Supporting Information For:
Palladium-catalyzed Intramolecular Cyanoamidation of Alkynyl and Alkenyl
Cyanoformamides

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General. Nominal (LR-MS) and exact mass (HR-MS) spectra were recorded on a JEOL JMS-01SG-2 or JMS-HX/HX 110A mass spectrometer. ¹H NMR and ¹³C NMR spectra were registered on JEOL JNM-LA500 using TMS as an internal standard. (s = singlet, d = doublet, dd = double doublet, ddd = doublet of double doublets, t = triplet, q = quartet, m = multiplet, br = broad). Optical rotations were measured in CHCl₃ unless otherwise noted with a JASCO DIP-360 digital polarimeter. For column chromatography, Kanto Silica gel 60 (spherical, 63-210 μm) was employed and preparative thin-layer chromatography (PTLC) was carried out using Silica gel 60 (Merck).

Materials. Unless otherwise noted, materials were purchased from Tokyo Kasei Co., Aldrich Inc., and other commercial suppliers and were used without purification. *N*-benzyl-2-iodoaniline was prepared by the known procedure.¹ TCNEO (=tetracyanoethyleneoxide) was prepared according to the literature procedure.²

General procedure for preparing cyanoformamides³

Under an argon atmosphere, to a solution of TCNEO (2.79 g, 19.4 mmol) in dry ether (30 mL) was added Me₂S (1.85 mL, 24.3 mmol) at 0 °C, and the reaction mixture was stirred at 0 °C for 1h. To the crude solution, was added a solution of *N*-benzyl-2-iodoaniline (5.00g, 16.2 mmol) in ether (30 mL) at 0 °C, and the whole was stirred at room temperature for 8h. The reaction mixture was filtered through a pad of Celite and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (AcOEt/Hexane = 1/5 as eluent) to afford *N*-benzyl-*N*-(2-iodophenyl)cyanoformamide (3.98 g, 68%) as a white solid.

Caution! Although the TCNEO can be handled in air for a short period, for example, to be weighed, all operations should be carried out in a fume hood to avoid inhalation of hydrogen cyanide, which may be generated during the reactions.

***N*-benzyl-*N*-(2-iodophenyl)cyanoformamide:** white solid: m.p. 84-87 °C; ¹H NMR (CDCl₃,

500 Hz) δ : 4.27 (d, 1H, J = 14.0 Hz), 5.51 (d, 1H, J = 14.0 Hz), 6.87 (d, 1H, J = 7.6 Hz), 7.18 (t, 1H, J = 7.8 Hz), 7.24 (m, 2H), 7.34 (m, 4H), 8.00 (d, 1H, J = 7.9 Hz); ^{13}C NMR (CDCl_3 , 126Hz) δ : 51.9, 99.6, 110.4, 128.6, 128.8, 129.5, 129.7, 131.2, 131.7, 133.9, 140.0, 140.5, 145.1; IR (CHCl_3): 2232.2, 1692.2, 1469.5, 1394.3, 1280.5 cm^{-1} ; MS (EI) m/z (relative intensity) 362 (M^+ , 5), 91 (100); *Anal.* Calcd. for $\text{C}_{15}\text{H}_{11}\text{IN}_2\text{O}$: C, 49.75; H, 3.06; N, 7.74. Found: C, 49.75; H, 3.21; N, 7.74.

To a solution of *N*-benzyl-*N*-(2-iodophenyl)cynoformamide (1.00 g, 2.76 mmol) prepared above, 1-hexyne (464 mg, 5.52 mmol) and Et_3N (559 mg, 5.52 mmol) in dry DMF (10 mL) was added $\text{Pd}(\text{PPh}_3)_4$ (319 mg, 0.276 mmol) and CuI (105 mg, 0.552 mmol) at room temperature and the whole was stirred at the same temperature for 24 h under an argon atmosphere. The crude residue was purified by column chromatography (AcOEt/Hexane = 1/2 as eluent) to give **1a** (680 mg, 78%) as a colorless oil.

1a: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 0.96 (m, 3H), 1.46 (m, 2H), 1.57 (m, 2H), 2.40 (t, 2H, J = 7.2 Hz), 4.49 (d, 1H, J = 14.0 Hz), 5.31 (d, 1H, J = 14.0 Hz), 6.86 (d, 1H, J = 7.9 Hz), 7.16-7.36 (m, 7 H), 7.51 (dd, 1H, J = 1.4, 7.8 Hz); ^{13}C NMR (CDCl_3 , 126Hz) δ : 13.4, 19.1, 21.9, 30.4, 52.0, 75.7, 97.9, 110.8, 124.4, 128.3, 128.6, 129.4, 129.5, 129.8, 133.5, 134.5, 139.1, 145.3; IR (CHCl_3): 2232.2, 1680.7 cm^{-1} ; MS (EI^+) m/z (relative intensity) 316 (M^+ , 25), 184 (100); HRMS (EI^+) $\text{C}_{21}\text{H}_{20}\text{N}_2\text{O}$: (M^+) 316.1576. Found: 316.1569.

1b: red oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 4.63 (d, 1H, J = 14.3 Hz), 5.29 (d, 1H, J = 14.3 Hz), 6.95 (d, 1H, J = 7.9 Hz), 7.21 (m, 6H), 7.35 (m, 4H), 7.48 (m, 2H), 7.59 (dd, 1H, J = 1.5, 7.6 Hz); ^{13}C NMR (CDCl_3 , 126Hz) δ : 52.1, 84.1, 95.9, 110.7, 121.8, 123.5, 128.3, 128.4, 128.5, 129.0, 129.3, 129.4, 129.9, 131.6, 133.1, 134.1, 138.9, 145.2; IR (CHCl_3): 2220.6, 1680.7, 1496.5, 1394.3 cm^{-1} ; MS (EI^+) m/z (relative intensity) 336 (M^+ , 22), 91 (100); HRMS (EI^+) $\text{C}_{23}\text{H}_{16}\text{N}_2\text{O}$: (M^+) 336.1263. Found: 336.1257.

1c: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 0.01 (s, 6H), 0.78 (s, 9H), 4.30 (d, 1H, J = 14.3 Hz), 4.35 (s, 2H), 5.21 (d, 1H, J = 14.0 Hz), 6.69 (d, 1H, J = 7.9 Hz), 7.00 (m, 2H), 7.11 (m, 4H), 7.22 (t, 1H, J = 7.6 Hz), 7.41 (d, 1H, J = 7.6 Hz); ^{13}C NMR (CDCl_3 , 126 Hz) δ : 5.3, 18.2, 25.7, 51.9, 52.0, 79.5, 94.8, 110.6, 123.2, 128.4, 128.7, 129.4, 129.5, 129.9, 130.0, 133.8, 134.5, 139.0, 145.1; IR (CHCl_3): 2232.2, 1680.7 cm^{-1} ; MS (FAB^+) m/z (relative intensity) 405 (M^+ , 4), 91 (100); HRMS (FAB^+) $\text{C}_{24}\text{H}_{28}\text{N}_2\text{OSi}$: (MH^+) 405.1998. Found: 405.1983.

1d: white solid; m.p. 63-65 °C; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.80 (m, 3H), 2.43 (m, 2H), 3.43 (t, 1H, $J = 6.9$ Hz), 3.62 (t, 1H, $J = 6.4$ Hz), 4.65 (s, 1H), 4.90 (s, 1H), 7.21-7.46 (m, 5H); ^{13}C NMR (CDCl_3 , 126Hz, mixture of rotamers) δ : 3.4, 17.0, 18.7, 43.9, 46.8, 47.7, 53.2, 74.0, 75.0, 78.1, 80.5, 110.6, 110.7, 127.7, 128.3, 128.4, 128.7, 128.8, 128.9, 129.0, 129.2, 134.0, 134.4, 144.8, 145.6; IR (CHCl_3): 2232.2, 1684.5 cm^{-1} ; MS (FAB^+) m/z (relative intensity) 227 (M^+ , 41), 91 (100); HRMS (FAB^+) $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}$: (MH^+) 227.1184. Found: 227.1190.

1e: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 2.65 (t, 1H, $J = 6.1$ Hz), 2.70 (t, 1H, $J = 6.3$ Hz), 3.54 (t, 1H, $J = 6.7$ Hz), 3.73 (t, 1H, $J = 6.4$ Hz), 4.69 (s, 1H), 4.93 (s, 1H), 7.25-7.44 (m, 10H); ^{13}C NMR (CDCl_3 , 126Hz, mixture of rotamers) δ : 17.7, 19.4, 43.6, 47.9, 53.2, 82.7, 84.4, 85.6, 110.7, 122.6, 122.8, 127.7, 128.2, 128.3, 128.4, 128.8, 129.0, 129.2, 131.4, 131.5, 133.9, 134.4, 145.0, 145.6; IR (CHCl_3): 2232.2, 1675.9, 1427.1 cm^{-1} ; MS (EI^+) m/z (relative intensity) 288 (M^+ , 100), 234 (30), 205 (50); HRMS (EI^+) $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}$: (M^+) 288.1263. Found: 288.1266.

1f: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 0.82-0.95 (m, 6H), 0.96-1.08 (m, 3H), 1.40 (m, 2H), 1.50 (m, 2H), 2.14-2.37 (m, 3H), 2.97- 3.24 (m, 3H), 3.35 (m, 3H), 3.69 (dd, 1H, $J = 10.4$ Hz, 3.7 Hz), 4.17-4.36 (m, 1H); ^{13}C NMR (CDCl_3 , 126Hz, mixture of rotamers) δ : 13.4, 18.2, 19.0, 19.1, 19.6, 19.9, 21.8, 21.9, 25.2, 25.7, 29.9, 30.3, 30.5, 56.8, 57.0, 69.4, 70.9, 71.7, 75.0, 88.8, 90.6, 110.8, 110.9, 146.4, 147.2; IR (CHCl_3): 2360.4, 1670.1 cm^{-1} ; MS (EI^+) m/z (relative intensity) 264 (M^+ , 1), 207 (21), 44 (100).

1g: colorless oil; $[\alpha]_{\text{D}}^{24} -106$ (c 0.81, CHCl_3); ^1H NMR (CDCl_3 , 500 Hz) δ : -0.07-0.15 (m, 6H), 0.74-0.96 (m, 12H), 1.26-1.54 (m, 4H), 1.79 (m, 1H), 1.99-2.19 (m, 4H), 2.31 (m, 1H), 3.23-3.90 (m, 2H), 3.96-4.28 (m, 1H), 4.40-5.03 (m, 1H); ^{13}C NMR (CDCl_3 , 126Hz, mixture of rotamers) δ : -5.5, -5.4, -5.1, -5.0, 13.3, 17.7, 17.8, 18.0, 18.1, 21.6, 21.7, 22.4, 23.9, 25.4, 25.5, 26.3, 30.1, 30.3, 46.9, 49.8, 61.2, 62.7, 64.1, 65.4, 77.9, 78.3, 86.6, 88.1, 110.9, 111.3, 142.6; IR (CHCl_3): 2360.4, 2232.2, 1672.0 cm^{-1} ; MS (EI^+) m/z (relative intensity) 291 ($\text{M}-\text{Bu}^t$, 57), 225 (48), 73 (100).

1h: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.58 (s, 3H), 1.59 (s, 3H), 3.34 (s, 3H), 3.45 (s, 3H), 5.08 (s, 1H), 7.33 (m, 3H), 7.44 (m, 2H); ^{13}C NMR (CDCl_3 , 126Hz) δ : 22.0, 22.3, 35.6, 57.4, 64.3, 73.9, 84.9, 87.3, 111.4, 122.2, 128.4, 128.7, 131.8, 145.6; IR (CHCl_3): 2360.4, 2229.3, 1672.0 cm^{-1} ; MS (EI^+) m/z (relative intensity) 270 (M^+ , 1), 186 (42), 145

(100).

4: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.82 (m, 1H), 1.92 (m, 1H), 2.42 (t, 1H, $J = 6.9$ Hz), 2.49 (t, 1H, $J = 6.7$ Hz), 3.49 (m, 1H), 3.68 (m, 1H), 4.64 (s, 1H), 4.80 (s, 1H), 7.23-7.40 (m, 10H); ^{13}C NMR (CDCl_3 , 126Hz, mixture of rotamers) δ : 16.6, 16.8, 25.4, 27.1, 44.0, 47.0, 48.0, 52.8, 81.9, 82.3, 87.2, 88.0, 110.6, 110.8, 123.2, 123.3, 127.8, 127.9, 128.0, 128.3, 128.4, 128.5, 128.8, 129.0, 129.2, 131.5, 131.6, 134.0, 134.6, 144.9, 145.4; IR (CHCl_3): 2231.2, 1677.8, 1429.0 cm^{-1} ; MS (EI^+) m/z (relative intensity) 302 (M^+ , 8), 211 (47), 91 (100); HRMS (EI^+) $\text{C}_{20}\text{H}_{18}\text{N}_2\text{O}$: (M^+) 302.1419. Found: 302.1416.

6: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.51 (m, 1H), 1.58 (m, 1H), 1.66 (m, 1H), 1.77 (m, 1H), 2.37 (t, 1H, $J = 6.9$ Hz), 2.41 (t, 1H, $J = 6.9$ Hz), 3.33 (m, 1H), 3.50 (m, 1H), 4.58 (s, 1H), 4.71 (s, 1H), 7.20-7.39 (m, 10H); ^{13}C NMR (CDCl_3 , 126Hz, mixture of rotamers) δ : 18.6, 25.1, 25.4, 27.1, 44.1, 47.6, 47.7, 52.2, 81.2, 81.4, 88.6, 88.9, 110.6, 110.8, 123.5, 123.6, 127.4, 127.6, 128.0, 128.1, 128.2, 128.6, 128.8, 129.0, 131.4, 134.5, 144.7, 145.1; IR (CHCl_3): 2232.2, 1675.8 cm^{-1} ; MS (EI^+) m/z (relative intensity) 316 (M^+ , 9), 225 (20), 91 (100); HRMS (EI^+) $\text{C}_{21}\text{H}_{20}\text{N}_2\text{O}$: (M^+) 316.1576. Found: 316.1567.

8a: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 2.11 (s, 3H), 4.09 (d, 1H, $J = 14.3$ Hz), 5.08 (s, 1H), 5.34 (s, 1H), 5.50 (d, 1H, $J = 14.0$ Hz), 6.75 (d, 1H, $J = 7.9$ Hz), 7.15 (m, 1H), 7.18 (m, 1H), 7.28 (m, 3H), 7.38 (m, 2H); ^{13}C NMR (CDCl_3 , 126Hz) δ : 23.5, 52.2, 110.8, 118.2, 128.3, 128.4, 128.7, 129.3, 130.2, 130.3, 130.5, 134.5, 134.8, 141.9, 142.2, 145.4; IR (CHCl_3): 2231.2, 1677.8 cm^{-1} ; MS (EI^+) m/z (relative intensity) 276 (M^+ , 1), 184 (64), 130 (100); HRMS (EI^+) $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}$: (M^+) 276.1263. Found: 276.1267.

8b: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 2.11 (s, 3H), 5.07 (m, 1H), 5.49 (m, 1H), 7.24 (m, 2H), 7.31 (m, 1H), 8.10 (d, 1H, $J = 8.2$ Hz), 8.31 (br, 1H); ^{13}C NMR (CDCl_3 , 126Hz) δ : 24.3, 111.6, 118.1, 121.7, 121.8, 126.3, 128.1, 131.4, 134.5, 140.4, 141.6; IR (CHCl_3): 3361.3, 1708.6, 1522.5 cm^{-1} ; MS (EI^+) m/z (relative intensity) 186 (M^+ , 13), 117 (100); HRMS (EI^+) $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}$: (M^+) 186.0793. Found: 186.0796.

General procedure for the palladium-catalyzed intramolecular cyanoamidation

Under an argon atmosphere, a solution of **1a** (50.0 mg, 0.158 mmol) and $\text{Pd}(\text{PPh}_3)_4$ (18.2 mg, 10 mol%) in toluene (1.6 mL) was stirred at 100 °C for 2 h. Purification by column chromatograph on silica gel (AcOEt/Hexane = 1/10 to 1/3 as eluent) gave the products **(Z)-2a** (35.3 mg, 71%) and **(E)-2a** (12.9 mg, 26%) as yellow solids, respectively.

(Z)-2a: yellow solid; m.p. 123-124 °C; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.00 (m, 3H), 1.53 (m, 2H), 1.81 (m, 2H), 2.83 (t, 2H, $J = 7.2$ Hz), 4.95 (s, 2H), 6.77 (d, 1H, $J = 7.9$ Hz), 7.04 (dd, 1H, $J = 7.6, 7.6$ Hz), 7.26-7.34 (m, 6 H), 7.52 (d, 1H, $J = 7.6$ Hz); ^{13}C NMR (CDCl_3 , 126Hz) δ : 13.7, 22.4, 29.3, 32.5, 43.8, 109.8, 117.4, 119.8, 120.6, 122.7, 125.4, 127.6, 127.9, 128.9, 132.1, 135.4, 136.7, 143.8, 164.6; IR (CHCl_3): 2210.9, 1713.4, 1606.4, 1467.6, 1379.8, 1354.8 cm^{-1} ; MS (EI^+) m/z (relative intensity) 316 (M^+ , 12), 91 (100); *Anal.* Calcd. for $\text{C}_{21}\text{H}_{20}\text{N}_2\text{O}$: C, 79.72; H, 6.37; N, 8.85. Found: C, 79.94; H, 6.33; N, 8.86.

(E)-2a: yellow solid; m.p. 102-103 °C; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.03 (m, 3H), 1.51 (m, 2H), 1.68 (m, 2H), 3.23 (m, 2H), 4.92 (s, 2H), 6.72 (d, 1H, $J = 7.9$ Hz), 7.07 (dd, 1H, $J = 7.8, 7.8$ Hz), 7.26-7.34 (m, 6 H), 8.23 (d, 1H, $J = 7.6$ Hz); ^{13}C NMR (CDCl_3 , 126Hz) δ : 13.7, 22.3, 29.3, 30.4, 43.5, 109.2, 118.1, 120.2, 121.4, 122.9, 123.8, 127.3, 127.8, 128.9, 131.9, 135.3, 135.4, 142.9, 166.0; *Anal.* Cald. for $\text{C}_{21}\text{H}_{20}\text{N}_2\text{O}$: C, 9.72; H, 6.37; N, 8.85. Found: C, 79.42; H, 6.26; N, 8.83.

2b: red solid; m.p. 170-172 °C; ^1H NMR (CDCl_3 , 500 Hz) δ : 4.99 (s, 2H), 6.72 (t, 2H, $J = 7.3$ Hz), 6.86 (m, 1H), 7.21 (m, 1H), 7.30 (m, 1H), 7.32-7.40 (m, 4 H), 7.51-7.58 (m, 3H), 7.60 (m, 2H); ^{13}C NMR (CDCl_3 , 126Hz) δ : 43.9, 109.7, 117.0, 117.1, 120.0, 122.3, 124.8, 127.6, 127.9, 128.8, 129.5, 130.8, 132.9, 135.3, 137.3, 144.1, 164.9; IR (CHCl_3): 2212.0, 1713.4, 1603.5, 1469.5, 1353.8 cm^{-1} ; MS (EI^+) m/z (relative intensity) 336 (M^+ , 28), 91 (100); HRMS (EI^+) $\text{C}_{23}\text{H}_{16}\text{N}_2\text{O}$: (M^+) 336.1263. Found: 336.1266.

2c: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 0.20 (s, 6H), 0.95 (s, 9H), 4.77 (s, 2H), 4.95 (s, 2H), 6.76 (d, 1H, $J = 7.9$ Hz), 7.05 (t, 1H, $J = 7.3$ Hz), 7.30 (m, 6H), 7.46 (d, 1H, $J = 7.6$ Hz); ^{13}C NMR (CDCl_3 , 126Hz) δ : -5.3, 18.2, 25.7, 43.8, 61.3, 109.7, 115.8, 118.6, 120.1, 122.8, 126.8, 127.5, 127.9, 128.9, 132.8, 135.3, 137.5, 143.9, 164.3; IR (CHCl_3): 2232.2, 1680.7 cm^{-1} ; MS (FAB^+) m/z (relative intensity) 405 (M^+ , 14), 91 (100); HRMS (FAB^+) $\text{C}_{24}\text{H}_{28}\text{N}_2\text{OSi}$: (MH^+) 405.1998. Found: 405.2002.

2d: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 2.04 (s, 3H), 2.78 (t, 2H, $J = 4.7$ Hz), 3.35 (t, 2H, $J = 6.1$ Hz), 4.57 (s, 2H), 7.22-7.36 (m, 5H); ^{13}C NMR (CDCl_3 , 126Hz) δ : 18.8, 23.8, 42.8, 47.2, 108.9, 117.2, 127.9, 128.4, 128.7, 135.6, 146.3, 163.9; IR (CHCl_3): 2218.7, 1692.2 cm^{-1} ; MS (EI^+) m/z (relative intensity) 226 (M^+ , 72), 91 (100); *Anal.* Calcd. for $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}$: C, 74.31; H, 6.24; N, 12.38. Found: C, 74.04; H, 6.24; N, 12.12.

2e: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 3.02 (t, 2H, $J = 6.1$ Hz), 3.34 (t, 2H, $J = 6.0$ Hz), 4.62 (s, 2H), 7.33 (m, 5H), 7.44 (m, 3H), 7.55 (d, 2H, $J = 7.0$ Hz); ^{13}C NMR (CDCl_3 , 126Hz) δ : 26.3, 43.2, 47.5, 114.1, 116.3, 128.0, 128.4, 128.6, 128.8, 128.9, 130.0, 133.5, 135.6, 146.2, 164.6; IR (CHCl_3): 3015.2, 1692.2, 1440.6, 1298.8, 1281.5 cm^{-1} ; MS (EI^+) m/z (relative intensity) 288 (M^+ , 53), 91 (100); HRMS (EI^+) $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}$: (M^+) 288.1263. Found: 288.1269.

3e: colorless oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 3.85 (m, 2H), 4.52 (d, 1H, $J = 14.7$ Hz), 4.70 (d, 1H, $J = 14.7$ Hz), 5.02 (s, 1H), 7.05 (d, 1H, $J = 1.8$ Hz), 7.21 (d, 2H, $J = 6.7$ Hz), 7.25-7.39 (m, 6H), 7.48 (d, 2H, $J = 7.3$ Hz); ^{13}C NMR (CDCl_3 , 126Hz) δ : 34.3, 46.5, 50.4, 50.4, 118.5, 127.7, 127.9, 128.1, 128.6, 128.9, 129.2, 133.4, 135.7, 136.6, 138.4, 168.3; IR (CHCl_3): 3067.2, 1689.3, 1454.1, 1243.9 cm^{-1} ; MS (EI^+) m/z (relative intensity) 288 (M^+ , 100), 261 (15); HRMS (EI^+) $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}$: (M^+) 288.1263. Found: 288.1258.

2f: colorless oil; $[\alpha]_{\text{D}}^{20} -0.24$ (c 0.81, CHCl_3); ^1H NMR (CDCl_3 , 500 Hz) δ : 0.85 (d, 3H, $J = 7.0$ Hz), 0.94 (t, 3H, $J = 7.3$ Hz), 1.09 (d, 3H, $J = 7.3$ Hz), 1.38 (m, 2H), 1.63 (m, 2H), 2.12 (m, 1H), 2.49 (m, 2H), 3.02 (s, 3H), 3.46 (s, 2H), 3.65 (dd, 1H, $J = 7.0, 2.1$ Hz), 4.58 (d, 1H, $J = 7.0$ Hz); ^{13}C NMR (CDCl_3 , 126Hz) δ : 13.7, 16.7, 20.6, 22.2, 28.7, 29.8, 30.6, 31.2, 58.7, 65.3, 78.8, 116.7, 117.4, 144.0, 163.9; IR (CHCl_3): 2360.4, 1692.2 cm^{-1} ; MS (EI^+) m/z (relative intensity) 264 (M^+ , 7), 98 (100); HRMS (EI^+) $\text{C}_{15}\text{H}_{24}\text{N}_2\text{O}_2$: (M^+) 264.1838. Found: 264.1840.

3f: colorless oil; $[\alpha]_{\text{D}}^{20} +42.7$ (c 0.49, CHCl_3); ^1H NMR (CDCl_3 , 500 Hz) δ : 0.85-0.97 (m, 6H), 1.00 (t, 3H, $J = 7.3$ Hz), 1.27-1.54 (m, 4H), 1.63 (m, 1H), 1.81 (m, 1H), 1.96 (m, 1H), 2.22 (m, 1H), 2.95 (s, 3H), 3.81 (m, 1H), 3.99 (s, 3H); ^{13}C NMR (CDCl_3 , 126Hz) δ : 13.7, 16.3, 18.2, 21.9, 25.5, 28.6, 29.0, 29.5, 32.3, 59.6, 65.6, 106.4, 120.3, 169.5, 170.2; IR (CHCl_3): 2360.4, 1676.8 cm^{-1} ; MS (EI^+) m/z (relative intensity) 264 (M^+ , 11), 262 (100); HRMS (EI^+) $\text{C}_{15}\text{H}_{24}\text{N}_2\text{O}_2$: (M^+) 264.1838. Found: 264.1832.

2g: white solid; $[\alpha]_{\text{D}}^{20} +46.1$ (c 0.70, CHCl_3); m.p. 113-115 $^{\circ}\text{C}$; ^1H NMR (CDCl_3 , 500 Hz) δ : -0.01 (s, 3H), 0.00 (s, 3H), 0.75 (s, 9H), 1.12 (m, 1H), 1.21 (m, 2H), 1.46 (m, 2H), 1.86 (m, 1H), 1.93 (m, 1H), 2.03 (m, 1H), 2.28 (t, 2H, $J = 7.8$ Hz), 3.06 (m, 1H), 3.41 (m, 1H), 3.56 (m, 1H), 4.55 (s, 1H); ^{13}C NMR (CDCl_3 , 126Hz) δ : -5.0, -4.0, 13.7, 17.7, 22.3, 25.2, 25.5, 29.5, 29.8, 31.2, 42.0, 68.0, 72.3, 116.2, 120.0, 149.2, 164.1; IR (CHCl_3): 1693.2 cm^{-1} ; MS (EI^+) m/z (relative intensity) 348 (M^+ , 1), 291 (55), 69 (100); *Anal.* Calcd. for $\text{C}_{19}\text{H}_{32}\text{N}_2\text{O}_2\text{Si}$: C, 65.47; H, 9.25; N, 8.04. Found: C, 65.37; H, 9.35; N, 7.91.

2h: pale yellow solid; m.p. 172-178 °C; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.24 (s, 3H), 1.30 (s, 3H), 2.92 (s, 3H), 3.12 (s, 3H), 4.21 (s, 1H), 7.47 (m, 3H), 7.56 (m, 2H); ^{13}C NMR (CDCl_3 , 126Hz) δ : 19.9, 24.6, 25.5, 58.0, 62.1, 82.0, 116.2, 118.9, 128.8, 128.9, 130.1, 133.3, 145.2, 163.0; IR (CHCl_3): 1690.3 cm^{-1} ; MS (EI^+) m/z (relative intensity) 270 (M^+ , 100), 199 (55), 143 (54).

5: yellow oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.79 (dd, 2H, $J = 12.1, 5.7$ Hz), 2.63 (m, 2H), 3.33 (m, 2H), 4.74 (s, 2H), 7.26-7.44 (m, 10H); ^{13}C NMR (CDCl_3 , 126Hz) δ : 22.3, 28.2, 46.8, 51.0, 118.5, 118.8, 127.7, 128.5, 128.7, 128.8, 129.0, 129.4, 134.4, 136.5, 144.7, 161.6; IR (CHCl_3): 3013.2, 1645.0, 1599.0, 1490.7, 1450.2 cm^{-1} ; MS (EI^+) m/z (relative intensity) 302 (M^+ , 29), 91 (100); HRMS (EI^+) $\text{C}_{20}\text{H}_{18}\text{N}_2\text{O}$: (M^+) 302.1419. Found: 302.1424.

7: colorless crystal; m.p. 142-143 °C; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.55 (m, 2H), 1.71 (m, 2H), 2.49 (m, 2H), 3.32 (m, 2H), 4.72 (s, 2H), 7.30-7.44 (m, 10H); ^{13}C NMR (CDCl_3 , 126Hz) δ : 26.1, 27.1, 28.5, 47.3, 50.0, 113.8, 117.4, 127.8, 128.4, 128.6, 128.8, 129.0, 129.3, 132.2, 136.7, 156.3, 169.6; IR (CHCl_3): 1641.1 cm^{-1} ; MS (EI^+) m/z (relative intensity) 316 (M^+ , 18), 91 (100); HRMS (EI^+) $\text{C}_{21}\text{H}_{20}\text{N}_2\text{O}$: (M^+) 316.1576. Found: 316.1582.

9a: yellow oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.57 (s, 3H), 2.64 (d, 1H, $J = 16.5$ Hz), 2.90 (d, 1H, $J = 16.5$ Hz), 4.93 (s, 2H), 6.78 (d, 1H, $J = 7.6$ Hz), 7.09 (t, 1H, $J = 7.6$ Hz), 7.27 (m, 6H), 7.47 (m, 1H); ^{13}C NMR (CDCl_3 , 126 Hz) δ : 22.4, 26.2, 43.8, 44.8, 109.7, 116.6, 123.1, 123.2, 127.1, 127.8, 128.9, 129.2, 130.9, 135.3, 141.8, 177.7; IR (CHCl_3): 1714.4 cm^{-1} ; MS (EI^+) m/z (relative intensity) 276 (M^+ , 19), 236 (23), 91 (100); HRMS (EI^+) $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}$: (M^+) 276.1263. Found: 276.1261.

9b: yellow oil; ^1H NMR (CDCl_3 , 500 Hz) δ : 1.56 (s, 3H), 2.64 (d, 1H, $J = 16.8$ Hz), 2.85 (d, 1H, $J = 16.5$ Hz), 7.00 (d, 1H, $J = 7.6$ Hz), 7.12 (t, 1H, $J = 7.6$ Hz), 7.30 (t, 1H, $J = 7.8$ Hz), 7.45 (d, 1H, $J = 7.3$ Hz), 9.15 (br, 1H); ^{13}C NMR (CDCl_3 , 126Hz) δ : 22.1, 26.1, 45.3, 110.6, 116.5, 123.2, 123.4, 129.2, 131.4, 139.9, 180.2; IR (CHCl_3): 3208.7, 1719.2 cm^{-1} ; MS (EI^+) m/z (relative intensity) 186 (M^+ , 62), 145 (100), 128 (95); HRMS (EI^+) $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}$: (M^+) 186.0793. Found: 186.0790.

References

1. Roesch, K. R.; Larock , R. C. *J. Org. Chem.* **2001**, 66, 412.
2. Linn, W. J.; Webster, O. W.; Benson, R. E. *J. Am. Chem. Soc.* **1965**, 87, 3651.
3. Amines or anilines were cyanocarbonylated by a modified procedure of the following paper. See; Ford, R. E.; Knowles, P.; Lunt, E.; Marshall, S. M.; Penrose, A. J.; Ramsden, C. A.; Summers, A. J. H.; Walker, J. L.; Wrigh, D. E. *J. Med. Chem.* **1986**, 29, 538.

Acquisition Time (min)	0.0087
Conc'd	Yes
Frequency (MHz)	125.65
Pulse Width (ms)	3.0000
Precursor delay (s)	0.000
Date	Fri Jul 29 16:44:41 2005
Number of Transients	30
Original F2 (kHz)	30793
Procs Count	30796
Solvent	CH ₃ COOCCl ₃ D
File Name	C:\Documents and Settings\Gowdy\Desktop\1-9\ADAM_18010126.D2C.midas

N-benzyl-N-(2-iodophenyl)cyanofornamide

 $C_{15}H_{11}IN_2O$

Exact Mass: 361.9916

Mol. Wt.: 362,1652

C, 49.75; H, 3.06; I, 35.04; N, 7.74; O, 4.42

Acquisition Time (sec)	0.0057	Core	Top Exp 20.11.20.07.2003	File Name	C:\Documents and Settings\Owner\My Documents\14001447-04-Exp.C.mda
Frequency (MHz)	125.65	Nucleus	Number of Transients	27	Original Photo Count
				27168	Summed Photo Count

Age	Age (yr)	Height (m)	HTL (cm)	HTL (in)	Height (m)	HTL (cm)	HTL (in)
1	13.65	160.63	0.4320	17.12	124.42	1002.30	0.7590
2	15.05	170.41	0.4949	17.12	124.42	1012.23	0.8240
3	16.45	179.19	0.5578	17.12	124.42	1022.16	0.8890
4	17.85	187.97	0.6207	17.12	124.42	1032.09	0.9540
5	19.25	196.75	0.6836	17.12	124.42	1042.02	1.0190
6	20.65	205.53	0.7465	17.12	124.42	1051.95	1.0840
7	22.05	214.31	0.8094	17.12	124.42	1061.88	1.1490
8	23.45	223.09	0.8723	17.12	124.42	1071.81	1.2140
9	24.85	231.87	0.9352	17.12	124.42	1081.74	1.2790
10	26.25	240.65	0.9981	17.12	124.42	1091.67	1.3440
11	27.65	249.43	1.0610	17.12	124.42	1101.60	1.4090
12	29.05	258.21	1.1239	17.12	124.42	1111.53	1.4740
13	30.45	266.99	1.1868	17.12	124.42	1121.46	1.5390
14	31.85	275.77	1.2497	17.12	124.42	1131.39	1.6040
15	33.25	284.55	1.3126	17.12	124.42	1141.32	1.6690
16	34.65	293.33	1.3755	17.12	124.42	1151.25	1.7340
17	36.05	302.11	1.4384	17.12	124.42	1161.18	1.7990
18	37.45	310.89	1.5013	17.12	124.42	1171.11	1.8640
19	38.85	319.67	1.5642	17.12	124.42	1181.04	1.9290
20	40.25	328.45	1.6271	17.12	124.42	1190.97	1.9940
21	41.65	337.23	1.6900	17.12	124.42	1200.90	2.0590
22	43.05	346.01	1.7529	17.12	124.42	1210.83	2.1240
23	44.45	354.79	1.8158	17.12	124.42	1220.76	2.1890
24	45.85	363.57	1.8787	17.12	124.42	1230.69	2.2540
25	47.25	372.35	1.9416	17.12	124.42	1240.62	2.3190
26	48.65	381.13	2.0045	17.12	124.42	1250.55	2.3840
27	50.05	389.91	2.0674	17.12	124.42	1260.48	2.4490
28	51.45	398.69	2.1303	17.12	124.42	1270.41	2.5140
29	52.85	407.47	2.1932	17.12	124.42	1280.34	2.5790
30	54.25	416.25	2.2561	17.12	124.42	1290.27	2.6440
31	55.65	425.03	2.3190	17.12	124.42	1300.20	2.7090
32	57.05	433.81	2.3819	17.12	124.42	1310.13	2.7740
33	58.45	442.59	2.4448	17.12	124.42	1320.06	2.8390
34	59.85	451.37	2.5077	17.12	124.42	1330.00	2.9040
35	61.25	460.15	2.5706	17.12	124.42	1339.93	2.9690
36	62.65	468.93	2.6335	17.12	124.42	1349.86	3.0340
37	64.05	477.71	2.6964	17.12	124.42	1359.79	3.0990
38	65.45	486.49	2.7593	17.12	124.42	1369.72	3.1640
39	66.85	495.27	2.8222	17.12	124.42	1379.65	3.2290
40	68.25	504.05	2.8851	17.12	124.42	1389.58	3.2940
41	69.65	512.83	2.9480	17.12	124.42	1399.51	3.35

Application Time (sec)	Rate	Date	Time	File Name	Comment
Frequency (MHz)	111	Thursday, 18 May 2006	10:00:00	Original_Freqs_Count	33706
Frequency (MHz)	1000.00			Pruned_Count	33706
Frequency (MHz)	1000.00			Pruned_Count	33706

¹H NMR (500 MHz, CHLOROFORM-D) δ ppm 4.67 (d, *J* = 14.34 Hz, 1 H) 5.29 (d, *J* = 14.34 Hz, 1 H) 5.29 (d, *J* = 14.34 Hz, 1 H) 6.95 (d, *J* = 7.93 Hz, 1 H) 7.21 (m, 6 H) 7.35 (m, 4 H) 7.48 (m, 2 H) 7.59 (dd, *J* = 7.63, 1.53 Hz, 1 H)

Acquisition Time (sec): 0.0957	Comments: nm	0018	Thu Jan 5 18:18:32 2000	File Name	C:\Documents and Settings\Owner\My Documents\1-1-000000011-Cyph-C.mn	Acq. Name	000000011-Cyph-C.mn
Frequency (MHz): 125.65	Mode: 13C	Number of Transients: 12	Original Pulse Count: 32768	Pulse Count	32768	Acq. Name	000000011-Cyph-C.mn
Sample Width (µs): 3.300000	Temperature (deg): 0.000

Acquisition Time (hrs)	3.2708	Comment	run	Date	Mon Dec 5 15:38:12 2005	File Name	C:\Documents and Settings\Chemistry\Documents\10001860-407785-11.msdata
Frequency (MHz)	500.00	Machine	1H	Number of Transients	4	Original Photo Count	30756
Temp (K)	300.00	Temperature (K)	300.00				

¹H NMR (500 MHz, CHLOROFORM-D) δ ppm 0.01 (s, 6 H) 0.78 (m, 9 H) 4.30 (d, *J*=14.34 Hz, 1 H) 4.35 (s, 2 H) 5.21 (d, *J*=14.04 Hz, 1 H) 6.69 (d, *J*=7.93 Hz, 1 H) 7.09 (m, 2 H) 7.11 (m, 4 H) 7.22 (t, *J*=7.63 Hz, 1 H) 7.41 (d, *J*=7.63 Hz, 1 H)

Algorithm Time (sec)	0.987	Comment		Date	Mon Dec 11 13:40:36 2006	All Memo	C:\Documents and Settings\Owner My Documents\1\WAMM\100011006-CQ-TB6-C-Verifile
Nucleus Frequency (MHz)	125.66	Nucleus	132	Number of Transitions	31	Points Count	32168
							Subfile
							C:\CH\CF\CH64-D

$C_{24}H_{28}N_2O_2Si$
Exact Mass: 404.1920
Mol. Wt.: 404.5769
C, 71.25; H, 6.98; N, 6.92; O, 7.91; Si, 6.94

No.	Age	Sex	Height	Weight	Height	Weight
1	23	M	170	65	170	65
2	24	F	165	55	165	55
3	25	M	175	70	175	70
4	26	F	160	50	160	50
5	27	M	180	75	180	75
6	28	F	165	55	165	55
7	29	M	175	70	175	70
8	30	F	160	50	160	50
9	31	M	180	75	180	75
10	32	F	165	55	165	55
11	33	M	175	70	175	70
12	34	F	160	50	160	50
13	35	M	180	75	180	75
14	36	F	165	55	165	55
15	37	M	175	70	175	70
16	38	F	160	50	160	50
17	39	M	180	75	180	75
18	40	F	165	55	165	55
19	41	M	175	70	175	70
20	42	F	160	50	160	50

Acquisition Date (mm)	3-27-06	Comment	nmr
Frequency (MHz)	500.00	Machine	5H
Temp (K)	300.00	Temperature (K)	300.00
1H NMR (500 MHz, CHLOROFORM-D) δ ppm 1.89 (m, $J=12.21$ Hz, 3 H) 2.42 (m, 2 H) 3.52 (m, 2 H) 4.77 (m, 2 H) 7.26 (m, 2 H) 7.36 (m, 3 H)			
File Name	32706	Original F2 Data	32706
File Name	32706	Original F2 Data	32706
File Name	32706	Original F2 Data	32706

1d

$C_{14}H_{14}N_2O$
Exact Mass: 226.1106
Mol. Wt.: 226.2738
C, 74.31; H, 6.24; N, 12.38; O, 7.07

31 Mar 2008
cui

Acquisition Time (sec): 0.0957	Comments: 13C	Date: Fri Mar 31 17:00:32 2006	File Name: C:\Documents and Settings\Cui\My Documents\15001813-Cui\cui.ms
Frequency (MHz): 125.05	Acq. Method: 13C	Original Pulse Count: 32768	Subs: 32768
Sample Name (mg): 3.0000 (30)	Integration (mg/100): 0.000		

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	3.33	416.1	0.2131	14	86.49	10713.7	0.7760
2	18.86	2353.4	0.1827	15	110.85	13861.1	0.1980
3	18.86	2353.4	0.4135	16	112.25	13973.3	0.2566
4	48.87	6093.1	0.2177	17	127.73	15948.6	0.3883
5	48.73	6071.1	0.4337	18	128.38	16137.3	0.8333
6	47.70	5953.2	0.4585	19	128.46	16143.8	0.4685
7	53.20	6644.2	0.2080	20	129.81	16289.3	0.2337
8	74.84	9352.8	0.2020	21	128.38	16137.3	0.8333
9	74.86	9421.8	0.0765	22	129.25	16240.2	0.4762
10	75.74	9493.2	0.3886	23	134.32	16828.1	0.2334
11	77.50	9675.1	1.0000	24	134.47	16850.5	0.1943
12	77.26	9777.1	0.9811	25	144.81	18277.8	0.2584
13	76.13	9546.8	0.0635	26	145.84	18393.5	0.1542

1d
 $C_{14}H_{11}N_2O$
 Exact Mass: 226.1106
 Mol. Wt.: 226.2738
 C, 74.31; H, 6.24; N, 12.38; O, 7.07

C:\Documents and Settings\Cui\My Documents\15001813-Cui\cui.ms

Acquisition Time (min): 0.0001	Comment: 100	DATE: Thu Sep 1 15:45:27 2005	File Name: C:\Documents and Settings\Owner\My Documents\15001462-C\mdata
Frequency (MHz): 125.85	Nucleus: ¹³ C	Number of Transients: 37	Points/Channel: 32768
Sample Width (Hz): 33000.00	Temperature (degrees C): 0.000	Original Points/Channel: 32768	Solvent: CD ₃ Cl ₂ (CDCl ₃)

Acquisition Time (min)	3.2780	Comment	nmr
Frequency (MHz)	500.00	Nucleus	¹ H
Sample (mg)	100.000	Temperature (deg C)	0.000
File Name	32780	Proton Count	32780
Chemical Shift (ppm)	0.000	Chemical Shift (ppm)	0.000

¹H NMR (500 MHz, CHLOROFORM-D) δ ppm 0.90 (m, 6 H), 1.01 (m, 3 H), 1.40 (m, 2 H), 1.59 (m, 2 H), 2.25 (m, 3 H), 2.97 (s, 2 H), 3.24 (s, 1 H), 3.36 (d, *J* = 7.63 Hz, 3 H), 3.69 (dd, *J* = 10.38, 3.66 Hz, 1 H) + 28 (m, 1 H)

$C_{15}H_{24}N_2O_2$
Exact Mass: 264.1838
Mol. Wt.: 264.3633
C, 68.15; H, 9.15; N, 10.60; O, 12.10

[illegible]

Sex	Length (cm)	Pin	Height (cm)	Pin	Length (cm)	Pin	Height (cm)
1	13.41	1184.4	2.423	13	68.36	8711.0	0.3105
2	16.95	2262.3	3.4075	18	68.36	8908.0	0.1163
3	18.06	2262.3	2.182	18	71.75	8973.0	0.4382
4	16.70	2262.3	3.4654	18	74.86	9215.5	0.0155
5	16.95	2448.2	2.220	23	72.32	8424.0	0.1760
6	18.06	2504.8	2.4308	21	76.74	8643.0	0.0000
7	21.83	2545.8	2.2138	23	76.74	8651.5	0.3843
8	21.88	2748.9	2.4609	23	77.26	8787.1	0.0428
9	22.22	3258.8	2.1976	24	88.11	11148.0	0.0162
10	25.66	3272.9	2.3671	25	96.50	11382.0	0.1426
11	29.64	3761.7	2.2587	28	110.77	13817.6	0.0049
12	30.28	3808.2	2.4034	27	140.82	13833.2	0.1260
13	35.23	5891.2	2.2168	28	146.42	14057.1	0.0008
14	36.78	7734.3	2.3003	29	147.21	15066.4	0.0257

Acquisition Time (mm)	8.6530	Comment	nmr	Date	16/03/06	File Name	C:\Documents and Settings\ChemM\My Documents\17031727_Aldrich\methyl
Frequency (MHz)	500.00	Nucleus	¹ H	Number of Transients	4	Points Count	83238
Sample Name (nmr)	12000.00	Temperature (degC)	0.000	Original Points Count	83238	Solvent	CD ₃ COCD ₃ DMSO-d ₆

¹H NMR (500 MHz, CDCl₃) δ ppm: 1.58 (s, 3 H), 1.58 (s, 3 H), 3.34 (s, 3 H), 3.45 (s, 3 H), 5.06 (s, 1 H), 7.34 (m, 3 H), 7.44 (m, 2 H)

1h
C₁₈H₁₈N₂O₂
Exact Mass: 270.1368
Mol. Wt.: 270.3264
C, 71.09; H, 6.71; N, 10.36; O, 11.84

31 Mar 2008
raw

Acquisition Time (mm)	0.0007	Conc (mg/ml)	1004	Date	Wed Mar 20 18:17:04 2008	File Name	C:\Documents and Settings\Oscar\My Documents\17001727-Cyline-C-metabolite
Frequency (MHz)	125.80	Mod (mm)	130	Number of Transients	83	Points Collected	32768
Sample Width (Hz)	330000.00	Temperature (deg C)	0.000	Original Points Collected	32768	Subs	C14.cdc\c14m.d

No.	Shift (ppm)	Integ.	Height
1	21.87	2.0623	0.5064
2	22.39	3931.7	0.9400
3	23.58	4471.4	0.4306
4	27.42	7214.0	0.9095
5	64.34	8993.9	0.2009
6	73.84	3256.2	0.5223
7	76.74	9643.0	0.9423
8	77.02	9679.1	0.9381
9	77.28	3020.1	0.9427
10	84.89	10965.1	0.1907
11	87.34	10874.4	0.1916
12	111.36	13682.2	0.1071
13	132.18	15355.6	0.1900
14	138.47	16134.8	1.0000
15	155.73	16175.3	0.5451
16	171.78	10980.7	0.0941
17	168.07	10286.8	0.1453

1h
 $C_{16}H_{18}N_2O_2$
 Exact Mass: 270.1368
 Mol. Wt.: 270.3264
 C, 71.09; H, 6.71; N, 10.36; O, 11.84

Acquisition Title (acc)	3.7756	Comment	inst	Date	Mod Seq	7.30.25.24.2005	File Name	C:\Documents and Settings\GarryM\Documents\...
Nuclear	532.00		11		Number of Transients	4	Original Points Count	32768
Frequency (MHz)							Signal	01.04.0094-0

¹H NMR (500 MHz, CH₂Cl₂-CDCl₃-D₂O) δ ppm 1.32 (m, 1 H), 1.92 (m, 1 H), 2.42 (t, J = 6.87 Hz, 1 H), 2.49 (s, J = 6.71 Hz, 1 H), 3.40 (m, 1 H), 3.68 (m, 1 H), 4.64 (s, 1 H), 4.80 (s, 1 H), 7.32 (m, 1 H).

4

 $C_{20}H_{15}N_2O$

Exact Mass: 302.1419

Mol. Wt.: 302,3698

C, 79.44; H, 6.00; N, 9.26; O, 5.29

Acquisition Time (min)	3.2760	Comment	nm	Date	Fri Sep 23 00:23:00 2006	File Name	C:\Documents and Settings\Owner\My Documents\15001452-1454.ms
Frequency (MHz)	500.00	Nucleus	¹ H	Number of Transients	4	Points/Chan	32768
Sample Width (Hz)	13000.00	Temperature (deg C)	0.00	Original Points/Chan	32768	Solvent	CHLOROFORM-D

¹H NMR (500 MHz, CHLOROFORM-D) δ ppm 1.51 (m, 1 H) 1.46 (m, 1 H) 1.66 (m, 1 H) 1.77 (m, 1 H) 2.37 (t, J=6.87 Hz, 1 H) 2.41 (t, J=6.87 Hz, 1 H) 3.33 (m, 1 H) 3.50 (m, 1 H) 4.58 (s, 1 H) 4.71 (s, 1 H) 7.30 (m, 10 H)

6
 $C_{21}H_{20}N_2O$
 Exact Mass: 316.1576
 Mol. Wt.: 316.3964
 C, 79.72; H, 6.37; N, 8.85; O, 5.06

C:\Documents and Settings\Owner\My Documents\15001452-1454.ms

Acquisition Date (MM/DD/YYYY)	09/09/08	Comment	13C	File Name	C:\Documents and Settings\Oscar\My Documents\18001457-CG.mvdata
Frequency (MHz)	125.80	Nucleus	13C	Probe Count	32198
Sample Name	330005-30	Temperature (degrees C)	0.000	Received	32198
Number of Transients	32	Original Points Count	32198		
FS Sep 23 00:24:41 2008

Acquisition Time (ms)	0.0087	Comment	on	Date	Sat Oct 8 12:16:13 2022	File Name	C:\Documents and Settings\Oscar M... Documents\11-19301499-001.mda
Frequency (MHz)	121.65	Methyl	13C	Number of Transients	20	Original F2/1H Count	32198
Temperature (K)	300.00	Transmitter channel C	0.000				CH-13C1H100MG

No.	Year1	Year2	Height
1	23.49	23.61	0.2085
2	5.15	6.05	0.4732
3	7.15	7.65	0.2414
4	77.00	90.14	0.1386
5	77.29	87.03	0.1205
6	15.00	13.21	0.1506
7	15.15	14.48	0.4705
8	129.28	107.18	0.8494
9	129.30	107.12	0.8324
10	129.69	105.82	1.8300

C₁₅H₁₆N₂O
Exact Mass: 276.1263
Mol. Wt.: 276.3325
C, 78.24; H, 5.84; N, 10.14; O, 5.79

Acquisition Date (MM/DD/YYYY)	02/08/07	Comment	1006	Date	Thu Oct 03 18:13 2008	File Name	C:\Documents and Settings\Owner\Mx Documents\1006\1006-0084-0084.d
Frequency (MHz)	125.80	Analysis	13C	Number of Transients	16	Probe Count	32768
Sweep Width (Hz)	33000.00	Temperature (degrees C)	0.000	Original Pulse Count	32768	Subset	CH40000000.d

No.	ppm	Height
1	24.32	3065.5
2	78.79	8443.4
3	77.26	8414.4
4	77.26	8706.5
5	111.88	16271.8
6	110.00	14813.0
7	121.71	15203.0
8	121.76	15206.1
9	120.32	15872.3
10	128.11	9606.8
11	131.38	10028.8
12	134.43	8903.7
13	140.38	11838.3
14	141.63	11754.5

$C_{11}H_{10}N_2O$
Exact Mass: 186.0793
Mol. Wt.: 186.2100
C, 70.95; H, 5.41; N, 15.04; O, 8.59

8b

Acquisition Time (sec)	0.0687	Date	Thu Jul 2 21:49:38 2009	File Name	C:\Documents and Settings\Glenice.Douglas\My Documents\14071408-Br-Glyn-C.midi
Frequency (MHz)	121.65	Number of Transients	119	Original Points Count	32768
		Absorbance		Points Count	32768
				Subplot	C:\CINEL-2004.D

No.	gender	height	weight	fat	mus	bone	fat0	height
1	M	172.17	78.602	15.1	120.80	11.0	181.128	1.1007
2	F	162.13	59.867	17.7	104.176	10.1	164.176	0.5469
3	F	158.13	56.896	16.1	101.161	10.1	157.161	0.4623
4	M	172.17	81.696	14	125.45	12.5	183.181	0.7308
5	M	163.17	64.967	13.7	109.171	10.7	169.171	0.4711
6	M	172.17	84.803	14	127.88	12.8	184.193	0.7458
7	F	160.18	58.801	18.1	102.18	11.1	165.18	0.4211
8	M	173.17	87.811	14.8	130.17	12.8	187.18	0.7885
9	F	157.13	54.866	20	93.17	11.7	157.17	0.2063
10	M	173.17	89.897	14	129.17	12.9	189.17	0.7844
11	M	171.18	84.897	21	104.18	10.7	176.18	0.7070
12	F	155.17	55.824	17.7	99.17	10.7	155.17	0.3700

C₂₁H₂₀N₂O
Exact Mass: 316.1576
Mol. Wt.: 316.3964
C, 79.72; H, 6.37; N, 8.85; O, 5.06

Acquisition Time (mm)	3.2790	Comments	700	Date	Wed Jul 23 16:52:58 2008
File Name	C:\Documents and Settings\Owner\My Documents\14501424-12M-40-E-H-DMF-40-E-H-remake	Frequency (MHz)	400.1450	Sample Name	14501424-12M-40-E-H-remake
Original F2 (Hz)	307.190	Phase Count	307190	Solvent	C14 (CDCl3)/CDCl3
				Temp (deg C)	100.00
				Temp (deg C)	100.00
				Number of Transients	4

$C_{21}H_{20}N_2O$
 Exact Mass: 316.1576
 Mol. Wt.: 316.3964
 C, 79.72; H, 6.37; N, 8.85; O, 5.06

[illegible]

Sex	Age (yr)	Height (m)	Weight (kg)	Max (g/min)	Max (g/min)	Height (m)	Weight (kg)
1	23.2	1.753	7.376	12	121.41	1.625	5.1467
2	33.2	2.009	8.936	14	124.51	1.944	6.4679
3	29.3	1.808	8.178	14	122.84	1.616	5.4863
4	29.3	1.808	8.178	14	122.84	1.616	5.4863
5	30.45	1.818	8.446	15	127.21	1.909	6.9000
6	43.48	1.843	8.4718	16	127.66	1.9993	7.4874
7	76.14	1.6643	7.5231	17	128.81	1.6919	7.0005
8	77.60	1.6815	7.587	17	131.71	1.6561	6.1258
9	77.26	1.6701	7.7166	19	130.35	1.7033	6.1266
10	100.23	1.7374	8.4607	20	135.26	1.7113	6.1176
11	110.17	1.8003	8.5961	21	142.87	1.7564	7.0079
12	120.23	1.8163	8.1128	22	146.86	1.8061	8.1128

Application Time (sec)	3.2790	Comment	run	Date	Fri Jan 8 10:51:14 2009	File Name	C:\Documents and Settings\Community Documents\10801812\Appl1.mcode
Frequency (MHz)	500.00	Acoustic	1H	Number of Transients	4	Original Points Count	30798
Time (min)	12:50:33	Non-House	☐	Transients (House)	☐		CH1.GFQF084-2
Time (min)	15:04:38						

¹H NMR (500 MHz, CHLOROFORM-D): d ppm 4.99 (s, 2 H) 6.72 (t, *J*_{H-H} = 7.32 Hz, 2 H) 6.66 (m, 1 H) 7.21 (m, 1 H) 7.30 (m, 1 H) 7.36 (m, 4 H) 7.55 (m, 3 H) 7.60 (m, 2 H).

Acquisition Time (MM:SS.SS)	0.0007	Comment	004	Date	Tue Nov 20 12:50:11 2007	File Name	C:\Documents and Settings\Owner\Documents\16001812-C-nitrile-Compound
Frequency (MHz)	125.80	Modulation	15C	Number of Transients	323	Points Collected	32768
Sweep Width (Hz)	33000.00	Temperature (degrees C)	0.003	Original Points Collected	32768	Bolvent	CH ₂ Cl ₂ /CDCl ₃ /D ₂ O

No.	ppm	Height	No.	ppm	Height
1	43.00	5511.5	12	127.34	55075.1
2	70.74	9462.4	13	129.82	95080.8
3	77.00	8819.8	14	129.82	95080.8
4	77.25	9706.5	15	129.82	95080.8
5	100.08	13778.4	16	130.80	95080.8
6	117.07	18302.2	17	132.85	95080.8
7	117.12	14716.7	18	132.85	95080.8
8	120.03	18081.8	19	132.85	95080.8
9	122.32	15308.3	20	144.07	30702.7
10	124.52	15004.8	21	154.85	20714.9
11	127.69	18284.7

$C_{23}H_{16}N_2O$
 Exact Mass: 336.1263
 Mol. Wt.: 336.3860
 C, 82.12; H, 4.79; N, 8.33; O, 4.76

Application Time (sec)	Comment	File Name	File Size	File Date	File Type	File Path
3.2789	Initial	Initial	3.2789	3/27/08	Initial	Initial
532.00	Initial	Initial	532.00	3/27/08	Initial	Initial
1200.00	Initial	Initial	1200.00	3/27/08	Initial	Initial
1200.00	Initial	Initial	1200.00	3/27/08	Initial	Initial

¹H NMR (500 MHz, CHLOROFORM-D): δ ppm 0.20 (s, 6 H), 0.95 (s, 9 H), 4.77 (s, 2 H), 4.95 (s, 2 H), 6.76 (d, $J=7.95$ Hz, 1 H), 7.65 (t, $J=7.32$ Hz, 1 H), 7.30 (m, 6 H), 7.46 (d, $J=7.63$ Hz, 1 H).

2c

$C_{24}H_{28}N_2O_2Si$
Exact Mass: 404.1920
Mol. Wt.: 404.5769
C, 71.25; H, 6.98; N, 6.92; O, 7.91; Si, 6.94

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Acquisition Time (hrs): 0.0957	Comments: nm	Chem: C ₂₄ H ₂₈ N ₂ O ₂ Si	File Name: C:\Documents and Settings\ChemM\Documents\18001504-2-c5-c-mrdata
Frequency (MHz): 125.65	Analysis: 1.32	Exact Mass: 404.1920	Subject: CHLOROFORM-D
Sample Width (Hz): 3.188838	Temperature (deg): 0.000	Mol. Wt.: 404.5769	30768
		C, 71.25; H, 6.98; N, 6.92; O, 7.91; Si, 6.94	30768

No.	Chemical Shift (ppm)	Height	No.	Chemical Shift (ppm)	Height
1	0.33	0.0000	12	126.12	0.0000
2	18.28	0.0000	13	126.81	0.0000
3	29.67	0.0000	14	127.75	0.0000
4	44.51	0.0000	15	127.94	0.0000
5	61.28	0.0000	16	127.89	0.0000
6	71.19	0.0000	17	128.88	0.0000
7	77.00	0.0000	18	132.76	0.0000
8	77.28	0.0000	19	136.27	0.0000
9	108.86	0.0000	20	137.51	0.0000
10	118.78	0.0000	21	143.83	0.0000
11	118.86	0.0000	22	144.34	0.0000

Acquisition Time (min)	3.2780	Comment	100	Date	Tue Jan 10 18:03:03 2006	File Name	C:\Documents and Settings\ChemM\Documents\16001615\data-H11.mrdata
Frequency (MHz)	500.00	Nucleus	¹ H	Number of Transients	4	Original Points Count	32768
Sample Width (Hz)	13000.00	Temperature (deg C)	0.000			Solvent	CHLOROFORM-D

¹H NMR (500 MHz, CHLOROFORM-D) δ ppm 2.04 (m, *J*=1.53 Hz, 3 H), 2.78 (t, *J*=4.73 Hz, 2 H), 3.35 (s, *J*=6.10 Hz, 2 H), 4.57 (s, 2 H), 7.32 (m, 3 H)

Acquisition Date (MM/DD/YYYY)	01/08/08	Conc.	13C	Date	Tue Jan 08 10:49:43 2008	File Name	C:\Documents and Settings\Owner\My Documents\11001815-4796-4796-4796-4796
Frequency (MHz)	125.80	Nucleus	¹³ C	Number of Transmits	16	Points Count	32768
Sample Name	330000.30	Temperature (degree C)	0.000	Original Points Count	32768	Bucket	On Lock (18M D)

Bin	ppm	Hz	Height
1	16.71	2568.3	0.3031
2	23.84	3608.9	0.0507
3	42.75	6417.8	0.0076
4	47.17	7077.4	0.0044
5	76.74	11512.4	0.4770
6	77.30	11614.4	0.4731
7	77.25	11608.5	0.4662
8	109.68	16361.2	0.1163
9	117.28	17528.3	0.1157
10	127.65	19364.7	0.0440
11	128.43	19527.1	0.0502
12	128.72	19574.4	0.0462
13	135.06	20252.9	0.2098
14	140.37	21044.1	0.1181
15	163.89	24582.8	0.1400

2d
 $C_{14}H_{14}N_2O$
 Exact Mass: 226.1106
 Mol. Wt.: 226.2738
 C, 74.31; H, 6.24; N, 12.38; O, 7.07

Acquisition Time (min)	3.2780	Comment	nmr	Date	Wed Sep 3 03:33 2006	File Name	C:\Documents and Settings\Chemistry\Documents\15021464-2 H2-H.mr
Frequency (MHz)	500.00	Nucleus	¹ H	Number of Transients	4	Points Count	32768
Sample Name (nmr)	15021464	Temperature (Algebra C)	130.0	Original Points Count	32768	Solvent	CHLOROFORM-D

¹H NMR (500 MHz, CHLOROFORM-D) δ ppm 3.02 (s, 2H, $J=6.10$ Hz, 2H) 3.34 (t, $J=5.05$ Hz, 2H) 4.62 (s, 2H) 7.33 (m, 5H) 7.44 (m, 3H) 7.55 (d, $J=7.02$ Hz, 2H)

3 Sep 2008
10:00

Acquisition Time (MM:SS)	0.0007	DATE	Tue Nov 25 10:59:42 2003	File Name	C:\Documents and Settings\Owner\My Documents\1000-1404-2-C2-C.mn
Frequency (MHz)	125.80	INSTR	13C	Points Count	32768
Sample Width (Hz)	33000.00	Temperature (degC)	0.000	Number of Transients	41
				Original Points Count	32768
				Bucket	Chemical shift D

PK	10000	PK	Height
1	28.30	3358.7	0.4176
2	43.10	8429.0	0.5508
3	47.40	8893.0	0.4307
4	76.54	2642.4	0.5565
5	77.80	8874.4	0.5408
6	77.24	8702.5	0.3313
7	114.14	14342.2	0.5803
8	119.29	14807.1	0.1308
9	120.07	16084.4	0.3228
10	120.30	10128.8	0.5828
11	120.64	10156.7	1.0000
12	120.87	10162.3	0.5854
13	120.91	10198.2	0.2701
14	120.17	10320.8	0.4428
15	133.40	10708.2	0.1325
16	130.00	11707.2	0.1844
17	140.19	18308.8	0.1158
18	164.04	20807.5	0.5807

$C_{19}H_{16}N_2O$
Exact Mass: 288.1263
Mol. Wt.: 288.3432
C, 79.14; H, 5.59; N, 9.72; O, 5.55

2e

Acquisition Time (min)	3.2780	Comment	nmr	Date	Wed Sep 3 02:47:47 2009	File Name	C:\Documents and Settings\Chemistry\Documents\1500-484-1481-48.mrdata
Frequency (MHz)	500.00	Nucleus	¹ H	Number of Transients	4	Original Pulse Count	32768
Sample Name (nmr)	15000003	Temperature (deg C)	120.00			Solvent	CHLOROCL-DM-D

¹H NMR (500 MHz, CHLOROFORM-D) δ ppm 3.81 (d, J=20.45 Hz, 1 H), 3.87 (m, 1 H), 4.52 (d, J=14.65 Hz, 1 H), 4.70 (d, J=14.05 Hz, 1 H), 5.02 (s, 1 H), 7.05 (s, 1 H), 7.21 (d, J=6.71 Hz, 2 H), 7.33 (m, 6 H), 7.48 (d, J=7.32 Hz, 2 H).

Accession Time (ms)	0.0087	Comment	100
Modulus	110	Number of Treatments	45
Frequency (MHz)	120.65	Original Points Count	32768
Modulus (GPa)	330000.30	Points Count	32768
Transverse (shear) G (GPa)	0.303	File Name	C:\Documents and Settings\Omar\My Documents\1989-404-LQ-L2-modulus
			CH1 (channel 0) Data D

Pos.	Player	HS	Height
1	Sam Cook	4,006.4	6'38 1/2"
2	Earl Smith	3,848.7	6'47 1/2"
3	Earl Smith	3,848.7	6'47 1/2"
4	Earl Smith	3,848.7	6'47 1/2"
5	Earl Smith	3,848.7	6'47 1/2"
6	Earl Smith	3,848.7	6'47 1/2"
7	Earl Smith	3,848.7	6'47 1/2"
8	Earl Smith	3,848.7	6'47 1/2"
9	Earl Smith	3,848.7	6'47 1/2"
10	Earl Smith	3,848.7	6'47 1/2"
11	Earl Smith	3,848.7	6'47 1/2"
12	Earl Smith	3,848.7	6'47 1/2"
13	Earl Smith	3,848.7	6'47 1/2"
14	Earl Smith	3,848.7	6'47 1/2"
15	Earl Smith	3,848.7	6'47 1/2"
16	Earl Smith	3,848.7	6'47 1/2"
17	Earl Smith	3,848.7	6'47 1/2"
18	Earl Smith	3,848.7	6'47 1/2"
19	Earl Smith	3,848.7	6'47 1/2"
20	Earl Smith	3,848.7	6'47 1/2"

$C_{19}H_{16}N_2O$
Exact Mass: 288.1263
Mol. Wt.: 288.3432
C, 79.14; H, 5.59; N, 9.72; O, 5.55

Acquisition Date (mm)	3/27/06	Comment	rmb	Date	Time (mm)	14:18:00 (2006)	File Name	C:\Documents and Settings\ChemM\My Documents\11\11001081_2\11001081_2.ms	
Frequency (MHz)	500.00	Nucleus	¹ H	Number of Transients	4	Original Data Name	32758	Solvent	CDCl ₃ /CF ₃ CO ₂ D
Temp (K)	300.00	Temperature (K)	300.00						

¹H NMR (500 MHz, CHLOROFORM-D) δ ppm 0.85 (d, *J*=7.02 Hz, 3 H) 0.94 (t, *J*=7.32 Hz, 3 H) 1.09 (d, *J*=7.32 Hz, 3 H) 1.38 (m, 2 H) 1.63 (m, 1 H) 2.12 (m, 1 H) 2.49 (m, 2 H) 3.02 (s, 3 H) 3.46 (s, 2 H) 3.65 (dd, *J*=7.02, 2.14 Hz, 1 H) 4.58 (d, *J*=7.02 Hz, 1 H)

2f

$C_{15}H_{24}N_2O_2$
Exact Mass: 264.1838
Mol. Wt.: 264.3633
C, 68.15; H, 9.15; N, 10.60; O, 12.10

C:\Documents and Settings\ChemM\My Documents\11\11001081_2\11001081_2.ms

Acquisition Time (min): 0.0017	0.00	Date: Tue Nov 20 12:50:11 2007	File Name: C:\Documents and Settings\Oscar\My Documents\17001861-5-ortho-2.mn
Frequency (MHz): 125.80	150	Number of Transmits: 148	Pulses Count: 32768
Sample Width (Hz): 335000.00	Temperature (degrees C): 0.000	Original Points Count: 32768	Solvent: CH ₂ D ₂ O/CDCl ₃

Bin	Spent	Hz	Height
1	13.88	1718.4	0.2364
2	16.78	2008.2	0.2908
3	20.88	2688.4	0.2172
4	22.22	2797.3	0.2436
5	26.88	3603.4	0.2653
6	28.78	3708.8	0.2576
7	30.88	3845.5	0.2462
8	31.22	3873.1	0.1985
9	38.78	4918.4	0.1188
10	65.33	8208.1	0.2465
11	70.74	8842.8	1.0000
12	77.68	9673.1	0.6565
13	77.24	9708.1	0.6522
14	78.81	9922.8	0.1624
15	116.73	14687.7	0.0876
16	117.36	14745.3	0.0792
17	144.01	18086.1	0.0928
18	163.08	20386.3	0.0472

2f
 $C_{15}H_{24}N_2O_2$
 Exact Mass: 264.1838
 Mol. Wt.: 264.3633
 C, 68.15; H, 9.15; N, 10.60; O, 12.10

[illegible]

Age	Sex	Height	Weight	Arm span	Hand span	Hand length
1	Male	103.2	22.0	147.0	20.0	20.0
2	Female	107.2	22.0	150.0	20.0	20.0
3	Male	110.2	22.0	153.0	20.0	20.0
4	Female	113.2	22.0	156.0	20.0	20.0
5	Male	116.2	22.0	159.0	20.0	20.0
6	Female	119.2	22.0	162.0	20.0	20.0
7	Male	122.2	22.0	165.0	20.0	20.0
8	Female	125.2	22.0	168.0	20.0	20.0
9	Male	128.2	22.0	171.0	20.0	20.0
10	Female	131.2	22.0	174.0	20.0	20.0
11	Male	134.2	22.0	177.0	20.0	20.0
12	Female	137.2	22.0	180.0	20.0	20.0
13	Male	140.2	22.0	183.0	20.0	20.0
14	Female	143.2	22.0	186.0	20.0	20.0
15	Male	146.2	22.0	189.0	20.0	20.0
16	Female	149.2	22.0	192.0	20.0	20.0
17	Male	152.2	22.0	195.0	20.0	20.0
18	Female	155.2	22.0	198.0	20.0	20.0
19	Male	158.2	22.0	201.0	20.0	20.0
20	Female	161.2	22.0	204.0	20.0	20.0

$C_{19}H_{32}N_2O_2Si$
Exact Mass: 348.2233
Mol. Wt.: 348.5552
C, 65.47; H, 9.25; N, 8.04; O, 9.18

[illegible]¹H NMR (500 MHz, CHLOROFORM-D) δ ppm 1.24 (s, 3 H) 1.30 (s, 3 H) 2.02 (s, 3 H) 3.12 (s, 3 H) 4.21 (s, 1 H) 7.47 (m, 3 H) 7.56 (m, 2 H)

2h

 $C_{16}H_{12}N_2O_2$

Exact Mass: 270.1368

Mol. Wt.: 270.3264

C, 71.09; H, 6.71; N, 10.36; O, 11.84

1 - Documents and Settings\OwnerMy Documents\1 - 1500 x 1000 kb - 44 directory optimization - 01 results

Acquisition Time (sec)	0.0087		Date	Tue Nov 25 11:39:42 2003	File Name	C:\Programs and Settings\Oscar M\Documents\... \MyData\11_0903\475-254-C.mda
Frequency (MHz)	120.60		Number of Patients	80	Patient Count	32788
			Number of Patients	80	Original Patient Count	32788
						Chk (C)254-00M.D

$C_{20}H_{18}N_2O$
Exact Mass: 302.1419
Mol. Wt.: 302.3698
C, 79.44; H, 6.00; N, 9.26; O, 5.29

No.	Species	Alt	Height	No.	Species	Alt	Height
1	22.28	2789.0	0.4043	51	123.47	18142.3	0.0044
2	38.17	3339.7	0.4088	52	123.47	18142.3	0.0044
3	48.70	5017.7	0.4318	53	123.86	18162.3	1.0000
4	51.85	6411.6	0.3641	54	123.86	18167.7	0.0979
5	76.74	8642.8	0.3768	55	129.41	18262.2	0.4040
6	77.00	9073.4	0.3760	56	134.36	19062.6	0.1205
7	77.28	8709.6	0.3769	57	139.49	17748.8	0.1818
8	118.21	14065.5	0.2028	58	144.67	18173.8	0.1715
9	127.79	14062.6	0.1454	59	161.00	20500.2	0.1157
10	127.79	14062.6	0.4038

Acquisition Time (min)	3.2780	Comment	none	Date	Tue Sep 17 15:36:34 2006	File Name	C:\Documents and Settings\ChemM\Documents\15021458-14714-1.mvdata
Frequency (MHz)	500.00	Nucleus	¹ H	Number of Transients	4	SDTMR	CHLOROFORM-D
Sample Width (Hz)	13000.00	Temperature (deg C)	3.000	Original Pulse Count	32768	Pulse Count	

¹H NMR (500 MHz, CHLOROFORM-D) δ ppm 1.55 (m, 2 H), 1.71 (m, 2 H), 2.49 (m, 2 H), 3.32 (m, 2 H), 4.72 (s, 2 H), 7.36 (m, 10 H).

Acquisition Time (sec)	Conversion	Date	File Name
0.0087	cosmo	Sat Sep 17 10:47:24 2005	C:\Documents and Settings\Oswin\My Documents\...HMMs_1893-1896-QT-C.midi
Frequency (MHz)	Melodic	Number of Practises	Pieces Count
121.65		36	32788
		Original Pieces Count	Salvaged
		32788	Chk C:\D3-05M.D

$C_{21}H_{20}N_2O$
Exact Mass: 316.1576
Mol. Wt.: 316.3964
C, 79.72; H, 6.37; N, 8.85; O, 5.06

No.	Year	Area	Height	No.	Year	Area	Height
1	2014	3504.2	0.4231	11	129.0	9087.5	0.5029
2	210	3407.3	0.4339	12	128.1	9033.1	0.5103
3	285.2	3303.3	0.3833	13	133.1	9253.9	1.0000
4	272.5	3250.7	0.3933	14	129.1	9164.7	0.6761
5	47.25	5030.7	0.3030	14	129.1	9164.7	0.6761
6	498.7	6771.1	0.3981	15	129.0	9027.9	0.6881
7	167.5	6043.4	0.5482	16	126.2	8504.0	0.3319
8	77.20	8714.8	0.5413	17	132.10	9070.0	0.1154
9	77.20	8708.8	0.5413	18	132.10	9070.0	0.1154
10	133.75	14759.5	0.7127	19	156.20	9403.0	0.1166
11	177.48	14506.3	0.8141	20	156.20	9403.0	0.1166

Acquisition Date (MM/DD)	08/07	Conc.	nmr	DMF	Ref. C-13, 01-06-2005	Original Points Count	32768	File Name	C:\Documents and Settings\Chemistry\Documents\15001500-Copy-2.mr	15001500-Copy-2.mr
Frequency (MHz)	125.80	Nucleus	¹³ C	Number of Transients	30	Original Points Count	32768	Points Count	32768	Bulk File
Sample Name (Hz)	330000.00	Temperature (°C)	0.000							

No.	Height	Area	Height	No.	Height	Area	Height
1	25.41	2811.5	0.5305	11	123.33	55464.3	0.5093
2	26.17	3298.3	0.5339	12	127.34	59714.7	0.5099
3	43.83	5057.4	0.4833	13	127.76	58554.4	0.5057
4	44.82	5031.5	0.2054	14	128.86	57503.3	1.0000
5	76.74	8942.4	0.2199	15	129.89	56219.8	0.0825
6	77.60	9074.4	0.2032	16	130.82	54650.8	0.1482
7	77.25	9702.5	0.1698	17	132.26	58868.9	0.1855
8	109.19	17953.8	0.4292	18	141.77	17813.1	0.1429
9	113.58	14455.3	0.1655	19	177.86	22226.7	0.1342
10	123.12	14468.8	0.3955

9a
 $C_{15}H_{10}N_2O$
 Exact Mass: 276.1263
 Mol. Wt.: 276.3325
 C, 78.24; H, 5.84; N, 10.14; O, 5.79