c-D1: R_f = 0.40 (40:60 EtOAc:Hex); ^1H NMR (400 MHz, CDCl_3) δ 7.73 (m, 2H), 7.47 (dd, J = 8.2, 7.6 Hz, 1H), 7.32 (d, J = 8.5 Hz, 1H), 7.09 (dd, J = 7.8, 7.7 Hz, 1H), 6.56 (d, J = 5.9 Hz, 1H), 6.42 (d, J = 5.8 Hz, 1H), 4.97 (d, J = 5.0 Hz, 1H), 4.57 (s, 1H), 3.45 (d, J = 8.5 Hz, 1H), 2.98 (d, J = 8.2 Hz, 1H), 2.08 (dd, J = 4.9, 4.4 Hz, 1H), 1.32 (s, 9H), 1.28–1.23 (m, 1H), 1.08 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 166.9, 142.3, 139.0, 137.7, 133.6, 132.5, 126.5, 118.9, 116.2, 96.9, 80.7, 65.4, 62.9, 51.4, 49.1, 38.6, 28.5, 22.6; DIMS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{20}\text{H}_{26}\text{N}_3\text{O}_4$ 372.1923; found 372.1916.

1c-D2: R_f = 0.29 (40:60 EtOAc:Hex); ^1H NMR (400 MHz, CDCl_3) δ 7.78 (d, J = 8.2 Hz, 1H), 7.42 (dd, J = 8.1, 7.8 Hz, 1H), 7.07 (d, J = 8.5 Hz, 1H), 6.90 (dd, J = 7.9, 7.6 Hz, 1H), 6.56 (d, J = 5.6 Hz, 1H), 6.48 (d, J = 5.7 Hz, 1H), 6.45 (s, 1H), 5.08 (s, 1H), 4.75 (s, 1H), 3.70 (d, J = 9.6 Hz, 1H), 2.63 (d, J = 9.6 Hz, 1H), 2.19 (dd, J = 4.7, 4.6 Hz, 1H), 1.19 (s, 9H), 1.05 (d, J = 11.6 Hz, 1H), 0.82 (s, 3H); ^{13}C NMR (CDCl_3) δ 168.2, 142.1, 135.7, 134.0, 133.1, 125.8, 122.8,

121.9, 98.5, 79.7, 65.1, 65.3, 51.3, 48.6, 39.8, 29.3, 28.6, 23.2; HR-FAB MS $[M+Na]^+$ calcd for $C_{20}H_{25}N_3NaO_4$ 394.1743; found 394.1746.

Synthesis of *N*-cyclohexyl-7a-methyl-2-(2-nitrophenyl)-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisindole-3-carboxamide (1d).

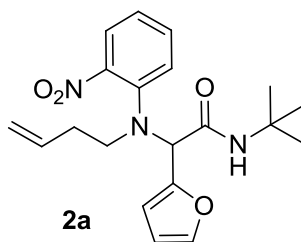


In a similar manner as described in [1], to a solution of 2-nitrophenol (69.8 mg, 0.50 mmol, 1 equiv) in methanol (0.50 mL) was added 2-furaldehyde (41.4 μ L, 0.5 mmol, 1 equiv), 2-methylallylamine (45.6 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (15% ethyl acetate in hexanes) to give epoxyisindolines **1d-D1** (36.9 mg, 19%) and **1d-D2** (67.5 mg, 34%).

1d-D1: $R_f = 0.35$ (50:50 EtOAc:Hex); 1H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, $J = 7.8$ Hz, 1H, NH), 7.72 (dd, $J = 8.1, 1.4$ Hz, 1H), 7.46 (dd, $J = 7.9, 7.7$ Hz, 1H), 7.31 (d, $J = 8.2$ Hz, 1H), 7.09 (dd, $J = 7.3, 7.3$ Hz, 1H), 6.56 (d, $J = 5.8$ Hz, 1H), 6.43 (dd, $J = 5.8, 1.6$ Hz, 1H), 4.98 (dd, $J = 4.6, 1.5$ Hz, 1H), 4.70 (s, 1H), 3.81-3.69 (m, 1H), 3.43 (d, $J = 8.4$ Hz, 1H), 3.00 (d, $J = 8.4$ Hz, 1H), 2.08 (dd, $J = 11.5, 4.8$ Hz, 1H), 1.95-1.87 (m, 1H), 1.74-1.59 (m, 4H), 1.41-1.11 (m, 5H), 1.00 (s, 3H), 0.94-0.79 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 141.8, 135.6, 133.9, 132.9, 125.6, 122.8, 121.9, 98.2, 79.6, 65.3, 64.7, 48.6, 48.0, 39.6, 32.9, 32.5, 30.9, 25.3, 24.6(2), 23.0; HR-FAB MS $[M+Na]^+$ calcd for $C_{22}H_{27}N_3NaO_4$ 420.1899; found 420.1907.

1d-D2: $R_f = 0.18$ (50:50 EtOAc:Hex); 1H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, $J = 8.2$ Hz, 1H), 7.42 (dd, $J = 7.8, 7.8$ Hz, 1H), 7.07 (d, $J = 8.4$ Hz, 1H), 6.90 (dd, $J = 7.4, 7.4$ Hz, 1H), 6.59 (d, $J = 5.7$ Hz, 1H), 6.54 (s, 1H), 6.50 (d, $J = 5.7$ Hz, 1H), 5.08 (s, 1H), 4.87 (s, 1H), 3.73-3.70 (m, 2H), 2.65 (d, $J = 9.6$ Hz, 1H), 2.23-2.14 (m, 1H), 1.85-1.76 (m, 1H), 1.65-1.49 (m, 2H), 1.49-1.35 (m, 2H), 1.35-1.00 (m, 5H), 0.94-0.78 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 142.2, 139.0, 137.8, 133.6, 132.4, 126.5, 118.9, 116.2, 96.9, 80.7, 65.3, 62.6, 49.0, 47.8, 38.6, 32.5, 32.5, 25.5, 24.3, 24.2, 22.5; HR-FAB MS $[M+Na]^+$ calcd for $C_{22}H_{27}N_3NaO_4$ 420.1899; found 420.1907.

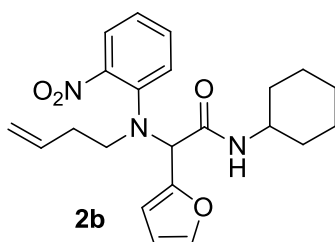
Synthesis of 2-(but-3-en-1-yl(2-nitrophenyl)amino)-*N*-(*tert*-butyl)-2-(furan-2-yl)acetamide (2a).



In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-furaldehyde (41.4 μ L, 0.5 mmol, 1 equiv), 3-

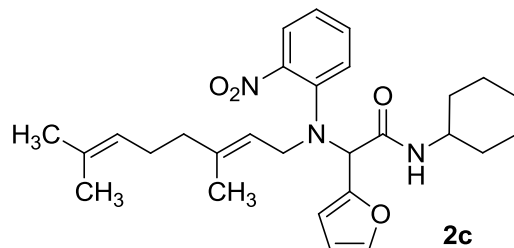
butenylamine (45.8 μL , 0.5 mmol, 1 equiv), and *tert*-butyl isocyanide (114 μL , 1.0 mmol, 2 equiv). The reaction mixture was warmed at 50 $^{\circ}\text{C}$ for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (10% ethyl acetate/hexanes) to afford *N*-arylamide **2a** (71.1 mg, 40%). $R_f = 0.20$ (20:80 EtOAc:Hex); ^1H NMR (400 MHz, CDCl_3) δ 7.73 (d, $J = 8.1$ Hz, 1H), 7.49 (dd, $J = 7.8, 7.7$ Hz, 1H), 7.40 (s, 1H), 7.34 (br s, 1H, NH), 7.25-7.18 (m, 2H), 6.36-6.28 (m, 2H), 5.69-5.52 (m, 1H), 4.97-4.82 (m, 3H), 3.03 (dd, $J = 7.7, 7.0$ Hz, 2H), 2.06-1.82 (m, 2H), 1.38 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 167.3, 149.4, 147.5, 142.8, 142.1, 135.0, 133.0, 126.9, 125.4, 125.1, 117.2, 111.4, 110.5, 66.6, 51.4, 50.8, 32.0, 28.7; HR-FAB MS $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{20}\text{H}_{25}\text{N}_3\text{NaO}_4$ 394.1743; found 394.1748.

Synthesis of 2-(but-3-en-1-yl(2-nitrophenyl)amino)-*N*-cyclohexyl-2-(furan-2-yl)acetamide (2b).



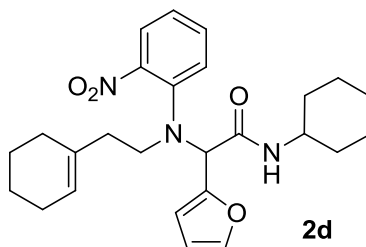
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-furaldehyde (41.5 μL , 0.5 mmol, 1 equiv), 3-butenylamine (45.8 μL , 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μL , 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 $^{\circ}\text{C}$ for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (20% ethyl acetate in hexanes) to afford *N*-arylamide **2b** (68.2 mg, 34%). $R_f = 0.51$ (50:50 EtOAc:Hex); ^1H NMR (400 MHz, CDCl_3) δ 7.70 (d, $J = 6.9$ Hz, 1H), 7.50-7.41 (m, 2H), 7.36 (s, 1H), 7.28 (d, $J = 7.3$ Hz, 1H), 7.22 (dd, $J = 7.4, 7.3$ Hz, 1H), 6.32 (s, 2H), 5.59-5.48 (m, 1H), 5.02 (s, 1H), 4.92 (d, $J = 10.1$ Hz, 1H), 4.84 (d, $J = 16.1$ Hz, 1H), 3.80-3.73 (m, 1H), 3.06-2.93 (m, 2H), 1.96-1.84 (m, 3H), 1.80-1.67 (m, 3H), 1.59 (d, $J = 12.5$ Hz, 1H), 1.40-1.11 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ 167.0, 149.1, 147.2, 142.6, 142.0, 134.7, 132.9, 126.6, 125.1, 124.9, 117.1, 111.2, 110.4, 65.7, 50.7, 48.3, 32.9, 32.5, 31.7, 25.4, 24.74, 24.67; HR-FAB MS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{28}\text{N}_3\text{O}_4$ 398.2080; found 398.2068.

Synthesis of (E)-N-cyclohexyl-2-((3,7-dimethylocta-2,6-dien-1-yl)(2-nitrophenyl)amino)-2-(furan-2-yl)acetamide (2c).



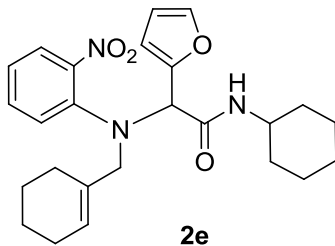
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-furaldehyde (41.5 μ L, 0.5 mmol, 1 equiv), geranylamine (92.4 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column on silica gel (40% ethyl acetate in hexanes) to afford *N*-arylamide **2c** (83.2 mg, 35%). $R_f = 0.16$ (40:60 EtOAc:Hex); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.66 (d, $J = 8.0$ Hz, 1H), 7.51 (d, $J = 8.2$ Hz, 1H), 7.44 (dd, $J = 8.2, 8.1$ Hz, 1H), 7.35-7.31 (m, 2H), 7.17 (dd, $J = 7.3, 7.2$ Hz, 1H), 6.40 (d, $J = 2.9$ Hz, 1H), 6.30 (d, $J = 3.0$ Hz, 1H), 5.06 (s, 1H), 4.95 (dd, $J = 6.9, 6.8$ Hz, 1H), 4.87 (dd, $J = 6.8, 6.7$ Hz, 1H), 3.73-3.66 (m, 1H), 3.55 (dd, $J = 14.9, 7.6$ Hz, 1H), 3.44 (dd, $J = 14.8, 6.8$ Hz, 1H), 1.91-1.84 (m, 5H), 1.72-1.51 (m, 10H), 1.37-1.13 (m, 7H), 1.12-1.01 (m, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.3, 149.6, 147.0, 142.7, 142.5, 141.3, 132.8, 131.7, 126.6, 124.74, 124.73, 123.9, 117.9, 110.9, 110.6, 64.8, 50.2, 48.2, 39.7, 32.8, 32.6, 26.3, 25.7, 25.5, 24.8, 24.7, 17.7, 15.9; HR-FAB MS $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{28}\text{H}_{37}\text{N}_3\text{NaO}_4$ 502.2682; found 502.2684.

Synthesis of 2-((2-(cyclohex-1-en-1-yl)ethyl)(2-nitrophenyl)amino)-N-cyclohexyl-2-(furan-2-yl)acetamide (2d).



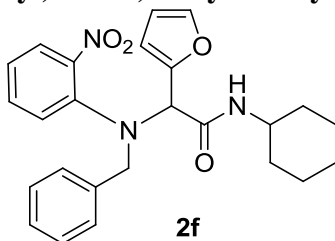
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-furaldehyde (41.5 μ L, 0.5 mmol, 1 equiv), 2-(1-cyclohexenyl)ethylamine (69.7 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (40% ethyl acetate in hexanes) to afford *N*-arylamide **2d** (85.8 mg, 35%). $R_f = 0.13$ (40:60 EtOAc:Hex); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.69 (d, $J = 8.1$ Hz, 1H), 7.49-7.45 (m, 2H), 7.37 (s, 1H), 7.33 (d, $J = 7.7$ Hz, 1H), 7.19 (dd, $J = 7.3, 7.3$ Hz, 1H), 6.38 (d, $J = 2.5$ Hz, 1H), 6.35-6.31 (m, 1H), 5.16 (s, 1H), 5.09 (s, 1H), 3.78-3.70 (m, 1H), 3.04-2.88 (m, 2H), 1.95-1.88 (m, 1H), 1.86-1.80 (m, 2H), 1.77-1.56 (m, 8H), 1.45-1.37 (m, 4H), 1.33-1.06 (m, 5H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.3, 149.3, 146.6, 142.7, 142.5, 134.3, 133.0, 126.4, 125.0, 124.7, 123.4, 111.3, 110.6, 65.2, 50.4, 48.3, 35.9, 32.9, 32.6, 28.1, 25.5, 25.2, 24.8, 24.7, 22.8, 22.2; HR-FAB MS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{26}\text{H}_{34}\text{N}_3\text{O}_4$ 452.2544; found 452.2560.

Synthesis of 2-((cyclohex-1-en-1-ylmethyl)(2-nitrophenyl)amino)-N-cyclohexyl-2-(furan-2-yl)acetamide (2e).



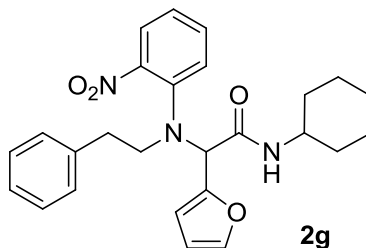
Cyclohex-1-en-1-ylmethyl amine hydrochloride (95.3 mg) was treated with aqueous NaOH (1.0 M, 1 equiv), extracted with diethyl ether, and concentrated *in vacuo* to afford the free cyclohex-1-en-1-ylmethyl amine (74.0 mg). In a similar manner as described in [1], to a solution of 2-nitrophenol (93.2 mg, 0.67 mmol, 1 equiv) in methanol (0.67 mL) was added 2-furaldehyde (55.5 μ L, 0.67 mmol, 1 equiv), cyclohex-1-en-1-ylmethyl amine (74.0 mg, 0.67 mmol, 1 equiv), and cyclohexyl isocyanide (83.5 μ L, 0.67 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (20% ethyl acetate in hexanes) to afford *N*-arylamide **2e** (105.1 mg, 36%). $R_f = 0.55$ (50:50 EtOAc:Hex); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.73 (d, $J = 6.9$ Hz, 1H), 7.52 (d, $J = 8.1$ Hz, 1H), 7.46 (dd, $J = 8.4, 8.4$ Hz, 1H), 7.37-7.33 (m, 2H), 7.13 (dd, $J = 7.3, 7.3$ Hz, 1H), 6.40 (d, $J = 2.9$ Hz, 1H), 6.34-6.31 (m, 1H), 5.28 (s, 1H), 5.16 (s, 1H), 3.81-3.73 (m, 1H), 3.50 (d, $J = 14.2$ Hz, 1H), 3.44 (d, $J = 14.2$ Hz, 1H), 1.97-1.90 (m, 1H), 1.78-1.58 (m, 6H), 1.52-1.49 (m, 2H), 1.42-1.24 (m, 7H), 1.20-1.11 (m, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 166.9, 149.5, 145.5, 142.6, 142.4, 133.1, 132.4, 128.4, 126.1, 125.2, 123.8, 111.3, 110.5, 66.0, 57.2, 48.4, 33.0, 32.6, 26.5, 25.5, 25.1, 24.80, 24.78, 22.4, 21.9; DIMS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{25}\text{H}_{32}\text{N}_3\text{O}_4$ 438.2393; found 438.2387.

Synthesis of 2-(benzyl(2-nitrophenyl)amino)-N-cyclohexyl-2-(furan-2-yl)acetamide (2f).



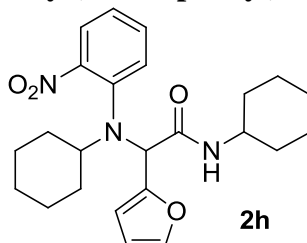
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-furaldehyde (41.5 μ L, 0.5 mmol, 1 equiv), benzylamine (54.6 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography (gradient 10-40% ethyl acetate in hexanes, 36 mL/min, Biotage Isolera, SNAP-Ultra cartridge) to afford *N*-arylamide **2f** (60.9 mg, 28%). $R_f = 0.62$ (50:50 EtOAc:Hex); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.62 (d, $J = 8.0$ Hz, 1H), 7.44 (br s, 1H, NH), 7.40-7.33 (m, 2H), 7.19-7.14 (m, 3H), 7.13-7.09 (m, 2H), 6.92-6.87 (m, 2H), 6.40 (d, $J = 2.8$ Hz, 1H), 6.35-6.32 (m, 1H), 5.06 (s, 1H), 4.20-4.06 (m, 2H), 3.80-3.69 (m, 1H), 1.93-1.84 (m, 1H), 1.77-1.64 (m, 3H), 1.63-1.58 (m, 1H), 1.36-1.28 (m, 2H), 1.27-1.21 (m, 2H), 1.18-1.10 (m, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.1, 149.3, 146.9, 142.9, 142.0, 135.6, 132.8, 129.0, 129.0, 128.4, 128.4, 127.7, 127.0, 125.1, 125.0, 111.4, 110.7, 65.7, 55.9, 48.4, 32.9, 32.7, 25.6, 24.9, 24.8; DIMS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{25}\text{H}_{28}\text{N}_3\text{O}_4$ 434.2080; found 434.2075.

Synthesis of *N*-cyclohexyl-2-(furan-2-yl)-2-((2-nitrophenyl)(phenethyl)amino)acetamide (2g).



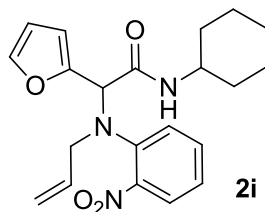
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-furaldehyde (41.5 μ L, 0.5 mmol, 1 equiv), phenethylamine (62.9 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography (gradient 13-40% ethyl acetate in hexanes, 36 mL/min, Biotage Isolera, SNAP-Ultra cartridge) to afford *N*-arylamide **2g** (62.7 mg, 28%). $R_f = 0.55$ (50:50 EtOAc:Hex); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.74 (d, $J = 8.0$ Hz, 1H), 7.52 (dd, $J = 7.8, 7.8$ Hz, 1H), 7.43-7.37 (m, 2H), 7.34 (br s, 1H, NH), 7.25-7.14 (m, 4H), 6.89 (d, $J = 6.8$ Hz, 2H), 6.40 (dd, $J = 11.3, 2.2$ Hz, 2H), 5.14 (s, 1H), 3.78-3.67 (m, 1H), 3.21-3.04 (m, 2H), 2.46-2.32 (m, 2H), 1.93-1.83 (m, 1H), 1.76-1.66 (m, 3H), 1.64-1.56 (m, 1H), 1.37-1.23 (m, 2H), 1.22-1.13 (m, 2H), 1.10-0.98 (m, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.0, 149.3, 146.7, 142.8, 142.2, 138.5, 133.2, 128.7, 128.6, 126.5, 126.2, 125.3, 125.0, 111.5, 110.7, 65.4, 53.0, 48.4, 33.9, 32.9, 32.5, 25.5, 24.9(2C); DIMS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{26}\text{H}_{30}\text{N}_3\text{O}_4$ 448.2236; found 448.2232.

Synthesis of *N*-cyclohexyl-2-(cyclohexyl(2-nitrophenyl)amino)-2-(furan-2-yl)acetamide (2h).



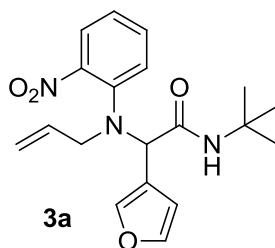
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-furaldehyde (41.5 μ L, 0.5 mmol, 1 equiv), cyclohexylamine (57.3 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography (gradient 12-40% ethyl acetate in hexanes, 36 mL/min, Biotage Isolera, SNAP-Ultra cartridge) to afford *N*-arylamide **2h** (53.2 mg, 25%). $R_f = 0.57$ (50:50 EtOAc:Hex); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.82 (br s, 1H, NH), 7.60 (d, $J = 8.0$ Hz, 1H), 7.37 (dd, $J = 7.4, 7.4$ Hz, 1H), 7.25-7.17 (m, 3H), 6.33 (d, $J = 2.9$ Hz, 1H), 6.18-6.14 (m, 1H), 5.06 (s, 1H), 3.77-3.65 (m, 1H), 2.80-2.70 (m, 1H), 1.91-1.83 (m, 2H), 1.77-1.62 (m, 6H), 1.61-1.54 (m, 1H), 1.52-1.45 (m, 1H), 1.36-1.18 (m, 4H), 1.16-1.05 (m, 3H), 0.96-0.74 (m, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.9, 150.1, 150.0, 142.3, 139.4, 131.8, 131.2, 126.4, 124.3, 110.8, 110.3, 64.8, 63.0, 48.1, 32.8, 32.7, 30.6, 29.2, 26.1, 25.9, 25.5, 24.9; DIMS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{24}\text{H}_{32}\text{N}_3\text{O}_4$ 426.2393; found 426.2388.

Synthesis of 2-(allyl(2-nitrophenyl)amino)-*N*-cyclohexyl-2-(furan-2-yl)acetamide (**2i**).



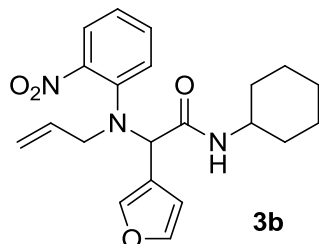
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.5 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-furaldehyde (41 μ L, 0.5 mmol, 1 equiv), allyl amine (38 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 6 h. Removal of volatiles gave the crude material, which was purified via flash column chromatography on silica gel (35% ethyl acetate in hexanes) to afford **2i** for characterization. $R_f = 0.10$ (40:60 Et₂O:Hex); ¹H NMR (400 MHz, CDCl₃) δ 7.70 (d, $J = 8.1$ Hz, 1H), 7.48 (dd, $J = 7.8, 7.8$ Hz, 1H), 7.38 (d, $J = 1.8$ Hz, 1H), 7.35 (d, $J = 8.2$ Hz, 1H), 7.19 (dd, $J = 7.8, 7.7$ Hz, 1H), 6.42 (d, $J = 3.2$ Hz, 1H), 6.33 (dd, $J = 3.3, 1.4$ Hz, 1H), 5.54-5.44 (m, 1H), 5.10 (s, 1H), 4.99 (d, $J = 10.2$ Hz, 1H), 4.92 (d, $J = 17.1$ Hz, 1H), 3.79-3.69 (m, 1H), 3.59-3.49 (m, 2H), 1.92-1.88 (m, 1H), 1.74-1.57 (m, 5H), 1.38-1.07 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 166.9, 149.2, 142.7, 142.1, 133.0, 132.2, 126.3, 125.0, 124.7, 119.5, 111.2, 110.6, 77.2, 65.0, 54.5, 48.2, 32.9, 32.5, 25.5, 24.8, 24.7.

Synthesis of 2-(allyl(2-nitrophenyl)amino)-*N*-(*tert*-butyl)-2-(furan-3-yl)acetamide (**3a**).



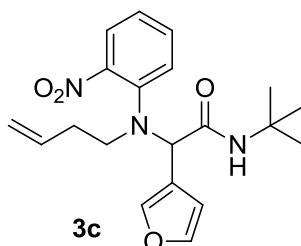
In a similar manner as described in [1], to a solution of 2-nitrophenol (50.1 mg, 0.37 mmol, 1 equiv) in methanol (0.37 mL) was added 3-furaldehyde (31.2 μ L, 0.37 mmol, 1 equiv), allylamine (27 μ L, 0.37 mmol, 1 equiv), and *tert*-butyl isocyanide (81.5 μ L, 0.74 mmol, 2 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (20% ethyl acetate in hexanes) to afford *N*-arylamide **3a** (79.9 mg, 45%). $R_f = 0.76$ (50:50 EtOAc:Hex); ¹H NMR (400 MHz, CDCl₃) δ 7.67 (d, $J = 7.4$ Hz, 1H), 7.47-7.39 (m, 2H), 7.33 (s, 1H), 7.24-7.15 (m, 3H), 6.35 (s, 1H), 5.66-5.53 (m, 1H), 5.04 (d, $J = 10.1$ Hz, 1H), 4.95-4.89 (m, 1H), 4.76 (s, 1H), 3.58 (dd, $J = 6.7, 6.6$ Hz, 1H), 3.47 (dd, $J = 6.5, 6.5$ Hz, 1H), 1.25 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 169.1, 147.2, 143.4, 142.2, 142.1, 132.7, 131.9, 126.6, 125.1, 124.8, 120.4, 120.0, 110.1, 64.0, 55.1, 51.1, 28.5; HR-FAB MS [M+H]⁺ calcd for C₁₉H₂₄N₃O₄ 358.1767; found 358.1767.

Synthesis of 2-(allyl(2-nitrophenyl)amino)-*N*-cyclohexyl-2-(furan-3-yl)acetamide (**3b**).



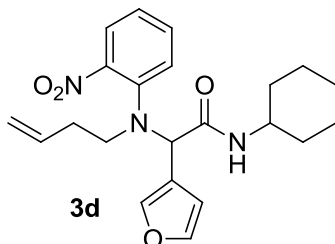
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 3-furaldehyde (43.3 μ L, 0.5 mmol, 1 equiv), allylamine (38.0 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μ L, 0.5 mmol, 1 equiv). The reaction mixture warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (15% ethyl acetate in hexanes) to afford *N*-arylamide **3b** (123.8 mg, 64%). $R_f = 0.51$ (50:50 EtOAc:Hex); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.75 (d, $J = 8.0$ Hz, 1H), 7.53-7.50 (m, 2H), 7.41 (s, 1H), 7.34-7.28 (m, 3H), 6.44 (s, 1H), 5.72-5.62 (m, 1H), 5.13 (d, $J = 10.1$ Hz, 1H), 5.02 (d, $J = 17.1$ Hz, 1H), 4.96 (s, 1H), 3.79-3.71 (m, 1H), 3.65 (dd, $J = 6.7, 6.6$ Hz, 1H), 3.55 (dd, $J = 6.6, 6.5$ Hz, 1H), 1.94-1.86 (m, 1H), 1.78-1.62 (m, 4H), 1.44-1.19 (m, 4H), 1.15-1.03 (m, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.8, 147.1, 143.3, 142.1, 141.8, 132.6, 131.6, 126.3, 125.0, 124.6, 120.3, 120.0, 109.9, 63.0, 55.1, 47.9, 32.7, 32.5, 25.4, 24.6, 24.5; HR-FAB MS $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{21}\text{H}_{25}\text{N}_3\text{NaO}_4$ 406.1743; found 406.1743.

Synthesis of 2-(but-3-en-1-yl(2-nitrophenyl)amino)-*N*-(*tert*-butyl)-2-(furan-3-yl)acetamide (**3c**).



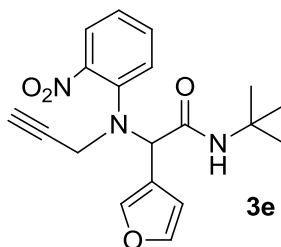
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 3-furaldehyde (43.2 μ L, 0.5 mmol, 1 equiv), 3-butenylamine (45.8 μ L, 0.5 mmol, 1 equiv), and *tert*-butyl isocyanide (113.1 μ L, 1.0 mmol, 2 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (15% ethyl acetate in hexanes) to afford *N*-arylamide **3c** (108.1 mg, 58%). $R_f = 0.18$ (20:80 EtOAc:Hex); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.64 (d, $J = 7.9$ Hz, 1H), 7.40 (dd, $J = 7.4, 7.4$ Hz, 1H), 7.30-7.23 (m, 2H), 7.23-7.08 (m, 3H), 6.28 (s, 1H), 5.61-5.46 (m, 1H), 4.92-4.79 (m, 2H), 4.67 (s, 1H), 3.06-2.94 (m, 1H), 2.91-2.79 (m, 1H), 2.03-1.81 (m, 2H), 1.24 (s, 9H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 169.1, 147.9, 143.2, 142.3, 141.9, 135.0, 132.7, 126.9, 125.6, 124.9, 119.5, 117.2, 110.6, 64.8, 51.2, 51.1, 31.3, 29.6; HR-FAB MS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{20}\text{H}_{26}\text{N}_3\text{O}_4$ 372.1923; found 372.1911.

Synthesis of 2-(but-3-en-1-yl(2-nitrophenyl)amino)-*N*-cyclohexyl-2-(furan-3-yl)acetamide (3d).



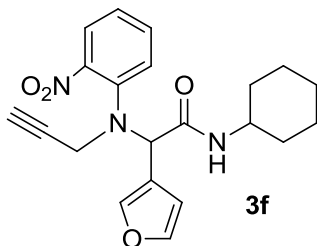
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 3-furaldehyde (43.3 μ L, 0.5 mmol, 1 equiv), 3-butenylamine (45.8 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (15% ethyl acetate in hexanes) to afford *N*-arylamide **3d** (103.3 mg, 52%). R_f = 0.51 (50:50 EtOAc:Hex); ^1H NMR (400 MHz, CDCl_3) δ 7.69 (d, J = 7.8 Hz, 1H), 7.47 (dd, J = 7.4, 7.4 Hz, 1H), 7.36 (s, 1H), 7.33 (s, 1H), 7.28-7.19 (m, 3H), 6.33 (s, 1H), 5.62-5.51 (m, 1H), 4.95-4.84 (m, 3H), 3.74-3.67 (m, 1H), 3.08-3.01 (m, 1H), 2.94-2.87 (m, 1H), 2.05-1.91 (m, 2H), 1.86 (d, J = 12.0 Hz, 1H), 1.75-1.54 (m, 5H), 1.38-1.12 (m, 3H), 1.09-1.00 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.8, 147.7, 143.1, 142.2, 141.8, 134.7, 132.7, 126.6, 125.4, 124.8, 119.5, 117.1, 110.3, 63.9, 51.1, 48.0, 32.8, 32.5, 31.0, 25.4, 24.7, 24.6; HR-FAB MS $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{22}\text{H}_{27}\text{N}_3\text{NaO}_4$ 420.1899; found 420.1918.

Synthesis of *N*-(*tert*-butyl)-2-(furan-3-yl)-2-((2-nitrophenyl)-(prop-2-yn-1-yl)amino)acetamide (3e).



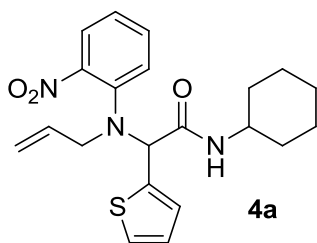
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.7 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 3-furaldehyde (43.2 μ L, 0.5 mmol, 1 equiv), propargylamine (32.0 μ L, 0.5 mmol, 1 equiv), and *tert*-butyl isocyanide (114 μ L, 1.0 mmol, 2 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (20% ethyl acetate in hexanes) to afford *N*-arylamide **3e** (40.7 mg, 23%). R_f = 0.70 (50:50 EtOAc:Hex); ^1H NMR (400 MHz, CDCl_3) δ 7.68 (d, J = 7.7 Hz, 1H), 7.58 (s, 1H), 7.54-7.49 (m, 2H), 7.37 (s, 1H), 7.34-7.28 (m, 1H), 6.89 (s, 1H), 6.41 (s, 1H), 4.95 (s, 1H), 3.61 (dd, J = 17.9, 2.2 Hz, 1H), 3.53 (dd, J = 17.8, 2.0 Hz, 1H), 2.27 (s, 1H), 1.12 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.7, 147.7, 143.9, 142.6, 141.1, 132.7, 126.7, 126.4, 124.3, 120.6, 109.2, 76.8, 75.2, 62.4, 51.2, 43.6, 28.4; DIMS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{22}\text{N}_3\text{O}_4$ 356.1610; found 356.1601.

Synthesis of *N*-cyclohexyl-2-(furan-3-yl)-2-((2-nitrophenyl)(prop-2-yn-1-yl)amino)acetamide (3f).



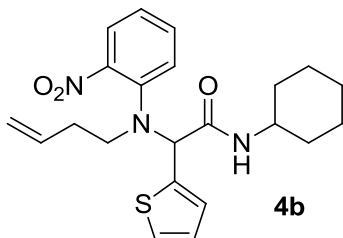
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.6 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 3-furaldehyde (43.3 μ L, 0.5 mmol, 1 equiv), propargylamine (32.1 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62.2 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (20% ethyl acetate in hexanes) to afford *N*-arylamide **3f** (92.2 mg, 48%). R_f = 0.47 (50:50 EtOAc:Hex); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.65 (d, J = 8.0 Hz, 1H), 7.59 (s, 1H), 7.51-7.50 (m, 2H), 7.36 (s, 1H), 7.33-7.30 (m, 1H), 7.02 (d, J = 8.3 Hz, 1H), 6.40 (s, 1H), 5.07 (s, 1H), 3.70-3.54 (m, 3H), 2.27 (s, 1H), 1.78-1.64 (m, 3H), 1.56-1.47 (m, 2H), 1.30-1.04 (m, 4H), 0.79-0.70 (m, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.5, 147.7, 143.8, 142.6, 140.9, 132.7, 126.4(2C), 124.2, 120.5, 109.1, 76.7, 75.2, 61.4, 47.9, 43.6, 32.7, 32.4, 25.4, 24.8, 24.7; HR-FAB MS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{21}\text{H}_{24}\text{N}_3\text{O}_4$ 382.1767; found 382.1768.

Synthesis of 2-(allyl(2-nitrophenyl)amino)-*N*-cyclohexyl-2-(thiophen-2-yl)acetamide (4a).



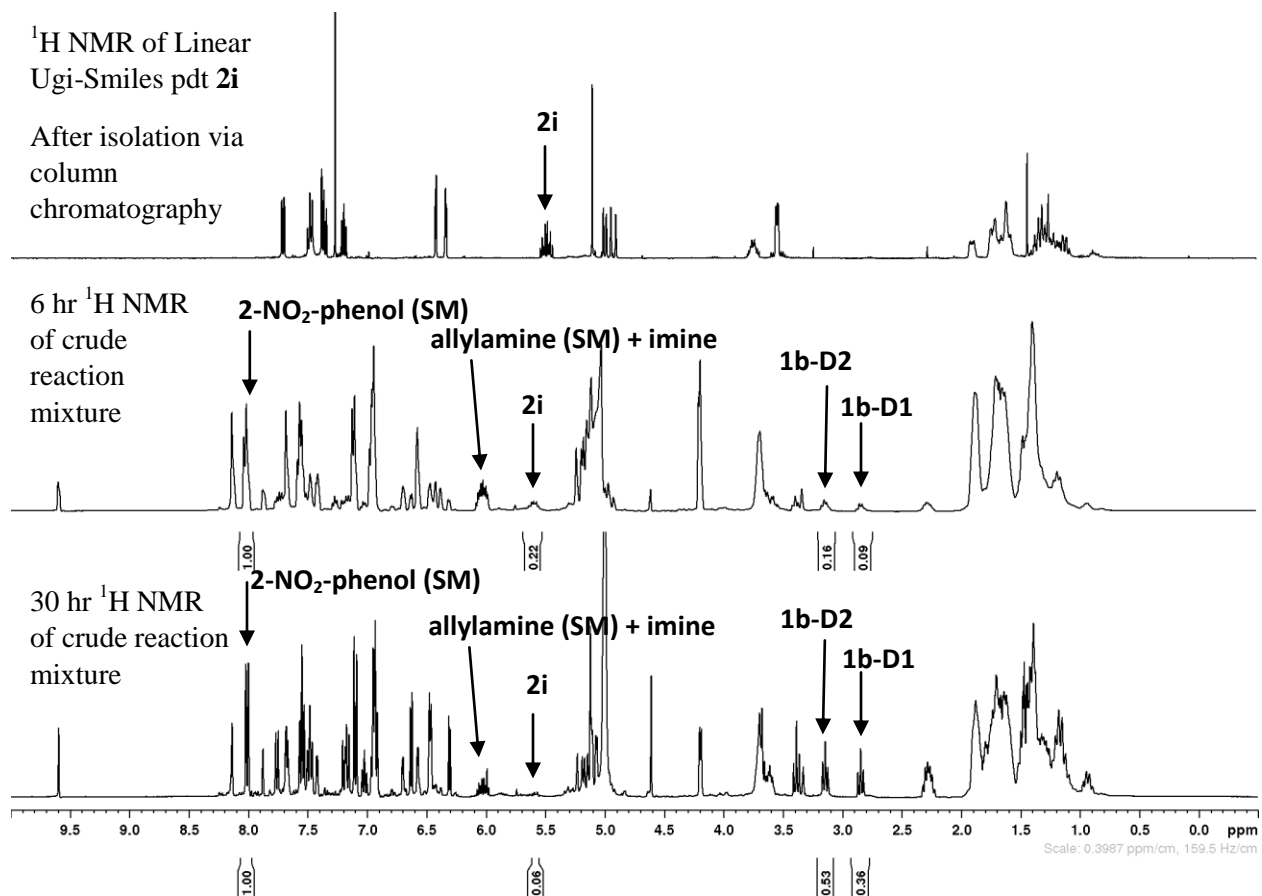
In a similar manner as described in [1], to a solution of 2-nitrophenol (69.8 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-thiophenecarboxaldehyde (46.7 μ L, 0.5 mmol, 1 equiv), allylamine (38 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (62 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 30 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (10% ethyl acetate in hexanes) to afford *N*-aryl amide **4a** (49.3 mg, 25%). R_f = 0.13 (20:80 EtOAc:Hex); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.69 (d, J = 8.0 Hz, 1H), 7.45 (dd, J = 8.0, 7.6 Hz, 1H), 7.29-7.19 (m, 4H), 7.05 (d, J = 2.6 Hz, 1H), 6.91 (dd, J = 4.3, 4.3 Hz, 1H), 5.65-5.55 (m, 1H), 5.22 (s, 1H), 5.06 (d, J = 10.1 Hz, 1H), 4.91 (d, J = 17.1 Hz, 1H), 3.67-3.62 (m, 1H), 3.60-3.46 (m, 2H), 1.86-1.77 (m, 1H), 1.73-1.64 (m, 1H), 1.60-1.50 (m, 3H), 1.33-1.09 (m, 4H), 0.96-0.88 (m, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 168.4, 147.1, 141.8, 138.4, 132.7, 131.4, 128.4, 126.5, 126.4 (2C), 125.3, 124.7, 120.3, 66.8, 55.4, 48.0, 32.5, 32.4, 25.4, 24.7, 24.6; DIMS $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{21}\text{H}_{26}\text{N}_3\text{O}_3\text{S}$ 400.1695; found 400.1690.

Synthesis of 2-(but-3-en-1-yl(2-nitrophenyl)amino)-*N*-cyclohexyl-2-(thiophen-2-yl)acetamide (**4b**).

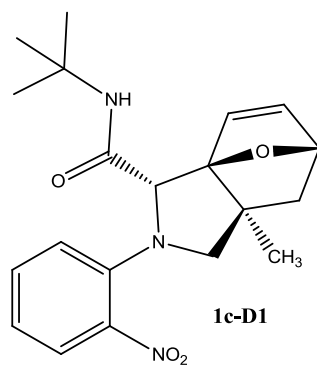


In a similar manner as described in [1], to a solution of 2-nitrophenol (69.8 mg, 0.5 mmol, 1 equiv) in methanol (0.50 mL) was added 2-thiophenecarboxaldehyde (46.7 μ L, 0.5 mmol, 1 equiv), 3-butenylamine (45.8 μ L, 0.5 mmol, 1 equiv), and cyclohexyl isocyanide (61.3 μ L, 0.5 mmol, 1 equiv). The reaction mixture was warmed at 50 °C for 48 h. Removal of volatiles gave crude material, which was purified via flash column chromatography on silica gel (20% ethyl ether in hexanes) to afford *N*-aryl amide **4b** (47.5 mg, 23%). $R_f = 0.10$ (40:60 Et₂O:Hex); ¹H NMR (400 MHz, CDCl₃) δ 7.70 (dd, $J = 8.1, 1.6$ Hz, 1H), 7.46 (dd, $J = 8.7, 7.0$ Hz, 1H), 7.30-7.18 (m, 4H), 6.96 (d, $J = 3.5$ Hz, 1H), 6.91 (dd, $J = 5.1, 3.5$ Hz, 1H), 5.60-5.49 (m, 1H), 5.20 (s, 1H), 4.92 (dd, $J = 10.2, 1.6$ Hz, 1H), 4.86 (dd, $J = 17.1, 1.6$ Hz, 1H), 3.74-3.64 (m, 1H), 3.08-2.89 (m, 2H), 2.10-1.99 (m, 1H), 1.98-1.90 (m, 1H), 1.89-1.82 (m, 1H), 1.74-1.66 (m, 1H), 1.66-1.56 (m, 2H), 1.35-1.13 (m, 5H), 1.06-0.96 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 168.5, 147.8, 141.8, 137.6, 134.9, 132.8, 128.7, 126.9, 126.6, 126.4, 125.6, 124.9, 117.2, 67.5, 51.3, 48.2, 32.8, 32.6, 31.0, 25.6, 24.8, 24.7; DIMS [M+H]⁺ calcd for C₂₂H₂₈N₃O₃S 414.1851; found 414.1845.

Stacked ^1H NMRs for reaction monitoring (related to Scheme 2)

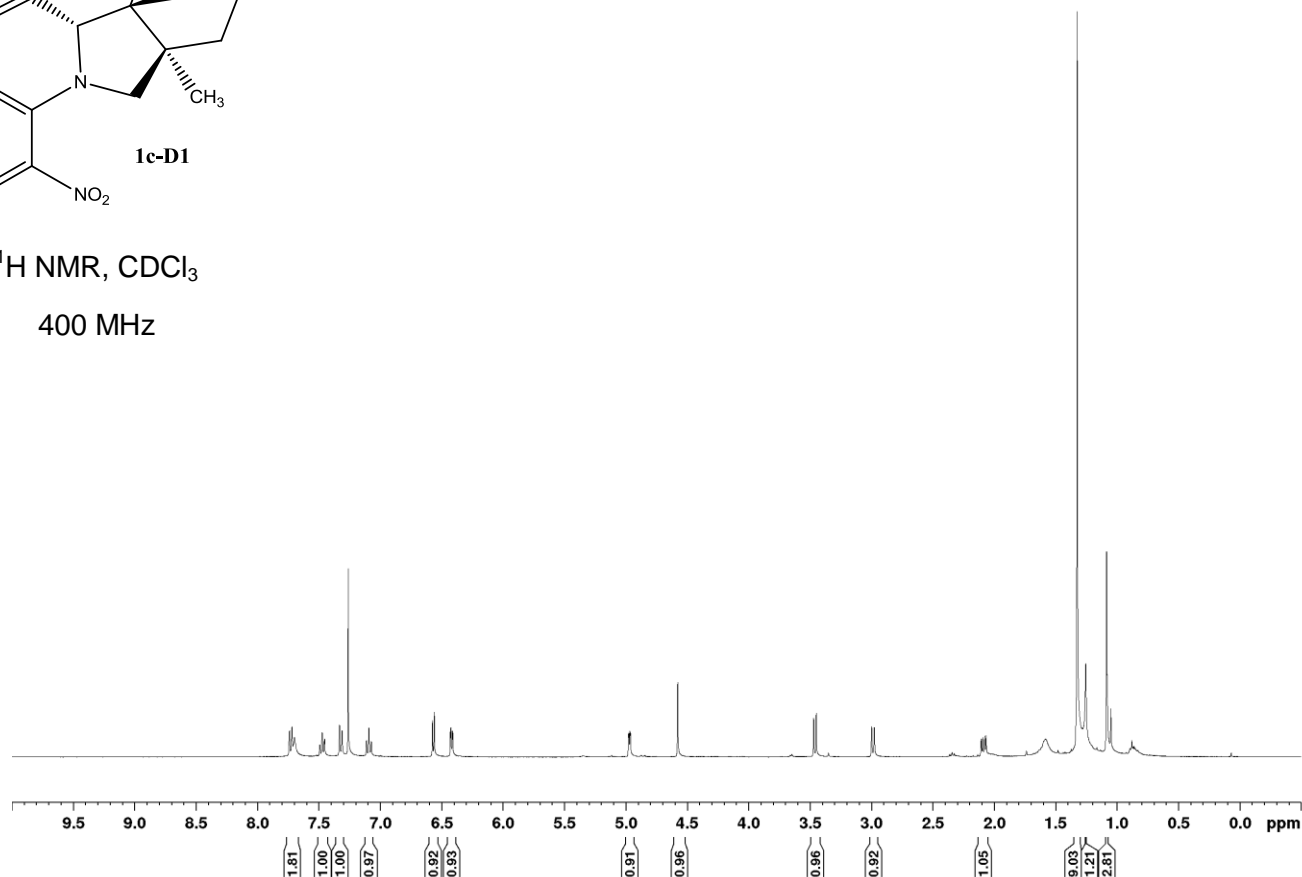


All ^1H spectra were acquired in CDCl_3 . Formation of linear Ugi-Smiles adduct **2i** was tracked by the appearance of the representative diagnostic allylic peak (marked **2i** above), as that peak did not overlap with other starting material or US-IMDA product peaks. Formation of diastereomers **1b-D1** and **1b-D2** were tracked by the diagnostic dd between 2.5-3.2 ppm, as these did not overlap with starting material or linear **2i** product peaks. Conversion was estimated by integrations.



¹H NMR, CDCl₃

400 MHz

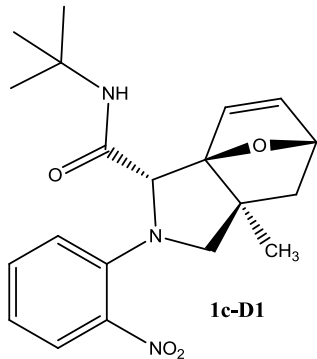


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EXPNO 1
PROCNO 1

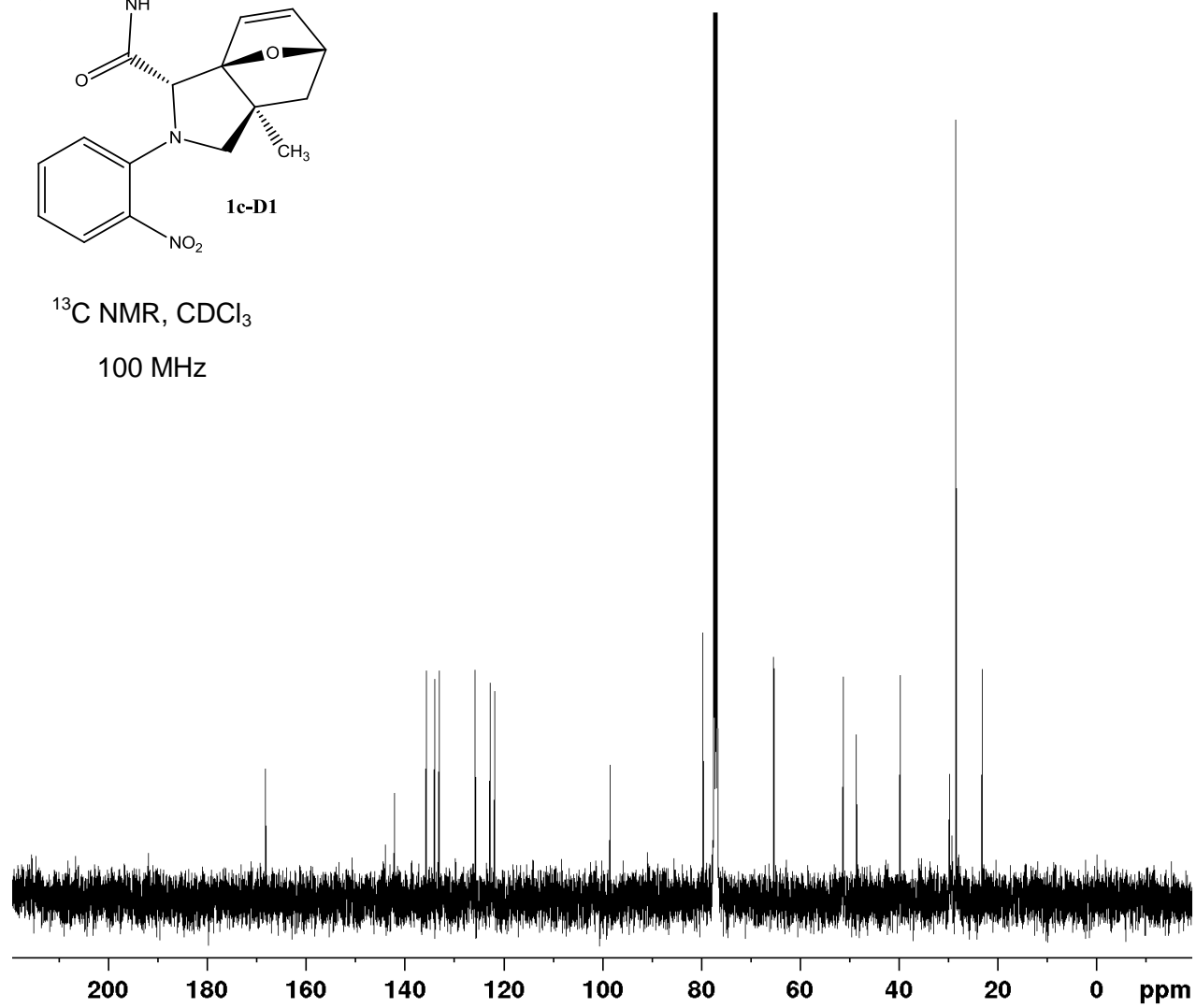
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DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1524711 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1500099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR, CDCl₃
100 MHz



```

Current Data Parameters
NAME      KM-35-D1-C-again
EXPNO     20
PROCNO    1

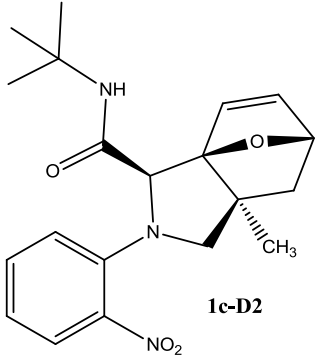
F2 - Acquisition Parameters
Date_     20150526
Time      21.41
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         2048
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         210.96
DW         20.800 usec
DE         10.00 usec
TE         293.3 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      100.6278588 MHz
NUC1       13C
P1         10.00 usec
PLW1       48.20000076 W

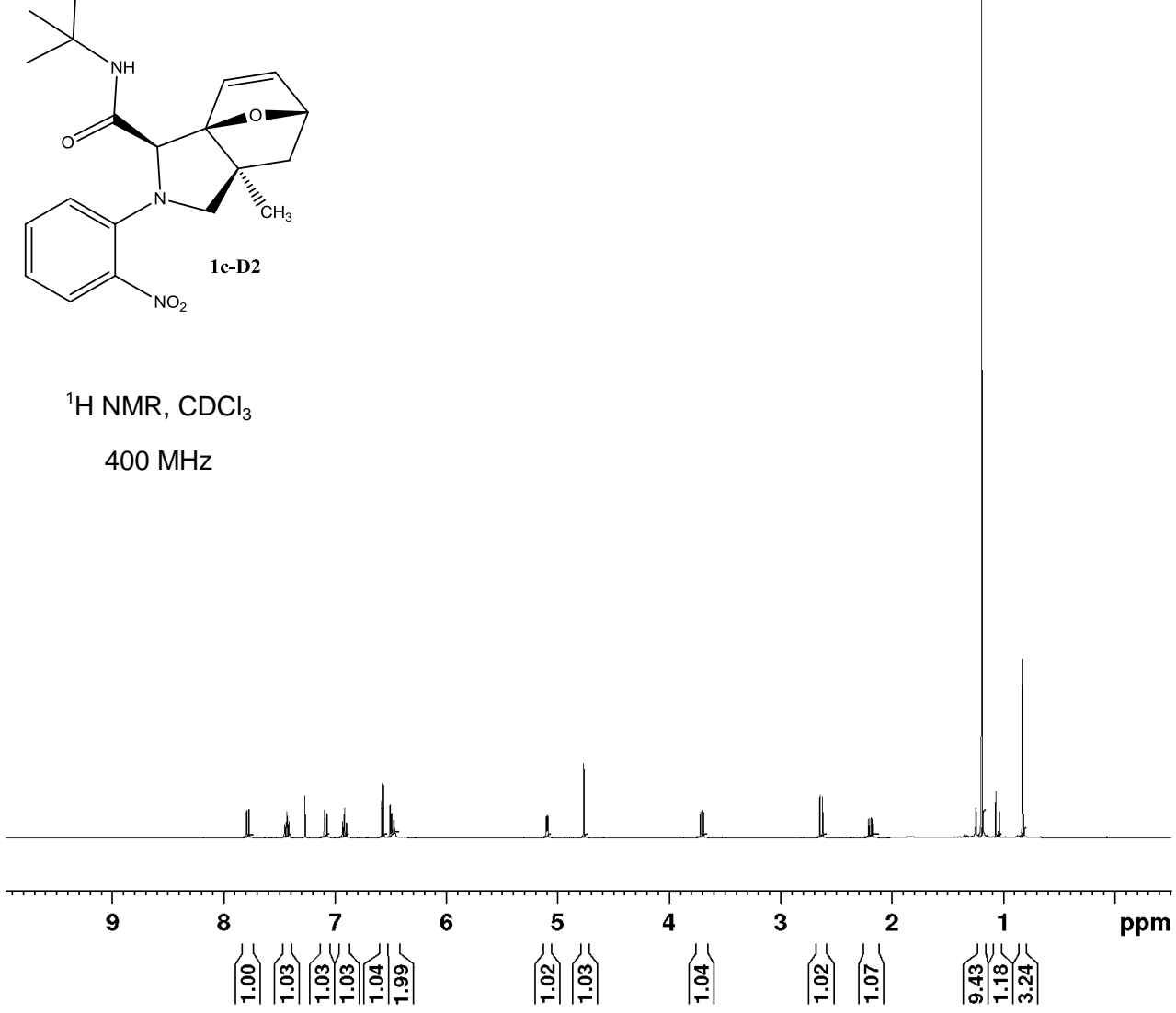
===== CHANNEL f2 =====
SFO2      400.1516006 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2     90.00 usec
PLW2       9.80000019 W
PLW12     0.27221999 W
PLW13     0.22050001 W

F2 - Processing parameters
SI         32768
SF         100.6177873 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



¹H NMR, CDCl₃
400 MHz

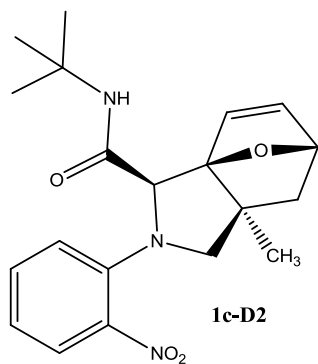


Current Data Parameters
 NAME KM-35-D2
 EXPNO 1
 PROCNO 1

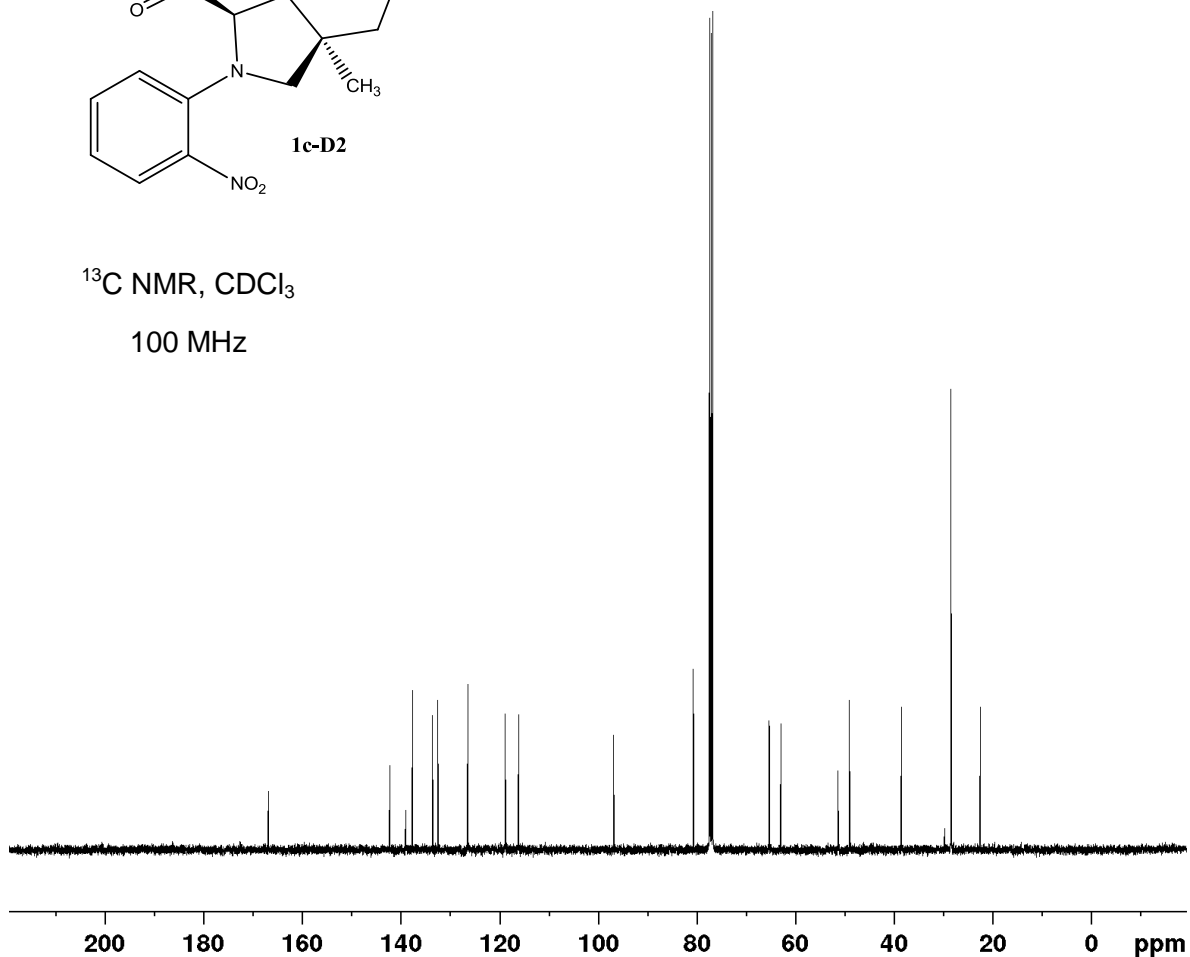
F2 - Acquisition Parameters
 Date_ 20150427
 Time 11.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 95.15
 DW 62.400 usec
 DE 6.50 usec
 TE 292.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500076 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3
100 MHz



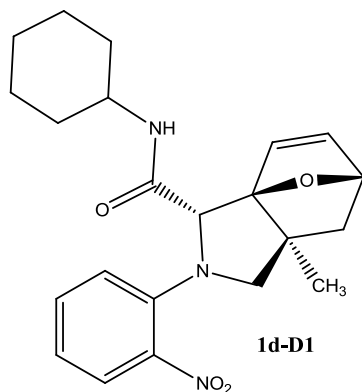
Current Data Parameters
NAME KM-35-D2-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150522
Time 12.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 210.96
DW 20.800 usec
DE 10.00 usec
TE 293.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

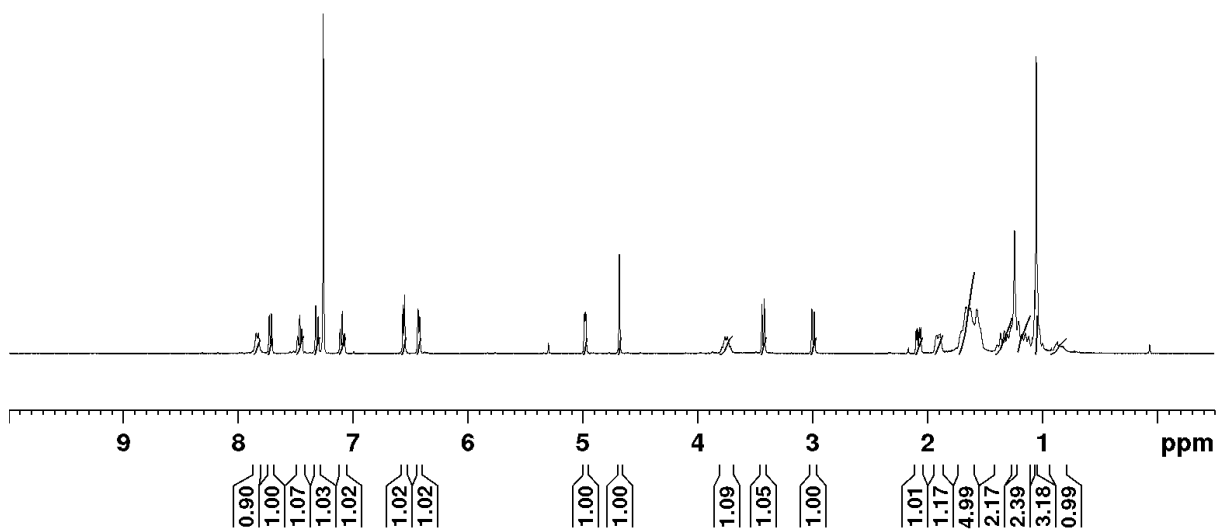
===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 48.20000076 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 9.80000019 W
PLW12 0.27221999 W
PLW13 0.22050001 W

F2 - Processing parameters
SI 32768
SF 100.6177874 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



^1H NMR, CDCl_3
400 MHz

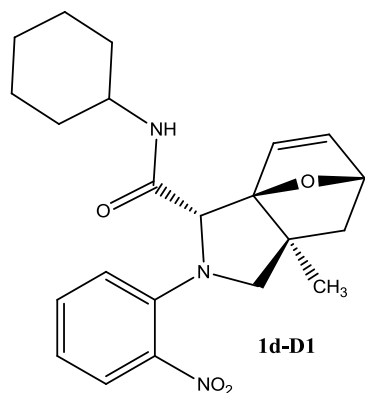


Current Data Parameters
 NAME KM-38-D1R-2-F23-25
 EXPNO 10
 PROCNO 1

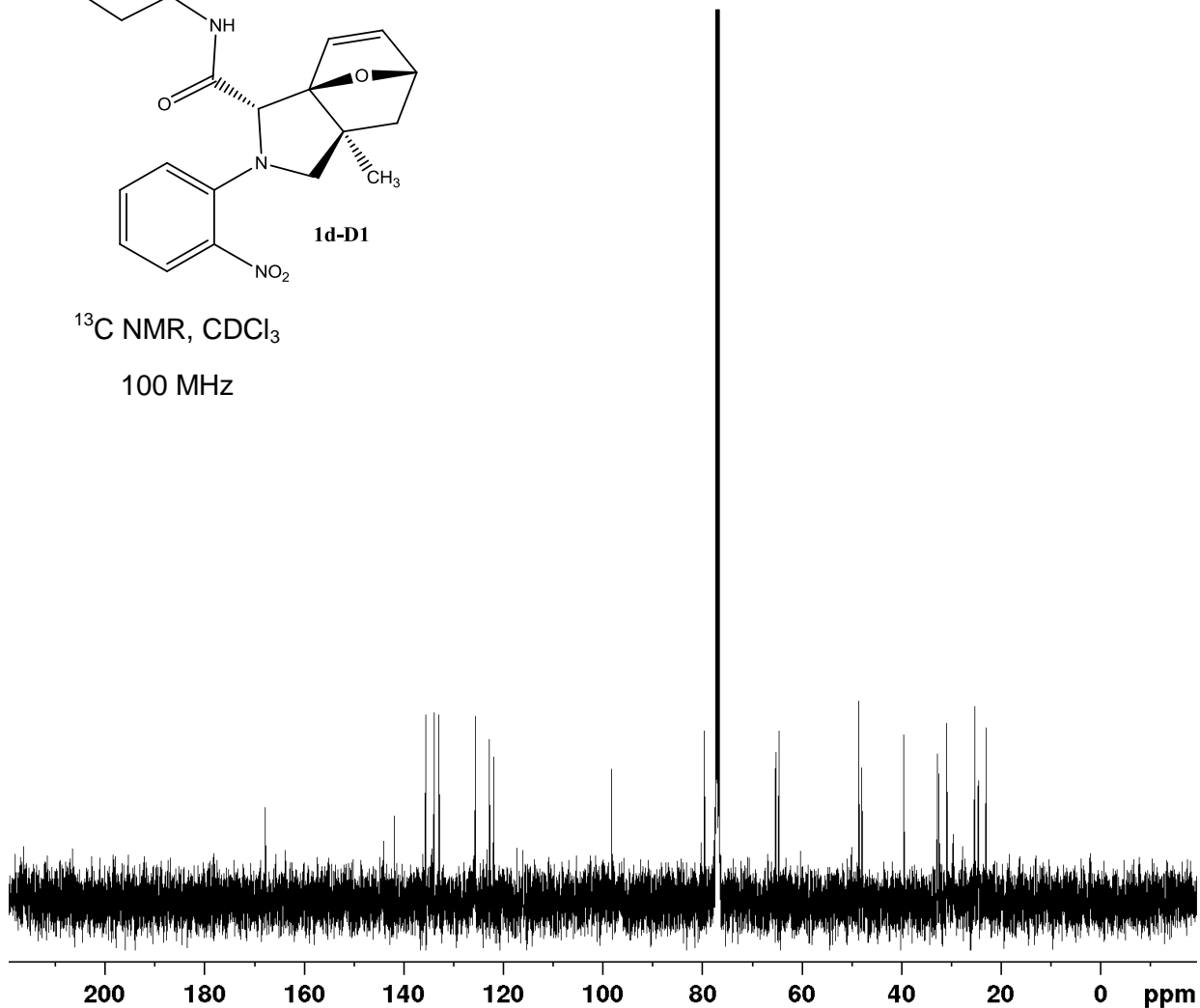
F2 - Acquisition Parameters
 Date_ 20150515
 Time 11.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl_3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 166.66
 DW 62.400 usec
 DE 6.50 usec
 TE 292.3 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500120 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3
100 MHz



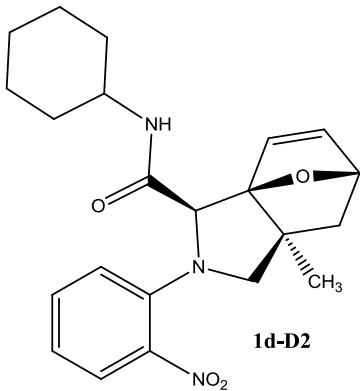
Current Data Parameters
NAME KM-38-D1R-2-F23-25-C2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150519
Time 13.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl_3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 210.96
DW 20.800 usec
DE 10.00 usec
TE 293.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

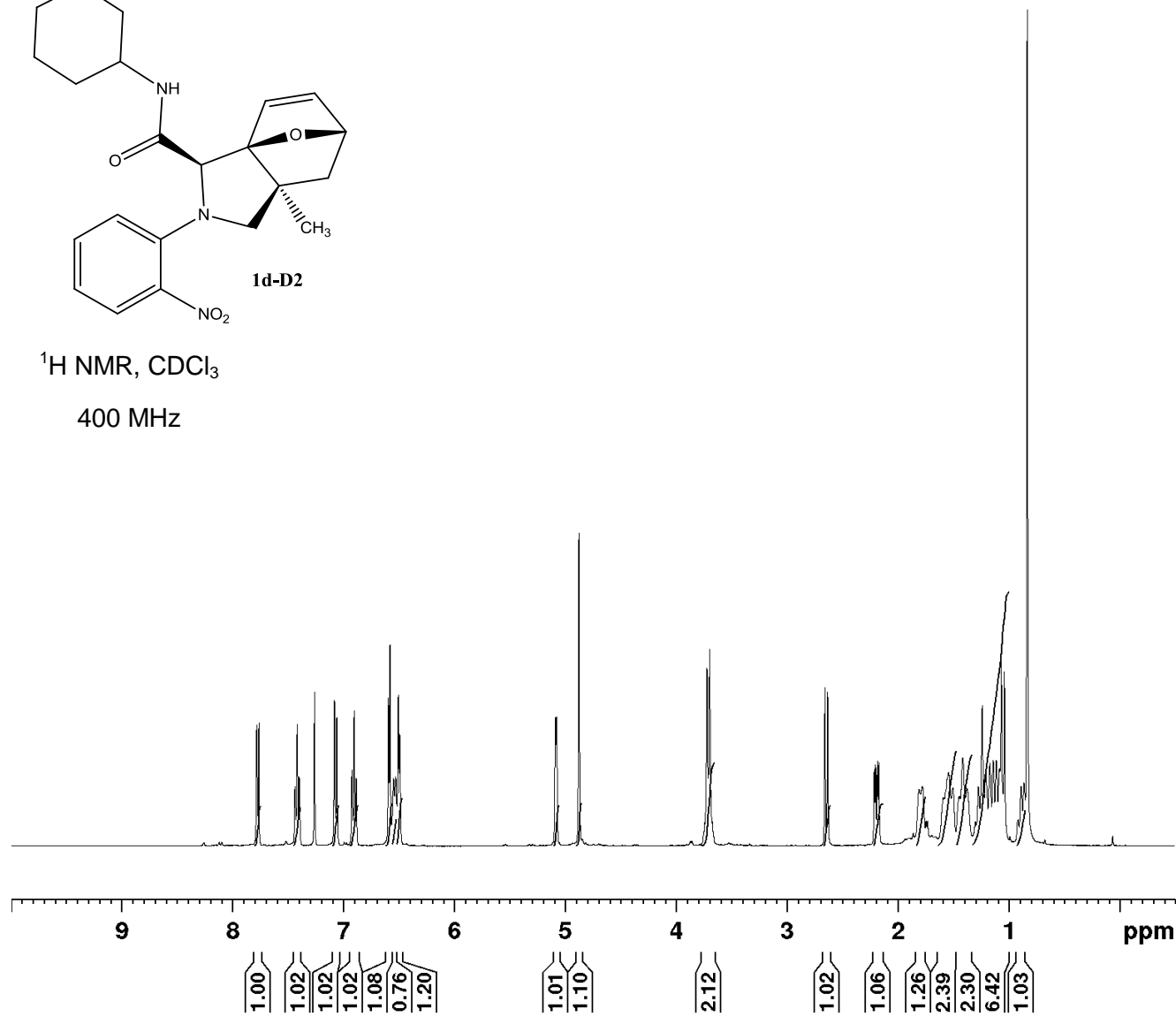
===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 ^{13}C
P1 10.00 usec
PLW1 48.20000076 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 ^1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 9.80000019 W
PLW12 0.27221999 W
PLW13 0.22050001 W

F2 - Processing parameters
SI 32768
SF 100.6178032 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹H NMR, CDCl₃
400 MHz

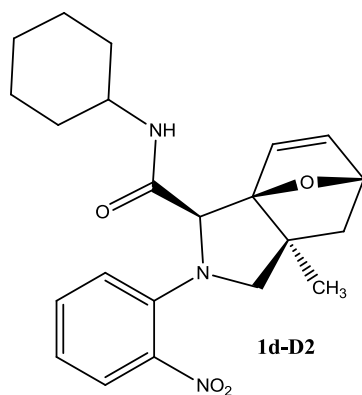


Current Data Parameters
 NAME KM-38-F63-80-D2
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150512
 Time 14.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 120.42
 DW 62.400 usec
 DE 6.50 usec
 TE 292.4 K
 D1 1.00000000 sec
 TD0 1

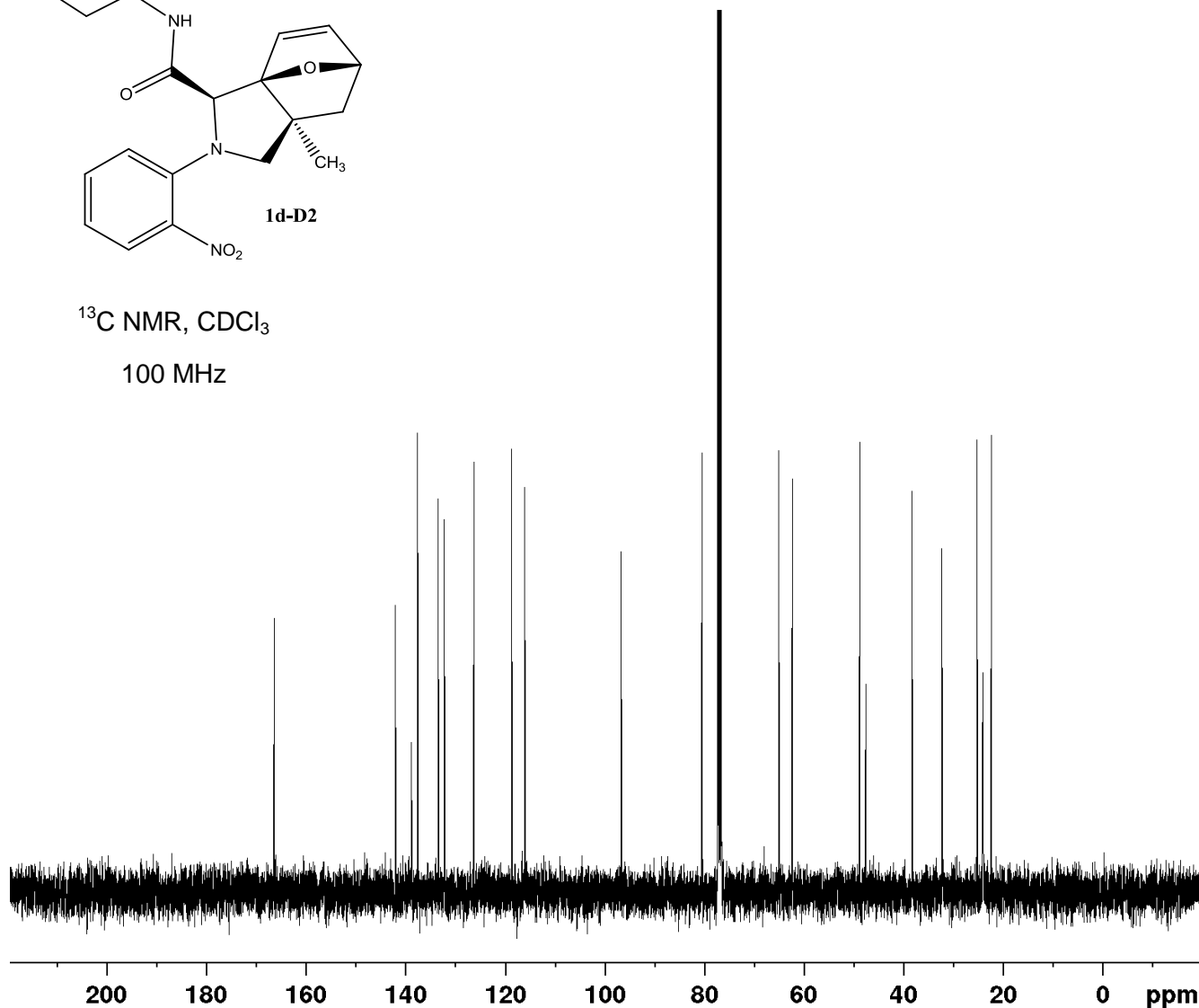
===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500104 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3

100 MHz



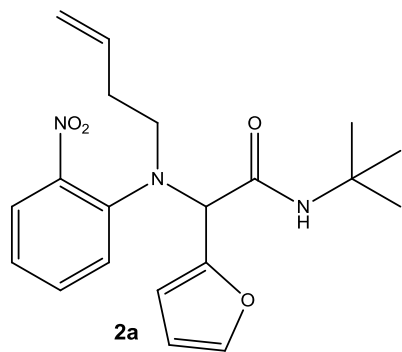
Current Data Parameters
 NAME KM-38-F63-80-D2
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150512
 Time 14.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 128
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 210.96
 DW 20.800 usec
 DE 10.00 usec
 TE 293.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 ^{13}C
 P1 10.00 usec
 PLW1 48.20000076 W

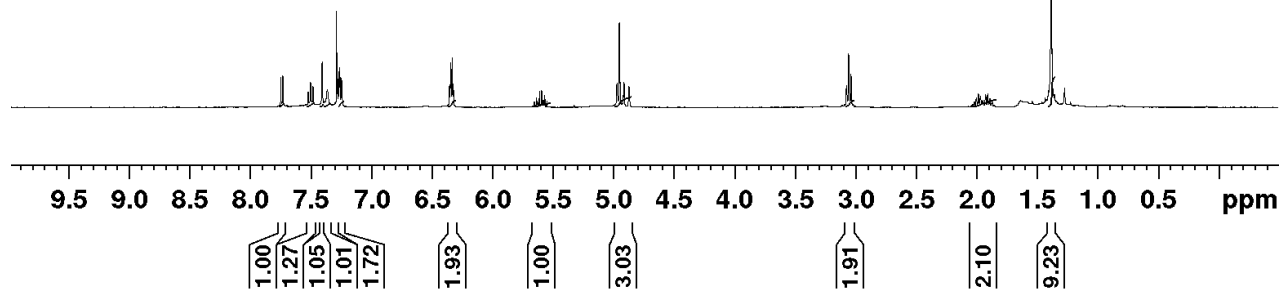
===== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 ^1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.80000019 W
 PLW12 0.27221999 W
 PLW13 0.22050001 W

F2 - Processing parameters
 SI 32768
 SF 100.6177903 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



¹H NMR, CDCl₃

400 MHz

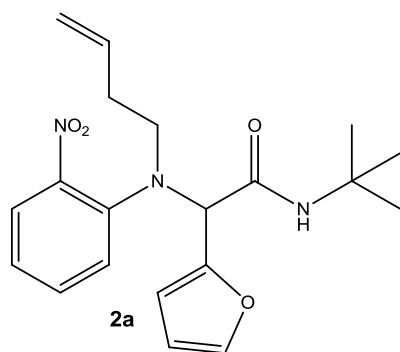


Current Data Parameters
 NAME KM-34-F31-41-test
 EXPNO 10
 PROCNO 1

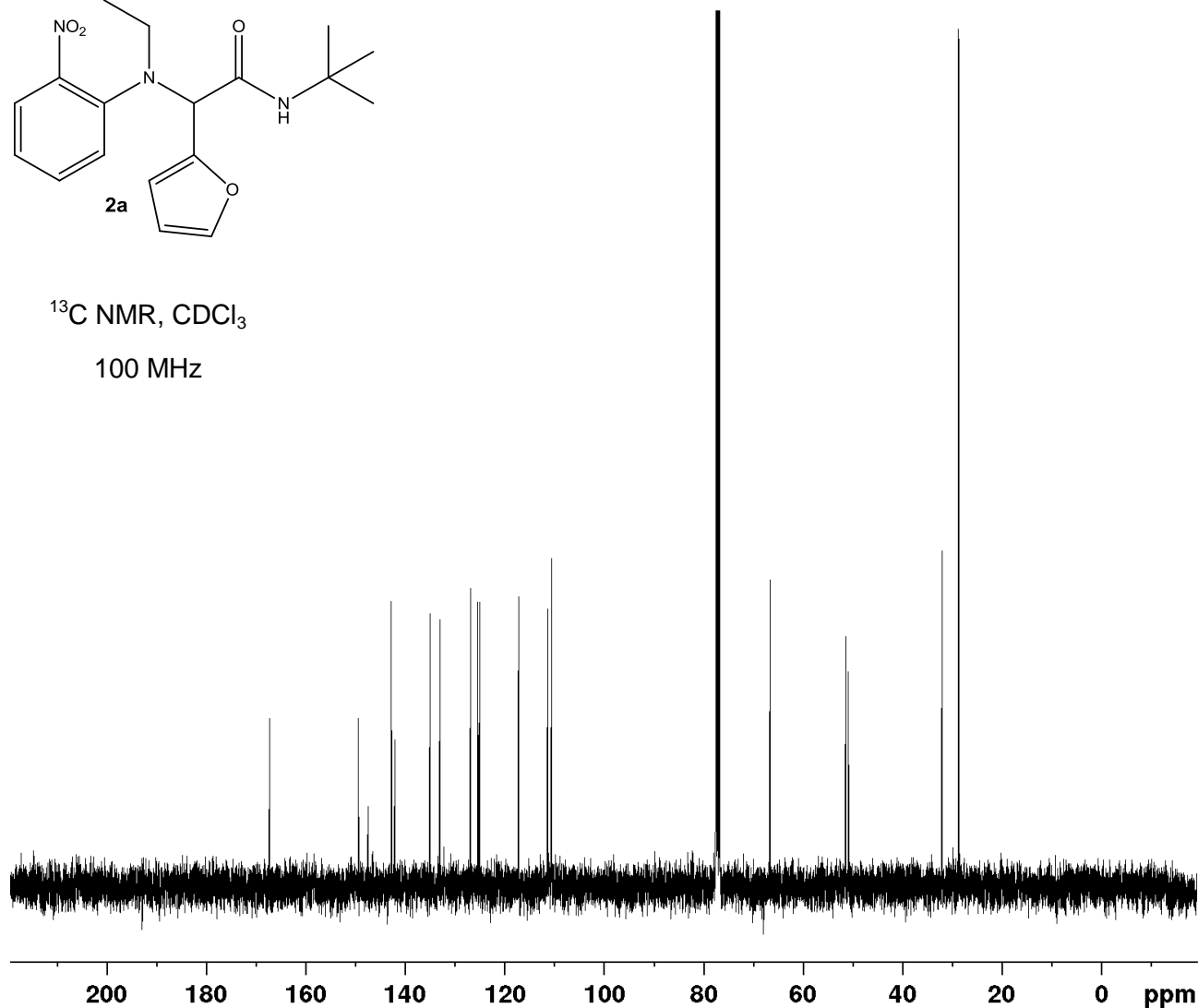
F2 - Acquisition Parameters
 Date_ 20150204
 Time 15.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 134.4
 DW 62.400 usec
 DE 6.50 usec
 TE 293.6 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3
100 MHz



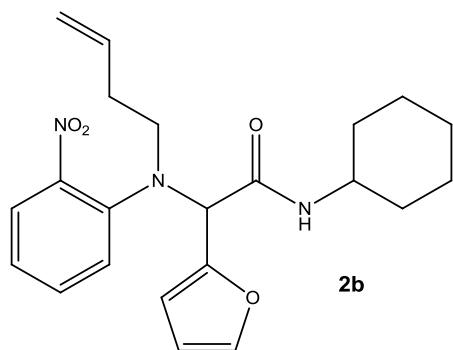
Current Data Parameters
NAME KM-34-F31-41-C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150202
Time 10.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl_3
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 210.96
DW 20.800 usec
DE 10.00 usec
TE 294.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

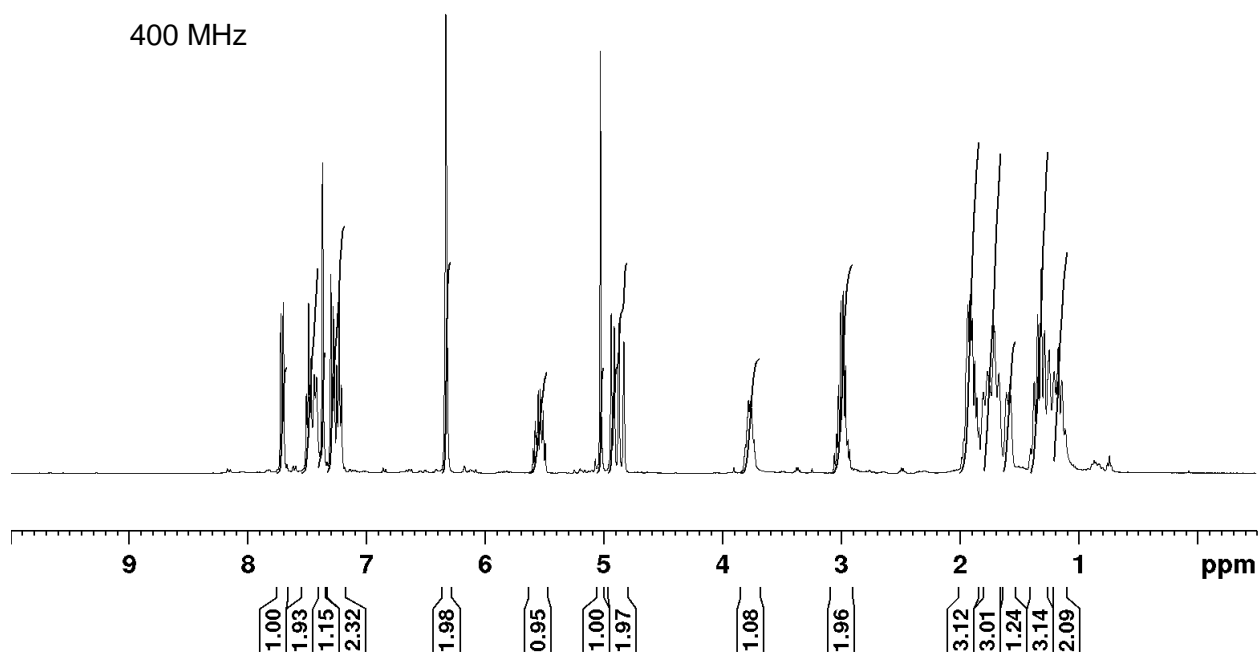
===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 ^{13}C
P1 10.00 usec
PLW1 48.20000076 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 ^1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 9.80000019 W
PLW12 0.27221999 W
PLW13 0.22050001 W

F2 - Processing parameters
SI 32768
SF 100.6177859 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



$^1\text{H NMR}$, CDCl_3
400 MHz

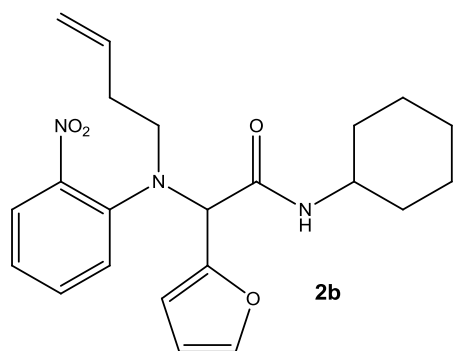


Current Data Parameters
NAME MM-2-70
EXPNO 1
PROCNO 1

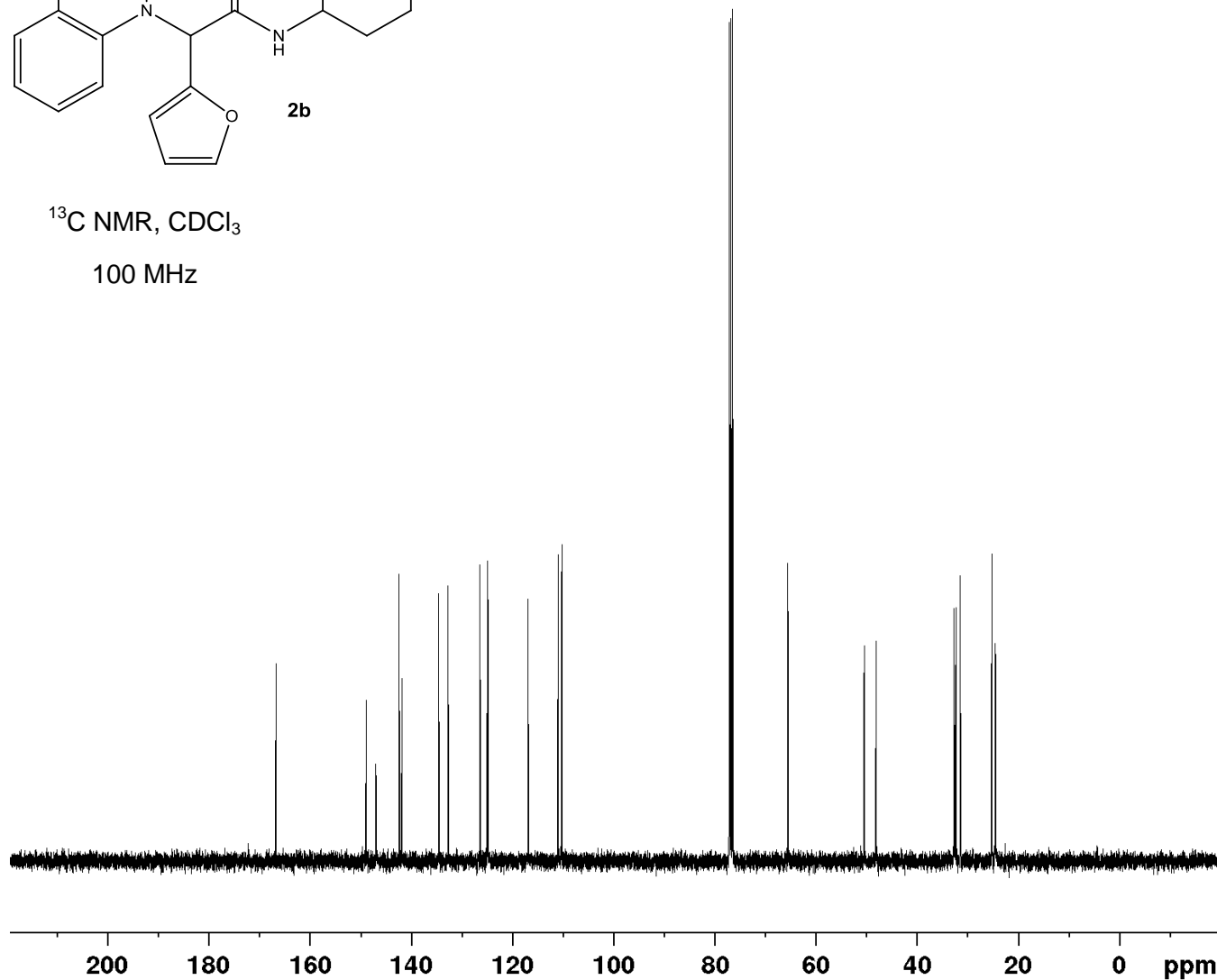
F2 - Acquisition Parameters
Date_ 20160307
Time 20.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 75.54
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1524711 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1500081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



^{13}C NMR, CDCl_3
100 MHz



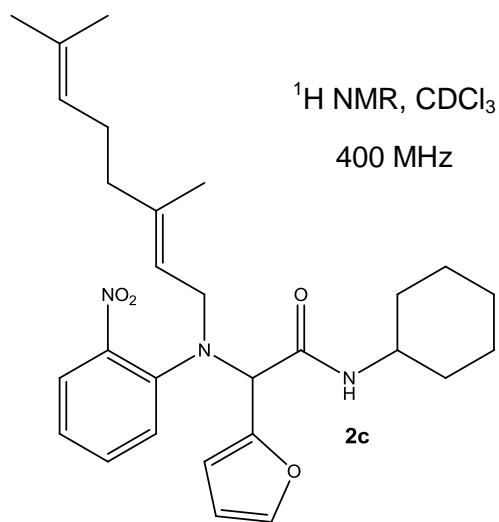
Current Data Parameters
NAME MM-2-70
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160307
Time 20.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl_3
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 210.96
DW 20.800 usec
DE 10.00 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 ^{13}C
P1 10.00 usec
PLW1 48.20000076 W

===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 ^1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 9.80000019 W
PLW12 0.27221999 W
PLW13 0.22050001 W

F2 - Processing parameters
SI 32768
SF 100.6178041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

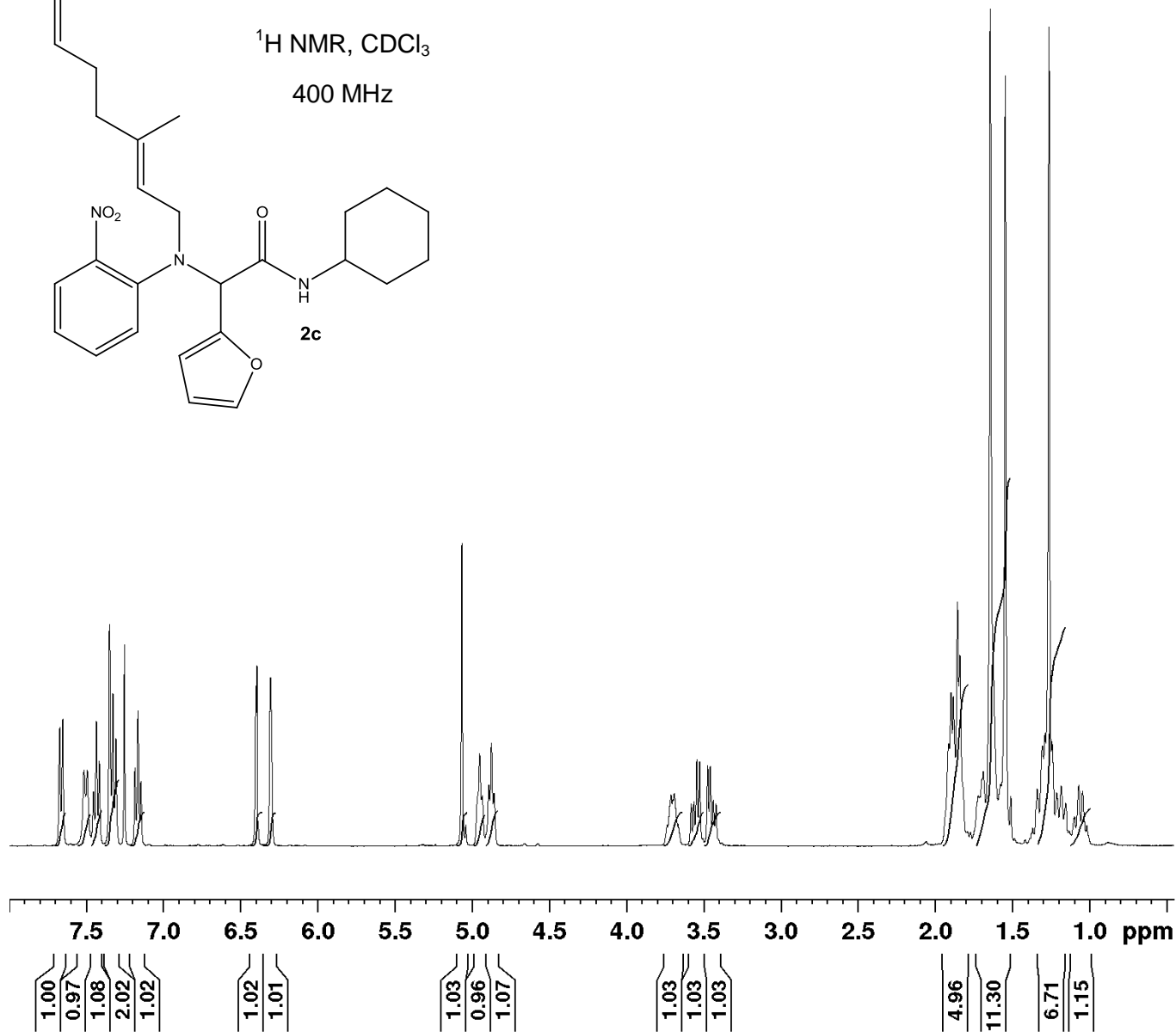


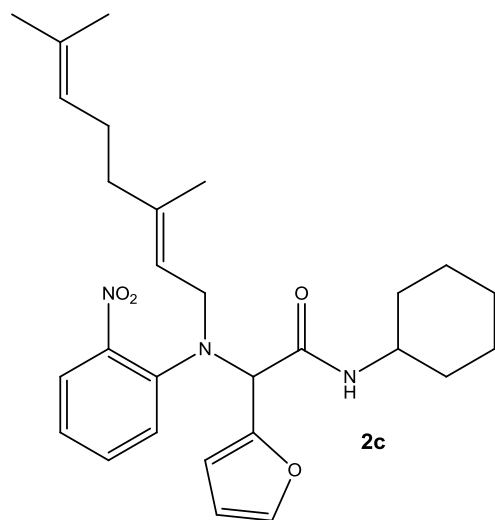
Current Data Parameters
 NAME MM-2-63
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160307
 Time 20.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 120.42
 DW 62.400 usec
 DE 6.50 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

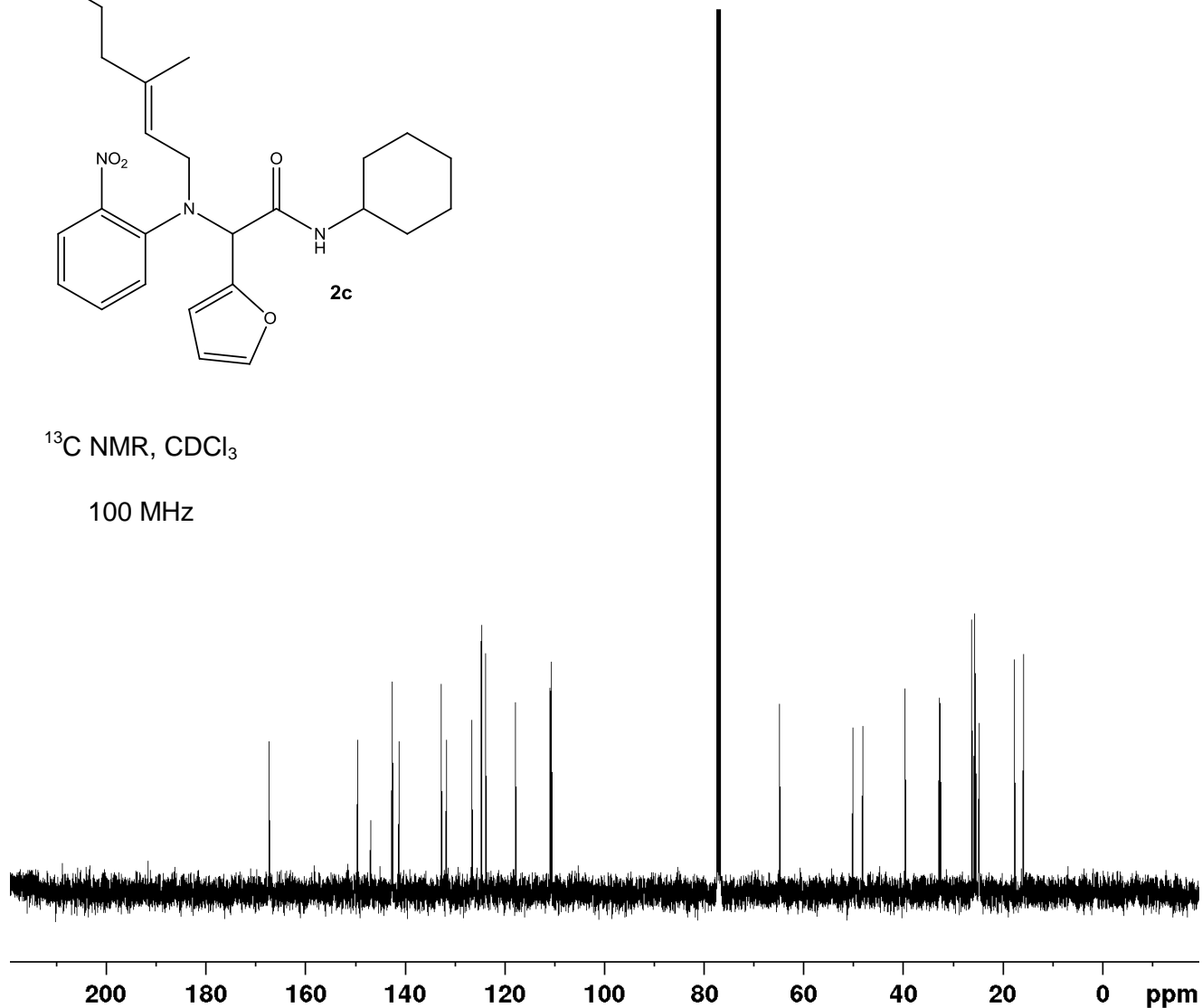
===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500122 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





¹³C NMR, CDCl₃
100 MHz



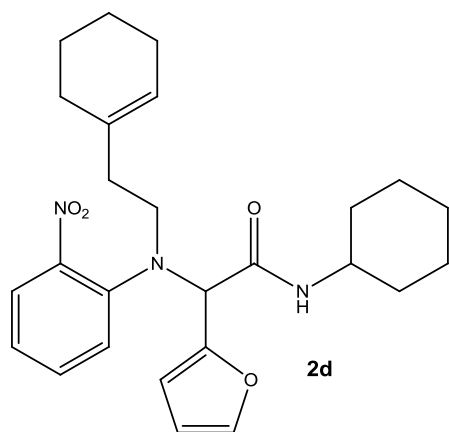
Current Data Parameters
NAME MM-2-63
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160307
Time 20.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 210.96
DW 20.800 usec
DE 10.00 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

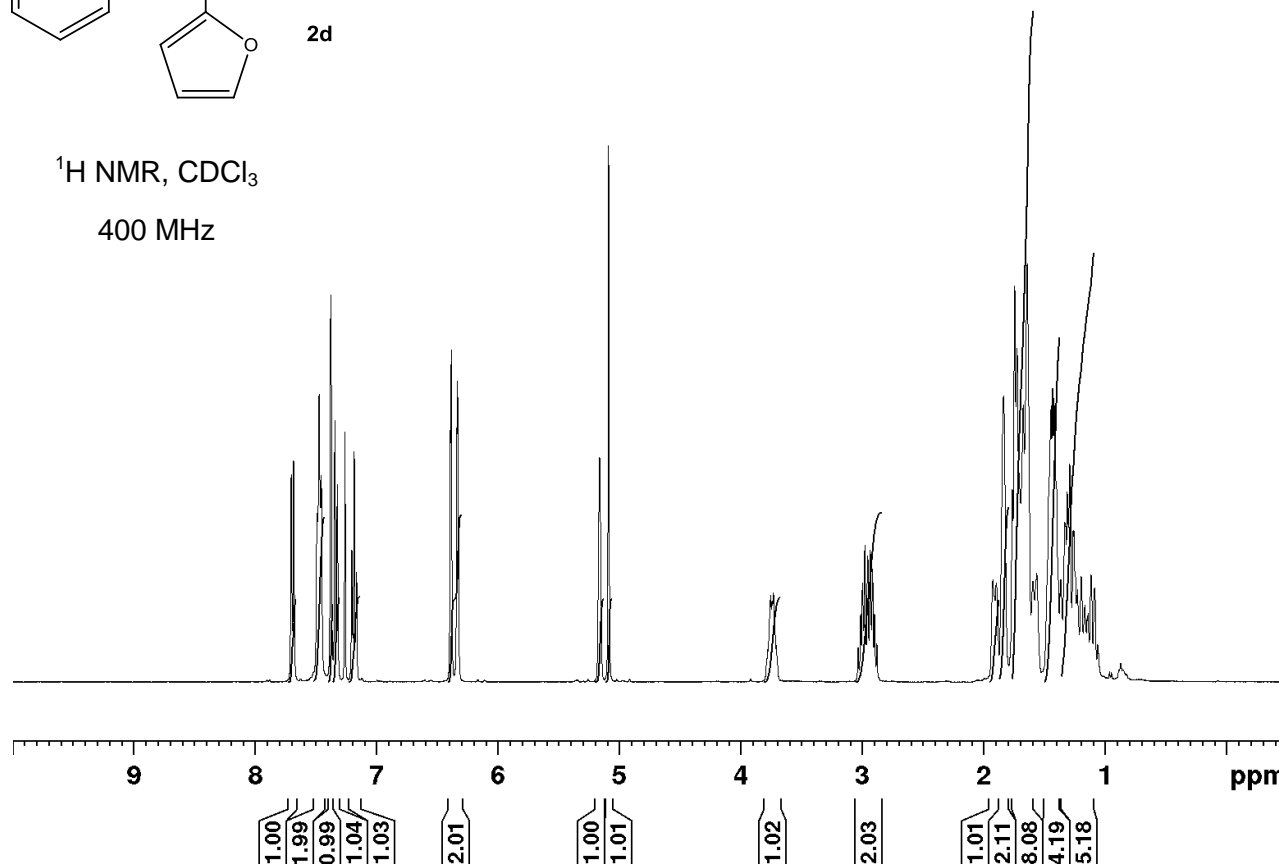
=====
CHANNEL f1
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 48.20000076 W

=====
CHANNEL f2
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 9.80000019 W
PLW12 0.27221999 W
PLW13 0.22050001 W

F2 - Processing parameters
SI 32768
SF 100.6177919 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹H NMR, CDCl₃
400 MHz

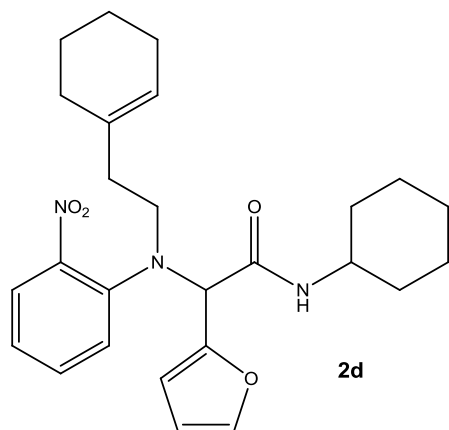


Current Data Parameters
NAME MM-2-64
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160309
Time 11.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 105.13
DW 62.400 usec
DE 6.50 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1

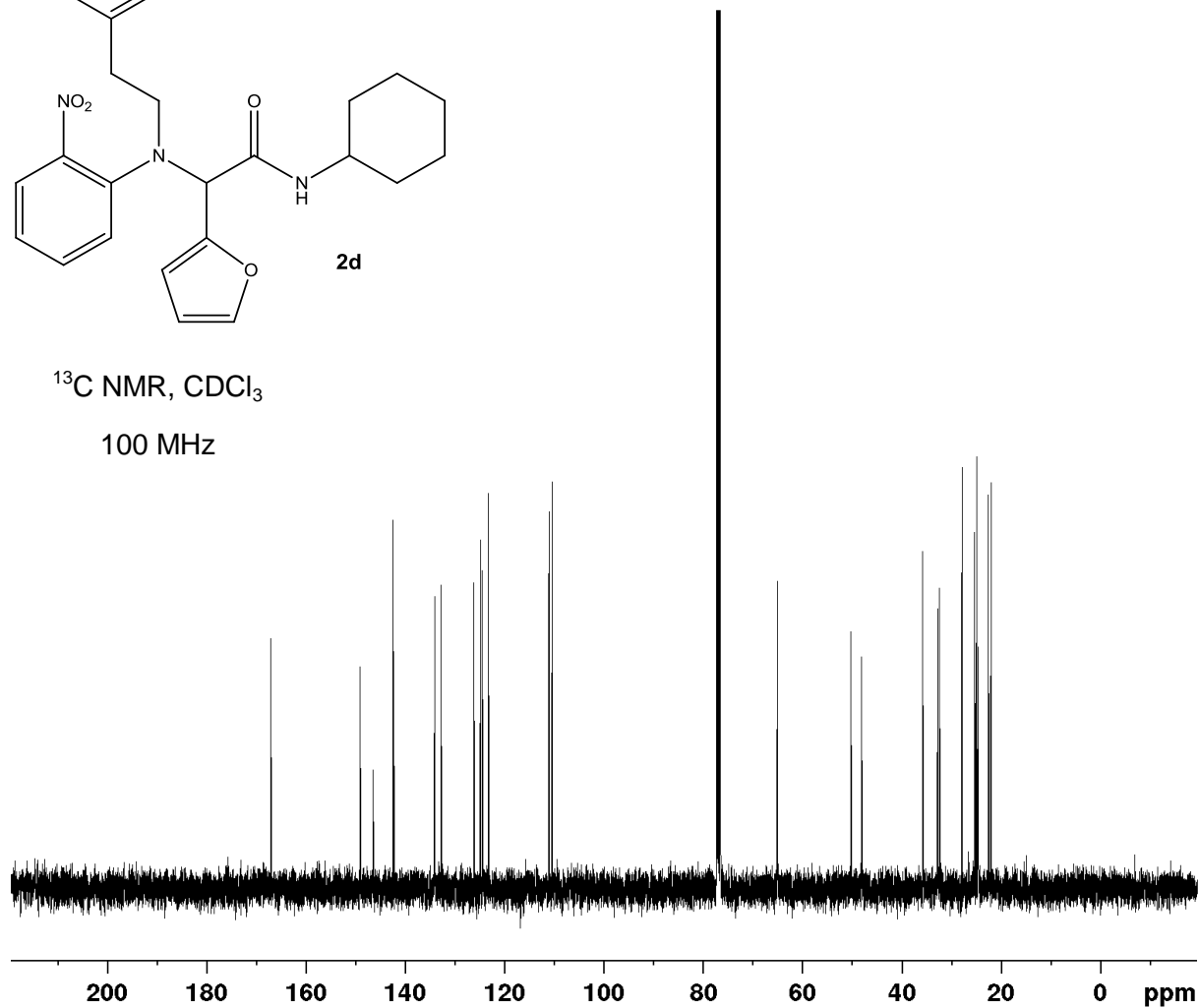
===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1500112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR, CDCl₃

100 MHz



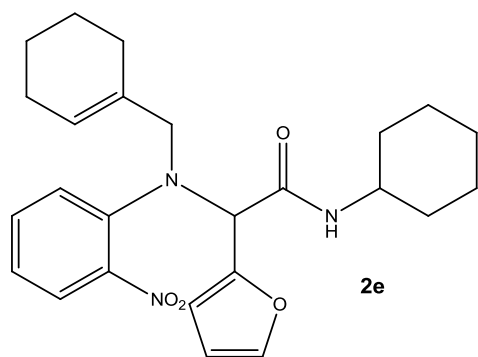
Current Data Parameters
NAME MM-2-64
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160309
Time 11.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 210.96
DW 20.800 usec
DE 10.00 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 48.20000076 W

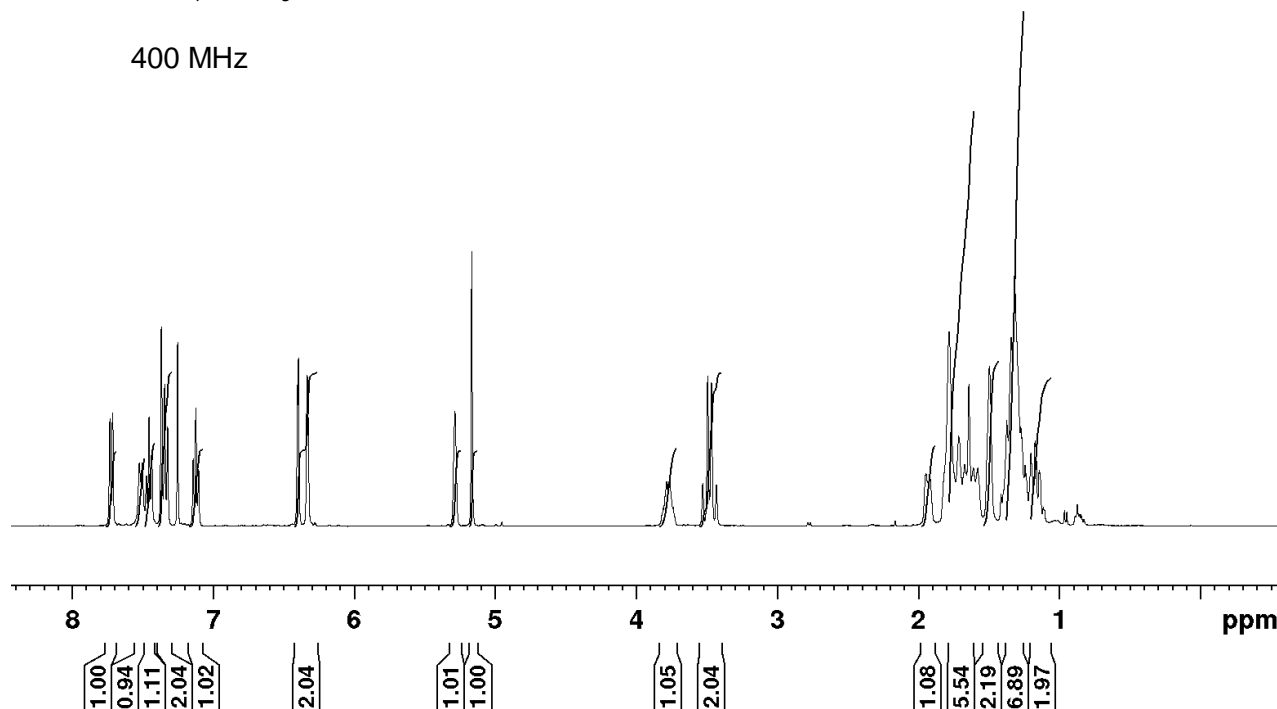
===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 9.80000019 W
PLW12 0.27221999 W
PLW13 0.22050001 W

F2 - Processing parameters
SI 32768
SF 100.6177941 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹H NMR, CDCl₃

400 MHz

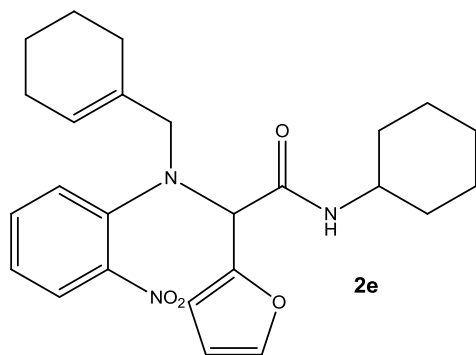


Current Data Parameters
 NAME MM-2-79
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160308
 Time 15.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 134.4
 DW 62.400 usec
 DE 6.50 usec
 TE 293.9 K
 D1 1.00000000 sec
 TDO 1

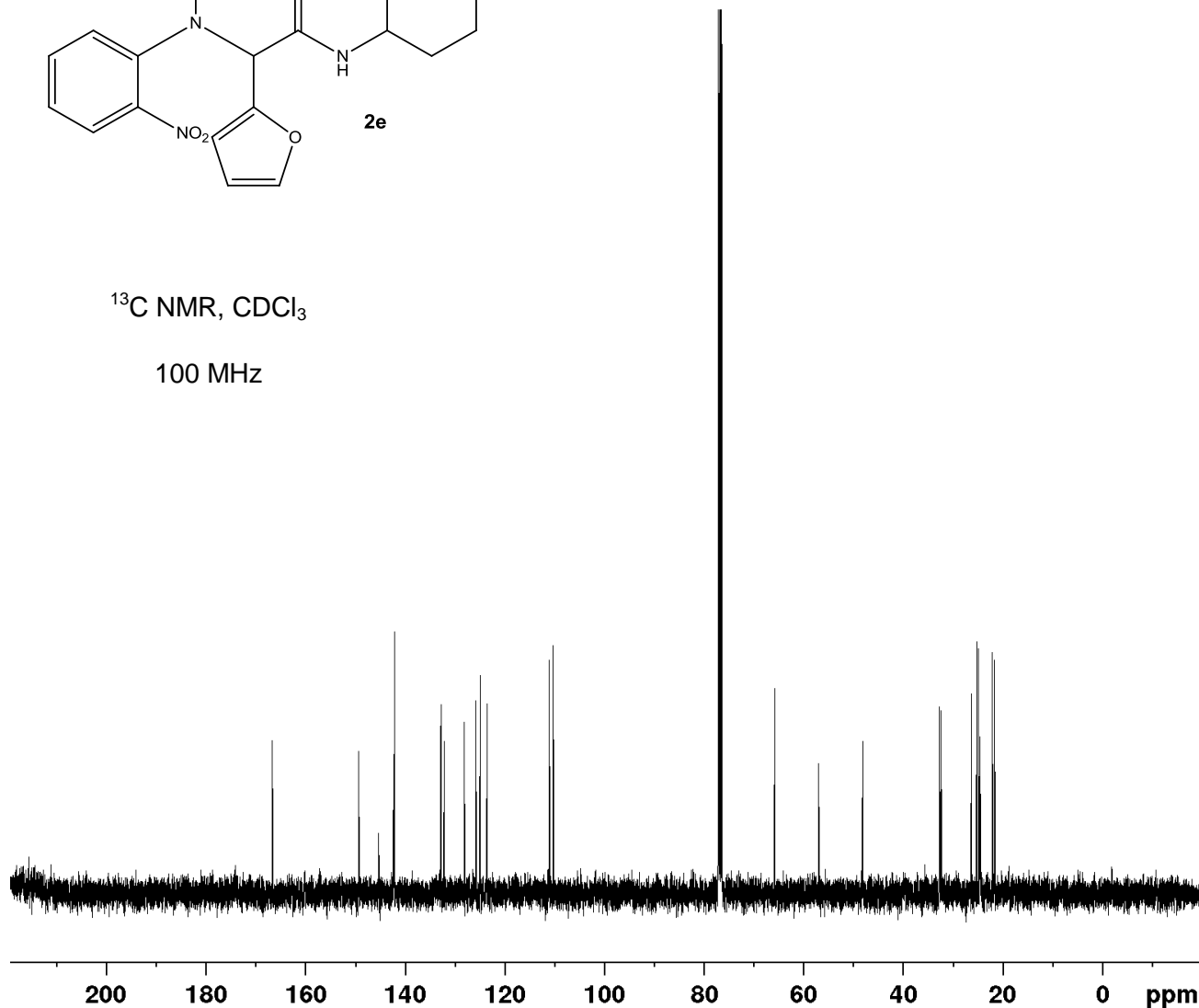
===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500119 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3

100 MHz



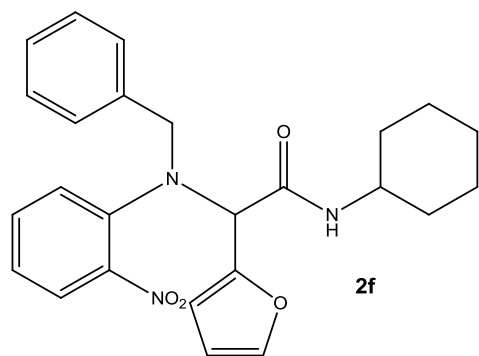
Current Data Parameters
 NAME MM-2-79
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160308
 Time 15.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 128
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 210.96
 DW 20.800 usec
 DE 10.00 usec
 TE 294.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 48.20000076 W

===== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.80000019 W
 PLW12 0.27221999 W
 PLW13 0.22050001 W

F2 - Processing parameters
 SI 32768
 SF 100.6178041 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



¹H NMR, CDCl₃

400 MHz

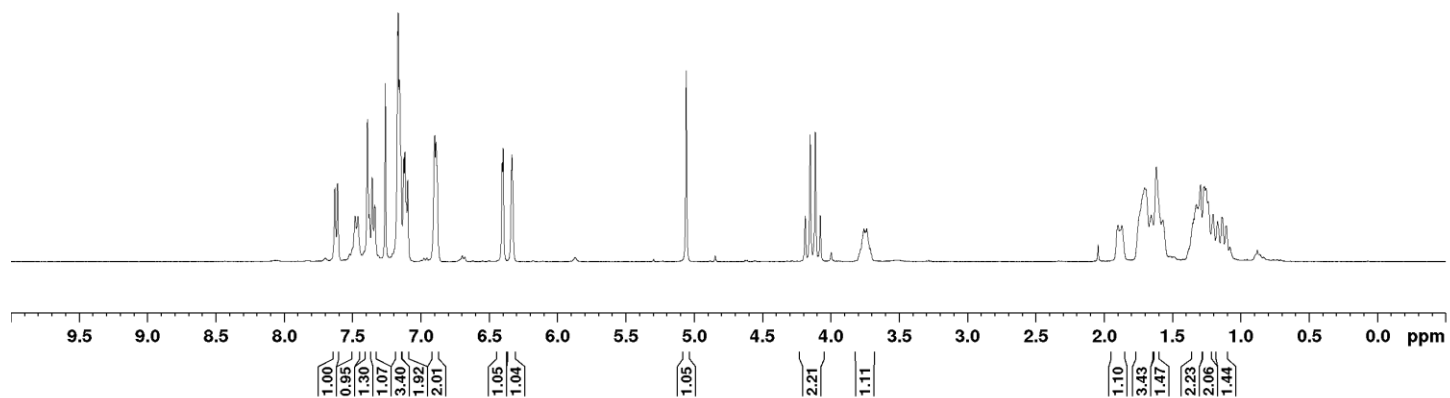


Current Data Parameters
 NAME a4 good
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160710
 Time 14.36
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 134.4
 DW 62.400 usec
 DE 6.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500106 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





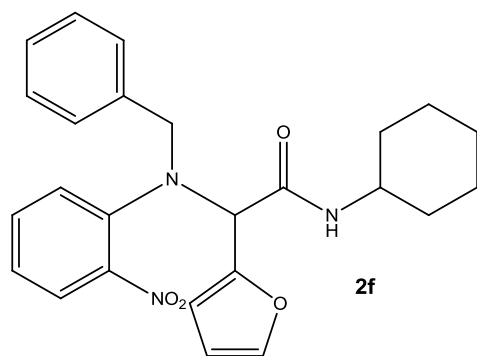
Current Data Parameters
NAME ad carbon
EXPNO 1
PROCNO 1

F2 Acquisition Parameters
Date_ 20160710
Time 23.39
INSTRUM spect
PROBHD 5 mm PABBO 5B7
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 210.96
BW 20.800 usec
DE 10.00 usec
TE 293.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 48.20000076 W

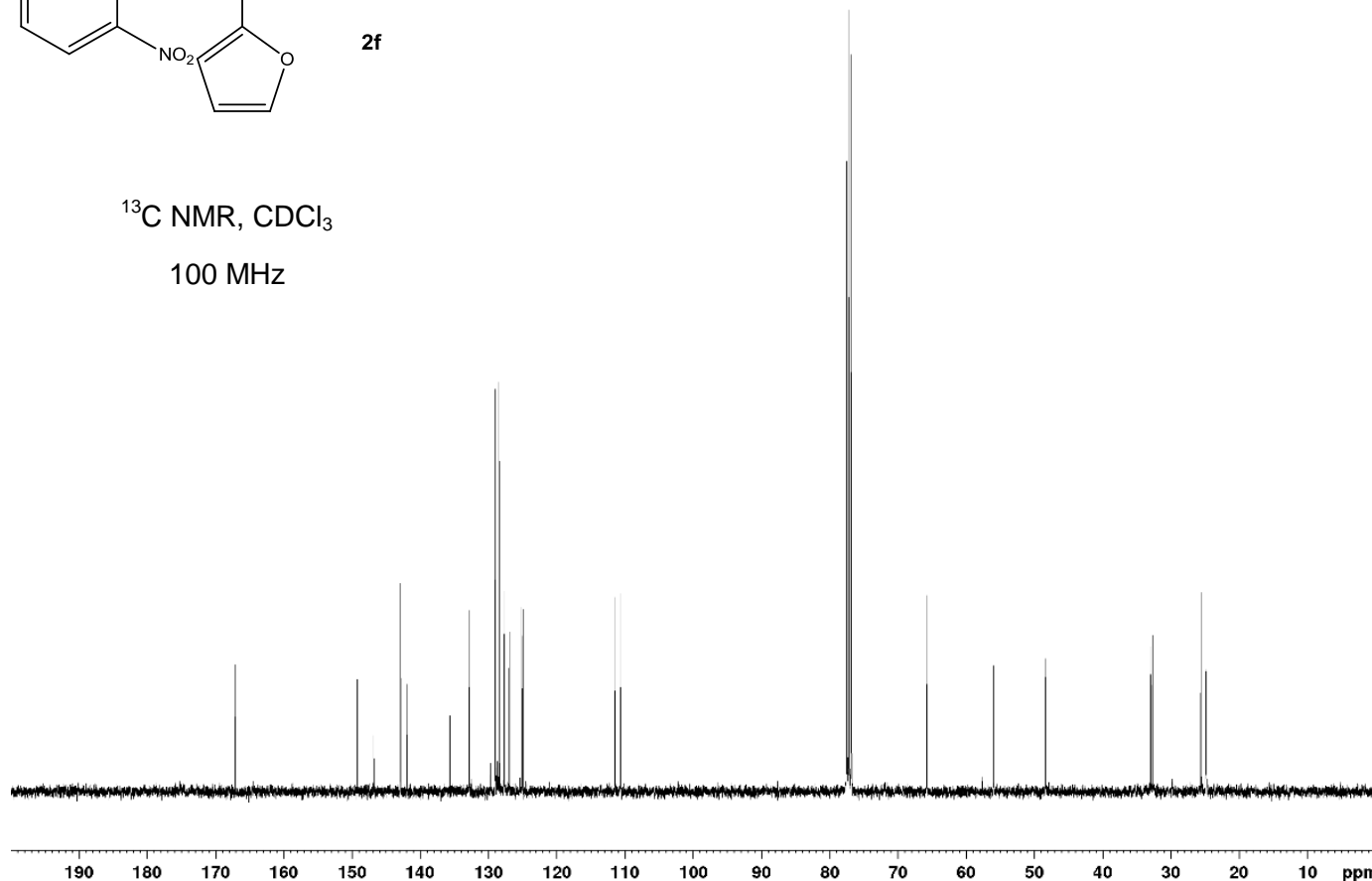
===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
PULPROG2 waltz16
PCPD2 80.00 usec
PLW2 9.80000019 W
PLW12 0.27221999 W
PLW13 0.22030001 W

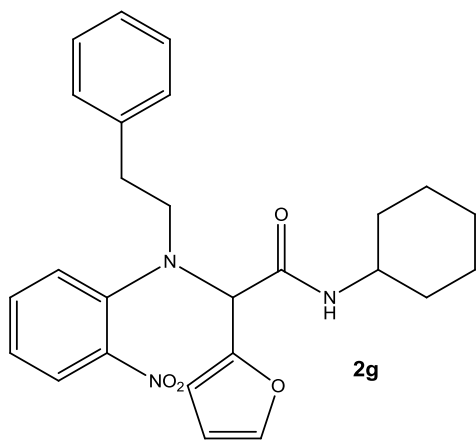
F2 Processing parameters
SI 32768
SF 100.6177879 MHz
WDW RM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



^{13}C NMR, CDCl_3

100 MHz





$^1\text{H NMR}$, CDCl_3

400 MHz

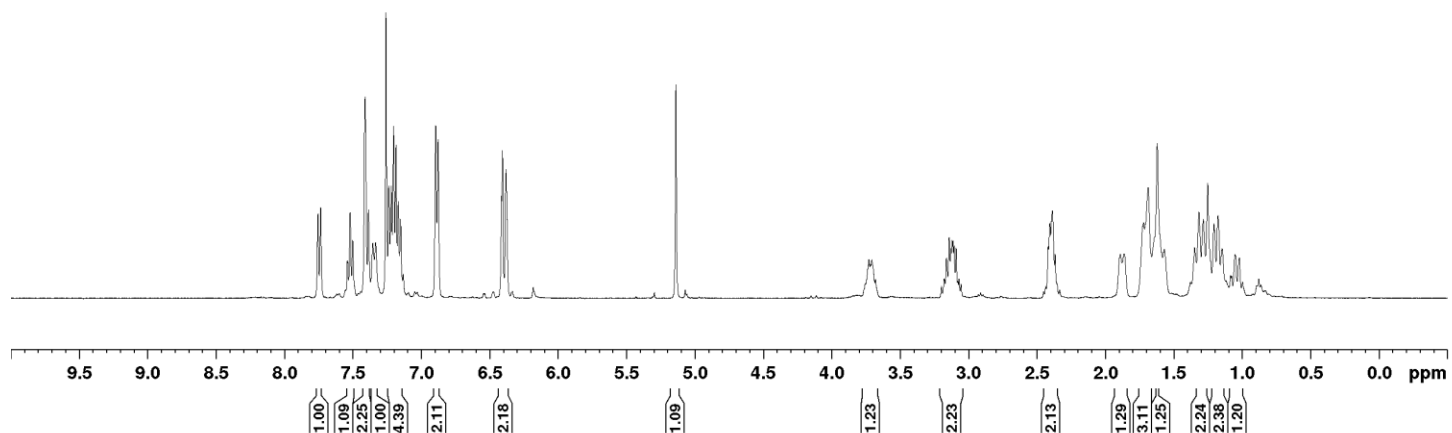


Current Data Parameters
 NAME al good
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160710
 Time 14.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 134.4
 DW 62.400 usec
 DE 6.50 usec
 TE 294.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500109 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





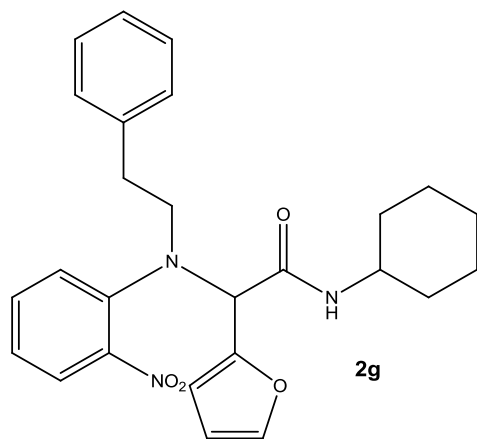
Current Data Parameters
NAME al-Carbon
EXPNO 1
PROCNO 1

F2 Acquisition Parameters
Date_ 20160711
Time 16.03
INSTRUM spect
PROBHD 5 mm PARR0 61/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 210.96
BW 20.800 usec
BE 10.00 usec
TE 293.3 K
E1 2.0000000 sec
E11 0.0300000 sec
TD0 1

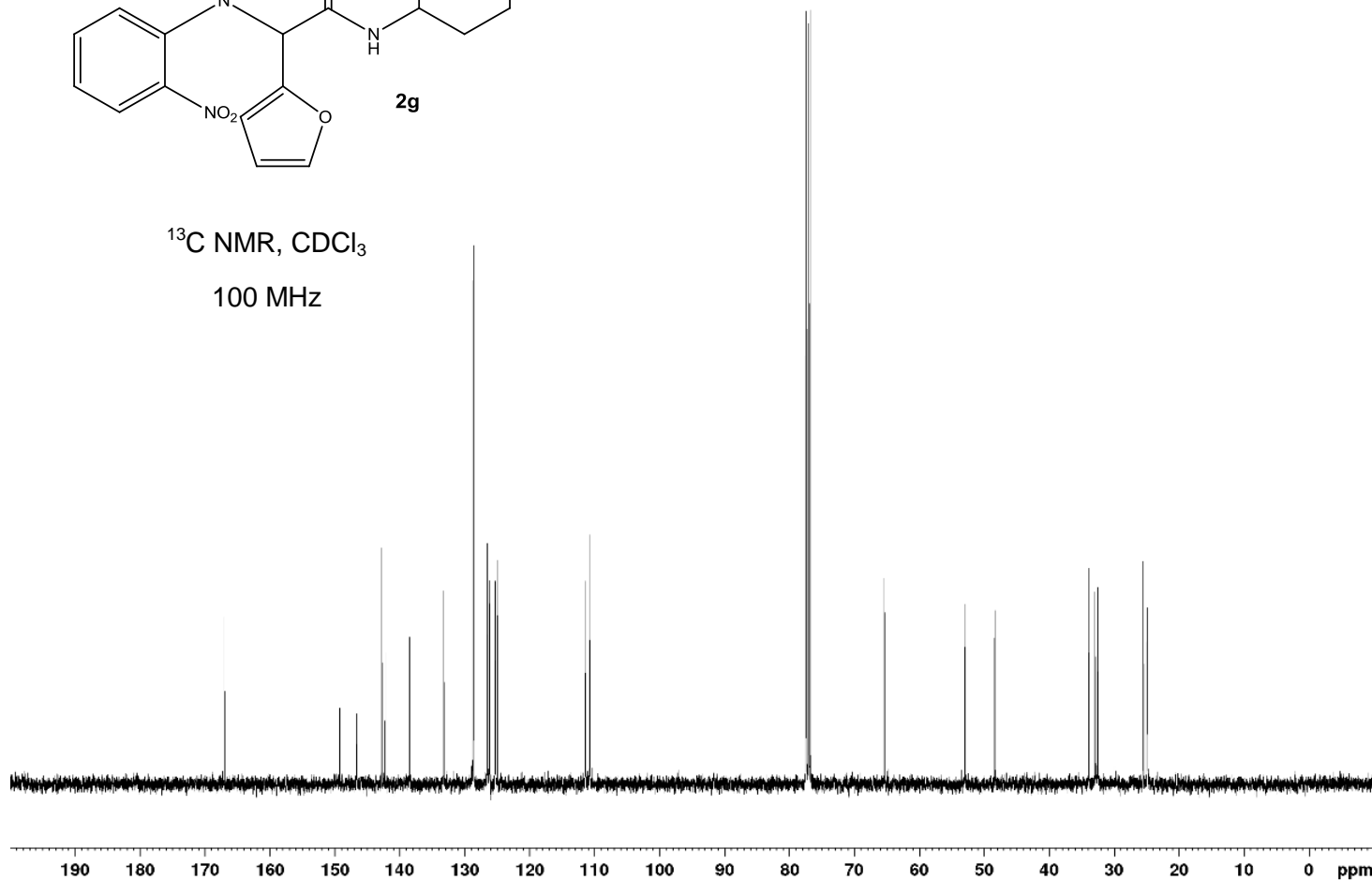
===== CHANNEL #1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 48.20000076 W

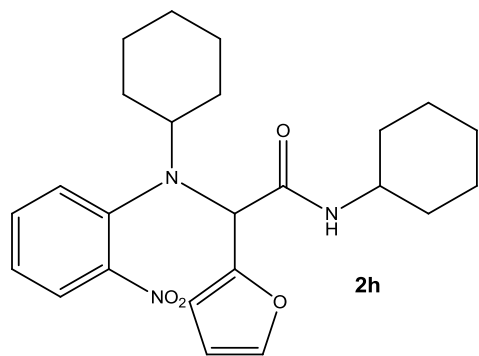
===== CHANNEL #2 =====
SFO2 400.1516006 MHz
NUC2 1H
PCPDPRG12 waltz16
PCPD2 80.00 usec
PLW2 9.80000019 W
PLW12 0.27221999 W
PLW13 0.22030001 W

F2 Processing parameters
SI 32768
SF 100.6177906 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



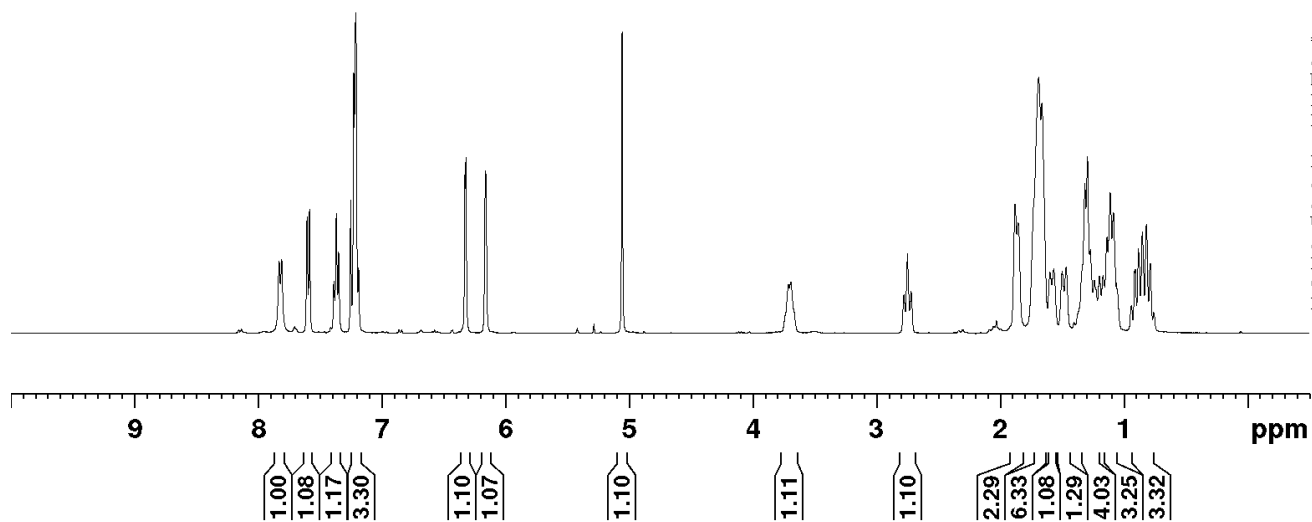
¹³C NMR, CDCl₃
100 MHz





¹H NMR, CDCl₃

400 MHz



Current Data Parameters
 NAME A2-Better
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160711
 Time 18.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 105.13
 DW 62.400 usec
 DE 6.50 usec
 TE 293.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500136 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



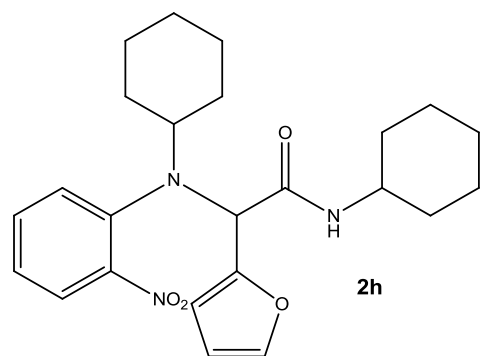
Current Data Parameters
NAME a2 carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160710
Time 21.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 210.96
DW 20.800 usec
DE 10.00 usec
TE 295.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

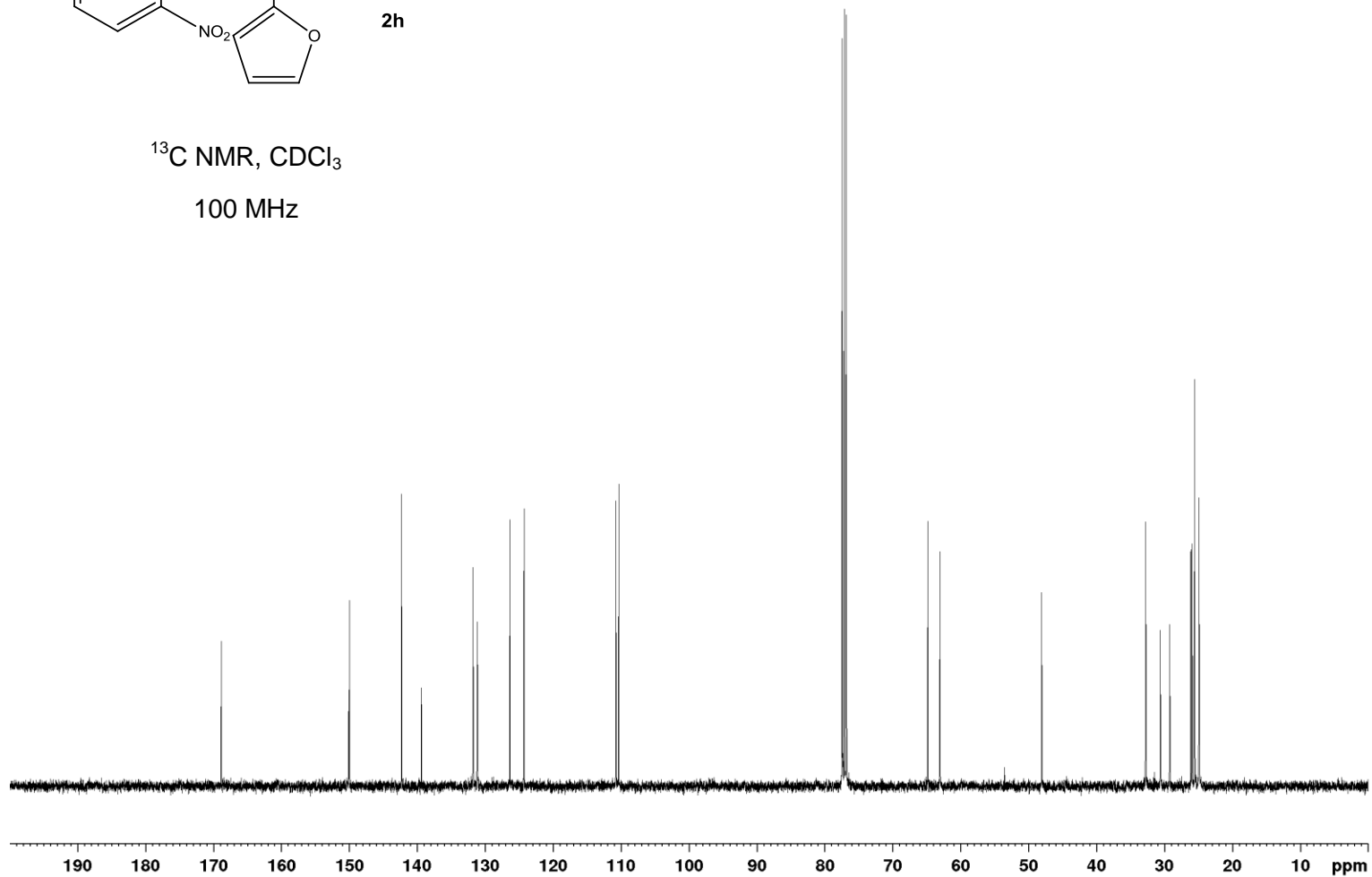
===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 48.20000076 W

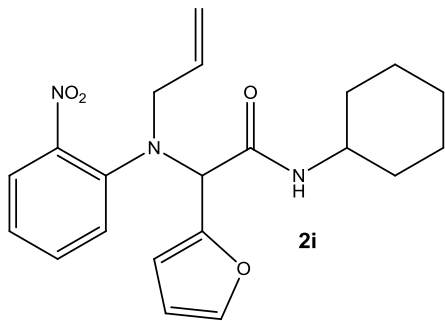
===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 9.80000019 W
PLW12 0.27221999 W
PLW13 0.22050001 W

F2 - Processing parameters
SI 32768
SF 100.6177898 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

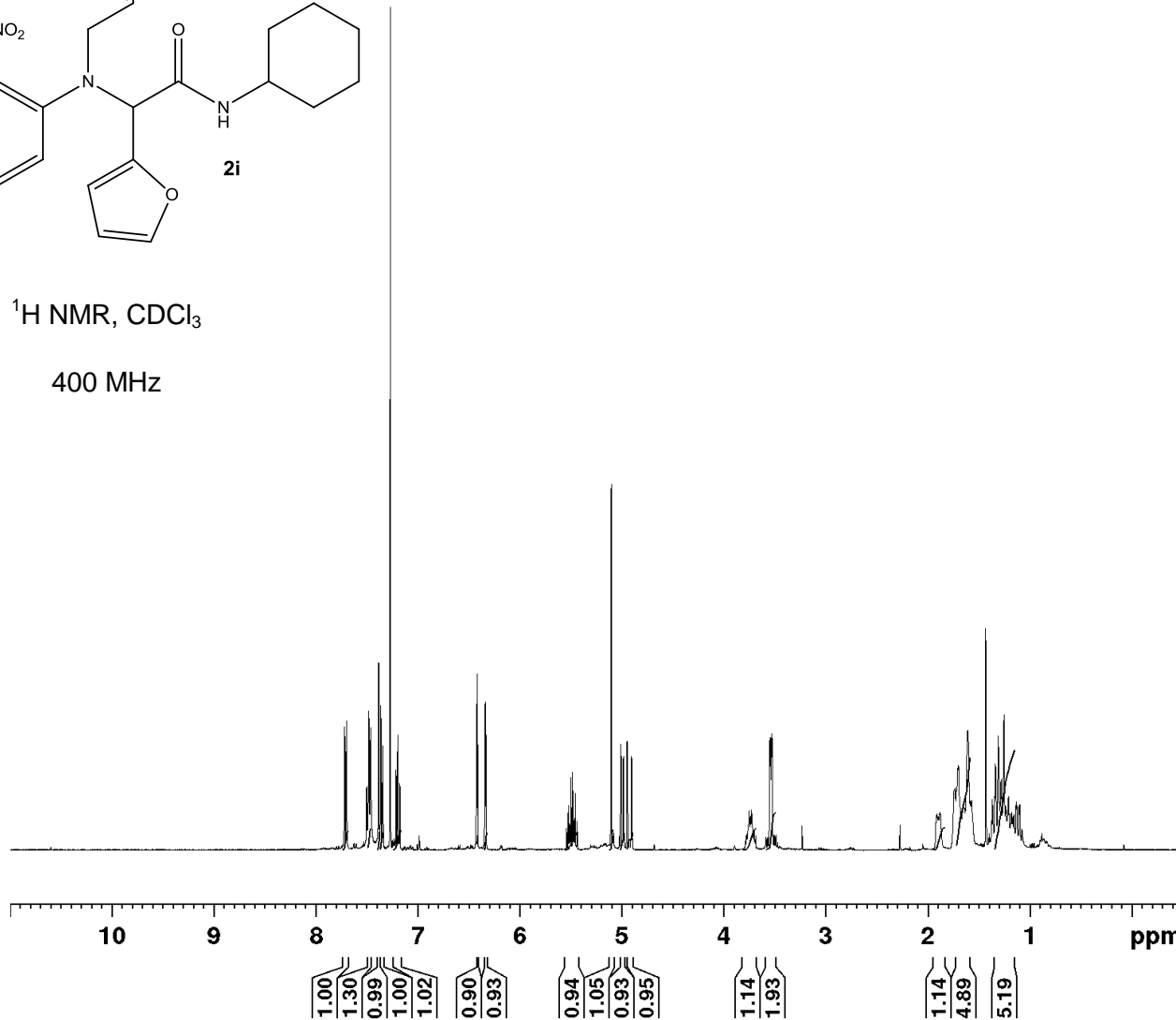


¹³C NMR, CDCl₃
100 MHz





¹H NMR, CDCl₃
400 MHz

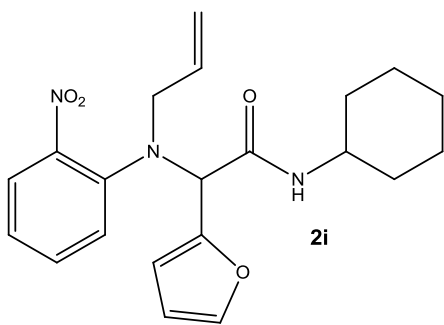


Current Data Parameters
 NAME MM-2-6Hr-F10-14
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160129
 Time 18.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 166.66
 DW 62.400 usec
 DE 6.50 usec
 TE 293.4 K
 D1 1.00000000 sec
 TD0 1

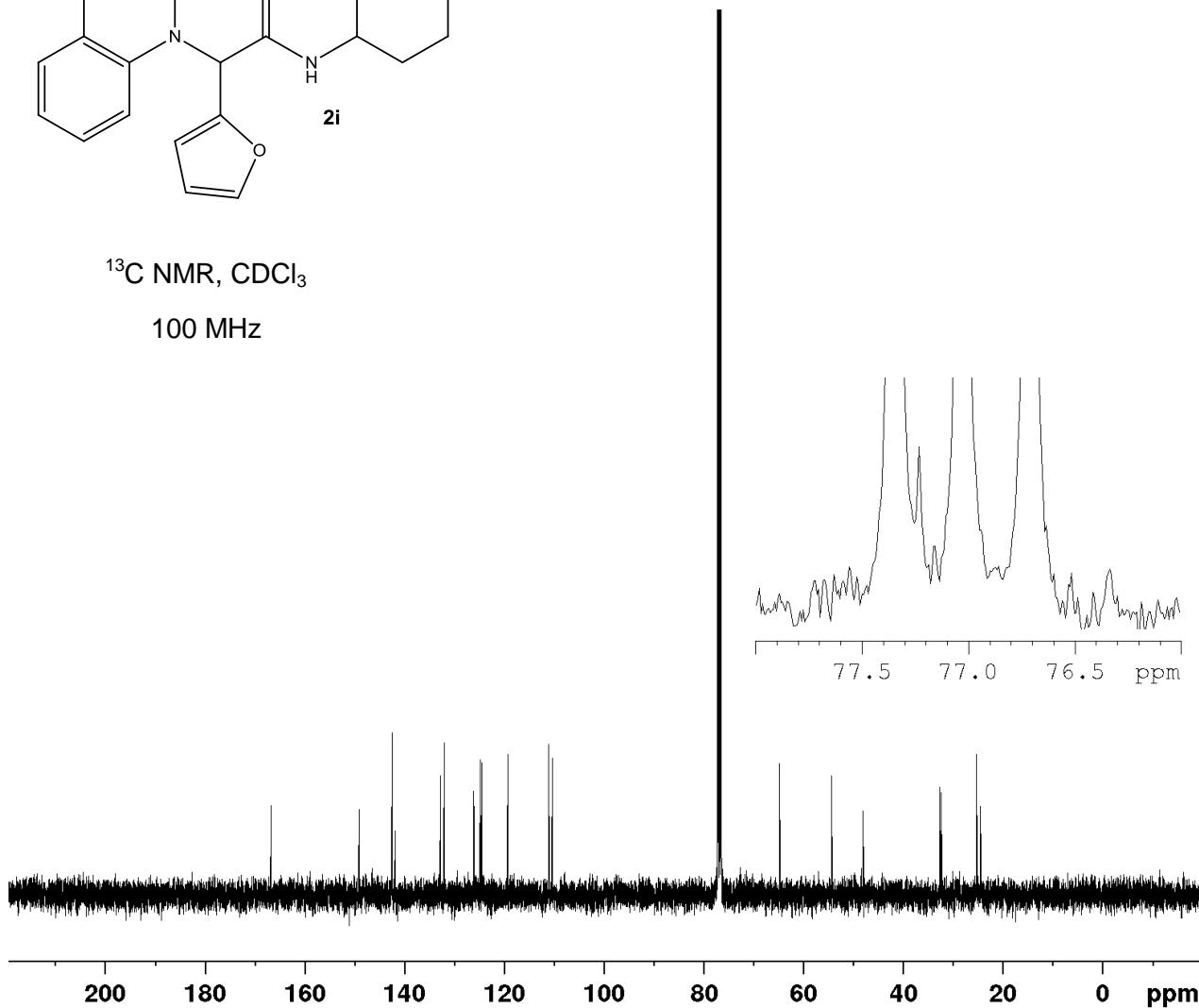
===== CHANNEL f1 =====
 SF01 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500082 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3

100 MHz



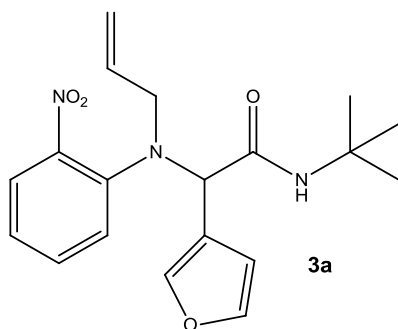
Current Data Parameters
 NAME MM-2-6Hr-F10-14
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160129
 Time 19.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 210.96
 DW 20.800 usec
 DE 10.00 usec
 TE 294.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

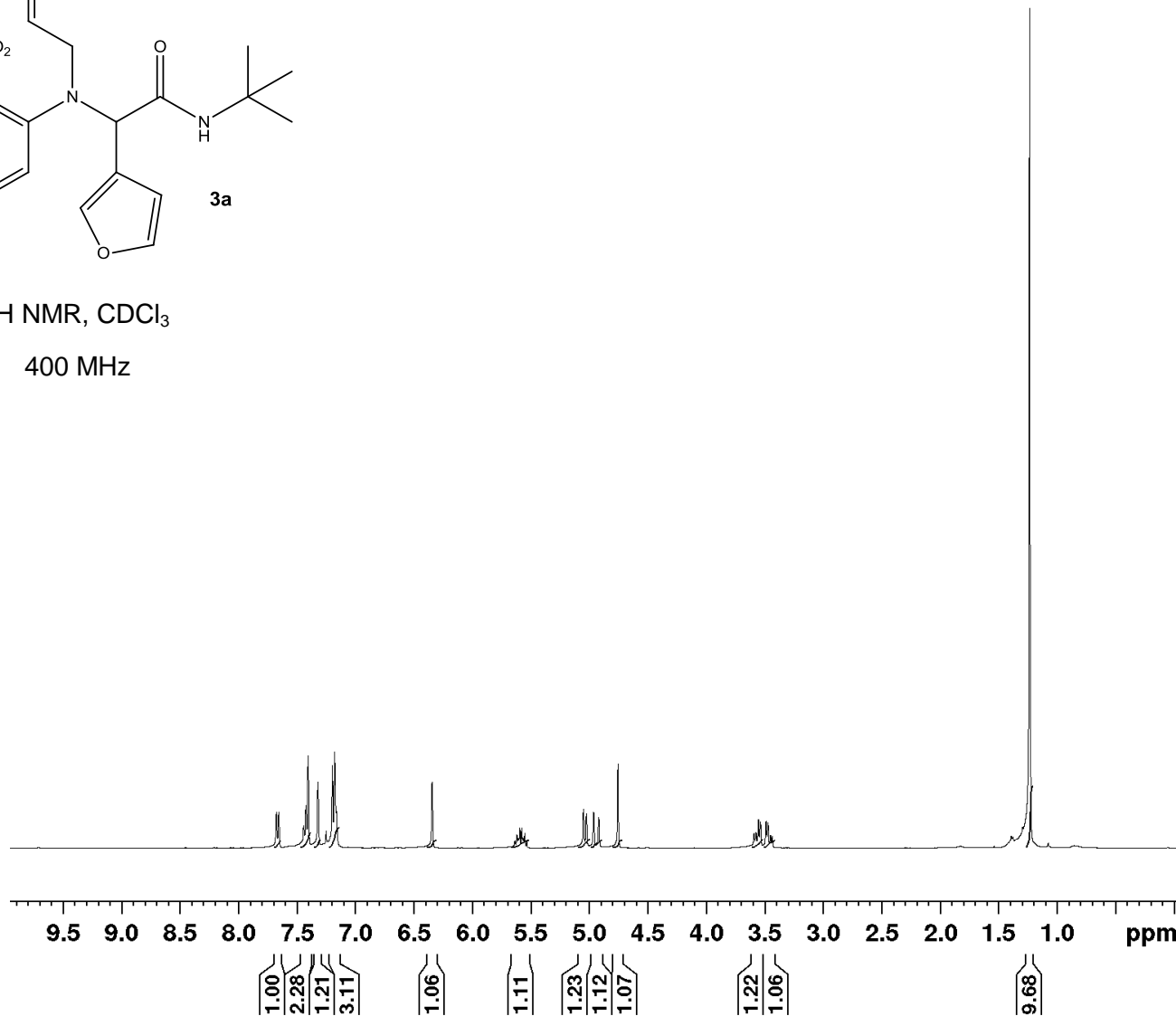
===== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 48.20000076 W

===== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.80000019 W
 PLW12 0.27221999 W
 PLW13 0.22050001 W

F2 - Processing parameters
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



^1H NMR, CDCl_3
400 MHz

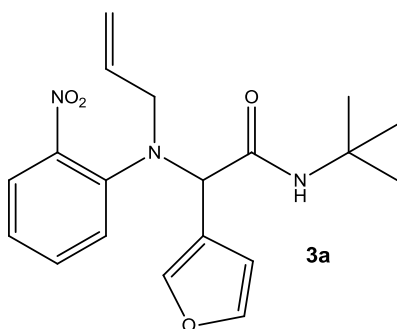


Current Data Parameters
NAME KM-11-9-14R-F9-16
EXPNO 10
PROCNO 1

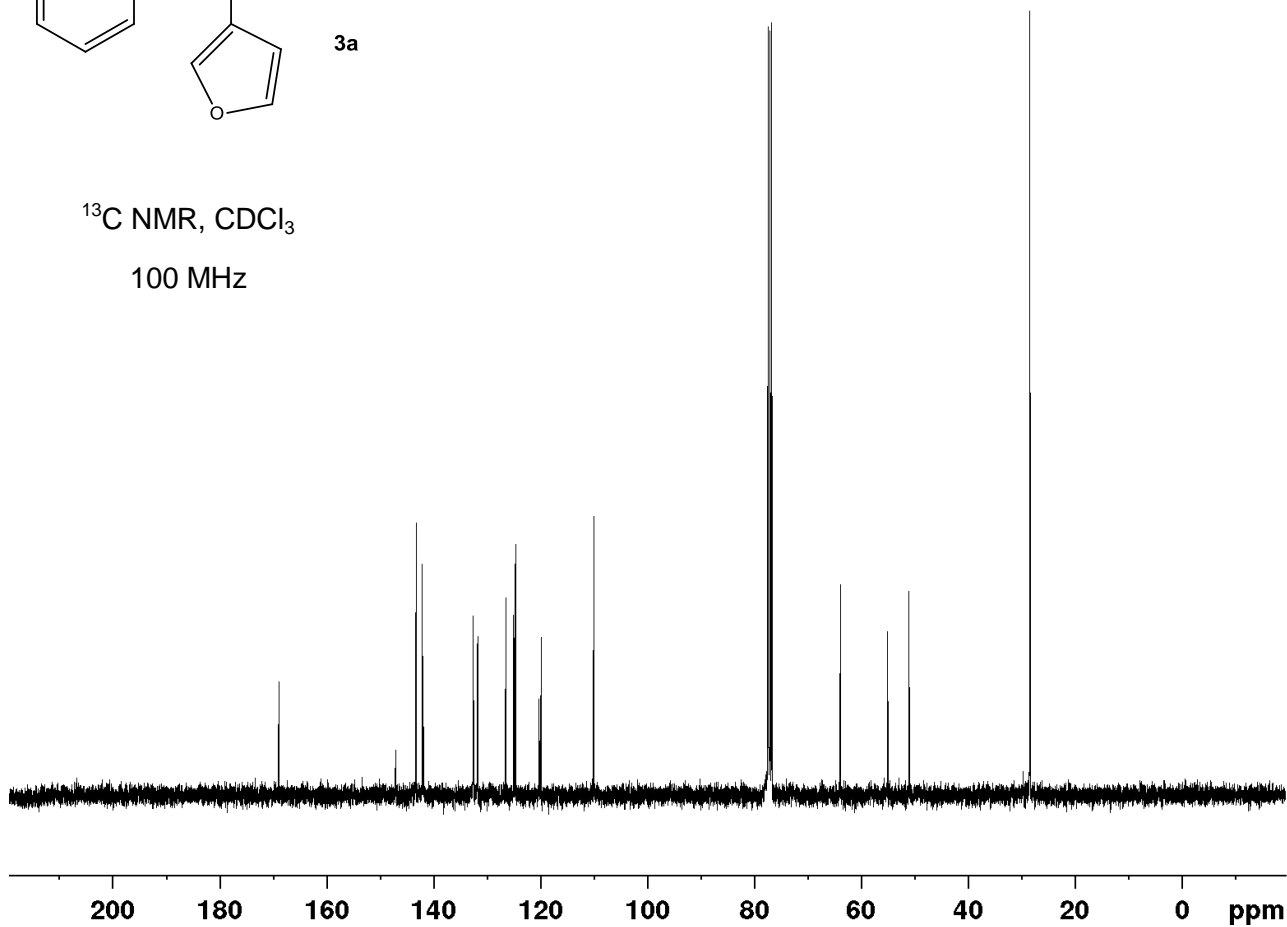
F2 - Acquisition Parameters
Date_ 20150105
Time 12.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 57.34
DW 62.400 usec
DE 6.50 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 ^1H
P1 15.00 usec
PLW1 9.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1500149 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



^{13}C NMR, CDCl_3
100 MHz



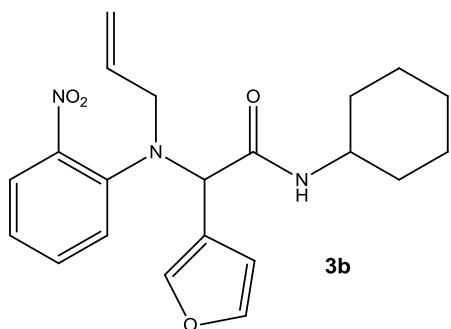
Current Data Parameters
NAME KM-11-9-14R-F9-16-C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150106
Time 14.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl_3
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 210.96
DW 20.800 usec
DE 10.00 usec
TE 294.3 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6278588 MHz
NUC1 13C
P1 10.00 usec
PLW1 48.20000076 W

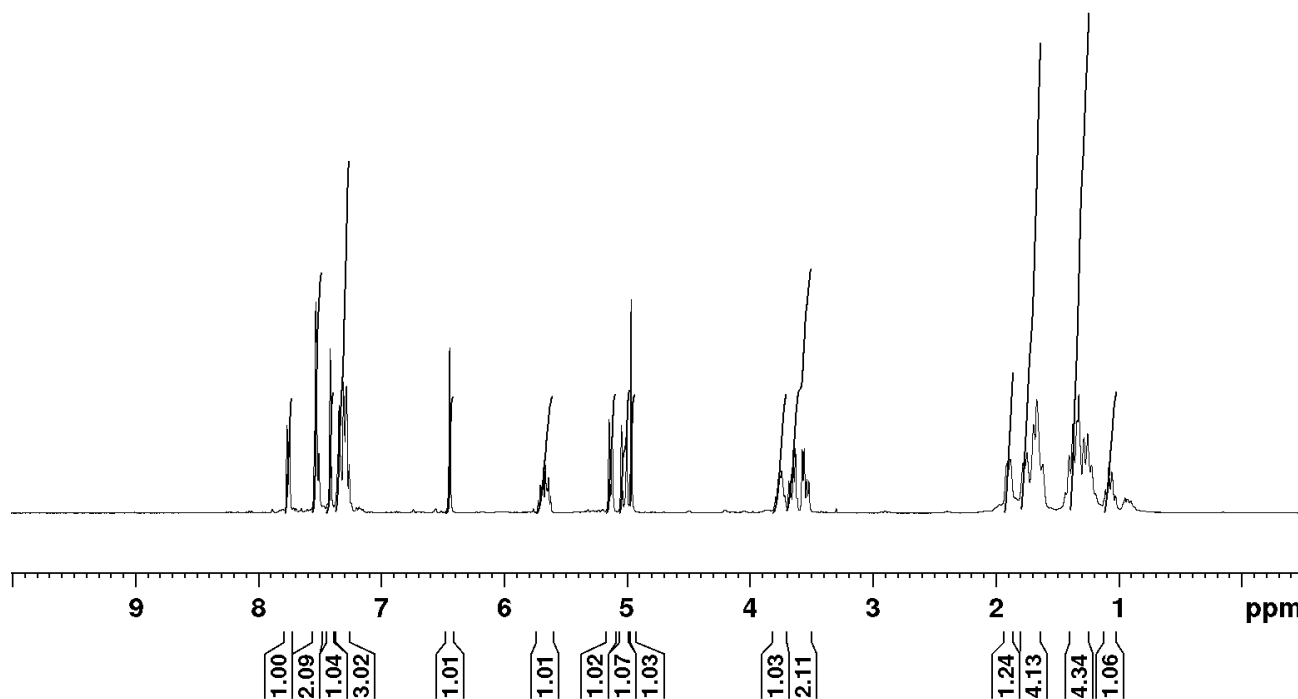
===== CHANNEL f2 =====
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 9.80000019 W
PLW12 0.27221999 W
PLW13 0.22050001 W

F2 - Processing parameters
SI 32768
SF 100.6177971 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹H NMR, CDCl₃

400 MHz

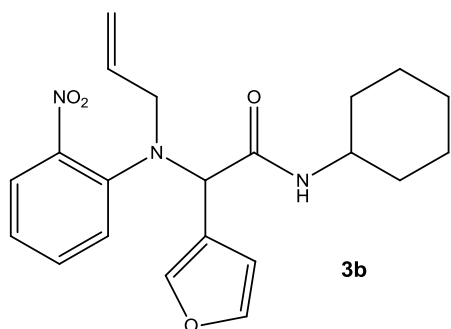


Current Data Parameters
 NAME MM-2-71
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160307
 Time 20.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 51.73
 DW 62.400 usec
 DE 6.50 usec
 TE 296.3 K
 D1 1.00000000 sec
 TD0 1

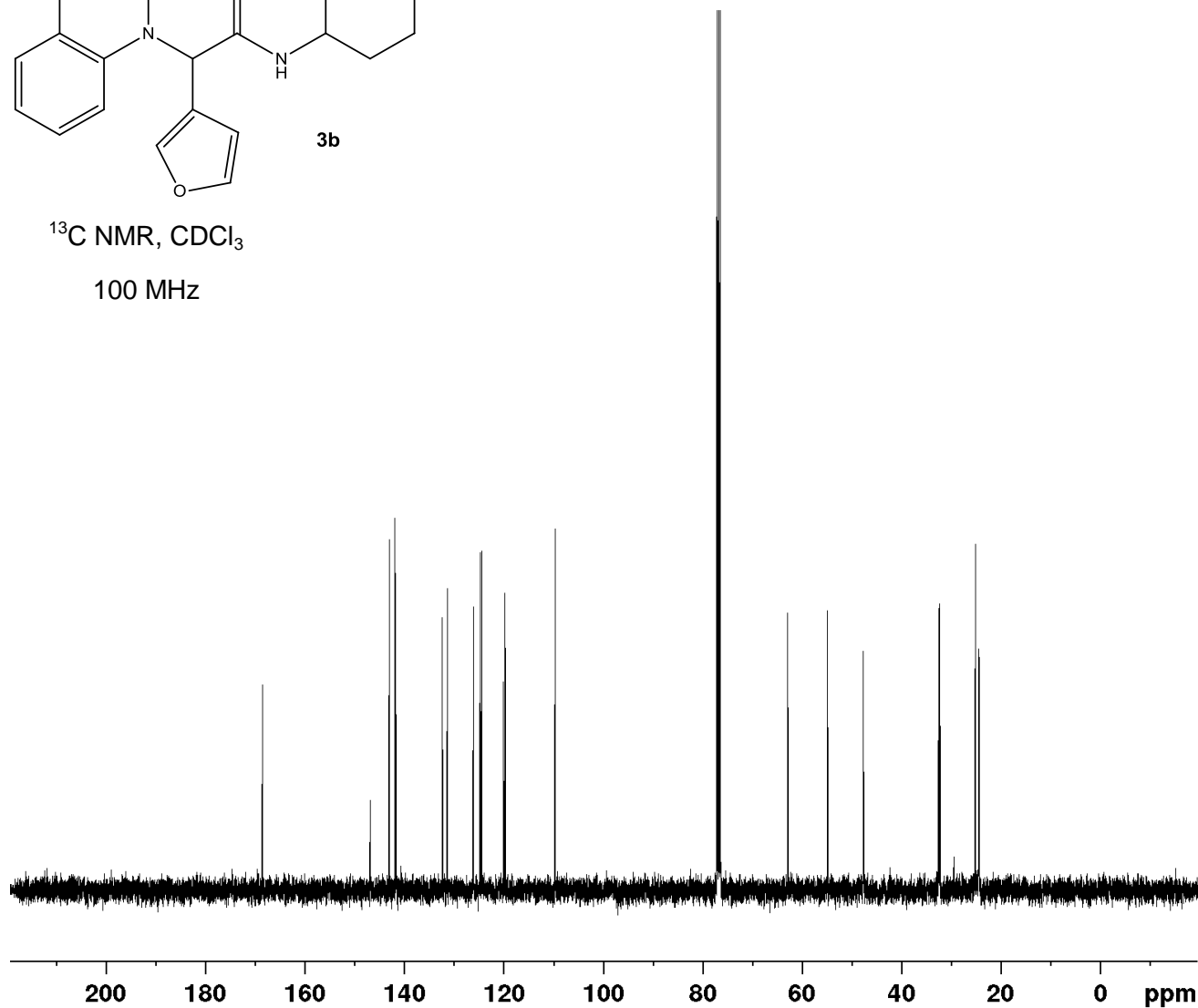
===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1499781 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3

100 MHz



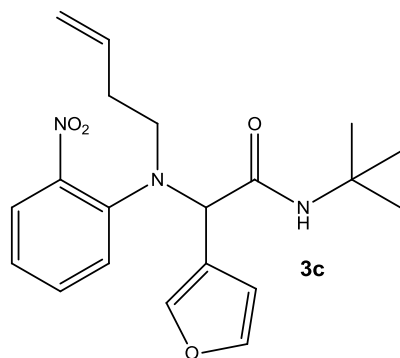
Current Data Parameters
 NAME MM-2-71
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160307
 Time 20.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 128
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 210.96
 DW 20.800 usec
 DE 10.00 usec
 TE 297.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

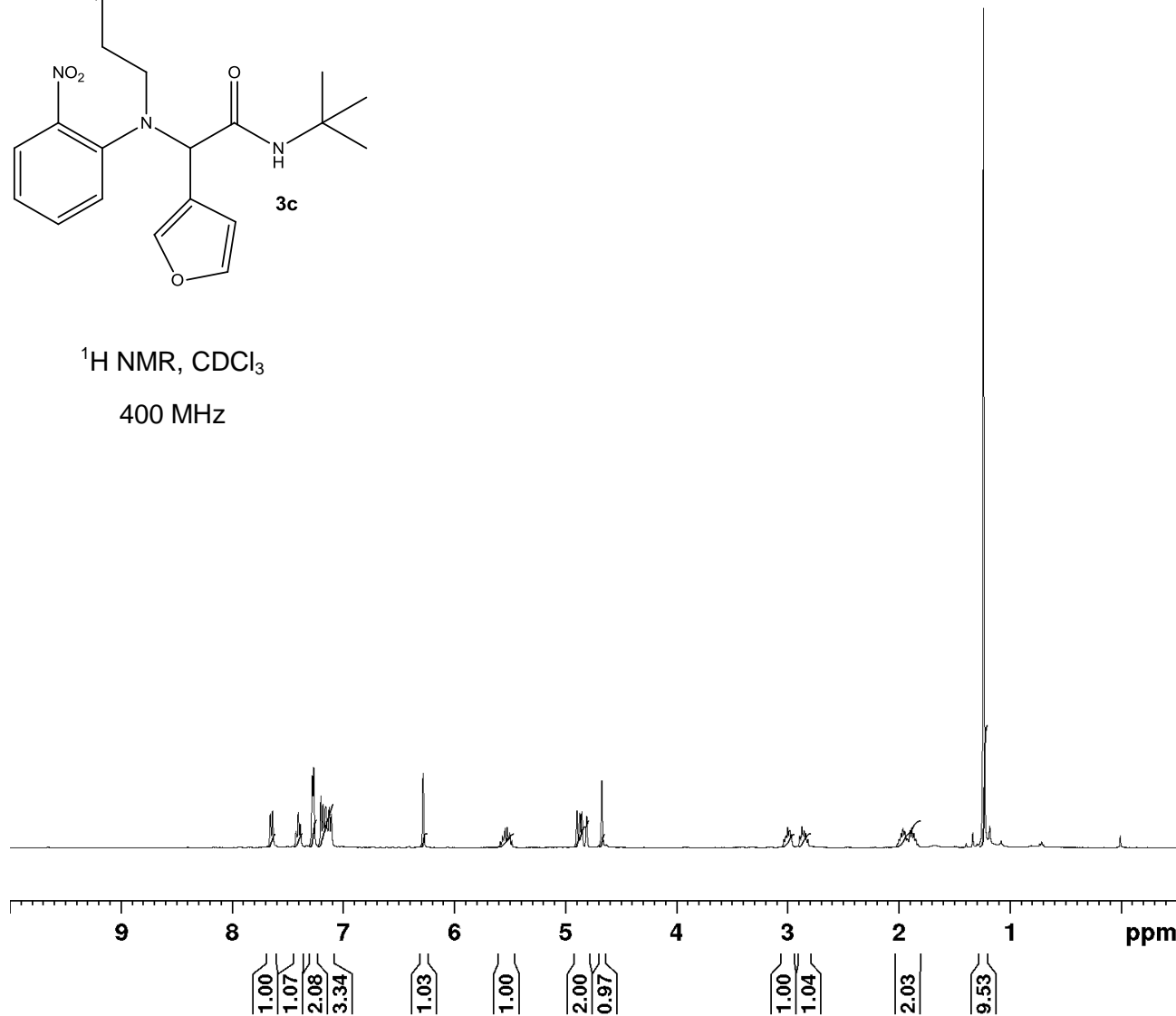
==== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 ^{13}C
 P1 10.00 usec
 PLW1 48.20000076 W

==== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 ^1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.80000019 W
 PLW12 0.27221999 W
 PLW13 0.22050001 W

F2 - Processing parameters
 SI 32768
 SF 100.6178041 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



^1H NMR, CDCl_3
400 MHz

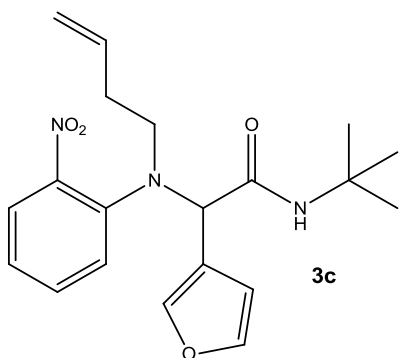


Current Data Parameters
NAME KM-37R-F12-35-3
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150513
Time 13.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 95.15
DW 62.400 usec
DE 6.50 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1

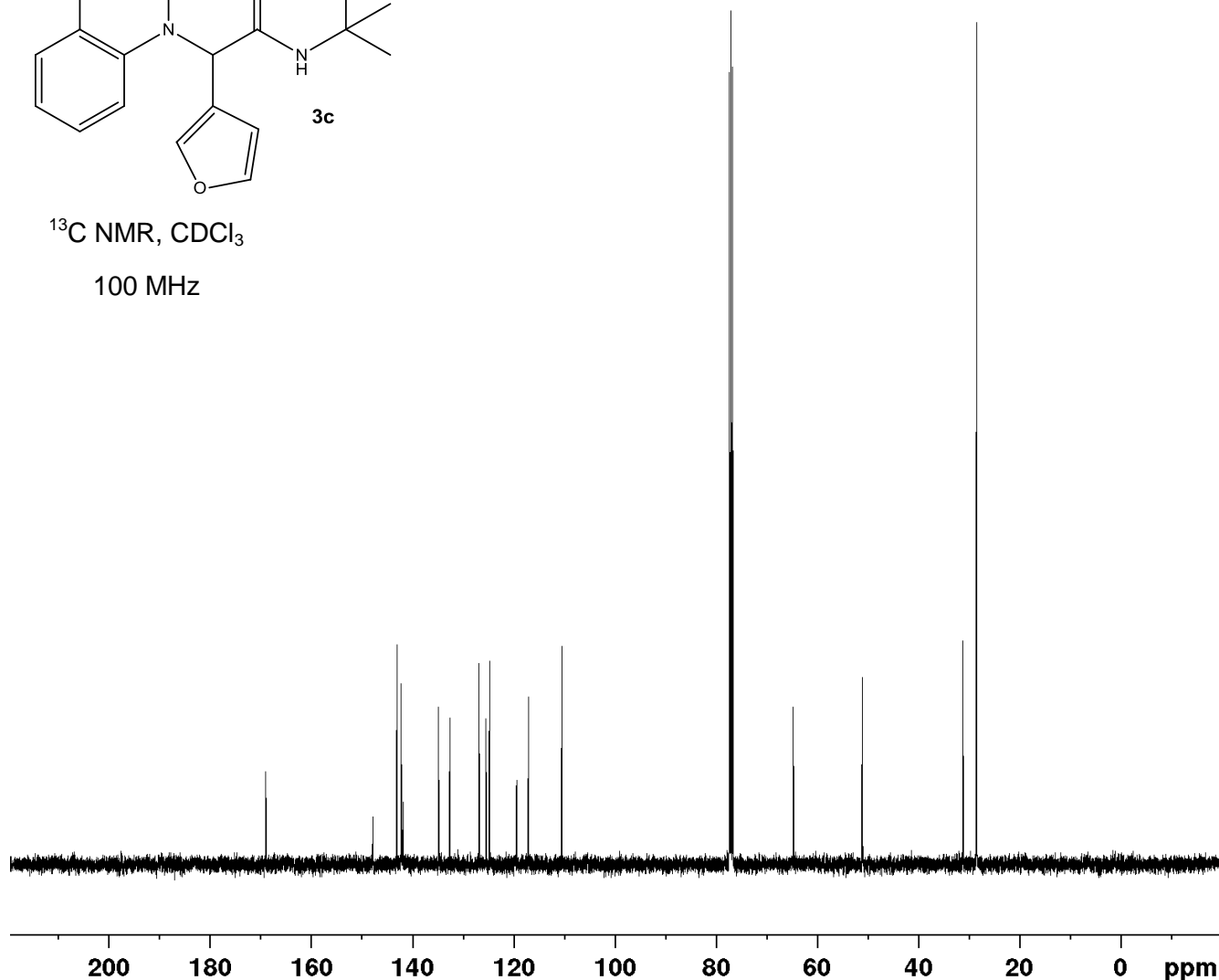
===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 ^1H
P1 15.00 usec
PLW1 9.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1500353 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



^{13}C NMR, CDCl_3

100 MHz



Current Data Parameters
 NAME KM-37R-F12-35-3
 EXPNO 20
 PROCNO 1

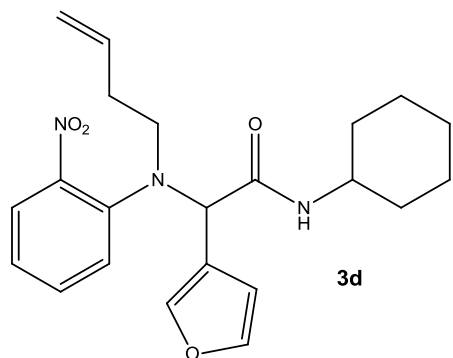
F2 - Acquisition Parameters

Date_ 20150513
 Time 13.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 128
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 210.96
 DW 20.800 usec
 DE 10.00 usec
 TE 293.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 48.20000076 W

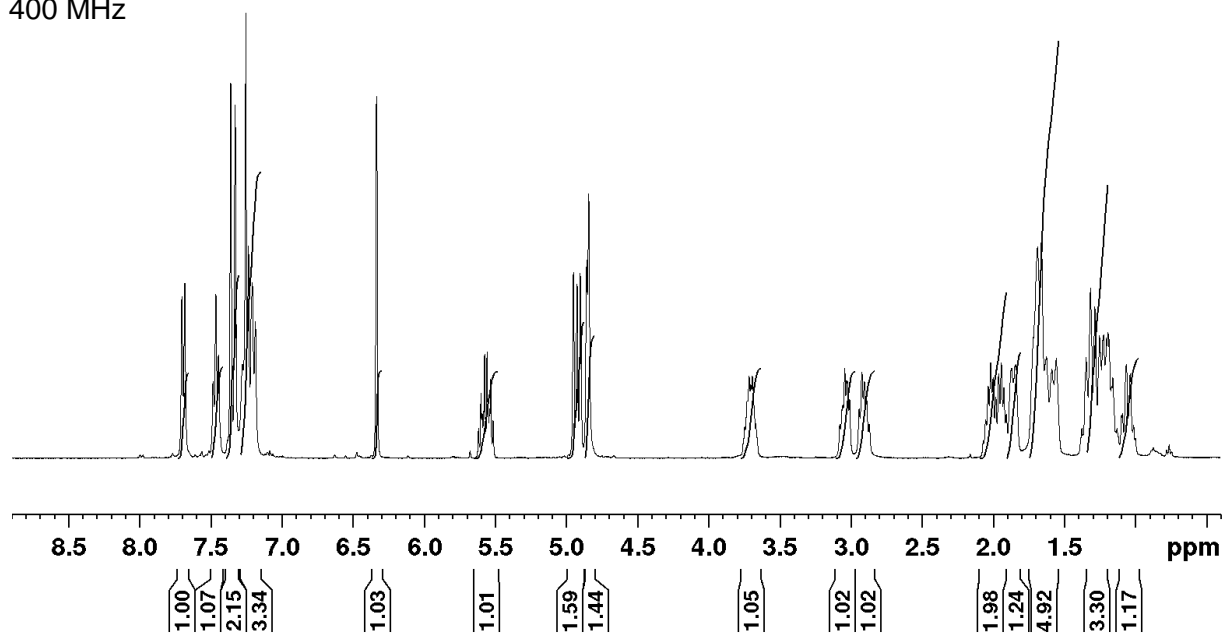
===== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.80000019 W
 PLW12 0.27221999 W
 PLW13 0.22050001 W

F2 - Processing parameters
 SI 32768
 SF 100.6177903 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



¹H NMR, CDCl₃

400 MHz

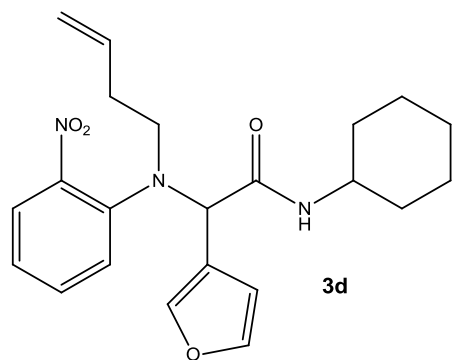


Current Data Parameters
 NAME MM-2-73
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160308
 Time 15.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 120.42
 DW 62.400 usec
 DE 6.50 usec
 TE 293.9 K
 D1 1.00000000 sec
 TD0 1

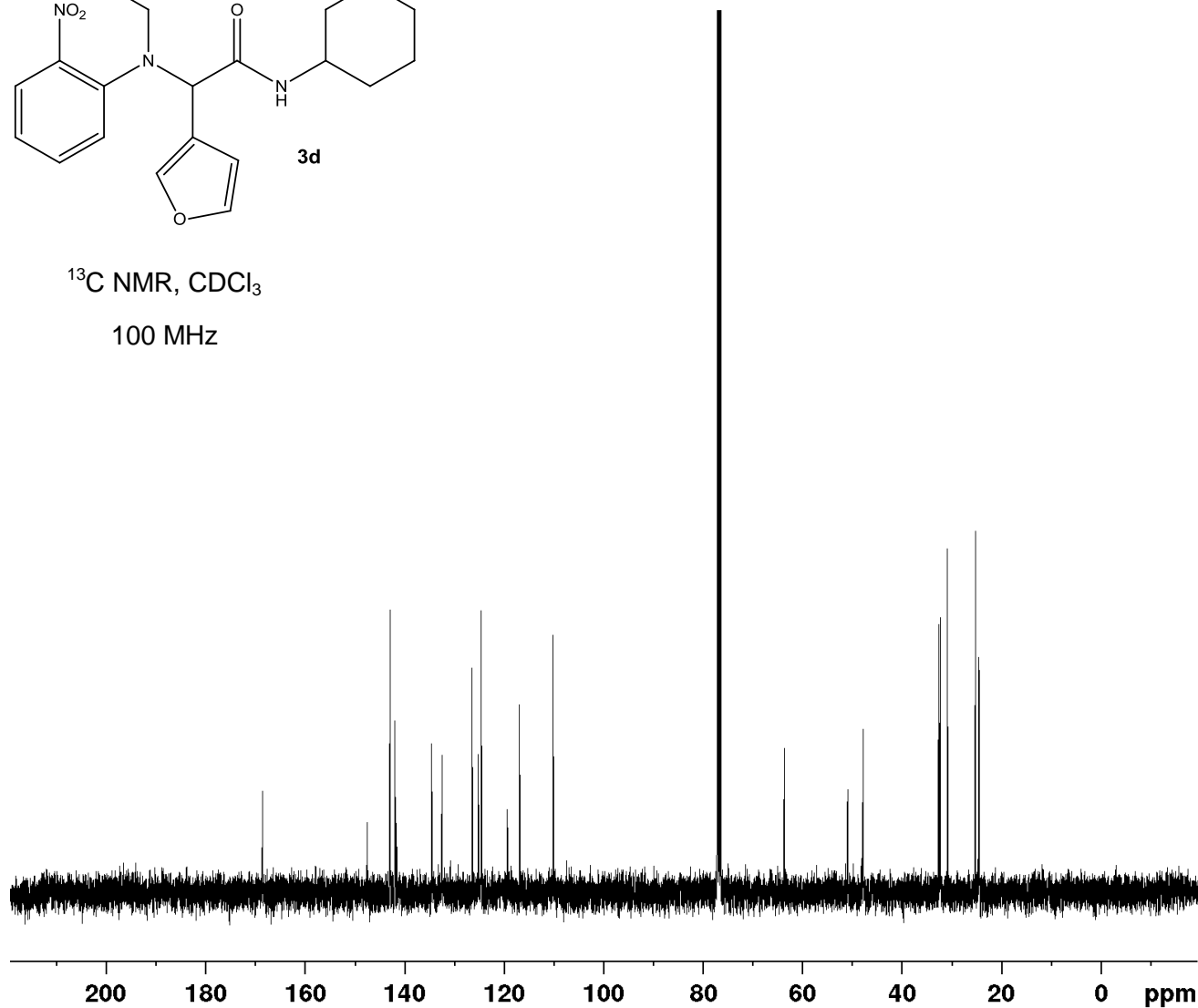
===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500119 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3

100 MHz



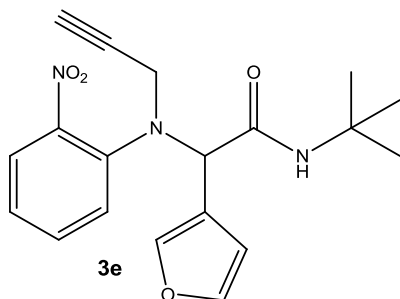
Current Data Parameters
 NAME MM-2-73
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160308
 Time 15.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 128
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 210.96
 DW 20.800 usec
 DE 10.00 usec
 TE 294.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 ^{13}C
 P1 10.00 usec
 PLW1 48.20000076 W

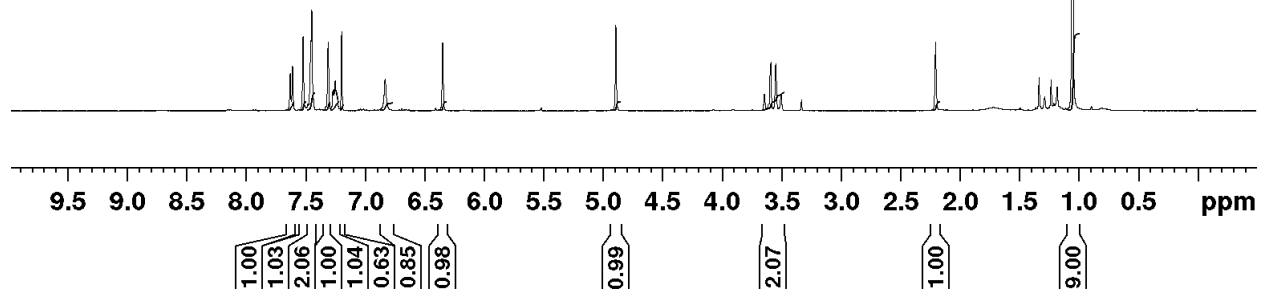
===== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 ^1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.80000019 W
 PLW12 0.27221999 W
 PLW13 0.22050001 W

F2 - Processing parameters
 SI 32768
 SF 100.6178041 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



$^1\text{H NMR}$, CDCl_3

400 MHz

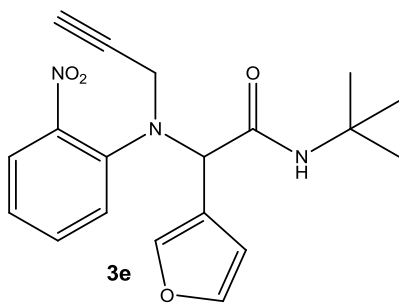


Current Data Parameters
 NAME KM-36R-F61-70-3
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150513
 Time 13.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl_3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 152.01
 DW 62.400 usec
 DE 6.50 usec
 TE 292.6 K
 D1 1.00000000 sec
 TD0 1

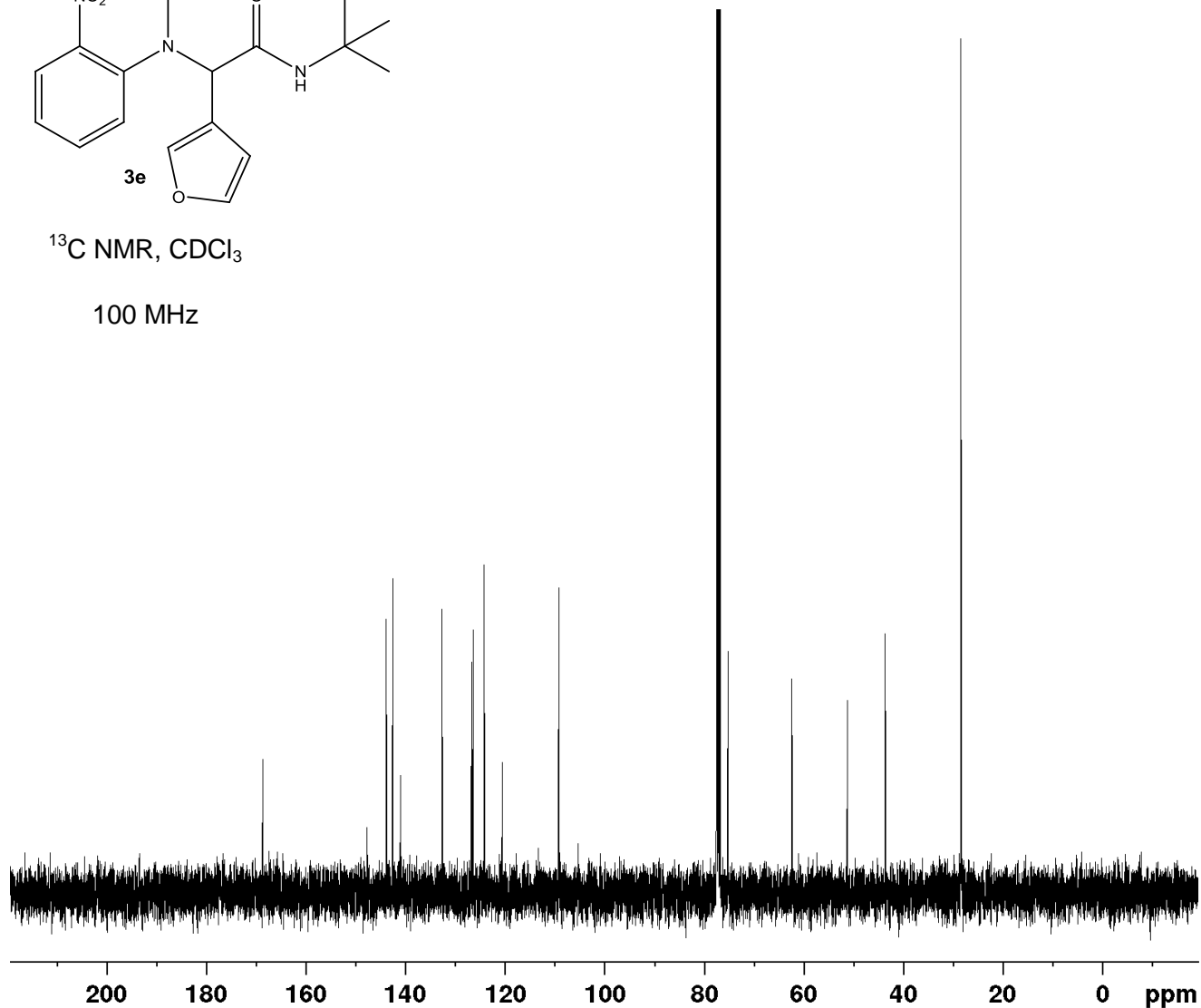
===== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500364 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3

100 MHz



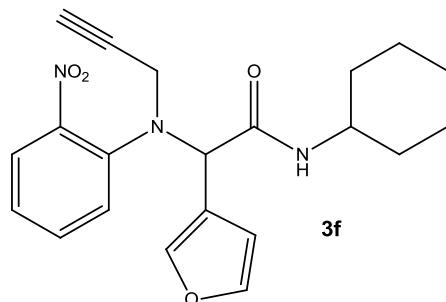
Current Data Parameters
 NAME KM-36R-F61-70-3
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150513
 Time 13.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 128
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 210.96
 DW 20.800 usec
 DE 10.00 usec
 TE 293.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 ^{13}C
 P1 10.00 usec
 PLW1 48.20000076 W

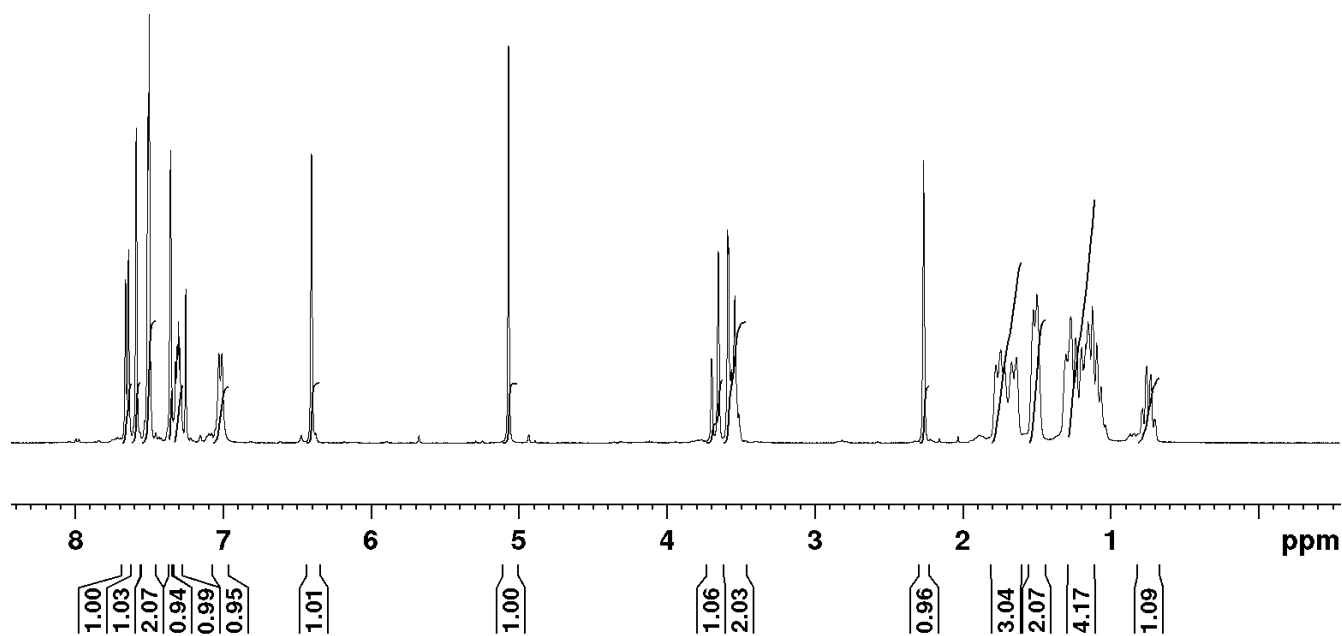
===== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 ^1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.80000019 W
 PLW12 0.27221999 W
 PLW13 0.22050001 W

F2 - Processing parameters
 SI 32768
 SF 100.6177852 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



¹H NMR, CDCl₃

400 MHz

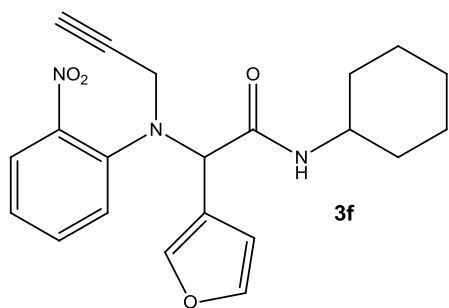


Current Data Parameters
 NAME MM-2-72
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160308
 Time 14.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 57.34
 DW 62.400 usec
 DE 6.50 usec
 TE 293.8 K
 D1 1.00000000 sec
 TDO 1

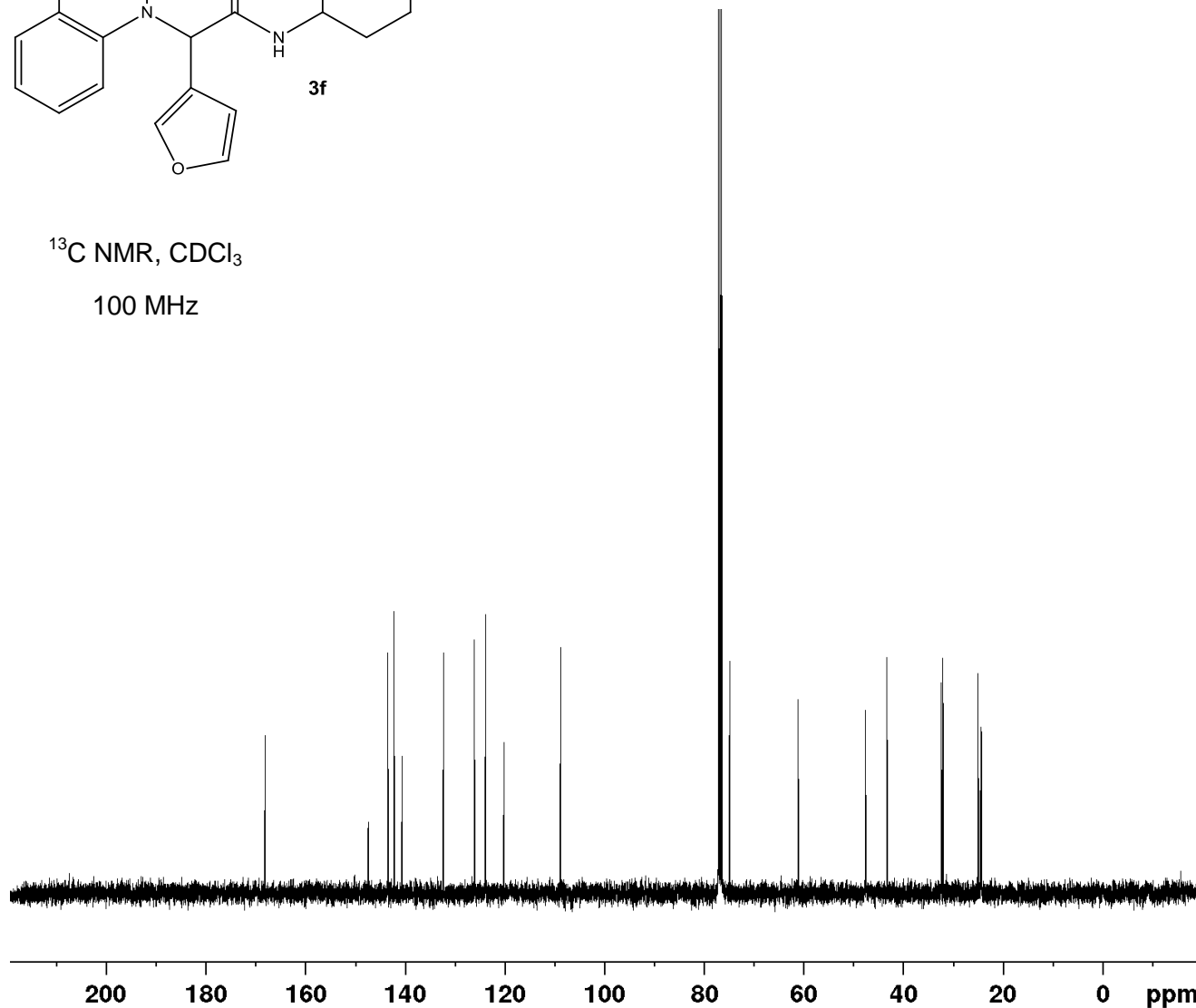
==== CHANNEL f1 =====
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500119 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3

100 MHz



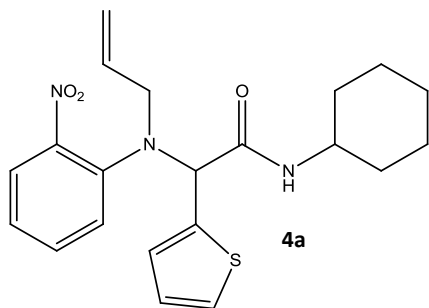
Current Data Parameters
 NAME MM-2-72
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160307
 Time 21.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 128
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 210.96
 DW 20.800 usec
 DE 10.00 usec
 TE 297.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 48.20000076 W

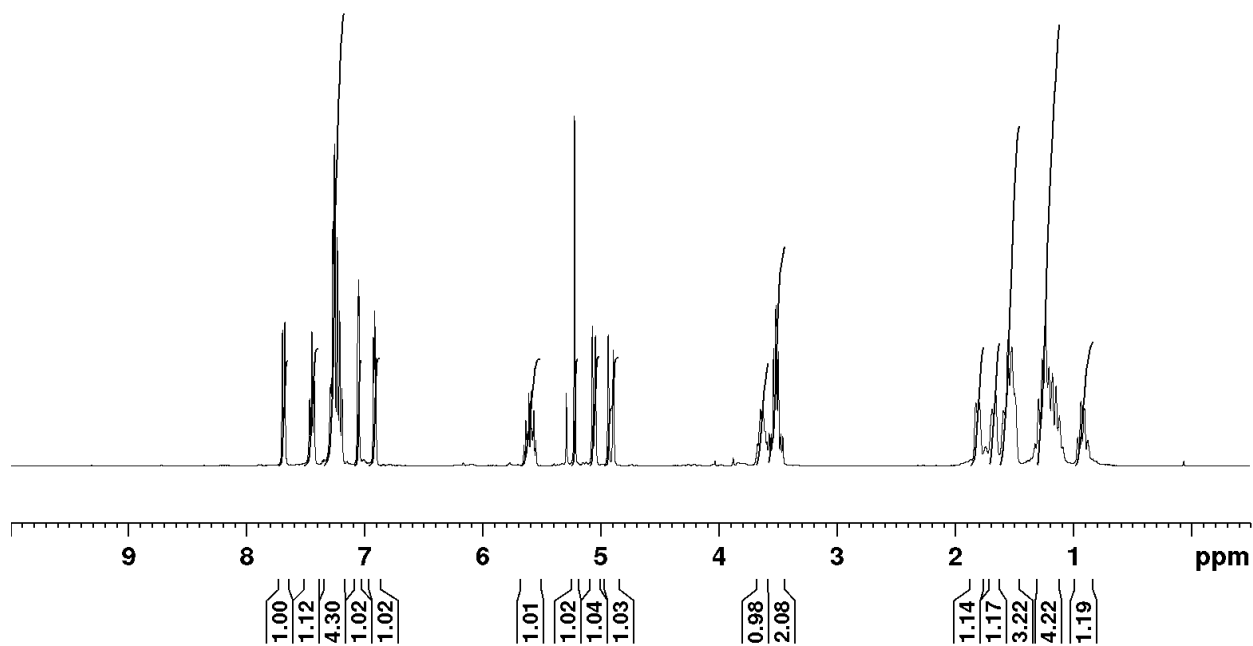
===== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.80000019 W
 PLW12 0.27221999 W
 PLW13 0.22050001 W

F2 - Processing parameters
 SI 32768
 SF 100.6178041 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



^1H NMR, CDCl_3

400 MHz

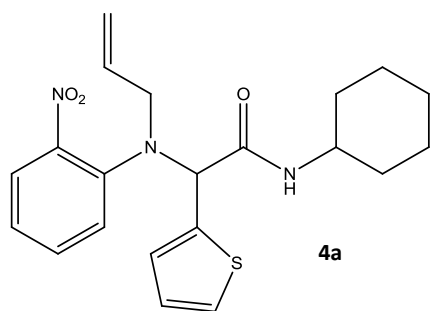


Current Data Parameters
 NAME MM-2-26-2-F14-21
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150512
 Time 13.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl_3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 82.91
 DW 62.400 usec
 DE 6.50 usec
 TE 292.2 K
 D1 1.00000000 sec
 TD0 1

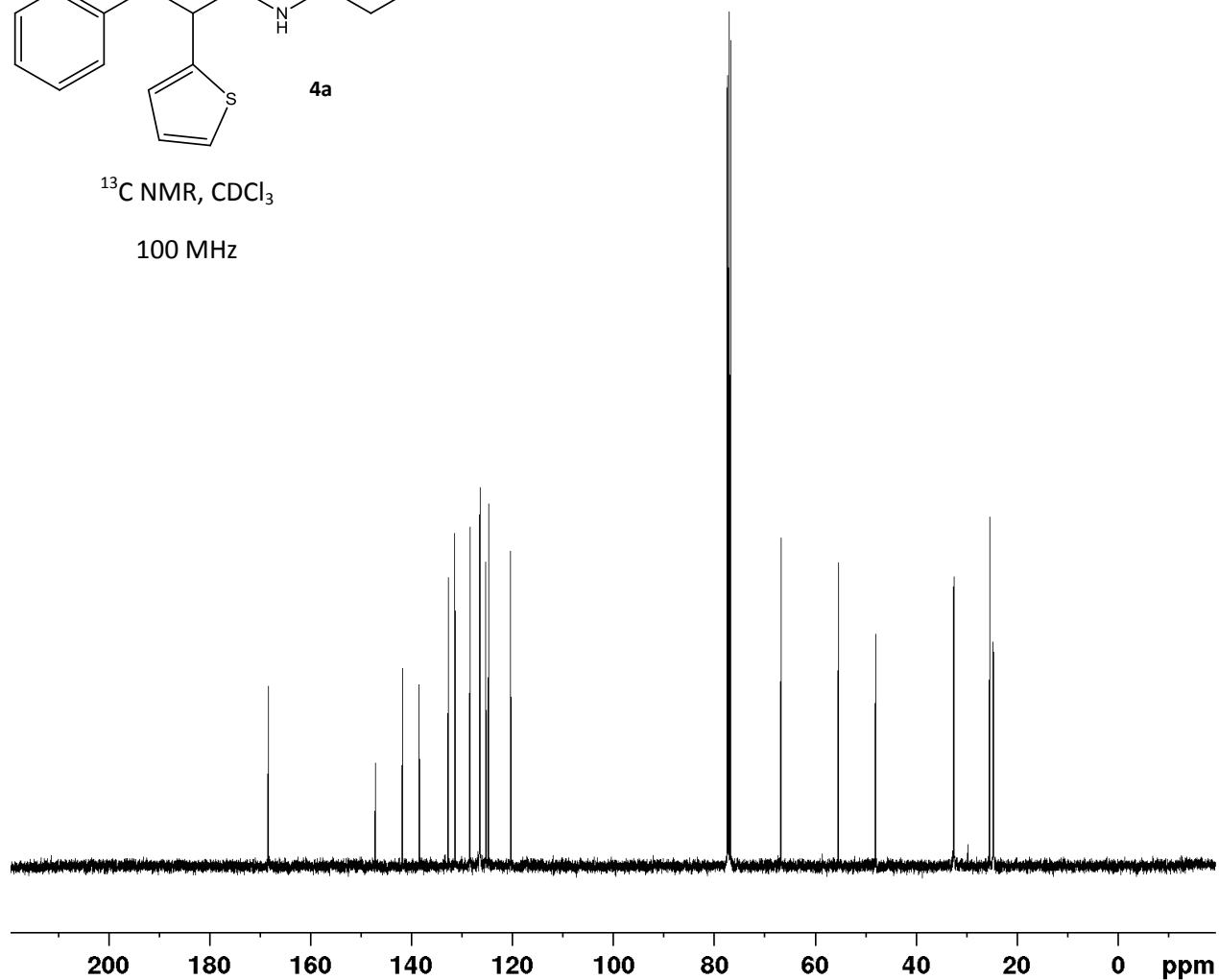
----- CHANNEL f1 -----
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.80000019 W

F2 - Processing parameters
 SI 65536
 SF 400.1500108 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



^{13}C NMR, CDCl_3

100 MHz



Current Data Parameters
 NAME MM-2-26-2-F14-21
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150904
 Time 17.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 210.96
 DW 20.800 usec
 DE 10.00 usec
 TE 294.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 48.20000076 W

===== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.80000019 W
 PLW12 0.27221999 W
 PLW13 0.22050001 W

F2 - Processing parameters
 SI 32768
 SF 100.6177926 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

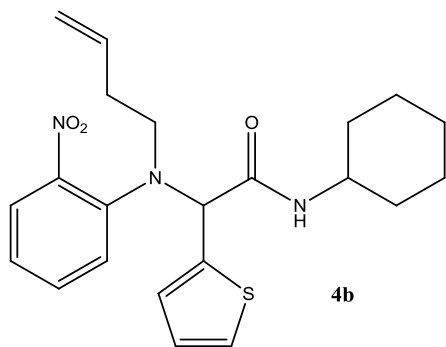


Current Data Parameters
NAME AF 1-10-1 R15-34
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160527
Time 13.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 66.61
DW 62.400 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1

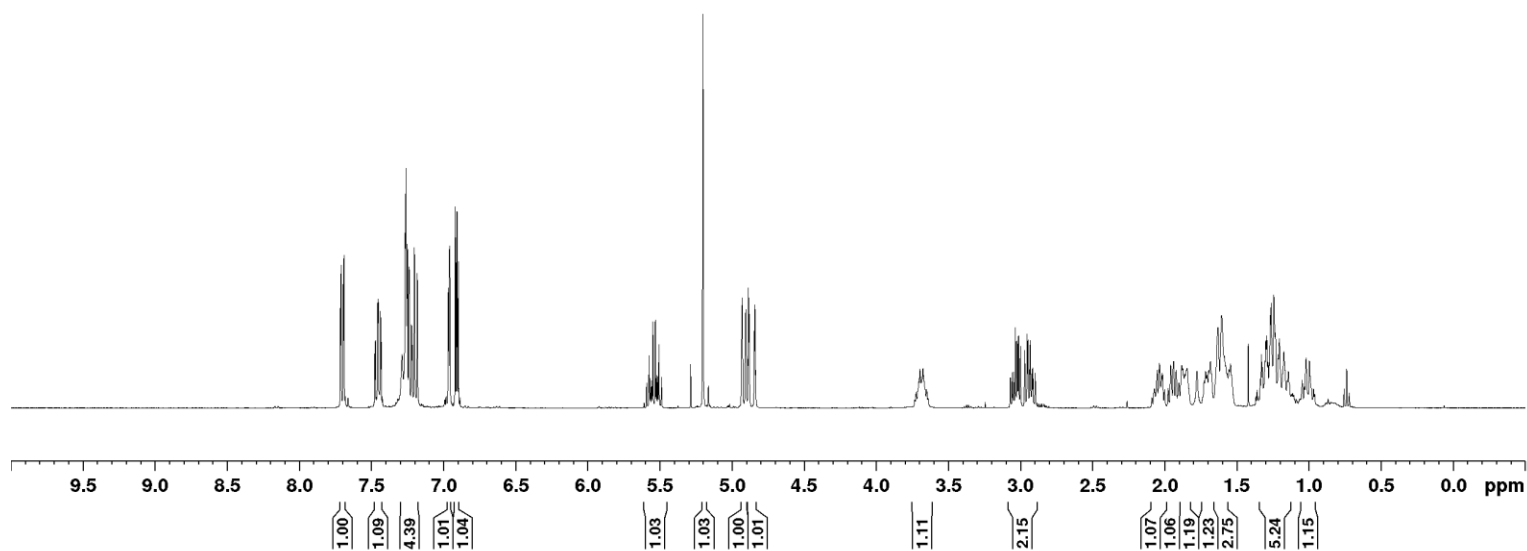
===== CHANNEL f1 =====
SFO1 400.1524711 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.80000019 W

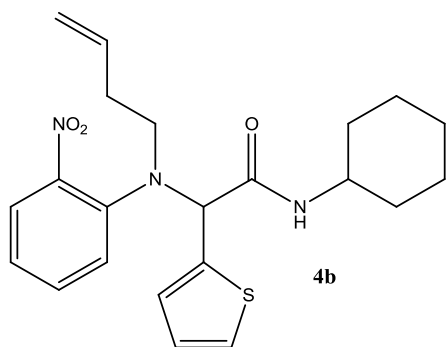
F2 - Processing parameters
SI 65536
SF 400.1500102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



^1H NMR, CDCl_3

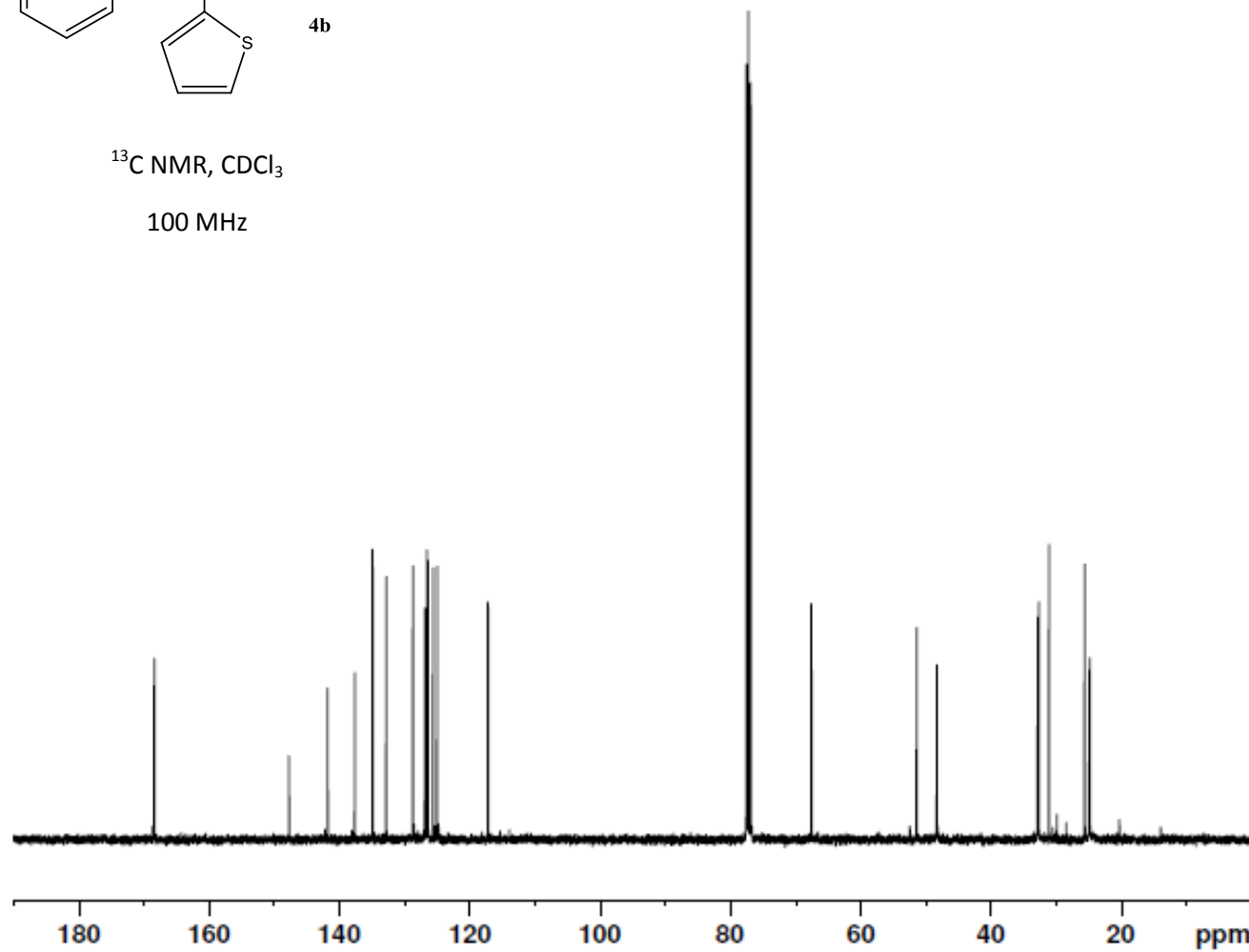
400 MHz





^{13}C NMR, CDCl_3

100 MHz



Current Data Parameters
 NAME AF 1-10-1 pure pdct
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160529
 Time 13.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl_3
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 210.96
 DW 20.800 usec
 DE 10.00 usec
 TE 295.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 100.6278588 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 48.20000076 W

==== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 9.80000019 W
 PLW12 0.27221999 W
 PLW13 0.22050001 W

F2 - Processing parameters
 SI 32768
 SF 100.6177865 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40